



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 07:00 AM UTC

PDB ID : 7ZQ9 / pdb_00007zq9
EMDB ID : EMD-14867
Title : Dimeric PSI of Chlamydomonas reinhardtii at 2.74 Å resolution (symmetry expanded)
Authors : Naschberger, A.; Amunts, A.
Deposited on : 2022-04-29
Resolution : 2.74 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:

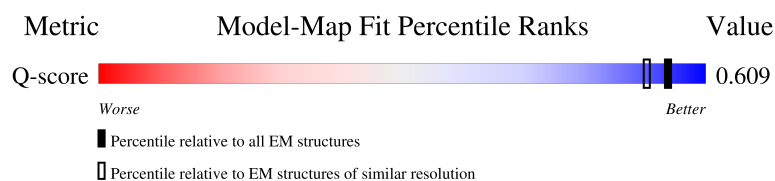
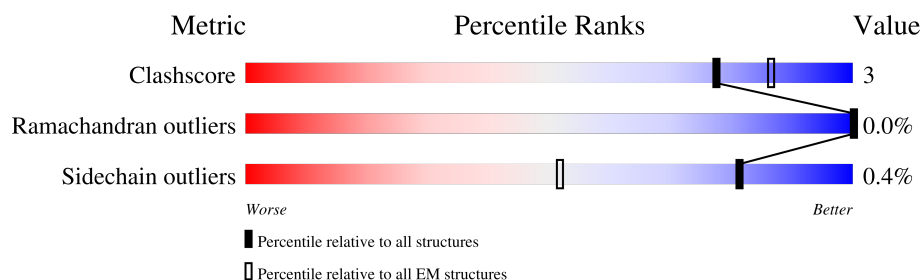
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

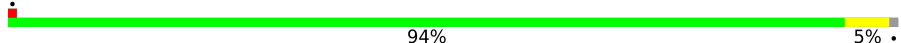
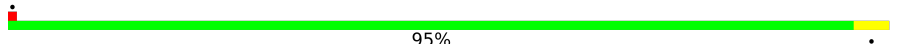
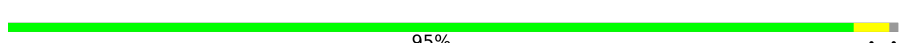
The reported resolution of this entry is 2.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	 94% 5% .
2	B	735	 95% .
3	C	81	 95% . .
4	D	196	 70% . 27%

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Mol	Chain	Length	Quality of chain
5	E	97	
6	F	227	
7	G	126	
8	I	106	
8	I2	106	
9	J	40	
10	L	196	
10	L2	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	
19	92	213	
20	B2	180	

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
21	CL0	A	801	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	604	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	609	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	1	616	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	609	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	611	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	613	X	-	-	-
22	CLA	3	614	X	-	-	-
22	CLA	3	615	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	613	X	-	-	-
22	CLA	4	614	X	-	-	-
22	CLA	4	616	X	-	-	-
22	CLA	5	601	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	613	X	-	-	-
22	CLA	5	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	5	616	X	-	-	-
22	CLA	5	617	X	-	-	-
22	CLA	5	621	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-
22	CLA	6	614	X	-	-	-
22	CLA	6	617	X	-	-	-
22	CLA	6	622	X	-	-	-
22	CLA	7	602	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	608	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	610	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	613	X	-	-	-
22	CLA	7	614	X	-	-	-
22	CLA	7	616	X	-	-	-
22	CLA	7	620	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	604	X	-	-	-
22	CLA	8	608	X	-	-	-
22	CLA	8	609	X	-	-	-
22	CLA	8	610	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-
22	CLA	8	613	X	-	-	-
22	CLA	8	614	X	-	-	-
22	CLA	8	616	X	-	-	-
22	CLA	9	601	X	-	-	-
22	CLA	9	602	X	-	-	-
22	CLA	9	603	X	-	-	-
22	CLA	9	604	X	-	-	-
22	CLA	9	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	9	610	X	-	-	-
22	CLA	9	611	X	-	-	-
22	CLA	9	612	X	-	-	-
22	CLA	9	613	X	-	-	-
22	CLA	9	614	X	-	-	-
22	CLA	92	601	X	-	-	-
22	CLA	92	602	X	-	-	-
22	CLA	92	603	X	-	-	-
22	CLA	92	604	X	-	-	-
22	CLA	92	609	X	-	-	-
22	CLA	92	610	X	-	-	-
22	CLA	92	611	X	-	-	-
22	CLA	92	612	X	-	-	-
22	CLA	92	613	X	-	-	-
22	CLA	92	614	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B2	804	X	-	-	-
22	CLA	B2	805	X	-	-	-
22	CLA	B2	806	X	-	-	-
22	CLA	B2	807	X	-	-	-
22	CLA	B2	808	X	-	-	-
22	CLA	B2	809	X	-	-	-
22	CLA	B2	810	X	-	-	-
22	CLA	B2	811	X	-	-	-
22	CLA	B2	812	X	-	-	-
22	CLA	B2	813	X	-	-	-
22	CLA	B2	814	X	-	-	-
22	CLA	B2	815	X	-	-	-
22	CLA	B2	820	X	-	-	-
22	CLA	B2	828	X	-	-	-
22	CLA	B2	829	X	-	-	-
22	CLA	B2	839	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	J	101	X	-	-	-
22	CLA	K	201	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	L	204	X	-	-	-
22	CLA	L2	203	X	-	-	-
22	CLA	L2	204	X	-	-	-
22	CLA	Z	602	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	608	X	-	-	-
22	CLA	Z	609	X	-	-	-
22	CLA	Z	610	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-
22	CLA	Z	613	X	-	-	-
22	CLA	Z	614	X	-	-	-
22	CLA	Z	616	X	-	-	-
31	CHL	1	601	X	-	-	-
31	CHL	1	606	X	-	-	-
31	CHL	1	607	X	-	-	-
31	CHL	3	608	X	-	-	-
31	CHL	4	601	X	-	-	-
31	CHL	4	606	X	-	-	-
31	CHL	4	607	X	-	-	-
31	CHL	4	608	X	-	-	-
31	CHL	4	618	X	-	-	-
31	CHL	5	606	X	-	-	-
31	CHL	5	607	X	-	-	-
31	CHL	5	608	X	-	-	-
31	CHL	5	618	X	-	-	-
31	CHL	6	601	X	-	-	-
31	CHL	6	606	X	-	-	-
31	CHL	6	607	X	-	-	-
31	CHL	6	608	X	-	-	-
31	CHL	6	616	X	-	-	-
31	CHL	6	618	X	-	-	-
31	CHL	7	601	X	-	-	-
31	CHL	7	606	X	-	-	-
31	CHL	7	607	X	-	-	-
31	CHL	8	601	X	-	-	-
31	CHL	8	606	X	-	-	-
31	CHL	8	607	X	-	-	-
31	CHL	9	606	X	-	-	-
31	CHL	9	607	X	-	-	-
31	CHL	92	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CHL	92	607	X	-	-	-
31	CHL	Z	601	X	-	-	-
31	CHL	Z	606	X	-	-	-
31	CHL	Z	607	X	-	-	-
32	XAT	1	618	X	-	-	-
32	XAT	5	624	X	-	-	-
33	NEX	6	625	X	-	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 113459 atoms, of which 56999 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
			11500	3808	5675	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	95	Total	C	H	N	O	0	0
			1393	452	687	119	135		

- 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		
8	I2	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		
10	L2	102	Total	C	H	N	O S	0	0
			1487	487	748	120	130 2		

- 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
			3280	1073	1630	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		

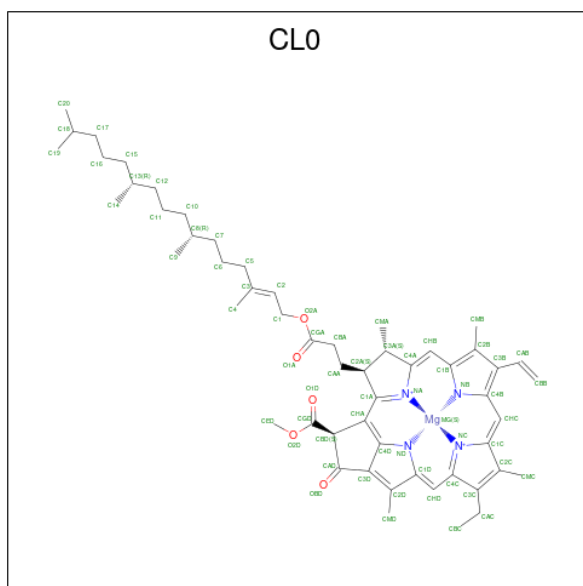
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	9	186	Total	C	H	N	O	S	0	0
			2820	918	1400	238	257	7		
19	92	184	Total	C	H	N	O	S	0	0
			2802	913	1392	236	254	7		

- Molecule 20 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

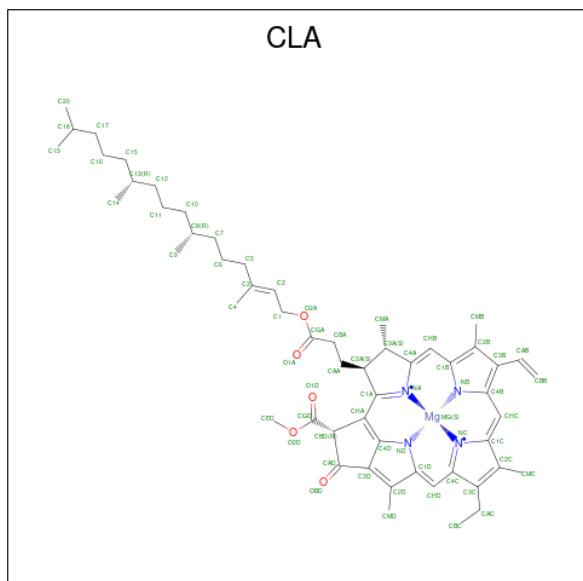
Mol	Chain	Residues	Atoms					AltConf	Trace
20	B2	180	Total	C	H	N	O	S	
			2865	972	1396	247	247	3	
								0	0

- Molecule 21 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
21	A	1	Total	C	H	Mg	N	O
			137	55	72	1	4	5
								0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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

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

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Mol	Chain	Residues	Atoms						AltConf
22	B	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	F	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	G	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	G	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	J	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	L	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	L	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	K	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	K	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
22	3	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
22	7	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	5	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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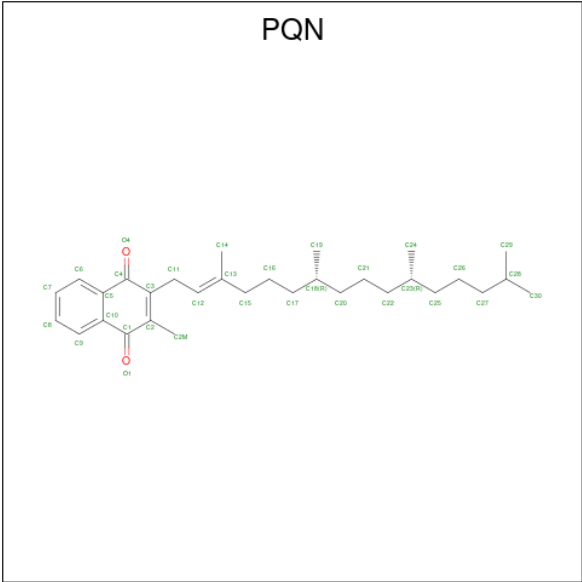
Mol	Chain	Residues	Atoms						AltConf
22	9	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			100	44	46	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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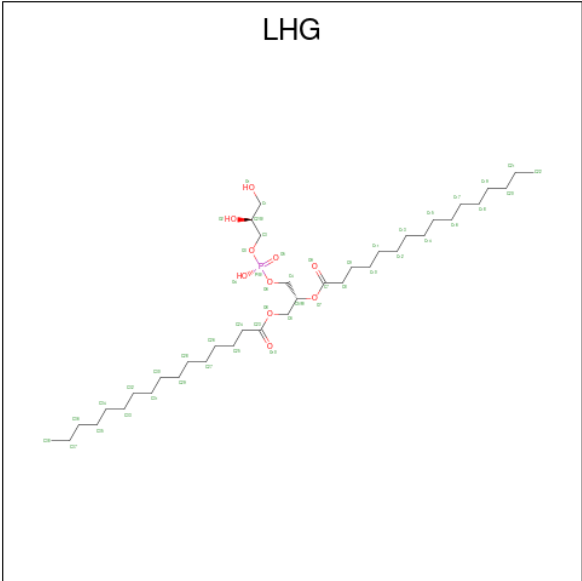
Mol	Chain	Residues	Atoms						AltConf
22	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
22	L2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	L2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



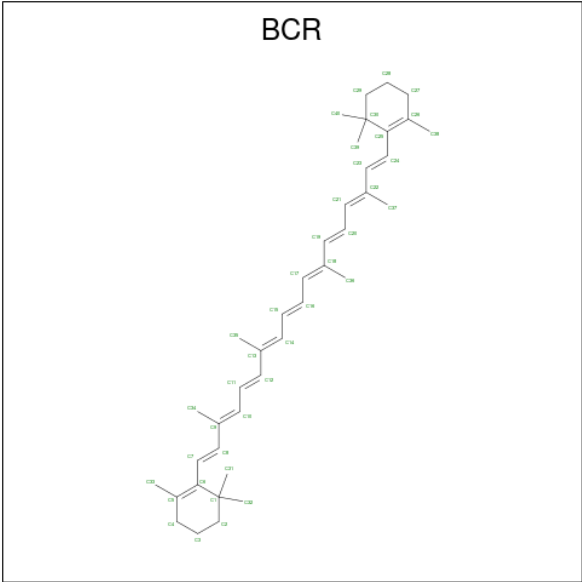
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	H	O	P	0
			87	27	49	10	1	
24	B	1	Total	C	H	O	P	0
			108	34	63	10	1	
24	1	1	Total	C	H	O	P	0
			87	28	48	10	1	
24	3	1	Total	C	H	O	P	0
			63	20	32	10	1	
24	3	1	Total	C	H	O	P	0
			114	36	67	10	1	
24	7	1	Total	C	H	O	P	0
			123	38	74	10	1	
24	8	1	Total	C	H	O	P	0
			105	33	61	10	1	
24	Z	1	Total	C	H	O	P	0
			87	28	48	10	1	
24	4	1	Total	C	H	O	P	0
			123	38	74	10	1	
24	4	1	Total	C	H	O	P	0
			87	27	49	10	1	
24	5	1	Total	C	H	O	P	0
			81	26	44	10	1	
24	6	1	Total	C	H	O	P	0
			123	38	74	10	1	
24	6	1	Total	C	H	O	P	0
			78	25	42	10	1	
24	9	1	Total	C	H	O	P	0
			96	30	55	10	1	
24	92	1	Total	C	H	O	P	0
			57	18	28	10	1	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	H	0
			96	40	56	
25	A	1	Total	C	H	0
			96	40	56	
25	A	1	Total	C	H	0
			96	40	56	
25	A	1	Total	C	H	0
			96	40	56	
25	A	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	G	1	Total	C	H	0
			96	40	56	
25	I	1	Total	C	H	0
			96	40	56	

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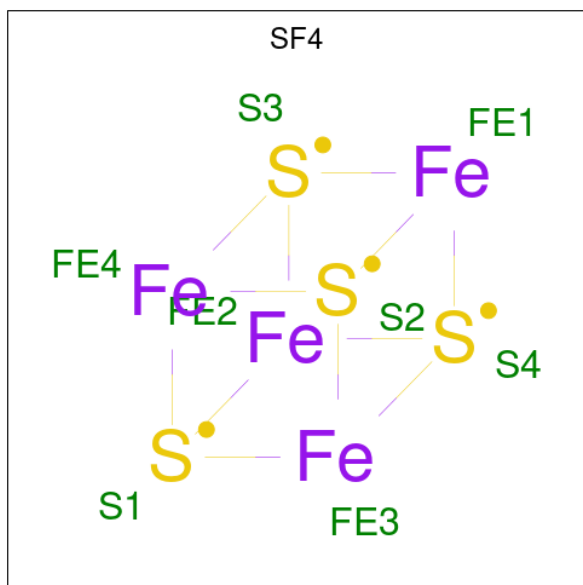
Mol	Chain	Residues	Atoms			AltConf
25	J	1	Total	C	H	0
			96	40	56	
25	L	1	Total	C	H	0
			96	40	56	
25	L	1	Total	C	H	0
			96	40	56	
25	K	1	Total	C	H	0
			96	40	56	
25	K	1	Total	C	H	0
			96	40	56	
25	3	1	Total	C	H	0
			96	40	56	
25	3	1	Total	C	H	0
			96	40	56	
25	3	1	Total	C	H	0
			96	40	56	
25	7	1	Total	C	H	0
			96	40	56	
25	8	1	Total	C	H	0
			96	40	56	
25	4	1	Total	C	H	0
			96	40	56	
25	5	1	Total	C	H	0
			96	40	56	
25	6	1	Total	C	H	0
			96	40	56	
25	9	1	Total	C	H	0
			96	40	56	
25	B2	1	Total	C	H	0
			47	20	27	
25	B2	1	Total	C	H	0
			96	40	56	
25	B2	1	Total	C	H	0
			96	40	56	
25	B2	1	Total	C	H	0
			34	14	20	
25	I2	1	Total	C	H	0
			96	40	56	
25	L2	1	Total	C	H	0
			96	40	56	
25	L2	1	Total	C	H	0
			96	40	56	

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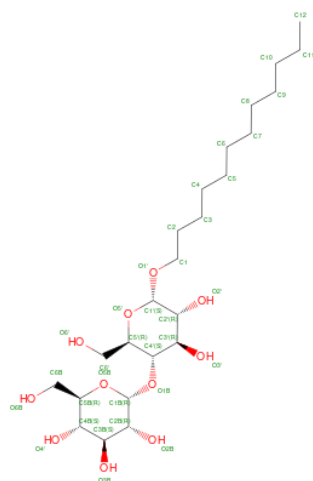
Mol	Chain	Residues	Atoms			AltConf
25	92	1	Total	C	H	0
			96	40	56	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$) (labeled as "Ligand of Interest" by depositor).

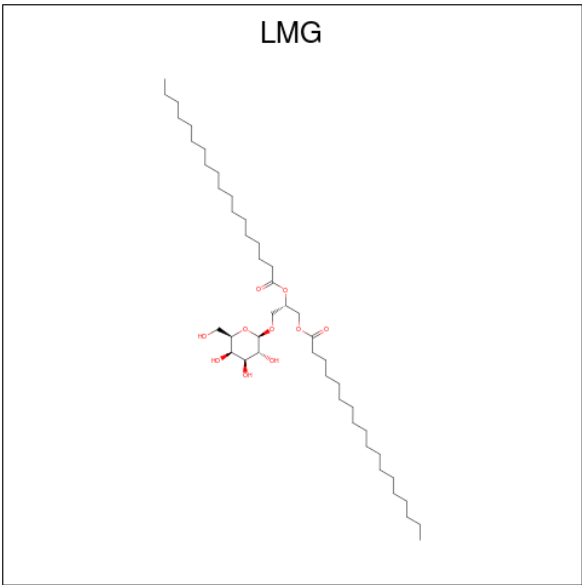


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Mol	Chain	Residues	Atoms				AltConf
27	1	1	Total	C	H	O	0
			59	18	35	6	
27	1	1	Total	C	H	O	0
			59	18	35	6	
27	7	1	Total	C	H	O	0
			69	21	37	11	
27	7	1	Total	C	H	O	0
			50	16	28	6	
27	7	1	Total	C	H	O	0
			54	16	27	11	
27	8	1	Total	C	H	O	0
			59	18	35	6	
27	8	1	Total	C	H	O	0
			59	18	35	6	
27	8	1	Total	C	H	O	0
			81	24	46	11	
27	8	1	Total	C	H	O	0
			59	18	35	6	
27	Z	1	Total	C	H	O	0
			66	20	35	11	
27	Z	1	Total	C	H	O	0
			50	16	28	6	
27	4	1	Total	C	H	O	0
			72	22	39	11	
27	4	1	Total	C	H	O	0
			44	14	24	6	
27	5	1	Total	C	H	O	0
			59	18	35	6	
27	6	1	Total	C	H	O	0
			59	18	35	6	
27	6	1	Total	C	H	O	0
			44	14	24	6	
27	6	1	Total	C	H	O	0
			59	18	35	6	
27	6	1	Total	C	H	O	0
			59	18	35	6	
27	9	1	Total	C	H	O	0
			59	18	35	6	
27	92	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



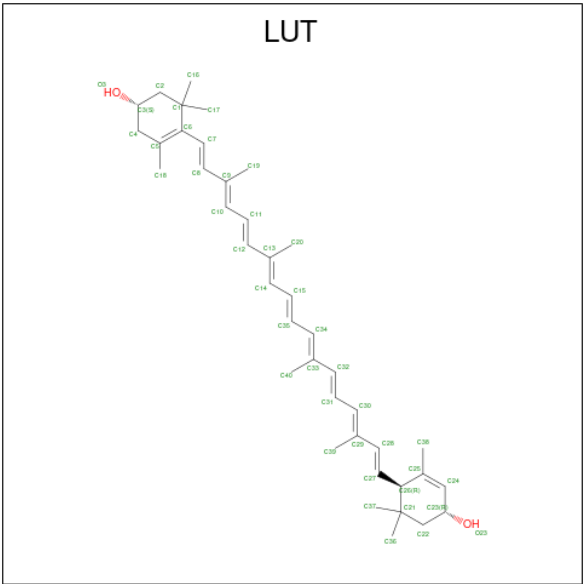
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	H	O	0
			117	38	69	10	
28	A	1	Total	C	H	O	0
			78	26	42	10	
28	B	1	Total	C	H	O	0
			99	33	56	10	
28	B	1	Total	C	H	O	0
			78	26	42	10	
28	J	1	Total	C	H	O	0
			99	32	57	10	
28	J	1	Total	C	H	O	0
			75	25	40	10	
28	1	1	Total	C	H	O	0
			78	26	42	10	
28	1	1	Total	C	H	O	0
			96	32	54	10	
28	3	1	Total	C	H	O	0
			120	40	75	5	
28	7	1	Total	C	H	O	0
			81	27	44	10	
28	8	1	Total	C	H	O	0
			66	22	34	10	
28	8	1	Total	C	H	O	0
			99	32	57	10	
28	4	1	Total	C	H	O	0
			96	31	55	10	
28	6	1	Total	C	H	O	0
			55	18	35	2	

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Mol	Chain	Residues	Atoms				AltConf
28	9	1	Total	C	H	O	0
			105	34	61	10	
28	B2	1	Total	C	H	O	0
			99	33	56	10	
28	B2	1	Total	C	H	O	0
			63	21	32	10	

- Molecule 29 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).



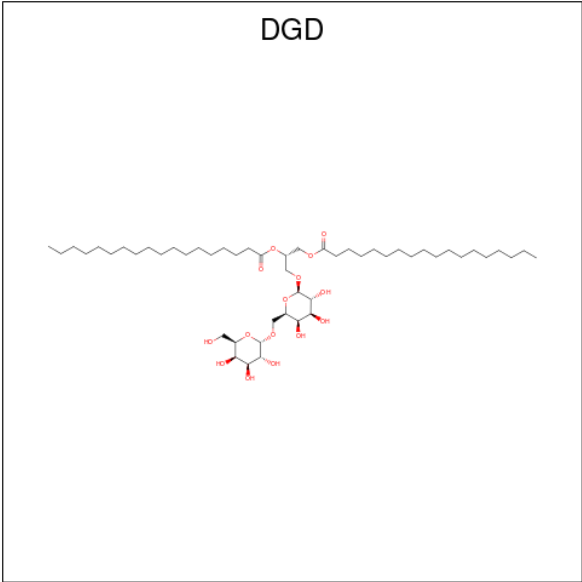
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	H	O	0
			98	40	56	2	
29	F	1	Total	C	H	O	0
			98	40	56	2	
29	1	1	Total	C	H	O	0
			98	40	56	2	
29	1	1	Total	C	H	O	0
			98	40	56	2	
29	3	1	Total	C	H	O	0
			98	40	56	2	
29	3	1	Total	C	H	O	0
			98	40	56	2	
29	3	1	Total	C	H	O	0
			98	40	56	2	

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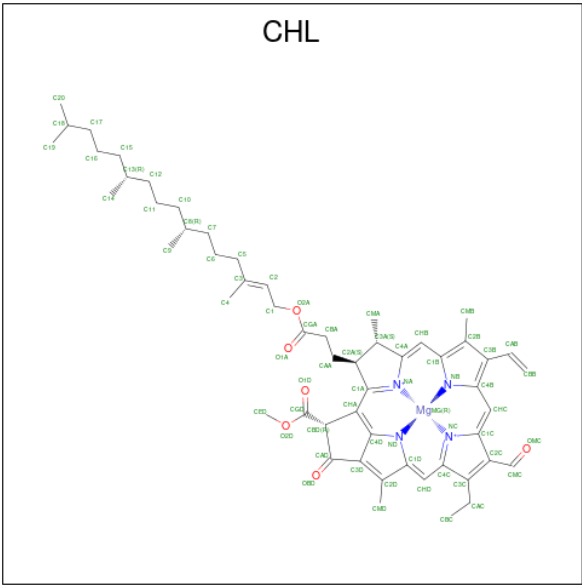
Mol	Chain	Residues	Atoms				AltConf
29	7	1	Total	C	H	O	0
			98	40	56	2	
29	7	1	Total	C	H	O	0
			98	40	56	2	
29	8	1	Total	C	H	O	0
			98	40	56	2	
29	Z	1	Total	C	H	O	0
			98	40	56	2	
29	Z	1	Total	C	H	O	0
			59	25	33	1	
29	4	1	Total	C	H	O	0
			98	40	56	2	
29	5	1	Total	C	H	O	0
			98	40	56	2	
29	5	1	Total	C	H	O	0
			98	40	56	2	
29	6	1	Total	C	H	O	0
			98	40	56	2	
29	9	1	Total	C	H	O	0
			98	40	56	2	
29	9	1	Total	C	H	O	0
			98	40	56	2	
29	92	1	Total	C	H	O	0
			98	40	56	2	
29	92	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
31	1	1	136	55	70	1	4	6	0
31	1	1	77	35	31	1	4	6	0
31	1	1	77	35	31	1	4	6	0

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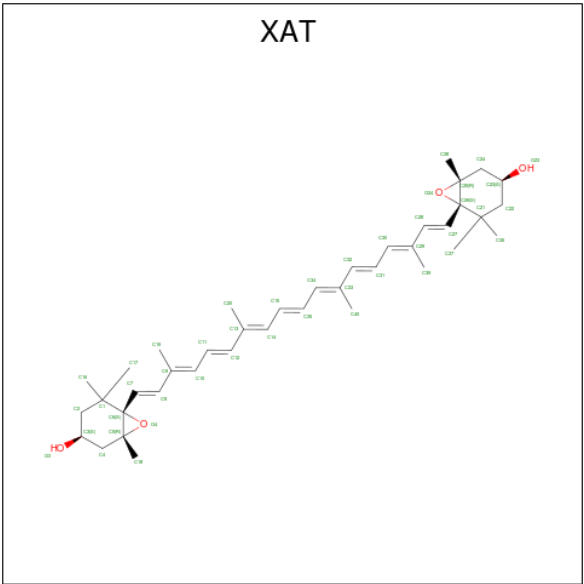
Mol	Chain	Residues	Atoms						AltConf
31	3	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	7	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	7	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	7	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	8	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	8	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	8	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	Z	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	Z	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	Z	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	4	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	4	1	Total 103	C 45	H 47	Mg 1	N 4	O 6	0
31	4	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	4	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	4	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	5	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	5	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	5	1	Total 88	C 40	H 37	Mg 1	N 4	O 6	0
31	5	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
31	6	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	6	1	Total 109	C 47	H 51	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms						AltConf
31	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
31	6	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
31	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
31	6	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
31	9	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
31	9	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
31	92	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
31	92	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	

- Molecule 32 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).



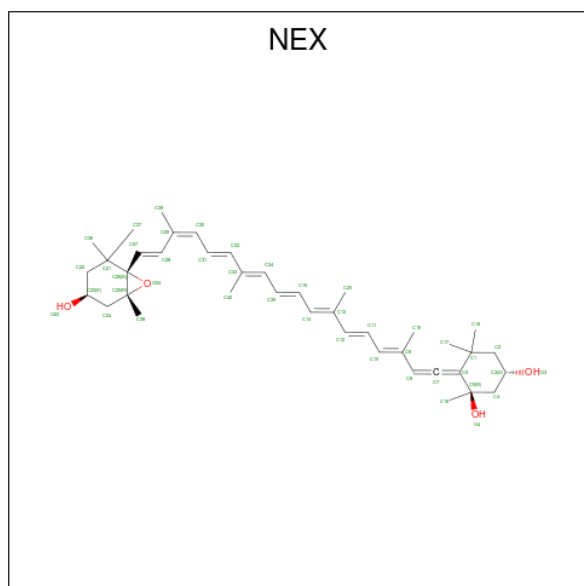
Mol	Chain	Residues	Atoms				AltConf
32	1	1	Total	C	H	O	0
			100	40	56	4	
32	7	1	Total	C	H	O	0
			100	40	56	4	

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Mol	Chain	Residues	Atoms				AltConf
32	8	1	Total	C	H	O	0
			100	40	56	4	
32	Z	1	Total	C	H	O	0
			100	40	56	4	
32	4	1	Total	C	H	O	0
			100	40	56	4	
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 (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
33	5	1	Total	C	H	O	0
			100	40	56	4	
33	6	1	Total	C	H	O	0
			100	40	56	4	

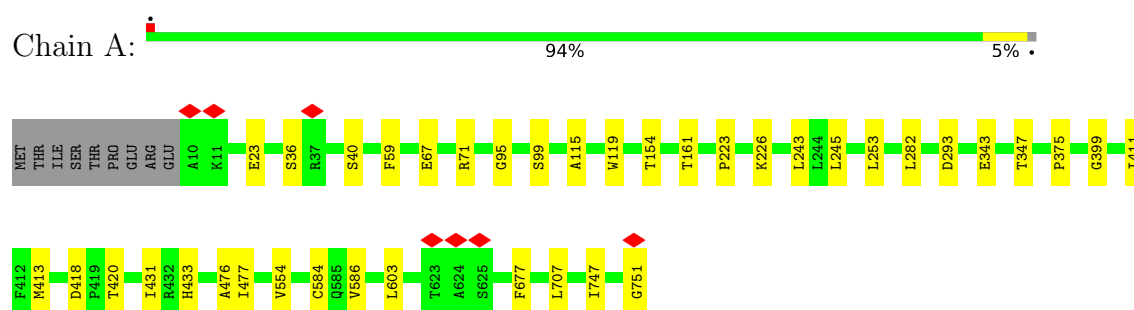
- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	H	11	Total 11	O 11	0
34	H	20	Total 20	O 20	0
34	H	1	Total 1	O 1	0
34	H	1	Total 1	O 1	0
34	H	4	Total 4	O 4	0
34	H	2	Total 2	O 2	0
34	H	7	Total 7	O 7	0
34	H	6	Total 6	O 6	0
34	H	7	Total 7	O 7	0
34	H	7	Total 7	O 7	0
34	H	5	Total 5	O 5	0
34	H	4	Total 4	O 4	0
34	H	7	Total 7	O 7	0
34	H	5	Total 5	O 5	0
34	H	1	Total 1	O 1	0

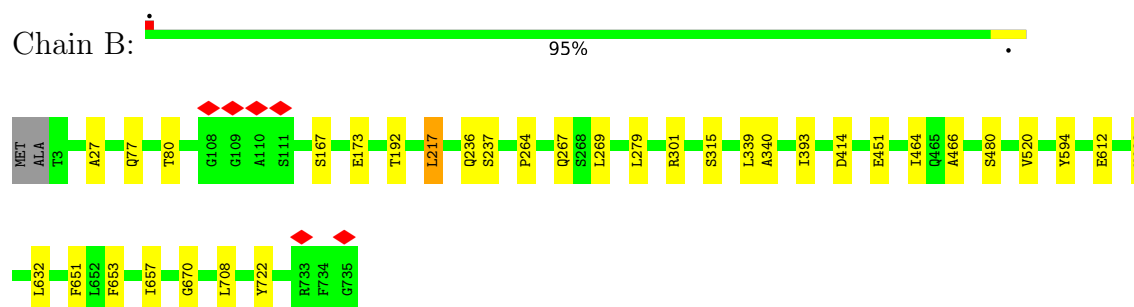
3 Residue-property plots

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

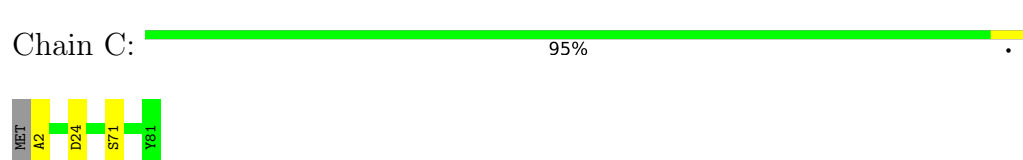
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



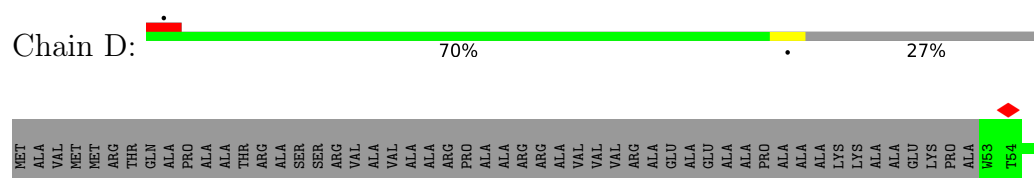
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

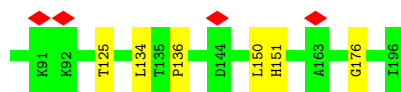


- Molecule 3: Photosystem I iron-sulfur center

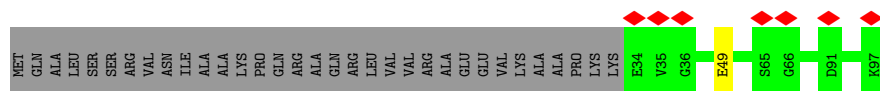


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

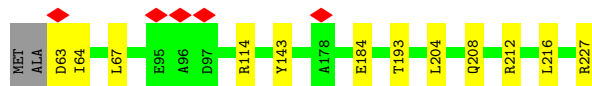
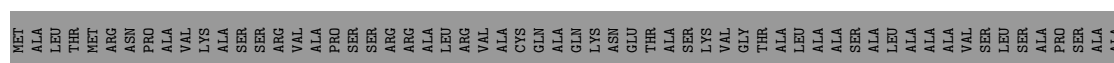




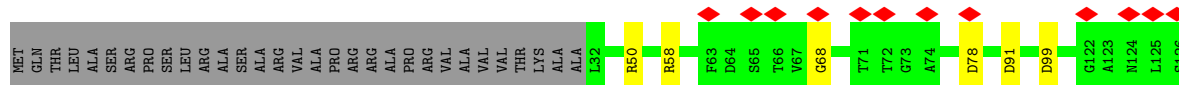
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



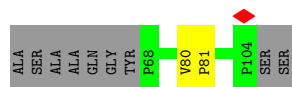
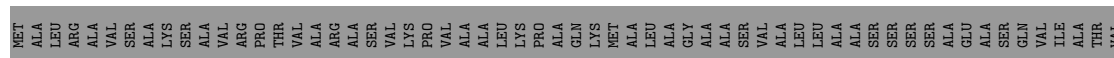
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



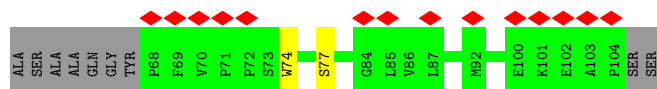
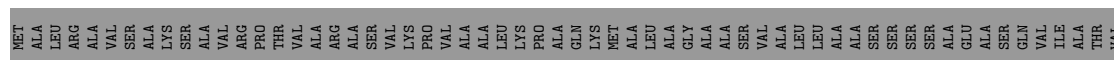
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



- Molecule 8: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit VIII



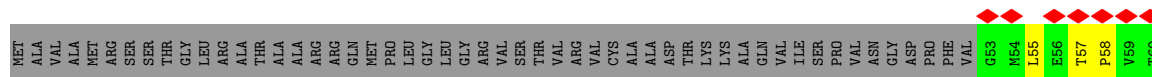
- Molecule 9: Photosystem I reaction center subunit IX

Chain J:  88% 12%



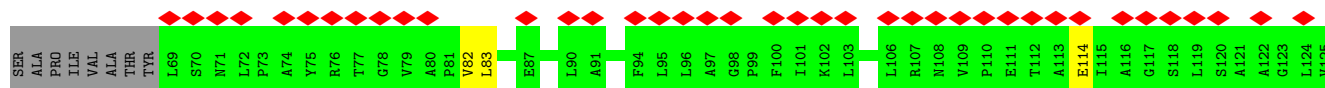
- Molecule 10: PSI subunit V

Chain L:  8% 60% 37%



- Molecule 10: PSI subunit V

Chain L2:  28% 51% 48%



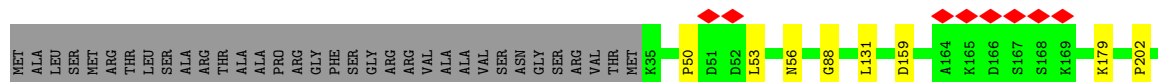
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  18% 69% 7% 24%

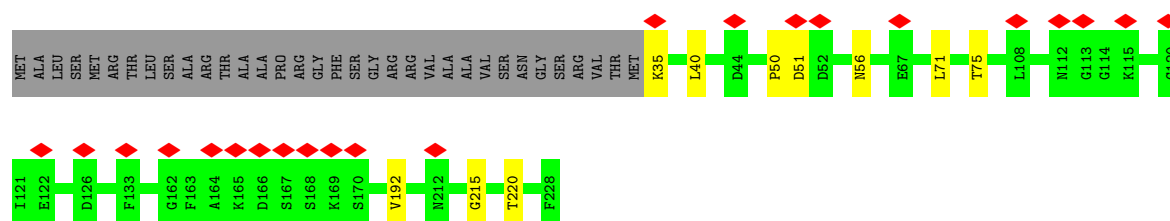
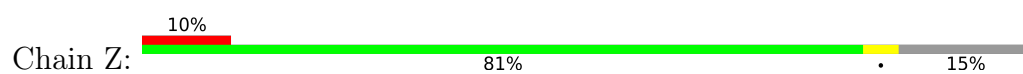


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

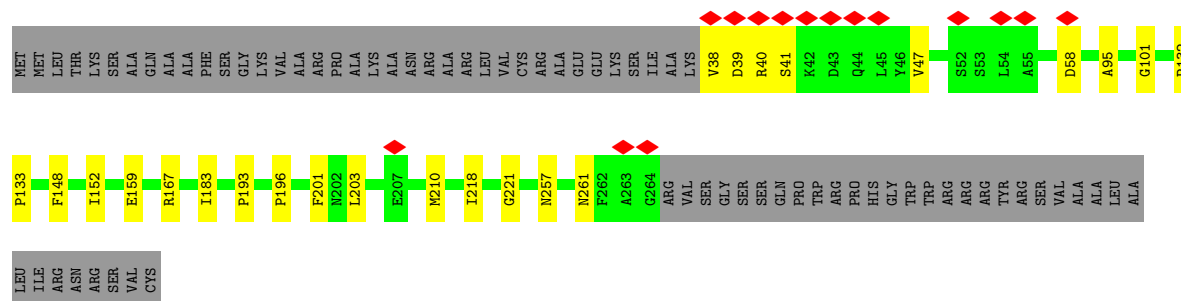
Chain 1:  81% 15%



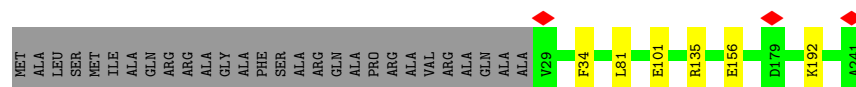
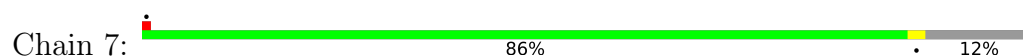
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic



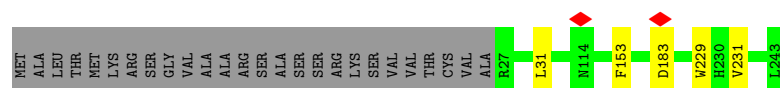
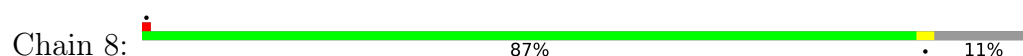
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic



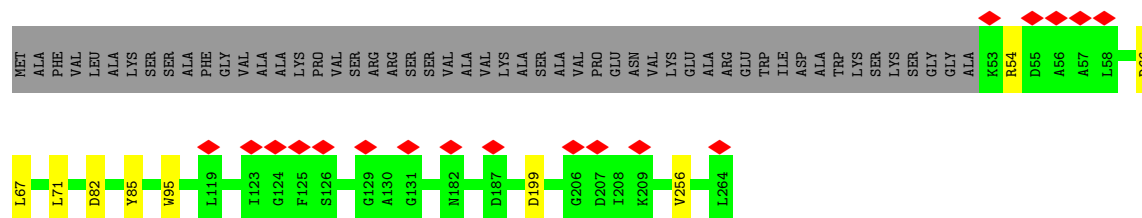
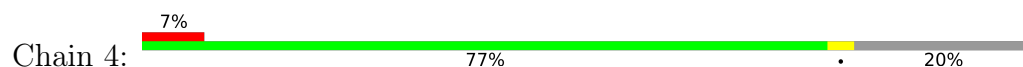
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



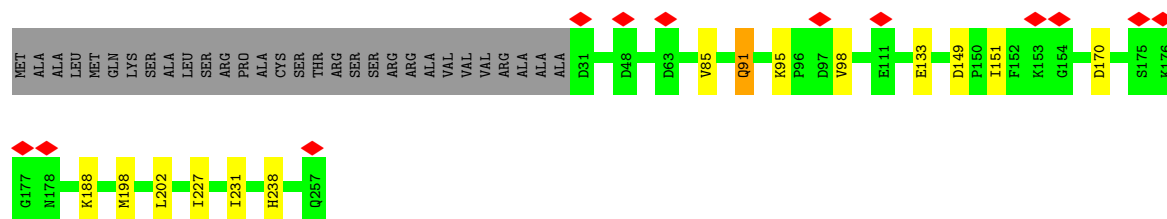
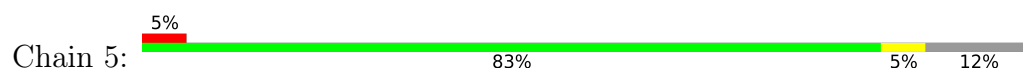
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



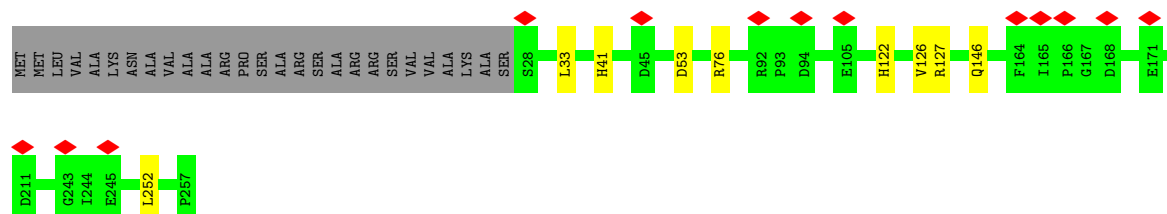
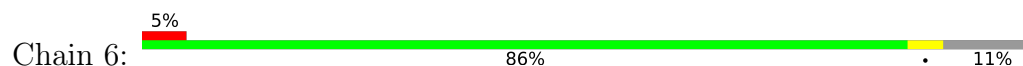
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)



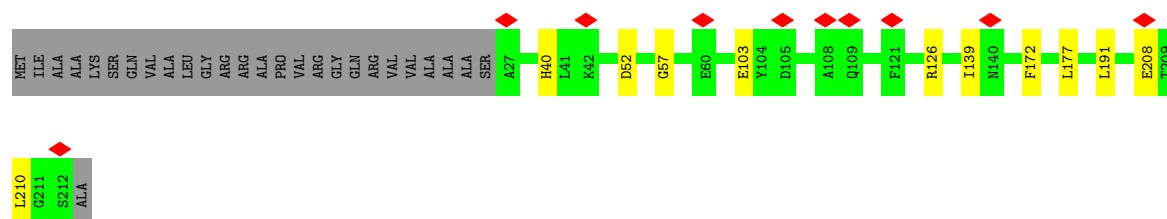
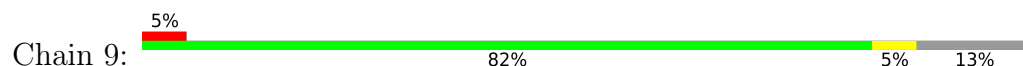
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



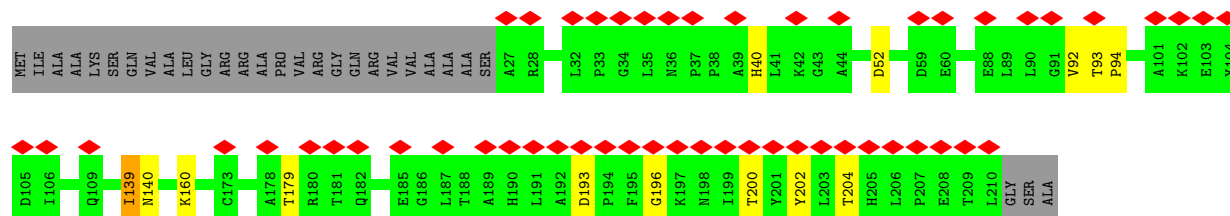
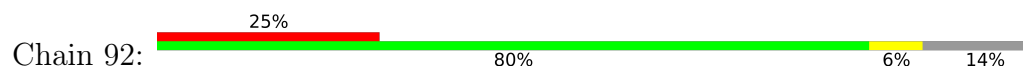
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



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



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



- Molecule 20: Photosystem I P700 chlorophyll a apoprotein A2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28346	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	0.175	Depositor
Minimum map value	-0.075	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.031	Depositor
Map size ($\text{\AA}$)	588.0, 588.0, 588.0	wwPDB
Map dimensions	700, 700, 700	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: CL0, DGD, AME, CLA, CHL, SF4, BCR, LUT, PQN, NEX, LMG, LMU, LHG, XAT

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	0.17	0/6021	0.23	0/8208
2	B	0.18	0/6036	0.23	0/8240
3	C	0.16	0/611	0.29	0/826
4	D	0.14	0/1161	0.24	0/1567
5	E	0.15	0/516	0.18	0/700
6	F	0.14	0/1292	0.21	0/1747
7	G	0.15	0/721	0.19	0/980
8	I	0.15	0/293	0.26	0/406
8	I2	0.10	0/293	0.24	0/406
9	J	0.17	0/329	0.23	0/452
10	L	0.15	0/920	0.20	0/1257
10	L2	0.10	0/757	0.17	0/1031
11	K	0.15	0/588	0.18	0/795
12	1	0.15	0/1491	0.21	0/2028
12	Z	0.13	0/1491	0.19	0/2028
13	3	0.16	0/1784	0.24	0/2420
14	7	0.17	0/1702	0.21	0/2310
15	8	0.17	0/1701	0.23	0/2315
16	4	0.13	0/1703	0.20	0/2321
17	5	0.14	0/1830	0.22	0/2492
18	6	0.14	0/1834	0.21	0/2505
19	9	0.14	0/1461	0.21	0/1987
19	92	0.12	0/1451	0.20	0/1974
20	B2	0.09	0/1522	0.19	0/2071
All	All	0.15	0/37508	0.22	0/51066

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	5675	5675	26	0
2	B	5824	5576	5577	31	0
3	C	601	582	581	2	0
4	D	1133	1151	1150	4	0
5	E	506	505	504	1	0
6	F	1266	1302	1301	9	0
7	G	706	687	686	4	0
8	I	281	292	292	1	0
8	I2	281	292	292	1	0
9	J	329	328	328	2	0
10	L	899	907	905	7	0
10	L2	739	748	747	2	0
11	K	583	620	620	7	0
12	1	1445	1397	1396	8	0
12	Z	1445	1397	1396	7	0
13	3	1736	1695	1694	15	0
14	7	1650	1590	1589	7	0
15	8	1650	1630	1629	5	0
16	4	1648	1603	1602	7	0
17	5	1775	1747	1746	14	0
18	6	1772	1770	1770	9	0
19	9	1420	1400	1399	10	0
19	92	1410	1392	1391	9	0
20	B2	1469	1396	1395	4	0
21	A	65	72	72	0	0
22	1	639	625	625	5	0
22	3	740	718	718	12	0
22	4	565	534	534	3	0
22	5	740	712	712	10	0
22	6	628	605	605	1	0
22	7	652	598	598	5	0
22	8	614	578	578	4	0
22	9	565	535	535	2	0
22	92	545	505	505	4	0
22	A	2718	2856	2856	28	0
22	B	2463	2580	2580	25	0
22	B2	919	891	891	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	175	177	177	1	0
22	G	106	92	92	0	0
22	J	55	49	49	1	0
22	K	196	158	158	3	0
22	L	110	105	105	1	0
22	L2	90	66	66	0	0
22	Z	627	593	593	6	0
23	A	33	46	46	0	0
23	B	33	46	46	0	0
24	1	39	48	48	1	0
24	3	78	99	99	1	0
24	4	87	123	123	1	0
24	5	37	44	44	1	0
24	6	85	116	116	1	0
24	7	49	74	74	1	0
24	8	44	61	61	0	0
24	9	41	55	55	0	0
24	92	29	28	28	1	0
24	A	87	123	123	0	0
24	B	45	63	63	0	0
24	Z	39	48	48	0	0
25	3	120	168	168	7	0
25	4	40	56	56	0	0
25	5	40	56	56	0	0
25	6	40	56	56	2	0
25	7	40	56	56	0	0
25	8	40	56	56	2	0
25	9	40	56	56	2	0
25	92	40	56	56	3	0
25	A	200	280	280	12	0
25	B	280	392	392	11	0
25	B2	114	159	159	6	0
25	G	40	56	56	0	0
25	I	40	56	56	1	0
25	I2	40	56	56	0	0
25	J	40	56	56	1	0
25	K	80	112	112	6	0
25	L	80	112	112	5	0
25	L2	80	112	112	3	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	1	148	201	201	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	4	53	63	63	0	0
27	5	24	35	35	0	0
27	6	92	129	129	1	0
27	7	81	92	92	1	0
27	8	107	151	151	1	0
27	9	24	35	35	1	0
27	92	35	46	46	2	0
27	A	196	262	262	4	0
27	B	35	46	46	3	0
27	G	24	35	35	0	0
27	K	24	35	35	0	0
27	Z	53	63	63	1	0
28	1	78	96	96	0	0
28	3	45	75	75	1	0
28	4	41	55	55	1	0
28	6	20	35	35	0	0
28	7	37	44	44	0	0
28	8	74	91	91	0	0
28	9	44	61	61	1	0
28	A	84	111	111	1	0
28	B	79	98	98	1	0
28	B2	74	88	88	0	0
28	J	77	97	97	2	0
29	1	84	112	112	2	0
29	3	126	168	168	2	0
29	4	42	56	56	1	0
29	5	84	112	112	4	0
29	6	42	56	56	1	0
29	7	84	112	112	4	0
29	8	42	56	56	0	0
29	9	84	112	112	3	0
29	92	84	112	112	0	0
29	A	42	56	56	1	0
29	F	42	56	56	3	0
29	Z	68	89	89	1	0
30	B	59	79	79	1	0
31	1	158	132	132	1	0
31	3	66	70	70	1	0
31	4	300	288	288	3	0
31	5	206	167	167	2	0
31	6	350	327	327	7	0
31	7	158	132	132	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	8	198	210	210	3	0
31	9	93	64	64	0	0
31	92	88	58	58	0	0
31	Z	178	171	171	1	0
32	1	44	56	56	1	0
32	4	44	56	56	0	0
32	5	44	56	56	0	0
32	6	44	56	56	0	0
32	7	44	56	56	0	0
32	8	44	56	56	0	0
32	Z	44	56	56	0	0
33	5	44	56	56	0	0
33	6	44	56	56	1	0
34	H	88	0	0	12	0
All	All	56460	56999	56982	324	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 (324) 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)
29:7:624:LUT:H381	29:7:624:LUT:H28	1.51	0.92
27:B:853:LMU:H2O1	27:B:853:LMU:H6'	1.15	0.87
1:A:95:GLY:O	1:A:99:SER:OG	1.94	0.83
17:5:170:ASP:OD1	29:5:620:LUT:O23	1.96	0.82
2:B:301:ARG:NH1	7:G:68:GLY:O	2.15	0.80
2:B:628:ASN:O	34:H:14:HOH:O	2.00	0.79
2:B:167:SER:OG	7:G:78:ASP:OD1	2.00	0.78
19:92:40:HIS:NE2	19:92:52:ASP:OD2	2.17	0.78
27:A:862:LMU:H2O2	27:A:863:LMU:H6B	1.21	0.77
31:8:606:CHL:O1D	34:H:91:HOH:O	2.03	0.77
6:F:184:GLU:OE1	34:H:88:HOH:O	2.03	0.76
7:G:58:ARG:NH2	7:G:99:ASP:OD2	2.21	0.73
27:7:628:LMU:O6'	34:H:81:HOH:O	2.05	0.73
12:1:179:LYS:NZ	24:1:620:LHG:O5	2.21	0.73
31:4:601:CHL:OBD	18:6:127:ARG:NH1	2.22	0.72
1:A:226:LYS:NZ	1:A:253:LEU:O	2.22	0.72
2:B:269:LEU:O	34:H:12:HOH:O	2.07	0.71
13:3:40:ARG:O	13:3:41:SER:OG	2.06	0.69
1:A:23:GLU:OE2	28:A:860:LMG:O5	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:7:624:LUT:H381	29:7:624:LUT:C28	2.19	0.69
6:F:63:ASP:N	6:F:67:LEU:O	2.26	0.69
31:6:606:CHL:OMC	34:H:73:HOH:O	2.12	0.68
13:3:159:GLU:OE2	34:H:37:HOH:O	2.12	0.67
2:B:27:ALA:HA	22:B:829:CLA:H43	1.77	0.66
22:A:803:CLA:HMB1	22:A:803:CLA:HBB1	1.77	0.66
22:A:811:CLA:H11	22:A:813:CLA:H42	1.79	0.64
2:B:217:LEU:CD1	19:9:210:LEU:HD23	2.28	0.64
11:K:78:SER:OG	22:K:201:CLA:O1D	2.16	0.64
19:9:208:GLU:N	19:9:208:GLU:OE1	2.31	0.64
22:5:621:CLA:HED2	22:5:621:CLA:O1A	1.98	0.63
22:Z:616:CLA:H72	22:Z:616:CLA:H41	1.79	0.63
13:3:148:PHE:CE2	13:3:152:ILE:HD11	2.32	0.63
22:Z:616:CLA:H41	22:Z:616:CLA:C7	2.29	0.63
29:5:626:LUT:H1	27:6:628:LMU:H6'	1.42	0.62
2:B:315:SER:OG	22:B:841:CLA:O1A	2.07	0.62
31:6:607:CHL:H42	33:6:625:NEX:H403	1.79	0.62
22:Z:603:CLA:HED2	22:Z:603:CLA:H43	1.80	0.62
14:7:192:LYS:NZ	24:7:625:LHG:O5	2.33	0.62
12:Z:40:LEU:HD13	31:Z:601:CHL:HMA3	1.81	0.61
18:6:146:GLN:OE1	18:6:146:GLN:N	2.33	0.61
22:3:607:CLA:H93	25:3:719:BCR:H392	1.83	0.61
12:Z:50:PRO:O	12:Z:56:ASN:ND2	2.33	0.60
19:92:160:LYS:NZ	24:92:622:LHG:O5	2.35	0.60
22:7:620:CLA:O1A	18:6:252:LEU:N	2.35	0.60
16:4:54:ARG:NH1	16:4:71:LEU:O	2.35	0.59
13:3:257:ASN:O	13:3:261:ASN:ND2	2.36	0.59
18:6:41:HIS:NE2	18:6:53:ASP:OD2	2.31	0.58
22:B:816:CLA:H101	22:B:816:CLA:H142	1.86	0.58
2:B:708:LEU:HD23	30:B:850:DGD:HA22	1.85	0.58
13:3:167:ARG:NH1	28:3:722:LMG:O1	2.37	0.57
14:7:101:GLU:N	14:7:101:GLU:OE1	2.37	0.57
2:B:393:ILE:HD13	22:B:829:CLA:HED1	1.87	0.57
1:A:161:THR:HG21	22:A:817:CLA:HBA1	1.85	0.57
31:8:606:CHL:OMC	34:H:55:HOH:O	2.18	0.57
2:B:339:LEU:HD21	22:B:829:CLA:HAB	1.86	0.57
22:1:603:CLA:HED2	22:1:603:CLA:H43	1.84	0.57
25:A:851:BCR:H23C	25:A:851:BCR:H403	1.87	0.57
22:5:602:CLA:H41	22:5:603:CLA:O1A	2.05	0.57
20:B2:33:GLU:OE1	20:B2:33:GLU:N	2.37	0.56
19:92:139:ILE:HG22	19:92:140:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:53:LEU:HD23	22:1:602:CLA:HED2	1.87	0.56
13:3:95:ALA:HB1	13:3:221:GLY:HA3	1.88	0.56
16:4:256:VAL:N	22:4:613:CLA:O1A	2.38	0.56
11:K:89:VAL:HG22	22:K:201:CLA:HMD2	1.89	0.55
12:1:220:THR:O	12:1:220:THR:HG22	2.05	0.55
22:A:840:CLA:H42	22:A:840:CLA:O1A	2.07	0.55
31:4:606:CHL:C4A	34:H:64:HOH:O	2.26	0.55
4:D:125:THR:HG23	4:D:136:PRO:HG2	1.88	0.55
29:7:624:LUT:H383	15:8:229:TRP:CE2	2.42	0.55
10:L2:114:GLU:N	10:L2:114:GLU:OE1	2.40	0.55
22:1:613:CLA:H102	22:1:613:CLA:H143	1.87	0.55
20:B2:60:LEU:O	20:B2:63:SER:OG	2.24	0.55
19:92:179:THR:HG21	22:92:613:CLA:O1D	2.07	0.55
22:Z:603:CLA:H43	22:Z:603:CLA:CED	2.36	0.55
22:A:829:CLA:HBB1	22:A:829:CLA:HMB1	1.88	0.54
14:7:156:GLU:N	14:7:156:GLU:OE1	2.39	0.54
22:3:615:CLA:H193	17:5:227:ILE:HG21	1.89	0.54
2:B:722:TYR:HB2	22:B:802:CLA:HED2	1.90	0.54
19:92:92:VAL:HG12	19:92:94:PRO:HD2	1.89	0.54
22:A:833:CLA:OBD	10:L:57:THR:HG21	2.07	0.54
6:F:64:ILE:HD11	6:F:143:TYR:CD2	2.43	0.54
22:1:603:CLA:H43	22:1:603:CLA:CED	2.38	0.54
12:1:159:ASP:OD1	29:1:617:LUT:O23	2.23	0.54
2:B:217:LEU:HD13	19:9:210:LEU:HD23	1.90	0.54
2:B:464:ILE:HD11	22:B:836:CLA:H12	1.90	0.54
25:L2:205:BCR:C23	25:L2:205:BCR:H403	2.38	0.54
27:B:853:LMU:O6'	27:B:853:LMU:O2B	1.99	0.53
25:B2:844:BCR:H331	25:B2:844:BCR:C8	2.38	0.53
25:L:205:BCR:C23	25:L:205:BCR:H403	2.39	0.53
8:I2:74:TRP:O	8:I2:77:SER:OG	2.26	0.53
2:B:653:PHE:CZ	2:B:657:ILE:HD11	2.43	0.53
2:B:393:ILE:HG21	22:B:829:CLA:HED1	1.90	0.53
31:5:606:CHL:C4C	34:H:67:HOH:O	2.34	0.53
22:Z:608:CLA:H12	29:Z:617:LUT:H383	1.90	0.52
25:B:843:BCR:H331	25:B:843:BCR:C8	2.39	0.52
12:Z:71:LEU:O	12:Z:75:THR:HG23	2.09	0.52
31:6:608:CHL:H11	29:6:621:LUT:H383	1.91	0.52
20:B2:158:LEU:O	20:B2:163:GLN:NE2	2.43	0.52
6:F:208:GLN:OE1	6:F:212:ARG:NH2	2.43	0.52
22:B:834:CLA:H141	28:B:854:LMG:C34	2.39	0.52
27:A:858:LMU:O3'	27:A:858:LMU:O2B	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:304:CLA:O1A	22:F:304:CLA:C2	2.58	0.52
25:A:848:BCR:H362	25:A:849:BCR:H21C	1.92	0.51
31:4:606:CHL:C1A	34:H:64:HOH:O	2.34	0.51
25:B:801:BCR:H331	25:B:801:BCR:C8	2.40	0.51
25:J:102:BCR:H331	25:J:102:BCR:C8	2.40	0.51
22:3:615:CLA:H42	17:5:231:ILE:CG1	2.40	0.51
7:G:50:ARG:NH2	7:G:91:ASP:OD1	2.43	0.51
13:3:210:MET:CE	22:3:610:CLA:HED3	2.41	0.51
22:3:602:CLA:HBA1	29:3:622:LUT:H182	1.93	0.51
6:F:204:LEU:HA	22:8:603:CLA:H42	1.92	0.51
16:4:82:ASP:OD1	16:4:85:TYR:N	2.44	0.51
28:9:620:LMG:O2	28:9:620:LMG:O9	2.29	0.51
22:A:818:CLA:H91	25:K:207:BCR:HC21	1.93	0.51
18:6:33:LEU:HD13	31:6:601:CHL:HMA3	1.91	0.51
25:L2:205:BCR:C8	25:L2:205:BCR:H331	2.41	0.50
22:A:802:CLA:H141	22:A:804:CLA:H191	1.93	0.50
22:4:613:CLA:H43	22:4:614:CLA:OBD	2.11	0.50
1:A:67:GLU:OE2	1:A:71:ARG:NH2	2.45	0.50
22:A:825:CLA:H41	22:A:825:CLA:H72	1.94	0.50
2:B:520:VAL:HG11	2:B:594:TYR:CG	2.47	0.49
25:A:852:BCR:H331	25:A:852:BCR:C8	2.42	0.49
22:B2:828:CLA:H141	22:B2:828:CLA:H171	1.93	0.49
10:L:128:LEU:HD22	25:L:205:BCR:H401	1.95	0.49
18:6:76:ARG:NH1	31:6:608:CHL:OBD	2.39	0.49
22:A:843:CLA:H93	22:A:843:CLA:H121	1.93	0.49
13:3:39:ASP:HB2	13:3:47:VAL:HG23	1.95	0.48
25:B:844:BCR:H382	25:B:844:BCR:H23C	1.94	0.48
22:8:604:CLA:H43	25:8:619:BCR:H272	1.94	0.48
19:9:40:HIS:ND1	19:9:57:GLY:O	2.46	0.48
15:8:31:LEU:HD13	31:8:601:CHL:HMA3	1.94	0.48
13:3:201:PHE:O	13:3:203:LEU:N	2.46	0.48
19:9:103:GLU:N	19:9:103:GLU:OE1	2.46	0.48
22:B:839:CLA:H93	25:I:172:BCR:H333	1.96	0.48
22:3:611:CLA:H41	22:3:611:CLA:H71	1.95	0.48
15:8:183:ASP:N	15:8:183:ASP:OD1	2.44	0.48
29:F:305:LUT:C28	29:F:305:LUT:H381	2.41	0.48
27:92:624:LMU:H82	25:92:623:BCR:H362	1.95	0.48
25:L:205:BCR:H331	25:L:205:BCR:C8	2.43	0.47
16:4:199:ASP:OD1	29:4:619:LUT:O23	2.29	0.47
2:B:466:ALA:O	2:B:480:SER:OG	2.28	0.47
22:92:611:CLA:H93	22:92:611:CLA:H121	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:ALA:HB2	25:B:847:BCR:H372	1.96	0.47
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.95	0.47
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.96	0.47
22:B:806:CLA:H2	22:B:806:CLA:HED3	1.96	0.47
17:5:85:VAL:HG11	29:5:620:LUT:H12	1.95	0.47
19:92:179:THR:HG22	19:92:202:TYR:CG	2.50	0.47
4:D:176:GLY:N	5:E:49:GLU:OE1	2.48	0.47
20:B2:27:ALA:HA	22:B2:829:CLA:H42	1.97	0.47
22:A:854:CLA:HBB1	22:A:854:CLA:HMB1	1.96	0.46
10:L:58:PRO:O	10:L:62:ALA:HB2	2.15	0.46
11:K:57:VAL:HG23	11:K:88:ASP:OD1	2.14	0.46
12:1:88:GLY:HA2	32:1:618:XAT:H181	1.98	0.46
17:5:188:LYS:NZ	24:5:623:LHG:O5	2.48	0.46
22:5:617:CLA:HED1	24:6:619:LHG:H311	1.98	0.46
1:A:433:HIS:HB3	10:L:55:LEU:HD22	1.96	0.46
22:B:841:CLA:HBC1	27:B:853:LMU:H2'	1.97	0.46
2:B:236:GLN:O	2:B:237:SER:OG	2.32	0.46
2:B:269:LEU:HD13	22:B:817:CLA:HMA2	1.97	0.46
2:B:632:LEU:HD21	2:B:651:PHE:CD1	2.51	0.46
22:A:811:CLA:HBA1	22:A:813:CLA:HMD2	1.97	0.46
14:7:81:LEU:HD22	22:7:610:CLA:H201	1.98	0.46
25:9:623:BCR:H362	27:9:624:LMU:H82	1.97	0.46
1:A:677:PHE:CG	25:A:852:BCR:H363	2.51	0.46
10:L:57:THR:HG22	10:L:58:PRO:HD2	1.98	0.46
19:92:200:THR:O	19:92:204:THR:OG1	2.29	0.46
1:A:59:PHE:CD2	22:A:806:CLA:HMC2	2.51	0.45
1:A:223:PRO:HB2	1:A:243:LEU:HD13	1.98	0.45
22:B:829:CLA:HBB1	22:B:829:CLA:HMB1	1.96	0.45
25:B:845:BCR:H331	25:B:845:BCR:C8	2.46	0.45
25:6:623:BCR:H331	25:6:623:BCR:C8	2.45	0.45
17:5:91:GLN:CD	17:5:98:VAL:HG21	2.41	0.45
14:7:135:ARG:NH1	22:7:609:CLA:O1D	2.46	0.45
25:B:845:BCR:H342	19:9:177:LEU:HD21	1.99	0.45
25:K:202:BCR:H392	25:K:202:BCR:C23	2.46	0.45
13:3:193:PRO:CG	31:3:608:CHL:HMD1	2.47	0.45
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.98	0.45
1:A:245:LEU:O	27:A:857:LMU:O2B	2.35	0.45
22:1:603:CLA:H61	22:1:603:CLA:H41	1.87	0.45
27:92:624:LMU:C8	25:92:623:BCR:H362	2.47	0.45
22:A:809:CLA:H91	22:A:812:CLA:H201	1.99	0.45
22:B:821:CLA:H191	12:1:131:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:844:BCR:H331	25:B:844:BCR:C8	2.46	0.45
19:9:52:ASP:OD1	29:9:617:LUT:O23	2.34	0.45
8:I:80:VAL:HB	8:I:81:PRO:HD3	1.98	0.44
25:K:202:BCR:H331	25:K:202:BCR:C8	2.47	0.44
29:7:624:LUT:H383	15:8:229:TRP:CZ2	2.52	0.44
2:B:414:ASP:O	6:F:227:ARG:NH1	2.51	0.44
2:B:451:GLU:OE2	6:F:114:ARG:NH1	2.50	0.44
22:3:615:CLA:H42	17:5:231:ILE:HG13	1.98	0.44
1:A:418:ASP:OD2	1:A:420:THR:OG1	2.30	0.44
2:B:632:LEU:HD21	2:B:651:PHE:CG	2.52	0.44
12:1:202:PRO:O	29:1:617:LUT:O3	2.33	0.44
1:A:413:MET:CE	1:A:431:ILE:HD11	2.47	0.44
22:3:603:CLA:HBC1	22:3:609:CLA:CBC	2.48	0.44
19:92:93:THR:OG1	19:92:94:PRO:HD3	2.17	0.44
1:A:119:TRP:CD2	22:A:810:CLA:HED3	2.53	0.44
27:A:862:LMU:O2'	27:A:863:LMU:O6B	2.04	0.44
22:7:608:CLA:O1A	22:7:610:CLA:HMD2	2.18	0.44
17:5:198:MET:HE3	22:5:603:CLA:CAB	2.48	0.44
2:B:173:GLU:OE1	2:B:173:GLU:N	2.49	0.44
3:C:2:ALA:N	3:C:71:SER:O	2.51	0.44
12:Z:35:LYS:N	12:Z:51:ASP:OD1	2.51	0.44
22:5:621:CLA:CBD	22:5:621:CLA:HAA2	2.48	0.44
18:6:122:HIS:O	18:6:126:VAL:HG23	2.17	0.44
25:9:623:BCR:H20C	25:9:623:BCR:H361	1.86	0.44
22:B:827:CLA:H141	22:B:829:CLA:H143	2.00	0.44
3:C:24:ASP:OD2	4:D:151:HIS:ND1	2.46	0.44
15:8:231:VAL:HG12	22:8:613:CLA:HED1	1.99	0.44
17:5:198:MET:HE3	22:5:603:CLA:HAB	1.99	0.44
25:K:202:BCR:H23C	25:K:202:BCR:H403	1.99	0.43
25:A:850:BCR:C8	25:A:850:BCR:H331	2.48	0.43
25:L:201:BCR:H24C	25:L:201:BCR:H371	1.90	0.43
13:3:101:GLY:HA2	29:3:622:LUT:H381	1.99	0.43
17:5:95:LYS:HB3	17:5:98:VAL:HG13	1.99	0.43
17:5:149:ASP:OD1	17:5:151:ILE:N	2.51	0.43
22:B:816:CLA:H142	22:B:816:CLA:C10	2.49	0.43
6:F:193:THR:HG21	28:J:104:LMG:H142	1.99	0.43
2:B:77:GLN:OE1	2:B:77:GLN:N	2.48	0.43
22:A:833:CLA:H42	10:L:65:VAL:HG13	2.00	0.43
13:3:183:ILE:HG22	13:3:196:PRO:HG2	2.00	0.43
22:3:603:CLA:HMD1	25:3:719:BCR:H403	2.01	0.43
1:A:343:GLU:O	1:A:347:THR:OG1	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:VAL:HG11	22:A:822:CLA:H203	2.01	0.43
22:L:203:CLA:H62	22:L:203:CLA:H41	1.89	0.43
25:3:719:BCR:C8	25:3:719:BCR:H331	2.47	0.43
25:B2:845:BCR:H24C	25:B2:845:BCR:H371	1.87	0.43
22:B:840:CLA:H122	22:B:840:CLA:H91	2.01	0.43
18:6:33:LEU:HD13	31:6:601:CHL:CMA	2.48	0.43
13:3:210:MET:HE2	22:3:610:CLA:HED3	2.01	0.43
1:A:411:ILE:HD13	22:A:831:CLA:CED	2.49	0.43
25:A:849:BCR:H331	25:A:849:BCR:C8	2.49	0.43
25:K:207:BCR:H24C	25:K:207:BCR:H371	1.88	0.43
22:7:610:CLA:H13	22:6:603:CLA:H142	2.00	0.43
12:Z:215:GLY:O	12:Z:220:THR:HG21	2.19	0.43
2:B:264:PRO:O	2:B:267:GLN:NE2	2.51	0.42
31:1:601:CHL:H62	31:1:601:CHL:H41	1.77	0.42
22:B:808:CLA:CGA	22:B:808:CLA:C1A	2.97	0.42
22:3:615:CLA:C19	17:5:227:ILE:HG21	2.49	0.42
1:A:586:VAL:HG13	2:B:670:GLY:HA3	2.00	0.42
1:A:707:LEU:HD23	6:F:216:LEU:HD23	2.01	0.42
25:B:848:BCR:H24C	25:B:848:BCR:H371	1.91	0.42
25:3:719:BCR:H20C	25:3:719:BCR:H361	1.90	0.42
14:7:34:PHE:HE1	31:7:601:CHL:HED2	1.85	0.42
17:5:133:GLU:OE2	34:H:86:HOH:O	2.21	0.42
19:9:126:ARG:NH2	22:9:609:CLA:O1D	2.53	0.42
22:B2:828:CLA:H101	25:B2:845:BCR:H372	2.00	0.42
1:A:476:ALA:O	1:A:477:ILE:C	2.63	0.42
22:A:802:CLA:CGA	22:A:802:CLA:H3A	2.50	0.42
16:4:54:ARG:HD3	16:4:67:LEU:HD12	2.00	0.42
22:3:615:CLA:HAA2	22:5:616:CLA:HED2	2.01	0.42
16:4:66:ASP:O	24:4:623:LHG:O4	2.38	0.42
22:5:616:CLA:H62	22:5:616:CLA:H41	1.92	0.42
29:9:617:LUT:C28	29:9:617:LUT:H381	2.48	0.42
22:A:823:CLA:H42	11:K:65:LEU:HD21	2.01	0.42
22:A:843:CLA:H61	22:A:843:CLA:H41	1.87	0.42
25:3:718:BCR:H24C	25:3:718:BCR:H371	1.90	0.42
22:92:602:CLA:H62	22:92:602:CLA:H41	1.82	0.42
22:A:843:CLA:H52	22:B:839:CLA:H43	2.01	0.42
13:3:58:ASP:OD1	13:3:58:ASP:N	2.53	0.42
22:92:613:CLA:C1A	22:92:613:CLA:CGA	2.98	0.42
14:7:34:PHE:CE1	31:7:601:CHL:HED2	2.54	0.42
22:5:617:CLA:H61	22:5:617:CLA:H41	1.90	0.42
28:J:103:LMG:HC61	28:J:103:LMG:O1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:69:ASP:OD1	11:K:70:SER:N	2.53	0.42
22:Z:613:CLA:CGA	22:Z:613:CLA:C1A	2.98	0.42
16:4:95:TRP:CD1	28:4:624:LMG:HO4	2.38	0.42
25:92:623:BCR:H361	25:92:623:BCR:H20C	1.84	0.42
25:A:848:BCR:H24C	25:A:848:BCR:H371	1.87	0.42
22:B:837:CLA:H41	29:F:305:LUT:C37	2.50	0.42
25:B:843:BCR:H24C	25:B:843:BCR:H371	1.92	0.42
4:D:88:TRP:CD1	4:D:134:LEU:HD13	2.55	0.42
25:L:205:BCR:H403	25:L:205:BCR:H23C	2.02	0.42
24:3:623:LHG:H111	22:5:616:CLA:HMC2	2.01	0.42
22:B2:828:CLA:H142	25:B2:844:BCR:C15	2.50	0.42
22:A:820:CLA:CAD	22:A:830:CLA:H41	2.50	0.41
18:6:33:LEU:HD12	31:6:601:CHL:HED2	2.01	0.41
22:A:829:CLA:H72	22:A:829:CLA:C12	2.50	0.41
29:A:856:LUT:H171	29:A:856:LUT:H8	2.02	0.41
25:3:620:BCR:H24C	25:3:620:BCR:H371	1.92	0.41
31:5:608:CHL:H12	29:5:620:LUT:H383	2.01	0.41
25:B2:844:BCR:H20C	25:B2:844:BCR:H361	1.95	0.41
25:A:851:BCR:H371	25:A:851:BCR:H24C	1.89	0.41
11:K:65:LEU:N	11:K:65:LEU:HD12	2.36	0.41
12:Z:220:THR:HG22	12:Z:220:THR:O	2.21	0.41
19:9:172:PHE:CE1	29:9:616:LUT:H182	2.55	0.41
1:A:584:CYS:O	2:B:670:GLY:N	2.53	0.41
1:A:747:ILE:O	1:A:751:GLY:N	2.52	0.41
22:A:811:CLA:C1	22:A:813:CLA:H42	2.49	0.41
25:3:719:BCR:H24C	25:3:719:BCR:H371	1.86	0.41
19:9:191:LEU:HD21	22:9:614:CLA:HMC2	2.03	0.41
1:A:343:GLU:OE1	1:A:343:GLU:N	2.48	0.41
11:K:35:ASN:ND2	22:K:204:CLA:OBD	2.53	0.41
25:L2:205:BCR:H20C	25:L2:205:BCR:H361	1.92	0.41
25:8:619:BCR:HC8	25:8:619:BCR:H311	2.01	0.41
25:A:848:BCR:H20C	25:A:848:BCR:H361	1.85	0.41
22:B:840:CLA:H91	22:B:840:CLA:C12	2.51	0.41
9:J:32:TYR:OH	22:J:101:CLA:HED3	2.21	0.41
1:A:115:ALA:HB3	22:A:809:CLA:HED3	2.03	0.41
25:A:851:BCR:H20C	25:A:851:BCR:H361	1.94	0.41
25:A:852:BCR:H20C	25:A:852:BCR:H361	1.87	0.41
31:7:601:CHL:H61	31:7:601:CHL:H41	1.83	0.41
19:92:193:ASP:OD2	19:92:196:GLY:N	2.53	0.41
22:A:833:CLA:C4	10:L:65:VAL:HG13	2.51	0.41
25:A:852:BCR:H24C	25:A:852:BCR:H371	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:GLN:O	2:B:80:THR:OG1	2.35	0.41
22:B:837:CLA:H41	29:F:305:LUT:H371	2.03	0.41
25:6:623:BCR:H20C	25:6:623:BCR:H361	1.96	0.41
12:1:50:PRO:O	12:1:56:ASN:ND2	2.54	0.40
9:J:8:LEU:HA	9:J:13:VAL:HG11	2.03	0.40
22:8:612:CLA:H43	22:4:609:CLA:H11	2.03	0.40
27:8:627:LMU:H2'	27:8:627:LMU:H6D	2.03	0.40
22:B2:828:CLA:H142	25:B2:844:BCR:H15C	2.04	0.40
22:B:823:CLA:H3A	22:B:841:CLA:HED3	2.04	0.40
22:B:832:CLA:HBB1	25:B:801:BCR:H323	2.02	0.40
25:B:845:BCR:H24C	25:B:845:BCR:H371	1.84	0.40
22:A:839:CLA:C1A	22:A:839:CLA:CGA	3.00	0.40
12:Z:192:VAL:HG13	27:Z:622:LMU:O2'	2.20	0.40
1:A:36:SER:O	1:A:40:SER:OG	2.32	0.40
25:K:207:BCR:H20C	25:K:207:BCR:H361	1.90	0.40
13:3:132:PRO:N	13:3:133:PRO:CD	2.84	0.40
17:5:95:LYS:O	17:5:98:VAL:HG22	2.21	0.40
10:L2:82:VAL:HG13	10:L2:83:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/751 (98%)	729 (98%)	11 (2%)	0	100	100
2	B	731/735 (100%)	718 (98%)	13 (2%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	93/126 (74%)	93 (100%)	0	0	100	100
8	I	35/106 (33%)	35 (100%)	0	0	100	100
8	I2	35/106 (33%)	34 (97%)	1 (3%)	0	100	100
9	J	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	L	120/196 (61%)	117 (98%)	3 (2%)	0	100	100
10	L2	98/196 (50%)	95 (97%)	3 (3%)	0	100	100
11	K	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
12	1	192/228 (84%)	192 (100%)	0	0	100	100
12	Z	192/228 (84%)	189 (98%)	3 (2%)	0	100	100
13	3	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
14	7	211/241 (88%)	210 (100%)	1 (0%)	0	100	100
15	8	215/243 (88%)	213 (99%)	2 (1%)	0	100	100
16	4	210/264 (80%)	207 (99%)	3 (1%)	0	100	100
17	5	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
18	6	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
19	9	184/213 (86%)	179 (97%)	4 (2%)	1 (0%)	24	40
19	92	182/213 (85%)	178 (98%)	3 (2%)	1 (0%)	24	40
20	B2	166/180 (92%)	164 (99%)	2 (1%)	0	100	100
All	All	4649/5592 (83%)	4572 (98%)	75 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	92	139	ILE
19	9	139	ILE

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%)	599 (100%)	2 (0%)	86	92
2	B	596/597 (100%)	594 (100%)	2 (0%)	86	92
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	121/152 (80%)	120 (99%)	1 (1%)	73	83
5	E	55/81 (68%)	55 (100%)	0	100	100
6	F	127/169 (75%)	127 (100%)	0	100	100
7	G	71/94 (76%)	71 (100%)	0	100	100
8	I	31/76 (41%)	31 (100%)	0	100	100
8	I2	31/76 (41%)	31 (100%)	0	100	100
9	J	35/35 (100%)	34 (97%)	1 (3%)	37	59
10	L	90/148 (61%)	89 (99%)	1 (1%)	65	79
10	L2	72/148 (49%)	72 (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%)	172 (99%)	2 (1%)	65	79
14	7	164/181 (91%)	164 (100%)	0	100	100
15	8	163/183 (89%)	162 (99%)	1 (1%)	78	87
16	4	166/205 (81%)	166 (100%)	0	100	100
17	5	184/206 (89%)	181 (98%)	3 (2%)	55	72
18	6	184/203 (91%)	184 (100%)	0	100	100
19	9	142/159 (89%)	142 (100%)	0	100	100
19	92	141/159 (89%)	141 (100%)	0	100	100
20	B2	153/153 (100%)	152 (99%)	1 (1%)	76	85
All	All	3703/4339 (85%)	3689 (100%)	14 (0%)	81	90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	THR
1	A	293	ASP
2	B	217	LEU
2	B	612	GLU
4	D	150	LEU
9	J	38	VAL

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Mol	Chain	Res	Type
10	L	64	ILE
13	3	38	VAL
13	3	218	ILE
15	8	153	PHE
17	5	91	GLN
17	5	202	LEU
17	5	238	HIS
20	B2	17	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	HIS
1	A	488	GLN
1	A	659	GLN
2	B	157	HIS
2	B	159	GLN
2	B	369	GLN
2	B	606	ASN
2	B	609	GLN
2	B	631	GLN
6	F	93	GLN
10	L	108	ASN
12	1	195	HIS
15	8	220	ASN
12	Z	194	GLN
16	4	166	GLN
17	5	72	GLN
17	5	257	GLN
18	6	88	GLN
19	92	140	ASN

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	0.55	0	9,11,13	0.88	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	-	3/9/10/12	-

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	-2.57	118.15	124.77

There are no chirality outliers.

All (3) 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	CB-CA-N-CT1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

397 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	92	602	19	69,73,73	1.18	5 (7%)	82,113,113	0.85	3 (3%)
28	LMG	1	628	-	42,42,55	0.19	0	50,50,63	0.29	0
30	DGD	B	850	-	60,60,67	0.17	0	74,74,81	0.33	0
22	CLA	K	204	-	50,54,73	1.38	5 (10%)	59,90,113	0.99	3 (5%)
22	CLA	L2	203	-	49,53,73	1.39	4 (8%)	58,89,113	0.97	3 (5%)
31	CHL	8	607	34	60,74,74	1.91	10 (16%)	58,114,114	1.11	5 (8%)
27	LMU	K	208	-	24,24,36	0.10	0	29,29,47	0.31	0
22	CLA	B2	814	-	64,68,73	1.22	4 (6%)	76,107,113	0.84	3 (3%)
22	CLA	A	854	34	69,73,73	1.23	5 (7%)	82,113,113	0.79	3 (3%)
24	LHG	6	629	-	35,35,48	0.26	0	38,41,54	0.29	0
22	CLA	A	823	-	69,73,73	1.18	5 (7%)	82,113,113	0.80	3 (3%)
28	LMG	A	860	-	36,36,55	0.20	0	44,44,63	0.24	0
29	LUT	1	617	-	42,43,43	0.28	0	51,60,60	0.42	0
31	CHL	4	606	34	50,64,74	2.16	10 (20%)	46,102,114	1.26	6 (13%)
25	BCR	K	202	-	41,41,41	0.16	0	56,56,56	0.37	0
25	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.46	0
29	LUT	6	621	-	42,43,43	0.26	0	51,60,60	0.40	0
31	CHL	8	606	34	60,74,74	1.97	10 (16%)	58,114,114	1.08	5 (8%)
22	CLA	B2	805	-	69,73,73	1.16	4 (5%)	82,113,113	0.81	3 (3%)
22	CLA	4	611	24	64,68,73	1.24	4 (6%)	76,107,113	0.85	3 (3%)
22	CLA	8	611	24	49,53,73	1.43	5 (10%)	58,89,113	0.98	3 (5%)
22	CLA	Z	611	24	64,68,73	1.22	4 (6%)	76,107,113	0.86	3 (3%)
28	LMG	7	626	-	37,37,55	0.19	0	45,45,63	0.26	0
28	LMG	8	629	-	42,42,55	0.18	0	50,50,63	0.16	0
22	CLA	B2	828	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	3 (3%)
22	CLA	8	608	34	54,58,73	1.34	5 (9%)	64,95,113	0.93	2 (3%)
26	SF4	C	102	3	0,12,12	-	-	-	-	-
27	LMU	Z	622	-	32,32,36	0.10	0	43,43,47	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	7	614	-	47,51,73	1.46	5 (10%)	55,86,113	1.02	4 (7%)
24	LHG	9	622	22	40,40,48	0.25	0	43,46,54	0.29	0
22	CLA	9	612	19	69,73,73	1.16	4 (5%)	82,113,113	0.80	2 (2%)
22	CLA	A	822	34	69,73,73	1.18	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	4	616	16	49,53,73	1.40	4 (8%)	58,89,113	0.96	3 (5%)
22	CLA	6	613	34	69,73,73	1.18	5 (7%)	82,113,113	0.84	3 (3%)
22	CLA	9	601	19	50,54,73	1.40	4 (8%)	59,90,113	0.98	3 (5%)
25	BCR	I2	172	-	41,41,41	0.12	0	56,56,56	0.32	0
22	CLA	1	613	34	69,73,73	1.16	5 (7%)	82,113,113	0.84	3 (3%)
22	CLA	7	603	-	56,60,73	1.31	5 (8%)	65,97,113	0.92	3 (4%)
25	BCR	B2	843	-	20,20,41	0.82	1 (5%)	27,27,56	0.25	0
25	BCR	K	207	-	41,41,41	0.14	0	56,56,56	0.28	0
22	CLA	3	617	13	50,54,73	1.37	4 (8%)	59,90,113	0.98	2 (3%)
22	CLA	4	609	16	64,68,73	1.25	4 (6%)	76,107,113	0.86	2 (2%)
22	CLA	B	841	24	69,73,73	1.18	5 (7%)	82,113,113	0.84	4 (4%)
33	NEX	5	625	-	40,46,46	0.45	1 (2%)	50,70,70	0.77	4 (8%)
31	CHL	1	601	12	60,74,74	1.95	10 (16%)	58,114,114	1.05	4 (6%)
31	CHL	7	606	34	40,54,74	2.42	10 (25%)	34,90,114	1.41	5 (14%)
25	BCR	A	850	-	41,41,41	0.16	0	56,56,56	0.24	0
22	CLA	A	820	-	69,73,73	1.16	5 (7%)	82,113,113	0.84	3 (3%)
22	CLA	A	843	34	69,73,73	1.17	5 (7%)	82,113,113	0.85	3 (3%)
27	LMU	8	625	-	24,24,36	0.12	0	29,29,47	0.28	0
32	XAT	1	618	-	41,47,47	0.14	0	54,74,74	0.71	1 (1%)
31	CHL	4	607	34	60,74,74	1.97	10 (16%)	58,114,114	1.04	5 (8%)
22	CLA	9	604	19	57,61,73	1.27	5 (8%)	67,98,113	0.90	3 (4%)
22	CLA	A	827	34	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	6	610	18	64,68,73	1.22	5 (7%)	76,107,113	0.85	3 (3%)
31	CHL	8	601	15	60,74,74	1.97	10 (16%)	58,114,114	1.10	4 (6%)
22	CLA	1	610	12	69,73,73	1.17	5 (7%)	82,113,113	0.80	3 (3%)
25	BCR	7	623	-	41,41,41	0.16	0	56,56,56	0.38	0
22	CLA	B	828	-	69,73,73	1.15	5 (7%)	82,113,113	0.80	3 (3%)
31	CHL	4	618	16	40,54,74	2.40	10 (25%)	34,90,114	1.36	5 (14%)
23	PQN	A	844	-	34,34,34	0.32	0	43,45,45	0.44	0
22	CLA	6	622	34	59,63,73	1.29	4 (6%)	70,101,113	0.88	2 (2%)
22	CLA	B	838	-	54,58,73	1.36	4 (7%)	64,95,113	0.92	2 (3%)
22	CLA	6	604	-	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	8	619	-	41,41,41	0.15	0	56,56,56	0.32	0
22	CLA	8	603	-	69,73,73	1.21	5 (7%)	82,113,113	0.79	2 (2%)
22	CLA	A	832	-	59,63,73	1.25	5 (8%)	70,101,113	0.90	2 (2%)
25	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.35	0
22	CLA	B	817	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
27	LMU	Z	621	-	22,22,36	0.13	0	27,27,47	0.27	0
31	CHL	Z	606	34	40,54,74	2.36	10 (25%)	34,90,114	1.44	5 (14%)
31	CHL	92	606	-	36,50,74	2.52	10 (27%)	29,85,114	1.37	4 (13%)
29	LUT	Z	617	-	42,43,43	0.28	0	51,60,60	0.45	0
28	LMG	4	624	-	41,41,55	0.18	0	49,49,63	0.26	0
29	LUT	A	856	-	42,43,43	0.29	0	51,60,60	0.42	0
22	CLA	92	611	24	69,73,73	1.20	5 (7%)	82,113,113	0.82	2 (2%)
26	SF4	C	101	3	0,12,12	-	-	-	-	-
22	CLA	B	819	34	64,68,73	1.23	5 (7%)	76,107,113	0.84	3 (3%)
22	CLA	3	609	13	65,69,73	1.20	5 (7%)	77,108,113	0.83	2 (2%)
24	LHG	5	623	22	36,36,48	0.26	0	39,42,54	0.29	0
22	CLA	B	805	-	69,73,73	1.14	5 (7%)	82,113,113	0.84	3 (3%)
29	LUT	5	620	-	42,43,43	0.27	0	51,60,60	0.49	0
25	BCR	I	172	-	41,41,41	0.20	0	56,56,56	0.37	0
25	BCR	B	848	-	41,41,41	0.13	0	56,56,56	0.47	0
27	LMU	1	623	-	24,24,36	0.13	0	29,29,47	0.26	0
22	CLA	5	613	17	60,64,73	1.26	5 (8%)	71,102,113	0.88	3 (4%)
22	CLA	B2	820	-	60,64,73	1.25	4 (6%)	71,102,113	0.89	3 (4%)
22	CLA	1	608	34	69,73,73	1.19	5 (7%)	82,113,113	0.83	3 (3%)
22	CLA	A	835	-	69,73,73	1.17	5 (7%)	82,113,113	0.83	3 (3%)
22	CLA	L2	204	-	49,53,73	1.39	4 (8%)	58,89,113	0.98	3 (5%)
22	CLA	B	821	-	69,73,73	1.21	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	B	810	-	69,73,73	1.17	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	B	834	-	64,68,73	1.23	5 (7%)	76,107,113	0.85	3 (3%)
22	CLA	5	601	17	69,73,73	1.18	4 (5%)	82,113,113	0.84	2 (2%)
25	BCR	A	852	-	41,41,41	0.13	0	56,56,56	0.38	0
22	CLA	A	805	-	59,63,73	1.28	5 (8%)	70,101,113	0.85	2 (2%)
22	CLA	B	806	2	69,73,73	1.18	5 (7%)	82,113,113	0.77	2 (2%)
22	CLA	A	815	-	59,63,73	1.28	5 (8%)	70,101,113	0.88	2 (2%)
25	BCR	A	851	-	41,41,41	0.15	0	56,56,56	0.33	0
25	BCR	G	205	-	41,41,41	0.15	0	56,56,56	0.31	0
22	CLA	8	604	34	64,68,73	1.24	5 (7%)	76,107,113	0.87	3 (3%)
22	CLA	Z	604	34	61,65,73	1.25	5 (8%)	72,103,113	0.88	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Z	602	12	64,68,73	1.24	5 (7%)	76,107,113	0.88	3 (3%)
22	CLA	3	614	-	49,53,73	1.40	5 (10%)	58,89,113	0.97	3 (5%)
22	CLA	7	602	14	69,73,73	1.17	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	3	603	-	69,73,73	1.18	5 (7%)	82,113,113	0.80	2 (2%)
27	LMU	B	853	-	36,36,36	0.12	0	47,47,47	0.70	2 (4%)
24	LHG	1	620	22	38,38,48	0.28	0	41,44,54	0.31	0
29	LUT	F	305	-	42,43,43	0.39	0	51,60,60	0.88	2 (3%)
22	CLA	B	820	-	60,64,73	1.28	5 (8%)	71,102,113	0.86	2 (2%)
25	BCR	B	843	-	41,41,41	0.17	0	56,56,56	0.32	0
26	SF4	A	853	1,2	0,12,12	-	-	-		
22	CLA	8	616	15	49,53,73	1.38	5 (10%)	58,89,113	0.97	3 (5%)
22	CLA	B	808	-	69,73,73	1.15	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	5	604	34	59,63,73	1.29	5 (8%)	70,101,113	0.89	3 (4%)
27	LMU	1	622	-	19,19,36	0.13	0	24,24,47	0.30	0
22	CLA	6	609	18	59,63,73	1.26	5 (8%)	70,101,113	0.92	4 (5%)
22	CLA	92	603	19	49,53,73	1.40	5 (10%)	58,89,113	0.98	3 (5%)
29	LUT	3	621	-	42,43,43	0.31	0	51,60,60	0.40	0
22	CLA	1	609	12	69,73,73	1.17	5 (7%)	82,113,113	0.83	2 (2%)
25	BCR	B2	845	-	41,41,41	0.14	0	56,56,56	0.32	0
22	CLA	B2	807	-	59,63,73	1.28	4 (6%)	70,101,113	0.87	3 (4%)
28	LMG	J	104	-	35,35,55	0.19	0	43,43,63	0.20	0
22	CLA	A	831	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	92	604	19	54,58,73	1.34	4 (7%)	64,95,113	0.92	3 (4%)
22	CLA	8	609	15	49,53,73	1.42	5 (10%)	58,89,113	0.95	2 (3%)
22	CLA	B	811	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	2 (2%)
27	LMU	A	862	-	20,20,36	0.13	0	25,25,47	0.28	0
25	BCR	B2	848	-	14,14,41	0.38	0	20,20,56	0.32	0
27	LMU	A	865	-	24,24,36	0.12	0	29,29,47	0.46	0
31	CHL	1	607	34	40,54,74	2.42	10 (25%)	34,90,114	1.28	4 (11%)
22	CLA	A	808	-	54,58,73	1.32	5 (9%)	64,95,113	0.90	2 (3%)
24	LHG	3	623	-	46,46,48	0.24	0	49,52,54	0.28	0
22	CLA	3	607	13	59,63,73	1.28	5 (8%)	70,101,113	0.89	3 (4%)
22	CLA	B	840	-	69,73,73	1.15	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	J	101	9	59,63,73	1.29	4 (6%)	70,101,113	0.88	2 (2%)
22	CLA	9	613	19	69,73,73	1.17	5 (7%)	82,113,113	0.85	4 (4%)
25	BCR	3	719	-	41,41,41	0.12	0	56,56,56	0.41	0
24	LHG	6	619	22	48,48,48	0.23	0	51,54,54	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	3	613	13	64,68,73	1.23	5 (7%)	76,107,113	0.84	3 (3%)
28	LMG	8	626	-	32,32,55	0.20	0	40,40,63	0.19	0
22	CLA	K	203	34	64,68,73	1.24	4 (6%)	76,107,113	0.86	3 (3%)
22	CLA	B	818	-	69,73,73	1.17	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	A	814	-	69,73,73	1.17	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	5	612	17	49,53,73	1.38	4 (8%)	58,89,113	0.95	2 (3%)
22	CLA	G	203	-	64,68,73	1.23	4 (6%)	76,107,113	0.81	2 (2%)
22	CLA	3	604	34	69,73,73	1.18	5 (7%)	82,113,113	0.81	2 (2%)
27	LMU	8	624	-	24,24,36	0.13	0	29,29,47	0.27	0
28	LMG	3	722	-	44,44,55	0.20	0	46,46,63	0.26	0
22	CLA	B	832	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	1	611	24	65,69,73	1.22	5 (7%)	77,108,113	0.83	2 (2%)
22	CLA	6	614	-	54,58,73	1.33	5 (9%)	64,95,113	0.93	3 (4%)
22	CLA	B	807	-	59,63,73	1.31	5 (8%)	70,101,113	0.88	3 (4%)
22	CLA	A	819	-	64,68,73	1.25	5 (7%)	76,107,113	0.87	2 (2%)
22	CLA	B2	839	-	49,53,73	1.42	4 (8%)	58,89,113	1.00	3 (5%)
22	CLA	B	831	-	59,63,73	1.26	5 (8%)	70,101,113	0.86	3 (4%)
25	BCR	L	201	-	41,41,41	0.18	0	56,56,56	0.35	0
22	CLA	6	603	-	69,73,73	1.18	5 (7%)	82,113,113	0.79	2 (2%)
22	CLA	9	610	19	64,68,73	1.22	5 (7%)	76,107,113	0.88	3 (3%)
25	BCR	5	622	-	41,41,41	0.16	0	56,56,56	0.32	0
22	CLA	9	609	19	55,59,73	1.32	5 (9%)	64,96,113	0.92	3 (4%)
22	CLA	6	602	18	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
27	LMU	7	628	-	22,22,36	0.14	0	27,27,47	0.32	0
22	CLA	Z	616	12	64,68,73	1.24	4 (6%)	76,107,113	0.86	3 (3%)
27	LMU	6	632	-	20,20,36	0.15	0	25,25,47	0.25	0
22	CLA	7	616	14	50,54,73	1.38	5 (10%)	59,90,113	0.94	3 (5%)
22	CLA	A	842	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	B	835	34	49,53,73	1.39	4 (8%)	58,89,113	0.97	2 (3%)
31	CHL	9	606	-	36,50,74	2.54	10 (27%)	29,85,114	1.42	4 (13%)
31	CHL	9	607	34	45,59,74	2.32	10 (22%)	40,96,114	1.22	4 (10%)
25	BCR	B	801	-	41,41,41	0.17	0	56,56,56	0.38	0
25	BCR	92	623	-	41,41,41	0.14	0	56,56,56	0.33	0
27	LMU	7	627	-	33,33,36	0.10	0	44,44,47	0.18	0
25	BCR	A	849	-	41,41,41	0.18	0	56,56,56	0.32	0
24	LHG	A	847	22	37,37,48	0.28	0	40,43,54	0.31	0
31	CHL	6	606	34	52,66,74	2.13	10 (19%)	48,104,114	1.18	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMU	A	864	-	24,24,36	0.11	0	29,29,47	0.31	0
22	CLA	6	611	24	62,66,73	1.26	4 (6%)	73,104,113	0.86	2 (2%)
22	CLA	A	826	34	69,73,73	1.19	4 (5%)	82,113,113	0.81	2 (2%)
22	CLA	B2	810	-	69,73,73	1.18	4 (5%)	82,113,113	0.81	3 (3%)
22	CLA	5	621	34	50,54,73	1.42	4 (8%)	59,90,113	1.07	5 (8%)
32	XAT	Z	618	-	41,47,47	0.16	0	54,74,74	0.62	0
22	CLA	7	611	24	69,73,73	1.18	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	B2	811	-	58,62,73	1.32	4 (6%)	71,100,113	0.97	4 (5%)
21	CL0	A	801	-	58,73,73	1.50	6 (10%)	60,113,113	1.56	3 (5%)
25	BCR	3	620	-	41,41,41	0.21	0	56,56,56	0.36	0
29	LUT	92	617	-	42,43,43	0.21	0	51,60,60	0.40	0
28	LMG	B2	855	-	31,31,55	0.20	0	39,39,63	0.17	0
22	CLA	5	614	-	49,53,73	1.40	4 (8%)	58,89,113	0.96	3 (5%)
24	LHG	4	623	-	37,37,48	0.25	0	40,43,54	0.31	0
22	CLA	3	611	-	69,73,73	1.18	5 (7%)	82,113,113	0.82	3 (3%)
31	CHL	5	606	34	40,54,74	2.39	10 (25%)	34,90,114	1.39	5 (14%)
29	LUT	7	624	-	42,43,43	0.23	0	51,60,60	0.43	0
22	CLA	8	602	15	66,70,73	1.22	5 (7%)	78,109,113	0.85	2 (2%)
22	CLA	7	610	14	69,73,73	1.21	5 (7%)	82,113,113	0.85	3 (3%)
31	CHL	1	606	34	40,54,74	2.42	10 (25%)	34,90,114	1.39	5 (14%)
22	CLA	B2	815	-	61,65,73	1.24	4 (6%)	72,103,113	0.86	3 (4%)
22	CLA	B	822	-	63,67,73	1.22	5 (7%)	74,105,113	0.87	3 (4%)
22	CLA	B	830	-	49,53,73	1.36	5 (10%)	58,89,113	0.97	2 (3%)
22	CLA	4	610	16	64,68,73	1.22	4 (6%)	76,107,113	0.82	2 (2%)
22	CLA	L	203	-	69,73,73	1.17	5 (7%)	82,113,113	0.80	3 (3%)
22	CLA	4	603	16	69,73,73	1.18	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	92	612	19	69,73,73	1.15	4 (5%)	82,113,113	0.81	2 (2%)
22	CLA	Z	608	34	54,58,73	1.35	5 (9%)	64,95,113	0.94	4 (6%)
24	LHG	7	625	22	48,48,48	0.24	0	51,54,54	0.23	0
29	LUT	5	626	-	42,43,43	0.25	0	51,60,60	0.40	0
22	CLA	7	608	34	54,58,73	1.34	5 (9%)	64,95,113	0.90	2 (3%)
29	LUT	3	720	-	42,43,43	0.22	0	51,60,60	0.34	0
31	CHL	6	618	18	37,51,74	2.50	10 (27%)	30,86,114	1.49	5 (16%)
31	CHL	6	616	18	60,74,74	1.98	10 (16%)	58,114,114	1.09	6 (10%)
25	BCR	B	847	-	41,41,41	0.20	0	56,56,56	0.41	0
22	CLA	A	830	-	69,73,73	1.17	5 (7%)	82,113,113	0.81	2 (2%)
25	BCR	L	205	-	41,41,41	0.15	0	56,56,56	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	1	603	-	61,65,73	1.26	5 (8%)	72,103,113	0.87	2 (2%)
22	CLA	4	613	16	69,73,73	1.19	5 (7%)	82,113,113	0.84	2 (2%)
27	LMU	92	624	-	36,36,36	0.09	0	47,47,47	0.23	0
22	CLA	B2	809	20	56,60,73	1.33	4 (7%)	65,97,113	0.90	2 (3%)
29	LUT	1	619	-	42,43,43	0.21	0	51,60,60	0.41	0
22	CLA	8	614	-	61,65,73	1.26	5 (8%)	72,103,113	0.86	3 (4%)
22	CLA	B	824	34	69,73,73	1.21	4 (5%)	82,113,113	0.83	2 (2%)
22	CLA	1	604	34	54,58,73	1.34	5 (9%)	64,95,113	0.94	3 (4%)
22	CLA	B2	813	-	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
22	CLA	1	602	12	64,68,73	1.23	5 (7%)	76,107,113	0.87	3 (3%)
22	CLA	B	827	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	2 (2%)
22	CLA	8	612	15	59,63,73	1.24	5 (8%)	70,101,113	0.86	2 (2%)
25	BCR	4	621	-	41,41,41	0.15	0	56,56,56	0.35	0
22	CLA	A	838	-	55,59,73	1.29	5 (9%)	64,96,113	0.93	2 (3%)
22	CLA	3	606	34	46,50,73	1.47	5 (10%)	53,85,113	1.00	2 (3%)
29	LUT	4	619	-	42,43,43	0.27	0	51,60,60	0.49	0
31	CHL	5	618	17	37,51,74	2.50	10 (27%)	30,86,114	1.49	5 (16%)
28	LMG	6	633	-	19,19,55	0.30	0	19,19,63	0.29	0
22	CLA	K	201	11	49,53,73	1.42	4 (8%)	58,89,113	0.98	1 (1%)
28	LMG	A	859	-	48,48,55	0.18	0	56,56,63	0.18	0
22	CLA	Z	609	12	69,73,73	1.21	4 (5%)	82,113,113	0.82	2 (2%)
22	CLA	B	814	-	64,68,73	1.20	5 (7%)	76,107,113	0.86	3 (3%)
22	CLA	K	206	11	49,53,73	1.40	4 (8%)	58,89,113	0.97	2 (3%)
22	CLA	A	824	-	49,53,73	1.39	5 (10%)	58,89,113	0.99	3 (5%)
32	XAT	4	620	-	41,47,47	0.13	0	54,74,74	0.69	0
22	CLA	7	609	14	49,53,73	1.43	5 (10%)	58,89,113	0.95	3 (5%)
22	CLA	4	602	16	64,68,73	1.24	5 (7%)	76,107,113	0.84	3 (3%)
27	LMU	6	631	-	24,24,36	0.13	0	29,29,47	0.27	0
22	CLA	Z	613	34	69,73,73	1.17	5 (7%)	82,113,113	0.85	3 (3%)
22	CLA	B2	808	-	49,53,73	1.39	4 (8%)	58,89,113	0.97	2 (3%)
22	CLA	7	613	14	69,73,73	1.18	5 (7%)	82,113,113	0.84	2 (2%)
31	CHL	Z	607	34	60,74,74	1.98	10 (16%)	58,114,114	1.09	6 (10%)
22	CLA	B	839	34	69,73,73	1.19	5 (7%)	82,113,113	0.84	2 (2%)
22	CLA	B	815	-	69,73,73	1.17	4 (5%)	82,113,113	0.80	2 (2%)
22	CLA	92	610	19	64,68,73	1.23	5 (7%)	76,107,113	0.87	3 (3%)
22	CLA	A	811	-	69,73,73	1.15	5 (7%)	82,113,113	0.82	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CHL	7	607	34	40,54,74	2.40	10 (25%)	34,90,114	1.43	5 (14%)
32	XAT	7	622	-	41,47,47	0.15	0	54,74,74	0.62	1 (1%)
22	CLA	5	617	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	3 (3%)
22	CLA	B	825	34	69,73,73	1.16	5 (7%)	82,113,113	0.79	2 (2%)
27	LMU	1	625	-	24,24,36	0.11	0	29,29,47	0.31	0
31	CHL	7	601	14	60,74,74	1.99	10 (16%)	58,114,114	1.05	5 (8%)
22	CLA	A	833	-	69,73,73	1.20	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	5	602	17	69,73,73	1.18	4 (5%)	82,113,113	0.82	2 (2%)
24	LHG	Z	620	22	38,38,48	0.26	0	41,44,54	0.30	0
22	CLA	9	602	19	64,68,73	1.23	5 (7%)	76,107,113	0.85	3 (3%)
22	CLA	5	616	17	57,61,73	1.29	5 (8%)	67,98,113	0.90	3 (4%)
22	CLA	A	812	-	69,73,73	1.15	5 (7%)	82,113,113	0.79	3 (3%)
25	BCR	6	623	-	41,41,41	0.18	0	56,56,56	0.34	0
24	LHG	3	721	-	30,30,48	0.26	0	33,36,54	0.36	0
28	LMG	B	854	-	36,36,55	0.19	0	44,44,63	0.17	0
28	LMG	J	103	-	42,42,55	0.18	0	50,50,63	0.39	0
22	CLA	B	803	-	69,73,73	1.19	4 (5%)	82,113,113	0.78	2 (2%)
29	LUT	3	622	-	42,43,43	0.31	0	51,60,60	0.49	0
22	CLA	A	836	-	69,73,73	1.19	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	7	620	34	57,61,73	1.29	4 (7%)	67,98,113	0.90	2 (2%)
22	CLA	9	611	24	69,73,73	1.19	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	5	609	17	69,73,73	1.16	5 (7%)	82,113,113	0.80	3 (3%)
27	LMU	5	627	-	24,24,36	0.11	0	29,29,47	0.25	0
27	LMU	6	628	-	24,24,36	0.12	0	29,29,47	0.30	0
27	LMU	7	629	-	28,28,36	0.10	0	39,39,47	0.27	0
22	CLA	5	611	24	59,63,73	1.26	5 (8%)	70,101,113	0.88	3 (4%)
27	LMU	A	863	-	36,36,36	0.09	0	47,47,47	0.27	0
33	NEX	6	625	-	40,46,46	0.30	0	50,70,70	0.86	4 (8%)
22	CLA	A	845	24	49,53,73	1.39	4 (8%)	58,89,113	0.94	2 (3%)
22	CLA	7	612	14	56,60,73	1.29	5 (8%)	65,97,113	0.89	2 (3%)
29	LUT	7	621	-	42,43,43	0.27	0	51,60,60	0.39	0
27	LMU	9	624	-	24,24,36	0.13	0	29,29,47	0.28	0
32	XAT	8	618	-	41,47,47	0.17	0	54,74,74	0.61	0
22	CLA	A	829	-	69,73,73	1.22	5 (7%)	82,113,113	0.82	3 (3%)
25	BCR	L2	201	-	41,41,41	0.14	0	56,56,56	0.36	0
27	LMU	A	858	-	36,36,36	0.09	0	47,47,47	0.19	0
31	CHL	5	608	34	45,59,74	2.29	10 (22%)	40,96,114	1.33	6 (15%)
27	LMU	4	626	-	20,20,36	0.15	0	25,25,47	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMU	1	627	-	22,22,36	0.13	0	27,27,47	0.30	0
27	LMU	A	857	-	35,35,36	0.09	0	46,46,47	0.18	0
25	BCR	J	102	-	41,41,41	0.15	0	56,56,56	0.31	0
22	CLA	5	610	17	64,68,73	1.20	4 (6%)	76,107,113	0.83	2 (2%)
22	CLA	A	839	-	69,73,73	1.17	5 (7%)	82,113,113	0.83	4 (4%)
22	CLA	A	804	-	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	B	816	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	A	840	-	69,73,73	1.18	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	A	813	-	69,73,73	1.17	5 (7%)	82,113,113	0.86	3 (3%)
22	CLA	Z	612	12	49,53,73	1.36	4 (8%)	58,89,113	0.95	2 (3%)
22	CLA	1	612	12	49,53,73	1.39	4 (8%)	58,89,113	0.97	3 (5%)
22	CLA	B2	804	-	49,53,73	1.37	4 (8%)	58,89,113	0.97	3 (5%)
22	CLA	3	602	13	64,68,73	1.22	5 (7%)	76,107,113	0.84	3 (3%)
24	LHG	4	622	22	48,48,48	0.23	0	51,54,54	0.28	0
22	CLA	8	613	15	69,73,73	1.17	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	1	616	12	50,54,73	1.41	5 (10%)	59,90,113	0.97	3 (5%)
22	CLA	B2	806	20	69,73,73	1.16	4 (5%)	82,113,113	0.81	2 (2%)
31	CHL	6	608	34	45,59,74	2.29	10 (22%)	40,96,114	1.29	6 (15%)
22	CLA	9	614	-	49,53,73	1.43	4 (8%)	58,89,113	0.96	3 (5%)
22	CLA	3	615	34	69,73,73	1.20	4 (5%)	82,113,113	0.84	3 (3%)
28	LMG	9	620	22	44,44,55	0.17	0	52,52,63	0.37	0
31	CHL	3	608	34	60,74,74	2.00	10 (16%)	58,114,114	1.12	5 (8%)
22	CLA	A	806	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	3 (3%)
22	CLA	B	833	-	62,66,73	1.22	5 (8%)	73,104,113	0.89	3 (4%)
28	LMG	B	852	-	43,43,55	0.17	0	51,51,63	0.23	0
22	CLA	4	612	16	49,53,73	1.39	4 (8%)	58,89,113	0.96	2 (3%)
31	CHL	4	601	16	60,74,74	1.97	10 (16%)	58,114,114	1.12	5 (8%)
22	CLA	5	603	-	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
25	BCR	B2	844	-	41,41,41	0.14	0	56,56,56	0.30	0
22	CLA	9	603	19,28	59,63,73	1.26	5 (8%)	70,101,113	0.90	4 (5%)
22	CLA	A	821	-	59,63,73	1.28	5 (8%)	70,101,113	0.85	2 (2%)
27	LMU	4	625	-	34,34,36	0.10	0	45,45,47	0.19	0
22	CLA	92	614	-	49,53,73	1.41	4 (8%)	58,89,113	0.98	3 (5%)
22	CLA	4	614	-	59,63,73	1.29	4 (6%)	70,101,113	0.87	2 (2%)
22	CLA	L	204	-	49,53,73	1.40	4 (8%)	58,89,113	0.99	3 (5%)
22	CLA	B	802	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	837	-	69,73,73	1.19	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	A	810	1	69,73,73	1.20	4 (5%)	82,113,113	0.85	2 (2%)
32	XAT	6	624	-	41,47,47	0.14	0	54,74,74	0.65	0
22	CLA	Z	610	12	64,68,73	1.22	5 (7%)	76,107,113	0.84	3 (3%)
22	CLA	92	609	19	49,53,73	1.40	4 (8%)	58,89,113	0.99	2 (3%)
22	CLA	F	304	6	69,73,73	1.17	4 (5%)	82,113,113	0.90	4 (4%)
22	CLA	6	617	-	49,53,73	1.42	4 (8%)	58,89,113	0.96	3 (5%)
29	LUT	9	616	-	42,43,43	0.28	0	51,60,60	0.39	0
24	LHG	B	851	22	44,44,48	0.26	0	47,50,54	0.32	0
22	CLA	Z	614	-	54,58,73	1.32	5 (9%)	64,95,113	0.93	3 (4%)
22	CLA	4	604	34	54,58,73	1.33	5 (9%)	64,95,113	0.93	3 (4%)
31	CHL	Z	601	12	60,74,74	1.96	10 (16%)	58,114,114	1.10	5 (8%)
31	CHL	6	607	34	60,74,74	1.95	10 (16%)	58,114,114	1.10	5 (8%)
22	CLA	92	613	19	64,68,73	1.21	4 (6%)	76,107,113	0.86	3 (3%)
22	CLA	G	204	7	50,54,73	1.38	4 (8%)	59,90,113	0.96	3 (5%)
22	CLA	A	809	1	69,73,73	1.15	5 (7%)	82,113,113	0.89	4 (4%)
22	CLA	A	802	-	69,73,73	1.16	5 (7%)	82,113,113	0.77	2 (2%)
22	CLA	F	301	34	69,73,73	1.14	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	A	837	1	61,65,73	1.31	4 (6%)	72,103,113	0.90	3 (4%)
22	CLA	7	604	34	55,59,73	1.29	5 (9%)	64,96,113	0.92	3 (4%)
27	LMU	G	206	-	24,24,36	0.13	0	29,29,47	0.24	0
31	CHL	92	607	-	40,54,74	2.38	10 (25%)	34,90,114	1.33	5 (14%)
22	CLA	B2	829	-	69,73,73	1.17	4 (5%)	82,113,113	0.82	3 (3%)
27	LMU	8	628	-	24,24,36	0.15	0	29,29,47	0.33	0
28	LMG	B2	852	-	43,43,55	0.17	0	51,51,63	0.18	0
22	CLA	A	803	34	69,73,73	1.25	5 (7%)	82,113,113	0.85	4 (4%)
29	LUT	92	616	-	42,43,43	0.26	0	51,60,60	0.34	0
22	CLA	Z	603	-	59,63,73	1.29	5 (8%)	70,101,113	0.86	2 (2%)
22	CLA	3	612	13	50,54,73	1.37	5 (10%)	59,90,113	0.94	3 (5%)
25	BCR	L2	205	-	41,41,41	0.15	0	56,56,56	0.35	0
28	LMG	1	624	-	36,36,55	0.19	0	44,44,63	0.18	0
22	CLA	B	812	-	69,73,73	1.19	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	B2	812	-	64,68,73	1.19	4 (6%)	76,107,113	0.86	3 (3%)
25	BCR	B	845	-	41,41,41	0.14	0	56,56,56	0.37	0
24	LHG	92	622	22	28,28,48	0.29	0	31,34,54	0.31	0
22	CLA	A	825	-	59,63,73	1.30	5 (8%)	70,101,113	0.89	2 (2%)
22	CLA	A	841	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMU	8	627	-	36,36,36	0.10	0	47,47,47	0.38	0
22	CLA	B	823	-	69,73,73	1.19	5 (7%)	82,113,113	0.84	3 (3%)
25	BCR	3	718	-	41,41,41	0.17	0	56,56,56	0.35	0
27	LMU	1	621	-	36,36,36	0.10	0	47,47,47	0.29	0
22	CLA	92	601	19	49,53,73	1.38	4 (8%)	58,89,113	0.94	2 (3%)
27	LMU	1	626	-	24,24,36	0.12	0	29,29,47	0.27	0
25	BCR	9	623	-	41,41,41	0.13	0	56,56,56	0.35	0
22	CLA	3	610	13	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
29	LUT	Z	619	-	26,26,43	0.38	0	33,35,60	0.38	0
22	CLA	A	828	-	69,73,73	1.18	5 (7%)	82,113,113	0.77	2 (2%)
32	XAT	5	624	-	41,47,47	0.13	0	54,74,74	0.66	0
22	CLA	F	303	34	49,53,73	1.40	5 (10%)	58,89,113	0.98	3 (5%)
31	CHL	4	608	-	60,74,74	1.99	10 (16%)	58,114,114	1.06	5 (8%)
22	CLA	B	804	-	49,53,73	1.41	4 (8%)	58,89,113	0.94	2 (3%)
22	CLA	A	834	-	69,73,73	1.19	5 (7%)	82,113,113	0.84	3 (3%)
24	LHG	8	620	22	43,43,48	0.27	0	46,49,54	0.27	0
22	CLA	A	818	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	A	816	-	69,73,73	1.16	4 (5%)	82,113,113	0.83	3 (3%)
22	CLA	A	817	34	59,63,73	1.29	5 (8%)	70,101,113	0.88	2 (2%)
22	CLA	B	813	-	69,73,73	1.16	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	A	807	1	69,73,73	1.19	5 (7%)	82,113,113	0.78	2 (2%)
29	LUT	9	617	-	42,43,43	0.21	0	51,60,60	0.41	0
27	LMU	A	861	-	24,24,36	0.12	0	29,29,47	0.30	0
31	CHL	5	607	34	60,74,74	2.01	10 (16%)	58,114,114	0.99	4 (6%)
22	CLA	8	610	15	69,73,73	1.16	4 (5%)	82,113,113	0.80	2 (2%)
22	CLA	6	612	18	49,53,73	1.38	4 (8%)	58,89,113	0.97	2 (3%)
22	CLA	B	829	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)
27	LMU	6	630	-	24,24,36	0.14	0	29,29,47	0.28	0
22	CLA	B	809	2	69,73,73	1.19	5 (7%)	82,113,113	0.79	2 (2%)
22	CLA	B	836	-	64,68,73	1.21	5 (7%)	76,107,113	0.87	3 (3%)
23	PQN	B	842	-	34,34,34	0.32	0	43,45,45	0.44	0
31	CHL	6	601	18	60,74,74	1.98	10 (16%)	58,114,114	1.00	4 (6%)
22	CLA	B	826	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
29	LUT	8	617	-	42,43,43	0.31	0	51,60,60	0.45	0
24	LHG	A	846	-	48,48,48	0.24	0	51,54,54	0.30	0
25	BCR	A	848	-	41,41,41	0.15	0	56,56,56	0.30	0
22	CLA	1	614	-	64,68,73	1.22	5 (7%)	76,107,113	0.87	3 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	92	602	19	1/1/20/20	7/39/115/115	-
28	LMG	1	628	-	-	5/37/57/70	0/1/1/1
30	DGD	B	850	-	-	10/48/88/95	0/2/2/2
22	CLA	K	204	-	1/1/15/20	4/17/93/115	-
22	CLA	L2	203	-	1/1/15/20	4/15/91/115	-
31	CHL	8	607	34	3/3/26/26	8/39/137/137	-
27	LMU	K	208	-	-	3/15/35/61	0/1/1/2
22	CLA	B2	814	-	1/1/19/20	3/33/109/115	-
22	CLA	A	854	34	1/1/20/20	1/39/115/115	-
24	LHG	6	629	-	-	10/40/40/53	-
22	CLA	A	823	-	1/1/20/20	6/39/115/115	-
28	LMG	A	860	-	-	6/31/51/70	0/1/1/1
29	LUT	1	617	-	-	2/29/67/67	0/2/2/2
31	CHL	4	606	34	3/3/24/26	1/27/125/137	-
25	BCR	K	202	-	-	2/29/63/63	0/2/2/2
25	BCR	B	844	-	-	0/29/63/63	0/2/2/2
29	LUT	6	621	-	-	2/29/67/67	0/2/2/2
31	CHL	8	606	34	3/3/26/26	2/39/137/137	-
22	CLA	B2	805	-	1/1/20/20	2/39/115/115	-
22	CLA	4	611	24	1/1/19/20	5/33/109/115	-
22	CLA	8	611	24	1/1/15/20	2/15/91/115	-
22	CLA	Z	611	24	1/1/19/20	5/33/109/115	-
28	LMG	7	626	-	-	8/32/52/70	0/1/1/1
28	LMG	8	629	-	-	9/37/57/70	0/1/1/1
22	CLA	B2	828	-	1/1/20/20	6/39/115/115	-
22	CLA	8	608	34	1/1/17/20	2/21/97/115	-
26	SF4	C	102	3	-	-	0/6/5/5
27	LMU	Z	622	-	-	3/17/57/61	0/2/2/2
22	CLA	7	614	-	1/1/14/20	5/13/89/115	-
24	LHG	9	622	22	-	12/45/45/53	-
22	CLA	9	612	19	1/1/20/20	5/39/115/115	-
22	CLA	A	822	34	1/1/20/20	0/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	616	16	1/1/15/20	0/15/91/115	-
22	CLA	6	613	34	1/1/20/20	4/39/115/115	-
22	CLA	9	601	19	1/1/15/20	2/17/93/115	-
25	BCR	I2	172	-	-	0/29/63/63	0/2/2/2
22	CLA	1	613	34	1/1/20/20	5/39/115/115	-
22	CLA	7	603	-	1/1/17/20	4/24/100/115	-
25	BCR	B2	843	-	-	0/13/30/63	0/1/1/2
25	BCR	K	207	-	-	4/29/63/63	0/2/2/2
22	CLA	3	617	13	1/1/15/20	2/17/93/115	-
22	CLA	4	609	16	1/1/19/20	6/33/109/115	-
22	CLA	B	841	24	1/1/20/20	8/39/115/115	-
33	NEX	5	625	-	-	2/27/83/83	1/3/3/3
31	CHL	1	601	12	3/3/26/26	8/39/137/137	-
31	CHL	7	606	34	3/3/21/26	2/15/113/137	-
25	BCR	A	850	-	-	0/29/63/63	0/2/2/2
22	CLA	A	820	-	1/1/20/20	6/39/115/115	-
22	CLA	A	843	34	1/1/20/20	7/39/115/115	-
27	LMU	8	625	-	-	2/15/35/61	0/1/1/2
32	XAT	1	618	-	1/1/26/26	0/31/93/93	0/4/4/4
31	CHL	4	607	34	3/3/26/26	1/39/137/137	-
22	CLA	9	604	19	1/1/17/20	0/25/101/115	-
22	CLA	A	827	34	1/1/20/20	2/39/115/115	-
22	CLA	6	610	18	1/1/19/20	0/33/109/115	-
31	CHL	8	601	15	3/3/26/26	7/39/137/137	-
22	CLA	1	610	12	1/1/20/20	2/39/115/115	-
25	BCR	7	623	-	-	2/29/63/63	0/2/2/2
22	CLA	B	828	-	1/1/20/20	4/39/115/115	-
31	CHL	4	618	16	3/3/21/26	0/15/113/137	-
23	PQN	A	844	-	-	3/23/43/43	0/2/2/2
22	CLA	6	622	34	1/1/18/20	2/27/103/115	-
22	CLA	B	838	-	1/1/17/20	1/21/97/115	-
22	CLA	6	604	-	1/1/20/20	2/39/115/115	-
25	BCR	8	619	-	-	4/29/63/63	0/2/2/2
22	CLA	8	603	-	1/1/20/20	5/39/115/115	-
22	CLA	A	832	-	1/1/18/20	0/27/103/115	-
25	BCR	B	846	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	817	-	1/1/20/20	8/39/115/115	-
27	LMU	Z	621	-	-	2/13/33/61	0/1/1/2
31	CHL	Z	606	34	3/3/21/26	5/15/113/137	-
31	CHL	92	606	-	3/3/20/26	0/10/108/137	-
29	LUT	Z	617	-	-	2/29/67/67	0/2/2/2
28	LMG	4	624	-	-	6/36/56/70	0/1/1/1
29	LUT	A	856	-	-	4/29/67/67	0/2/2/2
22	CLA	92	611	24	1/1/20/20	4/39/115/115	-
26	SF4	C	101	3	-	-	0/6/5/5
22	CLA	B	819	34	1/1/19/20	5/33/109/115	-
22	CLA	3	609	13	1/1/19/20	2/35/111/115	-
24	LHG	5	623	22	-	11/41/41/53	-
22	CLA	B	805	-	1/1/20/20	8/39/115/115	-
29	LUT	5	620	-	-	2/29/67/67	0/2/2/2
25	BCR	I	172	-	-	0/29/63/63	0/2/2/2
25	BCR	B	848	-	-	2/29/63/63	0/2/2/2
27	LMU	1	623	-	-	1/15/35/61	0/1/1/2
22	CLA	5	613	17	1/1/18/20	4/29/105/115	-
22	CLA	B2	820	-	1/1/18/20	7/29/105/115	-
22	CLA	1	608	34	1/1/20/20	2/39/115/115	-
22	CLA	A	835	-	1/1/20/20	6/39/115/115	-
22	CLA	L2	204	-	1/1/15/20	6/15/91/115	-
22	CLA	B	821	-	1/1/20/20	5/39/115/115	-
22	CLA	B	810	-	1/1/20/20	2/39/115/115	-
22	CLA	B	834	-	1/1/19/20	8/33/109/115	-
22	CLA	5	601	17	1/1/20/20	5/39/115/115	-
25	BCR	A	852	-	-	4/29/63/63	0/2/2/2
22	CLA	A	805	-	1/1/18/20	1/27/103/115	-
22	CLA	B	806	2	1/1/20/20	2/39/115/115	-
22	CLA	A	815	-	1/1/18/20	2/27/103/115	-
25	BCR	A	851	-	-	2/29/63/63	0/2/2/2
25	BCR	G	205	-	-	1/29/63/63	0/2/2/2
22	CLA	8	604	34	1/1/19/20	2/33/109/115	-
22	CLA	Z	604	34	1/1/18/20	2/30/106/115	-
22	CLA	Z	602	12	1/1/19/20	2/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	614	-	1/1/15/20	2/15/91/115	-
22	CLA	7	602	14	1/1/20/20	2/39/115/115	-
22	CLA	3	603	-	1/1/20/20	5/39/115/115	-
27	LMU	B	853	-	-	7/21/61/61	0/2/2/2
24	LHG	1	620	22	-	7/43/43/53	-
29	LUT	F	305	-	-	5/29/67/67	0/2/2/2
22	CLA	B	820	-	1/1/18/20	5/29/105/115	-
25	BCR	B	843	-	-	0/29/63/63	0/2/2/2
26	SF4	A	853	1,2	-	-	0/6/5/5
22	CLA	8	616	15	1/1/15/20	0/15/91/115	-
22	CLA	B	808	-	1/1/20/20	9/39/115/115	-
22	CLA	5	604	34	1/1/18/20	5/27/103/115	-
27	LMU	1	622	-	-	4/10/30/61	0/1/1/2
22	CLA	6	609	18	1/1/18/20	4/27/103/115	-
22	CLA	92	603	19	1/1/15/20	4/15/91/115	-
29	LUT	3	621	-	-	2/29/67/67	0/2/2/2
22	CLA	1	609	12	1/1/20/20	5/39/115/115	-
25	BCR	B2	845	-	-	4/29/63/63	0/2/2/2
22	CLA	B2	807	-	1/1/18/20	2/27/103/115	-
28	LMG	J	104	-	-	8/30/50/70	0/1/1/1
22	CLA	A	831	-	1/1/20/20	2/39/115/115	-
22	CLA	92	604	19	1/1/17/20	4/21/97/115	-
22	CLA	8	609	15	1/1/15/20	0/15/91/115	-
22	CLA	B	811	-	1/1/20/20	7/39/115/115	-
31	CHL	1	607	34	3/3/21/26	2/15/113/137	-
25	BCR	B2	848	-	-	2/5/22/63	0/1/1/2
27	LMU	A	862	-	-	2/11/31/61	0/1/1/2
27	LMU	A	865	-	-	3/15/35/61	0/1/1/2
22	CLA	A	808	-	1/1/17/20	0/21/97/115	-
24	LHG	3	623	-	-	12/51/51/53	-
22	CLA	3	607	13	1/1/18/20	5/27/103/115	-
22	CLA	B	840	-	1/1/20/20	7/39/115/115	-
22	CLA	J	101	9	1/1/18/20	3/27/103/115	-
22	CLA	9	613	19	1/1/20/20	4/39/115/115	-
25	BCR	3	719	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	6	619	22	-	6/53/53/53	-
22	CLA	3	613	13	1/1/19/20	5/33/109/115	-
28	LMG	8	626	-	-	6/27/47/70	0/1/1/1
22	CLA	K	203	34	1/1/19/20	1/33/109/115	-
22	CLA	B	818	-	1/1/20/20	4/39/115/115	-
22	CLA	A	814	-	1/1/20/20	5/39/115/115	-
22	CLA	5	612	17	1/1/15/20	5/15/91/115	-
22	CLA	G	203	-	1/1/19/20	2/33/109/115	-
22	CLA	3	604	34	1/1/20/20	1/39/115/115	-
27	LMU	8	624	-	-	1/15/35/61	0/1/1/2
28	LMG	3	722	-	-	5/46/46/70	-
22	CLA	B	832	-	1/1/20/20	5/39/115/115	-
22	CLA	1	611	24	1/1/19/20	4/35/111/115	-
22	CLA	6	614	-	1/1/17/20	2/21/97/115	-
22	CLA	B	807	-	1/1/18/20	3/27/103/115	-
22	CLA	A	819	-	1/1/19/20	3/33/109/115	-
22	CLA	B2	839	-	1/1/15/20	5/15/91/115	-
22	CLA	B	831	-	1/1/18/20	1/27/103/115	-
25	BCR	L	201	-	-	4/29/63/63	0/2/2/2
22	CLA	6	603	-	1/1/20/20	7/39/115/115	-
22	CLA	9	610	19	1/1/19/20	0/33/109/115	-
25	BCR	5	622	-	-	2/29/63/63	0/2/2/2
22	CLA	9	609	19	1/1/17/20	4/23/99/115	-
22	CLA	6	602	18	1/1/20/20	2/39/115/115	-
27	LMU	7	628	-	-	3/13/33/61	0/1/1/2
22	CLA	Z	616	12	1/1/19/20	4/33/109/115	-
27	LMU	6	632	-	-	3/11/31/61	0/1/1/2
22	CLA	7	616	14	1/1/15/20	3/17/93/115	-
22	CLA	A	842	-	1/1/20/20	3/39/115/115	-
22	CLA	B	835	34	1/1/15/20	2/15/91/115	-
31	CHL	9	606	-	3/3/20/26	0/10/108/137	-
31	CHL	9	607	34	3/3/23/26	1/21/119/137	-
25	BCR	B	801	-	-	0/29/63/63	0/2/2/2
25	BCR	92	623	-	-	4/29/63/63	0/2/2/2
27	LMU	7	627	-	-	2/18/58/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	A	849	-	-	0/29/63/63	0/2/2/2
24	LHG	A	847	22	-	4/42/42/53	-
31	CHL	6	606	34	3/3/24/26	2/30/128/137	-
27	LMU	A	864	-	-	2/15/35/61	0/1/1/2
22	CLA	6	611	24	1/1/18/20	4/31/107/115	-
22	CLA	A	826	34	1/1/20/20	7/39/115/115	-
22	CLA	B2	810	-	1/1/20/20	4/39/115/115	-
22	CLA	5	621	34	1/1/15/20	11/17/93/115	-
32	XAT	Z	618	-	-	0/31/93/93	0/4/4/4
22	CLA	7	611	24	1/1/20/20	7/39/115/115	-
22	CLA	B2	811	-	1/1/17/20	2/25/101/115	-
21	CL0	A	801	-	3/3/25/25	3/37/135/135	-
25	BCR	3	620	-	-	4/29/63/63	0/2/2/2
29	LUT	92	617	-	-	0/29/67/67	0/2/2/2
28	LMG	B2	855	-	-	2/26/46/70	0/1/1/1
22	CLA	5	614	-	1/1/15/20	4/15/91/115	-
24	LHG	4	623	-	-	15/42/42/53	-
22	CLA	3	611	-	1/1/20/20	6/39/115/115	-
31	CHL	5	606	34	3/3/21/26	2/15/113/137	-
29	LUT	7	624	-	-	4/29/67/67	0/2/2/2
22	CLA	8	602	15	1/1/19/20	3/36/112/115	-
22	CLA	7	610	14	1/1/20/20	7/39/115/115	-
31	CHL	1	606	34	3/3/21/26	0/15/113/137	-
22	CLA	B2	815	-	1/1/18/20	4/30/106/115	-
22	CLA	B	822	-	1/1/18/20	3/32/108/115	-
22	CLA	B	830	-	1/1/15/20	0/15/91/115	-
22	CLA	4	610	16	1/1/19/20	3/33/109/115	-
22	CLA	L	203	-	1/1/20/20	6/39/115/115	-
22	CLA	4	603	16	1/1/20/20	7/39/115/115	-
22	CLA	92	612	19	1/1/20/20	7/39/115/115	-
22	CLA	Z	608	34	1/1/17/20	2/21/97/115	-
24	LHG	7	625	22	-	13/53/53/53	-
29	LUT	5	626	-	-	4/29/67/67	0/2/2/2
22	CLA	7	608	34	1/1/17/20	0/21/97/115	-
29	LUT	3	720	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CHL	6	618	18	3/3/20/26	2/12/110/137	-
31	CHL	6	616	18	3/3/26/26	3/39/137/137	-
25	BCR	B	847	-	-	2/29/63/63	0/2/2/2
22	CLA	A	830	-	1/1/20/20	4/39/115/115	-
25	BCR	L	205	-	-	2/29/63/63	0/2/2/2
22	CLA	1	603	-	1/1/18/20	6/30/106/115	-
22	CLA	4	613	16	1/1/20/20	6/39/115/115	-
27	LMU	92	624	-	-	1/21/61/61	0/2/2/2
22	CLA	B2	809	20	1/1/17/20	2/24/100/115	-
29	LUT	1	619	-	-	2/29/67/67	0/2/2/2
22	CLA	8	614	-	1/1/18/20	7/30/106/115	-
22	CLA	B	824	34	1/1/20/20	3/39/115/115	-
22	CLA	1	604	34	1/1/17/20	0/21/97/115	-
22	CLA	B2	813	-	1/1/20/20	3/39/115/115	-
22	CLA	1	602	12	1/1/19/20	2/33/109/115	-
22	CLA	B	827	-	1/1/20/20	5/39/115/115	-
22	CLA	8	612	15	1/1/18/20	4/27/103/115	-
25	BCR	4	621	-	-	2/29/63/63	0/2/2/2
22	CLA	A	838	-	1/1/17/20	0/23/99/115	-
22	CLA	3	606	34	1/1/14/20	0/12/88/115	-
29	LUT	4	619	-	-	1/29/67/67	0/2/2/2
31	CHL	5	618	17	3/3/20/26	2/12/110/137	-
28	LMG	6	633	-	-	1/17/17/70	-
22	CLA	K	201	11	1/1/15/20	2/15/91/115	-
28	LMG	A	859	-	-	9/43/63/70	0/1/1/1
22	CLA	Z	609	12	1/1/20/20	8/39/115/115	-
22	CLA	B	814	-	1/1/19/20	3/33/109/115	-
22	CLA	K	206	11	1/1/15/20	4/15/91/115	-
22	CLA	A	824	-	1/1/15/20	4/15/91/115	-
32	XAT	4	620	-	-	0/31/93/93	0/4/4/4
22	CLA	7	609	14	1/1/15/20	1/15/91/115	-
22	CLA	4	602	16	1/1/19/20	2/33/109/115	-
27	LMU	6	631	-	-	4/15/35/61	0/1/1/2
22	CLA	Z	613	34	1/1/20/20	2/39/115/115	-
22	CLA	B2	808	-	1/1/15/20	4/15/91/115	-
22	CLA	7	613	14	1/1/20/20	0/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CHL	Z	607	34	3/3/26/26	4/39/137/137	-
22	CLA	B	839	34	1/1/20/20	5/39/115/115	-
22	CLA	B	815	-	1/1/20/20	4/39/115/115	-
22	CLA	92	610	19	1/1/19/20	0/33/109/115	-
22	CLA	A	811	-	1/1/20/20	4/39/115/115	-
31	CHL	7	607	34	3/3/21/26	0/15/113/137	-
32	XAT	7	622	-	-	0/31/93/93	0/4/4/4
22	CLA	5	617	-	1/1/20/20	5/39/115/115	-
22	CLA	B	825	34	1/1/20/20	2/39/115/115	-
27	LMU	1	625	-	-	5/15/35/61	0/1/1/2
31	CHL	7	601	14	3/3/26/26	4/39/137/137	-
22	CLA	A	833	-	1/1/20/20	1/39/115/115	-
22	CLA	5	602	17	1/1/20/20	1/39/115/115	-
24	LHG	Z	620	22	-	6/43/43/53	-
22	CLA	9	602	19	1/1/19/20	2/33/109/115	-
22	CLA	5	616	17	1/1/17/20	6/25/101/115	-
22	CLA	A	812	-	1/1/20/20	7/39/115/115	-
25	BCR	6	623	-	-	2/29/63/63	0/2/2/2
24	LHG	3	721	-	-	12/35/35/53	-
28	LMG	B	854	-	-	2/31/51/70	0/1/1/1
28	LMG	J	103	-	-	3/37/57/70	0/1/1/1
22	CLA	B	803	-	1/1/20/20	3/39/115/115	-
29	LUT	3	622	-	-	2/29/67/67	0/2/2/2
22	CLA	A	836	-	1/1/20/20	5/39/115/115	-
22	CLA	7	620	34	1/1/17/20	6/25/101/115	-
22	CLA	9	611	24	1/1/20/20	6/39/115/115	-
22	CLA	5	609	17	1/1/20/20	3/39/115/115	-
27	LMU	5	627	-	-	1/15/35/61	0/1/1/2
27	LMU	6	628	-	-	2/15/35/61	0/1/1/2
27	LMU	7	629	-	-	4/13/53/61	0/2/2/2
22	CLA	5	611	24	1/1/18/20	4/27/103/115	-
27	LMU	A	863	-	-	7/21/61/61	0/2/2/2
33	NEX	6	625	-	1/1/25/25	4/27/83/83	0/3/3/3
22	CLA	A	845	24	1/1/15/20	2/15/91/115	-
22	CLA	7	612	14	1/1/17/20	3/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LUT	7	621	-	-	2/29/67/67	0/2/2/2
27	LMU	9	624	-	-	4/15/35/61	0/1/1/2
32	XAT	8	618	-	-	0/31/93/93	0/4/4/4
22	CLA	A	829	-	1/1/20/20	8/39/115/115	-
25	BCR	L2	201	-	-	4/29/63/63	0/2/2/2
27	LMU	A	858	-	-	6/21/61/61	0/2/2/2
31	CHL	5	608	34	3/3/23/26	0/21/119/137	-
27	LMU	4	626	-	-	0/11/31/61	0/1/1/2
27	LMU	1	627	-	-	3/13/33/61	0/1/1/2
27	LMU	A	857	-	-	3/20/60/61	0/2/2/2
25	BCR	J	102	-	-	2/29/63/63	0/2/2/2
22	CLA	5	610	17	1/1/19/20	2/33/109/115	-
22	CLA	A	839	-	1/1/20/20	2/39/115/115	-
22	CLA	A	804	-	1/1/20/20	4/39/115/115	-
22	CLA	B	816	-	1/1/20/20	0/39/115/115	-
22	CLA	A	840	-	1/1/20/20	6/39/115/115	-
22	CLA	A	813	-	1/1/20/20	3/39/115/115	-
22	CLA	Z	612	12	1/1/15/20	5/15/91/115	-
22	CLA	1	612	12	1/1/15/20	6/15/91/115	-
22	CLA	B2	804	-	1/1/15/20	2/15/91/115	-
22	CLA	3	602	13	1/1/19/20	2/33/109/115	-
24	LHG	4	622	22	-	13/53/53/53	-
22	CLA	8	613	15	1/1/20/20	7/39/115/115	-
22	CLA	1	616	12	1/1/15/20	2/17/93/115	-
22	CLA	B2	806	20	1/1/20/20	6/39/115/115	-
31	CHL	6	608	34	3/3/23/26	0/21/119/137	-
22	CLA	9	614	-	1/1/15/20	4/15/91/115	-
22	CLA	3	615	34	1/1/20/20	5/39/115/115	-
28	LMG	9	620	22	-	7/39/59/70	0/1/1/1
31	CHL	3	608	34	3/3/26/26	3/39/137/137	-
22	CLA	A	806	-	1/1/20/20	10/39/115/115	-
22	CLA	B	833	-	1/1/18/20	4/31/107/115	-
28	LMG	B	852	-	-	5/38/58/70	0/1/1/1
22	CLA	4	612	16	1/1/15/20	4/15/91/115	-
31	CHL	4	601	16	3/3/26/26	6/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	603	-	1/1/20/20	15/39/115/115	-
25	BCR	B2	844	-	-	0/29/63/63	0/2/2/2
22	CLA	9	603	19,28	1/1/18/20	5/27/103/115	-
22	CLA	A	821	-	1/1/18/20	4/27/103/115	-
27	LMU	4	625	-	-	3/19/59/61	0/2/2/2
22	CLA	92	614	-	1/1/15/20	4/15/91/115	-
22	CLA	4	614	-	1/1/18/20	5/27/103/115	-
22	CLA	L	204	-	1/1/15/20	1/15/91/115	-
22	CLA	B	802	-	1/1/20/20	5/39/115/115	-
22	CLA	B	837	-	1/1/20/20	0/39/115/115	-
22	CLA	A	810	1	1/1/20/20	8/39/115/115	-
32	XAT	6	624	-	-	0/31/93/93	0/4/4/4
22	CLA	Z	610	12	1/1/19/20	0/33/109/115	-
22	CLA	92	609	19	1/1/15/20	8/15/91/115	-
22	CLA	F	304	6	1/1/20/20	8/39/115/115	-
22	CLA	6	617	-	1/1/15/20	2/15/91/115	-
29	LUT	9	616	-	-	2/29/67/67	0/2/2/2
24	LHG	B	851	22	-	12/49/49/53	-
22	CLA	Z	614	-	1/1/17/20	0/21/97/115	-
22	CLA	4	604	34	1/1/17/20	1/21/97/115	-
31	CHL	Z	601	12	3/3/26/26	7/39/137/137	-
31	CHL	6	607	34	3/3/26/26	8/39/137/137	-
22	CLA	92	613	19	1/1/19/20	2/33/109/115	-
22	CLA	G	204	7	1/1/15/20	4/17/93/115	-
22	CLA	A	809	1	1/1/20/20	6/39/115/115	-
22	CLA	A	802	-	1/1/20/20	0/39/115/115	-
22	CLA	F	301	34	1/1/20/20	3/39/115/115	-
22	CLA	A	837	1	1/1/18/20	1/30/106/115	-
22	CLA	7	604	34	1/1/17/20	1/23/99/115	-
27	LMU	G	206	-	-	4/15/35/61	0/1/1/2
31	CHL	92	607	-	3/3/21/26	2/15/113/137	-
22	CLA	B2	829	-	1/1/20/20	2/39/115/115	-
27	LMU	8	628	-	-	4/15/35/61	0/1/1/2
28	LMG	B2	852	-	-	3/38/58/70	0/1/1/1
22	CLA	A	803	34	1/1/20/20	2/39/115/115	-
29	LUT	92	616	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Z	603	-	1/1/18/20	6/27/103/115	-
22	CLA	3	612	13	1/1/15/20	2/17/93/115	-
25	BCR	L2	205	-	-	2/29/63/63	0/2/2/2
28	LMG	1	624	-	-	4/31/51/70	0/1/1/1
22	CLA	B	812	-	1/1/20/20	2/39/115/115	-
22	CLA	B2	812	-	1/1/19/20	3/33/109/115	-
25	BCR	B	845	-	-	4/29/63/63	0/2/2/2
24	LHG	92	622	22	-	9/33/33/53	-
22	CLA	A	825	-	1/1/18/20	7/27/103/115	-
22	CLA	A	841	-	1/1/20/20	7/39/115/115	-
27	LMU	8	627	-	-	9/21/61/61	0/2/2/2
22	CLA	B	823	-	1/1/20/20	4/39/115/115	-
25	BCR	3	718	-	-	2/29/63/63	0/2/2/2
27	LMU	1	621	-	-	6/21/61/61	0/2/2/2
22	CLA	92	601	19	1/1/15/20	4/15/91/115	-
27	LMU	1	626	-	-	0/15/35/61	0/1/1/2
25	BCR	9	623	-	-	2/29/63/63	0/2/2/2
22	CLA	3	610	13	1/1/20/20	0/39/115/115	-
29	LUT	Z	619	-	-	2/18/37/67	0/1/1/2
22	CLA	A	828	-	1/1/20/20	5/39/115/115	-
32	XAT	5	624	-	1/1/26/26	0/31/93/93	0/4/4/4
22	CLA	F	303	34	1/1/15/20	1/15/91/115	-
31	CHL	4	608	-	3/3/26/26	5/39/137/137	-
22	CLA	B	804	-	1/1/15/20	4/15/91/115	-
22	CLA	A	834	-	1/1/20/20	6/39/115/115	-
24	LHG	8	620	22	-	14/48/48/53	-
22	CLA	A	818	-	1/1/20/20	2/39/115/115	-
22	CLA	A	816	-	1/1/20/20	4/39/115/115	-
22	CLA	A	817	34	1/1/18/20	4/27/103/115	-
22	CLA	B	813	-	1/1/20/20	3/39/115/115	-
22	CLA	A	807	1	1/1/20/20	3/39/115/115	-
29	LUT	9	617	-	-	0/29/67/67	0/2/2/2
27	LMU	A	861	-	-	2/15/35/61	0/1/1/2
31	CHL	5	607	34	3/3/26/26	11/39/137/137	-
22	CLA	8	610	15	1/1/20/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	612	18	1/1/15/20	2/15/91/115	-
22	CLA	B	829	-	1/1/20/20	3/39/115/115	-
27	LMU	6	630	-	-	1/15/35/61	0/1/1/2
22	CLA	B	809	2	1/1/20/20	6/39/115/115	-
22	CLA	B	836	-	1/1/19/20	4/33/109/115	-
23	PQN	B	842	-	-	1/23/43/43	0/2/2/2
31	CHL	6	601	18	3/3/26/26	4/39/137/137	-
22	CLA	B	826	-	1/1/20/20	4/39/115/115	-
29	LUT	8	617	-	-	2/29/67/67	0/2/2/2
24	LHG	A	846	-	-	9/53/53/53	-
25	BCR	A	848	-	-	2/29/63/63	0/2/2/2
22	CLA	1	614	-	1/1/19/20	7/33/109/115	-

All (1385) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	601	CHL	MG-NB	-7.46	1.91	2.05
31	6	601	CHL	MG-NB	-7.44	1.91	2.05
31	8	601	CHL	MG-NB	-7.43	1.91	2.05
31	9	607	CHL	MG-NB	-7.43	1.91	2.05
31	4	606	CHL	MG-NB	-7.41	1.91	2.05
31	6	616	CHL	MG-NB	-7.40	1.91	2.05
31	1	607	CHL	MG-NB	-7.40	1.91	2.05
31	4	607	CHL	MG-NB	-7.37	1.91	2.05
31	Z	606	CHL	MG-NB	-7.36	1.91	2.05
31	5	608	CHL	MG-NB	-7.34	1.91	2.05
31	Z	607	CHL	MG-NB	-7.33	1.91	2.05
31	6	606	CHL	MG-NB	-7.32	1.91	2.05
31	3	608	CHL	MG-NB	-7.32	1.91	2.05
31	4	618	CHL	MG-NB	-7.31	1.91	2.05
31	4	601	CHL	MG-NB	-7.30	1.91	2.05
31	92	606	CHL	MG-NB	-7.29	1.91	2.05
31	5	606	CHL	MG-NB	-7.29	1.91	2.05
31	5	618	CHL	MG-NB	-7.28	1.91	2.05
31	7	606	CHL	MG-NB	-7.27	1.91	2.05
31	8	607	CHL	MG-NB	-7.27	1.91	2.05
31	4	608	CHL	MG-NB	-7.27	1.91	2.05
31	7	601	CHL	MG-NB	-7.27	1.91	2.05
31	6	618	CHL	MG-NB	-7.26	1.91	2.05
31	92	607	CHL	MG-NB	-7.26	1.91	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	606	CHL	MG-NB	-7.25	1.91	2.05
31	1	606	CHL	MG-NB	-7.25	1.91	2.05
31	1	601	CHL	MG-NB	-7.24	1.91	2.05
31	5	607	CHL	MG-NB	-7.23	1.91	2.05
31	6	607	CHL	MG-NB	-7.22	1.91	2.05
31	7	607	CHL	MG-NB	-7.21	1.91	2.05
31	6	608	CHL	MG-NB	-7.17	1.91	2.05
31	8	606	CHL	MG-NB	-7.17	1.91	2.05
31	8	601	CHL	C1B-C2B	6.97	1.47	1.39
31	1	601	CHL	C1B-C2B	6.96	1.47	1.39
31	4	601	CHL	C1B-C2B	6.92	1.47	1.39
31	Z	601	CHL	C1B-C2B	6.92	1.47	1.39
31	4	618	CHL	C1B-C2B	6.87	1.47	1.39
31	9	606	CHL	C1B-C2B	6.80	1.47	1.39
31	92	607	CHL	C1B-C2B	6.77	1.47	1.39
31	7	606	CHL	C1B-C2B	6.76	1.47	1.39
31	5	618	CHL	C1B-C2B	6.75	1.47	1.39
31	8	606	CHL	C1B-C2B	6.74	1.47	1.39
31	Z	606	CHL	C1B-C2B	6.67	1.47	1.39
31	6	618	CHL	C1B-C2B	6.58	1.47	1.39
31	Z	607	CHL	C1B-C2B	6.55	1.47	1.39
31	92	606	CHL	C1B-C2B	6.54	1.47	1.39
31	4	608	CHL	C1B-C2B	6.52	1.47	1.39
31	6	608	CHL	C1B-C2B	6.49	1.46	1.39
31	7	607	CHL	C1B-C2B	6.49	1.46	1.39
31	6	606	CHL	C1B-C2B	6.49	1.46	1.39
31	9	607	CHL	C1B-C2B	6.45	1.46	1.39
31	1	607	CHL	C1B-C2B	6.42	1.46	1.39
31	4	607	CHL	C1B-C2B	6.40	1.46	1.39
31	6	607	CHL	C1B-C2B	6.37	1.46	1.39
31	5	607	CHL	C1B-C2B	6.35	1.46	1.39
31	3	608	CHL	C1B-C2B	6.34	1.46	1.39
31	7	601	CHL	C1B-C2B	6.29	1.46	1.39
31	5	606	CHL	C1B-C2B	6.28	1.46	1.39
31	6	616	CHL	C1B-C2B	6.28	1.46	1.39
31	6	601	CHL	C1B-C2B	6.28	1.46	1.39
31	4	606	CHL	C1B-C2B	6.19	1.46	1.39
31	1	606	CHL	C1B-C2B	6.17	1.46	1.39
31	3	608	CHL	MG-ND	-6.13	1.93	2.05
31	5	608	CHL	C1B-C2B	6.11	1.46	1.39
31	6	601	CHL	MG-ND	-6.10	1.93	2.05
31	Z	601	CHL	MG-ND	-6.08	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	607	CHL	MG-ND	-6.06	1.93	2.05
31	4	607	CHL	MG-ND	-6.04	1.93	2.05
31	4	601	CHL	MG-ND	-6.04	1.93	2.05
31	5	606	CHL	MG-ND	-6.02	1.93	2.05
31	5	608	CHL	MG-ND	-6.01	1.93	2.05
31	1	607	CHL	MG-ND	-6.01	1.93	2.05
31	8	601	CHL	MG-ND	-6.01	1.93	2.05
31	8	607	CHL	MG-ND	-6.00	1.93	2.05
31	4	606	CHL	MG-ND	-6.00	1.93	2.05
31	8	607	CHL	C1B-C2B	6.00	1.46	1.39
31	92	606	CHL	MG-ND	-6.00	1.93	2.05
31	7	601	CHL	MG-ND	-5.99	1.93	2.05
31	7	607	CHL	MG-ND	-5.99	1.93	2.05
31	4	608	CHL	MG-ND	-5.98	1.93	2.05
31	6	606	CHL	MG-ND	-5.97	1.93	2.05
31	1	606	CHL	MG-ND	-5.97	1.94	2.05
31	6	616	CHL	MG-ND	-5.96	1.94	2.05
31	9	607	CHL	MG-ND	-5.94	1.94	2.05
31	6	607	CHL	MG-ND	-5.94	1.94	2.05
31	6	608	CHL	MG-ND	-5.92	1.94	2.05
31	7	606	CHL	MG-ND	-5.87	1.94	2.05
22	A	803	CLA	MG-NB	-5.87	1.94	2.05
31	5	607	CHL	MG-ND	-5.87	1.94	2.05
31	92	607	CHL	MG-ND	-5.85	1.94	2.05
31	6	618	CHL	MG-ND	-5.84	1.94	2.05
31	9	606	CHL	MG-ND	-5.84	1.94	2.05
31	Z	606	CHL	MG-ND	-5.83	1.94	2.05
31	1	601	CHL	MG-ND	-5.82	1.94	2.05
31	5	618	CHL	MG-ND	-5.81	1.94	2.05
22	A	854	CLA	MG-NB	-5.77	1.94	2.05
22	A	829	CLA	MG-NB	-5.73	1.94	2.05
22	A	837	CLA	MG-NB	-5.73	1.94	2.05
31	8	606	CHL	MG-ND	-5.73	1.94	2.05
31	4	618	CHL	MG-ND	-5.71	1.94	2.05
22	B	821	CLA	MG-NB	-5.70	1.94	2.05
21	A	801	CL0	MG-NB	-5.63	1.94	2.05
22	B	824	CLA	MG-NB	-5.62	1.94	2.05
22	7	610	CLA	MG-NB	-5.62	1.94	2.05
22	B	803	CLA	MG-NB	-5.58	1.94	2.05
22	B	807	CLA	MG-NB	-5.56	1.94	2.05
22	B2	809	CLA	MG-NB	-5.54	1.94	2.05
22	7	609	CLA	MG-NB	-5.52	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	810	CLA	MG-NB	-5.51	1.94	2.05
22	3	606	CLA	MG-NB	-5.51	1.94	2.05
22	9	614	CLA	MG-NB	-5.48	1.94	2.05
22	A	819	CLA	MG-NB	-5.48	1.94	2.05
22	1	616	CLA	MG-NB	-5.46	1.95	2.05
21	A	801	CL0	C3A-C2A	-5.46	1.50	1.54
22	B	820	CLA	MG-NB	-5.44	1.95	2.05
22	A	834	CLA	MG-NB	-5.44	1.95	2.05
22	B	837	CLA	MG-NB	-5.43	1.95	2.05
22	9	602	CLA	MG-NB	-5.42	1.95	2.05
22	Z	602	CLA	MG-NB	-5.41	1.95	2.05
22	A	822	CLA	MG-NB	-5.41	1.95	2.05
22	1	602	CLA	MG-NB	-5.41	1.95	2.05
22	3	610	CLA	MG-NB	-5.41	1.95	2.05
22	B	841	CLA	MG-NB	-5.40	1.95	2.05
22	4	602	CLA	MG-NB	-5.40	1.95	2.05
22	8	603	CLA	MG-NB	-5.40	1.95	2.05
22	4	609	CLA	MG-NB	-5.40	1.95	2.05
22	A	805	CLA	MG-NB	-5.39	1.95	2.05
22	B	818	CLA	MG-NB	-5.39	1.95	2.05
22	7	603	CLA	MG-NB	-5.39	1.95	2.05
22	6	611	CLA	MG-NB	-5.38	1.95	2.05
22	9	601	CLA	MG-NB	-5.38	1.95	2.05
22	7	614	CLA	MG-NB	-5.38	1.95	2.05
22	5	603	CLA	MG-NB	-5.37	1.95	2.05
22	B	834	CLA	MG-NB	-5.37	1.95	2.05
22	8	609	CLA	MG-NB	-5.37	1.95	2.05
22	A	807	CLA	MG-NB	-5.36	1.95	2.05
22	3	603	CLA	MG-NB	-5.36	1.95	2.05
22	3	615	CLA	MG-NB	-5.36	1.95	2.05
22	92	611	CLA	MG-NB	-5.36	1.95	2.05
22	6	617	CLA	MG-NB	-5.36	1.95	2.05
22	92	602	CLA	MG-NB	-5.36	1.95	2.05
22	3	613	CLA	MG-NB	-5.35	1.95	2.05
22	A	833	CLA	MG-NB	-5.35	1.95	2.05
22	B	823	CLA	MG-NB	-5.35	1.95	2.05
22	B2	820	CLA	C1D-ND	5.35	1.44	1.37
22	1	604	CLA	MG-NB	-5.35	1.95	2.05
22	3	614	CLA	MG-NB	-5.35	1.95	2.05
22	1	610	CLA	MG-NB	-5.34	1.95	2.05
22	1	608	CLA	MG-NB	-5.34	1.95	2.05
22	7	616	CLA	MG-NB	-5.34	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	613	CLA	MG-NB	-5.34	1.95	2.05
22	Z	608	CLA	MG-NB	-5.34	1.95	2.05
22	L	203	CLA	MG-NB	-5.34	1.95	2.05
22	A	836	CLA	MG-NB	-5.33	1.95	2.05
22	A	823	CLA	MG-NB	-5.33	1.95	2.05
22	6	610	CLA	MG-NB	-5.33	1.95	2.05
22	J	101	CLA	MG-NB	-5.33	1.95	2.05
22	6	622	CLA	MG-NB	-5.33	1.95	2.05
22	A	817	CLA	MG-NB	-5.33	1.95	2.05
22	K	203	CLA	MG-NB	-5.33	1.95	2.05
22	92	610	CLA	MG-NB	-5.33	1.95	2.05
22	A	815	CLA	MG-NB	-5.33	1.95	2.05
22	B	831	CLA	MG-NB	-5.33	1.95	2.05
22	A	821	CLA	MG-NB	-5.32	1.95	2.05
22	B	804	CLA	MG-NB	-5.32	1.95	2.05
22	9	611	CLA	MG-NB	-5.32	1.95	2.05
22	4	611	CLA	MG-NB	-5.31	1.95	2.05
22	1	603	CLA	MG-NB	-5.31	1.95	2.05
22	Z	609	CLA	MG-NB	-5.31	1.95	2.05
22	9	613	CLA	MG-NB	-5.31	1.95	2.05
22	3	604	CLA	MG-NB	-5.31	1.95	2.05
22	B2	807	CLA	MG-NB	-5.31	1.95	2.05
22	3	602	CLA	MG-NB	-5.31	1.95	2.05
22	5	602	CLA	MG-NB	-5.31	1.95	2.05
22	6	602	CLA	MG-NB	-5.30	1.95	2.05
22	3	609	CLA	MG-NB	-5.30	1.95	2.05
22	A	825	CLA	MG-NB	-5.30	1.95	2.05
22	1	611	CLA	MG-NB	-5.30	1.95	2.05
31	6	601	CHL	C3A-C2A	-5.30	1.50	1.54
22	B2	839	CLA	MG-NB	-5.30	1.95	2.05
22	B	827	CLA	MG-NB	-5.29	1.95	2.05
22	B	812	CLA	MG-NB	-5.28	1.95	2.05
22	Z	616	CLA	MG-NB	-5.28	1.95	2.05
22	7	608	CLA	MG-NB	-5.28	1.95	2.05
22	8	602	CLA	MG-NB	-5.28	1.95	2.05
22	8	611	CLA	MG-NB	-5.28	1.95	2.05
22	B2	811	CLA	MG-NB	-5.27	1.95	2.05
22	5	604	CLA	MG-NB	-5.27	1.95	2.05
22	G	203	CLA	MG-NB	-5.27	1.95	2.05
22	9	609	CLA	MG-NB	-5.27	1.95	2.05
22	B	819	CLA	MG-NB	-5.27	1.95	2.05
22	B	809	CLA	MG-NB	-5.26	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	829	CLA	MG-NB	-5.26	1.95	2.05
22	B	838	CLA	MG-NB	-5.26	1.95	2.05
22	8	608	CLA	MG-NB	-5.26	1.95	2.05
22	B	839	CLA	MG-NB	-5.26	1.95	2.05
22	3	611	CLA	MG-NB	-5.26	1.95	2.05
22	Z	604	CLA	MG-NB	-5.26	1.95	2.05
22	A	826	CLA	MG-NB	-5.25	1.95	2.05
22	4	613	CLA	MG-NB	-5.25	1.95	2.05
22	4	614	CLA	MG-NB	-5.25	1.95	2.05
22	B	810	CLA	MG-NB	-5.25	1.95	2.05
22	92	604	CLA	MG-NB	-5.25	1.95	2.05
22	B2	828	CLA	C1D-ND	5.25	1.44	1.37
22	4	610	CLA	MG-NB	-5.24	1.95	2.05
22	6	603	CLA	MG-NB	-5.24	1.95	2.05
22	92	614	CLA	C1D-ND	5.24	1.44	1.37
22	5	610	CLA	MG-NB	-5.24	1.95	2.05
22	A	824	CLA	MG-NB	-5.24	1.95	2.05
22	A	802	CLA	MG-NB	-5.24	1.95	2.05
22	92	614	CLA	MG-NB	-5.24	1.95	2.05
22	A	840	CLA	MG-NB	-5.23	1.95	2.05
22	6	613	CLA	MG-NB	-5.23	1.95	2.05
22	K	206	CLA	MG-NB	-5.22	1.95	2.05
22	5	621	CLA	C1D-ND	5.22	1.44	1.37
22	L	204	CLA	C1D-ND	5.22	1.44	1.37
22	Z	603	CLA	MG-NB	-5.22	1.95	2.05
22	A	845	CLA	MG-NB	-5.21	1.95	2.05
22	7	611	CLA	MG-NB	-5.21	1.95	2.05
31	5	607	CHL	C3A-C2A	-5.21	1.50	1.54
22	K	204	CLA	MG-NB	-5.20	1.95	2.05
22	9	610	CLA	MG-NB	-5.20	1.95	2.05
22	7	613	CLA	MG-NB	-5.20	1.95	2.05
22	B2	810	CLA	MG-NB	-5.20	1.95	2.05
22	B	806	CLA	MG-NB	-5.20	1.95	2.05
22	5	614	CLA	MG-NB	-5.20	1.95	2.05
22	Z	611	CLA	MG-NB	-5.20	1.95	2.05
22	G	204	CLA	MG-NB	-5.20	1.95	2.05
22	K	201	CLA	MG-NB	-5.19	1.95	2.05
22	B2	804	CLA	C1D-ND	5.19	1.44	1.37
22	B2	813	CLA	MG-NB	-5.19	1.95	2.05
22	B2	808	CLA	C1D-ND	5.19	1.44	1.37
22	Z	610	CLA	MG-NB	-5.19	1.95	2.05
22	1	609	CLA	MG-NB	-5.18	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	301	CLA	MG-NB	-5.18	1.95	2.05
22	5	611	CLA	MG-NB	-5.18	1.95	2.05
22	7	602	CLA	MG-NB	-5.17	1.95	2.05
22	B2	813	CLA	C1D-ND	5.17	1.44	1.37
22	B	825	CLA	MG-NB	-5.17	1.95	2.05
22	4	616	CLA	MG-NB	-5.17	1.95	2.05
22	8	616	CLA	MG-NB	-5.17	1.95	2.05
22	B	811	CLA	MG-NB	-5.17	1.95	2.05
22	B2	815	CLA	C1D-ND	5.17	1.44	1.37
22	B	840	CLA	MG-NB	-5.17	1.95	2.05
22	7	620	CLA	MG-NB	-5.16	1.95	2.05
31	7	601	CHL	C3A-C2A	-5.16	1.50	1.54
22	8	614	CLA	MG-NB	-5.16	1.95	2.05
22	4	604	CLA	MG-NB	-5.16	1.95	2.05
22	5	613	CLA	MG-NB	-5.16	1.95	2.05
22	L2	203	CLA	MG-NB	-5.16	1.95	2.05
22	B	802	CLA	MG-NB	-5.15	1.95	2.05
22	A	841	CLA	MG-NB	-5.15	1.95	2.05
22	B2	814	CLA	MG-NB	-5.15	1.95	2.05
22	B2	805	CLA	C1D-ND	5.15	1.44	1.37
22	A	830	CLA	MG-NB	-5.15	1.95	2.05
22	6	604	CLA	MG-NB	-5.15	1.95	2.05
22	A	804	CLA	MG-NB	-5.14	1.95	2.05
22	5	616	CLA	MG-NB	-5.14	1.95	2.05
22	8	610	CLA	MG-NB	-5.14	1.95	2.05
22	B	813	CLA	MG-NB	-5.14	1.95	2.05
22	A	808	CLA	MG-NB	-5.14	1.95	2.05
22	Z	612	CLA	C1D-ND	5.14	1.44	1.37
22	3	607	CLA	MG-NB	-5.14	1.95	2.05
22	1	614	CLA	MG-NB	-5.13	1.95	2.05
22	B	817	CLA	MG-NB	-5.13	1.95	2.05
22	L2	204	CLA	MG-NB	-5.13	1.95	2.05
22	B	833	CLA	MG-NB	-5.13	1.95	2.05
22	Z	614	CLA	MG-NB	-5.13	1.95	2.05
22	A	842	CLA	MG-NB	-5.13	1.95	2.05
22	1	613	CLA	MG-NB	-5.12	1.95	2.05
22	B	826	CLA	MG-NB	-5.12	1.95	2.05
22	92	613	CLA	MG-NB	-5.12	1.95	2.05
22	A	806	CLA	MG-NB	-5.12	1.95	2.05
22	A	839	CLA	MG-NB	-5.12	1.95	2.05
22	A	835	CLA	MG-NB	-5.11	1.95	2.05
22	L	204	CLA	MG-NB	-5.11	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	827	CLA	MG-NB	-5.11	1.95	2.05
22	8	604	CLA	MG-NB	-5.11	1.95	2.05
22	6	614	CLA	C1D-ND	5.11	1.44	1.37
22	4	612	CLA	C1D-ND	5.10	1.44	1.37
22	92	609	CLA	MG-NB	-5.10	1.95	2.05
22	A	843	CLA	MG-NB	-5.10	1.95	2.05
22	3	617	CLA	MG-NB	-5.10	1.95	2.05
22	B2	829	CLA	MG-NB	-5.10	1.95	2.05
22	B2	806	CLA	MG-NB	-5.10	1.95	2.05
22	B2	828	CLA	MG-NB	-5.10	1.95	2.05
22	A	811	CLA	MG-NB	-5.08	1.95	2.05
22	A	818	CLA	MG-NB	-5.08	1.95	2.05
22	Z	613	CLA	MG-NB	-5.08	1.95	2.05
22	6	614	CLA	MG-NB	-5.08	1.95	2.05
22	B	836	CLA	MG-NB	-5.08	1.95	2.05
22	A	828	CLA	MG-NB	-5.07	1.95	2.05
22	5	621	CLA	MG-NB	-5.07	1.95	2.05
22	6	609	CLA	MG-NB	-5.07	1.95	2.05
22	A	820	CLA	MG-NB	-5.07	1.95	2.05
22	A	813	CLA	MG-NB	-5.05	1.95	2.05
22	K	203	CLA	C1D-ND	5.05	1.44	1.37
22	B	835	CLA	MG-NB	-5.05	1.95	2.05
22	5	601	CLA	MG-NB	-5.05	1.95	2.05
22	B2	809	CLA	C1D-ND	5.05	1.44	1.37
22	92	603	CLA	MG-NB	-5.05	1.95	2.05
22	B	814	CLA	MG-NB	-5.04	1.95	2.05
22	7	604	CLA	MG-NB	-5.04	1.95	2.05
22	F	303	CLA	MG-NB	-5.04	1.95	2.05
22	K	206	CLA	C1D-ND	5.04	1.44	1.37
22	B	805	CLA	MG-NB	-5.04	1.95	2.05
22	B2	805	CLA	MG-NB	-5.04	1.95	2.05
22	B2	829	CLA	C1D-ND	5.04	1.44	1.37
22	F	304	CLA	MG-NB	-5.03	1.95	2.05
22	B	815	CLA	MG-NB	-5.03	1.95	2.05
22	B	830	CLA	MG-NB	-5.03	1.95	2.05
22	6	612	CLA	MG-NB	-5.03	1.95	2.05
22	92	601	CLA	MG-NB	-5.03	1.95	2.05
22	4	603	CLA	C1D-ND	5.02	1.44	1.37
22	B2	808	CLA	MG-NB	-5.02	1.95	2.05
22	7	620	CLA	C1D-ND	5.02	1.44	1.37
22	B2	820	CLA	MG-NB	-5.02	1.95	2.05
31	5	608	CHL	C3A-C2A	-5.02	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	92	603	CLA	C1D-ND	5.01	1.44	1.37
22	B2	812	CLA	MG-NB	-5.01	1.95	2.05
22	6	612	CLA	C1D-ND	5.01	1.44	1.37
22	B2	804	CLA	MG-NB	-5.01	1.95	2.05
22	5	609	CLA	MG-NB	-5.01	1.95	2.05
31	3	608	CHL	C3A-C2A	-5.01	1.50	1.54
22	5	617	CLA	MG-NB	-5.00	1.95	2.05
22	G	204	CLA	C1D-ND	5.00	1.44	1.37
22	B	816	CLA	MG-NB	-5.00	1.95	2.05
22	9	604	CLA	MG-NB	-5.00	1.95	2.05
22	B	835	CLA	C1D-ND	4.99	1.44	1.37
22	B2	806	CLA	C1D-ND	4.99	1.44	1.37
22	5	612	CLA	MG-NB	-4.99	1.95	2.05
22	A	812	CLA	MG-NB	-4.99	1.95	2.05
22	A	814	CLA	MG-NB	-4.99	1.95	2.05
22	B	822	CLA	C1D-ND	4.98	1.44	1.37
22	5	601	CLA	C1D-ND	4.98	1.44	1.37
22	B	822	CLA	MG-NB	-4.98	1.95	2.05
22	5	612	CLA	C1D-ND	4.97	1.44	1.37
22	6	611	CLA	C1D-ND	4.97	1.44	1.37
22	8	612	CLA	C1D-ND	4.96	1.44	1.37
22	1	612	CLA	C1D-ND	4.96	1.44	1.37
22	K	201	CLA	C1D-ND	4.95	1.44	1.37
22	B2	815	CLA	MG-NB	-4.95	1.96	2.05
22	Z	603	CLA	C1D-ND	4.95	1.44	1.37
22	1	612	CLA	MG-NB	-4.95	1.96	2.05
22	J	101	CLA	C1D-ND	4.95	1.44	1.37
22	F	303	CLA	C1D-ND	4.95	1.44	1.37
22	9	601	CLA	C1D-ND	4.94	1.44	1.37
22	Z	609	CLA	C1D-ND	4.94	1.44	1.37
22	B2	810	CLA	C1D-ND	4.94	1.44	1.37
22	92	613	CLA	C1D-ND	4.94	1.44	1.37
22	B	828	CLA	MG-NB	-4.93	1.96	2.05
22	9	612	CLA	MG-NB	-4.93	1.96	2.05
22	9	603	CLA	C1D-ND	4.93	1.44	1.37
22	9	603	CLA	MG-NB	-4.93	1.96	2.05
22	B	832	CLA	MG-NB	-4.93	1.96	2.05
22	92	604	CLA	C1D-ND	4.92	1.44	1.37
22	4	616	CLA	C1D-ND	4.91	1.44	1.37
22	7	612	CLA	C1D-ND	4.91	1.44	1.37
22	Z	602	CLA	C1D-ND	4.91	1.44	1.37
22	A	816	CLA	MG-NB	-4.91	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	604	CLA	C1D-ND	4.90	1.44	1.37
22	8	608	CLA	C1D-ND	4.90	1.44	1.37
22	3	612	CLA	MG-NB	-4.90	1.96	2.05
22	A	832	CLA	MG-NB	-4.90	1.96	2.05
22	3	612	CLA	C1D-ND	4.89	1.44	1.37
22	5	614	CLA	C1D-ND	4.89	1.44	1.37
22	L2	204	CLA	C1D-ND	4.89	1.44	1.37
22	B2	807	CLA	C1D-ND	4.89	1.44	1.37
22	B	824	CLA	C1D-ND	4.89	1.44	1.37
22	A	809	CLA	MG-NB	-4.89	1.96	2.05
22	B	812	CLA	C1D-ND	4.89	1.44	1.37
22	9	612	CLA	C1D-ND	4.88	1.44	1.37
22	A	831	CLA	MG-NB	-4.88	1.96	2.05
22	B2	814	CLA	C1D-ND	4.88	1.44	1.37
22	B2	811	CLA	C1D-ND	4.88	1.44	1.37
22	A	826	CLA	C1D-ND	4.88	1.44	1.37
22	5	602	CLA	C1D-ND	4.87	1.44	1.37
22	92	612	CLA	MG-NB	-4.87	1.96	2.05
22	3	606	CLA	C1D-ND	4.86	1.44	1.37
22	8	603	CLA	C1D-ND	4.86	1.44	1.37
22	4	603	CLA	MG-NB	-4.86	1.96	2.05
22	8	611	CLA	C1D-ND	4.86	1.44	1.37
22	7	614	CLA	C1D-ND	4.86	1.44	1.37
22	92	601	CLA	C1D-ND	4.86	1.44	1.37
22	A	817	CLA	C1D-ND	4.86	1.44	1.37
22	5	613	CLA	C1D-ND	4.86	1.44	1.37
22	7	613	CLA	C1D-ND	4.85	1.44	1.37
22	F	304	CLA	C1D-ND	4.85	1.44	1.37
22	9	614	CLA	C1D-ND	4.85	1.44	1.37
22	3	615	CLA	C1D-ND	4.85	1.44	1.37
22	A	832	CLA	C1D-ND	4.84	1.44	1.37
22	6	622	CLA	C1D-ND	4.84	1.44	1.37
22	Z	616	CLA	C1D-ND	4.84	1.44	1.37
22	B	815	CLA	C1D-ND	4.83	1.44	1.37
22	B2	839	CLA	C1D-ND	4.83	1.44	1.37
22	A	838	CLA	MG-NB	-4.83	1.96	2.05
22	4	604	CLA	C1D-ND	4.83	1.44	1.37
22	4	611	CLA	C1D-ND	4.83	1.44	1.37
31	4	608	CHL	C3A-C2A	-4.82	1.50	1.54
22	7	611	CLA	C1D-ND	4.82	1.44	1.37
22	B	827	CLA	C1D-ND	4.81	1.44	1.37
22	Z	611	CLA	C1D-ND	4.81	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	614	CLA	C1D-ND	4.81	1.44	1.37
22	K	204	CLA	C1D-ND	4.81	1.44	1.37
22	A	819	CLA	C1D-ND	4.81	1.44	1.37
22	3	607	CLA	C1D-ND	4.81	1.44	1.37
22	7	602	CLA	C1D-ND	4.81	1.44	1.37
22	1	609	CLA	C1D-ND	4.81	1.44	1.37
22	4	612	CLA	MG-NB	-4.80	1.96	2.05
22	B	839	CLA	C1D-ND	4.80	1.44	1.37
22	7	612	CLA	MG-NB	-4.80	1.96	2.05
22	A	816	CLA	C1D-ND	4.80	1.44	1.37
22	4	614	CLA	C1D-ND	4.80	1.44	1.37
31	1	606	CHL	C3A-C2A	-4.80	1.50	1.54
22	92	612	CLA	C1D-ND	4.80	1.44	1.37
22	A	845	CLA	C1D-ND	4.80	1.44	1.37
22	6	613	CLA	C1D-ND	4.80	1.44	1.37
22	9	604	CLA	C1D-ND	4.79	1.44	1.37
31	6	608	CHL	C3A-C2A	-4.79	1.50	1.54
22	B	808	CLA	MG-NB	-4.79	1.96	2.05
22	8	602	CLA	C1D-ND	4.79	1.44	1.37
22	5	616	CLA	C1D-ND	4.79	1.44	1.37
22	A	835	CLA	C1D-ND	4.79	1.44	1.37
22	3	613	CLA	C1D-ND	4.78	1.44	1.37
22	4	613	CLA	C1D-ND	4.78	1.44	1.37
31	9	607	CHL	C3A-C2A	-4.78	1.50	1.54
22	B	832	CLA	C1D-ND	4.78	1.44	1.37
22	A	803	CLA	MG-ND	-4.78	1.96	2.05
22	B2	812	CLA	C1D-ND	4.77	1.44	1.37
22	1	614	CLA	C1D-ND	4.77	1.44	1.37
22	A	828	CLA	C1D-ND	4.77	1.44	1.37
22	B	808	CLA	C1D-ND	4.77	1.44	1.37
22	6	617	CLA	C1D-ND	4.77	1.44	1.37
22	1	611	CLA	C1D-ND	4.76	1.44	1.37
22	A	814	CLA	C1D-ND	4.76	1.44	1.37
22	5	617	CLA	C1D-ND	4.76	1.44	1.37
22	5	604	CLA	C1D-ND	4.75	1.44	1.37
22	8	612	CLA	MG-NB	-4.75	1.96	2.05
22	A	831	CLA	C1D-ND	4.75	1.44	1.37
22	1	608	CLA	C1D-ND	4.75	1.44	1.37
22	Z	604	CLA	C1D-ND	4.75	1.44	1.37
22	B	809	CLA	C1D-ND	4.75	1.44	1.37
22	5	603	CLA	C1D-ND	4.75	1.44	1.37
22	G	203	CLA	C1D-ND	4.74	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	603	CLA	C1D-ND	4.74	1.44	1.37
22	8	613	CLA	C1D-ND	4.74	1.44	1.37
22	A	839	CLA	C1D-ND	4.74	1.44	1.37
22	3	614	CLA	C1D-ND	4.74	1.44	1.37
22	9	609	CLA	C1D-ND	4.73	1.44	1.37
22	L2	203	CLA	C1D-ND	4.73	1.44	1.37
22	A	815	CLA	C1D-ND	4.73	1.44	1.37
22	B	804	CLA	C1D-ND	4.72	1.44	1.37
22	B	841	CLA	C1D-ND	4.72	1.44	1.37
22	3	611	CLA	C1D-ND	4.72	1.44	1.37
22	A	825	CLA	C1D-ND	4.72	1.44	1.37
22	A	830	CLA	C1D-ND	4.71	1.44	1.37
22	A	840	CLA	C1D-ND	4.71	1.44	1.37
22	8	604	CLA	C1D-ND	4.71	1.44	1.37
22	92	611	CLA	C1D-ND	4.71	1.44	1.37
31	8	606	CHL	C3A-C2A	-4.71	1.50	1.54
22	Z	613	CLA	C1D-ND	4.70	1.44	1.37
22	4	610	CLA	C1D-ND	4.70	1.44	1.37
22	A	803	CLA	C1D-ND	4.70	1.44	1.37
22	A	838	CLA	C1D-ND	4.70	1.44	1.37
22	8	614	CLA	C1D-ND	4.69	1.44	1.37
22	6	602	CLA	C1D-ND	4.69	1.44	1.37
22	B	838	CLA	C1D-ND	4.69	1.44	1.37
22	6	603	CLA	C1D-ND	4.69	1.44	1.37
22	B	820	CLA	C1D-ND	4.69	1.44	1.37
31	5	607	CHL	CHB-C4A	-4.68	1.33	1.38
22	B	836	CLA	C1D-ND	4.68	1.44	1.37
22	A	854	CLA	C1D-ND	4.68	1.44	1.37
22	A	829	CLA	C1D-ND	4.68	1.44	1.37
22	6	610	CLA	C1D-ND	4.68	1.44	1.37
22	92	609	CLA	C1D-ND	4.67	1.44	1.37
31	6	616	CHL	C3A-C2A	-4.67	1.50	1.54
22	A	833	CLA	C1D-ND	4.67	1.44	1.37
22	3	604	CLA	C1D-ND	4.67	1.44	1.37
22	4	609	CLA	C1D-ND	4.66	1.44	1.37
31	9	607	CHL	CHB-C4A	-4.66	1.33	1.38
22	A	837	CLA	MG-ND	-4.65	1.96	2.05
22	B	811	CLA	C1D-ND	4.65	1.44	1.37
22	3	617	CLA	C1D-ND	4.65	1.44	1.37
22	Z	610	CLA	C1D-ND	4.65	1.44	1.37
31	7	606	CHL	CHB-C4A	-4.65	1.33	1.38
22	8	609	CLA	C1D-ND	4.65	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	201	CLA	MG-ND	-4.65	1.96	2.05
22	4	602	CLA	C1D-ND	4.65	1.44	1.37
22	1	604	CLA	C1D-ND	4.64	1.44	1.37
22	5	609	CLA	C1D-ND	4.64	1.44	1.37
22	Z	612	CLA	MG-NB	-4.64	1.96	2.05
22	B	837	CLA	C1D-ND	4.64	1.44	1.37
22	A	808	CLA	C1D-ND	4.64	1.44	1.37
22	B	821	CLA	MG-ND	-4.63	1.96	2.05
22	A	810	CLA	MG-ND	-4.63	1.96	2.05
22	7	603	CLA	C1D-ND	4.63	1.43	1.37
22	A	821	CLA	C1D-ND	4.63	1.43	1.37
22	9	602	CLA	C1D-ND	4.63	1.43	1.37
31	6	616	CHL	CHB-C4A	-4.62	1.33	1.38
22	B	816	CLA	C1D-ND	4.62	1.43	1.37
22	7	604	CLA	C1D-ND	4.62	1.43	1.37
22	7	608	CLA	C1D-ND	4.62	1.43	1.37
22	1	613	CLA	C1D-ND	4.61	1.43	1.37
22	5	611	CLA	C1D-ND	4.61	1.43	1.37
22	A	805	CLA	C1D-ND	4.60	1.43	1.37
21	A	801	CL0	MG-ND	-4.60	1.96	2.05
22	A	837	CLA	C1D-ND	4.60	1.43	1.37
22	B	813	CLA	C1D-ND	4.60	1.43	1.37
22	B	810	CLA	C1D-ND	4.60	1.43	1.37
22	A	804	CLA	C1D-ND	4.60	1.43	1.37
22	A	843	CLA	C1D-ND	4.60	1.43	1.37
22	1	616	CLA	C1D-ND	4.60	1.43	1.37
22	7	610	CLA	MG-ND	-4.59	1.96	2.05
22	A	813	CLA	C1D-ND	4.59	1.43	1.37
22	A	834	CLA	C1D-ND	4.58	1.43	1.37
22	7	609	CLA	C1D-ND	4.58	1.43	1.37
22	B	828	CLA	C1D-ND	4.57	1.43	1.37
22	Z	608	CLA	C1D-ND	4.57	1.43	1.37
22	A	818	CLA	C1D-ND	4.57	1.43	1.37
22	B	814	CLA	C1D-ND	4.57	1.43	1.37
31	4	606	CHL	CHB-C4A	-4.57	1.33	1.38
31	Z	607	CHL	CHB-C4A	-4.57	1.33	1.38
22	B	838	CLA	MG-ND	-4.57	1.96	2.05
22	7	616	CLA	C1D-ND	4.55	1.43	1.37
22	B	807	CLA	C1D-ND	4.55	1.43	1.37
31	1	606	CHL	CHB-C4A	-4.55	1.33	1.38
22	A	841	CLA	C1D-ND	4.55	1.43	1.37
22	9	610	CLA	C1D-ND	4.55	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	613	CLA	C1D-ND	4.55	1.43	1.37
22	B	826	CLA	C1D-ND	4.55	1.43	1.37
22	B	819	CLA	C1D-ND	4.54	1.43	1.37
22	6	609	CLA	C1D-ND	4.54	1.43	1.37
22	A	807	CLA	C1D-ND	4.54	1.43	1.37
22	5	621	CLA	MG-ND	-4.54	1.96	2.05
31	6	606	CHL	CHB-C4A	-4.54	1.33	1.38
22	A	820	CLA	C1D-ND	4.54	1.43	1.37
22	A	836	CLA	C1D-ND	4.53	1.43	1.37
22	A	854	CLA	MG-ND	-4.53	1.96	2.05
22	9	611	CLA	C1D-ND	4.53	1.43	1.37
22	A	812	CLA	C1D-ND	4.52	1.43	1.37
31	92	606	CHL	C2A-C3A	-4.52	1.51	1.54
22	92	602	CLA	C1D-ND	4.52	1.43	1.37
31	7	607	CHL	C3A-C2A	-4.51	1.50	1.54
22	3	602	CLA	C1D-ND	4.51	1.43	1.37
31	6	607	CHL	CHB-C4A	-4.51	1.33	1.38
22	B	802	CLA	C1D-ND	4.51	1.43	1.37
22	A	827	CLA	C1D-ND	4.51	1.43	1.37
31	4	607	CHL	C3A-C2A	-4.50	1.50	1.54
22	A	823	CLA	MG-ND	-4.50	1.96	2.05
22	B	803	CLA	MG-ND	-4.50	1.96	2.05
22	1	616	CLA	MG-ND	-4.50	1.96	2.05
22	B	834	CLA	C1D-ND	4.50	1.43	1.37
22	A	811	CLA	C1D-ND	4.50	1.43	1.37
22	A	822	CLA	C1D-ND	4.50	1.43	1.37
31	8	607	CHL	CHB-C4A	-4.49	1.33	1.38
31	6	608	CHL	CHB-C4A	-4.49	1.33	1.38
22	A	809	CLA	C1D-ND	4.48	1.43	1.37
22	8	616	CLA	C1D-ND	4.48	1.43	1.37
22	5	610	CLA	C1D-ND	4.48	1.43	1.37
22	B	805	CLA	C1D-ND	4.47	1.43	1.37
22	A	824	CLA	C1D-ND	4.47	1.43	1.37
22	A	829	CLA	MG-ND	-4.46	1.96	2.05
22	B	806	CLA	C1D-ND	4.46	1.43	1.37
22	A	825	CLA	MG-ND	-4.46	1.96	2.05
22	B	818	CLA	C1D-ND	4.46	1.43	1.37
22	1	602	CLA	C1D-ND	4.46	1.43	1.37
22	A	833	CLA	MG-ND	-4.46	1.96	2.05
22	A	842	CLA	C1D-ND	4.46	1.43	1.37
22	8	610	CLA	C1D-ND	4.46	1.43	1.37
22	7	609	CLA	MG-ND	-4.45	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	607	CHL	CHB-C4A	-4.45	1.33	1.38
31	6	618	CHL	CHB-C4A	-4.45	1.33	1.38
22	B	830	CLA	C1D-ND	4.44	1.43	1.37
31	5	606	CHL	CHB-C4A	-4.44	1.33	1.38
22	L	203	CLA	C1D-ND	4.43	1.43	1.37
31	4	601	CHL	C3A-C2A	-4.43	1.50	1.54
22	B	839	CLA	MG-ND	-4.43	1.97	2.05
31	7	601	CHL	CHB-C4A	-4.43	1.33	1.38
22	A	810	CLA	C1D-ND	4.42	1.43	1.37
22	92	610	CLA	MG-ND	-4.42	1.97	2.05
31	5	608	CHL	CHB-C4A	-4.42	1.33	1.38
22	7	610	CLA	C1D-ND	4.42	1.43	1.37
22	B	807	CLA	MG-ND	-4.42	1.97	2.05
22	B	821	CLA	C1D-ND	4.41	1.43	1.37
22	92	610	CLA	C1D-ND	4.41	1.43	1.37
22	B	831	CLA	C1D-ND	4.41	1.43	1.37
22	7	608	CLA	MG-ND	-4.41	1.97	2.05
22	7	614	CLA	MG-ND	-4.41	1.97	2.05
22	B	833	CLA	C1D-ND	4.41	1.43	1.37
22	B	806	CLA	MG-ND	-4.41	1.97	2.05
22	4	602	CLA	MG-ND	-4.41	1.97	2.05
22	1	610	CLA	C1D-ND	4.41	1.43	1.37
31	4	607	CHL	CHB-C4A	-4.41	1.33	1.38
22	Z	608	CLA	MG-ND	-4.40	1.97	2.05
22	3	617	CLA	MG-ND	-4.40	1.97	2.05
22	A	802	CLA	MG-ND	-4.40	1.97	2.05
31	6	618	CHL	C3A-C2A	-4.40	1.50	1.54
22	A	843	CLA	MG-ND	-4.39	1.97	2.05
31	8	606	CHL	CHB-C4A	-4.39	1.33	1.38
22	8	611	CLA	MG-ND	-4.38	1.97	2.05
22	Z	609	CLA	MG-ND	-4.37	1.97	2.05
31	4	606	CHL	C3A-C2A	-4.37	1.50	1.54
22	B	812	CLA	MG-ND	-4.37	1.97	2.05
22	3	610	CLA	C1D-ND	4.37	1.43	1.37
22	A	819	CLA	MG-ND	-4.36	1.97	2.05
31	6	606	CHL	C3A-C2A	-4.36	1.50	1.54
22	3	609	CLA	C1D-ND	4.36	1.43	1.37
22	4	613	CLA	MG-ND	-4.36	1.97	2.05
31	1	607	CHL	C3A-C2A	-4.36	1.50	1.54
22	1	611	CLA	MG-ND	-4.36	1.97	2.05
31	5	618	CHL	CHB-C4A	-4.36	1.33	1.38
22	A	824	CLA	MG-ND	-4.36	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	602	CLA	MG-ND	-4.35	1.97	2.05
22	B	819	CLA	MG-ND	-4.35	1.97	2.05
22	F	301	CLA	C1D-ND	4.35	1.43	1.37
22	92	609	CLA	MG-ND	-4.35	1.97	2.05
22	A	806	CLA	C1D-ND	4.35	1.43	1.37
22	B	840	CLA	C1D-ND	4.35	1.43	1.37
22	3	603	CLA	C1D-ND	4.35	1.43	1.37
22	1	608	CLA	MG-ND	-4.34	1.97	2.05
22	Z	616	CLA	MG-ND	-4.34	1.97	2.05
22	G	203	CLA	MG-ND	-4.34	1.97	2.05
22	B	820	CLA	MG-ND	-4.34	1.97	2.05
22	3	603	CLA	MG-ND	-4.33	1.97	2.05
22	8	603	CLA	MG-ND	-4.33	1.97	2.05
22	92	602	CLA	MG-ND	-4.33	1.97	2.05
22	B	833	CLA	MG-ND	-4.33	1.97	2.05
31	4	608	CHL	CHB-C4A	-4.33	1.33	1.38
22	B	829	CLA	MG-ND	-4.33	1.97	2.05
22	B	823	CLA	MG-ND	-4.32	1.97	2.05
22	A	836	CLA	MG-ND	-4.32	1.97	2.05
22	4	611	CLA	MG-ND	-4.32	1.97	2.05
22	A	823	CLA	C1D-ND	4.32	1.43	1.37
22	A	807	CLA	MG-ND	-4.32	1.97	2.05
31	9	606	CHL	C2A-C3A	-4.32	1.51	1.54
31	9	606	CHL	CHB-C4A	-4.32	1.33	1.38
22	7	611	CLA	MG-ND	-4.32	1.97	2.05
22	3	611	CLA	MG-ND	-4.32	1.97	2.05
22	B	817	CLA	C1D-ND	4.32	1.43	1.37
22	9	602	CLA	MG-ND	-4.31	1.97	2.05
22	B	809	CLA	MG-ND	-4.31	1.97	2.05
22	A	817	CLA	MG-ND	-4.31	1.97	2.05
22	8	604	CLA	MG-ND	-4.31	1.97	2.05
22	9	613	CLA	MG-ND	-4.31	1.97	2.05
22	A	813	CLA	MG-ND	-4.31	1.97	2.05
22	8	602	CLA	MG-ND	-4.31	1.97	2.05
22	3	609	CLA	MG-ND	-4.30	1.97	2.05
22	A	808	CLA	MG-ND	-4.30	1.97	2.05
22	6	617	CLA	MG-ND	-4.30	1.97	2.05
22	5	611	CLA	MG-ND	-4.30	1.97	2.05
22	B	825	CLA	C1D-ND	4.30	1.43	1.37
22	B	813	CLA	MG-ND	-4.30	1.97	2.05
22	4	609	CLA	MG-ND	-4.30	1.97	2.05
22	92	611	CLA	MG-ND	-4.30	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	613	CLA	MG-ND	-4.29	1.97	2.05
22	L	203	CLA	MG-ND	-4.29	1.97	2.05
22	3	615	CLA	MG-ND	-4.29	1.97	2.05
22	8	609	CLA	MG-ND	-4.29	1.97	2.05
22	3	613	CLA	MG-ND	-4.29	1.97	2.05
22	9	611	CLA	MG-ND	-4.29	1.97	2.05
31	3	608	CHL	CHB-C4A	-4.29	1.33	1.38
22	A	828	CLA	MG-ND	-4.28	1.97	2.05
22	5	602	CLA	MG-ND	-4.28	1.97	2.05
22	A	815	CLA	MG-ND	-4.28	1.97	2.05
22	9	601	CLA	MG-ND	-4.28	1.97	2.05
22	A	805	CLA	MG-ND	-4.28	1.97	2.05
22	B	815	CLA	MG-ND	-4.28	1.97	2.05
22	3	607	CLA	MG-ND	-4.27	1.97	2.05
22	1	614	CLA	MG-ND	-4.27	1.97	2.05
22	4	616	CLA	MG-ND	-4.27	1.97	2.05
22	1	604	CLA	MG-ND	-4.27	1.97	2.05
22	6	613	CLA	MG-ND	-4.27	1.97	2.05
22	1	603	CLA	MG-ND	-4.27	1.97	2.05
22	B	834	CLA	MG-ND	-4.26	1.97	2.05
22	4	604	CLA	MG-ND	-4.26	1.97	2.05
22	L2	203	CLA	MG-ND	-4.26	1.97	2.05
22	J	101	CLA	MG-ND	-4.26	1.97	2.05
22	4	614	CLA	MG-ND	-4.26	1.97	2.05
22	4	603	CLA	MG-ND	-4.26	1.97	2.05
22	A	826	CLA	MG-ND	-4.25	1.97	2.05
22	5	601	CLA	MG-ND	-4.25	1.97	2.05
22	B2	829	CLA	MG-ND	-4.25	1.97	2.05
22	6	603	CLA	MG-ND	-4.25	1.97	2.05
22	9	614	CLA	MG-ND	-4.25	1.97	2.05
22	5	604	CLA	MG-ND	-4.25	1.97	2.05
22	6	622	CLA	MG-ND	-4.25	1.97	2.05
22	B	826	CLA	MG-ND	-4.25	1.97	2.05
22	92	603	CLA	MG-ND	-4.25	1.97	2.05
22	Z	613	CLA	MG-ND	-4.24	1.97	2.05
22	B	830	CLA	MG-ND	-4.24	1.97	2.05
22	92	601	CLA	MG-ND	-4.24	1.97	2.05
22	B2	807	CLA	MG-ND	-4.24	1.97	2.05
22	92	604	CLA	MG-ND	-4.24	1.97	2.05
22	B	817	CLA	MG-ND	-4.24	1.97	2.05
22	B2	810	CLA	MG-ND	-4.24	1.97	2.05
22	B2	839	CLA	MG-ND	-4.23	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	814	CLA	MG-ND	-4.23	1.97	2.05
22	1	610	CLA	MG-ND	-4.23	1.97	2.05
22	A	845	CLA	MG-ND	-4.23	1.97	2.05
22	K	203	CLA	MG-ND	-4.22	1.97	2.05
31	6	607	CHL	C3A-C2A	-4.22	1.51	1.54
22	7	612	CLA	MG-ND	-4.22	1.97	2.05
22	A	821	CLA	MG-ND	-4.22	1.97	2.05
22	3	606	CLA	MG-ND	-4.22	1.97	2.05
22	Z	610	CLA	MG-ND	-4.22	1.97	2.05
22	A	839	CLA	MG-ND	-4.22	1.97	2.05
22	A	822	CLA	MG-ND	-4.22	1.97	2.05
22	Z	603	CLA	MG-ND	-4.22	1.97	2.05
22	8	610	CLA	MG-ND	-4.21	1.97	2.05
22	6	604	CLA	MG-ND	-4.21	1.97	2.05
22	B	837	CLA	MG-ND	-4.21	1.97	2.05
22	3	610	CLA	MG-ND	-4.21	1.97	2.05
22	7	616	CLA	MG-ND	-4.21	1.97	2.05
22	4	612	CLA	MG-ND	-4.20	1.97	2.05
22	5	616	CLA	MG-ND	-4.20	1.97	2.05
22	B	841	CLA	MG-ND	-4.20	1.97	2.05
22	6	611	CLA	MG-ND	-4.20	1.97	2.05
22	A	831	CLA	MG-ND	-4.20	1.97	2.05
31	Z	607	CHL	C3A-C2A	-4.20	1.51	1.54
22	B2	812	CLA	MG-ND	-4.19	1.97	2.05
22	1	613	CLA	MG-ND	-4.19	1.97	2.05
22	A	818	CLA	MG-ND	-4.19	1.97	2.05
22	5	617	CLA	MG-ND	-4.19	1.97	2.05
22	B	818	CLA	MG-ND	-4.19	1.97	2.05
22	B	824	CLA	MG-ND	-4.19	1.97	2.05
22	B2	814	CLA	MG-ND	-4.18	1.97	2.05
31	5	606	CHL	C3A-C2A	-4.18	1.51	1.54
22	B2	809	CLA	MG-ND	-4.18	1.97	2.05
22	6	610	CLA	MG-ND	-4.18	1.97	2.05
22	92	612	CLA	MG-ND	-4.18	1.97	2.05
22	B	835	CLA	MG-ND	-4.18	1.97	2.05
22	K	206	CLA	MG-ND	-4.18	1.97	2.05
22	A	834	CLA	MG-ND	-4.18	1.97	2.05
22	B	825	CLA	MG-ND	-4.18	1.97	2.05
22	Z	614	CLA	MG-ND	-4.18	1.97	2.05
31	5	607	CHL	C1A-CHA	-4.18	1.35	1.40
22	1	609	CLA	MG-ND	-4.18	1.97	2.05
31	7	607	CHL	CHB-C4A	-4.18	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	803	CLA	C1D-ND	4.18	1.43	1.37
22	B	828	CLA	MG-ND	-4.18	1.97	2.05
22	3	604	CLA	MG-ND	-4.18	1.97	2.05
22	A	832	CLA	MG-ND	-4.18	1.97	2.05
22	3	614	CLA	MG-ND	-4.18	1.97	2.05
22	F	303	CLA	MG-ND	-4.17	1.97	2.05
22	6	609	CLA	MG-ND	-4.17	1.97	2.05
22	B	811	CLA	MG-ND	-4.17	1.97	2.05
31	4	618	CHL	CHB-C4A	-4.17	1.33	1.38
31	5	618	CHL	C3A-C2A	-4.17	1.51	1.54
22	B	810	CLA	MG-ND	-4.17	1.97	2.05
22	9	609	CLA	MG-ND	-4.17	1.97	2.05
22	5	610	CLA	MG-ND	-4.17	1.97	2.05
22	3	602	CLA	MG-ND	-4.16	1.97	2.05
22	Z	602	CLA	MG-ND	-4.16	1.97	2.05
31	92	607	CHL	CHB-C4A	-4.16	1.33	1.38
22	B	832	CLA	MG-ND	-4.16	1.97	2.05
22	8	614	CLA	MG-ND	-4.16	1.97	2.05
22	5	614	CLA	MG-ND	-4.16	1.97	2.05
22	B	816	CLA	MG-ND	-4.16	1.97	2.05
22	F	304	CLA	MG-ND	-4.15	1.97	2.05
22	A	816	CLA	MG-ND	-4.15	1.97	2.05
22	K	204	CLA	MG-ND	-4.15	1.97	2.05
22	7	604	CLA	MG-ND	-4.15	1.97	2.05
22	9	604	CLA	MG-ND	-4.15	1.97	2.05
22	B2	806	CLA	MG-ND	-4.15	1.97	2.05
22	7	603	CLA	MG-ND	-4.14	1.97	2.05
22	A	804	CLA	MG-ND	-4.14	1.97	2.05
22	3	612	CLA	MG-ND	-4.14	1.97	2.05
22	6	602	CLA	MG-ND	-4.14	1.97	2.05
22	Z	611	CLA	MG-ND	-4.14	1.97	2.05
22	9	612	CLA	MG-ND	-4.14	1.97	2.05
22	7	620	CLA	MG-ND	-4.14	1.97	2.05
22	92	613	CLA	MG-ND	-4.14	1.97	2.05
22	7	602	CLA	MG-ND	-4.14	1.97	2.05
22	9	610	CLA	MG-ND	-4.14	1.97	2.05
22	B	831	CLA	MG-ND	-4.14	1.97	2.05
22	B2	813	CLA	MG-ND	-4.13	1.97	2.05
22	A	811	CLA	MG-ND	-4.13	1.97	2.05
22	5	609	CLA	MG-ND	-4.13	1.97	2.05
22	A	827	CLA	MG-ND	-4.13	1.97	2.05
22	A	840	CLA	MG-ND	-4.13	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	604	CLA	MG-ND	-4.13	1.97	2.05
22	B	822	CLA	MG-ND	-4.12	1.97	2.05
22	A	820	CLA	MG-ND	-4.12	1.97	2.05
22	B	804	CLA	MG-ND	-4.12	1.97	2.05
22	L2	204	CLA	MG-ND	-4.12	1.97	2.05
22	A	841	CLA	MG-ND	-4.12	1.97	2.05
22	A	830	CLA	MG-ND	-4.12	1.97	2.05
22	5	613	CLA	MG-ND	-4.12	1.97	2.05
22	B	814	CLA	MG-ND	-4.11	1.97	2.05
22	A	802	CLA	C1D-ND	4.11	1.43	1.37
22	4	610	CLA	MG-ND	-4.11	1.97	2.05
31	6	601	CHL	CHB-C4A	-4.11	1.33	1.38
22	A	842	CLA	MG-ND	-4.11	1.97	2.05
22	G	204	CLA	MG-ND	-4.11	1.97	2.05
31	1	601	CHL	CHB-C4A	-4.11	1.33	1.38
22	B	836	CLA	MG-ND	-4.11	1.97	2.05
22	B2	815	CLA	MG-ND	-4.11	1.97	2.05
31	4	607	CHL	C1A-CHA	-4.10	1.35	1.40
31	92	606	CHL	CHB-C4A	-4.10	1.33	1.38
22	5	612	CLA	MG-ND	-4.10	1.97	2.05
22	B	829	CLA	C1D-ND	4.10	1.43	1.37
22	A	838	CLA	MG-ND	-4.09	1.97	2.05
22	B2	811	CLA	MG-ND	-4.09	1.97	2.05
31	1	601	CHL	C1A-CHA	-4.09	1.35	1.40
31	6	608	CHL	C1A-CHA	-4.09	1.35	1.40
22	1	612	CLA	MG-ND	-4.09	1.97	2.05
22	8	608	CLA	MG-ND	-4.09	1.97	2.05
22	B	823	CLA	C1D-ND	4.09	1.43	1.37
31	8	606	CHL	C1A-CHA	-4.09	1.35	1.40
22	8	613	CLA	MG-ND	-4.08	1.97	2.05
22	8	616	CLA	MG-ND	-4.08	1.97	2.05
22	A	812	CLA	MG-ND	-4.07	1.97	2.05
22	A	835	CLA	MG-ND	-4.07	1.97	2.05
22	A	806	CLA	MG-ND	-4.07	1.97	2.05
31	9	607	CHL	C1A-CHA	-4.07	1.35	1.40
31	4	618	CHL	C3A-C2A	-4.06	1.51	1.54
22	A	809	CLA	MG-ND	-4.06	1.97	2.05
22	6	612	CLA	MG-ND	-4.06	1.97	2.05
31	5	608	CHL	C1A-CHA	-4.06	1.35	1.40
22	9	603	CLA	MG-ND	-4.05	1.97	2.05
22	B	808	CLA	MG-ND	-4.05	1.97	2.05
22	B2	828	CLA	MG-ND	-4.05	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	607	CHL	C1A-CHA	-4.04	1.35	1.40
22	B	805	CLA	MG-ND	-4.03	1.97	2.05
31	92	607	CHL	C1A-CHA	-4.03	1.35	1.40
31	6	618	CHL	C1A-CHA	-4.02	1.35	1.40
22	92	614	CLA	MG-ND	-4.02	1.97	2.05
31	5	618	CHL	C1A-CHA	-4.02	1.35	1.40
22	6	614	CLA	MG-ND	-4.02	1.97	2.05
31	3	608	CHL	C1A-CHA	-4.01	1.35	1.40
31	7	606	CHL	C1A-CHA	-4.01	1.35	1.40
22	F	301	CLA	MG-ND	-4.01	1.97	2.05
22	B2	805	CLA	MG-ND	-4.01	1.97	2.05
31	4	608	CHL	C1A-CHA	-4.01	1.35	1.40
31	5	606	CHL	C1A-CHA	-4.00	1.35	1.40
22	B2	808	CLA	MG-ND	-4.00	1.97	2.05
31	6	616	CHL	C1A-CHA	-3.99	1.35	1.40
31	4	606	CHL	C1A-CHA	-3.99	1.35	1.40
22	L	204	CLA	MG-ND	-3.99	1.97	2.05
22	5	603	CLA	MG-ND	-3.99	1.97	2.05
31	9	606	CHL	C1A-CHA	-3.98	1.35	1.40
31	6	606	CHL	C1A-CHA	-3.98	1.35	1.40
31	Z	606	CHL	C1A-CHA	-3.97	1.35	1.40
31	8	601	CHL	CHB-C4A	-3.97	1.33	1.38
22	B	827	CLA	MG-ND	-3.97	1.97	2.05
31	7	601	CHL	C1A-CHA	-3.96	1.35	1.40
31	Z	607	CHL	C1A-CHA	-3.96	1.35	1.40
31	8	601	CHL	C1A-CHA	-3.96	1.35	1.40
22	B2	820	CLA	MG-ND	-3.96	1.97	2.05
31	1	607	CHL	C1A-CHA	-3.96	1.35	1.40
31	7	607	CHL	C1A-CHA	-3.94	1.35	1.40
31	7	606	CHL	C3A-C2A	-3.93	1.51	1.54
22	Z	612	CLA	MG-ND	-3.93	1.98	2.05
31	4	601	CHL	C1A-CHA	-3.93	1.35	1.40
31	Z	601	CHL	C1A-CHA	-3.92	1.35	1.40
31	92	606	CHL	C1A-CHA	-3.92	1.35	1.40
31	Z	606	CHL	CHB-C4A	-3.90	1.33	1.38
22	B	840	CLA	MG-ND	-3.90	1.98	2.05
31	1	606	CHL	C1A-CHA	-3.90	1.35	1.40
31	4	618	CHL	C1A-CHA	-3.90	1.35	1.40
21	A	801	CL0	C1A-CHA	-3.89	1.35	1.40
22	8	612	CLA	MG-ND	-3.88	1.98	2.05
22	B2	804	CLA	MG-ND	-3.87	1.98	2.05
31	4	601	CHL	CHB-C4A	-3.86	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	802	CLA	MG-ND	-3.85	1.98	2.05
31	6	601	CHL	C1A-CHA	-3.82	1.35	1.40
31	Z	601	CHL	C3A-C2A	-3.80	1.51	1.54
31	Z	601	CHL	CHB-C4A	-3.77	1.34	1.38
31	8	607	CHL	C1A-CHA	-3.69	1.35	1.40
31	92	607	CHL	C3A-C2A	-3.63	1.51	1.54
31	6	608	CHL	C3B-C4B	3.58	1.44	1.41
31	6	616	CHL	C3B-C4B	3.54	1.44	1.41
31	1	601	CHL	C3A-C2A	-3.54	1.51	1.54
31	4	606	CHL	C3B-C4B	3.52	1.44	1.41
31	Z	606	CHL	C3A-C2A	-3.52	1.51	1.54
31	1	606	CHL	C3B-C4B	3.51	1.44	1.41
31	6	606	CHL	C3B-C4B	3.50	1.44	1.41
31	7	606	CHL	C3B-C4B	3.50	1.44	1.41
31	5	618	CHL	C3B-C4B	3.49	1.44	1.41
31	4	608	CHL	C3B-C4B	3.49	1.44	1.41
31	6	618	CHL	C3B-C4B	3.48	1.44	1.41
31	9	606	CHL	C3B-C4B	3.48	1.44	1.41
31	92	606	CHL	C3B-C4B	3.46	1.44	1.41
31	6	601	CHL	C3B-C4B	3.46	1.44	1.41
31	4	618	CHL	C3B-C4B	3.46	1.44	1.41
31	5	607	CHL	C3B-C4B	3.46	1.44	1.41
31	5	608	CHL	C3B-C4B	3.45	1.44	1.41
31	4	601	CHL	C3B-C4B	3.44	1.44	1.41
31	3	608	CHL	C3B-C4B	3.41	1.44	1.41
31	8	601	CHL	C3A-C2A	-3.41	1.51	1.54
31	Z	607	CHL	C3B-C4B	3.39	1.44	1.41
31	6	607	CHL	C3B-C4B	3.38	1.44	1.41
31	8	601	CHL	C3B-C4B	3.37	1.44	1.41
31	8	607	CHL	C3A-C2A	-3.32	1.51	1.54
31	92	607	CHL	C3B-C4B	3.31	1.44	1.41
31	8	606	CHL	C3B-C4B	3.31	1.44	1.41
31	Z	606	CHL	C3B-C4B	3.30	1.44	1.41
31	1	607	CHL	C3B-C4B	3.30	1.44	1.41
25	B2	843	BCR	C17-C18	3.29	1.36	1.33
31	5	606	CHL	C3B-C2B	-3.29	1.35	1.40
31	9	607	CHL	C3B-C4B	3.27	1.44	1.41
31	1	601	CHL	C3B-C2B	-3.25	1.36	1.40
31	8	607	CHL	C3B-C4B	3.25	1.44	1.41
31	8	607	CHL	C3B-C2B	-3.24	1.36	1.40
31	7	601	CHL	C3B-C4B	3.22	1.44	1.41
31	9	607	CHL	C3B-C2B	-3.22	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	606	CHL	C3B-C2B	-3.22	1.36	1.40
31	5	606	CHL	C3B-C4B	3.22	1.44	1.41
31	4	607	CHL	C3B-C4B	3.21	1.44	1.41
31	7	607	CHL	C3B-C4B	3.20	1.44	1.41
31	Z	607	CHL	C3B-C2B	-3.20	1.36	1.40
31	1	607	CHL	C3B-C2B	-3.20	1.36	1.40
31	1	606	CHL	C3B-C2B	-3.18	1.36	1.40
31	7	607	CHL	C3B-C2B	-3.18	1.36	1.40
31	Z	601	CHL	C3B-C4B	3.18	1.44	1.41
31	5	607	CHL	C3B-C2B	-3.17	1.36	1.40
31	3	608	CHL	C3B-C2B	-3.16	1.36	1.40
31	6	608	CHL	C3B-C2B	-3.15	1.36	1.40
31	5	618	CHL	C3B-C2B	-3.15	1.36	1.40
31	1	601	CHL	C3B-C4B	3.14	1.44	1.41
31	4	618	CHL	C3B-C2B	-3.14	1.36	1.40
31	6	618	CHL	C3B-C2B	-3.14	1.36	1.40
31	6	606	CHL	C3B-C2B	-3.14	1.36	1.40
31	5	608	CHL	C3B-C2B	-3.13	1.36	1.40
31	6	607	CHL	C3B-C2B	-3.13	1.36	1.40
31	92	607	CHL	C3B-C2B	-3.11	1.36	1.40
31	9	606	CHL	C3B-C2B	-3.10	1.36	1.40
31	4	607	CHL	C3B-C2B	-3.10	1.36	1.40
31	6	616	CHL	C3B-C2B	-3.08	1.36	1.40
31	8	601	CHL	C3B-C2B	-3.08	1.36	1.40
31	8	606	CHL	C3B-C2B	-3.07	1.36	1.40
31	4	608	CHL	C3B-C2B	-3.05	1.36	1.40
31	4	606	CHL	C3B-C2B	-3.04	1.36	1.40
31	7	601	CHL	C3B-C2B	-3.02	1.36	1.40
31	Z	601	CHL	C3B-C2B	-3.02	1.36	1.40
31	7	606	CHL	C3B-C2B	-3.02	1.36	1.40
31	4	601	CHL	C3B-C2B	-3.00	1.36	1.40
31	92	606	CHL	C3B-C2B	-2.95	1.36	1.40
31	6	601	CHL	C3B-C2B	-2.92	1.36	1.40
31	Z	601	CHL	CHC-C4B	-2.74	1.35	1.39
33	5	625	NEX	C1-C6	-2.70	1.50	1.54
31	1	601	CHL	CHC-C4B	-2.59	1.35	1.39
22	B	803	CLA	C1D-C2D	-2.57	1.40	1.45
22	B	806	CLA	C1D-C2D	-2.57	1.40	1.45
31	1	607	CHL	CHC-C4B	-2.57	1.35	1.39
22	B	802	CLA	C1D-C2D	-2.57	1.40	1.45
31	3	608	CHL	CHC-C4B	-2.55	1.35	1.39
22	A	829	CLA	C1D-C2D	-2.54	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	828	CLA	C1D-C2D	-2.54	1.40	1.45
31	8	607	CHL	CHB-C1B	-2.54	1.35	1.39
22	B	809	CLA	C1D-C2D	-2.53	1.40	1.45
31	7	607	CHL	CHC-C4B	-2.53	1.35	1.39
21	A	801	CL0	CHB-C4A	-2.53	1.35	1.38
22	A	807	CLA	C1D-C2D	-2.52	1.40	1.45
22	A	819	CLA	C1D-C2D	-2.52	1.40	1.45
31	8	601	CHL	CHC-C4B	-2.52	1.35	1.39
31	4	618	CHL	CHC-C4B	-2.52	1.35	1.39
22	B	808	CLA	C1D-C2D	-2.51	1.40	1.45
22	K	201	CLA	C1D-C2D	-2.51	1.40	1.45
31	4	606	CHL	CHC-C4B	-2.51	1.35	1.39
22	7	612	CLA	C1D-C2D	-2.51	1.40	1.45
31	9	607	CHL	CHC-C4B	-2.51	1.35	1.39
31	Z	607	CHL	CHC-C4B	-2.51	1.35	1.39
31	8	607	CHL	CHC-C4B	-2.51	1.35	1.39
22	A	805	CLA	C1D-C2D	-2.50	1.40	1.45
31	4	606	CHL	CHB-C1B	-2.50	1.35	1.39
22	A	854	CLA	C1D-C2D	-2.50	1.40	1.45
31	6	606	CHL	CHC-C4B	-2.50	1.35	1.39
31	6	606	CHL	CHB-C1B	-2.50	1.35	1.39
22	3	603	CLA	C1D-C2D	-2.50	1.40	1.45
31	7	606	CHL	CHC-C4B	-2.49	1.35	1.39
22	8	610	CLA	C1D-C2D	-2.49	1.40	1.45
31	9	606	CHL	CHC-C4B	-2.49	1.35	1.39
31	6	618	CHL	CHC-C4B	-2.49	1.35	1.39
31	7	601	CHL	CHC-C4B	-2.49	1.35	1.39
22	8	608	CLA	C1D-C2D	-2.49	1.40	1.45
22	B	816	CLA	C1D-C2D	-2.48	1.40	1.45
22	A	802	CLA	C1D-C2D	-2.48	1.40	1.45
22	A	842	CLA	C1D-C2D	-2.48	1.40	1.45
31	4	608	CHL	CHC-C4B	-2.48	1.35	1.39
22	B	825	CLA	C1D-C2D	-2.47	1.40	1.45
22	1	611	CLA	C1D-C2D	-2.47	1.40	1.45
31	5	608	CHL	CHB-C1B	-2.47	1.35	1.39
31	5	606	CHL	CHC-C4B	-2.47	1.35	1.39
22	A	830	CLA	C1D-C2D	-2.47	1.40	1.45
22	A	808	CLA	C1D-C2D	-2.46	1.40	1.45
22	A	814	CLA	C1D-C2D	-2.46	1.40	1.45
22	4	602	CLA	C1D-C2D	-2.46	1.40	1.45
31	Z	606	CHL	CHC-C4B	-2.46	1.35	1.39
22	B	820	CLA	C1D-C2D	-2.46	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	827	CLA	C1D-C2D	-2.46	1.40	1.45
22	B	838	CLA	C1D-C2D	-2.46	1.40	1.45
22	A	821	CLA	C1D-C2D	-2.46	1.40	1.45
22	F	301	CLA	C1D-C2D	-2.46	1.40	1.45
22	9	603	CLA	C1D-C2D	-2.46	1.40	1.45
22	A	813	CLA	C1D-C2D	-2.46	1.40	1.45
22	5	617	CLA	C1D-C2D	-2.46	1.40	1.45
22	B	821	CLA	C1D-C2D	-2.46	1.40	1.45
22	B	829	CLA	C1D-C2D	-2.45	1.40	1.45
22	J	101	CLA	C1D-C2D	-2.45	1.40	1.45
22	A	812	CLA	C1D-C2D	-2.45	1.40	1.45
31	9	607	CHL	CHB-C1B	-2.45	1.35	1.39
22	A	826	CLA	C1D-C2D	-2.45	1.40	1.45
22	B	813	CLA	C1D-C2D	-2.45	1.40	1.45
31	92	607	CHL	CHC-C4B	-2.45	1.35	1.39
22	B	824	CLA	C1D-C2D	-2.45	1.40	1.45
22	3	606	CLA	C1D-C2D	-2.45	1.40	1.45
31	8	606	CHL	CHC-C4B	-2.44	1.35	1.39
22	B	835	CLA	C1D-C2D	-2.44	1.40	1.45
22	5	621	CLA	C1D-C2D	-2.44	1.40	1.45
22	A	815	CLA	C1D-C2D	-2.44	1.40	1.45
22	A	817	CLA	C1D-C2D	-2.44	1.40	1.45
22	A	810	CLA	C1D-C2D	-2.44	1.40	1.45
22	8	612	CLA	C1D-C2D	-2.44	1.40	1.45
22	3	615	CLA	C1D-C2D	-2.44	1.40	1.45
22	7	614	CLA	C1D-C2D	-2.44	1.40	1.45
22	5	601	CLA	C1D-C2D	-2.44	1.40	1.45
22	B	810	CLA	C1D-C2D	-2.44	1.40	1.45
22	8	613	CLA	C1D-C2D	-2.44	1.40	1.45
31	4	607	CHL	CHC-C4B	-2.43	1.35	1.39
22	3	617	CLA	C1D-C2D	-2.43	1.40	1.45
22	5	612	CLA	C1D-C2D	-2.43	1.40	1.45
22	B	840	CLA	C1D-C2D	-2.43	1.40	1.45
22	1	612	CLA	C1D-C2D	-2.43	1.40	1.45
31	6	607	CHL	CHB-C1B	-2.43	1.35	1.39
22	A	822	CLA	C1D-C2D	-2.43	1.40	1.45
31	6	601	CHL	CHC-C4B	-2.43	1.35	1.39
22	G	203	CLA	C1D-C2D	-2.43	1.40	1.45
31	1	606	CHL	CHB-C1B	-2.43	1.35	1.39
22	92	609	CLA	C1D-C2D	-2.43	1.40	1.45
22	B	807	CLA	C1D-C2D	-2.43	1.40	1.45
22	9	612	CLA	C1D-C2D	-2.43	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	607	CHL	CHC-C4B	-2.42	1.35	1.39
22	B	815	CLA	C1D-C2D	-2.42	1.40	1.45
22	B	804	CLA	C1D-C2D	-2.42	1.40	1.45
22	A	818	CLA	C1D-C2D	-2.42	1.40	1.45
22	F	304	CLA	C1D-C2D	-2.42	1.40	1.45
22	B	837	CLA	C1D-C2D	-2.42	1.40	1.45
22	A	827	CLA	C1D-C2D	-2.42	1.40	1.45
22	4	613	CLA	C1D-C2D	-2.42	1.40	1.45
22	1	616	CLA	C1D-C2D	-2.42	1.40	1.45
22	Z	612	CLA	C1D-C2D	-2.42	1.40	1.45
22	Z	609	CLA	C1D-C2D	-2.42	1.40	1.45
31	4	601	CHL	CHC-C4B	-2.42	1.35	1.39
22	A	834	CLA	C1D-C2D	-2.42	1.40	1.45
22	4	603	CLA	C1D-C2D	-2.42	1.40	1.45
22	F	303	CLA	C1D-C2D	-2.41	1.40	1.45
22	7	602	CLA	C1D-C2D	-2.41	1.40	1.45
22	A	839	CLA	C1D-C2D	-2.41	1.40	1.45
22	A	838	CLA	C1D-C2D	-2.41	1.40	1.45
22	8	602	CLA	C1D-C2D	-2.41	1.40	1.45
22	5	613	CLA	C1D-C2D	-2.41	1.40	1.45
22	B	826	CLA	C1D-C2D	-2.41	1.40	1.45
22	6	603	CLA	C1D-C2D	-2.41	1.40	1.45
22	7	608	CLA	C1D-C2D	-2.41	1.40	1.45
22	A	845	CLA	C1D-C2D	-2.41	1.40	1.45
22	A	832	CLA	C1D-C2D	-2.40	1.40	1.45
22	6	610	CLA	C1D-C2D	-2.40	1.40	1.45
22	B	841	CLA	C1D-C2D	-2.40	1.40	1.45
22	B	812	CLA	C1D-C2D	-2.40	1.40	1.45
22	6	611	CLA	C1D-C2D	-2.40	1.40	1.45
22	B	805	CLA	C1D-C2D	-2.40	1.40	1.45
31	1	606	CHL	CHC-C4B	-2.40	1.35	1.39
22	A	806	CLA	C1D-C2D	-2.40	1.40	1.45
22	B	836	CLA	C1D-C2D	-2.40	1.40	1.45
22	Z	610	CLA	C1D-C2D	-2.40	1.40	1.45
22	1	609	CLA	C1D-C2D	-2.40	1.40	1.45
22	92	603	CLA	C1D-C2D	-2.40	1.40	1.45
22	4	614	CLA	C1D-C2D	-2.39	1.40	1.45
22	6	609	CLA	C1D-C2D	-2.39	1.40	1.45
31	6	608	CHL	CHC-C4B	-2.39	1.35	1.39
22	A	816	CLA	C1D-C2D	-2.39	1.40	1.45
22	7	613	CLA	C1D-C2D	-2.39	1.40	1.45
22	6	604	CLA	C1D-C2D	-2.39	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	616	CHL	CHC-C4B	-2.39	1.35	1.39
22	3	604	CLA	C1D-C2D	-2.39	1.40	1.45
22	4	612	CLA	C1D-C2D	-2.39	1.40	1.45
22	9	611	CLA	C1D-C2D	-2.39	1.40	1.45
22	9	602	CLA	C1D-C2D	-2.39	1.40	1.45
22	5	616	CLA	C1D-C2D	-2.39	1.40	1.45
22	5	609	CLA	C1D-C2D	-2.39	1.40	1.45
22	9	604	CLA	C1D-C2D	-2.39	1.40	1.45
22	8	609	CLA	C1D-C2D	-2.39	1.40	1.45
22	A	837	CLA	C1D-C2D	-2.39	1.40	1.45
22	B	832	CLA	C1D-C2D	-2.38	1.40	1.45
22	8	603	CLA	C1D-C2D	-2.38	1.40	1.45
22	A	833	CLA	C1D-C2D	-2.38	1.40	1.45
22	5	602	CLA	C1D-C2D	-2.38	1.40	1.45
22	A	803	CLA	C1D-C2D	-2.38	1.40	1.45
22	B	831	CLA	C1D-C2D	-2.38	1.40	1.45
22	3	612	CLA	C1D-C2D	-2.38	1.40	1.45
22	B	811	CLA	C1D-C2D	-2.38	1.40	1.45
22	7	620	CLA	C1D-C2D	-2.38	1.40	1.45
22	A	820	CLA	C1D-C2D	-2.38	1.40	1.45
22	B	830	CLA	C1D-C2D	-2.38	1.40	1.45
22	8	616	CLA	C1D-C2D	-2.38	1.40	1.45
22	3	613	CLA	C1D-C2D	-2.38	1.40	1.45
31	5	608	CHL	CHC-C4B	-2.38	1.35	1.39
22	Z	616	CLA	C1D-C2D	-2.38	1.40	1.45
31	92	606	CHL	CHC-C4B	-2.38	1.35	1.39
22	A	825	CLA	C1D-C2D	-2.38	1.40	1.45
22	3	602	CLA	C1D-C2D	-2.38	1.40	1.45
22	5	611	CLA	C1D-C2D	-2.38	1.40	1.45
22	8	611	CLA	C1D-C2D	-2.38	1.40	1.45
22	6	612	CLA	C1D-C2D	-2.38	1.40	1.45
31	6	618	CHL	CHB-C1B	-2.38	1.35	1.39
22	B	834	CLA	C1D-C2D	-2.38	1.40	1.45
22	7	609	CLA	C1D-C2D	-2.38	1.40	1.45
22	1	602	CLA	C1D-C2D	-2.37	1.40	1.45
31	7	601	CHL	CHB-C1B	-2.37	1.35	1.39
22	1	614	CLA	C1D-C2D	-2.37	1.40	1.45
22	Z	611	CLA	C1D-C2D	-2.37	1.40	1.45
22	B	818	CLA	C1D-C2D	-2.37	1.40	1.45
22	5	614	CLA	C1D-C2D	-2.37	1.40	1.45
22	B	823	CLA	C1D-C2D	-2.37	1.40	1.45
22	9	613	CLA	C1D-C2D	-2.37	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	836	CLA	C1D-C2D	-2.37	1.40	1.45
31	6	616	CHL	CHB-C1B	-2.37	1.35	1.39
22	6	602	CLA	C1D-C2D	-2.37	1.40	1.45
22	1	603	CLA	C1D-C2D	-2.37	1.40	1.45
22	9	609	CLA	C1D-C2D	-2.37	1.40	1.45
31	Z	607	CHL	CHB-C1B	-2.36	1.35	1.39
22	6	613	CLA	C1D-C2D	-2.36	1.40	1.45
22	A	843	CLA	C1D-C2D	-2.36	1.40	1.45
22	B	833	CLA	C1D-C2D	-2.36	1.40	1.45
22	K	206	CLA	C1D-C2D	-2.36	1.40	1.45
31	8	606	CHL	CHB-C1B	-2.36	1.35	1.39
22	A	840	CLA	C1D-C2D	-2.36	1.40	1.45
22	Z	603	CLA	C1D-C2D	-2.36	1.40	1.45
22	92	612	CLA	C1D-C2D	-2.36	1.40	1.45
22	7	611	CLA	C1D-C2D	-2.36	1.40	1.45
22	92	611	CLA	C1D-C2D	-2.36	1.40	1.45
22	4	610	CLA	C1D-C2D	-2.36	1.40	1.45
22	8	614	CLA	C1D-C2D	-2.36	1.40	1.45
22	6	622	CLA	C1D-C2D	-2.36	1.40	1.45
22	B2	820	CLA	C1D-C2D	-2.36	1.40	1.45
22	B	828	CLA	C1D-C2D	-2.35	1.40	1.45
22	K	203	CLA	C1D-C2D	-2.35	1.40	1.45
31	5	607	CHL	CHB-C1B	-2.35	1.35	1.39
22	1	610	CLA	C1D-C2D	-2.35	1.40	1.45
22	3	611	CLA	C1D-C2D	-2.35	1.40	1.45
31	5	618	CHL	CHC-C4B	-2.35	1.35	1.39
22	3	609	CLA	C1D-C2D	-2.35	1.40	1.45
22	3	610	CLA	C1D-C2D	-2.35	1.40	1.45
22	7	616	CLA	C1D-C2D	-2.35	1.40	1.45
22	9	614	CLA	C1D-C2D	-2.35	1.40	1.45
22	4	609	CLA	C1D-C2D	-2.35	1.40	1.45
31	9	606	CHL	CHB-C1B	-2.35	1.35	1.39
22	5	604	CLA	C1D-C2D	-2.35	1.40	1.45
31	4	618	CHL	CHB-C1B	-2.35	1.35	1.39
22	B	819	CLA	C1D-C2D	-2.35	1.40	1.45
31	5	606	CHL	CHB-C1B	-2.35	1.35	1.39
22	A	835	CLA	C1D-C2D	-2.35	1.40	1.45
22	G	204	CLA	C1D-C2D	-2.35	1.40	1.45
22	5	610	CLA	C1D-C2D	-2.35	1.40	1.45
22	92	601	CLA	C1D-C2D	-2.35	1.40	1.45
22	B	839	CLA	C1D-C2D	-2.34	1.40	1.45
22	A	809	CLA	C1D-C2D	-2.34	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	92	602	CLA	C1D-C2D	-2.34	1.40	1.45
31	92	607	CHL	CHB-C1B	-2.34	1.35	1.39
22	B2	808	CLA	C1D-C2D	-2.34	1.40	1.45
22	92	613	CLA	C1D-C2D	-2.34	1.40	1.45
22	A	831	CLA	C1D-C2D	-2.34	1.40	1.45
22	4	604	CLA	C1D-C2D	-2.34	1.40	1.45
22	7	603	CLA	C1D-C2D	-2.34	1.40	1.45
22	A	824	CLA	C1D-C2D	-2.34	1.40	1.45
22	K	204	CLA	C1D-C2D	-2.34	1.40	1.45
22	B	814	CLA	C1D-C2D	-2.33	1.40	1.45
22	L	203	CLA	C1D-C2D	-2.33	1.40	1.45
22	4	611	CLA	C1D-C2D	-2.33	1.40	1.45
22	B2	807	CLA	C1D-C2D	-2.33	1.40	1.45
22	6	614	CLA	C1D-C2D	-2.33	1.40	1.45
22	1	613	CLA	C1D-C2D	-2.33	1.40	1.45
22	B2	813	CLA	C1D-C2D	-2.33	1.40	1.45
22	7	610	CLA	C1D-C2D	-2.33	1.40	1.45
22	92	610	CLA	C1D-C2D	-2.33	1.40	1.45
22	1	608	CLA	C1D-C2D	-2.33	1.40	1.45
22	B2	806	CLA	C1D-C2D	-2.33	1.40	1.45
22	B2	810	CLA	C1D-C2D	-2.33	1.40	1.45
22	Z	608	CLA	C1D-C2D	-2.33	1.40	1.45
22	8	604	CLA	C1D-C2D	-2.33	1.40	1.45
22	4	616	CLA	C1D-C2D	-2.33	1.40	1.45
22	A	811	CLA	C1D-C2D	-2.33	1.40	1.45
22	7	604	CLA	C1D-C2D	-2.33	1.40	1.45
22	Z	604	CLA	C1D-C2D	-2.33	1.40	1.45
22	B	817	CLA	C1D-C2D	-2.33	1.40	1.45
31	5	618	CHL	CHB-C1B	-2.32	1.35	1.39
31	8	601	CHL	CHB-C1B	-2.32	1.35	1.39
22	A	804	CLA	C1D-C2D	-2.32	1.40	1.45
22	A	823	CLA	C1D-C2D	-2.32	1.40	1.45
22	3	614	CLA	C1D-C2D	-2.32	1.40	1.45
22	6	617	CLA	C1D-C2D	-2.32	1.40	1.45
22	B2	812	CLA	C1D-C2D	-2.32	1.40	1.45
22	3	607	CLA	C1D-C2D	-2.31	1.40	1.45
22	Z	602	CLA	C1D-C2D	-2.31	1.40	1.45
22	92	604	CLA	C1D-C2D	-2.31	1.40	1.45
31	6	608	CHL	CHB-C1B	-2.31	1.35	1.39
22	9	601	CLA	C1D-C2D	-2.31	1.40	1.45
31	6	607	CHL	CHC-C4B	-2.31	1.35	1.39
31	1	601	CHL	CHB-C1B	-2.31	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	841	CLA	C1D-C2D	-2.31	1.40	1.45
22	B2	811	CLA	C1D-C2D	-2.30	1.40	1.45
31	3	608	CHL	CHB-C1B	-2.30	1.35	1.39
31	7	606	CHL	CHB-C1B	-2.30	1.35	1.39
31	4	608	CHL	CHB-C1B	-2.30	1.35	1.39
22	B2	805	CLA	C1D-C2D	-2.30	1.40	1.45
22	B	822	CLA	C1D-C2D	-2.30	1.40	1.45
31	1	607	CHL	CHB-C1B	-2.30	1.35	1.39
22	B2	804	CLA	C1D-C2D	-2.29	1.40	1.45
22	Z	614	CLA	C1D-C2D	-2.29	1.40	1.45
22	B2	839	CLA	C1D-C2D	-2.29	1.40	1.45
22	B2	828	CLA	C1D-C2D	-2.29	1.40	1.45
22	B2	814	CLA	C1D-C2D	-2.29	1.40	1.45
22	92	614	CLA	C1D-C2D	-2.29	1.40	1.45
22	Z	613	CLA	C1D-C2D	-2.29	1.40	1.45
22	B2	809	CLA	C1D-C2D	-2.29	1.40	1.45
31	4	607	CHL	CHB-C1B	-2.28	1.35	1.39
31	7	607	CHL	CHB-C1B	-2.27	1.36	1.39
31	92	606	CHL	CHB-C1B	-2.27	1.36	1.39
22	L2	203	CLA	C1D-C2D	-2.27	1.40	1.45
22	5	603	CLA	C1D-C2D	-2.27	1.40	1.45
22	B2	829	CLA	C1D-C2D	-2.27	1.40	1.45
22	L2	204	CLA	C1D-C2D	-2.26	1.40	1.45
22	L	204	CLA	C1D-C2D	-2.26	1.40	1.45
22	9	610	CLA	C1D-C2D	-2.26	1.40	1.45
22	B2	815	CLA	C1D-C2D	-2.26	1.40	1.45
22	1	604	CLA	C1D-C2D	-2.25	1.40	1.45
31	6	601	CHL	CHB-C1B	-2.25	1.36	1.39
31	Z	606	CHL	CHB-C1B	-2.23	1.36	1.39
31	4	601	CHL	CHB-C1B	-2.23	1.36	1.39
31	Z	601	CHL	CHB-C1B	-2.20	1.36	1.39
22	B	823	CLA	C3D-C4D	-2.17	1.39	1.44
22	B	840	CLA	C3D-C4D	-2.16	1.39	1.44
22	A	827	CLA	C3D-C4D	-2.16	1.39	1.44
22	A	806	CLA	C3D-C4D	-2.13	1.39	1.44
22	B	825	CLA	C3D-C4D	-2.12	1.39	1.44
22	3	602	CLA	C3D-C4D	-2.11	1.39	1.44
22	1	602	CLA	C3D-C4D	-2.11	1.39	1.44
22	B	818	CLA	C3D-C4D	-2.11	1.39	1.44
22	B	808	CLA	C3D-C4D	-2.11	1.39	1.44
22	A	807	CLA	C3D-C4D	-2.11	1.39	1.44
22	A	842	CLA	C3D-C4D	-2.11	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	831	CLA	C3D-C4D	-2.11	1.39	1.44
22	A	820	CLA	C3D-C4D	-2.11	1.39	1.44
22	Z	613	CLA	C3D-C4D	-2.10	1.39	1.44
22	A	808	CLA	C3D-C4D	-2.10	1.39	1.44
22	A	823	CLA	C3D-C4D	-2.10	1.39	1.44
22	1	613	CLA	C3D-C4D	-2.10	1.39	1.44
22	8	602	CLA	C3D-C4D	-2.10	1.39	1.44
22	B	837	CLA	C3D-C4D	-2.10	1.39	1.44
22	B	830	CLA	C3D-C4D	-2.10	1.39	1.44
22	3	610	CLA	C3D-C4D	-2.10	1.39	1.44
22	1	610	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	832	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	834	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	803	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	825	CLA	C3D-C4D	-2.09	1.39	1.44
22	B	806	CLA	C3D-C4D	-2.09	1.39	1.44
22	B	802	CLA	C3D-C4D	-2.09	1.39	1.44
22	B	819	CLA	C3D-C4D	-2.09	1.39	1.44
22	B	810	CLA	C3D-C4D	-2.09	1.39	1.44
22	A	821	CLA	C3D-C4D	-2.09	1.39	1.44
22	9	603	CLA	C3D-C4D	-2.08	1.39	1.44
22	92	602	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	814	CLA	C3D-C4D	-2.08	1.39	1.44
22	A	822	CLA	C3D-C4D	-2.08	1.39	1.44
22	A	841	CLA	C3D-C4D	-2.08	1.39	1.44
22	A	818	CLA	C3D-C4D	-2.08	1.39	1.44
22	7	616	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	821	CLA	C3D-C4D	-2.08	1.39	1.44
22	8	616	CLA	C3D-C4D	-2.08	1.39	1.44
22	A	809	CLA	C3D-C4D	-2.08	1.39	1.44
22	B	829	CLA	C3D-C4D	-2.07	1.39	1.44
22	B	807	CLA	C3D-C4D	-2.07	1.39	1.44
22	B	817	CLA	C3D-C4D	-2.07	1.39	1.44
22	A	813	CLA	C3D-C4D	-2.07	1.39	1.44
22	4	603	CLA	C3D-C4D	-2.07	1.39	1.44
22	9	610	CLA	C3D-C4D	-2.07	1.39	1.44
22	A	836	CLA	C3D-C4D	-2.07	1.39	1.44
22	A	843	CLA	C3D-C4D	-2.07	1.39	1.44
22	7	603	CLA	C3D-C4D	-2.07	1.39	1.44
22	9	604	CLA	C3D-C4D	-2.07	1.39	1.44
22	92	610	CLA	C3D-C4D	-2.07	1.39	1.44
22	B	833	CLA	C3D-C4D	-2.06	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	811	CLA	C3D-C4D	-2.06	1.39	1.44
22	5	616	CLA	C3D-C4D	-2.06	1.39	1.44
22	A	804	CLA	C3D-C4D	-2.06	1.39	1.44
22	L	203	CLA	C3D-C4D	-2.06	1.39	1.44
22	1	608	CLA	C3D-C4D	-2.06	1.39	1.44
22	A	802	CLA	C3D-C4D	-2.06	1.39	1.44
22	B	826	CLA	C3D-C4D	-2.06	1.39	1.44
22	3	612	CLA	C3D-C4D	-2.06	1.39	1.44
22	B	828	CLA	C3D-C4D	-2.05	1.39	1.44
22	5	609	CLA	C3D-C4D	-2.05	1.39	1.44
22	B	813	CLA	C3D-C4D	-2.05	1.39	1.44
22	1	614	CLA	C3D-C4D	-2.05	1.39	1.44
22	7	602	CLA	C3D-C4D	-2.05	1.39	1.44
22	3	604	CLA	C3D-C4D	-2.05	1.39	1.44
22	A	833	CLA	C3D-C4D	-2.05	1.39	1.44
22	8	603	CLA	C3D-C4D	-2.05	1.39	1.44
22	A	839	CLA	C3D-C4D	-2.05	1.39	1.44
22	3	609	CLA	C3D-C4D	-2.05	1.39	1.44
22	3	611	CLA	C3D-C4D	-2.05	1.39	1.44
22	A	828	CLA	C3D-C4D	-2.04	1.39	1.44
22	K	204	CLA	C3D-C4D	-2.04	1.39	1.44
22	A	831	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	812	CLA	C3D-C4D	-2.04	1.39	1.44
22	6	610	CLA	C3D-C4D	-2.04	1.39	1.44
22	A	805	CLA	C3D-C4D	-2.04	1.39	1.44
22	3	607	CLA	C3D-C4D	-2.04	1.39	1.44
22	Z	608	CLA	C3D-C4D	-2.04	1.39	1.44
22	5	611	CLA	C3D-C4D	-2.04	1.39	1.44
22	A	854	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	816	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	841	CLA	C3D-C4D	-2.04	1.39	1.44
22	8	612	CLA	C3D-C4D	-2.04	1.39	1.44
22	7	609	CLA	C3D-C4D	-2.04	1.39	1.44
22	7	610	CLA	C3D-C4D	-2.04	1.39	1.44
22	9	613	CLA	C3D-C4D	-2.04	1.39	1.44
22	5	613	CLA	C3D-C4D	-2.04	1.39	1.44
22	6	614	CLA	C3D-C4D	-2.04	1.39	1.44
22	9	611	CLA	C3D-C4D	-2.04	1.39	1.44
22	A	814	CLA	C3D-C4D	-2.04	1.39	1.44
22	B	839	CLA	C3D-C4D	-2.04	1.39	1.44
22	8	609	CLA	C3D-C4D	-2.04	1.39	1.44
21	A	801	CL0	CHD-C4C	-2.04	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	303	CLA	C3D-C4D	-2.04	1.39	1.44
22	1	603	CLA	C3D-C4D	-2.03	1.39	1.44
22	6	603	CLA	C3D-C4D	-2.03	1.39	1.44
22	7	613	CLA	C3D-C4D	-2.03	1.39	1.44
22	8	611	CLA	C3D-C4D	-2.03	1.39	1.44
22	B	822	CLA	C3D-C4D	-2.03	1.39	1.44
22	8	608	CLA	C3D-C4D	-2.03	1.39	1.44
22	A	830	CLA	C3D-C4D	-2.03	1.39	1.44
22	A	812	CLA	C3D-C4D	-2.03	1.39	1.44
22	Z	610	CLA	C3D-C4D	-2.03	1.39	1.44
22	3	614	CLA	C3D-C4D	-2.03	1.39	1.44
22	B	832	CLA	C3D-C4D	-2.03	1.39	1.44
22	1	611	CLA	C3D-C4D	-2.03	1.39	1.44
22	7	604	CLA	C3D-C4D	-2.03	1.39	1.44
22	5	603	CLA	C3D-C4D	-2.03	1.39	1.44
22	B	820	CLA	C3D-C4D	-2.02	1.39	1.44
22	6	609	CLA	C3D-C4D	-2.02	1.39	1.44
22	1	609	CLA	C3D-C4D	-2.02	1.39	1.44
22	3	606	CLA	C3D-C4D	-2.02	1.39	1.44
22	Z	602	CLA	C3D-C4D	-2.02	1.39	1.44
22	3	613	CLA	C3D-C4D	-2.02	1.39	1.44
22	6	602	CLA	C3D-C4D	-2.02	1.39	1.44
22	7	611	CLA	C3D-C4D	-2.02	1.39	1.44
22	A	824	CLA	C3D-C4D	-2.02	1.39	1.44
22	7	614	CLA	C3D-C4D	-2.02	1.39	1.44
22	Z	604	CLA	C3D-C4D	-2.02	1.39	1.44
22	7	612	CLA	C3D-C4D	-2.02	1.39	1.44
22	8	604	CLA	C3D-C4D	-2.02	1.39	1.44
22	4	604	CLA	C3D-C4D	-2.02	1.39	1.44
22	8	613	CLA	C3D-C4D	-2.02	1.39	1.44
22	4	602	CLA	C3D-C4D	-2.02	1.39	1.44
22	B	811	CLA	C3D-C4D	-2.02	1.39	1.44
22	1	604	CLA	C3D-C4D	-2.02	1.39	1.44
22	9	609	CLA	C3D-C4D	-2.02	1.39	1.44
22	4	613	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	805	CLA	C3D-C4D	-2.01	1.39	1.44
22	92	603	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	836	CLA	C3D-C4D	-2.01	1.39	1.44
22	Z	603	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	817	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	834	CLA	C3D-C4D	-2.01	1.39	1.44
22	6	604	CLA	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	301	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	819	CLA	C3D-C4D	-2.01	1.39	1.44
22	Z	614	CLA	C3D-C4D	-2.01	1.39	1.44
22	7	608	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	809	CLA	C3D-C4D	-2.01	1.39	1.44
22	3	603	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	840	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	835	CLA	C3D-C4D	-2.01	1.39	1.44
22	8	614	CLA	C3D-C4D	-2.01	1.39	1.44
22	1	616	CLA	C3D-C4D	-2.01	1.39	1.44
22	5	604	CLA	C3D-C4D	-2.01	1.39	1.44
22	9	602	CLA	C3D-C4D	-2.00	1.39	1.44
22	A	815	CLA	C3D-C4D	-2.00	1.39	1.44
22	A	829	CLA	C3D-C4D	-2.00	1.39	1.44
22	6	613	CLA	C3D-C4D	-2.00	1.39	1.44
22	A	838	CLA	C3D-C4D	-2.00	1.39	1.44
22	92	611	CLA	C3D-C4D	-2.00	1.39	1.44

All (765) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	801	CL0	C1B-CHB-C4A	9.95	127.72	121.32
31	8	601	CHL	C1B-CHB-C4A	5.02	124.55	121.32
31	4	601	CHL	C1B-CHB-C4A	4.98	124.53	121.32
31	3	608	CHL	C1B-CHB-C4A	4.86	124.45	121.32
31	8	607	CHL	C1B-CHB-C4A	4.72	124.36	121.32
31	7	606	CHL	C1B-CHB-C4A	4.69	124.34	121.32
31	Z	601	CHL	C1B-CHB-C4A	4.64	124.31	121.32
31	Z	606	CHL	C1B-CHB-C4A	4.59	124.28	121.32
31	8	606	CHL	C1B-CHB-C4A	4.56	124.26	121.32
22	9	610	CLA	C1D-ND-C4D	-4.50	103.16	106.31
22	Z	613	CLA	C1D-ND-C4D	-4.44	103.20	106.31
31	1	606	CHL	C1B-CHB-C4A	4.41	124.16	121.32
22	9	604	CLA	C1D-ND-C4D	-4.38	103.24	106.31
31	7	607	CHL	C1B-CHB-C4A	4.37	124.13	121.32
31	5	606	CHL	C1B-CHB-C4A	4.35	124.12	121.32
31	9	606	CHL	C1B-CHB-C4A	4.35	124.12	121.32
22	L	204	CLA	C1D-ND-C4D	-4.34	103.27	106.31
22	F	303	CLA	C1D-ND-C4D	-4.33	103.27	106.31
22	1	613	CLA	C1D-ND-C4D	-4.33	103.27	106.31
22	4	604	CLA	C1D-ND-C4D	-4.33	103.27	106.31
22	9	603	CLA	C1D-ND-C4D	-4.32	103.28	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	614	CLA	C1D-ND-C4D	-4.31	103.29	106.31
22	92	614	CLA	C1D-ND-C4D	-4.31	103.29	106.31
22	B	814	CLA	C1D-ND-C4D	-4.31	103.29	106.31
22	B2	804	CLA	C1D-ND-C4D	-4.31	103.29	106.31
22	5	617	CLA	C1D-ND-C4D	-4.30	103.29	106.31
22	5	603	CLA	C1D-ND-C4D	-4.30	103.30	106.31
31	6	606	CHL	C1B-CHB-C4A	4.30	124.09	121.32
22	A	816	CLA	C1D-ND-C4D	-4.30	103.30	106.31
31	4	606	CHL	C1B-CHB-C4A	4.29	124.08	121.32
22	Z	602	CLA	C1D-ND-C4D	-4.28	103.31	106.31
22	B	822	CLA	C1D-ND-C4D	-4.28	103.31	106.31
22	A	809	CLA	C1D-ND-C4D	-4.28	103.31	106.31
22	K	204	CLA	C1D-ND-C4D	-4.28	103.31	106.31
22	Z	614	CLA	C1D-ND-C4D	-4.27	103.31	106.31
22	92	604	CLA	C1D-ND-C4D	-4.27	103.32	106.31
22	92	602	CLA	C1D-ND-C4D	-4.26	103.32	106.31
22	92	613	CLA	C1D-ND-C4D	-4.26	103.33	106.31
22	1	602	CLA	C1D-ND-C4D	-4.24	103.34	106.31
22	5	609	CLA	C1D-ND-C4D	-4.24	103.34	106.31
22	Z	612	CLA	C1D-ND-C4D	-4.23	103.34	106.31
22	A	804	CLA	C1D-ND-C4D	-4.23	103.34	106.31
22	5	613	CLA	C1D-ND-C4D	-4.23	103.34	106.31
31	5	618	CHL	C1B-CHB-C4A	4.23	124.04	121.32
22	92	610	CLA	C1D-ND-C4D	-4.22	103.35	106.31
22	6	609	CLA	C1D-ND-C4D	-4.22	103.35	106.31
22	B2	812	CLA	C1D-ND-C4D	-4.21	103.36	106.31
22	7	614	CLA	C1D-ND-C4D	-4.20	103.36	106.31
22	6	612	CLA	C1D-ND-C4D	-4.20	103.36	106.31
31	4	618	CHL	C1B-CHB-C4A	4.20	124.03	121.32
22	8	616	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	B	808	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	9	601	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	B2	820	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	Z	611	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	L2	204	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	B	833	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	B2	814	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	5	616	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	B2	815	CLA	C1D-ND-C4D	-4.19	103.37	106.31
22	3	612	CLA	C1D-ND-C4D	-4.18	103.38	106.31
22	4	612	CLA	C1D-ND-C4D	-4.18	103.38	106.31
22	A	820	CLA	C1D-ND-C4D	-4.18	103.38	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	614	CLA	C1D-ND-C4D	-4.18	103.38	106.31
22	1	614	CLA	C1D-ND-C4D	-4.18	103.38	106.31
22	B2	813	CLA	C1D-ND-C4D	-4.18	103.38	106.31
22	3	614	CLA	C1D-ND-C4D	-4.18	103.38	106.31
22	4	611	CLA	C1D-ND-C4D	-4.18	103.38	106.31
22	Z	604	CLA	C1D-ND-C4D	-4.17	103.38	106.31
22	B2	828	CLA	C1D-ND-C4D	-4.17	103.38	106.31
22	3	602	CLA	C1D-ND-C4D	-4.17	103.39	106.31
22	3	607	CLA	C1D-ND-C4D	-4.17	103.39	106.31
22	L2	203	CLA	C1D-ND-C4D	-4.17	103.39	106.31
22	6	610	CLA	C1D-ND-C4D	-4.17	103.39	106.31
22	6	617	CLA	C1D-ND-C4D	-4.16	103.39	106.31
22	4	603	CLA	C1D-ND-C4D	-4.16	103.39	106.31
22	A	831	CLA	C1D-ND-C4D	-4.16	103.39	106.31
22	3	611	CLA	C1D-ND-C4D	-4.16	103.39	106.31
22	7	603	CLA	C1D-ND-C4D	-4.16	103.39	106.31
22	8	611	CLA	C1D-ND-C4D	-4.16	103.39	106.31
31	6	618	CHL	C1B-CHB-C4A	4.16	124.00	121.32
22	A	834	CLA	C1D-ND-C4D	-4.16	103.39	106.31
22	7	616	CLA	C1D-ND-C4D	-4.15	103.40	106.31
22	9	609	CLA	C1D-ND-C4D	-4.15	103.40	106.31
22	B2	805	CLA	C1D-ND-C4D	-4.15	103.40	106.31
31	4	608	CHL	C1B-CHB-C4A	4.15	123.99	121.32
22	A	835	CLA	C1D-ND-C4D	-4.15	103.40	106.31
22	7	604	CLA	C1D-ND-C4D	-4.15	103.40	106.31
22	6	604	CLA	C1D-ND-C4D	-4.15	103.40	106.31
31	1	601	CHL	C1B-CHB-C4A	4.15	123.99	121.32
31	5	608	CHL	C1B-CHB-C4A	4.15	123.99	121.32
22	7	602	CLA	C1D-ND-C4D	-4.15	103.40	106.31
22	Z	610	CLA	C1D-ND-C4D	-4.14	103.40	106.31
22	6	602	CLA	C1D-ND-C4D	-4.14	103.40	106.31
22	B2	808	CLA	C1D-ND-C4D	-4.14	103.41	106.31
22	A	839	CLA	C1D-ND-C4D	-4.14	103.41	106.31
22	B	836	CLA	C1D-ND-C4D	-4.14	103.41	106.31
22	B	840	CLA	C1D-ND-C4D	-4.14	103.41	106.31
22	F	304	CLA	C1D-ND-C4D	-4.14	103.41	106.31
22	4	616	CLA	C1D-ND-C4D	-4.14	103.41	106.31
22	5	611	CLA	C1D-ND-C4D	-4.14	103.41	106.31
22	7	612	CLA	C1D-ND-C4D	-4.13	103.41	106.31
22	A	806	CLA	C1D-ND-C4D	-4.13	103.41	106.31
22	A	830	CLA	C1D-ND-C4D	-4.13	103.41	106.31
22	1	616	CLA	C1D-ND-C4D	-4.13	103.41	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B2	811	CLA	C1D-ND-C4D	-4.13	103.41	106.31
22	8	613	CLA	C1D-ND-C4D	-4.13	103.42	106.31
22	5	601	CLA	C1D-ND-C4D	-4.13	103.42	106.31
22	A	813	CLA	C1D-ND-C4D	-4.13	103.42	106.31
22	Z	616	CLA	C1D-ND-C4D	-4.13	103.42	106.31
22	1	610	CLA	C1D-ND-C4D	-4.13	103.42	106.31
22	7	620	CLA	C1D-ND-C4D	-4.13	103.42	106.31
31	6	616	CHL	C1B-CHB-C4A	4.12	123.97	121.32
22	A	827	CLA	C1D-ND-C4D	-4.12	103.42	106.31
22	1	612	CLA	C1D-ND-C4D	-4.12	103.42	106.31
22	5	614	CLA	C1D-ND-C4D	-4.12	103.42	106.31
22	A	818	CLA	C1D-ND-C4D	-4.12	103.42	106.31
22	6	611	CLA	C1D-ND-C4D	-4.12	103.42	106.31
22	A	843	CLA	C1D-ND-C4D	-4.11	103.42	106.31
22	B	835	CLA	C1D-ND-C4D	-4.11	103.42	106.31
22	92	603	CLA	C1D-ND-C4D	-4.11	103.42	106.31
22	A	822	CLA	C1D-ND-C4D	-4.11	103.43	106.31
22	A	811	CLA	C1D-ND-C4D	-4.11	103.43	106.31
22	B	831	CLA	C1D-ND-C4D	-4.11	103.43	106.31
22	G	204	CLA	C1D-ND-C4D	-4.11	103.43	106.31
22	3	610	CLA	C1D-ND-C4D	-4.11	103.43	106.31
22	B2	829	CLA	C1D-ND-C4D	-4.11	103.43	106.31
31	6	607	CHL	C1B-CHB-C4A	4.11	123.97	121.32
22	6	613	CLA	C1D-ND-C4D	-4.10	103.43	106.31
22	8	604	CLA	C1D-ND-C4D	-4.10	103.44	106.31
22	9	613	CLA	C1D-ND-C4D	-4.10	103.44	106.31
22	B2	839	CLA	C1D-ND-C4D	-4.10	103.44	106.31
31	Z	607	CHL	C1B-CHB-C4A	4.10	123.96	121.32
22	7	611	CLA	C1D-ND-C4D	-4.10	103.44	106.31
22	7	613	CLA	C1D-ND-C4D	-4.10	103.44	106.31
22	K	203	CLA	C1D-ND-C4D	-4.09	103.44	106.31
22	K	206	CLA	C1D-ND-C4D	-4.09	103.44	106.31
22	1	604	CLA	C1D-ND-C4D	-4.09	103.44	106.31
22	8	614	CLA	C1D-ND-C4D	-4.09	103.44	106.31
22	6	622	CLA	C1D-ND-C4D	-4.09	103.44	106.31
22	B	816	CLA	C1D-ND-C4D	-4.09	103.44	106.31
22	5	612	CLA	C1D-ND-C4D	-4.09	103.44	106.31
22	A	832	CLA	C1D-ND-C4D	-4.08	103.45	106.31
22	A	808	CLA	C1D-ND-C4D	-4.08	103.45	106.31
22	B	834	CLA	C1D-ND-C4D	-4.08	103.45	106.31
22	B	805	CLA	C1D-ND-C4D	-4.08	103.45	106.31
22	8	609	CLA	C1D-ND-C4D	-4.08	103.45	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	602	CLA	C1D-ND-C4D	-4.08	103.45	106.31
22	B2	807	CLA	C1D-ND-C4D	-4.08	103.45	106.31
22	B2	810	CLA	C1D-ND-C4D	-4.07	103.45	106.31
22	1	609	CLA	C1D-ND-C4D	-4.07	103.45	106.31
31	6	608	CHL	C1B-CHB-C4A	4.07	123.94	121.32
22	92	612	CLA	C1D-ND-C4D	-4.07	103.46	106.31
22	A	824	CLA	C1D-ND-C4D	-4.07	103.46	106.31
22	8	602	CLA	C1D-ND-C4D	-4.07	103.46	106.31
22	1	608	CLA	C1D-ND-C4D	-4.07	103.46	106.31
22	8	612	CLA	C1D-ND-C4D	-4.07	103.46	106.31
22	1	611	CLA	C1D-ND-C4D	-4.06	103.46	106.31
22	A	842	CLA	C1D-ND-C4D	-4.06	103.46	106.31
31	7	601	CHL	C1B-CHB-C4A	4.06	123.93	121.32
22	L	203	CLA	C1D-ND-C4D	-4.05	103.47	106.31
22	B2	809	CLA	C1D-ND-C4D	-4.05	103.47	106.31
22	92	609	CLA	C1D-ND-C4D	-4.05	103.47	106.31
22	A	823	CLA	C1D-ND-C4D	-4.05	103.47	106.31
22	B	828	CLA	C1D-ND-C4D	-4.05	103.47	106.31
22	1	603	CLA	C1D-ND-C4D	-4.05	103.47	106.31
22	5	604	CLA	C1D-ND-C4D	-4.05	103.47	106.31
22	Z	603	CLA	C1D-ND-C4D	-4.04	103.47	106.31
22	9	602	CLA	C1D-ND-C4D	-4.04	103.47	106.31
22	Z	608	CLA	C1D-ND-C4D	-4.04	103.48	106.31
22	A	838	CLA	C1D-ND-C4D	-4.04	103.48	106.31
22	B	832	CLA	C1D-ND-C4D	-4.04	103.48	106.31
22	B	810	CLA	C1D-ND-C4D	-4.04	103.48	106.31
22	B	837	CLA	C1D-ND-C4D	-4.04	103.48	106.31
22	4	602	CLA	C1D-ND-C4D	-4.04	103.48	106.31
22	B	804	CLA	C1D-ND-C4D	-4.04	103.48	106.31
22	B	807	CLA	C1D-ND-C4D	-4.03	103.48	106.31
22	A	841	CLA	C1D-ND-C4D	-4.03	103.48	106.31
22	3	604	CLA	C1D-ND-C4D	-4.03	103.48	106.31
22	5	610	CLA	C1D-ND-C4D	-4.03	103.48	106.31
22	9	612	CLA	C1D-ND-C4D	-4.02	103.49	106.31
22	B	819	CLA	C1D-ND-C4D	-4.02	103.49	106.31
22	92	601	CLA	C1D-ND-C4D	-4.02	103.49	106.31
22	4	610	CLA	C1D-ND-C4D	-4.02	103.49	106.31
22	A	833	CLA	C1D-ND-C4D	-4.02	103.49	106.31
22	B2	806	CLA	C1D-ND-C4D	-4.02	103.49	106.31
22	3	606	CLA	C1D-ND-C4D	-4.01	103.50	106.31
22	8	603	CLA	C1D-ND-C4D	-4.01	103.50	106.31
22	B	841	CLA	C1D-ND-C4D	-4.01	103.50	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	92	611	CLA	C1D-ND-C4D	-4.00	103.51	106.31
22	A	814	CLA	C1D-ND-C4D	-4.00	103.51	106.31
22	A	845	CLA	C1D-ND-C4D	-4.00	103.51	106.31
22	A	821	CLA	C1D-ND-C4D	-3.99	103.51	106.31
22	8	608	CLA	C1D-ND-C4D	-3.99	103.51	106.31
22	4	614	CLA	C1D-ND-C4D	-3.99	103.51	106.31
22	A	803	CLA	C1D-ND-C4D	-3.99	103.51	106.31
22	9	611	CLA	C1D-ND-C4D	-3.99	103.51	106.31
22	A	815	CLA	C1D-ND-C4D	-3.99	103.51	106.31
22	B	813	CLA	C1D-ND-C4D	-3.99	103.52	106.31
22	4	613	CLA	C1D-ND-C4D	-3.99	103.52	106.31
22	7	608	CLA	C1D-ND-C4D	-3.98	103.52	106.31
22	J	101	CLA	C1D-ND-C4D	-3.98	103.52	106.31
22	B	812	CLA	C1D-ND-C4D	-3.97	103.52	106.31
22	3	613	CLA	C1D-ND-C4D	-3.97	103.53	106.31
22	B	839	CLA	C1D-ND-C4D	-3.97	103.53	106.31
22	A	812	CLA	C1D-ND-C4D	-3.97	103.53	106.31
22	B	826	CLA	C1D-ND-C4D	-3.96	103.53	106.31
22	A	840	CLA	C1D-ND-C4D	-3.96	103.53	106.31
22	6	603	CLA	C1D-ND-C4D	-3.96	103.53	106.31
22	3	617	CLA	C1D-ND-C4D	-3.95	103.54	106.31
22	B	823	CLA	C1D-ND-C4D	-3.94	103.55	106.31
22	B	811	CLA	C1D-ND-C4D	-3.94	103.55	106.31
22	B	827	CLA	C1D-ND-C4D	-3.94	103.55	106.31
22	A	825	CLA	C1D-ND-C4D	-3.94	103.55	106.31
22	7	609	CLA	C1D-ND-C4D	-3.93	103.55	106.31
31	4	607	CHL	C1B-CHB-C4A	3.93	123.85	121.32
22	B	830	CLA	C1D-ND-C4D	-3.93	103.56	106.31
22	3	615	CLA	C1D-ND-C4D	-3.93	103.56	106.31
22	A	817	CLA	C1D-ND-C4D	-3.92	103.56	106.31
22	A	836	CLA	C1D-ND-C4D	-3.92	103.56	106.31
22	A	805	CLA	C1D-ND-C4D	-3.91	103.57	106.31
22	3	609	CLA	C1D-ND-C4D	-3.91	103.57	106.31
22	B	820	CLA	C1D-ND-C4D	-3.91	103.57	106.31
22	B	818	CLA	C1D-ND-C4D	-3.90	103.57	106.31
22	A	819	CLA	C1D-ND-C4D	-3.90	103.58	106.31
22	B	817	CLA	C1D-ND-C4D	-3.89	103.58	106.31
22	F	301	CLA	C1D-ND-C4D	-3.89	103.59	106.31
22	8	610	CLA	C1D-ND-C4D	-3.88	103.59	106.31
22	4	609	CLA	C1D-ND-C4D	-3.88	103.59	106.31
22	B	825	CLA	C1D-ND-C4D	-3.86	103.60	106.31
22	B	802	CLA	C1D-ND-C4D	-3.86	103.60	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	203	CLA	C1D-ND-C4D	-3.85	103.61	106.31
22	A	854	CLA	C1D-ND-C4D	-3.85	103.61	106.31
31	92	606	CHL	C1B-CHB-C4A	3.85	123.80	121.32
22	B	829	CLA	C1D-ND-C4D	-3.82	103.63	106.31
22	B	815	CLA	C1D-ND-C4D	-3.81	103.64	106.31
22	Z	609	CLA	C1D-ND-C4D	-3.81	103.64	106.31
22	B	809	CLA	C1D-ND-C4D	-3.81	103.64	106.31
22	A	807	CLA	C1D-ND-C4D	-3.80	103.64	106.31
22	B	838	CLA	C1D-ND-C4D	-3.80	103.64	106.31
22	B	821	CLA	C1D-ND-C4D	-3.79	103.65	106.31
22	B	824	CLA	C1D-ND-C4D	-3.78	103.66	106.31
22	A	826	CLA	C1D-ND-C4D	-3.75	103.68	106.31
22	A	828	CLA	C1D-ND-C4D	-3.75	103.68	106.31
31	1	607	CHL	C1B-CHB-C4A	3.74	123.73	121.32
22	A	802	CLA	C1D-ND-C4D	-3.71	103.71	106.31
22	3	603	CLA	C1D-ND-C4D	-3.68	103.73	106.31
31	6	601	CHL	C1B-CHB-C4A	3.68	123.69	121.32
22	K	201	CLA	C1D-ND-C4D	-3.68	103.73	106.31
22	A	837	CLA	C1D-ND-C4D	-3.67	103.73	106.31
22	5	621	CLA	C1D-ND-C4D	-3.65	103.75	106.31
22	B	806	CLA	C1D-ND-C4D	-3.65	103.75	106.31
22	A	810	CLA	C1D-ND-C4D	-3.64	103.76	106.31
22	7	610	CLA	C1D-ND-C4D	-3.62	103.77	106.31
22	A	829	CLA	C1D-ND-C4D	-3.60	103.78	106.31
31	92	607	CHL	C1B-CHB-C4A	3.56	123.61	121.32
33	6	625	NEX	C5-C6-C1	3.43	123.10	119.70
31	9	607	CHL	C1B-CHB-C4A	3.43	123.53	121.32
31	Z	606	CHL	CHA-C1A-C2A	-3.27	125.63	133.31
31	7	606	CHL	CHA-C1A-C2A	-3.26	125.65	133.31
22	B	803	CLA	C1D-ND-C4D	-3.24	104.04	106.31
21	A	801	CL0	CHA-C1A-C2A	-3.23	125.72	133.31
31	8	606	CHL	CHA-C1A-C2A	-3.17	125.87	133.31
31	7	601	CHL	CHA-C1A-C2A	-3.15	125.91	133.31
31	6	608	CHL	CHA-C1A-C2A	-3.15	125.91	133.31
31	1	601	CHL	CHA-C1A-C2A	-3.13	125.96	133.31
31	4	601	CHL	CHA-C1A-C2A	-3.13	125.96	133.31
31	5	608	CHL	CHA-C1A-C2A	-3.13	125.97	133.31
31	5	607	CHL	C1B-CHB-C4A	3.12	123.33	121.32
31	4	606	CHL	CHA-C1A-C2A	-3.10	126.03	133.31
31	6	618	CHL	CHA-C1A-C2A	-3.10	126.04	133.31
33	6	625	NEX	O24-C25-C24	-3.10	110.59	113.49
31	7	607	CHL	CHA-C1A-C2A	-3.08	126.07	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1	606	CHL	CHA-C1A-C2A	-3.06	126.13	133.31
31	Z	607	CHL	CHA-C1A-C2A	-3.05	126.14	133.31
31	3	608	CHL	CHA-C1A-C2A	-3.05	126.14	133.31
31	4	608	CHL	CHA-C1A-C2A	-3.05	126.15	133.31
31	6	607	CHL	CHA-C1A-C2A	-3.03	126.20	133.31
31	5	606	CHL	CHA-C1A-C2A	-3.00	126.27	133.31
31	6	616	CHL	CHA-C1A-C2A	-2.99	126.29	133.31
31	6	606	CHL	CHA-C1A-C2A	-2.97	126.33	133.31
31	5	618	CHL	CHA-C1A-C2A	-2.97	126.33	133.31
31	4	618	CHL	CHA-C1A-C2A	-2.95	126.38	133.31
31	92	607	CHL	CHA-C1A-C2A	-2.91	126.47	133.31
31	4	607	CHL	CHA-C1A-C2A	-2.91	126.48	133.31
31	9	607	CHL	CHA-C1A-C2A	-2.88	126.55	133.31
31	Z	601	CHL	CHA-C1A-C2A	-2.87	126.57	133.31
31	8	601	CHL	CHA-C1A-C2A	-2.85	126.62	133.31
33	5	625	NEX	O24-C25-C24	-2.83	110.84	113.49
31	8	607	CHL	C3D-C4D-CHA	2.79	112.78	108.54
31	Z	601	CHL	C3D-C4D-CHA	2.78	112.77	108.54
31	1	607	CHL	C3D-C4D-CHA	2.72	112.67	108.54
31	6	601	CHL	C3D-C4D-CHA	2.71	112.66	108.54
22	B	833	CLA	CHD-C1D-ND	-2.70	121.00	124.80
31	92	607	CHL	C3D-C4D-CHA	2.69	112.63	108.54
31	6	606	CHL	C3D-C4D-CHA	2.69	112.62	108.54
31	9	606	CHL	C3D-C4D-CHA	2.66	112.58	108.54
22	7	610	CLA	CHD-C1D-ND	-2.66	121.06	124.80
31	92	606	CHL	C3D-C4D-CHA	2.65	112.57	108.54
31	5	618	CHL	C3D-C4D-CHA	2.65	112.56	108.54
22	A	809	CLA	CHD-C1D-ND	-2.64	121.08	124.80
31	4	618	CHL	C3D-C4D-CHA	2.64	112.55	108.54
31	6	618	CHL	C3D-C4D-CHA	2.64	112.55	108.54
22	9	610	CLA	CHD-C1D-ND	-2.63	121.10	124.80
31	8	607	CHL	CHA-C1A-C2A	-2.63	127.13	133.31
31	Z	606	CHL	C3D-C4D-CHA	2.62	112.52	108.54
22	1	604	CLA	CHD-C1D-ND	-2.61	121.12	124.80
31	Z	607	CHL	C3D-C4D-CHA	2.61	112.51	108.54
31	6	607	CHL	C3D-C4D-CHA	2.61	112.50	108.54
31	7	607	CHL	C3D-C4D-CHA	2.61	112.50	108.54
31	5	606	CHL	C3D-C4D-CHA	2.60	112.49	108.54
31	7	601	CHL	C3D-C4D-CHA	2.60	112.49	108.54
31	1	601	CHL	C3D-C4D-CHA	2.60	112.49	108.54
31	4	608	CHL	C3D-C4D-CHA	2.60	112.48	108.54
31	4	606	CHL	C3D-C4D-CHA	2.59	112.47	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	606	CHL	C3D-C4D-CHA	2.58	112.47	108.54
31	8	601	CHL	C3D-C4D-CHA	2.58	112.47	108.54
22	B	822	CLA	CHD-C1D-ND	-2.58	121.17	124.80
31	1	606	CHL	C3D-C4D-CHA	2.58	112.46	108.54
22	A	823	CLA	CHD-C1D-ND	-2.57	121.18	124.80
22	B2	811	CLA	CAB-C3B-C2B	2.57	130.35	123.53
31	5	607	CHL	CHA-C1A-C2A	-2.56	127.30	133.31
22	A	806	CLA	CHD-C1D-ND	-2.55	121.21	124.80
31	9	607	CHL	C3D-C4D-CHA	2.55	112.42	108.54
31	4	607	CHL	C3D-C4D-CHA	2.55	112.41	108.54
31	5	608	CHL	C3D-C4D-CHA	2.55	112.41	108.54
22	A	827	CLA	CHD-C1D-ND	-2.55	121.22	124.80
22	Z	602	CLA	CHD-C1D-ND	-2.54	121.22	124.80
22	5	603	CLA	CHD-C1D-ND	-2.54	121.23	124.80
31	5	607	CHL	C3D-C4D-CHA	2.53	112.39	108.54
22	8	602	CLA	CHD-C1D-ND	-2.53	121.24	124.80
22	A	836	CLA	CHD-C1D-ND	-2.53	121.24	124.80
22	B	803	CLA	CHD-C1D-ND	-2.53	121.24	124.80
22	L2	203	CLA	CHD-C1D-ND	-2.53	121.24	124.80
22	B	841	CLA	CHD-C1D-ND	-2.53	121.24	124.80
31	6	616	CHL	C3D-C4D-CHA	2.53	112.38	108.54
22	92	604	CLA	CHD-C1D-ND	-2.53	121.25	124.80
22	L	203	CLA	CHD-C1D-ND	-2.52	121.25	124.80
22	A	812	CLA	CHD-C1D-ND	-2.52	121.25	124.80
22	B	805	CLA	CHD-C1D-ND	-2.52	121.25	124.80
22	B	819	CLA	CHD-C1D-ND	-2.52	121.25	124.80
22	92	614	CLA	CHD-C1D-ND	-2.52	121.26	124.80
22	1	610	CLA	CHD-C1D-ND	-2.52	121.26	124.80
22	7	603	CLA	CHD-C1D-ND	-2.52	121.26	124.80
22	B	834	CLA	CHD-C1D-ND	-2.52	121.26	124.80
22	1	608	CLA	CHD-C1D-ND	-2.52	121.26	124.80
22	Z	604	CLA	CHD-C1D-ND	-2.51	121.27	124.80
22	5	616	CLA	CHD-C1D-ND	-2.51	121.27	124.80
22	A	835	CLA	CHD-C1D-ND	-2.51	121.27	124.80
22	8	616	CLA	CHD-C1D-ND	-2.51	121.27	124.80
22	A	804	CLA	CHD-C1D-ND	-2.51	121.27	124.80
31	4	601	CHL	C3D-C4D-CHA	2.51	112.35	108.54
22	6	610	CLA	CHD-C1D-ND	-2.51	121.27	124.80
22	4	610	CLA	CHD-C1D-ND	-2.50	121.28	124.80
22	5	610	CLA	CHD-C1D-ND	-2.50	121.28	124.80
21	A	801	CL0	C3D-C4D-CHA	2.50	112.34	108.54
22	Z	610	CLA	CHD-C1D-ND	-2.50	121.28	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	802	CLA	CHD-C1D-ND	-2.50	121.28	124.80
22	B	829	CLA	CHD-C1D-ND	-2.50	121.28	124.80
31	7	606	CHL	C3D-C4D-CHA	2.50	112.34	108.54
22	A	803	CLA	CHD-C1D-ND	-2.50	121.29	124.80
31	3	608	CHL	C3D-C4D-CHA	2.50	112.34	108.54
22	L2	204	CLA	CHD-C1D-ND	-2.50	121.29	124.80
22	A	809	CLA	C1-C2-C3	-2.50	122.11	126.20
22	8	604	CLA	CHD-C1D-ND	-2.50	121.29	124.80
22	Z	613	CLA	CHD-C1D-ND	-2.49	121.29	124.80
22	6	614	CLA	CHD-C1D-ND	-2.49	121.29	124.80
22	4	604	CLA	CHD-C1D-ND	-2.49	121.30	124.80
22	5	621	CLA	C2A-C1A-CHA	2.49	128.19	123.87
22	9	604	CLA	CHD-C1D-ND	-2.49	121.30	124.80
22	9	609	CLA	CHD-C1D-ND	-2.49	121.31	124.80
22	Z	614	CLA	CHD-C1D-ND	-2.48	121.31	124.80
22	B2	839	CLA	CHD-C1D-ND	-2.48	121.31	124.80
22	A	811	CLA	CHD-C1D-ND	-2.48	121.31	124.80
22	92	610	CLA	CHD-C1D-ND	-2.48	121.31	124.80
22	B	839	CLA	CHD-C1D-ND	-2.48	121.31	124.80
22	9	614	CLA	CHD-C1D-ND	-2.48	121.32	124.80
31	6	608	CHL	C3D-C4D-CHA	2.47	112.30	108.54
22	3	602	CLA	CHD-C1D-ND	-2.47	121.32	124.80
22	6	617	CLA	CHD-C1D-ND	-2.47	121.32	124.80
22	7	616	CLA	CHD-C1D-ND	-2.47	121.32	124.80
22	A	816	CLA	CHD-C1D-ND	-2.47	121.33	124.80
22	5	613	CLA	CHD-C1D-ND	-2.46	121.33	124.80
22	A	833	CLA	CHD-C1D-ND	-2.46	121.33	124.80
22	B2	829	CLA	CHD-C1D-ND	-2.46	121.34	124.80
22	B	826	CLA	CHD-C1D-ND	-2.46	121.34	124.80
22	L	204	CLA	CHD-C1D-ND	-2.46	121.34	124.80
22	A	837	CLA	CHD-C1D-ND	-2.46	121.34	124.80
22	Z	603	CLA	CHD-C1D-ND	-2.46	121.34	124.80
22	B	814	CLA	CHD-C1D-ND	-2.46	121.35	124.80
22	92	602	CLA	CHD-C1D-ND	-2.46	121.35	124.80
22	A	830	CLA	CHD-C1D-ND	-2.45	121.35	124.80
22	3	610	CLA	CHD-C1D-ND	-2.45	121.35	124.80
27	B	853	LMU	C1B-O5B-C5B	2.45	118.51	113.72
22	6	609	CLA	CHD-C1D-ND	-2.45	121.35	124.80
22	K	204	CLA	CHD-C1D-ND	-2.45	121.35	124.80
22	3	614	CLA	CHD-C1D-ND	-2.45	121.35	124.80
22	A	841	CLA	CHD-C1D-ND	-2.45	121.35	124.80
22	B	830	CLA	CHD-C1D-ND	-2.45	121.35	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	832	CLA	CHD-C1D-ND	-2.45	121.36	124.80
22	8	614	CLA	CHD-C1D-ND	-2.45	121.36	124.80
22	B	840	CLA	CHD-C1D-ND	-2.45	121.36	124.80
22	8	609	CLA	CHD-C1D-ND	-2.45	121.36	124.80
22	92	613	CLA	CHD-C1D-ND	-2.45	121.36	124.80
22	B2	805	CLA	CHD-C1D-ND	-2.44	121.36	124.80
22	A	820	CLA	CHD-C1D-ND	-2.44	121.37	124.80
22	B	831	CLA	CHD-C1D-ND	-2.44	121.37	124.80
22	3	611	CLA	CHD-C1D-ND	-2.44	121.37	124.80
22	B	832	CLA	CHD-C1D-ND	-2.44	121.37	124.80
22	A	840	CLA	CHD-C1D-ND	-2.44	121.37	124.80
22	B	807	CLA	CHD-C1D-ND	-2.44	121.37	124.80
22	B2	814	CLA	CHD-C1D-ND	-2.44	121.38	124.80
22	9	613	CLA	CHD-C1D-ND	-2.43	121.38	124.80
22	1	613	CLA	CHD-C1D-ND	-2.43	121.38	124.80
22	5	617	CLA	CHD-C1D-ND	-2.43	121.38	124.80
22	9	611	CLA	CHD-C1D-ND	-2.43	121.39	124.80
22	8	613	CLA	CHD-C1D-ND	-2.43	121.39	124.80
22	B	812	CLA	CHD-C1D-ND	-2.43	121.39	124.80
22	5	604	CLA	CHD-C1D-ND	-2.42	121.39	124.80
22	4	616	CLA	CHD-C1D-ND	-2.42	121.39	124.80
22	B	835	CLA	CHD-C1D-ND	-2.42	121.40	124.80
22	F	303	CLA	CHD-C1D-ND	-2.42	121.40	124.80
22	K	203	CLA	CHD-C1D-ND	-2.42	121.40	124.80
22	B	823	CLA	CHD-C1D-ND	-2.42	121.40	124.80
22	1	602	CLA	CHD-C1D-ND	-2.42	121.40	124.80
22	A	815	CLA	CHD-C1D-ND	-2.42	121.40	124.80
22	1	609	CLA	CHD-C1D-ND	-2.42	121.40	124.80
22	A	831	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	A	834	CLA	CHD-C1D-ND	-2.41	121.41	124.80
33	5	625	NEX	C2-C1-C6	-2.41	106.86	109.21
22	6	602	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	7	611	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	6	622	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	92	611	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	8	610	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	92	601	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	5	609	CLA	CHD-C1D-ND	-2.41	121.41	124.80
22	B	828	CLA	CHD-C1D-ND	-2.41	121.42	124.80
22	3	604	CLA	CHD-C1D-ND	-2.40	121.42	124.80
22	3	609	CLA	CHD-C1D-ND	-2.40	121.42	124.80
22	B	838	CLA	CHD-C1D-ND	-2.40	121.42	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	603	CLA	CHD-C1D-ND	-2.40	121.43	124.80
22	9	602	CLA	CHD-C1D-ND	-2.40	121.43	124.80
22	B	821	CLA	CHD-C1D-ND	-2.40	121.43	124.80
22	3	607	CLA	CHD-C1D-ND	-2.40	121.43	124.80
22	8	603	CLA	CHD-C1D-ND	-2.39	121.43	124.80
22	Z	608	CLA	CHD-C1D-ND	-2.39	121.43	124.80
22	A	822	CLA	CHD-C1D-ND	-2.39	121.43	124.80
22	7	602	CLA	CHD-C1D-ND	-2.39	121.43	124.80
22	6	613	CLA	CHD-C1D-ND	-2.39	121.44	124.80
22	B	818	CLA	CHD-C1D-ND	-2.39	121.44	124.80
22	B2	807	CLA	CHD-C1D-ND	-2.39	121.44	124.80
22	7	608	CLA	CHD-C1D-ND	-2.39	121.45	124.80
22	4	602	CLA	CHD-C1D-ND	-2.38	121.45	124.80
32	1	618	XAT	C7-C8-C9	2.38	129.23	125.53
22	A	843	CLA	CHD-C1D-ND	-2.38	121.45	124.80
22	B	810	CLA	CHD-C1D-ND	-2.38	121.45	124.80
22	B2	811	CLA	CHD-C1D-ND	-2.38	121.45	124.80
22	4	613	CLA	CHD-C1D-ND	-2.38	121.45	124.80
22	5	621	CLA	CAA-C2A-C1A	2.38	119.77	111.97
22	7	613	CLA	CHD-C1D-ND	-2.38	121.46	124.80
22	B	804	CLA	CHD-C1D-ND	-2.37	121.46	124.80
22	6	611	CLA	CHD-C1D-ND	-2.37	121.46	124.80
22	Z	616	CLA	CHD-C1D-ND	-2.37	121.46	124.80
22	92	609	CLA	CHD-C1D-ND	-2.37	121.46	124.80
22	7	614	CLA	CHD-C1D-ND	-2.37	121.47	124.80
22	B2	804	CLA	CHD-C1D-ND	-2.37	121.47	124.80
22	A	839	CLA	CHD-C1D-ND	-2.37	121.47	124.80
22	B	802	CLA	CHD-C1D-ND	-2.37	121.47	124.80
22	5	614	CLA	CHD-C1D-ND	-2.37	121.47	124.80
22	7	609	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	B2	809	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	B	837	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	4	609	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	B2	810	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	B2	828	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	8	608	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	5	602	CLA	CHD-C1D-ND	-2.36	121.48	124.80
22	A	824	CLA	CHD-C1D-ND	-2.36	121.49	124.80
22	B	817	CLA	CHD-C1D-ND	-2.36	121.49	124.80
22	4	611	CLA	CHD-C1D-ND	-2.36	121.49	124.80
22	1	614	CLA	CHD-C1D-ND	-2.35	121.49	124.80
22	3	612	CLA	CHD-C1D-ND	-2.35	121.49	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	808	CLA	CHD-C1D-ND	-2.35	121.49	124.80
22	7	604	CLA	CHD-C1D-ND	-2.35	121.50	124.80
22	A	825	CLA	CHD-C1D-ND	-2.35	121.50	124.80
22	4	614	CLA	CHD-C1D-ND	-2.35	121.50	124.80
22	9	601	CLA	CHD-C1D-ND	-2.35	121.50	124.80
22	A	807	CLA	CHD-C1D-ND	-2.35	121.50	124.80
22	A	821	CLA	CHD-C1D-ND	-2.35	121.50	124.80
22	A	805	CLA	CHD-C1D-ND	-2.35	121.50	124.80
22	B	815	CLA	CHD-C1D-ND	-2.35	121.50	124.80
22	K	206	CLA	CHD-C1D-ND	-2.34	121.50	124.80
31	6	616	CHL	C1-C2-C3	-2.34	122.36	126.20
22	B2	815	CLA	CHD-C1D-ND	-2.34	121.50	124.80
22	B	836	CLA	CHD-C1D-ND	-2.34	121.51	124.80
22	9	603	CLA	CHD-C1D-ND	-2.34	121.51	124.80
22	A	813	CLA	CHD-C1D-ND	-2.34	121.51	124.80
22	B	811	CLA	CHD-C1D-ND	-2.34	121.51	124.80
22	B2	820	CLA	CHD-C1D-ND	-2.34	121.52	124.80
22	6	604	CLA	CHD-C1D-ND	-2.33	121.52	124.80
22	3	606	CLA	CHD-C1D-ND	-2.33	121.53	124.80
22	A	842	CLA	CHD-C1D-ND	-2.33	121.53	124.80
22	B	816	CLA	CHD-C1D-ND	-2.33	121.53	124.80
31	1	607	CHL	CHA-C1A-C2A	-2.33	127.85	133.31
22	A	818	CLA	CHD-C1D-ND	-2.32	121.53	124.80
22	B2	808	CLA	CHD-C1D-ND	-2.32	121.53	124.80
22	F	301	CLA	CHD-C1D-ND	-2.32	121.53	124.80
22	9	610	CLA	C3D-C4D-ND	2.32	113.76	109.99
22	1	612	CLA	CHD-C1D-ND	-2.32	121.53	124.80
31	4	606	CHL	C1-C2-C3	-2.32	122.40	126.20
22	A	817	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	1	611	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	A	838	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	1	616	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	G	203	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	8	611	CLA	CHD-C1D-ND	-2.32	121.54	124.80
29	F	305	LUT	C8-C7-C6	2.32	133.19	127.00
22	A	845	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	Z	609	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	B2	813	CLA	CHD-C1D-ND	-2.31	121.55	124.80
22	9	612	CLA	CHD-C1D-ND	-2.31	121.55	124.80
22	Z	611	CLA	CHD-C1D-ND	-2.31	121.55	124.80
22	5	601	CLA	CHD-C1D-ND	-2.31	121.55	124.80
22	B	806	CLA	CHD-C1D-ND	-2.31	121.56	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	825	CLA	CHD-C1D-ND	-2.31	121.56	124.80
22	B2	812	CLA	CHD-C1D-ND	-2.30	121.56	124.80
22	4	603	CLA	CHD-C1D-ND	-2.30	121.56	124.80
22	B2	806	CLA	CHD-C1D-ND	-2.30	121.56	124.80
22	7	620	CLA	CHD-C1D-ND	-2.30	121.57	124.80
22	6	603	CLA	CHD-C1D-ND	-2.30	121.57	124.80
22	Z	612	CLA	CHD-C1D-ND	-2.30	121.57	124.80
22	92	612	CLA	CHD-C1D-ND	-2.29	121.58	124.80
22	3	615	CLA	CHD-C1D-ND	-2.29	121.58	124.80
22	8	612	CLA	CHD-C1D-ND	-2.29	121.58	124.80
22	B	808	CLA	CHD-C1D-ND	-2.29	121.58	124.80
22	6	612	CLA	CHD-C1D-ND	-2.29	121.58	124.80
22	A	814	CLA	CHD-C1D-ND	-2.29	121.58	124.80
33	5	625	NEX	O24-C26-C27	-2.29	110.32	116.88
22	B	841	CLA	C1-C2-C3	-2.29	122.45	126.20
22	A	854	CLA	CHD-C1D-ND	-2.28	121.59	124.80
22	G	204	CLA	CHD-C1D-ND	-2.28	121.59	124.80
22	3	617	CLA	CHD-C1D-ND	-2.28	121.60	124.80
22	A	826	CLA	CHD-C1D-ND	-2.28	121.60	124.80
22	5	611	CLA	CHD-C1D-ND	-2.27	121.60	124.80
22	A	828	CLA	CHD-C1D-ND	-2.27	121.60	124.80
22	B	814	CLA	C3D-C4D-ND	2.27	113.68	109.99
31	5	608	CHL	C1A-CHA-C4D	2.27	122.77	118.98
22	B	809	CLA	CHD-C1D-ND	-2.27	121.61	124.80
22	7	612	CLA	CHD-C1D-ND	-2.27	121.61	124.80
22	Z	613	CLA	C3D-C4D-ND	2.27	113.67	109.99
22	B	827	CLA	CHD-C1D-ND	-2.27	121.61	124.80
22	4	612	CLA	CHD-C1D-ND	-2.27	121.61	124.80
22	B	820	CLA	CHD-C1D-ND	-2.26	121.62	124.80
22	3	613	CLA	CHD-C1D-ND	-2.26	121.62	124.80
22	5	612	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	4	607	CHL	C4C-CHD-C1D	2.25	124.11	116.07
31	6	601	CHL	CHA-C1A-C2A	-2.24	128.04	133.31
22	B	826	CLA	C3B-C4B-NB	-2.24	108.53	110.53
22	A	810	CLA	CHD-C1D-ND	-2.24	121.65	124.80
22	J	101	CLA	CHD-C1D-ND	-2.24	121.65	124.80
31	Z	601	CHL	C1A-CHA-C4D	2.23	122.71	118.98
22	92	603	CLA	CHD-C1D-ND	-2.23	121.66	124.80
29	F	305	LUT	C27-C28-C29	2.23	131.13	126.32
22	A	829	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	1	601	CHL	C4C-CHD-C1D	2.23	124.04	116.07
31	9	606	CHL	C1A-CHA-C4D	2.23	122.70	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	304	CLA	CHD-C1D-ND	-2.23	121.67	124.80
31	5	606	CHL	C1A-CHA-C4D	2.23	122.70	118.98
31	7	601	CHL	C4C-CHD-C1D	2.23	124.03	116.07
31	6	616	CHL	C4C-CHD-C1D	2.23	124.03	116.07
22	92	610	CLA	C3D-C4D-ND	2.22	113.60	109.99
31	6	618	CHL	C1A-CHA-C4D	2.22	122.69	118.98
31	Z	607	CHL	C4C-CHD-C1D	2.22	124.01	116.07
31	8	607	CHL	C1A-CHA-C4D	2.22	122.69	118.98
27	B	853	LMU	C1B-O1B-C4'	2.22	123.24	117.98
22	B	824	CLA	CHD-C1D-ND	-2.22	121.69	124.80
31	8	606	CHL	C4C-CHD-C1D	2.21	123.99	116.07
31	4	606	CHL	C4C-CHD-C1D	2.21	123.98	116.07
31	3	608	CHL	C4C-CHD-C1D	2.21	123.97	116.07
31	4	606	CHL	C1A-CHA-C4D	2.21	122.67	118.98
31	6	606	CHL	C4C-CHD-C1D	2.21	123.97	116.07
31	1	606	CHL	C4C-CHD-C1D	2.21	123.96	116.07
22	92	602	CLA	C3D-C4D-ND	2.21	113.57	109.99
31	4	618	CHL	C4C-CHD-C1D	2.20	123.95	116.07
31	9	607	CHL	C4C-CHD-C1D	2.20	123.94	116.07
31	9	606	CHL	C4C-CHD-C1D	2.20	123.94	116.07
31	7	607	CHL	C4C-CHD-C1D	2.20	123.94	116.07
31	4	601	CHL	C1A-CHA-C4D	2.20	122.65	118.98
22	L	204	CLA	C3D-C4D-ND	2.20	113.56	109.99
31	8	601	CHL	C4C-CHD-C1D	2.20	123.93	116.07
31	8	606	CHL	C1A-CHA-C4D	2.20	122.65	118.98
31	4	601	CHL	C4C-CHD-C1D	2.20	123.92	116.07
22	B	813	CLA	CHD-C1D-ND	-2.19	121.72	124.80
31	Z	606	CHL	C1A-CHA-C4D	2.19	122.64	118.98
31	6	618	CHL	C4C-CHD-C1D	2.19	123.91	116.07
31	5	607	CHL	C4C-CHD-C1D	2.19	123.90	116.07
31	6	601	CHL	C4C-CHD-C1D	2.19	123.90	116.07
31	4	608	CHL	C4C-CHD-C1D	2.19	123.90	116.07
22	A	806	CLA	C3D-C4D-ND	2.19	113.54	109.99
31	7	606	CHL	C4C-CHD-C1D	2.19	123.89	116.07
31	5	608	CHL	C4C-CHD-C1D	2.18	123.88	116.07
22	1	613	CLA	C3D-C4D-ND	2.18	113.53	109.99
22	4	604	CLA	C3D-C4D-ND	2.18	113.53	109.99
22	9	604	CLA	C3D-C4D-ND	2.18	113.53	109.99
22	L2	203	CLA	C3D-C4D-ND	2.18	113.53	109.99
31	5	618	CHL	C4C-CHD-C1D	2.18	123.86	116.07
31	6	608	CHL	C1A-CHA-C4D	2.18	122.61	118.98
22	3	603	CLA	CHD-C1D-ND	-2.17	121.74	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	6	608	CHL	C4C-CHD-C1D	2.17	123.84	116.07
31	6	607	CHL	C4C-CHD-C1D	2.17	123.84	116.07
22	Z	614	CLA	C3D-C4D-ND	2.17	113.52	109.99
31	Z	601	CHL	C4C-CHD-C1D	2.17	123.84	116.07
31	Z	606	CHL	C4C-CHD-C1D	2.17	123.84	116.07
22	A	820	CLA	C3D-C4D-ND	2.17	113.51	109.99
31	5	606	CHL	C4C-CHD-C1D	2.17	123.81	116.07
22	L2	204	CLA	C3D-C4D-ND	2.16	113.50	109.99
31	1	606	CHL	C1A-CHA-C4D	2.16	122.59	118.98
22	A	823	CLA	C3D-C4D-ND	2.16	113.49	109.99
22	A	804	CLA	C3D-C4D-ND	2.16	113.49	109.99
22	5	603	CLA	C3D-C4D-ND	2.15	113.49	109.99
31	4	608	CHL	C1A-CHA-C4D	2.15	122.58	118.98
33	6	625	NEX	O24-C26-C27	-2.15	110.70	116.88
31	3	608	CHL	C1A-CHA-C4D	2.15	122.57	118.98
22	3	614	CLA	C3D-C4D-ND	2.15	113.48	109.99
31	6	606	CHL	C1A-CHA-C4D	2.15	122.56	118.98
31	5	618	CHL	C1A-CHA-C4D	2.15	122.56	118.98
22	6	617	CLA	C3D-C4D-ND	2.15	113.47	109.99
22	92	613	CLA	C3D-C4D-ND	2.14	113.47	109.99
22	A	809	CLA	C3D-C4D-ND	2.14	113.47	109.99
31	1	607	CHL	C4C-CHD-C1D	2.14	123.73	116.07
22	Z	604	CLA	C3D-C4D-ND	2.14	113.47	109.99
22	1	604	CLA	C3D-C4D-ND	2.14	113.47	109.99
31	8	607	CHL	C4C-CHD-C1D	2.14	123.73	116.07
31	7	607	CHL	C1A-CHA-C4D	2.14	122.55	118.98
22	B	831	CLA	C3D-C4D-ND	2.14	113.46	109.99
31	92	607	CHL	C4C-CHD-C1D	2.13	123.70	116.07
22	A	819	CLA	CHD-C1D-ND	-2.13	121.80	124.80
31	Z	607	CHL	C1-C2-C3	-2.13	122.70	126.20
22	K	204	CLA	C3D-C4D-ND	2.13	113.45	109.99
22	8	616	CLA	C3D-C4D-ND	2.13	113.45	109.99
22	4	611	CLA	C3D-C4D-ND	2.13	113.45	109.99
22	5	617	CLA	C3D-C4D-ND	2.13	113.45	109.99
22	92	603	CLA	CHC-C4B-NB	2.13	127.24	124.05
31	92	606	CHL	C1A-CHA-C4D	2.13	122.53	118.98
22	5	609	CLA	C3D-C4D-ND	2.13	113.44	109.99
22	7	614	CLA	CHC-C4B-NB	2.13	127.24	124.05
22	6	609	CLA	C3D-C4D-ND	2.13	113.44	109.99
22	B2	839	CLA	C3D-C4D-ND	2.12	113.43	109.99
22	5	621	CLA	CHA-C1A-NA	-2.12	121.59	126.39
22	7	616	CLA	C3D-C4D-ND	2.12	113.43	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	614	CLA	C3D-C4D-ND	2.12	113.43	109.99
22	3	607	CLA	C3D-C4D-ND	2.11	113.42	109.99
22	Z	602	CLA	C3D-C4D-ND	2.11	113.42	109.99
22	3	602	CLA	C3D-C4D-ND	2.11	113.42	109.99
31	6	607	CHL	C1A-CHA-C4D	2.11	122.51	118.98
22	A	822	CLA	C3D-C4D-ND	2.11	113.42	109.99
22	A	829	CLA	C3B-C4B-NB	-2.11	108.65	110.53
22	6	609	CLA	CAA-C2A-C1A	-2.11	105.07	111.97
31	92	606	CHL	C4C-CHD-C1D	2.11	123.61	116.07
22	A	834	CLA	C3D-C4D-ND	2.11	113.41	109.99
22	3	611	CLA	C3D-C4D-ND	2.11	113.41	109.99
22	B2	804	CLA	C3D-C4D-ND	2.11	113.41	109.99
22	A	837	CLA	C3B-C4B-NB	-2.10	108.65	110.53
22	9	614	CLA	C3D-C4D-ND	2.10	113.41	109.99
31	Z	607	CHL	C1A-CHA-C4D	2.10	122.49	118.98
22	8	604	CLA	C3D-C4D-ND	2.10	113.40	109.99
22	92	604	CLA	C3D-C4D-ND	2.10	113.40	109.99
22	A	816	CLA	C3D-C4D-ND	2.10	113.40	109.99
22	B2	812	CLA	C3D-C4D-ND	2.10	113.40	109.99
31	4	618	CHL	C1A-CHA-C4D	2.10	122.48	118.98
22	9	601	CLA	C3D-C4D-ND	2.10	113.40	109.99
31	92	607	CHL	C1A-CHA-C4D	2.10	122.48	118.98
22	92	614	CLA	C3D-C4D-ND	2.10	113.39	109.99
22	A	843	CLA	C3D-C4D-ND	2.09	113.39	109.99
22	Z	610	CLA	C3D-C4D-ND	2.09	113.39	109.99
22	B2	814	CLA	C3D-C4D-ND	2.09	113.39	109.99
22	B	819	CLA	C3D-C4D-ND	2.09	113.39	109.99
22	9	613	CLA	C3D-C4D-ND	2.09	113.39	109.99
22	5	611	CLA	C3D-C4D-ND	2.09	113.38	109.99
22	A	811	CLA	C3D-C4D-ND	2.09	113.38	109.99
22	1	614	CLA	C3D-C4D-ND	2.09	113.38	109.99
22	9	603	CLA	C3D-C4D-ND	2.08	113.38	109.99
22	L	203	CLA	C3D-C4D-ND	2.08	113.37	109.99
22	Z	611	CLA	C3D-C4D-ND	2.08	113.37	109.99
22	A	803	CLA	C3B-C4B-NB	-2.08	108.67	110.53
22	1	602	CLA	C3D-C4D-ND	2.08	113.37	109.99
22	9	609	CLA	C3D-C4D-ND	2.08	113.37	109.99
22	B2	811	CLA	C3D-C4D-ND	2.08	113.37	109.99
22	B2	815	CLA	C3D-C4D-ND	2.08	113.37	109.99
22	B	833	CLA	C3D-C4D-ND	2.08	113.37	109.99
22	5	621	CLA	CHD-C1D-ND	-2.08	121.88	124.80
22	F	303	CLA	C3D-C4D-ND	2.08	113.36	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	610	CLA	C3D-C4D-ND	2.08	113.36	109.99
22	A	824	CLA	C3D-C4D-ND	2.07	113.36	109.99
22	5	613	CLA	C3D-C4D-ND	2.07	113.36	109.99
22	9	603	CLA	CHC-C4B-NB	2.07	127.16	124.05
22	8	611	CLA	C3D-C4D-ND	2.07	113.35	109.99
22	1	612	CLA	CHC-C4B-NB	2.07	127.15	124.05
33	5	625	NEX	O24-C25-C26	-2.07	57.29	58.93
22	A	827	CLA	C3D-C4D-ND	2.07	113.35	109.99
22	7	604	CLA	C3D-C4D-ND	2.07	113.35	109.99
22	B	823	CLA	C3D-C4D-ND	2.07	113.34	109.99
31	7	606	CHL	C1A-CHA-C4D	2.06	122.42	118.98
22	6	614	CLA	C3D-C4D-ND	2.06	113.33	109.99
22	B	828	CLA	C3D-C4D-ND	2.06	113.33	109.99
22	Z	608	CLA	C3D-C4D-ND	2.06	113.33	109.99
22	B	834	CLA	C3D-C4D-ND	2.06	113.33	109.99
22	B2	829	CLA	C3D-C4D-ND	2.05	113.33	109.99
22	6	602	CLA	C3D-C4D-ND	2.05	113.32	109.99
22	B	836	CLA	C3D-C4D-ND	2.05	113.32	109.99
22	3	612	CLA	C3D-C4D-ND	2.05	113.32	109.99
22	1	616	CLA	C3D-C4D-ND	2.05	113.31	109.99
22	B	822	CLA	C3D-C4D-ND	2.05	113.31	109.99
33	6	625	NEX	O24-C25-C26	-2.05	57.31	58.93
31	7	601	CHL	C1A-CHA-C4D	2.05	122.40	118.98
22	F	304	CLA	C3D-C4D-ND	2.05	113.31	109.99
22	8	614	CLA	C3D-C4D-ND	2.05	113.31	109.99
32	7	622	XAT	O4-C5-C6	-2.04	57.31	58.93
22	7	603	CLA	C3D-C4D-ND	2.04	113.31	109.99
22	Z	616	CLA	C3D-C4D-ND	2.04	113.31	109.99
22	5	614	CLA	C3D-C4D-ND	2.04	113.31	109.99
22	B	817	CLA	C3D-C4D-ND	2.04	113.31	109.99
22	3	610	CLA	C3D-C4D-ND	2.04	113.31	109.99
22	4	616	CLA	C3D-C4D-ND	2.04	113.31	109.99
22	F	304	CLA	O2A-C1-C2	2.04	115.97	108.11
22	B2	805	CLA	C3D-C4D-ND	2.04	113.30	109.99
22	7	609	CLA	C3D-C4D-ND	2.04	113.30	109.99
22	6	613	CLA	C3D-C4D-ND	2.03	113.29	109.99
22	6	610	CLA	C3D-C4D-ND	2.03	113.29	109.99
22	B	807	CLA	C3D-C4D-ND	2.03	113.29	109.99
22	1	608	CLA	C3D-C4D-ND	2.03	113.29	109.99
22	A	835	CLA	C3D-C4D-ND	2.03	113.28	109.99
22	B2	810	CLA	C3D-C4D-ND	2.03	113.28	109.99
22	A	813	CLA	C3D-C4D-ND	2.03	113.28	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	613	CLA	CHC-C4B-NB	2.03	127.09	124.05
22	9	613	CLA	CHC-C4B-NB	2.03	127.09	124.05
22	B	840	CLA	C3D-C4D-ND	2.03	113.28	109.99
22	A	839	CLA	CHC-C4B-NB	2.03	127.09	124.05
22	6	604	CLA	C3D-C4D-ND	2.03	113.28	109.99
22	B2	807	CLA	C3D-C4D-ND	2.03	113.28	109.99
22	A	803	CLA	C3D-C4D-ND	2.02	113.28	109.99
22	7	610	CLA	C3B-C4B-NB	-2.02	108.72	110.53
22	B	805	CLA	C3D-C4D-ND	2.02	113.28	109.99
22	4	602	CLA	C3D-C4D-ND	2.02	113.28	109.99
22	A	854	CLA	C3B-C4B-NB	-2.02	108.72	110.53
22	A	841	CLA	C3D-C4D-ND	2.02	113.27	109.99
22	B	841	CLA	C3D-C4D-ND	2.02	113.27	109.99
22	A	839	CLA	C3D-C4D-ND	2.02	113.27	109.99
22	Z	608	CLA	CHC-C4B-NB	2.02	127.08	124.05
22	B2	828	CLA	C3D-C4D-ND	2.02	113.27	109.99
31	4	607	CHL	C1A-CHA-C4D	2.02	122.35	118.98
22	5	604	CLA	C3D-C4D-ND	2.01	113.26	109.99
31	6	616	CHL	C1A-CHA-C4D	2.01	122.34	118.98
31	6	608	CHL	C4D-ND-C1D	-2.01	103.69	105.22
22	B2	813	CLA	C3D-C4D-ND	2.01	113.25	109.99
22	5	616	CLA	C3D-C4D-ND	2.01	113.25	109.99
22	9	602	CLA	C3D-C4D-ND	2.01	113.25	109.99
22	A	818	CLA	C3D-C4D-ND	2.01	113.25	109.99
22	3	615	CLA	CHC-C4B-NB	2.01	127.06	124.05
31	5	608	CHL	C4D-ND-C1D	-2.01	103.70	105.22
22	G	204	CLA	C3D-C4D-ND	2.00	113.24	109.99
22	A	812	CLA	CHC-C4B-NB	2.00	127.05	124.05
22	K	203	CLA	C3D-C4D-ND	2.00	113.24	109.99
22	B2	820	CLA	C3D-C4D-ND	2.00	113.24	109.99

All (328) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	801	CL0	ND
21	A	801	CL0	NA
21	A	801	CL0	NC
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND
22	A	805	CLA	ND
22	A	806	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	807	CLA	ND
22	A	808	CLA	ND
22	A	809	CLA	ND
22	A	810	CLA	ND
22	A	811	CLA	ND
22	A	812	CLA	ND
22	A	813	CLA	ND
22	A	814	CLA	ND
22	A	815	CLA	ND
22	A	816	CLA	ND
22	A	817	CLA	ND
22	A	818	CLA	ND
22	A	819	CLA	ND
22	A	820	CLA	ND
22	A	821	CLA	ND
22	A	822	CLA	ND
22	A	823	CLA	ND
22	A	824	CLA	ND
22	A	825	CLA	ND
22	A	826	CLA	ND
22	A	827	CLA	ND
22	A	828	CLA	ND
22	A	829	CLA	ND
22	A	830	CLA	ND
22	A	831	CLA	ND
22	A	832	CLA	ND
22	A	833	CLA	ND
22	A	834	CLA	ND
22	A	835	CLA	ND
22	A	836	CLA	ND
22	A	837	CLA	ND
22	A	838	CLA	ND
22	A	839	CLA	ND
22	A	840	CLA	ND
22	A	841	CLA	ND
22	A	842	CLA	ND
22	A	843	CLA	ND
22	A	845	CLA	ND
22	A	854	CLA	ND
22	B	802	CLA	ND
22	B	803	CLA	ND
22	B	804	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	805	CLA	ND
22	B	806	CLA	ND
22	B	807	CLA	ND
22	B	808	CLA	ND
22	B	809	CLA	ND
22	B	810	CLA	ND
22	B	811	CLA	ND
22	B	812	CLA	ND
22	B	813	CLA	ND
22	B	814	CLA	ND
22	B	815	CLA	ND
22	B	816	CLA	ND
22	B	817	CLA	ND
22	B	818	CLA	ND
22	B	819	CLA	ND
22	B	820	CLA	ND
22	B	821	CLA	ND
22	B	822	CLA	ND
22	B	823	CLA	ND
22	B	824	CLA	ND
22	B	825	CLA	ND
22	B	826	CLA	ND
22	B	827	CLA	ND
22	B	828	CLA	ND
22	B	829	CLA	ND
22	B	830	CLA	ND
22	B	831	CLA	ND
22	B	832	CLA	ND
22	B	833	CLA	ND
22	B	834	CLA	ND
22	B	835	CLA	ND
22	B	836	CLA	ND
22	B	837	CLA	ND
22	B	838	CLA	ND
22	B	839	CLA	ND
22	B	840	CLA	ND
22	B	841	CLA	ND
22	F	301	CLA	ND
22	F	303	CLA	ND
22	F	304	CLA	ND
22	G	203	CLA	ND
22	G	204	CLA	ND

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Mol	Chain	Res	Type	Atom
22	J	101	CLA	ND
22	L	203	CLA	ND
22	L	204	CLA	ND
22	K	201	CLA	ND
22	K	203	CLA	ND
22	K	204	CLA	ND
22	K	206	CLA	ND
22	1	602	CLA	ND
22	1	603	CLA	ND
22	1	604	CLA	ND
22	1	608	CLA	ND
22	1	609	CLA	ND
22	1	610	CLA	ND
22	1	611	CLA	ND
22	1	612	CLA	ND
22	1	613	CLA	ND
22	1	614	CLA	ND
22	1	616	CLA	ND
22	3	602	CLA	ND
22	3	603	CLA	ND
22	3	604	CLA	ND
22	3	606	CLA	ND
22	3	607	CLA	ND
22	3	609	CLA	ND
22	3	610	CLA	ND
22	3	611	CLA	ND
22	3	612	CLA	ND
22	3	613	CLA	ND
22	3	614	CLA	ND
22	3	617	CLA	ND
22	3	615	CLA	ND
22	7	602	CLA	ND
22	7	603	CLA	ND
22	7	604	CLA	ND
22	7	608	CLA	ND
22	7	609	CLA	ND
22	7	610	CLA	ND
22	7	611	CLA	ND
22	7	612	CLA	ND
22	7	613	CLA	ND
22	7	614	CLA	ND
22	7	616	CLA	ND

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Mol	Chain	Res	Type	Atom
22	7	620	CLA	ND
22	8	602	CLA	ND
22	8	603	CLA	ND
22	8	604	CLA	ND
22	8	608	CLA	ND
22	8	609	CLA	ND
22	8	610	CLA	ND
22	8	611	CLA	ND
22	8	612	CLA	ND
22	8	613	CLA	ND
22	8	614	CLA	ND
22	8	616	CLA	ND
22	Z	602	CLA	ND
22	Z	603	CLA	ND
22	Z	604	CLA	ND
22	Z	608	CLA	ND
22	Z	609	CLA	ND
22	Z	610	CLA	ND
22	Z	611	CLA	ND
22	Z	612	CLA	ND
22	Z	613	CLA	ND
22	Z	614	CLA	ND
22	Z	616	CLA	ND
22	4	602	CLA	ND
22	4	603	CLA	ND
22	4	604	CLA	ND
22	4	609	CLA	ND
22	4	610	CLA	ND
22	4	611	CLA	ND
22	4	612	CLA	ND
22	4	613	CLA	ND
22	4	614	CLA	ND
22	4	616	CLA	ND
22	5	601	CLA	ND
22	5	602	CLA	ND
22	5	603	CLA	ND
22	5	604	CLA	ND
22	5	609	CLA	ND
22	5	610	CLA	ND
22	5	611	CLA	ND
22	5	612	CLA	ND
22	5	613	CLA	ND

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Mol	Chain	Res	Type	Atom
22	5	614	CLA	ND
22	5	616	CLA	ND
22	5	617	CLA	ND
22	5	621	CLA	ND
22	6	602	CLA	ND
22	6	603	CLA	ND
22	6	604	CLA	ND
22	6	609	CLA	ND
22	6	610	CLA	ND
22	6	611	CLA	ND
22	6	612	CLA	ND
22	6	613	CLA	ND
22	6	614	CLA	ND
22	6	617	CLA	ND
22	6	622	CLA	ND
22	9	601	CLA	ND
22	9	602	CLA	ND
22	9	603	CLA	ND
22	9	604	CLA	ND
22	9	609	CLA	ND
22	9	610	CLA	ND
22	9	611	CLA	ND
22	9	612	CLA	ND
22	9	613	CLA	ND
22	9	614	CLA	ND
22	B2	804	CLA	ND
22	B2	805	CLA	ND
22	B2	806	CLA	ND
22	B2	807	CLA	ND
22	B2	808	CLA	ND
22	B2	809	CLA	ND
22	B2	810	CLA	ND
22	B2	811	CLA	ND
22	B2	813	CLA	ND
22	B2	814	CLA	ND
22	B2	815	CLA	ND
22	B2	828	CLA	ND
22	B2	829	CLA	ND
22	B2	839	CLA	ND
22	B2	812	CLA	ND
22	B2	820	CLA	ND
22	L2	203	CLA	ND

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Mol	Chain	Res	Type	Atom
22	L2	204	CLA	ND
22	92	601	CLA	ND
22	92	602	CLA	ND
22	92	603	CLA	ND
22	92	604	CLA	ND
22	92	609	CLA	ND
22	92	610	CLA	ND
22	92	611	CLA	ND
22	92	612	CLA	ND
22	92	613	CLA	ND
22	92	614	CLA	ND
31	1	601	CHL	ND
31	1	601	CHL	NA
31	1	601	CHL	NC
31	1	606	CHL	ND
31	1	606	CHL	NA
31	1	606	CHL	NC
31	1	607	CHL	ND
31	1	607	CHL	NA
31	1	607	CHL	NC
31	3	608	CHL	ND
31	3	608	CHL	NA
31	3	608	CHL	NC
31	7	601	CHL	ND
31	7	601	CHL	NA
31	7	601	CHL	NC
31	7	606	CHL	ND
31	7	606	CHL	NA
31	7	606	CHL	NC
31	7	607	CHL	ND
31	7	607	CHL	NA
31	7	607	CHL	NC
31	8	601	CHL	ND
31	8	601	CHL	NA
31	8	601	CHL	NC
31	8	606	CHL	ND
31	8	606	CHL	NA
31	8	606	CHL	NC
31	8	607	CHL	ND
31	8	607	CHL	NA
31	8	607	CHL	NC
31	Z	601	CHL	ND

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Mol	Chain	Res	Type	Atom
31	Z	601	CHL	NA
31	Z	601	CHL	NC
31	Z	606	CHL	ND
31	Z	606	CHL	NA
31	Z	606	CHL	NC
31	Z	607	CHL	ND
31	Z	607	CHL	NA
31	Z	607	CHL	NC
31	4	601	CHL	ND
31	4	601	CHL	NA
31	4	601	CHL	NC
31	4	606	CHL	ND
31	4	606	CHL	NA
31	4	606	CHL	NC
31	4	607	CHL	ND
31	4	607	CHL	NA
31	4	607	CHL	NC
31	4	608	CHL	ND
31	4	608	CHL	NA
31	4	608	CHL	NC
31	4	618	CHL	ND
31	4	618	CHL	NA
31	4	618	CHL	NC
31	5	606	CHL	ND
31	5	606	CHL	NA
31	5	606	CHL	NC
31	5	607	CHL	ND
31	5	607	CHL	NA
31	5	607	CHL	NC
31	5	608	CHL	ND
31	5	608	CHL	NA
31	5	608	CHL	NC
31	5	618	CHL	ND
31	5	618	CHL	NA
31	5	618	CHL	NC
31	6	601	CHL	ND
31	6	601	CHL	NA
31	6	601	CHL	NC
31	6	606	CHL	ND
31	6	606	CHL	NA
31	6	606	CHL	NC
31	6	607	CHL	ND

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Mol	Chain	Res	Type	Atom
31	6	607	CHL	NA
31	6	607	CHL	NC
31	6	608	CHL	ND
31	6	608	CHL	NA
31	6	608	CHL	NC
31	6	616	CHL	ND
31	6	616	CHL	NA
31	6	616	CHL	NC
31	6	618	CHL	ND
31	6	618	CHL	NA
31	6	618	CHL	NC
31	9	606	CHL	ND
31	9	606	CHL	NA
31	9	606	CHL	NC
31	9	607	CHL	ND
31	9	607	CHL	NA
31	9	607	CHL	NC
31	92	606	CHL	ND
31	92	606	CHL	NA
31	92	606	CHL	NC
31	92	607	CHL	ND
31	92	607	CHL	NA
31	92	607	CHL	NC
32	1	618	XAT	C6
32	5	624	XAT	C26
33	6	625	NEX	C25

All (1439) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	806	CLA	CAD-CBD-CGD-O1D
22	A	806	CLA	CAD-CBD-CGD-O2D
22	A	806	CLA	C2-C3-C5-C6
22	A	806	CLA	C4-C3-C5-C6
22	A	809	CLA	CHA-CBD-CGD-O1D
22	A	809	CLA	CHA-CBD-CGD-O2D
22	A	816	CLA	O2A-C1-C2-C3
22	A	817	CLA	CHA-CBD-CGD-O1D
22	A	817	CLA	CHA-CBD-CGD-O2D
22	A	821	CLA	C2B-C3B-CAB-CBB
22	A	821	CLA	C4B-C3B-CAB-CBB
22	A	823	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	A	823	CLA	C4B-C3B-CAB-CBB
22	A	825	CLA	C4B-C3B-CAB-CBB
22	A	831	CLA	CHA-CBD-CGD-O1D
22	A	831	CLA	CHA-CBD-CGD-O2D
22	A	834	CLA	C2B-C3B-CAB-CBB
22	A	834	CLA	C4B-C3B-CAB-CBB
22	A	835	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	841	CLA	C2B-C3B-CAB-CBB
22	A	841	CLA	C4B-C3B-CAB-CBB
22	A	842	CLA	C2B-C3B-CAB-CBB
22	A	842	CLA	C4B-C3B-CAB-CBB
22	A	845	CLA	CAD-CBD-CGD-O1D
22	A	845	CLA	CAD-CBD-CGD-O2D
22	B	804	CLA	CHA-CBD-CGD-O1D
22	B	804	CLA	CHA-CBD-CGD-O2D
22	B	808	CLA	CHA-CBD-CGD-O1D
22	B	808	CLA	CHA-CBD-CGD-O2D
22	B	815	CLA	CHA-CBD-CGD-O1D
22	B	815	CLA	CHA-CBD-CGD-O2D
22	B	817	CLA	C2B-C3B-CAB-CBB
22	B	817	CLA	C4B-C3B-CAB-CBB
22	B	819	CLA	C2B-C3B-CAB-CBB
22	B	819	CLA	C4B-C3B-CAB-CBB
22	B	821	CLA	C4B-C3B-CAB-CBB
22	B	825	CLA	CHA-CBD-CGD-O1D
22	B	825	CLA	CHA-CBD-CGD-O2D
22	B	828	CLA	C4B-C3B-CAB-CBB
22	B	833	CLA	CHA-CBD-CGD-O1D
22	B	833	CLA	CHA-CBD-CGD-O2D
22	F	304	CLA	C1A-C2A-CAA-CBA
22	F	304	CLA	C2-C1-O2A-CGA
22	G	204	CLA	CHA-CBD-CGD-O1D
22	G	204	CLA	CHA-CBD-CGD-O2D
22	K	201	CLA	C2B-C3B-CAB-CBB
22	K	201	CLA	C4B-C3B-CAB-CBB
22	1	610	CLA	C2B-C3B-CAB-CBB
22	1	610	CLA	C4B-C3B-CAB-CBB
22	1	611	CLA	C2B-C3B-CAB-CBB
22	1	611	CLA	C4B-C3B-CAB-CBB
22	1	613	CLA	C2B-C3B-CAB-CBB
22	1	613	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	1	614	CLA	C2B-C3B-CAB-CBB
22	1	614	CLA	C4B-C3B-CAB-CBB
22	3	611	CLA	C2B-C3B-CAB-CBB
22	3	611	CLA	C4B-C3B-CAB-CBB
22	3	613	CLA	C4B-C3B-CAB-CBB
22	3	614	CLA	C2B-C3B-CAB-CBB
22	3	614	CLA	C4B-C3B-CAB-CBB
22	7	602	CLA	CHA-CBD-CGD-O1D
22	7	602	CLA	CHA-CBD-CGD-O2D
22	7	610	CLA	C1A-C2A-CAA-CBA
22	7	610	CLA	C3A-C2A-CAA-CBA
22	7	611	CLA	C2B-C3B-CAB-CBB
22	7	611	CLA	C4B-C3B-CAB-CBB
22	7	614	CLA	C2B-C3B-CAB-CBB
22	7	614	CLA	C4B-C3B-CAB-CBB
22	7	620	CLA	C2B-C3B-CAB-CBB
22	7	620	CLA	C4B-C3B-CAB-CBB
22	8	602	CLA	CHA-CBD-CGD-O2D
22	8	612	CLA	CHA-CBD-CGD-O1D
22	8	612	CLA	CHA-CBD-CGD-O2D
22	8	613	CLA	C2B-C3B-CAB-CBB
22	8	613	CLA	C4B-C3B-CAB-CBB
22	Z	602	CLA	CHA-CBD-CGD-O2D
22	Z	609	CLA	C1A-C2A-CAA-CBA
22	Z	613	CLA	C4B-C3B-CAB-CBB
22	4	602	CLA	CHA-CBD-CGD-O1D
22	4	602	CLA	CHA-CBD-CGD-O2D
22	4	609	CLA	C4B-C3B-CAB-CBB
22	4	610	CLA	C4-C3-C5-C6
22	4	612	CLA	CHA-CBD-CGD-O1D
22	4	612	CLA	CHA-CBD-CGD-O2D
22	4	613	CLA	C2B-C3B-CAB-CBB
22	4	613	CLA	C4B-C3B-CAB-CBB
22	4	613	CLA	C4-C3-C5-C6
22	5	603	CLA	CHA-CBD-CGD-O1D
22	5	603	CLA	CHA-CBD-CGD-O2D
22	6	602	CLA	CHA-CBD-CGD-O1D
22	6	602	CLA	CHA-CBD-CGD-O2D
22	6	609	CLA	C2B-C3B-CAB-CBB
22	6	609	CLA	C4B-C3B-CAB-CBB
22	9	602	CLA	CHA-CBD-CGD-O1D
22	9	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	9	609	CLA	C2B-C3B-CAB-CBB
22	9	609	CLA	C4B-C3B-CAB-CBB
22	9	609	CLA	C4-C3-C5-C6
22	9	611	CLA	C2B-C3B-CAB-CBB
22	9	611	CLA	C4B-C3B-CAB-CBB
22	9	612	CLA	CHA-CBD-CGD-O1D
22	9	612	CLA	CHA-CBD-CGD-O2D
22	9	614	CLA	C2B-C3B-CAB-CBB
22	9	614	CLA	C4B-C3B-CAB-CBB
22	B2	807	CLA	C4B-C3B-CAB-CBB
22	B2	808	CLA	CHA-CBD-CGD-O1D
22	B2	808	CLA	CHA-CBD-CGD-O2D
22	B2	810	CLA	C1A-C2A-CAA-CBA
22	B2	814	CLA	CAD-CBD-CGD-O1D
22	B2	814	CLA	CAD-CBD-CGD-O2D
22	B2	815	CLA	CHA-CBD-CGD-O1D
22	B2	815	CLA	CHA-CBD-CGD-O2D
22	L2	204	CLA	C4B-C3B-CAB-CBB
22	L2	204	CLA	CHA-CBD-CGD-O1D
22	L2	204	CLA	CHA-CBD-CGD-O2D
22	92	601	CLA	CHA-CBD-CGD-O1D
22	92	601	CLA	CHA-CBD-CGD-O2D
22	92	602	CLA	CHA-CBD-CGD-O1D
22	92	602	CLA	CHA-CBD-CGD-O2D
22	92	602	CLA	C2-C3-C5-C6
22	92	602	CLA	C4-C3-C5-C6
22	92	604	CLA	C2B-C3B-CAB-CBB
22	92	604	CLA	C4B-C3B-CAB-CBB
22	92	604	CLA	CHA-CBD-CGD-O1D
22	92	604	CLA	CHA-CBD-CGD-O2D
22	92	609	CLA	C1A-C2A-CAA-CBA
22	92	609	CLA	C2B-C3B-CAB-CBB
22	92	609	CLA	C4B-C3B-CAB-CBB
22	92	611	CLA	C2B-C3B-CAB-CBB
22	92	611	CLA	C4B-C3B-CAB-CBB
24	A	846	LHG	C3-O3-P-O5
24	A	846	LHG	C4-O6-P-O3
24	A	846	LHG	C4-O6-P-O5
24	A	847	LHG	C4-O6-P-O3
24	1	620	LHG	C3-O3-P-O6
24	3	721	LHG	C2-C3-O3-P
24	3	721	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
24	3	721	LHG	C4-O6-P-O3
24	3	721	LHG	C4-O6-P-O5
24	3	623	LHG	O2-C2-C3-O3
24	3	623	LHG	C3-O3-P-O5
24	3	623	LHG	C3-O3-P-O6
24	3	623	LHG	O6-C4-C5-O7
24	7	625	LHG	C1-C2-C3-O3
24	7	625	LHG	C3-O3-P-O4
24	7	625	LHG	C3-O3-P-O5
24	7	625	LHG	C3-O3-P-O6
24	8	620	LHG	C3-O3-P-O5
24	8	620	LHG	C3-O3-P-O6
24	8	620	LHG	C4-O6-P-O3
24	8	620	LHG	C4-O6-P-O4
24	4	622	LHG	C2-C3-O3-P
24	4	622	LHG	C3-O3-P-O4
24	4	622	LHG	C3-O3-P-O6
24	4	623	LHG	C3-O3-P-O4
24	4	623	LHG	C3-O3-P-O5
24	4	623	LHG	C3-O3-P-O6
24	4	623	LHG	C4-O6-P-O3
24	4	623	LHG	C4-O6-P-O4
24	4	623	LHG	C4-O6-P-O5
24	5	623	LHG	C3-O3-P-O5
24	5	623	LHG	C3-O3-P-O6
24	5	623	LHG	C4-O6-P-O3
24	5	623	LHG	C4-O6-P-O4
24	5	623	LHG	C4-O6-P-O5
24	6	629	LHG	C1-C2-C3-O3
24	6	629	LHG	C4-O6-P-O3
24	6	629	LHG	C4-O6-P-O4
24	6	629	LHG	C4-O6-P-O5
24	9	622	LHG	C1-C2-C3-O3
24	9	622	LHG	C3-O3-P-O5
24	9	622	LHG	C4-O6-P-O4
24	92	622	LHG	C1-C2-C3-O3
24	92	622	LHG	C4-O6-P-O3
24	92	622	LHG	C4-O6-P-O4
25	A	851	BCR	C23-C24-C25-C26
25	A	851	BCR	C23-C24-C25-C30
25	J	102	BCR	C23-C24-C25-C26
25	3	620	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	3	620	BCR	C5-C6-C7-C8
25	8	619	BCR	C1-C6-C7-C8
25	8	619	BCR	C5-C6-C7-C8
25	9	623	BCR	C23-C24-C25-C26
25	92	623	BCR	C23-C24-C25-C26
27	A	858	LMU	O5'-C1'-O1'-C1
27	A	865	LMU	C2'-C1'-O1'-C1
27	A	865	LMU	O5'-C1'-O1'-C1
27	B	853	LMU	O5'-C1'-O1'-C1
27	1	627	LMU	C2'-C1'-O1'-C1
27	1	627	LMU	O5'-C1'-O1'-C1
27	7	628	LMU	C2'-C1'-O1'-C1
27	7	628	LMU	O5'-C1'-O1'-C1
27	7	628	LMU	C2-C1-O1'-C1'
27	7	629	LMU	C2'-C1'-O1'-C1
27	7	629	LMU	O5'-C1'-O1'-C1
27	5	627	LMU	C2-C1-O1'-C1'
27	6	632	LMU	O5'-C1'-O1'-C1
27	6	632	LMU	C2-C1-O1'-C1'
27	6	628	LMU	O5'-C1'-O1'-C1
28	A	859	LMG	O6-C1-O1-C7
28	B	854	LMG	C2-C1-O1-C7
28	B	854	LMG	O6-C1-O1-C7
28	8	626	LMG	C2-C1-O1-C7
28	8	626	LMG	O6-C1-O1-C7
28	8	629	LMG	C2-C1-O1-C7
28	8	629	LMG	O6-C1-O1-C7
28	B2	852	LMG	O6-C1-O1-C7
29	A	856	LUT	C5-C6-C7-C8
29	A	856	LUT	C21-C26-C27-C28
29	A	856	LUT	C25-C26-C27-C28
29	F	305	LUT	C1-C6-C7-C8
29	F	305	LUT	C5-C6-C7-C8
29	F	305	LUT	C25-C26-C27-C28
29	7	624	LUT	C21-C26-C27-C28
29	7	624	LUT	C25-C26-C27-C28
29	7	624	LUT	C27-C28-C29-C30
29	5	626	LUT	C21-C26-C27-C28
29	5	626	LUT	C25-C26-C27-C28
30	B	850	DGD	O6D-C1D-O3G-C3G
31	8	601	CHL	CAD-CBD-CGD-O1D
31	8	601	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	5	607	CHL	CHA-CBD-CGD-O1D
31	5	607	CHL	CHA-CBD-CGD-O2D
27	A	858	LMU	O5B-C1B-O1B-C4'
27	A	858	LMU	C2B-C1B-O1B-C4'
22	B	806	CLA	C3-C5-C6-C7
27	A	863	LMU	O5B-C1B-O1B-C4'
27	8	627	LMU	O5B-C1B-O1B-C4'
22	A	829	CLA	C4-C3-C5-C6
22	B	822	CLA	C4-C3-C5-C6
22	B	840	CLA	C4-C3-C5-C6
22	J	101	CLA	C4-C3-C5-C6
22	L	203	CLA	C4-C3-C5-C6
22	1	603	CLA	C4-C3-C5-C6
22	5	611	CLA	C4-C3-C5-C6
22	5	617	CLA	C4-C3-C5-C6
31	1	601	CHL	C4-C3-C5-C6
31	8	607	CHL	C4-C3-C5-C6
22	A	829	CLA	C2-C3-C5-C6
22	B	822	CLA	C2-C3-C5-C6
22	J	101	CLA	C2-C3-C5-C6
22	1	603	CLA	C2-C3-C5-C6
22	4	610	CLA	C2-C3-C5-C6
22	4	613	CLA	C2-C3-C5-C6
22	5	611	CLA	C2-C3-C5-C6
22	5	617	CLA	C2-C3-C5-C6
31	1	601	CHL	C2-C3-C5-C6
31	8	607	CHL	C2-C3-C5-C6
22	5	603	CLA	C2A-CAA-CBA-CGA
27	A	863	LMU	C2B-C1B-O1B-C4'
27	8	627	LMU	C2B-C1B-O1B-C4'
22	5	621	CLA	C2C-C3C-CAC-CBC
22	B	808	CLA	C3-C5-C6-C7
27	B	853	LMU	C2B-C1B-O1B-C4'
24	3	721	LHG	O2-C2-C3-O3
24	7	625	LHG	O2-C2-C3-O3
24	4	623	LHG	O2-C2-C3-O3
24	6	629	LHG	O2-C2-C3-O3
24	9	622	LHG	O2-C2-C3-O3
24	92	622	LHG	O2-C2-C3-O3
22	B	833	CLA	C4-C3-C5-C6
22	8	612	CLA	C4-C3-C5-C6
31	7	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	833	CLA	C2-C3-C5-C6
22	B	840	CLA	C2-C3-C5-C6
22	7	612	CLA	C2-C3-C5-C6
22	8	612	CLA	C2-C3-C5-C6
24	6	629	LHG	C2-C3-O3-P
27	A	864	LMU	O5'-C1'-O1'-C1
27	G	206	LMU	O5'-C1'-O1'-C1
27	1	622	LMU	O5'-C1'-O1'-C1
27	7	627	LMU	O5'-C1'-O1'-C1
27	Z	621	LMU	O5'-C1'-O1'-C1
27	4	625	LMU	O5'-C1'-O1'-C1
27	6	631	LMU	O5'-C1'-O1'-C1
28	A	860	LMG	O6-C1-O1-C7
28	7	626	LMG	O6-C1-O1-C7
28	9	620	LMG	O6-C1-O1-C7
27	8	627	LMU	C5'-C4'-O1B-C1B
24	1	620	LHG	C1-C2-C3-O3
24	3	623	LHG	C1-C2-C3-O3
22	7	612	CLA	C4-C3-C5-C6
22	Z	603	CLA	C4-C3-C5-C6
22	L	203	CLA	C2-C3-C5-C6
22	Z	603	CLA	C2-C3-C5-C6
31	7	601	CHL	C2-C3-C5-C6
22	A	806	CLA	C11-C10-C8-C9
22	B	808	CLA	C14-C13-C15-C16
22	B	809	CLA	C6-C7-C8-C9
22	G	203	CLA	C6-C7-C8-C9
22	1	609	CLA	C11-C10-C8-C9
22	4	609	CLA	C11-C10-C8-C9
22	5	603	CLA	C11-C10-C8-C9
22	5	603	CLA	C14-C13-C15-C16
31	1	601	CHL	C6-C7-C8-C9
27	A	858	LMU	C2'-C1'-O1'-C1
27	G	206	LMU	C2'-C1'-O1'-C1
27	1	622	LMU	C2'-C1'-O1'-C1
27	7	627	LMU	C2'-C1'-O1'-C1
27	8	628	LMU	C2'-C1'-O1'-C1
27	Z	621	LMU	C2'-C1'-O1'-C1
27	4	625	LMU	C2'-C1'-O1'-C1
27	6	632	LMU	C2'-C1'-O1'-C1
27	6	628	LMU	C2'-C1'-O1'-C1
27	6	631	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
28	A	859	LMG	C2-C1-O1-C7
28	A	860	LMG	C2-C1-O1-C7
28	7	626	LMG	C2-C1-O1-C7
28	9	620	LMG	C2-C1-O1-C7
30	B	850	DGD	C2D-C1D-O3G-C3G
24	1	620	LHG	O2-C2-C3-O3
29	7	624	LUT	C27-C28-C29-C39
22	A	830	CLA	C2A-CAA-CBA-CGA
28	4	624	LMG	C10-C11-C12-C13
27	8	627	LMU	C3'-C4'-O1B-C1B
27	B	853	LMU	O5B-C1B-O1B-C4'
31	6	616	CHL	C8-C10-C11-C12
22	B	839	CLA	C2A-CAA-CBA-CGA
22	B	818	CLA	C13-C15-C16-C17
27	A	862	LMU	O5'-C1'-O1'-C1
27	A	861	LMU	O5'-C1'-O1'-C1
27	8	628	LMU	O5'-C1'-O1'-C1
22	B	803	CLA	C10-C11-C12-C13
22	5	609	CLA	C10-C11-C12-C13
24	8	620	LHG	O2-C2-C3-O3
22	5	617	CLA	C8-C10-C11-C12
22	4	603	CLA	C3-C5-C6-C7
22	A	840	CLA	C15-C16-C17-C18
24	8	620	LHG	C1-C2-C3-O3
24	4	623	LHG	C1-C2-C3-O3
22	7	616	CLA	C2A-CAA-CBA-CGA
22	B2	805	CLA	C2A-CAA-CBA-CGA
22	5	621	CLA	C4C-C3C-CAC-CBC
22	A	818	CLA	C3-C5-C6-C7
22	A	813	CLA	C15-C16-C17-C18
27	A	862	LMU	C2'-C1'-O1'-C1
27	A	863	LMU	C2'-C1'-O1'-C1
27	B	853	LMU	C2'-C1'-O1'-C1
27	K	208	LMU	C2'-C1'-O1'-C1
24	B	851	LHG	O2-C2-C3-O3
22	1	614	CLA	C2A-CAA-CBA-CGA
22	3	603	CLA	C8-C10-C11-C12
22	A	825	CLA	C3-C5-C6-C7
31	Z	607	CHL	C10-C11-C12-C13
28	6	633	LMG	C17-C18-C19-C20
27	92	624	LMU	O5'-C5'-C6'-O6'
27	1	627	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
27	Z	622	LMU	C2-C1-O1'-C1'
22	B	820	CLA	C5-C6-C7-C8
22	A	836	CLA	C4B-C3B-CAB-CBB
22	B	808	CLA	C4B-C3B-CAB-CBB
22	B	839	CLA	C4B-C3B-CAB-CBB
22	B	841	CLA	C4B-C3B-CAB-CBB
22	F	304	CLA	C4B-C3B-CAB-CBB
22	K	204	CLA	C4B-C3B-CAB-CBB
22	7	610	CLA	C4B-C3B-CAB-CBB
22	Z	608	CLA	C4B-C3B-CAB-CBB
22	6	617	CLA	C4B-C3B-CAB-CBB
22	9	601	CLA	C4B-C3B-CAB-CBB
22	B2	808	CLA	C4B-C3B-CAB-CBB
22	B2	809	CLA	C4B-C3B-CAB-CBB
22	B2	828	CLA	C4B-C3B-CAB-CBB
22	92	601	CLA	C4B-C3B-CAB-CBB
22	92	614	CLA	C4B-C3B-CAB-CBB
27	7	629	LMU	O5'-C5'-C6'-O6'
22	B	823	CLA	C2A-CAA-CBA-CGA
22	A	834	CLA	C3A-C2A-CAA-CBA
22	B	823	CLA	C3A-C2A-CAA-CBA
22	3	611	CLA	C3A-C2A-CAA-CBA
22	7	616	CLA	C3A-C2A-CAA-CBA
22	9	603	CLA	C3A-C2A-CAA-CBA
22	B2	810	CLA	C3A-C2A-CAA-CBA
31	Z	606	CHL	C3A-C2A-CAA-CBA
22	9	612	CLA	C13-C15-C16-C17
24	B	851	LHG	C1-C2-C3-O3
22	1	611	CLA	C5-C6-C7-C8
22	A	825	CLA	C2B-C3B-CAB-CBB
22	B	808	CLA	C2B-C3B-CAB-CBB
22	B	821	CLA	C2B-C3B-CAB-CBB
22	B	828	CLA	C2B-C3B-CAB-CBB
22	F	304	CLA	C2B-C3B-CAB-CBB
22	3	613	CLA	C2B-C3B-CAB-CBB
22	7	610	CLA	C2B-C3B-CAB-CBB
22	Z	613	CLA	C2B-C3B-CAB-CBB
22	4	609	CLA	C2B-C3B-CAB-CBB
22	6	617	CLA	C2B-C3B-CAB-CBB
22	9	601	CLA	C2B-C3B-CAB-CBB
22	B2	807	CLA	C2B-C3B-CAB-CBB
22	B2	828	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	L2	204	CLA	C2B-C3B-CAB-CBB
22	92	601	CLA	C2B-C3B-CAB-CBB
25	B	846	BCR	C23-C24-C25-C30
25	B	847	BCR	C23-C24-C25-C30
25	J	102	BCR	C23-C24-C25-C30
25	K	202	BCR	C23-C24-C25-C26
25	K	202	BCR	C23-C24-C25-C30
25	K	207	BCR	C23-C24-C25-C26
25	K	207	BCR	C23-C24-C25-C30
25	3	620	BCR	C23-C24-C25-C26
25	3	620	BCR	C23-C24-C25-C30
25	3	719	BCR	C23-C24-C25-C26
25	3	719	BCR	C23-C24-C25-C30
25	7	623	BCR	C23-C24-C25-C30
25	8	619	BCR	C23-C24-C25-C26
25	8	619	BCR	C23-C24-C25-C30
25	4	621	BCR	C23-C24-C25-C26
25	4	621	BCR	C23-C24-C25-C30
25	5	622	BCR	C23-C24-C25-C26
25	5	622	BCR	C23-C24-C25-C30
25	9	623	BCR	C23-C24-C25-C30
25	92	623	BCR	C1-C6-C7-C8
25	92	623	BCR	C5-C6-C7-C8
25	92	623	BCR	C23-C24-C25-C30
29	A	856	LUT	C1-C6-C7-C8
29	1	619	LUT	C1-C6-C7-C8
29	Z	619	LUT	C1-C6-C7-C8
29	Z	619	LUT	C5-C6-C7-C8
29	5	620	LUT	C1-C6-C7-C8
29	5	626	LUT	C1-C6-C7-C8
29	5	626	LUT	C5-C6-C7-C8
29	9	616	LUT	C1-C6-C7-C8
29	92	616	LUT	C1-C6-C7-C8
22	A	806	CLA	C5-C6-C7-C8
24	8	620	LHG	C23-C24-C25-C26
22	B2	810	CLA	C4-C3-C5-C6
24	6	619	LHG	C26-C27-C28-C29
22	B	829	CLA	C5-C6-C7-C8
27	1	621	LMU	O5B-C1B-O1B-C4'
22	6	613	CLA	C11-C10-C8-C9
27	A	863	LMU	O5'-C1'-O1'-C1
27	K	208	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
22	9	611	CLA	C10-C11-C12-C13
24	A	846	LHG	C23-C24-C25-C26
28	A	860	LMG	C8-C7-O1-C1
22	B2	810	CLA	C2-C3-C5-C6
28	B	852	LMG	C11-C12-C13-C14
22	Z	609	CLA	C13-C15-C16-C17
22	4	609	CLA	C5-C6-C7-C8
24	8	620	LHG	C17-C18-C19-C20
22	B	817	CLA	C2C-C3C-CAC-CBC
22	Z	604	CLA	C3-C5-C6-C7
27	A	864	LMU	O5'-C5'-C6'-O6'
27	B	853	LMU	O5'-C5'-C6'-O6'
27	6	630	LMU	O5'-C5'-C6'-O6'
28	1	628	LMG	O6-C5-C6-O5
28	7	626	LMG	O6-C5-C6-O5
22	3	607	CLA	C2C-C3C-CAC-CBC
28	B2	855	LMG	O6-C5-C6-O5
27	1	622	LMU	O5'-C5'-C6'-O6'
28	A	860	LMG	O6-C5-C6-O5
28	8	626	LMG	O6-C5-C6-O5
24	5	623	LHG	O7-C5-C6-O8
31	6	607	CHL	C15-C16-C17-C18
28	J	104	LMG	O6-C5-C6-O5
28	8	629	LMG	O6-C5-C6-O5
22	A	806	CLA	C2-C1-O2A-CGA
27	1	625	LMU	O5'-C5'-C6'-O6'
28	9	620	LMG	O6-C5-C6-O5
22	B	820	CLA	C4-C3-C5-C6
22	B2	806	CLA	C4-C3-C5-C6
22	5	603	CLA	C3-C5-C6-C7
22	A	843	CLA	C2-C3-C5-C6
22	B	820	CLA	C2-C3-C5-C6
22	A	854	CLA	C2A-CAA-CBA-CGA
27	A	861	LMU	O5'-C5'-C6'-O6'
24	B	851	LHG	C17-C18-C19-C20
22	A	826	CLA	C10-C11-C12-C13
22	A	836	CLA	C8-C10-C11-C12
22	B	840	CLA	C15-C16-C17-C18
22	K	203	CLA	C5-C6-C7-C8
22	1	608	CLA	C10-C11-C12-C13
24	4	622	LHG	C9-C10-C11-C12
31	4	608	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	4	624	LMG	O6-C5-C6-O5
22	B	827	CLA	C3-C5-C6-C7
22	A	812	CLA	C1A-C2A-CAA-CBA
22	A	834	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	C1A-C2A-CAA-CBA
22	B	838	CLA	C1A-C2A-CAA-CBA
22	J	101	CLA	C1A-C2A-CAA-CBA
22	1	611	CLA	C1A-C2A-CAA-CBA
22	3	611	CLA	C1A-C2A-CAA-CBA
22	9	603	CLA	C1A-C2A-CAA-CBA
27	8	627	LMU	O5B-C5B-C6B-O6B
22	A	834	CLA	C13-C15-C16-C17
22	B	836	CLA	C10-C11-C12-C13
24	A	847	LHG	O6-C4-C5-C6
24	3	721	LHG	O6-C4-C5-C6
24	5	623	LHG	O6-C4-C5-C6
27	8	625	LMU	O5'-C5'-C6'-O6'
22	A	834	CLA	C11-C10-C8-C7
22	1	614	CLA	C6-C7-C8-C10
22	5	603	CLA	C11-C10-C8-C7
23	A	844	PQN	C17-C18-C20-C21
31	Z	601	CHL	C6-C7-C8-C10
27	A	857	LMU	O5B-C5B-C6B-O6B
22	A	835	CLA	C4-C3-C5-C6
22	B	828	CLA	C4-C3-C5-C6
22	9	611	CLA	C4-C3-C5-C6
31	6	607	CHL	C4-C3-C5-C6
22	A	835	CLA	C2-C3-C5-C6
22	B	828	CLA	C2-C3-C5-C6
22	6	613	CLA	C2-C3-C5-C6
31	6	607	CHL	C2-C3-C5-C6
27	A	858	LMU	O5B-C5B-C6B-O6B
22	B	824	CLA	C8-C10-C11-C12
22	B	805	CLA	C14-C13-C15-C16
22	B	827	CLA	C11-C10-C8-C9
22	B	834	CLA	C11-C10-C8-C9
22	Z	609	CLA	C11-C12-C13-C14
31	5	607	CHL	C6-C7-C8-C9
27	9	624	LMU	C4-C5-C6-C7
31	8	607	CHL	C15-C16-C17-C18
24	7	625	LHG	C4-C5-C6-O8
28	J	104	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	4	624	LMG	O1-C7-C8-C9
28	3	722	LMG	C33-C34-C35-C36
27	G	206	LMU	O5'-C5'-C6'-O6'
27	8	628	LMU	O5'-C5'-C6'-O6'
28	J	103	LMG	C16-C17-C18-C19
22	Z	611	CLA	C10-C11-C12-C13
31	5	618	CHL	CHA-CBD-CGD-O2D
22	A	833	CLA	C3-C5-C6-C7
27	9	624	LMU	O5'-C5'-C6'-O6'
22	A	826	CLA	C4-C3-C5-C6
22	A	826	CLA	C2-C3-C5-C6
22	B	839	CLA	C2-C3-C5-C6
27	6	631	LMU	O5'-C5'-C6'-O6'
22	5	601	CLA	C10-C11-C12-C13
22	6	603	CLA	C5-C6-C7-C8
22	A	806	CLA	C2A-CAA-CBA-CGA
22	A	810	CLA	C2A-CAA-CBA-CGA
22	A	826	CLA	O2A-C1-C2-C3
22	A	843	CLA	O2A-C1-C2-C3
22	9	609	CLA	O2A-C1-C2-C3
22	9	613	CLA	O2A-C1-C2-C3
31	Z	601	CHL	O2A-C1-C2-C3
24	A	847	LHG	O6-C4-C5-O7
22	B	811	CLA	C15-C16-C17-C18
22	B	821	CLA	C10-C11-C12-C13
22	5	603	CLA	C5-C6-C7-C8
22	B	839	CLA	C4-C3-C5-C6
22	A	817	CLA	C2-C3-C5-C6
22	9	611	CLA	C2-C3-C5-C6
22	B2	806	CLA	C2-C3-C5-C6
27	1	623	LMU	C11-C10-C9-C8
24	B	851	LHG	O7-C5-C6-O8
22	8	603	CLA	C15-C16-C17-C18
22	A	829	CLA	C5-C6-C7-C8
22	B	817	CLA	C13-C15-C16-C17
22	A	817	CLA	C4-C3-C5-C6
22	A	820	CLA	C4-C3-C5-C6
22	A	828	CLA	C4-C3-C5-C6
22	A	830	CLA	C4-C3-C5-C6
22	A	840	CLA	C4-C3-C5-C6
22	A	841	CLA	C4-C3-C5-C6
22	B	807	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	812	CLA	C4-C3-C5-C6
22	3	603	CLA	C4-C3-C5-C6
22	6	613	CLA	C4-C3-C5-C6
22	9	612	CLA	C4-C3-C5-C6
22	92	612	CLA	C4-C3-C5-C6
31	6	601	CHL	C4-C3-C5-C6
27	B	853	LMU	C2-C1-O1'-C1'
27	G	206	LMU	C2-C1-O1'-C1'
27	1	621	LMU	C2-C1-O1'-C1'
27	1	622	LMU	C2-C1-O1'-C1'
27	8	625	LMU	C2-C1-O1'-C1'
23	A	844	PQN	C19-C18-C20-C21
31	Z	601	CHL	C6-C7-C8-C9
22	8	602	CLA	C8-C10-C11-C12
22	92	611	CLA	C15-C16-C17-C18
22	A	835	CLA	C4B-C3B-CAB-CBB
22	B	802	CLA	C4B-C3B-CAB-CBB
22	B	818	CLA	C4B-C3B-CAB-CBB
22	B	832	CLA	C4B-C3B-CAB-CBB
22	B	834	CLA	C4B-C3B-CAB-CBB
22	L	203	CLA	C4B-C3B-CAB-CBB
22	K	206	CLA	C4B-C3B-CAB-CBB
22	3	612	CLA	C4B-C3B-CAB-CBB
22	Z	611	CLA	C4B-C3B-CAB-CBB
22	4	611	CLA	C4B-C3B-CAB-CBB
22	5	612	CLA	C4B-C3B-CAB-CBB
22	5	614	CLA	C4B-C3B-CAB-CBB
22	6	611	CLA	C4B-C3B-CAB-CBB
22	9	613	CLA	C4B-C3B-CAB-CBB
22	B2	806	CLA	C4B-C3B-CAB-CBB
22	B2	839	CLA	C4B-C3B-CAB-CBB
22	L2	203	CLA	C4B-C3B-CAB-CBB
22	A	816	CLA	C13-C15-C16-C17
22	B	826	CLA	C8-C10-C11-C12
27	9	624	LMU	C2'-C1'-O1'-C1
22	A	828	CLA	C8-C10-C11-C12
22	7	611	CLA	C8-C10-C11-C12
24	9	622	LHG	C25-C26-C27-C28
24	B	851	LHG	O6-C4-C5-C6
24	Z	620	LHG	O6-C4-C5-C6
24	92	622	LHG	O6-C4-C5-C6
24	B	851	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	5	607	CHL	CAA-CBA-CGA-O2A
22	A	804	CLA	C11-C12-C13-C15
22	A	811	CLA	C6-C7-C8-C10
22	A	829	CLA	C6-C7-C8-C10
22	B	827	CLA	C11-C10-C8-C7
22	B	834	CLA	C11-C10-C8-C7
22	F	301	CLA	C11-C10-C8-C7
22	Z	609	CLA	C11-C12-C13-C15
31	1	601	CHL	C11-C12-C13-C15
24	5	623	LHG	O2-C2-C3-O3
28	A	859	LMG	C40-C41-C42-C43
22	A	810	CLA	C4-C3-C5-C6
22	A	815	CLA	C4-C3-C5-C6
22	B	805	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C4-C3-C5-C6
22	B	829	CLA	C4-C3-C5-C6
22	1	609	CLA	C4-C3-C5-C6
22	1	614	CLA	C4-C3-C5-C6
22	A	830	CLA	C2-C3-C5-C6
22	92	609	CLA	C4C-C3C-CAC-CBC
22	7	604	CLA	C4-C3-C5-C6
24	4	622	LHG	C1-C2-C3-O3
31	Z	606	CHL	C1A-C2A-CAA-CBA
22	5	610	CLA	C4-C3-C5-C6
24	4	623	LHG	C13-C14-C15-C16
22	A	840	CLA	C2-C3-C5-C6
22	B	808	CLA	C2-C3-C5-C6
22	B	829	CLA	C2-C3-C5-C6
22	3	603	CLA	C2-C3-C5-C6
22	9	612	CLA	C2-C3-C5-C6
22	92	612	CLA	C2-C3-C5-C6
24	B	851	LHG	O6-C4-C5-O7
24	6	629	LHG	O6-C4-C5-O7
22	B	832	CLA	C2B-C3B-CAB-CBB
22	3	612	CLA	C2B-C3B-CAB-CBB
22	Z	611	CLA	C2B-C3B-CAB-CBB
22	4	611	CLA	C2B-C3B-CAB-CBB
22	5	612	CLA	C2B-C3B-CAB-CBB
22	6	611	CLA	C2B-C3B-CAB-CBB
25	A	848	BCR	C1-C6-C7-C8
25	B	846	BCR	C23-C24-C25-C26
25	B	848	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	L	201	BCR	C1-C6-C7-C8
25	3	718	BCR	C23-C24-C25-C30
25	6	623	BCR	C23-C24-C25-C30
25	B2	848	BCR	C1-C6-C7-C8
25	L2	201	BCR	C1-C6-C7-C8
29	1	617	LUT	C1-C6-C7-C8
29	3	621	LUT	C1-C6-C7-C8
29	8	617	LUT	C1-C6-C7-C8
29	Z	617	LUT	C1-C6-C7-C8
29	6	621	LUT	C1-C6-C7-C8
31	3	608	CHL	C15-C16-C17-C18
24	8	620	LHG	C26-C27-C28-C29
22	3	603	CLA	C2C-C3C-CAC-CBC
22	1	609	CLA	C15-C16-C17-C18
28	3	722	LMG	C8-C7-O1-C1
22	Z	609	CLA	C4-C3-C5-C6
22	A	828	CLA	C2-C3-C5-C6
22	A	841	CLA	C2-C3-C5-C6
22	B	807	CLA	C2-C3-C5-C6
22	B	812	CLA	C2-C3-C5-C6
22	1	609	CLA	C2-C3-C5-C6
22	1	614	CLA	C2-C3-C5-C6
22	Z	609	CLA	C2-C3-C5-C6
31	6	601	CHL	C2-C3-C5-C6
24	8	620	LHG	C15-C16-C17-C18
24	A	846	LHG	C27-C28-C29-C30
22	A	812	CLA	C15-C16-C17-C18
22	A	811	CLA	C6-C7-C8-C9
22	A	828	CLA	C14-C13-C15-C16
22	A	829	CLA	C6-C7-C8-C9
22	B	802	CLA	C11-C10-C8-C9
30	B	850	DGD	C2A-C3A-C4A-C5A
28	1	628	LMG	C11-C12-C13-C14
22	A	809	CLA	C2A-CAA-CBA-CGA
27	B	853	LMU	C2-C3-C4-C5
28	7	626	LMG	O8-C28-C29-C30
22	A	815	CLA	C2-C3-C5-C6
22	92	612	CLA	C13-C15-C16-C17
24	1	620	LHG	O6-C4-C5-C6
22	B	819	CLA	C11-C10-C8-C7
22	8	613	CLA	C12-C13-C15-C16
31	8	607	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	6	616	CHL	C12-C13-C15-C16
28	J	104	LMG	C8-C7-O1-C1
28	B2	855	LMG	C8-C7-O1-C1
22	A	803	CLA	C2A-CAA-CBA-CGA
22	B	831	CLA	C2A-CAA-CBA-CGA
28	3	722	LMG	O8-C28-C29-C30
22	A	820	CLA	C2-C3-C5-C6
22	A	823	CLA	O2A-C1-C2-C3
22	A	827	CLA	O2A-C1-C2-C3
31	8	607	CHL	O2A-C1-C2-C3
31	4	606	CHL	O2A-C1-C2-C3
27	4	625	LMU	C3-C4-C5-C6
22	A	812	CLA	C13-C15-C16-C17
24	Z	620	LHG	O6-C4-C5-O7
24	4	623	LHG	O6-C4-C5-O7
24	92	622	LHG	O6-C4-C5-O7
22	A	811	CLA	C4-C3-C5-C6
22	A	821	CLA	C4-C3-C5-C6
22	B	813	CLA	C4-C3-C5-C6
22	B	815	CLA	C4-C3-C5-C6
22	1	613	CLA	C4-C3-C5-C6
22	A	810	CLA	C2-C3-C5-C6
22	Z	611	CLA	C5-C6-C7-C8
24	7	625	LHG	O7-C5-C6-O8
28	8	626	LMG	O7-C8-C9-O8
22	5	617	CLA	C10-C11-C12-C13
22	A	823	CLA	C11-C12-C13-C14
31	8	607	CHL	C6-C7-C8-C9
22	A	836	CLA	CAA-CBA-CGA-O2A
22	5	603	CLA	C2-C1-O2A-CGA
22	3	613	CLA	C4-C3-C5-C6
22	7	620	CLA	C4-C3-C5-C6
22	B	819	CLA	C3-C5-C6-C7
24	4	622	LHG	C19-C20-C21-C22
22	B	813	CLA	C2-C3-C5-C6
22	B	815	CLA	C2-C3-C5-C6
22	7	603	CLA	C2-C3-C5-C6
22	7	610	CLA	CBA-CGA-O2A-C1
31	Z	607	CHL	C4C-C3C-CAC-CBC
31	5	607	CHL	C4C-C3C-CAC-CBC
31	9	607	CHL	C4C-C3C-CAC-CBC
27	A	863	LMU	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
27	A	863	LMU	C2-C1-O1'-C1'
27	1	625	LMU	C2-C1-O1'-C1'
27	8	624	LMU	C2-C1-O1'-C1'
22	A	806	CLA	C3-C5-C6-C7
28	A	859	LMG	C32-C33-C34-C35
22	92	609	CLA	C2C-C3C-CAC-CBC
27	8	627	LMU	C7-C8-C9-C10
22	A	819	CLA	C4B-C3B-CAB-CBB
22	B	805	CLA	C1A-C2A-CAA-CBA
22	B	826	CLA	C4B-C3B-CAB-CBB
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	840	CLA	C4B-C3B-CAB-CBB
22	7	616	CLA	C1A-C2A-CAA-CBA
22	4	603	CLA	C4B-C3B-CAB-CBB
22	5	613	CLA	C4B-C3B-CAB-CBB
22	5	616	CLA	C4B-C3B-CAB-CBB
22	5	621	CLA	C4B-C3B-CAB-CBB
22	B2	815	CLA	C4B-C3B-CAB-CBB
22	B2	820	CLA	C1A-C2A-CAA-CBA
22	B2	820	CLA	C4B-C3B-CAB-CBB
24	4	623	LHG	C9-C10-C11-C12
22	B	805	CLA	C4-C3-C5-C6
22	B2	812	CLA	C4-C3-C5-C6
22	92	613	CLA	C4-C3-C5-C6
22	B	817	CLA	C4C-C3C-CAC-CBC
22	9	613	CLA	C2A-CAA-CBA-CGA
24	7	625	LHG	C34-C35-C36-C37
24	3	623	LHG	O6-C4-C5-C6
24	4	623	LHG	O6-C4-C5-C6
24	9	622	LHG	O6-C4-C5-C6
22	A	809	CLA	C12-C13-C15-C16
22	A	816	CLA	C12-C13-C15-C16
22	A	820	CLA	C6-C7-C8-C10
22	A	828	CLA	C12-C13-C15-C16
22	B	802	CLA	C11-C10-C8-C7
22	B	832	CLA	C11-C12-C13-C15
22	4	609	CLA	C11-C10-C8-C7
31	4	601	CHL	C11-C10-C8-C7
31	6	607	CHL	C12-C13-C15-C16
22	3	607	CLA	C4C-C3C-CAC-CBC
22	3	607	CLA	C4-C3-C5-C6
22	7	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	1	628	LMG	C14-C15-C16-C17
30	B	850	DGD	C3A-C4A-C5A-C6A
24	1	620	LHG	O6-C4-C5-O7
24	3	721	LHG	O6-C4-C5-O7
24	5	623	LHG	O6-C4-C5-O7
22	A	804	CLA	C11-C12-C13-C14
22	B	819	CLA	C11-C10-C8-C9
22	Z	616	CLA	C5-C6-C7-C8
22	A	830	CLA	C13-C15-C16-C17
28	A	859	LMG	C12-C13-C14-C15
22	3	611	CLA	C3-C5-C6-C7
24	7	625	LHG	C31-C32-C33-C34
28	7	626	LMG	O7-C8-C9-O8
28	4	624	LMG	O1-C7-C8-O7
22	A	841	CLA	C16-C17-C18-C20
28	7	626	LMG	C7-C8-C9-O8
22	6	604	CLA	C4-C3-C5-C6
22	A	811	CLA	C2-C3-C5-C6
22	A	804	CLA	CAD-CBD-CGD-O2D
22	B	805	CLA	CAD-CBD-CGD-O2D
22	B	841	CLA	CAD-CBD-CGD-O2D
22	7	614	CLA	CAD-CBD-CGD-O2D
22	7	620	CLA	CAD-CBD-CGD-O2D
22	6	622	CLA	CAD-CBD-CGD-O2D
22	B2	820	CLA	CAD-CBD-CGD-O2D
31	1	601	CHL	CAD-CBD-CGD-O2D
31	1	607	CHL	CAD-CBD-CGD-O2D
31	Z	601	CHL	CAD-CBD-CGD-O2D
31	4	601	CHL	CAD-CBD-CGD-O2D
31	6	601	CHL	CAD-CBD-CGD-O2D
24	3	623	LHG	C32-C33-C34-C35
27	A	863	LMU	C3'-C4'-O1B-C1B
31	4	608	CHL	C2A-CAA-CBA-CGA
22	B	832	CLA	C15-C16-C17-C18
21	A	801	CL0	CHA-CBD-CGD-O1D
21	A	801	CL0	CHA-CBD-CGD-O2D
22	A	804	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CAD-CBD-CGD-O1D
22	B	805	CLA	CAD-CBD-CGD-O1D
22	B	811	CLA	CHA-CBD-CGD-O1D
22	B	814	CLA	CHA-CBD-CGD-O1D
22	B	821	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	821	CLA	CHA-CBD-CGD-O2D
22	B	841	CLA	CAD-CBD-CGD-O1D
22	K	204	CLA	CHA-CBD-CGD-O1D
22	K	204	CLA	CHA-CBD-CGD-O2D
22	1	602	CLA	CHA-CBD-CGD-O1D
22	1	602	CLA	CHA-CBD-CGD-O2D
22	1	603	CLA	CHA-CBD-CGD-O1D
22	1	603	CLA	CHA-CBD-CGD-O2D
22	1	612	CLA	CHA-CBD-CGD-O1D
22	1	612	CLA	CHA-CBD-CGD-O2D
22	3	602	CLA	CHA-CBD-CGD-O1D
22	3	602	CLA	CHA-CBD-CGD-O2D
22	7	614	CLA	CAD-CBD-CGD-O1D
22	7	620	CLA	CAD-CBD-CGD-O1D
22	8	602	CLA	CHA-CBD-CGD-O1D
22	8	603	CLA	CHA-CBD-CGD-O1D
22	8	603	CLA	CHA-CBD-CGD-O2D
22	Z	602	CLA	CHA-CBD-CGD-O1D
22	Z	603	CLA	CHA-CBD-CGD-O1D
22	Z	603	CLA	CHA-CBD-CGD-O2D
22	Z	612	CLA	CHA-CBD-CGD-O1D
22	Z	612	CLA	CHA-CBD-CGD-O2D
22	5	621	CLA	CHA-CBD-CGD-O1D
22	5	621	CLA	CHA-CBD-CGD-O2D
22	6	603	CLA	CAD-CBD-CGD-O1D
22	6	622	CLA	CAD-CBD-CGD-O1D
22	9	603	CLA	CHA-CBD-CGD-O1D
22	9	603	CLA	CHA-CBD-CGD-O2D
22	B2	820	CLA	CAD-CBD-CGD-O1D
22	92	612	CLA	CHA-CBD-CGD-O1D
22	92	612	CLA	CHA-CBD-CGD-O2D
24	A	846	LHG	C4-O6-P-O4
24	A	847	LHG	C3-O3-P-O5
24	3	721	LHG	C3-O3-P-O5
24	3	721	LHG	C4-O6-P-O4
24	3	623	LHG	C3-O3-P-O4
24	3	623	LHG	C4-O6-P-O3
24	3	623	LHG	C4-O6-P-O4
24	3	623	LHG	C4-O6-P-O5
24	8	620	LHG	C3-O3-P-O4
24	8	620	LHG	C4-O6-P-O5
24	Z	620	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
24	Z	620	LHG	C4-O6-P-O4
24	Z	620	LHG	C4-O6-P-O5
24	6	619	LHG	C4-O6-P-O5
24	9	622	LHG	C4-O6-P-O5
24	92	622	LHG	C4-O6-P-O5
31	1	601	CHL	CAD-CBD-CGD-O1D
31	1	607	CHL	CAD-CBD-CGD-O1D
31	7	601	CHL	CAD-CBD-CGD-O1D
31	8	607	CHL	CHA-CBD-CGD-O2D
31	Z	601	CHL	CAD-CBD-CGD-O1D
31	4	601	CHL	CAD-CBD-CGD-O1D
31	4	607	CHL	CHA-CBD-CGD-O2D
31	4	608	CHL	CHA-CBD-CGD-O2D
31	5	618	CHL	CHA-CBD-CGD-O1D
31	6	601	CHL	CAD-CBD-CGD-O1D
22	B	826	CLA	C13-C15-C16-C17
22	B	834	CLA	C4-C3-C5-C6
22	5	613	CLA	C4-C3-C5-C6
31	8	601	CHL	C4-C3-C5-C6
22	A	836	CLA	C2B-C3B-CAB-CBB
22	B	834	CLA	C2B-C3B-CAB-CBB
22	B	839	CLA	C2B-C3B-CAB-CBB
22	B	841	CLA	C2B-C3B-CAB-CBB
22	K	204	CLA	C2B-C3B-CAB-CBB
22	Z	608	CLA	C2B-C3B-CAB-CBB
22	B2	808	CLA	C2B-C3B-CAB-CBB
22	B2	809	CLA	C2B-C3B-CAB-CBB
22	B2	815	CLA	C2B-C3B-CAB-CBB
22	92	614	CLA	C2B-C3B-CAB-CBB
25	7	623	BCR	C23-C24-C25-C26
29	1	619	LUT	C5-C6-C7-C8
29	3	622	LUT	C1-C6-C7-C8
29	92	616	LUT	C5-C6-C7-C8
22	B2	828	CLA	C5-C6-C7-C8
22	B	818	CLA	C10-C11-C12-C13
22	A	812	CLA	C3-C5-C6-C7
24	4	623	LHG	C6-C5-O7-C7
31	Z	607	CHL	CAA-CBA-CGA-O2A
22	A	829	CLA	C8-C10-C11-C12
22	B	805	CLA	C2-C3-C5-C6
24	6	629	LHG	C13-C14-C15-C16
24	6	629	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	841	CLA	C14-C13-C15-C16
22	8	613	CLA	C11-C12-C13-C14
31	1	601	CHL	C11-C12-C13-C14
31	8	601	CHL	C14-C13-C15-C16
31	5	607	CHL	C11-C10-C8-C9
31	6	607	CHL	C6-C7-C8-C9
31	6	616	CHL	C14-C13-C15-C16
22	A	823	CLA	C11-C12-C13-C15
24	3	721	LHG	C1-C2-C3-O3
24	9	622	LHG	O6-C4-C5-O7
27	1	621	LMU	O5'-C1'-O1'-C1
27	9	624	LMU	O5'-C1'-O1'-C1
22	6	609	CLA	C2A-CAA-CBA-CGA
22	B	805	CLA	CAA-CBA-CGA-O2A
30	B	850	DGD	O2G-C1B-C2B-C3B
22	6	603	CLA	C4-C3-C5-C6
31	4	601	CHL	C4-C3-C5-C6
22	5	601	CLA	C16-C17-C18-C19
28	B	852	LMG	O1-C7-C8-O7
28	J	104	LMG	O1-C7-C8-O7
22	3	615	CLA	CAA-CBA-CGA-O2A
24	5	623	LHG	C4-C5-C6-O8
28	8	629	LMG	C14-C15-C16-C17
22	92	603	CLA	C2C-C3C-CAC-CBC
22	4	603	CLA	C10-C11-C12-C13
22	A	823	CLA	C2A-CAA-CBA-CGA
22	5	621	CLA	C2A-CAA-CBA-CGA
28	B	852	LMG	O6-C1-O1-C7
22	A	843	CLA	C4-C3-C5-C6
22	1	613	CLA	C2-C3-C5-C6
22	7	620	CLA	C2-C3-C5-C6
27	A	857	LMU	O1'-C1-C2-C3
27	A	857	LMU	C2-C1-O1'-C1'
27	A	858	LMU	C2-C1-O1'-C1'
27	7	629	LMU	C2-C1-O1'-C1'
27	8	628	LMU	C2-C1-O1'-C1'
27	8	627	LMU	C2-C1-O1'-C1'
31	8	601	CHL	CAA-CBA-CGA-O2A
22	A	809	CLA	C14-C13-C15-C16
22	A	840	CLA	C14-C13-C15-C16
22	F	301	CLA	C11-C10-C8-C9
22	7	611	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	8	613	CLA	C14-C13-C15-C16
24	4	622	LHG	C27-C28-C29-C30
22	5	617	CLA	C4B-C3B-CAB-CBB
22	5	601	CLA	C16-C17-C18-C20
22	B	840	CLA	C10-C11-C12-C13
22	B	810	CLA	C4-C3-C5-C6
22	4	603	CLA	C4-C3-C5-C6
22	4	611	CLA	C4-C3-C5-C6
22	5	603	CLA	C4-C3-C5-C6
22	1	609	CLA	CAA-CBA-CGA-O2A
22	B	810	CLA	C2-C3-C5-C6
22	B	834	CLA	C2-C3-C5-C6
22	5	610	CLA	C2-C3-C5-C6
22	5	613	CLA	C2-C3-C5-C6
22	6	603	CLA	C2-C3-C5-C6
22	92	613	CLA	C2-C3-C5-C6
24	4	622	LHG	O6-C4-C5-O7
24	4	622	LHG	O6-C4-C5-C6
27	Z	622	LMU	C5'-C4'-O1B-C1B
22	A	840	CLA	C12-C13-C15-C16
22	7	611	CLA	C6-C7-C8-C10
22	5	601	CLA	C6-C7-C8-C10
31	8	601	CHL	C11-C12-C13-C15
24	4	622	LHG	O2-C2-C3-O3
27	8	627	LMU	C2-C3-C4-C5
22	4	609	CLA	C3A-C2A-CAA-CBA
22	5	621	CLA	C3A-C2A-CAA-CBA
22	3	607	CLA	C2-C3-C5-C6
22	6	604	CLA	C2-C3-C5-C6
28	1	628	LMG	C12-C13-C14-C15
25	A	852	BCR	C11-C10-C9-C34
25	A	852	BCR	C16-C17-C18-C36
25	B	845	BCR	C11-C10-C9-C34
25	B	845	BCR	C20-C21-C22-C37
25	L	201	BCR	C11-C10-C9-C34
25	B2	845	BCR	C11-C10-C9-C34
25	B2	845	BCR	C20-C21-C22-C37
25	L2	201	BCR	C11-C10-C9-C34
29	F	305	LUT	C20-C13-C14-C15
33	5	625	NEX	C39-C29-C30-C31
33	6	625	NEX	C39-C29-C30-C31
28	8	629	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
22	3	603	CLA	C4C-C3C-CAC-CBC
22	6	612	CLA	CAA-CBA-CGA-O1A
31	92	607	CHL	CAA-CBA-CGA-O1A
22	B	803	CLA	C8-C10-C11-C12
31	5	607	CHL	C4-C3-C5-C6
22	A	821	CLA	C2-C3-C5-C6
22	3	613	CLA	C2-C3-C5-C6
22	B2	812	CLA	C2-C3-C5-C6
31	8	601	CHL	C2-C3-C5-C6
24	B	851	LHG	O9-C7-C8-C9
31	5	607	CHL	CAA-CBA-CGA-O1A
24	5	623	LHG	C1-C2-C3-O3
27	Z	622	LMU	C3'-C4'-O1B-C1B
22	8	611	CLA	CAA-CBA-CGA-O1A
28	8	629	LMG	C15-C16-C17-C18
22	4	612	CLA	CAA-CBA-CGA-O1A
22	A	810	CLA	C11-C10-C8-C9
22	A	812	CLA	C14-C13-C15-C16
22	A	820	CLA	C6-C7-C8-C9
22	A	820	CLA	C11-C12-C13-C14
22	B	811	CLA	C11-C10-C8-C9
22	B	817	CLA	C11-C10-C8-C9
22	B	840	CLA	C11-C12-C13-C14
22	B	841	CLA	C11-C10-C8-C9
22	5	601	CLA	C6-C7-C8-C9
22	B2	806	CLA	C11-C12-C13-C14
31	4	601	CHL	C11-C10-C8-C9
24	4	623	LHG	C4-C5-O7-C7
24	6	629	LHG	C4-C5-O7-C7
30	B	850	DGD	C1G-C2G-O2G-C1B
22	A	810	CLA	C5-C6-C7-C8
22	A	841	CLA	C10-C11-C12-C13
22	92	611	CLA	C8-C10-C11-C12
22	B	836	CLA	C4-C3-C5-C6
22	8	613	CLA	C4-C3-C5-C6
31	Z	601	CHL	C4-C3-C5-C6
22	B	804	CLA	CAA-CBA-CGA-O1A
22	4	612	CLA	CAA-CBA-CGA-O2A
22	L2	204	CLA	CAA-CBA-CGA-O1A
22	A	819	CLA	C1A-C2A-CAA-CBA
22	7	614	CLA	C1A-C2A-CAA-CBA
22	5	621	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	A	852	BCR	C11-C10-C9-C8
25	A	852	BCR	C16-C17-C18-C19
25	B	845	BCR	C11-C10-C9-C8
25	B	845	BCR	C20-C21-C22-C23
25	L	201	BCR	C11-C10-C9-C8
25	B2	845	BCR	C11-C10-C9-C8
25	B2	845	BCR	C20-C21-C22-C23
25	L2	201	BCR	C11-C10-C9-C8
29	F	305	LUT	C12-C13-C14-C15
33	5	625	NEX	C28-C29-C30-C31
33	6	625	NEX	C28-C29-C30-C31
22	5	612	CLA	CAA-CBA-CGA-O1A
22	L2	203	CLA	CAA-CBA-CGA-O1A
31	3	608	CHL	C13-C15-C16-C17
22	A	819	CLA	C2B-C3B-CAB-CBB
22	A	824	CLA	C2B-C3B-CAB-CBB
22	A	835	CLA	C2B-C3B-CAB-CBB
22	B	818	CLA	C2B-C3B-CAB-CBB
22	B	826	CLA	C2B-C3B-CAB-CBB
22	B	840	CLA	C2B-C3B-CAB-CBB
22	K	206	CLA	C2B-C3B-CAB-CBB
22	1	612	CLA	C2B-C3B-CAB-CBB
22	1	616	CLA	C2B-C3B-CAB-CBB
22	8	608	CLA	C2B-C3B-CAB-CBB
22	Z	609	CLA	C2B-C3B-CAB-CBB
22	Z	616	CLA	C2B-C3B-CAB-CBB
22	5	613	CLA	C2B-C3B-CAB-CBB
22	5	616	CLA	C2B-C3B-CAB-CBB
22	5	621	CLA	C2B-C3B-CAB-CBB
22	6	614	CLA	C2B-C3B-CAB-CBB
22	9	613	CLA	C2B-C3B-CAB-CBB
22	B2	806	CLA	C2B-C3B-CAB-CBB
22	B2	820	CLA	C2B-C3B-CAB-CBB
25	A	848	BCR	C5-C6-C7-C8
25	B	847	BCR	C23-C24-C25-C26
25	B	848	BCR	C5-C6-C7-C8
25	L	205	BCR	C23-C24-C25-C26
25	6	623	BCR	C23-C24-C25-C26
25	L2	205	BCR	C23-C24-C25-C30
29	1	617	LUT	C5-C6-C7-C8
29	3	621	LUT	C5-C6-C7-C8
29	7	621	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	8	617	LUT	C5-C6-C7-C8
29	Z	617	LUT	C5-C6-C7-C8
29	5	620	LUT	C5-C6-C7-C8
29	6	621	LUT	C5-C6-C7-C8
29	9	616	LUT	C5-C6-C7-C8
27	1	621	LMU	C3'-C4'-O1B-C1B
22	6	612	CLA	CAA-CBA-CGA-O2A
31	92	607	CHL	CAA-CBA-CGA-O2A
22	K	206	CLA	CAA-CBA-CGA-O1A
22	8	611	CLA	CAA-CBA-CGA-O2A
22	F	301	CLA	C4-C3-C5-C6
22	Z	604	CLA	C4-C3-C5-C6
22	5	609	CLA	C4-C3-C5-C6
31	8	606	CHL	C4-C3-C5-C6
22	8	613	CLA	C2-C3-C5-C6
31	4	601	CHL	C2-C3-C5-C6
22	A	824	CLA	CAA-CBA-CGA-O2A
22	L2	204	CLA	CAA-CBA-CGA-O2A
24	A	846	LHG	C11-C12-C13-C14
33	6	625	NEX	C9-C10-C11-C12
22	B	808	CLA	C12-C13-C15-C16
22	B	809	CLA	C6-C7-C8-C10
22	G	203	CLA	C6-C7-C8-C10
22	1	613	CLA	C11-C12-C13-C15
22	4	611	CLA	C6-C7-C8-C10
22	B2	828	CLA	C12-C13-C15-C16
22	A	827	CLA	C13-C15-C16-C17
24	9	622	LHG	O7-C5-C6-O8
30	B	850	DGD	O1G-C1G-C2G-O2G
22	B2	839	CLA	CAA-CBA-CGA-O1A
31	7	606	CHL	CAA-CBA-CGA-O2A
24	3	623	LHG	C28-C29-C30-C31
22	92	603	CLA	C4C-C3C-CAC-CBC
22	A	824	CLA	CAA-CBA-CGA-O1A
22	1	612	CLA	CAA-CBA-CGA-O2A
22	5	612	CLA	CAA-CBA-CGA-O2A
22	9	614	CLA	CAA-CBA-CGA-O2A
31	Z	606	CHL	CAA-CBA-CGA-O2A
22	B	823	CLA	C4-C3-C5-C6
22	B	841	CLA	C4-C3-C5-C6
22	5	604	CLA	C4-C3-C5-C6
22	6	611	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	811	CLA	C2-C3-C5-C6
22	4	603	CLA	C2-C3-C5-C6
22	4	611	CLA	C2-C3-C5-C6
22	5	603	CLA	C2-C3-C5-C6
31	5	607	CHL	C2-C3-C5-C6
22	1	612	CLA	CAA-CBA-CGA-O1A
22	B	834	CLA	C8-C10-C11-C12
22	B2	839	CLA	CAA-CBA-CGA-O2A
31	7	606	CHL	CAA-CBA-CGA-O1A
22	A	840	CLA	C11-C10-C8-C9
22	3	615	CLA	C11-C10-C8-C9
22	8	610	CLA	C11-C12-C13-C14
30	B	850	DGD	C9B-CAB-CBB-CCB
33	6	625	NEX	C33-C34-C35-C15
31	Z	606	CHL	CAA-CBA-CGA-O1A
22	A	814	CLA	C4-C3-C5-C6
22	B	811	CLA	C4-C3-C5-C6
22	8	614	CLA	C4-C3-C5-C6
22	5	616	CLA	C4-C3-C5-C6
22	B2	814	CLA	C4-C3-C5-C6
22	B	804	CLA	CAA-CBA-CGA-O2A
22	9	614	CLA	CAA-CBA-CGA-O1A
24	6	619	LHG	C2-C3-O3-P
24	9	622	LHG	C5-C4-O6-P
22	6	611	CLA	C2-C3-C5-C6
28	7	626	LMG	C14-C15-C16-C17
22	7	610	CLA	O1A-CGA-O2A-C1
22	4	613	CLA	CAA-CBA-CGA-O2A
24	B	851	LHG	C4-C5-C6-O8
28	B	852	LMG	O1-C7-C8-C9
28	8	626	LMG	C7-C8-C9-O8
22	K	206	CLA	CAA-CBA-CGA-O2A
22	Z	612	CLA	CAA-CBA-CGA-O1A
22	3	609	CLA	C4C-C3C-CAC-CBC
24	7	625	LHG	O6-C4-C5-O7
22	A	825	CLA	C4-C3-C5-C6
22	3	615	CLA	C4-C3-C5-C6
28	8	629	LMG	C21-C22-C23-C24
22	A	809	CLA	C4B-C3B-CAB-CBB
22	A	843	CLA	C4B-C3B-CAB-CBB
22	B	807	CLA	C4B-C3B-CAB-CBB
22	B	820	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	1	616	CLA	C4B-C3B-CAB-CBB
22	8	608	CLA	C4B-C3B-CAB-CBB
22	Z	609	CLA	C4B-C3B-CAB-CBB
22	Z	616	CLA	C4B-C3B-CAB-CBB
22	6	614	CLA	C4B-C3B-CAB-CBB
22	L2	203	CLA	CAA-CBA-CGA-O2A
24	B	851	LHG	C23-C24-C25-C26
27	K	208	LMU	C5-C6-C7-C8
31	4	608	CHL	CHA-CBD-CGD-O1D
31	5	606	CHL	CHA-CBD-CGD-O1D
31	5	606	CHL	CHA-CBD-CGD-O2D
31	6	606	CHL	CHA-CBD-CGD-O1D
31	6	606	CHL	CHA-CBD-CGD-O2D
31	6	607	CHL	CHA-CBD-CGD-O1D
31	6	607	CHL	CHA-CBD-CGD-O2D
31	6	618	CHL	CHA-CBD-CGD-O1D
31	6	618	CHL	CHA-CBD-CGD-O2D
22	92	602	CLA	CAA-CBA-CGA-O2A
27	6	631	LMU	C3-C4-C5-C6
22	6	609	CLA	C4-C3-C5-C6
24	1	620	LHG	O7-C5-C6-O8
24	4	623	LHG	O7-C5-C6-O8
28	9	620	LMG	O1-C7-C8-O7
22	B	817	CLA	CAA-CBA-CGA-O2A
22	A	814	CLA	C2-C3-C5-C6
22	8	614	CLA	C2-C3-C5-C6
27	1	621	LMU	C5'-C4'-O1B-C1B
22	B	817	CLA	C11-C10-C8-C7
22	B2	806	CLA	C11-C12-C13-C15
31	5	607	CHL	C11-C10-C8-C7
22	A	829	CLA	C10-C11-C12-C13
22	A	825	CLA	C2C-C3C-CAC-CBC
22	A	826	CLA	C11-C10-C8-C9
22	A	839	CLA	C11-C12-C13-C14
22	A	843	CLA	C11-C12-C13-C14
22	L	203	CLA	C14-C13-C15-C16
22	7	611	CLA	C11-C12-C13-C14
22	92	602	CLA	C14-C13-C15-C16
22	A	825	CLA	C2-C1-O2A-CGA
22	A	843	CLA	C2-C1-O2A-CGA
22	B	836	CLA	C2-C1-O2A-CGA
22	B2	805	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	F	304	CLA	C3A-C2A-CAA-CBA
22	B	836	CLA	C2-C3-C5-C6
22	3	617	CLA	C2C-C3C-CAC-CBC
22	B	824	CLA	O2A-C1-C2-C3
31	Z	607	CHL	O2A-C1-C2-C3
22	92	609	CLA	CAA-CBA-CGA-O2A
24	8	620	LHG	C12-C13-C14-C15
28	J	103	LMG	C22-C23-C24-C25
28	8	626	LMG	O8-C28-C29-C30
24	4	622	LHG	C5-C4-O6-P
22	6	603	CLA	C13-C15-C16-C17
28	A	859	LMG	C13-C14-C15-C16
28	1	624	LMG	C31-C32-C33-C34
27	1	621	LMU	C2B-C1B-O1B-C4'
31	3	608	CHL	C4-C3-C5-C6
22	92	609	CLA	CAA-CBA-CGA-O1A
22	92	614	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	CAA-CBA-CGA-O2A
22	5	616	CLA	CAA-CBA-CGA-O2A
28	A	860	LMG	O1-C7-C8-O7
22	B	827	CLA	C8-C10-C11-C12
22	A	813	CLA	C6-C7-C8-C9
22	B	832	CLA	C11-C12-C13-C14
22	1	603	CLA	CAA-CBA-CGA-O2A
22	B2	813	CLA	CAA-CBA-CGA-O2A
24	A	846	LHG	O8-C23-C24-C25
24	6	619	LHG	O7-C7-C8-C9
24	7	625	LHG	O6-C4-C5-C6
22	B	811	CLA	CAA-CBA-CGA-O2A
22	5	604	CLA	C2-C3-C5-C6
22	92	614	CLA	CAA-CBA-CGA-O1A
22	A	810	CLA	C11-C10-C8-C7
22	A	820	CLA	C11-C12-C13-C15
22	A	839	CLA	C11-C12-C13-C15
22	A	843	CLA	C11-C10-C8-C7
22	3	615	CLA	C11-C10-C8-C7
22	8	610	CLA	C11-C12-C13-C15
31	5	607	CHL	C6-C7-C8-C10
22	3	604	CLA	C3-C5-C6-C7
22	92	612	CLA	C4C-C3C-CAC-CBC
22	Z	612	CLA	CAA-CBA-CGA-O2A
22	5	614	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	B	802	CLA	C2B-C3B-CAB-CBB
22	B	820	CLA	C2B-C3B-CAB-CBB
22	L	203	CLA	C2B-C3B-CAB-CBB
22	8	614	CLA	C2B-C3B-CAB-CBB
22	5	611	CLA	C2B-C3B-CAB-CBB
22	5	614	CLA	C2B-C3B-CAB-CBB
22	B2	829	CLA	C2B-C3B-CAB-CBB
22	B2	839	CLA	C2B-C3B-CAB-CBB
22	L2	203	CLA	C2B-C3B-CAB-CBB
22	92	603	CLA	C2B-C3B-CAB-CBB
25	G	205	BCR	C1-C6-C7-C8
25	L	205	BCR	C23-C24-C25-C30
25	L	201	BCR	C5-C6-C7-C8
25	K	207	BCR	C1-C6-C7-C8
25	K	207	BCR	C5-C6-C7-C8
25	3	718	BCR	C23-C24-C25-C26
25	B2	848	BCR	C5-C6-C7-C8
25	L2	205	BCR	C23-C24-C25-C26
25	L2	201	BCR	C5-C6-C7-C8
29	3	622	LUT	C5-C6-C7-C8
29	7	621	LUT	C5-C6-C7-C8
29	4	619	LUT	C1-C6-C7-C8
28	J	104	LMG	O7-C10-C11-C12
28	B	852	LMG	C12-C13-C14-C15
22	A	812	CLA	C2-C1-O2A-CGA
28	9	620	LMG	O7-C10-C11-C12
27	1	625	LMU	C2-C3-C4-C5
22	B	834	CLA	CAA-CBA-CGA-O2A
22	5	604	CLA	CAA-CBA-CGA-O2A
31	Z	601	CHL	C2-C3-C5-C6
27	A	865	LMU	C5-C6-C7-C8
21	A	801	CL0	C5-C6-C7-C8
24	B	851	LHG	C25-C26-C27-C28
28	7	626	LMG	O10-C28-C29-C30
22	A	803	CLA	C4-C3-C5-C6
22	B	824	CLA	C4-C3-C5-C6
22	B	814	CLA	CAA-CBA-CGA-O2A
24	4	622	LHG	O8-C23-C24-C25
22	5	616	CLA	C2-C3-C5-C6
24	1	620	LHG	C11-C10-C9-C8
22	B2	804	CLA	CAA-CBA-CGA-O1A
22	A	806	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	6	607	CHL	C14-C13-C15-C16
22	8	604	CLA	CAA-CBA-CGA-O2A
22	8	614	CLA	CAA-CBA-CGA-O2A
24	3	721	LHG	O7-C7-C8-C9
28	1	624	LMG	O7-C10-C11-C12
28	3	722	LMG	O1-C7-C8-C9
22	A	807	CLA	C4B-C3B-CAB-CBB
22	A	824	CLA	C4B-C3B-CAB-CBB
22	1	612	CLA	C4B-C3B-CAB-CBB
22	3	607	CLA	C4B-C3B-CAB-CBB
22	7	609	CLA	C4B-C3B-CAB-CBB
22	8	614	CLA	C4B-C3B-CAB-CBB
22	Z	611	CLA	C1A-C2A-CAA-CBA
22	Z	612	CLA	C4B-C3B-CAB-CBB
22	5	603	CLA	C1A-C2A-CAA-CBA
22	5	611	CLA	C4B-C3B-CAB-CBB
22	6	613	CLA	C4B-C3B-CAB-CBB
22	9	603	CLA	C4B-C3B-CAB-CBB
22	B2	829	CLA	C4B-C3B-CAB-CBB
22	92	603	CLA	C4B-C3B-CAB-CBB
22	A	810	CLA	C8-C10-C11-C12
27	1	625	LMU	O5'-C1'-O1'-C1
28	4	624	LMG	O6-C1-O1-C7
22	B	809	CLA	CAA-CBA-CGA-O2A
22	G	204	CLA	CAA-CBA-CGA-O2A
22	7	603	CLA	CAA-CBA-CGA-O2A
22	5	603	CLA	CAA-CBA-CGA-O2A
22	B2	820	CLA	CAA-CBA-CGA-O2A
24	92	622	LHG	O7-C7-C8-C9
28	1	624	LMG	O1-C7-C8-O7
27	1	625	LMU	C2'-C1'-O1'-C1
22	B	835	CLA	CAA-CBA-CGA-O2A
22	F	304	CLA	CAA-CBA-CGA-O2A
22	4	614	CLA	CAA-CBA-CGA-O2A
22	3	613	CLA	C10-C11-C12-C13
22	B	809	CLA	C3-C5-C6-C7
22	A	829	CLA	C2-C1-O2A-CGA
22	7	610	CLA	C2-C1-O2A-CGA
31	8	607	CHL	C2-C1-O2A-CGA
31	4	608	CHL	C2-C1-O2A-CGA
22	A	826	CLA	CAA-CBA-CGA-O2A
28	J	104	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
22	B	822	CLA	C6-C7-C8-C10
22	L	203	CLA	C12-C13-C15-C16
22	7	611	CLA	C11-C12-C13-C15
22	5	603	CLA	C12-C13-C15-C16
23	A	844	PQN	C21-C22-C23-C25
23	B	842	PQN	C16-C17-C18-C20
31	1	601	CHL	C11-C10-C8-C7
22	B	841	CLA	C2-C3-C5-C6
28	9	620	LMG	C7-C8-O7-C10
30	B	850	DGD	C3G-C2G-O2G-C1B
22	8	603	CLA	CAA-CBA-CGA-O2A
22	B2	811	CLA	CAA-CBA-CGA-O2A
27	8	627	LMU	C4-C5-C6-C7
22	A	818	CLA	C2A-CAA-CBA-CGA
22	92	602	CLA	C2A-CAA-CBA-CGA
28	A	859	LMG	C29-C30-C31-C32
22	A	836	CLA	C3A-C2A-CAA-CBA
22	3	615	CLA	C3A-C2A-CAA-CBA
22	8	614	CLA	C3A-C2A-CAA-CBA
22	4	613	CLA	C3A-C2A-CAA-CBA
22	4	614	CLA	C3A-C2A-CAA-CBA
22	5	603	CLA	C3A-C2A-CAA-CBA
22	5	604	CLA	C3A-C2A-CAA-CBA
22	9	611	CLA	C3A-C2A-CAA-CBA
22	B2	828	CLA	C4-C3-C5-C6
24	4	622	LHG	O10-C23-C24-C25
22	B2	812	CLA	C2C-C3C-CAC-CBC
22	5	609	CLA	C2-C3-C5-C6
24	7	625	LHG	C10-C11-C12-C13
22	5	614	CLA	CAA-CBA-CGA-O1A
22	B2	804	CLA	CAA-CBA-CGA-O2A
22	A	825	CLA	C4C-C3C-CAC-CBC
22	3	617	CLA	C4C-C3C-CAC-CBC
22	F	304	CLA	CAA-CBA-CGA-O1A
24	A	846	LHG	O10-C23-C24-C25
28	3	722	LMG	O10-C28-C29-C30
28	A	859	LMG	C30-C31-C32-C33
24	9	622	LHG	C29-C30-C31-C32
22	Z	603	CLA	CAA-CBA-CGA-O2A
28	8	629	LMG	O8-C28-C29-C30
22	3	609	CLA	C2C-C3C-CAC-CBC
22	4	614	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	5	604	CLA	CAA-CBA-CGA-O1A
24	3	721	LHG	O9-C7-C8-C9
28	J	104	LMG	O9-C10-C11-C12
22	92	612	CLA	C2C-C3C-CAC-CBC
22	B2	813	CLA	C2A-CAA-CBA-CGA
22	A	812	CLA	C6-C7-C8-C9
22	A	816	CLA	C14-C13-C15-C16
22	B2	828	CLA	C14-C13-C15-C16
22	5	621	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	CAA-CBA-CGA-O1A
22	B	811	CLA	CAA-CBA-CGA-O1A
24	6	619	LHG	O9-C7-C8-C9
24	6	619	LHG	C9-C10-C11-C12
24	9	622	LHG	C26-C27-C28-C29
22	Z	616	CLA	C3-C5-C6-C7
28	J	104	LMG	O10-C28-C29-C30
22	4	603	CLA	CAA-CBA-CGA-O2A
24	7	625	LHG	O8-C23-C24-C25
22	A	826	CLA	CAA-CBA-CGA-O1A
22	1	603	CLA	CAA-CBA-CGA-O1A
22	8	604	CLA	CAA-CBA-CGA-O1A
22	8	614	CLA	CAA-CBA-CGA-O1A
22	B	802	CLA	C8-C10-C11-C12
24	Z	620	LHG	C5-C6-O8-C23
28	B2	852	LMG	O7-C10-C11-C12
22	B	835	CLA	CAA-CBA-CGA-O1A
22	B	809	CLA	C8-C10-C11-C12
28	J	103	LMG	C8-C7-O1-C1
28	8	629	LMG	C8-C7-O1-C1
28	4	624	LMG	C8-C7-O1-C1
22	B	814	CLA	CAA-CBA-CGA-O1A
22	5	616	CLA	CAA-CBA-CGA-O1A
22	B2	813	CLA	CAA-CBA-CGA-O1A
28	9	620	LMG	O9-C10-C11-C12
22	4	610	CLA	C5-C6-C7-C8
28	A	859	LMG	C7-C8-C9-O8
22	L	204	CLA	CAA-CBA-CGA-O2A
22	B	809	CLA	CAA-CBA-CGA-O1A
24	92	622	LHG	O9-C7-C8-C9
22	4	614	CLA	C4-C3-C5-C6
22	F	304	CLA	C15-C16-C17-C18
22	3	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	8	606	CHL	C2-C3-C5-C6
22	A	805	CLA	CAD-CBD-CGD-O2D
22	A	810	CLA	CAD-CBD-CGD-O2D
22	A	814	CLA	CAD-CBD-CGD-O2D
22	A	842	CLA	CAD-CBD-CGD-O2D
22	B	803	CLA	CAD-CBD-CGD-O2D
22	1	608	CLA	CAD-CBD-CGD-O2D
22	4	604	CLA	CAD-CBD-CGD-O2D
22	4	614	CLA	CAD-CBD-CGD-O2D
22	5	602	CLA	CAD-CBD-CGD-O2D
22	5	612	CLA	CAD-CBD-CGD-O2D
22	6	603	CLA	CAD-CBD-CGD-O2D
22	B2	839	CLA	CAD-CBD-CGD-O2D
22	92	609	CLA	CAD-CBD-CGD-O2D
31	7	601	CHL	CAD-CBD-CGD-O2D
31	Z	606	CHL	CAD-CBD-CGD-O2D
22	B	813	CLA	C8-C10-C11-C12
22	A	813	CLA	CAA-CBA-CGA-O2A
22	B	806	CLA	CAA-CBA-CGA-O2A
28	1	628	LMG	O8-C28-C29-C30
22	Z	603	CLA	CAA-CBA-CGA-O1A
28	1	624	LMG	O9-C10-C11-C12
22	8	603	CLA	CAA-CBA-CGA-O1A
22	4	603	CLA	CAA-CBA-CGA-O1A
22	B2	811	CLA	CAA-CBA-CGA-O1A
28	B2	852	LMG	O9-C10-C11-C12
22	A	841	CLA	C11-C10-C8-C7
22	A	814	CLA	CAA-CBA-CGA-O2A
22	1	614	CLA	CAA-CBA-CGA-O2A
22	6	603	CLA	CAA-CBA-CGA-O2A
24	8	620	LHG	O7-C7-C8-C9
28	A	860	LMG	O8-C28-C29-C30
30	B	850	DGD	C7B-C8B-C9B-CAB
22	G	204	CLA	CAA-CBA-CGA-O1A
22	5	621	CLA	CAA-CBA-CGA-O1A
22	A	837	CLA	CAA-CBA-CGA-O2A
22	7	612	CLA	CAA-CBA-CGA-O2A
24	B	851	LHG	O8-C23-C24-C25
22	F	303	CLA	CAA-CBA-CGA-O2A
22	7	603	CLA	CAA-CBA-CGA-O1A
22	B2	820	CLA	CAA-CBA-CGA-O1A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	5	625	NEX	C1-C2-C3-C4-C5-C6

163 monomers are involved in 223 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	92	602	CLA	1	0
30	B	850	DGD	1	0
22	K	204	CLA	1	0
22	A	854	CLA	1	0
22	A	823	CLA	1	0
28	A	860	LMG	1	0
29	1	617	LUT	2	0
31	4	606	CHL	2	0
25	K	202	BCR	3	0
25	B	844	BCR	2	0
29	6	621	LUT	1	0
31	8	606	CHL	2	0
22	B2	828	CLA	4	0
27	Z	622	LMU	1	0
22	A	822	CLA	1	0
22	1	613	CLA	1	0
25	K	207	BCR	3	0
22	4	609	CLA	1	0
22	B	841	CLA	3	0
31	1	601	CHL	1	0
25	A	850	BCR	1	0
22	A	820	CLA	1	0
22	A	843	CLA	3	0
32	1	618	XAT	1	0
31	8	601	CHL	1	0
25	8	619	BCR	2	0
22	8	603	CLA	1	0
22	B	817	CLA	1	0
29	Z	617	LUT	1	0
28	4	624	LMG	1	0
29	A	856	LUT	1	0
22	92	611	CLA	1	0
22	3	609	CLA	1	0
24	5	623	LHG	1	0
29	5	620	LUT	3	0
25	I	172	BCR	1	0
25	B	848	BCR	1	0
22	B	821	CLA	1	0
22	B	834	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	852	BCR	4	0
22	B	806	CLA	1	0
25	A	851	BCR	3	0
22	8	604	CLA	1	0
22	3	603	CLA	2	0
27	B	853	LMU	3	0
24	1	620	LHG	1	0
29	F	305	LUT	3	0
25	B	843	BCR	2	0
22	B	808	CLA	1	0
25	B2	845	BCR	2	0
28	J	104	LMG	1	0
22	A	831	CLA	1	0
27	A	862	LMU	2	0
24	3	623	LHG	1	0
22	3	607	CLA	1	0
22	B	840	CLA	2	0
22	J	101	CLA	1	0
25	3	719	BCR	5	0
24	6	619	LHG	1	0
28	3	722	LMG	1	0
22	B	832	CLA	1	0
25	L	201	BCR	1	0
22	6	603	CLA	1	0
22	9	609	CLA	1	0
27	7	628	LMU	1	0
22	Z	616	CLA	2	0
25	B	801	BCR	2	0
25	92	623	BCR	3	0
25	A	849	BCR	2	0
31	6	606	CHL	1	0
22	5	621	CLA	2	0
25	3	620	BCR	1	0
24	4	623	LHG	1	0
22	3	611	CLA	1	0
31	5	606	CHL	1	0
29	7	624	LUT	4	0
22	7	610	CLA	3	0
22	L	203	CLA	1	0
22	Z	608	CLA	1	0
24	7	625	LHG	1	0
29	5	626	LUT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	7	608	CLA	1	0
25	B	847	BCR	1	0
22	A	830	CLA	1	0
25	L	205	BCR	4	0
22	1	603	CLA	3	0
22	4	613	CLA	2	0
27	92	624	LMU	2	0
22	1	602	CLA	1	0
22	B	827	CLA	1	0
22	8	612	CLA	1	0
29	4	619	LUT	1	0
22	K	201	CLA	2	0
22	7	609	CLA	1	0
22	Z	613	CLA	1	0
22	B	839	CLA	2	0
22	A	811	CLA	3	0
22	5	617	CLA	2	0
31	7	601	CHL	3	0
22	A	833	CLA	3	0
22	5	602	CLA	1	0
22	5	616	CLA	3	0
22	A	812	CLA	1	0
25	6	623	BCR	2	0
28	B	854	LMG	1	0
28	J	103	LMG	1	0
29	3	622	LUT	2	0
22	7	620	CLA	1	0
27	6	628	LMU	1	0
27	A	863	LMU	2	0
33	6	625	NEX	1	0
27	9	624	LMU	1	0
22	A	829	CLA	2	0
27	A	858	LMU	1	0
31	5	608	CHL	1	0
27	A	857	LMU	1	0
25	J	102	BCR	1	0
22	A	839	CLA	1	0
22	A	804	CLA	1	0
22	B	816	CLA	2	0
22	A	840	CLA	1	0
22	A	813	CLA	3	0
22	3	602	CLA	1	0

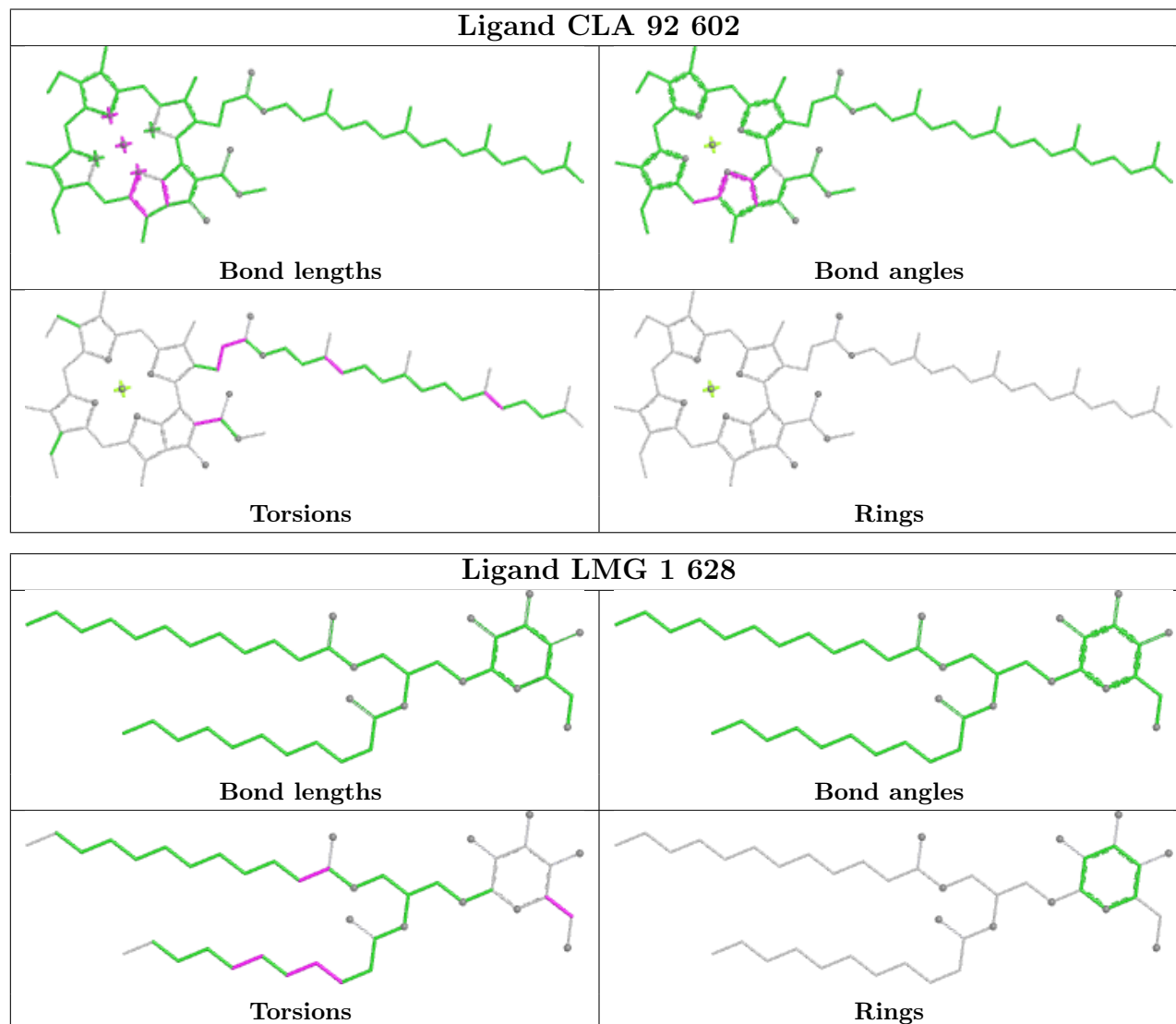
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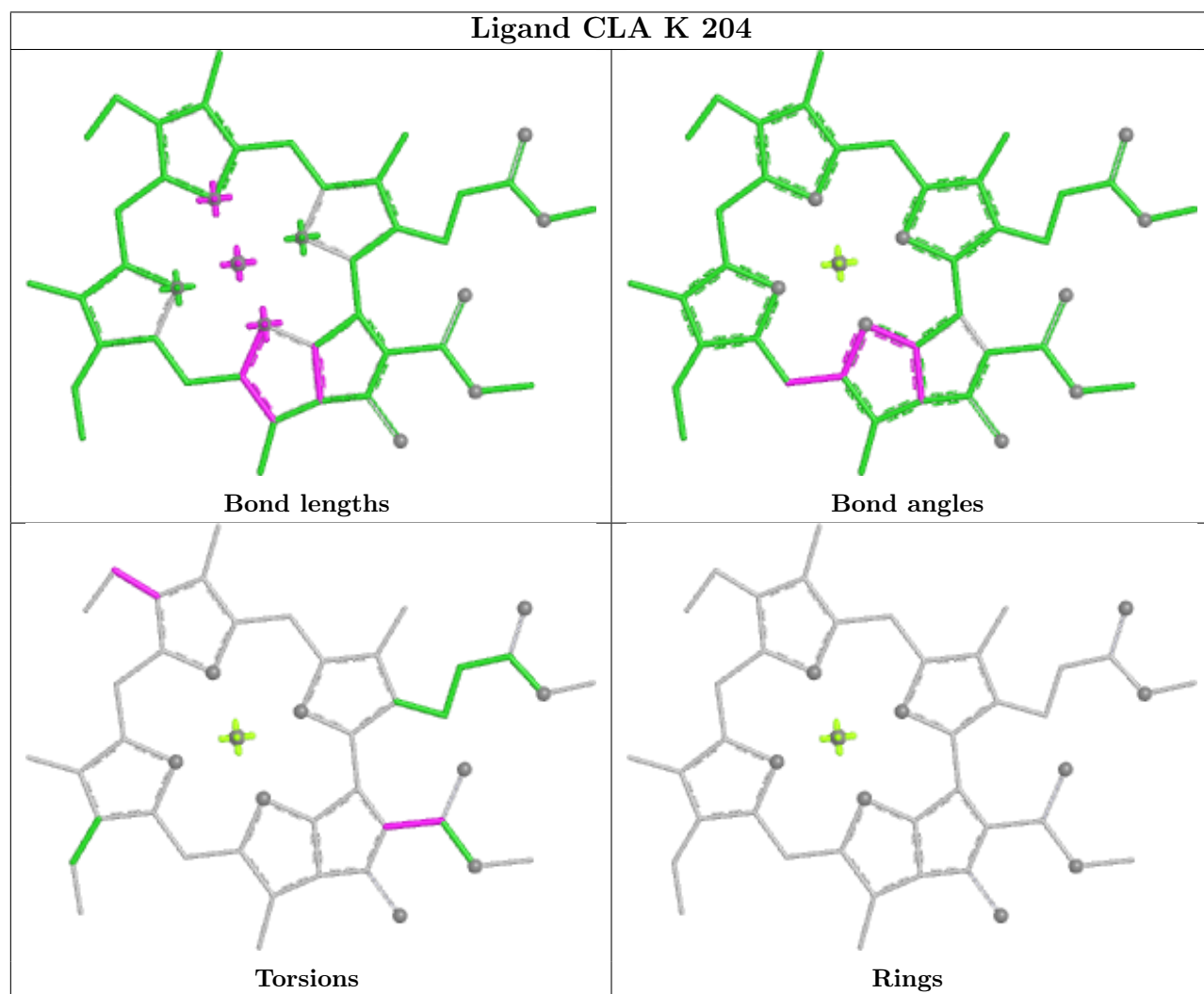
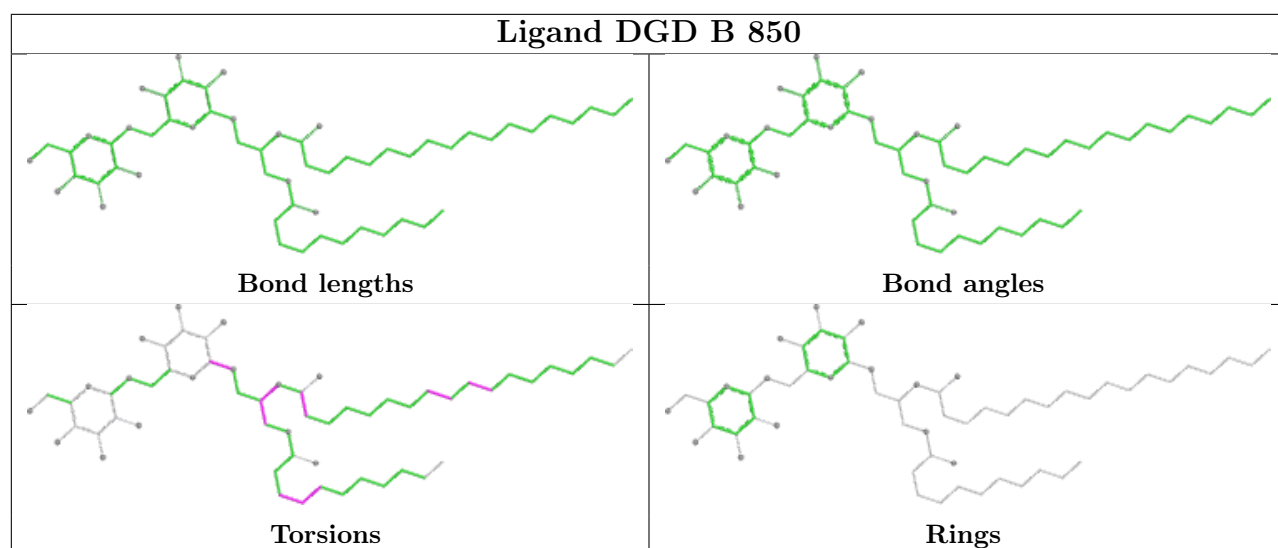
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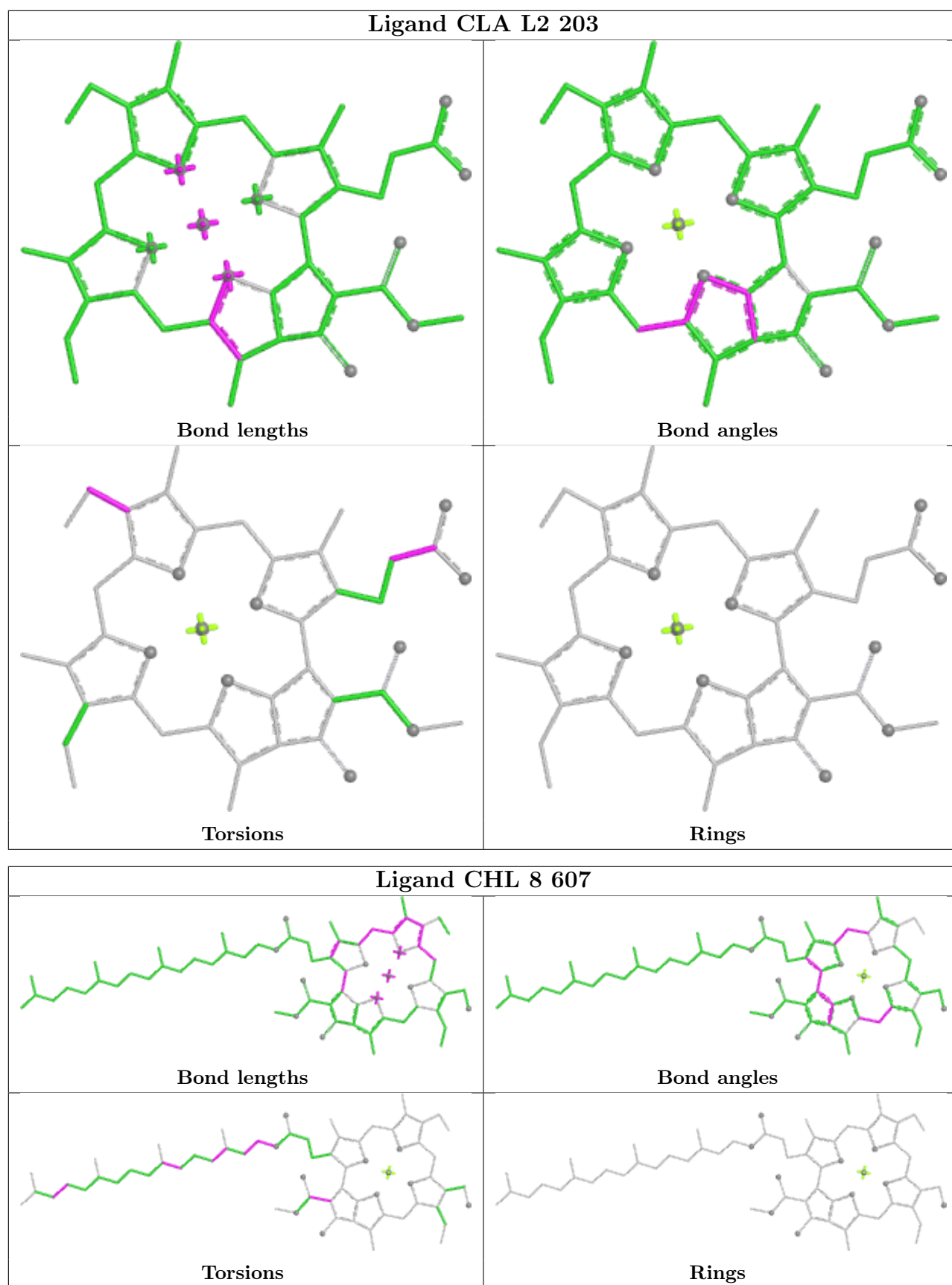
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	613	CLA	1	0
31	6	608	CHL	2	0
22	9	614	CLA	1	0
22	3	615	CLA	5	0
28	9	620	LMG	1	0
31	3	608	CHL	1	0
22	A	806	CLA	1	0
31	4	601	CHL	1	0
22	5	603	CLA	3	0
25	B2	844	BCR	4	0
22	4	614	CLA	1	0
22	B	802	CLA	1	0
22	B	837	CLA	2	0
22	A	810	CLA	1	0
22	F	304	CLA	1	0
29	9	616	LUT	1	0
31	Z	601	CHL	1	0
31	6	607	CHL	1	0
22	92	613	CLA	2	0
22	A	809	CLA	2	0
22	A	802	CLA	2	0
22	B2	829	CLA	1	0
22	A	803	CLA	1	0
22	Z	603	CLA	2	0
25	L2	205	BCR	3	0
25	B	845	BCR	3	0
24	92	622	LHG	1	0
22	A	825	CLA	1	0
27	8	627	LMU	1	0
22	B	823	CLA	1	0
25	3	718	BCR	1	0
25	9	623	BCR	2	0
22	3	610	CLA	2	0
22	A	818	CLA	1	0
22	A	817	CLA	1	0
29	9	617	LUT	2	0
22	B	829	CLA	6	0
22	B	836	CLA	1	0
31	6	601	CHL	3	0
25	A	848	BCR	3	0

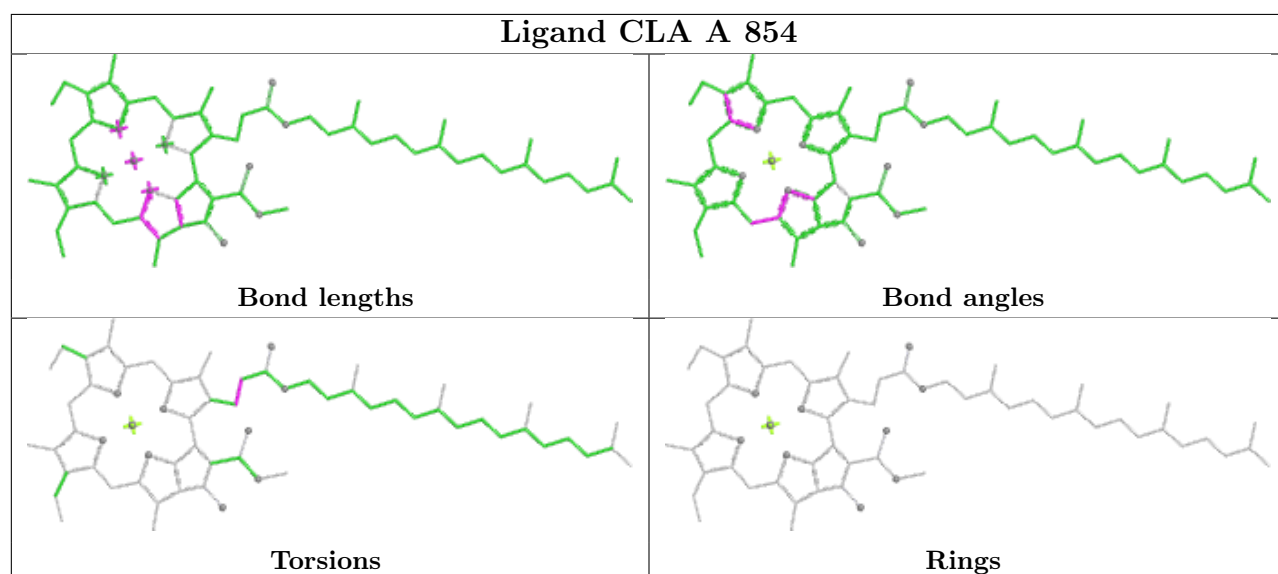
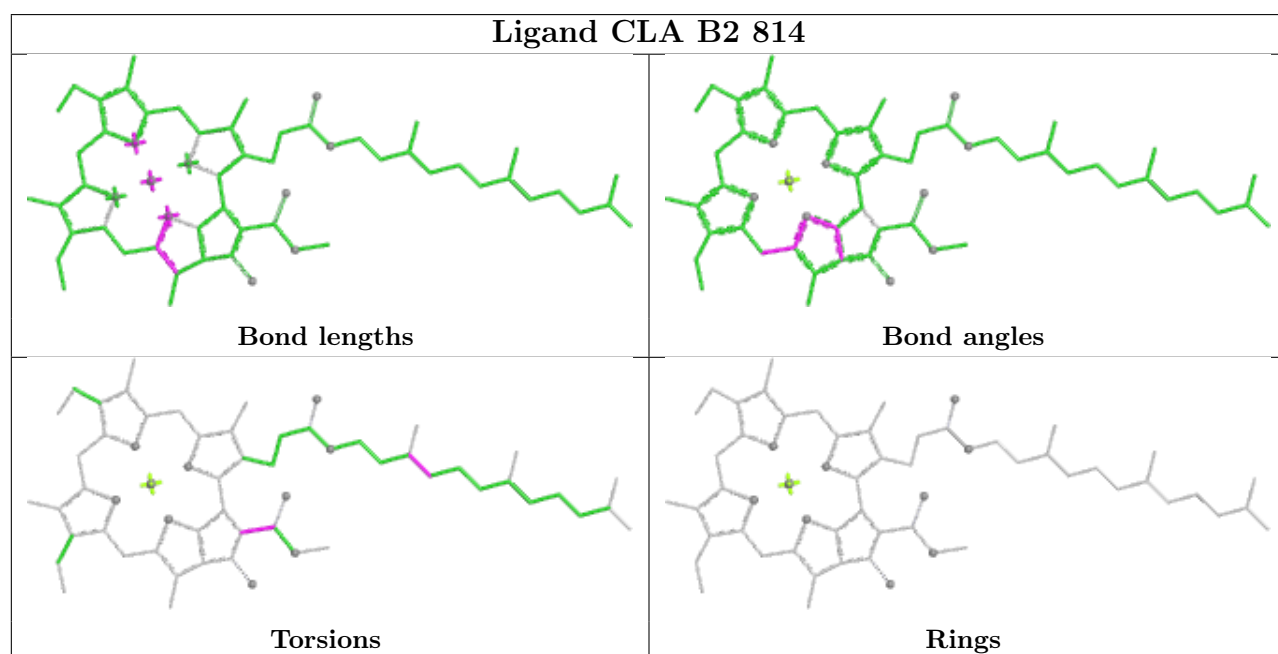
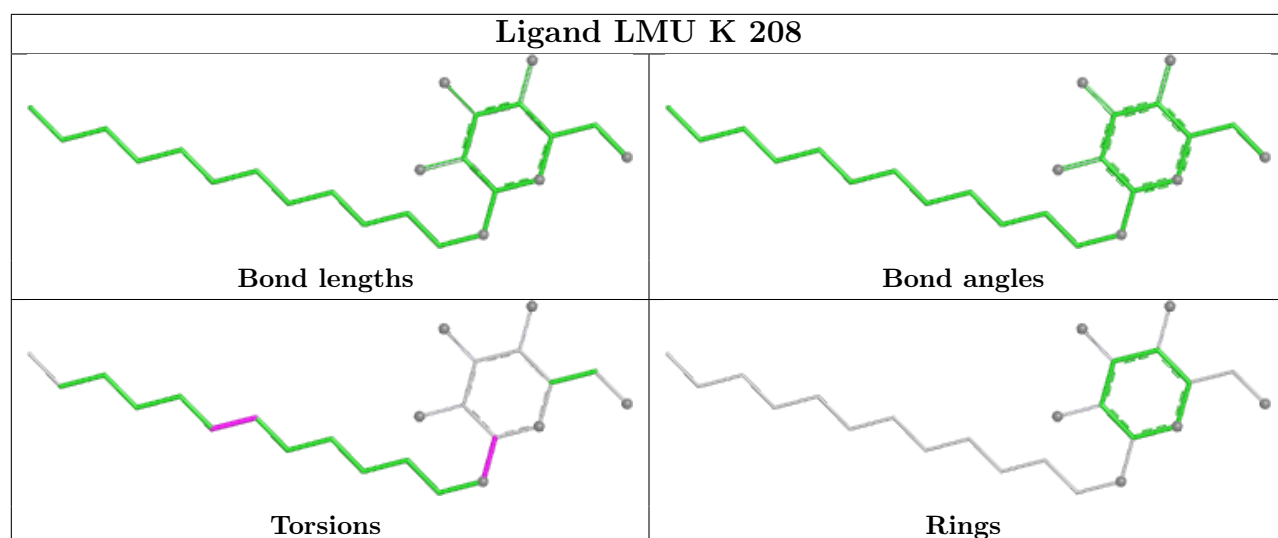
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

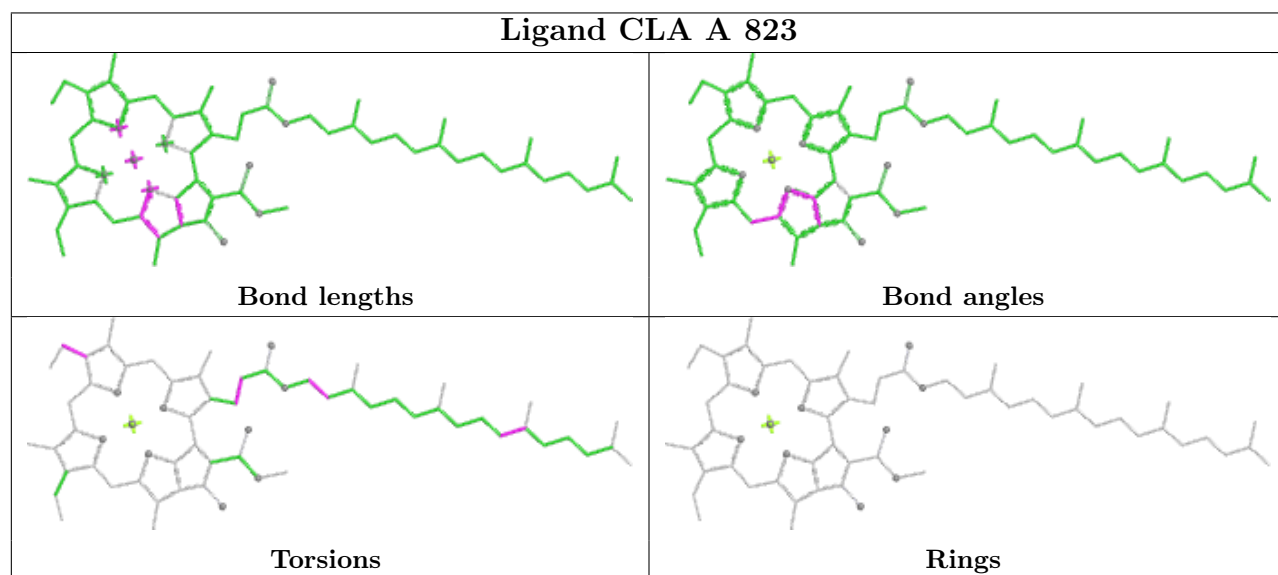
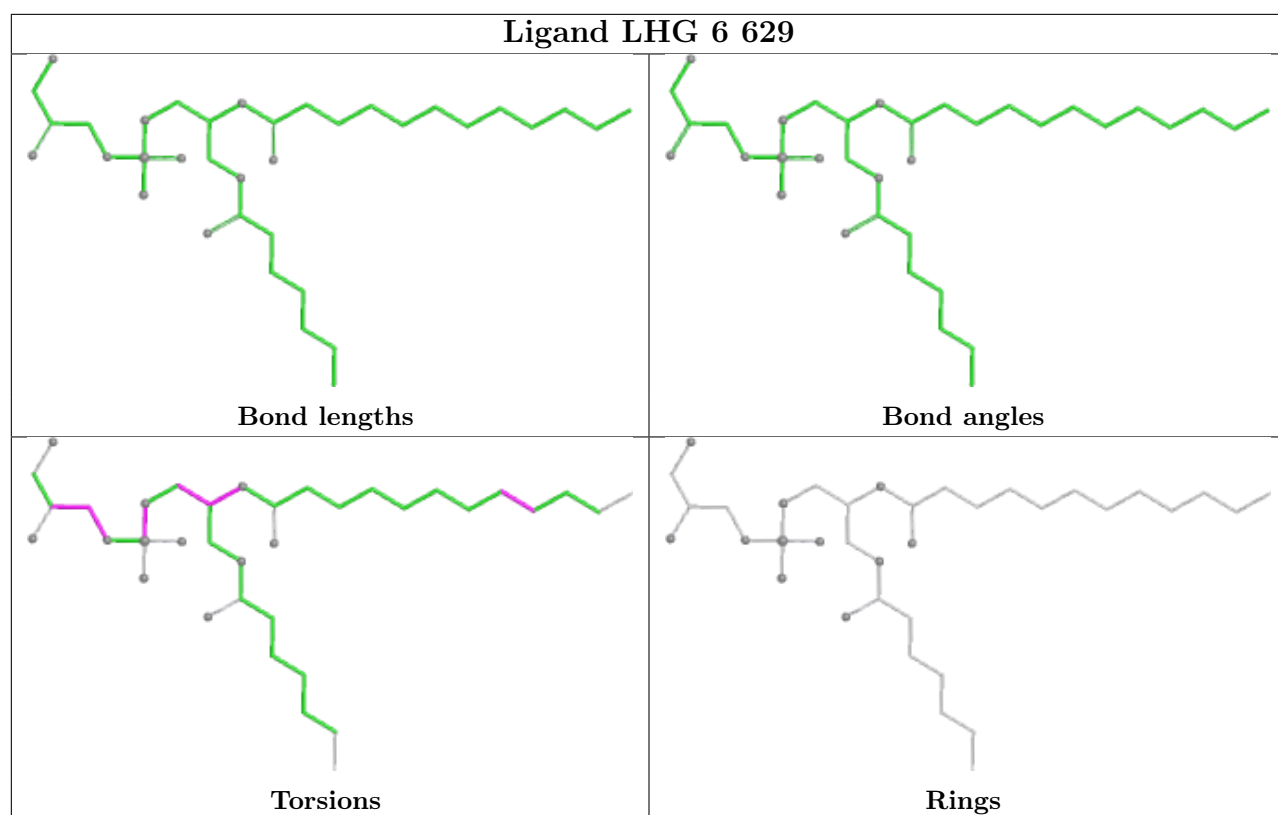
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

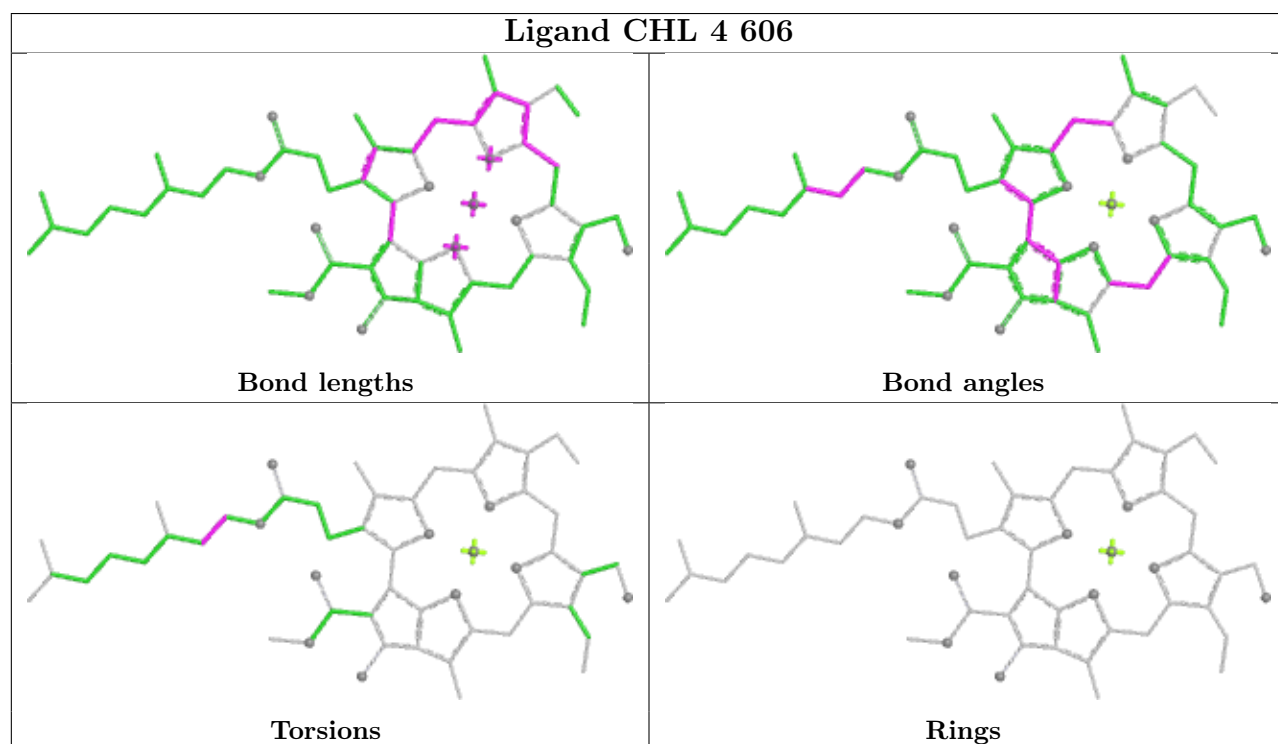
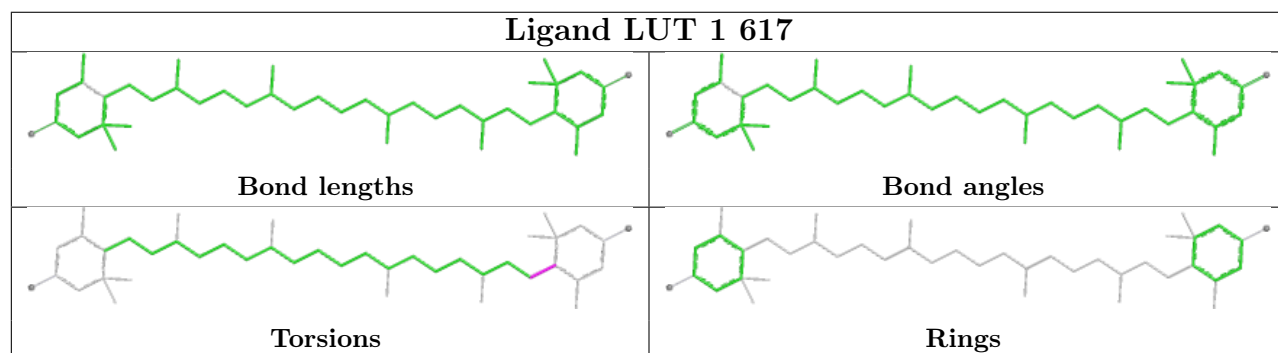
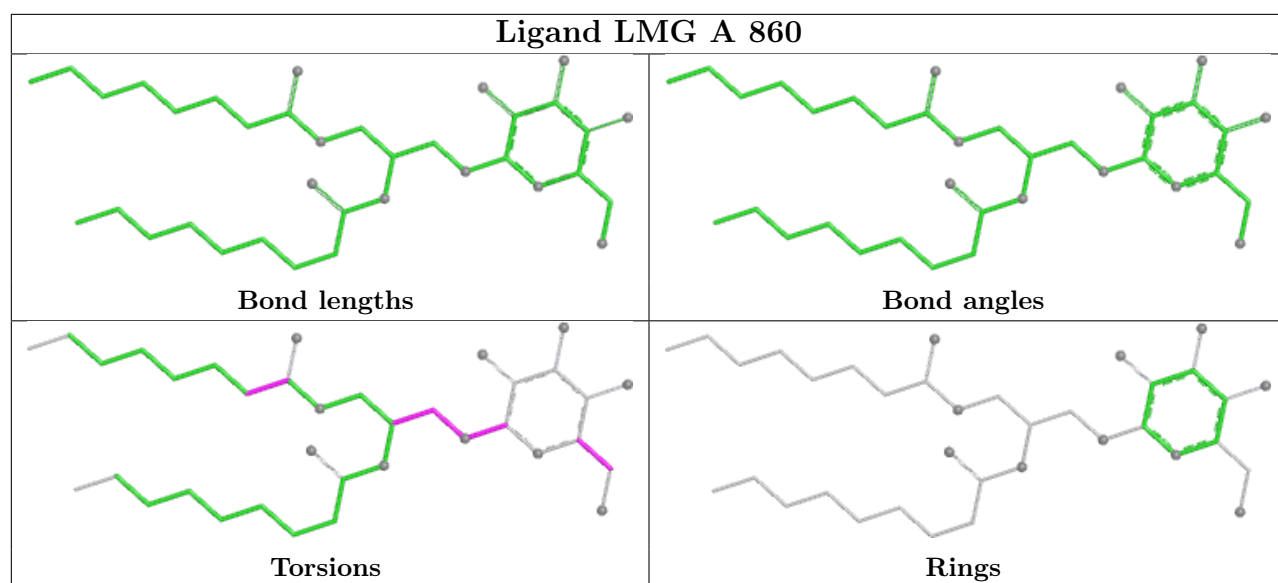


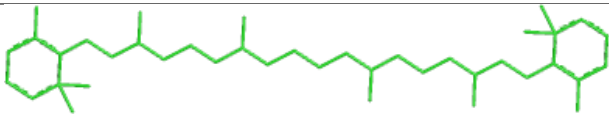
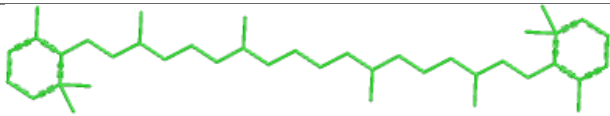
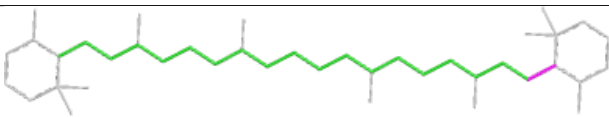
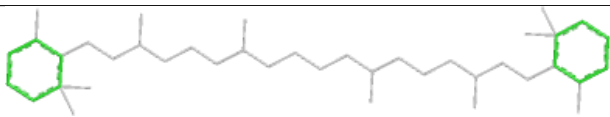


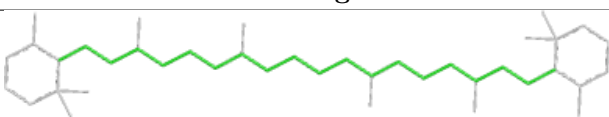
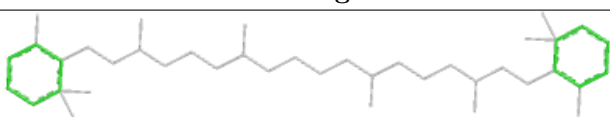


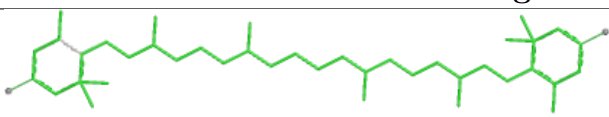
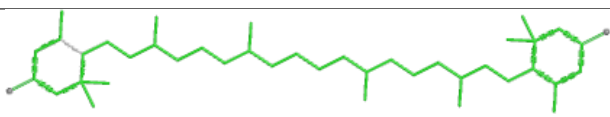
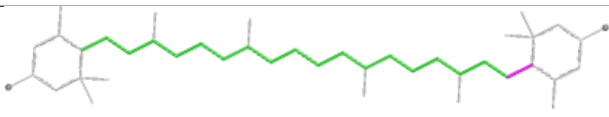
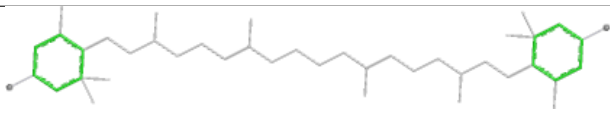


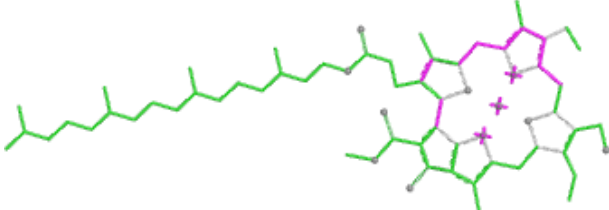
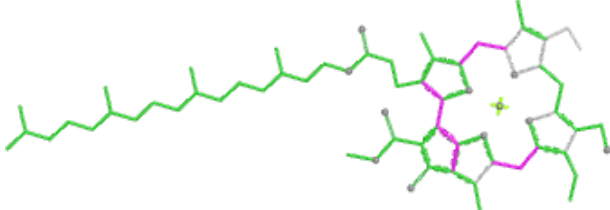
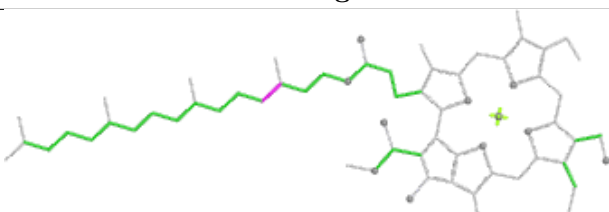
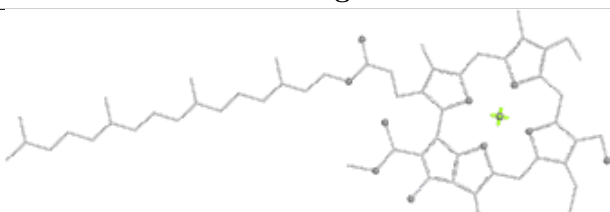


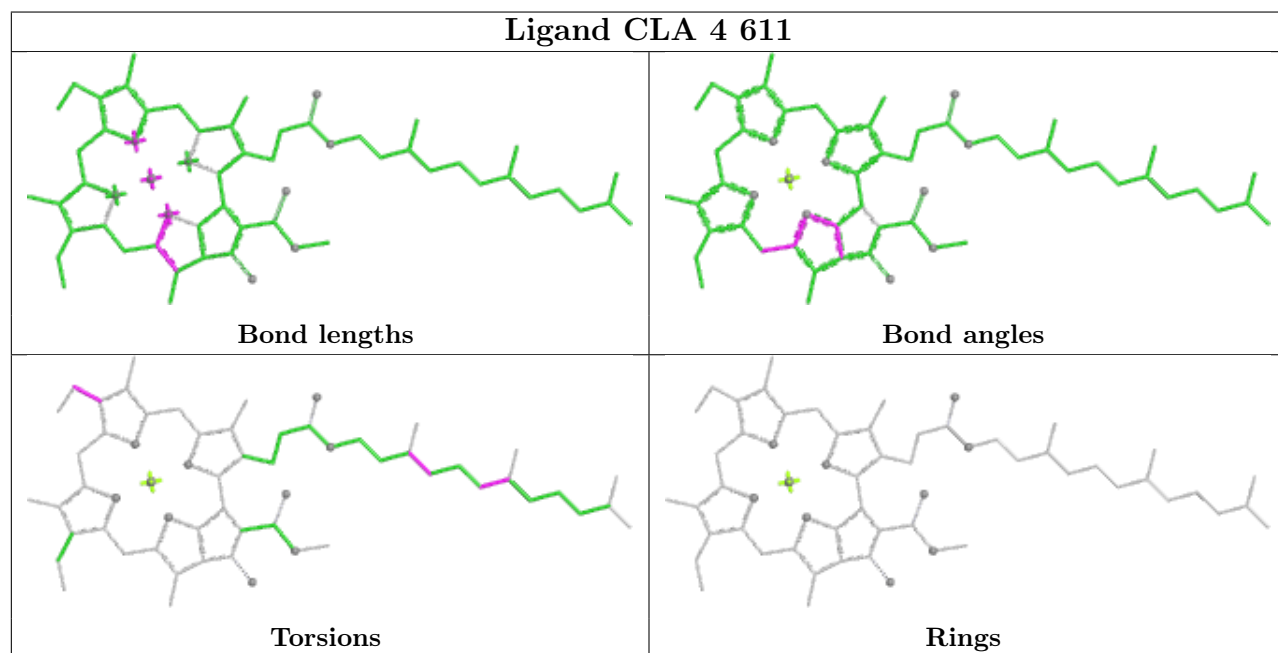
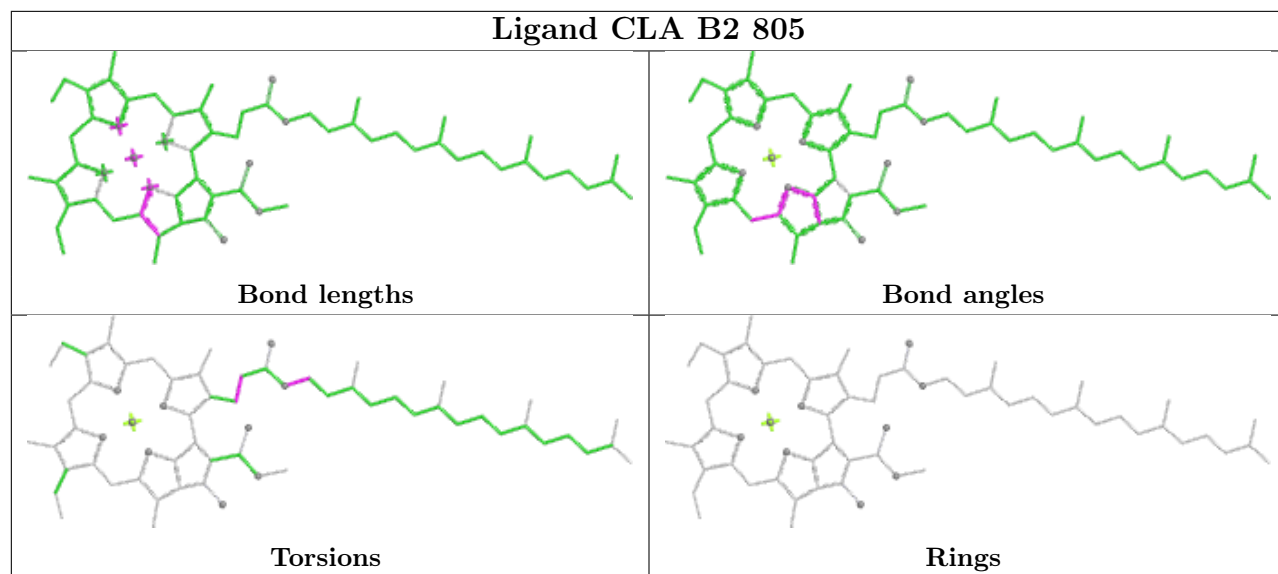


Ligand BCR K 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

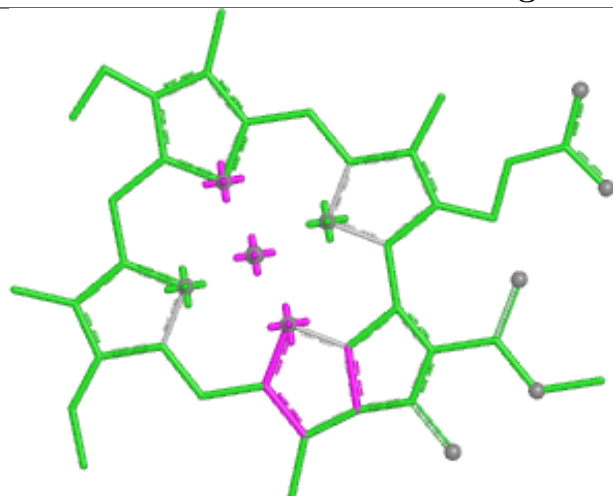
Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 6 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

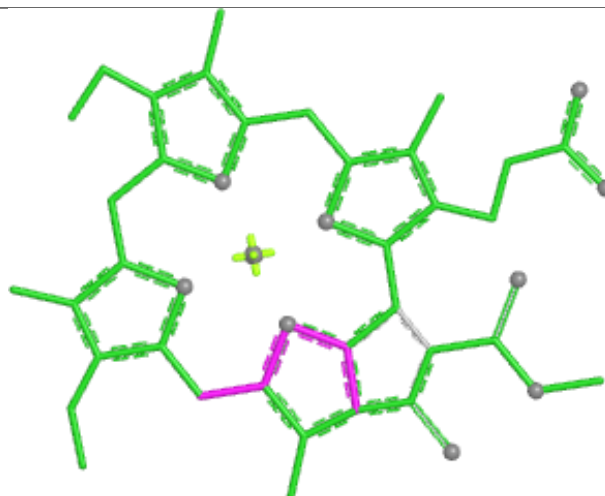
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Bond lengths	Bond angles
	
Torsions	Rings



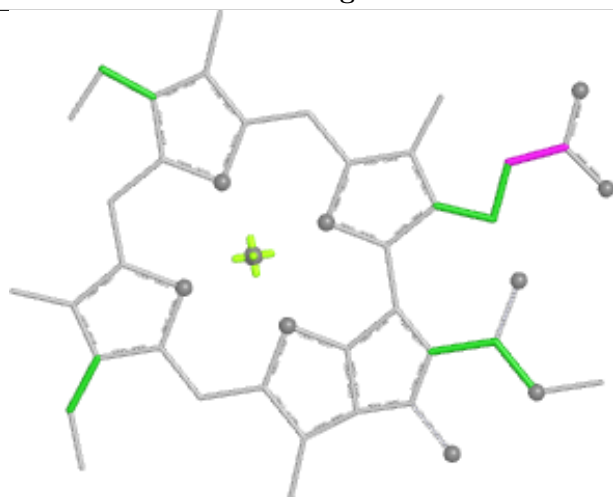
Ligand CLA 8 611



Bond lengths



Bond angles

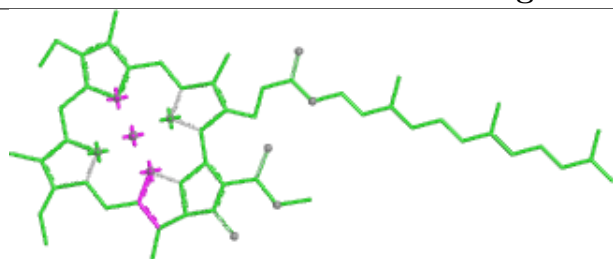


Torsions

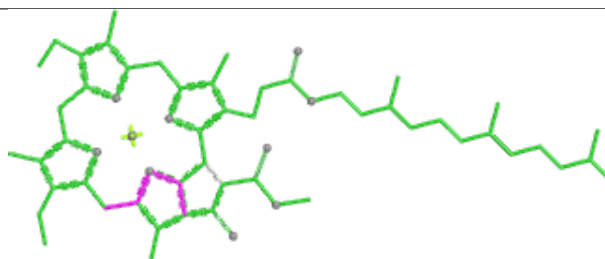


Rings

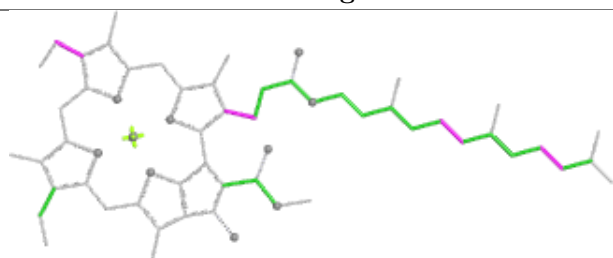
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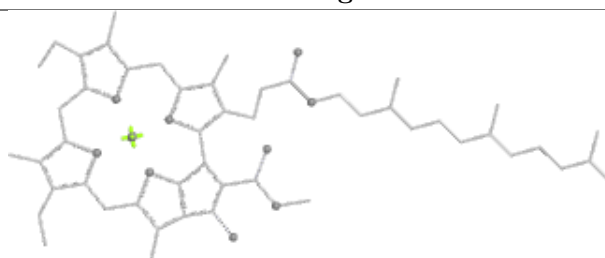
Bond lengths



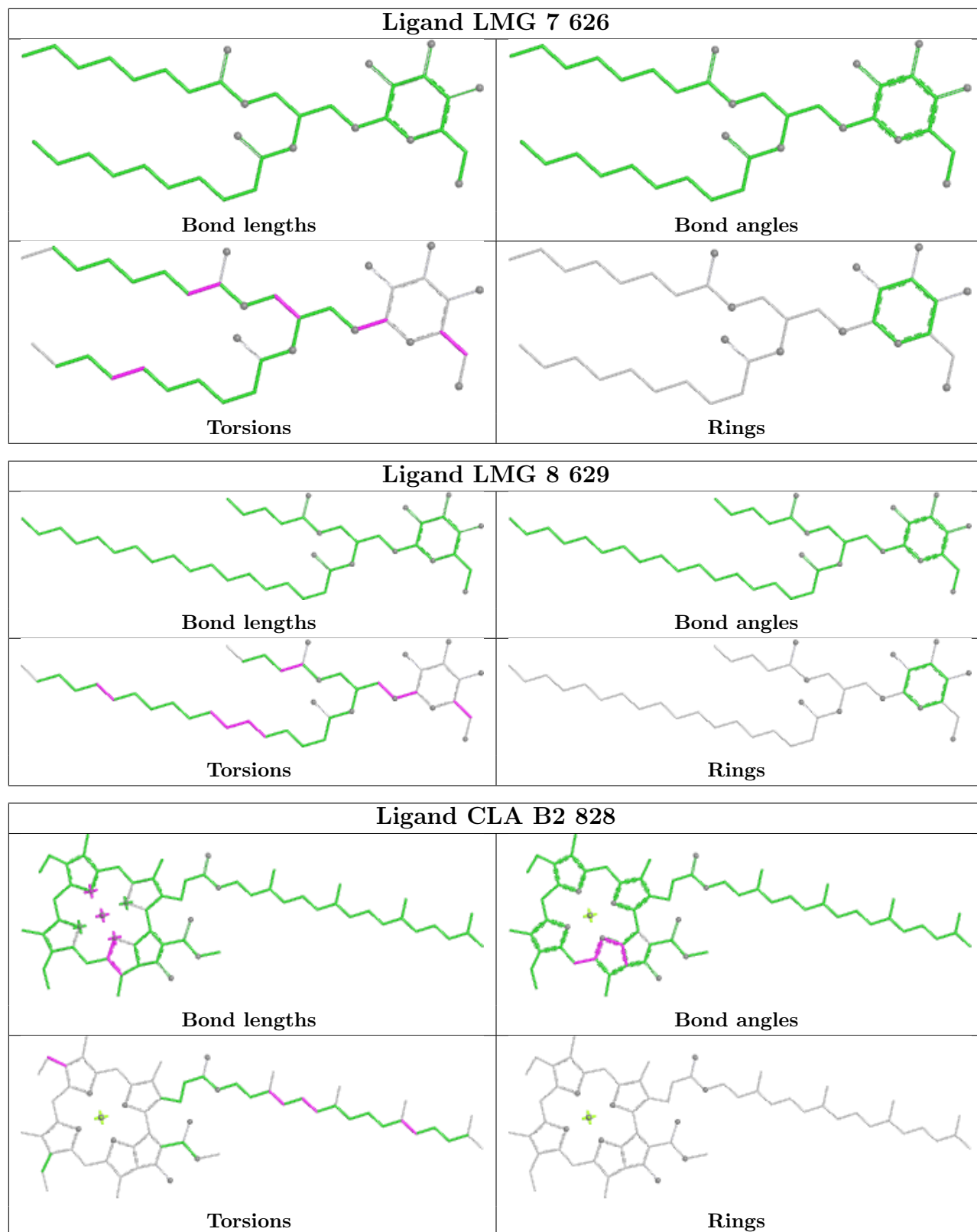
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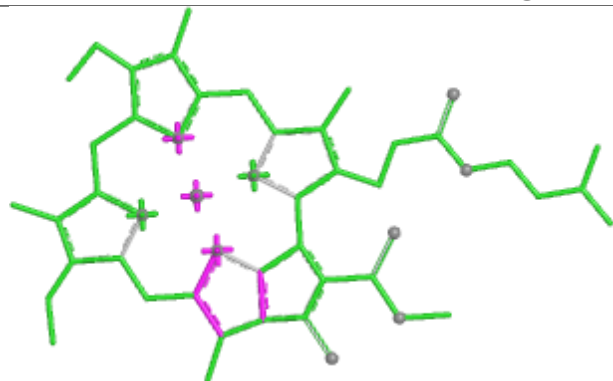
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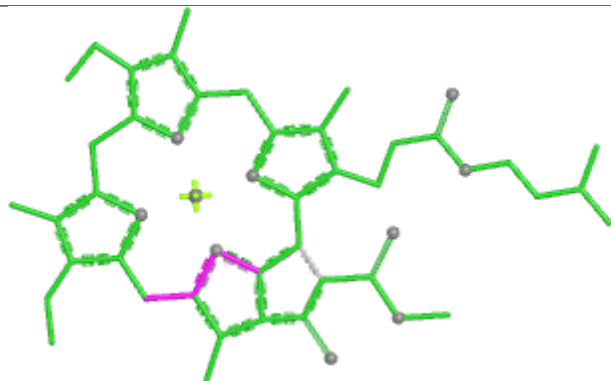
Rings



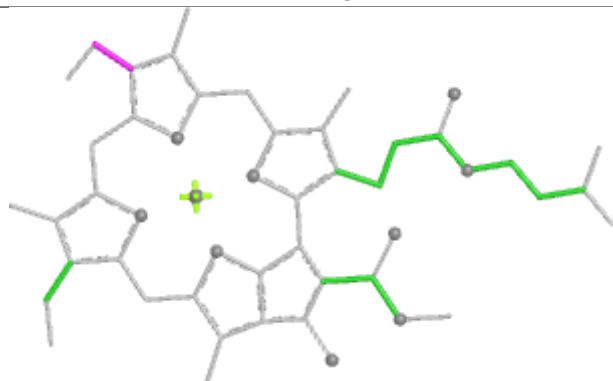
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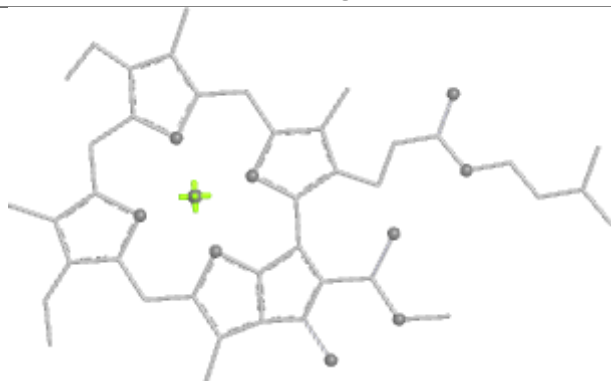
Bond lengths



Bond angles

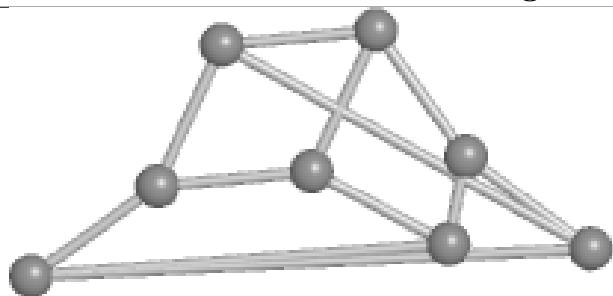


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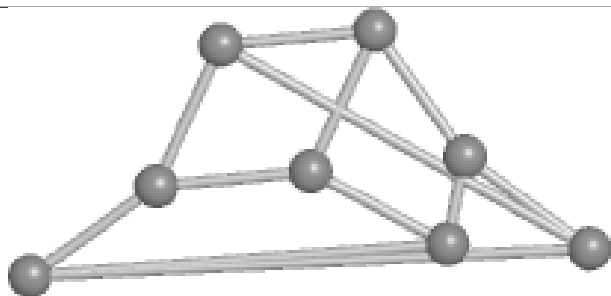


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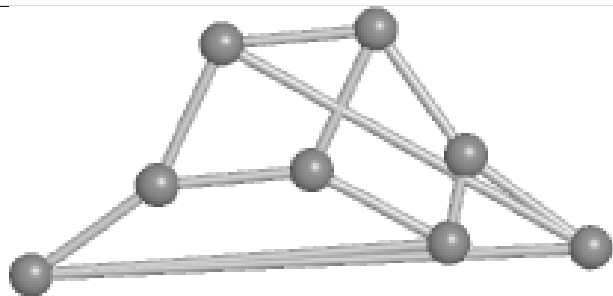
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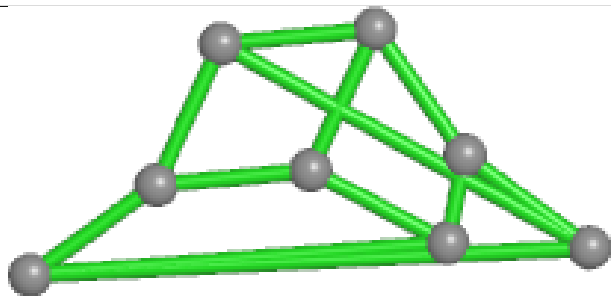
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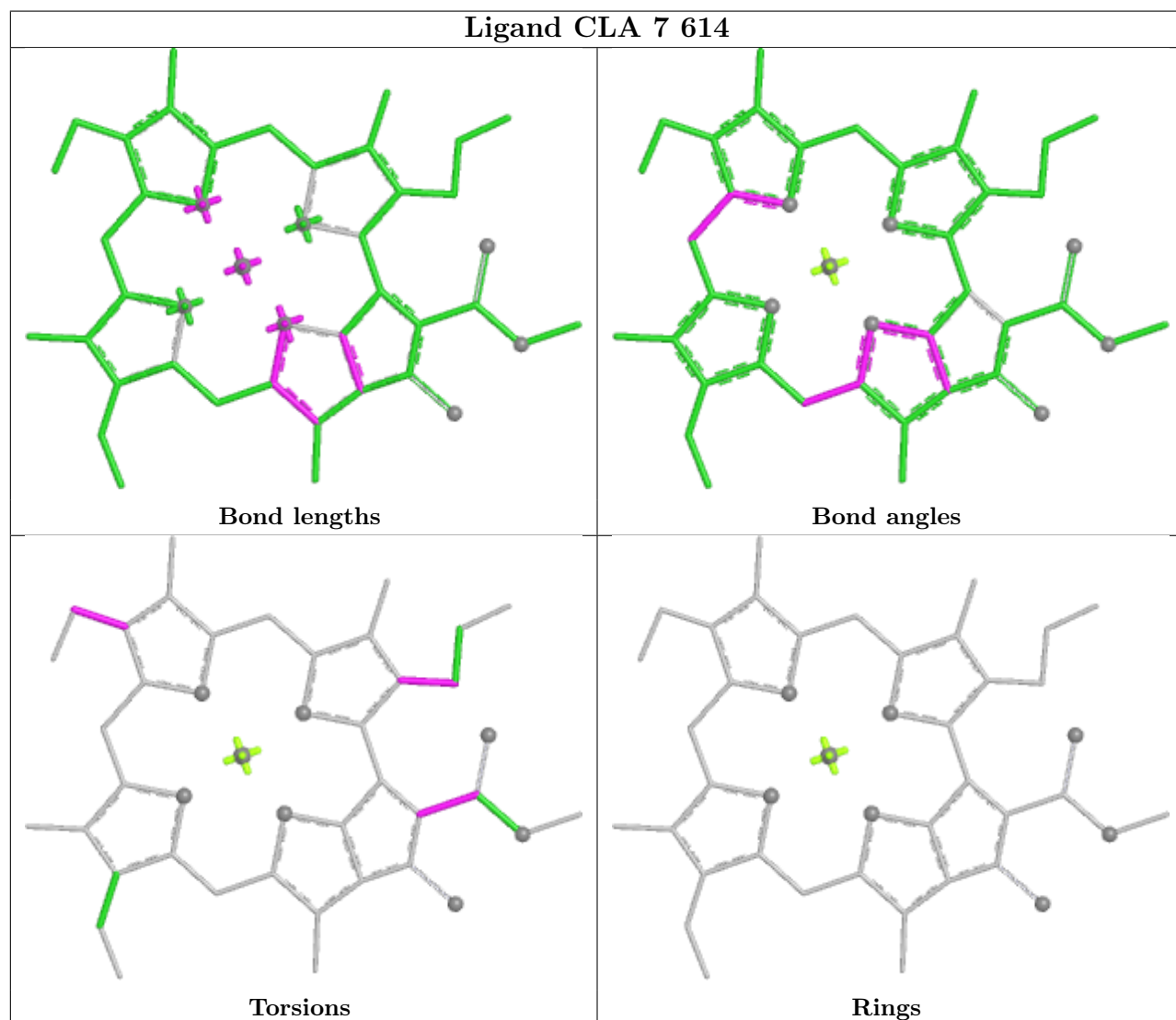
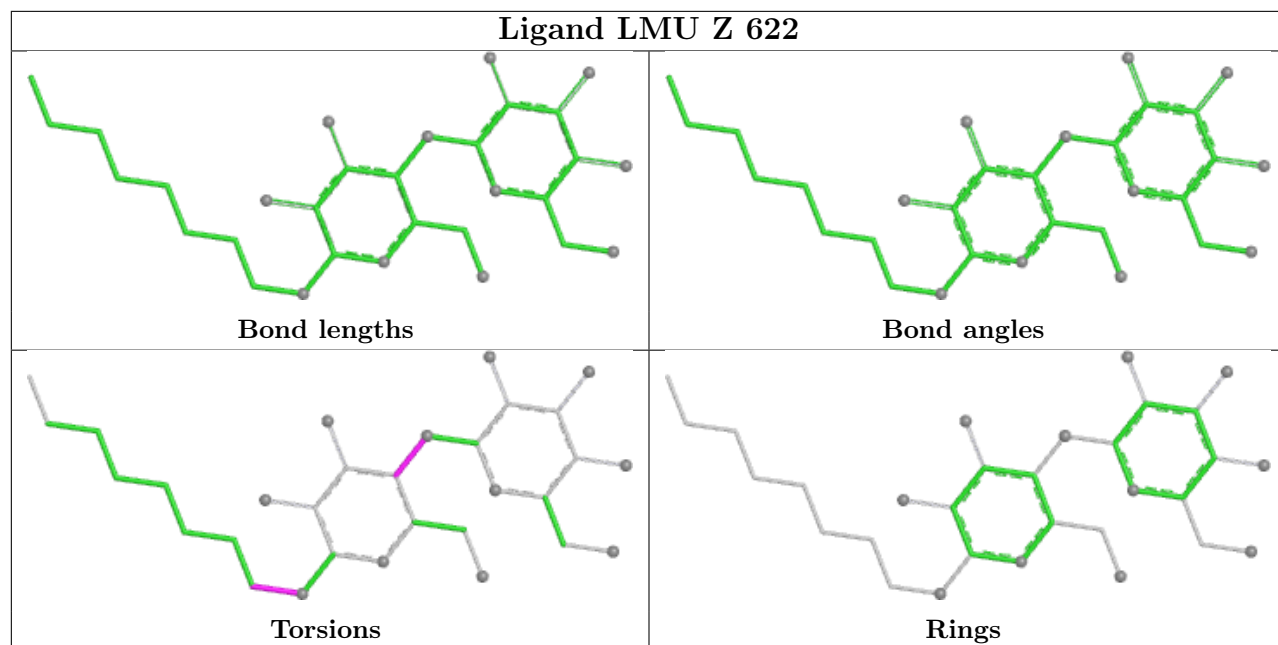
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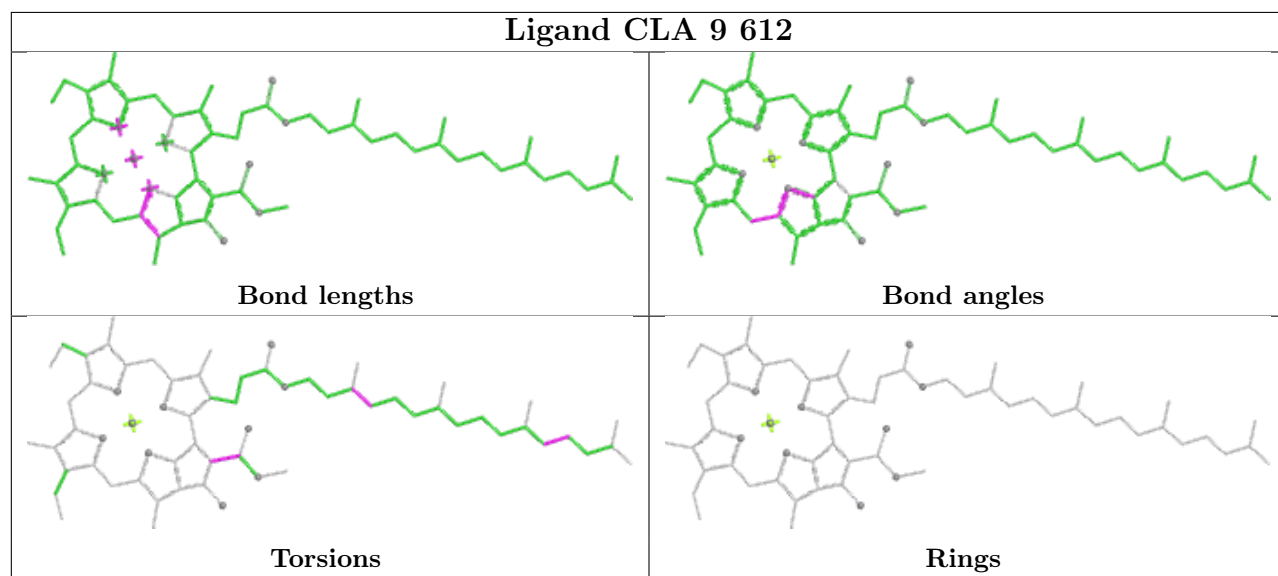
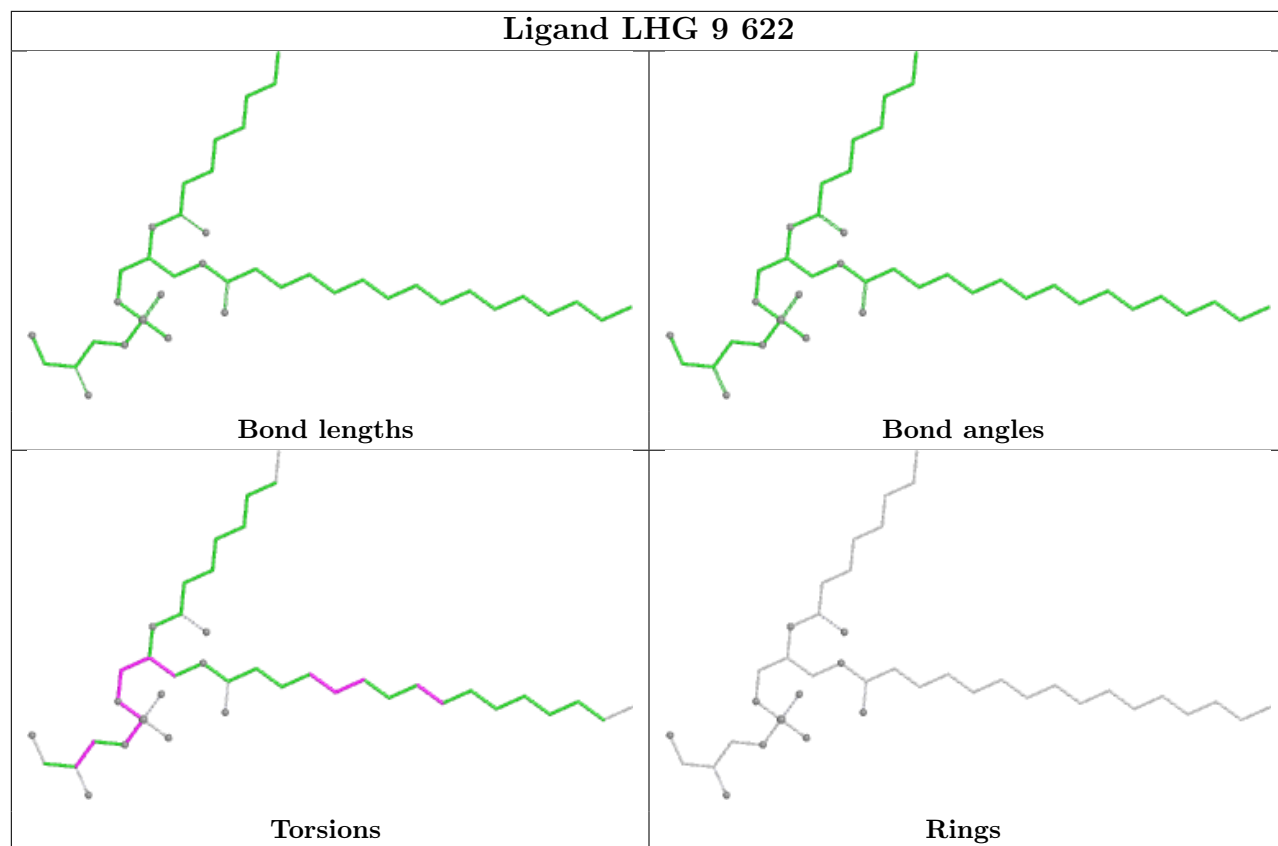


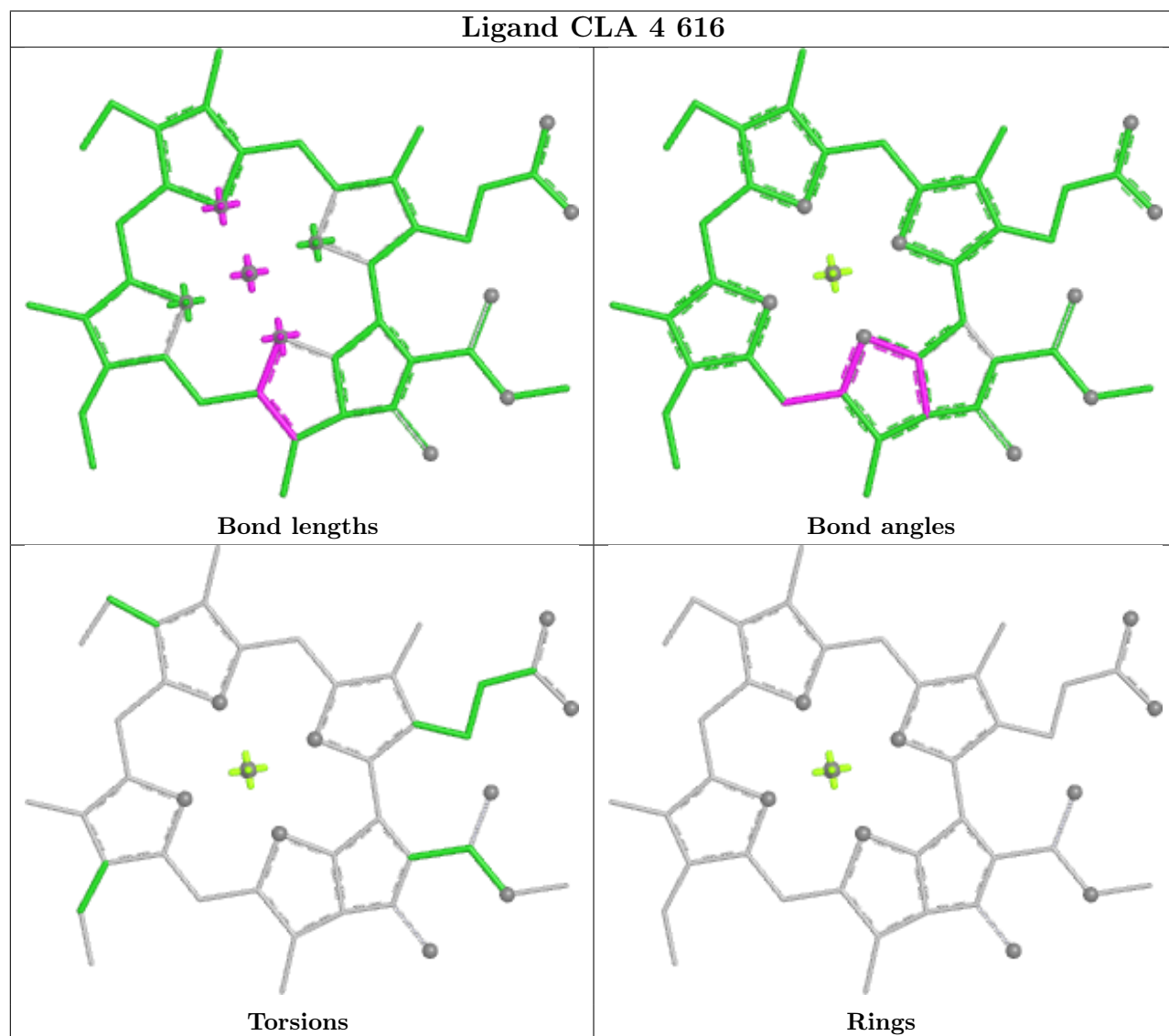
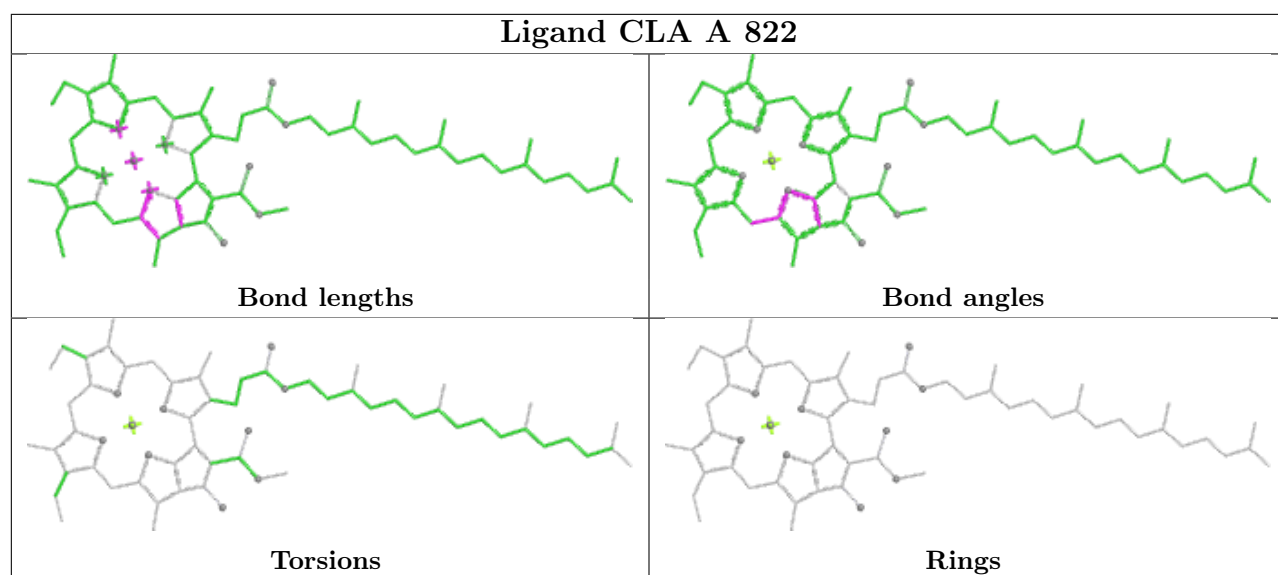
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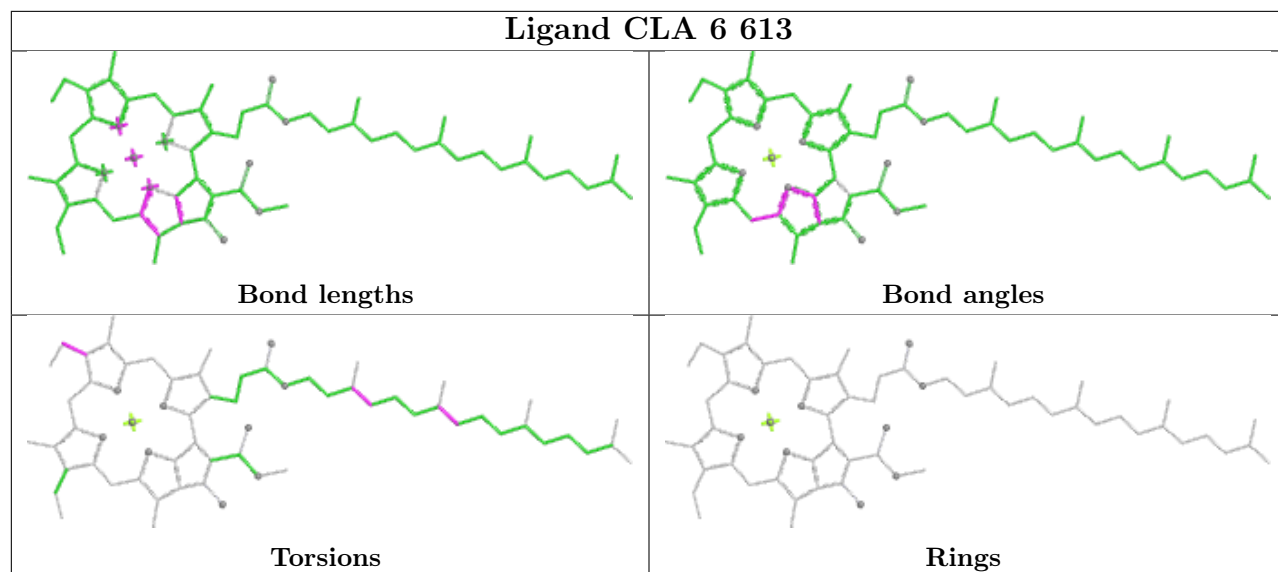
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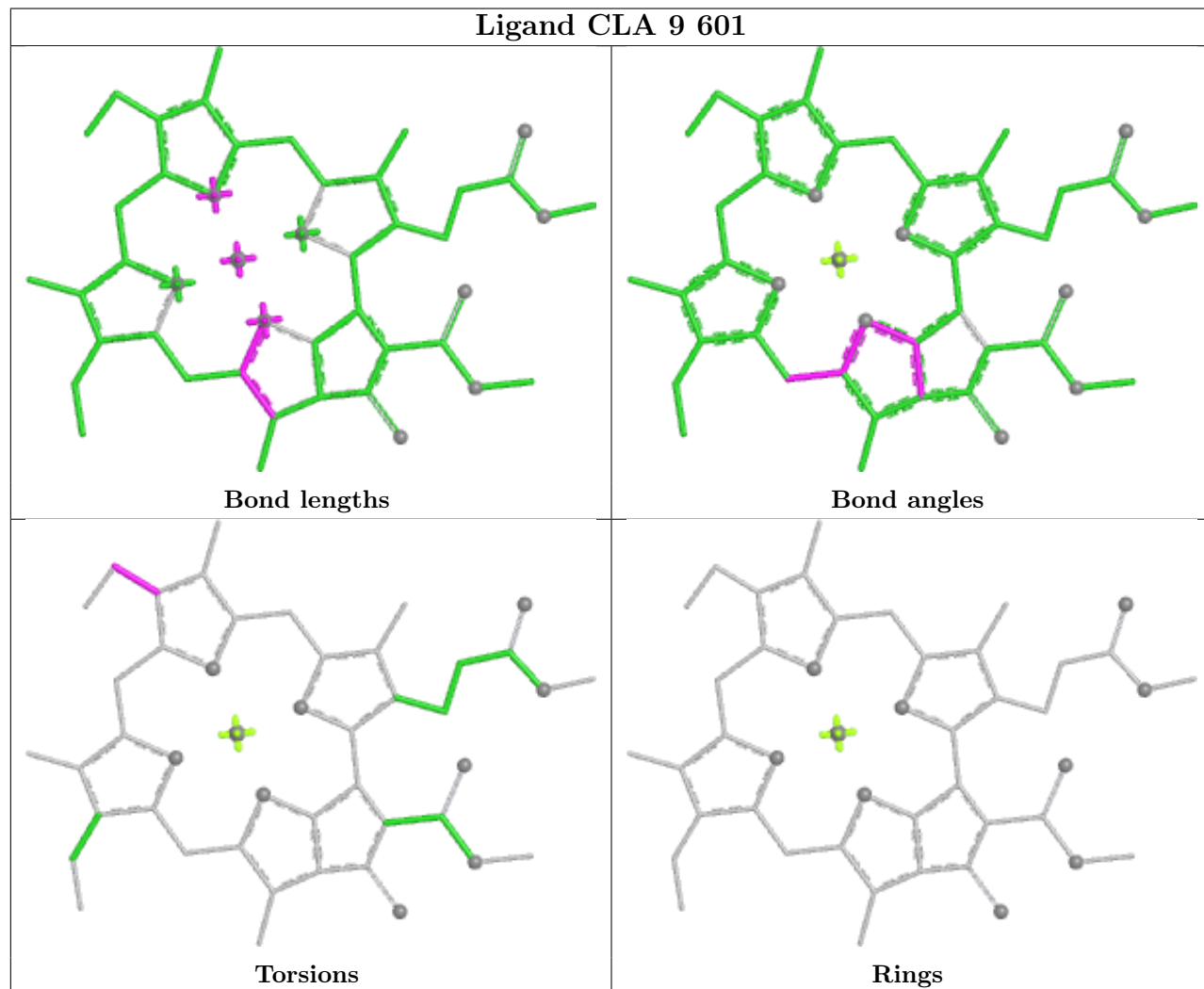


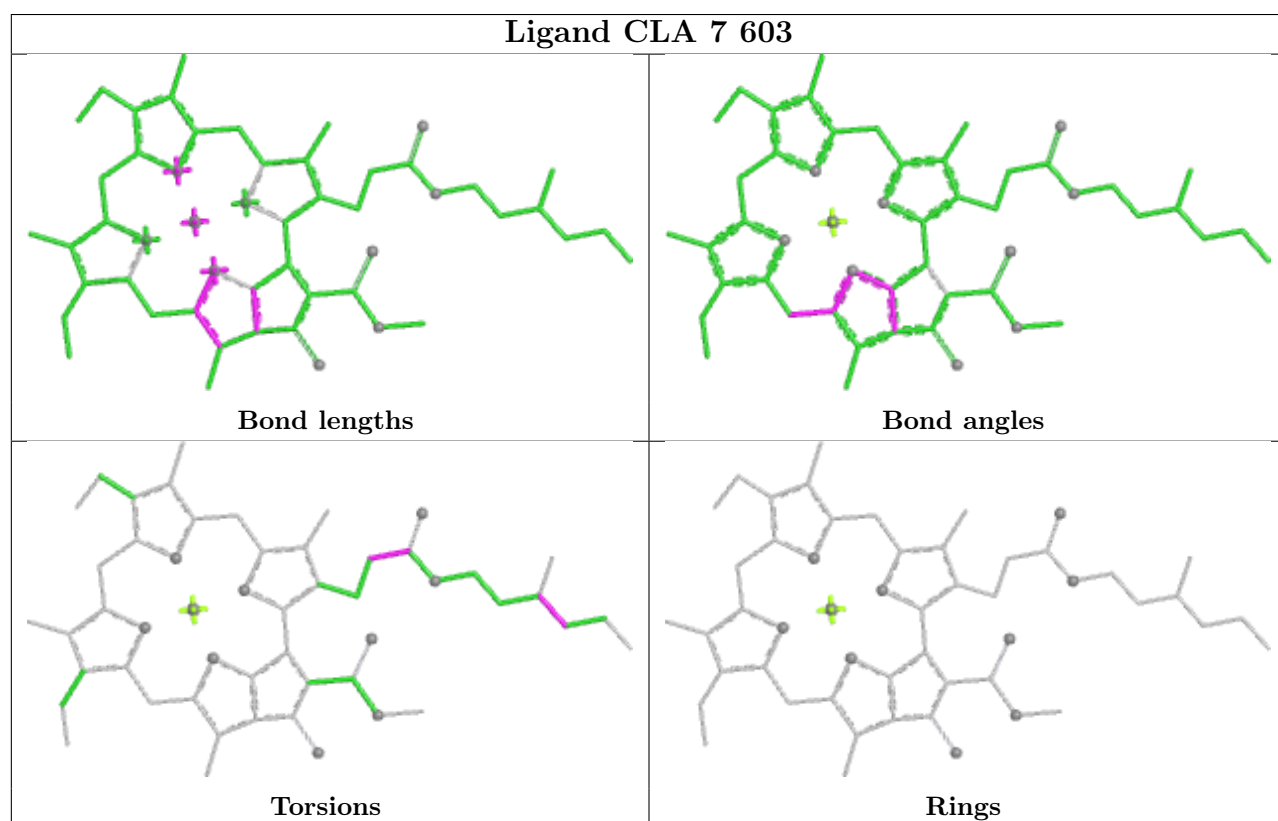
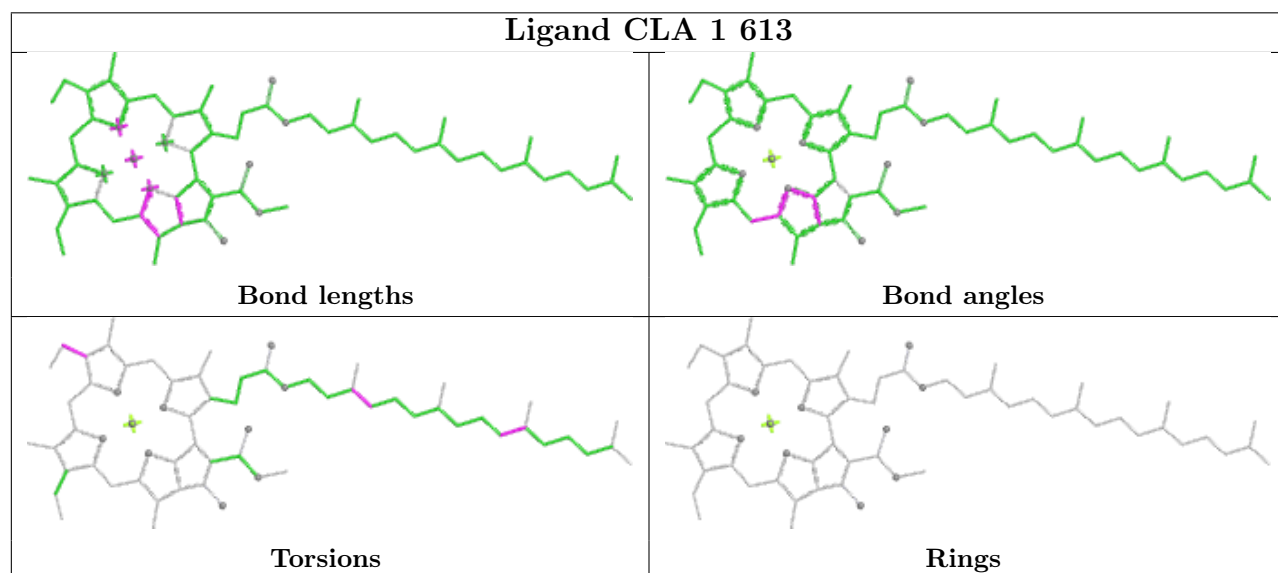
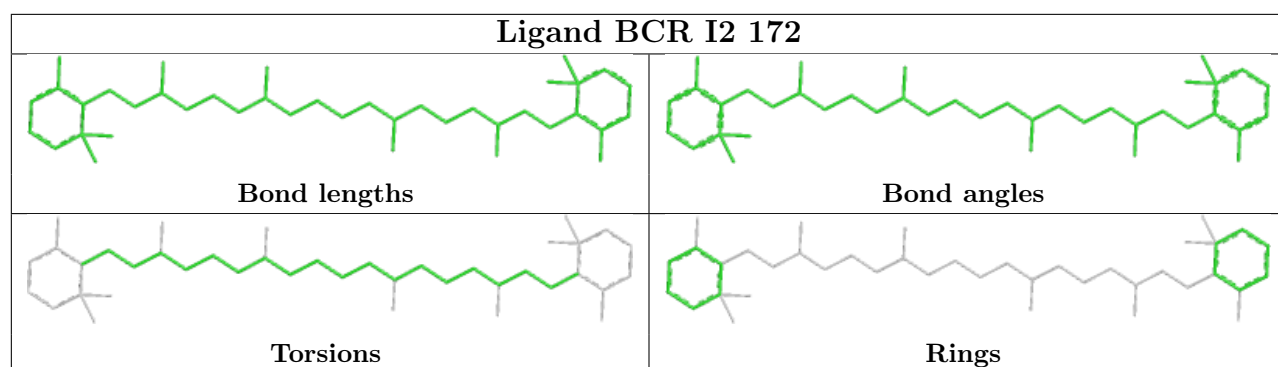


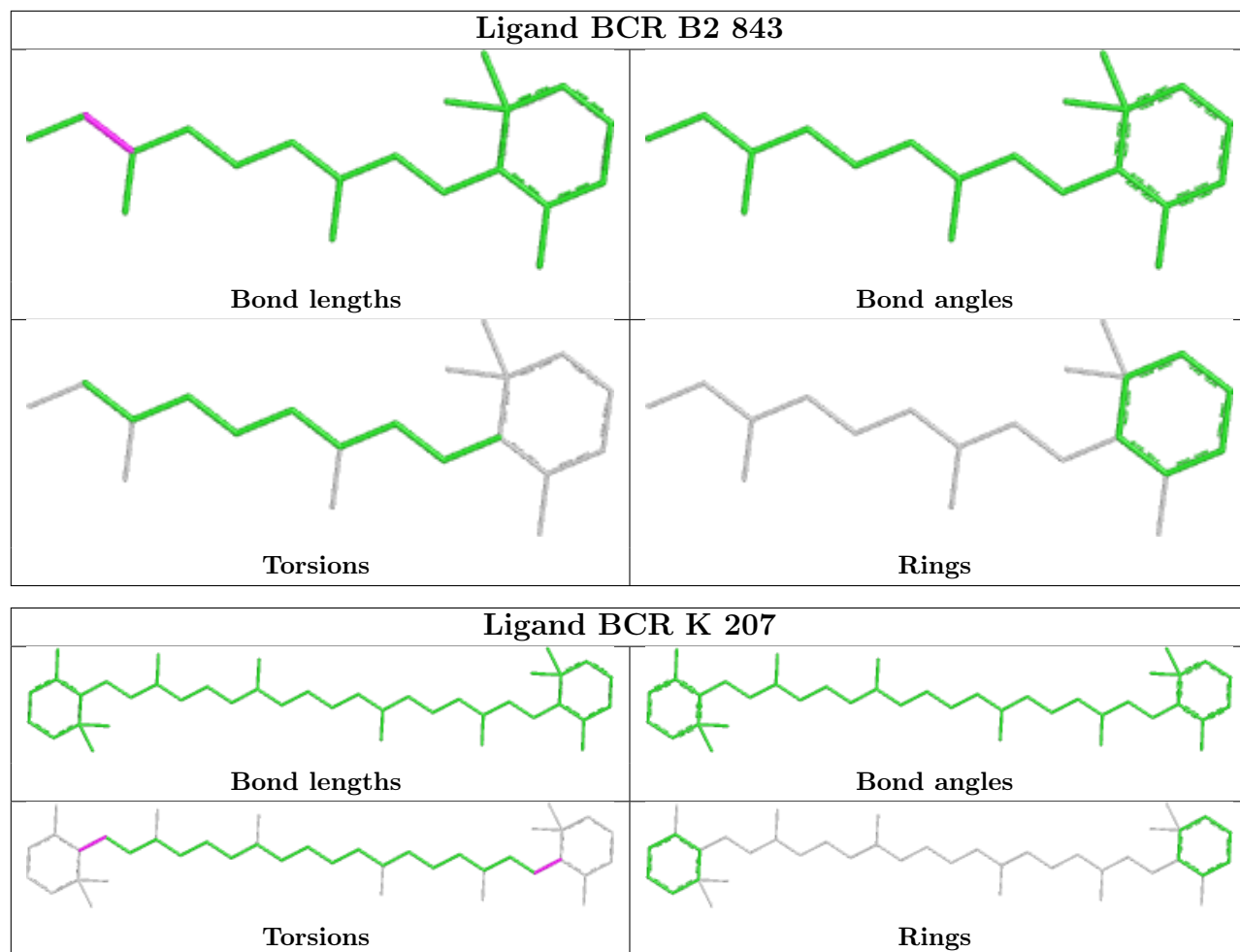
Ligand CLA 6 613



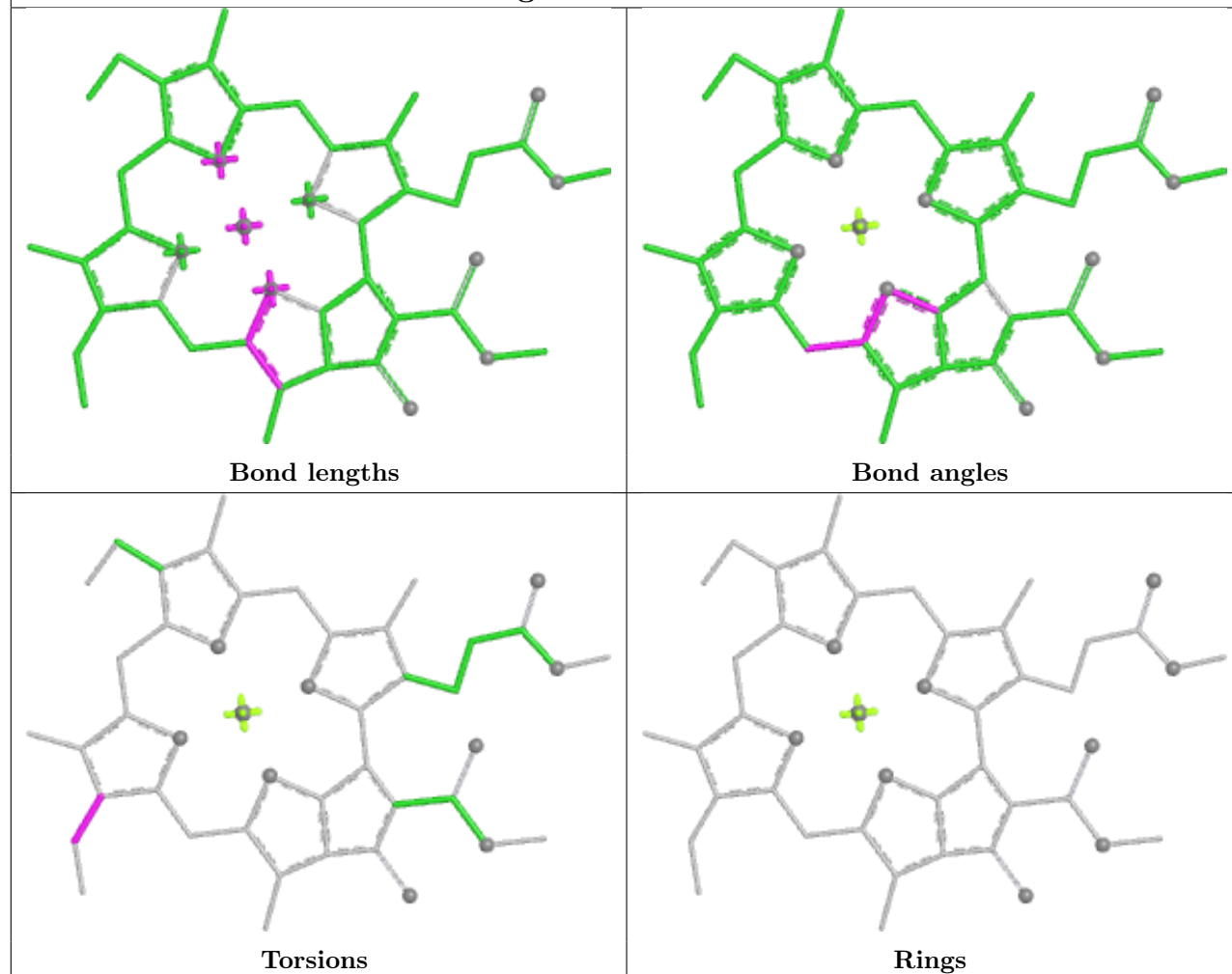
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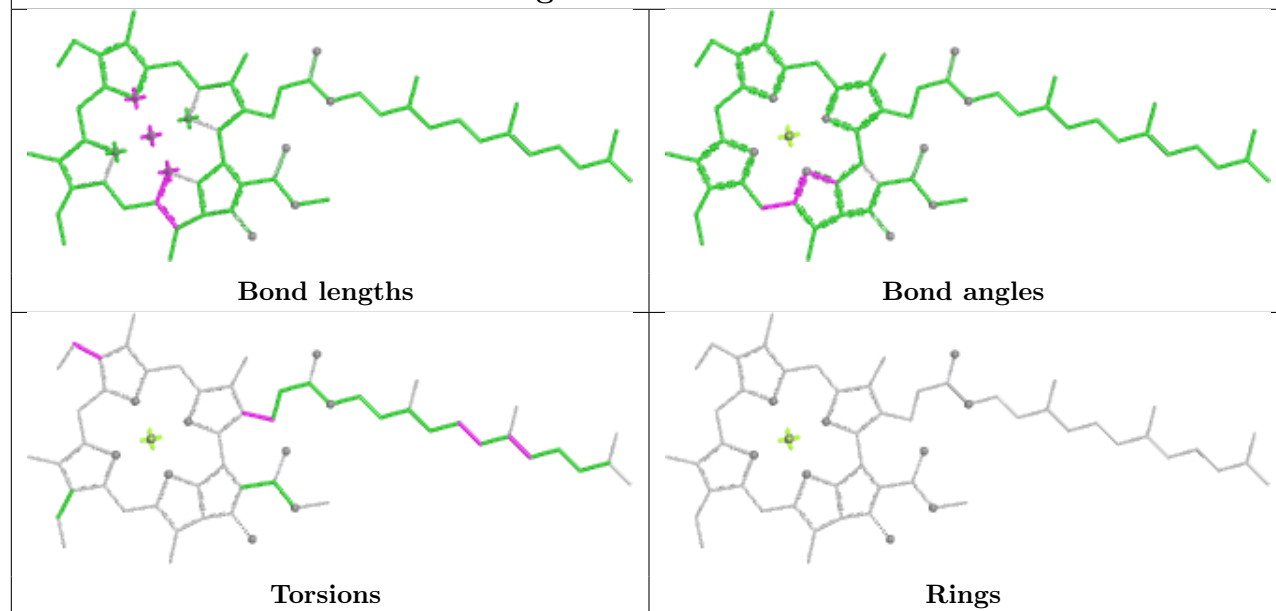


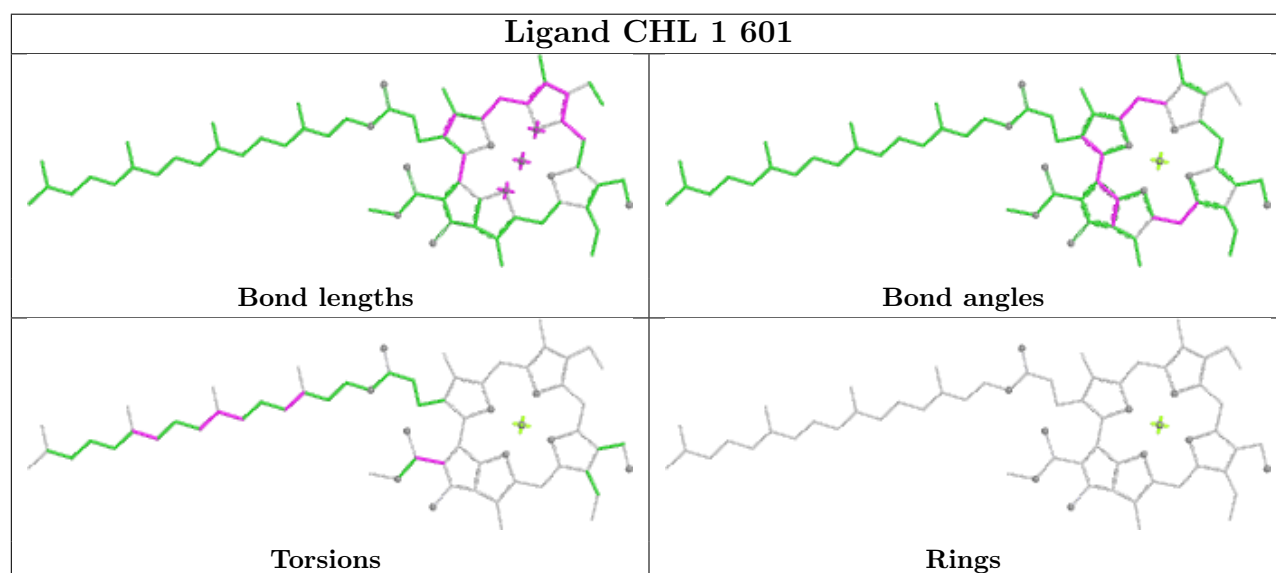
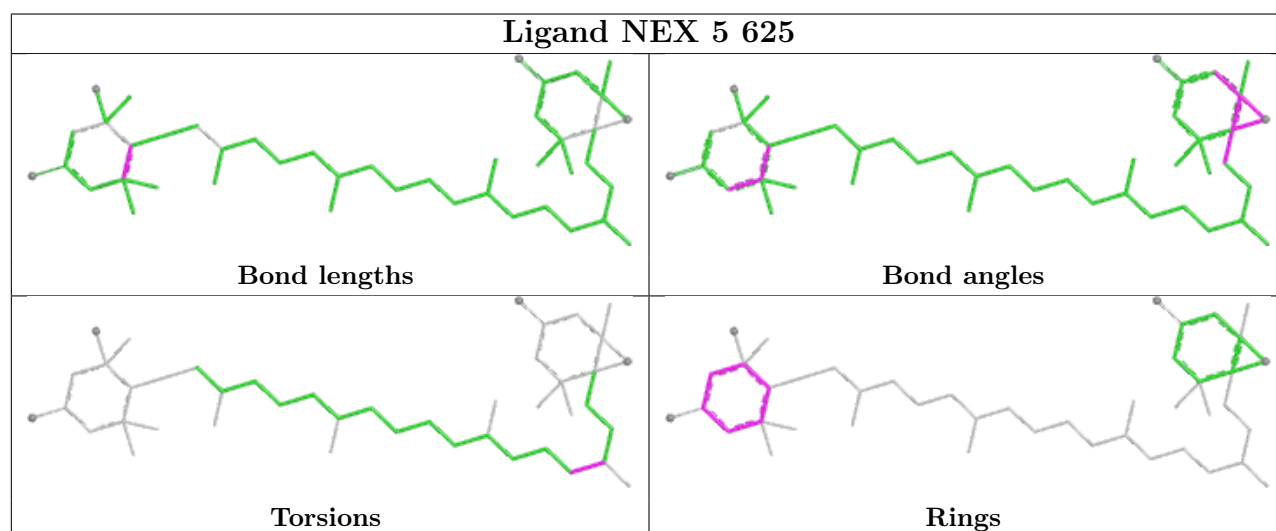
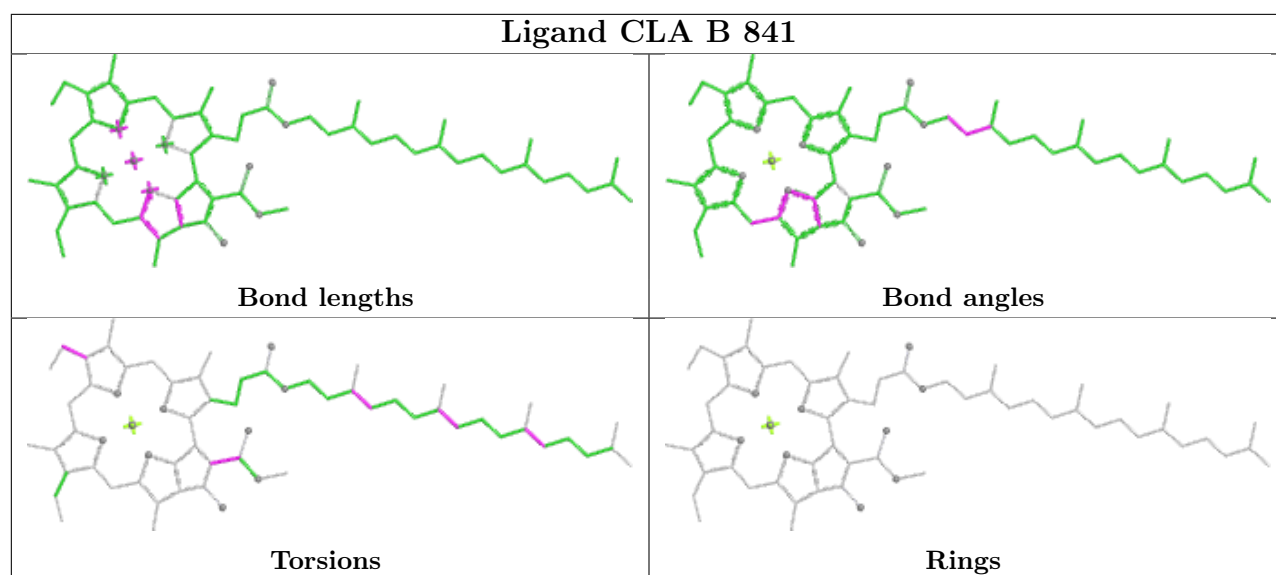


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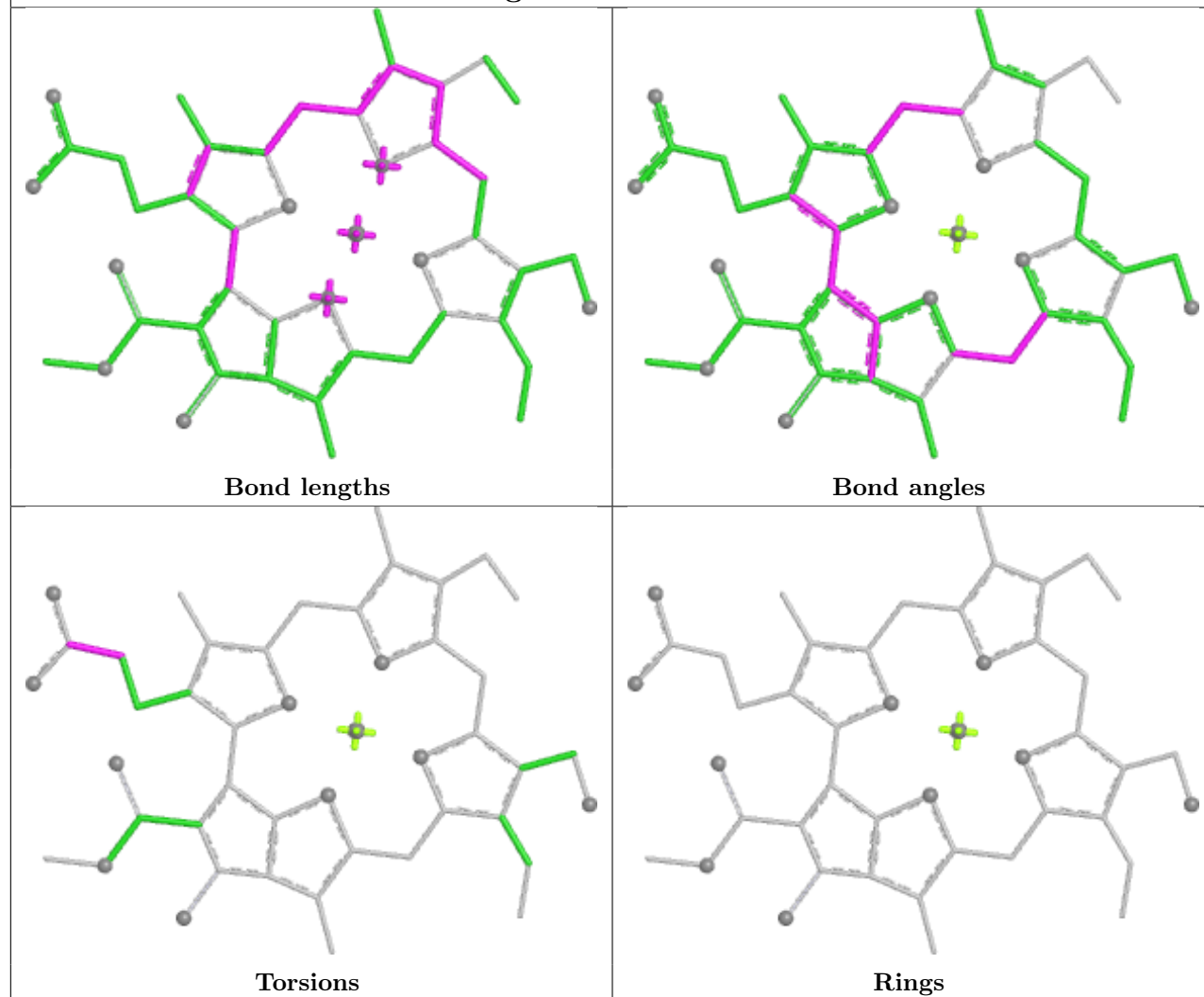


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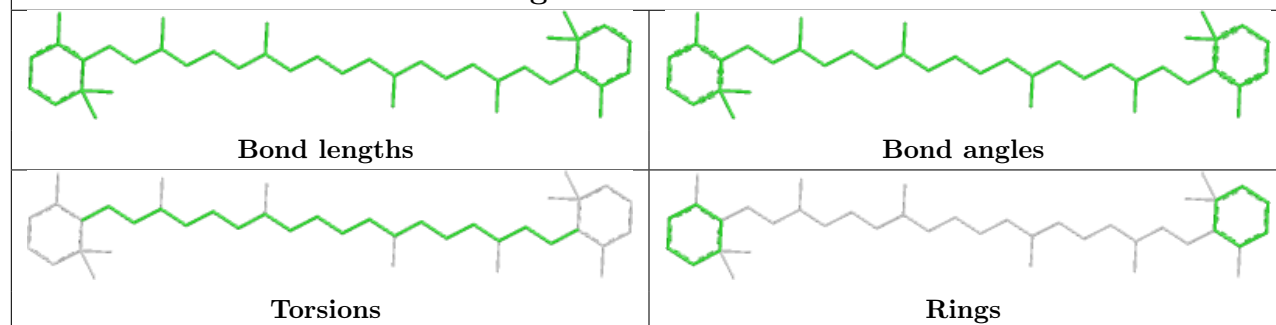


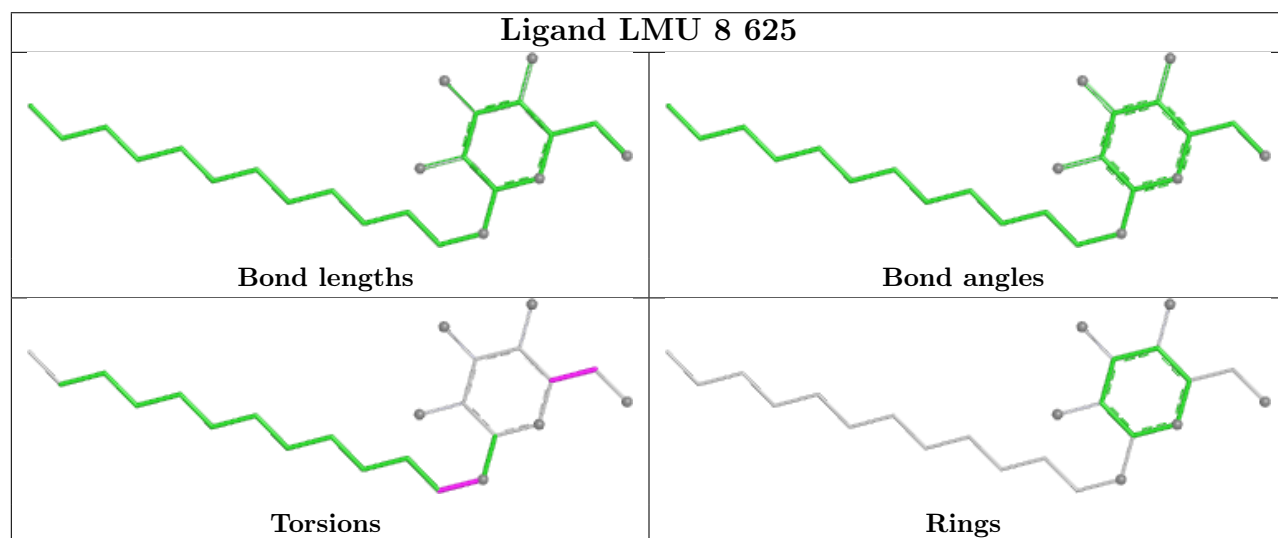
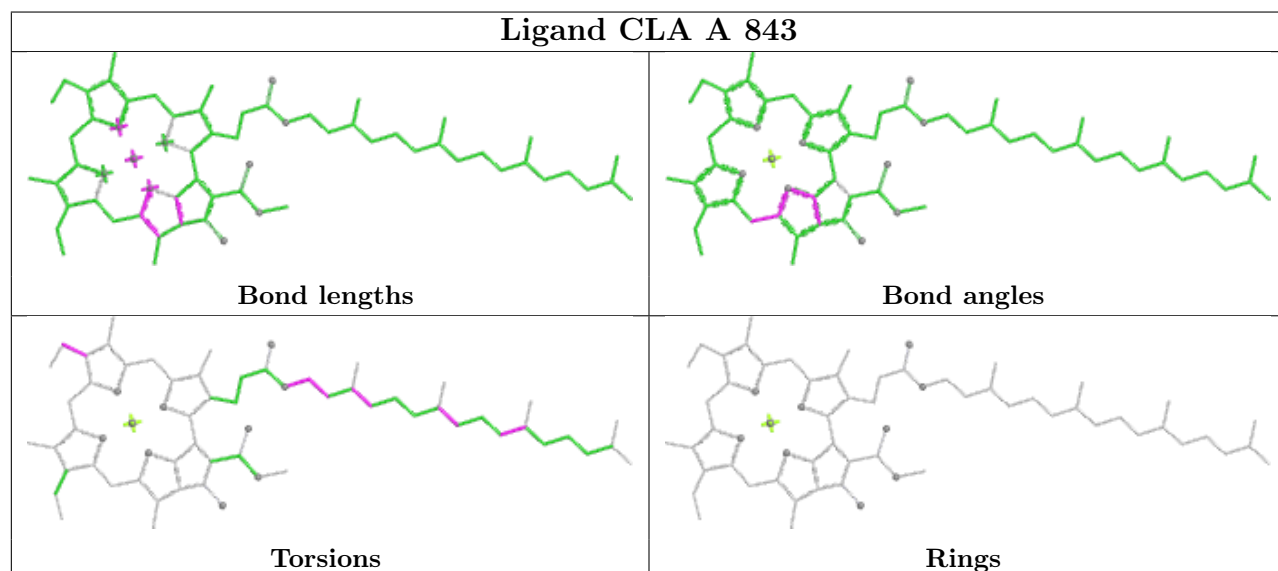
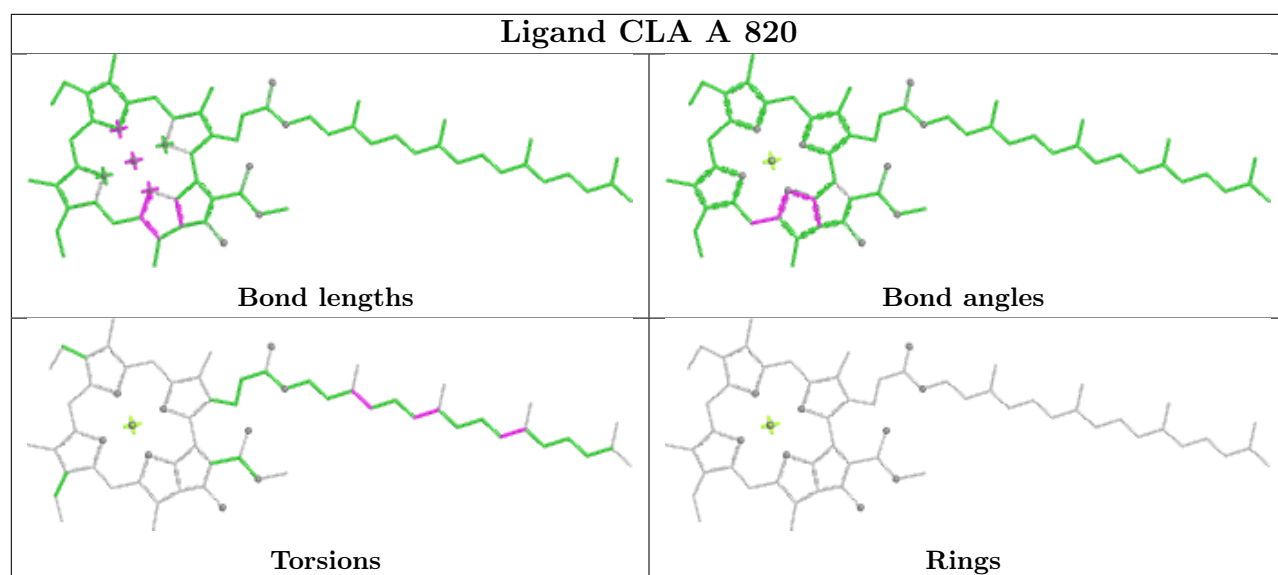


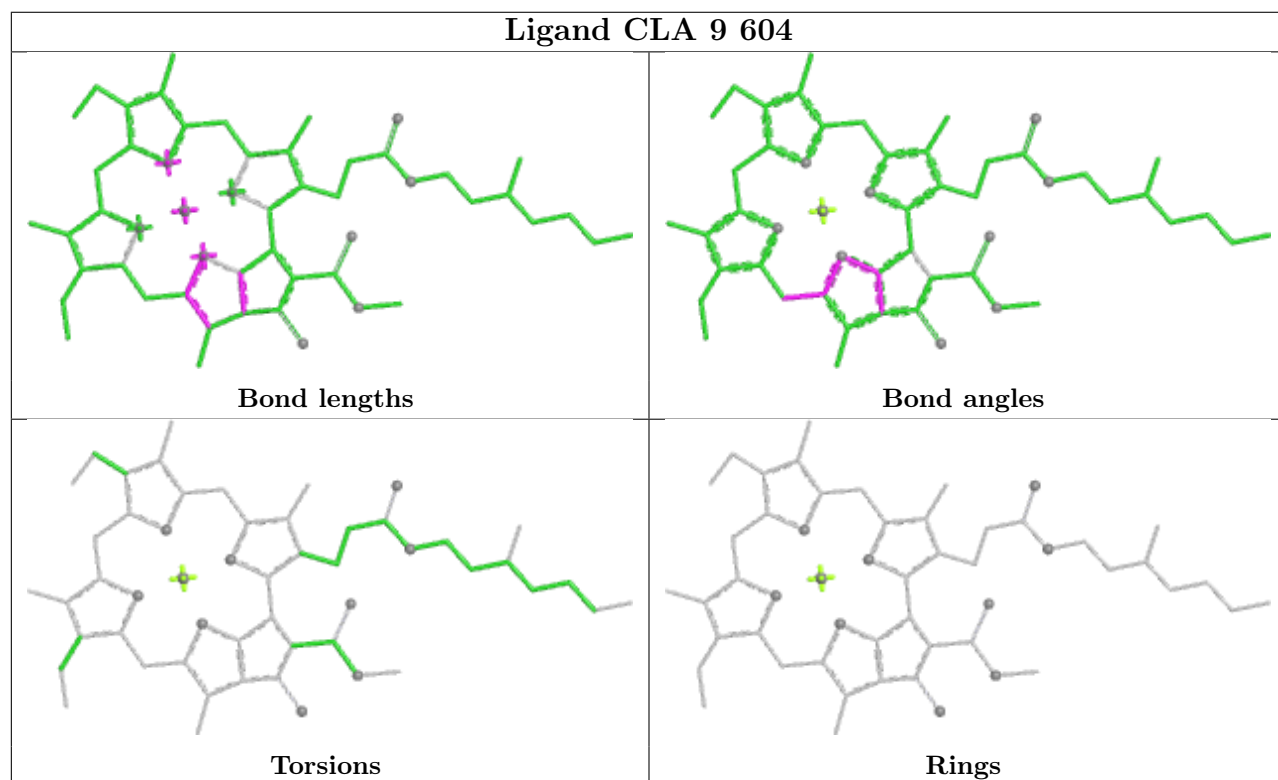
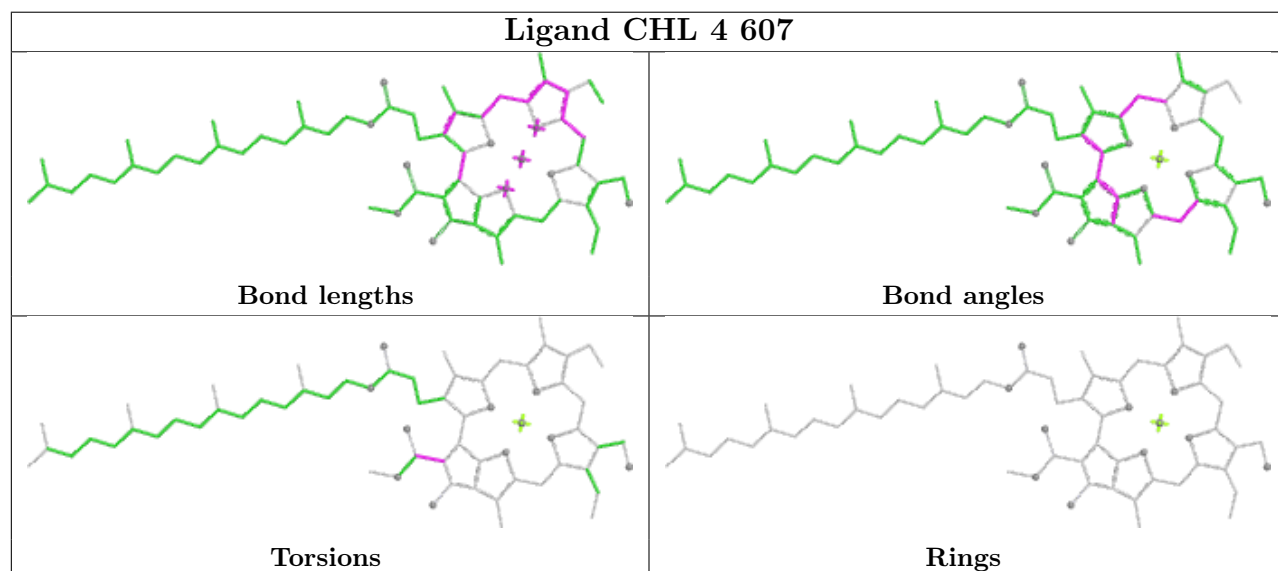
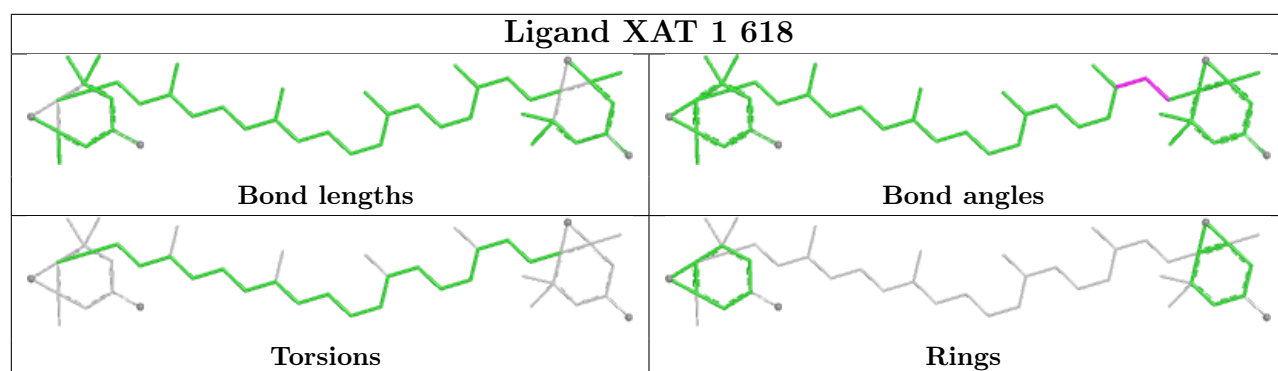
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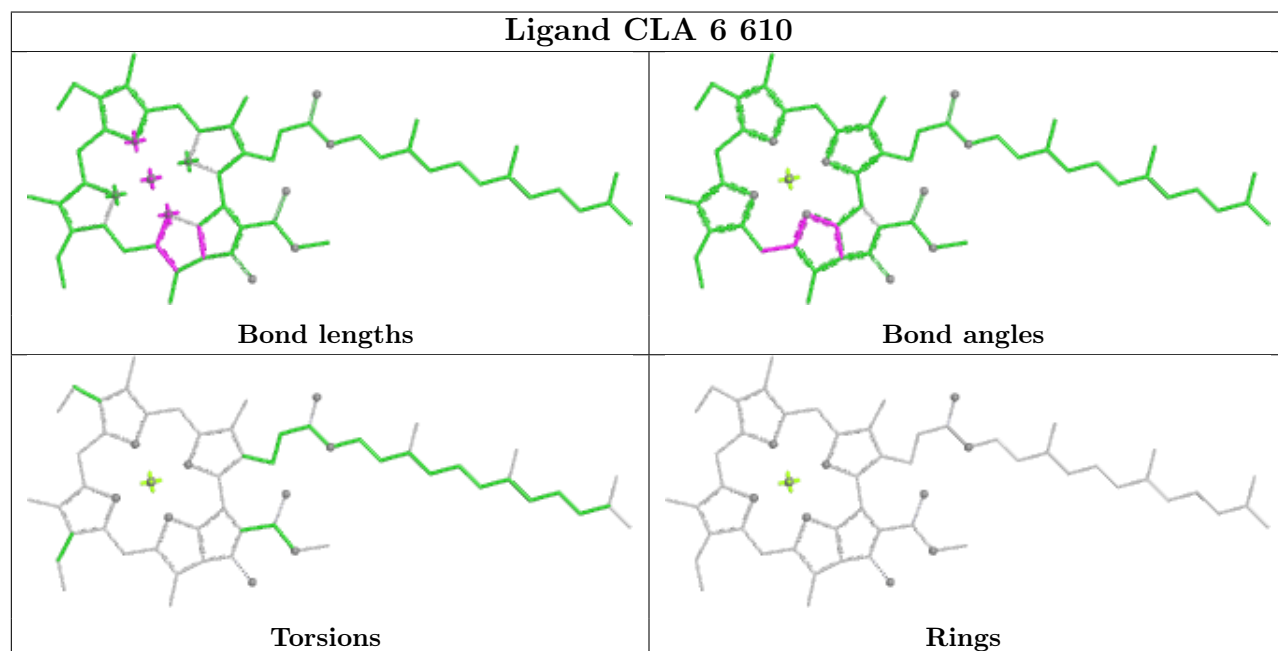
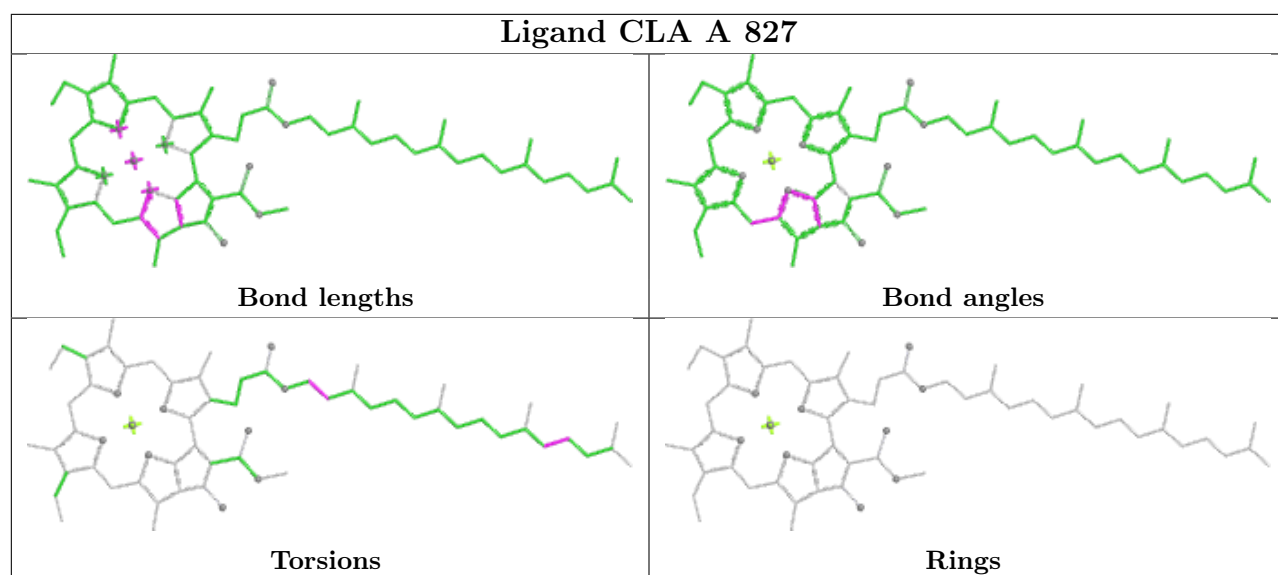


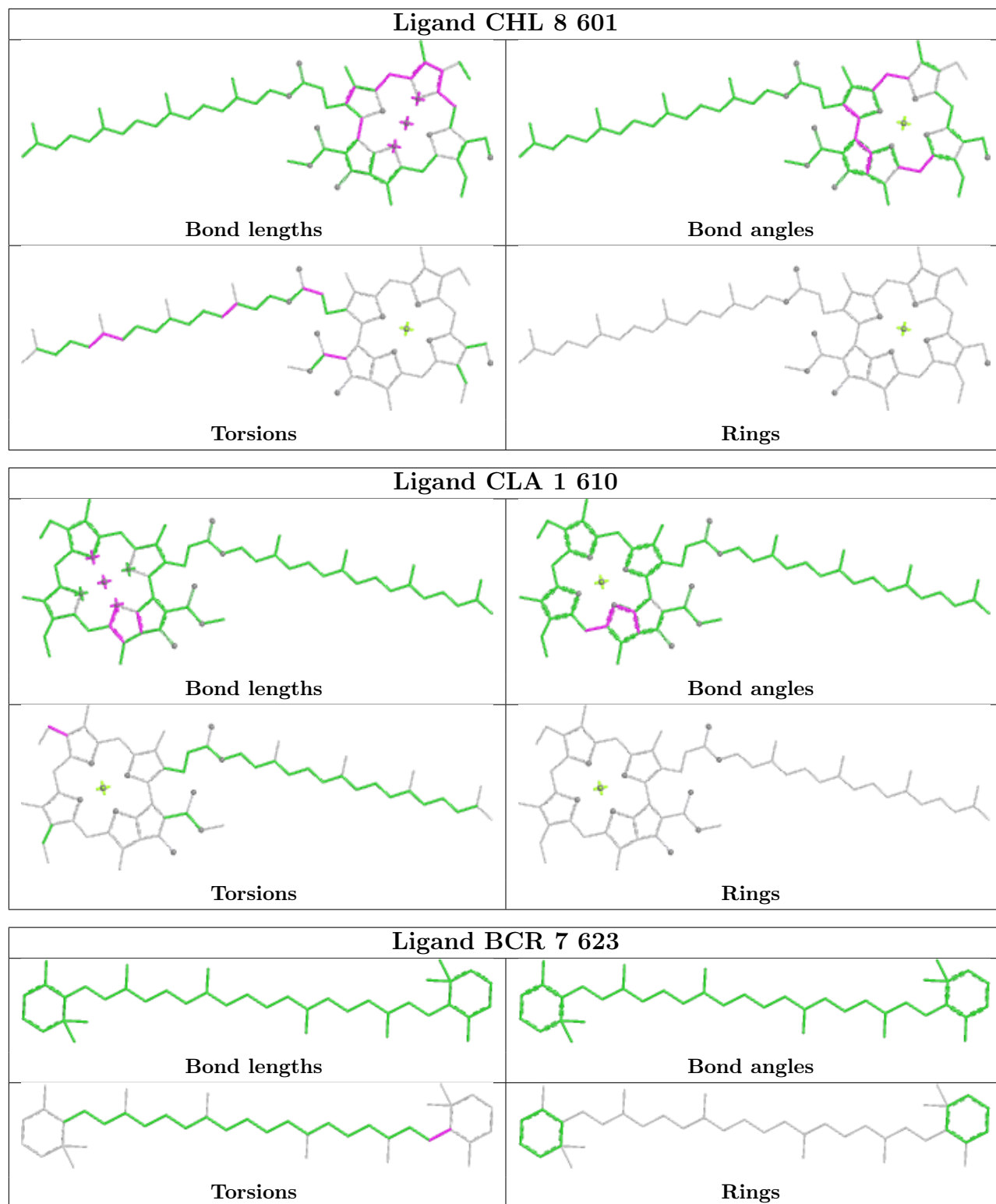
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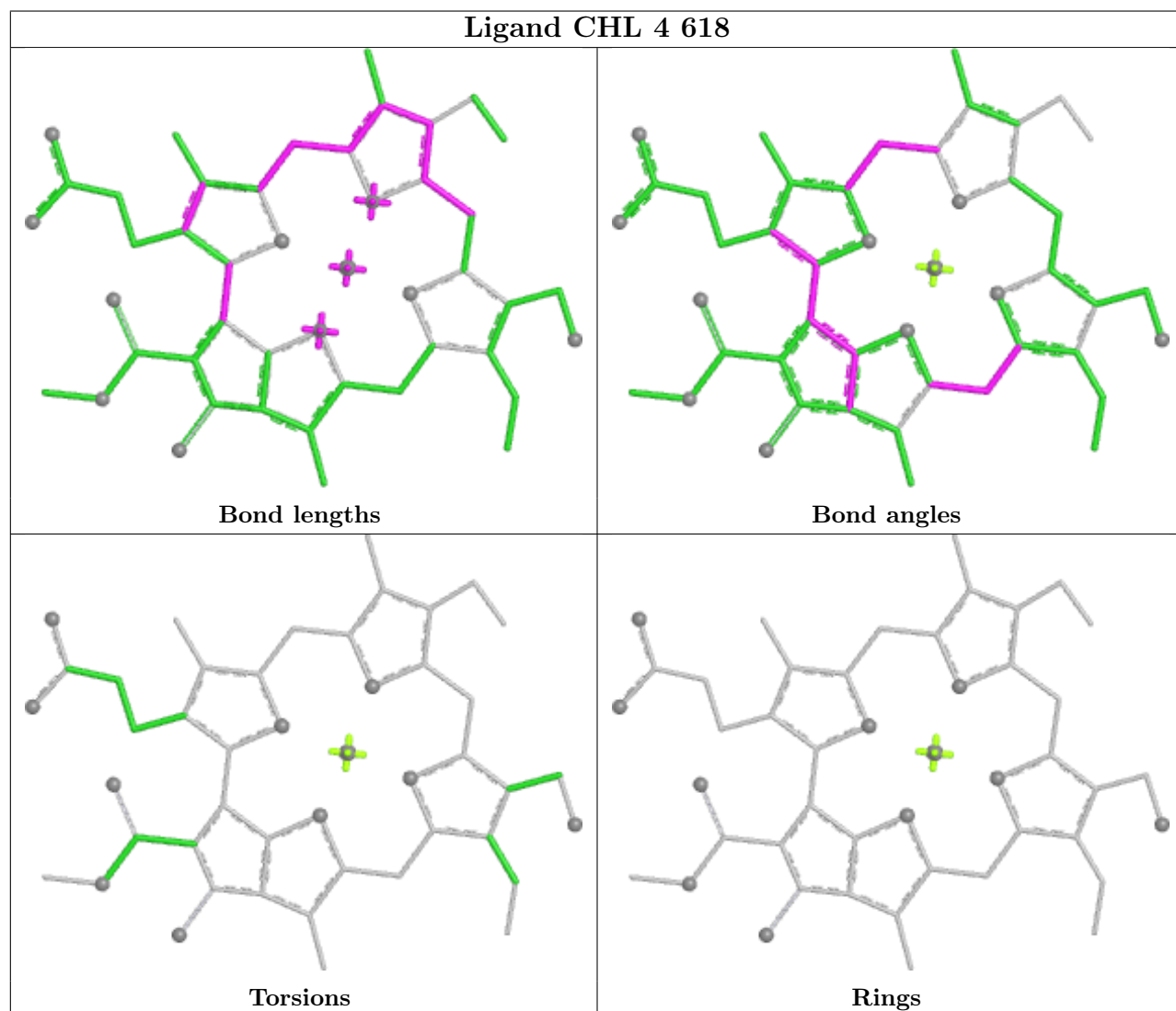
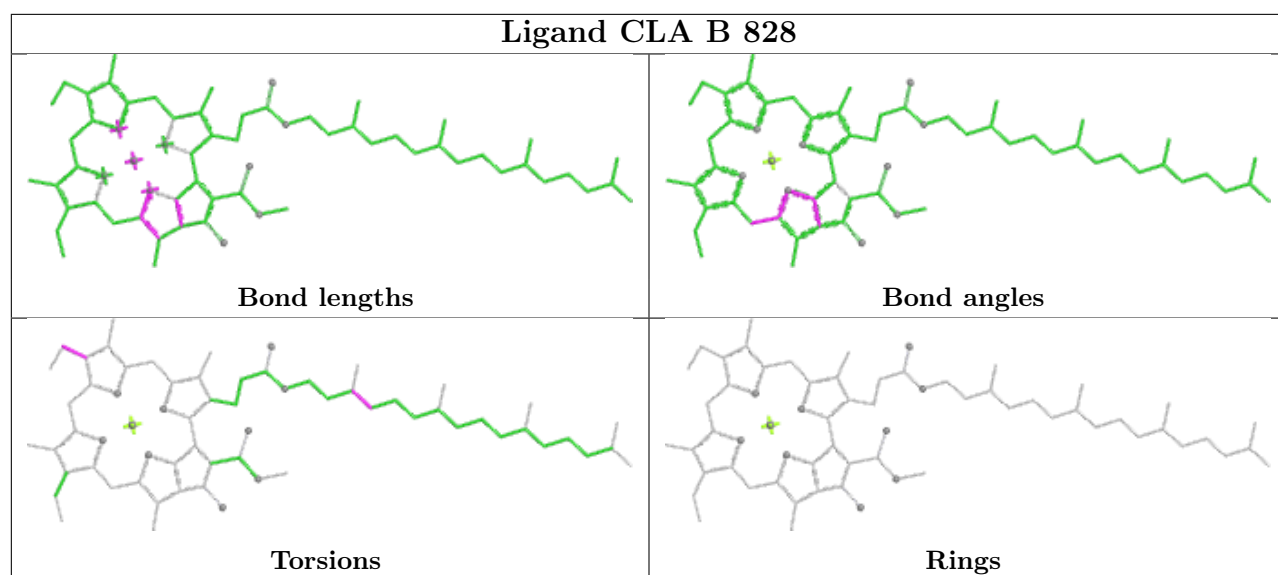


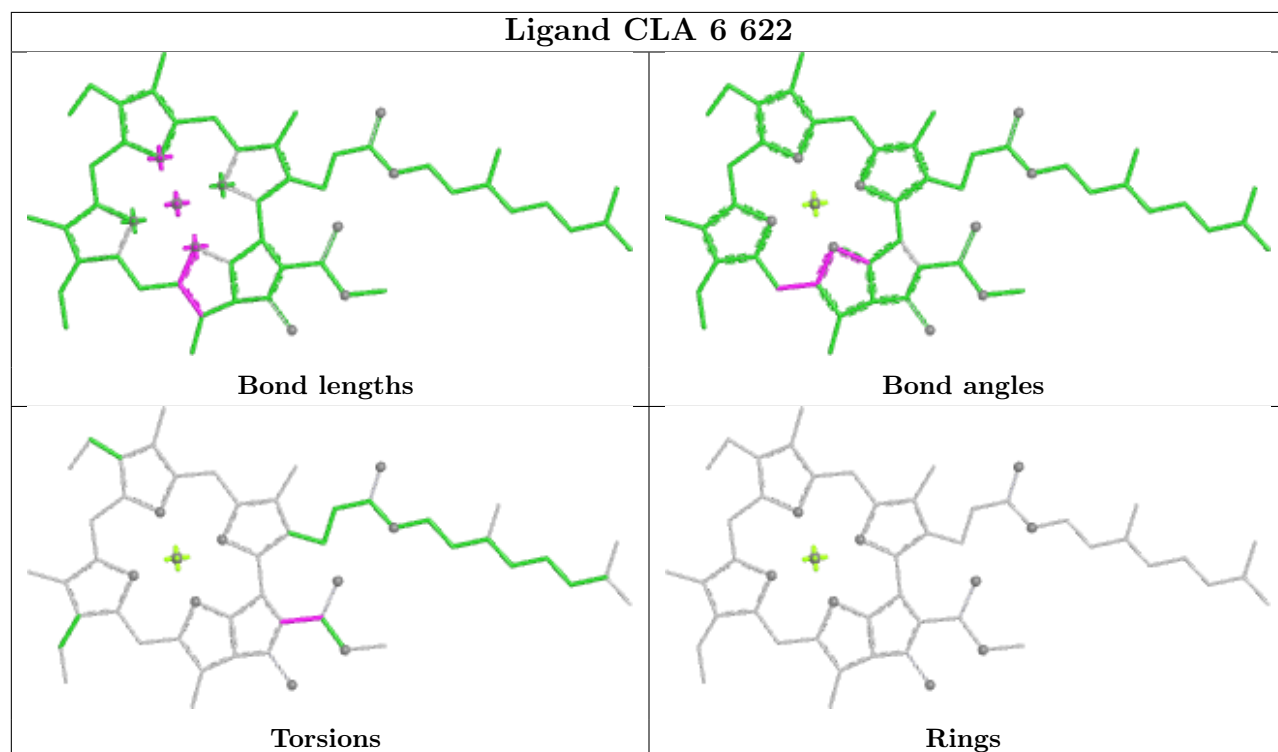
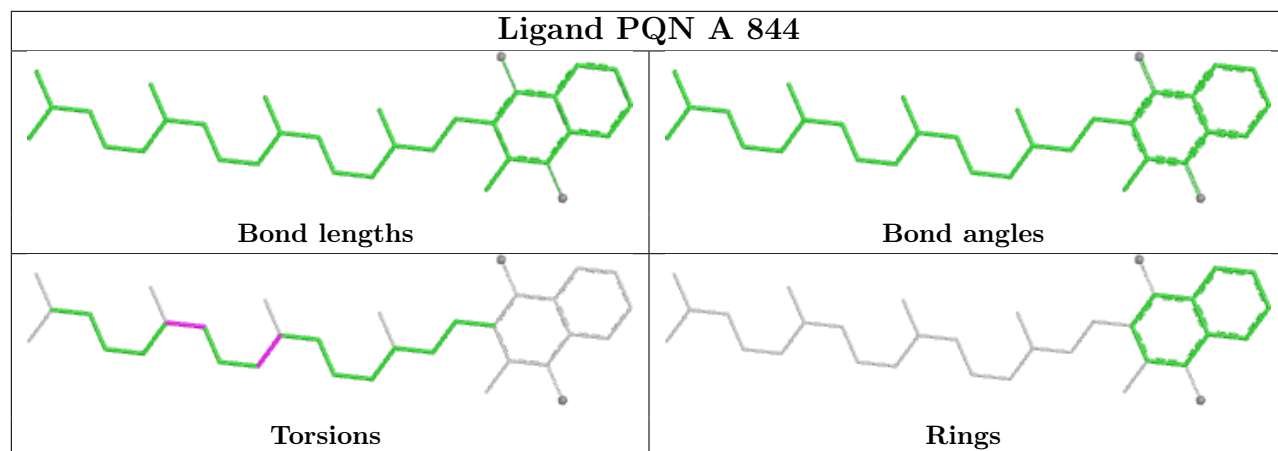




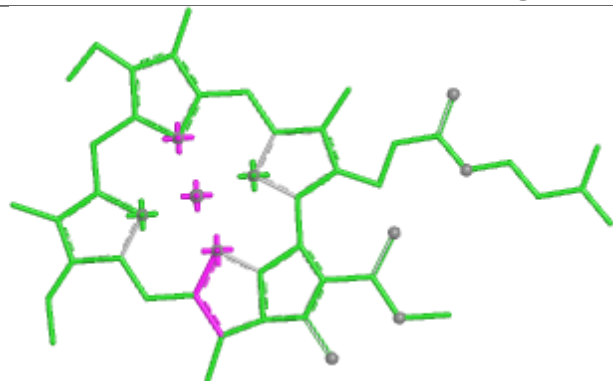




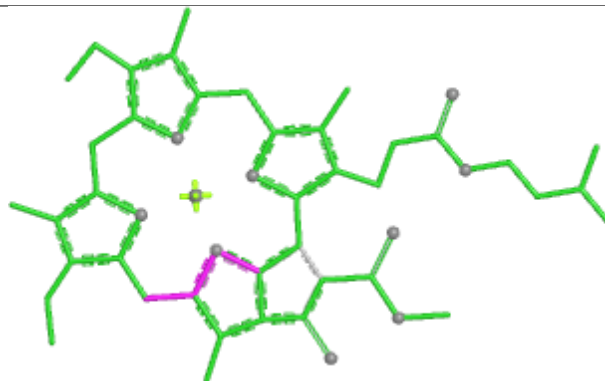




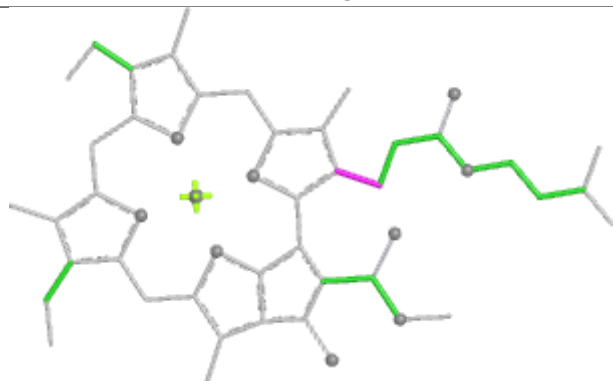
Ligand CLA B 838



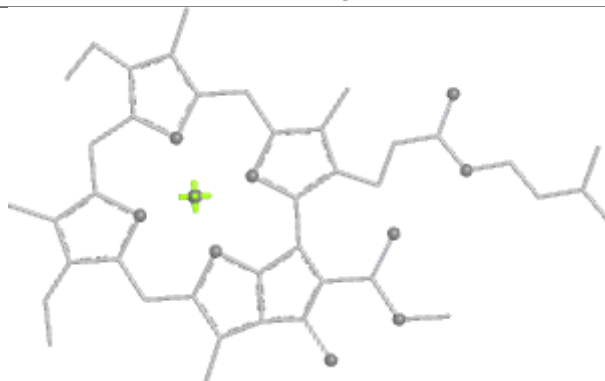
Bond lengths



Bond angles

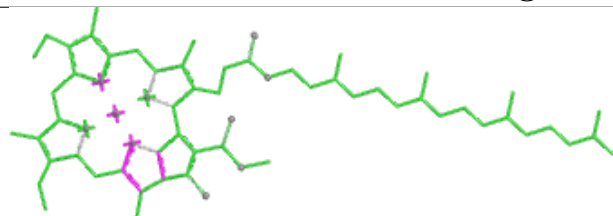


Torsions

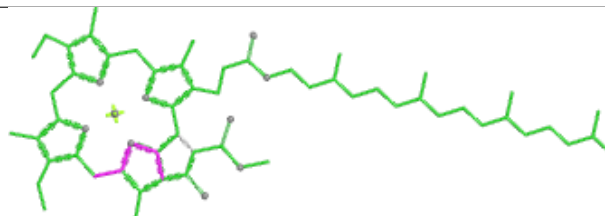


Rings

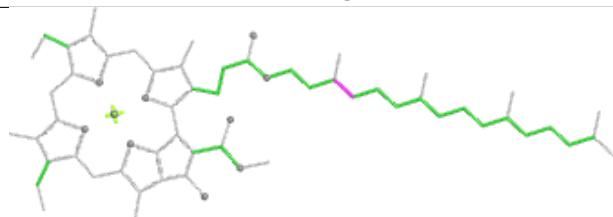
Ligand CLA 6 604



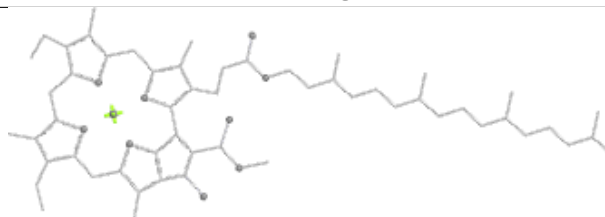
Bond lengths



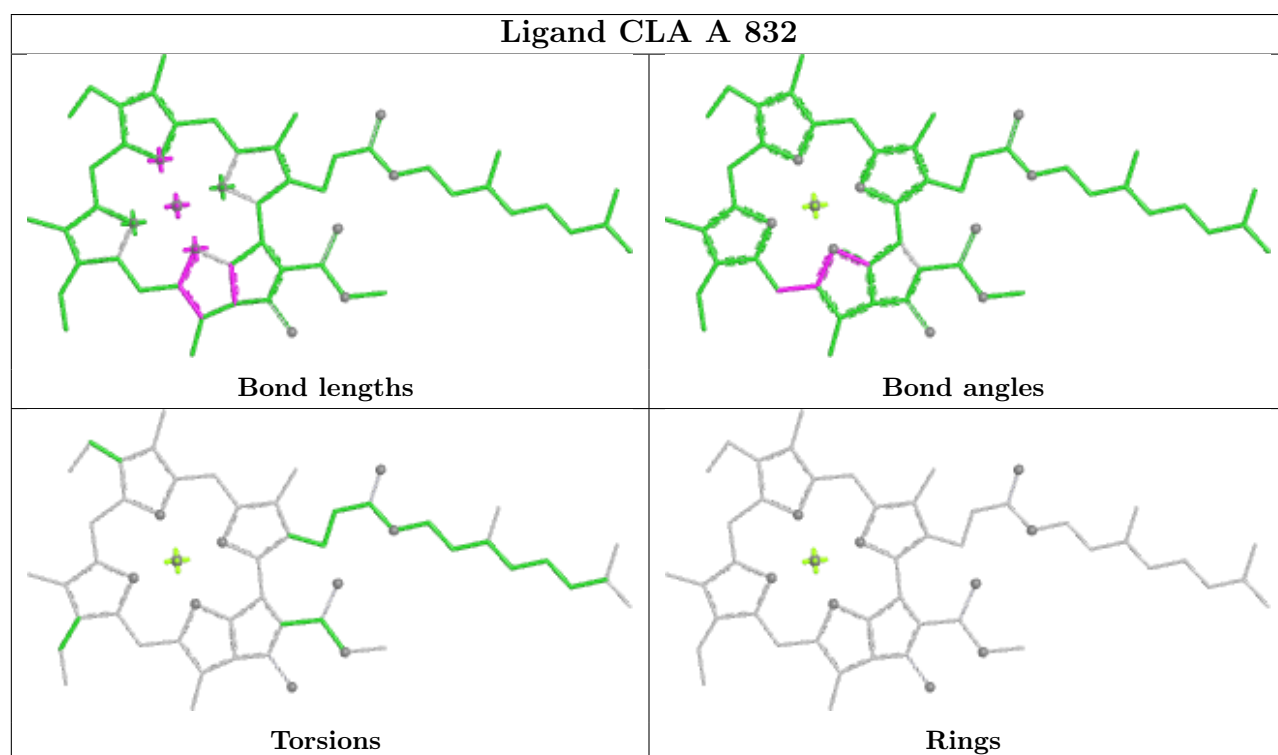
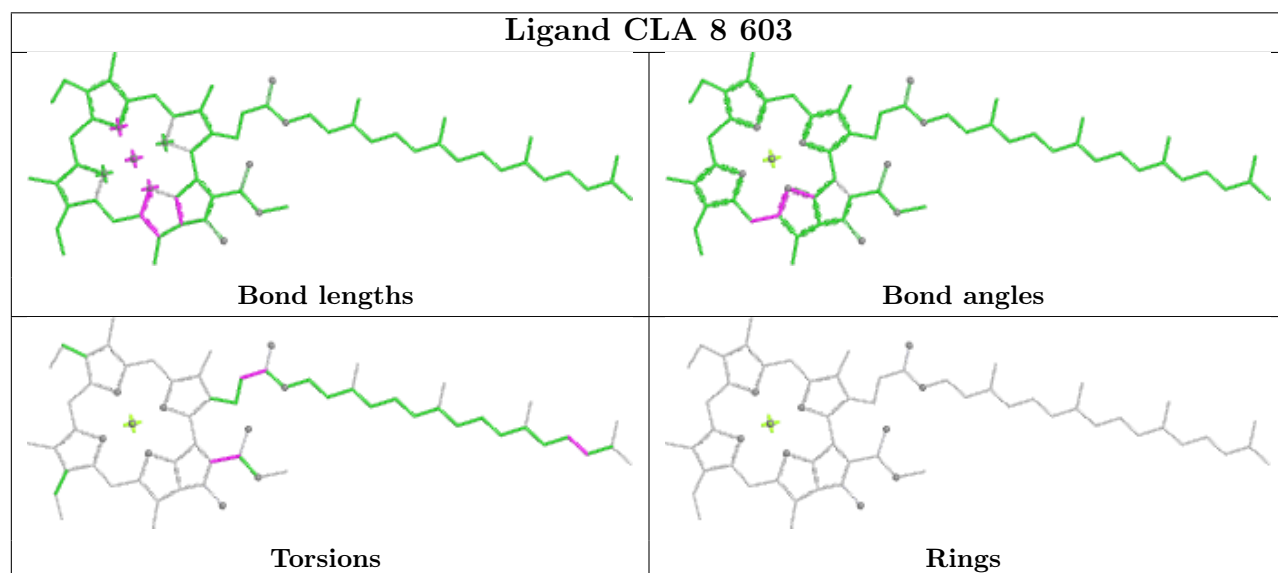
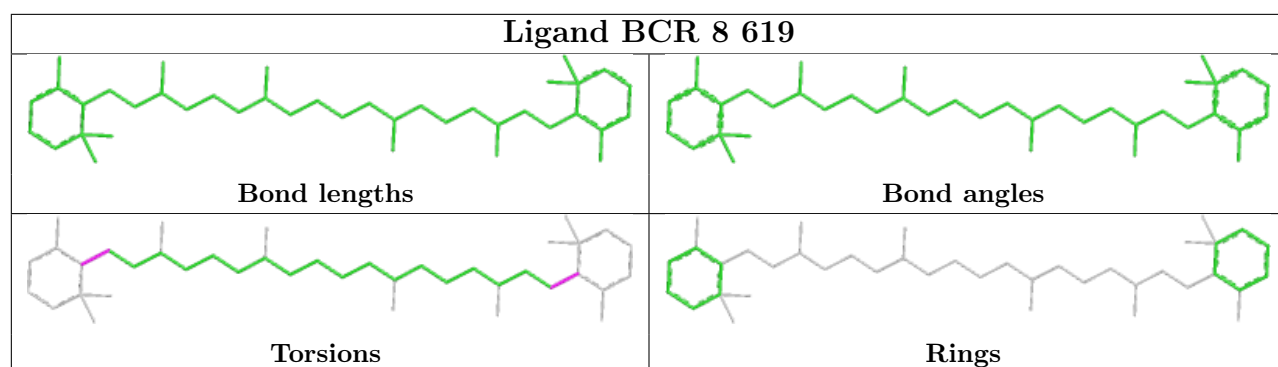
Bond angles

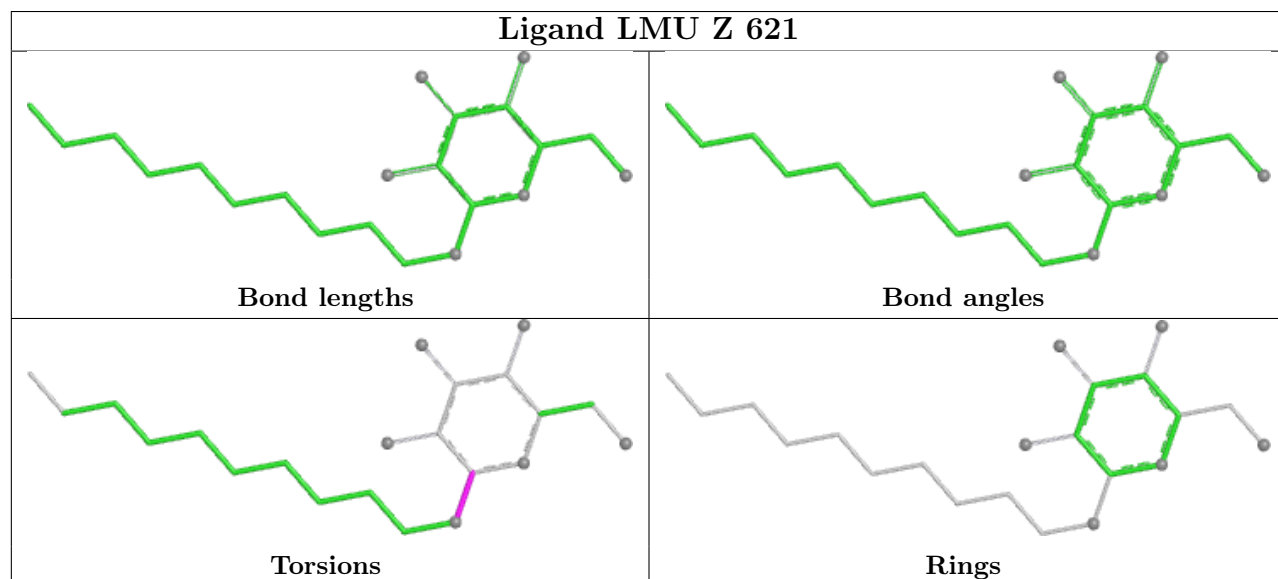
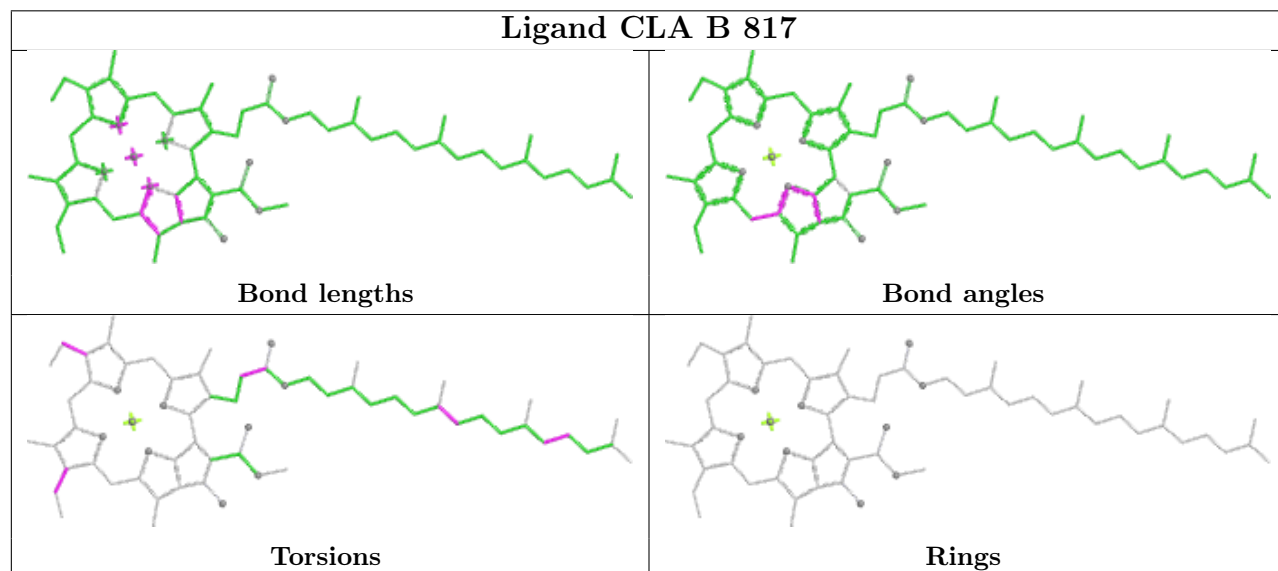
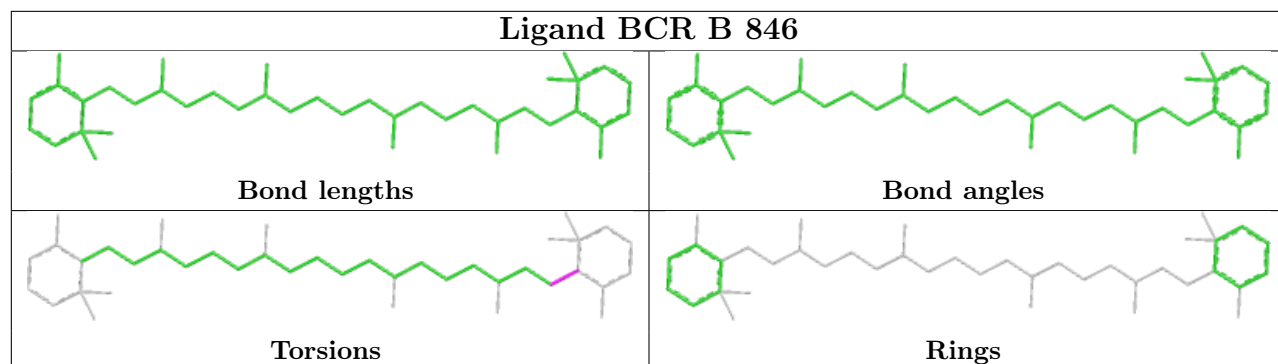


Torsions

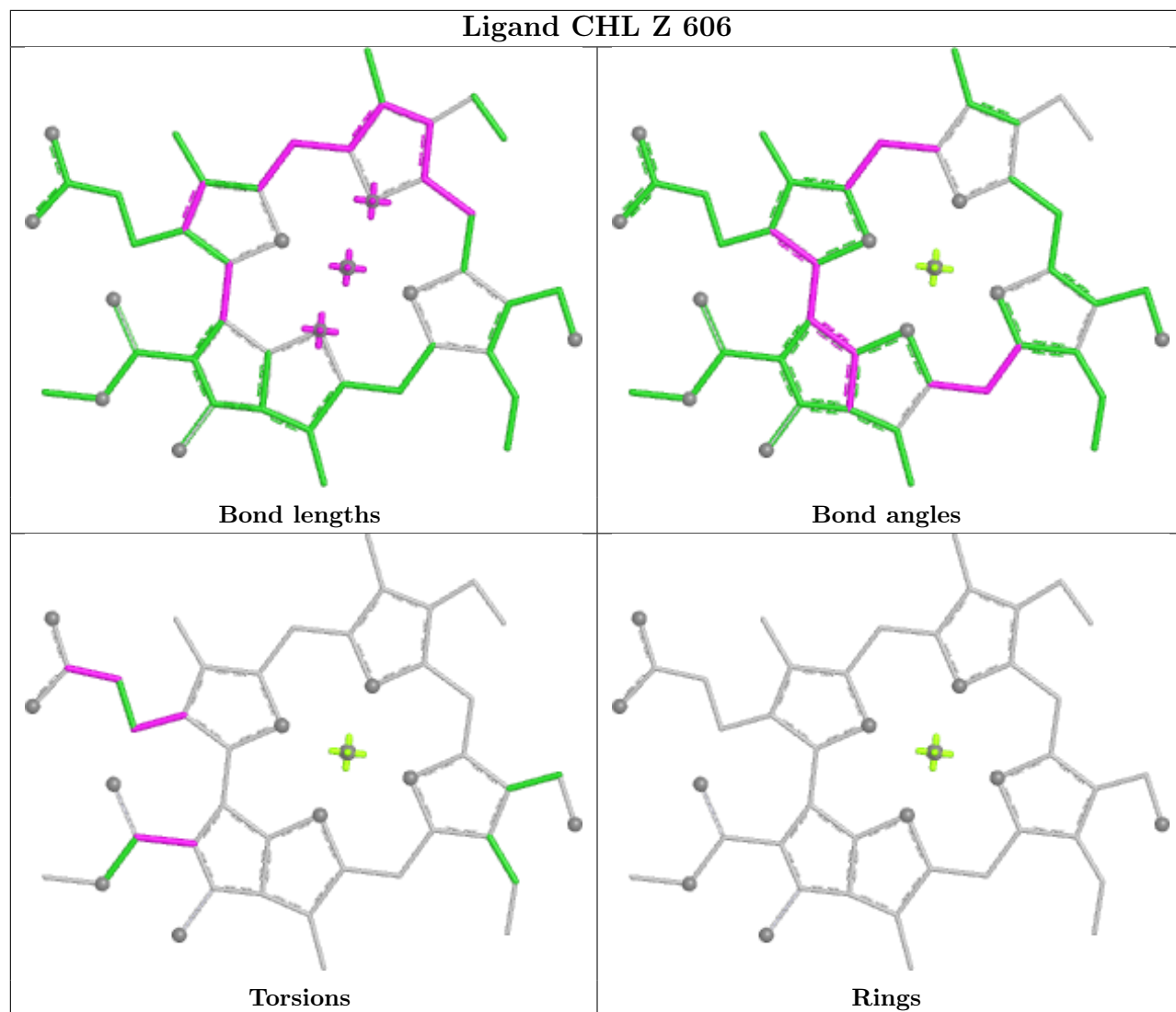


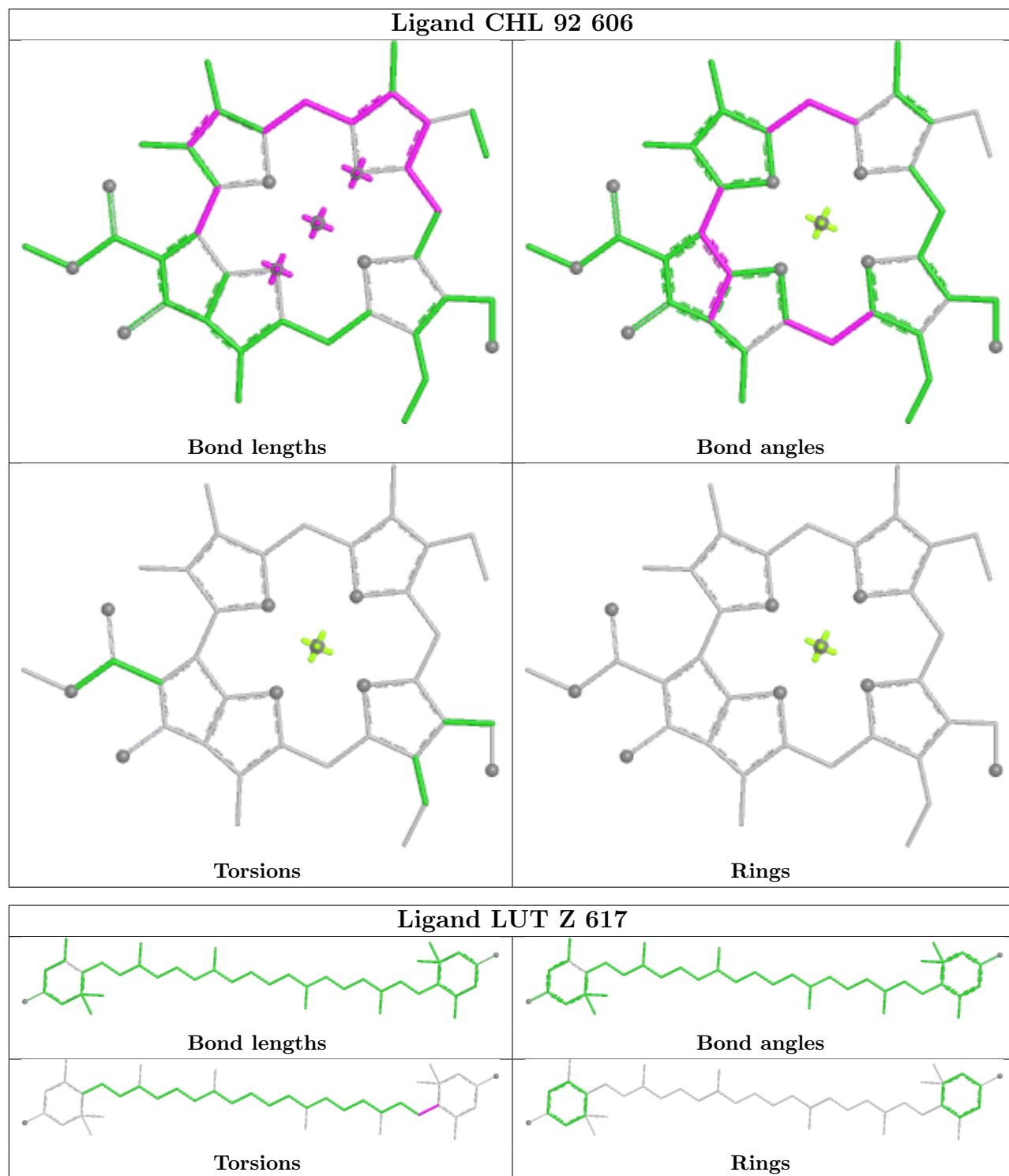
Rings

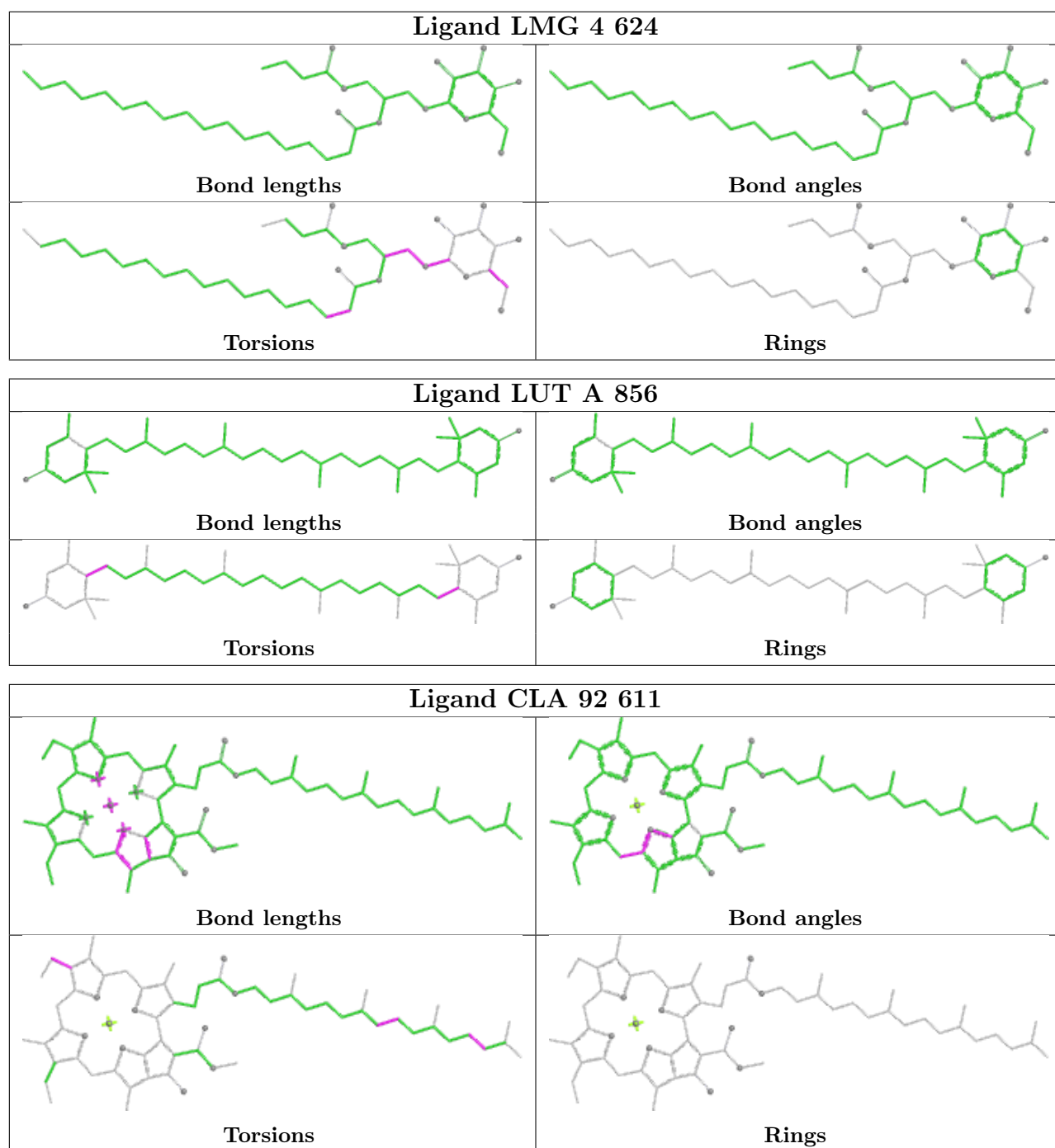


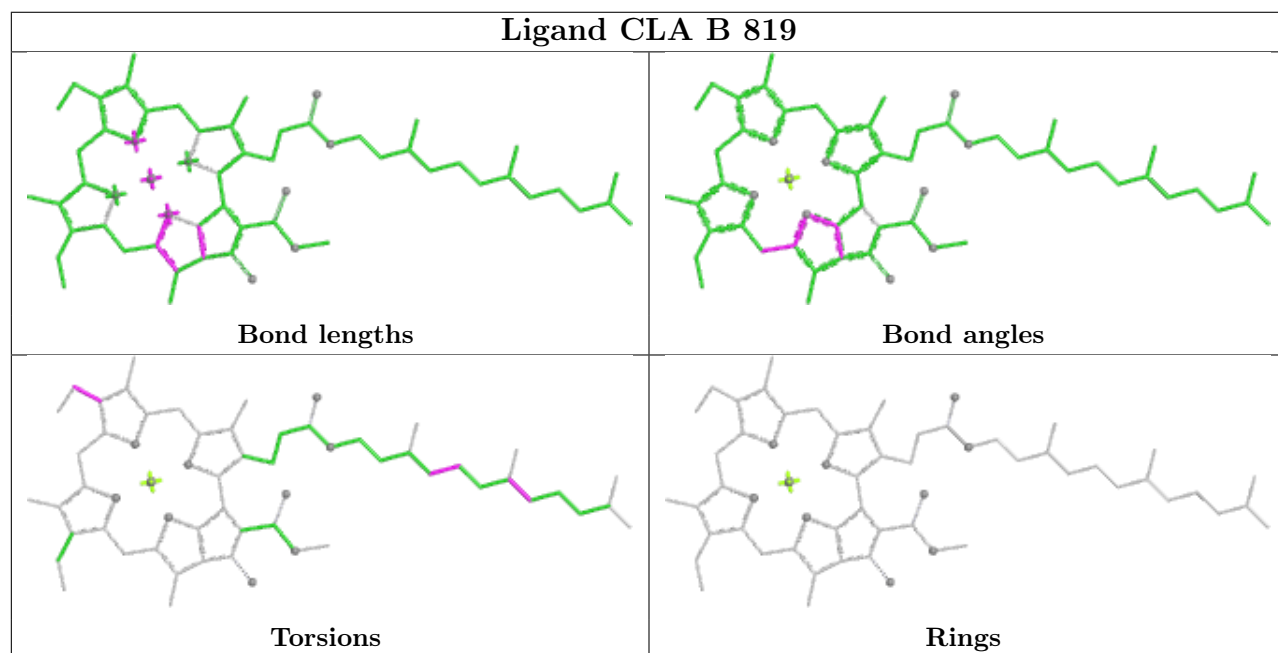
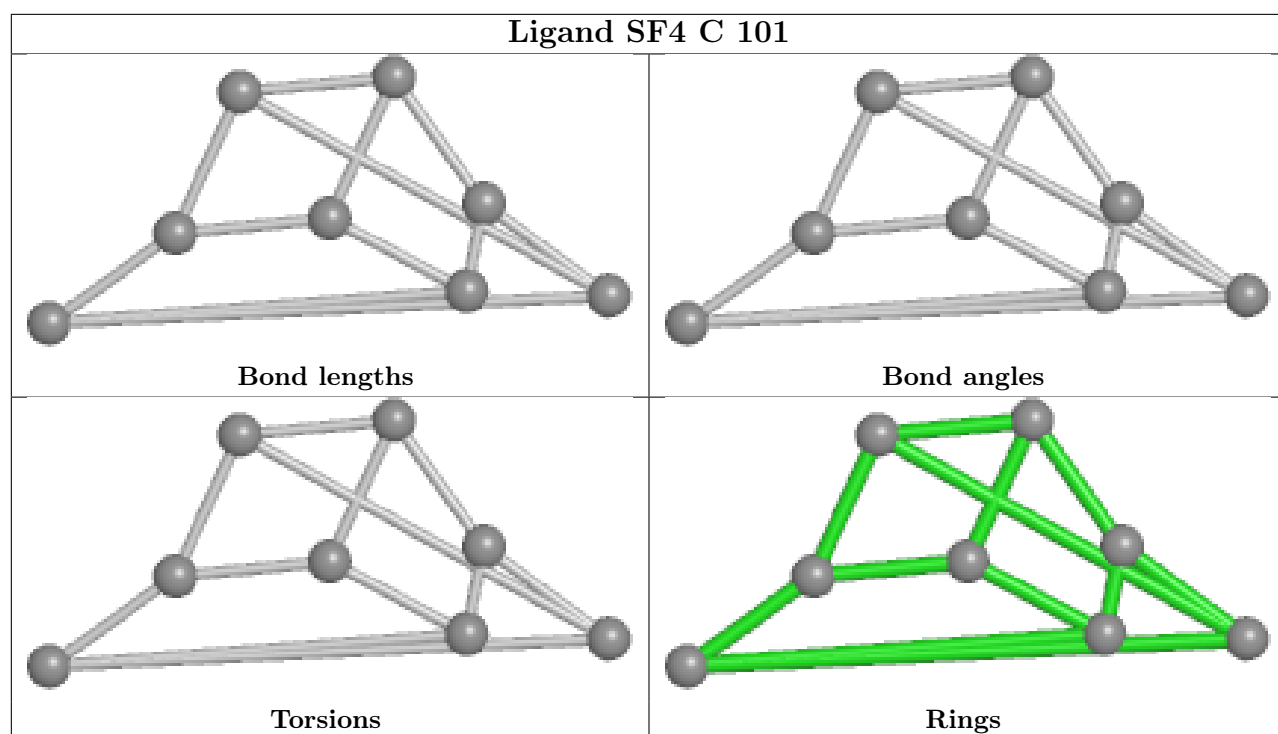


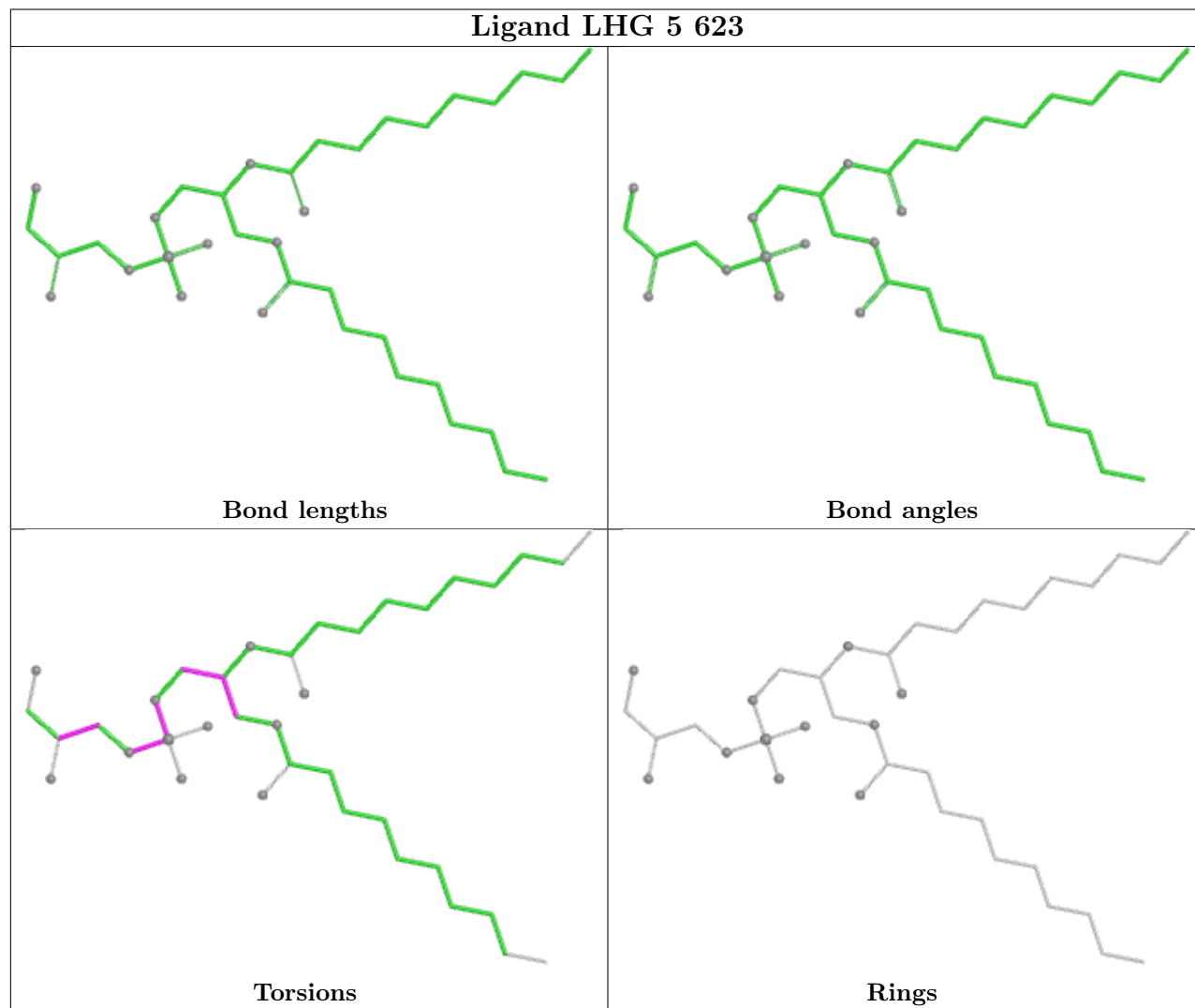
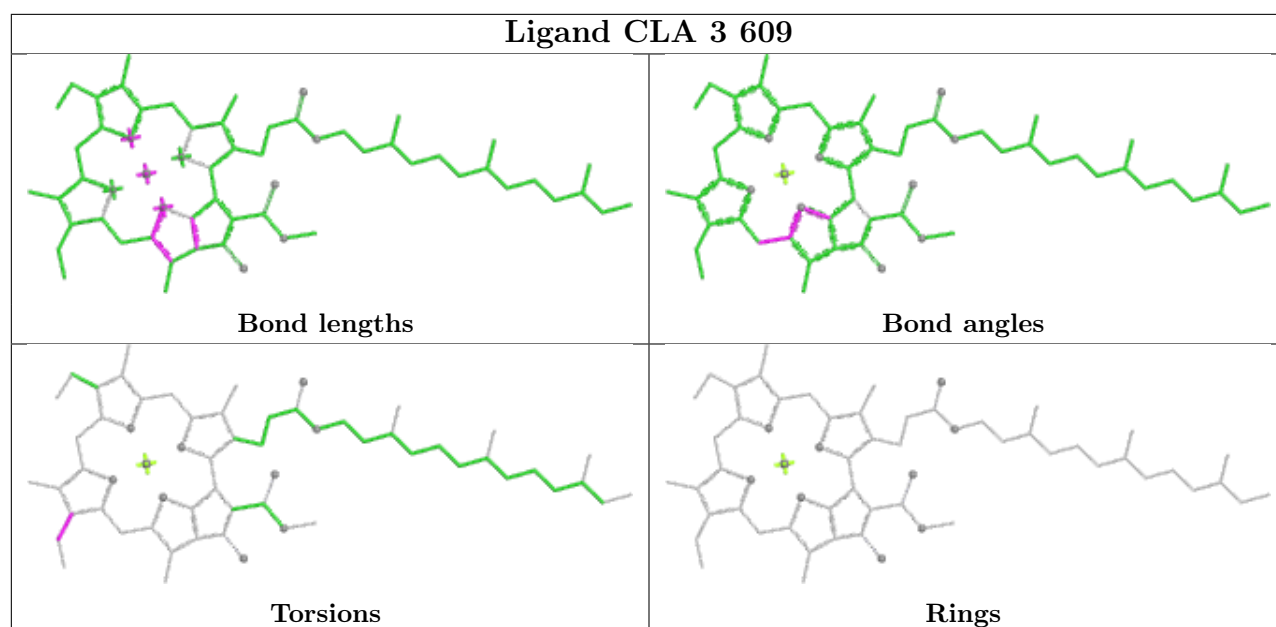
Ligand CHL Z 606

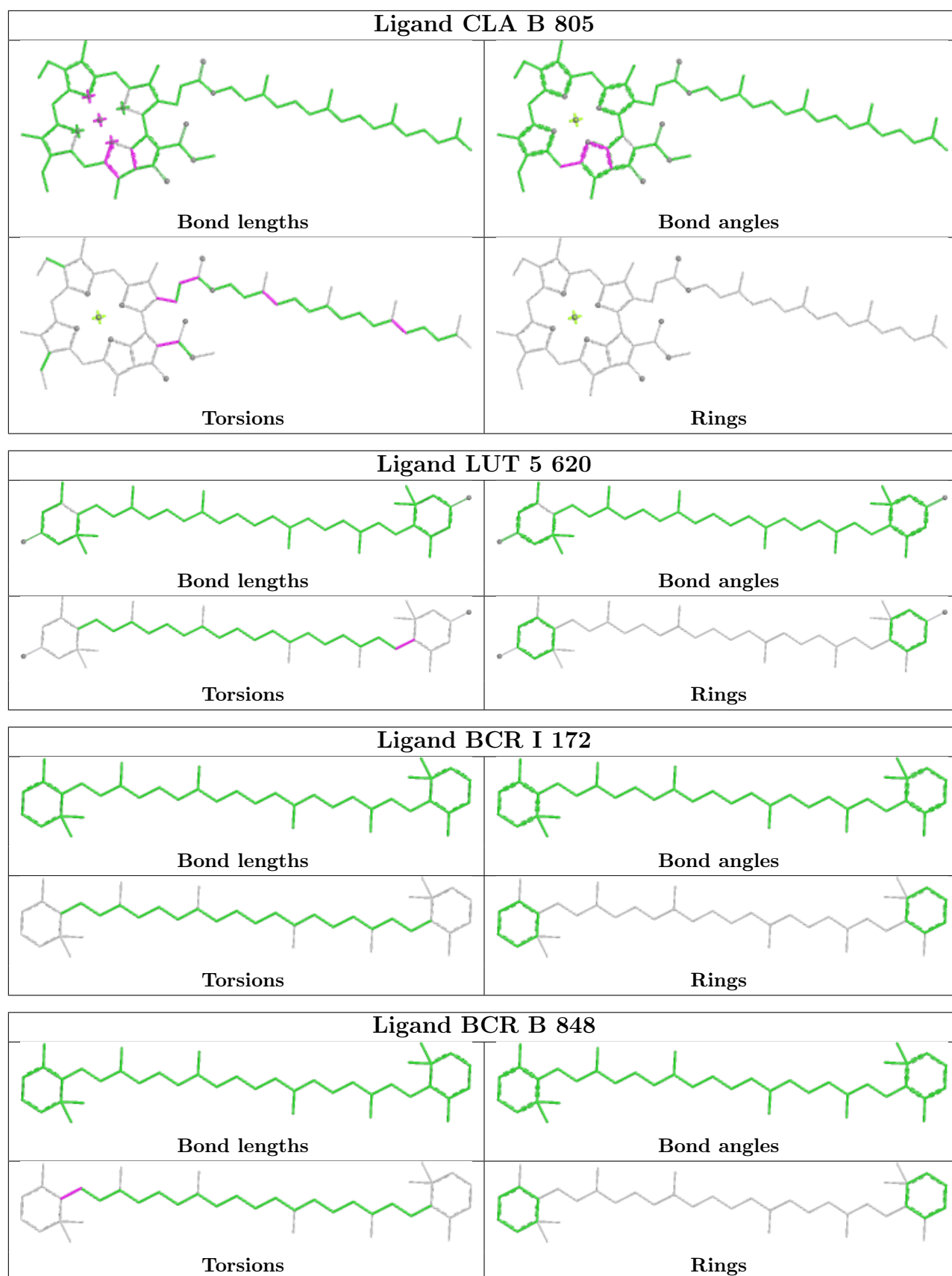


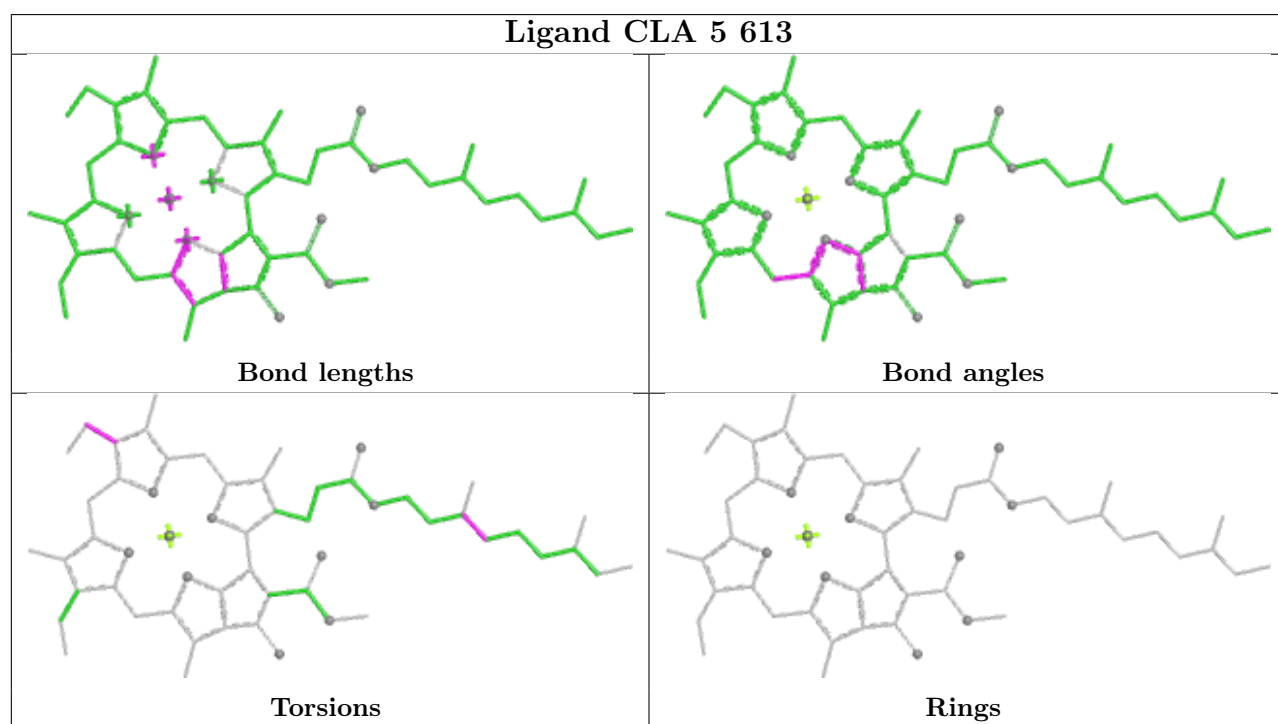
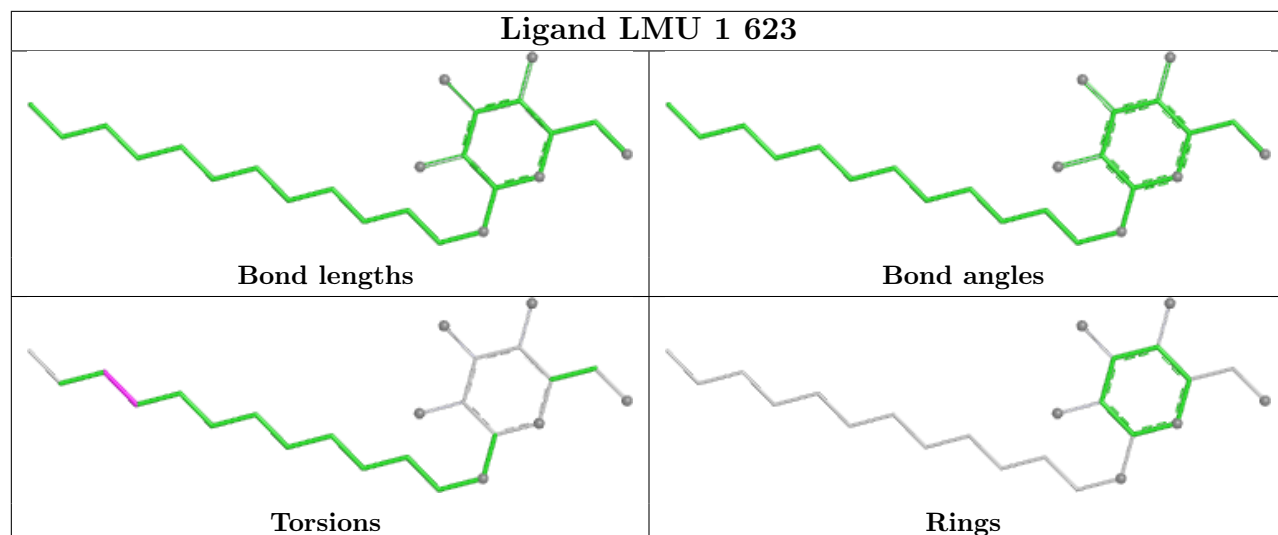


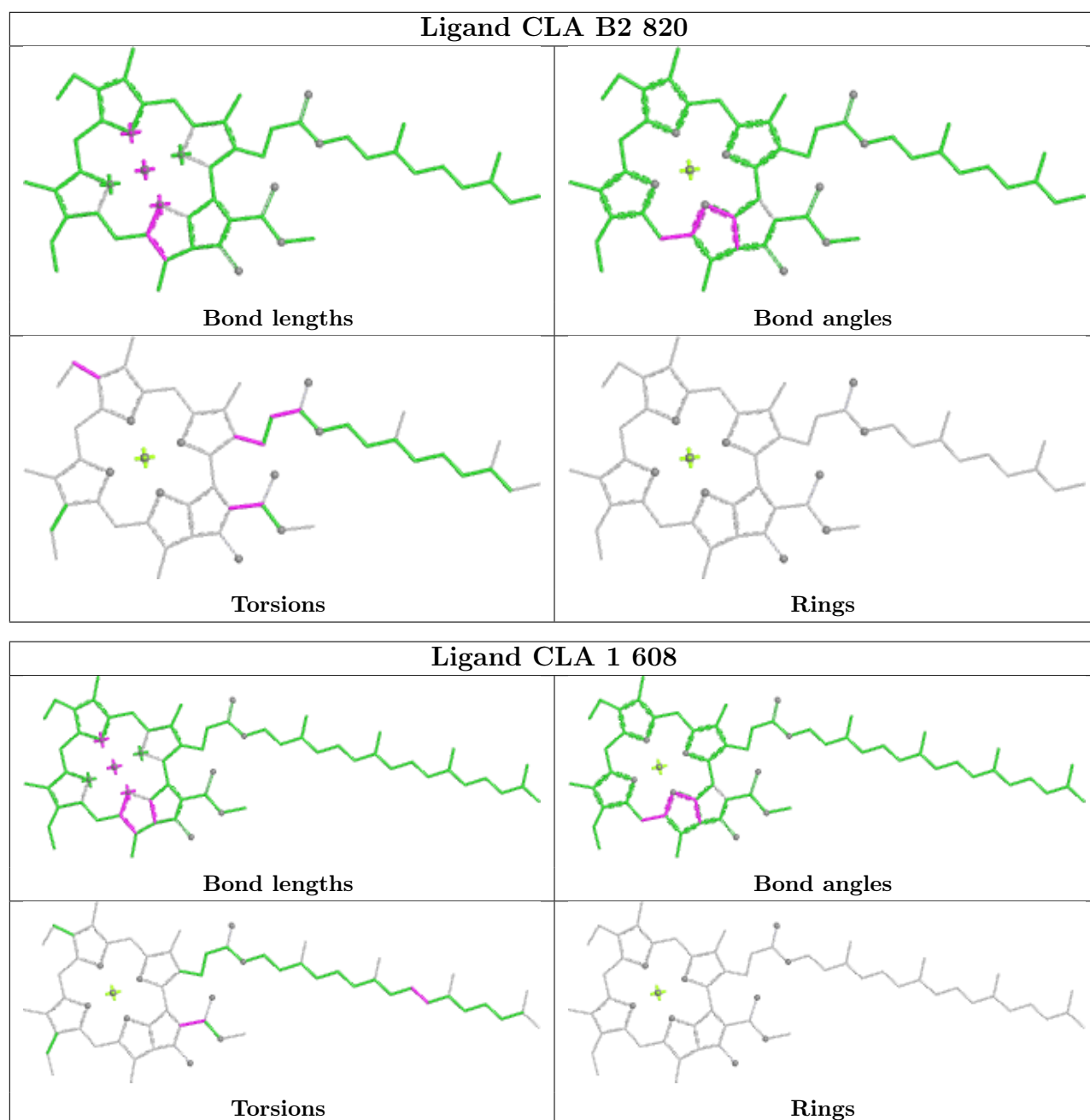


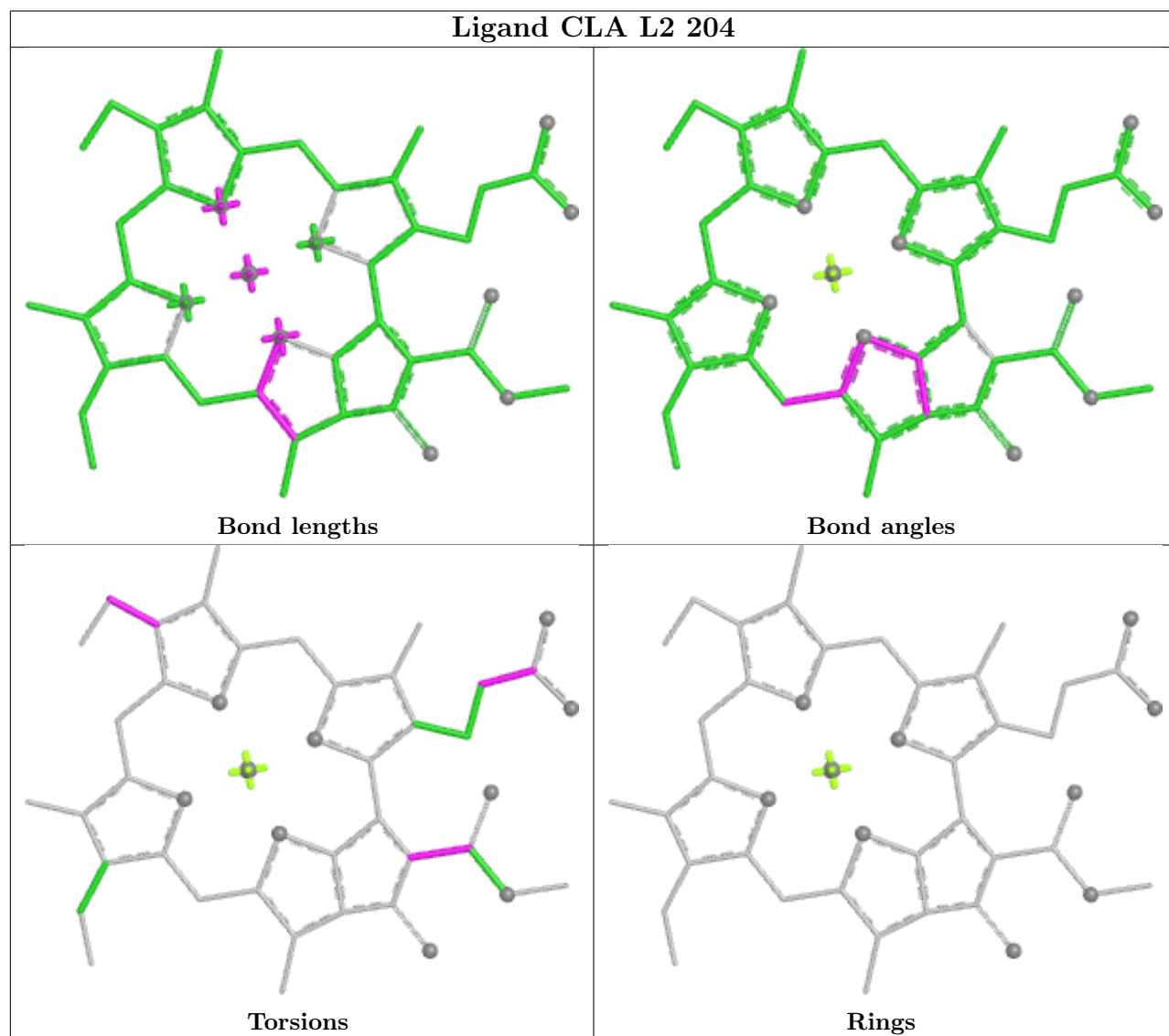
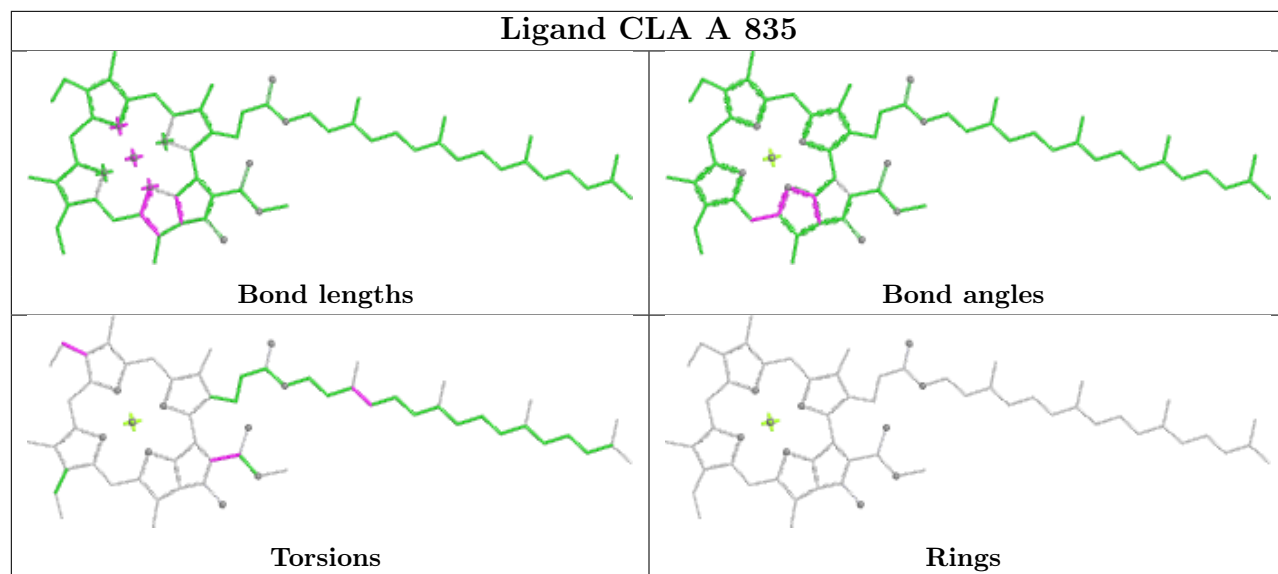


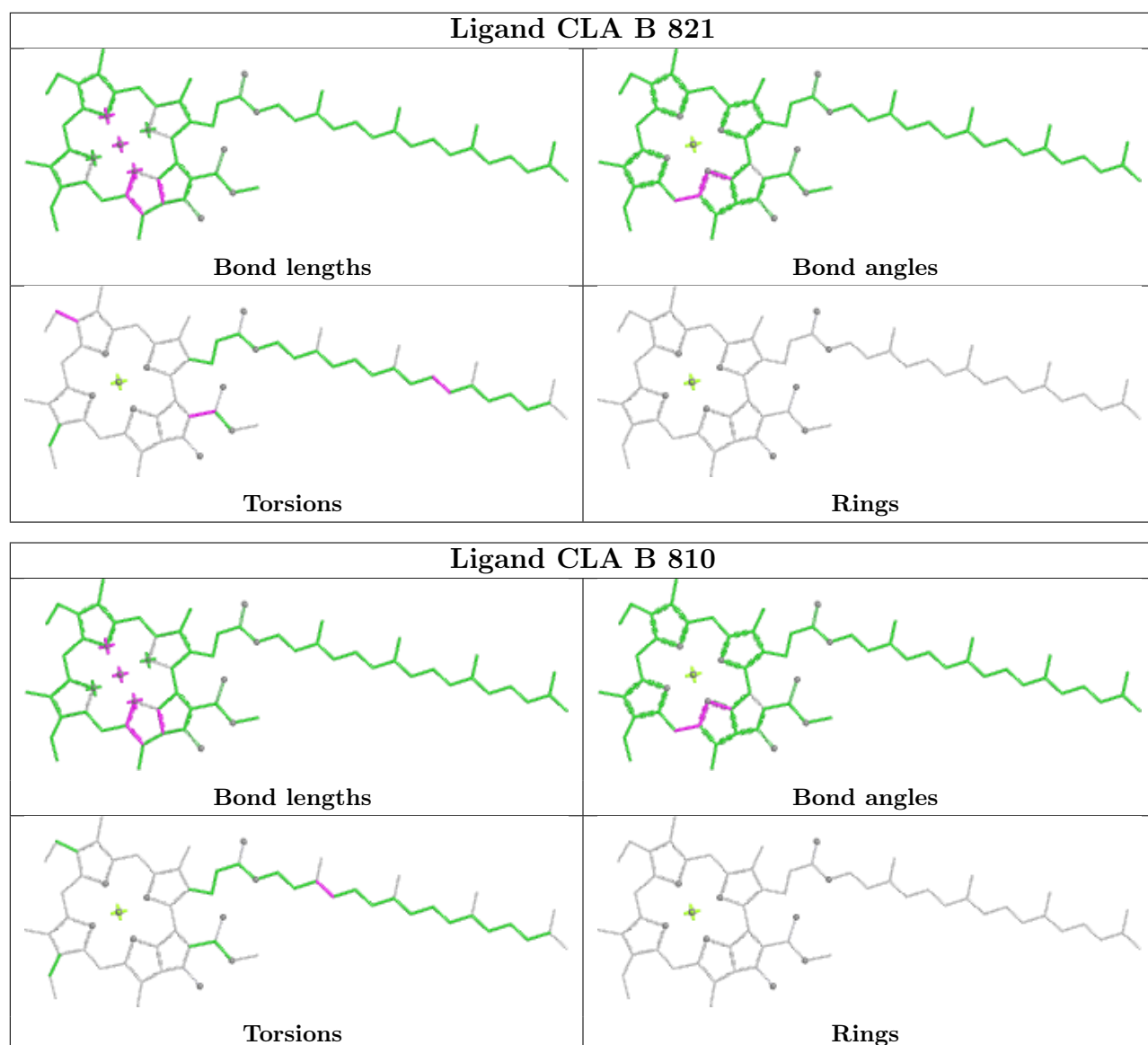


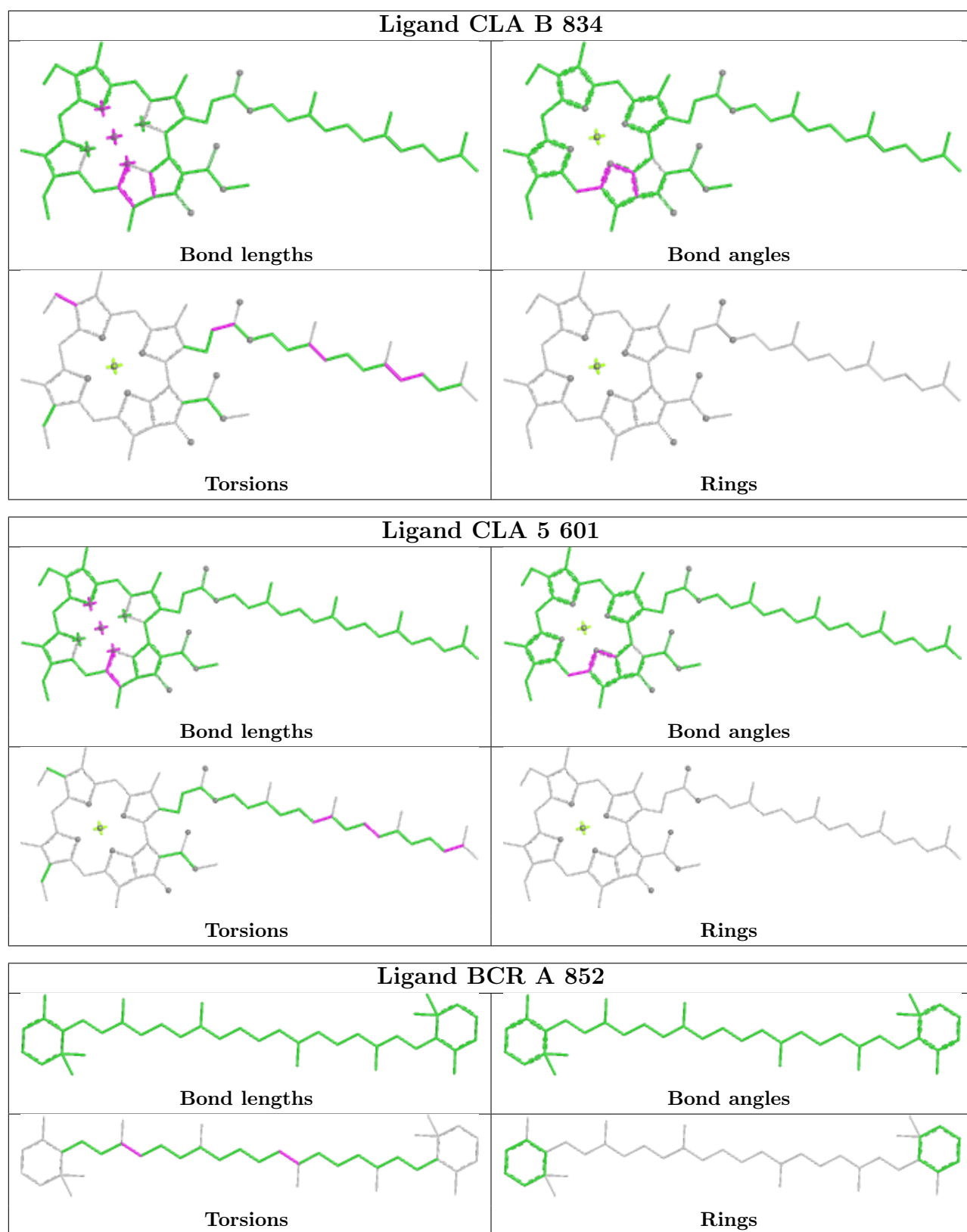




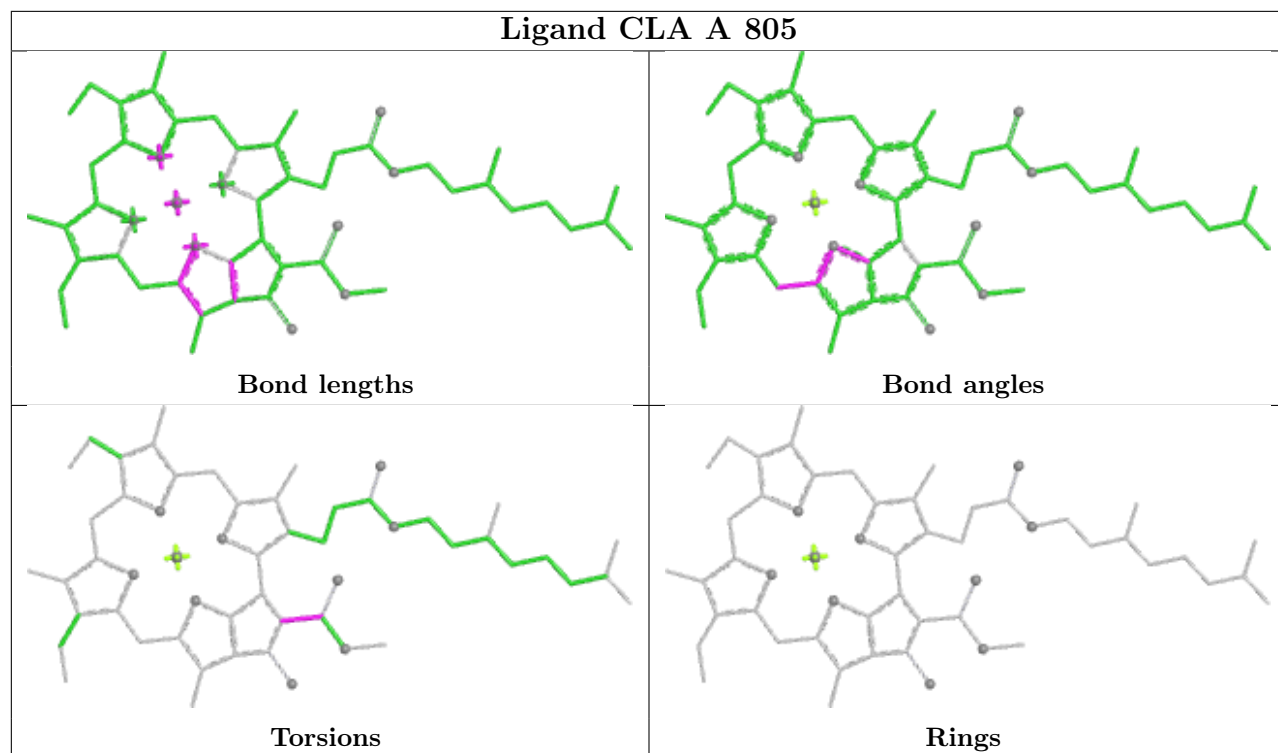




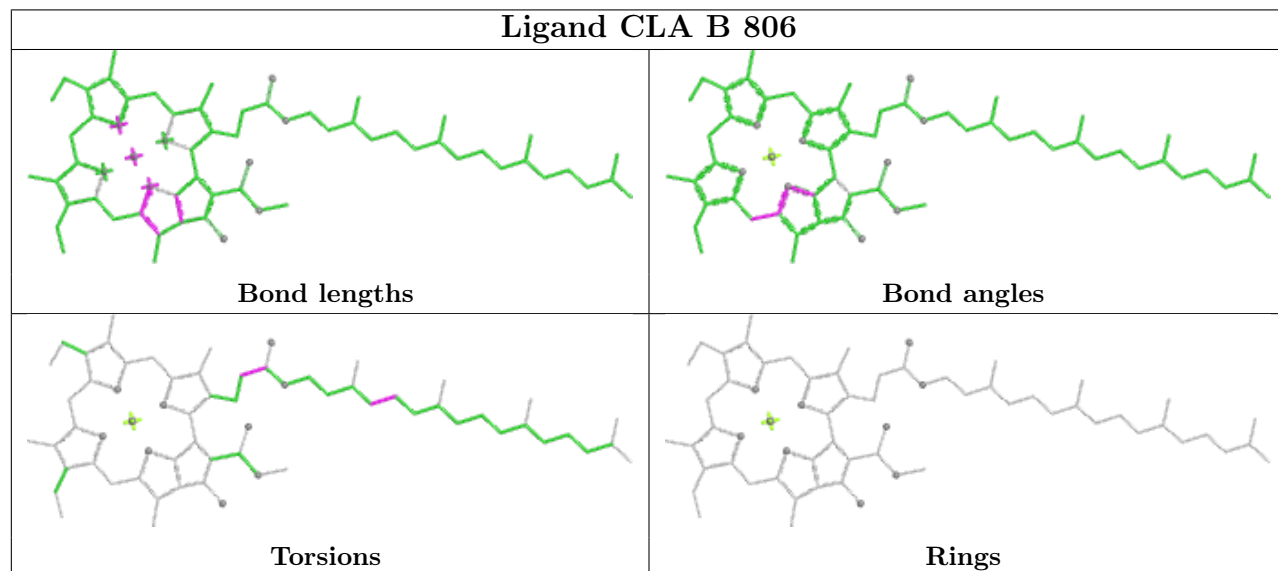


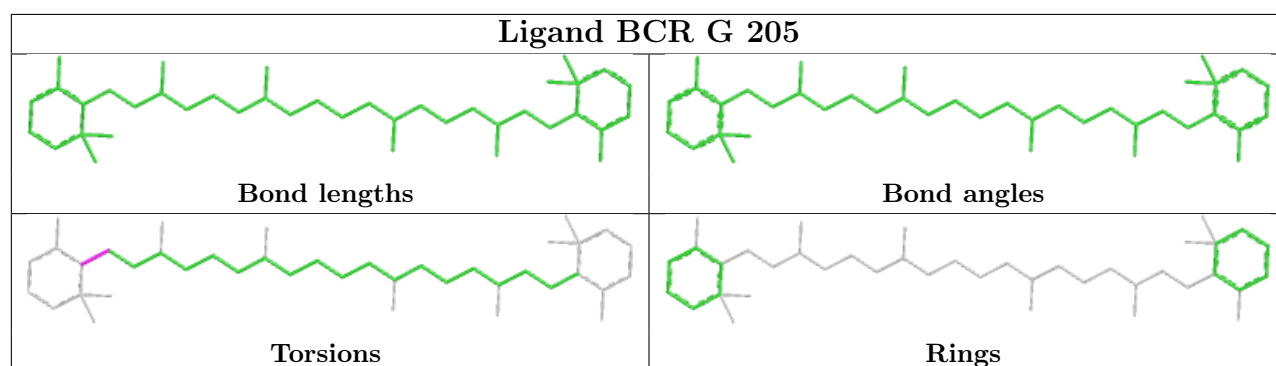
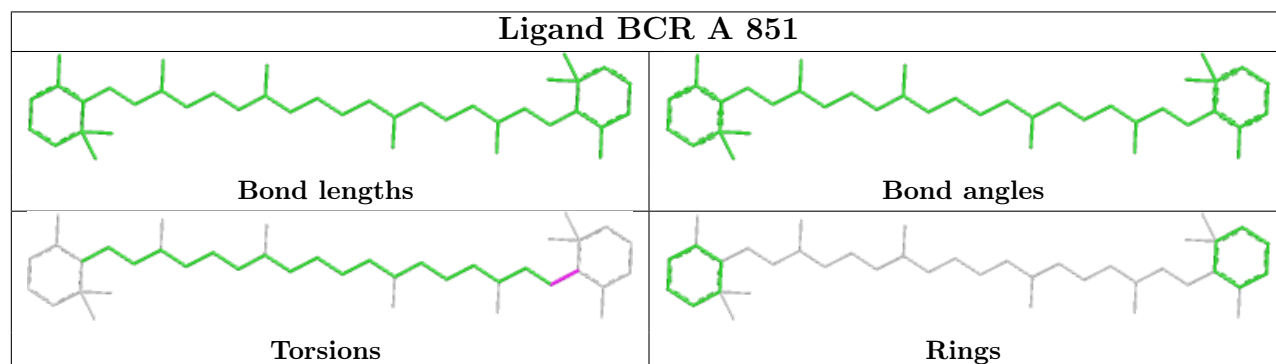
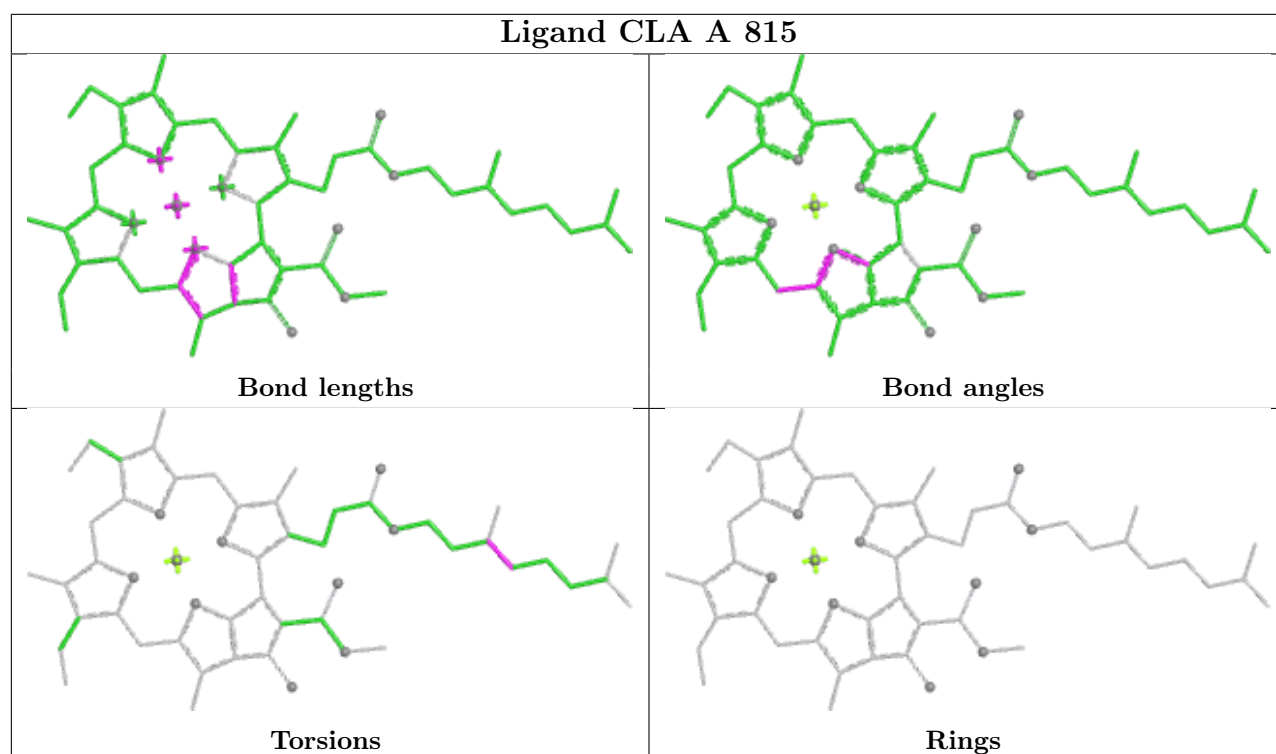


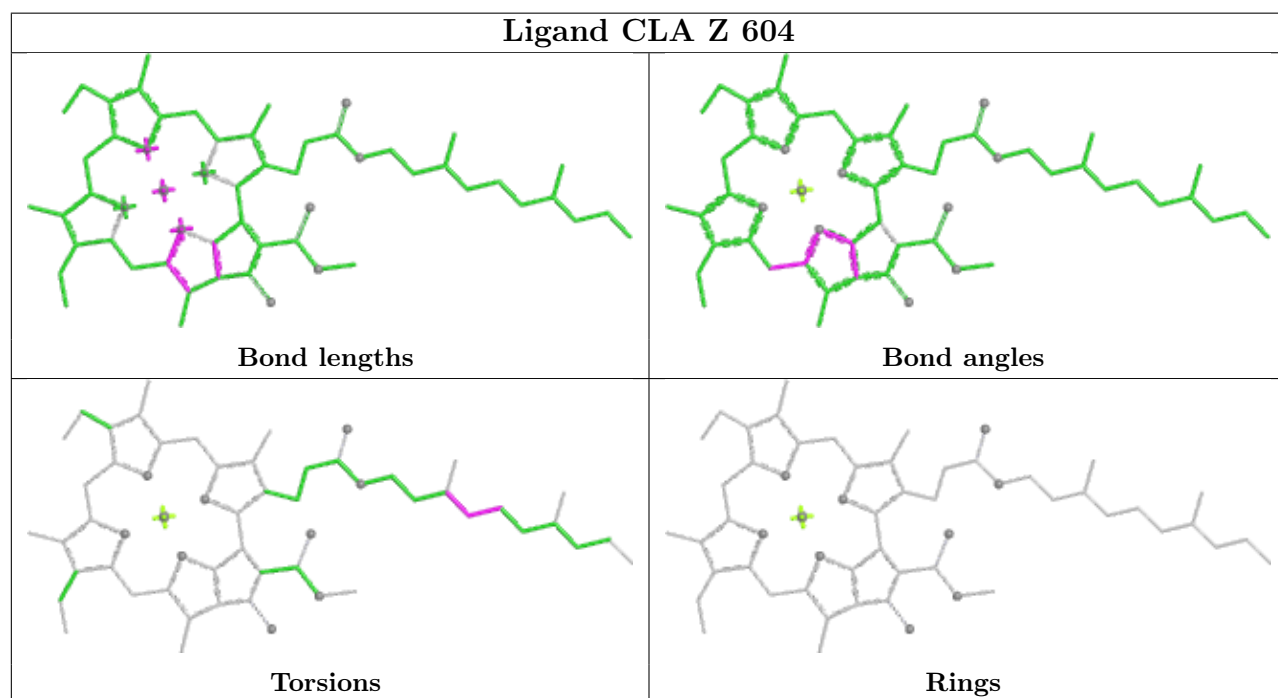
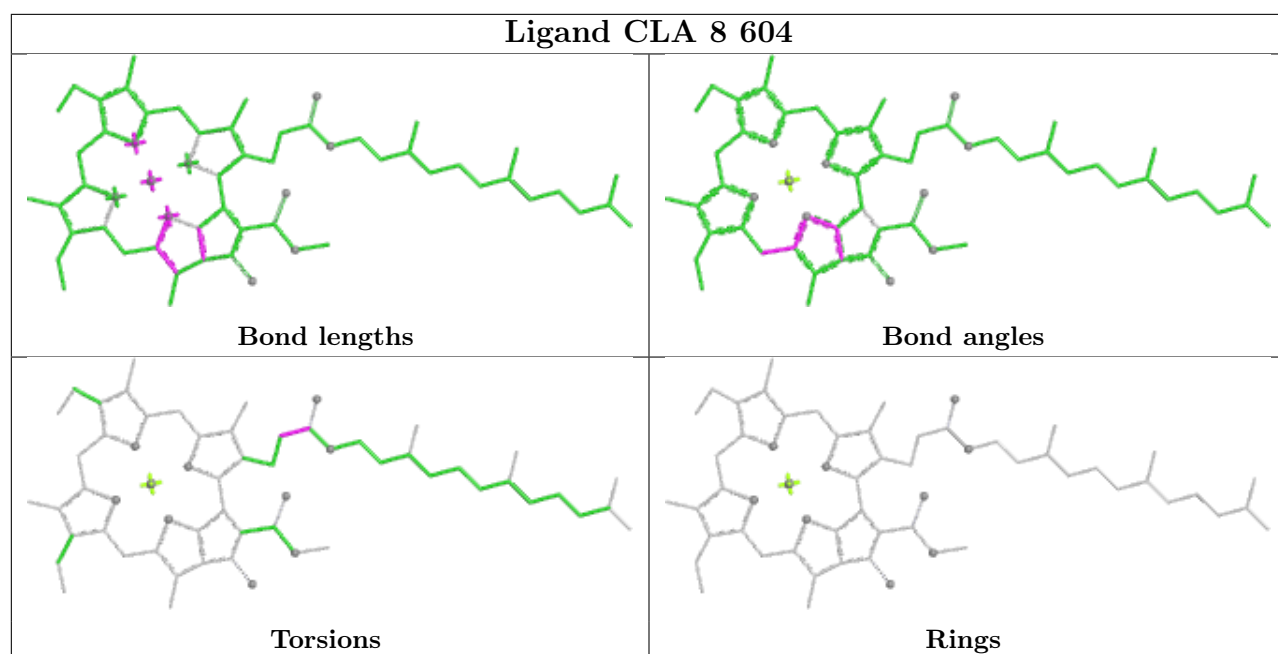
Ligand CLA A 805



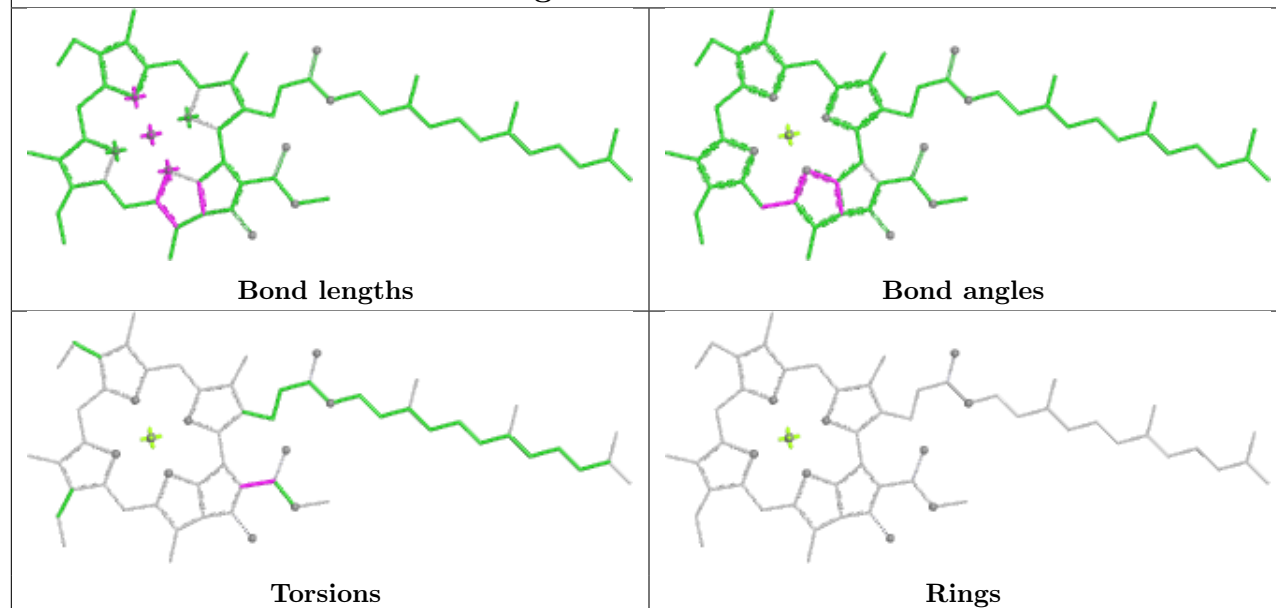
Ligand CLA B 806



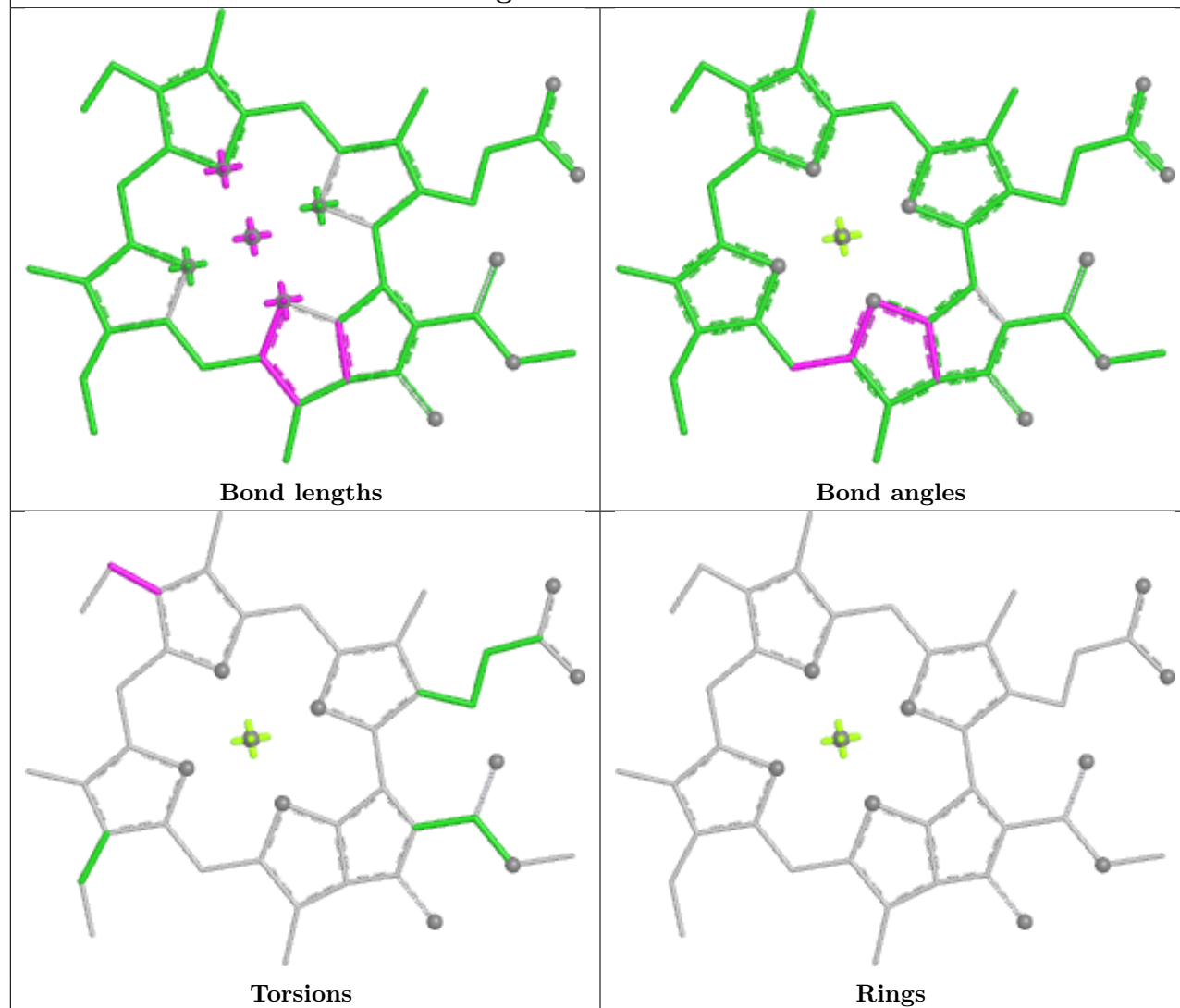


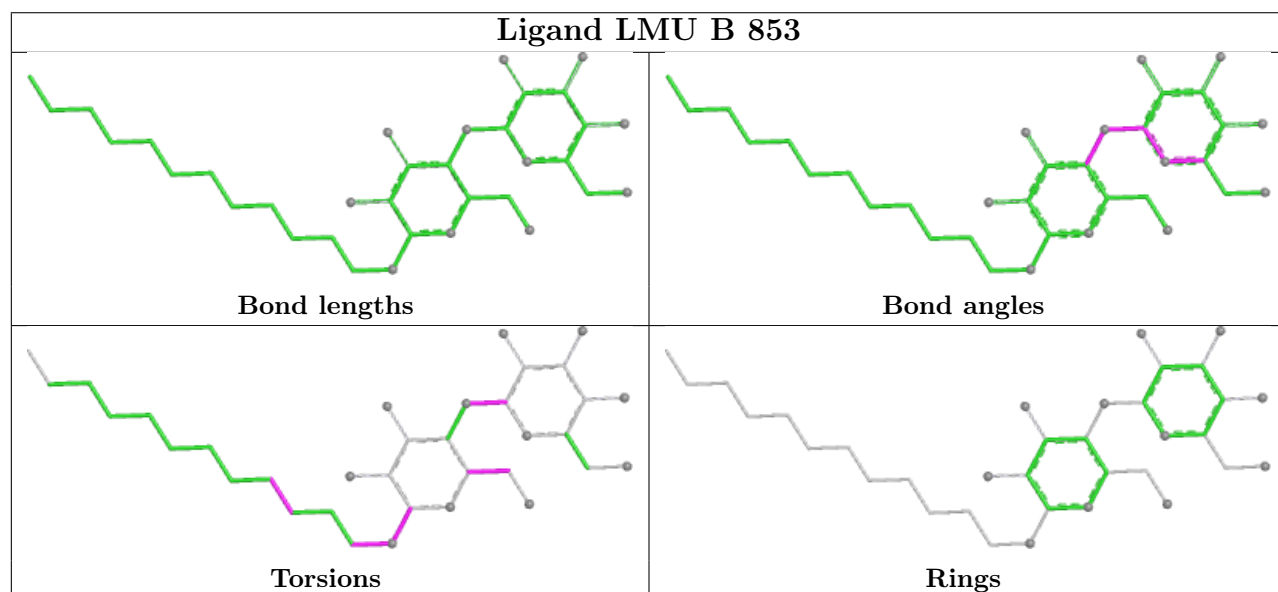
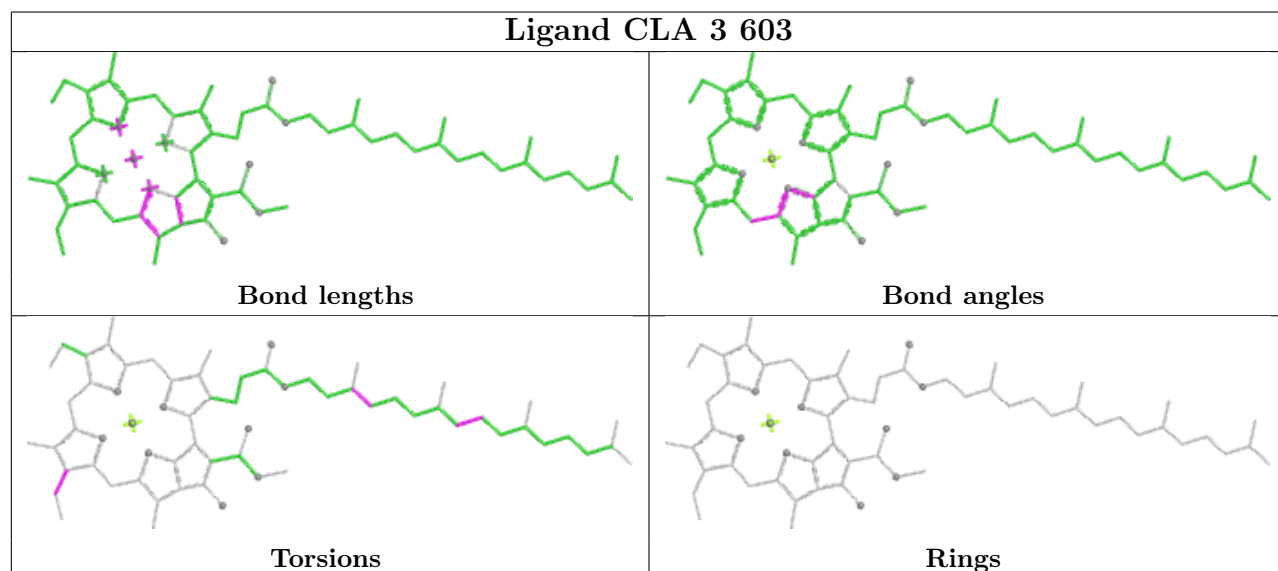
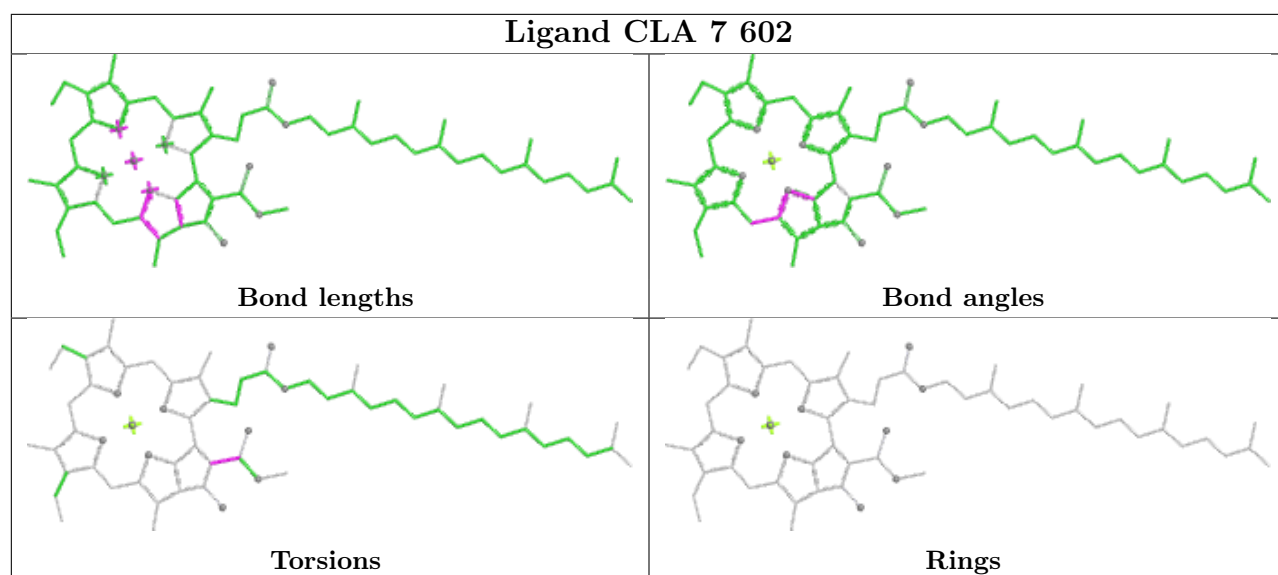


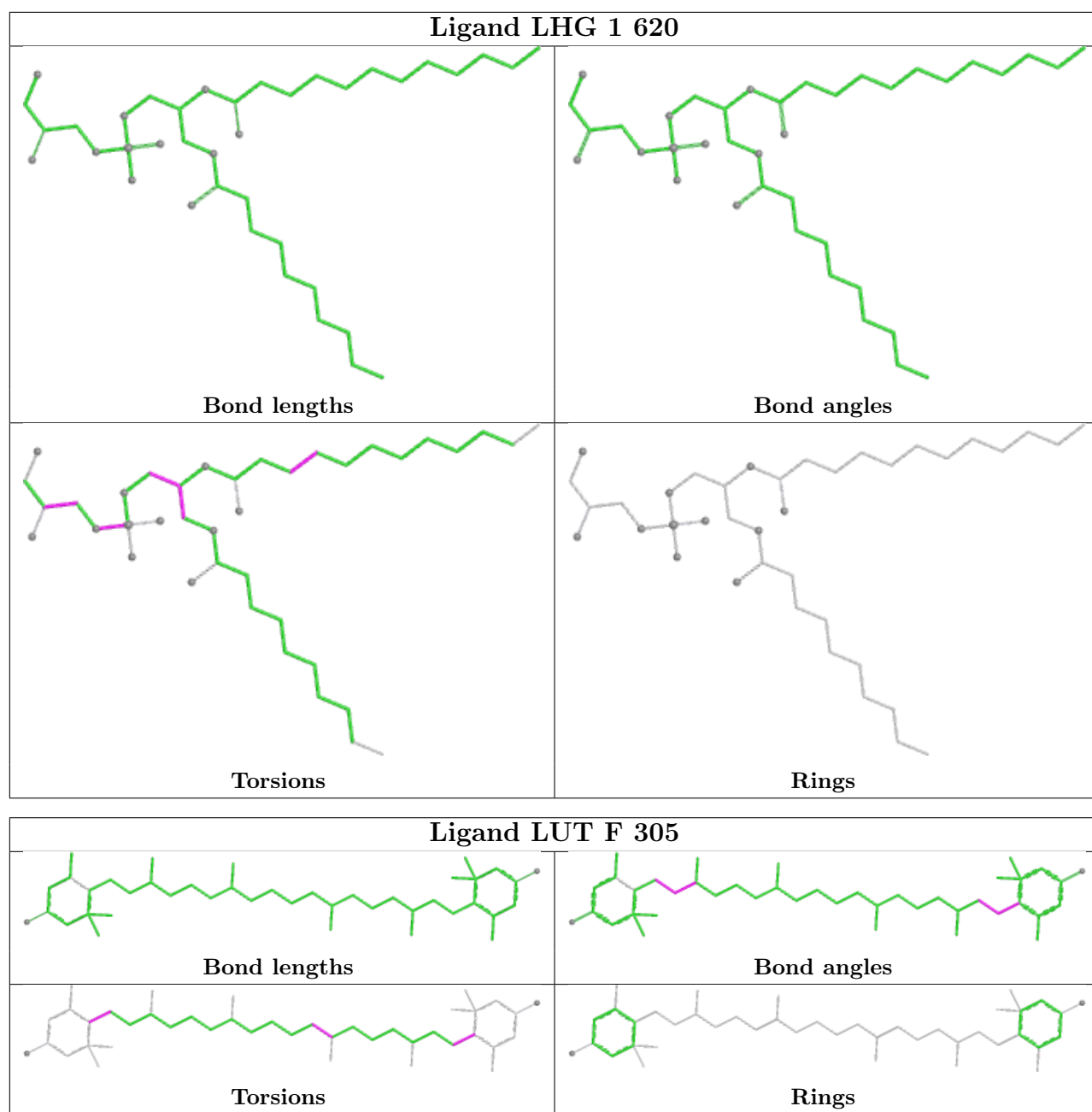
Ligand CLA Z 602

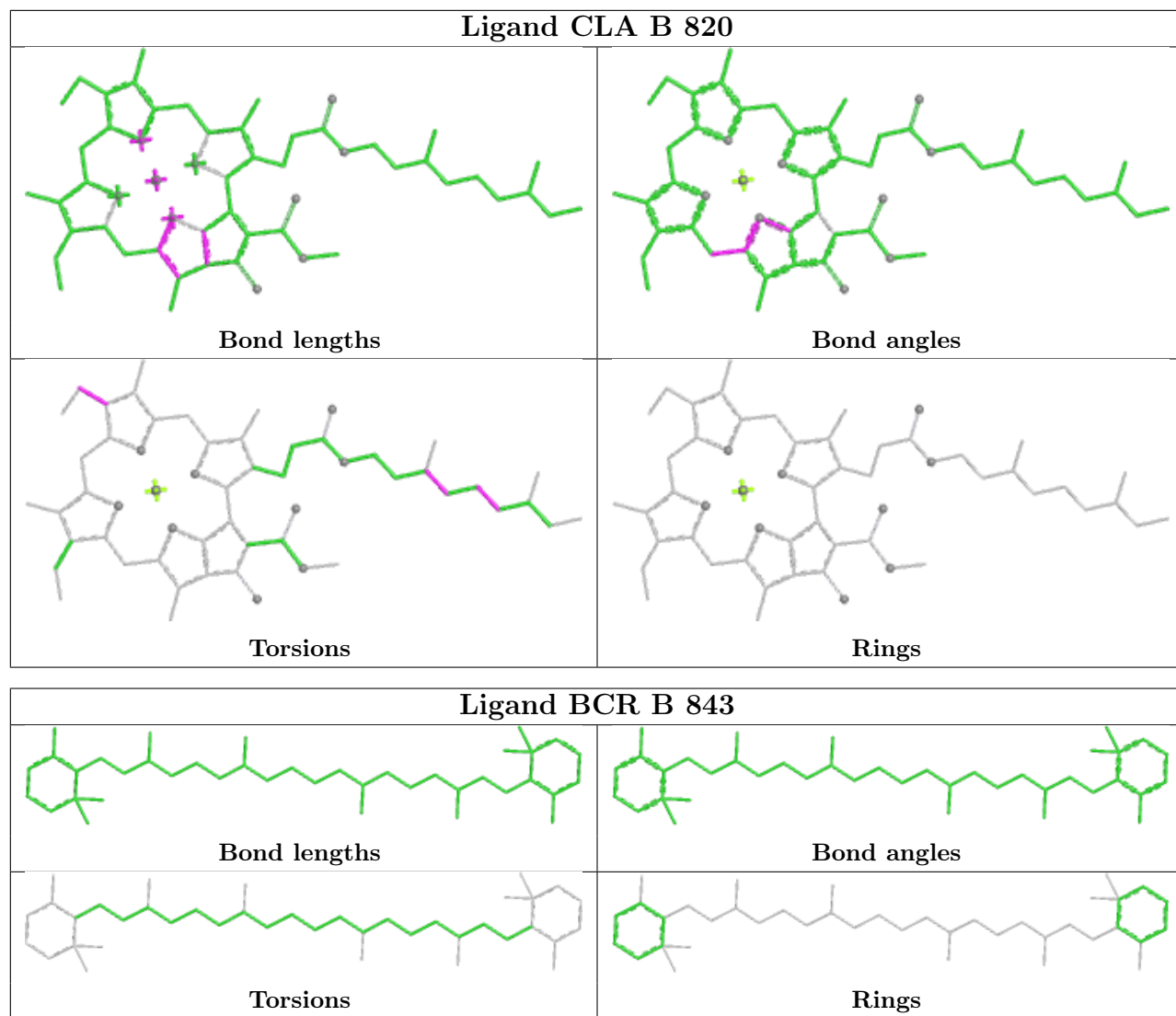


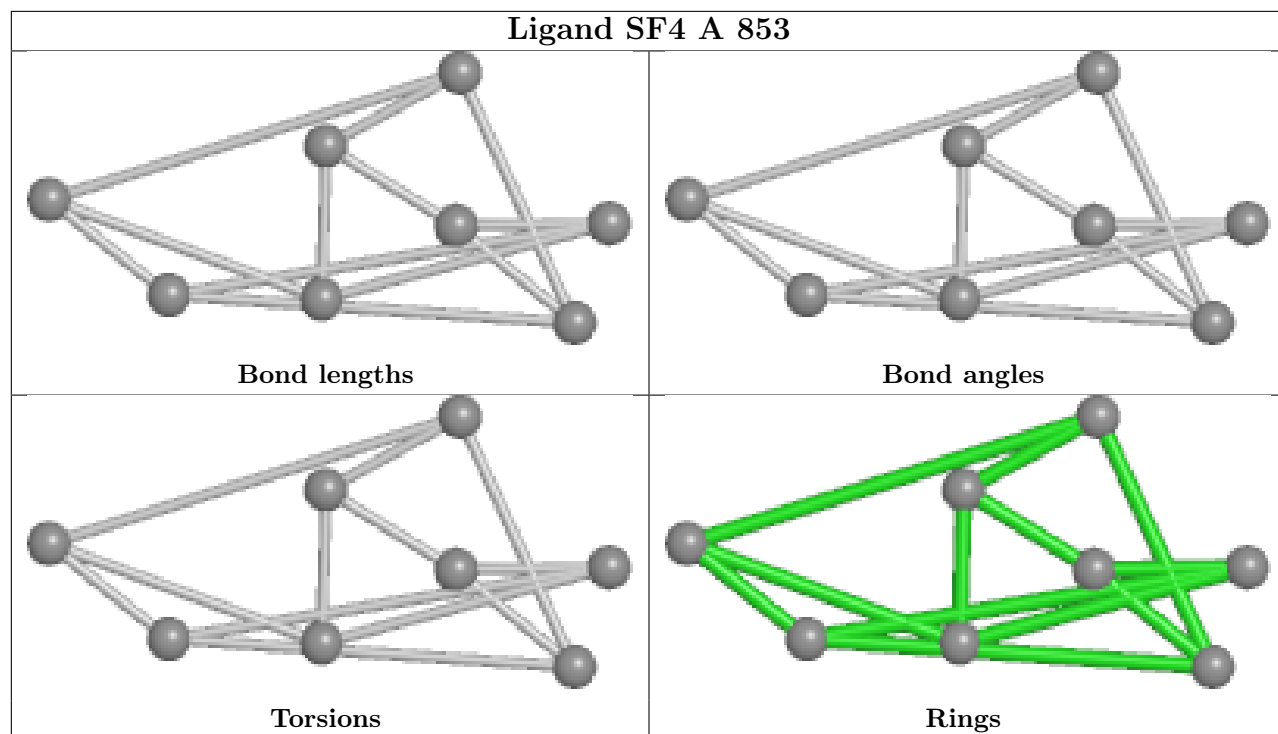
Ligand CLA 3 614



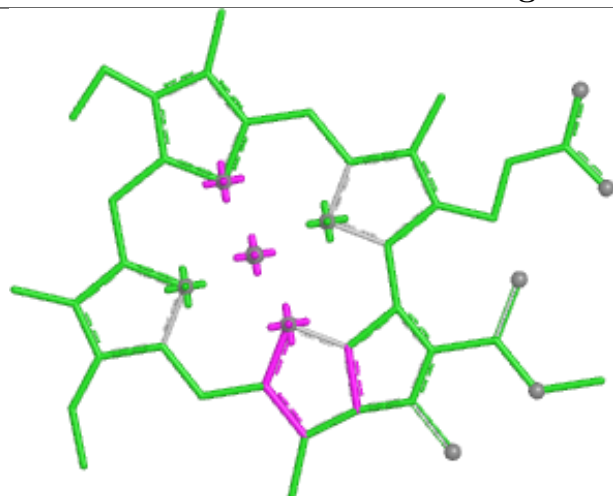




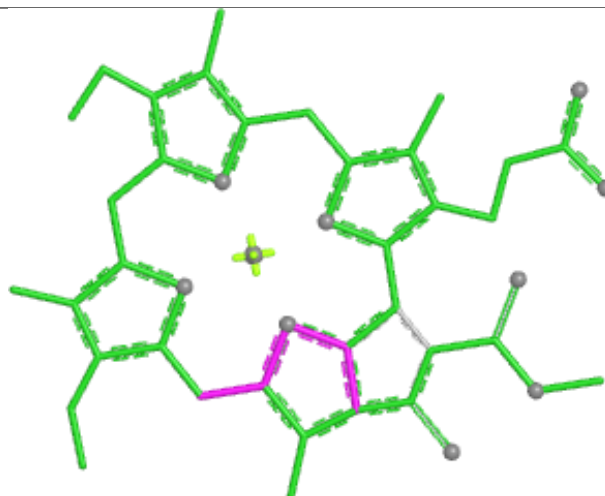




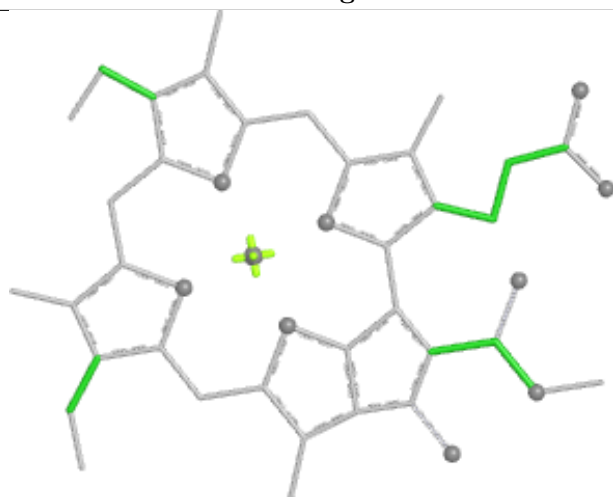
Ligand CLA 8 616



Bond lengths



Bond angles

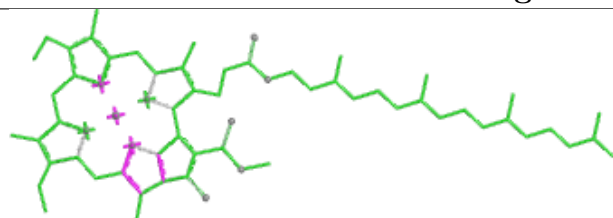


Torsions

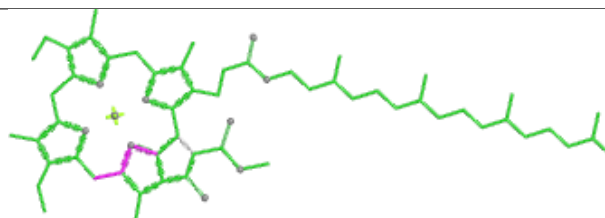


Rings

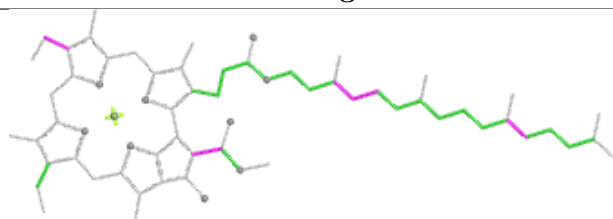
Ligand CLA B 808



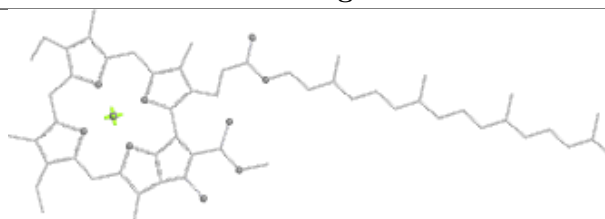
Bond lengths



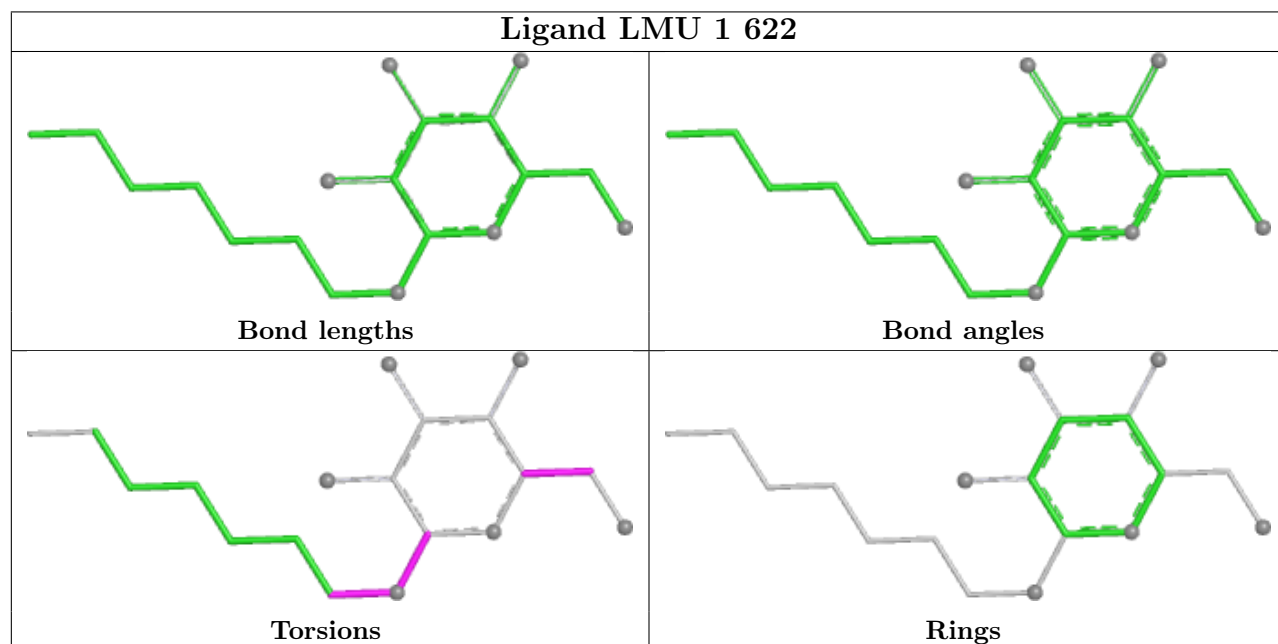
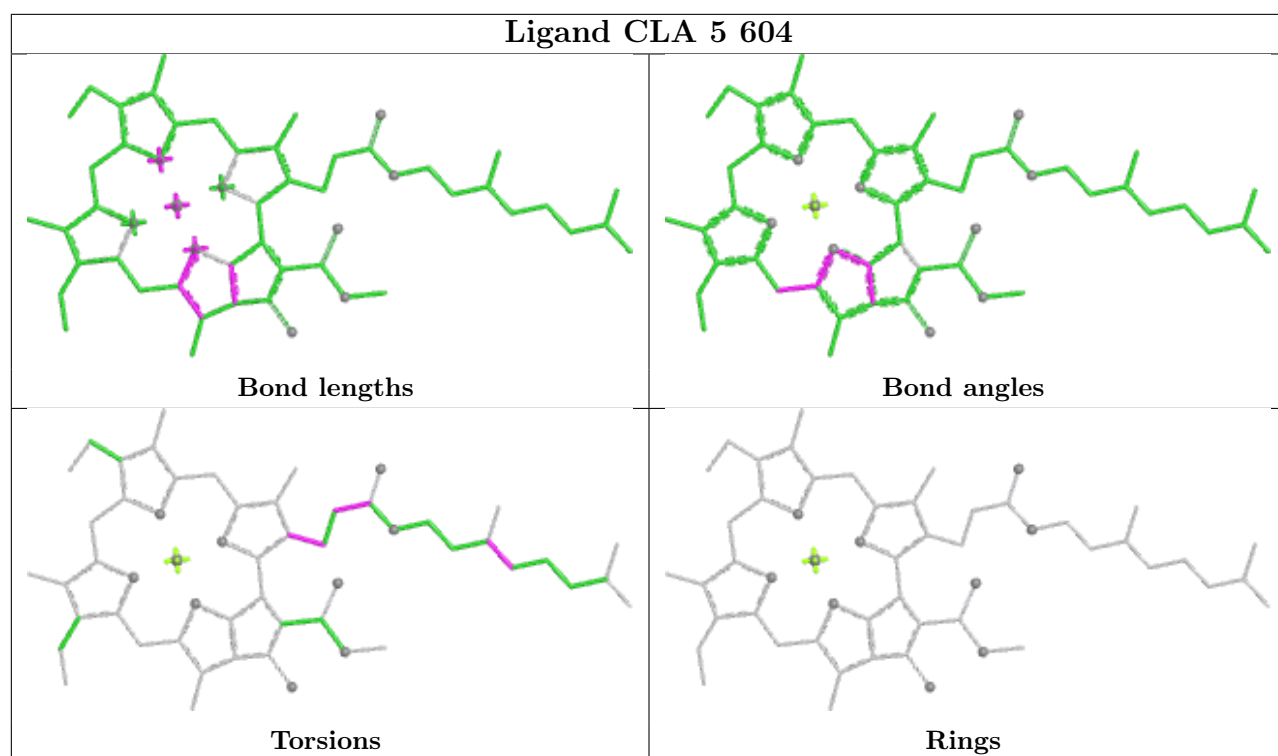
Bond angles

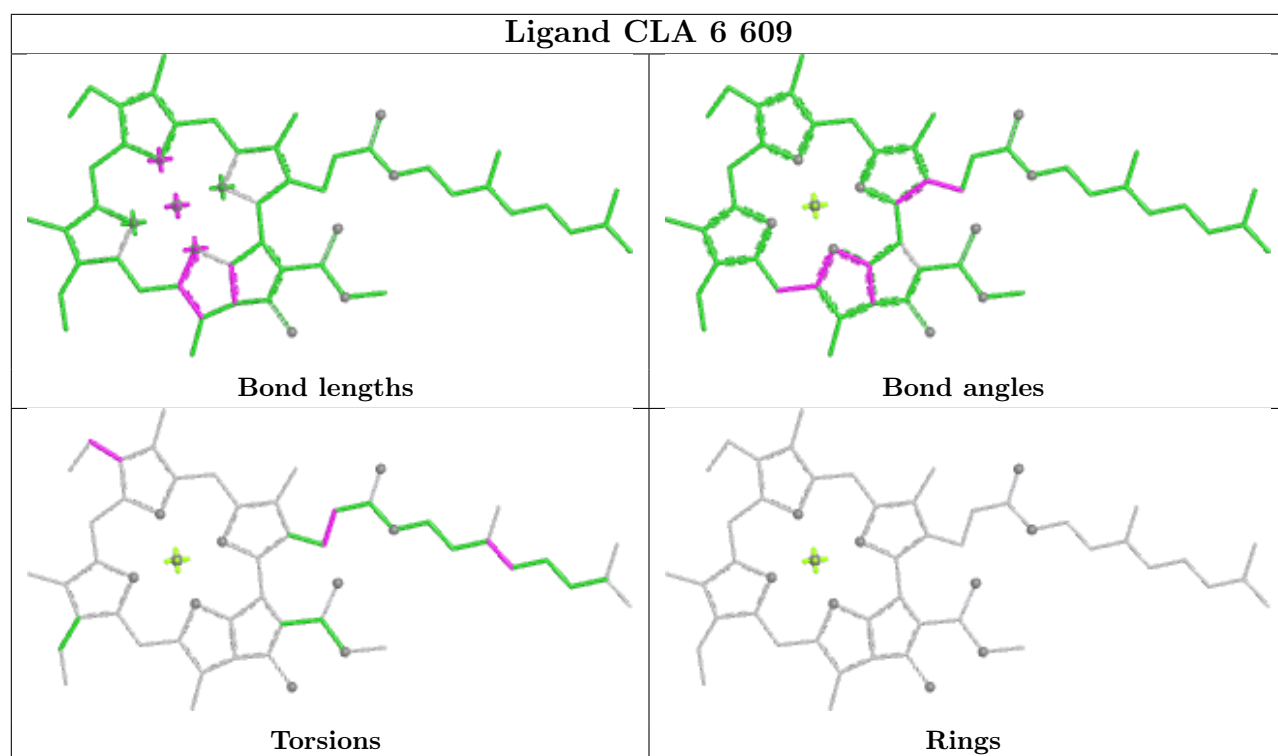


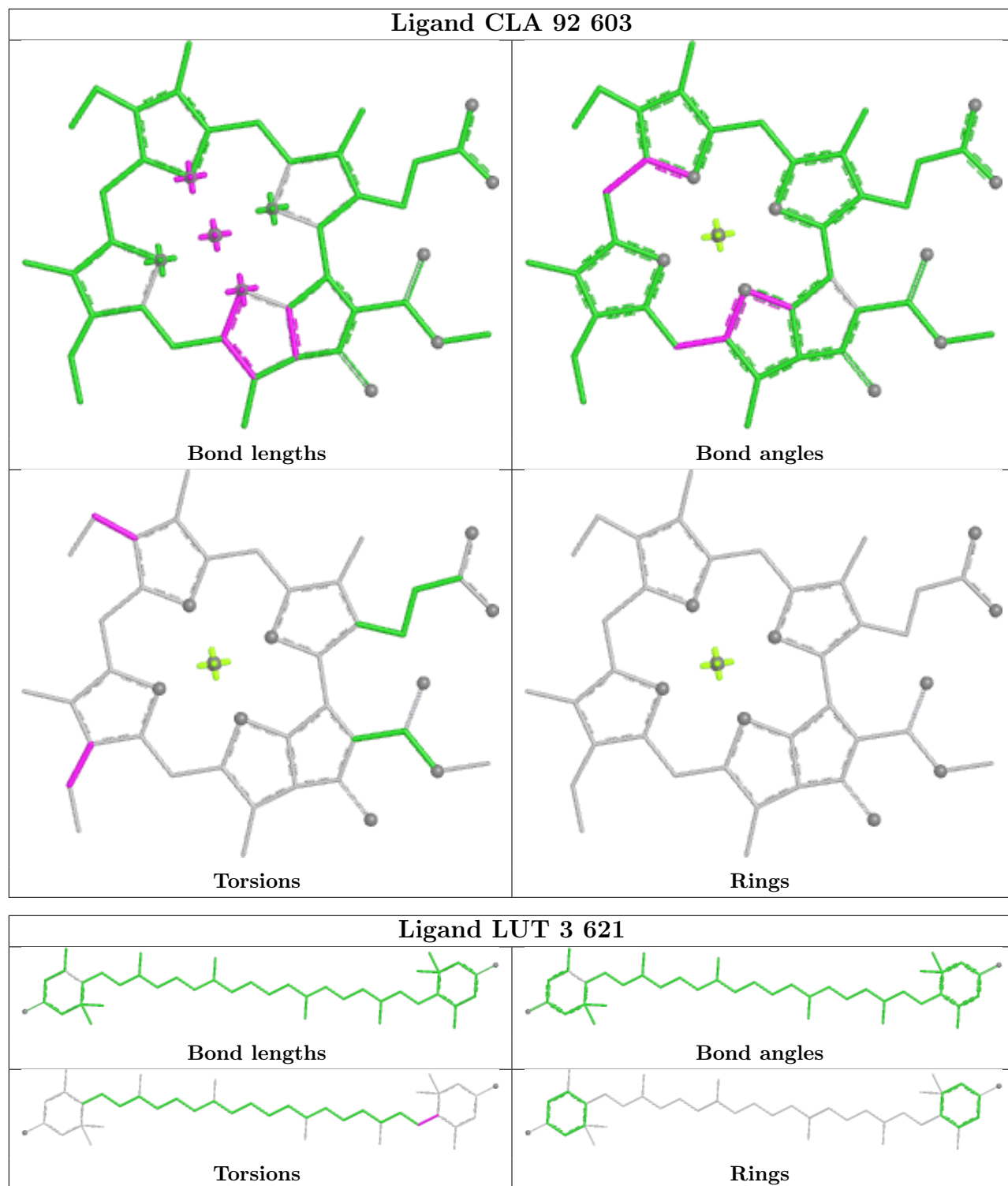
Torsions

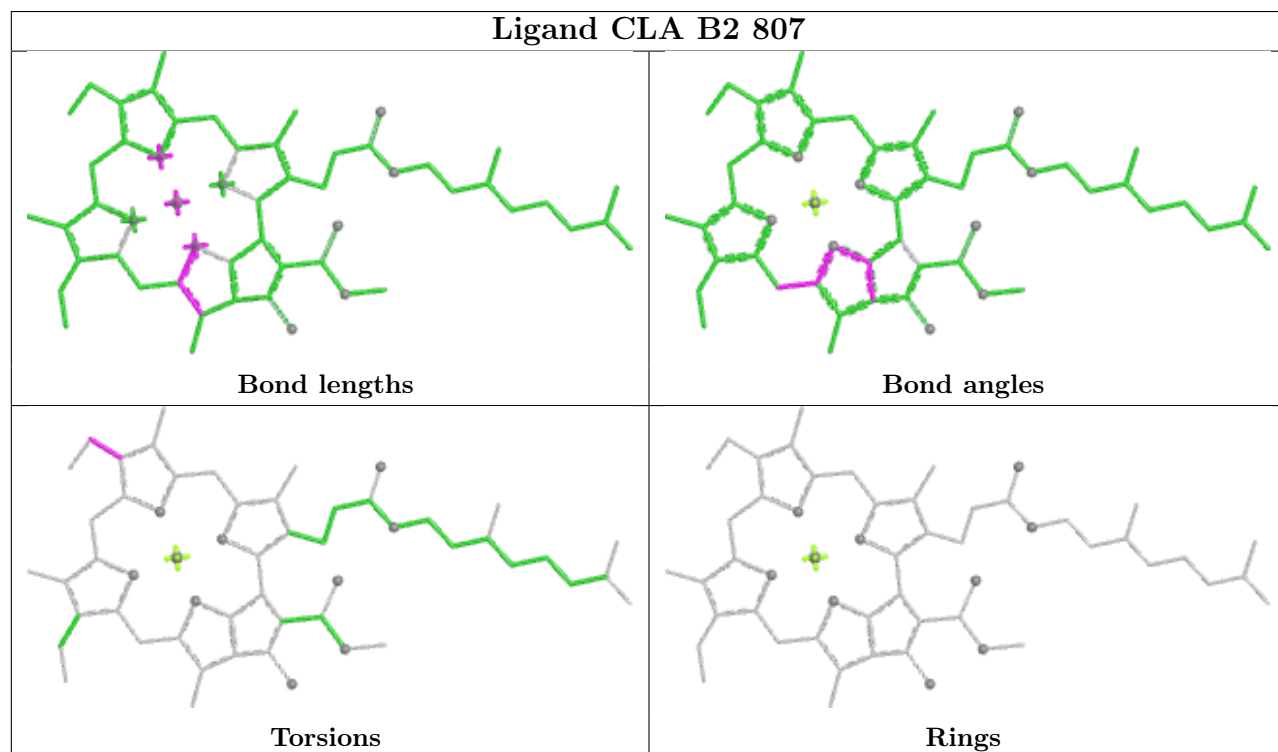
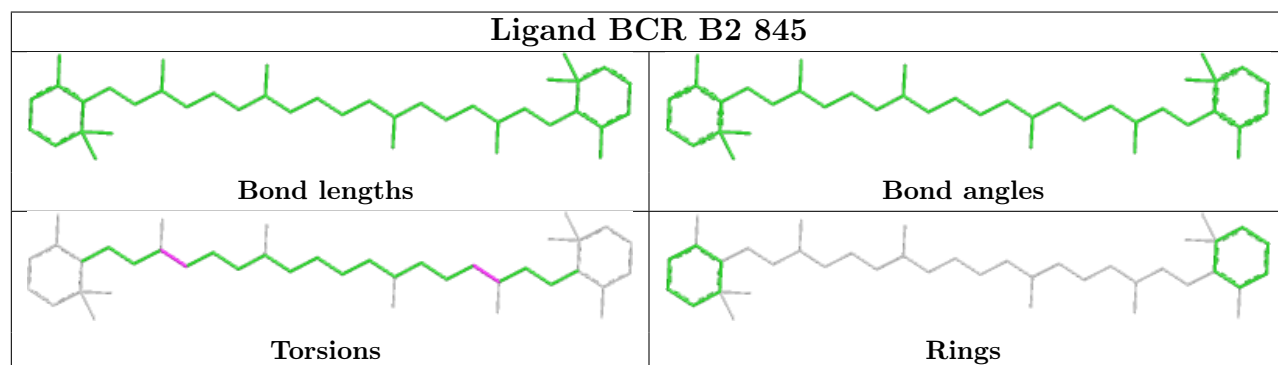
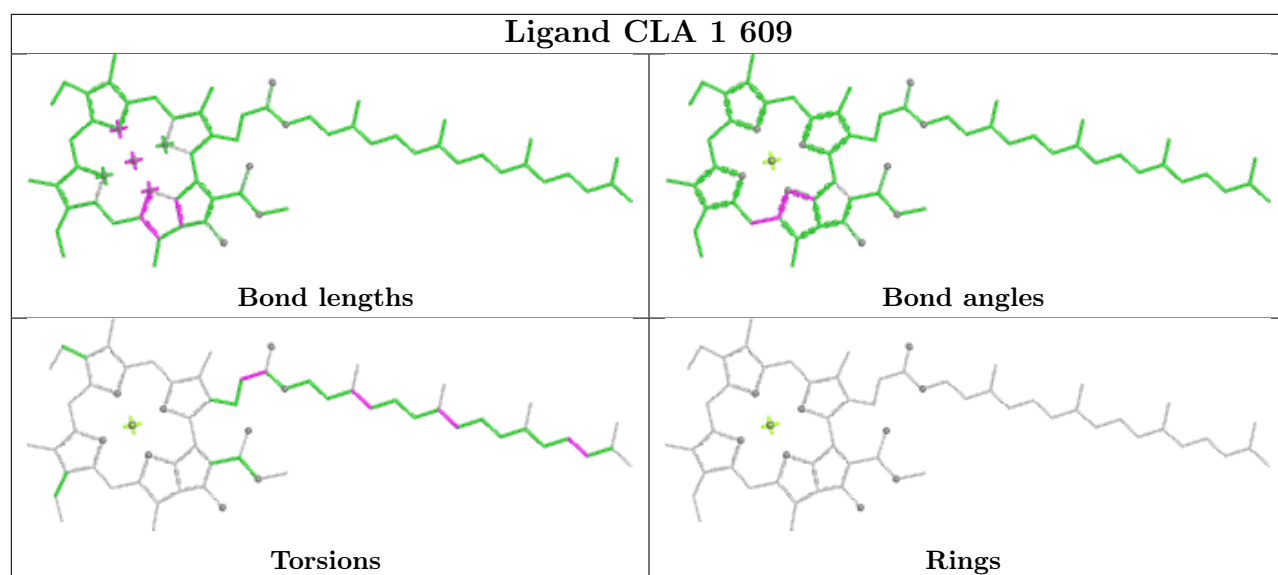


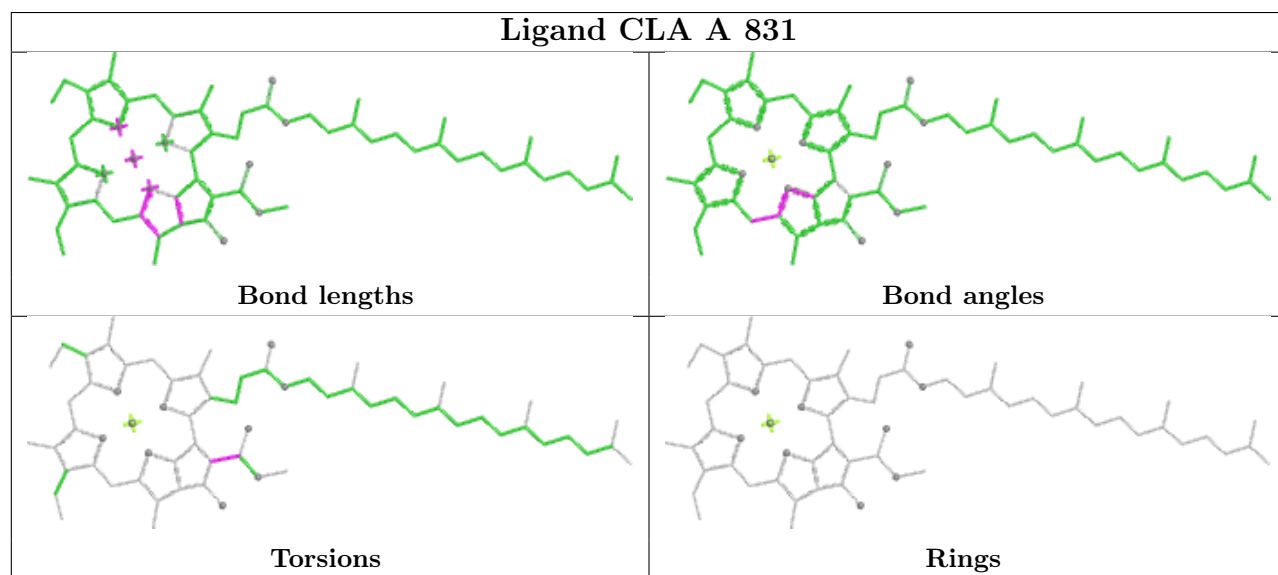
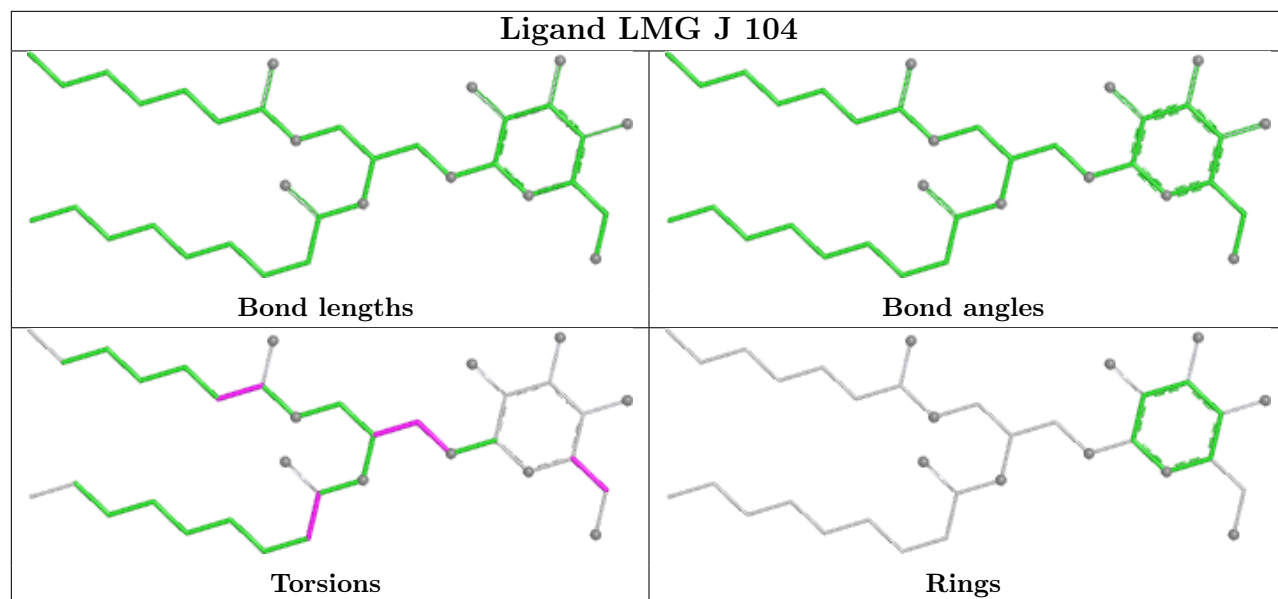
Rings

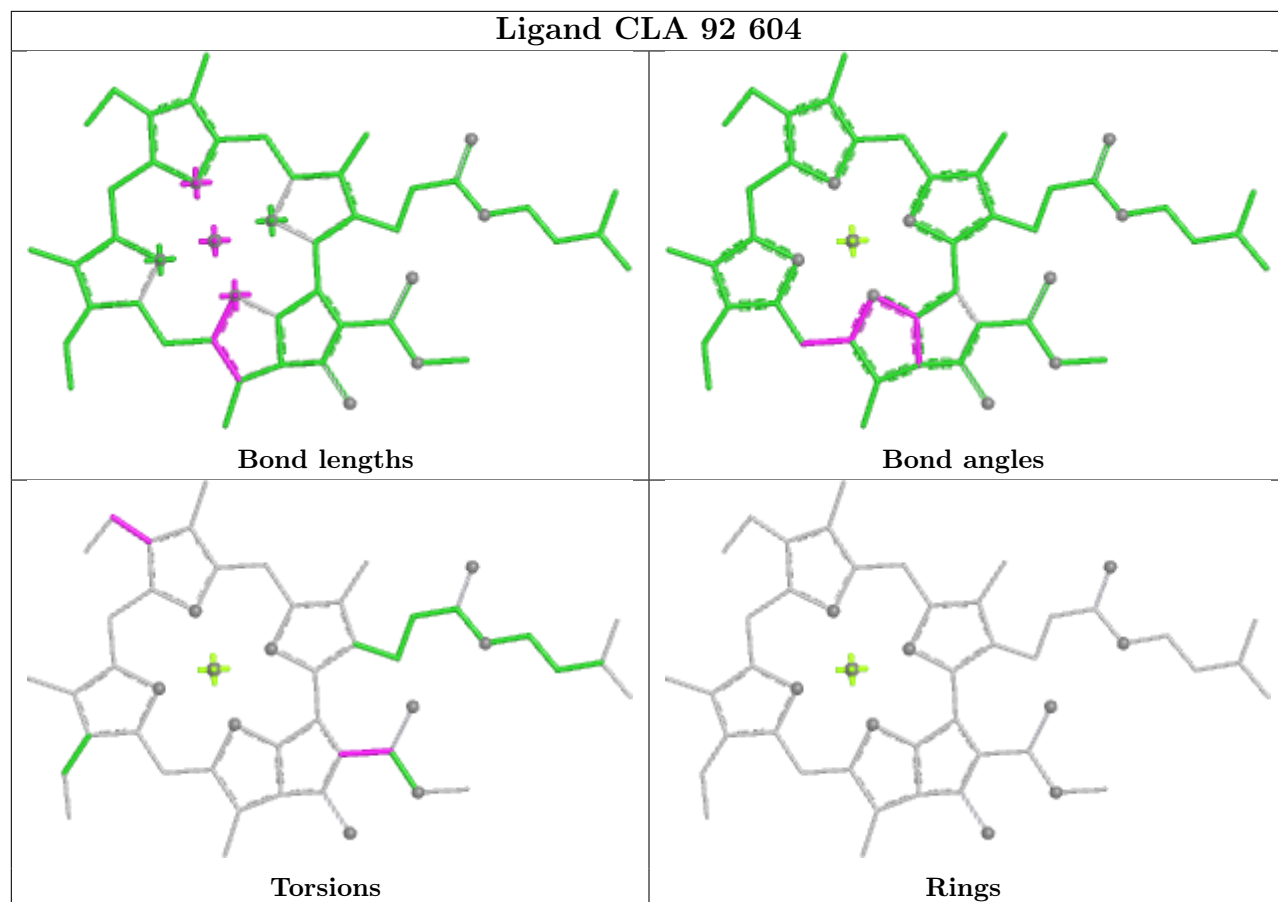




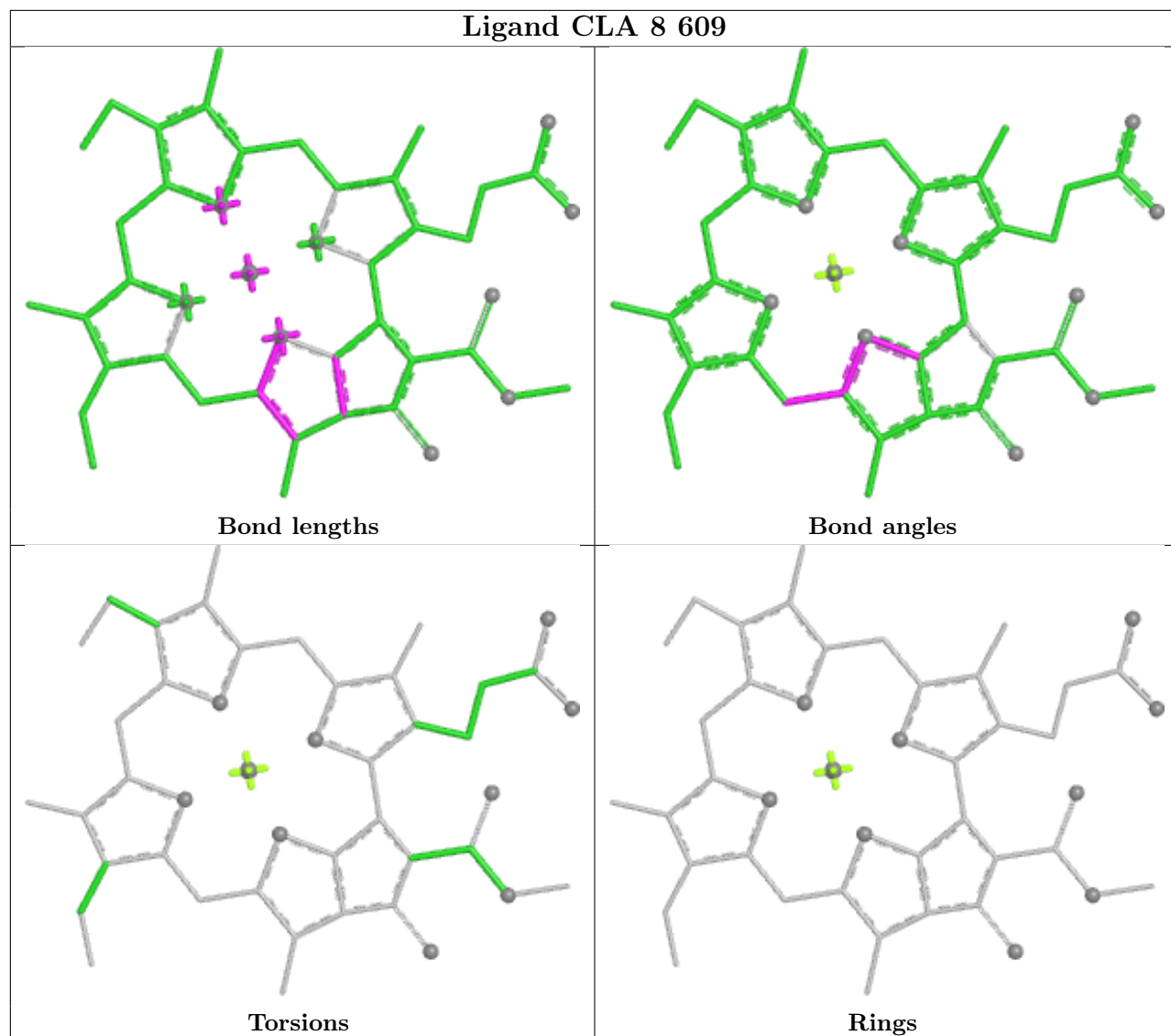




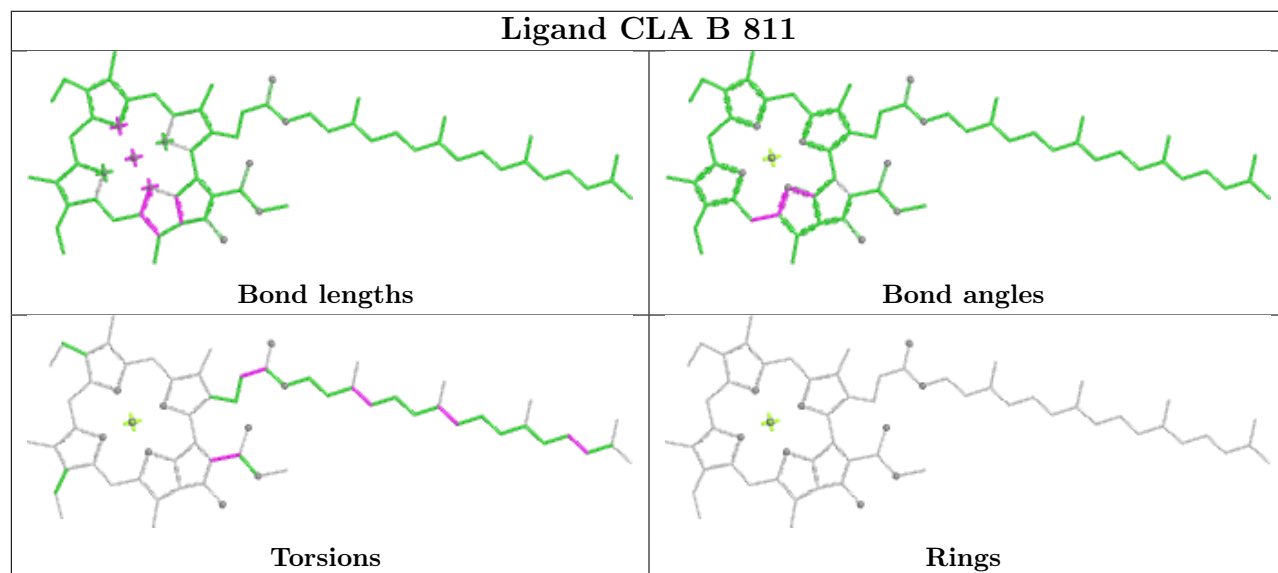


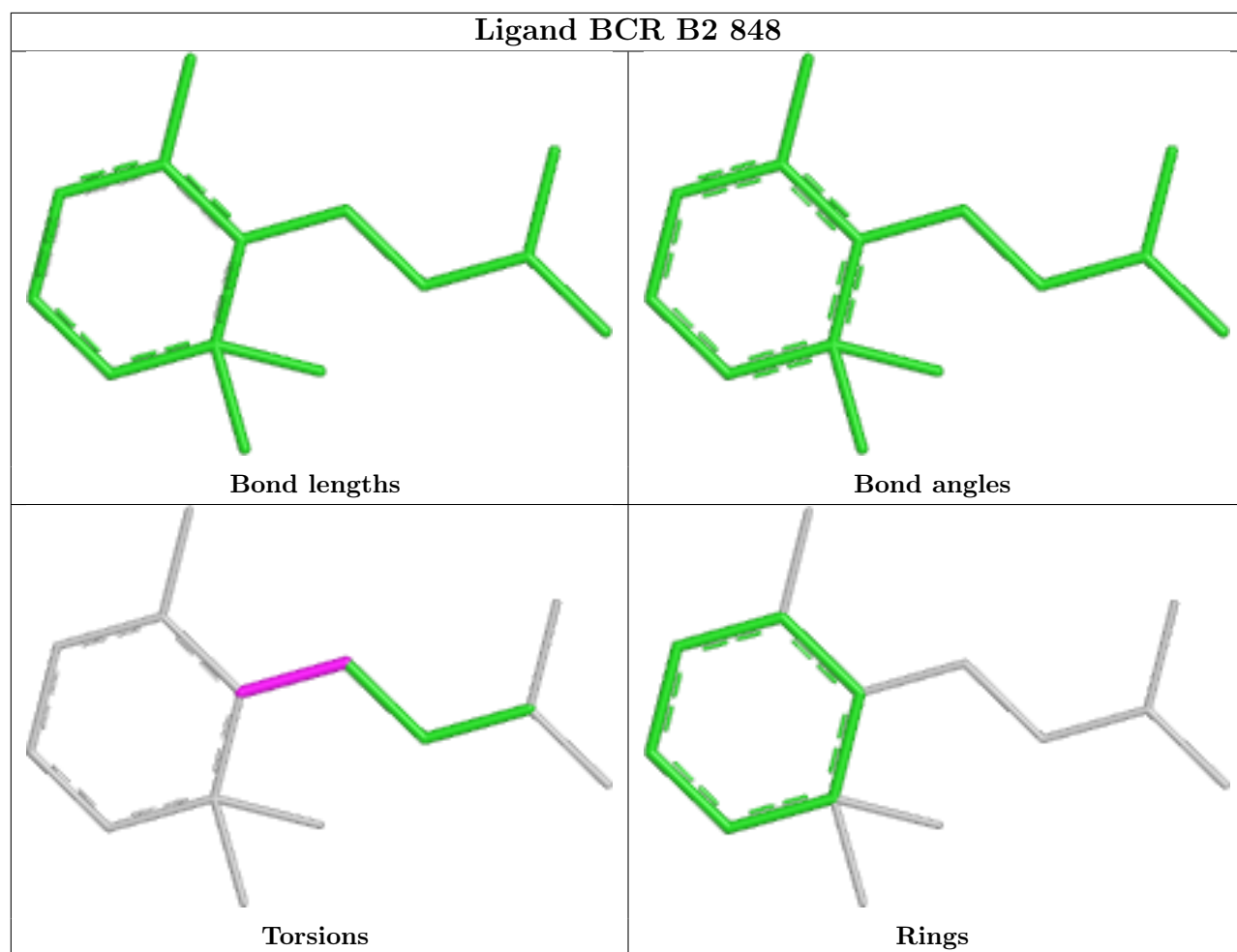
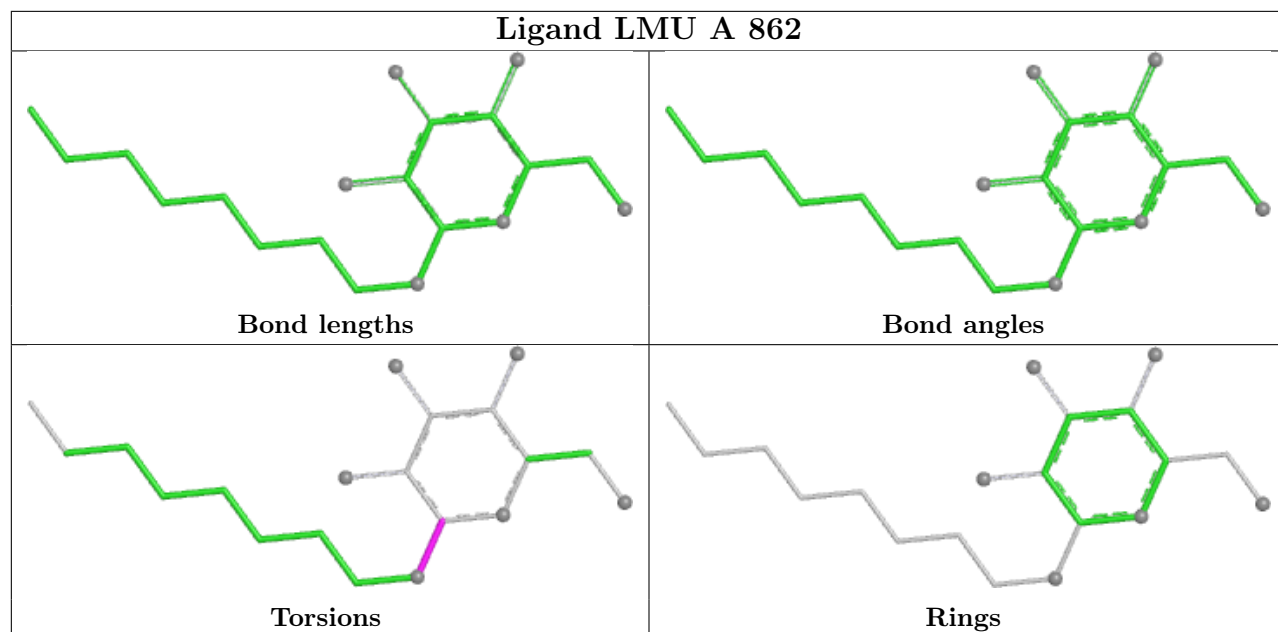


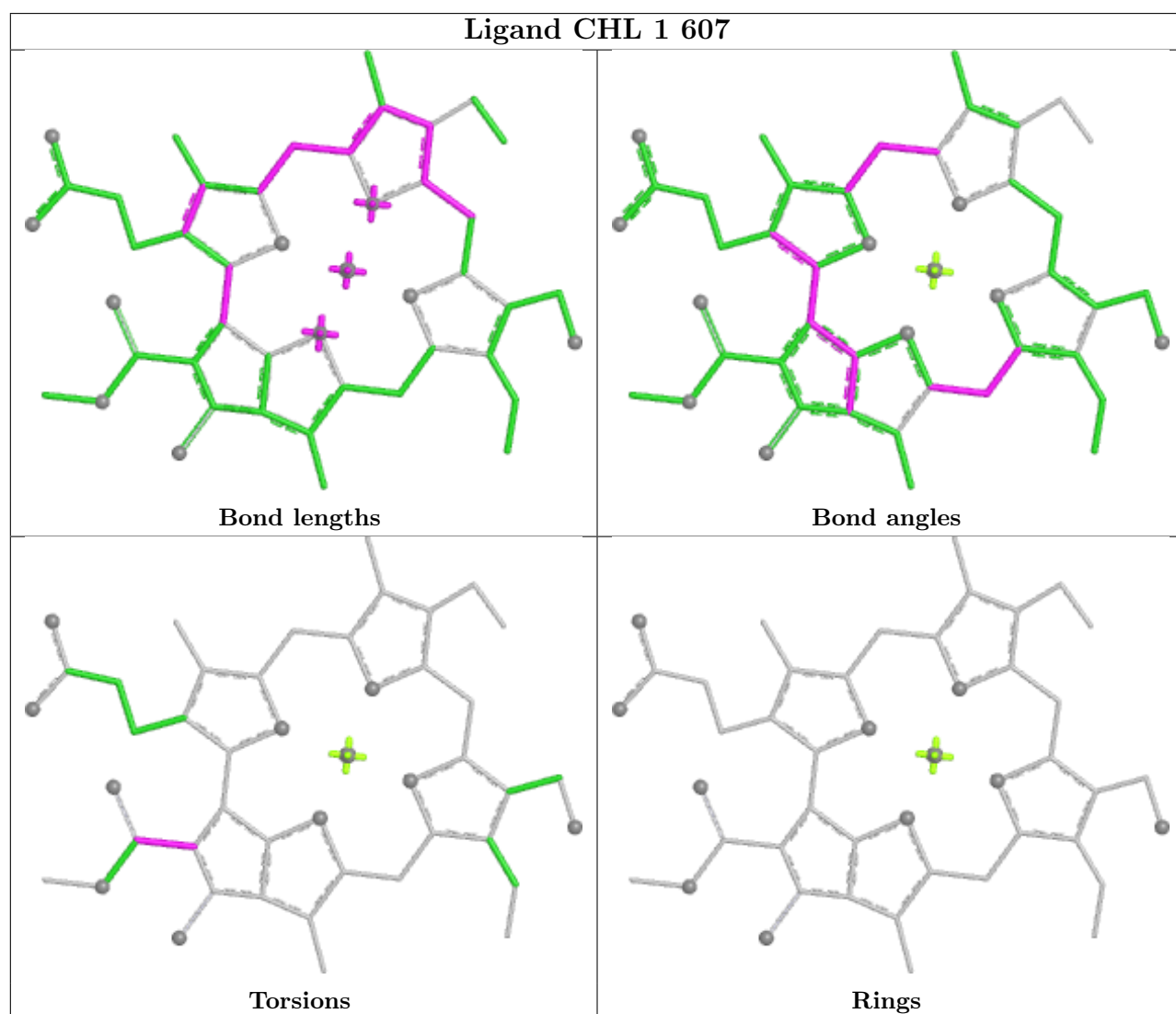
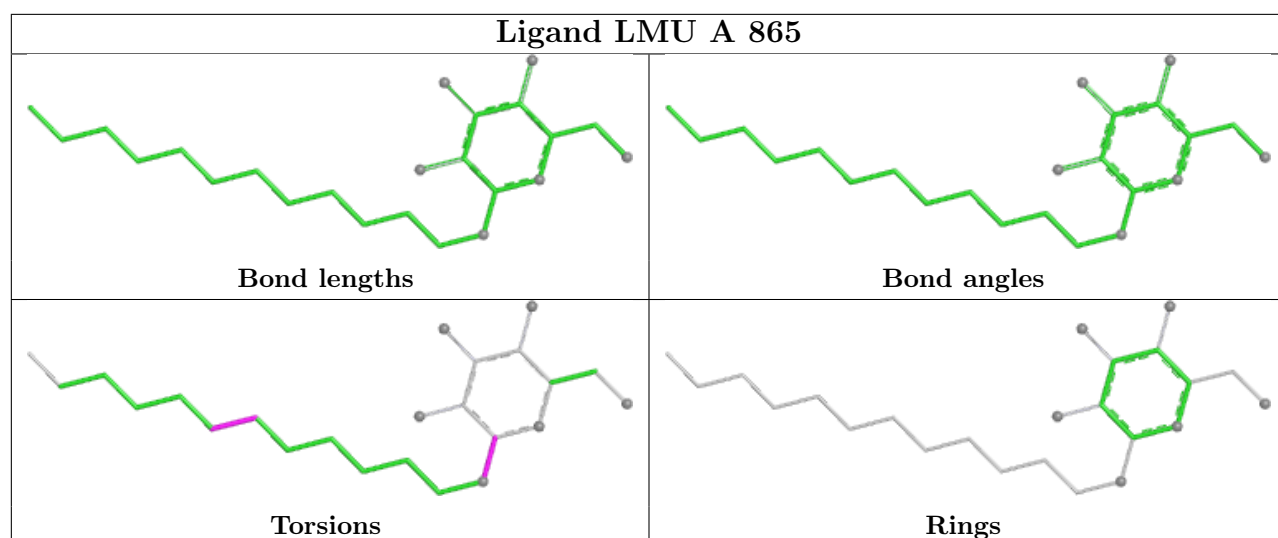
Ligand CLA 8 609

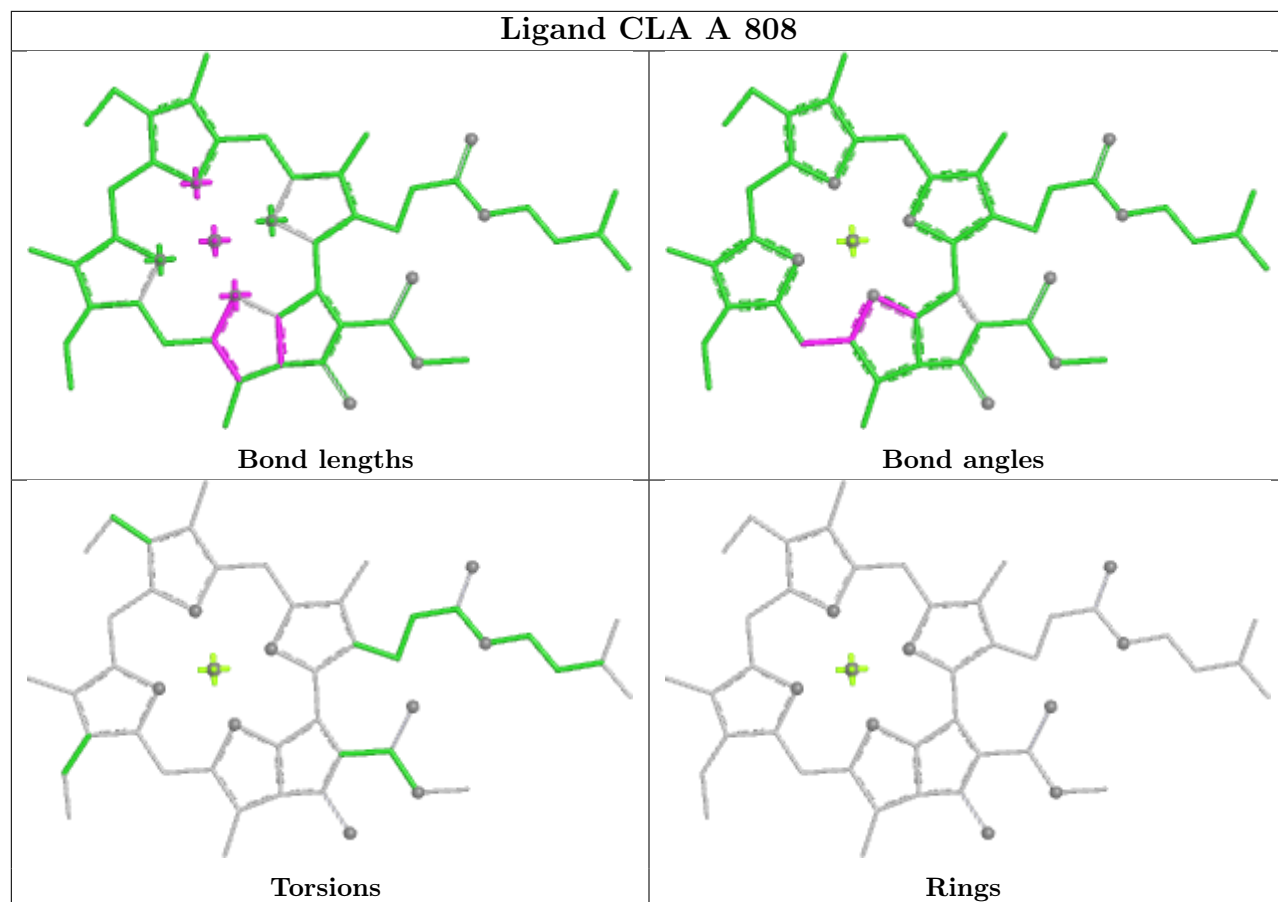


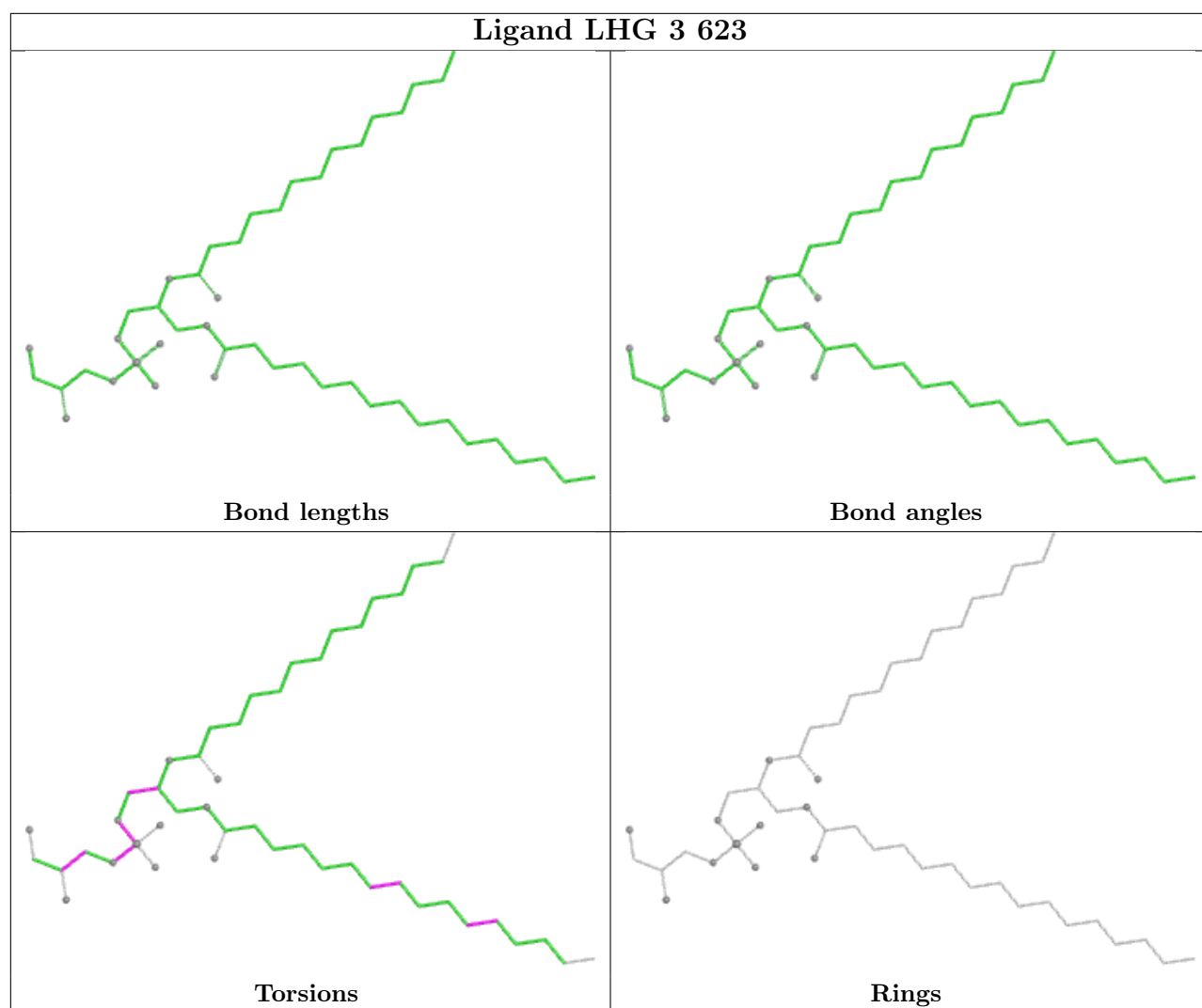
Ligand CLA B 811



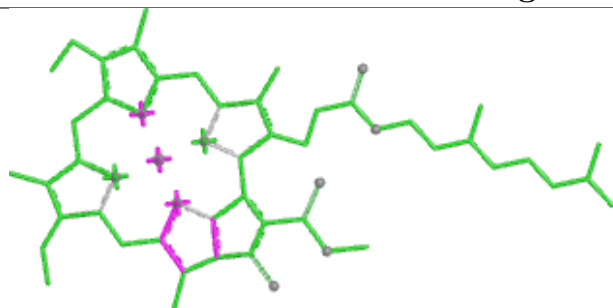




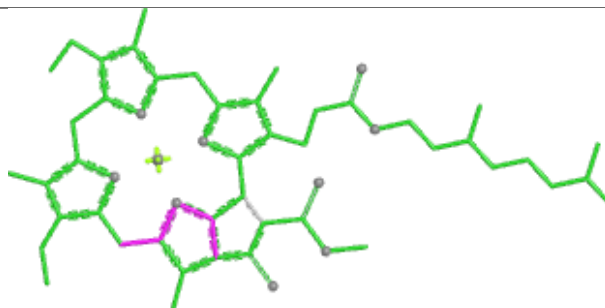




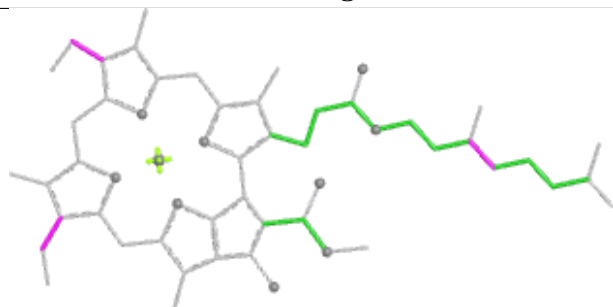
Ligand CLA 3 607



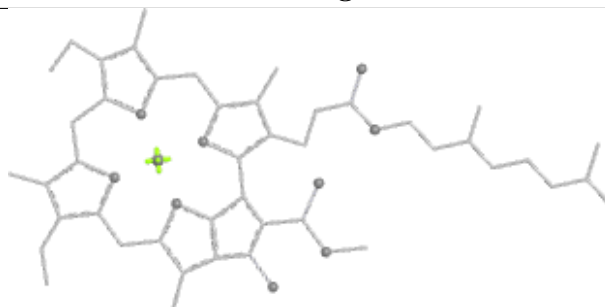
Bond lengths



Bond angles

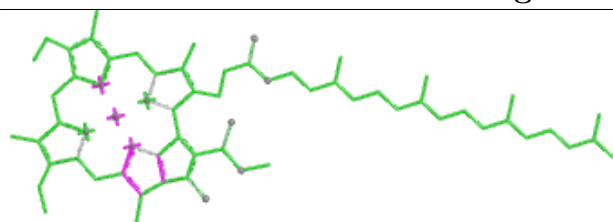


Torsions

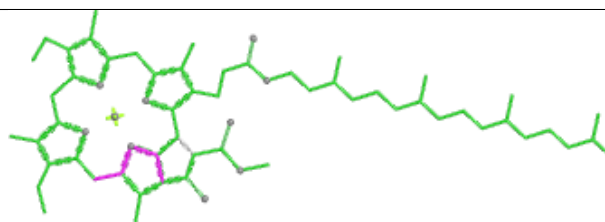


Rings

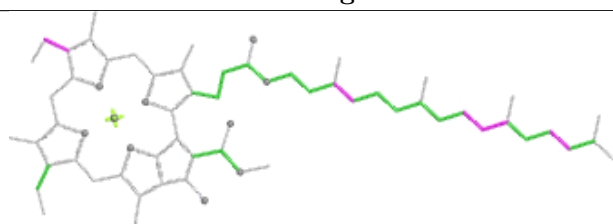
Ligand CLA B 840



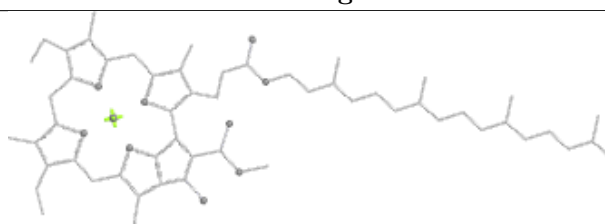
Bond lengths



Bond angles

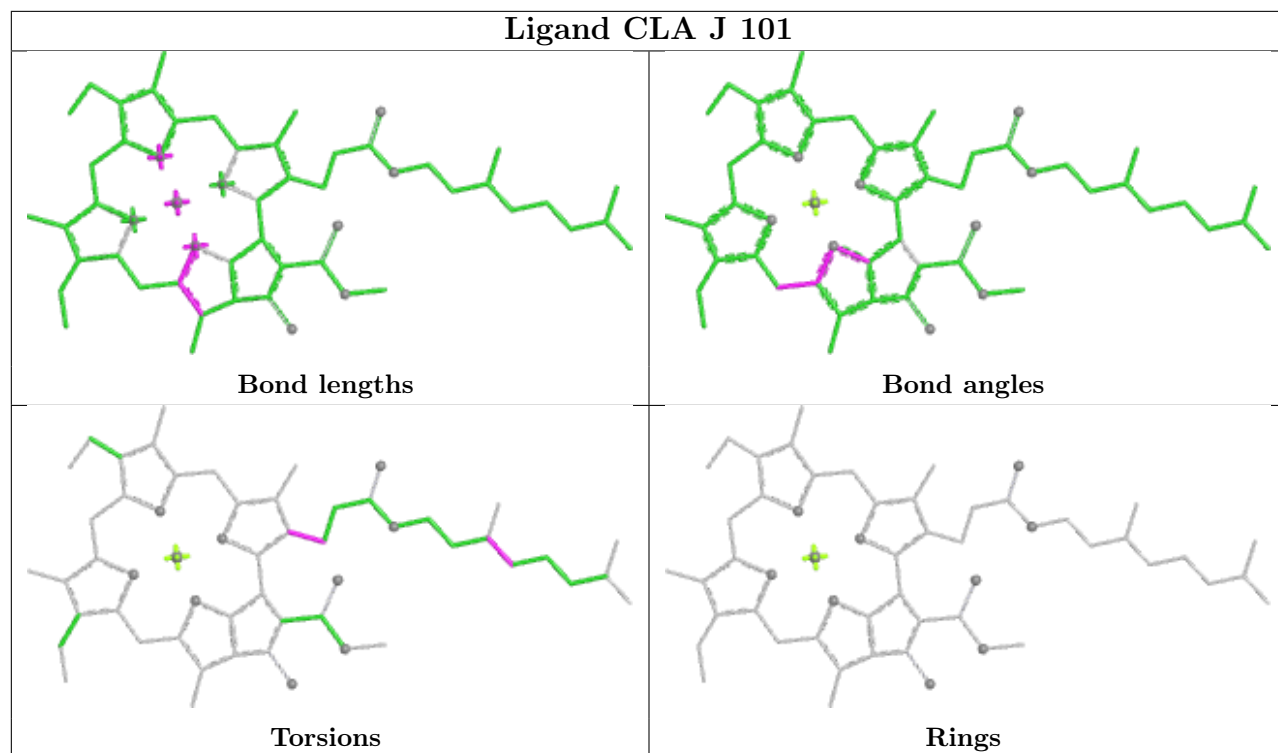


Torsions

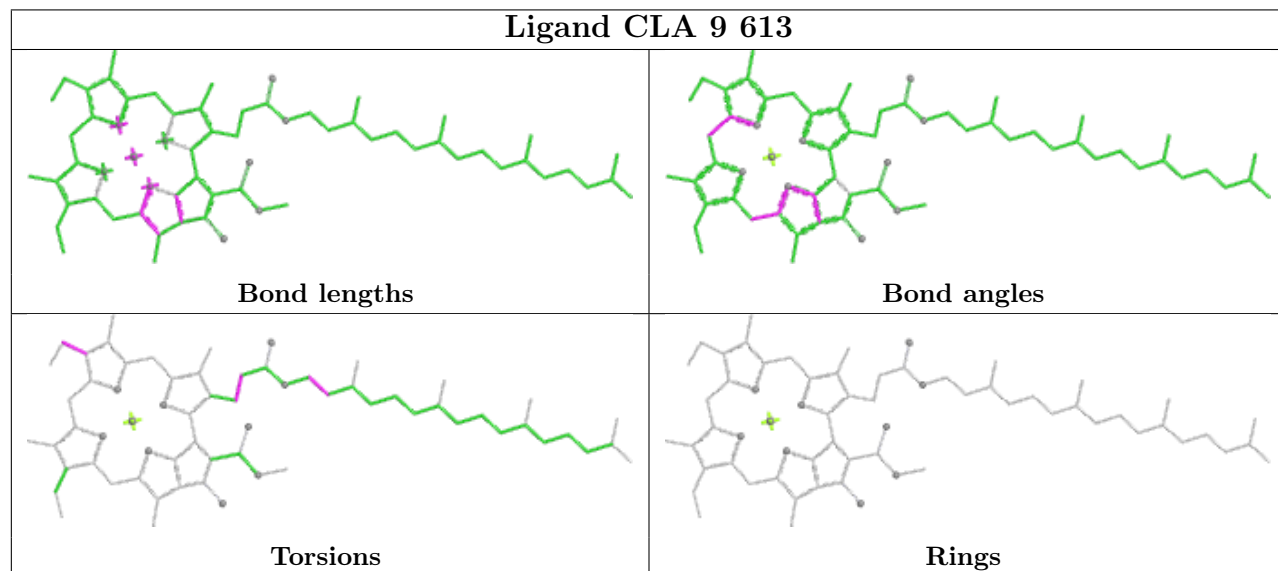


Rings

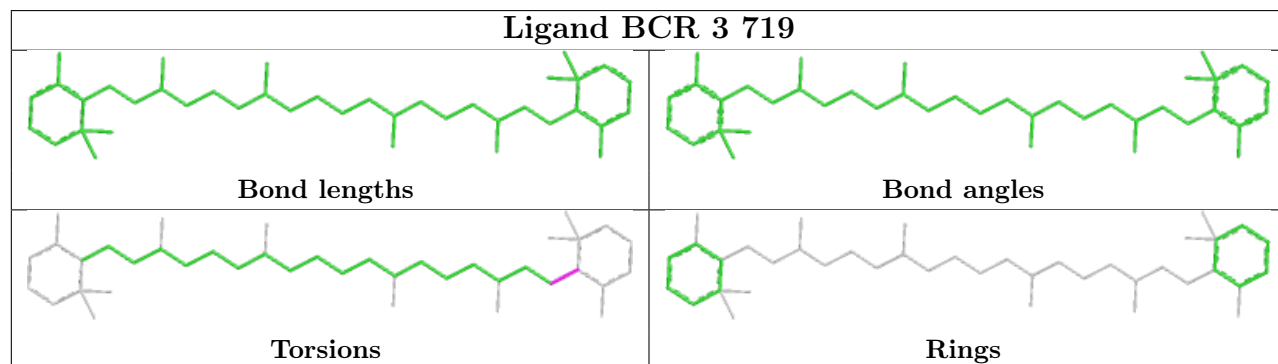
Ligand CLA J 101

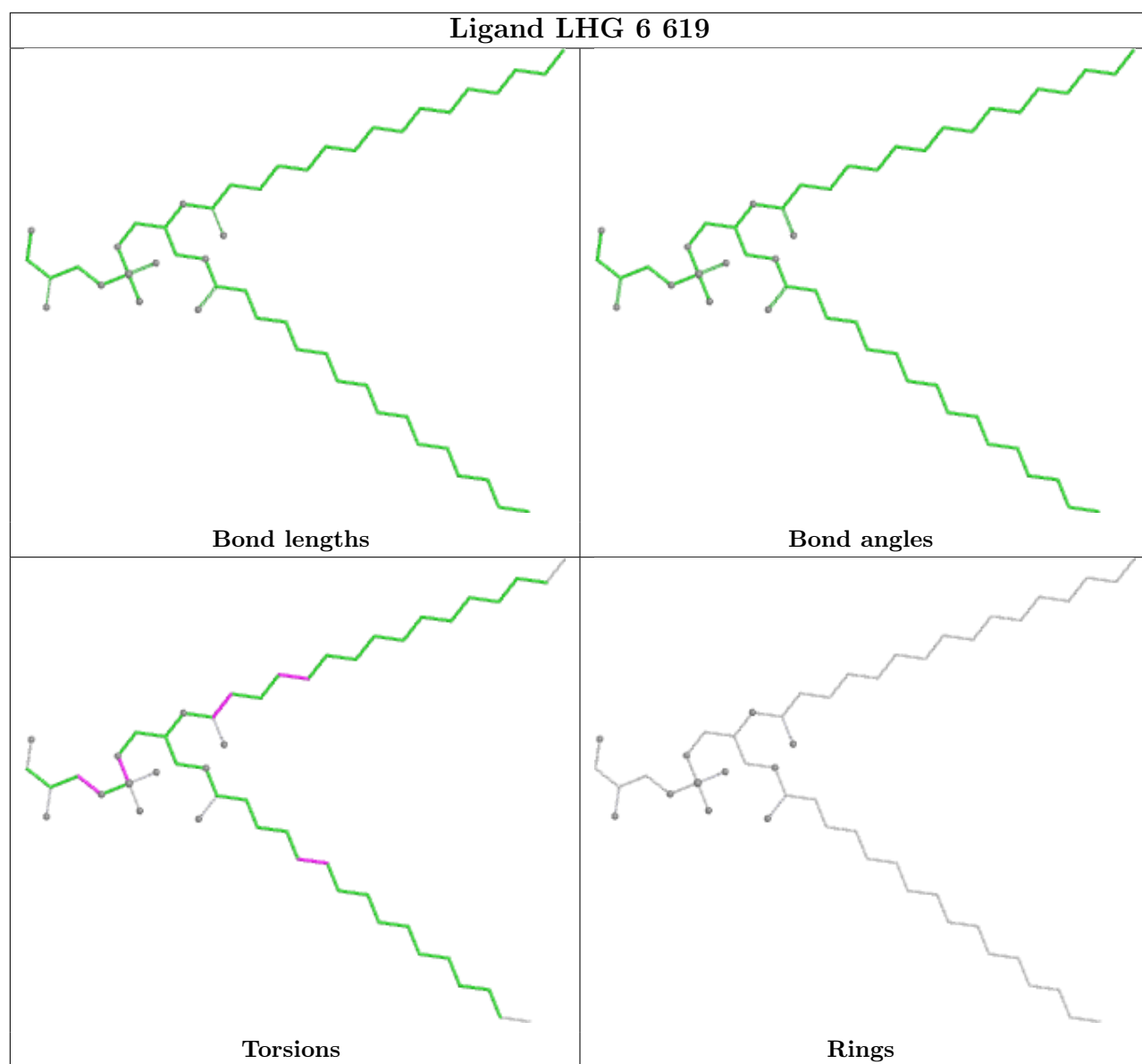


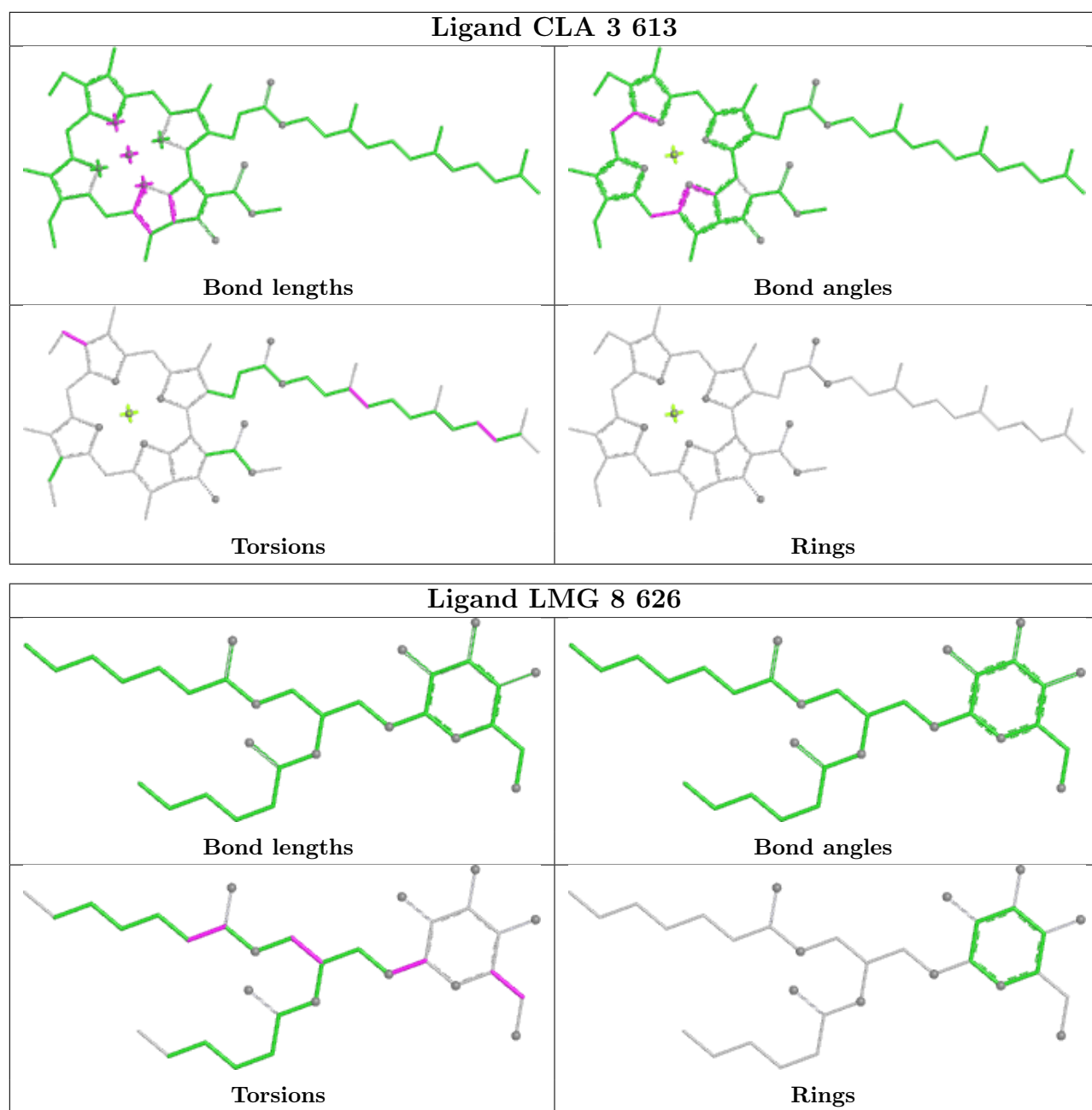
Ligand CLA 9 613



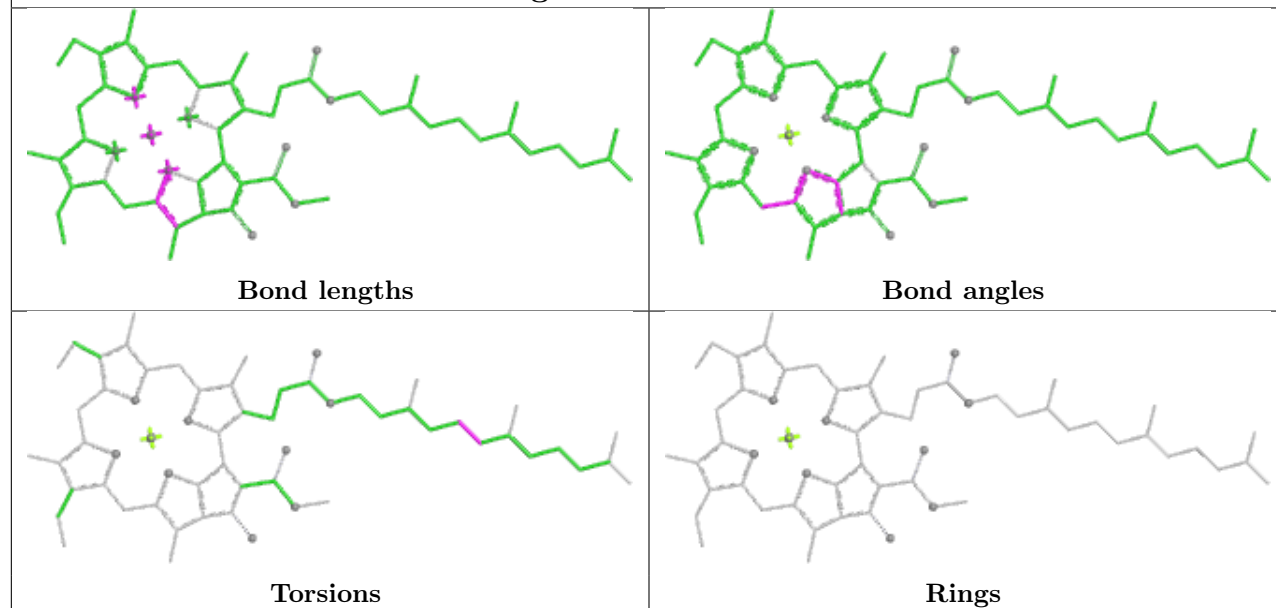
Ligand BCR 3 719



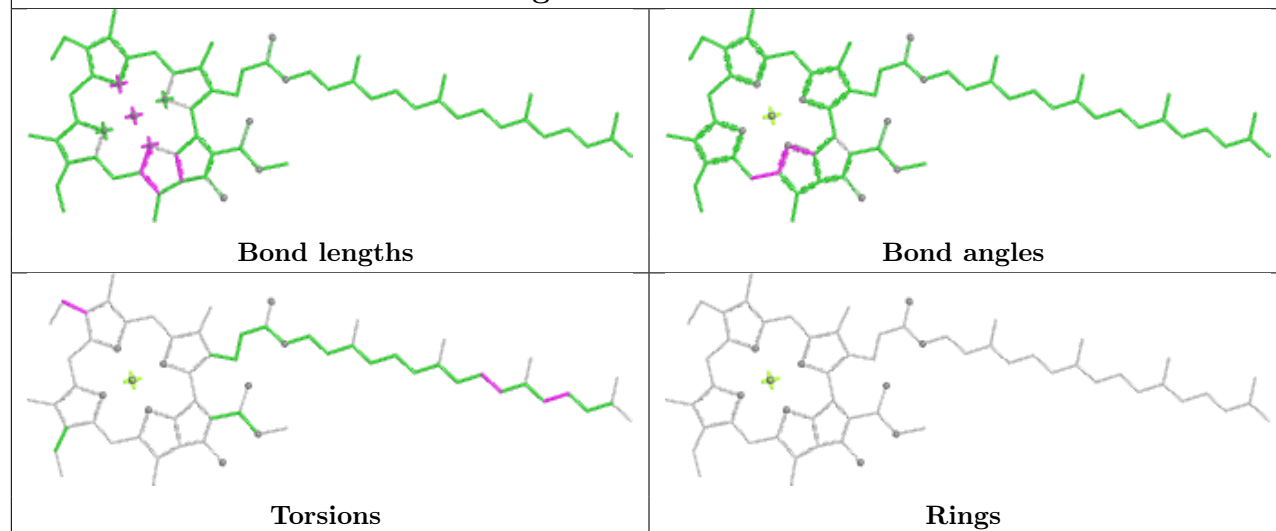


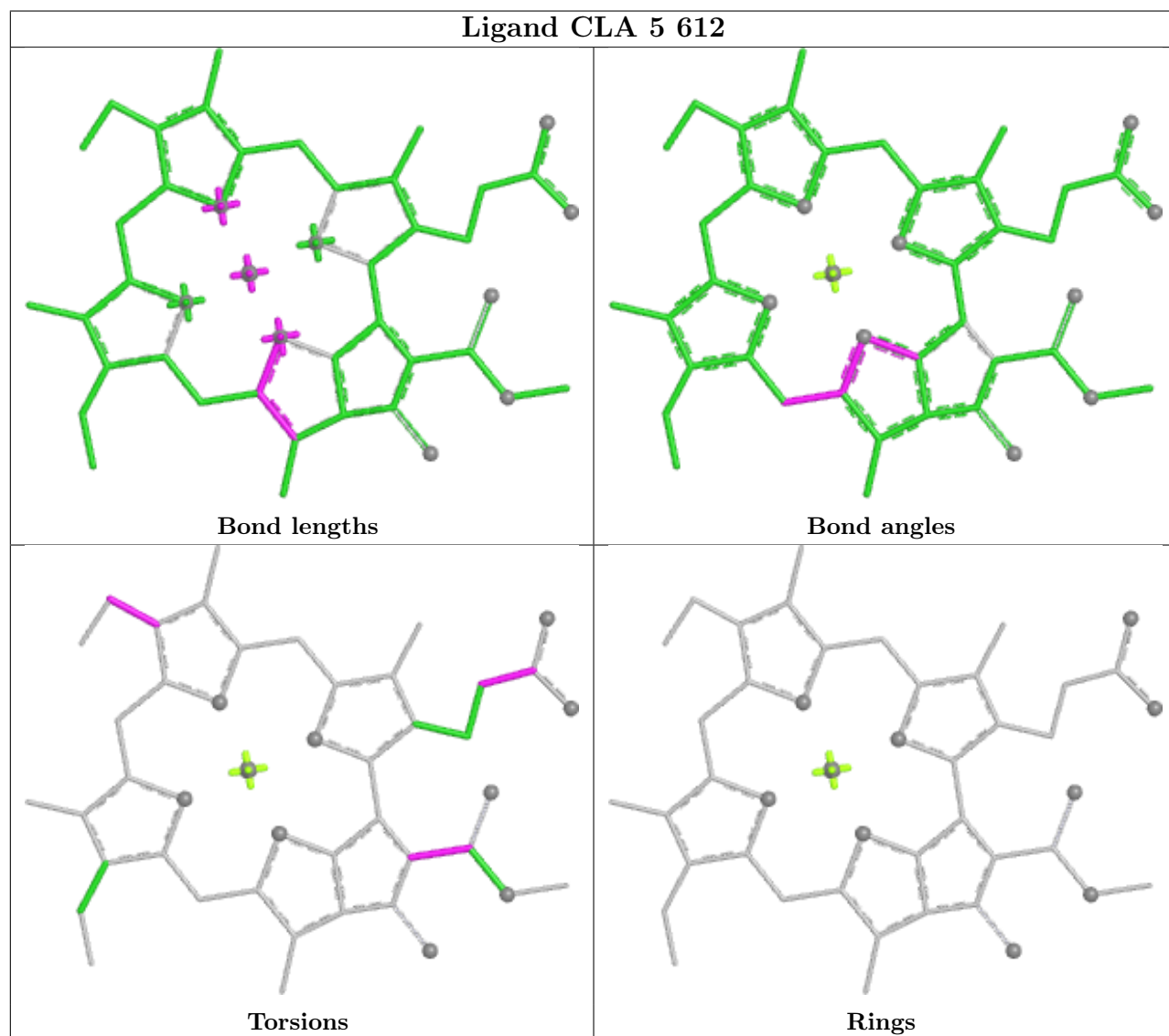
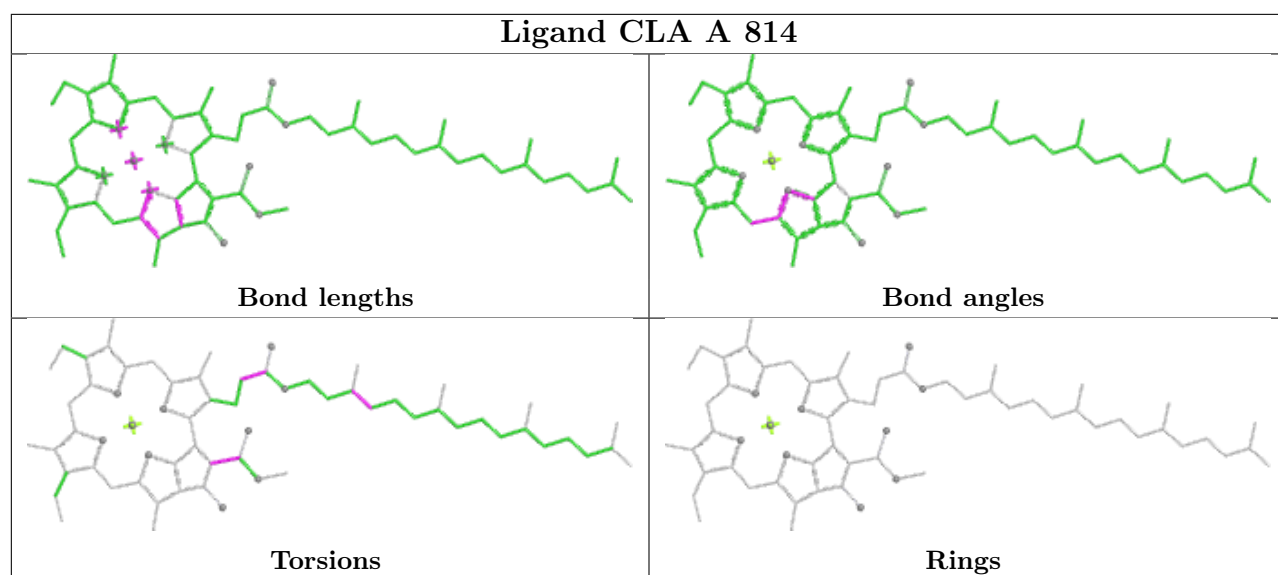


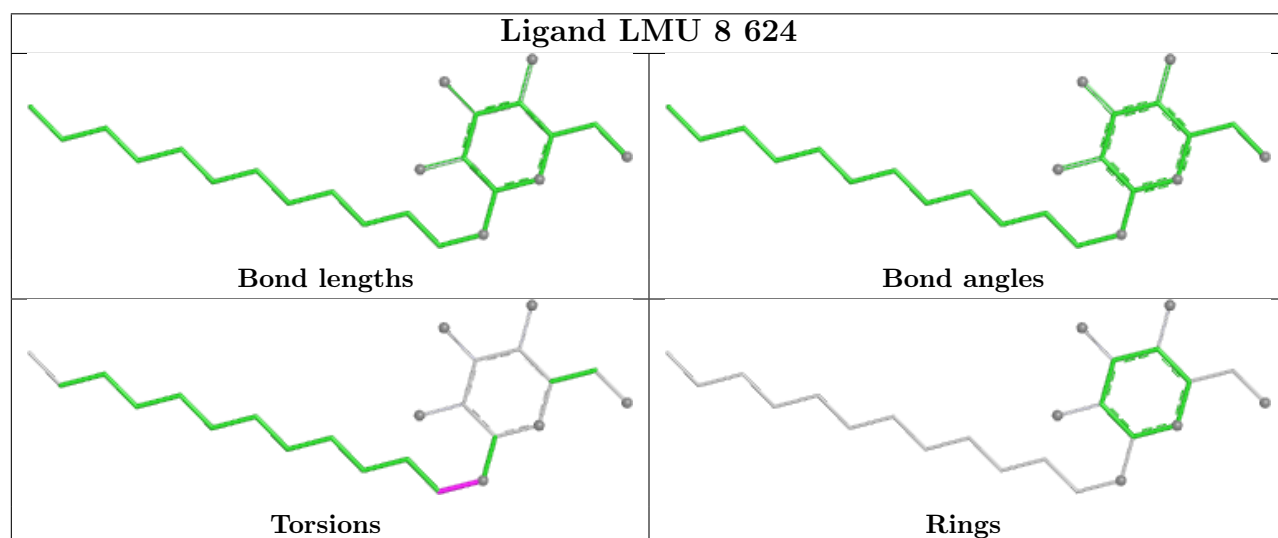
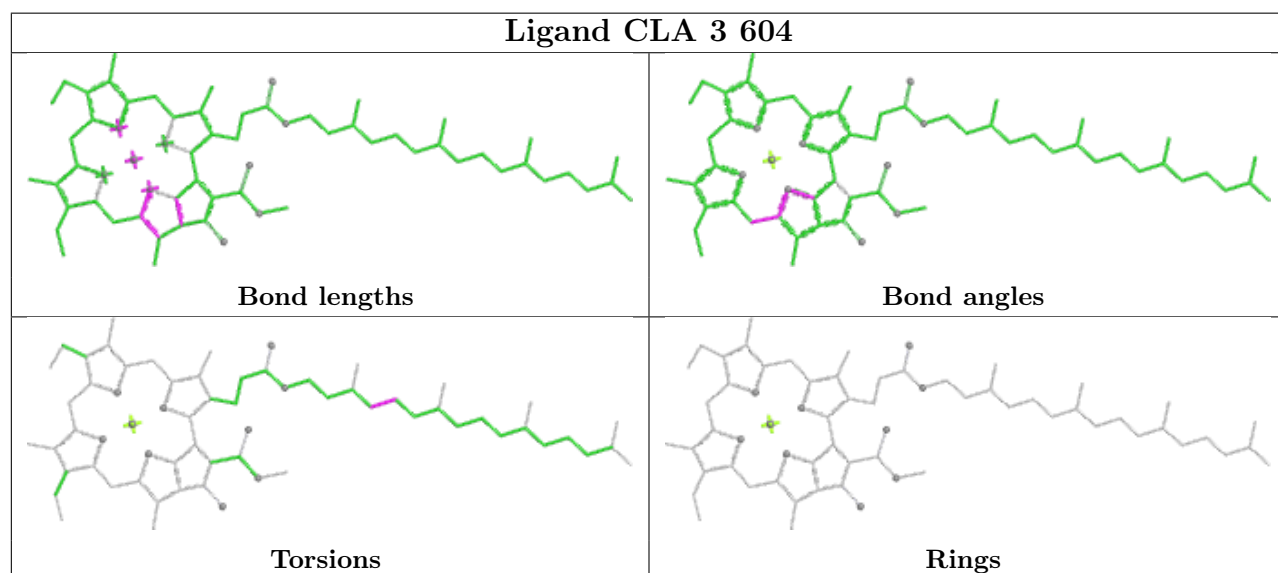
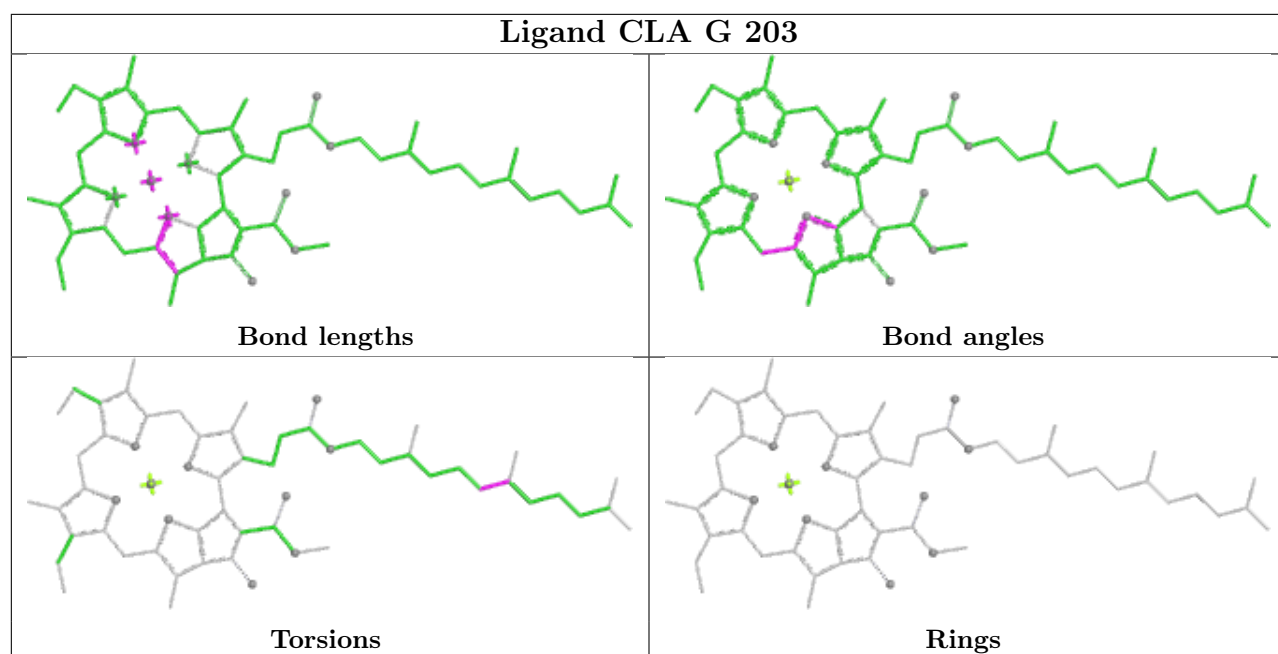
Ligand CLA K 203

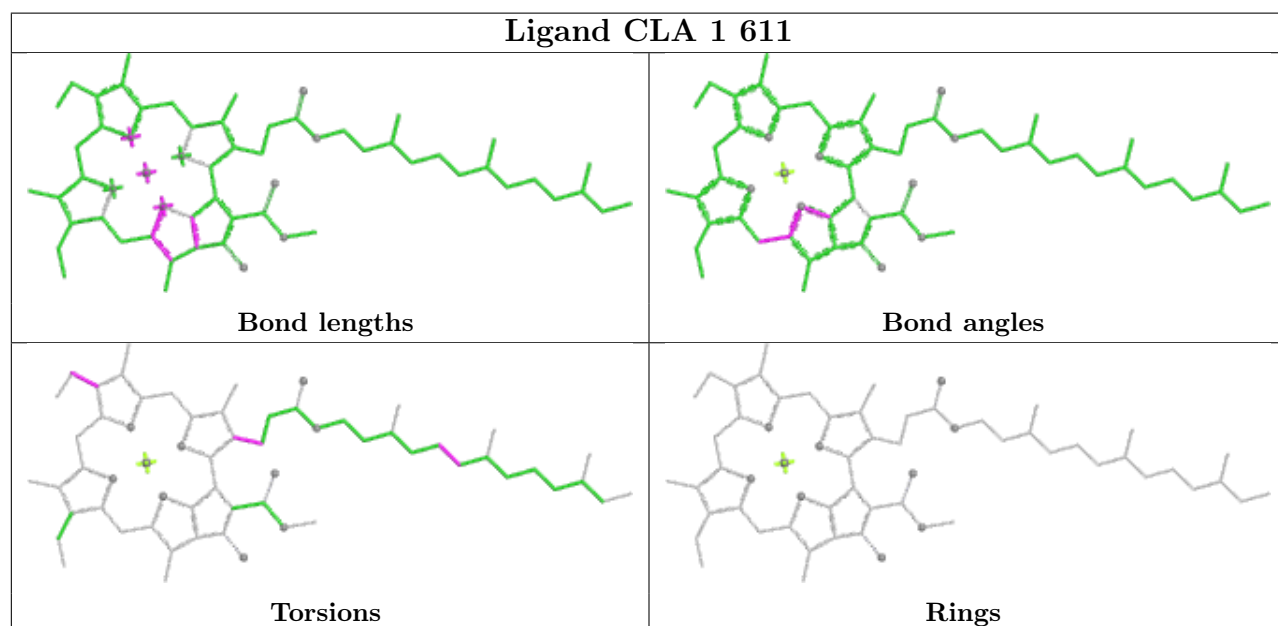
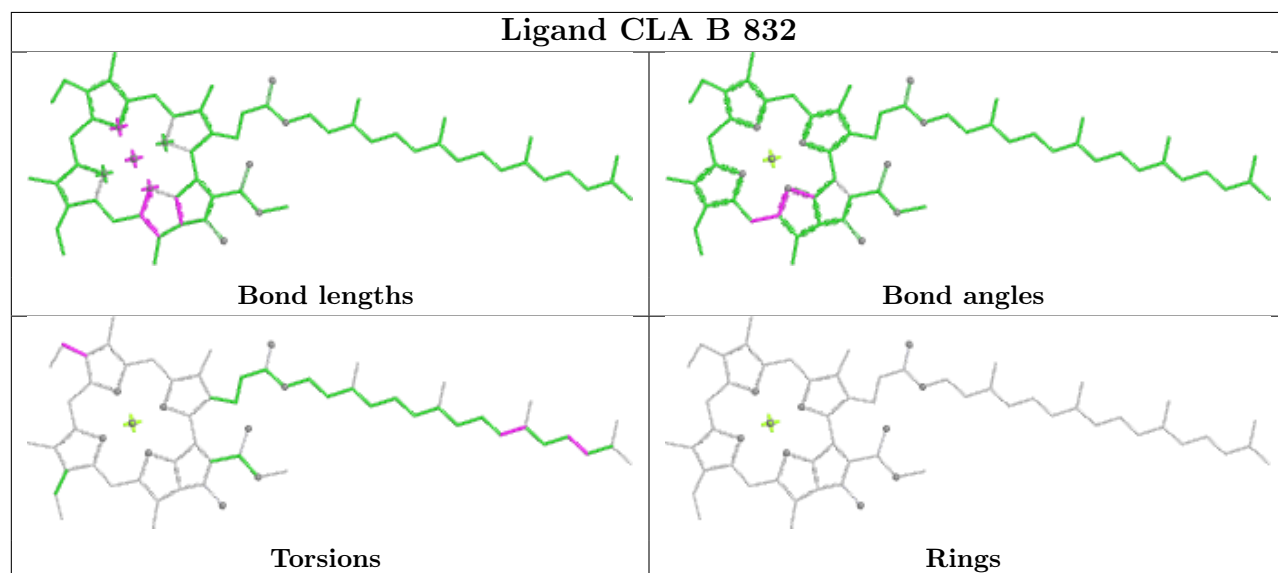
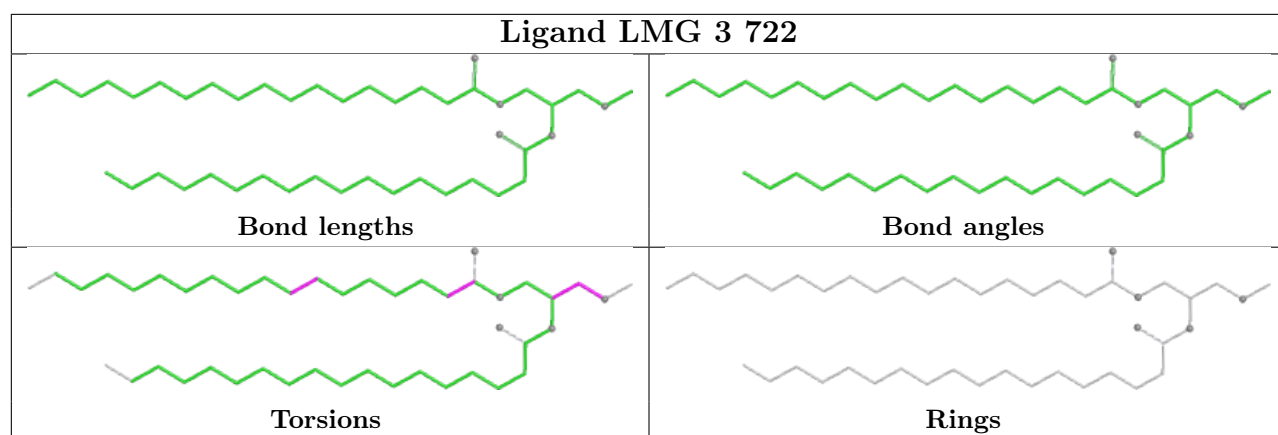


Ligand CLA B 818

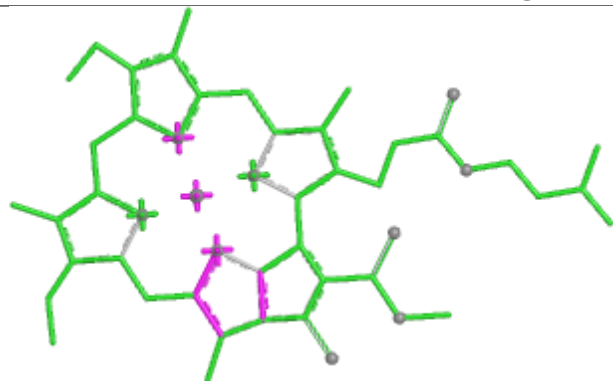




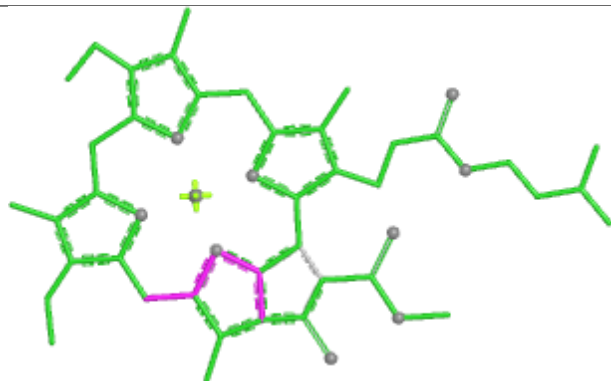




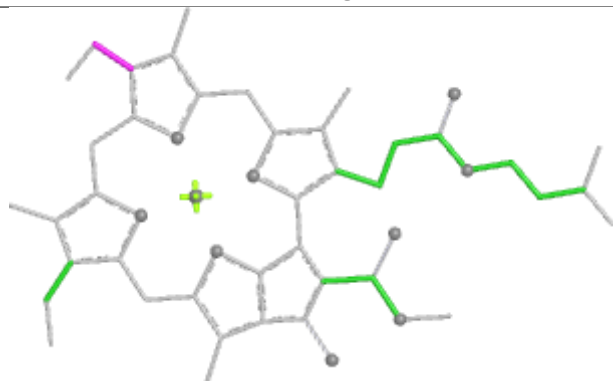
Ligand CLA 6 614



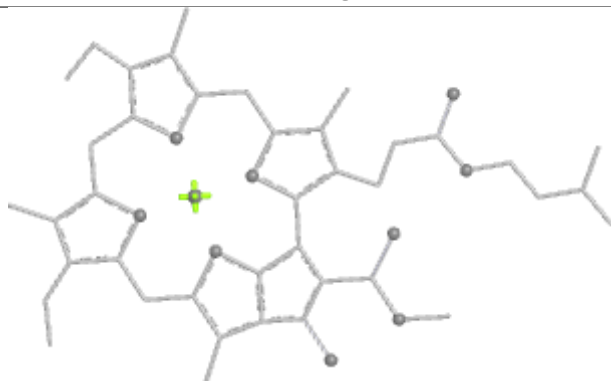
Bond lengths



Bond angles

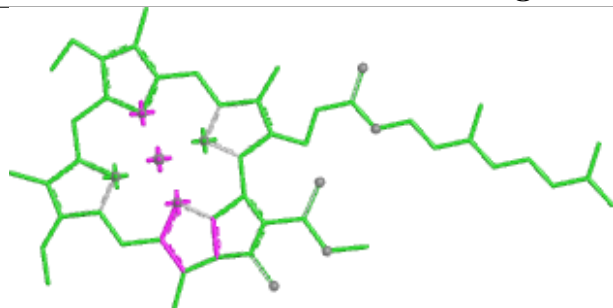


Torsions

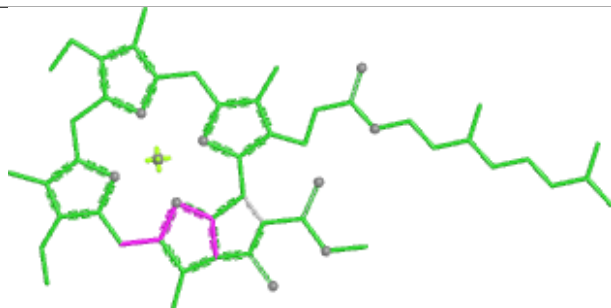


Rings

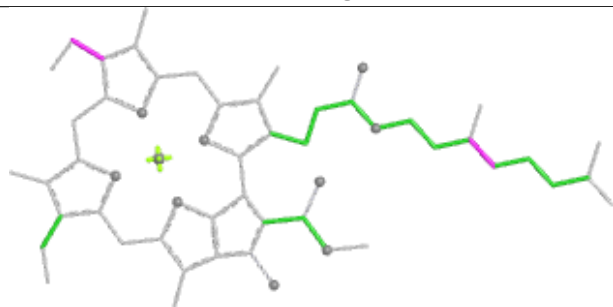
Ligand CLA B 807



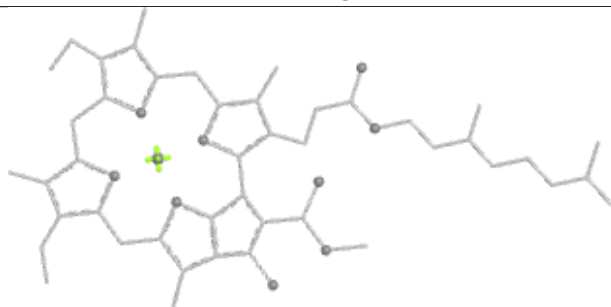
Bond lengths



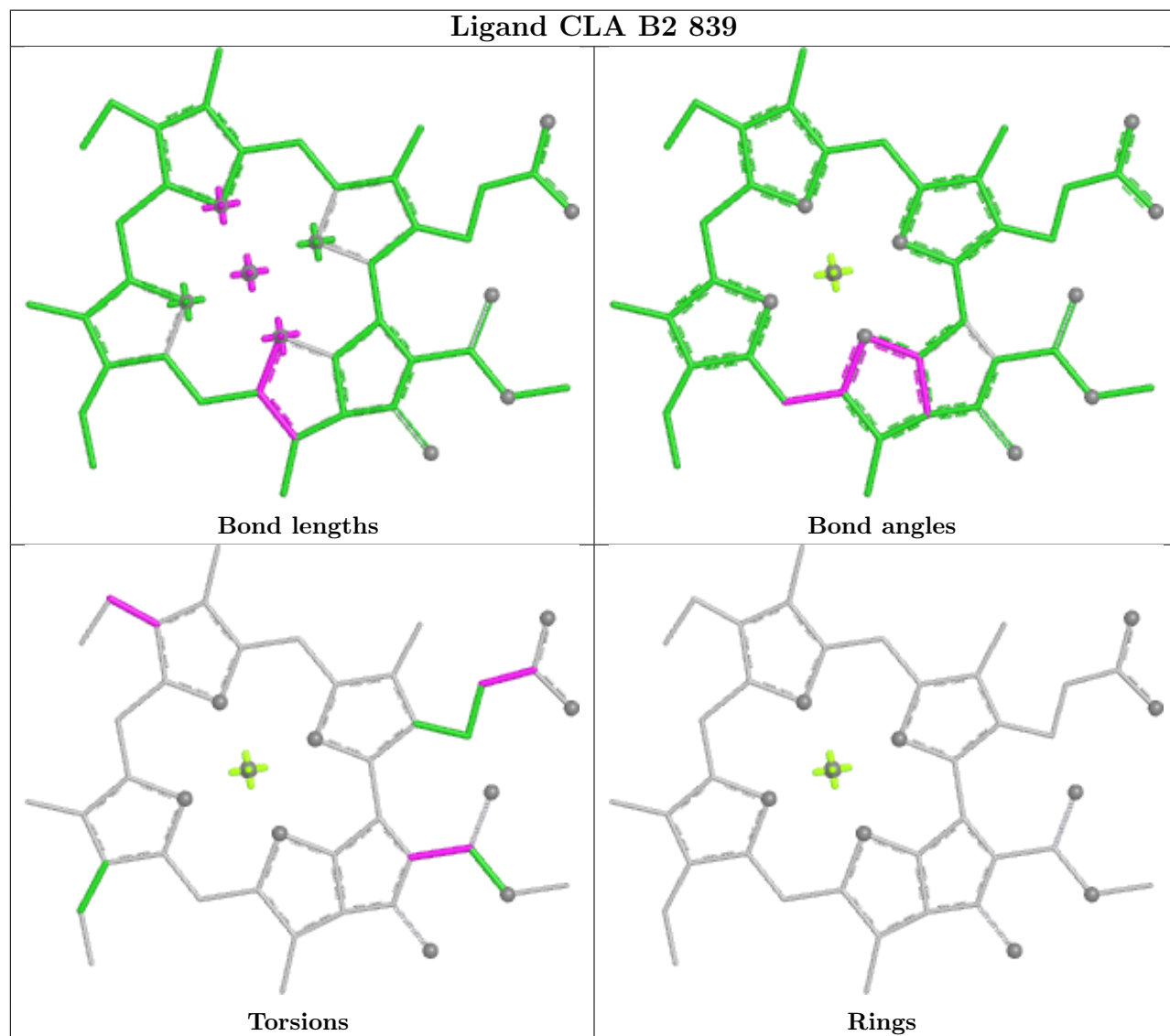
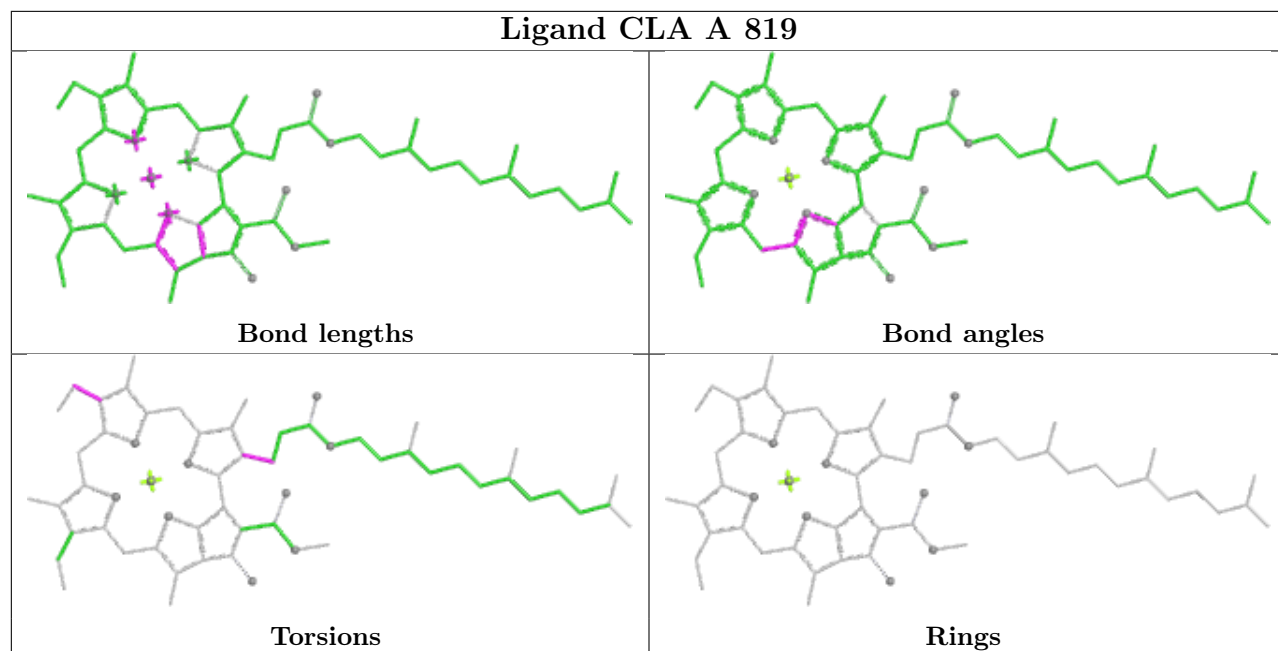
Bond angles

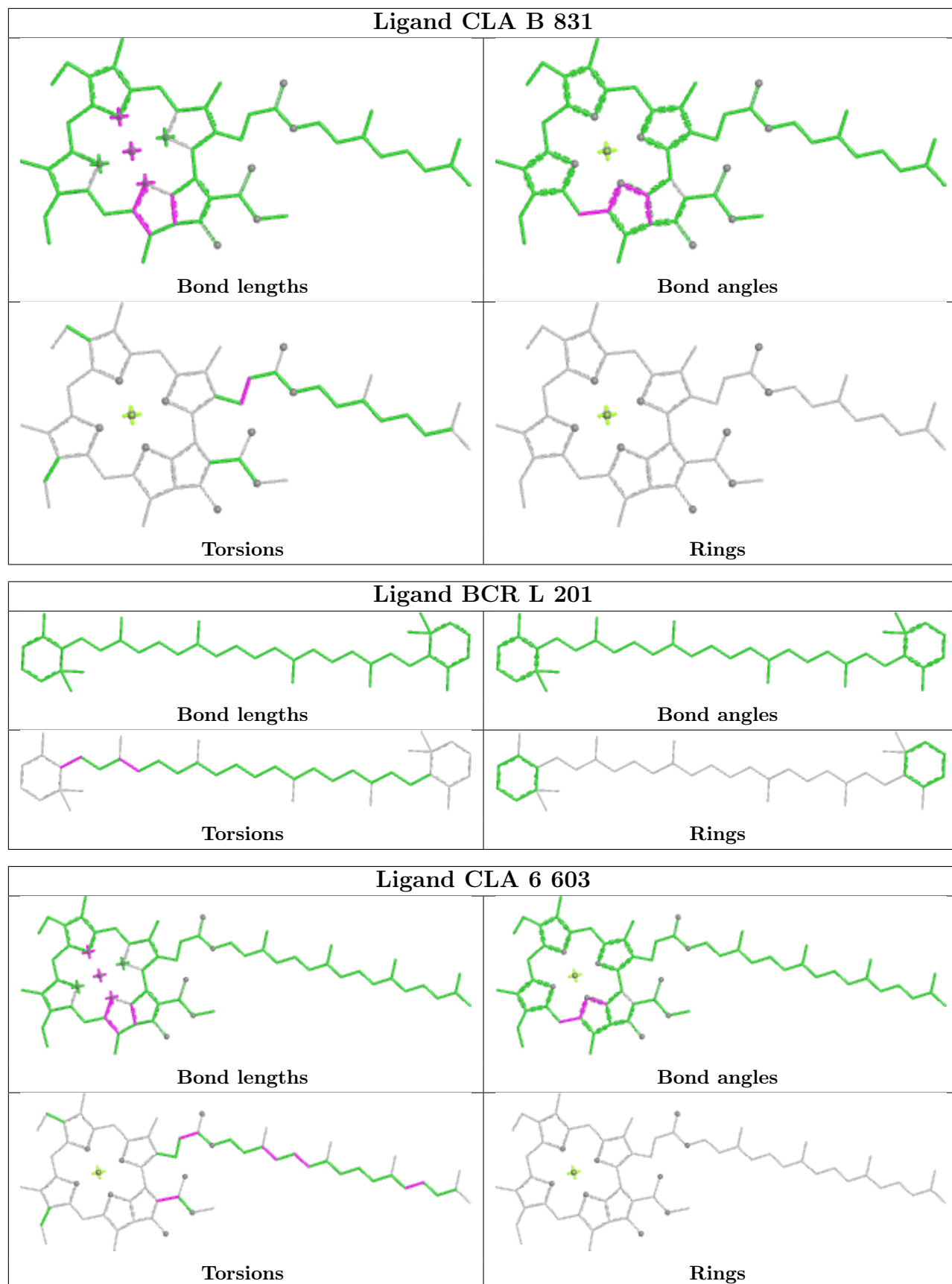


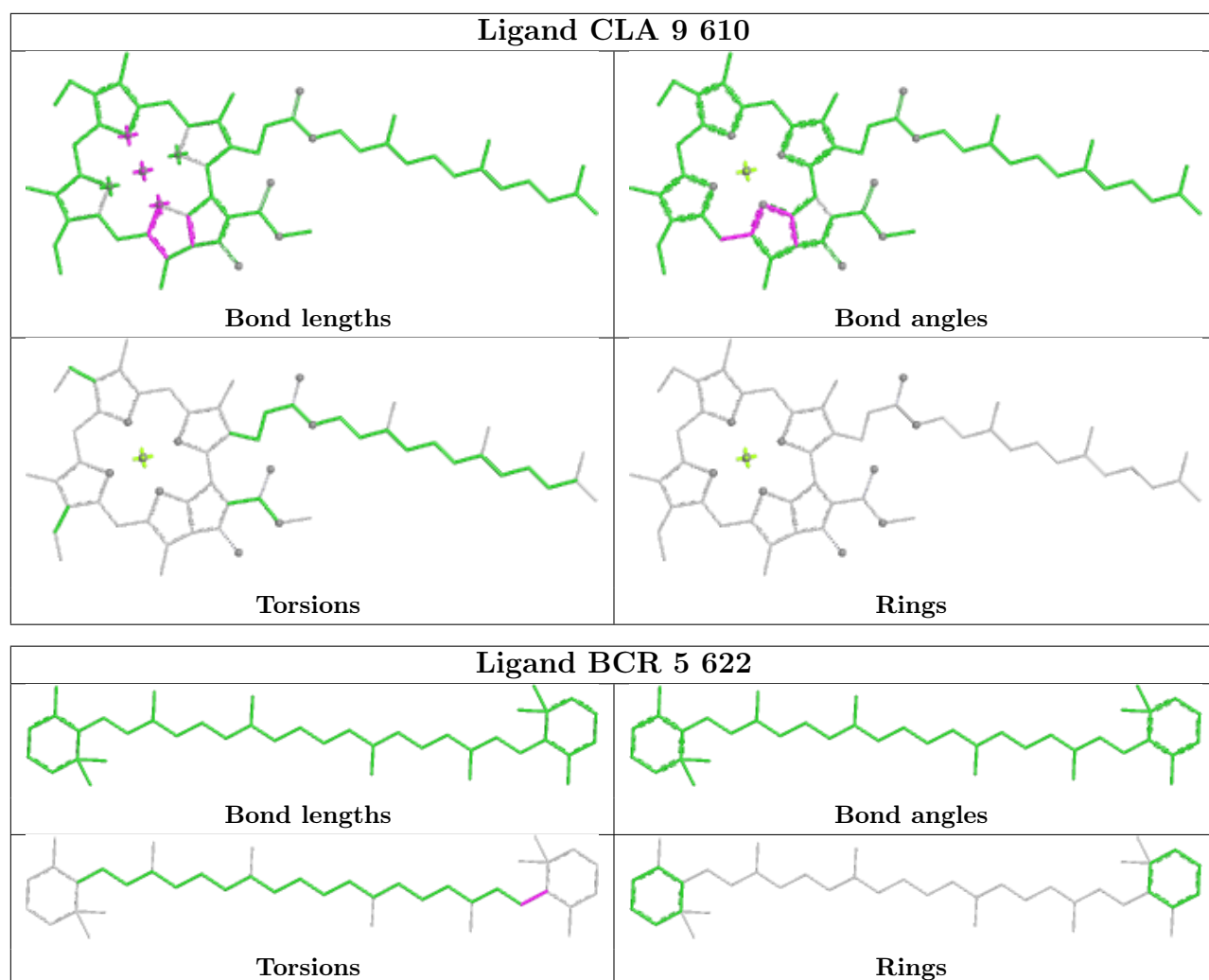
Torsions



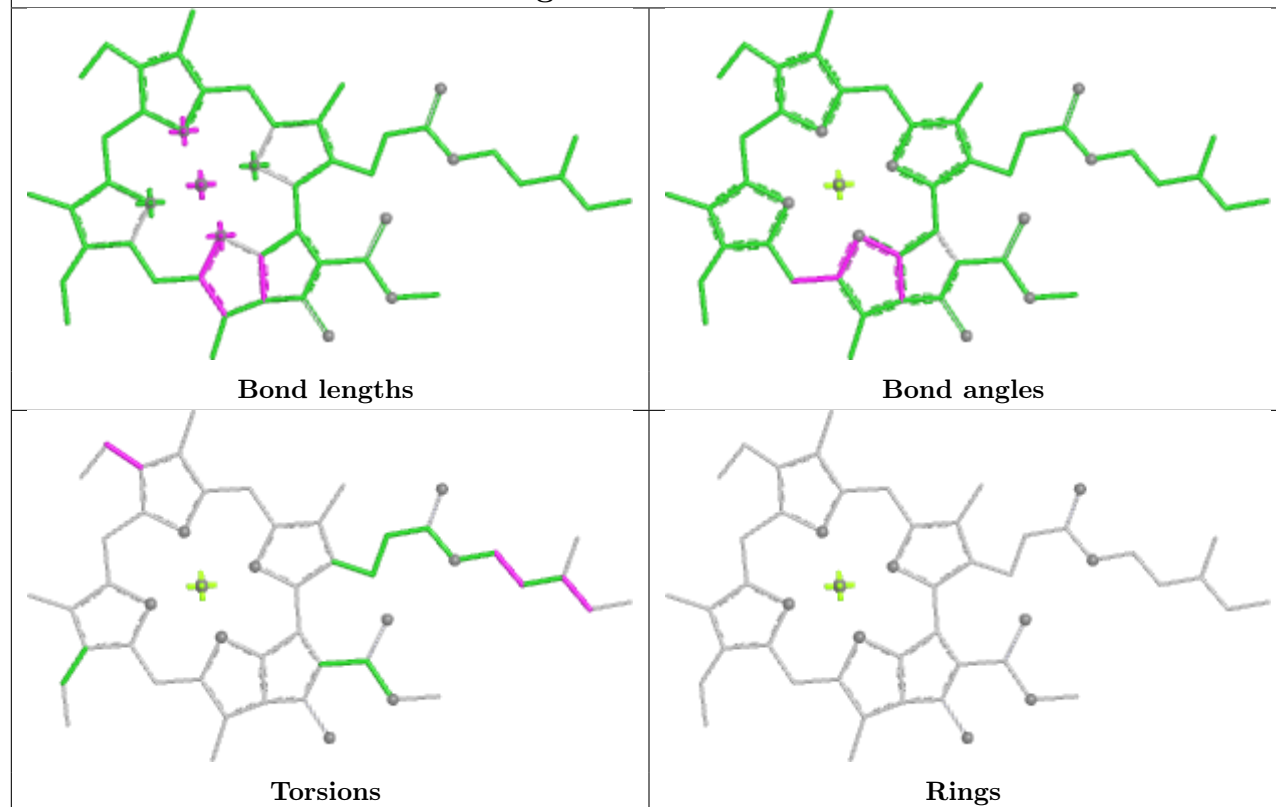
Rings



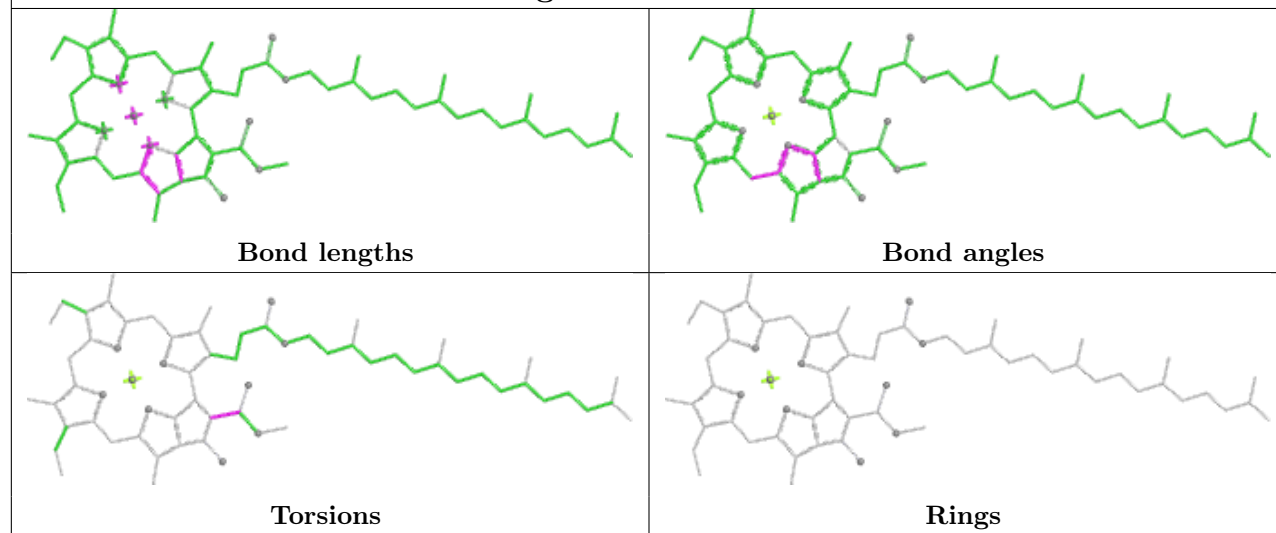


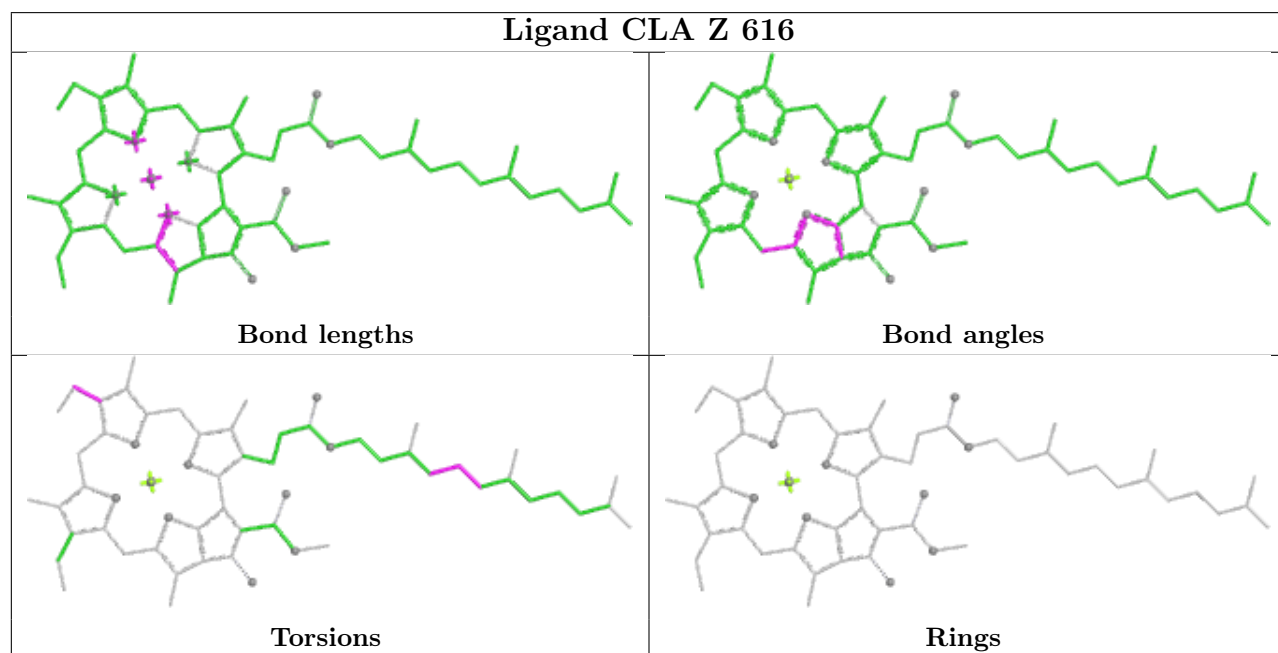
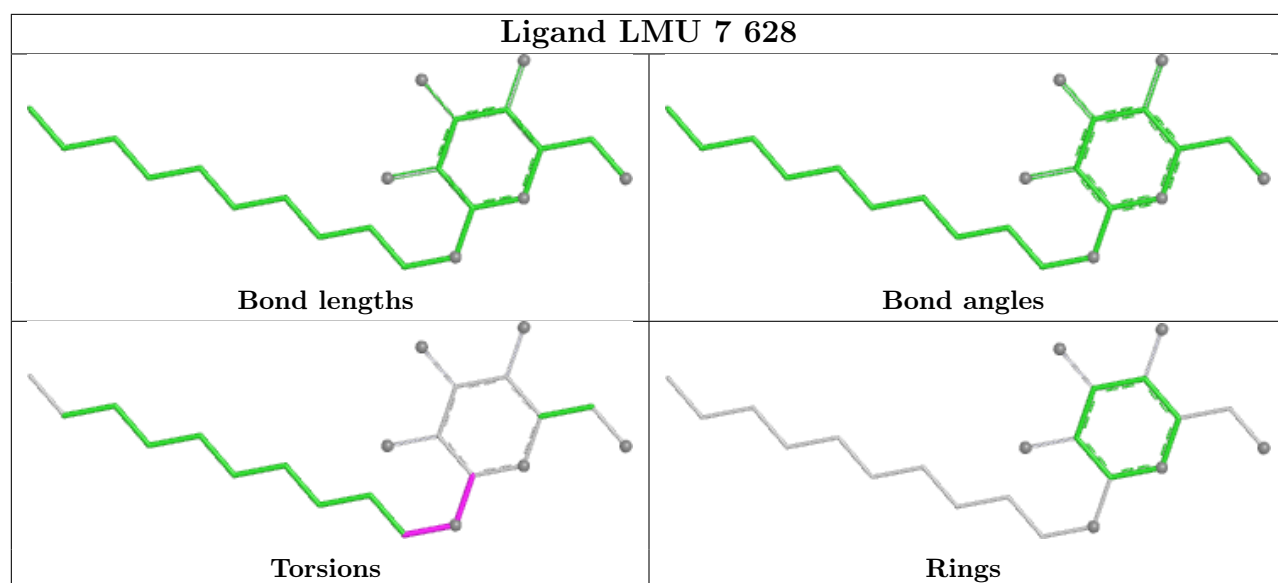


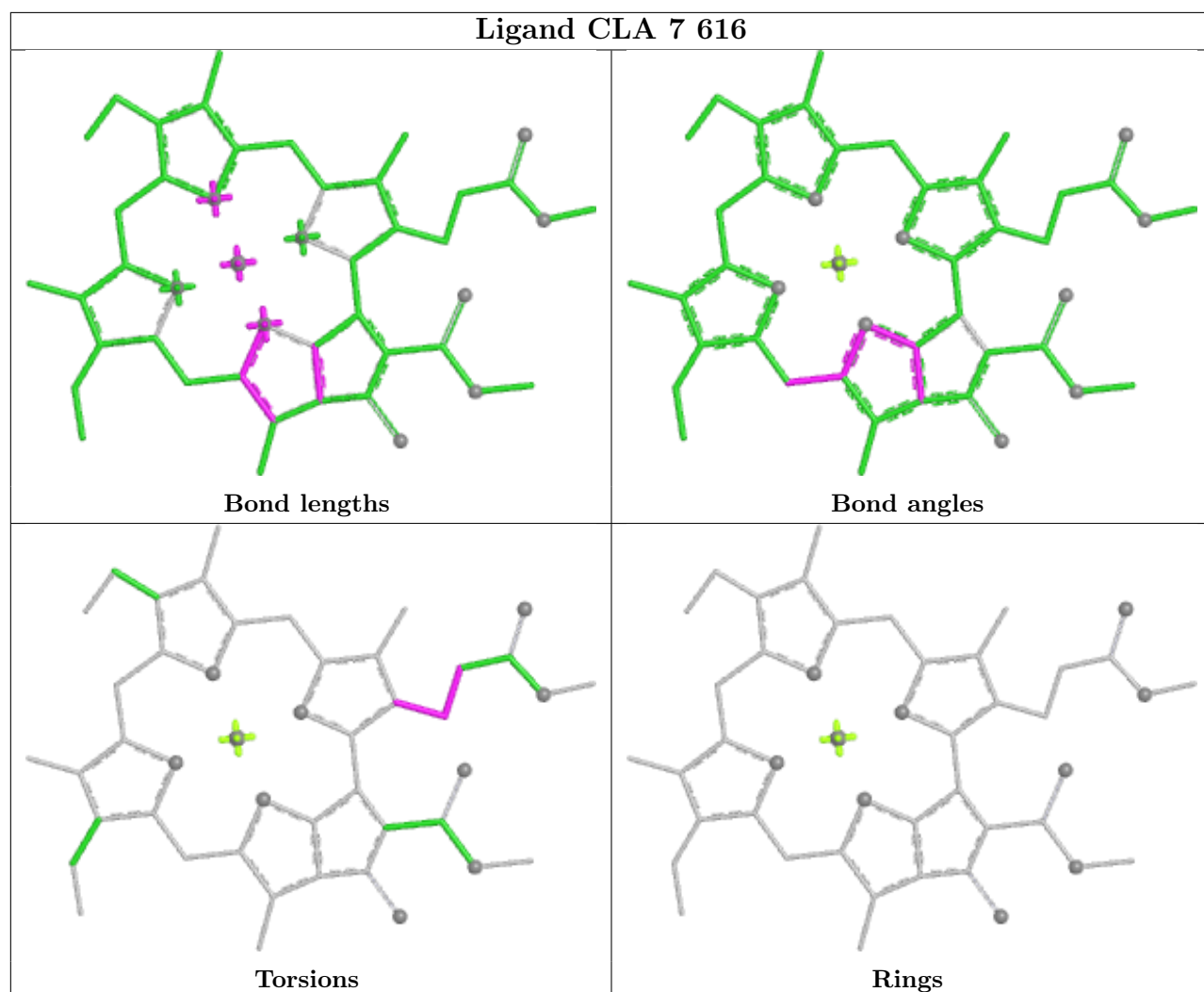
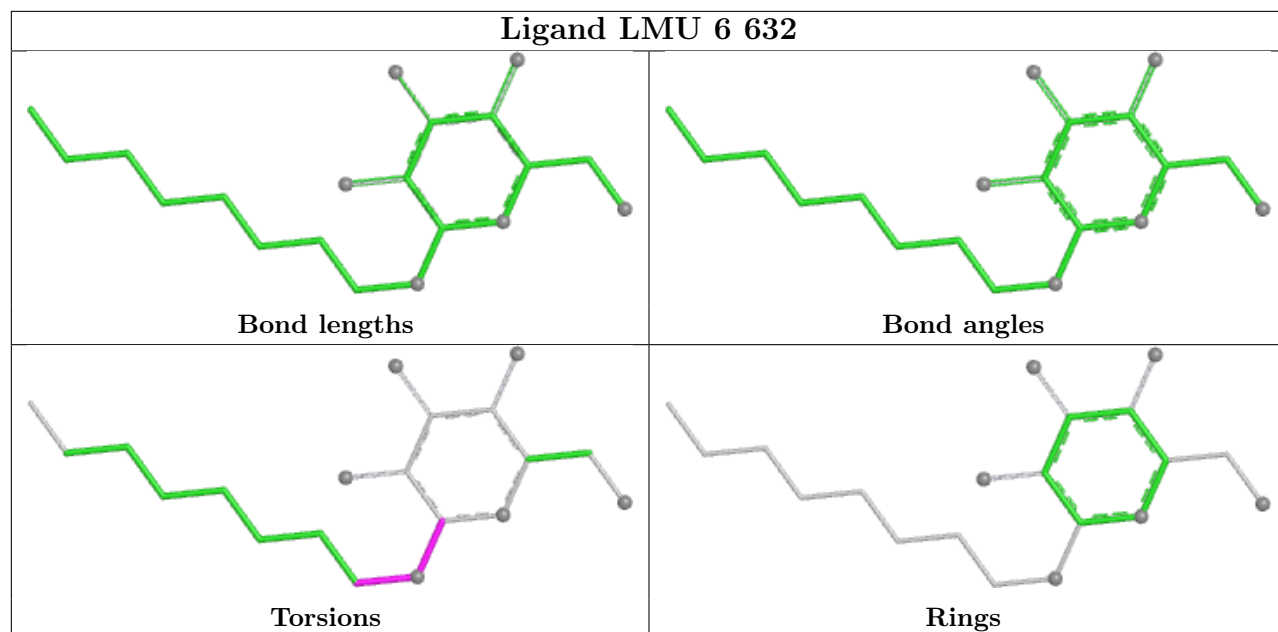
Ligand CLA 9 609

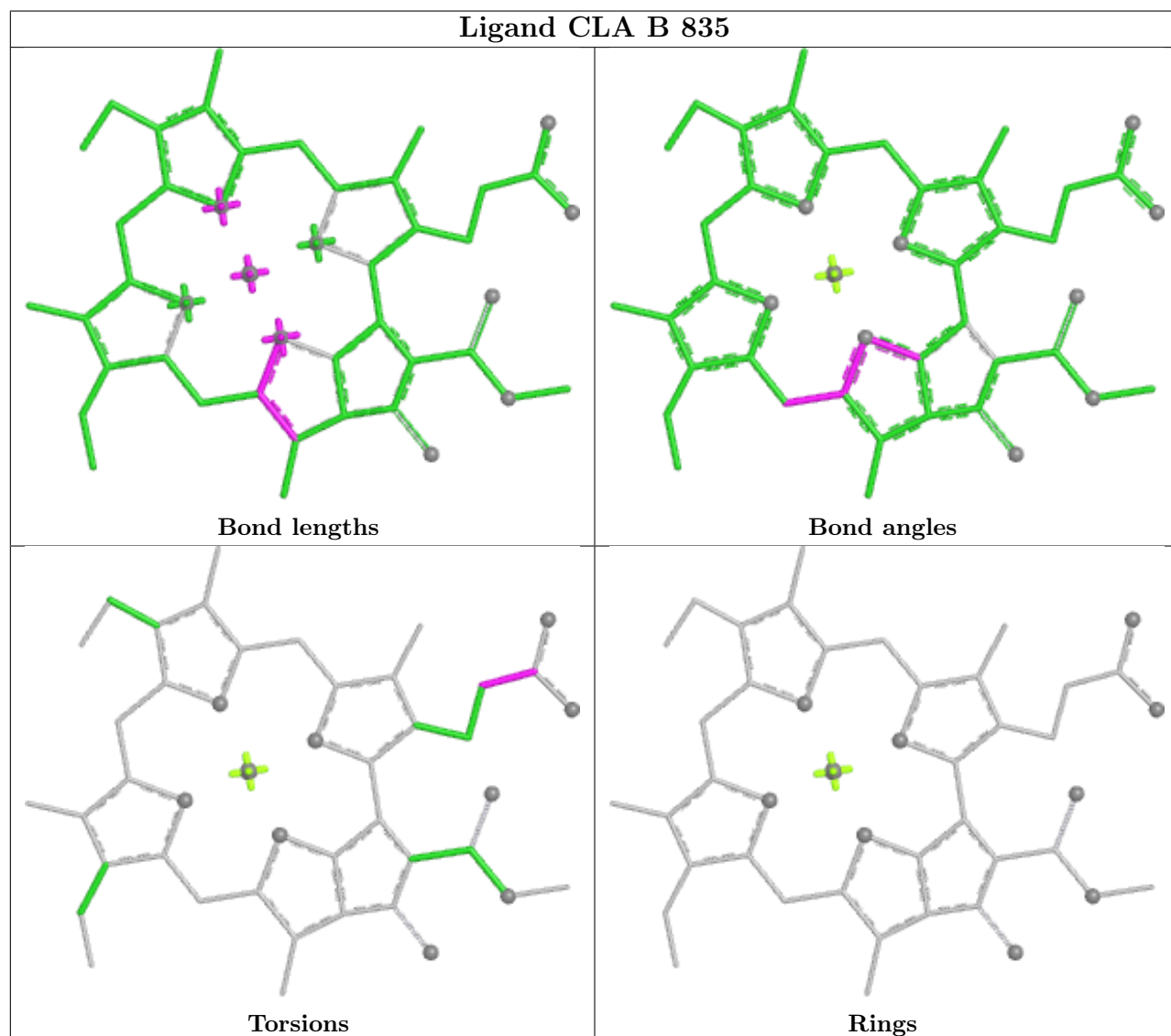
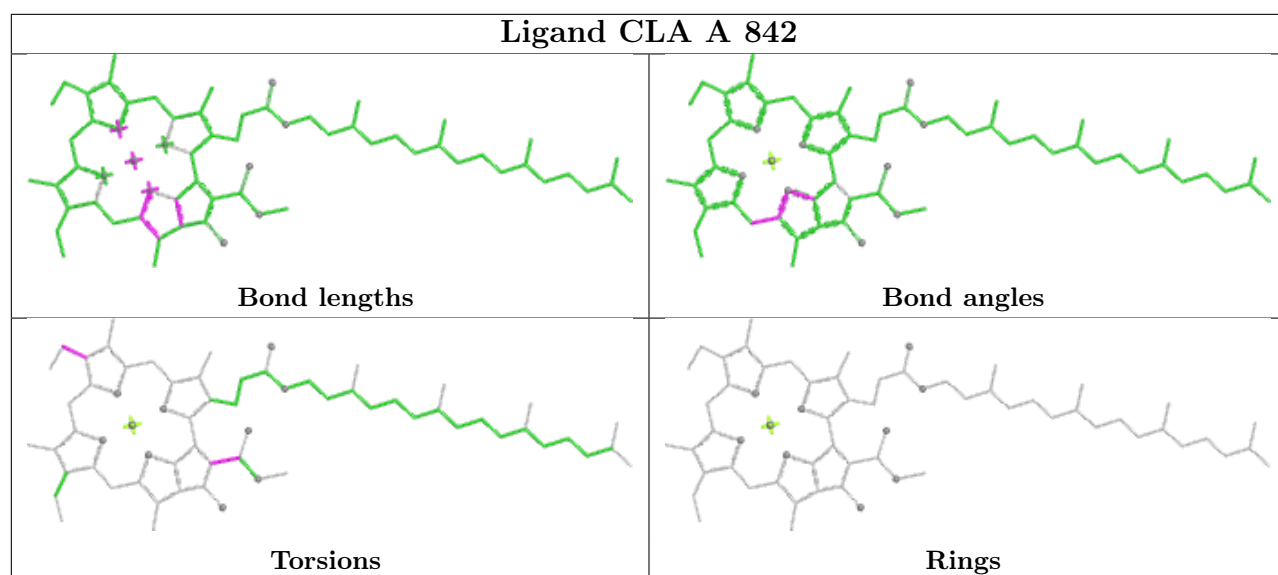


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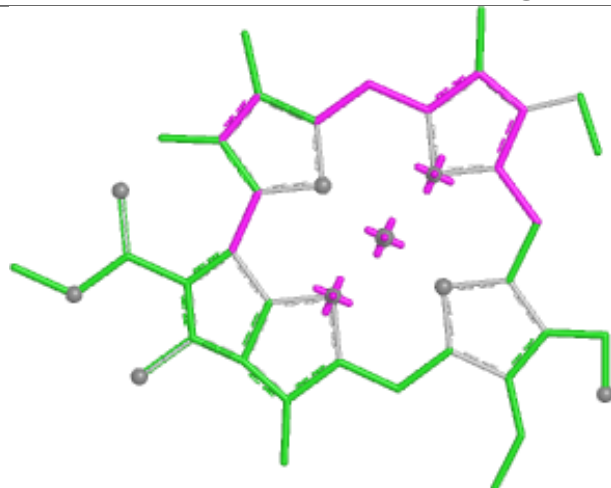




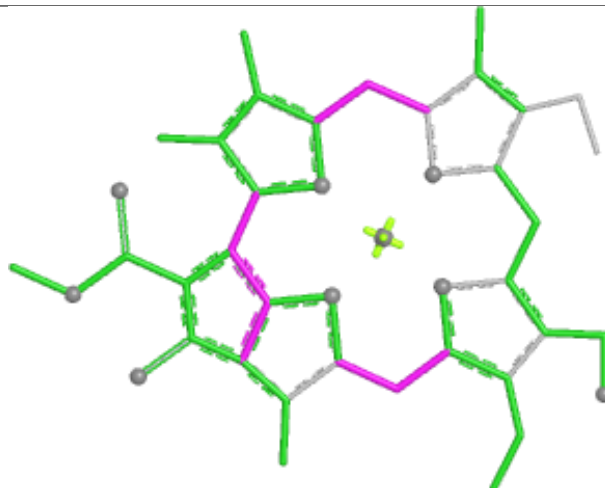




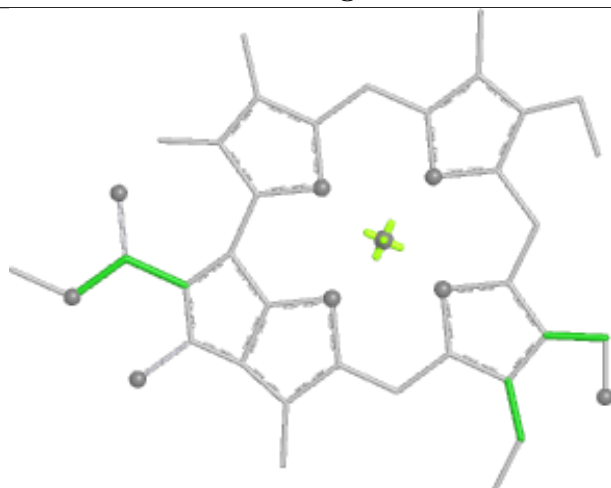
Ligand CHL 9 606



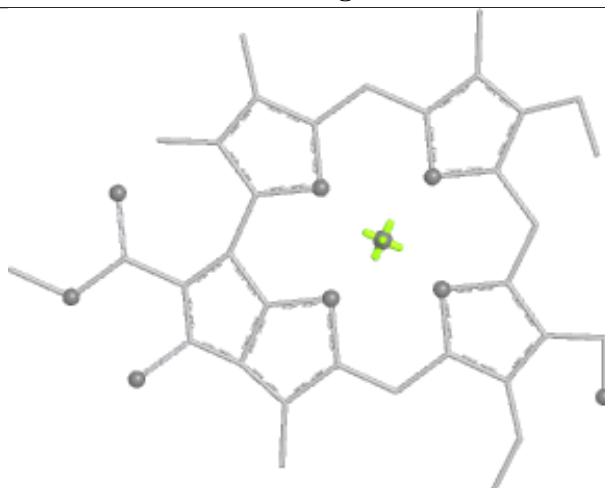
Bond lengths



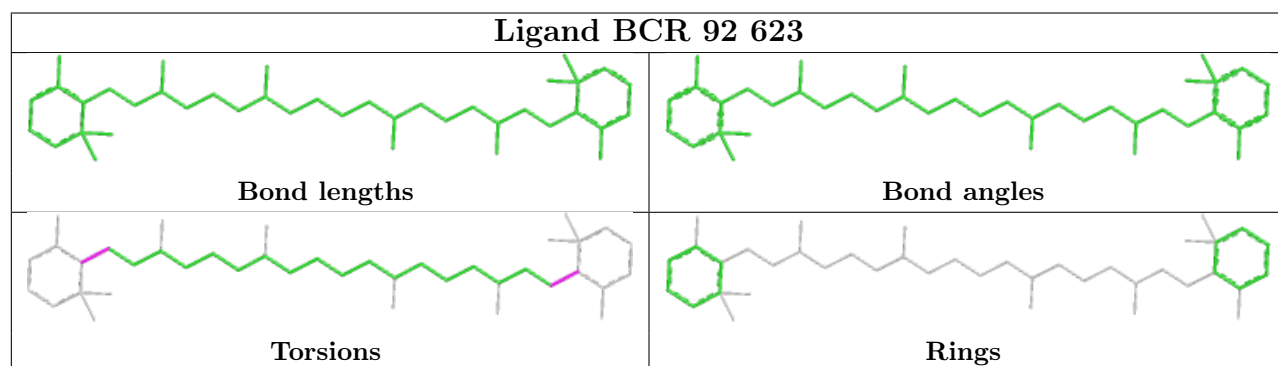
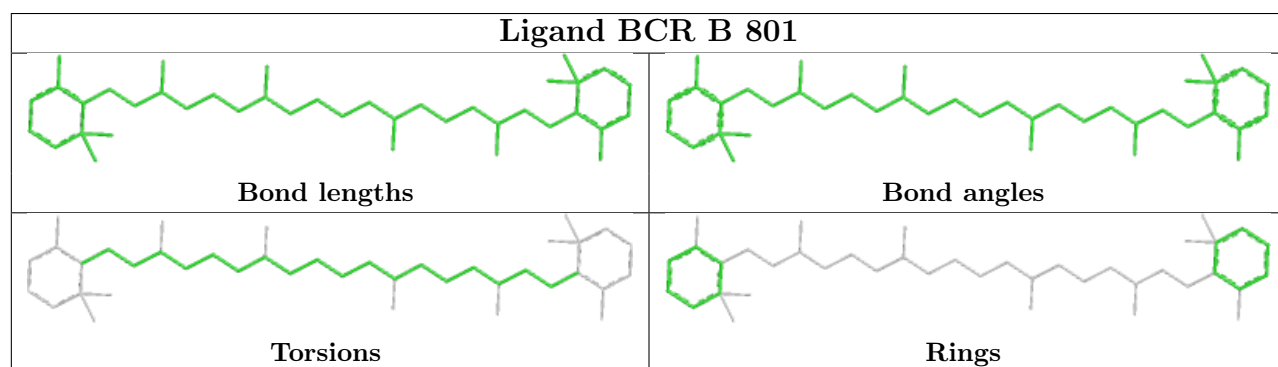
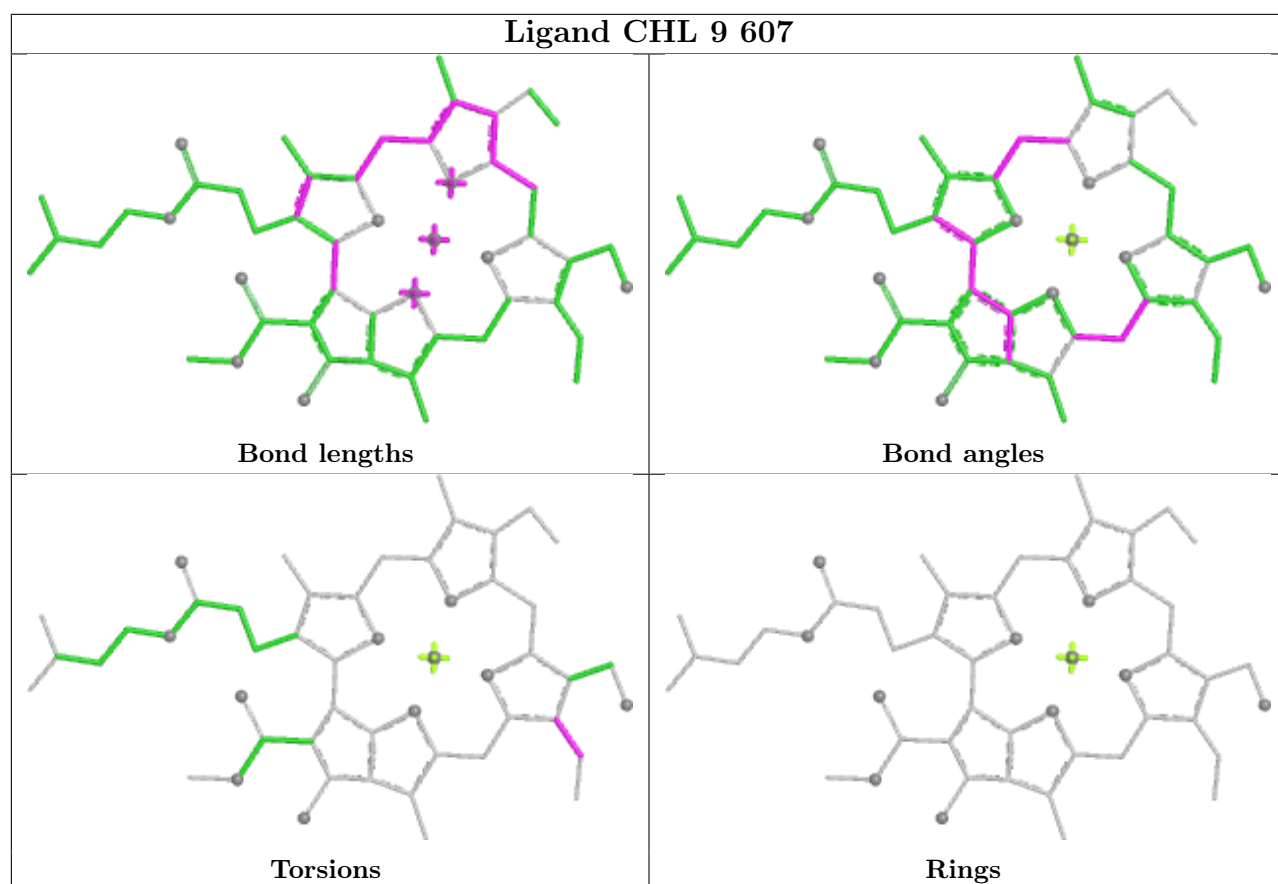
Bond angles

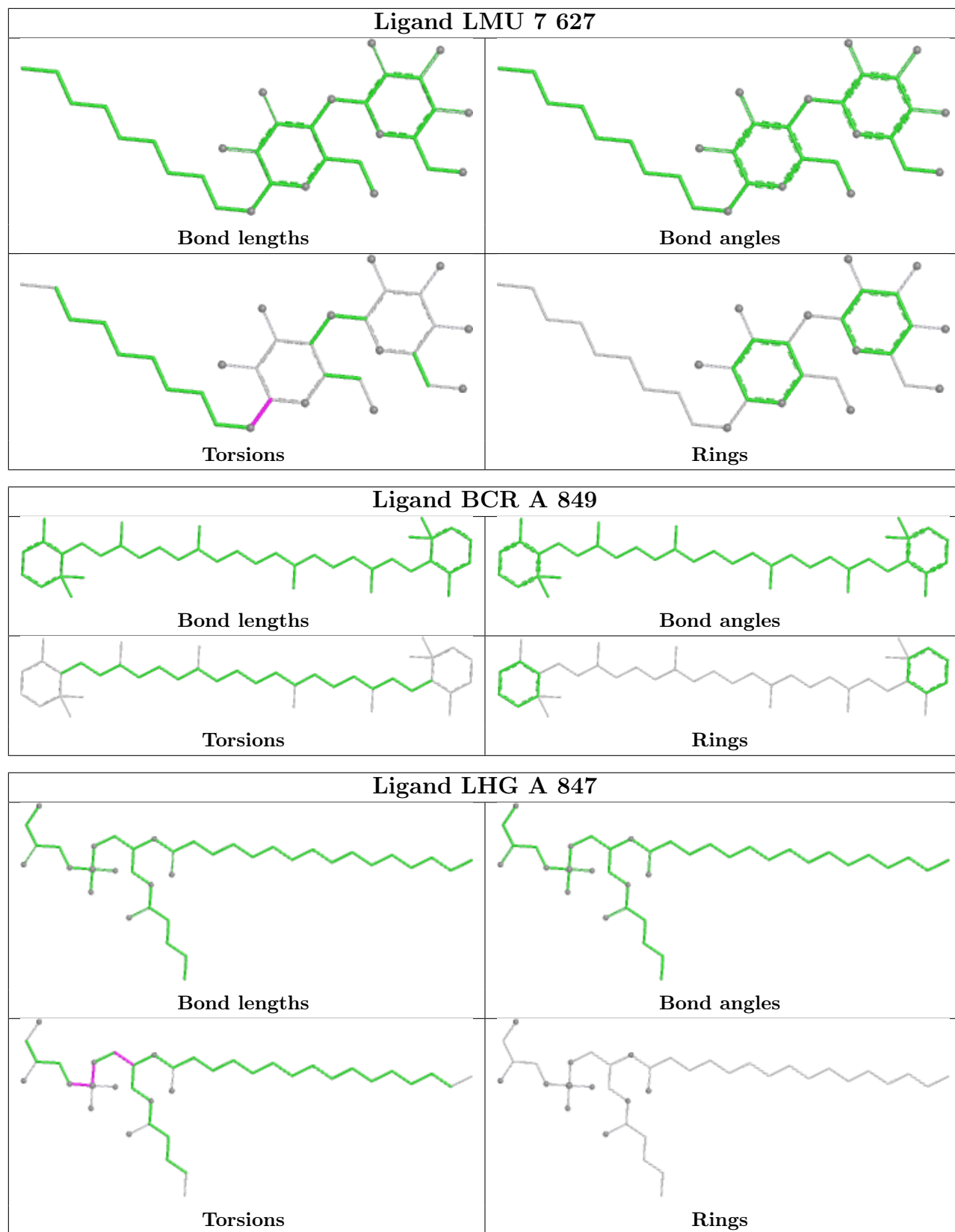


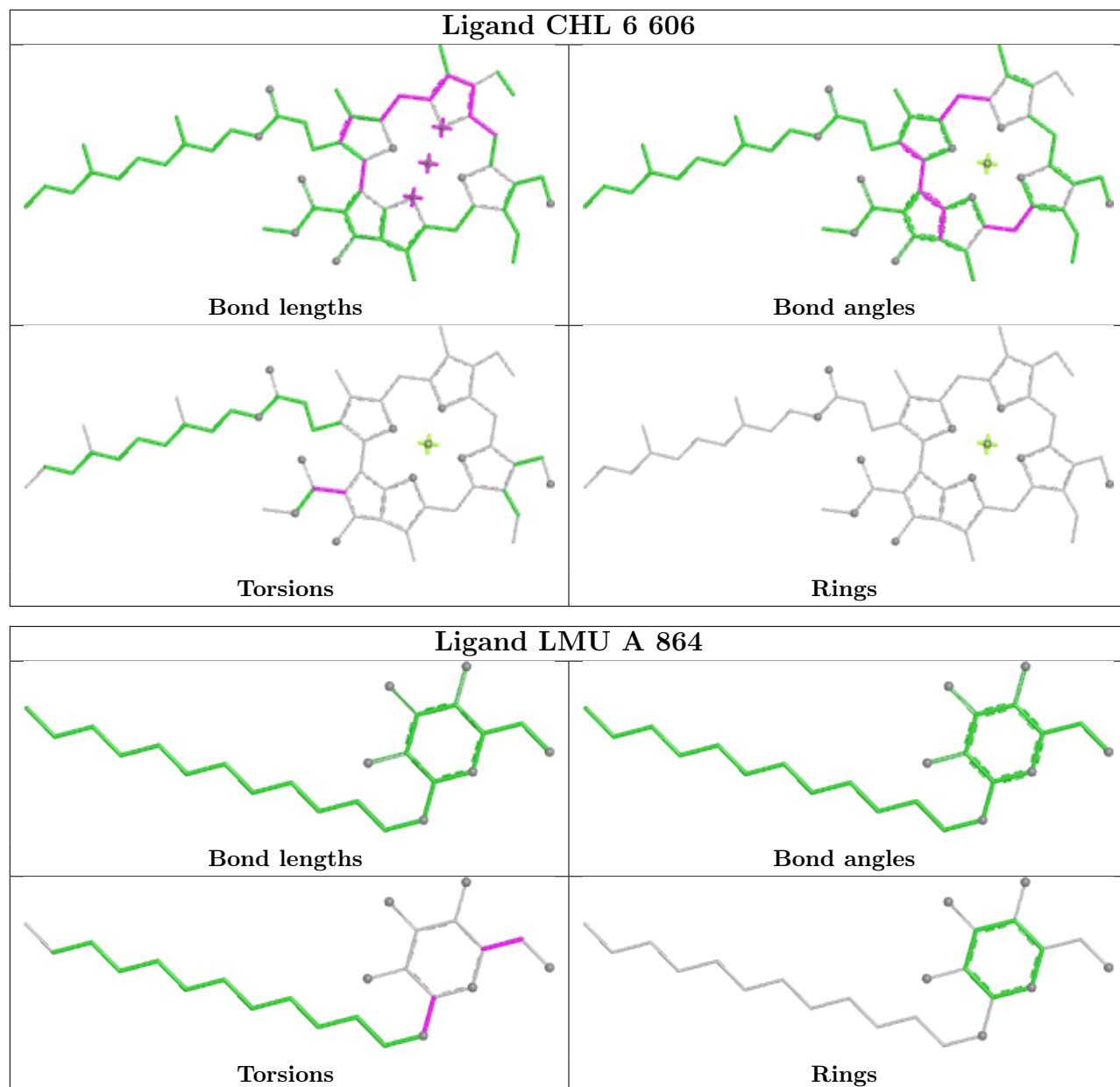
Torsions



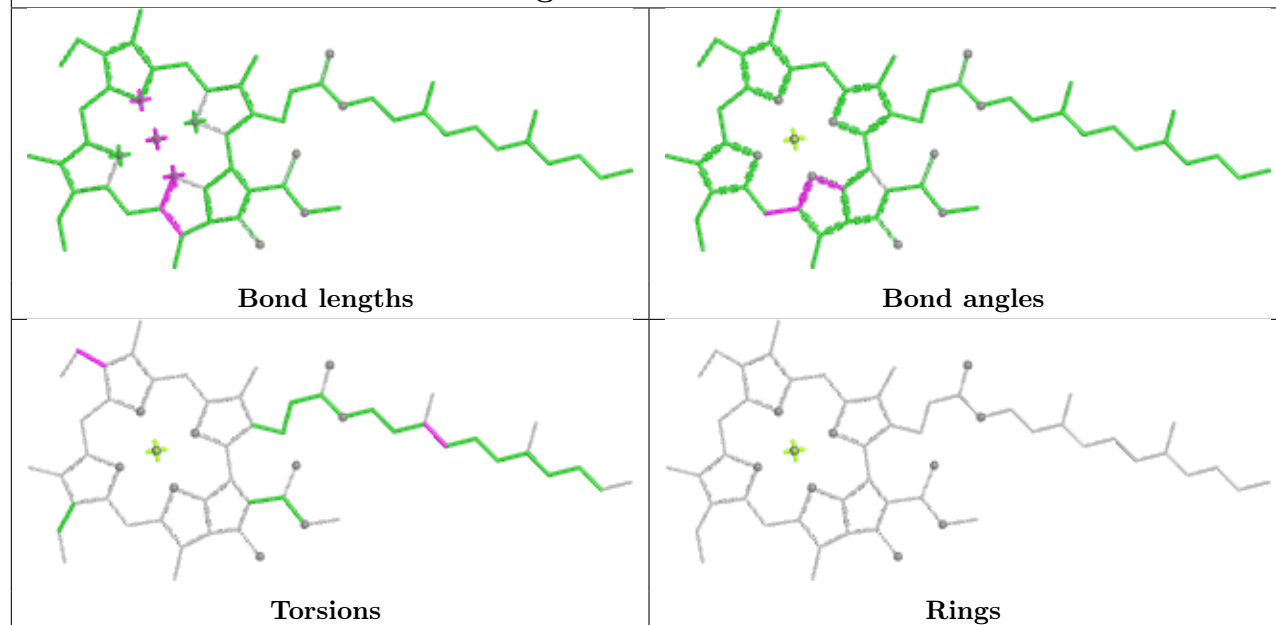
Rings



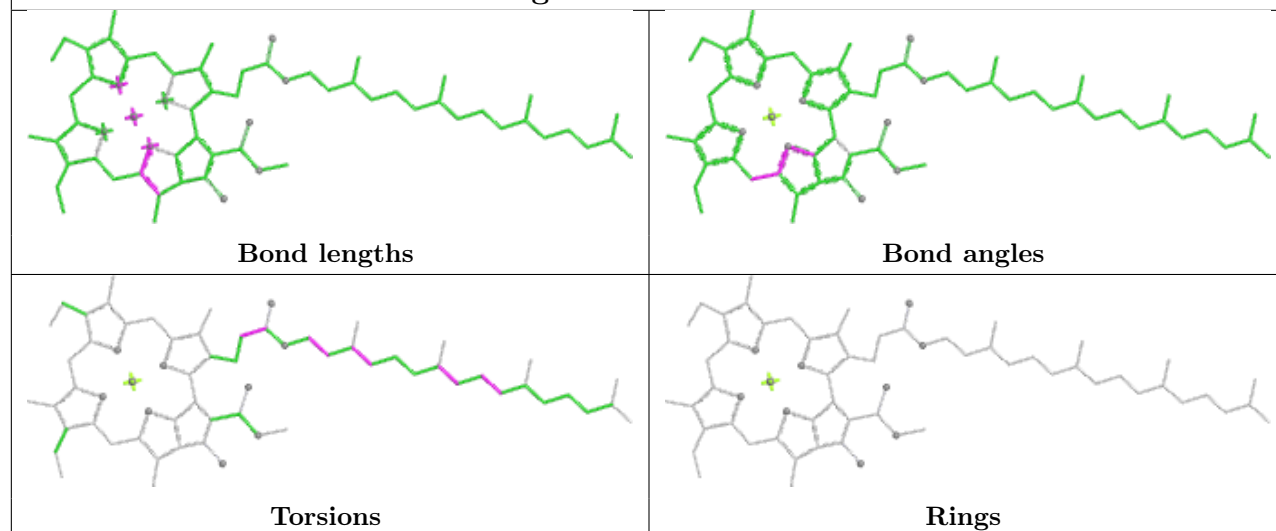


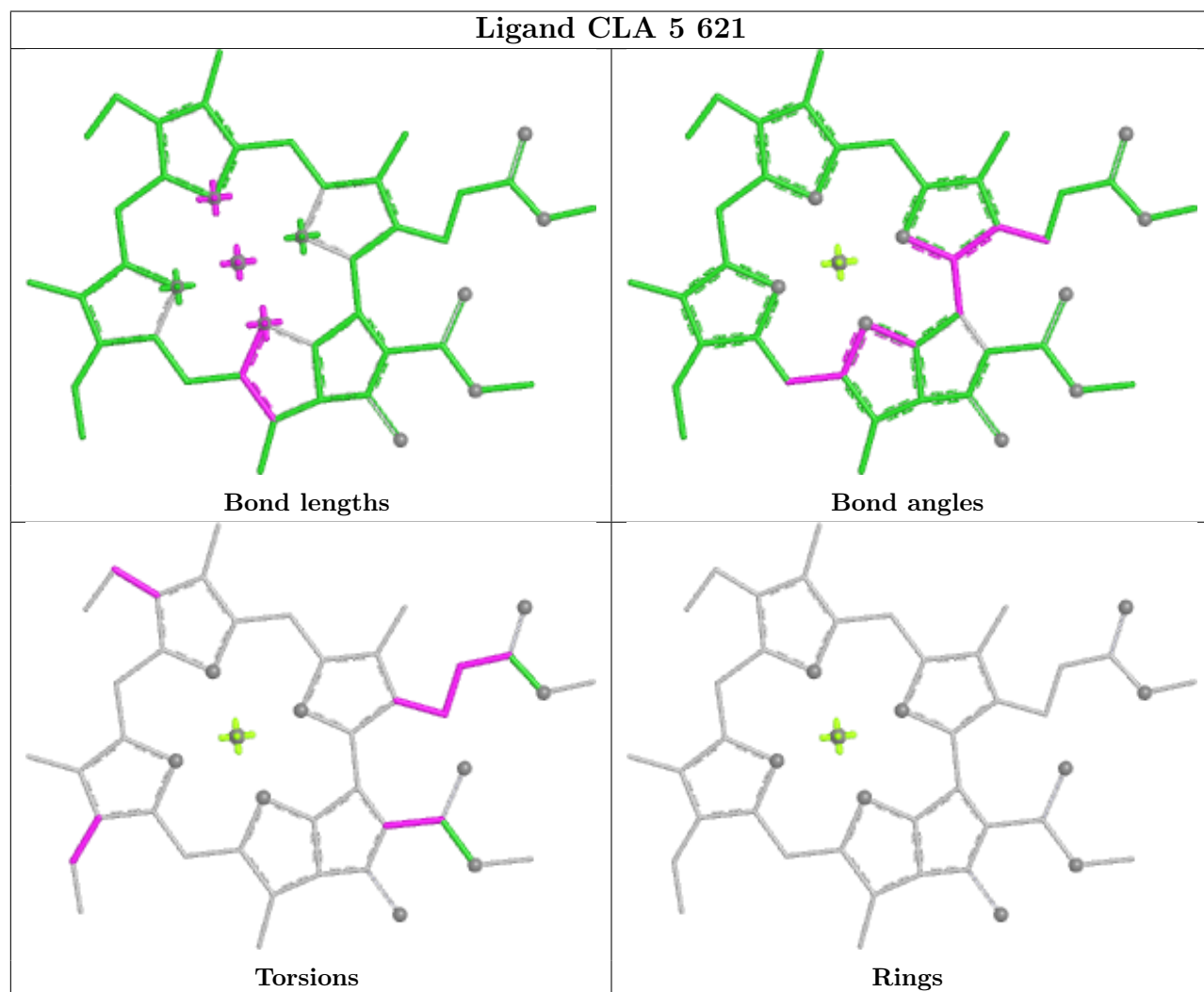
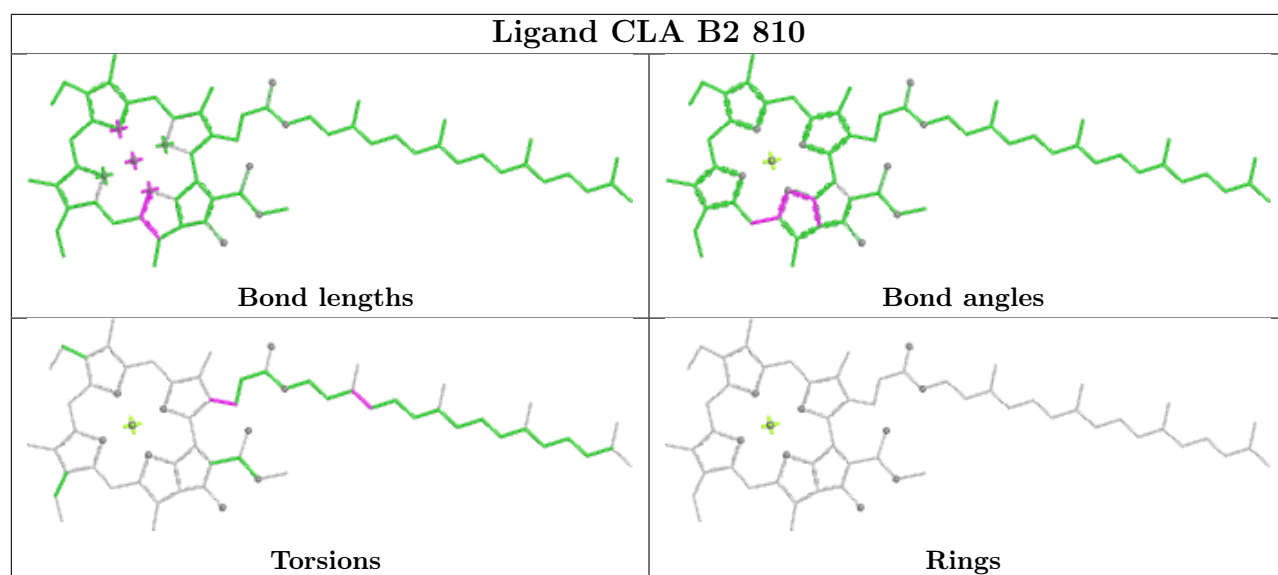


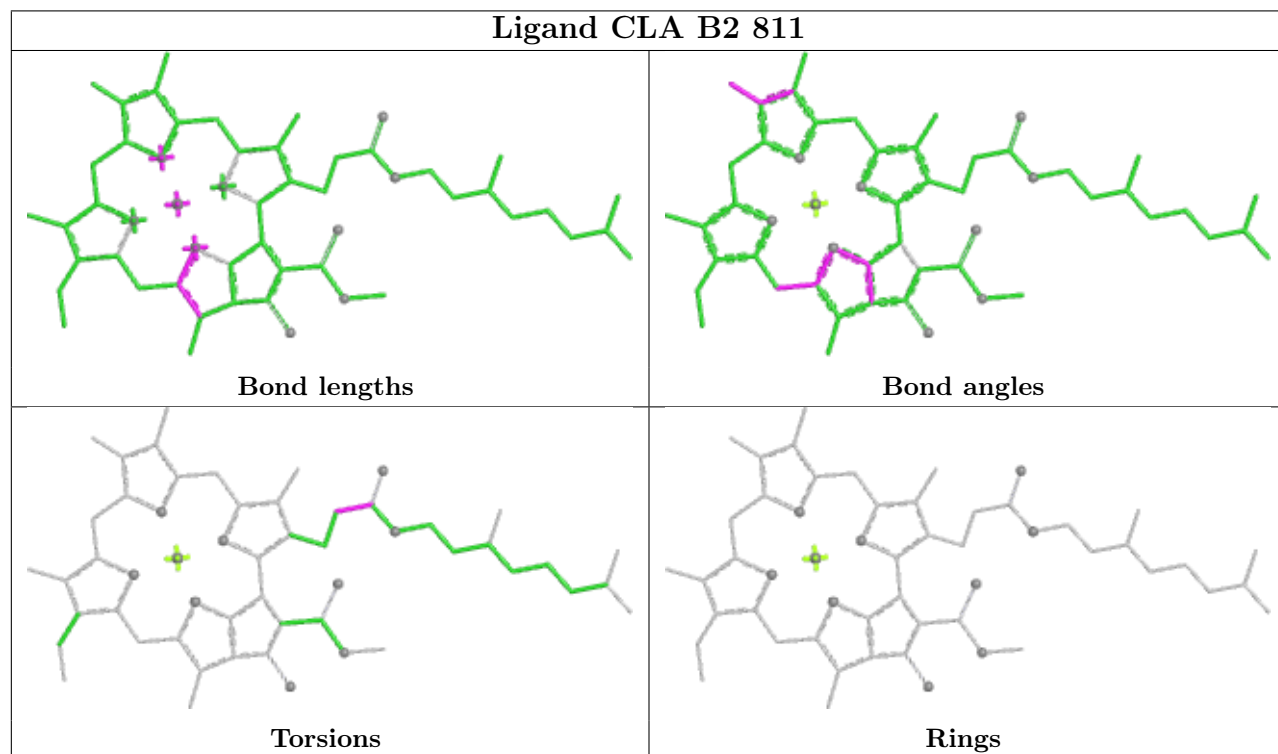
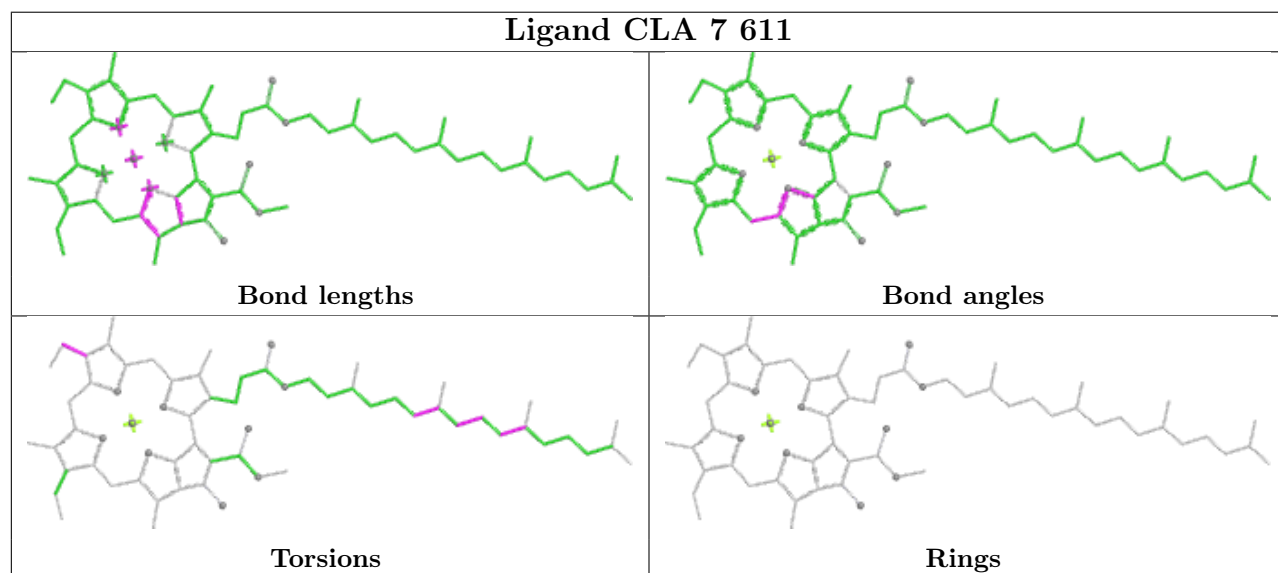
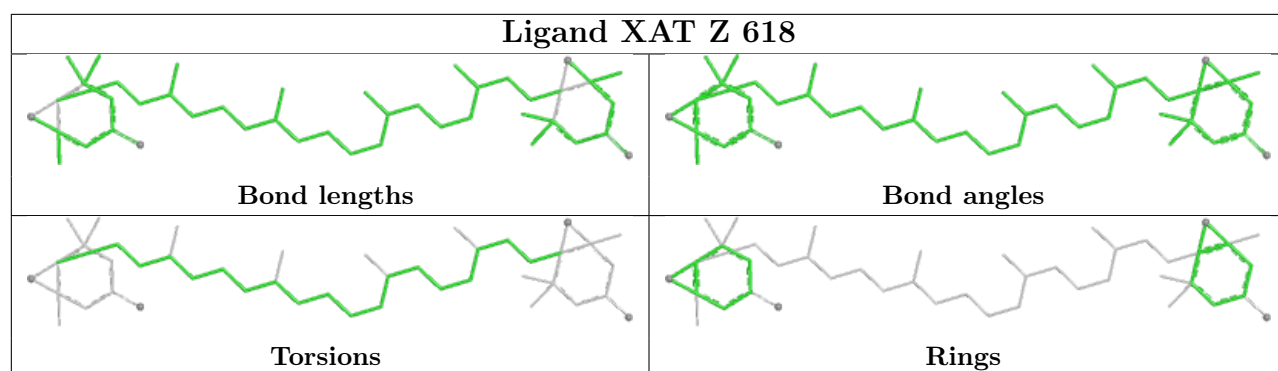
Ligand CLA 6 611

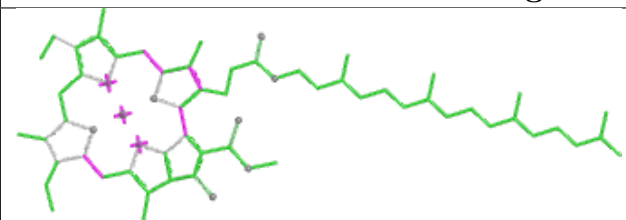
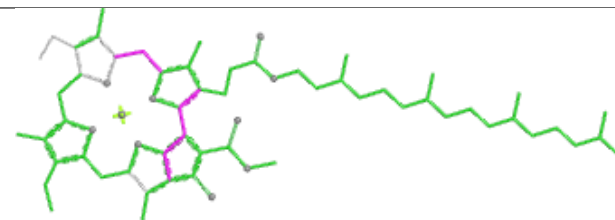
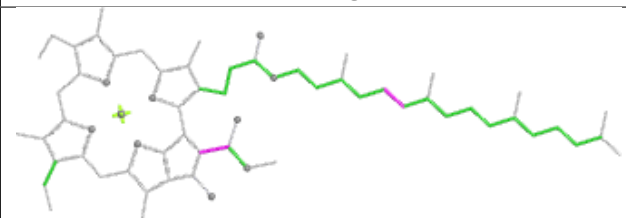
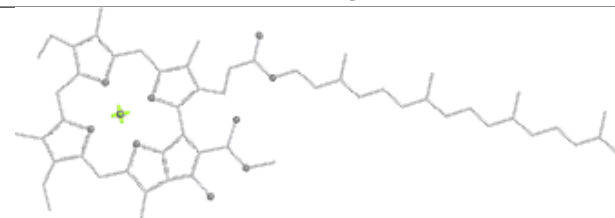


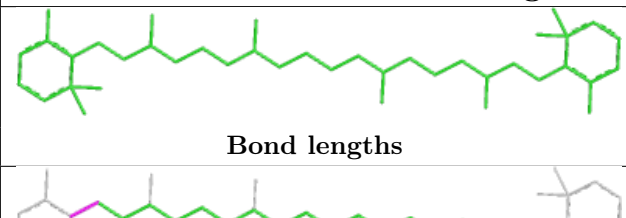
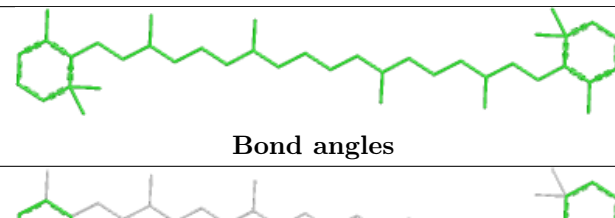
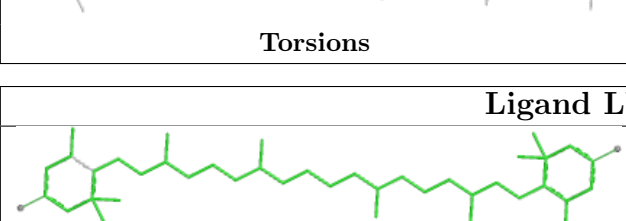
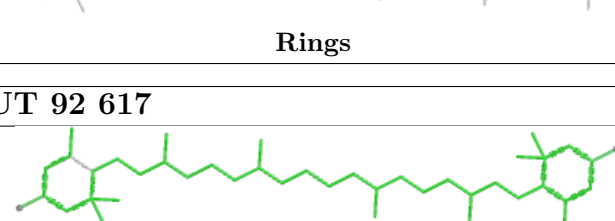
Ligand CLA A 826

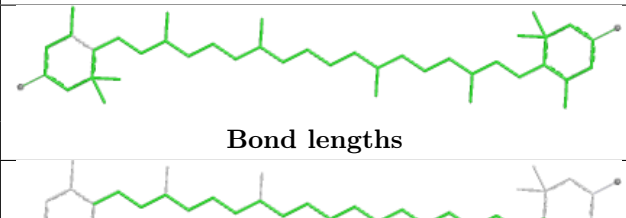
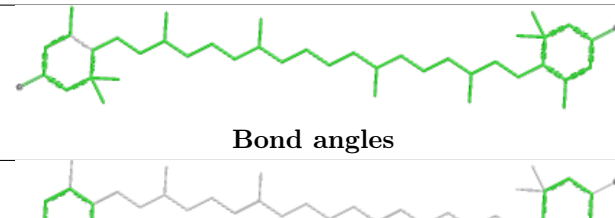
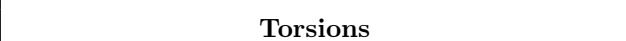


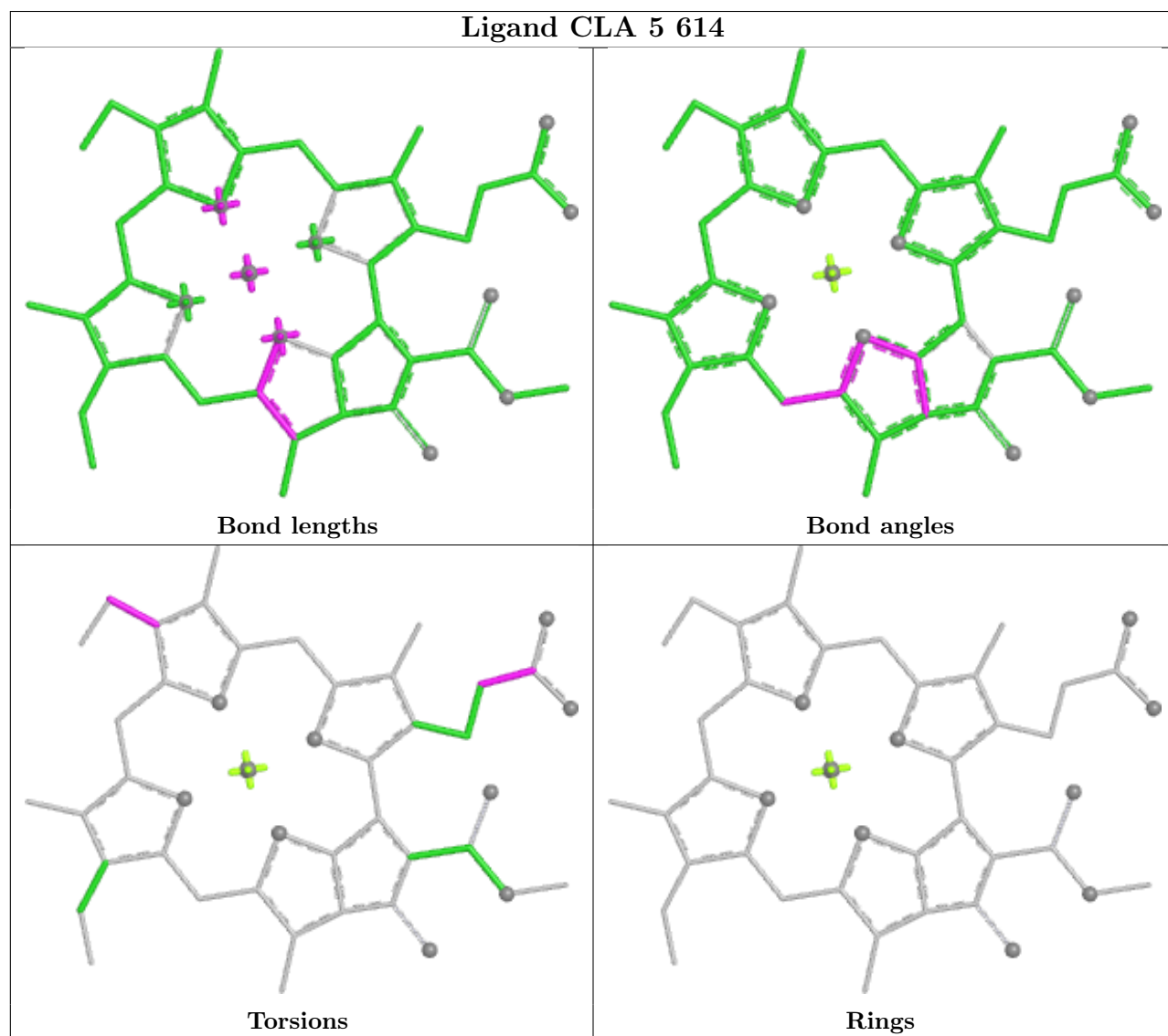
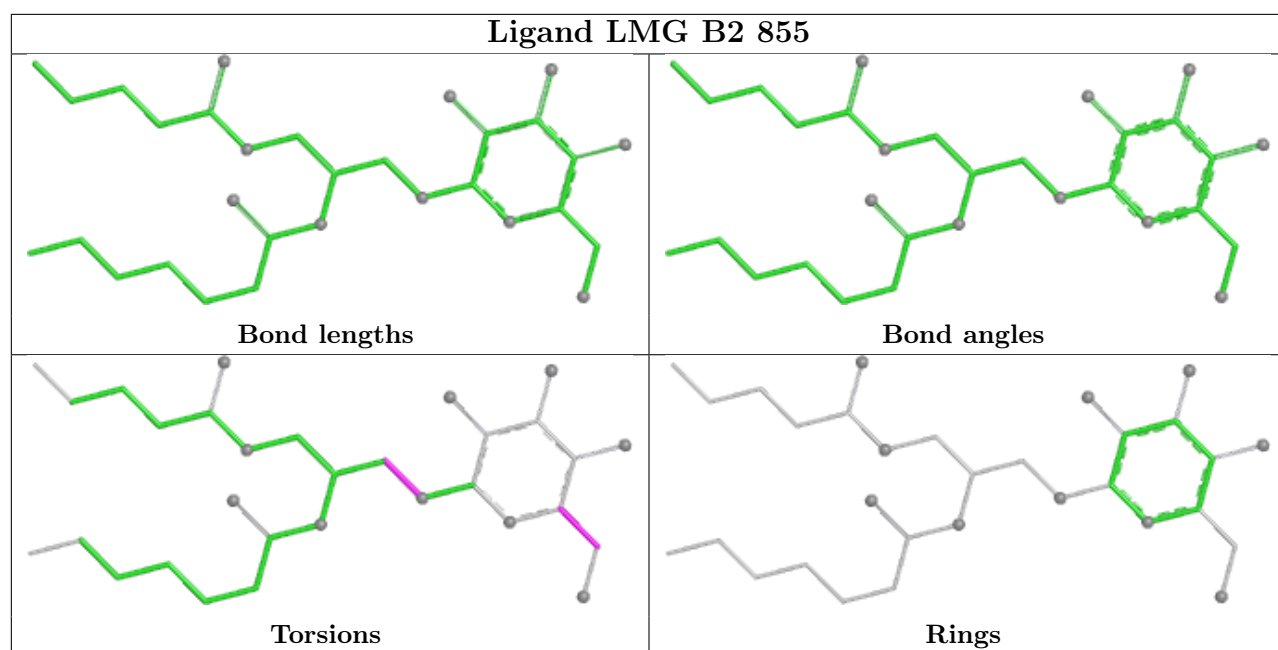


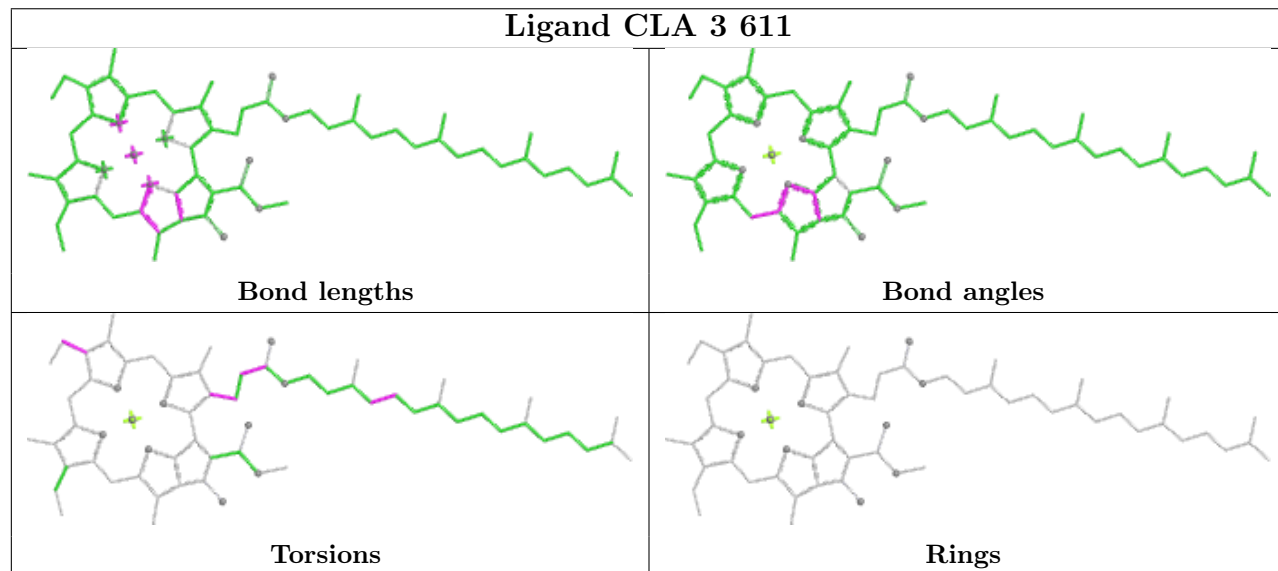
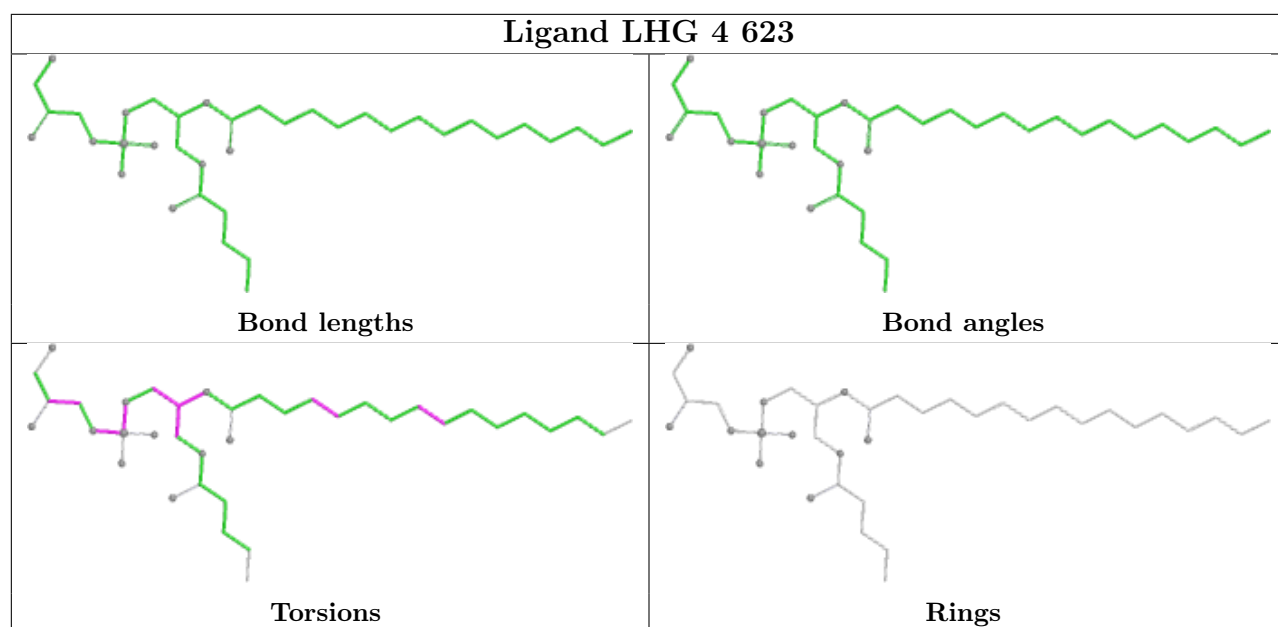


Ligand CL0 A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

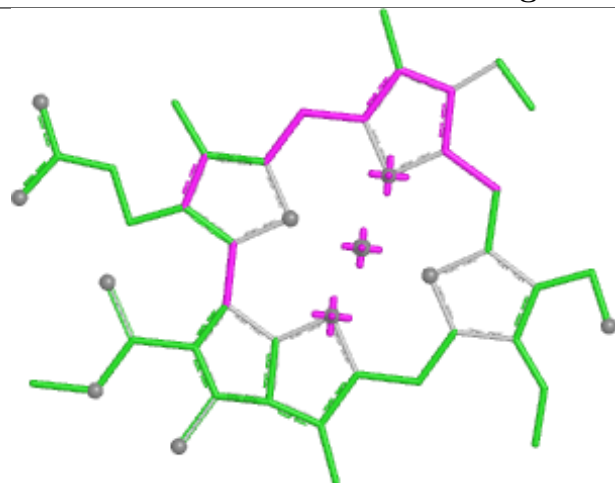
Ligand BCR 3 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 92 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

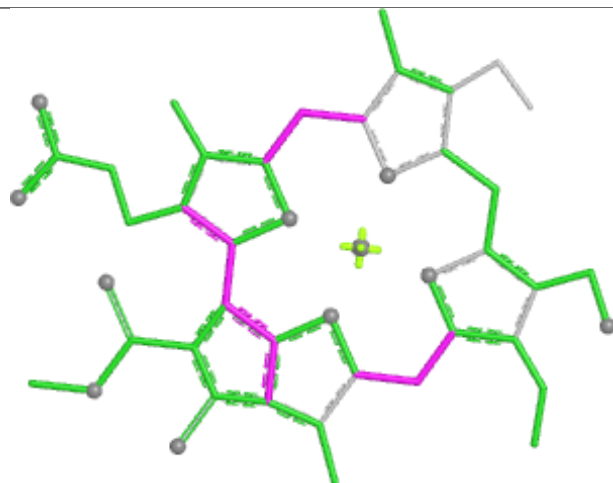




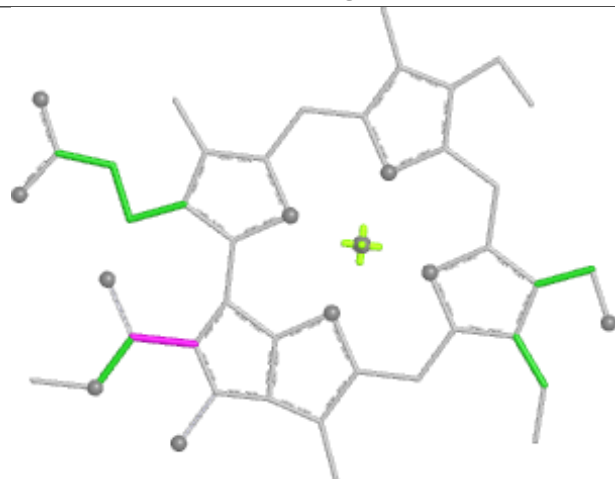
Ligand CHL 5 606



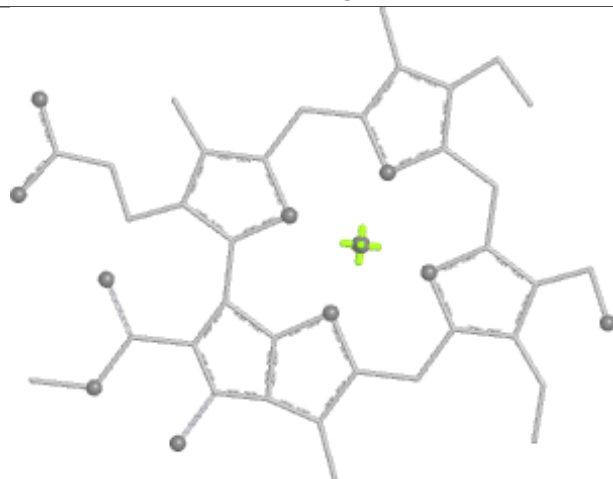
Bond lengths



Bond angles



Torsions



Rings

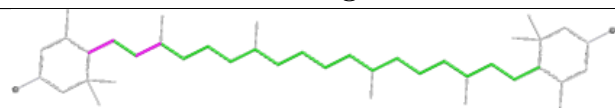
Ligand LUT 7 624



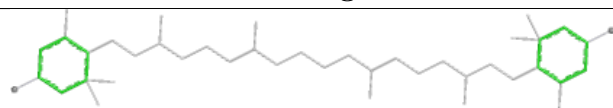
Bond lengths



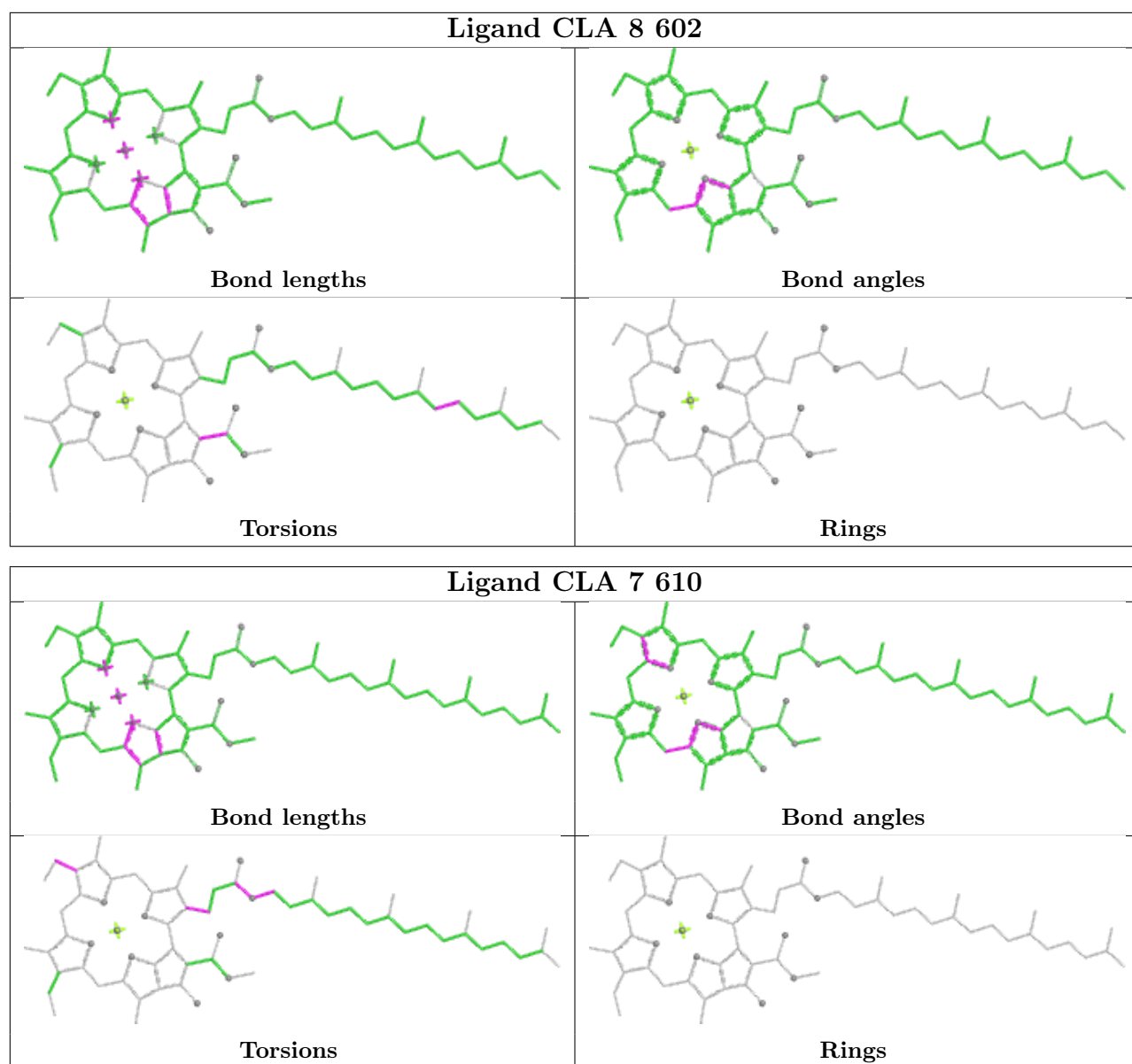
Bond angles



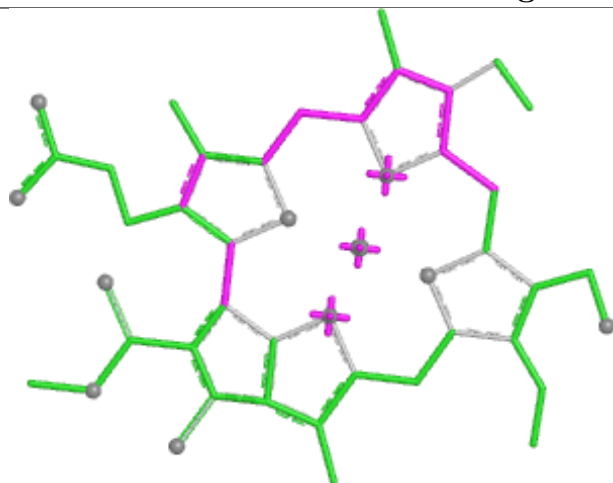
Torsions



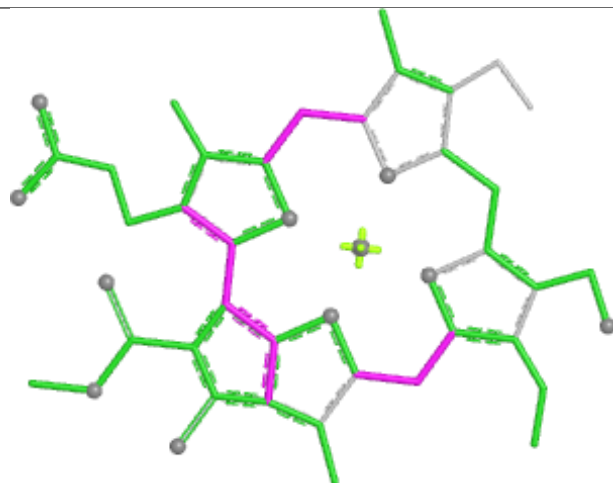
Rings



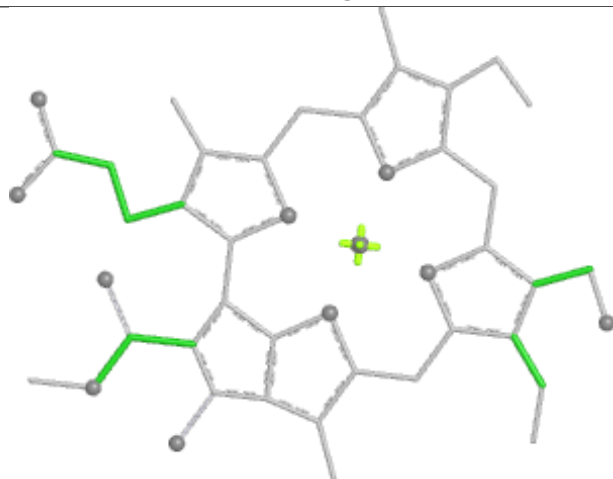
Ligand CHL 1 606



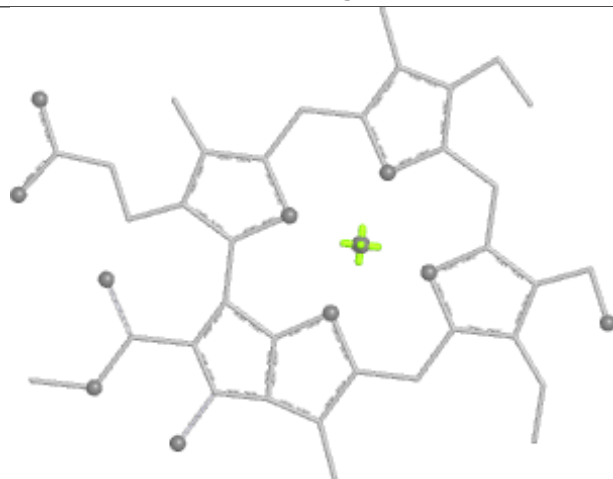
Bond lengths



Bond angles

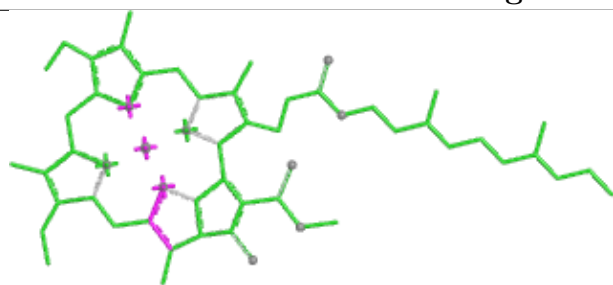


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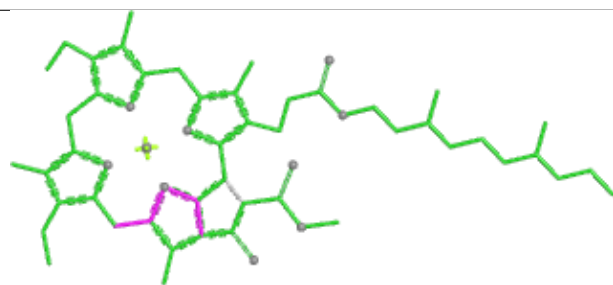


Rings

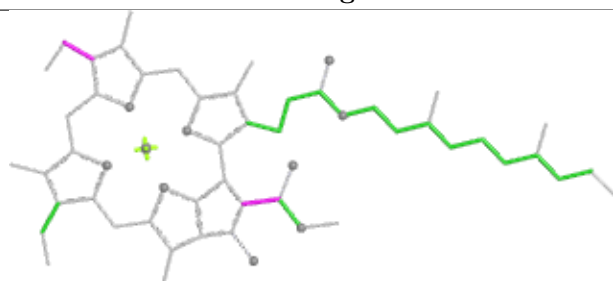
Ligand CLA B2 815



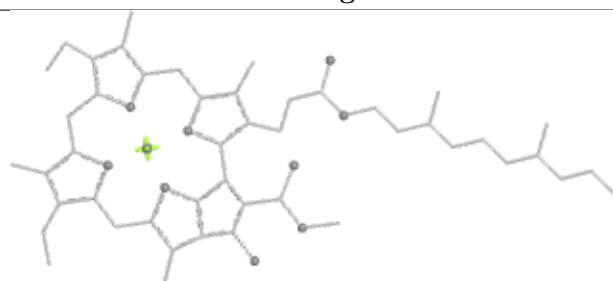
Bond lengths



Bond angles

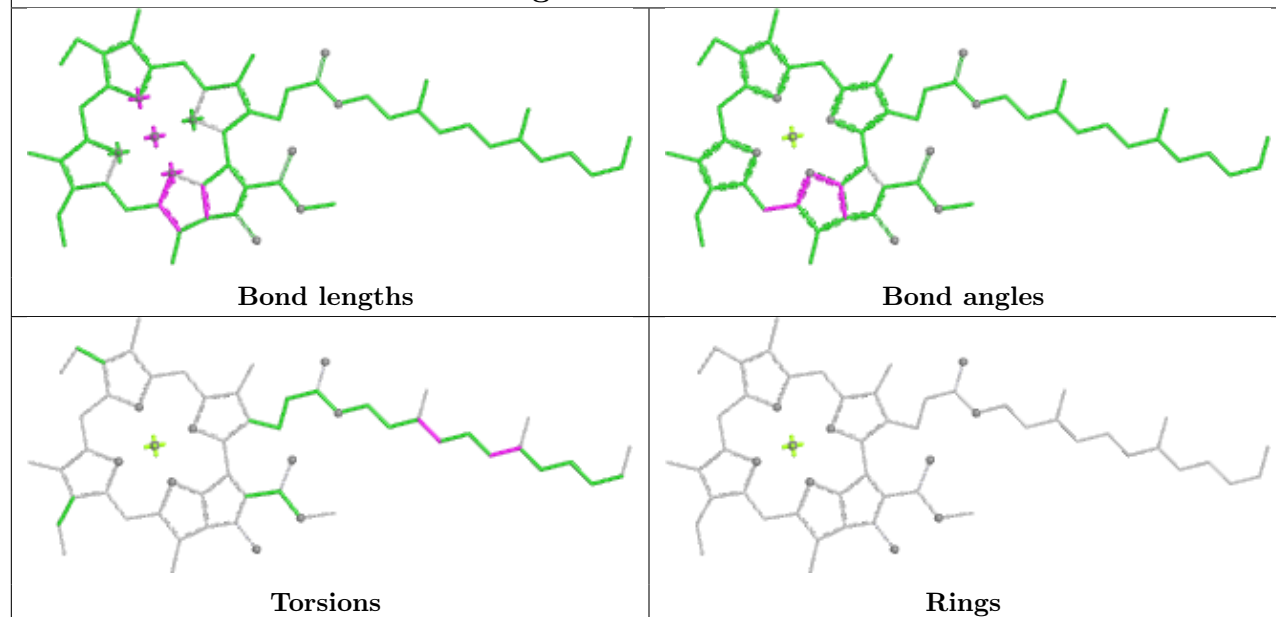


Torsions

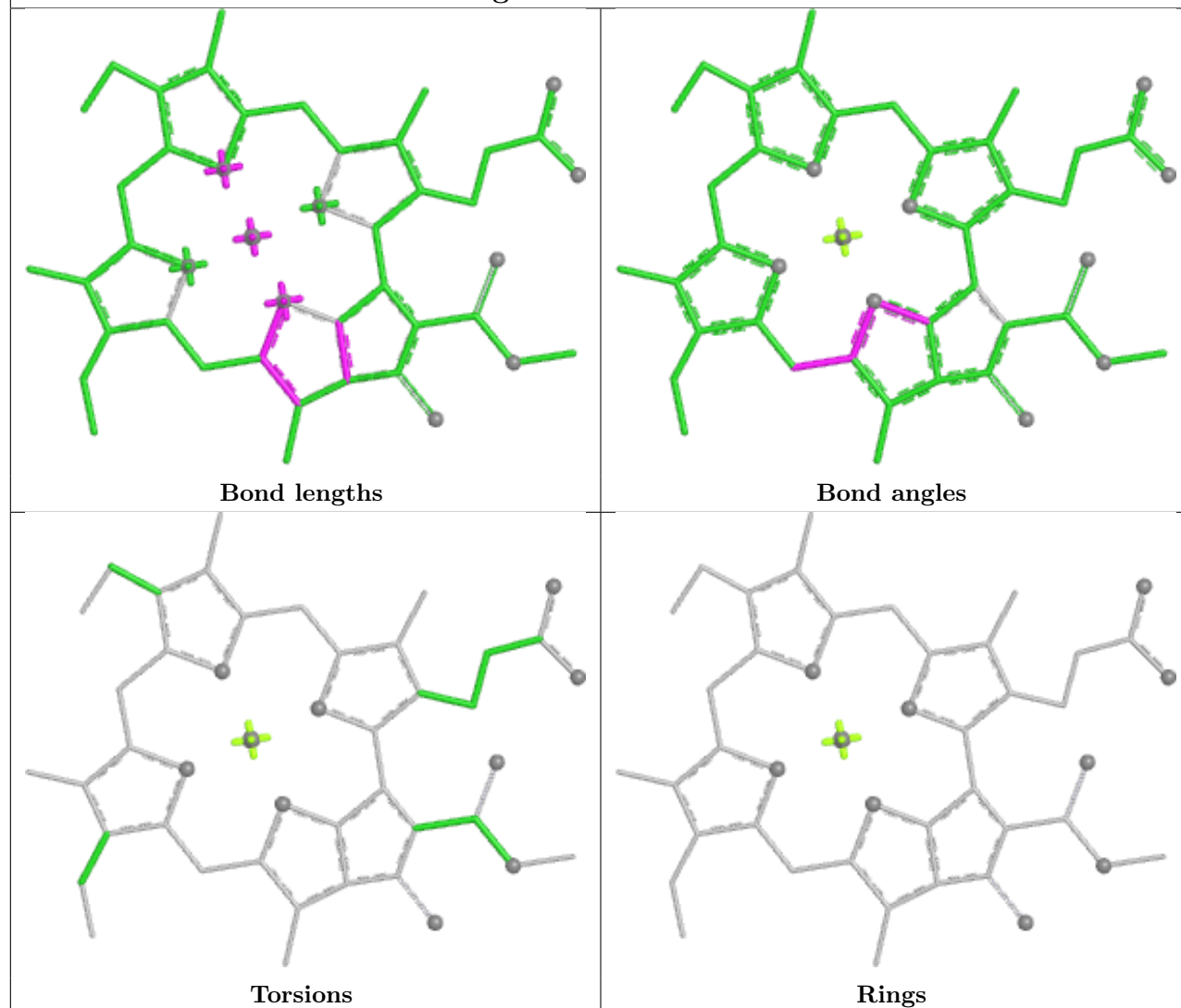


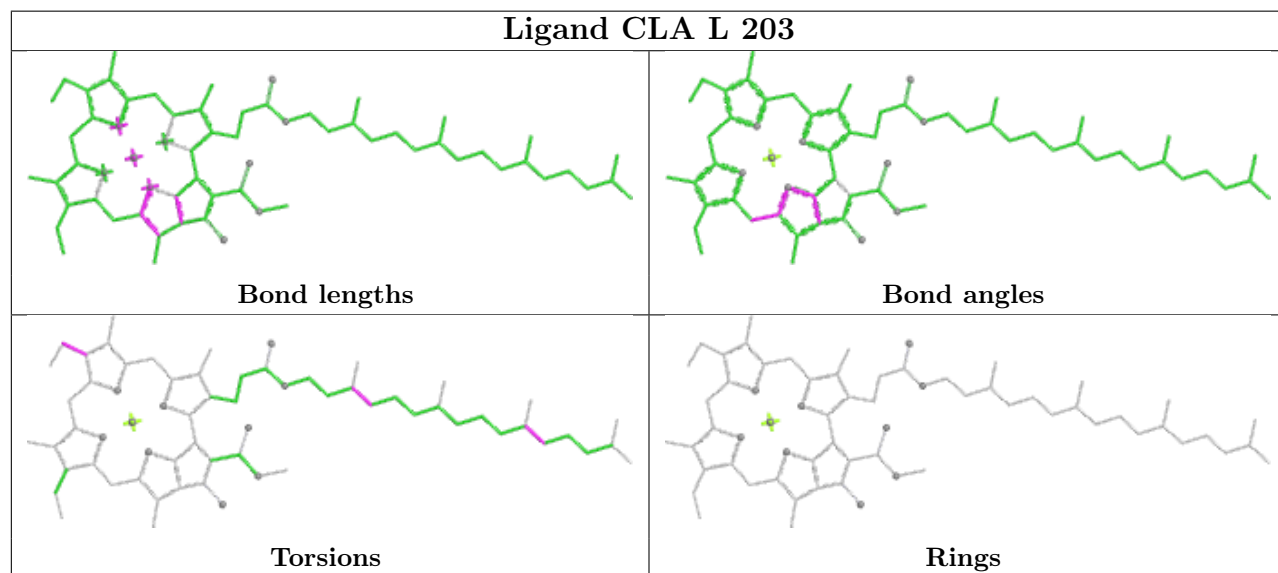
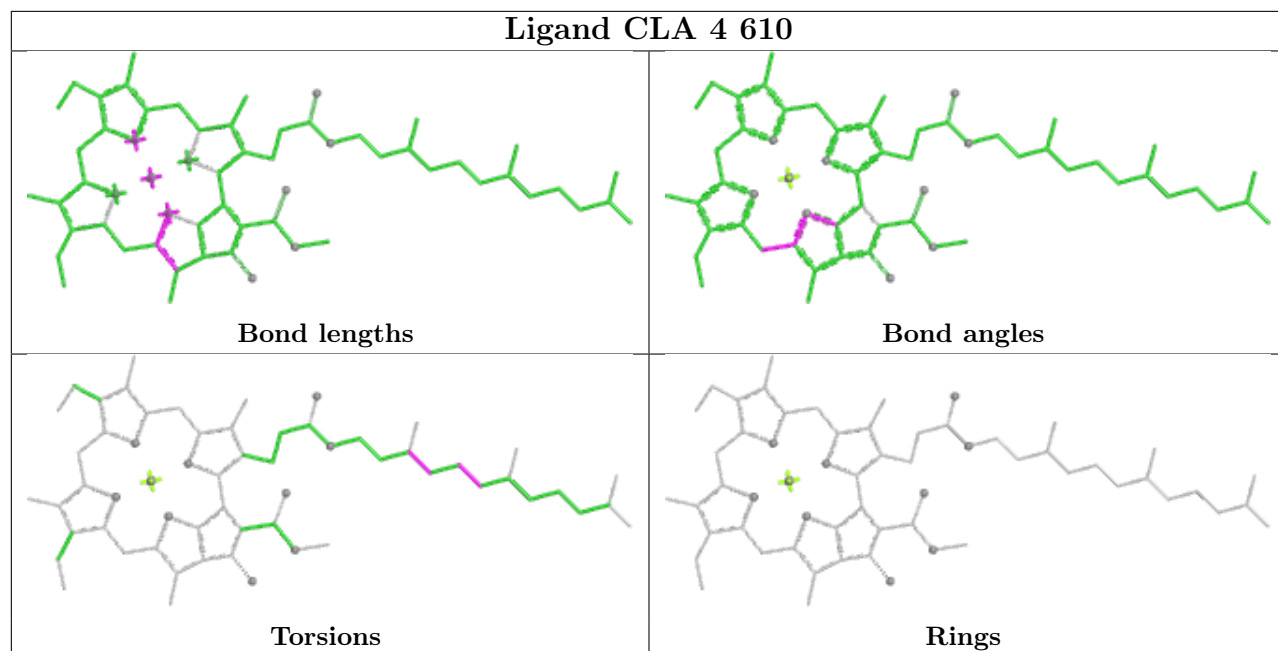
Rings

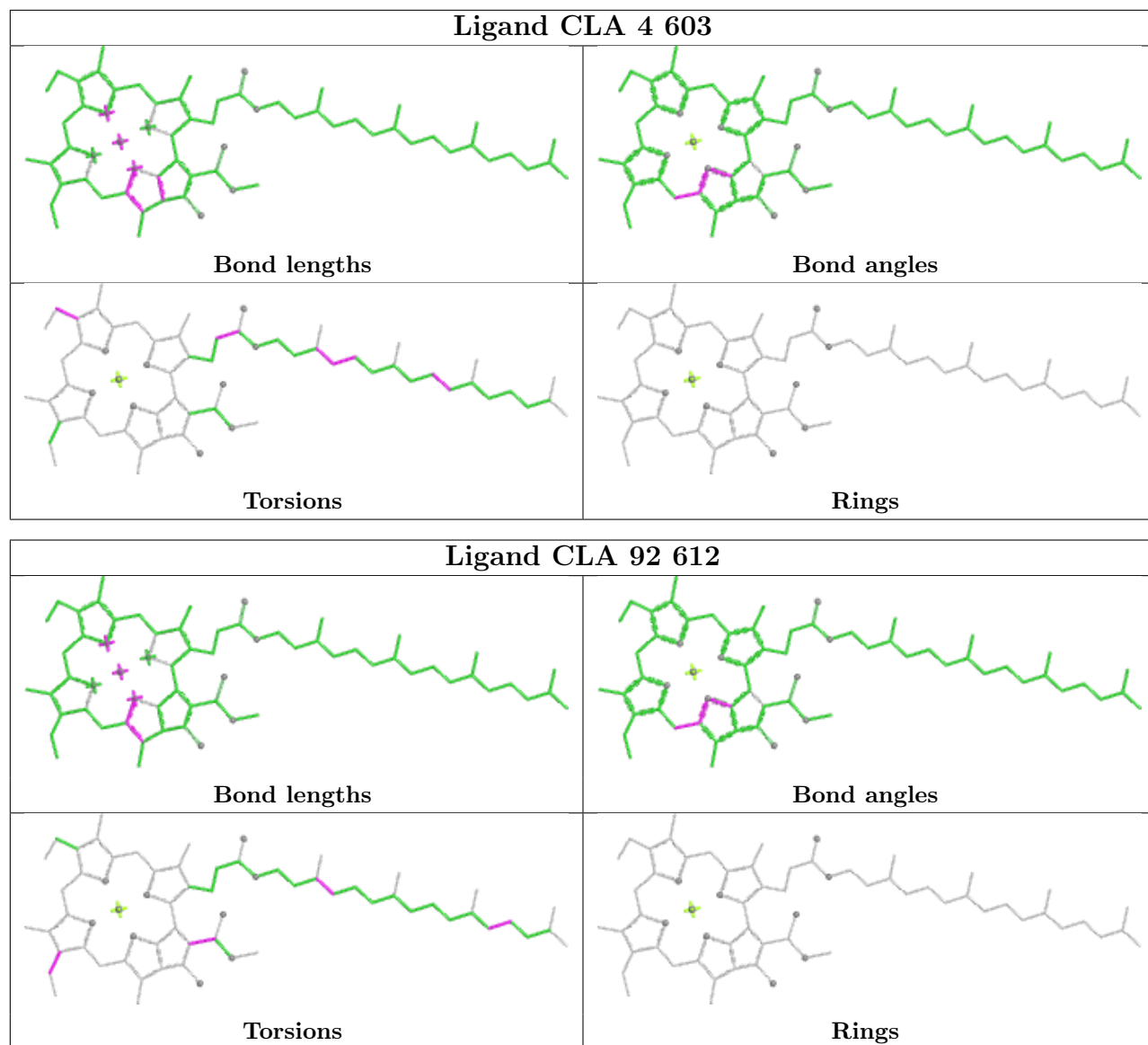
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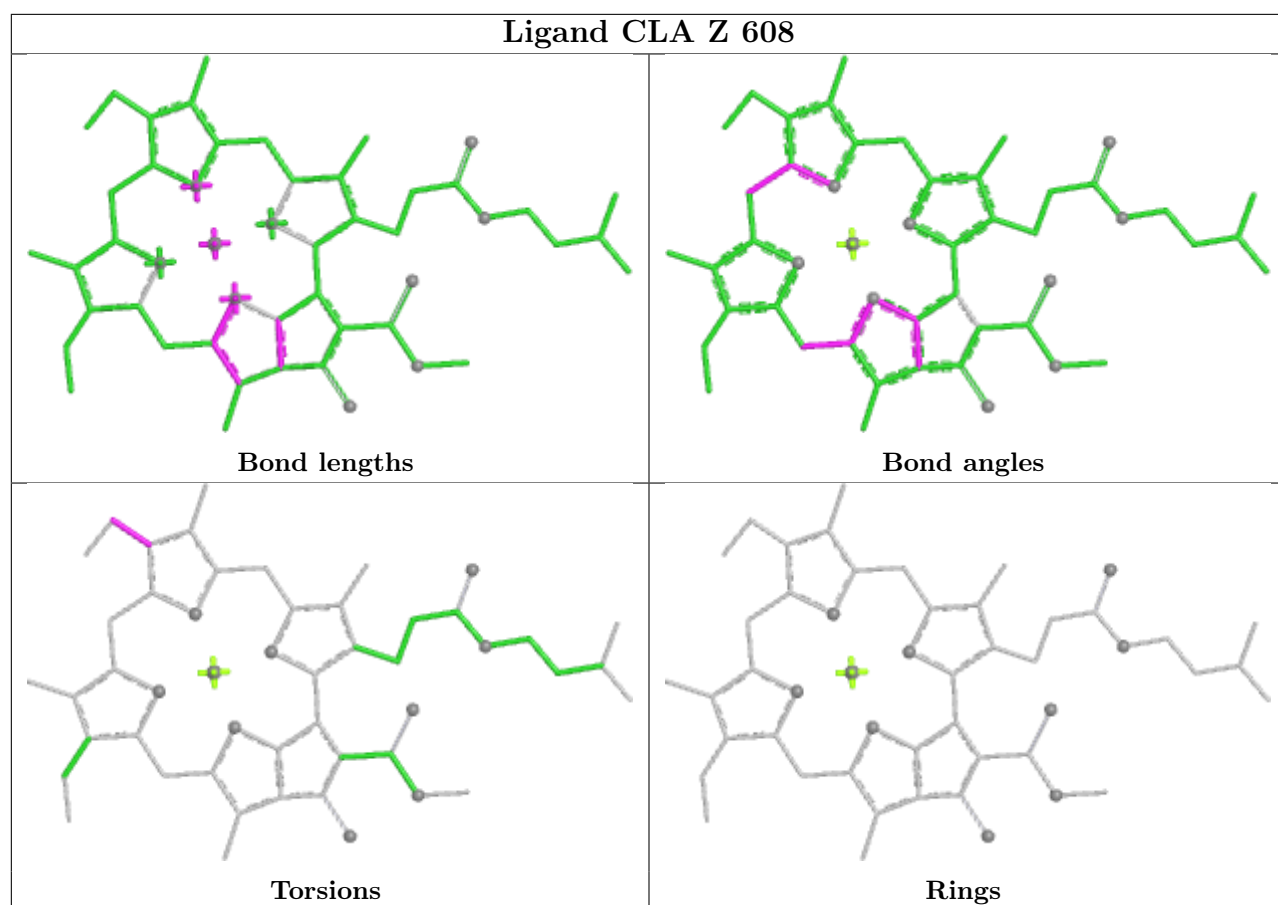


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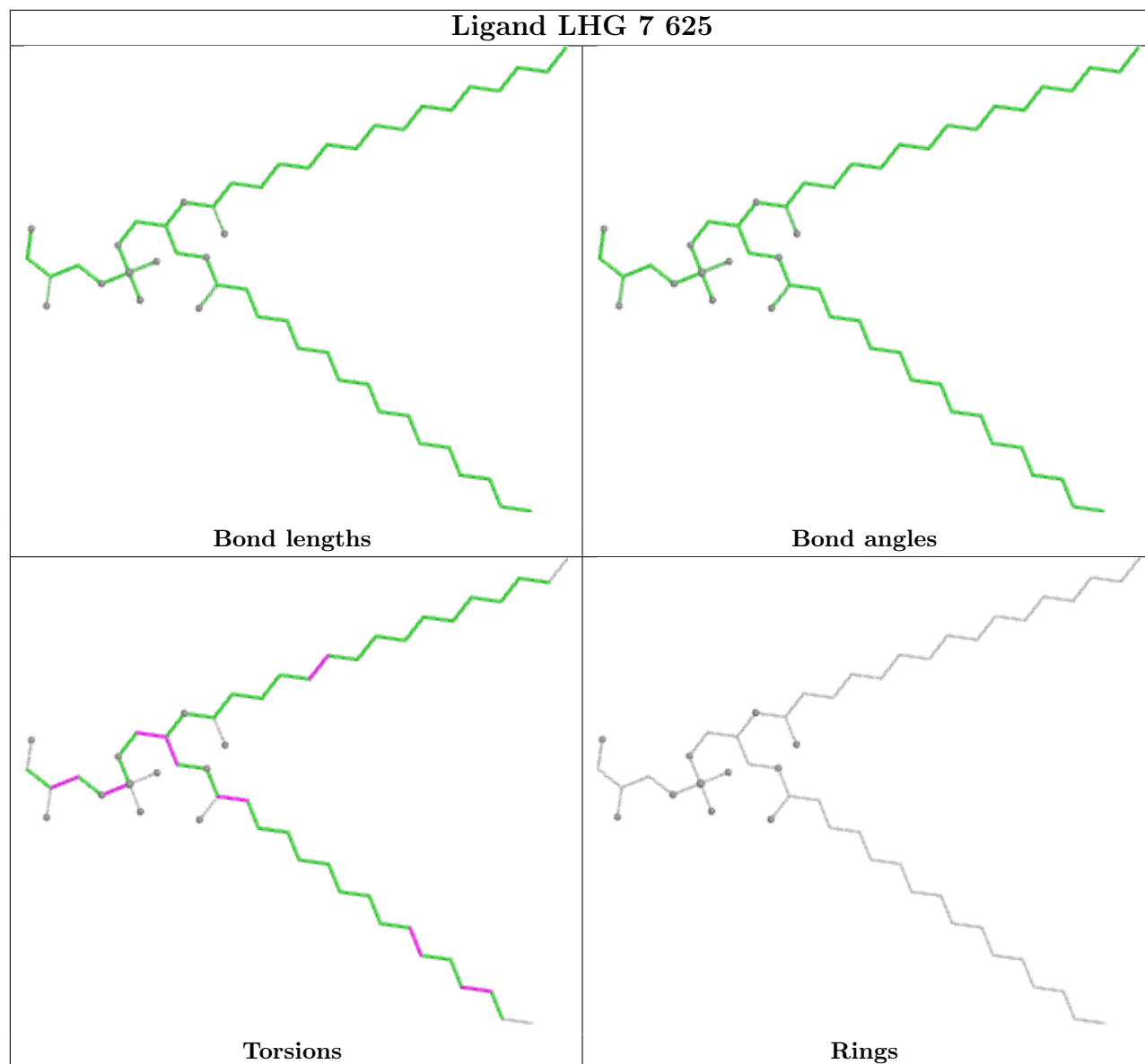




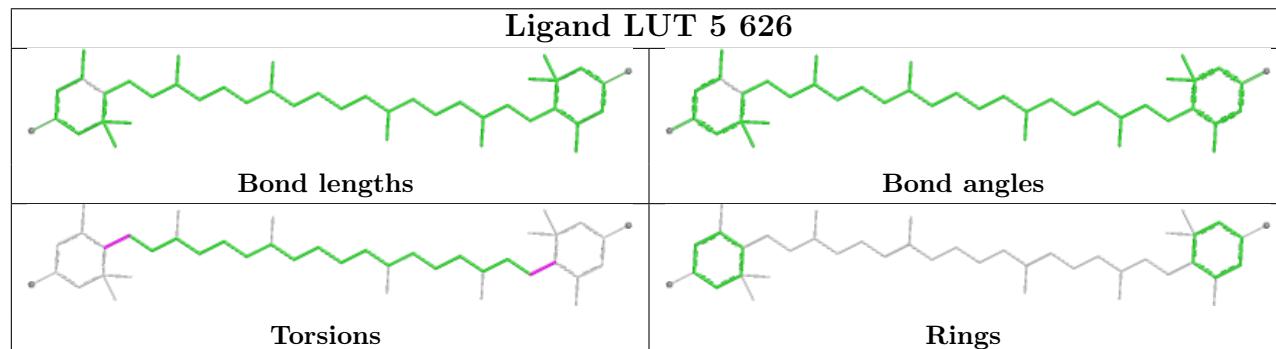




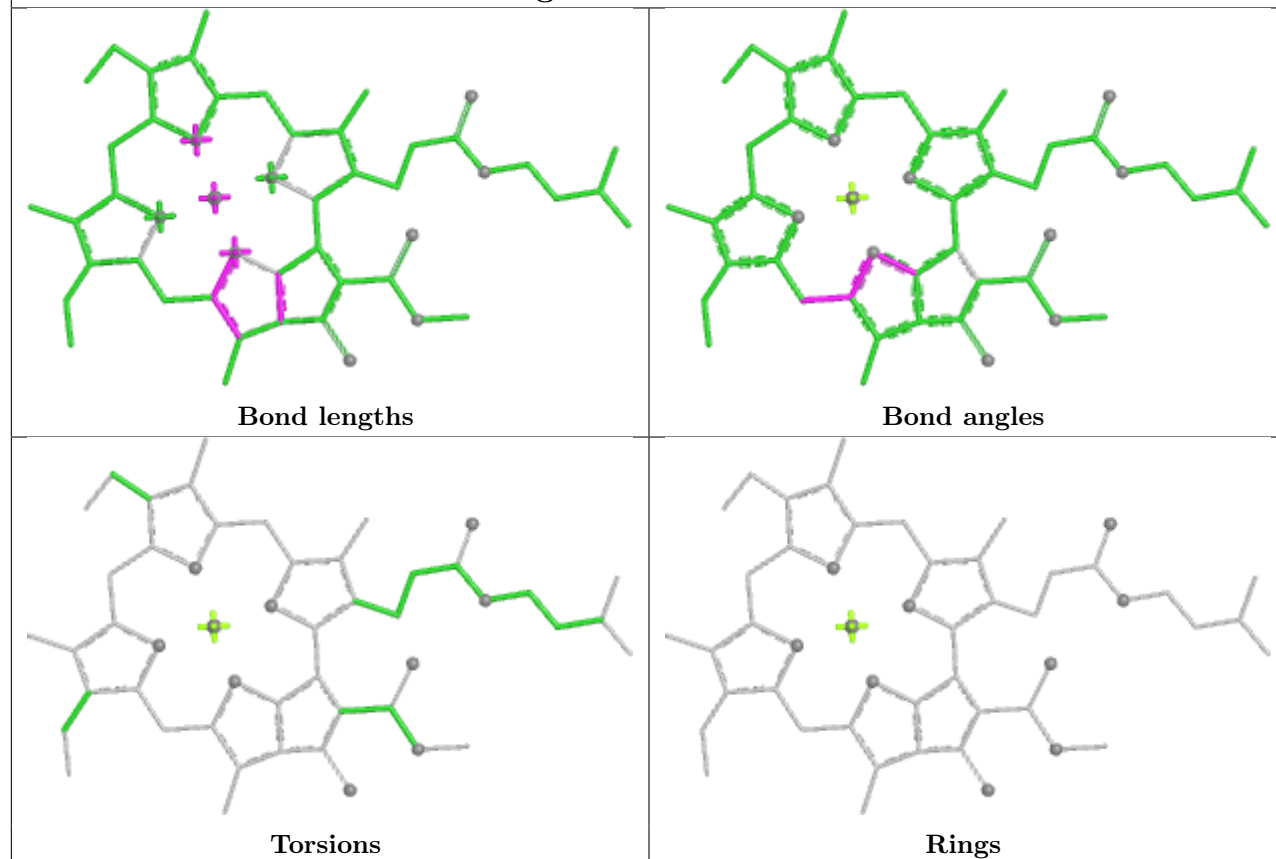
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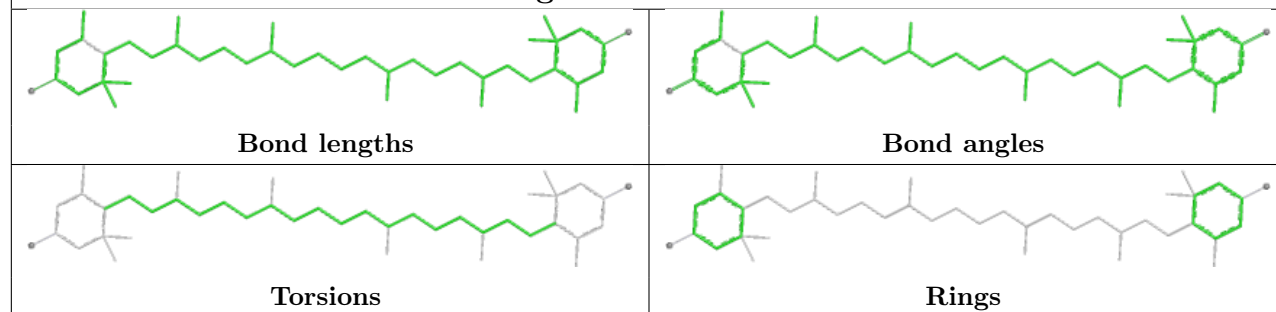
Ligand LUT 5 626



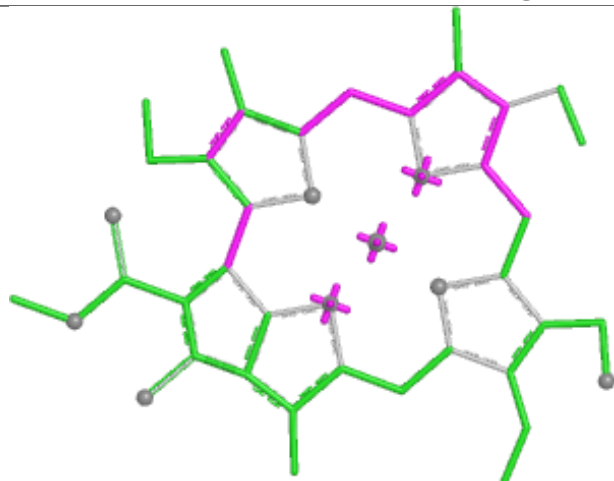
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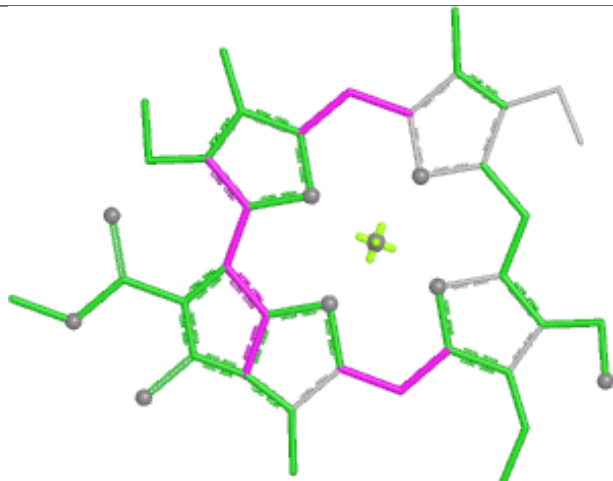
Ligand LUT 3 720



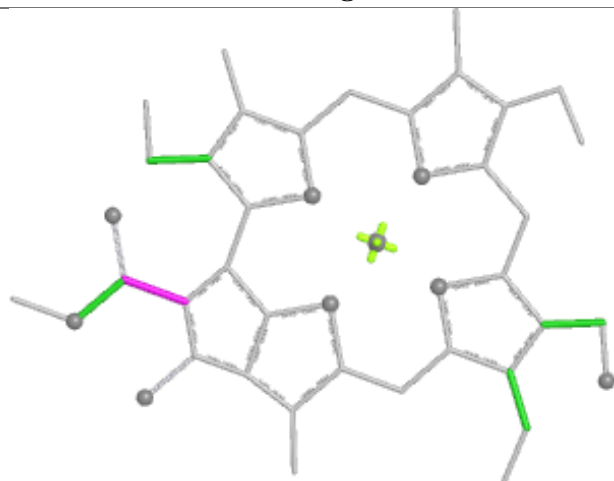
Ligand CHL 6 618



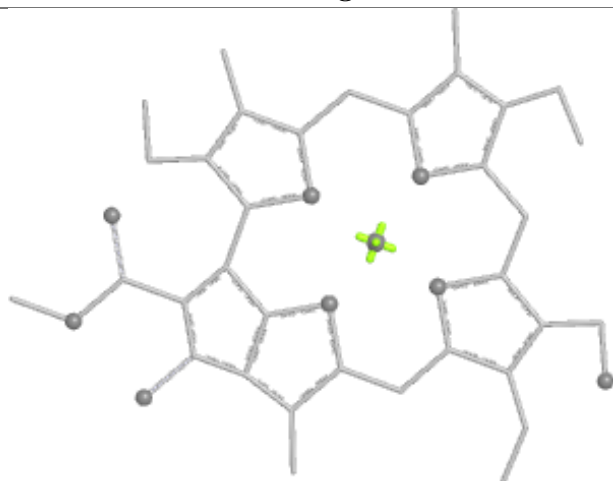
Bond lengths



Bond angles

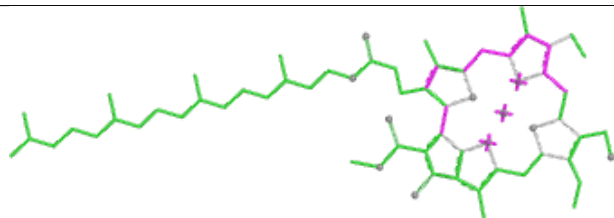


Torsions

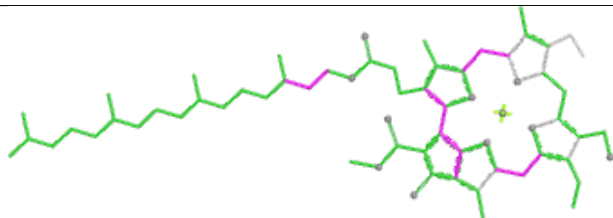


Rings

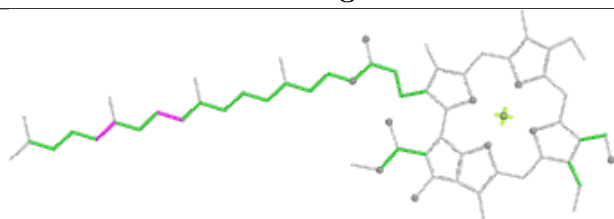
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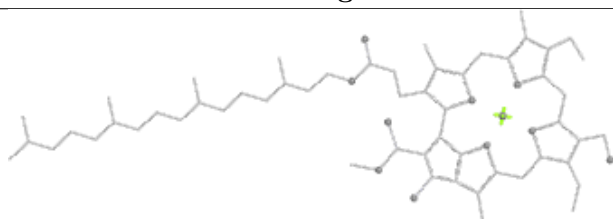
Bond lengths



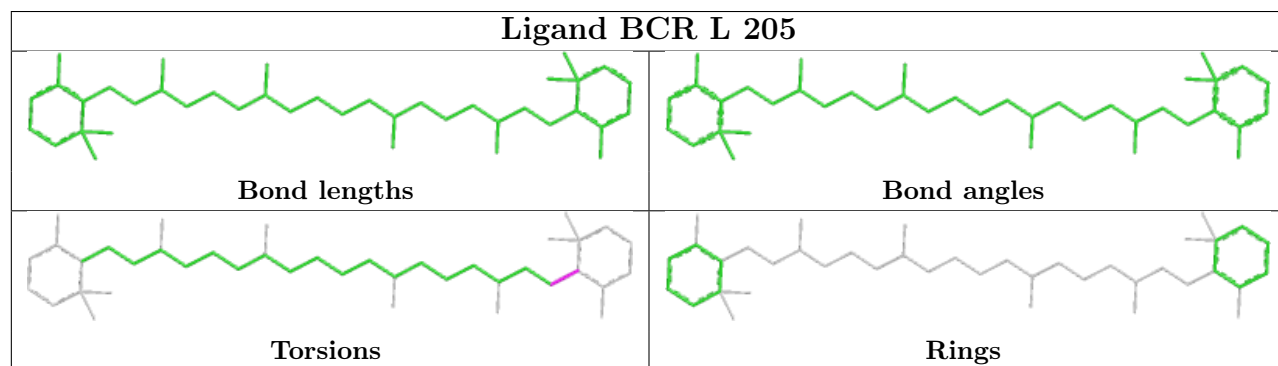
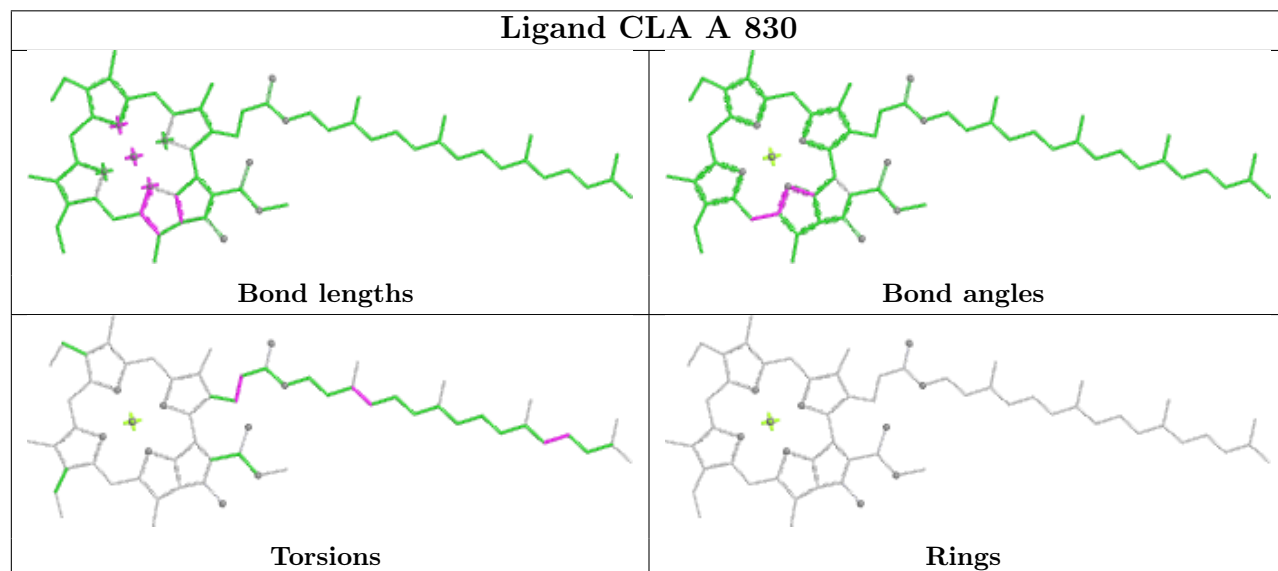
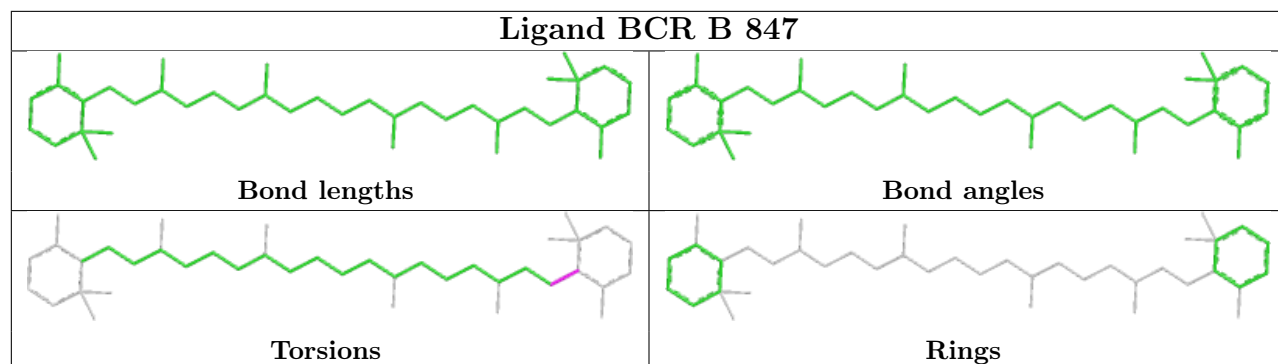
Bond angles

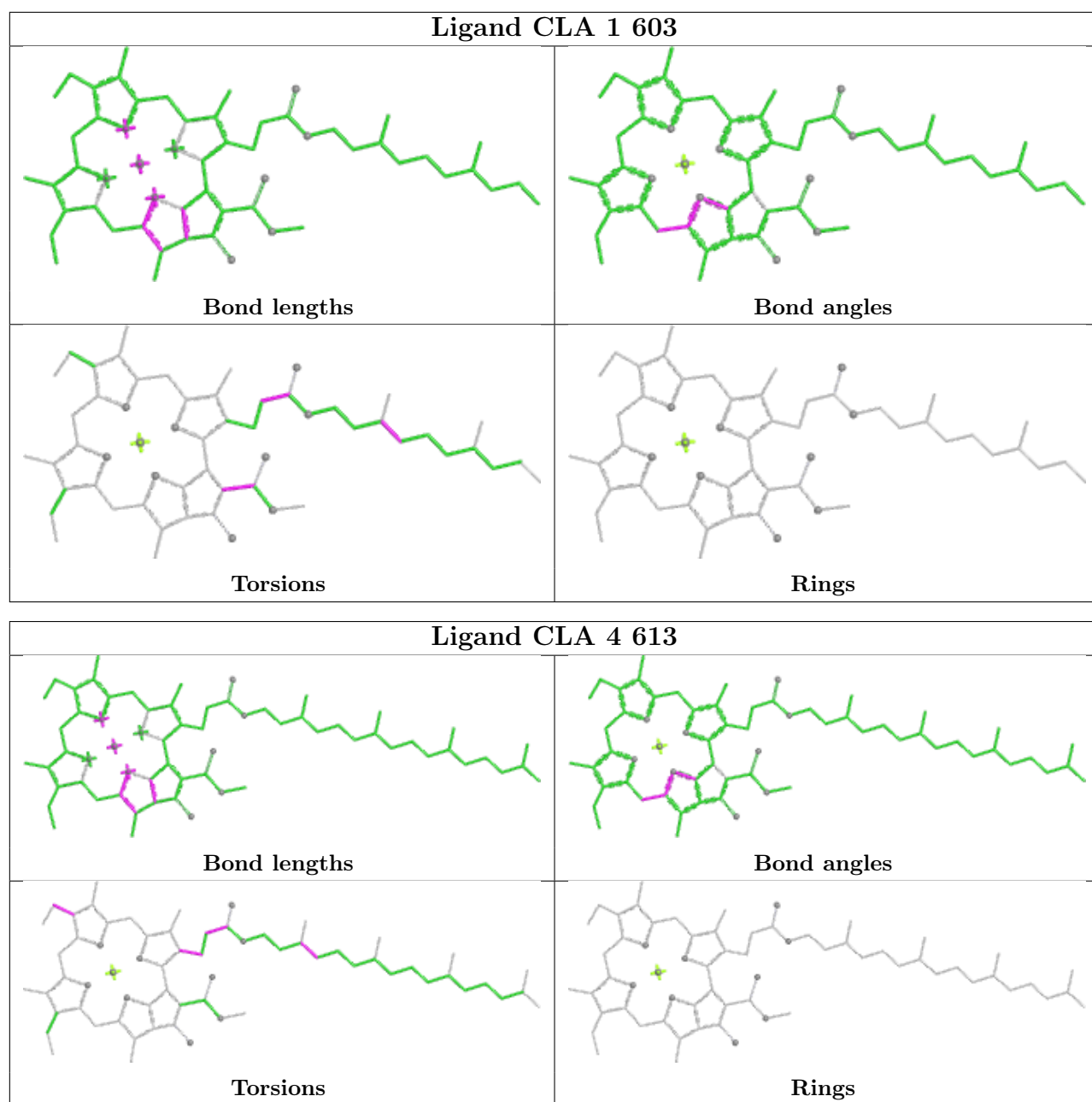


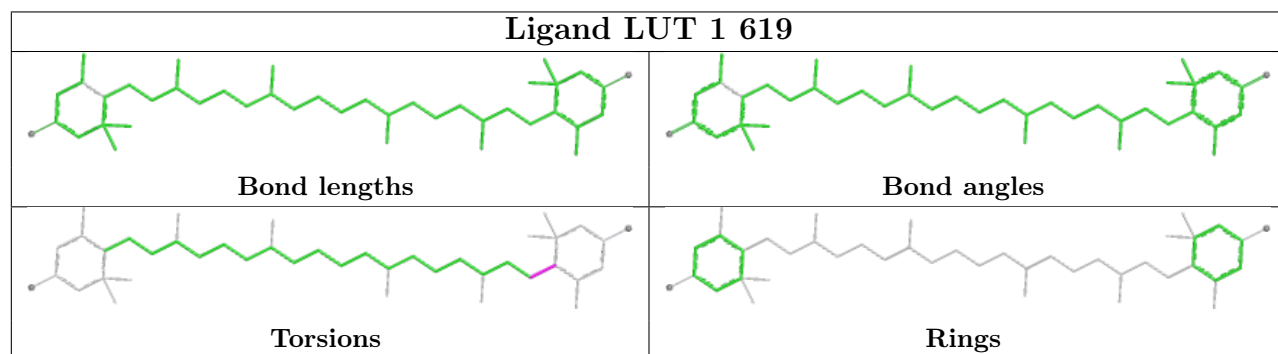
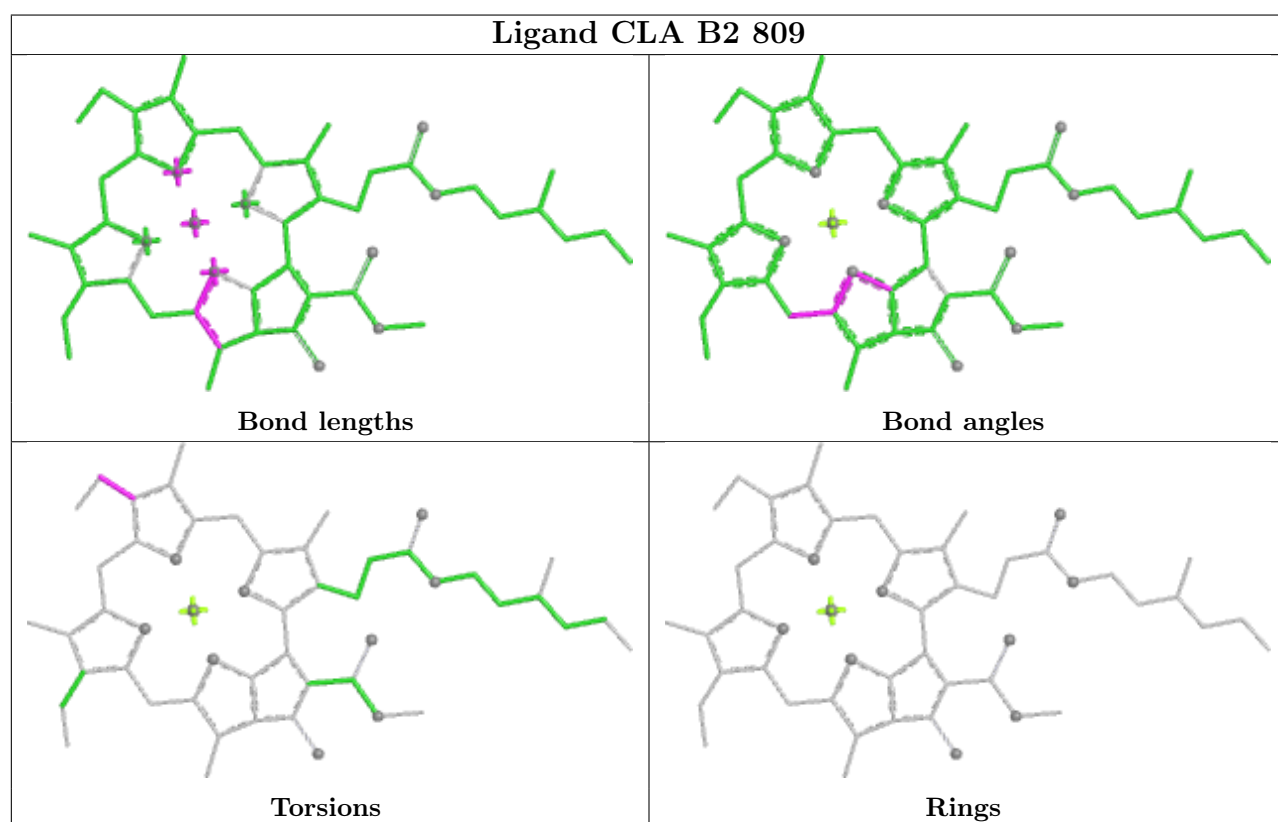
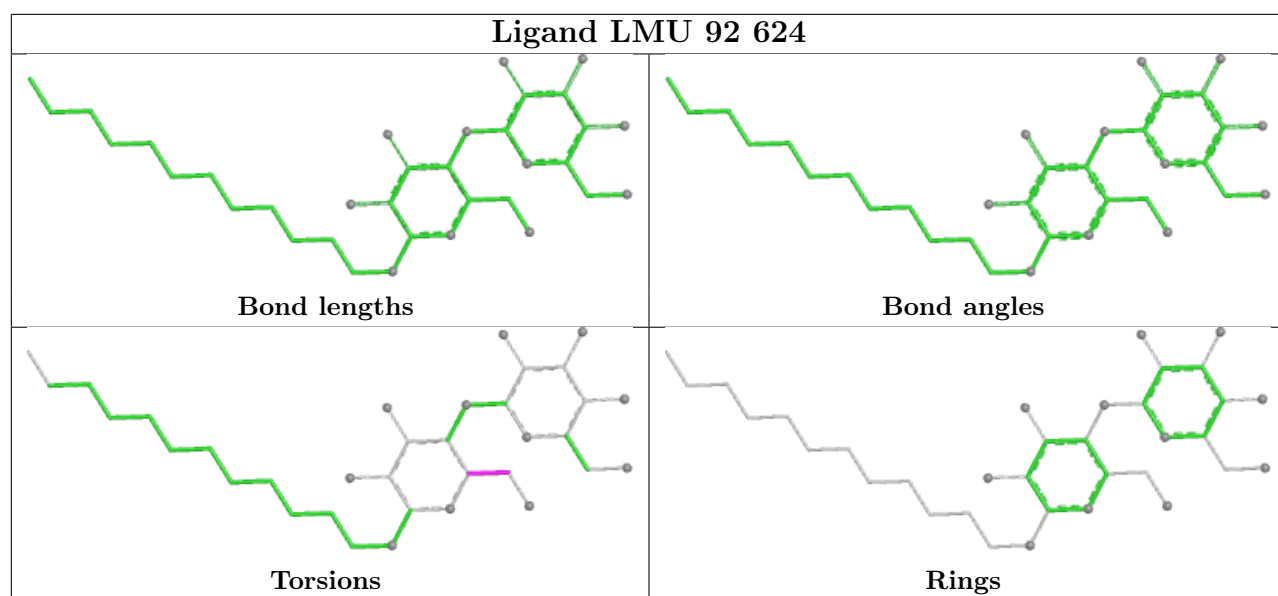
Torsions

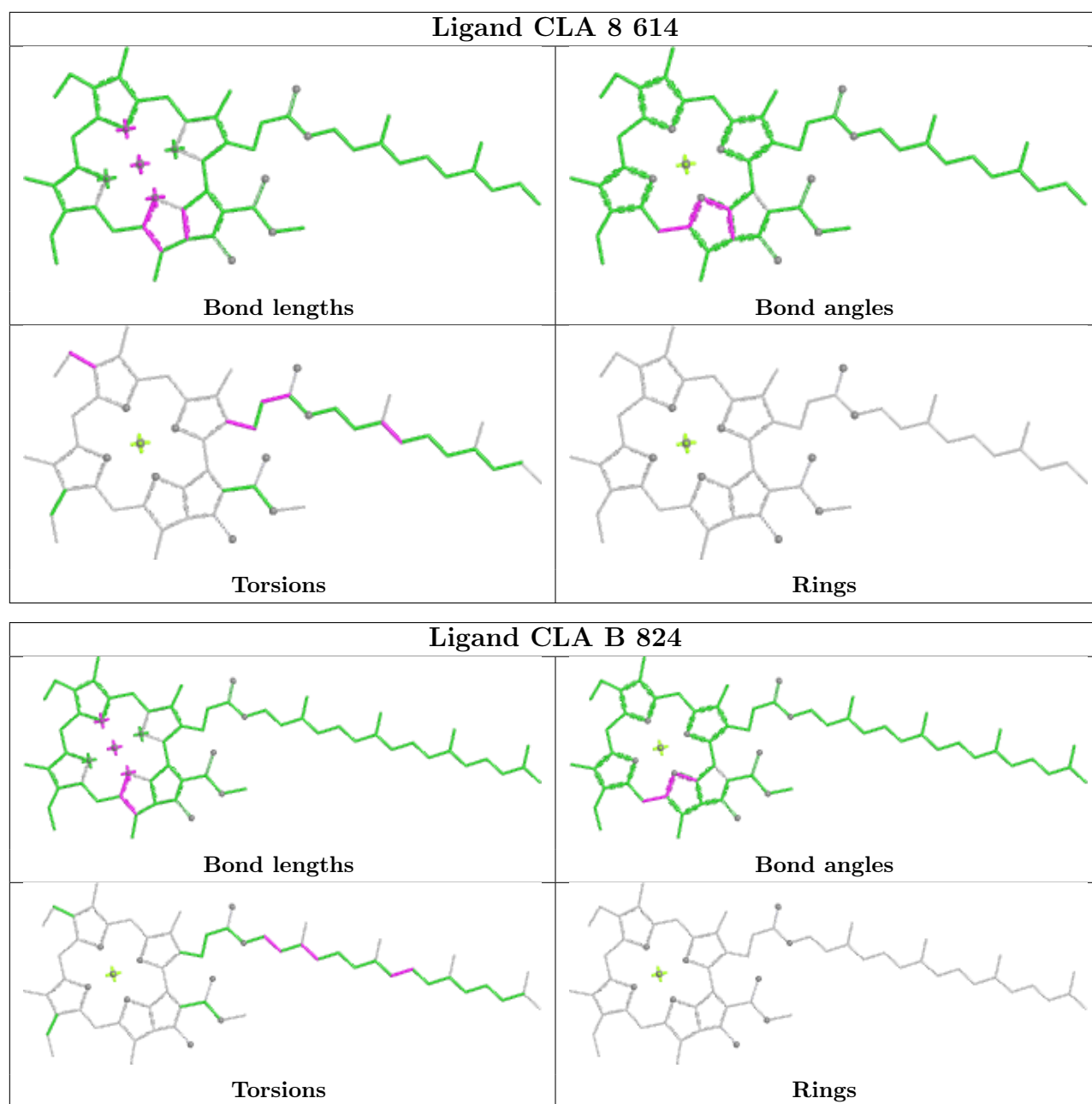


Rings

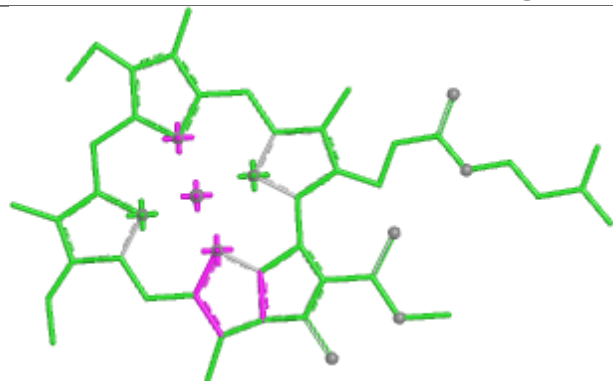




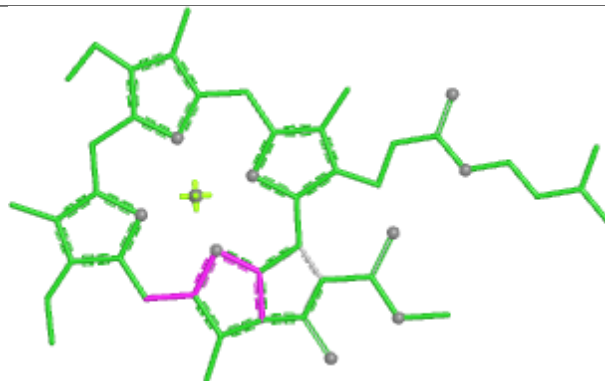




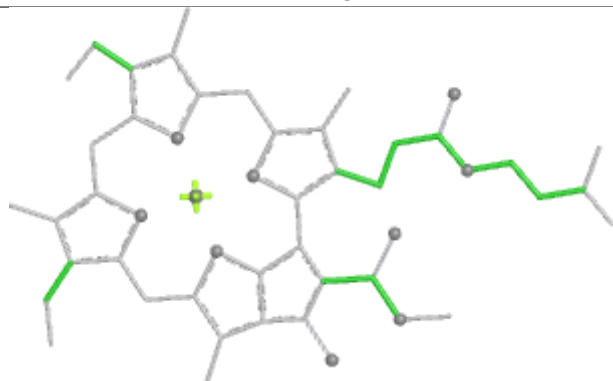
Ligand CLA 1 604



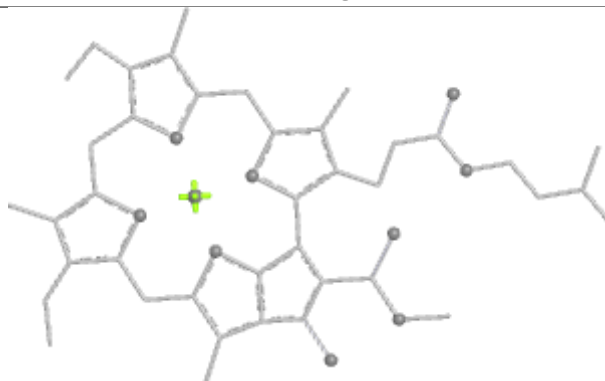
Bond lengths



Bond angles

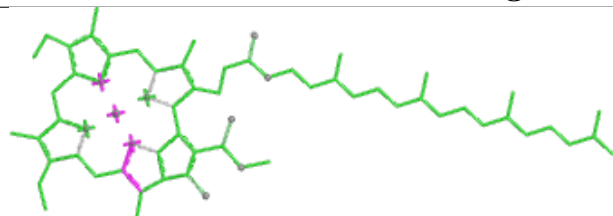


Torsions

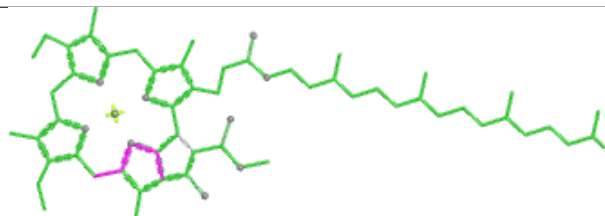


Rings

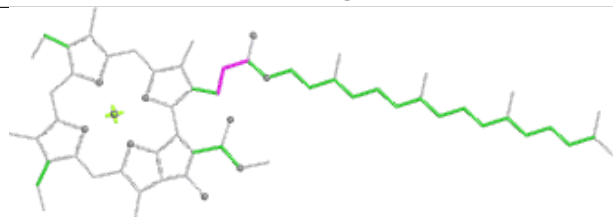
Ligand CLA B2 813



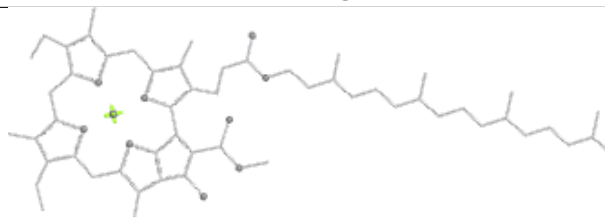
Bond lengths



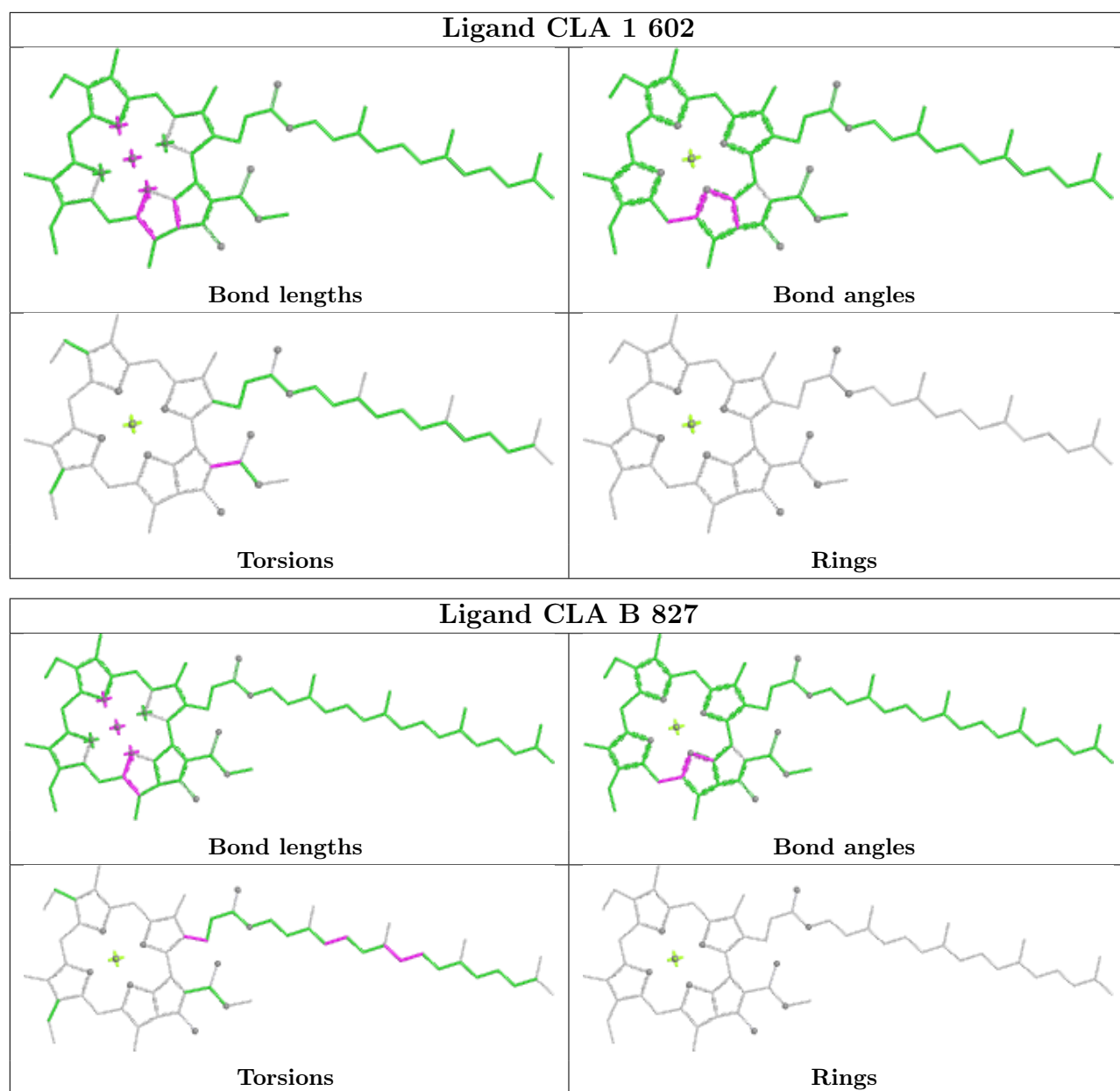
Bond angles

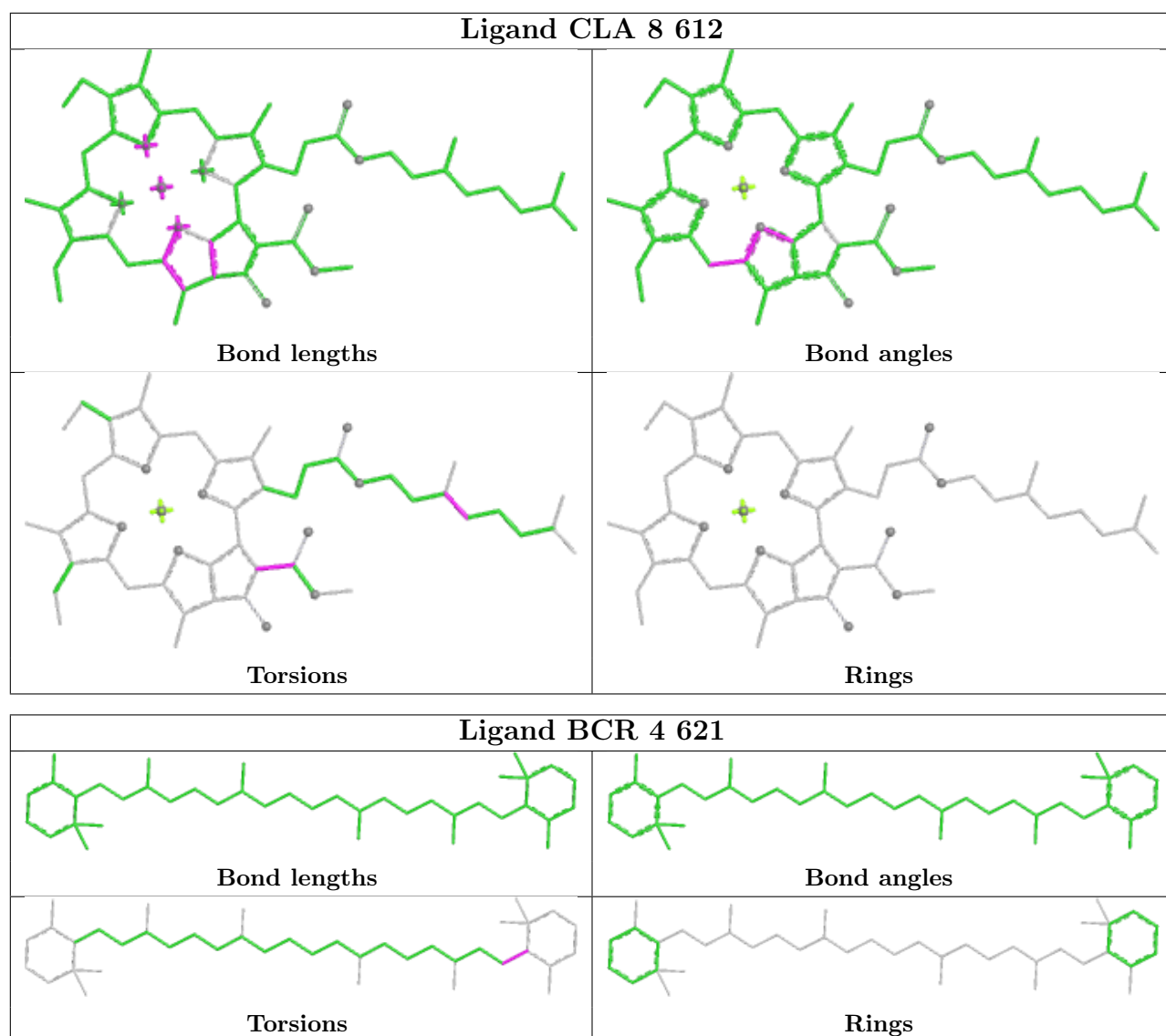


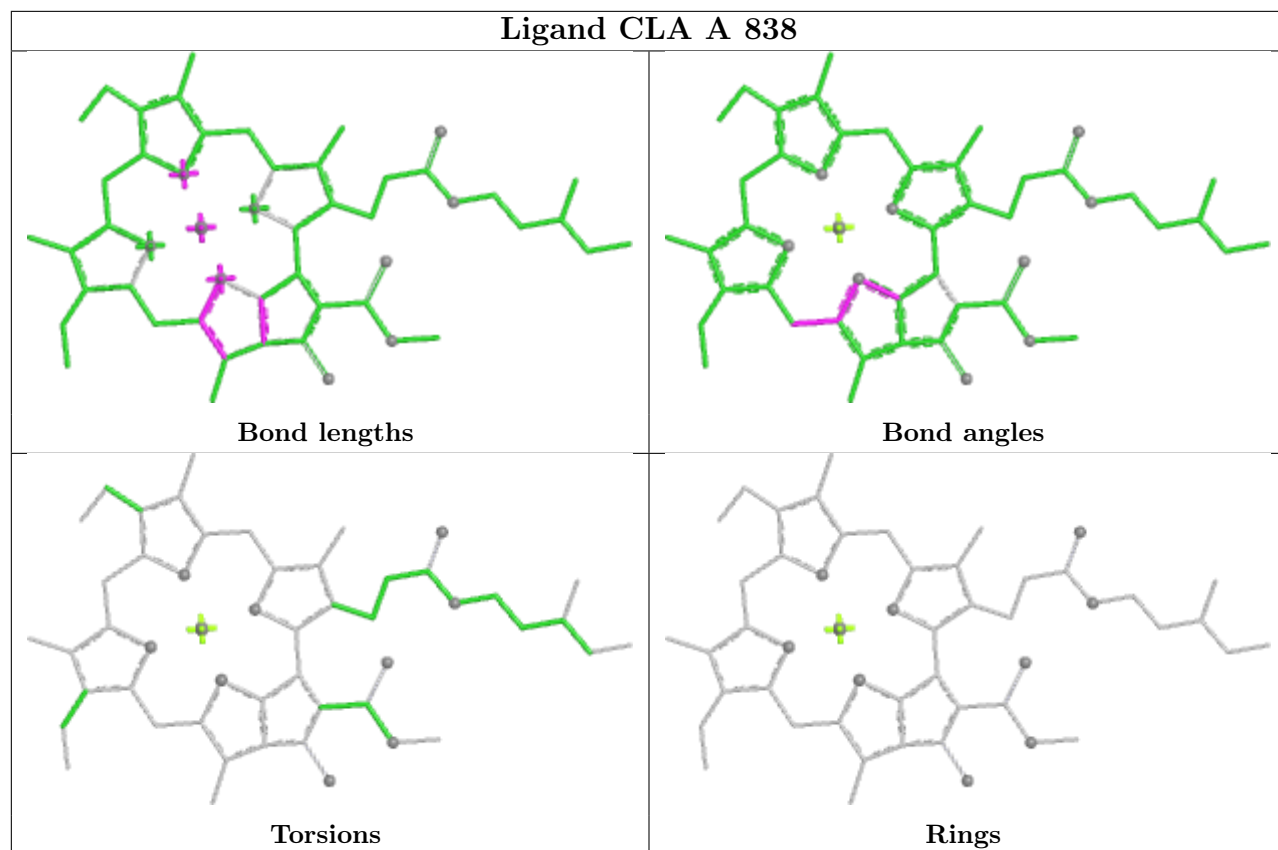
Torsions



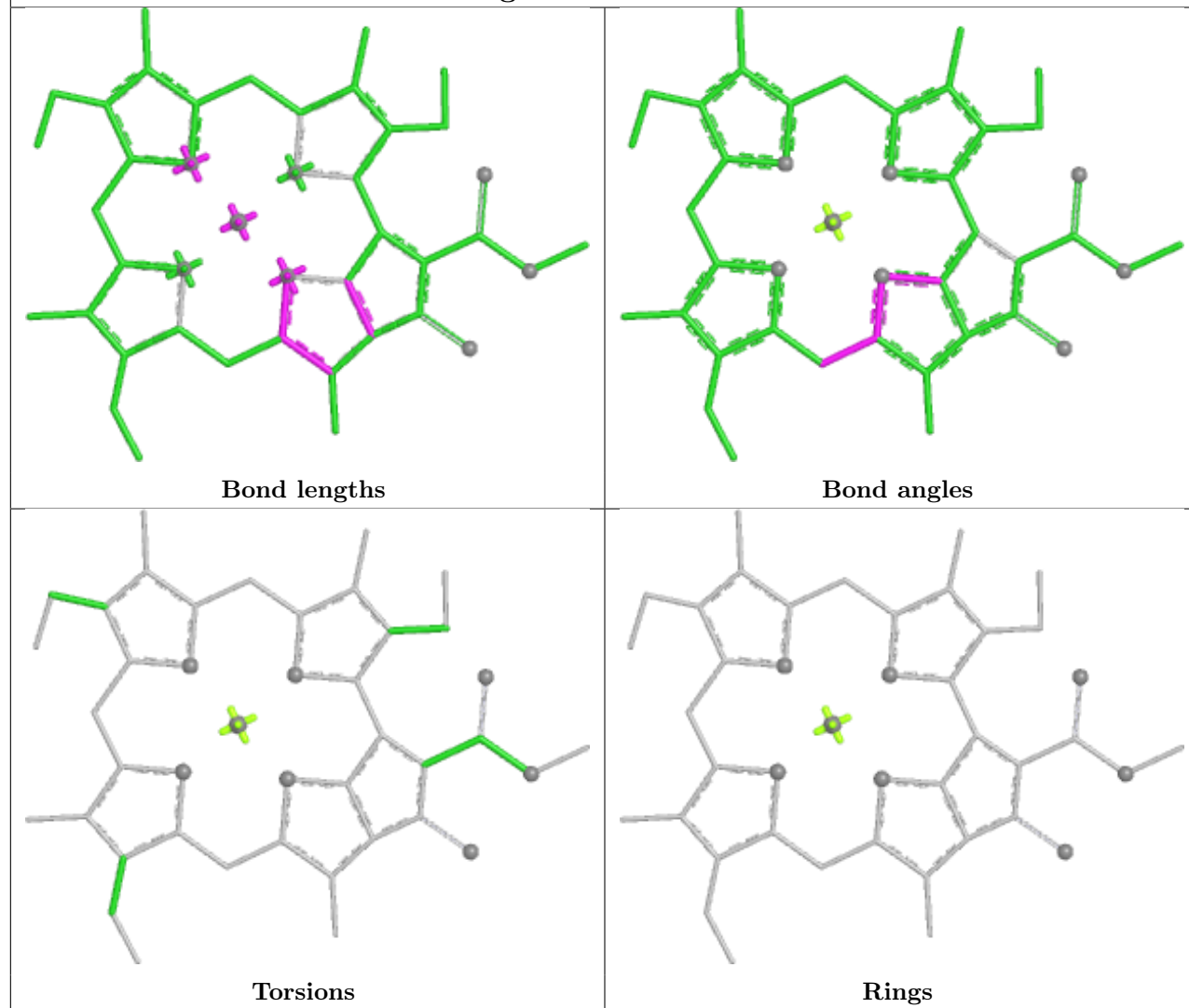
Rings



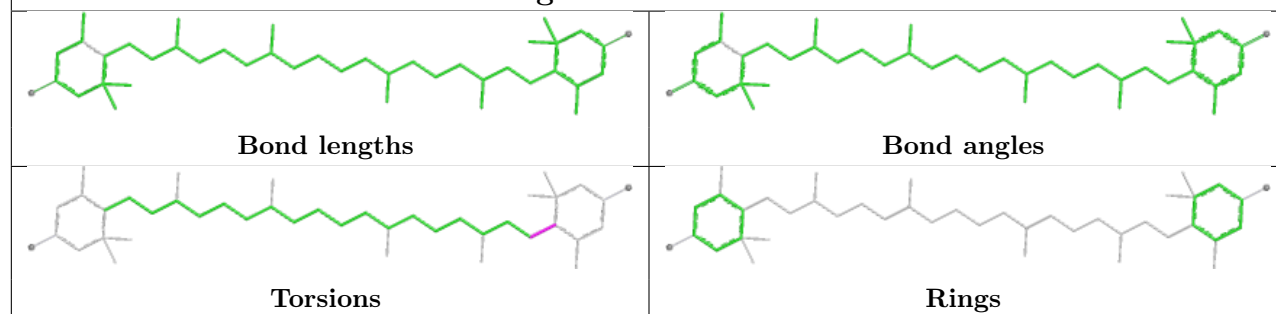


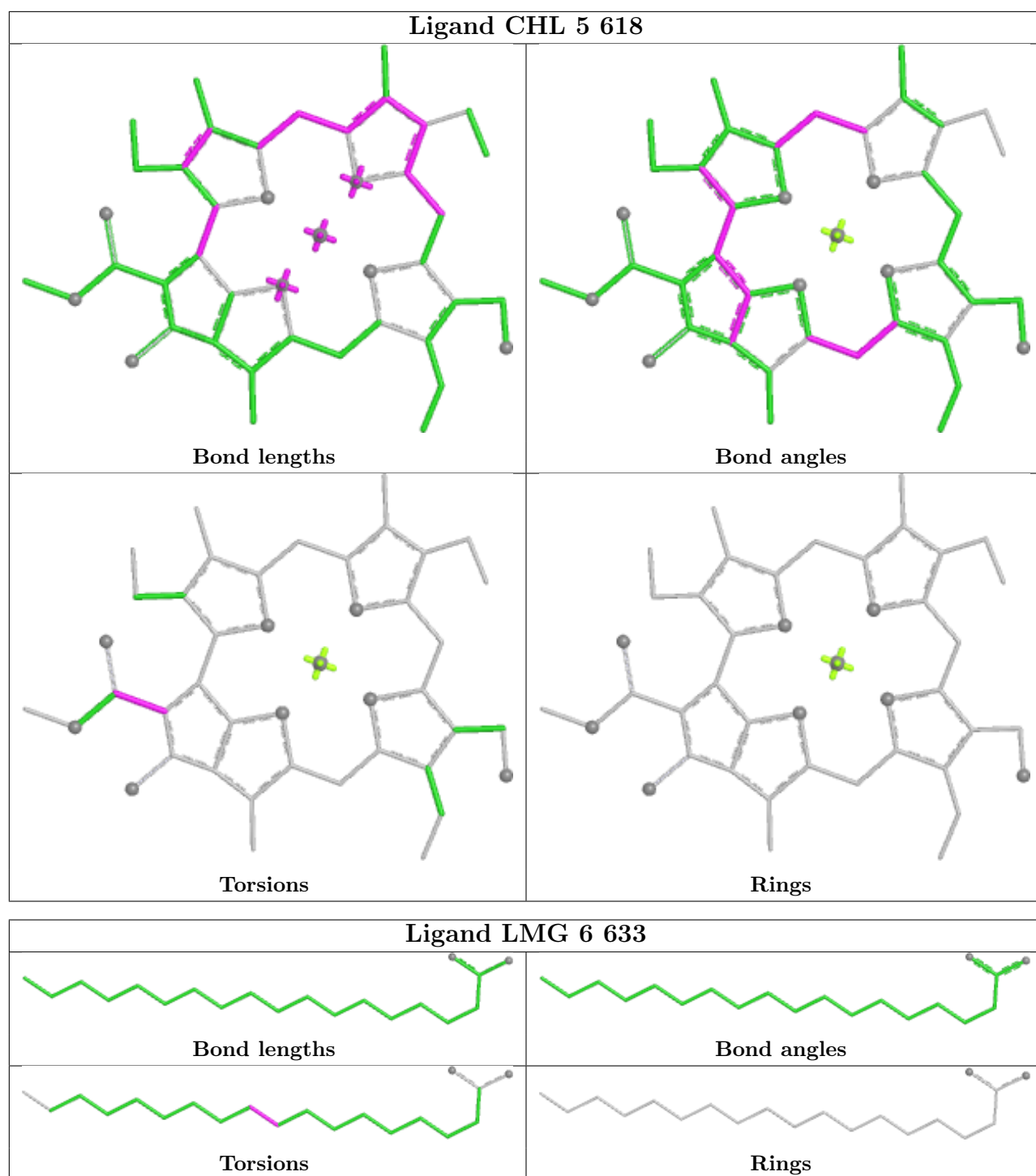


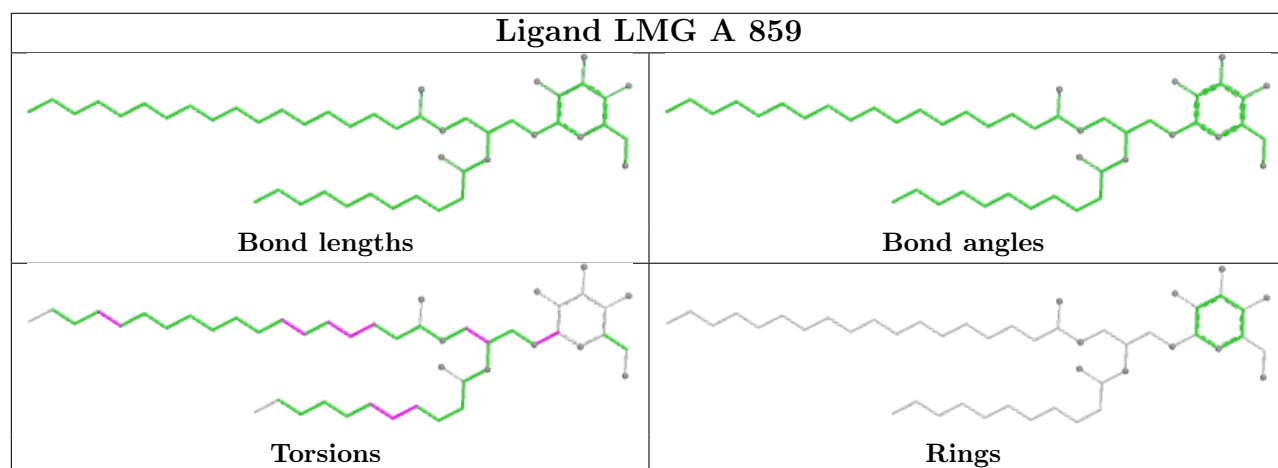
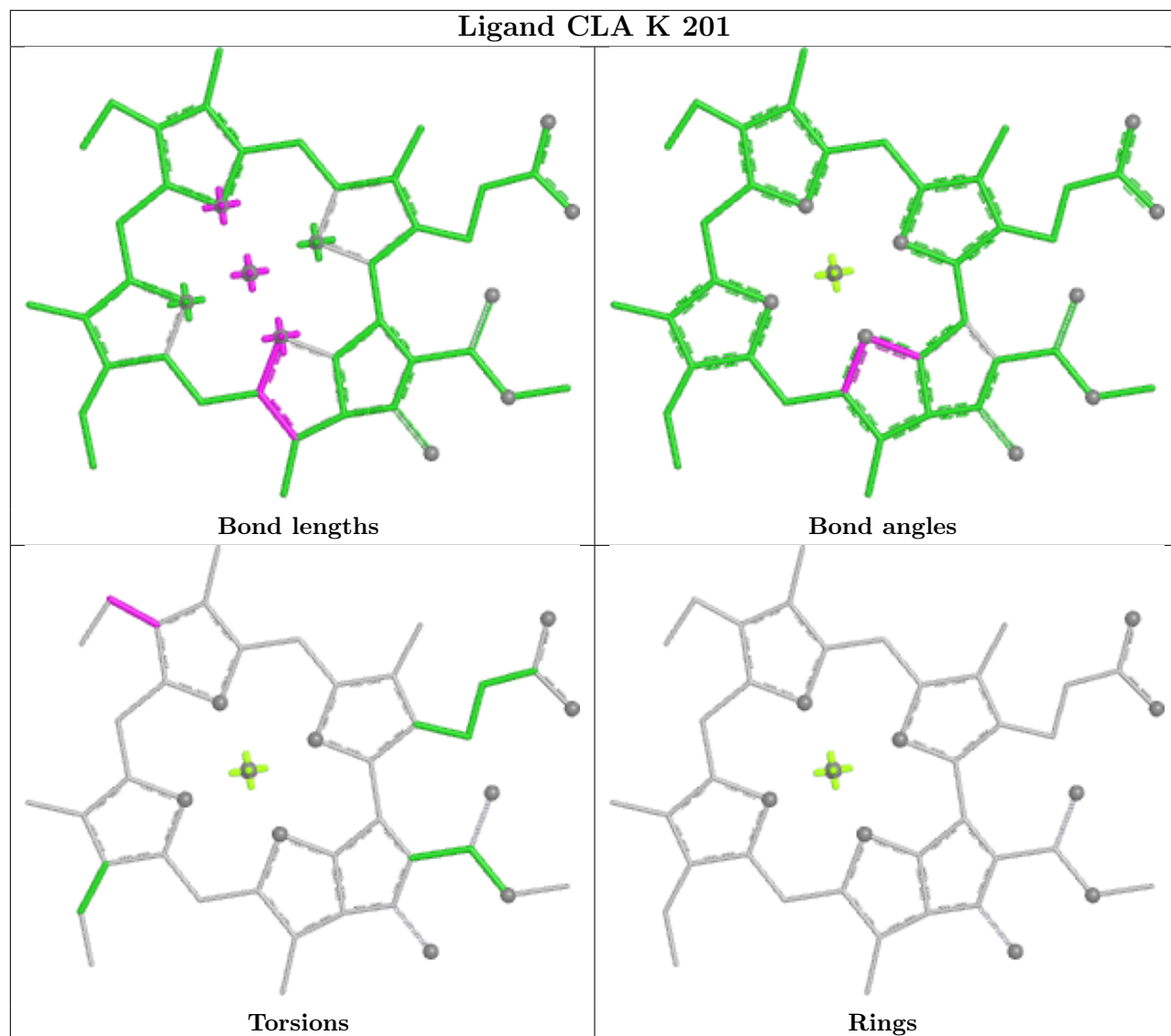
Ligand CLA 3 606

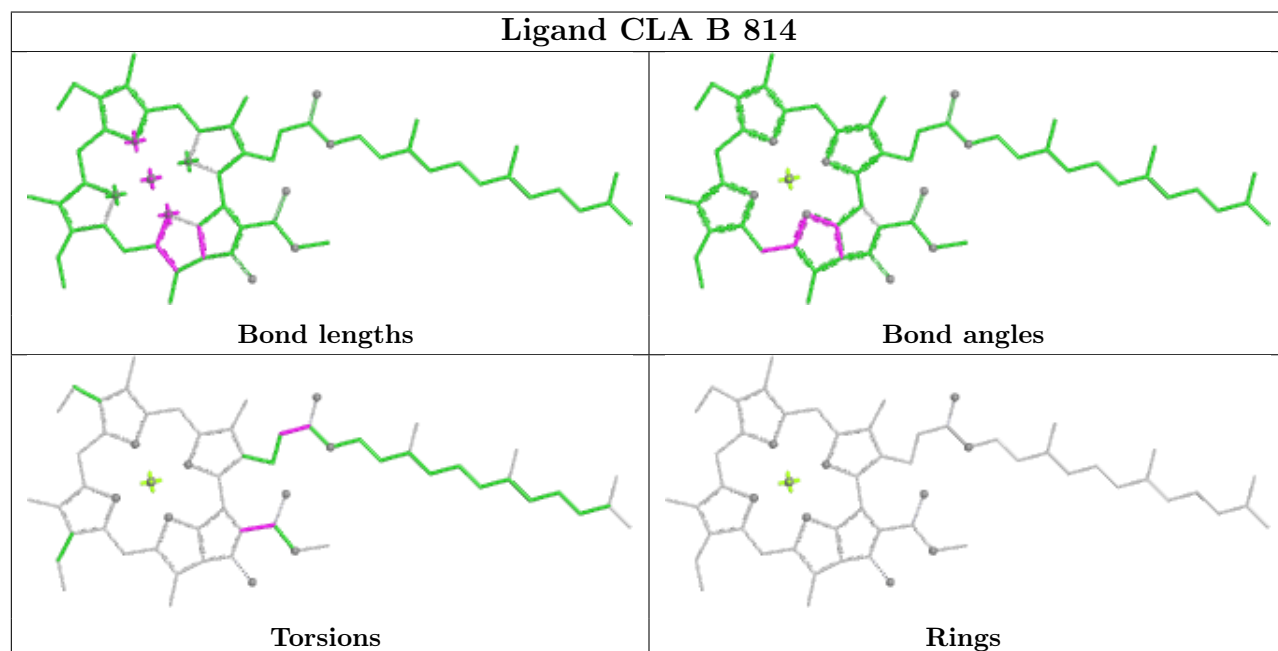
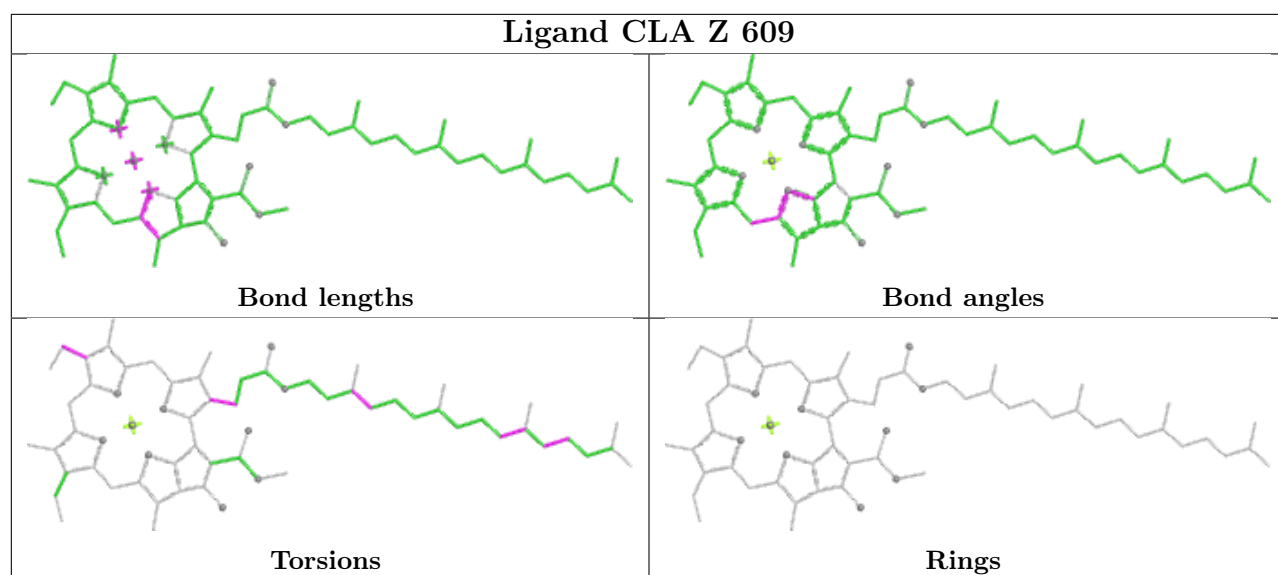


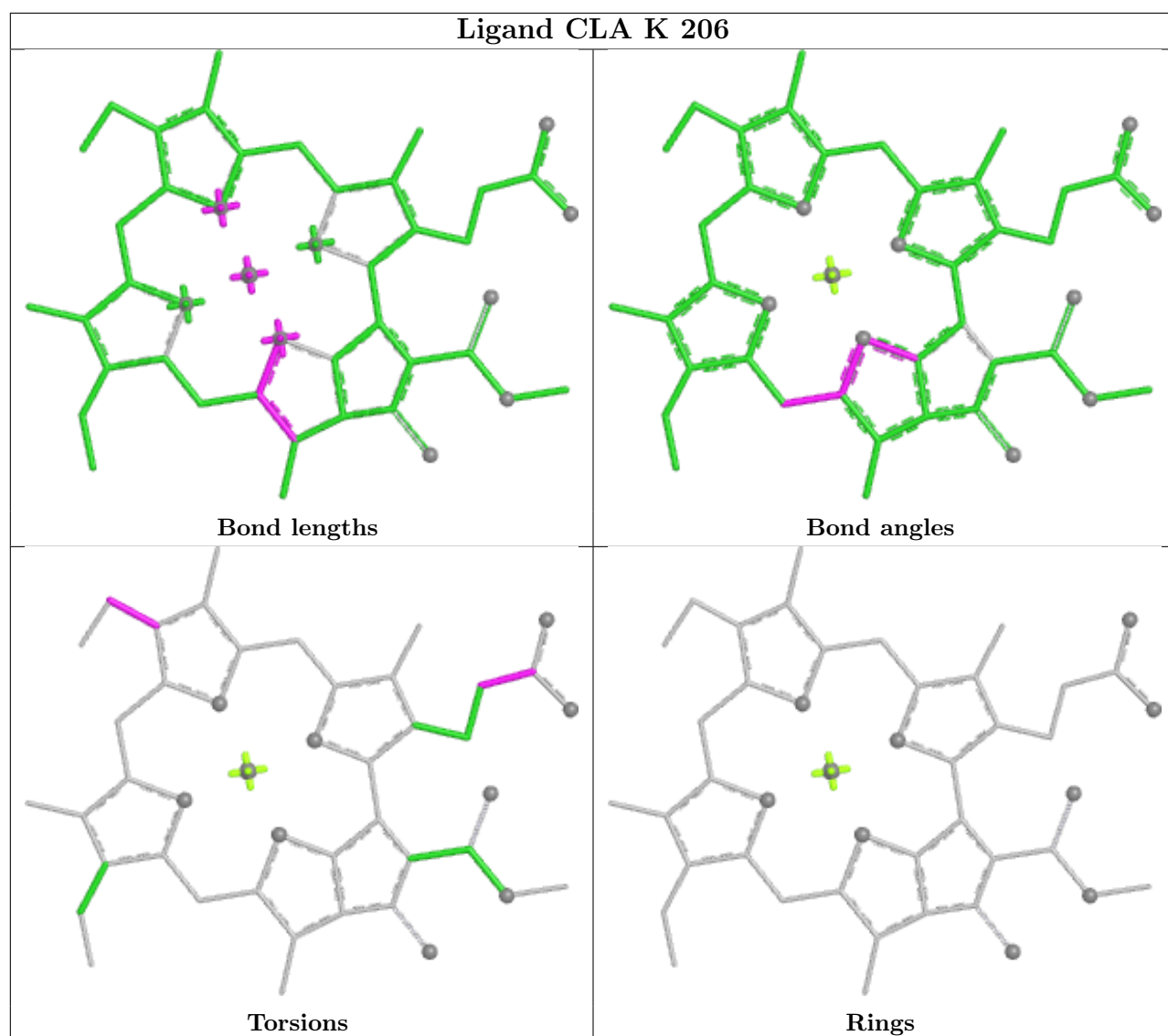
Ligand LUT 4 619



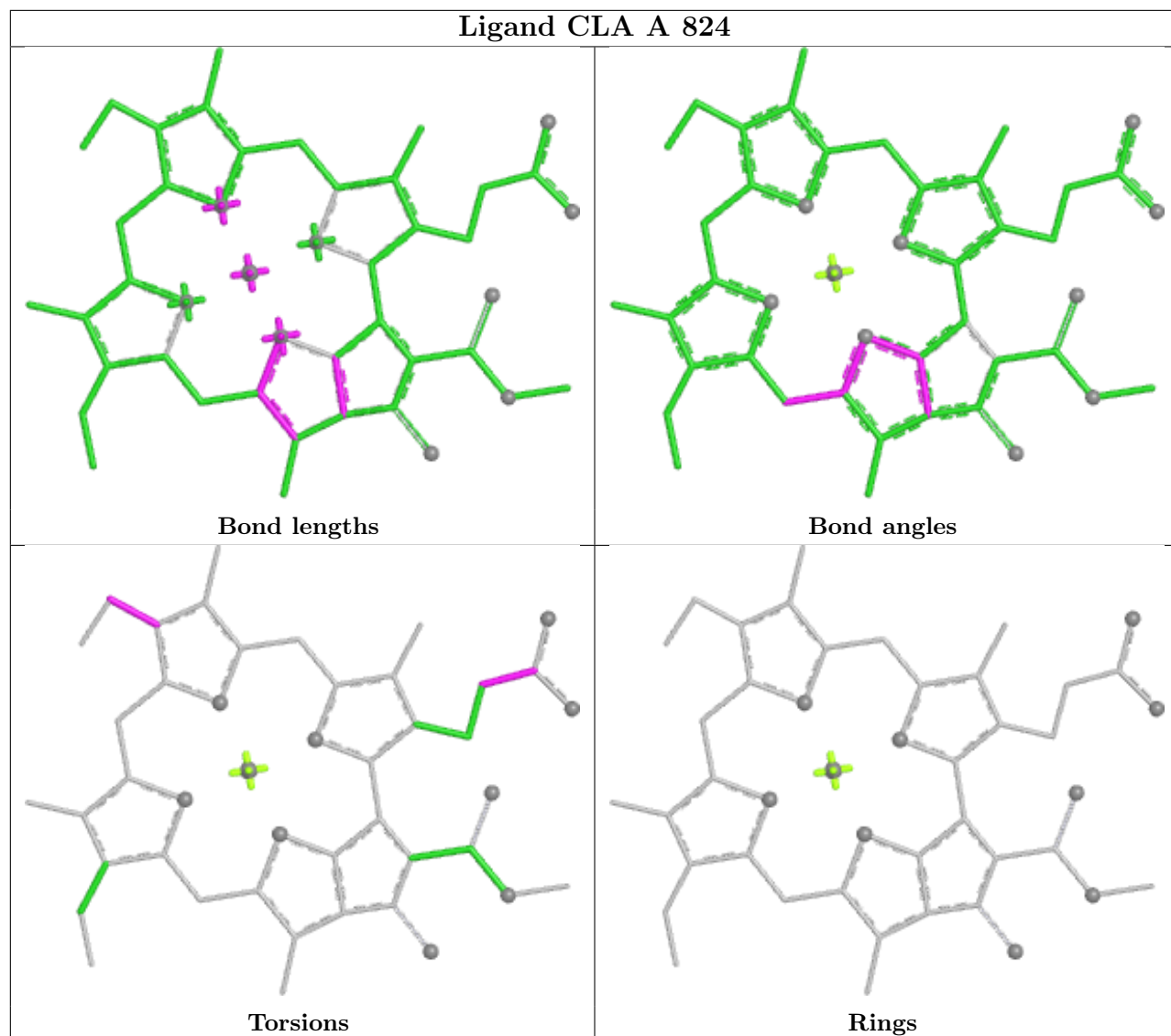




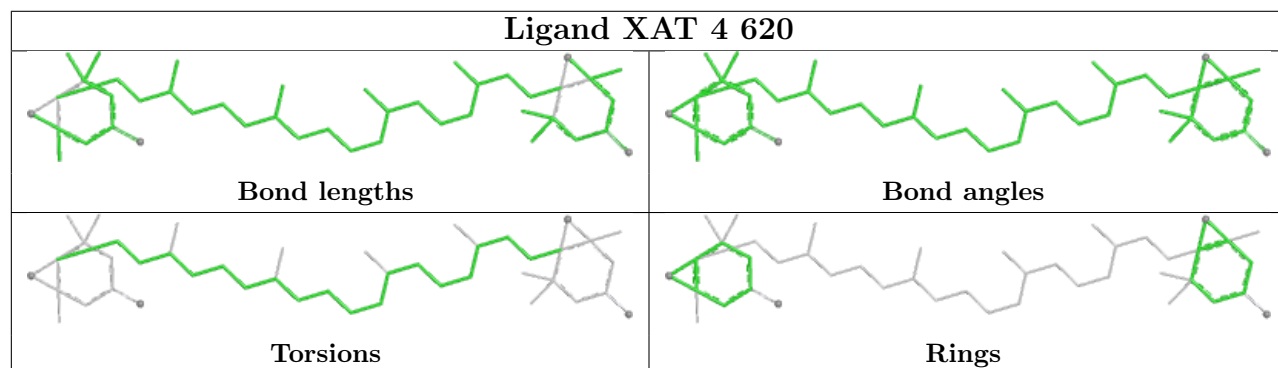




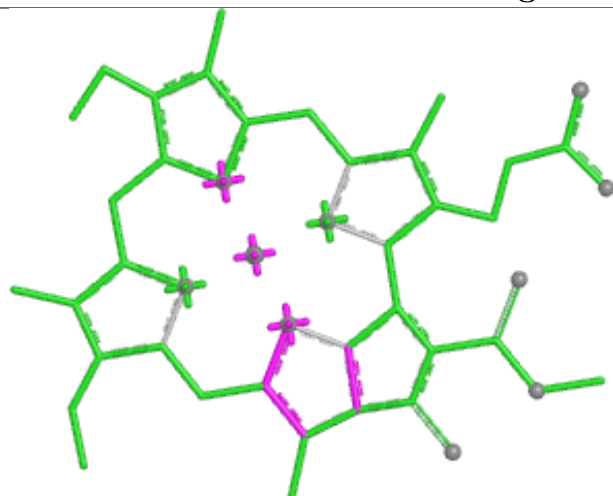
Ligand CLA A 824



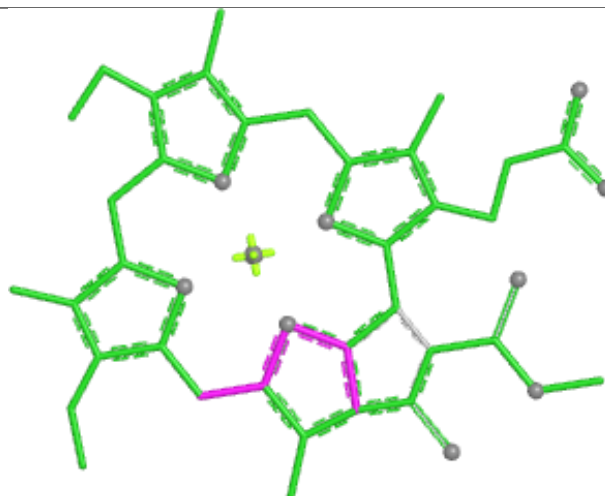
Ligand XAT 4 620



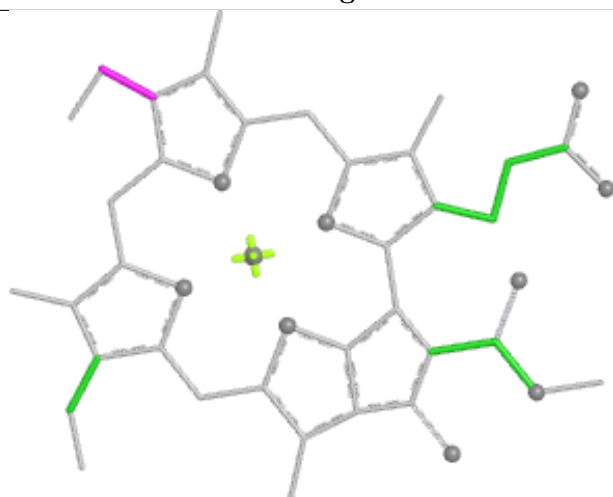
Ligand CLA 7 609



Bond lengths



Bond angles

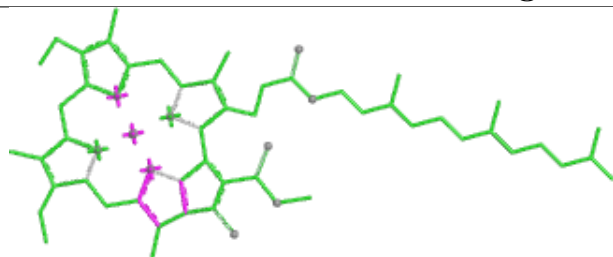


Torsions

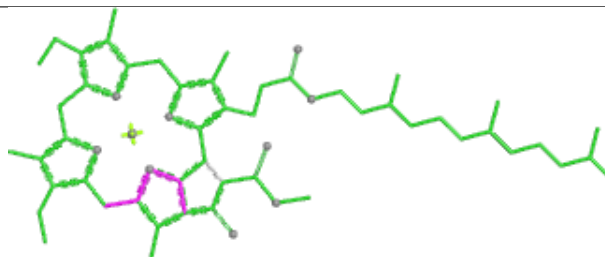


Rings

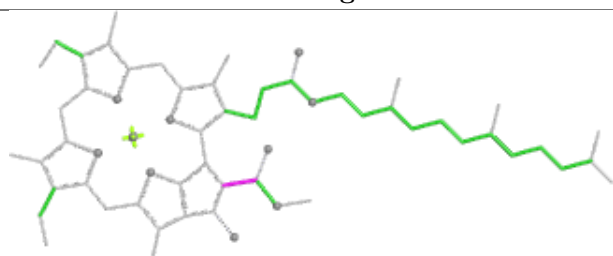
Ligand CLA 4 602



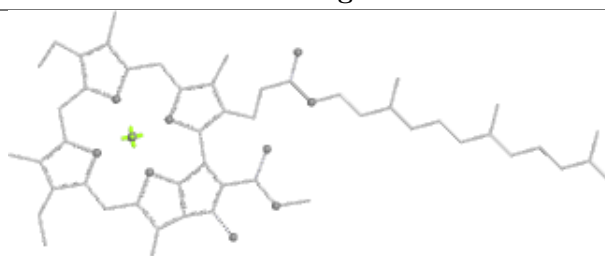
Bond lengths



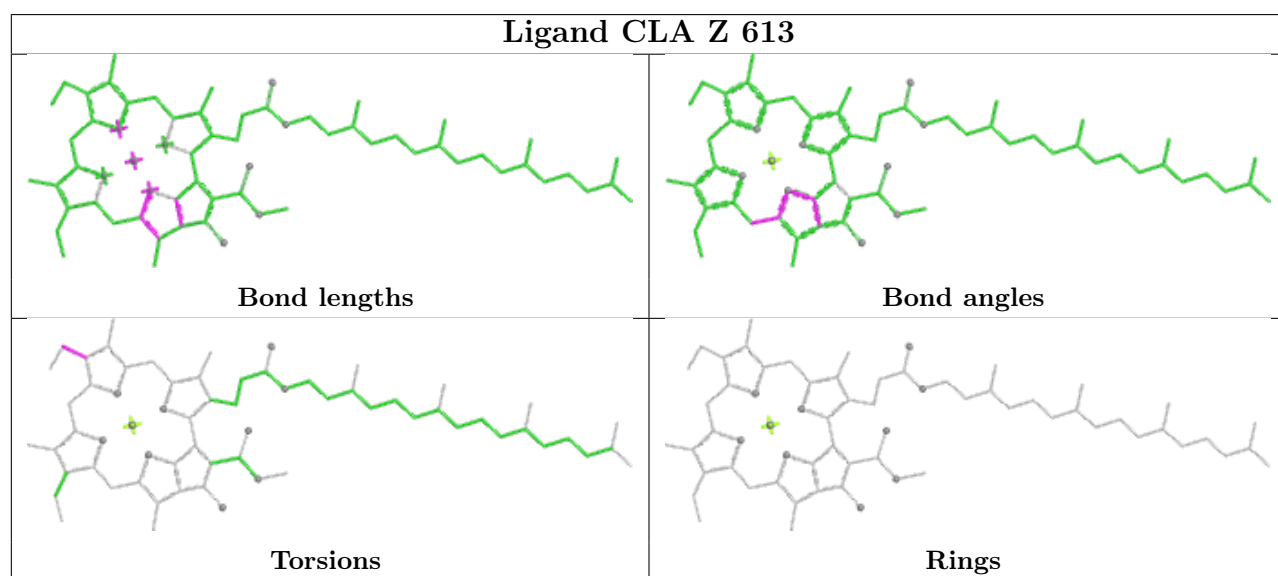
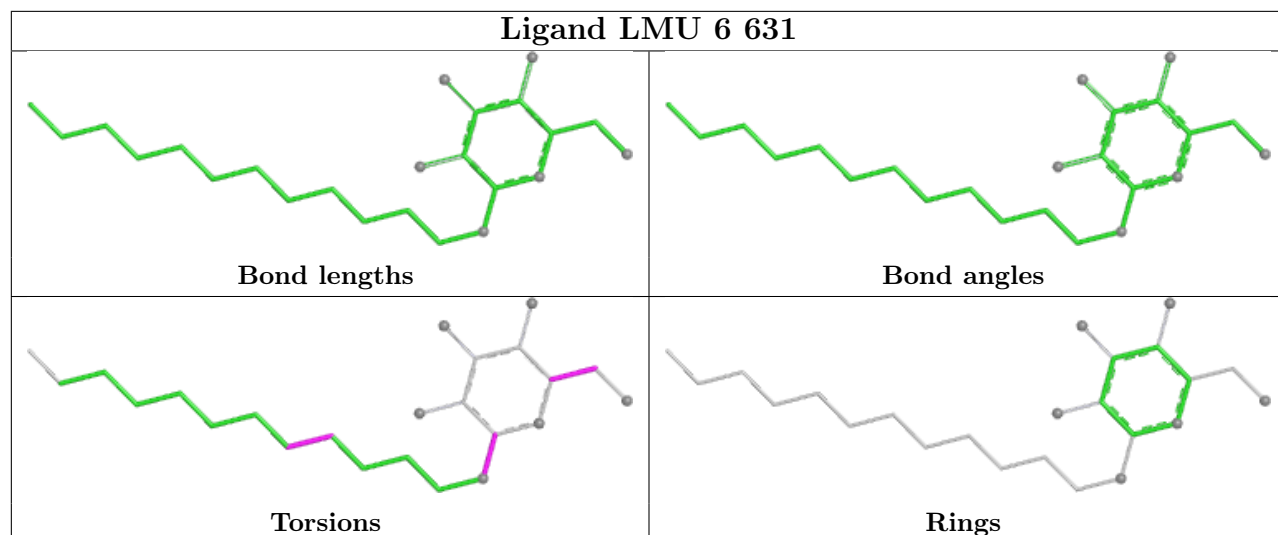
Bond angles



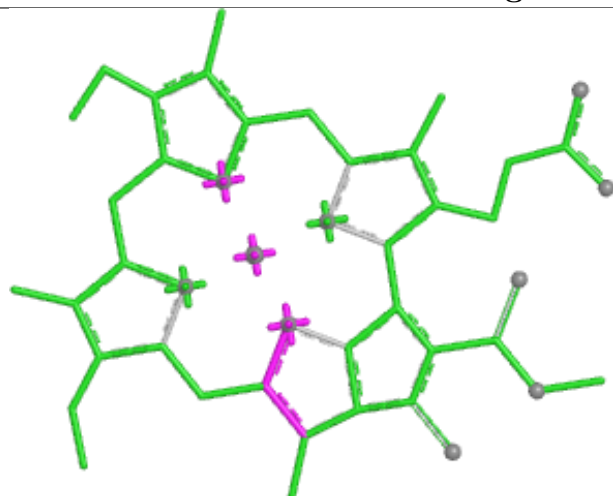
Torsions



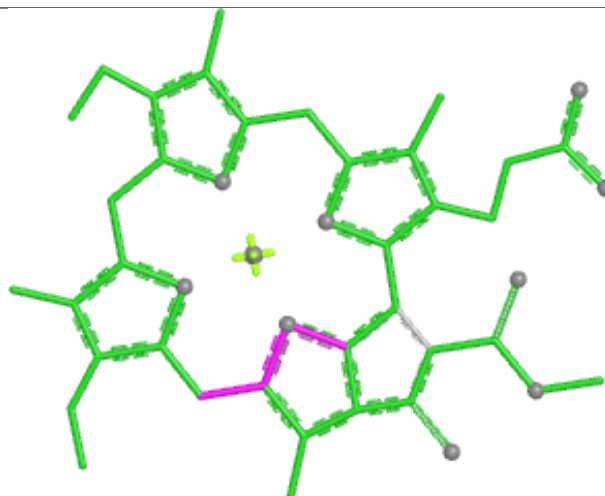
Rings



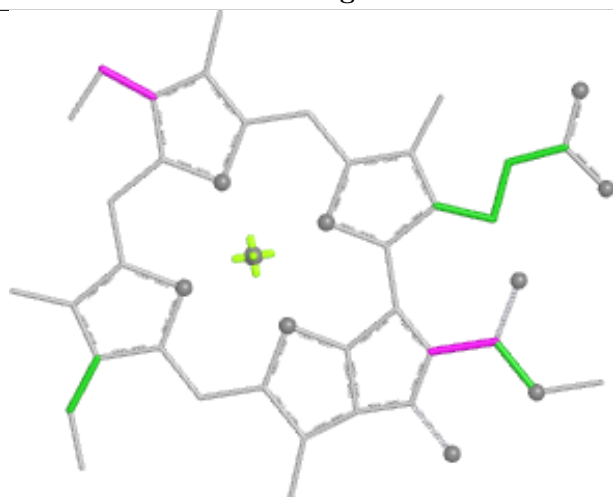
Ligand CLA B2 808



Bond lengths



Bond angles

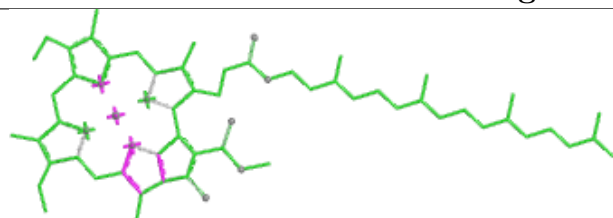


Torsions

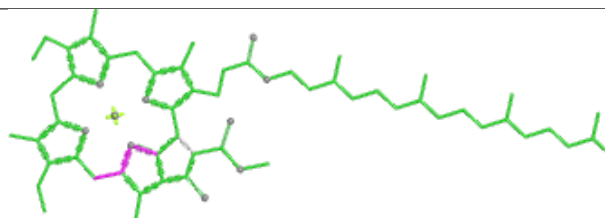


Rings

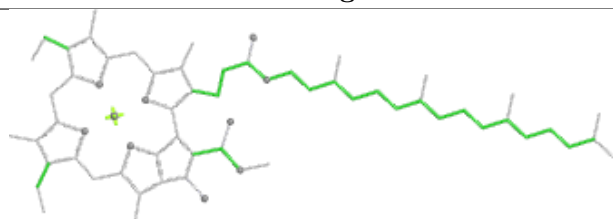
Ligand CLA 7 613



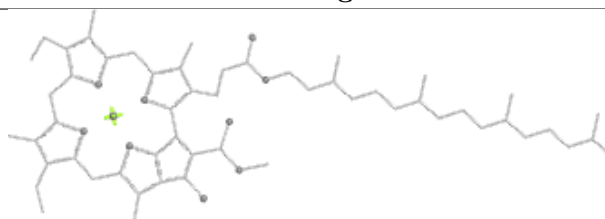
Bond lengths



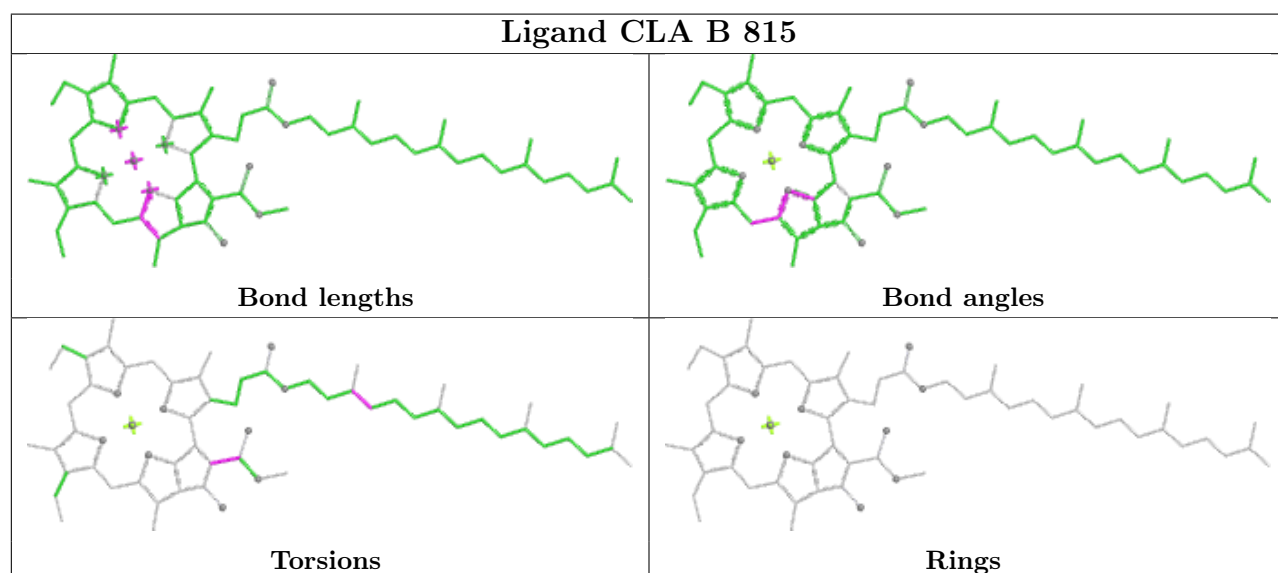
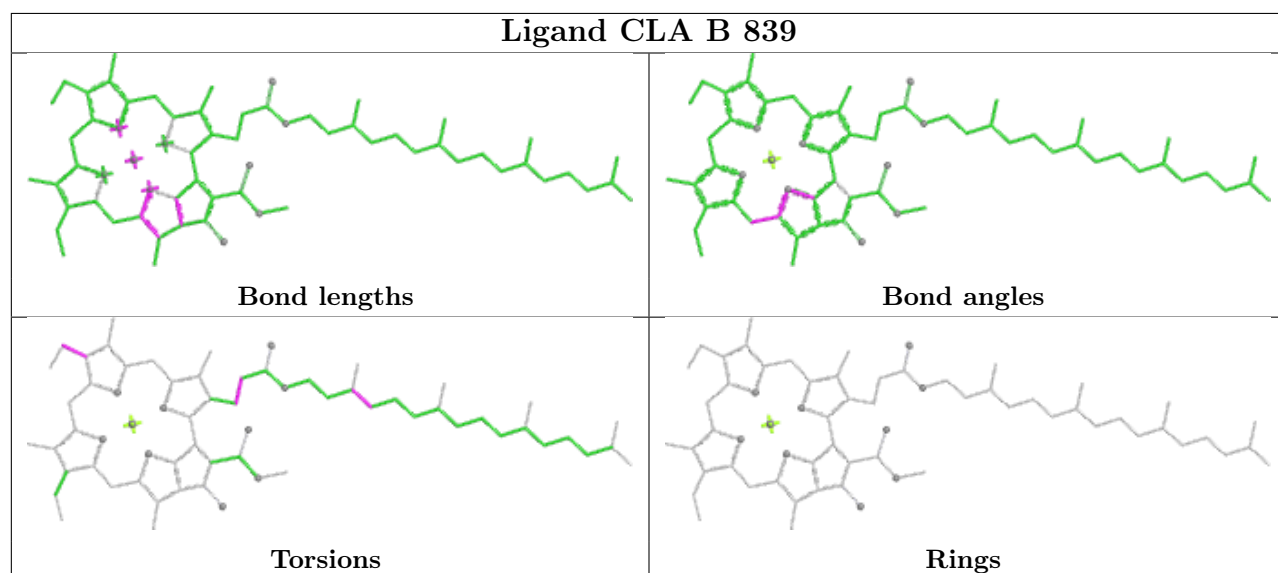
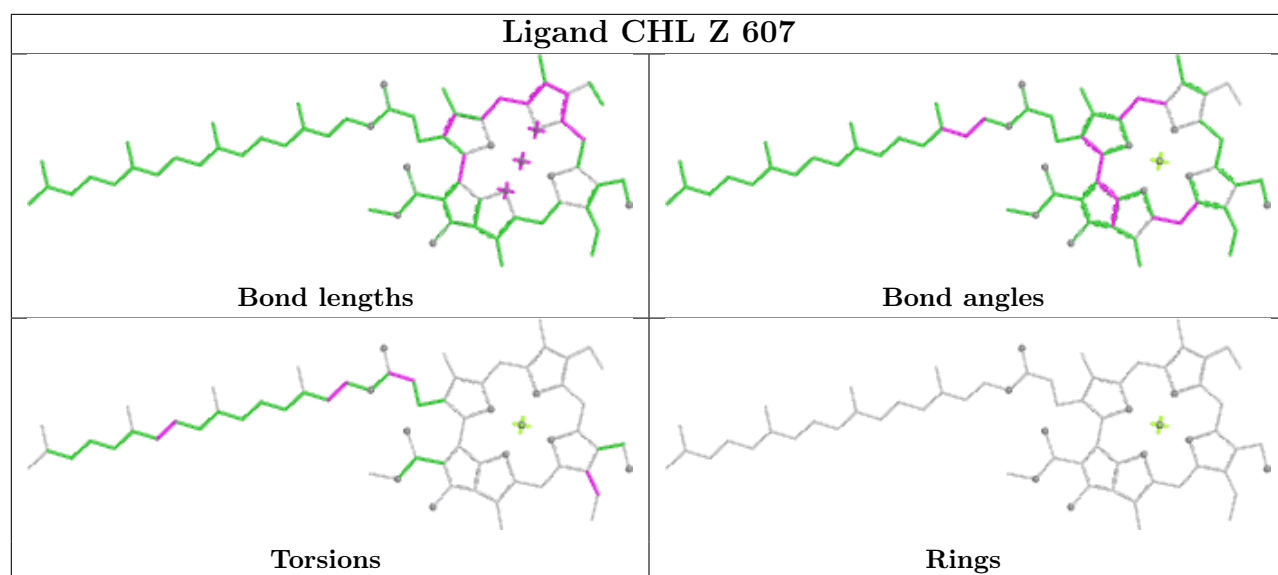
Bond angles

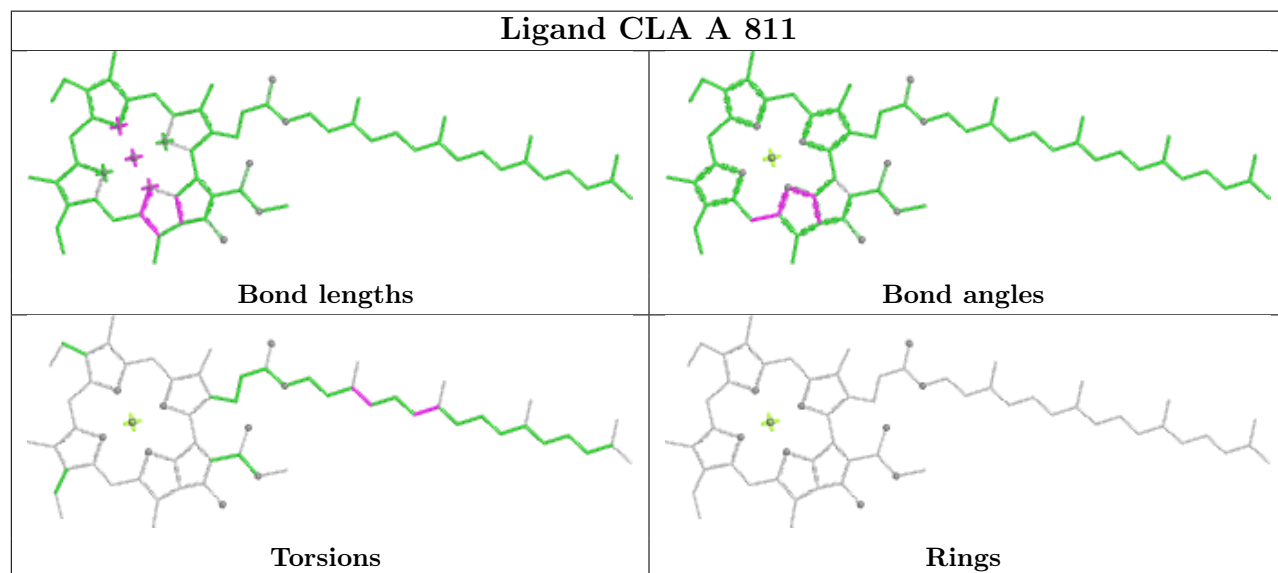
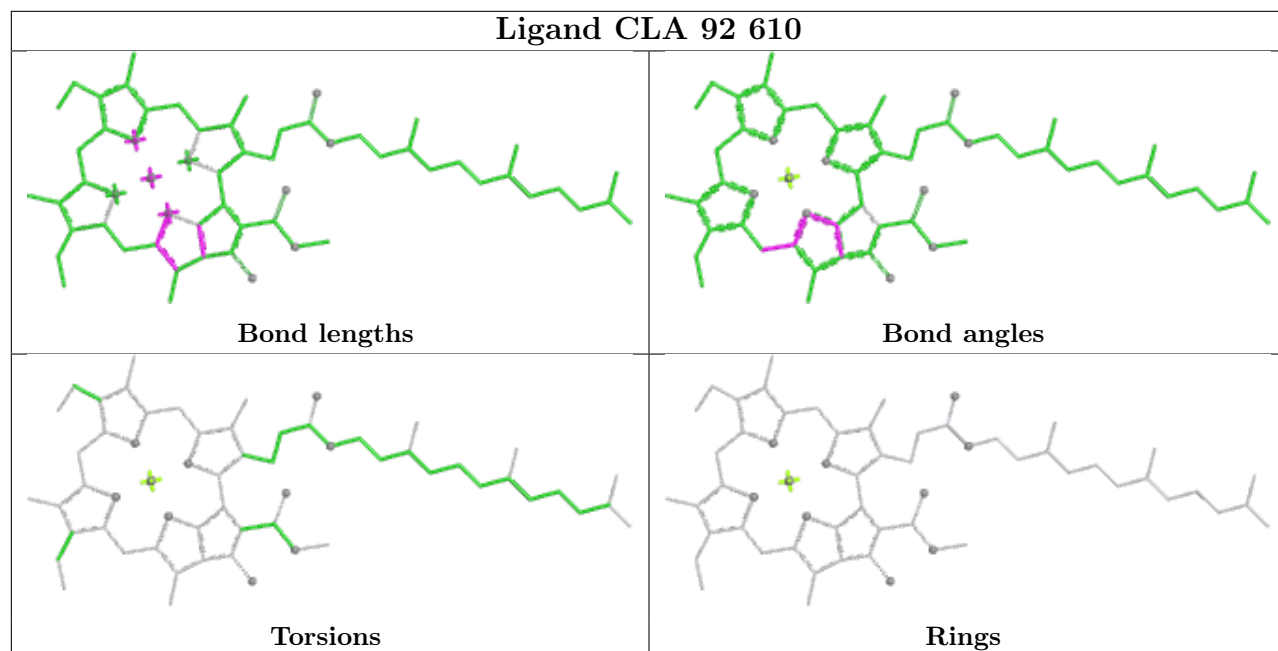


Torsions

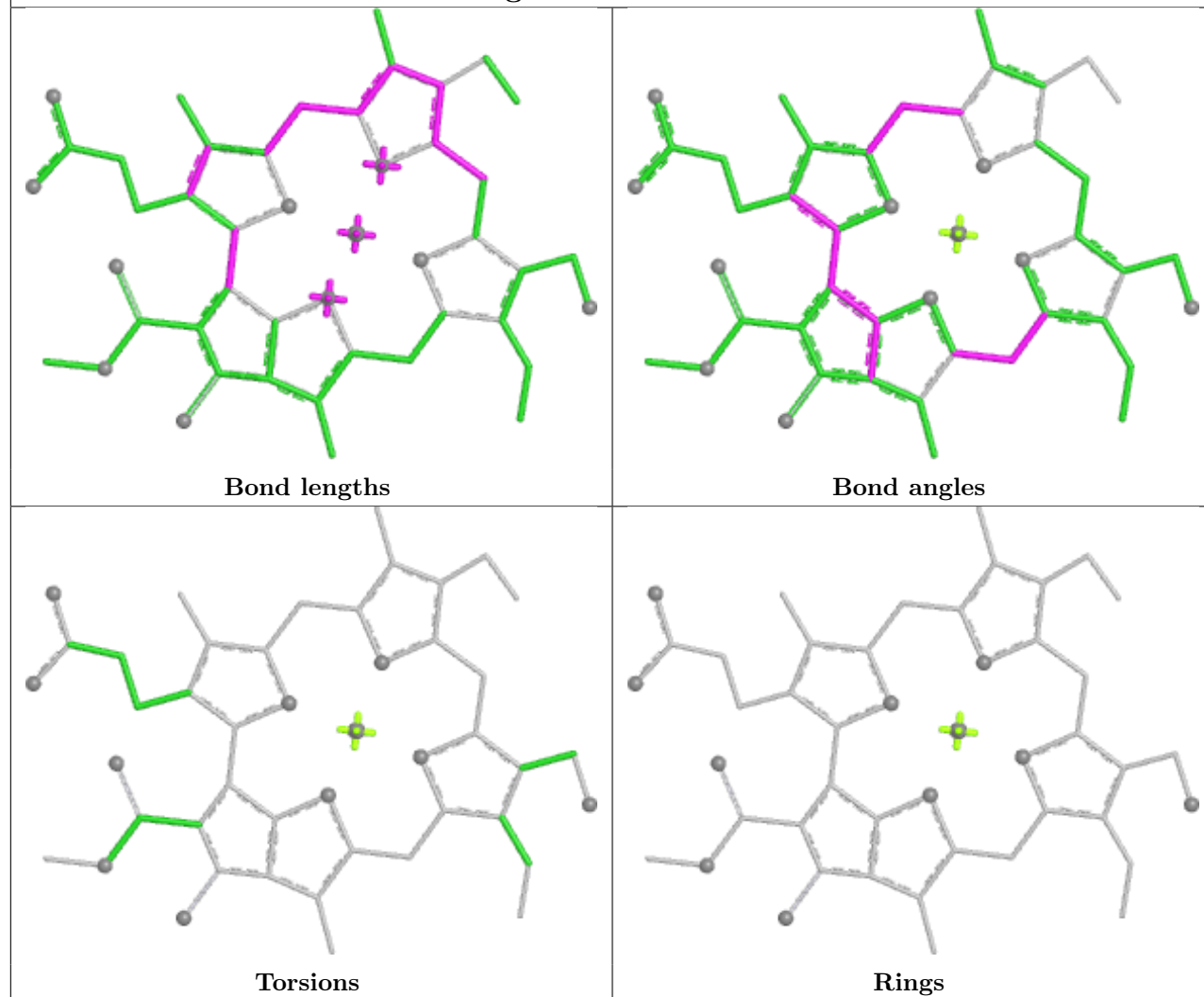


Rings

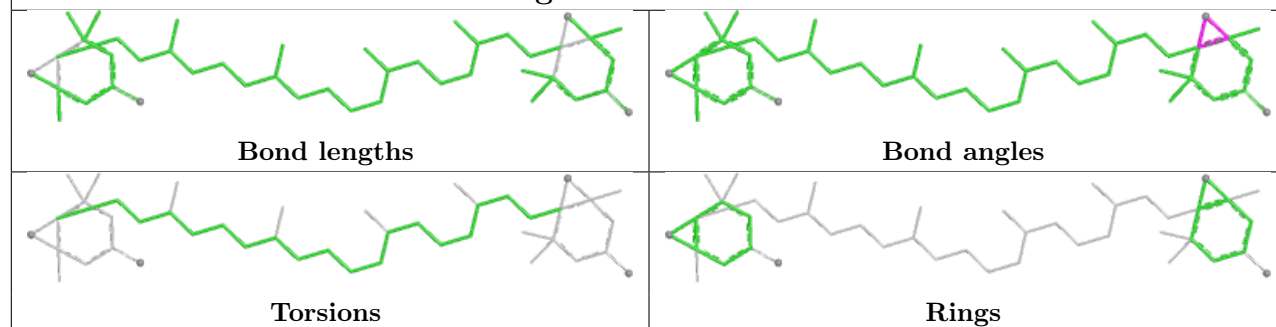


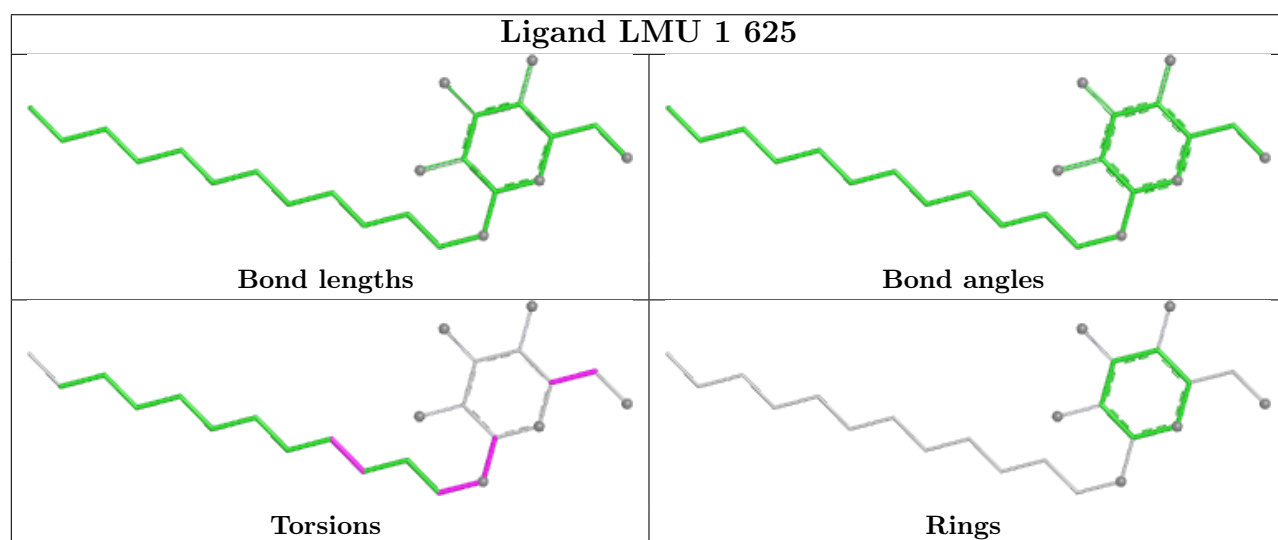
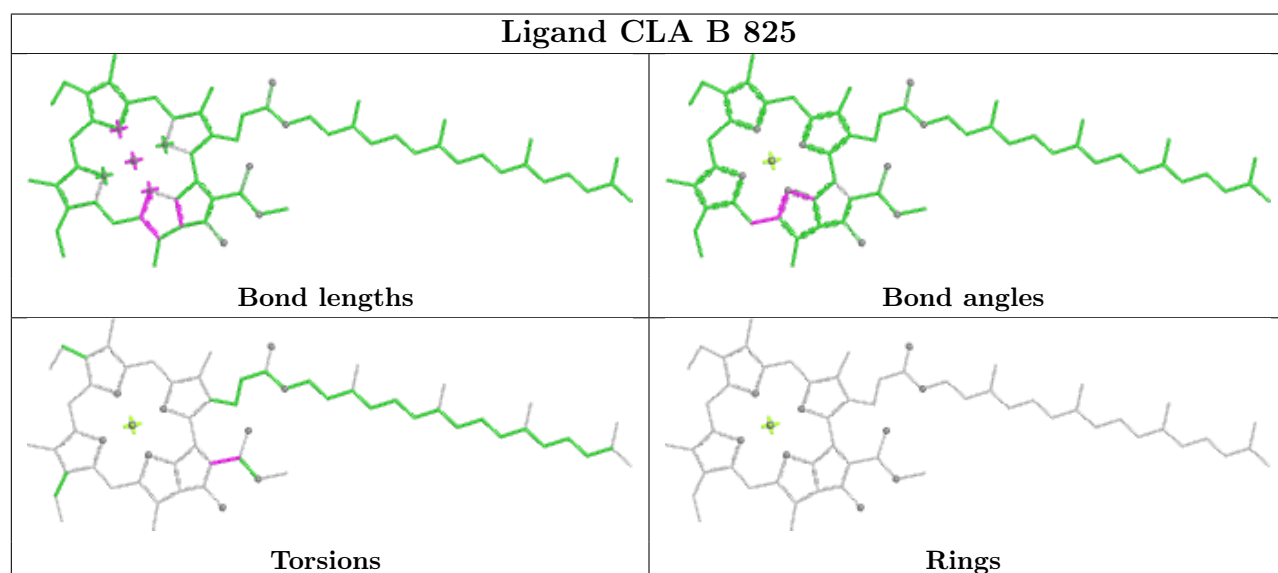
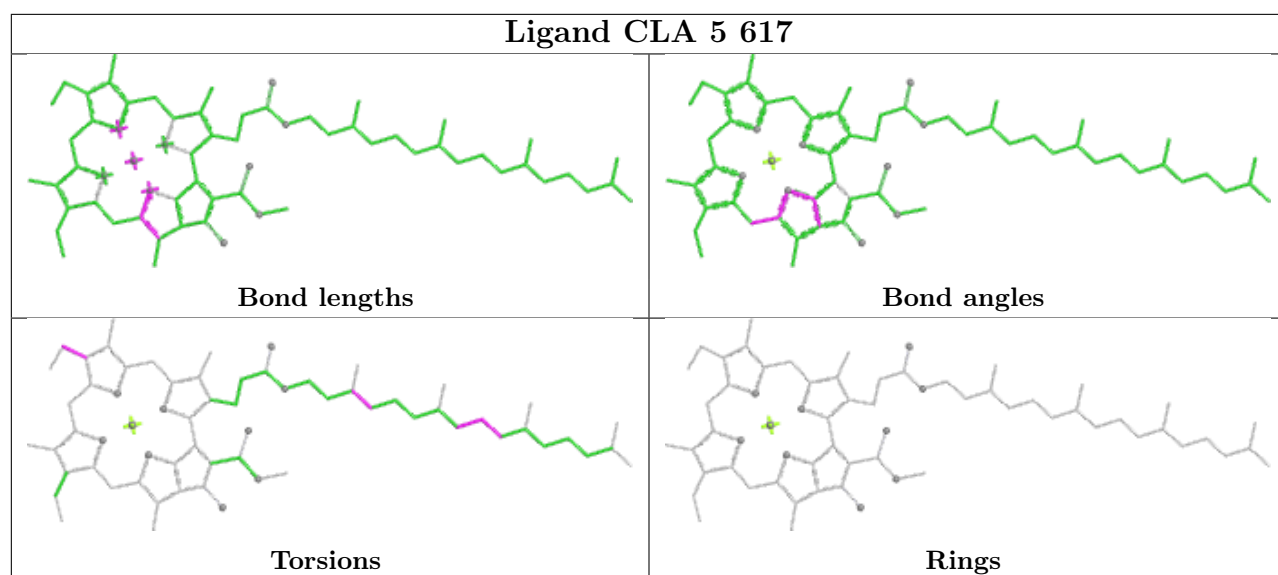


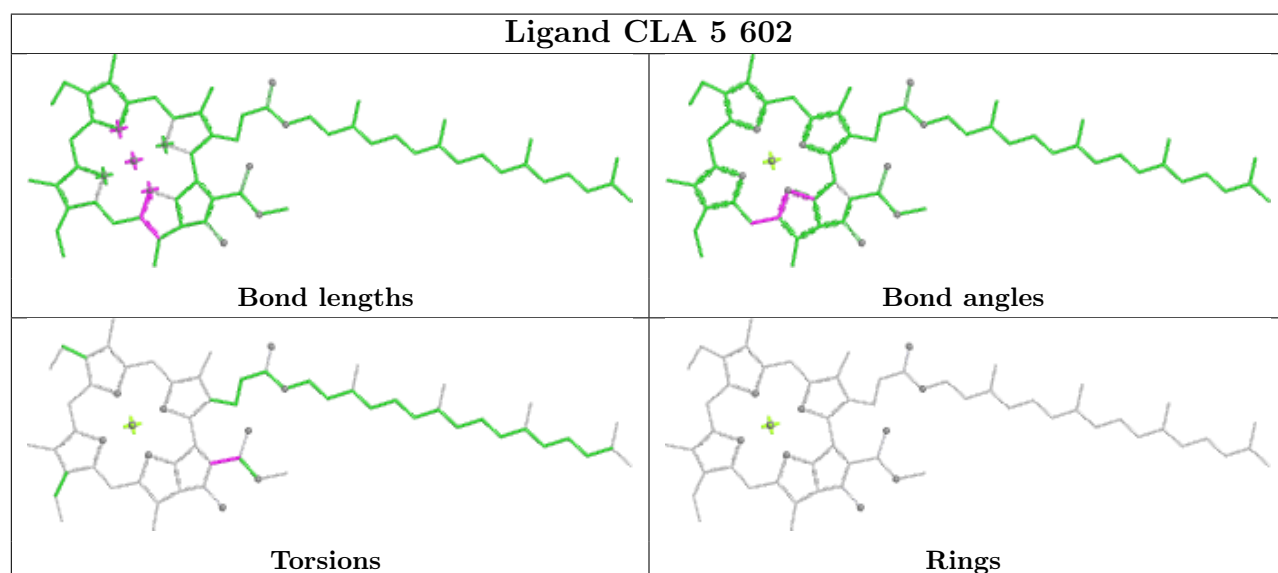
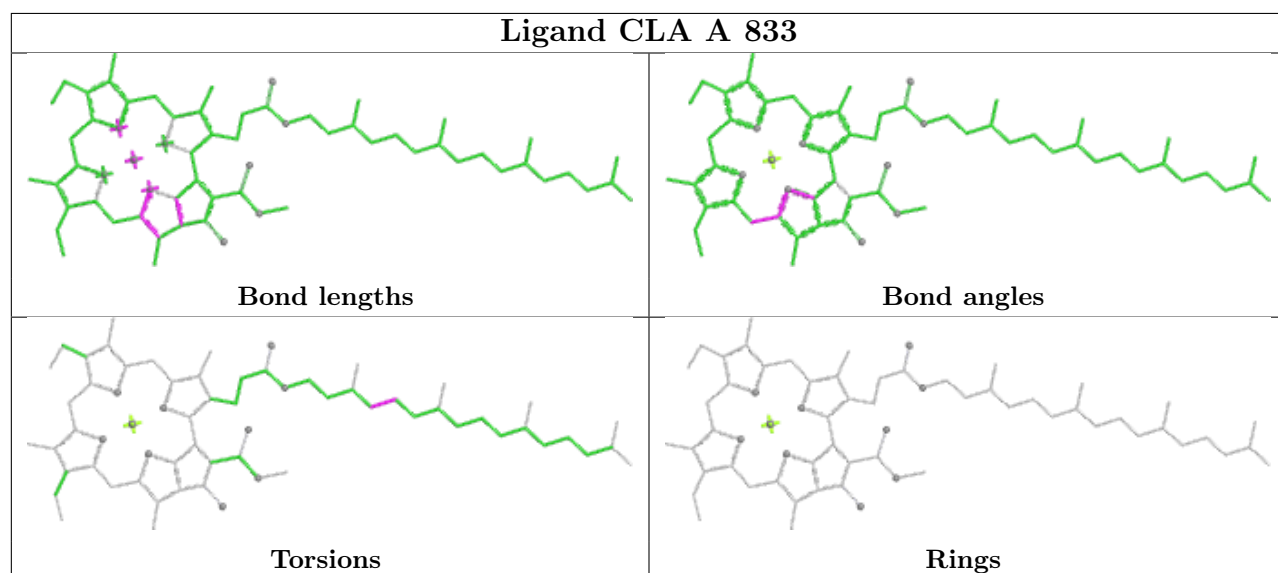
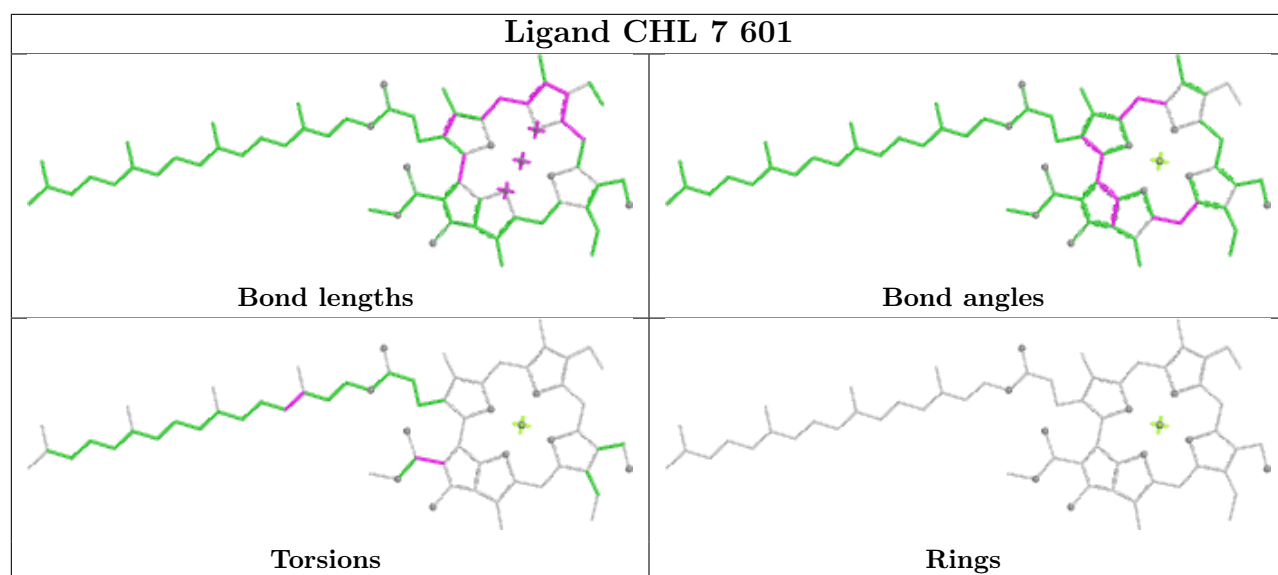
Ligand CHL 7 607

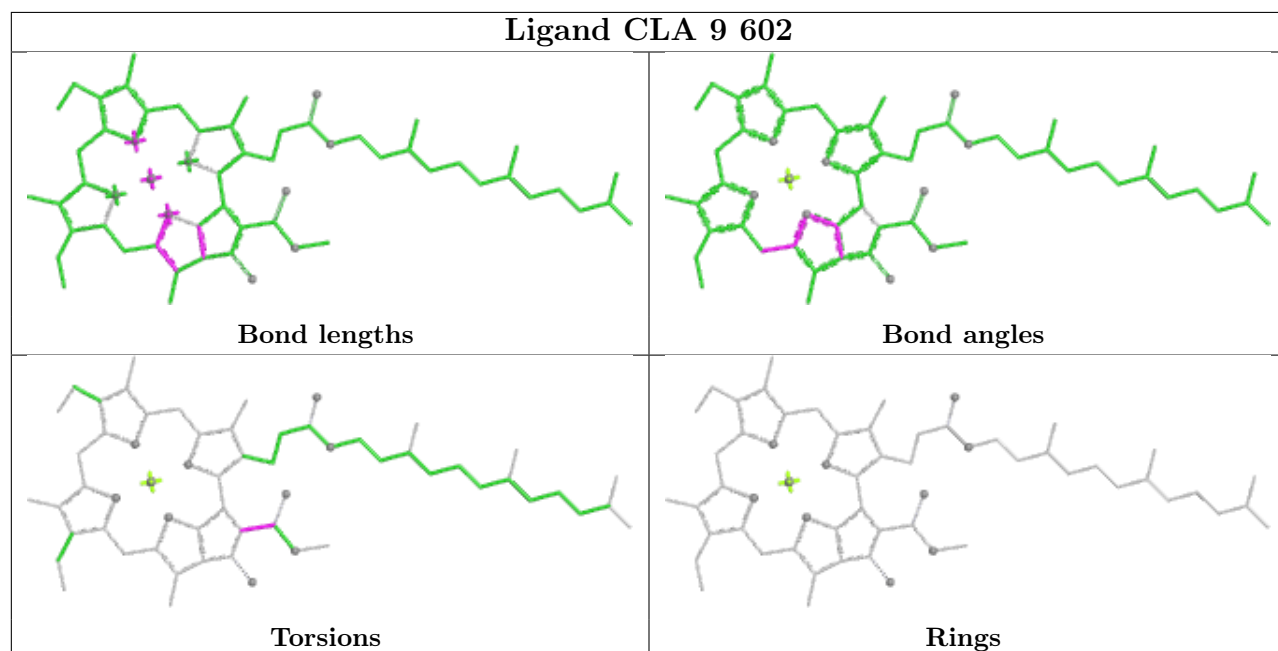
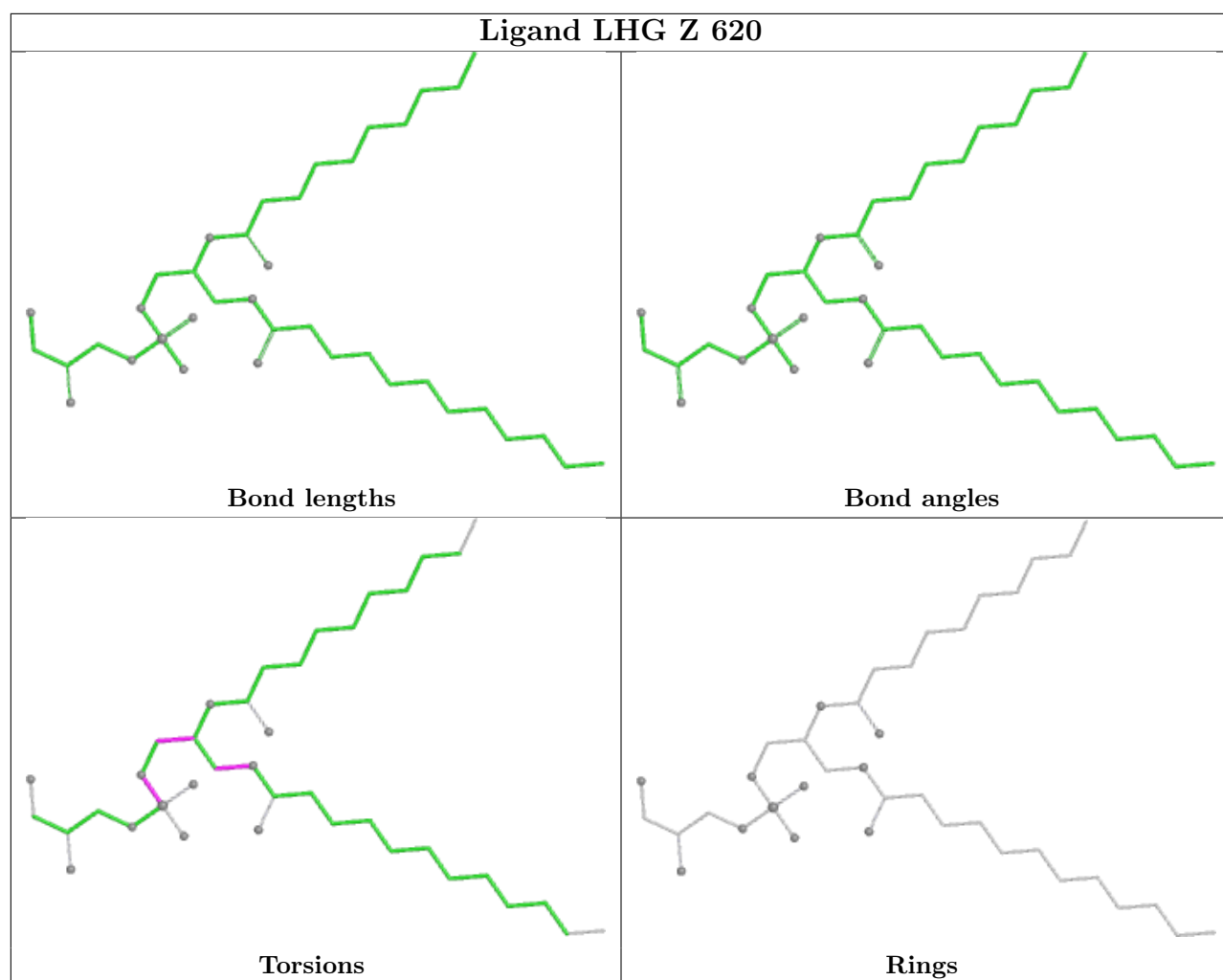


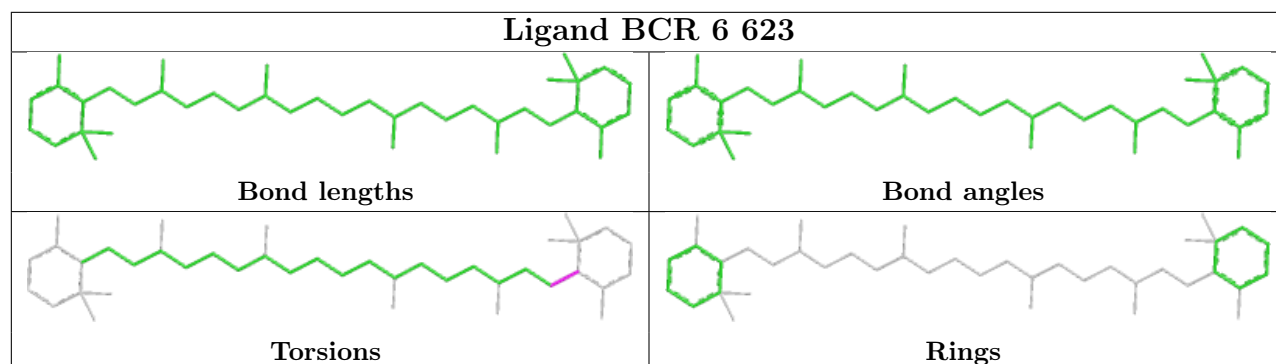
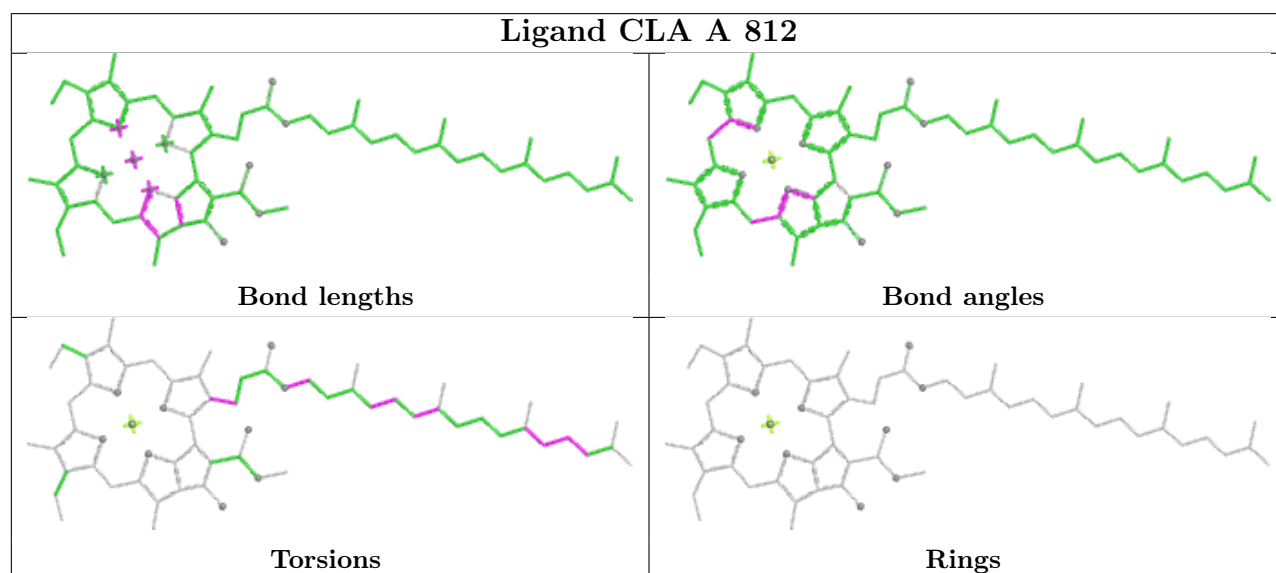
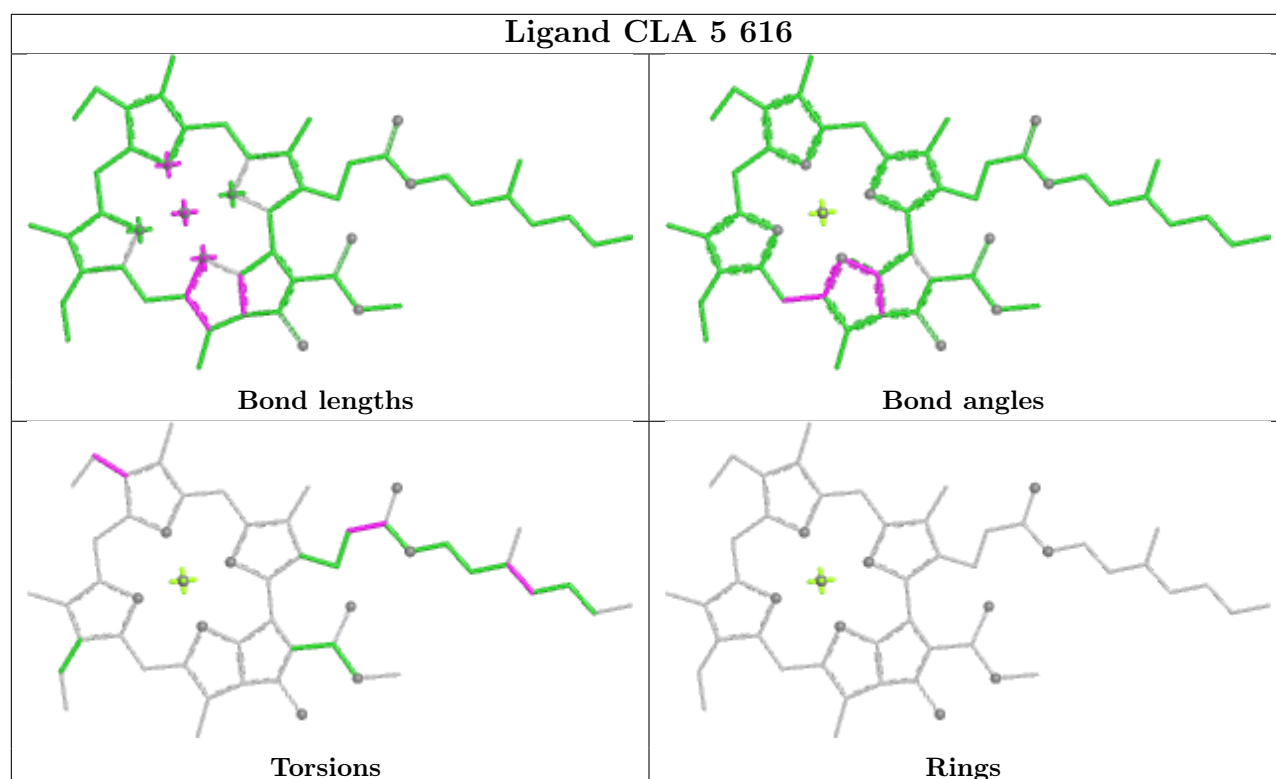
Ligand XAT 7 622

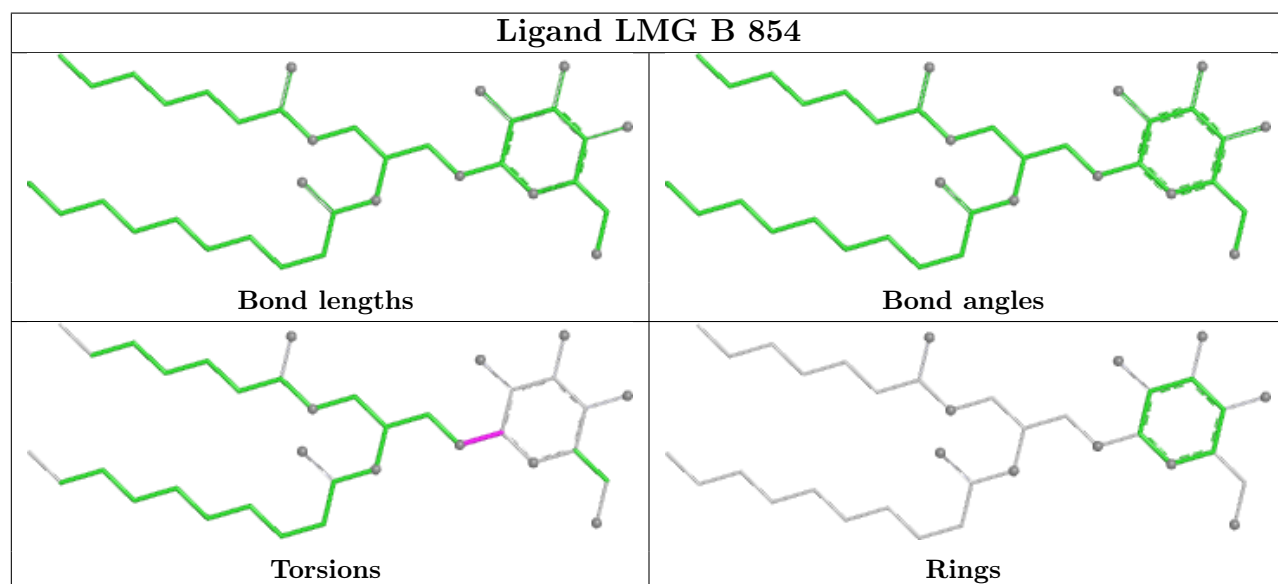
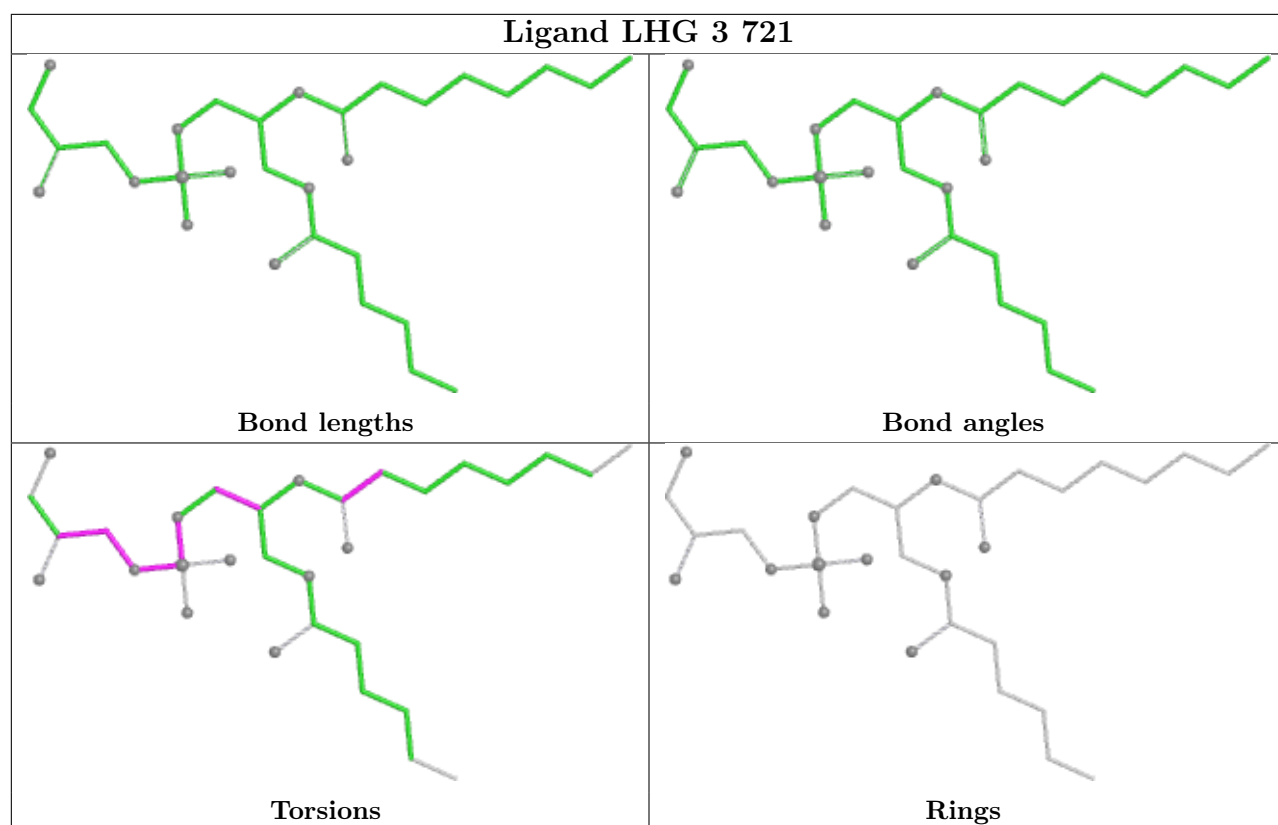


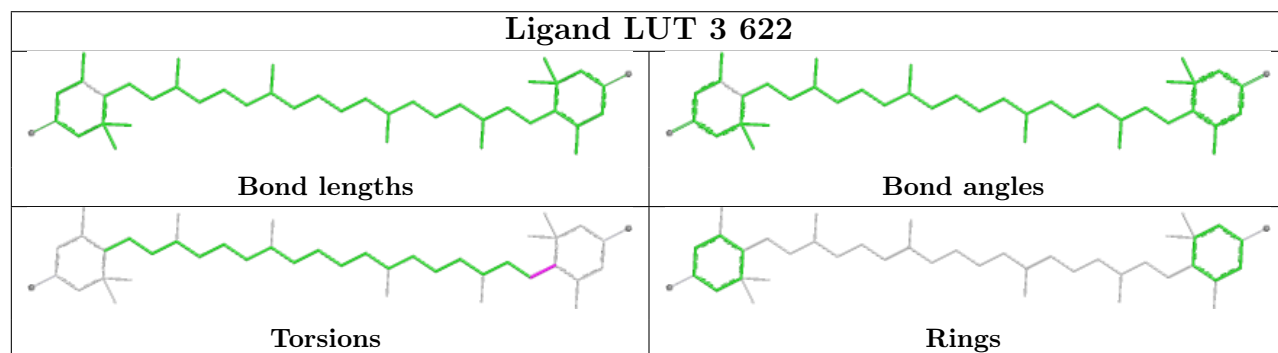
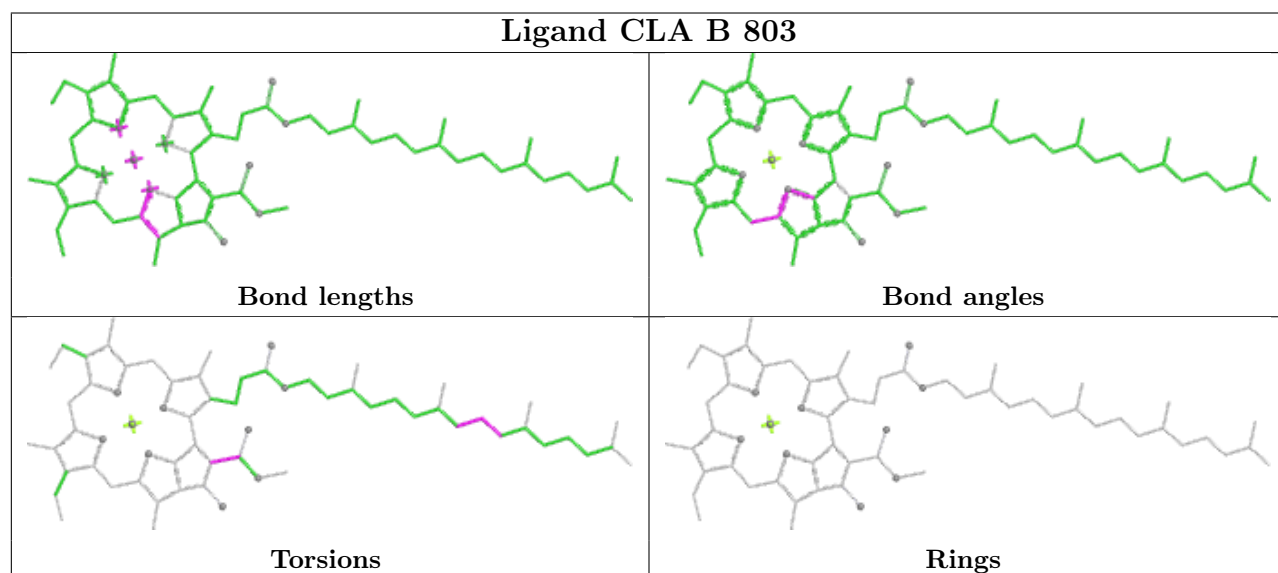
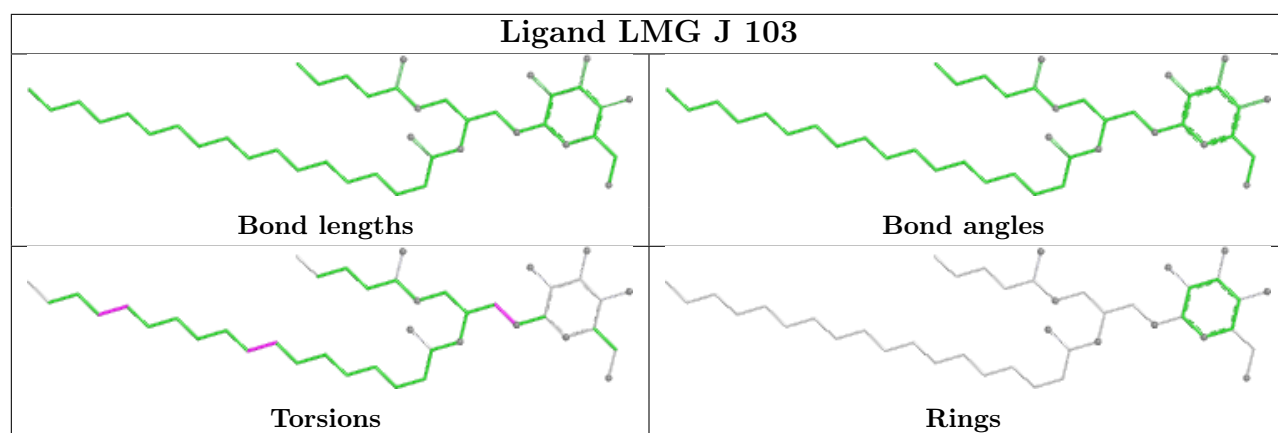


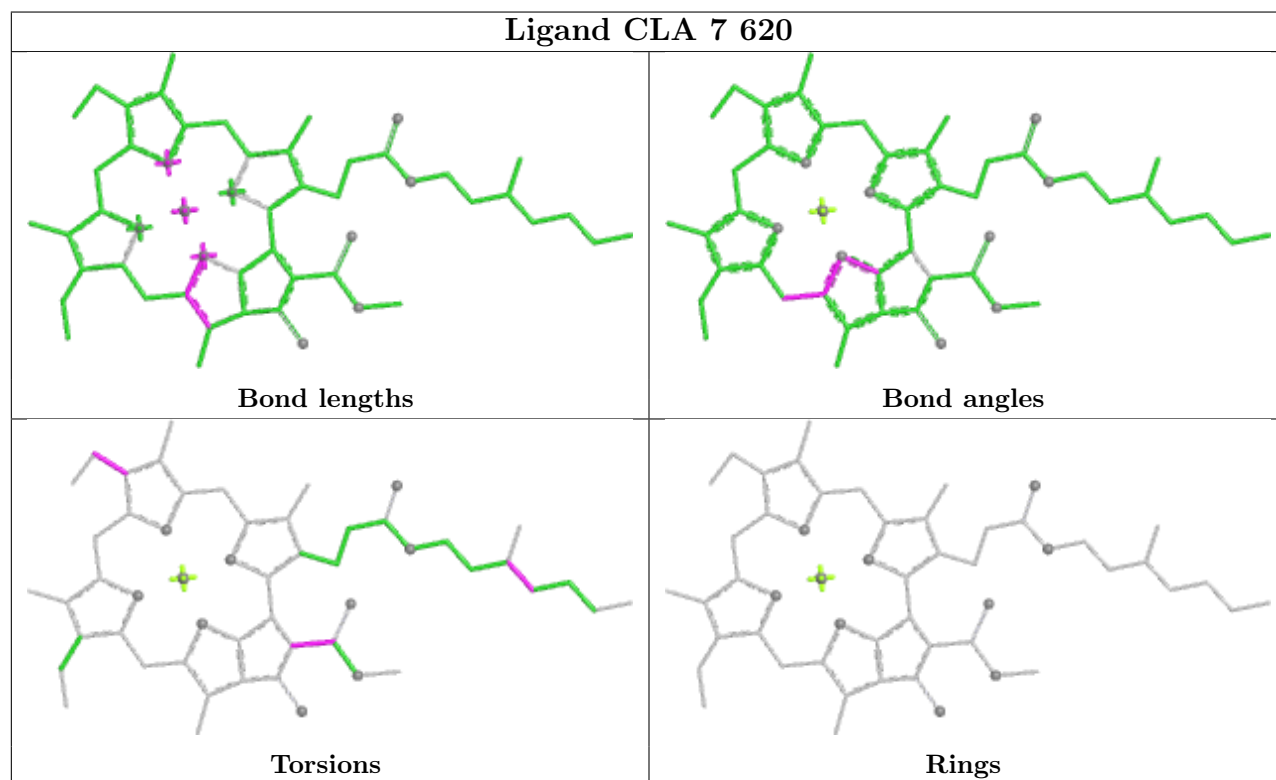
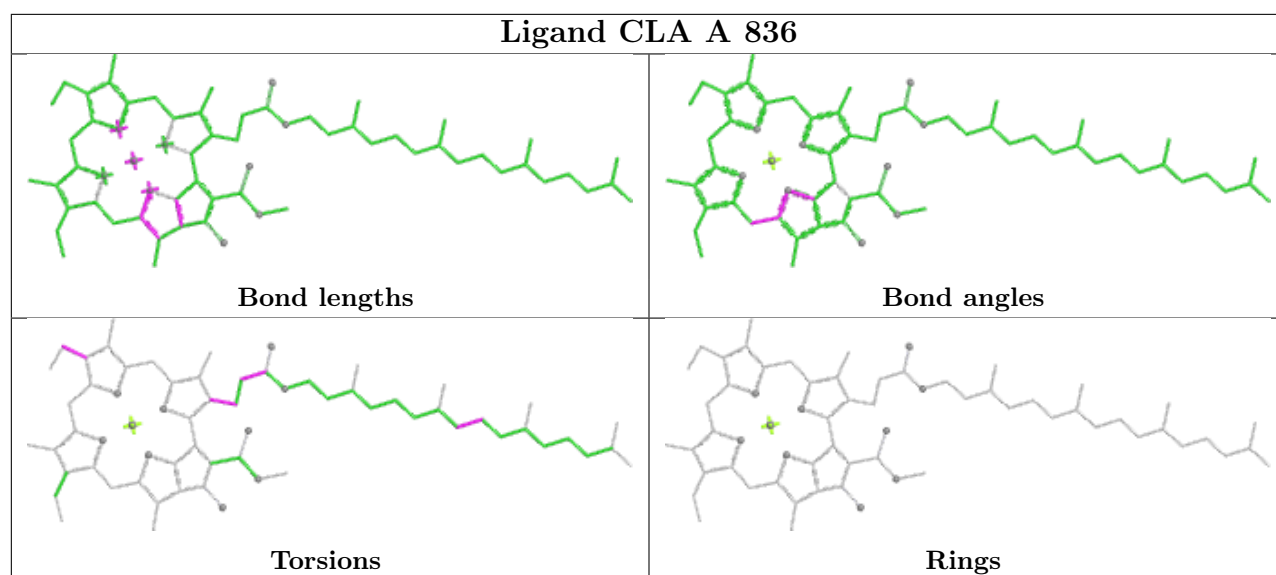


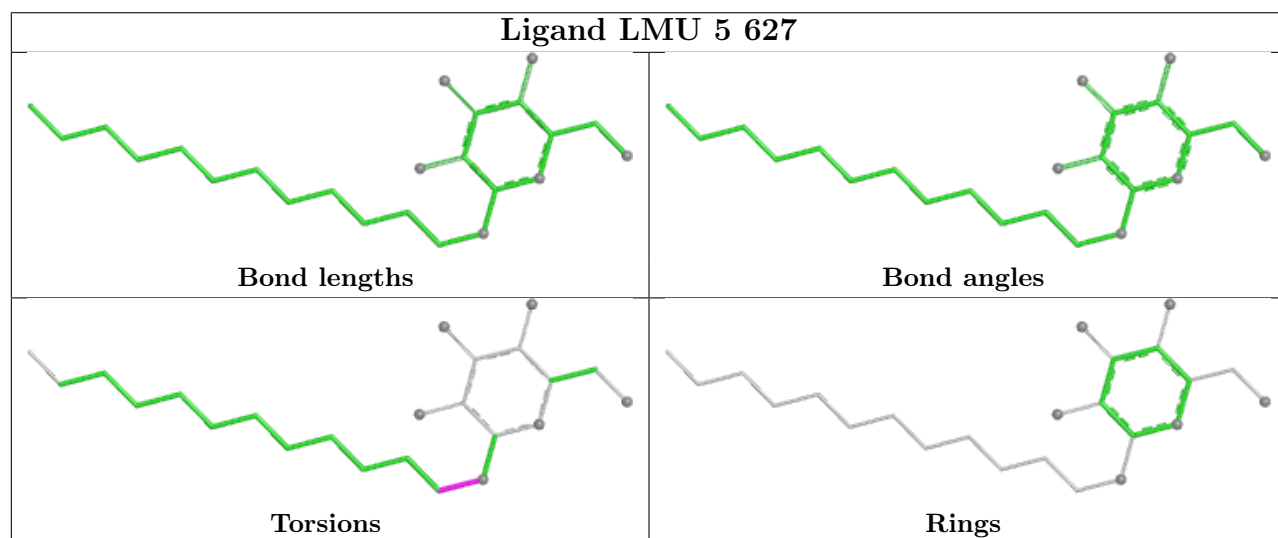
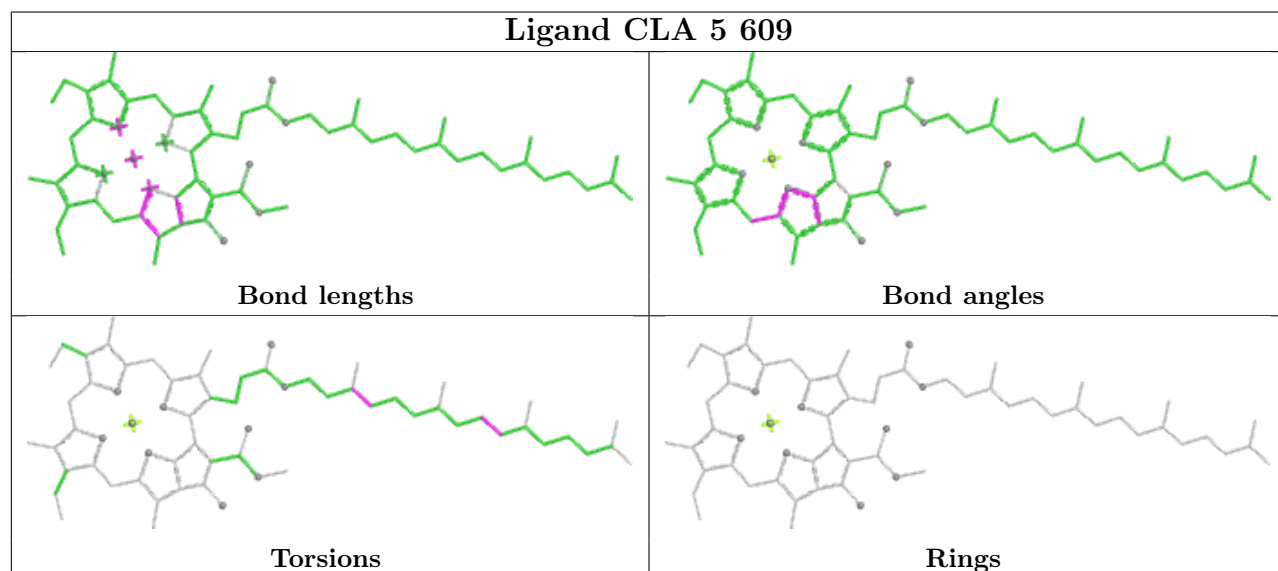
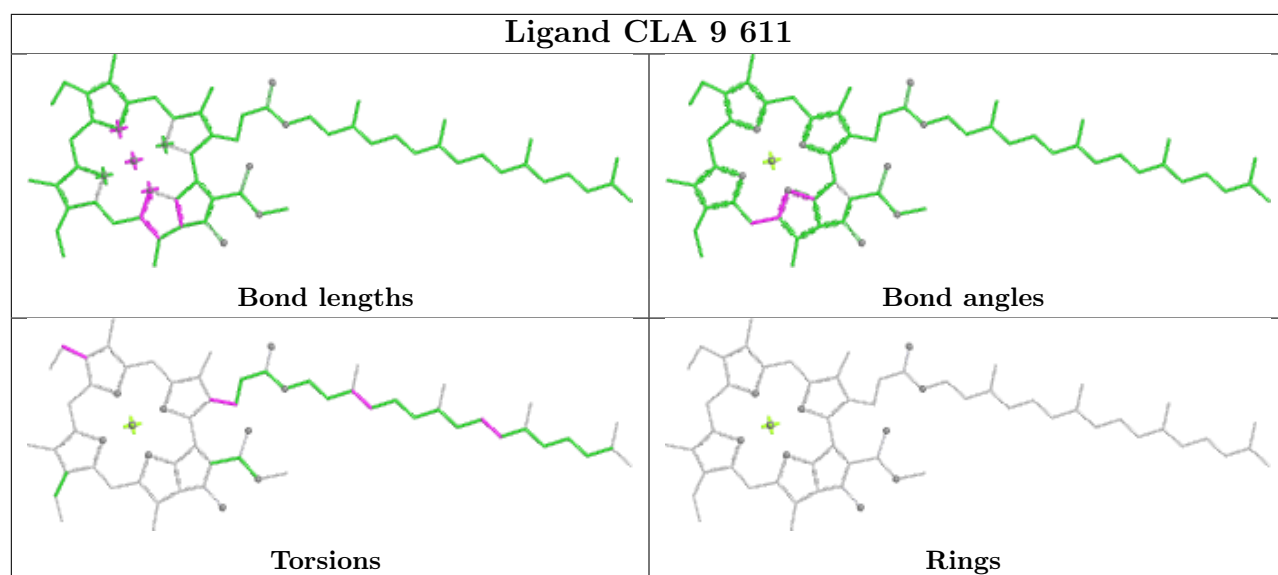


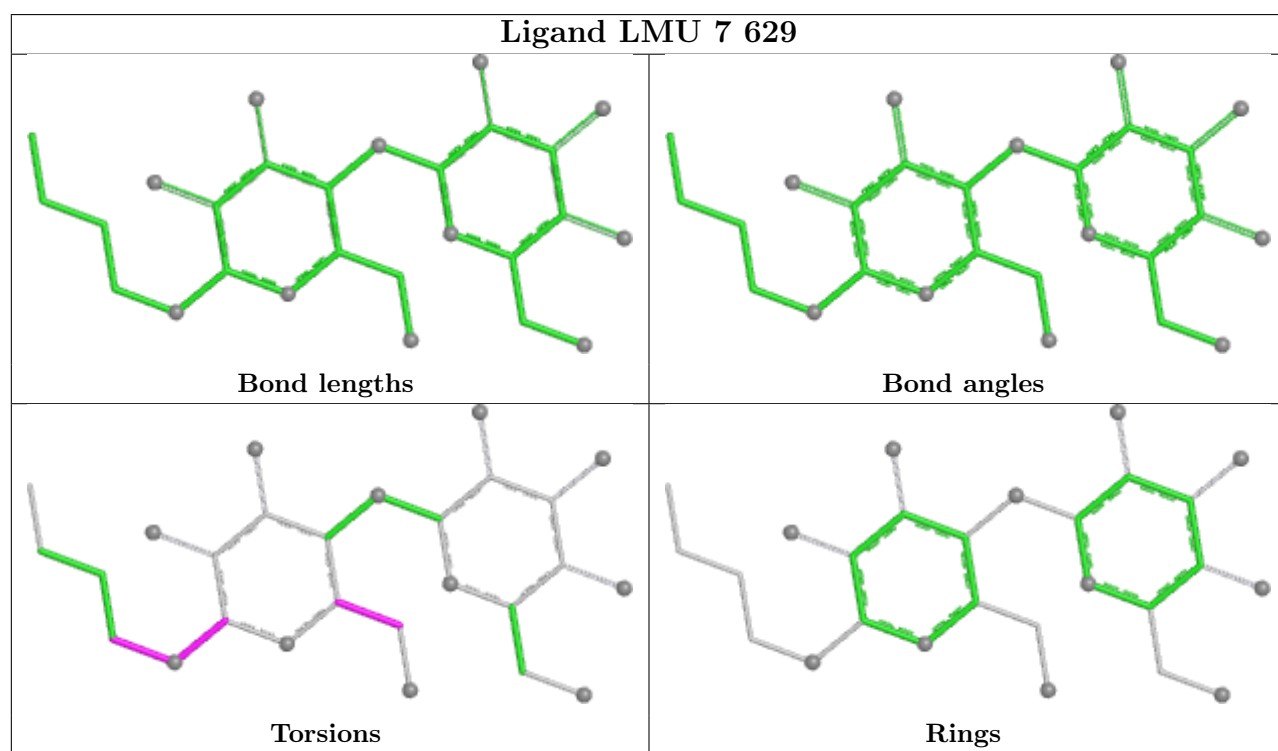
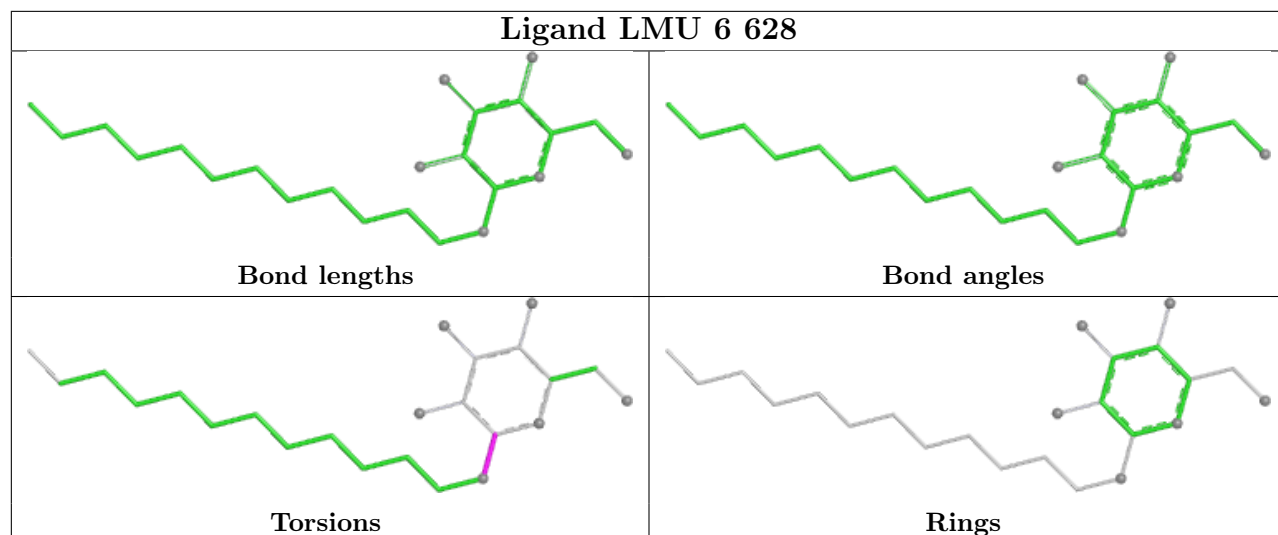


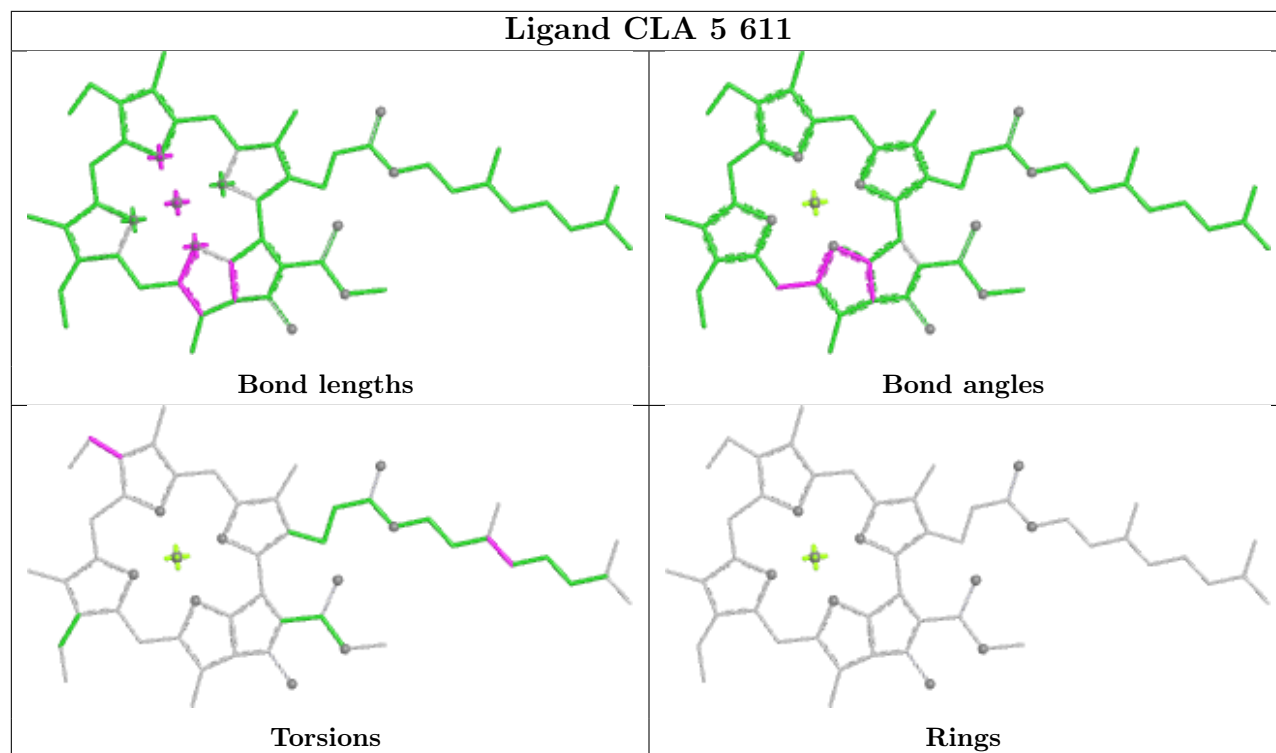
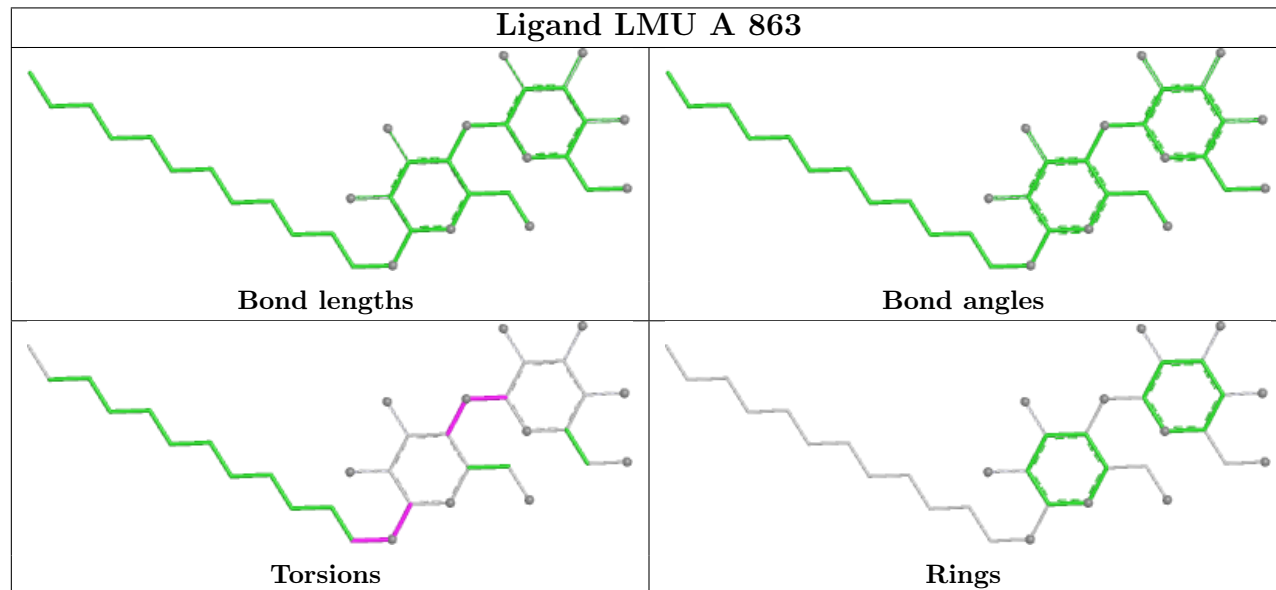




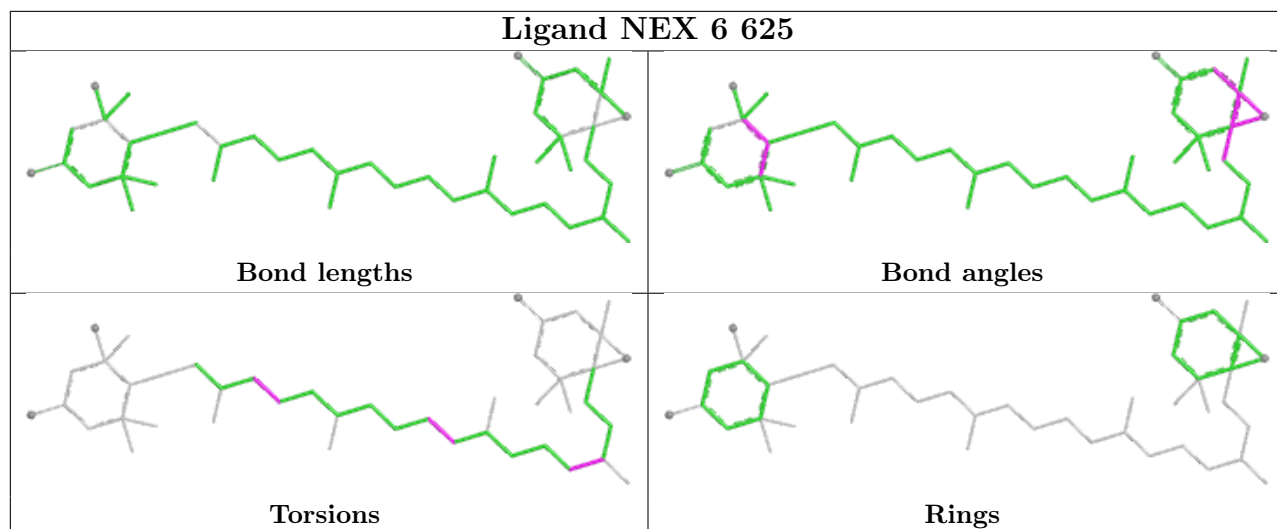




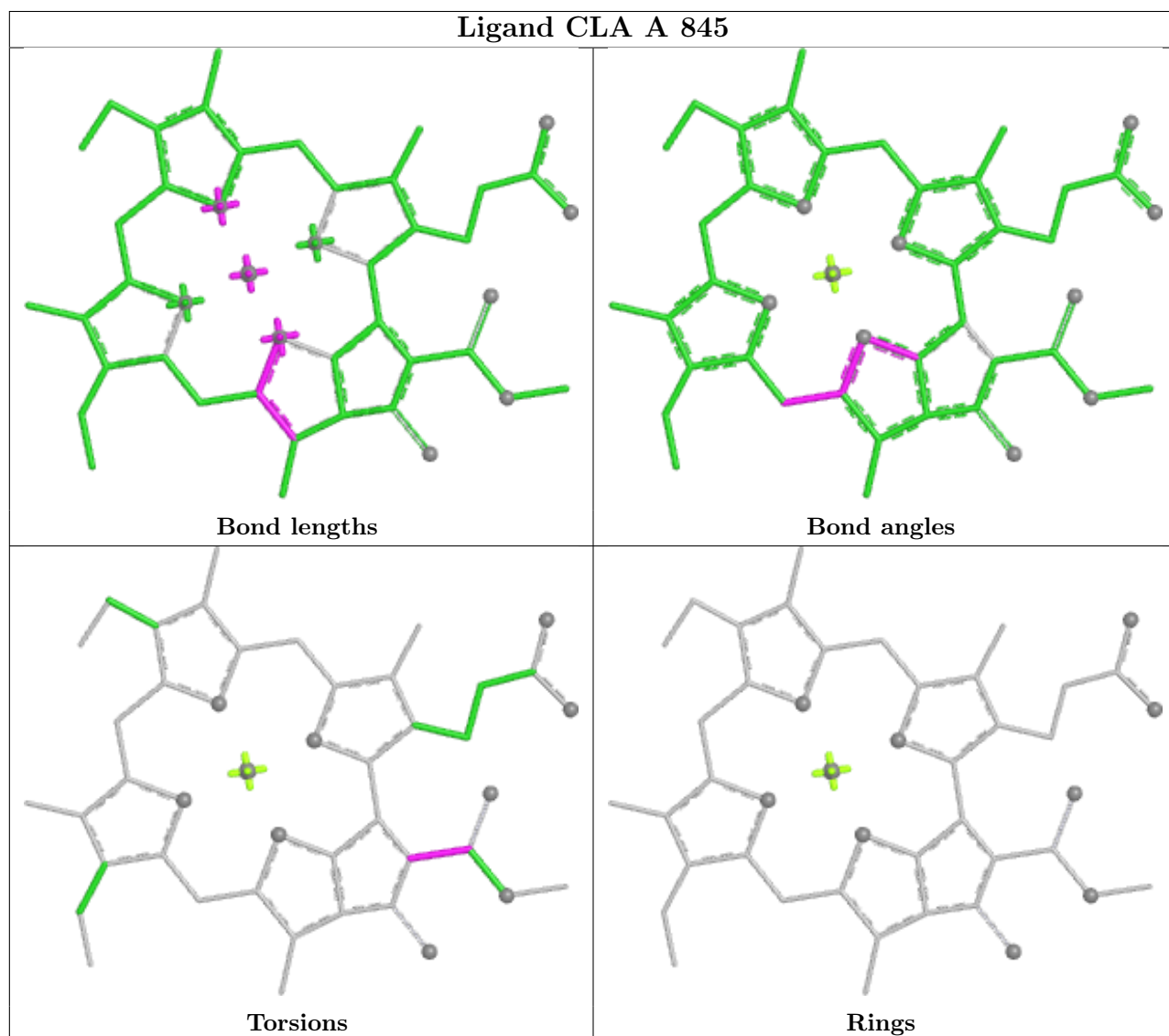


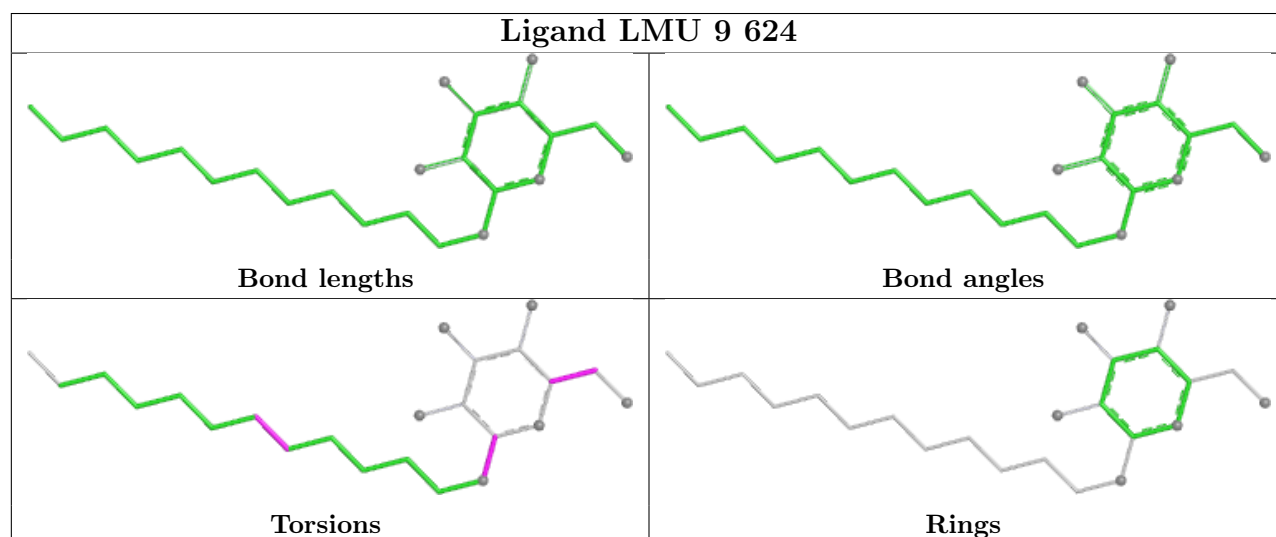
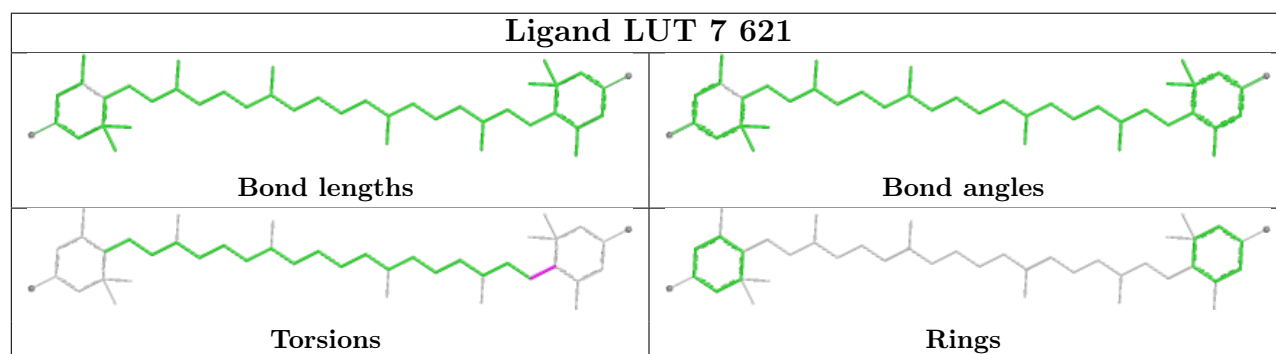
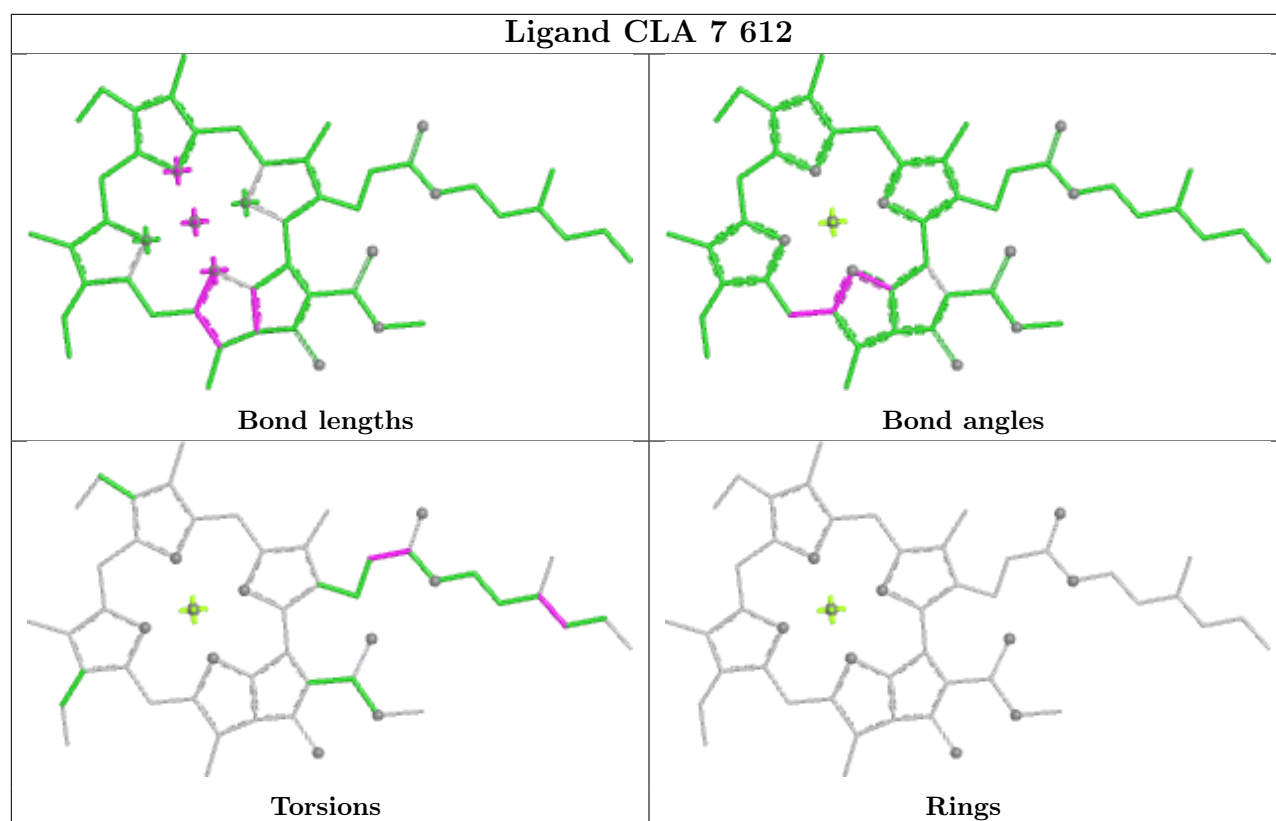
Ligand CLA 5 611**Ligand LMU A 863**

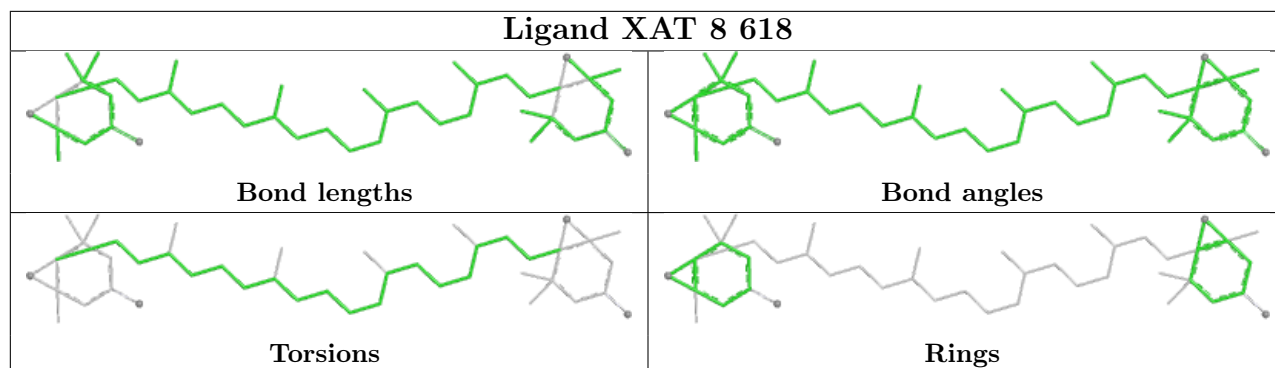
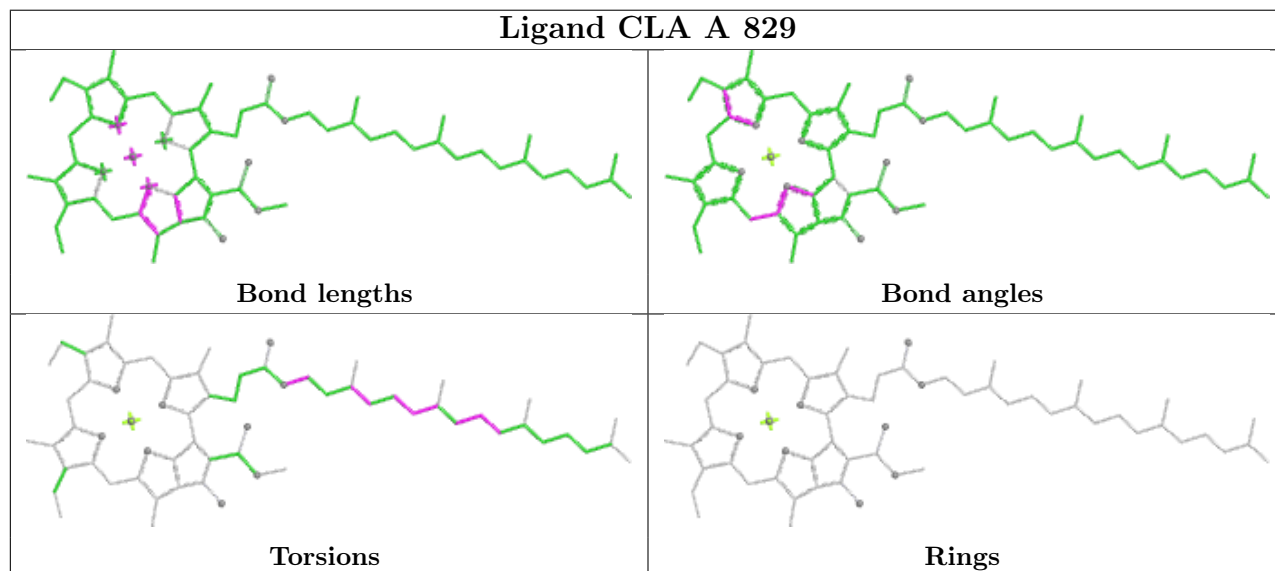
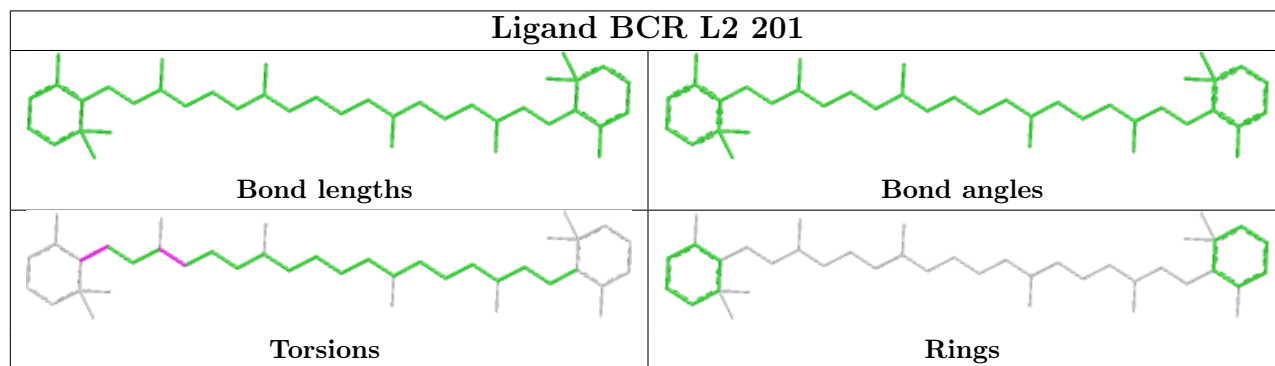
Ligand NEX 6 625

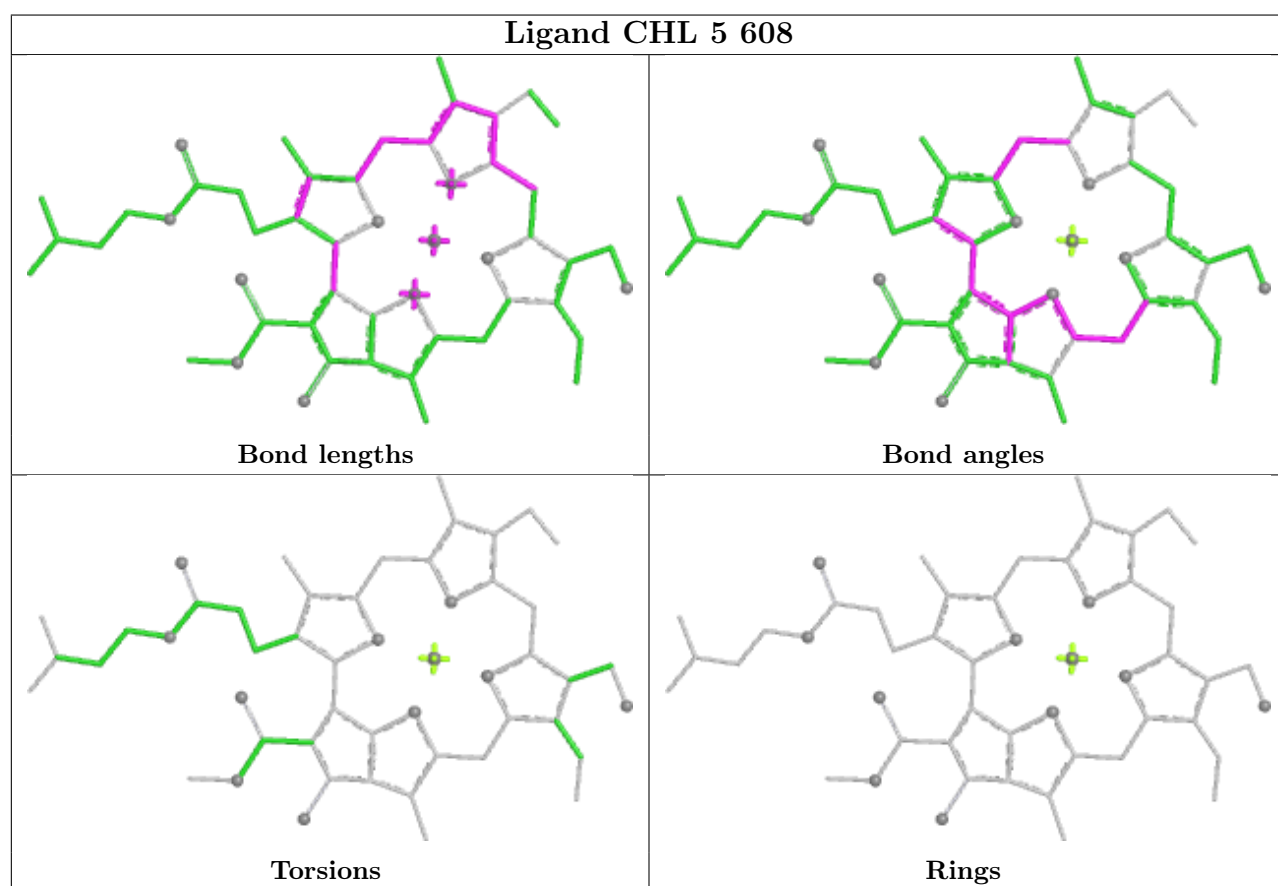
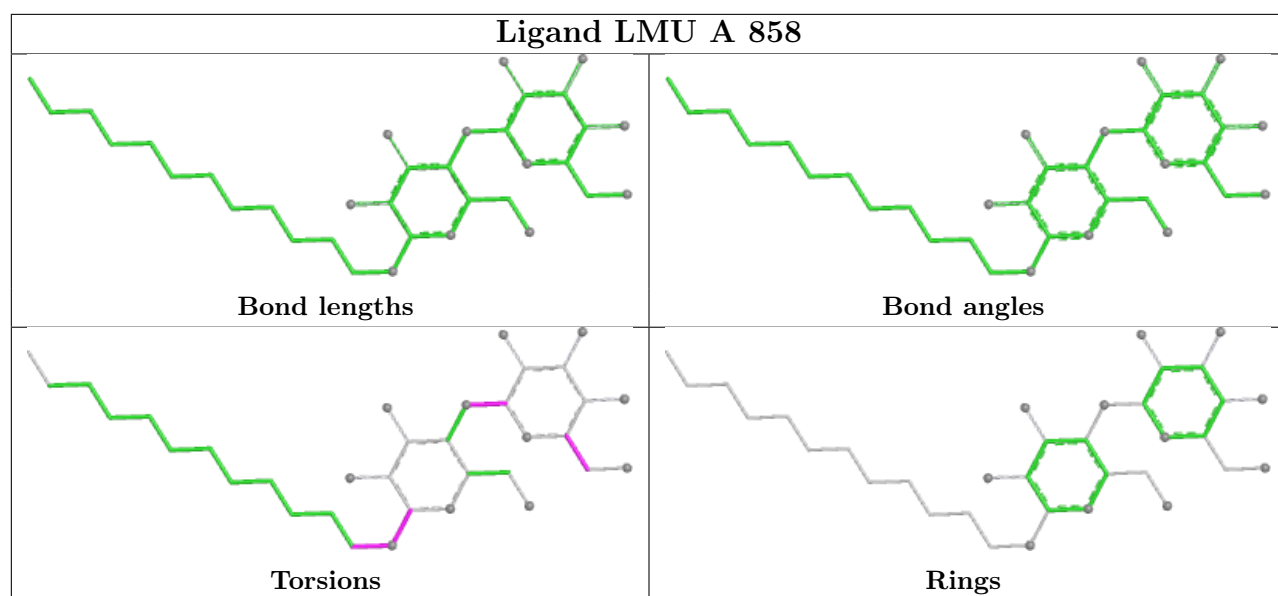


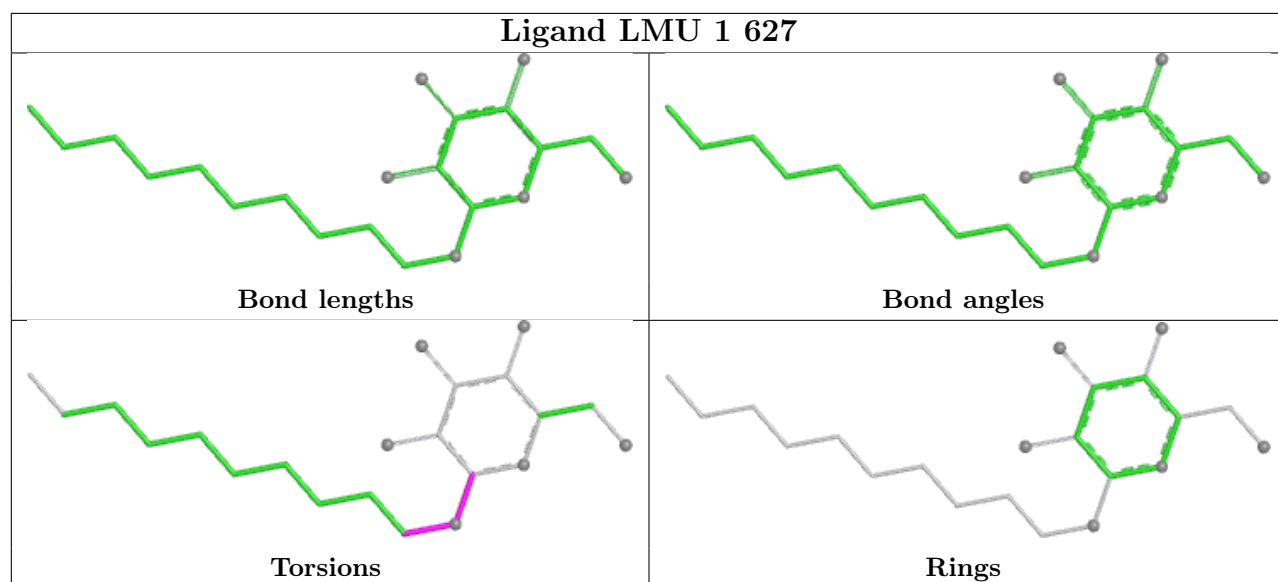
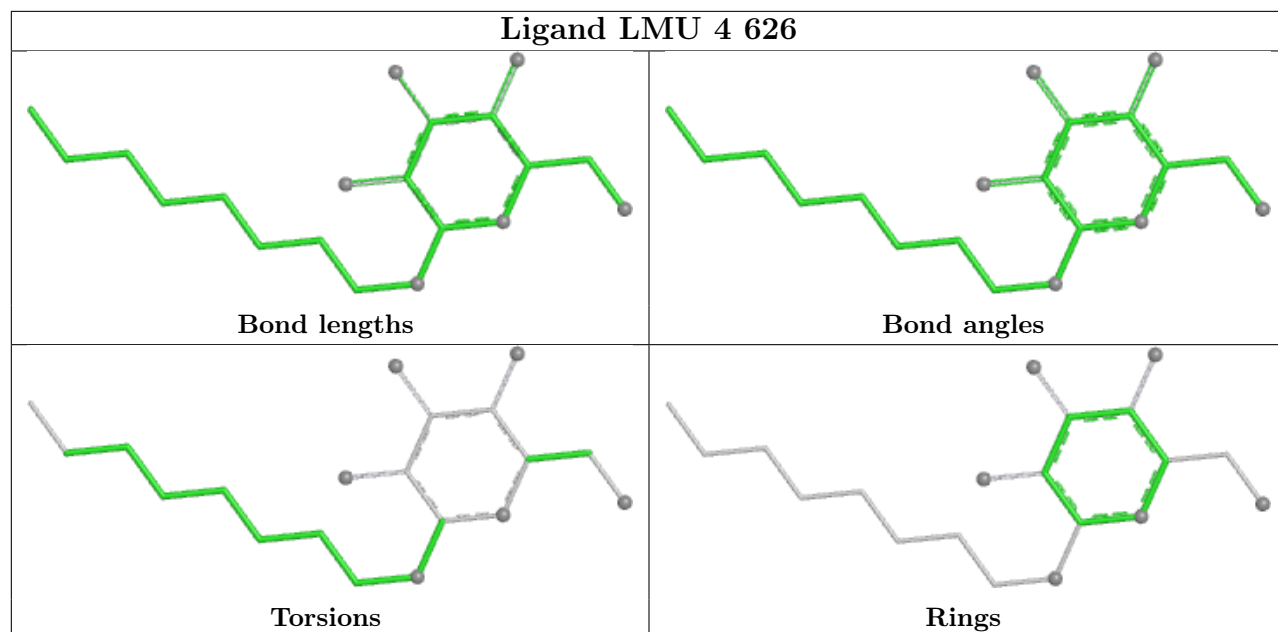
Ligand CLA A 845

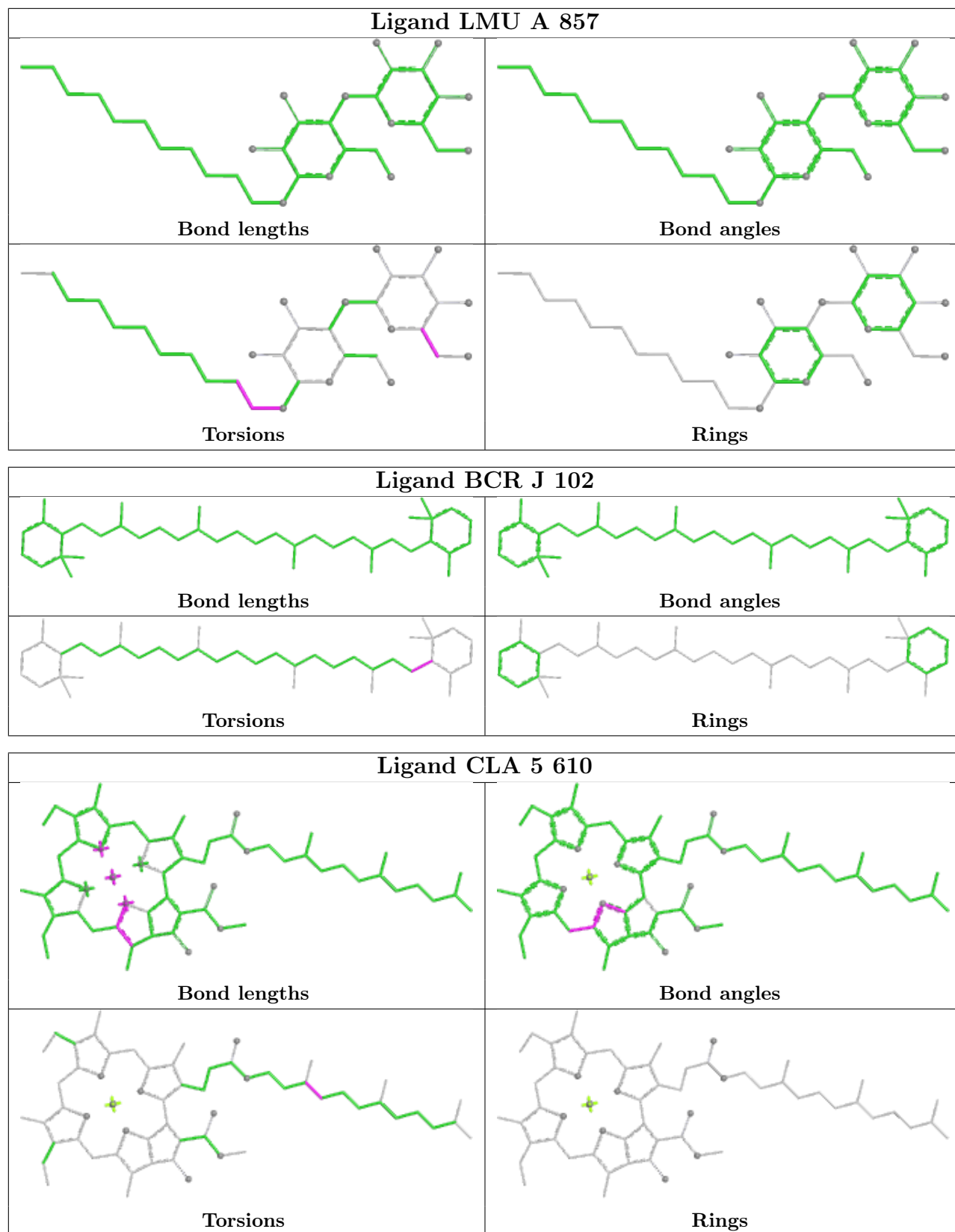


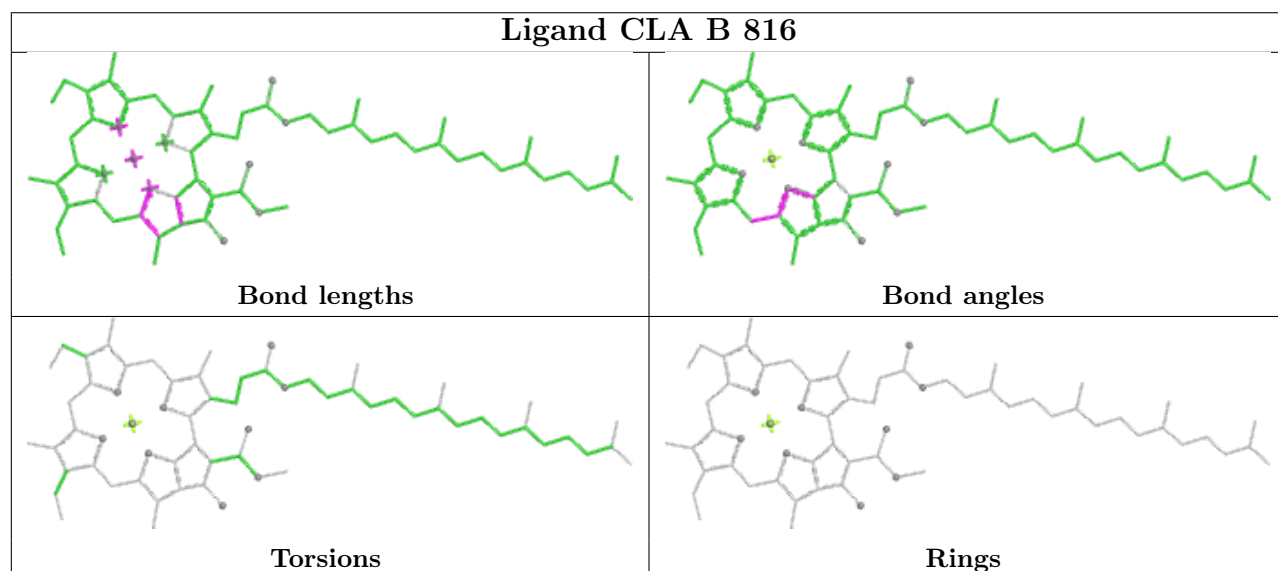
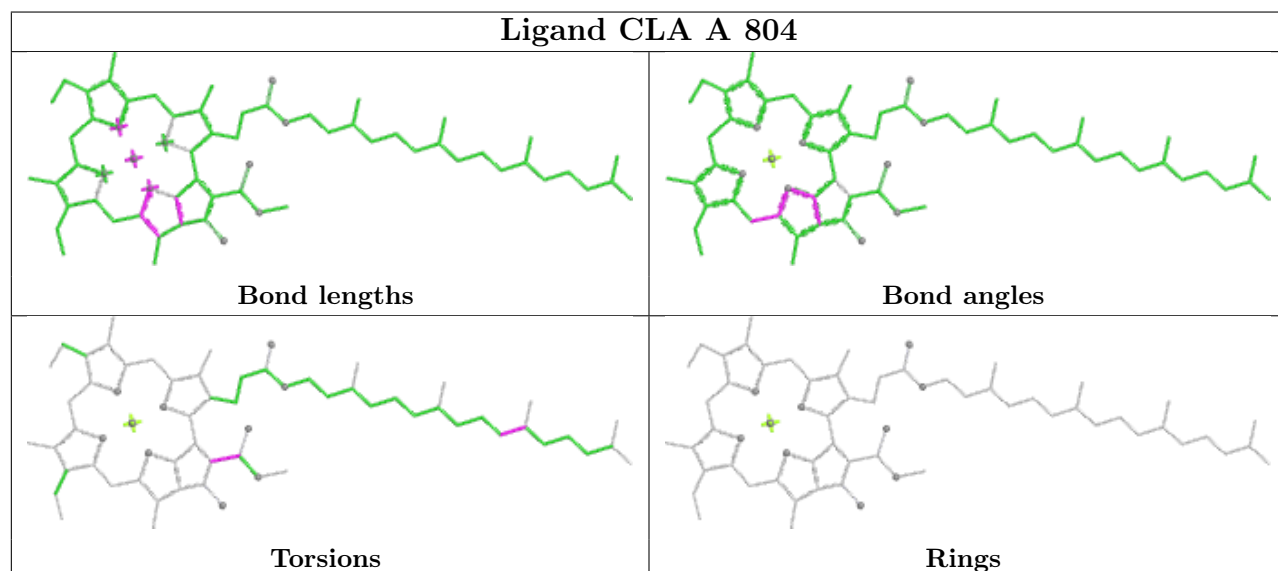
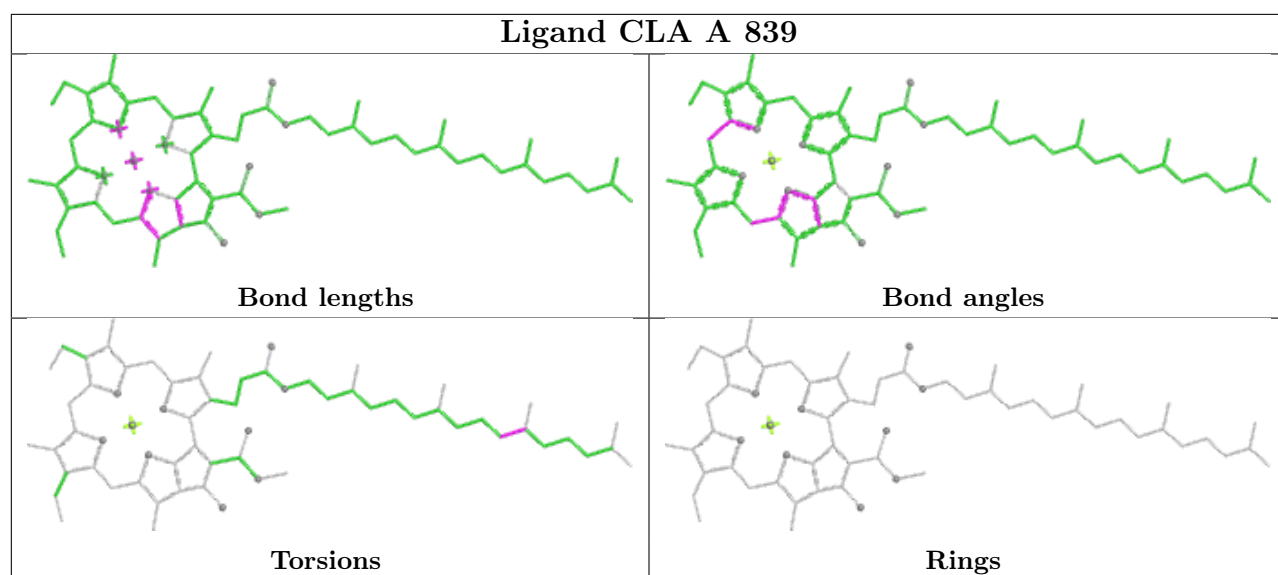


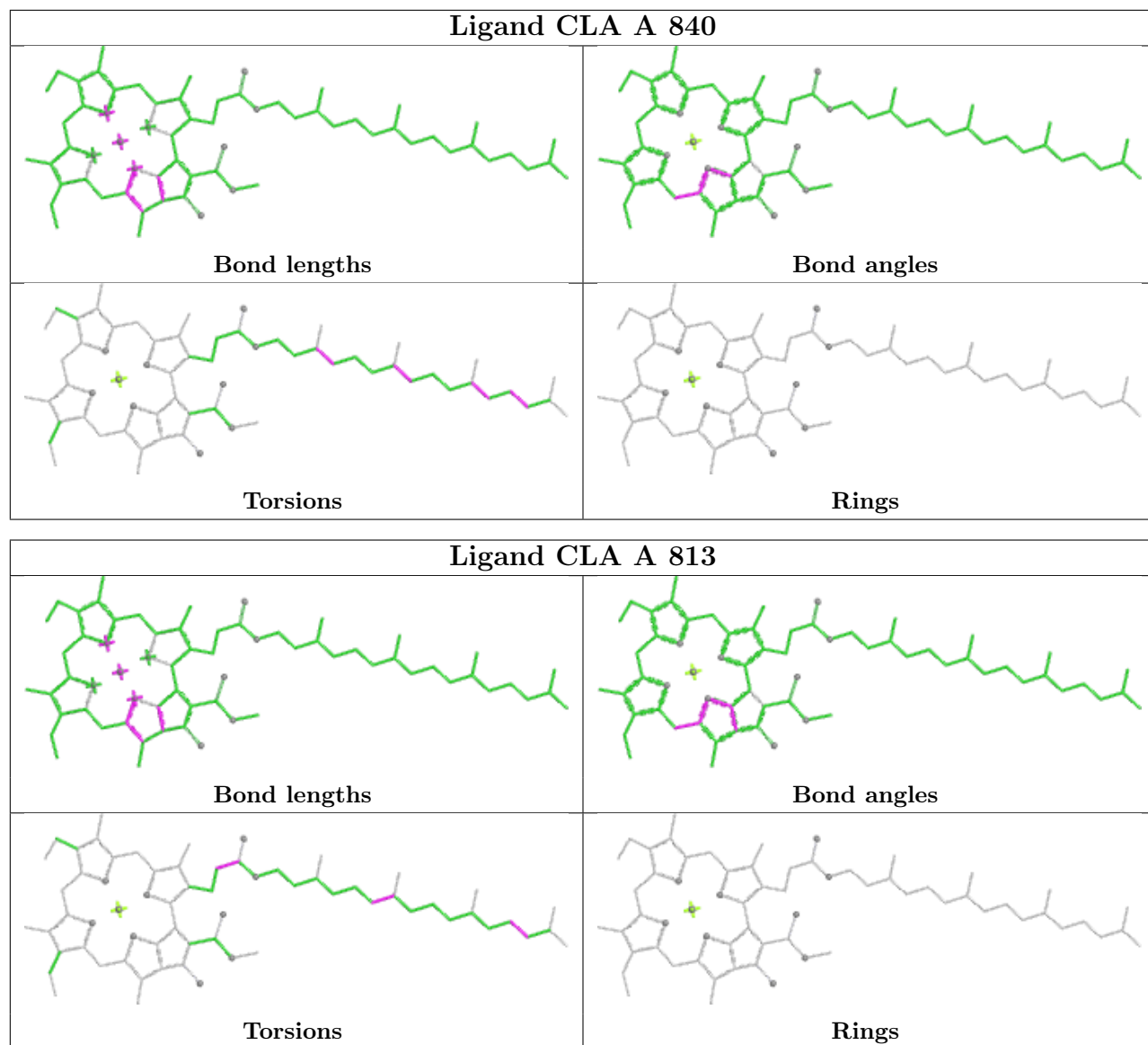
Ligand XAT 8 618**Ligand CLA A 829****Ligand BCR L2 201**



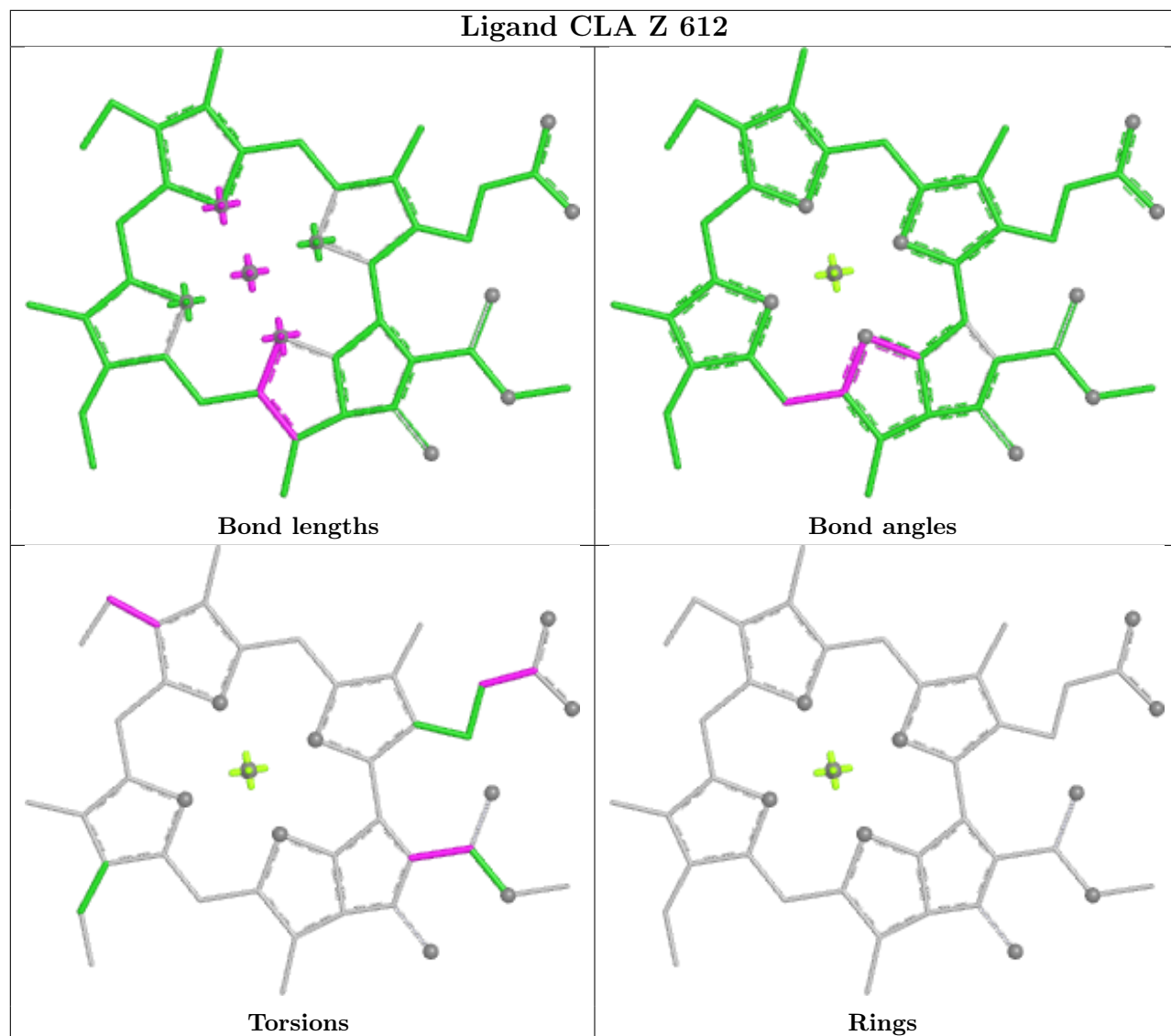




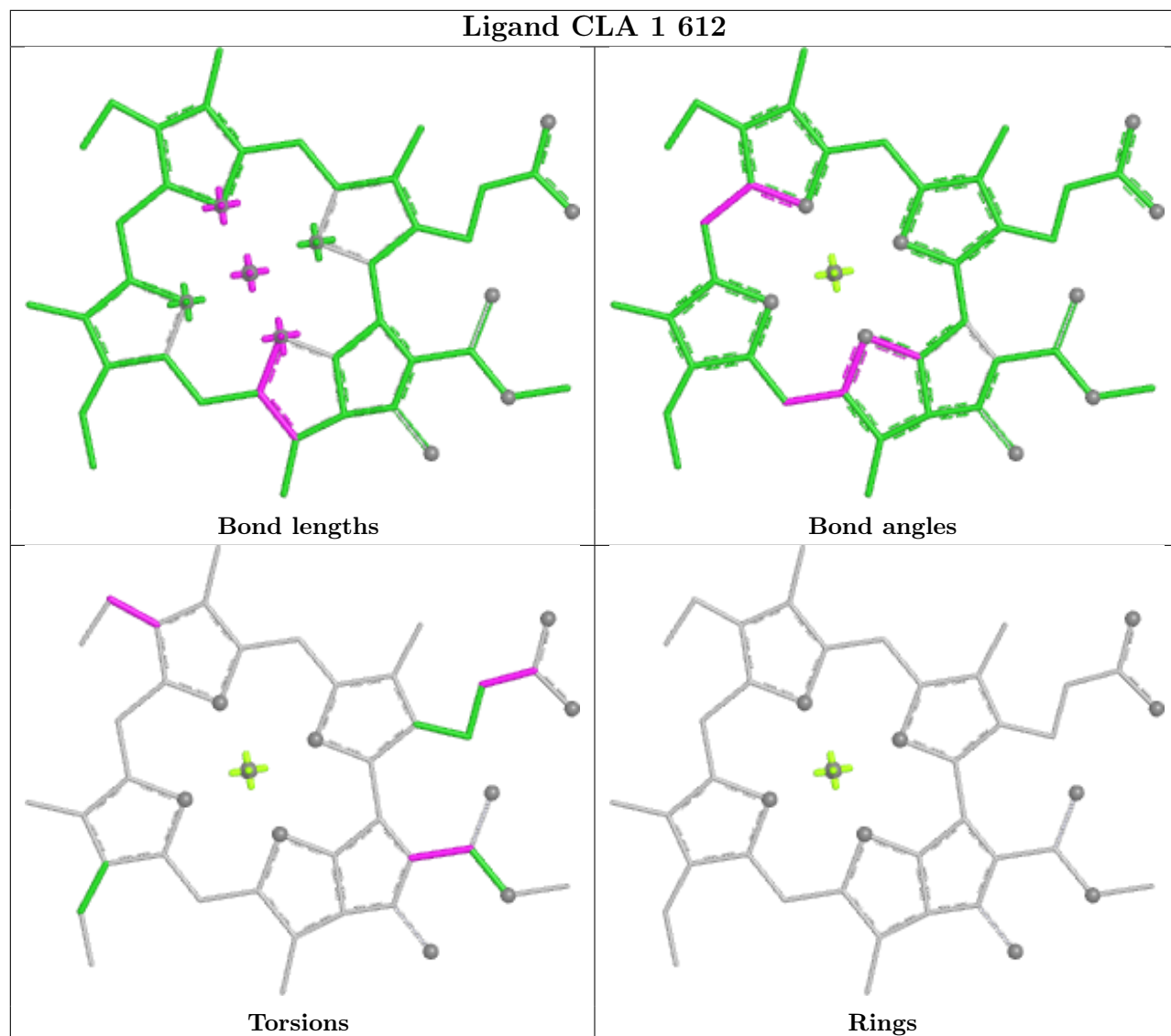




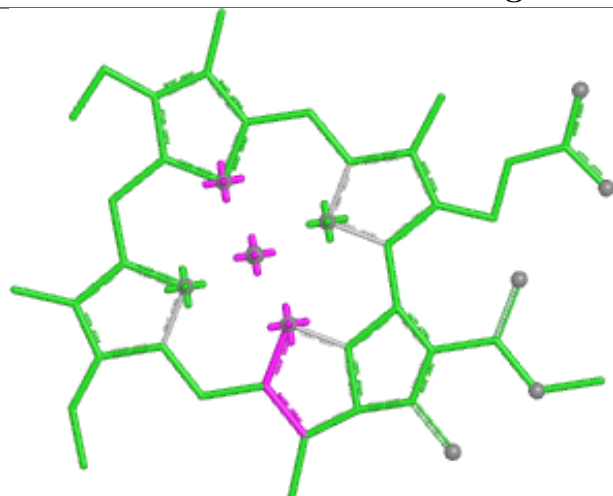
Ligand CLA Z 612



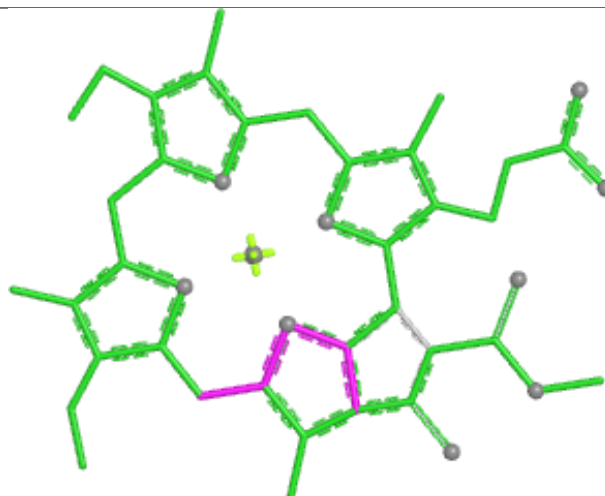
Ligand CLA 1 612



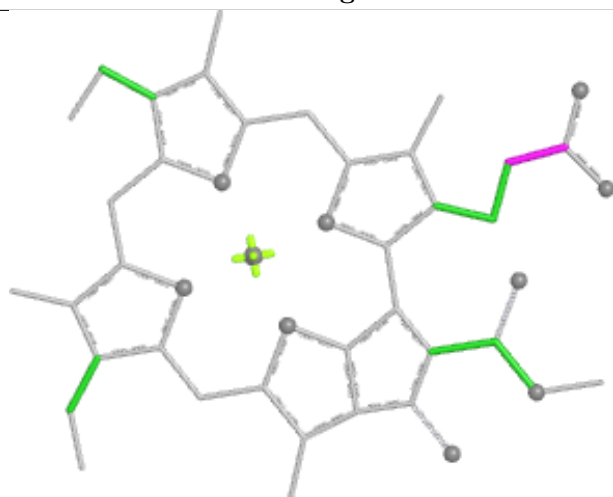
Ligand CLA B2 804



Bond lengths



Bond angles

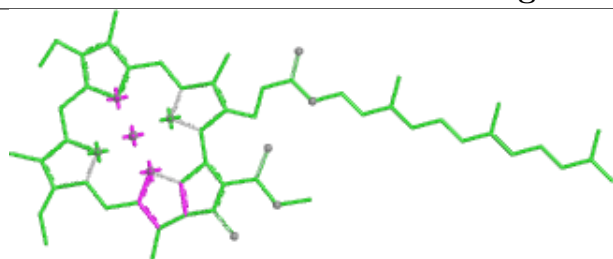


Torsions

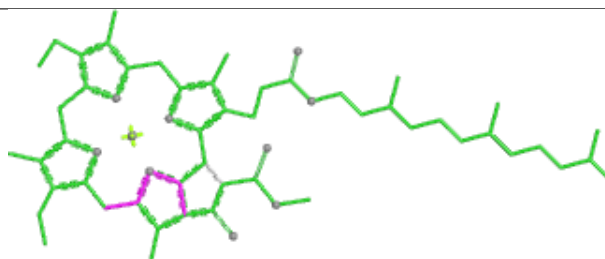


Rings

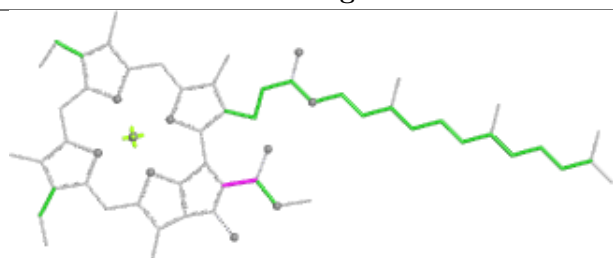
Ligand CLA 3 602



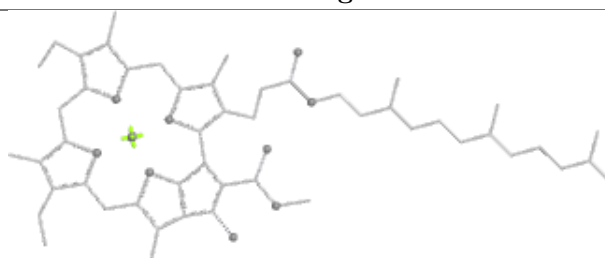
Bond lengths



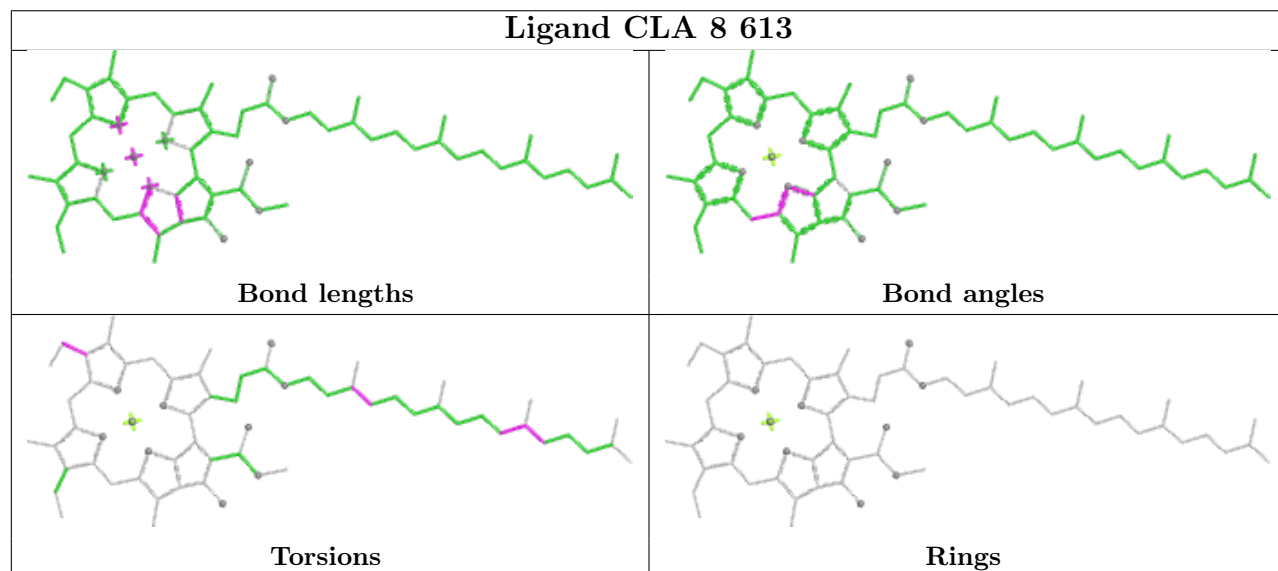
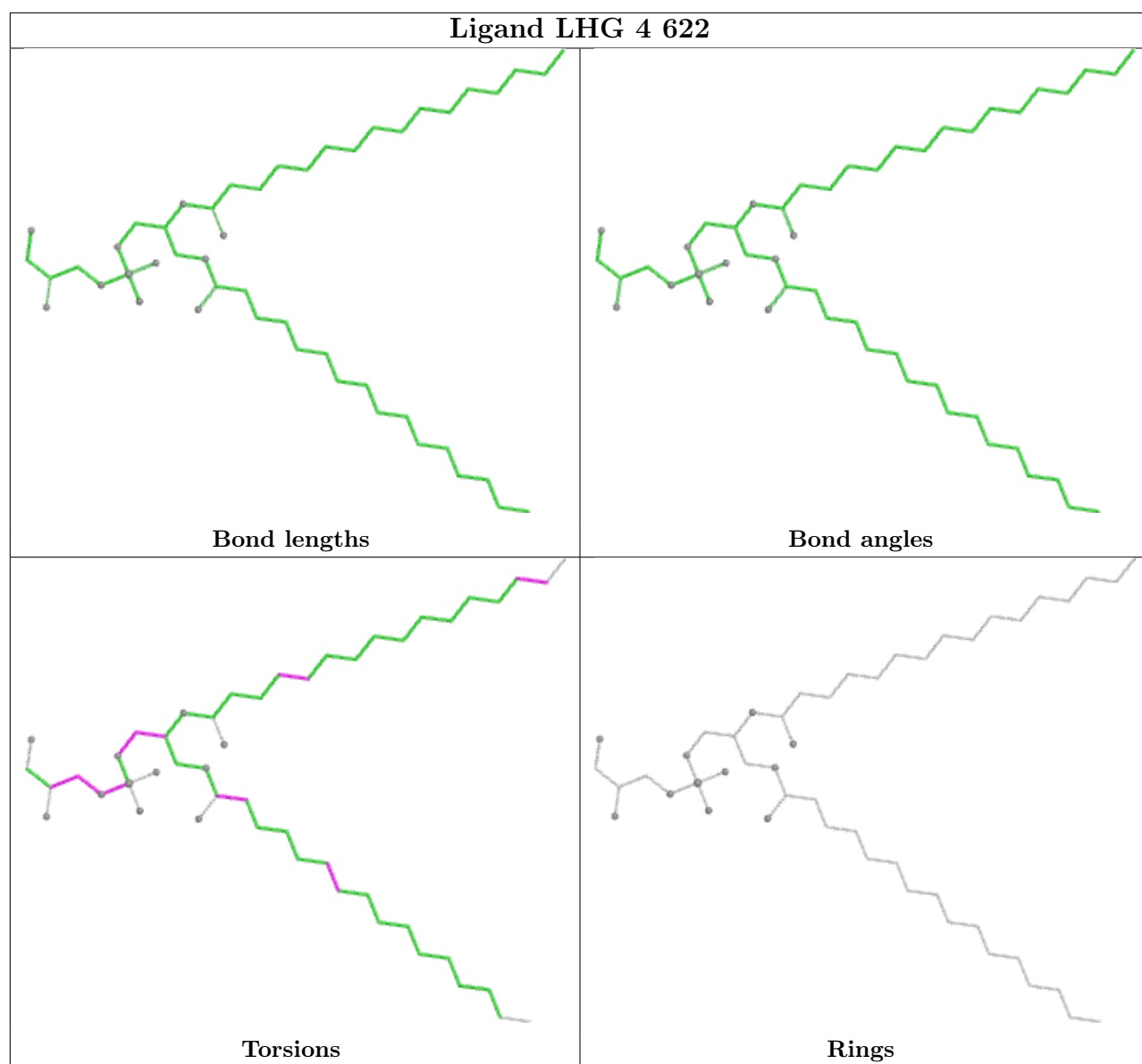
Bond angles



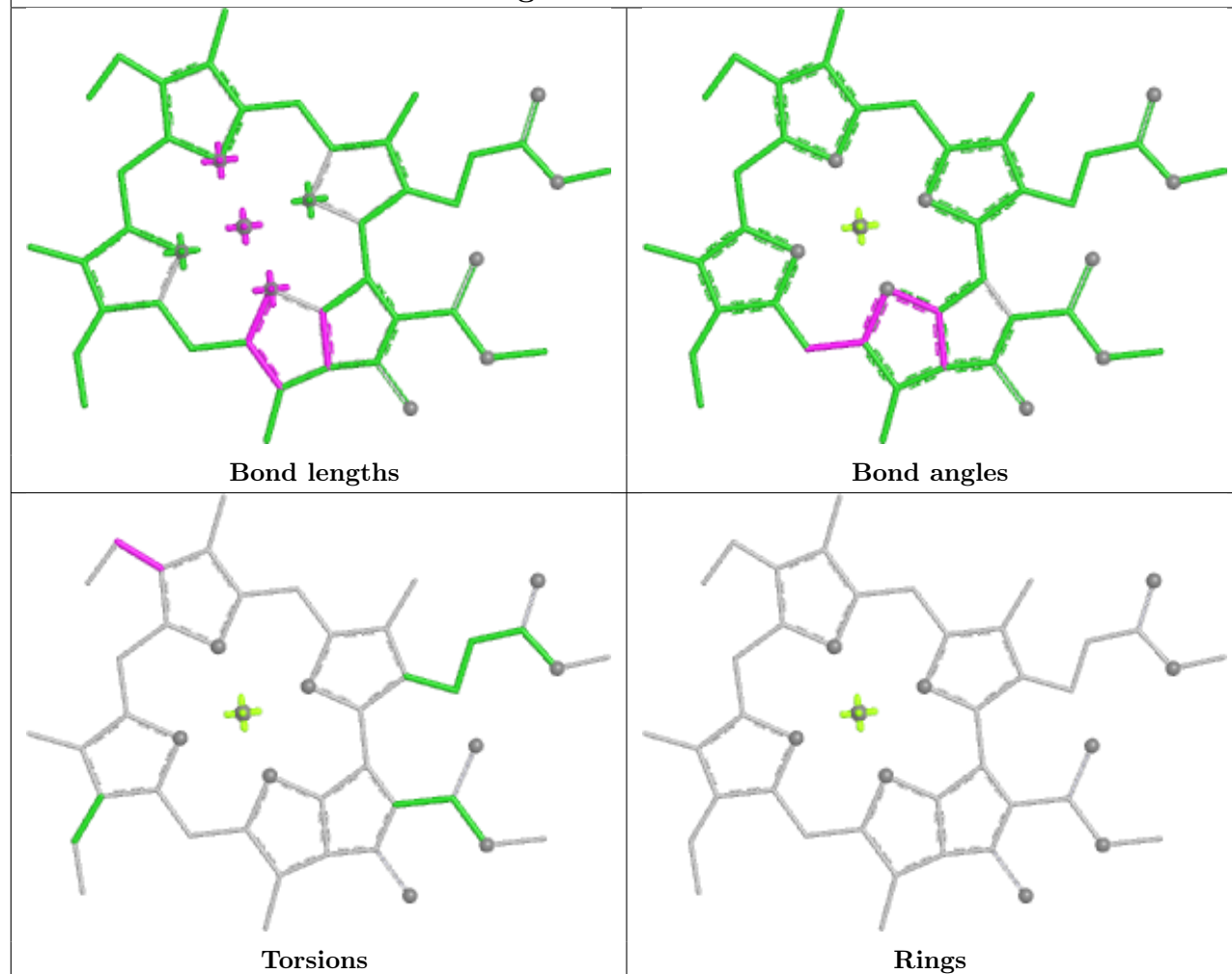
Torsions



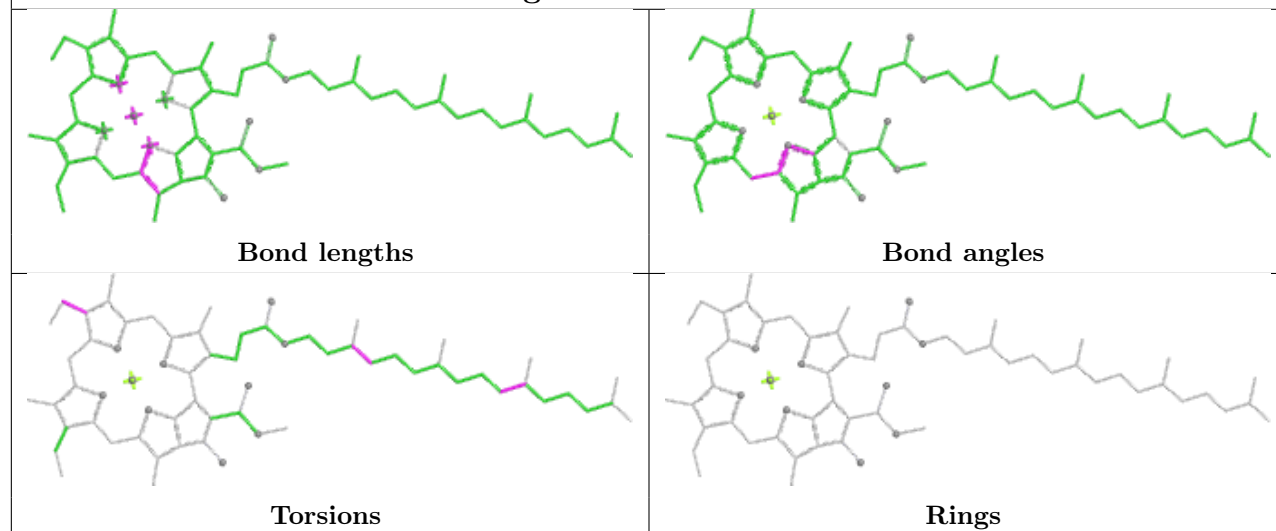
Rings

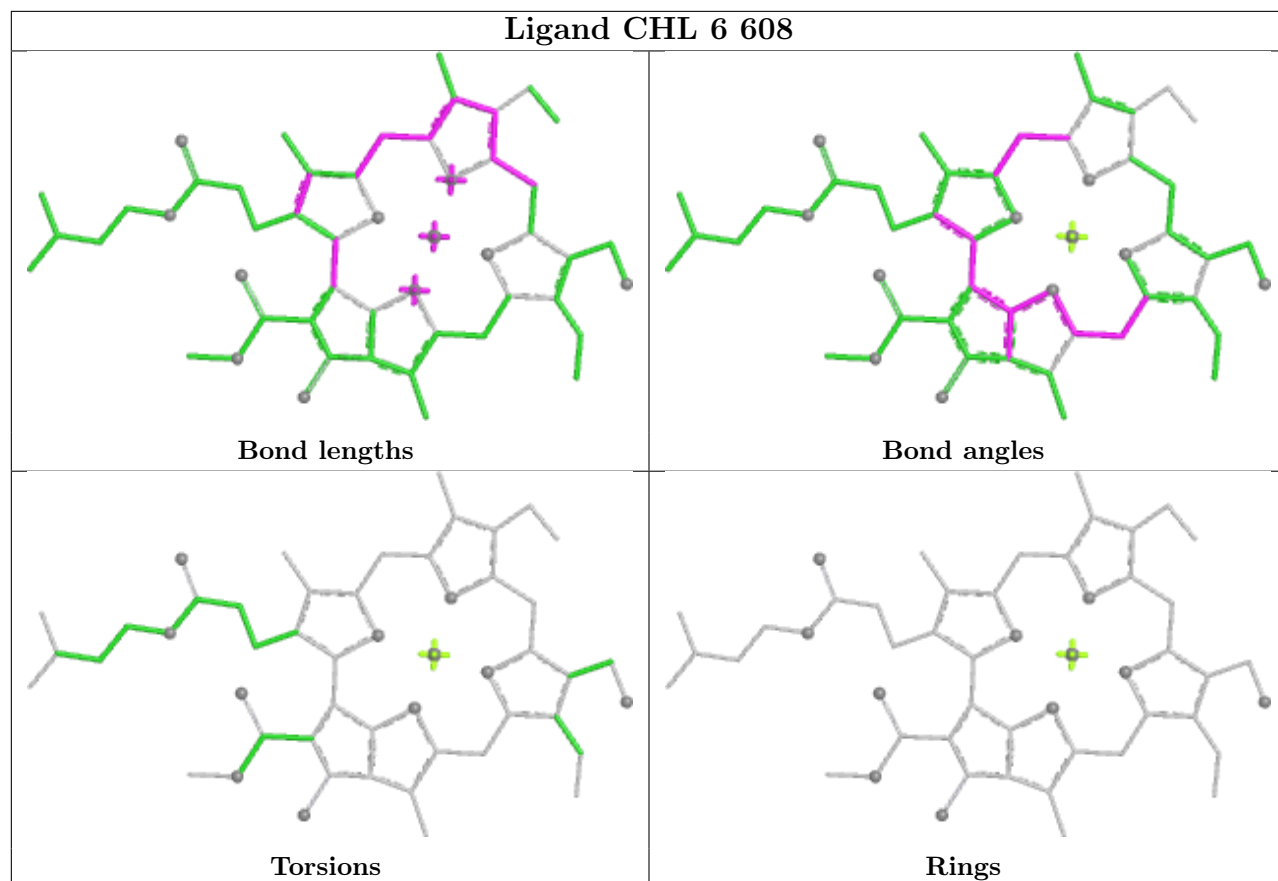


Ligand CLA 1 616

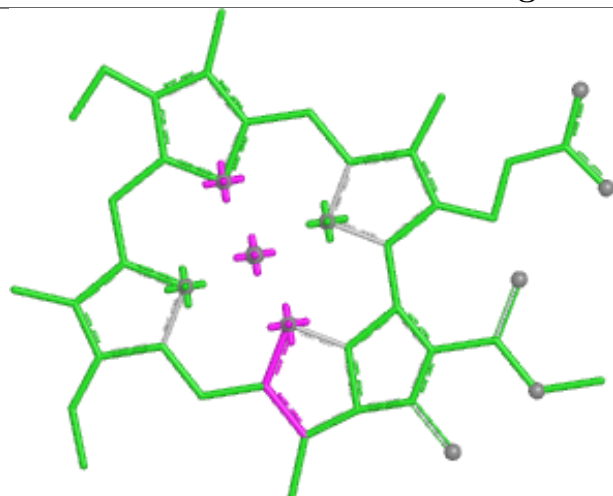


Ligand CLA B2 806

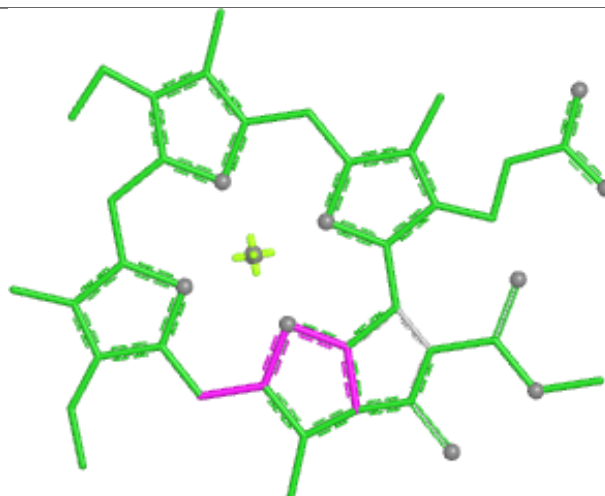




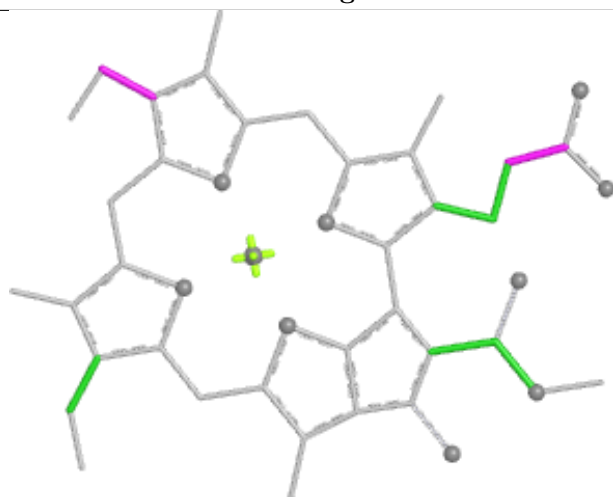
Ligand CLA 9 614



Bond lengths



Bond angles

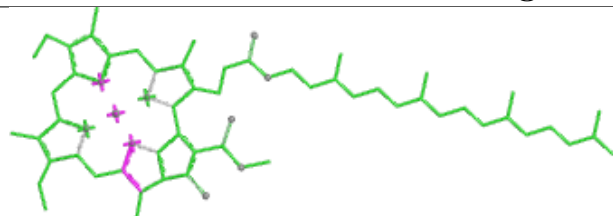


Torsions

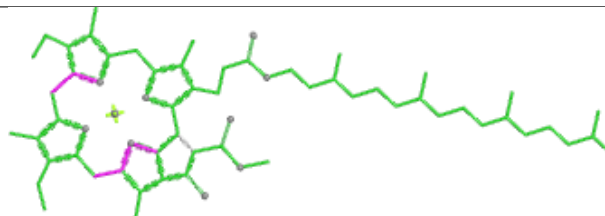


Rings

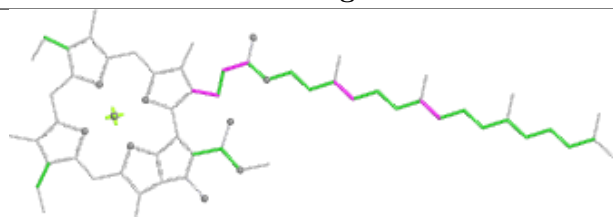
Ligand CLA 3 615



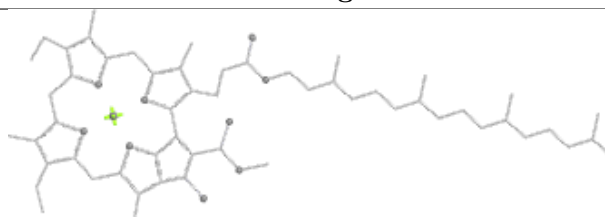
Bond lengths



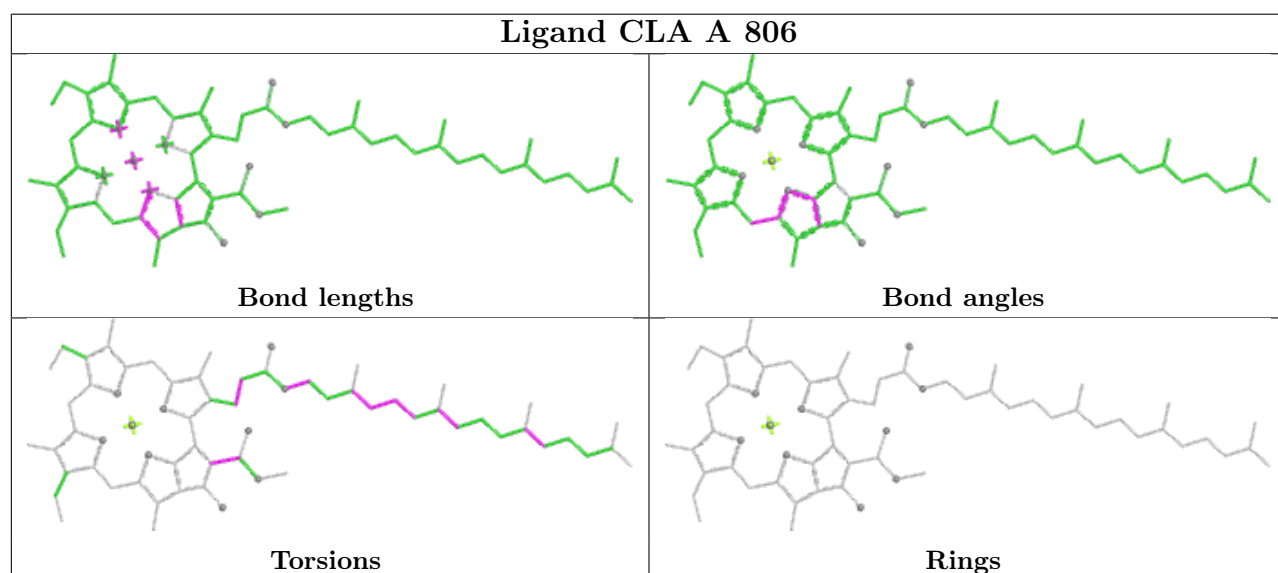
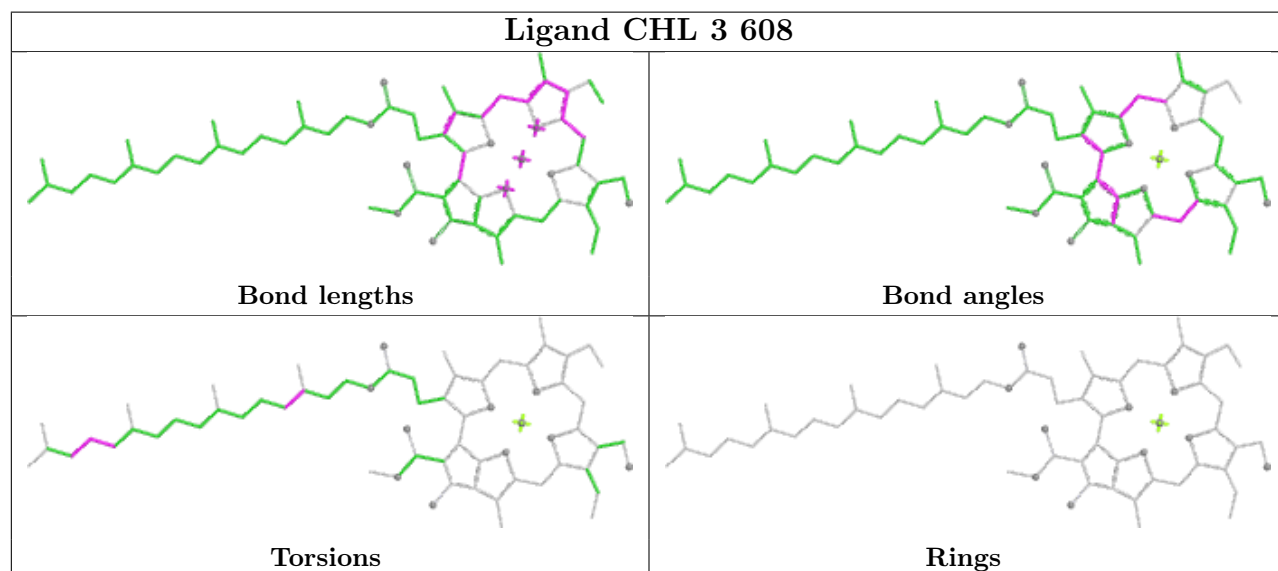
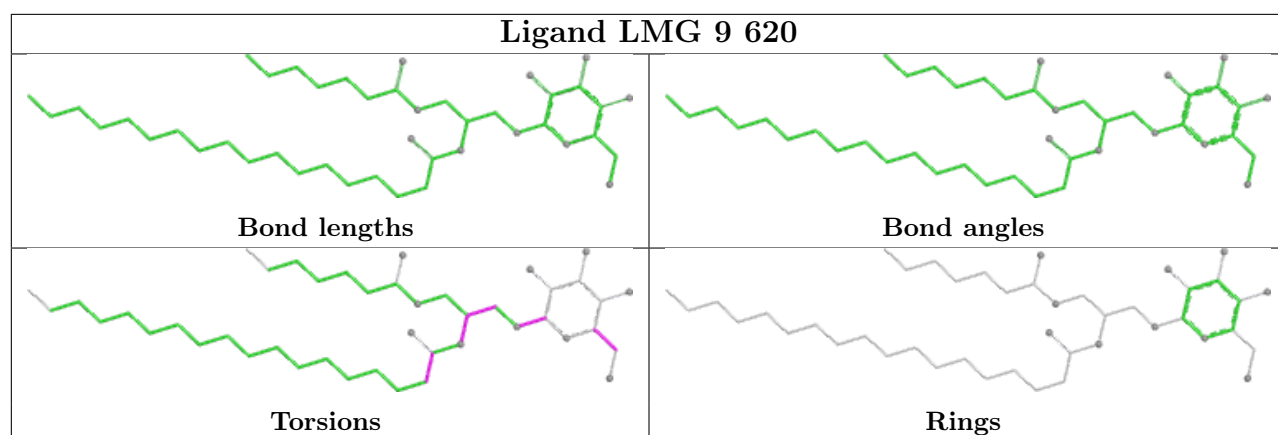
Bond angles

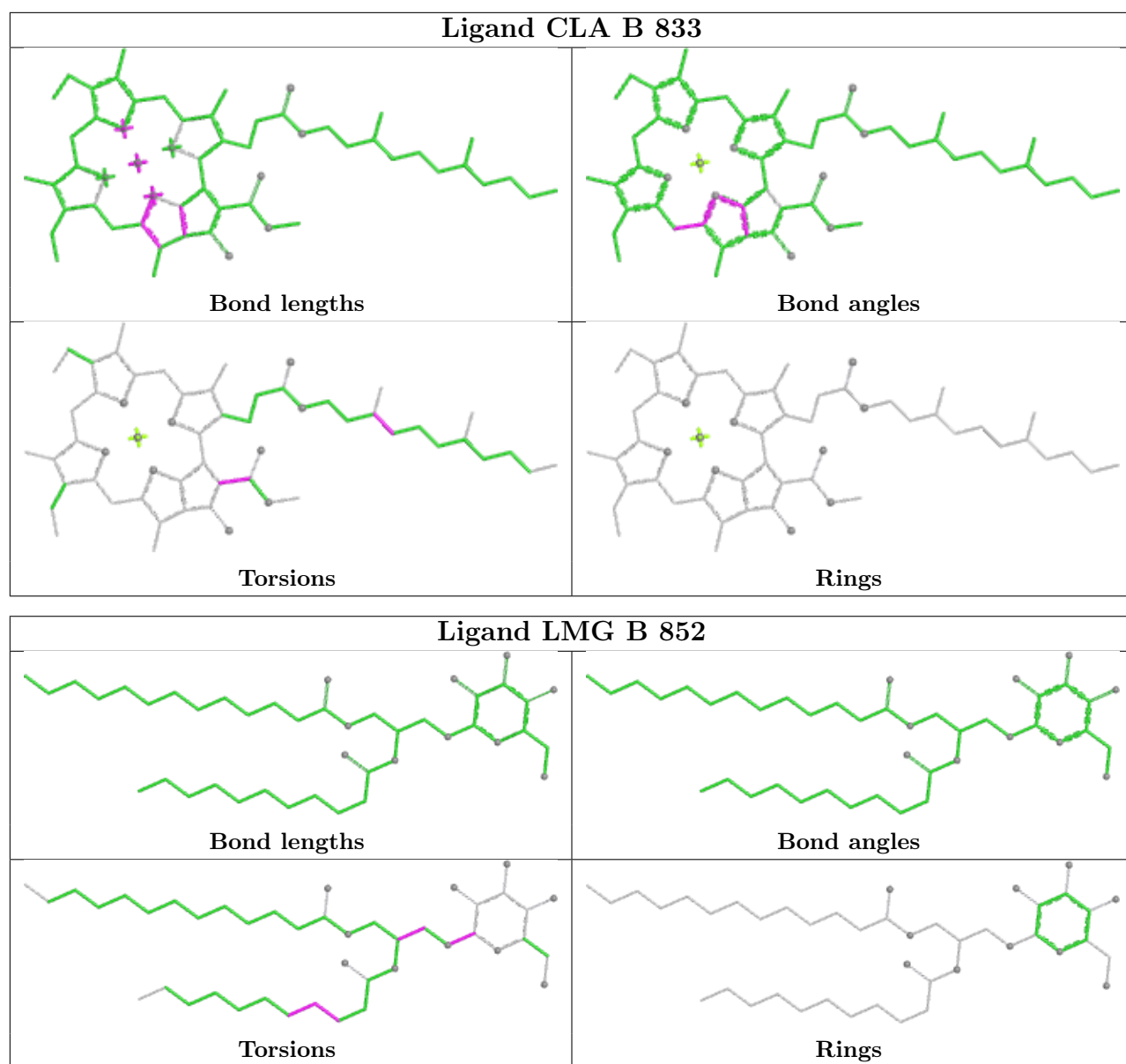


Torsions

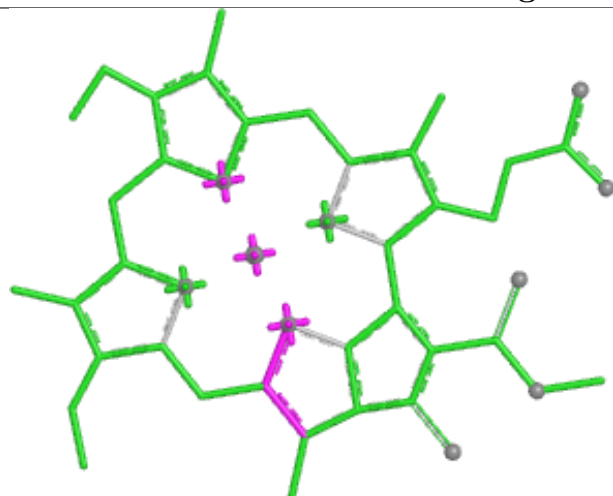


Rings

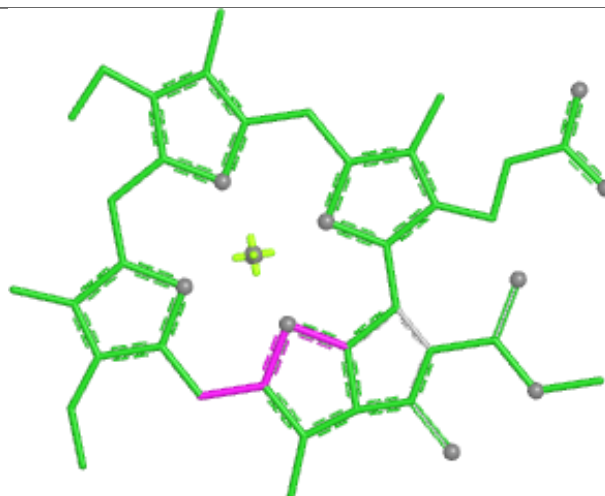




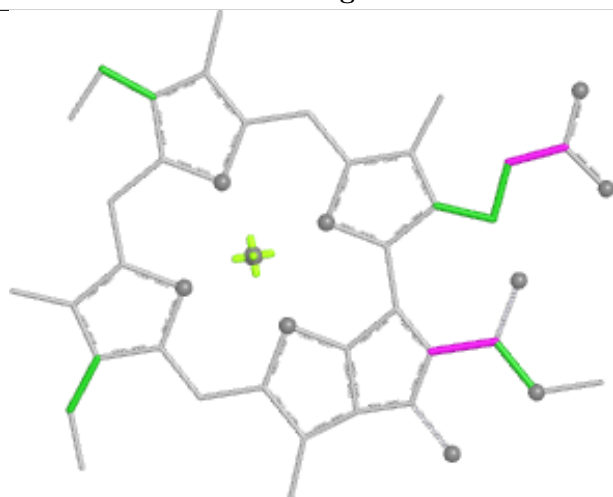
Ligand CLA 4 612



Bond lengths



Bond angles

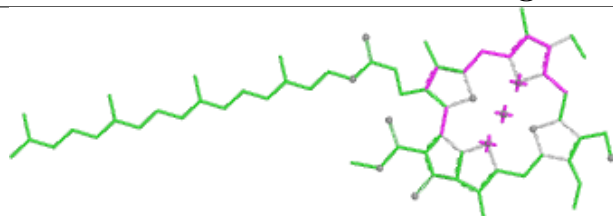


Torsions

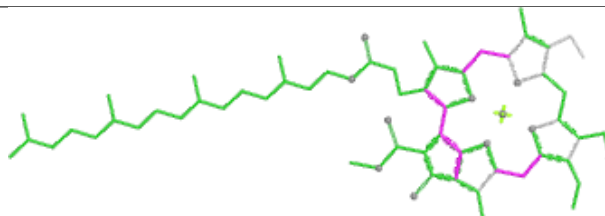


Rings

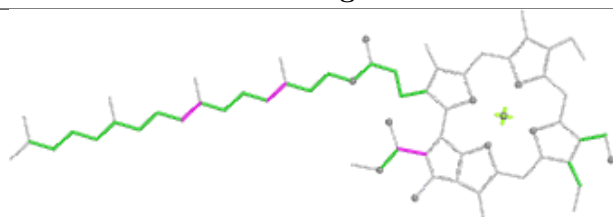
Ligand CHL 4 601



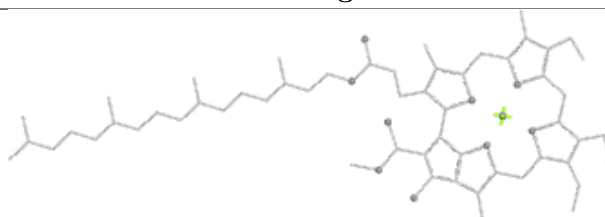
Bond lengths



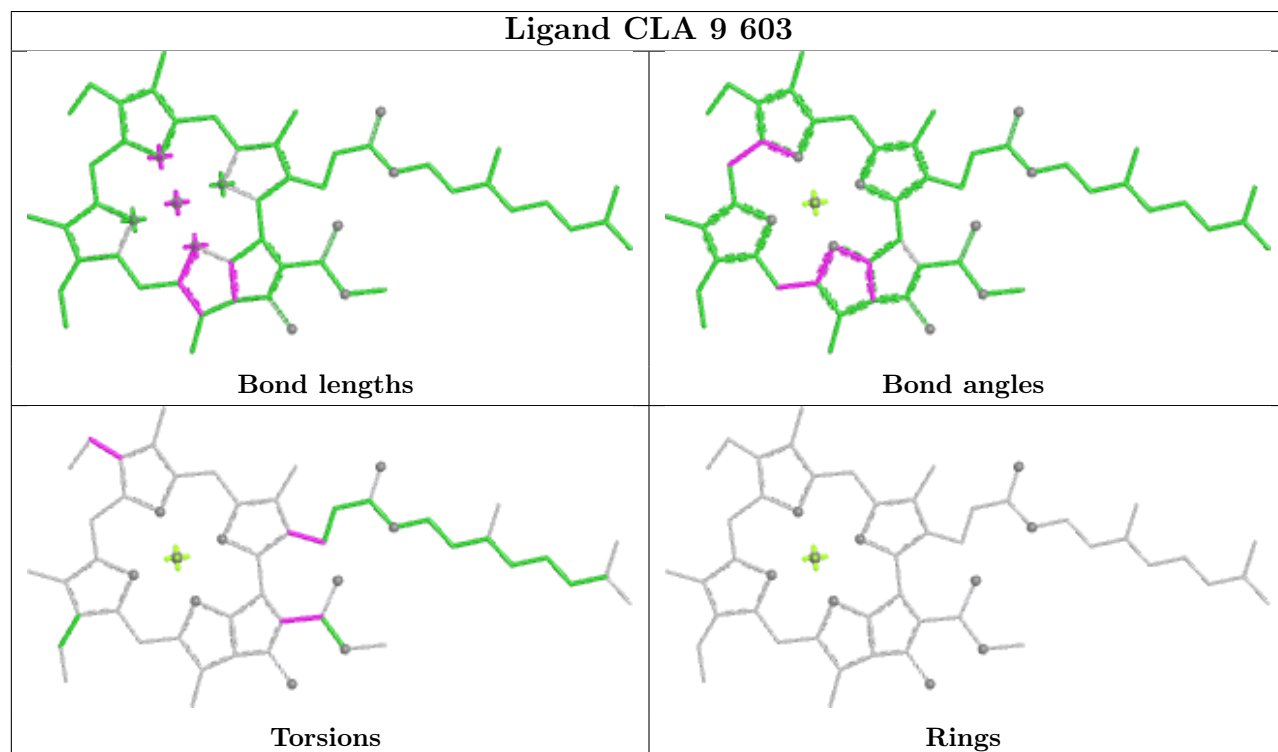
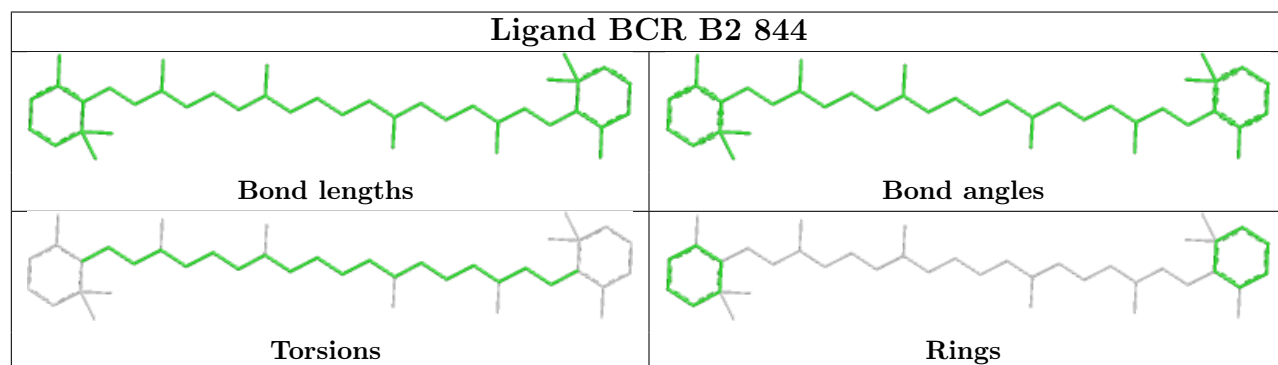
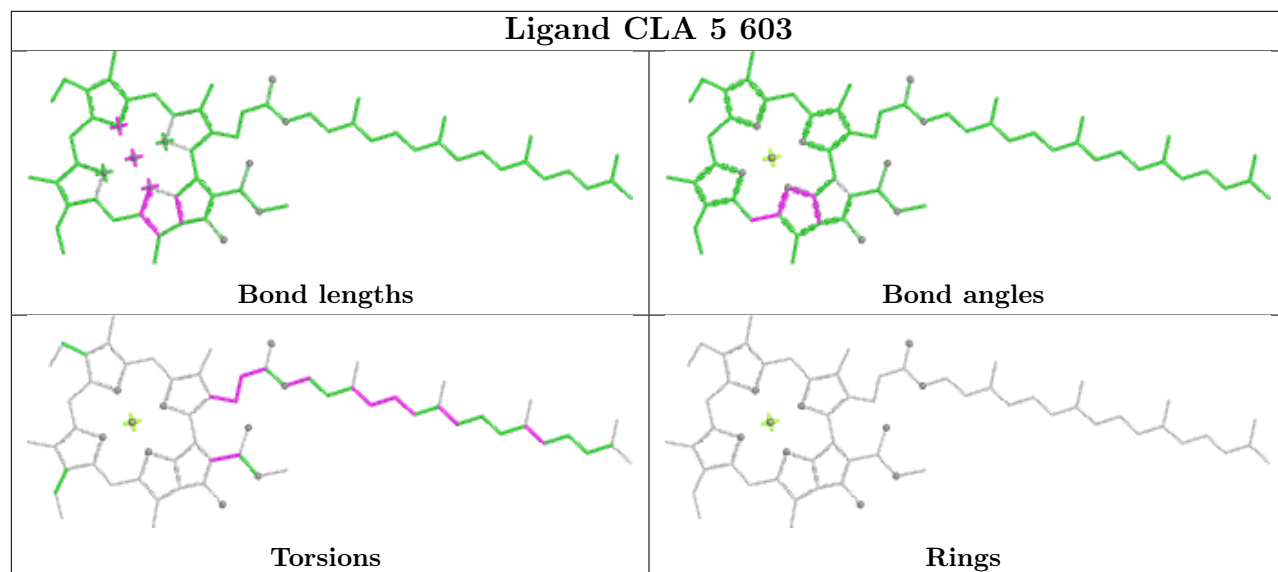
Bond angles

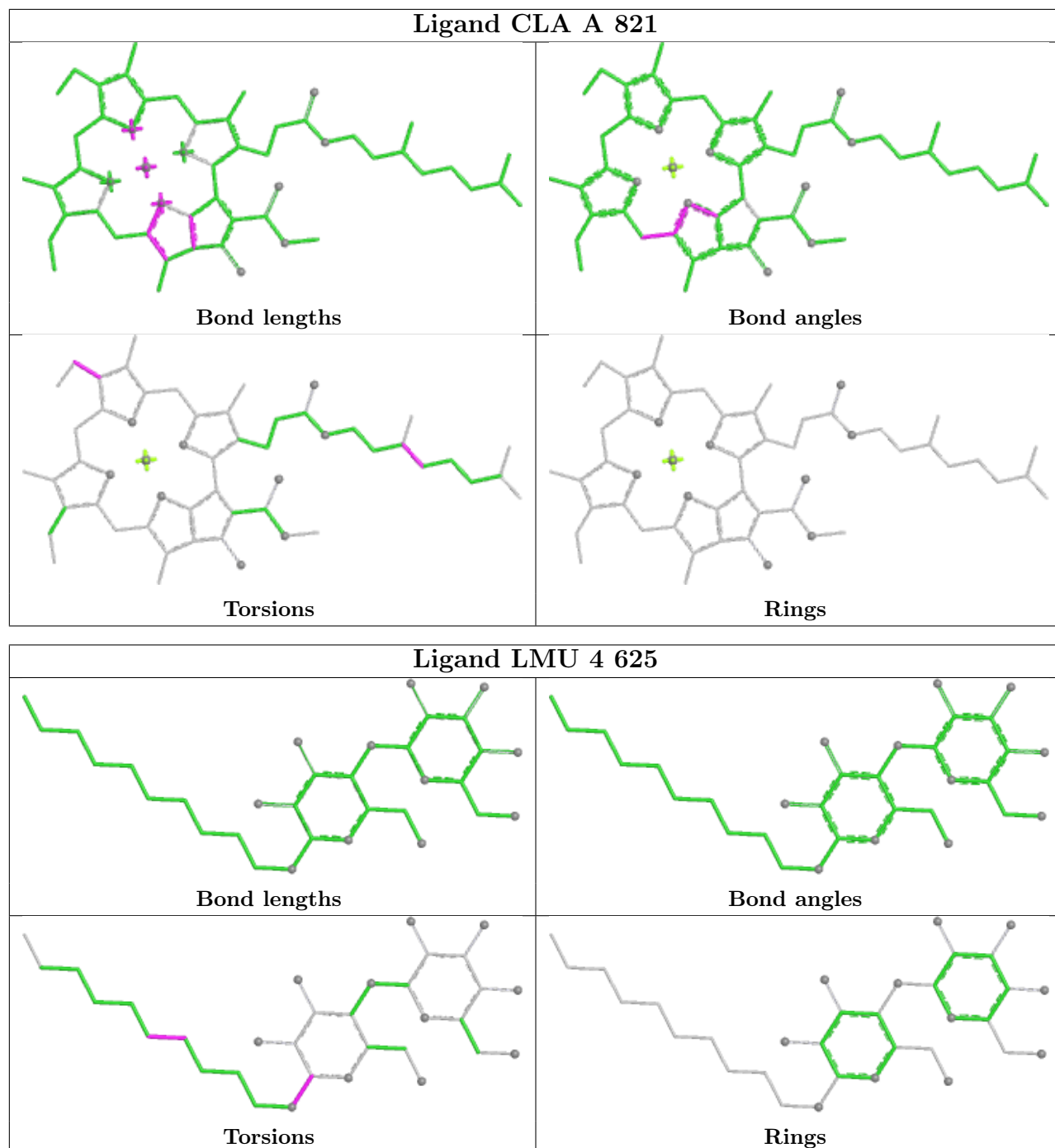


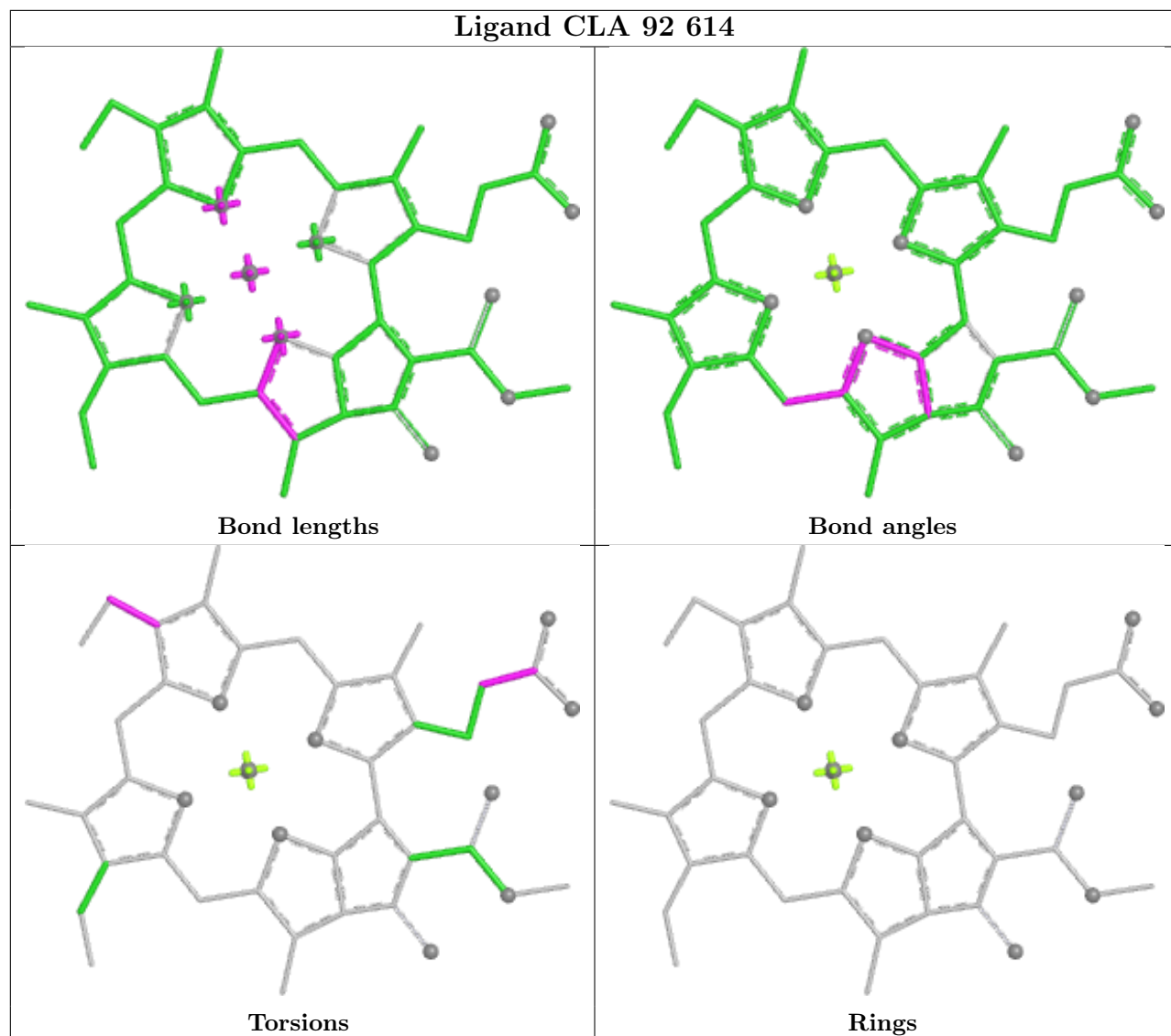
Torsions

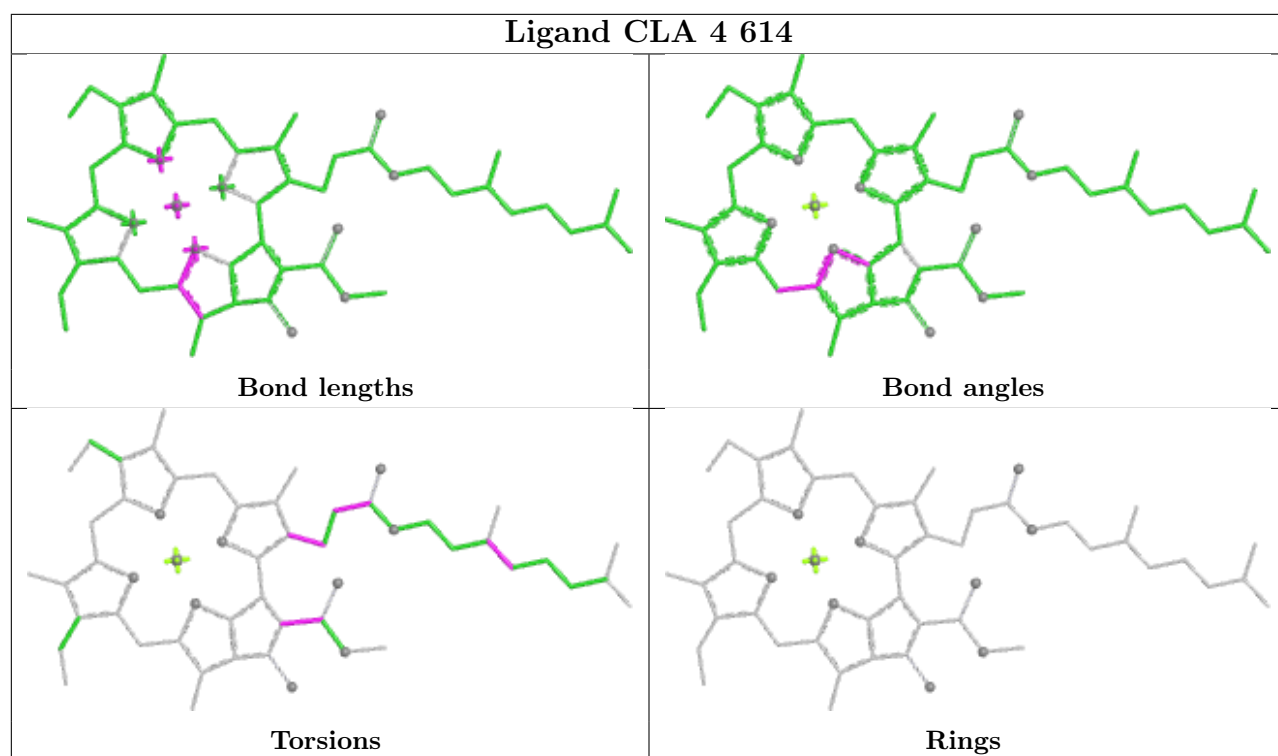


Rings

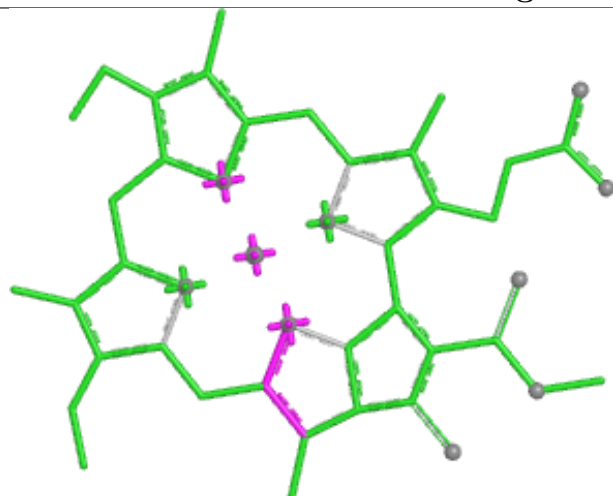




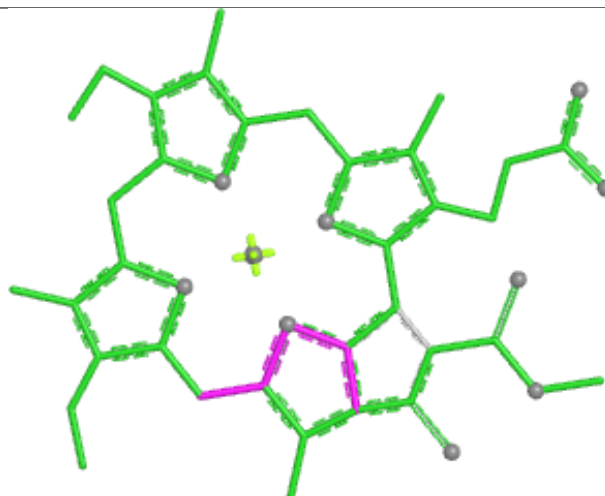




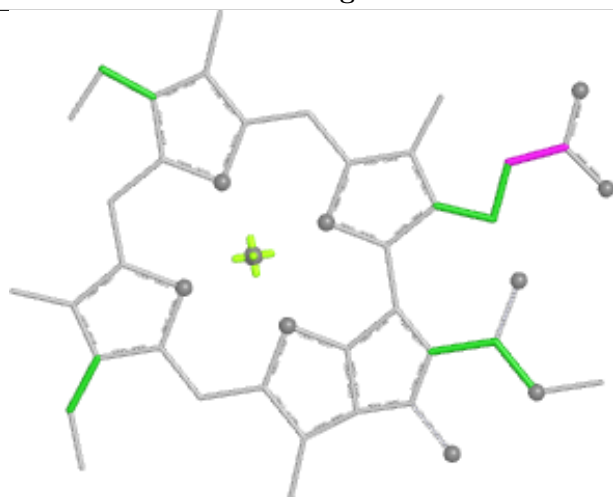
Ligand CLA L 204



Bond lengths



Bond angles

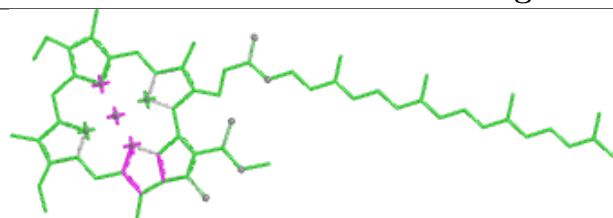


Torsions

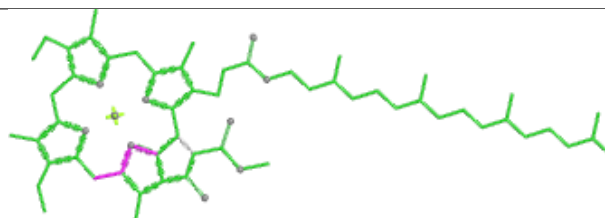


Rings

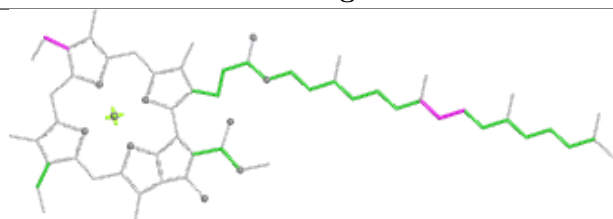
Ligand CLA B 802



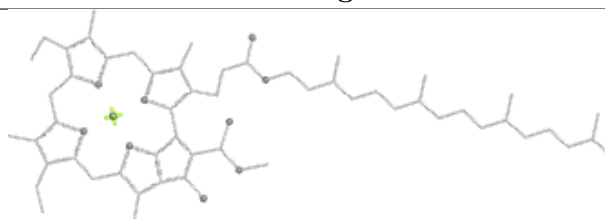
Bond lengths



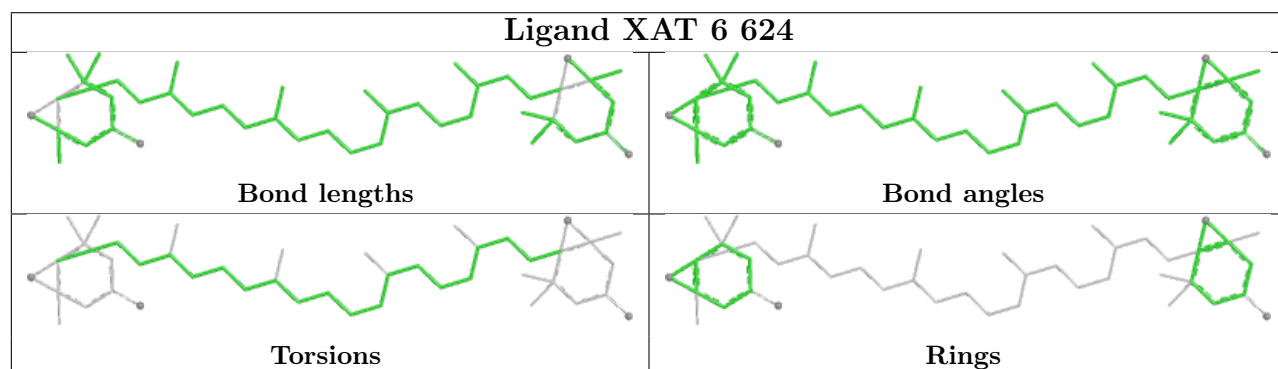
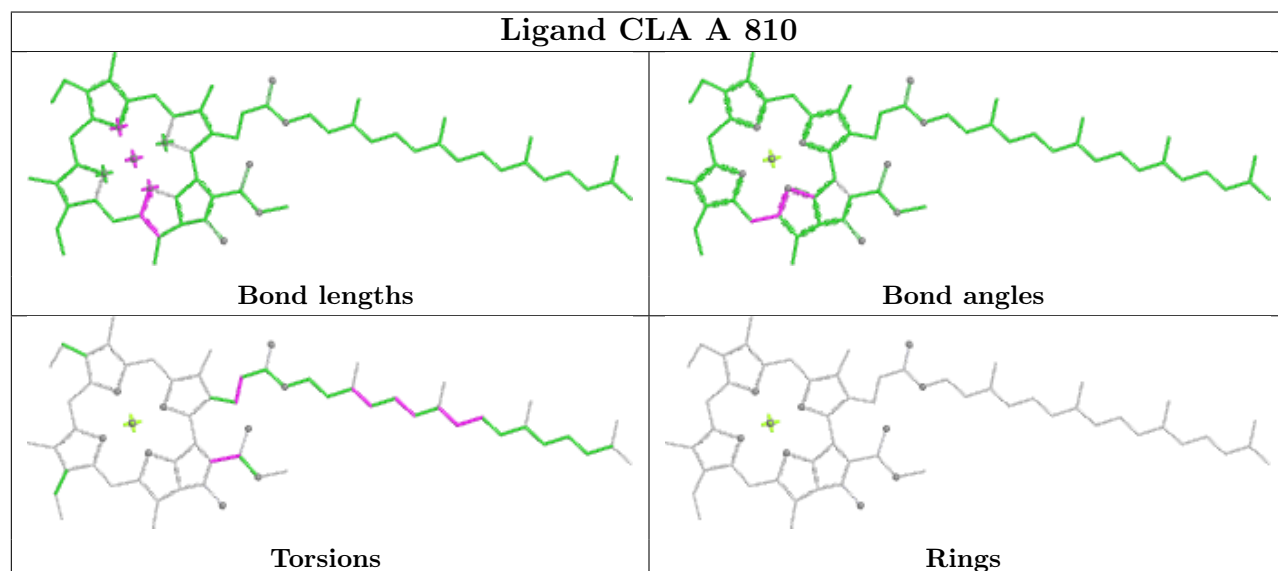
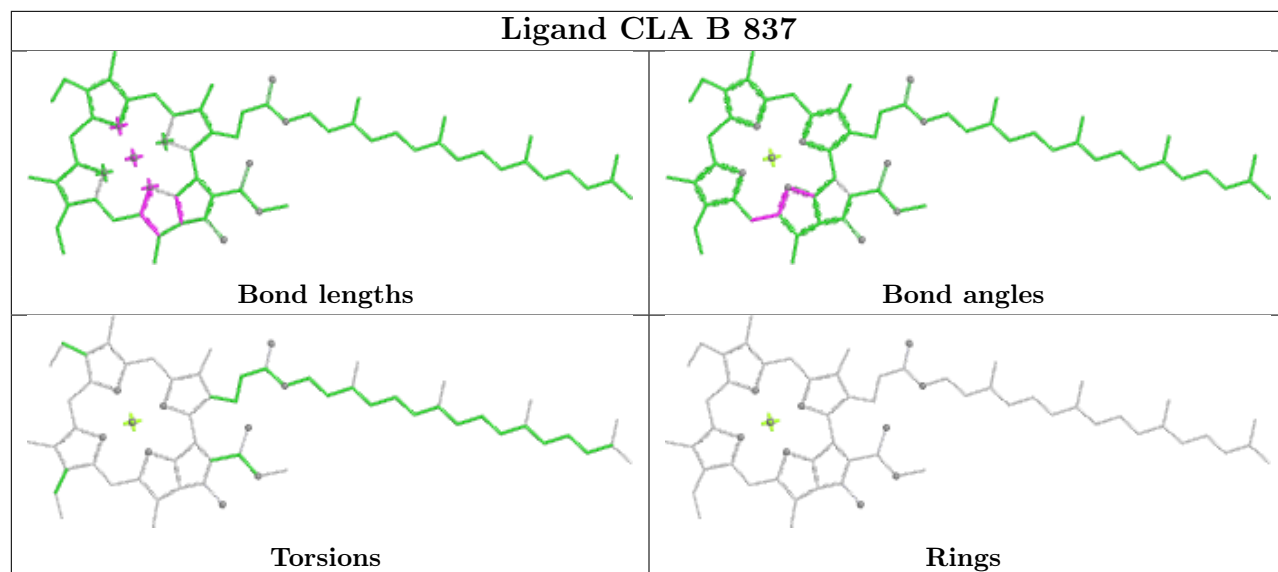
Bond angles



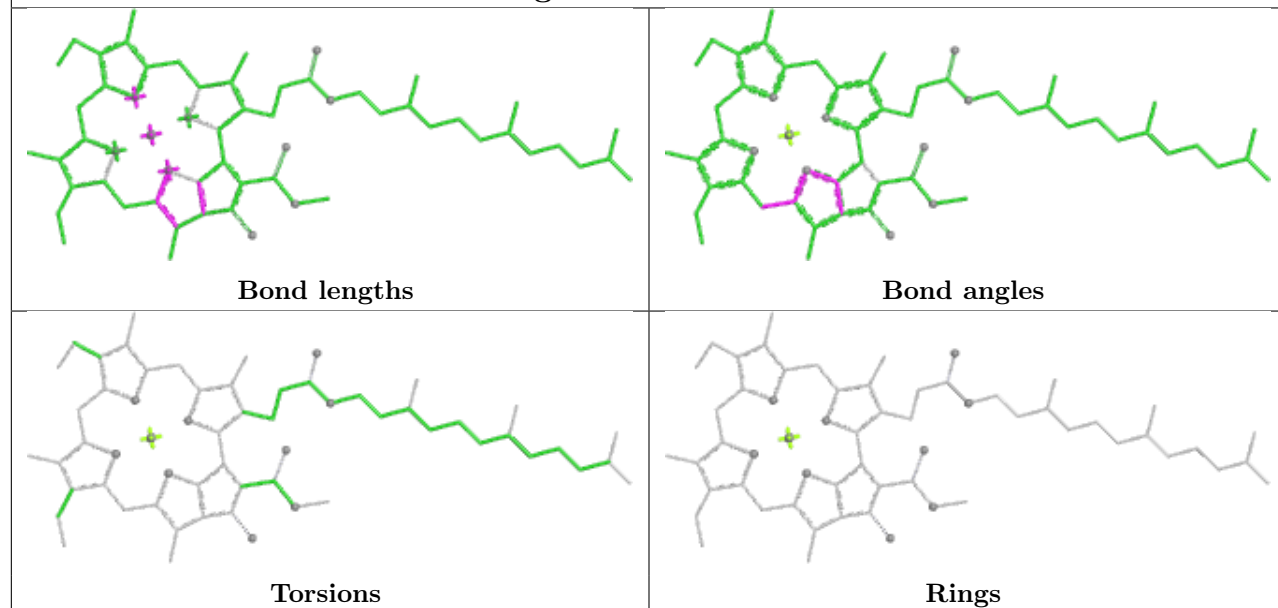
Torsions



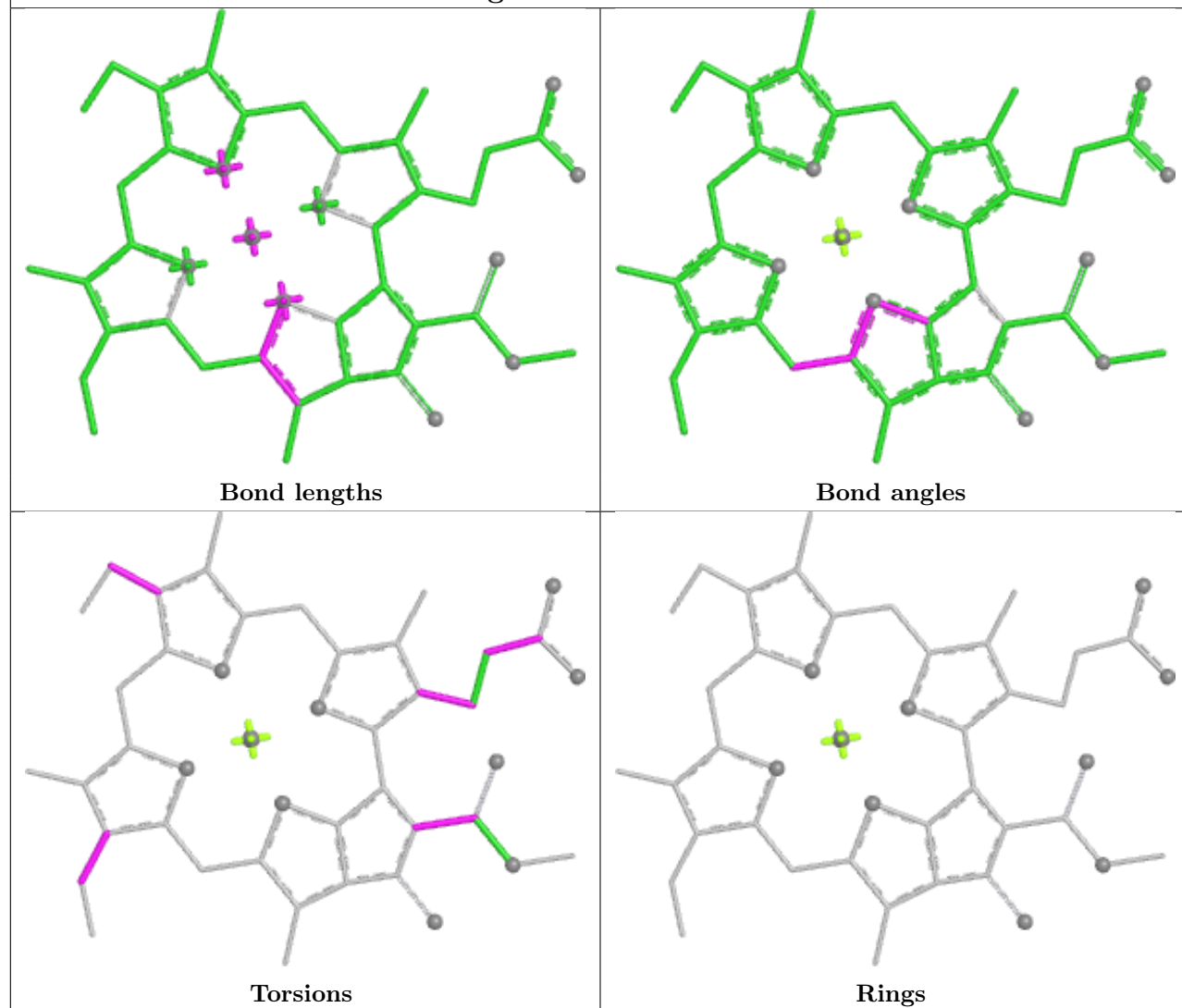
Rings



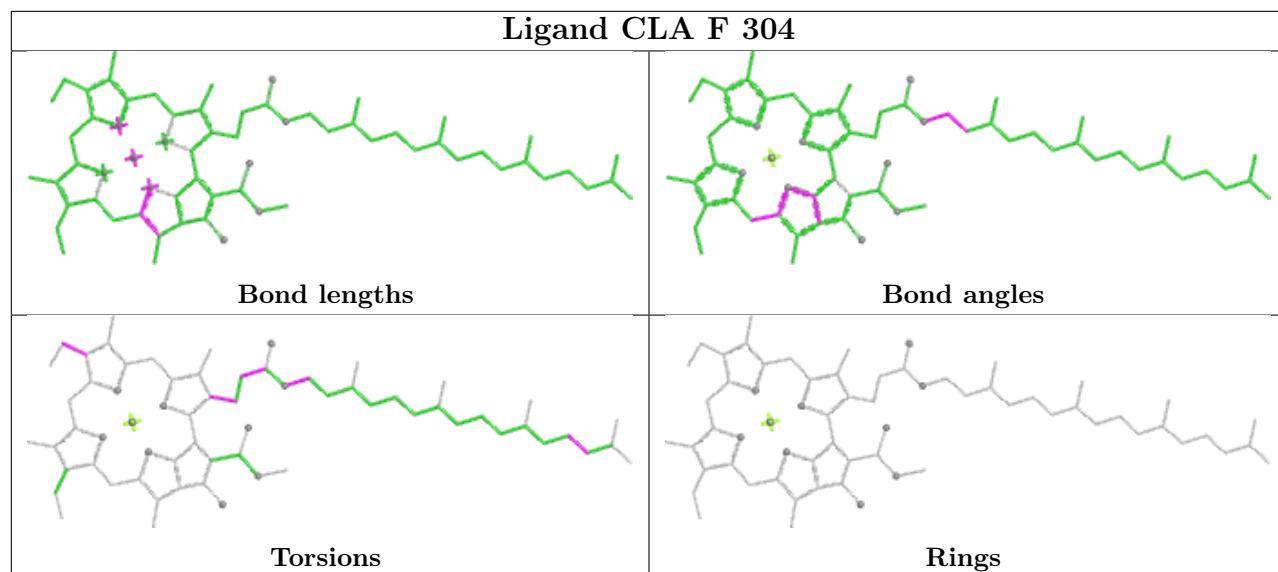
Ligand CLA Z 610



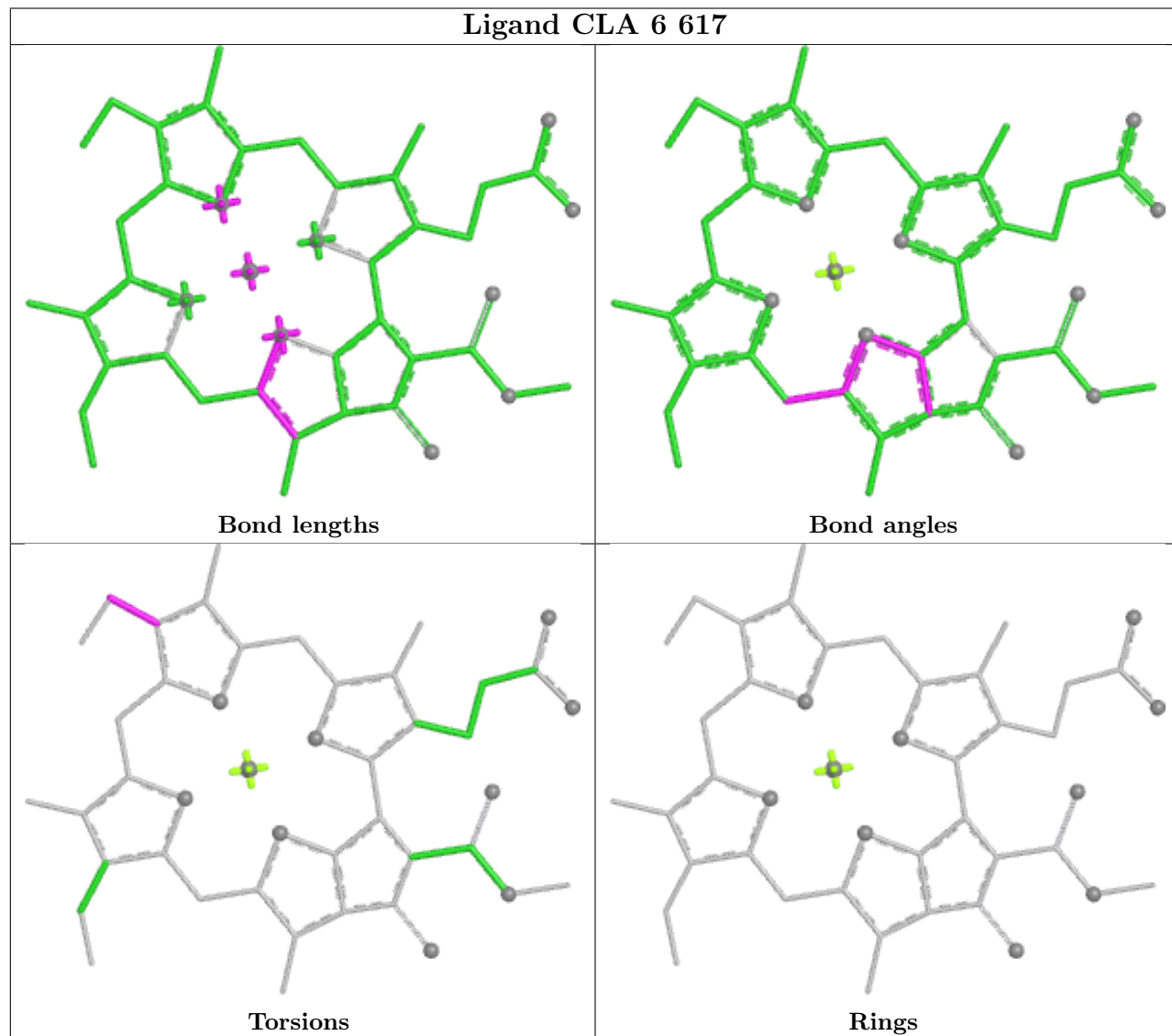
Ligand CLA 92 609

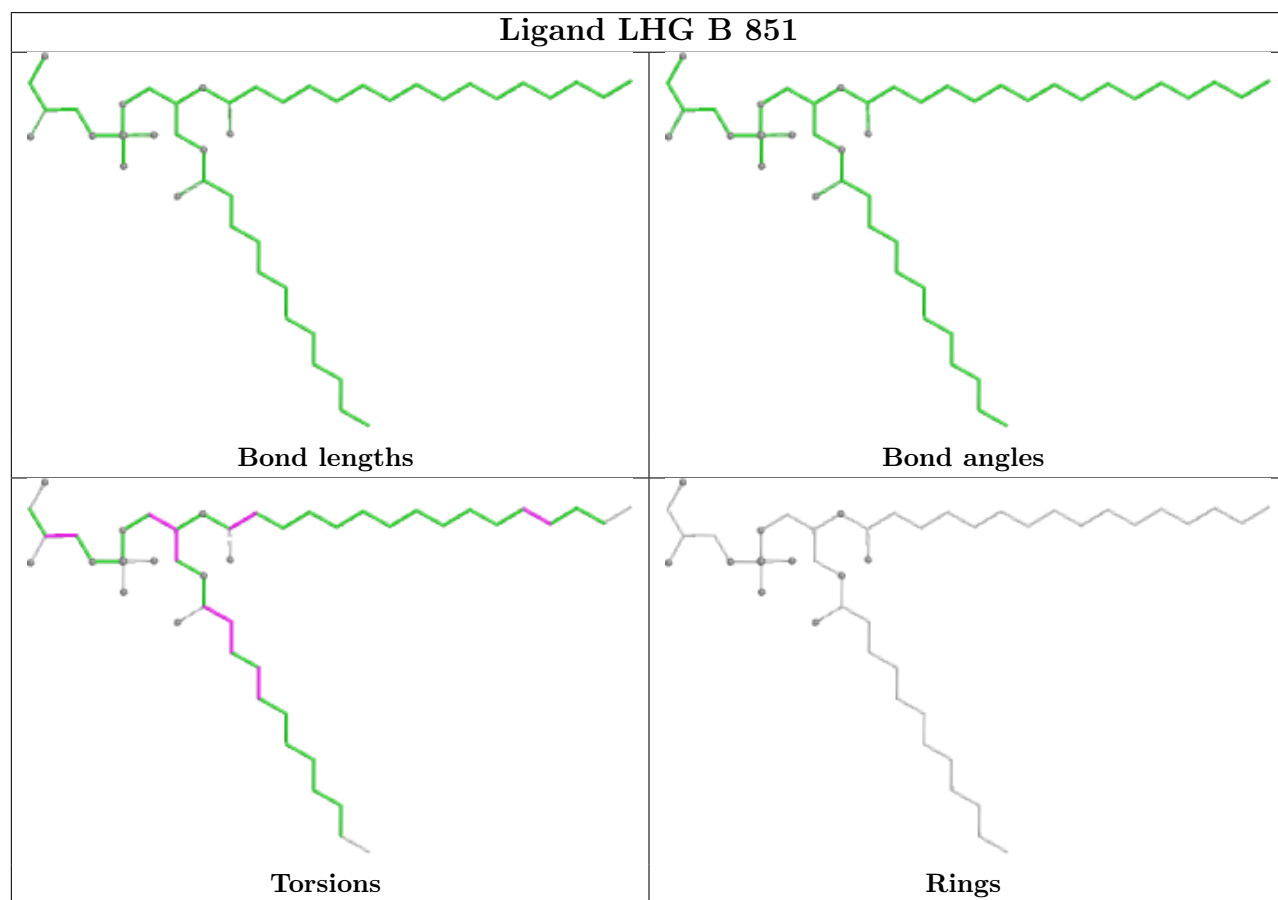
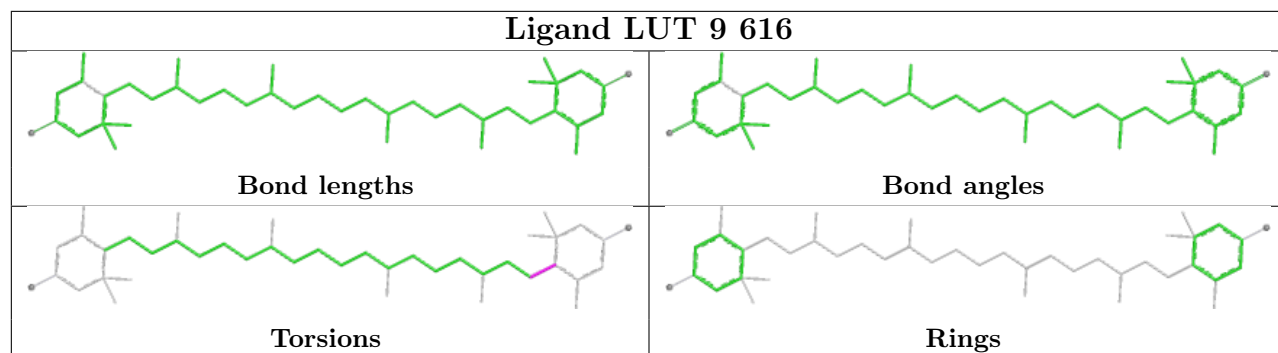


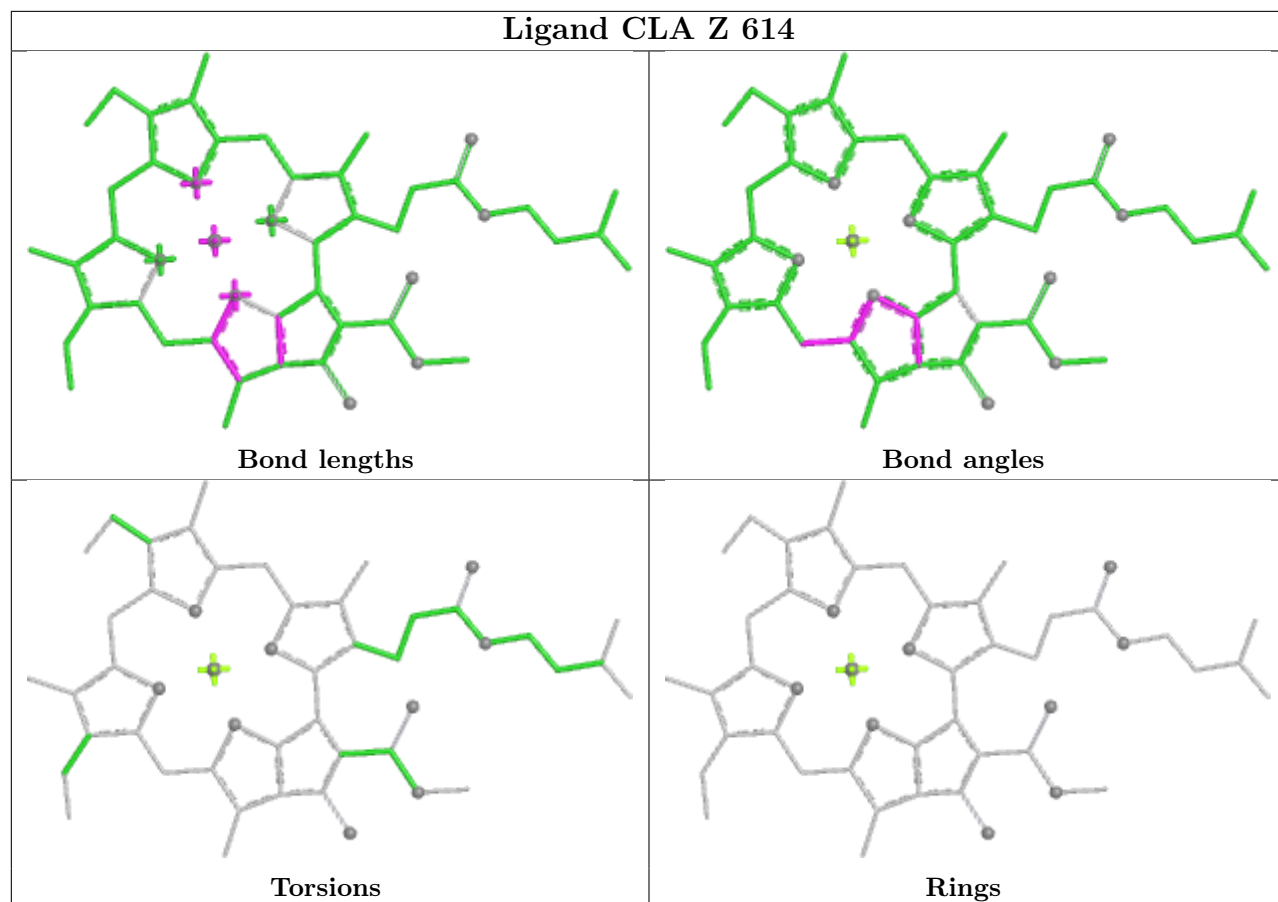
Ligand CLA F 304



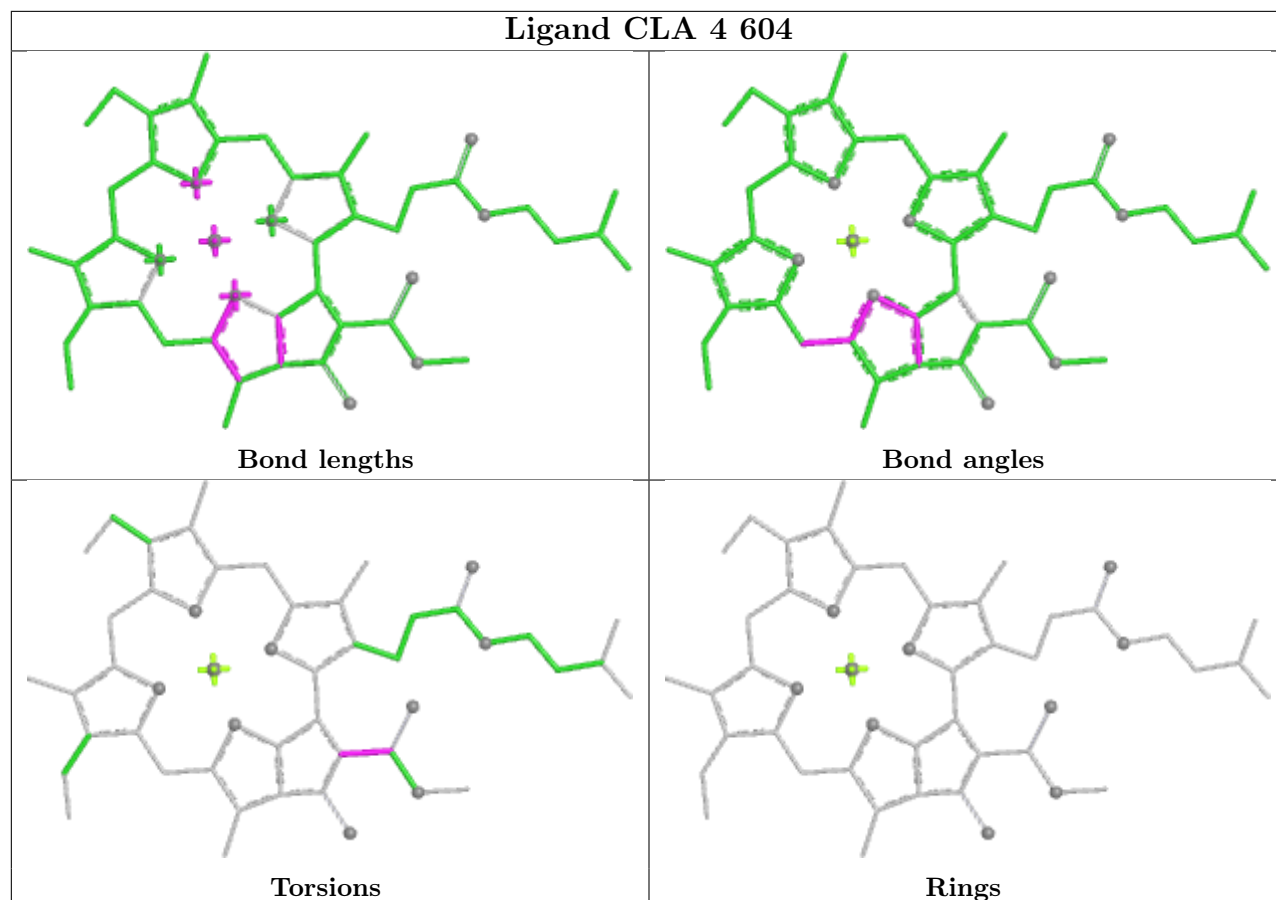
Ligand CLA 6 617



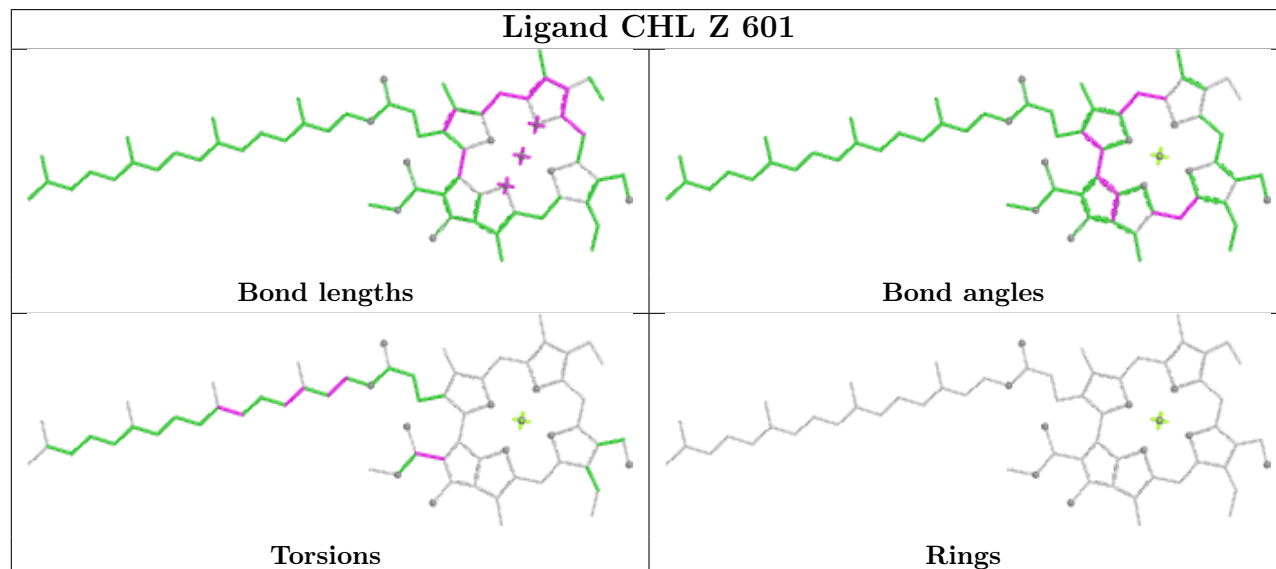


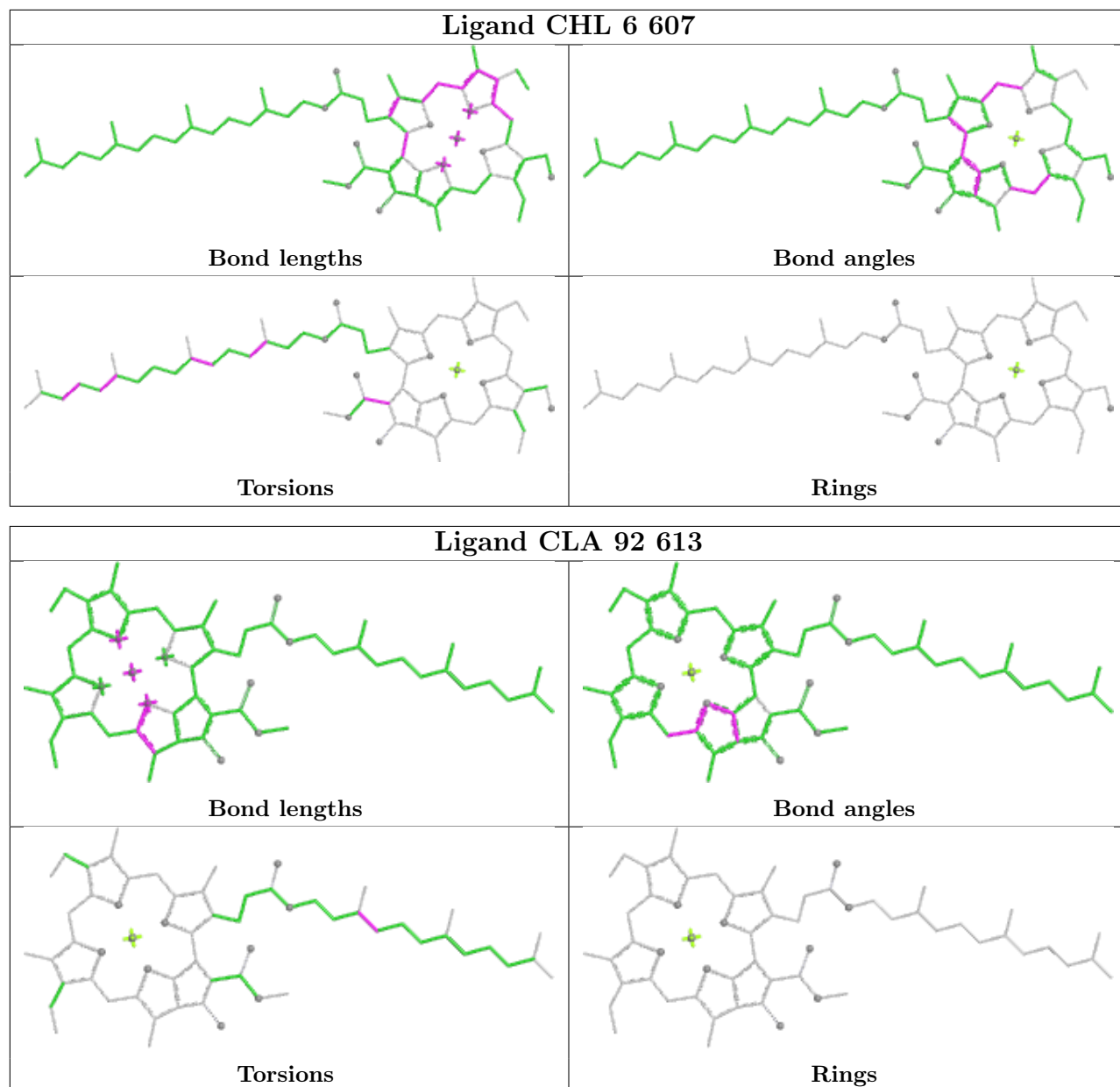


Ligand CLA 4 604

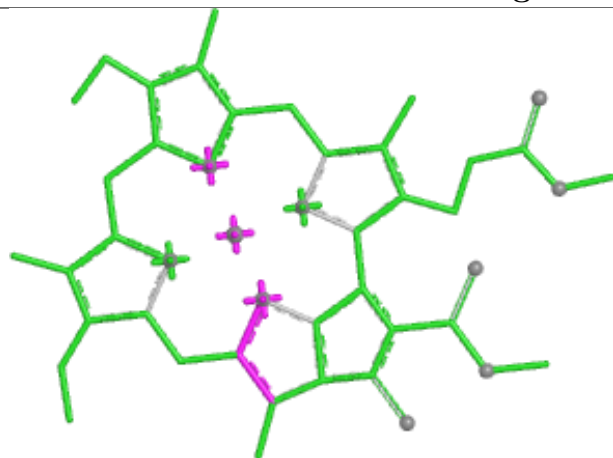


Ligand CHL Z 601

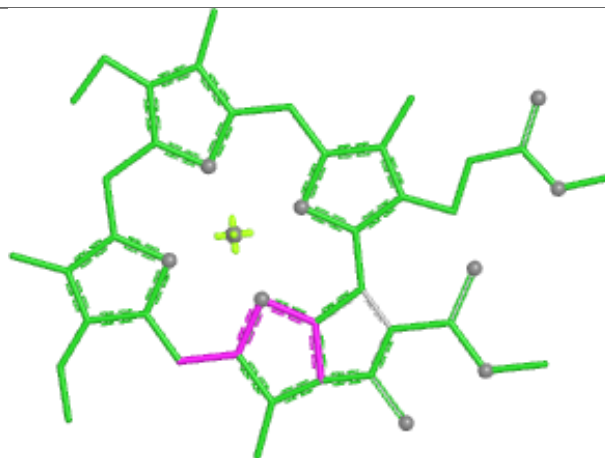




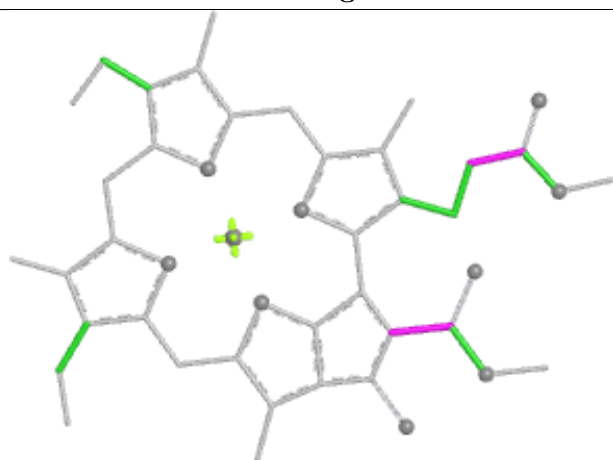
Ligand CLA G 204



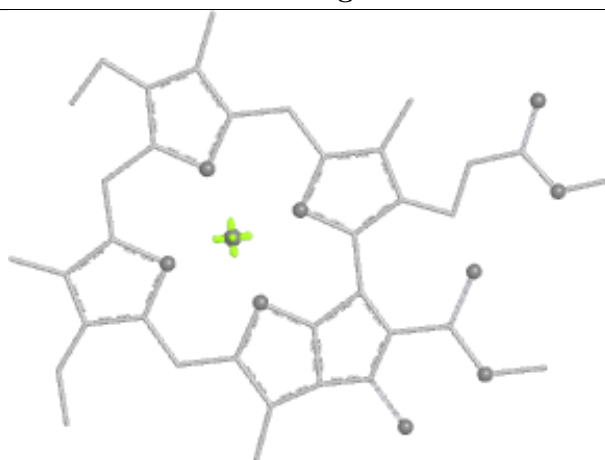
Bond lengths



Bond angles

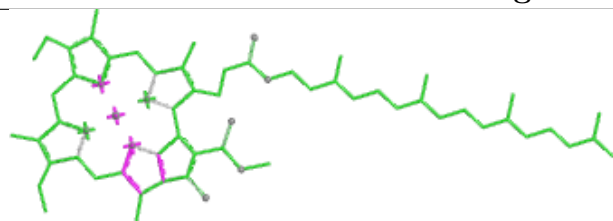


Torsions

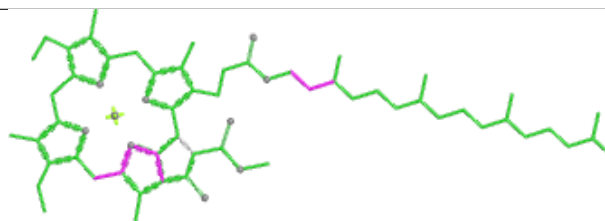


Rings

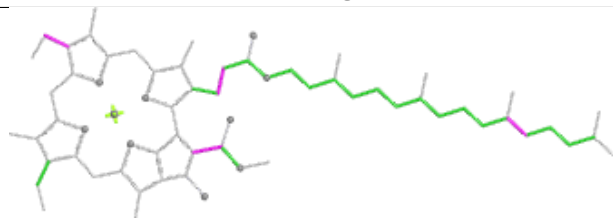
Ligand CLA A 809



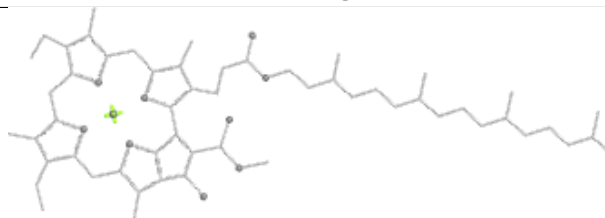
Bond lengths



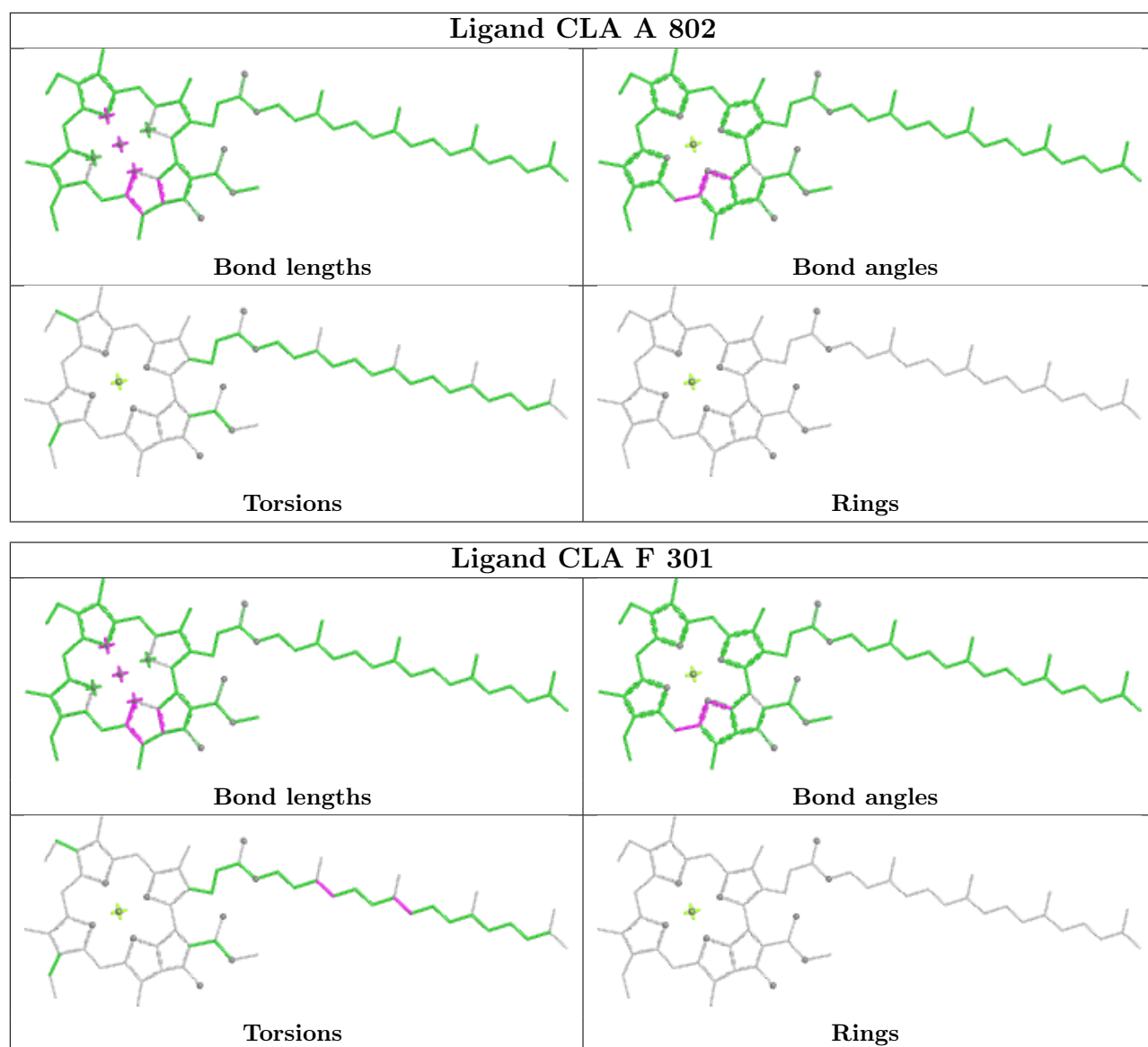
Bond angles



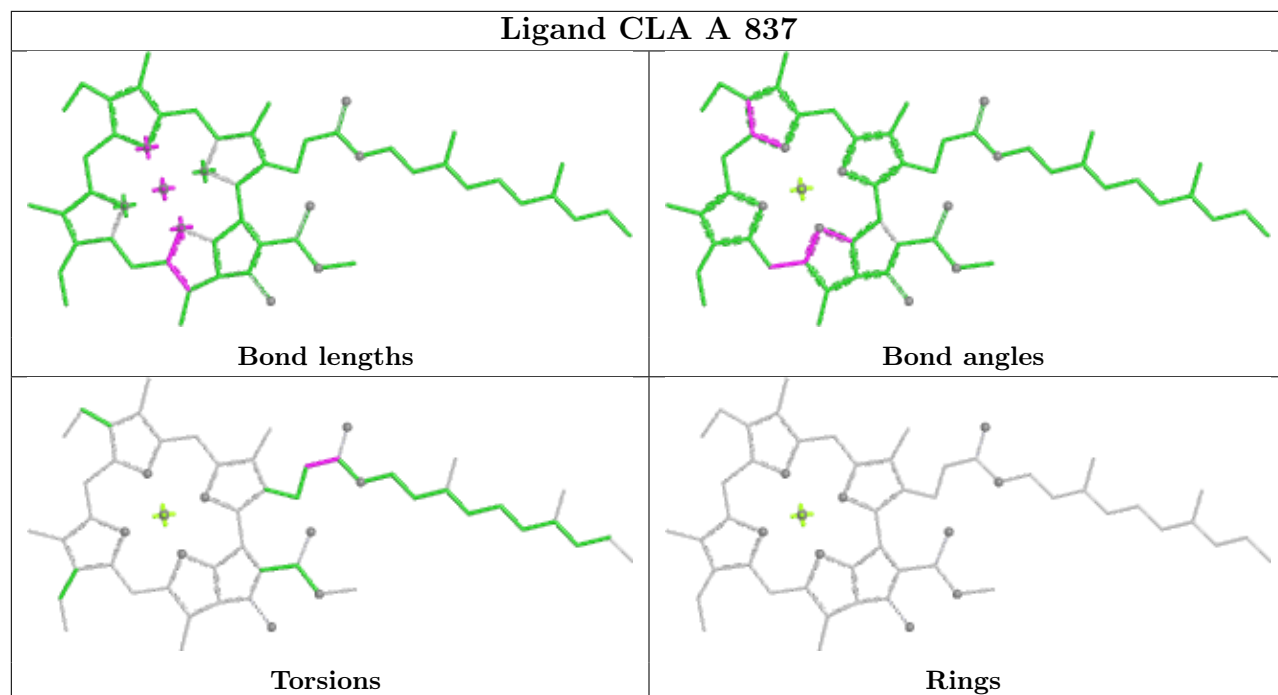
Torsions



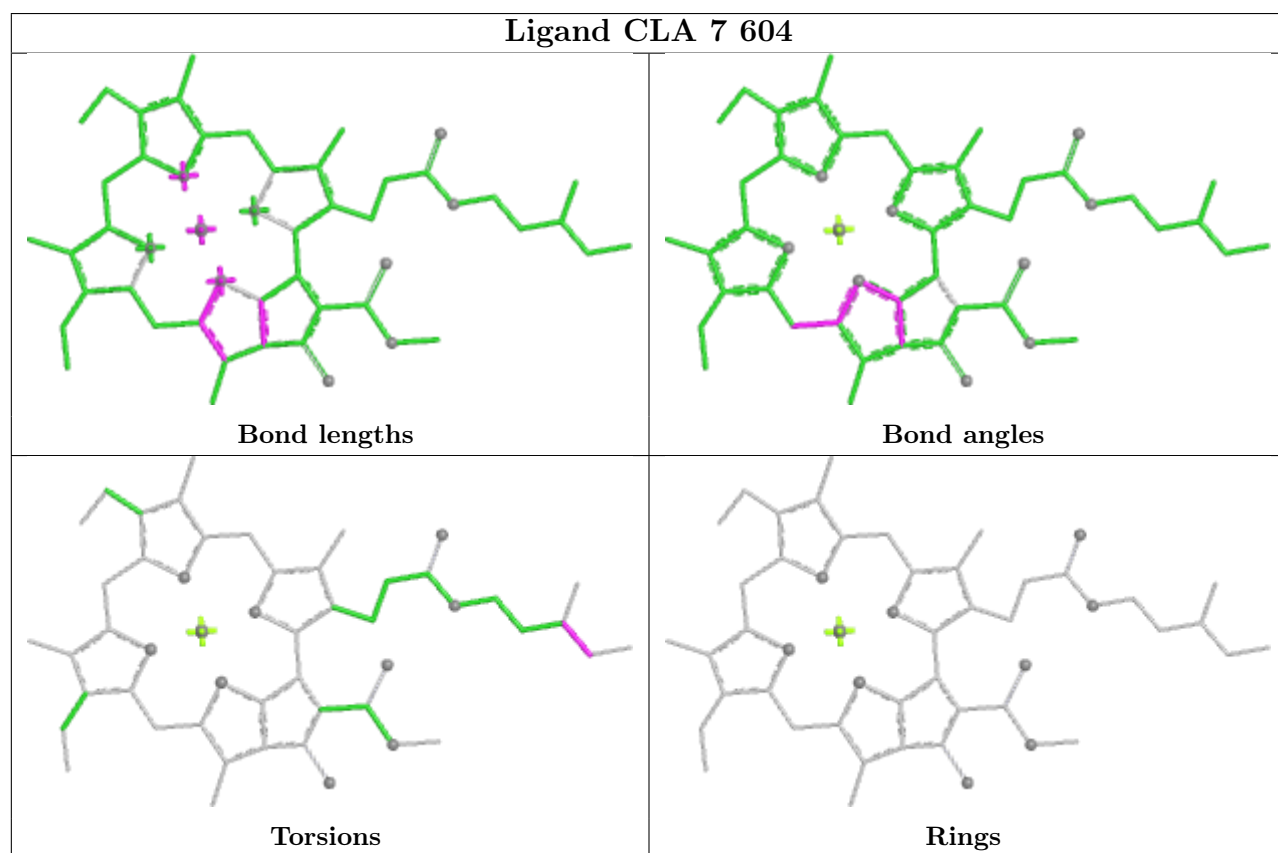
Rings

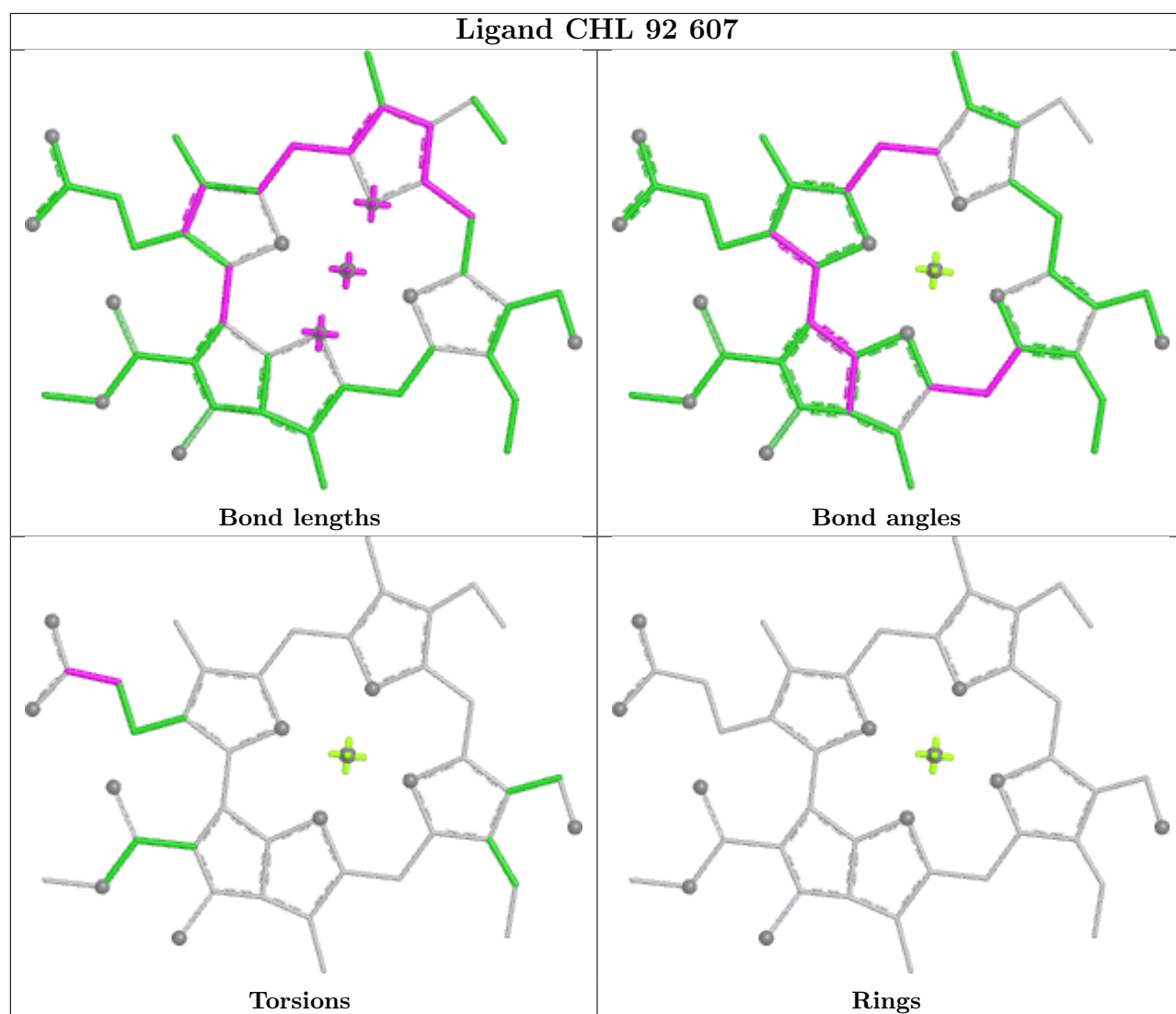
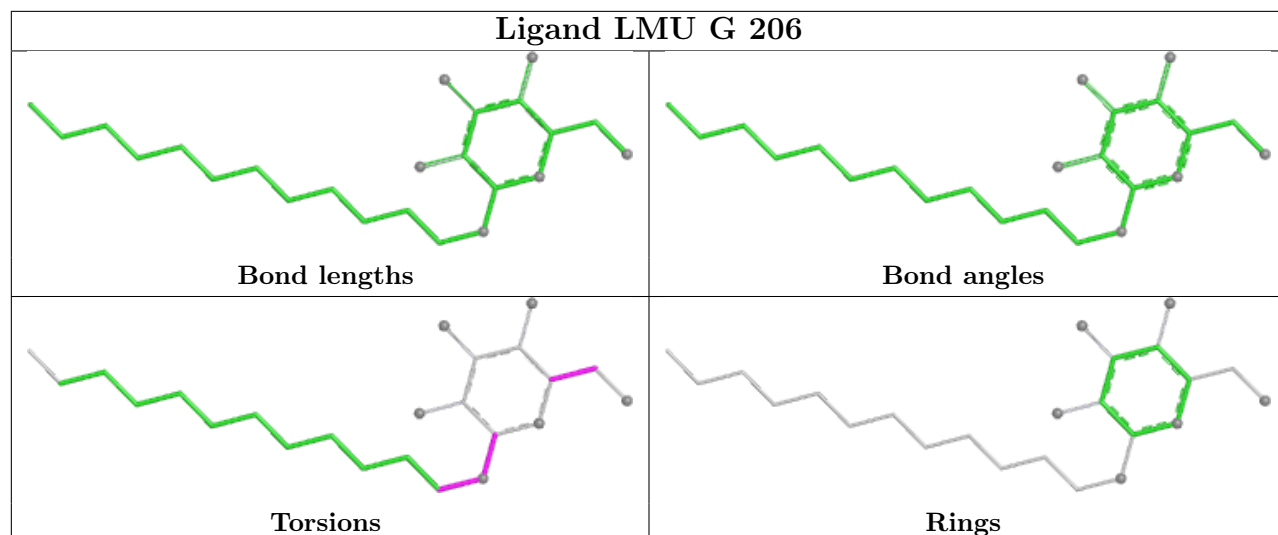


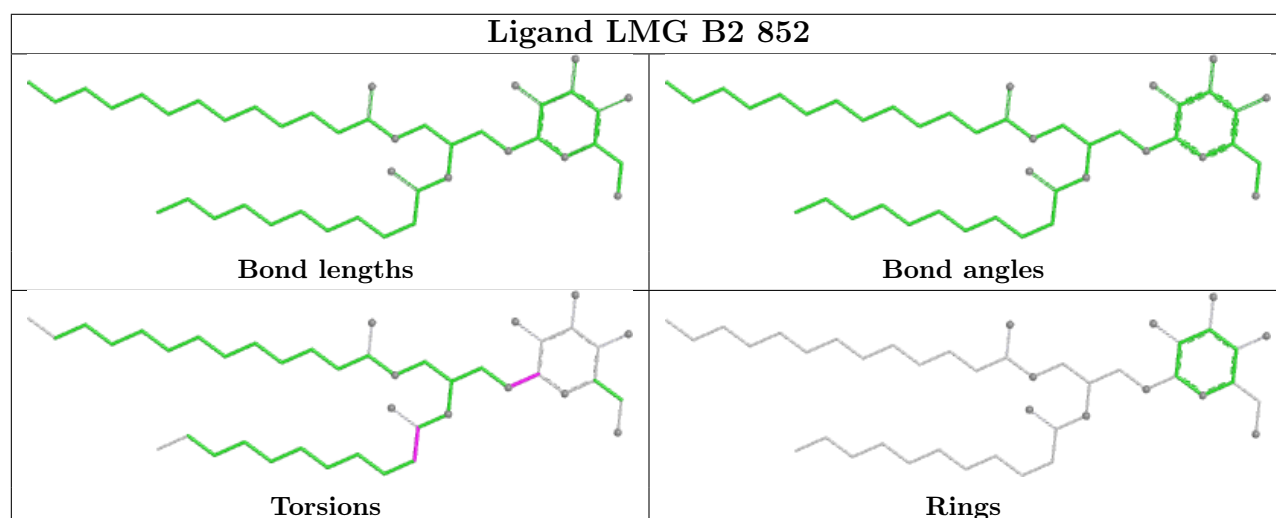
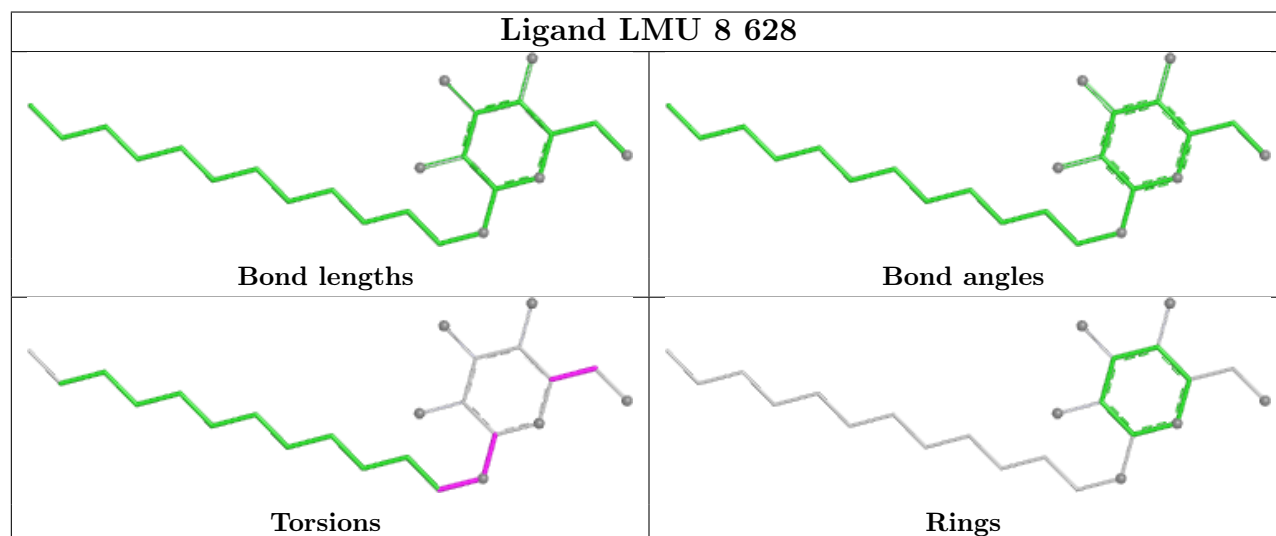
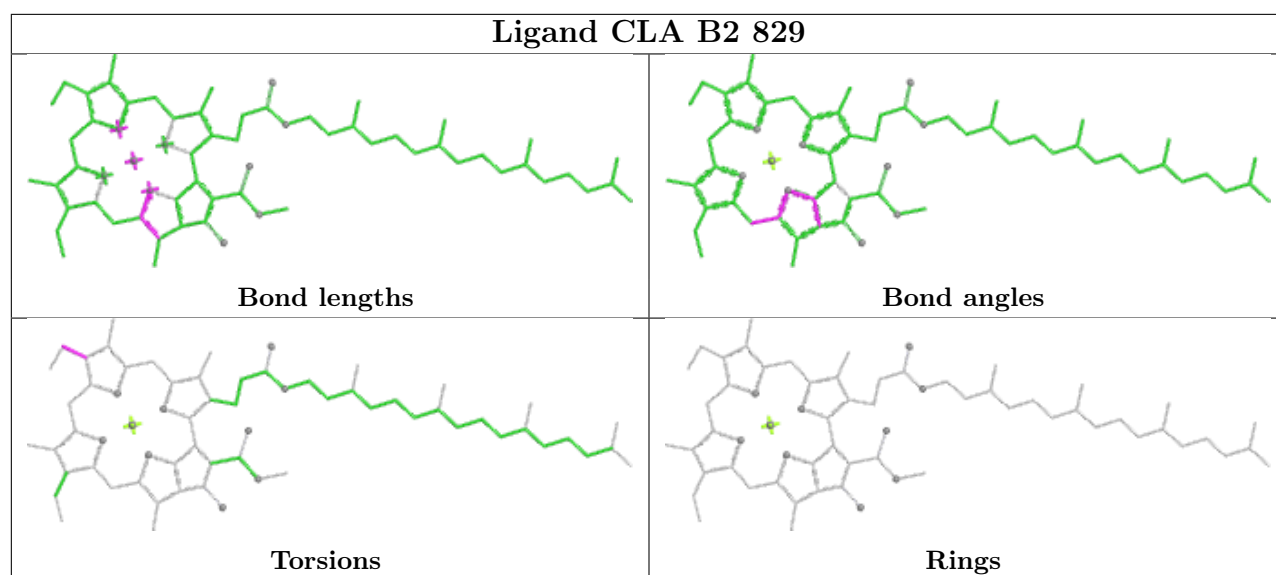
Ligand CLA A 837

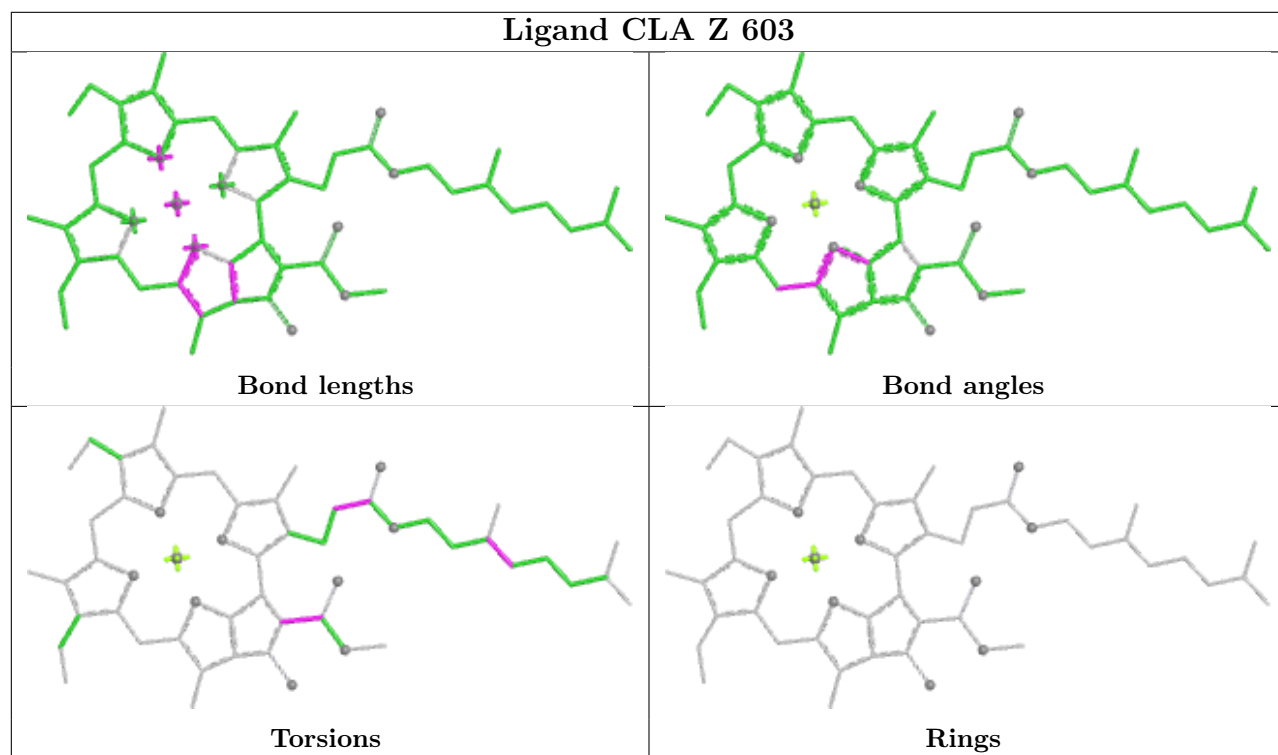
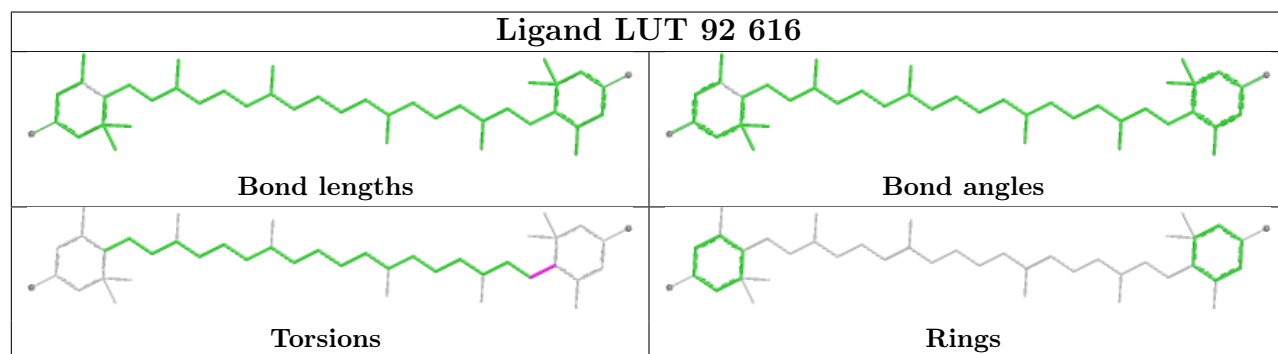
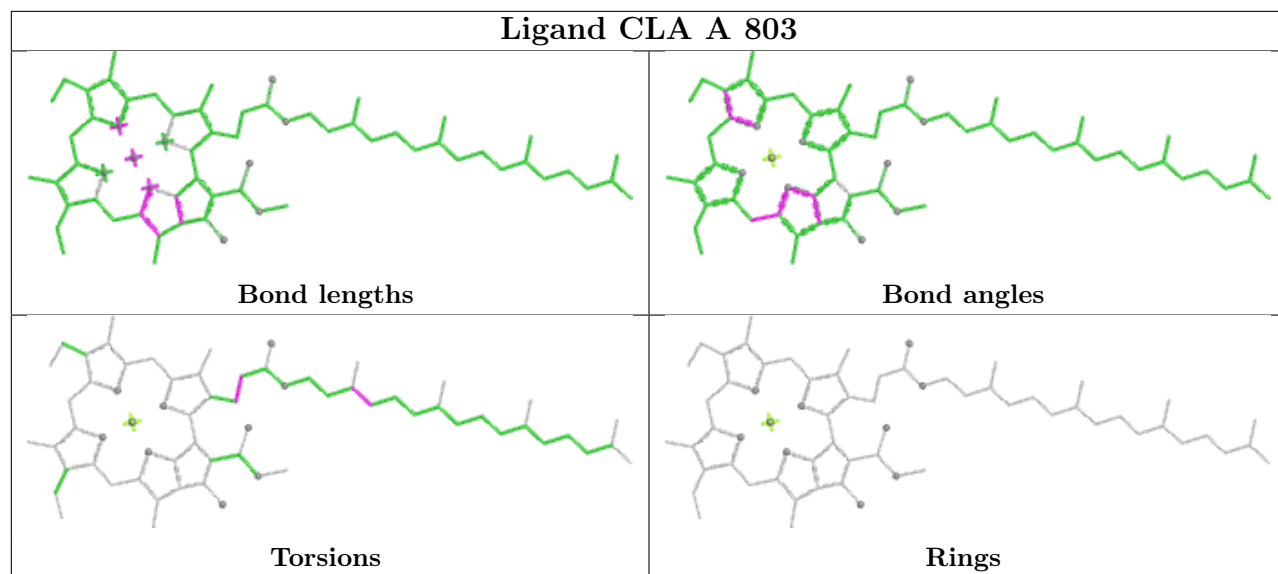


Ligand CLA 7 604

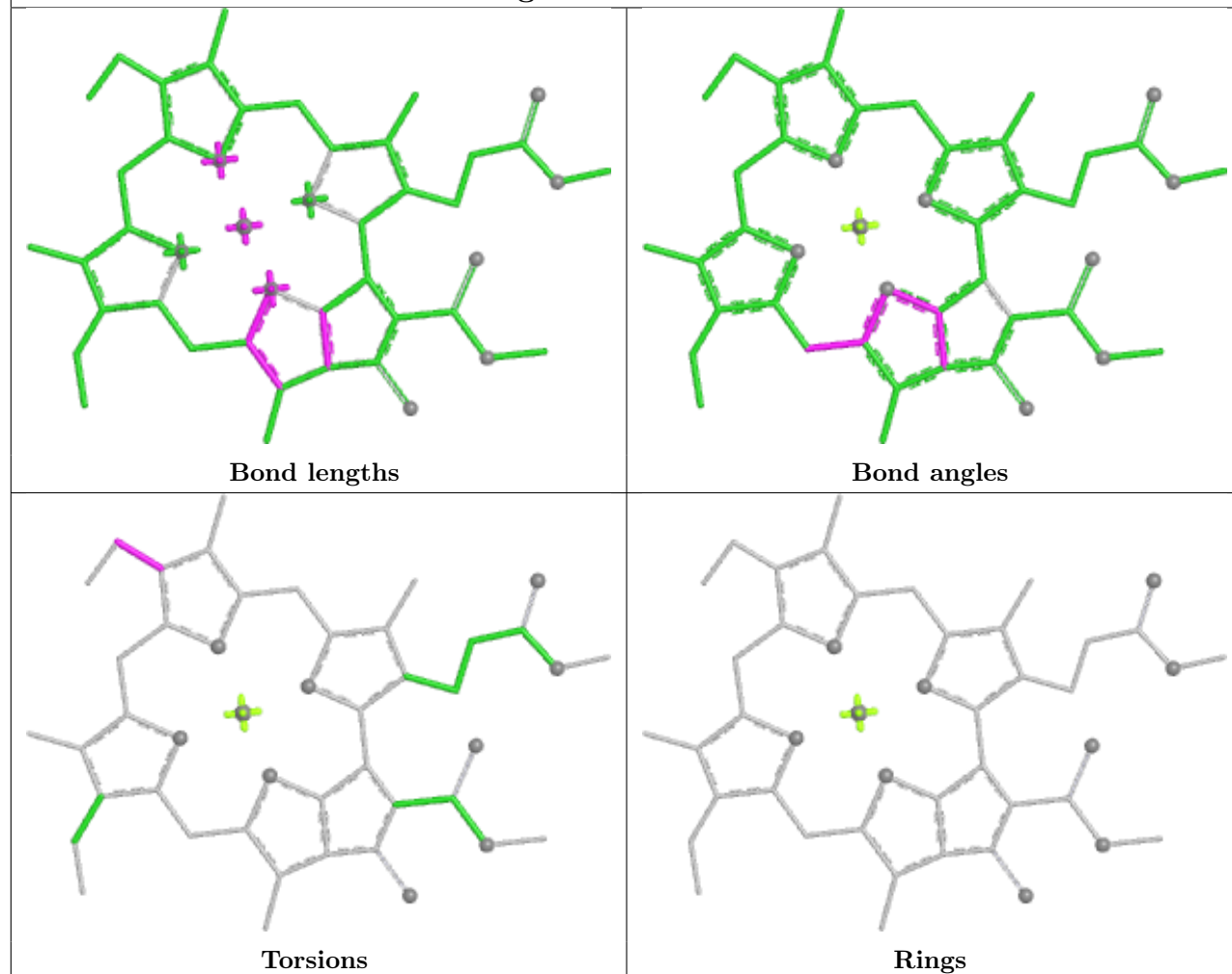




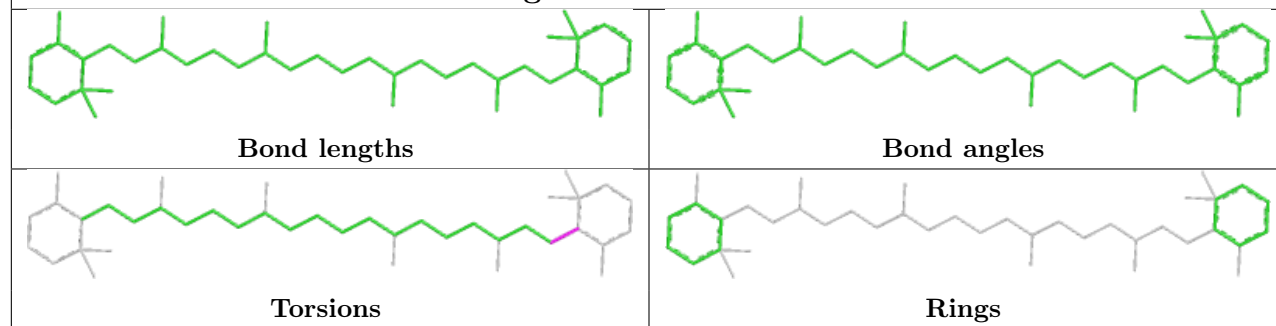


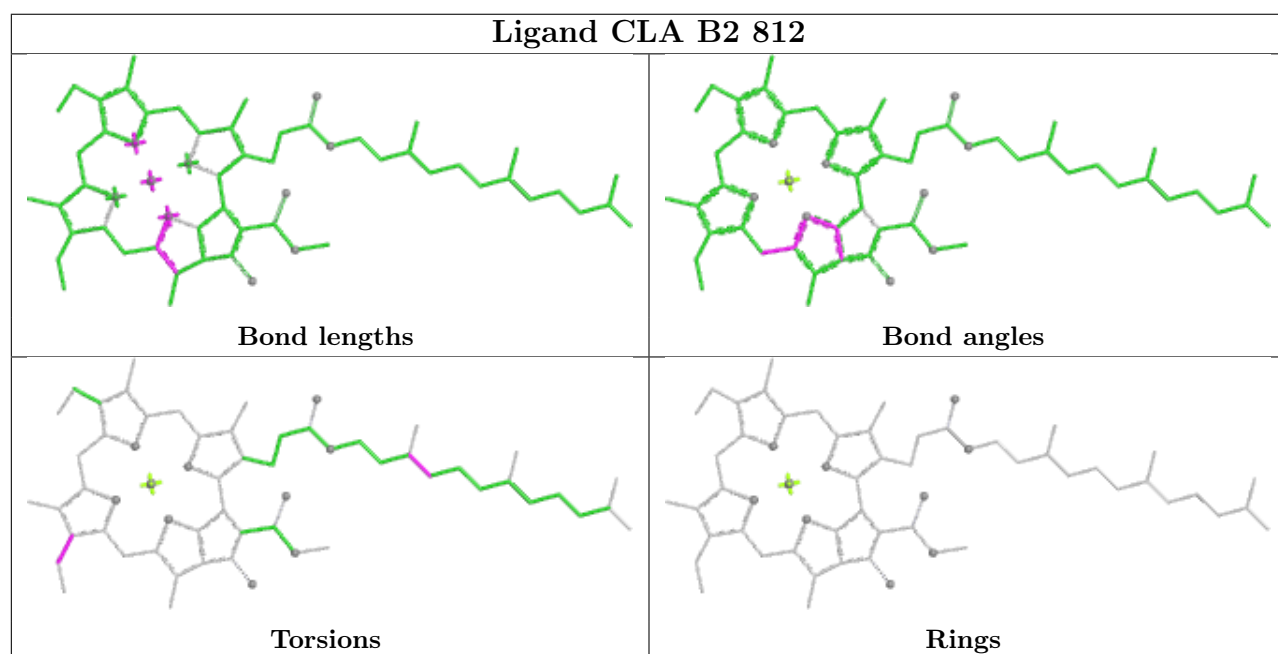
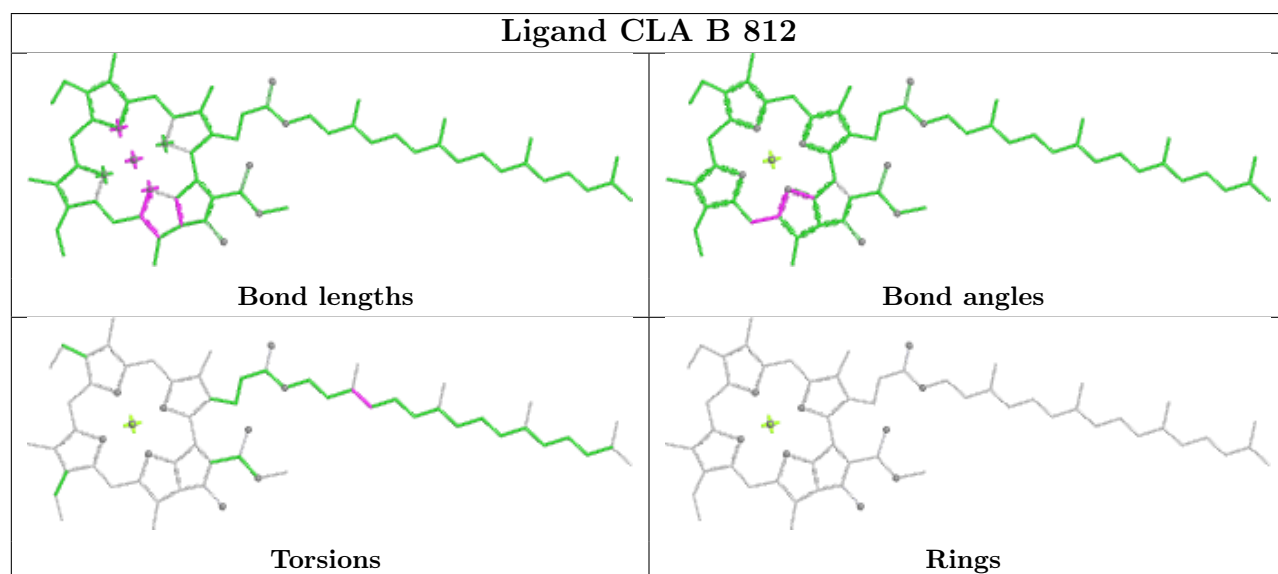
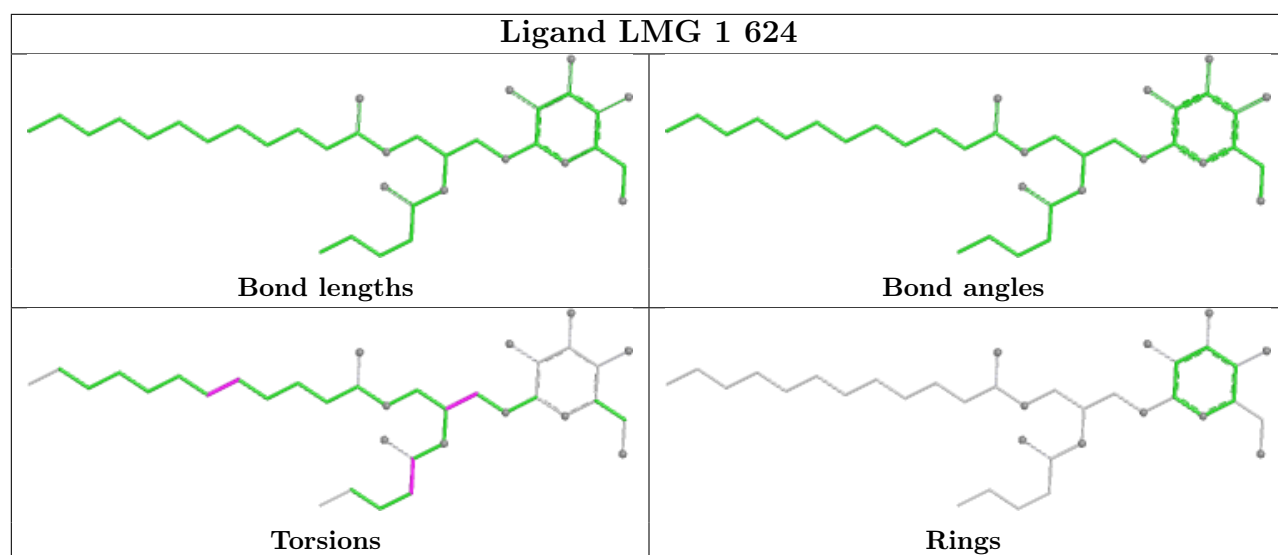


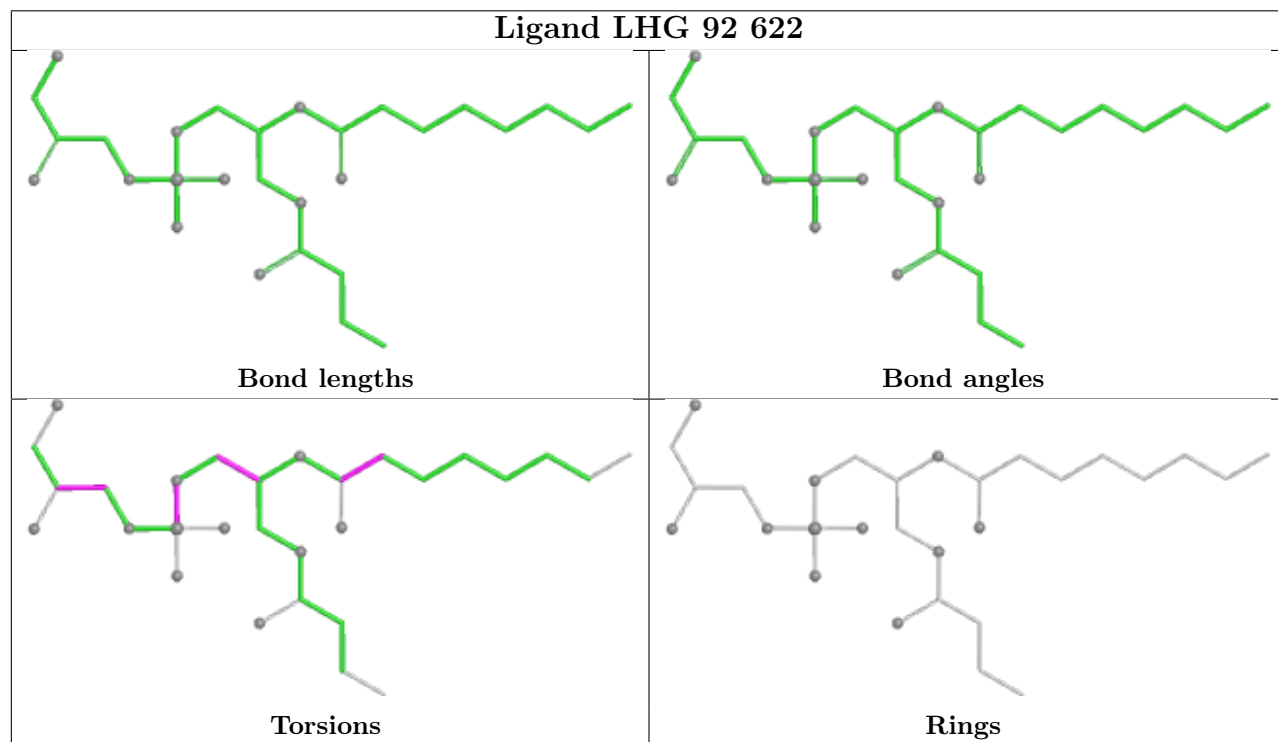
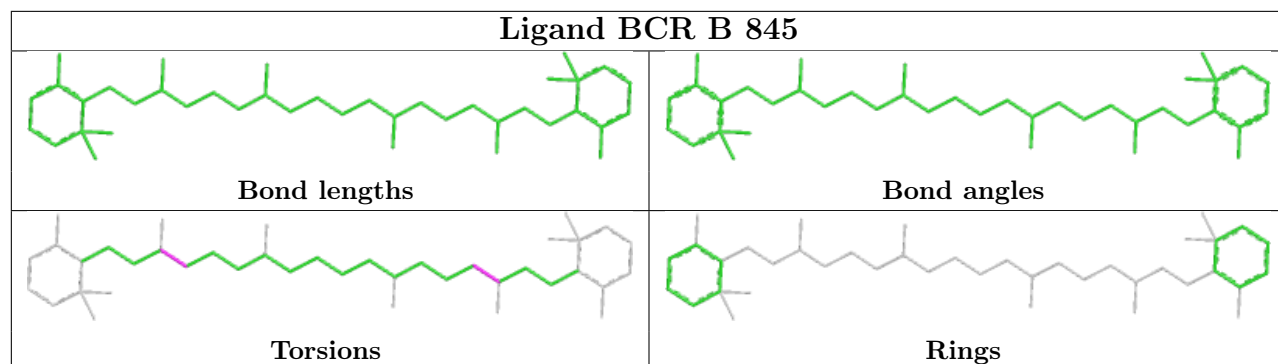
Ligand CLA 3 612

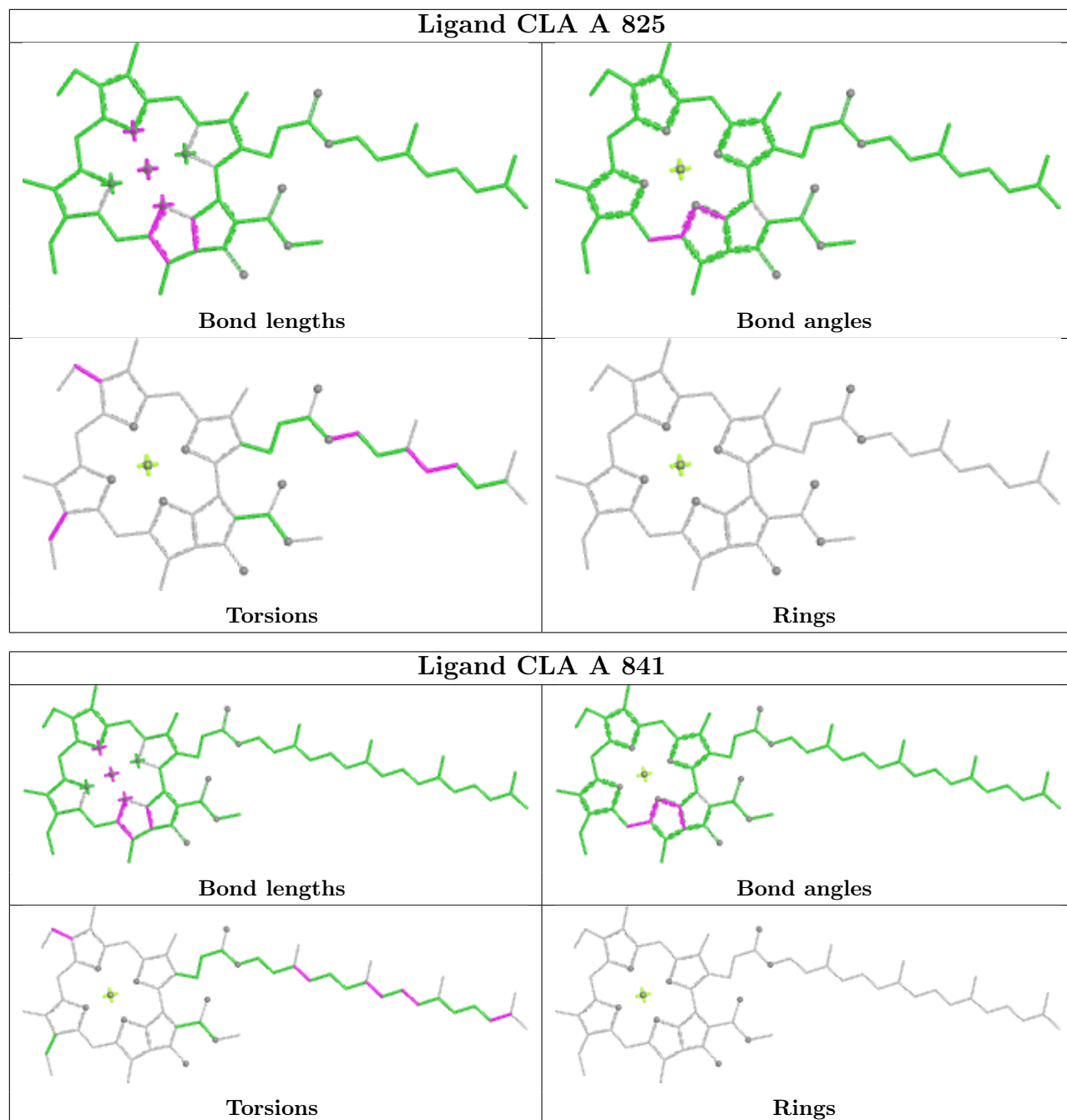


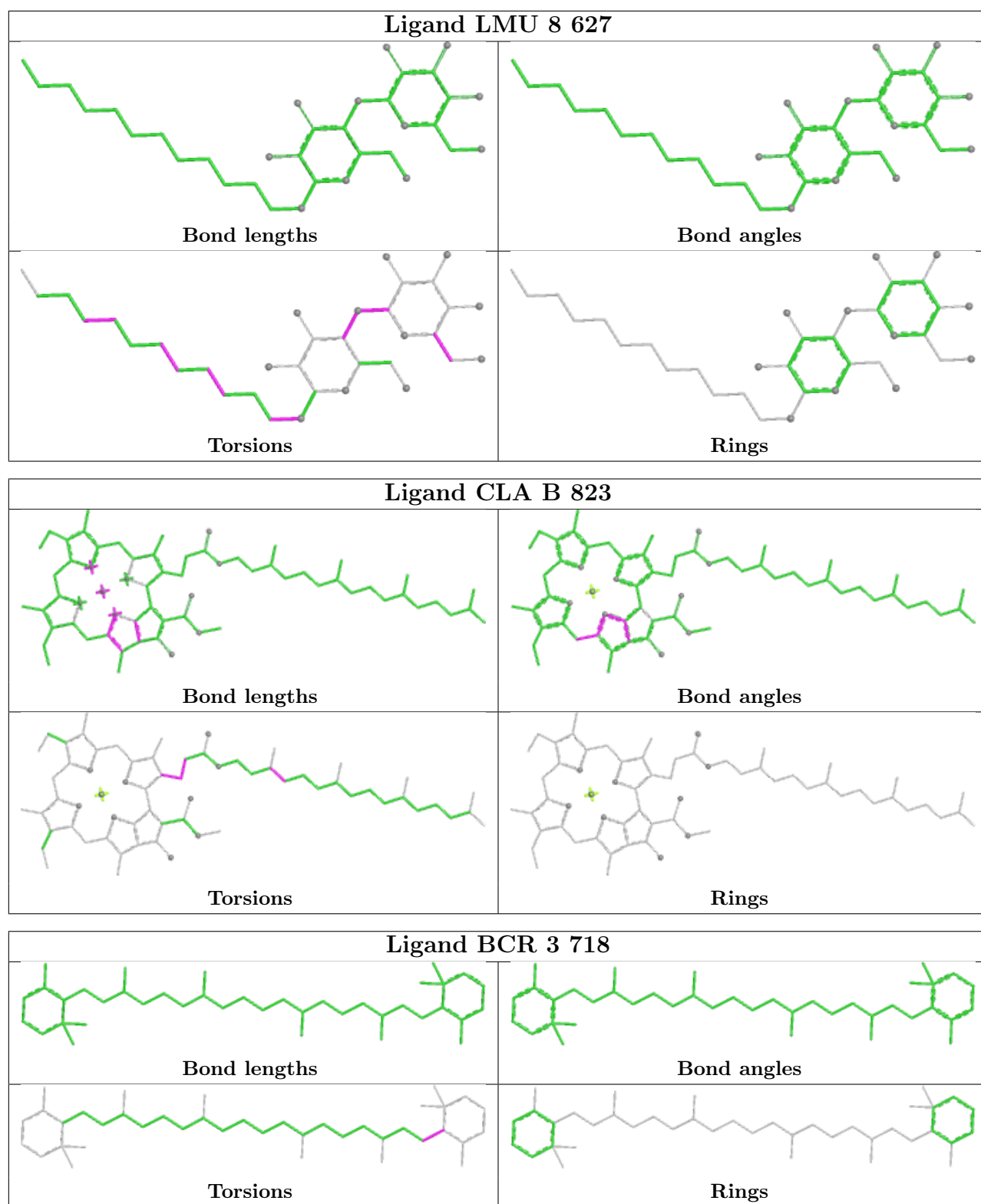
Ligand BCR L2 205

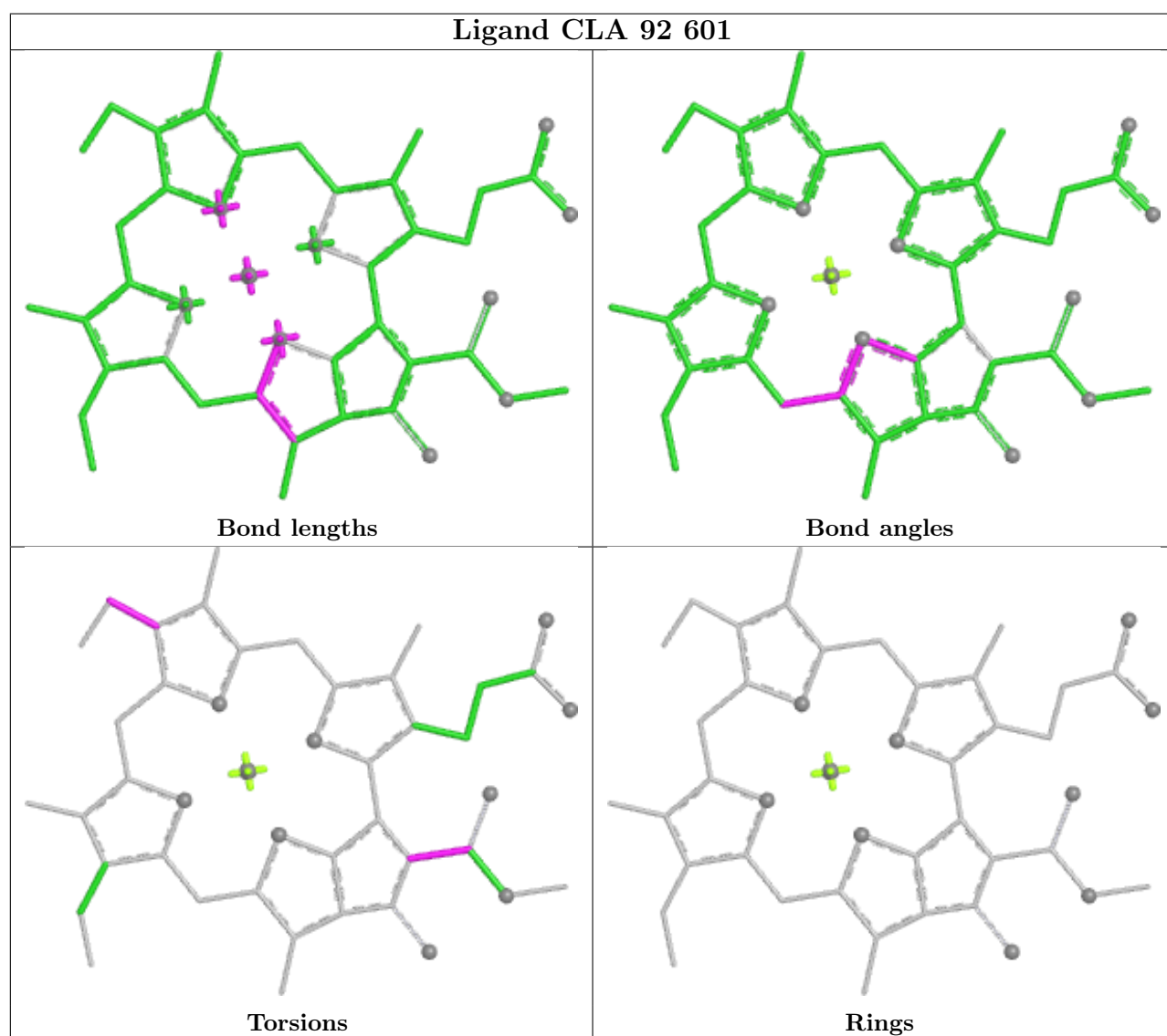
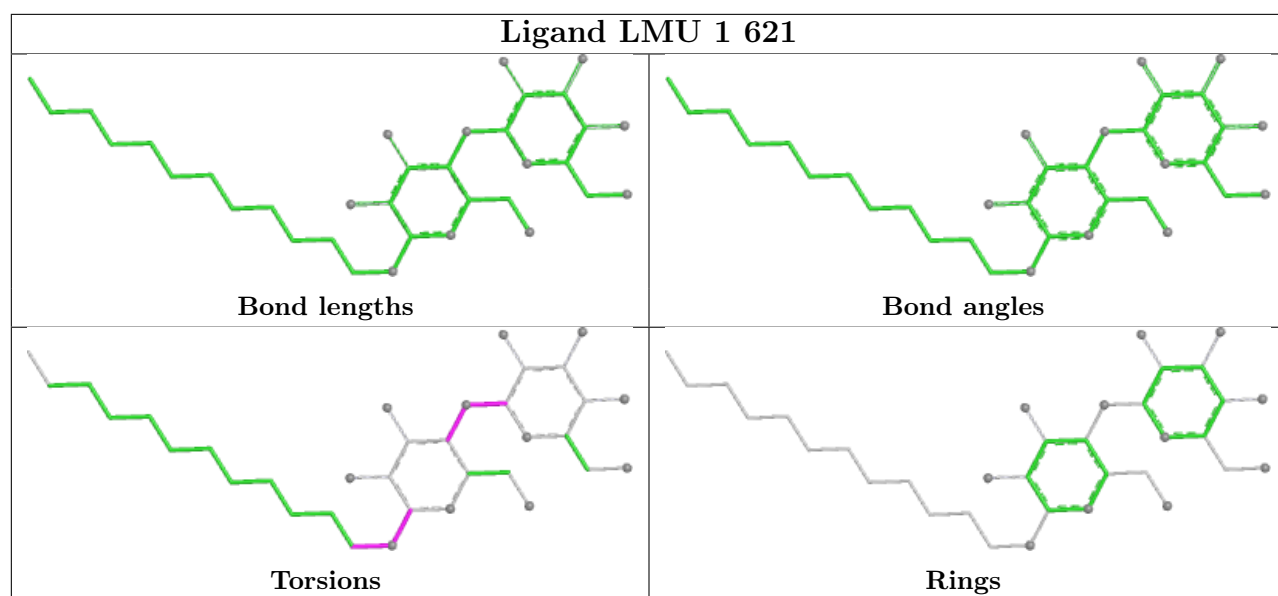


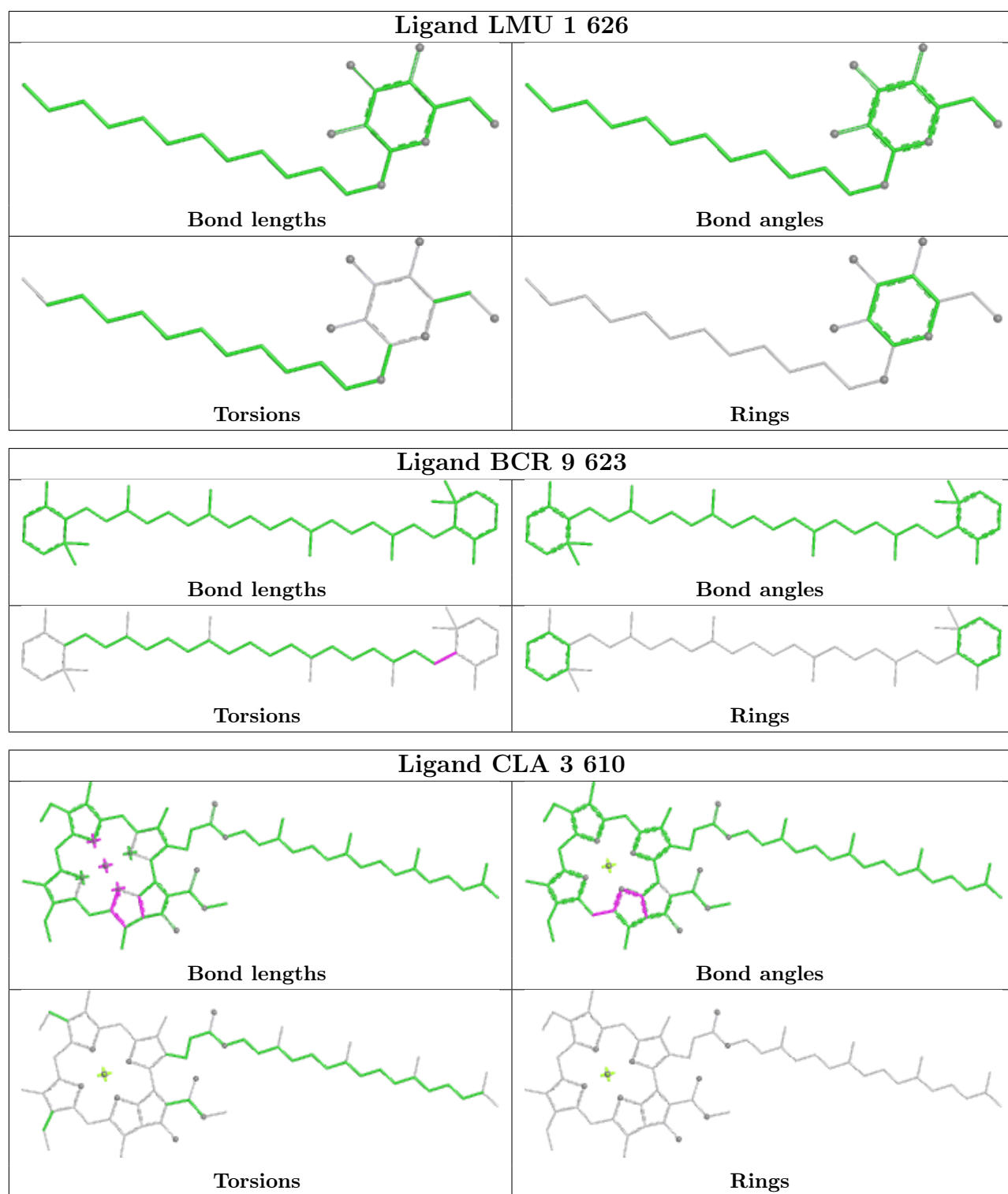




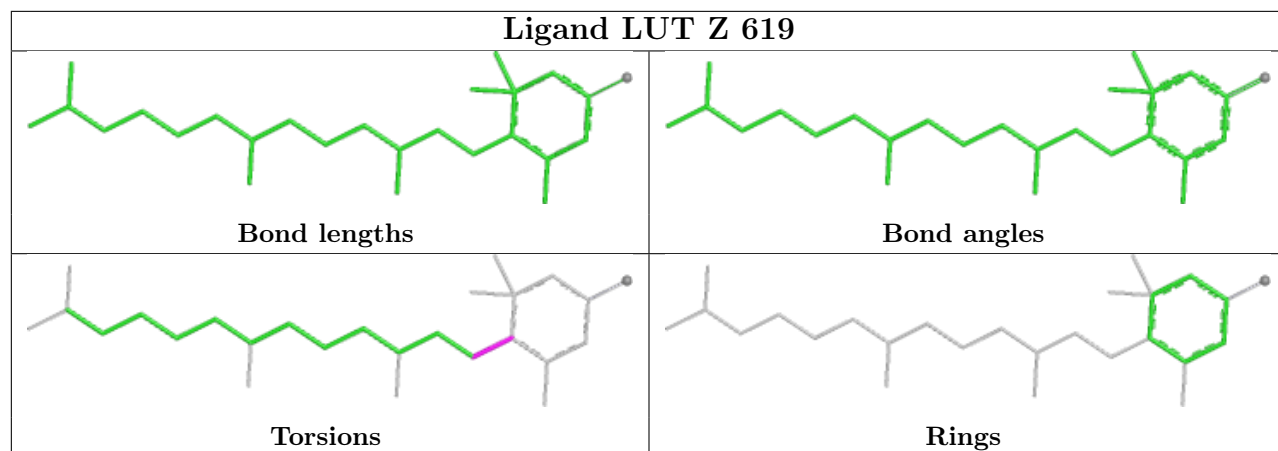




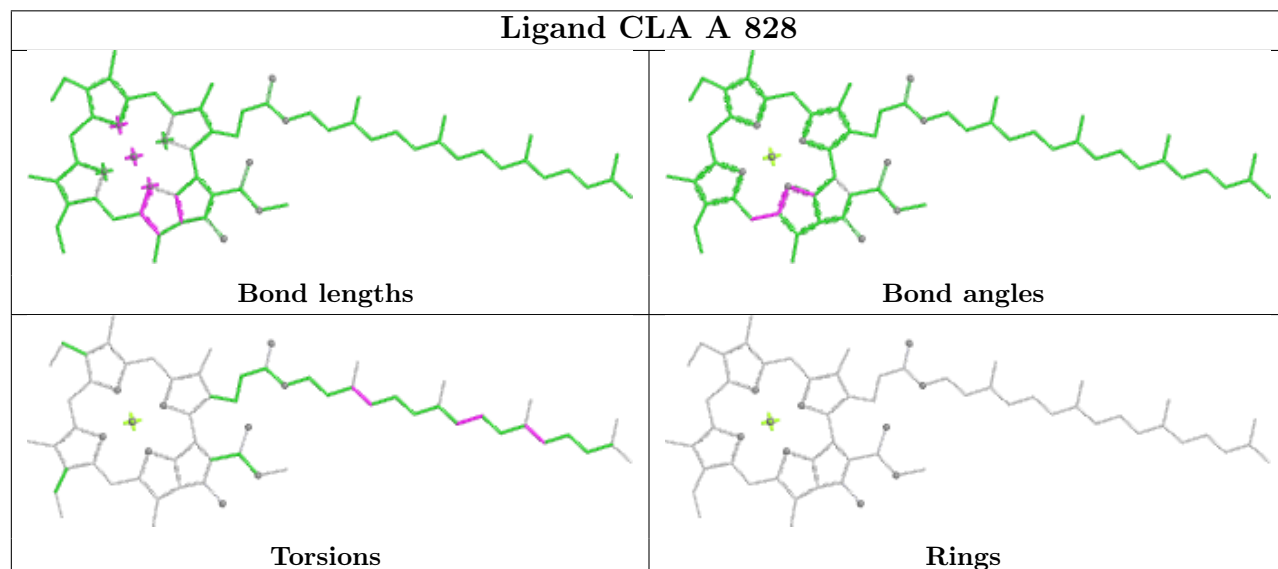




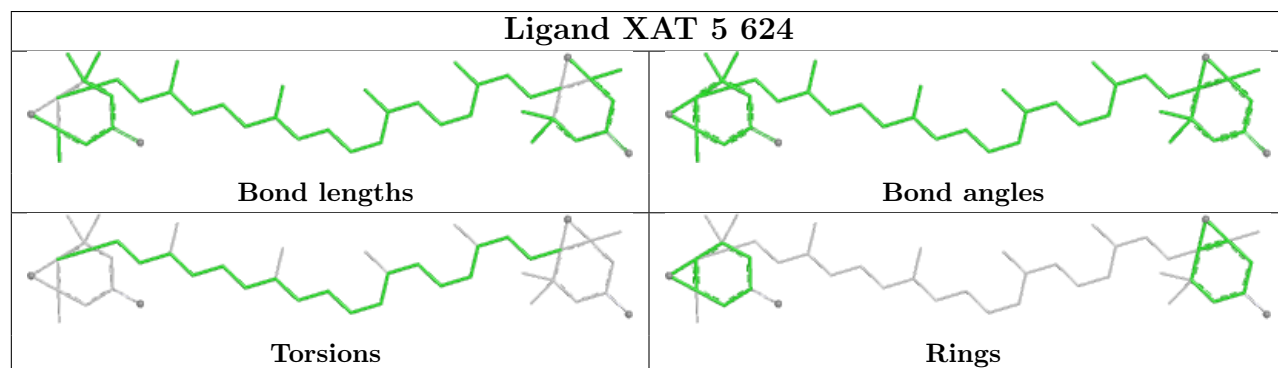
Ligand LUT Z 619



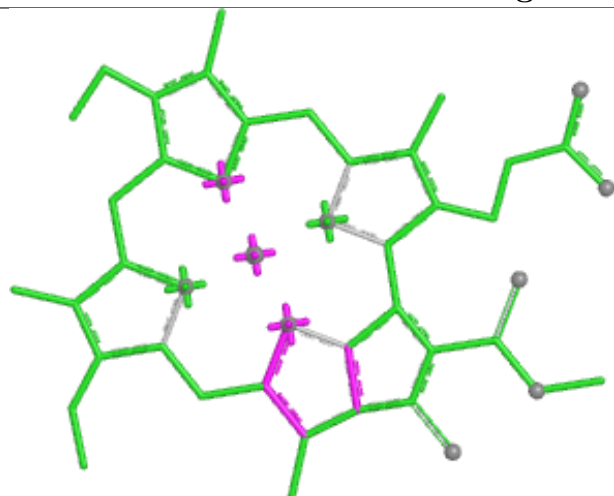
Ligand CLA A 828



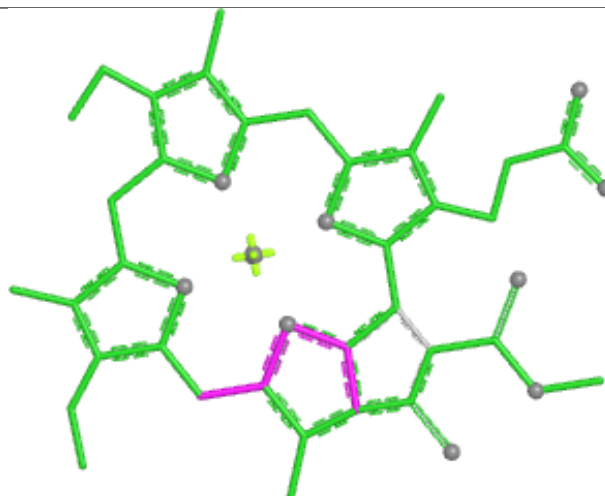
Ligand XAT 5 624



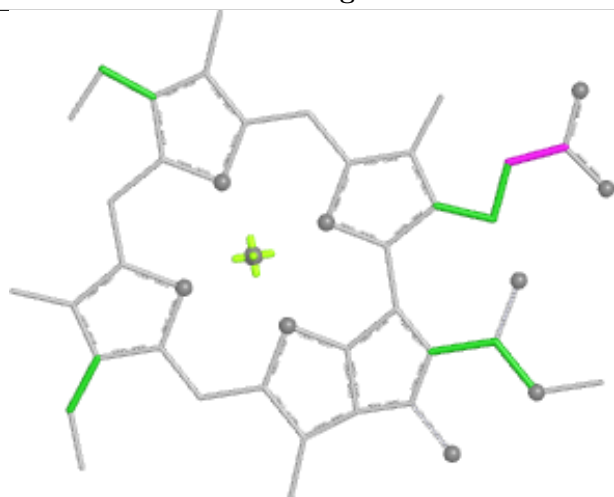
Ligand CLA F 303



Bond lengths



Bond angles

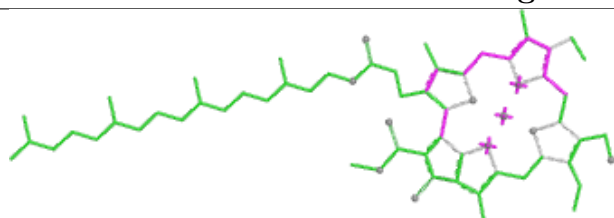


Torsions

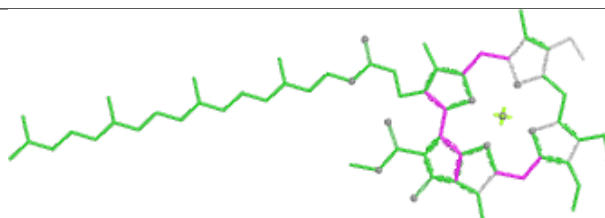


Rings

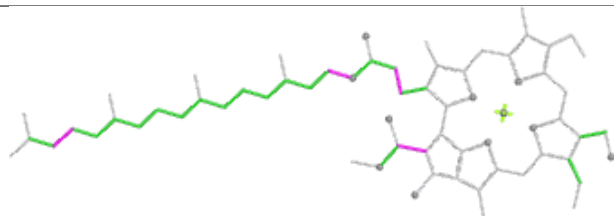
Ligand CHL 4 608



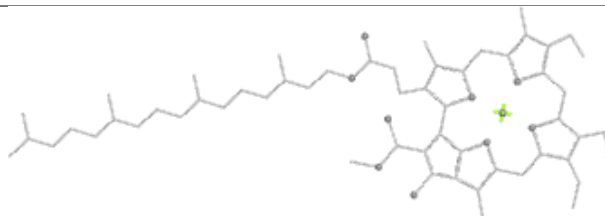
Bond lengths



Bond angles

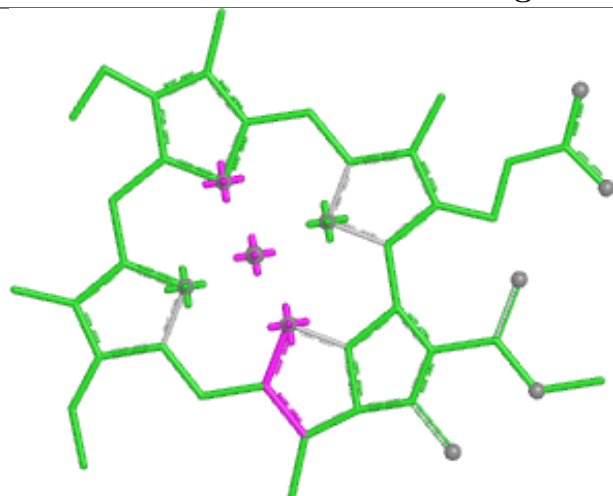


Torsions

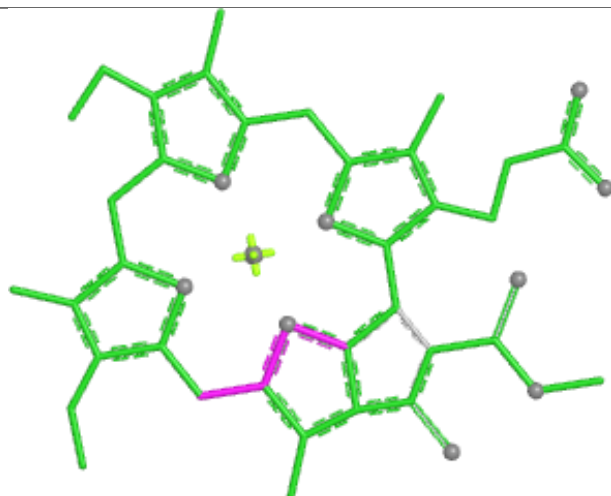


Rings

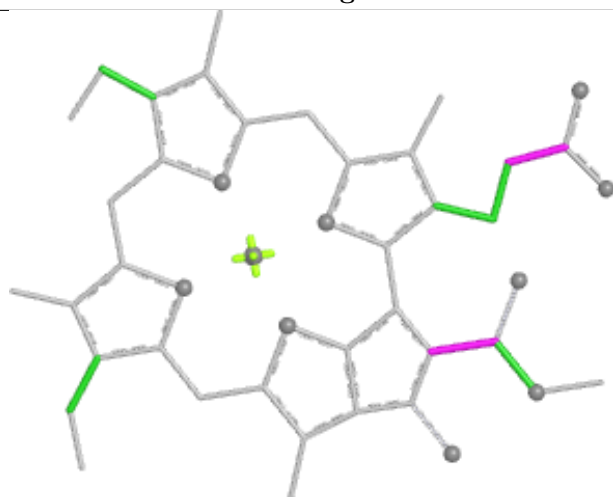
Ligand CLA B 804



Bond lengths



Bond angles

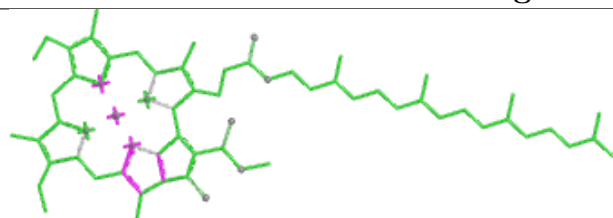


Torsions

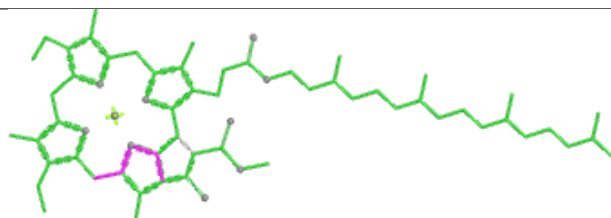


Rings

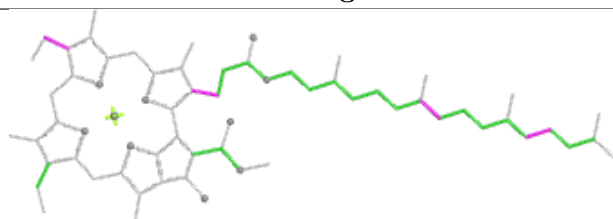
Ligand CLA A 834



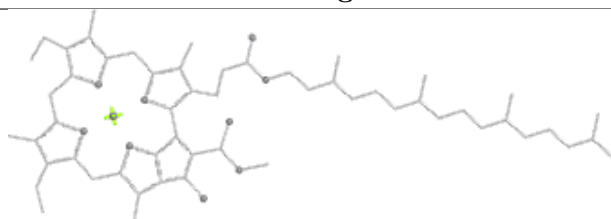
Bond lengths



Bond angles

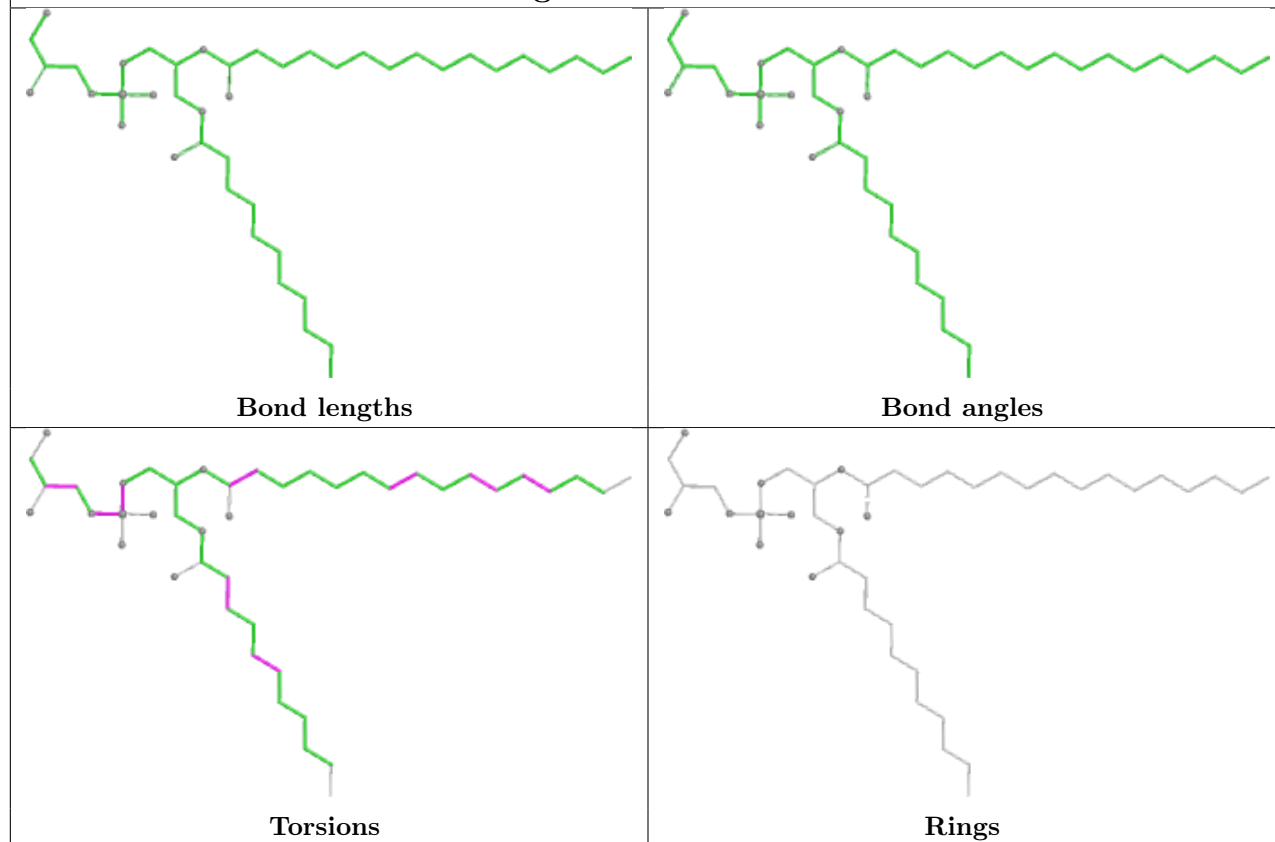


Torsions

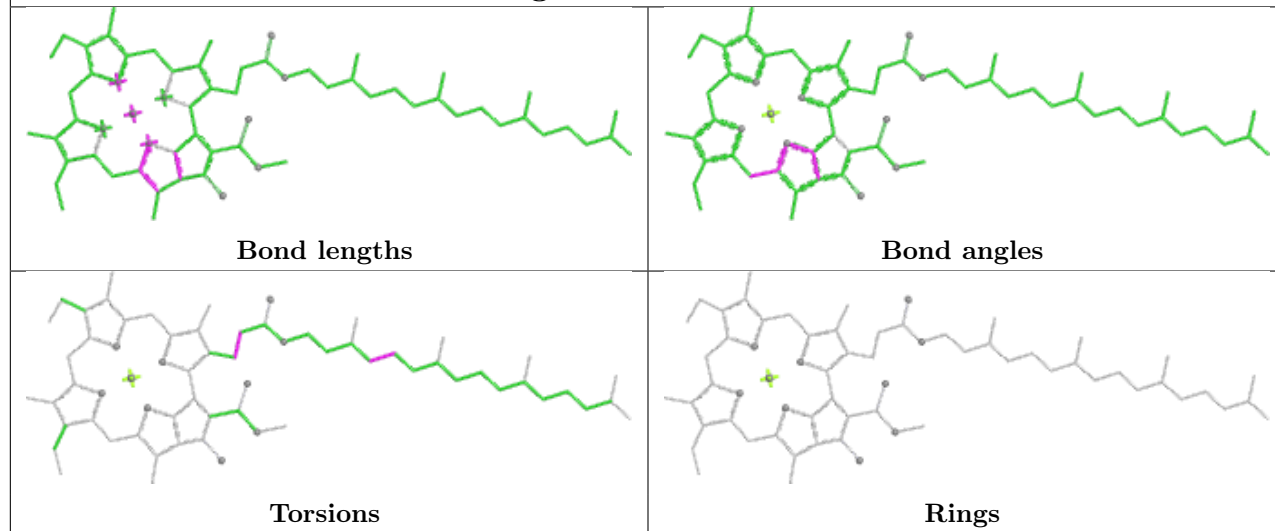


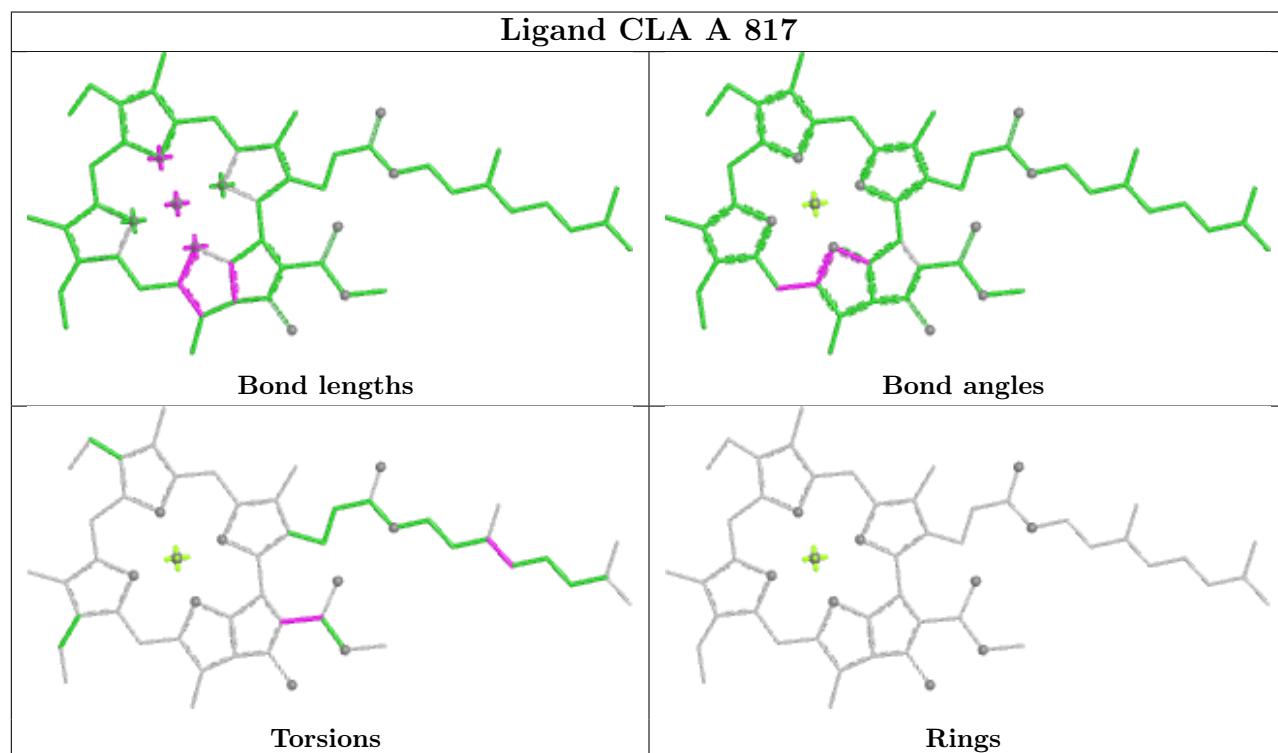
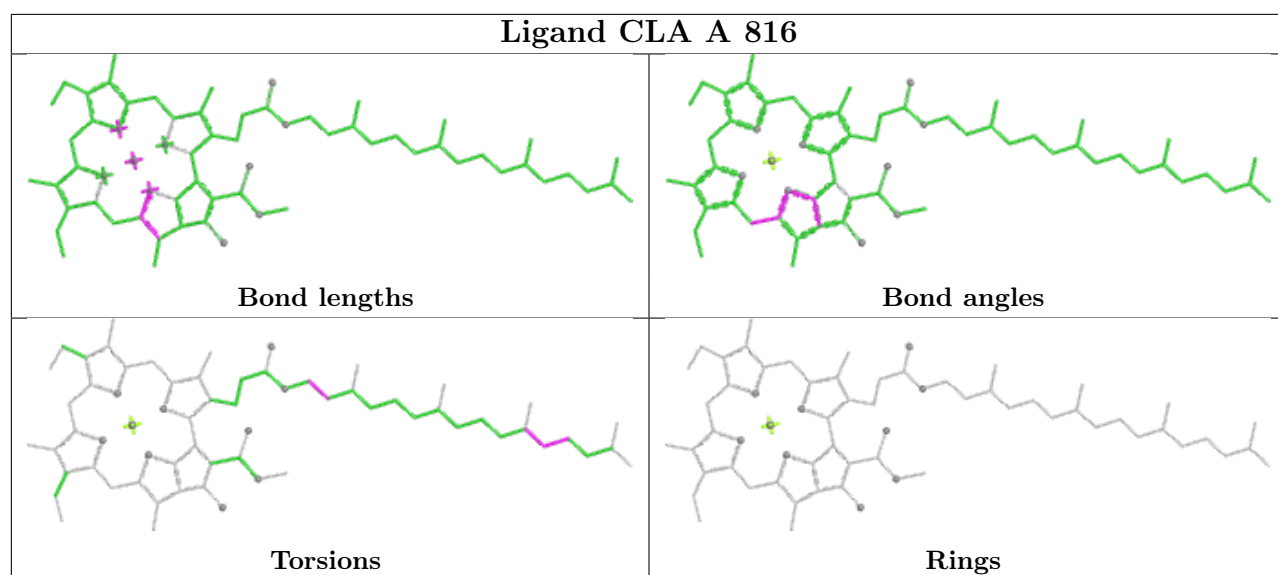
Rings

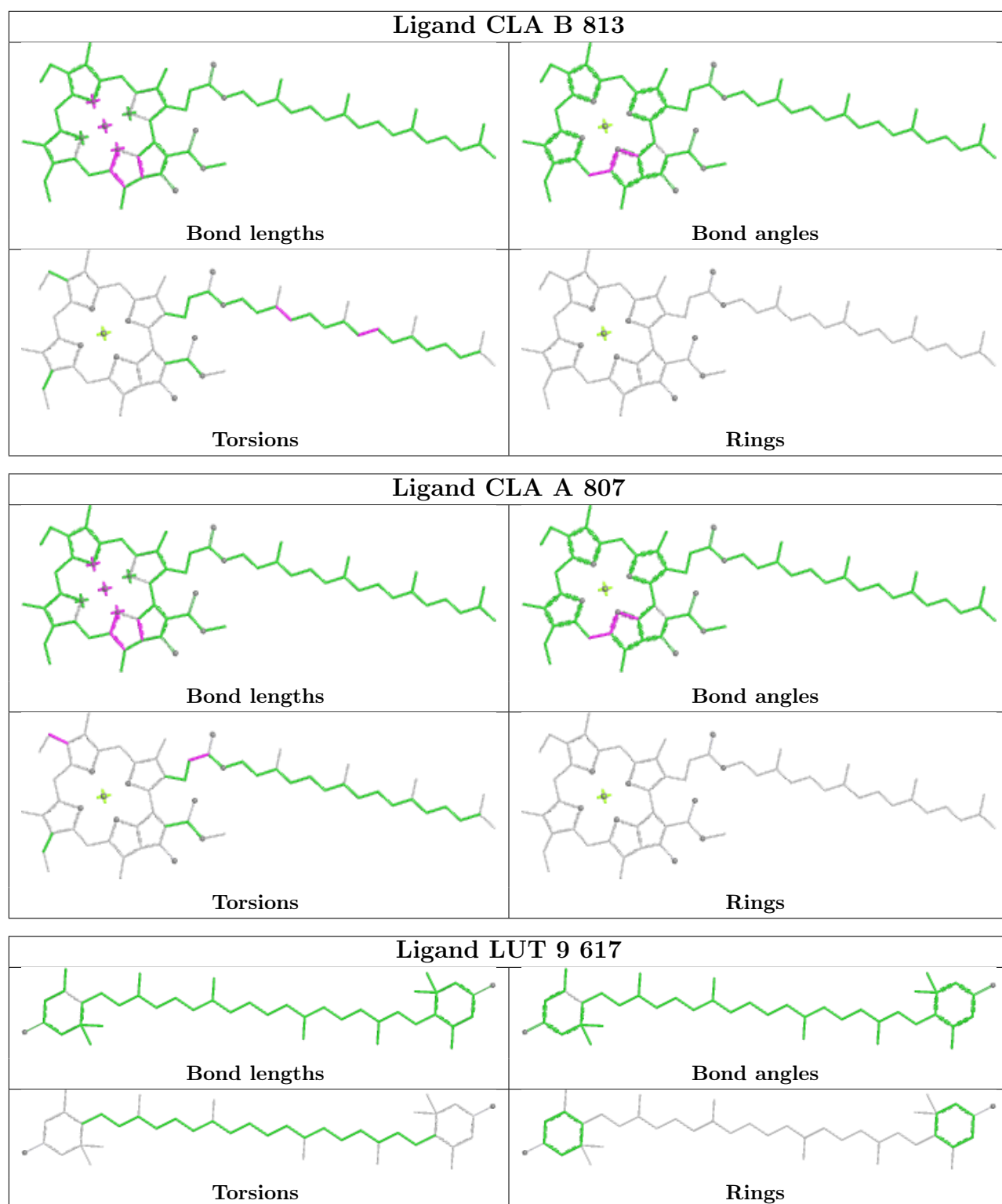
Ligand LHG 8 620

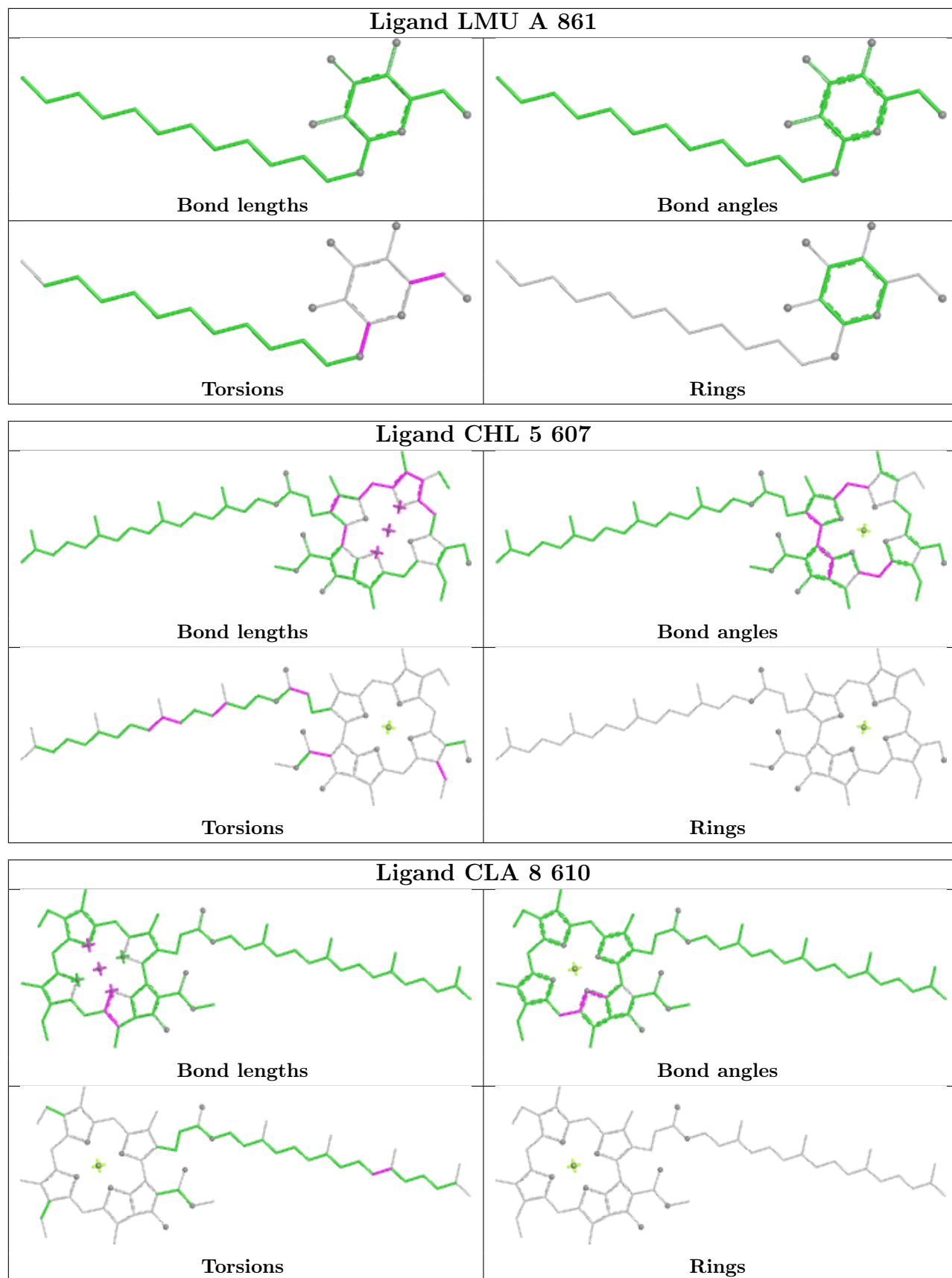


Ligand CLA A 818

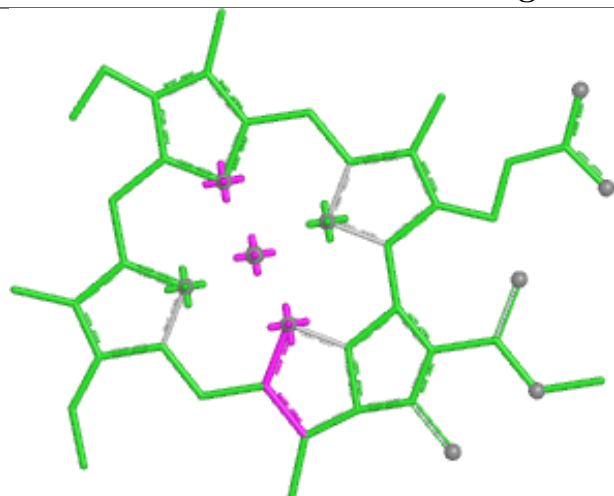




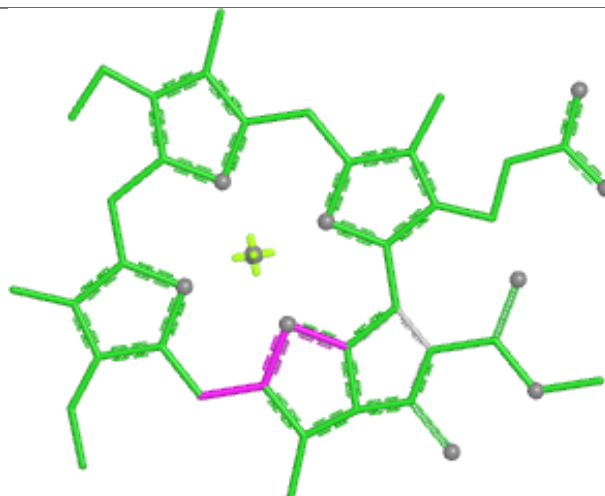




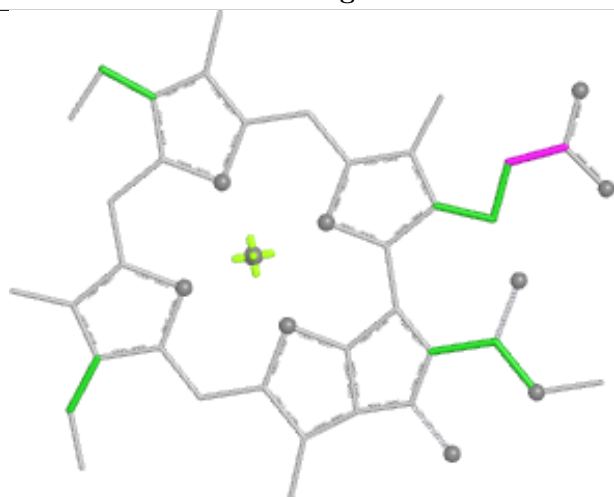
Ligand CLA 6 612



Bond lengths



Bond angles

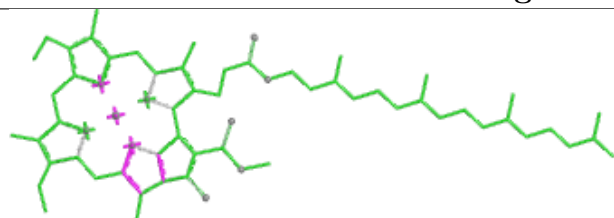


Torsions

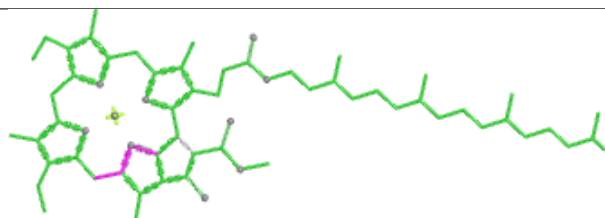


Rings

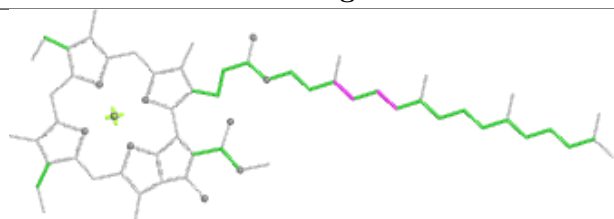
Ligand CLA B 829



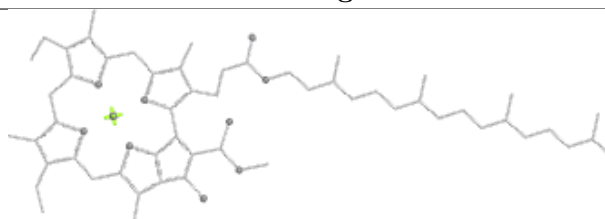
Bond lengths



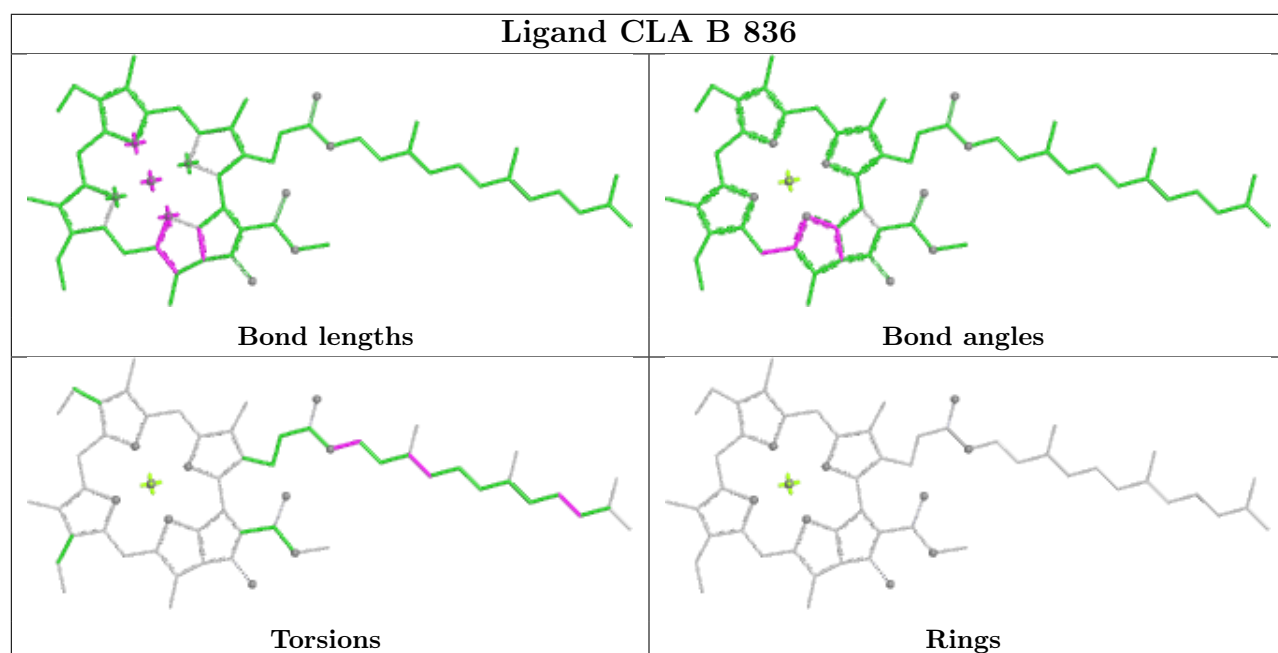
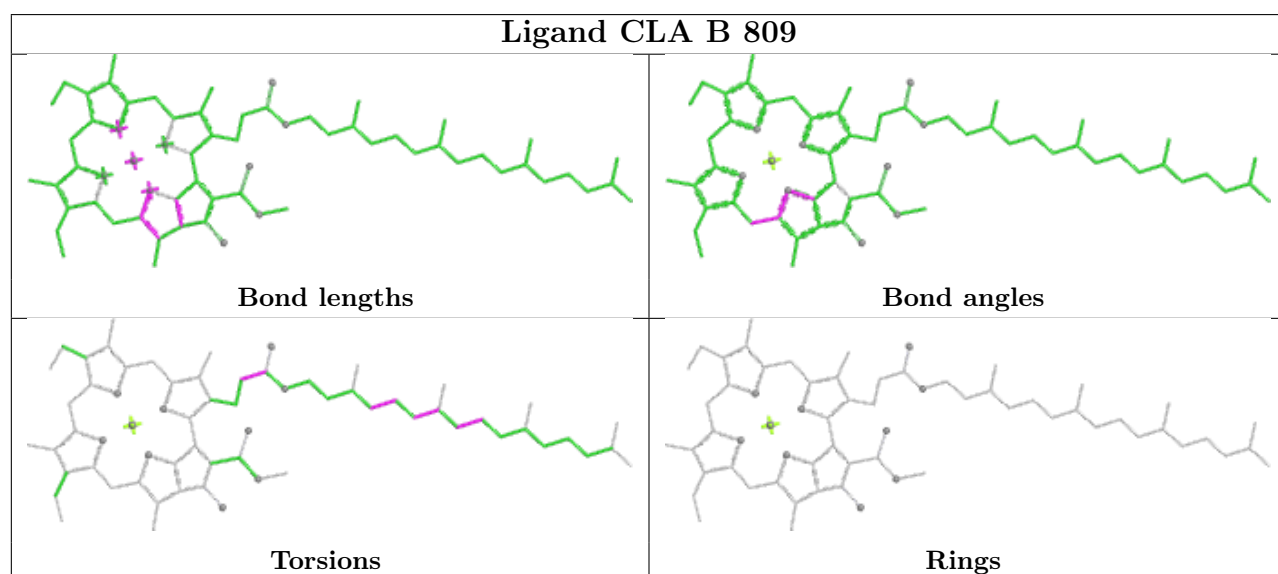
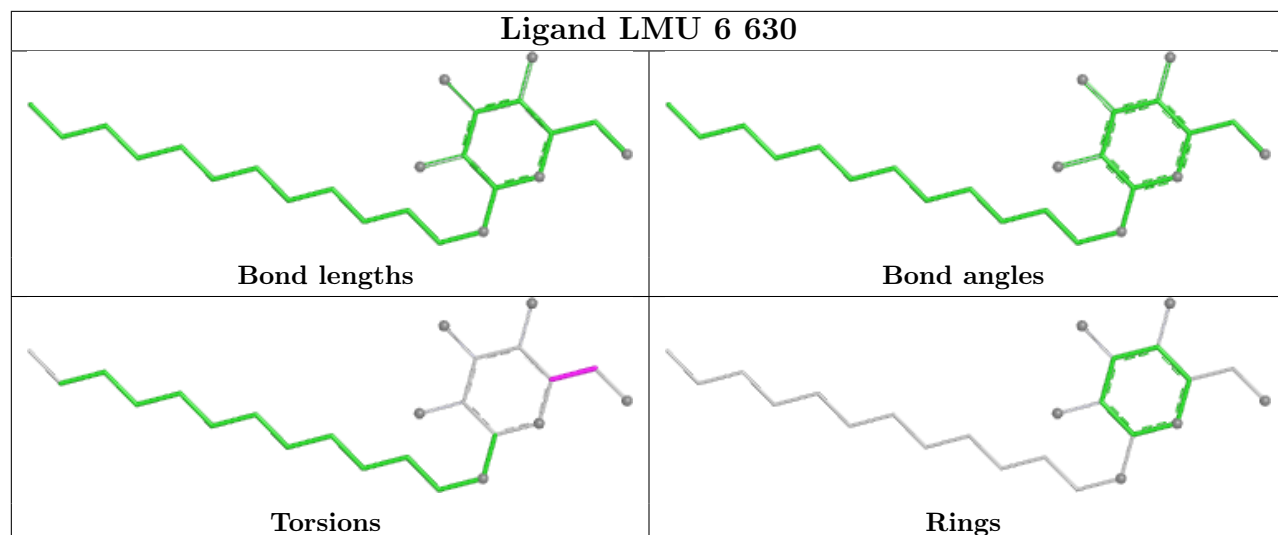
Bond angles

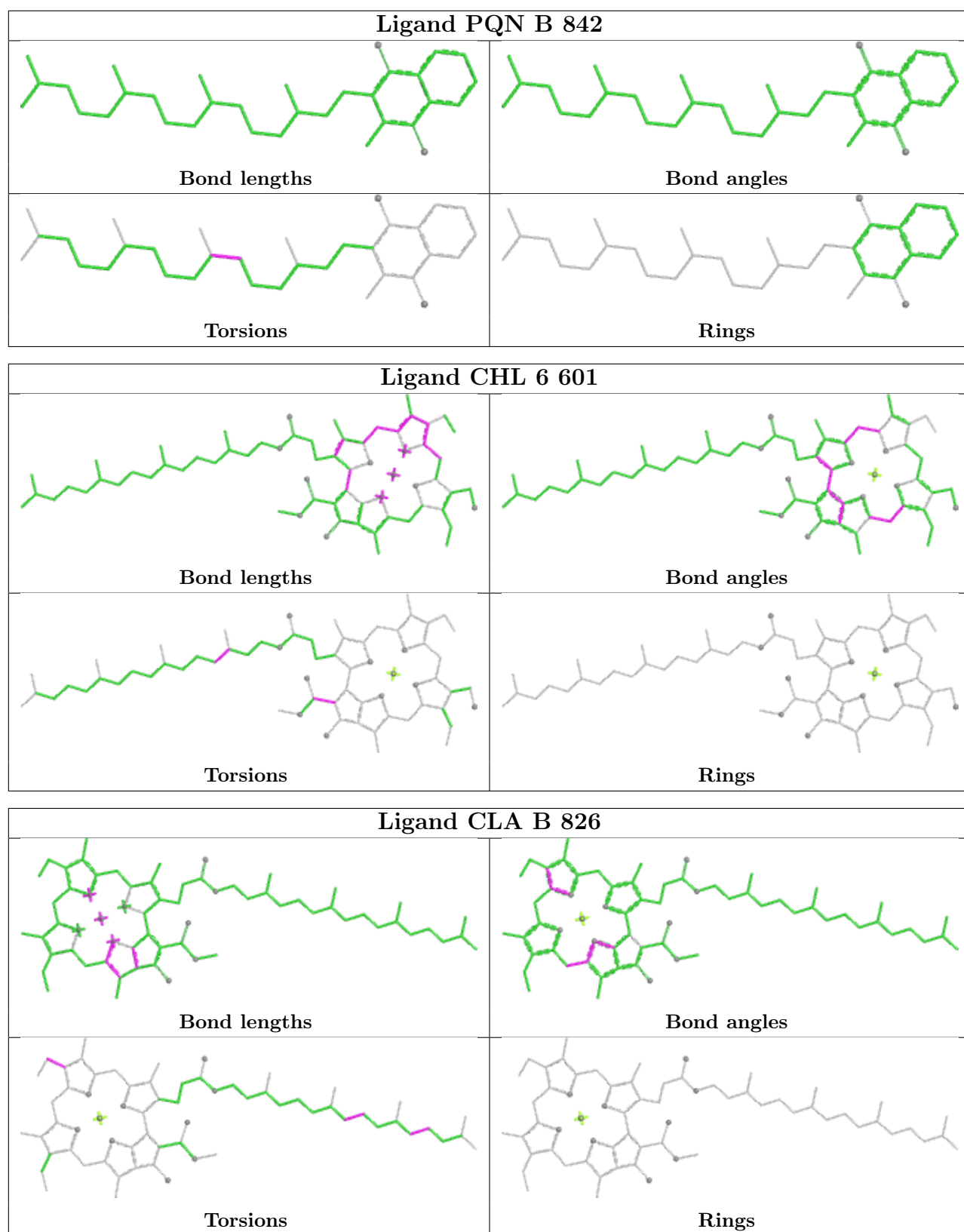


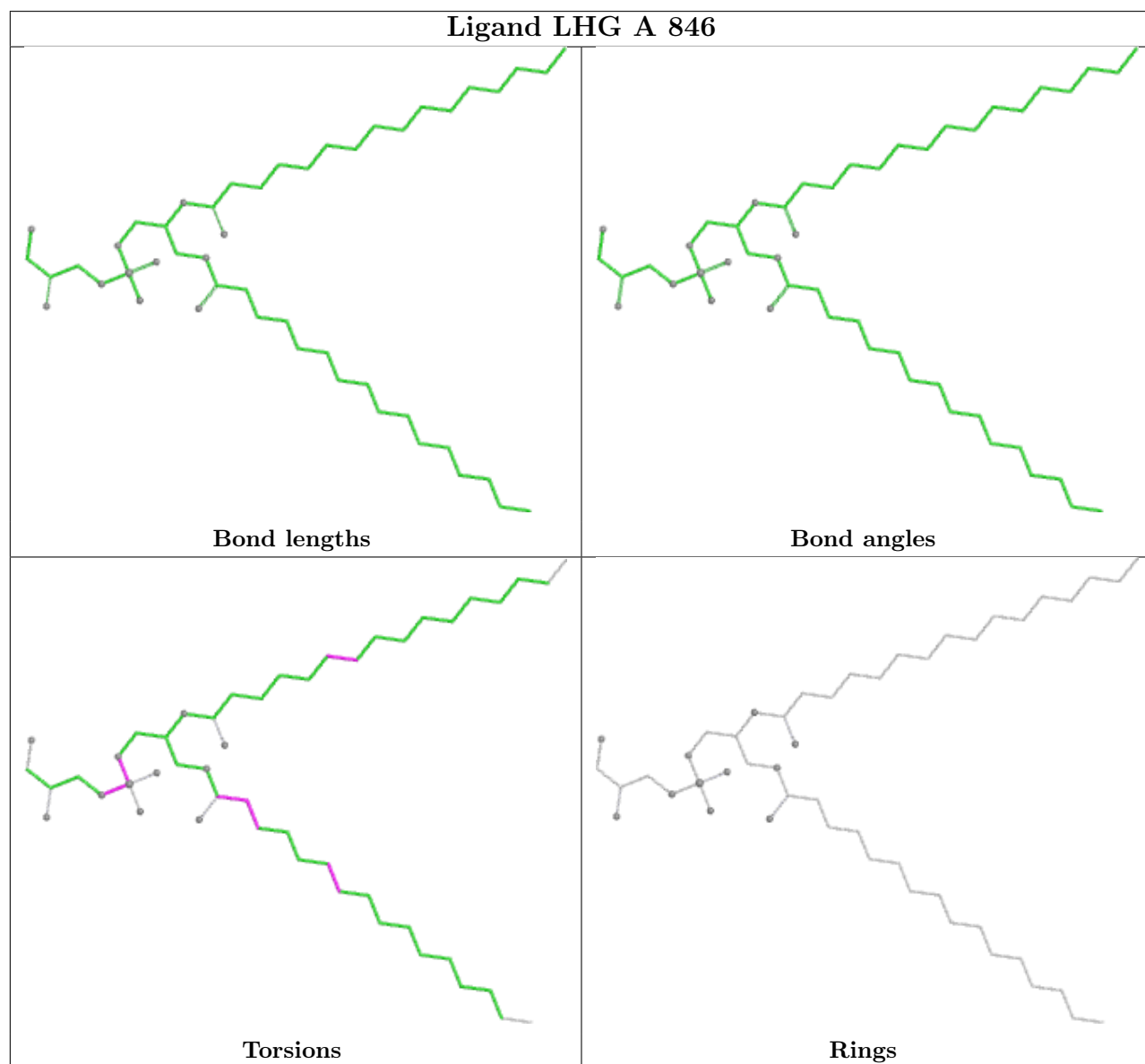
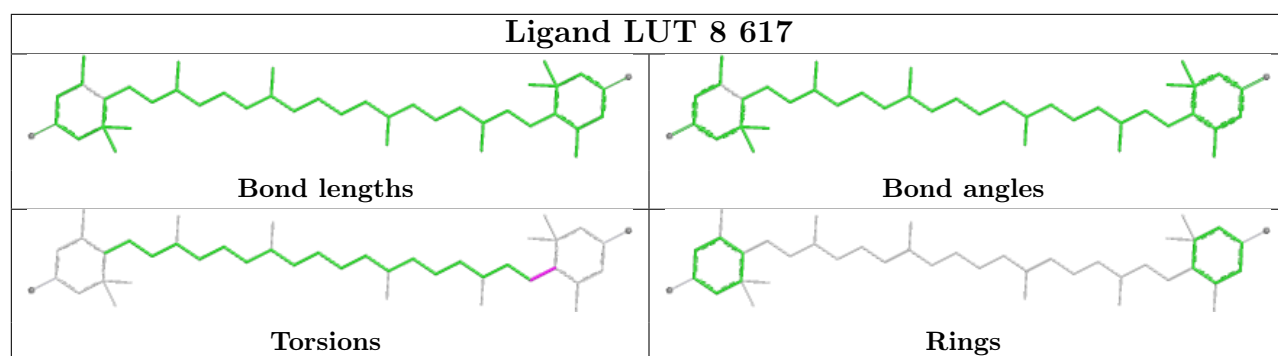
Torsions

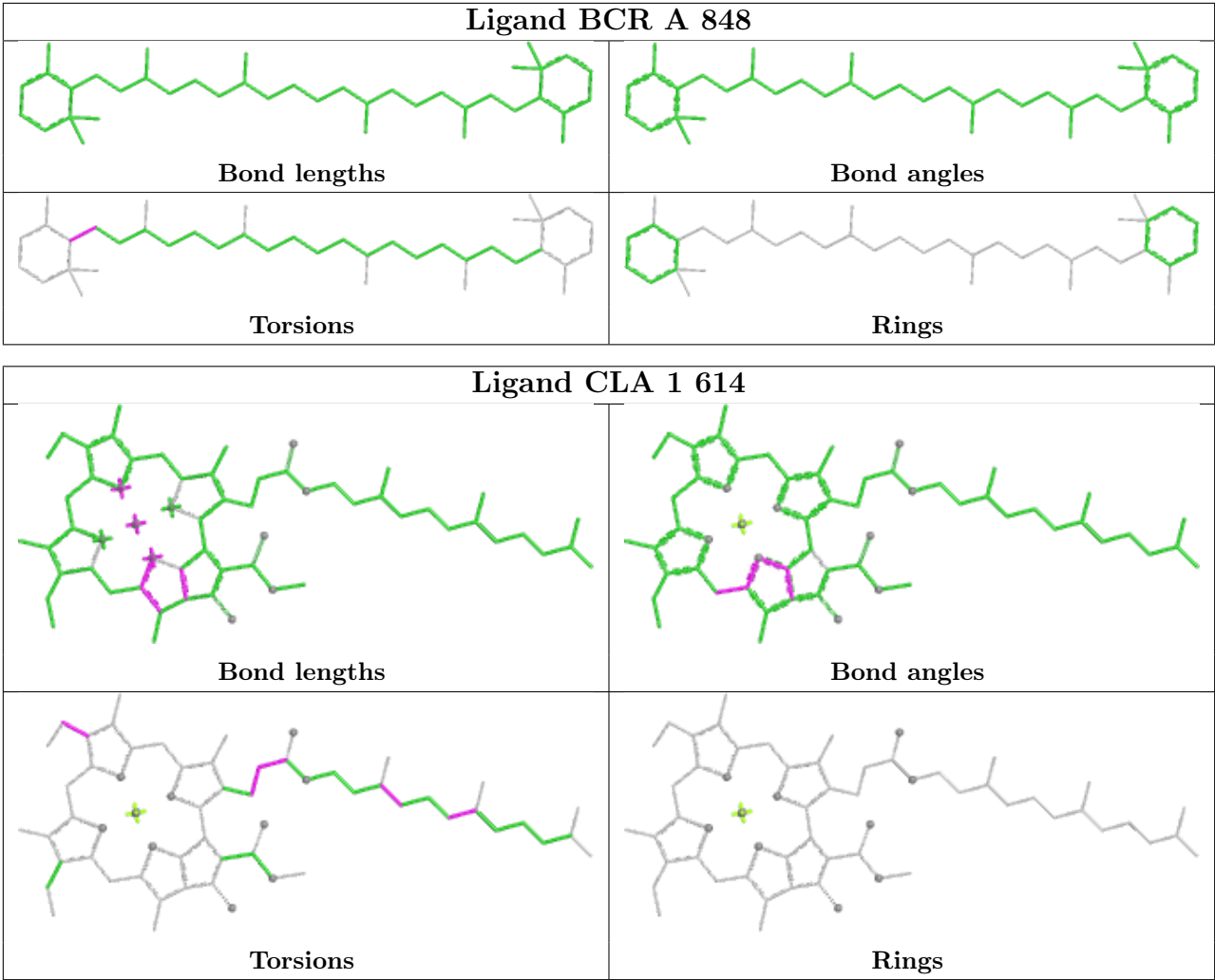


Rings









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	B2	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B2	218:PRO	C	683:HIS	N	78.76
1	B2	169:PHE	C	191:TRP	N	27.65

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B2	115:ASN	C	128:ILE	N	22.89
1	B2	77:GLN	C	88:ILE	N	9.86
1	B2	107:ARG	C	112:GLY	N	7.45
1	B2	201:PRO	C	207:HIS	N	6.93

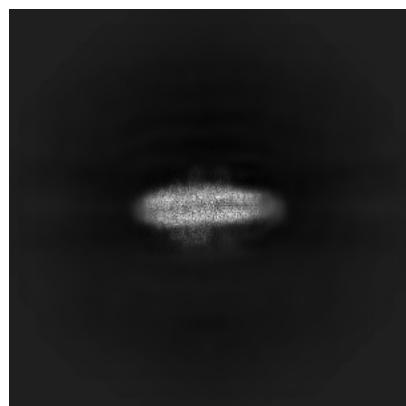
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14867. These allow visual inspection of the internal detail of the map and identification of artifacts.

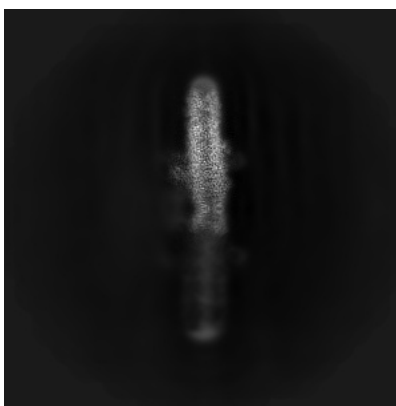
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

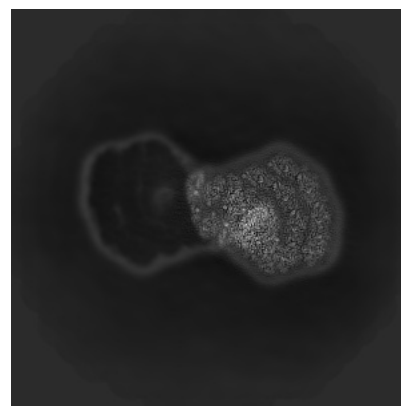
6.1.1 Primary map



X

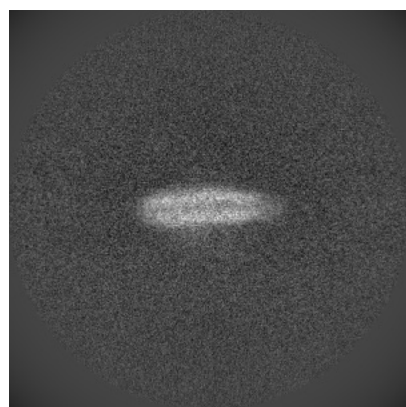


Y

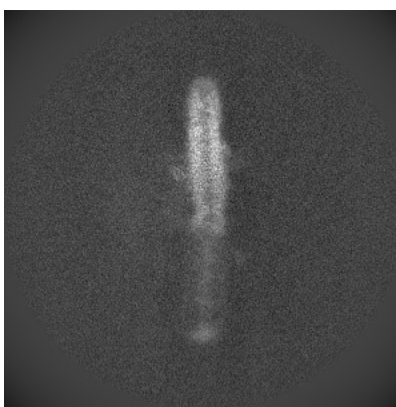


Z

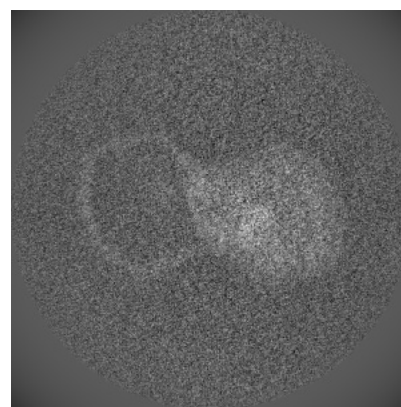
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

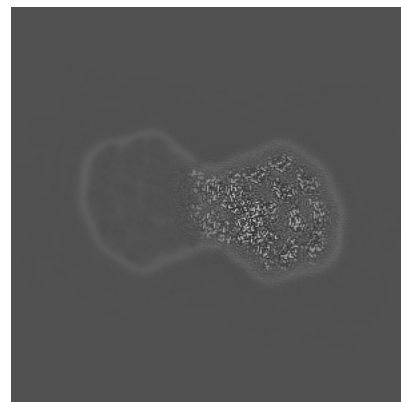
6.2.1 Primary map



X Index: 350

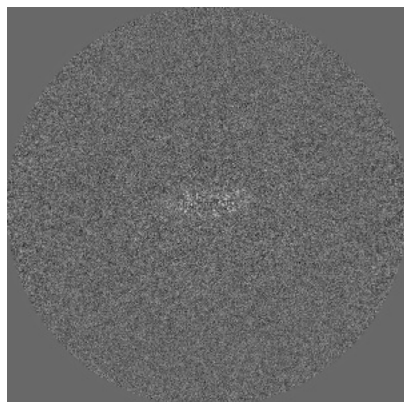


Y Index: 350

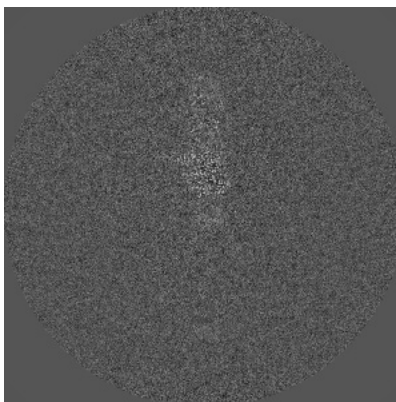


Z Index: 350

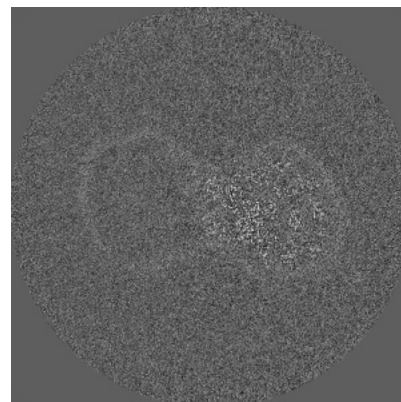
6.2.2 Raw map



X Index: 350



Y Index: 350



Z Index: 350

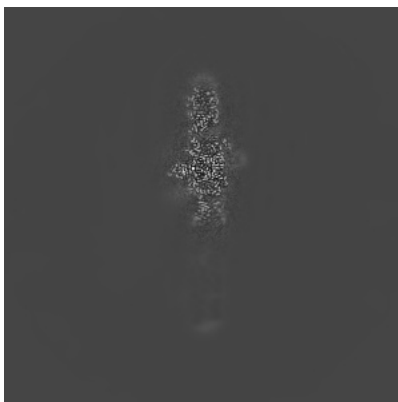
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

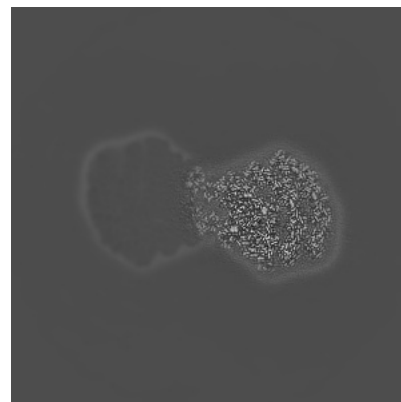
6.3.1 Primary map



X Index: 416

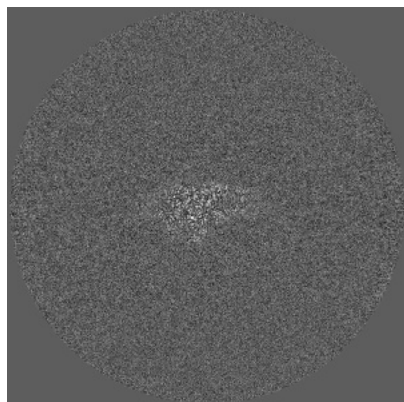


Y Index: 323

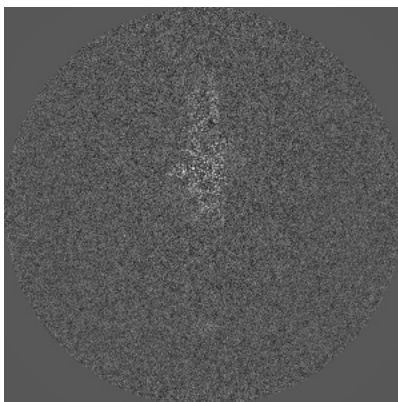


Z Index: 340

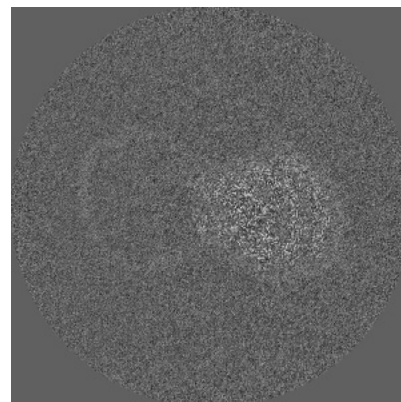
6.3.2 Raw map



X Index: 415



Y Index: 323

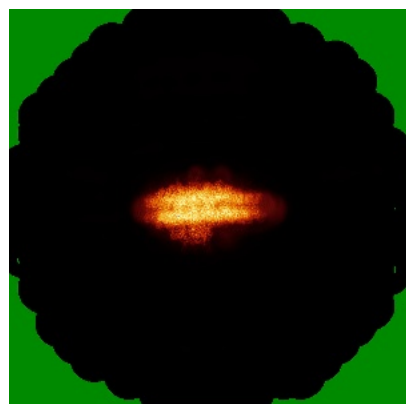


Z Index: 340

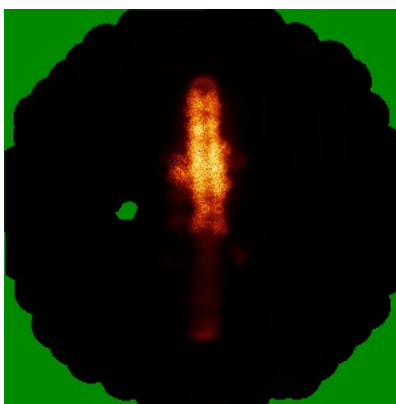
The images above show the largest variance slices of the map in three orthogonal directions.

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

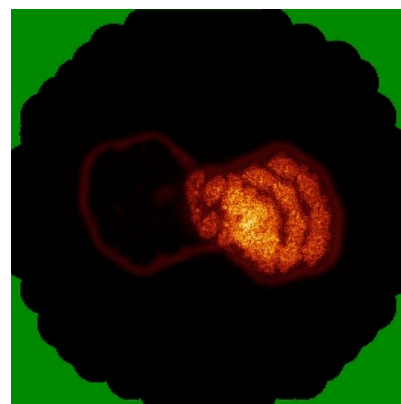
6.4.1 Primary map



X

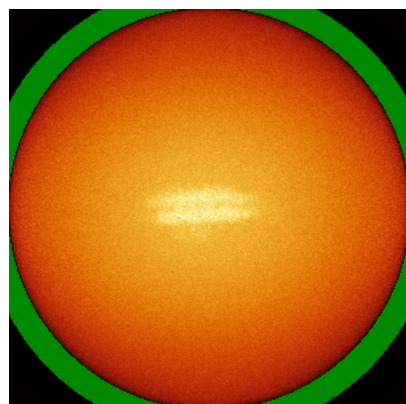


Y

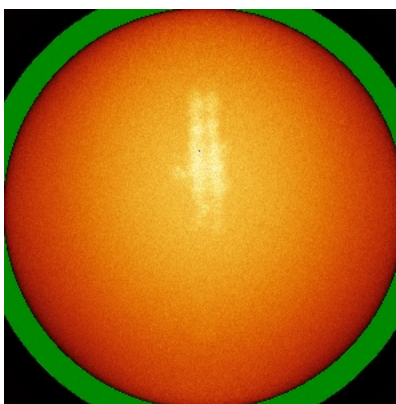


Z

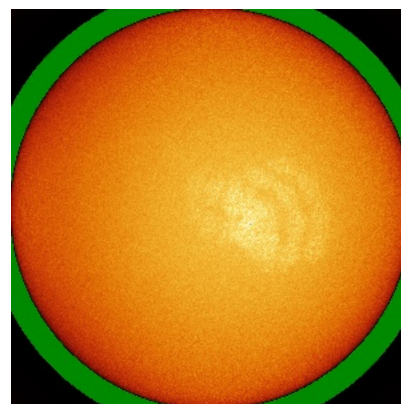
6.4.2 Raw map



X



Y

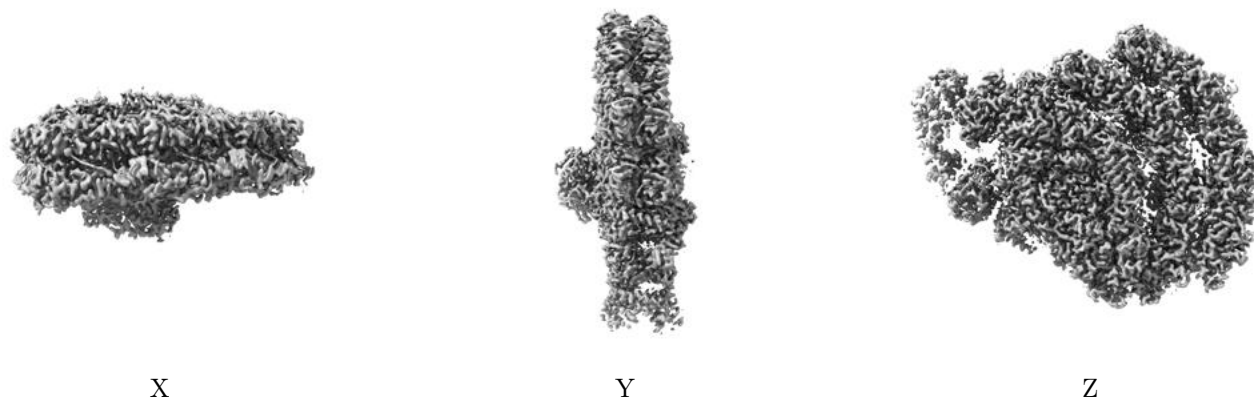


Z

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.

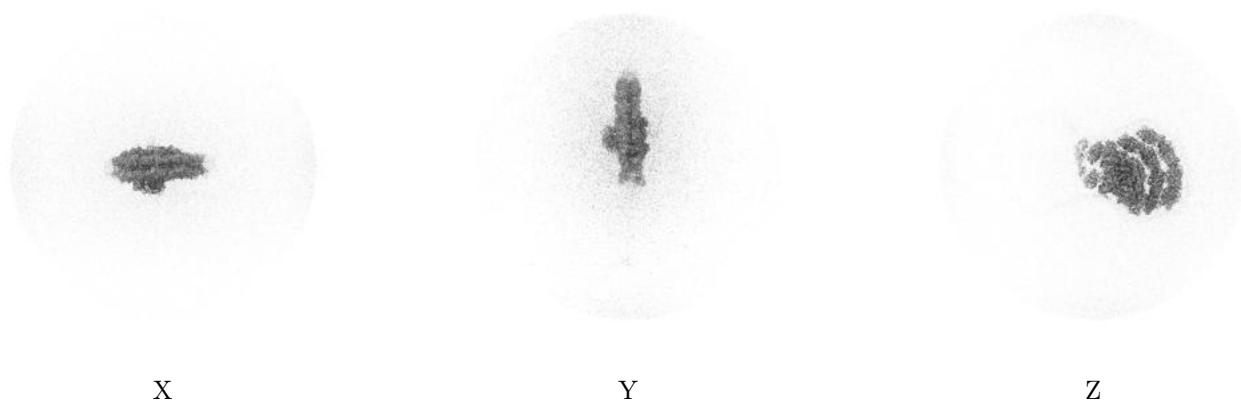
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.031. 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.

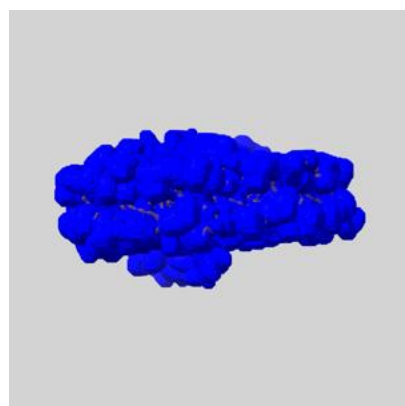
6.6 Mask visualisation [i](#)

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

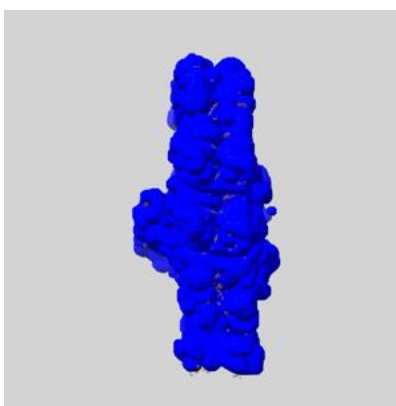
A mask typically either:

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

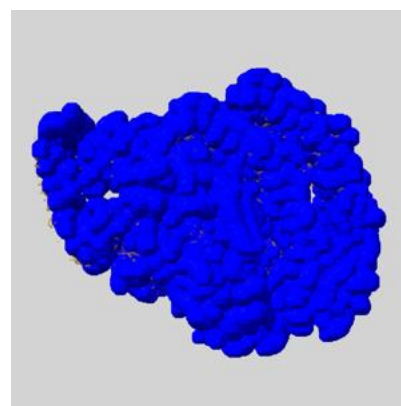
6.6.1 emd_14867_msk_1.map [i](#)



X



Y

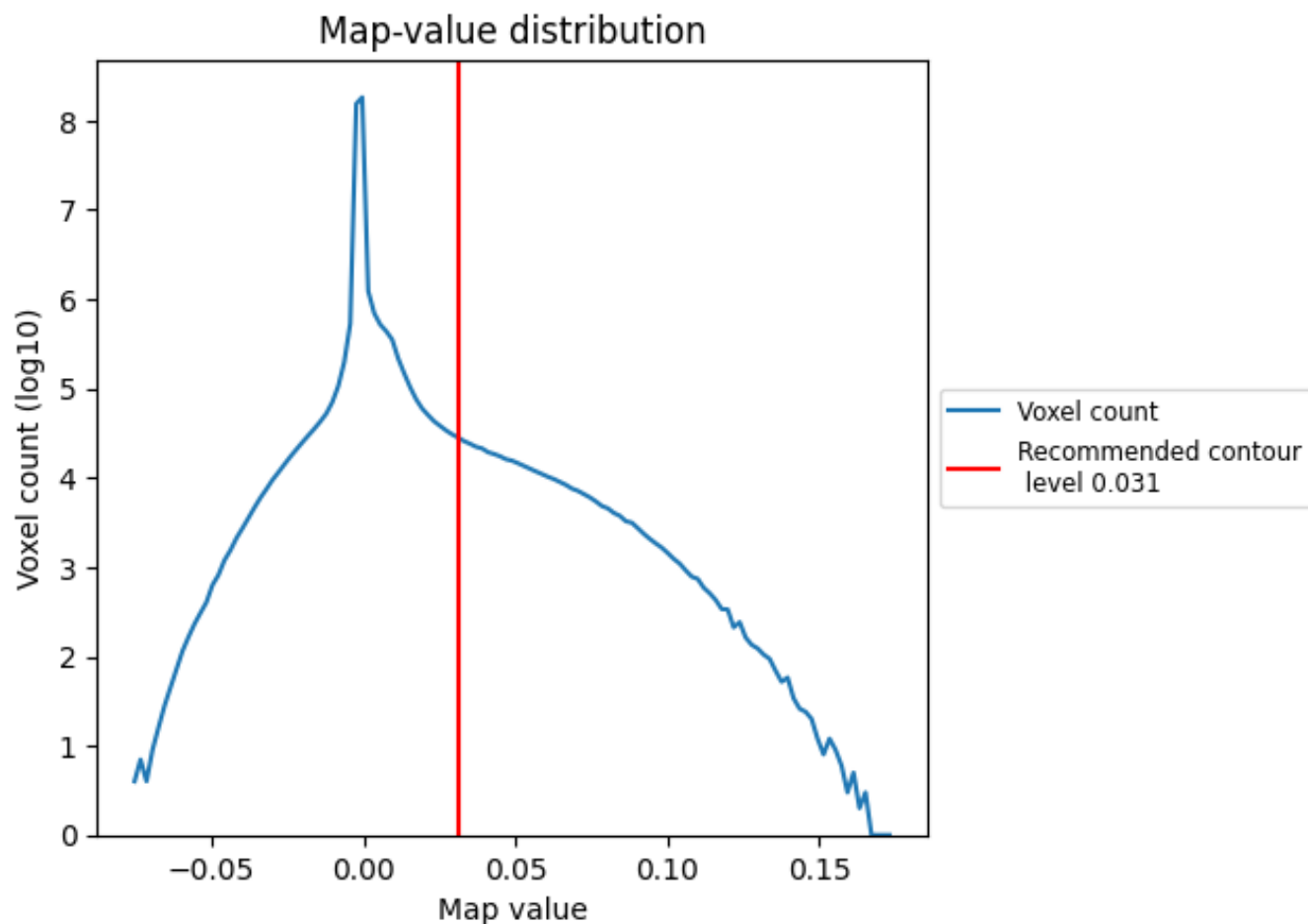


Z

7 Map analysis [i](#)

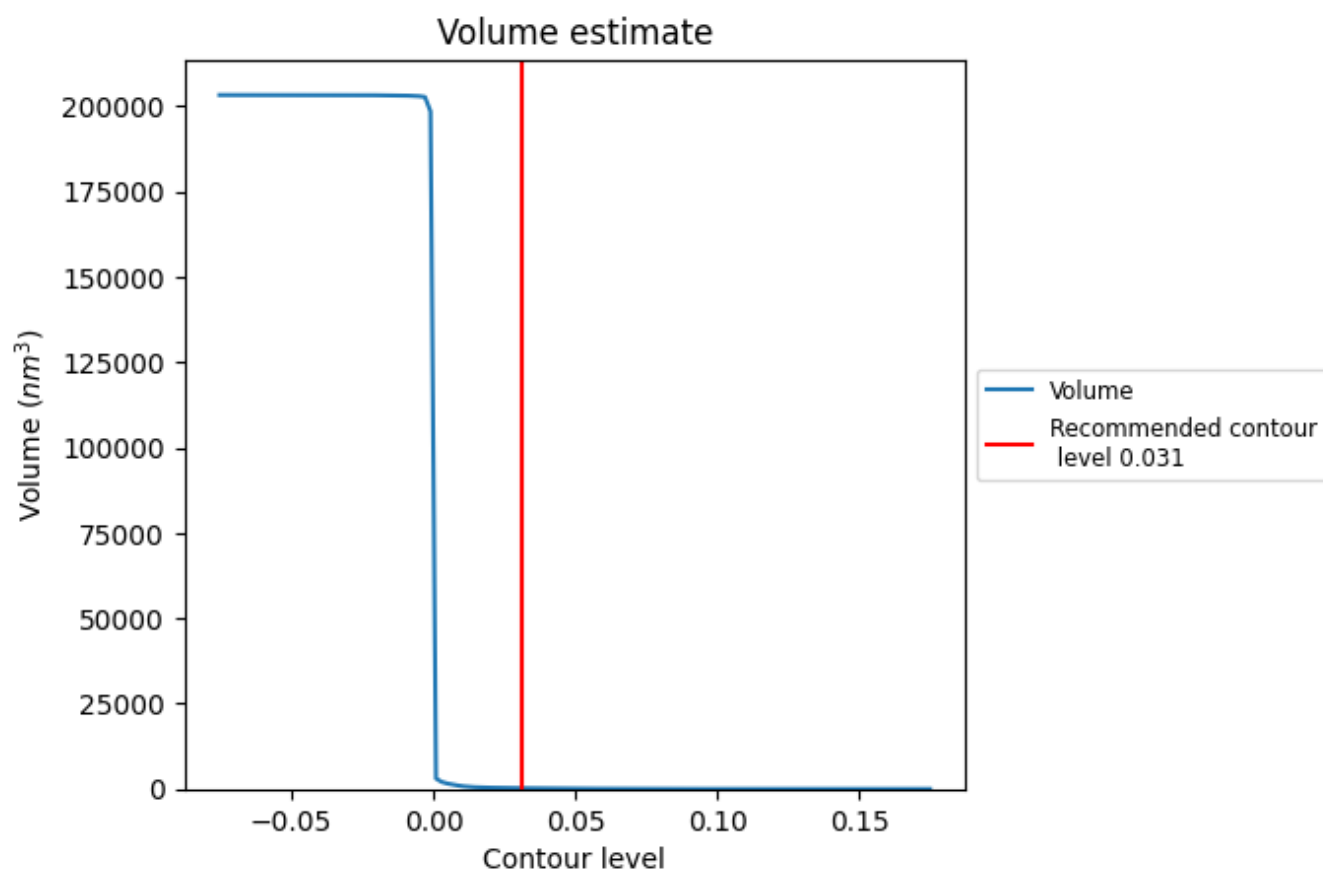
This section contains the results of statistical analysis of the map.

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.

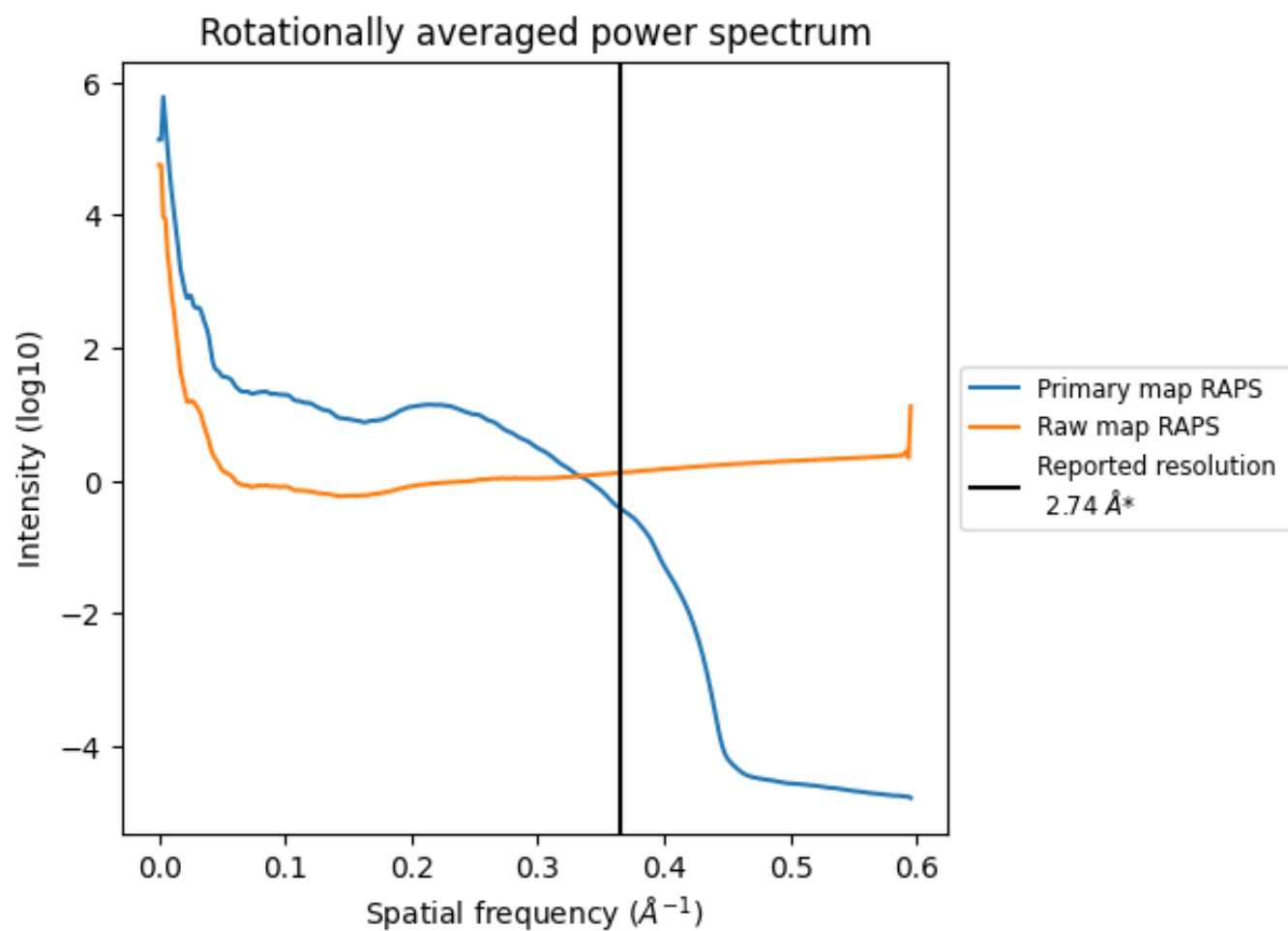
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 231 nm³; this corresponds to an approximate mass of 209 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 ⓘ

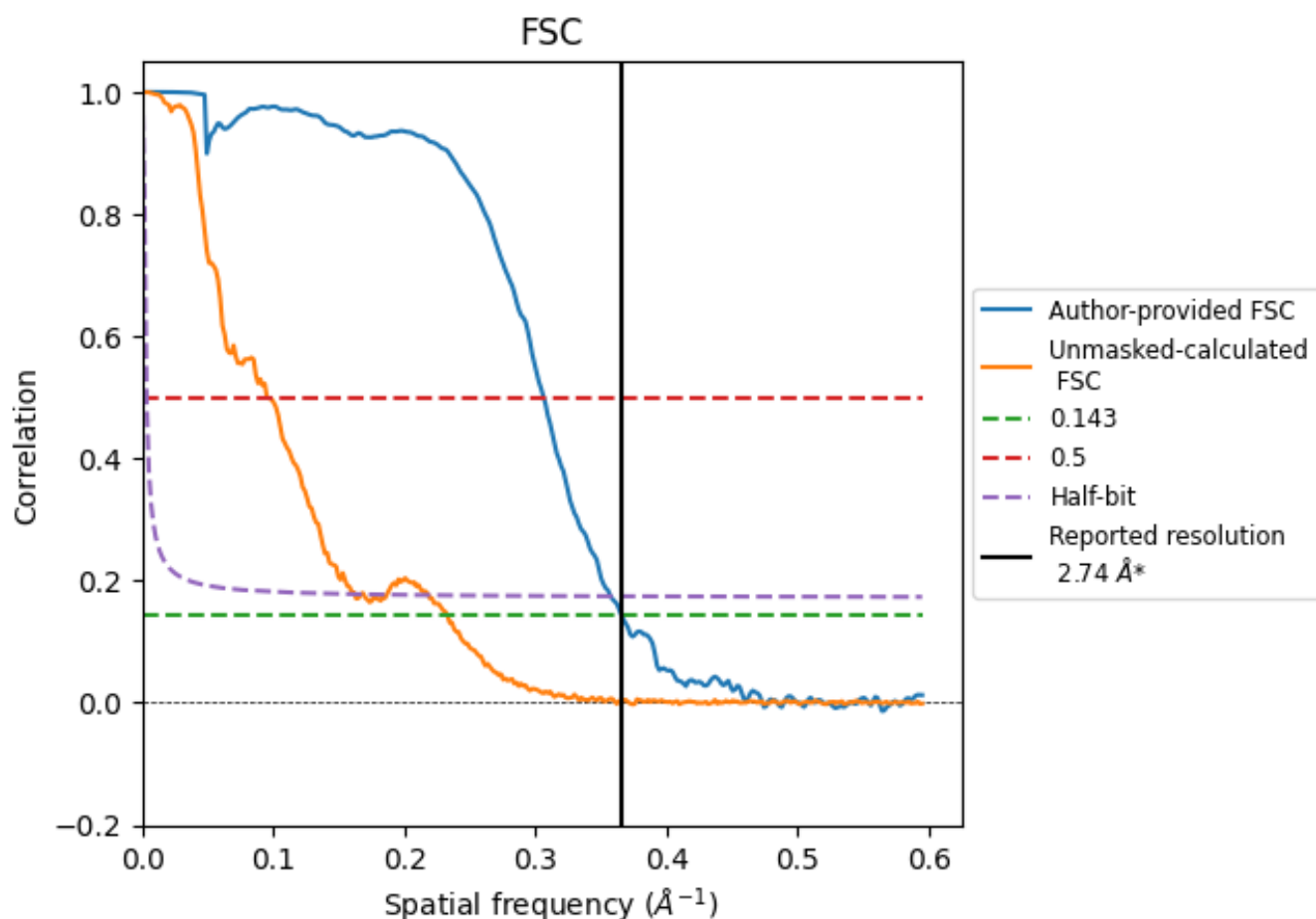


*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

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 0.365 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

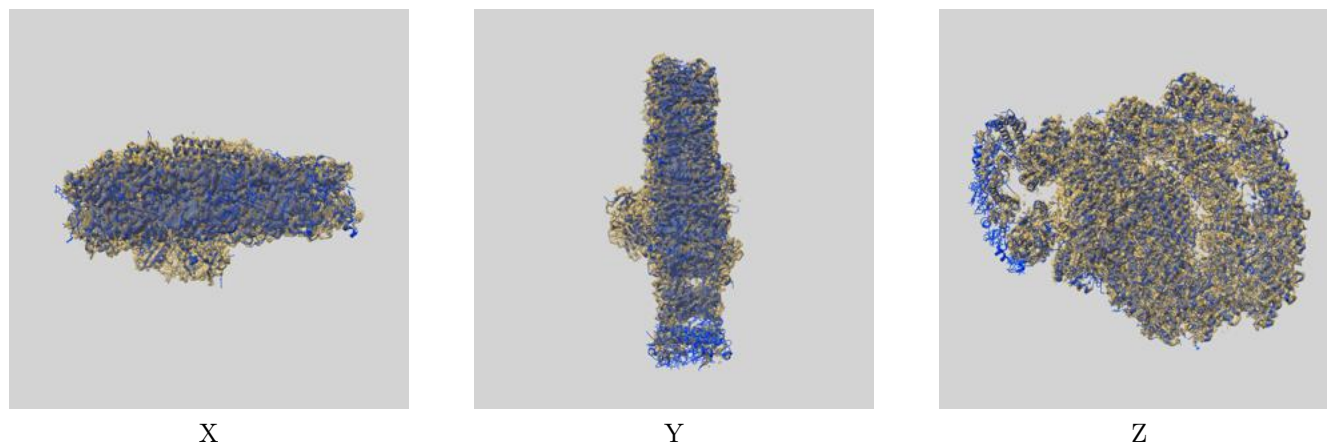
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.26	2.80
Unmasked-calculated*	4.30	10.50	6.17

*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 4.30 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

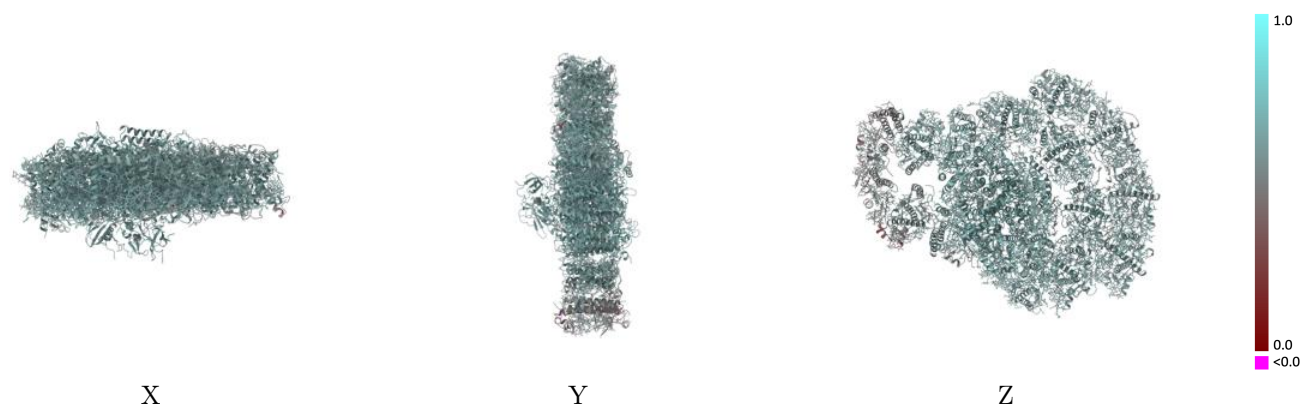
This section contains information regarding the fit between EMDB map EMD-14867 and PDB model 7ZQ9. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

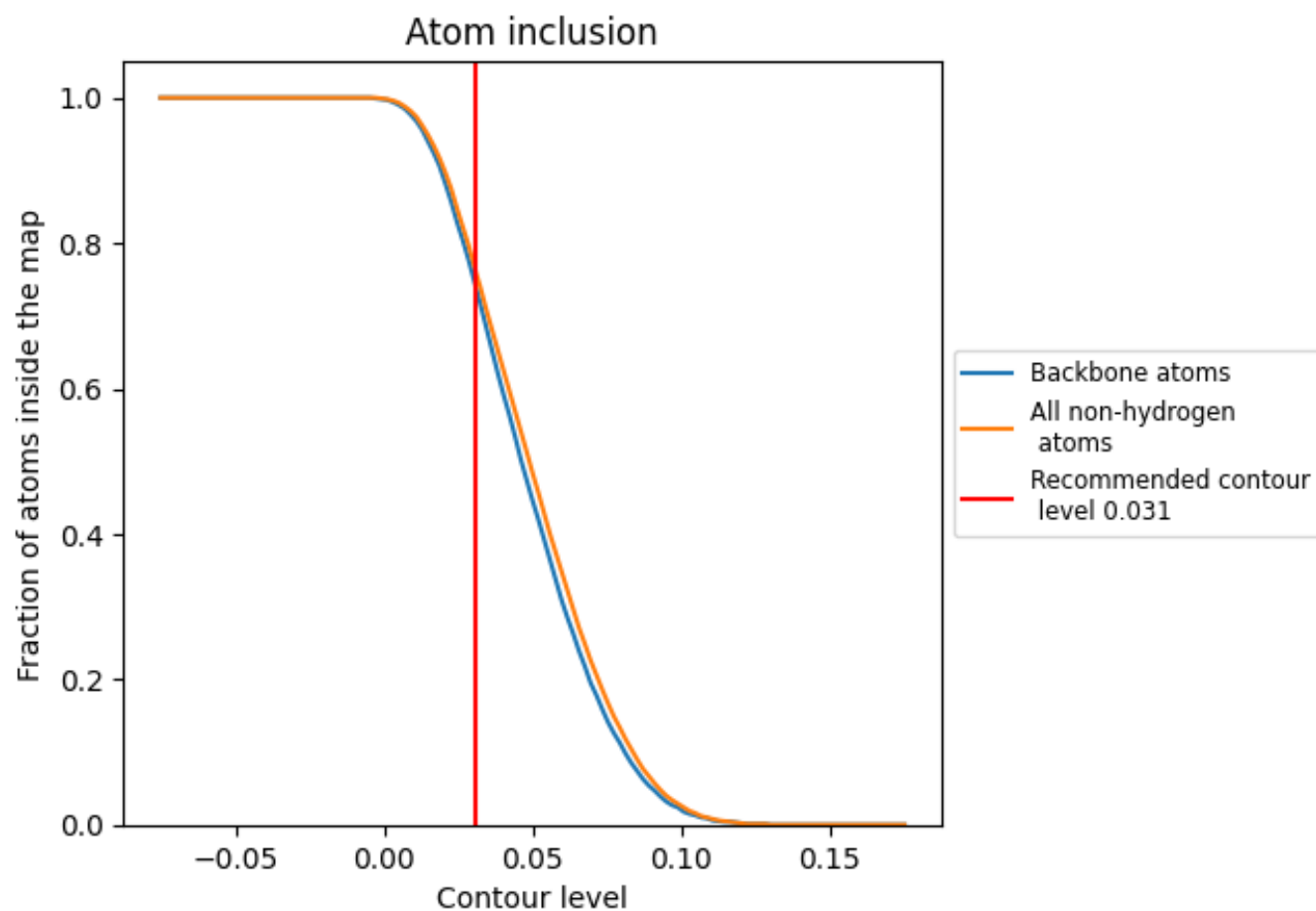


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.6090
1	 0.7690	 0.6100
3	 0.7890	 0.6130
4	 0.6760	 0.5800
5	 0.7360	 0.5940
6	 0.6910	 0.5870
7	 0.8220	 0.6170
8	 0.8330	 0.6210
9	 0.7150	 0.5960
92	 0.5280	 0.5380
A	 0.8970	 0.6530
B	 0.9100	 0.6580
B2	 0.2380	 0.4950
C	 0.9070	 0.6460
D	 0.7900	 0.6170
E	 0.7730	 0.6160
F	 0.8130	 0.6180
G	 0.7110	 0.6000
I	 0.8020	 0.6160
I2	 0.3950	 0.5110
J	 0.8420	 0.6240
K	 0.6190	 0.5850
L	 0.6650	 0.5780
L2	 0.3430	 0.4920
Z	 0.6750	 0.5840

