



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:53 PM UTC

PDB ID : 9UAS / pdb\_00009uas  
EMDB ID : EMD-63994  
Title : PSI-LHCE-LHCII from Euglena gracilis  
Authors : Feng, Y.  
Deposited on : 2025-04-01  
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

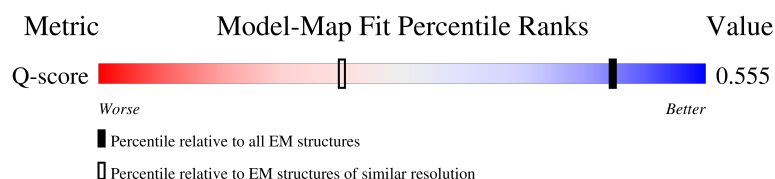
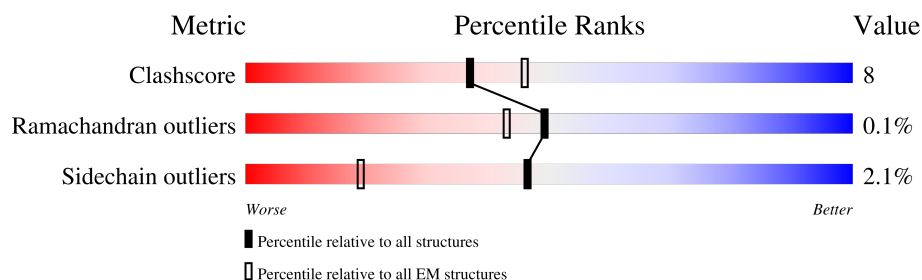
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.35 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	4607 ( 1.85 - 2.85 )

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

Mol	Chain	Length	Quality of chain
1	B	734	
2	C	81	
3	D	193	
4	E	158	

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Mol	Chain	Length	Quality of chain
5	F	325	
6	G	184	
6	P	184	
7	H	185	
8	I	184	
8	N	184	
9	J	39	
10	K	184	
10	Q	184	
11	L	187	
11	R	187	
12	M	31	
13	O	177	
14	S	180	
15	T	173	
16	U	209	
17	V	196	
18	W	228	
19	X	223	
20	A	756	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	801	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	844	X	-	-	-
22	CLA	A	852	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	859	X	-	-	-
22	CLA	F	403	X	-	-	-
22	CLA	F	404	X	-	-	-
22	CLA	F	405	X	-	-	-
22	CLA	G	601	X	-	-	-
22	CLA	G	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	G	603	X	-	-	-
22	CLA	G	604	X	-	-	-
22	CLA	G	605	X	-	-	-
22	CLA	G	606	X	-	-	-
22	CLA	G	607	X	-	-	-
22	CLA	G	608	X	-	-	-
22	CLA	G	609	X	-	-	-
22	CLA	G	610	X	-	-	-
22	CLA	G	611	X	-	-	-
22	CLA	H	302	X	-	-	-
22	CLA	H	303	X	-	-	-
22	CLA	H	304	X	-	-	-
22	CLA	H	305	X	-	-	-
22	CLA	H	306	X	-	-	-
22	CLA	H	307	X	-	-	-
22	CLA	H	308	X	-	-	-
22	CLA	H	309	X	-	-	-
22	CLA	H	310	X	-	-	-
22	CLA	H	311	X	-	-	-
22	CLA	H	312	X	-	-	-
22	CLA	H	313	X	-	-	-
22	CLA	H	318	X	-	-	-
22	CLA	I	601	X	-	-	-
22	CLA	I	602	X	-	-	-
22	CLA	I	603	X	-	-	-
22	CLA	I	604	X	-	-	-
22	CLA	I	605	X	-	-	-
22	CLA	I	606	X	-	-	-
22	CLA	I	607	X	-	-	-
22	CLA	I	608	X	-	-	-
22	CLA	I	609	X	-	-	-
22	CLA	I	610	X	-	-	-
22	CLA	I	611	X	-	-	-
22	CLA	J	102	X	-	-	-
22	CLA	K	602	X	-	-	-
22	CLA	K	603	X	-	-	-
22	CLA	K	604	X	-	-	-
22	CLA	K	605	X	-	-	-
22	CLA	K	606	X	-	-	-
22	CLA	K	607	X	-	-	-
22	CLA	K	608	X	-	-	-
22	CLA	K	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	K	610	X	-	-	-
22	CLA	K	611	X	-	-	-
22	CLA	K	612	X	-	-	-
22	CLA	K	613	X	-	-	-
22	CLA	K	617	X	-	-	-
22	CLA	L	402	X	-	-	-
22	CLA	L	403	X	-	-	-
22	CLA	L	404	X	-	-	-
22	CLA	L	405	X	-	-	-
22	CLA	L	406	X	-	-	-
22	CLA	L	407	X	-	-	-
22	CLA	L	408	X	-	-	-
22	CLA	L	409	X	-	-	-
22	CLA	L	410	X	-	-	-
22	CLA	L	411	X	-	-	-
22	CLA	L	412	X	-	-	-
22	CLA	L	417	X	-	-	-
22	CLA	N	601	X	-	-	-
22	CLA	N	602	X	-	-	-
22	CLA	N	603	X	-	-	-
22	CLA	N	604	X	-	-	-
22	CLA	N	605	X	-	-	-
22	CLA	N	606	X	-	-	-
22	CLA	N	607	X	-	-	-
22	CLA	N	608	X	-	-	-
22	CLA	N	609	X	-	-	-
22	CLA	N	610	X	-	-	-
22	CLA	N	611	X	-	-	-
22	CLA	O	305	X	-	-	-
22	CLA	O	306	X	-	-	-
22	CLA	O	307	X	-	-	-
22	CLA	O	308	X	-	-	-
22	CLA	O	309	X	-	-	-
22	CLA	O	310	X	-	-	-
22	CLA	O	311	X	-	-	-
22	CLA	O	312	X	-	-	-
22	CLA	O	313	X	-	-	-
22	CLA	O	314	X	-	-	-
22	CLA	O	315	X	-	-	-
22	CLA	O	319	X	-	-	-
22	CLA	P	602	X	-	-	-
22	CLA	P	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	P	605	X	-	-	-
22	CLA	P	606	X	-	-	-
22	CLA	P	607	X	-	-	-
22	CLA	P	608	X	-	-	-
22	CLA	P	609	X	-	-	-
22	CLA	P	610	X	-	-	-
22	CLA	P	611	X	-	-	-
22	CLA	Q	601	X	-	-	-
22	CLA	Q	603	X	-	-	-
22	CLA	Q	604	X	-	-	-
22	CLA	Q	605	X	-	-	-
22	CLA	Q	606	X	-	-	-
22	CLA	Q	607	X	-	-	-
22	CLA	Q	608	X	-	-	-
22	CLA	Q	609	X	-	-	-
22	CLA	Q	610	X	-	-	-
22	CLA	Q	611	X	-	-	-
22	CLA	Q	612	X	-	-	-
22	CLA	Q	613	X	-	-	-
22	CLA	Q	617	X	-	-	-
22	CLA	Q	618	X	-	-	-
22	CLA	R	601	X	-	-	-
22	CLA	R	602	X	-	-	-
22	CLA	R	603	X	-	-	-
22	CLA	R	604	X	-	-	-
22	CLA	R	605	X	-	-	-
22	CLA	R	606	X	-	-	-
22	CLA	R	607	X	-	-	-
22	CLA	R	608	X	-	-	-
22	CLA	R	609	X	-	-	-
22	CLA	R	610	X	-	-	-
22	CLA	R	611	X	-	-	-
22	CLA	R	615	X	-	-	-
22	CLA	S	601	X	-	-	-
22	CLA	S	602	X	-	-	-
22	CLA	S	603	X	-	-	-
22	CLA	S	604	X	-	-	-
22	CLA	S	605	X	-	-	-
22	CLA	S	606	X	-	-	-
22	CLA	S	607	X	-	-	-
22	CLA	S	608	X	-	-	-
22	CLA	S	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	S	614	X	-	-	-
22	CLA	S	615	X	-	-	-
22	CLA	T	601	X	-	-	-
22	CLA	T	602	X	-	-	-
22	CLA	T	603	X	-	-	-
22	CLA	T	604	X	-	-	-
22	CLA	T	605	X	-	-	-
22	CLA	T	606	X	-	-	-
22	CLA	T	607	X	-	-	-
22	CLA	T	608	X	-	-	-
22	CLA	T	609	X	-	-	-
22	CLA	T	610	X	-	-	-
22	CLA	T	611	X	-	-	-
22	CLA	U	401	X	-	-	-
22	CLA	U	403	X	-	-	-
22	CLA	U	404	X	-	-	-
22	CLA	U	405	X	-	-	-
22	CLA	U	406	X	-	-	-
22	CLA	U	409	X	-	-	-
22	CLA	U	410	X	-	-	-
22	CLA	U	411	X	-	-	-
22	CLA	U	412	X	-	-	-
22	CLA	U	413	X	-	-	-
22	CLA	U	414	X	-	-	-
22	CLA	U	415	X	-	-	-
22	CLA	U	420	X	-	-	-
22	CLA	V	601	X	-	-	-
22	CLA	V	602	X	-	-	-
22	CLA	V	603	X	-	-	-
22	CLA	V	604	X	-	-	-
22	CLA	V	607	X	-	-	-
22	CLA	V	608	X	-	-	-
22	CLA	V	609	X	-	-	-
22	CLA	V	610	X	-	-	-
22	CLA	V	611	X	-	-	-
22	CLA	V	612	X	-	-	-
22	CLA	V	613	X	-	-	-
22	CLA	V	617	X	-	-	-
22	CLA	W	402	X	-	-	-
22	CLA	W	403	X	-	-	-
22	CLA	W	404	X	-	-	-
22	CLA	W	405	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	W	406	X	-	-	-
22	CLA	W	409	X	-	-	-
22	CLA	W	410	X	-	-	-
22	CLA	W	411	X	-	-	-
22	CLA	W	412	X	-	-	-
22	CLA	W	413	X	-	-	-
22	CLA	W	414	X	-	-	-
22	CLA	W	415	X	-	-	-
22	CLA	W	419	X	-	-	-
22	CLA	X	402	X	-	-	-
22	CLA	X	403	X	-	-	-
22	CLA	X	404	X	-	-	-
22	CLA	X	405	X	-	-	-
22	CLA	X	407	X	-	-	-
22	CLA	X	408	X	-	-	-
22	CLA	X	409	X	-	-	-
22	CLA	X	410	X	-	-	-
22	CLA	X	411	X	-	-	-
22	CLA	X	412	X	-	-	-
22	CLA	X	413	X	-	-	-
22	CLA	X	417	X	-	-	-
22	CLA	X	419	X	-	-	-
31	CHL	U	407	X	-	-	-
31	CHL	U	408	X	-	-	-
31	CHL	V	605	X	-	-	-
31	CHL	V	606	X	-	-	-
31	CHL	W	407	X	-	-	-
31	CHL	W	408	X	-	-	-
31	CHL	W	422	X	-	-	-
31	CHL	X	406	X	-	-	-
33	CL0	A	802	X	-	-	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 60137 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	732	Total	C	N	O	S	0	0
			5868	3859	985	1009	15		

- Molecule 2 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	80	Total	C	N	O	S	0	0
			596	363	104	118	11		

- Molecule 3 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	190	Total	C	N	O	S	0	0
			1489	948	254	285	2		

- Molecule 4 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	63	Total	C	N	O	0	0
			509	324	86	99		

- Molecule 5 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	166	Total	C	N	O	S	0	0
			1262	811	210	239	2		

- Molecule 6 is a protein called Lhce5.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	175	Total	C	N	O	S	0	0
			1323	853	224	242	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	164	Total	C	N	O	S	0	0
			1243	803	209	227	4		

- Molecule 7 is a protein called Lhce7.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	173	Total	C	N	O	S	0	0
			1342	862	233	242	5		

- Molecule 8 is a protein called Lhce5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	165	Total	C	N	O	S	0	0
			1242	801	212	225	4		
8	N	170	Total	C	N	O	S	0	0
			1271	819	215	233	4		

- Molecule 9 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	37	Total	C	N	O	S	0	0
			305	209	43	52	1		

- Molecule 10 is a protein called LhcE6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	182	Total	C	N	O	S	0	0
			1444	939	246	253	6		
10	Q	182	Total	C	N	O	S	0	0
			1440	938	245	251	6		

- Molecule 11 is a protein called Lhce8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	178	Total	C	N	O	S	0	0
			1364	876	237	247	4		
11	R	174	Total	C	N	O	S	0	0
			1331	852	232	243	4		

- Molecule 12 is a protein called PsaM.



Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			242	162	37	42	1		

- Molecule 13 is a protein called LhcE7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	175	Total	C	N	O	S	0	0
			1359	870	234	250	5		

- Molecule 14 is a protein called Lhce10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	172	Total	C	N	O	S	0	0
			1327	858	219	246	4		

- Molecule 15 is a protein called Lhce11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	167	Total	C	N	O	S	0	0
			1283	824	221	231	7		

- Molecule 16 is a protein called LhcbM4.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	199	Total	C	N	O	S	0	0
			1517	981	256	275	5		

- Molecule 17 is a protein called LhcbM4.10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	196	Total	C	N	O	S	0	0
			1513	990	253	265	5		

- Molecule 18 is a protein called LhcbM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	220	Total	C	N	O	S	0	0
			1669	1088	275	302	4		

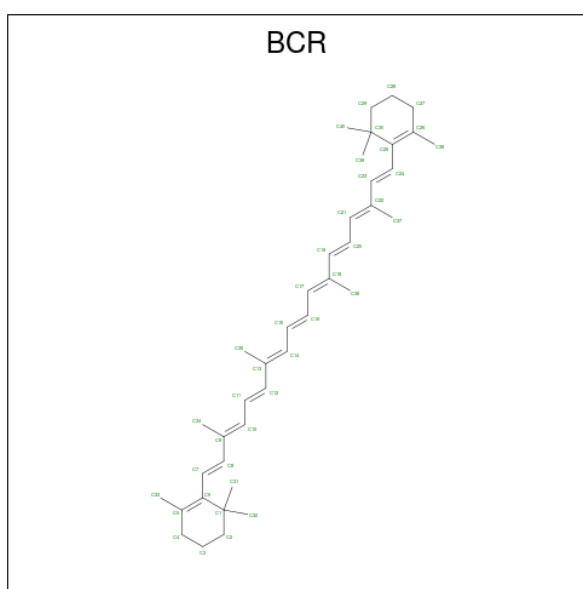
- Molecule 19 is a protein called LhcbM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	223	Total	C	N	O	S	0	0
			1688	1093	284	306	5		

- Molecule 20 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A	740	Total	C	N	O	S	0	0
			5872	3855	992	1004	21		

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



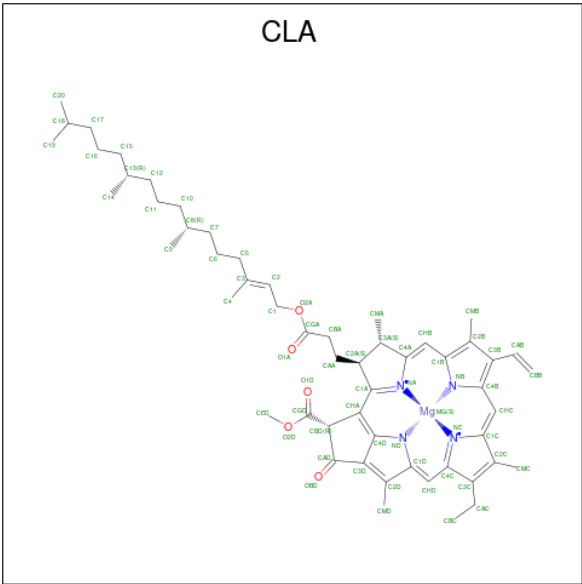
Mol	Chain	Residues	Atoms		AltConf
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	J	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms		AltConf
21	M	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	K	1	Total 64	C 55	Mg 1	N 4	O 4	0
22	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	K	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	K	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	K	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	L	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	N	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	O	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Q	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	R	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	R	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	R	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	T	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	U	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	U	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	U	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	V	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	V	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	V	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	W	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	W	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	W	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	X	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

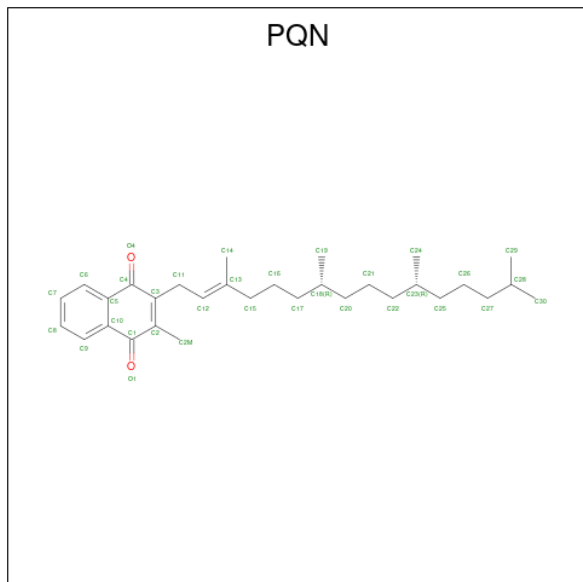
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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

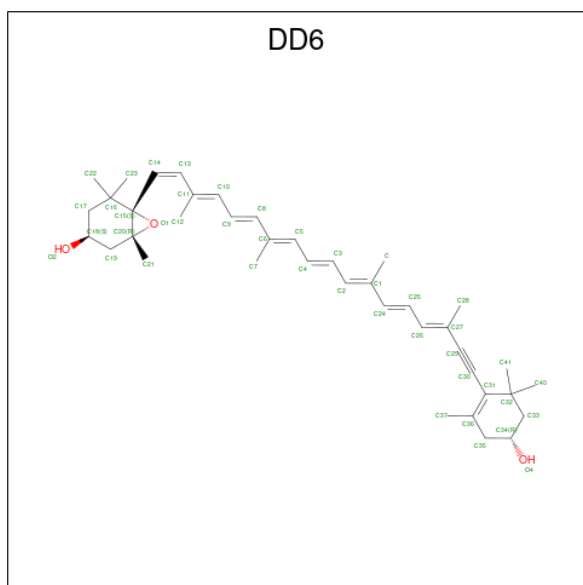


- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 24 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula:  $C_{40}H_{54}O_3$ ) (labeled as "Ligand of Interest" by depositor).



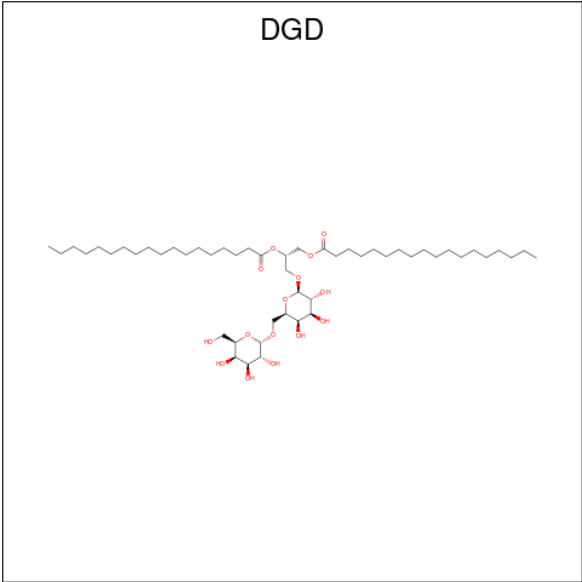
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			43	40	3	
24	F	1	Total	C	O	0
			43	40	3	
24	G	1	Total	C	O	0
			43	40	3	
24	G	1	Total	C	O	0
			43	40	3	
24	H	1	Total	C	O	0
			43	40	3	
24	H	1	Total	C	O	0
			43	40	3	
24	I	1	Total	C	O	0
			43	40	3	
24	I	1	Total	C	O	0
			43	40	3	
24	J	1	Total	C	O	0
			43	40	3	
24	K	1	Total	C	O	0
			43	40	3	
24	K	1	Total	C	O	0
			43	40	3	
24	L	1	Total	C	O	0
			43	40	3	
24	L	1	Total	C	O	0
			43	40	3	
24	L	1	Total	C	O	0
			43	40	3	
24	N	1	Total	C	O	0
			43	40	3	
24	N	1	Total	C	O	0
			43	40	3	
24	O	1	Total	C	O	0
			43	40	3	
24	O	1	Total	C	O	0
			43	40	3	
24	P	1	Total	C	O	0
			43	40	3	
24	P	1	Total	C	O	0
			43	40	3	
24	Q	1	Total	C	O	0
			43	40	3	
24	Q	1	Total	C	O	0
			43	40	3	

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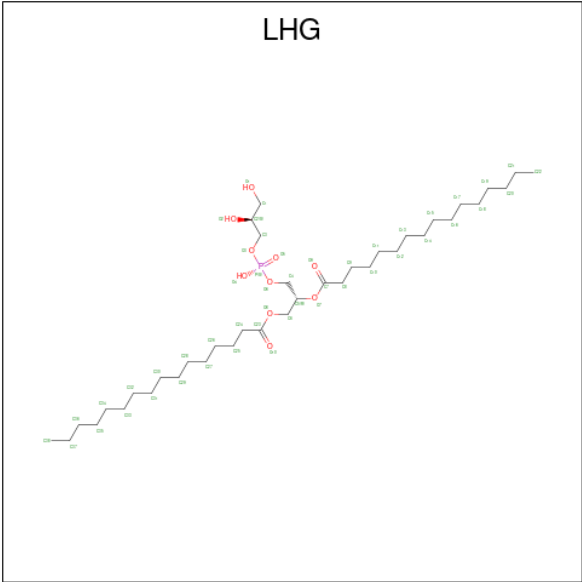
Mol	Chain	Residues	Atoms			AltConf
24	R	1	Total 43	C 40	O 3	0
24	R	1	Total 43	C 40	O 3	0
24	S	1	Total 43	C 40	O 3	0
24	S	1	Total 43	C 40	O 3	0
24	T	1	Total 43	C 40	O 3	0
24	T	1	Total 43	C 40	O 3	0
24	U	1	Total 43	C 40	O 3	0
24	U	1	Total 43	C 40	O 3	0
24	V	1	Total 43	C 40	O 3	0
24	V	1	Total 43	C 40	O 3	0
24	W	1	Total 43	C 40	O 3	0
24	W	1	Total 43	C 40	O 3	0
24	W	1	Total 43	C 40	O 3	0
24	X	1	Total 43	C 40	O 3	0
24	X	1	Total 43	C 40	O 3	0
24	X	1	Total 43	C 40	O 3	0
24	X	1	Total 43	C 40	O 3	0
24	A	1	Total 43	C 40	O 3	0
24	A	1	Total 43	C 40	O 3	0
24	A	1	Total 43	C 40	O 3	0

- Molecule 25 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
25	B	1	Total	C	O	0
			66	51	15	
25	F	1	Total	C	O	0
			34	29	5	
25	O	1	Total	C	O	0
			60	45	15	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



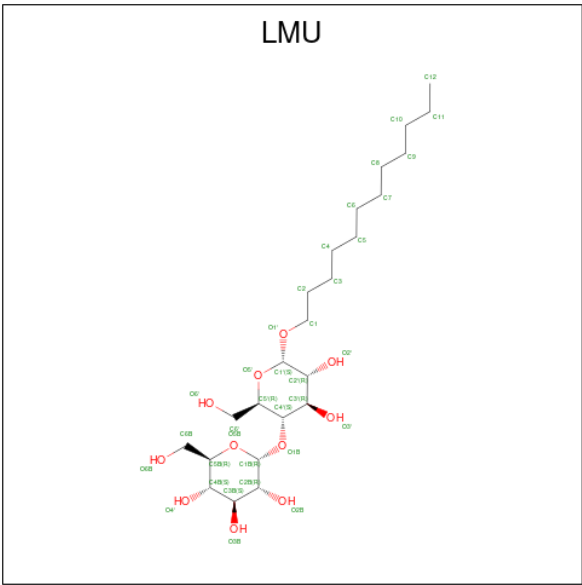
Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	P	0
			27	16	10	1	
26	B	1	Total	C	O	P	0
			42	31	10	1	
26	G	1	Total	C	O	P	0
			32	21	10	1	
26	H	1	Total	C	O	P	0
			27	16	10	1	
26	K	1	Total	C	O	P	0
			39	28	10	1	
26	K	1	Total	C	O	P	0
			33	22	10	1	
26	L	1	Total	C	O	P	0
			42	31	10	1	
26	N	1	Total	C	O	P	0
			28	17	10	1	
26	N	1	Total	C	O	P	0
			43	32	10	1	
26	O	1	Total	C	O	P	0
			34	23	10	1	
26	O	1	Total	C	O	P	0
			49	38	10	1	
26	O	1	Total	C	O	P	0
			43	32	10	1	
26	O	1	Total	C	O	P	0
			42	31	10	1	
26	P	1	Total	C	O	P	0
			40	29	10	1	
26	Q	1	Total	C	O	P	0
			44	33	10	1	
26	R	1	Total	C	O	P	0
			42	31	10	1	
26	S	1	Total	C	O	P	0
			32	21	10	1	
26	T	1	Total	C	O	P	0
			42	31	10	1	
26	U	1	Total	C	O	P	0
			25	16	8	1	
26	W	1	Total	C	O	P	0
			42	31	10	1	
26	X	1	Total	C	O	P	0
			42	31	10	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			19	14	5	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			15	14	1	
27	F	1	Total	C	O	0
			21	15	6	
27	F	1	Total	C	O	0
			21	15	6	
27	G	1	Total	C	O	0
			21	15	6	

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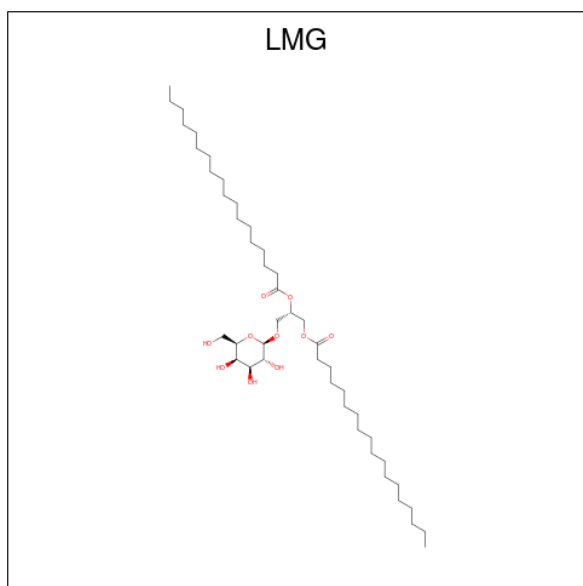
Mol	Chain	Residues	Atoms			AltConf
27	H	1	Total	C	O	0
			21	15	6	
27	H	1	Total	C	O	0
			24	18	6	
27	H	1	Total	C	O	0
			33	23	10	
27	J	1	Total	C	O	0
			34	24	10	
27	K	1	Total	C	O	0
			33	23	10	
27	L	1	Total	C	O	0
			24	18	6	
27	L	1	Total	C	O	0
			27	21	6	
27	L	1	Total	C	O	0
			34	24	10	
27	M	1	Total	C	O	0
			24	18	6	
27	O	1	Total	C	O	0
			24	18	6	
27	O	1	Total	C	O	0
			35	24	11	
27	O	1	Total	C	O	0
			26	22	4	
27	O	1	Total	C	O	0
			35	24	11	
27	T	1	Total	C	O	0
			21	15	6	
27	T	1	Total	C	O	0
			24	18	6	
27	T	1	Total	C	O	0
			24	18	6	
27	U	1	Total	C	O	0
			35	24	11	
27	U	1	Total	C	O	0
			35	24	11	
27	U	1	Total	C	O	0
			24	18	6	
27	W	1	Total	C	O	0
			24	18	6	
27	X	1	Total	C	O	0
			24	18	6	

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Mol	Chain	Residues	Atoms			AltConf
27	X	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			24	18	6	
27	A	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			21	15	6	
27	A	1	Total	C	O	0
			24	18	6	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			43	33	10	
28	B	1	Total	C	O	0
			53	43	10	
28	F	1	Total	C	O	0
			42	32	10	
28	G	1	Total	C	O	0
			46	36	10	
28	H	1	Total	C	O	0
			43	33	10	
28	H	1	Total	C	O	0
			40	30	10	

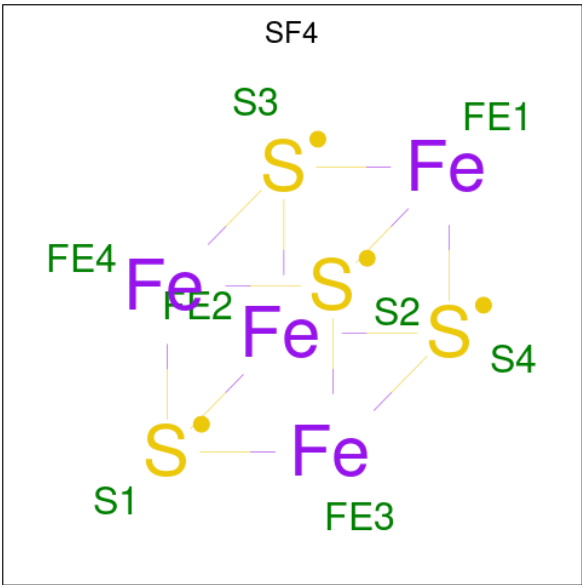
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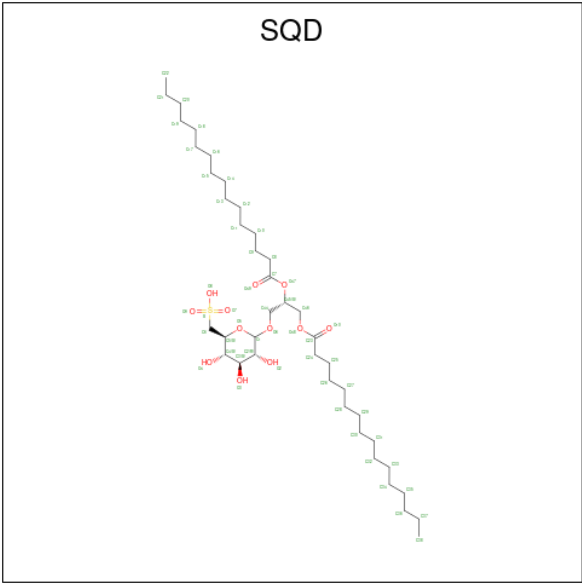
Mol	Chain	Residues	Atoms			AltConf
28	H	1	Total	C	O	0
			37	27	10	
28	I	1	Total	C	O	0
			37	27	10	
28	I	1	Total	C	O	0
			50	41	9	
28	J	1	Total	C	O	0
			55	45	10	
28	K	1	Total	C	O	0
			43	33	10	
28	K	1	Total	C	O	0
			49	39	10	
28	K	1	Total	C	O	0
			43	33	10	
28	L	1	Total	C	O	0
			51	41	10	
28	N	1	Total	C	O	0
			44	34	10	
28	Q	1	Total	C	O	0
			37	27	10	
28	T	1	Total	C	O	0
			41	31	10	
28	U	1	Total	C	O	0
			53	43	10	
28	U	1	Total	C	O	0
			49	39	10	
28	W	1	Total	C	O	0
			48	38	10	
28	A	1	Total	C	O	0
			41	31	10	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



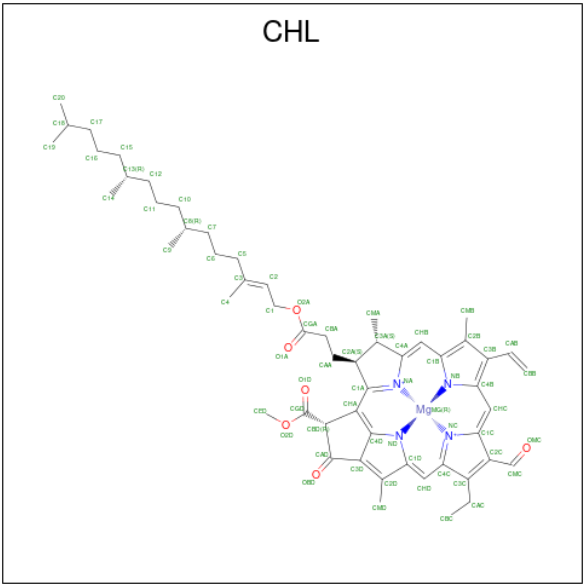
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	F	1	Total	C	O	S	0
			42	29	12	1	
30	K	1	Total	C	O	S	0
			43	30	12	1	
30	O	1	Total	C	O	S	0
			42	29	12	1	
30	V	1	Total	C	O	S	0
			27	16	10	1	

- Molecule 31 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



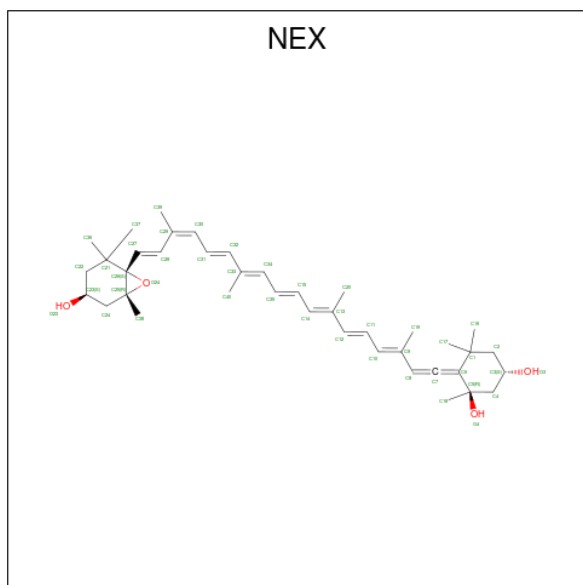
Mol	Chain	Residues	Atoms				AltConf
31	U	1	Total	C	Mg	N	O
			46	35	1	4	6
31	U	1	Total	C	Mg	N	O
			46	35	1	4	6
31	V	1	Total	C	Mg	N	O
			46	35	1	4	6
31	V	1	Total	C	Mg	N	O
			46	35	1	4	6
31	W	1	Total	C	Mg	N	O
			46	35	1	4	6
31	W	1	Total	C	Mg	N	O
			66	55	1	4	6
31	W	1	Total	C	Mg	N	O
			66	55	1	4	6

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Mol	Chain	Residues	Atoms					AltConf
31	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 32 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula:  $C_{40}H_{56}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
32	U	1	Total	C	O	0
			44	40	4	
32	V	1	Total	C	O	0
			44	40	4	

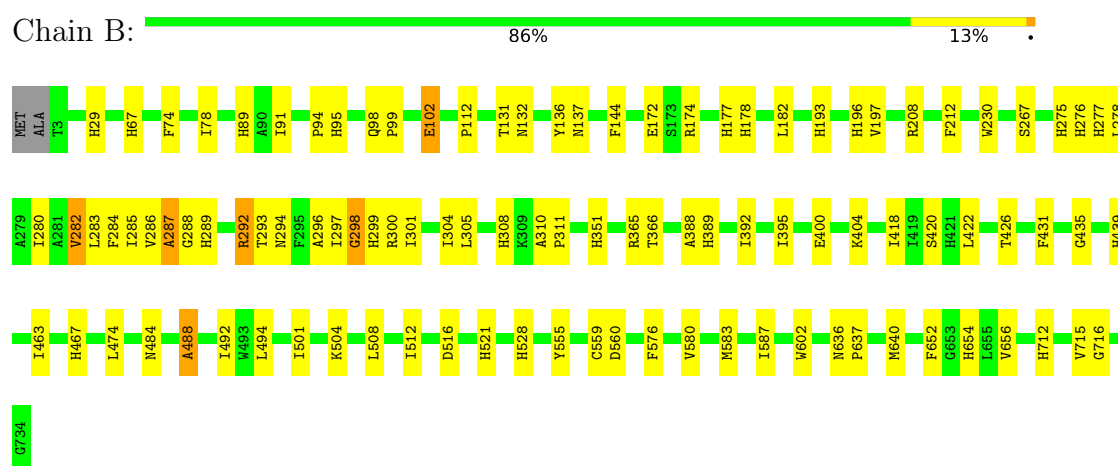
- Molecule 33 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



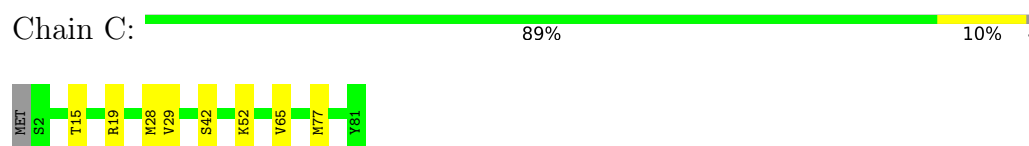
### 3 Residue-property plots

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.

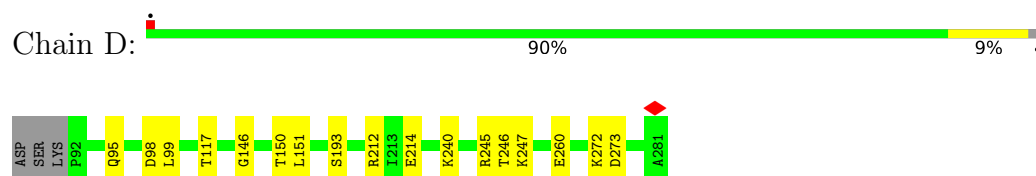
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2



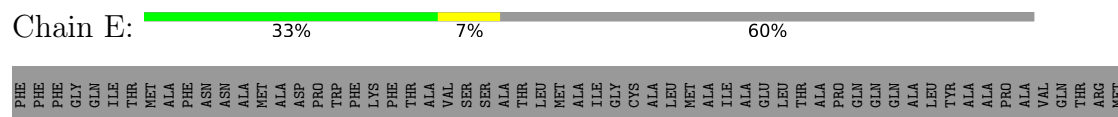
- Molecule 2: Photosystem I iron-sulfur center

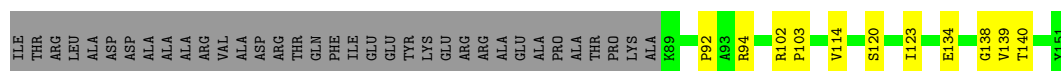


- Molecule 3: PsaD

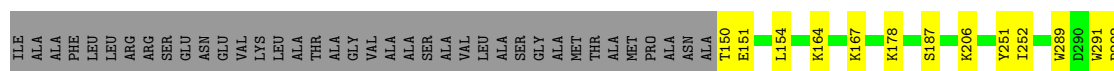
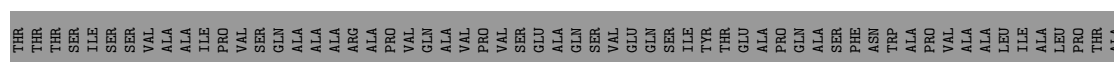


- Molecule 4: PsaE

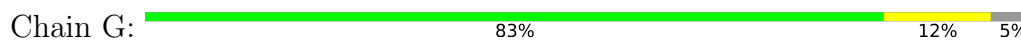




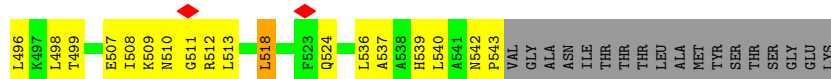
- Molecule 5: PsaF



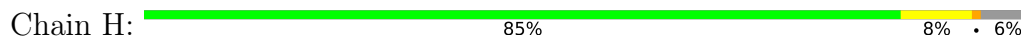
- Molecule 6: Lhce5.7



- Molecule 6: Lhce5.7



- Molecule 7: Lhce7.3



- Molecule 8: Lhce5



THR  
THR  
THR  
LEU  
ALA  
MET  
TVR  
SER  
THR  
SER  
GLY  
ASP  
LYS

• Molecule 8: Lhce5

Chain N: 75% 16% 8%

HIS  
LYS  
D66  
G67  
V68  
W69  
F70  
F71  
H78  
E108  
S115  
M116  
L117  
V120  
A132  
E135  
D141  
K144  
M150  
A151  
I152  
A153  
A154  
P155  
T156  
E157  
Y158  
W159  
R160  
G178  
F179  
D180  
L184  
T185  
T186  
D187  
Y188  
T189  
G197  
M201  
E216  
L222  
L226

T235  
THR  
THR  
LEU  
ALA  
MET  
TVR  
SER  
THR  
SER  
GLY  
ASP  
LYS

• Molecule 9: PsaJ

Chain J: 87% 8% 5%

LEU  
THR  
M7  
V20  
R37  
I42  
L43

• Molecule 10: LhcE6

Chain K: 88% 10% ..

E377  
P390  
L393  
V434  
E471  
R474  
W481  
K486  
Y487  
P492  
P496  
E508  
G521  
L522  
E523  
V524  
Q525  
V528  
H543  
P544  
L545  
A546  
A547  
N548  
T549  
P558  
PRO  
VAL

• Molecule 10: LhcE6

Chain Q: 83% 15% ..

GLU  
LYS  
Y379  
R380  
W383  
F384  
P385  
N386  
I387  
T388  
L408  
M418  
N425  
G426  
R458  
L461  
I462  
S463  
L464  
Q465  
V467  
T504  
I509  
R513  
M516  
V524  
L537  
I538  
E539  
H540  
L541  
R542  
L545  
A546  
A547  
N548  
I549  
G550  
V560

• Molecule 11: Lhce8

Chain L: 78% 16% 5%

VAL  
D194  
R195  
G201  
D226  
P227  
K228  
E231  
M245  
L257  
Y263  
V285  
V288  
L292  
N301  
F305  
T315  
E319  
G332  
L333  
E334  
V335  
Q336  
R337  
H338  
V339  
V342  
V346  
N347  
L348  
V349  
E350  
H351  
V352  
A361  
H366  
Q367  
V368  
F369  
V370  
A371  
MET

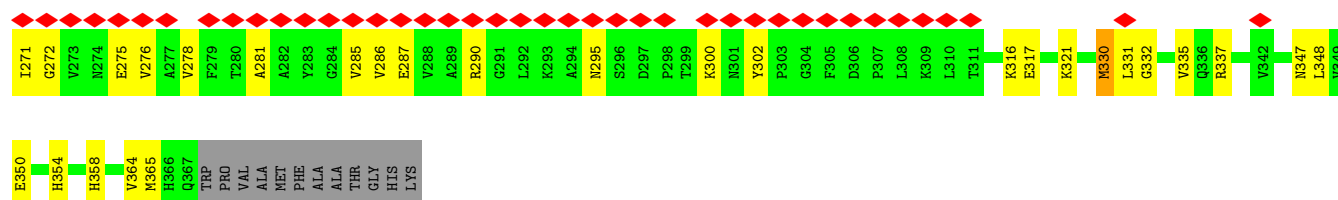
PHE  
ALA  
ALA  
THR  
GLY  
HIS  
LYS

• Molecule 11: Lhce8

Chain R: 38% 66% 25% 7%

VAL  
D194  
R195  
P196  
F199  
S206  
Y207  
L208  
T209  
G210  
Q211  
Y212  
F213  
F218  
A225  
D226  
P227  
K228  
V229  
R232  
M233  
R234  
V235  
S236  
E237  
V238  
Y239  
H240  
G241  
R242  
L243  
A244  
M245  
L246  
A247  
I248  
V253  
P254  
D255  
I256  
L257  
G258  
K259  
G260  
A261  
V262  
Y263  
E264  
A265  
A266  
Q267  
N268  
A269  
G270





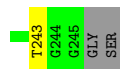
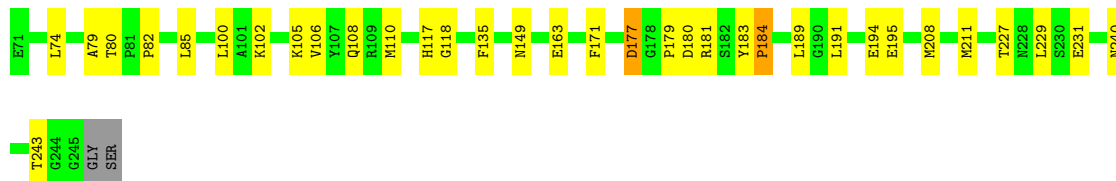
- Molecule 12: PsaM

Chain M: 84% 16%



- Molecule 13: LhcE7

Chain O: 80% 18% ..



- Molecule 14: Lhce10

Chain S: 81% 14% . .



- Molecule 15: Lhce11

Chain T: 92% 5% .



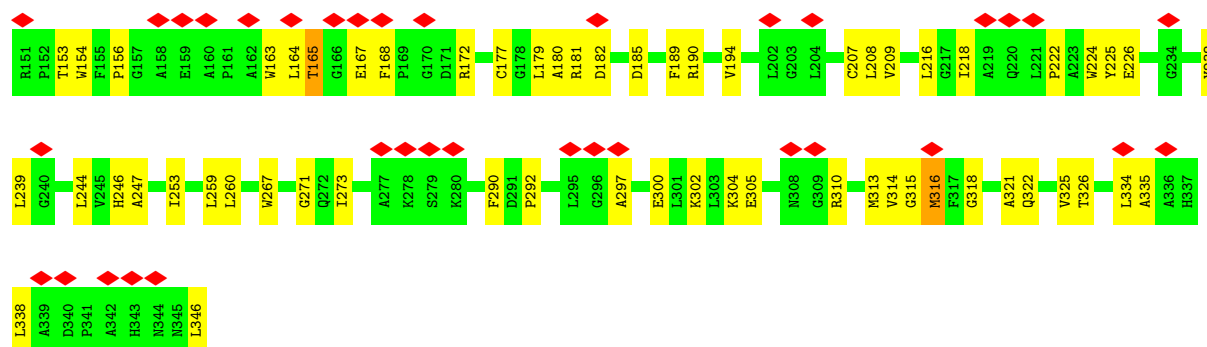
- Molecule 16: LhcbM4.6

Chain U: 88% 8% 5%



- Molecule 17: LhcbM4.10

Chain V: 18% 70% 29% .



• Molecule 18: LhcbM2

Chain W: 87% 9% .



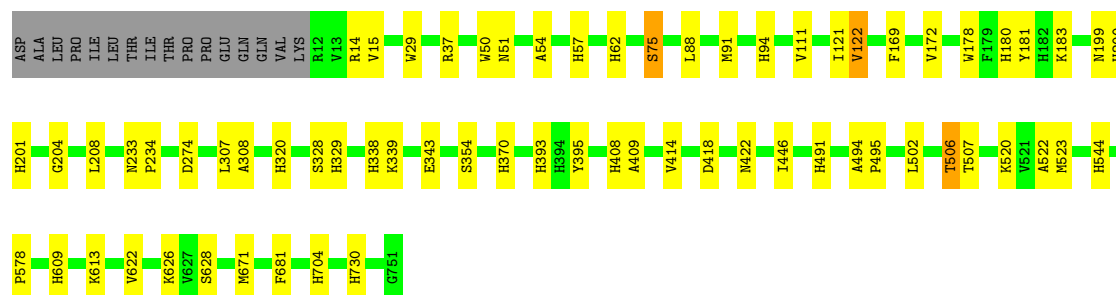
• Molecule 19: LhcbM8

Chain X: 93% 7% .



• Molecule 20: PsaA

Chain A: 89% 9% .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.393	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	496.64, 496.64, 496.64	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	B	0.35	1/6078 (0.0%)	0.49	4/8287 (0.0%)
2	C	0.33	0/606	0.53	0/819
3	D	0.14	0/1525	0.38	0/2065
4	E	0.13	0/521	0.31	0/707
5	F	0.17	0/1288	0.46	0/1747
6	G	0.17	0/1360	0.39	0/1855
6	P	0.41	0/1279	0.68	1/1744 (0.1%)
7	H	0.32	0/1381	0.52	3/1876 (0.2%)
8	I	0.31	0/1278	0.56	0/1741
8	N	0.24	0/1307	0.46	0/1784
9	J	0.14	0/314	0.32	0/429
10	K	0.21	0/1492	0.49	0/2035
10	Q	0.20	0/1489	0.48	0/2034
11	L	0.35	0/1401	0.58	2/1910 (0.1%)
11	R	0.16	0/1365	0.41	0/1858
12	M	0.13	0/246	0.32	0/332
13	O	0.20	0/1397	0.46	0/1898
14	S	0.26	0/1370	0.46	0/1865
15	T	0.16	0/1320	0.40	0/1784
16	U	0.15	0/1566	0.37	0/2141
17	V	0.14	0/1566	0.33	0/2141
18	W	0.16	0/1719	0.38	0/2343
19	X	0.17	0/1731	0.37	0/2351
20	A	0.35	0/6073	0.49	1/8279 (0.0%)
All	All	0.27	1/39672 (0.0%)	0.47	11/54025 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	ALA	CA-C	-6.82	1.46	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	395	GLY	N-CA-C	-9.42	102.67	114.92
1	B	298	GLY	N-CA-C	8.87	120.52	111.56
1	B	287	ALA	N-CA-C	-6.79	102.39	111.96
7	H	149	GLY	O-C-N	-6.78	115.67	122.18
7	H	152	VAL	CB-CA-C	-5.83	104.18	112.22
1	B	282	VAL	N-CA-C	-5.81	97.26	109.34
11	L	361	ALA	N-CA-C	5.73	117.61	111.36
11	L	332	GLY	O-C-N	-5.67	116.24	122.24
20	A	446	ILE	O-C-N	-5.62	116.41	121.91
7	H	150	LEU	N-CA-C	5.60	118.15	111.71
1	B	292	ARG	N-CA-C	5.53	117.67	110.43

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	B	5868	0	5667	91	0
2	C	596	0	571	6	0
3	D	1489	0	1462	9	0
4	E	509	0	489	5	0
5	F	1262	0	1293	10	0
6	G	1323	0	1305	15	0
6	P	1243	0	1218	39	0
7	H	1342	0	1315	9	0
8	I	1242	0	1213	25	0
8	N	1271	0	1245	27	0
9	J	305	0	314	4	0
10	K	1444	0	1391	17	0
10	Q	1440	0	1388	26	0
11	L	1364	0	1346	27	0
11	R	1331	0	1315	45	0
12	M	242	0	258	8	0
13	O	1359	0	1328	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	S	1327	0	1271	18	0
15	T	1283	0	1238	6	0
16	U	1517	0	1466	14	0
17	V	1513	0	1467	56	0
18	W	1669	0	1647	15	0
19	X	1688	0	1693	10	0
20	A	5872	0	5735	55	0
21	A	160	0	224	8	0
21	B	240	0	336	21	0
21	J	40	0	56	1	0
21	M	40	0	56	3	0
22	A	2638	0	2742	77	0
22	B	2341	0	2395	78	0
22	F	165	0	154	6	0
22	G	571	0	498	10	0
22	H	698	0	626	10	0
22	I	567	0	490	17	0
22	J	50	0	39	1	0
22	K	765	0	758	33	0
22	L	703	0	694	30	0
22	N	570	0	504	19	0
22	O	651	0	585	20	0
22	P	446	0	326	10	0
22	Q	738	0	655	20	0
22	R	678	0	653	29	0
22	S	621	0	530	14	0
22	T	625	0	603	10	0
22	U	676	0	586	14	0
22	V	625	0	548	32	0
22	W	733	0	694	18	0
22	X	741	0	716	7	0
23	A	33	0	46	2	0
23	B	33	0	46	1	0
24	A	129	0	0	0	0
24	B	43	0	0	1	0
24	F	43	0	0	0	0
24	G	86	0	0	0	0
24	H	86	0	0	0	0
24	I	86	0	0	0	0
24	J	43	0	0	0	0
24	K	86	0	0	0	0
24	L	129	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	N	86	0	0	0	0
24	O	86	0	0	0	0
24	P	86	0	0	0	0
24	Q	86	0	0	1	0
24	R	86	0	0	0	0
24	S	86	0	0	1	0
24	T	86	0	0	0	0
24	U	86	0	0	0	0
24	V	86	0	0	0	0
24	W	129	0	0	0	0
24	X	172	0	0	0	0
25	B	66	0	96	6	0
25	F	34	0	50	2	0
25	O	60	0	81	3	0
26	A	98	0	148	3	0
26	B	69	0	81	8	0
26	G	32	0	34	0	0
26	H	27	0	24	0	0
26	K	72	0	84	3	0
26	L	42	0	57	3	0
26	N	71	0	82	2	0
26	O	168	0	228	4	0
26	P	40	0	53	1	0
26	Q	44	0	61	1	0
26	R	42	0	57	3	0
26	S	32	0	34	2	0
26	T	42	0	57	1	0
26	U	25	0	21	0	0
26	W	42	0	57	2	0
26	X	42	0	57	0	0
27	A	104	0	142	2	0
27	B	165	0	233	10	0
27	F	42	0	52	1	0
27	G	21	0	26	0	0
27	H	78	0	103	2	0
27	J	34	0	44	0	0
27	K	33	0	42	2	0
27	L	85	0	110	6	0
27	M	24	0	35	1	0
27	O	120	0	155	4	0
27	T	69	0	96	2	0
27	U	94	0	127	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	W	24	0	35	0	0
27	X	59	0	81	0	0
28	A	41	0	52	0	0
28	B	96	0	138	4	0
28	F	42	0	54	3	0
28	G	46	0	65	0	0
28	H	120	0	150	2	0
28	I	87	0	117	1	0
28	J	55	0	86	1	0
28	K	135	0	183	3	0
28	L	51	0	75	0	0
28	N	44	0	61	1	0
28	Q	37	0	44	2	0
28	T	41	0	52	2	0
28	U	102	0	150	4	0
28	W	48	0	69	3	0
29	B	8	0	0	0	0
29	C	16	0	0	0	0
30	F	42	0	48	2	0
30	K	43	0	50	1	0
30	O	42	0	48	8	0
30	V	27	0	25	1	0
31	U	92	0	62	7	0
31	V	92	0	62	14	0
31	W	178	0	171	10	0
31	X	46	0	31	0	0
32	U	44	0	56	4	0
32	V	44	0	56	9	0
33	A	65	0	72	6	0
All	All	60137	0	57815	901	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 8.

All (901) 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)
23:B:840:PQN:H291	25:B:847:DGD:HBT1	1.23	1.10
31:V:605:CHL:HAB	31:V:606:CHL:OMC	1.50	1.08
8:N:184:LEU:HD12	22:N:607:CLA:H42	1.41	1.01
6:P:391:ALA:HB2	6:P:404:ASP:HB3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:THR:HB	12:M:1:MET:HE1	1.46	0.94
28:F:408:LMG:H122	22:W:402:CLA:HAB	1.55	0.89
13:O:135:PHE:HE2	30:O:302:SQD:H82	1.38	0.89
13:O:135:PHE:CE2	30:O:302:SQD:H82	2.09	0.88
11:L:315:THR:HG21	22:L:408:CLA:H12	1.54	0.87
22:L:404:CLA:HMC1	22:L:417:CLA:HBB2	1.57	0.87
33:A:802:CL0:H2	33:A:802:CL0:H15	1.57	0.85
1:B:293:THR:HG22	1:B:294:ASN:H	1.41	0.85
31:V:605:CHL:CAB	31:V:606:CHL:OMC	2.24	0.84
17:V:273:ILE:HG21	32:V:616:NEX:H172	1.60	0.83
22:V:604:CLA:C1C	32:V:616:NEX:H222	2.08	0.83
22:L:404:CLA:CMC	22:L:417:CLA:CBB	2.57	0.83
8:I:222:LEU:HD11	22:I:611:CLA:HBC2	1.62	0.82
14:S:223:VAL:HG21	22:S:610:CLA:HAC2	1.62	0.81
22:V:604:CLA:CHC	32:V:616:NEX:H362	2.12	0.80
11:R:233:MET:HE1	22:R:602:CLA:H3A	1.63	0.79
22:B:833:CLA:H203	31:U:408:CHL:HMD1	1.67	0.77
22:A:828:CLA:HED1	22:A:836:CLA:HAB	1.65	0.76
22:L:404:CLA:HMC1	22:L:417:CLA:CBB	2.16	0.76
12:M:20:PHE:CD2	22:O:311:CLA:H42	2.21	0.75
28:K:601:LMG:H302	22:K:613:CLA:HMA2	1.69	0.75
20:A:408:HIS:HE1	22:A:831:CLA:NA	1.85	0.74
6:P:388:GLN:O	6:P:390:PRO:HD3	1.87	0.74
22:B:822:CLA:HAB	22:B:829:CLA:HMD1	1.69	0.74
8:I:65:LYS:HE2	8:I:65:LYS:H	1.53	0.74
1:B:95:HIS:HE1	22:B:809:CLA:NB	1.83	0.73
8:I:158:TYR:CE2	22:K:607:CLA:HBA1	2.24	0.73
22:A:819:CLA:HBB1	22:A:819:CLA:HHC	1.69	0.73
11:L:315:THR:CG2	22:L:408:CLA:H12	2.18	0.73
31:V:605:CHL:CMC	31:V:606:CHL:C4C	2.67	0.73
22:L:404:CLA:HMC3	22:L:417:CLA:CBB	2.18	0.72
17:V:305:GLU:OE2	22:V:609:CLA:NB	2.22	0.72
6:P:383:TRP:HE3	6:P:384:PHE:H	1.35	0.72
3:D:212:ARG:NH2	3:D:214:GLU:OE2	2.23	0.72
1:B:292:ARG:HD3	1:B:300:ARG:HD3	1.70	0.72
1:B:389:HIS:HE1	22:B:828:CLA:NA	1.88	0.71
8:I:193:GLU:OE2	22:I:607:CLA:NB	2.24	0.71
11:R:195:ARG:HH21	11:R:210:GLY:H	1.38	0.71
20:A:121:ILE:HG13	20:A:122:VAL:HG13	1.72	0.71
1:B:230:TRP:HB2	22:B:815:CLA:H12	1.72	0.70
31:V:605:CHL:C1C	31:V:606:CHL:HBC2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:335:VAL:HG11	22:R:610:CLA:HAC2	1.71	0.70
8:N:68:VAL:HG12	8:N:70:PHE:H	1.57	0.70
1:B:292:ARG:HD3	1:B:300:ARG:CD	2.22	0.69
5:F:307:ASP:OD2	5:F:308:ALA:N	2.25	0.69
28:H:319:LMG:H132	30:K:621:SQD:H121	1.75	0.69
8:N:160:ARG:NH2	22:N:606:CLA:O1D	2.25	0.69
17:V:334:LEU:HD11	22:V:613:CLA:HBB1	1.75	0.69
1:B:178:HIS:CD2	22:B:812:CLA:NB	2.61	0.69
10:K:390:PRO:HG2	10:K:393:LEU:HD12	1.74	0.69
20:A:94:HIS:HE1	22:A:809:CLA:NA	1.91	0.68
22:N:610:CLA:HBA1	22:N:610:CLA:HBD	1.75	0.68
11:R:232:ARG:HB3	11:R:295:ASN:HD22	1.58	0.68
22:R:604:CLA:H3A	22:R:605:CLA:H152	1.74	0.68
1:B:282:VAL:HG13	24:B:841:DD6:C7	2.23	0.67
22:K:613:CLA:H42	22:L:417:CLA:OBD	1.94	0.67
22:A:811:CLA:HBD	22:A:811:CLA:HBA1	1.77	0.67
1:B:292:ARG:HH21	1:B:296:ALA:HA	1.60	0.67
10:Q:418:MET:HE1	22:Q:604:CLA:H43	1.75	0.67
1:B:287:ALA:O	1:B:289:HIS:N	2.27	0.67
6:P:537:ALA:O	6:P:540:LEU:HB3	1.95	0.67
11:R:229:VAL:HA	11:R:232:ARG:HG2	1.76	0.67
22:A:822:CLA:H171	22:A:832:CLA:HBC1	1.77	0.67
8:I:65:LYS:HE2	8:I:65:LYS:N	2.09	0.66
2:C:15:THR:HG22	2:C:28:MET:HE2	1.78	0.66
17:V:315:GLY:HA2	22:V:612:CLA:HBB1	1.76	0.66
22:Q:610:CLA:NB	26:Q:616:LHG:O4	2.29	0.66
28:N:615:LMG:H211	22:O:315:CLA:HBB1	1.76	0.66
1:B:94:PRO:HB3	27:B:854:LMU:H51	1.78	0.66
22:G:603:CLA:H93	22:K:603:CLA:H112	1.78	0.66
10:K:496:PRO:HA	27:K:620:LMU:H3'	1.77	0.66
6:P:381:GLY:HA3	22:P:608:CLA:HBB1	1.77	0.66
12:M:24:LYS:HE3	27:M:102:LMU:H6E	1.79	0.65
11:R:272:GLY:H	11:R:275:GLU:HB2	1.61	0.65
10:Q:425:ASN:HD22	22:Q:604:CLA:HBB2	1.61	0.65
28:T:616:LMG:H371	22:A:816:CLA:H141	1.76	0.65
20:A:704:HIS:HE1	22:A:841:CLA:C4D	2.10	0.65
26:B:851:LHG:H131	27:L:419:LMU:H12	1.78	0.65
6:P:411:ASP:HB3	6:P:414:VAL:HG12	1.79	0.65
22:V:604:CLA:NC	32:V:616:NEX:H222	2.11	0.64
6:P:399:ALA:O	22:P:602:CLA:HED1	1.96	0.64
22:N:606:CLA:HHC	22:N:606:CLA:HBB1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:233:MET:CE	22:R:602:CLA:H3A	2.28	0.64
13:O:135:PHE:CZ	30:O:302:SQD:H111	2.34	0.63
6:P:391:ALA:HB2	6:P:404:ASP:CB	2.25	0.63
20:A:704:HIS:HE1	22:A:841:CLA:ND	1.97	0.63
6:P:474:ARG:HH12	22:P:606:CLA:HED1	1.62	0.63
6:G:426:ALA:HB1	6:G:511:GLY:HA3	1.81	0.63
13:O:100:LEU:CD2	22:V:603:CLA:H43	2.27	0.63
22:W:412:CLA:H8	22:W:413:CLA:C4D	2.26	0.63
10:K:544:PRO:HB2	10:K:545:LEU:HD13	1.81	0.62
20:A:329:HIS:HD2	22:A:824:CLA:NB	1.97	0.62
1:B:144:PHE:HB2	28:B:856:LMG:H222	1.80	0.62
19:X:301:HIS:CD2	22:X:413:CLA:NC	2.67	0.62
22:A:840:CLA:H122	21:A:849:BCR:H312	1.82	0.62
11:L:231:GLU:N	11:L:231:GLU:OE1	2.31	0.62
17:V:156:PRO:HG2	22:V:601:CLA:HBB1	1.82	0.62
1:B:287:ALA:C	1:B:289:HIS:H	2.08	0.61
5:F:293:ASN:ND2	22:W:410:CLA:O1A	2.31	0.61
31:V:605:CHL:C2C	31:V:606:CHL:HBC2	2.29	0.61
22:B:833:CLA:H203	31:U:408:CHL:CMD	2.29	0.61
31:V:605:CHL:HAB	31:V:606:CHL:CMC	2.27	0.61
22:K:607:CLA:HHC	22:K:607:CLA:HBB1	1.82	0.61
11:R:302:TYR:OH	11:R:316:LYS:NZ	2.28	0.61
22:B:859:CLA:HBA1	22:B:859:CLA:HBD	1.83	0.61
7:H:12:ILE:HG13	7:H:13:PRO:HD2	1.82	0.61
8:I:195:LYS:HB3	22:I:608:CLA:HMD2	1.83	0.61
15:T:372:LEU:HB2	15:T:374:MET:HE2	1.83	0.61
27:H:321:LMU:H123	22:A:824:CLA:H203	1.82	0.61
19:X:211:LYS:H	22:X:419:CLA:HBB1	1.65	0.61
11:R:253:VAL:HG11	22:R:604:CLA:HAC2	1.83	0.60
8:I:154:ALA:HA	22:I:606:CLA:HAB	1.82	0.60
1:B:196:HIS:HE1	22:B:814:CLA:C1C	2.05	0.60
8:I:201:MET:HE1	22:I:602:CLA:HAB	1.84	0.60
30:O:302:SQD:O7	10:Q:545:LEU:HB2	2.01	0.60
1:B:560:ASP:OD1	2:C:52:LYS:NZ	2.30	0.60
7:H:42:VAL:O	7:H:46:MET:HG2	2.01	0.60
22:P:608:CLA:HBD	22:P:609:CLA:HMD3	1.84	0.59
17:V:335:ALA:HA	17:V:338:LEU:HD12	1.84	0.59
11:R:261:ALA:O	11:R:265:ALA:N	2.29	0.59
11:R:233:MET:HA	11:R:236:SER:HB3	1.85	0.59
19:X:257:LYS:HA	19:X:257:LYS:HE2	1.82	0.59
27:L:420:LMU:H51	22:A:834:CLA:HBB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:334:GLU:O	11:L:334:GLU:HG3	2.02	0.59
22:Q:607:CLA:HBB1	11:R:199:PHE:CE1	2.38	0.59
17:V:322:GLN:NE2	22:V:612:CLA:O1D	2.36	0.59
18:W:179:GLU:OE2	18:W:179:GLU:N	2.30	0.59
22:A:839:CLA:HBC2	27:A:854:LMU:H91	1.85	0.59
17:V:179:LEU:HD13	22:V:602:CLA:H42	1.85	0.59
22:B:829:CLA:HBB1	22:B:829:CLA:HMB1	1.85	0.59
7:H:38:LYS:HE2	7:H:38:LYS:HA	1.85	0.58
14:S:208:ILE:HD12	14:S:208:ILE:H	1.68	0.58
17:V:165:THR:OG1	17:V:167:GLU:OE2	2.20	0.58
17:V:207:CYS:HG	17:V:224:TRP:CD1	2.22	0.58
31:V:605:CHL:HMC	31:V:606:CHL:C1C	2.34	0.58
8:I:150:MET:HE1	28:K:601:LMG:H172	1.85	0.58
13:O:106:VAL:O	13:O:110:MET:HG2	2.03	0.58
6:G:446:ALA:HB3	6:G:449:GLU:HG2	1.86	0.58
13:O:177:ASP:OD1	13:O:177:ASP:N	2.36	0.57
6:P:460:GLY:C	10:Q:461:LEU:HD21	2.29	0.57
13:O:179:PRO:HD3	10:Q:386:ASN:O	2.03	0.57
1:B:275:HIS:HE1	22:B:815:CLA:C4D	2.18	0.57
8:I:64:HIS:N	8:I:65:LYS:HZ3	2.02	0.57
1:B:193:HIS:HB2	22:B:813:CLA:CHC	2.34	0.57
1:B:712:HIS:HE1	22:B:838:CLA:ND	2.02	0.57
22:V:612:CLA:H62	22:V:612:CLA:H193	1.86	0.57
22:B:802:CLA:HMB2	22:A:804:CLA:OBD	2.05	0.57
22:R:610:CLA:HAB	22:R:610:CLA:H121	1.87	0.57
11:R:226:ASP:HB3	11:R:229:VAL:HB	1.86	0.57
21:B:801:BCR:HC8	21:B:801:BCR:H331	1.86	0.57
31:V:605:CHL:HMC	31:V:606:CHL:NC	2.20	0.57
8:N:154:ALA:HB3	8:N:155:PRO:HD3	1.87	0.57
1:B:463:ILE:HD11	22:B:834:CLA:H2	1.87	0.56
10:K:523:GLU:OE2	22:K:617:CLA:NA	2.38	0.56
8:N:184:LEU:HG	22:N:607:CLA:H11	1.87	0.56
8:N:197:GLY:O	8:N:201:MET:HG3	2.05	0.56
22:G:608:CLA:H71	22:G:609:CLA:C4D	2.35	0.56
11:R:331:LEU:HD21	22:R:615:CLA:H52	1.86	0.56
17:V:346:LEU:HD22	22:V:612:CLA:H43	1.87	0.56
1:B:654:HIS:NE2	22:B:802:CLA:NA	2.53	0.56
13:O:195:GLU:OE2	27:O:301:LMU:C2'	2.52	0.56
6:P:539:HIS:HA	6:P:542:ASN:CG	2.31	0.56
10:Q:461:LEU:O	10:Q:465:GLN:HG2	2.06	0.56
22:U:406:CLA:H2	31:U:407:CHL:HBD	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:150:THR:OG1	5:F:151:GLU:N	2.33	0.56
3:D:150:THR:OG1	3:D:151:LEU:N	2.39	0.56
1:B:174:ARG:O	1:B:178:HIS:HB2	2.06	0.56
6:P:393:LEU:HD11	6:P:402:GLY:HA2	1.88	0.56
6:P:542:ASN:HB2	6:P:543:PRO:HD2	1.88	0.56
1:B:29:HIS:HE1	22:B:803:CLA:NB	2.00	0.56
10:Q:504:THR:HG22	22:Q:609:CLA:HHB	1.87	0.56
20:A:37:ARG:HH22	20:A:62:HIS:HA	1.70	0.56
17:V:325:VAL:HG23	17:V:326:THR:HG23	1.88	0.56
11:R:248:ILE:HA	11:R:330:MET:HE1	1.87	0.55
1:B:488:ALA:HB2	16:U:232:ASN:OD1	2.06	0.55
8:I:183:LYS:HE2	8:I:183:LYS:N	2.20	0.55
1:B:292:ARG:NH1	1:B:292:ARG:HB3	2.21	0.55
1:B:293:THR:HG22	1:B:294:ASN:N	2.17	0.55
7:H:168:HIS:CD2	22:H:312:CLA:NC	2.74	0.55
14:S:164:MET:HB3	15:T:337:MET:HE3	1.88	0.55
4:E:134:GLU:OE2	4:E:138:GLY:HA2	2.07	0.55
9:J:37:ARG:NH2	22:J:102:CLA:O1D	2.31	0.55
14:S:220:GLY:O	14:S:224:GLN:HG3	2.07	0.55
19:X:258:ASP:OD1	19:X:259:GLU:N	2.39	0.55
31:V:605:CHL:C2C	31:V:606:CHL:CBC	2.85	0.55
22:B:830:CLA:O1A	5:F:305:LEU:HD11	2.06	0.55
6:P:433:ILE:HG12	6:P:518:LEU:HD22	1.88	0.55
26:B:851:LHG:H292	27:B:854:LMU:H12	1.89	0.54
8:N:144:LYS:HG3	13:O:149:ASN:ND2	2.22	0.54
22:O:305:CLA:HBA2	26:O:318:LHG:H251	1.89	0.54
10:K:521:GLY:O	10:K:525:GLN:HG3	2.07	0.54
6:P:398:PRO:O	6:P:399:ALA:C	2.51	0.54
6:P:391:ALA:C	6:P:392:HIS:CG	2.85	0.54
20:A:201:HIS:CD2	22:A:815:CLA:NB	2.74	0.54
10:Q:539:GLU:HG3	10:Q:547:ALA:HB1	1.90	0.54
33:A:802:CL0:CGD	33:A:802:CL0:H8	2.38	0.54
8:I:132:ALA:N	8:I:135:GLU:OE2	2.40	0.54
22:K:609:CLA:HMB2	22:A:844:CLA:H11	1.89	0.54
22:L:408:CLA:CGA	22:L:408:CLA:H3A	2.38	0.54
10:Q:548:ASN:HD21	28:Q:602:LMG:HC8	1.71	0.54
1:B:283:LEU:C	1:B:285:ILE:N	2.66	0.54
22:L:408:CLA:H43	22:L:410:CLA:H11	1.90	0.54
13:O:180:ASP:OD2	13:O:181:ARG:N	2.40	0.54
6:G:494:ASP:OD2	6:G:499:THR:OG1	2.22	0.53
22:L:404:CLA:CMC	22:L:417:CLA:HBB2	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:178:GLY:HA2	22:N:607:CLA:HED1	1.90	0.53
20:A:75:SER:OG	20:A:181:TYR:HB2	2.08	0.53
1:B:102:GLU:N	1:B:102:GLU:OE1	2.41	0.53
16:U:251:SER:HB3	22:U:401:CLA:HBD	1.89	0.53
20:A:491:HIS:HE1	22:A:836:CLA:NB	2.05	0.53
8:I:195:LYS:HE3	22:I:608:CLA:C3D	2.39	0.53
10:K:543:HIS:HB3	10:K:546:ALA:HB3	1.89	0.53
1:B:712:HIS:HE1	22:B:838:CLA:C4D	2.21	0.53
26:R:614:LHG:H112	26:R:614:LHG:H291	1.89	0.53
17:V:267:TRP:HH2	32:V:616:NEX:C19	2.21	0.53
21:B:801:BCR:H331	23:A:843:PQN:H193	1.90	0.53
26:N:614:LHG:O3	26:N:614:LHG:O1	2.24	0.53
13:O:184:PRO:HB3	22:Q:601:CLA:HBC2	1.89	0.53
22:Q:607:CLA:HBB1	11:R:199:PHE:HE1	1.74	0.53
11:L:335:VAL:O	11:L:339:VAL:HG23	2.09	0.53
22:P:602:CLA:HMB1	22:P:602:CLA:HBB1	1.90	0.53
11:R:354:HIS:HB2	11:R:358:HIS:CE1	2.43	0.53
8:N:216:GLU:N	8:N:216:GLU:OE1	2.41	0.53
1:B:431:PHE:HZ	21:B:801:BCR:H341	1.74	0.53
13:O:227:THR:O	13:O:231:GLU:HG2	2.09	0.53
22:R:605:CLA:O2A	22:R:605:CLA:H2A	2.09	0.52
33:A:802:CL0:H2	33:A:802:CL0:CBB	2.36	0.52
5:F:164:LYS:HA	5:F:167:LYS:HE2	1.90	0.52
11:L:351:HIS:CD2	22:L:412:CLA:NC	2.78	0.52
10:Q:458:ARG:NH2	11:R:364:VAL:O	2.39	0.52
18:W:303:PHE:HE1	22:W:409:CLA:HBA2	1.75	0.52
22:W:414:CLA:H202	22:W:415:CLA:HBC1	1.91	0.52
31:W:407:CHL:C3C	31:W:408:CHL:HBC3	2.39	0.52
10:K:486:LYS:HD2	10:K:486:LYS:N	2.24	0.52
11:L:301:ASN:OD1	11:L:301:ASN:N	2.39	0.52
11:L:315:THR:HG22	22:L:408:CLA:HHB	1.91	0.52
6:P:395:GLY:HA2	6:P:400:ASP:HB3	1.90	0.52
1:B:292:ARG:HG3	1:B:299:HIS:N	2.25	0.52
1:B:528:HIS:CD2	22:B:836:CLA:NB	2.77	0.52
22:B:806:CLA:H43	27:B:855:LMU:H111	1.92	0.52
6:G:530:GLU:OE1	6:G:530:GLU:N	2.43	0.52
15:T:261:LYS:H	27:A:857:LMU:H2'	1.74	0.52
28:W:401:LMG:H341	31:W:408:CHL:C4	2.39	0.52
20:A:308:ALA:HB2	22:A:822:CLA:HBC2	1.92	0.52
6:P:542:ASN:O	6:P:543:PRO:C	2.52	0.51
1:B:467:HIS:CD2	22:B:833:CLA:ND	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:189:THR:HG22	22:I:607:CLA:HBB	1.91	0.51
33:A:802:CL0:H13	22:A:852:CLA:OBD	2.09	0.51
1:B:278:LEU:O	1:B:278:LEU:HG	2.09	0.51
1:B:418:ILE:HG23	22:B:836:CLA:HBB2	1.91	0.51
6:G:546:ALA:HB1	22:G:610:CLA:HED1	1.92	0.51
17:V:224:TRP:CZ3	31:V:606:CHL:HMA1	2.45	0.51
1:B:512:ILE:HG22	1:B:516:ASP:OD2	2.10	0.51
6:P:457:ILE:HG23	10:Q:461:LEU:HD12	1.92	0.51
10:Q:425:ASN:ND2	22:Q:604:CLA:HBB2	2.24	0.51
31:V:605:CHL:HBC2	31:V:606:CHL:HBC3	1.92	0.51
1:B:285:ILE:HG22	1:B:285:ILE:O	2.10	0.51
30:O:302:SQD:H132	22:O:308:CLA:CBC	2.41	0.51
6:P:382:VAL:HG22	6:P:383:TRP:CD2	2.45	0.51
20:A:57:HIS:HE1	22:A:806:CLA:NB	2.05	0.51
20:A:199:ASN:HB3	22:A:821:CLA:HMD1	1.93	0.51
6:P:539:HIS:O	6:P:540:LEU:C	2.54	0.51
11:R:236:SER:HB2	22:R:606:CLA:HED3	1.91	0.51
17:V:189:PHE:CD2	22:V:602:CLA:H12	2.46	0.51
30:O:302:SQD:H132	22:O:308:CLA:HBC2	1.93	0.51
10:K:492:PRO:HB3	22:K:606:CLA:HBC2	1.92	0.51
14:S:104:THR:O	14:S:108:MET:HG2	2.11	0.50
22:A:806:CLA:HBD	22:A:813:CLA:H2	1.92	0.50
1:B:299:HIS:HD1	1:B:304:ILE:HD11	1.76	0.50
21:B:843:BCR:H311	22:Q:613:CLA:HBB2	1.94	0.50
6:P:414:VAL:HG22	6:P:418:MET:SD	2.51	0.50
17:V:318:GLY:O	17:V:322:GLN:HG3	2.12	0.50
1:B:559:CYS:SG	20:A:578:PRO:HG3	2.51	0.50
16:U:267:TRP:HH2	32:U:418:NEX:C19	2.24	0.50
22:B:815:CLA:CHA	22:B:815:CLA:HBA1	2.41	0.50
11:L:348:LEU:HD13	22:L:412:CLA:HBC2	1.93	0.50
25:O:304:DGD:O1A	25:O:304:DGD:HE5	2.11	0.50
6:P:494:ASP:OD2	6:P:499:THR:OG1	2.29	0.50
14:S:72:VAL:HG11	14:S:77:ALA:HB3	1.92	0.50
16:U:188:LYS:HZ1	22:U:405:CLA:HBA1	1.75	0.50
26:K:616:LHG:O1	26:K:616:LHG:O3	2.26	0.50
22:S:610:CLA:HBA1	22:S:610:CLA:HBD	1.92	0.50
10:Q:524:VAL:HG11	22:Q:612:CLA:HAC2	1.94	0.50
22:V:601:CLA:HAA2	22:V:601:CLA:HED2	1.93	0.50
20:A:37:ARG:H	20:A:37:ARG:HD2	1.77	0.50
20:A:408:HIS:HE1	22:A:831:CLA:C4A	2.24	0.50
1:B:521:HIS:CD2	22:B:835:CLA:NB	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:50:TRP:O	20:A:51:ASN:HB2	2.12	0.50
1:B:283:LEU:O	1:B:285:ILE:N	2.46	0.49
22:L:408:CLA:H51	22:L:410:CLA:HMA3	1.92	0.49
8:N:158:TYR:CE2	22:O:309:CLA:HBA1	2.47	0.49
14:S:204:LYS:O	14:S:208:ILE:HD12	2.11	0.49
31:U:407:CHL:O2A	32:U:418:NEX:H403	2.12	0.49
13:O:229:LEU:HD13	22:O:314:CLA:HBC2	1.94	0.49
22:V:604:CLA:C1B	32:V:616:NEX:H383	2.42	0.49
11:R:243:LEU:HD13	22:R:606:CLA:HMD3	1.94	0.49
16:U:267:TRP:HH2	32:U:418:NEX:H191	1.78	0.49
1:B:297:ILE:HG13	22:B:819:CLA:HED2	1.93	0.49
11:L:370:VAL:HG22	11:L:371:ALA:N	2.27	0.49
12:M:20:PHE:CE2	22:O:311:CLA:H11	2.47	0.49
13:O:163:GLU:HG2	22:O:309:CLA:C1B	2.42	0.49
20:A:29:TRP:HH2	22:A:806:CLA:H42	1.76	0.49
22:B:830:CLA:HMB1	22:B:830:CLA:HBB1	1.94	0.49
26:B:851:LHG:H112	27:L:419:LMU:H1'	1.94	0.49
19:X:174:ALA:HB2	19:X:181:PHE:HD2	1.77	0.49
17:V:225:TYR:HA	31:V:606:CHL:CMA	2.42	0.49
22:F:403:CLA:H142	9:J:20:VAL:HG13	1.95	0.49
22:A:825:CLA:H141	26:A:846:LHG:H192	1.93	0.49
22:B:809:CLA:CMA	27:B:854:LMU:H71	2.42	0.49
28:W:401:LMG:H341	31:W:408:CHL:H42	1.95	0.49
6:G:511:GLY:O	6:G:515:MET:HG3	2.13	0.49
8:N:189:THR:HG22	22:N:607:CLA:HHB	1.94	0.49
1:B:292:ARG:HD3	1:B:300:ARG:HD2	1.95	0.49
3:D:272:LYS:HG3	3:D:273:ASP:OD2	2.13	0.49
5:F:251:TYR:CE2	22:F:404:CLA:HBA1	2.48	0.49
11:L:346:VAL:O	11:L:350:GLU:HG2	2.13	0.49
22:X:404:CLA:H13	22:X:408:CLA:H112	1.93	0.49
20:A:57:HIS:HE1	22:A:806:CLA:C4B	2.26	0.49
8:I:173:ASP:OD1	8:I:174:ARG:N	2.45	0.48
28:K:601:LMG:O5	28:K:601:LMG:O4	2.28	0.48
22:N:606:CLA:H121	22:O:315:CLA:HAB	1.94	0.48
17:V:313:MET:HE1	22:V:602:CLA:HHC	1.94	0.48
17:V:321:ALA:O	17:V:325:VAL:HG22	2.13	0.48
1:B:292:ARG:HA	1:B:297:ILE:O	2.13	0.48
22:K:605:CLA:H151	22:K:605:CLA:H112	1.53	0.48
22:R:601:CLA:O1A	26:R:614:LHG:O2	2.31	0.48
14:S:164:MET:HE2	14:S:164:MET:HA	1.94	0.48
1:B:29:HIS:HE1	22:B:803:CLA:C4B	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:407:SQD:H151	22:X:403:CLA:H93	1.95	0.48
18:W:284:GLU:O	18:W:296:LYS:NZ	2.39	0.48
1:B:292:ARG:HG2	1:B:298:GLY:CA	2.44	0.48
22:K:604:CLA:HED3	22:K:607:CLA:H43	1.95	0.48
11:R:347:ASN:HB3	22:R:610:CLA:HED2	1.95	0.48
22:B:809:CLA:H43	11:L:352:VAL:HG21	1.94	0.48
8:N:116:MET:O	8:N:120:VAL:HG23	2.14	0.48
22:V:608:CLA:HBA2	22:V:608:CLA:H3A	1.61	0.48
22:B:823:CLA:H171	22:B:823:CLA:H13	1.63	0.48
26:B:851:LHG:H252	27:B:854:LMU:H22	1.96	0.48
17:V:267:TRP:O	17:V:271:GLY:N	2.41	0.48
17:V:267:TRP:CD1	17:V:273:ILE:HA	2.49	0.48
1:B:172:GLU:OE2	1:B:301:ILE:HG13	2.13	0.48
11:R:254:PRO:O	11:R:258:GLY:N	2.47	0.48
26:W:420:LHG:HC81	26:W:420:LHG:H111	1.56	0.48
22:A:832:CLA:H62	26:A:846:LHG:H131	1.96	0.48
22:B:834:CLA:H142	22:B:839:CLA:H193	1.95	0.48
22:K:605:CLA:H3A	22:K:605:CLA:HBA2	1.45	0.48
13:O:195:GLU:OE2	27:O:301:LMU:H2'	2.13	0.48
6:P:496:LEU:HB2	6:P:498:LEU:HD23	1.95	0.48
19:X:197:GLU:OE1	19:X:197:GLU:N	2.41	0.48
1:B:308:HIS:HE1	22:B:821:CLA:ND	2.09	0.48
1:B:435:GLY:HA3	22:B:832:CLA:HAB	1.96	0.48
22:L:411:CLA:H2	22:L:411:CLA:H61	1.67	0.48
17:V:222:PRO:HB3	17:V:226:GLU:HB2	1.95	0.48
22:A:803:CLA:H142	21:A:851:BCR:H23C	1.96	0.48
1:B:98:GLN:HB3	1:B:99:PRO:HD3	1.96	0.47
1:B:576:PHE:O	1:B:580:VAL:HG23	2.14	0.47
22:L:402:CLA:H41	22:L:402:CLA:H61	1.48	0.47
20:A:370:HIS:CD2	22:A:828:CLA:NC	2.81	0.47
1:B:277:HIS:HA	1:B:280:ILE:HG12	1.95	0.47
1:B:286:VAL:HG12	1:B:286:VAL:O	2.14	0.47
22:B:831:CLA:H62	22:B:831:CLA:H2	1.67	0.47
6:P:424:PHE:O	6:P:425:HIS:C	2.54	0.47
22:P:605:CLA:HBA1	22:P:605:CLA:H3A	1.50	0.47
26:B:851:LHG:H262	27:B:854:LMU:H22	1.96	0.47
22:K:604:CLA:H143	22:K:604:CLA:H162	1.76	0.47
1:B:193:HIS:HB2	22:B:813:CLA:C1C	2.44	0.47
7:H:169:LEU:HD11	22:H:312:CLA:HMC2	1.96	0.47
8:I:78:HIS:NE2	8:I:90:ASP:OD2	2.41	0.47
6:P:397:TYR:O	6:P:400:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:216:LEU:HB3	17:V:218:ILE:HG12	1.97	0.47
17:V:325:VAL:HG21	22:V:612:CLA:HMD2	1.97	0.47
27:O:301:LMU:H102	22:O:312:CLA:H2	1.97	0.47
31:V:605:CHL:CMC	31:V:606:CHL:NC	2.77	0.47
20:A:393:HIS:HE1	22:A:829:CLA:C1D	2.15	0.47
1:B:74:PHE:O	1:B:78:ILE:HG12	2.14	0.47
22:F:404:CLA:H91	22:W:410:CLA:H143	1.96	0.47
11:L:305:PHE:CE2	26:O:321:LHG:H361	2.49	0.47
22:S:608:CLA:NB	26:S:613:LHG:O4	2.48	0.47
20:A:178:TRP:HB2	22:A:813:CLA:CMC	2.45	0.47
1:B:283:LEU:C	1:B:285:ILE:H	2.21	0.47
22:B:806:CLA:H2	22:B:806:CLA:H61	1.63	0.47
22:B:816:CLA:H3A	22:B:816:CLA:HBA2	1.46	0.47
22:B:822:CLA:O1A	21:B:844:BCR:H14C	2.15	0.47
22:B:834:CLA:H41	22:B:834:CLA:H61	1.67	0.47
25:B:847:DGD:HB82	25:B:847:DGD:HBE1	1.49	0.47
28:B:856:LMG:H342	28:B:856:LMG:H202	1.97	0.47
5:F:289:TRP:HE1	30:F:407:SQD:H462	1.79	0.47
25:F:401:DGD:HAF2	25:F:401:DGD:HAV2	1.63	0.47
22:F:403:CLA:H162	22:F:403:CLA:H122	1.62	0.47
8:I:155:PRO:HG2	22:K:607:CLA:H72	1.96	0.47
8:N:67:GLY:HA3	22:N:601:CLA:HED2	1.96	0.47
22:R:601:CLA:H171	22:R:601:CLA:H13	1.65	0.47
16:U:337:HIS:CD2	22:U:415:CLA:NC	2.82	0.47
17:V:154:TRP:CE3	22:V:601:CLA:HAA1	2.50	0.47
17:V:273:ILE:HD11	22:V:607:CLA:HAB	1.97	0.47
22:N:610:CLA:HBA1	22:N:610:CLA:CBD	2.43	0.47
11:R:228:LYS:H	11:R:228:LYS:HD3	1.80	0.47
18:W:319:LYS:O	18:W:323:VAL:HG23	2.14	0.47
6:G:455:ASP:OD1	6:G:455:ASP:N	2.46	0.47
22:G:608:CLA:H121	22:G:609:CLA:C4B	2.45	0.47
22:H:311:CLA:HBB1	22:H:311:CLA:H8	1.97	0.47
6:P:422:GLU:O	6:P:423:VAL:C	2.56	0.47
20:A:274:ASP:N	20:A:274:ASP:OD1	2.47	0.47
20:A:506:THR:HG22	20:A:507:THR:HG22	1.96	0.47
12:M:13:LEU:HD21	21:M:101:BCR:H281	1.96	0.47
22:O:308:CLA:H2	10:Q:550:GLY:O	2.15	0.47
15:T:261:LYS:HE2	15:T:261:LYS:HA	1.96	0.46
27:T:618:LMU:H12	22:A:812:CLA:H42	1.96	0.46
22:L:408:CLA:O1D	22:L:408:CLA:H2A	2.15	0.46
8:N:132:ALA:HB3	8:N:135:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:118:GLY:HA2	13:O:208:MET:HE2	1.97	0.46
17:V:189:PHE:HD2	22:V:602:CLA:H12	1.79	0.46
31:W:407:CHL:C1C	31:W:408:CHL:HBC2	2.45	0.46
1:B:351:HIS:HE1	22:B:825:CLA:C1B	2.13	0.46
30:O:302:SQD:H241	30:O:302:SQD:H462	1.47	0.46
11:R:350:GLU:HB3	11:R:358:HIS:CG	2.50	0.46
22:R:604:CLA:HBB	22:R:605:CLA:H152	1.97	0.46
17:V:267:TRP:HH2	32:V:616:NEX:H192	1.79	0.46
18:W:311:ASP:N	18:W:311:ASP:OD2	2.48	0.46
6:P:507:GLU:CD	22:P:607:CLA:NB	2.72	0.46
10:Q:463:SER:O	10:Q:467:VAL:HG23	2.16	0.46
22:Q:605:CLA:H61	22:Q:605:CLA:H2	1.59	0.46
11:R:365:MET:HE3	11:R:365:MET:HA	1.97	0.46
7:H:131:ASP:OD2	7:H:135:ARG:NH1	2.47	0.46
8:I:183:LYS:HE2	8:I:183:LYS:H	1.81	0.46
11:L:285:VAL:HG22	17:V:259:LEU:HA	1.98	0.46
8:N:222:LEU:O	8:N:226:LEU:HB2	2.16	0.46
11:R:264:GLU:O	11:R:268:ASN:ND2	2.48	0.46
31:V:605:CHL:CMC	31:V:606:CHL:C3C	2.93	0.46
22:A:822:CLA:H141	22:A:822:CLA:H162	1.74	0.46
22:B:807:CLA:H8	22:B:807:CLA:HBB1	1.98	0.46
25:B:847:DGD:HBW1	25:B:847:DGD:HGB3	1.97	0.46
6:G:418:MET:HE1	22:G:602:CLA:H43	1.96	0.46
22:I:611:CLA:HAC2	28:I:615:LMG:H401	1.97	0.46
22:S:605:CLA:H8	22:S:605:CLA:C2C	2.46	0.46
17:V:260:LEU:HD12	17:V:260:LEU:H	1.81	0.46
18:W:191:LEU:HD13	22:W:404:CLA:H42	1.97	0.46
1:B:132:ASN:HB2	12:M:1:MET:HE2	1.97	0.46
1:B:636:ASN:HB2	1:B:637:PRO:HD2	1.97	0.46
11:L:366:HIS:O	11:L:367:GLN:C	2.58	0.46
11:R:262:TRP:CH2	11:R:337:ARG:HD3	2.50	0.46
28:J:101:LMG:H232	28:J:101:LMG:H262	1.77	0.46
22:K:604:CLA:HMD3	22:K:607:CLA:ND	2.30	0.46
22:K:613:CLA:H2	22:K:613:CLA:H61	1.68	0.46
6:P:382:VAL:HG22	6:P:383:TRP:H	1.80	0.46
11:R:300:LYS:HD3	11:R:300:LYS:HA	1.80	0.46
20:A:730:HIS:HE1	22:A:842:CLA:C4D	2.29	0.46
1:B:395:ILE:HD12	1:B:555:TYR:HD1	1.81	0.46
1:B:422:LEU:O	1:B:426:THR:HG23	2.16	0.46
22:B:818:CLA:HBB1	22:B:818:CLA:HMB3	1.97	0.46
22:B:829:CLA:HBA2	22:B:829:CLA:H3A	1.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:508:GLU:OE2	22:K:608:CLA:NB	2.48	0.46
11:R:287:GLU:HG2	11:R:290:ARG:HH12	1.80	0.46
16:U:278:LYS:HD2	16:U:278:LYS:N	2.31	0.46
17:V:290:PHE:O	17:V:292:PRO:HD3	2.15	0.46
20:A:91:MET:HE2	20:A:91:MET:HA	1.98	0.46
1:B:292:ARG:HB3	1:B:292:ARG:CZ	2.45	0.46
27:B:854:LMU:H51	27:B:854:LMU:H22	1.82	0.46
13:O:135:PHE:CE2	30:O:302:SQD:H111	2.51	0.46
6:P:472:TYR:CE2	22:Q:608:CLA:HBA1	2.50	0.46
18:W:217:LEU:HB3	22:W:406:CLA:HMC2	1.97	0.46
21:B:845:BCR:H15C	21:B:845:BCR:H351	1.72	0.45
22:G:603:CLA:H101	22:K:603:CLA:C15	2.46	0.45
22:K:604:CLA:H91	22:K:604:CLA:H111	1.62	0.45
13:O:74:LEU:HD13	13:O:79:ALA:HB3	1.98	0.45
11:R:195:ARG:O	11:R:196:PRO:C	2.58	0.45
11:R:248:ILE:CA	11:R:330:MET:HE1	2.47	0.45
14:S:98:LEU:HD13	22:S:602:CLA:H42	1.98	0.45
17:V:247:ALA:HB1	17:V:253:ILE:HD11	1.97	0.45
20:A:37:ARG:H	20:A:37:ARG:CD	2.29	0.45
1:B:144:PHE:HD1	28:B:856:LMG:H242	1.81	0.45
27:K:620:LMU:H102	26:L:416:LHG:H141	1.98	0.45
22:L:408:CLA:HMB2	22:L:408:CLA:H2	1.98	0.45
14:S:184:GLU:C	14:S:185:LYS:HD2	2.41	0.45
18:W:371:ALA:HB2	31:W:422:CHL:HAA2	1.97	0.45
20:A:520:LYS:HE2	20:A:520:LYS:HB3	1.77	0.45
22:A:814:CLA:H161	22:A:814:CLA:H141	1.67	0.45
21:B:844:BCR:HC42	28:U:402:LMG:H182	1.99	0.45
11:L:288:VAL:O	11:L:292:LEU:HG	2.16	0.45
13:O:105:LYS:HD2	13:O:105:LYS:HA	1.65	0.45
10:Q:541:LEU:HD23	10:Q:541:LEU:HA	1.73	0.45
11:R:271:ILE:HD11	11:R:276:VAL:HG22	1.98	0.45
20:A:343:GLU:OE1	20:A:343:GLU:N	2.48	0.45
22:A:817:CLA:H141	22:A:817:CLA:H161	1.64	0.45
1:B:474:LEU:HD11	5:F:154:LEU:HD23	1.97	0.45
27:B:858:LMU:H52	27:B:858:LMU:H81	1.76	0.45
3:D:240:LYS:HE3	3:D:240:LYS:HB3	1.66	0.45
22:A:844:CLA:HBA1	22:A:844:CLA:H3A	1.45	0.45
22:B:835:CLA:HBB1	22:B:835:CLA:HMB3	1.97	0.45
10:K:474:ARG:HG3	22:K:606:CLA:CHD	2.47	0.45
22:S:605:CLA:H62	22:S:605:CLA:H41	1.75	0.45
20:A:338:HIS:CD2	22:A:825:CLA:ND	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ARG:HB3	1:B:602:TRP:CZ3	2.51	0.45
22:B:806:CLA:H141	22:B:806:CLA:H162	1.72	0.45
21:B:846:BCR:H15C	21:B:846:BCR:H351	1.85	0.45
26:B:851:LHG:H262	27:B:854:LMU:C2	2.46	0.45
8:N:70:PHE:CG	8:N:71:PRO:HD2	2.52	0.45
6:P:406:LEU:HB2	6:P:408:LEU:HG	1.98	0.45
19:X:101:LEU:HD11	19:X:260:THR:HG23	1.99	0.45
22:A:842:CLA:O1A	26:A:845:LHG:H131	2.17	0.45
22:B:810:CLA:H61	22:B:810:CLA:H92	1.70	0.45
25:B:847:DGD:O2D	25:B:847:DGD:HG31	2.16	0.45
4:E:94:ARG:HB3	4:E:94:ARG:NH1	2.32	0.45
6:G:539:HIS:CD2	22:G:611:CLA:NC	2.85	0.45
22:K:609:CLA:CHB	22:A:844:CLA:H42	2.46	0.45
13:O:183:TYR:HB3	22:O:310:CLA:HED2	1.98	0.45
6:P:510:ASN:O	6:P:513:LEU:HG	2.16	0.45
11:R:317:GLU:O	11:R:321:LYS:HG3	2.17	0.45
22:R:611:CLA:H3A	22:R:611:CLA:HBA2	1.48	0.45
14:S:210:ASN:ND2	22:S:609:CLA:NB	2.65	0.45
20:A:522:ALA:O	20:A:523:MET:HE2	2.17	0.45
22:B:805:CLA:H203	22:B:805:CLA:H161	1.84	0.45
8:I:193:GLU:HG3	22:I:607:CLA:C1B	2.47	0.45
26:N:616:LHG:H122	26:N:616:LHG:H152	1.83	0.45
13:O:171:PHE:CE2	10:Q:383:TRP:CH2	3.05	0.45
22:Q:611:CLA:H2	22:Q:611:CLA:H62	1.62	0.45
22:R:604:CLA:C3A	22:R:605:CLA:H152	2.45	0.45
22:W:404:CLA:H142	22:W:404:CLA:H112	1.78	0.45
31:W:407:CHL:C2C	31:W:408:CHL:HBC3	2.46	0.45
22:L:409:CLA:H143	27:L:419:LMU:H121	1.98	0.45
8:N:189:THR:HG21	22:N:607:CLA:H12	1.98	0.45
22:R:601:CLA:H52	26:R:614:LHG:H101	1.99	0.45
22:T:604:CLA:H142	22:T:604:CLA:H111	1.76	0.45
17:V:310:ARG:O	17:V:314:VAL:HG23	2.17	0.45
22:A:817:CLA:H62	22:A:817:CLA:H102	1.79	0.45
1:B:583:MET:O	1:B:587:ILE:HG12	2.17	0.45
17:V:297:ALA:HB1	17:V:302:LYS:HE3	1.98	0.45
22:B:804:CLA:H61	22:B:804:CLA:H2	1.67	0.44
18:W:303:PHE:CE2	22:W:409:CLA:NC	2.85	0.44
10:K:487:TYR:CE1	11:L:201:GLY:HA3	2.53	0.44
11:L:368:TRP:CH2	11:L:370:VAL:HA	2.53	0.44
8:N:115:SER:CB	8:N:201:MET:HG2	2.48	0.44
10:Q:426:GLY:HA2	10:Q:516:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:604:CLA:HMB1	22:R:605:CLA:H162	1.98	0.44
14:S:75:PRO:HD3	22:S:601:CLA:HMA1	2.00	0.44
1:B:656:VAL:HG23	1:B:716:GLY:HA2	1.98	0.44
2:C:29:VAL:HG12	3:D:245:ARG:HB3	2.00	0.44
11:L:245:MET:SD	22:L:408:CLA:HAB	2.57	0.44
10:Q:546:ALA:HB2	28:Q:602:LMG:HC5	1.99	0.44
20:A:169:PHE:O	20:A:172:VAL:HG22	2.17	0.44
22:A:824:CLA:H91	22:A:824:CLA:H111	1.60	0.44
1:B:89:HIS:CD2	22:B:807:CLA:NA	2.85	0.44
1:B:276:HIS:O	1:B:280:ILE:HG23	2.16	0.44
22:K:607:CLA:HHC	22:K:607:CLA:CBB	2.47	0.44
8:N:150:MET:HE3	8:N:150:MET:HB3	1.80	0.44
17:V:168:PHE:CE2	17:V:190:ARG:HD2	2.52	0.44
17:V:180:ALA:HB2	22:V:602:CLA:HAA2	1.99	0.44
19:X:207:LEU:O	19:X:209:HIS:N	2.51	0.44
21:B:801:BCR:H331	21:B:801:BCR:C8	2.48	0.44
22:B:839:CLA:HBA1	26:B:848:LHG:HC41	2.00	0.44
21:B:843:BCR:H24C	21:B:843:BCR:H371	1.61	0.44
22:H:305:CLA:HBA2	22:H:305:CLA:H3A	1.79	0.44
22:I:601:CLA:H61	22:I:601:CLA:H2	1.79	0.44
10:K:549:ILE:HG21	22:K:611:CLA:H42	1.98	0.44
10:Q:384:PHE:HD2	10:Q:387:ILE:HD13	1.82	0.44
11:R:253:VAL:HA	11:R:256:ILE:HD12	1.98	0.44
28:U:402:LMG:H392	28:U:402:LMG:H362	1.81	0.44
22:U:415:CLA:H3A	22:U:415:CLA:HBA2	1.44	0.44
20:A:14:ARG:HG2	20:A:15:VAL:H	1.82	0.44
22:A:833:CLA:H162	22:A:833:CLA:H121	1.77	0.44
1:B:420:SER:HB2	22:A:841:CLA:HED2	1.99	0.44
21:B:844:BCR:H15C	21:B:844:BCR:H351	1.82	0.44
6:P:509:LYS:HA	6:P:512:ARG:HD2	1.99	0.44
22:T:605:CLA:H62	22:T:605:CLA:H41	1.67	0.44
22:U:404:CLA:HMB1	22:U:404:CLA:HBB1	2.00	0.44
22:B:820:CLA:H62	22:B:820:CLA:H41	1.53	0.44
7:H:131:ASP:O	7:H:135:ARG:HG3	2.18	0.44
22:K:613:CLA:H42	11:L:370:VAL:HG23	2.00	0.44
22:L:417:CLA:H202	22:L:417:CLA:H162	1.83	0.44
11:R:196:PRO:HB2	22:R:601:CLA:HED2	2.00	0.44
11:R:232:ARG:HG3	11:R:233:MET:N	2.32	0.44
14:S:113:VAL:HG12	14:S:117:ARG:HD2	1.99	0.44
31:W:407:CHL:CBC	31:W:408:CHL:HBC3	2.48	0.44
20:A:51:ASN:N	20:A:51:ASN:HD22	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:820:CLA:HAB	22:A:820:CLA:H8	2.00	0.44
22:A:832:CLA:H41	22:A:832:CLA:H61	1.78	0.44
1:B:652:PHE:O	1:B:656:VAL:HG22	2.17	0.44
22:B:828:CLA:H162	22:B:828:CLA:H141	1.78	0.44
25:B:847:DGD:HA51	25:B:847:DGD:HA21	1.40	0.44
10:Q:542:ARG:HH11	10:Q:542:ARG:HG2	1.83	0.44
22:T:605:CLA:H162	22:T:605:CLA:H192	1.74	0.44
22:T:611:CLA:HBA1	22:T:611:CLA:H3A	1.44	0.44
2:C:77:MET:HE3	2:C:77:MET:HB3	1.90	0.44
22:H:313:CLA:H62	22:H:313:CLA:H41	1.87	0.44
11:L:228:LYS:HB3	11:L:228:LYS:HE3	1.80	0.44
6:P:536:LEU:HD12	6:P:536:LEU:HA	1.81	0.44
22:P:606:CLA:HBA1	22:P:606:CLA:H3A	1.68	0.44
16:U:290:PHE:CE2	22:U:409:CLA:NC	2.86	0.44
28:U:423:LMG:H142	28:U:423:LMG:H111	1.79	0.44
17:V:267:TRP:CH2	32:V:616:NEX:H192	2.53	0.44
22:V:609:CLA:H62	22:V:609:CLA:H41	1.85	0.44
22:A:824:CLA:H141	22:A:828:CLA:H151	2.00	0.44
8:I:154:ALA:HB3	8:I:155:PRO:HD3	2.00	0.43
8:I:222:LEU:CD1	22:I:611:CLA:HBC2	2.42	0.43
11:L:263:TYR:CD2	11:L:337:ARG:HD2	2.52	0.43
22:W:402:CLA:H41	22:W:402:CLA:H62	1.72	0.43
20:A:626:LYS:HE2	20:A:626:LYS:N	2.33	0.43
22:A:814:CLA:H41	22:A:814:CLA:H62	1.70	0.43
22:F:404:CLA:H62	22:F:404:CLA:H41	1.74	0.43
6:P:409:ALA:HB1	6:P:415:TYR:HD1	1.82	0.43
14:S:103:ALA:O	14:S:106:GLU:HG3	2.18	0.43
17:V:238:TYR:CD1	17:V:239:LEU:HG	2.53	0.43
22:X:419:CLA:H3A	22:X:419:CLA:HBA1	1.62	0.43
20:A:204:GLY:O	20:A:208:LEU:HB2	2.18	0.43
20:A:320:HIS:HE1	22:A:823:CLA:C4A	2.32	0.43
1:B:136:TYR:CZ	12:M:7:GLN:HB3	2.53	0.43
1:B:178:HIS:O	1:B:182:LEU:HB3	2.18	0.43
22:B:833:CLA:H192	22:B:833:CLA:H162	1.69	0.43
13:O:163:GLU:HG2	22:O:309:CLA:NB	2.32	0.43
6:G:383:TRP:O	22:G:601:CLA:NA	2.51	0.43
25:O:304:DGD:HA52	25:O:304:DGD:HA81	1.31	0.43
10:Q:509:ILE:HG22	10:Q:513:ARG:HE	1.84	0.43
22:R:601:CLA:H41	22:R:601:CLA:H62	1.44	0.43
16:U:238:TYR:HB3	16:U:244:LEU:HD13	1.99	0.43
17:V:224:TRP:HE3	17:V:225:TYR:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:409:CLA:H162	22:X:409:CLA:H122	1.73	0.43
22:A:805:CLA:H92	22:A:805:CLA:H62	1.73	0.43
22:A:852:CLA:H161	22:A:852:CLA:H141	1.79	0.43
1:B:91:ILE:HD12	1:B:112:PRO:HB2	2.00	0.43
1:B:208:ARG:O	1:B:212:PHE:HB3	2.18	0.43
22:B:824:CLA:HAA2	22:B:825:CLA:OBD	2.18	0.43
25:B:847:DGD:HE61	25:B:847:DGD:HE1	1.68	0.43
3:D:95:GLN:OE1	3:D:95:GLN:N	2.49	0.43
22:L:410:CLA:HMA1	22:L:410:CLA:H2	2.01	0.43
22:U:411:CLA:H92	22:U:411:CLA:H61	1.71	0.43
17:V:238:TYR:HB3	17:V:244:LEU:HD12	2.01	0.43
22:W:411:CLA:H41	22:W:411:CLA:H62	1.77	0.43
22:B:827:CLA:H92	22:B:827:CLA:H61	1.81	0.43
22:H:307:CLA:H61	22:H:307:CLA:H2	1.67	0.43
8:N:141:ASP:OD1	8:N:144:LYS:HB3	2.18	0.43
22:N:603:CLA:H141	22:N:603:CLA:H161	1.78	0.43
22:N:603:CLA:H142	22:N:603:CLA:H112	1.86	0.43
22:O:313:CLA:H92	22:O:313:CLA:H61	1.77	0.43
22:O:313:CLA:H161	22:O:313:CLA:H141	1.66	0.43
18:W:174:GLU:N	18:W:174:GLU:OE1	2.51	0.43
20:A:671:MET:HE3	20:A:671:MET:HB3	1.76	0.43
21:A:849:BCR:H24C	21:A:849:BCR:H371	1.77	0.43
1:B:439:HIS:HE1	22:B:832:CLA:C1A	2.16	0.43
12:M:20:PHE:CG	22:O:311:CLA:H42	2.53	0.43
13:O:189:LEU:HD12	13:O:191:LEU:HD11	2.00	0.43
22:U:405:CLA:H51	27:U:421:LMU:H82	2.00	0.43
22:V:603:CLA:H112	22:V:603:CLA:H72	1.89	0.43
22:W:406:CLA:H101	22:W:409:CLA:H151	2.01	0.43
22:A:801:CLA:H62	22:A:801:CLA:H41	1.77	0.43
21:B:801:BCR:H12C	23:A:843:PQN:H291	2.01	0.43
22:B:804:CLA:H162	22:B:804:CLA:H141	1.75	0.43
10:K:508:GLU:HG3	22:K:608:CLA:C1B	2.49	0.43
26:K:616:LHG:H272	26:K:616:LHG:H242	1.80	0.43
22:O:313:CLA:H111	22:O:313:CLA:H71	1.56	0.43
11:R:195:ARG:NH2	11:R:210:GLY:H	2.13	0.43
22:R:601:CLA:H111	22:R:601:CLA:H72	1.59	0.43
22:R:615:CLA:HBA1	22:R:615:CLA:H3A	1.80	0.43
17:V:224:TRP:CE3	17:V:225:TYR:HB3	2.54	0.43
22:V:604:CLA:H93	22:V:604:CLA:H62	1.71	0.43
22:B:817:CLA:H141	22:B:817:CLA:H161	1.83	0.43
27:H:301:LMU:H31	28:H:322:LMG:H112	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:614:LHG:H271	26:T:614:LHG:H242	1.86	0.43
22:V:601:CLA:HED2	22:V:601:CLA:HBD	1.69	0.43
22:A:844:CLA:H61	22:A:844:CLA:H92	1.80	0.43
1:B:308:HIS:HE1	22:B:821:CLA:C4D	2.31	0.43
22:B:830:CLA:H201	22:W:410:CLA:H91	2.01	0.43
6:G:464:MET:CE	7:H:93:GLN:HG3	2.48	0.43
22:G:608:CLA:H62	22:G:608:CLA:H41	1.49	0.43
22:K:605:CLA:H112	22:K:605:CLA:H91	1.76	0.43
13:O:82:PRO:HG2	13:O:85:LEU:HD12	2.01	0.43
22:R:607:CLA:H91	22:R:607:CLA:H111	1.77	0.43
17:V:238:TYR:HD1	17:V:239:LEU:HG	1.83	0.43
20:A:681:PHE:HZ	22:A:842:CLA:HBC2	1.83	0.43
22:A:840:CLA:H112	22:A:840:CLA:H143	1.74	0.43
25:F:401:DGD:HA32	9:J:42:ILE:HG22	2.01	0.42
22:O:308:CLA:HBA2	22:O:308:CLA:H3A	1.85	0.42
6:P:524:GLN:OE1	22:P:610:CLA:C1A	2.67	0.42
22:V:612:CLA:H111	22:V:612:CLA:H91	1.81	0.42
20:A:418:ASP:O	20:A:422:ASN:ND2	2.48	0.42
33:A:802:CL0:CMB	22:A:852:CLA:OBD	2.66	0.42
21:A:848:BCR:H11C	21:A:848:BCR:H341	1.80	0.42
1:B:67:HIS:HE1	22:B:806:CLA:C4D	2.32	0.42
4:E:92:PRO:HB2	4:E:114:VAL:HG21	2.02	0.42
28:F:408:LMG:H132	27:U:424:LMU:H21	2.01	0.42
22:I:601:CLA:CHA	22:I:601:CLA:HBA1	2.50	0.42
22:I:603:CLA:H2	22:I:603:CLA:H61	1.76	0.42
13:O:194:GLU:OE1	13:O:194:GLU:N	2.52	0.42
6:P:426:ALA:HB1	6:P:511:GLY:HA3	2.00	0.42
22:Q:610:CLA:H112	22:Q:610:CLA:H172	2.01	0.42
11:R:348:LEU:HD13	22:R:611:CLA:HBC2	2.01	0.42
22:T:605:CLA:H92	22:T:605:CLA:H61	1.74	0.42
17:V:209:VAL:HG21	22:V:604:CLA:HAC2	2.01	0.42
22:A:812:CLA:H61	22:A:812:CLA:H2	1.81	0.42
6:G:415:TYR:O	6:G:419:ARG:HG3	2.19	0.42
22:L:402:CLA:HBA2	26:L:416:LHG:HC81	2.00	0.42
22:S:608:CLA:C1B	26:S:613:LHG:HC32	2.50	0.42
22:W:409:CLA:H61	22:W:409:CLA:H2	1.72	0.42
22:A:808:CLA:H151	22:A:808:CLA:H112	1.44	0.42
22:A:827:CLA:HAA2	22:A:828:CLA:OBD	2.20	0.42
1:B:504:LYS:HA	1:B:504:LYS:HD3	1.86	0.42
21:B:801:BCR:H15C	21:B:801:BCR:H351	1.67	0.42
28:F:408:LMG:H152	28:F:408:LMG:H182	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F:409:LMU:H12	27:F:409:LMU:H41	1.84	0.42
22:K:604:CLA:HMD1	22:K:607:CLA:C1D	2.49	0.42
10:Q:408:LEU:HD13	22:Q:604:CLA:H42	2.00	0.42
22:S:605:CLA:H3A	22:S:605:CLA:HBA2	1.43	0.42
22:S:607:CLA:HAB	24:S:611:DD6:C24	2.49	0.42
22:T:608:CLA:CED	22:T:608:CLA:H2A	2.49	0.42
18:W:295:ASP:OD1	18:W:296:LYS:N	2.52	0.42
33:A:802:CL0:H40	22:A:804:CLA:O1D	2.20	0.42
22:A:838:CLA:H41	22:A:838:CLA:H61	1.66	0.42
6:G:433:ILE:HD13	6:G:518:LEU:HG	2.01	0.42
11:L:231:GLU:H	11:L:231:GLU:CD	2.26	0.42
22:L:408:CLA:HBB1	22:L:408:CLA:HMB1	2.01	0.42
10:Q:516:MET:HG2	24:Q:614:DD6:C5	2.50	0.42
22:Q:603:CLA:HBB1	22:Q:603:CLA:HMB3	2.00	0.42
11:R:281:ALA:O	11:R:285:VAL:HG23	2.19	0.42
22:S:606:CLA:HBA1	22:S:606:CLA:H3A	1.83	0.42
22:T:605:CLA:H142	22:T:605:CLA:H111	1.83	0.42
16:U:211:GLU:HB3	16:U:331:LEU:HD12	2.02	0.42
18:W:345:GLN:OE1	18:W:345:GLN:N	2.52	0.42
21:A:851:BCR:H361	21:A:851:BCR:H20C	1.77	0.42
21:B:842:BCR:H20C	21:B:842:BCR:H361	1.91	0.42
2:C:15:THR:O	2:C:19:ARG:HG3	2.18	0.42
4:E:120:SER:HB3	4:E:123:ILE:HG12	2.00	0.42
8:I:224:ALA:C	8:I:226:LEU:N	2.76	0.42
22:Q:604:CLA:H61	22:Q:604:CLA:H41	1.76	0.42
17:V:208:LEU:HD23	17:V:208:LEU:HA	1.86	0.42
22:B:816:CLA:H161	22:B:816:CLA:H121	1.68	0.42
22:H:308:CLA:HBB1	22:H:310:CLA:H3A	2.02	0.42
8:I:186:THR:O	8:I:190:LYS:HG3	2.20	0.42
22:I:603:CLA:H92	22:I:603:CLA:H62	1.91	0.42
26:O:321:LHG:HC62	26:O:321:LHG:H241	1.75	0.42
20:A:183:LYS:HE3	20:A:183:LYS:HB3	1.84	0.42
20:A:544:HIS:CD2	22:A:840:CLA:NB	2.86	0.42
20:A:613:LYS:HG2	22:A:838:CLA:HBC1	2.02	0.42
1:B:712:HIS:CE1	22:B:838:CLA:C4D	3.03	0.42
10:K:547:ALA:HB1	22:K:611:CLA:HED1	2.02	0.42
22:N:610:CLA:HBA1	22:N:610:CLA:CHA	2.49	0.42
15:T:304:LEU:HD11	22:T:607:CLA:HAC1	2.02	0.42
17:V:163:TRP:CD1	17:V:164:LEU:HG	2.55	0.42
17:V:290:PHE:CE1	22:V:607:CLA:NC	2.88	0.42
1:B:400:GLU:O	1:B:404:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:822:CLA:H51	22:B:823:CLA:H143	2.01	0.42
22:K:604:CLA:CMD	22:K:607:CLA:C1D	2.97	0.42
21:M:101:BCR:H24C	21:M:101:BCR:H371	1.79	0.42
8:N:178:GLY:HA2	22:N:607:CLA:CED	2.50	0.42
22:V:604:CLA:HHC	32:V:616:NEX:H362	1.96	0.42
18:W:235:GLU:HG2	18:W:240:LYS:HB3	2.02	0.42
22:A:814:CLA:H102	22:A:814:CLA:H61	1.83	0.42
1:B:137:ASN:HB3	28:B:856:LMG:H132	2.01	0.42
8:N:108:GLU:HG3	22:N:602:CLA:C1B	2.49	0.42
14:S:168:TYR:HB2	22:T:606:CLA:HAB	2.01	0.42
22:A:842:CLA:H141	22:A:842:CLA:H161	1.60	0.42
5:F:291:TRP:CG	5:F:292:PRO:HD3	2.55	0.41
22:H:311:CLA:H141	22:H:311:CLA:H161	1.87	0.41
13:O:171:PHE:HE2	10:Q:383:TRP:CH2	2.37	0.41
16:U:307:LYS:HB3	22:U:412:CLA:HMD1	2.01	0.41
16:U:347:LEU:HD23	16:U:347:LEU:HA	1.89	0.41
17:V:181:ARG:NH2	30:V:618:SQD:O8	2.53	0.41
31:W:407:CHL:C2C	31:W:408:CHL:CBC	2.97	0.41
22:A:805:CLA:H142	22:A:805:CLA:H112	1.79	0.41
22:A:815:CLA:H141	22:A:815:CLA:H162	1.90	0.41
22:B:824:CLA:H142	22:B:824:CLA:H111	1.78	0.41
21:B:844:BCR:H341	21:B:844:BCR:H11C	1.81	0.41
13:O:191:LEU:HD22	27:O:301:LMU:H72	2.01	0.41
6:P:479:PHE:HB3	26:P:601:LHG:O4	2.21	0.41
31:W:407:CHL:HAB	31:W:408:CHL:OMC	2.20	0.41
26:W:420:LHG:H131	26:W:420:LHG:H102	1.77	0.41
20:A:51:ASN:HA	20:A:54:ALA:HB3	2.02	0.41
21:A:848:BCR:H371	21:A:848:BCR:H24C	1.79	0.41
22:G:608:CLA:H121	22:G:609:CLA:CHC	2.50	0.41
11:L:226:ASP:OD2	11:L:226:ASP:C	2.64	0.41
22:L:412:CLA:H3A	22:L:412:CLA:HBA2	1.71	0.41
8:N:189:THR:CG2	22:N:607:CLA:HHB	2.51	0.41
22:Q:608:CLA:HBA1	22:Q:608:CLA:H3A	1.94	0.41
22:T:608:CLA:H2A	22:T:608:CLA:HED3	2.01	0.41
17:V:207:CYS:HB3	17:V:224:TRP:HD1	1.85	0.41
17:V:267:TRP:CE2	17:V:273:ILE:HG23	2.56	0.41
22:A:804:CLA:H142	22:A:804:CLA:H111	1.77	0.41
22:A:852:CLA:H91	22:A:852:CLA:H111	1.79	0.41
8:I:111:HIS:CE1	22:I:603:CLA:C4A	2.95	0.41
22:I:606:CLA:HED3	10:K:481:TRP:CZ3	2.56	0.41
22:L:406:CLA:H111	22:L:406:CLA:H72	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:408:CLA:CGA	22:L:408:CLA:C3A	2.99	0.41
22:P:603:CLA:HMD1	22:P:606:CLA:C1D	2.50	0.41
20:A:233:ASN:OD1	20:A:233:ASN:C	2.63	0.41
20:A:494:ALA:N	20:A:495:PRO:HD2	2.36	0.41
22:A:830:CLA:HBA1	22:A:830:CLA:HBD	2.02	0.41
1:B:516:ASP:N	1:B:516:ASP:OD1	2.54	0.41
1:B:640:MET:HE2	1:B:640:MET:HB2	1.83	0.41
6:G:440:GLU:OE2	6:G:446:ALA:HA	2.20	0.41
22:K:617:CLA:H92	22:K:617:CLA:H62	1.74	0.41
14:S:74:PHE:CD1	14:S:75:PRO:HD2	2.55	0.41
15:T:353:GLY:H	15:T:358:GLU:CD	2.27	0.41
31:U:407:CHL:CBA	32:U:418:NEX:H403	2.50	0.41
17:V:316:MET:HE2	17:V:316:MET:HB2	1.87	0.41
31:W:422:CHL:H141	19:X:221:ILE:HG13	2.01	0.41
22:A:807:CLA:H3A	22:A:807:CLA:HBA1	1.47	0.41
21:A:851:BCR:H24C	21:A:851:BCR:H371	1.81	0.41
22:B:809:CLA:HMA1	27:B:854:LMU:H71	2.01	0.41
26:K:616:LHG:HC82	26:K:616:LHG:H281	2.02	0.41
11:L:319:GLU:HG3	22:L:408:CLA:C1B	2.51	0.41
8:N:157:GLU:OE2	22:N:606:CLA:C1C	2.67	0.41
6:P:392:HIS:CD2	6:P:409:ALA:O	2.74	0.41
11:R:218:PHE:HB3	22:R:602:CLA:CAD	2.50	0.41
28:W:401:LMG:H342	28:W:401:LMG:H311	1.69	0.41
22:W:411:CLA:H142	22:W:411:CLA:H111	1.79	0.41
20:A:354:SER:OG	20:A:409:ALA:HB2	2.21	0.41
22:A:827:CLA:HBA2	22:A:827:CLA:H3A	1.69	0.41
21:A:849:BCR:H11C	21:A:849:BCR:H341	1.84	0.41
2:C:29:VAL:HG21	3:D:247:LYS:HG2	2.01	0.41
3:D:98:ASP:OD2	3:D:99:LEU:N	2.54	0.41
11:L:257:LEU:HA	27:L:419:LMU:H6D	2.01	0.41
22:L:404:CLA:H2	22:L:404:CLA:H61	1.75	0.41
11:R:233:MET:HE2	22:R:602:CLA:H12	2.03	0.41
14:S:150:ASN:HB2	14:S:152:GLU:OE2	2.20	0.41
16:U:188:LYS:NZ	22:U:405:CLA:HBA1	2.34	0.41
20:A:233:ASN:HA	20:A:234:PRO:HD3	1.91	0.41
22:A:816:CLA:H151	22:A:816:CLA:H112	1.66	0.41
22:B:823:CLA:H62	22:B:823:CLA:H41	1.85	0.41
22:B:834:CLA:HBB1	22:B:834:CLA:HMB3	2.02	0.41
8:N:180:ASP:OD2	8:N:185:THR:OG1	2.38	0.41
11:R:286:VAL:O	11:R:290:ARG:HG3	2.20	0.41
16:U:261:MET:HE3	16:U:261:MET:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:U:408:CHL:HMA2	28:U:423:LMG:O2	2.21	0.41
17:V:314:VAL:HG12	22:V:612:CLA:HBB2	2.03	0.41
22:W:412:CLA:H121	22:W:413:CLA:C4B	2.50	0.41
20:A:200:HIS:CE1	22:A:814:CLA:NA	2.88	0.41
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.93	0.41
1:B:310:ALA:HA	1:B:311:PRO:HD3	1.94	0.41
1:B:494:LEU:HD12	1:B:494:LEU:HA	1.86	0.41
22:B:813:CLA:H2	22:B:813:CLA:H61	1.59	0.41
22:B:824:CLA:HMA1	21:B:845:BCR:H14C	2.03	0.41
22:B:825:CLA:H122	21:B:844:BCR:H373	2.03	0.41
21:B:843:BCR:H24C	21:B:843:BCR:H402	1.73	0.41
26:B:851:LHG:H161	26:B:851:LHG:H192	1.84	0.41
8:I:79:LEU:HD11	8:I:90:ASP:HB2	2.03	0.41
10:K:525:GLN:HG2	22:K:611:CLA:C1D	2.50	0.41
22:K:608:CLA:H41	22:K:608:CLA:H62	1.87	0.41
8:N:117:LEU:HD22	22:N:604:CLA:HAB	2.03	0.41
13:O:117:HIS:HE1	22:O:307:CLA:C4D	2.34	0.41
11:R:195:ARG:HB2	11:R:195:ARG:HH11	1.86	0.41
22:R:607:CLA:H52	22:R:607:CLA:HBB1	2.03	0.41
14:S:136:ALA:O	14:S:139:THR:OG1	2.38	0.41
27:T:618:LMU:H31	27:T:618:LMU:H62	1.73	0.41
22:U:401:CLA:HBA1	22:U:401:CLA:H3A	1.89	0.41
19:X:268:LYS:HD3	22:X:411:CLA:HAA2	2.02	0.41
20:A:88:LEU:HD23	20:A:88:LEU:HA	1.90	0.41
20:A:339:LYS:HB2	20:A:339:LYS:HE2	1.94	0.41
1:B:177:HIS:HE1	22:B:811:CLA:C4A	2.34	0.41
22:B:830:CLA:HBC3	22:B:830:CLA:HHD	2.03	0.41
6:G:447:TRP:CE2	6:G:448:PHE:HD2	2.39	0.41
11:L:338:HIS:HB3	11:L:368:TRP:HZ3	1.85	0.41
22:L:409:CLA:NC	26:L:416:LHG:HC41	2.36	0.41
21:M:101:BCR:H11C	21:M:101:BCR:H341	1.85	0.41
10:Q:537:LEU:HD13	22:Q:613:CLA:HBC2	2.02	0.41
22:S:605:CLA:O1D	22:S:605:CLA:H2A	2.21	0.41
17:V:182:ASP:HB3	17:V:185:ASP:CG	2.46	0.41
17:V:190:ARG:O	17:V:194:VAL:HG23	2.21	0.41
17:V:246:HIS:HB2	22:V:617:CLA:C1B	2.51	0.41
17:V:300:GLU:O	17:V:304:LYS:HG3	2.21	0.41
20:A:609:HIS:NE2	22:A:838:CLA:HBC3	2.36	0.41
21:B:801:BCR:H272	22:B:831:CLA:HBB2	2.03	0.40
21:B:842:BCR:H341	21:B:842:BCR:H11C	1.82	0.40
10:K:545:LEU:H	10:K:545:LEU:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:243:LEU:HD11	22:R:606:CLA:HBC3	2.03	0.40
22:S:604:CLA:H112	22:S:604:CLA:H91	1.82	0.40
28:T:616:LMG:HC1	28:T:616:LMG:HC8	1.79	0.40
22:U:404:CLA:H92	22:U:404:CLA:H61	1.66	0.40
18:W:198:PHE:O	18:W:202:ARG:HG3	2.21	0.40
1:B:388:ALA:O	1:B:392:ILE:HG13	2.19	0.40
22:B:832:CLA:H12	9:J:42:ILE:HD12	2.04	0.40
4:E:102:ARG:HA	4:E:103:PRO:HD3	1.98	0.40
22:H:308:CLA:H92	22:H:308:CLA:H61	1.79	0.40
27:L:420:LMU:H51	27:L:420:LMU:H22	1.82	0.40
26:O:321:LHG:H372	26:O:321:LHG:H342	1.84	0.40
11:R:332:GLY:HA2	11:R:335:VAL:HG12	2.02	0.40
22:R:607:CLA:H92	22:R:607:CLA:H61	1.70	0.40
21:B:801:BCR:H24C	21:B:801:BCR:H371	1.90	0.40
3:D:117:THR:O	3:D:146:GLY:HA3	2.22	0.40
7:H:165:LEU:HD13	22:H:312:CLA:HBC2	2.03	0.40
22:I:611:CLA:HBA2	22:I:611:CLA:H3A	1.67	0.40
25:O:304:DGD:HB71	25:O:304:DGD:HB41	1.13	0.40
22:B:859:CLA:H142	22:B:859:CLA:H111	1.79	0.40
22:K:607:CLA:H93	22:K:607:CLA:H111	1.79	0.40
8:N:152:ILE:HA	8:N:152:ILE:HD13	1.85	0.40
13:O:240:ASN:OD1	13:O:243:THR:HG23	2.22	0.40
22:Q:608:CLA:HHC	22:Q:608:CLA:HBB1	2.03	0.40
17:V:153:THR:HA	17:V:172:ARG:O	2.22	0.40
22:W:406:CLA:H92	22:W:406:CLA:H62	1.92	0.40
20:A:37:ARG:NH2	20:A:62:HIS:O	2.54	0.40
1:B:293:THR:CG2	1:B:294:ASN:H	2.22	0.40
1:B:484:ASN:ND2	31:U:408:CHL:OBD	2.54	0.40
22:B:834:CLA:H51	22:B:834:CLA:H11	1.87	0.40
5:F:252:ILE:HD13	22:F:404:CLA:C1D	2.32	0.40
21:J:103:BCR:H24C	21:J:103:BCR:H371	1.92	0.40
22:K:608:CLA:H3A	22:K:608:CLA:CGA	2.51	0.40
22:U:420:CLA:HBA2	22:U:420:CLA:H3A	1.30	0.40
18:W:221:ALA:HB3	18:W:222:PRO:HD3	2.04	0.40
20:A:180:HIS:HE1	22:A:812:CLA:C1A	2.34	0.40
20:A:502:LEU:HD23	20:A:502:LEU:HA	1.87	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	B	730/734 (100%)	698 (96%)	29 (4%)	3 (0%)	30	34
2	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	D	188/193 (97%)	182 (97%)	6 (3%)	0	100	100
4	E	61/158 (39%)	61 (100%)	0	0	100	100
5	F	164/325 (50%)	161 (98%)	3 (2%)	0	100	100
6	G	173/184 (94%)	169 (98%)	4 (2%)	0	100	100
6	P	162/184 (88%)	146 (90%)	16 (10%)	0	100	100
7	H	171/185 (92%)	165 (96%)	6 (4%)	0	100	100
8	I	163/184 (89%)	160 (98%)	3 (2%)	0	100	100
8	N	168/184 (91%)	155 (92%)	13 (8%)	0	100	100
9	J	35/39 (90%)	35 (100%)	0	0	100	100
10	K	180/184 (98%)	175 (97%)	5 (3%)	0	100	100
10	Q	180/184 (98%)	168 (93%)	12 (7%)	0	100	100
11	L	176/187 (94%)	167 (95%)	8 (4%)	1 (1%)	21	24
11	R	172/187 (92%)	163 (95%)	8 (5%)	1 (1%)	21	24
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	O	173/177 (98%)	160 (92%)	12 (7%)	1 (1%)	21	24
14	S	170/180 (94%)	166 (98%)	4 (2%)	0	100	100
15	T	165/173 (95%)	158 (96%)	7 (4%)	0	100	100
16	U	197/209 (94%)	186 (94%)	11 (6%)	0	100	100
17	V	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
18	W	218/228 (96%)	209 (96%)	9 (4%)	0	100	100
19	X	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
20	A	738/756 (98%)	715 (97%)	22 (3%)	1 (0%)	48	59
All	All	4906/5366 (91%)	4700 (96%)	199 (4%)	7 (0%)	49	59



All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	R	196	PRO
1	B	288	GLY
1	B	284	PHE
11	L	367	GLN
1	B	488	ALA
13	O	184	PRO
20	A	122	VAL

### 5.3.2 Protein sidechains [i](#)

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	B	608/609 (100%)	600 (99%)	8 (1%)	61	76
2	C	69/70 (99%)	67 (97%)	2 (3%)	37	49
3	D	157/160 (98%)	154 (98%)	3 (2%)	50	65
4	E	54/124 (44%)	52 (96%)	2 (4%)	30	40
5	F	132/251 (53%)	129 (98%)	3 (2%)	44	58
6	G	133/140 (95%)	132 (99%)	1 (1%)	73	84
6	P	124/140 (89%)	118 (95%)	6 (5%)	23	29
7	H	141/149 (95%)	139 (99%)	2 (1%)	59	73
8	I	120/136 (88%)	114 (95%)	6 (5%)	22	27
8	N	124/136 (91%)	120 (97%)	4 (3%)	34	46
9	J	34/36 (94%)	34 (100%)	0	100	100
10	K	144/146 (99%)	139 (96%)	5 (4%)	32	42
10	Q	144/146 (99%)	141 (98%)	3 (2%)	47	61
11	L	139/145 (96%)	134 (96%)	5 (4%)	31	41
11	R	136/145 (94%)	132 (97%)	4 (3%)	37	49
12	M	26/26 (100%)	26 (100%)	0	100	100
13	O	143/144 (99%)	138 (96%)	5 (4%)	32	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	S	133/137 (97%)	130 (98%)	3 (2%)	44	58
15	T	126/131 (96%)	125 (99%)	1 (1%)	73	84
16	U	152/158 (96%)	150 (99%)	2 (1%)	61	76
17	V	151/151 (100%)	148 (98%)	3 (2%)	48	63
18	W	167/172 (97%)	165 (99%)	2 (1%)	63	77
19	X	173/173 (100%)	171 (99%)	2 (1%)	63	77
20	A	621/636 (98%)	612 (99%)	9 (1%)	59	73
All	All	3951/4261 (93%)	3870 (98%)	81 (2%)	46	61

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	GLU
1	B	197	VAL
1	B	267	SER
1	B	366	THR
1	B	492	ILE
1	B	501	ILE
1	B	508	LEU
1	B	715	VAL
2	C	42	SER
2	C	65	VAL
3	D	193	SER
3	D	246	THR
3	D	260	GLU
4	E	139	VAL
4	E	140	THR
5	F	178	LYS
5	F	187	SER
5	F	206	LYS
6	G	438	VAL
7	H	12	ILE
7	H	137	ILE
8	I	120	VAL
8	I	123	ILE
8	I	124	VAL
8	I	145	LEU
8	I	152	ILE
8	I	185	THR
10	K	434	VAL

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Mol	Chain	Res	Type
10	K	471	GLU
10	K	523	GLU
10	K	528	VAL
10	K	545	LEU
11	L	195	ARG
11	L	301	ASN
11	L	342	VAL
11	L	368	TRP
11	L	370	VAL
8	N	78	HIS
8	N	152	ILE
8	N	184	LEU
8	N	187	ASP
13	O	80	THR
13	O	102	LYS
13	O	108	GLN
13	O	177	ASP
13	O	211	MET
6	P	383	TRP
6	P	392	HIS
6	P	393	LEU
6	P	433	ILE
6	P	508	ILE
6	P	518	LEU
10	Q	380	ARG
10	Q	387	ILE
10	Q	388	THR
11	R	195	ARG
11	R	229	VAL
11	R	278	VAL
11	R	330	MET
14	S	78	THR
14	S	168	TYR
14	S	203	THR
15	T	281	PHE
16	U	284	THR
16	U	349	THR
17	V	165	THR
17	V	177	CYS
17	V	316	MET
18	W	342	VAL
18	W	369	THR

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Mol	Chain	Res	Type
19	X	306	THR
19	X	320	ASP
20	A	75	SER
20	A	111	VAL
20	A	307	LEU
20	A	328	SER
20	A	395	TYR
20	A	414	VAL
20	A	506	THR
20	A	622	VAL
20	A	628	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	672	GLN
1	B	704	GLN
6	G	378	HIS
6	G	524	GLN
6	G	542	ASN
7	H	93	GLN
7	H	139	ASN
7	H	153	GLN
10	K	425	ASN
10	K	511	ASN
10	K	525	GLN
11	L	211	GLN
11	L	336	GLN
8	N	196	ASN
13	O	203	ASN
13	O	217	GLN
13	O	235	HIS
10	Q	425	ASN
10	Q	511	ASN
10	Q	525	GLN
10	Q	526	ASN
11	R	268	ASN
11	R	336	GLN
14	S	210	ASN
14	S	224	GLN
14	S	225	HIS
15	T	386	ASN

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Mol	Chain	Res	Type
17	V	232	ASN
17	V	322	GLN
19	X	123	HIS
19	X	200	ASN
19	X	204	ASN
20	A	34	HIS
20	A	51	ASN
20	A	116	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

436 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	F	404	-	59,63,73	1.26	6 (10%)	70,101,113	1.35	6 (8%)
22	CLA	K	604	-	68,72,73	1.18	8 (11%)	80,111,113	1.26	6 (7%)
22	CLA	B	821	1	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)
22	CLA	W	403	18	56,60,73	1.31	8 (14%)	65,97,113	1.38	6 (9%)
28	LMG	I	615	-	50,50,55	1.04	1 (2%)	56,57,63	1.41	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	819	20	62,66,73	1.22	8 (12%)	73,104,113	1.44	7 (9%)
22	CLA	A	820	20	69,73,73	1.17	8 (11%)	82,113,113	1.25	7 (8%)
26	LHG	K	619	-	32,32,48	1.36	6 (18%)	35,38,54	1.12	2 (5%)
22	CLA	P	604	-	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	B	831	1	69,73,73	1.16	8 (11%)	82,113,113	1.24	8 (9%)
22	CLA	I	604	-	49,53,73	1.39	9 (18%)	58,89,113	1.42	4 (6%)
22	CLA	O	319	13	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
28	LMG	T	616	-	41,41,55	0.83	1 (2%)	49,49,63	1.24	3 (6%)
27	LMU	B	849	-	24,24,36	0.45	0	29,29,47	0.64	0
22	CLA	P	609	-	49,53,73	1.39	8 (16%)	58,89,113	1.39	3 (5%)
22	CLA	X	405	-	60,64,73	1.25	8 (13%)	71,102,113	1.32	5 (7%)
21	BCR	A	848	-	41,41,41	0.71	0	56,56,56	1.81	10 (17%)
22	CLA	S	610	14	49,53,73	1.40	7 (14%)	58,89,113	1.49	5 (8%)
22	CLA	W	412	26	64,68,73	1.23	8 (12%)	76,107,113	1.30	6 (7%)
22	CLA	A	818	20	57,61,73	1.28	8 (14%)	67,98,113	1.34	7 (10%)
22	CLA	I	607	8	59,63,73	1.26	8 (13%)	70,101,113	1.34	7 (10%)
24	DD6	S	611	-	40,45,45	1.54	2 (5%)	51,67,67	1.81	13 (25%)
22	CLA	A	844	26	59,63,73	1.27	9 (15%)	70,101,113	1.38	7 (10%)
28	LMG	H	322	-	37,37,55	0.84	1 (2%)	45,45,63	1.24	3 (6%)
28	LMG	I	614	-	37,37,55	0.85	1 (2%)	45,45,63	1.28	5 (11%)
22	CLA	Q	617	10	56,60,73	1.30	7 (12%)	65,97,113	1.38	6 (9%)
22	CLA	B	807	1	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
31	CHL	U	408	-	40,54,74	2.38	10 (25%)	34,90,114	1.35	5 (14%)
22	CLA	K	606	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	6 (9%)
24	DD6	U	416	-	40,45,45	1.57	2 (5%)	51,67,67	1.79	12 (23%)
22	CLA	W	410	18	64,68,73	1.21	8 (12%)	76,107,113	1.30	6 (7%)
22	CLA	U	420	16	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
26	LHG	K	616	22	38,38,48	1.27	6 (15%)	41,44,54	1.04	3 (7%)
22	CLA	B	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	7 (8%)
22	CLA	R	604	-	49,53,73	1.40	7 (14%)	58,89,113	1.37	5 (8%)
22	CLA	W	411	18	64,68,73	1.21	9 (14%)	76,107,113	1.26	7 (9%)
27	LMU	H	321	-	34,34,36	0.48	0	42,44,47	0.77	2 (4%)
22	CLA	B	810	-	60,64,73	1.25	8 (13%)	71,102,113	1.30	5 (7%)
21	BCR	M	101	-	41,41,41	0.74	1 (2%)	56,56,56	2.02	15 (26%)
24	DD6	W	418	-	40,45,45	1.57	3 (7%)	51,67,67	1.88	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LHG	N	616	-	42,42,48	1.21	6 (14%)	45,48,54	0.99	2 (4%)
22	CLA	H	311	7	69,73,73	1.19	7 (10%)	82,113,113	1.27	6 (7%)
22	CLA	R	607	11	64,68,73	1.24	9 (14%)	76,107,113	1.30	6 (7%)
22	CLA	X	413	19	49,53,73	1.39	6 (12%)	58,89,113	1.40	4 (6%)
27	LMU	B	855	-	24,24,36	0.46	0	29,29,47	0.66	0
22	CLA	O	306	13	64,68,73	1.21	9 (14%)	76,107,113	1.27	6 (7%)
26	LHG	S	613	22	31,31,48	1.37	6 (19%)	34,37,54	1.14	3 (8%)
22	CLA	J	102	9	54,58,73	1.31	8 (14%)	64,95,113	1.38	5 (7%)
27	LMU	B	857	-	36,36,36	0.42	0	47,47,47	0.74	1 (2%)
24	DD6	V	614	-	40,45,45	1.53	2 (5%)	51,67,67	2.01	15 (29%)
22	CLA	X	412	19	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	B	817	1	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	T	606	15	54,58,73	1.31	7 (12%)	64,95,113	1.37	6 (9%)
22	CLA	S	602	14	64,68,73	1.22	7 (10%)	76,107,113	1.31	8 (10%)
22	CLA	V	609	17	61,65,73	1.25	8 (13%)	72,103,113	1.32	6 (8%)
27	LMU	T	615	-	21,21,36	0.47	0	26,26,47	0.58	0
27	LMU	H	301	-	21,21,36	0.50	0	26,26,47	0.71	0
22	CLA	X	411	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	6 (10%)
22	CLA	N	606	8	69,73,73	1.19	7 (10%)	82,113,113	1.25	6 (7%)
27	LMU	B	854	-	24,24,36	0.46	0	29,29,47	0.80	1 (3%)
30	SQD	F	407	-	40,42,54	0.43	1 (2%)	50,53,65	0.47	1 (2%)
31	CHL	W	422	-	60,74,74	1.92	10 (16%)	58,114,114	1.12	5 (8%)
21	BCR	B	843	-	41,41,41	0.72	0	56,56,56	3.46	25 (44%)
31	CHL	X	406	-	40,54,74	2.36	10 (25%)	34,90,114	1.40	5 (14%)
22	CLA	B	829	-	49,53,73	1.34	9 (18%)	58,89,113	1.50	5 (8%)
27	LMU	A	854	-	36,36,36	0.42	0	47,47,47	0.70	1 (2%)
24	DD6	X	401	-	40,45,45	1.51	2 (5%)	51,67,67	1.81	11 (21%)
22	CLA	X	403	19	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
27	LMU	G	615	-	21,21,36	0.46	0	26,26,47	0.50	0
22	CLA	G	604	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	6 (10%)
22	CLA	L	411	11	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
22	CLA	N	607	-	64,68,73	1.22	9 (14%)	76,107,113	1.26	6 (7%)
22	CLA	A	803	-	69,73,73	1.19	8 (11%)	82,113,113	1.25	7 (8%)
22	CLA	H	308	7	64,68,73	1.20	7 (10%)	76,107,113	1.28	7 (9%)
22	CLA	A	813	20	69,73,73	1.16	7 (10%)	82,113,113	1.18	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	806	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
27	LMU	J	104	-	35,35,36	0.40	0	44,45,47	0.93	2 (4%)
28	LMG	A	855	-	41,41,55	0.84	0	49,49,63	1.26	6 (12%)
22	CLA	B	833	1	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
22	CLA	O	311	26	64,68,73	1.21	7 (10%)	76,107,113	1.27	6 (7%)
27	LMU	F	402	-	21,21,36	0.47	0	26,26,47	0.68	0
24	DD6	L	413	-	40,45,45	1.53	2 (5%)	51,67,67	1.76	13 (25%)
22	CLA	B	813	1	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
22	CLA	H	302	7	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
22	CLA	S	606	14	54,58,73	1.33	6 (11%)	64,95,113	1.36	6 (9%)
22	CLA	B	808	1	59,63,73	1.27	9 (15%)	70,101,113	1.32	6 (8%)
22	CLA	B	835	1	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
22	CLA	H	312	7	49,53,73	1.39	7 (14%)	58,89,113	1.37	4 (6%)
26	LHG	B	848	22	26,26,48	1.36	6 (23%)	29,32,54	1.17	2 (6%)
22	CLA	N	604	-	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	P	608	-	49,53,73	1.41	9 (18%)	58,89,113	1.42	5 (8%)
22	CLA	V	612	-	69,73,73	1.19	8 (11%)	82,113,113	1.24	4 (4%)
25	DGD	O	304	-	61,61,67	0.87	3 (4%)	75,75,81	1.13	6 (8%)
22	CLA	V	602	17	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	V	608	17	59,63,73	1.27	8 (13%)	70,101,113	1.30	5 (7%)
22	CLA	S	605	-	64,68,73	1.21	7 (10%)	76,107,113	1.42	5 (6%)
27	LMU	T	618	-	24,24,36	0.45	0	29,29,47	0.65	0
22	CLA	H	313	7	62,66,73	1.24	7 (11%)	73,104,113	1.30	6 (8%)
24	DD6	H	315	-	40,45,45	1.53	2 (5%)	51,67,67	1.79	14 (27%)
22	CLA	K	613	-	57,61,73	1.29	9 (15%)	67,98,113	1.33	5 (7%)
22	CLA	G	601	6	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
26	LHG	T	614	22	41,41,48	1.24	6 (14%)	44,47,54	0.99	2 (4%)
27	LMU	O	322	-	36,36,36	0.49	0	47,47,47	1.10	5 (10%)
22	CLA	A	811	20	61,65,73	1.24	7 (11%)	72,103,113	1.39	9 (12%)
22	CLA	U	415	16	49,53,73	1.40	8 (16%)	58,89,113	1.38	4 (6%)
22	CLA	A	824	20	69,73,73	1.17	7 (10%)	82,113,113	1.26	7 (8%)
27	LMU	F	409	-	21,21,36	0.50	0	26,26,47	0.56	0
22	CLA	W	415	18	49,53,73	1.44	8 (16%)	58,89,113	1.42	5 (8%)
22	CLA	G	608	26	64,68,73	1.21	8 (12%)	76,107,113	1.33	5 (6%)
24	DD6	X	416	-	40,45,45	1.57	1 (2%)	51,67,67	2.21	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	822	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	P	606	6	49,53,73	1.38	7 (14%)	58,89,113	1.42	5 (8%)
24	DD6	S	612	-	40,45,45	1.53	2 (5%)	51,67,67	1.81	13 (25%)
27	LMU	B	850	-	24,24,36	0.45	0	29,29,47	0.55	0
28	LMG	W	401	-	48,48,55	0.72	0	56,56,63	1.33	7 (12%)
22	CLA	V	607	-	49,53,73	1.39	6 (12%)	58,89,113	1.42	5 (8%)
24	DD6	W	417	-	40,45,45	1.52	2 (5%)	51,67,67	1.72	12 (23%)
22	CLA	G	605	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
22	CLA	L	402	11	69,73,73	1.16	8 (11%)	82,113,113	1.25	4 (4%)
22	CLA	R	610	11	69,73,73	1.19	7 (10%)	82,113,113	1.21	5 (6%)
22	CLA	W	402	18	59,63,73	1.26	8 (13%)	70,101,113	1.29	6 (8%)
22	CLA	Q	606	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
22	CLA	R	608	26	58,62,73	1.29	8 (13%)	68,99,113	1.30	5 (7%)
25	DGD	B	847	-	67,67,67	0.84	4 (5%)	81,81,81	1.01	5 (6%)
22	CLA	L	407	-	61,65,73	1.25	8 (13%)	72,103,113	1.31	5 (6%)
28	LMG	H	319	-	40,40,55	0.81	1 (2%)	48,48,63	1.21	3 (6%)
27	LMU	T	617	-	24,24,36	0.43	0	29,29,47	0.65	0
22	CLA	H	303	7	64,68,73	1.22	8 (12%)	76,107,113	1.28	5 (6%)
27	LMU	K	620	-	34,34,36	0.50	0	42,44,47	0.99	4 (9%)
26	LHG	A	845	-	48,48,48	1.15	6 (12%)	51,54,54	0.95	3 (5%)
22	CLA	A	852	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	5 (6%)
22	CLA	U	405	16	61,65,73	1.26	8 (13%)	72,103,113	1.31	5 (6%)
22	CLA	A	806	20	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
22	CLA	U	401	-	59,63,73	1.27	9 (15%)	70,101,113	1.32	5 (7%)
24	DD6	P	613	-	40,45,45	1.55	2 (5%)	51,67,67	1.94	18 (35%)
24	DD6	A	858	-	40,45,45	1.53	2 (5%)	51,67,67	2.53	21 (41%)
22	CLA	N	608	26	49,53,73	1.39	7 (14%)	58,89,113	1.39	4 (6%)
22	CLA	Q	613	10	49,53,73	1.38	8 (16%)	58,89,113	1.43	5 (8%)
22	CLA	I	608	-	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	A	807	20	69,73,73	1.17	9 (13%)	82,113,113	1.30	5 (6%)
22	CLA	I	605	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	5 (8%)
29	SF4	C	102	2	0,12,12	-	-	-	-	-
22	CLA	R	606	11	61,65,73	1.25	5 (8%)	72,103,113	1.27	5 (6%)
22	CLA	B	830	1	69,73,73	1.14	8 (11%)	82,113,113	1.31	8 (9%)
22	CLA	T	609	15	49,53,73	1.38	7 (14%)	58,89,113	1.42	6 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	U	404	16	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
22	CLA	W	409	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	7 (8%)
22	CLA	T	611	15	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	T	601	15	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
22	CLA	T	603	15	64,68,73	1.22	8 (12%)	76,107,113	1.28	7 (9%)
27	LMU	U	424	-	24,24,36	0.43	0	29,29,47	0.57	0
27	LMU	B	853	-	19,19,36	0.47	0	23,23,47	0.43	0
22	CLA	K	602	10	64,68,73	1.21	8 (12%)	76,107,113	1.28	7 (9%)
28	LMG	B	856	-	53,53,55	0.73	0	61,61,63	1.38	8 (13%)
26	LHG	O	323	-	42,42,48	1.23	6 (14%)	45,48,54	0.96	2 (4%)
26	LHG	O	318	22	33,33,48	1.34	6 (18%)	36,39,54	1.07	3 (8%)
27	LMU	X	418	-	24,24,36	0.44	0	29,29,47	0.54	0
22	CLA	H	309	26	59,63,73	1.28	8 (13%)	70,101,113	1.32	6 (8%)
22	CLA	T	608	26	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)
28	LMG	F	408	-	42,42,55	0.85	2 (4%)	50,50,63	1.33	4 (8%)
22	CLA	F	405	5	49,53,73	1.40	8 (16%)	58,89,113	1.35	4 (6%)
22	CLA	G	603	6	60,64,73	1.26	8 (13%)	71,102,113	1.30	6 (8%)
22	CLA	B	819	1	57,61,73	1.33	6 (10%)	67,98,113	1.37	3 (4%)
22	CLA	A	841	20	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
22	CLA	A	808	20	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	Q	605	-	60,64,73	1.26	6 (10%)	71,102,113	1.32	7 (9%)
22	CLA	A	805	20	65,69,73	1.20	6 (9%)	77,108,113	1.28	7 (9%)
31	CHL	W	407	-	40,54,74	2.36	10 (25%)	34,90,114	1.42	5 (14%)
21	BCR	A	850	-	41,41,41	0.70	0	56,56,56	1.97	13 (23%)
22	CLA	O	308	-	65,69,73	1.21	7 (10%)	77,108,113	1.28	7 (9%)
22	CLA	V	610	-	49,53,73	1.40	6 (12%)	58,89,113	1.39	4 (6%)
24	DD6	A	859	-	40,45,45	1.58	2 (5%)	51,67,67	1.89	14 (27%)
22	CLA	W	404	18	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
26	LHG	L	416	22	41,41,48	1.22	6 (14%)	44,47,54	1.01	2 (4%)
22	CLA	V	611	-	49,53,73	1.41	7 (14%)	58,89,113	1.41	4 (6%)
22	CLA	N	601	8	49,53,73	1.38	8 (16%)	58,89,113	1.39	4 (6%)
22	CLA	H	304	7	49,53,73	1.38	7 (14%)	58,89,113	1.40	6 (10%)
26	LHG	O	324	-	41,41,48	1.23	5 (12%)	44,47,54	0.98	2 (4%)
22	CLA	B	823	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	4 (4%)
22	CLA	B	826	1	62,66,73	1.24	7 (11%)	73,104,113	1.31	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LHG	H	316	22	26,26,48	1.45	6 (23%)	29,32,54	1.18	2 (6%)
28	LMG	Q	602	-	37,37,55	0.84	1 (2%)	45,45,63	1.29	6 (13%)
22	CLA	Q	604	10	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
30	SQD	K	621	-	41,43,54	0.43	1 (2%)	51,54,65	0.53	0
22	CLA	S	603	14	49,53,73	1.38	7 (14%)	58,89,113	1.40	6 (10%)
22	CLA	A	809	20	57,61,73	1.29	8 (14%)	67,98,113	1.34	5 (7%)
22	CLA	X	410	26	64,68,73	1.21	7 (10%)	76,107,113	1.29	5 (6%)
22	CLA	Q	618	-	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
21	BCR	B	846	-	41,41,41	0.68	0	56,56,56	1.84	17 (30%)
22	CLA	A	815	20	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
24	DD6	W	416	-	40,45,45	1.50	2 (5%)	51,67,67	1.77	11 (21%)
25	DGD	F	401	-	33,33,67	1.08	2 (6%)	35,35,81	1.33	5 (14%)
24	DD6	L	414	-	40,45,45	1.55	2 (5%)	51,67,67	1.80	15 (29%)
27	LMU	X	421	-	36,36,36	0.40	0	47,47,47	0.68	1 (2%)
22	CLA	A	827	-	66,70,73	1.18	7 (10%)	78,109,113	1.29	5 (6%)
24	DD6	N	613	-	40,45,45	1.54	2 (5%)	51,67,67	1.85	15 (29%)
22	CLA	I	610	8	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	F	403	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
31	CHL	V	606	-	40,54,74	2.39	10 (25%)	34,90,114	1.33	5 (14%)
24	DD6	O	316	-	40,45,45	1.53	2 (5%)	51,67,67	1.69	13 (25%)
27	LMU	O	320	-	27,27,36	0.54	0	30,31,47	0.80	1 (3%)
22	CLA	B	832	1	66,70,73	1.19	8 (12%)	78,109,113	1.32	6 (7%)
22	CLA	A	817	20	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
22	CLA	A	804	-	69,73,73	1.17	7 (10%)	82,113,113	1.19	5 (6%)
22	CLA	A	816	20	65,69,73	1.20	9 (13%)	77,108,113	1.40	7 (9%)
22	CLA	W	419	18	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	R	603	-	60,64,73	1.26	7 (11%)	71,102,113	1.33	5 (7%)
24	DD6	A	847	-	40,45,45	1.53	2 (5%)	51,67,67	1.83	14 (27%)
22	CLA	T	602	15	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	T	604	15	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
21	BCR	A	851	-	41,41,41	0.70	0	56,56,56	2.11	16 (28%)
24	DD6	G	613	-	40,45,45	1.56	2 (5%)	51,67,67	1.90	16 (31%)
27	LMU	U	421	-	36,36,36	0.41	0	47,47,47	0.66	1 (2%)
22	CLA	A	842	20	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
22	CLA	S	604	-	64,68,73	1.22	8 (12%)	76,107,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	H	310	7	49,53,73	1.38	7 (14%)	58,89,113	1.40	4 (6%)
22	CLA	A	826	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
26	LHG	R	614	22	41,41,48	1.22	6 (14%)	44,47,54	0.97	2 (4%)
21	BCR	A	849	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
22	CLA	K	610	10	60,64,73	1.25	8 (13%)	71,102,113	1.30	6 (8%)
32	NEX	V	616	-	40,46,46	0.36	1 (2%)	50,70,70	0.66	1 (2%)
24	DD6	K	614	-	40,45,45	1.57	3 (7%)	51,67,67	1.83	14 (27%)
26	LHG	P	601	-	39,39,48	1.25	6 (15%)	42,45,54	1.00	2 (4%)
28	LMG	K	618	-	49,49,55	0.75	0	57,57,63	1.32	7 (12%)
22	CLA	O	315	13	54,58,73	1.34	8 (14%)	64,95,113	1.34	6 (9%)
22	CLA	P	607	6	49,53,73	1.39	8 (16%)	58,89,113	1.42	5 (8%)
21	BCR	B	844	-	41,41,41	0.69	0	56,56,56	1.81	12 (21%)
22	CLA	A	821	20	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
24	DD6	P	612	-	40,45,45	1.56	1 (2%)	51,67,67	2.93	17 (33%)
22	CLA	K	607	10	61,65,73	1.22	9 (14%)	72,103,113	1.44	6 (8%)
22	CLA	K	609	26	64,68,73	1.21	8 (12%)	76,107,113	1.28	4 (5%)
22	CLA	K	603	10	64,68,73	1.21	9 (14%)	76,107,113	1.28	5 (6%)
27	LMU	M	102	-	24,24,36	0.44	0	29,29,47	0.60	0
22	CLA	X	407	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
24	DD6	V	615	-	40,45,45	1.50	2 (5%)	51,67,67	1.85	14 (27%)
24	DD6	F	406	-	40,45,45	1.55	2 (5%)	51,67,67	1.88	16 (31%)
22	CLA	R	605	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
31	CHL	W	408	-	60,74,74	1.89	10 (16%)	58,114,114	1.16	6 (10%)
28	LMG	K	601	-	43,43,55	0.76	0	51,51,63	1.28	5 (9%)
22	CLA	G	610	6	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	X	404	19	64,68,73	1.23	7 (10%)	76,107,113	1.25	5 (6%)
22	CLA	N	602	8	64,68,73	1.21	9 (14%)	76,107,113	1.31	6 (7%)
31	CHL	V	605	-	40,54,74	2.36	10 (25%)	34,90,114	1.38	5 (14%)
22	CLA	G	606	6	69,73,73	1.17	7 (10%)	82,113,113	1.22	5 (6%)
21	BCR	B	801	-	41,41,41	0.69	0	56,56,56	1.97	17 (30%)
22	CLA	B	838	1	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
22	CLA	X	417	19	54,58,73	1.33	6 (11%)	64,95,113	1.38	7 (10%)
24	DD6	R	612	-	40,45,45	1.52	2 (5%)	51,67,67	1.84	11 (21%)
22	CLA	Q	611	10	59,63,73	1.27	7 (11%)	70,101,113	1.32	6 (8%)
22	CLA	L	410	11	64,68,73	1.21	7 (10%)	76,107,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	837	20	54,58,73	1.32	8 (14%)	64,95,113	1.37	6 (9%)
22	CLA	B	814	1	49,53,73	1.37	7 (14%)	58,89,113	1.40	7 (12%)
22	CLA	Q	609	10	64,68,73	1.21	8 (12%)	76,107,113	1.26	6 (7%)
22	CLA	R	611	11	49,53,73	1.39	7 (14%)	58,89,113	1.38	4 (6%)
22	CLA	P	610	6	45,49,73	1.44	6 (13%)	54,84,113	1.51	6 (11%)
22	CLA	T	605	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
22	CLA	B	809	1	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
22	CLA	O	314	13	49,53,73	1.39	8 (16%)	58,89,113	1.38	4 (6%)
26	LHG	W	420	22	41,41,48	1.23	6 (14%)	44,47,54	0.91	2 (4%)
22	CLA	L	403	11	64,68,73	1.21	8 (12%)	76,107,113	1.30	8 (10%)
22	CLA	A	810	20	69,73,73	1.16	8 (11%)	82,113,113	1.26	7 (8%)
22	CLA	B	811	1	49,53,73	1.38	7 (14%)	58,89,113	1.45	6 (10%)
24	DD6	H	314	-	40,45,45	1.53	2 (5%)	51,67,67	1.87	15 (29%)
22	CLA	I	606	8	65,69,73	1.21	9 (13%)	77,108,113	1.27	5 (6%)
22	CLA	U	403	16	49,53,73	1.40	7 (14%)	58,89,113	1.46	5 (8%)
21	BCR	J	103	-	41,41,41	0.67	0	56,56,56	1.78	13 (23%)
22	CLA	B	859	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)
22	CLA	K	608	10	69,73,73	1.14	8 (11%)	82,113,113	1.25	8 (9%)
22	CLA	Q	612	10	69,73,73	1.16	7 (10%)	82,113,113	1.26	4 (4%)
22	CLA	O	312	13	64,68,73	1.20	7 (10%)	76,107,113	1.31	8 (10%)
26	LHG	X	420	22	41,41,48	1.24	6 (14%)	44,47,54	1.00	2 (4%)
28	LMG	J	101	-	55,55,55	0.70	1 (1%)	63,63,63	1.35	8 (12%)
31	CHL	U	407	-	40,54,74	2.36	10 (25%)	34,90,114	1.39	5 (14%)
22	CLA	B	836	1	55,59,73	1.30	8 (14%)	64,96,113	1.36	6 (9%)
22	CLA	Q	608	10	54,58,73	1.32	7 (12%)	64,95,113	1.36	6 (9%)
22	CLA	R	609	-	45,49,73	1.42	7 (15%)	54,84,113	1.48	7 (12%)
22	CLA	A	832	20	56,60,73	1.29	7 (12%)	65,97,113	1.35	6 (9%)
22	CLA	A	840	20	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	R	601	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	7 (8%)
22	CLA	R	615	11	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
26	LHG	O	321	-	48,48,48	1.15	6 (12%)	51,54,54	0.93	2 (3%)
22	CLA	U	413	16	49,53,73	1.39	8 (16%)	58,89,113	1.45	5 (8%)
22	CLA	A	822	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
24	DD6	G	612	-	40,45,45	1.56	2 (5%)	51,67,67	1.75	12 (23%)
22	CLA	T	607	15	64,68,73	1.22	8 (12%)	76,107,113	1.28	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	T	610	-	49,53,73	1.39	7 (14%)	58,89,113	1.39	4 (6%)
22	CLA	H	307	7	64,68,73	1.23	7 (10%)	76,107,113	1.28	6 (7%)
27	LMU	U	422	-	36,36,36	0.44	0	47,47,47	0.80	2 (4%)
26	LHG	A	846	22	48,48,48	1.15	6 (12%)	51,54,54	0.93	2 (3%)
24	DD6	K	615	-	40,45,45	1.58	3 (7%)	51,67,67	1.69	12 (23%)
22	CLA	K	617	10	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	I	602	8	64,68,73	1.22	8 (12%)	76,107,113	1.30	7 (9%)
22	CLA	U	410	16	59,63,73	1.27	8 (13%)	70,101,113	1.31	5 (7%)
22	CLA	V	617	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
22	CLA	B	805	1	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
22	CLA	A	814	20	69,73,73	1.16	6 (8%)	82,113,113	1.26	6 (7%)
26	LHG	Q	616	22	43,43,48	1.20	6 (13%)	46,49,54	0.95	2 (4%)
24	DD6	I	612	-	40,45,45	1.53	2 (5%)	51,67,67	1.69	10 (19%)
24	DD6	X	414	-	40,45,45	1.52	2 (5%)	51,67,67	1.79	13 (25%)
22	CLA	O	310	13	64,68,73	1.21	8 (12%)	76,107,113	1.33	6 (7%)
22	CLA	P	602	6	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
22	CLA	A	831	20	69,73,73	1.16	7 (10%)	82,113,113	1.28	7 (8%)
22	CLA	W	406	-	60,64,73	1.25	7 (11%)	71,102,113	1.30	4 (5%)
22	CLA	U	411	16	61,65,73	1.23	7 (11%)	72,103,113	1.30	7 (9%)
22	CLA	B	839	26	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
22	CLA	G	611	6	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
28	LMG	L	401	-	51,51,55	0.71	1 (1%)	59,59,63	1.32	5 (8%)
24	DD6	X	415	-	40,45,45	1.50	2 (5%)	51,67,67	1.68	11 (21%)
28	LMG	H	317	-	43,43,55	0.79	1 (2%)	51,51,63	1.32	8 (15%)
22	CLA	G	607	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	5 (6%)
22	CLA	S	608	26	49,53,73	1.41	8 (16%)	58,89,113	1.39	5 (8%)
22	CLA	H	306	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
22	CLA	W	413	-	49,53,73	1.38	8 (16%)	58,89,113	1.40	4 (6%)
22	CLA	A	833	20	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	N	610	8	59,63,73	1.27	7 (11%)	70,101,113	1.42	7 (10%)
22	CLA	S	609	14	59,63,73	1.27	7 (11%)	70,101,113	1.30	7 (10%)
22	CLA	H	318	7	49,53,73	1.39	8 (16%)	58,89,113	1.42	5 (8%)
24	DD6	Q	614	-	40,45,45	1.53	2 (5%)	51,67,67	1.76	11 (21%)
22	CLA	N	609	8	49,53,73	1.39	7 (14%)	58,89,113	1.38	4 (6%)
22	CLA	A	835	20	65,69,73	1.20	8 (12%)	77,108,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMU	L	419	-	27,27,36	0.42	0	29,30,47	0.75	0
24	DD6	Q	615	-	40,45,45	1.55	2 (5%)	51,67,67	1.87	13 (25%)
22	CLA	S	601	14	49,53,73	1.39	6 (12%)	58,89,113	1.44	4 (6%)
22	CLA	Q	603	10	49,53,73	1.38	7 (14%)	58,89,113	1.45	6 (10%)
22	CLA	R	602	-	64,68,73	1.22	7 (10%)	76,107,113	1.26	5 (6%)
22	CLA	S	615	-	55,59,73	1.31	7 (12%)	64,96,113	1.38	6 (9%)
22	CLA	O	313	13	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
27	LMU	L	420	-	35,35,36	0.37	0	44,45,47	0.83	2 (4%)
22	CLA	I	601	8	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
22	CLA	W	405	18	64,68,73	1.22	9 (14%)	76,107,113	1.27	5 (6%)
22	CLA	B	812	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
22	CLA	I	603	8	60,64,73	1.27	8 (13%)	71,102,113	1.29	6 (8%)
22	CLA	V	603	17	61,65,73	1.25	7 (11%)	72,103,113	1.29	6 (8%)
24	DD6	L	415	-	40,45,45	1.54	2 (5%)	51,67,67	1.95	14 (27%)
22	CLA	G	609	-	49,53,73	1.39	7 (14%)	58,89,113	1.39	5 (8%)
22	CLA	B	828	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	9 (10%)
27	LMU	O	303	-	36,36,36	0.42	0	47,47,47	0.72	1 (2%)
28	LMG	U	423	-	49,49,55	0.73	1 (2%)	57,57,63	1.31	3 (5%)
21	BCR	B	842	-	41,41,41	0.71	0	56,56,56	2.00	16 (28%)
22	CLA	K	605	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
30	SQD	V	618	-	25,27,54	0.54	1 (4%)	33,36,65	0.46	0
22	CLA	A	839	20	69,73,73	1.16	5 (7%)	82,113,113	1.38	8 (9%)
21	BCR	B	845	-	41,41,41	0.66	0	56,56,56	1.91	14 (25%)
22	CLA	O	305	13	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
22	CLA	I	609	8	49,53,73	1.39	7 (14%)	58,89,113	1.45	6 (10%)
22	CLA	S	614	-	49,53,73	1.38	7 (14%)	58,89,113	1.43	6 (10%)
22	CLA	L	406	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
22	CLA	A	828	20	69,73,73	1.17	9 (13%)	82,113,113	1.27	7 (8%)
23	PQN	B	840	-	34,34,34	1.64	2 (5%)	43,45,45	1.11	4 (9%)
22	CLA	V	613	-	49,53,73	1.41	7 (14%)	58,89,113	1.47	4 (6%)
22	CLA	U	414	16	65,69,73	1.22	8 (12%)	77,108,113	1.29	5 (6%)
22	CLA	V	601	17	49,53,73	1.41	6 (12%)	58,89,113	1.42	4 (6%)
27	LMU	A	856	-	21,21,36	0.47	0	26,26,47	0.49	0
32	NEX	U	418	-	40,46,46	0.35	1 (2%)	50,70,70	0.64	1 (2%)
22	CLA	A	838	20	56,60,73	1.30	8 (14%)	65,97,113	1.41	7 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	801	-	69,73,73	1.13	8 (11%)	82,113,113	1.34	9 (10%)
22	CLA	B	804	1	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
28	LMG	B	852	-	43,43,55	0.84	0	51,51,63	1.27	4 (7%)
22	CLA	B	816	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
22	CLA	B	825	1	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
22	CLA	L	409	26	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)
22	CLA	K	611	10	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
22	CLA	L	404	-	60,64,73	1.25	7 (11%)	71,102,113	1.34	5 (7%)
27	LMU	L	418	-	24,24,36	0.48	0	29,29,47	0.73	0
22	CLA	L	405	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
28	LMG	N	615	-	44,44,55	0.78	0	52,52,63	1.26	4 (7%)
22	CLA	P	605	-	49,53,73	1.38	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	G	602	6	64,68,73	1.21	8 (12%)	76,107,113	1.32	8 (10%)
22	CLA	X	402	19	59,63,73	1.26	8 (13%)	70,101,113	1.34	5 (7%)
24	DD6	T	612	-	40,45,45	1.55	2 (5%)	51,67,67	1.86	14 (27%)
22	CLA	B	837	-	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
22	CLA	I	611	8	49,53,73	1.43	8 (16%)	58,89,113	1.42	7 (12%)
24	DD6	B	841	-	40,45,45	1.53	2 (5%)	51,67,67	1.99	15 (29%)
22	CLA	B	820	1	57,61,73	1.31	6 (10%)	67,98,113	1.48	6 (8%)
22	CLA	O	309	13	54,58,73	1.31	8 (14%)	64,95,113	1.39	5 (7%)
24	DD6	N	612	-	40,45,45	1.57	3 (7%)	51,67,67	1.83	13 (25%)
27	LMU	O	301	-	24,24,36	0.44	0	29,29,47	0.56	0
22	CLA	L	412	11	49,53,73	1.39	8 (16%)	58,89,113	1.35	4 (6%)
22	CLA	H	305	7	64,68,73	1.22	7 (10%)	76,107,113	1.30	7 (9%)
26	LHG	U	419	22	24,24,48	1.49	6 (25%)	27,29,54	1.24	2 (7%)
22	CLA	N	611	-	44,48,73	1.45	6 (13%)	51,82,113	1.49	5 (9%)
22	CLA	B	827	1	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
22	CLA	P	611	6	49,53,73	1.40	6 (12%)	58,89,113	1.48	5 (8%)
22	CLA	A	823	20	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
22	CLA	N	603	8	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
22	CLA	L	408	11	64,68,73	1.20	9 (14%)	76,107,113	1.40	10 (13%)
22	CLA	P	603	6	49,53,73	1.40	6 (12%)	58,89,113	1.28	4 (6%)
22	CLA	V	604	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	6 (8%)
22	CLA	B	818	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
27	LMU	B	858	-	14,14,36	0.30	0	13,13,47	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMU	W	421	-	24,24,36	0.44	0	29,29,47	0.56	0
22	CLA	X	409	19	69,73,73	1.17	7 (10%)	82,113,113	1.25	7 (8%)
24	DD6	T	613	-	40,45,45	1.52	2 (5%)	51,67,67	1.69	12 (23%)
22	CLA	A	812	20	61,65,73	1.23	8 (13%)	72,103,113	1.28	5 (6%)
23	PQN	A	843	-	34,34,34	1.62	2 (5%)	43,45,45	1.14	4 (9%)
22	CLA	Q	607	-	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
27	LMU	A	857	-	24,24,36	0.45	0	29,29,47	0.65	0
22	CLA	Q	610	26	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
29	SF4	B	860	1,20	0,12,12	-	-	-	-	-
22	CLA	B	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
22	CLA	B	815	1	56,60,73	1.30	8 (14%)	65,97,113	1.30	4 (6%)
24	DD6	O	317	-	40,45,45	1.55	2 (5%)	51,67,67	1.81	11 (21%)
29	SF4	C	101	2	0,12,12	-	-	-	-	-
28	LMG	K	622	-	43,43,55	0.80	1 (2%)	51,51,63	1.28	5 (9%)
22	CLA	X	408	19	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	A	829	20	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
26	LHG	N	614	22	27,27,48	1.43	6 (22%)	30,33,54	1.12	2 (6%)
22	CLA	K	612	10	49,53,73	1.39	7 (14%)	58,89,113	1.36	6 (10%)
28	LMG	G	616	-	46,46,55	0.81	1 (2%)	54,54,63	1.29	7 (12%)
22	CLA	W	414	18	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
24	DD6	J	105	-	40,45,45	1.52	2 (5%)	51,67,67	1.87	13 (25%)
22	CLA	U	406	-	60,64,73	1.26	8 (13%)	71,102,113	1.31	6 (8%)
22	CLA	B	802	1	69,73,73	1.18	10 (14%)	82,113,113	1.30	6 (7%)
22	CLA	Q	601	-	49,53,73	1.41	9 (18%)	58,89,113	1.40	4 (6%)
26	LHG	G	614	22	31,31,48	1.37	6 (19%)	34,37,54	1.07	2 (5%)
24	DD6	I	613	-	40,45,45	1.58	2 (5%)	51,67,67	1.91	16 (31%)
33	CL0	A	802	20	58,73,73	2.85	19 (32%)	60,113,113	1.76	11 (18%)
22	CLA	A	836	20	69,73,73	1.16	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	B	803	1	60,64,73	1.25	7 (11%)	71,102,113	1.32	6 (8%)
22	CLA	X	419	19	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
22	CLA	A	830	20	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
28	LMG	U	402	-	53,53,55	0.72	0	61,61,63	1.31	4 (6%)
27	LMU	H	320	-	24,24,36	0.44	0	29,29,47	0.59	0
22	CLA	L	417	11	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
22	CLA	N	605	-	49,53,73	1.38	7 (14%)	58,89,113	1.45	6 (10%)
22	CLA	A	825	20	65,69,73	1.19	7 (10%)	77,108,113	1.27	5 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	DD6	U	417	-	40,45,45	1.50	2 (5%)	51,67,67	1.79	16 (31%)
22	CLA	O	307	13	49,53,73	1.39	7 (14%)	58,89,113	1.39	5 (8%)
26	LHG	B	851	-	41,41,48	1.22	6 (14%)	44,47,54	1.00	3 (6%)
30	SQD	O	302	-	40,42,54	0.44	1 (2%)	50,53,65	0.51	1 (2%)
22	CLA	A	834	20	49,53,73	1.38	8 (16%)	58,89,113	1.38	4 (6%)
22	CLA	S	607	14	64,68,73	1.22	6 (9%)	76,107,113	1.28	5 (6%)
27	LMU	A	853	-	24,24,36	0.44	0	29,29,47	0.56	0
22	CLA	U	409	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
24	DD6	R	613	-	40,45,45	1.55	2 (5%)	51,67,67	2.03	17 (33%)
22	CLA	U	412	26	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	F	404	-	1/1/13/20	10/27/103/115	-
22	CLA	K	604	-	1/1/14/20	19/37/113/115	-
22	CLA	B	821	1	1/1/14/20	8/33/109/115	-
22	CLA	W	403	18	1/1/12/20	6/24/100/115	-
28	LMG	I	615	-	-	26/46/62/70	0/1/1/1
22	CLA	A	819	20	1/1/13/20	11/31/107/115	-
22	CLA	A	820	20	1/1/15/20	10/39/115/115	-
26	LHG	K	619	-	-	18/37/37/53	-
22	CLA	P	604	-	1/1/11/20	5/15/91/115	-
22	CLA	B	831	1	1/1/15/20	6/39/115/115	-
22	CLA	I	604	-	1/1/11/20	1/15/91/115	-
22	CLA	O	319	13	1/1/11/20	0/15/91/115	-
28	LMG	T	616	-	-	16/36/56/70	0/1/1/1
27	LMU	B	849	-	-	1/15/35/61	0/1/1/2
22	CLA	P	609	-	1/1/11/20	9/15/91/115	-
22	CLA	X	405	-	1/1/13/20	8/29/105/115	-
21	BCR	A	848	-	-	0/29/63/63	0/2/2/2
22	CLA	S	610	14	1/1/11/20	3/15/91/115	-
22	CLA	W	412	26	1/1/14/20	5/33/109/115	-
22	CLA	A	818	20	1/1/12/20	3/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	I	607	8	1/1/13/20	3/27/103/115	-
24	DD6	S	611	-	-	1/26/80/80	0/3/3/3
22	CLA	A	844	26	1/1/13/20	11/27/103/115	-
28	LMG	H	322	-	-	15/32/52/70	0/1/1/1
28	LMG	I	614	-	-	12/32/52/70	0/1/1/1
22	CLA	Q	617	10	1/1/12/20	4/24/100/115	-
22	CLA	B	807	1	1/1/15/20	15/39/115/115	-
31	CHL	U	408	-	3/3/16/26	1/15/113/137	-
22	CLA	K	606	-	1/1/12/20	0/21/97/115	-
24	DD6	U	416	-	-	1/26/80/80	0/3/3/3
22	CLA	W	410	18	1/1/14/20	9/33/109/115	-
22	CLA	U	420	16	1/1/11/20	7/15/91/115	-
26	LHG	K	616	22	-	15/43/43/53	-
22	CLA	B	824	-	1/1/15/20	11/39/115/115	-
22	CLA	R	604	-	1/1/11/20	5/15/91/115	-
22	CLA	W	411	18	1/1/14/20	9/33/109/115	-
27	LMU	H	321	-	-	1/19/56/61	0/2/2/2
22	CLA	B	810	-	1/1/13/20	4/29/105/115	-
21	BCR	M	101	-	-	2/29/63/63	0/2/2/2
24	DD6	W	418	-	-	1/26/80/80	0/3/3/3
26	LHG	N	616	-	-	23/47/47/53	-
22	CLA	H	311	7	1/1/15/20	13/39/115/115	-
22	CLA	R	607	11	1/1/14/20	14/33/109/115	-
22	CLA	X	413	19	1/1/11/20	3/15/91/115	-
27	LMU	B	855	-	-	2/15/35/61	0/1/1/2
22	CLA	O	306	13	1/1/14/20	7/33/109/115	-
26	LHG	S	613	22	-	13/36/36/53	-
22	CLA	J	102	9	1/1/12/20	7/21/97/115	-
27	LMU	B	857	-	-	4/21/61/61	0/2/2/2
24	DD6	V	614	-	-	1/26/80/80	0/3/3/3
22	CLA	X	412	19	1/1/15/20	10/39/115/115	-
22	CLA	B	817	1	1/1/15/20	15/39/115/115	-
22	CLA	T	606	15	1/1/12/20	4/21/97/115	-
22	CLA	S	602	14	1/1/14/20	7/33/109/115	-
22	CLA	V	609	17	1/1/13/20	7/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMU	T	615	-	-	0/12/32/61	0/1/1/2
27	LMU	H	301	-	-	1/12/32/61	0/1/1/2
22	CLA	X	411	-	1/1/11/20	2/15/91/115	-
22	CLA	N	606	8	1/1/15/20	9/39/115/115	-
27	LMU	B	854	-	-	3/15/35/61	0/1/1/2
30	SQD	F	407	-	-	3/37/57/69	0/1/1/1
31	CHL	W	422	-	3/3/20/26	8/39/137/137	-
21	BCR	B	843	-	-	4/29/63/63	0/2/2/2
31	CHL	X	406	-	3/3/16/26	0/15/113/137	-
22	CLA	B	829	-	1/1/11/20	6/15/91/115	-
27	LMU	A	854	-	-	2/21/61/61	0/2/2/2
24	DD6	X	401	-	-	0/26/80/80	0/3/3/3
22	CLA	X	403	19	1/1/15/20	8/39/115/115	-
27	LMU	G	615	-	-	0/12/32/61	0/1/1/2
22	CLA	G	604	-	1/1/11/20	0/15/91/115	-
22	CLA	L	411	11	1/1/15/20	11/39/115/115	-
22	CLA	N	607	-	1/1/14/20	13/33/109/115	-
22	CLA	A	803	-	1/1/15/20	12/39/115/115	-
22	CLA	H	308	7	1/1/14/20	5/33/109/115	-
22	CLA	A	813	20	1/1/15/20	10/39/115/115	-
22	CLA	B	806	1	1/1/15/20	11/39/115/115	-
27	LMU	J	104	-	-	9/21/57/61	0/2/2/2
28	LMG	A	855	-	-	12/36/56/70	0/1/1/1
22	CLA	B	833	1	1/1/15/20	9/39/115/115	-
22	CLA	O	311	26	1/1/14/20	9/33/109/115	-
27	LMU	F	402	-	-	1/12/32/61	0/1/1/2
24	DD6	L	413	-	-	1/26/80/80	0/3/3/3
22	CLA	B	813	1	1/1/15/20	9/39/115/115	-
22	CLA	H	302	7	1/1/11/20	2/15/91/115	-
22	CLA	S	606	14	1/1/12/20	4/21/97/115	-
22	CLA	B	808	1	1/1/13/20	6/27/103/115	-
22	CLA	B	835	1	1/1/15/20	11/39/115/115	-
22	CLA	H	312	7	1/1/11/20	3/15/91/115	-
26	LHG	B	848	22	-	10/31/31/53	-
22	CLA	N	604	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	P	608	-	1/1/11/20	9/15/91/115	-
22	CLA	V	612	-	1/1/15/20	13/39/115/115	-
25	DGD	O	304	-	-	31/49/89/95	0/2/2/2
22	CLA	V	602	17	1/1/15/20	7/39/115/115	-
22	CLA	V	608	17	1/1/13/20	9/27/103/115	-
22	CLA	S	605	-	1/1/14/20	13/33/109/115	-
27	LMU	T	618	-	-	1/15/35/61	0/1/1/2
22	CLA	H	313	7	1/1/13/20	10/31/107/115	-
24	DD6	H	315	-	-	1/26/80/80	0/3/3/3
22	CLA	K	613	-	1/1/12/20	4/25/101/115	-
22	CLA	G	601	6	1/1/11/20	4/15/91/115	-
26	LHG	T	614	22	-	27/46/46/53	-
27	LMU	O	322	-	-	4/21/61/61	0/2/2/2
22	CLA	A	811	20	1/1/13/20	10/30/106/115	-
22	CLA	U	415	16	1/1/11/20	7/15/91/115	-
22	CLA	A	824	20	1/1/15/20	21/39/115/115	-
27	LMU	F	409	-	-	4/12/32/61	0/1/1/2
22	CLA	W	415	18	1/1/11/20	6/15/91/115	-
22	CLA	G	608	26	1/1/14/20	16/33/109/115	-
24	DD6	X	416	-	-	5/26/80/80	0/3/3/3
22	CLA	B	822	1	1/1/15/20	10/39/115/115	-
22	CLA	P	606	6	1/1/11/20	6/15/91/115	-
24	DD6	S	612	-	-	1/26/80/80	0/3/3/3
27	LMU	B	850	-	-	3/15/35/61	0/1/1/2
28	LMG	W	401	-	-	18/43/63/70	0/1/1/1
22	CLA	V	607	-	1/1/11/20	3/15/91/115	-
24	DD6	W	417	-	-	1/26/80/80	0/3/3/3
22	CLA	G	605	-	1/1/11/20	2/15/91/115	-
22	CLA	L	402	11	1/1/15/20	14/39/115/115	-
22	CLA	R	610	11	1/1/15/20	14/39/115/115	-
22	CLA	W	402	18	1/1/13/20	2/27/103/115	-
22	CLA	Q	606	-	1/1/11/20	6/15/91/115	-
22	CLA	R	608	26	1/1/12/20	10/26/102/115	-
25	DGD	B	847	-	-	33/55/95/95	0/2/2/2
22	CLA	L	407	-	1/1/13/20	5/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	H	319	-	-	19/35/55/70	0/1/1/1
27	LMU	T	617	-	-	3/15/35/61	0/1/1/2
22	CLA	H	303	7	1/1/14/20	9/33/109/115	-
27	LMU	K	620	-	-	6/19/56/61	0/2/2/2
26	LHG	A	845	-	-	25/53/53/53	-
22	CLA	A	852	-	1/1/15/20	14/39/115/115	-
22	CLA	U	405	16	1/1/13/20	2/30/106/115	-
22	CLA	A	806	20	1/1/15/20	12/39/115/115	-
22	CLA	U	401	-	1/1/13/20	9/27/103/115	-
24	DD6	P	613	-	-	4/26/80/80	0/3/3/3
24	DD6	A	858	-	-	5/26/80/80	0/3/3/3
22	CLA	N	608	26	1/1/11/20	7/15/91/115	-
22	CLA	Q	613	10	1/1/11/20	6/15/91/115	-
22	CLA	I	608	-	1/1/11/20	4/15/91/115	-
22	CLA	A	807	20	1/1/15/20	8/39/115/115	-
22	CLA	I	605	-	1/1/11/20	2/15/91/115	-
29	SF4	C	102	2	-	-	0/6/5/5
22	CLA	R	606	11	1/1/13/20	9/30/106/115	-
22	CLA	B	830	1	1/1/15/20	8/39/115/115	-
22	CLA	T	609	15	1/1/11/20	4/15/91/115	-
22	CLA	U	404	16	1/1/15/20	12/39/115/115	-
22	CLA	W	409	-	1/1/15/20	9/39/115/115	-
22	CLA	T	611	15	1/1/15/20	13/39/115/115	-
22	CLA	T	601	15	1/1/11/20	3/15/91/115	-
22	CLA	T	603	15	1/1/14/20	8/33/109/115	-
27	LMU	U	424	-	-	2/15/35/61	0/1/1/2
27	LMU	B	853	-	-	0/10/27/61	0/1/1/2
22	CLA	K	602	10	1/1/14/20	9/33/109/115	-
28	LMG	B	856	-	-	27/48/68/70	0/1/1/1
26	LHG	O	323	-	-	18/47/47/53	-
26	LHG	O	318	22	-	16/38/38/53	-
27	LMU	X	418	-	-	1/15/35/61	0/1/1/2
22	CLA	H	309	26	1/1/13/20	9/27/103/115	-
22	CLA	T	608	26	1/1/14/20	2/33/109/115	-
28	LMG	F	408	-	-	18/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	F	405	5	1/1/11/20	6/15/91/115	-
22	CLA	G	603	6	1/1/13/20	6/29/105/115	-
22	CLA	B	819	1	1/1/12/20	10/25/101/115	-
22	CLA	A	841	20	1/1/15/20	10/39/115/115	-
22	CLA	A	808	20	1/1/15/20	10/39/115/115	-
22	CLA	Q	605	-	1/1/13/20	3/29/105/115	-
22	CLA	A	805	20	1/1/14/20	11/35/111/115	-
31	CHL	W	407	-	3/3/16/26	2/15/113/137	-
22	CLA	O	308	-	1/1/14/20	14/35/111/115	-
21	BCR	A	850	-	-	4/29/63/63	0/2/2/2
22	CLA	V	610	-	1/1/11/20	4/15/91/115	-
24	DD6	A	859	-	-	1/26/80/80	0/3/3/3
22	CLA	W	404	18	1/1/15/20	7/39/115/115	-
26	LHG	L	416	22	-	20/46/46/53	-
22	CLA	V	611	-	1/1/11/20	6/15/91/115	-
22	CLA	N	601	8	1/1/11/20	6/15/91/115	-
22	CLA	H	304	7	1/1/11/20	7/15/91/115	-
26	LHG	O	324	-	-	25/46/46/53	-
22	CLA	B	823	-	1/1/15/20	11/39/115/115	-
22	CLA	B	826	1	1/1/13/20	10/31/107/115	-
26	LHG	H	316	22	-	5/31/31/53	-
28	LMG	Q	602	-	-	11/32/52/70	0/1/1/1
22	CLA	Q	604	10	1/1/15/20	15/39/115/115	-
30	SQD	K	621	-	-	3/38/58/69	0/1/1/1
22	CLA	S	603	14	1/1/11/20	2/15/91/115	-
22	CLA	A	809	20	1/1/12/20	0/25/101/115	-
22	CLA	X	410	26	1/1/14/20	10/33/109/115	-
22	CLA	Q	618	-	1/1/11/20	9/15/91/115	-
21	BCR	B	846	-	-	6/29/63/63	0/2/2/2
22	CLA	A	815	20	1/1/15/20	5/39/115/115	-
24	DD6	W	416	-	-	1/26/80/80	0/3/3/3
25	DGD	F	401	-	-	19/35/35/95	-
24	DD6	L	414	-	-	2/26/80/80	0/3/3/3
27	LMU	X	421	-	-	2/21/61/61	0/2/2/2
22	CLA	A	827	-	1/1/14/20	4/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DD6	N	613	-	-	4/26/80/80	0/3/3/3
22	CLA	I	610	8	1/1/11/20	5/15/91/115	-
22	CLA	F	403	-	1/1/15/20	9/39/115/115	-
31	CHL	V	606	-	3/3/16/26	1/15/113/137	-
24	DD6	O	316	-	-	1/26/80/80	0/3/3/3
27	LMU	O	320	-	-	0/17/35/61	1/2/2/2
22	CLA	B	832	1	1/1/14/20	13/36/112/115	-
22	CLA	A	817	20	1/1/15/20	13/39/115/115	-
22	CLA	A	804	-	1/1/15/20	6/39/115/115	-
22	CLA	A	816	20	1/1/14/20	14/35/111/115	-
22	CLA	W	419	18	1/1/11/20	5/15/91/115	-
22	CLA	R	603	-	1/1/13/20	9/29/105/115	-
24	DD6	A	847	-	-	1/26/80/80	0/3/3/3
22	CLA	T	602	15	1/1/15/20	7/39/115/115	-
22	CLA	T	604	15	1/1/15/20	17/39/115/115	-
21	BCR	A	851	-	-	4/29/63/63	0/2/2/2
24	DD6	G	613	-	-	0/26/80/80	0/3/3/3
27	LMU	U	421	-	-	7/21/61/61	0/2/2/2
22	CLA	A	842	20	1/1/15/20	12/39/115/115	-
22	CLA	S	604	-	1/1/14/20	9/33/109/115	-
22	CLA	H	310	7	1/1/11/20	4/15/91/115	-
22	CLA	A	826	-	1/1/15/20	9/39/115/115	-
26	LHG	R	614	22	-	19/46/46/53	-
21	BCR	A	849	-	-	0/29/63/63	0/2/2/2
22	CLA	K	610	10	1/1/13/20	8/29/105/115	-
32	NEX	V	616	-	-	4/27/83/83	0/3/3/3
24	DD6	K	614	-	-	0/26/80/80	0/3/3/3
26	LHG	P	601	-	-	22/44/44/53	-
28	LMG	K	618	-	-	24/44/64/70	0/1/1/1
22	CLA	O	315	13	1/1/12/20	4/21/97/115	-
22	CLA	P	607	6	1/1/11/20	4/15/91/115	-
21	BCR	B	844	-	-	0/29/63/63	0/2/2/2
22	CLA	A	821	20	1/1/15/20	12/39/115/115	-
24	DD6	P	612	-	-	6/26/80/80	0/3/3/3
22	CLA	K	607	10	1/1/13/20	8/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	609	26	1/1/14/20	11/33/109/115	-
22	CLA	K	603	10	1/1/14/20	6/33/109/115	-
27	LMU	M	102	-	-	4/15/35/61	0/1/1/2
22	CLA	X	407	-	1/1/15/20	4/39/115/115	-
24	DD6	V	615	-	-	3/26/80/80	0/3/3/3
24	DD6	F	406	-	-	8/26/80/80	0/3/3/3
22	CLA	R	605	-	1/1/15/20	15/39/115/115	-
31	CHL	W	408	-	3/3/20/26	4/39/137/137	-
28	LMG	K	601	-	-	24/38/58/70	0/1/1/1
22	CLA	G	610	6	1/1/11/20	5/15/91/115	-
22	CLA	X	404	19	1/1/14/20	9/33/109/115	-
22	CLA	N	602	8	1/1/14/20	3/33/109/115	-
31	CHL	V	605	-	3/3/16/26	0/15/113/137	-
22	CLA	G	606	6	1/1/15/20	12/39/115/115	-
21	BCR	B	801	-	-	4/29/63/63	0/2/2/2
22	CLA	B	838	1	1/1/11/20	6/15/91/115	-
22	CLA	X	417	19	1/1/12/20	3/21/97/115	-
24	DD6	R	612	-	-	1/26/80/80	0/3/3/3
22	CLA	Q	611	10	1/1/13/20	8/27/103/115	-
22	CLA	L	410	11	1/1/14/20	9/33/109/115	-
22	CLA	A	837	20	1/1/12/20	4/21/97/115	-
22	CLA	B	814	1	1/1/11/20	7/15/91/115	-
22	CLA	Q	609	10	1/1/14/20	8/33/109/115	-
22	CLA	R	611	11	1/1/11/20	4/15/91/115	-
22	CLA	P	610	6	1/1/10/20	4/10/86/115	-
22	CLA	T	605	-	1/1/15/20	15/39/115/115	-
22	CLA	B	809	1	1/1/15/20	3/39/115/115	-
22	CLA	O	314	13	1/1/11/20	0/15/91/115	-
26	LHG	W	420	22	-	21/46/46/53	-
22	CLA	L	403	11	1/1/14/20	6/33/109/115	-
22	CLA	A	810	20	1/1/15/20	10/39/115/115	-
22	CLA	B	811	1	1/1/11/20	1/15/91/115	-
24	DD6	H	314	-	-	1/26/80/80	0/3/3/3
22	CLA	I	606	8	1/1/14/20	11/35/111/115	-
22	CLA	U	403	16	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2
22	CLA	B	859	-	1/1/15/20	11/39/115/115	-
22	CLA	K	608	10	1/1/15/20	9/39/115/115	-
22	CLA	Q	612	10	1/1/15/20	14/39/115/115	-
22	CLA	O	312	13	1/1/14/20	6/33/109/115	-
26	LHG	X	420	22	-	27/46/46/53	-
28	LMG	J	101	-	-	24/50/70/70	0/1/1/1
31	CHL	U	407	-	3/3/16/26	0/15/113/137	-
22	CLA	B	836	1	1/1/12/20	1/23/99/115	-
22	CLA	Q	608	10	1/1/12/20	2/21/97/115	-
22	CLA	R	609	-	1/1/10/20	4/10/86/115	-
22	CLA	A	832	20	1/1/12/20	4/24/100/115	-
22	CLA	A	840	20	1/1/15/20	14/39/115/115	-
22	CLA	R	601	-	1/1/15/20	15/39/115/115	-
22	CLA	R	615	11	1/1/15/20	11/39/115/115	-
26	LHG	O	321	-	-	29/53/53/53	-
22	CLA	U	413	16	1/1/11/20	4/15/91/115	-
22	CLA	A	822	-	1/1/15/20	8/39/115/115	-
24	DD6	G	612	-	-	0/26/80/80	0/3/3/3
22	CLA	T	607	15	1/1/14/20	9/33/109/115	-
22	CLA	T	610	-	1/1/11/20	6/15/91/115	-
22	CLA	H	307	7	1/1/14/20	8/33/109/115	-
27	LMU	U	422	-	-	5/21/61/61	0/2/2/2
26	LHG	A	846	22	-	26/53/53/53	-
24	DD6	K	615	-	-	0/26/80/80	0/3/3/3
22	CLA	K	617	10	1/1/15/20	8/39/115/115	-
22	CLA	I	602	8	1/1/14/20	1/33/109/115	-
22	CLA	U	410	16	1/1/13/20	6/27/103/115	-
22	CLA	V	617	-	1/1/11/20	8/15/91/115	-
22	CLA	B	805	1	1/1/15/20	7/39/115/115	-
22	CLA	A	814	20	1/1/15/20	7/39/115/115	-
26	LHG	Q	616	22	-	15/48/48/53	-
24	DD6	I	612	-	-	0/26/80/80	0/3/3/3
24	DD6	X	414	-	-	1/26/80/80	0/3/3/3
22	CLA	O	310	13	1/1/14/20	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	P	602	6	1/1/11/20	9/15/91/115	-
22	CLA	A	831	20	1/1/15/20	6/39/115/115	-
22	CLA	W	406	-	1/1/13/20	2/29/105/115	-
22	CLA	U	411	16	1/1/13/20	7/30/106/115	-
22	CLA	B	839	26	1/1/15/20	2/39/115/115	-
22	CLA	G	611	6	1/1/11/20	5/15/91/115	-
28	LMG	L	401	-	-	19/46/66/70	0/1/1/1
24	DD6	X	415	-	-	1/26/80/80	0/3/3/3
28	LMG	H	317	-	-	13/38/58/70	0/1/1/1
22	CLA	G	607	-	1/1/14/20	2/33/109/115	-
22	CLA	S	608	26	1/1/11/20	8/15/91/115	-
22	CLA	H	306	-	1/1/13/20	9/27/103/115	-
22	CLA	W	413	-	1/1/11/20	4/15/91/115	-
22	CLA	A	833	20	1/1/15/20	6/39/115/115	-
22	CLA	N	610	8	1/1/13/20	16/27/103/115	-
22	CLA	S	609	14	-	9/27/103/115	-
22	CLA	H	318	7	1/1/11/20	6/15/91/115	-
24	DD6	Q	614	-	-	0/26/80/80	0/3/3/3
22	CLA	N	609	8	1/1/11/20	4/15/91/115	-
22	CLA	A	835	20	1/1/14/20	9/35/111/115	-
27	LMU	L	419	-	-	6/21/34/61	1/1/1/2
24	DD6	Q	615	-	-	0/26/80/80	0/3/3/3
22	CLA	S	601	14	1/1/11/20	6/15/91/115	-
22	CLA	Q	603	10	1/1/11/20	4/15/91/115	-
22	CLA	R	602	-	1/1/14/20	11/33/109/115	-
22	CLA	S	615	-	1/1/12/20	4/23/99/115	-
22	CLA	O	313	13	1/1/15/20	14/39/115/115	-
27	LMU	L	420	-	-	4/21/57/61	0/2/2/2
22	CLA	I	601	8	1/1/15/20	14/39/115/115	-
22	CLA	W	405	18	1/1/14/20	1/33/109/115	-
22	CLA	B	812	1	1/1/15/20	17/39/115/115	-
22	CLA	I	603	8	1/1/13/20	7/29/105/115	-
22	CLA	V	603	17	1/1/13/20	10/30/106/115	-
22	CLA	G	609	-	1/1/11/20	4/15/91/115	-
24	DD6	L	415	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	828	1	1/1/15/20	12/39/115/115	-
27	LMU	O	303	-	-	2/21/61/61	0/2/2/2
28	LMG	U	423	-	-	20/44/64/70	0/1/1/1
21	BCR	B	842	-	-	2/29/63/63	0/2/2/2
22	CLA	K	605	-	1/1/15/20	18/39/115/115	-
30	SQD	V	618	-	-	4/19/39/69	0/1/1/1
22	CLA	A	839	20	1/1/15/20	5/39/115/115	-
21	BCR	B	845	-	-	2/29/63/63	0/2/2/2
22	CLA	O	305	13	1/1/12/20	2/21/97/115	-
22	CLA	I	609	8	1/1/11/20	4/15/91/115	-
22	CLA	S	614	-	1/1/11/20	0/15/91/115	-
22	CLA	L	406	-	1/1/15/20	8/39/115/115	-
22	CLA	A	828	20	1/1/15/20	7/39/115/115	-
23	PQN	B	840	-	-	0/23/43/43	0/2/2/2
22	CLA	V	613	-	1/1/11/20	9/15/91/115	-
22	CLA	U	414	16	1/1/14/20	14/35/111/115	-
22	CLA	V	601	17	1/1/11/20	6/15/91/115	-
27	LMU	A	856	-	-	0/12/32/61	0/1/1/2
32	NEX	U	418	-	-	4/27/83/83	0/3/3/3
22	CLA	A	838	20	1/1/12/20	5/24/100/115	-
22	CLA	A	801	-	1/1/15/20	15/39/115/115	-
22	CLA	B	804	1	1/1/15/20	13/39/115/115	-
28	LMG	B	852	-	-	15/38/58/70	0/1/1/1
22	CLA	B	816	1	1/1/15/20	10/39/115/115	-
22	CLA	B	825	1	1/1/15/20	6/39/115/115	-
22	CLA	L	409	26	1/1/14/20	5/33/109/115	-
22	CLA	K	611	10	1/1/15/20	10/39/115/115	-
22	CLA	L	404	-	1/1/13/20	11/29/105/115	-
27	LMU	L	418	-	-	0/15/35/61	0/1/1/2
22	CLA	L	405	-	1/1/11/20	2/15/91/115	-
28	LMG	N	615	-	-	24/39/59/70	0/1/1/1
22	CLA	P	605	-	1/1/11/20	5/15/91/115	-
22	CLA	G	602	6	1/1/14/20	4/33/109/115	-
22	CLA	X	402	19	1/1/13/20	9/27/103/115	-
24	DD6	T	612	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	837	-	1/1/11/20	2/15/91/115	-
22	CLA	I	611	8	1/1/11/20	4/15/91/115	-
24	DD6	B	841	-	-	1/26/80/80	0/3/3/3
22	CLA	B	820	1	1/1/12/20	9/25/101/115	-
22	CLA	O	309	13	1/1/12/20	4/21/97/115	-
24	DD6	N	612	-	-	0/26/80/80	0/3/3/3
27	LMU	O	301	-	-	1/15/35/61	0/1/1/2
22	CLA	L	412	11	1/1/11/20	5/15/91/115	-
22	CLA	H	305	7	1/1/14/20	10/33/109/115	-
26	LHG	U	419	22	-	15/28/28/53	-
22	CLA	N	611	-	1/1/9/20	4/10/82/115	-
22	CLA	B	827	1	1/1/15/20	6/39/115/115	-
22	CLA	P	611	6	1/1/11/20	7/15/91/115	-
22	CLA	A	823	20	1/1/11/20	5/15/91/115	-
22	CLA	N	603	8	1/1/15/20	8/39/115/115	-
22	CLA	L	408	11	1/1/14/20	5/33/109/115	-
22	CLA	P	603	6	-	6/15/91/115	-
22	CLA	V	604	-	1/1/13/20	7/29/105/115	-
22	CLA	B	818	-	1/1/15/20	11/39/115/115	-
27	LMU	B	858	-	-	2/12/12/61	-
27	LMU	W	421	-	-	4/15/35/61	0/1/1/2
22	CLA	X	409	19	1/1/15/20	9/39/115/115	-
24	DD6	T	613	-	-	1/26/80/80	0/3/3/3
22	CLA	A	812	20	1/1/13/20	7/30/106/115	-
23	PQN	A	843	-	-	4/23/43/43	0/2/2/2
22	CLA	Q	607	-	1/1/11/20	4/15/91/115	-
27	LMU	A	857	-	-	3/15/35/61	0/1/1/2
22	CLA	Q	610	26	1/1/15/20	12/39/115/115	-
29	SF4	B	860	1,20	-	-	0/6/5/5
22	CLA	B	834	1	1/1/15/20	6/39/115/115	-
22	CLA	B	815	1	1/1/12/20	3/24/100/115	-
24	DD6	O	317	-	-	0/26/80/80	0/3/3/3
29	SF4	C	101	2	-	-	0/6/5/5
28	LMG	K	622	-	-	15/38/58/70	0/1/1/1
22	CLA	X	408	19	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	829	20	1/1/15/20	14/39/115/115	-
26	LHG	N	614	22	-	9/32/32/53	-
22	CLA	K	612	10	1/1/11/20	2/15/91/115	-
28	LMG	G	616	-	-	21/41/61/70	0/1/1/1
22	CLA	W	414	18	1/1/15/20	9/39/115/115	-
24	DD6	J	105	-	-	3/26/80/80	0/3/3/3
22	CLA	U	406	-	1/1/13/20	7/29/105/115	-
22	CLA	B	802	1	1/1/15/20	5/39/115/115	-
22	CLA	Q	601	-	1/1/11/20	5/15/91/115	-
26	LHG	G	614	22	-	13/36/36/53	-
24	DD6	I	613	-	-	0/26/80/80	0/3/3/3
33	CL0	A	802	20	3/3/20/25	8/37/135/135	-
22	CLA	A	836	20	1/1/15/20	10/39/115/115	-
22	CLA	B	803	1	1/1/13/20	7/29/105/115	-
22	CLA	X	419	19	1/1/11/20	8/15/91/115	-
22	CLA	A	830	20	1/1/15/20	13/39/115/115	-
28	LMG	U	402	-	-	26/48/68/70	0/1/1/1
27	LMU	H	320	-	-	2/15/35/61	0/1/1/2
22	CLA	L	417	11	1/1/15/20	8/39/115/115	-
22	CLA	N	605	-	1/1/11/20	2/15/91/115	-
22	CLA	A	825	20	1/1/14/20	14/35/111/115	-
24	DD6	U	417	-	-	1/26/80/80	0/3/3/3
22	CLA	O	307	13	1/1/11/20	5/15/91/115	-
26	LHG	B	851	-	-	22/46/46/53	-
30	SQD	O	302	-	-	5/37/57/69	0/1/1/1
22	CLA	A	834	20	1/1/11/20	4/15/91/115	-
22	CLA	S	607	14	1/1/14/20	10/33/109/115	-
27	LMU	A	853	-	-	0/15/35/61	0/1/1/2
22	CLA	U	409	-	1/1/11/20	5/15/91/115	-
24	DD6	R	613	-	-	1/26/80/80	0/3/3/3
22	CLA	U	412	26	1/1/11/20	3/15/91/115	-

All (2484) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	859	DD6	C30-C31	-8.58	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	612	DD6	C30-C31	-8.58	1.25	1.42
24	P	613	DD6	C30-C31	-8.56	1.25	1.42
24	N	612	DD6	C30-C31	-8.54	1.25	1.42
24	G	613	DD6	C30-C31	-8.51	1.26	1.42
24	Q	615	DD6	C30-C31	-8.49	1.26	1.42
24	L	414	DD6	C30-C31	-8.48	1.26	1.42
24	T	612	DD6	C30-C31	-8.48	1.26	1.42
24	O	317	DD6	C30-C31	-8.48	1.26	1.42
24	I	613	DD6	C30-C31	-8.43	1.26	1.42
24	S	611	DD6	C30-C31	-8.43	1.26	1.42
24	X	416	DD6	C30-C31	-8.43	1.26	1.42
24	S	612	DD6	C30-C31	-8.42	1.26	1.42
24	L	415	DD6	C30-C31	-8.42	1.26	1.42
24	R	613	DD6	C30-C31	-8.41	1.26	1.42
24	G	612	DD6	C30-C31	-8.40	1.26	1.42
24	V	614	DD6	C30-C31	-8.39	1.26	1.42
24	U	416	DD6	C30-C31	-8.38	1.26	1.42
24	A	847	DD6	C30-C31	-8.37	1.26	1.42
24	R	612	DD6	C30-C31	-8.37	1.26	1.42
24	F	406	DD6	C30-C31	-8.35	1.26	1.42
24	B	841	DD6	C30-C31	-8.35	1.26	1.42
24	I	612	DD6	C30-C31	-8.34	1.26	1.42
24	N	613	DD6	C30-C31	-8.33	1.26	1.42
24	Q	614	DD6	C30-C31	-8.30	1.26	1.42
24	H	314	DD6	C30-C31	-8.30	1.26	1.42
24	L	413	DD6	C30-C31	-8.30	1.26	1.42
24	K	615	DD6	C30-C31	-8.30	1.26	1.42
24	W	418	DD6	C30-C31	-8.28	1.26	1.42
24	H	315	DD6	C30-C31	-8.28	1.26	1.42
24	T	613	DD6	C30-C31	-8.26	1.26	1.42
24	O	316	DD6	C30-C31	-8.26	1.26	1.42
24	X	414	DD6	C30-C31	-8.25	1.26	1.42
24	K	614	DD6	C30-C31	-8.24	1.26	1.42
24	X	401	DD6	C30-C31	-8.24	1.26	1.42
24	J	105	DD6	C30-C31	-8.23	1.26	1.42
24	W	416	DD6	C30-C31	-8.22	1.26	1.42
24	A	858	DD6	C30-C31	-8.19	1.26	1.42
24	W	417	DD6	C30-C31	-8.17	1.26	1.42
24	V	615	DD6	C30-C31	-8.14	1.26	1.42
24	X	415	DD6	C30-C31	-8.10	1.26	1.42
24	U	417	DD6	C30-C31	-7.97	1.27	1.42
33	A	802	CL0	C1B-C2B	7.93	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	840	PQN	C3-C2	7.84	1.49	1.35
23	A	843	PQN	C3-C2	7.75	1.49	1.35
33	A	802	CL0	C1D-C2D	7.32	1.47	1.39
31	V	606	CHL	MG-NB	-7.28	1.91	2.05
31	W	408	CHL	MG-NB	-7.15	1.91	2.05
31	U	408	CHL	MG-NB	-7.14	1.91	2.05
33	A	802	CL0	C1A-CHA	7.10	1.48	1.40
31	V	605	CHL	MG-NB	-7.05	1.91	2.05
31	W	408	CHL	C1B-C2B	7.02	1.47	1.39
31	W	407	CHL	MG-NB	-7.00	1.91	2.05
31	W	422	CHL	MG-NB	-6.98	1.91	2.05
31	U	407	CHL	MG-NB	-6.98	1.92	2.05
31	W	422	CHL	C1B-C2B	6.96	1.47	1.39
33	A	802	CL0	C3B-C4B	6.96	1.48	1.41
31	W	407	CHL	C1B-C2B	6.95	1.47	1.39
31	X	406	CHL	MG-NB	-6.92	1.92	2.05
31	X	406	CHL	C1B-C2B	6.89	1.47	1.39
31	V	606	CHL	C1B-C2B	6.88	1.47	1.39
31	V	605	CHL	C1B-C2B	6.86	1.47	1.39
31	U	407	CHL	C1B-C2B	6.75	1.47	1.39
31	U	408	CHL	C1B-C2B	6.71	1.47	1.39
31	W	407	CHL	MG-ND	-5.84	1.94	2.05
31	X	406	CHL	MG-ND	-5.76	1.94	2.05
31	W	408	CHL	MG-ND	-5.74	1.94	2.05
33	A	802	CL0	C3A-C2A	-5.73	1.49	1.54
31	U	407	CHL	MG-ND	-5.72	1.94	2.05
31	W	422	CHL	MG-ND	-5.71	1.94	2.05
31	V	605	CHL	MG-ND	-5.69	1.94	2.05
31	U	408	CHL	MG-ND	-5.66	1.94	2.05
31	V	606	CHL	MG-ND	-5.64	1.94	2.05
33	A	802	CL0	CHB-C4A	-5.42	1.32	1.38
28	I	615	LMG	C1-C2	5.11	1.55	1.52
23	B	840	PQN	C10-C5	4.98	1.48	1.40
23	A	843	PQN	C10-C5	4.88	1.48	1.40
33	A	802	CL0	C3D-C2D	4.57	1.47	1.39
33	A	802	CL0	CHB-C1B	4.52	1.46	1.39
33	A	802	CL0	O2D-CGD	4.28	1.43	1.33
25	F	401	DGD	O1G-C1A	4.25	1.45	1.33
33	A	802	CL0	C3B-C2B	4.24	1.46	1.40
33	A	802	CL0	O2A-CGA	4.21	1.45	1.33
31	U	408	CHL	CHB-C4A	-4.16	1.33	1.38
31	V	606	CHL	CHB-C4A	-4.12	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	U	407	CHL	CHB-C4A	-4.10	1.33	1.38
31	V	606	CHL	C3A-C2A	-4.07	1.51	1.54
31	V	605	CHL	CHB-C4A	-4.03	1.33	1.38
31	X	406	CHL	CHB-C4A	-4.03	1.33	1.38
31	U	408	CHL	C1A-CHA	-4.02	1.35	1.40
25	O	304	DGD	O1G-C1A	4.01	1.45	1.33
25	B	847	DGD	O1G-C1A	3.99	1.45	1.33
31	U	408	CHL	C3A-C2A	-3.98	1.51	1.54
31	V	605	CHL	C1A-CHA	-3.97	1.35	1.40
31	W	422	CHL	CHB-C4A	-3.97	1.33	1.38
31	W	407	CHL	CHB-C4A	-3.96	1.33	1.38
25	F	401	DGD	O2G-C1B	3.94	1.45	1.34
31	W	408	CHL	CHB-C4A	-3.91	1.33	1.38
31	W	422	CHL	C1A-CHA	-3.91	1.35	1.40
31	U	407	CHL	C3B-C4B	3.90	1.45	1.41
31	X	406	CHL	C3A-C2A	-3.90	1.51	1.54
31	V	606	CHL	C1A-CHA	-3.89	1.35	1.40
22	I	611	CLA	C1D-ND	3.88	1.43	1.37
31	U	407	CHL	C3A-C2A	-3.88	1.51	1.54
22	W	415	CLA	C1D-ND	3.87	1.42	1.37
31	V	606	CHL	C3B-C4B	3.84	1.45	1.41
31	W	407	CHL	C1A-CHA	-3.84	1.35	1.40
31	X	406	CHL	C1A-CHA	-3.81	1.35	1.40
31	U	408	CHL	C3B-C4B	3.81	1.45	1.41
31	V	605	CHL	C3B-C4B	3.81	1.45	1.41
31	W	408	CHL	C1A-CHA	-3.81	1.35	1.40
33	A	802	CL0	CHC-C4B	3.80	1.45	1.39
31	X	406	CHL	C3B-C4B	3.80	1.45	1.41
22	P	603	CLA	C1D-ND	3.79	1.42	1.37
25	O	304	DGD	O2G-C1B	3.78	1.44	1.34
22	B	820	CLA	C1D-ND	3.78	1.42	1.37
31	U	407	CHL	C1A-CHA	-3.78	1.35	1.40
22	A	803	CLA	C1D-ND	3.78	1.42	1.37
31	V	605	CHL	C3A-C2A	-3.74	1.51	1.54
33	A	802	CL0	CHD-C1D	3.74	1.45	1.39
22	A	839	CLA	C1D-ND	3.73	1.42	1.37
22	A	838	CLA	C1D-ND	3.73	1.42	1.37
22	P	611	CLA	C1D-ND	3.69	1.42	1.37
31	W	422	CHL	C3A-C2A	-3.69	1.51	1.54
25	B	847	DGD	O2G-C1B	3.69	1.44	1.34
22	P	608	CLA	C1D-ND	3.68	1.42	1.37
33	A	802	CL0	OBD-CAD	3.68	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	819	CLA	C1D-ND	3.68	1.42	1.37
22	B	826	CLA	C1D-ND	3.68	1.42	1.37
31	W	407	CHL	C3B-C4B	3.68	1.45	1.41
22	X	417	CLA	C1D-ND	3.67	1.42	1.37
22	V	601	CLA	C1D-ND	3.67	1.42	1.37
22	P	610	CLA	C1D-ND	3.66	1.42	1.37
22	R	610	CLA	C1D-ND	3.66	1.42	1.37
22	V	613	CLA	C1D-ND	3.65	1.42	1.37
22	R	606	CLA	C1D-ND	3.65	1.42	1.37
22	X	409	CLA	C1D-ND	3.63	1.42	1.37
22	U	404	CLA	C1D-ND	3.63	1.42	1.37
22	Q	618	CLA	C1D-ND	3.63	1.42	1.37
22	I	603	CLA	C1D-ND	3.63	1.42	1.37
22	R	611	CLA	C1D-ND	3.63	1.42	1.37
22	B	859	CLA	C1D-ND	3.62	1.42	1.37
22	I	609	CLA	C1D-ND	3.62	1.42	1.37
22	Q	608	CLA	C1D-ND	3.62	1.42	1.37
22	S	608	CLA	C1D-ND	3.62	1.42	1.37
22	A	840	CLA	C1D-ND	3.62	1.42	1.37
22	P	604	CLA	C1D-ND	3.62	1.42	1.37
22	T	607	CLA	C1D-ND	3.62	1.42	1.37
22	I	601	CLA	C1D-ND	3.62	1.42	1.37
22	S	610	CLA	C1D-ND	3.61	1.42	1.37
22	B	804	CLA	C1D-ND	3.61	1.42	1.37
22	U	414	CLA	C1D-ND	3.61	1.42	1.37
22	V	604	CLA	C1D-ND	3.61	1.42	1.37
22	V	609	CLA	C1D-ND	3.61	1.42	1.37
22	R	607	CLA	C1D-ND	3.60	1.42	1.37
22	S	602	CLA	C1D-ND	3.60	1.42	1.37
22	V	607	CLA	C1D-ND	3.60	1.42	1.37
22	B	816	CLA	C1D-ND	3.60	1.42	1.37
22	R	605	CLA	C1D-ND	3.60	1.42	1.37
22	R	615	CLA	C1D-ND	3.60	1.42	1.37
22	X	404	CLA	C1D-ND	3.60	1.42	1.37
22	O	315	CLA	C1D-ND	3.60	1.42	1.37
22	Q	613	CLA	C1D-ND	3.60	1.42	1.37
22	B	836	CLA	C1D-ND	3.60	1.42	1.37
22	H	302	CLA	C1D-ND	3.60	1.42	1.37
22	N	602	CLA	C1D-ND	3.60	1.42	1.37
22	N	603	CLA	C1D-ND	3.59	1.42	1.37
22	W	414	CLA	C1D-ND	3.59	1.42	1.37
22	H	307	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	311	CLA	C1D-ND	3.59	1.42	1.37
22	A	829	CLA	C1D-ND	3.59	1.42	1.37
31	W	422	CHL	C3B-C4B	3.59	1.44	1.41
22	A	826	CLA	C1D-ND	3.59	1.42	1.37
31	W	407	CHL	C3A-C2A	-3.59	1.51	1.54
22	B	806	CLA	C1D-ND	3.59	1.42	1.37
22	U	405	CLA	C1D-ND	3.59	1.42	1.37
22	G	604	CLA	C1D-ND	3.59	1.42	1.37
22	N	609	CLA	C1D-ND	3.58	1.42	1.37
22	A	842	CLA	C1D-ND	3.58	1.42	1.37
22	S	609	CLA	C1D-ND	3.58	1.42	1.37
22	G	602	CLA	C1D-ND	3.58	1.42	1.37
22	A	815	CLA	C1D-ND	3.58	1.42	1.37
22	H	313	CLA	C1D-ND	3.58	1.42	1.37
22	L	417	CLA	C1D-ND	3.58	1.42	1.37
22	B	821	CLA	C1D-ND	3.58	1.42	1.37
22	K	611	CLA	C1D-ND	3.58	1.42	1.37
22	R	609	CLA	C1D-ND	3.58	1.42	1.37
22	V	603	CLA	C1D-ND	3.57	1.42	1.37
22	O	319	CLA	C1D-ND	3.57	1.42	1.37
22	R	603	CLA	C1D-ND	3.57	1.42	1.37
22	X	412	CLA	C1D-ND	3.57	1.42	1.37
33	A	802	CL0	CHD-C4C	3.57	1.46	1.39
22	T	611	CLA	C1D-ND	3.57	1.42	1.37
22	X	408	CLA	C1D-ND	3.57	1.42	1.37
22	L	405	CLA	C1D-ND	3.57	1.42	1.37
22	R	608	CLA	C1D-ND	3.57	1.42	1.37
22	V	617	CLA	C1D-ND	3.57	1.42	1.37
22	W	419	CLA	C1D-ND	3.56	1.42	1.37
22	S	606	CLA	C1D-ND	3.56	1.42	1.37
22	K	604	CLA	C1D-ND	3.56	1.42	1.37
22	N	606	CLA	C1D-ND	3.56	1.42	1.37
22	U	413	CLA	C1D-ND	3.56	1.42	1.37
22	A	841	CLA	C1D-ND	3.56	1.42	1.37
22	U	403	CLA	C1D-ND	3.56	1.42	1.37
22	A	844	CLA	C1D-ND	3.56	1.42	1.37
22	K	613	CLA	C1D-ND	3.56	1.42	1.37
22	V	602	CLA	C1D-ND	3.56	1.42	1.37
22	I	602	CLA	C1D-ND	3.56	1.42	1.37
22	U	415	CLA	C1D-ND	3.56	1.42	1.37
22	V	611	CLA	C1D-ND	3.56	1.42	1.37
22	A	824	CLA	C1D-ND	3.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	612	CLA	C1D-ND	3.55	1.42	1.37
22	B	834	CLA	C1D-ND	3.55	1.42	1.37
22	N	610	CLA	C1D-ND	3.55	1.42	1.37
22	U	412	CLA	C1D-ND	3.55	1.42	1.37
22	X	411	CLA	C1D-ND	3.55	1.42	1.37
22	W	403	CLA	C1D-ND	3.55	1.42	1.37
22	H	318	CLA	C1D-ND	3.55	1.42	1.37
22	N	601	CLA	C1D-ND	3.54	1.42	1.37
22	R	602	CLA	C1D-ND	3.54	1.42	1.37
22	X	419	CLA	C1D-ND	3.54	1.42	1.37
22	H	303	CLA	C1D-ND	3.54	1.42	1.37
22	X	407	CLA	C1D-ND	3.54	1.42	1.37
22	B	817	CLA	C1D-ND	3.54	1.42	1.37
22	N	611	CLA	C1D-ND	3.54	1.42	1.37
22	S	607	CLA	C1D-ND	3.54	1.42	1.37
22	F	405	CLA	C1D-ND	3.54	1.42	1.37
22	V	610	CLA	C1D-ND	3.54	1.42	1.37
22	K	612	CLA	C1D-ND	3.54	1.42	1.37
22	X	403	CLA	C1D-ND	3.54	1.42	1.37
22	U	411	CLA	C1D-ND	3.54	1.42	1.37
22	T	606	CLA	C1D-ND	3.54	1.42	1.37
22	U	401	CLA	C1D-ND	3.54	1.42	1.37
22	A	833	CLA	C1D-ND	3.54	1.42	1.37
22	B	825	CLA	C1D-ND	3.53	1.42	1.37
22	B	815	CLA	C1D-ND	3.53	1.42	1.37
22	R	601	CLA	C1D-ND	3.53	1.42	1.37
22	X	413	CLA	C1D-ND	3.53	1.42	1.37
22	X	410	CLA	C1D-ND	3.53	1.42	1.37
22	G	609	CLA	C1D-ND	3.53	1.42	1.37
22	G	611	CLA	C1D-ND	3.53	1.42	1.37
22	T	602	CLA	C1D-ND	3.53	1.42	1.37
22	H	304	CLA	C1D-ND	3.53	1.42	1.37
22	W	412	CLA	C1D-ND	3.53	1.42	1.37
22	A	827	CLA	C1D-ND	3.53	1.42	1.37
22	B	832	CLA	C1D-ND	3.53	1.42	1.37
22	H	309	CLA	C1D-ND	3.53	1.42	1.37
22	A	807	CLA	C1D-ND	3.53	1.42	1.37
22	O	313	CLA	C1D-ND	3.52	1.42	1.37
22	S	614	CLA	C1D-ND	3.52	1.42	1.37
22	F	403	CLA	C1D-ND	3.52	1.42	1.37
22	A	813	CLA	C1D-ND	3.52	1.42	1.37
22	L	409	CLA	C1D-ND	3.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	817	CLA	C1D-ND	3.52	1.42	1.37
22	V	608	CLA	C1D-ND	3.52	1.42	1.37
22	B	812	CLA	C1D-ND	3.52	1.42	1.37
22	W	404	CLA	C1D-ND	3.52	1.42	1.37
22	B	808	CLA	C1D-ND	3.52	1.42	1.37
22	N	604	CLA	C1D-ND	3.52	1.42	1.37
22	A	831	CLA	C1D-ND	3.52	1.42	1.37
22	H	308	CLA	C1D-ND	3.52	1.42	1.37
22	Q	611	CLA	C1D-ND	3.52	1.42	1.37
22	U	406	CLA	C1D-ND	3.52	1.42	1.37
22	S	601	CLA	C1D-ND	3.51	1.42	1.37
22	R	604	CLA	C1D-ND	3.51	1.42	1.37
22	B	828	CLA	C1D-ND	3.51	1.42	1.37
22	B	835	CLA	C1D-ND	3.51	1.42	1.37
22	H	305	CLA	C1D-ND	3.51	1.42	1.37
22	G	601	CLA	C1D-ND	3.51	1.42	1.37
22	A	818	CLA	C1D-ND	3.51	1.42	1.37
22	Q	601	CLA	C1D-ND	3.51	1.42	1.37
22	T	610	CLA	C1D-ND	3.51	1.42	1.37
22	N	607	CLA	C1D-ND	3.50	1.42	1.37
22	O	308	CLA	C1D-ND	3.50	1.42	1.37
22	X	405	CLA	C1D-ND	3.50	1.42	1.37
22	A	808	CLA	C1D-ND	3.50	1.42	1.37
22	B	837	CLA	C1D-ND	3.50	1.42	1.37
22	B	809	CLA	C1D-ND	3.50	1.42	1.37
22	G	603	CLA	C1D-ND	3.50	1.42	1.37
22	B	839	CLA	C1D-ND	3.50	1.42	1.37
22	O	312	CLA	C1D-ND	3.50	1.42	1.37
22	B	818	CLA	C1D-ND	3.50	1.42	1.37
22	A	832	CLA	C1D-ND	3.50	1.42	1.37
22	I	610	CLA	C1D-ND	3.50	1.42	1.37
22	B	831	CLA	C1D-ND	3.49	1.42	1.37
22	L	410	CLA	C1D-ND	3.49	1.42	1.37
22	O	314	CLA	C1D-ND	3.49	1.42	1.37
22	T	609	CLA	C1D-ND	3.49	1.42	1.37
22	I	604	CLA	C1D-ND	3.49	1.42	1.37
22	N	605	CLA	C1D-ND	3.49	1.42	1.37
22	P	607	CLA	C1D-ND	3.49	1.42	1.37
22	A	837	CLA	C1D-ND	3.49	1.42	1.37
22	A	809	CLA	C1D-ND	3.49	1.42	1.37
22	I	606	CLA	C1D-ND	3.49	1.42	1.37
22	A	828	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	606	CLA	C1D-ND	3.49	1.42	1.37
22	K	603	CLA	C1D-ND	3.49	1.42	1.37
22	Q	605	CLA	C1D-ND	3.49	1.42	1.37
22	P	605	CLA	C1D-ND	3.49	1.42	1.37
22	Q	603	CLA	C1D-ND	3.49	1.42	1.37
22	L	407	CLA	C1D-ND	3.49	1.42	1.37
22	A	804	CLA	C1D-ND	3.48	1.42	1.37
22	T	605	CLA	C1D-ND	3.48	1.42	1.37
22	W	405	CLA	C1D-ND	3.48	1.42	1.37
22	Q	606	CLA	C1D-ND	3.48	1.42	1.37
22	O	307	CLA	C1D-ND	3.48	1.42	1.37
22	K	609	CLA	C1D-ND	3.48	1.42	1.37
22	L	404	CLA	C1D-ND	3.48	1.42	1.37
22	B	805	CLA	C1D-ND	3.48	1.42	1.37
22	L	412	CLA	C1D-ND	3.48	1.42	1.37
22	B	813	CLA	C1D-ND	3.48	1.42	1.37
22	T	604	CLA	C1D-ND	3.48	1.42	1.37
22	B	838	CLA	C1D-ND	3.48	1.42	1.37
31	W	408	CHL	C3B-C4B	3.48	1.44	1.41
22	S	615	CLA	C1D-ND	3.48	1.42	1.37
22	J	102	CLA	C1D-ND	3.48	1.42	1.37
22	U	420	CLA	C1D-ND	3.48	1.42	1.37
22	A	825	CLA	C1D-ND	3.48	1.42	1.37
22	Q	617	CLA	C1D-ND	3.47	1.42	1.37
22	Q	607	CLA	C1D-ND	3.47	1.42	1.37
22	A	835	CLA	C1D-ND	3.47	1.42	1.37
22	B	803	CLA	C1D-ND	3.47	1.42	1.37
22	Q	604	CLA	C1D-ND	3.47	1.42	1.37
22	G	607	CLA	C1D-ND	3.47	1.42	1.37
22	B	822	CLA	C1D-ND	3.47	1.42	1.37
22	W	411	CLA	C1D-ND	3.47	1.42	1.37
22	L	411	CLA	C1D-ND	3.47	1.42	1.37
22	P	609	CLA	C1D-ND	3.47	1.42	1.37
22	S	604	CLA	C1D-ND	3.47	1.42	1.37
22	W	410	CLA	C1D-ND	3.47	1.42	1.37
22	W	413	CLA	C1D-ND	3.47	1.42	1.37
22	K	606	CLA	C1D-ND	3.47	1.42	1.37
22	K	605	CLA	C1D-ND	3.46	1.42	1.37
22	T	603	CLA	C1D-ND	3.46	1.42	1.37
22	X	402	CLA	C1D-ND	3.46	1.42	1.37
22	H	310	CLA	C1D-ND	3.46	1.42	1.37
22	A	806	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	410	CLA	C1D-ND	3.46	1.42	1.37
22	B	827	CLA	C1D-ND	3.46	1.42	1.37
22	Q	610	CLA	C1D-ND	3.46	1.42	1.37
22	I	607	CLA	C1D-ND	3.46	1.42	1.37
22	A	823	CLA	C1D-ND	3.46	1.42	1.37
22	B	824	CLA	C1D-ND	3.45	1.42	1.37
22	H	306	CLA	C1D-ND	3.45	1.42	1.37
22	B	833	CLA	C1D-ND	3.45	1.42	1.37
22	O	311	CLA	C1D-ND	3.45	1.42	1.37
22	W	406	CLA	C1D-ND	3.45	1.42	1.37
22	T	608	CLA	C1D-ND	3.45	1.42	1.37
22	K	602	CLA	C1D-ND	3.44	1.42	1.37
22	K	617	CLA	C1D-ND	3.44	1.42	1.37
22	A	836	CLA	C1D-ND	3.44	1.42	1.37
22	N	606	CLA	C4B-NB	3.44	1.42	1.37
22	W	402	CLA	C1D-ND	3.44	1.42	1.37
22	O	310	CLA	C1D-ND	3.44	1.42	1.37
22	F	404	CLA	C1D-ND	3.44	1.42	1.37
22	K	610	CLA	C1D-ND	3.44	1.42	1.37
22	L	406	CLA	C1D-ND	3.44	1.42	1.37
22	B	823	CLA	C1D-ND	3.43	1.42	1.37
22	O	306	CLA	C1D-ND	3.43	1.42	1.37
22	O	309	CLA	C1D-ND	3.43	1.42	1.37
22	H	312	CLA	C1D-ND	3.43	1.42	1.37
22	L	403	CLA	C1D-ND	3.43	1.42	1.37
22	S	603	CLA	C1D-ND	3.43	1.42	1.37
22	U	409	CLA	C1D-ND	3.43	1.42	1.37
22	B	811	CLA	C1D-ND	3.42	1.42	1.37
22	A	810	CLA	C1D-ND	3.42	1.42	1.37
22	A	812	CLA	C1D-ND	3.42	1.42	1.37
22	A	852	CLA	C1D-ND	3.42	1.42	1.37
22	G	610	CLA	C1D-ND	3.42	1.42	1.37
22	N	608	CLA	C1D-ND	3.42	1.42	1.37
22	A	834	CLA	C1D-ND	3.42	1.42	1.37
22	A	811	CLA	C1D-ND	3.42	1.42	1.37
22	Q	609	CLA	C1D-ND	3.41	1.42	1.37
22	A	830	CLA	C1D-ND	3.41	1.42	1.37
22	L	402	CLA	C1D-ND	3.41	1.42	1.37
22	G	608	CLA	C1D-ND	3.41	1.42	1.37
22	A	805	CLA	C1D-ND	3.41	1.42	1.37
22	B	807	CLA	C1D-ND	3.41	1.42	1.37
22	A	814	CLA	C1D-ND	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	605	CLA	C1D-ND	3.39	1.42	1.37
22	A	822	CLA	C1D-ND	3.39	1.42	1.37
22	A	821	CLA	C1D-ND	3.39	1.42	1.37
22	G	605	CLA	C1D-ND	3.38	1.42	1.37
22	B	810	CLA	C1D-ND	3.38	1.42	1.37
22	A	820	CLA	C1D-ND	3.37	1.42	1.37
22	Q	612	CLA	C1D-ND	3.37	1.42	1.37
22	B	814	CLA	C1D-ND	3.37	1.42	1.37
22	T	601	CLA	C1D-ND	3.37	1.42	1.37
22	O	305	CLA	C1D-ND	3.35	1.42	1.37
22	S	605	CLA	C1D-ND	3.33	1.42	1.37
22	O	315	CLA	C4B-NB	3.31	1.42	1.37
22	B	838	CLA	C4B-NB	3.31	1.42	1.37
33	A	802	CL0	CHC-C1C	3.31	1.45	1.39
22	P	602	CLA	C1D-ND	3.30	1.42	1.37
22	A	803	CLA	C4B-NB	3.29	1.42	1.37
22	W	409	CLA	C1D-ND	3.28	1.42	1.37
22	V	601	CLA	C4B-NB	3.28	1.42	1.37
22	S	609	CLA	C4B-NB	3.27	1.42	1.37
22	P	606	CLA	C1D-ND	3.26	1.42	1.37
22	V	613	CLA	C4B-NB	3.26	1.42	1.37
22	W	405	CLA	C4B-NB	3.25	1.42	1.37
22	I	608	CLA	C1D-ND	3.25	1.42	1.37
26	U	419	LHG	C26-C25	-3.24	1.35	1.51
26	H	316	LHG	C26-C25	-3.24	1.35	1.51
22	R	610	CLA	C4B-NB	3.24	1.42	1.37
22	P	608	CLA	C4B-NB	3.23	1.42	1.37
22	A	842	CLA	C4B-NB	3.23	1.42	1.37
22	B	819	CLA	C4B-NB	3.23	1.42	1.37
26	X	420	LHG	C26-C25	-3.23	1.35	1.51
26	L	416	LHG	C26-C25	-3.23	1.35	1.51
22	B	820	CLA	C4B-NB	3.23	1.42	1.37
22	B	825	CLA	C4B-NB	3.23	1.42	1.37
22	H	311	CLA	C4B-NB	3.23	1.42	1.37
22	X	404	CLA	C4B-NB	3.22	1.42	1.37
26	P	601	LHG	C26-C25	-3.22	1.35	1.51
26	N	614	LHG	C26-C25	-3.22	1.35	1.51
26	T	614	LHG	C26-C25	-3.22	1.35	1.51
22	I	601	CLA	C4B-NB	3.22	1.42	1.37
26	B	851	LHG	C26-C25	-3.22	1.35	1.51
26	O	323	LHG	C26-C25	-3.21	1.35	1.51
26	Q	616	LHG	C26-C25	-3.21	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	601	CLA	C4B-NB	3.21	1.42	1.37
26	O	318	LHG	C26-C25	-3.21	1.35	1.51
26	O	324	LHG	C26-C25	-3.21	1.35	1.51
26	A	845	LHG	C26-C25	-3.21	1.35	1.51
26	R	614	LHG	C26-C25	-3.21	1.35	1.51
26	K	619	LHG	C26-C25	-3.21	1.35	1.51
22	A	819	CLA	C1D-ND	3.21	1.42	1.37
22	P	610	CLA	C4B-NB	3.21	1.42	1.37
26	K	616	LHG	C26-C25	-3.20	1.35	1.51
22	P	609	CLA	C4B-NB	3.20	1.42	1.37
22	X	419	CLA	C4B-NB	3.20	1.42	1.37
26	W	420	LHG	C26-C25	-3.20	1.35	1.51
26	O	321	LHG	C26-C25	-3.20	1.35	1.51
26	N	616	LHG	C26-C25	-3.20	1.35	1.51
26	A	846	LHG	C26-C25	-3.19	1.35	1.51
22	R	608	CLA	C4B-NB	3.19	1.42	1.37
26	S	613	LHG	C26-C25	-3.19	1.35	1.51
26	G	614	LHG	C26-C25	-3.19	1.35	1.51
22	U	403	CLA	C4B-NB	3.19	1.42	1.37
22	V	611	CLA	C4B-NB	3.18	1.42	1.37
22	U	415	CLA	C4B-NB	3.18	1.42	1.37
22	Q	610	CLA	C4B-NB	3.17	1.42	1.37
22	A	806	CLA	C4B-NB	3.17	1.42	1.37
22	V	617	CLA	C4B-NB	3.16	1.42	1.37
22	P	603	CLA	C4B-NB	3.16	1.42	1.37
22	F	405	CLA	C4B-NB	3.16	1.42	1.37
22	Q	618	CLA	C4B-NB	3.16	1.42	1.37
22	W	415	CLA	C4B-NB	3.16	1.42	1.37
22	V	612	CLA	C4B-NB	3.15	1.42	1.37
22	S	610	CLA	C4B-NB	3.15	1.42	1.37
22	T	606	CLA	C4B-NB	3.14	1.42	1.37
22	V	610	CLA	C4B-NB	3.14	1.42	1.37
22	B	833	CLA	C4B-NB	3.14	1.42	1.37
22	X	412	CLA	C4B-NB	3.13	1.42	1.37
22	T	610	CLA	C4B-NB	3.13	1.42	1.37
22	A	834	CLA	C4B-NB	3.13	1.42	1.37
22	W	414	CLA	C4B-NB	3.13	1.42	1.37
22	H	307	CLA	C4B-NB	3.13	1.42	1.37
22	T	605	CLA	C4B-NB	3.13	1.42	1.37
22	S	608	CLA	C4B-NB	3.13	1.42	1.37
22	H	309	CLA	C4B-NB	3.13	1.42	1.37
22	A	816	CLA	C1D-ND	3.12	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	607	CLA	C4B-NB	3.12	1.42	1.37
22	R	615	CLA	C4B-NB	3.12	1.42	1.37
22	G	606	CLA	C4B-NB	3.12	1.42	1.37
22	S	606	CLA	C4B-NB	3.12	1.42	1.37
22	K	610	CLA	C4B-NB	3.12	1.42	1.37
22	X	410	CLA	C4B-NB	3.12	1.42	1.37
31	W	422	CHL	C3B-C2B	-3.12	1.36	1.40
22	F	403	CLA	C4B-NB	3.12	1.42	1.37
22	N	611	CLA	C4B-NB	3.11	1.42	1.37
22	A	820	CLA	C4B-NB	3.11	1.42	1.37
22	O	313	CLA	C4B-NB	3.11	1.41	1.37
22	H	313	CLA	C4B-NB	3.11	1.41	1.37
22	R	606	CLA	C4B-NB	3.11	1.41	1.37
22	R	607	CLA	C4B-NB	3.11	1.41	1.37
22	R	611	CLA	C4B-NB	3.11	1.41	1.37
22	G	603	CLA	C4B-NB	3.11	1.41	1.37
22	A	824	CLA	C4B-NB	3.11	1.41	1.37
22	N	604	CLA	C4B-NB	3.10	1.41	1.37
22	B	803	CLA	C4B-NB	3.10	1.41	1.37
22	I	608	CLA	C4B-NB	3.10	1.41	1.37
22	A	804	CLA	C4B-NB	3.10	1.41	1.37
22	A	852	CLA	C4B-NB	3.10	1.41	1.37
22	T	603	CLA	C4B-NB	3.10	1.41	1.37
22	V	603	CLA	C4B-NB	3.10	1.41	1.37
22	B	806	CLA	C4B-NB	3.09	1.41	1.37
22	B	828	CLA	C4B-NB	3.09	1.41	1.37
22	Q	607	CLA	C4B-NB	3.09	1.41	1.37
22	I	606	CLA	C4B-NB	3.09	1.41	1.37
22	N	608	CLA	C4B-NB	3.09	1.41	1.37
22	O	307	CLA	C4B-NB	3.08	1.41	1.37
22	U	406	CLA	C4B-NB	3.08	1.41	1.37
22	T	601	CLA	C4B-NB	3.08	1.41	1.37
22	I	603	CLA	C4B-NB	3.08	1.41	1.37
22	H	302	CLA	C4B-NB	3.08	1.41	1.37
22	R	609	CLA	C4B-NB	3.08	1.41	1.37
22	B	837	CLA	C4B-NB	3.08	1.41	1.37
22	V	602	CLA	C4B-NB	3.08	1.41	1.37
22	W	403	CLA	C4B-NB	3.08	1.41	1.37
22	B	821	CLA	C4B-NB	3.07	1.41	1.37
22	Q	605	CLA	C4B-NB	3.07	1.41	1.37
22	R	605	CLA	C4B-NB	3.07	1.41	1.37
22	L	409	CLA	C4B-NB	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	603	CLA	C4B-NB	3.07	1.41	1.37
31	U	407	CHL	C3B-C2B	-3.07	1.36	1.40
22	B	817	CLA	C4B-NB	3.07	1.41	1.37
22	A	809	CLA	C4B-NB	3.07	1.41	1.37
22	B	826	CLA	C4B-NB	3.07	1.41	1.37
22	H	318	CLA	C4B-NB	3.07	1.41	1.37
22	Q	608	CLA	C4B-NB	3.07	1.41	1.37
31	W	407	CHL	C3B-C2B	-3.06	1.36	1.40
22	A	836	CLA	C4B-NB	3.06	1.41	1.37
22	B	807	CLA	C4B-NB	3.06	1.41	1.37
22	K	604	CLA	C4B-NB	3.06	1.41	1.37
22	B	835	CLA	C4B-NB	3.06	1.41	1.37
22	V	604	CLA	C4B-NB	3.06	1.41	1.37
22	K	613	CLA	C4B-NB	3.06	1.41	1.37
22	A	829	CLA	C4B-NB	3.06	1.41	1.37
22	A	837	CLA	C4B-NB	3.06	1.41	1.37
22	K	602	CLA	C4B-NB	3.06	1.41	1.37
22	W	406	CLA	C4B-NB	3.06	1.41	1.37
22	B	812	CLA	C4B-NB	3.06	1.41	1.37
22	B	831	CLA	C4B-NB	3.06	1.41	1.37
22	R	601	CLA	C4B-NB	3.06	1.41	1.37
22	R	604	CLA	C4B-NB	3.06	1.41	1.37
22	V	607	CLA	C4B-NB	3.05	1.41	1.37
22	X	417	CLA	C4B-NB	3.05	1.41	1.37
22	B	859	CLA	C4B-NB	3.05	1.41	1.37
22	S	607	CLA	C4B-NB	3.05	1.41	1.37
22	A	831	CLA	C4B-NB	3.05	1.41	1.37
22	G	611	CLA	C4B-NB	3.05	1.41	1.37
22	U	405	CLA	C4B-NB	3.05	1.41	1.37
22	L	417	CLA	C4B-NB	3.05	1.41	1.37
22	A	839	CLA	C4B-NB	3.05	1.41	1.37
22	A	814	CLA	C4B-NB	3.04	1.41	1.37
22	A	807	CLA	C4B-NB	3.04	1.41	1.37
22	R	602	CLA	C4B-NB	3.04	1.41	1.37
22	I	611	CLA	C4B-NB	3.04	1.41	1.37
22	S	601	CLA	C4B-NB	3.04	1.41	1.37
22	S	604	CLA	C4B-NB	3.04	1.41	1.37
22	S	615	CLA	C4B-NB	3.04	1.41	1.37
22	N	607	CLA	C4B-NB	3.04	1.41	1.37
22	B	815	CLA	C4B-NB	3.03	1.41	1.37
22	Q	606	CLA	C4B-NB	3.03	1.41	1.37
22	A	805	CLA	C4B-NB	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	U	408	CHL	C3B-C2B	-3.03	1.36	1.40
22	I	605	CLA	C4B-NB	3.03	1.41	1.37
22	W	412	CLA	C4B-NB	3.03	1.41	1.37
22	B	814	CLA	C4B-NB	3.03	1.41	1.37
22	V	609	CLA	C4B-NB	3.03	1.41	1.37
22	B	836	CLA	C4B-NB	3.03	1.41	1.37
22	A	841	CLA	C4B-NB	3.03	1.41	1.37
22	U	420	CLA	C4B-NB	3.02	1.41	1.37
22	I	609	CLA	C4B-NB	3.02	1.41	1.37
22	W	419	CLA	C4B-NB	3.02	1.41	1.37
22	L	412	CLA	C4B-NB	3.02	1.41	1.37
22	T	608	CLA	C4B-NB	3.02	1.41	1.37
22	B	824	CLA	C4B-NB	3.02	1.41	1.37
22	F	404	CLA	C4B-NB	3.02	1.41	1.37
22	G	604	CLA	C4B-NB	3.02	1.41	1.37
22	H	312	CLA	C4B-NB	3.02	1.41	1.37
22	L	405	CLA	C4B-NB	3.02	1.41	1.37
22	X	413	CLA	C4B-NB	3.02	1.41	1.37
22	L	411	CLA	C4B-NB	3.02	1.41	1.37
22	U	414	CLA	C4B-NB	3.02	1.41	1.37
22	P	611	CLA	C4B-NB	3.02	1.41	1.37
22	U	413	CLA	C4B-NB	3.02	1.41	1.37
22	V	608	CLA	C4B-NB	3.02	1.41	1.37
22	G	609	CLA	C4B-NB	3.01	1.41	1.37
22	U	409	CLA	C4B-NB	3.01	1.41	1.37
22	Q	603	CLA	C4B-NB	3.01	1.41	1.37
22	U	410	CLA	C4B-NB	3.01	1.41	1.37
22	H	310	CLA	C4B-NB	3.01	1.41	1.37
22	A	823	CLA	C4B-NB	3.01	1.41	1.37
22	K	606	CLA	C4B-NB	3.01	1.41	1.37
22	K	611	CLA	C4B-NB	3.01	1.41	1.37
22	X	409	CLA	C4B-NB	3.00	1.41	1.37
22	I	604	CLA	C4B-NB	3.00	1.41	1.37
22	B	809	CLA	C4B-NB	3.00	1.41	1.37
22	B	808	CLA	C4B-NB	3.00	1.41	1.37
22	N	610	CLA	C4B-NB	3.00	1.41	1.37
22	Q	617	CLA	C4B-NB	3.00	1.41	1.37
22	S	603	CLA	C4B-NB	2.99	1.41	1.37
22	T	611	CLA	C4B-NB	2.99	1.41	1.37
22	A	830	CLA	C4B-NB	2.99	1.41	1.37
22	B	822	CLA	C4B-NB	2.99	1.41	1.37
22	O	305	CLA	C4B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	409	CLA	C4B-NB	2.99	1.41	1.37
22	B	810	CLA	C4B-NB	2.99	1.41	1.37
22	A	810	CLA	C4B-NB	2.99	1.41	1.37
22	U	401	CLA	C4B-NB	2.99	1.41	1.37
22	L	407	CLA	C4B-NB	2.99	1.41	1.37
22	B	816	CLA	C4B-NB	2.98	1.41	1.37
22	P	604	CLA	C4B-NB	2.98	1.41	1.37
22	G	601	CLA	C4B-NB	2.98	1.41	1.37
22	P	606	CLA	C4B-NB	2.98	1.41	1.37
22	O	319	CLA	C4B-NB	2.98	1.41	1.37
22	B	805	CLA	C4B-NB	2.98	1.41	1.37
22	A	835	CLA	C4B-NB	2.98	1.41	1.37
22	B	823	CLA	C4B-NB	2.98	1.41	1.37
22	O	311	CLA	C4B-NB	2.98	1.41	1.37
22	I	607	CLA	C4B-NB	2.98	1.41	1.37
22	H	305	CLA	C4B-NB	2.97	1.41	1.37
22	W	410	CLA	C4B-NB	2.97	1.41	1.37
22	N	609	CLA	C4B-NB	2.97	1.41	1.37
22	B	811	CLA	C4B-NB	2.97	1.41	1.37
22	B	818	CLA	C4B-NB	2.97	1.41	1.37
22	U	411	CLA	C4B-NB	2.97	1.41	1.37
22	A	833	CLA	C4B-NB	2.97	1.41	1.37
31	X	406	CHL	C3B-C2B	-2.97	1.36	1.40
22	B	804	CLA	C4B-NB	2.97	1.41	1.37
22	B	813	CLA	C4B-NB	2.97	1.41	1.37
22	W	413	CLA	C4B-NB	2.97	1.41	1.37
22	K	605	CLA	C4B-NB	2.97	1.41	1.37
22	H	306	CLA	C4B-NB	2.96	1.41	1.37
22	L	406	CLA	C4B-NB	2.96	1.41	1.37
22	O	308	CLA	C4B-NB	2.96	1.41	1.37
22	T	602	CLA	C4B-NB	2.96	1.41	1.37
22	X	402	CLA	C4B-NB	2.96	1.41	1.37
22	A	828	CLA	C4B-NB	2.96	1.41	1.37
22	A	818	CLA	C4B-NB	2.96	1.41	1.37
22	G	608	CLA	C4B-NB	2.96	1.41	1.37
22	L	410	CLA	C4B-NB	2.96	1.41	1.37
22	X	405	CLA	C4B-NB	2.96	1.41	1.37
22	A	813	CLA	C4B-NB	2.95	1.41	1.37
22	K	612	CLA	C4B-NB	2.95	1.41	1.37
22	L	403	CLA	C4B-NB	2.95	1.41	1.37
22	A	844	CLA	C4B-NB	2.95	1.41	1.37
22	X	403	CLA	C4B-NB	2.95	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	815	CLA	C4B-NB	2.95	1.41	1.37
22	U	412	CLA	C4B-NB	2.95	1.41	1.37
22	Q	611	CLA	C4B-NB	2.95	1.41	1.37
22	A	812	CLA	C4B-NB	2.95	1.41	1.37
22	S	614	CLA	C4B-NB	2.95	1.41	1.37
22	X	407	CLA	C4B-NB	2.95	1.41	1.37
22	A	822	CLA	C4B-NB	2.95	1.41	1.37
31	W	408	CHL	C3B-C2B	-2.95	1.36	1.40
22	A	840	CLA	C4B-NB	2.95	1.41	1.37
22	W	411	CLA	C4B-NB	2.95	1.41	1.37
22	A	832	CLA	C4B-NB	2.95	1.41	1.37
22	H	303	CLA	C4B-NB	2.94	1.41	1.37
31	V	605	CHL	C3B-C2B	-2.94	1.36	1.40
22	Q	609	CLA	C4B-NB	2.94	1.41	1.37
22	R	603	CLA	C4B-NB	2.93	1.41	1.37
22	A	811	CLA	C4B-NB	2.93	1.41	1.37
22	L	402	CLA	C4B-NB	2.93	1.41	1.37
22	A	821	CLA	C4B-NB	2.93	1.41	1.37
22	A	838	CLA	C4B-NB	2.93	1.41	1.37
22	T	604	CLA	C4B-NB	2.92	1.41	1.37
22	W	402	CLA	C4B-NB	2.92	1.41	1.37
22	O	309	CLA	C4B-NB	2.92	1.41	1.37
22	A	826	CLA	C4B-NB	2.92	1.41	1.37
22	G	610	CLA	C4B-NB	2.92	1.41	1.37
22	N	605	CLA	C4B-NB	2.92	1.41	1.37
22	X	411	CLA	C4B-NB	2.92	1.41	1.37
22	H	304	CLA	C4B-NB	2.92	1.41	1.37
22	I	610	CLA	C4B-NB	2.92	1.41	1.37
22	X	408	CLA	C4B-NB	2.92	1.41	1.37
22	J	102	CLA	C4B-NB	2.92	1.41	1.37
22	B	832	CLA	C4B-NB	2.92	1.41	1.37
22	U	404	CLA	C4B-NB	2.92	1.41	1.37
22	B	839	CLA	C4B-NB	2.91	1.41	1.37
22	L	404	CLA	C4B-NB	2.91	1.41	1.37
22	O	310	CLA	C4B-NB	2.91	1.41	1.37
31	V	606	CHL	C3B-C2B	-2.91	1.36	1.40
22	W	404	CLA	C4B-NB	2.91	1.41	1.37
22	T	607	CLA	C4B-NB	2.91	1.41	1.37
22	T	609	CLA	C4B-NB	2.90	1.41	1.37
22	K	607	CLA	C1D-ND	2.90	1.41	1.37
22	K	617	CLA	C4B-NB	2.90	1.41	1.37
22	A	825	CLA	C4B-NB	2.90	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	601	CLA	C4B-NB	2.90	1.41	1.37
22	K	609	CLA	C4B-NB	2.90	1.41	1.37
22	A	817	CLA	C4B-NB	2.90	1.41	1.37
22	O	314	CLA	C4B-NB	2.90	1.41	1.37
22	G	605	CLA	C4B-NB	2.89	1.41	1.37
22	I	602	CLA	C4B-NB	2.89	1.41	1.37
22	H	308	CLA	C4B-NB	2.89	1.41	1.37
22	P	605	CLA	C4B-NB	2.89	1.41	1.37
22	Q	612	CLA	C4B-NB	2.89	1.41	1.37
22	K	603	CLA	C4B-NB	2.89	1.41	1.37
22	A	827	CLA	C4B-NB	2.89	1.41	1.37
22	N	610	CLA	C1B-C2B	2.88	1.49	1.43
22	G	607	CLA	C4B-NB	2.88	1.41	1.37
22	B	827	CLA	C4B-NB	2.88	1.41	1.37
22	O	312	CLA	C4B-NB	2.88	1.41	1.37
22	Q	613	CLA	C4B-NB	2.88	1.41	1.37
22	R	607	CLA	C1B-C2B	2.88	1.49	1.43
22	Q	604	CLA	C4B-NB	2.87	1.41	1.37
22	N	602	CLA	C4B-NB	2.87	1.41	1.37
22	B	829	CLA	C1D-ND	2.86	1.41	1.37
22	S	602	CLA	C4B-NB	2.86	1.41	1.37
22	B	834	CLA	C4B-NB	2.85	1.41	1.37
22	S	609	CLA	C1B-C2B	2.85	1.49	1.43
22	O	306	CLA	C4B-NB	2.84	1.41	1.37
22	A	808	CLA	C4B-NB	2.83	1.41	1.37
22	P	611	CLA	C1B-C2B	2.83	1.49	1.43
22	V	612	CLA	C1B-C2B	2.82	1.49	1.43
22	V	602	CLA	C1B-C2B	2.82	1.49	1.43
22	P	603	CLA	C1B-C2B	2.81	1.49	1.43
22	G	602	CLA	C4B-NB	2.80	1.41	1.37
22	K	608	CLA	C1D-ND	2.80	1.41	1.37
22	R	615	CLA	C1B-C2B	2.80	1.49	1.43
22	S	601	CLA	C1B-C2B	2.79	1.49	1.43
22	B	802	CLA	C1D-ND	2.79	1.41	1.37
22	B	819	CLA	C1B-C2B	2.79	1.49	1.43
22	S	602	CLA	C1B-C2B	2.79	1.49	1.43
24	K	614	DD6	C28-C27	-2.78	1.49	1.50
22	R	602	CLA	C1B-C2B	2.78	1.49	1.43
22	B	830	CLA	C1D-ND	2.78	1.41	1.37
22	B	802	CLA	MG-NB	-2.78	2.00	2.05
22	V	608	CLA	C1B-C2B	2.77	1.49	1.43
22	V	610	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	412	CLA	C1B-C2B	2.77	1.49	1.43
24	K	615	DD6	C28-C27	-2.77	1.49	1.50
22	O	310	CLA	C1B-C2B	2.76	1.49	1.43
22	T	611	CLA	C1B-C2B	2.76	1.49	1.43
22	X	402	CLA	C1B-C2B	2.76	1.49	1.43
22	P	602	CLA	C4B-NB	2.76	1.41	1.37
22	R	611	CLA	C1B-C2B	2.76	1.49	1.43
22	U	413	CLA	C1B-C2B	2.76	1.49	1.43
22	A	806	CLA	C1B-C2B	2.75	1.49	1.43
22	B	811	CLA	C1B-C2B	2.75	1.49	1.43
22	V	617	CLA	C1B-C2B	2.75	1.49	1.43
22	L	405	CLA	C1B-C2B	2.75	1.49	1.43
22	I	604	CLA	C1B-C2B	2.75	1.49	1.43
22	U	414	CLA	C1B-C2B	2.75	1.49	1.43
22	T	610	CLA	C1B-C2B	2.75	1.49	1.43
22	H	305	CLA	C1B-C2B	2.74	1.49	1.43
22	V	604	CLA	C1B-C2B	2.74	1.49	1.43
22	Q	601	CLA	C1B-C2B	2.74	1.49	1.43
22	A	831	CLA	C1B-C2B	2.74	1.49	1.43
22	L	408	CLA	C1D-ND	2.74	1.41	1.37
22	I	609	CLA	C1B-C2B	2.74	1.49	1.43
22	R	601	CLA	C1B-C2B	2.74	1.49	1.43
22	A	841	CLA	C1B-C2B	2.74	1.49	1.43
22	I	610	CLA	C1B-C2B	2.74	1.49	1.43
22	V	613	CLA	C1B-C2B	2.74	1.49	1.43
22	Q	606	CLA	C1B-C2B	2.73	1.49	1.43
22	J	102	CLA	C1B-C2B	2.73	1.49	1.43
22	O	319	CLA	C1B-C2B	2.73	1.49	1.43
22	P	608	CLA	C1B-C2B	2.73	1.49	1.43
22	N	611	CLA	C1B-C2B	2.73	1.49	1.43
22	X	411	CLA	C1B-C2B	2.73	1.49	1.43
22	S	604	CLA	C1B-C2B	2.73	1.49	1.43
22	K	605	CLA	C1B-C2B	2.73	1.49	1.43
22	A	824	CLA	C1B-C2B	2.73	1.49	1.43
22	X	413	CLA	C1B-C2B	2.73	1.49	1.43
33	A	802	CL0	CHA-CBD	-2.73	1.48	1.51
22	Q	618	CLA	C1B-C2B	2.73	1.49	1.43
22	W	412	CLA	C1B-C2B	2.73	1.49	1.43
22	L	407	CLA	C1B-C2B	2.72	1.49	1.43
22	N	604	CLA	C1B-C2B	2.72	1.49	1.43
22	O	313	CLA	C1B-C2B	2.72	1.49	1.43
22	A	819	CLA	C4B-NB	2.72	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	406	CLA	C1B-C2B	2.72	1.49	1.43
22	U	420	CLA	C1B-C2B	2.72	1.49	1.43
22	K	606	CLA	C1B-C2B	2.72	1.49	1.43
22	S	608	CLA	C1B-C2B	2.72	1.49	1.43
22	V	609	CLA	C1B-C2B	2.72	1.49	1.43
22	A	839	CLA	C1B-C2B	2.72	1.49	1.43
22	N	607	CLA	C1B-C2B	2.72	1.49	1.43
22	Q	603	CLA	C1B-C2B	2.71	1.49	1.43
22	U	412	CLA	C1B-C2B	2.71	1.49	1.43
22	L	417	CLA	C1B-C2B	2.71	1.49	1.43
22	A	840	CLA	C1B-C2B	2.71	1.49	1.43
22	A	833	CLA	C1B-C2B	2.71	1.49	1.43
22	B	810	CLA	C1B-C2B	2.71	1.49	1.43
22	F	403	CLA	C1B-C2B	2.71	1.49	1.43
22	P	606	CLA	C1B-C2B	2.71	1.49	1.43
22	P	610	CLA	C1B-C2B	2.71	1.49	1.43
22	R	609	CLA	C1B-C2B	2.71	1.49	1.43
22	R	608	CLA	C1B-C2B	2.71	1.49	1.43
22	U	401	CLA	C1B-C2B	2.71	1.49	1.43
22	R	605	CLA	C1B-C2B	2.71	1.49	1.43
22	H	310	CLA	C1B-C2B	2.71	1.49	1.43
22	H	312	CLA	C1B-C2B	2.71	1.49	1.43
22	T	601	CLA	C1B-C2B	2.71	1.49	1.43
22	U	410	CLA	C1B-C2B	2.70	1.49	1.43
22	A	814	CLA	C1B-C2B	2.70	1.49	1.43
22	A	805	CLA	C1B-C2B	2.70	1.49	1.43
22	A	821	CLA	C1B-C2B	2.70	1.49	1.43
22	G	611	CLA	C1B-C2B	2.70	1.49	1.43
22	A	835	CLA	C1B-C2B	2.70	1.49	1.43
22	W	414	CLA	C1B-C2B	2.70	1.49	1.43
22	T	609	CLA	C1B-C2B	2.70	1.49	1.43
22	A	813	CLA	C1B-C2B	2.70	1.49	1.43
22	H	311	CLA	C1B-C2B	2.70	1.49	1.43
22	P	605	CLA	C1B-C2B	2.70	1.49	1.43
22	R	603	CLA	C1B-C2B	2.70	1.49	1.43
22	I	608	CLA	C1B-C2B	2.70	1.49	1.43
22	T	605	CLA	C1B-C2B	2.70	1.49	1.43
22	V	611	CLA	C1B-C2B	2.70	1.49	1.43
22	A	844	CLA	C1B-C2B	2.70	1.49	1.43
22	G	602	CLA	C1B-C2B	2.70	1.49	1.43
22	G	604	CLA	C1B-C2B	2.70	1.49	1.43
22	X	419	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	610	CLA	C1B-C2B	2.70	1.49	1.43
22	T	608	CLA	C1B-C2B	2.70	1.49	1.43
22	B	818	CLA	C1B-C2B	2.70	1.49	1.43
22	P	604	CLA	C1B-C2B	2.70	1.49	1.43
22	Q	617	CLA	C1B-C2B	2.69	1.49	1.43
22	B	825	CLA	C1B-C2B	2.69	1.49	1.43
22	N	608	CLA	C1B-C2B	2.69	1.49	1.43
22	V	607	CLA	C1B-C2B	2.69	1.49	1.43
22	B	833	CLA	C1B-C2B	2.69	1.49	1.43
22	Q	607	CLA	C1B-C2B	2.69	1.49	1.43
22	H	309	CLA	C1B-C2B	2.69	1.49	1.43
22	B	816	CLA	C1B-C2B	2.69	1.49	1.43
22	X	407	CLA	C1B-C2B	2.69	1.49	1.43
22	L	409	CLA	C1B-C2B	2.69	1.49	1.43
22	W	419	CLA	C1B-C2B	2.69	1.49	1.43
22	A	807	CLA	C1B-C2B	2.69	1.49	1.43
22	I	605	CLA	C1B-C2B	2.69	1.49	1.43
22	X	403	CLA	C1B-C2B	2.69	1.49	1.43
22	I	606	CLA	C1B-C2B	2.69	1.49	1.43
22	A	801	CLA	C1D-ND	2.69	1.41	1.37
22	R	604	CLA	C1B-C2B	2.69	1.49	1.43
22	K	611	CLA	C1B-C2B	2.69	1.49	1.43
22	N	601	CLA	C1B-C2B	2.68	1.49	1.43
22	I	602	CLA	C1B-C2B	2.68	1.49	1.43
22	H	303	CLA	C1B-C2B	2.68	1.49	1.43
22	O	311	CLA	C1B-C2B	2.68	1.49	1.43
22	L	406	CLA	C1B-C2B	2.68	1.49	1.43
22	A	818	CLA	C1B-C2B	2.68	1.49	1.43
22	N	609	CLA	C1B-C2B	2.68	1.49	1.43
22	V	601	CLA	C1B-C2B	2.68	1.49	1.43
22	F	404	CLA	C1B-C2B	2.68	1.49	1.43
22	U	415	CLA	C1B-C2B	2.68	1.49	1.43
22	U	409	CLA	C1B-C2B	2.68	1.49	1.43
22	B	831	CLA	C1B-C2B	2.68	1.49	1.43
22	A	808	CLA	C1B-C2B	2.68	1.49	1.43
22	R	606	CLA	C1B-C2B	2.68	1.49	1.43
22	A	823	CLA	C1B-C2B	2.68	1.49	1.43
22	B	809	CLA	C1B-C2B	2.68	1.49	1.43
22	I	603	CLA	C1B-C2B	2.68	1.49	1.43
22	O	305	CLA	C1B-C2B	2.68	1.49	1.43
22	Q	612	CLA	C1B-C2B	2.68	1.49	1.43
22	W	415	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	404	CLA	C1B-C2B	2.67	1.49	1.43
22	X	405	CLA	C1B-C2B	2.67	1.49	1.43
22	B	826	CLA	C1B-C2B	2.67	1.49	1.43
22	B	803	CLA	C1B-C2B	2.67	1.49	1.43
22	B	832	CLA	C1B-C2B	2.67	1.49	1.43
22	B	839	CLA	C1B-C2B	2.67	1.49	1.43
22	A	803	CLA	C1B-C2B	2.67	1.49	1.43
22	N	605	CLA	C1B-C2B	2.67	1.49	1.43
22	G	610	CLA	C1B-C2B	2.67	1.49	1.43
22	B	804	CLA	C1B-C2B	2.67	1.49	1.43
22	I	607	CLA	C1B-C2B	2.67	1.49	1.43
22	K	613	CLA	C1B-C2B	2.67	1.49	1.43
22	W	413	CLA	C1B-C2B	2.67	1.49	1.43
22	O	314	CLA	C1B-C2B	2.67	1.49	1.43
22	Q	610	CLA	C1B-C2B	2.67	1.49	1.43
22	B	821	CLA	C1B-C2B	2.67	1.49	1.43
22	B	808	CLA	C1B-C2B	2.67	1.49	1.43
22	V	603	CLA	C1B-C2B	2.67	1.49	1.43
22	A	837	CLA	C1B-C2B	2.67	1.49	1.43
22	B	837	CLA	C1B-C2B	2.67	1.49	1.43
22	U	405	CLA	C1B-C2B	2.66	1.49	1.43
22	O	309	CLA	C1B-C2B	2.66	1.49	1.43
22	B	823	CLA	C1B-C2B	2.66	1.49	1.43
22	H	302	CLA	C1B-C2B	2.66	1.49	1.43
22	B	859	CLA	C1B-C2B	2.66	1.49	1.43
22	P	609	CLA	C1B-C2B	2.66	1.49	1.43
22	S	615	CLA	C1B-C2B	2.66	1.49	1.43
22	G	608	CLA	C1B-C2B	2.66	1.49	1.43
22	L	411	CLA	C1B-C2B	2.66	1.49	1.43
22	S	614	CLA	C1B-C2B	2.66	1.49	1.43
22	X	409	CLA	C1B-C2B	2.66	1.49	1.43
22	B	824	CLA	C1B-C2B	2.66	1.49	1.43
22	O	308	CLA	C1B-C2B	2.66	1.49	1.43
22	L	404	CLA	C1B-C2B	2.66	1.49	1.43
22	A	832	CLA	C1B-C2B	2.66	1.49	1.43
22	H	318	CLA	C1B-C2B	2.66	1.49	1.43
22	B	807	CLA	C1B-C2B	2.66	1.49	1.43
22	A	810	CLA	C1B-C2B	2.66	1.49	1.43
22	A	829	CLA	C1B-C2B	2.66	1.49	1.43
22	Q	605	CLA	C1B-C2B	2.66	1.49	1.43
22	N	603	CLA	C1B-C2B	2.66	1.49	1.43
22	X	410	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	307	CLA	C1B-C2B	2.65	1.49	1.43
22	T	603	CLA	C1B-C2B	2.65	1.49	1.43
22	I	601	CLA	C1B-C2B	2.65	1.49	1.43
22	A	852	CLA	C1B-C2B	2.65	1.49	1.43
22	S	607	CLA	C1B-C2B	2.65	1.49	1.43
22	S	610	CLA	C1B-C2B	2.65	1.49	1.43
22	H	306	CLA	C1B-C2B	2.65	1.49	1.43
22	W	409	CLA	C1B-C2B	2.65	1.49	1.43
22	N	606	CLA	C1B-C2B	2.65	1.49	1.43
22	X	408	CLA	C1B-C2B	2.65	1.49	1.43
22	A	827	CLA	C1B-C2B	2.65	1.49	1.43
22	F	405	CLA	C1B-C2B	2.65	1.49	1.43
22	K	612	CLA	C1B-C2B	2.65	1.49	1.43
22	B	806	CLA	C1B-C2B	2.65	1.49	1.43
22	U	403	CLA	C1B-C2B	2.65	1.49	1.43
22	A	815	CLA	C1B-C2B	2.65	1.49	1.43
22	N	602	CLA	C1B-C2B	2.65	1.49	1.43
22	G	609	CLA	C1B-C2B	2.65	1.49	1.43
22	W	406	CLA	C1B-C2B	2.65	1.49	1.43
22	G	607	CLA	C1B-C2B	2.64	1.49	1.43
22	H	307	CLA	C1B-C2B	2.64	1.49	1.43
22	U	411	CLA	C1B-C2B	2.64	1.49	1.43
22	G	605	CLA	C1B-C2B	2.64	1.49	1.43
22	L	402	CLA	C1B-C2B	2.64	1.49	1.43
22	O	315	CLA	C1B-C2B	2.64	1.49	1.43
22	Q	611	CLA	C1B-C2B	2.64	1.49	1.43
22	W	403	CLA	C1B-C2B	2.64	1.49	1.43
22	A	809	CLA	C1B-C2B	2.64	1.49	1.43
22	T	602	CLA	C1B-C2B	2.64	1.49	1.43
22	S	606	CLA	C1B-C2B	2.64	1.49	1.43
22	X	417	CLA	C1B-C2B	2.64	1.49	1.43
22	H	313	CLA	C1B-C2B	2.64	1.49	1.43
22	K	617	CLA	C1B-C2B	2.64	1.49	1.43
22	A	817	CLA	C1B-C2B	2.64	1.49	1.43
22	W	405	CLA	C1B-C2B	2.64	1.49	1.43
22	B	812	CLA	C1B-C2B	2.64	1.49	1.43
22	P	607	CLA	C1B-C2B	2.64	1.49	1.43
22	B	836	CLA	C1B-C2B	2.64	1.49	1.43
22	G	601	CLA	C1B-C2B	2.63	1.49	1.43
22	W	404	CLA	C1B-C2B	2.63	1.49	1.43
22	A	828	CLA	C1B-C2B	2.63	1.49	1.43
22	A	826	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	805	CLA	C1B-C2B	2.63	1.49	1.43
22	T	607	CLA	C1B-C2B	2.63	1.49	1.43
22	L	412	CLA	C1B-C2B	2.63	1.49	1.43
22	O	312	CLA	C1B-C2B	2.63	1.49	1.43
22	B	822	CLA	C1B-C2B	2.63	1.49	1.43
22	L	403	CLA	C1B-C2B	2.63	1.49	1.43
22	B	817	CLA	C1B-C2B	2.63	1.49	1.43
22	B	838	CLA	C1B-C2B	2.63	1.49	1.43
22	H	308	CLA	C1B-C2B	2.63	1.49	1.43
22	K	609	CLA	C1B-C2B	2.62	1.49	1.43
22	K	610	CLA	C1B-C2B	2.62	1.49	1.43
22	S	603	CLA	C1B-C2B	2.62	1.49	1.43
22	B	835	CLA	C1B-C2B	2.62	1.49	1.43
22	Q	604	CLA	C1B-C2B	2.62	1.49	1.43
22	B	828	CLA	C1B-C2B	2.61	1.49	1.43
22	W	411	CLA	C1B-C2B	2.61	1.49	1.43
22	Q	608	CLA	C1B-C2B	2.61	1.49	1.43
22	X	404	CLA	C1B-C2B	2.61	1.49	1.43
22	A	822	CLA	C1B-C2B	2.61	1.49	1.43
22	L	410	CLA	C1B-C2B	2.61	1.49	1.43
22	B	814	CLA	C1B-C2B	2.61	1.49	1.43
22	K	602	CLA	C1B-C2B	2.61	1.49	1.43
22	Q	609	CLA	C1B-C2B	2.61	1.49	1.43
22	A	811	CLA	C1B-C2B	2.60	1.49	1.43
22	A	812	CLA	C1B-C2B	2.60	1.49	1.43
22	K	604	CLA	C1B-C2B	2.60	1.49	1.43
22	T	606	CLA	C1B-C2B	2.60	1.49	1.43
22	P	602	CLA	C1B-C2B	2.60	1.49	1.43
22	A	838	CLA	C1B-C2B	2.60	1.49	1.43
22	K	608	CLA	CMD-C2D	-2.60	1.45	1.50
22	O	306	CLA	C1B-C2B	2.60	1.49	1.43
22	G	603	CLA	C1B-C2B	2.60	1.49	1.43
22	A	836	CLA	C1B-C2B	2.60	1.49	1.43
22	H	304	CLA	C1B-C2B	2.60	1.49	1.43
22	B	827	CLA	C1B-C2B	2.59	1.49	1.43
22	K	603	CLA	C1B-C2B	2.59	1.49	1.43
22	B	813	CLA	C1B-C2B	2.59	1.49	1.43
22	G	606	CLA	C1B-C2B	2.59	1.49	1.43
22	W	402	CLA	C1B-C2B	2.59	1.49	1.43
22	N	606	CLA	C3B-C4B	2.59	1.50	1.42
22	B	830	CLA	MG-NB	-2.58	2.00	2.05
22	S	605	CLA	C4B-NB	2.58	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	T	604	CLA	C1B-C2B	2.58	1.49	1.43
22	B	815	CLA	C1B-C2B	2.58	1.49	1.43
22	A	834	CLA	C1B-C2B	2.57	1.49	1.43
22	A	842	CLA	C1B-C2B	2.57	1.49	1.43
22	B	834	CLA	C1B-C2B	2.57	1.49	1.43
22	W	410	CLA	C1B-C2B	2.57	1.49	1.43
22	B	802	CLA	CMD-C2D	-2.56	1.45	1.50
33	A	802	CL0	CBD-CGD	-2.56	1.49	1.52
22	Q	613	CLA	C1B-C2B	2.55	1.49	1.43
22	A	825	CLA	C1B-C2B	2.55	1.49	1.43
22	A	830	CLA	C1B-C2B	2.55	1.49	1.43
22	B	820	CLA	C1B-C2B	2.54	1.49	1.43
22	A	804	CLA	C1B-C2B	2.53	1.49	1.43
26	K	616	LHG	O8-C6	-2.52	1.39	1.45
22	I	611	CLA	C1B-C2B	2.52	1.49	1.43
22	L	408	CLA	CHC-C1C	2.52	1.43	1.38
24	F	406	DD6	O1-C20	-2.52	1.43	1.46
22	T	606	CLA	C3B-C4B	2.51	1.50	1.42
22	A	803	CLA	CHC-C1C	2.51	1.43	1.38
24	Q	615	DD6	O1-C20	-2.51	1.43	1.46
22	P	607	CLA	CHC-C1C	2.51	1.43	1.38
26	T	614	LHG	O8-C6	-2.50	1.39	1.45
22	A	839	CLA	CHC-C1C	2.49	1.43	1.38
26	G	614	LHG	O8-C6	-2.49	1.39	1.45
22	Q	608	CLA	C3B-C4B	2.49	1.50	1.42
24	A	859	DD6	O1-C20	-2.48	1.43	1.46
22	U	403	CLA	C3B-C4B	2.48	1.50	1.42
24	H	315	DD6	O1-C20	-2.48	1.43	1.46
26	Q	616	LHG	O8-C6	-2.47	1.39	1.45
24	S	611	DD6	O1-C20	-2.47	1.43	1.46
22	X	410	CLA	C3B-C4B	2.47	1.49	1.42
22	H	311	CLA	C3B-C4B	2.46	1.49	1.42
22	A	842	CLA	C3B-C4B	2.46	1.49	1.42
26	A	846	LHG	O8-C6	-2.46	1.39	1.45
26	A	845	LHG	O8-C6	-2.45	1.39	1.45
26	O	318	LHG	O8-C6	-2.45	1.39	1.45
22	W	405	CLA	C3B-C4B	2.45	1.49	1.42
22	B	829	CLA	CMD-C2D	-2.45	1.45	1.50
22	G	606	CLA	C3B-C4B	2.45	1.49	1.42
26	O	324	LHG	O7-C7	2.45	1.41	1.34
22	X	404	CLA	C3B-C4B	2.45	1.49	1.42
26	W	420	LHG	O8-C6	-2.44	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	419	LHG	O7-C7	2.44	1.41	1.34
22	B	802	CLA	MG-ND	-2.44	2.00	2.05
22	L	408	CLA	CMD-C2D	-2.44	1.45	1.50
24	T	612	DD6	O1-C20	-2.44	1.43	1.46
22	P	603	CLA	C3B-C4B	2.44	1.49	1.42
26	W	420	LHG	O7-C7	2.44	1.41	1.34
22	B	830	CLA	CMD-C2D	-2.43	1.45	1.50
24	G	613	DD6	O1-C20	-2.43	1.43	1.46
26	R	614	LHG	O8-C6	-2.43	1.39	1.45
22	A	816	CLA	MG-NB	-2.43	2.01	2.05
22	S	605	CLA	C1B-C2B	2.43	1.48	1.43
22	A	816	CLA	CMD-C2D	-2.42	1.45	1.50
22	H	307	CLA	C3B-C4B	2.42	1.49	1.42
22	Q	618	CLA	C3B-C4B	2.42	1.49	1.42
22	B	802	CLA	CMB-C2B	-2.42	1.45	1.50
22	P	607	CLA	C3B-C4B	2.42	1.49	1.42
31	W	407	CHL	CHC-C4B	-2.42	1.35	1.39
26	U	419	LHG	O8-C6	-2.42	1.39	1.45
22	P	611	CLA	C3B-C4B	2.42	1.49	1.42
22	V	601	CLA	C3B-C4B	2.42	1.49	1.42
22	K	608	CLA	CMB-C2B	-2.42	1.45	1.50
22	X	412	CLA	C3B-C4B	2.42	1.49	1.42
22	W	414	CLA	C3B-C4B	2.42	1.49	1.42
22	B	813	CLA	CHC-C1C	2.41	1.43	1.38
22	S	608	CLA	C3B-C4B	2.41	1.49	1.42
24	O	317	DD6	O1-C20	-2.41	1.43	1.46
22	H	312	CLA	C3B-C4B	2.41	1.49	1.42
22	A	820	CLA	C1B-C2B	2.41	1.48	1.43
22	A	819	CLA	CHC-C1C	2.41	1.43	1.38
22	Q	610	CLA	C3B-C4B	2.41	1.49	1.42
22	W	403	CLA	C3B-C4B	2.40	1.49	1.42
26	P	601	LHG	O7-C5	-2.40	1.40	1.46
26	X	420	LHG	O8-C6	-2.40	1.39	1.45
22	S	606	CLA	C3B-C4B	2.40	1.49	1.42
22	Q	607	CLA	C3B-C4B	2.40	1.49	1.42
24	W	418	DD6	O1-C20	-2.40	1.43	1.46
31	V	605	CHL	CHC-C4B	-2.40	1.35	1.39
22	R	608	CLA	C3B-C4B	2.40	1.49	1.42
22	H	308	CLA	C3B-C4B	2.39	1.49	1.42
22	V	617	CLA	C3B-C4B	2.39	1.49	1.42
22	V	610	CLA	C3B-C4B	2.39	1.49	1.42
26	O	324	LHG	O8-C6	-2.39	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	607	CLA	CMB-C2B	-2.39	1.45	1.50
22	K	607	CLA	CMD-C2D	-2.39	1.45	1.50
22	N	607	CLA	C3B-C4B	2.39	1.49	1.42
22	P	610	CLA	C3B-C4B	2.39	1.49	1.42
22	S	607	CLA	C3B-C4B	2.39	1.49	1.42
24	H	314	DD6	O1-C20	-2.39	1.43	1.46
22	X	419	CLA	C3B-C4B	2.39	1.49	1.42
22	B	830	CLA	CMB-C2B	-2.39	1.45	1.50
22	A	819	CLA	C3B-C4B	2.39	1.49	1.42
22	I	601	CLA	C3B-C4B	2.39	1.49	1.42
24	P	613	DD6	O1-C20	-2.39	1.43	1.46
26	K	619	LHG	O8-C6	-2.39	1.39	1.45
31	X	406	CHL	CHB-C1B	-2.39	1.35	1.39
22	I	607	CLA	CHC-C1C	2.39	1.43	1.38
22	B	820	CLA	C3B-C4B	2.38	1.49	1.42
22	A	819	CLA	CMB-C2B	-2.38	1.45	1.50
22	R	604	CLA	CHC-C1C	2.38	1.43	1.38
22	A	801	CLA	CMD-C2D	-2.38	1.45	1.50
26	O	323	LHG	O8-C23	2.38	1.40	1.33
22	K	608	CLA	CMC-C2C	-2.38	1.45	1.50
26	B	848	LHG	O8-C6	-2.38	1.39	1.45
26	O	321	LHG	O8-C6	-2.38	1.39	1.45
22	I	608	CLA	CMD-C2D	-2.38	1.45	1.50
26	B	851	LHG	O8-C6	-2.38	1.39	1.45
31	U	408	CHL	CHB-C1B	-2.38	1.35	1.39
26	P	601	LHG	O8-C6	-2.38	1.39	1.45
26	O	323	LHG	O8-C6	-2.38	1.39	1.45
24	X	414	DD6	O1-C20	-2.38	1.43	1.46
22	H	302	CLA	C3B-C4B	2.38	1.49	1.42
26	O	321	LHG	O8-C23	2.37	1.40	1.33
22	V	603	CLA	C3B-C4B	2.37	1.49	1.42
22	S	607	CLA	CHC-C1C	2.37	1.43	1.38
22	V	611	CLA	C3B-C4B	2.37	1.49	1.42
26	L	416	LHG	O8-C6	-2.37	1.39	1.45
26	K	616	LHG	O7-C5	-2.37	1.41	1.46
22	S	615	CLA	C3B-C4B	2.37	1.49	1.42
26	B	848	LHG	O7-C5	-2.37	1.41	1.46
22	R	602	CLA	C3B-C4B	2.37	1.49	1.42
24	B	841	DD6	O1-C20	-2.37	1.43	1.46
24	V	615	DD6	O1-C20	-2.37	1.43	1.46
22	X	409	CLA	C3B-C4B	2.37	1.49	1.42
22	B	829	CLA	CMB-C2B	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	846	LHG	O7-C5	-2.37	1.41	1.46
26	N	614	LHG	O7-C5	-2.37	1.41	1.46
22	F	405	CLA	C3B-C4B	2.36	1.49	1.42
22	N	608	CLA	C3B-C4B	2.36	1.49	1.42
22	R	603	CLA	C3B-C4B	2.36	1.49	1.42
22	R	605	CLA	C3B-C4B	2.36	1.49	1.42
22	V	609	CLA	C3B-C4B	2.36	1.49	1.42
22	H	312	CLA	CHC-C1C	2.36	1.43	1.38
31	X	406	CHL	CHC-C4B	-2.36	1.35	1.39
22	P	608	CLA	C3B-C4B	2.36	1.49	1.42
24	G	612	DD6	O1-C20	-2.36	1.43	1.46
24	R	612	DD6	O1-C20	-2.36	1.43	1.46
22	R	610	CLA	C3B-C4B	2.36	1.49	1.42
26	P	601	LHG	O8-C23	2.36	1.40	1.33
22	V	613	CLA	C3B-C4B	2.36	1.49	1.42
31	W	408	CHL	CHB-C1B	-2.36	1.35	1.39
22	U	406	CLA	C3B-C4B	2.36	1.49	1.42
22	B	814	CLA	CHC-C1C	2.36	1.43	1.38
22	H	309	CLA	C3B-C4B	2.36	1.49	1.42
22	L	409	CLA	C3B-C4B	2.36	1.49	1.42
26	S	613	LHG	O8-C6	-2.35	1.39	1.45
22	R	606	CLA	C3B-C4B	2.35	1.49	1.42
22	L	408	CLA	CMB-C2B	-2.35	1.45	1.50
22	U	420	CLA	C3B-C4B	2.35	1.49	1.42
33	A	802	CL0	C3D-C4D	-2.35	1.37	1.41
26	R	614	LHG	O7-C5	-2.35	1.41	1.46
31	U	407	CHL	CHC-C4B	-2.35	1.35	1.39
22	B	811	CLA	C3B-C4B	2.35	1.49	1.42
24	V	614	DD6	O1-C20	-2.35	1.43	1.46
22	K	607	CLA	MG-NB	-2.35	2.01	2.05
22	T	611	CLA	C3B-C4B	2.35	1.49	1.42
22	U	405	CLA	C3B-C4B	2.35	1.49	1.42
26	X	420	LHG	O8-C23	2.35	1.40	1.33
22	A	834	CLA	C3B-C4B	2.35	1.49	1.42
22	R	604	CLA	C3B-C4B	2.35	1.49	1.42
22	U	415	CLA	C3B-C4B	2.35	1.49	1.42
22	S	606	CLA	CHC-C1C	2.35	1.43	1.38
26	H	316	LHG	O8-C6	-2.35	1.39	1.45
22	P	611	CLA	CHC-C1C	2.35	1.43	1.38
22	I	607	CLA	C3B-C4B	2.35	1.49	1.42
22	P	604	CLA	C3B-C4B	2.35	1.49	1.42
24	N	613	DD6	O1-C20	-2.34	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	614	LHG	O7-C5	-2.34	1.41	1.46
22	A	836	CLA	C3B-C4B	2.34	1.49	1.42
22	S	603	CLA	C3B-C4B	2.34	1.49	1.42
22	Q	601	CLA	C3B-C4B	2.34	1.49	1.42
22	Q	613	CLA	C3B-C4B	2.34	1.49	1.42
22	A	837	CLA	C3B-C4B	2.34	1.49	1.42
22	B	822	CLA	CHC-C1C	2.34	1.43	1.38
22	R	601	CLA	C3B-C4B	2.34	1.49	1.42
26	L	416	LHG	O8-C23	2.34	1.40	1.33
24	K	614	DD6	O1-C20	-2.34	1.43	1.46
22	T	609	CLA	C3B-C4B	2.34	1.49	1.42
22	N	607	CLA	CHC-C1C	2.34	1.43	1.38
22	K	613	CLA	C3B-C4B	2.34	1.49	1.42
24	Q	614	DD6	O1-C20	-2.34	1.43	1.46
22	O	307	CLA	C3B-C4B	2.34	1.49	1.42
22	B	824	CLA	C3B-C4B	2.34	1.49	1.42
22	O	315	CLA	C3B-C4B	2.34	1.49	1.42
22	A	824	CLA	C3B-C4B	2.34	1.49	1.42
22	S	601	CLA	C3B-C4B	2.34	1.49	1.42
26	L	416	LHG	O7-C5	-2.34	1.41	1.46
22	X	408	CLA	C3B-C4B	2.33	1.49	1.42
22	B	825	CLA	CHC-C1C	2.33	1.43	1.38
22	T	610	CLA	C3B-C4B	2.33	1.49	1.42
26	N	614	LHG	O7-C7	2.33	1.40	1.34
22	I	608	CLA	C3B-C4B	2.33	1.49	1.42
26	O	318	LHG	O7-C7	2.33	1.40	1.34
22	X	417	CLA	C3B-C4B	2.33	1.49	1.42
22	K	611	CLA	C3B-C4B	2.33	1.49	1.42
22	R	609	CLA	C3B-C4B	2.33	1.49	1.42
26	K	619	LHG	O8-C23	2.33	1.40	1.33
26	K	619	LHG	O7-C7	2.33	1.40	1.34
22	A	817	CLA	C3B-C4B	2.33	1.49	1.42
26	T	614	LHG	O7-C5	-2.33	1.41	1.46
22	V	609	CLA	CHC-C1C	2.33	1.43	1.38
22	A	801	CLA	C1B-C2B	2.33	1.48	1.43
24	N	612	DD6	O1-C20	-2.33	1.43	1.46
24	X	401	DD6	O1-C20	-2.33	1.43	1.46
26	X	420	LHG	O7-C5	-2.33	1.41	1.46
22	Q	609	CLA	C3B-C4B	2.33	1.49	1.42
26	N	614	LHG	O8-C6	-2.33	1.40	1.45
26	B	848	LHG	O8-C23	2.33	1.40	1.33
22	F	403	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	405	CLA	C3B-C4B	2.33	1.49	1.42
22	R	615	CLA	C3B-C4B	2.33	1.49	1.42
22	Q	607	CLA	CHC-C1C	2.33	1.43	1.38
22	A	803	CLA	C3B-C4B	2.33	1.49	1.42
26	Q	616	LHG	O7-C5	-2.33	1.41	1.46
22	B	818	CLA	C3B-C4B	2.33	1.49	1.42
22	T	607	CLA	C3B-C4B	2.33	1.49	1.42
22	S	605	CLA	CMD-C2D	-2.33	1.46	1.50
26	A	845	LHG	O7-C5	-2.33	1.41	1.46
22	N	611	CLA	C3B-C4B	2.33	1.49	1.42
22	B	859	CLA	C3B-C4B	2.33	1.49	1.42
22	S	608	CLA	CHC-C1C	2.33	1.43	1.38
22	N	609	CLA	C3B-C4B	2.32	1.49	1.42
22	T	603	CLA	C3B-C4B	2.32	1.49	1.42
22	B	802	CLA	CMC-C2C	-2.32	1.46	1.50
22	S	610	CLA	C3B-C4B	2.32	1.49	1.42
22	V	607	CLA	C3B-C4B	2.32	1.49	1.42
22	B	828	CLA	C3B-C4B	2.32	1.49	1.42
26	Q	616	LHG	O7-C7	2.32	1.40	1.34
22	S	605	CLA	MG-NB	-2.32	2.01	2.05
22	L	406	CLA	C3B-C4B	2.32	1.49	1.42
31	V	606	CHL	CHB-C1B	-2.32	1.35	1.39
22	F	404	CLA	C3B-C4B	2.32	1.49	1.42
26	B	851	LHG	O7-C7	2.32	1.40	1.34
26	B	851	LHG	O8-C23	2.32	1.40	1.33
22	T	611	CLA	CHC-C1C	2.32	1.43	1.38
24	I	613	DD6	O1-C20	-2.32	1.43	1.46
26	S	613	LHG	O8-C23	2.32	1.40	1.33
22	B	822	CLA	C3B-C4B	2.32	1.49	1.42
26	O	324	LHG	O8-C23	2.32	1.40	1.33
22	X	413	CLA	C3B-C4B	2.32	1.49	1.42
22	H	308	CLA	CHC-C1C	2.32	1.43	1.38
22	O	309	CLA	CHC-C1C	2.32	1.43	1.38
22	Q	605	CLA	C3B-C4B	2.32	1.49	1.42
22	O	309	CLA	C3B-C4B	2.32	1.49	1.42
22	T	608	CLA	C3B-C4B	2.32	1.49	1.42
22	N	605	CLA	C3B-C4B	2.32	1.49	1.42
22	S	609	CLA	C3B-C4B	2.32	1.49	1.42
22	I	605	CLA	C3B-C4B	2.32	1.49	1.42
22	V	612	CLA	C3B-C4B	2.32	1.49	1.42
26	K	619	LHG	O7-C5	-2.32	1.41	1.46
22	H	309	CLA	CHC-C1C	2.32	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	859	CLA	CHC-C1C	2.32	1.43	1.38
22	I	609	CLA	C3B-C4B	2.32	1.49	1.42
26	O	321	LHG	O7-C5	-2.32	1.41	1.46
26	N	616	LHG	O8-C6	-2.32	1.40	1.45
22	T	604	CLA	C3B-C4B	2.32	1.49	1.42
22	O	312	CLA	C3B-C4B	2.32	1.49	1.42
22	L	411	CLA	C3B-C4B	2.32	1.49	1.42
22	Q	603	CLA	C3B-C4B	2.32	1.49	1.42
22	B	820	CLA	CHC-C1C	2.32	1.43	1.38
22	V	611	CLA	CHC-C1C	2.31	1.43	1.38
22	I	606	CLA	C3B-C4B	2.31	1.49	1.42
22	H	305	CLA	C3B-C4B	2.31	1.49	1.42
26	G	614	LHG	O7-C7	2.31	1.40	1.34
22	I	611	CLA	C3B-C4B	2.31	1.49	1.42
26	H	316	LHG	O7-C5	-2.31	1.41	1.46
26	W	420	LHG	O8-C23	2.31	1.40	1.33
22	B	834	CLA	C3B-C4B	2.31	1.49	1.42
22	H	313	CLA	C3B-C4B	2.31	1.49	1.42
22	O	314	CLA	C3B-C4B	2.31	1.49	1.42
22	B	812	CLA	CHC-C1C	2.31	1.43	1.38
26	A	846	LHG	O8-C23	2.31	1.40	1.33
26	O	323	LHG	O7-C7	2.31	1.40	1.34
22	U	411	CLA	C3B-C4B	2.31	1.49	1.42
22	G	609	CLA	CHC-C1C	2.31	1.43	1.38
22	B	839	CLA	C3B-C4B	2.31	1.49	1.42
22	G	604	CLA	C3B-C4B	2.31	1.49	1.42
22	W	409	CLA	C3B-C4B	2.31	1.49	1.42
22	A	806	CLA	CHC-C1C	2.31	1.43	1.38
22	P	606	CLA	C3B-C4B	2.31	1.49	1.42
26	N	614	LHG	O8-C23	2.31	1.40	1.33
22	B	833	CLA	C3B-C4B	2.31	1.49	1.42
22	L	403	CLA	C3B-C4B	2.31	1.49	1.42
22	A	822	CLA	C3B-C4B	2.31	1.49	1.42
22	S	614	CLA	C3B-C4B	2.31	1.49	1.42
22	A	830	CLA	C3B-C4B	2.31	1.49	1.42
22	G	607	CLA	C3B-C4B	2.30	1.49	1.42
22	R	611	CLA	C3B-C4B	2.30	1.49	1.42
31	W	422	CHL	CHC-C4B	-2.30	1.35	1.39
22	N	601	CLA	C3B-C4B	2.30	1.49	1.42
26	N	616	LHG	O7-C7	2.30	1.40	1.34
26	N	616	LHG	O7-C5	-2.30	1.41	1.46
22	A	814	CLA	C3B-C4B	2.30	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	801	CLA	CMC-C2C	-2.30	1.46	1.50
26	Q	616	LHG	O8-C23	2.30	1.40	1.33
22	P	604	CLA	CHC-C1C	2.30	1.43	1.38
26	S	613	LHG	O7-C5	-2.30	1.41	1.46
22	O	306	CLA	MG-NB	-2.30	2.01	2.05
22	I	603	CLA	C3B-C4B	2.30	1.49	1.42
22	A	809	CLA	C3B-C4B	2.30	1.49	1.42
22	A	825	CLA	C3B-C4B	2.30	1.49	1.42
22	B	812	CLA	C3B-C4B	2.30	1.49	1.42
22	A	811	CLA	CHC-C1C	2.30	1.43	1.38
22	A	829	CLA	C3B-C4B	2.30	1.49	1.42
22	B	837	CLA	C3B-C4B	2.30	1.49	1.42
22	A	827	CLA	C3B-C4B	2.30	1.49	1.42
22	N	606	CLA	CHC-C1C	2.30	1.43	1.38
26	U	419	LHG	O8-C23	2.30	1.40	1.33
22	B	823	CLA	C3B-C4B	2.30	1.49	1.42
22	G	611	CLA	C3B-C4B	2.30	1.49	1.42
22	L	410	CLA	C3B-C4B	2.30	1.49	1.42
26	A	845	LHG	O7-C7	2.30	1.40	1.34
22	L	404	CLA	C3B-C4B	2.30	1.49	1.42
22	G	603	CLA	C3B-C4B	2.30	1.49	1.42
22	A	852	CLA	C3B-C4B	2.30	1.49	1.42
22	U	405	CLA	CHC-C1C	2.30	1.43	1.38
26	R	614	LHG	O7-C7	2.30	1.40	1.34
22	A	832	CLA	C3B-C4B	2.30	1.49	1.42
22	W	415	CLA	CHC-C1C	2.30	1.43	1.38
22	O	305	CLA	C3B-C4B	2.30	1.49	1.42
24	O	316	DD6	O1-C20	-2.30	1.43	1.46
22	P	605	CLA	C3B-C4B	2.30	1.49	1.42
22	W	419	CLA	C3B-C4B	2.30	1.49	1.42
22	B	821	CLA	C3B-C4B	2.30	1.49	1.42
22	R	606	CLA	CHC-C1C	2.30	1.43	1.38
26	H	316	LHG	O8-C23	2.30	1.40	1.33
22	H	318	CLA	C3B-C4B	2.29	1.49	1.42
22	I	608	CLA	CHC-C1C	2.29	1.43	1.38
22	W	406	CLA	C3B-C4B	2.29	1.49	1.42
26	O	318	LHG	O8-C23	2.29	1.40	1.33
24	R	613	DD6	O1-C20	-2.29	1.43	1.46
22	V	613	CLA	CHC-C1C	2.29	1.43	1.38
22	X	411	CLA	CHC-C1C	2.29	1.43	1.38
22	L	412	CLA	CHC-C1C	2.29	1.43	1.38
22	K	610	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	311	CLA	CHC-C1C	2.29	1.43	1.38
22	Q	611	CLA	C3B-C4B	2.29	1.49	1.42
22	K	607	CLA	C4B-NB	2.29	1.40	1.37
22	B	825	CLA	C3B-C4B	2.29	1.49	1.42
22	G	610	CLA	C3B-C4B	2.29	1.49	1.42
22	W	411	CLA	C3B-C4B	2.29	1.49	1.42
22	T	602	CLA	CHC-C1C	2.29	1.43	1.38
22	T	607	CLA	CHC-C1C	2.29	1.43	1.38
31	W	408	CHL	C3A-C2A	-2.29	1.52	1.54
22	R	608	CLA	CHC-C1C	2.29	1.43	1.38
22	B	838	CLA	C3B-C4B	2.29	1.49	1.42
22	B	804	CLA	C3B-C4B	2.29	1.49	1.42
22	X	407	CLA	C3B-C4B	2.29	1.49	1.42
22	A	811	CLA	C3B-C4B	2.29	1.49	1.42
24	U	416	DD6	O1-C20	-2.29	1.43	1.46
22	V	607	CLA	CHC-C1C	2.29	1.43	1.38
22	N	602	CLA	C3B-C4B	2.29	1.49	1.42
26	X	420	LHG	O7-C7	2.29	1.40	1.34
22	I	611	CLA	CHC-C1C	2.29	1.43	1.38
22	R	605	CLA	CHC-C1C	2.29	1.43	1.38
26	G	614	LHG	O8-C23	2.29	1.40	1.33
26	B	851	LHG	O7-C5	-2.29	1.41	1.46
22	B	831	CLA	C3B-C4B	2.29	1.49	1.42
22	P	606	CLA	CMD-C2D	-2.29	1.46	1.50
22	N	604	CLA	C3B-C4B	2.29	1.49	1.42
22	R	611	CLA	CHC-C1C	2.29	1.43	1.38
22	A	833	CLA	C3B-C4B	2.29	1.49	1.42
22	U	409	CLA	CHC-C1C	2.29	1.43	1.38
22	B	814	CLA	C3B-C4B	2.29	1.49	1.42
22	Q	601	CLA	CHC-C1C	2.29	1.43	1.38
22	Q	618	CLA	CHC-C1C	2.29	1.43	1.38
22	K	602	CLA	C3B-C4B	2.29	1.49	1.42
22	U	414	CLA	C3B-C4B	2.29	1.49	1.42
22	N	609	CLA	CHC-C1C	2.29	1.43	1.38
22	W	406	CLA	CHC-C1C	2.29	1.43	1.38
26	N	616	LHG	O8-C23	2.29	1.40	1.33
22	B	817	CLA	C3B-C4B	2.29	1.49	1.42
22	U	410	CLA	C3B-C4B	2.29	1.49	1.42
22	O	311	CLA	CHC-C1C	2.29	1.43	1.38
22	W	403	CLA	CHC-C1C	2.29	1.43	1.38
24	L	414	DD6	O1-C20	-2.29	1.43	1.46
22	K	606	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	405	CLA	C3B-C4B	2.29	1.49	1.42
22	A	830	CLA	CHC-C1C	2.28	1.43	1.38
22	A	831	CLA	C3B-C4B	2.28	1.49	1.42
22	X	402	CLA	C3B-C4B	2.28	1.49	1.42
26	R	614	LHG	O8-C23	2.28	1.40	1.33
22	H	306	CLA	C3B-C4B	2.28	1.49	1.42
22	K	604	CLA	C3B-C4B	2.28	1.49	1.42
22	H	304	CLA	C3B-C4B	2.28	1.49	1.42
22	L	409	CLA	CHC-C1C	2.28	1.43	1.38
22	R	602	CLA	CHC-C1C	2.28	1.43	1.38
22	N	603	CLA	C3B-C4B	2.28	1.49	1.42
22	V	602	CLA	CHC-C1C	2.28	1.43	1.38
22	P	609	CLA	C3B-C4B	2.28	1.49	1.42
22	B	836	CLA	MG-NB	-2.28	2.01	2.05
22	G	609	CLA	C3B-C4B	2.28	1.49	1.42
22	A	829	CLA	CHC-C1C	2.28	1.43	1.38
22	A	815	CLA	C3B-C4B	2.28	1.49	1.42
24	S	612	DD6	O1-C20	-2.28	1.43	1.46
22	B	803	CLA	CHC-C1C	2.28	1.43	1.38
22	B	835	CLA	C3B-C4B	2.28	1.49	1.42
26	T	614	LHG	O8-C23	2.28	1.40	1.33
22	L	403	CLA	CHC-C1C	2.28	1.43	1.38
22	R	601	CLA	CHC-C1C	2.28	1.43	1.38
26	H	316	LHG	O7-C7	2.28	1.40	1.34
22	L	406	CLA	CMD-C2D	-2.28	1.46	1.50
22	A	834	CLA	CHC-C1C	2.28	1.43	1.38
22	U	412	CLA	C3B-C4B	2.28	1.49	1.42
22	N	604	CLA	CHC-C1C	2.28	1.43	1.38
22	A	828	CLA	CHC-C1C	2.28	1.43	1.38
22	S	604	CLA	C3B-C4B	2.28	1.49	1.42
24	I	612	DD6	O1-C20	-2.28	1.43	1.46
26	B	848	LHG	O7-C7	2.28	1.40	1.34
22	I	604	CLA	C3B-C4B	2.28	1.49	1.42
22	O	315	CLA	CHC-C1C	2.28	1.43	1.38
22	O	319	CLA	C3B-C4B	2.28	1.49	1.42
22	B	827	CLA	C3B-C4B	2.28	1.49	1.42
22	U	401	CLA	C3B-C4B	2.28	1.49	1.42
22	W	410	CLA	C3B-C4B	2.28	1.49	1.42
22	A	806	CLA	C3B-C4B	2.28	1.49	1.42
22	W	413	CLA	C3B-C4B	2.28	1.49	1.42
22	X	411	CLA	C3B-C4B	2.28	1.49	1.42
22	A	844	CLA	CMC-C2C	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	613	LHG	O7-C7	2.28	1.40	1.34
22	V	604	CLA	CHC-C1C	2.28	1.43	1.38
22	X	409	CLA	CHC-C1C	2.28	1.43	1.38
22	W	404	CLA	C3B-C4B	2.28	1.49	1.42
22	L	408	CLA	MG-NB	-2.28	2.01	2.05
22	X	413	CLA	CHC-C1C	2.28	1.43	1.38
22	B	835	CLA	CHC-C1C	2.27	1.43	1.38
22	A	804	CLA	CHC-C1C	2.27	1.43	1.38
22	V	602	CLA	C3B-C4B	2.27	1.49	1.42
24	W	417	DD6	O1-C20	-2.27	1.43	1.46
22	P	603	CLA	CHC-C1C	2.27	1.43	1.38
22	A	837	CLA	CHC-C1C	2.27	1.43	1.38
22	T	601	CLA	C3B-C4B	2.27	1.49	1.42
22	A	823	CLA	C3B-C4B	2.27	1.49	1.42
22	S	604	CLA	CHC-C1C	2.27	1.43	1.38
22	U	410	CLA	CHC-C1C	2.27	1.43	1.38
22	Q	617	CLA	C3B-C4B	2.27	1.49	1.42
22	U	406	CLA	CHC-C1C	2.27	1.43	1.38
22	O	311	CLA	C3B-C4B	2.27	1.49	1.42
22	B	815	CLA	CHC-C1C	2.27	1.43	1.38
22	O	310	CLA	C3B-C4B	2.27	1.49	1.42
22	A	828	CLA	C3B-C4B	2.27	1.49	1.42
22	T	605	CLA	C3B-C4B	2.27	1.49	1.42
22	H	318	CLA	CHC-C1C	2.27	1.43	1.38
22	B	807	CLA	CHC-C1C	2.27	1.43	1.38
22	S	605	CLA	CMC-C2C	-2.27	1.46	1.50
22	G	605	CLA	C3B-C4B	2.27	1.49	1.42
22	O	306	CLA	CHC-C1C	2.27	1.43	1.38
22	U	420	CLA	CHC-C1C	2.27	1.43	1.38
22	Q	604	CLA	CHC-C1C	2.27	1.43	1.38
31	W	408	CHL	CHC-C4B	-2.27	1.36	1.39
26	O	318	LHG	O7-C5	-2.27	1.41	1.46
22	W	415	CLA	C3B-C4B	2.27	1.49	1.42
22	B	816	CLA	CHC-C1C	2.27	1.43	1.38
22	B	833	CLA	CHC-C1C	2.27	1.43	1.38
22	V	604	CLA	C3B-C4B	2.27	1.49	1.42
22	A	804	CLA	C3B-C4B	2.27	1.49	1.42
22	G	610	CLA	CHC-C1C	2.27	1.43	1.38
22	V	601	CLA	CHC-C1C	2.27	1.43	1.38
22	P	602	CLA	CMD-C2D	-2.27	1.46	1.50
26	A	846	LHG	O7-C7	2.27	1.40	1.34
22	B	810	CLA	C3B-C4B	2.27	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	612	CLA	C3B-C4B	2.27	1.49	1.42
22	O	308	CLA	C3B-C4B	2.27	1.49	1.42
22	K	610	CLA	CHC-C1C	2.27	1.43	1.38
22	P	610	CLA	CHC-C1C	2.27	1.43	1.38
22	I	602	CLA	C3B-C4B	2.27	1.49	1.42
22	U	409	CLA	C3B-C4B	2.27	1.49	1.42
24	W	416	DD6	O1-C20	-2.27	1.43	1.46
22	N	605	CLA	CHC-C1C	2.27	1.43	1.38
22	W	413	CLA	CHC-C1C	2.27	1.43	1.38
22	A	807	CLA	CHC-C1C	2.27	1.43	1.38
22	A	827	CLA	CHC-C1C	2.27	1.43	1.38
22	B	813	CLA	C3B-C4B	2.27	1.49	1.42
31	V	606	CHL	CHC-C4B	-2.27	1.36	1.39
22	K	603	CLA	C3B-C4B	2.27	1.49	1.42
22	W	402	CLA	C3B-C4B	2.27	1.49	1.42
22	B	818	CLA	CHC-C1C	2.26	1.43	1.38
22	S	602	CLA	C3B-C4B	2.26	1.49	1.42
22	B	808	CLA	C3B-C4B	2.26	1.49	1.42
22	Q	606	CLA	C3B-C4B	2.26	1.49	1.42
22	L	405	CLA	CHC-C1C	2.26	1.43	1.38
22	O	308	CLA	CHC-C1C	2.26	1.43	1.38
22	L	406	CLA	CHC-C1C	2.26	1.43	1.38
22	V	610	CLA	CHC-C1C	2.26	1.43	1.38
22	N	602	CLA	CHC-C1C	2.26	1.43	1.38
26	T	614	LHG	O7-C7	2.26	1.40	1.34
22	R	603	CLA	CHC-C1C	2.26	1.43	1.38
24	U	417	DD6	O1-C20	-2.26	1.43	1.46
22	A	852	CLA	CHC-C1C	2.26	1.43	1.38
22	A	810	CLA	C3B-C4B	2.26	1.49	1.42
26	O	321	LHG	O7-C7	2.26	1.40	1.34
22	O	313	CLA	C3B-C4B	2.26	1.49	1.42
22	B	827	CLA	CHC-C1C	2.26	1.43	1.38
22	U	401	CLA	CHC-C1C	2.26	1.43	1.38
22	W	412	CLA	C3B-C4B	2.26	1.49	1.42
22	A	808	CLA	C3B-C4B	2.26	1.49	1.42
22	B	826	CLA	C3B-C4B	2.26	1.49	1.42
22	K	609	CLA	C3B-C4B	2.26	1.49	1.42
22	B	831	CLA	CHC-C1C	2.26	1.43	1.38
22	O	314	CLA	CHC-C1C	2.26	1.43	1.38
22	B	829	CLA	C1B-C2B	2.26	1.48	1.43
22	A	826	CLA	C3B-C4B	2.26	1.49	1.42
22	B	824	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	603	CLA	CHC-C1C	2.26	1.43	1.38
22	Q	610	CLA	CHC-C1C	2.26	1.43	1.38
26	P	601	LHG	O7-C7	2.26	1.40	1.34
22	A	820	CLA	C3B-C4B	2.26	1.49	1.42
22	B	815	CLA	C3B-C4B	2.26	1.49	1.42
22	V	612	CLA	CHC-C1C	2.26	1.43	1.38
22	H	310	CLA	C3B-C4B	2.26	1.49	1.42
26	L	416	LHG	O7-C7	2.26	1.40	1.34
22	I	602	CLA	CHC-C1C	2.26	1.43	1.38
22	A	826	CLA	CHC-C1C	2.26	1.43	1.38
22	U	404	CLA	C3B-C4B	2.26	1.49	1.42
22	K	605	CLA	C3B-C4B	2.26	1.49	1.42
22	A	821	CLA	C3B-C4B	2.26	1.49	1.42
22	G	602	CLA	CHC-C1C	2.26	1.43	1.38
22	A	832	CLA	CHC-C1C	2.26	1.43	1.38
22	K	611	CLA	CHC-C1C	2.25	1.43	1.38
22	L	417	CLA	C3B-C4B	2.25	1.49	1.42
22	B	839	CLA	CHC-C1C	2.25	1.43	1.38
22	P	605	CLA	CHC-C1C	2.25	1.43	1.38
22	A	810	CLA	CHC-C1C	2.25	1.43	1.38
22	L	408	CLA	CMC-C2C	-2.25	1.46	1.50
22	Q	609	CLA	CHC-C1C	2.25	1.43	1.38
22	T	609	CLA	CHC-C1C	2.25	1.43	1.38
22	X	407	CLA	CHC-C1C	2.25	1.43	1.38
22	A	819	CLA	CMD-C2D	-2.25	1.46	1.50
22	U	413	CLA	C3B-C4B	2.25	1.49	1.42
22	X	403	CLA	C3B-C4B	2.25	1.49	1.42
28	F	408	LMG	C4-C5	2.25	1.57	1.53
22	A	817	CLA	CHC-C1C	2.25	1.43	1.38
22	R	609	CLA	CHC-C1C	2.25	1.43	1.38
22	L	417	CLA	MG-NB	-2.25	2.01	2.05
24	L	413	DD6	O1-C20	-2.25	1.43	1.46
22	G	601	CLA	CHC-C1C	2.25	1.43	1.38
22	W	410	CLA	CHC-C1C	2.25	1.43	1.38
31	V	605	CHL	CHB-C1B	-2.25	1.36	1.39
22	A	844	CLA	C3B-C4B	2.25	1.49	1.42
22	T	604	CLA	CHC-C1C	2.25	1.43	1.38
22	V	603	CLA	CHC-C1C	2.25	1.43	1.38
22	A	814	CLA	CHC-C1C	2.25	1.43	1.38
22	Q	612	CLA	C3B-C4B	2.25	1.49	1.42
22	V	617	CLA	CHC-C1C	2.25	1.43	1.38
22	L	410	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	601	CLA	C3B-C4B	2.25	1.49	1.42
22	K	617	CLA	CHC-C1C	2.25	1.43	1.38
22	A	809	CLA	CHC-C1C	2.25	1.43	1.38
26	A	845	LHG	O8-C23	2.25	1.39	1.33
22	K	606	CLA	CHC-C1C	2.25	1.43	1.38
22	B	808	CLA	CHC-C1C	2.25	1.43	1.38
22	A	807	CLA	C3B-C4B	2.25	1.49	1.42
22	F	405	CLA	CHC-C1C	2.25	1.43	1.38
22	I	610	CLA	C3B-C4B	2.25	1.49	1.42
22	I	606	CLA	CHC-C1C	2.24	1.43	1.38
22	P	602	CLA	CHC-C1C	2.24	1.43	1.38
22	T	605	CLA	CHC-C1C	2.24	1.43	1.38
24	A	847	DD6	O1-C20	-2.24	1.43	1.46
22	A	835	CLA	C3B-C4B	2.24	1.49	1.42
22	H	313	CLA	CHC-C1C	2.24	1.43	1.38
22	A	823	CLA	CHC-C1C	2.24	1.43	1.38
22	Q	603	CLA	CHC-C1C	2.24	1.43	1.38
22	U	415	CLA	CHC-C1C	2.24	1.43	1.38
22	B	806	CLA	C3B-C4B	2.24	1.49	1.42
22	S	614	CLA	CHC-C1C	2.24	1.43	1.38
22	A	813	CLA	C3B-C4B	2.24	1.49	1.42
22	W	412	CLA	CHC-C1C	2.24	1.43	1.38
22	T	601	CLA	CHC-C1C	2.24	1.43	1.38
22	B	830	CLA	CMC-C2C	-2.24	1.46	1.50
22	I	610	CLA	CHC-C1C	2.24	1.43	1.38
22	A	820	CLA	CHC-C1C	2.24	1.43	1.38
22	A	831	CLA	CHC-C1C	2.24	1.43	1.38
22	T	602	CLA	C3B-C4B	2.24	1.49	1.42
22	B	828	CLA	CHC-C1C	2.24	1.43	1.38
22	W	411	CLA	CHC-C1C	2.24	1.43	1.38
22	H	306	CLA	CHC-C1C	2.24	1.43	1.38
22	L	402	CLA	CHC-C1C	2.24	1.43	1.38
22	B	807	CLA	C3B-C4B	2.24	1.49	1.42
22	U	414	CLA	CHC-C1C	2.24	1.43	1.38
22	L	412	CLA	C3B-C4B	2.24	1.49	1.42
22	K	608	CLA	C4B-NB	2.24	1.40	1.37
22	H	302	CLA	CHC-C1C	2.24	1.43	1.38
22	X	405	CLA	CHC-C1C	2.24	1.43	1.38
22	P	606	CLA	MG-NB	-2.24	2.01	2.05
22	X	408	CLA	CHC-C1C	2.24	1.43	1.38
22	L	408	CLA	C4B-NB	2.24	1.40	1.37
22	S	605	CLA	CMB-C2B	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	617	CLA	CHC-C1C	2.24	1.43	1.38
22	S	603	CLA	CHC-C1C	2.24	1.43	1.38
22	H	303	CLA	CHC-C1C	2.24	1.43	1.38
22	W	402	CLA	CHC-C1C	2.24	1.43	1.38
22	A	805	CLA	CHC-C1C	2.24	1.43	1.38
22	G	608	CLA	C3B-C4B	2.24	1.49	1.42
22	O	313	CLA	CHC-C1C	2.23	1.43	1.38
22	H	303	CLA	C3B-C4B	2.23	1.49	1.42
22	F	404	CLA	CHC-C1C	2.23	1.43	1.38
24	T	613	DD6	O1-C20	-2.23	1.43	1.46
22	B	834	CLA	CHC-C1C	2.23	1.43	1.38
22	B	816	CLA	C3B-C4B	2.23	1.49	1.42
22	S	610	CLA	CHC-C1C	2.23	1.43	1.38
22	U	412	CLA	CHC-C1C	2.23	1.43	1.38
22	A	833	CLA	CHC-C1C	2.23	1.43	1.38
22	G	604	CLA	CHC-C1C	2.23	1.43	1.38
22	S	609	CLA	CHC-C1C	2.23	1.43	1.38
22	B	811	CLA	CHC-C1C	2.23	1.43	1.38
22	A	822	CLA	CHC-C1C	2.23	1.43	1.38
22	A	801	CLA	MG-NB	-2.23	2.01	2.05
22	R	610	CLA	CHC-C1C	2.23	1.43	1.38
22	X	404	CLA	CHC-C1C	2.23	1.43	1.38
22	B	803	CLA	C3B-C4B	2.23	1.49	1.42
22	A	842	CLA	CHC-C1C	2.23	1.43	1.38
22	G	608	CLA	MG-NB	-2.23	2.01	2.05
22	B	809	CLA	C3B-C4B	2.23	1.49	1.42
22	G	611	CLA	CHC-C1C	2.23	1.43	1.38
22	A	839	CLA	C3B-C4B	2.23	1.49	1.42
22	I	603	CLA	CHC-C1C	2.23	1.43	1.38
22	A	840	CLA	MG-NB	-2.23	2.01	2.05
22	A	824	CLA	CHC-C1C	2.23	1.42	1.38
22	Q	604	CLA	MG-NB	-2.23	2.01	2.05
22	I	601	CLA	CHC-C1C	2.23	1.42	1.38
22	O	305	CLA	CHC-C1C	2.23	1.42	1.38
22	B	805	CLA	C3B-C4B	2.23	1.49	1.42
22	K	617	CLA	MG-NB	-2.22	2.01	2.05
22	A	816	CLA	C1B-C2B	2.22	1.48	1.43
22	J	102	CLA	CHC-C1C	2.22	1.42	1.38
22	R	615	CLA	CHC-C1C	2.22	1.42	1.38
22	K	617	CLA	C3B-C4B	2.22	1.49	1.42
22	O	319	CLA	CHC-C1C	2.22	1.42	1.38
22	B	820	CLA	CMD-C2D	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	305	CLA	CHC-C1C	2.22	1.42	1.38
22	I	605	CLA	CHC-C1C	2.22	1.42	1.38
22	A	815	CLA	CHC-C1C	2.22	1.42	1.38
22	B	832	CLA	C3B-C4B	2.22	1.49	1.42
22	K	607	CLA	C3B-C4B	2.22	1.49	1.42
22	T	608	CLA	CHC-C1C	2.22	1.42	1.38
22	V	608	CLA	C3B-C4B	2.22	1.49	1.42
22	T	603	CLA	CHC-C1C	2.22	1.42	1.38
22	X	412	CLA	CHC-C1C	2.22	1.42	1.38
26	K	616	LHG	O8-C23	2.22	1.39	1.33
22	A	808	CLA	CHC-C1C	2.22	1.42	1.38
26	O	323	LHG	O7-C5	-2.22	1.41	1.46
22	Q	608	CLA	CHC-C1C	2.22	1.42	1.38
22	L	407	CLA	C3B-C4B	2.22	1.49	1.42
22	B	815	CLA	MG-NB	-2.22	2.01	2.05
22	K	602	CLA	CHC-C1C	2.22	1.42	1.38
22	U	403	CLA	CHC-C1C	2.22	1.42	1.38
22	U	411	CLA	CHC-C1C	2.22	1.42	1.38
22	X	402	CLA	CHC-C1C	2.22	1.42	1.38
22	L	408	CLA	C3B-C4B	2.22	1.49	1.42
22	B	805	CLA	CHC-C1C	2.22	1.42	1.38
22	B	823	CLA	CHC-C1C	2.22	1.42	1.38
22	A	838	CLA	C3B-C4B	2.22	1.49	1.42
22	L	411	CLA	CHC-C1C	2.22	1.42	1.38
22	I	611	CLA	MG-NB	-2.22	2.01	2.05
24	L	415	DD6	O1-C20	-2.22	1.43	1.46
22	A	801	CLA	CMB-C2B	-2.22	1.46	1.50
22	A	812	CLA	C3B-C4B	2.22	1.49	1.42
22	A	835	CLA	CHC-C1C	2.22	1.42	1.38
22	G	605	CLA	CHC-C1C	2.21	1.42	1.38
22	K	613	CLA	CHC-C1C	2.21	1.42	1.38
22	O	306	CLA	C3B-C4B	2.21	1.49	1.42
22	Q	605	CLA	CHC-C1C	2.21	1.42	1.38
22	W	409	CLA	CHC-C1C	2.21	1.42	1.38
22	B	830	CLA	C4B-NB	2.21	1.40	1.37
22	A	819	CLA	CMC-C2C	-2.21	1.46	1.50
24	K	615	DD6	O1-C20	-2.21	1.43	1.46
22	B	810	CLA	CHC-C1C	2.21	1.42	1.38
22	L	402	CLA	C3B-C4B	2.21	1.49	1.42
22	O	307	CLA	CHC-C1C	2.21	1.42	1.38
22	B	809	CLA	CHC-C1C	2.21	1.42	1.38
22	B	819	CLA	C3B-C4B	2.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	841	CLA	C3B-C4B	2.21	1.49	1.42
22	T	607	CLA	MG-NB	-2.21	2.01	2.05
22	N	608	CLA	CMD-C2D	-2.21	1.46	1.50
22	L	404	CLA	CHC-C1C	2.21	1.42	1.38
22	G	606	CLA	CHC-C1C	2.21	1.42	1.38
22	Q	606	CLA	CHC-C1C	2.21	1.42	1.38
22	A	825	CLA	CHC-C1C	2.21	1.42	1.38
22	H	304	CLA	CHC-C1C	2.20	1.42	1.38
22	A	841	CLA	CHC-C1C	2.20	1.42	1.38
22	K	607	CLA	CMC-C2C	-2.20	1.46	1.50
22	B	804	CLA	CHC-C1C	2.20	1.42	1.38
22	T	610	CLA	CHC-C1C	2.20	1.42	1.38
22	Q	604	CLA	C3B-C4B	2.20	1.49	1.42
22	K	612	CLA	CHC-C1C	2.20	1.42	1.38
22	A	805	CLA	C3B-C4B	2.20	1.49	1.42
22	L	407	CLA	CHC-C1C	2.20	1.42	1.38
22	A	813	CLA	CHC-C1C	2.20	1.42	1.38
22	O	312	CLA	CHC-C1C	2.20	1.42	1.38
22	R	607	CLA	CMB-C2B	-2.20	1.46	1.50
31	U	407	CHL	CHB-C1B	-2.20	1.36	1.39
22	A	818	CLA	C3B-C4B	2.20	1.49	1.42
22	B	802	CLA	C1B-C2B	2.20	1.48	1.43
22	B	826	CLA	CHC-C1C	2.20	1.42	1.38
22	T	609	CLA	MG-NB	-2.20	2.01	2.05
22	G	608	CLA	CHC-C1C	2.20	1.42	1.38
22	I	604	CLA	CHC-C1C	2.20	1.42	1.38
22	N	601	CLA	CHC-C1C	2.20	1.42	1.38
22	P	606	CLA	CHC-C1C	2.20	1.42	1.38
26	K	616	LHG	O7-C7	2.20	1.40	1.34
22	N	603	CLA	CHC-C1C	2.20	1.42	1.38
22	N	611	CLA	CHC-C1C	2.20	1.42	1.38
22	W	419	CLA	CHC-C1C	2.20	1.42	1.38
22	N	608	CLA	CHC-C1C	2.20	1.42	1.38
22	A	816	CLA	C1B-NB	-2.20	1.35	1.37
22	B	837	CLA	CHC-C1C	2.20	1.42	1.38
22	G	607	CLA	CHC-C1C	2.20	1.42	1.38
22	K	605	CLA	CHC-C1C	2.20	1.42	1.38
22	K	608	CLA	MG-NB	-2.20	2.01	2.05
31	U	408	CHL	CHC-C4B	-2.20	1.36	1.39
22	J	102	CLA	C3B-C4B	2.20	1.49	1.42
22	O	310	CLA	CMD-C2D	-2.20	1.46	1.50
22	G	602	CLA	MG-NB	-2.20	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	W	422	CHL	CHB-C1B	-2.19	1.36	1.39
22	L	417	CLA	CHC-C1C	2.19	1.42	1.38
22	G	602	CLA	C3B-C4B	2.19	1.49	1.42
22	U	404	CLA	CHC-C1C	2.19	1.42	1.38
22	N	602	CLA	MG-NB	-2.19	2.01	2.05
22	S	602	CLA	CHC-C1C	2.19	1.42	1.38
22	P	609	CLA	CHC-C1C	2.19	1.42	1.38
22	B	838	CLA	CHC-C1C	2.19	1.42	1.38
22	I	609	CLA	CHC-C1C	2.19	1.42	1.38
22	A	816	CLA	C4B-NB	2.19	1.40	1.37
22	B	821	CLA	CHC-C1C	2.19	1.42	1.38
22	N	610	CLA	C3B-C4B	2.19	1.49	1.42
22	A	844	CLA	CHC-C1C	2.19	1.42	1.38
22	P	602	CLA	C3B-C4B	2.19	1.49	1.42
22	R	607	CLA	C3B-C4B	2.19	1.49	1.42
22	B	817	CLA	CHC-C1C	2.18	1.42	1.38
22	G	603	CLA	CHC-C1C	2.18	1.42	1.38
22	B	829	CLA	CMC-C2C	-2.18	1.46	1.50
22	R	607	CLA	CHC-C1C	2.18	1.42	1.38
22	S	601	CLA	CHC-C1C	2.18	1.42	1.38
24	X	415	DD6	O1-C20	-2.18	1.43	1.46
22	X	419	CLA	CHC-C1C	2.18	1.42	1.38
22	N	610	CLA	CMB-C2B	-2.18	1.46	1.50
22	A	812	CLA	CHC-C1C	2.18	1.42	1.38
22	A	820	CLA	CMB-C2B	-2.18	1.46	1.50
22	Q	613	CLA	CHC-C1C	2.18	1.42	1.38
22	H	304	CLA	CMD-C2D	-2.18	1.46	1.50
22	U	413	CLA	CHC-C1C	2.18	1.42	1.38
22	G	609	CLA	CMD-C2D	-2.18	1.46	1.50
22	B	806	CLA	CHC-C1C	2.18	1.42	1.38
22	W	415	CLA	MG-NB	-2.18	2.01	2.05
22	W	414	CLA	CHC-C1C	2.17	1.42	1.38
22	X	410	CLA	CHC-C1C	2.17	1.42	1.38
22	A	816	CLA	CMB-C2B	-2.17	1.46	1.50
22	A	836	CLA	CHC-C1C	2.17	1.42	1.38
22	H	307	CLA	CHC-C1C	2.17	1.42	1.38
22	V	608	CLA	CHC-C1C	2.17	1.42	1.38
22	A	809	CLA	MG-NB	-2.17	2.01	2.05
22	R	603	CLA	CMD-C2D	-2.17	1.46	1.50
26	K	619	LHG	P-O6	2.17	1.67	1.59
22	N	609	CLA	MG-NB	-2.17	2.01	2.05
22	B	830	CLA	C1B-C2B	2.17	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	612	CLA	MG-NB	-2.17	2.01	2.05
22	N	607	CLA	MG-NB	-2.17	2.01	2.05
22	K	607	CLA	C1B-C2B	2.17	1.48	1.43
22	W	404	CLA	CHC-C1C	2.17	1.42	1.38
22	G	603	CLA	CMD-C2D	-2.17	1.46	1.50
22	A	808	CLA	MG-NB	-2.17	2.01	2.05
22	F	403	CLA	CHC-C1C	2.17	1.42	1.38
22	S	615	CLA	CHC-C1C	2.17	1.42	1.38
22	I	611	CLA	CMB-C2B	-2.17	1.46	1.50
22	L	407	CLA	MG-NB	-2.17	2.01	2.05
22	A	838	CLA	CHC-C1C	2.17	1.42	1.38
22	A	821	CLA	CHC-C1C	2.16	1.42	1.38
22	W	413	CLA	MG-NB	-2.16	2.01	2.05
22	H	310	CLA	CHC-C1C	2.16	1.42	1.38
22	P	608	CLA	CHC-C1C	2.16	1.42	1.38
22	B	829	CLA	C4B-NB	2.16	1.40	1.37
22	H	305	CLA	MG-NB	-2.16	2.01	2.05
22	W	404	CLA	MG-NB	-2.16	2.01	2.05
22	H	304	CLA	MG-NB	-2.16	2.01	2.05
22	A	820	CLA	MG-NB	-2.16	2.01	2.05
26	W	420	LHG	O7-C5	-2.16	1.41	1.46
28	H	317	LMG	O7-C8	-2.16	1.41	1.46
22	B	805	CLA	MG-NB	-2.16	2.01	2.05
22	L	403	CLA	MG-NB	-2.16	2.01	2.05
22	A	816	CLA	CMC-C2C	-2.16	1.46	1.50
22	L	404	CLA	CMD-C2D	-2.16	1.46	1.50
22	B	839	CLA	MG-NB	-2.16	2.01	2.05
22	T	606	CLA	CHC-C1C	2.16	1.42	1.38
22	K	609	CLA	CHC-C1C	2.16	1.42	1.38
22	B	829	CLA	MG-NB	-2.16	2.01	2.05
22	L	410	CLA	MG-NB	-2.16	2.01	2.05
22	W	405	CLA	CMD-C2D	-2.16	1.46	1.50
22	K	608	CLA	C1B-C2B	2.16	1.48	1.43
22	X	403	CLA	MG-NB	-2.16	2.01	2.05
22	A	838	CLA	MG-NB	-2.16	2.01	2.05
22	W	410	CLA	MG-NB	-2.16	2.01	2.05
22	Q	611	CLA	CHC-C1C	2.15	1.42	1.38
22	L	408	CLA	C1B-C2B	2.15	1.48	1.43
22	A	840	CLA	C3B-C4B	2.15	1.49	1.42
22	K	602	CLA	MG-NB	-2.15	2.01	2.05
25	O	304	DGD	O5D-C1E	2.15	1.43	1.40
22	K	604	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	V	618	SQD	O8-S	2.15	1.55	1.47
22	T	602	CLA	MG-NB	-2.15	2.01	2.05
24	W	418	DD6	C28-C27	-2.15	1.49	1.50
22	O	305	CLA	MG-NB	-2.15	2.01	2.05
22	B	834	CLA	MG-NB	-2.15	2.01	2.05
22	P	607	CLA	MG-NB	-2.15	2.01	2.05
22	X	417	CLA	CHC-C1C	2.15	1.42	1.38
22	K	609	CLA	MG-NB	-2.15	2.01	2.05
22	N	603	CLA	MG-NB	-2.15	2.01	2.05
22	B	807	CLA	CMC-C2C	-2.15	1.46	1.50
22	T	602	CLA	CMD-C2D	-2.15	1.46	1.50
22	H	303	CLA	MG-NB	-2.15	2.01	2.05
22	P	602	CLA	MG-NB	-2.15	2.01	2.05
22	K	604	CLA	CHC-C1C	2.14	1.42	1.38
22	J	102	CLA	MG-NB	-2.14	2.01	2.05
22	G	603	CLA	MG-NB	-2.14	2.01	2.05
22	B	821	CLA	MG-NB	-2.14	2.01	2.05
22	A	818	CLA	MG-NB	-2.14	2.01	2.05
22	A	804	CLA	MG-NB	-2.14	2.01	2.05
22	Q	601	CLA	CMD-C2D	-2.14	1.46	1.50
22	X	407	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	835	CLA	MG-NB	-2.14	2.01	2.05
22	B	807	CLA	CMD-C2D	-2.14	1.46	1.50
22	P	602	CLA	CMC-C2C	-2.14	1.46	1.50
28	Q	602	LMG	O7-C8	-2.14	1.41	1.46
22	X	405	CLA	CMB-C2B	-2.14	1.46	1.50
22	X	403	CLA	CHC-C1C	2.14	1.42	1.38
22	H	305	CLA	CMD-C2D	-2.14	1.46	1.50
26	O	323	LHG	P-O6	2.14	1.67	1.59
22	X	407	CLA	MG-NB	-2.14	2.01	2.05
26	O	321	LHG	P-O6	2.14	1.67	1.59
22	I	602	CLA	CMD-C2D	-2.14	1.46	1.50
22	I	602	CLA	MG-NB	-2.14	2.01	2.05
22	K	603	CLA	MG-NB	-2.14	2.01	2.05
22	K	610	CLA	MG-NB	-2.14	2.01	2.05
26	B	851	LHG	P-O6	2.14	1.67	1.59
22	K	606	CLA	CMD-C2D	-2.14	1.46	1.50
26	H	316	LHG	P-O6	2.14	1.67	1.59
26	N	616	LHG	P-O6	2.14	1.67	1.59
22	T	603	CLA	MG-NB	-2.14	2.01	2.05
22	U	404	CLA	MG-NB	-2.14	2.01	2.05
22	B	833	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	810	CLA	MG-NB	-2.13	2.01	2.05
22	H	318	CLA	MG-NB	-2.13	2.01	2.05
22	I	607	CLA	MG-NB	-2.13	2.01	2.05
22	N	605	CLA	MG-NB	-2.13	2.01	2.05
22	A	840	CLA	CHC-C1C	2.13	1.42	1.38
22	W	412	CLA	MG-NB	-2.13	2.01	2.05
26	N	614	LHG	P-O6	2.13	1.67	1.59
22	B	828	CLA	CMB-C2B	-2.13	1.46	1.50
22	B	838	CLA	CMB-C2B	-2.13	1.46	1.50
22	F	405	CLA	CMD-C2D	-2.13	1.46	1.50
26	P	601	LHG	P-O6	2.13	1.67	1.59
22	K	610	CLA	CMD-C2D	-2.13	1.46	1.50
22	S	604	CLA	MG-NB	-2.13	2.01	2.05
22	P	607	CLA	CMC-C2C	-2.13	1.46	1.50
22	T	603	CLA	CMD-C2D	-2.13	1.46	1.50
22	O	310	CLA	CHC-C1C	2.13	1.42	1.38
22	Q	612	CLA	CHC-C1C	2.13	1.42	1.38
22	X	404	CLA	CMD-C2D	-2.13	1.46	1.50
22	B	816	CLA	MG-NB	-2.13	2.01	2.05
22	K	605	CLA	MG-NB	-2.13	2.01	2.05
24	A	858	DD6	O1-C20	-2.13	1.43	1.46
22	A	822	CLA	MG-NB	-2.13	2.01	2.05
22	Q	617	CLA	MG-NB	-2.13	2.01	2.05
22	O	319	CLA	MG-NB	-2.13	2.01	2.05
22	L	412	CLA	MG-NB	-2.13	2.01	2.05
22	B	802	CLA	C4B-NB	2.13	1.40	1.37
22	B	806	CLA	MG-NB	-2.13	2.01	2.05
22	I	603	CLA	MG-NB	-2.13	2.01	2.05
22	L	402	CLA	MG-NB	-2.13	2.01	2.05
22	A	818	CLA	CHC-C1C	2.12	1.42	1.38
22	G	607	CLA	MG-NB	-2.12	2.01	2.05
22	Q	605	CLA	CMD-C2D	-2.12	1.46	1.50
25	B	847	DGD	O2G-C2G	-2.12	1.41	1.46
22	O	312	CLA	MG-NB	-2.12	2.01	2.05
22	K	613	CLA	CMD-C2D	-2.12	1.46	1.50
22	A	824	CLA	CMB-C2B	-2.12	1.46	1.50
22	A	823	CLA	CMD-C2D	-2.12	1.46	1.50
22	O	308	CLA	MG-NB	-2.12	2.01	2.05
22	A	840	CLA	CMD-C2D	-2.12	1.46	1.50
22	I	605	CLA	CMD-C2D	-2.12	1.46	1.50
22	G	607	CLA	CMD-C2D	-2.12	1.46	1.50
22	A	817	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	608	CLA	MG-NB	-2.12	2.01	2.05
22	R	605	CLA	CMD-C2D	-2.12	1.46	1.50
26	O	324	LHG	P-O6	2.12	1.67	1.59
22	A	816	CLA	CHC-C1C	2.12	1.42	1.38
22	B	837	CLA	CMB-C2B	-2.12	1.46	1.50
22	X	402	CLA	MG-NB	-2.12	2.01	2.05
22	B	804	CLA	CMD-C2D	-2.12	1.46	1.50
22	A	817	CLA	MG-NB	-2.12	2.01	2.05
22	A	833	CLA	MG-NB	-2.12	2.01	2.05
22	L	409	CLA	CMD-C2D	-2.11	1.46	1.50
22	N	604	CLA	MG-NB	-2.11	2.01	2.05
22	G	606	CLA	CMD-C2D	-2.11	1.46	1.50
22	R	607	CLA	CMC-C2C	-2.11	1.46	1.50
22	H	310	CLA	CMD-C2D	-2.11	1.46	1.50
28	J	101	LMG	O7-C8	-2.11	1.41	1.46
22	U	413	CLA	MG-NB	-2.11	2.01	2.05
22	K	603	CLA	CMB-C2B	-2.11	1.46	1.50
22	H	311	CLA	CMB-C2B	-2.11	1.46	1.50
22	B	819	CLA	CHC-C1C	2.11	1.42	1.38
30	O	302	SQD	O8-S	2.11	1.55	1.47
22	V	612	CLA	CMB-C2B	-2.11	1.46	1.50
22	B	832	CLA	CHC-C1C	2.11	1.42	1.38
22	A	801	CLA	C3B-C4B	2.11	1.48	1.42
22	O	307	CLA	CMD-C2D	-2.11	1.46	1.50
22	Q	603	CLA	CMD-C2D	-2.11	1.46	1.50
22	W	409	CLA	CMB-C2B	-2.11	1.46	1.50
22	U	412	CLA	MG-NB	-2.11	2.01	2.05
26	R	614	LHG	P-O6	2.11	1.67	1.59
22	B	834	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	835	CLA	CMD-C2D	-2.11	1.46	1.50
30	K	621	SQD	O8-S	2.11	1.55	1.47
22	S	606	CLA	CMD-C2D	-2.11	1.46	1.50
22	W	409	CLA	MG-NB	-2.11	2.01	2.05
22	B	822	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	827	CLA	CMD-C2D	-2.11	1.46	1.50
22	L	412	CLA	CMD-C2D	-2.11	1.46	1.50
22	A	834	CLA	MG-NB	-2.11	2.01	2.05
28	I	614	LMG	O7-C8	-2.11	1.41	1.46
26	U	419	LHG	P-O6	2.11	1.67	1.59
22	Q	611	CLA	CMD-C2D	-2.11	1.46	1.50
22	R	603	CLA	MG-NB	-2.11	2.01	2.05
22	L	405	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	309	CLA	CMB-C2B	-2.11	1.46	1.50
22	A	841	CLA	CMB-C2B	-2.11	1.46	1.50
22	N	605	CLA	CMD-C2D	-2.11	1.46	1.50
22	S	603	CLA	CMD-C2D	-2.11	1.46	1.50
22	A	838	CLA	CMD-C2D	-2.11	1.46	1.50
22	A	832	CLA	MG-NB	-2.11	2.01	2.05
22	B	806	CLA	CMD-C2D	-2.11	1.46	1.50
22	Q	606	CLA	MG-NB	-2.11	2.01	2.05
22	B	819	CLA	CMB-C2B	-2.11	1.46	1.50
22	B	837	CLA	CMD-C2D	-2.11	1.46	1.50
22	A	819	CLA	C1B-C2B	2.11	1.48	1.43
22	I	605	CLA	MG-NB	-2.11	2.01	2.05
30	F	407	SQD	O8-S	2.10	1.55	1.47
22	O	308	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	836	CLA	C3B-C4B	2.10	1.48	1.42
22	A	830	CLA	CMD-C2D	-2.10	1.46	1.50
22	W	411	CLA	MG-NB	-2.10	2.01	2.05
22	O	309	CLA	CMD-C2D	-2.10	1.46	1.50
22	K	617	CLA	CMD-C2D	-2.10	1.46	1.50
26	S	613	LHG	P-O6	2.10	1.67	1.59
26	G	614	LHG	P-O6	2.10	1.67	1.59
22	S	615	CLA	CMD-C2D	-2.10	1.46	1.50
22	P	609	CLA	CMB-C2B	-2.10	1.46	1.50
22	G	605	CLA	MG-NB	-2.10	2.01	2.05
22	Q	609	CLA	MG-NB	-2.10	2.01	2.05
22	A	810	CLA	MG-NB	-2.10	2.01	2.05
22	A	815	CLA	MG-NB	-2.10	2.01	2.05
22	A	829	CLA	MG-NB	-2.10	2.01	2.05
22	O	312	CLA	CMD-C2D	-2.10	1.46	1.50
22	G	601	CLA	MG-NB	-2.10	2.01	2.05
22	I	610	CLA	MG-NB	-2.10	2.01	2.05
22	A	811	CLA	MG-NB	-2.10	2.01	2.05
22	Q	613	CLA	CMB-C2B	-2.10	1.46	1.50
22	A	812	CLA	CMD-C2D	-2.10	1.46	1.50
22	I	606	CLA	CMD-C2D	-2.10	1.46	1.50
22	Q	610	CLA	CMD-C2D	-2.10	1.46	1.50
22	T	601	CLA	MG-NB	-2.10	2.01	2.05
22	Q	612	CLA	CMD-C2D	-2.10	1.46	1.50
22	L	406	CLA	MG-NB	-2.10	2.01	2.05
22	S	603	CLA	MG-NB	-2.10	2.01	2.05
28	L	401	LMG	O7-C8	-2.10	1.41	1.46
22	K	617	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	813	CLA	CMB-C2B	-2.10	1.46	1.50
22	X	412	CLA	CMB-C2B	-2.10	1.46	1.50
22	R	601	CLA	MG-NB	-2.10	2.01	2.05
22	G	605	CLA	CMB-C2B	-2.10	1.46	1.50
22	K	609	CLA	CMD-C2D	-2.10	1.46	1.50
22	A	836	CLA	CMB-C2B	-2.10	1.46	1.50
31	W	407	CHL	CHB-C1B	-2.10	1.36	1.39
22	F	403	CLA	CMD-C2D	-2.09	1.46	1.50
22	L	411	CLA	CMD-C2D	-2.09	1.46	1.50
22	Q	609	CLA	CMB-C2B	-2.09	1.46	1.50
22	U	409	CLA	CMD-C2D	-2.09	1.46	1.50
22	X	411	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	832	CLA	CMD-C2D	-2.09	1.46	1.50
22	H	303	CLA	CMB-C2B	-2.09	1.46	1.50
22	V	604	CLA	CMB-C2B	-2.09	1.46	1.50
22	F	404	CLA	CMD-C2D	-2.09	1.46	1.50
22	O	314	CLA	MG-NB	-2.09	2.01	2.05
22	U	409	CLA	MG-NB	-2.09	2.01	2.05
26	O	318	LHG	P-O6	2.09	1.67	1.59
22	X	403	CLA	CMD-C2D	-2.09	1.46	1.50
22	G	604	CLA	MG-NB	-2.09	2.01	2.05
22	U	420	CLA	MG-NB	-2.09	2.01	2.05
22	B	816	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	818	CLA	CMD-C2D	-2.09	1.46	1.50
26	X	420	LHG	P-O6	2.09	1.67	1.59
22	B	821	CLA	CMB-C2B	-2.09	1.46	1.50
22	G	606	CLA	CMB-C2B	-2.09	1.46	1.50
22	A	831	CLA	CMD-C2D	-2.09	1.46	1.50
22	R	608	CLA	MG-NB	-2.09	2.01	2.05
22	W	406	CLA	MG-NB	-2.09	2.01	2.05
22	B	859	CLA	CMD-C2D	-2.09	1.46	1.50
22	H	307	CLA	CMB-C2B	-2.09	1.46	1.50
22	U	410	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	817	CLA	MG-NB	-2.09	2.01	2.05
22	O	307	CLA	MG-NB	-2.09	2.01	2.05
22	A	818	CLA	CMB-C2B	-2.09	1.46	1.50
22	T	608	CLA	MG-NB	-2.09	2.01	2.05
22	B	805	CLA	CMD-C2D	-2.09	1.46	1.50
22	I	610	CLA	CMD-C2D	-2.09	1.46	1.50
22	A	808	CLA	CMD-C2D	-2.09	1.46	1.50
22	W	409	CLA	CMD-C2D	-2.09	1.46	1.50
22	G	602	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	809	CLA	CMD-C2D	-2.09	1.46	1.50
22	Q	601	CLA	CMB-C2B	-2.09	1.46	1.50
22	X	411	CLA	MG-NB	-2.09	2.01	2.05
22	W	412	CLA	CMB-C2B	-2.09	1.46	1.50
26	A	845	LHG	P-O6	2.09	1.67	1.59
22	O	313	CLA	MG-NB	-2.09	2.01	2.05
22	O	313	CLA	CMD-C2D	-2.09	1.46	1.50
22	P	609	CLA	CMD-C2D	-2.09	1.46	1.50
22	X	419	CLA	CMD-C2D	-2.09	1.46	1.50
24	N	612	DD6	C28-C27	-2.09	1.49	1.50
22	S	601	CLA	MG-NB	-2.09	2.01	2.05
22	A	807	CLA	MG-NB	-2.09	2.01	2.05
22	Q	617	CLA	CMD-C2D	-2.09	1.46	1.50
22	U	412	CLA	CMB-C2B	-2.09	1.46	1.50
22	A	831	CLA	CMB-C2B	-2.09	1.46	1.50
22	X	405	CLA	MG-NB	-2.08	2.01	2.05
22	O	310	CLA	CMB-C2B	-2.08	1.46	1.50
22	P	605	CLA	CMD-C2D	-2.08	1.46	1.50
22	W	403	CLA	CMB-C2B	-2.08	1.46	1.50
22	B	824	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	814	CLA	CMD-C2D	-2.08	1.46	1.50
22	H	309	CLA	CMD-C2D	-2.08	1.46	1.50
22	L	402	CLA	CMB-C2B	-2.08	1.46	1.50
22	A	821	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	818	CLA	MG-NB	-2.08	2.01	2.05
22	V	609	CLA	MG-NB	-2.08	2.01	2.05
22	H	306	CLA	CMB-C2B	-2.08	1.46	1.50
22	B	810	CLA	CMD-C2D	-2.08	1.46	1.50
22	H	313	CLA	CMD-C2D	-2.08	1.46	1.50
22	O	314	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	835	CLA	CMD-C2D	-2.08	1.46	1.50
22	K	612	CLA	CMD-C2D	-2.08	1.46	1.50
22	W	402	CLA	CMD-C2D	-2.08	1.46	1.50
22	W	413	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	802	CLA	CHC-C1C	2.08	1.42	1.38
22	B	838	CLA	CMD-C2D	-2.08	1.46	1.50
22	U	415	CLA	CMB-C2B	-2.08	1.46	1.50
22	W	406	CLA	CMB-C2B	-2.08	1.46	1.50
22	B	815	CLA	CMB-C2B	-2.08	1.46	1.50
22	B	817	CLA	CMB-C2B	-2.08	1.46	1.50
22	A	829	CLA	CMD-C2D	-2.08	1.46	1.50
22	N	608	CLA	MG-NB	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	603	CLA	CMD-C2D	-2.08	1.46	1.50
22	R	602	CLA	CMD-C2D	-2.08	1.46	1.50
22	T	607	CLA	CMB-C2B	-2.08	1.46	1.50
26	A	846	LHG	P-O6	2.08	1.67	1.59
22	T	605	CLA	CMB-C2B	-2.08	1.46	1.50
22	U	410	CLA	MG-NB	-2.08	2.01	2.05
22	B	818	CLA	CMB-C2B	-2.08	1.46	1.50
22	W	415	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	806	CLA	CMD-C2D	-2.08	1.46	1.50
22	Q	611	CLA	MG-NB	-2.08	2.01	2.05
22	B	807	CLA	CMB-C2B	-2.08	1.46	1.50
22	P	608	CLA	CMC-C2C	-2.08	1.46	1.50
26	T	614	LHG	P-O6	2.08	1.67	1.59
26	B	848	LHG	P-O6	2.08	1.67	1.59
22	V	612	CLA	MG-NB	-2.08	2.01	2.05
22	A	835	CLA	MG-NB	-2.08	2.01	2.05
22	V	611	CLA	CMD-C2D	-2.08	1.46	1.50
22	W	414	CLA	CMD-C2D	-2.08	1.46	1.50
22	X	412	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	842	CLA	CMB-C2B	-2.08	1.46	1.50
22	A	844	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	832	CLA	CMD-C2D	-2.08	1.46	1.50
22	F	405	CLA	MG-NB	-2.08	2.01	2.05
22	N	606	CLA	CMD-C2D	-2.08	1.46	1.50
22	W	402	CLA	MG-NB	-2.08	2.01	2.05
22	K	602	CLA	CMD-C2D	-2.07	1.46	1.50
22	O	306	CLA	CMD-C2D	-2.07	1.46	1.50
22	O	315	CLA	CMB-C2B	-2.07	1.46	1.50
22	G	604	CLA	CMD-C2D	-2.07	1.46	1.50
22	P	610	CLA	CMD-C2D	-2.07	1.46	1.50
22	V	603	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	813	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	808	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	814	CLA	CMD-C2D	-2.07	1.46	1.50
22	I	609	CLA	CMD-C2D	-2.07	1.46	1.50
22	L	403	CLA	CMD-C2D	-2.07	1.46	1.50
22	N	609	CLA	CMD-C2D	-2.07	1.46	1.50
22	O	305	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	844	CLA	MG-NB	-2.07	2.01	2.05
22	L	405	CLA	CMD-C2D	-2.07	1.46	1.50
22	L	409	CLA	CMB-C2B	-2.07	1.46	1.50
22	K	608	CLA	C3B-C4B	2.07	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	608	CLA	MG-NB	-2.07	2.01	2.05
22	R	610	CLA	CMD-C2D	-2.07	1.46	1.50
22	T	605	CLA	CMD-C2D	-2.07	1.46	1.50
22	P	605	CLA	MG-NB	-2.07	2.01	2.05
22	B	816	CLA	CMB-C2B	-2.07	1.46	1.50
22	N	603	CLA	CMD-C2D	-2.07	1.46	1.50
22	T	601	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	838	CLA	CMB-C2B	-2.07	1.46	1.50
22	R	601	CLA	CMD-C2D	-2.07	1.46	1.50
22	W	410	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	826	CLA	CMD-C2D	-2.07	1.46	1.50
22	I	607	CLA	CMC-C2C	-2.07	1.46	1.50
22	J	102	CLA	CMD-C2D	-2.07	1.46	1.50
22	S	615	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	804	CLA	MG-NB	-2.07	2.01	2.05
22	B	814	CLA	MG-NB	-2.07	2.01	2.05
22	O	309	CLA	MG-NB	-2.07	2.01	2.05
22	P	604	CLA	MG-NB	-2.07	2.01	2.05
22	O	315	CLA	CMD-C2D	-2.07	1.46	1.50
22	P	607	CLA	CMD-C2D	-2.07	1.46	1.50
28	K	622	LMG	O7-C8	-2.07	1.41	1.46
22	U	415	CLA	MG-NB	-2.07	2.01	2.05
22	L	404	CLA	MG-NB	-2.07	2.01	2.05
22	R	607	CLA	MG-NB	-2.07	2.01	2.05
22	K	611	CLA	MG-NB	-2.07	2.01	2.05
22	H	302	CLA	CMB-C2B	-2.07	1.46	1.50
22	S	614	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	828	CLA	CMD-C2D	-2.07	1.46	1.50
22	X	410	CLA	CMB-C2B	-2.07	1.46	1.50
22	A	808	CLA	CMB-C2B	-2.07	1.46	1.50
22	A	821	CLA	CMB-C2B	-2.07	1.46	1.50
22	H	306	CLA	CMD-C2D	-2.07	1.46	1.50
22	R	608	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	822	CLA	MG-NB	-2.07	2.01	2.05
22	K	606	CLA	MG-NB	-2.07	2.01	2.05
22	U	414	CLA	MG-NB	-2.07	2.01	2.05
22	A	828	CLA	MG-NB	-2.07	2.01	2.05
22	I	608	CLA	CMB-C2B	-2.07	1.46	1.50
22	U	403	CLA	CMD-C2D	-2.07	1.46	1.50
22	U	414	CLA	CMB-C2B	-2.07	1.46	1.50
22	I	606	CLA	CMB-C2B	-2.07	1.46	1.50
22	I	610	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	408	CLA	CMD-C2D	-2.07	1.46	1.50
22	L	411	CLA	MG-NB	-2.07	2.01	2.05
22	Q	608	CLA	CMB-C2B	-2.07	1.46	1.50
22	W	414	CLA	CMB-C2B	-2.07	1.46	1.50
22	X	409	CLA	MG-NB	-2.07	2.01	2.05
22	I	601	CLA	CMB-C2B	-2.07	1.46	1.50
22	I	601	CLA	CMD-C2D	-2.07	1.46	1.50
22	I	609	CLA	MG-NB	-2.07	2.01	2.05
22	A	833	CLA	CMD-C2D	-2.07	1.46	1.50
22	I	604	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	837	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	811	CLA	MG-NB	-2.06	2.01	2.05
22	B	809	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	859	CLA	CMB-C2B	-2.06	1.46	1.50
22	N	602	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	809	CLA	CMD-C2D	-2.06	1.46	1.50
22	P	602	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	829	CLA	MG-ND	-2.06	2.01	2.05
22	Q	613	CLA	MG-NB	-2.06	2.01	2.05
22	A	807	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	811	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	841	CLA	MG-NB	-2.06	2.01	2.05
22	B	815	CLA	CMD-C2D	-2.06	1.46	1.50
22	S	604	CLA	CMD-C2D	-2.06	1.46	1.50
22	U	401	CLA	CMB-C2B	-2.06	1.46	1.50
22	W	412	CLA	CMD-C2D	-2.06	1.46	1.50
22	H	303	CLA	CMD-C2D	-2.06	1.46	1.50
22	O	311	CLA	CMD-C2D	-2.06	1.46	1.50
22	Q	606	CLA	CMB-C2B	-2.06	1.46	1.50
22	V	609	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	834	CLA	CMB-C2B	-2.06	1.46	1.50
22	K	613	CLA	MG-NB	-2.06	2.01	2.05
22	N	601	CLA	CMD-C2D	-2.06	1.46	1.50
22	N	604	CLA	CMD-C2D	-2.06	1.46	1.50
22	V	607	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	803	CLA	CMC-C2C	-2.06	1.46	1.50
22	T	604	CLA	MG-NB	-2.06	2.01	2.05
22	K	602	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	823	CLA	CMB-C2B	-2.06	1.46	1.50
22	U	405	CLA	CMD-C2D	-2.06	1.46	1.50
28	U	423	LMG	O7-C8	-2.06	1.41	1.46
22	U	401	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	836	CLA	CHC-C1C	2.06	1.42	1.38
22	W	403	CLA	CMD-C2D	-2.06	1.46	1.50
22	T	605	CLA	MG-NB	-2.06	2.01	2.05
22	B	836	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	805	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	824	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	834	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	841	CLA	CMD-C2D	-2.06	1.46	1.50
22	W	419	CLA	MG-NB	-2.06	2.01	2.05
22	Q	610	CLA	CMB-C2B	-2.06	1.46	1.50
22	U	404	CLA	CMD-C2D	-2.06	1.46	1.50
22	W	415	CLA	CMB-C2B	-2.06	1.46	1.50
22	X	409	CLA	CMD-C2D	-2.06	1.46	1.50
22	S	614	CLA	MG-NB	-2.06	2.01	2.05
22	L	407	CLA	CMD-C2D	-2.06	1.46	1.50
22	S	610	CLA	CMB-C2B	-2.06	1.46	1.50
22	U	420	CLA	CMD-C2D	-2.06	1.46	1.50
22	W	411	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	801	CLA	CHC-C1C	2.06	1.42	1.38
26	Q	616	LHG	P-O6	2.06	1.67	1.59
22	A	803	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	837	CLA	CMB-C2B	-2.06	1.46	1.50
22	H	308	CLA	MG-NB	-2.06	2.01	2.05
22	B	804	CLA	CMB-C2B	-2.06	1.46	1.50
22	T	609	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	839	CLA	CMD-C2D	-2.06	1.46	1.50
22	G	603	CLA	CMB-C2B	-2.06	1.46	1.50
22	Q	609	CLA	CMD-C2D	-2.06	1.46	1.50
22	L	402	CLA	CMD-C2D	-2.06	1.46	1.50
22	H	310	CLA	MG-NB	-2.06	2.01	2.05
22	R	615	CLA	MG-NB	-2.06	2.01	2.05
22	B	826	CLA	CMD-C2D	-2.06	1.46	1.50
22	G	611	CLA	MG-NB	-2.05	2.01	2.05
22	Q	603	CLA	MG-NB	-2.05	2.01	2.05
22	P	608	CLA	CMB-C2B	-2.05	1.46	1.50
22	W	411	CLA	CMB-C2B	-2.05	1.46	1.50
22	X	404	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	829	CLA	CMB-C2B	-2.05	1.46	1.50
22	S	607	CLA	MG-NB	-2.05	2.01	2.05
22	A	826	CLA	MG-NB	-2.05	2.01	2.05
22	A	827	CLA	MG-NB	-2.05	2.01	2.05
22	B	825	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	610	CLA	CHC-C1C	2.05	1.42	1.38
22	N	606	CLA	CMB-C2B	-2.05	1.46	1.50
22	S	609	CLA	CMB-C2B	-2.05	1.46	1.50
22	W	413	CLA	CMB-C2B	-2.05	1.46	1.50
28	F	408	LMG	O7-C8	-2.05	1.41	1.46
22	F	403	CLA	MG-NB	-2.05	2.01	2.05
22	K	609	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	812	CLA	CMB-C2B	-2.05	1.46	1.50
22	B	823	CLA	CMD-C2D	-2.05	1.46	1.50
22	I	607	CLA	CMD-C2D	-2.05	1.46	1.50
22	S	610	CLA	CMD-C2D	-2.05	1.46	1.50
22	U	414	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	831	CLA	MG-NB	-2.05	2.01	2.05
22	S	602	CLA	MG-NB	-2.05	2.01	2.05
32	V	616	NEX	C1-C6	-2.05	1.51	1.54
22	A	815	CLA	CMD-C2D	-2.05	1.46	1.50
22	V	611	CLA	MG-NB	-2.05	2.01	2.05
22	K	603	CLA	CMD-C2D	-2.05	1.46	1.50
22	U	401	CLA	CMD-C2D	-2.05	1.46	1.50
22	X	410	CLA	CMD-C2D	-2.05	1.46	1.50
22	A	836	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	838	CLA	MG-NB	-2.05	2.01	2.05
22	N	610	CLA	CMD-C2D	-2.05	1.46	1.50
22	A	827	CLA	CMD-C2D	-2.05	1.46	1.50
22	R	609	CLA	MG-NB	-2.05	2.01	2.05
22	H	313	CLA	CMB-C2B	-2.05	1.46	1.50
22	U	412	CLA	CMD-C2D	-2.05	1.46	1.50
22	A	810	CLA	CMD-C2D	-2.05	1.46	1.50
22	R	609	CLA	CMD-C2D	-2.05	1.46	1.50
22	W	405	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	830	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	835	CLA	CMB-C2B	-2.05	1.46	1.50
22	H	306	CLA	MG-NB	-2.05	2.01	2.05
22	L	405	CLA	MG-NB	-2.05	2.01	2.05
26	W	420	LHG	P-O6	2.05	1.67	1.59
22	O	306	CLA	CMB-C2B	-2.05	1.46	1.50
22	U	406	CLA	CMB-C2B	-2.05	1.46	1.50
22	B	813	CLA	MG-NB	-2.05	2.01	2.05
22	B	829	CLA	CHC-C1C	2.05	1.42	1.38
22	B	826	CLA	CMB-C2B	-2.05	1.46	1.50
22	B	832	CLA	CMB-C2B	-2.05	1.46	1.50
22	H	307	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	611	CLA	CMC-C2C	-2.05	1.46	1.50
22	J	102	CLA	CMB-C2B	-2.05	1.46	1.50
22	Q	604	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	806	CLA	CMB-C2B	-2.05	1.46	1.50
22	N	601	CLA	MG-NB	-2.05	2.01	2.05
22	B	813	CLA	CMD-C2D	-2.05	1.46	1.50
22	S	604	CLA	CMB-C2B	-2.05	1.46	1.50
22	U	410	CLA	CMB-C2B	-2.05	1.46	1.50
22	F	403	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	818	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	812	CLA	MG-NB	-2.05	2.01	2.05
26	L	416	LHG	P-O6	2.05	1.67	1.59
22	G	610	CLA	CMB-C2B	-2.05	1.46	1.50
22	W	404	CLA	CMD-C2D	-2.05	1.46	1.50
22	I	604	CLA	MG-NB	-2.05	2.01	2.05
22	S	608	CLA	MG-NB	-2.05	2.01	2.05
22	U	405	CLA	MG-NB	-2.05	2.01	2.05
22	V	613	CLA	CMB-C2B	-2.05	1.46	1.50
22	B	803	CLA	CMB-C2B	-2.05	1.46	1.50
22	A	810	CLA	CMB-C2B	-2.05	1.46	1.50
22	W	403	CLA	MG-NB	-2.04	2.01	2.05
22	B	821	CLA	CMD-C2D	-2.04	1.46	1.50
22	T	604	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	808	CLA	MG-NB	-2.04	2.01	2.05
22	N	604	CLA	CMB-C2B	-2.04	1.46	1.50
22	T	610	CLA	CMB-C2B	-2.04	1.46	1.50
22	V	604	CLA	MG-NB	-2.04	2.01	2.05
22	F	405	CLA	CMB-C2B	-2.04	1.46	1.50
22	G	602	CLA	CMB-C2B	-2.04	1.46	1.50
22	G	608	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	822	CLA	CMD-C2D	-2.04	1.46	1.50
28	H	319	LMG	O7-C8	-2.04	1.41	1.46
22	V	608	CLA	CMB-C2B	-2.04	1.46	1.50
22	A	828	CLA	CMC-C2C	-2.04	1.46	1.50
22	P	608	CLA	MG-NB	-2.04	2.01	2.05
22	L	412	CLA	CMB-C2B	-2.04	1.46	1.50
22	U	405	CLA	CMB-C2B	-2.04	1.46	1.50
22	G	605	CLA	CMD-C2D	-2.04	1.46	1.50
22	I	604	CLA	CMD-C2D	-2.04	1.46	1.50
22	P	608	CLA	CMD-C2D	-2.04	1.46	1.50
22	U	415	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	842	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	315	CLA	MG-NB	-2.04	2.01	2.05
22	B	833	CLA	MG-NB	-2.04	2.01	2.05
22	I	601	CLA	MG-NB	-2.04	2.01	2.05
22	Q	607	CLA	CMD-C2D	-2.04	1.46	1.50
22	U	403	CLA	CMB-C2B	-2.04	1.46	1.50
22	K	610	CLA	CMB-C2B	-2.04	1.46	1.50
26	B	848	LHG	C26-C25	-2.04	1.35	1.50
25	B	847	DGD	O5D-C1E	2.04	1.43	1.40
22	G	611	CLA	CMD-C2D	-2.04	1.46	1.50
22	T	601	CLA	CMB-C2B	-2.04	1.46	1.50
22	T	611	CLA	MG-NB	-2.04	2.01	2.05
22	L	407	CLA	CMB-C2B	-2.04	1.46	1.50
22	N	602	CLA	CMC-C2C	-2.04	1.46	1.50
22	A	825	CLA	CMB-C2B	-2.04	1.46	1.50
22	U	413	CLA	CMB-C2B	-2.04	1.46	1.50
22	X	419	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	802	CLA	C1B-NB	-2.04	1.35	1.37
22	O	311	CLA	CMB-C2B	-2.04	1.46	1.50
22	T	611	CLA	CMB-C2B	-2.04	1.46	1.50
22	A	826	CLA	CMB-C2B	-2.04	1.46	1.50
22	T	603	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	803	CLA	CMD-C2D	-2.04	1.46	1.50
22	H	302	CLA	CMD-C2D	-2.04	1.46	1.50
22	I	606	CLA	CMC-C2C	-2.04	1.46	1.50
22	A	828	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	827	CLA	MG-NB	-2.04	2.01	2.05
22	K	613	CLA	CMB-C2B	-2.04	1.46	1.50
22	T	602	CLA	CMB-C2B	-2.04	1.46	1.50
22	Q	601	CLA	CMC-C2C	-2.04	1.46	1.50
22	Q	606	CLA	CMD-C2D	-2.04	1.46	1.50
22	T	610	CLA	CMD-C2D	-2.04	1.46	1.50
22	H	309	CLA	MG-NB	-2.04	2.01	2.05
22	A	830	CLA	MG-NB	-2.04	2.01	2.05
28	T	616	LMG	O7-C8	-2.04	1.41	1.46
22	Q	618	CLA	CMB-C2B	-2.04	1.46	1.50
22	A	807	CLA	CMD-C2D	-2.04	1.46	1.50
22	I	606	CLA	MG-NB	-2.03	2.01	2.05
24	J	105	DD6	O1-C20	-2.03	1.43	1.46
22	G	608	CLA	CMB-C2B	-2.03	1.46	1.50
22	I	603	CLA	CMB-C2B	-2.03	1.46	1.50
22	S	609	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	837	CLA	MG-NB	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	810	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	831	CLA	CMD-C2D	-2.03	1.46	1.50
22	R	607	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	844	CLA	CMB-C2B	-2.03	1.46	1.50
22	W	411	CLA	CMC-C2C	-2.03	1.46	1.50
22	A	813	CLA	CMB-C2B	-2.03	1.46	1.50
22	R	604	CLA	MG-NB	-2.03	2.01	2.05
22	B	812	CLA	CMD-C2D	-2.03	1.46	1.50
22	G	601	CLA	CMD-C2D	-2.03	1.46	1.50
22	Q	607	CLA	CMB-C2B	-2.03	1.46	1.50
21	M	101	BCR	C30-C25	-2.03	1.51	1.53
22	W	402	CLA	CMB-C2B	-2.03	1.46	1.50
22	A	807	CLA	CMC-C2C	-2.03	1.46	1.50
28	H	322	LMG	O7-C8	-2.03	1.41	1.46
22	B	827	CLA	CMB-C2B	-2.03	1.46	1.50
22	K	604	CLA	CMB-C2B	-2.03	1.46	1.50
22	Q	608	CLA	CMD-C2D	-2.03	1.46	1.50
22	S	602	CLA	CMD-C2D	-2.03	1.46	1.50
22	P	609	CLA	MG-NB	-2.03	2.01	2.05
22	T	608	CLA	CMD-C2D	-2.03	1.46	1.50
22	I	602	CLA	CMB-C2B	-2.03	1.46	1.50
22	W	410	CLA	CMB-C2B	-2.03	1.46	1.50
22	X	403	CLA	CMB-C2B	-2.03	1.46	1.50
22	R	605	CLA	MG-NB	-2.03	2.01	2.05
22	T	611	CLA	CMD-C2D	-2.03	1.46	1.50
22	V	610	CLA	CMB-C2B	-2.03	1.46	1.50
22	G	610	CLA	MG-NB	-2.03	2.01	2.05
22	U	411	CLA	CMD-C2D	-2.03	1.46	1.50
22	X	405	CLA	CMD-C2D	-2.03	1.46	1.50
22	X	408	CLA	MG-NB	-2.03	2.01	2.05
22	Q	618	CLA	CMD-C2D	-2.03	1.46	1.50
22	V	617	CLA	CMB-C2B	-2.03	1.46	1.50
22	Q	610	CLA	MG-NB	-2.03	2.01	2.05
22	A	825	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	836	CLA	CMD-C2D	-2.03	1.46	1.50
22	K	606	CLA	CMB-C2B	-2.03	1.46	1.50
22	L	410	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	804	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	812	CLA	MG-NB	-2.03	2.01	2.05
26	K	616	LHG	P-O6	2.03	1.67	1.59
22	A	828	CLA	CMB-C2B	-2.03	1.46	1.50
22	R	601	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	809	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	812	CLA	CMB-C2B	-2.03	1.46	1.50
22	P	604	CLA	CMD-C2D	-2.03	1.46	1.50
22	H	312	CLA	MG-NB	-2.03	2.01	2.05
22	V	612	CLA	CMD-C2D	-2.03	1.46	1.50
22	V	609	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	852	CLA	MG-NB	-2.02	2.01	2.05
22	S	608	CLA	CMB-C2B	-2.02	1.46	1.50
22	G	609	CLA	MG-NB	-2.02	2.01	2.05
22	W	405	CLA	MG-NB	-2.02	2.01	2.05
22	X	419	CLA	MG-NB	-2.02	2.01	2.05
22	H	318	CLA	CMB-C2B	-2.02	1.46	1.50
22	R	611	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	833	CLA	CMB-C2B	-2.02	1.46	1.50
22	T	607	CLA	CMD-C2D	-2.02	1.46	1.50
22	W	405	CLA	CHC-C1C	2.02	1.42	1.38
22	Q	618	CLA	MG-NB	-2.02	2.01	2.05
22	H	311	CLA	CMD-C2D	-2.02	1.46	1.50
22	R	615	CLA	CMB-C2B	-2.02	1.46	1.50
22	R	611	CLA	MG-NB	-2.02	2.01	2.05
22	B	808	CLA	CMD-C2D	-2.02	1.46	1.50
22	P	603	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	828	CLA	MG-NB	-2.02	2.01	2.05
22	K	611	CLA	CMD-C2D	-2.02	1.46	1.50
22	T	608	CLA	CMB-C2B	-2.02	1.46	1.50
22	N	611	CLA	MG-NB	-2.02	2.01	2.05
22	G	607	CLA	CMB-C2B	-2.02	1.46	1.50
22	L	417	CLA	CMC-C2C	-2.02	1.46	1.50
22	L	409	CLA	MG-NB	-2.02	2.01	2.05
22	A	821	CLA	MG-NB	-2.02	2.01	2.05
22	L	417	CLA	CMD-C2D	-2.02	1.46	1.50
22	N	607	CLA	CMD-C2D	-2.02	1.46	1.50
22	R	608	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	837	CLA	MG-NB	-2.02	2.01	2.05
22	K	607	CLA	CHC-C1C	2.02	1.42	1.38
22	H	308	CLA	CMD-C2D	-2.02	1.46	1.50
28	G	616	LMG	O7-C8	-2.02	1.41	1.46
22	H	302	CLA	MG-NB	-2.02	2.01	2.05
22	F	403	CLA	CMC-C2C	-2.02	1.46	1.50
22	A	817	CLA	CMB-C2B	-2.02	1.46	1.50
22	K	604	CLA	MG-NB	-2.02	2.01	2.05
22	O	310	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	610	CLA	CMD-C2D	-2.02	1.46	1.50
22	X	413	CLA	CMD-C2D	-2.02	1.46	1.50
22	K	605	CLA	CMB-C2B	-2.02	1.46	1.50
22	Q	604	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	834	CLA	CMB-C2B	-2.02	1.46	1.50
22	G	601	CLA	CMB-C2B	-2.02	1.46	1.50
22	L	406	CLA	CMB-C2B	-2.02	1.46	1.50
22	O	313	CLA	CMC-C2C	-2.02	1.46	1.50
22	A	803	CLA	MG-NB	-2.02	2.01	2.05
22	H	312	CLA	CMD-C2D	-2.02	1.46	1.50
22	U	413	CLA	CMD-C2D	-2.02	1.46	1.50
22	T	606	CLA	CMD-C2D	-2.02	1.46	1.50
22	R	602	CLA	MG-NB	-2.02	2.01	2.05
22	L	411	CLA	CMB-C2B	-2.01	1.46	1.50
22	W	405	CLA	CMC-C2C	-2.01	1.46	1.50
22	A	806	CLA	CMC-C2C	-2.01	1.46	1.50
22	O	306	CLA	CMC-C2C	-2.01	1.46	1.50
22	S	608	CLA	CMD-C2D	-2.01	1.46	1.50
22	V	613	CLA	CMD-C2D	-2.01	1.46	1.50
22	Q	613	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	822	CLA	CMC-C2C	-2.01	1.46	1.50
22	V	602	CLA	MG-NB	-2.01	2.01	2.05
22	B	805	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	840	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	823	CLA	MG-NB	-2.01	2.01	2.05
22	Q	601	CLA	MG-NB	-2.01	2.01	2.05
22	B	859	CLA	MG-NB	-2.01	2.01	2.05
22	U	406	CLA	MG-NB	-2.01	2.01	2.05
32	U	418	NEX	C1-C6	-2.01	1.51	1.54
22	R	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	R	615	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	824	CLA	MG-NB	-2.01	2.01	2.05
22	B	831	CLA	CMC-C2C	-2.01	1.46	1.50
22	I	604	CLA	CMC-C2C	-2.01	1.46	1.50
22	T	606	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	822	CLA	CMB-C2B	-2.01	1.46	1.50
22	H	309	CLA	CMB-C2B	-2.01	1.46	1.50
22	N	607	CLA	CMB-C2B	-2.01	1.46	1.50
22	U	409	CLA	CMB-C2B	-2.01	1.46	1.50
22	P	611	CLA	CMD-C2D	-2.01	1.46	1.50
22	Q	607	CLA	MG-NB	-2.01	2.01	2.05
22	I	605	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	314	CLA	CMB-C2B	-2.01	1.46	1.50
22	V	617	CLA	MG-NB	-2.01	2.01	2.05
22	B	817	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	825	CLA	CMB-C2B	-2.01	1.46	1.50
22	K	613	CLA	CMC-C2C	-2.01	1.46	1.50
22	B	824	CLA	CMB-C2B	-2.01	1.46	1.50
22	V	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	822	CLA	CMB-C2B	-2.01	1.46	1.50
22	L	403	CLA	CMB-C2B	-2.01	1.46	1.50
22	N	602	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	832	CLA	MG-NB	-2.01	2.01	2.05
22	B	806	CLA	CMB-C2B	-2.01	1.46	1.50
22	H	318	CLA	CMD-C2D	-2.01	1.46	1.50
22	X	402	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	833	CLA	CMB-C2B	-2.01	1.46	1.50
22	R	610	CLA	CMB-C2B	-2.01	1.46	1.50
22	V	601	CLA	CMD-C2D	-2.01	1.46	1.50
22	U	420	CLA	CMB-C2B	-2.01	1.46	1.50
22	K	603	CLA	CMC-C2C	-2.01	1.46	1.50
22	N	601	CLA	CMB-C2B	-2.01	1.46	1.50
22	Q	612	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	823	CLA	CMC-C2C	-2.01	1.46	1.50
22	W	419	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	852	CLA	CMD-C2D	-2.01	1.46	1.50
22	U	406	CLA	CMD-C2D	-2.01	1.46	1.50
22	X	417	CLA	CMC-C2C	-2.01	1.46	1.50
22	A	852	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	808	CLA	CMC-C2C	-2.00	1.46	1.50
22	B	839	CLA	CMC-C2C	-2.00	1.46	1.50
22	K	605	CLA	CMD-C2D	-2.00	1.46	1.50
22	N	607	CLA	CMC-C2C	-2.00	1.46	1.50
22	O	305	CLA	CMB-C2B	-2.00	1.46	1.50
22	V	608	CLA	CMD-C2D	-2.00	1.46	1.50
22	X	408	CLA	CMB-C2B	-2.00	1.46	1.50
22	V	602	CLA	CMD-C2D	-2.00	1.46	1.50
22	K	611	CLA	CMC-C2C	-2.00	1.46	1.50
22	O	319	CLA	CMD-C2D	-2.00	1.46	1.50
22	A	820	CLA	CMD-C2D	-2.00	1.46	1.50
26	U	419	LHG	O7-C5	-2.00	1.41	1.46
22	B	830	CLA	C1B-NB	-2.00	1.35	1.37
22	X	402	CLA	CMD-C2D	-2.00	1.46	1.50
22	B	833	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	T	604	CLA	CMB-C2B	-2.00	1.46	1.50
22	V	603	CLA	CMC-C2C	-2.00	1.46	1.50
22	U	411	CLA	MG-NB	-2.00	2.01	2.05
22	B	811	CLA	CMB-C2B	-2.00	1.46	1.50
22	U	401	CLA	CMC-C2C	-2.00	1.46	1.50

All (2573) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	843	BCR	C40-C30-C25	-13.78	88.64	110.24
24	P	612	DD6	C9-C10-C11	-10.08	113.14	127.28
24	P	612	DD6	C4-C5-C6	-9.22	114.35	127.28
21	B	843	BCR	C40-C30-C39	-9.02	82.82	108.63
24	X	416	DD6	C4-C5-C6	-8.51	115.34	127.28
24	A	858	DD6	C4-C5-C6	-7.81	116.32	127.28
24	P	612	DD6	C14-C13-C11	-7.43	114.00	125.53
22	A	839	CLA	C4A-NA-C1A	7.32	110.02	106.68
22	B	820	CLA	C4A-NA-C1A	7.27	109.99	106.68
22	B	829	CLA	C4A-NA-C1A	7.18	109.95	106.68
22	B	804	CLA	C4A-NA-C1A	7.13	109.93	106.68
22	K	607	CLA	C4A-NA-C1A	7.13	109.93	106.68
22	P	611	CLA	C4A-NA-C1A	7.13	109.93	106.68
24	A	858	DD6	C9-C10-C11	-7.13	117.28	127.28
22	V	613	CLA	C4A-NA-C1A	7.12	109.93	106.68
22	B	819	CLA	C4A-NA-C1A	7.03	109.88	106.68
22	B	835	CLA	C4A-NA-C1A	7.02	109.88	106.68
22	A	807	CLA	C4A-NA-C1A	6.99	109.87	106.68
22	N	610	CLA	C4A-NA-C1A	6.99	109.87	106.68
22	R	607	CLA	C4A-NA-C1A	6.97	109.86	106.68
22	P	602	CLA	C4A-NA-C1A	6.97	109.86	106.68
22	I	609	CLA	C4A-NA-C1A	6.89	109.82	106.68
21	B	843	BCR	C39-C30-C25	6.83	120.95	110.24
22	O	310	CLA	C4A-NA-C1A	6.82	109.79	106.68
22	B	802	CLA	C4A-NA-C1A	6.81	109.78	106.68
22	B	824	CLA	C4A-NA-C1A	6.75	109.76	106.68
22	L	409	CLA	C4A-NA-C1A	6.72	109.75	106.68
22	U	403	CLA	C4A-NA-C1A	6.72	109.75	106.68
22	A	844	CLA	C4A-NA-C1A	6.72	109.74	106.68
22	L	417	CLA	C4A-NA-C1A	6.70	109.74	106.68
22	A	841	CLA	C4A-NA-C1A	6.70	109.73	106.68
22	B	837	CLA	C4A-NA-C1A	6.69	109.73	106.68
22	B	809	CLA	C4A-NA-C1A	6.68	109.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	U	413	CLA	C4A-NA-C1A	6.68	109.72	106.68
22	L	405	CLA	C4A-NA-C1A	6.67	109.72	106.68
22	A	821	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	A	838	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	P	610	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	S	601	CLA	C4A-NA-C1A	6.65	109.72	106.68
22	O	309	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	X	408	CLA	C4A-NA-C1A	6.63	109.70	106.68
22	L	404	CLA	C4A-NA-C1A	6.63	109.70	106.68
22	B	817	CLA	C4A-NA-C1A	6.63	109.70	106.68
22	Q	603	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	B	826	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	A	814	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	B	838	CLA	C4A-NA-C1A	6.61	109.69	106.68
22	X	413	CLA	C4A-NA-C1A	6.61	109.69	106.68
24	A	858	DD6	C3-C2-C1	-6.61	118.01	127.28
22	K	611	CLA	C4A-NA-C1A	6.60	109.69	106.68
22	V	609	CLA	C4A-NA-C1A	6.60	109.69	106.68
22	B	803	CLA	C4A-NA-C1A	6.60	109.69	106.68
22	B	821	CLA	C4A-NA-C1A	6.59	109.69	106.68
22	L	402	CLA	C4A-NA-C1A	6.59	109.69	106.68
22	O	313	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	Q	617	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	T	606	CLA	C4A-NA-C1A	6.57	109.68	106.68
22	B	836	CLA	C4A-NA-C1A	6.56	109.67	106.68
22	U	414	CLA	C4A-NA-C1A	6.56	109.67	106.68
22	V	604	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	S	605	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	A	801	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	B	825	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	I	608	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	V	611	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	B	823	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	B	806	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	H	311	CLA	C4A-NA-C1A	6.52	109.66	106.68
22	X	411	CLA	C4A-NA-C1A	6.52	109.66	106.68
22	F	403	CLA	C4A-NA-C1A	6.52	109.65	106.68
22	A	831	CLA	C4A-NA-C1A	6.52	109.65	106.68
22	A	819	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	V	617	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	G	608	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	N	602	CLA	C4A-NA-C1A	6.51	109.65	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	608	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	N	606	CLA	C4A-NA-C1A	6.50	109.65	106.68
22	W	410	CLA	C4A-NA-C1A	6.50	109.65	106.68
22	A	840	CLA	C4A-NA-C1A	6.50	109.64	106.68
22	O	319	CLA	C4A-NA-C1A	6.50	109.64	106.68
22	I	605	CLA	C4A-NA-C1A	6.50	109.64	106.68
22	T	604	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	U	401	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	B	807	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	G	605	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	U	412	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	T	608	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	N	605	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	V	612	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	A	826	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	X	412	CLA	C4A-NA-C1A	6.48	109.64	106.68
22	X	402	CLA	C4A-NA-C1A	6.48	109.64	106.68
22	B	805	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	H	318	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	K	605	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	K	606	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	S	615	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	H	308	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	W	405	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	A	828	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	S	606	CLA	C4A-NA-C1A	6.46	109.63	106.68
22	T	601	CLA	C4A-NA-C1A	6.46	109.63	106.68
22	R	603	CLA	C4A-NA-C1A	6.46	109.63	106.68
22	S	614	CLA	C4A-NA-C1A	6.46	109.63	106.68
22	B	811	CLA	C4A-NA-C1A	6.46	109.62	106.68
22	H	309	CLA	C4A-NA-C1A	6.46	109.62	106.68
22	W	414	CLA	C4A-NA-C1A	6.46	109.62	106.68
22	X	419	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	B	808	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	I	610	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	A	816	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	I	606	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	J	102	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	O	305	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	P	606	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	W	404	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	N	611	CLA	C4A-NA-C1A	6.43	109.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	611	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	K	609	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	N	608	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	X	403	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	H	305	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	K	608	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	T	610	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	L	406	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	S	602	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	W	419	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	A	833	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	B	818	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	Q	610	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	R	605	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	H	307	CLA	C4A-NA-C1A	6.42	109.61	106.68
24	R	613	DD6	C3-C2-C1	-6.41	118.28	127.28
22	R	611	CLA	C4A-NA-C1A	6.41	109.60	106.68
22	P	607	CLA	C4A-NA-C1A	6.41	109.60	106.68
22	X	410	CLA	C4A-NA-C1A	6.41	109.60	106.68
22	R	615	CLA	C4A-NA-C1A	6.41	109.60	106.68
22	G	601	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	P	605	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	W	412	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	H	313	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	S	604	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	I	601	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	V	602	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	B	810	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	B	816	CLA	C4A-NA-C1A	6.38	109.59	106.68
22	G	611	CLA	C4A-NA-C1A	6.37	109.59	106.68
22	Q	612	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	A	810	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	R	609	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	B	832	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	O	312	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	X	405	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	Q	608	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	B	833	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	L	410	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	U	406	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	P	604	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	G	610	CLA	C4A-NA-C1A	6.35	109.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	604	CLA	C4A-NA-C1A	6.34	109.57	106.68
22	Q	606	CLA	C4A-NA-C1A	6.34	109.57	106.68
22	F	404	CLA	C4A-NA-C1A	6.34	109.57	106.68
22	Q	601	CLA	C4A-NA-C1A	6.34	109.57	106.68
22	V	601	CLA	C4A-NA-C1A	6.34	109.57	106.68
22	P	609	CLA	C4A-NA-C1A	6.34	109.57	106.68
22	A	823	CLA	C4A-NA-C1A	6.33	109.56	106.68
22	U	420	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	A	805	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	A	806	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	K	613	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	H	306	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	A	824	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	A	835	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	G	604	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	K	604	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	R	601	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	S	607	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	U	409	CLA	C4A-NA-C1A	6.30	109.56	106.68
22	O	311	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	B	839	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	L	408	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	Q	609	CLA	C4A-NA-C1A	6.29	109.55	106.68
22	A	829	CLA	C4A-NA-C1A	6.29	109.55	106.68
22	N	601	CLA	C4A-NA-C1A	6.29	109.55	106.68
22	W	406	CLA	C4A-NA-C1A	6.29	109.55	106.68
22	N	604	CLA	C4A-NA-C1A	6.28	109.55	106.68
22	A	815	CLA	C4A-NA-C1A	6.28	109.55	106.68
22	B	812	CLA	C4A-NA-C1A	6.28	109.55	106.68
22	O	308	CLA	C4A-NA-C1A	6.28	109.55	106.68
22	W	403	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	R	608	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	I	607	CLA	C4A-NA-C1A	6.27	109.54	106.68
22	V	607	CLA	C4A-NA-C1A	6.27	109.54	106.68
22	A	834	CLA	C4A-NA-C1A	6.27	109.54	106.68
22	Q	618	CLA	C4A-NA-C1A	6.27	109.54	106.68
22	H	302	CLA	C4A-NA-C1A	6.26	109.54	106.68
22	A	836	CLA	C4A-NA-C1A	6.26	109.54	106.68
22	A	842	CLA	C4A-NA-C1A	6.26	109.54	106.68
21	A	851	BCR	C7-C8-C9	-6.26	116.97	126.23
22	U	404	CLA	C4A-NA-C1A	6.26	109.54	106.68
22	K	603	CLA	C4A-NA-C1A	6.26	109.53	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	407	CLA	C4A-NA-C1A	6.26	109.53	106.68
22	V	610	CLA	C4A-NA-C1A	6.26	109.53	106.68
22	X	409	CLA	C4A-NA-C1A	6.26	109.53	106.68
22	G	607	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	A	827	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	H	303	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	U	410	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	A	837	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	G	606	CLA	C4A-NA-C1A	6.24	109.53	106.68
22	L	407	CLA	C4A-NA-C1A	6.24	109.53	106.68
22	H	310	CLA	C4A-NA-C1A	6.24	109.53	106.68
22	K	617	CLA	C4A-NA-C1A	6.24	109.52	106.68
22	W	413	CLA	C4A-NA-C1A	6.24	109.52	106.68
22	G	602	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	K	602	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	S	608	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	Q	607	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	U	411	CLA	C4A-NA-C1A	6.22	109.52	106.68
22	T	605	CLA	C4A-NA-C1A	6.22	109.52	106.68
22	T	607	CLA	C4A-NA-C1A	6.22	109.52	106.68
22	U	405	CLA	C4A-NA-C1A	6.22	109.52	106.68
22	T	609	CLA	C4A-NA-C1A	6.21	109.51	106.68
22	V	608	CLA	C4A-NA-C1A	6.21	109.51	106.68
22	B	822	CLA	C4A-NA-C1A	6.20	109.51	106.68
22	A	809	CLA	C4A-NA-C1A	6.20	109.51	106.68
22	Q	611	CLA	C4A-NA-C1A	6.20	109.51	106.68
22	L	411	CLA	C4A-NA-C1A	6.20	109.51	106.68
22	B	859	CLA	C4A-NA-C1A	6.19	109.50	106.68
22	V	603	CLA	C4A-NA-C1A	6.19	109.50	106.68
22	B	834	CLA	C4A-NA-C1A	6.17	109.50	106.68
22	S	609	CLA	C4A-NA-C1A	6.17	109.50	106.68
22	A	817	CLA	C4A-NA-C1A	6.17	109.50	106.68
22	N	607	CLA	C4A-NA-C1A	6.17	109.49	106.68
22	A	852	CLA	C4A-NA-C1A	6.17	109.49	106.68
22	A	822	CLA	C4A-NA-C1A	6.16	109.49	106.68
22	K	610	CLA	C4A-NA-C1A	6.16	109.49	106.68
22	Q	604	CLA	C4A-NA-C1A	6.15	109.49	106.68
22	X	404	CLA	C4A-NA-C1A	6.15	109.49	106.68
22	A	808	CLA	C4A-NA-C1A	6.15	109.48	106.68
22	F	405	CLA	C4A-NA-C1A	6.14	109.48	106.68
22	T	602	CLA	C4A-NA-C1A	6.14	109.48	106.68
22	W	415	CLA	C4A-NA-C1A	6.14	109.48	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	828	CLA	C4A-NA-C1A	6.14	109.48	106.68
22	I	602	CLA	C4A-NA-C1A	6.13	109.48	106.68
22	A	825	CLA	C4A-NA-C1A	6.12	109.47	106.68
22	L	403	CLA	C4A-NA-C1A	6.12	109.47	106.68
22	T	603	CLA	C4A-NA-C1A	6.11	109.47	106.68
22	U	415	CLA	C4A-NA-C1A	6.11	109.47	106.68
22	O	306	CLA	C4A-NA-C1A	6.09	109.46	106.68
22	O	315	CLA	C4A-NA-C1A	6.08	109.45	106.68
22	Q	613	CLA	C4A-NA-C1A	6.07	109.45	106.68
22	A	832	CLA	C4A-NA-C1A	6.07	109.45	106.68
22	W	411	CLA	C4A-NA-C1A	6.05	109.44	106.68
22	B	831	CLA	C4A-NA-C1A	6.05	109.44	106.68
24	P	613	DD6	C3-C2-C1	-6.04	118.81	127.28
22	N	603	CLA	C4A-NA-C1A	6.04	109.43	106.68
22	N	609	CLA	C4A-NA-C1A	6.04	109.43	106.68
21	B	843	BCR	C24-C23-C22	-6.03	117.31	126.23
22	A	812	CLA	C4A-NA-C1A	6.03	109.43	106.68
22	R	606	CLA	C4A-NA-C1A	6.01	109.42	106.68
33	A	802	CL0	CHA-C1A-C2A	-5.99	119.24	133.31
22	H	312	CLA	C4A-NA-C1A	5.99	109.41	106.68
22	S	610	CLA	C4A-NA-C1A	5.98	109.41	106.68
22	O	314	CLA	C4A-NA-C1A	5.97	109.40	106.68
21	B	843	BCR	C40-C30-C29	-5.96	86.06	108.95
22	Q	605	CLA	C4A-NA-C1A	5.96	109.40	106.68
22	R	604	CLA	C4A-NA-C1A	5.96	109.40	106.68
22	A	818	CLA	C4A-NA-C1A	5.95	109.39	106.68
22	A	811	CLA	C4A-NA-C1A	5.94	109.39	106.68
22	W	402	CLA	C4A-NA-C1A	5.93	109.39	106.68
22	R	602	CLA	C4A-NA-C1A	5.93	109.39	106.68
22	S	603	CLA	C4A-NA-C1A	5.93	109.38	106.68
22	X	417	CLA	C4A-NA-C1A	5.91	109.38	106.68
22	W	409	CLA	C4A-NA-C1A	5.90	109.37	106.68
22	G	609	CLA	C4A-NA-C1A	5.90	109.37	106.68
22	G	603	CLA	C4A-NA-C1A	5.89	109.37	106.68
22	R	610	CLA	C4A-NA-C1A	5.86	109.35	106.68
24	J	105	DD6	C9-C10-C11	-5.86	119.06	127.28
22	I	611	CLA	C4A-NA-C1A	5.85	109.35	106.68
21	A	850	BCR	C24-C23-C22	-5.81	117.64	126.23
22	B	814	CLA	C4A-NA-C1A	5.81	109.33	106.68
22	A	803	CLA	C4A-NA-C1A	5.78	109.32	106.68
22	H	304	CLA	C4A-NA-C1A	5.75	109.30	106.68
21	B	843	BCR	C7-C8-C9	-5.74	117.74	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	830	CLA	C4A-NA-C1A	5.74	109.30	106.68
22	K	612	CLA	C4A-NA-C1A	5.71	109.29	106.68
22	O	307	CLA	C4A-NA-C1A	5.71	109.29	106.68
22	I	603	CLA	C4A-NA-C1A	5.67	109.27	106.68
22	B	815	CLA	C4A-NA-C1A	5.60	109.23	106.68
22	L	412	CLA	C4A-NA-C1A	5.56	109.22	106.68
22	A	804	CLA	C4A-NA-C1A	5.53	109.20	106.68
22	A	820	CLA	C4A-NA-C1A	5.51	109.19	106.68
22	A	813	CLA	C4A-NA-C1A	5.50	109.19	106.68
21	B	801	BCR	C7-C8-C9	-5.47	118.14	126.23
21	B	801	BCR	C11-C10-C9	-5.47	119.60	127.28
21	B	843	BCR	C30-C25-C26	-5.42	115.23	122.64
21	B	801	BCR	C15-C14-C13	-5.42	119.68	127.28
24	A	847	DD6	C4-C5-C6	-5.41	119.69	127.28
22	P	603	CLA	C4A-NA-C1A	5.40	109.14	106.68
24	B	841	DD6	C3-C2-C1	-5.36	119.77	127.28
24	L	415	DD6	C3-C2-C1	-5.32	119.82	127.28
22	B	827	CLA	C4A-NA-C1A	5.30	109.10	106.68
24	T	612	DD6	C3-C2-C1	-5.30	119.85	127.28
21	M	101	BCR	C20-C21-C22	-5.29	119.86	127.28
21	A	850	BCR	C20-C21-C22	-5.28	119.87	127.28
24	G	613	DD6	C3-C2-C1	-5.27	119.88	127.28
24	J	105	DD6	C4-C5-C6	-5.26	119.90	127.28
24	P	612	DD6	C4-C3-C2	-5.24	112.79	123.52
24	V	614	DD6	C4-C5-C6	-5.22	119.95	127.28
24	I	613	DD6	C3-C2-C1	-5.22	119.96	127.28
21	B	843	BCR	C3-C4-C5	-5.18	104.83	114.06
22	B	813	CLA	C4A-NA-C1A	5.12	109.02	106.68
24	V	614	DD6	C21-C20-C19	5.11	119.98	114.24
22	A	830	CLA	C4A-NA-C1A	5.10	109.01	106.68
24	W	418	DD6	C21-C20-C19	5.09	119.95	114.24
21	M	101	BCR	C16-C17-C18	-5.08	120.16	127.28
21	A	851	BCR	C28-C27-C26	-5.06	105.03	114.06
24	S	611	DD6	C3-C2-C1	-5.06	120.19	127.28
24	H	314	DD6	C21-C20-C19	5.03	119.89	114.24
24	Q	615	DD6	C21-C20-C19	5.03	119.89	114.24
24	N	613	DD6	C3-C2-C1	-5.02	120.23	127.28
24	L	414	DD6	C3-C2-C1	-5.02	120.24	127.28
21	B	845	BCR	C15-C14-C13	-5.01	120.25	127.28
24	I	613	DD6	C21-C20-C19	5.00	119.86	114.24
24	R	613	DD6	C21-C20-C19	4.99	119.85	114.24
24	U	416	DD6	C21-C20-C19	4.98	119.83	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	O	317	DD6	C21-C20-C19	4.96	119.81	114.24
24	X	401	DD6	C4-C5-C6	-4.95	120.33	127.28
24	G	613	DD6	C21-C20-C19	4.94	119.79	114.24
24	N	612	DD6	C21-C20-C19	4.92	119.77	114.24
24	Q	615	DD6	C3-C2-C1	-4.92	120.39	127.28
24	K	614	DD6	C21-C20-C19	4.91	119.75	114.24
24	L	415	DD6	C9-C10-C11	-4.89	120.43	127.28
24	H	315	DD6	C21-C20-C19	4.86	119.70	114.24
24	W	418	DD6	C3-C2-C1	-4.85	120.47	127.28
33	A	802	CL0	C1B-CHB-C4A	4.85	124.44	121.32
24	A	859	DD6	C3-C2-C1	-4.85	120.48	127.28
24	A	858	DD6	C21-C20-C19	4.85	119.69	114.24
24	S	612	DD6	C21-C20-C19	4.85	119.69	114.24
24	N	613	DD6	C21-C20-C19	4.84	119.68	114.24
24	T	612	DD6	C21-C20-C19	4.84	119.67	114.24
24	F	406	DD6	C21-C20-C19	4.81	119.64	114.24
24	P	613	DD6	C21-C20-C19	4.81	119.64	114.24
24	O	317	DD6	C3-C2-C1	-4.80	120.54	127.28
24	S	611	DD6	C21-C20-C19	4.80	119.63	114.24
24	L	414	DD6	C21-C20-C19	4.79	119.62	114.24
24	F	406	DD6	C4-C5-C6	-4.79	120.56	127.28
24	X	401	DD6	C21-C20-C19	4.79	119.62	114.24
21	B	842	BCR	C15-C14-C13	-4.78	120.57	127.28
24	V	615	DD6	C21-C20-C19	4.76	119.59	114.24
24	R	612	DD6	C21-C20-C19	4.76	119.59	114.24
24	X	414	DD6	C21-C20-C19	4.71	119.53	114.24
24	W	416	DD6	C21-C20-C19	4.68	119.50	114.24
21	M	101	BCR	C24-C23-C22	-4.67	119.33	126.23
24	L	415	DD6	C21-C20-C19	4.67	119.48	114.24
31	W	408	CHL	C1B-CHB-C4A	4.65	124.31	121.32
21	A	849	BCR	C15-C14-C13	-4.59	120.83	127.28
24	H	314	DD6	C4-C5-C6	-4.59	120.84	127.28
21	B	846	BCR	C24-C23-C22	-4.56	119.49	126.23
21	B	846	BCR	C16-C17-C18	-4.56	120.89	127.28
24	B	841	DD6	C21-C20-C19	4.54	119.34	114.24
24	A	847	DD6	C21-C20-C19	4.53	119.33	114.24
31	W	422	CHL	C1B-CHB-C4A	4.49	124.21	121.32
24	I	612	DD6	C21-C20-C19	4.47	119.26	114.24
24	L	413	DD6	C21-C20-C19	4.45	119.24	114.24
24	N	612	DD6	C4-C5-C6	-4.45	121.04	127.28
33	A	802	CL0	O2D-CGD-CBD	4.44	115.83	110.95
24	A	859	DD6	C4-C5-C6	-4.44	121.06	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	415	DD6	C4-C5-C6	-4.42	121.08	127.28
24	X	414	DD6	C4-C5-C6	-4.42	121.08	127.28
24	G	612	DD6	C21-C20-C19	4.40	119.18	114.24
22	S	605	CLA	C1-C2-C3	-4.38	119.02	126.20
31	W	407	CHL	C1B-CHB-C4A	4.37	124.14	121.32
24	W	417	DD6	C21-C20-C19	4.37	119.15	114.24
24	P	612	DD6	C9-C8-C6	-4.36	114.40	126.36
22	A	819	CLA	O2D-CGD-O1D	-4.36	115.37	123.85
21	A	850	BCR	C16-C17-C18	-4.33	121.20	127.28
24	B	841	DD6	C4-C5-C6	-4.29	121.26	127.28
24	X	415	DD6	C21-C20-C19	4.28	119.05	114.24
24	R	612	DD6	C3-C2-C1	-4.28	121.28	127.28
24	W	416	DD6	C4-C5-C6	-4.27	121.28	127.28
24	K	615	DD6	C4-C5-C6	-4.27	121.29	127.28
24	K	615	DD6	C21-C20-C19	4.26	119.03	114.24
24	U	417	DD6	C21-C20-C19	4.26	119.03	114.24
22	A	819	CLA	C3B-C4B-NB	-4.26	106.73	110.53
24	P	612	DD6	C21-C20-C19	4.25	119.02	114.24
21	A	848	BCR	C33-C5-C6	-4.25	119.85	124.48
24	B	841	DD6	C9-C10-C11	-4.23	121.34	127.28
24	N	613	DD6	C9-C10-C11	-4.22	121.36	127.28
24	Q	614	DD6	C21-C20-C19	4.21	118.97	114.24
25	F	401	DGD	O2G-C1B-C2B	4.21	120.59	111.48
24	F	406	DD6	C14-C13-C11	-4.20	119.01	125.53
24	R	612	DD6	C4-C5-C6	-4.19	121.40	127.28
31	U	407	CHL	C1B-CHB-C4A	4.18	124.01	121.32
24	A	859	DD6	C21-C20-C19	4.16	118.92	114.24
24	T	613	DD6	C21-C20-C19	4.15	118.91	114.24
24	L	413	DD6	C4-C5-C6	-4.15	121.46	127.28
33	A	802	CL0	O2D-CGD-O1D	-4.15	115.78	123.85
31	X	406	CHL	C1B-CHB-C4A	4.14	123.99	121.32
21	A	851	BCR	C20-C21-C22	-4.14	121.47	127.28
21	B	842	BCR	C33-C5-C6	-4.13	119.98	124.48
31	V	605	CHL	C1B-CHB-C4A	4.13	123.98	121.32
24	V	614	DD6	O1-C20-C19	-4.13	109.62	113.49
26	L	416	LHG	O7-C7-C8	4.12	120.40	111.48
24	K	614	DD6	C4-C5-C6	-4.12	121.50	127.28
24	O	316	DD6	C21-C20-C19	4.10	118.85	114.24
26	N	616	LHG	O7-C7-C8	4.10	120.36	111.48
21	B	843	BCR	C16-C17-C18	-4.10	121.53	127.28
26	U	419	LHG	O7-C7-C8	4.09	120.34	111.48
24	P	612	DD6	C13-C11-C10	4.09	125.44	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	315	DD6	C3-C2-C1	-4.09	121.55	127.28
26	O	324	LHG	O7-C7-C8	4.08	120.31	111.48
21	A	848	BCR	C16-C17-C18	-4.08	121.56	127.28
26	S	613	LHG	O7-C7-C8	4.08	120.30	111.48
21	B	844	BCR	C7-C8-C9	-4.08	120.20	126.23
26	A	845	LHG	O7-C7-C8	4.06	120.27	111.48
21	A	850	BCR	C38-C26-C25	-4.06	120.06	124.48
24	X	415	DD6	C4-C5-C6	-4.04	121.61	127.28
26	X	420	LHG	O7-C7-C8	4.04	120.22	111.48
24	X	416	DD6	C8-C6-C5	4.04	125.36	119.01
24	G	612	DD6	C4-C5-C6	-4.04	121.62	127.28
26	K	619	LHG	O7-C7-C8	4.03	120.21	111.48
24	X	416	DD6	C12-C11-C13	4.03	124.24	118.09
24	V	614	DD6	C9-C10-C11	-4.03	121.63	127.28
26	H	316	LHG	O7-C7-C8	4.03	120.19	111.48
21	A	851	BCR	C16-C17-C18	-4.02	121.64	127.28
21	A	849	BCR	C24-C23-C22	-4.01	120.30	126.23
24	S	612	DD6	C4-C5-C6	-4.01	121.66	127.28
26	T	614	LHG	O7-C7-C8	4.00	120.14	111.48
24	Q	614	DD6	C4-C5-C6	-4.00	121.67	127.28
21	A	849	BCR	C16-C17-C18	-4.00	121.67	127.28
24	R	612	DD6	C9-C10-C11	-4.00	121.67	127.28
24	U	416	DD6	C4-C5-C6	-4.00	121.67	127.28
24	A	858	DD6	C-C1-C24	3.98	124.17	118.09
26	B	851	LHG	O7-C7-C8	3.98	120.10	111.48
26	A	846	LHG	O7-C7-C8	3.98	120.09	111.48
21	B	845	BCR	C24-C23-C22	-3.98	120.35	126.23
24	P	612	DD6	C25-C24-C1	-3.98	115.46	126.36
31	U	408	CHL	C1B-CHB-C4A	3.97	123.88	121.32
26	K	616	LHG	O7-C7-C8	3.97	120.06	111.48
26	G	614	LHG	O7-C7-C8	3.96	120.04	111.48
24	V	615	DD6	C4-C5-C6	-3.95	121.73	127.28
24	S	612	DD6	C3-C2-C1	-3.95	121.74	127.28
26	O	321	LHG	O7-C7-C8	3.94	120.01	111.48
21	B	845	BCR	C11-C10-C9	-3.94	121.76	127.28
21	A	848	BCR	C11-C10-C9	-3.93	121.77	127.28
21	A	848	BCR	C7-C8-C9	-3.93	120.42	126.23
24	L	413	DD6	C3-C2-C1	-3.91	121.79	127.28
24	W	417	DD6	O1-C20-C19	-3.91	109.83	113.49
21	A	849	BCR	C20-C21-C22	-3.91	121.80	127.28
24	W	417	DD6	C4-C5-C6	-3.88	121.83	127.28
26	B	848	LHG	O7-C7-C8	3.87	119.86	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	416	DD6	C3-C2-C1	-3.87	121.85	127.28
21	J	103	BCR	C15-C14-C13	-3.87	121.85	127.28
24	V	615	DD6	C3-C2-C1	-3.87	121.85	127.28
22	A	839	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
21	B	842	BCR	C24-C23-C22	-3.86	120.52	126.23
26	O	318	LHG	O7-C7-C8	3.86	119.84	111.48
21	B	844	BCR	C11-C10-C9	-3.86	121.86	127.28
21	A	851	BCR	C15-C14-C13	-3.86	121.87	127.28
31	V	606	CHL	C1B-CHB-C4A	3.85	123.80	121.32
24	X	416	DD6	C21-C20-C19	3.84	118.56	114.24
26	O	323	LHG	O7-C7-C8	3.84	119.79	111.48
24	X	416	DD6	C14-C13-C11	3.83	131.47	125.53
21	B	844	BCR	C15-C14-C13	-3.83	121.91	127.28
21	A	851	BCR	C27-C26-C25	-3.82	117.54	122.70
24	U	417	DD6	C4-C5-C6	-3.81	121.94	127.28
26	P	601	LHG	O7-C7-C8	3.81	119.72	111.48
26	N	614	LHG	O7-C7-C8	3.80	119.70	111.48
26	Q	616	LHG	O7-C7-C8	3.80	119.70	111.48
24	T	613	DD6	C3-C2-C1	-3.80	121.95	127.28
24	Q	615	DD6	C15-C14-C13	-3.79	117.97	125.99
21	B	842	BCR	C30-C25-C26	-3.79	117.45	122.64
22	K	607	CLA	C3B-C4B-NB	-3.79	107.15	110.53
26	R	614	LHG	O7-C7-C8	3.79	119.68	111.48
21	B	845	BCR	C3-C4-C5	-3.78	107.32	114.06
21	B	842	BCR	C16-C17-C18	-3.77	121.99	127.28
24	A	847	DD6	C9-C10-C11	-3.76	122.00	127.28
21	B	845	BCR	C7-C8-C9	-3.76	120.68	126.23
21	M	101	BCR	C15-C14-C13	-3.76	122.01	127.28
21	A	848	BCR	C24-C23-C22	-3.75	120.68	126.23
24	R	613	DD6	C15-C14-C13	-3.74	118.08	125.99
24	Q	614	DD6	C3-C2-C1	-3.74	122.03	127.28
21	B	844	BCR	C16-C17-C18	-3.74	122.03	127.28
24	V	614	DD6	C3-C2-C1	-3.74	122.04	127.28
24	W	418	DD6	C4-C5-C6	-3.72	122.06	127.28
21	B	842	BCR	C11-C10-C9	-3.71	122.08	127.28
21	B	843	BCR	C39-C30-C29	3.70	123.16	108.95
21	A	848	BCR	C15-C14-C13	-3.70	122.09	127.28
21	A	850	BCR	C15-C14-C13	-3.69	122.10	127.28
24	H	314	DD6	C3-C2-C1	-3.68	122.11	127.28
21	A	850	BCR	C33-C5-C6	-3.67	120.48	124.48
24	S	611	DD6	C15-C14-C13	-3.67	118.24	125.99
24	X	416	DD6	C10-C9-C8	-3.66	112.60	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	844	BCR	C24-C23-C22	-3.65	120.83	126.23
24	V	614	DD6	C15-C14-C13	-3.65	118.28	125.99
21	B	843	BCR	C15-C14-C13	-3.64	122.17	127.28
24	X	414	DD6	C3-C2-C1	-3.64	122.17	127.28
24	X	401	DD6	C9-C10-C11	-3.63	122.19	127.28
21	B	846	BCR	C20-C21-C22	-3.63	122.19	127.28
24	N	612	DD6	C3-C2-C1	-3.62	122.21	127.28
21	B	844	BCR	C33-C5-C6	-3.61	120.54	124.48
21	A	849	BCR	C38-C26-C25	-3.61	120.55	124.48
21	B	842	BCR	C20-C21-C22	-3.61	122.22	127.28
22	A	816	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
21	M	101	BCR	C7-C8-C9	-3.60	120.91	126.23
22	B	802	CLA	C3B-C4B-NB	-3.60	107.32	110.53
25	O	304	DGD	O2G-C1B-C2B	3.60	119.26	111.48
22	A	831	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
24	X	401	DD6	C3-C2-C1	-3.58	122.26	127.28
22	A	816	CLA	C3B-C4B-NB	-3.57	107.34	110.53
21	B	801	BCR	C28-C27-C26	-3.56	107.70	114.06
22	L	408	CLA	C3B-C4B-NB	-3.56	107.36	110.53
24	A	858	DD6	C9-C8-C6	-3.55	116.62	126.36
21	J	103	BCR	C16-C17-C18	-3.55	122.30	127.28
22	B	820	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
22	A	816	CLA	CAA-CBA-CGA	-3.55	103.14	113.21
24	I	613	DD6	C15-C14-C13	-3.54	118.51	125.99
24	H	315	DD6	C15-C14-C13	-3.52	118.56	125.99
26	W	420	LHG	O7-C7-C8	3.52	119.09	111.48
24	H	314	DD6	C15-C14-C13	-3.50	118.58	125.99
21	M	101	BCR	C33-C5-C6	-3.50	120.67	124.48
24	U	416	DD6	C3-C2-C1	-3.50	122.37	127.28
21	A	849	BCR	C11-C10-C9	-3.50	122.37	127.28
24	O	317	DD6	C15-C14-C13	-3.50	118.60	125.99
24	G	613	DD6	C15-C14-C13	-3.49	118.61	125.99
28	I	615	LMG	C6-C5-C4	-3.49	108.76	113.53
24	B	841	DD6	O1-C20-C19	-3.47	110.24	113.49
24	T	612	DD6	C15-C14-C13	-3.46	118.67	125.99
21	B	846	BCR	C33-C5-C6	-3.46	120.71	124.48
24	Q	614	DD6	O1-C20-C19	-3.44	110.26	113.49
24	A	858	DD6	C-C1-C2	-3.44	117.24	122.82
24	T	613	DD6	C4-C5-C6	-3.43	122.47	127.28
24	U	416	DD6	C9-C10-C11	-3.43	122.47	127.28
24	V	614	DD6	O1-C15-C14	-3.42	107.07	116.88
22	S	610	CLA	CAA-C2A-C3A	-3.42	103.75	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	846	BCR	C15-C14-C13	-3.41	122.49	127.28
24	I	612	DD6	O1-C20-C19	-3.41	110.30	113.49
25	B	847	DGD	O2G-C1B-C2B	3.40	118.84	111.48
22	I	611	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
21	J	103	BCR	C33-C5-C6	-3.40	120.78	124.48
24	N	612	DD6	C9-C10-C11	-3.38	122.54	127.28
24	I	612	DD6	C4-C5-C6	-3.37	122.55	127.28
24	P	613	DD6	C4-C5-C6	-3.37	122.55	127.28
24	J	105	DD6	C3-C2-C1	-3.36	122.57	127.28
21	A	851	BCR	C24-C23-C22	-3.35	121.28	126.23
24	G	612	DD6	C3-C2-C1	-3.35	122.59	127.28
24	A	859	DD6	C15-C14-C13	-3.34	118.92	125.99
22	A	824	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
21	M	101	BCR	C11-C10-C9	-3.34	122.59	127.28
22	Q	613	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
24	L	415	DD6	C14-C13-C11	-3.33	120.36	125.53
22	B	830	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
24	G	613	DD6	C4-C5-C6	-3.33	122.61	127.28
21	J	103	BCR	C3-C4-C5	-3.32	108.13	114.06
21	M	101	BCR	C30-C25-C26	-3.32	118.10	122.64
24	U	417	DD6	O1-C20-C19	-3.32	110.38	113.49
25	B	847	DGD	O1G-C1A-C2A	3.32	121.95	111.83
24	X	415	DD6	O1-C20-C19	-3.32	110.38	113.49
21	J	103	BCR	C28-C27-C26	-3.31	108.15	114.06
24	W	417	DD6	C3-C2-C1	-3.31	122.63	127.28
21	A	848	BCR	C38-C26-C25	-3.31	120.87	124.48
24	V	615	DD6	C15-C14-C13	-3.31	118.99	125.99
24	U	417	DD6	C37-C36-C31	-3.31	117.98	124.16
22	B	824	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
22	B	828	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
24	O	316	DD6	C3-C2-C1	-3.30	122.65	127.28
21	A	849	BCR	C7-C8-C9	-3.28	121.39	126.23
22	B	830	CLA	C3B-C4B-NB	-3.27	107.61	110.53
24	O	316	DD6	C9-C10-C11	-3.27	122.69	127.28
22	B	803	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
24	S	612	DD6	C15-C14-C13	-3.27	119.09	125.99
24	N	613	DD6	C4-C5-C6	-3.27	122.70	127.28
24	W	416	DD6	C9-C10-C11	-3.26	122.70	127.28
22	U	403	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
21	B	842	BCR	C7-C8-C9	-3.26	121.42	126.23
21	B	845	BCR	C28-C27-C26	-3.25	108.25	114.06
25	O	304	DGD	O1G-C1A-C2A	3.25	121.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	103	BCR	C7-C8-C9	-3.25	121.43	126.23
25	F	401	DGD	O1G-C1A-C2A	3.25	121.74	111.83
28	U	402	LMG	O6-C1-O1	-3.25	102.37	110.04
24	S	612	DD6	C9-C10-C11	-3.25	122.73	127.28
27	O	322	LMU	C1-O1'-C1'	-3.24	108.14	113.68
24	V	615	DD6	C9-C10-C11	-3.24	122.73	127.28
21	A	848	BCR	C20-C21-C22	-3.24	122.73	127.28
21	J	103	BCR	C11-C10-C9	-3.24	122.74	127.28
24	I	612	DD6	C3-C2-C1	-3.24	122.74	127.28
22	S	609	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
31	U	407	CHL	CHA-C1A-C2A	-3.23	125.72	133.31
24	W	418	DD6	C15-C14-C13	-3.23	119.17	125.99
22	P	608	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
21	B	845	BCR	C38-C26-C25	-3.23	120.96	124.48
21	A	849	BCR	C33-C5-C6	-3.22	120.97	124.48
24	X	416	DD6	C37-C36-C35	3.22	120.35	114.42
24	K	614	DD6	C15-C14-C13	-3.22	119.18	125.99
24	L	414	DD6	C15-C14-C13	-3.22	119.19	125.99
22	A	801	CLA	C3B-C4B-NB	-3.22	107.66	110.53
24	H	315	DD6	O1-C20-C21	-3.21	111.46	115.05
22	P	610	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
21	B	846	BCR	C3-C4-C5	-3.20	108.34	114.06
24	X	416	DD6	C4-C3-C2	-3.20	116.96	123.52
22	A	810	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
24	G	612	DD6	O1-C20-C19	-3.20	110.49	113.49
22	A	838	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
22	A	811	CLA	CAA-C2A-C3A	-3.20	104.36	113.00
24	P	612	DD6	O1-C20-C21	-3.20	111.47	115.05
31	V	605	CHL	CHA-C1A-C2A	-3.20	125.80	133.31
22	A	835	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
24	O	317	DD6	C4-C5-C6	-3.18	122.81	127.28
22	B	804	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	K	614	DD6	C37-C36-C31	-3.18	118.22	124.16
24	N	612	DD6	C15-C14-C13	-3.17	119.28	125.99
24	O	316	DD6	C4-C5-C6	-3.17	122.83	127.28
21	B	842	BCR	C27-C26-C25	-3.17	118.43	122.70
22	A	816	CLA	O2D-CGD-CBD	3.16	116.76	111.23
24	K	614	DD6	C3-C2-C1	-3.16	122.85	127.28
22	B	835	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
22	A	806	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
22	B	819	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
31	X	406	CHL	CHA-C1A-C2A	-3.15	125.90	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	S	611	DD6	O1-C15-C14	-3.15	107.85	116.88
24	B	841	DD6	O1-C15-C14	-3.15	107.85	116.88
24	W	418	DD6	O1-C20-C19	-3.15	110.54	113.49
31	W	407	CHL	CHA-C1A-C2A	-3.14	125.93	133.31
22	G	603	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
24	B	841	DD6	C25-C26-C27	-3.14	117.83	126.61
22	A	842	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
31	W	408	CHL	CHA-C1A-C2A	-3.14	125.94	133.31
22	H	313	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
22	W	415	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
21	B	843	BCR	C33-C5-C4	3.13	120.26	113.60
24	J	105	DD6	C21-C20-C19	3.13	117.75	114.24
21	B	844	BCR	C20-C21-C22	-3.13	122.89	127.28
24	I	613	DD6	C4-C5-C6	-3.13	122.89	127.28
24	I	613	DD6	C9-C10-C11	-3.12	122.90	127.28
28	F	408	LMG	O6-C5-C4	3.12	115.33	109.70
22	T	608	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
24	L	414	DD6	C4-C5-C6	-3.12	122.90	127.28
22	I	607	CLA	C1-C2-C3	-3.12	121.09	126.20
22	U	405	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
24	H	314	DD6	C9-C10-C11	-3.11	122.91	127.28
22	Q	604	CLA	C3B-C4B-NB	-3.11	107.75	110.53
22	B	832	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
22	B	836	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
22	I	608	CLA	C3B-C4B-NB	-3.11	107.76	110.53
21	B	842	BCR	C3-C4-C5	-3.11	108.52	114.06
24	S	611	DD6	C4-C5-C6	-3.11	122.92	127.28
24	R	612	DD6	C15-C14-C13	-3.10	119.43	125.99
28	H	319	LMG	O6-C1-O1	-3.10	102.72	110.04
24	Q	615	DD6	C37-C36-C31	-3.10	118.37	124.16
21	B	843	BCR	C4-C5-C6	-3.09	118.53	122.70
24	Q	615	DD6	C4-C5-C6	-3.09	122.94	127.28
22	B	831	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
25	F	401	DGD	C2G-O2G-C1B	-3.09	110.40	117.80
22	B	817	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
22	A	833	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	R	613	DD6	C3-C4-C5	-3.09	117.20	123.52
22	A	844	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
22	K	608	CLA	C3B-C4B-NB	-3.09	107.78	110.53
22	Q	607	CLA	C3B-C4B-NB	-3.08	107.78	110.53
24	X	414	DD6	C9-C10-C11	-3.08	122.96	127.28
24	R	613	DD6	C4-C5-C6	-3.08	122.96	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	103	BCR	C24-C23-C22	-3.08	121.68	126.23
21	A	849	BCR	C3-C4-C5	-3.07	108.57	114.06
24	H	314	DD6	O1-C15-C14	-3.07	108.07	116.88
24	U	416	DD6	C15-C14-C13	-3.07	119.50	125.99
21	A	851	BCR	C33-C5-C6	-3.07	121.13	124.48
22	B	827	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
22	A	827	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
24	X	414	DD6	C15-C14-C13	-3.07	119.50	125.99
22	O	307	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
21	B	842	BCR	C28-C27-C26	-3.07	108.58	114.06
24	U	417	DD6	C3-C2-C1	-3.07	122.98	127.28
24	O	316	DD6	O1-C20-C19	-3.07	110.62	113.49
22	B	815	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
24	L	413	DD6	C9-C10-C11	-3.06	122.98	127.28
22	O	309	CLA	C3B-C4B-NB	-3.06	107.80	110.53
24	K	615	DD6	C3-C2-C1	-3.06	122.98	127.28
24	T	612	DD6	C3-C4-C5	-3.06	117.25	123.52
22	Q	604	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
24	R	613	DD6	C10-C9-C8	-3.06	114.34	123.20
22	B	812	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
22	B	813	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
24	I	613	DD6	C37-C36-C35	3.06	120.04	114.42
31	W	422	CHL	CHA-C1A-C2A	-3.06	126.13	133.31
22	I	603	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
22	S	614	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
28	W	401	LMG	O6-C1-O1	-3.05	102.83	110.04
24	R	613	DD6	O1-C20-C21	-3.05	111.64	115.05
22	B	811	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
22	B	814	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
24	N	613	DD6	C15-C14-C13	-3.04	119.56	125.99
22	Q	618	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
22	A	808	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
22	A	828	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
22	P	607	CLA	C3B-C4B-NB	-3.04	107.82	110.53
22	B	807	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
22	N	605	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
22	A	821	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
22	B	806	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
22	N	606	CLA	C3B-C4B-NB	-3.03	107.82	110.53
22	V	617	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
22	X	410	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
22	A	840	CLA	O2D-CGD-O1D	-3.03	117.95	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	I	612	DD6	C9-C10-C11	-3.03	123.03	127.28
22	A	852	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
22	B	813	CLA	C3B-C4B-NB	-3.03	107.83	110.53
22	W	403	CLA	C3B-C4B-NB	-3.03	107.83	110.53
22	A	801	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
31	U	408	CHL	CHA-C1A-C2A	-3.03	126.19	133.31
24	T	613	DD6	O1-C20-C19	-3.03	110.65	113.49
22	A	830	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
24	L	413	DD6	C15-C14-C13	-3.03	119.59	125.99
24	X	416	DD6	C3-C2-C1	-3.02	123.04	127.28
22	A	837	CLA	C3B-C4B-NB	-3.02	107.83	110.53
22	A	814	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
21	B	843	BCR	C33-C5-C6	-3.02	121.19	124.48
22	L	412	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
22	A	825	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
22	A	823	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
22	B	834	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
22	P	611	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
22	T	604	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
22	L	408	CLA	C6-C5-C3	-3.02	106.12	113.47
24	X	415	DD6	C3-C2-C1	-3.01	123.05	127.28
22	T	601	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
21	A	851	BCR	C29-C30-C25	3.01	114.82	110.44
22	O	312	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
24	A	859	DD6	C9-C10-C11	-3.01	123.05	127.28
24	G	612	DD6	C15-C14-C13	-3.01	119.62	125.99
22	F	405	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
22	J	102	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
22	Q	605	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
22	A	817	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
22	A	809	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
22	G	602	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
22	U	406	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
22	X	404	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
24	O	317	DD6	O1-C20-C21	-3.00	111.70	115.05
22	I	602	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
22	K	604	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
22	P	606	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
22	L	407	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
22	W	403	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
21	B	843	BCR	C27-C26-C25	-2.99	118.66	122.70
22	T	610	CLA	O2D-CGD-O1D	-2.99	118.02	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	U	415	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
22	L	406	CLA	C3B-C4B-NB	-2.99	107.86	110.53
24	P	613	DD6	C9-C10-C11	-2.99	123.08	127.28
22	A	807	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	B	841	DD6	C15-C14-C13	-2.99	119.68	125.99
22	B	823	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
22	G	605	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
31	V	606	CHL	CHA-C1A-C2A	-2.99	126.30	133.31
22	A	826	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
22	A	834	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
22	L	417	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
22	B	838	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
24	P	612	DD6	C-C1-C2	-2.98	117.99	122.82
22	W	409	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	B	809	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	S	601	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	G	609	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	T	602	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	W	404	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	A	842	CLA	CAA-C2A-C3A	-2.98	104.95	113.00
22	T	605	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	K	603	CLA	C3B-C4B-NB	-2.98	107.87	110.53
22	B	859	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
22	S	615	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
22	L	409	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
22	N	607	CLA	C3B-C4B-NB	-2.97	107.88	110.53
22	Q	610	CLA	C3B-C4B-NB	-2.97	107.88	110.53
22	B	825	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
22	B	826	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
22	N	603	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
24	F	406	DD6	C25-C24-C1	-2.97	118.22	126.36
22	B	810	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
22	B	829	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
22	N	604	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
22	W	405	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
22	H	309	CLA	C3B-C4B-NB	-2.97	107.88	110.53
22	B	803	CLA	C3B-C4B-NB	-2.97	107.88	110.53
24	R	613	DD6	C37-C36-C35	2.96	119.87	114.42
24	P	612	DD6	C7-C6-C5	-2.96	118.01	122.82
22	V	602	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
22	N	610	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
22	W	419	CLA	O2D-CGD-O1D	-2.96	118.09	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	403	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	R	606	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	K	617	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	T	603	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	V	615	DD6	O1-C15-C14	-2.96	108.41	116.88
22	H	306	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	A	809	CLA	C3B-C4B-NB	-2.95	107.89	110.53
22	U	413	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
21	A	850	BCR	C7-C8-C9	-2.95	121.87	126.23
22	A	837	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
21	B	801	BCR	C3-C4-C5	-2.95	108.79	114.06
22	H	311	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
22	A	831	CLA	O2D-CGD-CBD	2.95	116.39	111.23
24	V	615	DD6	O1-C20-C19	-2.95	110.73	113.49
22	G	604	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
24	P	612	DD6	C8-C6-C5	2.95	123.65	119.01
24	W	418	DD6	O1-C15-C14	-2.95	108.43	116.88
22	B	816	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	K	611	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	X	419	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	Q	603	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	Q	613	CLA	C3B-C4B-NB	-2.94	107.90	110.53
21	B	843	BCR	C2-C1-C6	2.94	114.72	110.44
22	L	406	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	X	409	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	X	408	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
24	G	612	DD6	C9-C10-C11	-2.94	123.15	127.28
22	U	409	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	W	410	CLA	C3B-C4B-NB	-2.94	107.90	110.53
24	I	612	DD6	C15-C14-C13	-2.94	119.77	125.99
22	B	821	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
21	B	801	BCR	C24-C23-C22	-2.94	121.89	126.23
22	O	306	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	S	602	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
22	G	607	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	K	613	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
24	Q	614	DD6	C9-C10-C11	-2.94	123.16	127.28
22	B	833	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	V	613	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	K	612	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	U	406	CLA	C3B-C4B-NB	-2.94	107.91	110.53
22	K	603	CLA	O2D-CGD-O1D	-2.94	118.13	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	820	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
24	X	401	DD6	C15-C14-C13	-2.93	119.79	125.99
22	B	822	CLA	C3B-C4B-NB	-2.93	107.91	110.53
22	S	603	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	U	412	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
21	B	845	BCR	C15-C16-C17	-2.93	117.52	123.52
22	I	604	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	A	812	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	O	315	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	K	614	DD6	C37-C36-C35	2.93	119.81	114.42
22	O	311	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
22	T	609	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
22	K	605	CLA	C3B-C4B-NB	-2.93	107.92	110.53
22	U	420	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
21	M	101	BCR	C27-C26-C25	-2.92	118.75	122.70
22	A	813	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
24	A	858	DD6	O1-C20-C19	-2.92	110.75	113.49
22	A	818	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	K	610	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	O	310	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
28	B	852	LMG	O6-C1-O1	-2.92	103.14	110.04
22	H	309	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	I	607	CLA	C3B-C4B-NB	-2.92	107.93	110.53
22	Q	608	CLA	C3B-C4B-NB	-2.92	107.93	110.53
22	L	405	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	G	605	CLA	C3B-C4B-NB	-2.92	107.93	110.53
24	Q	615	DD6	O1-C20-C21	-2.92	111.79	115.05
22	A	836	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	A	836	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	B	837	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	R	603	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	Q	606	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	A	832	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	B	818	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	B	802	CLA	O2A-CGA-O1A	-2.91	116.34	123.63
22	G	608	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	H	305	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	L	403	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	V	601	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	V	610	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	P	604	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
22	R	604	CLA	O2D-CGD-O1D	-2.91	118.19	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	610	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
22	O	314	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
22	V	612	CLA	C3B-C4B-NB	-2.91	107.94	110.53
22	K	609	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	W	411	CLA	C3B-C4B-NB	-2.90	107.94	110.53
24	N	613	DD6	C21-C20-C15	-2.90	117.52	122.30
22	I	606	CLA	C3B-C4B-NB	-2.90	107.94	110.53
21	B	801	BCR	C15-C16-C17	-2.90	117.58	123.52
24	K	614	DD6	C9-C10-C11	-2.90	123.21	127.28
22	A	811	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
22	V	609	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	W	412	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	W	413	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	F	404	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
22	U	404	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
22	X	405	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
22	H	307	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
23	A	843	PQN	C14-C13-C15	2.90	120.26	115.23
22	N	611	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	A	810	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	U	415	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	H	314	DD6	O1-C20-C19	-2.89	110.78	113.49
22	O	306	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	I	613	DD6	O1-C15-C14	-2.89	108.59	116.88
22	T	602	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	V	617	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	X	410	CLA	C3B-C4B-NB	-2.89	107.95	110.53
27	J	104	LMU	C6B-C5B-C4B	-2.89	109.58	113.53
22	Q	606	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	U	412	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	H	303	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	S	608	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	R	615	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	Q	614	DD6	C15-C14-C13	-2.89	119.89	125.99
22	N	602	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
22	A	804	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
24	X	416	DD6	C21-C20-C15	-2.88	117.56	122.30
22	W	414	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	L	411	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	Q	611	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	Q	601	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	B	820	CLA	CHB-C4A-NA	2.88	128.56	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	306	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
22	T	611	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
22	U	410	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
22	T	606	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
24	A	859	DD6	O1-C15-C14	-2.88	108.64	116.88
22	Q	609	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	L	404	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
22	O	308	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
22	W	413	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
22	H	303	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	P	605	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	X	407	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	S	608	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	N	611	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	T	606	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	I	610	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	U	403	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	A	822	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	U	411	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	G	601	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
22	G	611	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
21	A	851	BCR	C34-C9-C10	-2.87	118.17	122.82
22	Q	601	CLA	C3B-C4B-NB	-2.87	107.97	110.53
24	Q	615	DD6	C10-C9-C8	-2.87	114.90	123.20
24	H	315	DD6	C4-C5-C6	-2.87	123.26	127.28
22	X	413	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
22	H	310	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
22	W	412	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
22	A	827	CLA	C3B-C4B-NB	-2.86	107.97	110.53
22	X	402	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
22	O	309	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
24	P	613	DD6	C15-C14-C13	-2.86	119.94	125.99
24	N	612	DD6	C21-C20-C15	-2.86	117.59	122.30
22	G	608	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	A	807	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	V	607	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	A	851	BCR	C38-C26-C27	2.86	119.69	113.60
22	B	859	CLA	CAA-C2A-C3A	-2.86	105.28	113.00
22	F	403	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	H	307	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	A	822	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
22	H	312	CLA	O2D-CGD-O1D	-2.86	118.29	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	311	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	U	420	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	W	411	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
24	A	859	DD6	C4-C3-C2	-2.85	117.68	123.52
22	A	842	CLA	O2A-CGA-O1A	-2.85	116.49	123.63
22	I	605	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	L	410	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	X	407	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	B	837	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	S	615	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	T	611	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	U	411	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	Q	612	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	B	859	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	G	606	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	B	805	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	A	843	PQN	C11-C3-C2	-2.85	120.00	124.89
22	I	607	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	S	604	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	V	608	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	W	410	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
22	P	602	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
22	Q	612	CLA	C3B-C4B-NB	-2.85	107.99	110.53
22	A	824	CLA	C3B-C4B-NB	-2.85	107.99	110.53
24	F	406	DD6	C21-C20-C15	-2.84	117.62	122.30
22	N	609	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
22	W	404	CLA	C3B-C4B-NB	-2.84	107.99	110.53
24	T	613	DD6	C15-C14-C13	-2.84	119.98	125.99
22	B	812	CLA	C3B-C4B-NB	-2.84	107.99	110.53
22	Q	617	CLA	C3B-C4B-NB	-2.84	107.99	110.53
22	T	608	CLA	C3B-C4B-NB	-2.84	107.99	110.53
27	O	322	LMU	O1B-C4'-C3'	2.84	114.45	107.23
22	B	829	CLA	C3B-C4B-NB	-2.84	108.00	110.53
22	S	607	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
22	V	611	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
22	R	608	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
22	V	604	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
22	V	602	CLA	C3B-C4B-NB	-2.84	108.00	110.53
22	V	609	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
22	L	402	CLA	C3B-C4B-NB	-2.83	108.00	110.53
24	K	615	DD6	O1-C20-C19	-2.83	110.84	113.49
22	A	815	CLA	O2D-CGD-O1D	-2.83	118.33	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	415	DD6	C21-C20-C15	-2.83	117.64	122.30
22	L	409	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	X	412	CLA	C3B-C4B-NB	-2.83	108.00	110.53
24	G	613	DD6	C37-C36-C31	-2.83	118.87	124.16
22	I	608	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
22	W	402	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
22	W	406	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
22	R	611	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
24	T	612	DD6	O1-C20-C19	-2.83	110.84	113.49
24	A	847	DD6	C14-C13-C11	-2.83	121.14	125.53
22	H	318	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
22	U	401	CLA	C3B-C4B-NB	-2.82	108.01	110.53
22	R	609	CLA	CAA-C2A-C3A	-2.82	109.75	116.23
22	F	403	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	R	613	DD6	O1-C15-C14	-2.82	108.79	116.88
22	K	605	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	N	607	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	P	604	CLA	C3B-C4B-NB	-2.82	108.01	110.53
22	S	605	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	U	417	DD6	C9-C10-C11	-2.82	123.33	127.28
22	B	822	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	S	606	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	V	603	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	H	315	DD6	O1-C15-C14	-2.82	108.81	116.88
22	N	610	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	V	610	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	B	825	CLA	C3B-C4B-NB	-2.82	108.02	110.53
22	L	417	CLA	C3B-C4B-NB	-2.82	108.02	110.53
22	N	608	CLA	C3B-C4B-NB	-2.82	108.02	110.53
22	R	605	CLA	C3B-C4B-NB	-2.82	108.02	110.53
22	R	608	CLA	C3B-C4B-NB	-2.82	108.02	110.53
22	K	602	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
24	K	614	DD6	O1-C15-C14	-2.81	108.82	116.88
22	K	606	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
22	B	839	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	K	613	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	P	609	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
21	M	101	BCR	C28-C27-C26	-2.81	109.04	114.06
22	T	604	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	U	410	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	A	823	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	X	403	CLA	O2D-CGD-O1D	-2.81	118.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	609	CLA	C3B-C4B-NB	-2.81	108.03	110.53
22	L	407	CLA	C3B-C4B-NB	-2.81	108.03	110.53
22	O	305	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
22	W	414	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
26	K	619	LHG	O8-C23-C24	2.80	120.38	111.83
22	G	607	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	O	314	CLA	C3B-C4B-NB	-2.80	108.03	110.53
28	Q	602	LMG	O6-C1-O1	-2.80	103.42	110.04
24	J	105	DD6	C14-C13-C11	-2.80	121.18	125.53
22	X	411	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
28	L	401	LMG	O6-C1-O1	-2.80	103.43	110.04
22	R	607	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
22	R	609	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
22	N	610	CLA	CHB-C4A-NA	2.80	128.44	124.40
33	A	802	CL0	O2A-CGA-O1A	-2.80	116.63	123.63
22	L	408	CLA	C1-C2-C3	-2.80	121.61	126.20
22	R	602	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
21	B	844	BCR	C38-C26-C25	-2.80	121.43	124.48
24	T	612	DD6	O1-C15-C14	-2.80	108.86	116.88
26	B	848	LHG	O8-C23-C24	2.80	120.37	111.83
22	G	610	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
28	K	618	LMG	O6-C1-O1	-2.80	103.44	110.04
22	H	308	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
22	B	839	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
22	A	841	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
24	W	416	DD6	C14-C13-C11	-2.79	121.20	125.53
22	R	605	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
22	A	803	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
22	B	816	CLA	C3B-C4B-NB	-2.79	108.04	110.53
24	Q	615	DD6	C37-C36-C35	2.79	119.55	114.42
22	R	610	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	B	808	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	N	602	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	R	615	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	V	611	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	O	313	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	H	304	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	O	317	DD6	O1-C15-C14	-2.79	108.89	116.88
26	O	318	LHG	O8-C23-C24	2.79	120.33	111.83
22	Q	609	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
22	G	608	CLA	C11-C10-C8	-2.79	106.71	115.97
22	I	609	CLA	O2D-CGD-O1D	-2.79	118.43	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I	614	LMG	O6-C1-O1	-2.78	103.47	110.04
22	N	606	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
22	S	604	CLA	C3B-C4B-NB	-2.78	108.05	110.53
28	I	615	LMG	O6-C1-O1	-2.78	103.47	110.04
21	B	801	BCR	C11-C12-C13	-2.78	118.73	126.36
22	G	610	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	Q	610	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
24	P	612	DD6	C12-C11-C10	-2.78	118.31	122.82
22	B	809	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	S	606	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	W	406	CLA	C3B-C4B-NB	-2.78	108.05	110.53
31	X	406	CHL	C3D-C4D-CHA	2.78	112.77	108.54
22	P	607	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
22	L	403	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	W	409	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	A	808	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	S	612	DD6	O1-C20-C19	-2.78	110.89	113.49
22	X	412	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
22	K	609	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
22	H	302	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
22	Q	607	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
22	S	609	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	S	610	CLA	C3B-C4B-NB	-2.77	108.06	110.53
21	B	801	BCR	C38-C26-C25	-2.77	121.46	124.48
24	S	611	DD6	C37-C36-C35	2.77	119.51	114.42
24	S	612	DD6	O1-C15-C14	-2.77	108.94	116.88
24	H	315	DD6	C37-C36-C31	-2.77	118.99	124.16
24	N	613	DD6	C37-C36-C31	-2.77	118.99	124.16
22	T	607	CLA	C3B-C4B-NB	-2.76	108.06	110.53
22	N	601	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
22	U	414	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
26	O	321	LHG	O8-C23-C24	2.76	120.26	111.83
22	A	828	CLA	C3B-C4B-NB	-2.76	108.06	110.53
33	A	802	CL0	C4D-CHA-CBD	-2.76	106.18	108.97
22	B	833	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	U	401	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
21	B	843	BCR	C34-C9-C10	-2.76	118.35	122.82
22	I	604	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	T	607	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
22	W	419	CLA	C3B-C4B-NB	-2.75	108.07	110.53
21	B	843	BCR	C38-C26-C27	2.75	119.46	113.60
24	A	847	DD6	C4-C3-C2	-2.75	117.89	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	418	DD6	C37-C36-C35	2.75	119.48	114.42
22	A	817	CLA	C3B-C4B-NB	-2.75	108.07	110.53
22	N	611	CLA	C3A-C2A-C1A	-2.75	103.49	106.30
22	V	608	CLA	C3B-C4B-NB	-2.75	108.08	110.53
22	O	319	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
27	L	420	LMU	C1B-O1B-C4'	-2.75	111.46	117.98
22	B	810	CLA	C3B-C4B-NB	-2.75	108.08	110.53
21	J	103	BCR	C20-C21-C22	-2.75	123.42	127.28
24	T	612	DD6	C4-C5-C6	-2.75	123.42	127.28
24	X	401	DD6	C14-C13-C11	-2.75	121.27	125.53
24	X	415	DD6	O1-C15-C14	-2.75	109.00	116.88
26	H	316	LHG	O8-C23-C24	2.75	120.21	111.83
22	I	606	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
22	I	601	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
22	A	821	CLA	C1-C2-C3	-2.75	121.70	126.20
22	A	829	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
23	B	840	PQN	C14-C13-C15	2.75	119.99	115.23
22	I	605	CLA	C3B-C4B-NB	-2.75	108.08	110.53
22	A	839	CLA	CHB-C4A-NA	2.75	128.36	124.40
26	U	419	LHG	O8-C23-C24	2.74	120.20	111.83
22	N	604	CLA	C3B-C4B-NB	-2.74	108.08	110.53
22	Q	617	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
22	S	614	CLA	C3B-C4B-NB	-2.74	108.08	110.53
22	N	608	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
22	B	832	CLA	C3B-C4B-NB	-2.74	108.08	110.53
21	B	845	BCR	C20-C21-C22	-2.74	123.44	127.28
22	G	611	CLA	C3B-C4B-NB	-2.74	108.09	110.53
22	P	605	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
22	A	806	CLA	C3B-C4B-NB	-2.74	108.09	110.53
22	L	404	CLA	C3B-C4B-NB	-2.73	108.09	110.53
22	P	610	CLA	CHB-C4A-NA	2.73	128.35	124.40
22	H	311	CLA	C3B-C4B-NB	-2.73	108.09	110.53
24	V	615	DD6	C37-C36-C35	2.73	119.44	114.42
28	T	616	LMG	O6-C1-O1	-2.73	103.59	110.04
24	L	414	DD6	O1-C20-C21	-2.73	112.00	115.05
22	L	411	CLA	C3B-C4B-NB	-2.73	108.09	110.53
22	T	605	CLA	C3B-C4B-NB	-2.73	108.09	110.53
22	A	839	CLA	O1D-CGD-CBD	2.73	129.90	124.52
22	V	612	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
28	J	101	LMG	O6-C1-O1	-2.73	103.60	110.04
22	L	402	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
22	I	610	CLA	C3B-C4B-NB	-2.73	108.10	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	605	CLA	C3B-C4B-NB	-2.73	108.10	110.53
24	A	858	DD6	C21-C20-C15	-2.73	117.81	122.30
22	A	821	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	S	613	LHG	O8-C23-C24	2.72	120.14	111.83
22	Q	608	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
22	I	602	CLA	C3B-C4B-NB	-2.72	108.10	110.53
31	W	422	CHL	C3D-C4D-CHA	2.72	112.67	108.54
24	N	612	DD6	O1-C15-C14	-2.72	109.09	116.88
22	O	319	CLA	C3B-C4B-NB	-2.72	108.10	110.53
26	P	601	LHG	O8-C23-C24	2.72	120.12	111.83
22	B	804	CLA	C3B-C4B-NB	-2.72	108.10	110.53
22	A	813	CLA	C3B-C4B-NB	-2.72	108.10	110.53
24	F	406	DD6	C9-C10-C11	-2.72	123.47	127.28
22	H	302	CLA	C3B-C4B-NB	-2.72	108.11	110.53
24	G	612	DD6	C37-C36-C31	-2.71	119.08	124.16
21	B	845	BCR	C2-C1-C6	2.71	114.38	110.44
24	K	615	DD6	C15-C14-C13	-2.71	120.25	125.99
22	O	305	CLA	C1-C2-C3	-2.71	122.37	126.76
24	G	613	DD6	C37-C36-C35	2.71	119.41	114.42
26	Q	616	LHG	O8-C23-C24	2.71	120.10	111.83
22	R	601	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
22	X	417	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
24	U	417	DD6	C15-C14-C13	-2.71	120.27	125.99
28	A	855	LMG	O6-C1-O1	-2.70	103.65	110.04
22	B	814	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	X	415	DD6	C9-C10-C11	-2.70	123.49	127.28
22	G	604	CLA	C3B-C4B-NB	-2.70	108.12	110.53
26	L	416	LHG	O8-C23-C24	2.70	120.07	111.83
22	B	808	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
22	O	305	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	F	406	DD6	C3-C2-C1	-2.70	123.49	127.28
22	T	610	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	X	402	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	X	416	DD6	C7-C6-C5	-2.70	118.45	122.82
22	P	606	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	A	811	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	G	606	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
24	W	417	DD6	C15-C14-C13	-2.70	120.29	125.99
22	U	409	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	X	411	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	X	416	DD6	O1-C20-C21	-2.69	112.04	115.05
22	L	405	CLA	C3B-C4B-NB	-2.69	108.13	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	414	DD6	O1-C15-C14	-2.69	109.17	116.88
24	I	613	DD6	C3-C4-C5	-2.69	118.01	123.52
24	A	847	DD6	C15-C14-C13	-2.69	120.31	125.99
22	G	601	CLA	C3B-C4B-NB	-2.69	108.13	110.53
24	P	613	DD6	C3-C4-C5	-2.69	118.02	123.52
24	Q	615	DD6	C3-C4-C5	-2.69	118.02	123.52
24	U	416	DD6	C14-C13-C11	-2.69	121.36	125.53
24	X	401	DD6	C21-C20-C15	-2.69	117.88	122.30
22	A	825	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	A	830	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
22	B	823	CLA	C3B-C4B-NB	-2.69	108.13	110.53
26	T	614	LHG	O8-C23-C24	2.68	120.02	111.83
22	R	601	CLA	C3B-C4B-NB	-2.68	108.13	110.53
27	A	854	LMU	C1B-O1B-C4'	-2.68	111.62	117.98
24	X	414	DD6	O1-C20-C19	-2.68	110.98	113.49
24	A	858	DD6	C8-C6-C5	2.68	123.23	119.01
22	X	409	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	K	610	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	V	601	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	X	408	CLA	C3B-C4B-NB	-2.68	108.14	110.53
24	B	841	DD6	C25-C24-C1	-2.68	119.01	126.36
21	A	850	BCR	C11-C10-C9	-2.68	123.52	127.28
31	W	408	CHL	C3D-C4D-CHA	2.68	112.61	108.54
24	P	612	DD6	C24-C1-C2	2.68	123.22	119.01
28	N	615	LMG	O6-C1-O1	-2.68	103.72	110.04
22	K	602	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	U	414	CLA	C3B-C4B-NB	-2.68	108.14	110.53
26	N	614	LHG	O8-C23-C24	2.67	119.99	111.83
26	A	846	LHG	O8-C23-C24	2.67	119.99	111.83
28	H	317	LMG	O6-C1-O1	-2.67	103.72	110.04
22	O	308	CLA	C3B-C4B-NB	-2.67	108.14	110.53
22	P	602	CLA	C3B-C4B-NB	-2.67	108.14	110.53
26	O	323	LHG	O8-C23-C24	2.67	119.98	111.83
24	G	613	DD6	C9-C10-C11	-2.67	123.54	127.28
22	T	601	CLA	C3B-C4B-NB	-2.67	108.15	110.53
24	R	612	DD6	C14-C13-C11	-2.67	121.39	125.53
22	P	611	CLA	CHB-C4A-NA	2.67	128.25	124.40
31	W	407	CHL	C3D-C4D-CHA	2.67	112.59	108.54
26	R	614	LHG	O8-C23-C24	2.66	119.96	111.83
22	I	611	CLA	C3B-C4B-NB	-2.66	108.15	110.53
22	J	102	CLA	C3B-C4B-NB	-2.66	108.15	110.53
22	K	611	CLA	C3B-C4B-NB	-2.66	108.15	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W	420	LHG	O8-C23-C24	2.66	119.95	111.83
22	Q	618	CLA	C3B-C4B-NB	-2.66	108.15	110.53
22	A	838	CLA	C3B-C4B-NB	-2.66	108.15	110.53
22	I	601	CLA	C3B-C4B-NB	-2.66	108.16	110.53
24	G	613	DD6	O1-C15-C14	-2.66	109.26	116.88
26	N	616	LHG	O8-C23-C24	2.66	119.94	111.83
24	R	613	DD6	C25-C24-C1	-2.66	119.07	126.36
24	W	416	DD6	C21-C20-C15	-2.66	117.93	122.30
22	O	310	CLA	CHB-C4A-NA	2.66	128.24	124.40
31	V	605	CHL	C3D-C4D-CHA	2.66	112.58	108.54
21	A	849	BCR	C33-C5-C4	2.66	119.26	113.60
24	U	417	DD6	C21-C20-C15	-2.66	117.93	122.30
24	F	406	DD6	O1-C15-C14	-2.66	109.27	116.88
26	K	616	LHG	O8-C23-C24	2.66	119.94	111.83
24	I	612	DD6	O1-C15-C14	-2.66	109.27	116.88
22	A	815	CLA	C3B-C4B-NB	-2.66	108.16	110.53
28	K	601	LMG	O6-C1-O1	-2.65	103.77	110.04
24	G	612	DD6	O1-C15-C14	-2.65	109.27	116.88
24	P	612	DD6	C37-C36-C31	-2.65	119.20	124.16
22	A	833	CLA	C3B-C4B-NB	-2.65	108.16	110.53
22	B	824	CLA	C3B-C4B-NB	-2.65	108.16	110.53
26	A	845	LHG	O8-C23-C24	2.65	119.92	111.83
22	G	602	CLA	C3B-C4B-NB	-2.65	108.16	110.53
22	H	312	CLA	C3B-C4B-NB	-2.65	108.16	110.53
22	R	603	CLA	C3B-C4B-NB	-2.65	108.16	110.53
22	K	607	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
22	S	610	CLA	CHB-C4A-NA	2.65	128.22	124.40
22	K	606	CLA	C3B-C4B-NB	-2.65	108.16	110.53
22	A	839	CLA	C3B-C4B-NB	-2.65	108.16	110.53
24	U	416	DD6	O1-C15-C14	-2.65	109.28	116.88
22	P	610	CLA	C3B-C4B-NB	-2.65	108.17	110.53
22	N	605	CLA	C3B-C4B-NB	-2.65	108.17	110.53
22	A	831	CLA	C3B-C4B-NB	-2.65	108.17	110.53
21	B	843	BCR	C37-C22-C21	-2.65	118.53	122.82
22	B	859	CLA	CHB-C4A-NA	2.64	128.22	124.40
27	J	104	LMU	C1B-O1B-C4'	-2.64	111.71	117.98
24	K	615	DD6	C9-C10-C11	-2.64	123.57	127.28
31	U	407	CHL	C3D-C4D-CHA	2.64	112.56	108.54
26	X	420	LHG	O8-C23-C24	2.64	119.89	111.83
22	Q	613	CLA	CHB-C4A-NA	2.64	128.21	124.40
22	I	607	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
24	P	613	DD6	C25-C26-C27	-2.64	119.23	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	807	CLA	C3B-C4B-NB	-2.64	108.17	110.53
22	S	601	CLA	C3B-C4B-NB	-2.64	108.17	110.53
21	B	843	BCR	C8-C9-C10	2.64	123.16	119.01
24	W	416	DD6	C15-C14-C13	-2.64	120.42	125.99
24	X	416	DD6	C13-C11-C10	-2.64	114.86	119.01
22	X	419	CLA	C3B-C4B-NB	-2.64	108.18	110.53
24	Q	614	DD6	O1-C15-C14	-2.64	109.33	116.88
24	S	611	DD6	C9-C10-C11	-2.63	123.58	127.28
24	Q	615	DD6	O1-C15-C14	-2.63	109.33	116.88
24	P	613	DD6	O1-C20-C21	-2.63	112.11	115.05
22	B	805	CLA	C3B-C4B-NB	-2.63	108.18	110.53
22	A	834	CLA	C3B-C4B-NB	-2.63	108.18	110.53
22	B	821	CLA	C3B-C4B-NB	-2.63	108.18	110.53
22	O	310	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	R	612	DD6	O1-C15-C14	-2.63	109.35	116.88
22	S	607	CLA	C3B-C4B-NB	-2.63	108.19	110.53
28	U	423	LMG	O6-C1-O1	-2.63	103.84	110.04
22	A	842	CLA	C3B-C4B-NB	-2.63	108.19	110.53
21	B	843	BCR	C29-C30-C25	2.62	114.25	110.44
22	N	601	CLA	C3B-C4B-NB	-2.62	108.19	110.53
22	K	606	CLA	C1-C2-C3	-2.62	122.52	126.76
22	X	408	CLA	CHB-C4A-NA	2.62	128.18	124.40
22	L	412	CLA	C3B-C4B-NB	-2.62	108.19	110.53
22	V	613	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	F	406	DD6	C-C1-C2	-2.62	118.57	122.82
24	L	415	DD6	C15-C14-C13	-2.62	120.46	125.99
22	B	828	CLA	CMB-C2B-C1B	-2.62	121.44	125.42
22	A	801	CLA	O1D-CGD-CBD	2.61	129.67	124.52
22	Q	603	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	R	607	CLA	C3B-C4B-NB	-2.61	108.20	110.53
24	O	316	DD6	C37-C36-C31	-2.61	119.28	124.16
22	V	617	CLA	CHB-C4A-NA	2.61	128.17	124.40
24	I	613	DD6	C21-C20-C15	-2.61	118.01	122.30
24	F	406	DD6	C25-C26-C27	-2.61	119.31	126.61
24	U	417	DD6	O1-C15-C14	-2.61	109.41	116.88
22	O	309	CLA	CHB-C4A-NA	2.61	128.16	124.40
24	T	612	DD6	C37-C36-C31	-2.61	119.28	124.16
24	W	418	DD6	C21-C20-C15	-2.61	118.01	122.30
22	H	318	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	H	308	CLA	C3B-C4B-NB	-2.60	108.20	110.53
22	V	609	CLA	C1-C2-C3	-2.60	121.93	126.20
24	N	612	DD6	O1-C20-C19	-2.60	111.05	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	305	CLA	C3B-C4B-NB	-2.60	108.21	110.53
24	V	615	DD6	C21-C20-C15	-2.60	118.02	122.30
21	A	851	BCR	C8-C9-C10	2.60	123.10	119.01
24	A	847	DD6	C3-C2-C1	-2.60	123.63	127.28
21	M	101	BCR	C38-C26-C27	2.60	119.14	113.60
24	K	615	DD6	O1-C15-C14	-2.60	109.43	116.88
23	B	840	PQN	C11-C12-C13	-2.60	122.35	126.83
22	P	608	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	P	610	CLA	O2D-CGD-CBD	2.60	115.77	111.23
24	W	418	DD6	C9-C10-C11	-2.59	123.64	127.28
22	A	819	CLA	O2D-CGD-CBD	2.59	115.77	111.23
24	J	105	DD6	C37-C36-C31	-2.59	119.31	124.16
22	X	417	CLA	C1-C2-C3	-2.59	122.57	126.76
24	O	317	DD6	C10-C9-C8	-2.59	115.69	123.20
22	G	602	CLA	C1-C2-C3	-2.59	121.95	126.20
26	O	324	LHG	O8-C23-C24	2.59	119.73	111.83
22	H	313	CLA	C3B-C4B-NB	-2.59	108.22	110.53
22	T	609	CLA	C3B-C4B-NB	-2.59	108.22	110.53
22	U	409	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	A	841	CLA	C3B-C4B-NB	-2.59	108.22	110.53
22	O	310	CLA	C1-C2-C3	-2.59	121.96	126.20
26	B	851	LHG	O8-C23-C24	2.59	119.73	111.83
22	H	310	CLA	C3B-C4B-NB	-2.59	108.22	110.53
22	R	602	CLA	C3B-C4B-NB	-2.59	108.22	110.53
31	U	408	CHL	C3D-C4D-CHA	2.59	112.47	108.54
22	X	404	CLA	C3B-C4B-NB	-2.58	108.22	110.53
22	A	805	CLA	C3B-C4B-NB	-2.58	108.22	110.53
22	B	824	CLA	CHB-C4A-NA	2.58	128.13	124.40
22	F	405	CLA	C3B-C4B-NB	-2.58	108.22	110.53
25	O	304	DGD	O6D-C1D-C2D	-2.58	105.07	110.37
24	B	841	DD6	C28-C27-C26	-2.58	119.17	124.18
24	H	314	DD6	C37-C36-C31	-2.58	119.34	124.16
22	B	805	CLA	CHB-C4A-NA	2.58	128.12	124.40
24	F	406	DD6	C37-C36-C31	-2.58	119.34	124.16
24	G	613	DD6	C3-C4-C5	-2.58	118.25	123.52
22	O	313	CLA	C3B-C4B-NB	-2.58	108.23	110.53
28	G	616	LMG	O6-C1-O1	-2.57	103.96	110.04
22	B	824	CLA	O2D-CGD-CBD	2.57	115.73	111.23
22	U	403	CLA	CHB-C4A-NA	2.57	128.11	124.40
24	J	105	DD6	C9-C8-C6	-2.57	119.32	126.36
22	B	834	CLA	C3B-C4B-NB	-2.57	108.24	110.53
22	W	402	CLA	C3B-C4B-NB	-2.57	108.24	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	604	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	B	828	CLA	C3B-C4B-NB	-2.57	108.24	110.53
22	B	815	CLA	C3B-C4B-NB	-2.57	108.24	110.53
22	R	610	CLA	C3B-C4B-NB	-2.56	108.24	110.53
21	J	103	BCR	C38-C26-C25	-2.56	121.69	124.48
22	V	607	CLA	C3B-C4B-NB	-2.56	108.24	110.53
21	B	845	BCR	C16-C17-C18	-2.56	123.69	127.28
24	W	417	DD6	O1-C15-C14	-2.56	109.54	116.88
22	B	804	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	F	404	CLA	CHB-C4A-NA	2.56	128.09	124.40
21	B	846	BCR	C10-C11-C12	-2.56	115.78	123.20
22	A	805	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
22	V	613	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	A	838	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	X	405	CLA	C3B-C4B-NB	-2.56	108.25	110.53
24	V	614	DD6	C37-C36-C31	-2.56	119.37	124.16
22	B	809	CLA	CHB-C4A-NA	2.56	128.09	124.40
28	H	322	LMG	O6-C1-O1	-2.56	104.00	110.04
22	R	604	CLA	C3B-C4B-NB	-2.56	108.25	110.53
22	A	835	CLA	C3B-C4B-NB	-2.56	108.25	110.53
22	B	830	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
24	J	105	DD6	C28-C27-C26	-2.55	119.23	124.18
22	B	818	CLA	C3B-C4B-NB	-2.55	108.25	110.53
22	K	617	CLA	C3B-C4B-NB	-2.55	108.25	110.53
22	L	409	CLA	CHB-C4A-NA	2.55	128.08	124.40
22	A	811	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
22	N	609	CLA	C3B-C4B-NB	-2.55	108.26	110.53
22	U	404	CLA	C3B-C4B-NB	-2.55	108.26	110.53
24	R	613	DD6	C25-C26-C27	-2.54	119.50	126.61
22	A	844	CLA	C3B-C4B-NB	-2.54	108.26	110.53
22	B	811	CLA	C3B-C4B-NB	-2.54	108.26	110.53
22	L	404	CLA	CHB-C4A-NA	2.54	128.06	124.40
31	V	606	CHL	C3D-C4D-CHA	2.54	112.40	108.54
21	B	843	BCR	C23-C22-C21	2.54	123.00	119.01
26	G	614	LHG	O8-C23-C24	2.54	119.57	111.83
24	J	105	DD6	C25-C26-C27	-2.54	119.52	126.61
27	X	421	LMU	C1B-O1B-C4'	-2.53	111.97	117.98
22	T	607	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
24	P	613	DD6	C25-C24-C1	-2.53	119.42	126.36
24	L	413	DD6	C37-C36-C31	-2.53	119.42	124.16
22	P	602	CLA	CHB-C4A-NA	2.53	128.05	124.40
21	A	850	BCR	C28-C27-C26	-2.53	109.54	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	613	DD6	C14-C13-C11	-2.53	121.61	125.53
22	B	811	CLA	CHB-C4A-NA	2.53	128.04	124.40
21	B	842	BCR	C8-C7-C6	-2.52	120.26	127.00
22	B	825	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	A	824	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	L	410	CLA	C3B-C4B-NB	-2.52	108.28	110.53
22	I	605	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	A	836	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	N	605	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	A	805	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	P	611	CLA	C3B-C4B-NB	-2.52	108.28	110.53
22	K	611	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	A	820	CLA	C1-C2-C3	-2.52	122.08	126.20
24	W	417	DD6	C9-C10-C11	-2.51	123.75	127.28
28	I	615	LMG	C3-C4-C5	-2.51	107.55	110.76
24	U	417	DD6	C37-C36-C35	2.51	119.04	114.42
24	R	612	DD6	C37-C36-C31	-2.51	119.46	124.16
22	A	825	CLA	CHB-C4A-NA	2.51	128.03	124.40
28	K	622	LMG	O6-C1-O1	-2.51	104.11	110.04
22	H	309	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	W	416	DD6	C37-C36-C31	-2.51	119.47	124.16
22	P	603	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
22	H	307	CLA	CHB-C4A-NA	2.51	128.02	124.40
23	A	843	PQN	C11-C12-C13	-2.51	122.51	126.83
22	L	405	CLA	CHB-C4A-NA	2.50	128.01	124.40
21	B	846	BCR	C7-C8-C9	-2.50	122.53	126.23
24	S	611	DD6	C3-C4-C5	-2.50	118.40	123.52
22	A	824	CLA	O2D-CGD-CBD	2.50	115.61	111.23
22	H	311	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	A	821	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	B	823	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	V	615	DD6	C37-C36-C31	-2.50	119.48	124.16
24	R	613	DD6	O1-C20-C19	-2.50	111.15	113.49
24	P	612	DD6	C21-C20-C15	-2.50	118.19	122.30
22	R	606	CLA	C3B-C4B-NB	-2.50	108.30	110.53
33	A	802	CL0	CMD-C2D-C3D	2.50	129.68	124.68
22	R	611	CLA	C3B-C4B-NB	-2.50	108.30	110.53
22	U	413	CLA	CHB-C4A-NA	2.50	128.00	124.40
24	L	414	DD6	C21-C20-C15	-2.50	118.19	122.30
22	O	315	CLA	C3B-C4B-NB	-2.50	108.30	110.53
24	A	859	DD6	C25-C26-C27	-2.49	119.64	126.61
22	L	406	CLA	CHB-C4A-NA	2.49	128.00	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	613	DD6	C21-C20-C15	-2.49	118.20	122.30
24	G	613	DD6	C21-C20-C15	-2.49	118.20	122.30
22	K	605	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	N	606	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	V	602	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	X	415	DD6	C21-C20-C15	-2.49	118.21	122.30
22	A	830	CLA	C3B-C4B-NB	-2.49	108.31	110.53
22	T	611	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	R	605	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	X	413	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	A	828	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	S	614	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	I	608	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	Q	603	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	Q	605	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	R	607	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	W	415	CLA	C3B-C4B-NB	-2.48	108.31	110.53
24	T	613	DD6	C9-C10-C11	-2.48	123.80	127.28
22	B	819	CLA	C3B-C4B-NB	-2.48	108.31	110.53
21	A	850	BCR	C38-C26-C27	2.48	118.88	113.60
22	N	602	CLA	CHB-C4A-NA	2.48	127.98	124.40
24	P	612	DD6	C37-C36-C35	2.48	118.98	114.42
22	W	403	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	A	826	CLA	C3B-C4B-NB	-2.48	108.32	110.53
27	U	421	LMU	C1B-O1B-C4'	-2.48	112.11	117.98
23	B	840	PQN	C11-C3-C2	-2.48	120.65	124.89
22	A	842	CLA	CHB-C4A-NA	2.48	127.97	124.40
28	B	856	LMG	C40-C39-C38	-2.47	101.86	114.37
22	G	608	CLA	CHB-C4A-NA	2.47	127.97	124.40
33	A	802	CL0	C1C-CHC-C4B	2.47	124.92	116.07
22	P	604	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	I	606	CLA	CHB-C4A-NA	2.47	127.97	124.40
24	A	847	DD6	C21-C20-C15	-2.47	118.23	122.30
22	A	815	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
27	B	857	LMU	C1B-O1B-C4'	-2.47	112.12	117.98
22	W	410	CLA	CHB-C4A-NA	2.47	127.97	124.40
24	O	316	DD6	O1-C15-C14	-2.47	109.80	116.88
22	B	804	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
21	B	844	BCR	C28-C27-C26	-2.47	109.65	114.06
22	X	402	CLA	CHB-C4A-NA	2.47	127.96	124.40
22	A	803	CLA	C1-C2-C3	-2.47	122.15	126.20
22	T	606	CLA	CHB-C4A-NA	2.47	127.96	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	S	611	DD6	C21-C20-C15	-2.47	118.24	122.30
22	A	826	CLA	CHB-C4A-NA	2.47	127.96	124.40
22	A	814	CLA	CHB-C4A-NA	2.46	127.96	124.40
24	L	413	DD6	C21-C20-C15	-2.46	118.25	122.30
27	K	620	LMU	C1-O1'-C1'	-2.46	109.47	113.68
22	A	839	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
22	U	412	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	L	402	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	O	311	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	O	316	DD6	C21-C20-C15	-2.46	118.25	122.30
22	T	603	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	L	414	DD6	C37-C36-C31	-2.46	119.56	124.16
22	N	610	CLA	C3B-C4B-NB	-2.46	108.33	110.53
22	K	613	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	V	607	CLA	CHB-C4A-NA	2.46	127.95	124.40
21	B	845	BCR	C21-C20-C19	-2.46	116.08	123.20
22	R	606	CLA	CHB-C4A-NA	2.46	127.95	124.40
22	N	603	CLA	CHB-C4A-NA	2.46	127.94	124.40
22	V	601	CLA	CHB-C4A-NA	2.46	127.94	124.40
24	U	416	DD6	C21-C20-C15	-2.46	118.26	122.30
22	G	601	CLA	CHB-C4A-NA	2.46	127.94	124.40
24	F	406	DD6	C19-C18-C17	2.46	115.38	110.79
22	B	829	CLA	CHB-C4A-NA	2.46	127.94	124.40
22	V	611	CLA	CHB-C4A-NA	2.46	127.94	124.40
24	Q	614	DD6	C21-C20-C15	-2.45	118.26	122.30
24	T	613	DD6	C37-C36-C35	2.45	118.93	114.42
22	O	312	CLA	CHB-C4A-NA	2.45	127.94	124.40
24	L	414	DD6	O1-C15-C14	-2.45	109.85	116.88
24	X	401	DD6	O1-C15-C14	-2.45	109.85	116.88
24	V	615	DD6	C28-C27-C26	-2.45	119.42	124.18
24	H	314	DD6	C21-C20-C15	-2.45	118.27	122.30
22	A	820	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
24	S	612	DD6	C21-C20-C15	-2.45	118.27	122.30
22	I	609	CLA	CHB-C4A-NA	2.45	127.94	124.40
22	L	411	CLA	CHB-C4A-NA	2.45	127.94	124.40
24	A	859	DD6	C25-C24-C1	-2.45	119.65	126.36
22	X	411	CLA	CHB-C4A-NA	2.45	127.93	124.40
22	A	808	CLA	CHB-C4A-NA	2.45	127.93	124.40
28	I	614	LMG	O1-C7-C8	-2.45	104.87	110.82
22	B	835	CLA	CHB-C4A-NA	2.45	127.93	124.40
22	X	405	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	I	613	DD6	C37-C36-C31	-2.45	119.58	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	843	PQN	C2M-C2-C3	-2.45	120.43	124.45
22	P	605	CLA	CHB-C4A-NA	2.45	127.93	124.40
22	Q	601	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	T	612	DD6	O1-C20-C21	-2.45	112.31	115.05
22	X	403	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	O	317	DD6	C21-C20-C15	-2.44	118.28	122.30
22	X	410	CLA	CHB-C4A-NA	2.44	127.93	124.40
22	V	604	CLA	C3B-C4B-NB	-2.44	108.35	110.53
24	W	418	DD6	C37-C36-C31	-2.44	119.59	124.16
22	A	811	CLA	CHB-C4A-NA	2.44	127.93	124.40
22	K	609	CLA	CHB-C4A-NA	2.44	127.93	124.40
28	H	317	LMG	C38-C37-C36	-2.44	102.02	114.37
22	H	308	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	Q	611	CLA	C3B-C4B-NB	-2.44	108.35	110.53
24	N	612	DD6	C37-C36-C31	-2.44	119.59	124.16
22	K	604	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	W	418	DD6	C10-C9-C8	-2.44	116.13	123.20
22	L	407	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	B	839	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	O	319	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	T	608	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	V	608	CLA	CHB-C4A-NA	2.44	127.92	124.40
21	B	801	BCR	C20-C21-C22	-2.44	123.86	127.28
22	G	605	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	A	827	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	U	404	CLA	CMB-C2B-C1B	-2.44	121.71	125.42
22	H	302	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	K	614	DD6	C21-C20-C15	-2.44	118.29	122.30
22	B	816	CLA	CHB-C4A-NA	2.44	127.91	124.40
22	R	603	CLA	CHB-C4A-NA	2.44	127.91	124.40
22	B	811	CLA	CMB-C2B-C1B	-2.43	121.71	125.42
24	X	415	DD6	C15-C14-C13	-2.43	120.85	125.99
22	X	417	CLA	CMB-C2B-C1B	-2.43	121.71	125.42
22	G	610	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	A	858	DD6	C7-C6-C5	-2.43	118.87	122.82
24	H	315	DD6	C10-C9-C8	-2.43	116.15	123.20
24	L	414	DD6	C10-C9-C8	-2.43	116.15	123.20
22	T	609	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	Q	612	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	T	601	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	B	807	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	N	601	CLA	CHB-C4A-NA	2.43	127.91	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	844	CLA	CHB-C4A-NA	2.43	127.91	124.40
28	J	101	LMG	C40-C39-C38	-2.43	102.08	114.37
22	B	818	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	A	829	CLA	C1-C2-C3	-2.43	122.22	126.20
24	W	417	DD6	C21-C20-C15	-2.43	118.31	122.30
24	R	612	DD6	O1-C20-C21	-2.43	112.33	115.05
24	T	613	DD6	O1-C15-C14	-2.43	109.92	116.88
24	N	613	DD6	C3-C4-C5	-2.43	118.55	123.52
28	B	856	LMG	O6-C5-C4	2.43	114.07	109.70
33	A	802	CL0	C3D-C4D-CHA	2.43	112.23	108.54
24	K	614	DD6	O1-C20-C19	-2.43	111.22	113.49
22	B	834	CLA	CHB-C4A-NA	2.43	127.90	124.40
21	B	846	BCR	C16-C15-C14	-2.43	118.56	123.52
22	O	315	CLA	C1-C2-C3	-2.43	122.84	126.76
24	Q	614	DD6	C37-C36-C31	-2.43	119.62	124.16
22	S	604	CLA	CHB-C4A-NA	2.43	127.90	124.40
22	A	837	CLA	CHB-C4A-NA	2.43	127.90	124.40
22	J	102	CLA	C1-C2-C3	-2.42	122.84	126.76
22	B	832	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	B	821	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	U	414	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	U	405	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	K	606	CLA	CHB-C4A-NA	2.42	127.89	124.40
21	B	842	BCR	C33-C5-C4	2.42	118.75	113.60
24	T	612	DD6	C10-C9-C8	-2.42	116.19	123.20
24	O	316	DD6	C15-C14-C13	-2.42	120.88	125.99
24	L	413	DD6	O1-C15-C14	-2.42	109.95	116.88
22	H	312	CLA	CHB-C4A-NA	2.42	127.89	124.40
21	B	846	BCR	C11-C10-C9	-2.42	123.89	127.28
27	U	422	LMU	C1B-O1B-C4'	-2.42	112.25	117.98
22	W	412	CLA	C11-C10-C8	-2.41	107.94	115.97
22	W	419	CLA	CHB-C4A-NA	2.41	127.89	124.40
22	I	610	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	S	607	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	X	413	CLA	C3B-C4B-NB	-2.41	108.38	110.53
22	A	820	CLA	C3B-C4B-NB	-2.41	108.38	110.53
22	B	802	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
22	W	412	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	P	610	CLA	CAA-C2A-C3A	-2.41	110.70	116.23
24	X	401	DD6	C37-C36-C31	-2.41	119.65	124.16
22	B	833	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	U	403	CLA	O2D-CGD-CBD	2.41	115.44	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	609	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	V	610	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	T	609	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
22	G	602	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	S	606	CLA	CHB-C4A-NA	2.41	127.88	124.40
24	P	613	DD6	O1-C15-C14	-2.41	109.98	116.88
24	X	414	DD6	C14-C13-C11	-2.41	121.79	125.53
24	X	415	DD6	C37-C36-C31	-2.41	119.66	124.16
22	R	615	CLA	CHB-C4A-NA	2.41	127.87	124.40
22	A	812	CLA	CHB-C4A-NA	2.41	127.87	124.40
22	G	611	CLA	CHB-C4A-NA	2.41	127.87	124.40
22	Q	604	CLA	CHB-C4A-NA	2.41	127.87	124.40
22	A	840	CLA	C3B-C4B-NB	-2.41	108.38	110.53
22	S	615	CLA	CHB-C4A-NA	2.41	127.87	124.40
21	M	101	BCR	C20-C19-C18	-2.41	119.77	126.36
22	X	412	CLA	CHB-C4A-NA	2.41	127.87	124.40
22	V	612	CLA	CHB-C4A-NA	2.40	127.87	124.40
33	A	802	CL0	O1D-CGD-CBD	2.40	128.37	124.72
22	W	403	CLA	C1-C2-C3	-2.40	122.26	126.20
22	W	409	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	N	612	DD6	C14-C13-C11	-2.40	121.80	125.53
22	S	608	CLA	CHB-C4A-NA	2.40	127.87	124.40
22	A	814	CLA	C3B-C4B-NB	-2.40	108.39	110.53
22	N	608	CLA	CHB-C4A-NA	2.40	127.87	124.40
22	Q	610	CLA	CHB-C4A-NA	2.40	127.87	124.40
22	H	310	CLA	CHB-C4A-NA	2.40	127.87	124.40
28	U	402	LMG	C40-C39-C38	-2.40	102.23	114.37
24	H	315	DD6	O1-C20-C19	-2.40	111.24	113.49
22	B	835	CLA	C3B-C4B-NB	-2.40	108.39	110.53
22	S	602	CLA	C3B-C4B-NB	-2.40	108.39	110.53
22	G	606	CLA	CHB-C4A-NA	2.40	127.86	124.40
22	F	403	CLA	CHB-C4A-NA	2.40	127.86	124.40
28	W	401	LMG	C38-C37-C36	-2.40	102.24	114.37
22	G	609	CLA	CHB-C4A-NA	2.40	127.86	124.40
22	X	404	CLA	CHB-C4A-NA	2.40	127.86	124.40
24	A	847	DD6	C26-C25-C24	-2.40	116.25	123.20
24	X	414	DD6	O1-C20-C21	-2.40	112.37	115.05
22	H	306	CLA	CHB-C4A-NA	2.40	127.86	124.40
22	Q	607	CLA	CHB-C4A-NA	2.40	127.86	124.40
24	X	414	DD6	C37-C36-C31	-2.40	119.68	124.16
24	B	841	DD6	C37-C36-C31	-2.40	119.68	124.16
22	W	404	CLA	CHB-C4A-NA	2.40	127.86	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	803	CLA	O2D-CGD-CBD	2.40	115.42	111.23
22	A	833	CLA	CHB-C4A-NA	2.39	127.86	124.40
22	B	820	CLA	O2D-CGD-CBD	2.39	115.42	111.23
22	P	608	CLA	O2D-CGD-CBD	2.39	115.42	111.23
24	T	612	DD6	C9-C10-C11	-2.39	123.92	127.28
21	A	849	BCR	C1-C6-C5	-2.39	119.36	122.64
22	A	822	CLA	CHB-C4A-NA	2.39	127.85	124.40
32	V	616	NEX	C5-C6-C1	2.39	122.07	119.70
22	Q	606	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	U	420	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	X	407	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	S	601	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	K	617	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
24	O	316	DD6	C14-C13-C11	-2.39	121.82	125.53
24	V	614	DD6	C4-C3-C2	-2.39	118.63	123.52
22	B	837	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	P	608	CLA	CHB-C4A-NA	2.39	127.85	124.40
27	K	620	LMU	O5'-C5'-C4'	2.39	114.35	109.51
22	B	808	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	A	819	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
22	V	604	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	W	414	CLA	CHB-C4A-NA	2.39	127.85	124.40
21	B	843	BCR	C38-C26-C25	-2.39	121.88	124.48
25	B	847	DGD	O1G-C1A-O1A	-2.39	117.65	123.63
24	R	613	DD6	C12-C11-C13	2.39	121.74	118.09
22	B	834	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
22	P	607	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	A	810	CLA	CHB-C4A-NA	2.39	127.85	124.40
28	K	618	LMG	C40-C39-C38	-2.39	102.30	114.37
24	A	858	DD6	C12-C11-C10	-2.39	118.95	122.82
22	B	803	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	B	827	CLA	C3B-C4B-NB	-2.39	108.40	110.53
22	R	610	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	R	608	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	S	602	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	S	603	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	G	604	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	H	313	CLA	CHB-C4A-NA	2.38	127.84	124.40
24	L	413	DD6	C37-C36-C35	2.38	118.81	114.42
24	R	613	DD6	C28-C27-C26	-2.38	119.55	124.18
27	K	620	LMU	C5'-O5'-C1'	2.38	117.05	112.21
24	L	415	DD6	C25-C26-C27	-2.38	119.94	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	802	CL0	C4C-C3C-C2C	-2.38	103.96	113.37
24	A	858	DD6	C15-C14-C13	-2.38	120.95	125.99
22	R	601	CLA	CHB-C4A-NA	2.38	127.84	124.40
22	N	609	CLA	CHB-C4A-NA	2.38	127.84	124.40
22	A	823	CLA	CHB-C4A-NA	2.38	127.84	124.40
22	Q	611	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	L	408	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
24	B	841	DD6	C14-C13-C11	-2.38	121.84	125.53
22	G	603	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	U	405	CLA	C3B-C4B-NB	-2.38	108.41	110.53
24	K	615	DD6	C21-C20-C15	-2.38	118.39	122.30
22	Q	608	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	A	831	CLA	CHB-C4A-NA	2.38	127.83	124.40
24	A	847	DD6	O1-C15-C14	-2.38	110.06	116.88
22	H	305	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	G	607	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	H	304	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	W	406	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	H	303	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	K	610	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	U	410	CLA	CHB-C4A-NA	2.38	127.83	124.40
24	F	406	DD6	C4-C3-C2	-2.38	118.66	123.52
22	K	603	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	A	841	CLA	CHB-C4A-NA	2.38	127.83	124.40
24	P	613	DD6	C10-C9-C8	-2.38	116.32	123.20
28	I	614	LMG	O1-C1-C2	-2.38	104.67	108.27
24	L	415	DD6	C37-C36-C35	2.37	118.79	114.42
22	A	835	CLA	CHB-C4A-NA	2.37	127.83	124.40
28	I	615	LMG	C38-C37-C36	-2.37	102.37	114.37
28	G	616	LMG	C40-C39-C38	-2.37	102.37	114.37
22	B	802	CLA	O1D-CGD-CBD	2.37	129.20	124.52
24	U	416	DD6	O1-C20-C19	-2.37	111.27	113.49
22	W	405	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	Q	615	DD6	C21-C20-C15	-2.37	118.40	122.30
22	Q	618	CLA	CHB-C4A-NA	2.37	127.82	124.40
22	A	818	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
24	W	418	DD6	C14-C13-C11	-2.37	121.85	125.53
21	B	844	BCR	C21-C20-C19	-2.37	116.33	123.20
22	I	602	CLA	CHB-C4A-NA	2.37	127.82	124.40
28	W	401	LMG	C40-C39-C38	-2.37	102.40	114.37
22	G	602	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
27	K	620	LMU	C1B-O1B-C4'	-2.37	111.31	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	810	CLA	CHB-C4A-NA	2.36	127.81	124.40
22	A	809	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
22	A	824	CLA	C1-C2-C3	-2.36	122.33	126.20
22	A	840	CLA	C1-C2-C3	-2.36	122.33	126.20
22	A	807	CLA	CHB-C4A-NA	2.36	127.81	124.40
24	L	413	DD6	O1-C20-C19	-2.36	111.28	113.49
24	A	859	DD6	O1-C20-C19	-2.36	111.28	113.49
22	I	604	CLA	CHB-C4A-NA	2.36	127.80	124.40
24	G	612	DD6	C37-C36-C35	2.36	118.76	114.42
25	O	304	DGD	O1G-C1A-O1A	-2.36	117.73	123.63
22	U	411	CLA	CHB-C4A-NA	2.36	127.80	124.40
22	B	822	CLA	CHB-C4A-NA	2.36	127.80	124.40
22	I	601	CLA	CHB-C4A-NA	2.36	127.80	124.40
22	L	417	CLA	CHB-C4A-NA	2.36	127.80	124.40
22	O	313	CLA	CHB-C4A-NA	2.36	127.80	124.40
24	S	612	DD6	C14-C13-C11	-2.35	121.88	125.53
24	T	613	DD6	C37-C36-C31	-2.35	119.76	124.16
22	O	307	CLA	CHB-C4A-NA	2.35	127.80	124.40
22	N	610	CLA	C1-C2-C3	-2.35	122.34	126.20
24	U	417	DD6	C28-C27-C26	-2.35	119.61	124.18
22	R	609	CLA	CHB-C4A-NA	2.35	127.80	124.40
22	G	604	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
22	H	308	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
22	Q	617	CLA	CHB-C4A-NA	2.35	127.79	124.40
22	A	832	CLA	CHB-C4A-NA	2.35	127.79	124.40
24	W	416	DD6	O1-C15-C14	-2.35	110.15	116.88
22	O	308	CLA	CHB-C4A-NA	2.35	127.79	124.40
22	H	305	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
21	B	846	BCR	C2-C1-C6	2.35	113.85	110.44
22	B	812	CLA	C1-C2-C3	-2.35	122.35	126.20
24	N	613	DD6	O1-C15-C14	-2.35	110.15	116.88
24	X	416	DD6	C37-C36-C31	-2.35	119.77	124.16
22	U	401	CLA	CHB-C4A-NA	2.35	127.79	124.40
22	X	417	CLA	CHB-C4A-NA	2.35	127.79	124.40
24	G	613	DD6	O1-C20-C21	-2.35	112.42	115.05
22	I	611	CLA	CMB-C2B-C1B	-2.35	121.85	125.42
22	O	307	CLA	C3B-C4B-NB	-2.34	108.44	110.53
22	Q	613	CLA	O1D-CGD-CBD	2.34	129.14	124.52
28	B	852	LMG	O1-C7-C8	-2.34	105.12	110.82
22	X	409	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	U	417	DD6	C-C1-C2	-2.34	119.02	122.82
21	A	851	BCR	C30-C25-C26	-2.34	119.44	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	610	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	A	806	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	I	612	DD6	C14-C13-C11	-2.34	121.90	125.53
24	A	859	DD6	C37-C36-C31	-2.34	119.78	124.16
22	A	839	CLA	CMB-C2B-C3B	2.34	132.05	126.55
22	B	827	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	W	413	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	A	812	CLA	C3B-C4B-NB	-2.34	108.44	110.53
22	K	602	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	N	604	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	A	817	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	B	817	CLA	CHB-C4A-NA	2.34	127.77	124.40
22	L	403	CLA	CHB-C4A-NA	2.34	127.77	124.40
24	I	613	DD6	C25-C24-C1	-2.34	119.95	126.36
22	A	818	CLA	C3B-C4B-NB	-2.34	108.44	110.53
21	M	101	BCR	C16-C15-C14	-2.34	118.74	123.52
22	L	403	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
31	W	408	CHL	C1-C2-C3	-2.34	122.37	126.20
24	L	415	DD6	C37-C36-C31	-2.33	119.80	124.16
22	H	318	CLA	CHB-C4A-NA	2.33	127.77	124.40
22	J	102	CLA	CHB-C4A-NA	2.33	127.77	124.40
22	A	806	CLA	O2D-CGD-CBD	2.33	115.31	111.23
22	R	609	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
22	L	410	CLA	CHB-C4A-NA	2.33	127.77	124.40
24	J	105	DD6	C13-C11-C10	2.33	122.67	119.01
22	A	803	CLA	C3B-C4B-NB	-2.33	108.45	110.53
24	O	317	DD6	C3-C4-C5	-2.33	118.75	123.52
28	G	616	LMG	C38-C37-C36	-2.33	102.60	114.37
24	I	613	DD6	C25-C26-C27	-2.33	120.10	126.61
22	A	830	CLA	C1-C2-C3	-2.33	122.38	126.20
24	J	105	DD6	O1-C20-C21	-2.33	112.45	115.05
22	Q	608	CLA	C1-C2-C3	-2.33	123.00	126.76
24	W	418	DD6	O1-C20-C21	-2.33	112.45	115.05
22	A	818	CLA	C1-C2-C3	-2.33	122.39	126.20
22	U	415	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	L	415	DD6	O1-C20-C21	-2.32	112.45	115.05
22	G	603	CLA	C3B-C4B-NB	-2.32	108.45	110.53
22	A	832	CLA	C3B-C4B-NB	-2.32	108.45	110.53
24	G	613	DD6	C25-C26-C27	-2.32	120.11	126.61
22	O	305	CLA	CHB-C4A-NA	2.32	127.75	124.40
22	B	836	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
28	J	101	LMG	C38-C37-C36	-2.32	102.62	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	105	DD6	C12-C11-C10	-2.32	119.05	122.82
21	B	842	BCR	C15-C16-C17	-2.32	118.77	123.52
22	B	806	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
22	U	406	CLA	CHB-C4A-NA	2.32	127.75	124.40
22	B	820	CLA	C3B-C4B-NB	-2.32	108.46	110.53
22	O	312	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
28	K	622	LMG	C38-C37-C36	-2.32	102.64	114.37
28	B	856	LMG	C38-C37-C36	-2.32	102.64	114.37
22	B	813	CLA	CHB-C4A-NA	2.32	127.75	124.40
22	U	404	CLA	CHB-C4A-NA	2.32	127.75	124.40
22	K	612	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	K	615	DD6	C28-C27-C26	-2.32	119.68	124.18
22	O	315	CLA	CHB-C4A-NA	2.32	127.74	124.40
22	P	606	CLA	CHB-C4A-NA	2.32	127.74	124.40
22	H	304	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
22	A	832	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
22	A	816	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
22	I	609	CLA	CMB-C2B-C1B	-2.31	121.89	125.42
22	N	607	CLA	CHB-C4A-NA	2.31	127.74	124.40
21	A	851	BCR	C10-C11-C12	-2.31	116.50	123.20
28	L	401	LMG	C38-C37-C36	-2.31	102.68	114.37
22	O	306	CLA	CHB-C4A-NA	2.31	127.74	124.40
22	R	607	CLA	C1-C2-C3	-2.31	122.41	126.20
22	K	607	CLA	CHB-C4A-NA	2.31	127.74	124.40
24	A	858	DD6	C37-C36-C31	-2.31	119.84	124.16
24	T	612	DD6	C21-C20-C15	-2.31	118.50	122.30
22	A	815	CLA	CHB-C4A-NA	2.31	127.73	124.40
22	A	838	CLA	C1-C2-C3	-2.31	122.41	126.20
24	X	414	DD6	C21-C20-C15	-2.31	118.50	122.30
22	P	606	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
22	W	411	CLA	CHB-C4A-NA	2.31	127.73	124.40
22	X	419	CLA	CHB-C4A-NA	2.31	127.73	124.40
21	B	846	BCR	C30-C25-C26	-2.31	119.48	122.64
22	Q	603	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
23	B	840	PQN	C2M-C2-C3	-2.31	120.66	124.45
22	S	603	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
22	B	812	CLA	CHB-C4A-NA	2.31	127.73	124.40
21	A	849	BCR	C8-C7-C6	-2.30	120.84	127.00
22	H	311	CLA	C1-C2-C3	-2.30	122.42	126.20
24	P	613	DD6	C37-C36-C31	-2.30	119.85	124.16
24	V	614	DD6	C14-C13-C11	-2.30	121.96	125.53
22	K	608	CLA	CHB-C4A-NA	2.30	127.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	817	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
22	R	605	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
24	L	414	DD6	C3-C4-C5	-2.30	118.81	123.52
22	U	413	CLA	C3B-C4B-NB	-2.30	108.48	110.53
22	N	605	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
22	T	603	CLA	C3B-C4B-NB	-2.30	108.48	110.53
22	W	411	CLA	C1-C2-C3	-2.30	122.43	126.20
21	B	801	BCR	C4-C5-C6	-2.30	119.60	122.70
22	O	314	CLA	CHB-C4A-NA	2.30	127.72	124.40
22	S	609	CLA	O2D-CGD-CBD	2.30	115.25	111.23
24	L	415	DD6	C25-C24-C1	-2.30	120.06	126.36
22	W	402	CLA	CHB-C4A-NA	2.30	127.71	124.40
22	S	602	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
22	A	828	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
21	B	845	BCR	C33-C5-C6	-2.30	121.98	124.48
24	A	858	DD6	C13-C11-C10	2.30	122.62	119.01
28	B	856	LMG	O2-C2-C1	-2.30	104.61	110.08
22	T	605	CLA	CHB-C4A-NA	2.29	127.71	124.40
21	B	842	BCR	C38-C26-C27	2.29	118.49	113.60
22	L	408	CLA	C6-C7-C8	-2.29	108.34	115.97
22	X	411	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
24	S	612	DD6	C37-C36-C31	-2.29	119.88	124.16
28	K	618	LMG	C38-C37-C36	-2.29	102.79	114.37
22	A	840	CLA	CHB-C4A-NA	2.29	127.70	124.40
31	X	406	CHL	C4C-CHD-C1D	2.29	124.25	116.07
24	G	613	DD6	C10-C9-C8	-2.29	116.57	123.20
24	G	612	DD6	C21-C20-C15	-2.29	118.54	122.30
22	K	608	CLA	O1D-CGD-CBD	2.29	129.03	124.52
24	U	417	DD6	C14-C13-C11	-2.29	121.98	125.53
31	W	422	CHL	C1A-CHA-C4D	2.28	122.79	118.98
22	T	602	CLA	CHB-C4A-NA	2.28	127.70	124.40
22	A	818	CLA	CHB-C4A-NA	2.28	127.70	124.40
28	U	402	LMG	C38-C37-C36	-2.28	102.83	114.37
22	T	607	CLA	CHB-C4A-NA	2.28	127.69	124.40
22	S	602	CLA	C1-C2-C3	-2.28	122.46	126.20
22	B	807	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
22	A	819	CLA	CHB-C4A-NA	2.28	127.69	124.40
22	B	804	CLA	C1-C2-C3	-2.28	122.47	126.20
32	U	418	NEX	C5-C6-C1	2.28	121.95	119.70
22	I	609	CLA	C3B-C4B-NB	-2.28	108.50	110.53
28	B	856	LMG	C42-C41-C40	-2.27	102.88	114.37
22	B	826	CLA	CHB-C4A-NA	2.27	127.68	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	858	DD6	C37-C36-C35	2.27	118.60	114.42
22	B	817	CLA	C3B-C4B-NB	-2.27	108.50	110.53
22	S	609	CLA	CHB-C4A-NA	2.27	127.68	124.40
28	I	614	LMG	O3-C3-C2	-2.27	105.02	110.38
22	B	824	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
24	A	847	DD6	O1-C20-C21	-2.27	112.51	115.05
22	L	408	CLA	CHD-C1D-ND	-2.27	121.61	124.80
22	Q	605	CLA	C3B-C4B-NB	-2.27	108.50	110.53
22	A	830	CLA	CHB-C4A-NA	2.27	127.67	124.40
22	B	812	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
31	W	408	CHL	C4C-CHD-C1D	2.27	124.18	116.07
22	B	829	CLA	O1D-CGD-CBD	2.27	128.99	124.52
21	A	851	BCR	C20-C19-C18	-2.27	120.15	126.36
22	B	828	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
22	A	835	CLA	O2D-CGD-CBD	2.27	115.19	111.23
22	R	615	CLA	C1-C2-C3	-2.27	122.49	126.20
24	A	859	DD6	C37-C36-C35	2.26	118.58	114.42
22	W	415	CLA	O1D-CGD-CBD	2.26	128.98	124.52
22	R	601	CLA	C1-C2-C3	-2.26	122.49	126.20
24	I	613	DD6	C10-C9-C8	-2.26	116.64	123.20
22	X	409	CLA	C1-C2-C3	-2.26	122.49	126.20
28	A	855	LMG	C38-C37-C36	-2.26	102.94	114.37
22	I	607	CLA	CHB-C4A-NA	2.26	127.66	124.40
22	A	834	CLA	CHB-C4A-NA	2.26	127.66	124.40
24	T	613	DD6	C21-C20-C15	-2.26	118.58	122.30
31	W	407	CHL	C4C-CHD-C1D	2.26	124.15	116.07
24	N	613	DD6	C25-C24-C1	-2.26	120.17	126.36
27	O	322	LMU	C3'-C4'-C5'	-2.26	105.92	110.93
24	A	847	DD6	C37-C36-C35	2.26	118.57	114.42
24	H	315	DD6	C3-C4-C5	-2.26	118.90	123.52
22	Q	609	CLA	CHB-C4A-NA	2.26	127.66	124.40
22	B	831	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
28	K	622	LMG	O3-C3-C2	-2.26	105.06	110.38
22	B	831	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
22	B	814	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
31	V	605	CHL	C4C-CHD-C1D	2.25	124.13	116.07
22	A	813	CLA	CHB-C4A-NA	2.25	127.65	124.40
21	B	801	BCR	C16-C17-C18	-2.25	124.12	127.28
22	F	404	CLA	C3B-C4B-NB	-2.25	108.52	110.53
22	R	611	CLA	CHB-C4A-NA	2.25	127.65	124.40
22	I	611	CLA	O1D-CGD-CBD	2.25	128.96	124.52
24	H	314	DD6	C28-C27-C26	-2.25	119.81	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	I	603	CLA	C3B-C4B-NB	-2.25	108.52	110.53
24	A	859	DD6	C28-C27-C26	-2.25	119.81	124.18
22	B	831	CLA	CHB-C4A-NA	2.25	127.65	124.40
22	B	839	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
24	V	614	DD6	O1-C20-C21	-2.25	112.53	115.05
24	A	847	DD6	O1-C20-C19	-2.25	111.39	113.49
22	B	825	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
24	U	417	DD6	C-C1-C24	2.25	121.52	118.09
22	N	611	CLA	CHB-C4A-NA	2.25	127.64	124.40
22	Q	604	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
28	J	101	LMG	C42-C41-C40	-2.24	103.02	114.37
22	Q	605	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
24	W	416	DD6	O1-C20-C19	-2.24	111.39	113.49
31	W	408	CHL	C1A-CHA-C4D	2.24	122.72	118.98
22	A	808	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
22	B	806	CLA	CHB-C4A-NA	2.24	127.63	124.40
22	R	602	CLA	CHB-C4A-NA	2.24	127.63	124.40
22	O	309	CLA	C1-C2-C3	-2.24	123.14	126.76
22	R	609	CLA	C3B-C4B-NB	-2.24	108.53	110.53
22	N	610	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
28	I	614	LMG	O2-C2-C1	-2.24	104.74	110.08
22	A	801	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
28	B	856	LMG	O3-C3-C2	-2.24	105.10	110.38
22	Q	617	CLA	C1-C2-C3	-2.24	122.53	126.20
22	B	835	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
24	F	406	DD6	C28-C27-C26	-2.24	119.84	124.18
31	W	407	CHL	C1A-CHA-C4D	2.24	122.72	118.98
24	H	314	DD6	C4-C3-C2	-2.24	118.94	123.52
21	B	844	BCR	C3-C4-C5	-2.24	110.07	114.06
28	L	401	LMG	O3-C3-C2	-2.24	105.11	110.38
22	B	830	CLA	CMB-C2B-C1B	-2.24	122.02	125.42
24	O	316	DD6	C37-C36-C35	2.24	118.53	114.42
24	F	406	DD6	C24-C1-C2	2.23	122.52	119.01
28	J	101	LMG	O3-C3-C2	-2.23	105.11	110.38
24	W	416	DD6	C37-C36-C35	2.23	118.53	114.42
31	U	407	CHL	C4C-CHD-C1D	2.23	124.05	116.07
28	J	101	LMG	O2-C2-C1	-2.23	104.76	110.08
22	B	818	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
22	A	820	CLA	CHB-C4A-NA	2.23	127.62	124.40
24	X	415	DD6	C28-C27-C26	-2.23	119.85	124.18
22	X	409	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
21	B	843	BCR	C10-C11-C12	-2.23	116.74	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	603	CLA	CHB-C4A-NA	2.23	127.61	124.40
22	P	607	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
21	M	101	BCR	C38-C26-C25	-2.23	122.06	124.48
28	H	317	LMG	C40-C39-C38	-2.23	103.12	114.37
28	T	616	LMG	O2-C2-C1	-2.23	104.77	110.08
22	A	844	CLA	C1-C2-C3	-2.23	122.55	126.20
24	O	317	DD6	C25-C26-C27	-2.22	120.39	126.61
22	B	822	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
24	H	315	DD6	C37-C36-C35	2.22	118.51	114.42
27	O	303	LMU	C1B-O1B-C4'	-2.22	112.71	117.98
28	B	852	LMG	O2-C2-C1	-2.22	104.78	110.08
28	K	618	LMG	C42-C41-C40	-2.22	103.13	114.37
22	B	831	CLA	C3B-C4B-NB	-2.22	108.55	110.53
22	B	838	CLA	C3B-C4B-NB	-2.22	108.55	110.53
22	O	310	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
22	O	312	CLA	C1-C2-C3	-2.22	122.56	126.20
22	A	840	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
22	W	414	CLA	C1-C2-C3	-2.22	122.56	126.20
24	I	613	DD6	O1-C20-C21	-2.22	112.57	115.05
24	L	413	DD6	C14-C13-C11	-2.22	122.08	125.53
28	U	423	LMG	O3-C3-C2	-2.22	105.14	110.38
22	W	415	CLA	CHB-C4A-NA	2.22	127.60	124.40
28	F	408	LMG	C1-C2-C3	-2.22	105.34	110.01
22	O	308	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
24	L	414	DD6	C25-C24-C1	-2.22	120.28	126.36
22	X	409	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
28	H	317	LMG	O3-C3-C2	-2.22	105.15	110.38
28	Q	602	LMG	O2-C2-C1	-2.22	104.79	110.08
22	B	828	CLA	CHB-C4A-NA	2.22	127.60	124.40
22	B	832	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
24	R	612	DD6	C21-C20-C15	-2.22	118.66	122.30
24	K	614	DD6	C14-C13-C11	-2.22	122.09	125.53
31	U	408	CHL	C4C-CHD-C1D	2.21	123.99	116.07
24	L	414	DD6	C25-C26-C27	-2.21	120.42	126.61
22	A	839	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
24	W	417	DD6	C37-C36-C31	-2.21	120.02	124.16
22	A	827	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
28	K	618	LMG	O2-C2-C1	-2.21	104.81	110.08
22	V	607	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
24	N	613	DD6	O1-C20-C21	-2.21	112.58	115.05
22	H	308	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
22	H	313	CLA	C1-C2-C3	-2.21	122.58	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	807	CLA	C1-C2-C3	-2.21	122.58	126.20
22	B	814	CLA	CHB-C4A-NA	2.21	127.59	124.40
22	F	403	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
22	O	312	CLA	C3B-C4B-NB	-2.21	108.56	110.53
24	A	858	DD6	O1-C15-C14	-2.21	110.55	116.88
24	V	615	DD6	C25-C26-C27	-2.21	120.44	126.61
24	V	614	DD6	C21-C20-C15	-2.21	118.67	122.30
22	S	604	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
22	P	609	CLA	CHB-C4A-NA	2.21	127.58	124.40
22	I	602	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
24	O	316	DD6	C4-C3-C2	-2.20	119.01	123.52
28	G	616	LMG	C42-C41-C40	-2.20	103.23	114.37
25	F	401	DGD	O2G-C1B-O1B	-2.20	118.56	123.70
22	A	809	CLA	CHB-C4A-NA	2.20	127.58	124.40
28	W	401	LMG	O7-C10-O9	-2.20	118.56	123.70
22	V	603	CLA	CHB-C4A-NA	2.20	127.58	124.40
27	B	854	LMU	C1-O1'-C1'	-2.20	109.92	113.68
24	R	613	DD6	C21-C20-C15	-2.20	118.68	122.30
24	L	414	DD6	C37-C36-C35	2.20	118.47	114.42
28	K	601	LMG	O7-C10-O9	-2.20	118.56	123.70
22	K	612	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
22	L	412	CLA	CHB-C4A-NA	2.20	127.57	124.40
21	B	846	BCR	C38-C26-C25	-2.20	122.08	124.48
21	A	848	BCR	C33-C5-C4	2.20	118.28	113.60
21	A	848	BCR	C28-C27-C26	-2.20	110.14	114.06
21	B	846	BCR	C34-C9-C8	2.20	121.44	118.09
22	I	602	CLA	CMB-C2B-C1B	-2.20	122.08	125.42
25	B	847	DGD	C3B-C2B-C1B	-2.20	105.65	113.69
22	H	306	CLA	C1-C2-C3	-2.20	122.60	126.20
27	O	322	LMU	O1'-C1'-C2'	2.20	111.61	108.27
22	P	611	CLA	O1D-CGD-CBD	2.20	128.85	124.52
21	A	849	BCR	C4-C5-C6	-2.20	119.74	122.70
22	A	829	CLA	C3B-C4B-NB	-2.20	108.57	110.53
24	F	406	DD6	C37-C36-C35	2.19	118.46	114.42
24	I	613	DD6	C14-C13-C11	-2.19	122.12	125.53
24	K	615	DD6	C14-C13-C11	-2.19	122.13	125.53
22	A	819	CLA	O1D-CGD-CBD	2.19	128.84	124.52
22	V	602	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
28	H	317	LMG	O2-C2-C1	-2.19	104.85	110.08
28	F	408	LMG	O2-C2-C1	-2.19	104.85	110.08
28	F	408	LMG	O3-C3-C2	-2.19	105.21	110.38
22	A	803	CLA	CHB-C4A-NA	2.19	127.56	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	604	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
22	W	405	CLA	C3B-C4B-NB	-2.19	108.58	110.53
22	A	824	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
24	S	611	DD6	C25-C24-C1	-2.19	120.36	126.36
28	K	622	LMG	O2-C2-C1	-2.19	104.86	110.08
22	B	826	CLA	C3B-C4B-NB	-2.19	108.58	110.53
22	S	605	CLA	CHB-C4A-NA	2.19	127.56	124.40
22	A	852	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
22	F	404	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
22	A	844	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
28	W	401	LMG	O3-C3-C2	-2.19	105.22	110.38
31	X	406	CHL	C1A-CHA-C4D	2.19	122.63	118.98
22	A	811	CLA	CMB-C2B-C3B	2.19	131.69	126.55
28	G	616	LMG	O1-C7-C8	-2.19	105.50	110.82
24	K	614	DD6	C26-C25-C24	-2.19	116.87	123.20
22	N	602	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
24	O	316	DD6	C28-C27-C26	-2.19	119.94	124.18
22	B	838	CLA	CHB-C4A-NA	2.18	127.55	124.40
22	Q	609	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
22	W	409	CLA	CMB-C2B-C1B	-2.18	122.09	125.42
31	V	606	CHL	C4C-CHD-C1D	2.18	123.88	116.07
22	K	604	CLA	CMB-C2B-C1B	-2.18	122.09	125.42
31	V	605	CHL	C1A-CHA-C4D	2.18	122.62	118.98
24	H	315	DD6	C28-C27-C26	-2.18	119.94	124.18
28	T	616	LMG	O3-C3-C2	-2.18	105.24	110.38
28	H	322	LMG	O2-C2-C1	-2.18	104.88	110.08
28	J	101	LMG	O1-C7-C8	-2.18	105.52	110.82
22	K	608	CLA	CHD-C1D-ND	-2.18	121.73	124.80
28	Q	602	LMG	O1-C7-C8	-2.18	105.52	110.82
22	U	411	CLA	C1-C2-C3	-2.18	122.63	126.20
22	S	606	CLA	C1-C2-C3	-2.18	123.24	126.76
24	R	613	DD6	C7-C6-C8	2.18	121.41	118.09
24	X	401	DD6	C4-C3-C2	-2.18	119.06	123.52
22	H	318	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
28	K	601	LMG	O3-C3-C2	-2.17	105.25	110.38
22	B	815	CLA	CHB-C4A-NA	2.17	127.54	124.40
24	W	417	DD6	C14-C13-C11	-2.17	122.16	125.53
22	A	810	CLA	O2D-CGD-CBD	2.17	115.03	111.23
28	K	601	LMG	O2-C2-C1	-2.17	104.90	110.08
24	S	611	DD6	C10-C9-C8	-2.17	116.91	123.20
31	V	606	CHL	C1A-CHA-C4D	2.17	122.60	118.98
24	Q	615	DD6	C12-C11-C13	2.17	121.40	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	613	DD6	C28-C27-C26	-2.17	119.97	124.18
31	U	407	CHL	C1A-CHA-C4D	2.17	122.60	118.98
24	T	612	DD6	C14-C13-C11	-2.17	122.17	125.53
24	I	613	DD6	C28-C27-C26	-2.17	119.97	124.18
22	H	311	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
28	H	322	LMG	O3-C3-C2	-2.17	105.27	110.38
22	A	810	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
22	B	827	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
22	L	403	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
28	K	618	LMG	O3-C3-C2	-2.17	105.27	110.38
22	V	603	CLA	C1-C2-C3	-2.16	122.65	126.20
24	N	613	DD6	C28-C27-C26	-2.16	119.98	124.18
24	N	613	DD6	C37-C36-C35	2.16	118.40	114.42
24	S	612	DD6	C26-C25-C24	-2.16	116.93	123.20
22	K	612	CLA	CHB-C4A-NA	2.16	127.52	124.40
24	K	614	DD6	O1-C20-C21	-2.16	112.63	115.05
24	A	847	DD6	C37-C36-C31	-2.16	120.12	124.16
24	Q	615	DD6	C7-C6-C8	2.16	121.39	118.09
28	W	401	LMG	O2-C2-C1	-2.16	104.92	110.08
22	K	617	CLA	CHB-C4A-NA	2.16	127.52	124.40
31	U	408	CHL	C1A-CHA-C4D	2.16	122.59	118.98
28	A	855	LMG	O2-C2-C1	-2.16	104.93	110.08
31	W	422	CHL	C4C-CHD-C1D	2.16	123.80	116.07
21	B	801	BCR	C21-C20-C19	-2.16	116.94	123.20
22	I	603	CLA	CHB-C4A-NA	2.16	127.52	124.40
22	A	825	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
28	Q	602	LMG	O3-C3-C2	-2.16	105.29	110.38
22	A	828	CLA	C1-C2-C3	-2.16	122.66	126.20
24	A	858	DD6	C28-C27-C26	-2.16	119.99	124.18
24	W	417	DD6	C37-C36-C35	2.16	118.38	114.42
24	N	613	DD6	C25-C26-C27	-2.15	120.58	126.61
22	R	615	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
22	B	805	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
24	G	613	DD6	C25-C24-C1	-2.15	120.46	126.36
24	A	859	DD6	O1-C20-C21	-2.15	112.64	115.05
22	L	403	CLA	C1-C2-C3	-2.15	122.67	126.20
24	P	613	DD6	C37-C36-C35	2.15	118.38	114.42
28	W	401	LMG	C42-C41-C40	-2.15	103.49	114.37
24	H	315	DD6	C21-C20-C15	-2.15	118.76	122.30
28	U	423	LMG	O2-C2-C1	-2.15	104.95	110.08
24	R	612	DD6	C37-C36-C35	2.15	118.38	114.42
22	X	403	CLA	O2A-CGA-O1A	-2.15	118.25	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	615	LMG	O3-C3-C2	-2.15	105.31	110.38
24	T	612	DD6	C37-C36-C35	2.15	118.37	114.42
22	N	603	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	W	402	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
24	G	612	DD6	C14-C13-C11	-2.15	122.20	125.53
22	K	608	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	L	410	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	V	603	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
22	G	607	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	W	411	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	A	811	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	U	411	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	A	829	CLA	CHB-C4A-NA	2.15	127.50	124.40
22	O	306	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	Q	611	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
28	N	615	LMG	O2-C2-C1	-2.14	104.97	110.08
22	F	405	CLA	CHB-C4A-NA	2.14	127.49	124.40
21	A	850	BCR	C10-C11-C12	-2.14	116.99	123.20
24	W	418	DD6	C3-C4-C5	-2.14	119.14	123.52
22	G	603	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
22	A	817	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
22	B	825	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
22	G	602	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
22	A	820	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
28	H	319	LMG	O3-C3-C2	-2.14	105.33	110.38
22	I	603	CLA	O2D-CGD-CBD	2.14	114.97	111.23
22	O	306	CLA	C1-C2-C3	-2.14	122.69	126.20
22	T	606	CLA	C1-C2-C3	-2.14	123.30	126.76
22	X	410	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
22	B	820	CLA	C1-C2-C3	-2.14	122.69	126.20
22	T	603	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
22	O	308	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
22	K	608	CLA	C1-C2-C3	-2.14	122.70	126.20
22	A	831	CLA	C1-C2-C3	-2.13	122.70	126.20
28	B	852	LMG	O3-C3-C2	-2.13	105.34	110.38
22	O	305	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
22	A	804	CLA	C3B-C4B-NB	-2.13	108.62	110.53
22	A	833	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
22	A	816	CLA	CHB-C4A-NA	2.13	127.48	124.40
22	B	821	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
22	R	608	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
28	H	319	LMG	O7-C10-O9	-2.13	118.72	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	603	CLA	C3B-C4B-NB	-2.13	108.63	110.53
22	K	607	CLA	O1D-CGD-CBD	2.13	128.72	124.52
22	B	828	CLA	CMB-C2B-C3B	2.13	131.56	126.55
28	A	855	LMG	O1-C7-C8	-2.13	105.64	110.82
21	J	103	BCR	C21-C20-C19	-2.13	117.03	123.20
22	W	410	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
24	K	614	DD6	C4-C3-C2	-2.13	119.16	123.52
22	A	833	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
22	B	834	CLA	CMB-C2B-C3B	2.13	131.56	126.55
22	A	828	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
21	M	101	BCR	C3-C4-C5	-2.13	110.27	114.06
24	W	417	DD6	C28-C27-C26	-2.13	120.05	124.18
24	A	858	DD6	C25-C26-C27	-2.13	120.67	126.61
22	B	818	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
22	Q	605	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
22	R	610	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
28	N	615	LMG	O1-C7-C8	-2.12	105.65	110.82
22	K	602	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
22	L	417	CLA	C1-C2-C3	-2.12	122.72	126.20
28	I	615	LMG	O2-C2-C1	-2.12	104.87	108.87
24	S	611	DD6	C28-C27-C26	-2.12	120.06	124.18
28	A	855	LMG	O3-C3-C2	-2.12	105.38	110.38
22	P	603	CLA	C3B-C4B-NB	-2.12	108.64	110.53
22	A	803	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
22	H	304	CLA	CMB-C2B-C3B	2.12	131.53	126.55
24	I	612	DD6	C37-C36-C31	-2.12	120.20	124.16
22	N	607	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	A	826	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
22	B	833	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	G	603	CLA	O2D-CGD-CBD	2.12	114.93	111.23
22	B	830	CLA	CHB-C4A-NA	2.12	127.45	124.40
22	K	604	CLA	C1-C2-C3	-2.12	122.73	126.20
24	N	612	DD6	C4-C3-C2	-2.12	119.19	123.52
22	A	813	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	T	607	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
22	B	839	CLA	C1-C2-C3	-2.12	122.73	126.20
22	K	607	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
22	T	607	CLA	CMB-C2B-C3B	2.11	131.52	126.55
28	G	616	LMG	O2-C2-C1	-2.11	105.04	110.08
22	A	817	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
22	U	404	CLA	CMB-C2B-C3B	2.11	131.52	126.55
22	A	801	CLA	CAC-C3C-C4C	2.11	127.54	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	O	317	DD6	C28-C27-C26	-2.11	120.08	124.18
22	B	836	CLA	C1-C2-C3	-2.11	122.74	126.20
22	Q	611	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
22	B	824	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
24	I	612	DD6	C21-C20-C15	-2.11	118.83	122.30
22	H	305	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
22	W	405	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
22	B	806	CLA	CMB-C2B-C3B	2.11	131.51	126.55
24	U	416	DD6	O1-C20-C21	-2.11	112.69	115.05
22	B	835	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
22	V	608	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
24	R	613	DD6	C9-C10-C11	-2.11	124.32	127.28
22	F	404	CLA	C1-C2-C3	-2.11	122.75	126.20
24	J	105	DD6	C4-C3-C2	-2.11	119.21	123.52
22	X	405	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
22	B	811	CLA	CMB-C2B-C3B	2.11	131.50	126.55
22	X	417	CLA	CMB-C2B-C3B	2.11	131.50	126.55
22	R	603	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
22	L	408	CLA	CHB-C4A-NA	2.10	127.44	124.40
24	H	315	DD6	C9-C10-C11	-2.10	124.33	127.28
28	U	402	LMG	O3-C3-C2	-2.10	105.42	110.38
24	N	612	DD6	C26-C25-C24	-2.10	117.11	123.20
24	U	416	DD6	C37-C36-C31	-2.10	120.23	124.16
28	K	618	LMG	O1-C1-C2	-2.10	105.08	108.27
22	N	607	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
21	B	843	BCR	C21-C20-C19	-2.10	117.12	123.20
22	V	609	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
22	W	412	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
24	V	614	DD6	C37-C36-C35	2.10	118.28	114.42
22	A	832	CLA	CMB-C2B-C3B	2.10	131.49	126.55
22	L	411	CLA	C1-C2-C3	-2.10	122.76	126.20
22	N	602	CLA	C1-C2-C3	-2.10	122.76	126.20
24	L	414	DD6	C9-C10-C11	-2.10	124.34	127.28
22	I	611	CLA	CHB-C4A-NA	2.10	127.43	124.40
22	A	852	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
22	A	831	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
22	K	617	CLA	CMB-C2B-C3B	2.10	131.48	126.55
22	O	312	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
24	X	415	DD6	C14-C13-C11	-2.09	122.28	125.53
22	A	837	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
28	L	401	LMG	O2-C2-C1	-2.09	105.08	110.08
22	W	403	CLA	O2A-CGA-O1A	-2.09	118.39	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	815	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
27	H	321	LMU	C1-O1'-C1'	-2.09	110.10	113.68
22	T	606	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
22	X	412	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
22	T	609	CLA	CMB-C2B-C3B	2.09	131.47	126.55
24	S	612	DD6	O1-C20-C21	-2.09	112.71	115.05
22	H	309	CLA	C1-C2-C3	-2.09	122.77	126.20
22	S	615	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	B	836	CLA	C3B-C4B-NB	-2.09	108.66	110.53
27	O	320	LMU	C1B-O1B-C4'	-2.09	111.03	115.20
22	N	606	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	K	610	CLA	C1-C2-C3	-2.09	122.77	126.20
24	N	612	DD6	C37-C36-C35	2.09	118.26	114.42
22	K	608	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
22	L	408	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
22	A	822	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
22	I	602	CLA	C1-C2-C3	-2.09	122.78	126.20
22	A	838	CLA	O2D-CGD-CBD	2.09	114.88	111.23
22	A	804	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
22	B	809	CLA	C1-C2-C3	-2.08	122.78	126.20
22	X	417	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	O	312	CLA	CMB-C2B-C3B	2.08	131.45	126.55
22	R	609	CLA	CMB-C2B-C3B	2.08	131.45	126.55
22	A	815	CLA	CMB-C2B-C3B	2.08	131.44	126.55
24	V	615	DD6	C14-C13-C11	-2.08	122.30	125.53
22	B	830	CLA	O2D-CGD-CBD	2.08	114.87	111.23
28	L	401	LMG	O1-C7-C8	-2.08	105.76	110.82
22	A	801	CLA	C2D-C1D-ND	-2.08	108.07	110.13
24	W	418	DD6	C25-C26-C27	-2.08	120.79	126.61
22	V	604	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
22	H	313	CLA	O2D-CGD-CBD	2.08	114.86	111.23
25	B	847	DGD	C2G-O2G-C1B	-2.08	112.82	117.80
22	A	836	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
30	F	407	SQD	O8-S-C6	-2.08	101.96	105.97
25	O	304	DGD	C3D-C4D-C5D	2.08	114.00	110.23
24	H	314	DD6	C37-C36-C35	2.08	118.24	114.42
28	Q	602	LMG	O1-C1-C2	-2.08	105.12	108.27
22	A	801	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
24	H	314	DD6	C25-C26-C27	-2.07	120.81	126.61
22	A	821	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	A	852	CLA	CHB-C4A-NA	2.07	127.39	124.40
25	O	304	DGD	O3G-C1D-C2D	2.07	111.42	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	805	CLA	C1-C2-C3	-2.07	122.80	126.20
22	K	602	CLA	C1-C2-C3	-2.07	122.80	126.20
22	S	609	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	B	809	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
24	V	615	DD6	C33-C32-C31	2.07	113.57	109.49
22	B	836	CLA	CHB-C4A-NA	2.07	127.39	124.40
22	A	811	CLA	C1-C2-C3	-2.07	122.80	126.20
24	L	413	DD6	C4-C3-C2	-2.07	119.28	123.52
24	P	613	DD6	C7-C6-C8	2.07	121.25	118.09
22	H	303	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	H	305	CLA	CMB-C2B-C3B	2.07	131.42	126.55
22	I	605	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
28	H	317	LMG	C42-C41-C40	-2.07	103.91	114.37
22	T	605	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	U	401	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	L	406	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	B	804	CLA	CMB-C2B-C3B	2.07	131.41	126.55
21	B	846	BCR	C21-C20-C19	-2.07	117.21	123.20
22	N	606	CLA	C1-C2-C3	-2.07	122.81	126.20
24	B	841	DD6	O1-C20-C21	-2.07	112.74	115.05
22	K	611	CLA	O1D-CGD-CBD	2.07	128.59	124.52
22	U	414	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
22	H	304	CLA	C3B-C4B-NB	-2.06	108.69	110.53
22	O	311	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
22	W	414	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
21	B	846	BCR	C8-C7-C6	-2.06	121.48	127.00
22	R	604	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
22	X	408	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
22	B	828	CLA	O2D-CGD-CBD	2.06	114.84	111.23
22	A	805	CLA	C1-C2-C3	-2.06	122.82	126.20
21	B	845	BCR	C38-C26-C27	2.06	117.99	113.60
22	U	413	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
22	A	805	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
22	T	611	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
28	G	616	LMG	O3-C3-C2	-2.06	105.52	110.38
22	L	404	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
26	A	845	LHG	C26-C25-C24	2.06	120.70	113.13
22	L	409	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
22	B	812	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
22	I	601	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
24	V	614	DD6	C28-C27-C26	-2.06	120.18	124.18
21	B	844	BCR	C15-C16-C17	-2.06	119.31	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	802	CLA	CHB-C4A-NA	2.06	127.37	124.40
22	B	803	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
22	G	604	CLA	CMB-C2B-C3B	2.06	131.39	126.55
22	X	407	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
22	K	602	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
21	B	801	BCR	C29-C30-C25	2.06	113.43	110.44
24	L	415	DD6	C9-C8-C6	-2.06	120.72	126.36
22	T	602	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
22	I	611	CLA	CMB-C2B-C3B	2.06	131.39	126.55
22	B	813	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
22	A	812	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
24	K	615	DD6	C37-C36-C31	-2.05	120.32	124.16
22	W	409	CLA	C1-C2-C3	-2.05	122.83	126.20
22	W	411	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
22	A	844	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
21	A	850	BCR	C20-C19-C18	-2.05	120.73	126.36
24	Q	614	DD6	C14-C13-C11	-2.05	122.34	125.53
28	I	615	LMG	O7-C10-O9	-2.05	118.90	123.70
21	B	801	BCR	C1-C6-C5	-2.05	119.83	122.64
27	U	422	LMU	C1-O1'-C1'	-2.05	110.17	113.68
22	B	825	CLA	O2D-CGD-CBD	2.05	114.82	111.23
22	B	814	CLA	CMB-C2B-C3B	2.05	131.38	126.55
22	B	831	CLA	CMB-C2B-C3B	2.05	131.38	126.55
22	U	406	CLA	C1-C2-C3	-2.05	122.83	126.20
24	B	841	DD6	C37-C36-C35	2.05	118.19	114.42
22	B	814	CLA	O2D-CGD-CBD	2.05	114.82	111.23
22	V	603	CLA	CMB-C2B-C3B	2.05	131.38	126.55
22	S	603	CLA	CMB-C2B-C3B	2.05	131.38	126.55
22	Q	608	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	R	607	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
24	L	415	DD6	C28-C27-C26	-2.05	120.20	124.18
22	X	411	CLA	CMB-C2B-C3B	2.05	131.37	126.55
22	B	832	CLA	CAA-CBA-CGA	-2.05	107.39	113.21
24	G	613	DD6	C14-C13-C11	-2.05	122.35	125.53
26	S	613	LHG	C26-C25-C24	2.05	120.66	113.13
22	N	603	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
22	L	411	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	L	417	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
27	L	420	LMU	C1-O1'-C1'	-2.05	110.02	113.79
22	A	801	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	K	615	DD6	C25-C26-C27	-2.05	120.88	126.61
24	X	414	DD6	C4-C3-C2	-2.05	119.33	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	804	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	R	601	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	Q	603	CLA	CMB-C2B-C3B	2.05	131.37	126.55
22	A	803	CLA	O1D-CGD-CBD	2.05	128.56	124.52
22	F	403	CLA	C1-C2-C3	-2.05	122.84	126.20
22	Q	605	CLA	CMB-C2B-C3B	2.05	131.37	126.55
22	S	602	CLA	CMB-C2B-C3B	2.05	131.36	126.55
22	B	828	CLA	C1-C2-C3	-2.05	122.85	126.20
24	T	613	DD6	C14-C13-C11	-2.04	122.36	125.53
22	B	807	CLA	C1-C2-C3	-2.04	122.85	126.20
22	S	608	CLA	O2A-CGA-O1A	-2.04	118.08	123.33
22	U	406	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
24	V	614	DD6	C25-C26-C27	-2.04	120.90	126.61
24	P	613	DD6	O1-C20-C19	-2.04	111.58	113.49
28	Q	602	LMG	O7-C10-O9	-2.04	118.93	123.70
24	U	416	DD6	C28-C27-C26	-2.04	120.22	124.18
22	U	411	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
27	H	321	LMU	C1B-O1B-C4'	-2.04	111.86	115.27
22	S	614	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
22	X	402	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
24	A	858	DD6	O1-C20-C21	-2.04	112.77	115.05
22	I	607	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
22	V	604	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
22	T	607	CLA	C1-C2-C3	-2.04	122.86	126.20
22	A	835	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	U	409	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
22	W	402	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
22	L	407	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	W	409	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	S	607	CLA	C1-C2-C3	-2.04	122.86	126.20
24	Q	614	DD6	C37-C36-C35	2.04	118.17	114.42
22	R	606	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	S	602	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
22	U	410	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
22	T	608	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
24	S	611	DD6	C25-C26-C27	-2.04	120.92	126.61
22	B	831	CLA	C1-C2-C3	-2.03	122.86	126.20
22	L	403	CLA	CMB-C2B-C3B	2.03	131.34	126.55
22	B	839	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
22	I	609	CLA	CMB-C2B-C3B	2.03	131.34	126.55
22	K	603	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
24	N	613	DD6	C32-C33-C34	-2.03	109.13	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	315	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
21	J	103	BCR	C33-C5-C4	2.03	117.93	113.60
22	A	838	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
21	B	801	BCR	C38-C26-C27	2.03	117.93	113.60
22	S	604	CLA	C1-C2-C3	-2.03	122.87	126.20
22	X	404	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
22	S	614	CLA	O2D-CGD-CBD	2.03	114.78	111.23
22	A	814	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
24	U	417	DD6	C40-C32-C31	-2.03	106.88	110.52
22	K	610	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	S	615	CLA	C1-C2-C3	-2.03	122.87	126.20
22	A	842	CLA	C1-C2-C3	-2.03	122.87	126.20
22	Q	617	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	V	617	CLA	O2D-CGD-CBD	2.03	114.78	111.23
22	G	609	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
22	K	606	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	T	603	CLA	O2D-CGD-CBD	2.03	114.78	111.23
22	B	826	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	I	603	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	O	311	CLA	C1-C2-C3	-2.03	122.87	126.20
28	A	855	LMG	O7-C10-O9	-2.03	118.96	123.70
22	W	404	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
22	G	606	CLA	C1-C2-C3	-2.03	122.88	126.20
28	K	601	LMG	O1-C1-C2	-2.03	105.19	108.27
28	B	856	LMG	O7-C10-O9	-2.03	118.97	123.70
22	B	827	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
22	B	805	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
24	H	314	DD6	O1-C20-C21	-2.02	112.79	115.05
24	S	612	DD6	C37-C36-C35	2.02	118.14	114.42
24	X	414	DD6	C28-C27-C26	-2.02	120.26	124.18
30	O	302	SQD	O8-S-C6	-2.02	102.07	105.97
22	O	313	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
22	Q	610	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
22	B	808	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
24	G	612	DD6	C26-C25-C24	-2.02	117.35	123.20
28	B	856	LMG	O1-C7-C8	-2.02	105.91	110.82
22	A	813	CLA	O1D-CGD-CBD	2.02	128.50	124.52
22	K	605	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	F	401	DGD	O1G-C1A-O1A	-2.02	118.58	123.63
22	H	309	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
24	H	314	DD6	C14-C13-C11	-2.02	122.40	125.53
24	T	613	DD6	C28-C27-C26	-2.02	120.27	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	308	CLA	CMB-C2B-C3B	2.02	131.29	126.55
21	A	850	BCR	C16-C15-C14	-2.02	119.40	123.52
22	N	605	CLA	CMB-C2B-C3B	2.01	131.29	126.55
26	B	851	LHG	C26-C25-C24	2.01	120.53	113.13
22	B	806	CLA	C1-C2-C3	-2.01	122.90	126.20
28	J	101	LMG	O1-C1-C2	-2.01	105.22	108.27
22	R	602	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
22	G	602	CLA	CMB-C2B-C3B	2.01	131.29	126.55
26	K	616	LHG	C26-C25-C24	2.01	120.52	113.13
24	U	417	DD6	C25-C26-C27	-2.01	120.98	126.61
22	S	603	CLA	C3B-C4B-NB	-2.01	108.73	110.53
28	H	317	LMG	O1-C1-C2	-2.01	105.22	108.27
22	B	826	CLA	C1-C2-C3	-2.01	122.90	126.20
22	A	826	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
28	K	622	LMG	O1-C7-C8	-2.01	105.92	110.82
22	R	604	CLA	CHB-C4A-NA	2.01	127.30	124.40
24	L	413	DD6	O1-C20-C21	-2.01	112.80	115.05
22	W	410	CLA	C1-C2-C3	-2.01	122.90	126.20
22	A	837	CLA	C1-C2-C3	-2.01	123.51	126.76
21	B	846	BCR	C28-C27-C26	-2.01	110.47	114.06
22	T	603	CLA	C1-C2-C3	-2.01	122.90	126.20
22	R	601	CLA	O2D-CGD-CBD	2.01	114.75	111.23
22	I	606	CLA	C1-C2-C3	-2.01	122.90	126.20
22	O	308	CLA	C1-C2-C3	-2.01	122.90	126.20
24	L	414	DD6	C28-C27-C26	-2.01	120.28	124.18
21	B	842	BCR	C21-C20-C19	-2.01	117.38	123.20
22	S	609	CLA	C1-C2-C3	-2.01	122.90	126.20
26	O	318	LHG	C26-C25-C24	2.01	120.51	113.13
22	A	810	CLA	C1-C2-C3	-2.01	122.91	126.20
22	K	611	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
22	K	604	CLA	CMB-C2B-C3B	2.01	131.27	126.55
22	B	810	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
22	B	808	CLA	C1-C2-C3	-2.01	122.91	126.20
27	O	322	LMU	C1B-O5B-C5B	2.01	117.64	113.72
22	O	307	CLA	O2D-CGD-CBD	2.01	114.74	111.23
22	S	606	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
28	H	317	LMG	O1-C7-C8	-2.01	105.94	110.82
22	T	611	CLA	C1-C2-C3	-2.01	122.91	126.20
22	B	830	CLA	CMB-C2B-C3B	2.01	131.27	126.55
24	X	401	DD6	O1-C20-C21	-2.01	112.81	115.05
22	A	805	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
22	A	806	CLA	O2A-CGA-O1A	-2.01	118.61	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	816	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
22	H	306	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
22	H	307	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
22	U	405	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
22	A	818	CLA	CMB-C2B-C3B	2.00	131.26	126.55
22	H	307	CLA	C1-C2-C3	-2.00	122.91	126.20
22	A	814	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
21	A	851	BCR	C36-C18-C17	-2.00	119.57	122.82
24	A	858	DD6	C26-C25-C24	2.00	129.00	123.20
22	A	804	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
24	G	613	DD6	C40-C32-C31	-2.00	106.93	110.52
22	K	613	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
22	A	841	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
22	K	612	CLA	CMB-C2B-C3B	2.00	131.26	126.55
22	L	408	CLA	CAA-CBA-CGA	-2.00	107.52	113.21
22	Q	609	CLA	C1-C2-C3	-2.00	122.92	126.20
22	L	410	CLA	CAA-C2A-C3A	-2.00	107.59	113.00
21	B	801	BCR	C23-C24-C25	-2.00	121.65	127.00
24	B	841	DD6	C21-C20-C15	-2.00	119.01	122.30
21	J	103	BCR	C2-C1-C6	2.00	113.34	110.44

All (304) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	802	CLA	ND
22	B	803	CLA	ND
22	B	804	CLA	ND
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

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Mol	Chain	Res	Type	Atom
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	859	CLA	ND
22	F	403	CLA	ND
22	F	404	CLA	ND
22	F	405	CLA	ND
22	G	601	CLA	ND
22	G	602	CLA	ND
22	G	603	CLA	ND
22	G	604	CLA	ND
22	G	605	CLA	ND
22	G	606	CLA	ND
22	G	607	CLA	ND
22	G	608	CLA	ND
22	G	609	CLA	ND
22	G	610	CLA	ND
22	G	611	CLA	ND
22	H	302	CLA	ND
22	H	303	CLA	ND
22	H	304	CLA	ND
22	H	305	CLA	ND
22	H	306	CLA	ND
22	H	307	CLA	ND
22	H	308	CLA	ND

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Mol	Chain	Res	Type	Atom
22	H	309	CLA	ND
22	H	310	CLA	ND
22	H	311	CLA	ND
22	H	312	CLA	ND
22	H	313	CLA	ND
22	H	318	CLA	ND
22	I	601	CLA	ND
22	I	602	CLA	ND
22	I	603	CLA	ND
22	I	604	CLA	ND
22	I	605	CLA	ND
22	I	606	CLA	ND
22	I	607	CLA	ND
22	I	608	CLA	ND
22	I	609	CLA	ND
22	I	610	CLA	ND
22	I	611	CLA	ND
22	J	102	CLA	ND
22	K	602	CLA	ND
22	K	603	CLA	ND
22	K	604	CLA	ND
22	K	605	CLA	ND
22	K	606	CLA	ND
22	K	607	CLA	ND
22	K	608	CLA	ND
22	K	609	CLA	ND
22	K	610	CLA	ND
22	K	611	CLA	ND
22	K	612	CLA	ND
22	K	613	CLA	ND
22	K	617	CLA	ND
22	L	402	CLA	ND
22	L	403	CLA	ND
22	L	404	CLA	ND
22	L	405	CLA	ND
22	L	406	CLA	ND
22	L	407	CLA	ND
22	L	408	CLA	ND
22	L	409	CLA	ND
22	L	410	CLA	ND
22	L	411	CLA	ND
22	L	412	CLA	ND

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Mol	Chain	Res	Type	Atom
22	L	417	CLA	ND
22	N	601	CLA	ND
22	N	602	CLA	ND
22	N	603	CLA	ND
22	N	604	CLA	ND
22	N	605	CLA	ND
22	N	606	CLA	ND
22	N	607	CLA	ND
22	N	608	CLA	ND
22	N	609	CLA	ND
22	N	610	CLA	ND
22	N	611	CLA	ND
22	O	305	CLA	ND
22	O	306	CLA	ND
22	O	307	CLA	ND
22	O	308	CLA	ND
22	O	309	CLA	ND
22	O	310	CLA	ND
22	O	311	CLA	ND
22	O	312	CLA	ND
22	O	313	CLA	ND
22	O	314	CLA	ND
22	O	315	CLA	ND
22	O	319	CLA	ND
22	P	602	CLA	ND
22	P	604	CLA	ND
22	P	605	CLA	ND
22	P	606	CLA	ND
22	P	607	CLA	ND
22	P	608	CLA	ND
22	P	609	CLA	ND
22	P	610	CLA	ND
22	P	611	CLA	ND
22	Q	601	CLA	ND
22	Q	603	CLA	ND
22	Q	604	CLA	ND
22	Q	605	CLA	ND
22	Q	606	CLA	ND
22	Q	607	CLA	ND
22	Q	608	CLA	ND
22	Q	609	CLA	ND
22	Q	610	CLA	ND

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Mol	Chain	Res	Type	Atom
22	Q	611	CLA	ND
22	Q	612	CLA	ND
22	Q	613	CLA	ND
22	Q	617	CLA	ND
22	Q	618	CLA	ND
22	R	601	CLA	ND
22	R	602	CLA	ND
22	R	603	CLA	ND
22	R	604	CLA	ND
22	R	605	CLA	ND
22	R	606	CLA	ND
22	R	607	CLA	ND
22	R	608	CLA	ND
22	R	609	CLA	ND
22	R	610	CLA	ND
22	R	611	CLA	ND
22	R	615	CLA	ND
22	S	601	CLA	ND
22	S	602	CLA	ND
22	S	603	CLA	ND
22	S	604	CLA	ND
22	S	605	CLA	ND
22	S	606	CLA	ND
22	S	607	CLA	ND
22	S	608	CLA	ND
22	S	610	CLA	ND
22	S	614	CLA	ND
22	S	615	CLA	ND
22	T	601	CLA	ND
22	T	602	CLA	ND
22	T	603	CLA	ND
22	T	604	CLA	ND
22	T	605	CLA	ND
22	T	606	CLA	ND
22	T	607	CLA	ND
22	T	608	CLA	ND
22	T	609	CLA	ND
22	T	610	CLA	ND
22	T	611	CLA	ND
22	U	401	CLA	ND
22	U	403	CLA	ND
22	U	404	CLA	ND

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Mol	Chain	Res	Type	Atom
22	U	405	CLA	ND
22	U	406	CLA	ND
22	U	409	CLA	ND
22	U	410	CLA	ND
22	U	411	CLA	ND
22	U	412	CLA	ND
22	U	413	CLA	ND
22	U	414	CLA	ND
22	U	415	CLA	ND
22	U	420	CLA	ND
22	V	601	CLA	ND
22	V	602	CLA	ND
22	V	603	CLA	ND
22	V	604	CLA	ND
22	V	607	CLA	ND
22	V	608	CLA	ND
22	V	609	CLA	ND
22	V	610	CLA	ND
22	V	611	CLA	ND
22	V	612	CLA	ND
22	V	613	CLA	ND
22	V	617	CLA	ND
22	W	402	CLA	ND
22	W	403	CLA	ND
22	W	404	CLA	ND
22	W	405	CLA	ND
22	W	406	CLA	ND
22	W	409	CLA	ND
22	W	410	CLA	ND
22	W	411	CLA	ND
22	W	412	CLA	ND
22	W	413	CLA	ND
22	W	414	CLA	ND
22	W	415	CLA	ND
22	W	419	CLA	ND
22	X	402	CLA	ND
22	X	403	CLA	ND
22	X	404	CLA	ND
22	X	405	CLA	ND
22	X	407	CLA	ND
22	X	408	CLA	ND
22	X	409	CLA	ND

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Mol	Chain	Res	Type	Atom
22	X	410	CLA	ND
22	X	411	CLA	ND
22	X	412	CLA	ND
22	X	413	CLA	ND
22	X	417	CLA	ND
22	X	419	CLA	ND
22	A	801	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND
22	A	805	CLA	ND
22	A	806	CLA	ND
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

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Mol	Chain	Res	Type	Atom
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	844	CLA	ND
22	A	852	CLA	ND
31	U	407	CHL	NC
31	U	407	CHL	NA
31	U	407	CHL	ND
31	U	408	CHL	NC
31	U	408	CHL	NA
31	U	408	CHL	ND
31	V	605	CHL	NC
31	V	605	CHL	NA
31	V	605	CHL	ND
31	V	606	CHL	NC
31	V	606	CHL	NA
31	V	606	CHL	ND
31	W	407	CHL	NC
31	W	407	CHL	NA
31	W	407	CHL	ND
31	W	408	CHL	NC
31	W	408	CHL	NA
31	W	408	CHL	ND
31	W	422	CHL	NC
31	W	422	CHL	NA
31	W	422	CHL	ND
31	X	406	CHL	NC
31	X	406	CHL	NA
31	X	406	CHL	ND
33	A	802	CL0	NC
33	A	802	CL0	NA
33	A	802	CL0	ND

All (3251) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	801	BCR	C7-C8-C9-C10
21	B	801	BCR	C7-C8-C9-C34
21	B	842	BCR	C21-C22-C23-C24
21	B	842	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	B	845	BCR	C21-C22-C23-C24
21	B	846	BCR	C21-C22-C23-C24
21	M	101	BCR	C23-C24-C25-C26
21	A	850	BCR	C37-C22-C23-C24
22	B	804	CLA	C3A-C2A-CAA-CBA
22	B	804	CLA	CAD-CBD-CGD-O1D
22	B	804	CLA	CAD-CBD-CGD-O2D
22	B	807	CLA	C2B-C3B-CAB-CBB
22	B	807	CLA	C4B-C3B-CAB-CBB
22	B	807	CLA	CHA-CBD-CGD-O1D
22	B	807	CLA	CHA-CBD-CGD-O2D
22	B	812	CLA	C1A-C2A-CAA-CBA
22	B	812	CLA	CAD-CBD-CGD-O1D
22	B	812	CLA	CAD-CBD-CGD-O2D
22	B	814	CLA	CHA-CBD-CGD-O2D
22	B	815	CLA	C1A-C2A-CAA-CBA
22	B	815	CLA	C3A-C2A-CAA-CBA
22	B	816	CLA	C3A-C2A-CAA-CBA
22	B	818	CLA	CBD-CGD-O2D-CED
22	B	824	CLA	C3A-C2A-CAA-CBA
22	B	824	CLA	CHA-CBD-CGD-O1D
22	B	824	CLA	CHA-CBD-CGD-O2D
22	B	825	CLA	C1A-C2A-CAA-CBA
22	B	828	CLA	CAD-CBD-CGD-O1D
22	B	828	CLA	CAD-CBD-CGD-O2D
22	B	829	CLA	C1A-C2A-CAA-CBA
22	B	829	CLA	C3A-C2A-CAA-CBA
22	B	830	CLA	C11-C12-C13-C14
22	B	832	CLA	CHA-CBD-CGD-O2D
22	B	833	CLA	C2B-C3B-CAB-CBB
22	B	833	CLA	C4B-C3B-CAB-CBB
22	B	859	CLA	C2B-C3B-CAB-CBB
22	B	859	CLA	C4B-C3B-CAB-CBB
22	G	606	CLA	C1A-C2A-CAA-CBA
22	G	606	CLA	C3A-C2A-CAA-CBA
22	G	608	CLA	C1A-C2A-CAA-CBA
22	G	608	CLA	C3A-C2A-CAA-CBA
22	G	609	CLA	CHA-CBD-CGD-O1D
22	G	609	CLA	CHA-CBD-CGD-O2D
22	H	307	CLA	C1A-C2A-CAA-CBA
22	H	307	CLA	C3A-C2A-CAA-CBA
22	H	309	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	H	309	CLA	C4B-C3B-CAB-CBB
22	H	312	CLA	C1A-C2A-CAA-CBA
22	H	312	CLA	C3A-C2A-CAA-CBA
22	I	601	CLA	C1A-C2A-CAA-CBA
22	I	606	CLA	C4B-C3B-CAB-CBB
22	I	609	CLA	CHA-CBD-CGD-O1D
22	I	609	CLA	CHA-CBD-CGD-O2D
22	I	611	CLA	C1A-C2A-CAA-CBA
22	I	611	CLA	C3A-C2A-CAA-CBA
22	J	102	CLA	C1A-C2A-CAA-CBA
22	K	605	CLA	C1A-C2A-CAA-CBA
22	K	605	CLA	C3A-C2A-CAA-CBA
22	K	605	CLA	CAD-CBD-CGD-O1D
22	K	605	CLA	CAD-CBD-CGD-O2D
22	K	605	CLA	C6-C7-C8-C9
22	K	607	CLA	C1A-C2A-CAA-CBA
22	K	607	CLA	C3A-C2A-CAA-CBA
22	K	609	CLA	C1A-C2A-CAA-CBA
22	L	403	CLA	CHA-CBD-CGD-O2D
22	L	407	CLA	C1A-C2A-CAA-CBA
22	L	407	CLA	C3A-C2A-CAA-CBA
22	L	408	CLA	CBD-CGD-O2D-CED
22	L	409	CLA	CBD-CGD-O2D-CED
22	L	410	CLA	C1A-C2A-CAA-CBA
22	N	607	CLA	C1A-C2A-CAA-CBA
22	N	609	CLA	CHA-CBD-CGD-O1D
22	N	609	CLA	CHA-CBD-CGD-O2D
22	N	611	CLA	CBD-CGD-O2D-CED
22	O	306	CLA	CHA-CBD-CGD-O1D
22	O	306	CLA	CHA-CBD-CGD-O2D
22	O	307	CLA	CHA-CBD-CGD-O2D
22	O	308	CLA	C3A-C2A-CAA-CBA
22	O	309	CLA	C1A-C2A-CAA-CBA
22	O	309	CLA	C3A-C2A-CAA-CBA
22	O	309	CLA	C2B-C3B-CAB-CBB
22	O	309	CLA	C4B-C3B-CAB-CBB
22	O	311	CLA	C2B-C3B-CAB-CBB
22	O	311	CLA	C4B-C3B-CAB-CBB
22	O	313	CLA	C11-C10-C8-C7
22	P	602	CLA	C3A-C2A-CAA-CBA
22	P	602	CLA	CBD-CGD-O2D-CED
22	P	606	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	P	606	CLA	C3A-C2A-CAA-CBA
22	P	607	CLA	C1A-C2A-CAA-CBA
22	P	608	CLA	CHA-CBD-CGD-O1D
22	P	608	CLA	CHA-CBD-CGD-O2D
22	P	609	CLA	CHA-CBD-CGD-O2D
22	P	611	CLA	C1A-C2A-CAA-CBA
22	P	611	CLA	C3A-C2A-CAA-CBA
22	Q	606	CLA	CAD-CBD-CGD-O2D
22	Q	608	CLA	C1A-C2A-CAA-CBA
22	Q	608	CLA	C3A-C2A-CAA-CBA
22	Q	613	CLA	C1A-C2A-CAA-CBA
22	Q	618	CLA	CHA-CBD-CGD-O1D
22	Q	618	CLA	CHA-CBD-CGD-O2D
22	R	603	CLA	CHA-CBD-CGD-O1D
22	R	603	CLA	CHA-CBD-CGD-O2D
22	R	606	CLA	C1A-C2A-CAA-CBA
22	R	606	CLA	C3A-C2A-CAA-CBA
22	R	606	CLA	CBD-CGD-O2D-CED
22	R	607	CLA	CBD-CGD-O2D-CED
22	R	611	CLA	C1A-C2A-CAA-CBA
22	R	611	CLA	C3A-C2A-CAA-CBA
22	S	601	CLA	CHA-CBD-CGD-O1D
22	S	601	CLA	CHA-CBD-CGD-O2D
22	S	605	CLA	C1A-C2A-CAA-CBA
22	S	605	CLA	C3A-C2A-CAA-CBA
22	S	605	CLA	C4-C3-C5-C6
22	S	606	CLA	C1A-C2A-CAA-CBA
22	S	607	CLA	C1A-C2A-CAA-CBA
22	S	608	CLA	C1A-C2A-CAA-CBA
22	S	608	CLA	C3A-C2A-CAA-CBA
22	T	603	CLA	CHA-CBD-CGD-O1D
22	T	603	CLA	CHA-CBD-CGD-O2D
22	T	606	CLA	C1A-C2A-CAA-CBA
22	T	606	CLA	C3A-C2A-CAA-CBA
22	T	611	CLA	C3A-C2A-CAA-CBA
22	T	611	CLA	CAD-CBD-CGD-O2D
22	T	611	CLA	CBD-CGD-O2D-CED
22	U	401	CLA	C1A-C2A-CAA-CBA
22	U	401	CLA	C3A-C2A-CAA-CBA
22	U	403	CLA	C1A-C2A-CAA-CBA
22	U	403	CLA	C3A-C2A-CAA-CBA
22	U	409	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	U	409	CLA	C3A-C2A-CAA-CBA
22	U	410	CLA	C1A-C2A-CAA-CBA
22	U	410	CLA	C3A-C2A-CAA-CBA
22	U	413	CLA	C1A-C2A-CAA-CBA
22	U	413	CLA	C3A-C2A-CAA-CBA
22	U	413	CLA	CBD-CGD-O2D-CED
22	U	415	CLA	C1A-C2A-CAA-CBA
22	U	415	CLA	C3A-C2A-CAA-CBA
22	U	415	CLA	CBD-CGD-O2D-CED
22	U	420	CLA	C1A-C2A-CAA-CBA
22	U	420	CLA	C3A-C2A-CAA-CBA
22	U	420	CLA	CBD-CGD-O2D-CED
22	V	601	CLA	CBD-CGD-O2D-CED
22	V	602	CLA	C4B-C3B-CAB-CBB
22	V	602	CLA	CBD-CGD-O2D-CED
22	V	604	CLA	CBD-CGD-O2D-CED
22	V	607	CLA	CBD-CGD-O2D-CED
22	V	608	CLA	CBD-CGD-O2D-CED
22	V	609	CLA	CBD-CGD-O2D-CED
22	V	611	CLA	CHA-CBD-CGD-O2D
22	V	612	CLA	CBD-CGD-O2D-CED
22	V	613	CLA	CAD-CBD-CGD-O1D
22	V	613	CLA	CAD-CBD-CGD-O2D
22	W	414	CLA	CBD-CGD-O2D-CED
22	X	402	CLA	C1A-C2A-CAA-CBA
22	X	402	CLA	C3A-C2A-CAA-CBA
22	X	402	CLA	O1A-CGA-O2A-C1
22	X	408	CLA	C1A-C2A-CAA-CBA
22	X	408	CLA	C3A-C2A-CAA-CBA
22	X	409	CLA	CBD-CGD-O2D-CED
22	X	413	CLA	C1A-C2A-CAA-CBA
22	X	413	CLA	C3A-C2A-CAA-CBA
22	X	417	CLA	CAD-CBD-CGD-O1D
22	X	417	CLA	CAD-CBD-CGD-O2D
22	X	419	CLA	C1A-C2A-CAA-CBA
22	X	419	CLA	C3A-C2A-CAA-CBA
22	X	419	CLA	CBD-CGD-O2D-CED
22	A	805	CLA	C1A-C2A-CAA-CBA
22	A	805	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	C1A-C2A-CAA-CBA
22	A	806	CLA	C3A-C2A-CAA-CBA
22	A	807	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	807	CLA	CAD-CBD-CGD-O1D
22	A	807	CLA	CAD-CBD-CGD-O2D
22	A	810	CLA	CHA-CBD-CGD-O1D
22	A	810	CLA	CHA-CBD-CGD-O2D
22	A	811	CLA	C1A-C2A-CAA-CBA
22	A	817	CLA	C2-C1-O2A-CGA
22	A	818	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	821	CLA	C1A-C2A-CAA-CBA
22	A	821	CLA	C3A-C2A-CAA-CBA
22	A	824	CLA	C2-C3-C5-C6
22	A	824	CLA	C4-C3-C5-C6
22	A	825	CLA	C1A-C2A-CAA-CBA
22	A	825	CLA	C3A-C2A-CAA-CBA
22	A	825	CLA	C2B-C3B-CAB-CBB
22	A	825	CLA	C4B-C3B-CAB-CBB
22	A	827	CLA	C3A-C2A-CAA-CBA
22	A	830	CLA	C1A-C2A-CAA-CBA
22	A	831	CLA	CHA-CBD-CGD-O1D
22	A	831	CLA	CHA-CBD-CGD-O2D
22	A	832	CLA	C1A-C2A-CAA-CBA
22	A	832	CLA	C3A-C2A-CAA-CBA
22	A	835	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	838	CLA	C1A-C2A-CAA-CBA
22	A	852	CLA	C1A-C2A-CAA-CBA
24	F	406	DD6	C5-C6-C8-C9
24	F	406	DD6	C7-C6-C8-C9
24	L	415	DD6	C10-C11-C13-C14
24	L	415	DD6	C12-C11-C13-C14
24	P	613	DD6	C-C1-C24-C25
24	P	613	DD6	C2-C1-C24-C25
24	P	613	DD6	C13-C14-C15-O1
24	R	613	DD6	C13-C14-C15-O1
24	X	416	DD6	C10-C11-C13-C14
24	A	858	DD6	C13-C14-C15-O1
25	B	847	DGD	O6D-C1D-O3G-C3G
25	B	847	DGD	C2E-C1E-O5D-C6D
25	B	847	DGD	O6E-C1E-O5D-C6D
25	O	304	DGD	O6D-C1D-O3G-C3G
26	B	848	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	B	848	LHG	O2-C2-C3-O3
26	B	848	LHG	C3-O3-P-O6
26	B	851	LHG	O2-C2-C3-O3
26	B	851	LHG	C3-O3-P-O4
26	B	851	LHG	C3-O3-P-O6
26	B	851	LHG	C4-O6-P-O3
26	B	851	LHG	C4-O6-P-O5
26	G	614	LHG	C3-O3-P-O5
26	H	316	LHG	C3-O3-P-O5
26	K	616	LHG	O7-C5-C6-O8
26	K	619	LHG	C1-C2-C3-O3
26	K	619	LHG	C3-O3-P-O4
26	K	619	LHG	C3-O3-P-O6
26	K	619	LHG	O6-C4-C5-O7
26	L	416	LHG	C3-O3-P-O5
26	L	416	LHG	C3-O3-P-O6
26	N	614	LHG	C3-O3-P-O5
26	N	616	LHG	C3-O3-P-O4
26	N	616	LHG	C3-O3-P-O6
26	N	616	LHG	C4-O6-P-O3
26	N	616	LHG	C4-O6-P-O4
26	N	616	LHG	C4-O6-P-O5
26	N	616	LHG	O9-C7-O7-C5
26	O	318	LHG	C4-O6-P-O3
26	O	318	LHG	C4-O6-P-O4
26	O	321	LHG	O1-C1-C2-O2
26	O	321	LHG	O1-C1-C2-C3
26	O	321	LHG	C3-O3-P-O4
26	O	321	LHG	C3-O3-P-O5
26	O	321	LHG	C3-O3-P-O6
26	O	321	LHG	O10-C23-O8-C6
26	O	321	LHG	C24-C23-O8-C6
26	O	323	LHG	O1-C1-C2-C3
26	O	323	LHG	O2-C2-C3-O3
26	O	323	LHG	C3-O3-P-O5
26	O	323	LHG	C3-O3-P-O6
26	O	323	LHG	C4-O6-P-O5
26	O	324	LHG	O1-C1-C2-C3
26	O	324	LHG	C3-O3-P-O5
26	O	324	LHG	C3-O3-P-O6
26	O	324	LHG	C4-O6-P-O3
26	O	324	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
26	P	601	LHG	O1-C1-C2-C3
26	P	601	LHG	O7-C5-C6-O8
26	P	601	LHG	C8-C7-O7-C5
26	Q	616	LHG	O1-C1-C2-C3
26	Q	616	LHG	C3-O3-P-O4
26	Q	616	LHG	C3-O3-P-O5
26	Q	616	LHG	C3-O3-P-O6
26	R	614	LHG	C3-O3-P-O4
26	R	614	LHG	C3-O3-P-O5
26	R	614	LHG	C3-O3-P-O6
26	S	613	LHG	O1-C1-C2-C3
26	S	613	LHG	C3-O3-P-O4
26	S	613	LHG	C3-O3-P-O5
26	S	613	LHG	C3-O3-P-O6
26	S	613	LHG	C4-O6-P-O3
26	S	613	LHG	C4-O6-P-O4
26	S	613	LHG	C4-O6-P-O5
26	T	614	LHG	C3-O3-P-O4
26	T	614	LHG	C3-O3-P-O5
26	T	614	LHG	C3-O3-P-O6
26	T	614	LHG	C4-O6-P-O4
26	T	614	LHG	C4-O6-P-O5
26	U	419	LHG	C4-O6-P-O3
26	U	419	LHG	C4-O6-P-O5
26	U	419	LHG	C8-C7-O7-C5
26	W	420	LHG	C3-O3-P-O5
26	W	420	LHG	C3-O3-P-O6
26	W	420	LHG	C4-O6-P-O3
26	W	420	LHG	C4-O6-P-O4
26	W	420	LHG	C4-O6-P-O5
26	X	420	LHG	C1-C2-C3-O3
26	A	845	LHG	O1-C1-C2-O2
26	A	845	LHG	O1-C1-C2-C3
26	A	845	LHG	C3-O3-P-O4
26	A	845	LHG	C3-O3-P-O6
26	A	845	LHG	C4-O6-P-O3
26	A	846	LHG	C4-O6-P-O3
26	A	846	LHG	C4-O6-P-O4
26	A	846	LHG	C4-O6-P-O5
26	A	846	LHG	C8-C7-O7-C5
27	J	104	LMU	C2-C1-O1'-C1'
27	K	620	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
28	B	852	LMG	C2-C1-O1-C7
28	B	856	LMG	O6-C1-O1-C7
28	F	408	LMG	O9-C10-O7-C8
28	H	317	LMG	O6-C1-O1-C7
28	H	317	LMG	O1-C7-C8-O7
28	H	319	LMG	C2-C1-O1-C7
28	H	319	LMG	O6-C1-O1-C7
28	H	319	LMG	O1-C7-C8-O7
28	K	601	LMG	O6-C1-O1-C7
28	K	601	LMG	O9-C10-O7-C8
28	K	601	LMG	C11-C10-O7-C8
28	K	618	LMG	O6-C1-O1-C7
28	N	615	LMG	O1-C7-C8-O7
28	N	615	LMG	C11-C10-O7-C8
28	U	402	LMG	C2-C1-O1-C7
28	U	402	LMG	O6-C1-O1-C7
28	U	402	LMG	O9-C10-O7-C8
28	U	402	LMG	C11-C10-O7-C8
28	W	401	LMG	C11-C10-O7-C8
30	O	302	SQD	O10-C23-O48-C46
30	O	302	SQD	C24-C23-O48-C46
31	W	422	CHL	C4-C3-C5-C6
22	R	606	CLA	O1D-CGD-O2D-CED
22	R	608	CLA	O1D-CGD-O2D-CED
22	I	610	CLA	O1D-CGD-O2D-CED
22	L	408	CLA	O1D-CGD-O2D-CED
22	P	602	CLA	O1D-CGD-O2D-CED
22	R	601	CLA	O1D-CGD-O2D-CED
22	R	609	CLA	O1D-CGD-O2D-CED
22	T	611	CLA	O1D-CGD-O2D-CED
22	U	415	CLA	O1D-CGD-O2D-CED
22	V	608	CLA	O1D-CGD-O2D-CED
22	V	612	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	CBD-CGD-O2D-CED
22	B	813	CLA	CBD-CGD-O2D-CED
22	B	821	CLA	CBD-CGD-O2D-CED
22	B	826	CLA	CBD-CGD-O2D-CED
22	F	405	CLA	CBD-CGD-O2D-CED
22	G	610	CLA	CBD-CGD-O2D-CED
22	H	307	CLA	CBD-CGD-O2D-CED
22	H	311	CLA	CBD-CGD-O2D-CED
22	I	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	I	607	CLA	CBD-CGD-O2D-CED
22	I	609	CLA	CBD-CGD-O2D-CED
22	I	610	CLA	CBD-CGD-O2D-CED
22	K	605	CLA	CBD-CGD-O2D-CED
22	L	406	CLA	CBD-CGD-O2D-CED
22	N	602	CLA	CBD-CGD-O2D-CED
22	N	607	CLA	CBD-CGD-O2D-CED
22	N	610	CLA	CBD-CGD-O2D-CED
22	Q	606	CLA	CBD-CGD-O2D-CED
22	R	601	CLA	CBD-CGD-O2D-CED
22	R	602	CLA	CBD-CGD-O2D-CED
22	R	604	CLA	CBD-CGD-O2D-CED
22	R	608	CLA	CBD-CGD-O2D-CED
22	R	609	CLA	CBD-CGD-O2D-CED
22	R	610	CLA	CBD-CGD-O2D-CED
22	R	615	CLA	CBD-CGD-O2D-CED
22	S	604	CLA	CBD-CGD-O2D-CED
22	S	605	CLA	CBD-CGD-O2D-CED
22	U	401	CLA	CBD-CGD-O2D-CED
22	U	404	CLA	CBD-CGD-O2D-CED
22	V	610	CLA	CBD-CGD-O2D-CED
22	V	613	CLA	CBD-CGD-O2D-CED
22	V	617	CLA	CBD-CGD-O2D-CED
22	W	410	CLA	CBD-CGD-O2D-CED
22	W	411	CLA	CBD-CGD-O2D-CED
22	A	801	CLA	CBD-CGD-O2D-CED
22	A	817	CLA	CBD-CGD-O2D-CED
22	A	824	CLA	CBD-CGD-O2D-CED
22	A	852	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	O1A-CGA-O2A-C1
22	X	405	CLA	O1A-CGA-O2A-C1
22	A	817	CLA	O1A-CGA-O2A-C1
22	A	824	CLA	O1A-CGA-O2A-C1
26	K	616	LHG	O10-C'23-O8-C6
28	H	322	LMG	O10-C'28-O8-C9
22	U	420	CLA	O1D-CGD-O2D-CED
22	V	601	CLA	O1D-CGD-O2D-CED
27	O	322	LMU	O5B-C1B-O1B-C4'
22	B	821	CLA	O1D-CGD-O2D-CED
22	R	615	CLA	O1D-CGD-O2D-CED
22	X	402	CLA	CBA-CGA-O2A-C1
22	X	405	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	K	616	LHG	C24-C23-O8-C6
22	F	403	CLA	CBD-CGD-O2D-CED
22	U	410	CLA	CBD-CGD-O2D-CED
22	B	817	CLA	O1A-CGA-O2A-C1
22	B	819	CLA	O1A-CGA-O2A-C1
22	O	308	CLA	O1A-CGA-O2A-C1
22	S	605	CLA	O1A-CGA-O2A-C1
22	S	609	CLA	O1A-CGA-O2A-C1
22	T	603	CLA	O1A-CGA-O2A-C1
22	A	805	CLA	O1A-CGA-O2A-C1
26	T	614	LHG	O10-C23-O8-C6
28	N	615	LMG	O10-C28-O8-C9
22	I	609	CLA	O1D-CGD-O2D-CED
22	L	409	CLA	O1D-CGD-O2D-CED
22	R	610	CLA	O1D-CGD-O2D-CED
22	A	801	CLA	O1D-CGD-O2D-CED
22	R	607	CLA	O1D-CGD-O2D-CED
22	V	602	CLA	O1D-CGD-O2D-CED
22	V	604	CLA	O1D-CGD-O2D-CED
22	V	607	CLA	O1D-CGD-O2D-CED
22	V	609	CLA	O1D-CGD-O2D-CED
22	W	414	CLA	O1D-CGD-O2D-CED
22	X	409	CLA	O1D-CGD-O2D-CED
26	O	324	LHG	O9-C7-O7-C5
26	P	601	LHG	O9-C7-O7-C5
26	U	419	LHG	O9-C7-O7-C5
26	A	846	LHG	O9-C7-O7-C5
28	I	615	LMG	O9-C10-O7-C8
28	N	615	LMG	O9-C10-O7-C8
28	W	401	LMG	O9-C10-O7-C8
22	U	413	CLA	O1D-CGD-O2D-CED
22	B	813	CLA	C3-C5-C6-C7
22	B	818	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	B	833	CLA	C3-C5-C6-C7
22	G	603	CLA	C3-C5-C6-C7
22	I	603	CLA	C3-C5-C6-C7
22	I	606	CLA	C3-C5-C6-C7
22	K	605	CLA	C3-C5-C6-C7
22	K	611	CLA	C3-C5-C6-C7
22	L	404	CLA	C3-C5-C6-C7
22	L	411	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	R	601	CLA	C3-C5-C6-C7
22	S	602	CLA	C3-C5-C6-C7
22	S	604	CLA	C3-C5-C6-C7
22	V	604	CLA	C3-C5-C6-C7
22	A	814	CLA	C3-C5-C6-C7
22	B	808	CLA	CBA-CGA-O2A-C1
22	B	817	CLA	CBA-CGA-O2A-C1
22	B	819	CLA	CBA-CGA-O2A-C1
22	K	610	CLA	CBA-CGA-O2A-C1
22	O	308	CLA	CBA-CGA-O2A-C1
22	S	605	CLA	CBA-CGA-O2A-C1
22	T	603	CLA	CBA-CGA-O2A-C1
22	V	603	CLA	CBA-CGA-O2A-C1
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	817	CLA	CBA-CGA-O2A-C1
22	A	821	CLA	CBA-CGA-O2A-C1
22	A	824	CLA	CBA-CGA-O2A-C1
28	N	615	LMG	C29-C28-O8-C9
22	B	805	CLA	CBD-CGD-O2D-CED
22	B	822	CLA	CBD-CGD-O2D-CED
22	G	607	CLA	CBD-CGD-O2D-CED
22	H	304	CLA	CBD-CGD-O2D-CED
22	H	318	CLA	CBD-CGD-O2D-CED
22	L	407	CLA	CBD-CGD-O2D-CED
22	L	411	CLA	CBD-CGD-O2D-CED
22	N	606	CLA	CBD-CGD-O2D-CED
22	O	308	CLA	CBD-CGD-O2D-CED
22	P	606	CLA	CBD-CGD-O2D-CED
22	Q	604	CLA	CBD-CGD-O2D-CED
22	Q	609	CLA	CBD-CGD-O2D-CED
22	Q	611	CLA	CBD-CGD-O2D-CED
22	Q	618	CLA	CBD-CGD-O2D-CED
22	S	607	CLA	CBD-CGD-O2D-CED
22	T	604	CLA	CBD-CGD-O2D-CED
22	T	606	CLA	CBD-CGD-O2D-CED
22	T	608	CLA	CBD-CGD-O2D-CED
22	U	403	CLA	CBD-CGD-O2D-CED
22	U	411	CLA	CBD-CGD-O2D-CED
22	U	414	CLA	CBD-CGD-O2D-CED
22	W	415	CLA	CBD-CGD-O2D-CED
22	X	405	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	812	CLA	CBD-CGD-O2D-CED
26	N	616	LHG	C8-C7-O7-C5
26	O	324	LHG	C8-C7-O7-C5
28	F	408	LMG	C11-C10-O7-C8
22	B	818	CLA	O1D-CGD-O2D-CED
22	N	611	CLA	O1D-CGD-O2D-CED
22	U	404	CLA	O1D-CGD-O2D-CED
22	V	613	CLA	O1D-CGD-O2D-CED
22	X	419	CLA	O1D-CGD-O2D-CED
22	B	820	CLA	C4-C3-C5-C6
22	B	832	CLA	C4-C3-C5-C6
22	B	834	CLA	C4-C3-C5-C6
22	L	402	CLA	C4-C3-C5-C6
22	R	602	CLA	C4-C3-C5-C6
22	U	411	CLA	C4-C3-C5-C6
22	A	811	CLA	C4-C3-C5-C6
22	A	814	CLA	C4-C3-C5-C6
22	B	820	CLA	C2-C3-C5-C6
22	B	832	CLA	C2-C3-C5-C6
22	B	834	CLA	C2-C3-C5-C6
22	L	402	CLA	C2-C3-C5-C6
22	R	602	CLA	C2-C3-C5-C6
22	S	605	CLA	C2-C3-C5-C6
31	W	422	CHL	C2-C3-C5-C6
22	F	405	CLA	O1D-CGD-O2D-CED
22	K	605	CLA	O1D-CGD-O2D-CED
22	W	411	CLA	O1D-CGD-O2D-CED
22	V	607	CLA	C2A-CAA-CBA-CGA
22	A	823	CLA	C2A-CAA-CBA-CGA
22	A	830	CLA	C2A-CAA-CBA-CGA
22	A	838	CLA	C3-C5-C6-C7
22	Q	605	CLA	C3-C5-C6-C7
33	A	802	CL0	C3-C5-C6-C7
22	B	830	CLA	CBA-CGA-O2A-C1
22	L	404	CLA	CBA-CGA-O2A-C1
22	R	615	CLA	CBA-CGA-O2A-C1
22	S	609	CLA	CBA-CGA-O2A-C1
25	F	401	DGD	C2A-C1A-O1G-C1G
26	T	614	LHG	C24-C23-O8-C6
28	H	322	LMG	C29-C28-O8-C9
26	B	851	LHG	C24-C25-C26-C27
26	G	614	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	T	614	LHG	C24-C25-C26-C27
26	U	419	LHG	C24-C25-C26-C27
26	K	616	LHG	C24-C25-C26-C27
26	O	321	LHG	C24-C25-C26-C27
26	W	420	LHG	C24-C25-C26-C27
26	A	846	LHG	C24-C25-C26-C27
25	B	847	DGD	O6E-C5E-C6E-O5E
22	B	830	CLA	O1A-CGA-O2A-C1
22	K	610	CLA	O1A-CGA-O2A-C1
22	L	404	CLA	O1A-CGA-O2A-C1
22	R	601	CLA	O1A-CGA-O2A-C1
22	R	608	CLA	O1A-CGA-O2A-C1
22	V	603	CLA	O1A-CGA-O2A-C1
26	B	848	LHG	O10-C23-O8-C6
28	H	317	LMG	O10-C28-O8-C9
28	K	618	LMG	O10-C28-O8-C9
28	U	402	LMG	O10-C28-O8-C9
22	W	410	CLA	O1D-CGD-O2D-CED
26	S	613	LHG	C24-C25-C26-C27
26	O	318	LHG	C24-C25-C26-C27
26	X	420	LHG	C24-C25-C26-C27
26	A	845	LHG	C24-C25-C26-C27
22	B	802	CLA	O1D-CGD-O2D-CED
22	G	610	CLA	O1D-CGD-O2D-CED
22	I	601	CLA	O1D-CGD-O2D-CED
22	N	602	CLA	O1D-CGD-O2D-CED
22	F	403	CLA	C3-C5-C6-C7
22	G	608	CLA	C3-C5-C6-C7
22	H	303	CLA	C3-C5-C6-C7
22	H	311	CLA	C3-C5-C6-C7
22	L	403	CLA	C3-C5-C6-C7
22	Q	611	CLA	C3-C5-C6-C7
22	U	401	CLA	C3-C5-C6-C7
22	X	410	CLA	C3-C5-C6-C7
22	G	611	CLA	CBD-CGD-O2D-CED
22	O	311	CLA	CBD-CGD-O2D-CED
22	P	610	CLA	CBD-CGD-O2D-CED
22	Q	603	CLA	CBD-CGD-O2D-CED
26	N	616	LHG	O2-C2-C3-O3
26	O	321	LHG	O2-C2-C3-O3
26	X	420	LHG	O2-C2-C3-O3
22	B	826	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	H	311	CLA	O1D-CGD-O2D-CED
22	Q	606	CLA	O1D-CGD-O2D-CED
22	S	605	CLA	O1D-CGD-O2D-CED
22	V	610	CLA	O1D-CGD-O2D-CED
22	V	617	CLA	O1D-CGD-O2D-CED
22	R	601	CLA	CBA-CGA-O2A-C1
22	R	608	CLA	CBA-CGA-O2A-C1
26	B	848	LHG	C24-C23-O8-C6
28	H	317	LMG	C29-C28-O8-C9
28	K	618	LMG	C29-C28-O8-C9
22	A	821	CLA	O1A-CGA-O2A-C1
22	H	307	CLA	O1D-CGD-O2D-CED
25	O	304	DGD	O6E-C5E-C6E-O5E
25	B	847	DGD	C4E-C5E-C6E-O5E
27	J	104	LMU	C4B-C5B-C6B-O6B
22	L	404	CLA	CBD-CGD-O2D-CED
22	W	409	CLA	CBD-CGD-O2D-CED
25	F	401	DGD	C2B-C1B-O2G-C2G
28	B	856	LMG	C11-C10-O7-C8
28	I	615	LMG	C11-C10-O7-C8
28	H	317	LMG	O6-C5-C6-O5
28	J	101	LMG	O6-C5-C6-O5
22	L	406	CLA	O1D-CGD-O2D-CED
22	N	607	CLA	O1D-CGD-O2D-CED
22	U	401	CLA	O1D-CGD-O2D-CED
22	A	824	CLA	O1D-CGD-O2D-CED
22	B	820	CLA	C3-C5-C6-C7
22	X	412	CLA	C3-C5-C6-C7
22	B	827	CLA	CBD-CGD-O2D-CED
22	G	608	CLA	CBD-CGD-O2D-CED
22	U	409	CLA	CBD-CGD-O2D-CED
27	B	857	LMU	O5'-C5'-C6'-O6'
28	N	615	LMG	O6-C5-C6-O5
22	I	607	CLA	O1D-CGD-O2D-CED
22	R	602	CLA	O1D-CGD-O2D-CED
22	G	608	CLA	C4-C3-C5-C6
22	G	608	CLA	C2-C3-C5-C6
22	T	605	CLA	C2-C3-C5-C6
22	U	411	CLA	C2-C3-C5-C6
22	A	814	CLA	C2-C3-C5-C6
22	R	615	CLA	O1A-CGA-O2A-C1
25	F	401	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
22	R	604	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	CBD-CGD-O2D-CED
22	N	610	CLA	O1D-CGD-O2D-CED
26	B	851	LHG	C5-C4-O6-P
22	J	102	CLA	C2A-CAA-CBA-CGA
22	B	813	CLA	O1D-CGD-O2D-CED
22	F	403	CLA	O1D-CGD-O2D-CED
22	S	604	CLA	O1D-CGD-O2D-CED
22	U	410	CLA	O1D-CGD-O2D-CED
22	A	817	CLA	O1D-CGD-O2D-CED
22	A	852	CLA	O1D-CGD-O2D-CED
25	O	304	DGD	O6E-C1E-O5D-C6D
28	B	852	LMG	O6-C1-O1-C7
28	L	401	LMG	O6-C1-O1-C7
28	T	616	LMG	O6-C1-O1-C7
28	U	423	LMG	O6-C1-O1-C7
28	W	401	LMG	O6-C1-O1-C7
22	A	813	CLA	CBA-CGA-O2A-C1
22	A	835	CLA	CBA-CGA-O2A-C1
28	U	402	LMG	C29-C28-O8-C9
22	B	829	CLA	CBD-CGD-O2D-CED
22	N	604	CLA	CBD-CGD-O2D-CED
22	P	608	CLA	CBD-CGD-O2D-CED
22	Q	612	CLA	CBD-CGD-O2D-CED
22	W	404	CLA	CBD-CGD-O2D-CED
22	A	823	CLA	CBD-CGD-O2D-CED
22	A	830	CLA	CBD-CGD-O2D-CED
28	A	855	LMG	O6-C5-C6-O5
25	O	304	DGD	C4E-C5E-C6E-O5E
25	O	304	DGD	C4B-C5B-C6B-C7B
22	H	309	CLA	CBD-CGD-O2D-CED
22	U	406	CLA	CBD-CGD-O2D-CED
22	A	819	CLA	CBD-CGD-O2D-CED
28	U	402	LMG	C4-C5-C6-O5
26	P	601	LHG	C15-C16-C17-C18
26	Q	616	LHG	C25-C26-C27-C28
24	F	406	DD6	C11-C10-C9-C8
24	P	612	DD6	C24-C25-C26-C27
26	B	848	LHG	C1-C2-C3-O3
26	B	851	LHG	C1-C2-C3-O3
26	L	416	LHG	C1-C2-C3-O3
26	O	323	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
22	H	306	CLA	CBA-CGA-O2A-C1
22	J	102	CLA	CBA-CGA-O2A-C1
22	K	602	CLA	CBA-CGA-O2A-C1
22	K	605	CLA	CBA-CGA-O2A-C1
22	N	610	CLA	CBA-CGA-O2A-C1
22	O	312	CLA	CBA-CGA-O2A-C1
22	Q	617	CLA	CBA-CGA-O2A-C1
22	U	406	CLA	CBA-CGA-O2A-C1
22	W	403	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	CBA-CGA-O2A-C1
22	A	825	CLA	CBA-CGA-O2A-C1
26	N	614	LHG	C24-C23-O8-C6
26	P	601	LHG	C24-C23-O8-C6
26	U	419	LHG	C24-C23-O8-C6
25	O	304	DGD	C5A-C6A-C7A-C8A
22	V	603	CLA	CBD-CGD-O2D-CED
22	X	410	CLA	CBD-CGD-O2D-CED
28	J	101	LMG	C4-C5-C6-O5
22	L	407	CLA	O1D-CGD-O2D-CED
22	U	414	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	O1D-CGD-O2D-CED
22	R	601	CLA	C4-C3-C5-C6
22	T	605	CLA	C4-C3-C5-C6
22	A	838	CLA	C4-C3-C5-C6
22	R	601	CLA	C2-C3-C5-C6
22	A	811	CLA	C2-C3-C5-C6
22	B	812	CLA	C3-C5-C6-C7
22	L	402	CLA	C3-C5-C6-C7
22	S	609	CLA	C3-C5-C6-C7
22	B	806	CLA	C14-C13-C15-C16
22	B	807	CLA	C14-C13-C15-C16
22	B	821	CLA	C11-C10-C8-C9
22	B	834	CLA	C14-C13-C15-C16
22	G	606	CLA	C11-C10-C8-C9
22	H	305	CLA	C6-C7-C8-C9
22	H	313	CLA	C11-C10-C8-C9
22	I	601	CLA	C6-C7-C8-C9
22	I	606	CLA	C11-C10-C8-C9
22	K	604	CLA	C11-C10-C8-C9
22	K	604	CLA	C11-C12-C13-C14
22	K	609	CLA	C6-C7-C8-C9
22	L	411	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	N	606	CLA	C11-C10-C8-C9
22	Q	609	CLA	C6-C7-C8-C9
22	Q	612	CLA	C14-C13-C15-C16
22	R	606	CLA	C6-C7-C8-C9
22	R	607	CLA	C6-C7-C8-C9
22	R	610	CLA	C14-C13-C15-C16
22	S	605	CLA	C11-C10-C8-C9
22	T	603	CLA	C11-C10-C8-C9
22	T	604	CLA	C11-C12-C13-C14
22	T	605	CLA	C6-C7-C8-C9
22	T	607	CLA	C11-C10-C8-C9
22	X	404	CLA	C11-C10-C8-C9
22	A	807	CLA	C14-C13-C15-C16
22	A	808	CLA	C14-C13-C15-C16
22	A	816	CLA	C6-C7-C8-C9
22	A	817	CLA	C14-C13-C15-C16
22	A	825	CLA	C11-C12-C13-C14
22	A	836	CLA	C11-C12-C13-C14
22	A	840	CLA	C11-C12-C13-C14
22	A	841	CLA	C11-C12-C13-C14
22	A	842	CLA	C14-C13-C15-C16
22	N	606	CLA	O1D-CGD-O2D-CED
22	T	606	CLA	O1D-CGD-O2D-CED
22	U	411	CLA	O1D-CGD-O2D-CED
22	W	415	CLA	O1D-CGD-O2D-CED
25	O	304	DGD	C2E-C1E-O5D-C6D
28	L	401	LMG	C2-C1-O1-C7
28	T	616	LMG	C2-C1-O1-C7
28	U	423	LMG	C2-C1-O1-C7
28	W	401	LMG	C2-C1-O1-C7
26	O	324	LHG	O2-C2-C3-O3
26	R	614	LHG	O2-C2-C3-O3
22	H	304	CLA	O1D-CGD-O2D-CED
22	Q	611	CLA	O1D-CGD-O2D-CED
25	O	304	DGD	C4D-C5D-C6D-O5D
22	W	403	CLA	O1A-CGA-O2A-C1
22	A	825	CLA	O1A-CGA-O2A-C1
22	A	835	CLA	O1A-CGA-O2A-C1
25	B	847	DGD	C8B-C9B-CAB-CBB
22	P	606	CLA	O1D-CGD-O2D-CED
21	B	845	BCR	C37-C22-C23-C24
21	B	846	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	X	416	DD6	C12-C11-C13-C14
21	A	850	BCR	C21-C22-C23-C24
22	K	602	CLA	O1A-CGA-O2A-C1
22	N	610	CLA	O1A-CGA-O2A-C1
26	P	601	LHG	O10-C23-O8-C6
22	H	307	CLA	C3-C5-C6-C7
22	V	603	CLA	C3-C5-C6-C7
22	W	404	CLA	C3-C5-C6-C7
27	J	104	LMU	C4'-C5'-C6'-O6'
25	F	401	DGD	O1B-C1B-O2G-C2G
22	R	605	CLA	CBD-CGD-O2D-CED
25	O	304	DGD	C2B-C1B-O2G-C2G
26	B	851	LHG	O7-C5-C6-O8
22	R	607	CLA	CBA-CGA-O2A-C1
22	S	607	CLA	CBA-CGA-O2A-C1
22	A	833	CLA	C13-C15-C16-C17
22	A	842	CLA	C15-C16-C17-C18
22	B	822	CLA	O1D-CGD-O2D-CED
22	H	318	CLA	O1D-CGD-O2D-CED
22	L	411	CLA	O1D-CGD-O2D-CED
22	T	604	CLA	O1D-CGD-O2D-CED
22	U	403	CLA	O1D-CGD-O2D-CED
22	G	601	CLA	CBD-CGD-O2D-CED
22	O	310	CLA	CBD-CGD-O2D-CED
26	O	323	LHG	C25-C26-C27-C28
22	P	611	CLA	C2C-C3C-CAC-CBC
22	K	608	CLA	C5-C6-C7-C8
22	V	612	CLA	C5-C6-C7-C8
22	X	403	CLA	C10-C11-C12-C13
22	X	409	CLA	C13-C15-C16-C17
22	A	815	CLA	C10-C11-C12-C13
22	A	825	CLA	C8-C10-C11-C12
22	A	840	CLA	C5-C6-C7-C8
31	W	408	CHL	C10-C11-C12-C13
25	O	304	DGD	O6D-C5D-C6D-O5D
26	X	420	LHG	O1-C1-C2-O2
22	B	806	CLA	C3-C5-C6-C7
27	B	857	LMU	C4'-C5'-C6'-O6'
22	Q	609	CLA	O1D-CGD-O2D-CED
22	Q	618	CLA	O1D-CGD-O2D-CED
22	A	811	CLA	O1D-CGD-O2D-CED
22	T	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	J	104	LMU	O5B-C5B-C6B-O6B
22	B	807	CLA	C6-C7-C8-C10
22	B	812	CLA	C12-C13-C15-C16
22	H	311	CLA	C6-C7-C8-C10
22	K	608	CLA	C11-C12-C13-C15
22	A	801	CLA	C11-C10-C8-C7
22	A	806	CLA	C11-C12-C13-C15
22	A	808	CLA	C11-C12-C13-C15
22	A	824	CLA	C6-C7-C8-C10
22	A	828	CLA	C6-C7-C8-C10
22	G	607	CLA	O1D-CGD-O2D-CED
22	B	826	CLA	CBA-CGA-O2A-C1
22	K	617	CLA	CBA-CGA-O2A-C1
25	F	401	DGD	CEA-CFA-CGA-CHA
28	T	616	LMG	O6-C5-C6-O5
22	K	609	CLA	C10-C11-C12-C13
26	G	614	LHG	C23-C24-C25-C26
22	Q	604	CLA	O1D-CGD-O2D-CED
22	T	608	CLA	O1D-CGD-O2D-CED
22	Q	610	CLA	C3-C5-C6-C7
22	B	818	CLA	C15-C16-C17-C18
22	B	834	CLA	C8-C10-C11-C12
22	K	604	CLA	C8-C10-C11-C12
26	W	420	LHG	C10-C11-C12-C13
26	B	851	LHG	C23-C24-C25-C26
28	H	317	LMG	C28-C29-C30-C31
28	H	322	LMG	C10-C11-C12-C13
28	I	615	LMG	C28-C29-C30-C31
22	K	605	CLA	O1A-CGA-O2A-C1
26	N	614	LHG	O10-C23-O8-C6
22	K	608	CLA	CBD-CGD-O2D-CED
22	T	607	CLA	CBD-CGD-O2D-CED
26	O	321	LHG	C8-C7-O7-C5
28	Q	602	LMG	C11-C10-O7-C8
22	B	805	CLA	O1D-CGD-O2D-CED
22	B	839	CLA	C13-C15-C16-C17
22	Q	609	CLA	C5-C6-C7-C8
22	R	601	CLA	C8-C10-C11-C12
22	S	604	CLA	C8-C10-C11-C12
22	A	813	CLA	C13-C15-C16-C17
22	A	830	CLA	C13-C15-C16-C17
22	A	841	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	A	842	CLA	C13-C15-C16-C17
27	U	422	LMU	O5'-C5'-C6'-O6'
22	B	814	CLA	C2A-CAA-CBA-CGA
22	B	817	CLA	C2A-CAA-CBA-CGA
22	P	604	CLA	C2A-CAA-CBA-CGA
22	T	605	CLA	C2A-CAA-CBA-CGA
22	U	409	CLA	C2A-CAA-CBA-CGA
22	W	415	CLA	C2A-CAA-CBA-CGA
22	W	419	CLA	C2A-CAA-CBA-CGA
22	X	402	CLA	C2A-CAA-CBA-CGA
22	X	417	CLA	C2A-CAA-CBA-CGA
22	A	810	CLA	C2A-CAA-CBA-CGA
22	A	818	CLA	C2A-CAA-CBA-CGA
22	A	821	CLA	C2A-CAA-CBA-CGA
22	B	818	CLA	C8-C10-C11-C12
22	Q	604	CLA	C15-C16-C17-C18
22	R	610	CLA	C8-C10-C11-C12
22	R	610	CLA	C10-C11-C12-C13
22	T	611	CLA	C5-C6-C7-C8
22	A	807	CLA	C8-C10-C11-C12
22	A	824	CLA	C8-C10-C11-C12
22	A	824	CLA	C10-C11-C12-C13
22	A	824	CLA	C13-C15-C16-C17
28	N	615	LMG	C4-C5-C6-O5
26	O	321	LHG	C7-C8-C9-C10
28	F	408	LMG	C28-C29-C30-C31
22	H	306	CLA	O1A-CGA-O2A-C1
22	J	102	CLA	O1A-CGA-O2A-C1
22	O	312	CLA	O1A-CGA-O2A-C1
22	U	406	CLA	O1A-CGA-O2A-C1
22	A	813	CLA	O1A-CGA-O2A-C1
26	U	419	LHG	O10-C23-O8-C6
22	A	835	CLA	CBD-CGD-O2D-CED
22	B	806	CLA	C13-C15-C16-C17
22	B	822	CLA	C5-C6-C7-C8
22	B	823	CLA	C5-C6-C7-C8
22	B	824	CLA	C8-C10-C11-C12
22	B	835	CLA	C5-C6-C7-C8
22	H	308	CLA	C5-C6-C7-C8
22	K	604	CLA	C5-C6-C7-C8
22	K	611	CLA	C8-C10-C11-C12
22	L	402	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	L	417	CLA	C5-C6-C7-C8
22	L	417	CLA	C10-C11-C12-C13
22	U	404	CLA	C5-C6-C7-C8
22	A	805	CLA	C8-C10-C11-C12
26	K	619	LHG	O2-C2-C3-O3
26	L	416	LHG	O2-C2-C3-O3
26	T	614	LHG	O2-C2-C3-O3
22	X	405	CLA	O1D-CGD-O2D-CED
22	O	311	CLA	CBA-CGA-O2A-C1
22	W	413	CLA	CBD-CGD-O2D-CED
22	Q	617	CLA	O1A-CGA-O2A-C1
22	A	812	CLA	O1A-CGA-O2A-C1
22	L	407	CLA	C8-C10-C11-C12
22	B	835	CLA	C10-C11-C12-C13
22	O	310	CLA	C5-C6-C7-C8
22	R	607	CLA	C8-C10-C11-C12
22	A	815	CLA	C15-C16-C17-C18
25	O	304	DGD	O1B-C1B-O2G-C2G
27	X	421	LMU	O1'-C1-C2-C3
22	O	308	CLA	O1D-CGD-O2D-CED
22	R	607	CLA	C5-C6-C7-C8
22	T	605	CLA	C15-C16-C17-C18
22	V	612	CLA	C10-C11-C12-C13
22	X	412	CLA	C8-C10-C11-C12
22	L	410	CLA	CBD-CGD-O2D-CED
22	Q	601	CLA	CBD-CGD-O2D-CED
22	R	607	CLA	O1A-CGA-O2A-C1
28	H	317	LMG	C4-C5-C6-O5
26	P	601	LHG	C25-C26-C27-C28
22	S	607	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	C8-C10-C11-C12
22	B	812	CLA	C10-C11-C12-C13
22	A	841	CLA	C15-C16-C17-C18
22	G	608	CLA	CBA-CGA-O2A-C1
22	X	408	CLA	CBA-CGA-O2A-C1
26	O	318	LHG	C24-C23-O8-C6
22	K	612	CLA	CBD-CGD-O2D-CED
22	P	609	CLA	CBD-CGD-O2D-CED
26	W	420	LHG	C8-C7-O7-C5
28	H	319	LMG	C11-C10-O7-C8
22	K	617	CLA	O1A-CGA-O2A-C1
22	Q	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	824	CLA	C10-C11-C12-C13
22	A	814	CLA	C13-C15-C16-C17
22	P	610	CLA	O1D-CGD-O2D-CED
27	J	104	LMU	O1'-C1-C2-C3
26	B	851	LHG	C26-C27-C28-C29
26	O	318	LHG	C10-C11-C12-C13
22	K	602	CLA	C5-C6-C7-C8
28	B	852	LMG	C28-C29-C30-C31
28	U	402	LMG	C10-C11-C12-C13
26	O	321	LHG	O9-C7-O7-C5
26	W	420	LHG	O9-C7-O7-C5
26	N	616	LHG	C1-C2-C3-O3
26	T	614	LHG	C1-C2-C3-O3
22	N	607	CLA	C2A-CAA-CBA-CGA
22	G	611	CLA	O1D-CGD-O2D-CED
22	O	311	CLA	O1D-CGD-O2D-CED
22	B	810	CLA	CBA-CGA-O2A-C1
22	R	602	CLA	CBA-CGA-O2A-C1
26	N	616	LHG	C12-C13-C14-C15
26	O	321	LHG	C34-C35-C36-C37
22	B	807	CLA	C10-C11-C12-C13
22	B	812	CLA	C5-C6-C7-C8
22	N	603	CLA	C15-C16-C17-C18
22	R	605	CLA	C15-C16-C17-C18
22	X	410	CLA	C10-C11-C12-C13
26	O	321	LHG	C32-C33-C34-C35
22	L	404	CLA	O1D-CGD-O2D-CED
22	W	409	CLA	O1D-CGD-O2D-CED
22	B	807	CLA	C5-C6-C7-C8
22	B	810	CLA	C5-C6-C7-C8
22	H	305	CLA	C5-C6-C7-C8
22	A	829	CLA	C13-C15-C16-C17
25	B	847	DGD	C2A-C3A-C4A-C5A
30	V	618	SQD	O6-C44-C45-O47
22	N	608	CLA	CBD-CGD-O2D-CED
22	P	604	CLA	CBD-CGD-O2D-CED
27	J	104	LMU	O5'-C5'-C6'-O6'
22	B	813	CLA	C10-C11-C12-C13
22	B	833	CLA	C13-C15-C16-C17
22	K	604	CLA	C13-C15-C16-C17
22	T	607	CLA	C8-C10-C11-C12
22	V	604	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	816	CLA	C10-C11-C12-C13
26	A	846	LHG	C24-C23-O8-C6
28	U	402	LMG	O6-C5-C6-O5
22	B	804	CLA	C3-C5-C6-C7
25	B	847	DGD	C2D-C1D-O3G-C3G
28	K	618	LMG	C2-C1-O1-C7
22	T	602	CLA	C15-C16-C17-C18
22	A	804	CLA	C10-C11-C12-C13
28	U	423	LMG	C28-C29-C30-C31
28	L	401	LMG	C4-C5-C6-O5
26	R	614	LHG	C25-C26-C27-C28
26	A	846	LHG	O2-C2-C3-O3
22	H	311	CLA	CBA-CGA-O2A-C1
26	G	614	LHG	C24-C23-O8-C6
22	B	812	CLA	C16-C17-C18-C20
22	L	402	CLA	C16-C17-C18-C20
28	K	618	LMG	C28-C29-C30-C31
22	G	608	CLA	O1D-CGD-O2D-CED
21	B	801	BCR	C11-C12-C13-C35
26	O	324	LHG	C2-C3-O3-P
22	B	826	CLA	O1A-CGA-O2A-C1
22	S	607	CLA	O1A-CGA-O2A-C1
22	B	808	CLA	C2A-CAA-CBA-CGA
22	U	420	CLA	C2A-CAA-CBA-CGA
22	A	805	CLA	C2A-CAA-CBA-CGA
26	H	316	LHG	O1-C1-C2-C3
26	N	616	LHG	O1-C1-C2-C3
26	T	614	LHG	O1-C1-C2-C3
26	X	420	LHG	O1-C1-C2-C3
26	U	419	LHG	C6-C5-O7-C7
28	I	615	LMG	C7-C8-O7-C10
28	W	401	LMG	C7-C8-O7-C10
22	Q	611	CLA	C6-C7-C8-C9
22	Q	611	CLA	C6-C7-C8-C10
22	T	602	CLA	C16-C17-C18-C19
22	X	410	CLA	C11-C12-C13-C14
22	X	410	CLA	C11-C12-C13-C15
22	A	806	CLA	C16-C17-C18-C20
22	A	821	CLA	C16-C17-C18-C19
22	A	824	CLA	C16-C17-C18-C20
22	B	827	CLA	O1D-CGD-O2D-CED
22	G	608	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	O	311	CLA	O1A-CGA-O2A-C1
22	B	831	CLA	C3-C5-C6-C7
22	L	417	CLA	C3-C5-C6-C7
22	O	308	CLA	C3-C5-C6-C7
22	R	602	CLA	C3-C5-C6-C7
22	X	404	CLA	C8-C10-C11-C12
22	A	838	CLA	C2-C3-C5-C6
26	T	614	LHG	C30-C31-C32-C33
22	U	409	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	O1D-CGD-O2D-CED
27	A	857	LMU	O5'-C5'-C6'-O6'
26	S	613	LHG	C11-C10-C9-C8
22	W	403	CLA	CBD-CGD-O2D-CED
22	A	803	CLA	CBD-CGD-O2D-CED
26	K	616	LHG	C23-C24-C25-C26
22	H	303	CLA	C11-C12-C13-C15
22	L	402	CLA	C16-C17-C18-C19
22	N	610	CLA	C6-C7-C8-C9
22	A	806	CLA	C16-C17-C18-C19
22	A	808	CLA	C16-C17-C18-C19
22	A	826	CLA	C16-C17-C18-C20
22	A	852	CLA	C16-C17-C18-C20
22	R	602	CLA	O1A-CGA-O2A-C1
26	L	416	LHG	C16-C17-C18-C19
26	N	616	LHG	C13-C14-C15-C16
26	W	420	LHG	C11-C10-C9-C8
28	B	852	LMG	C13-C14-C15-C16
28	K	601	LMG	C14-C15-C16-C17
25	B	847	DGD	C5B-C6B-C7B-C8B
26	K	616	LHG	C26-C27-C28-C29
26	O	318	LHG	C12-C13-C14-C15
26	O	321	LHG	C27-C28-C29-C30
26	O	324	LHG	C31-C32-C33-C34
27	B	855	LMU	C4-C5-C6-C7
27	U	421	LMU	C11-C10-C9-C8
22	A	823	CLA	O1D-CGD-O2D-CED
22	B	823	CLA	C10-C11-C12-C13
22	I	601	CLA	C5-C6-C7-C8
22	T	605	CLA	C5-C6-C7-C8
22	A	819	CLA	C8-C10-C11-C12
27	J	104	LMU	C2-C3-C4-C5
28	B	856	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
28	F	408	LMG	C30-C31-C32-C33
28	U	423	LMG	C17-C18-C19-C20
22	X	408	CLA	O1A-CGA-O2A-C1
22	B	835	CLA	CBA-CGA-O2A-C1
25	F	401	DGD	C7A-C8A-C9A-CAA
25	O	304	DGD	C5B-C6B-C7B-C8B
26	W	420	LHG	C30-C31-C32-C33
28	B	856	LMG	C19-C20-C21-C22
28	B	856	LMG	C41-C42-C43-C44
28	L	401	LMG	C31-C32-C33-C34
26	B	848	LHG	O1-C1-C2-O2
26	O	324	LHG	O1-C1-C2-O2
26	P	601	LHG	O1-C1-C2-O2
26	S	613	LHG	O1-C1-C2-O2
26	T	614	LHG	O1-C1-C2-O2
27	O	322	LMU	C2-C1-O1'-C1'
27	A	857	LMU	C2-C1-O1'-C1'
26	Q	616	LHG	C15-C16-C17-C18
26	A	845	LHG	C11-C10-C9-C8
28	G	616	LMG	C34-C35-C36-C37
28	U	402	LMG	C31-C32-C33-C34
22	A	840	CLA	C10-C11-C12-C13
22	F	405	CLA	C4B-C3B-CAB-CBB
22	H	306	CLA	C4B-C3B-CAB-CBB
22	H	313	CLA	C4B-C3B-CAB-CBB
22	L	409	CLA	C4B-C3B-CAB-CBB
22	Q	601	CLA	C4B-C3B-CAB-CBB
22	S	610	CLA	C4B-C3B-CAB-CBB
22	U	420	CLA	C4B-C3B-CAB-CBB
22	V	608	CLA	C4B-C3B-CAB-CBB
22	V	612	CLA	C4B-C3B-CAB-CBB
22	A	841	CLA	C4B-C3B-CAB-CBB
28	L	401	LMG	C10-C11-C12-C13
26	L	416	LHG	C17-C18-C19-C20
26	A	845	LHG	C31-C32-C33-C34
28	J	101	LMG	C11-C12-C13-C14
22	G	608	CLA	C11-C12-C13-C14
22	O	312	CLA	C11-C12-C13-C14
22	T	602	CLA	C16-C17-C18-C20
22	A	808	CLA	C16-C17-C18-C20
22	A	824	CLA	C16-C17-C18-C19
22	A	852	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	N	604	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	C2A-CAA-CBA-CGA
22	A	824	CLA	C2A-CAA-CBA-CGA
26	O	323	LHG	C26-C27-C28-C29
22	H	307	CLA	C5-C6-C7-C8
22	X	408	CLA	C15-C16-C17-C18
28	H	317	LMG	C11-C10-O7-C8
25	B	847	DGD	CCA-CDA-CEA-CFA
26	O	321	LHG	C11-C10-C9-C8
28	J	101	LMG	C13-C14-C15-C16
28	K	601	LMG	C30-C31-C32-C33
22	B	816	CLA	C12-C13-C15-C16
22	B	832	CLA	C6-C7-C8-C10
22	K	611	CLA	C6-C7-C8-C10
22	Q	609	CLA	C11-C10-C8-C7
22	R	601	CLA	C11-C10-C8-C7
22	A	816	CLA	C11-C12-C13-C15
26	P	601	LHG	C14-C15-C16-C17
27	F	409	LMU	C5-C6-C7-C8
22	B	807	CLA	C15-C16-C17-C18
25	B	847	DGD	C9A-CAA-CBA-CCA
25	B	847	DGD	C7B-C8B-C9B-CAB
28	H	322	LMG	C30-C31-C32-C33
28	I	615	LMG	C33-C34-C35-C36
28	K	601	LMG	C17-C18-C19-C20
28	L	401	LMG	C22-C23-C24-C25
26	O	318	LHG	O10-C23-O8-C6
26	A	846	LHG	O10-C23-O8-C6
22	B	812	CLA	C3A-C2A-CAA-CBA
22	B	817	CLA	C4-C3-C5-C6
22	B	825	CLA	C3A-C2A-CAA-CBA
22	B	859	CLA	C3A-C2A-CAA-CBA
22	F	404	CLA	C3A-C2A-CAA-CBA
22	H	318	CLA	C3A-C2A-CAA-CBA
22	I	601	CLA	C3A-C2A-CAA-CBA
22	K	617	CLA	C3A-C2A-CAA-CBA
22	L	410	CLA	C3A-C2A-CAA-CBA
22	N	610	CLA	C3A-C2A-CAA-CBA
22	P	609	CLA	C3A-C2A-CAA-CBA
22	Q	613	CLA	C3A-C2A-CAA-CBA
22	S	606	CLA	C3A-C2A-CAA-CBA
22	S	607	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	S	609	CLA	C3A-C2A-CAA-CBA
22	U	405	CLA	C3A-C2A-CAA-CBA
22	V	603	CLA	C3A-C2A-CAA-CBA
22	V	609	CLA	C4-C3-C5-C6
22	X	404	CLA	C3A-C2A-CAA-CBA
22	A	807	CLA	C3A-C2A-CAA-CBA
22	A	818	CLA	C3A-C2A-CAA-CBA
22	A	838	CLA	C3A-C2A-CAA-CBA
22	A	844	CLA	C3A-C2A-CAA-CBA
22	A	852	CLA	C3A-C2A-CAA-CBA
26	X	420	LHG	C28-C29-C30-C31
28	T	616	LMG	C29-C30-C31-C32
27	M	102	LMU	O1'-C1-C2-C3
28	I	614	LMG	C32-C33-C34-C35
22	Q	610	CLA	C13-C15-C16-C17
22	A	817	CLA	C13-C15-C16-C17
22	A	827	CLA	C8-C10-C11-C12
22	P	608	CLA	O1D-CGD-O2D-CED
26	O	323	LHG	C7-C8-C9-C10
26	O	324	LHG	C7-C8-C9-C10
28	T	616	LMG	C32-C33-C34-C35
28	T	616	LMG	C34-C35-C36-C37
28	W	401	LMG	C38-C39-C40-C41
22	G	608	CLA	C11-C12-C13-C15
22	O	312	CLA	C11-C12-C13-C15
22	S	605	CLA	C11-C12-C13-C14
22	X	408	CLA	C16-C17-C18-C20
22	A	821	CLA	C16-C17-C18-C20
28	U	402	LMG	C15-C16-C17-C18
26	G	614	LHG	C9-C10-C11-C12
26	W	420	LHG	C25-C26-C27-C28
28	G	616	LMG	C41-C42-C43-C44
28	I	615	LMG	C16-C17-C18-C19
28	L	401	LMG	C17-C18-C19-C20
26	O	321	LHG	C1-C2-C3-O3
22	B	803	CLA	CBA-CGA-O2A-C1
22	B	804	CLA	CBA-CGA-O2A-C1
22	H	309	CLA	CBA-CGA-O2A-C1
22	K	607	CLA	CBA-CGA-O2A-C1
26	O	318	LHG	C25-C26-C27-C28
26	A	846	LHG	C32-C33-C34-C35
28	I	615	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	K	601	LMG	C31-C32-C33-C34
22	A	841	CLA	C3-C5-C6-C7
26	S	613	LHG	C23-C24-C25-C26
26	U	419	LHG	C23-C24-C25-C26
26	W	420	LHG	C7-C8-C9-C10
28	T	616	LMG	C28-C29-C30-C31
26	R	614	LHG	C15-C16-C17-C18
26	A	845	LHG	C25-C26-C27-C28
27	F	402	LMU	C2-C3-C4-C5
28	J	101	LMG	C17-C18-C19-C20
28	J	101	LMG	C31-C32-C33-C34
28	W	401	LMG	C13-C14-C15-C16
22	B	810	CLA	O1A-CGA-O2A-C1
26	Q	616	LHG	C14-C15-C16-C17
28	N	615	LMG	C17-C18-C19-C20
22	B	829	CLA	O1D-CGD-O2D-CED
26	O	321	LHG	C14-C15-C16-C17
22	A	836	CLA	C15-C16-C17-C18
26	B	851	LHG	C12-C13-C14-C15
26	A	846	LHG	C31-C32-C33-C34
28	F	408	LMG	C16-C17-C18-C19
28	H	322	LMG	C29-C30-C31-C32
22	H	303	CLA	C11-C12-C13-C14
22	N	610	CLA	C6-C7-C8-C10
22	H	311	CLA	O1A-CGA-O2A-C1
26	G	614	LHG	O10-C23-O8-C6
21	B	846	BCR	C23-C24-C25-C26
21	B	846	BCR	C23-C24-C25-C30
21	M	101	BCR	C23-C24-C25-C30
21	A	850	BCR	C23-C24-C25-C26
21	A	850	BCR	C23-C24-C25-C30
22	F	405	CLA	C2B-C3B-CAB-CBB
22	H	302	CLA	C2B-C3B-CAB-CBB
22	H	306	CLA	C2B-C3B-CAB-CBB
22	H	313	CLA	C2B-C3B-CAB-CBB
22	I	606	CLA	C2B-C3B-CAB-CBB
22	L	409	CLA	C2B-C3B-CAB-CBB
22	P	610	CLA	C2B-C3B-CAB-CBB
22	Q	601	CLA	C2B-C3B-CAB-CBB
22	S	606	CLA	C2B-C3B-CAB-CBB
22	S	610	CLA	C2B-C3B-CAB-CBB
22	U	420	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	V	602	CLA	C2B-C3B-CAB-CBB
22	V	611	CLA	C2B-C3B-CAB-CBB
22	V	612	CLA	C2B-C3B-CAB-CBB
22	A	834	CLA	C2B-C3B-CAB-CBB
28	J	101	LMG	C33-C34-C35-C36
22	G	606	CLA	CBD-CGD-O2D-CED
22	A	816	CLA	CBD-CGD-O2D-CED
28	K	618	LMG	C11-C10-O7-C8
26	O	324	LHG	C24-C23-O8-C6
22	K	602	CLA	C10-C11-C12-C13
22	N	603	CLA	C10-C11-C12-C13
22	X	412	CLA	C5-C6-C7-C8
22	A	803	CLA	C5-C6-C7-C8
22	K	603	CLA	C3-C5-C6-C7
22	K	610	CLA	C3-C5-C6-C7
22	N	607	CLA	C3-C5-C6-C7
22	V	612	CLA	C3-C5-C6-C7
26	W	420	LHG	C34-C35-C36-C37
26	A	845	LHG	C14-C15-C16-C17
28	I	615	LMG	C18-C19-C20-C21
28	K	618	LMG	C36-C37-C38-C39
26	X	420	LHG	C11-C10-C9-C8
28	W	401	LMG	C30-C31-C32-C33
22	X	405	CLA	C2A-CAA-CBA-CGA
26	T	614	LHG	C23-C24-C25-C26
28	B	852	LMG	C18-C19-C20-C21
28	J	101	LMG	C18-C19-C20-C21
28	U	402	LMG	C33-C34-C35-C36
22	B	804	CLA	O1A-CGA-O2A-C1
22	B	835	CLA	O1A-CGA-O2A-C1
22	K	607	CLA	O1A-CGA-O2A-C1
26	A	845	LHG	C15-C16-C17-C18
28	U	402	LMG	C18-C19-C20-C21
28	U	402	LMG	C30-C31-C32-C33
28	B	856	LMG	O9-C10-O7-C8
22	O	308	CLA	C12-C13-C15-C16
22	R	603	CLA	C11-C10-C8-C7
22	A	835	CLA	C4-C3-C5-C6
22	Q	612	CLA	O1D-CGD-O2D-CED
28	K	618	LMG	C32-C33-C34-C35
28	T	616	LMG	C33-C34-C35-C36
22	U	411	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	844	CLA	C5-C6-C7-C8
26	B	851	LHG	C15-C16-C17-C18
26	K	616	LHG	C29-C30-C31-C32
26	K	616	LHG	C30-C31-C32-C33
28	K	622	LMG	C34-C35-C36-C37
28	U	423	LMG	C30-C31-C32-C33
22	W	404	CLA	O1D-CGD-O2D-CED
22	O	305	CLA	CBA-CGA-O2A-C1
22	R	603	CLA	CBA-CGA-O2A-C1
22	T	604	CLA	CBA-CGA-O2A-C1
22	T	605	CLA	CBA-CGA-O2A-C1
28	K	601	LMG	C29-C28-O8-C9
25	B	847	DGD	CAB-CBB-CCB-CDB
26	A	845	LHG	C12-C13-C14-C15
28	I	615	LMG	C17-C18-C19-C20
22	W	409	CLA	C8-C10-C11-C12
27	M	102	LMU	C5-C6-C7-C8
28	I	615	LMG	O6-C1-O1-C7
25	B	847	DGD	C6A-C7A-C8A-C9A
26	L	416	LHG	C15-C16-C17-C18
26	P	601	LHG	C12-C13-C14-C15
27	L	419	LMU	C4-C5-C6-C7
28	W	401	LMG	C36-C37-C38-C39
27	M	102	LMU	O5'-C5'-C6'-O6'
22	A	830	CLA	O1D-CGD-O2D-CED
28	B	856	LMG	C2-C1-O1-C7
28	K	601	LMG	C2-C1-O1-C7
28	N	615	LMG	C2-C1-O1-C7
22	Q	613	CLA	CBD-CGD-O2D-CED
22	B	833	CLA	C15-C16-C17-C18
22	W	411	CLA	C8-C10-C11-C12
25	O	304	DGD	C2B-C3B-C4B-C5B
26	R	614	LHG	C11-C10-C9-C8
28	H	319	LMG	C31-C32-C33-C34
25	B	847	DGD	CBA-CCA-CDA-CEA
26	O	321	LHG	C31-C32-C33-C34
22	B	832	CLA	C5-C6-C7-C8
22	U	406	CLA	C3-C5-C6-C7
22	A	811	CLA	C3-C5-C6-C7
22	B	832	CLA	CBA-CGA-O2A-C1
22	B	812	CLA	C16-C17-C18-C19
28	I	615	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
26	X	420	LHG	C8-C7-O7-C5
28	I	614	LMG	C11-C10-O7-C8
28	U	423	LMG	C11-C10-O7-C8
25	B	847	DGD	C1A-C2A-C3A-C4A
26	O	318	LHG	C23-C24-C25-C26
28	L	401	LMG	C28-C29-C30-C31
25	O	304	DGD	CDA-CEA-CFA-CGA
26	N	616	LHG	C26-C27-C28-C29
26	O	323	LHG	C10-C11-C12-C13
26	A	845	LHG	C28-C29-C30-C31
28	H	319	LMG	C29-C30-C31-C32
28	N	615	LMG	C13-C14-C15-C16
22	B	828	CLA	C13-C15-C16-C17
22	Q	610	CLA	C5-C6-C7-C8
22	W	405	CLA	C5-C6-C7-C8
24	J	105	DD6	C12-C11-C13-C14
22	B	859	CLA	C3-C5-C6-C7
24	J	105	DD6	C10-C11-C13-C14
25	O	304	DGD	C2G-C3G-O3G-C1D
28	H	322	LMG	C8-C7-O1-C1
28	W	401	LMG	C32-C33-C34-C35
22	B	811	CLA	C2A-CAA-CBA-CGA
22	I	603	CLA	C11-C10-C8-C9
22	X	408	CLA	C16-C17-C18-C19
22	A	810	CLA	C16-C17-C18-C20
22	A	820	CLA	C16-C17-C18-C19
22	A	820	CLA	C16-C17-C18-C20
25	B	847	DGD	C9B-CAB-CBB-CCB
26	A	846	LHG	C15-C16-C17-C18
22	Q	604	CLA	C4-C3-C5-C6
22	B	817	CLA	C2-C3-C5-C6
28	F	408	LMG	C12-C13-C14-C15
28	G	616	LMG	C14-C15-C16-C17
28	I	615	LMG	C31-C32-C33-C34
22	B	816	CLA	C13-C15-C16-C17
22	B	817	CLA	C15-C16-C17-C18
22	B	805	CLA	C15-C16-C17-C18
22	B	817	CLA	C8-C10-C11-C12
22	Q	612	CLA	C8-C10-C11-C12
22	W	414	CLA	C10-C11-C12-C13
22	H	313	CLA	CBA-CGA-O2A-C1
22	N	607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	A	855	LMG	C4-C5-C6-O5
26	G	614	LHG	C12-C13-C14-C15
27	B	855	LMU	O5'-C5'-C6'-O6'
27	H	320	LMU	O5'-C5'-C6'-O6'
28	I	614	LMG	C12-C13-C14-C15
22	K	604	CLA	CBD-CGD-O2D-CED
26	A	845	LHG	C8-C7-O7-C5
22	T	604	CLA	C10-C11-C12-C13
22	H	309	CLA	O1A-CGA-O2A-C1
22	H	309	CLA	O1D-CGD-O2D-CED
26	L	416	LHG	C14-C15-C16-C17
28	U	423	LMG	C10-C11-C12-C13
22	A	814	CLA	C15-C16-C17-C18
22	U	406	CLA	O1D-CGD-O2D-CED
22	F	404	CLA	C3-C5-C6-C7
25	F	401	DGD	O2G-C2G-C3G-O3G
26	O	321	LHG	O7-C5-C6-O8
28	B	852	LMG	O7-C8-C9-O8
28	B	856	LMG	O1-C7-C8-O7
28	G	616	LMG	O7-C8-C9-O8
28	Q	602	LMG	O1-C7-C8-O7
25	O	304	DGD	C3B-C4B-C5B-C6B
28	F	408	LMG	C18-C19-C20-C21
28	K	622	LMG	C29-C30-C31-C32
22	A	819	CLA	CBA-CGA-O2A-C1
22	B	803	CLA	O1A-CGA-O2A-C1
26	S	613	LHG	C10-C11-C12-C13
28	N	615	LMG	C19-C20-C21-C22
22	A	803	CLA	C8-C10-C11-C12
27	U	421	LMU	O5'-C5'-C6'-O6'
28	L	401	LMG	O6-C5-C6-O5
28	Q	602	LMG	C4-C5-C6-O5
28	K	618	LMG	C17-C18-C19-C20
26	O	321	LHG	C15-C16-C17-C18
28	H	322	LMG	C11-C12-C13-C14
28	J	101	LMG	C30-C31-C32-C33
28	N	615	LMG	C15-C16-C17-C18
28	Q	602	LMG	O6-C5-C6-O5
22	A	822	CLA	C16-C17-C18-C20
22	S	607	CLA	C8-C10-C11-C12
22	A	812	CLA	C5-C6-C7-C8
26	T	614	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	T	614	LHG	C28-C29-C30-C31
28	H	319	LMG	C14-C15-C16-C17
22	H	311	CLA	C4-C3-C5-C6
22	W	402	CLA	C4-C3-C5-C6
22	B	807	CLA	C3-C5-C6-C7
26	A	846	LHG	C1-C2-C3-O3
28	L	401	LMG	C34-C35-C36-C37
22	B	826	CLA	C2A-CAA-CBA-CGA
22	N	610	CLA	C2A-CAA-CBA-CGA
22	S	610	CLA	C2A-CAA-CBA-CGA
22	U	414	CLA	C2A-CAA-CBA-CGA
22	A	803	CLA	C2A-CAA-CBA-CGA
22	A	814	CLA	C2A-CAA-CBA-CGA
22	A	820	CLA	C2A-CAA-CBA-CGA
22	L	405	CLA	CBD-CGD-O2D-CED
22	X	402	CLA	CBD-CGD-O2D-CED
22	A	806	CLA	CBA-CGA-O2A-C1
28	U	423	LMG	C18-C19-C20-C21
26	O	324	LHG	O10-C23-O8-C6
22	X	410	CLA	O1D-CGD-O2D-CED
22	G	608	CLA	C8-C10-C11-C12
22	L	402	CLA	C8-C10-C11-C12
26	K	619	LHG	C10-C11-C12-C13
27	B	849	LMU	C1-C2-C3-C4
28	I	615	LMG	C22-C23-C24-C25
28	K	618	LMG	C39-C40-C41-C42
27	O	322	LMU	O5'-C5'-C6'-O6'
22	V	603	CLA	O1D-CGD-O2D-CED
26	O	323	LHG	O1-C1-C2-O2
26	Q	616	LHG	O1-C1-C2-O2
22	T	604	CLA	O1A-CGA-O2A-C1
22	B	804	CLA	C1A-C2A-CAA-CBA
22	B	816	CLA	C1A-C2A-CAA-CBA
22	B	819	CLA	C1A-C2A-CAA-CBA
22	B	824	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	859	CLA	C1A-C2A-CAA-CBA
22	F	404	CLA	C1A-C2A-CAA-CBA
22	G	611	CLA	C1A-C2A-CAA-CBA
22	H	318	CLA	C1A-C2A-CAA-CBA
22	K	617	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	L	412	CLA	C1A-C2A-CAA-CBA
22	N	610	CLA	C1A-C2A-CAA-CBA
22	O	308	CLA	C1A-C2A-CAA-CBA
22	P	602	CLA	C1A-C2A-CAA-CBA
22	P	608	CLA	C1A-C2A-CAA-CBA
22	P	609	CLA	C1A-C2A-CAA-CBA
22	Q	618	CLA	C1A-C2A-CAA-CBA
22	R	602	CLA	C1A-C2A-CAA-CBA
22	R	607	CLA	C1A-C2A-CAA-CBA
22	S	609	CLA	C1A-C2A-CAA-CBA
22	T	611	CLA	C1A-C2A-CAA-CBA
22	U	405	CLA	C1A-C2A-CAA-CBA
22	V	603	CLA	C1A-C2A-CAA-CBA
22	V	613	CLA	C1A-C2A-CAA-CBA
22	W	410	CLA	C1A-C2A-CAA-CBA
22	X	404	CLA	C1A-C2A-CAA-CBA
22	X	405	CLA	C1A-C2A-CAA-CBA
22	A	820	CLA	C1A-C2A-CAA-CBA
22	A	827	CLA	C1A-C2A-CAA-CBA
22	A	842	CLA	C1A-C2A-CAA-CBA
22	A	844	CLA	C1A-C2A-CAA-CBA
26	O	321	LHG	C9-C10-C11-C12
28	H	317	LMG	C30-C31-C32-C33
28	I	614	LMG	C31-C32-C33-C34
22	R	603	CLA	O1A-CGA-O2A-C1
22	A	829	CLA	C10-C11-C12-C13
26	K	619	LHG	O6-C4-C5-C6
26	X	420	LHG	O6-C4-C5-C6
22	B	820	CLA	CBD-CGD-O2D-CED
26	X	420	LHG	O9-C7-O7-C5
28	H	319	LMG	O9-C10-O7-C8
28	Q	602	LMG	O9-C10-O7-C8
26	P	601	LHG	C9-C10-C11-C12
26	T	614	LHG	C11-C12-C13-C14
22	K	613	CLA	C3-C5-C6-C7
22	B	824	CLA	C12-C13-C15-C16
22	B	830	CLA	C11-C12-C13-C15
22	B	832	CLA	C11-C10-C8-C7
22	B	835	CLA	C12-C13-C15-C16
22	G	606	CLA	C11-C12-C13-C15
22	G	608	CLA	C11-C10-C8-C7
22	I	606	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	L	402	CLA	C11-C10-C8-C7
22	L	402	CLA	C12-C13-C15-C16
22	L	408	CLA	C6-C7-C8-C10
22	L	417	CLA	C6-C7-C8-C10
22	Q	612	CLA	C12-C13-C15-C16
22	R	601	CLA	C6-C7-C8-C10
22	R	605	CLA	C6-C7-C8-C10
22	T	604	CLA	C12-C13-C15-C16
22	U	414	CLA	C11-C12-C13-C15
22	X	408	CLA	C6-C7-C8-C10
22	A	803	CLA	C12-C13-C15-C16
22	A	815	CLA	C11-C10-C8-C7
22	A	835	CLA	C11-C12-C13-C15
22	A	836	CLA	C11-C12-C13-C15
22	A	839	CLA	C12-C13-C15-C16
22	A	840	CLA	C11-C10-C8-C7
22	A	852	CLA	C11-C12-C13-C15
23	A	843	PQN	C17-C18-C20-C21
25	F	401	DGD	CBA-CCA-CDA-CEA
26	O	323	LHG	C28-C29-C30-C31
28	K	601	LMG	C29-C30-C31-C32
28	A	855	LMG	C33-C34-C35-C36
22	B	817	CLA	C16-C17-C18-C20
22	X	407	CLA	C15-C16-C17-C18
22	T	605	CLA	O1A-CGA-O2A-C1
28	U	402	LMG	C16-C17-C18-C19
25	F	401	DGD	C1A-C2A-C3A-C4A
28	U	423	LMG	C31-C32-C33-C34
22	I	603	CLA	C2-C3-C5-C6
22	I	606	CLA	C2-C3-C5-C6
22	A	820	CLA	C2-C3-C5-C6
22	A	828	CLA	C2-C3-C5-C6
22	A	835	CLA	C2-C3-C5-C6
26	B	851	LHG	C14-C15-C16-C17
22	B	832	CLA	O1A-CGA-O2A-C1
22	O	305	CLA	O1A-CGA-O2A-C1
27	F	409	LMU	O5'-C5'-C6'-O6'
26	B	851	LHG	C28-C29-C30-C31
22	P	611	CLA	C4C-C3C-CAC-CBC
22	U	404	CLA	C10-C11-C12-C13
22	A	821	CLA	C15-C16-C17-C18
22	A	819	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	831	CLA	C11-C10-C8-C9
22	B	832	CLA	C11-C10-C8-C9
22	B	859	CLA	C14-C13-C15-C16
22	H	308	CLA	C11-C10-C8-C9
22	I	606	CLA	C6-C7-C8-C9
22	L	402	CLA	C14-C13-C15-C16
22	L	408	CLA	C11-C10-C8-C9
22	L	410	CLA	C11-C10-C8-C9
22	R	601	CLA	C6-C7-C8-C9
22	T	604	CLA	C6-C7-C8-C9
22	T	604	CLA	C14-C13-C15-C16
22	U	404	CLA	C11-C10-C8-C9
22	X	407	CLA	C11-C12-C13-C14
22	A	803	CLA	C6-C7-C8-C9
22	A	803	CLA	C14-C13-C15-C16
22	A	810	CLA	C11-C12-C13-C14
22	A	824	CLA	C6-C7-C8-C9
22	A	829	CLA	C11-C12-C13-C14
22	A	852	CLA	C6-C7-C8-C9
23	A	843	PQN	C19-C18-C20-C21
27	U	422	LMU	O5B-C5B-C6B-O6B
25	B	847	DGD	CDA-CEA-CFA-CGA
28	K	601	LMG	C16-C17-C18-C19
28	Q	602	LMG	C29-C30-C31-C32
22	B	816	CLA	CBA-CGA-O2A-C1
22	B	827	CLA	CBA-CGA-O2A-C1
28	W	401	LMG	C31-C32-C33-C34
27	W	421	LMU	O5'-C5'-C6'-O6'
28	H	319	LMG	O6-C5-C6-O5
22	R	605	CLA	O1D-CGD-O2D-CED
27	A	854	LMU	C5-C6-C7-C8
28	J	101	LMG	C39-C40-C41-C42
28	K	622	LMG	C2-C1-O1-C7
22	W	411	CLA	C10-C11-C12-C13
28	J	101	LMG	C14-C15-C16-C17
22	R	603	CLA	C11-C10-C8-C9
22	V	604	CLA	C11-C10-C8-C9
25	O	304	DGD	O1G-C1G-C2G-C3G
26	B	851	LHG	C4-C5-C6-O8
26	K	616	LHG	C4-C5-C6-O8
26	L	416	LHG	C4-C5-C6-O8
26	N	614	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
26	R	614	LHG	C4-C5-C6-O8
28	B	852	LMG	C7-C8-C9-O8
28	B	856	LMG	O1-C7-C8-C9
28	H	319	LMG	O1-C7-C8-C9
28	H	322	LMG	C7-C8-C9-O8
28	N	615	LMG	O1-C7-C8-C9
28	U	402	LMG	C7-C8-C9-O8
30	K	621	SQD	C44-C45-C46-O48
26	X	420	LHG	C26-C27-C28-C29
28	G	616	LMG	C29-C30-C31-C32
22	N	607	CLA	O1A-CGA-O2A-C1
28	K	618	LMG	O6-C5-C6-O5
22	A	820	CLA	C15-C16-C17-C18
26	A	846	LHG	C28-C29-C30-C31
27	T	617	LMU	C2-C3-C4-C5
28	B	852	LMG	C21-C22-C23-C24
28	W	401	LMG	C29-C30-C31-C32
22	G	601	CLA	O1D-CGD-O2D-CED
22	V	612	CLA	CBA-CGA-O2A-C1
22	A	816	CLA	CBA-CGA-O2A-C1
28	A	855	LMG	C10-C11-C12-C13
27	K	620	LMU	O5B-C5B-C6B-O6B
27	O	303	LMU	O5B-C5B-C6B-O6B
22	Q	604	CLA	C16-C17-C18-C19
22	S	605	CLA	C11-C12-C13-C15
26	P	601	LHG	C10-C11-C12-C13
28	H	317	LMG	C39-C40-C41-C42
28	K	618	LMG	C31-C32-C33-C34
28	N	615	LMG	C12-C13-C14-C15
28	U	402	LMG	C17-C18-C19-C20
27	O	303	LMU	O5'-C5'-C6'-O6'
28	B	856	LMG	O6-C5-C6-O5
27	L	419	LMU	C7-C8-C9-C10
28	G	616	LMG	C36-C37-C38-C39
22	O	310	CLA	O1D-CGD-O2D-CED
33	A	802	CL0	CHA-CBD-CGD-O2D
22	B	828	CLA	C15-C16-C17-C18
22	L	410	CLA	C3-C5-C6-C7
26	O	318	LHG	C11-C10-C9-C8
27	L	419	LMU	O5'-C5'-C6'-O6'
27	U	424	LMU	O5'-C5'-C6'-O6'
22	H	313	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	Q	616	LHG	C29-C30-C31-C32
22	I	603	CLA	C4-C3-C5-C6
22	U	401	CLA	C4-C3-C5-C6
22	B	812	CLA	C2-C3-C5-C6
22	H	311	CLA	C2-C3-C5-C6
22	O	311	CLA	C2-C3-C5-C6
22	V	609	CLA	C2-C3-C5-C6
22	X	409	CLA	C5-C6-C7-C8
24	N	613	DD6	C12-C11-C13-C14
24	A	858	DD6	C12-C11-C13-C14
25	B	847	DGD	CCB-CDB-CEB-CFB
22	A	819	CLA	O1D-CGD-O2D-CED
25	F	401	DGD	CCA-CDA-CEA-CFA
24	F	406	DD6	C10-C11-C13-C14
24	N	613	DD6	C10-C11-C13-C14
24	A	858	DD6	C10-C11-C13-C14
22	A	806	CLA	O1A-CGA-O2A-C1
22	A	819	CLA	O1A-CGA-O2A-C1
22	B	812	CLA	C15-C16-C17-C18
28	K	601	LMG	O6-C5-C6-O5
22	R	615	CLA	C13-C15-C16-C17
22	A	831	CLA	C5-C6-C7-C8
28	U	402	LMG	C34-C35-C36-C37
27	X	421	LMU	C1-C2-C3-C4
26	U	419	LHG	C3-O3-P-O5
28	H	319	LMG	C10-C11-C12-C13
26	A	846	LHG	C14-C15-C16-C17
27	B	854	LMU	C6-C7-C8-C9
28	G	616	LMG	C31-C32-C33-C34
28	U	423	LMG	C19-C20-C21-C22
22	T	601	CLA	O1D-CGD-O2D-CED
22	B	809	CLA	CBA-CGA-O2A-C1
22	Q	612	CLA	CBA-CGA-O2A-C1
26	W	420	LHG	C6-C5-O7-C7
28	K	601	LMG	C9-C8-O7-C10
26	N	616	LHG	C15-C16-C17-C18
26	P	601	LHG	C11-C10-C9-C8
26	A	846	LHG	C34-C35-C36-C37
28	L	401	LMG	C32-C33-C34-C35
22	Q	604	CLA	C10-C11-C12-C13
28	B	856	LMG	C34-C35-C36-C37
28	F	408	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
22	B	817	CLA	C16-C17-C18-C19
22	Q	604	CLA	C16-C17-C18-C20
22	A	826	CLA	C16-C17-C18-C19
28	T	616	LMG	C4-C5-C6-O5
27	B	858	LMU	O1'-C1-C2-C3
22	B	859	CLA	CBD-CGD-O2D-CED
26	A	845	LHG	C17-C18-C19-C20
27	B	850	LMU	C3-C4-C5-C6
22	L	402	CLA	CBA-CGA-O2A-C1
22	S	604	CLA	CBA-CGA-O2A-C1
22	W	412	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	CBA-CGA-O2A-C1
28	F	408	LMG	C29-C30-C31-C32
26	K	616	LHG	C25-C26-C27-C28
22	O	311	CLA	C4-C3-C5-C6
22	A	832	CLA	C4-C3-C5-C6
22	G	603	CLA	C2-C3-C5-C6
25	O	304	DGD	C6B-C7B-C8B-C9B
26	R	614	LHG	C9-C10-C11-C12
22	O	306	CLA	C11-C12-C13-C15
26	X	420	LHG	C10-C11-C12-C13
28	F	408	LMG	C32-C33-C34-C35
26	R	614	LHG	C28-C29-C30-C31
28	I	614	LMG	C29-C30-C31-C32
25	O	304	DGD	O1G-C1G-C2G-O2G
26	K	619	LHG	O7-C5-C6-O8
28	F	408	LMG	O7-C8-C9-O8
30	O	302	SQD	O47-C45-C46-O48
28	K	622	LMG	C32-C33-C34-C35
28	I	615	LMG	C38-C39-C40-C41
28	U	402	LMG	C40-C41-C42-C43
25	O	304	DGD	C6A-C7A-C8A-C9A
22	T	607	CLA	O1D-CGD-O2D-CED
26	O	321	LHG	C33-C34-C35-C36
28	B	856	LMG	C37-C38-C39-C40
22	A	833	CLA	C2A-CAA-CBA-CGA
27	B	858	LMU	C2'-C1'-O1'-C1
22	O	313	CLA	C3-C5-C6-C7
22	W	413	CLA	O1D-CGD-O2D-CED
22	A	805	CLA	C5-C6-C7-C8
26	X	420	LHG	C12-C13-C14-C15
22	B	827	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	K	618	LMG	C18-C19-C20-C21
28	H	319	LMG	C28-C29-C30-C31
26	L	416	LHG	C12-C13-C14-C15
26	A	846	LHG	C25-C26-C27-C28
28	B	856	LMG	C38-C39-C40-C41
28	J	101	LMG	C34-C35-C36-C37
28	K	618	LMG	C38-C39-C40-C41
22	O	313	CLA	C13-C15-C16-C17
28	U	423	LMG	C34-C35-C36-C37
22	L	410	CLA	O1D-CGD-O2D-CED
22	A	835	CLA	O1D-CGD-O2D-CED
28	K	601	LMG	C10-C11-C12-C13
22	R	615	CLA	C8-C10-C11-C12
22	W	411	CLA	C5-C6-C7-C8
22	K	612	CLA	O1D-CGD-O2D-CED
22	P	609	CLA	O1D-CGD-O2D-CED
22	Q	601	CLA	O1D-CGD-O2D-CED
22	A	816	CLA	C14-C13-C15-C16
22	X	412	CLA	C16-C17-C18-C19
22	B	812	CLA	C4-C3-C5-C6
22	Q	617	CLA	C4-C3-C5-C6
22	W	411	CLA	C4-C3-C5-C6
22	A	828	CLA	C4-C3-C5-C6
22	A	836	CLA	C4-C3-C5-C6
33	A	802	CL0	C4-C3-C5-C6
28	N	615	LMG	C31-C32-C33-C34
22	V	612	CLA	O1A-CGA-O2A-C1
28	I	614	LMG	C30-C31-C32-C33
22	B	817	CLA	C13-C15-C16-C17
26	T	614	LHG	C35-C36-C37-C38
26	N	616	LHG	C7-C8-C9-C10
27	U	421	LMU	C2-C3-C4-C5
28	I	615	LMG	C37-C38-C39-C40
26	A	846	LHG	C12-C13-C14-C15
27	M	102	LMU	C4-C5-C6-C7
24	J	105	DD6	C27-C29-C30-C31
24	L	413	DD6	C27-C29-C30-C31
24	L	414	DD6	C27-C29-C30-C31
24	L	415	DD6	C27-C29-C30-C31
24	N	613	DD6	C27-C29-C30-C31
24	P	612	DD6	C27-C29-C30-C31
24	R	612	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	S	611	DD6	C27-C29-C30-C31
24	S	612	DD6	C27-C29-C30-C31
24	T	613	DD6	C27-C29-C30-C31
24	U	416	DD6	C27-C29-C30-C31
24	U	417	DD6	C27-C29-C30-C31
24	W	416	DD6	C27-C29-C30-C31
24	A	859	DD6	C27-C29-C30-C31
26	K	619	LHG	O1-C1-C2-O2
26	N	616	LHG	O1-C1-C2-O2
27	O	301	LMU	C2-C1-O1'-C1'
22	B	806	CLA	C6-C7-C8-C9
22	B	807	CLA	C6-C7-C8-C9
22	B	824	CLA	C14-C13-C15-C16
22	B	828	CLA	C11-C10-C8-C9
22	B	830	CLA	C14-C13-C15-C16
22	B	831	CLA	C6-C7-C8-C9
22	B	835	CLA	C11-C10-C8-C9
22	B	835	CLA	C14-C13-C15-C16
22	G	608	CLA	C6-C7-C8-C9
22	G	608	CLA	C11-C10-C8-C9
22	H	303	CLA	C6-C7-C8-C9
22	L	406	CLA	C6-C7-C8-C9
22	L	408	CLA	C6-C7-C8-C9
22	L	417	CLA	C6-C7-C8-C9
22	N	607	CLA	C6-C7-C8-C9
22	Q	609	CLA	C11-C10-C8-C9
22	R	605	CLA	C6-C7-C8-C9
22	U	414	CLA	C11-C12-C13-C14
22	W	404	CLA	C14-C13-C15-C16
22	X	408	CLA	C6-C7-C8-C9
22	A	801	CLA	C11-C10-C8-C9
22	A	801	CLA	C11-C12-C13-C14
22	A	815	CLA	C11-C10-C8-C9
22	A	829	CLA	C11-C10-C8-C9
22	A	839	CLA	C14-C13-C15-C16
22	A	840	CLA	C14-C13-C15-C16
22	A	852	CLA	C11-C12-C13-C14
22	L	417	CLA	C8-C10-C11-C12
22	B	837	CLA	C4B-C3B-CAB-CBB
22	H	302	CLA	C4B-C3B-CAB-CBB
22	K	605	CLA	C4B-C3B-CAB-CBB
22	P	603	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	P	610	CLA	C4B-C3B-CAB-CBB
22	Q	607	CLA	C4B-C3B-CAB-CBB
22	Q	613	CLA	C4B-C3B-CAB-CBB
22	R	607	CLA	C4B-C3B-CAB-CBB
22	S	606	CLA	C4B-C3B-CAB-CBB
22	S	609	CLA	C4B-C3B-CAB-CBB
22	T	610	CLA	C4B-C3B-CAB-CBB
22	U	415	CLA	C4B-C3B-CAB-CBB
22	V	601	CLA	C4B-C3B-CAB-CBB
22	V	610	CLA	C4B-C3B-CAB-CBB
22	V	611	CLA	C4B-C3B-CAB-CBB
22	A	824	CLA	C4B-C3B-CAB-CBB
22	A	834	CLA	C4B-C3B-CAB-CBB
22	A	837	CLA	C4B-C3B-CAB-CBB
26	O	321	LHG	C10-C11-C12-C13
27	W	421	LMU	C4-C5-C6-C7
28	B	856	LMG	C17-C18-C19-C20
28	N	615	LMG	C16-C17-C18-C19
22	A	816	CLA	C8-C10-C11-C12
28	G	616	LMG	C42-C43-C44-C45
22	H	305	CLA	CBA-CGA-O2A-C1
22	B	815	CLA	C2A-CAA-CBA-CGA
27	K	620	LMU	C2'-C1'-O1'-C1
25	B	847	DGD	CEA-CFA-CGA-CHA
22	B	832	CLA	C3-C5-C6-C7
22	N	610	CLA	C3-C5-C6-C7
22	O	312	CLA	C3-C5-C6-C7
28	G	616	LMG	C4-C5-C6-O5
26	P	601	LHG	O6-C4-C5-C6
25	O	304	DGD	CCA-CDA-CEA-CFA
28	H	319	LMG	C17-C18-C19-C20
26	B	848	LHG	O8-C23-C24-C25
22	B	806	CLA	C6-C7-C8-C10
22	B	806	CLA	C12-C13-C15-C16
22	B	813	CLA	C6-C7-C8-C10
22	B	817	CLA	C11-C10-C8-C7
22	B	821	CLA	C6-C7-C8-C10
22	B	830	CLA	C12-C13-C15-C16
22	B	831	CLA	C6-C7-C8-C10
22	B	831	CLA	C11-C10-C8-C7
22	B	835	CLA	C11-C10-C8-C7
22	B	859	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	H	303	CLA	C6-C7-C8-C10
22	H	308	CLA	C11-C10-C8-C7
22	H	313	CLA	C11-C10-C8-C7
22	K	603	CLA	C11-C10-C8-C7
22	K	604	CLA	C6-C7-C8-C10
22	L	406	CLA	C6-C7-C8-C10
22	L	410	CLA	C11-C10-C8-C7
22	N	607	CLA	C6-C7-C8-C10
22	Q	610	CLA	C12-C13-C15-C16
22	R	606	CLA	C6-C7-C8-C10
22	T	604	CLA	C6-C7-C8-C10
22	T	607	CLA	C11-C10-C8-C7
22	U	404	CLA	C11-C10-C8-C7
22	X	407	CLA	C11-C12-C13-C15
22	X	412	CLA	C11-C12-C13-C15
22	A	801	CLA	C11-C12-C13-C15
22	A	803	CLA	C6-C7-C8-C10
22	A	804	CLA	C11-C10-C8-C7
22	A	810	CLA	C11-C12-C13-C15
22	A	829	CLA	C11-C10-C8-C7
22	A	829	CLA	C11-C12-C13-C15
22	A	840	CLA	C12-C13-C15-C16
22	A	842	CLA	C6-C7-C8-C10
22	A	852	CLA	C6-C7-C8-C10
22	A	840	CLA	C8-C10-C11-C12
31	W	408	CHL	C8-C10-C11-C12
25	B	847	DGD	CFA-CGA-CHA-CIA
28	B	852	LMG	C19-C20-C21-C22
26	K	616	LHG	C28-C29-C30-C31
28	B	856	LMG	C16-C17-C18-C19
22	B	816	CLA	O1A-CGA-O2A-C1
22	A	816	CLA	O1A-CGA-O2A-C1
22	G	603	CLA	C4-C3-C5-C6
22	I	606	CLA	C4-C3-C5-C6
22	J	102	CLA	C3A-C2A-CAA-CBA
22	K	609	CLA	C3A-C2A-CAA-CBA
22	L	412	CLA	C3A-C2A-CAA-CBA
22	P	605	CLA	C3A-C2A-CAA-CBA
22	V	608	CLA	C3A-C2A-CAA-CBA
22	V	617	CLA	C3A-C2A-CAA-CBA
22	W	410	CLA	C3A-C2A-CAA-CBA
22	B	812	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	B	834	CLA	C13-C15-C16-C17
26	L	416	LHG	C27-C28-C29-C30
30	K	621	SQD	C11-C10-C9-C8
27	T	617	LMU	O5'-C1'-O1'-C1
28	F	408	LMG	O6-C1-O1-C7
28	N	615	LMG	O6-C1-O1-C7
28	N	615	LMG	C30-C31-C32-C33
22	B	809	CLA	O1A-CGA-O2A-C1
22	P	604	CLA	O1D-CGD-O2D-CED
22	U	414	CLA	CBA-CGA-O2A-C1
32	U	418	NEX	C9-C10-C11-C12
32	V	616	NEX	C9-C10-C11-C12
22	K	602	CLA	C11-C12-C13-C14
22	X	412	CLA	C16-C17-C18-C20
26	A	846	LHG	C11-C10-C9-C8
22	N	608	CLA	O1D-CGD-O2D-CED
28	H	322	LMG	C31-C32-C33-C34
22	O	313	CLA	CBD-CGD-O2D-CED
28	H	317	LMG	C36-C37-C38-C39
28	Q	602	LMG	C32-C33-C34-C35
27	U	421	LMU	C3'-C4'-O1B-C1B
27	O	322	LMU	C2B-C1B-O1B-C4'
22	G	608	CLA	C2A-CAA-CBA-CGA
28	K	622	LMG	C14-C15-C16-C17
28	W	401	LMG	C33-C34-C35-C36
25	F	401	DGD	C1G-C2G-C3G-O3G
25	O	304	DGD	C1G-C2G-C3G-O3G
26	O	321	LHG	C4-C5-C6-O8
26	P	601	LHG	C4-C5-C6-O8
26	W	420	LHG	C4-C5-C6-O8
28	F	408	LMG	C7-C8-C9-O8
28	G	616	LMG	O1-C7-C8-C9
28	H	319	LMG	C7-C8-C9-O8
28	K	601	LMG	O1-C7-C8-C9
28	K	601	LMG	C7-C8-C9-O8
28	Q	602	LMG	O1-C7-C8-C9
30	O	302	SQD	C44-C45-C46-O48
28	B	852	LMG	C30-C31-C32-C33
22	B	823	CLA	C16-C17-C18-C19
22	O	306	CLA	C11-C12-C13-C14
22	O	313	CLA	C5-C6-C7-C8
22	A	808	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	X	420	LHG	C9-C10-C11-C12
28	G	616	LMG	C40-C41-C42-C43
28	J	101	LMG	C29-C30-C31-C32
28	J	101	LMG	C35-C36-C37-C38
27	J	104	LMU	C7-C8-C9-C10
28	J	101	LMG	C37-C38-C39-C40
22	A	820	CLA	C4-C3-C5-C6
22	A	830	CLA	C4-C3-C5-C6
22	A	836	CLA	C2-C3-C5-C6
33	A	802	CL0	C2-C3-C5-C6
22	Q	612	CLA	O1A-CGA-O2A-C1
22	S	601	CLA	CBD-CGD-O2D-CED
26	N	616	LHG	C28-C29-C30-C31
28	G	616	LMG	C30-C31-C32-C33
28	H	322	LMG	C32-C33-C34-C35
28	K	618	LMG	C16-C17-C18-C19
22	S	604	CLA	C11-C12-C13-C14
25	F	401	DGD	C2G-C3G-O3G-C1D
30	F	407	SQD	C7-C8-C9-C10
26	O	324	LHG	O6-C4-C5-O7
26	Q	616	LHG	O6-C4-C5-O7
26	T	614	LHG	O6-C4-C5-O7
26	X	420	LHG	O6-C4-C5-O7
26	A	846	LHG	O6-C4-C5-O7
25	B	847	DGD	C4A-C5A-C6A-C7A
28	L	401	LMG	C15-C16-C17-C18
22	K	608	CLA	O1D-CGD-O2D-CED
22	W	403	CLA	O1D-CGD-O2D-CED
21	B	846	BCR	C1-C6-C7-C8
21	J	103	BCR	C1-C6-C7-C8
22	B	837	CLA	C2B-C3B-CAB-CBB
22	Q	607	CLA	C2B-C3B-CAB-CBB
22	Q	613	CLA	C2B-C3B-CAB-CBB
22	T	610	CLA	C2B-C3B-CAB-CBB
22	U	415	CLA	C2B-C3B-CAB-CBB
22	A	824	CLA	C2B-C3B-CAB-CBB
28	G	616	LMG	C32-C33-C34-C35
26	P	601	LHG	C5-C4-O6-P
26	K	616	LHG	C9-C10-C11-C12
26	A	846	LHG	C29-C30-C31-C32
22	N	603	CLA	C13-C15-C16-C17
25	B	847	DGD	CFB-CGB-CHB-CIB

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Mol	Chain	Res	Type	Atoms
28	I	615	LMG	C34-C35-C36-C37
26	P	601	LHG	O8-C23-C24-C25
26	N	614	LHG	O7-C5-C6-O8
26	T	614	LHG	O7-C5-C6-O8
26	U	419	LHG	O7-C5-C6-O8
28	H	319	LMG	O7-C8-C9-O8
28	H	322	LMG	O7-C8-C9-O8
28	K	618	LMG	O7-C8-C9-O8
28	U	402	LMG	O7-C8-C9-O8
28	U	423	LMG	O1-C7-C8-O7
22	U	414	CLA	C12-C13-C15-C16
22	A	825	CLA	C12-C13-C15-C16
26	O	324	LHG	C27-C28-C29-C30
26	O	318	LHG	C26-C27-C28-C29
28	N	615	LMG	C21-C22-C23-C24
27	U	421	LMU	C5'-C4'-O1B-C1B
25	F	401	DGD	C3A-C4A-C5A-C6A
22	B	812	CLA	C14-C13-C15-C16
22	B	817	CLA	C11-C10-C8-C9
22	B	828	CLA	C6-C7-C8-C9
22	K	603	CLA	C11-C10-C8-C9
22	K	604	CLA	C6-C7-C8-C9
22	K	608	CLA	C14-C13-C15-C16
22	L	406	CLA	C14-C13-C15-C16
22	O	313	CLA	C11-C10-C8-C9
22	Q	610	CLA	C14-C13-C15-C16
22	A	803	CLA	C11-C10-C8-C9
33	A	802	CL0	C6-C7-C8-C9
22	B	820	CLA	C5-C6-C7-C8
28	K	601	LMG	C32-C33-C34-C35
22	B	823	CLA	C16-C17-C18-C20
22	H	306	CLA	C6-C7-C8-C10
26	X	420	LHG	C27-C28-C29-C30
27	U	422	LMU	C5-C6-C7-C8
28	L	401	LMG	C30-C31-C32-C33
27	H	301	LMU	O1'-C1-C2-C3
22	R	602	CLA	C2A-CAA-CBA-CGA
22	I	601	CLA	C15-C16-C17-C18
28	Q	602	LMG	C34-C35-C36-C37
28	I	615	LMG	C24-C25-C26-C27
22	G	606	CLA	O1D-CGD-O2D-CED
22	S	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	A	855	LMG	C15-C16-C17-C18
22	H	307	CLA	C4-C3-C5-C6
25	O	304	DGD	C9B-CAB-CBB-CCB
22	Q	617	CLA	C2-C3-C5-C6
22	A	830	CLA	C2-C3-C5-C6
22	K	602	CLA	C11-C12-C13-C15
22	W	412	CLA	O1A-CGA-O2A-C1
22	A	803	CLA	O1D-CGD-O2D-CED
26	O	318	LHG	C11-C12-C13-C14
22	T	604	CLA	C15-C16-C17-C18
26	U	419	LHG	C26-C27-C28-C29
28	B	852	LMG	C17-C18-C19-C20
28	K	618	LMG	C34-C35-C36-C37
22	Q	611	CLA	CBA-CGA-O2A-C1
28	K	622	LMG	C17-C18-C19-C20
28	T	616	LMG	C30-C31-C32-C33
22	Q	613	CLA	O1D-CGD-O2D-CED
22	A	810	CLA	C16-C17-C18-C19
22	A	822	CLA	C16-C17-C18-C19
22	N	601	CLA	CBD-CGD-O2D-CED
26	O	324	LHG	C25-C26-C27-C28
22	O	310	CLA	C10-C11-C12-C13
24	F	406	DD6	C12-C11-C13-C14
24	X	416	DD6	C7-C6-C8-C9
25	B	847	DGD	C7A-C8A-C9A-CAA
26	G	614	LHG	C11-C10-C9-C8
22	B	807	CLA	C12-C13-C15-C16
22	B	818	CLA	C11-C10-C8-C7
22	B	828	CLA	C6-C7-C8-C10
22	G	606	CLA	C6-C7-C8-C10
22	G	606	CLA	C11-C10-C8-C7
22	H	305	CLA	C6-C7-C8-C10
22	K	609	CLA	C6-C7-C8-C10
22	L	403	CLA	C6-C7-C8-C10
22	L	411	CLA	C12-C13-C15-C16
22	N	606	CLA	C11-C10-C8-C7
22	O	310	CLA	C11-C10-C8-C7
22	R	605	CLA	C12-C13-C15-C16
22	R	615	CLA	C11-C10-C8-C7
22	T	603	CLA	C6-C7-C8-C10
22	T	604	CLA	C11-C12-C13-C15
22	X	403	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	A	801	CLA	C12-C13-C15-C16
22	A	808	CLA	C12-C13-C15-C16
22	A	841	CLA	C11-C10-C8-C7
33	A	802	CL0	C6-C7-C8-C10
28	B	856	LMG	C28-C29-C30-C31
28	J	101	LMG	C38-C39-C40-C41
22	A	833	CLA	C8-C10-C11-C12
21	B	801	BCR	C11-C12-C13-C14
24	X	416	DD6	C5-C6-C8-C9
22	K	608	CLA	CBA-CGA-O2A-C1
22	A	840	CLA	CBA-CGA-O2A-C1
26	A	846	LHG	C27-C28-C29-C30
25	B	847	DGD	C5D-C6D-O5D-C1E
26	O	324	LHG	C26-C27-C28-C29
22	I	610	CLA	C2A-CAA-CBA-CGA
22	Q	612	CLA	C2A-CAA-CBA-CGA
22	R	608	CLA	C2A-CAA-CBA-CGA
22	S	605	CLA	C2A-CAA-CBA-CGA
22	X	408	CLA	C2A-CAA-CBA-CGA
27	U	421	LMU	C6-C7-C8-C9
22	A	825	CLA	C14-C13-C15-C16
22	T	609	CLA	CBD-CGD-O2D-CED
26	A	845	LHG	O9-C7-O7-C5
28	K	601	LMG	C11-C12-C13-C14
22	F	404	CLA	C4-C3-C5-C6
22	A	801	CLA	C4-C3-C5-C6
22	A	844	CLA	C4-C3-C5-C6
22	L	402	CLA	O1A-CGA-O2A-C1
22	A	836	CLA	O1A-CGA-O2A-C1
22	T	611	CLA	C13-C15-C16-C17
22	A	833	CLA	CBD-CGD-O2D-CED
22	B	813	CLA	C8-C10-C11-C12
26	O	324	LHG	C6-C5-O7-C7
22	H	305	CLA	O1A-CGA-O2A-C1
22	O	313	CLA	C8-C10-C11-C12
22	A	816	CLA	O1D-CGD-O2D-CED
25	F	401	DGD	C4A-C5A-C6A-C7A
28	U	423	LMG	C16-C17-C18-C19
28	U	423	LMG	C23-C24-C25-C26
26	O	324	LHG	C12-C13-C14-C15
22	U	414	CLA	O1A-CGA-O2A-C1
22	B	808	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	K	604	CLA	C3-C5-C6-C7
25	O	304	DGD	C1A-C2A-C3A-C4A
25	F	401	DGD	CDA-CEA-CFA-CGA
28	B	856	LMG	C30-C31-C32-C33
26	P	601	LHG	O6-C4-C5-O7
22	K	604	CLA	O1D-CGD-O2D-CED
26	K	619	LHG	C4-C5-C6-O8
28	B	852	LMG	O1-C7-C8-C9
28	G	616	LMG	C7-C8-C9-O8
28	I	615	LMG	O1-C7-C8-C9
28	K	618	LMG	C7-C8-C9-O8
22	L	402	CLA	C13-C15-C16-C17
22	X	403	CLA	C8-C10-C11-C12
28	G	616	LMG	O6-C5-C6-O5
22	O	315	CLA	CBA-CGA-O2A-C1
22	L	404	CLA	C4-C3-C5-C6
22	H	307	CLA	C2-C3-C5-C6
22	Q	604	CLA	C2-C3-C5-C6
22	A	844	CLA	C2-C3-C5-C6
22	B	830	CLA	C2C-C3C-CAC-CBC
22	R	601	CLA	C5-C6-C7-C8
25	O	304	DGD	O2G-C2G-C3G-O3G
26	L	416	LHG	O7-C5-C6-O8
26	R	614	LHG	O7-C5-C6-O8
26	W	420	LHG	O7-C5-C6-O8
28	F	408	LMG	O1-C7-C8-O7
28	I	615	LMG	O1-C7-C8-O7
28	K	601	LMG	O1-C7-C8-O7
28	K	601	LMG	O7-C8-C9-O8
28	K	618	LMG	O1-C7-C8-O7
22	W	410	CLA	C5-C6-C7-C8
22	H	311	CLA	C11-C12-C13-C14
22	K	609	CLA	C11-C10-C8-C9
22	K	611	CLA	C14-C13-C15-C16
22	L	402	CLA	C11-C12-C13-C14
22	L	411	CLA	C11-C12-C13-C14
22	O	310	CLA	C11-C10-C8-C9
22	Q	612	CLA	C11-C12-C13-C14
22	R	615	CLA	C11-C10-C8-C9
22	U	404	CLA	C6-C7-C8-C9
22	V	602	CLA	C11-C12-C13-C14
22	V	604	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	824	CLA	C11-C10-C8-C9
22	A	841	CLA	C11-C10-C8-C9
22	S	604	CLA	C11-C12-C13-C15
22	T	607	CLA	C11-C12-C13-C14
28	W	401	LMG	O6-C5-C6-O5
26	O	323	LHG	C30-C31-C32-C33
28	W	401	LMG	C41-C42-C43-C44
31	W	422	CHL	C8-C10-C11-C12
22	X	402	CLA	O1D-CGD-O2D-CED
22	Q	611	CLA	O1A-CGA-O2A-C1
22	B	802	CLA	CAA-CBA-CGA-O2A
22	T	607	CLA	C11-C12-C13-C15
28	I	614	LMG	C4-C5-C6-O5
22	L	405	CLA	O1D-CGD-O2D-CED
28	H	319	LMG	C33-C34-C35-C36
22	L	406	CLA	C13-C15-C16-C17
22	A	807	CLA	C10-C11-C12-C13
25	B	847	DGD	C5A-C6A-C7A-C8A
22	R	604	CLA	C2A-CAA-CBA-CGA
22	W	414	CLA	C2A-CAA-CBA-CGA
26	W	420	LHG	C9-C10-C11-C12
28	B	852	LMG	C14-C15-C16-C17
22	B	821	CLA	C11-C12-C13-C15
28	K	618	LMG	C35-C36-C37-C38
26	X	420	LHG	C23-C24-C25-C26
26	O	323	LHG	C12-C13-C14-C15
26	X	420	LHG	C31-C32-C33-C34
26	A	845	LHG	C13-C14-C15-C16
22	A	852	CLA	C13-C15-C16-C17
22	X	404	CLA	C3-C5-C6-C7
22	U	414	CLA	C14-C13-C15-C16
30	F	407	SQD	C25-C26-C27-C28
27	B	854	LMU	C1-C2-C3-C4
28	I	615	LMG	C14-C15-C16-C17
22	B	823	CLA	C13-C15-C16-C17
24	O	316	DD6	C27-C29-C30-C31
24	X	415	DD6	C27-C29-C30-C31
22	A	840	CLA	O1A-CGA-O2A-C1
22	W	409	CLA	C3-C5-C6-C7
22	K	604	CLA	C2A-CAA-CBA-CGA
22	B	819	CLA	C4B-C3B-CAB-CBB
22	B	822	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	826	CLA	C1A-C2A-CAA-CBA
22	B	838	CLA	C4B-C3B-CAB-CBB
22	F	403	CLA	C4B-C3B-CAB-CBB
22	H	306	CLA	C1A-C2A-CAA-CBA
22	I	601	CLA	C4B-C3B-CAB-CBB
22	I	607	CLA	C1A-C2A-CAA-CBA
22	I	608	CLA	C4B-C3B-CAB-CBB
22	K	613	CLA	C4B-C3B-CAB-CBB
22	N	608	CLA	C4B-C3B-CAB-CBB
22	N	611	CLA	C4B-C3B-CAB-CBB
22	O	310	CLA	C1A-C2A-CAA-CBA
22	O	315	CLA	C4B-C3B-CAB-CBB
22	P	605	CLA	C1A-C2A-CAA-CBA
22	P	608	CLA	C4B-C3B-CAB-CBB
22	Q	610	CLA	C4B-C3B-CAB-CBB
22	Q	618	CLA	C4B-C3B-CAB-CBB
22	R	608	CLA	C4B-C3B-CAB-CBB
22	R	610	CLA	C4B-C3B-CAB-CBB
22	S	608	CLA	C4B-C3B-CAB-CBB
22	S	615	CLA	C4B-C3B-CAB-CBB
22	U	411	CLA	C1A-C2A-CAA-CBA
22	V	608	CLA	C1A-C2A-CAA-CBA
22	V	613	CLA	C4B-C3B-CAB-CBB
22	V	617	CLA	C4B-C3B-CAB-CBB
22	W	403	CLA	C4B-C3B-CAB-CBB
22	W	414	CLA	C4B-C3B-CAB-CBB
22	X	409	CLA	C1A-C2A-CAA-CBA
22	X	419	CLA	C4B-C3B-CAB-CBB
22	A	813	CLA	C1A-C2A-CAA-CBA
22	A	823	CLA	C1A-C2A-CAA-CBA
22	A	836	CLA	C4B-C3B-CAB-CBB
22	B	828	CLA	C4-C3-C5-C6
22	H	313	CLA	C4-C3-C5-C6
22	S	602	CLA	C4-C3-C5-C6
22	W	402	CLA	C2-C3-C5-C6
26	K	619	LHG	C25-C26-C27-C28
27	U	424	LMU	C2-C3-C4-C5
22	B	807	CLA	C16-C17-C18-C20
22	S	602	CLA	C11-C12-C13-C15
22	B	804	CLA	C2A-CAA-CBA-CGA
22	K	611	CLA	C2A-CAA-CBA-CGA
22	L	411	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	804	CLA	C2A-CAA-CBA-CGA
22	A	842	CLA	C2A-CAA-CBA-CGA
28	F	408	LMG	C33-C34-C35-C36
22	B	859	CLA	O1D-CGD-O2D-CED
26	T	614	LHG	O6-C4-C5-C6
22	O	306	CLA	C3-C5-C6-C7
22	B	805	CLA	C12-C13-C15-C16
22	B	806	CLA	C11-C10-C8-C7
22	B	832	CLA	C11-C12-C13-C15
22	B	834	CLA	C12-C13-C15-C16
22	H	313	CLA	C6-C7-C8-C10
22	I	601	CLA	C6-C7-C8-C10
22	K	608	CLA	C11-C10-C8-C7
22	L	409	CLA	C11-C10-C8-C7
22	N	606	CLA	C12-C13-C15-C16
22	R	605	CLA	C11-C12-C13-C15
22	R	610	CLA	C11-C10-C8-C7
22	T	611	CLA	C12-C13-C15-C16
22	V	602	CLA	C11-C12-C13-C15
22	A	816	CLA	C11-C10-C8-C7
22	A	817	CLA	C11-C12-C13-C15
22	A	817	CLA	C12-C13-C15-C16
22	A	820	CLA	C12-C13-C15-C16
22	A	841	CLA	C11-C12-C13-C15
26	A	845	LHG	C10-C11-C12-C13
28	J	101	LMG	C36-C37-C38-C39
22	H	306	CLA	C6-C7-C8-C9
22	K	603	CLA	C11-C12-C13-C15
22	W	411	CLA	C11-C12-C13-C14
26	L	416	LHG	C28-C29-C30-C31
22	B	820	CLA	O1D-CGD-O2D-CED
25	B	847	DGD	CEB-CFB-CGB-CHB
22	L	417	CLA	CBA-CGA-O2A-C1
27	U	422	LMU	C4'-C5'-C6'-O6'
26	K	619	LHG	C12-C13-C14-C15
27	B	857	LMU	C6-C7-C8-C9
22	O	313	CLA	O1D-CGD-O2D-CED
28	J	101	LMG	C12-C13-C14-C15
22	O	315	CLA	O1A-CGA-O2A-C1
22	B	859	CLA	C10-C11-C12-C13
26	P	601	LHG	C2-C3-O3-P
22	B	814	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	N	610	CLA	C4-C3-C5-C6
22	A	822	CLA	C4-C3-C5-C6
26	T	614	LHG	C29-C30-C31-C32
22	A	814	CLA	C5-C6-C7-C8
28	H	317	LMG	O9-C10-O7-C8
22	G	610	CLA	C2A-CAA-CBA-CGA
22	A	807	CLA	C2A-CAA-CBA-CGA
22	A	841	CLA	C2A-CAA-CBA-CGA
22	B	818	CLA	C11-C10-C8-C9
22	B	821	CLA	C6-C7-C8-C9
22	G	606	CLA	C6-C7-C8-C9
22	L	403	CLA	C6-C7-C8-C9
22	T	605	CLA	C11-C12-C13-C14
22	X	412	CLA	C11-C12-C13-C14
22	A	804	CLA	C11-C10-C8-C9
22	A	828	CLA	C6-C7-C8-C9
31	W	422	CHL	C11-C12-C13-C14
22	X	409	CLA	C15-C16-C17-C18
24	P	612	DD6	C11-C10-C9-C8
22	O	313	CLA	C16-C17-C18-C20
22	V	609	CLA	C5-C6-C7-C8
22	S	601	CLA	O1D-CGD-O2D-CED
22	T	605	CLA	C3-C5-C6-C7
28	L	401	LMG	C37-C38-C39-C40
26	T	614	LHG	C26-C27-C28-C29
26	X	420	LHG	C34-C35-C36-C37
28	G	616	LMG	O1-C7-C8-O7
28	U	402	LMG	O1-C7-C8-O7
28	A	855	LMG	O7-C8-C9-O8
30	K	621	SQD	O47-C45-C46-O48
26	O	324	LHG	C1-C2-C3-O3
22	R	610	CLA	C13-C15-C16-C17
22	F	404	CLA	CBD-CGD-O2D-CED
25	B	847	DGD	C1G-C2G-C3G-O3G
26	U	419	LHG	C4-C5-C6-O8
26	X	420	LHG	C4-C5-C6-O8
28	F	408	LMG	O1-C7-C8-C9
28	H	317	LMG	O1-C7-C8-C9
28	K	618	LMG	O1-C7-C8-C9
28	T	616	LMG	O1-C7-C8-C9
28	A	855	LMG	C7-C8-C9-O8
27	L	420	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
22	U	404	CLA	C8-C10-C11-C12
26	H	316	LHG	O8-C23-C24-C25
22	K	608	CLA	O1A-CGA-O2A-C1
28	U	402	LMG	C39-C40-C41-C42
22	F	405	CLA	CAD-CBD-CGD-O2D
22	L	404	CLA	CAD-CBD-CGD-O2D
22	N	605	CLA	CAD-CBD-CGD-O2D
22	P	602	CLA	CAD-CBD-CGD-O2D
22	T	610	CLA	CAD-CBD-CGD-O2D
22	W	419	CLA	CAD-CBD-CGD-O2D
22	A	844	CLA	CAD-CBD-CGD-O2D
22	T	609	CLA	O1D-CGD-O2D-CED
28	I	615	LMG	C13-C14-C15-C16
28	W	401	LMG	C29-C28-O8-C9
22	O	313	CLA	C10-C11-C12-C13
28	U	402	LMG	C19-C20-C21-C22
22	B	833	CLA	C16-C17-C18-C19
22	H	308	CLA	C11-C12-C13-C14
22	H	303	CLA	C2A-CAA-CBA-CGA
22	Q	604	CLA	C2A-CAA-CBA-CGA
22	B	827	CLA	C5-C6-C7-C8
27	L	419	LMU	O5B-C1B-O1B-C4'
22	K	604	CLA	CAA-CBA-CGA-O2A
28	H	319	LMG	C32-C33-C34-C35
27	K	620	LMU	C2-C3-C4-C5
22	B	814	CLA	CHA-CBD-CGD-O1D
22	B	819	CLA	CHA-CBD-CGD-O1D
22	B	819	CLA	CHA-CBD-CGD-O2D
22	B	820	CLA	CHA-CBD-CGD-O1D
22	B	820	CLA	CHA-CBD-CGD-O2D
22	B	823	CLA	CHA-CBD-CGD-O1D
22	B	823	CLA	CHA-CBD-CGD-O2D
22	B	832	CLA	CHA-CBD-CGD-O1D
22	F	405	CLA	CAD-CBD-CGD-O1D
22	H	304	CLA	CHA-CBD-CGD-O1D
22	H	304	CLA	CHA-CBD-CGD-O2D
22	H	310	CLA	CHA-CBD-CGD-O1D
22	H	310	CLA	CHA-CBD-CGD-O2D
22	K	604	CLA	CHA-CBD-CGD-O1D
22	K	604	CLA	CHA-CBD-CGD-O2D
22	K	610	CLA	CHA-CBD-CGD-O1D
22	K	610	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	L	403	CLA	CHA-CBD-CGD-O1D
22	L	404	CLA	CAD-CBD-CGD-O1D
22	L	410	CLA	CHA-CBD-CGD-O1D
22	L	410	CLA	CHA-CBD-CGD-O2D
22	N	605	CLA	CAD-CBD-CGD-O1D
22	O	307	CLA	CHA-CBD-CGD-O1D
22	O	308	CLA	CHA-CBD-CGD-O1D
22	O	308	CLA	CHA-CBD-CGD-O2D
22	P	602	CLA	CAD-CBD-CGD-O1D
22	P	603	CLA	CHA-CBD-CGD-O1D
22	P	603	CLA	CHA-CBD-CGD-O2D
22	P	609	CLA	CHA-CBD-CGD-O1D
22	P	611	CLA	CHA-CBD-CGD-O1D
22	Q	606	CLA	CAD-CBD-CGD-O1D
22	R	609	CLA	CHA-CBD-CGD-O1D
22	R	609	CLA	CHA-CBD-CGD-O2D
22	T	610	CLA	CAD-CBD-CGD-O1D
22	T	611	CLA	CAD-CBD-CGD-O1D
22	V	608	CLA	CHA-CBD-CGD-O1D
22	V	611	CLA	CHA-CBD-CGD-O1D
22	W	419	CLA	CAD-CBD-CGD-O1D
22	A	805	CLA	CHA-CBD-CGD-O1D
22	A	805	CLA	CHA-CBD-CGD-O2D
22	A	806	CLA	CHA-CBD-CGD-O1D
22	A	806	CLA	CHA-CBD-CGD-O2D
22	A	826	CLA	CHA-CBD-CGD-O1D
22	A	826	CLA	CHA-CBD-CGD-O2D
22	A	844	CLA	CAD-CBD-CGD-O1D
26	B	848	LHG	C4-O6-P-O5
26	G	614	LHG	C3-O3-P-O6
26	K	616	LHG	C3-O3-P-O5
26	K	619	LHG	C3-O3-P-O5
26	K	619	LHG	C4-O6-P-O5
26	L	416	LHG	C3-O3-P-O4
26	O	318	LHG	C4-O6-P-O5
26	O	323	LHG	C3-O3-P-O4
26	O	323	LHG	C4-O6-P-O3
26	O	323	LHG	C4-O6-P-O4
26	T	614	LHG	C4-O6-P-O3
26	W	420	LHG	C3-O3-P-O4
26	A	845	LHG	C4-O6-P-O4
33	A	802	CL0	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	821	CLA	CBD-CGD-O2D-CED
28	B	856	LMG	C40-C41-C42-C43
26	U	419	LHG	C3-O3-P-O6
22	B	826	CLA	C4-C3-C5-C6
22	K	611	CLA	C4-C3-C5-C6
22	A	833	CLA	O1D-CGD-O2D-CED
22	I	608	CLA	C2B-C3B-CAB-CBB
22	N	608	CLA	C2B-C3B-CAB-CBB
22	N	611	CLA	C2B-C3B-CAB-CBB
22	O	315	CLA	C2B-C3B-CAB-CBB
22	Q	610	CLA	C2B-C3B-CAB-CBB
22	Q	618	CLA	C2B-C3B-CAB-CBB
22	R	608	CLA	C2B-C3B-CAB-CBB
22	R	610	CLA	C2B-C3B-CAB-CBB
22	S	608	CLA	C2B-C3B-CAB-CBB
22	S	609	CLA	C2B-C3B-CAB-CBB
22	V	601	CLA	C2B-C3B-CAB-CBB
22	V	608	CLA	C2B-C3B-CAB-CBB
22	V	610	CLA	C2B-C3B-CAB-CBB
22	V	613	CLA	C2B-C3B-CAB-CBB
22	W	403	CLA	C2B-C3B-CAB-CBB
22	A	836	CLA	C2B-C3B-CAB-CBB
22	A	837	CLA	C2B-C3B-CAB-CBB
22	A	841	CLA	C2B-C3B-CAB-CBB
22	A	842	CLA	CAA-CBA-CGA-O2A
22	L	404	CLA	C2-C3-C5-C6
22	U	401	CLA	C2-C3-C5-C6
28	Q	602	LMG	C31-C32-C33-C34
22	K	617	CLA	C5-C6-C7-C8
22	A	808	CLA	C5-C6-C7-C8
26	U	419	LHG	C5-C4-O6-P
22	F	403	CLA	C13-C15-C16-C17
22	T	604	CLA	C16-C17-C18-C20
22	U	404	CLA	C16-C17-C18-C20
25	O	304	DGD	C7B-C8B-C9B-CAB
26	A	845	LHG	C27-C28-C29-C30
26	O	323	LHG	O8-C23-C24-C25
28	K	622	LMG	C31-C32-C33-C34
22	B	825	CLA	C2A-CAA-CBA-CGA
27	L	420	LMU	C3-C4-C5-C6
22	A	811	CLA	C5-C6-C7-C8
22	G	603	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
27	J	104	LMU	C9-C10-C11-C12
25	B	847	DGD	CAA-CBA-CCA-CDA
24	A	858	DD6	C1-C24-C25-C26
22	X	410	CLA	C8-C10-C11-C12
22	A	824	CLA	C5-C6-C7-C8
22	A	832	CLA	C2-C3-C5-C6
27	U	422	LMU	C1-C2-C3-C4
26	O	324	LHG	O6-C4-C5-C6
26	Q	616	LHG	O6-C4-C5-C6
22	K	607	CLA	C2C-C3C-CAC-CBC
22	B	813	CLA	C6-C7-C8-C9
22	B	822	CLA	C11-C12-C13-C14
22	I	601	CLA	C11-C10-C8-C9
22	K	608	CLA	C11-C10-C8-C9
22	N	603	CLA	C6-C7-C8-C9
22	O	313	CLA	C6-C7-C8-C9
22	O	313	CLA	C14-C13-C15-C16
22	R	603	CLA	C6-C7-C8-C9
22	T	603	CLA	C6-C7-C8-C9
22	U	414	CLA	C6-C7-C8-C9
22	W	414	CLA	C11-C12-C13-C14
22	W	414	CLA	C14-C13-C15-C16
22	A	801	CLA	C14-C13-C15-C16
22	H	305	CLA	C11-C10-C8-C7
22	K	602	CLA	C6-C7-C8-C10
22	K	605	CLA	C11-C12-C13-C15
22	K	609	CLA	C11-C10-C8-C7
22	K	611	CLA	C12-C13-C15-C16
22	L	411	CLA	C11-C12-C13-C15
22	N	603	CLA	C6-C7-C8-C10
22	A	842	CLA	C12-C13-C15-C16
28	I	615	LMG	C19-C20-C21-C22
22	T	605	CLA	C10-C11-C12-C13
22	L	417	CLA	O1A-CGA-O2A-C1
26	A	845	LHG	C16-C17-C18-C19
22	B	807	CLA	C16-C17-C18-C19
22	N	601	CLA	O1D-CGD-O2D-CED
26	S	613	LHG	O8-C23-C24-C25
22	Q	609	CLA	C8-C10-C11-C12
28	K	618	LMG	C13-C14-C15-C16
27	A	854	LMU	C7-C8-C9-C10
22	F	404	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	S	607	CLA	C11-C12-C13-C15
22	R	607	CLA	C10-C11-C12-C13
22	J	102	CLA	CBD-CGD-O2D-CED
28	L	401	LMG	C12-C13-C14-C15
28	L	401	LMG	C14-C15-C16-C17
22	S	604	CLA	CAA-CBA-CGA-O2A
27	A	857	LMU	C4'-C5'-C6'-O6'
28	T	616	LMG	C17-C18-C19-C20
26	B	851	LHG	C16-C17-C18-C19
22	S	615	CLA	O1A-CGA-O2A-C1
22	U	414	CLA	C5-C6-C7-C8
22	X	409	CLA	C10-C11-C12-C13
22	A	844	CLA	C3-C5-C6-C7
22	B	822	CLA	C4-C3-C5-C6
22	X	409	CLA	C4-C3-C5-C6
26	A	846	LHG	C13-C14-C15-C16
22	A	819	CLA	CAA-CBA-CGA-O2A
28	W	401	LMG	C16-C17-C18-C19
28	U	423	LMG	O1-C7-C8-C9
26	P	601	LHG	C26-C27-C28-C29
28	A	855	LMG	C31-C32-C33-C34
26	R	614	LHG	C24-C23-O8-C6
28	B	856	LMG	C11-C12-C13-C14
28	H	319	LMG	C11-C12-C13-C14
28	G	616	LMG	C8-C7-O1-C1
28	T	616	LMG	C8-C7-O1-C1
28	U	402	LMG	C8-C7-O1-C1
22	B	812	CLA	C2A-CAA-CBA-CGA
22	B	820	CLA	C2A-CAA-CBA-CGA
22	H	311	CLA	C2A-CAA-CBA-CGA
22	V	612	CLA	C2A-CAA-CBA-CGA
22	A	801	CLA	C2A-CAA-CBA-CGA
22	A	844	CLA	C2A-CAA-CBA-CGA
22	A	829	CLA	C4-C3-C5-C6
22	N	610	CLA	C2-C3-C5-C6
25	O	304	DGD	CEA-CFA-CGA-CHA
25	F	401	DGD	C4B-C5B-C6B-C7B
22	F	404	CLA	O1A-CGA-O2A-C1
26	R	614	LHG	O10-C23-O8-C6
24	B	841	DD6	C27-C29-C30-C31
24	H	315	DD6	C27-C29-C30-C31
24	X	414	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	R	614	LHG	C1-C2-C3-O3
28	J	101	LMG	C10-C11-C12-C13
22	B	805	CLA	C14-C13-C15-C16
22	B	816	CLA	C14-C13-C15-C16
22	B	832	CLA	C11-C12-C13-C14
22	H	313	CLA	C6-C7-C8-C9
22	R	605	CLA	C14-C13-C15-C16
22	A	810	CLA	C11-C10-C8-C9
22	A	816	CLA	C11-C10-C8-C9
22	A	819	CLA	C11-C10-C8-C9
22	A	820	CLA	C14-C13-C15-C16
22	A	831	CLA	C11-C10-C8-C9
22	S	615	CLA	CBA-CGA-O2A-C1
26	O	321	LHG	C2-C3-O3-P
22	N	601	CLA	C4B-C3B-CAB-CBB
22	N	610	CLA	C4B-C3B-CAB-CBB
22	U	406	CLA	C4B-C3B-CAB-CBB
22	X	412	CLA	C4B-C3B-CAB-CBB
28	F	408	LMG	C19-C20-C21-C22
26	Q	616	LHG	C9-C10-C11-C12
28	I	614	LMG	C15-C16-C17-C18
22	S	602	CLA	C11-C12-C13-C14
22	U	414	CLA	C4-C3-C5-C6
22	X	402	CLA	C4-C3-C5-C6
26	N	616	LHG	C27-C28-C29-C30
22	B	822	CLA	C2-C3-C5-C6
22	B	826	CLA	C2-C3-C5-C6
28	B	856	LMG	C29-C30-C31-C32
28	U	402	LMG	C37-C38-C39-C40
22	F	404	CLA	O1D-CGD-O2D-CED
22	B	822	CLA	C11-C12-C13-C15
22	B	833	CLA	C6-C7-C8-C10
22	F	403	CLA	C12-C13-C15-C16
22	Q	612	CLA	C11-C12-C13-C15
22	R	615	CLA	C12-C13-C15-C16
22	W	414	CLA	C11-C12-C13-C15
22	X	403	CLA	C12-C13-C15-C16
22	A	813	CLA	C11-C10-C8-C7
22	K	605	CLA	C10-C11-C12-C13
22	P	604	CLA	CAA-CBA-CGA-O2A
22	A	801	CLA	C2C-C3C-CAC-CBC
27	F	409	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
22	T	604	CLA	C16-C17-C18-C19
25	O	304	DGD	C7A-C8A-C9A-CAA
22	J	102	CLA	O1D-CGD-O2D-CED
28	T	616	LMG	O1-C7-C8-O7
22	H	309	CLA	C3A-C2A-CAA-CBA
22	A	812	CLA	C4-C3-C5-C6
25	B	847	DGD	CBB-CCB-CDB-CEB
22	K	611	CLA	C2-C3-C5-C6
22	W	411	CLA	C2-C3-C5-C6
22	A	822	CLA	C2-C3-C5-C6
22	A	821	CLA	O1D-CGD-O2D-CED
21	B	843	BCR	C11-C10-C9-C34
21	B	843	BCR	C20-C21-C22-C37
21	A	851	BCR	C11-C10-C9-C34
21	A	851	BCR	C16-C17-C18-C36
24	F	406	DD6	C-C1-C2-C3
24	P	612	DD6	C-C1-C2-C3
32	U	418	NEX	C39-C29-C30-C31
32	V	616	NEX	C39-C29-C30-C31
22	A	826	CLA	C10-C11-C12-C13
22	A	820	CLA	C2C-C3C-CAC-CBC
25	F	401	DGD	C9A-CAA-CBA-CCA
28	G	616	LMG	C13-C14-C15-C16
22	N	608	CLA	CAA-CBA-CGA-O2A
22	R	606	CLA	C2-C1-O2A-CGA
32	U	418	NEX	C33-C34-C35-C15
32	V	616	NEX	C33-C34-C35-C15
31	W	408	CHL	C3-C5-C6-C7
24	V	615	DD6	C7-C6-C8-C9
22	P	604	CLA	CAA-CBA-CGA-O1A
25	F	401	DGD	C2A-C3A-C4A-C5A
28	G	616	LMG	C15-C16-C17-C18
22	P	605	CLA	CAA-CBA-CGA-O1A
22	P	611	CLA	CAA-CBA-CGA-O1A
22	T	604	CLA	C4-C3-C5-C6
22	A	842	CLA	C4-C3-C5-C6
26	A	846	LHG	C30-C31-C32-C33
22	B	828	CLA	C2-C3-C5-C6
22	B	824	CLA	C16-C17-C18-C19
22	B	803	CLA	C2A-CAA-CBA-CGA
22	L	403	CLA	C2A-CAA-CBA-CGA
22	A	829	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	H	304	CLA	CAA-CBA-CGA-O2A
22	P	603	CLA	CAA-CBA-CGA-O2A
22	K	607	CLA	C4C-C3C-CAC-CBC
22	A	801	CLA	C3-C5-C6-C7
22	Q	610	CLA	C10-C11-C12-C13
22	B	809	CLA	C11-C10-C8-C9
22	B	810	CLA	C6-C7-C8-C9
22	K	604	CLA	C14-C13-C15-C16
22	K	605	CLA	C14-C13-C15-C16
22	O	308	CLA	C11-C10-C8-C9
22	O	308	CLA	C11-C12-C13-C14
22	Q	604	CLA	C11-C10-C8-C9
22	R	615	CLA	C14-C13-C15-C16
22	T	611	CLA	C14-C13-C15-C16
22	U	411	CLA	C6-C7-C8-C9
22	W	410	CLA	C6-C7-C8-C9
22	X	408	CLA	C11-C10-C8-C9
22	A	806	CLA	C6-C7-C8-C9
22	A	813	CLA	C11-C10-C8-C9
22	A	825	CLA	C11-C10-C8-C9
22	A	828	CLA	C11-C12-C13-C14
22	A	831	CLA	C6-C7-C8-C9
22	A	839	CLA	C11-C12-C13-C14
26	G	614	LHG	O1-C1-C2-C3
26	N	614	LHG	O1-C1-C2-C3
26	A	845	LHG	C23-C24-C25-C26
22	K	609	CLA	C11-C12-C13-C15
28	B	852	LMG	C23-C24-C25-C26
22	W	404	CLA	C8-C10-C11-C12
22	H	310	CLA	CAA-CBA-CGA-O2A
22	P	603	CLA	CAA-CBA-CGA-O1A
22	P	611	CLA	CAA-CBA-CGA-O2A
27	L	420	LMU	O5'-C1'-O1'-C1
22	A	829	CLA	CBD-CGD-O2D-CED
22	S	601	CLA	CAA-CBA-CGA-O2A
22	A	803	CLA	C4-C3-C5-C6
22	N	608	CLA	CAA-CBA-CGA-O1A
22	T	609	CLA	CAA-CBA-CGA-O2A
28	F	408	LMG	C34-C35-C36-C37
22	H	304	CLA	C2A-CAA-CBA-CGA
22	K	610	CLA	C2A-CAA-CBA-CGA
22	N	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	815	CLA	C2A-CAA-CBA-CGA
22	A	839	CLA	C2A-CAA-CBA-CGA
21	B	843	BCR	C11-C10-C9-C8
21	B	843	BCR	C20-C21-C22-C23
21	A	851	BCR	C11-C10-C9-C8
21	A	851	BCR	C16-C17-C18-C19
22	B	814	CLA	C1A-C2A-CAA-CBA
22	B	821	CLA	C1A-C2A-CAA-CBA
22	H	303	CLA	C1A-C2A-CAA-CBA
22	R	605	CLA	C1A-C2A-CAA-CBA
22	S	602	CLA	C1A-C2A-CAA-CBA
22	V	617	CLA	C1A-C2A-CAA-CBA
22	W	415	CLA	C1A-C2A-CAA-CBA
22	A	804	CLA	C1A-C2A-CAA-CBA
22	A	840	CLA	C1A-C2A-CAA-CBA
24	F	406	DD6	C24-C1-C2-C3
24	P	612	DD6	C24-C1-C2-C3
22	V	608	CLA	CBA-CGA-O2A-C1
28	J	101	LMG	C21-C22-C23-C24
22	H	304	CLA	CAA-CBA-CGA-O1A
23	A	843	PQN	C18-C20-C21-C22
21	B	846	BCR	C5-C6-C7-C8
21	J	103	BCR	C5-C6-C7-C8
22	B	803	CLA	C2B-C3B-CAB-CBB
22	B	819	CLA	C2B-C3B-CAB-CBB
22	B	838	CLA	C2B-C3B-CAB-CBB
22	F	403	CLA	C2B-C3B-CAB-CBB
22	I	601	CLA	C2B-C3B-CAB-CBB
22	K	605	CLA	C2B-C3B-CAB-CBB
22	K	613	CLA	C2B-C3B-CAB-CBB
22	N	601	CLA	C2B-C3B-CAB-CBB
22	N	610	CLA	C2B-C3B-CAB-CBB
22	P	608	CLA	C2B-C3B-CAB-CBB
22	R	607	CLA	C2B-C3B-CAB-CBB
22	S	615	CLA	C2B-C3B-CAB-CBB
22	U	406	CLA	C2B-C3B-CAB-CBB
22	V	617	CLA	C2B-C3B-CAB-CBB
22	W	414	CLA	C2B-C3B-CAB-CBB
22	X	403	CLA	C2B-C3B-CAB-CBB
22	X	419	CLA	C2B-C3B-CAB-CBB
22	T	609	CLA	CAA-CBA-CGA-O1A
26	L	416	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
26	N	614	LHG	C25-C26-C27-C28
22	G	603	CLA	C11-C10-C8-C9
22	A	828	CLA	C16-C17-C18-C20
28	A	855	LMG	C28-C29-C30-C31
22	B	838	CLA	CAA-CBA-CGA-O2A
22	B	823	CLA	C4-C3-C5-C6
22	W	406	CLA	C4-C3-C5-C6
22	T	604	CLA	C2-C3-C5-C6
26	B	851	LHG	C17-C18-C19-C20
22	W	404	CLA	C10-C11-C12-C13
22	N	610	CLA	C2C-C3C-CAC-CBC
22	W	413	CLA	CAA-CBA-CGA-O2A
22	B	813	CLA	C11-C10-C8-C7
22	B	817	CLA	C11-C12-C13-C15
22	B	833	CLA	C12-C13-C15-C16
22	F	403	CLA	C6-C7-C8-C10
22	K	604	CLA	C11-C10-C8-C7
22	R	607	CLA	C6-C7-C8-C10
22	A	806	CLA	C6-C7-C8-C10
22	A	811	CLA	C6-C7-C8-C10
22	A	813	CLA	C11-C12-C13-C15
22	A	819	CLA	C11-C10-C8-C7
22	A	822	CLA	C6-C7-C8-C10
22	A	825	CLA	C11-C10-C8-C7
22	A	826	CLA	C12-C13-C15-C16
22	A	829	CLA	C12-C13-C15-C16
22	A	831	CLA	C11-C10-C8-C7
26	L	416	LHG	C26-C27-C28-C29
28	A	855	LMG	C34-C35-C36-C37
22	B	818	CLA	C16-C17-C18-C19
22	S	607	CLA	C11-C12-C13-C14
22	L	412	CLA	C2A-CAA-CBA-CGA
22	R	610	CLA	C2A-CAA-CBA-CGA
22	S	602	CLA	C2A-CAA-CBA-CGA
22	U	415	CLA	C2A-CAA-CBA-CGA
22	W	404	CLA	C2A-CAA-CBA-CGA
28	K	622	LMG	C28-C29-C30-C31
25	B	847	DGD	O2G-C2G-C3G-O3G
26	X	420	LHG	O7-C5-C6-O8
28	B	852	LMG	O1-C7-C8-O7
28	Q	602	LMG	C33-C34-C35-C36
22	B	817	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	O	321	LHG	C30-C31-C32-C33
28	W	401	LMG	C37-C38-C39-C40
22	B	824	CLA	C3-C5-C6-C7
22	S	601	CLA	CAA-CBA-CGA-O1A
22	S	608	CLA	O1D-CGD-O2D-CED
22	I	603	CLA	C11-C10-C8-C7
22	V	604	CLA	C11-C10-C8-C7
22	A	816	CLA	C12-C13-C15-C16
22	B	819	CLA	C5-C6-C7-C8
22	W	419	CLA	CAA-CBA-CGA-O2A
22	O	306	CLA	C4-C3-C5-C6
22	Q	612	CLA	C4-C3-C5-C6
26	B	848	LHG	O10-C23-C24-C25
22	A	829	CLA	C8-C10-C11-C12
22	F	404	CLA	C2-C3-C5-C6
22	U	414	CLA	C2-C3-C5-C6
22	X	402	CLA	C2-C3-C5-C6
22	A	801	CLA	C2-C3-C5-C6
22	A	808	CLA	C15-C16-C17-C18
22	B	838	CLA	CAA-CBA-CGA-O1A
22	H	305	CLA	C11-C12-C13-C14
22	A	840	CLA	C16-C17-C18-C20
22	A	829	CLA	O1D-CGD-O2D-CED
22	A	837	CLA	CBA-CGA-O2A-C1
25	F	401	DGD	CFA-CGA-CHA-CIA
22	B	819	CLA	C2A-CAA-CBA-CGA
22	H	310	CLA	CAA-CBA-CGA-O1A
22	Q	618	CLA	CAA-CBA-CGA-O2A
22	W	413	CLA	CAA-CBA-CGA-O1A
22	B	826	CLA	C6-C7-C8-C9
22	T	607	CLA	C6-C7-C8-C9
22	A	811	CLA	C6-C7-C8-C9
22	A	830	CLA	C11-C12-C13-C14
28	L	401	LMG	C18-C19-C20-C21
28	K	622	LMG	C33-C34-C35-C36
22	H	311	CLA	C15-C16-C17-C18
27	T	618	LMU	C3-C4-C5-C6
22	G	601	CLA	CAA-CBA-CGA-O2A
26	O	324	LHG	C33-C34-C35-C36
22	B	825	CLA	C10-C11-C12-C13
22	O	312	CLA	C4-C3-C5-C6
22	A	805	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	W	419	CLA	CAA-CBA-CGA-O1A
26	B	851	LHG	C2-C3-O3-P
26	K	619	LHG	C2-C3-O3-P
26	Q	616	LHG	C2-C3-O3-P
22	H	313	CLA	C2-C3-C5-C6
22	W	406	CLA	C2-C3-C5-C6
22	A	803	CLA	C2-C3-C5-C6
22	A	812	CLA	C2-C3-C5-C6
22	B	838	CLA	CBD-CGD-O2D-CED
26	L	416	LHG	O10-C23-O8-C6
22	G	606	CLA	C15-C16-C17-C18
22	B	828	CLA	CBA-CGA-O2A-C1
22	V	613	CLA	CAA-CBA-CGA-O2A
22	B	828	CLA	O1A-CGA-O2A-C1
26	R	614	LHG	C12-C13-C14-C15
28	B	856	LMG	C7-C8-C9-O8
22	A	852	CLA	C8-C10-C11-C12
26	L	416	LHG	C19-C20-C21-C22
22	O	307	CLA	CAA-CBA-CGA-O2A
22	P	605	CLA	CAA-CBA-CGA-O2A
22	S	603	CLA	CAA-CBA-CGA-O2A
22	V	608	CLA	O1A-CGA-O2A-C1
22	B	835	CLA	C2A-CAA-CBA-CGA
22	G	602	CLA	C2A-CAA-CBA-CGA
22	O	307	CLA	C2A-CAA-CBA-CGA
22	O	313	CLA	C2A-CAA-CBA-CGA
26	K	616	LHG	C12-C13-C14-C15
22	G	605	CLA	CAA-CBA-CGA-O2A
22	N	601	CLA	CAA-CBA-CGA-O2A
22	V	613	CLA	CAA-CBA-CGA-O1A
22	X	411	CLA	CAA-CBA-CGA-O2A
22	R	605	CLA	O1A-CGA-O2A-C1
22	A	817	CLA	C5-C6-C7-C8
24	H	314	DD6	C27-C29-C30-C31
24	V	614	DD6	C27-C29-C30-C31
24	V	615	DD6	C27-C29-C30-C31
24	W	417	DD6	C27-C29-C30-C31
24	A	847	DD6	C27-C29-C30-C31
24	A	858	DD6	C27-C29-C30-C31
22	U	404	CLA	C4-C3-C5-C6
22	B	829	CLA	CAA-CBA-CGA-O2A
22	G	601	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	A	805	CLA	C2-C3-C5-C6
22	K	611	CLA	O1D-CGD-O2D-CED
22	B	804	CLA	C16-C17-C18-C20
22	X	404	CLA	C10-C11-C12-C13
22	X	407	CLA	C10-C11-C12-C13
27	X	418	LMU	C1-C2-C3-C4
26	O	321	LHG	C17-C18-C19-C20
25	O	304	DGD	CFA-CGA-CHA-CIA
22	B	803	CLA	C4B-C3B-CAB-CBB
22	K	609	CLA	C4B-C3B-CAB-CBB
22	Q	604	CLA	C4B-C3B-CAB-CBB
22	R	615	CLA	C4B-C3B-CAB-CBB
22	T	605	CLA	C4B-C3B-CAB-CBB
22	U	412	CLA	C4B-C3B-CAB-CBB
22	X	403	CLA	C4B-C3B-CAB-CBB
22	A	810	CLA	C4B-C3B-CAB-CBB
22	A	813	CLA	C4B-C3B-CAB-CBB
22	A	837	CLA	O1A-CGA-O2A-C1
28	K	601	LMG	O10-C28-O8-C9
22	S	608	CLA	CAA-CBA-CGA-O2A
22	K	611	CLA	CBD-CGD-O2D-CED
22	B	804	CLA	CAA-CBA-CGA-O2A
22	H	303	CLA	C5-C6-C7-C8
22	H	318	CLA	CAA-CBA-CGA-O2A
22	B	838	CLA	O1D-CGD-O2D-CED
22	B	830	CLA	C13-C15-C16-C17
22	G	609	CLA	CAA-CBA-CGA-O2A
22	Q	607	CLA	CAA-CBA-CGA-O2A
22	U	403	CLA	CAA-CBA-CGA-O2A
26	K	616	LHG	C10-C11-C12-C13
28	B	856	LMG	C14-C15-C16-C17
22	T	611	CLA	C16-C17-C18-C20
22	R	607	CLA	C4-C3-C5-C6
28	B	856	LMG	O7-C8-C9-O8
22	G	611	CLA	CAA-CBA-CGA-O2A
22	L	412	CLA	CAA-CBA-CGA-O2A
22	A	834	CLA	CAA-CBA-CGA-O2A
27	B	854	LMU	C4-C5-C6-C7
27	K	620	LMU	O5'-C1'-O1'-C1
26	X	420	LHG	C2-C3-O3-P
27	H	320	LMU	C4-C5-C6-C7
22	I	606	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	K	604	CLA	C11-C12-C13-C15
22	O	308	CLA	C11-C12-C13-C15
22	Q	604	CLA	C11-C10-C8-C7
22	X	404	CLA	C11-C10-C8-C7
22	A	824	CLA	C12-C13-C15-C16
22	N	604	CLA	CAA-CBA-CGA-O2A
22	P	607	CLA	CAA-CBA-CGA-O2A
22	P	609	CLA	CAA-CBA-CGA-O2A
22	A	829	CLA	CAA-CBA-CGA-O2A
26	Q	616	LHG	C28-C29-C30-C31
26	A	846	LHG	C7-C8-C9-C10
22	V	611	CLA	CAA-CBA-CGA-O2A
22	A	834	CLA	CAA-CBA-CGA-O1A
22	B	823	CLA	C14-C13-C15-C16
22	K	617	CLA	C11-C10-C8-C9
22	Q	604	CLA	C14-C13-C15-C16
22	R	610	CLA	C11-C10-C8-C9
22	A	824	CLA	C11-C12-C13-C14
22	L	411	CLA	C8-C10-C11-C12
30	F	407	SQD	C45-C44-O6-C1
30	O	302	SQD	C45-C44-O6-C1
25	B	847	DGD	C3A-C4A-C5A-C6A
28	B	856	LMG	C33-C34-C35-C36
22	Q	618	CLA	CAA-CBA-CGA-O1A
22	V	601	CLA	CAA-CBA-CGA-O2A
22	X	419	CLA	CAA-CBA-CGA-O2A
22	I	602	CLA	C2A-CAA-CBA-CGA
22	O	310	CLA	C2A-CAA-CBA-CGA
22	X	403	CLA	C2A-CAA-CBA-CGA
22	G	606	CLA	C2-C1-O2A-CGA
22	K	609	CLA	C2-C1-O2A-CGA
22	L	406	CLA	C2-C1-O2A-CGA
22	B	824	CLA	C16-C17-C18-C20
22	A	801	CLA	C16-C17-C18-C20
22	S	608	CLA	CBD-CGD-O2D-CED
26	N	616	LHG	C30-C31-C32-C33
28	J	101	LMG	C42-C43-C44-C45
28	T	616	LMG	C35-C36-C37-C38
22	W	412	CLA	C8-C10-C11-C12
22	A	839	CLA	C8-C10-C11-C12
22	R	605	CLA	CBA-CGA-O2A-C1
22	H	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	L	411	CLA	C4-C3-C5-C6
22	N	607	CLA	C3A-C2A-CAA-CBA
22	P	607	CLA	C3A-C2A-CAA-CBA
22	Q	610	CLA	C3A-C2A-CAA-CBA
22	A	804	CLA	C3A-C2A-CAA-CBA
22	B	829	CLA	CAA-CBA-CGA-O1A
22	N	601	CLA	CAA-CBA-CGA-O1A
22	N	609	CLA	CAA-CBA-CGA-O2A
22	X	411	CLA	CAA-CBA-CGA-O1A
22	S	602	CLA	C2-C3-C5-C6
28	I	614	LMG	C33-C34-C35-C36
27	L	420	LMU	C4-C5-C6-C7
28	K	622	LMG	C4-C5-C6-O5
26	P	601	LHG	O10-C23-C24-C25
22	H	318	CLA	CAA-CBA-CGA-O1A
22	O	307	CLA	CAA-CBA-CGA-O1A
22	Q	607	CLA	CAA-CBA-CGA-O1A
22	X	404	CLA	C11-C12-C13-C15
28	H	322	LMG	C12-C13-C14-C15
22	B	823	CLA	O2A-C1-C2-C3
31	W	422	CHL	O2A-C1-C2-C3
22	B	814	CLA	CAA-CBA-CGA-O2A
22	G	605	CLA	CAA-CBA-CGA-O1A
22	P	608	CLA	CAA-CBA-CGA-O2A
22	S	608	CLA	CAA-CBA-CGA-O1A
22	U	403	CLA	CAA-CBA-CGA-O1A
22	V	617	CLA	CAA-CBA-CGA-O2A
33	A	802	CL0	CAA-CBA-CGA-O2A
22	G	609	CLA	CAA-CBA-CGA-O1A
22	R	611	CLA	CAA-CBA-CGA-O2A
22	N	610	CLA	C4C-C3C-CAC-CBC
22	R	601	CLA	C13-C15-C16-C17
22	O	306	CLA	C2A-CAA-CBA-CGA
25	B	847	DGD	C6B-C7B-C8B-C9B
22	A	824	CLA	C3-C5-C6-C7
22	R	602	CLA	C5-C6-C7-C8
22	T	602	CLA	C5-C6-C7-C8
22	N	604	CLA	CAA-CBA-CGA-O1A
22	P	609	CLA	CAA-CBA-CGA-O1A
22	S	603	CLA	CAA-CBA-CGA-O1A
26	W	420	LHG	C24-C23-O8-C6
24	L	414	DD6	C13-C14-C15-O1

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Mol	Chain	Res	Type	Atoms
24	N	613	DD6	C13-C14-C15-O1
24	P	612	DD6	C13-C14-C15-O1
24	W	418	DD6	C13-C14-C15-O1
27	L	419	LMU	O1B-C1B-O5B-C5B
32	U	418	NEX	C28-C29-C30-C31
32	V	616	NEX	C28-C29-C30-C31
22	L	412	CLA	CAA-CBA-CGA-O1A
22	P	608	CLA	CAA-CBA-CGA-O1A
22	V	612	CLA	C8-C10-C11-C12
26	W	420	LHG	O10-C23-O8-C6
28	U	423	LMG	C14-C15-C16-C17
22	W	415	CLA	CAA-CBA-CGA-O1A
22	W	415	CLA	CAA-CBA-CGA-O2A
22	X	419	CLA	CAA-CBA-CGA-O1A
27	F	409	LMU	C4-C5-C6-C7
26	T	614	LHG	C4-C5-C6-O8
22	K	607	CLA	CBD-CGD-O2D-CED
22	B	816	CLA	C10-C11-C12-C13
22	T	602	CLA	C8-C10-C11-C12
22	V	601	CLA	CAA-CBA-CGA-O1A
27	T	617	LMU	C3-C4-C5-C6
22	I	606	CLA	O1D-CGD-O2D-CED
22	G	602	CLA	CBA-CGA-O2A-C1
22	B	808	CLA	C5-C6-C7-C8
27	H	321	LMU	C2-C3-C4-C5
28	K	601	LMG	C15-C16-C17-C18
22	U	410	CLA	C4-C3-C5-C6
22	H	309	CLA	C2A-CAA-CBA-CGA
22	I	608	CLA	CAA-CBA-CGA-O2A
22	N	609	CLA	CAA-CBA-CGA-O1A
22	B	818	CLA	C16-C17-C18-C20
22	A	801	CLA	C16-C17-C18-C19
22	A	822	CLA	C13-C15-C16-C17
28	B	856	LMG	C42-C43-C44-C45
22	X	410	CLA	O1A-CGA-O2A-C1
22	S	609	CLA	CAA-CBA-CGA-O2A
28	K	601	LMG	O8-C28-C29-C30
22	N	606	CLA	C15-C16-C17-C18
26	X	420	LHG	C25-C26-C27-C28
26	A	845	LHG	C32-C33-C34-C35
22	R	607	CLA	C3-C5-C6-C7
28	K	618	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
22	R	611	CLA	CAA-CBA-CGA-O1A
22	V	611	CLA	CAA-CBA-CGA-O1A
22	A	817	CLA	C10-C11-C12-C13
22	N	606	CLA	C14-C13-C15-C16
22	U	404	CLA	C11-C12-C13-C14
22	V	603	CLA	C6-C7-C8-C9
22	W	410	CLA	C11-C10-C8-C9
22	X	403	CLA	C11-C12-C13-C14
22	A	806	CLA	C11-C12-C13-C14
22	A	816	CLA	C11-C12-C13-C14
22	A	817	CLA	C11-C12-C13-C14
22	A	828	CLA	C16-C17-C18-C19
28	N	615	LMG	C14-C15-C16-C17
22	A	808	CLA	CAA-CBA-CGA-O2A
26	A	846	LHG	O6-C4-C5-C6
22	B	814	CLA	CAA-CBA-CGA-O1A
22	V	617	CLA	CAA-CBA-CGA-O1A
22	A	836	CLA	C5-C6-C7-C8
22	K	604	CLA	C4-C3-C5-C6
27	B	850	LMU	C4-C5-C6-C7
26	B	851	LHG	O7-C7-C8-C9
26	X	420	LHG	O7-C7-C8-C9
22	G	611	CLA	CAA-CBA-CGA-O1A
22	I	605	CLA	CAA-CBA-CGA-O2A
22	P	607	CLA	CAA-CBA-CGA-O1A
28	U	423	LMG	C35-C36-C37-C38
22	B	818	CLA	C6-C7-C8-C10
22	B	826	CLA	C6-C7-C8-C10
22	G	606	CLA	C12-C13-C15-C16
22	K	605	CLA	C6-C7-C8-C10
22	K	617	CLA	C11-C10-C8-C7
22	N	606	CLA	C6-C7-C8-C10
22	O	313	CLA	C11-C12-C13-C15
22	T	603	CLA	C11-C10-C8-C7
22	T	607	CLA	C6-C7-C8-C10
22	W	409	CLA	C11-C10-C8-C7
22	A	816	CLA	C6-C7-C8-C10
22	A	825	CLA	C6-C7-C8-C10
22	A	830	CLA	C11-C12-C13-C15
22	G	602	CLA	O1A-CGA-O2A-C1
26	N	616	LHG	C25-C26-C27-C28
22	P	603	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	Q	604	CLA	C2B-C3B-CAB-CBB
22	R	601	CLA	C2B-C3B-CAB-CBB
22	T	605	CLA	C2B-C3B-CAB-CBB
22	W	412	CLA	C2B-C3B-CAB-CBB
22	A	813	CLA	C2B-C3B-CAB-CBB
28	K	622	LMG	C11-C10-O7-C8
22	A	821	CLA	CAA-CBA-CGA-O2A
26	L	416	LHG	O8-C23-C24-C25
31	W	422	CHL	CAA-CBA-CGA-O2A
26	R	614	LHG	C17-C18-C19-C20
22	G	603	CLA	C2-C1-O2A-CGA
22	I	606	CLA	C2-C1-O2A-CGA
22	N	603	CLA	C2-C1-O2A-CGA
22	N	606	CLA	C2-C1-O2A-CGA
22	N	607	CLA	C2-C1-O2A-CGA
22	R	602	CLA	C2-C1-O2A-CGA
22	X	405	CLA	C2-C1-O2A-CGA
28	T	616	LMG	C16-C17-C18-C19
28	I	615	LMG	C2-C1-O1-C7
24	X	416	DD6	C11-C13-C14-C15
28	K	622	LMG	O6-C5-C6-O5
22	L	404	CLA	CAA-CBA-CGA-O2A
22	B	835	CLA	C8-C10-C11-C12
30	V	618	SQD	C45-C44-O6-C1
22	X	410	CLA	CBA-CGA-O2A-C1
28	L	401	LMG	C16-C17-C18-C19
22	K	609	CLA	C11-C12-C13-C14
22	B	821	CLA	C5-C6-C7-C8
22	B	803	CLA	C4-C3-C5-C6
22	B	804	CLA	C4-C3-C5-C6
26	T	614	LHG	C7-C8-C9-C10
22	K	605	CLA	CAA-CBA-CGA-O2A
22	B	804	CLA	C2-C3-C5-C6
22	K	604	CLA	C2-C3-C5-C6
22	L	411	CLA	C2-C3-C5-C6
28	U	423	LMG	O9-C10-O7-C8
22	B	807	CLA	C2A-CAA-CBA-CGA
22	F	404	CLA	C2A-CAA-CBA-CGA
22	X	412	CLA	C2A-CAA-CBA-CGA
22	T	611	CLA	C10-C11-C12-C13
31	W	407	CHL	CAA-CBA-CGA-O2A
22	U	401	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	840	CLA	C16-C17-C18-C19
26	O	318	LHG	O7-C7-C8-C9
30	V	618	SQD	C4-C5-C6-S
22	X	410	CLA	C4-C3-C5-C6
22	A	852	CLA	C4-C3-C5-C6
22	R	605	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	CAA-CBA-CGA-O2A
22	W	409	CLA	C2-C3-C5-C6
22	X	409	CLA	C2-C3-C5-C6
22	A	829	CLA	C2-C3-C5-C6
22	A	842	CLA	C2-C3-C5-C6
27	W	421	LMU	C7-C8-C9-C10
22	T	610	CLA	CAA-CBA-CGA-O2A
26	O	321	LHG	C28-C29-C30-C31
22	Q	610	CLA	O1A-CGA-O2A-C1
22	T	602	CLA	C2A-CAA-CBA-CGA
27	W	421	LMU	C1-C2-C3-C4
22	B	822	CLA	CAA-CBA-CGA-O2A
22	K	610	CLA	CAA-CBA-CGA-O2A
22	Q	605	CLA	CAA-CBA-CGA-O2A
24	T	612	DD6	C27-C29-C30-C31
27	B	857	LMU	C2-C1-O1'-C1'
22	B	813	CLA	C11-C10-C8-C9
22	B	828	CLA	C11-C12-C13-C14
22	G	602	CLA	C6-C7-C8-C9
22	H	308	CLA	C6-C7-C8-C9
22	K	602	CLA	C6-C7-C8-C9
22	R	605	CLA	C11-C12-C13-C14
22	A	813	CLA	C11-C12-C13-C14
22	A	826	CLA	C14-C13-C15-C16
25	O	304	DGD	C4A-C5A-C6A-C7A
28	H	319	LMG	C34-C35-C36-C37
22	N	603	CLA	CAA-CBA-CGA-O2A
22	R	603	CLA	CAA-CBA-CGA-O2A
27	U	421	LMU	C5-C6-C7-C8
22	T	604	CLA	C5-C6-C7-C8
22	H	305	CLA	C1A-C2A-CAA-CBA
22	H	309	CLA	C1A-C2A-CAA-CBA
22	H	311	CLA	C4B-C3B-CAB-CBB
22	K	602	CLA	C1A-C2A-CAA-CBA
22	R	601	CLA	C4B-C3B-CAB-CBB
22	V	609	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	W	411	CLA	C1A-C2A-CAA-CBA
22	W	412	CLA	C4B-C3B-CAB-CBB
22	I	608	CLA	CAA-CBA-CGA-O1A
27	L	419	LMU	C3-C4-C5-C6
22	N	607	CLA	C4-C3-C5-C6
22	W	409	CLA	C4-C3-C5-C6
31	W	422	CHL	C5-C6-C7-C8
28	G	616	LMG	O6-C1-O1-C7
28	H	322	LMG	O6-C1-O1-C7
22	B	805	CLA	CAA-CBA-CGA-O2A
22	H	306	CLA	CAA-CBA-CGA-O2A
22	I	601	CLA	CAA-CBA-CGA-O2A
22	Q	612	CLA	CAA-CBA-CGA-O2A
22	R	608	CLA	CAA-CBA-CGA-O2A
26	G	614	LHG	O8-C23-C24-C25
26	O	324	LHG	O7-C7-C8-C9
28	N	615	LMG	O7-C10-C11-C12
26	A	845	LHG	O7-C5-C6-O8
28	H	322	LMG	O1-C7-C8-O7
28	K	622	LMG	O7-C8-C9-O8
22	P	606	CLA	CAA-CBA-CGA-O2A
24	V	615	DD6	C5-C6-C8-C9
24	P	613	DD6	C1-C2-C3-C4
26	N	616	LHG	C9-C10-C11-C12
22	K	613	CLA	C5-C6-C7-C8
22	Q	603	CLA	CAA-CBA-CGA-O2A
22	Q	606	CLA	CAA-CBA-CGA-O2A
22	U	412	CLA	CAA-CBA-CGA-O2A
22	R	606	CLA	CAA-CBA-CGA-O2A
26	R	614	LHG	O8-C23-C24-C25
31	W	408	CHL	C2A-CAA-CBA-CGA
22	A	826	CLA	C15-C16-C17-C18
27	B	850	LMU	C6-C7-C8-C9
26	N	614	LHG	O8-C23-C24-C25
22	L	406	CLA	C15-C16-C17-C18
22	I	605	CLA	CAA-CBA-CGA-O1A
27	K	620	LMU	C2B-C1B-O1B-C4'
22	A	830	CLA	C15-C16-C17-C18
22	B	836	CLA	C2-C1-O2A-CGA
22	I	603	CLA	C2-C1-O2A-CGA
22	U	414	CLA	C2-C1-O2A-CGA
22	A	822	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
26	X	420	LHG	O8-C23-C24-C25
22	B	804	CLA	C11-C12-C13-C15
22	B	825	CLA	C12-C13-C15-C16
22	Q	604	CLA	C12-C13-C15-C16
22	T	602	CLA	C11-C10-C8-C7
22	T	605	CLA	C6-C7-C8-C10
22	V	603	CLA	C6-C7-C8-C10
22	V	612	CLA	C11-C12-C13-C15
22	X	408	CLA	C12-C13-C15-C16
22	A	840	CLA	C11-C12-C13-C15
22	U	401	CLA	CBA-CGA-O2A-C1
22	N	607	CLA	C5-C6-C7-C8
22	A	852	CLA	C15-C16-C17-C18
28	N	615	LMG	C10-C11-C12-C13
28	N	615	LMG	C28-C29-C30-C31
26	N	616	LHG	C4-C5-O7-C7
26	N	616	LHG	C6-C5-O7-C7
22	B	816	CLA	CAA-CBA-CGA-O2A
26	K	619	LHG	O7-C7-C8-C9
28	B	856	LMG	C15-C16-C17-C18
22	B	835	CLA	C13-C15-C16-C17
22	A	844	CLA	O1D-CGD-O2D-CED
22	P	602	CLA	C2A-CAA-CBA-CGA
22	P	605	CLA	C2A-CAA-CBA-CGA
22	U	404	CLA	C2A-CAA-CBA-CGA
22	V	602	CLA	C2A-CAA-CBA-CGA
22	V	609	CLA	C2A-CAA-CBA-CGA
28	K	618	LMG	O9-C10-O7-C8
22	H	305	CLA	C11-C12-C13-C15
22	T	605	CLA	C16-C17-C18-C19
22	U	410	CLA	C6-C7-C8-C10
31	W	407	CHL	CAA-CBA-CGA-O1A
28	L	401	LMG	C19-C20-C21-C22
28	H	322	LMG	O6-C5-C6-O5
26	Q	616	LHG	C12-C13-C14-C15
22	G	610	CLA	CAA-CBA-CGA-O1A
22	R	605	CLA	C3A-C2A-CAA-CBA
22	R	608	CLA	C4-C3-C5-C6
22	X	404	CLA	C4-C3-C5-C6
22	X	405	CLA	C3A-C2A-CAA-CBA
22	A	811	CLA	C3A-C2A-CAA-CBA
22	A	830	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	802	CLA	CAA-CBA-CGA-O1A
22	W	410	CLA	C8-C10-C11-C12
23	A	843	PQN	C25-C26-C27-C28
22	B	802	CLA	C16-C17-C18-C20
22	A	833	CLA	C16-C17-C18-C19
26	R	614	LHG	C14-C15-C16-C17
22	P	602	CLA	CAA-CBA-CGA-O2A
22	K	605	CLA	CAA-CBA-CGA-O1A
31	W	422	CHL	CAA-CBA-CGA-O1A
22	Q	610	CLA	CBA-CGA-O2A-C1
28	K	622	LMG	C29-C28-O8-C9
22	B	806	CLA	C5-C6-C7-C8
22	A	821	CLA	CAA-CBA-CGA-O1A
28	N	615	LMG	O9-C10-C11-C12
28	J	101	LMG	C15-C16-C17-C18
28	K	601	LMG	C12-C13-C14-C15
28	K	622	LMG	C37-C38-C39-C40
22	I	611	CLA	C2A-CAA-CBA-CGA
22	K	603	CLA	C2A-CAA-CBA-CGA
22	P	609	CLA	C2A-CAA-CBA-CGA
22	T	610	CLA	CAA-CBA-CGA-O1A
22	B	817	CLA	C11-C12-C13-C14
22	B	818	CLA	C6-C7-C8-C9
22	B	825	CLA	C11-C12-C13-C14
22	B	833	CLA	C14-C13-C15-C16
22	F	403	CLA	C6-C7-C8-C9
22	H	303	CLA	C11-C10-C8-C9
22	H	311	CLA	C6-C7-C8-C9
22	K	603	CLA	C6-C7-C8-C9
22	V	612	CLA	C14-C13-C15-C16
22	A	822	CLA	C6-C7-C8-C9
22	A	840	CLA	C11-C10-C8-C9
22	I	601	CLA	CAA-CBA-CGA-O1A
26	B	851	LHG	O9-C7-C8-C9
28	U	423	LMG	C32-C33-C34-C35
28	A	855	LMG	C13-C14-C15-C16
22	R	610	CLA	C4-C3-C5-C6
22	S	609	CLA	CAA-CBA-CGA-O1A
22	A	808	CLA	CAA-CBA-CGA-O1A
26	O	318	LHG	O9-C7-C8-C9
22	B	806	CLA	C2-C3-C5-C6
22	B	823	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	Q	610	CLA	C2-C3-C5-C6
24	F	406	DD6	C13-C14-C15-C16
30	V	618	SQD	O5-C5-C6-S
22	Q	601	CLA	CAA-CBA-CGA-O2A
22	N	603	CLA	CAA-CBA-CGA-O1A
26	O	324	LHG	O9-C7-C8-C9
22	K	607	CLA	O1D-CGD-O2D-CED
28	I	615	LMG	C21-C22-C23-C24
22	A	827	CLA	C3-C5-C6-C7
22	Q	609	CLA	O1A-CGA-O2A-C1
22	B	839	CLA	CAA-CBA-CGA-O2A
22	T	611	CLA	C16-C17-C18-C19
22	A	823	CLA	CAA-CBA-CGA-O2A
28	I	614	LMG	O6-C5-C6-O5
22	L	404	CLA	CAA-CBA-CGA-O1A
22	R	605	CLA	CAA-CBA-CGA-O1A
26	L	416	LHG	O10-C23-C24-C25
26	N	614	LHG	O10-C23-C24-C25
26	X	420	LHG	O9-C7-C8-C9
28	I	615	LMG	C23-C24-C25-C26
28	G	616	LMG	C11-C12-C13-C14
28	B	856	LMG	C8-C7-O1-C1
28	J	101	LMG	C8-C7-O1-C1
28	I	614	LMG	O9-C10-O7-C8
22	I	610	CLA	CAA-CBA-CGA-O2A
22	Q	603	CLA	CAA-CBA-CGA-O1A
22	R	604	CLA	CAA-CBA-CGA-O2A
22	B	805	CLA	CAA-CBA-CGA-O1A
22	Q	612	CLA	CAA-CBA-CGA-O1A
22	R	603	CLA	CAA-CBA-CGA-O1A
26	H	316	LHG	C4-C5-C6-O8
28	U	402	LMG	O1-C7-C8-C9
22	P	606	CLA	CAA-CBA-CGA-O1A
22	B	822	CLA	CAA-CBA-CGA-O1A
22	Q	605	CLA	CAA-CBA-CGA-O1A
22	R	608	CLA	CAA-CBA-CGA-O1A
26	K	619	LHG	O9-C7-C8-C9
22	B	806	CLA	C4-C3-C5-C6
22	B	859	CLA	C4-C3-C5-C6
22	I	603	CLA	CAA-CBA-CGA-O2A
26	A	845	LHG	O8-C23-C24-C25
26	G	614	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
22	P	602	CLA	CAA-CBA-CGA-O1A
22	Q	606	CLA	CAA-CBA-CGA-O1A
22	H	306	CLA	CAA-CBA-CGA-O1A
26	R	614	LHG	O10-C23-C24-C25
28	I	615	LMG	O9-C10-C11-C12
22	B	803	CLA	CAD-CBD-CGD-O2D
22	I	601	CLA	CAD-CBD-CGD-O2D
22	I	604	CLA	CAD-CBD-CGD-O2D
22	N	608	CLA	CAD-CBD-CGD-O2D
22	O	311	CLA	CAD-CBD-CGD-O2D
22	V	603	CLA	CAD-CBD-CGD-O2D
22	A	817	CLA	CAD-CBD-CGD-O2D
31	U	408	CHL	CAD-CBD-CGD-O2D
31	V	606	CHL	CAD-CBD-CGD-O2D
28	A	855	LMG	C12-C13-C14-C15
22	Q	611	CLA	CAA-CBA-CGA-O2A
22	S	605	CLA	CAA-CBA-CGA-O2A
22	W	409	CLA	CAA-CBA-CGA-O2A
22	I	610	CLA	CAA-CBA-CGA-O1A
22	U	412	CLA	CAA-CBA-CGA-O1A
26	O	318	LHG	O2-C2-C3-O3
22	A	810	CLA	C13-C15-C16-C17
22	W	409	CLA	O1A-CGA-O2A-C1
26	T	614	LHG	C25-C26-C27-C28
22	K	610	CLA	CAA-CBA-CGA-O1A
22	A	830	CLA	CAA-CBA-CGA-O1A
26	G	614	LHG	O10-C23-C24-C25
25	O	304	DGD	O2G-C1B-C2B-C3B
28	J	101	LMG	O7-C10-C11-C12
22	Q	612	CLA	C16-C17-C18-C19
26	B	851	LHG	C18-C19-C20-C21
26	H	316	LHG	C25-C26-C27-C28
22	K	617	CLA	CBD-CGD-O2D-CED
22	W	410	CLA	C11-C10-C8-C7
22	A	825	CLA	C11-C12-C13-C15
22	O	308	CLA	CAA-CBA-CGA-O2A
22	S	607	CLA	CAA-CBA-CGA-O2A
22	X	412	CLA	CAA-CBA-CGA-O2A
22	A	826	CLA	CAA-CBA-CGA-O2A
22	G	610	CLA	CAA-CBA-CGA-O2A
22	H	312	CLA	CAA-CBA-CGA-O2A
22	R	604	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	T	601	CLA	CAA-CBA-CGA-O2A
22	X	413	CLA	CAA-CBA-CGA-O2A
26	X	420	LHG	O10-C23-C24-C25
22	I	611	CLA	CBD-CGD-O2D-CED
22	A	844	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	CAA-CBA-CGA-O2A
22	R	610	CLA	CAA-CBA-CGA-O2A
28	I	614	LMG	O8-C28-C29-C30
28	U	423	LMG	O7-C10-C11-C12
22	R	610	CLA	O1A-CGA-O2A-C1
26	K	619	LHG	C23-C24-C25-C26
22	B	816	CLA	CAA-CBA-CGA-O1A
22	R	606	CLA	CAA-CBA-CGA-O1A

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	O	320	LMU	C1'-C2'-C3'-C4'-C5'-O5'
27	L	419	LMU	C1'-C2'-C3'-C4'-C5'-O5'

291 monomers are involved in 581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	404	CLA	4	0
22	K	604	CLA	6	0
22	B	821	CLA	2	0
28	I	615	LMG	1	0
22	A	819	CLA	1	0
22	A	820	CLA	1	0
22	B	831	CLA	2	0
28	T	616	LMG	2	0
22	P	609	CLA	1	0
21	A	848	BCR	2	0
22	S	610	CLA	2	0
22	W	412	CLA	2	0
22	I	607	CLA	3	0
24	S	611	DD6	1	0
22	A	844	CLA	4	0
28	H	322	LMG	1	0
22	B	807	CLA	2	0
31	U	408	CHL	4	0
22	K	606	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	W	410	CLA	3	0
22	U	420	CLA	1	0
26	K	616	LHG	3	0
22	B	824	CLA	3	0
22	R	604	CLA	5	0
22	W	411	CLA	2	0
27	H	321	LMU	1	0
22	B	810	CLA	1	0
21	M	101	BCR	3	0
26	N	616	LHG	1	0
22	H	311	CLA	2	0
22	R	607	CLA	3	0
22	X	413	CLA	1	0
27	B	855	LMU	1	0
26	S	613	LHG	2	0
22	J	102	CLA	1	0
22	B	817	CLA	1	0
22	T	606	CLA	1	0
22	S	602	CLA	1	0
22	V	609	CLA	2	0
27	H	301	LMU	1	0
22	X	411	CLA	1	0
22	N	606	CLA	4	0
27	B	854	LMU	8	0
30	F	407	SQD	2	0
31	W	422	CHL	2	0
21	B	843	BCR	3	0
22	B	829	CLA	3	0
27	A	854	LMU	1	0
22	X	403	CLA	1	0
22	L	411	CLA	1	0
22	N	607	CLA	7	0
22	A	803	CLA	1	0
22	H	308	CLA	2	0
22	A	813	CLA	2	0
22	B	806	CLA	4	0
22	B	833	CLA	4	0
22	O	311	CLA	3	0
22	B	813	CLA	3	0
22	S	606	CLA	1	0
22	B	835	CLA	2	0
22	H	312	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	848	LHG	1	0
22	N	604	CLA	1	0
22	P	608	CLA	2	0
22	V	612	CLA	7	0
25	O	304	DGD	3	0
22	V	602	CLA	5	0
22	V	608	CLA	1	0
22	S	605	CLA	4	0
27	T	618	LMU	2	0
22	H	313	CLA	1	0
22	K	613	CLA	4	0
22	G	601	CLA	1	0
26	T	614	LHG	1	0
22	A	811	CLA	1	0
22	U	415	CLA	2	0
22	A	824	CLA	4	0
27	F	409	LMU	1	0
22	W	415	CLA	1	0
22	G	608	CLA	4	0
22	B	822	CLA	3	0
22	P	606	CLA	3	0
28	W	401	LMG	3	0
22	V	607	CLA	2	0
22	L	402	CLA	2	0
22	R	610	CLA	3	0
22	W	402	CLA	2	0
25	B	847	DGD	6	0
28	H	319	LMG	1	0
27	K	620	LMU	2	0
26	A	845	LHG	1	0
22	A	852	CLA	4	0
22	U	405	CLA	3	0
22	A	806	CLA	4	0
22	U	401	CLA	2	0
22	Q	613	CLA	2	0
22	I	608	CLA	2	0
22	A	807	CLA	1	0
22	R	606	CLA	3	0
22	B	830	CLA	4	0
22	U	404	CLA	2	0
22	W	409	CLA	4	0
22	T	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	U	424	LMU	1	0
28	B	856	LMG	4	0
26	O	318	LHG	1	0
22	T	608	CLA	2	0
28	F	408	LMG	3	0
22	G	603	CLA	2	0
22	B	819	CLA	1	0
22	A	841	CLA	3	0
22	A	808	CLA	1	0
22	Q	605	CLA	1	0
22	A	805	CLA	2	0
31	W	407	CHL	6	0
22	O	308	CLA	4	0
22	W	404	CLA	2	0
26	L	416	LHG	3	0
22	N	601	CLA	1	0
22	B	823	CLA	3	0
28	Q	602	LMG	2	0
22	Q	604	CLA	5	0
30	K	621	SQD	1	0
22	A	809	CLA	1	0
21	B	846	BCR	1	0
22	A	815	CLA	2	0
25	F	401	DGD	2	0
22	A	827	CLA	2	0
22	F	403	CLA	2	0
31	V	606	CHL	14	0
22	B	832	CLA	3	0
22	A	817	CLA	2	0
22	A	804	CLA	3	0
22	A	816	CLA	2	0
22	T	604	CLA	1	0
21	A	851	BCR	3	0
27	U	421	LMU	1	0
22	A	842	CLA	4	0
22	S	604	CLA	1	0
22	H	310	CLA	1	0
26	R	614	LHG	3	0
21	A	849	BCR	3	0
32	V	616	NEX	9	0
26	P	601	LHG	1	0
22	O	315	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	P	607	CLA	1	0
21	B	844	BCR	5	0
22	A	821	CLA	1	0
22	K	607	CLA	9	0
22	K	609	CLA	2	0
22	K	603	CLA	2	0
27	M	102	LMU	1	0
22	R	605	CLA	5	0
31	W	408	CHL	8	0
28	K	601	LMG	3	0
22	G	610	CLA	1	0
22	X	404	CLA	1	0
22	N	602	CLA	1	0
31	V	605	CHL	12	0
21	B	801	BCR	8	0
22	B	838	CLA	3	0
22	Q	611	CLA	1	0
22	L	410	CLA	3	0
22	B	814	CLA	1	0
22	Q	609	CLA	1	0
22	R	611	CLA	2	0
22	P	610	CLA	1	0
22	T	605	CLA	4	0
22	B	809	CLA	4	0
22	O	314	CLA	1	0
26	W	420	LHG	2	0
22	B	811	CLA	1	0
22	I	606	CLA	2	0
21	J	103	BCR	1	0
22	B	859	CLA	2	0
22	K	608	CLA	4	0
22	Q	612	CLA	1	0
22	O	312	CLA	1	0
28	J	101	LMG	1	0
31	U	407	CHL	3	0
22	B	836	CLA	2	0
22	Q	608	CLA	3	0
22	A	832	CLA	3	0
22	A	840	CLA	3	0
22	R	601	CLA	6	0
22	R	615	CLA	2	0
26	O	321	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	822	CLA	3	0
22	T	607	CLA	1	0
22	H	307	CLA	1	0
26	A	846	LHG	2	0
22	K	617	CLA	2	0
22	I	602	CLA	1	0
22	V	617	CLA	1	0
22	B	805	CLA	1	0
22	A	814	CLA	4	0
26	Q	616	LHG	1	0
22	O	310	CLA	1	0
22	P	602	CLA	2	0
22	A	831	CLA	2	0
22	W	406	CLA	3	0
22	U	411	CLA	1	0
22	B	839	CLA	2	0
22	G	611	CLA	1	0
22	S	608	CLA	2	0
22	W	413	CLA	2	0
22	A	833	CLA	1	0
22	N	610	CLA	3	0
22	S	609	CLA	1	0
24	Q	614	DD6	1	0
27	L	419	LMU	4	0
22	S	601	CLA	1	0
22	Q	603	CLA	1	0
22	R	602	CLA	4	0
22	O	313	CLA	3	0
27	L	420	LMU	2	0
22	I	601	CLA	2	0
22	B	812	CLA	1	0
22	I	603	CLA	3	0
22	V	603	CLA	2	0
22	G	609	CLA	3	0
22	B	828	CLA	2	0
28	U	423	LMG	2	0
21	B	842	BCR	2	0
22	K	605	CLA	3	0
30	V	618	SQD	1	0
22	A	839	CLA	1	0
21	B	845	BCR	2	0
22	O	305	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	L	406	CLA	1	0
22	A	828	CLA	4	0
23	B	840	PQN	1	0
22	V	613	CLA	1	0
22	V	601	CLA	4	0
32	U	418	NEX	4	0
22	A	838	CLA	3	0
22	A	801	CLA	1	0
22	B	804	CLA	2	0
22	B	816	CLA	2	0
22	B	825	CLA	3	0
22	L	409	CLA	2	0
22	K	611	CLA	3	0
22	L	404	CLA	6	0
28	N	615	LMG	1	0
22	P	605	CLA	1	0
22	G	602	CLA	1	0
22	I	611	CLA	4	0
24	B	841	DD6	1	0
22	B	820	CLA	1	0
22	O	309	CLA	3	0
27	O	301	LMU	4	0
22	L	412	CLA	3	0
22	H	305	CLA	1	0
22	B	827	CLA	1	0
22	A	823	CLA	1	0
22	N	603	CLA	2	0
22	L	408	CLA	12	0
22	P	603	CLA	1	0
22	V	604	CLA	7	0
22	B	818	CLA	1	0
27	B	858	LMU	1	0
22	X	409	CLA	1	0
22	A	812	CLA	3	0
23	A	843	PQN	2	0
22	Q	607	CLA	2	0
27	A	857	LMU	1	0
22	Q	610	CLA	2	0
22	B	834	CLA	5	0
22	B	815	CLA	3	0
22	X	408	CLA	1	0
22	A	829	CLA	1	0

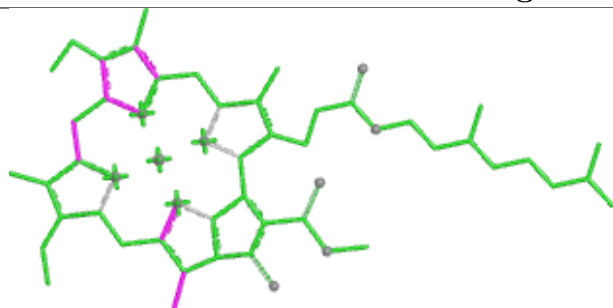
*Continued on next page...*

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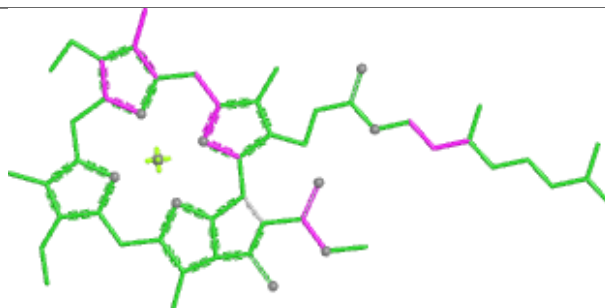
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	N	614	LHG	1	0
22	W	414	CLA	1	0
22	U	406	CLA	1	0
22	B	802	CLA	2	0
22	Q	601	CLA	1	0
33	A	802	CL0	6	0
22	A	836	CLA	2	0
22	B	803	CLA	2	0
22	X	419	CLA	2	0
22	A	830	CLA	1	0
28	U	402	LMG	2	0
22	L	417	CLA	7	0
22	A	825	CLA	2	0
22	O	307	CLA	1	0
26	B	851	LHG	7	0
30	O	302	SQD	8	0
22	A	834	CLA	1	0
22	S	607	CLA	1	0
22	U	409	CLA	1	0
22	U	412	CLA	1	0

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

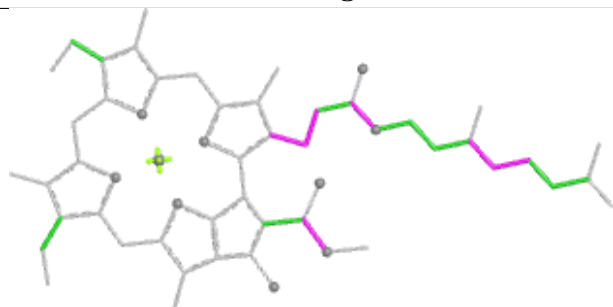
## Ligand CLA F 404



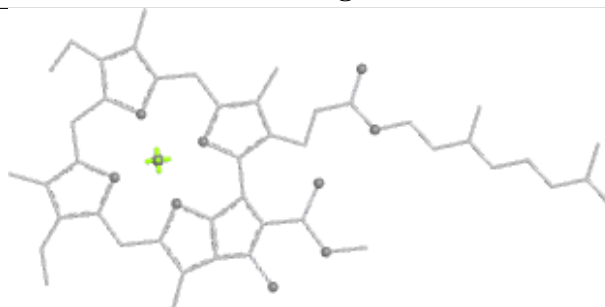
Bond lengths



Bond angles

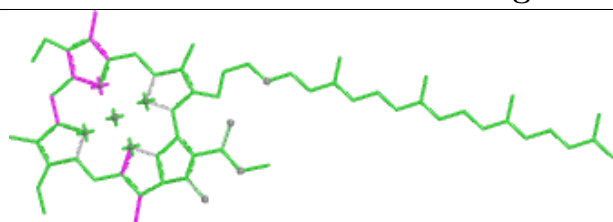


Torsions

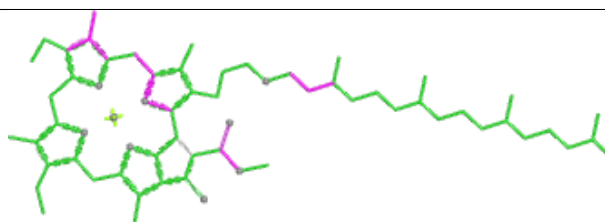


Rings

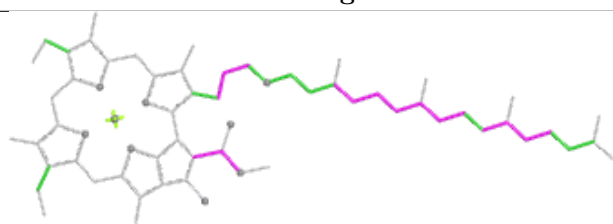
## Ligand CLA K 604



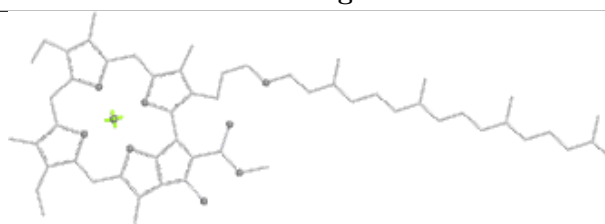
Bond lengths



Bond angles

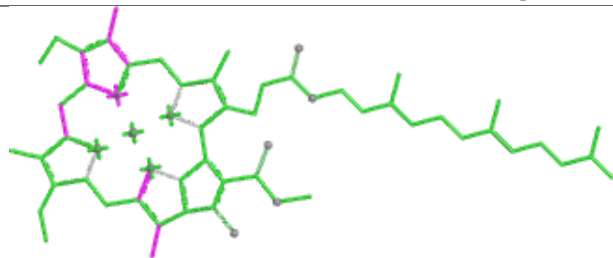


Torsions

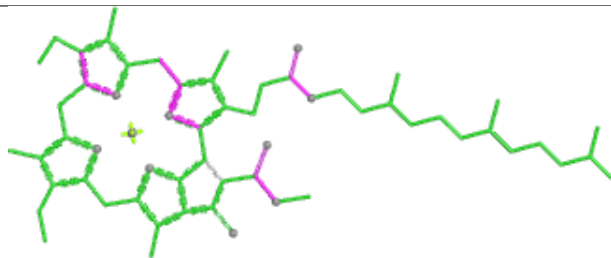


Rings

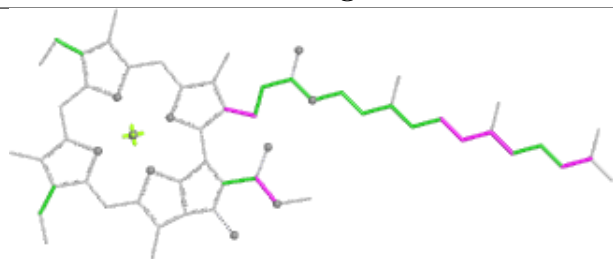
## Ligand CLA B 821



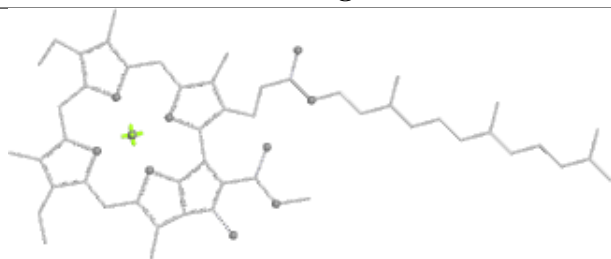
Bond lengths



Bond angles

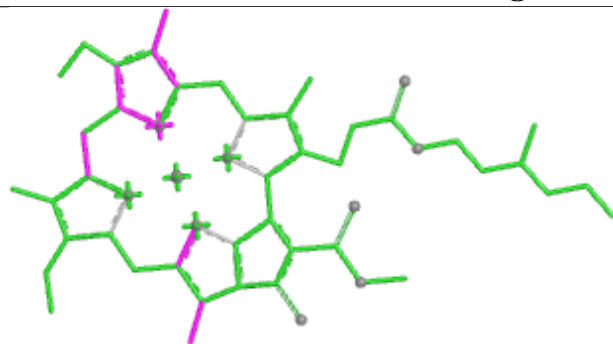


Torsions

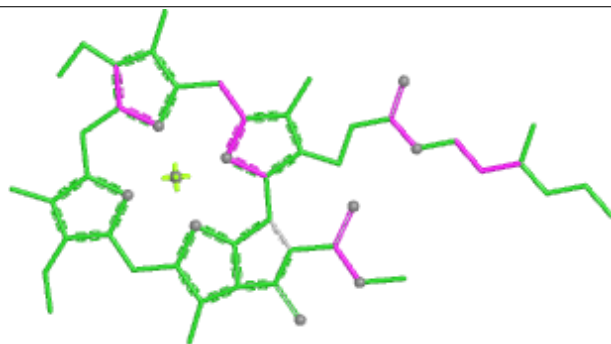


Rings

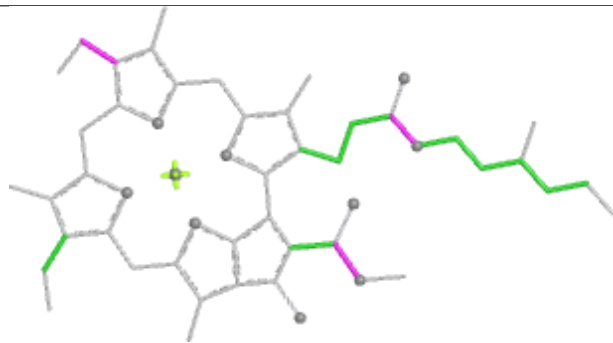
## Ligand CLA W 403



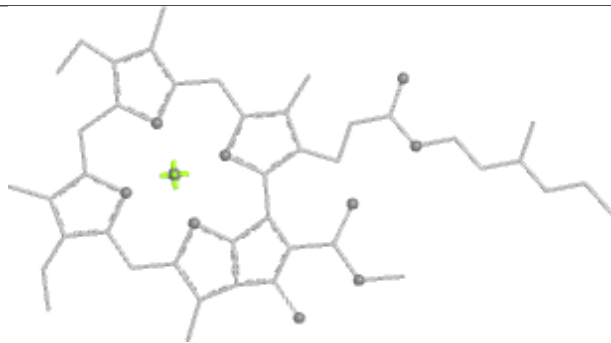
Bond lengths



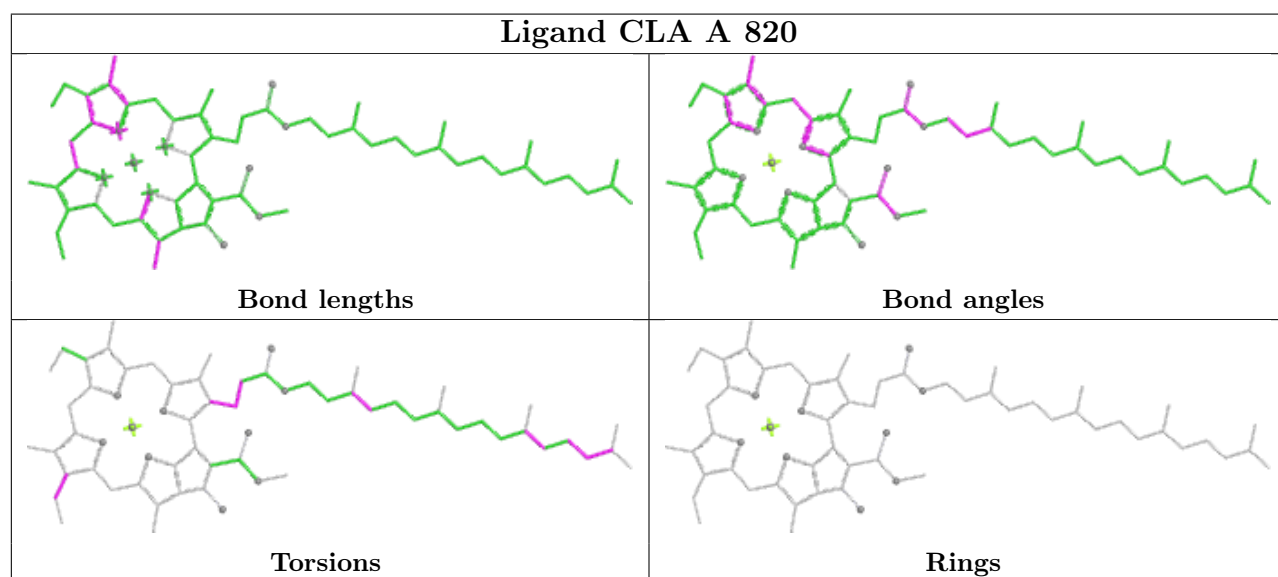
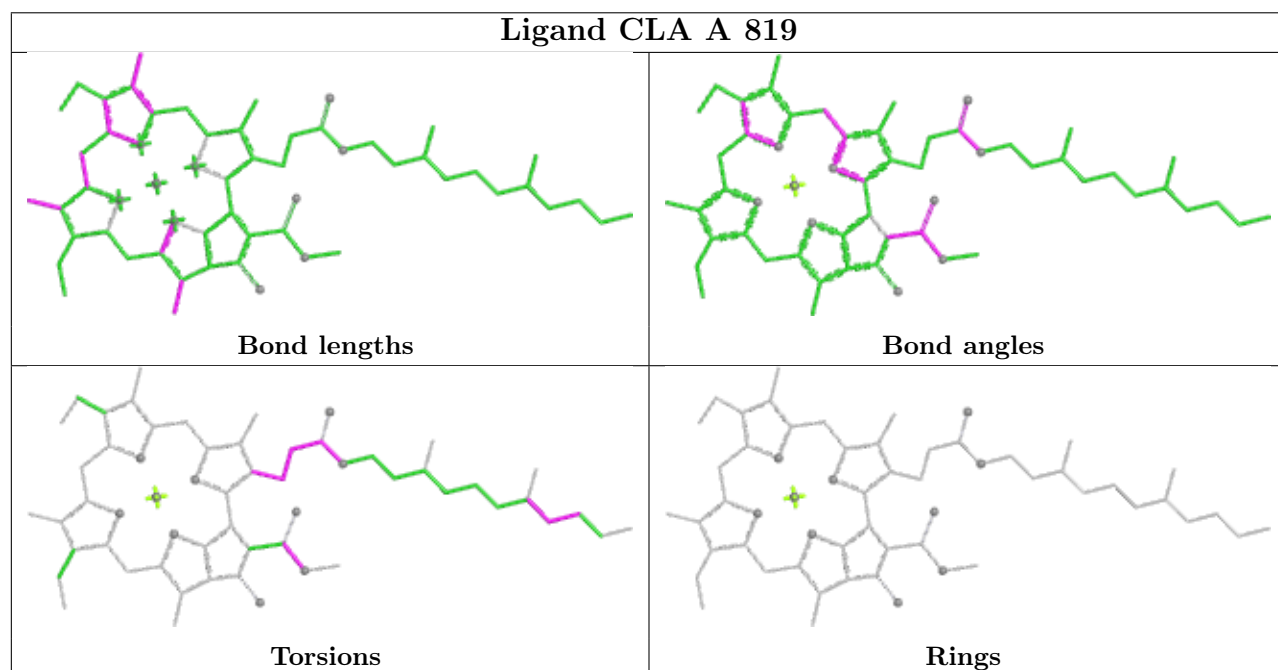
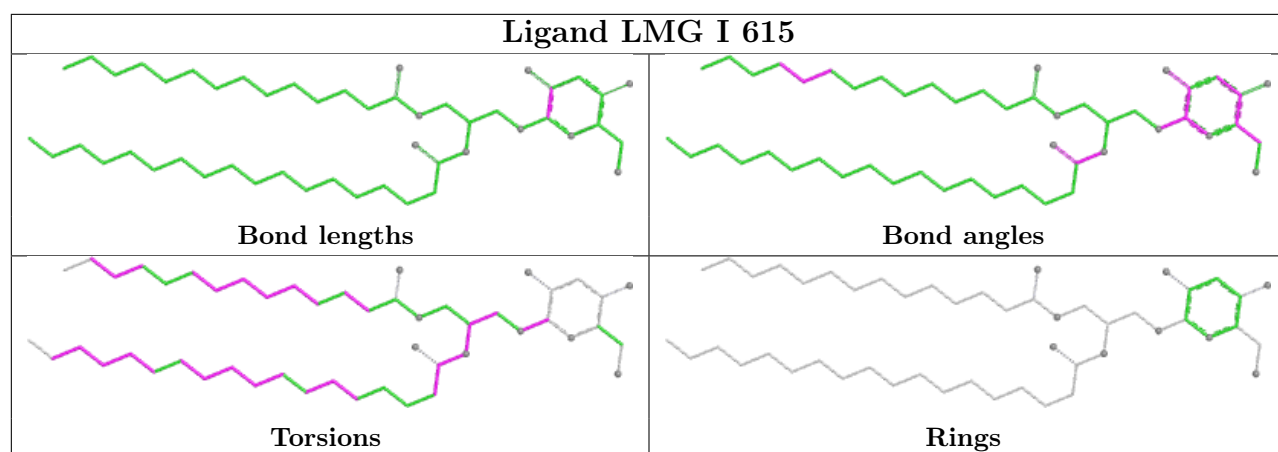
Bond angles

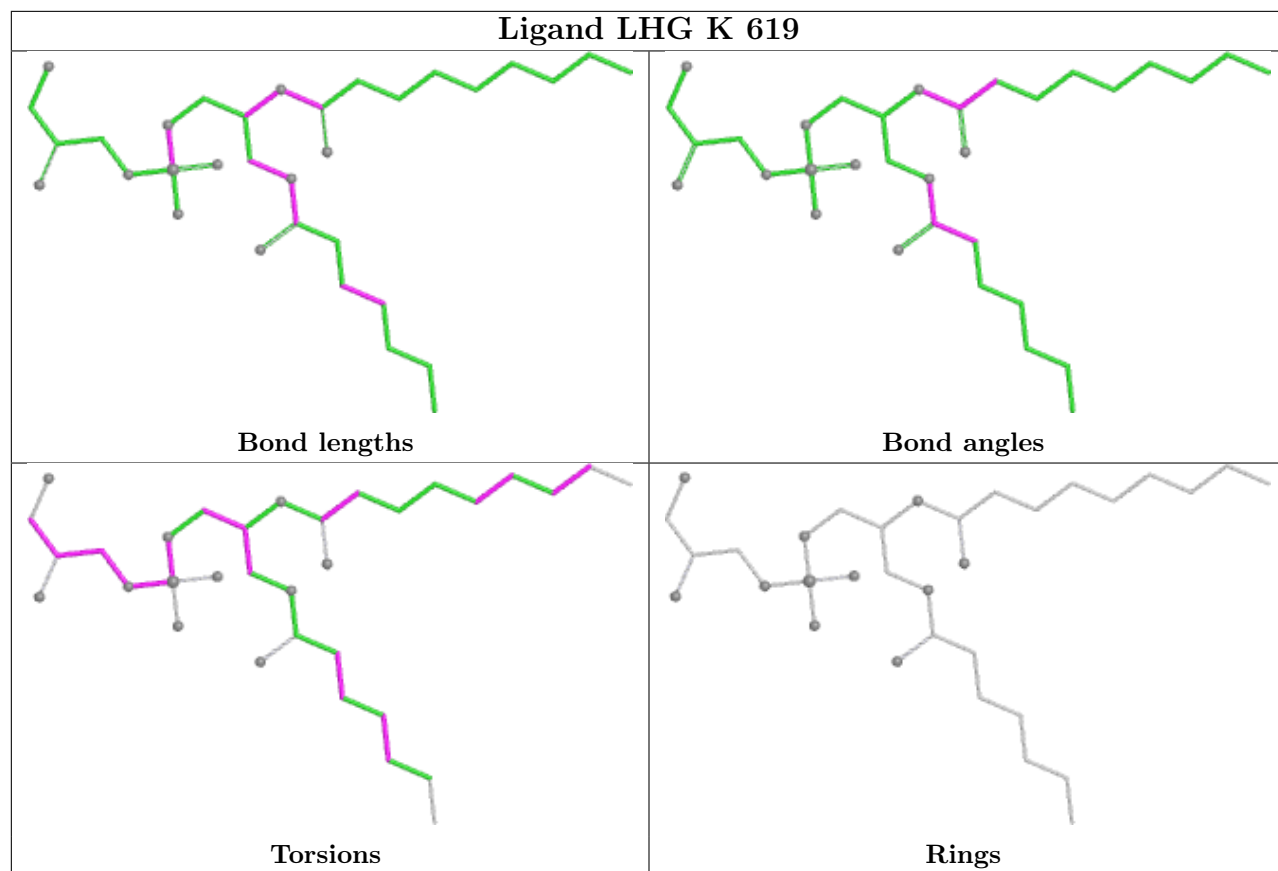


Torsions

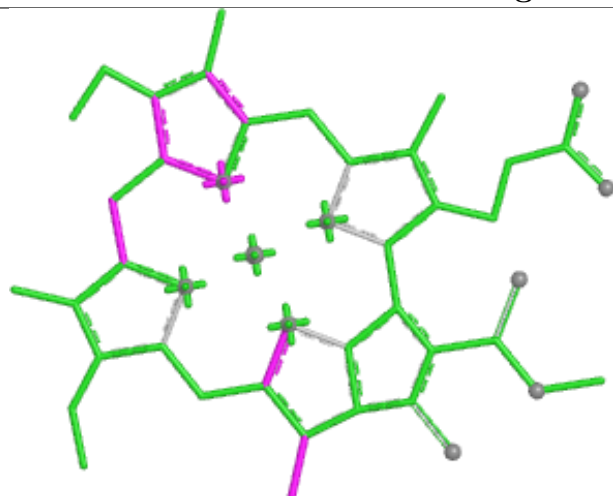


Rings

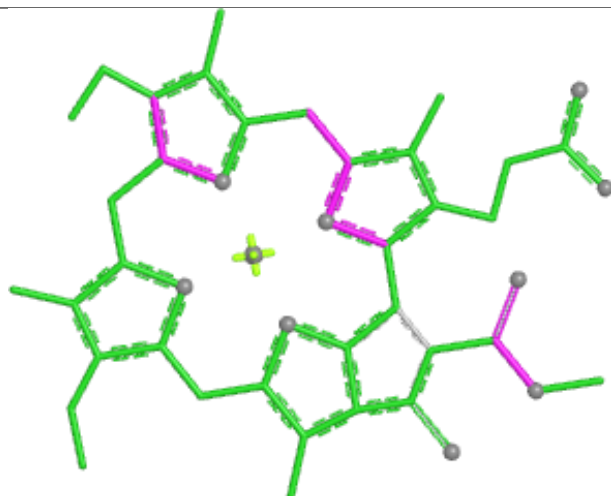




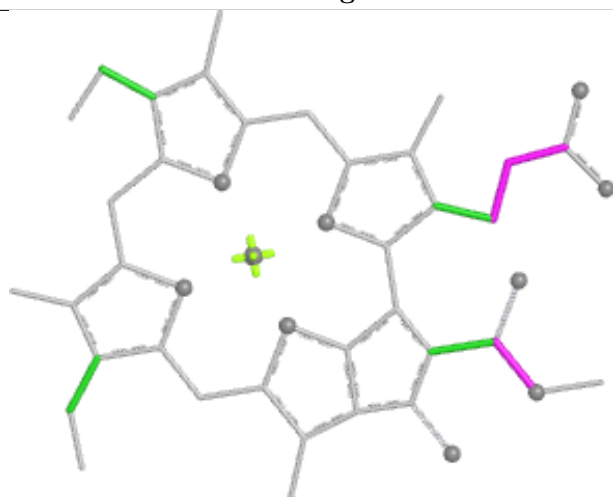
## Ligand CLA P 604



Bond lengths



Bond angles

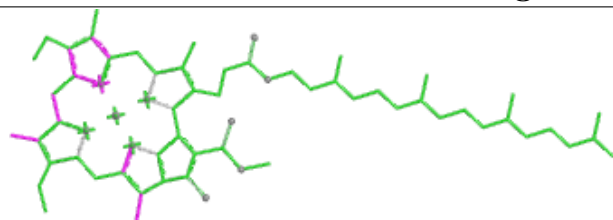


Torsions

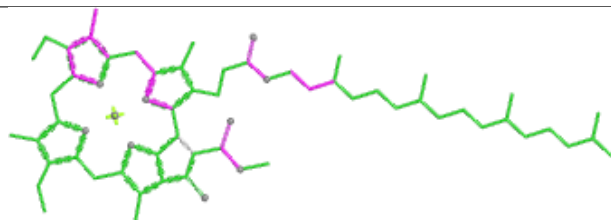


Rings

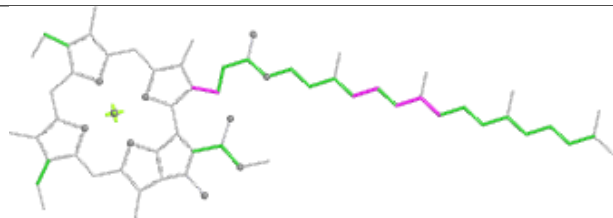
## Ligand CLA B 831



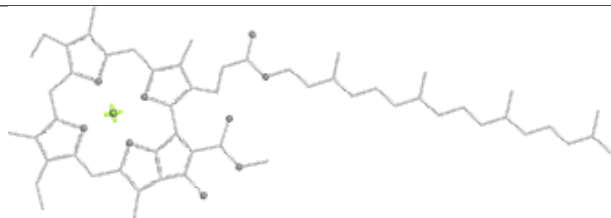
Bond lengths



Bond angles

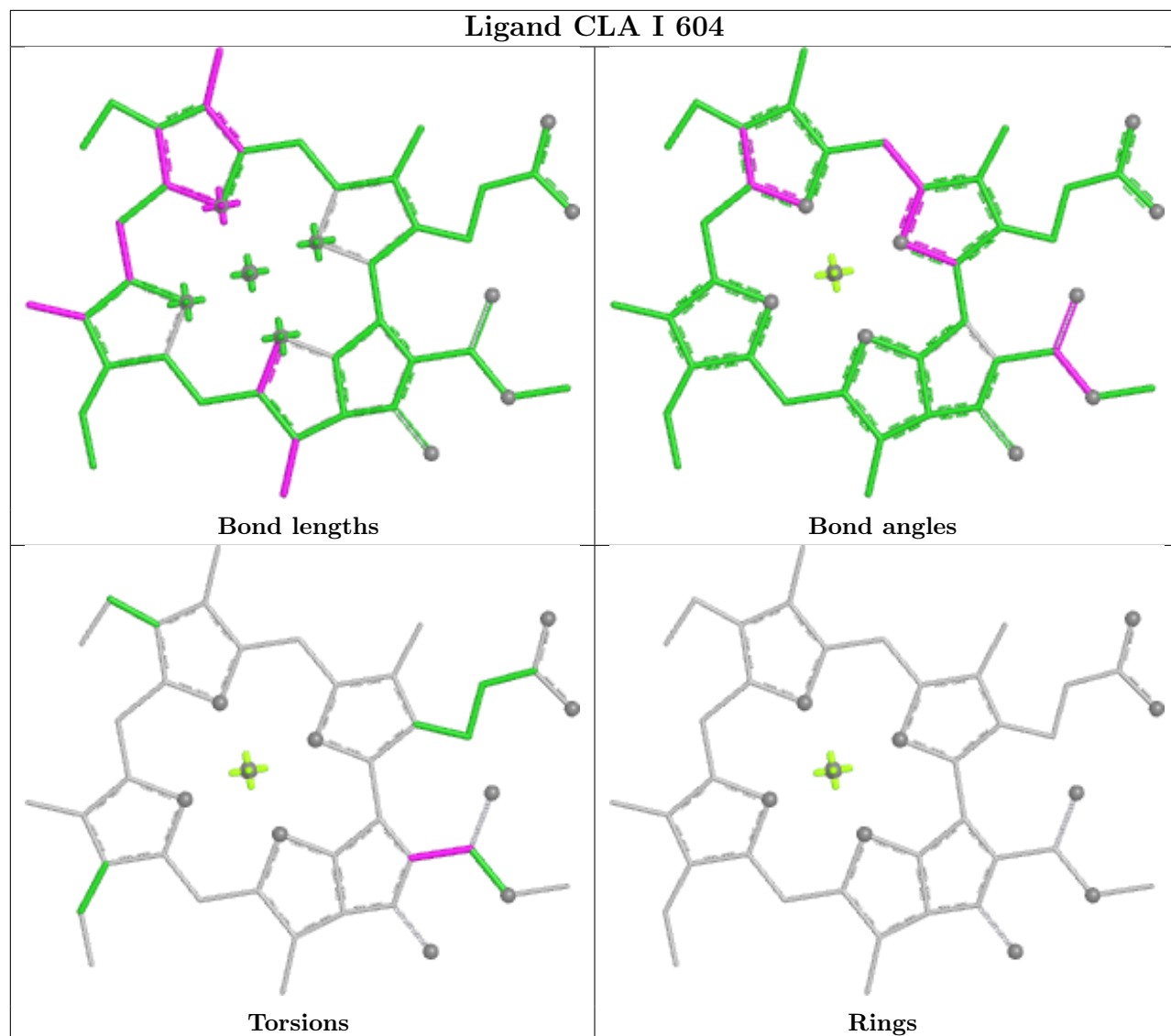


Torsions



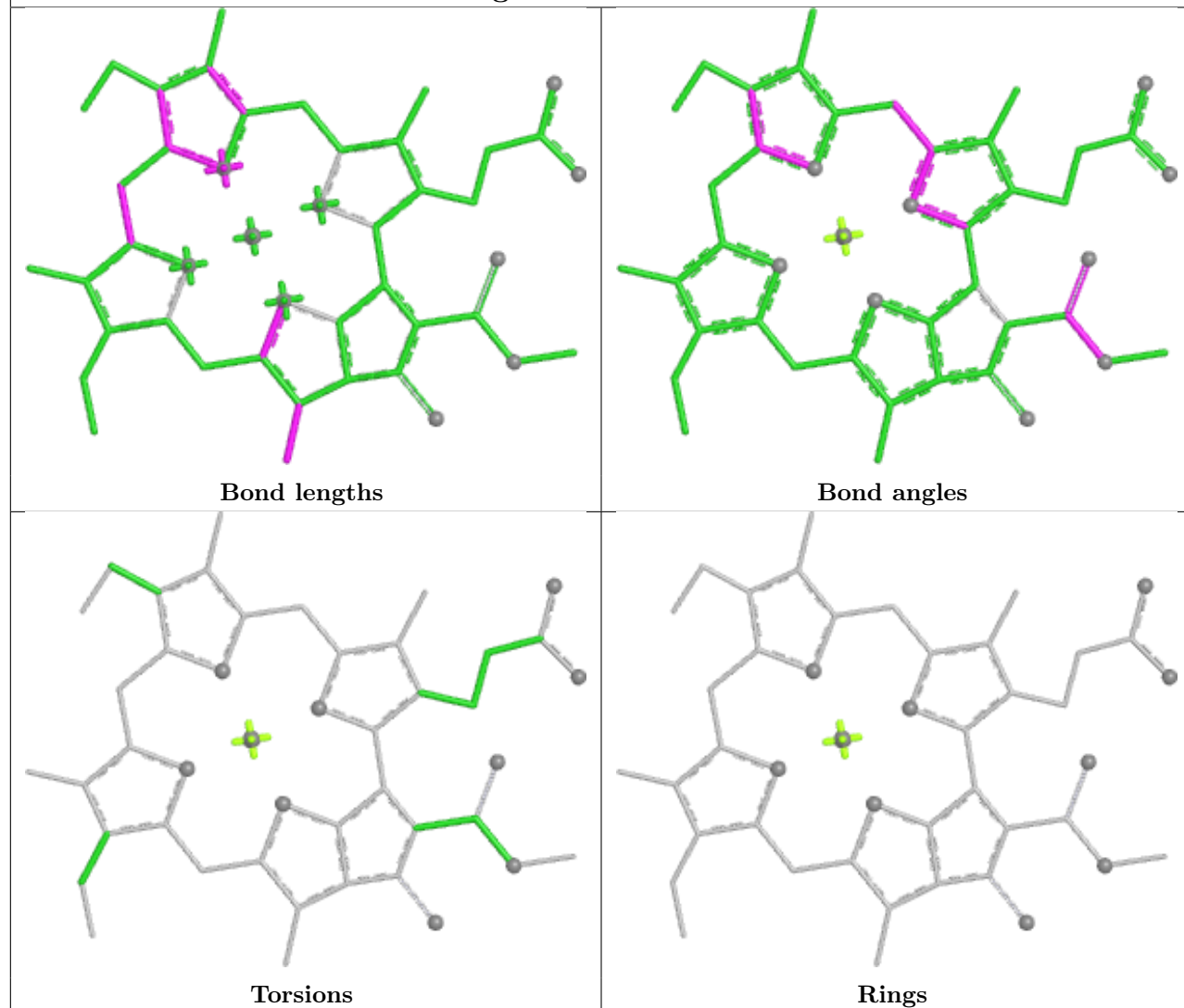
Rings

## Ligand CLA I 604

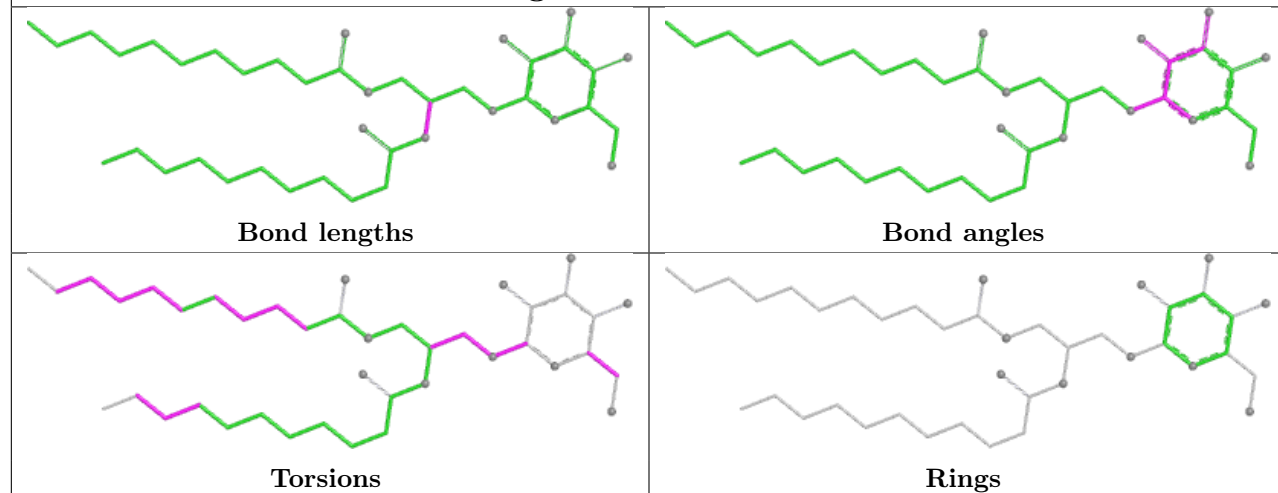


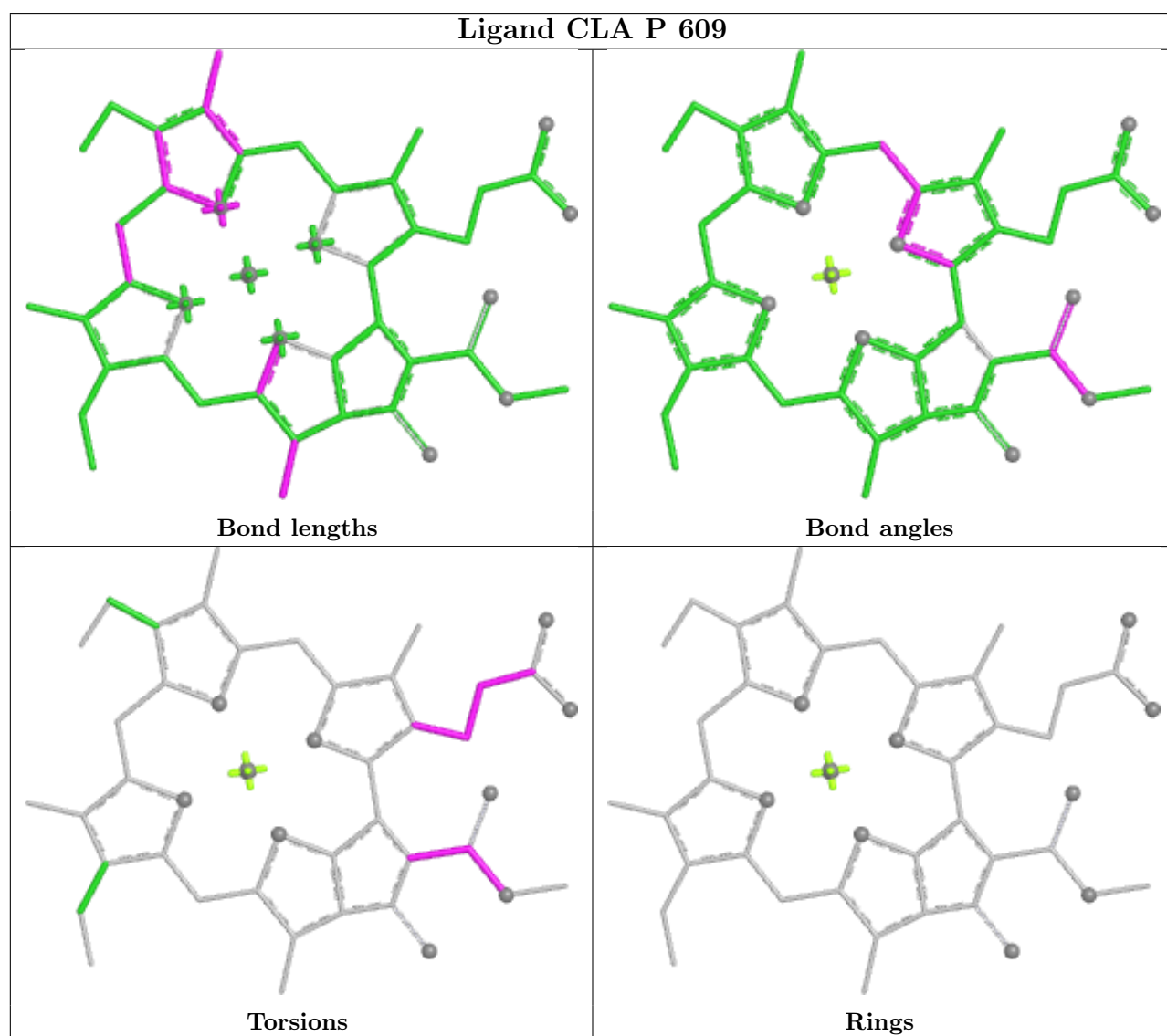
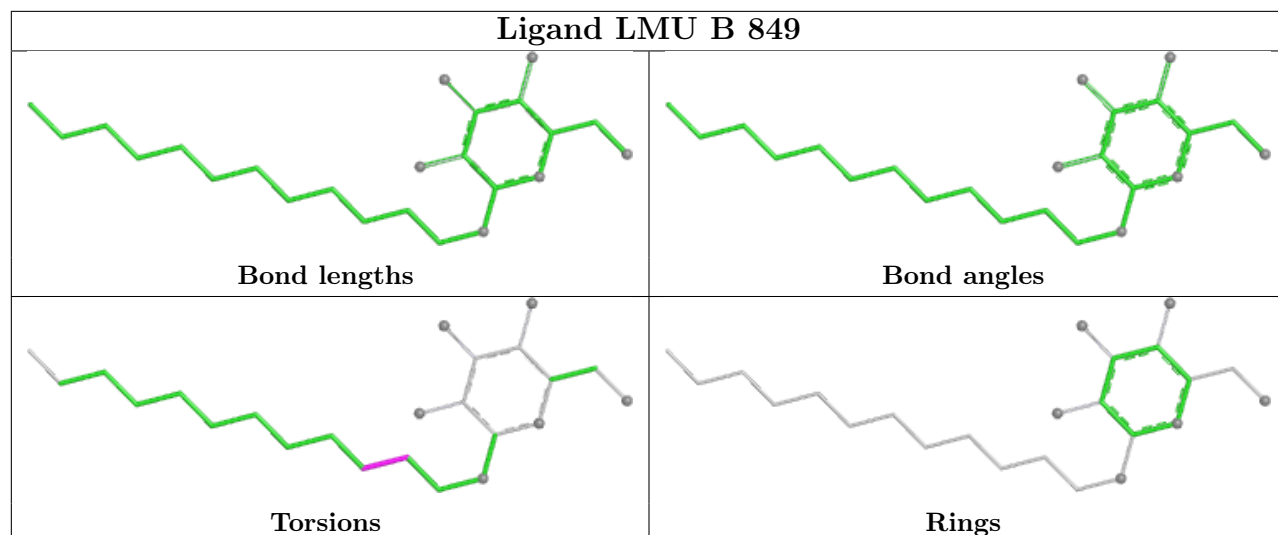


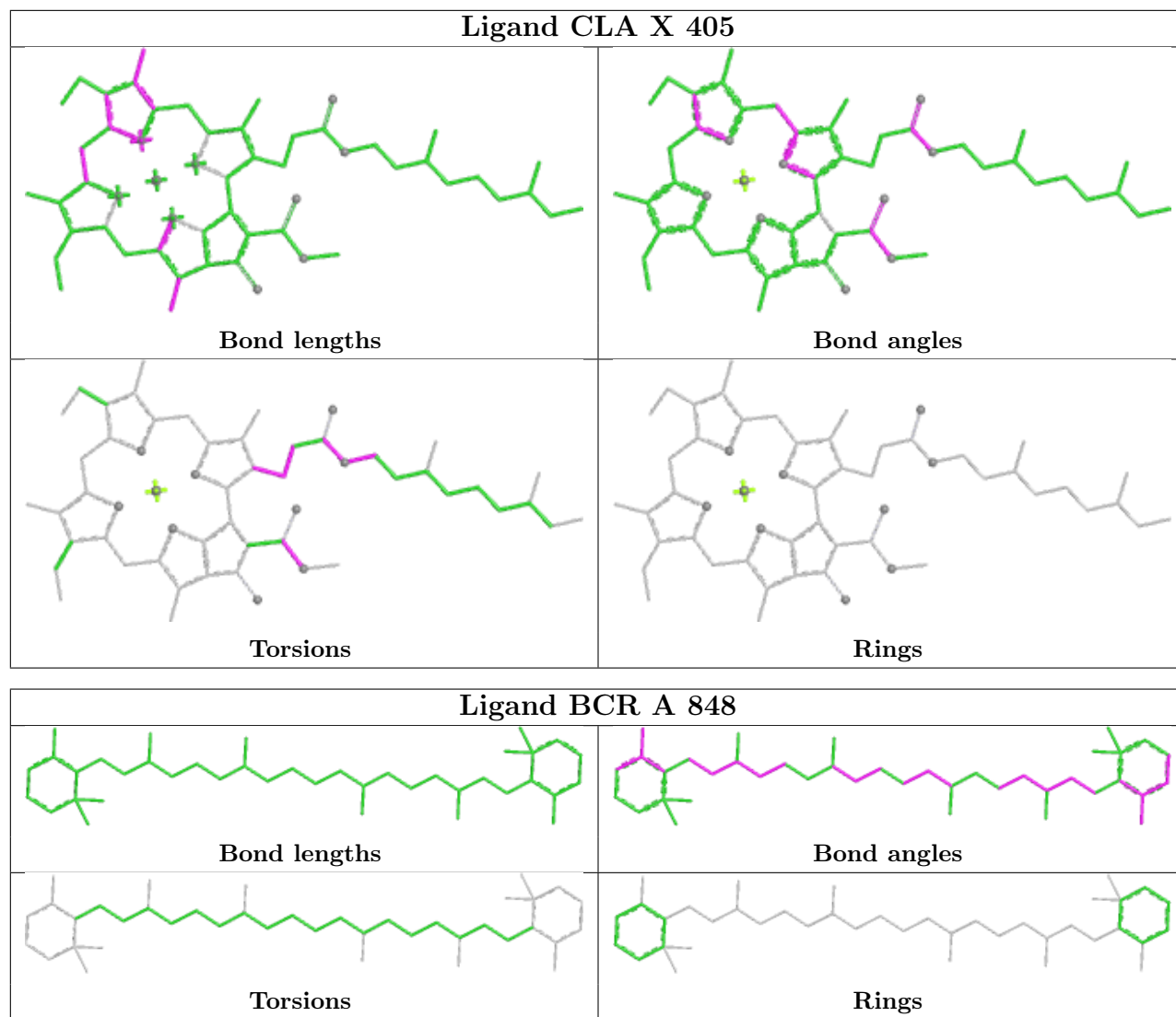
## Ligand CLA O 319



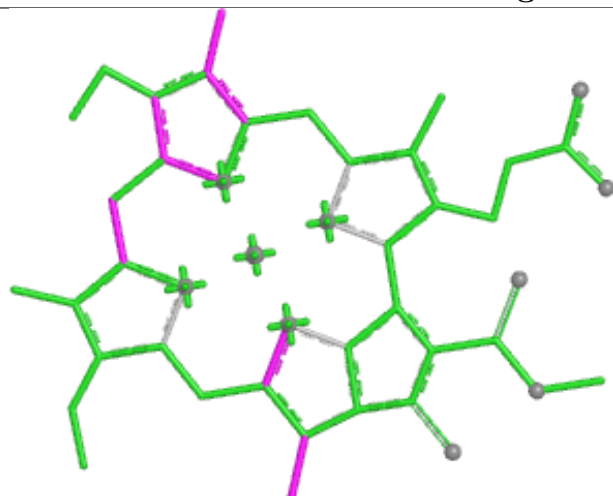
## Ligand LMG T 616



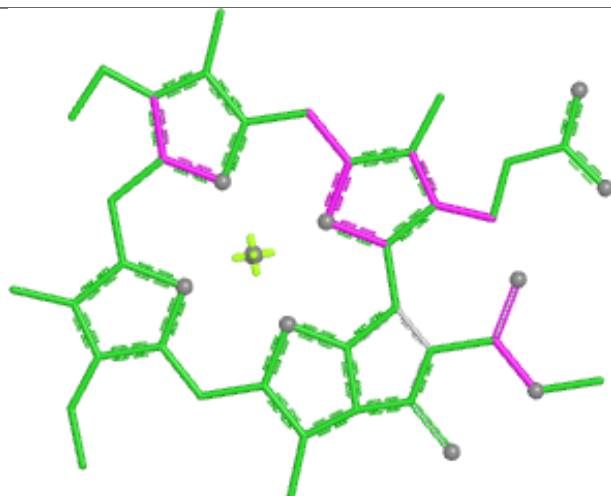




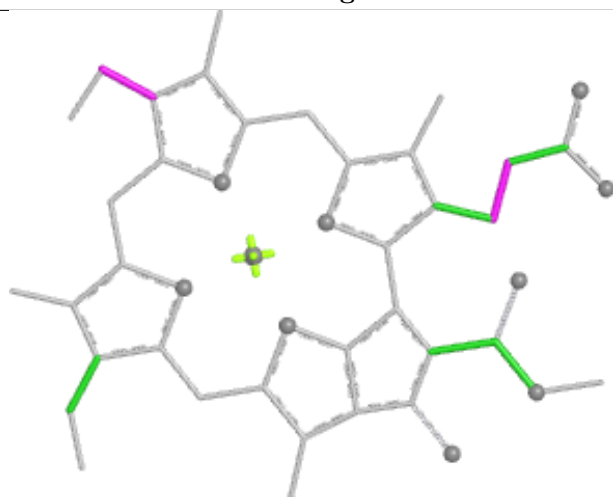
## Ligand CLA S 610



Bond lengths



Bond angles

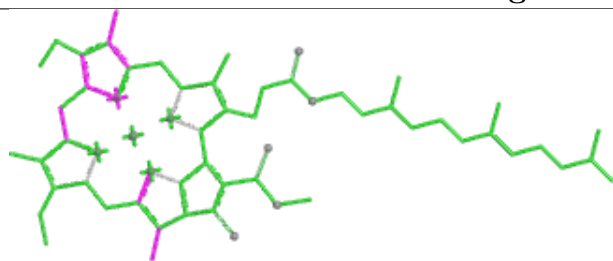


Torsions

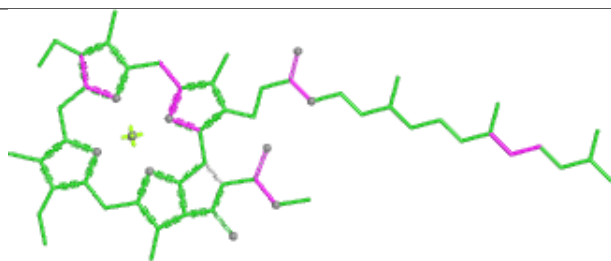


Rings

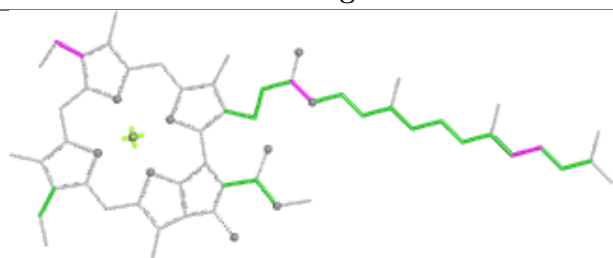
## Ligand CLA W 412



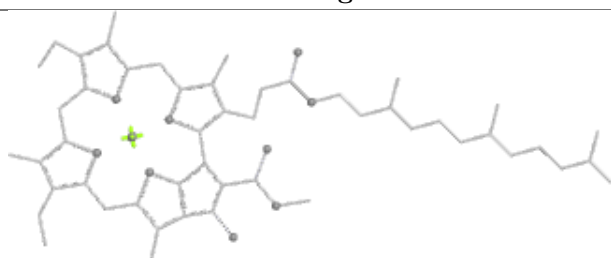
Bond lengths



Bond angles

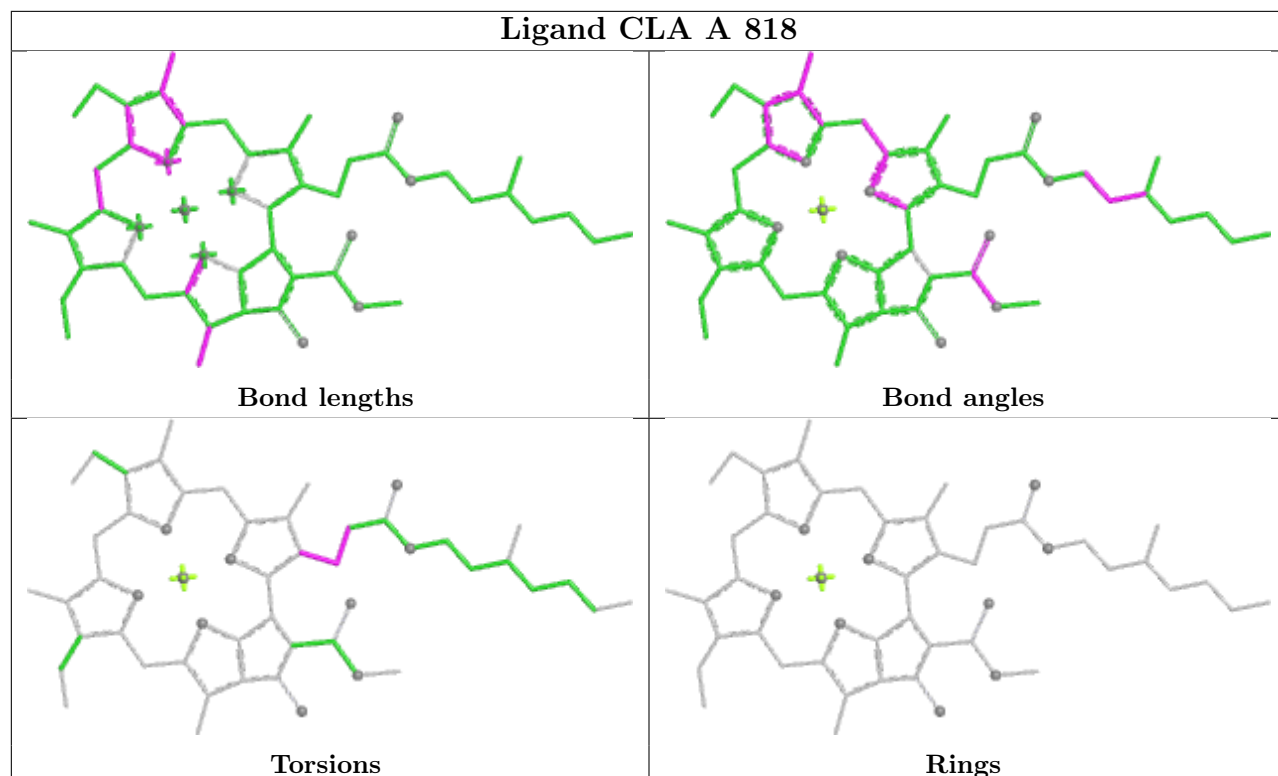


Torsions

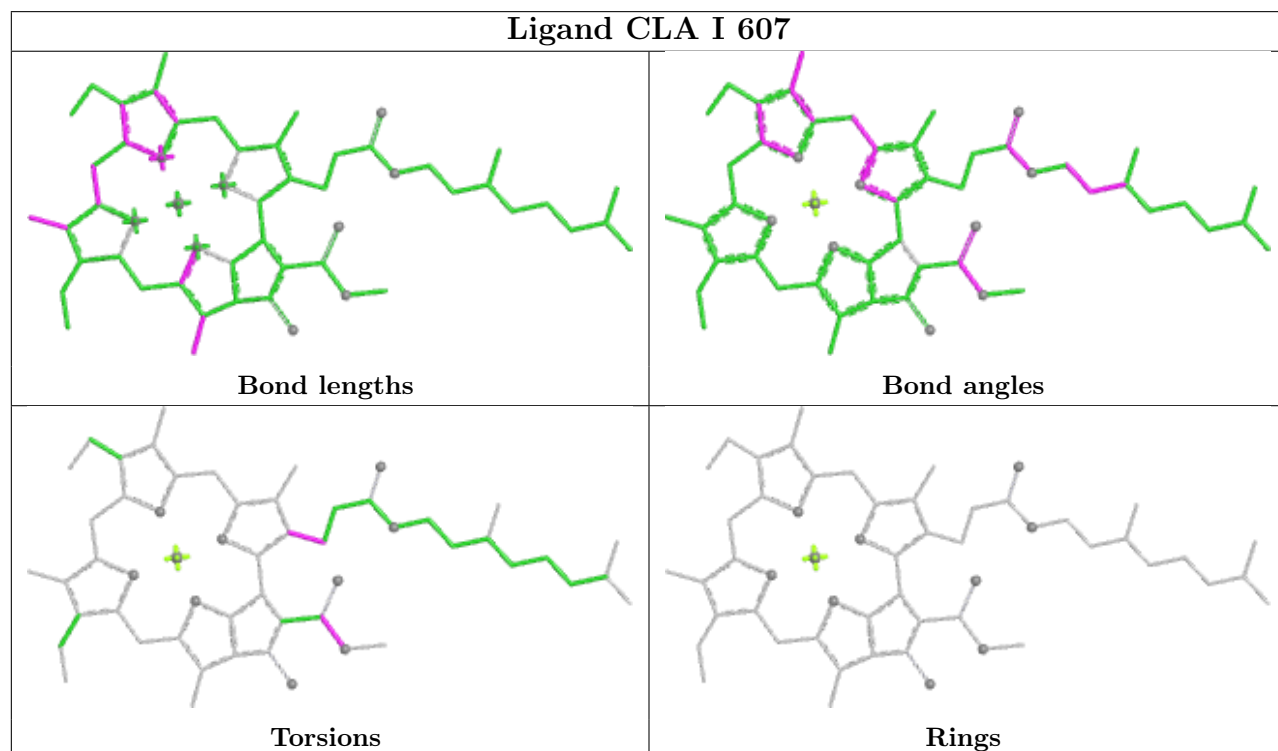


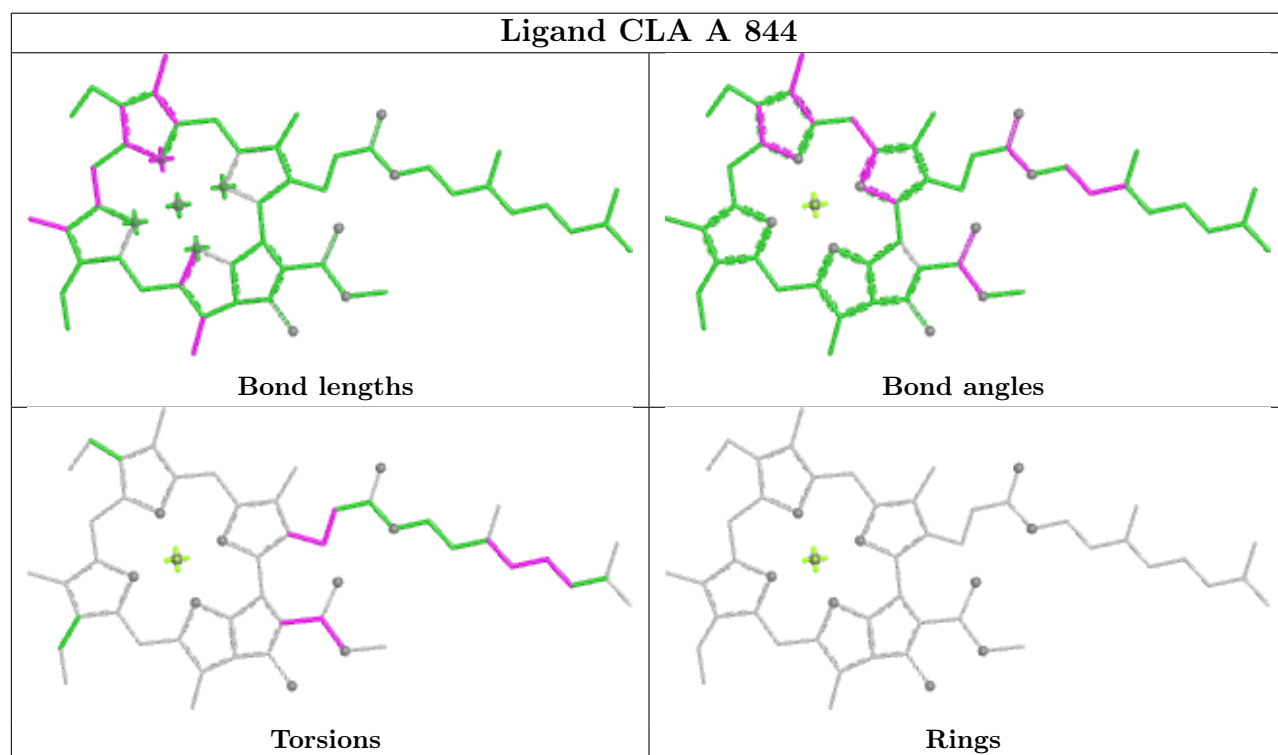
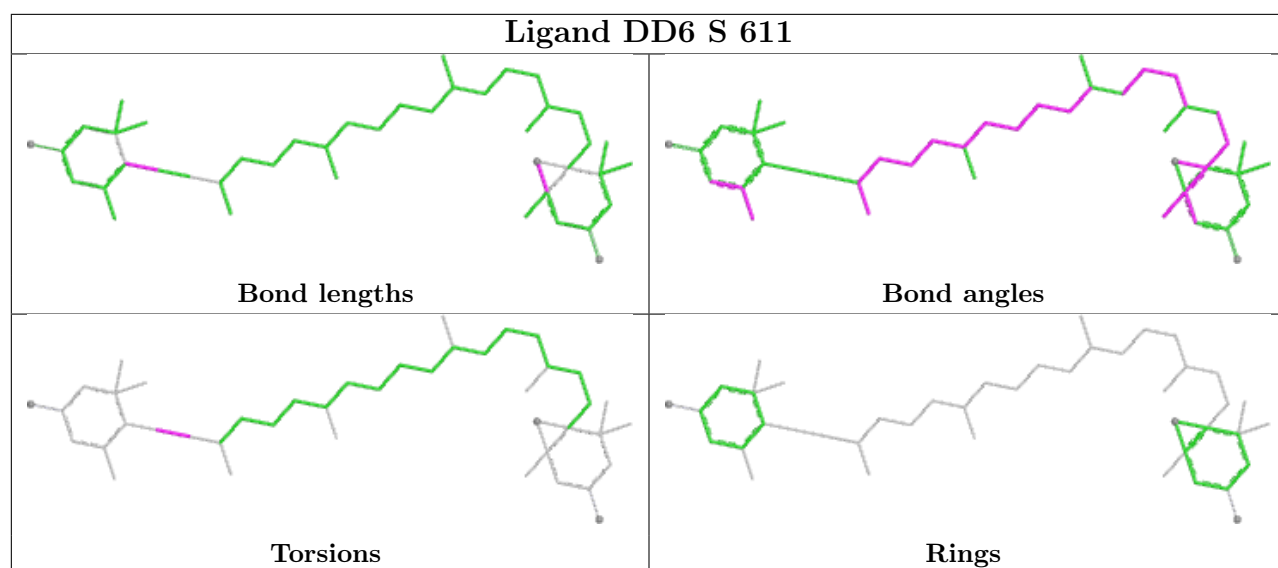
Rings

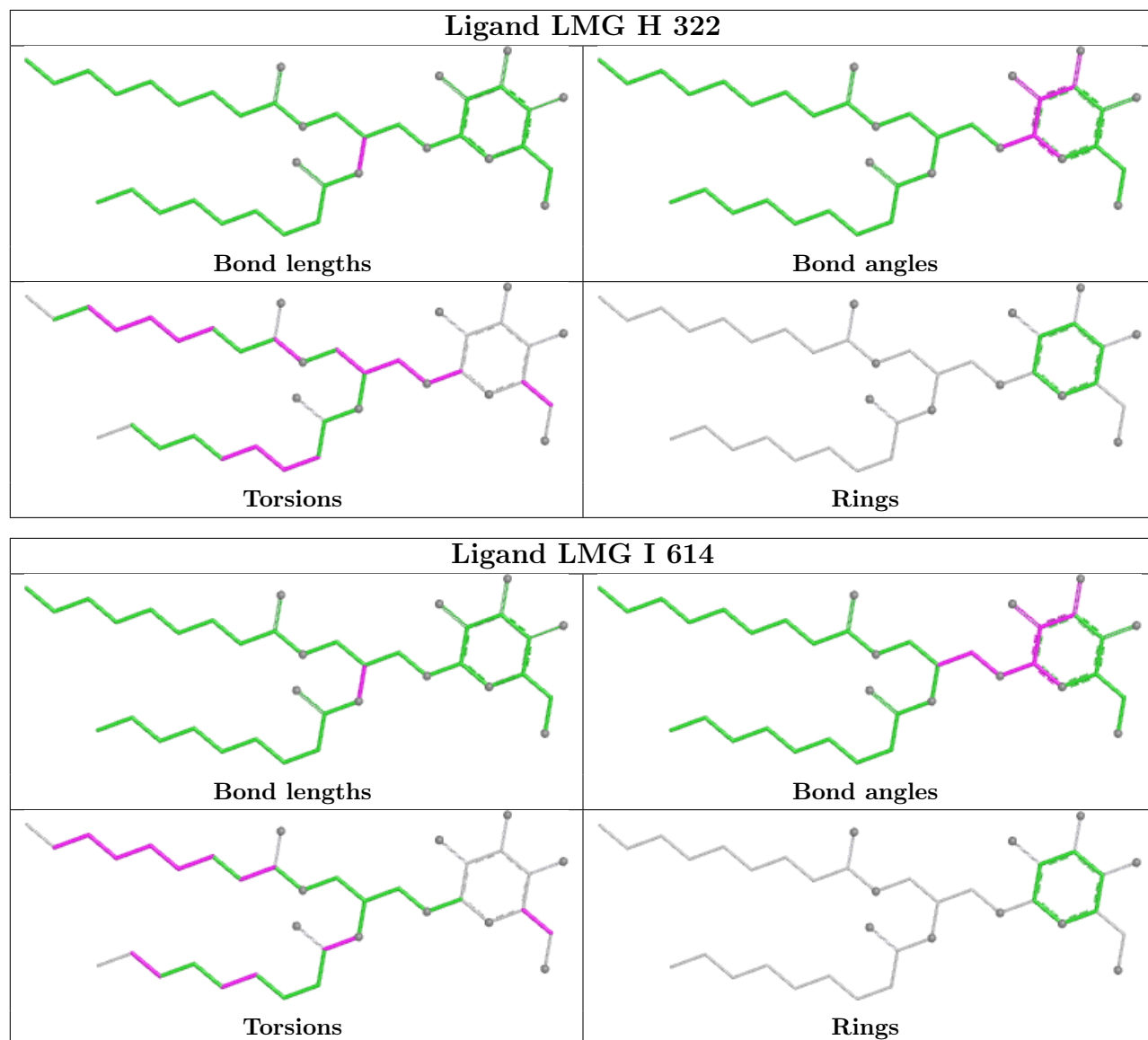
## Ligand CLA A 818

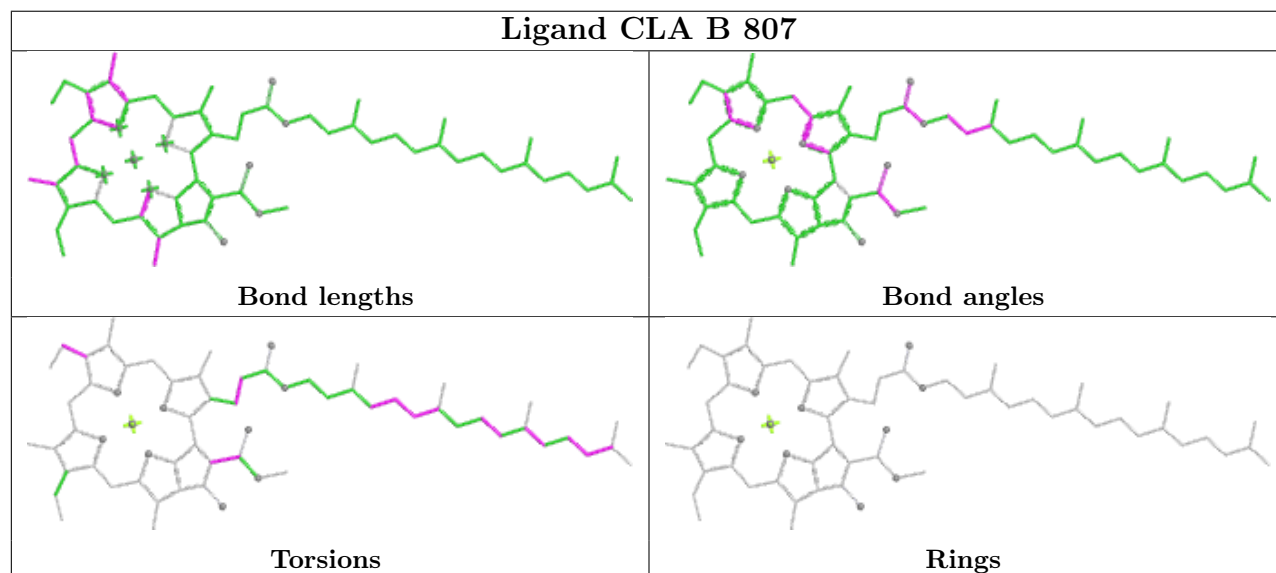
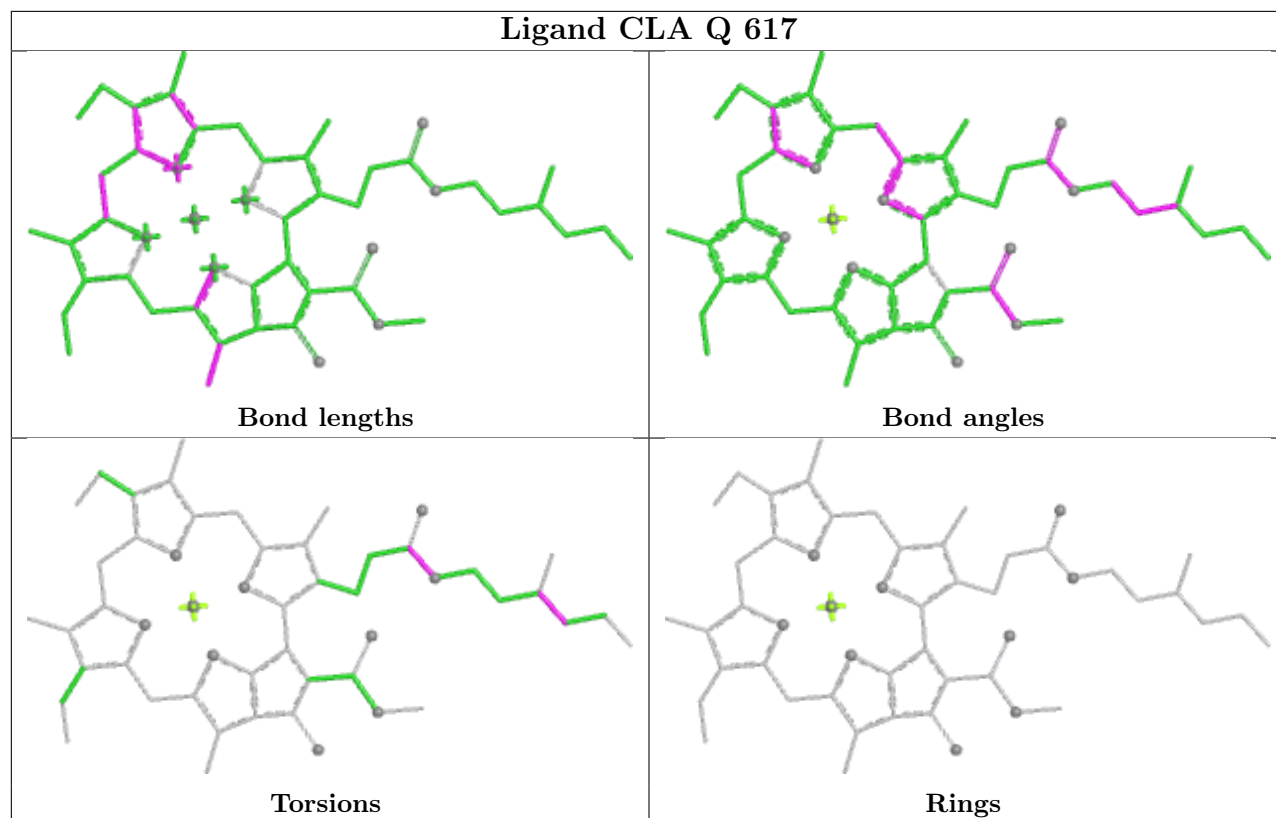


## Ligand CLA I 607

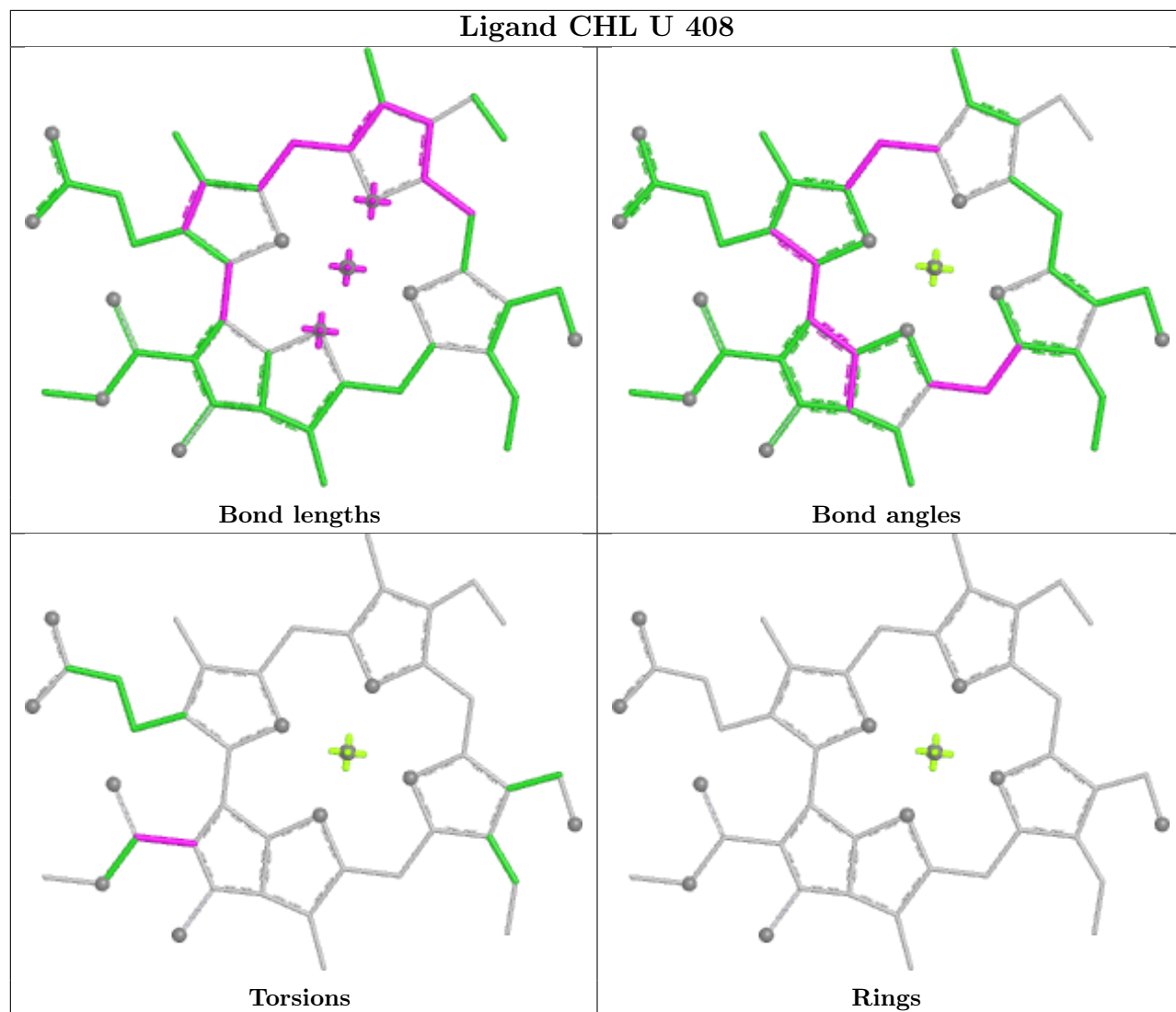




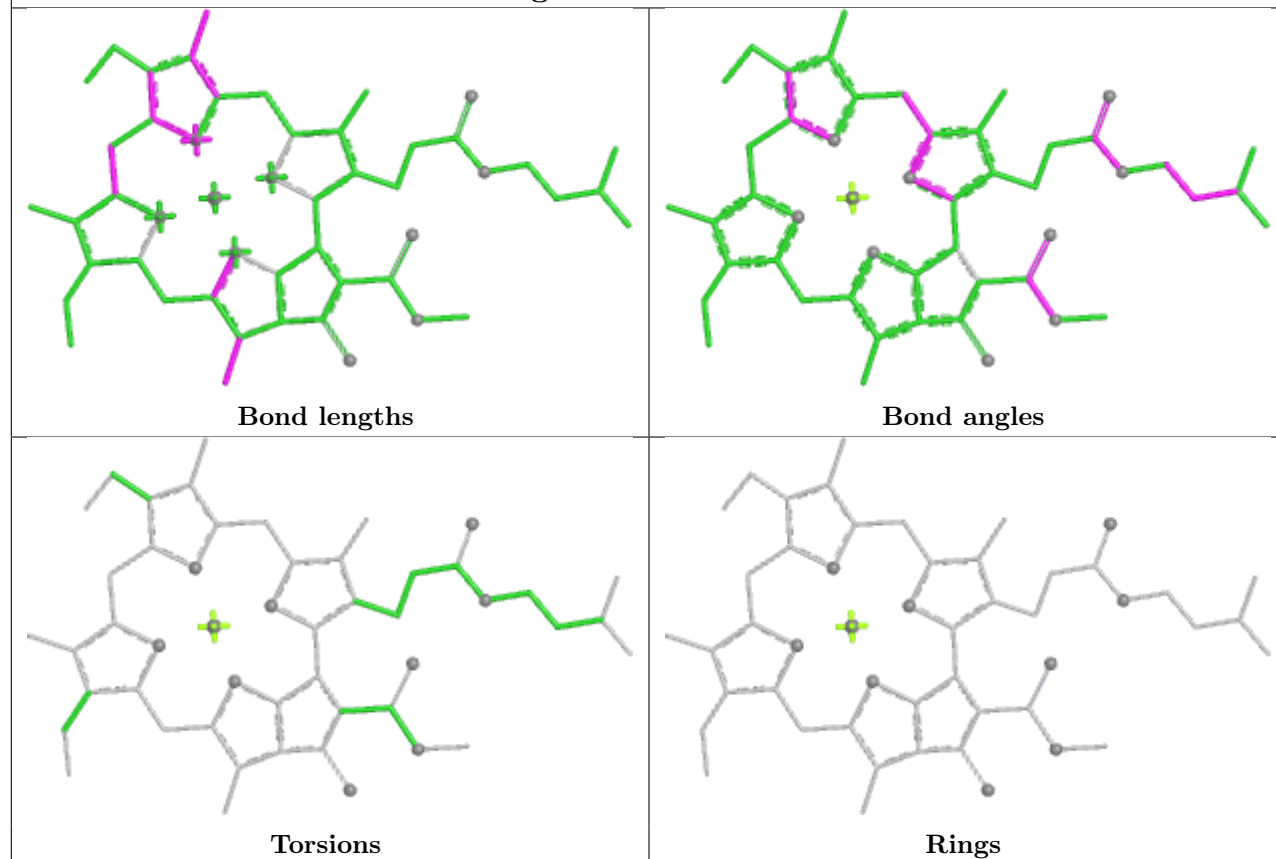




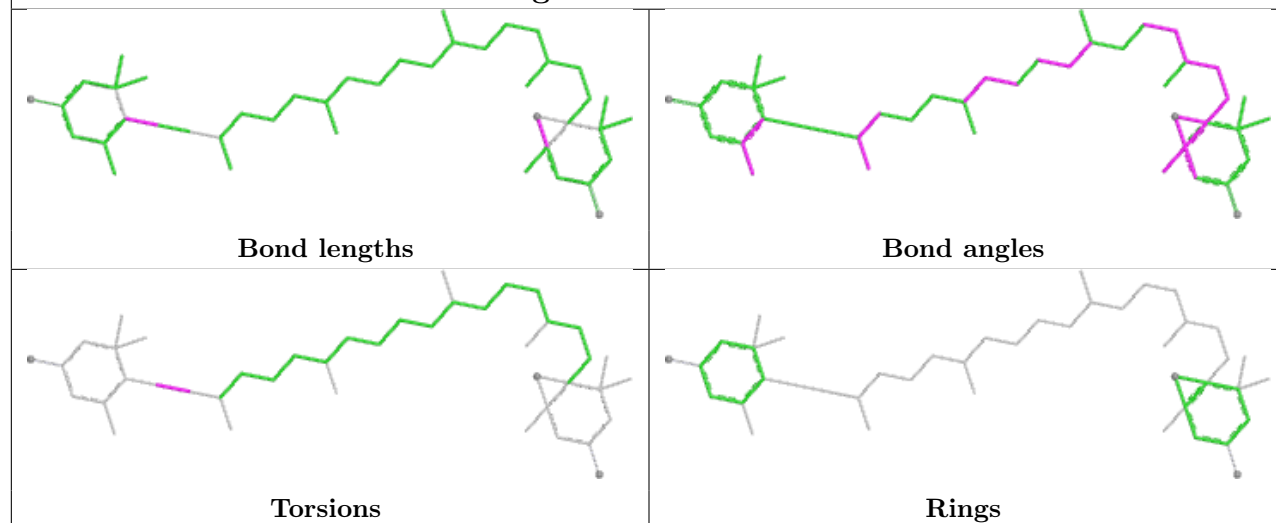


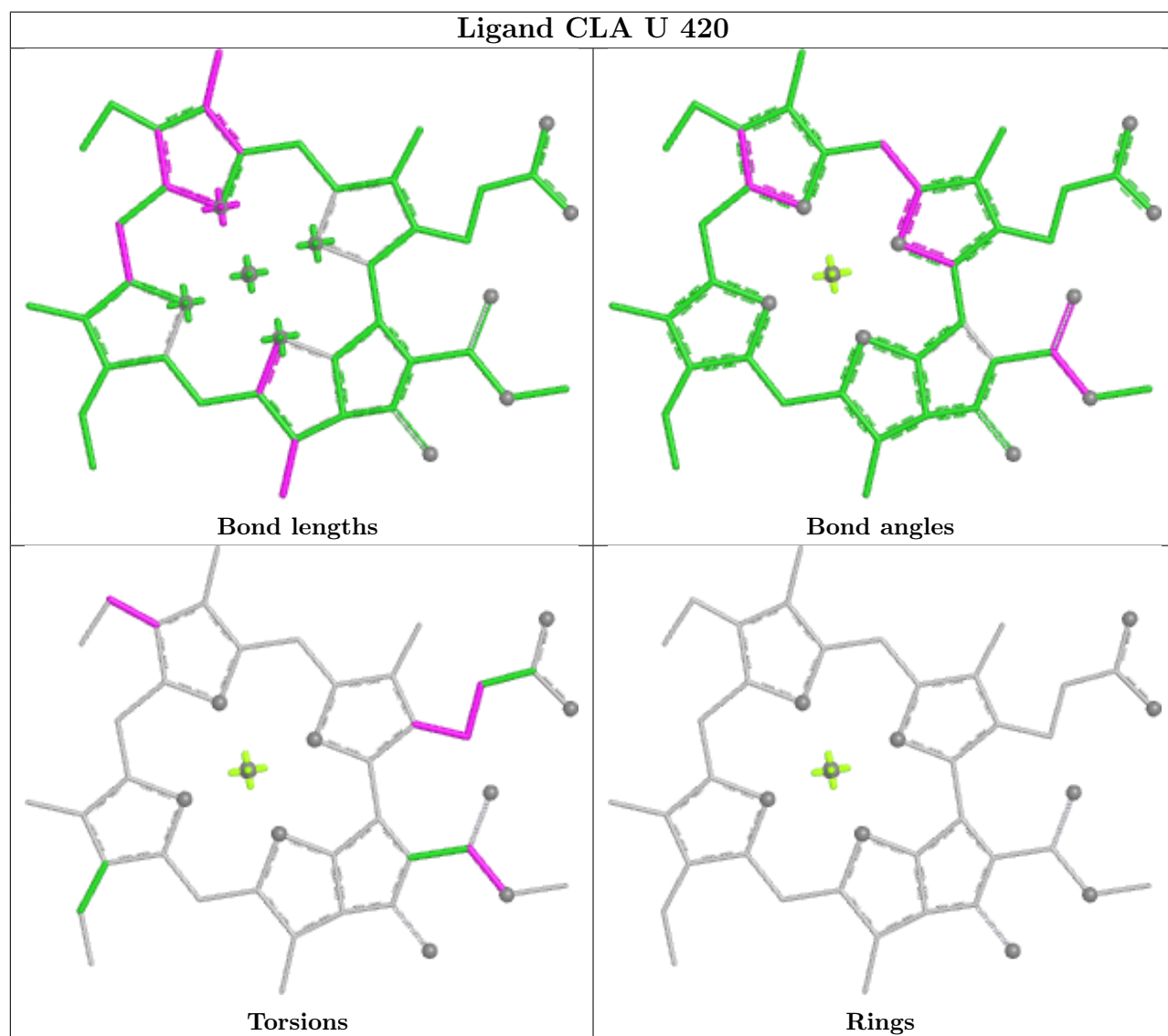
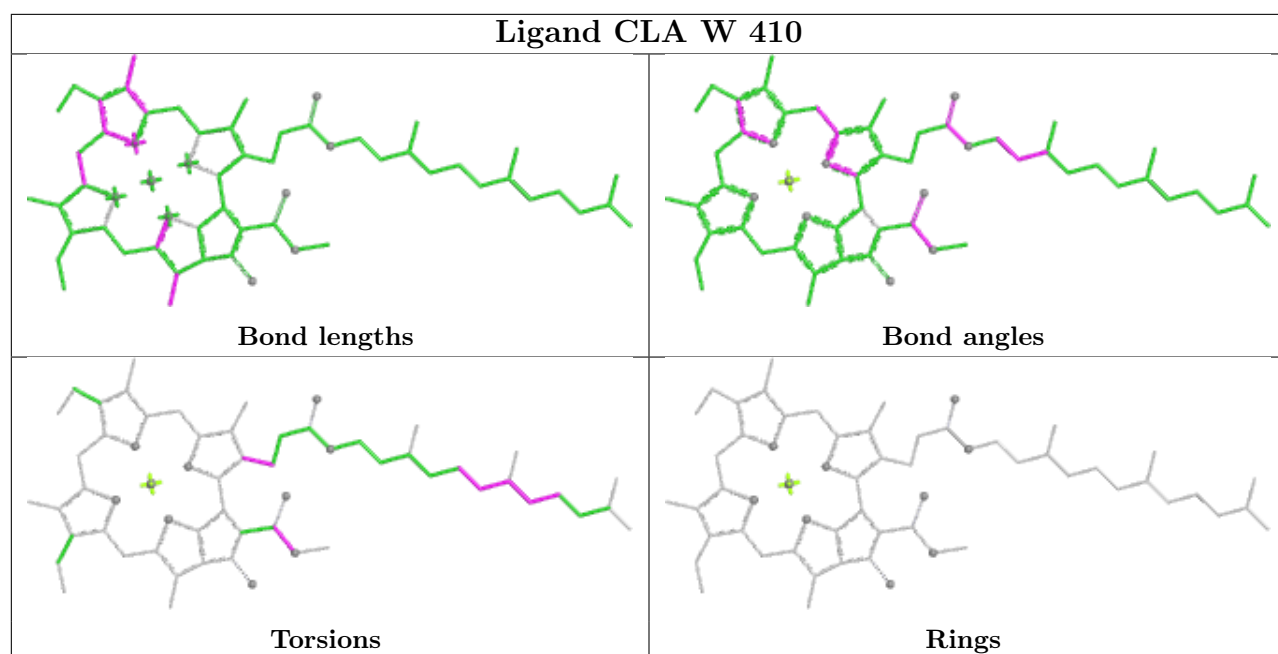


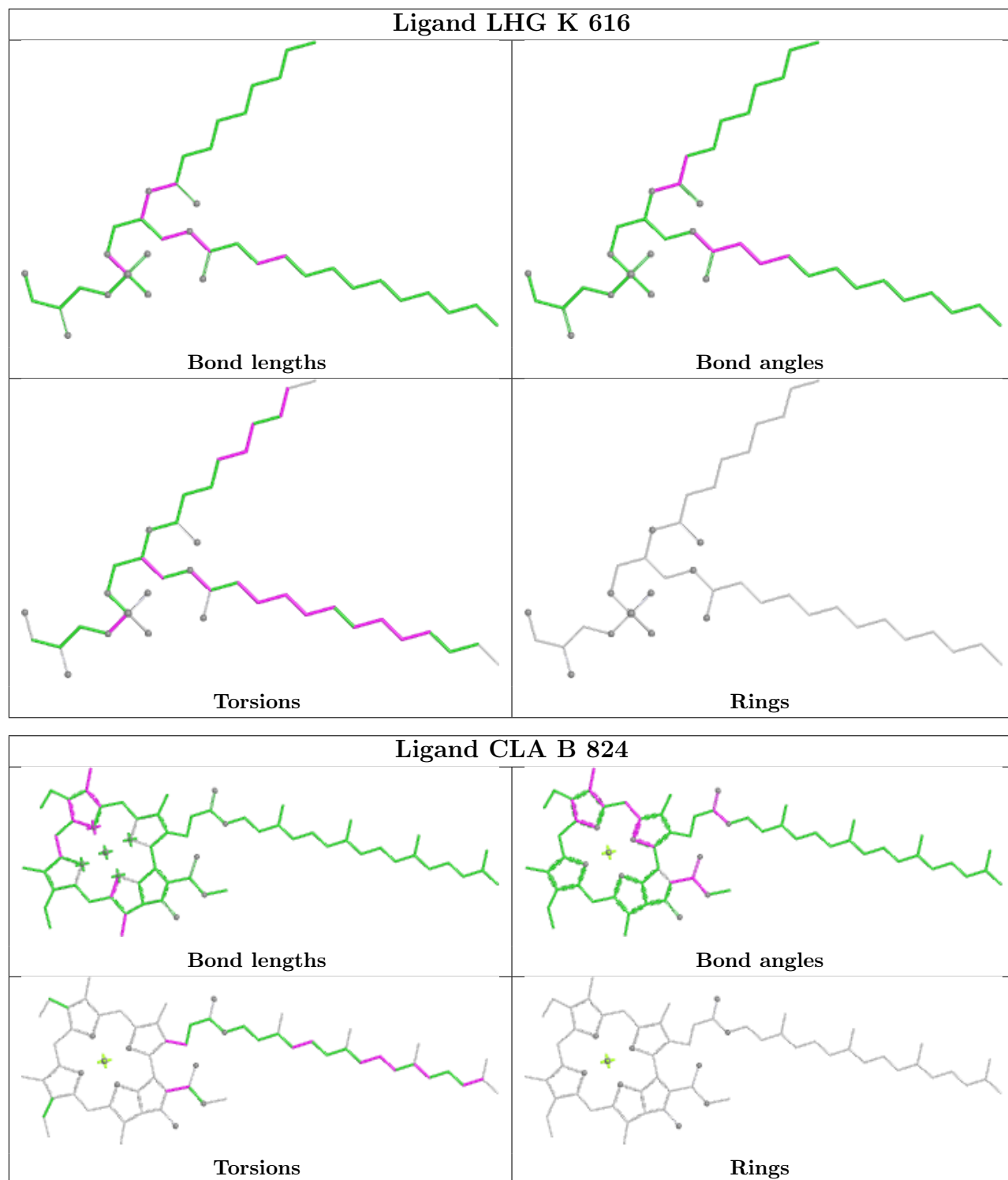
## Ligand CLA K 606



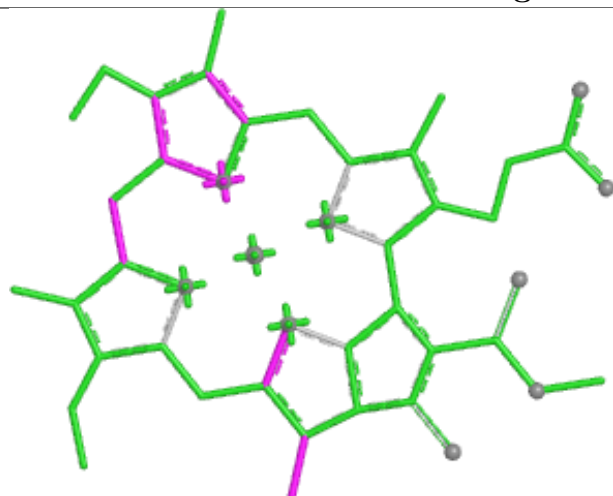
## Ligand DD6 U 416



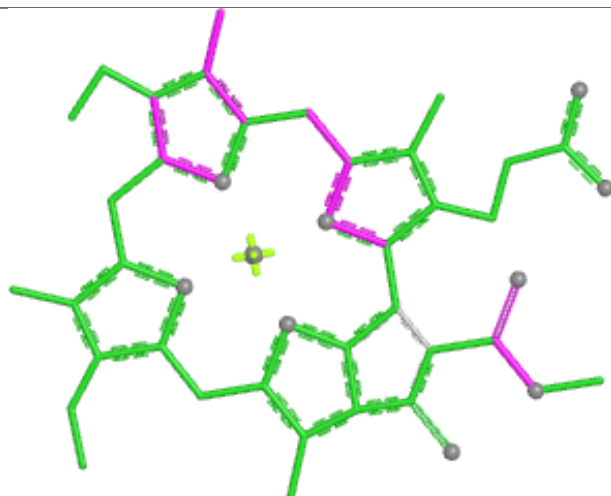




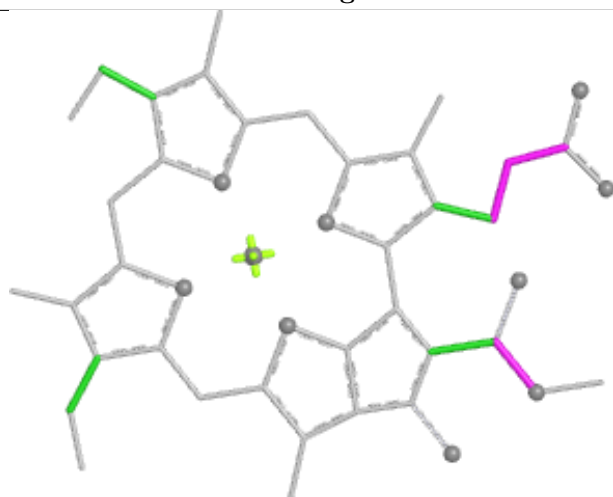
## Ligand CLA R 604



Bond lengths



Bond angles

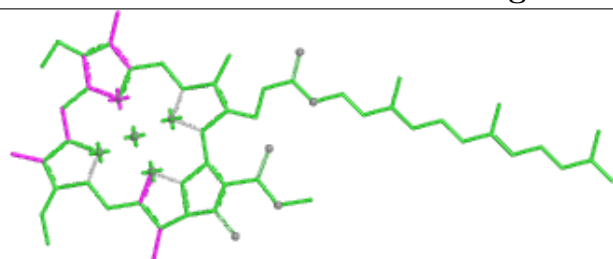


Torsions

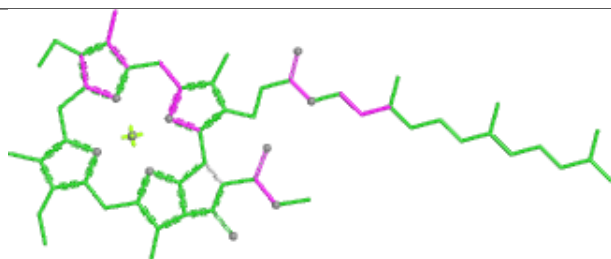


Rings

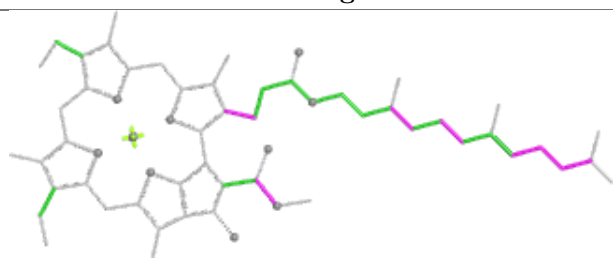
## Ligand CLA W 411



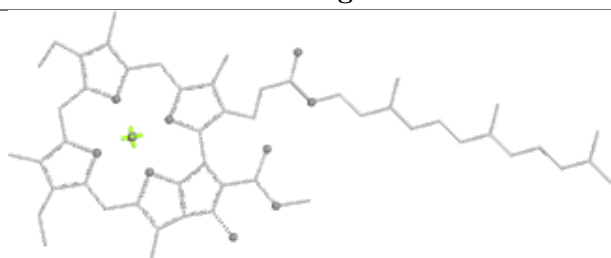
Bond lengths



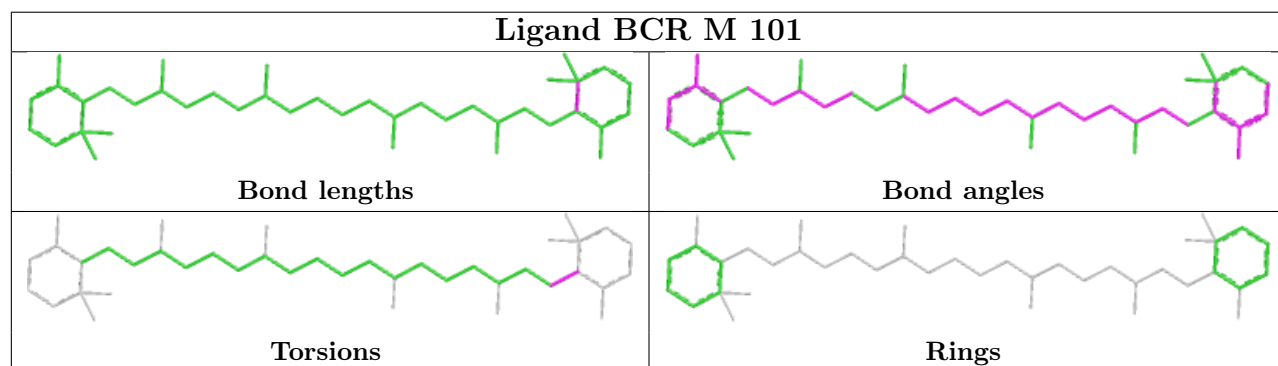
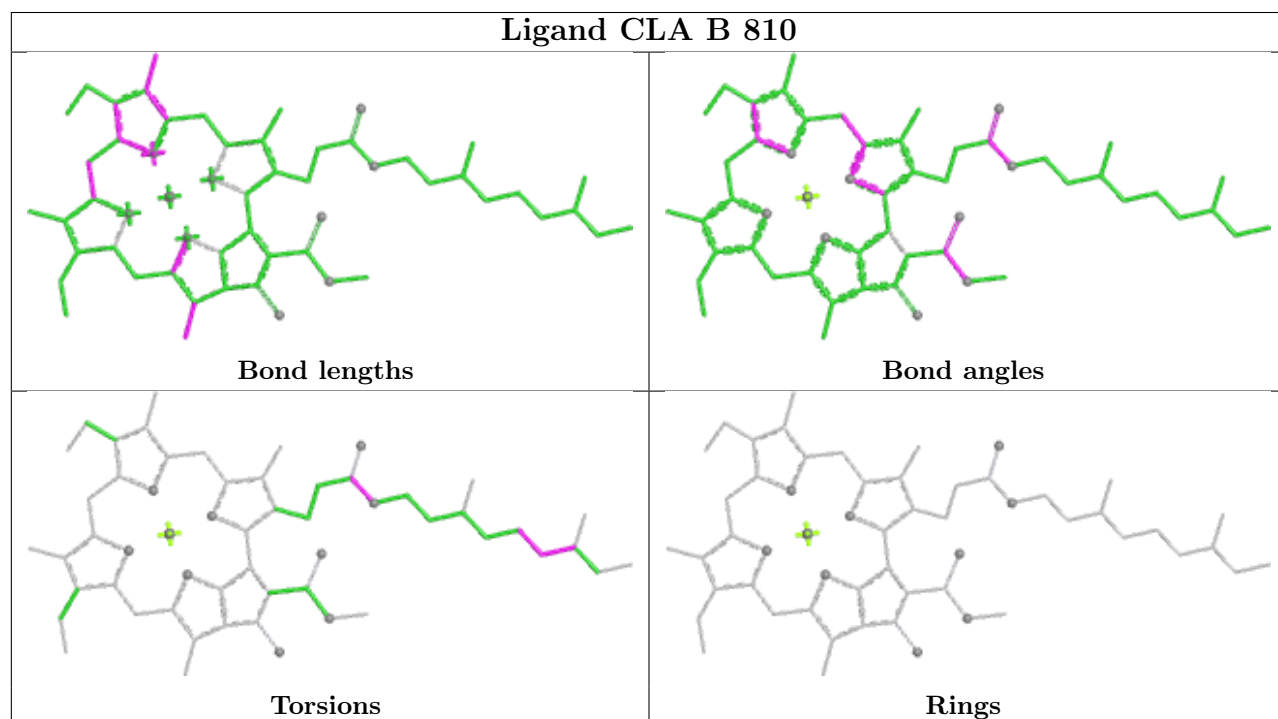
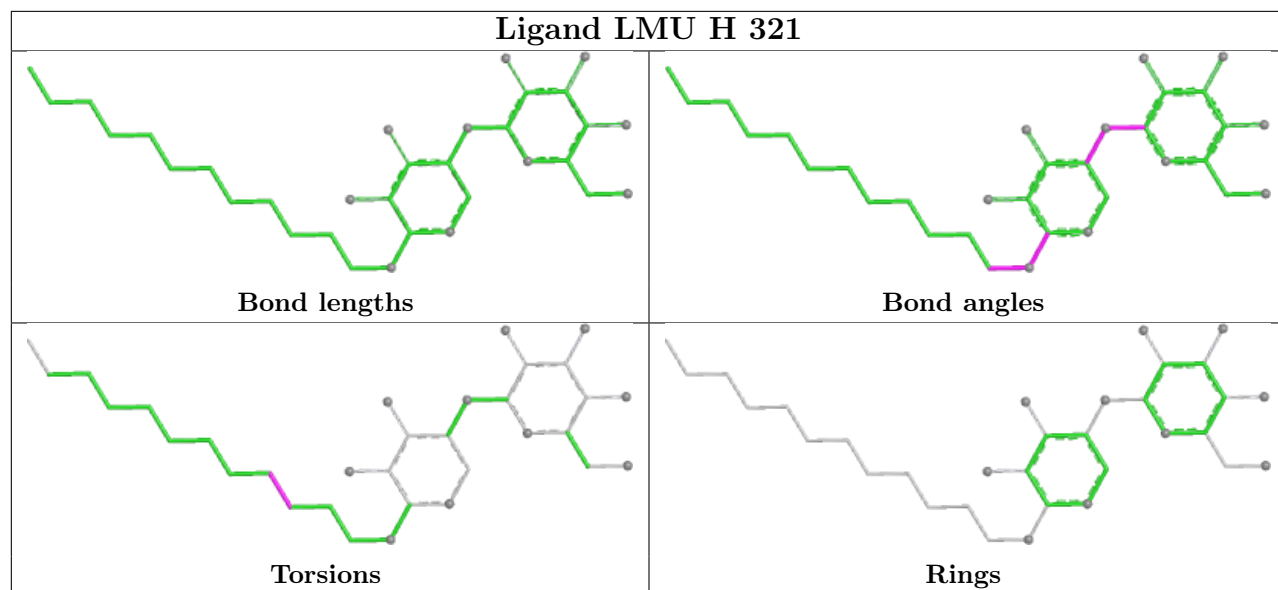
Bond angles

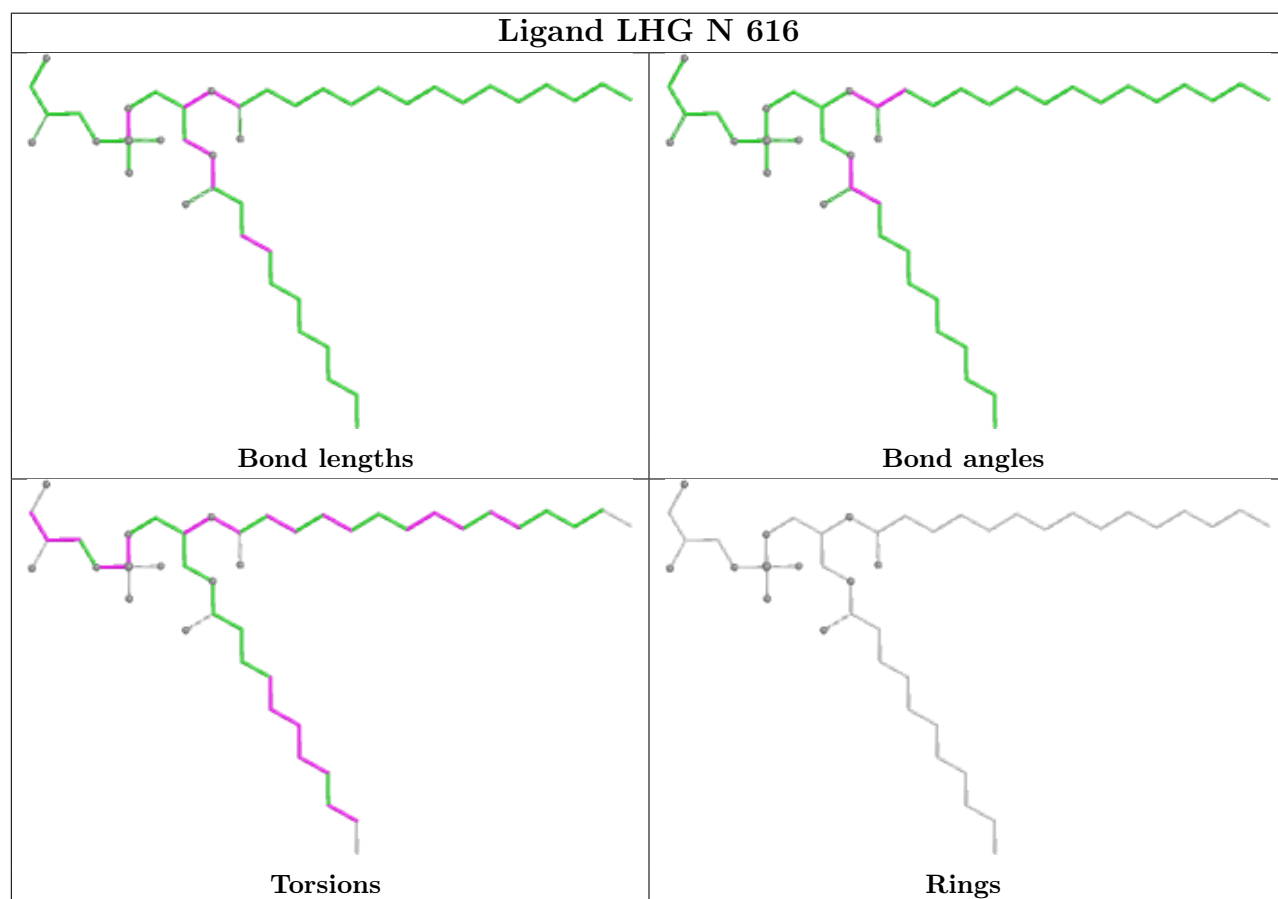
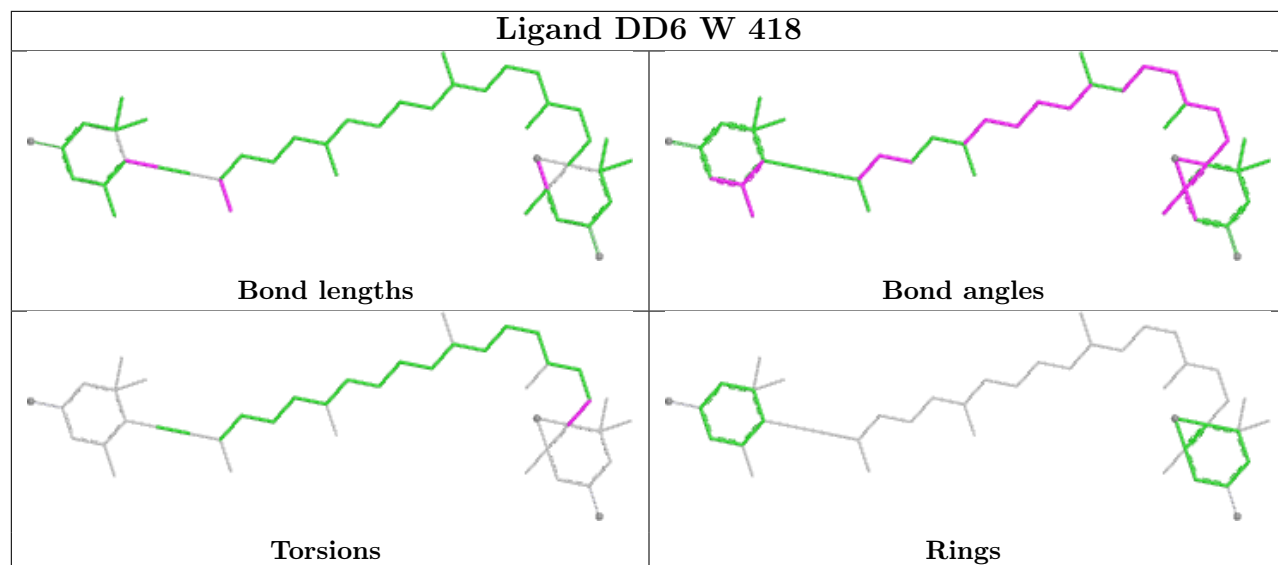


Torsions

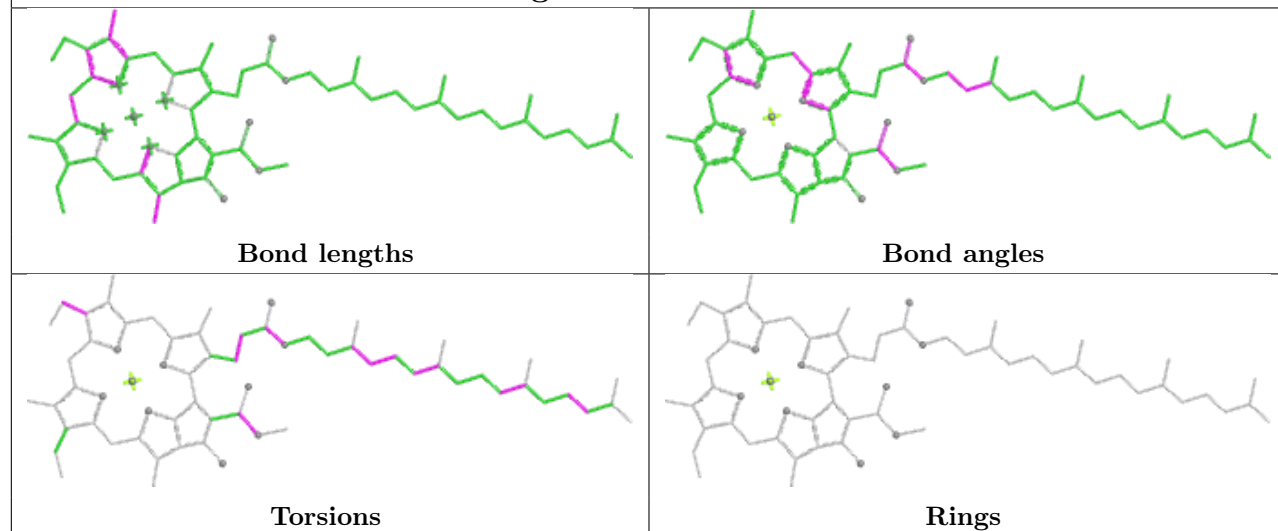


Rings

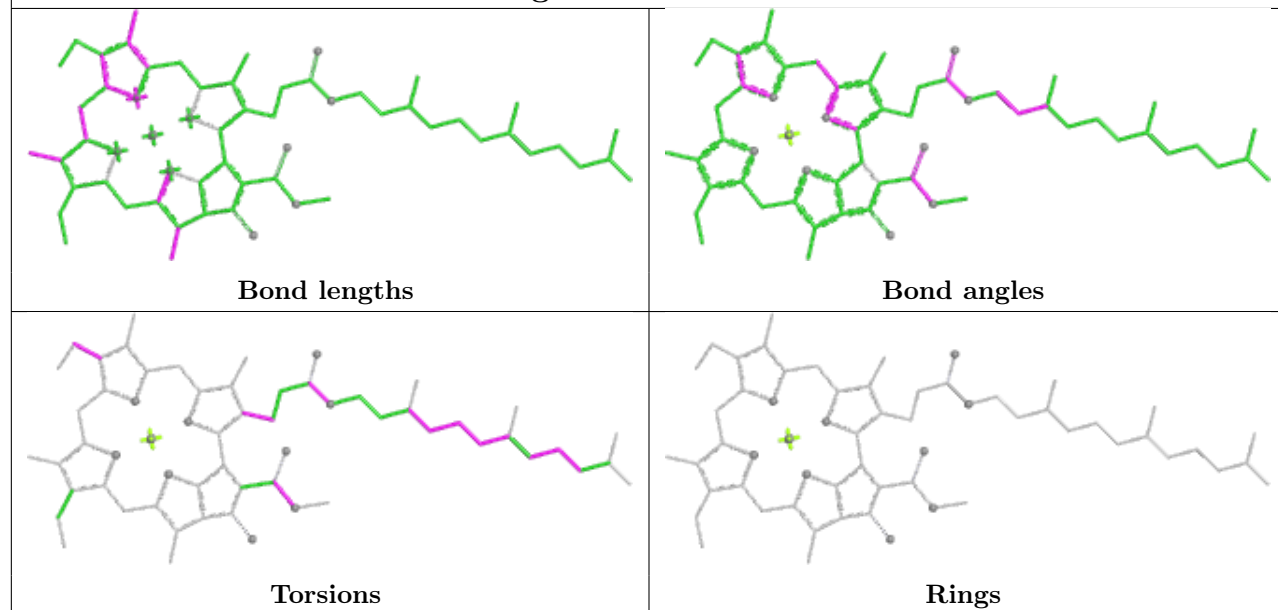




## Ligand CLA H 311

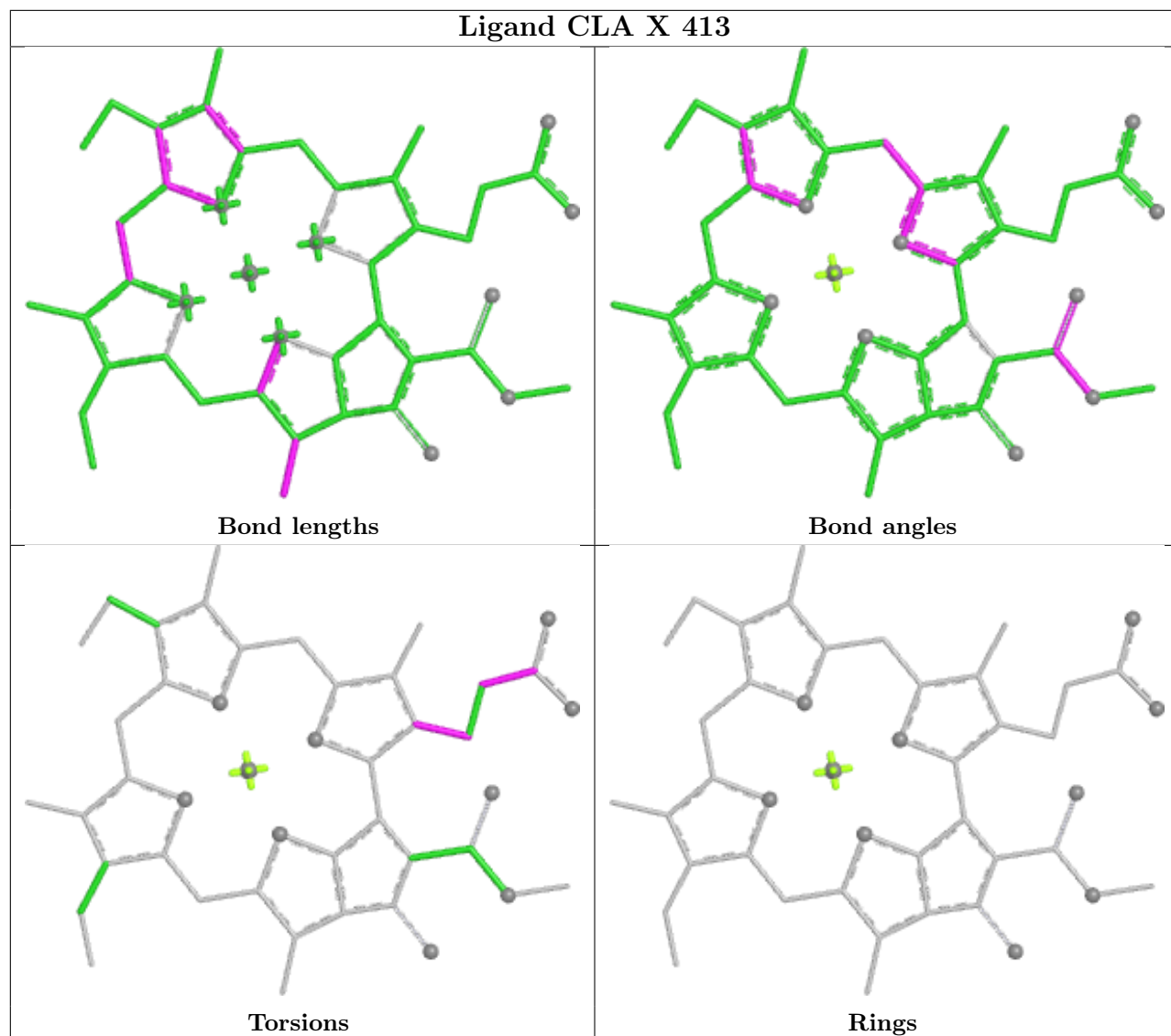


## Ligand CLA R 607

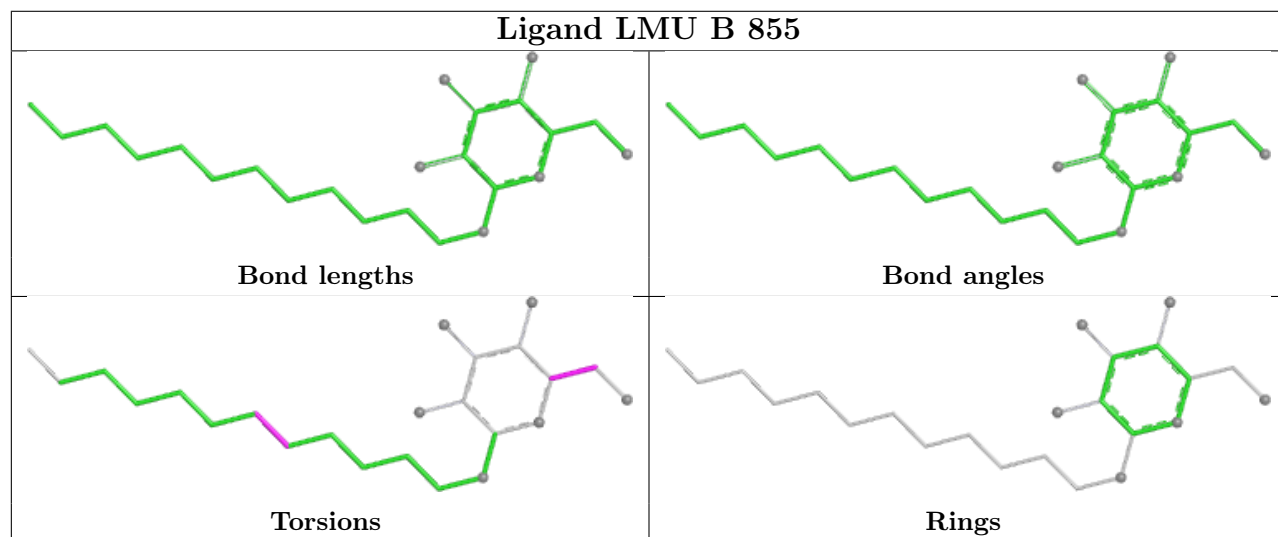


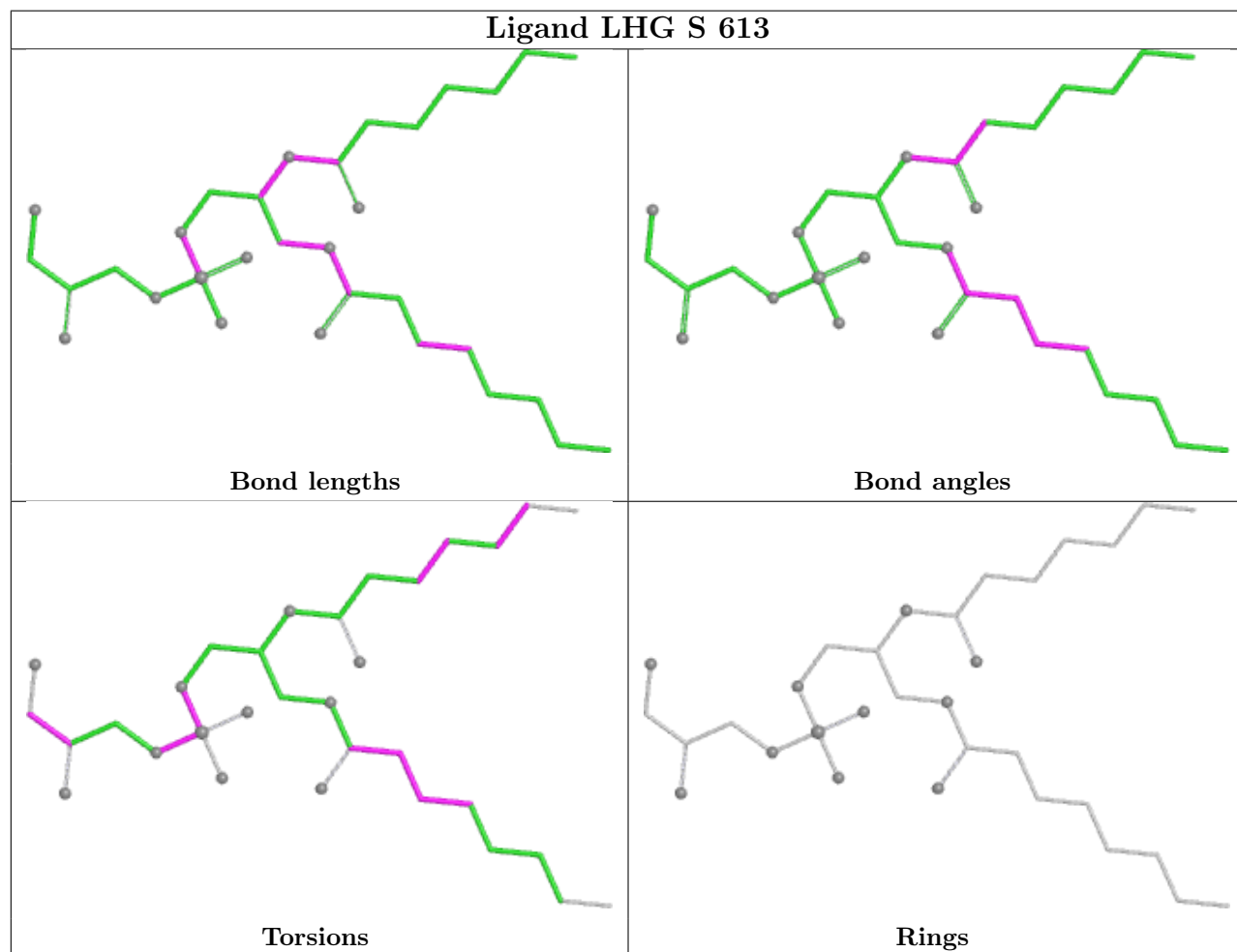
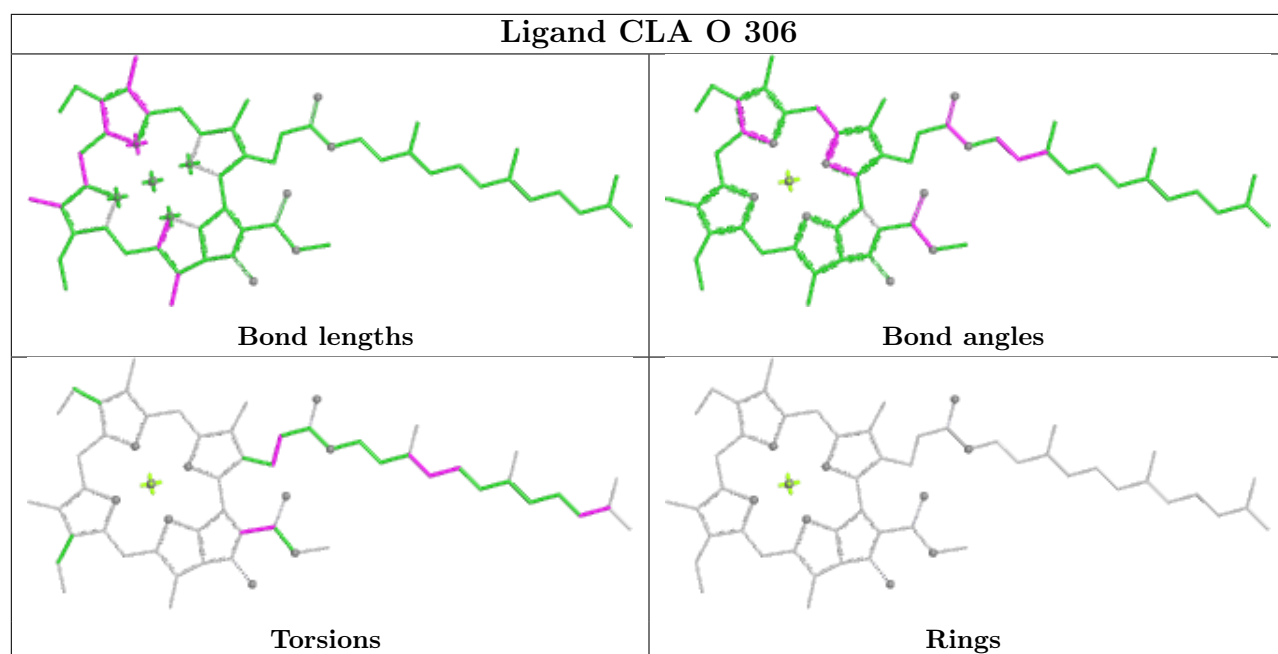


## Ligand CLA X 413

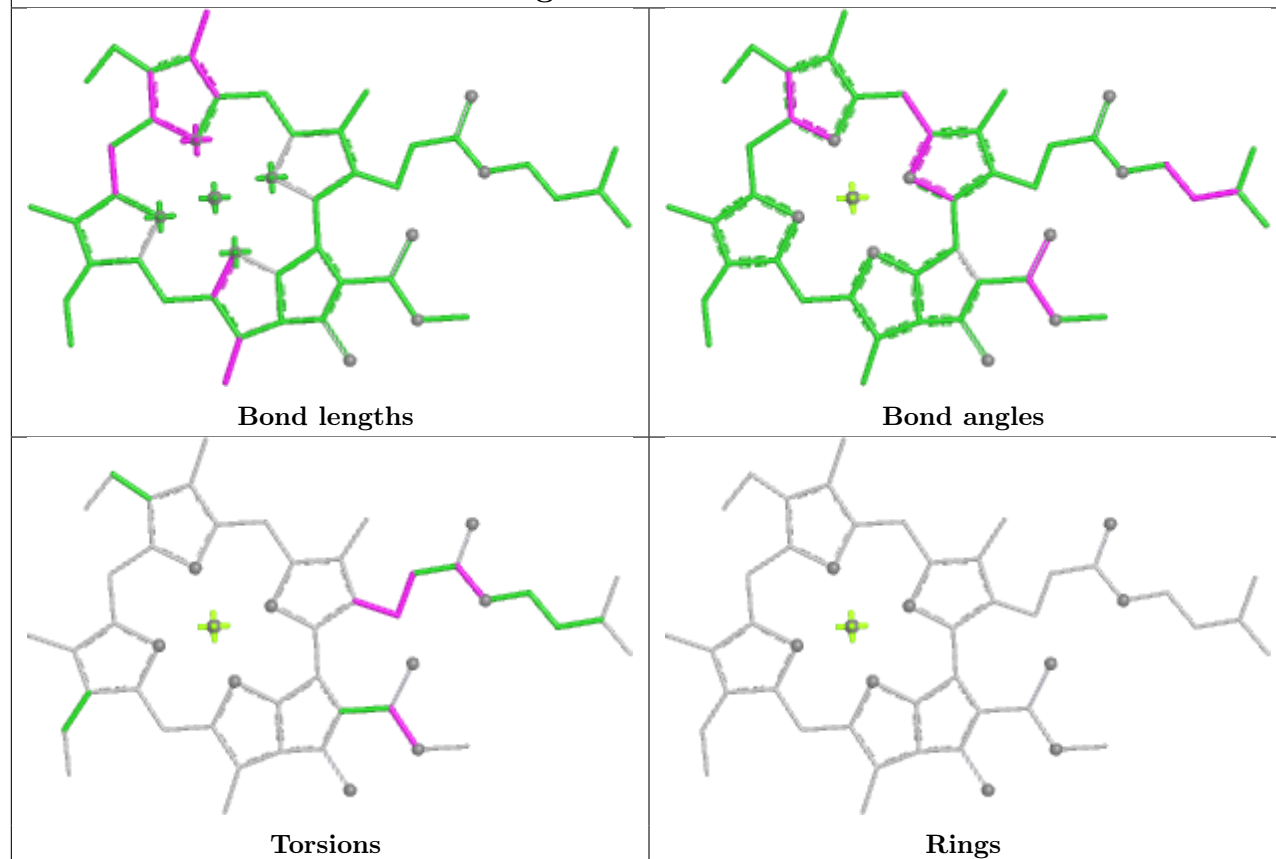


## Ligand LMU B 855

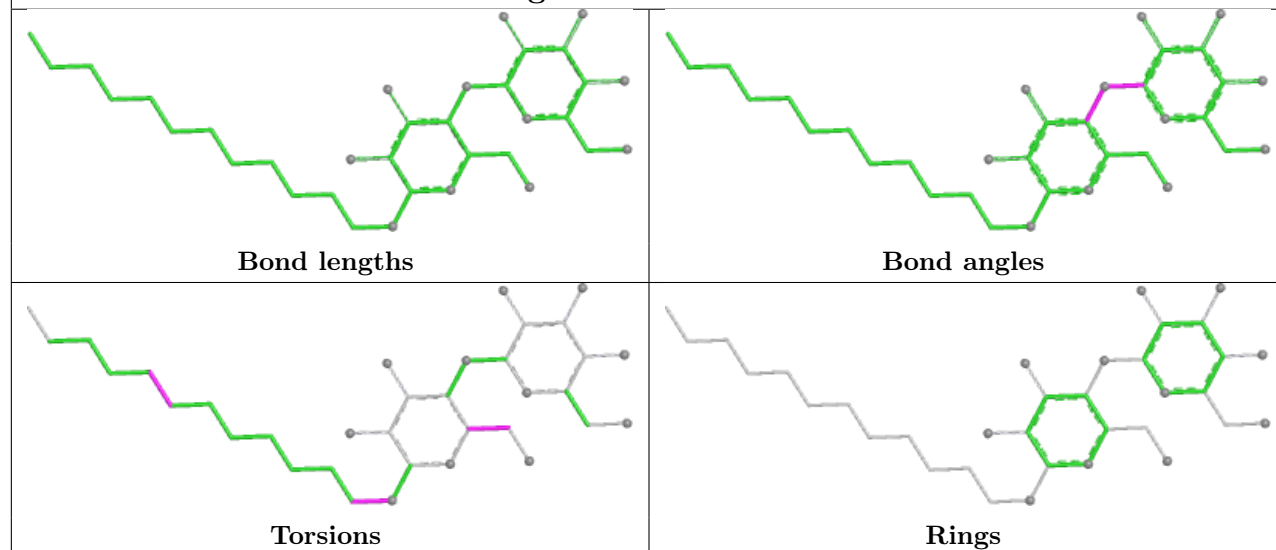


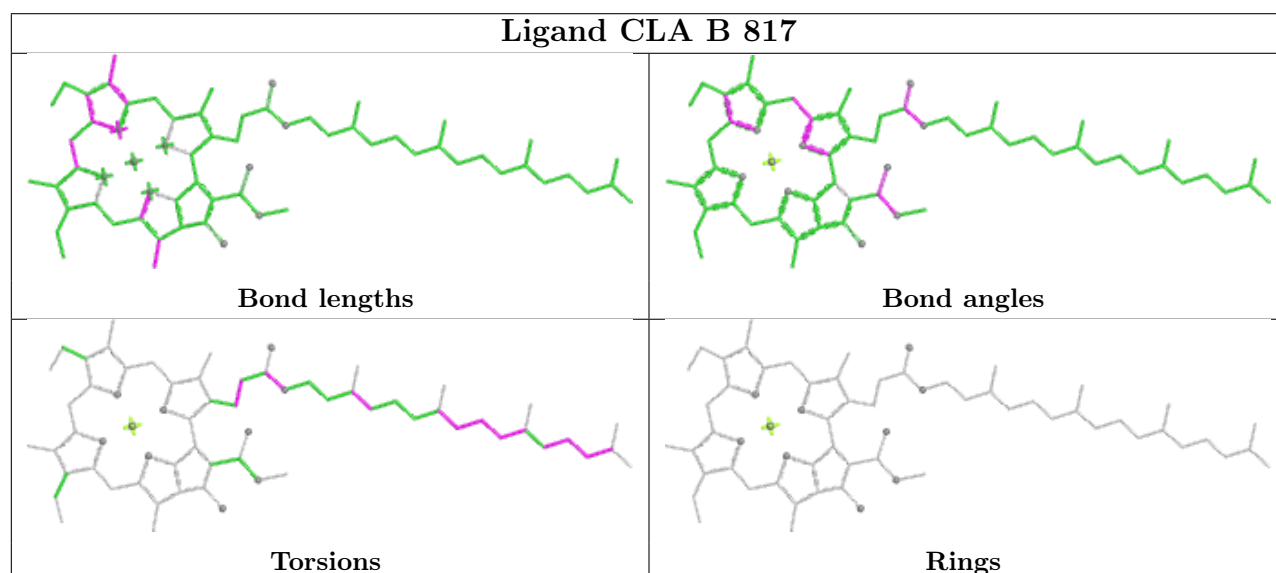
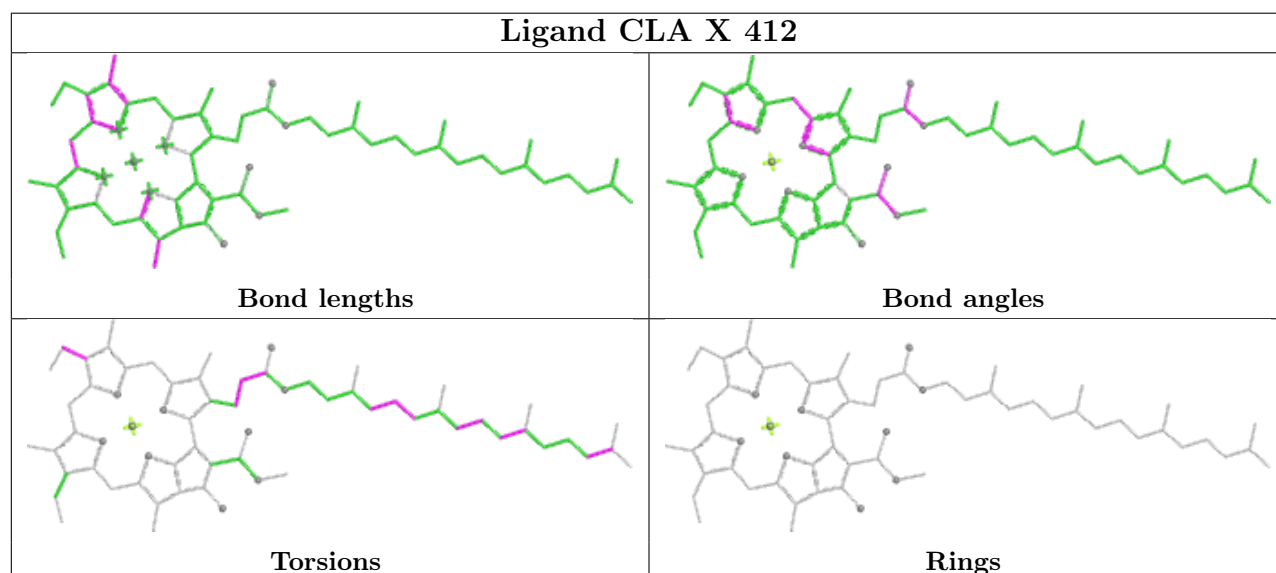
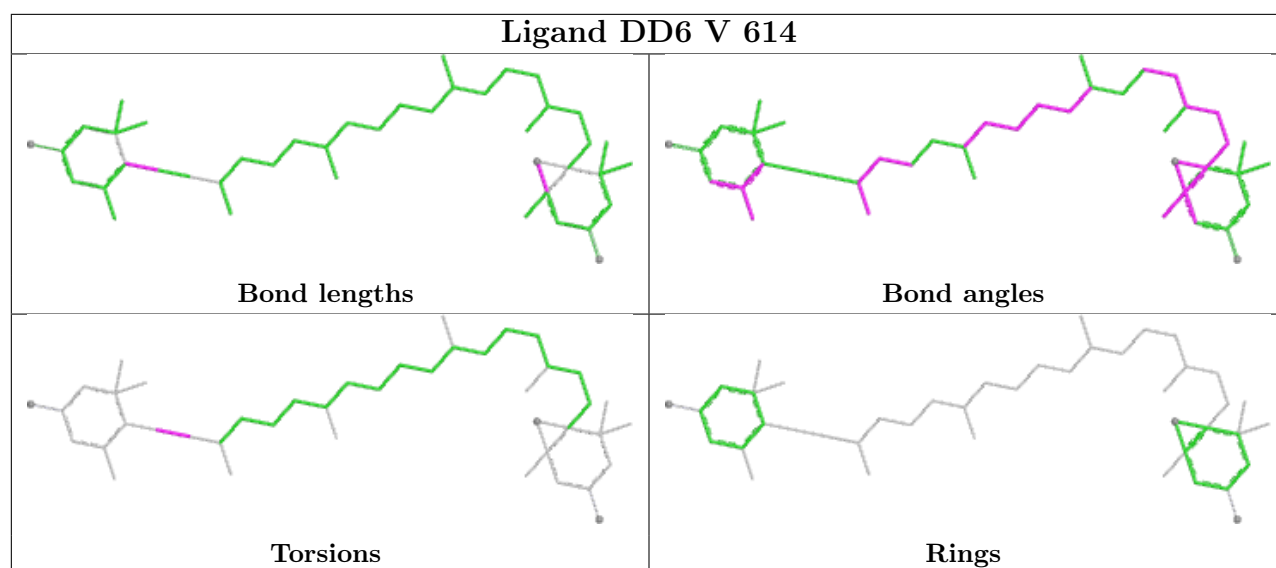


## Ligand CLA J 102

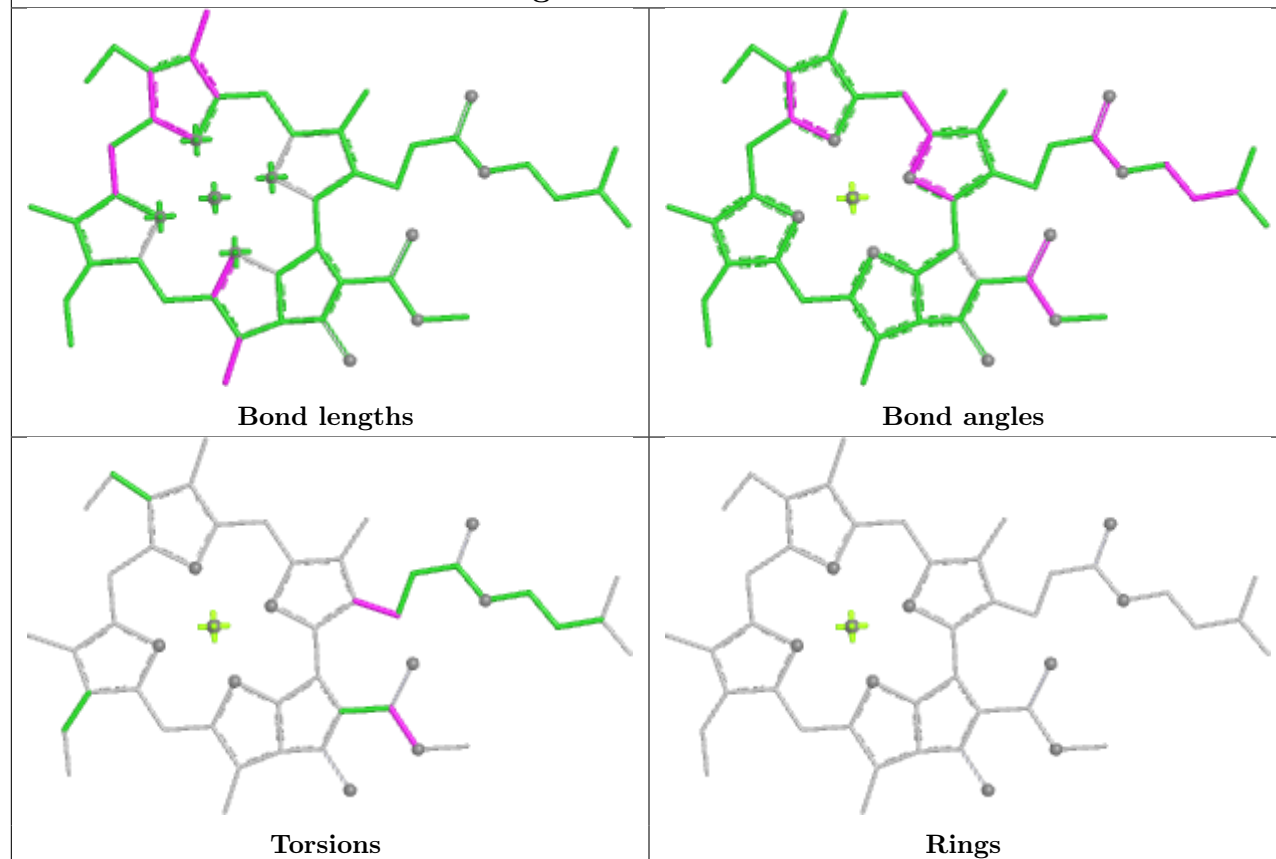


## Ligand LMU B 857

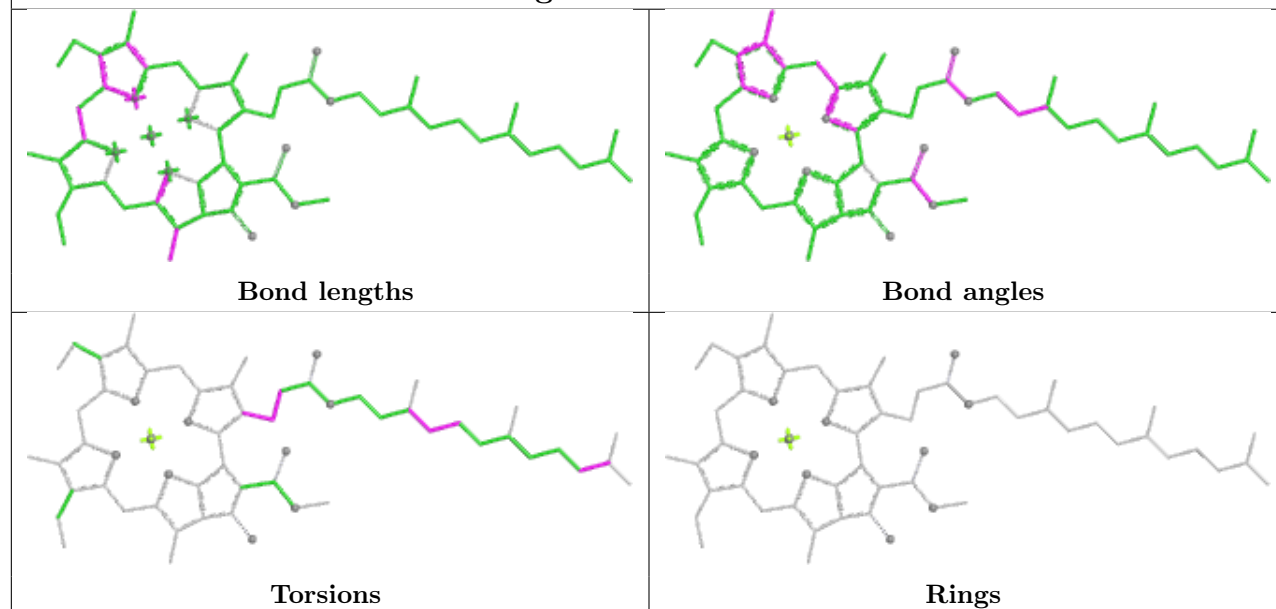


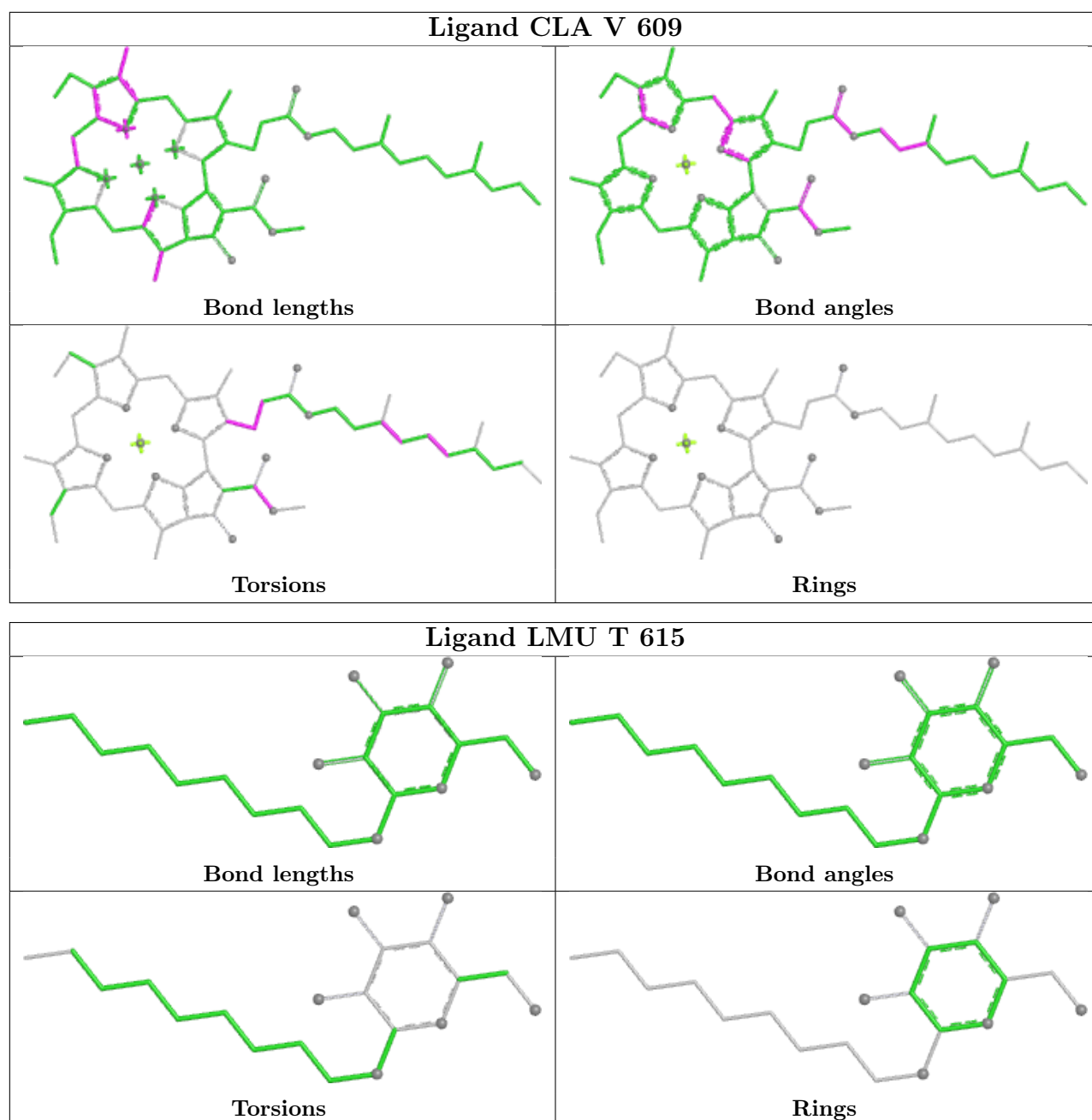


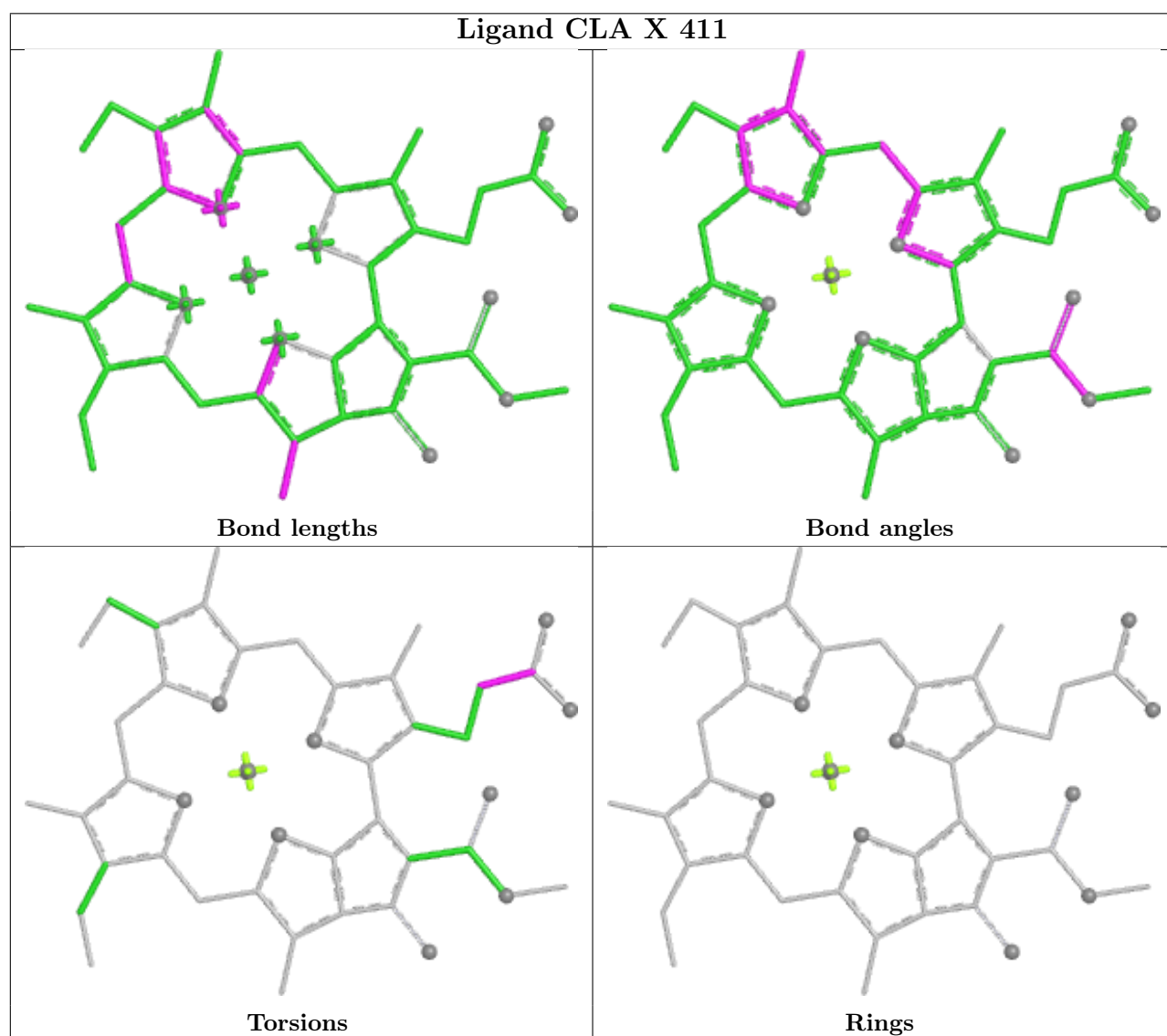
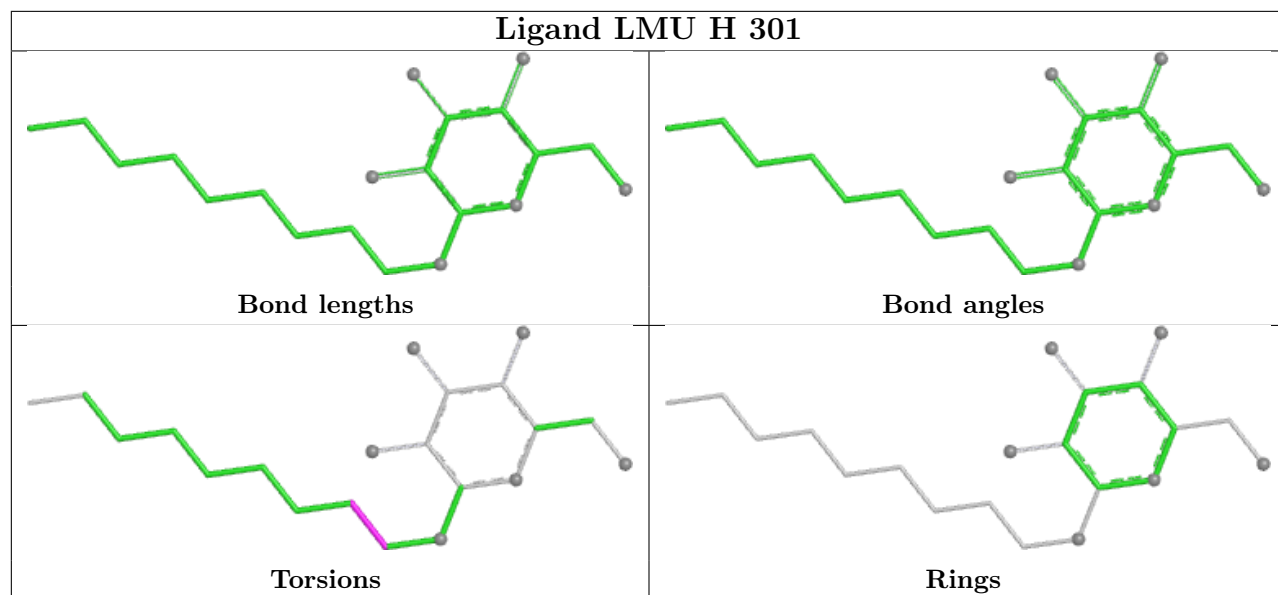
## Ligand CLA T 606

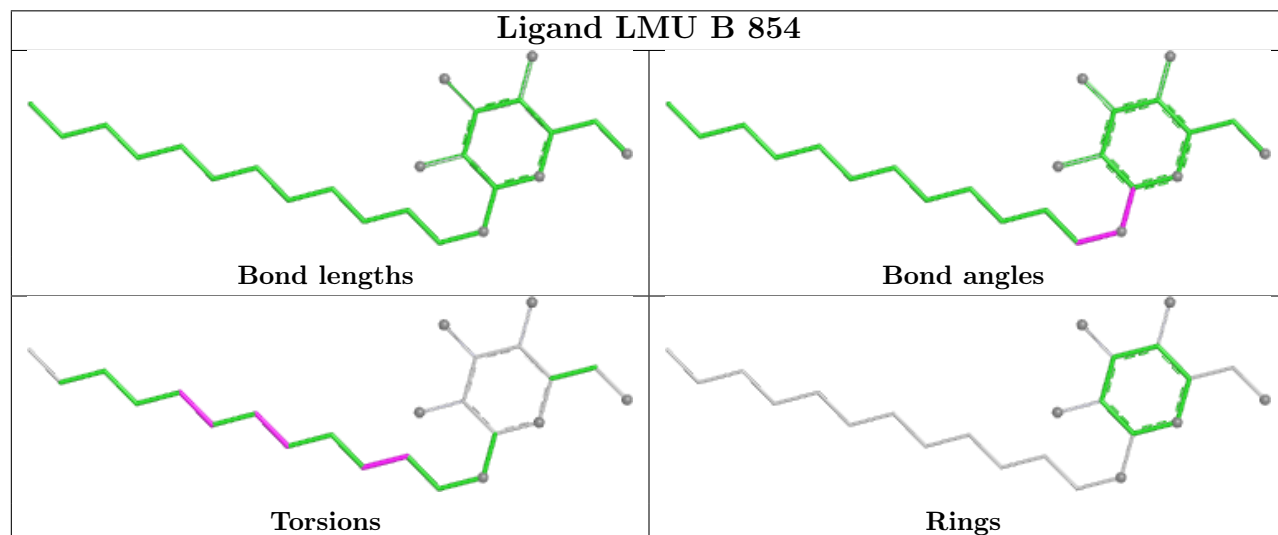
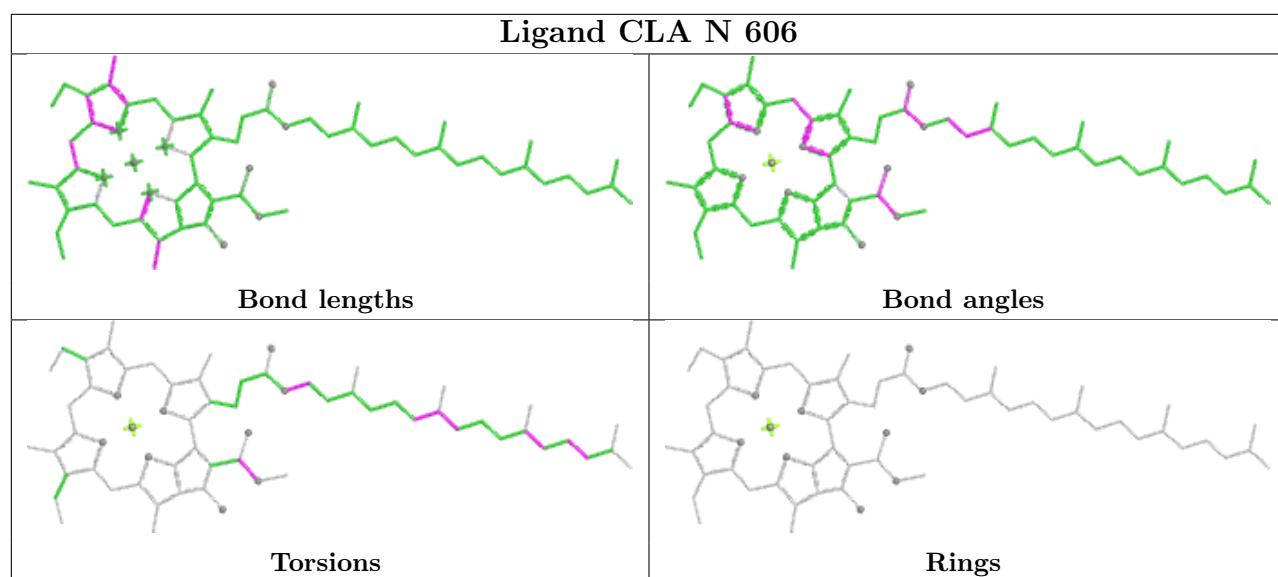


## Ligand CLA S 602

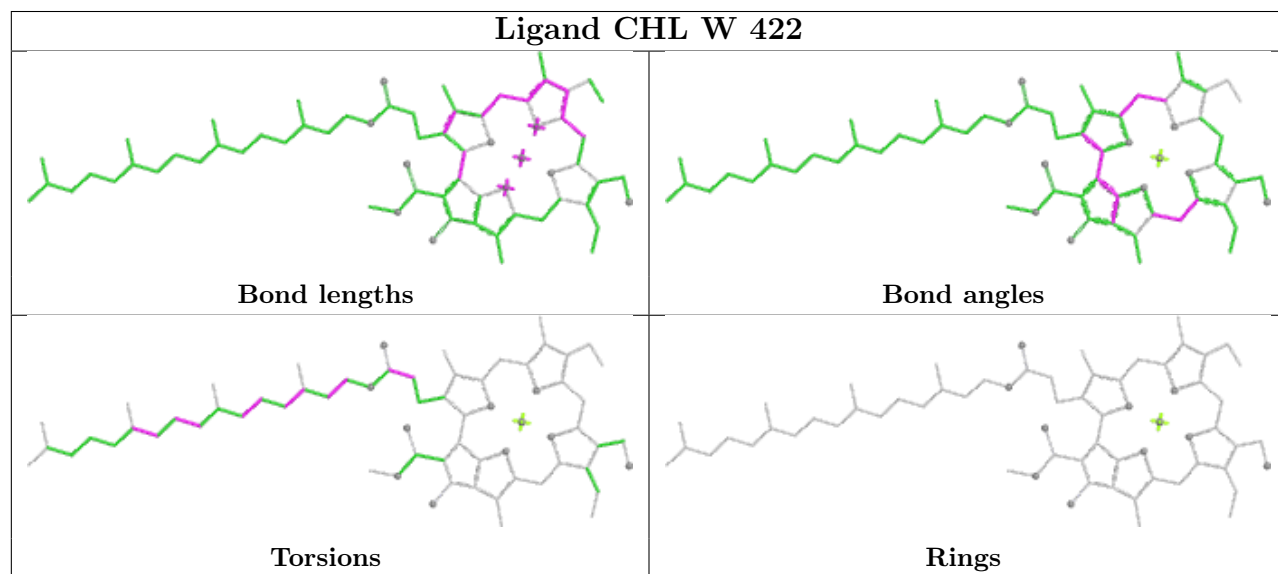
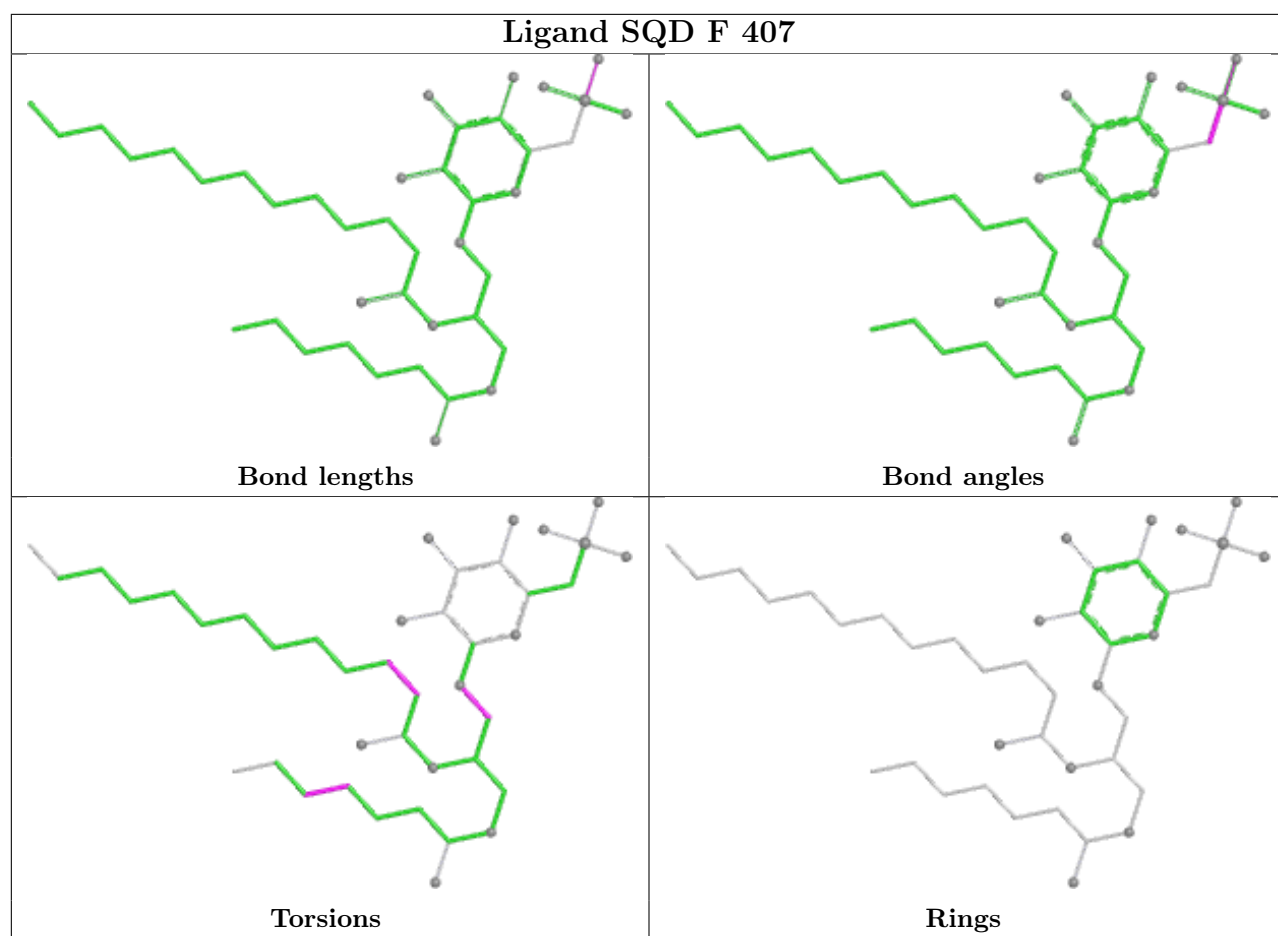


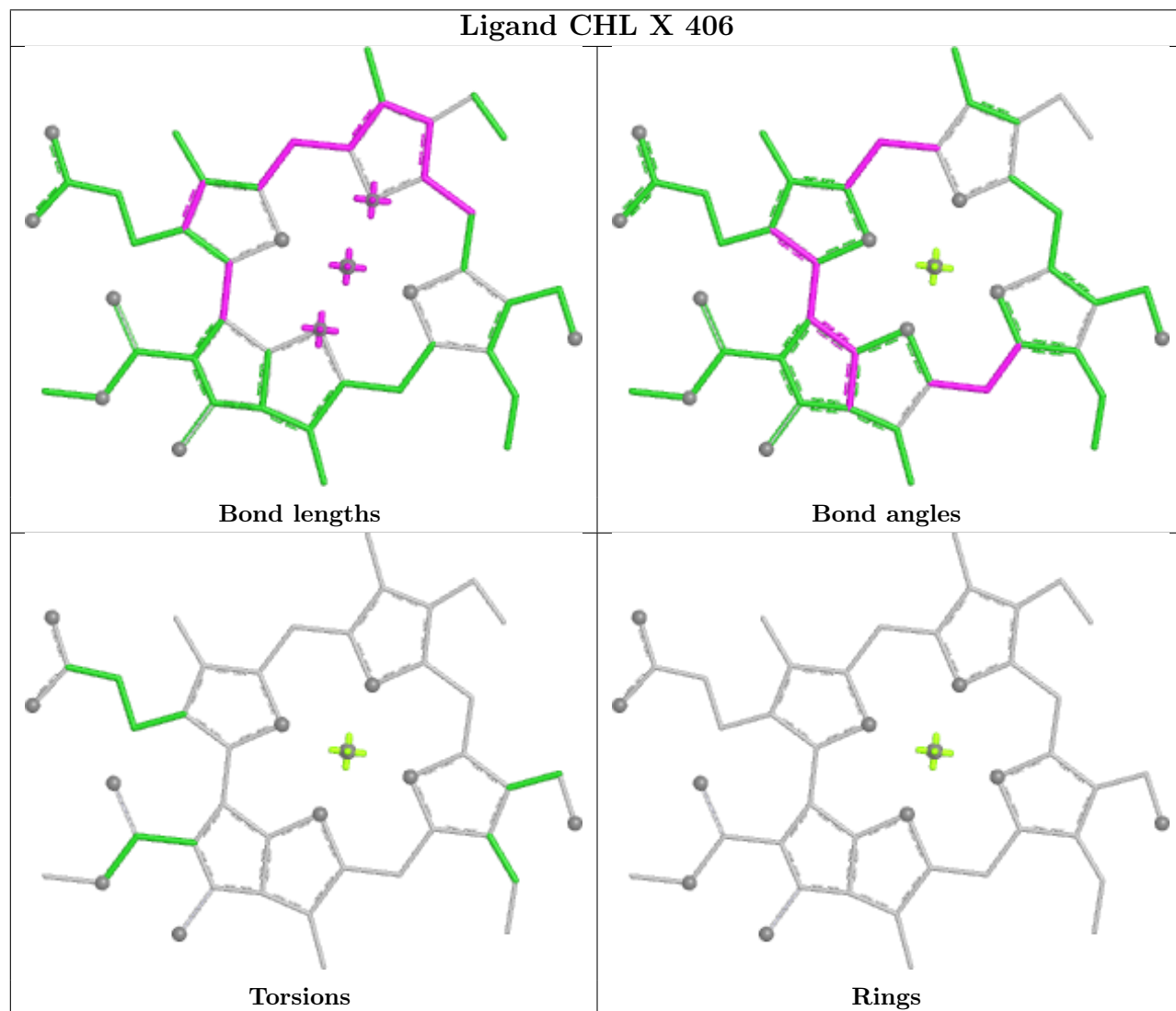
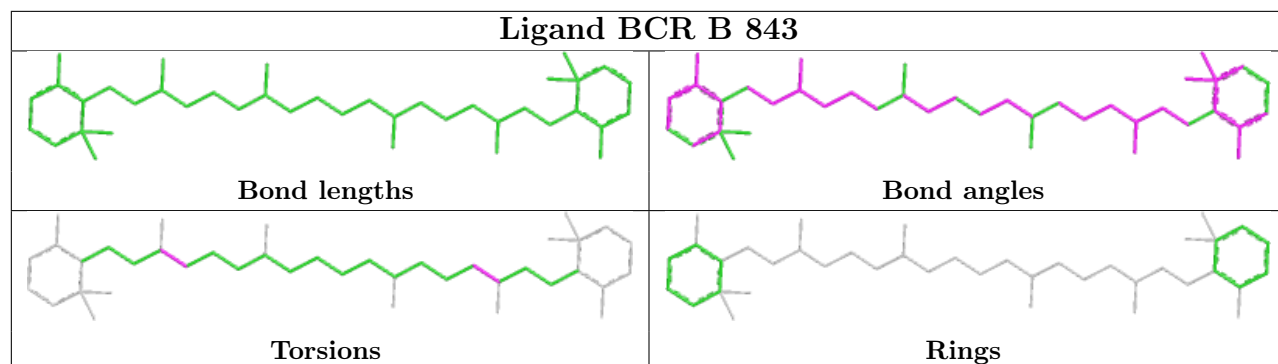




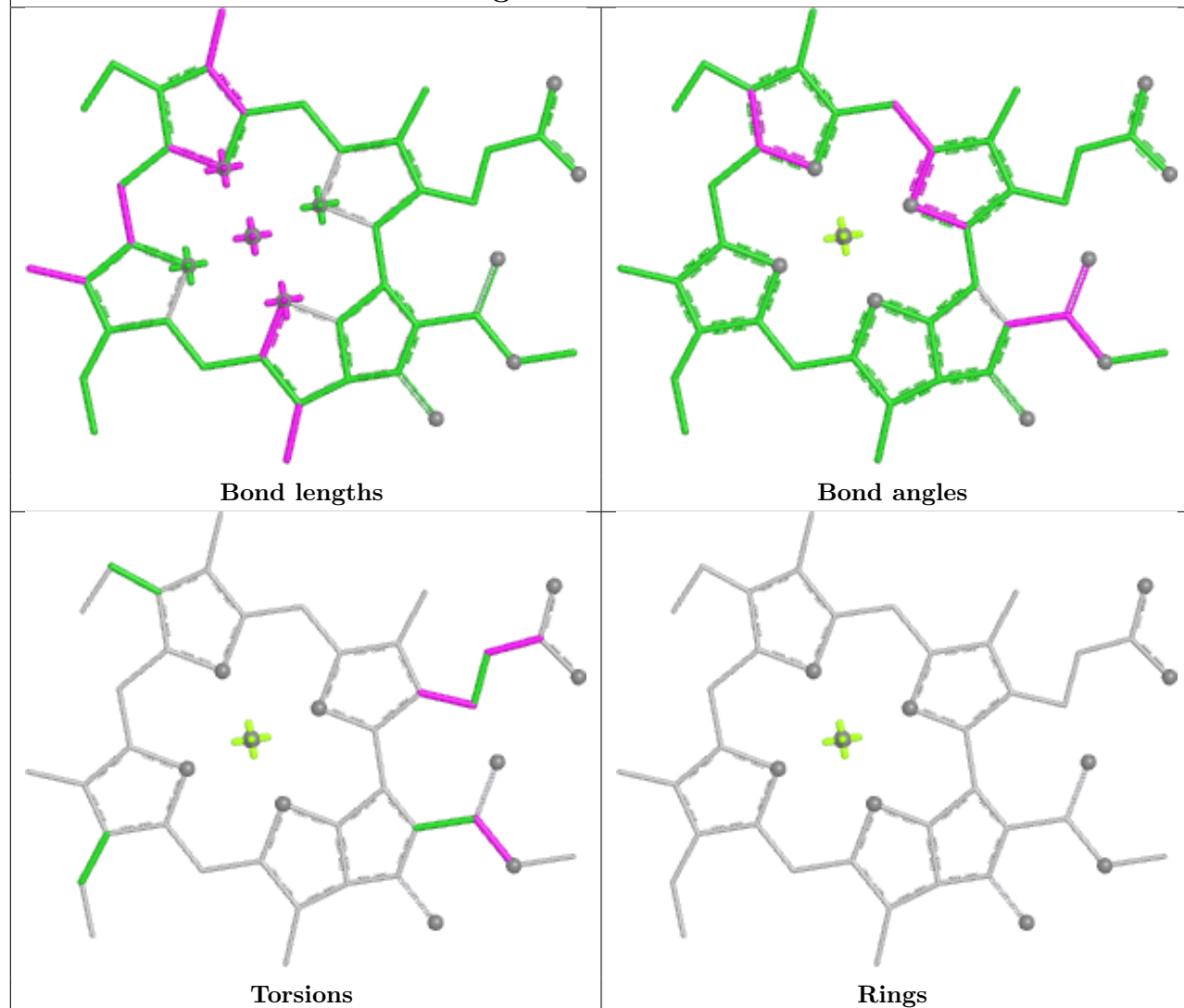




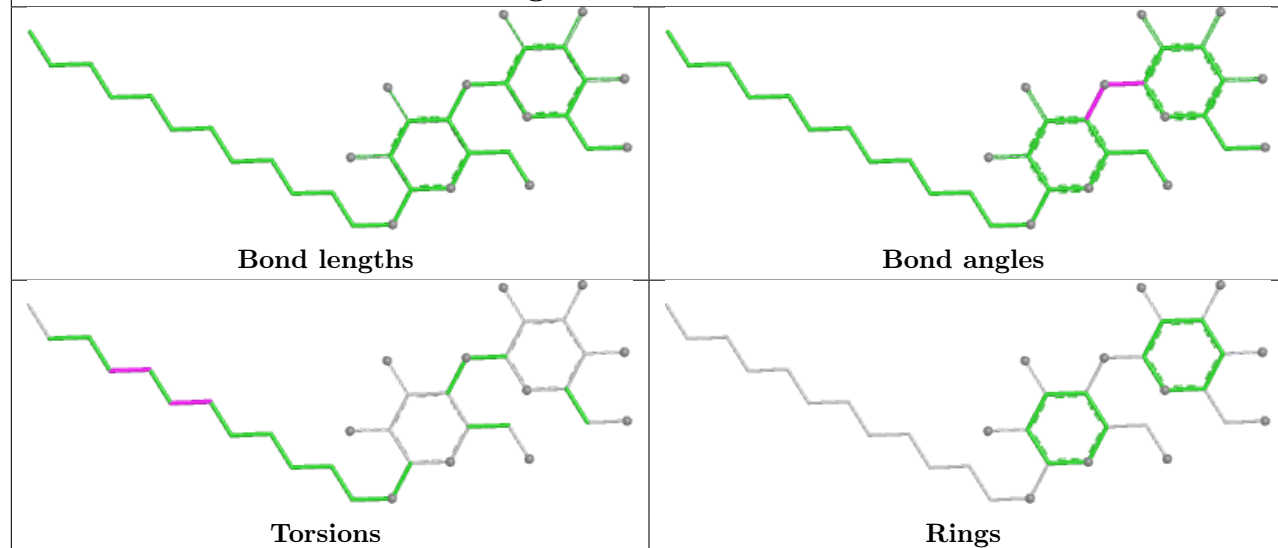


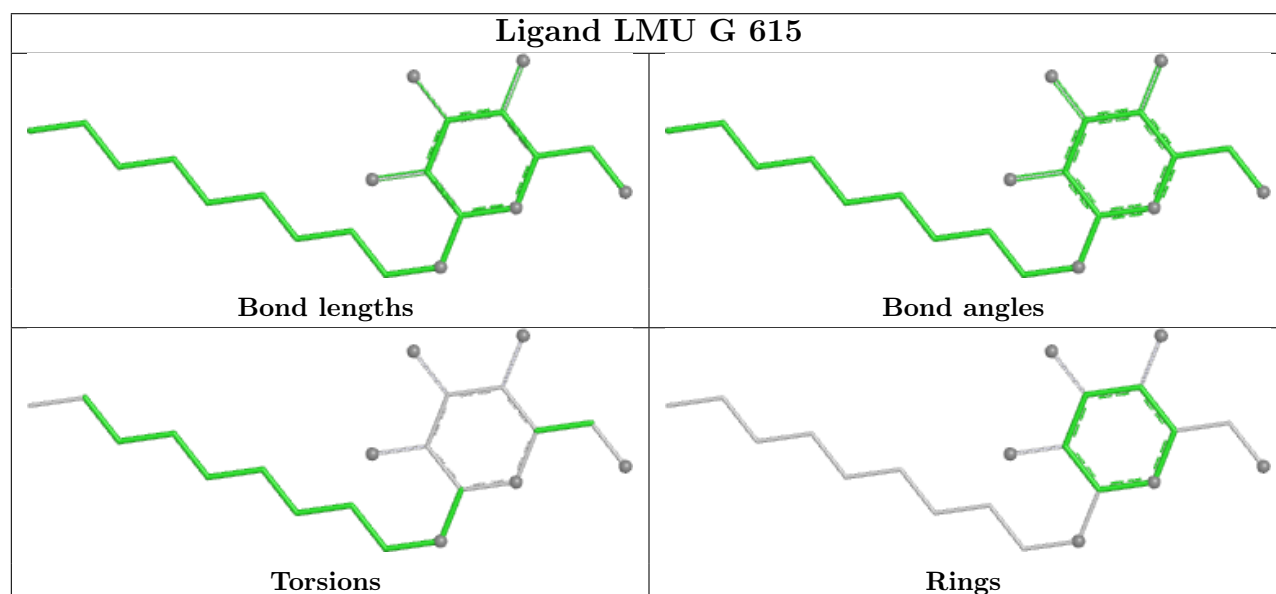
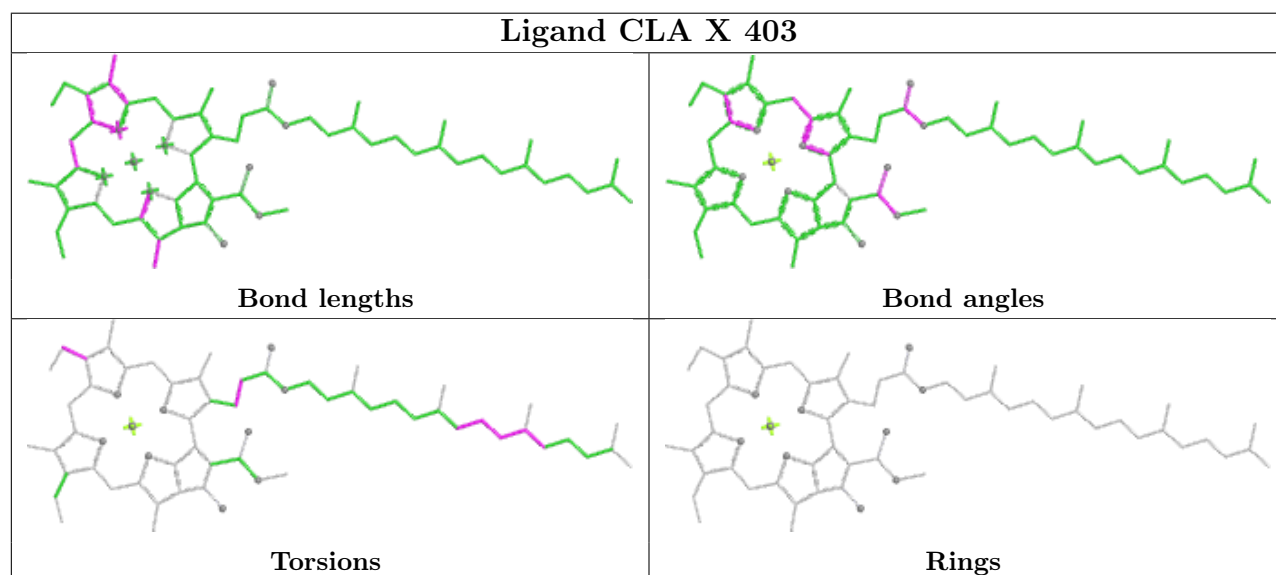
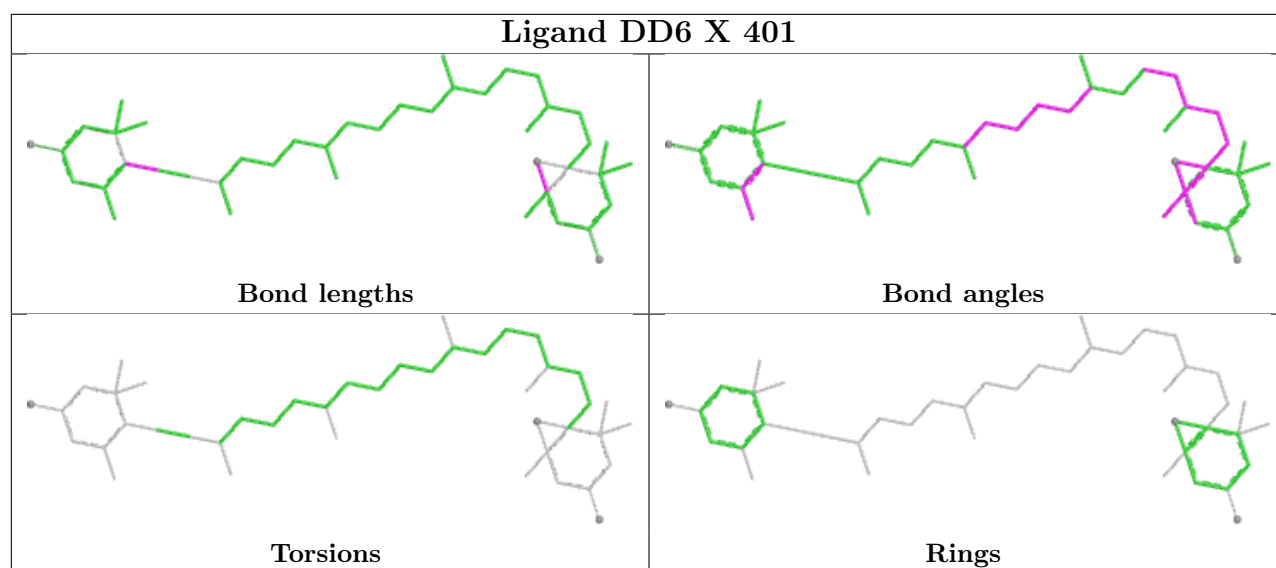


## Ligand CLA B 829

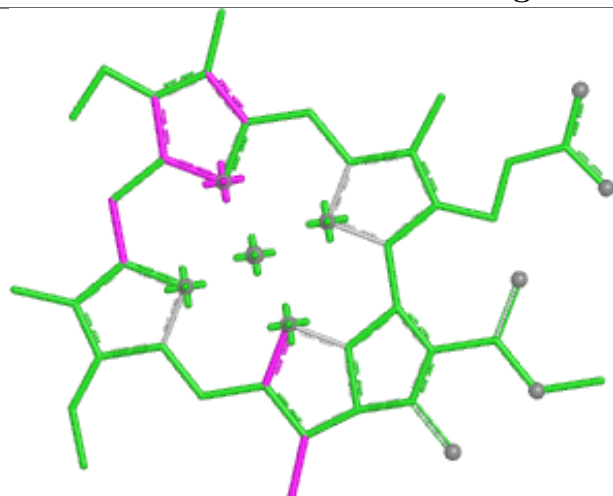


## Ligand LMU A 854

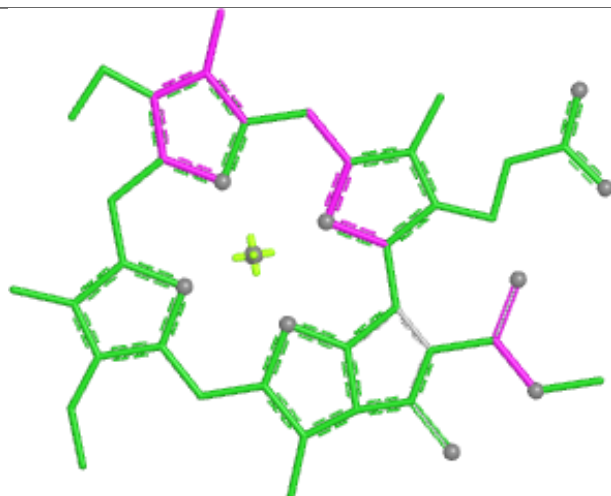




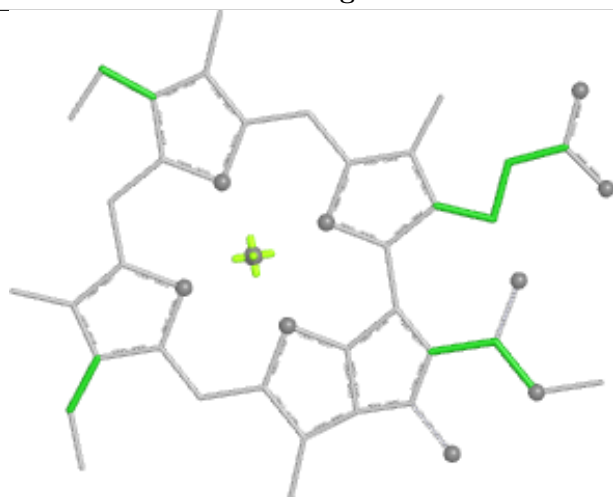
## Ligand CLA G 604



Bond lengths



Bond angles

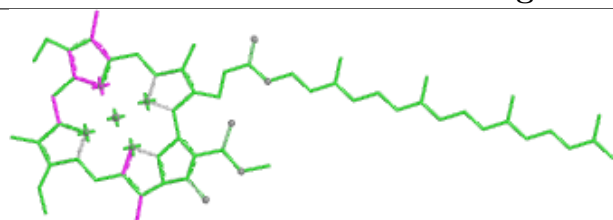


Torsions

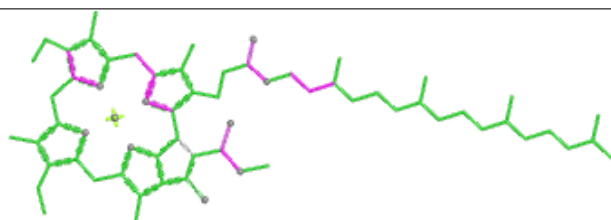


Rings

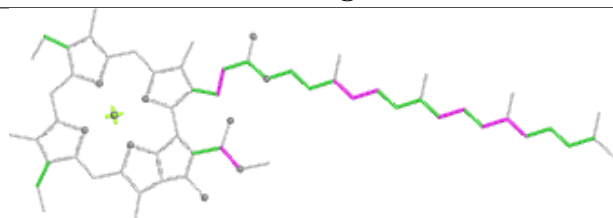
## Ligand CLA L 411



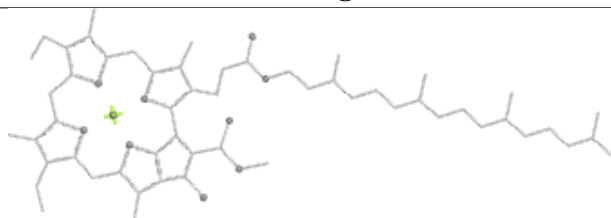
Bond lengths



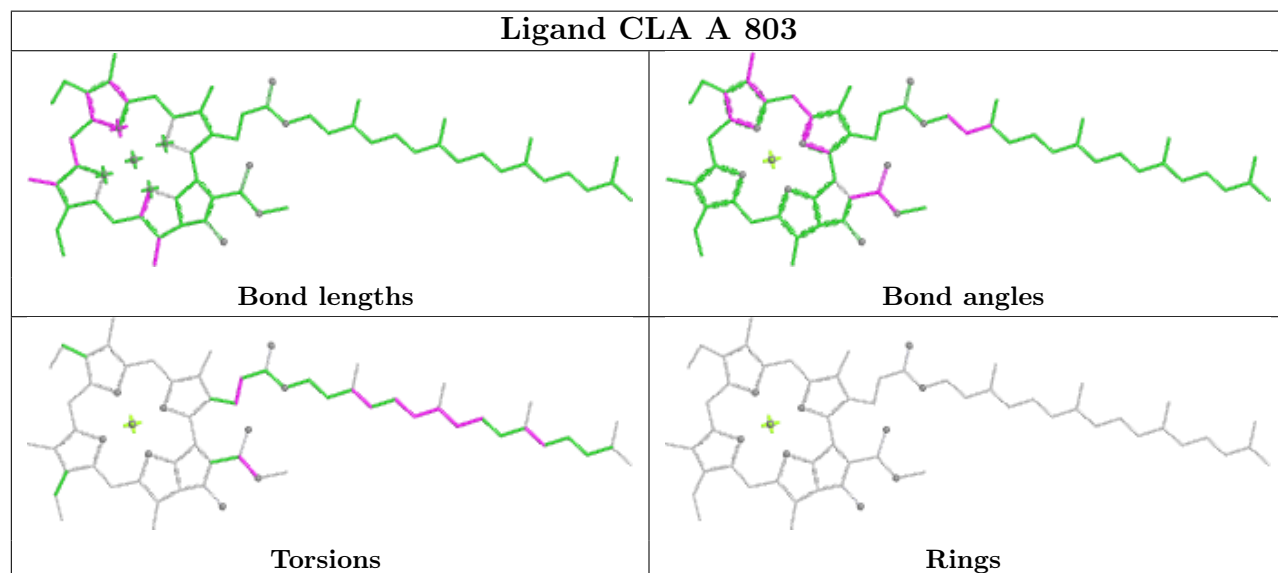
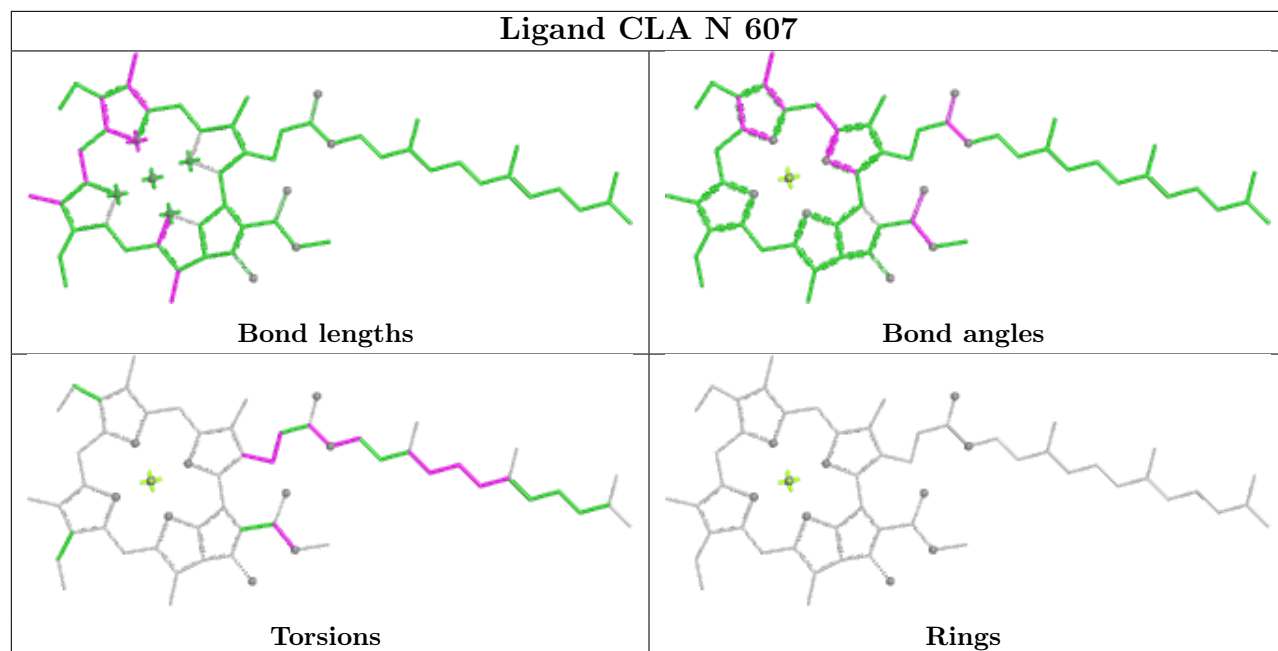
Bond angles



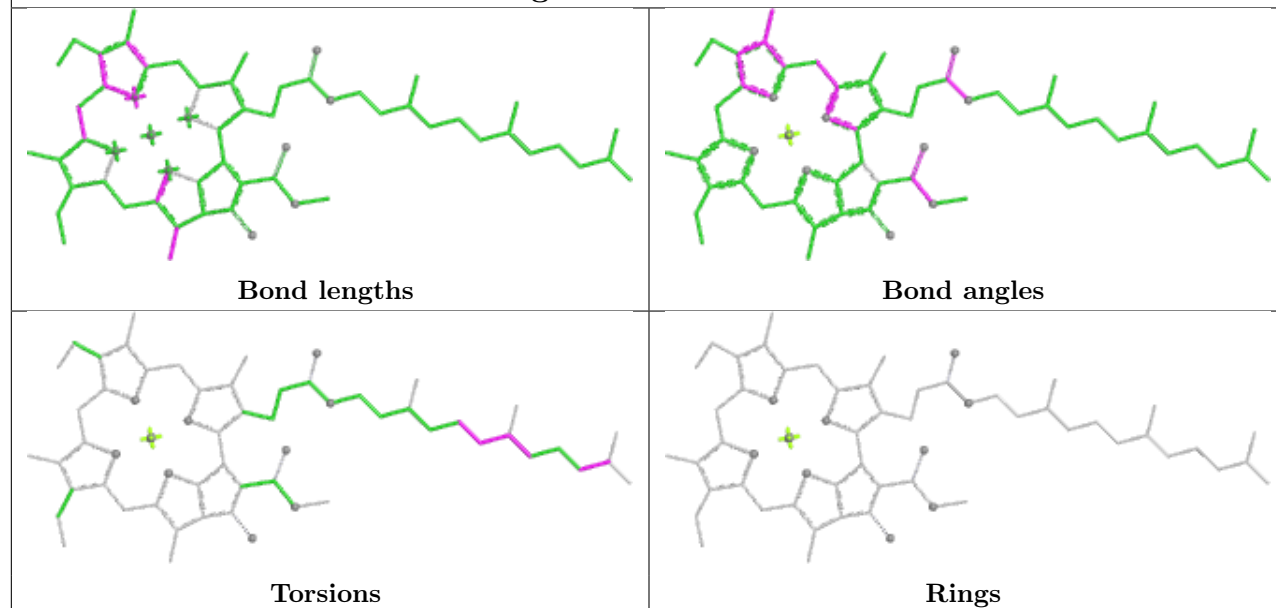
Torsions



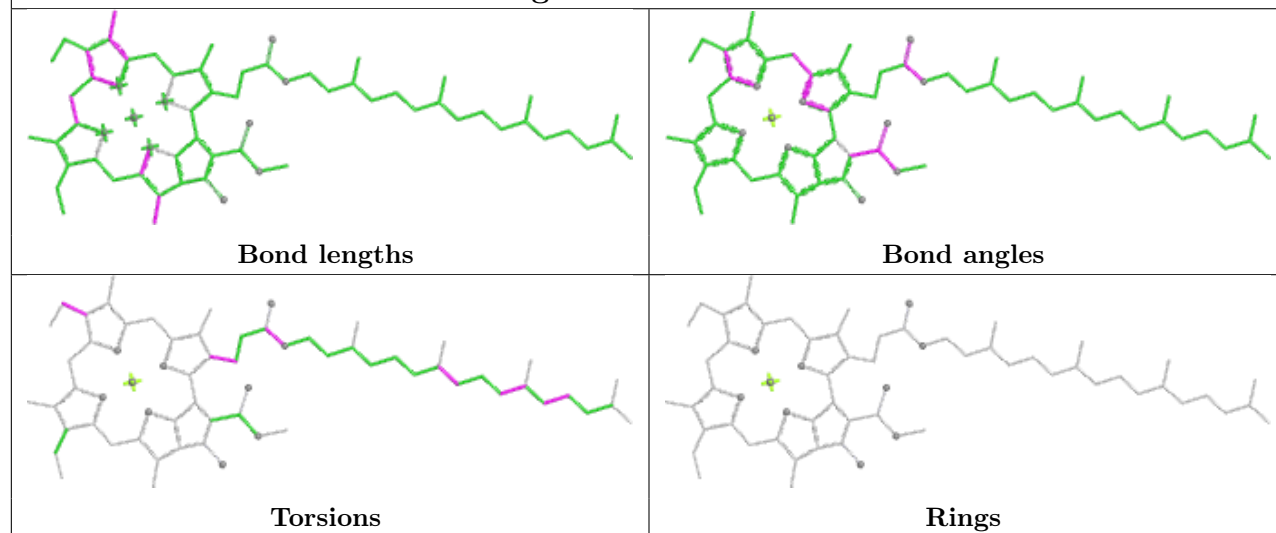
Rings

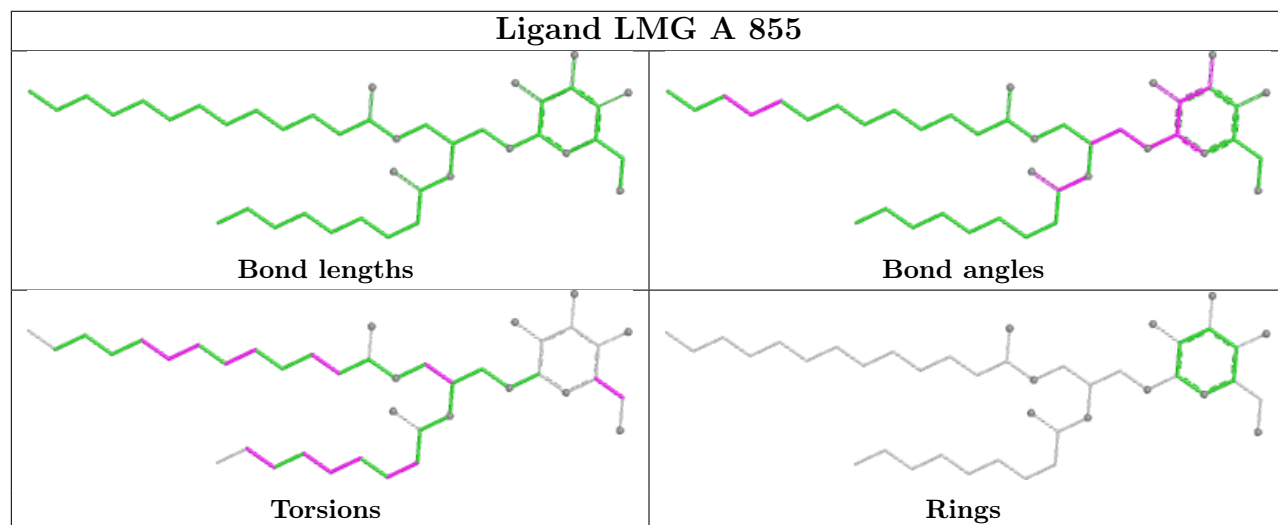
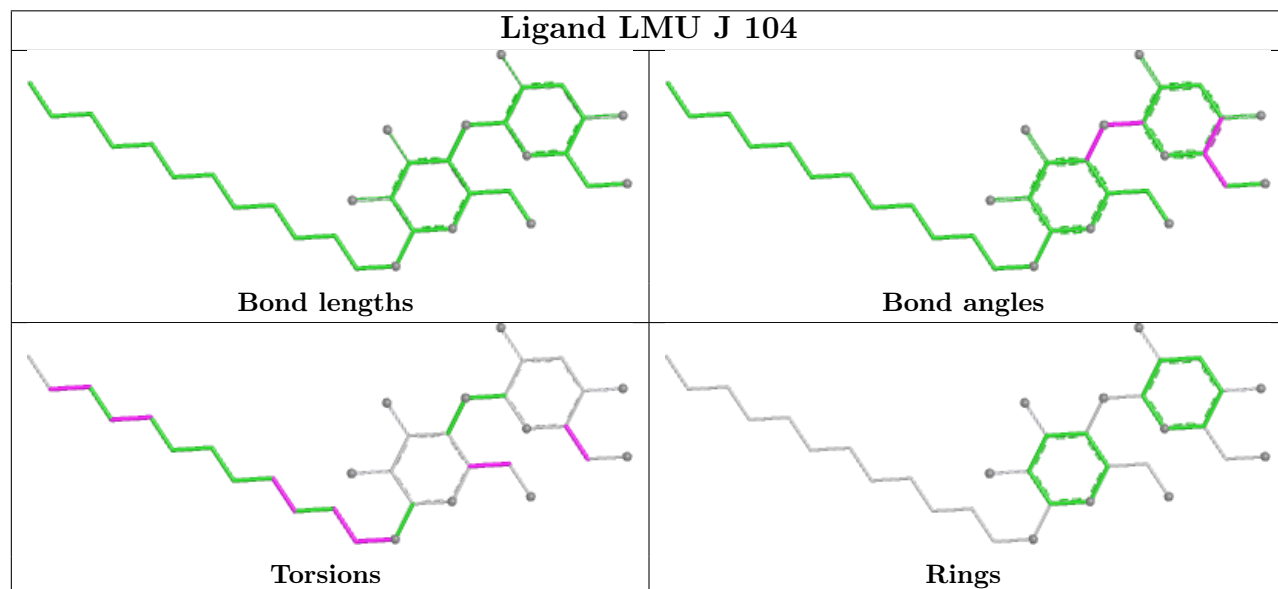
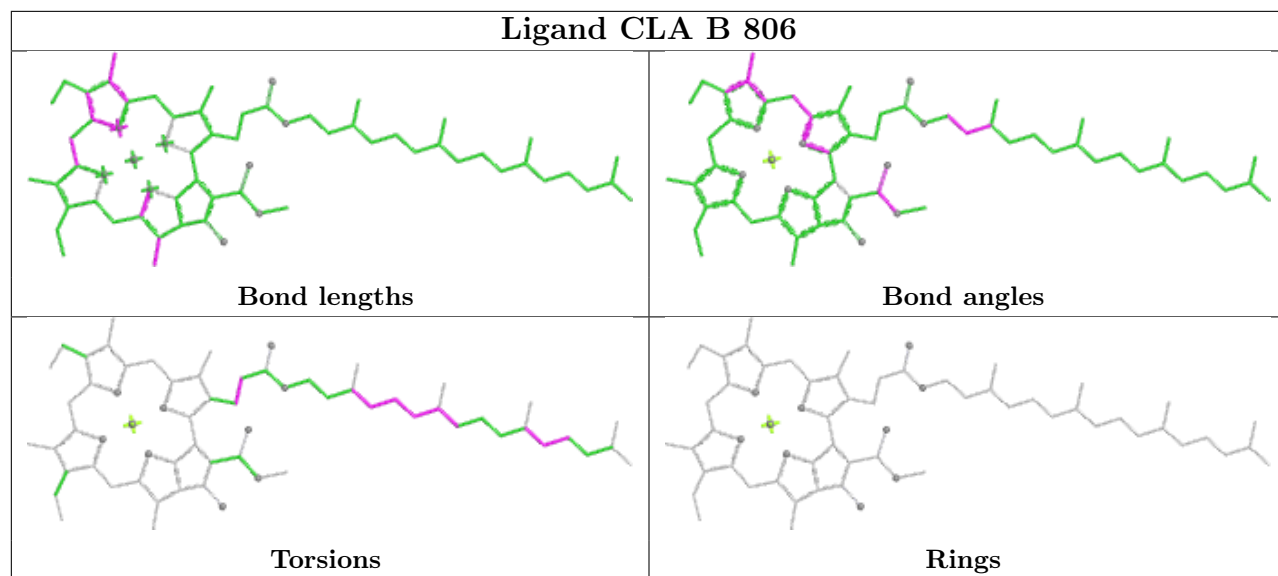


## Ligand CLA H 308

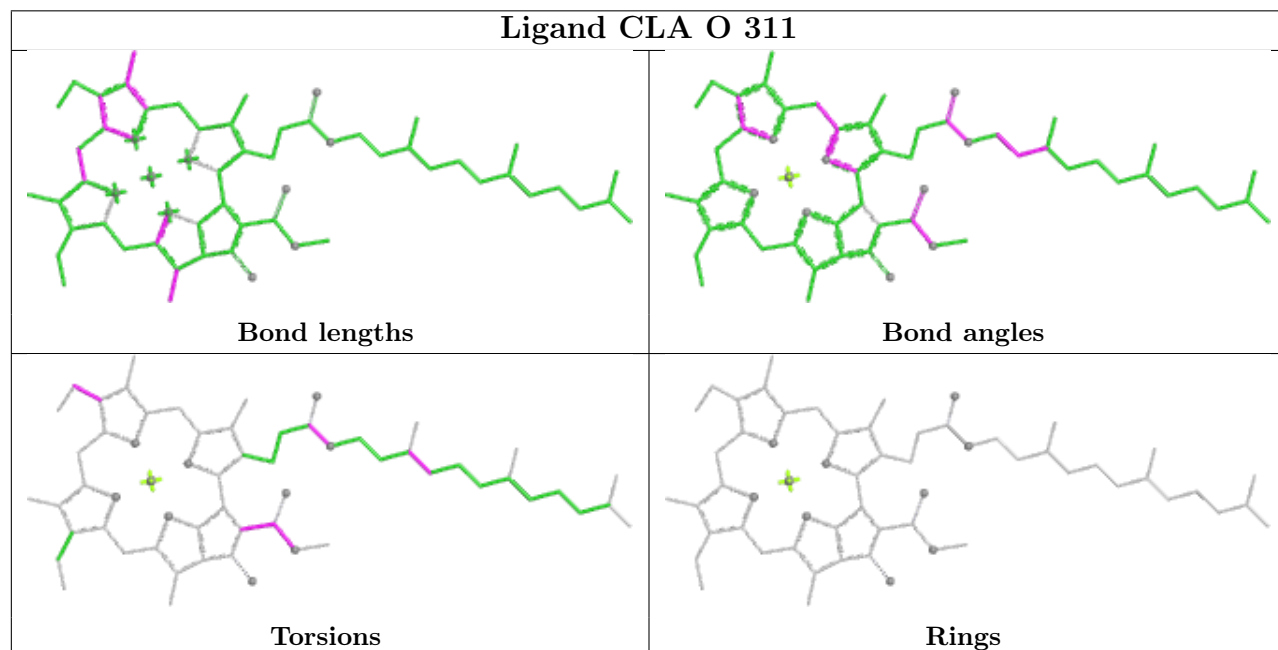
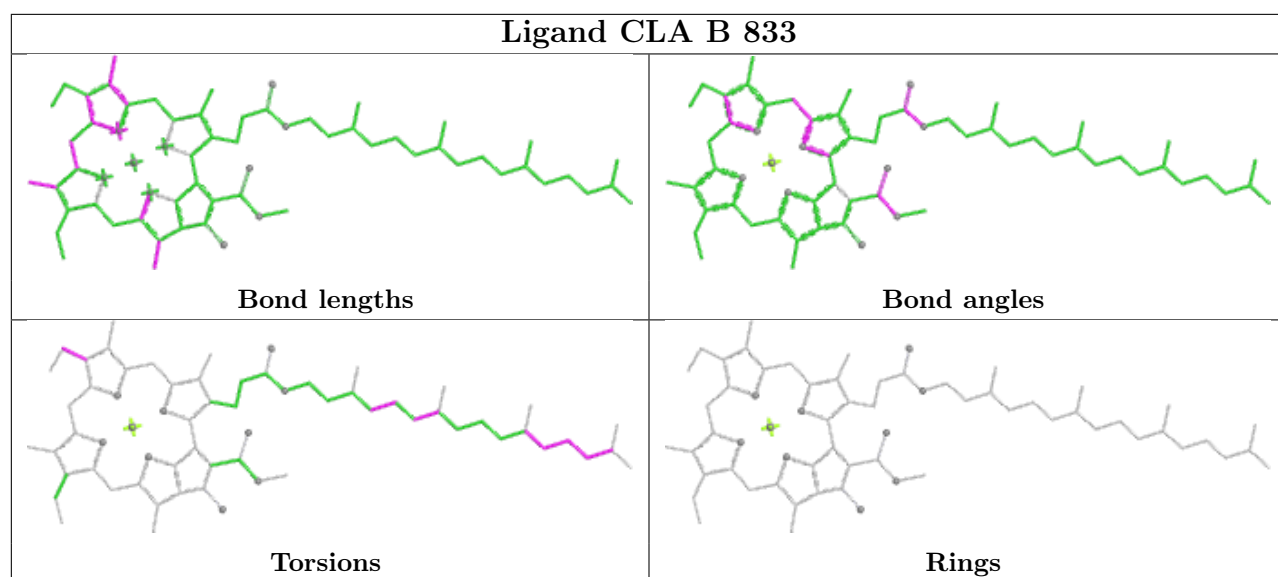


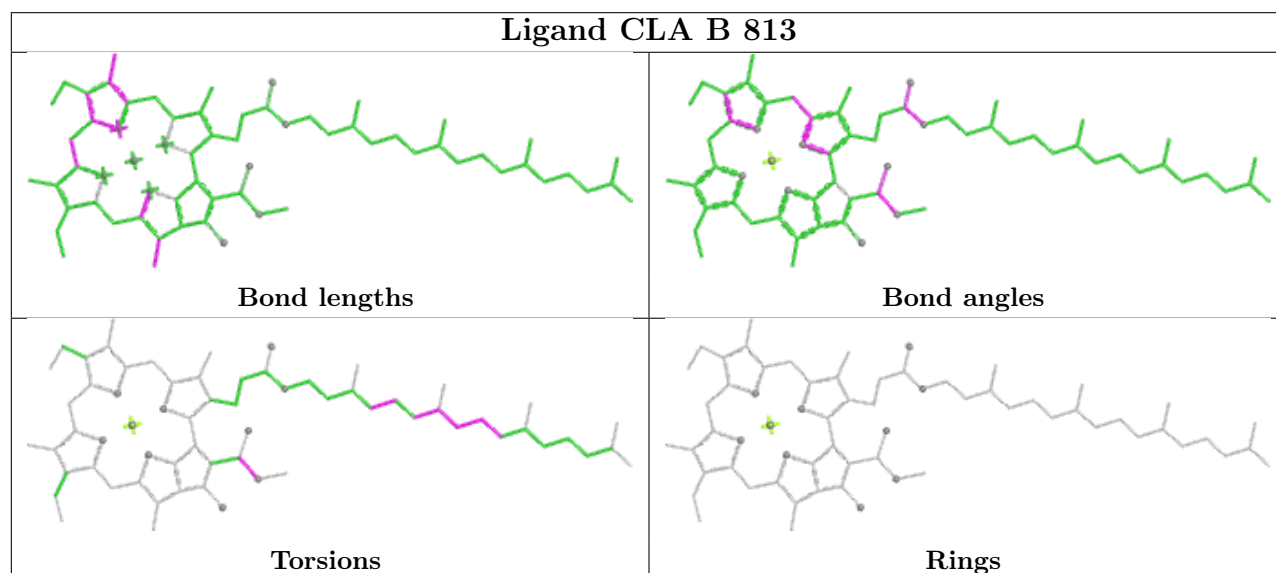
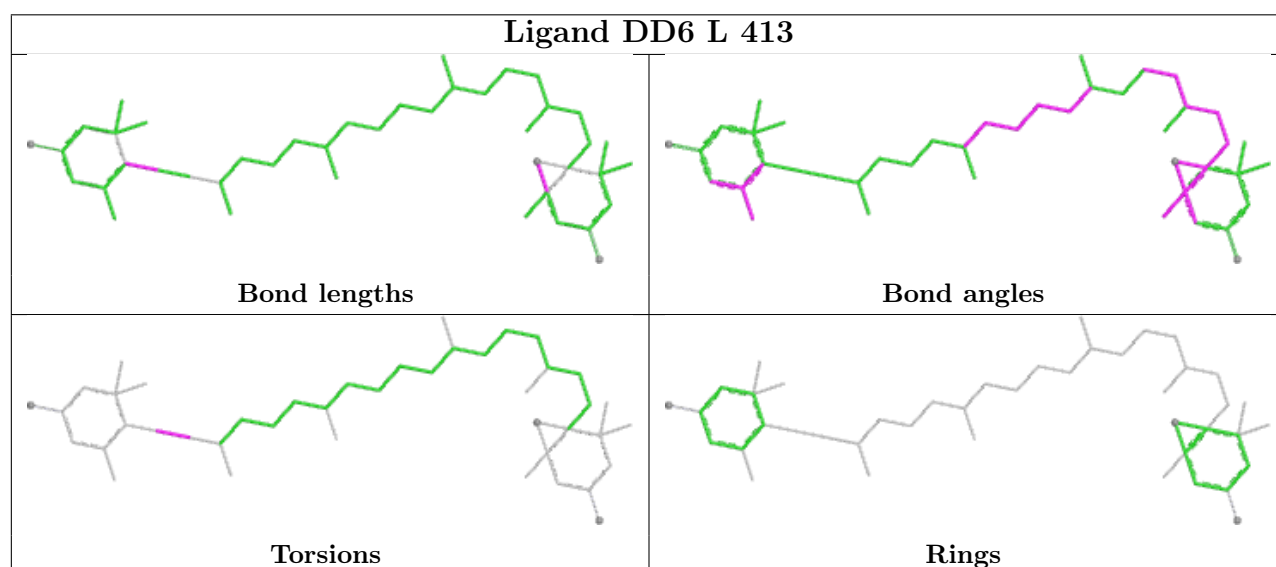
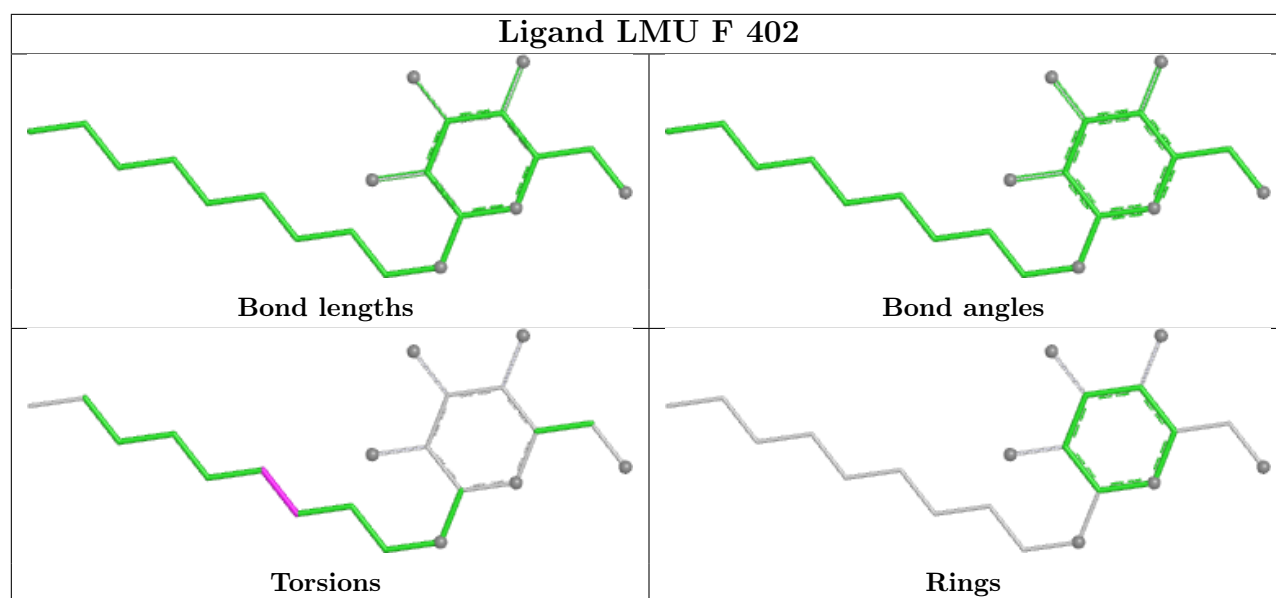
## Ligand CLA A 813

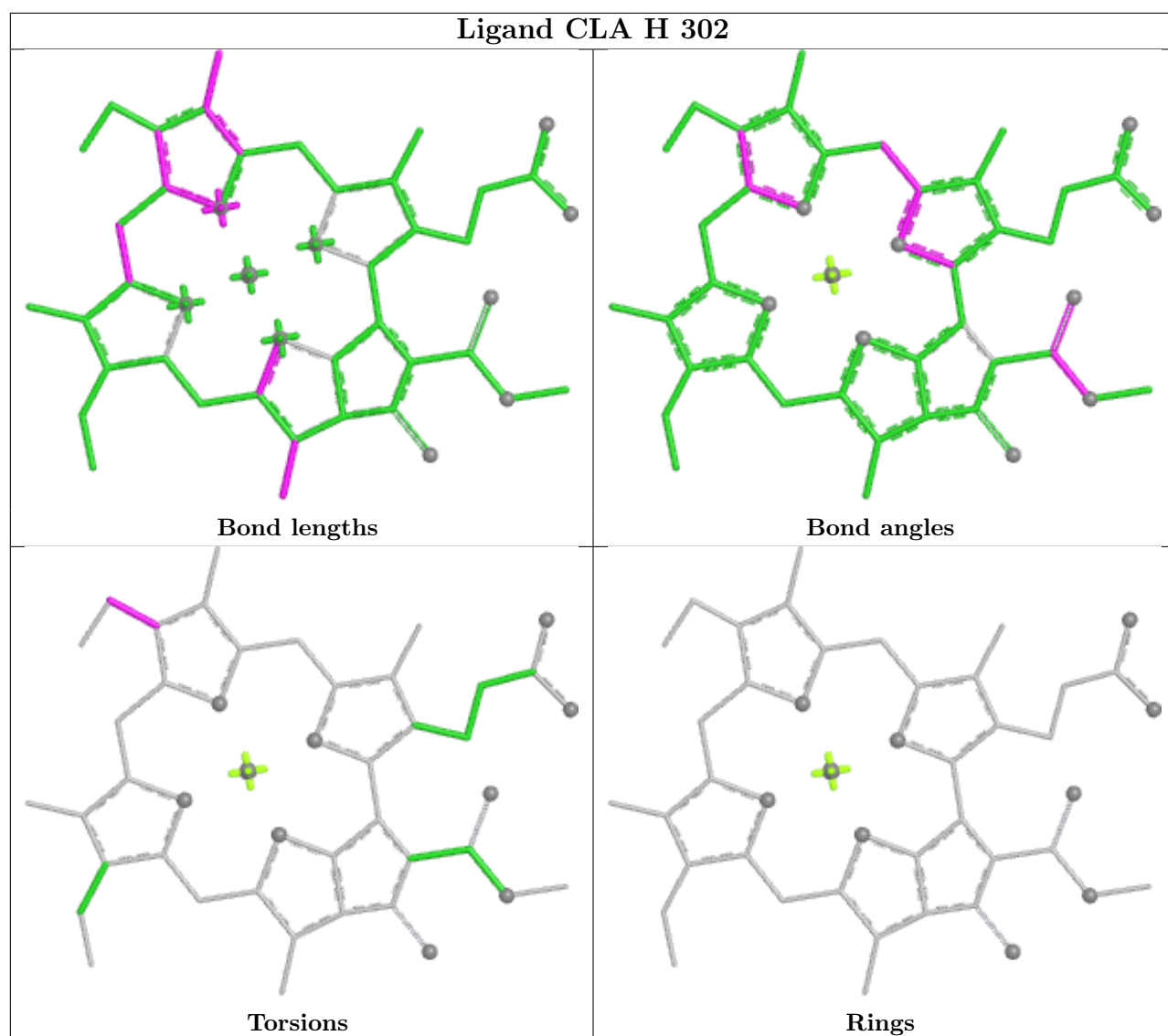




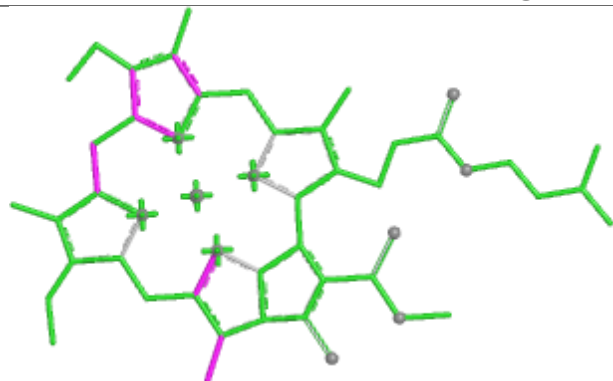




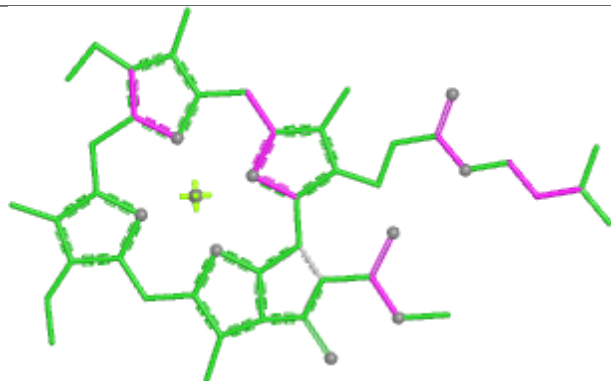




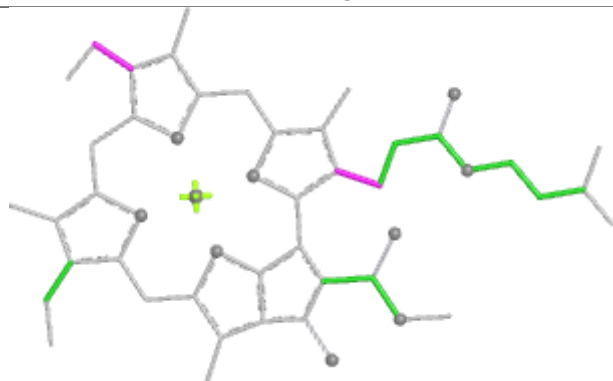
## Ligand CLA S 606



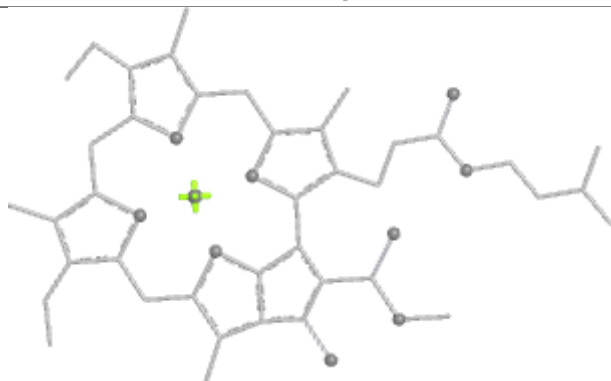
Bond lengths



Bond angles

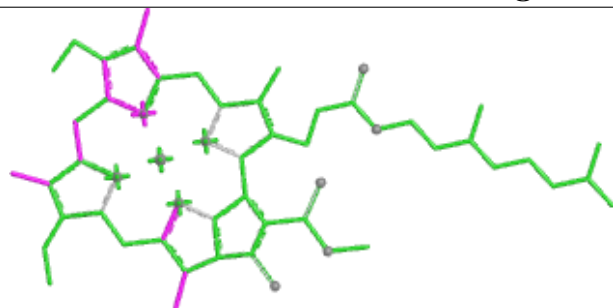


Torsions

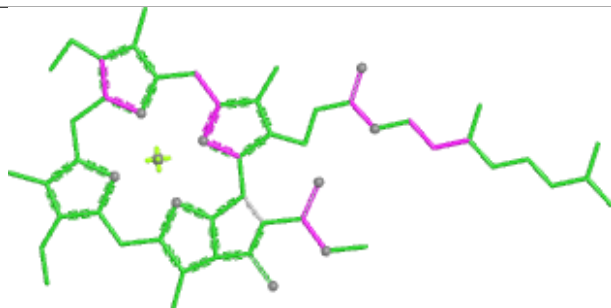


Rings

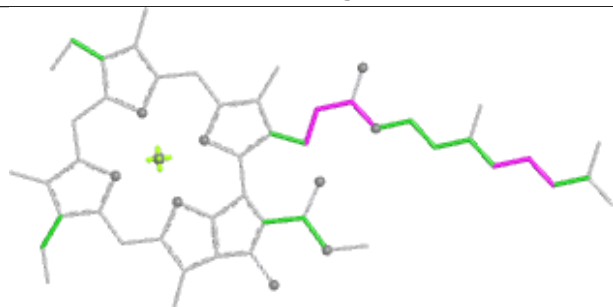
## Ligand CLA B 808



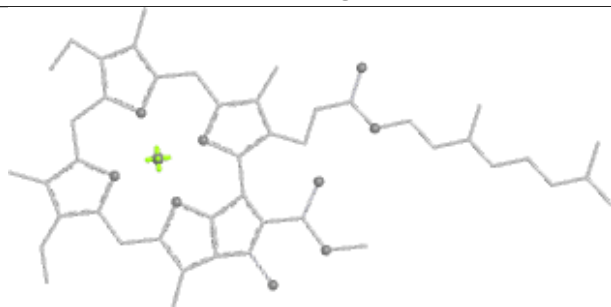
Bond lengths



Bond angles

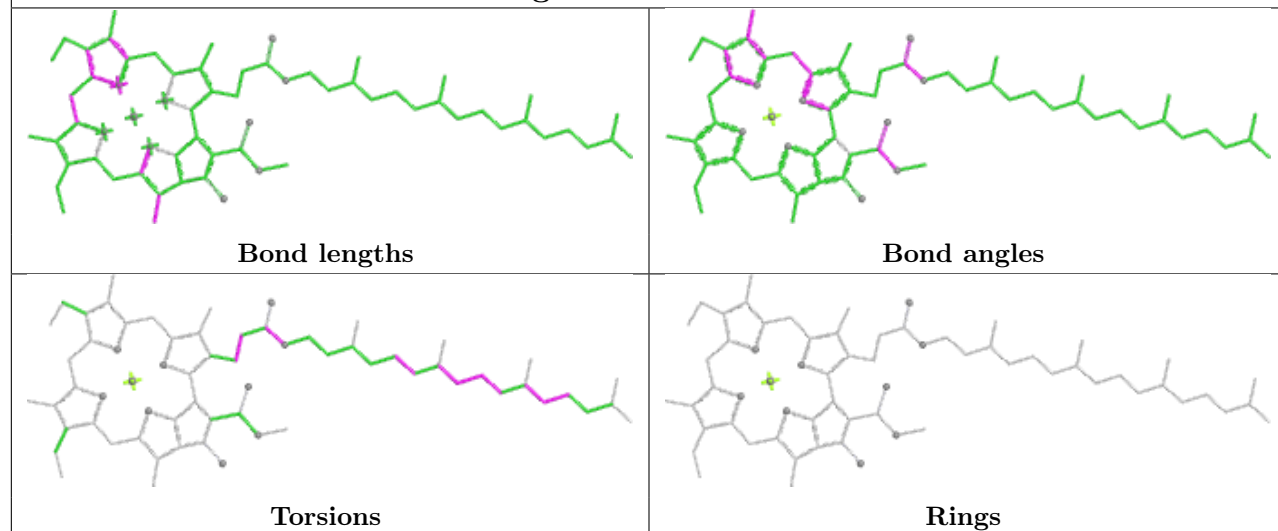


Torsions

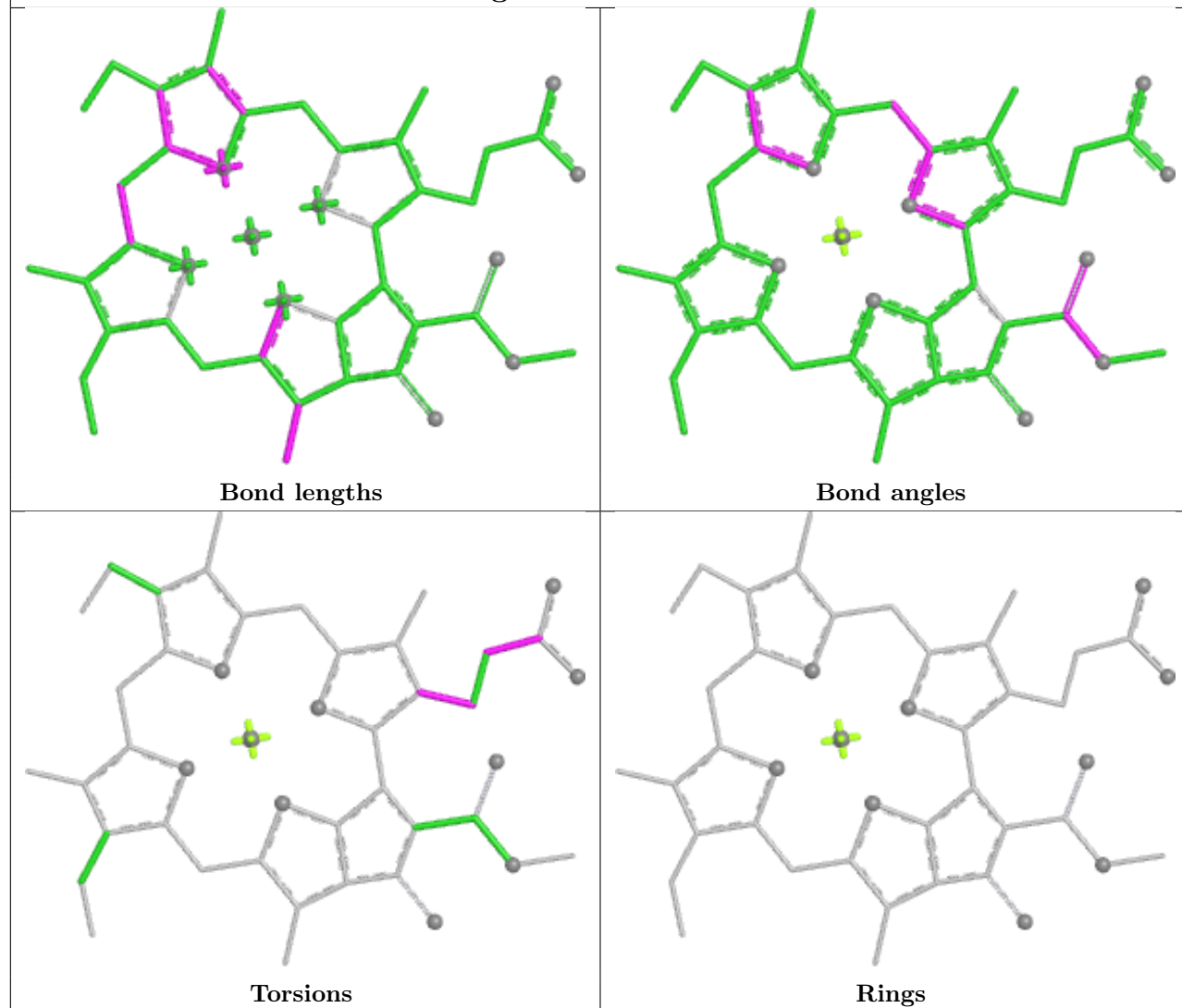


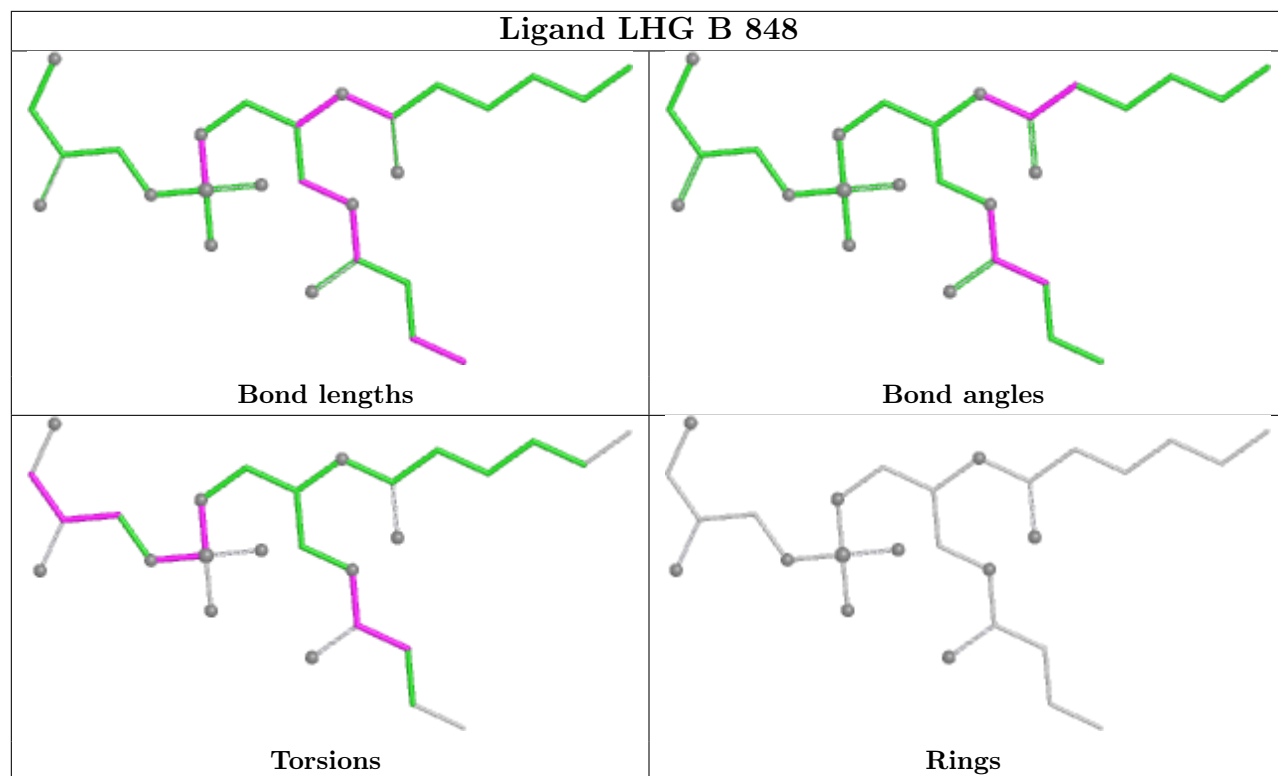
Rings

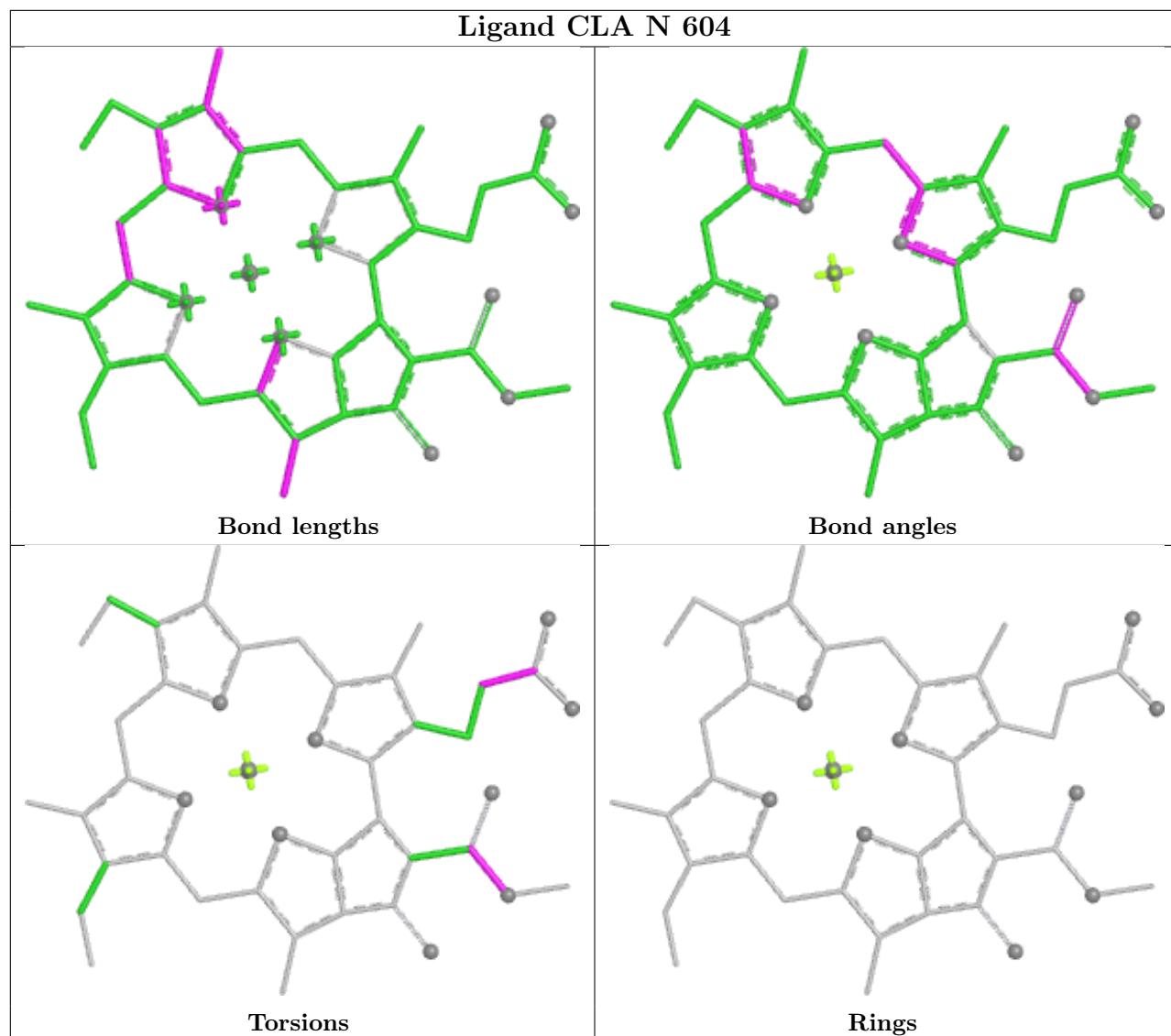
## Ligand CLA B 835



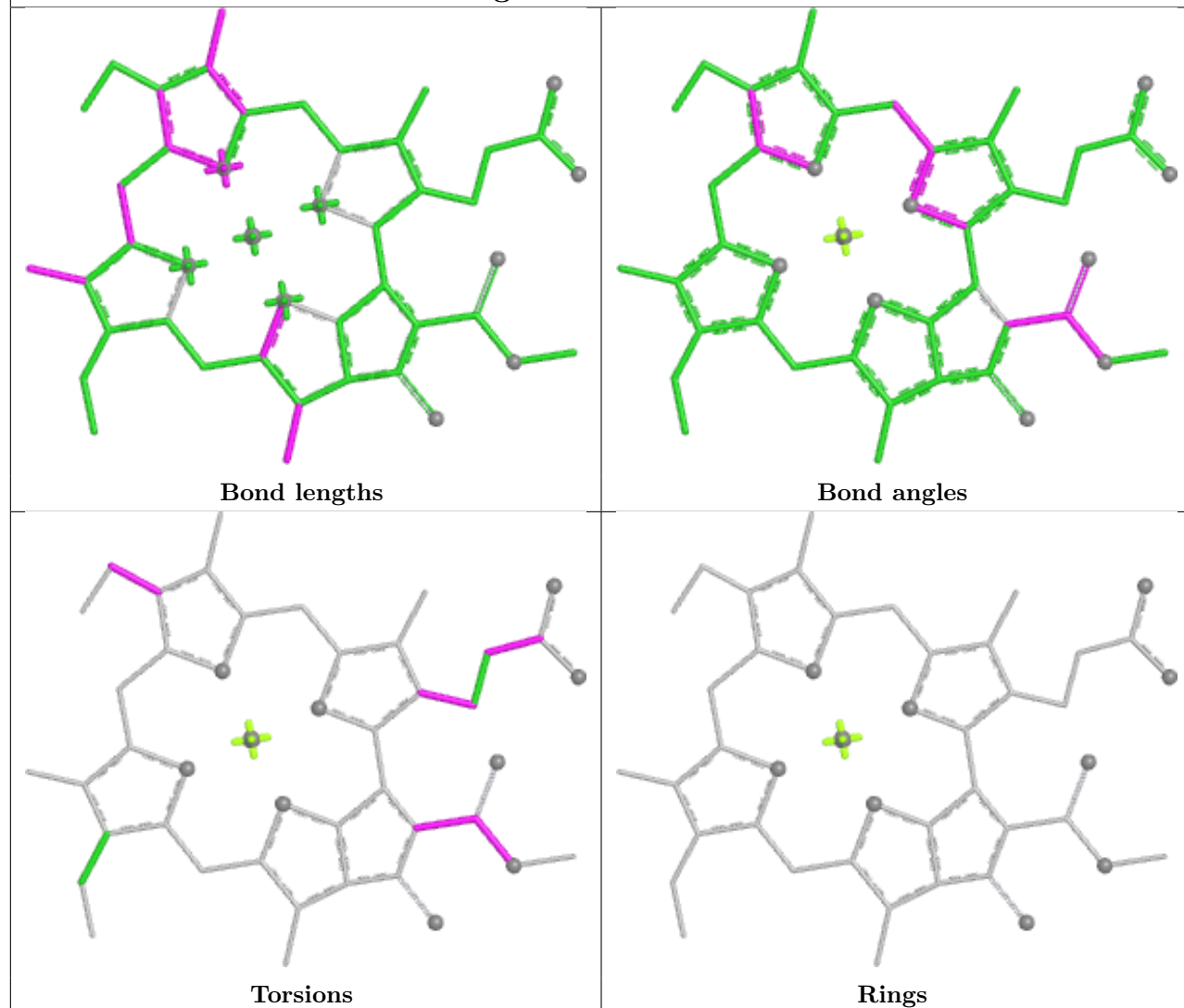
## Ligand CLA H 312



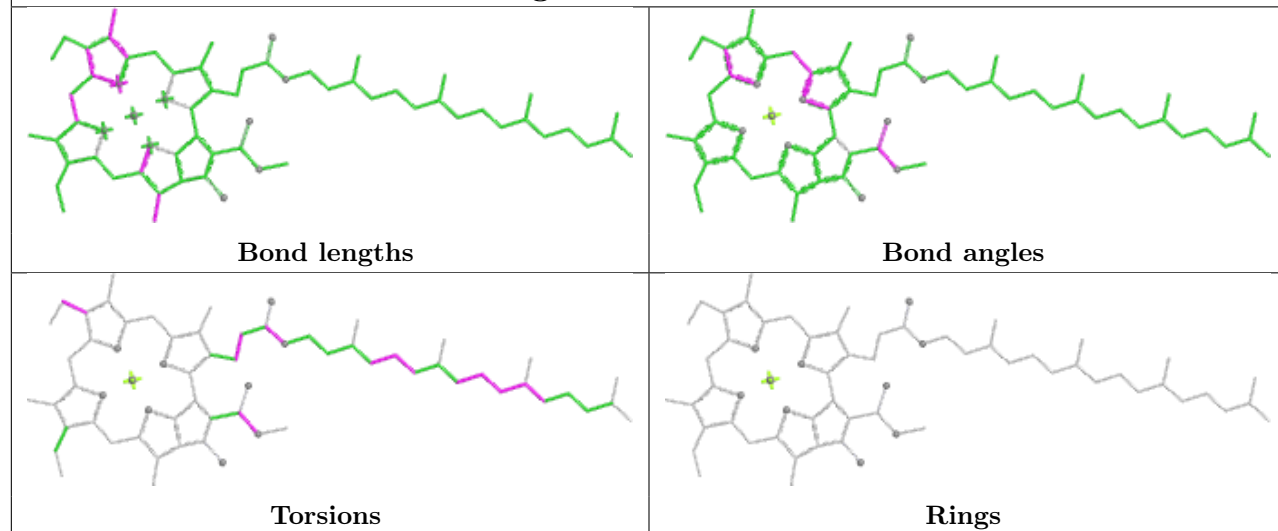




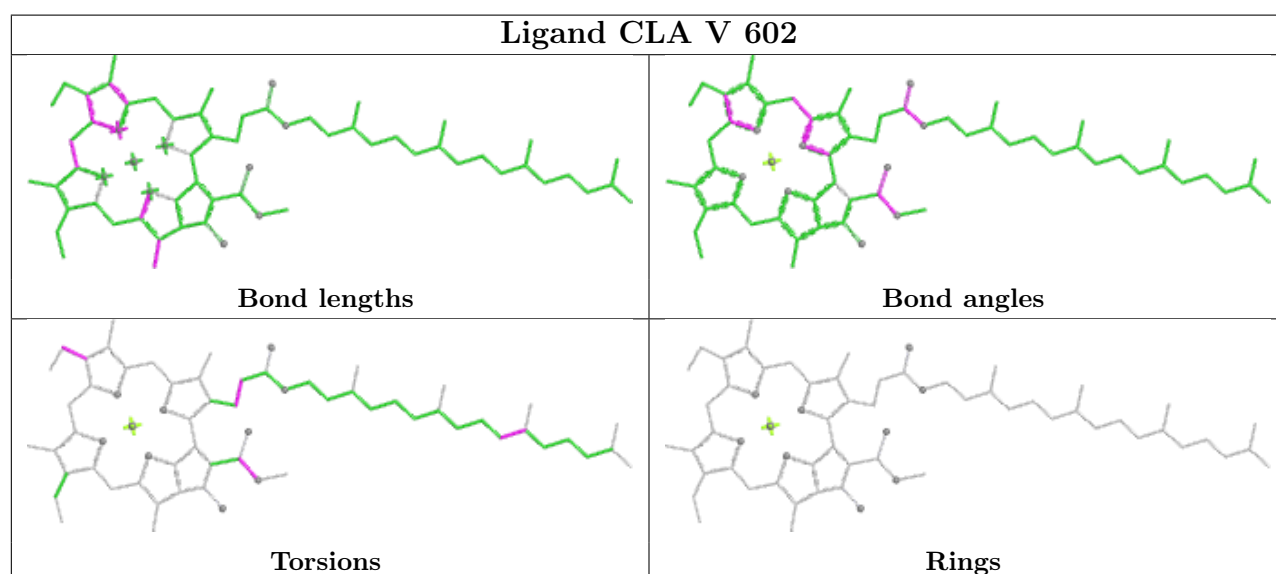
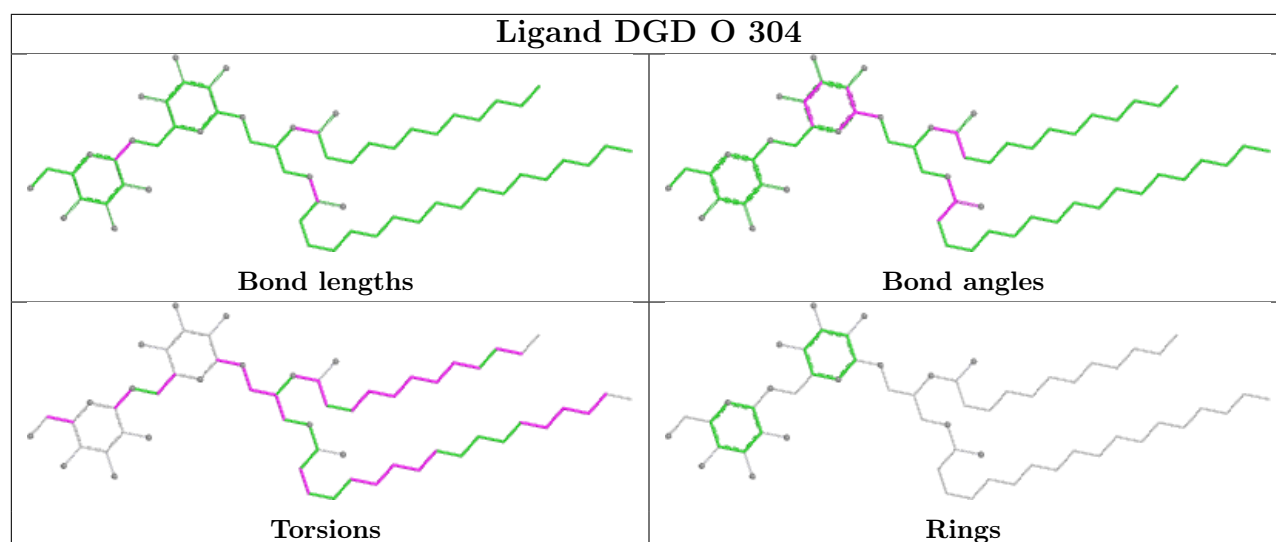
## Ligand CLA P 608



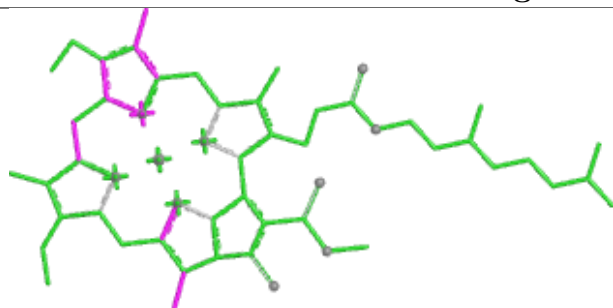
## Ligand CLA V 612



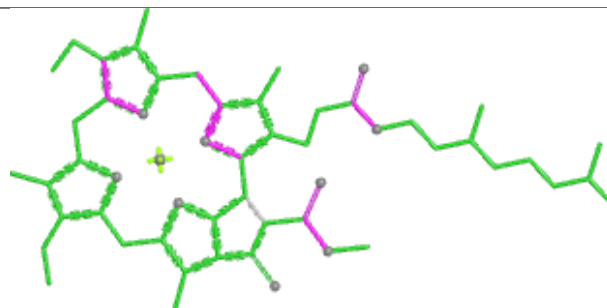




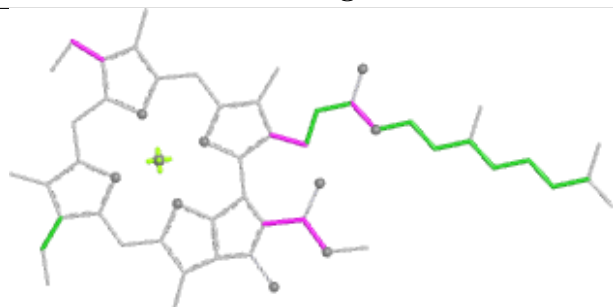
## Ligand CLA V 608



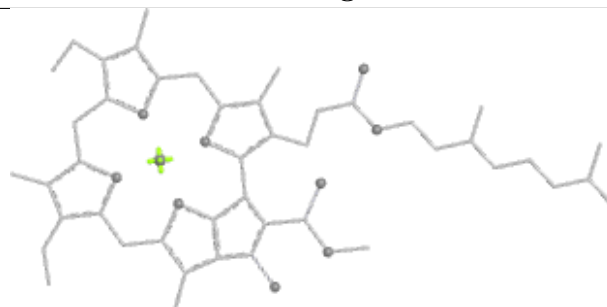
Bond lengths



Bond angles

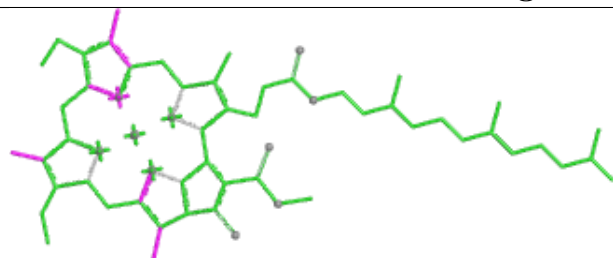


Torsions

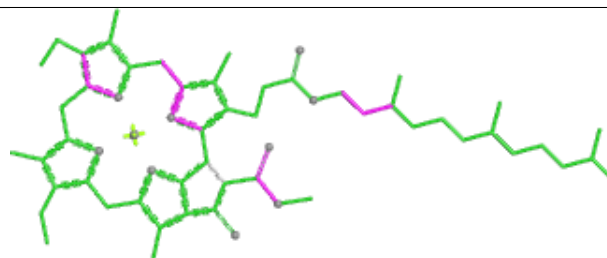


Rings

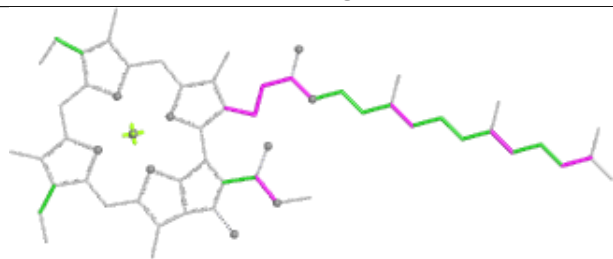
## Ligand CLA S 605



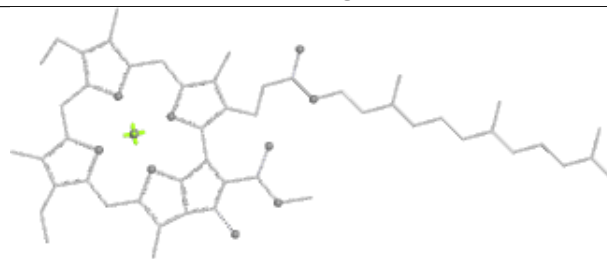
Bond lengths



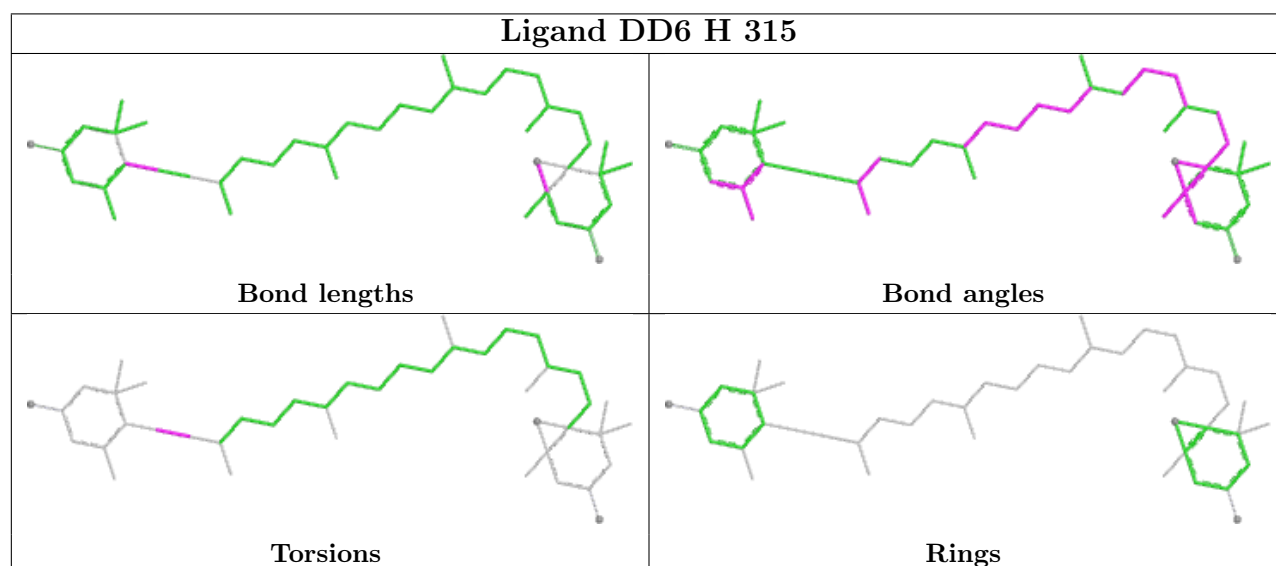
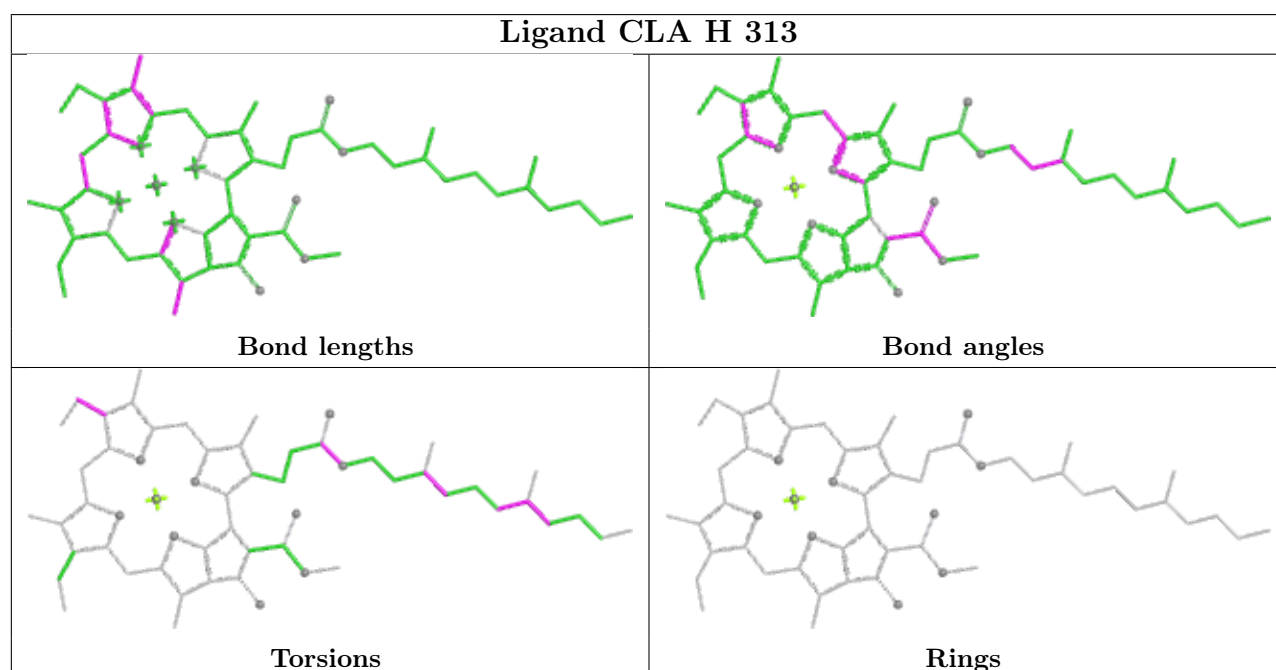
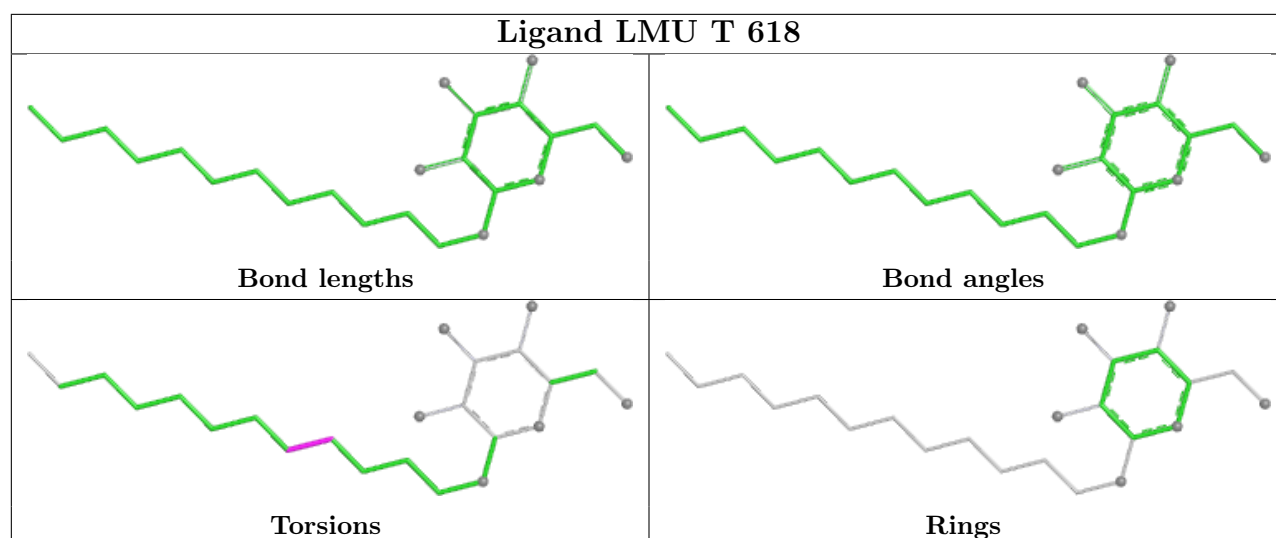
Bond angles

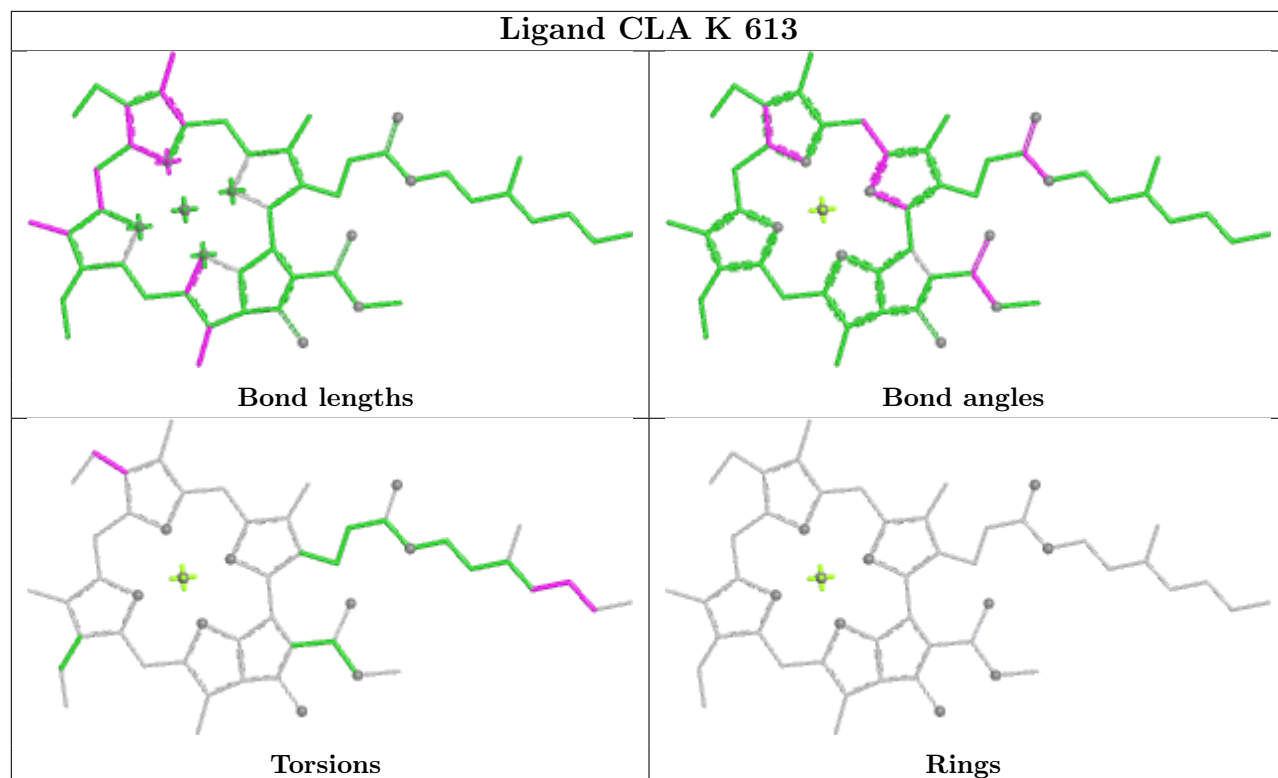


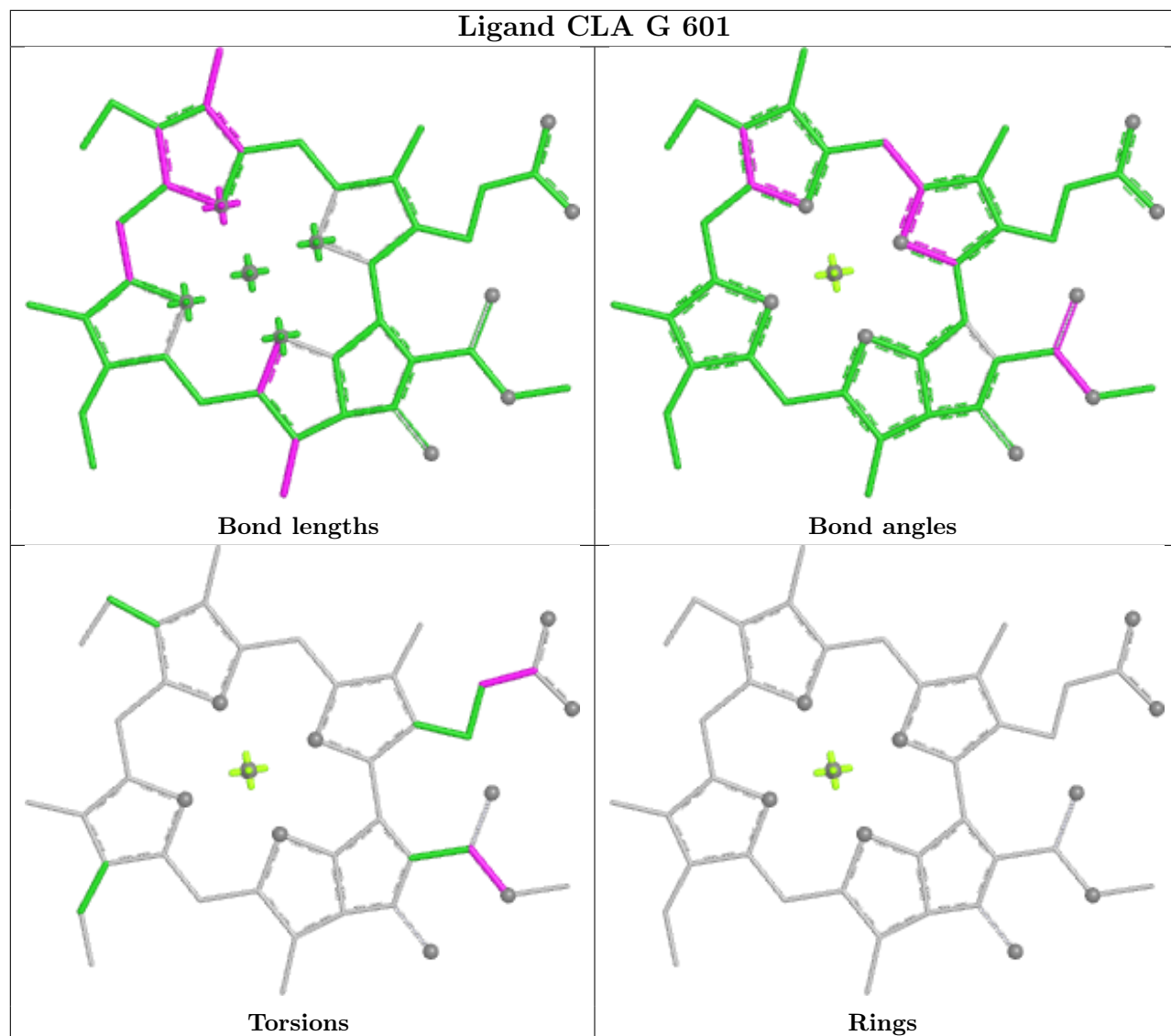
Torsions

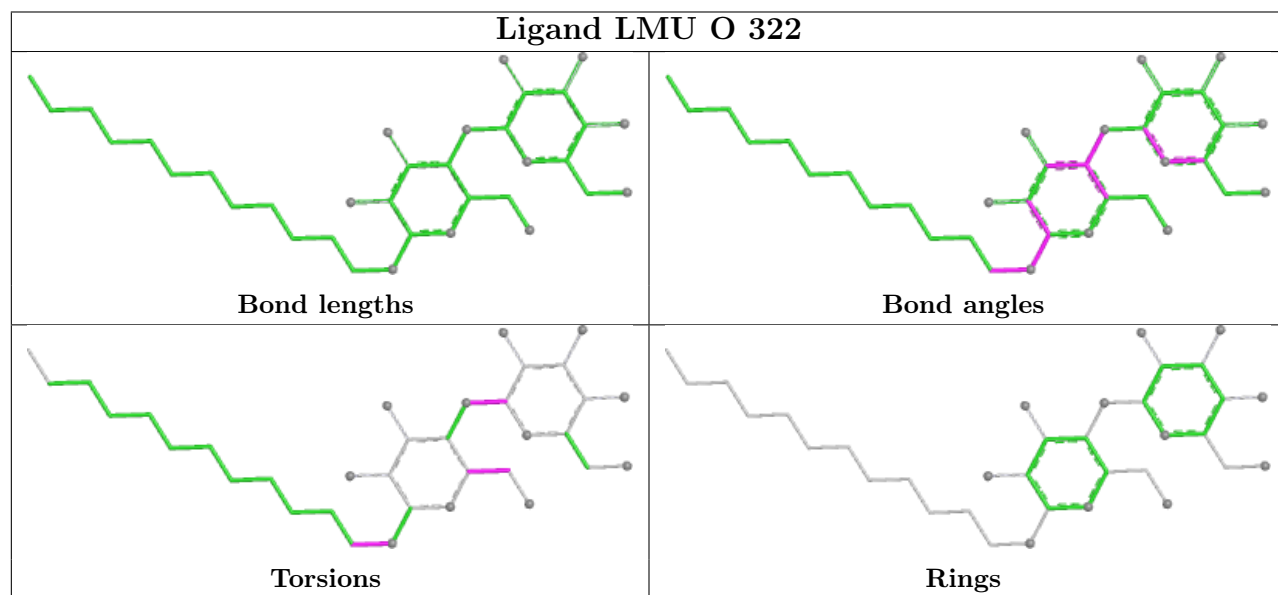
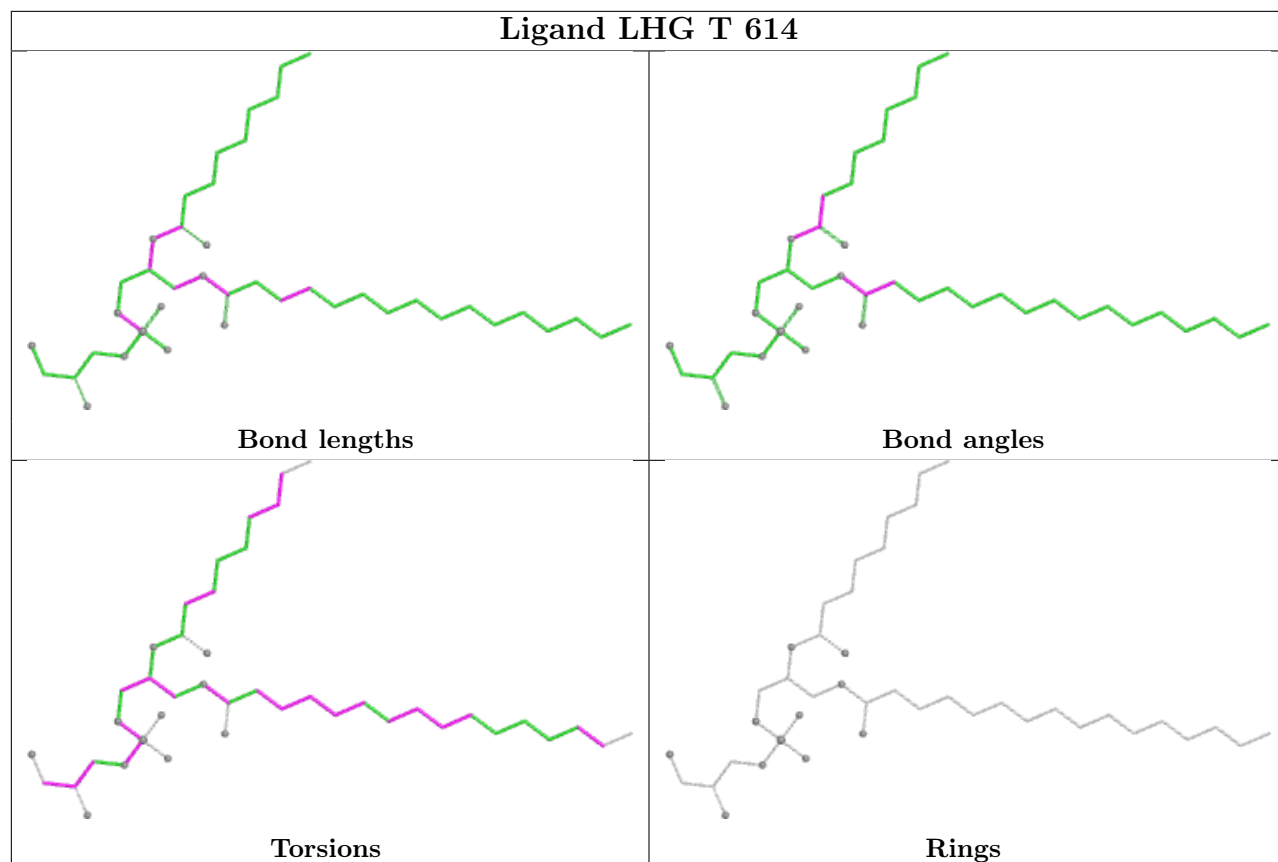


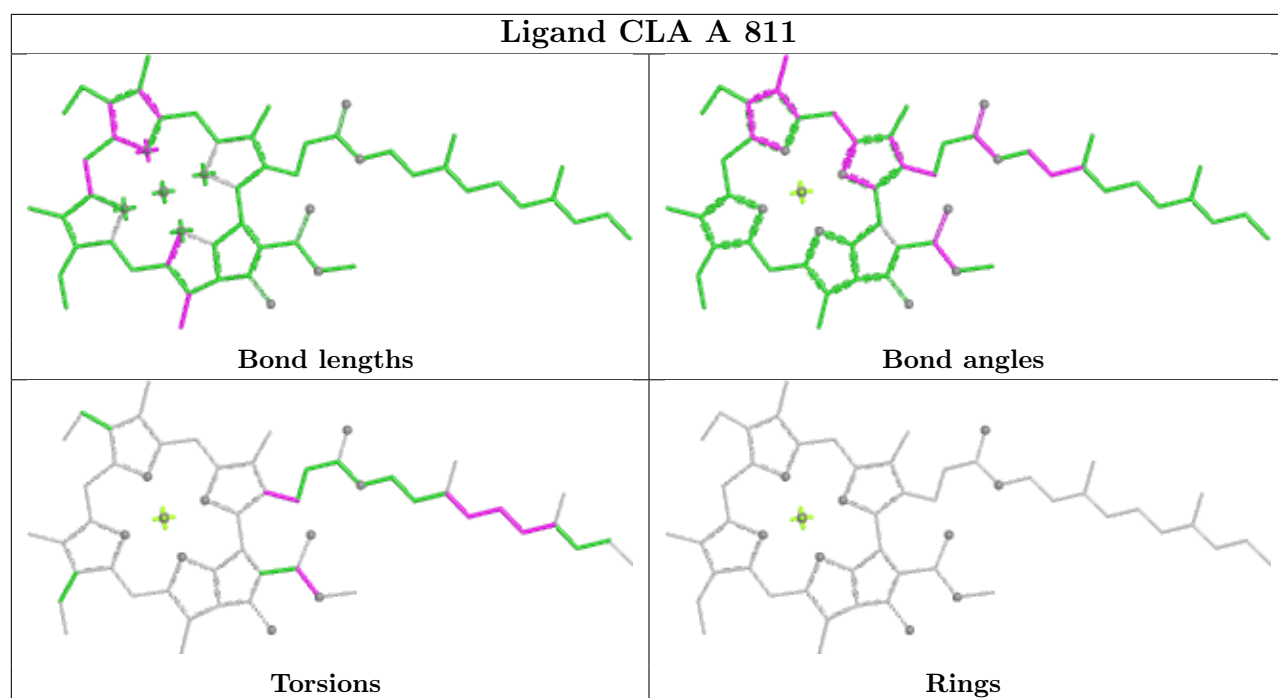
Rings



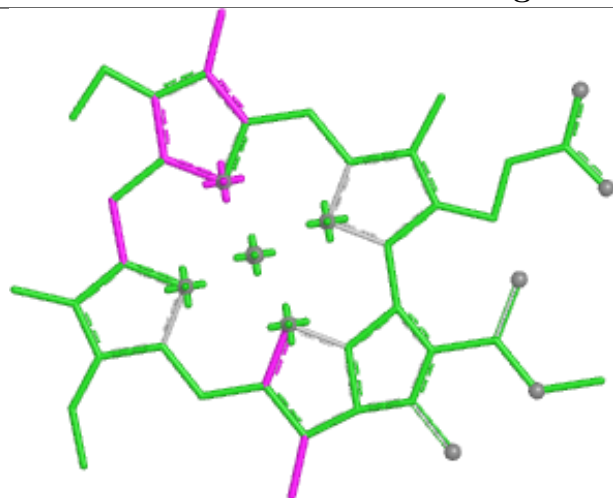




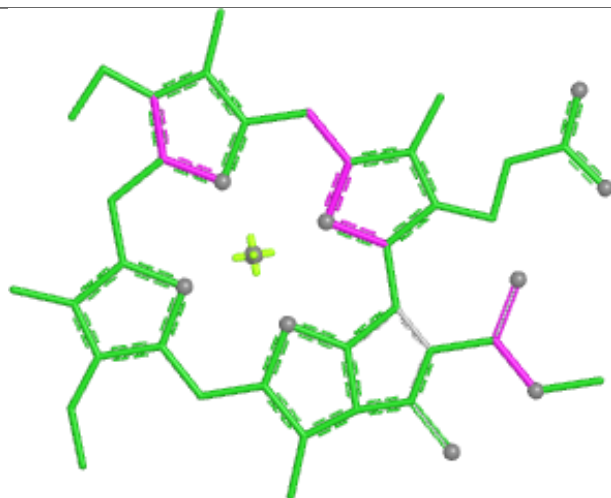




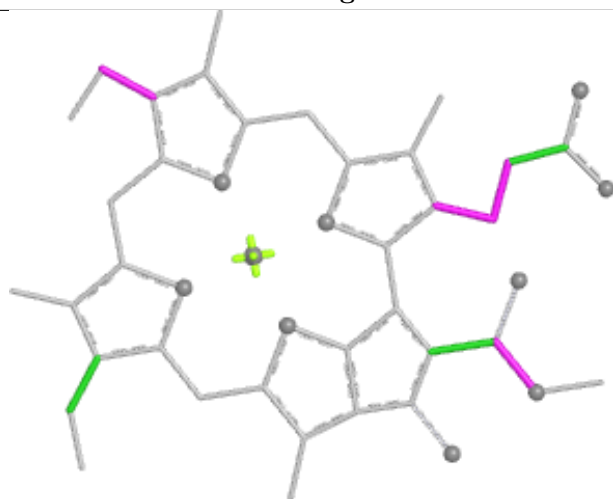
## Ligand CLA U 415



Bond lengths



Bond angles

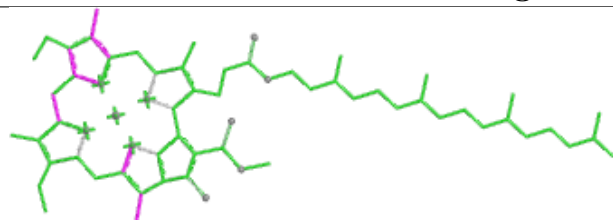


Torsions

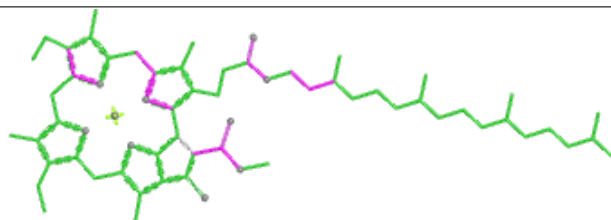


Rings

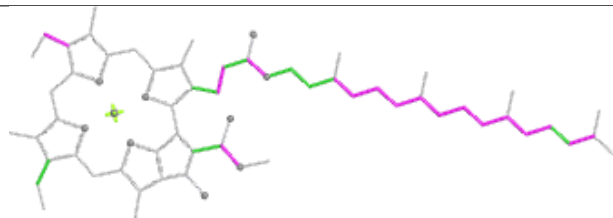
## Ligand CLA A 824



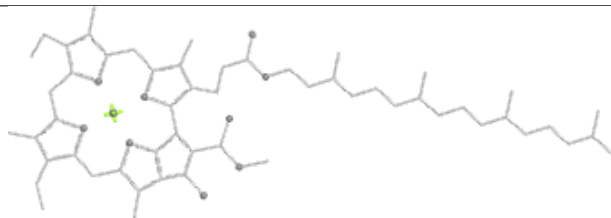
Bond lengths



Bond angles

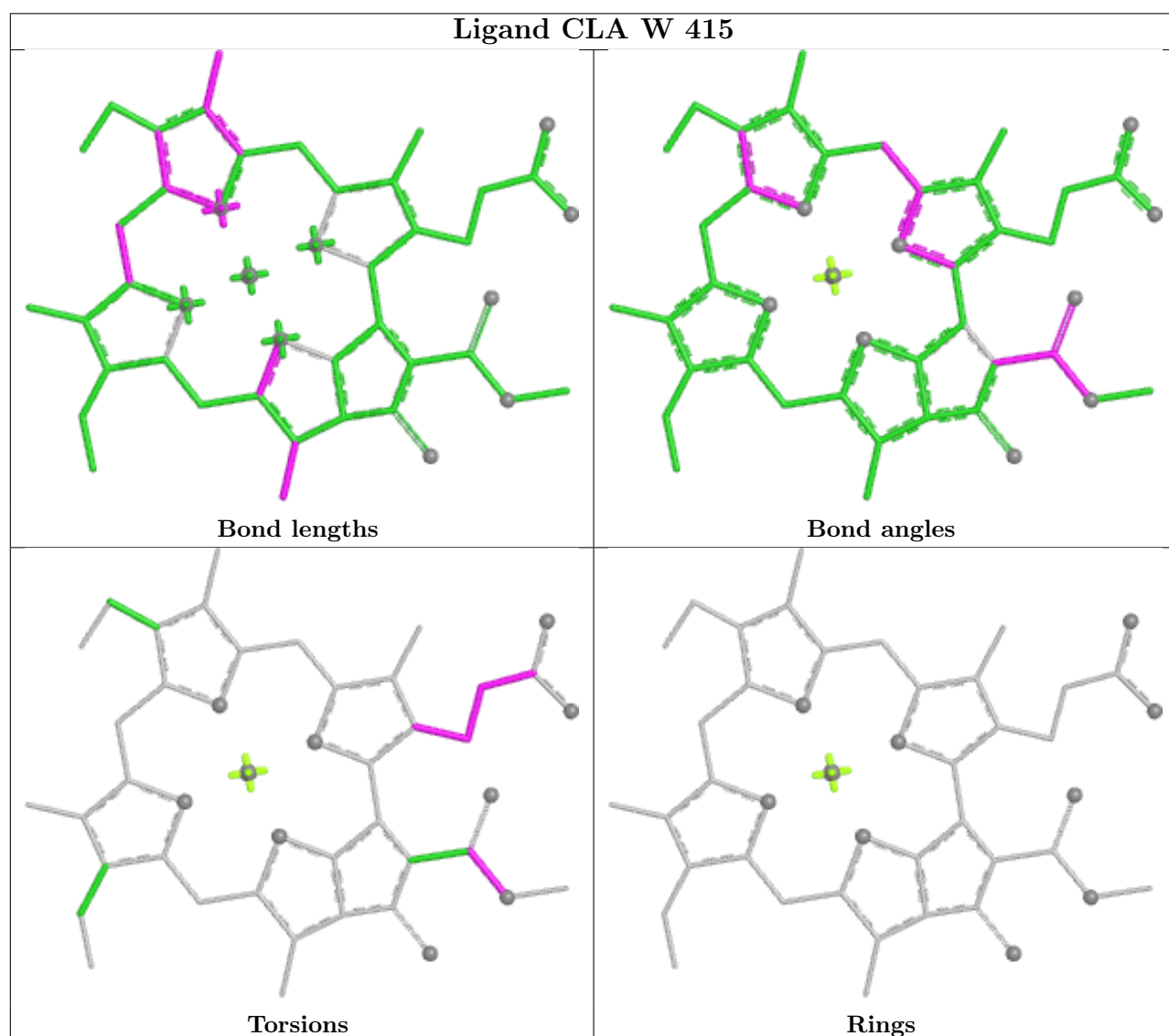
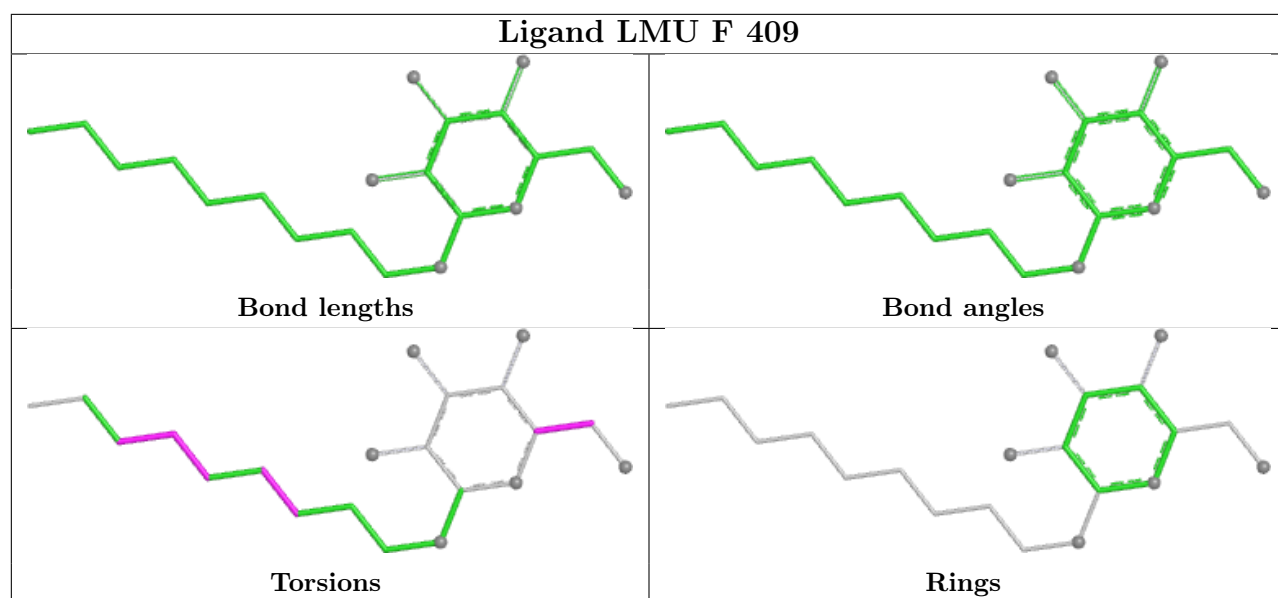


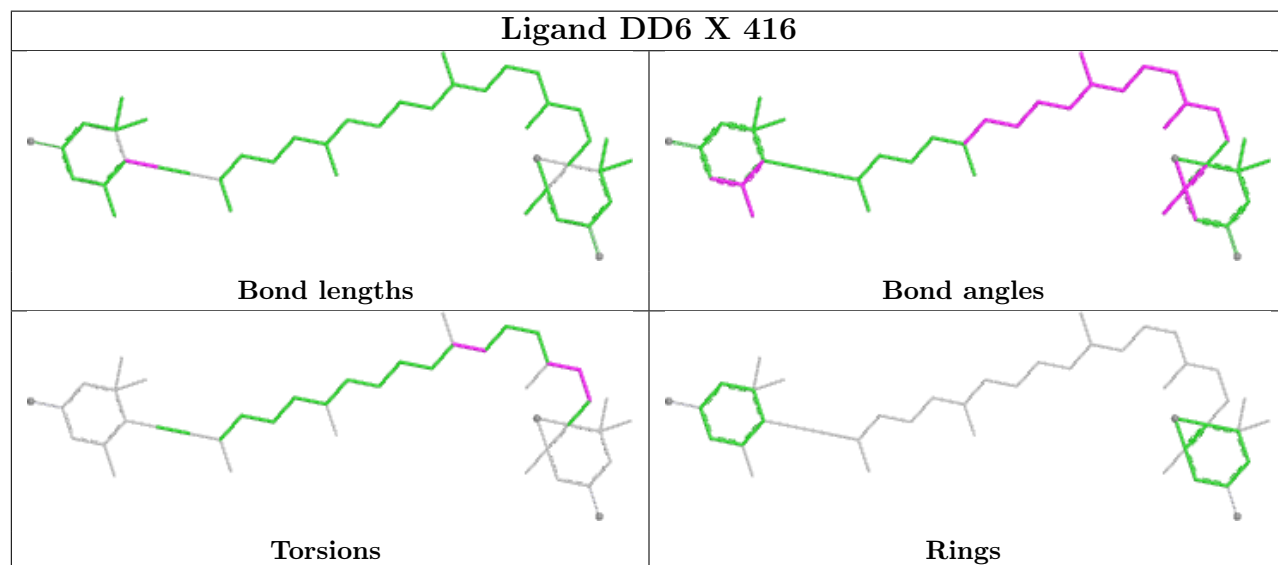
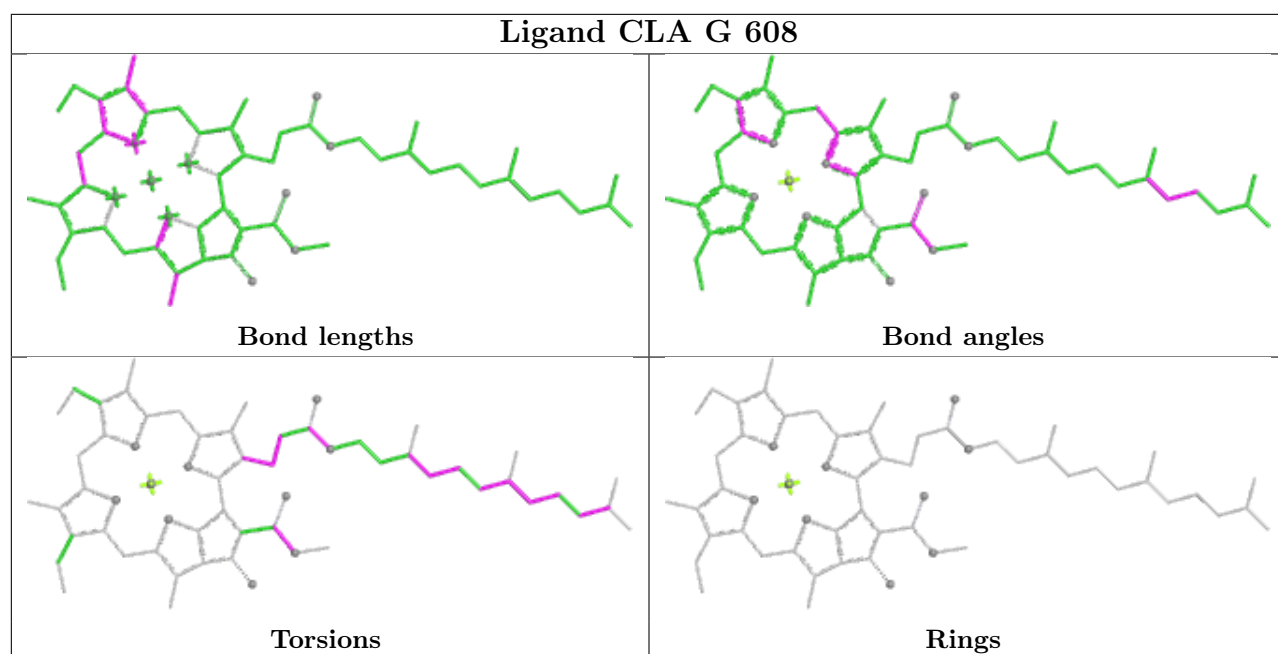
Torsions



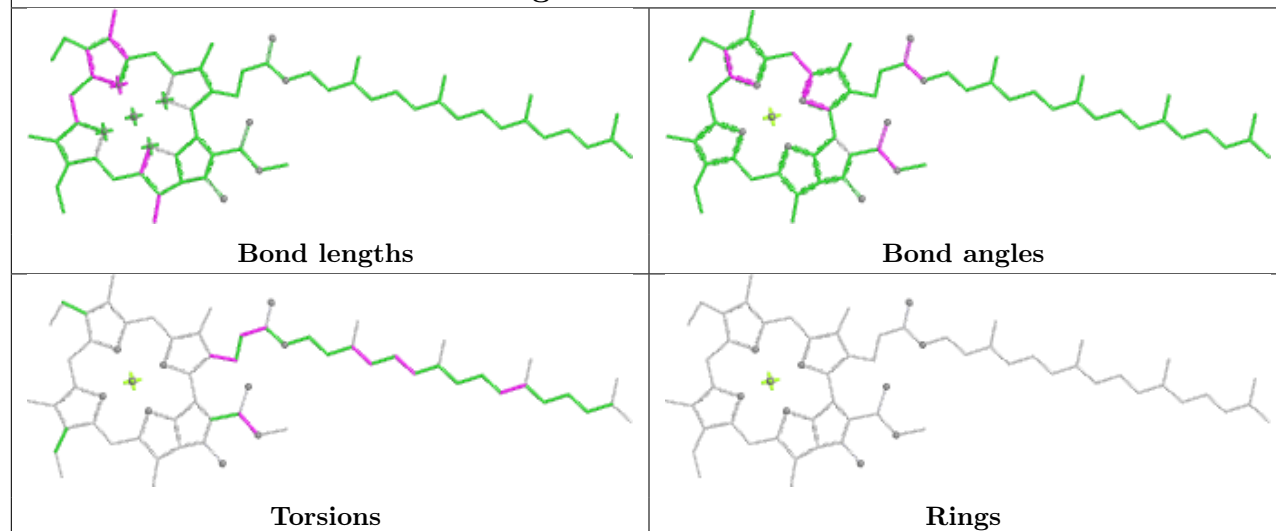
Rings



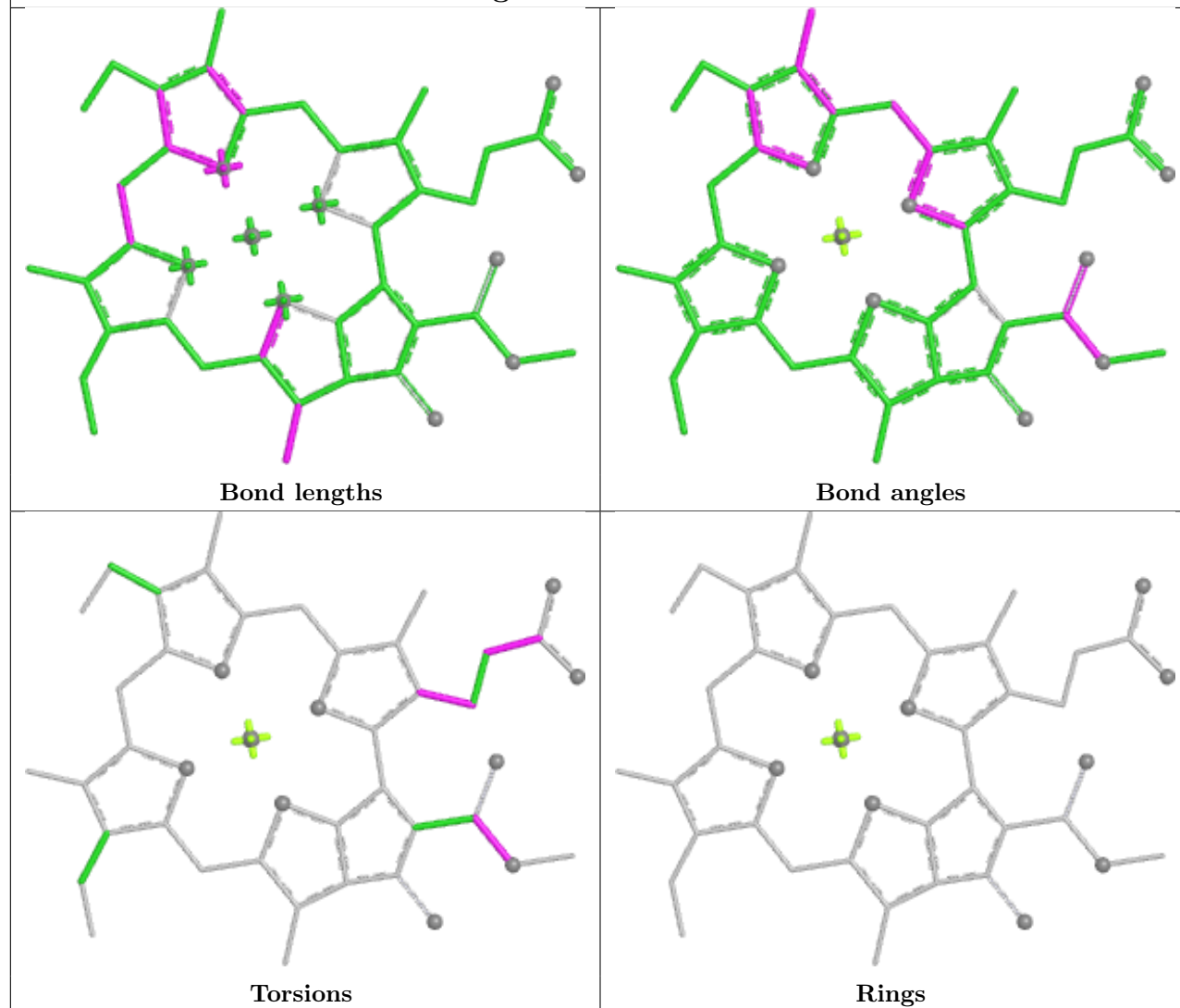


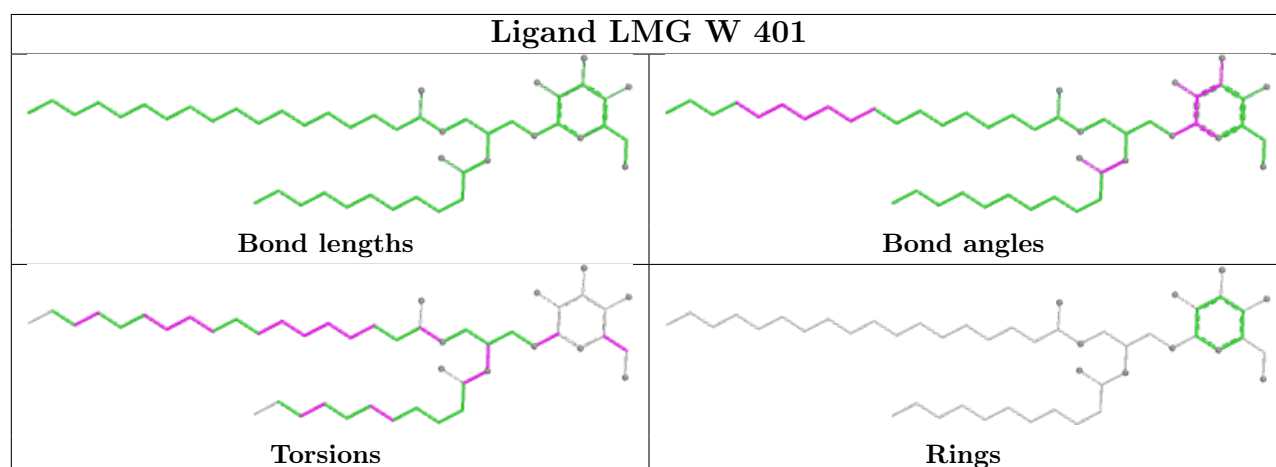
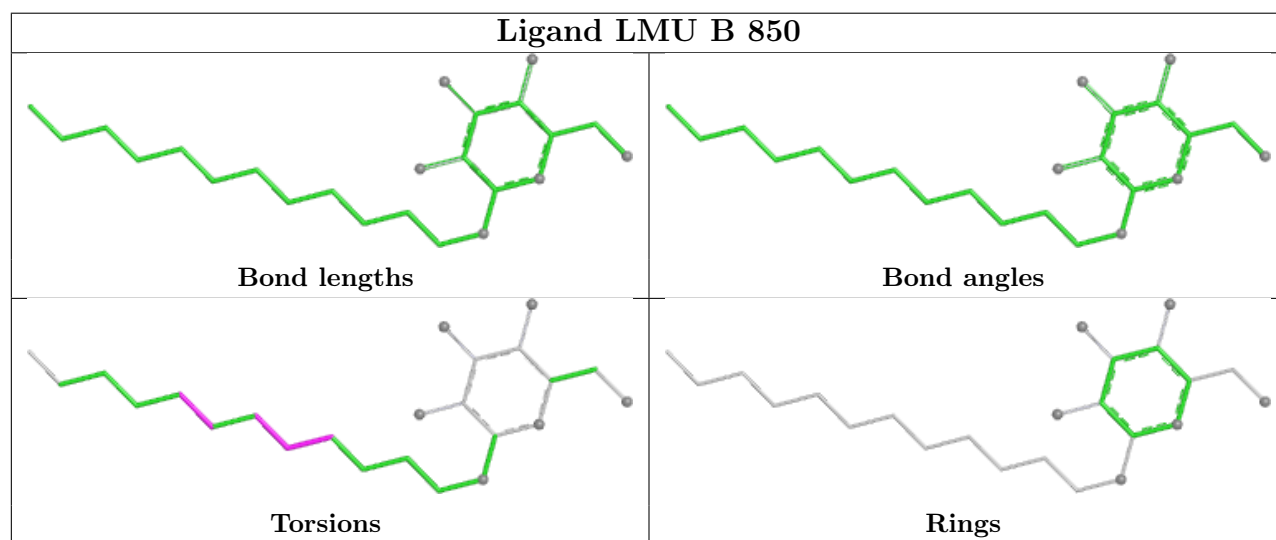
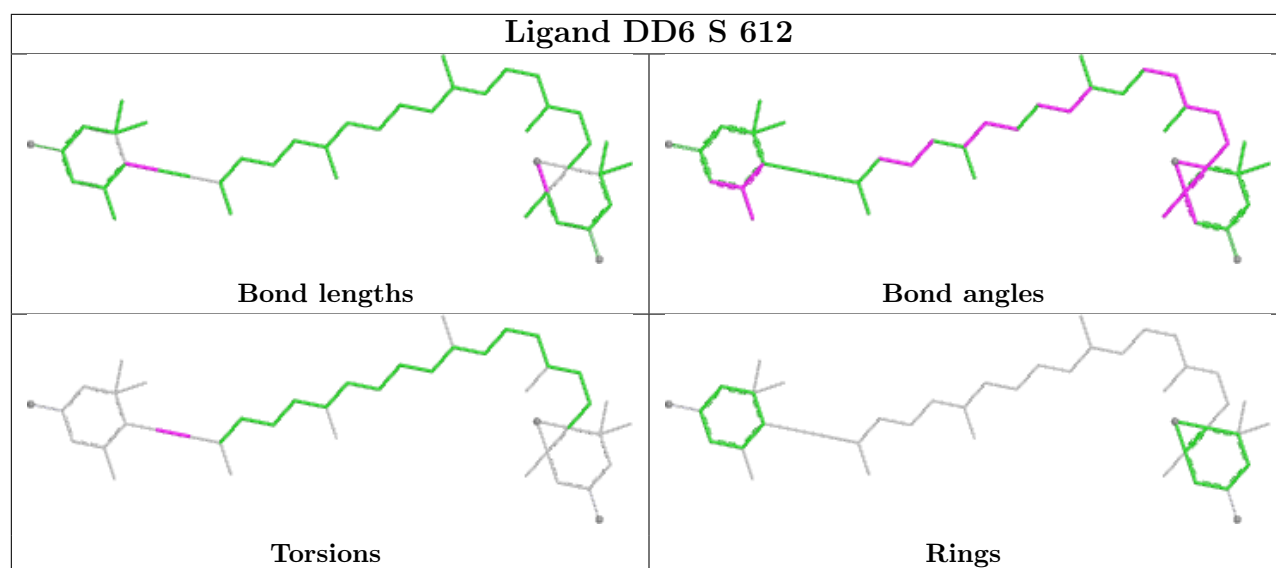


## Ligand CLA B 822

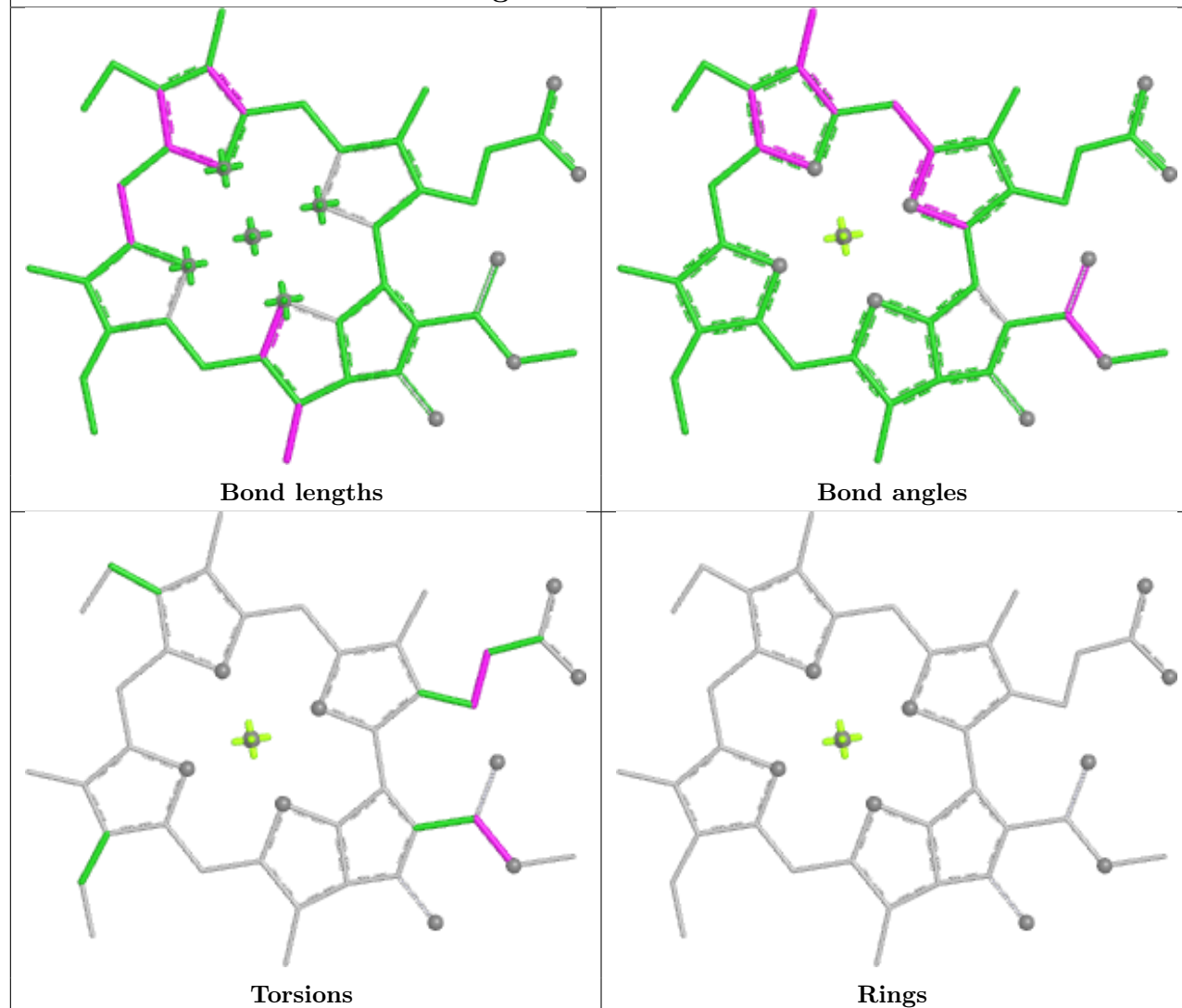


## Ligand CLA P 606

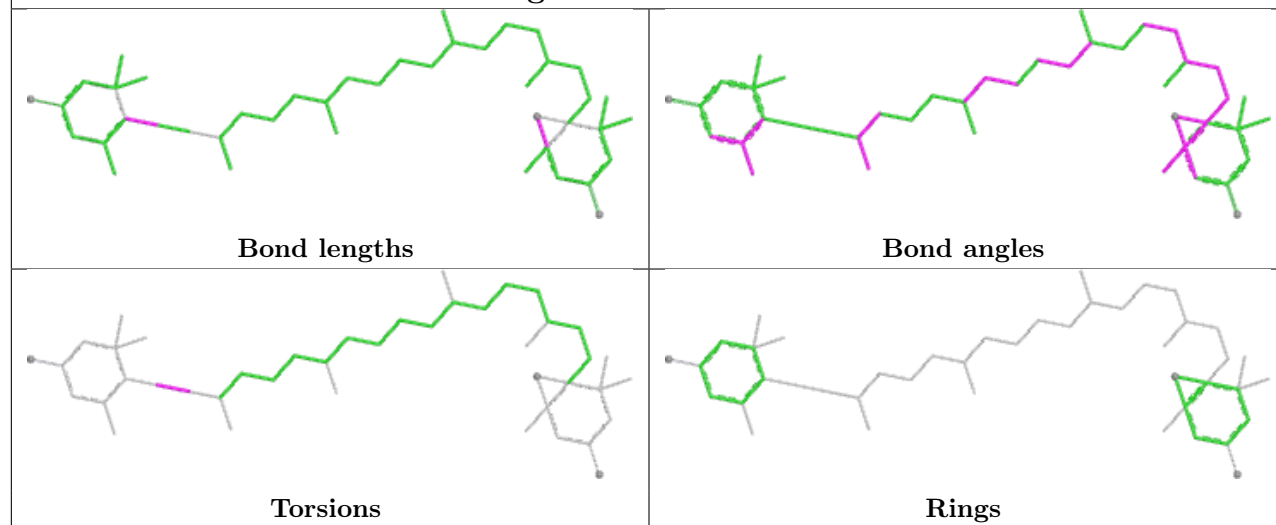




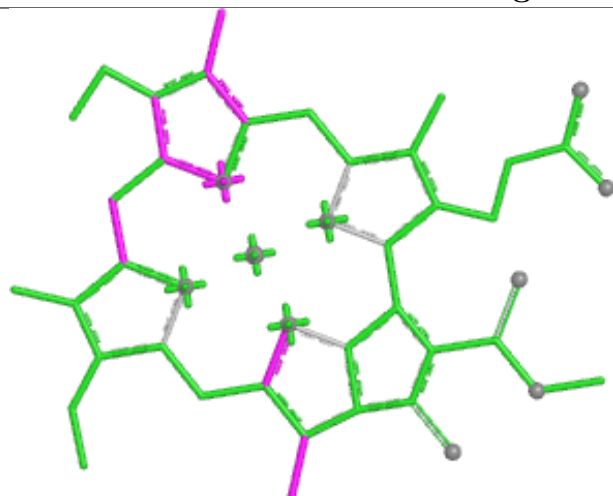
## Ligand CLA V 607



## Ligand DD6 W 417



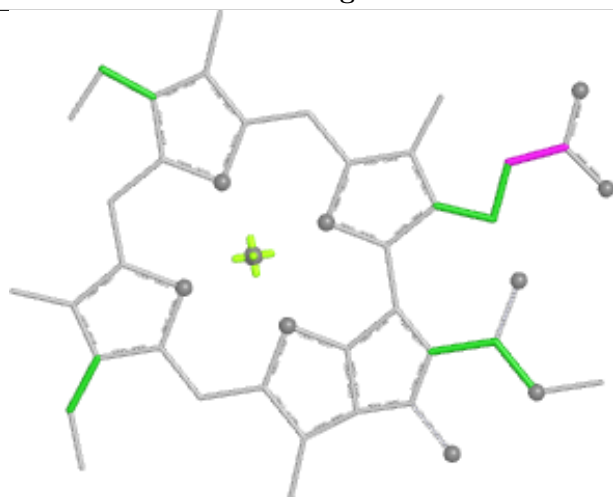
## Ligand CLA G 605



Bond lengths



Bond angles

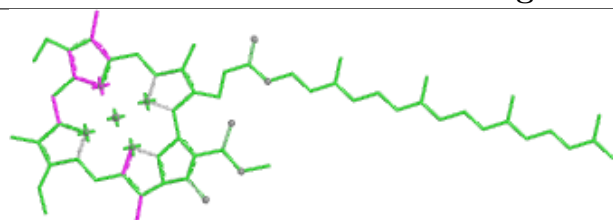


Torsions

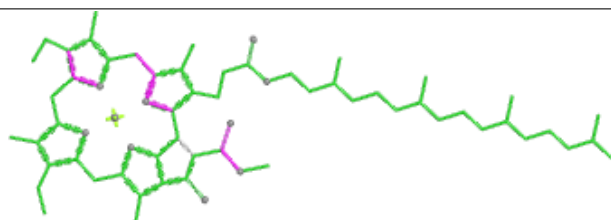


Rings

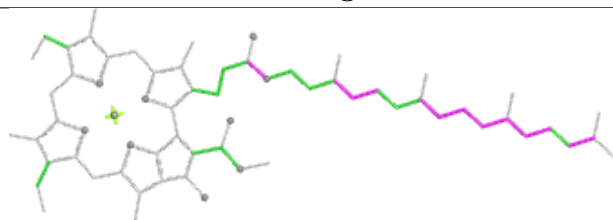
## Ligand CLA L 402



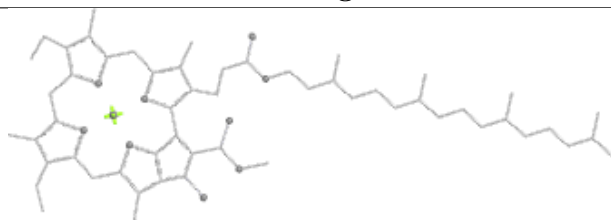
Bond lengths



Bond angles

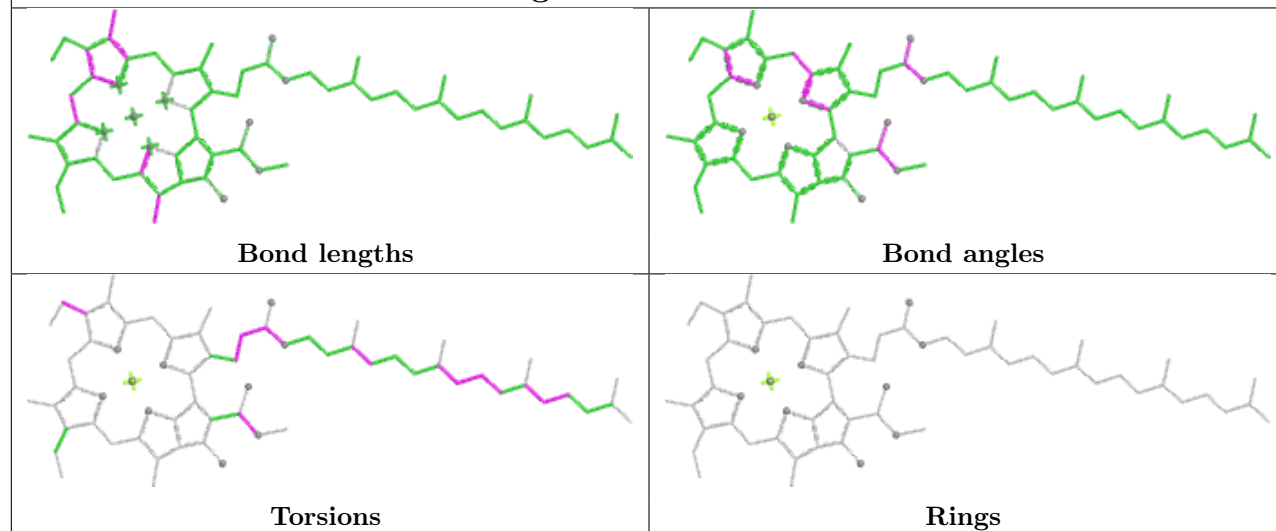


Torsions

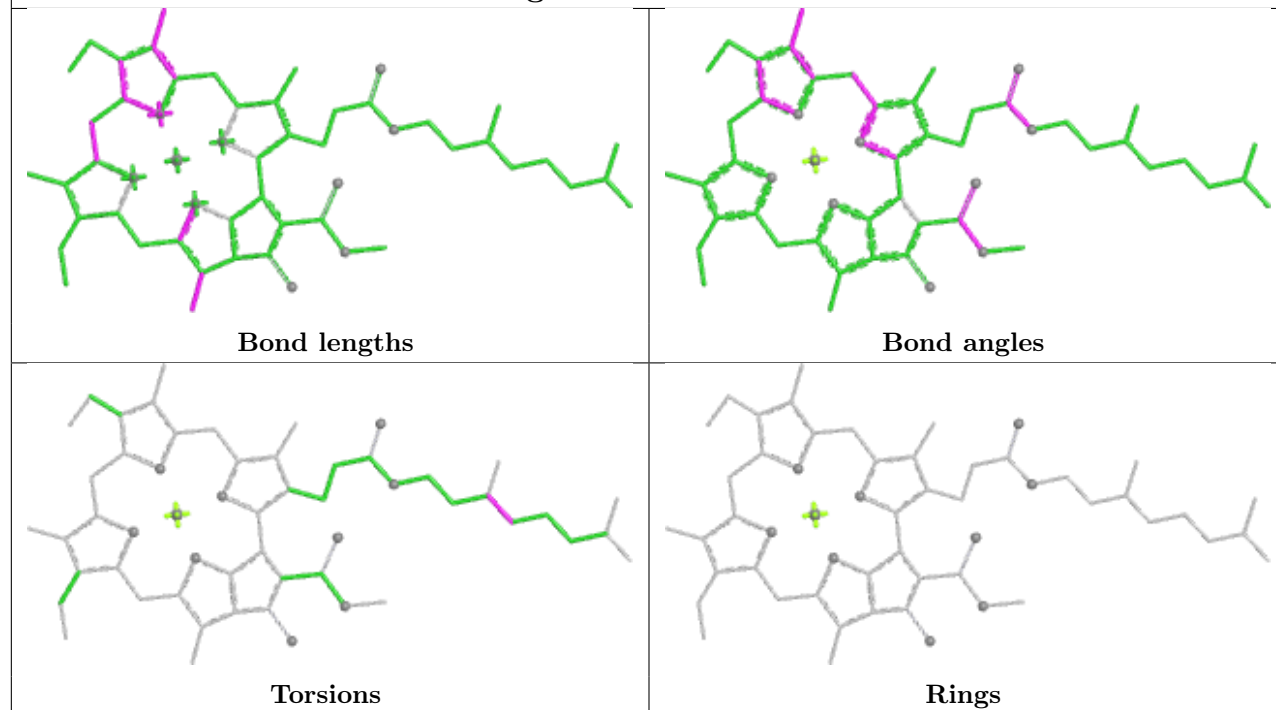


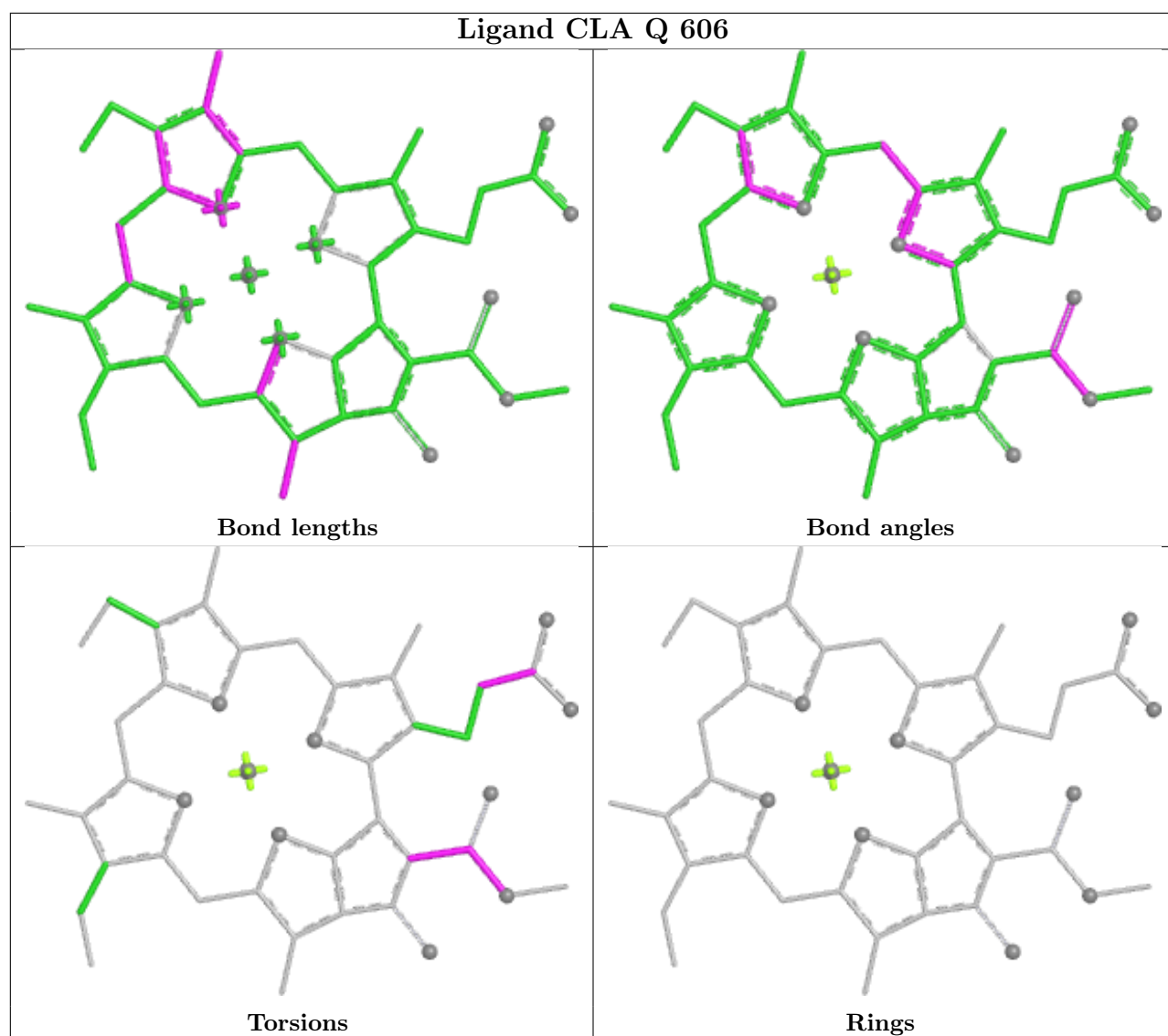
Rings

## Ligand CLA R 610

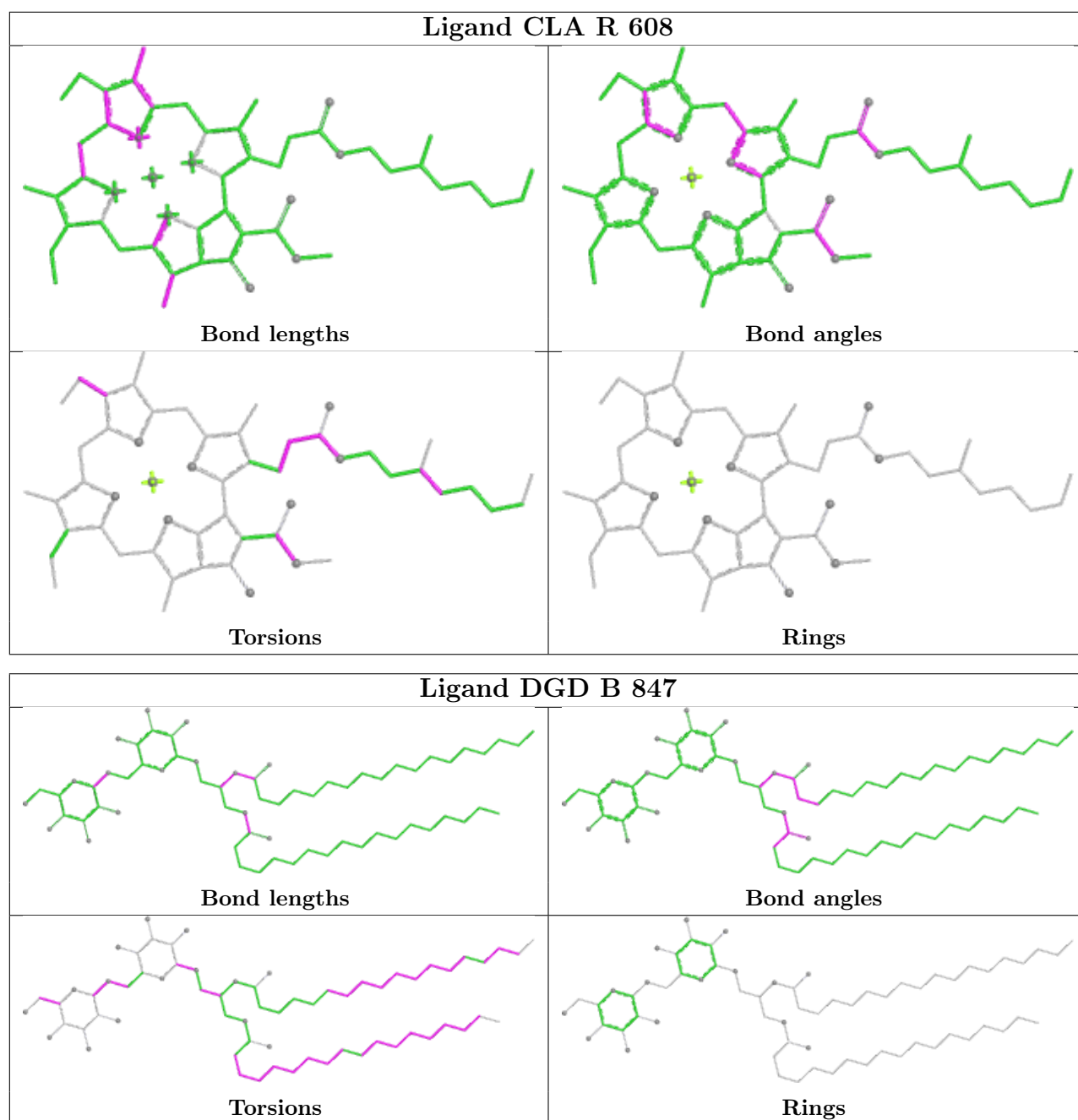


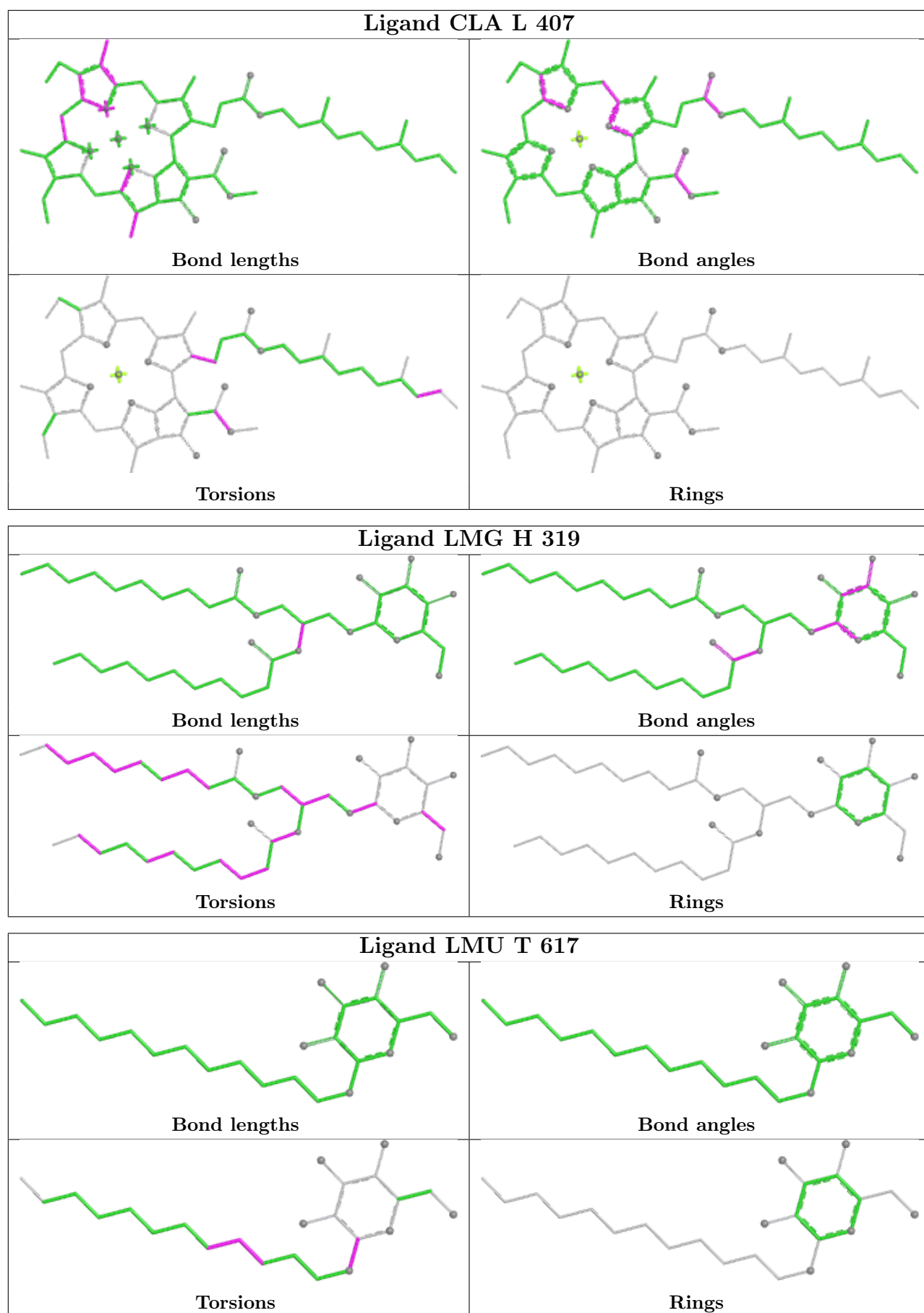
## Ligand CLA W 402

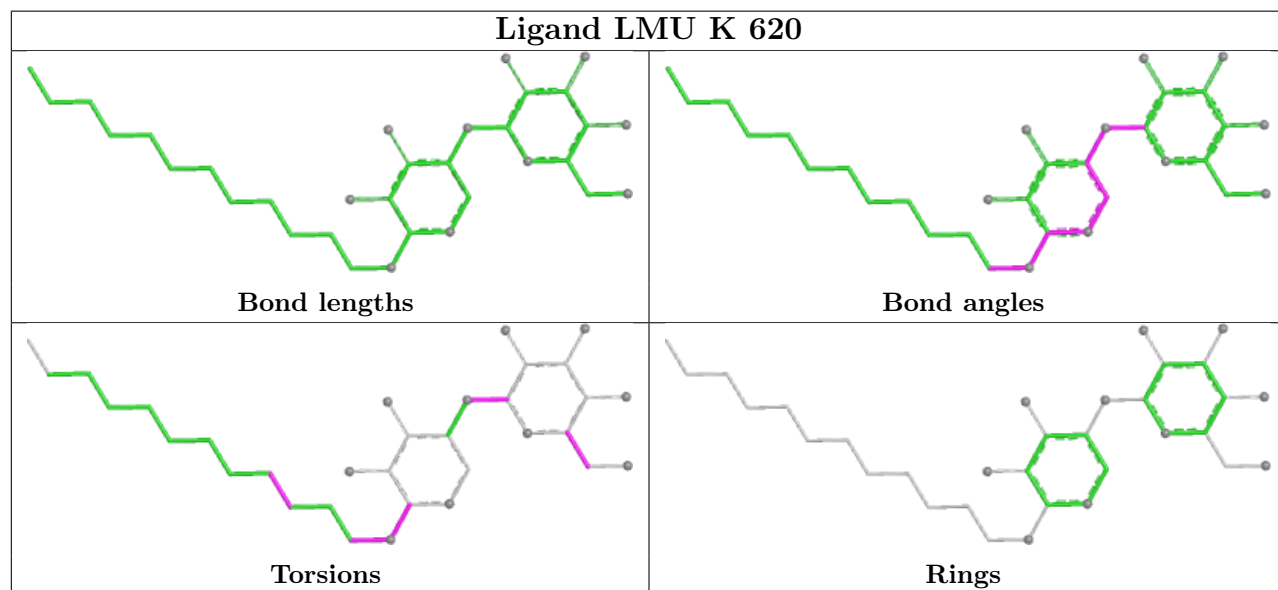
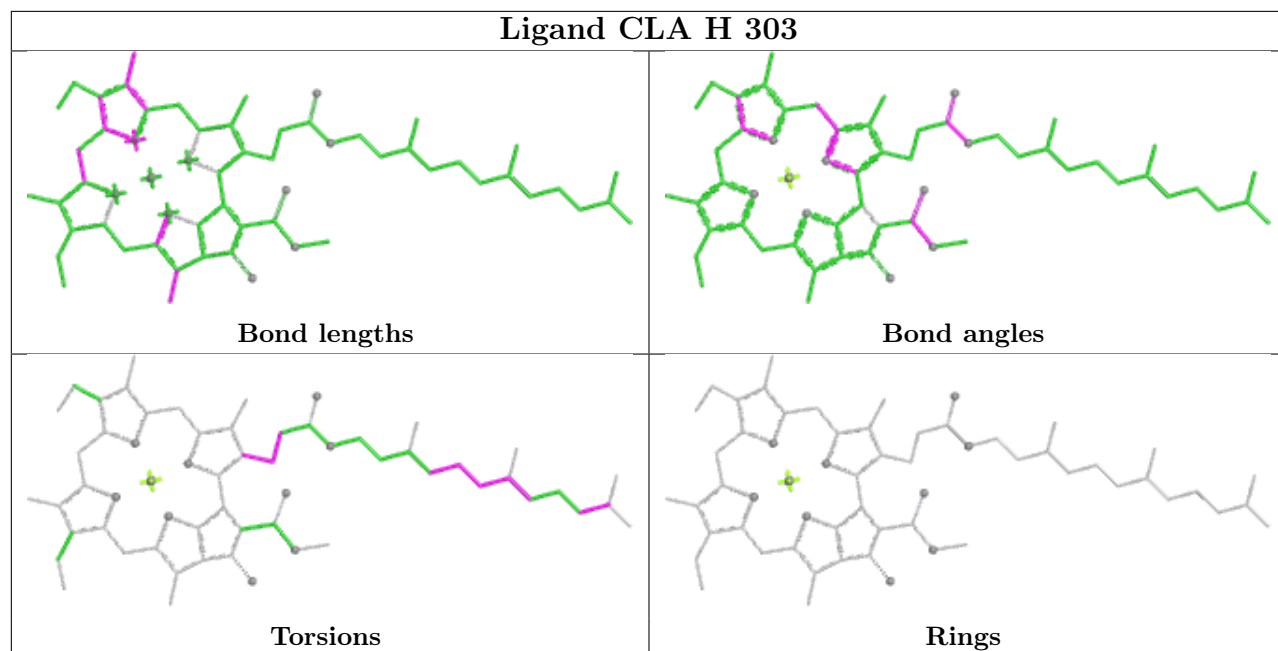


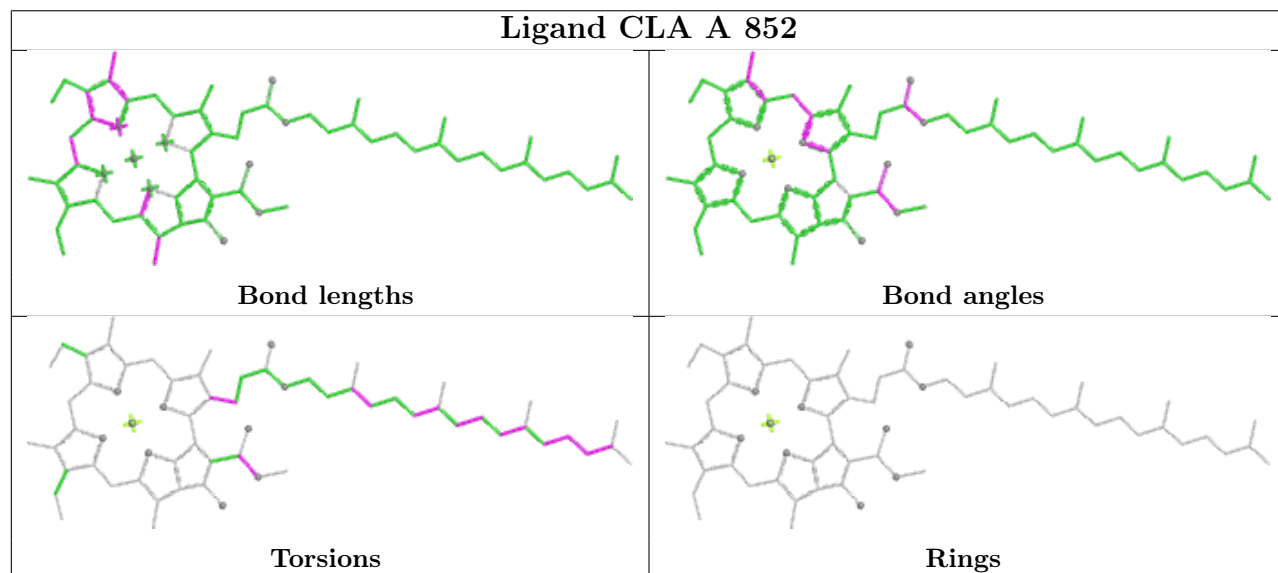
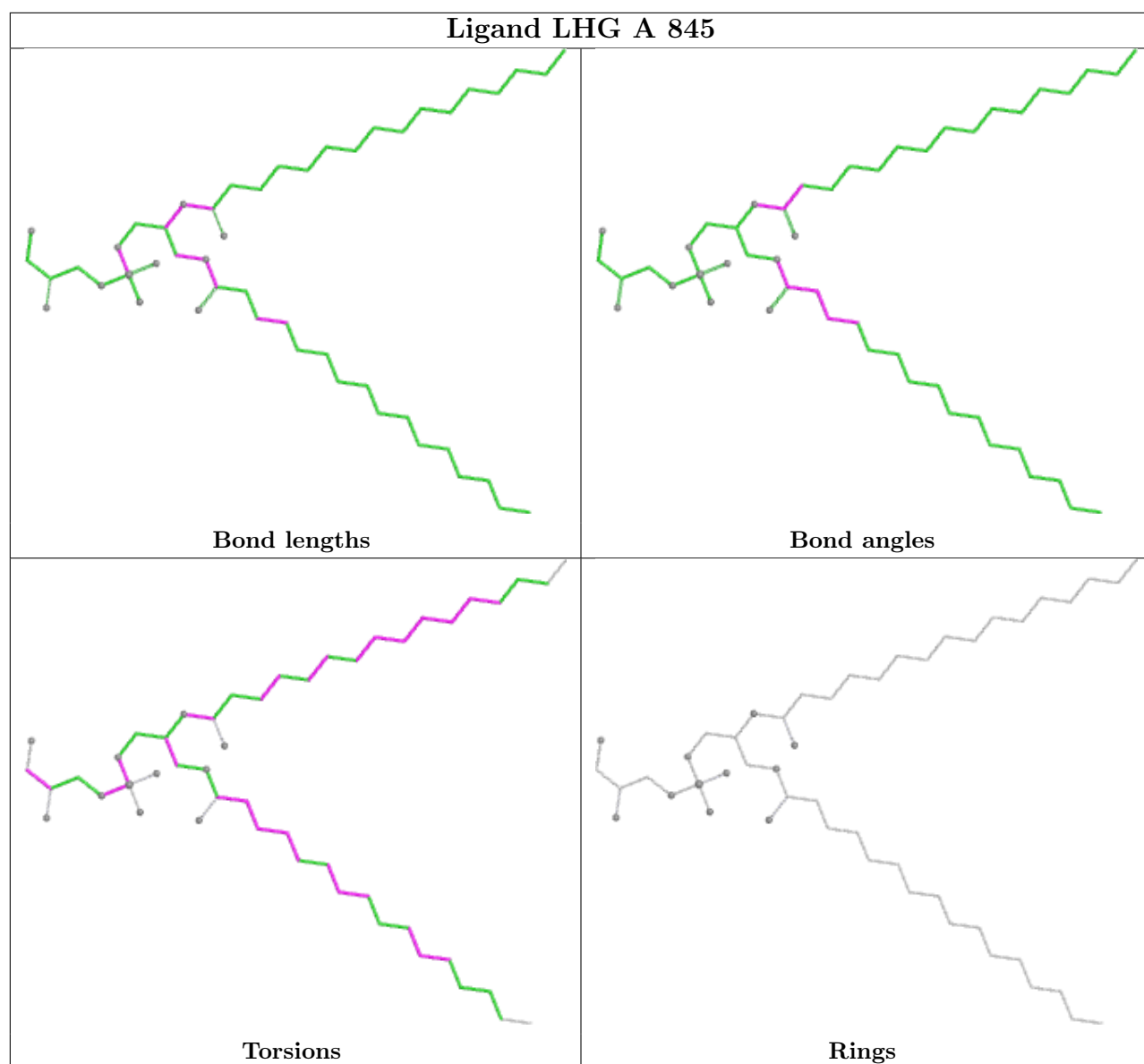


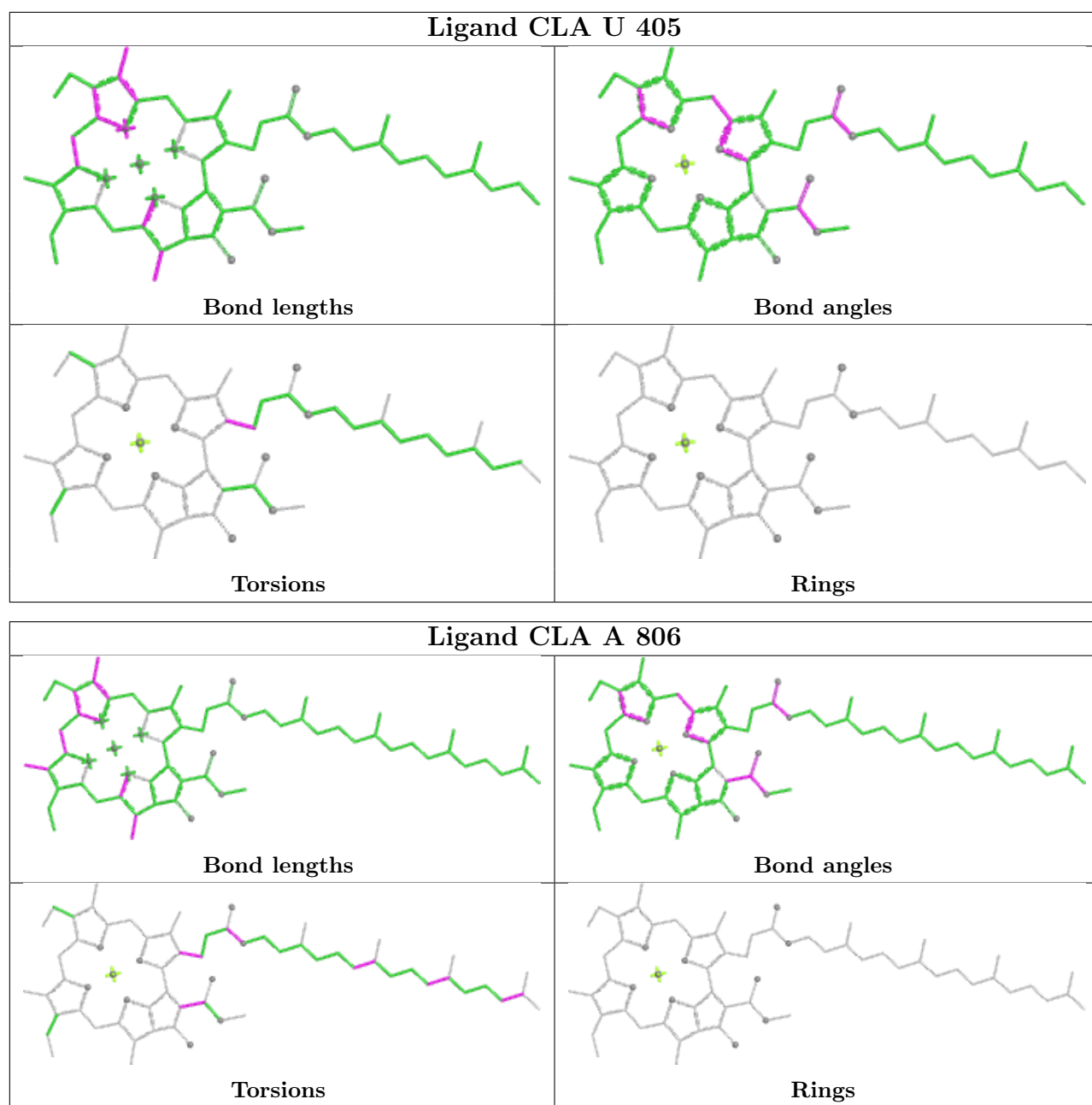


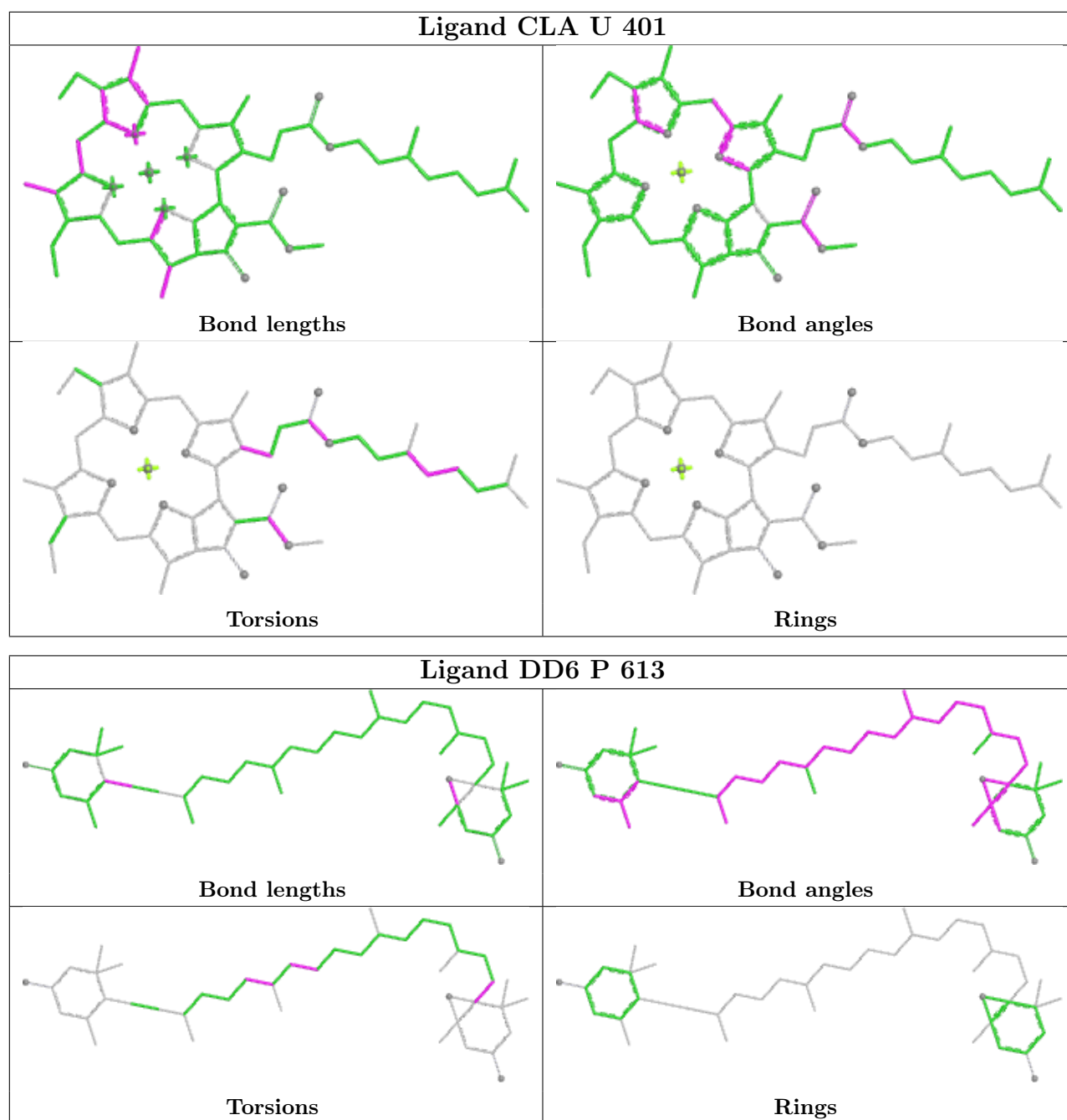


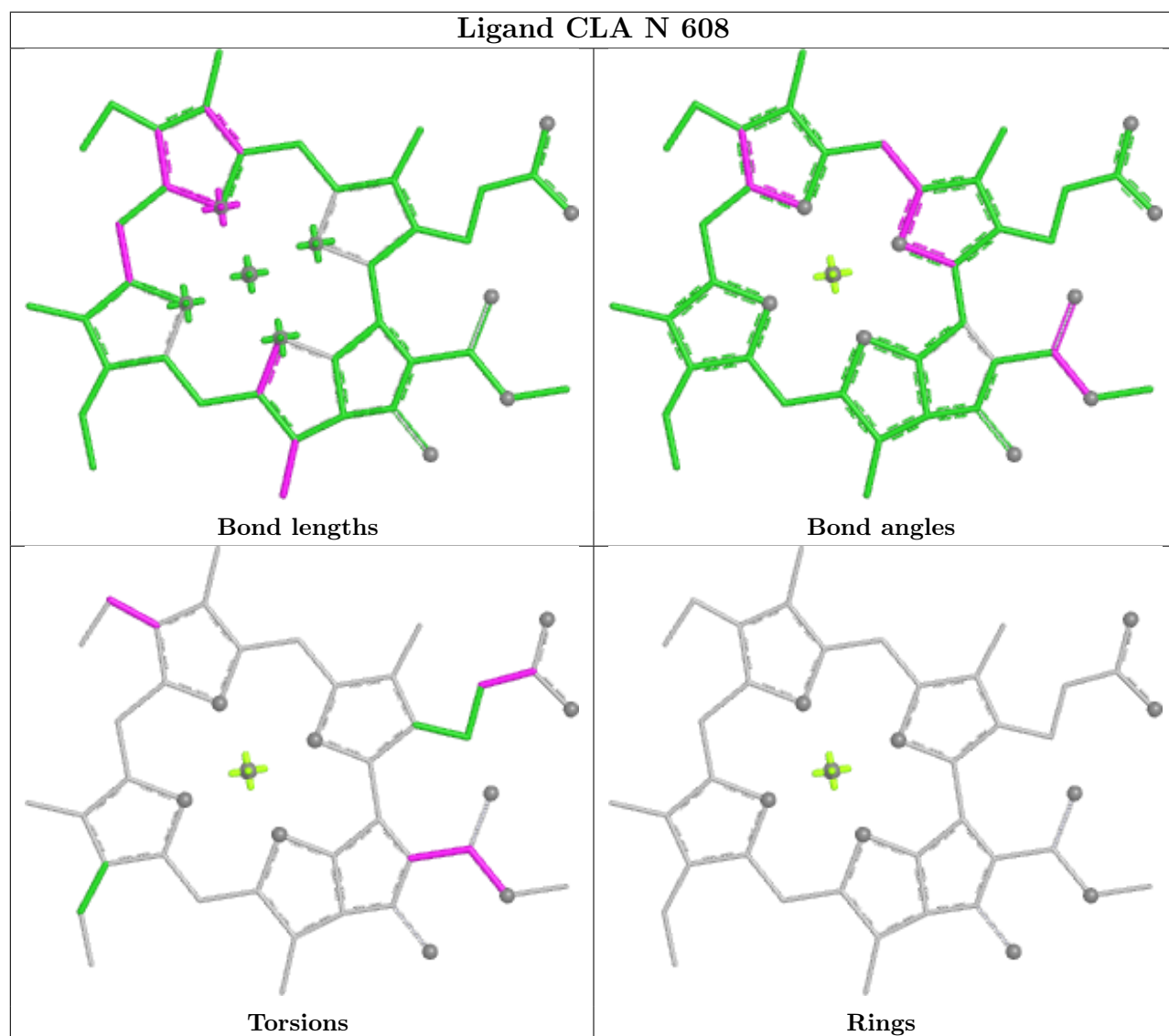
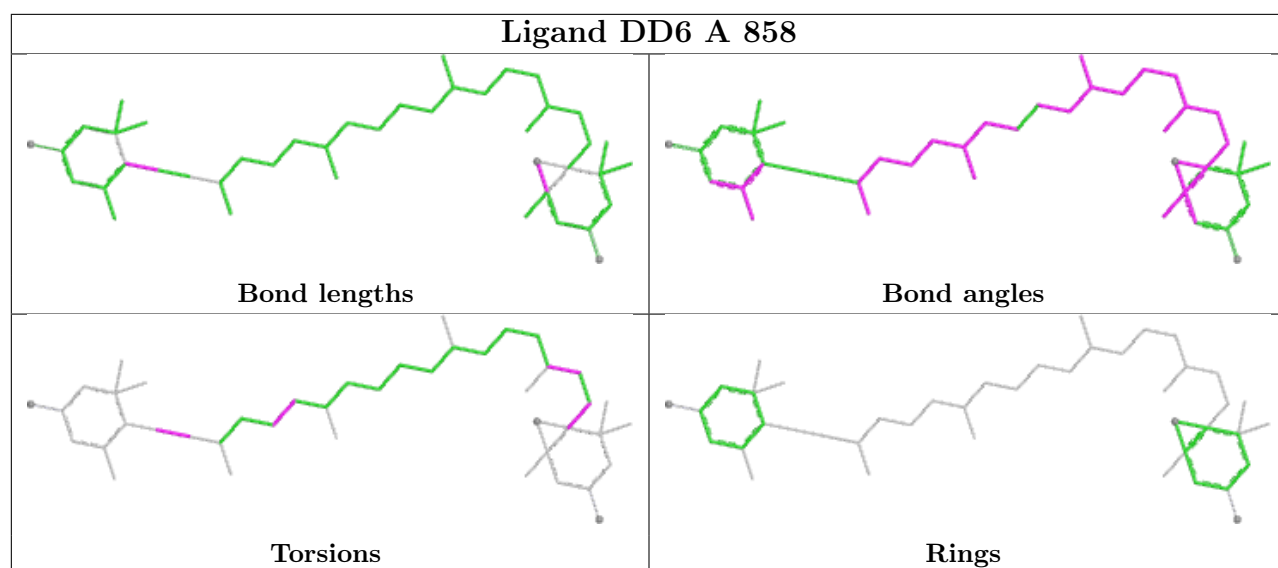


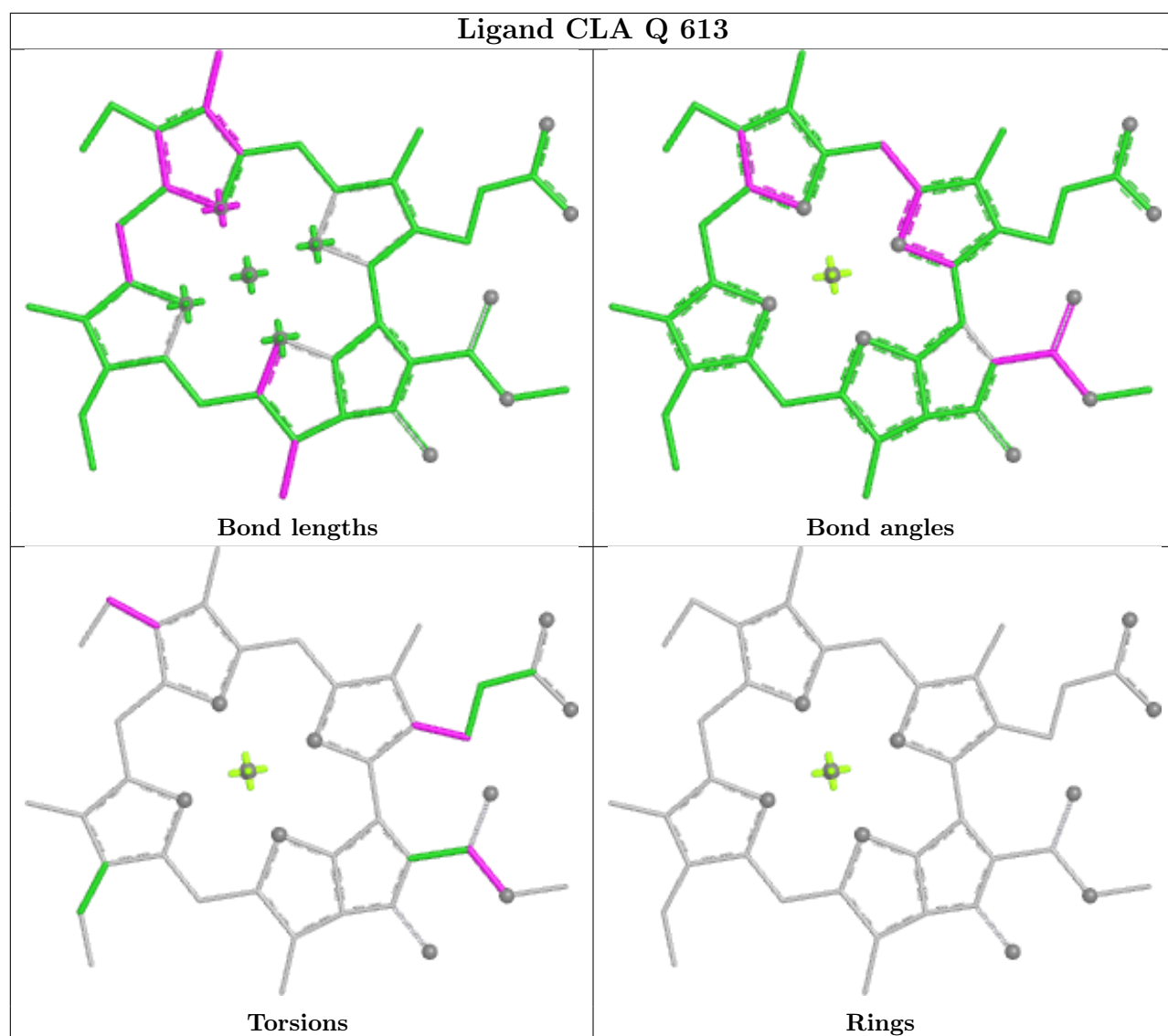






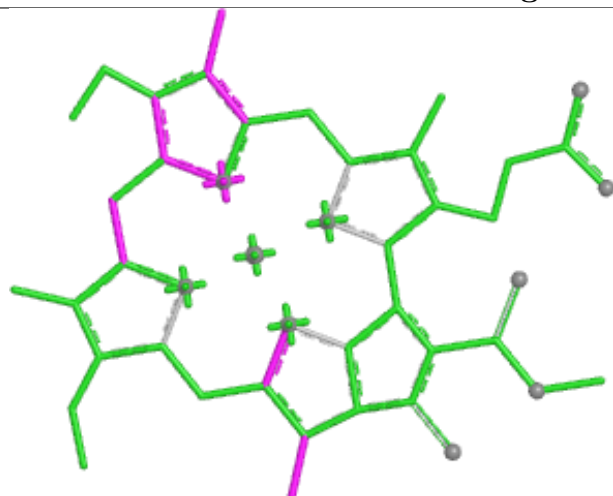




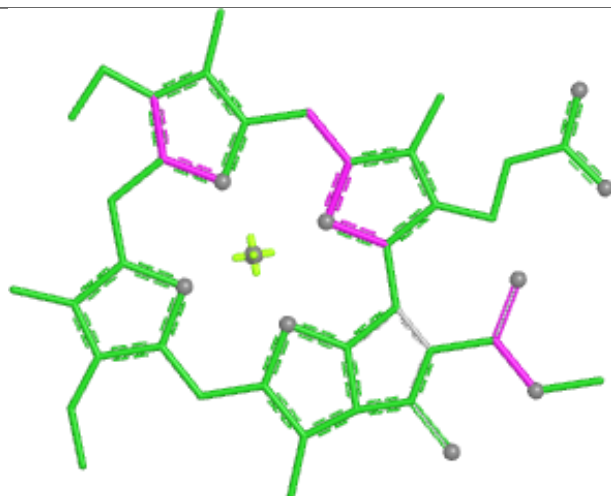




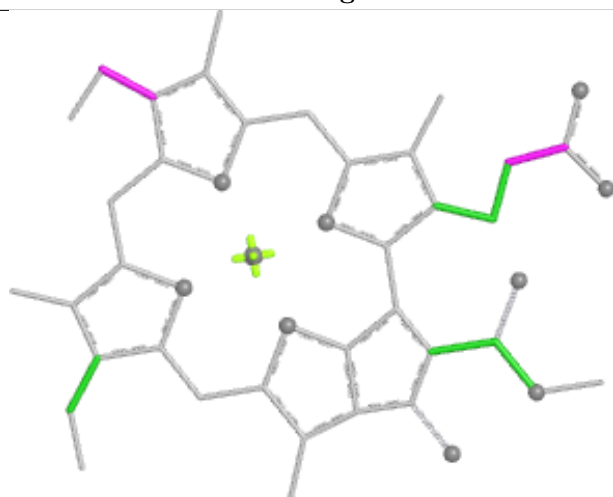
## Ligand CLA I 608



Bond lengths



Bond angles

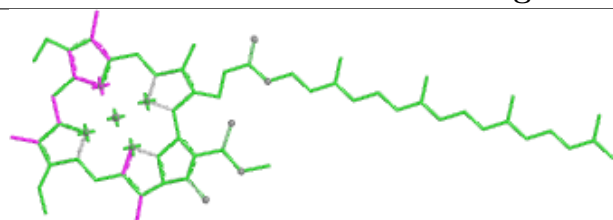


Torsions

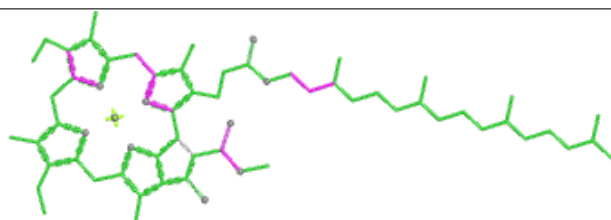


Rings

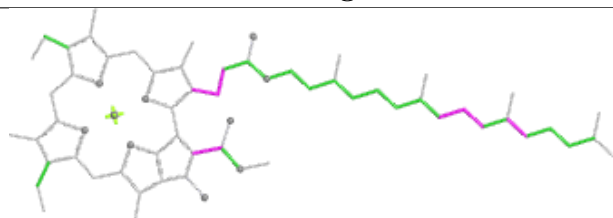
## Ligand CLA A 807



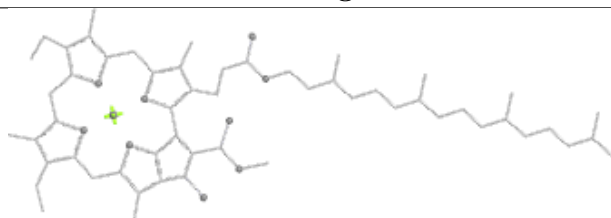
Bond lengths



Bond angles

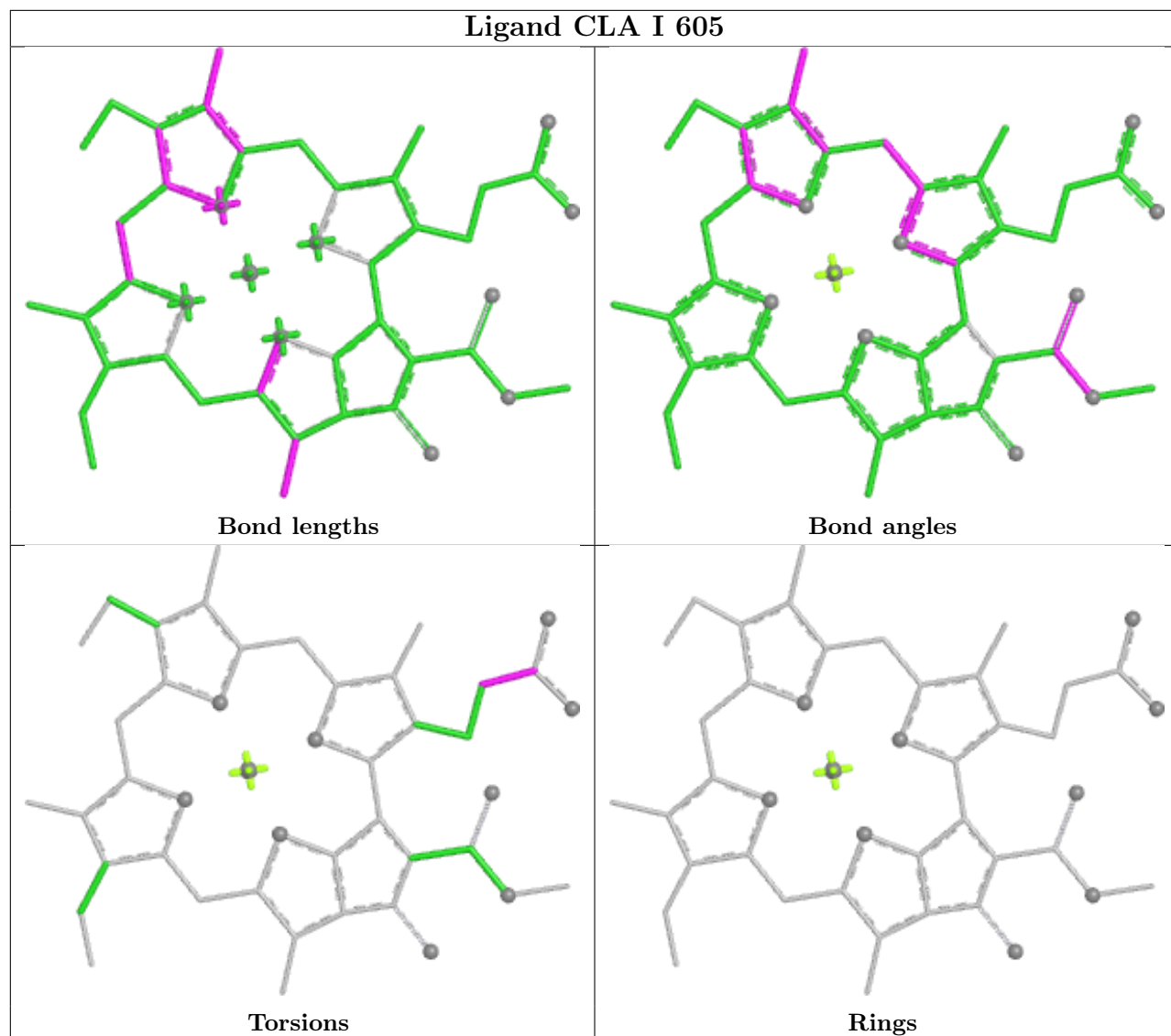


Torsions

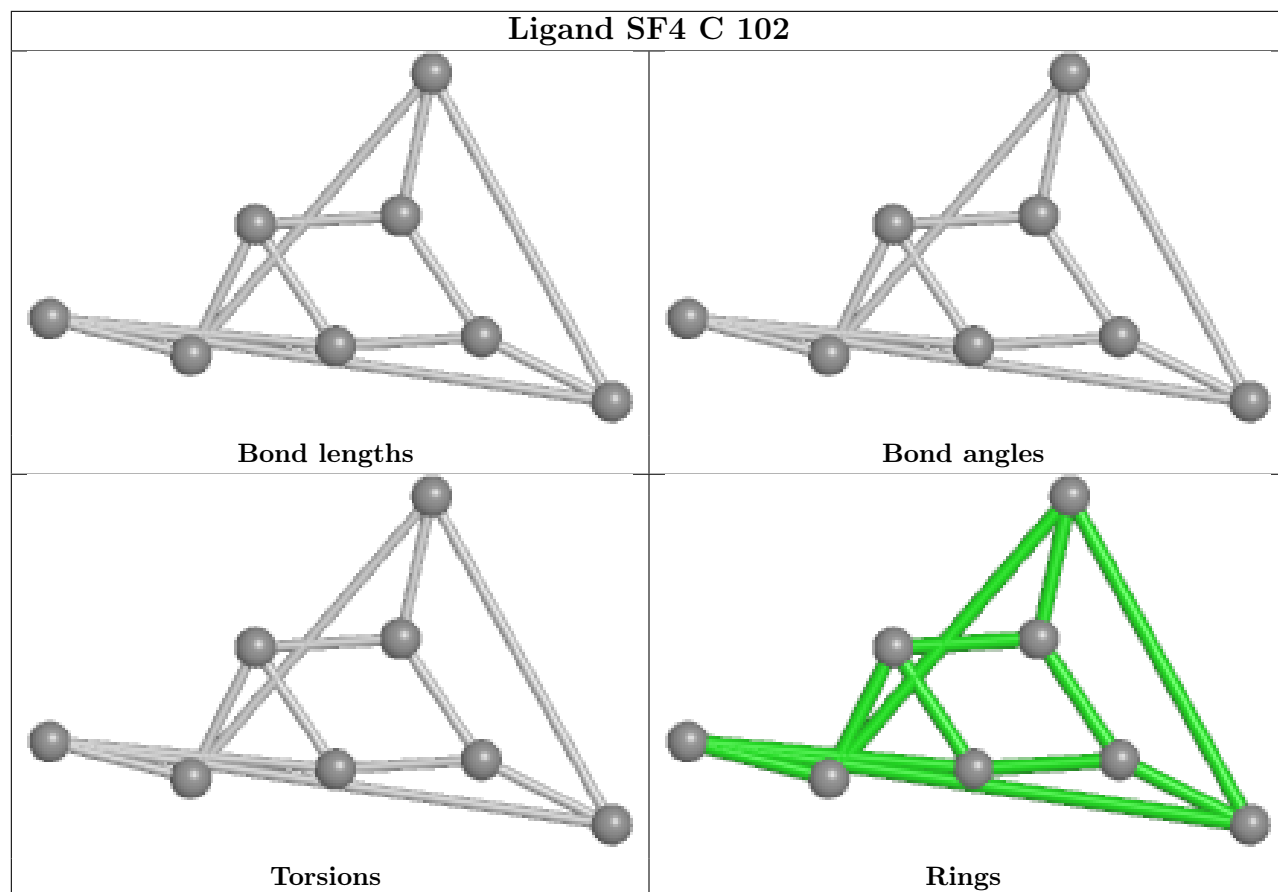


Rings

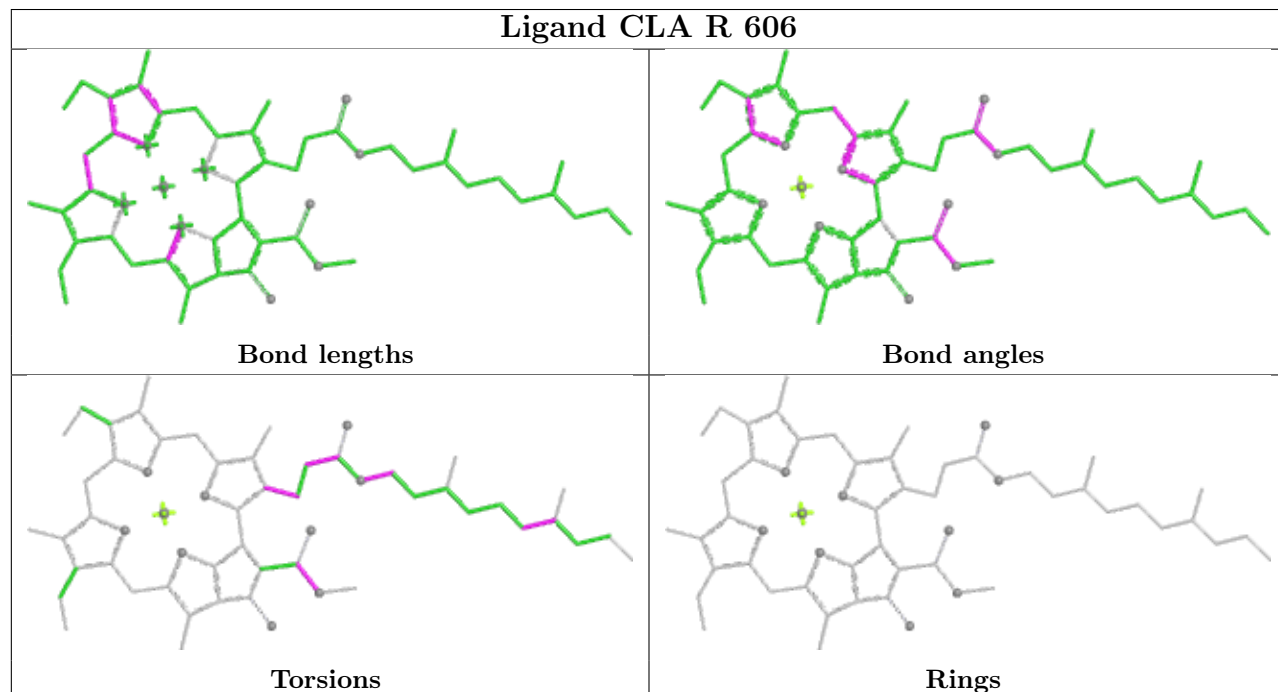
## Ligand CLA I 605



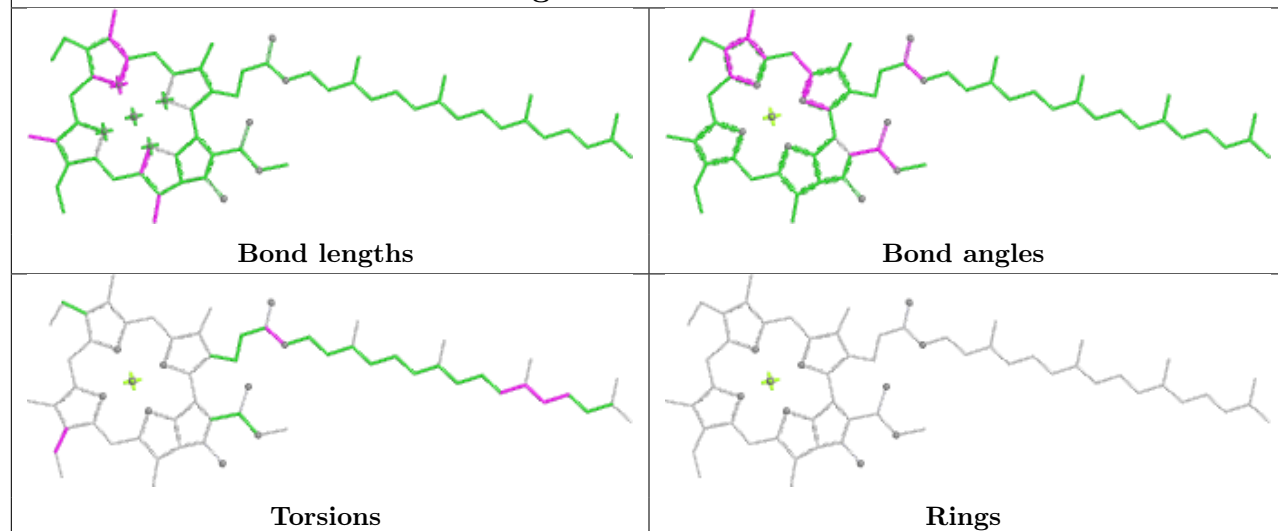
## Ligand SF4 C 102



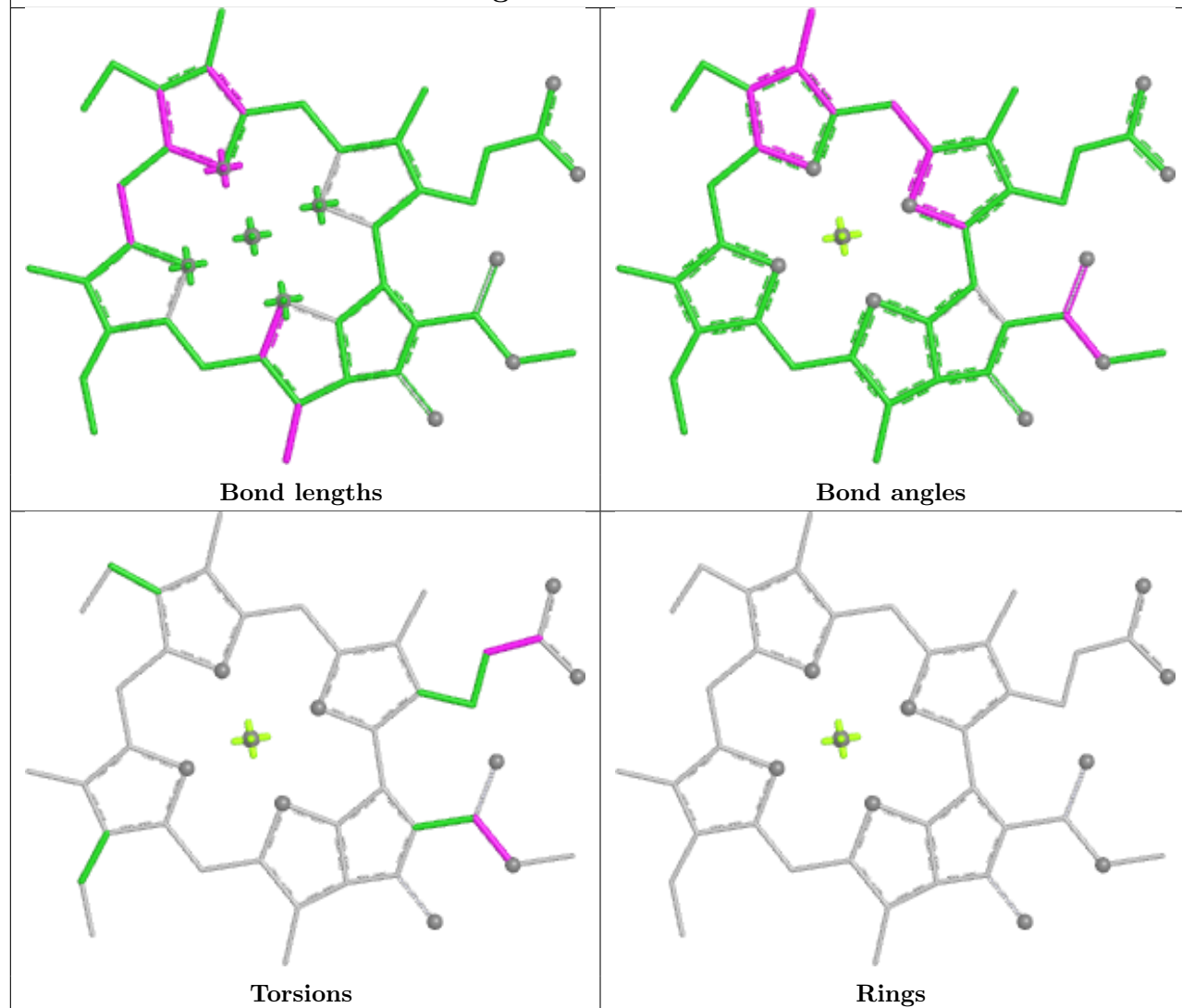
## Ligand CLA R 606

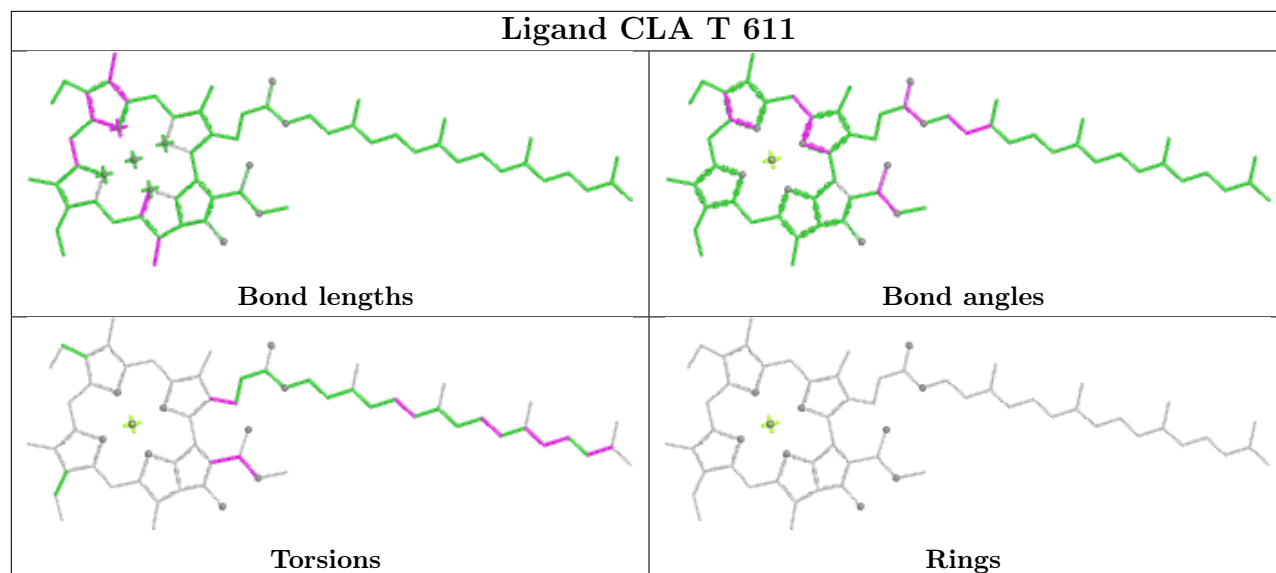
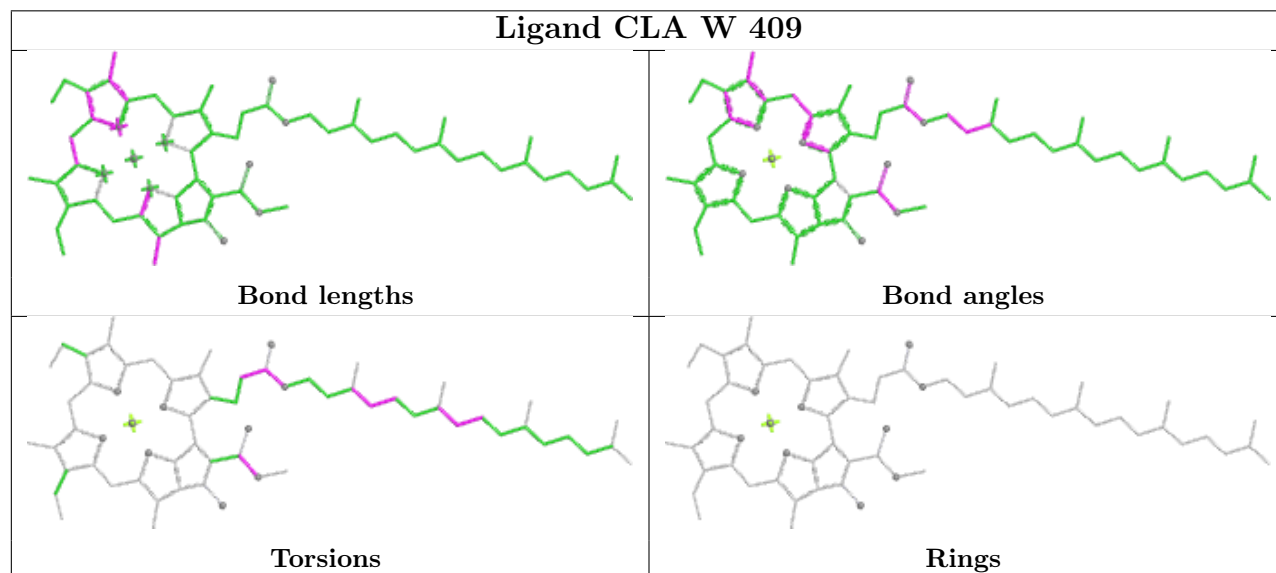
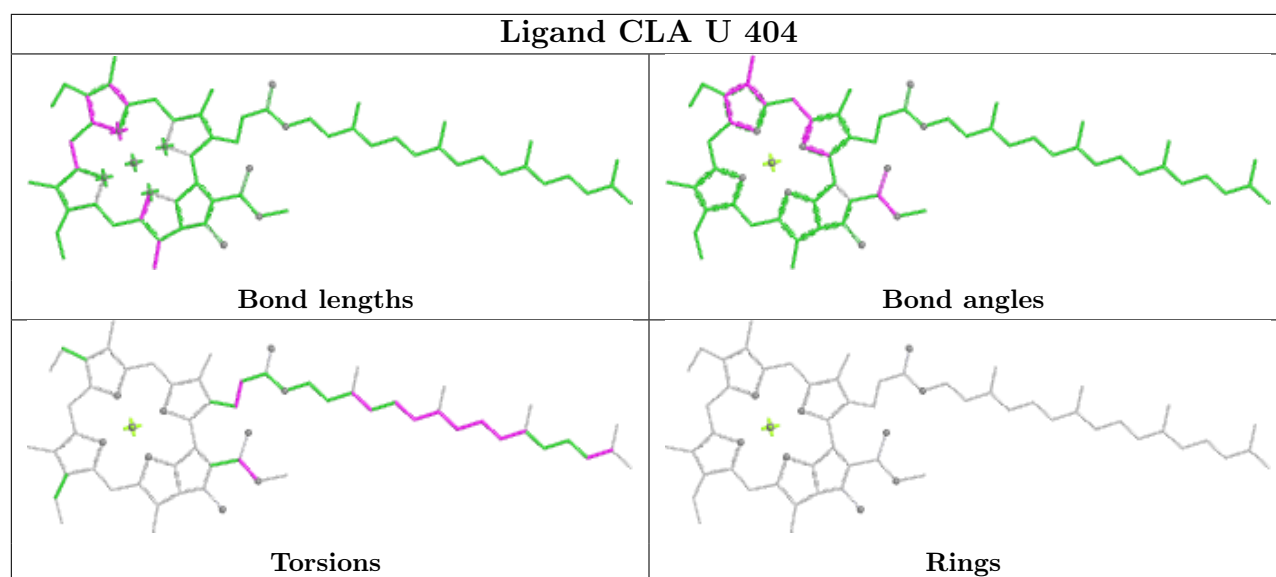


## Ligand CLA B 830

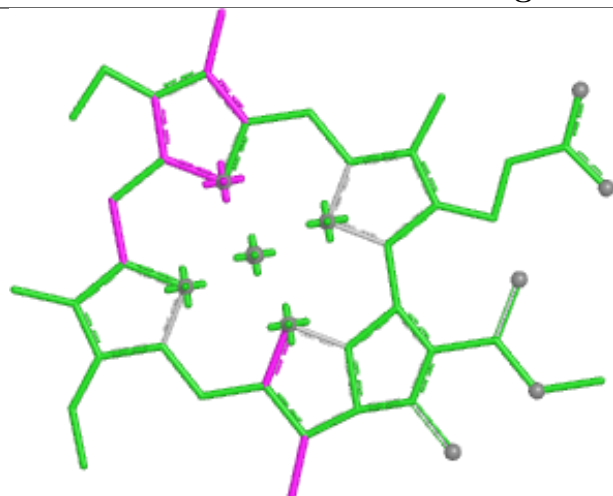


## Ligand CLA T 609





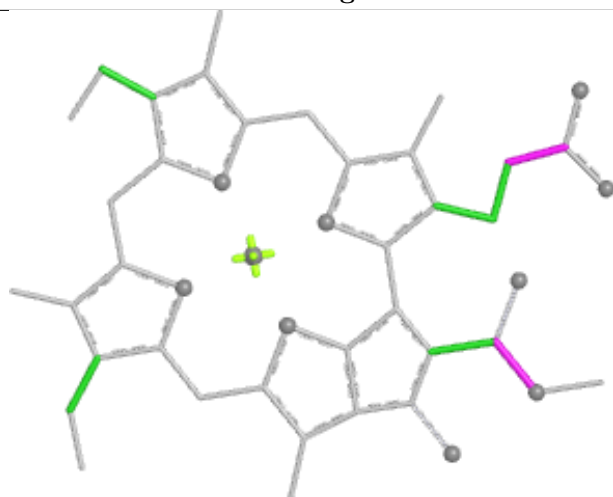
## Ligand CLA T 601



Bond lengths



Bond angles

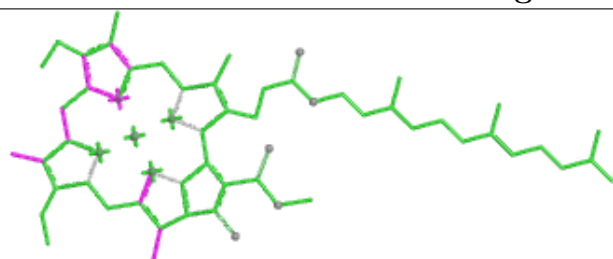


Torsions

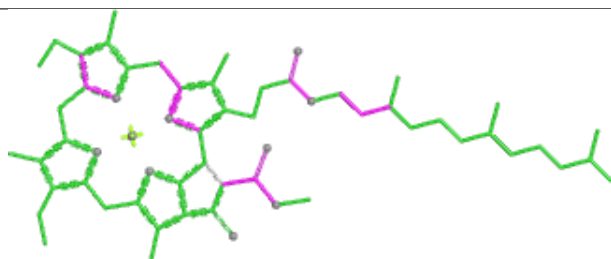


Rings

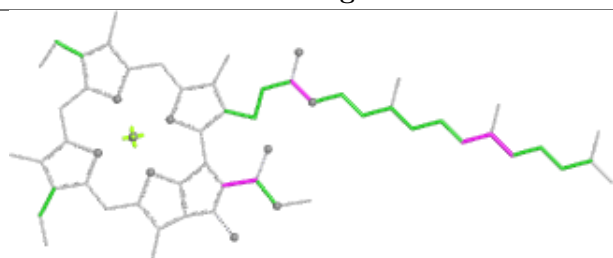
## Ligand CLA T 603



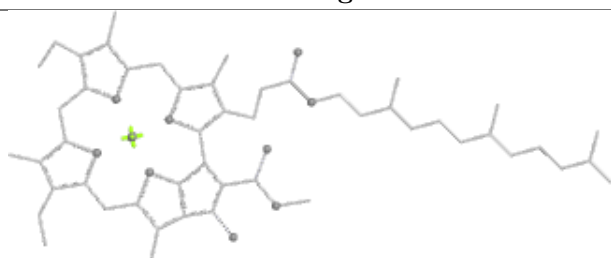
Bond lengths



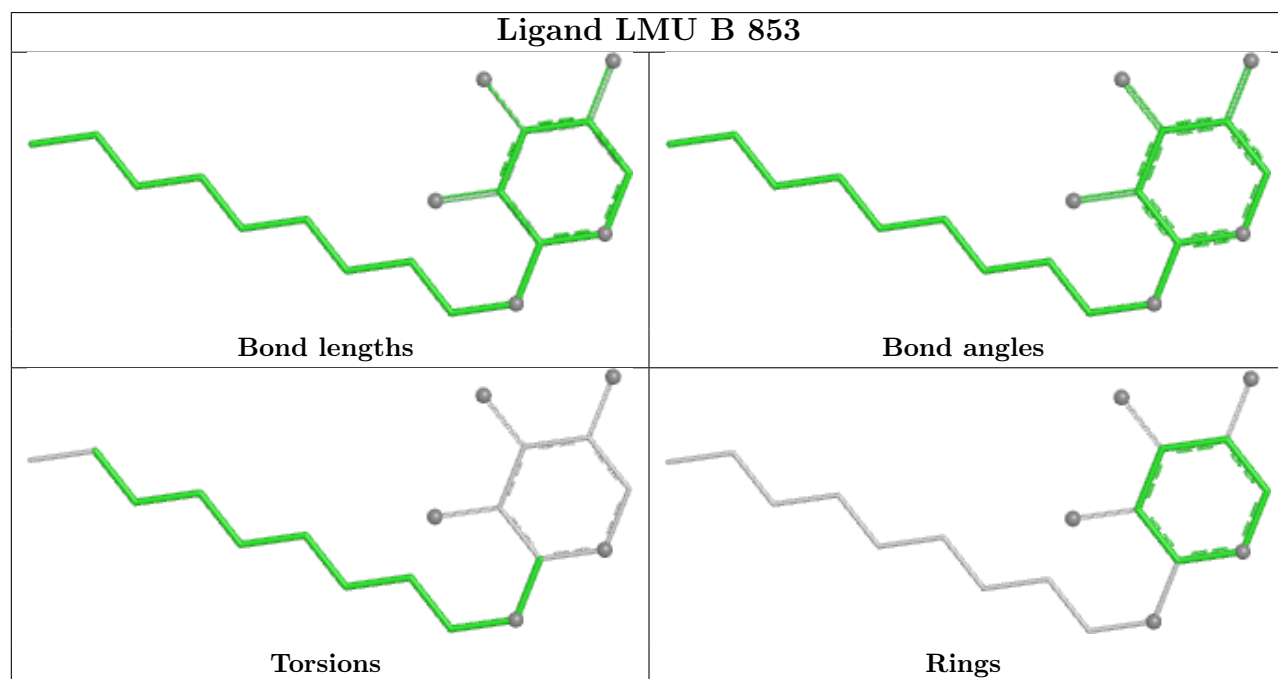
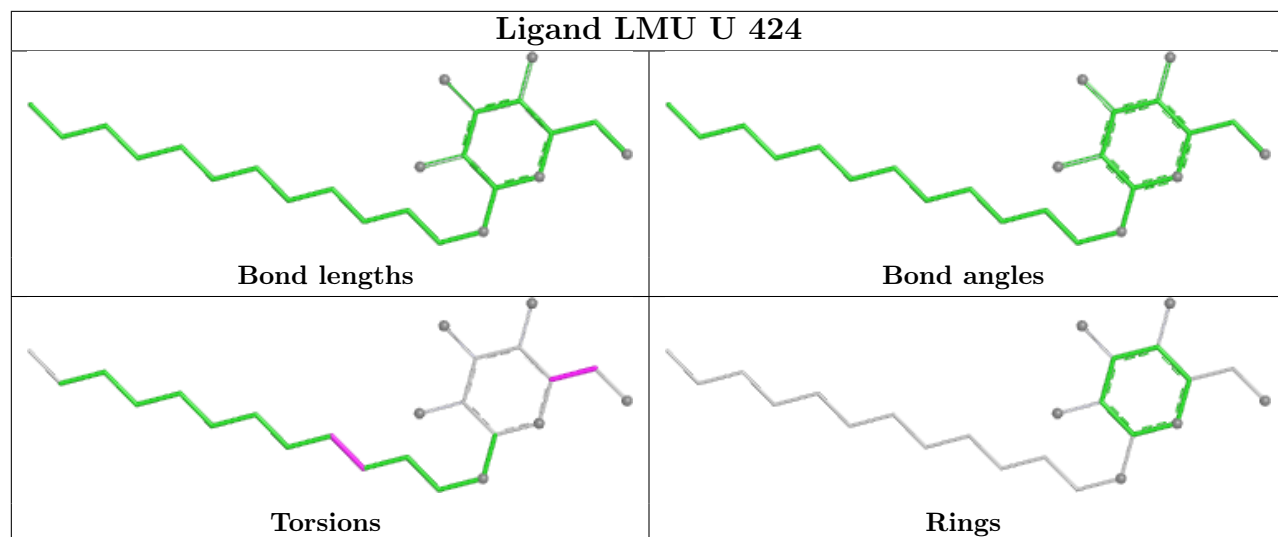
Bond angles

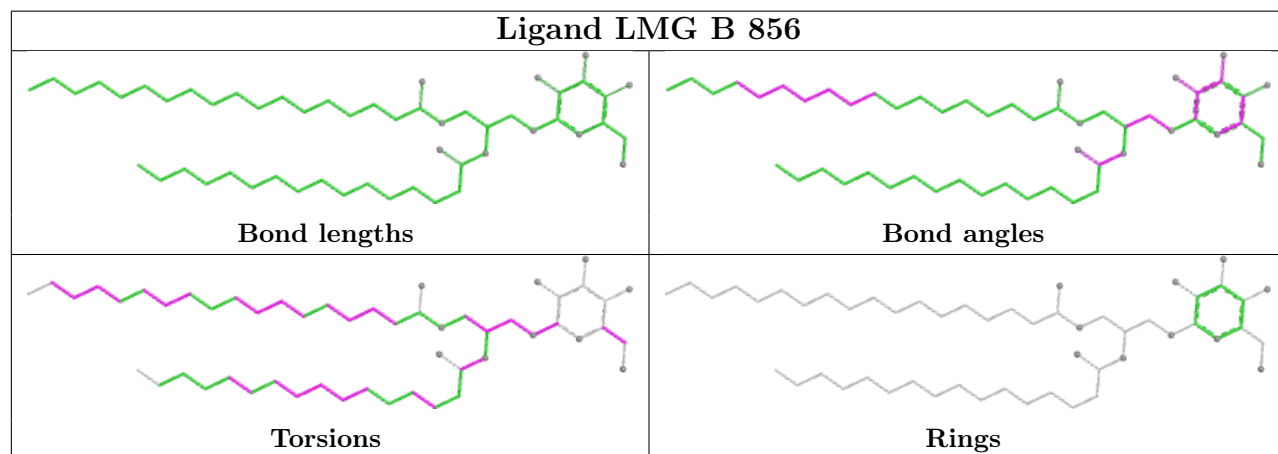
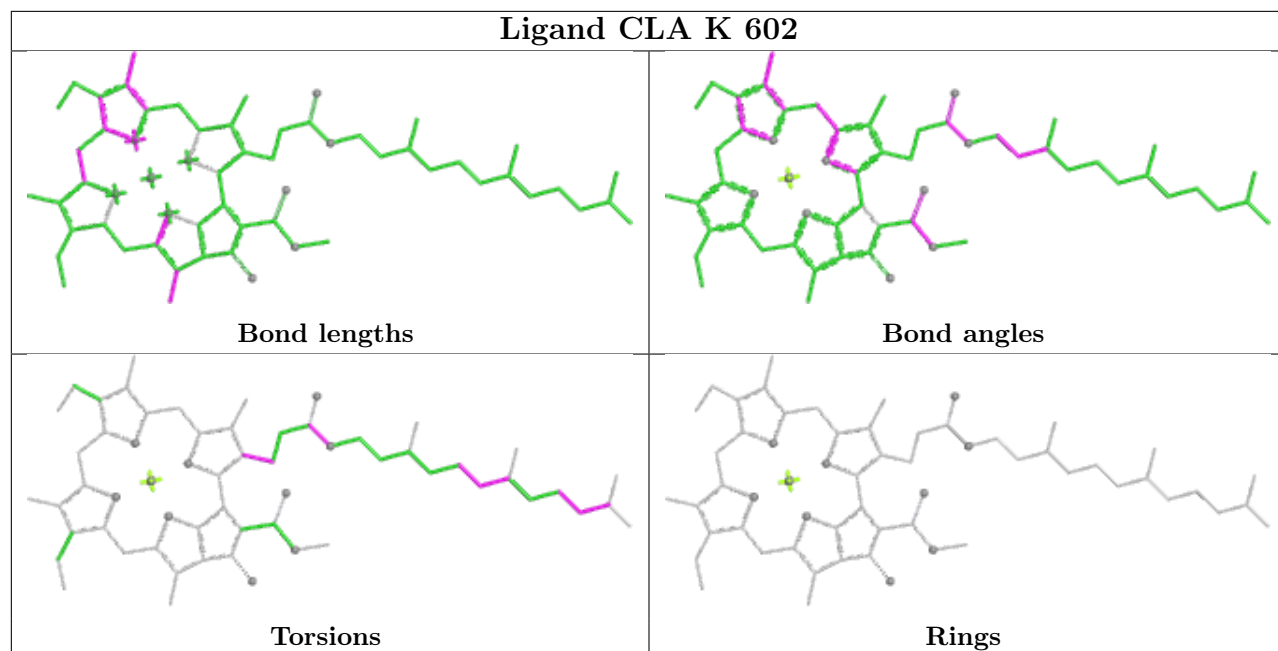


Torsions

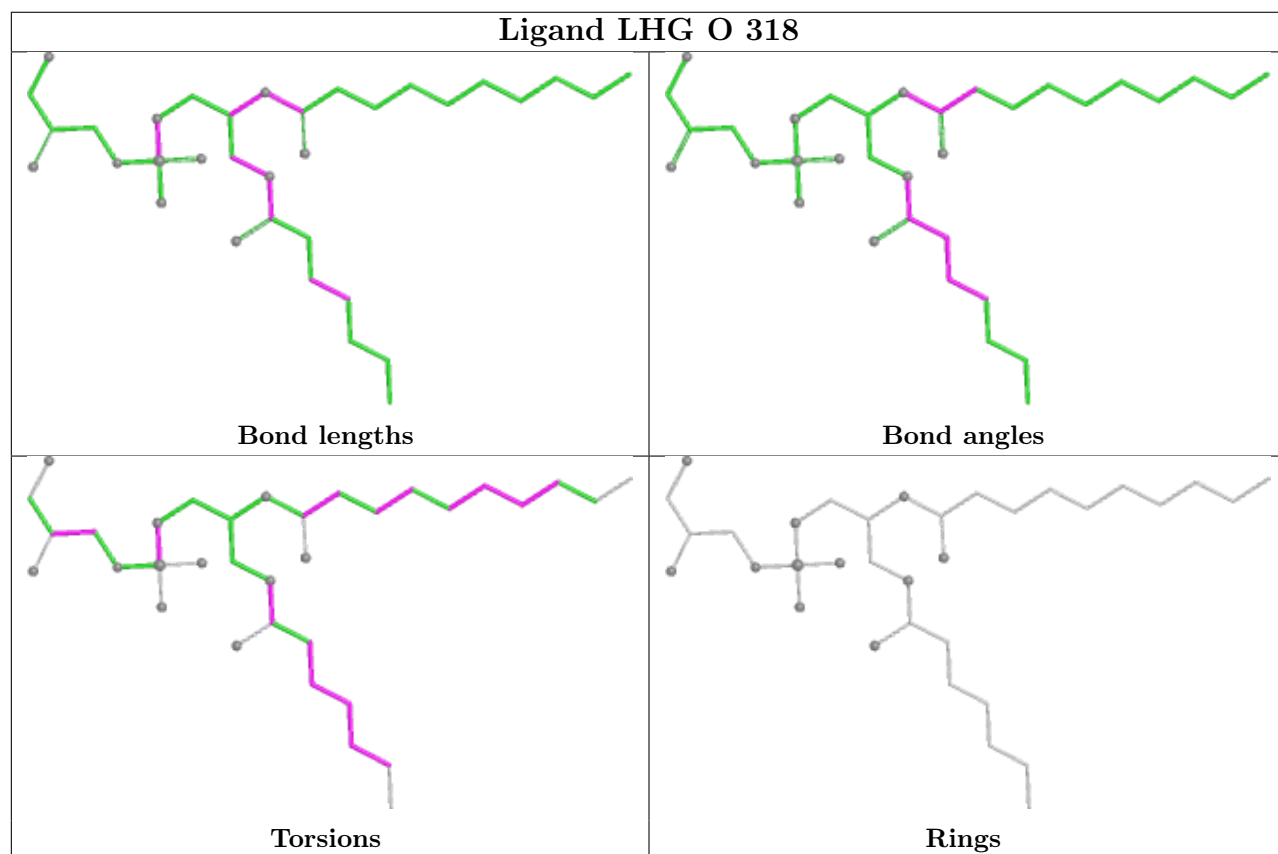
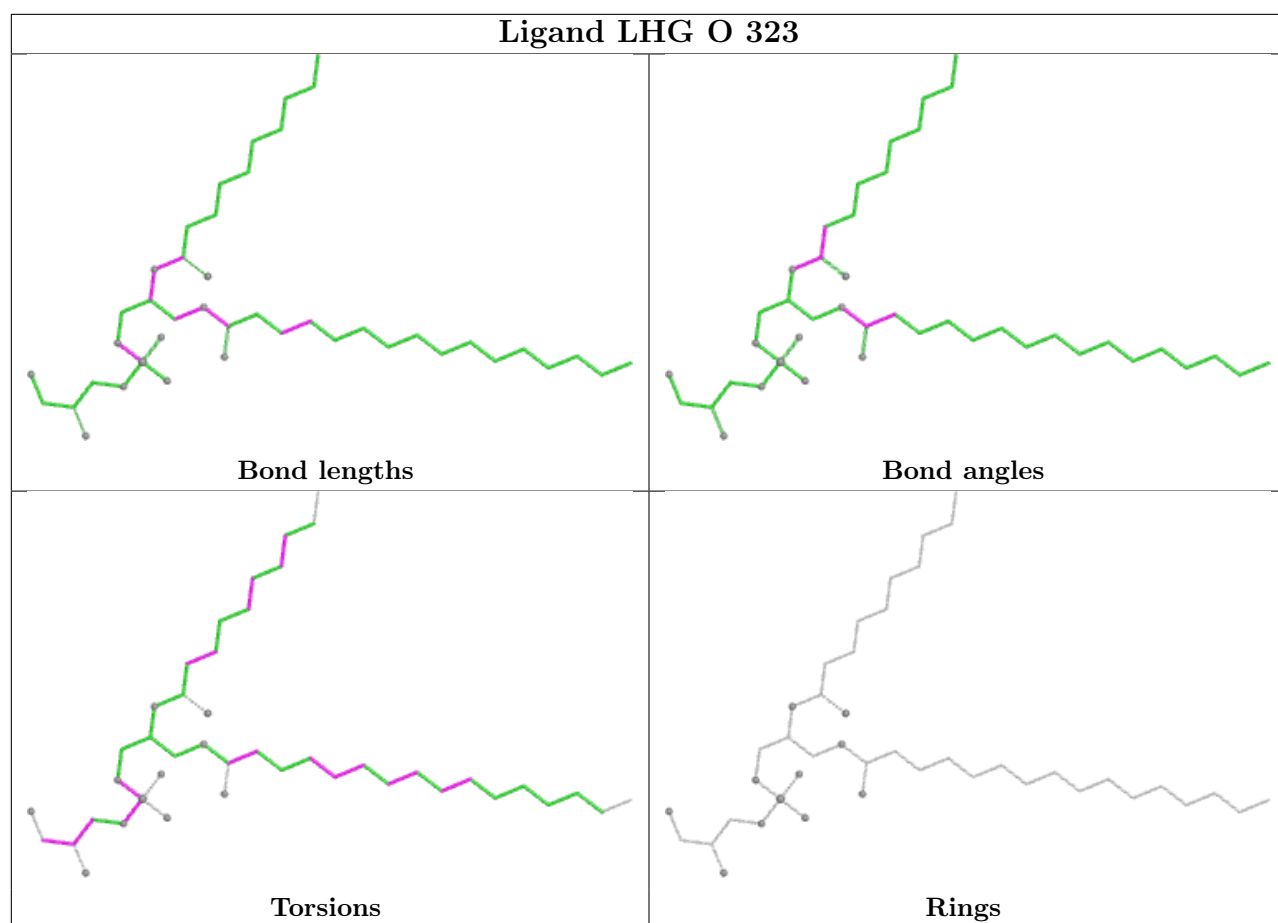


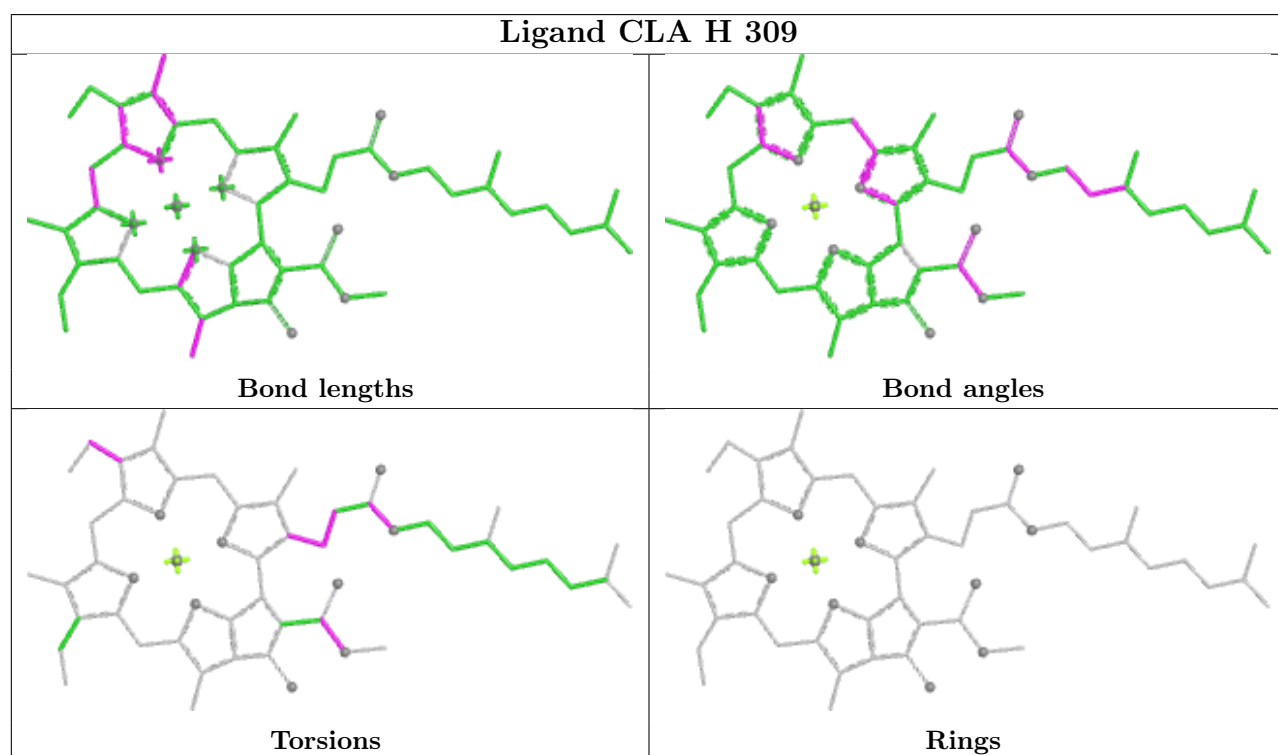
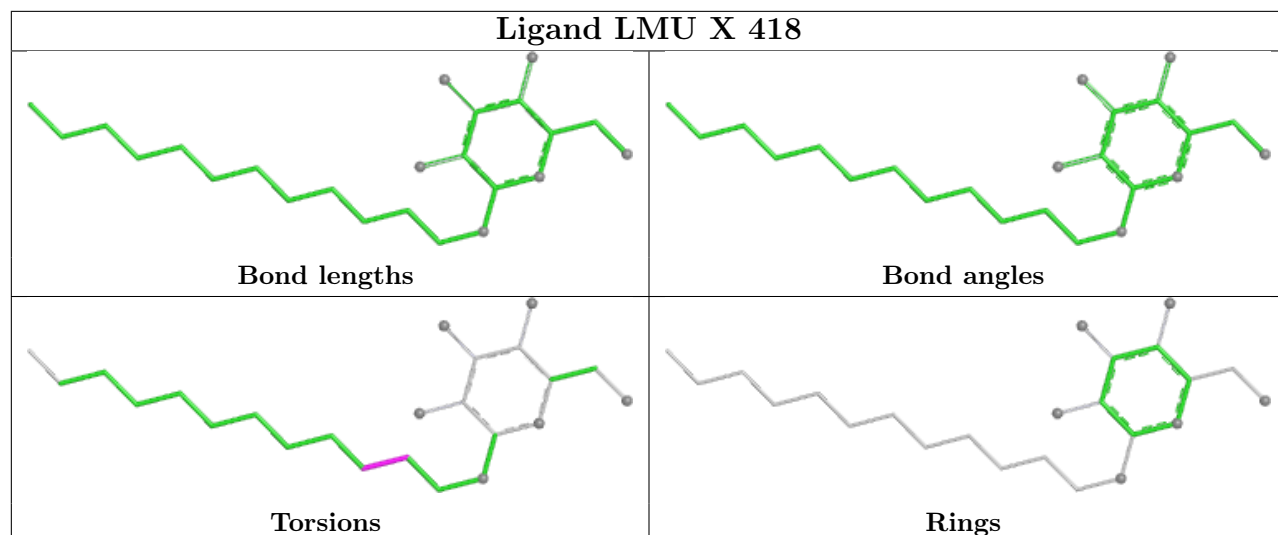
Rings

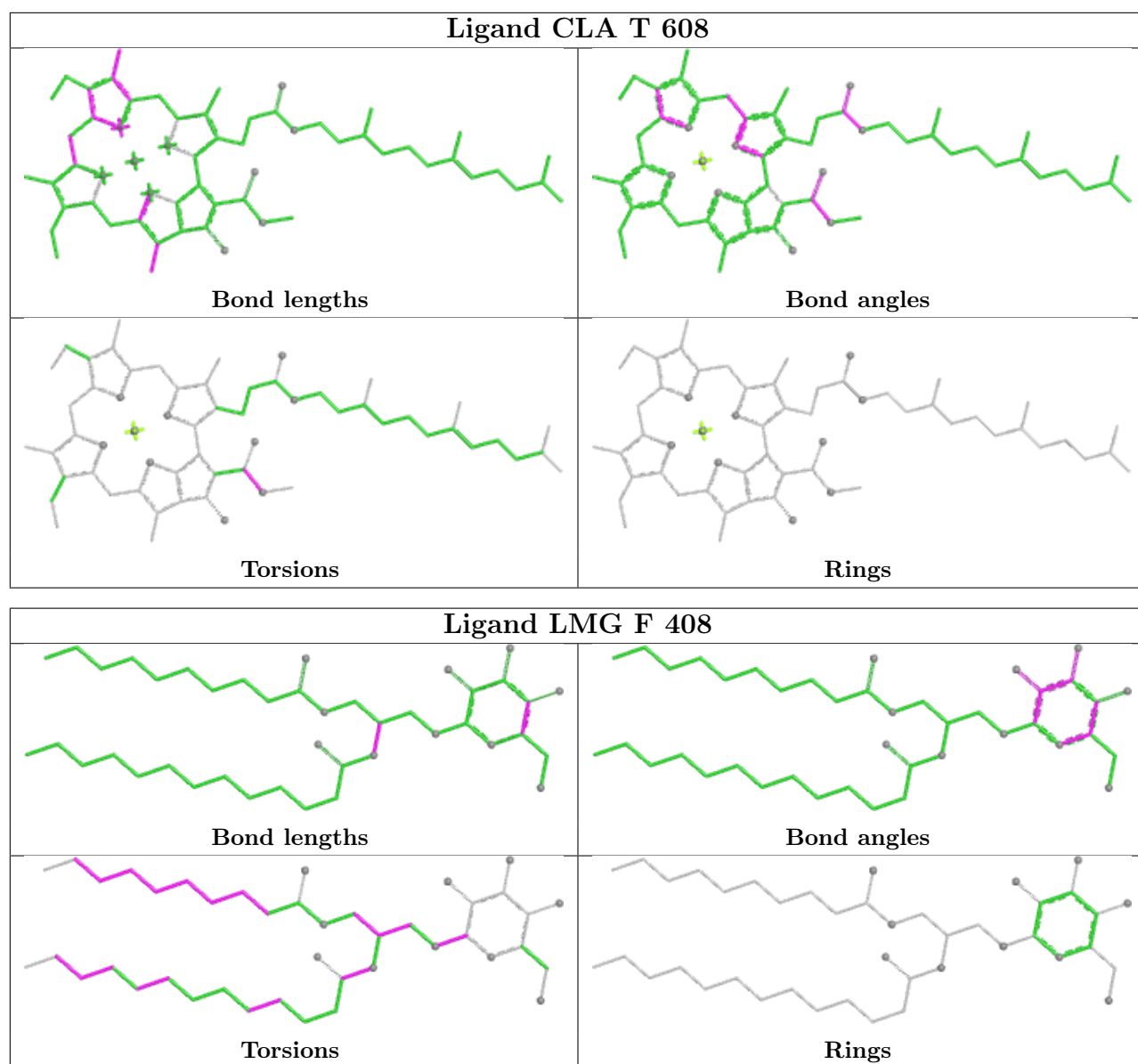




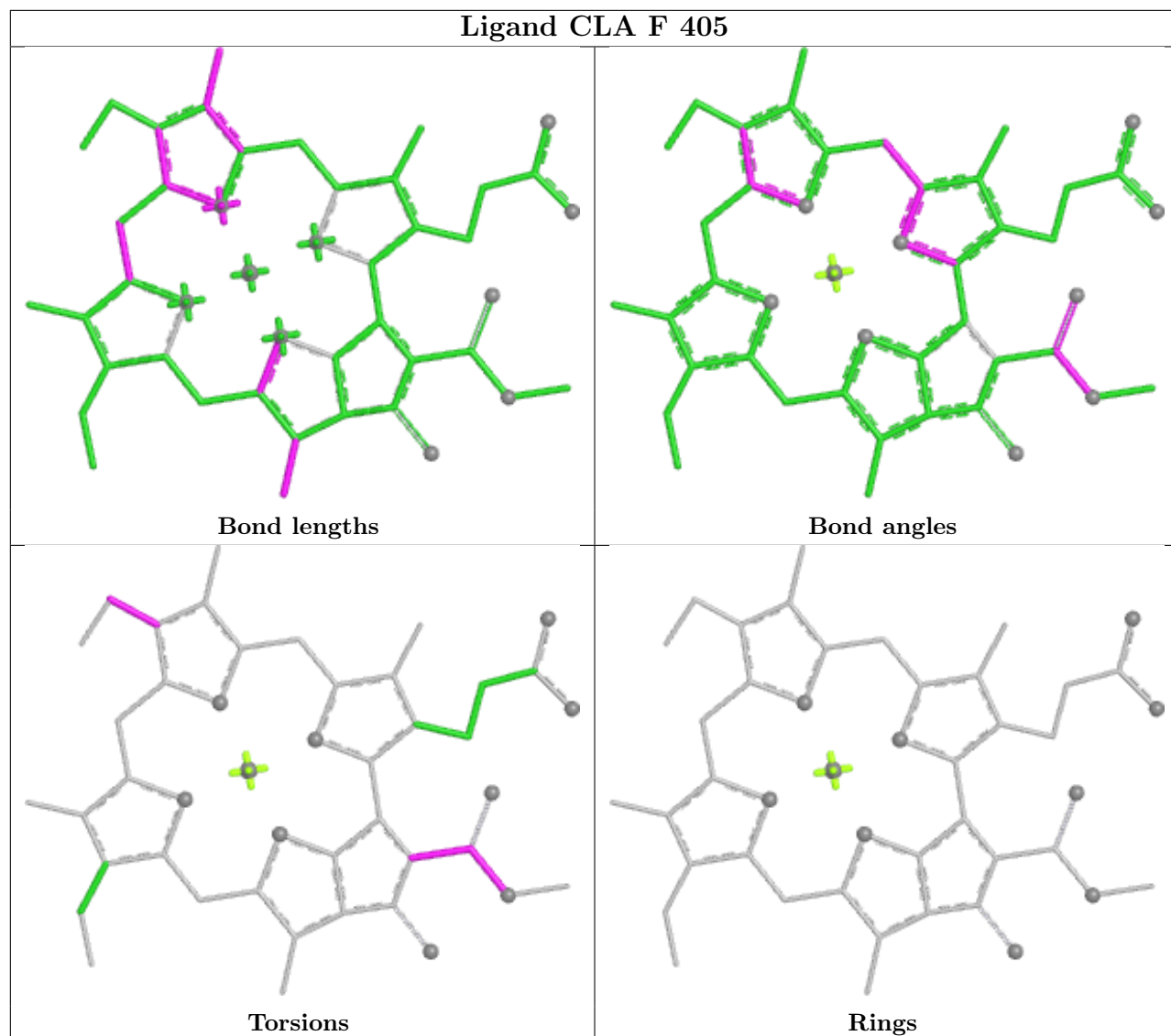


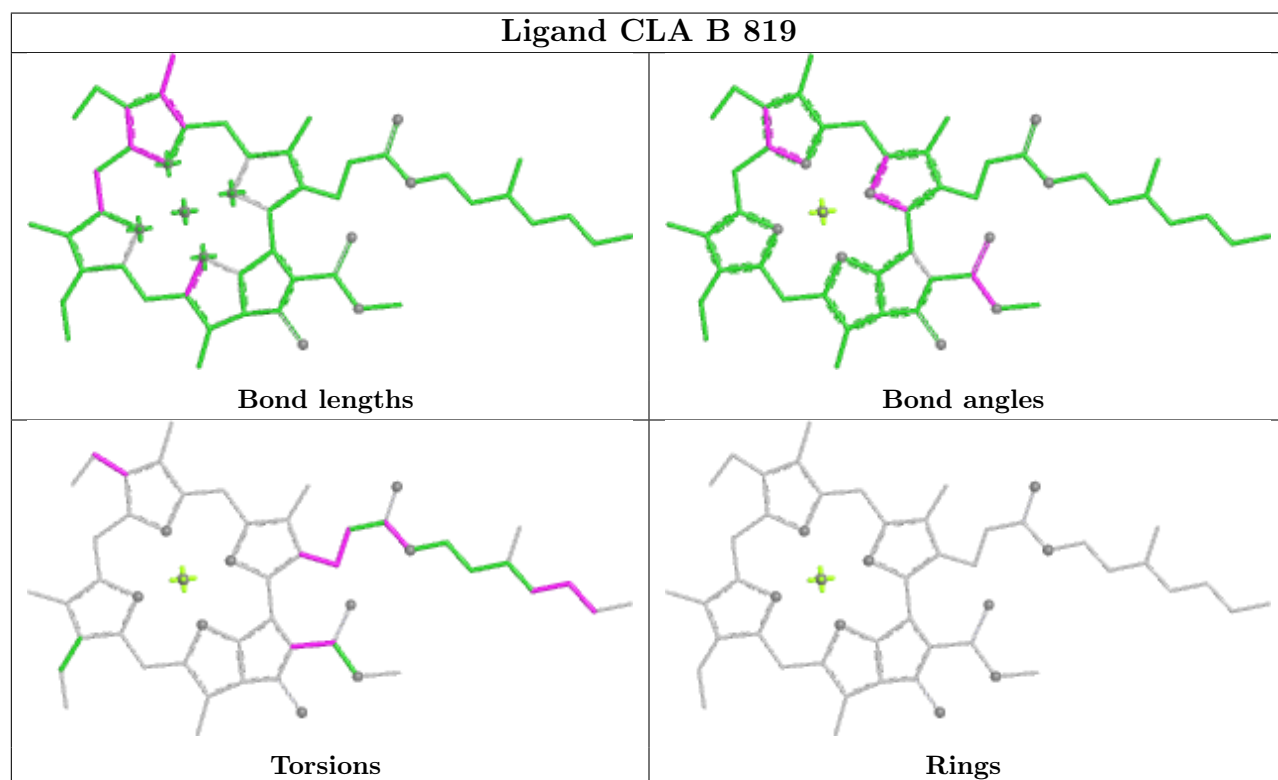
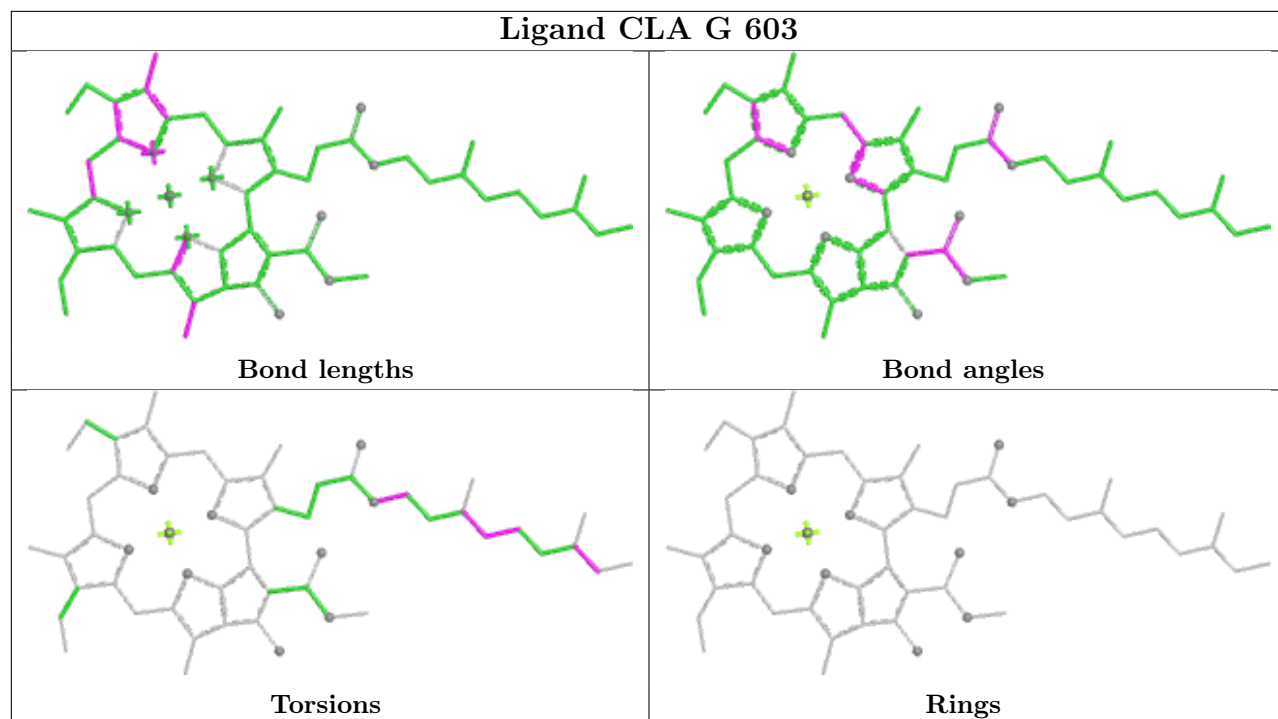


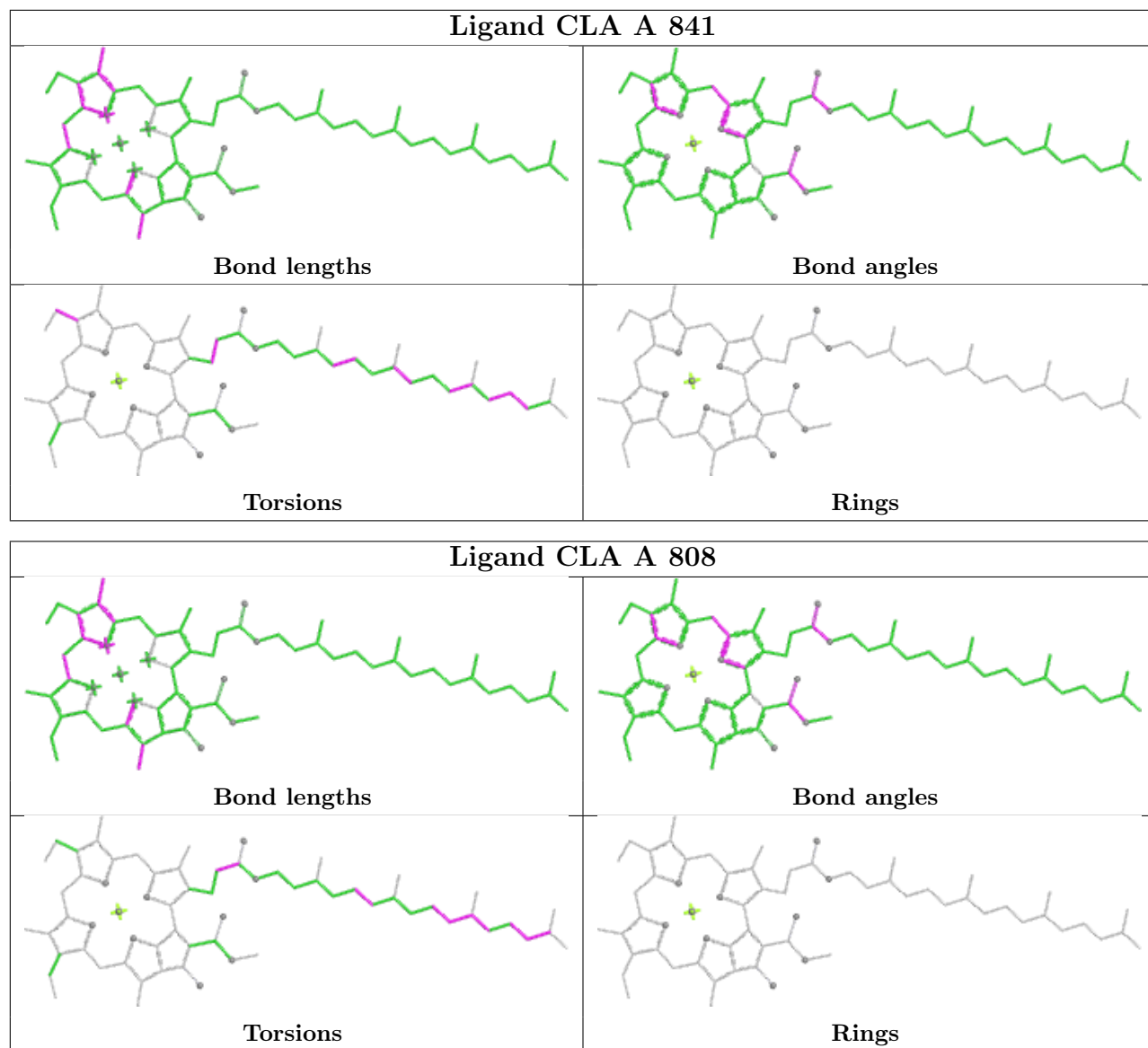


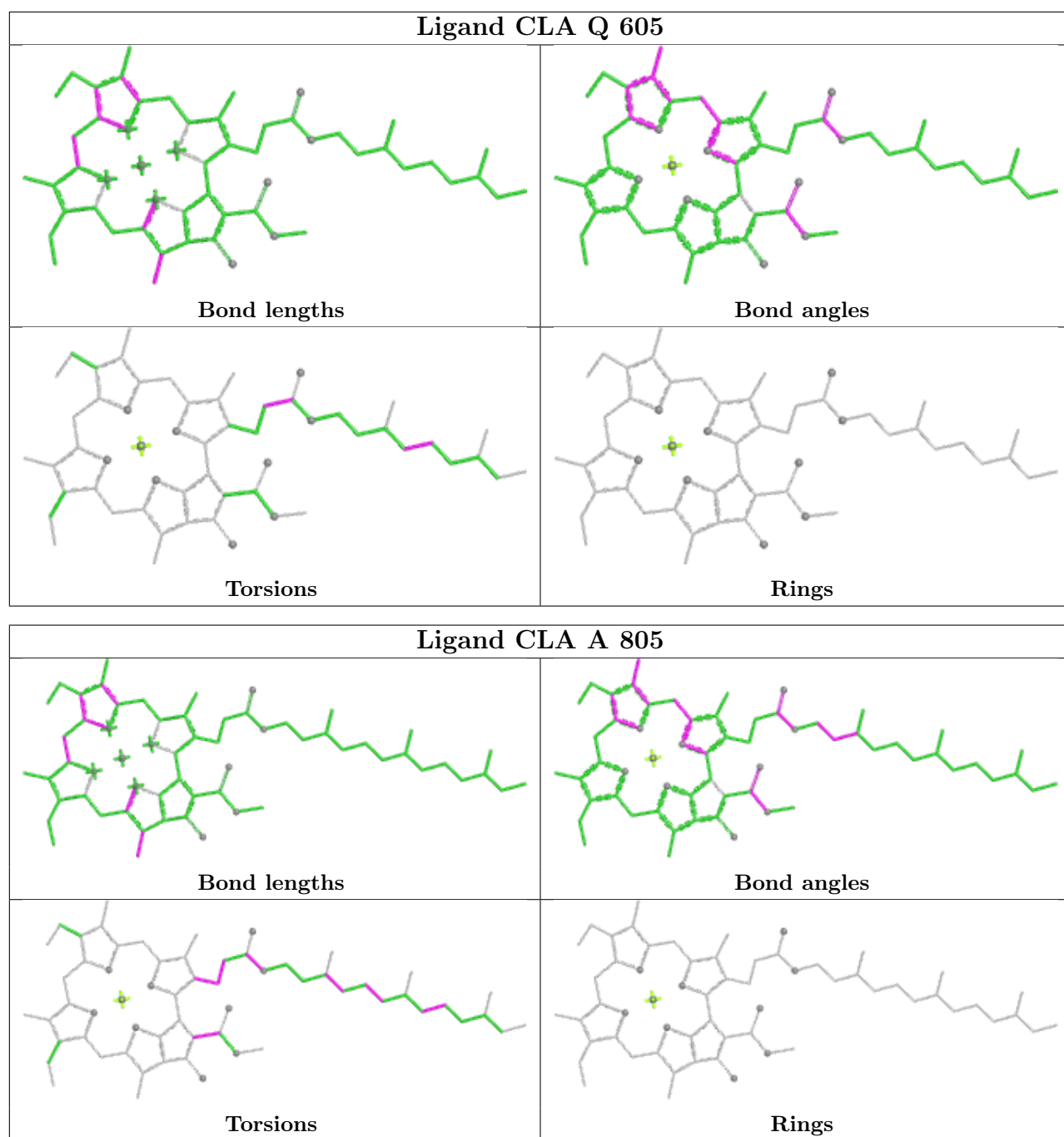


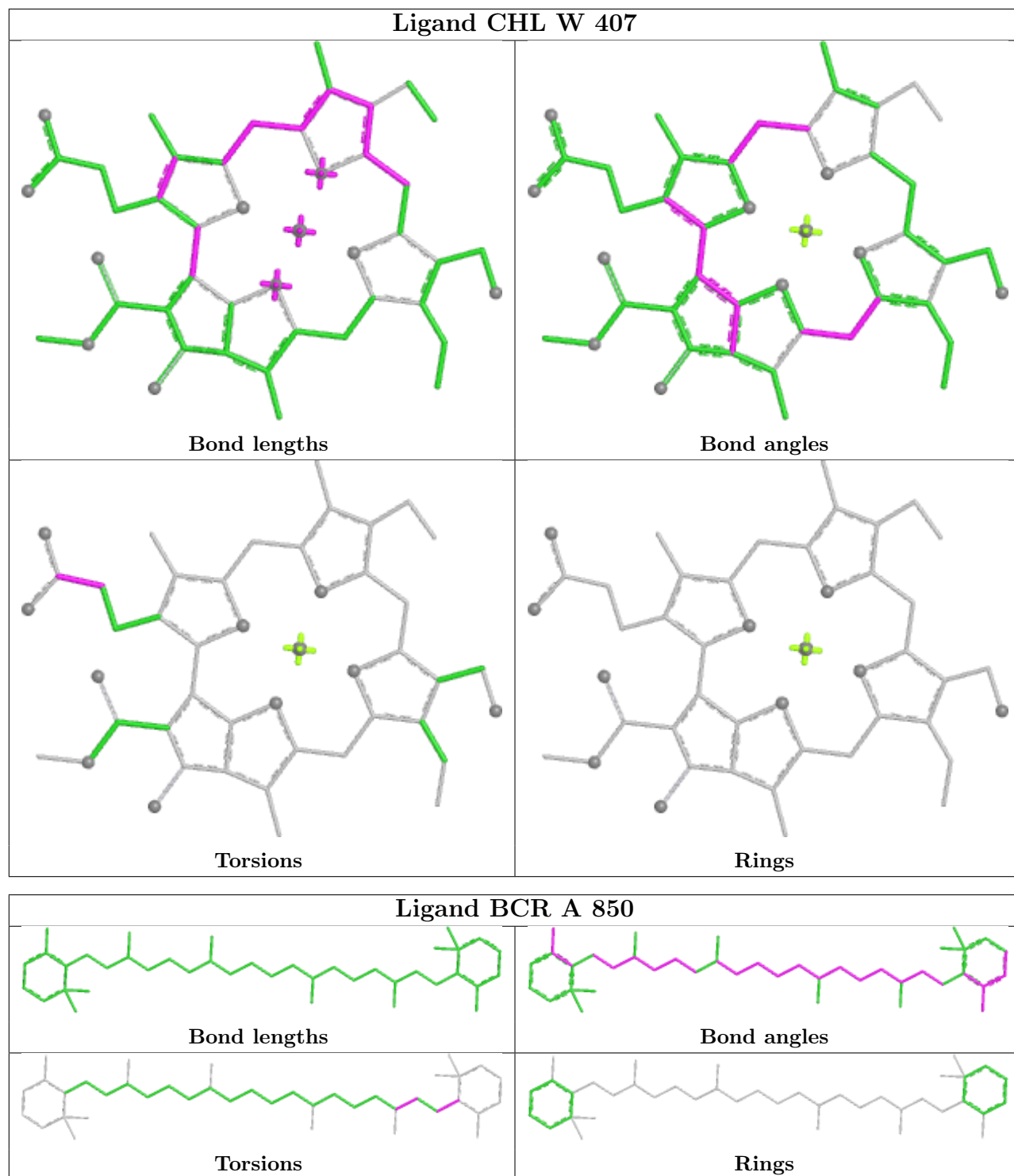
## Ligand CLA F 405





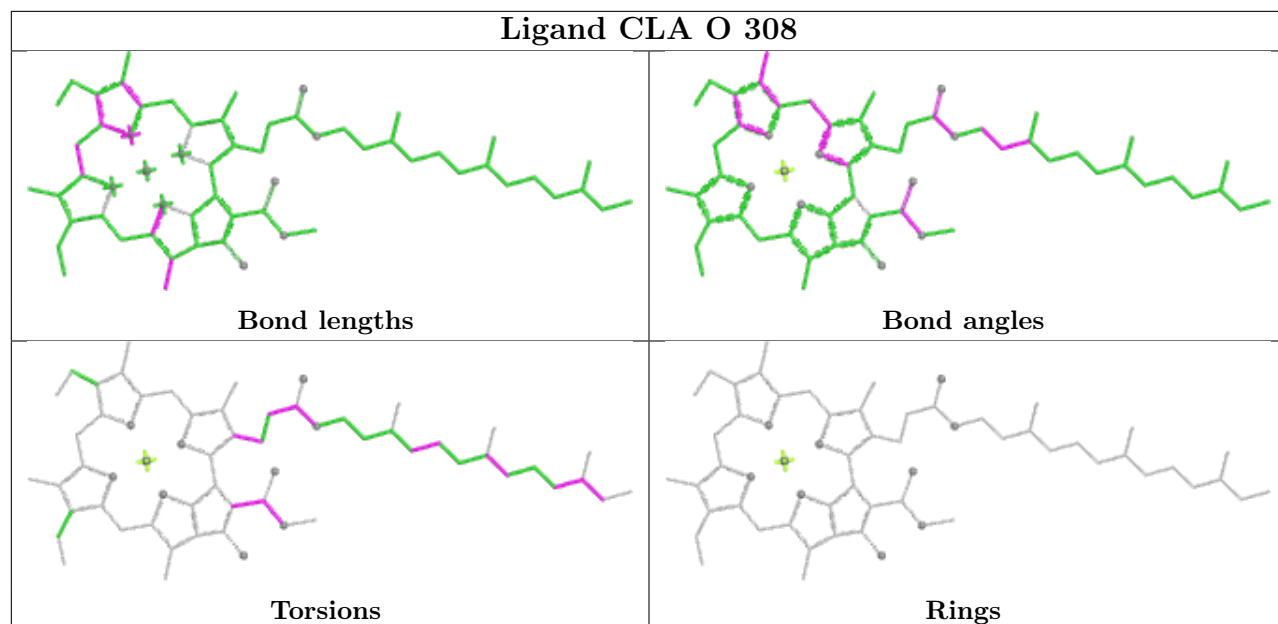




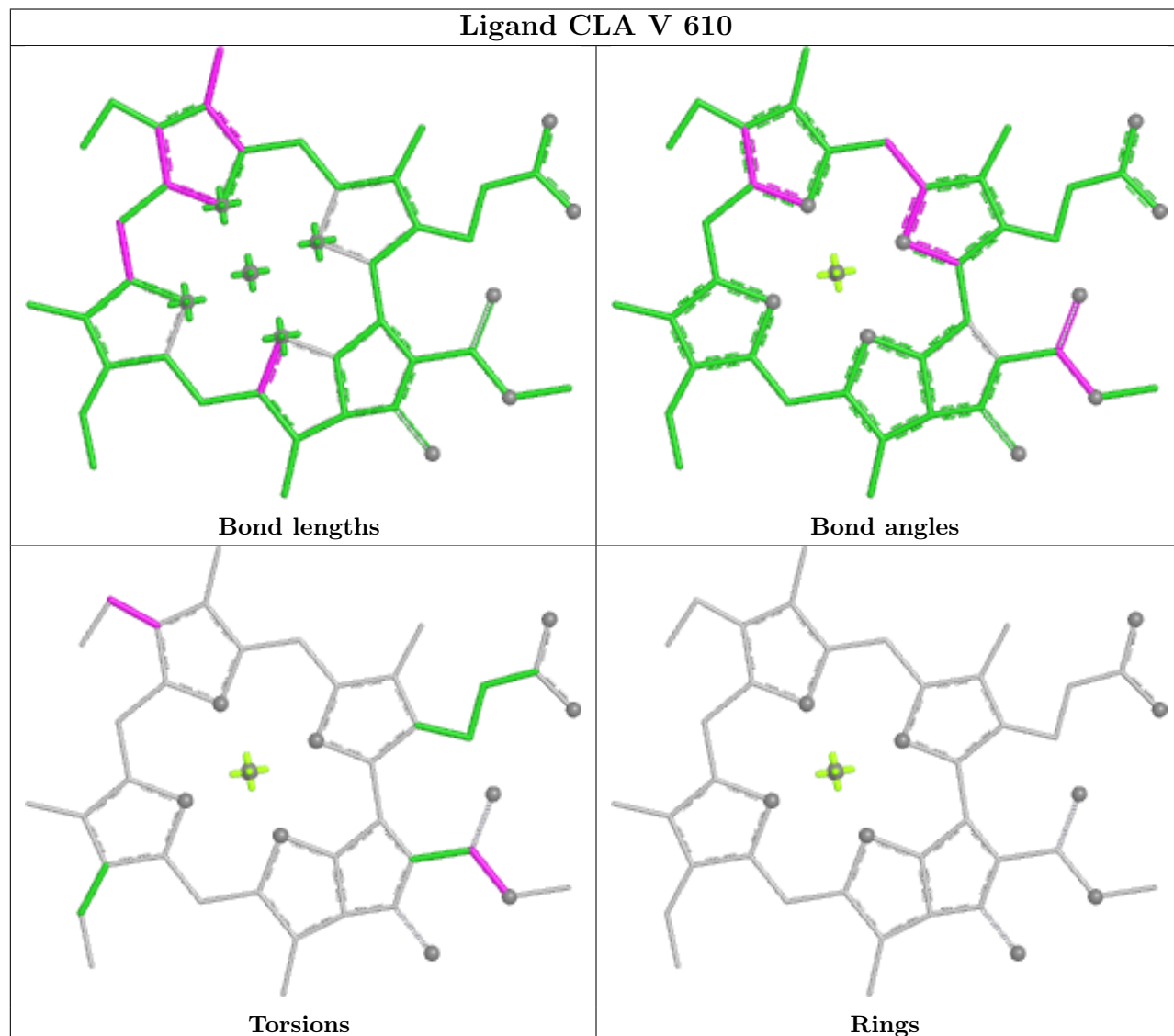


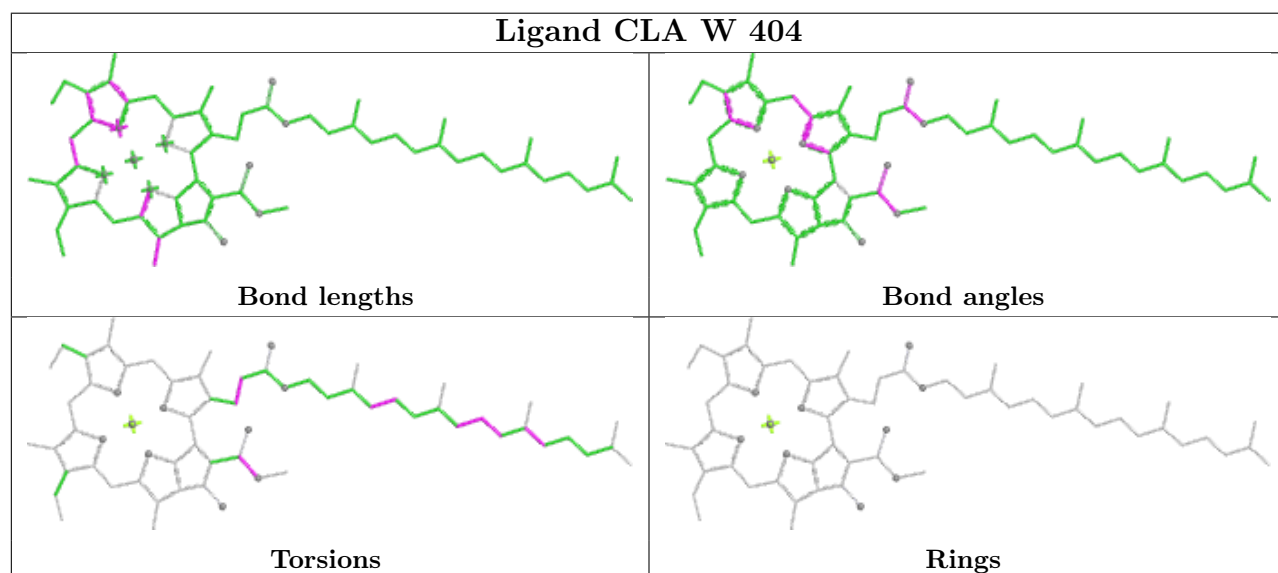
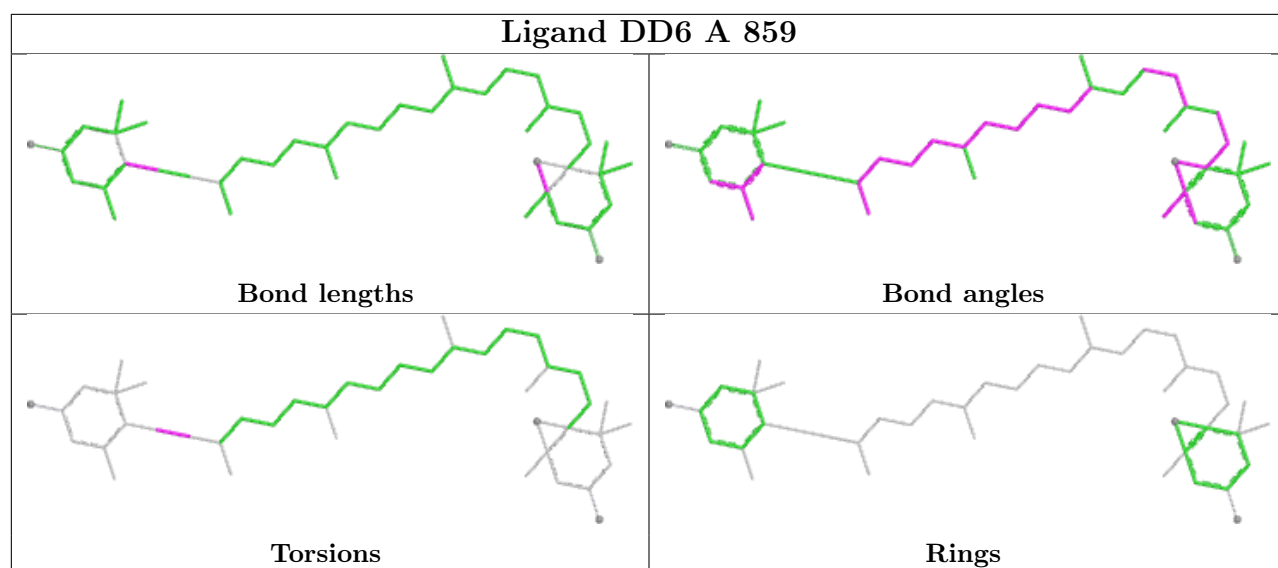


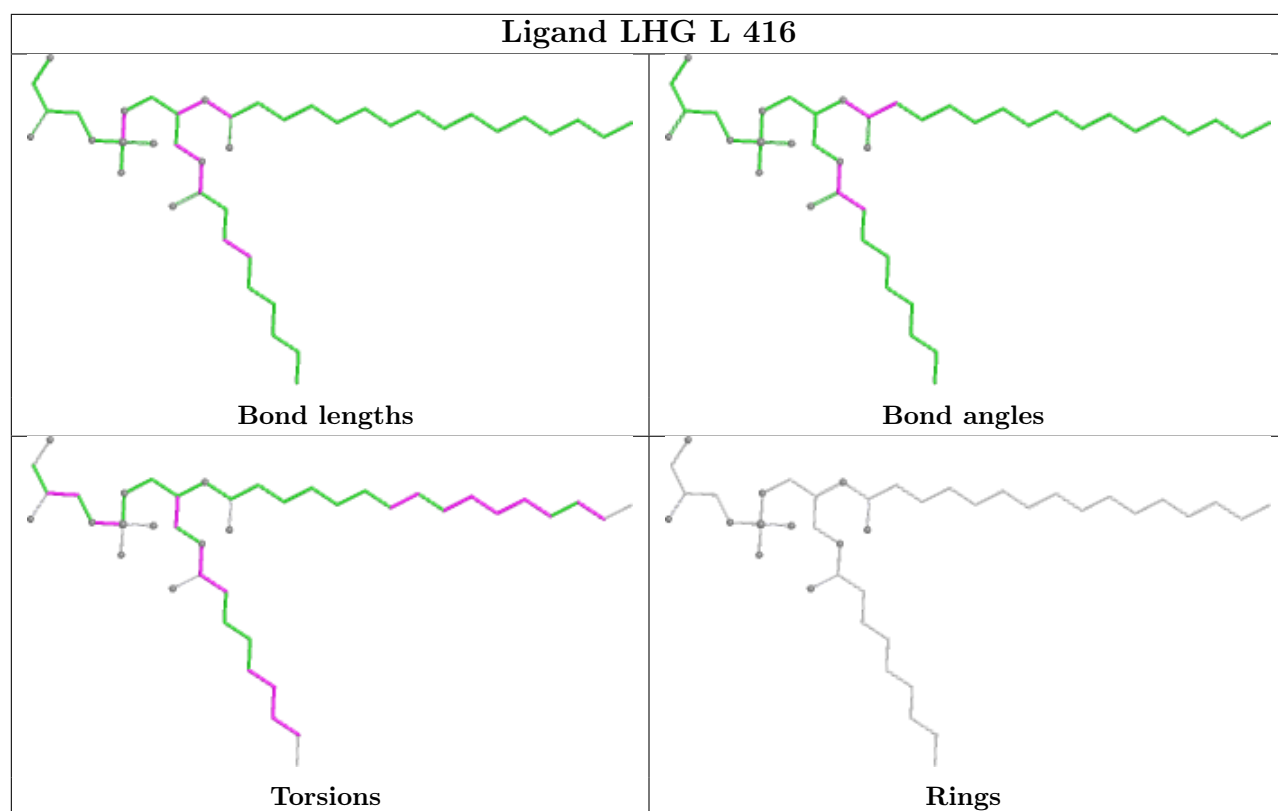
## Ligand CLA O 308

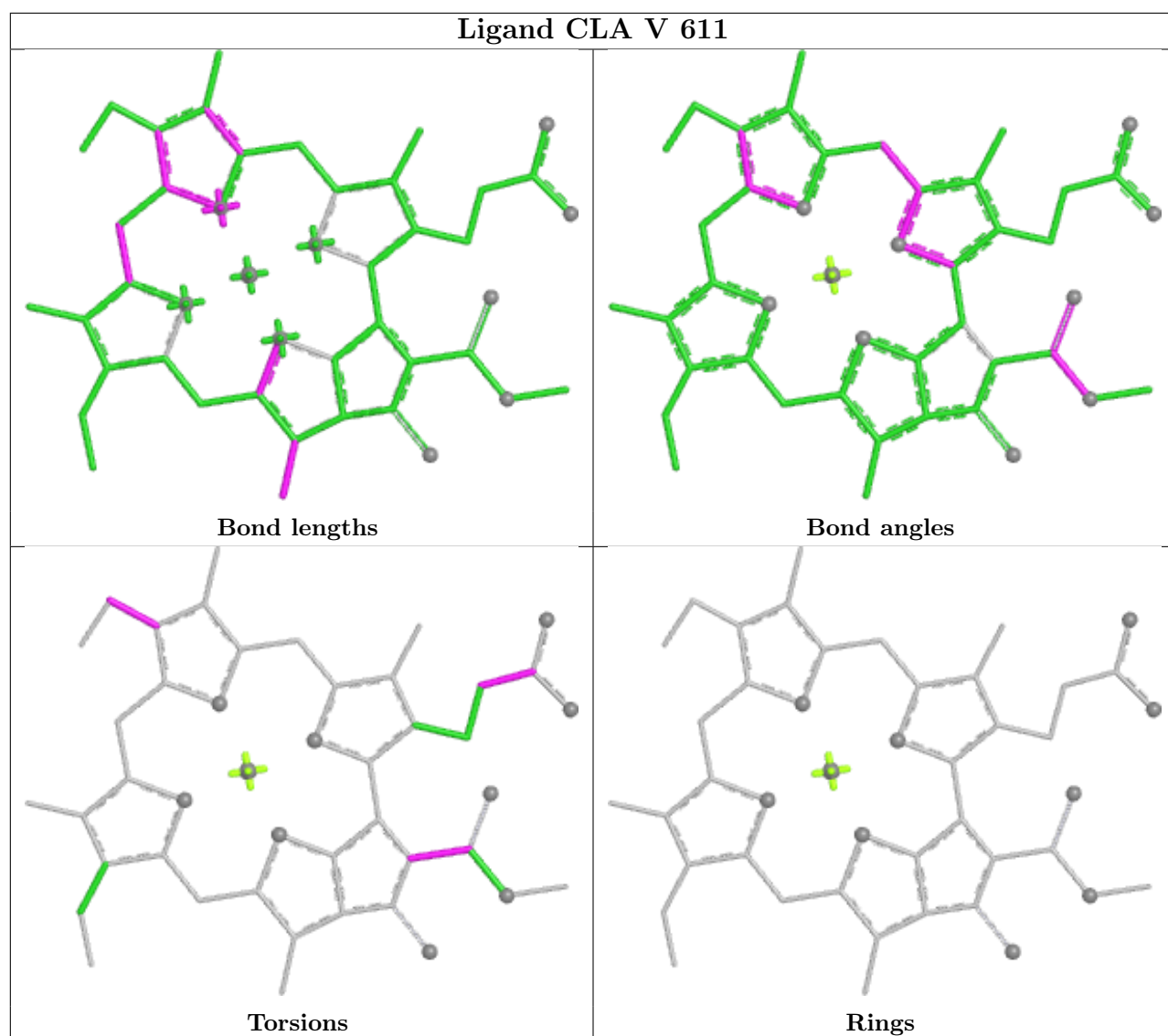


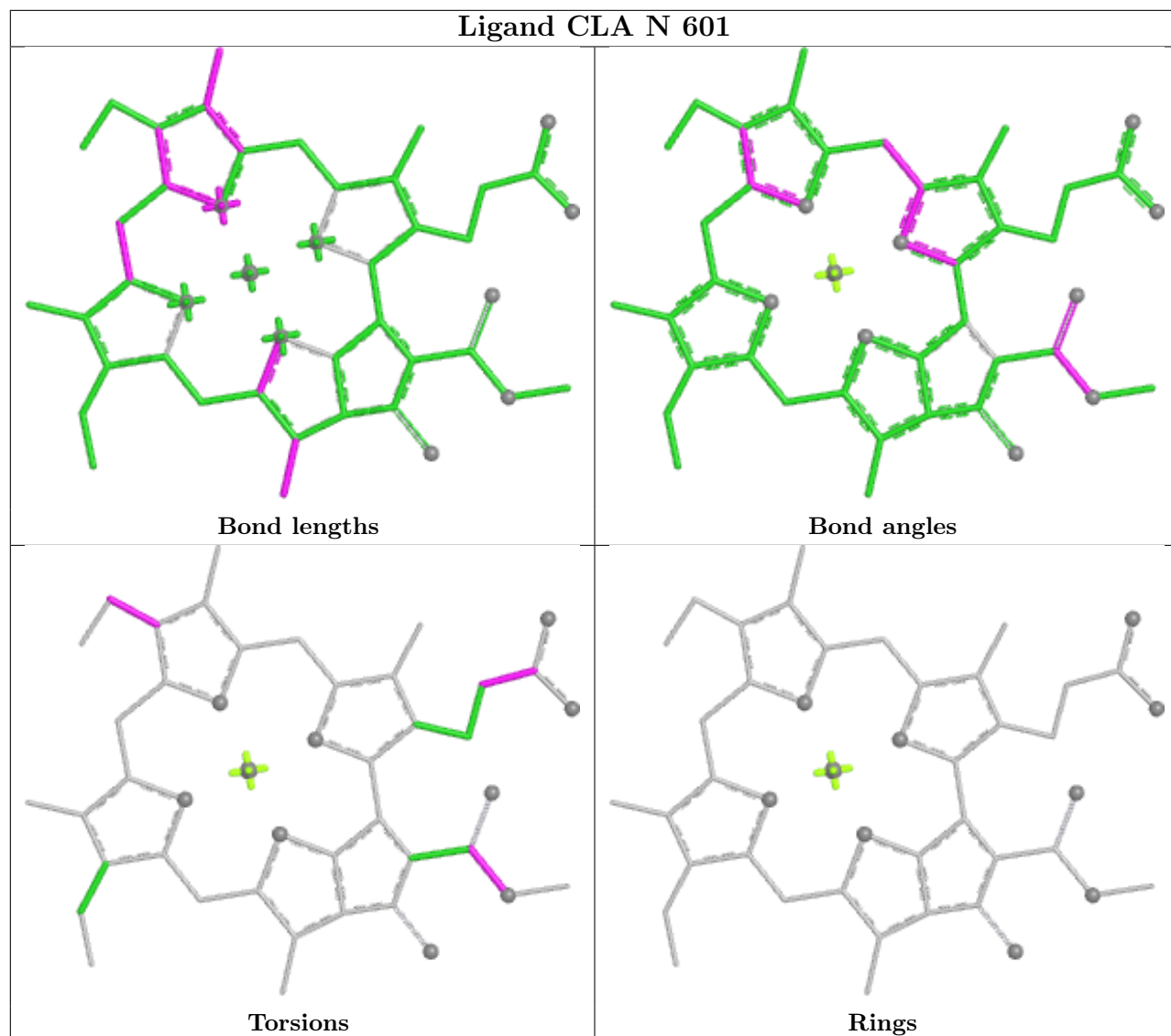
## Ligand CLA V 610

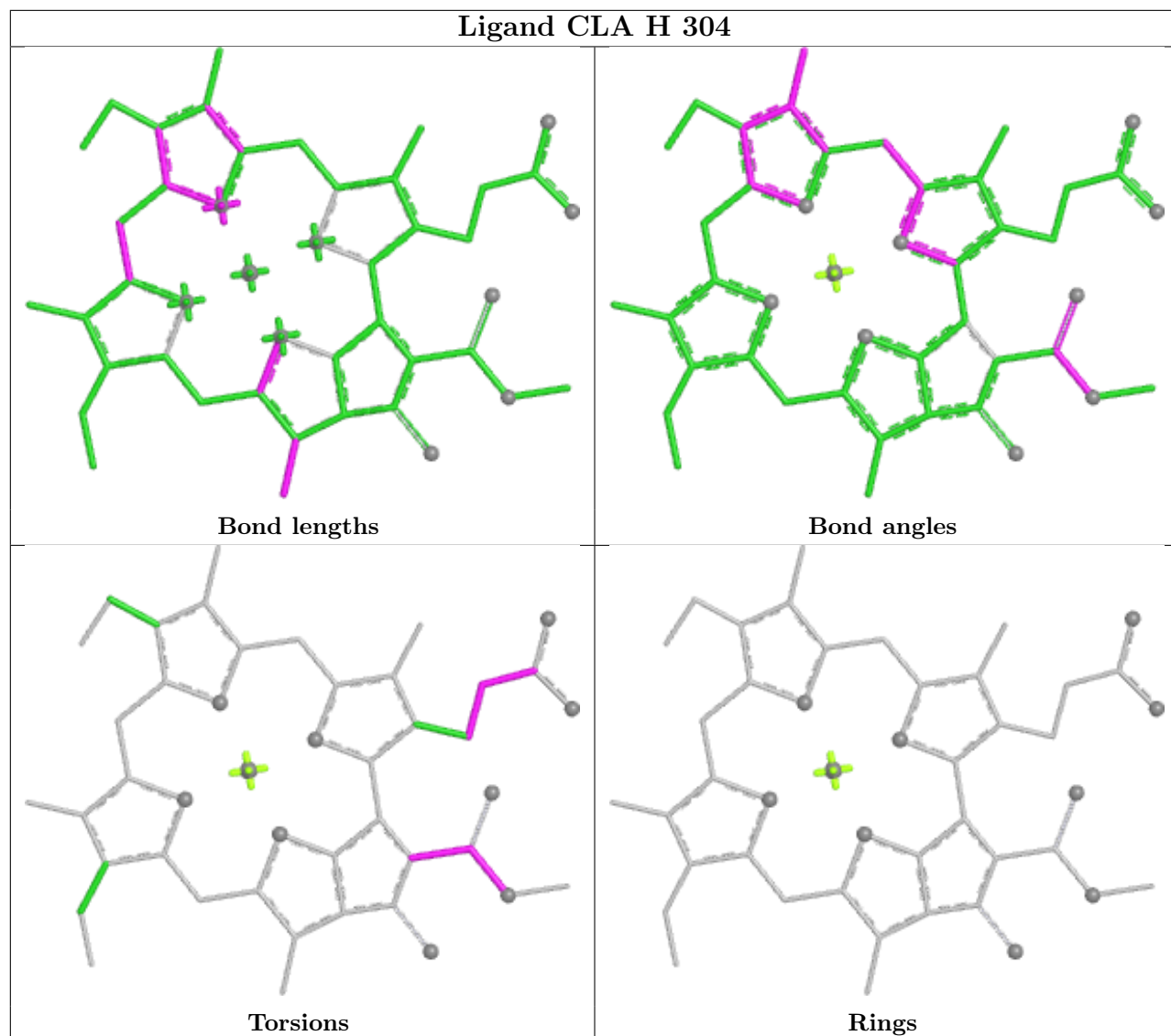


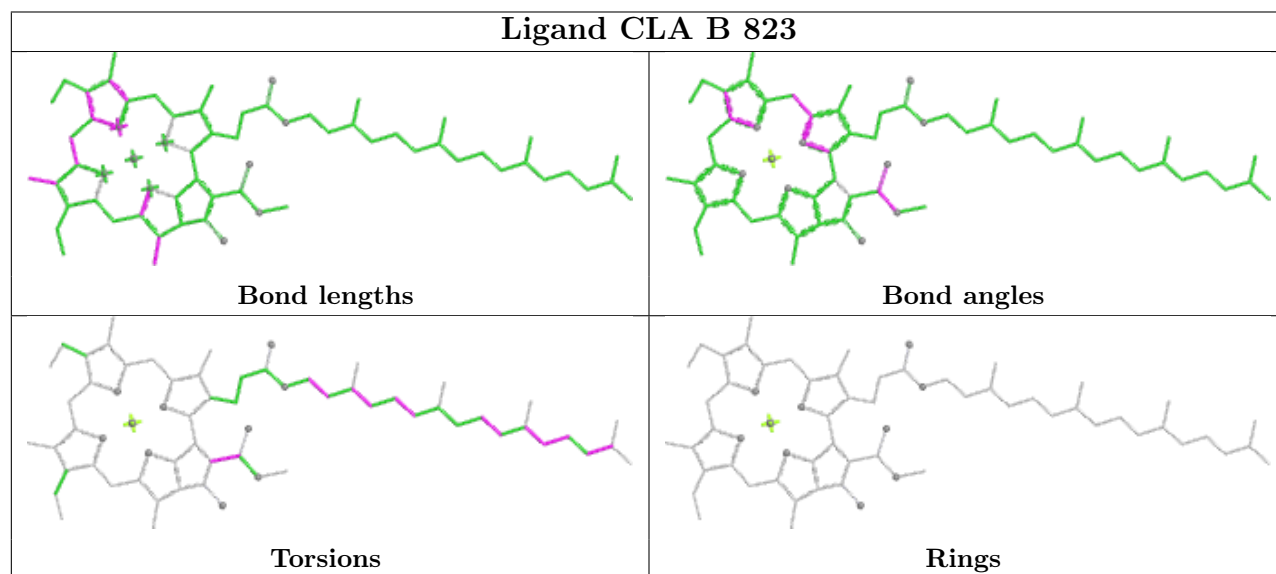
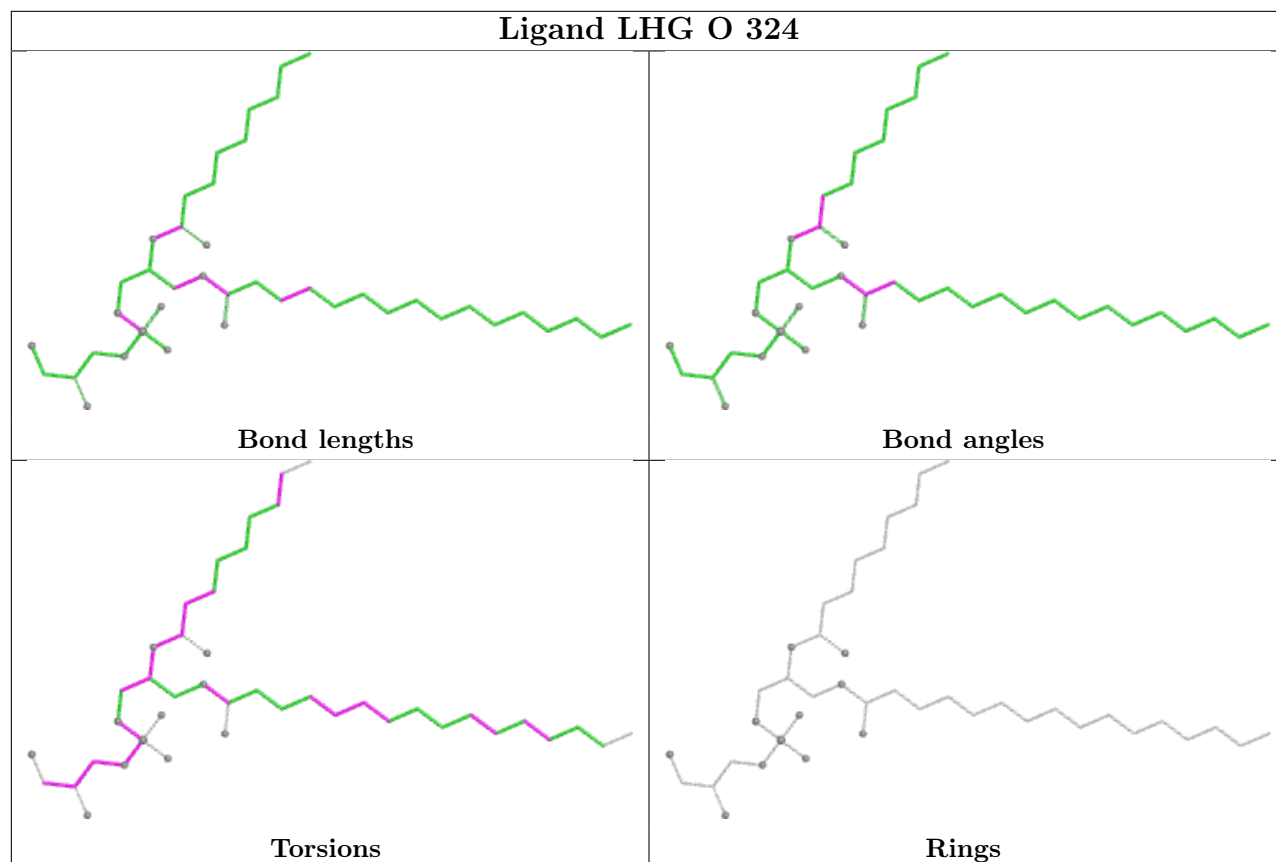




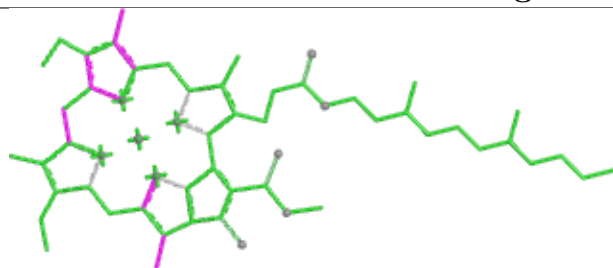




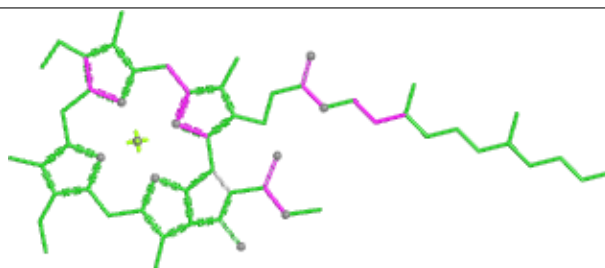




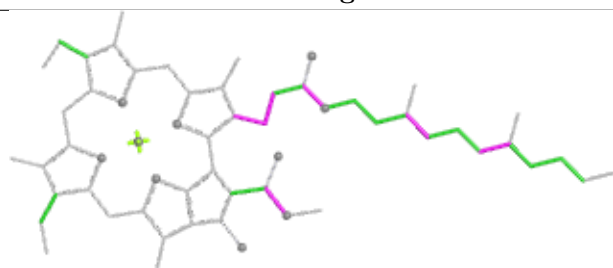
## Ligand CLA B 826



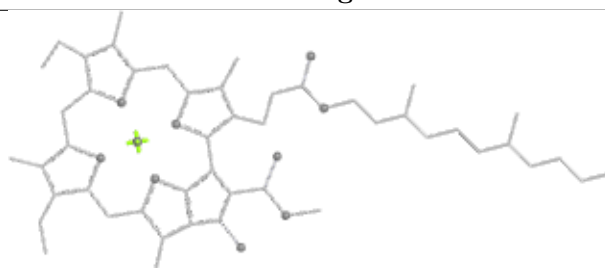
Bond lengths



Bond angles

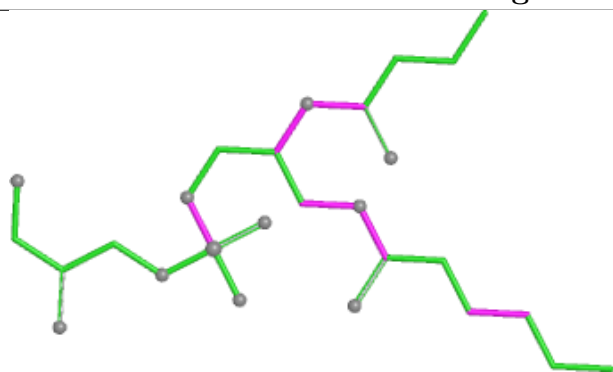


Torsions

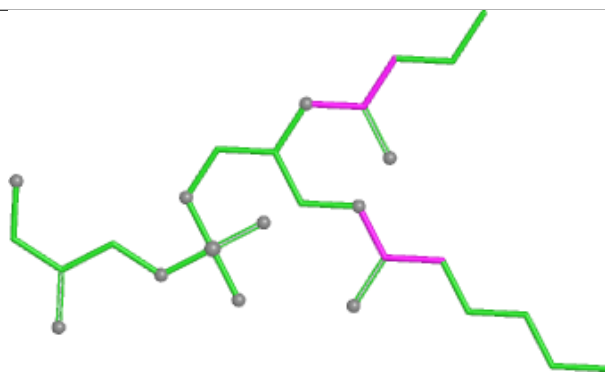


Rings

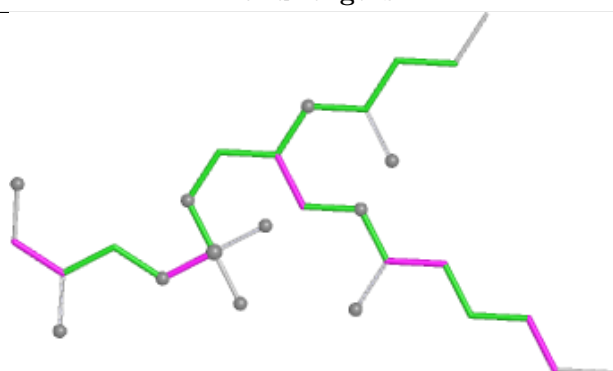
## Ligand LHG H 316



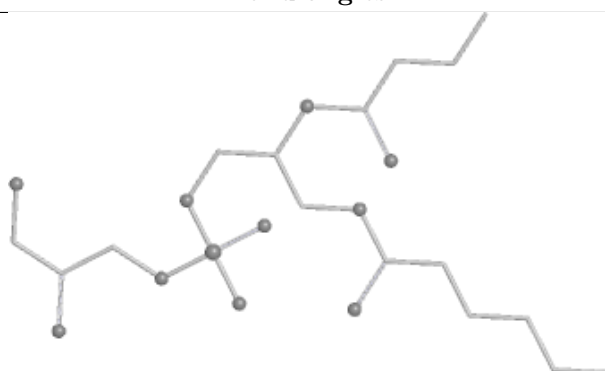
Bond lengths



Bond angles

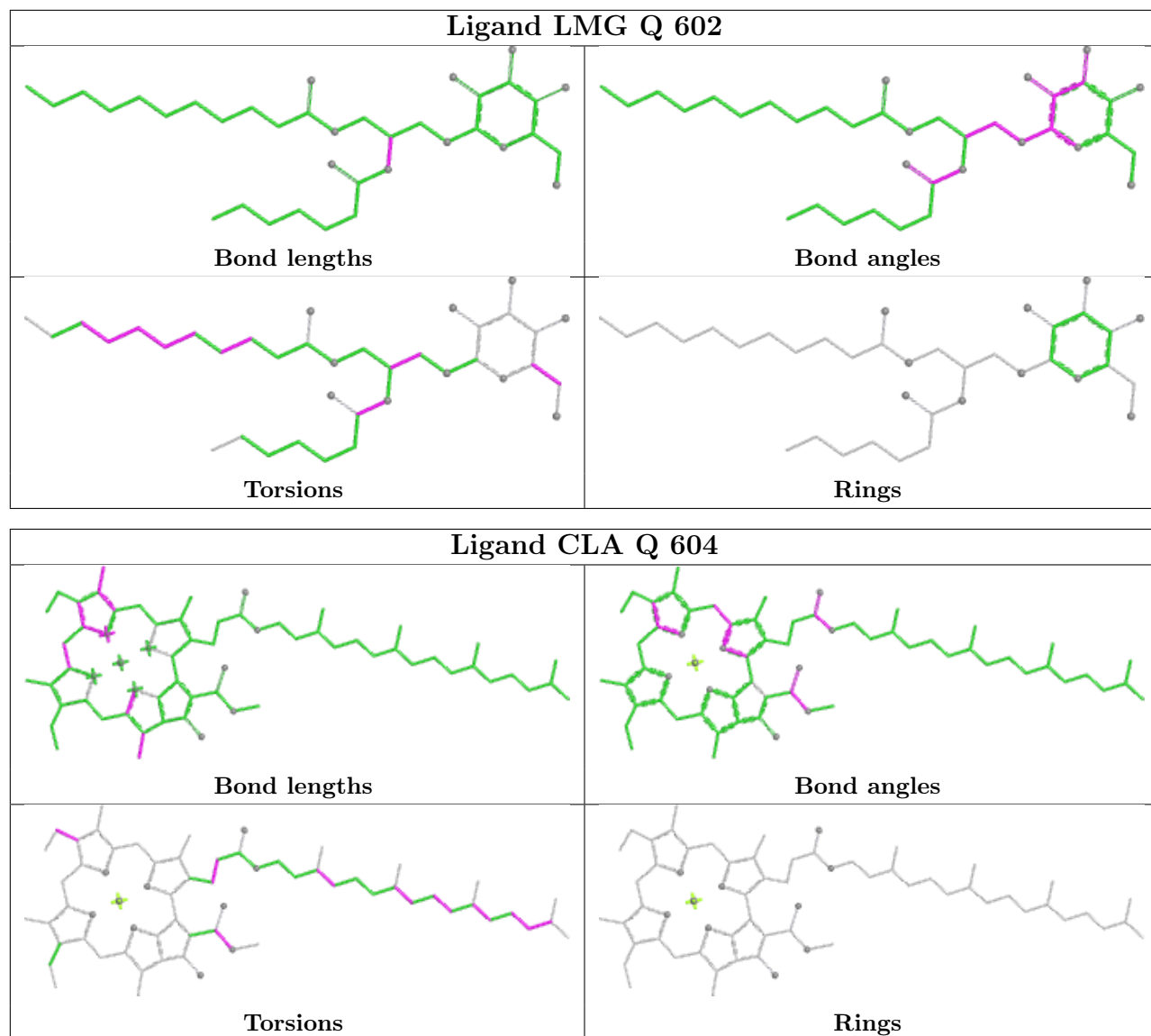


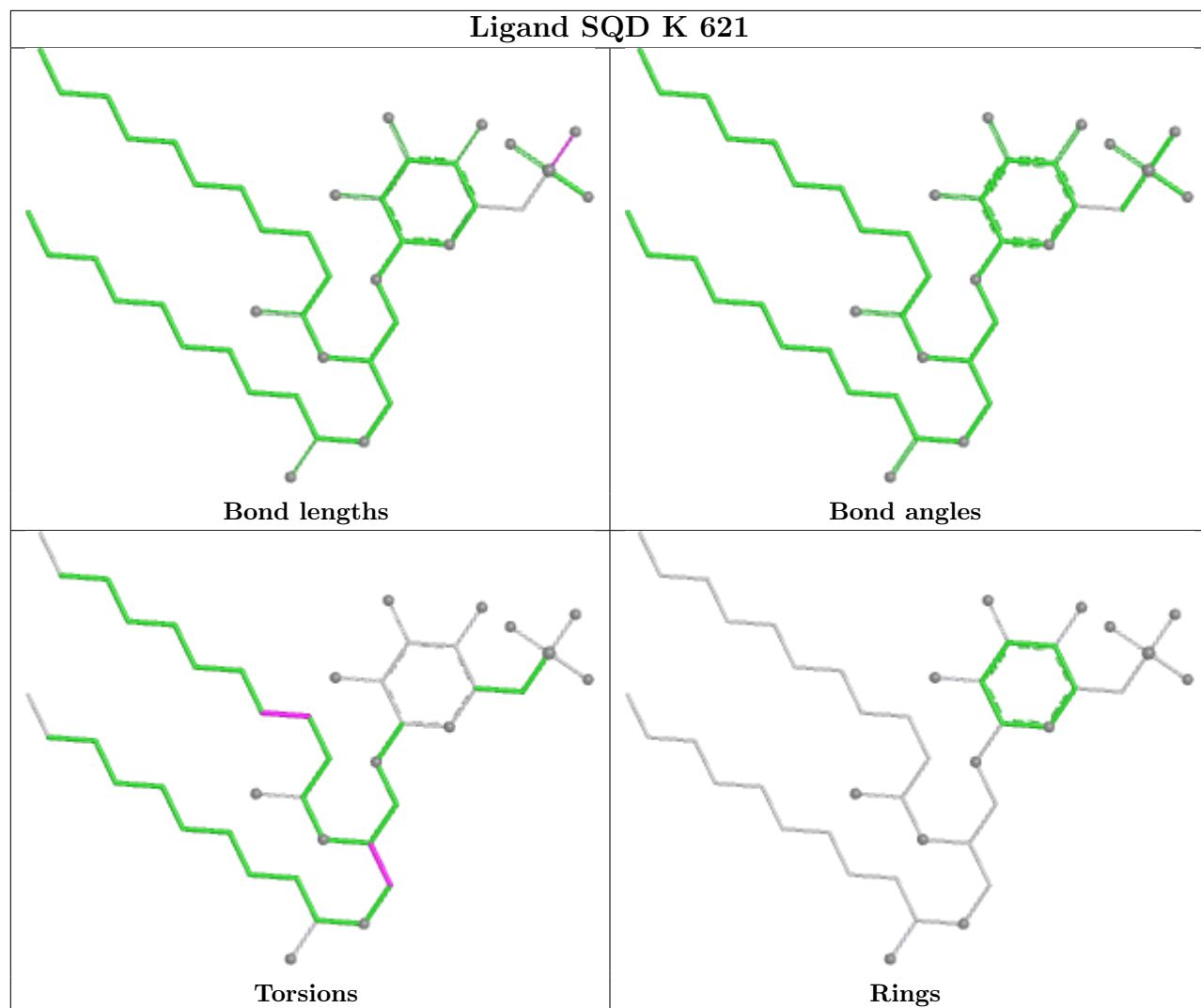
Torsions



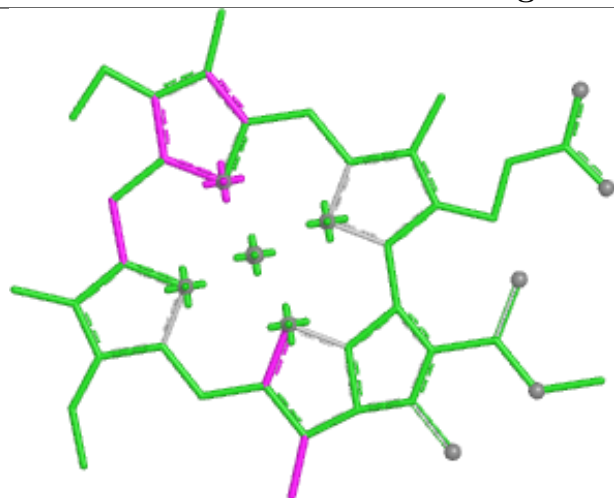
Rings



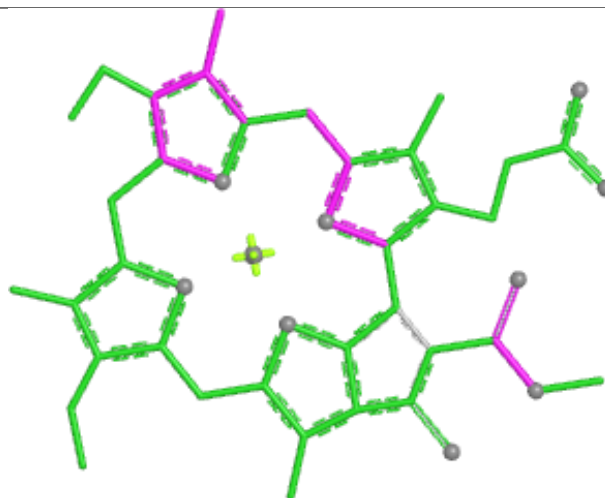




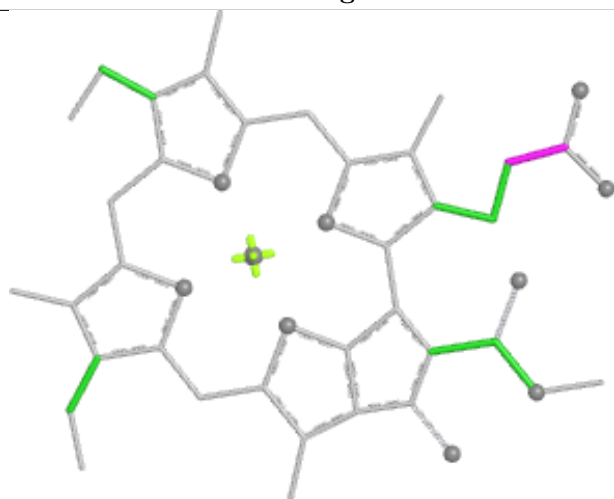
## Ligand CLA S 603



Bond lengths



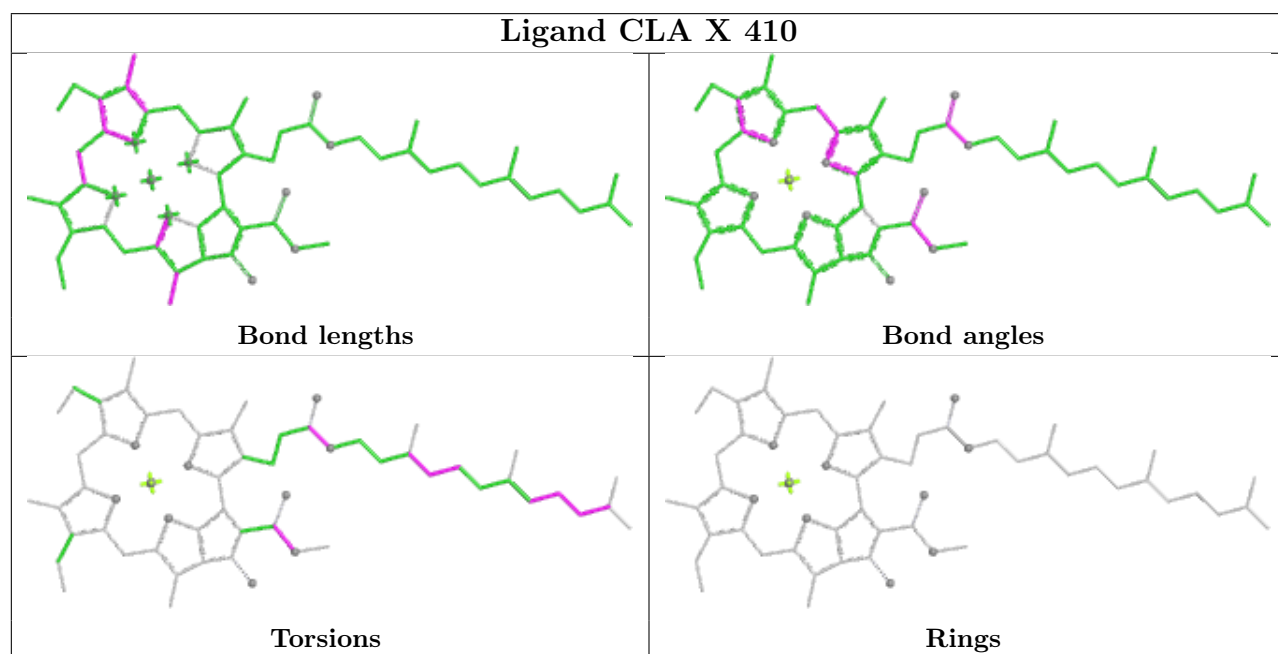
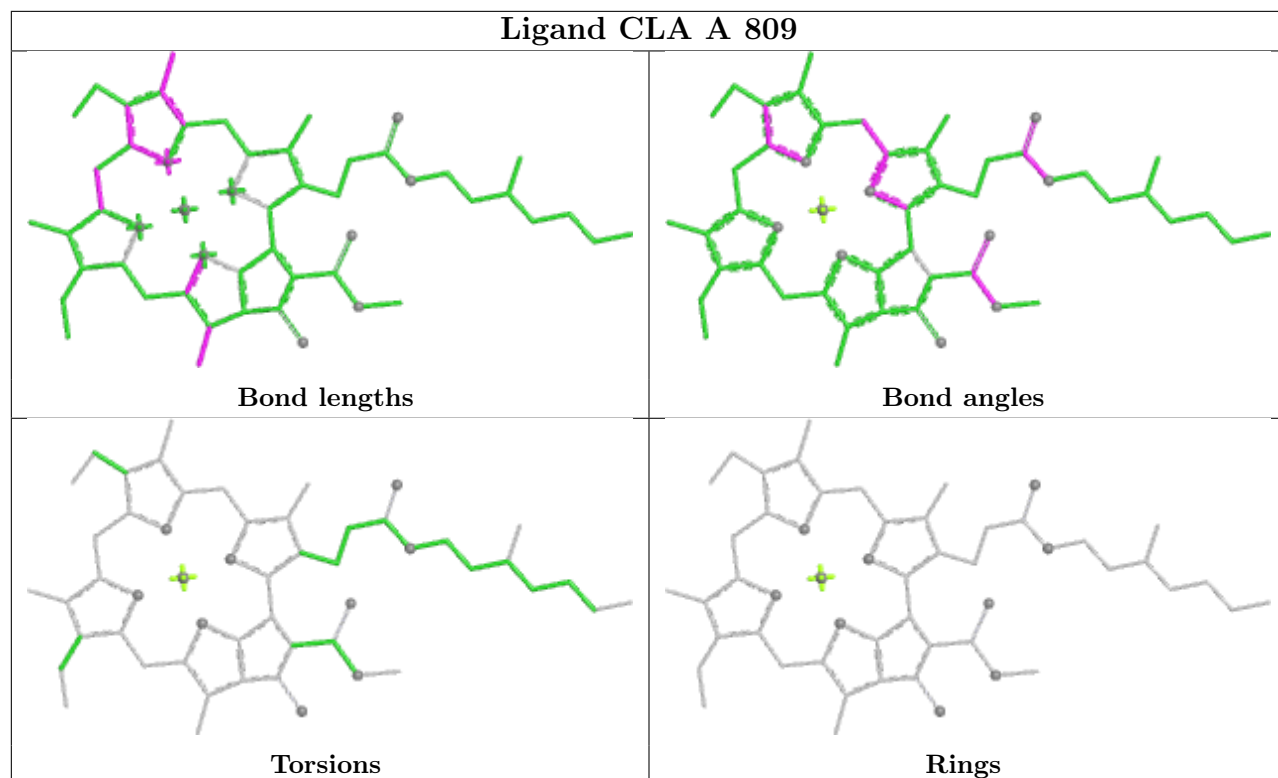
Bond angles



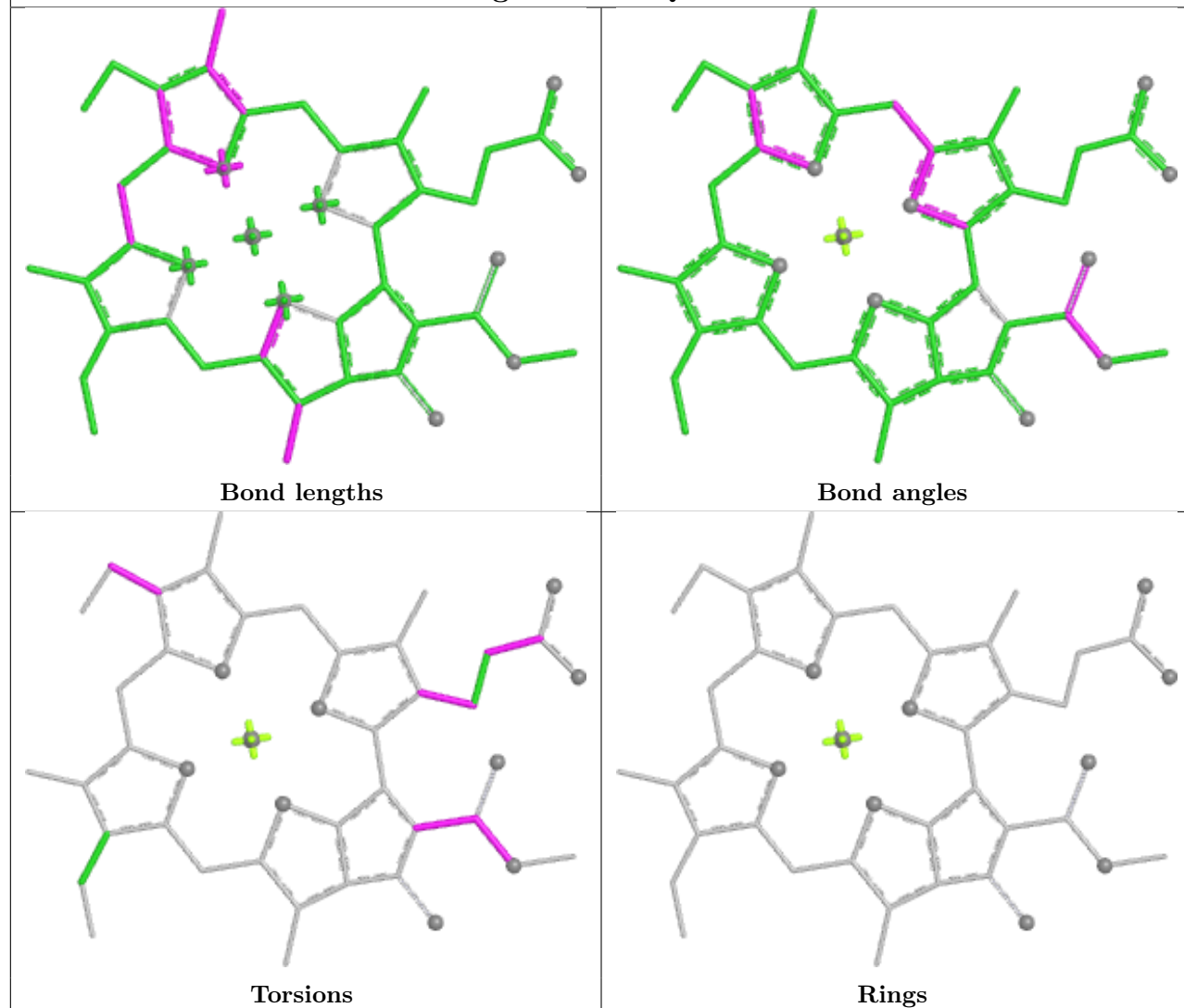
Torsions



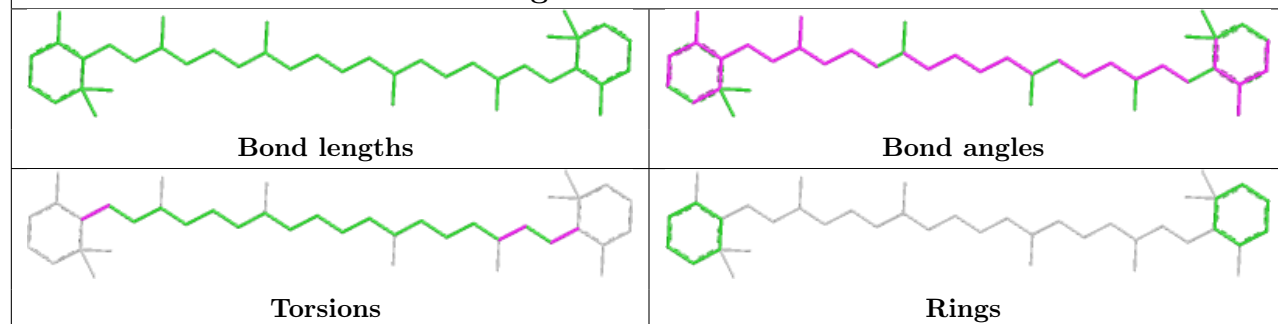
Rings

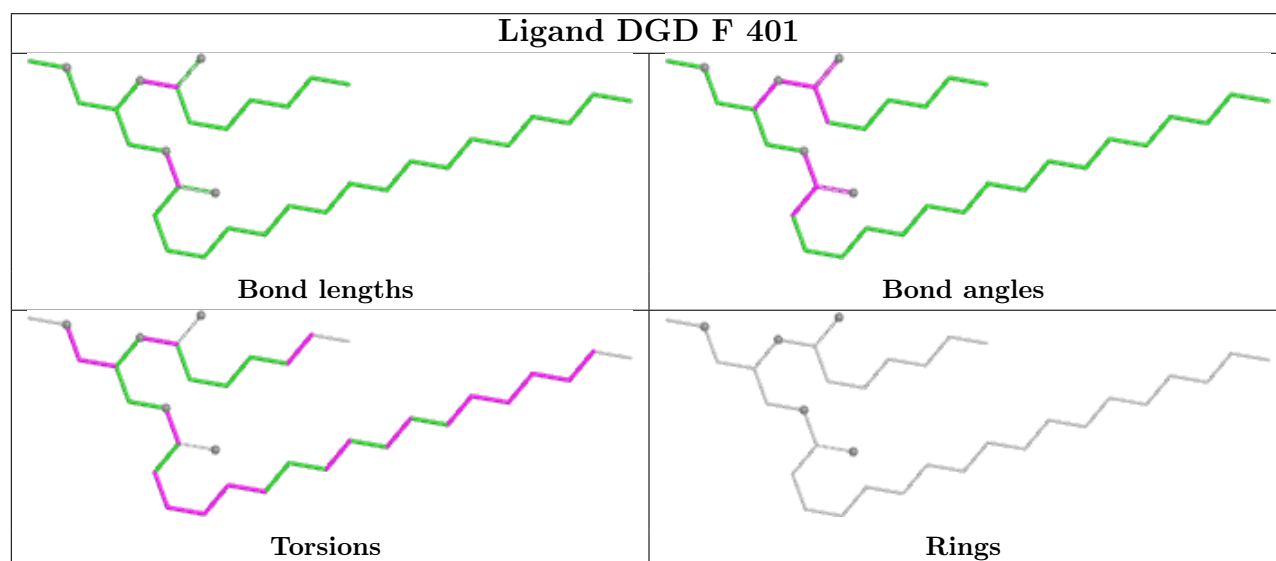
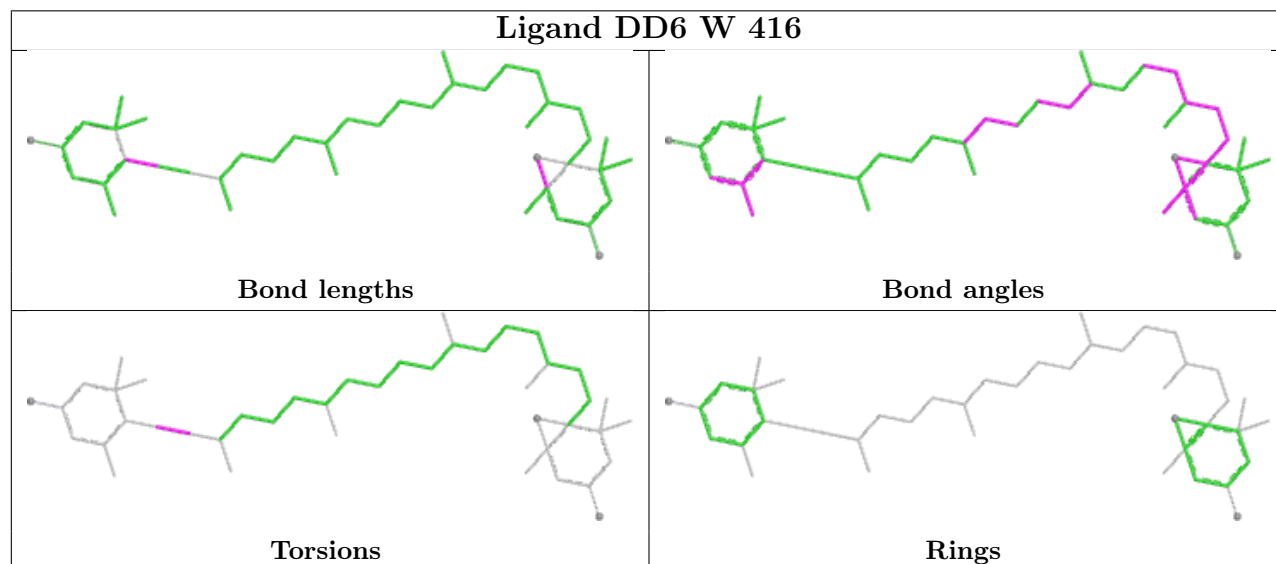
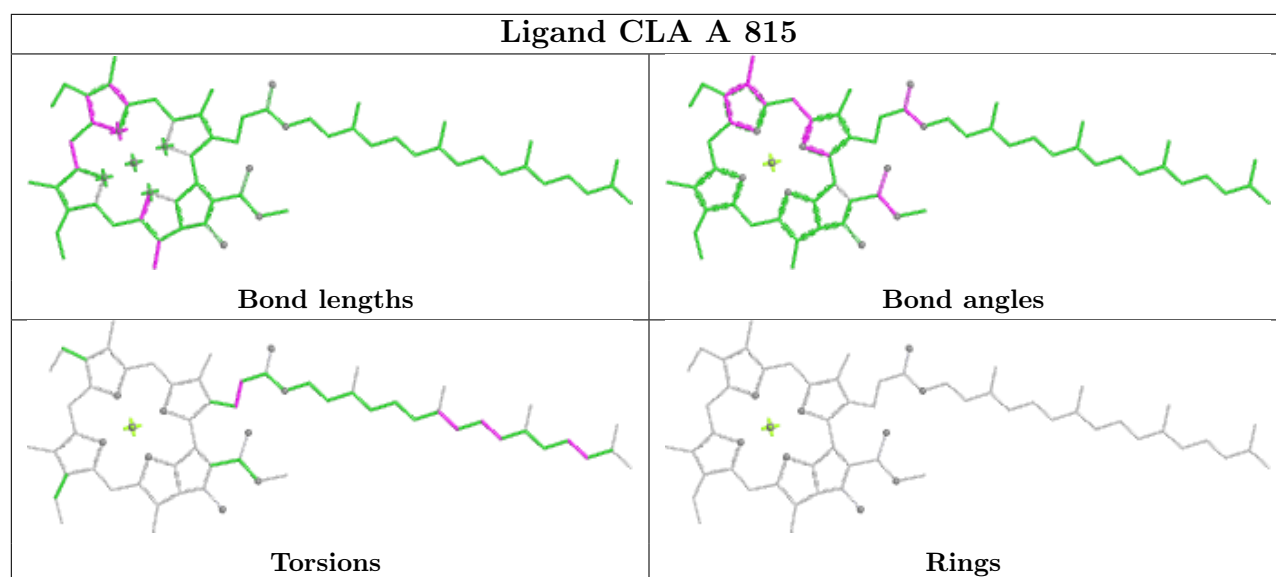


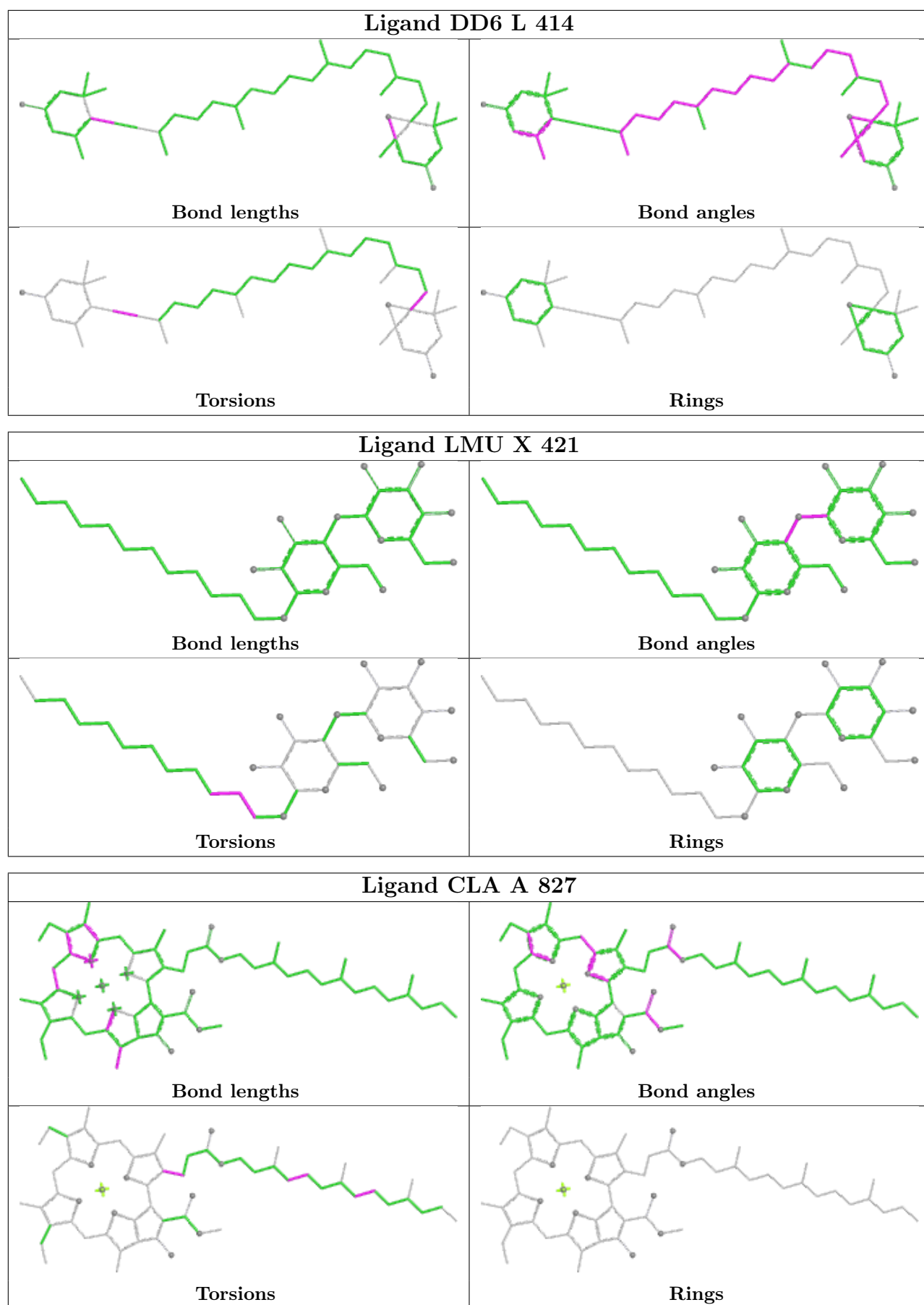
## Ligand CLA Q 618

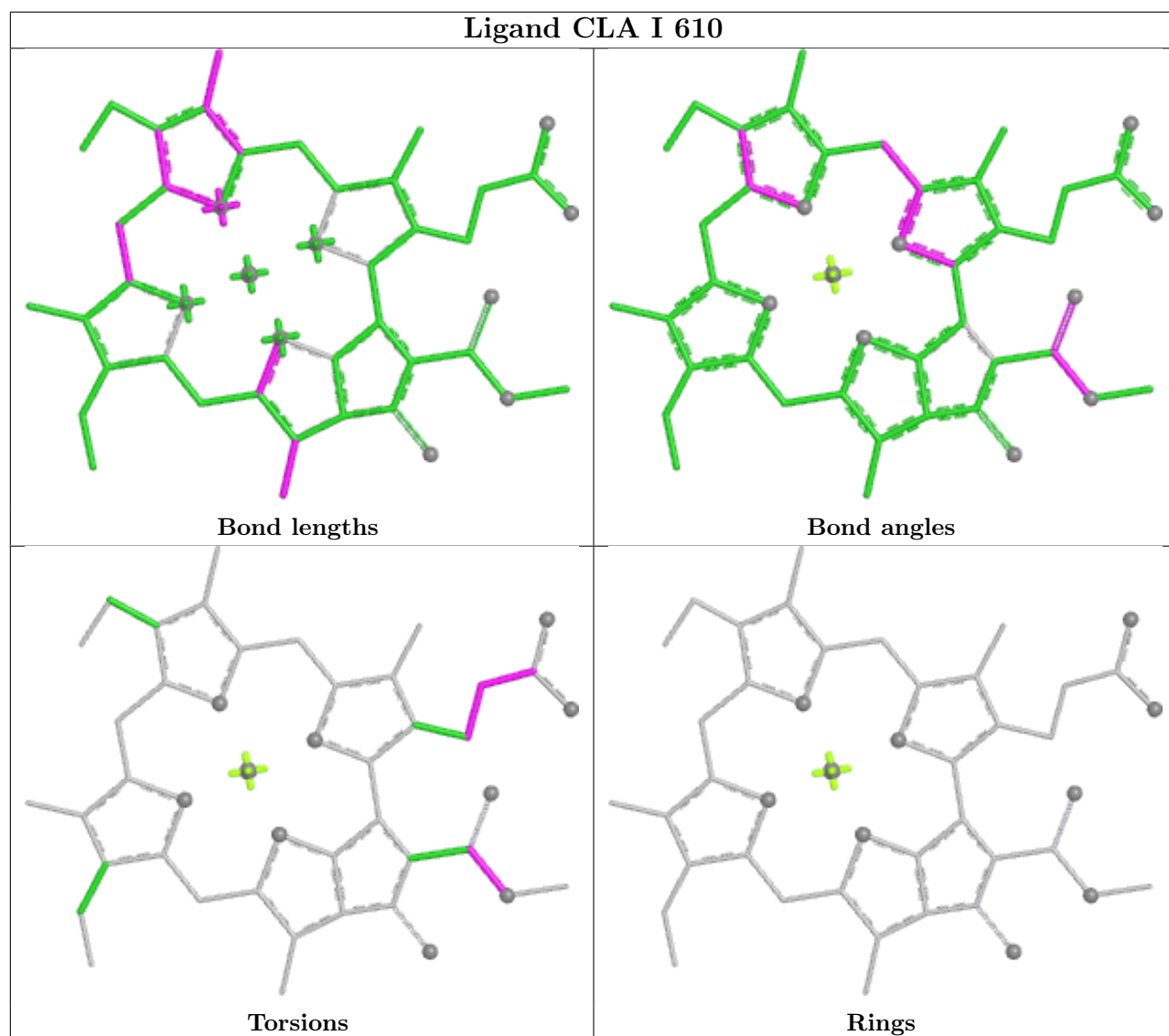
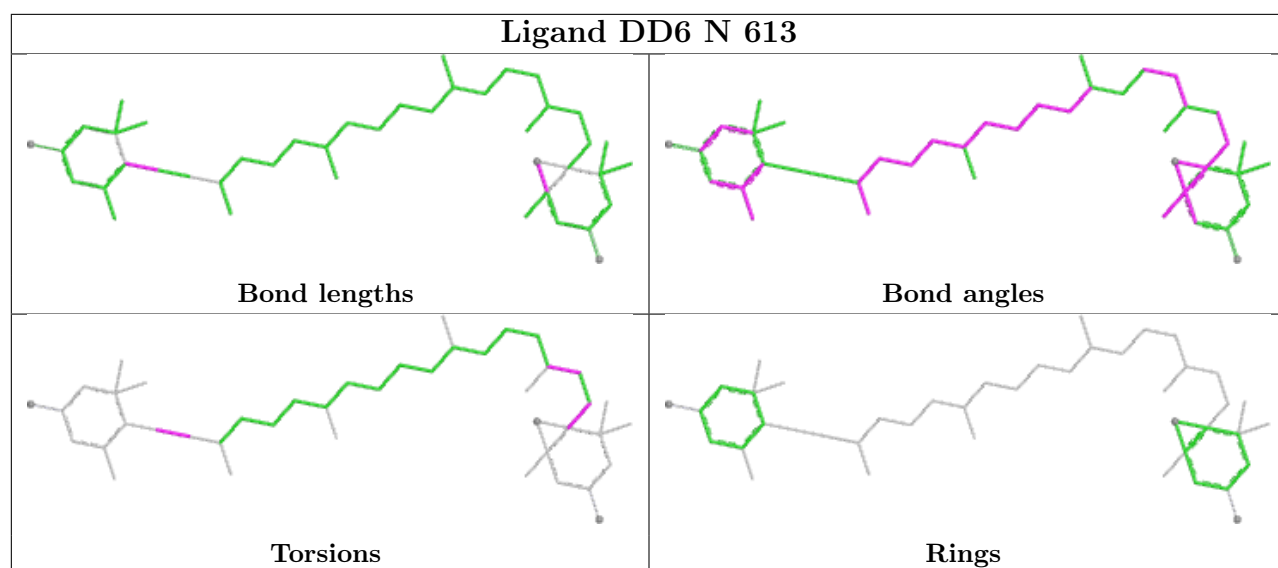


## Ligand BCR B 846



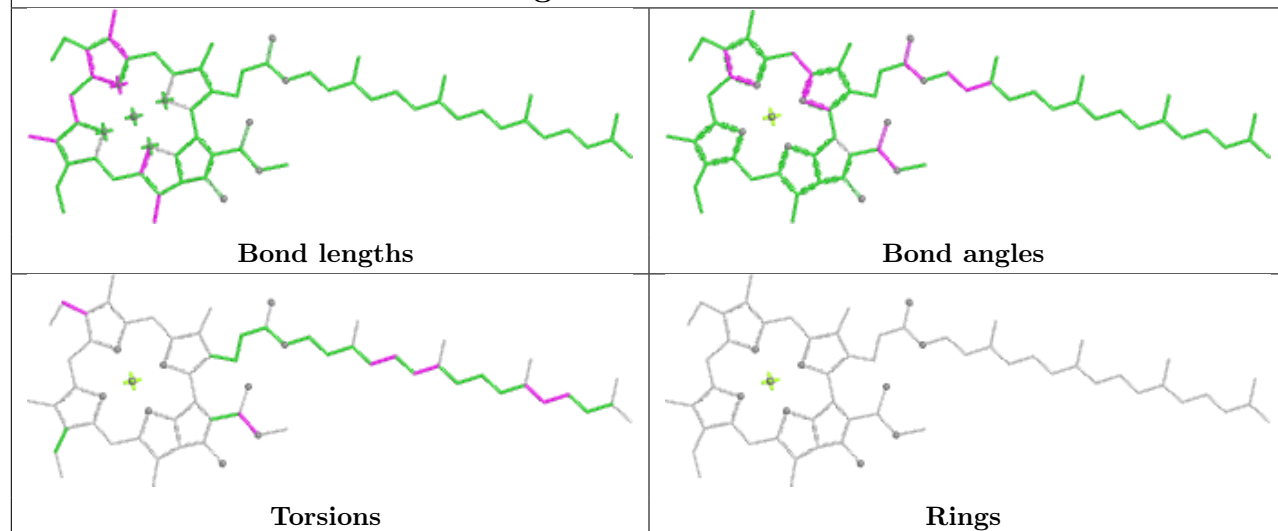




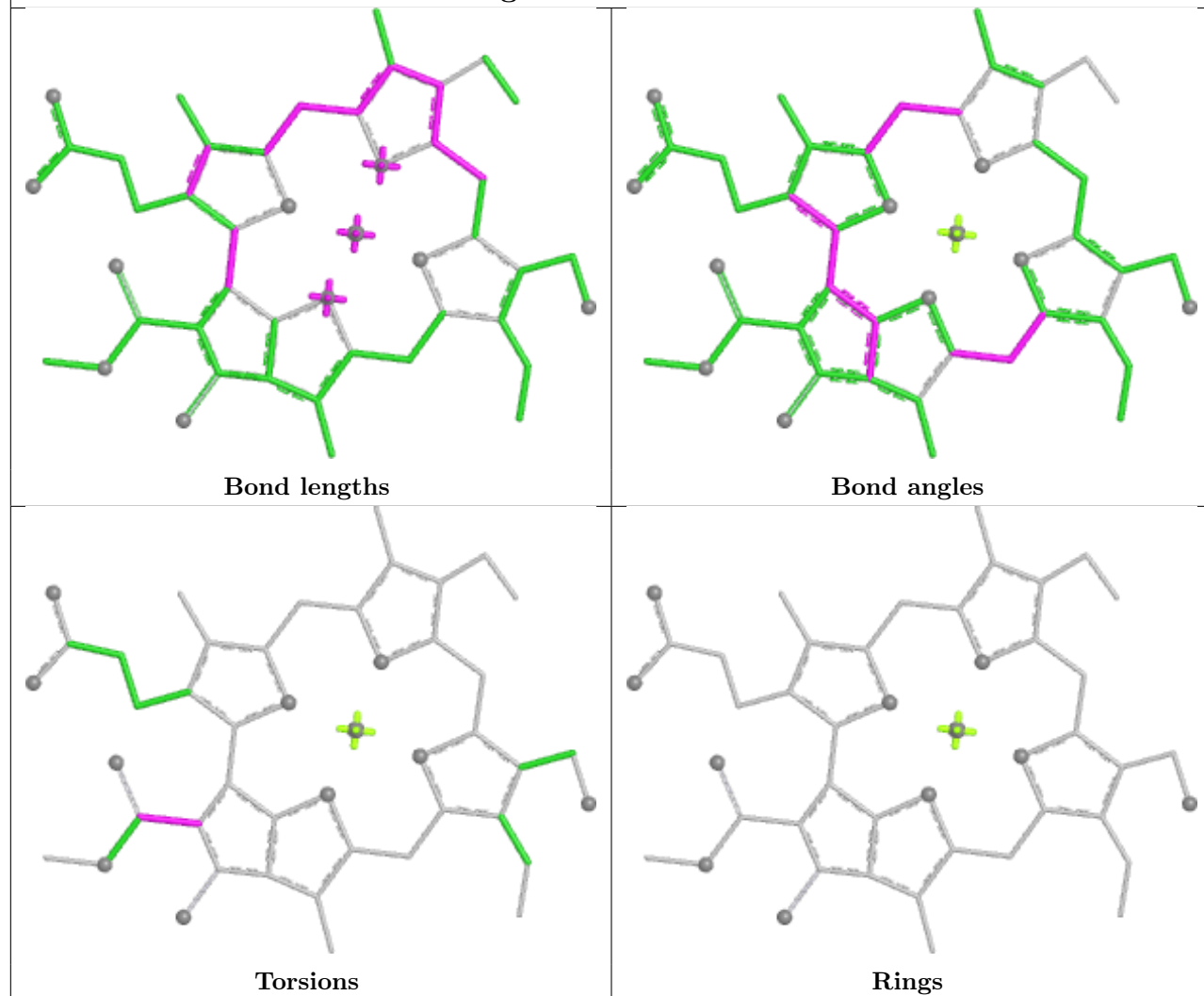


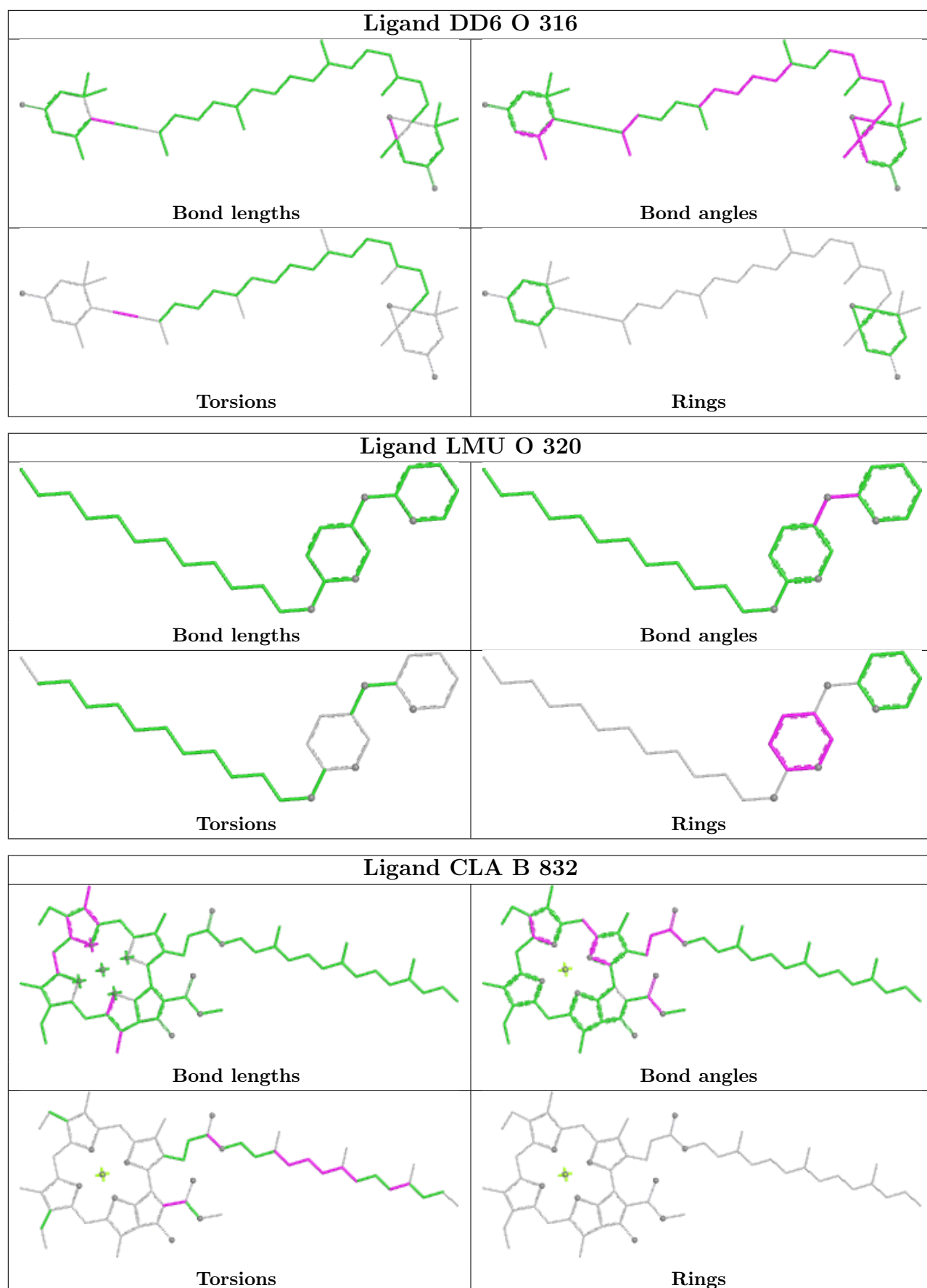


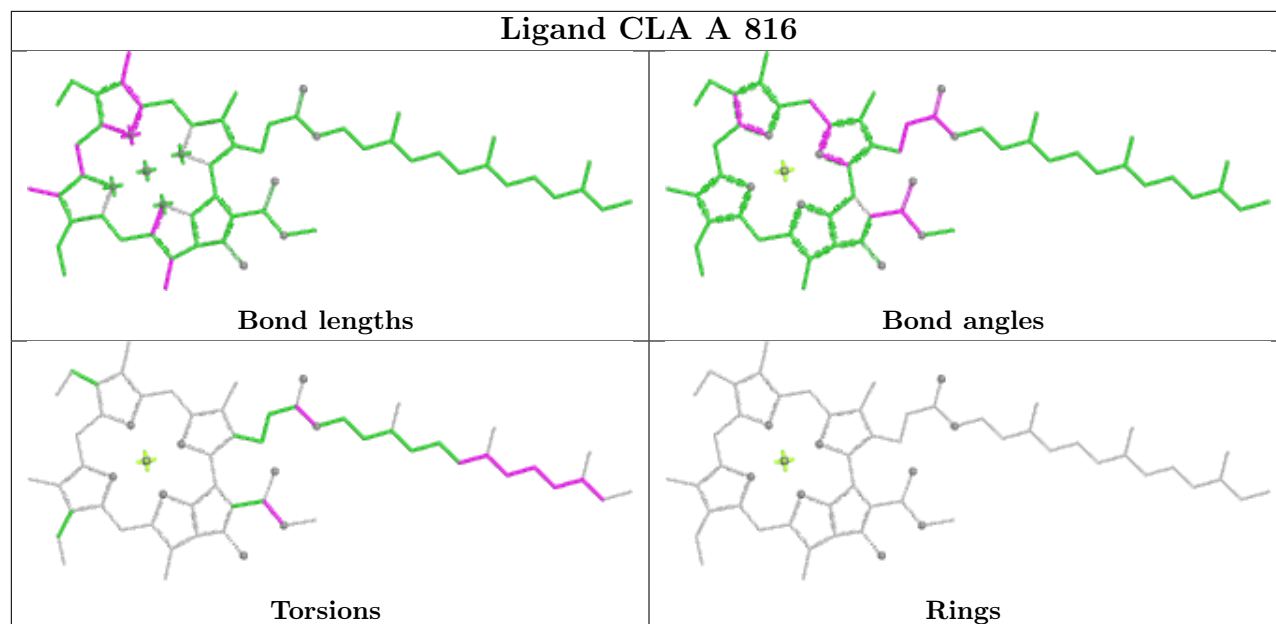
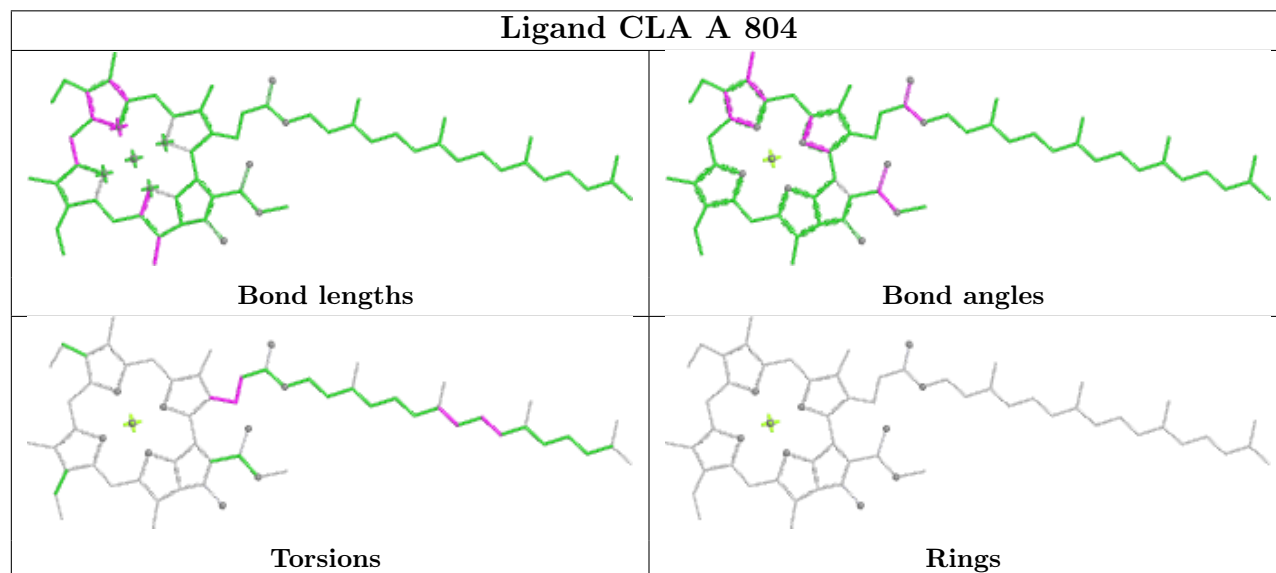
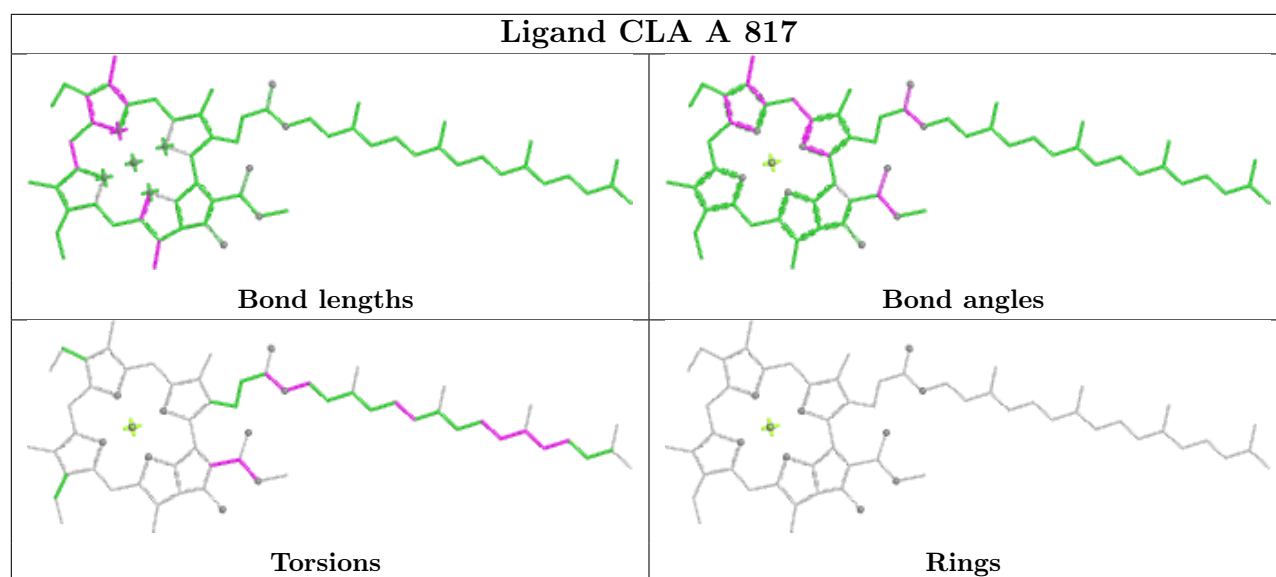
## Ligand CLA F 403

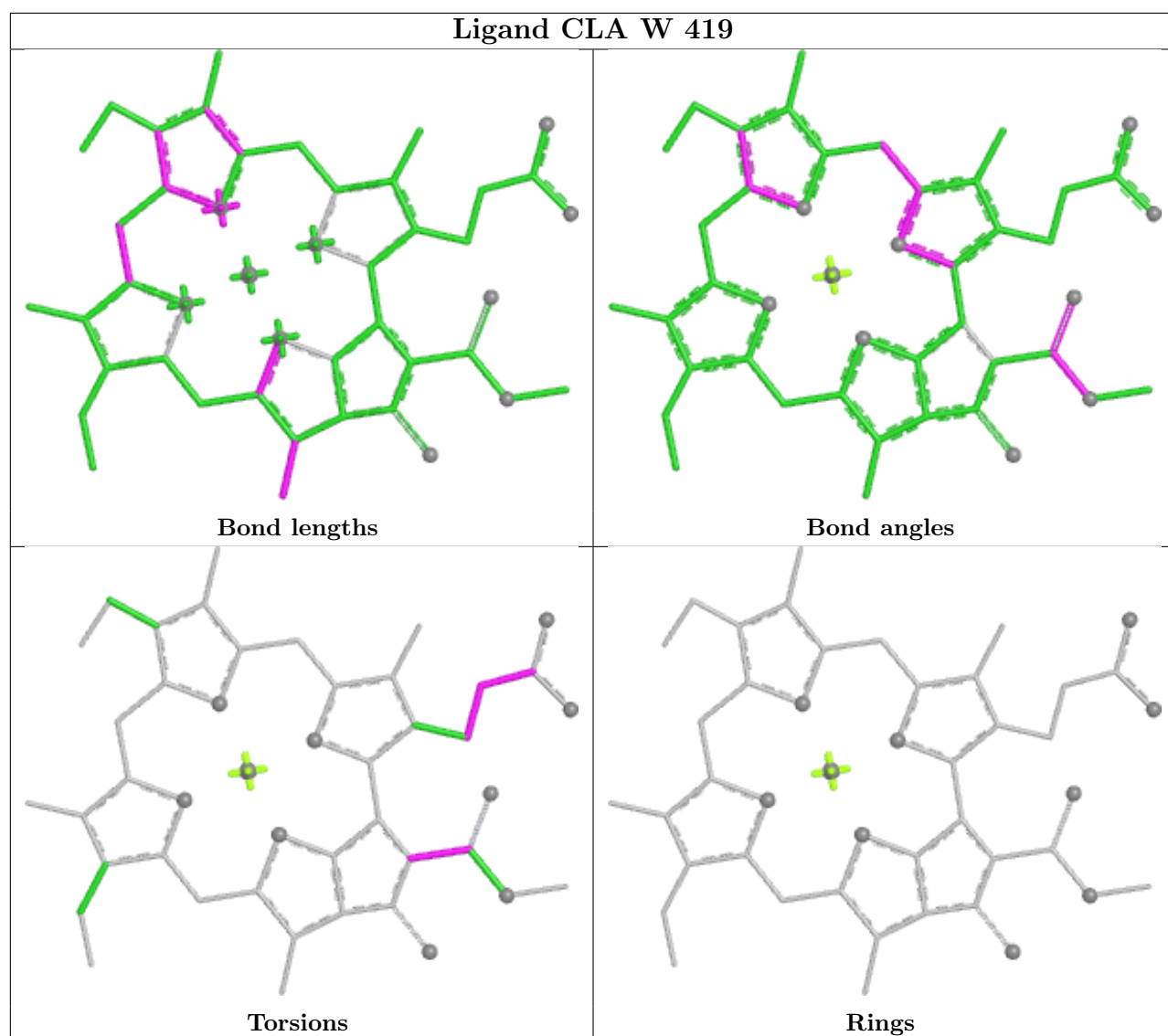


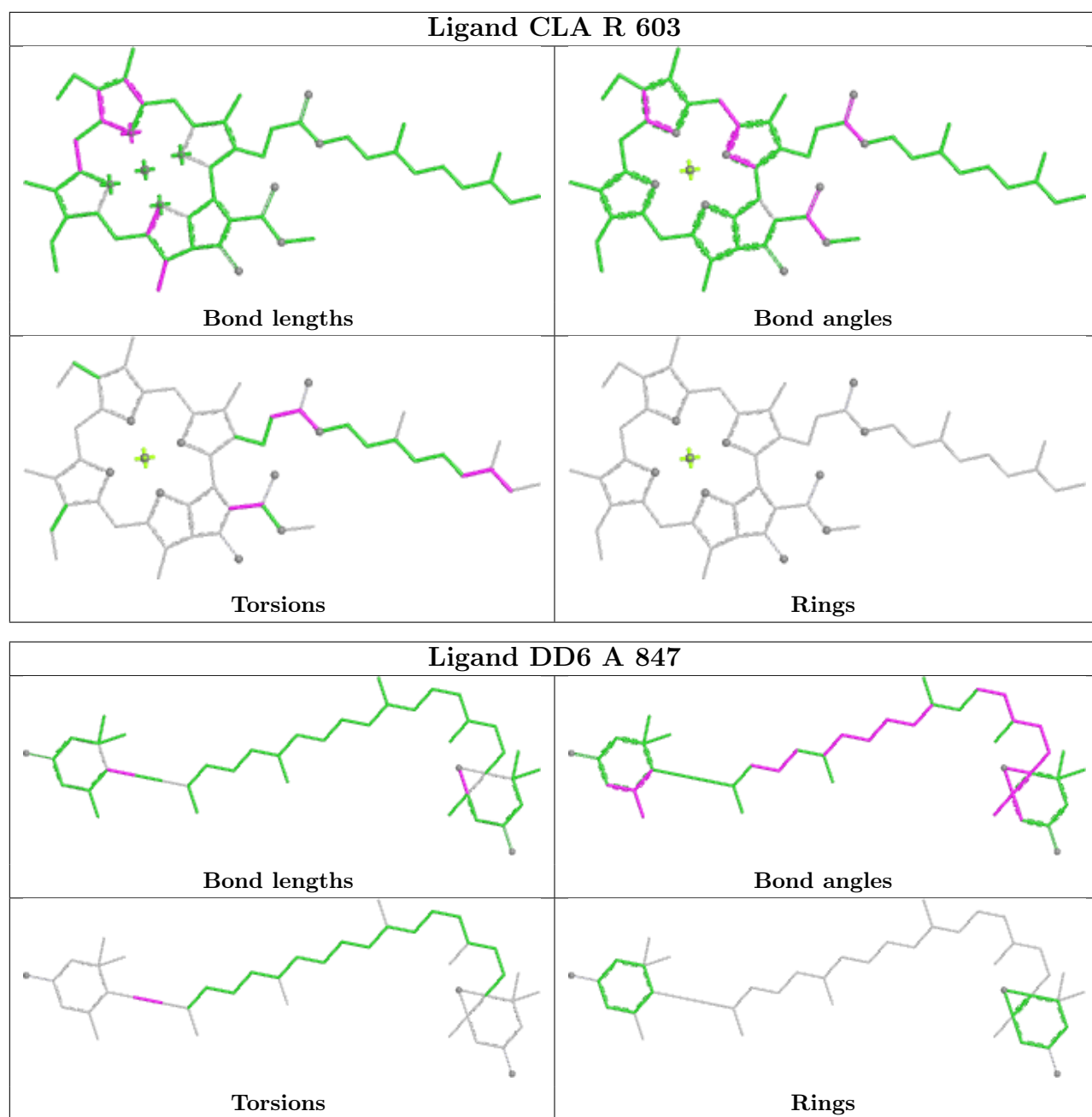
## Ligand CHL V 606

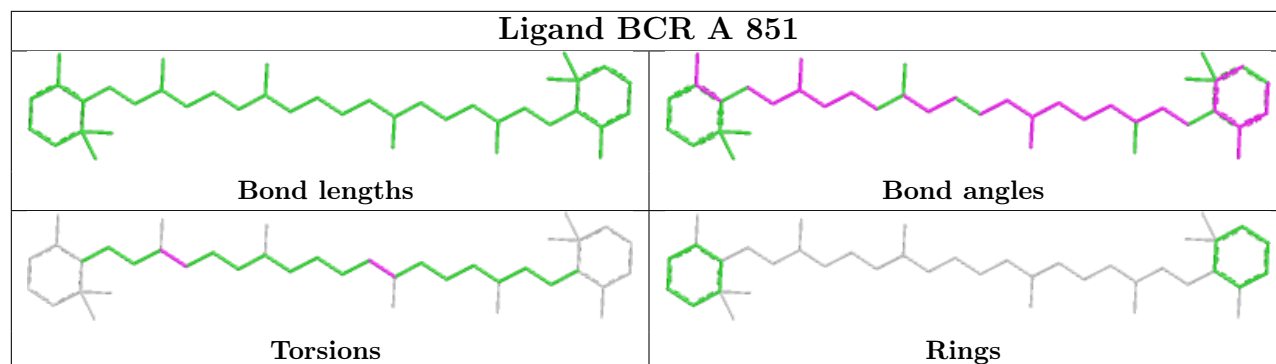
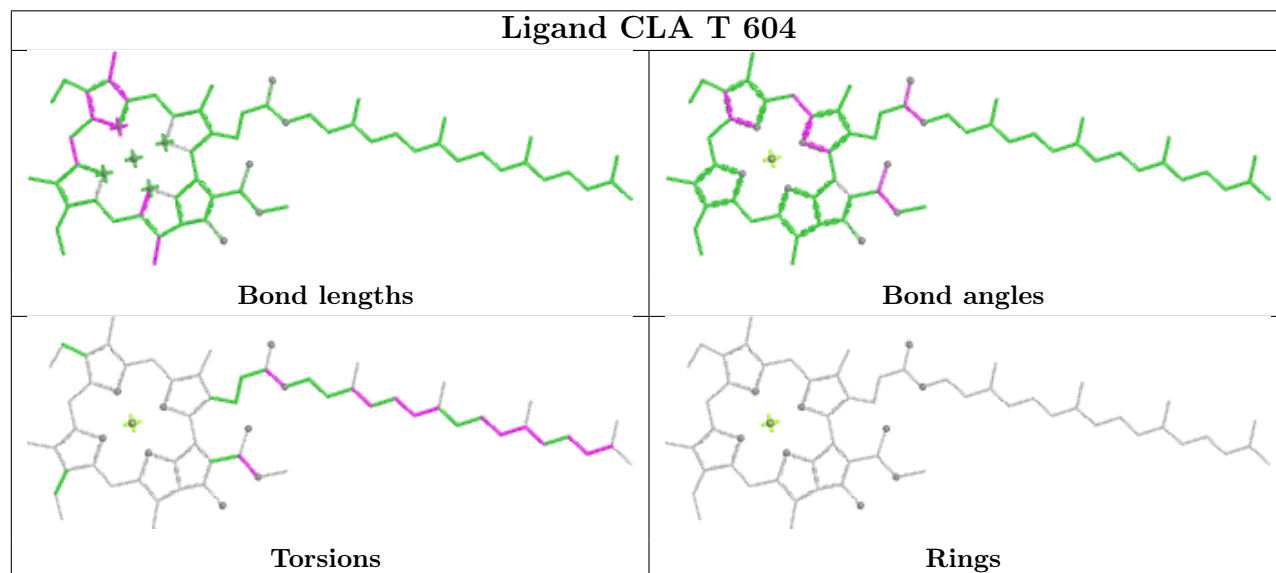
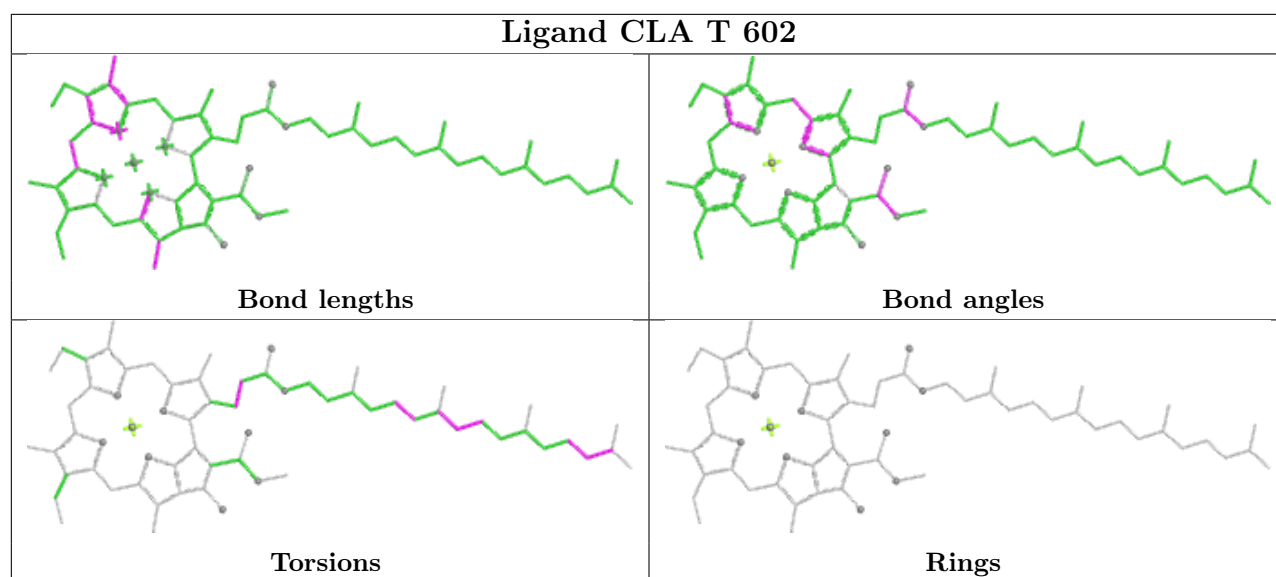


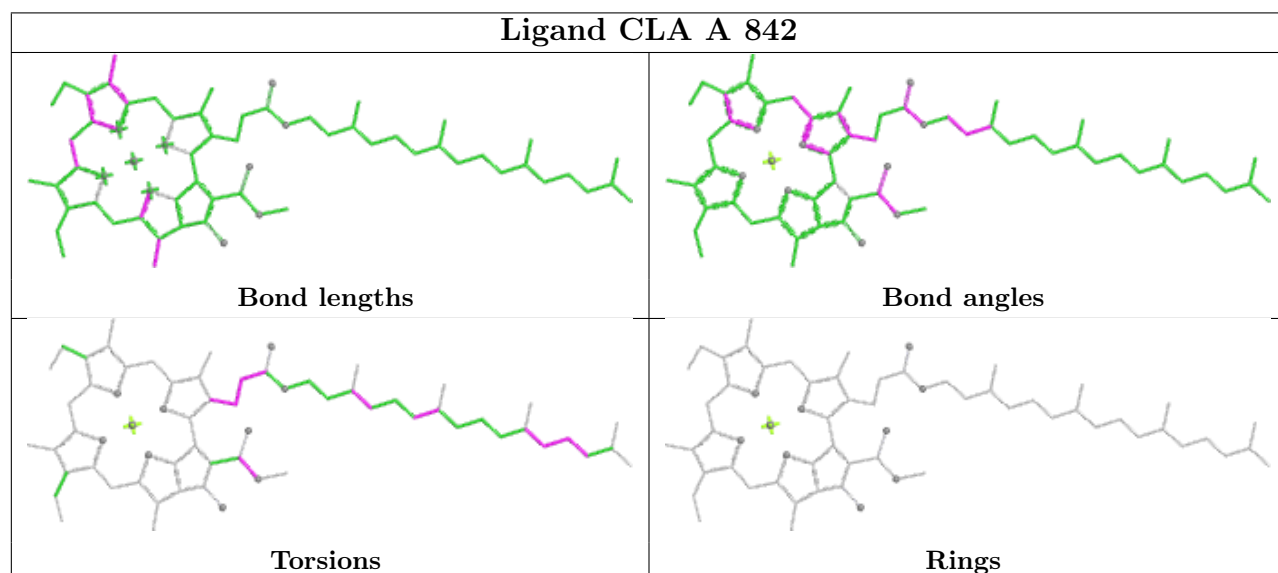
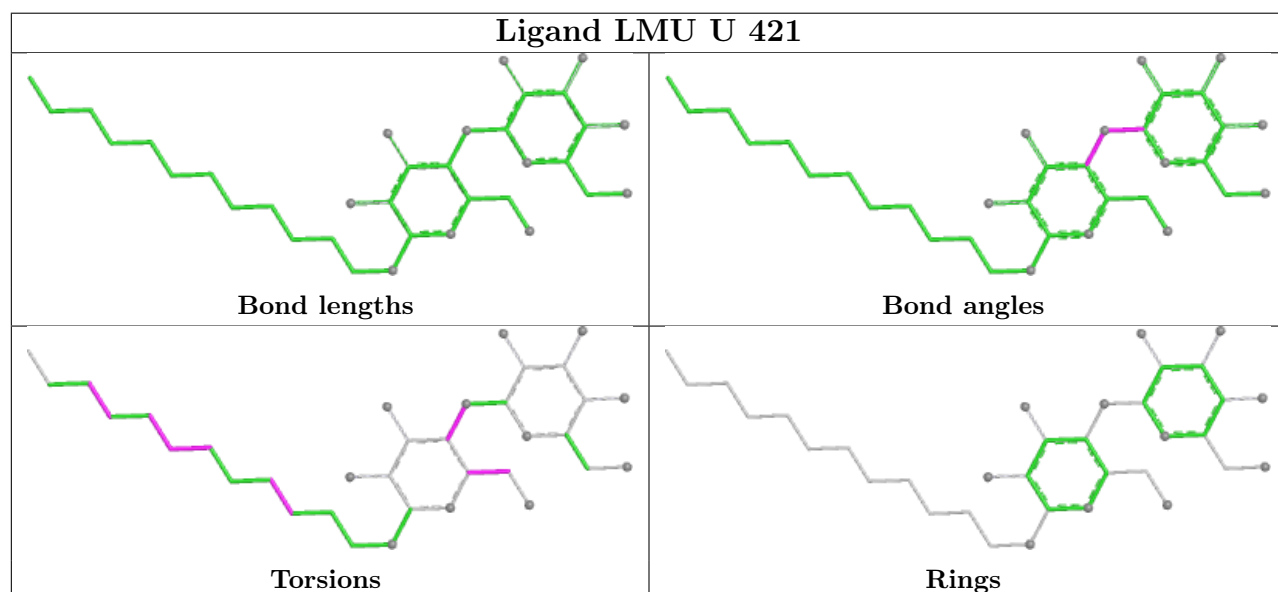
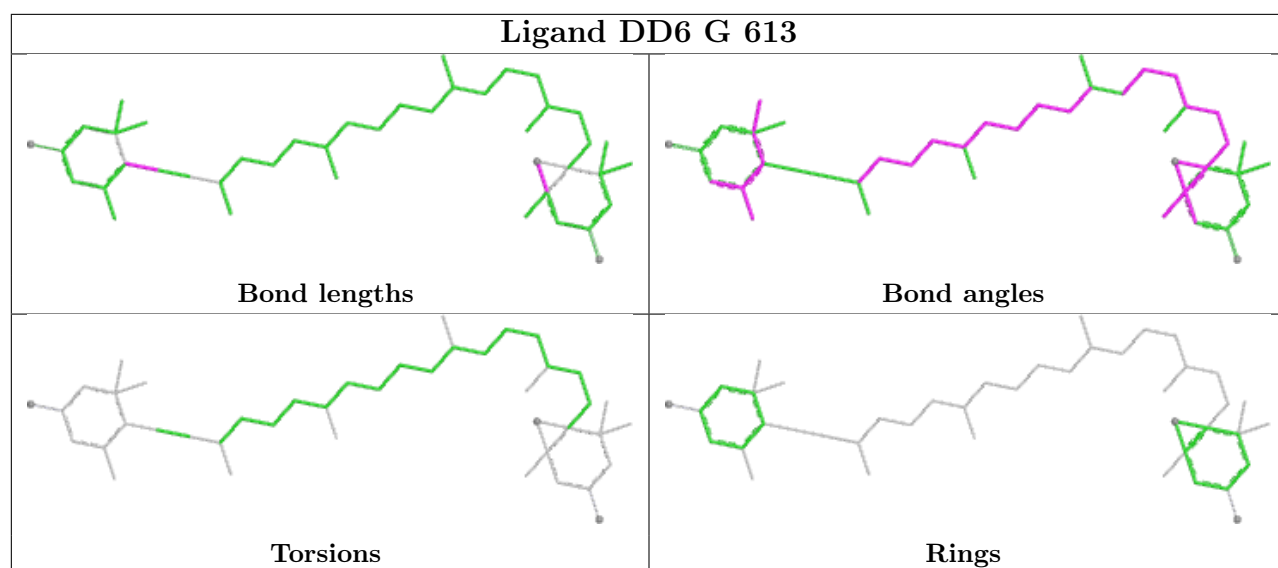




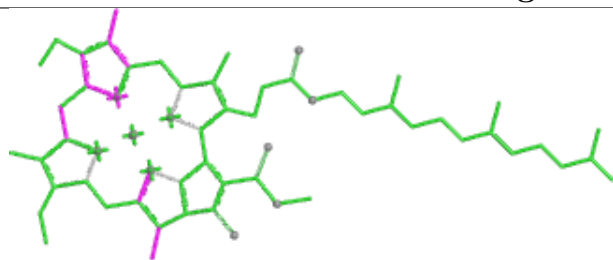




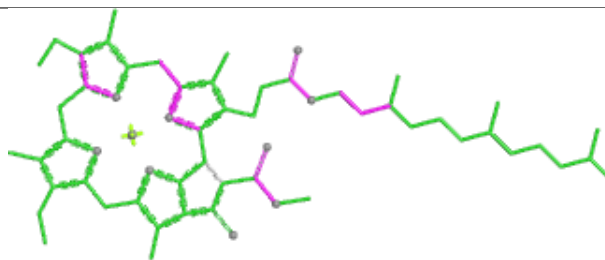




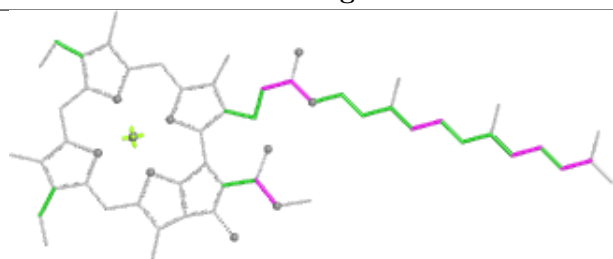
## Ligand CLA S 604



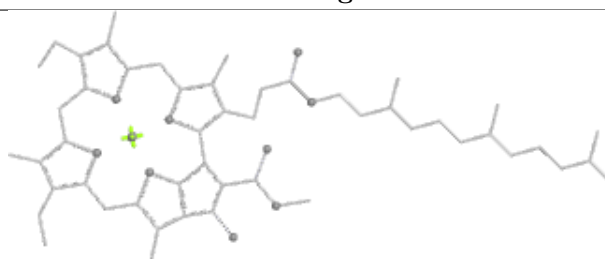
Bond lengths



Bond angles

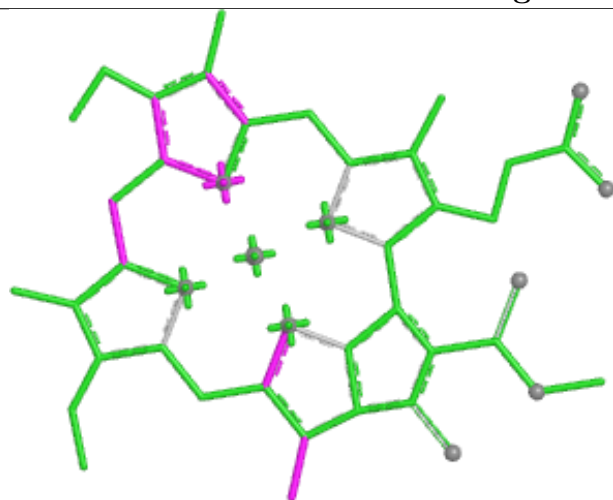


Torsions

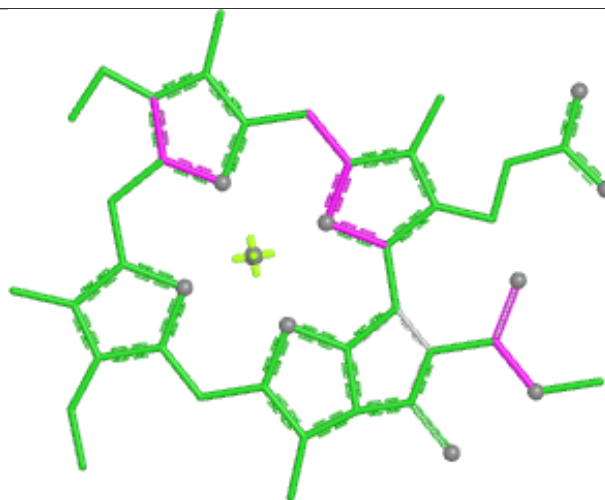


Rings

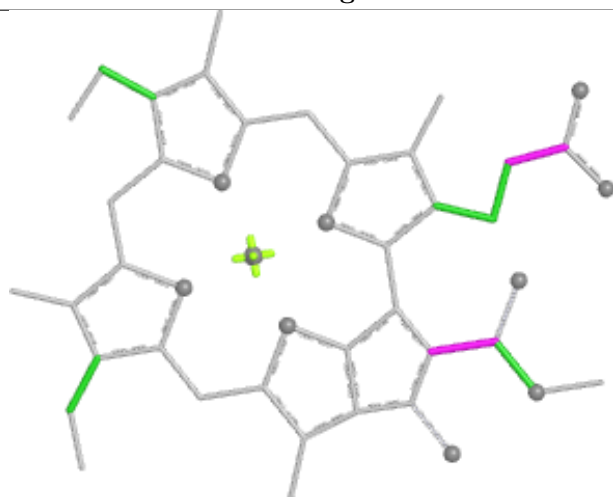
## Ligand CLA H 310



Bond lengths



Bond angles

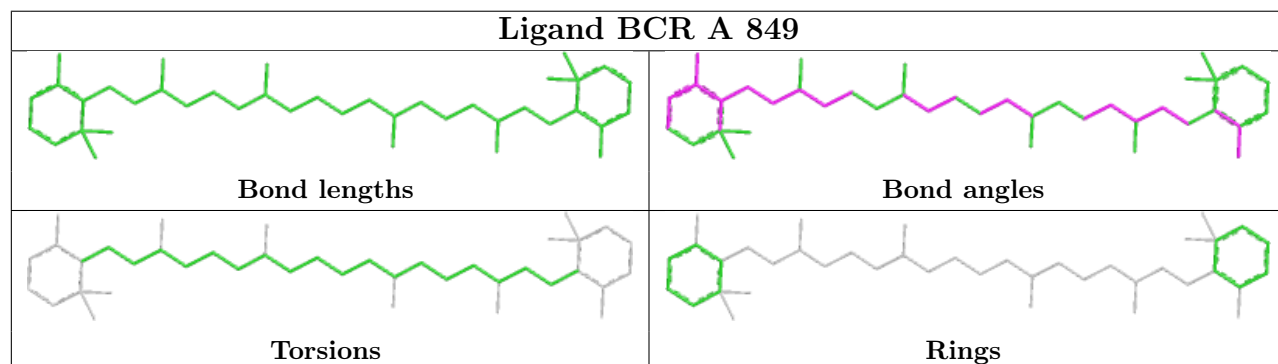
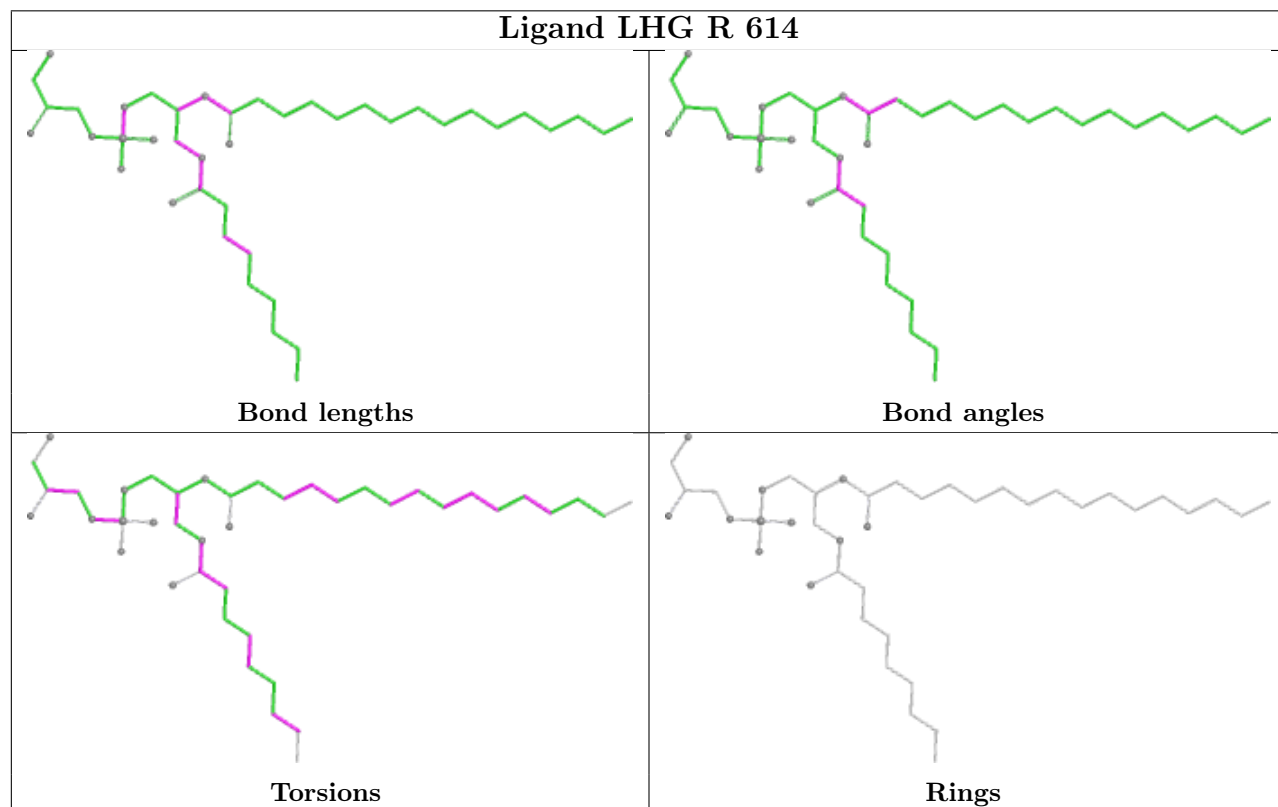
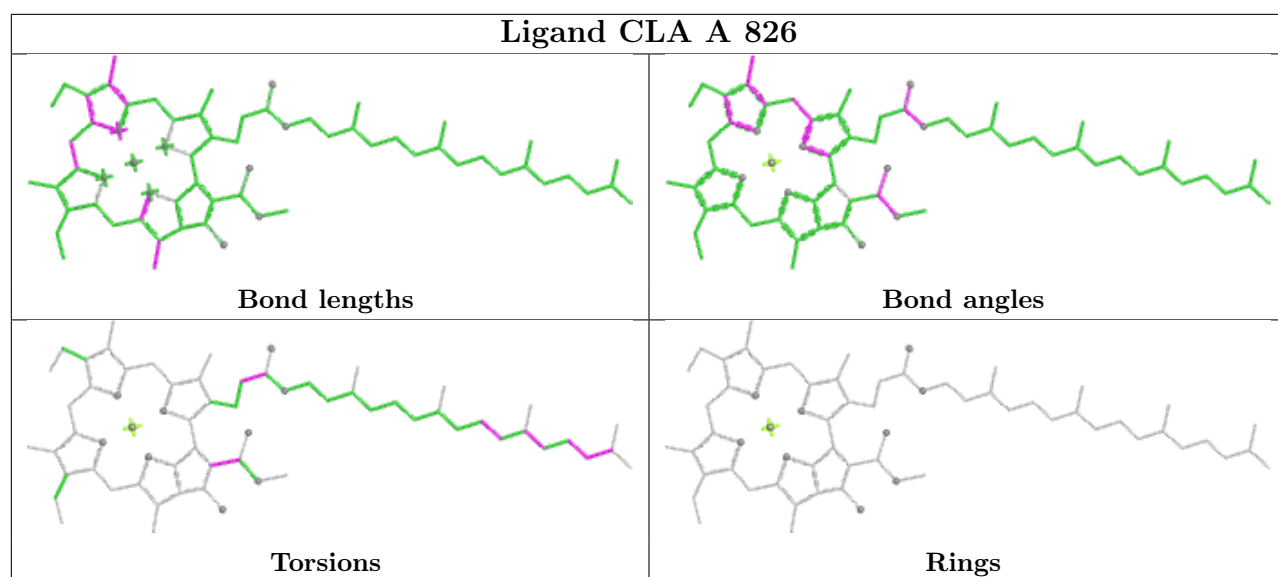


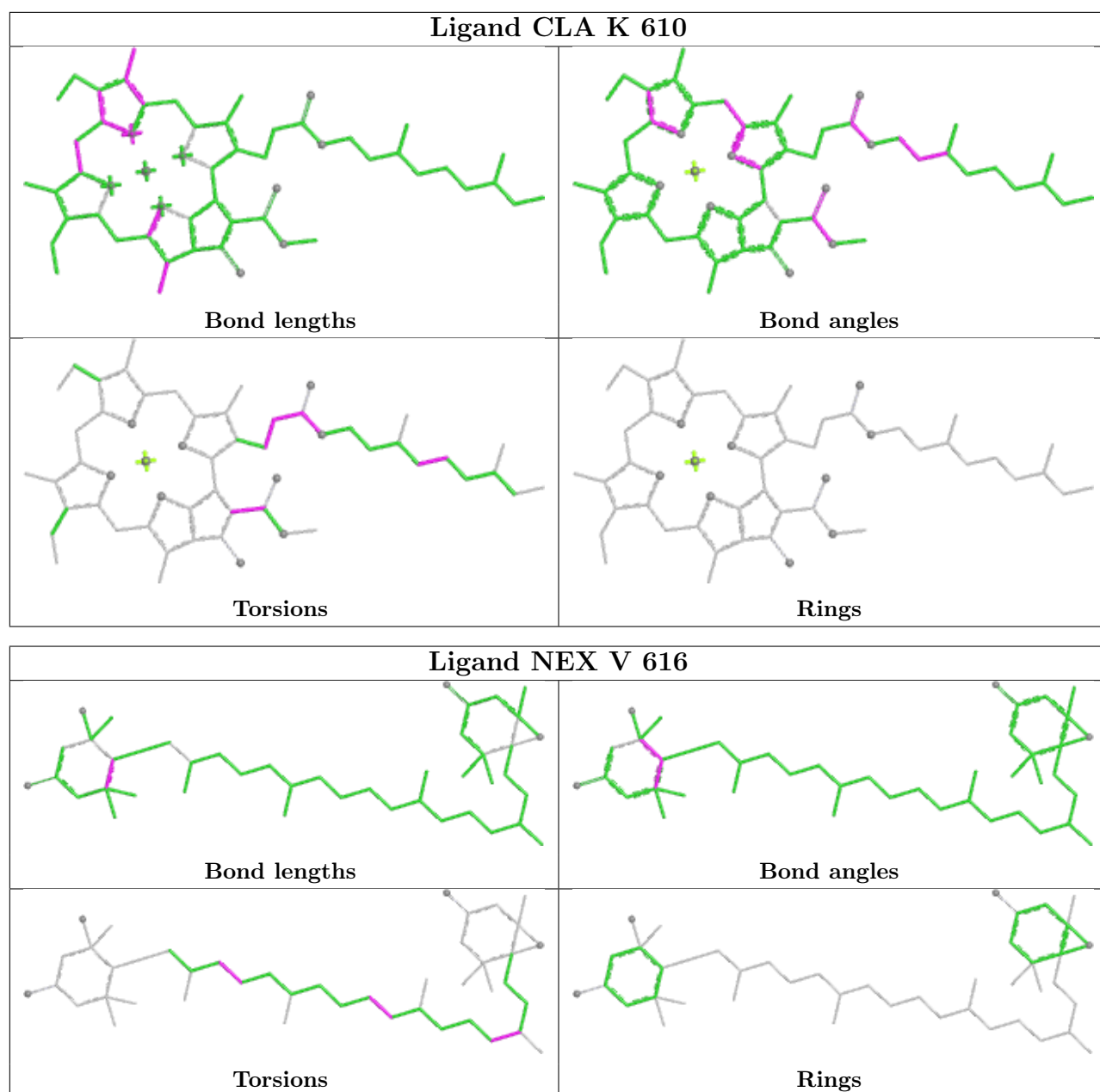
Torsions

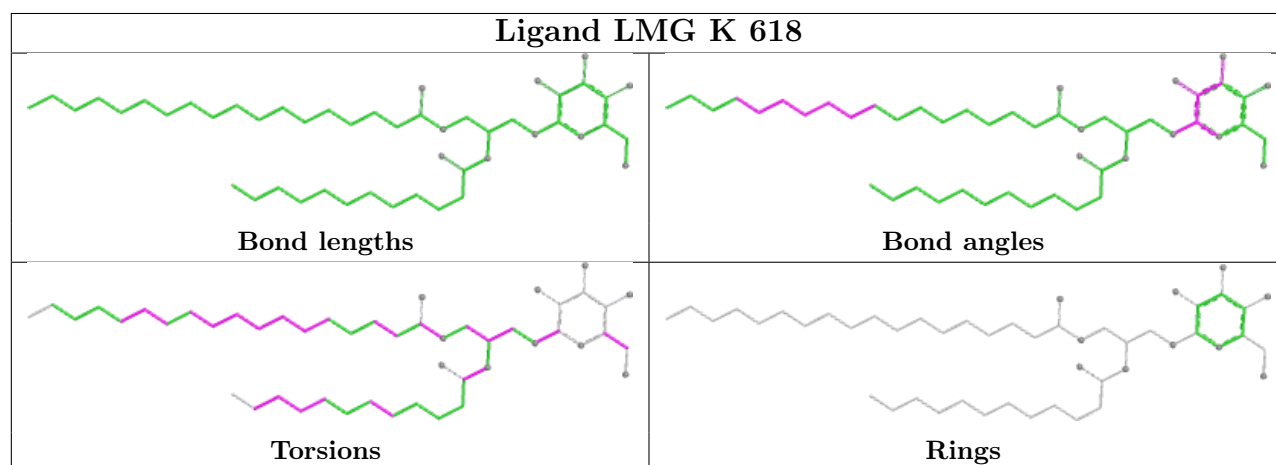
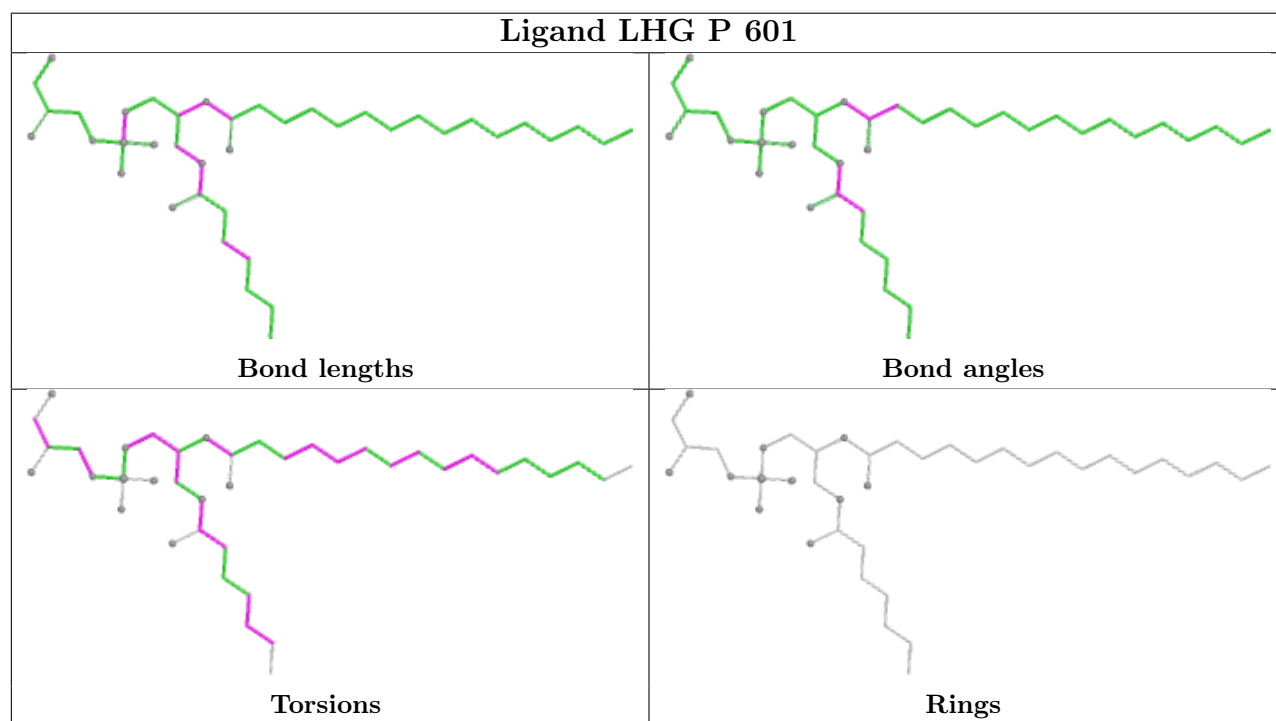
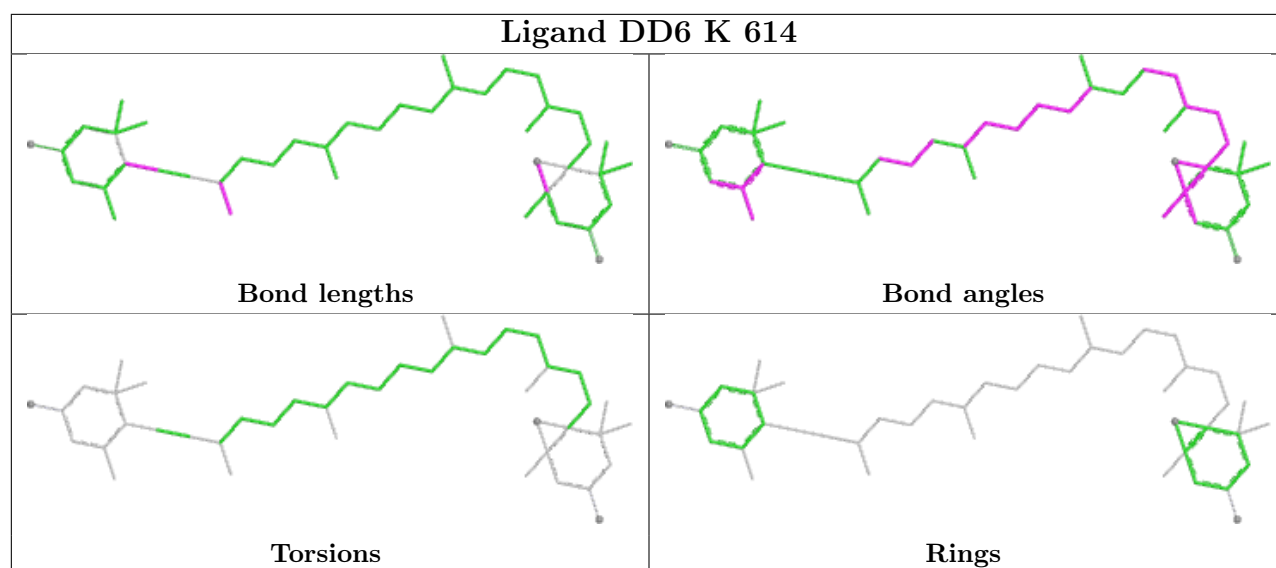


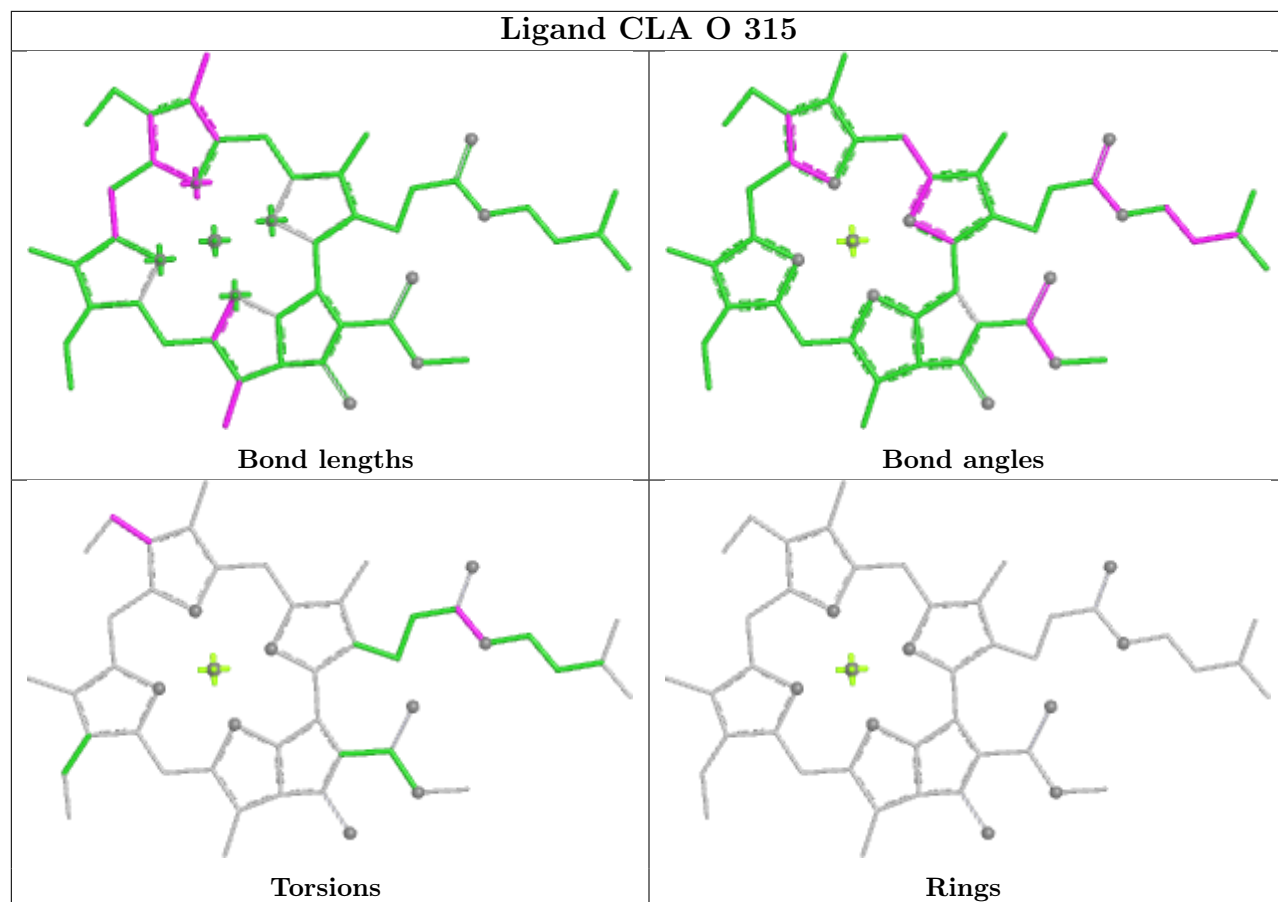
Rings



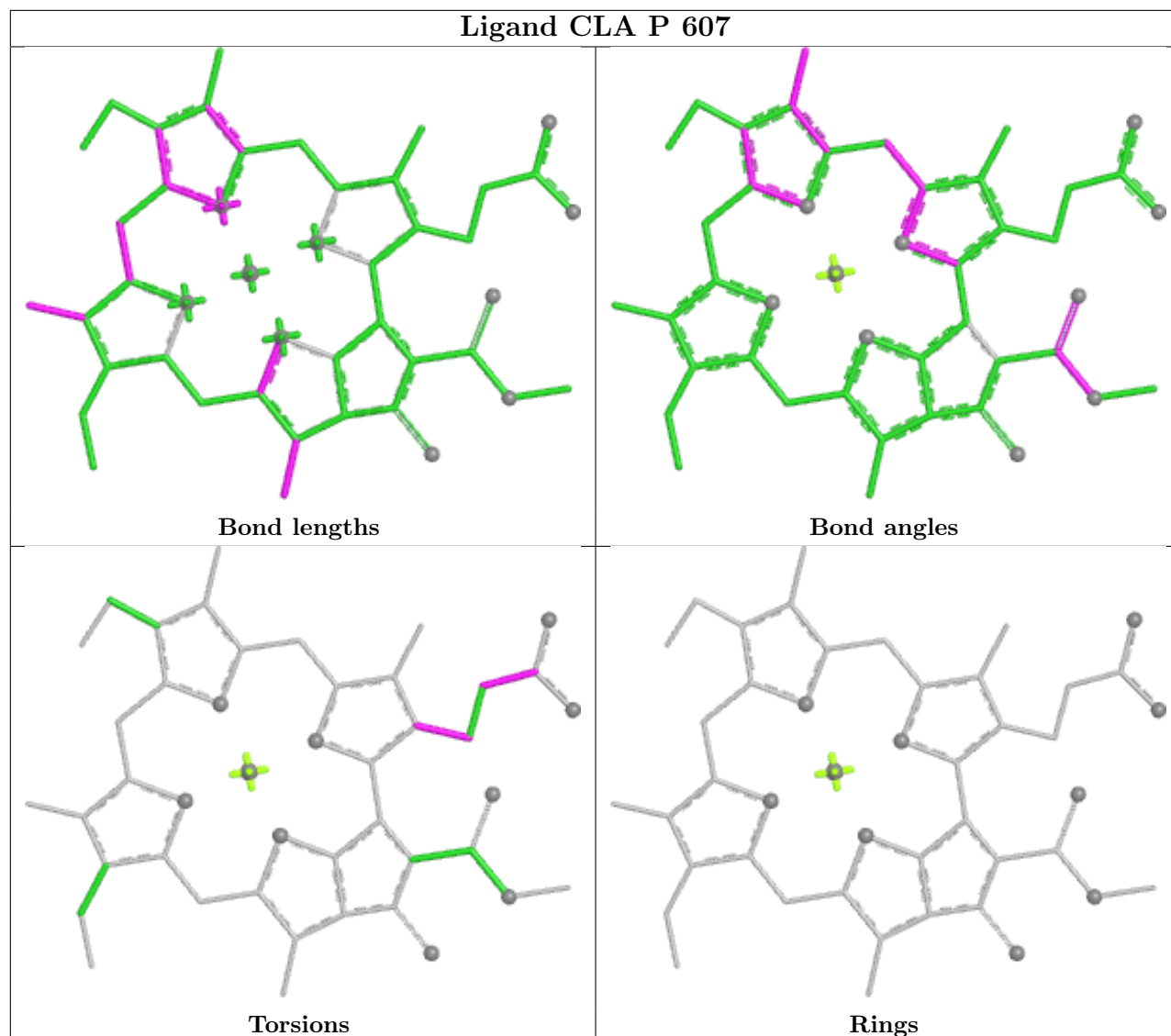




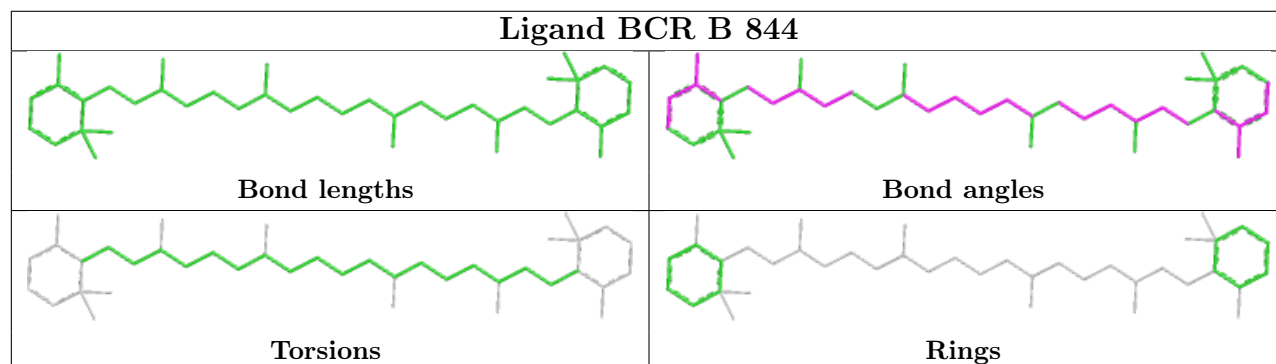


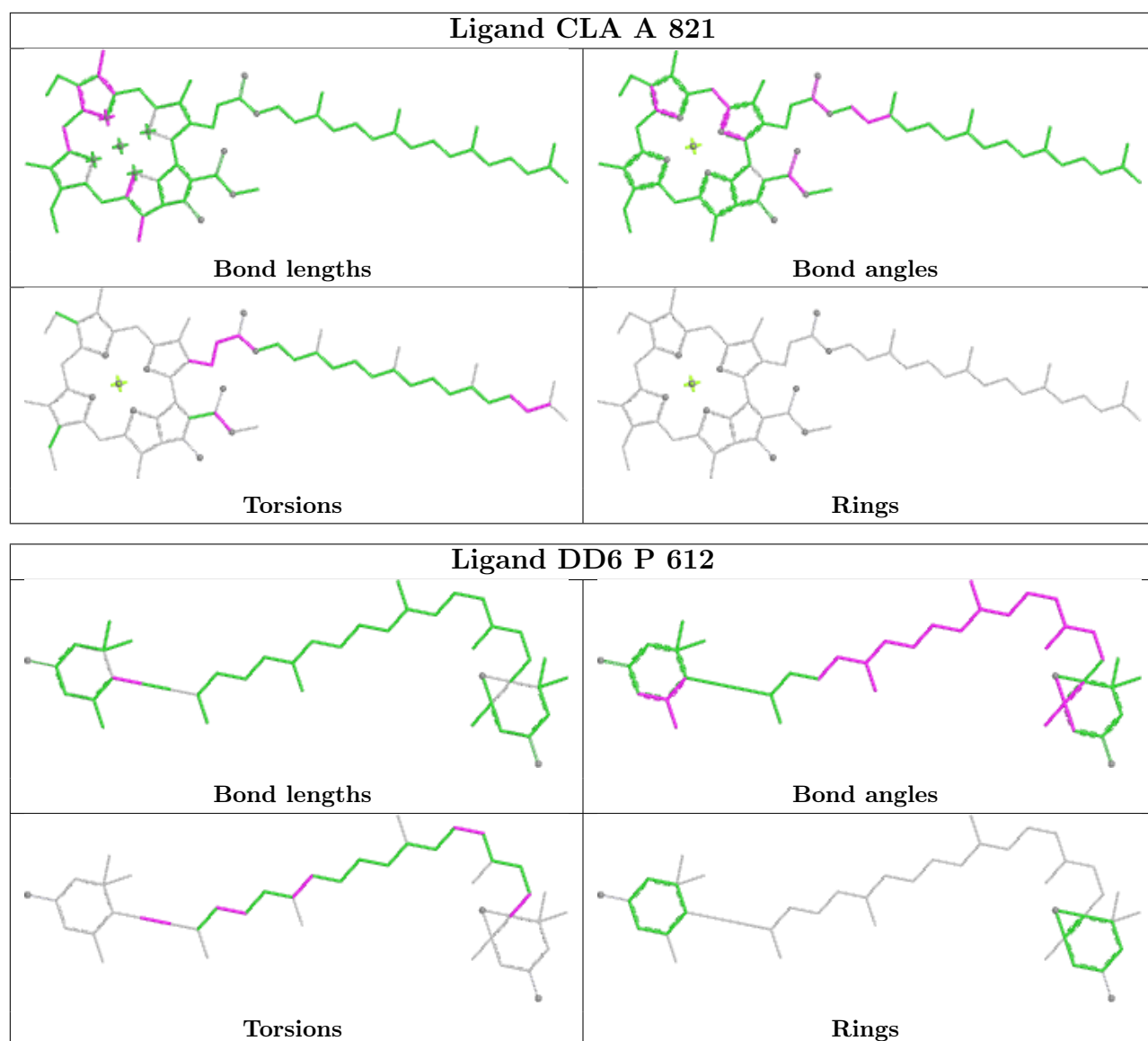


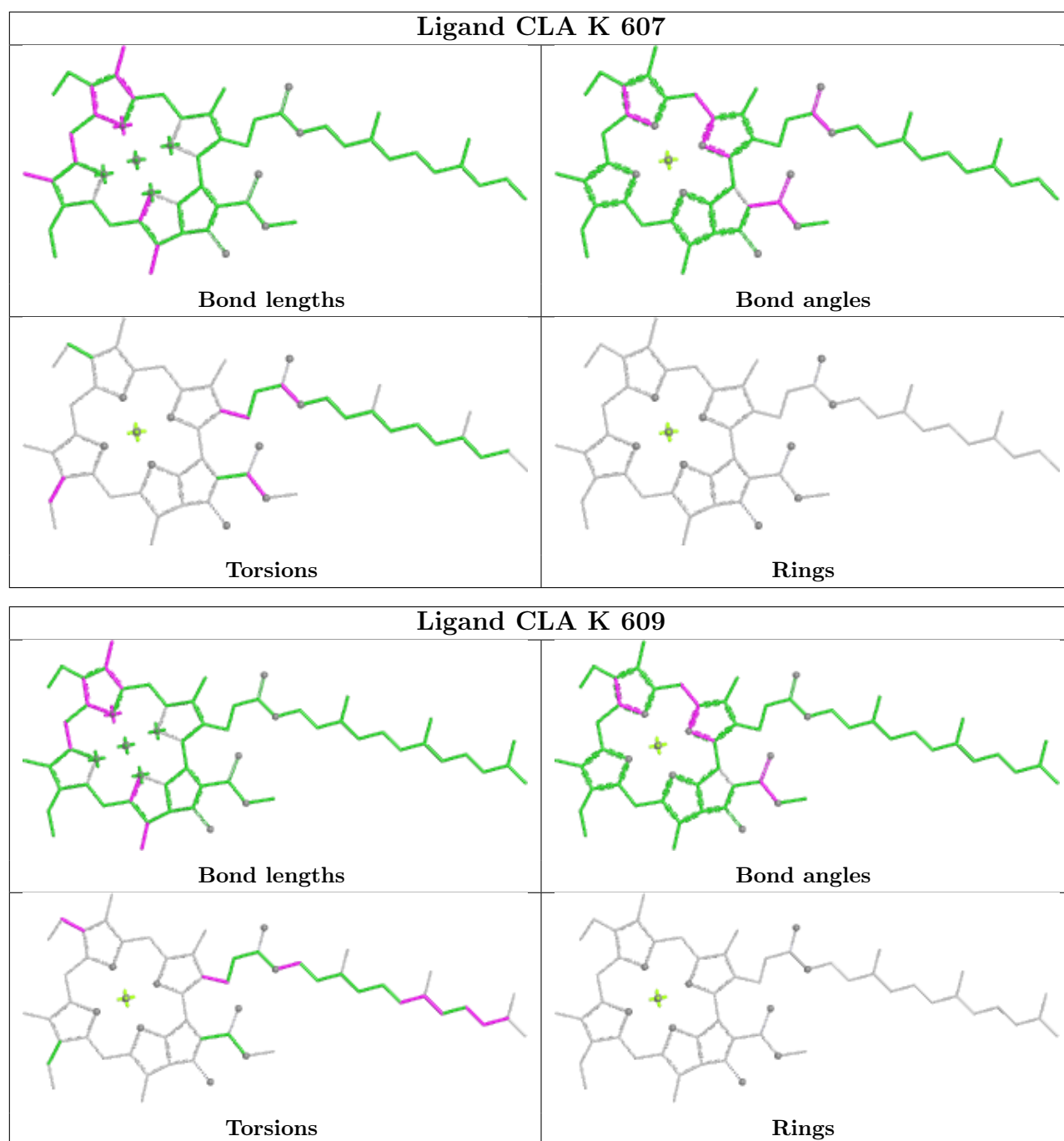
## Ligand CLA P 607

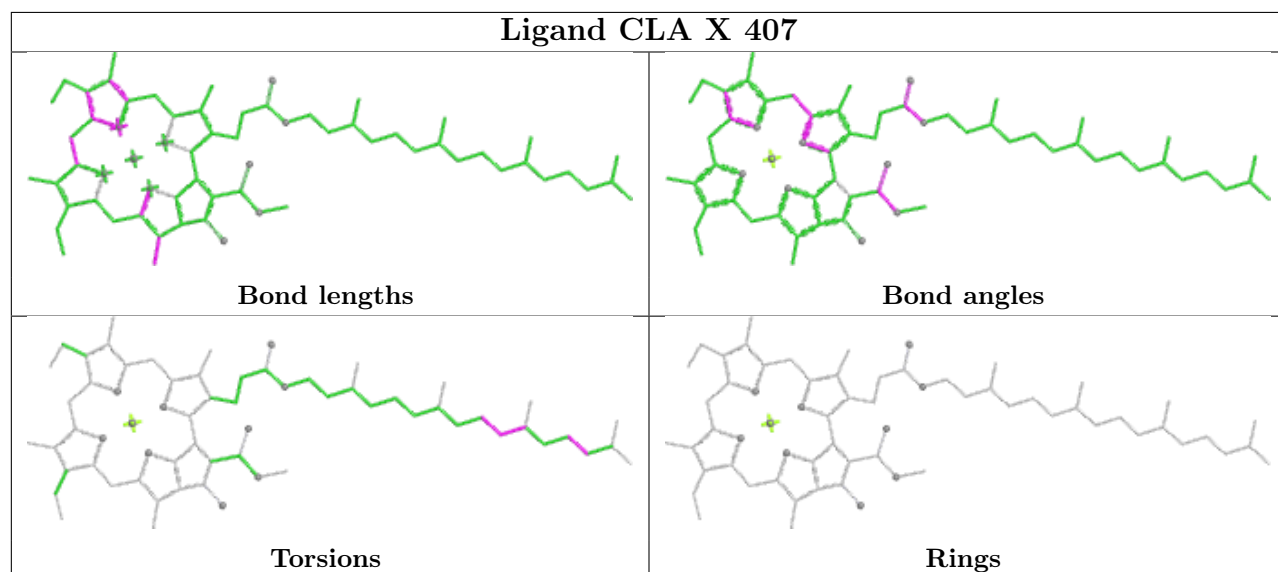
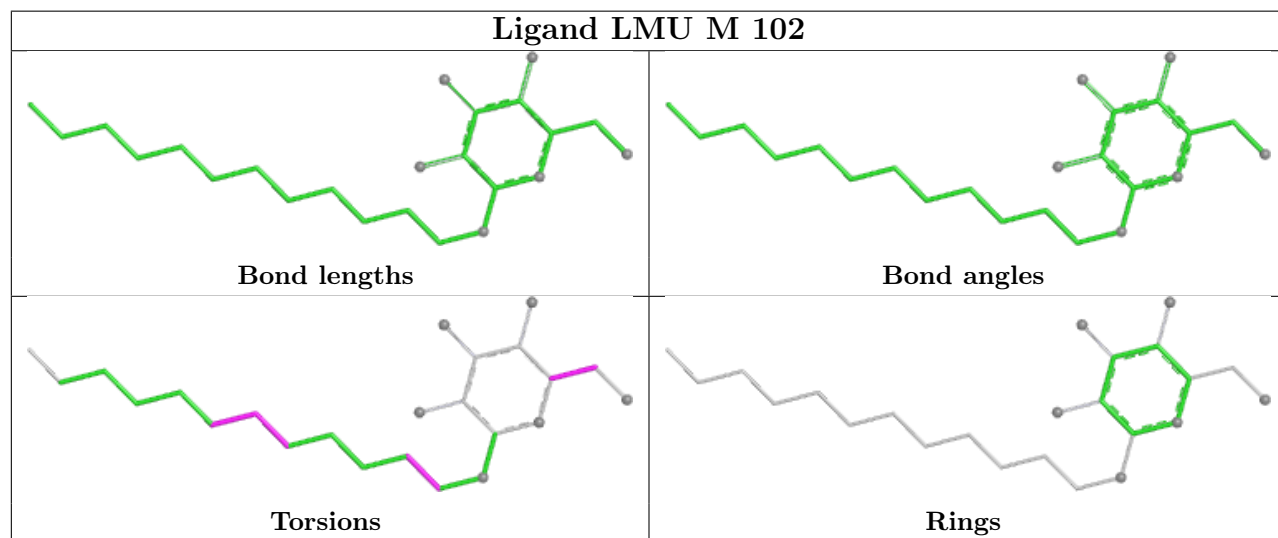
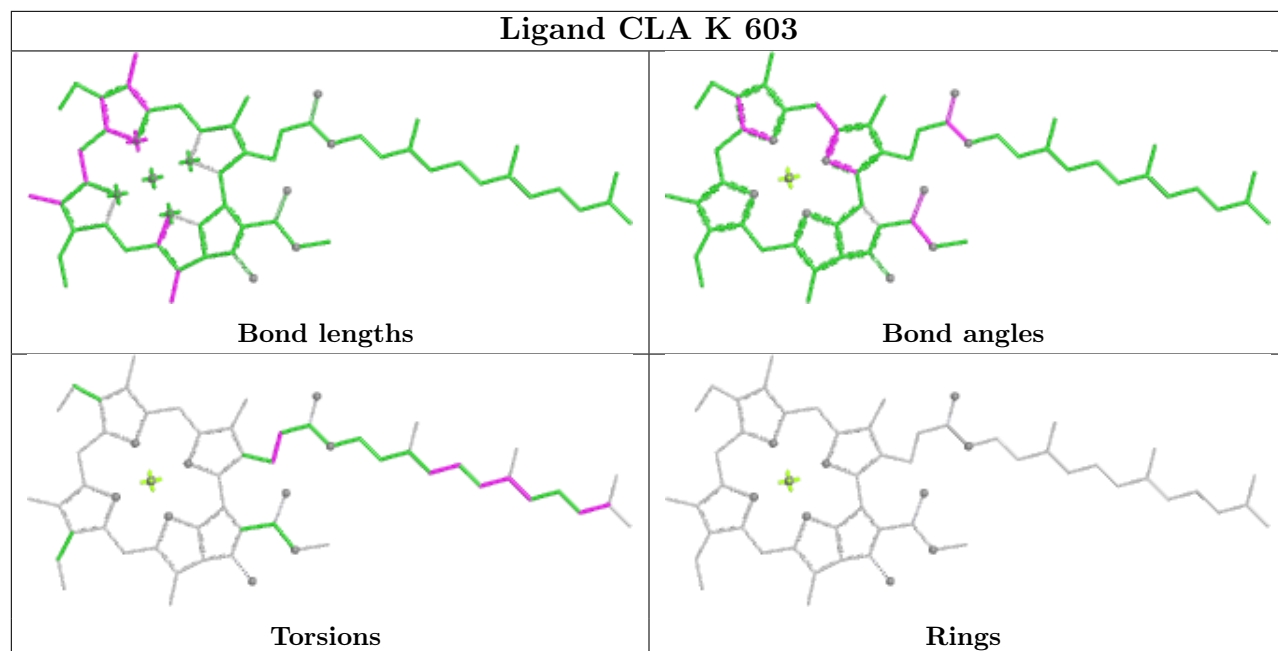


## Ligand BCR B 844

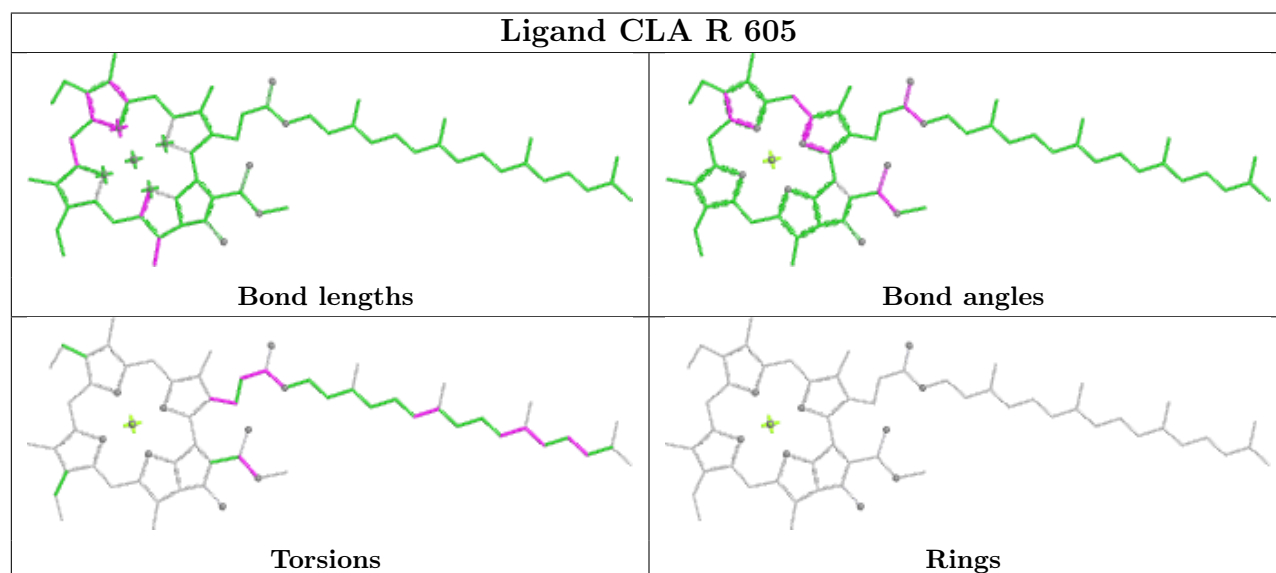
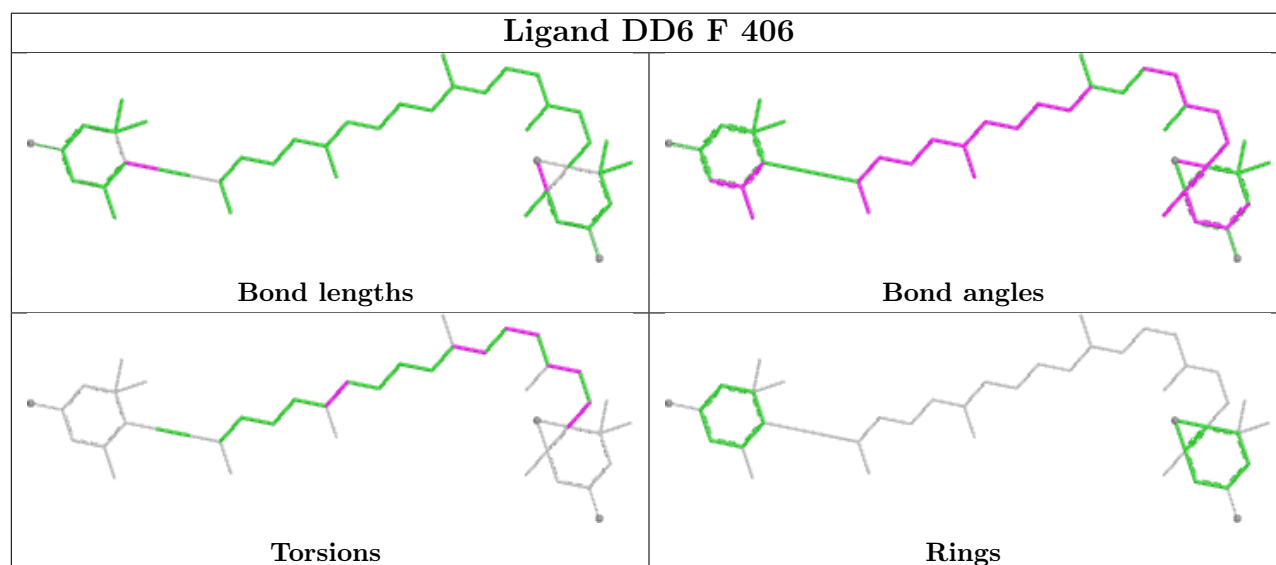
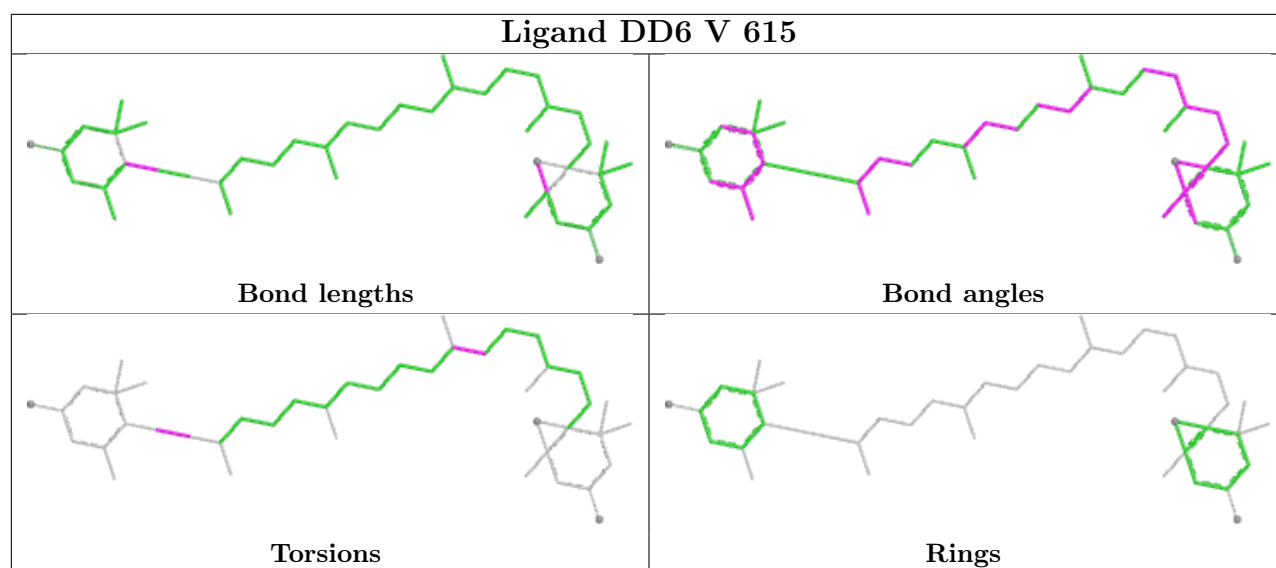


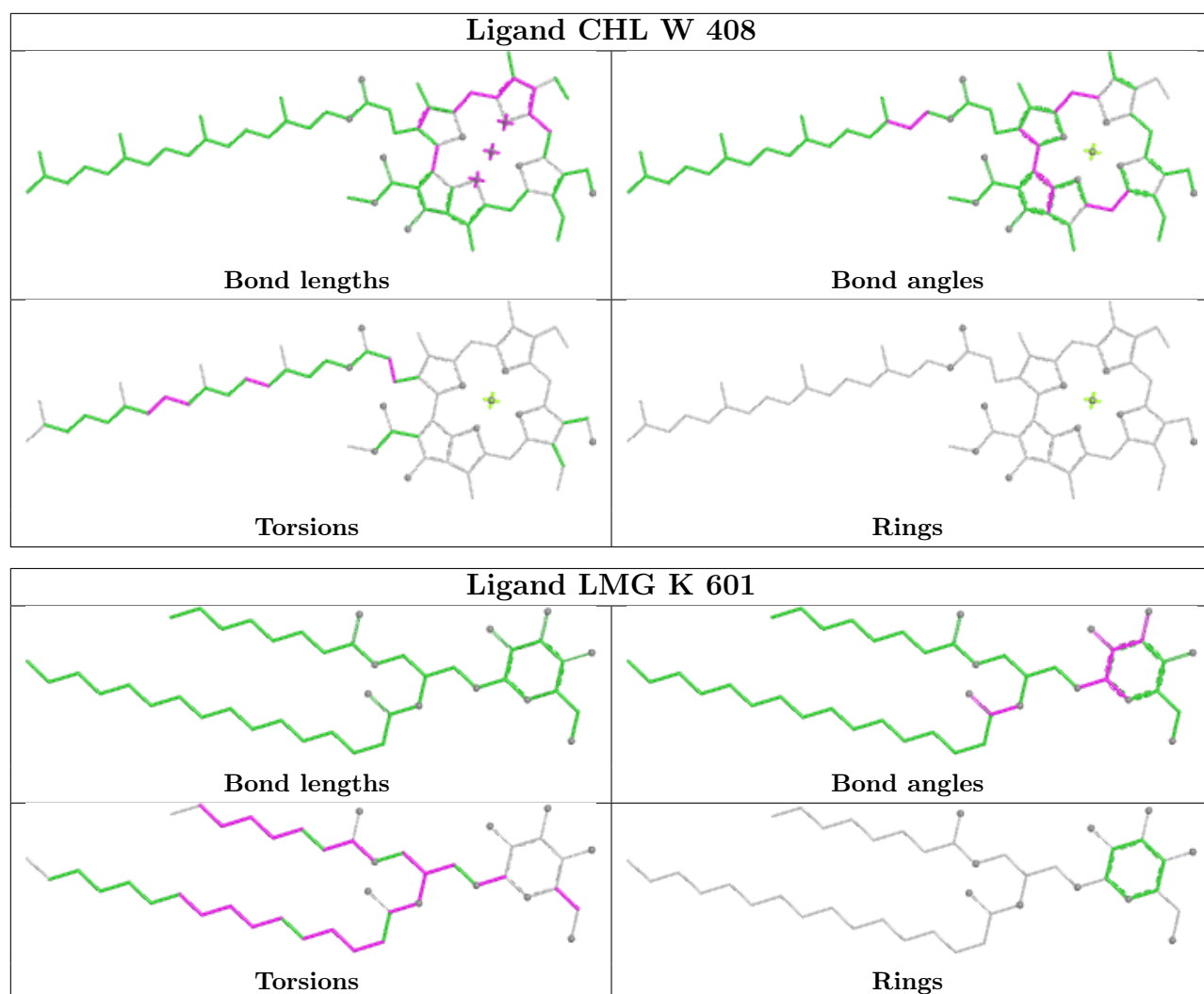




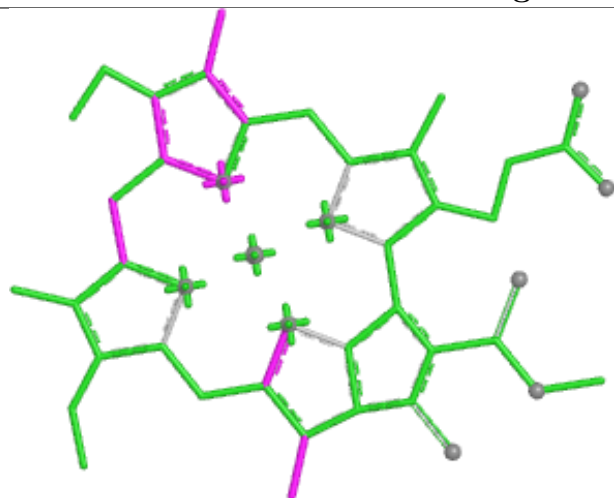




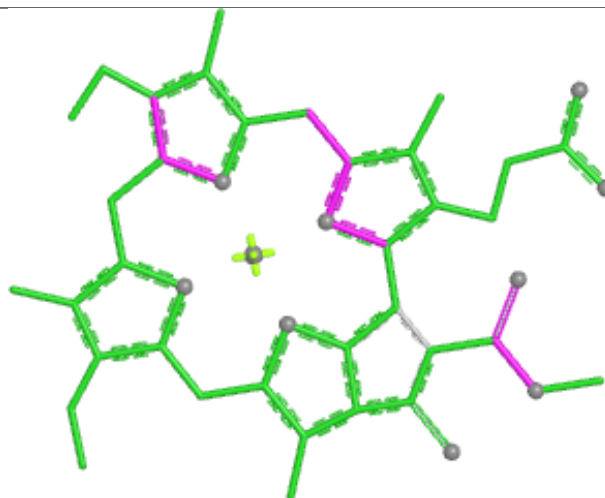




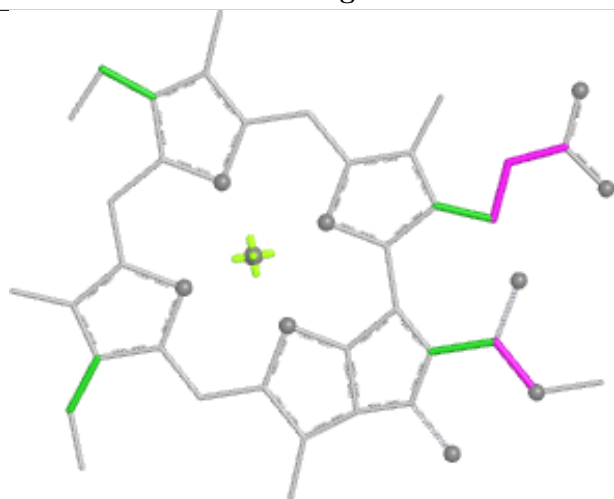
## Ligand CLA G 610



Bond lengths



Bond angles

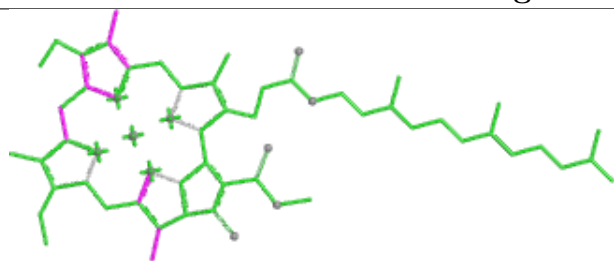


Torsions

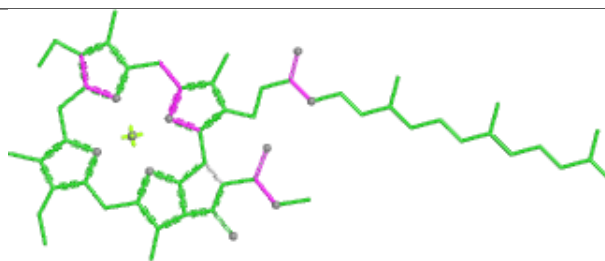


Rings

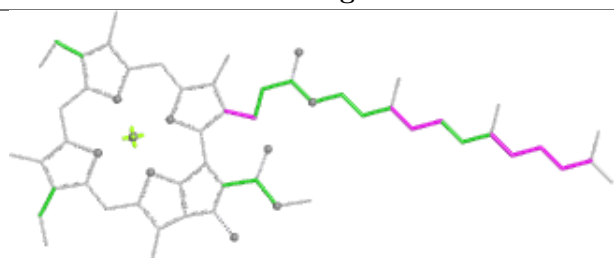
## Ligand CLA X 404



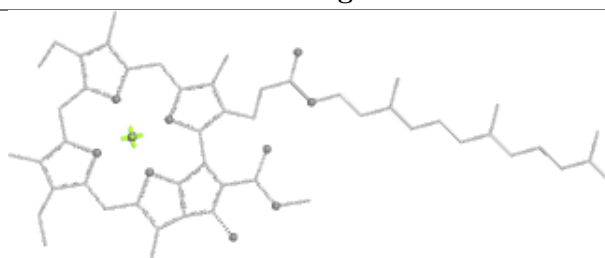
Bond lengths



Bond angles

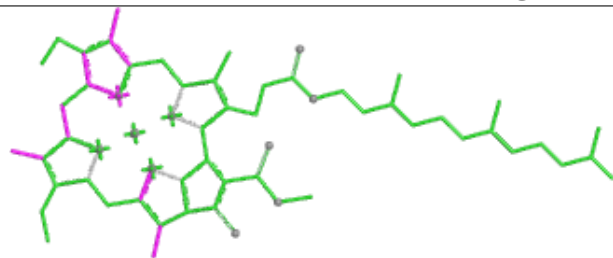


Torsions

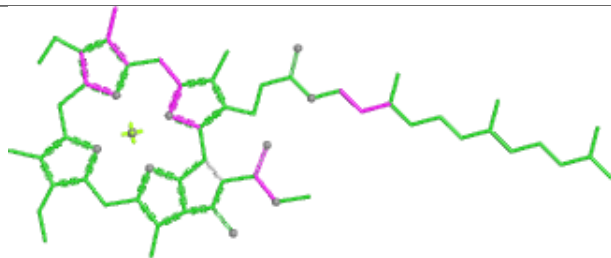


Rings

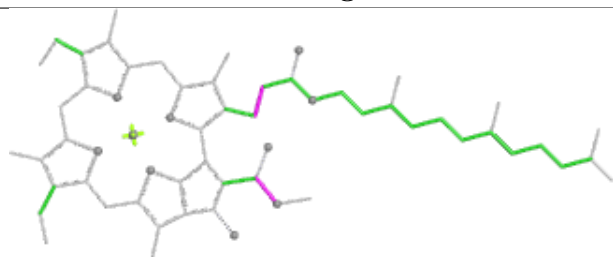
## Ligand CLA N 602



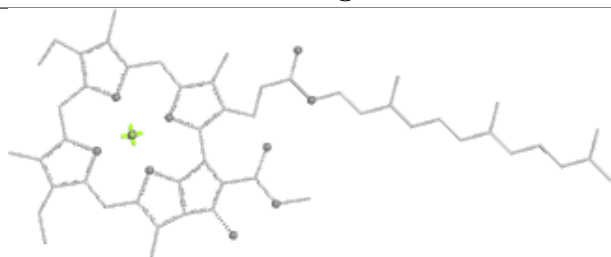
Bond lengths



Bond angles

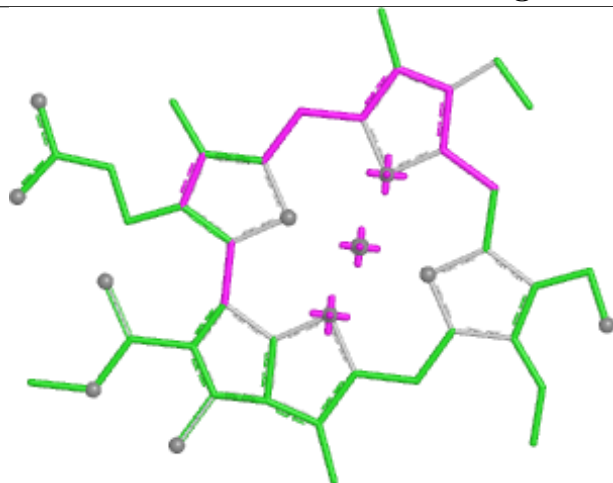


Torsions

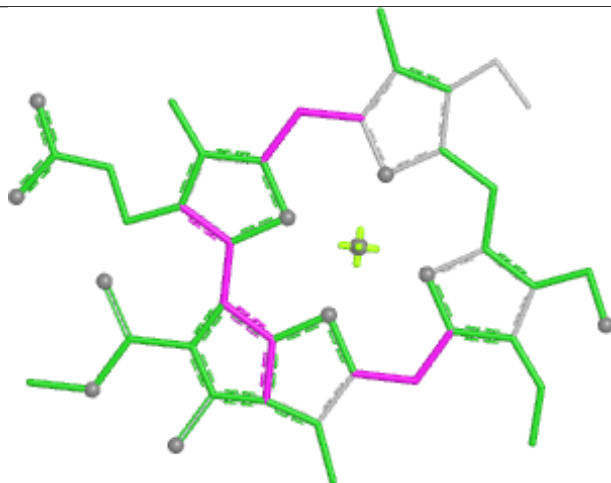


Rings

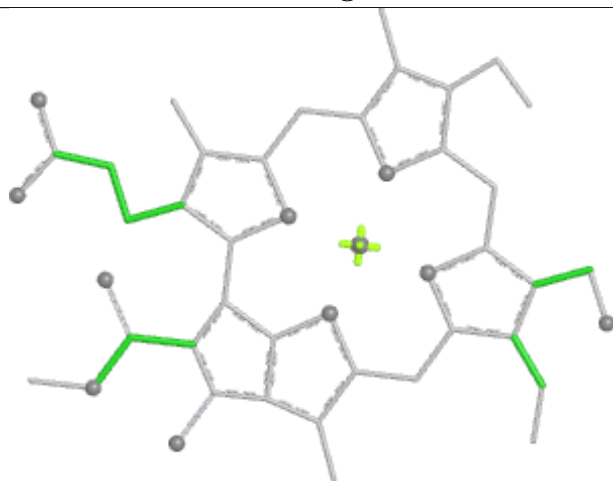
## Ligand CHL V 605



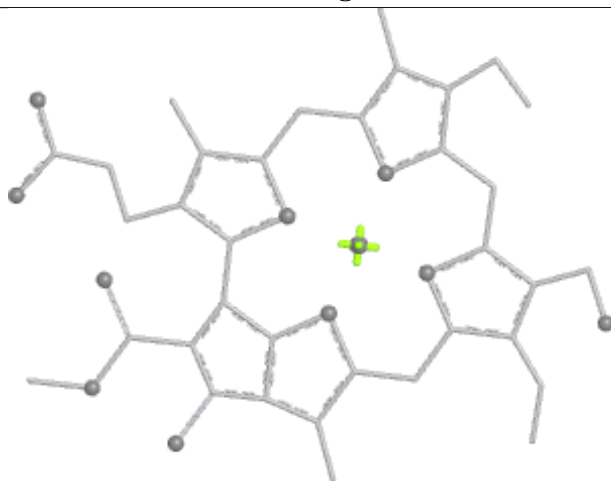
Bond lengths



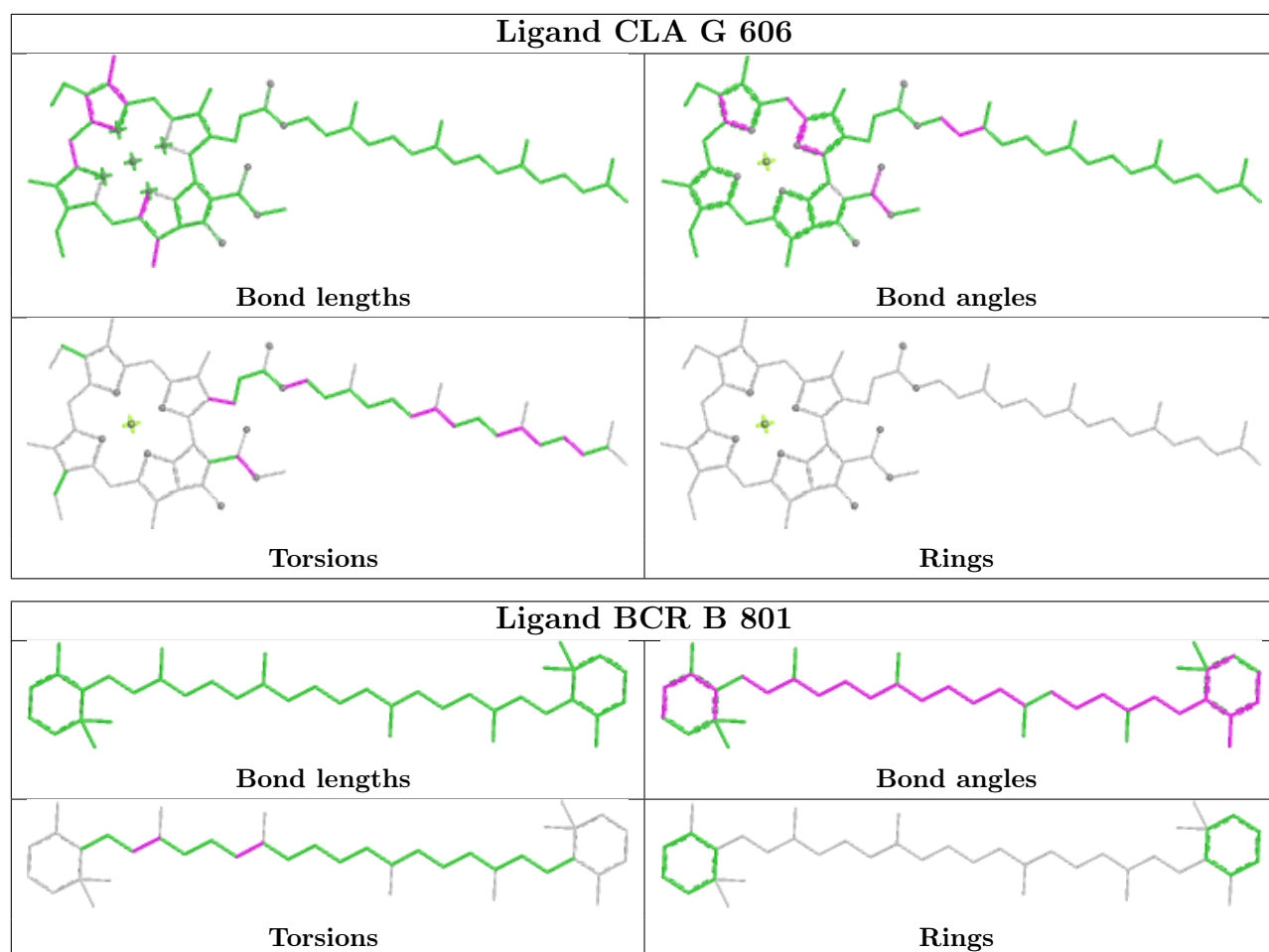
Bond angles



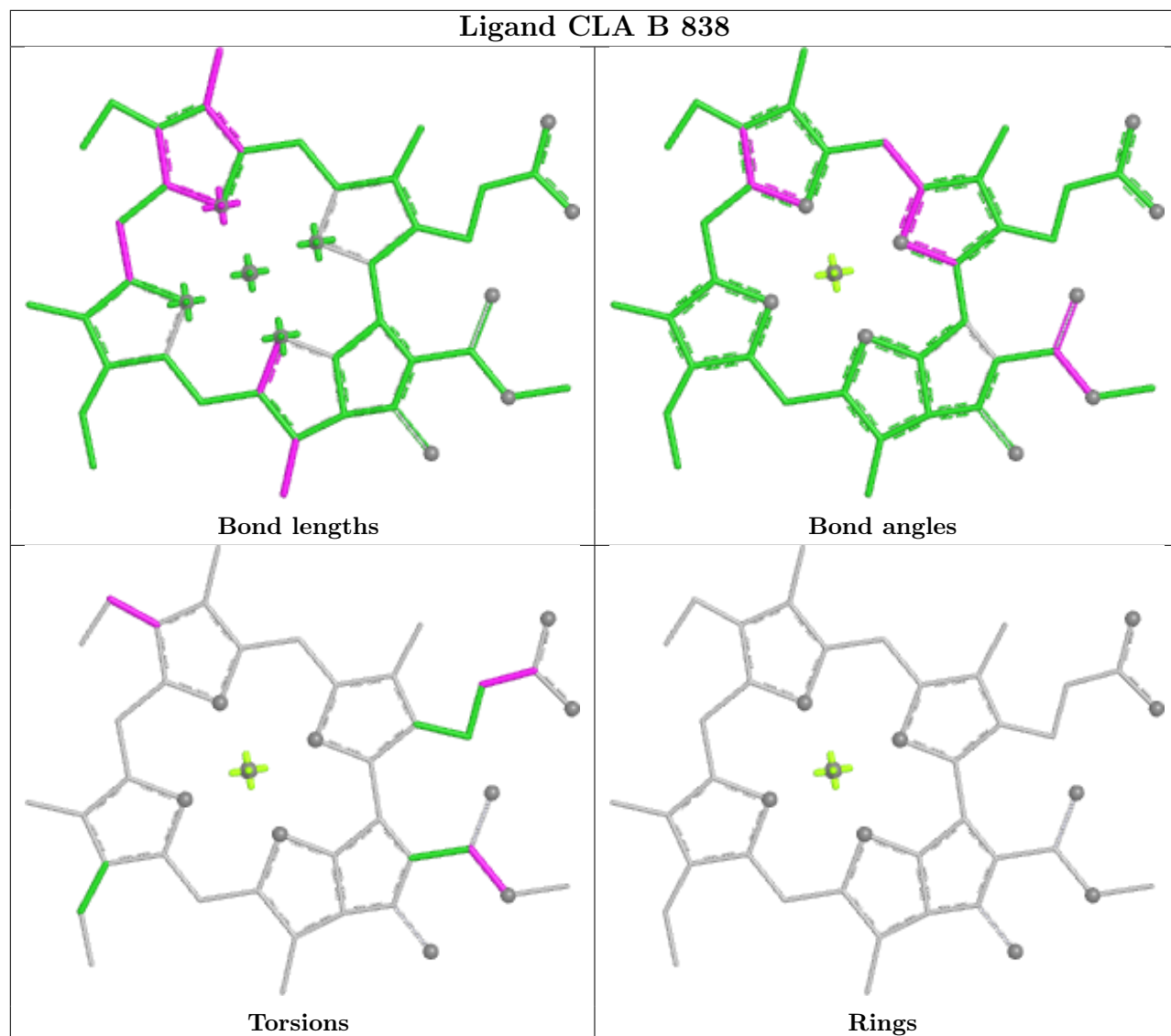
Torsions



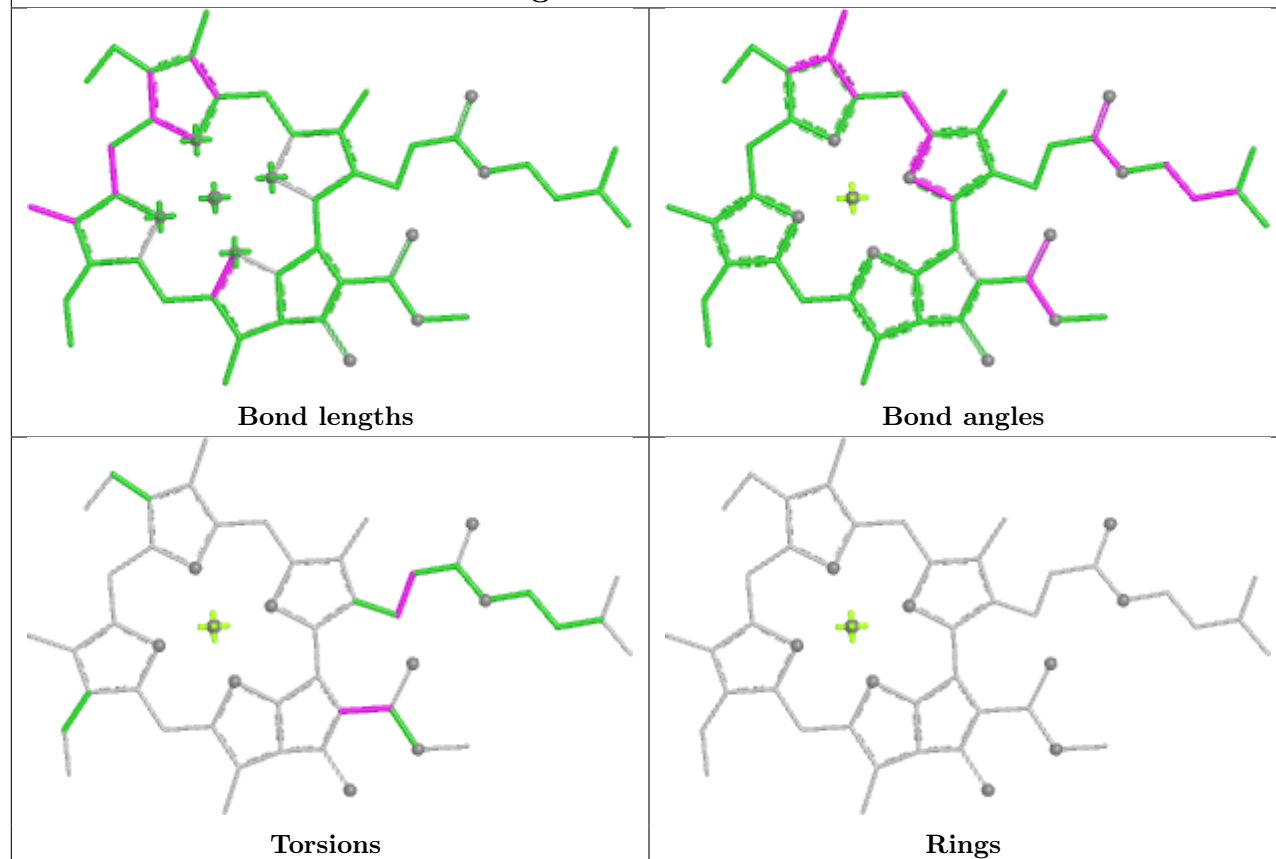
Rings



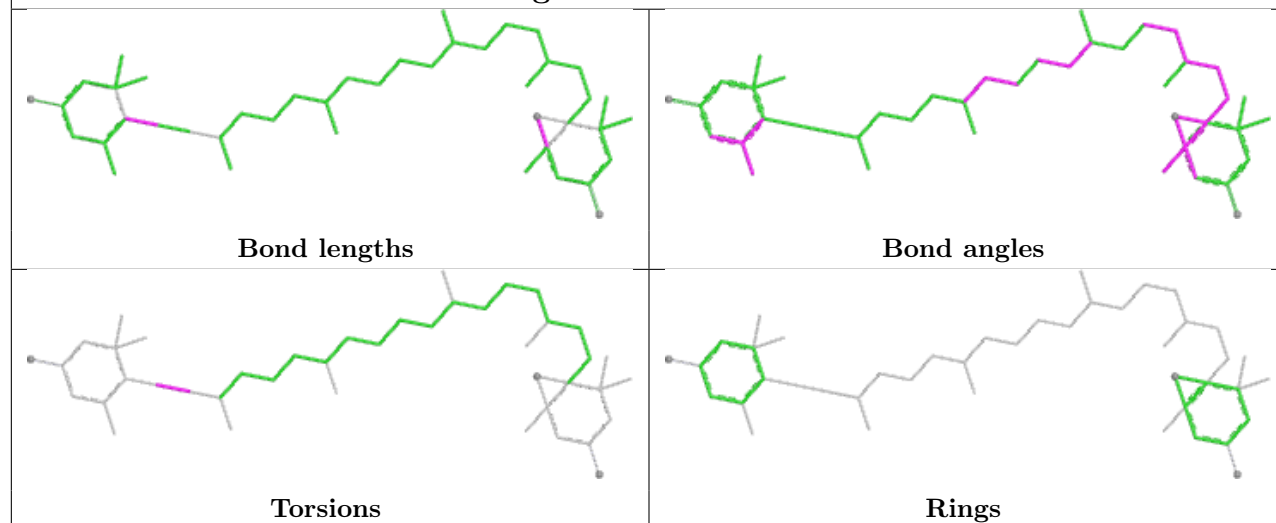
## Ligand CLA B 838



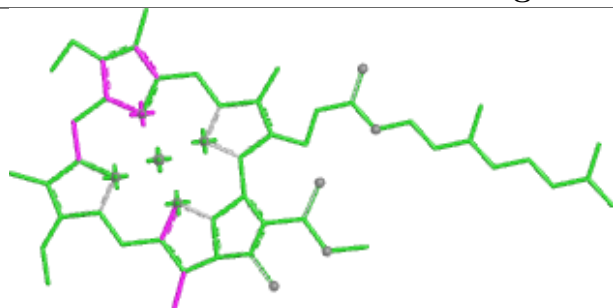
## Ligand CLA X 417



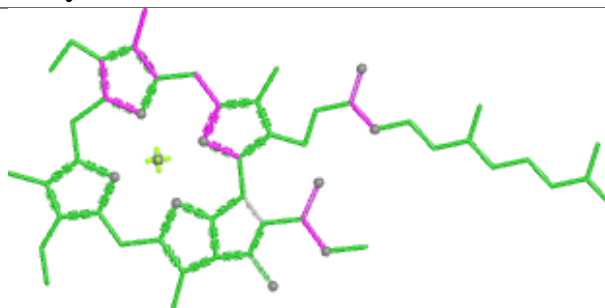
## Ligand DD6 R 612



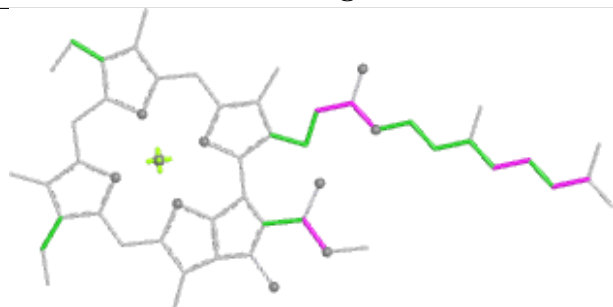
## Ligand CLA Q 611



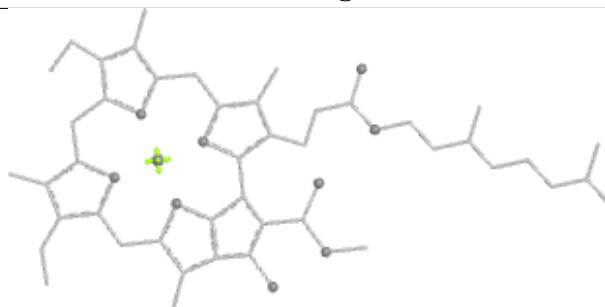
Bond lengths



Bond angles

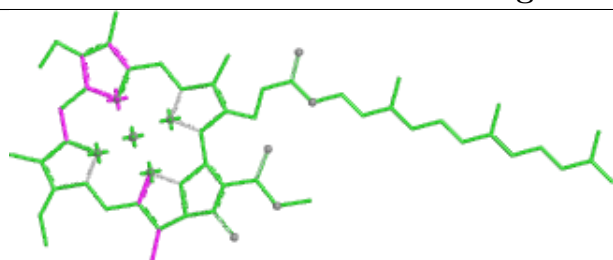


Torsions

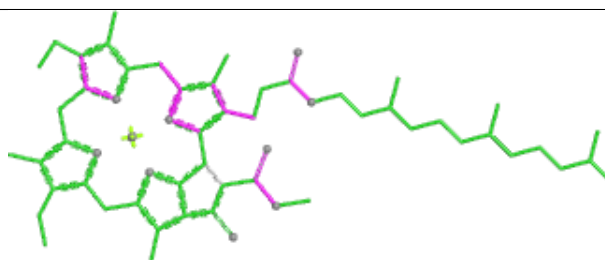


Rings

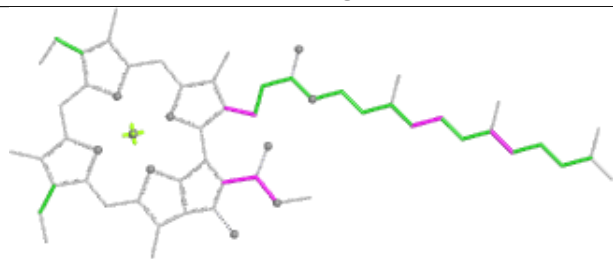
## Ligand CLA L 410



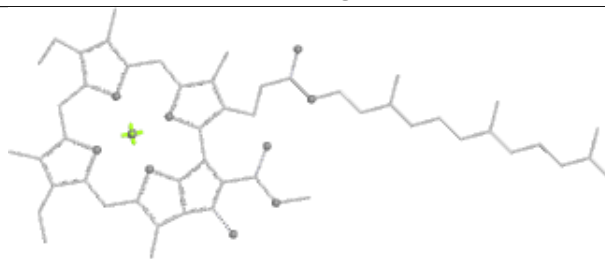
Bond lengths



Bond angles

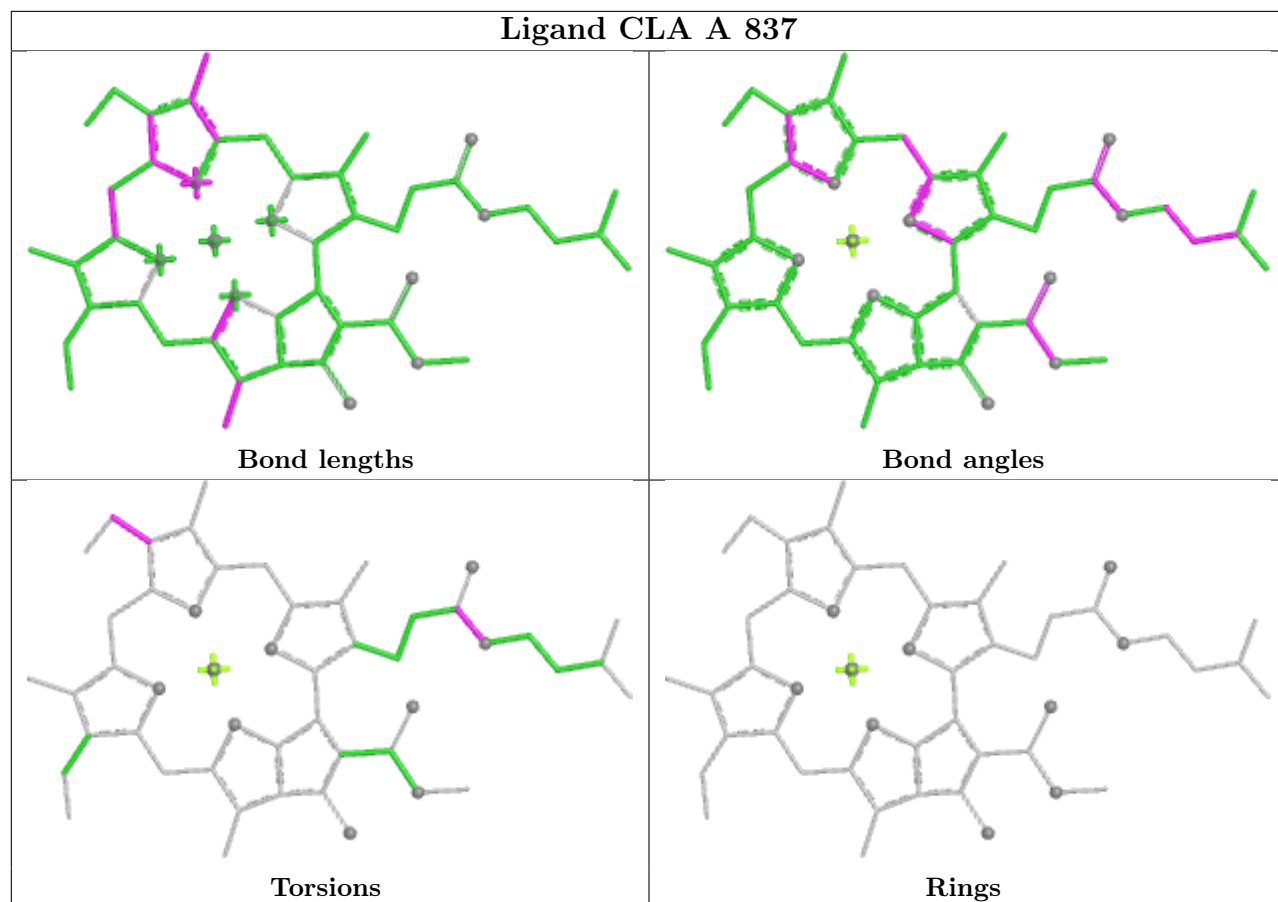


Torsions

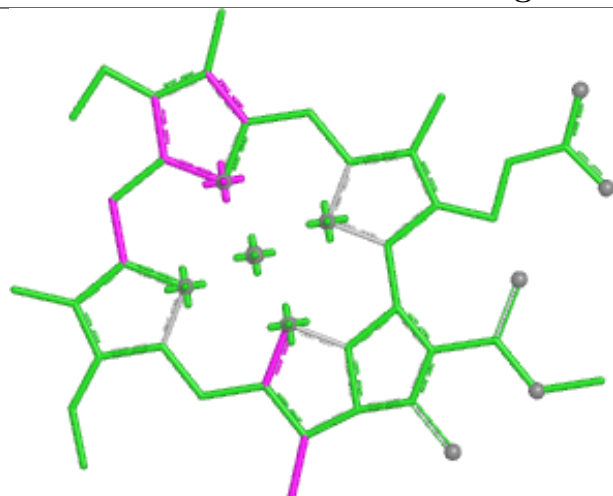


Rings

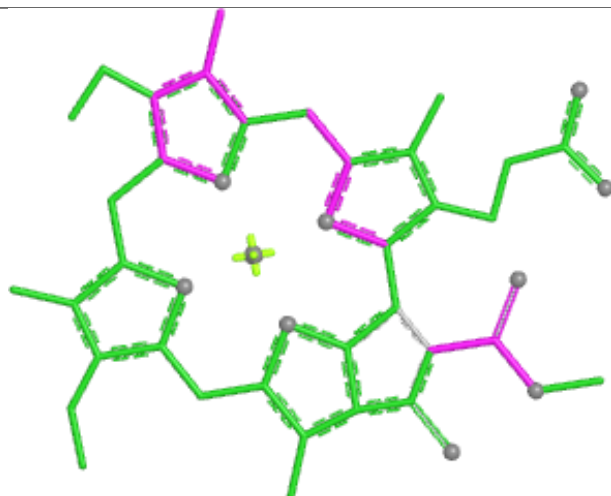




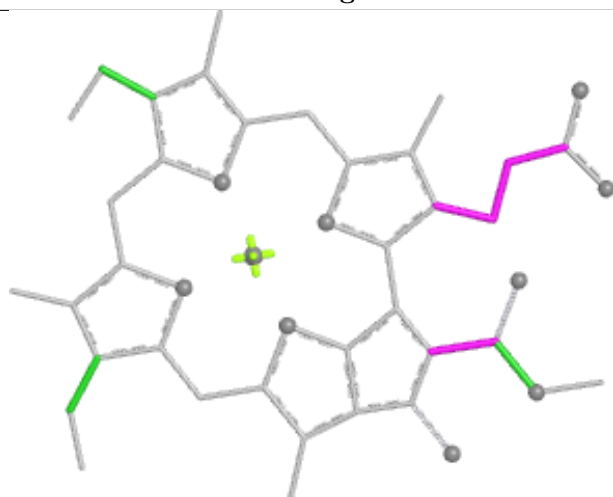
## Ligand CLA B 814



Bond lengths



Bond angles

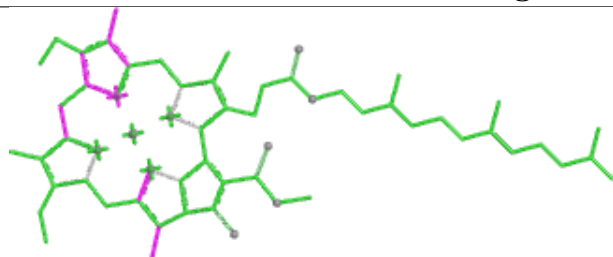


Torsions

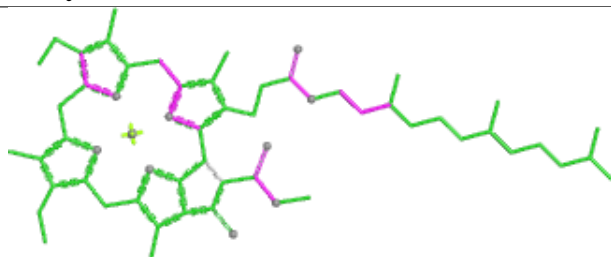


Rings

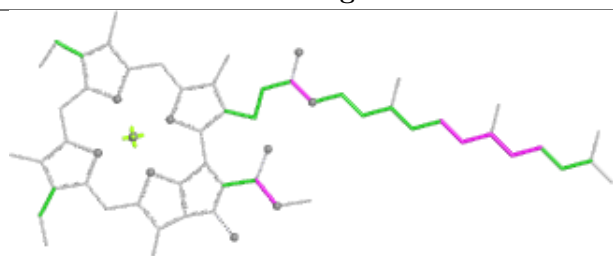
## Ligand CLA Q 609



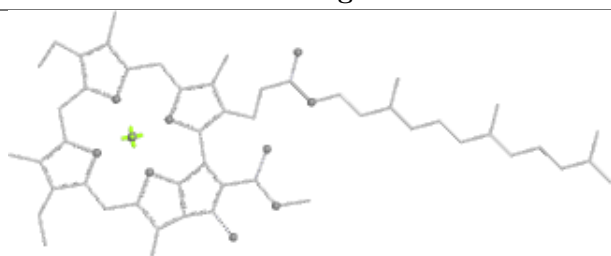
Bond lengths



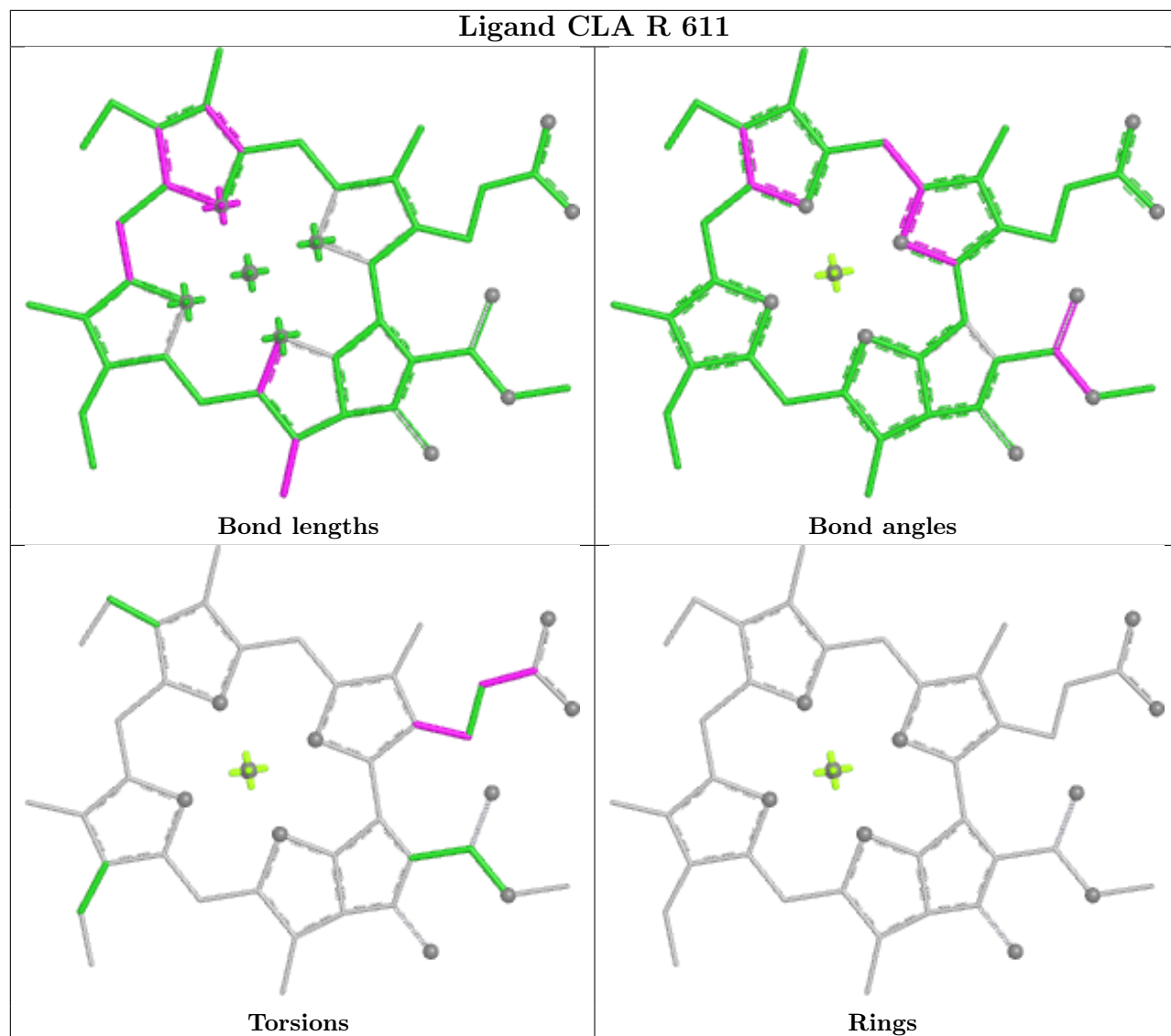
Bond angles



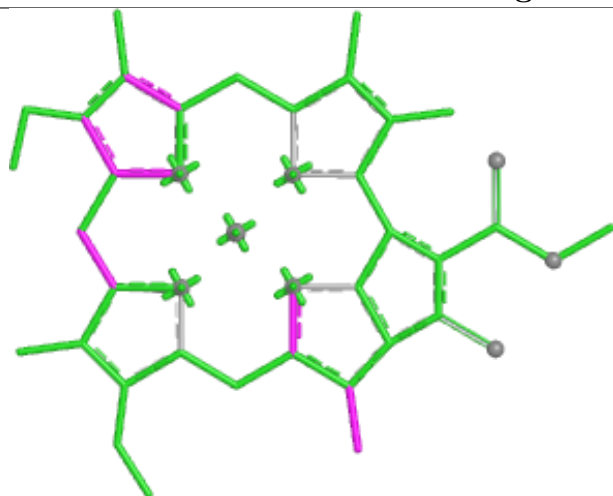
Torsions



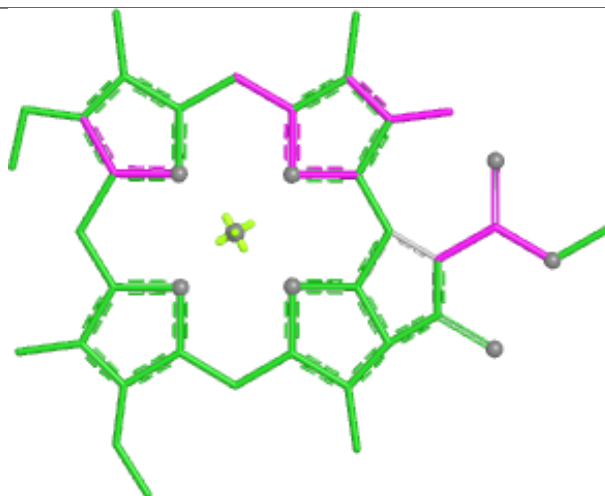
Rings



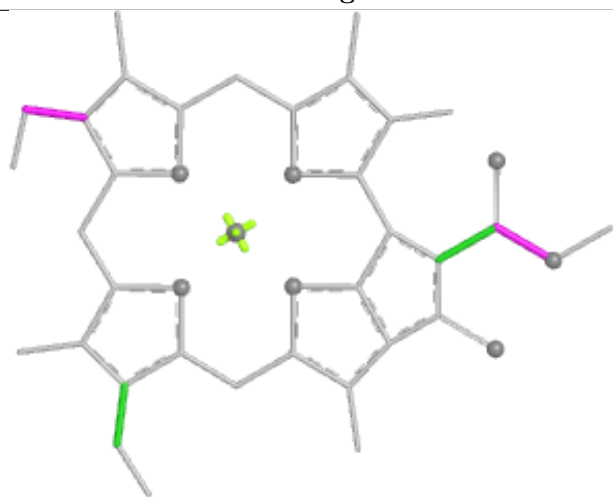
## Ligand CLA P 610



Bond lengths



Bond angles

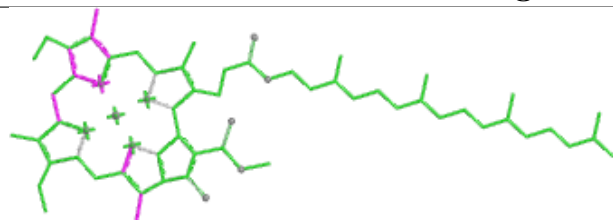


Torsions

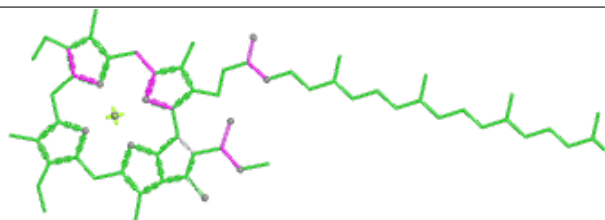


Rings

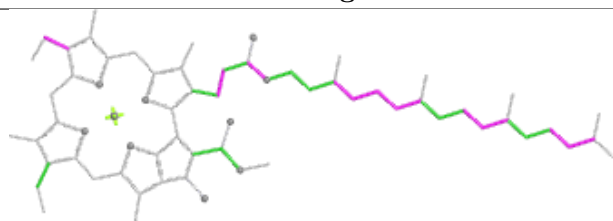
## Ligand CLA T 605



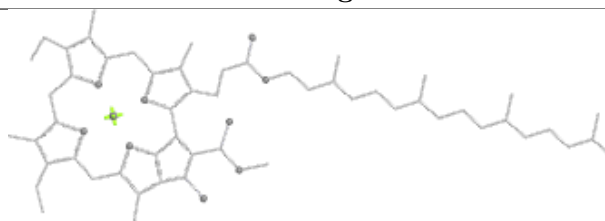
Bond lengths



Bond angles

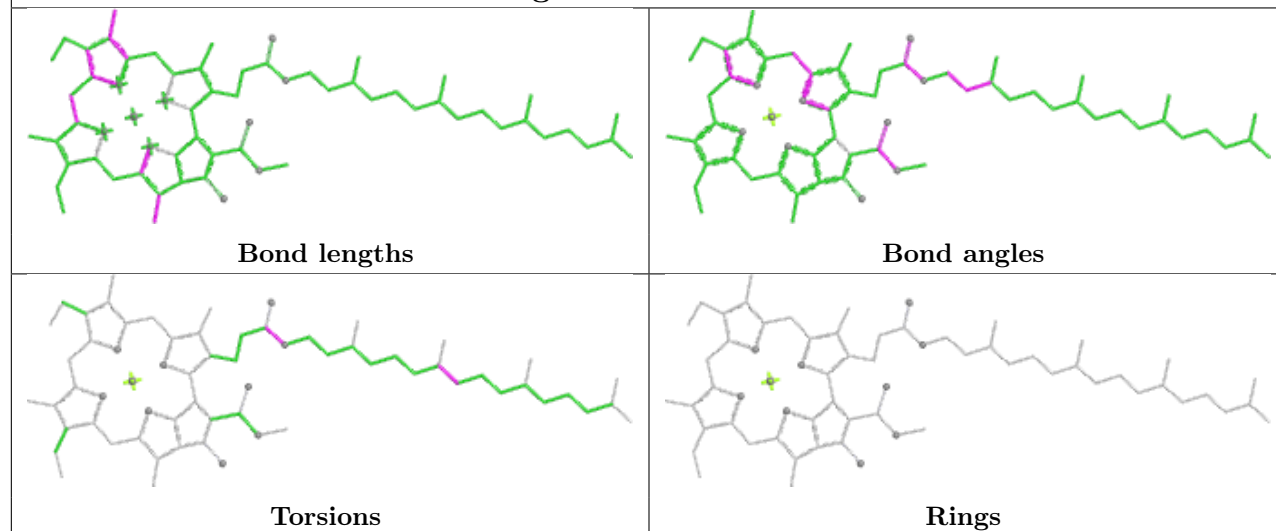


Torsions

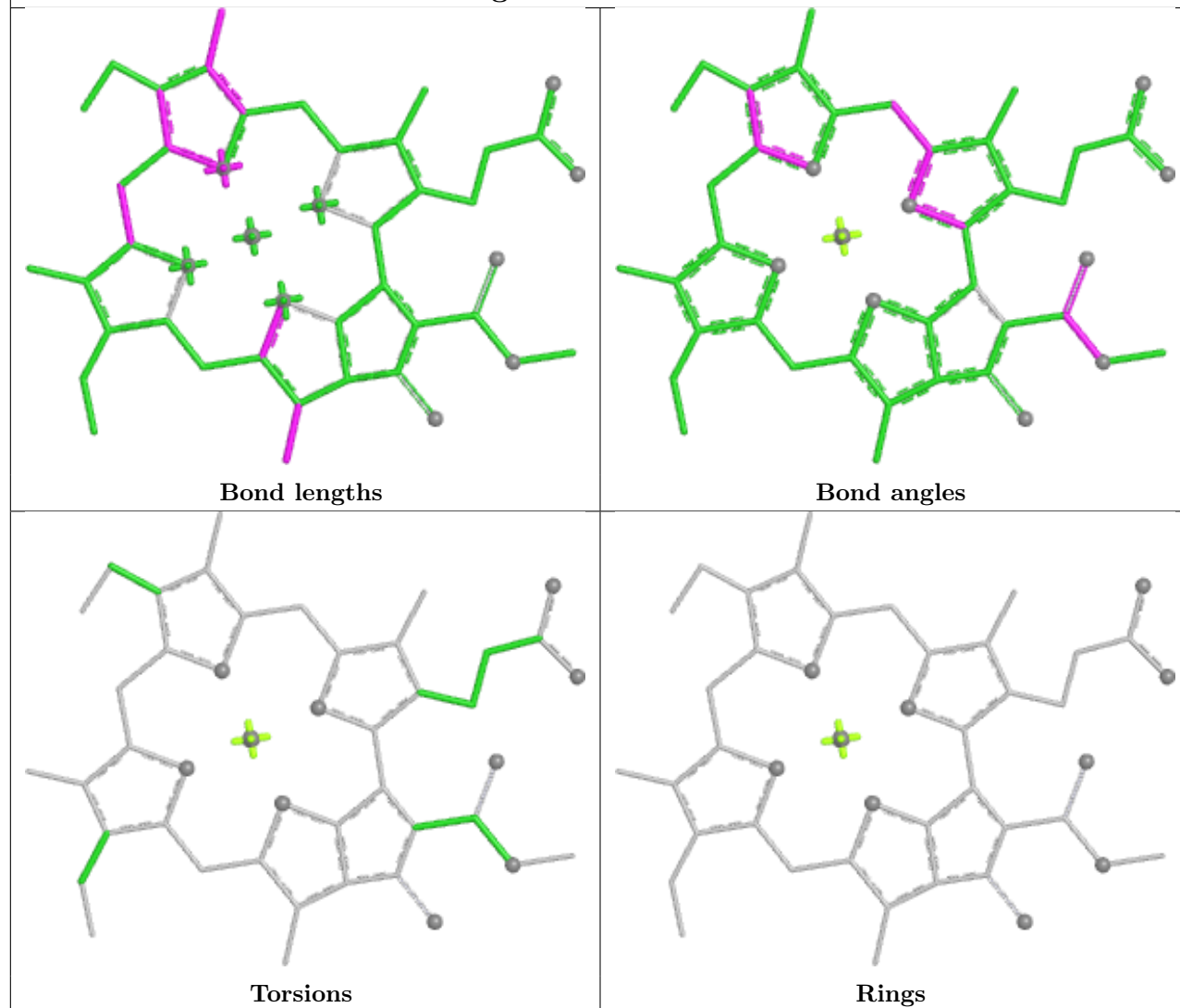


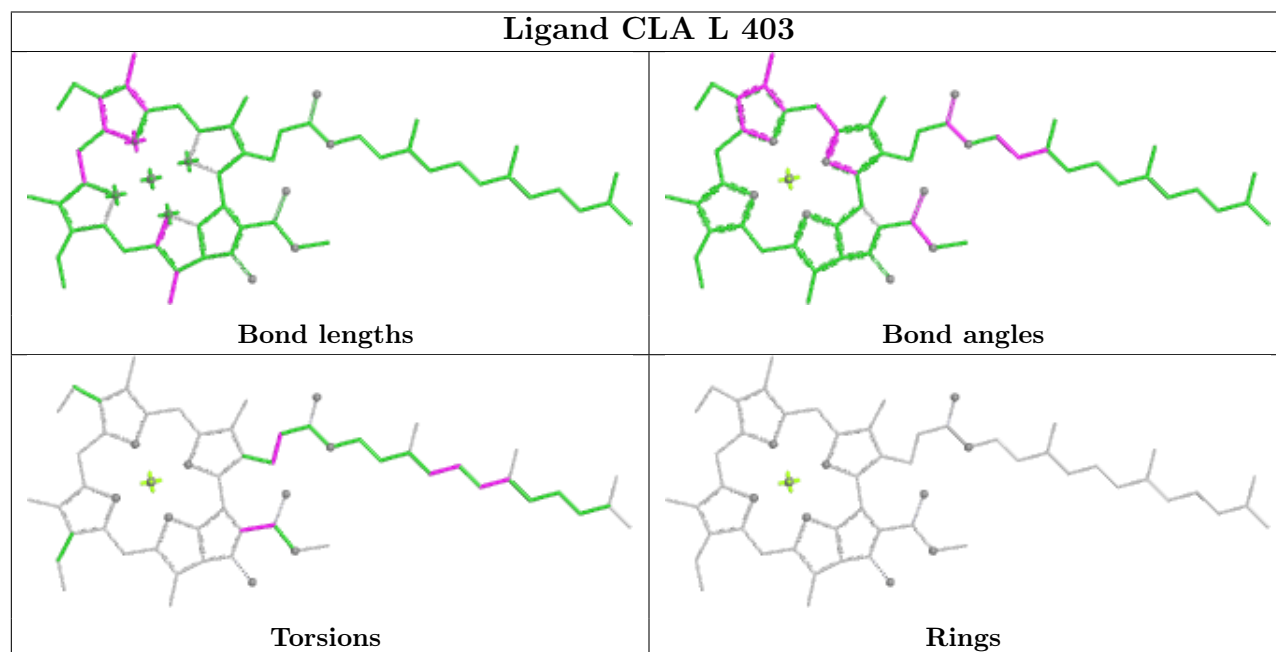
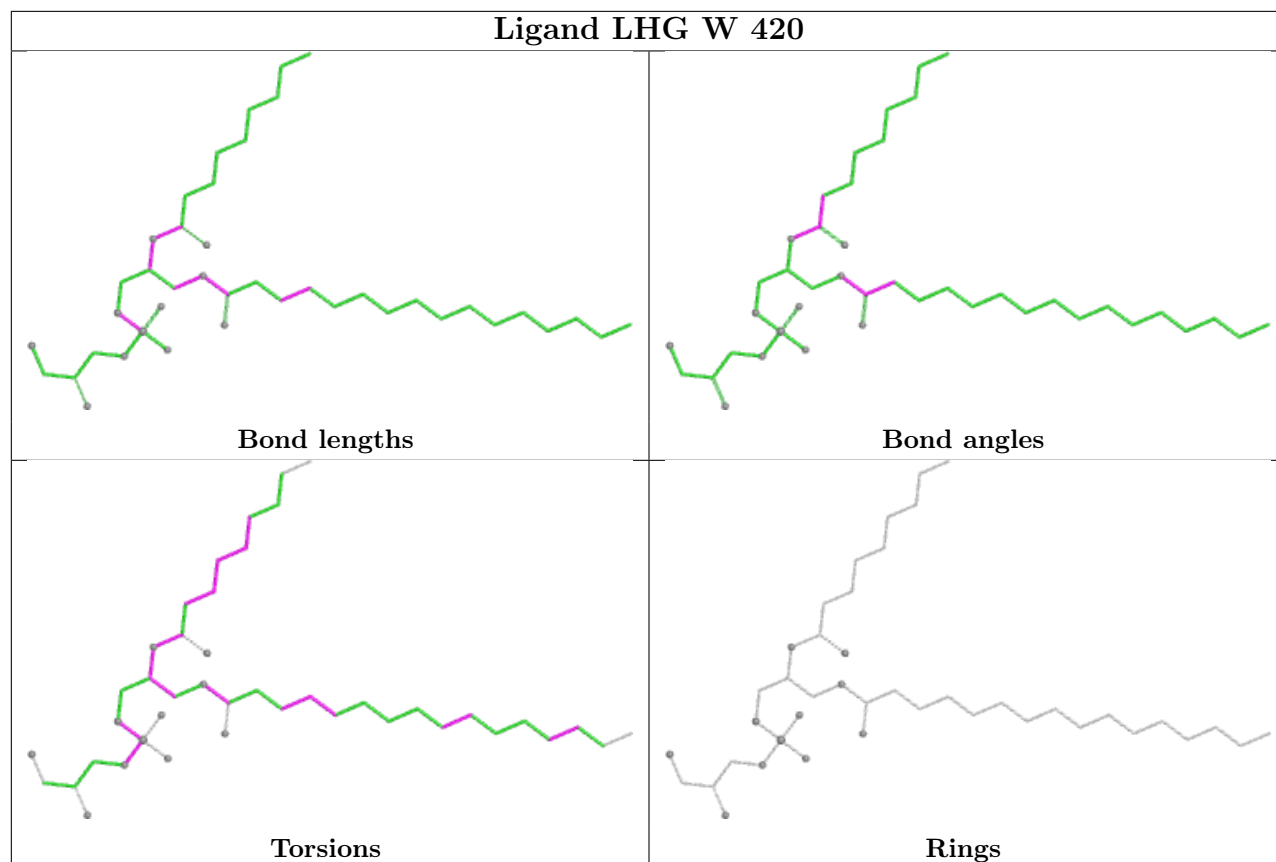
Rings

## Ligand CLA B 809

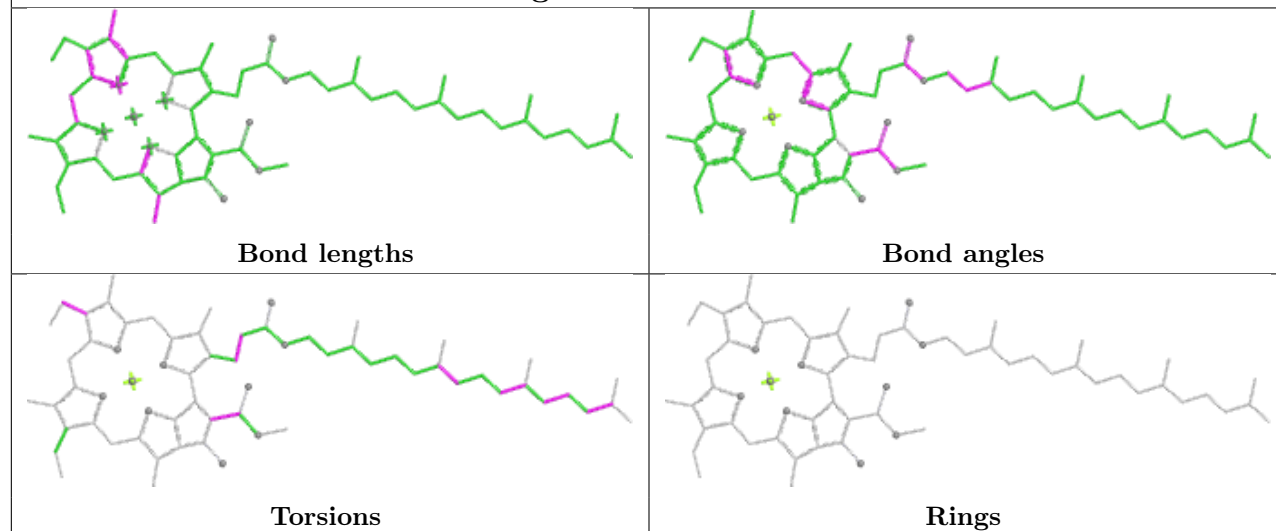


## Ligand CLA O 314

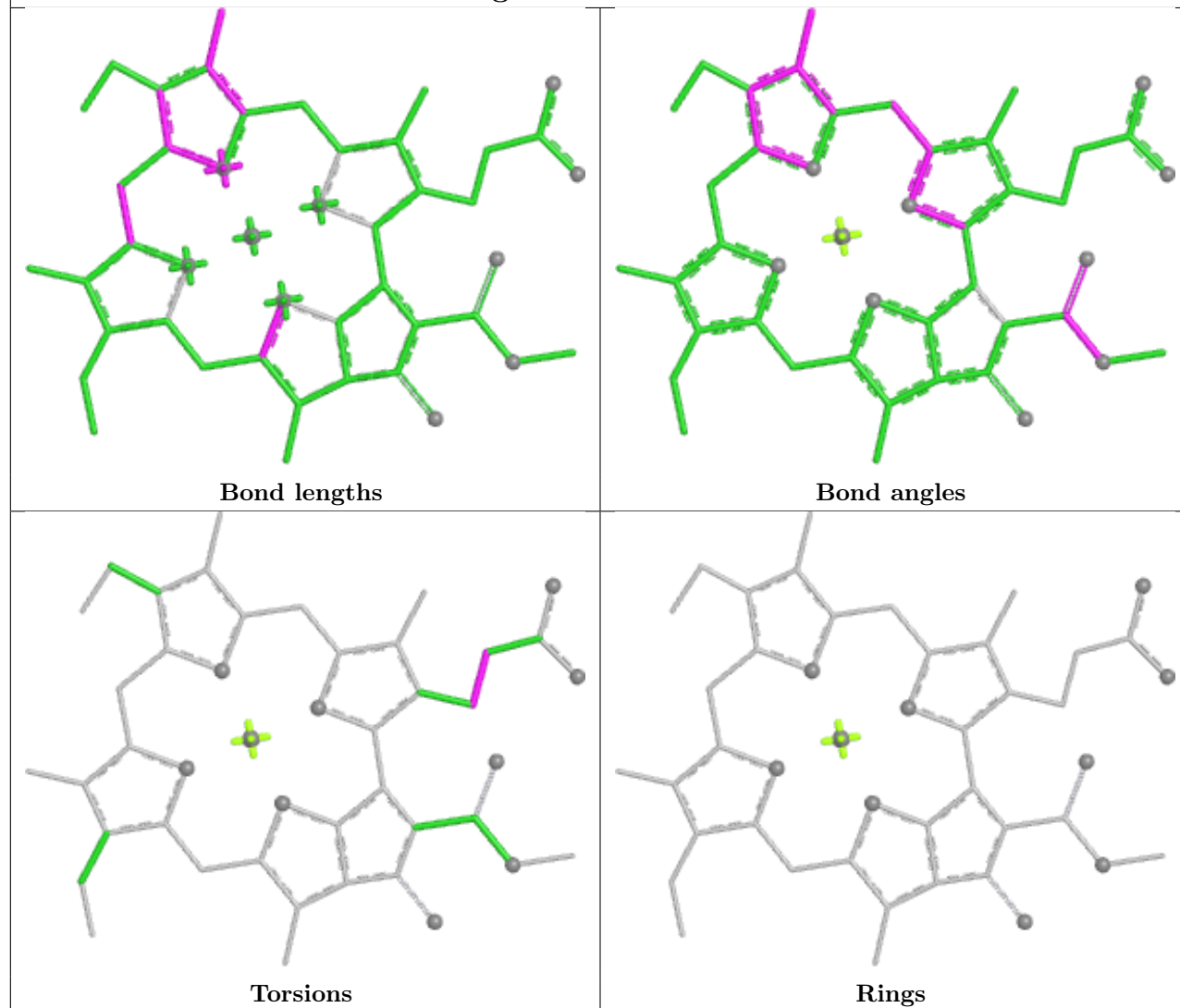


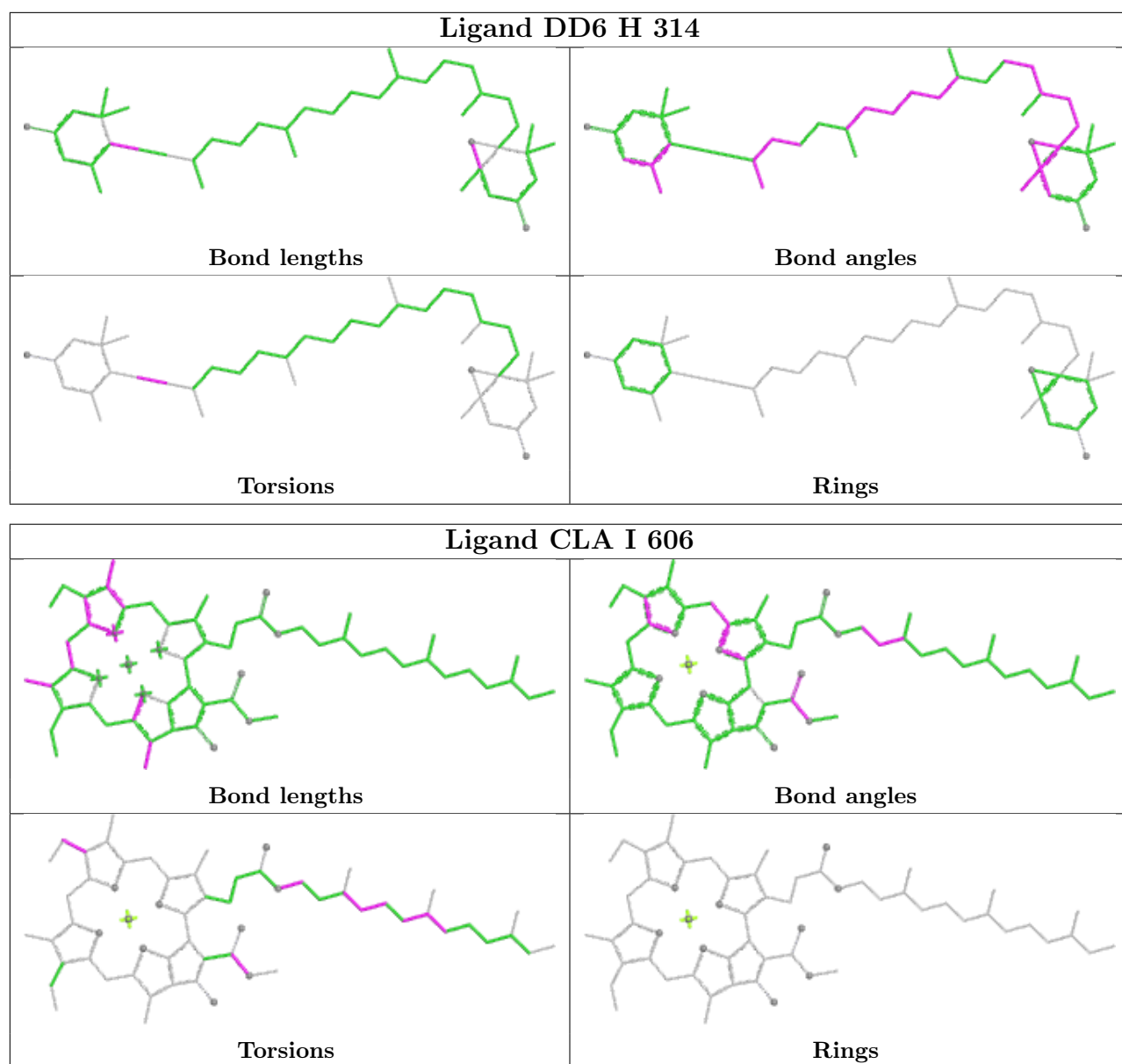


## Ligand CLA A 810



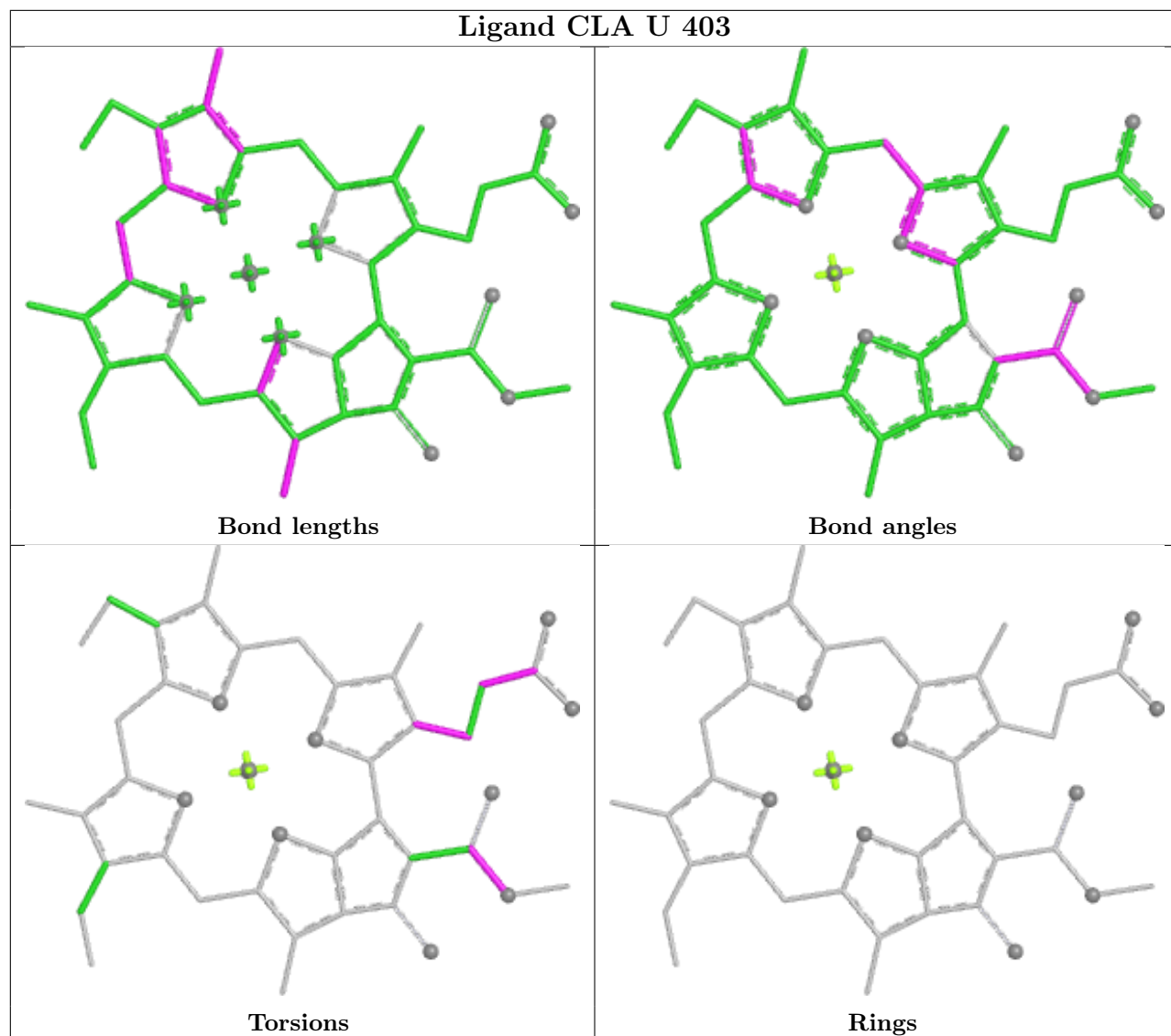
## Ligand CLA B 811



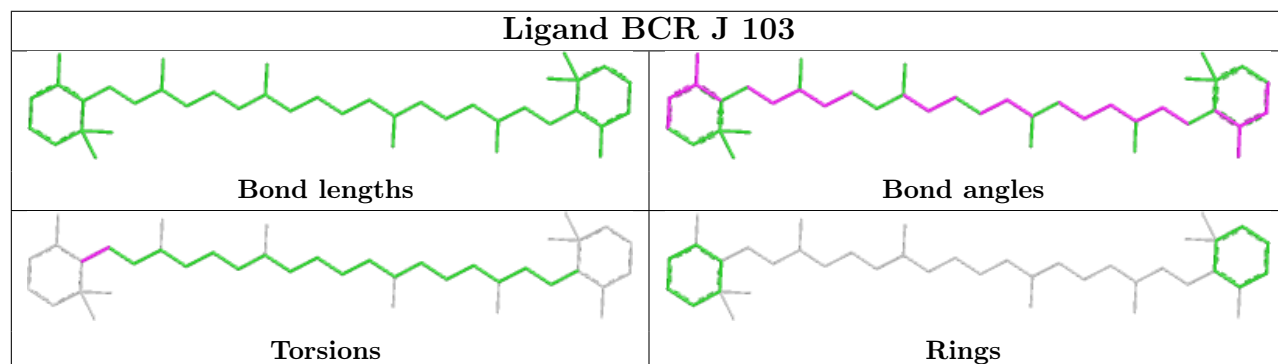


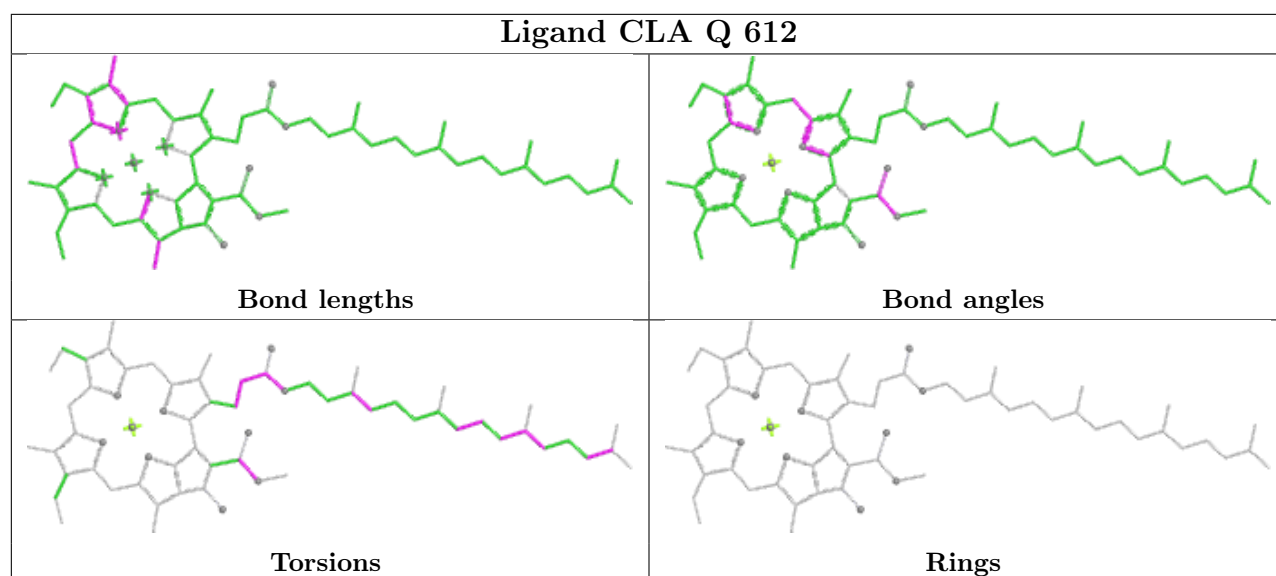
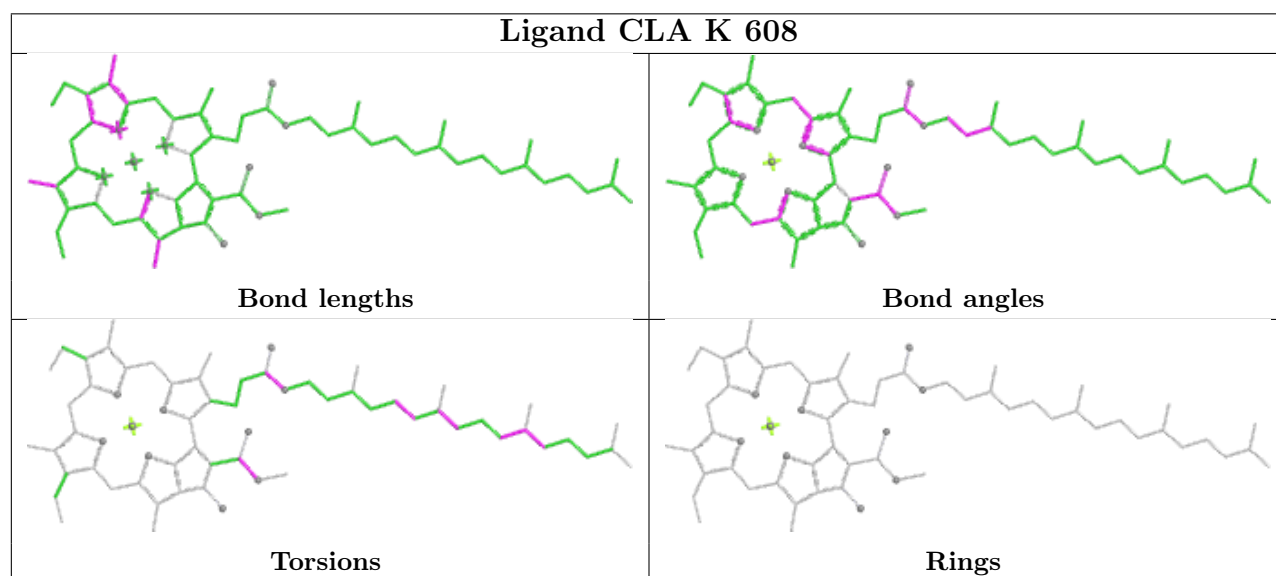
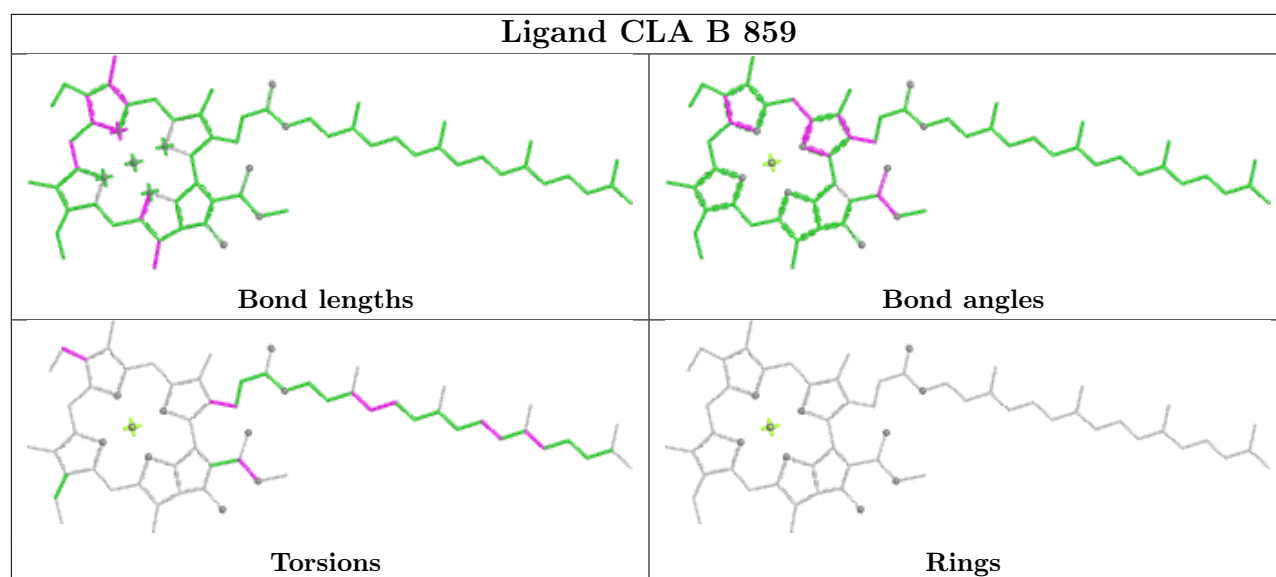


## Ligand CLA U 403

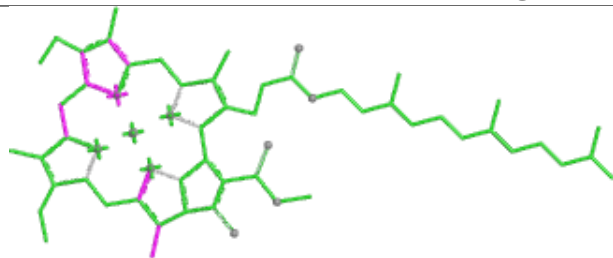


## Ligand BCR J 103

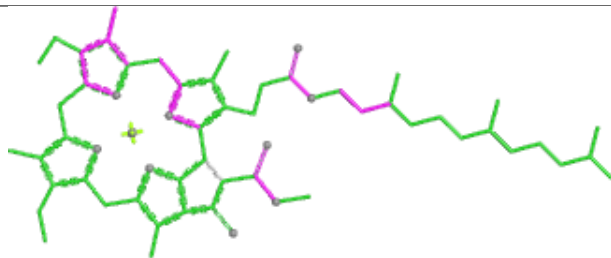




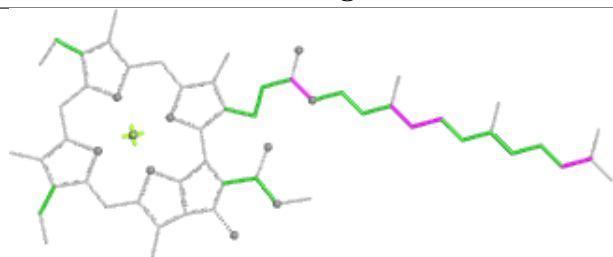
## Ligand CLA O 312



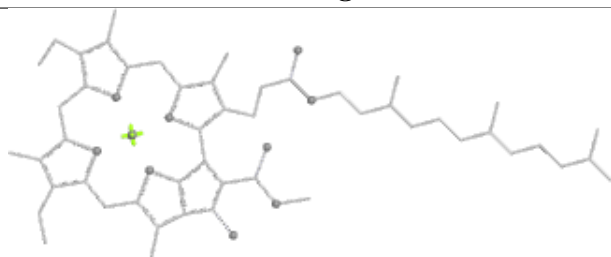
Bond lengths



Bond angles

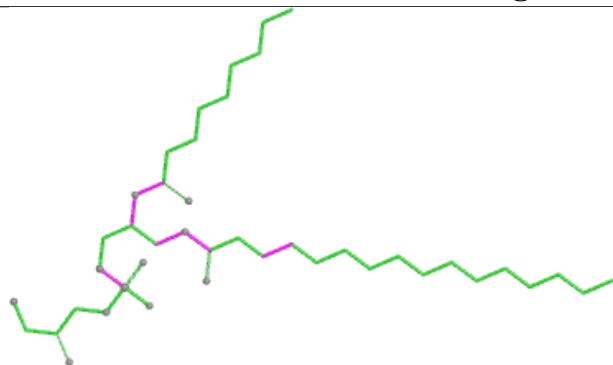


Torsions

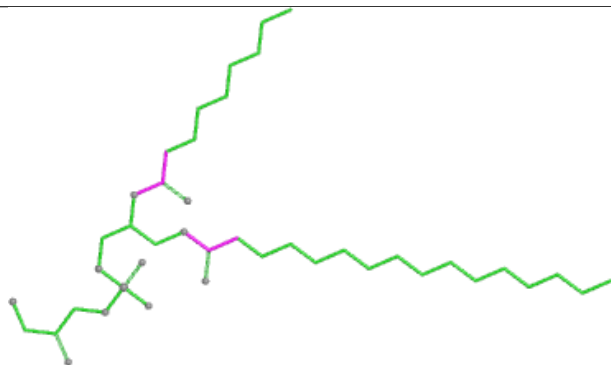


Rings

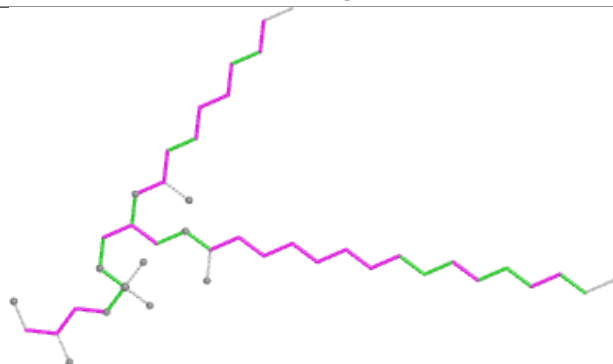
## Ligand LHG X 420



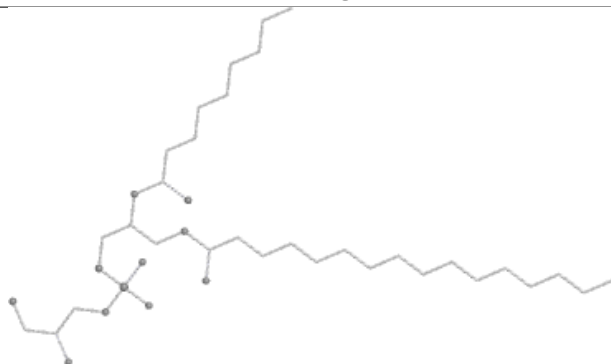
Bond lengths



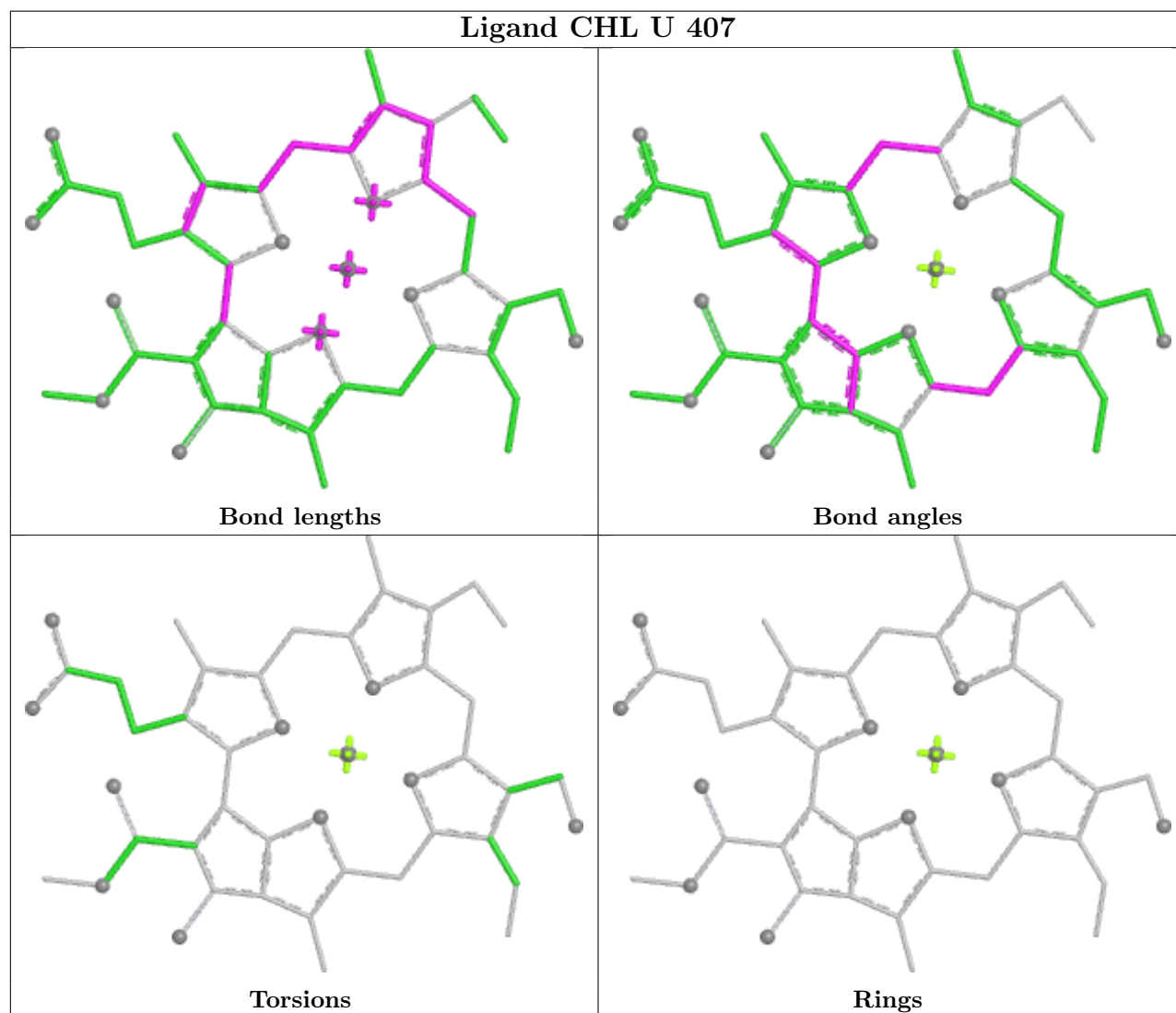
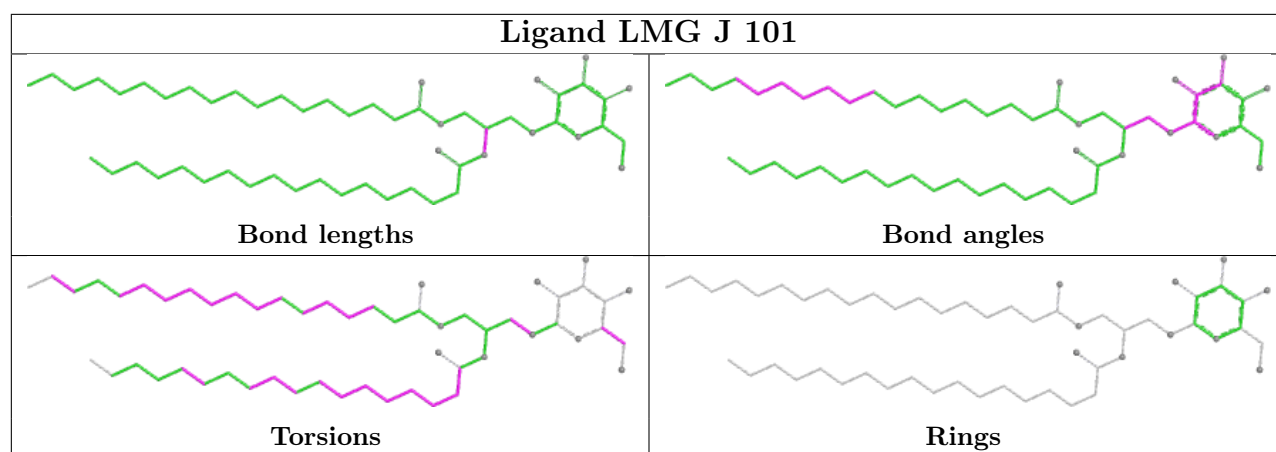
Bond angles



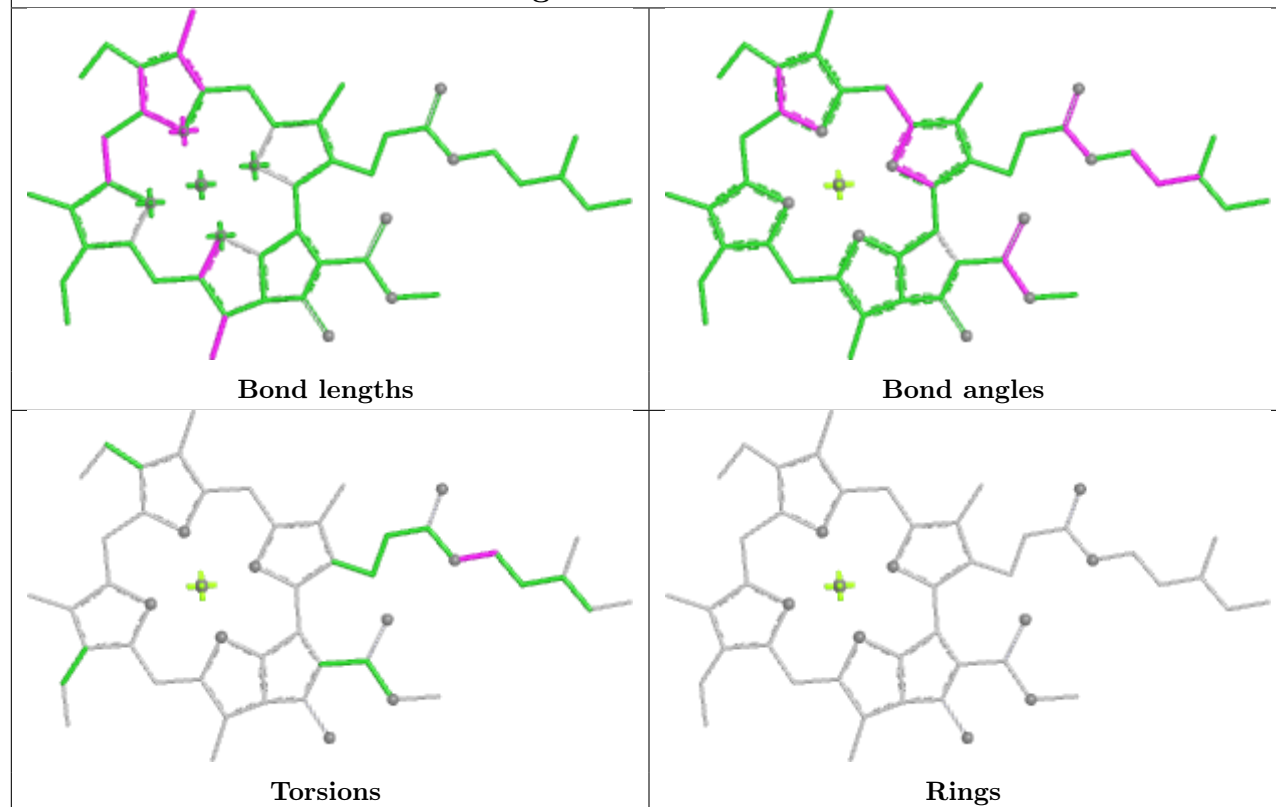
Torsions



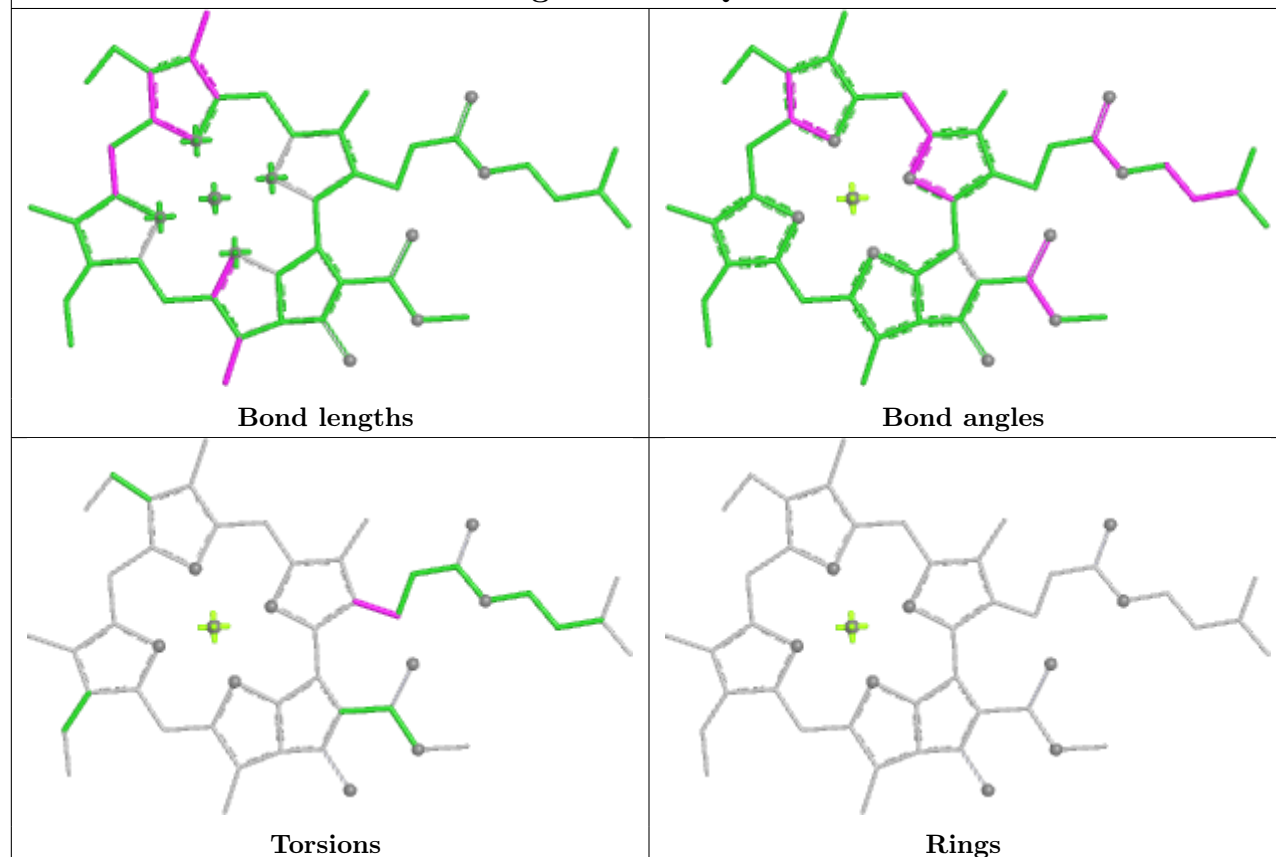
Rings



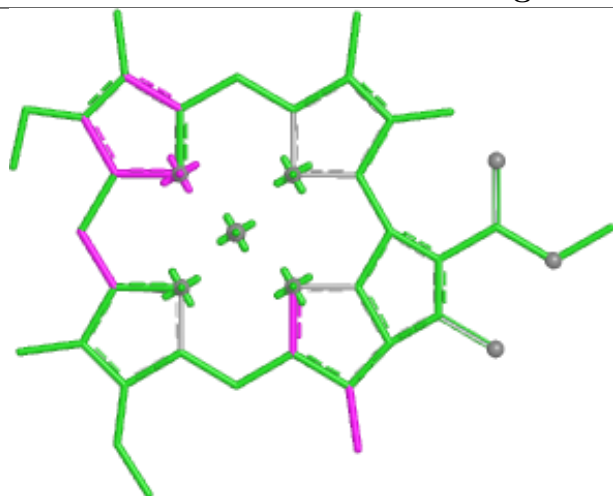
## Ligand CLA B 836



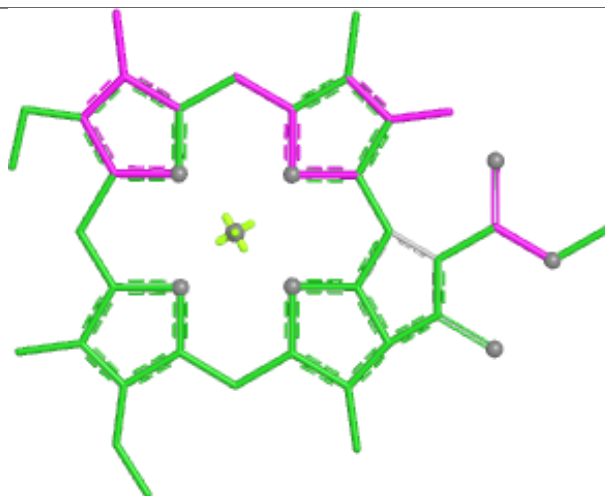
## Ligand CLA Q 608



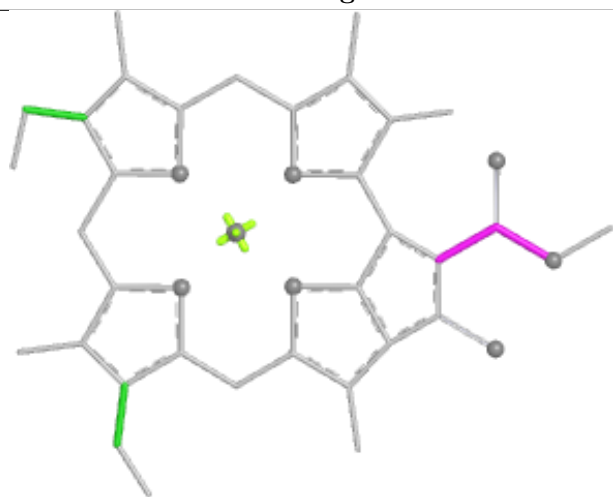
## Ligand CLA R 609



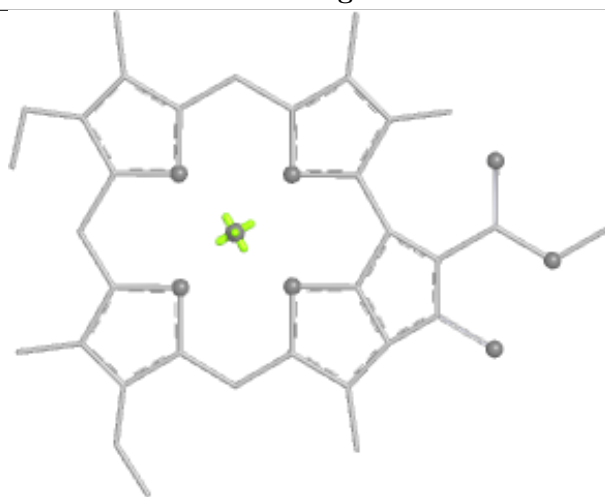
Bond lengths



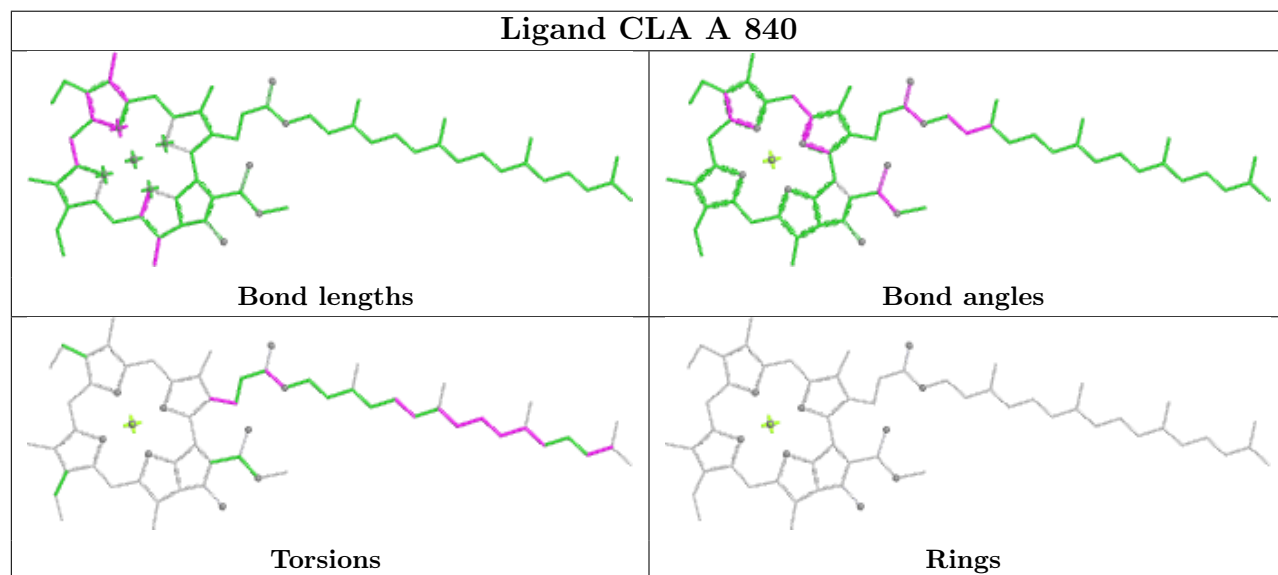
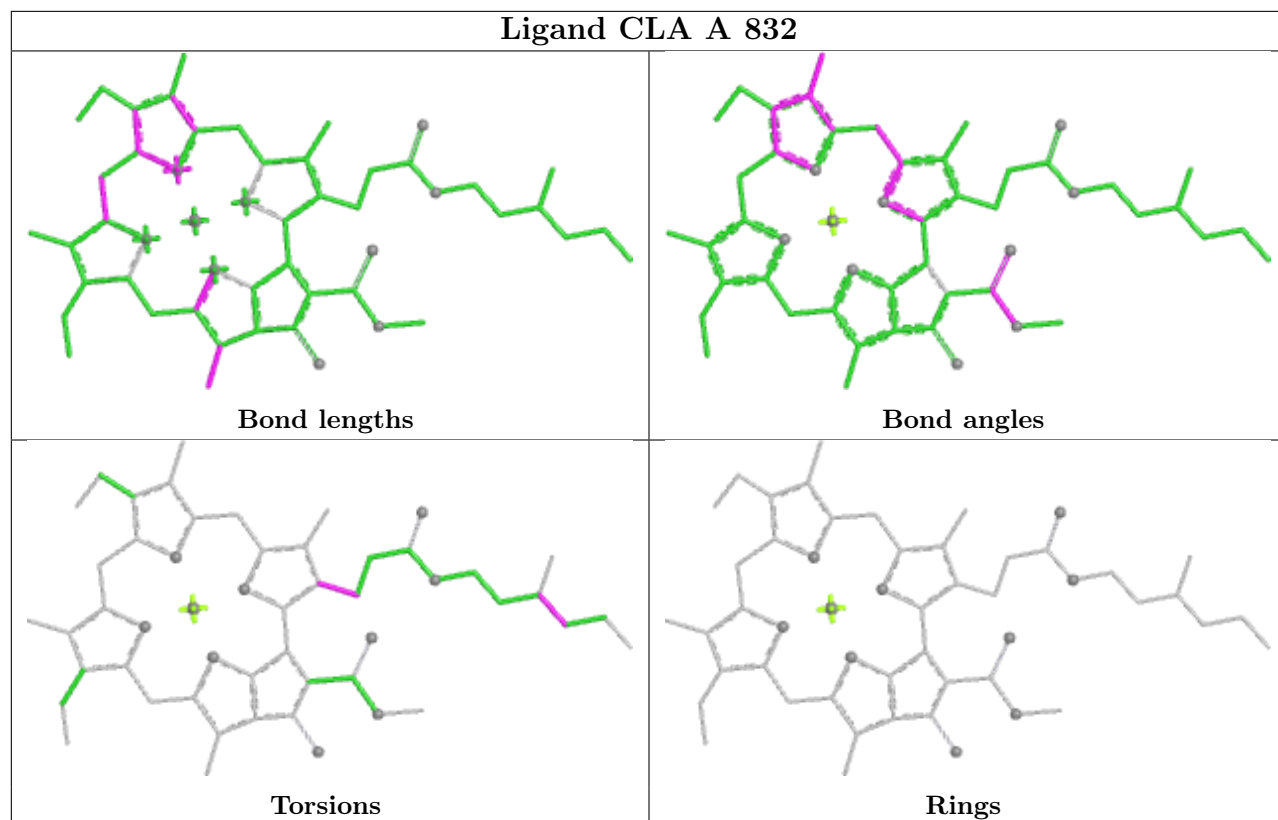
Bond angles

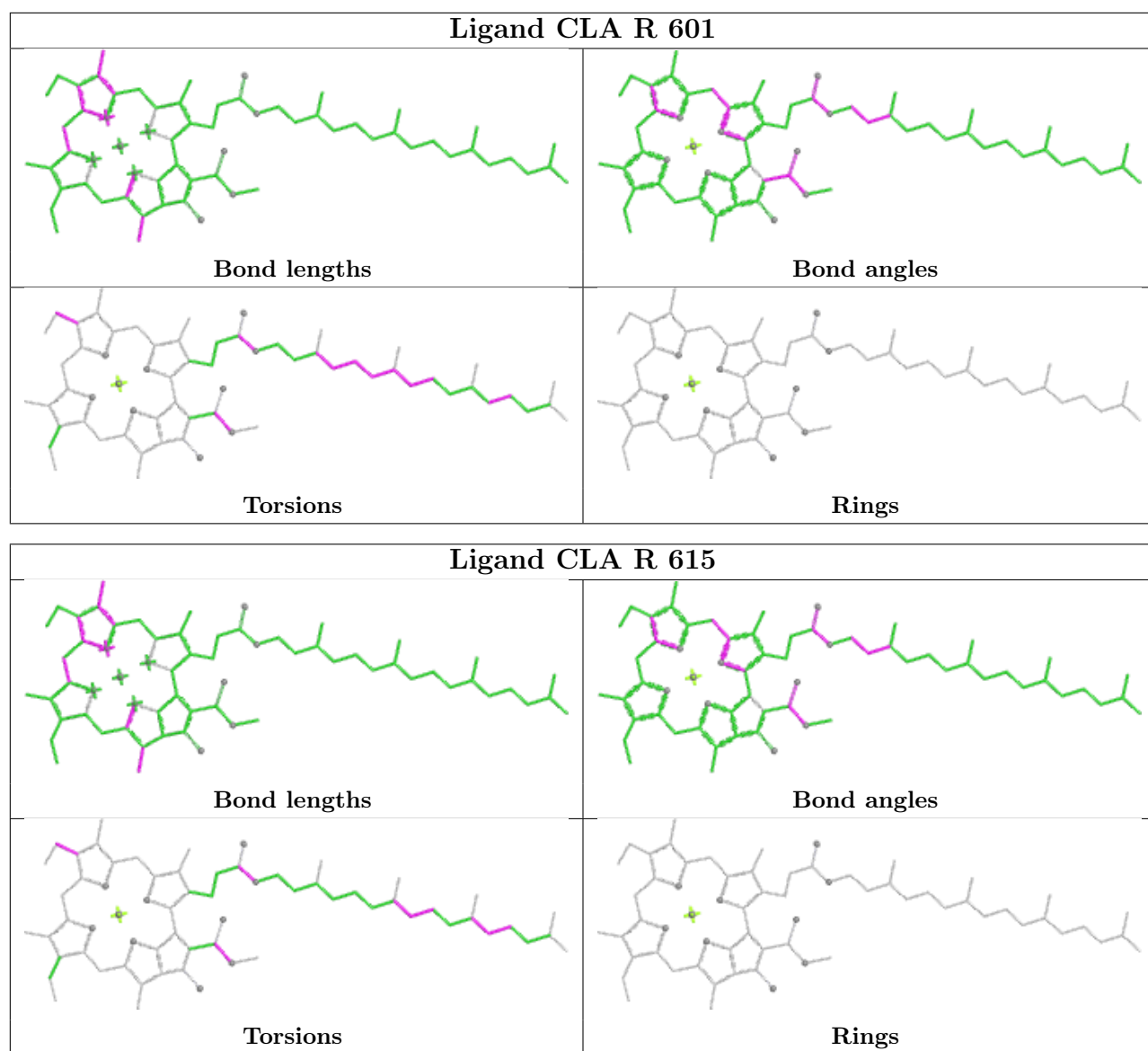


Torsions

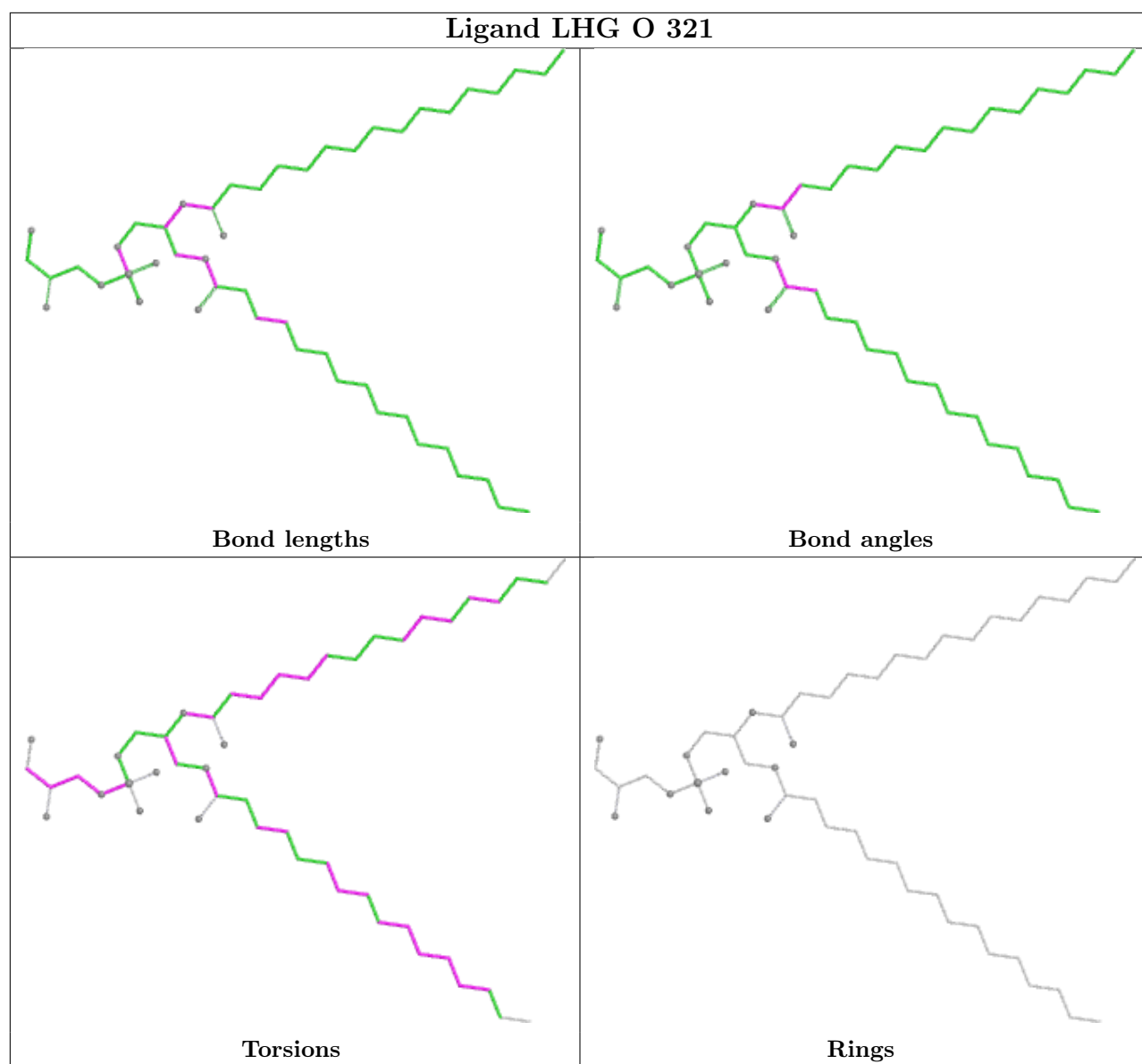


Rings

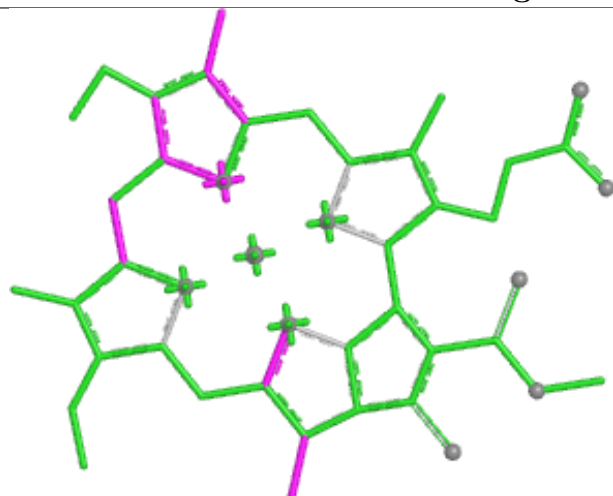




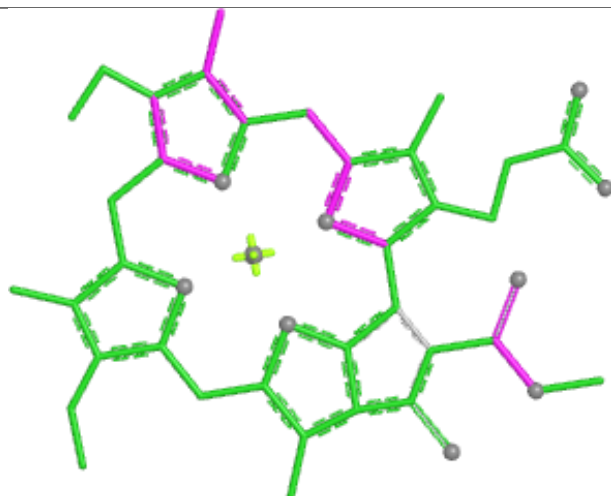




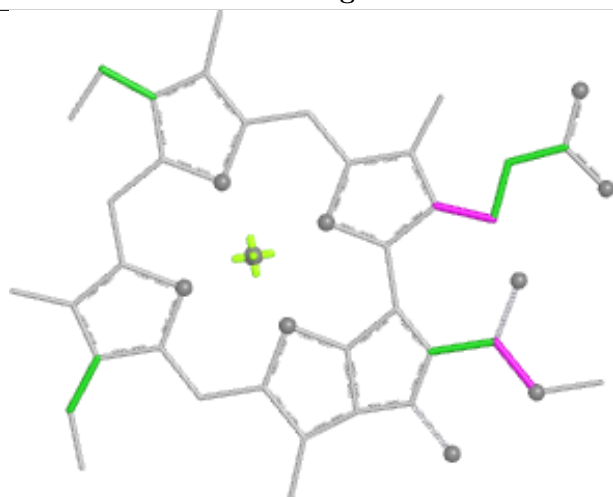
## Ligand CLA U 413



Bond lengths



Bond angles

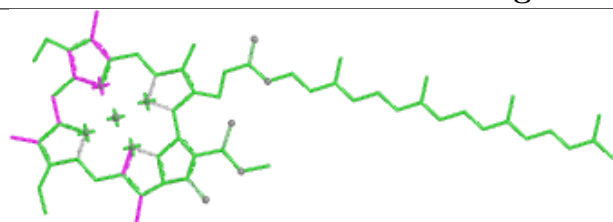


Torsions

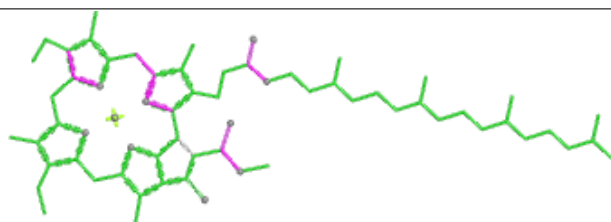


Rings

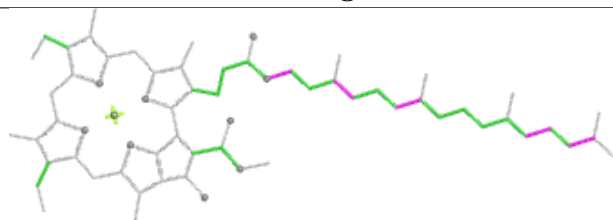
## Ligand CLA A 822



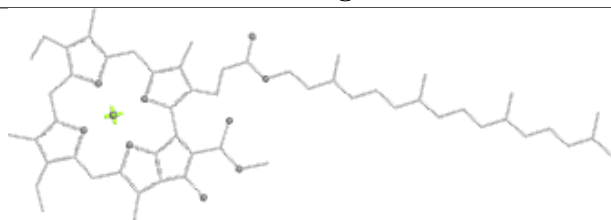
Bond lengths



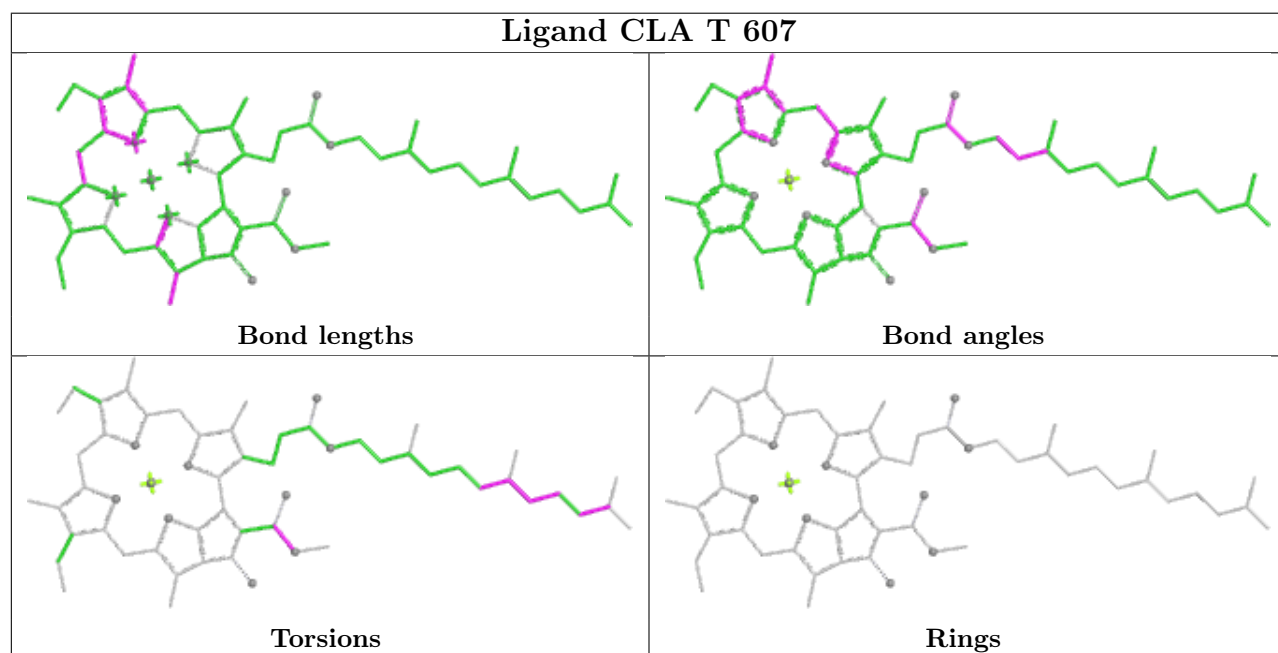
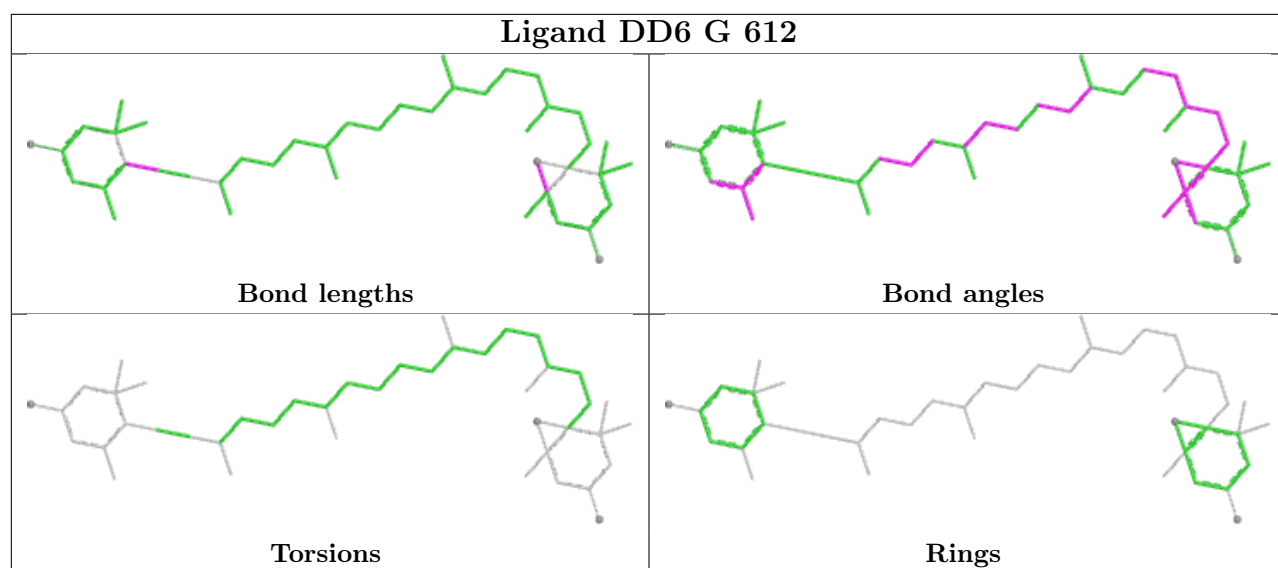
Bond angles



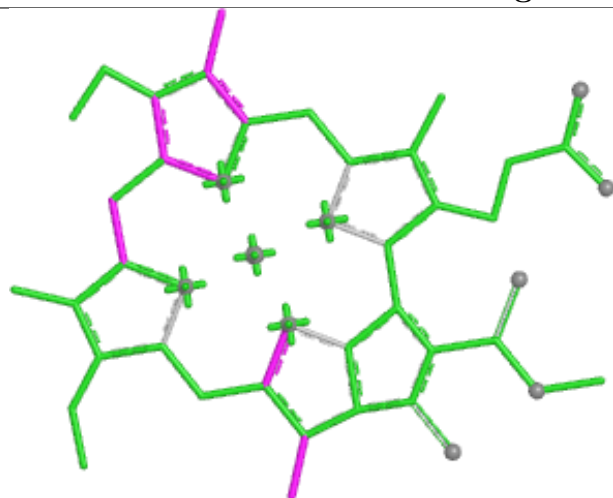
Torsions



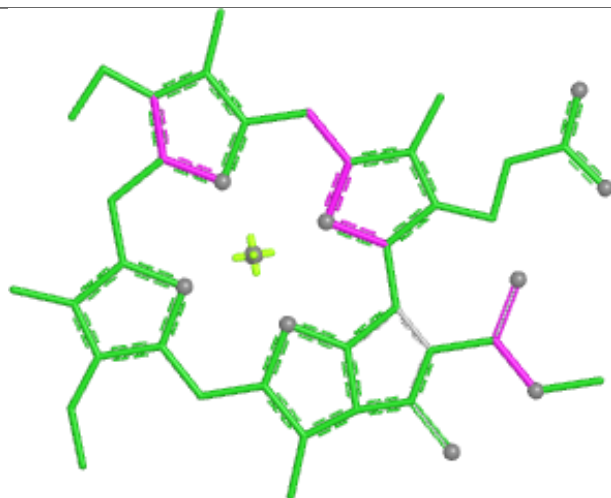
Rings



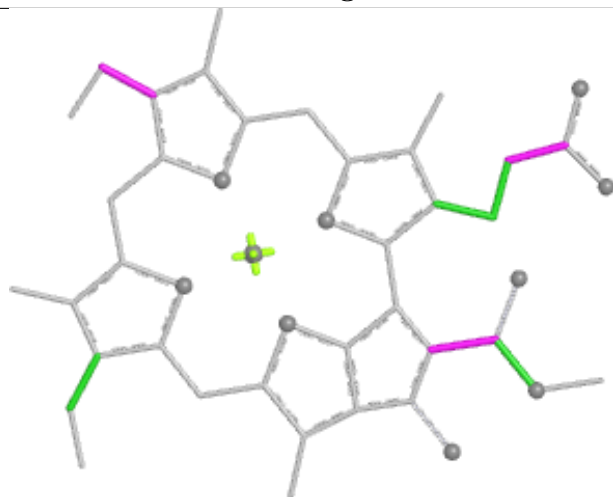
## Ligand CLA T 610



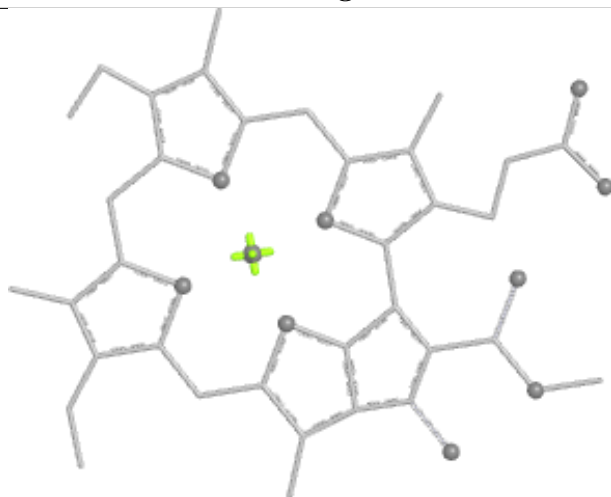
Bond lengths



Bond angles

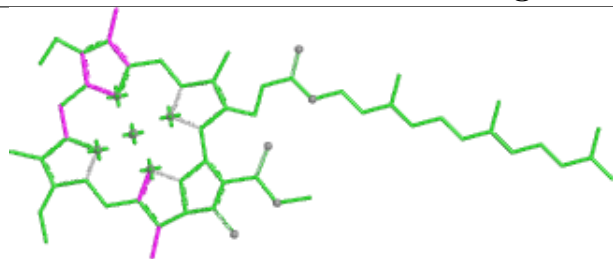


Torsions

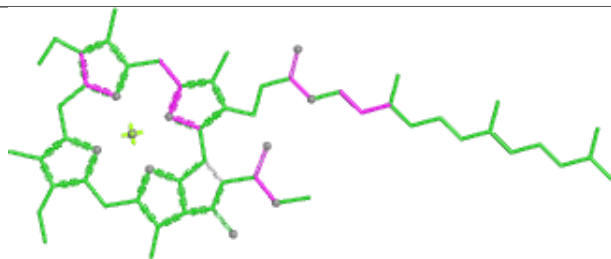


Rings

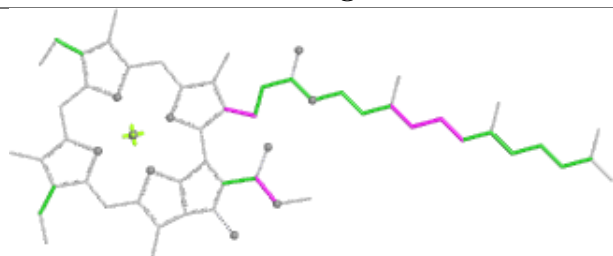
## Ligand CLA H 307



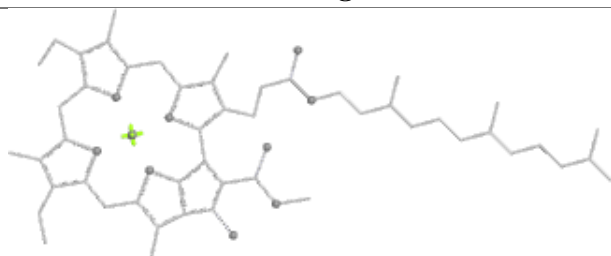
Bond lengths



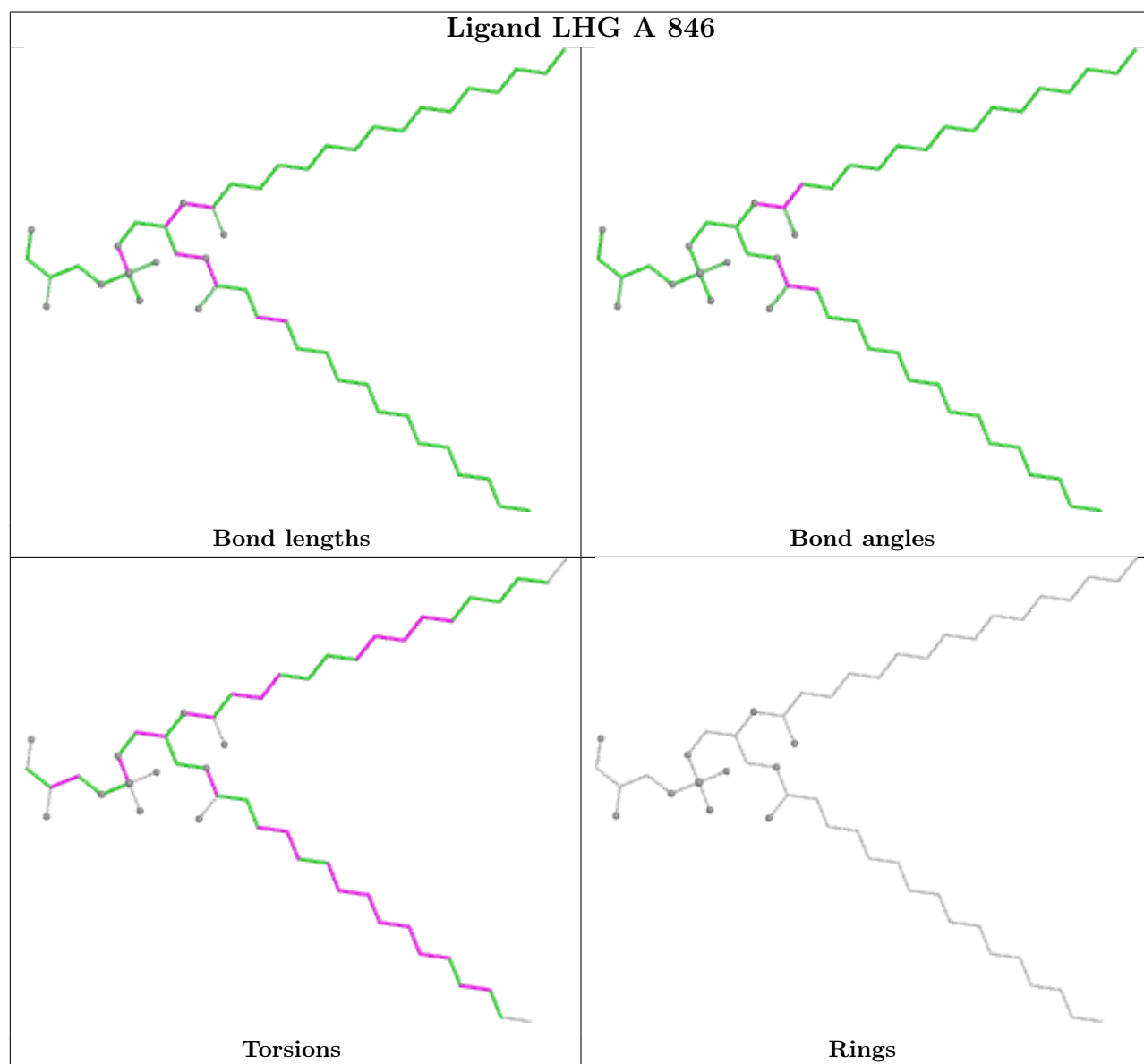
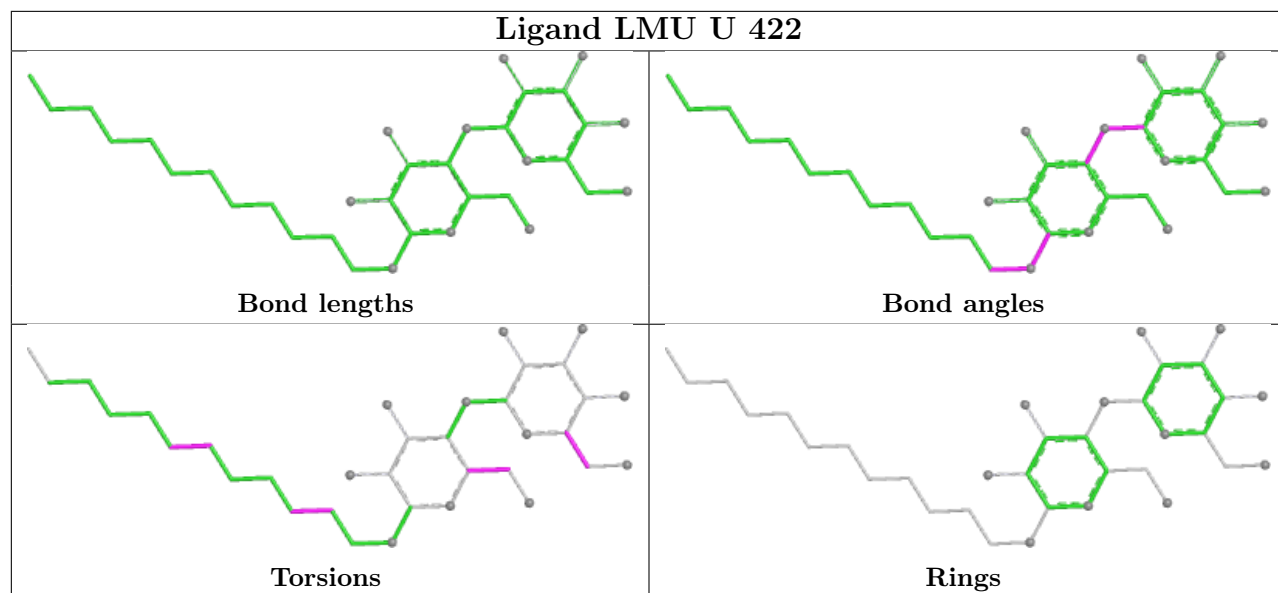
Bond angles

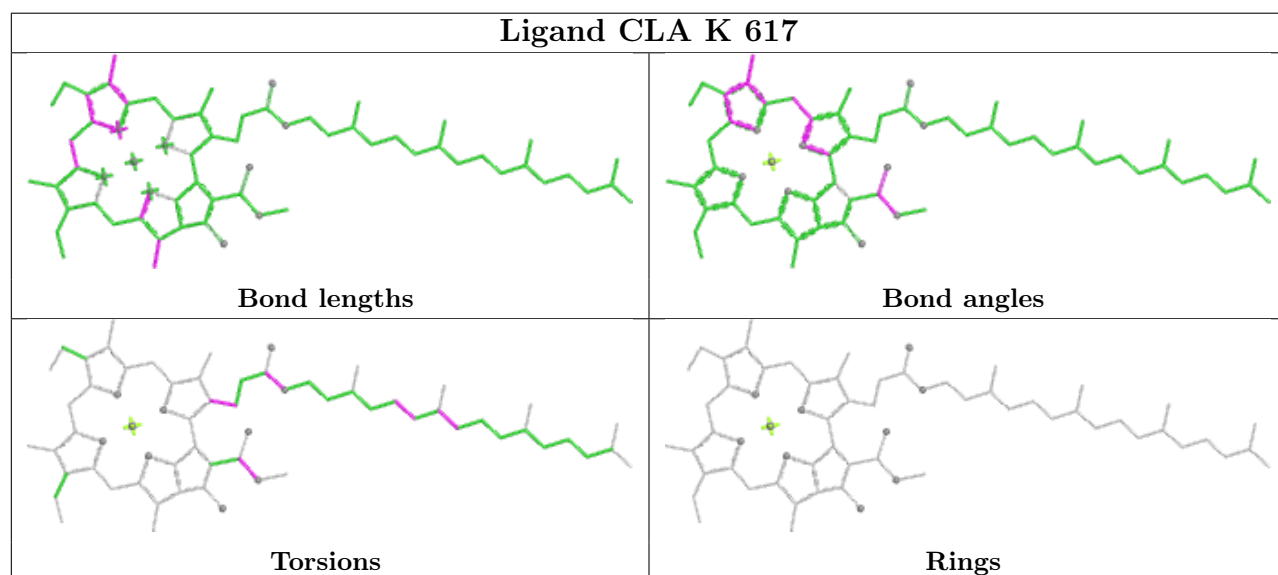
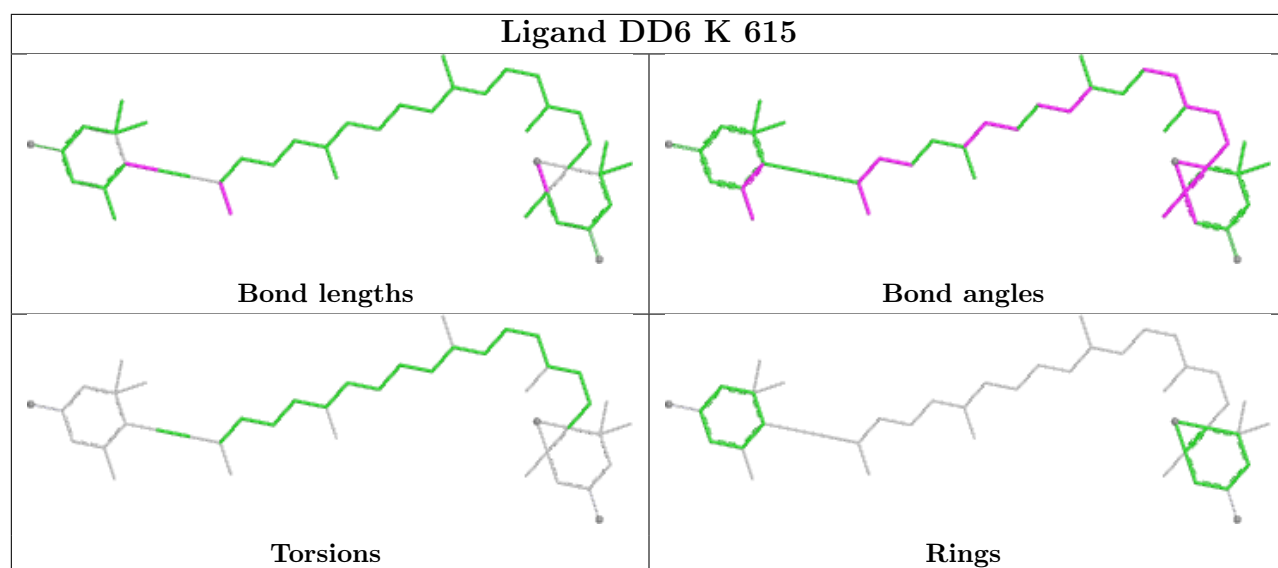


Torsions

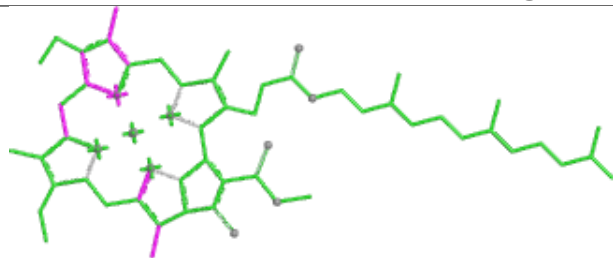


Rings

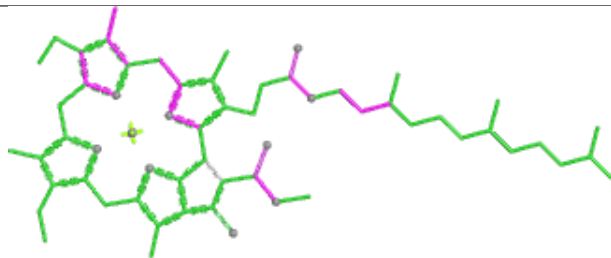




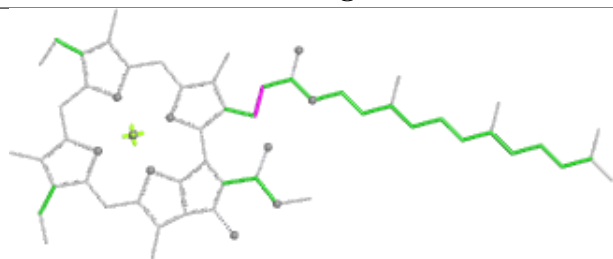
## Ligand CLA I 602



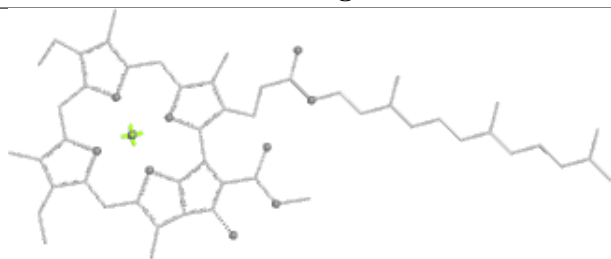
Bond lengths



Bond angles

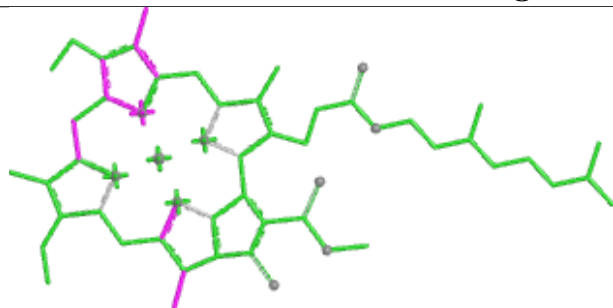


Torsions

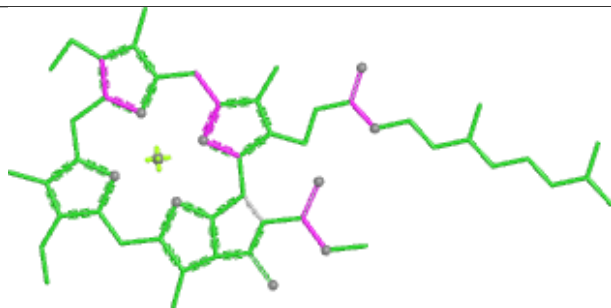


Rings

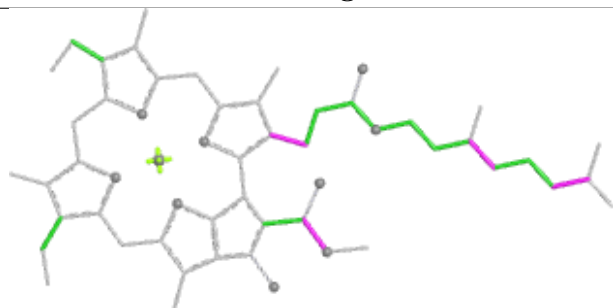
## Ligand CLA U 410



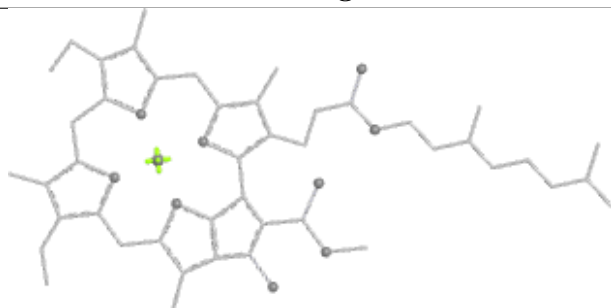
Bond lengths



Bond angles

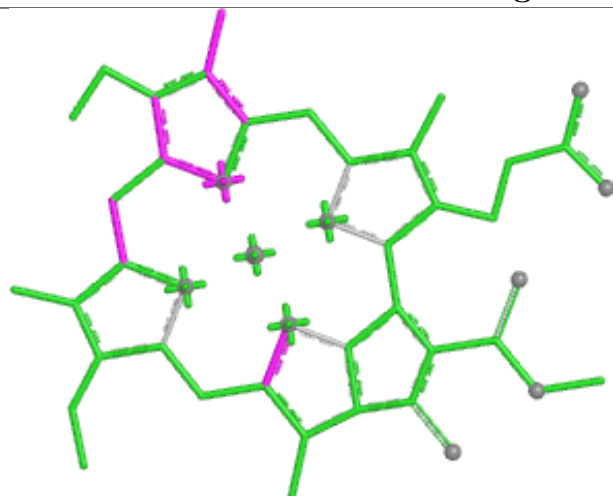


Torsions

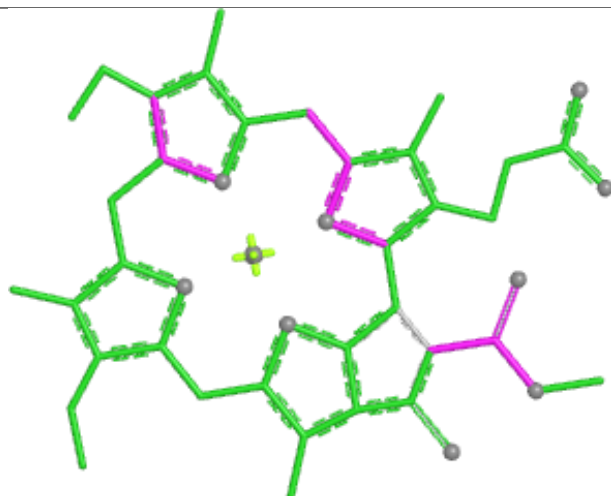


Rings

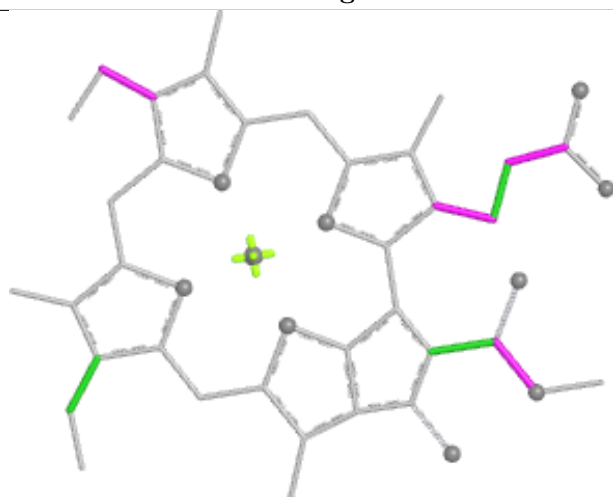
## Ligand CLA V 617



Bond lengths



Bond angles

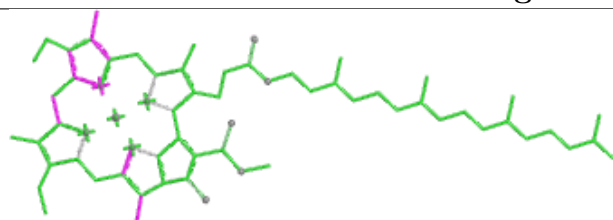


Torsions

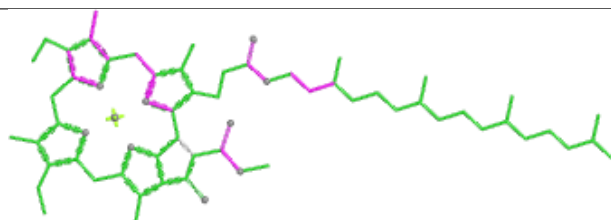


Rings

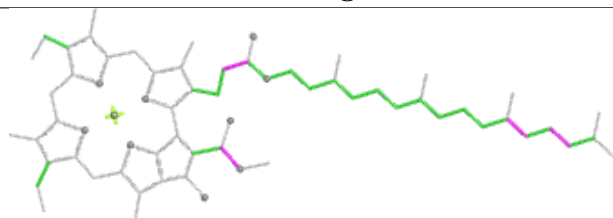
## Ligand CLA B 805



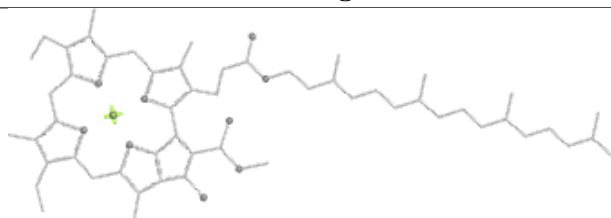
Bond lengths



Bond angles

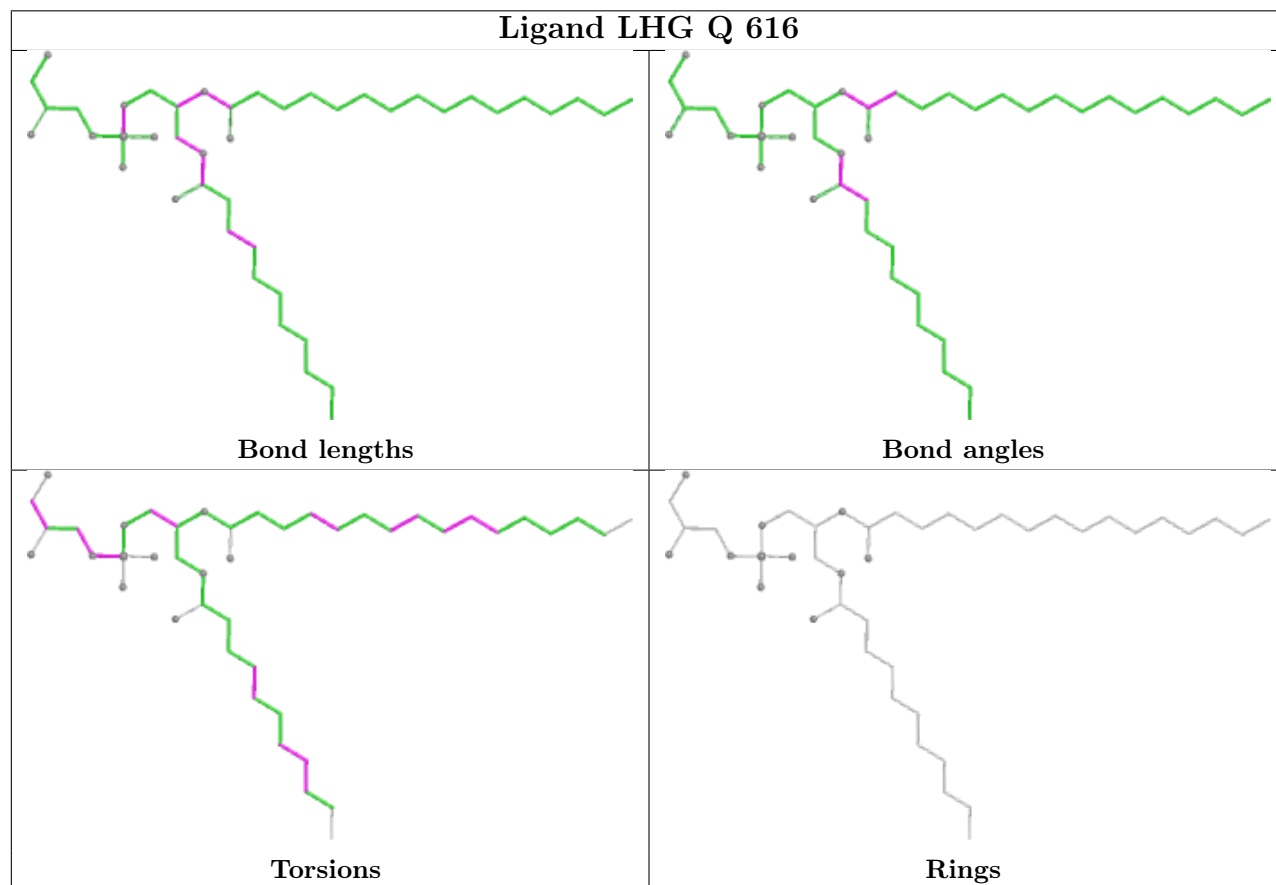
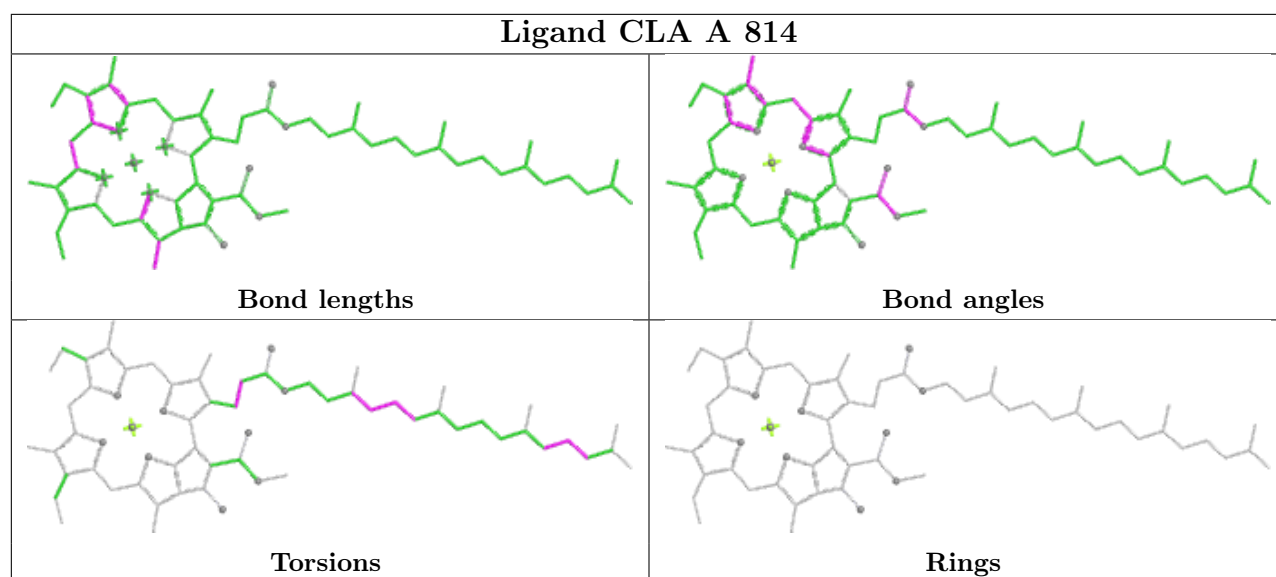


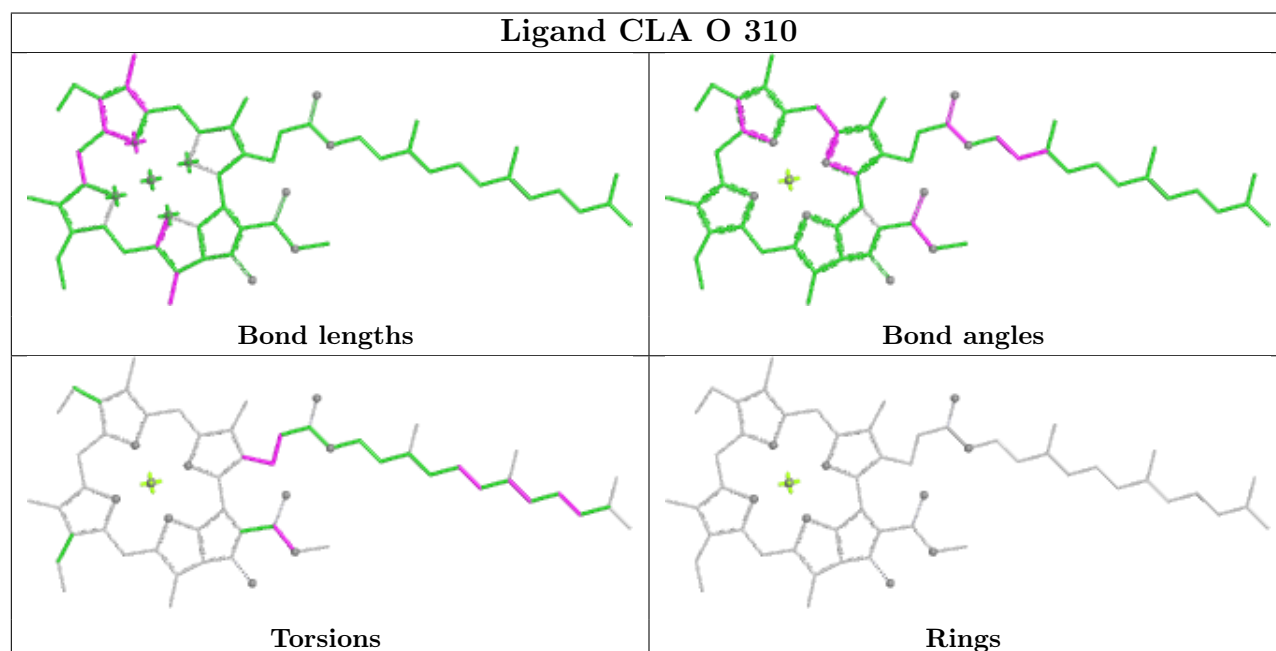
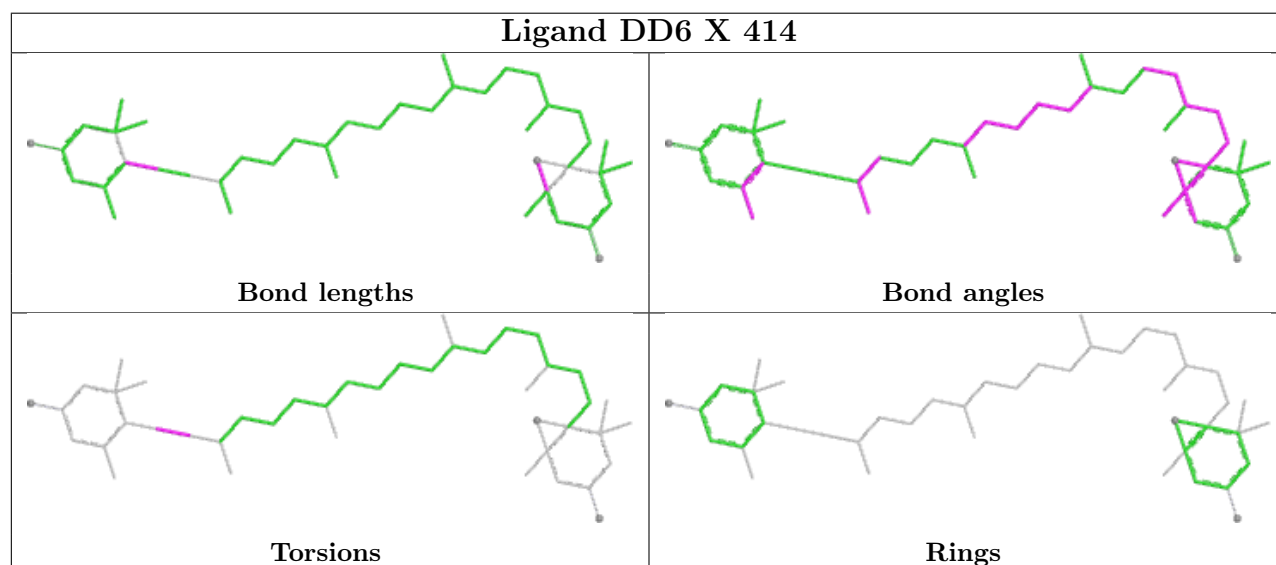
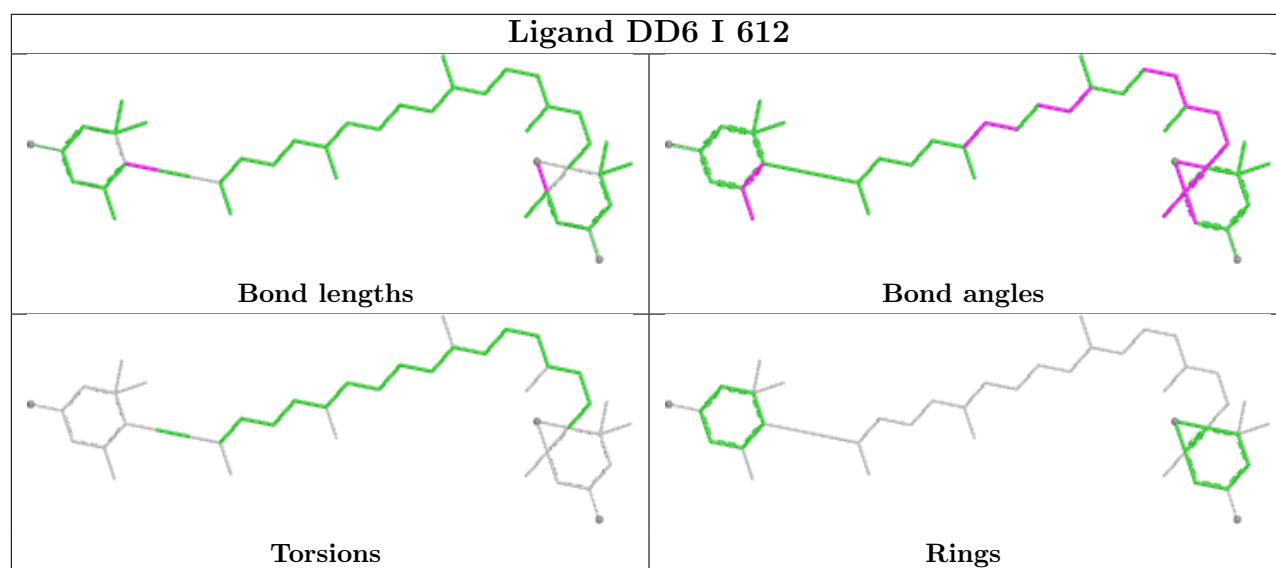
Torsions



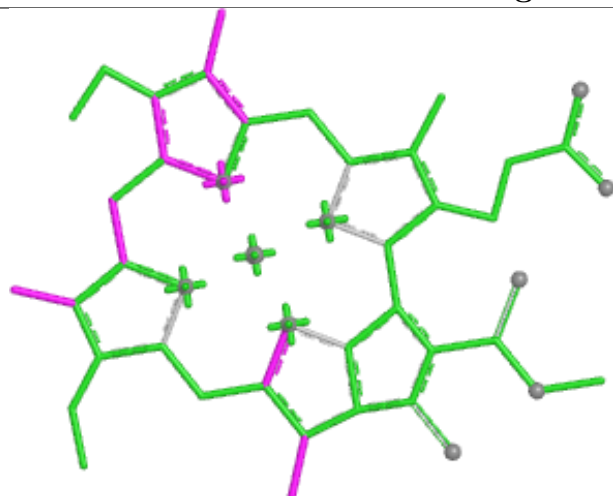
Rings







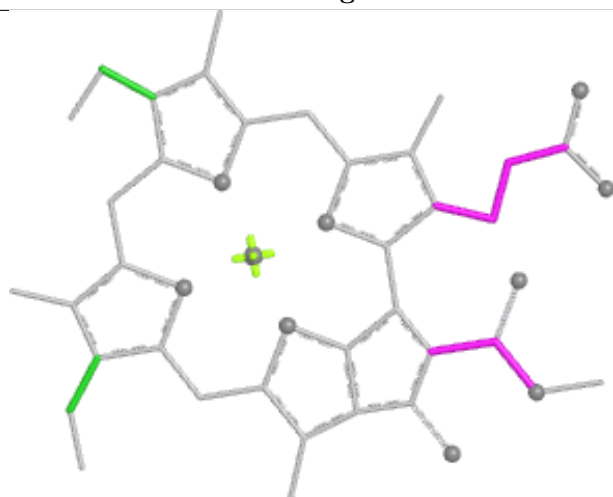
## Ligand CLA P 602



Bond lengths



Bond angles

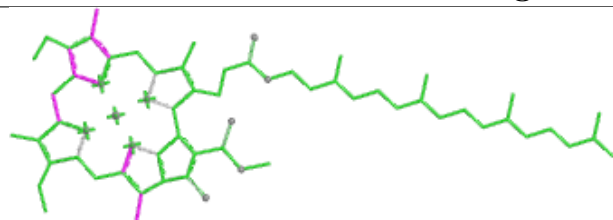


Torsions

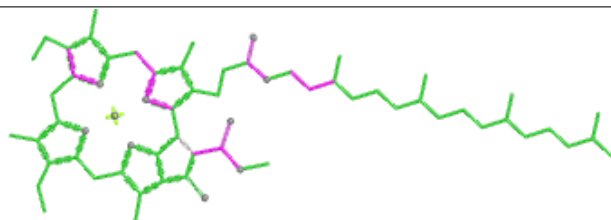


Rings

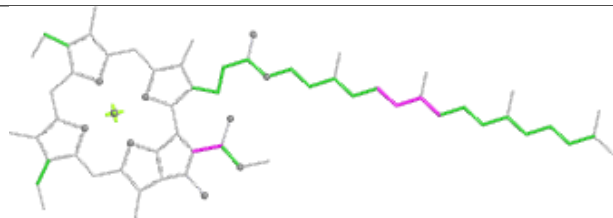
## Ligand CLA A 831



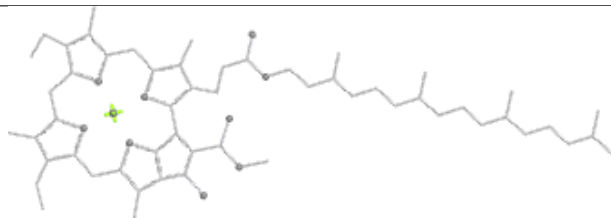
Bond lengths



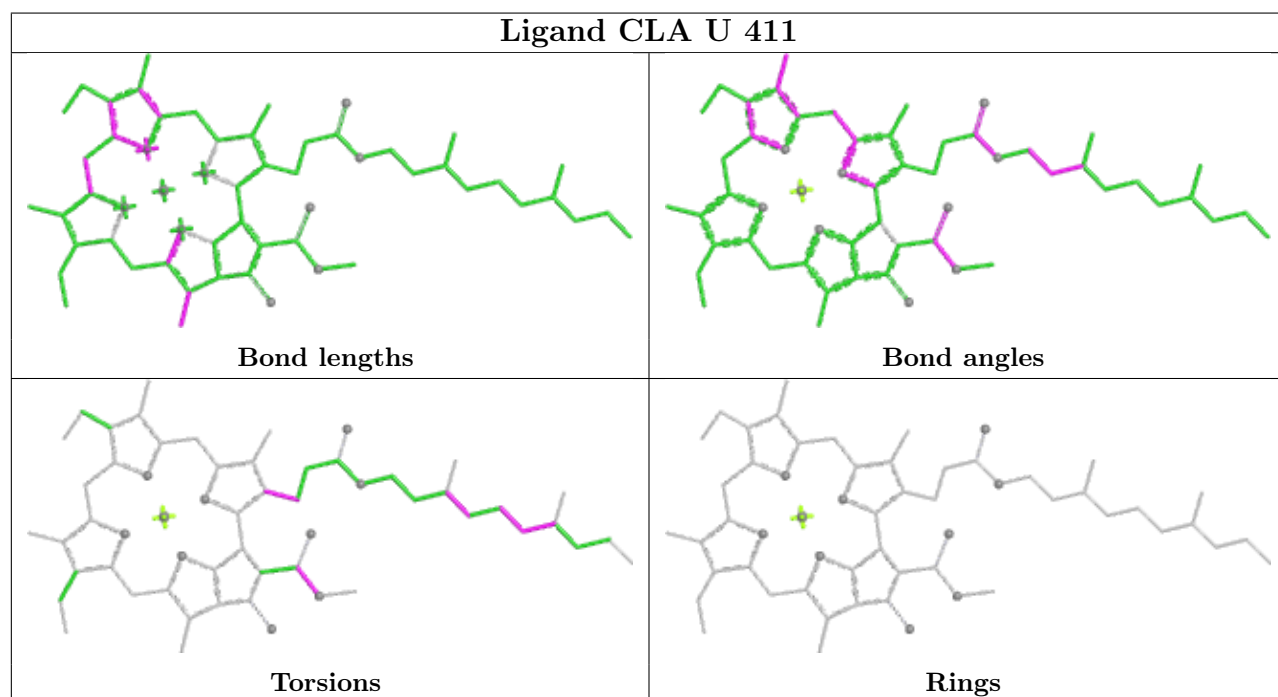
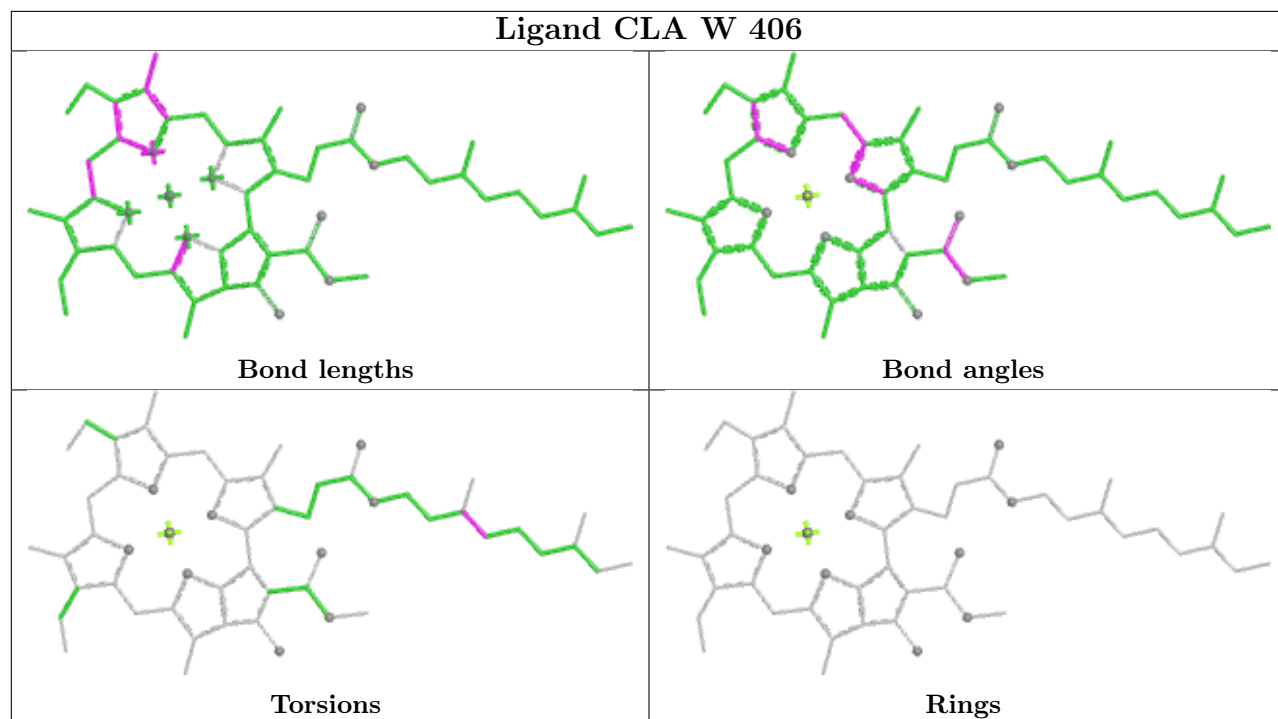
Bond angles



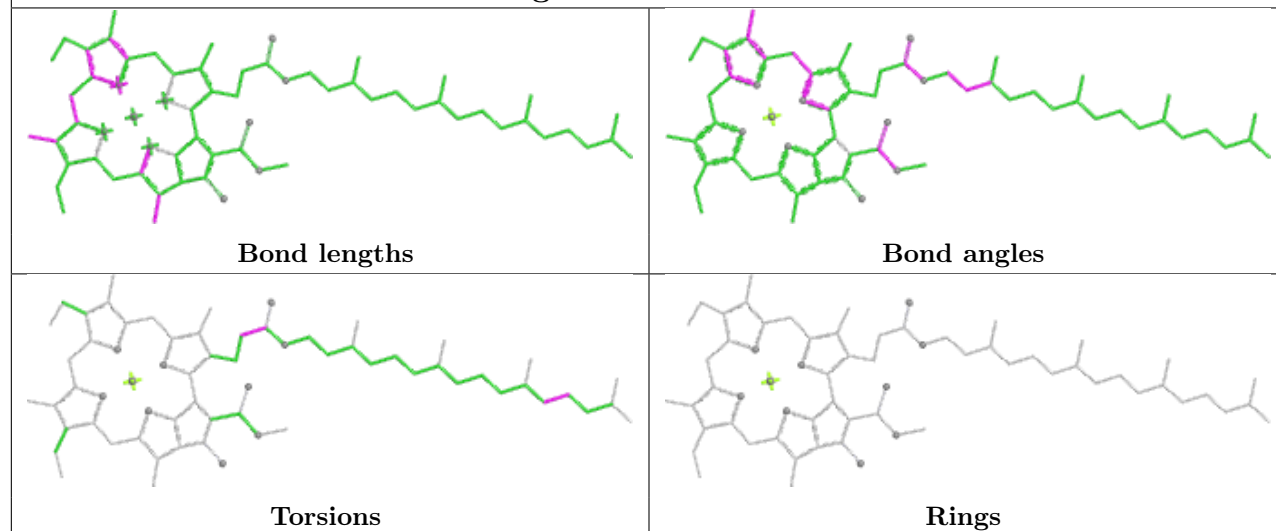
Torsions



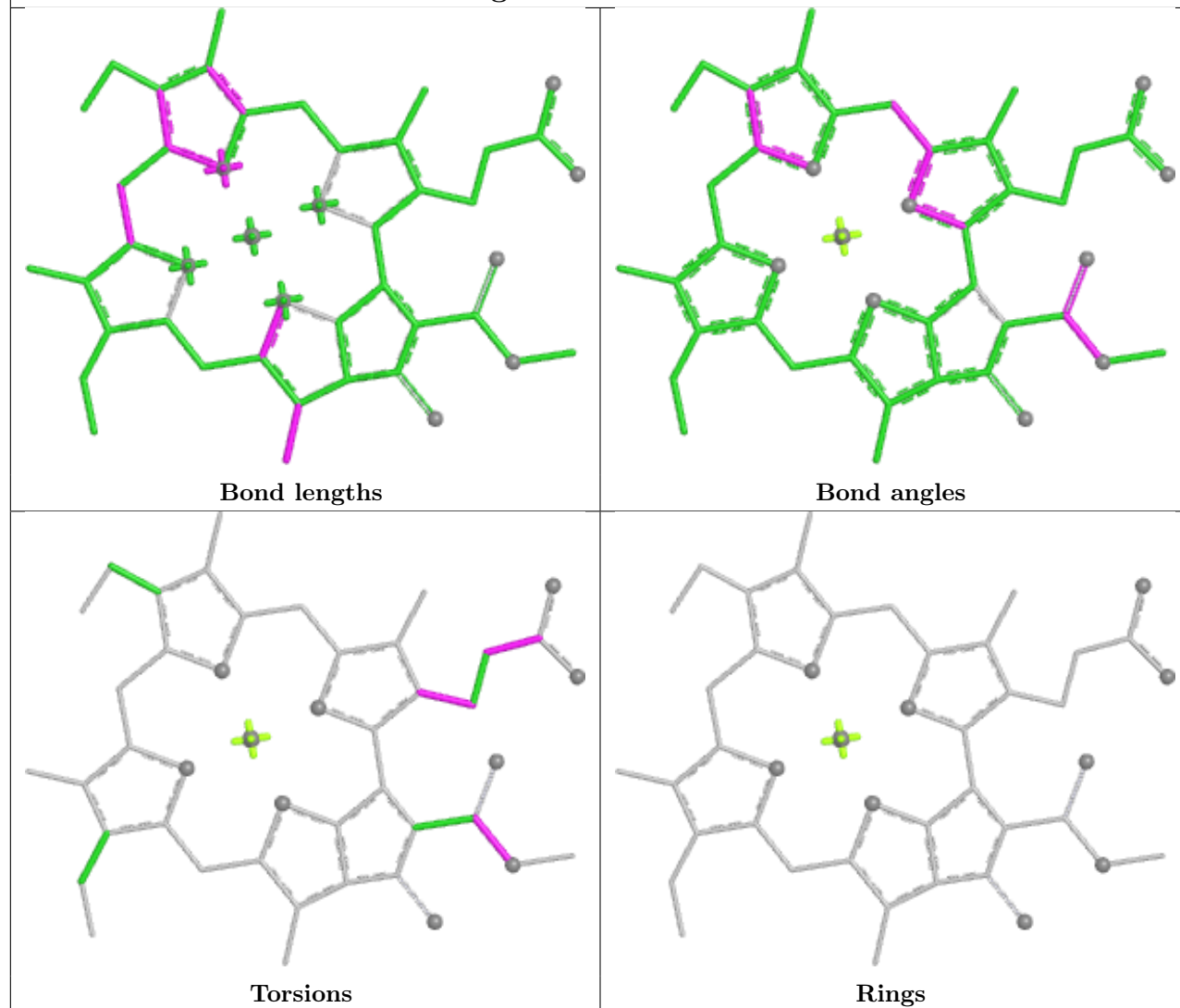
Rings

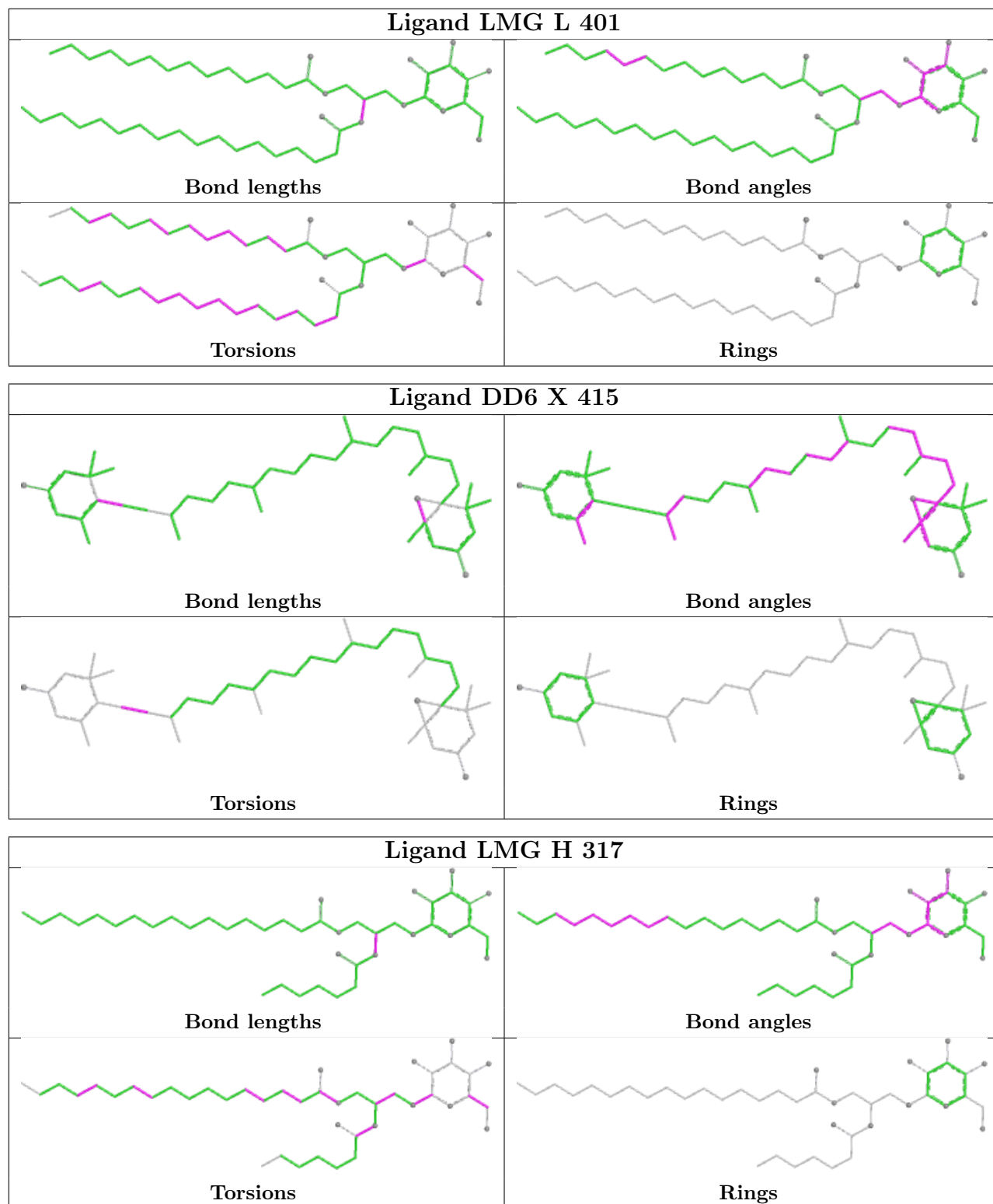


## Ligand CLA B 839

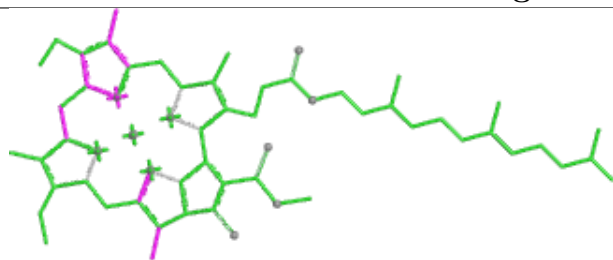


## Ligand CLA G 611

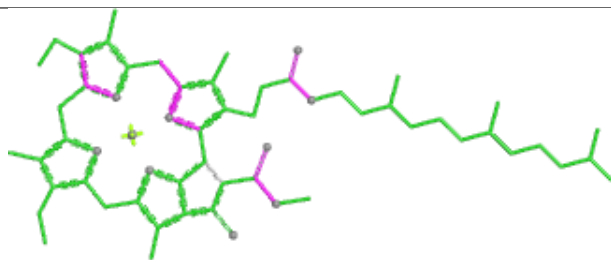




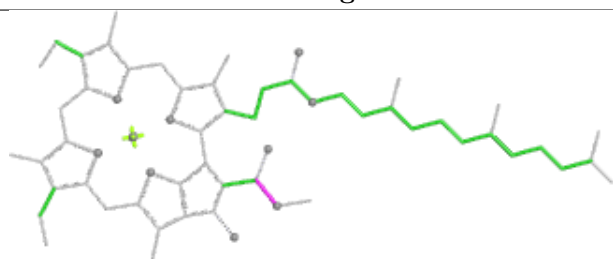
## Ligand CLA G 607



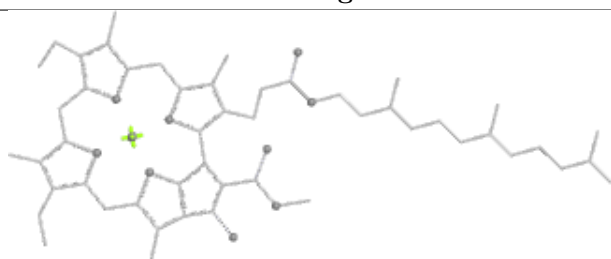
Bond lengths



Bond angles

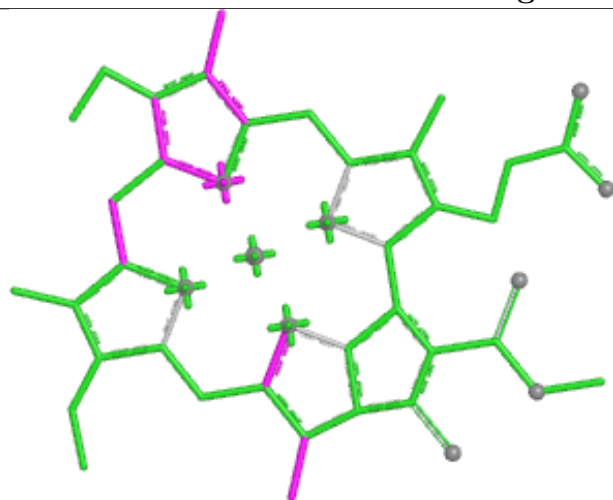


Torsions

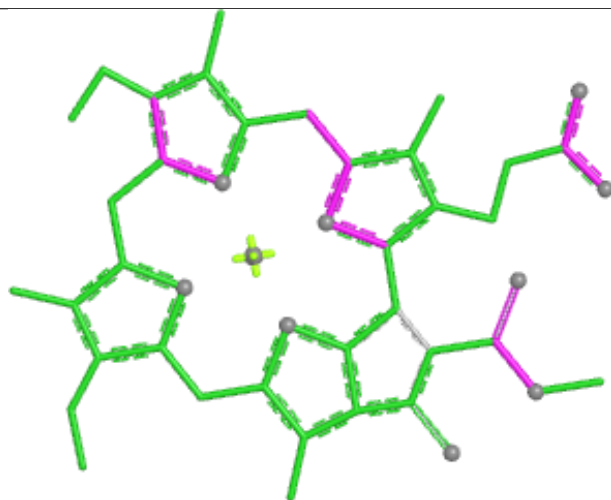


Rings

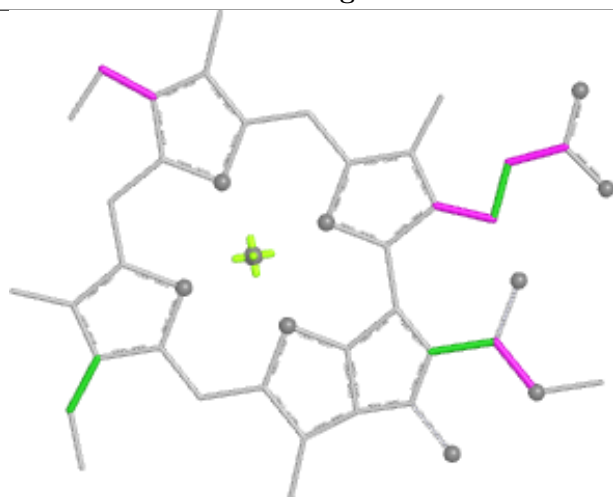
## Ligand CLA S 608



Bond lengths



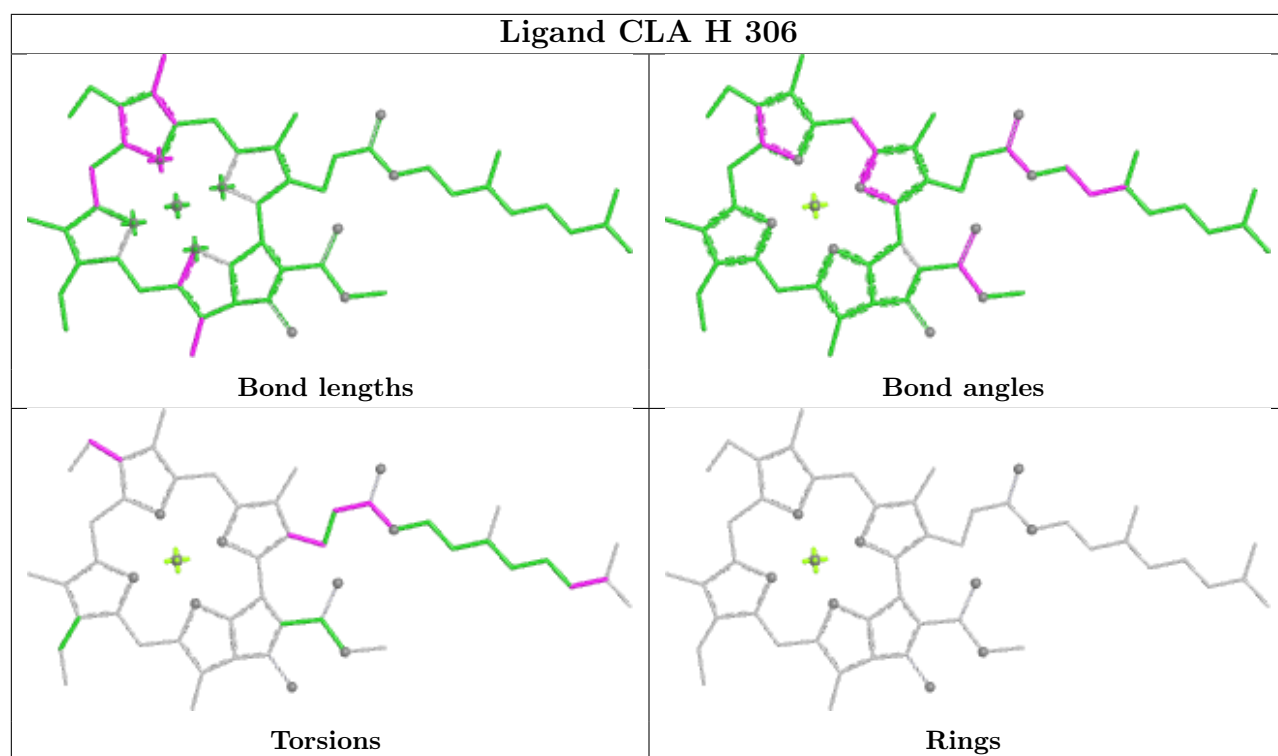
Bond angles



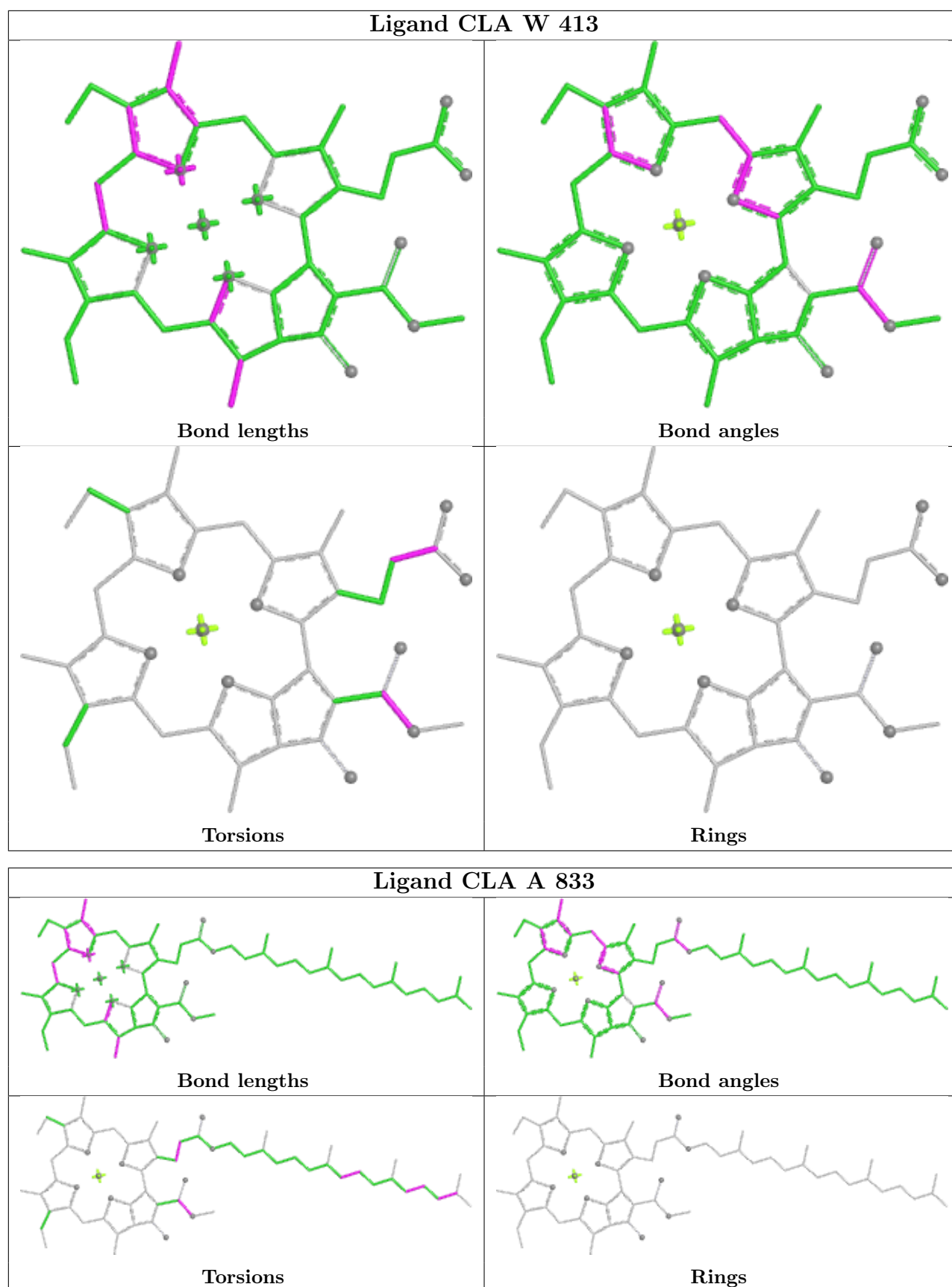
Torsions



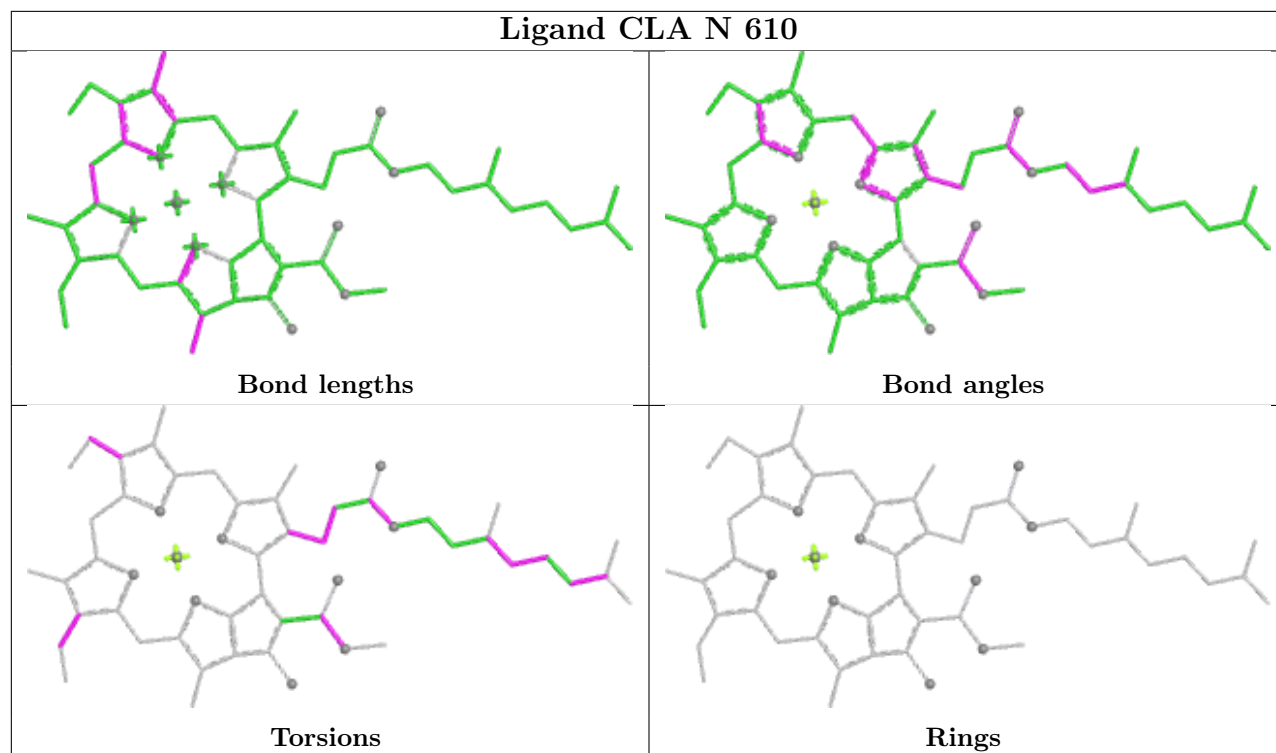
Rings



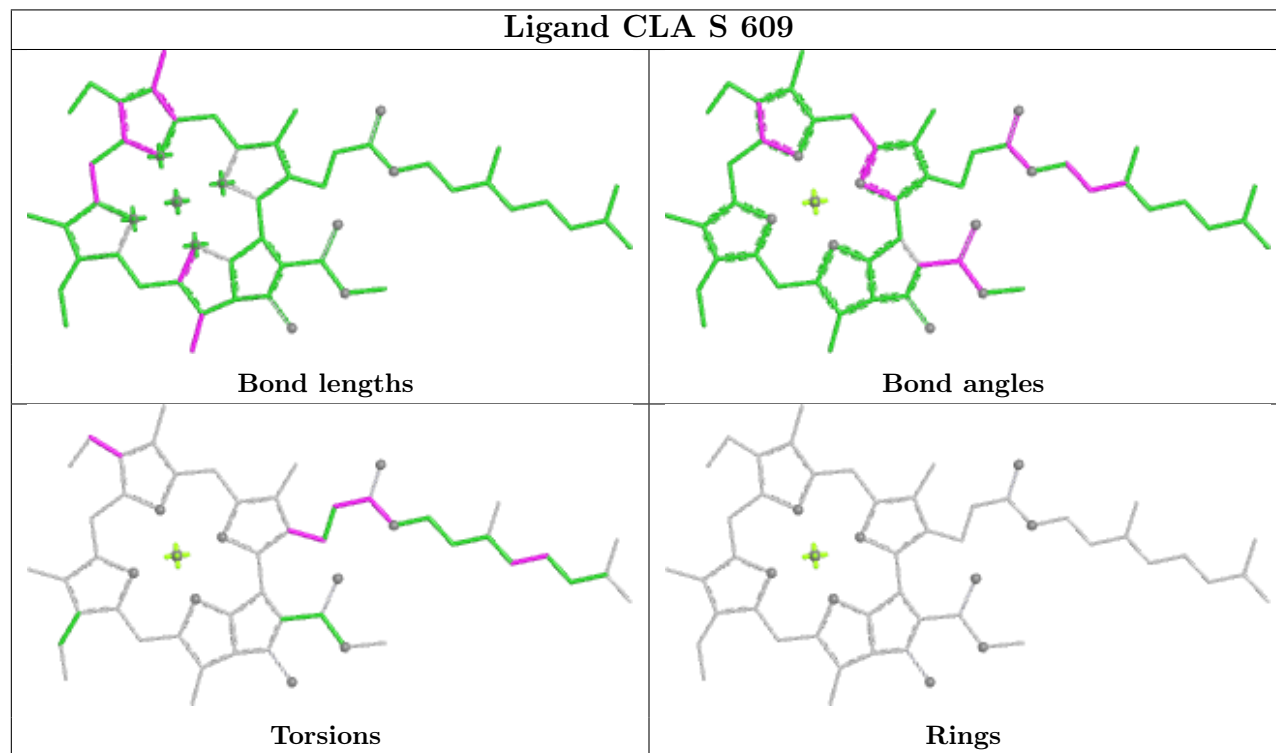




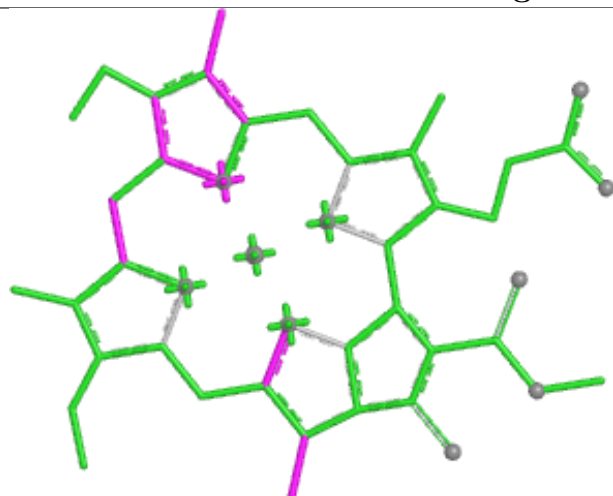
## Ligand CLA N 610



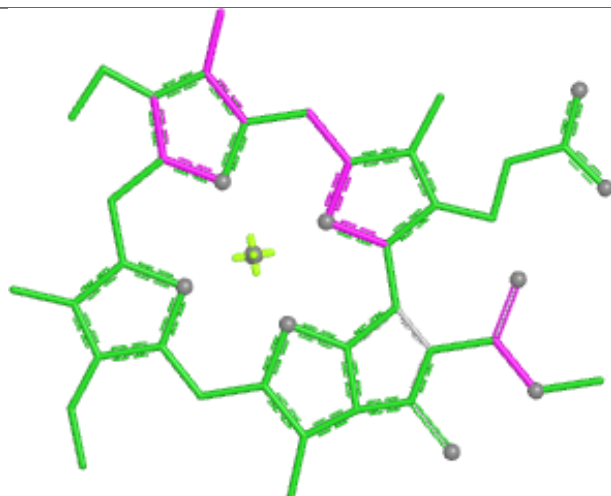
## Ligand CLA S 609



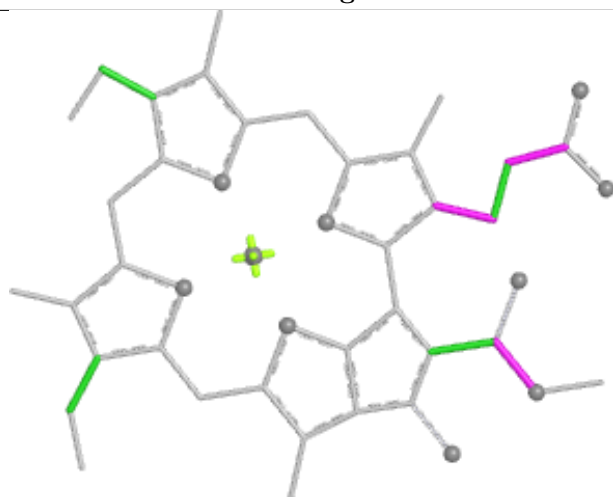
## Ligand CLA H 318



Bond lengths



Bond angles

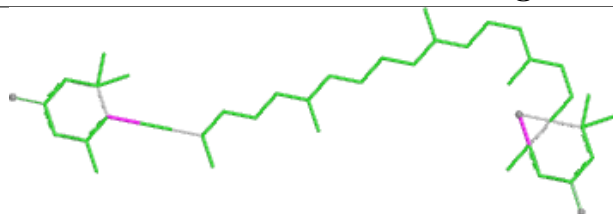


Torsions

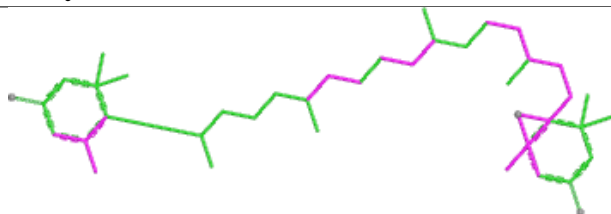


Rings

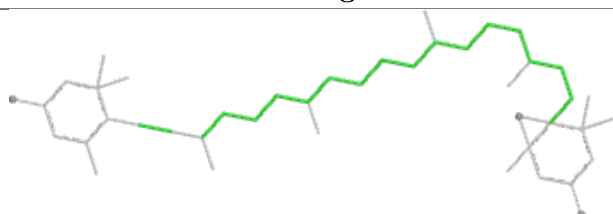
## Ligand DD6 Q 614



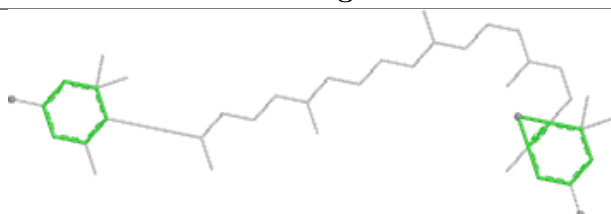
Bond lengths



Bond angles

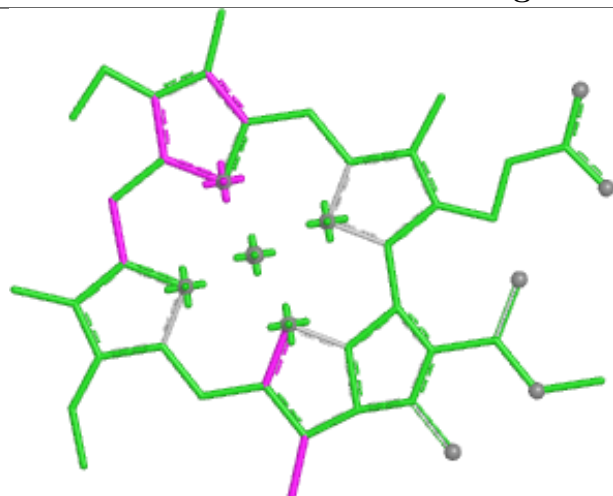


Torsions

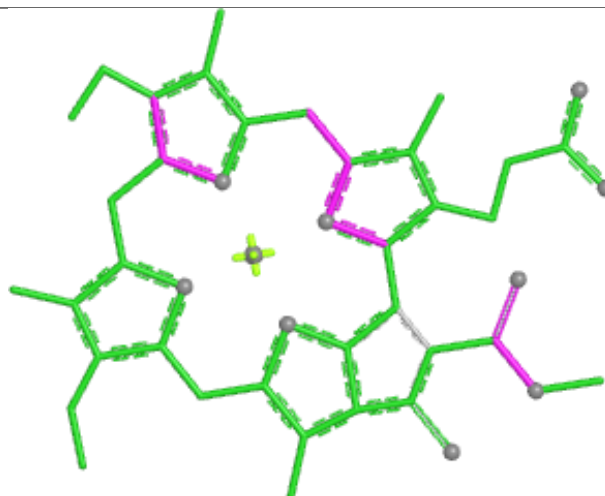


Rings

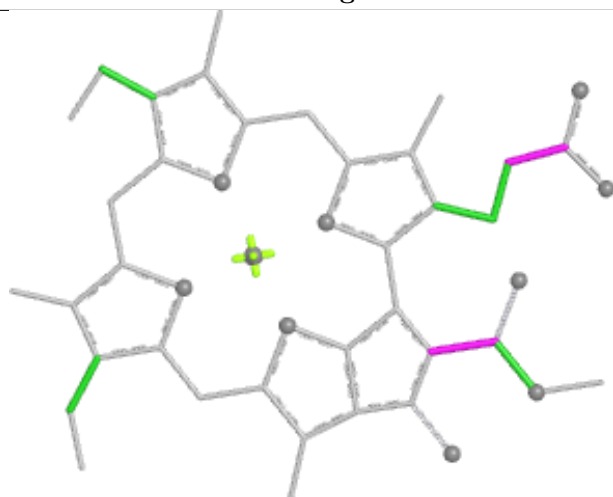
## Ligand CLA N 609



Bond lengths



Bond angles

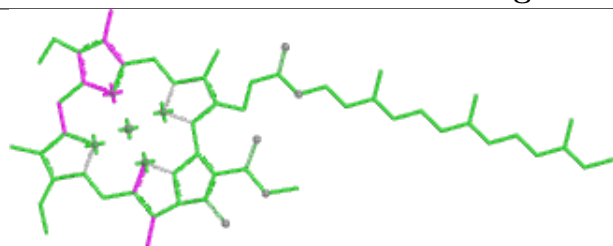


Torsions

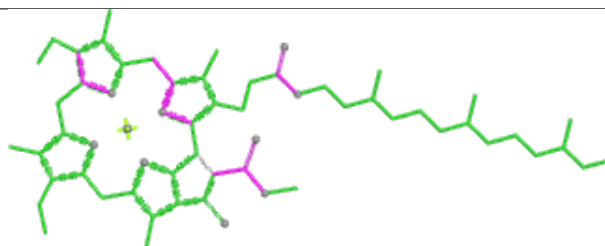


Rings

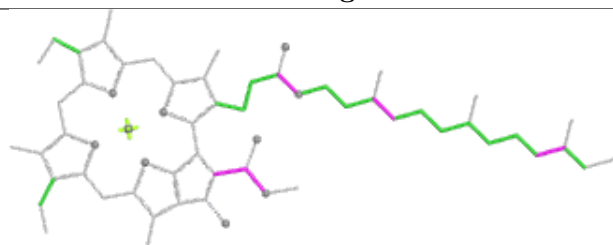
## Ligand CLA A 835



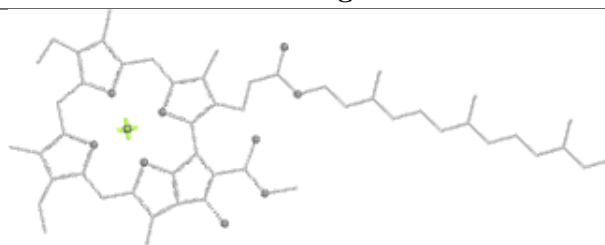
Bond lengths



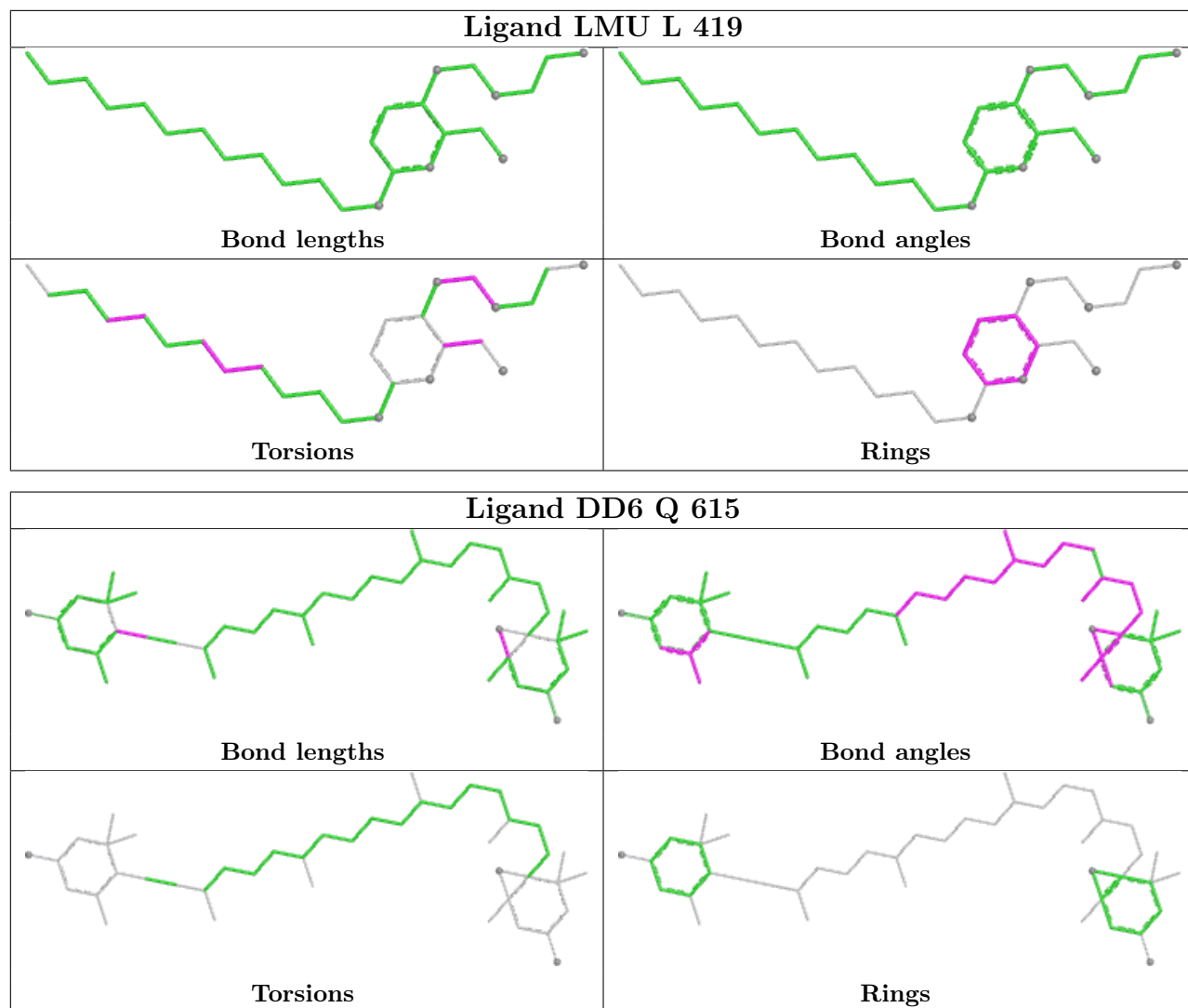
Bond angles

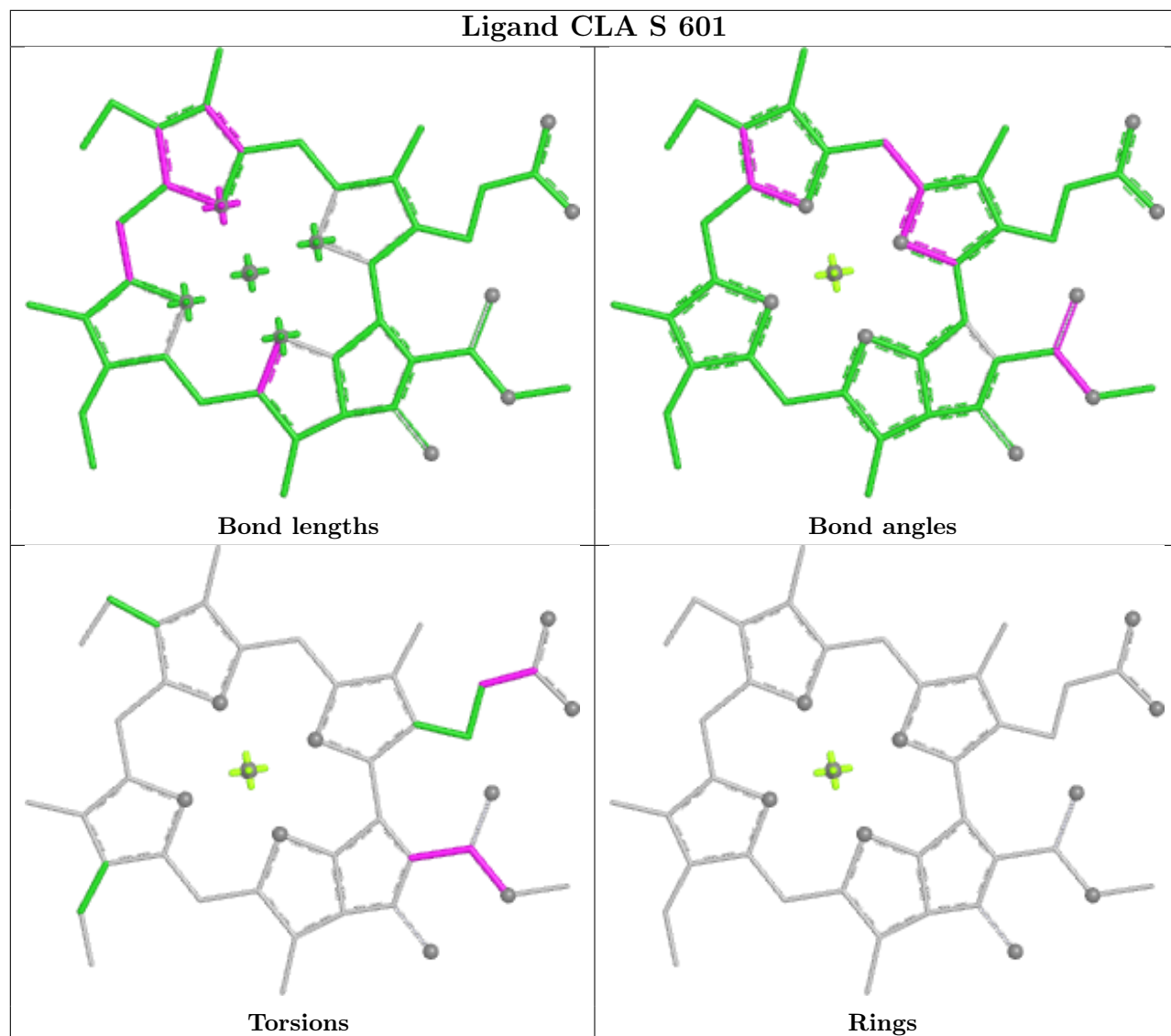


Torsions

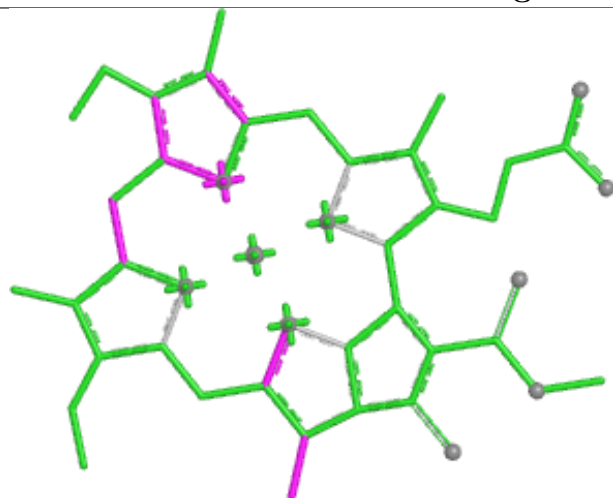


Rings

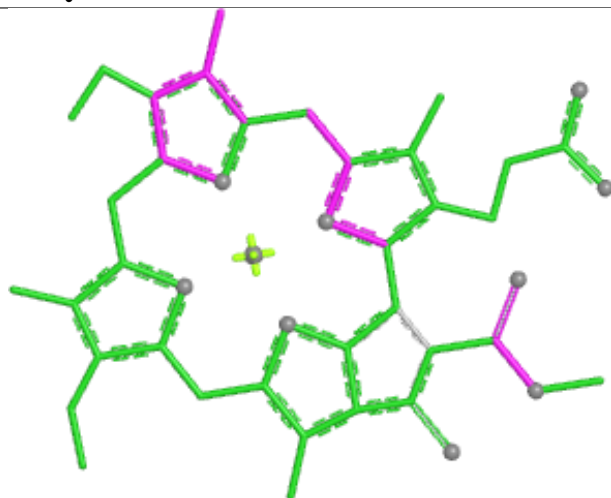




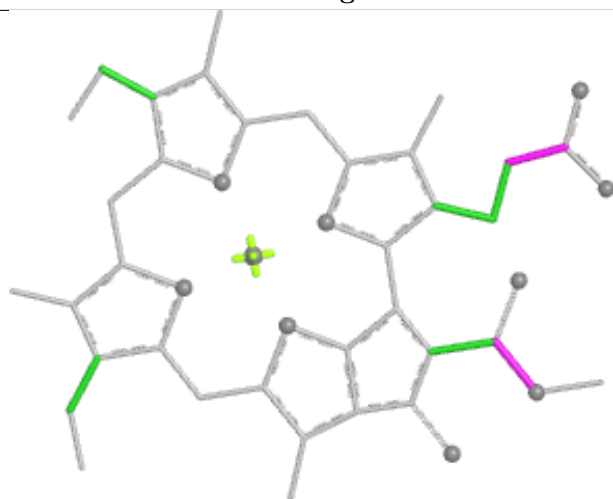
## Ligand CLA Q 603



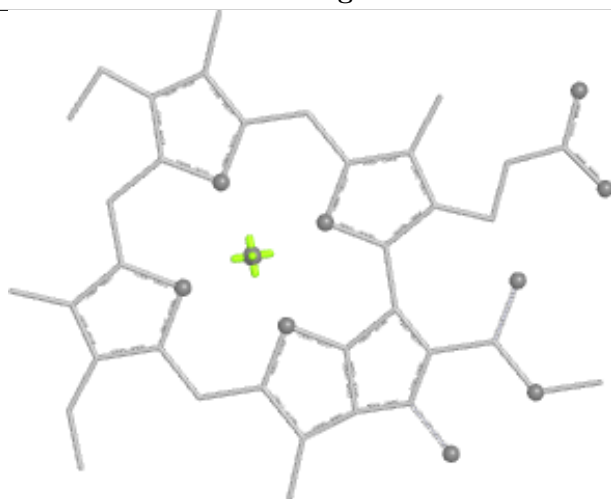
Bond lengths



Bond angles

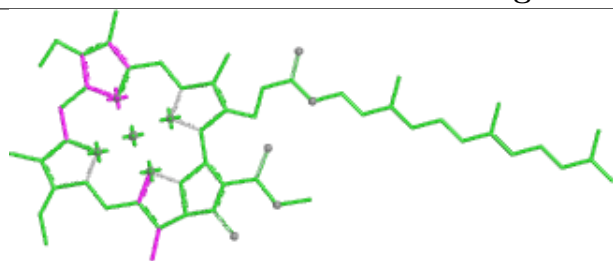


Torsions

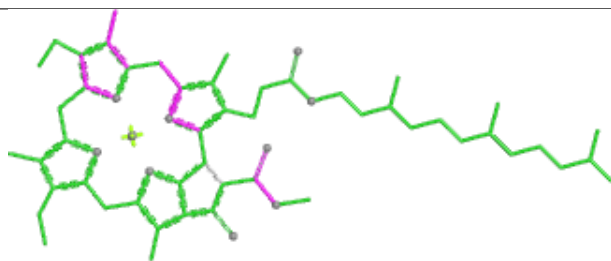


Rings

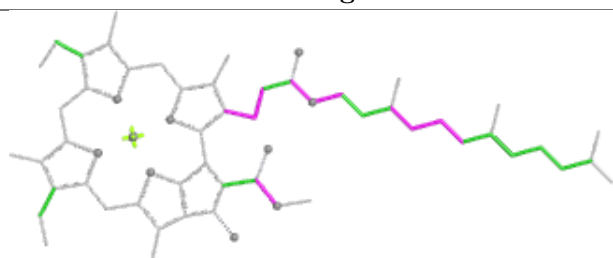
## Ligand CLA R 602



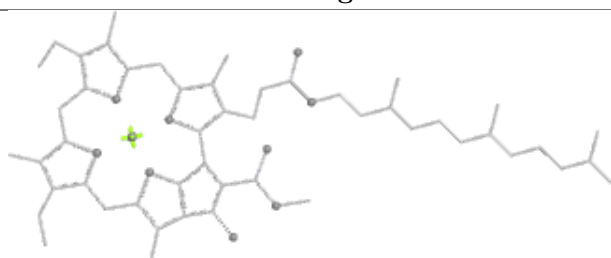
Bond lengths



Bond angles

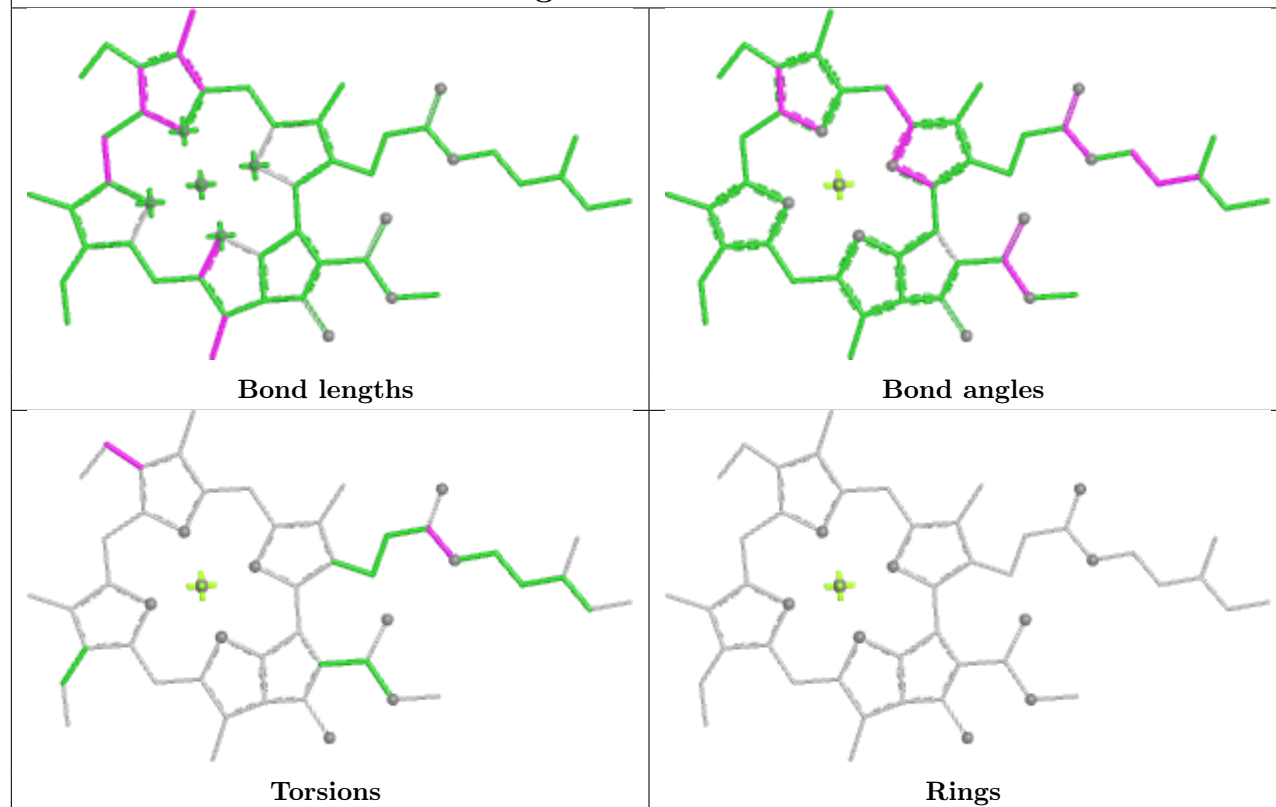


Torsions

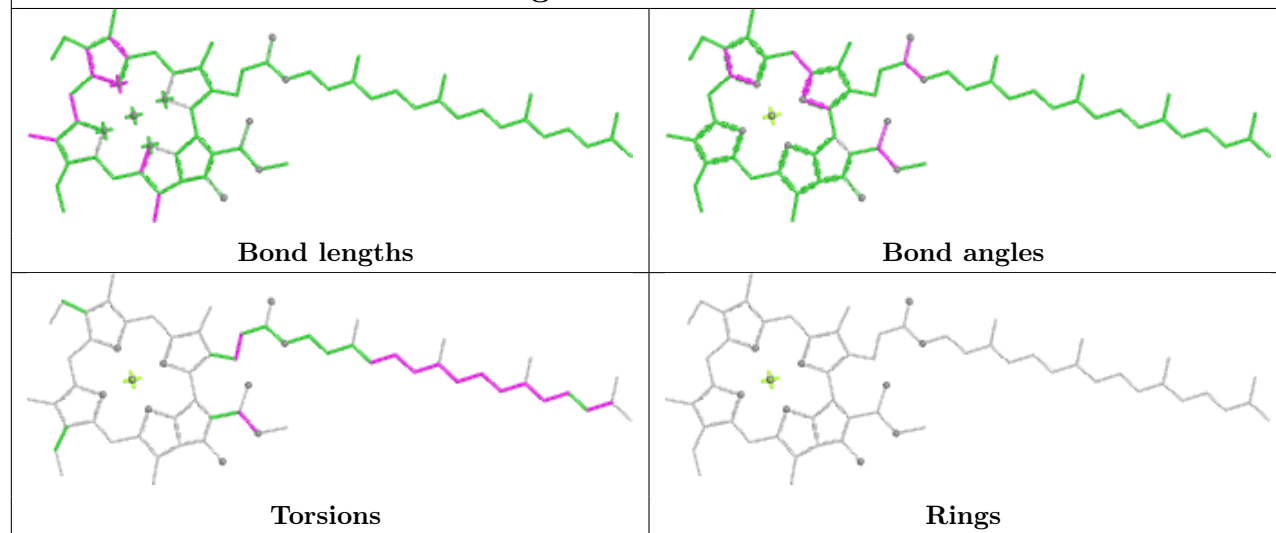


Rings

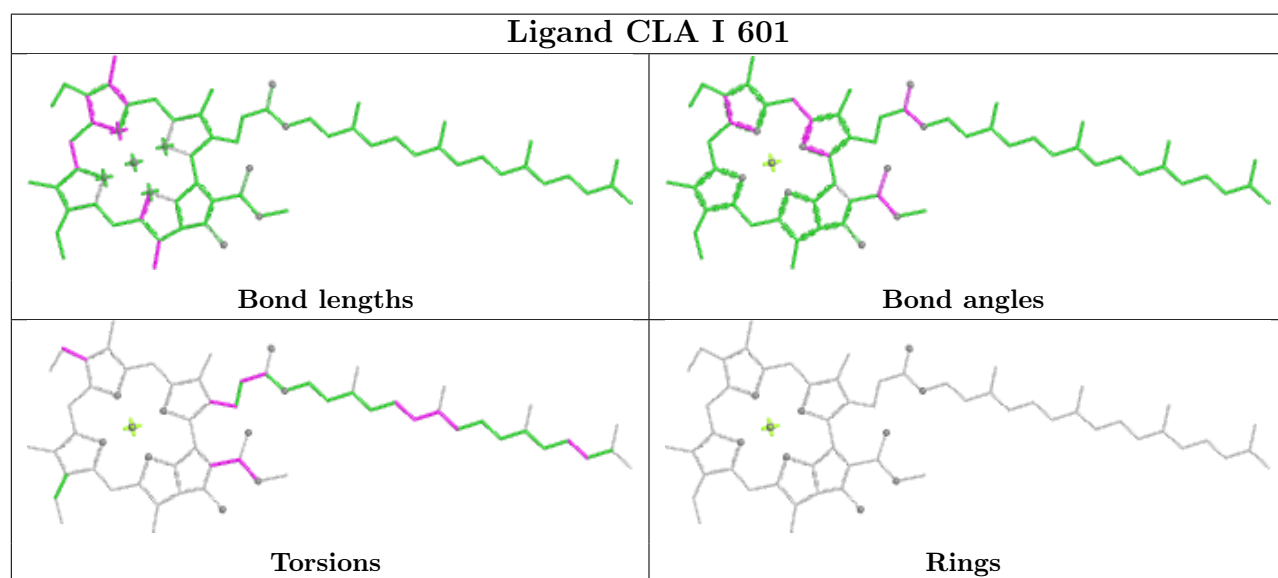
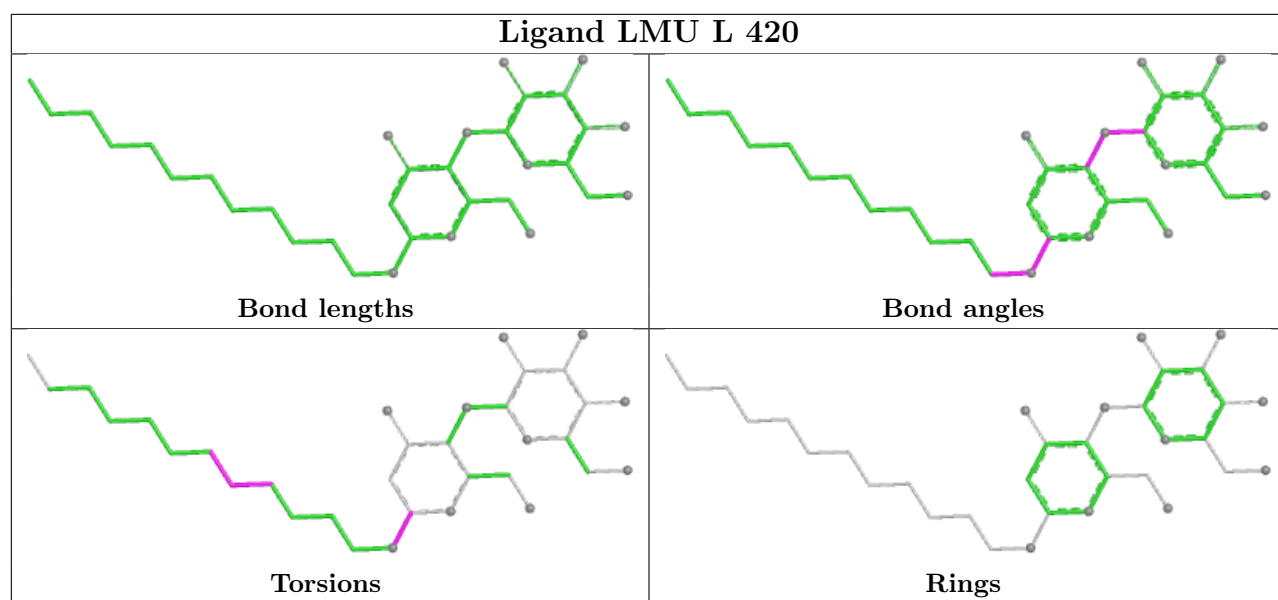
## Ligand CLA S 615

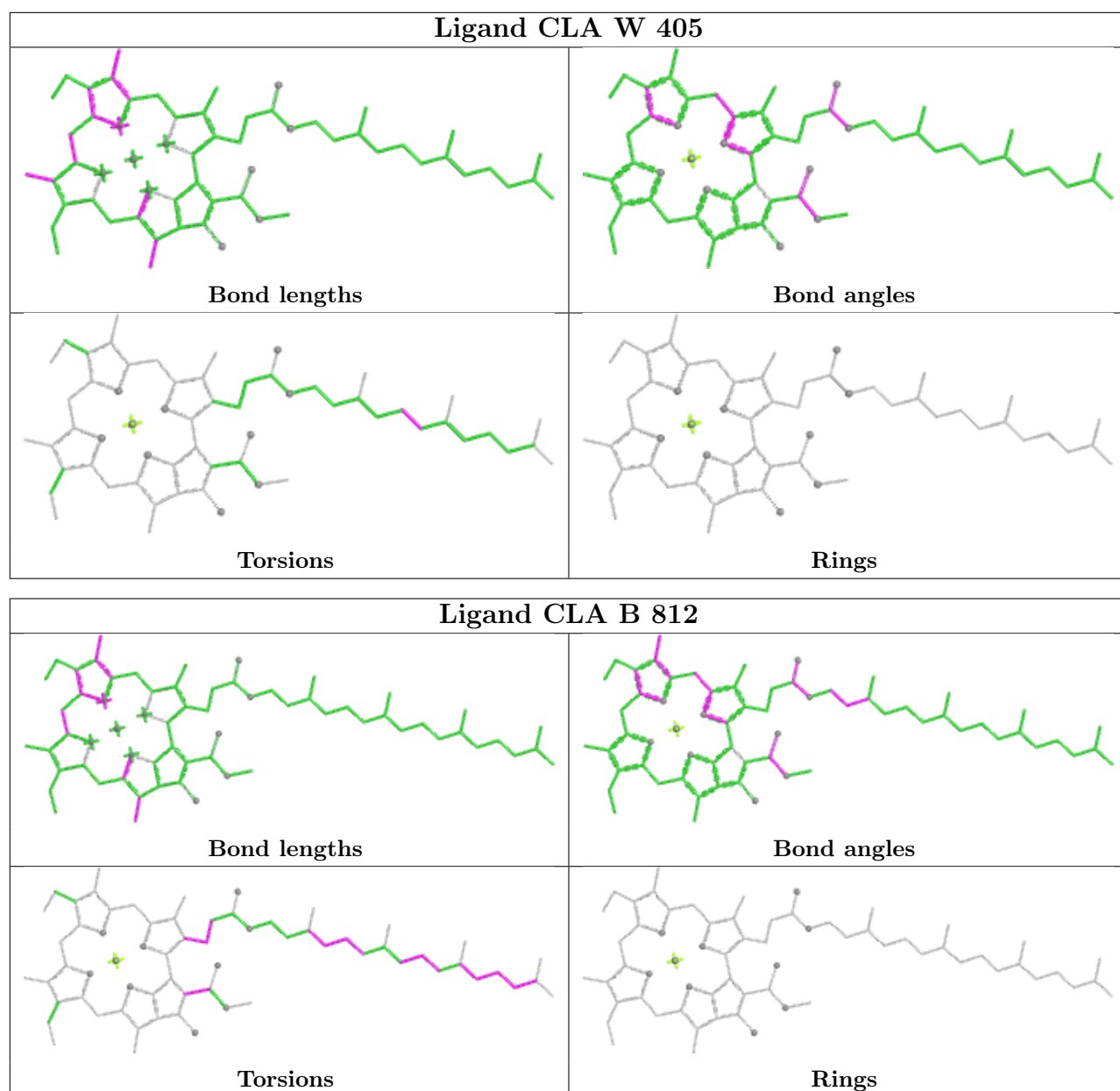


## Ligand CLA O 313

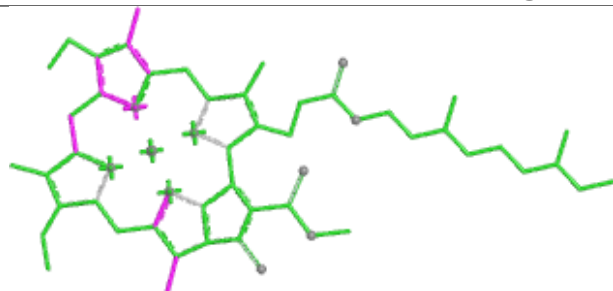




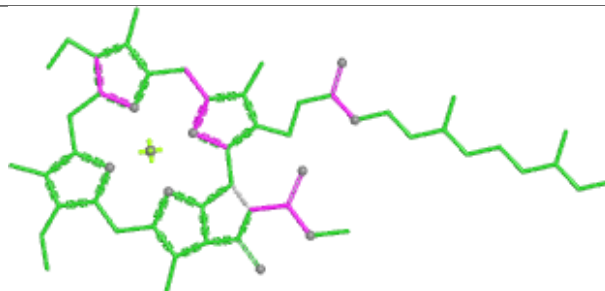




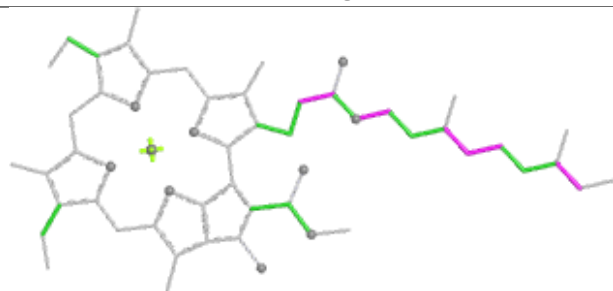
## Ligand CLA I 603



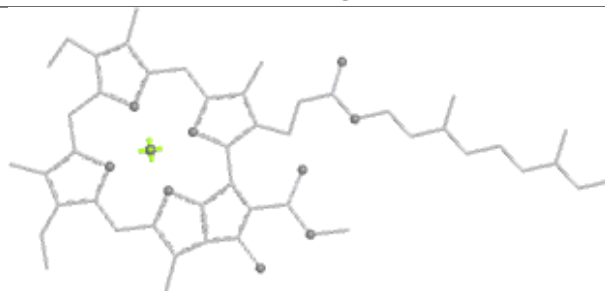
Bond lengths



Bond angles

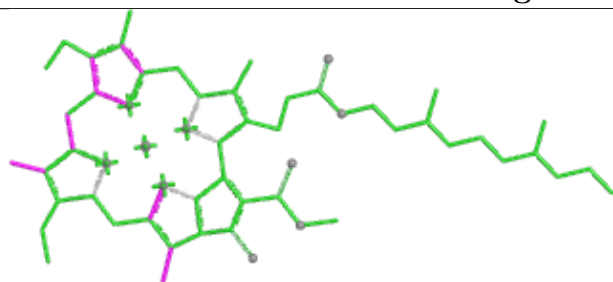


Torsions

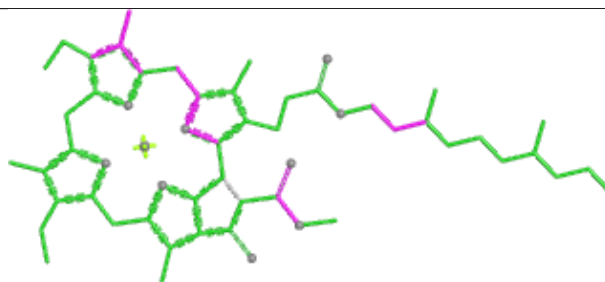


Rings

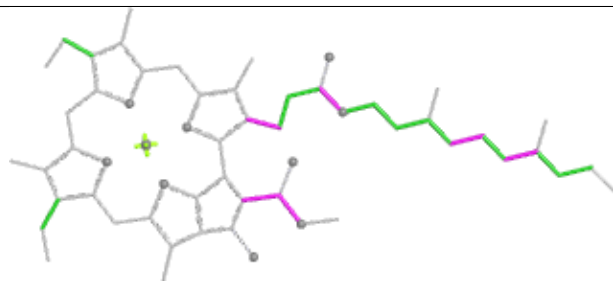
## Ligand CLA V 603



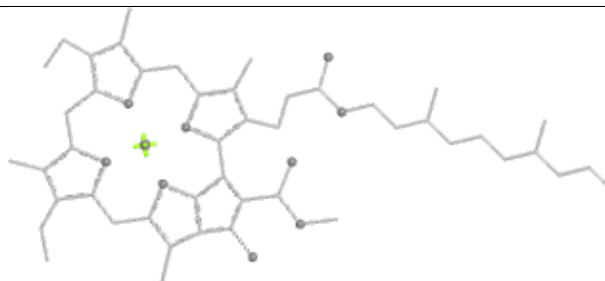
Bond lengths



Bond angles

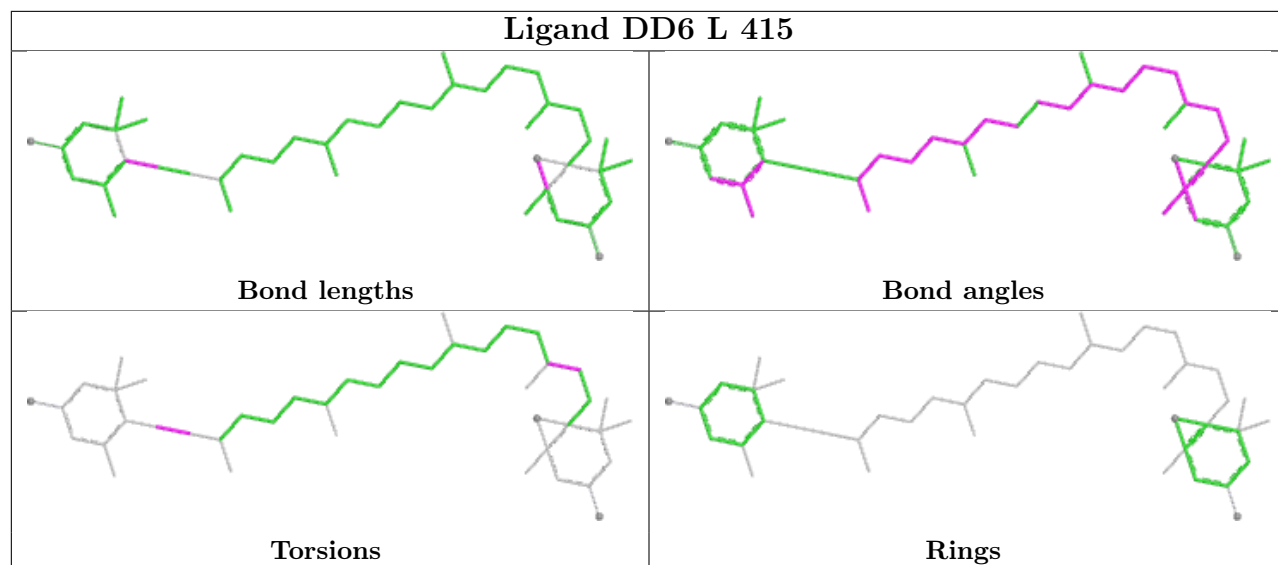


Torsions

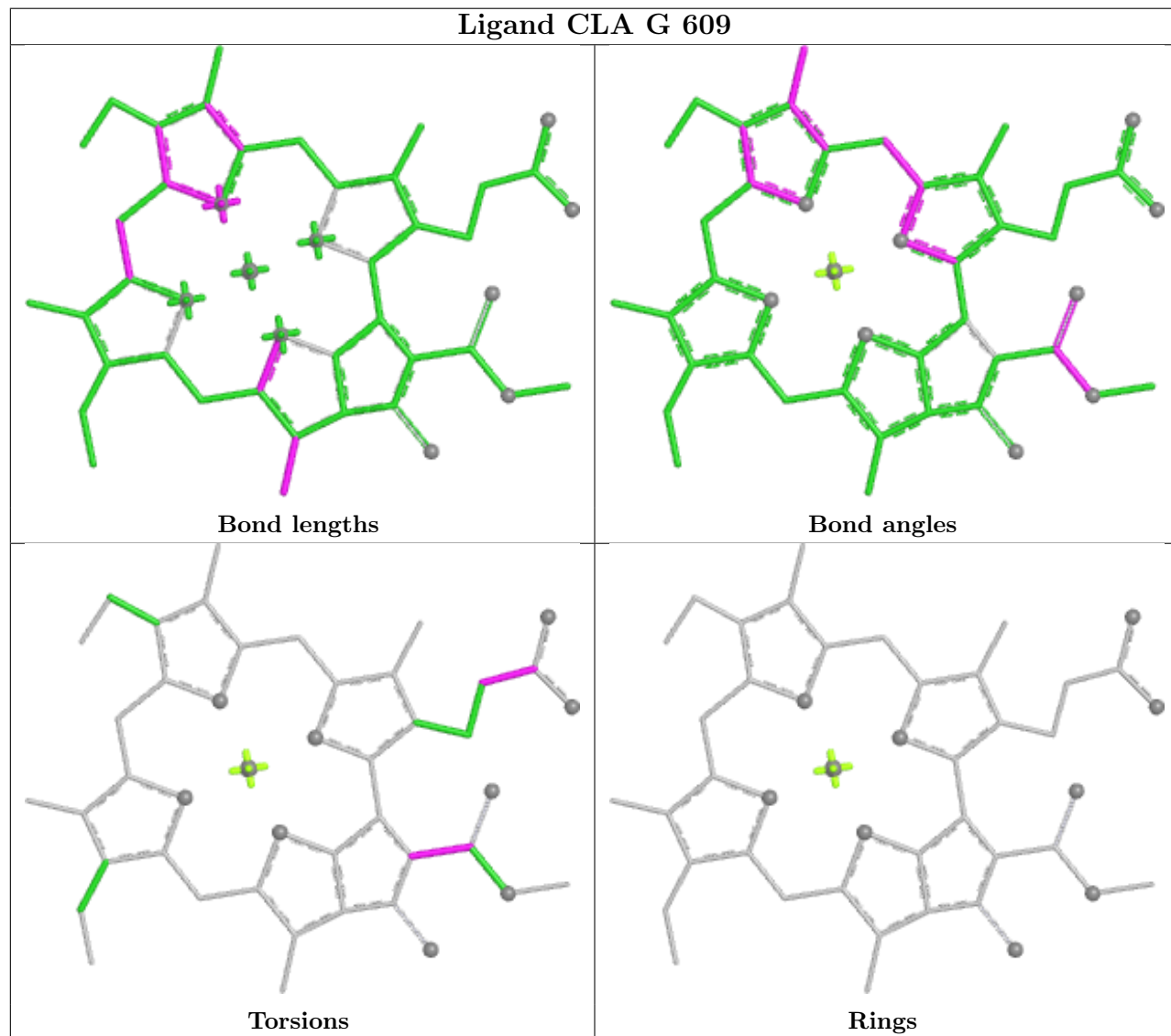


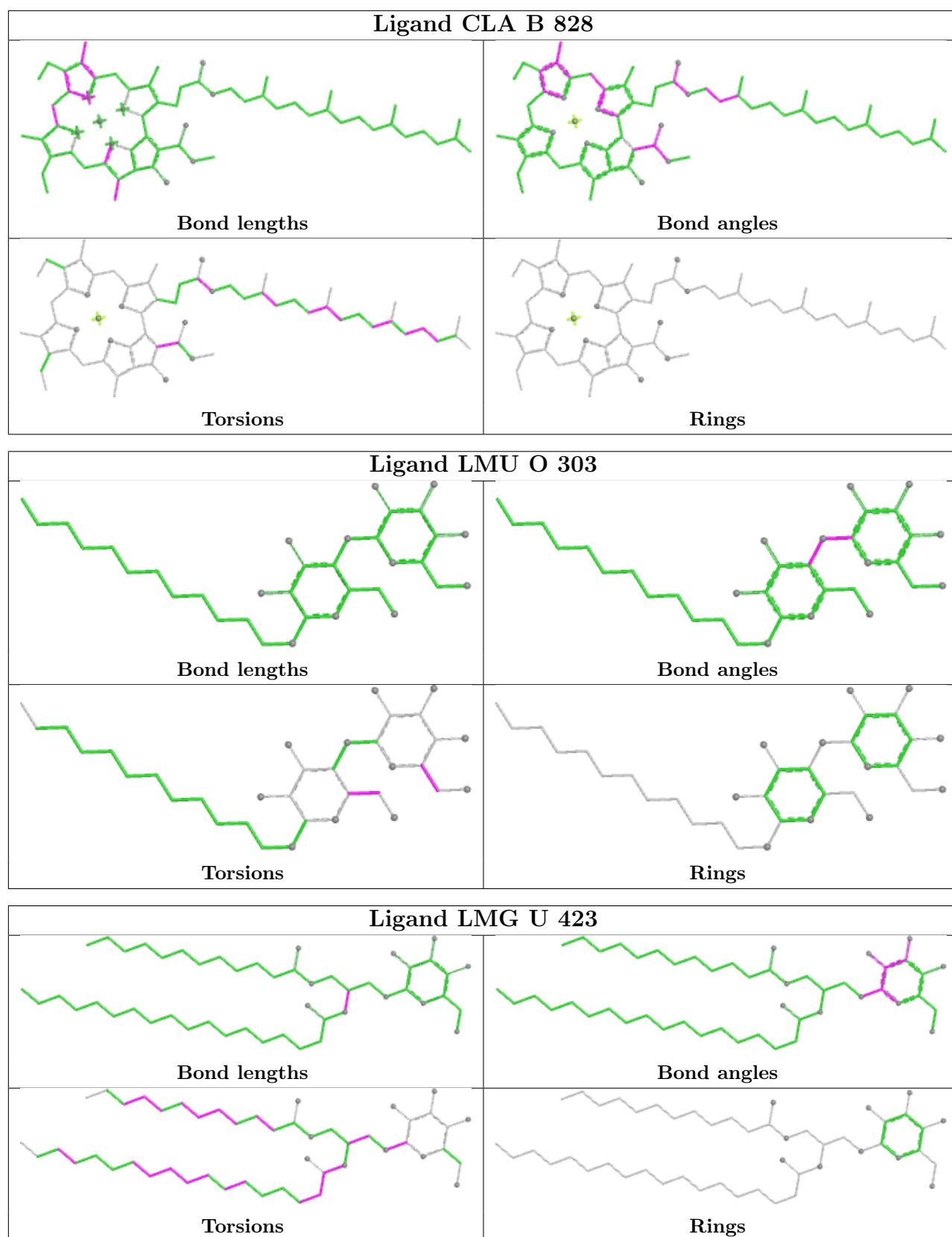
Rings

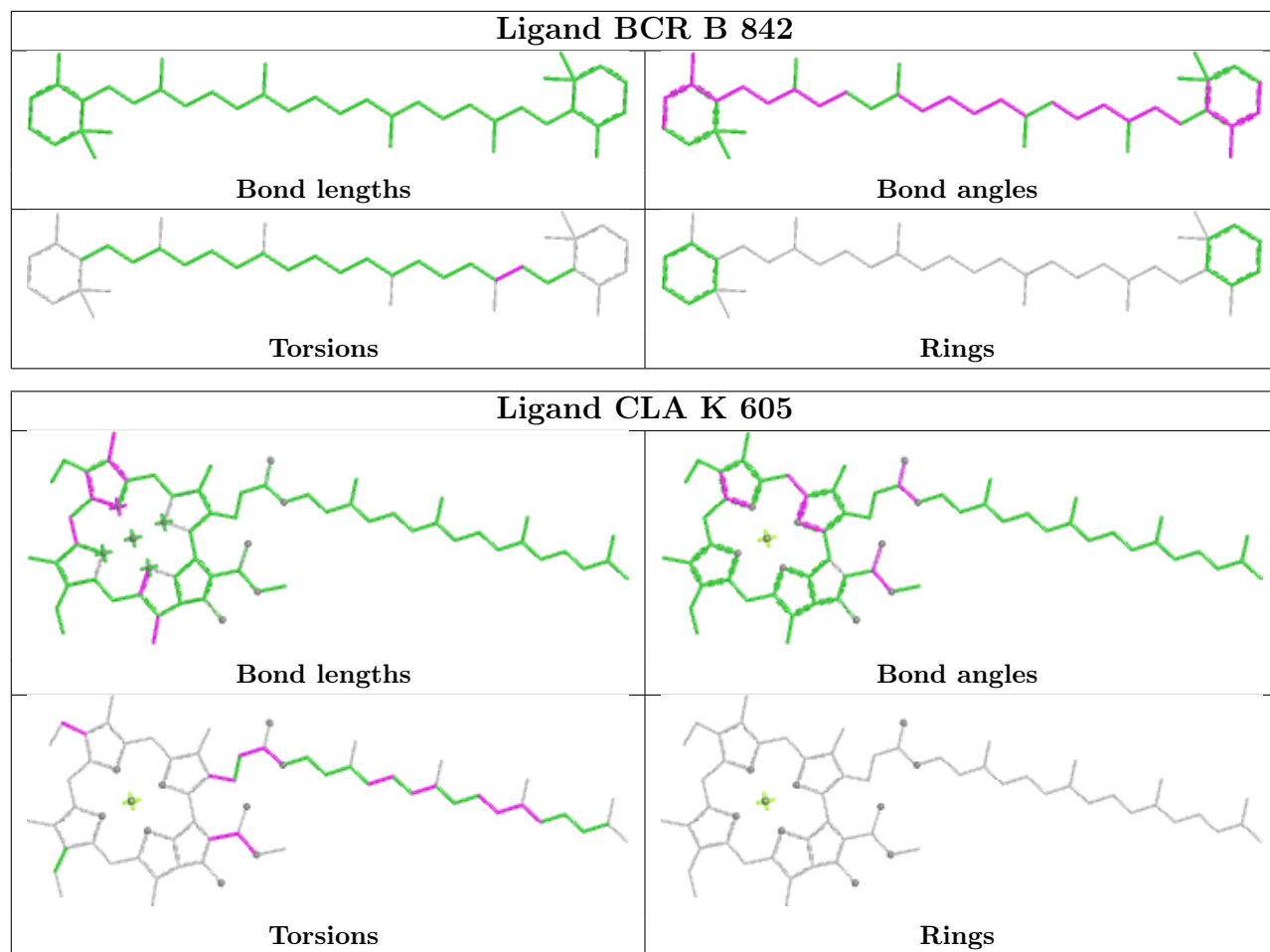
## Ligand DD6 L 415

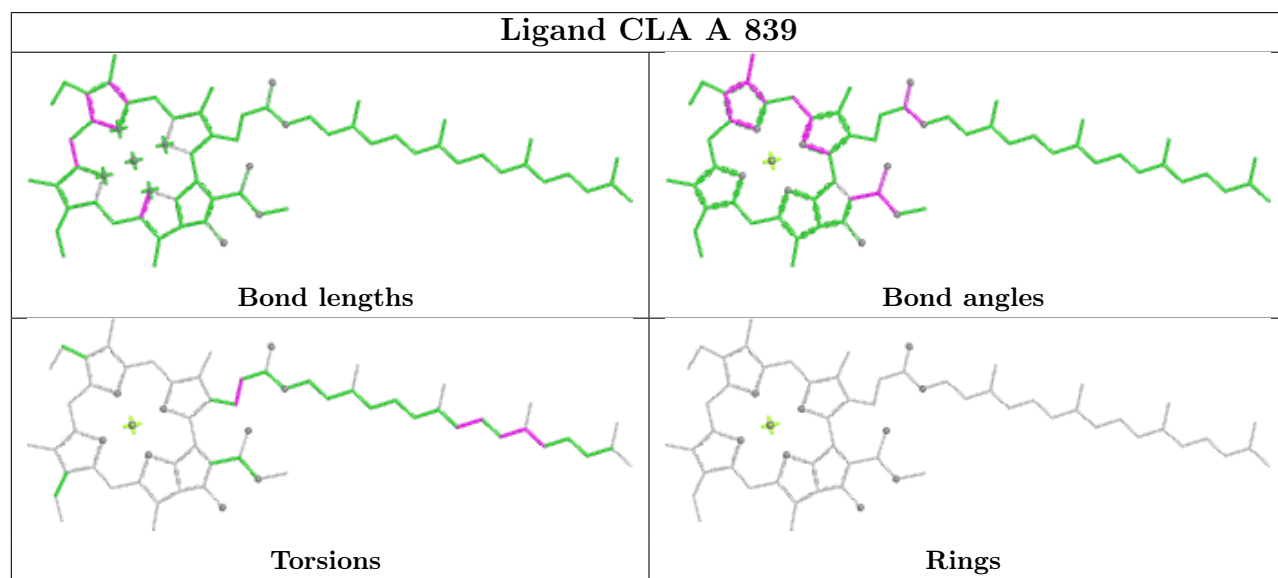
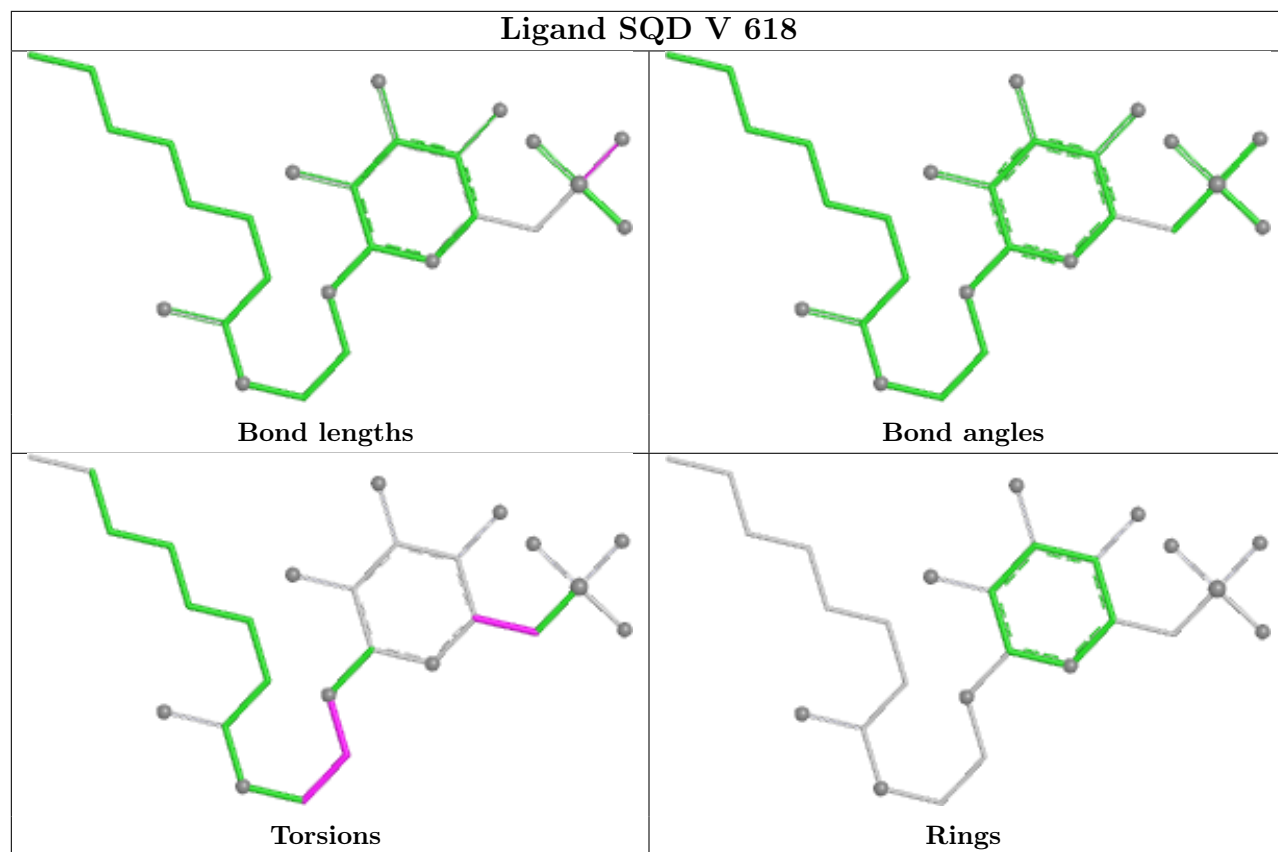


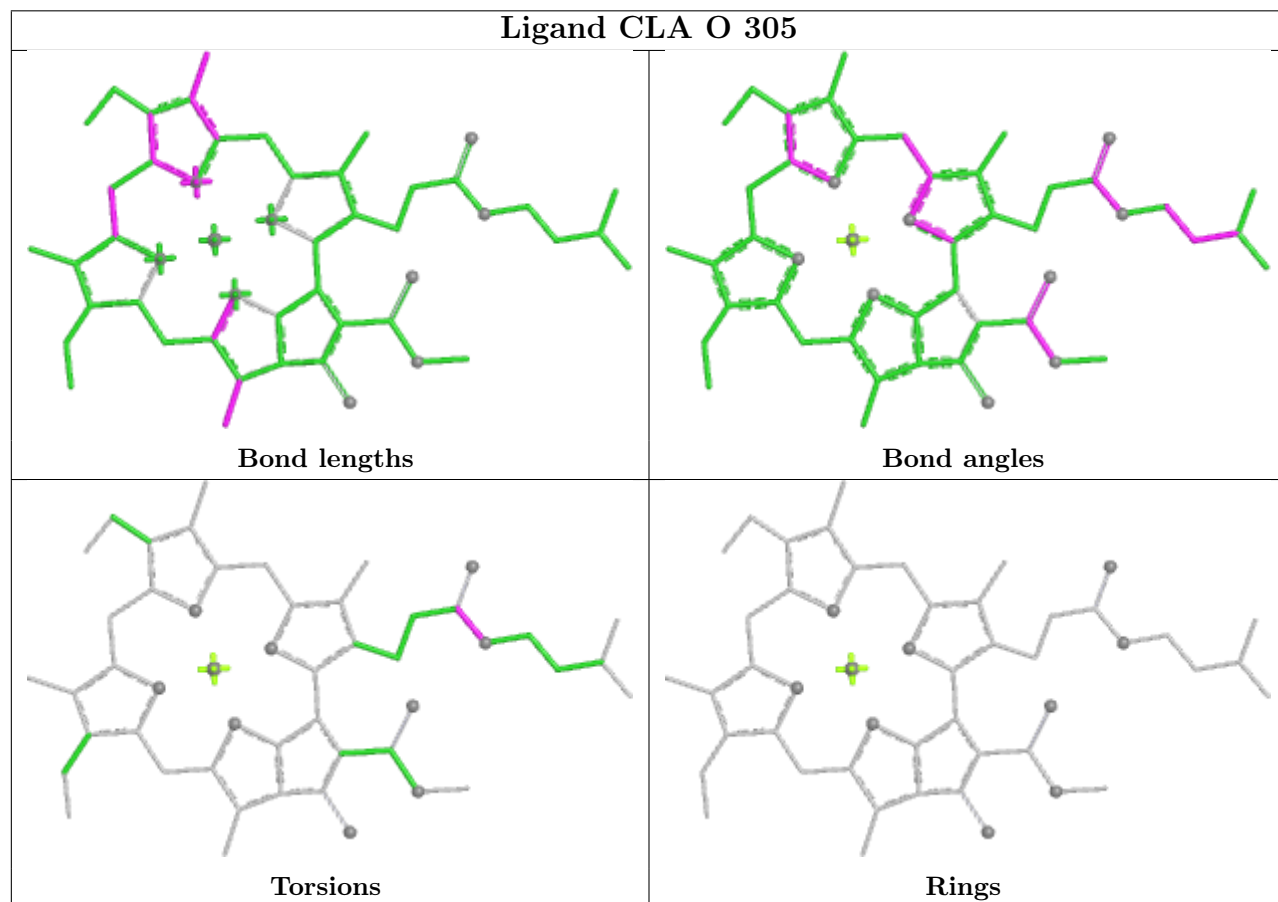
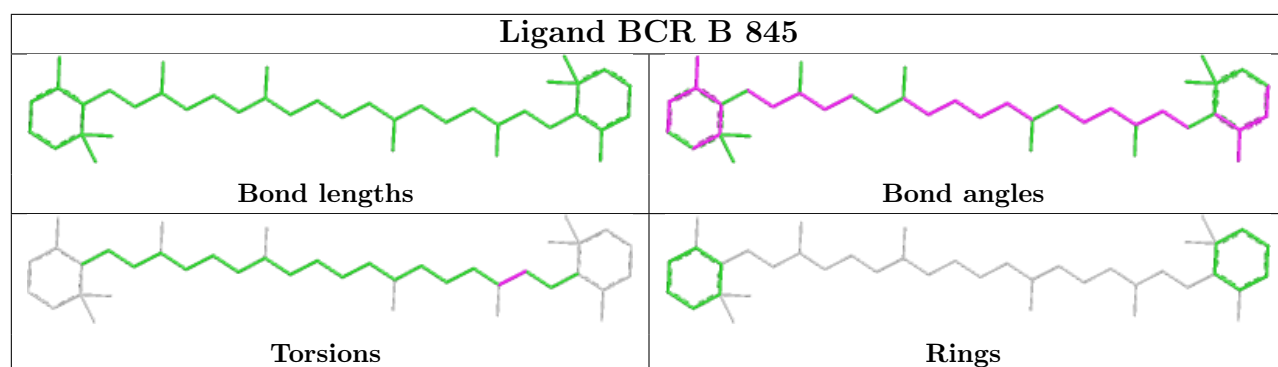
## Ligand CLA G 609





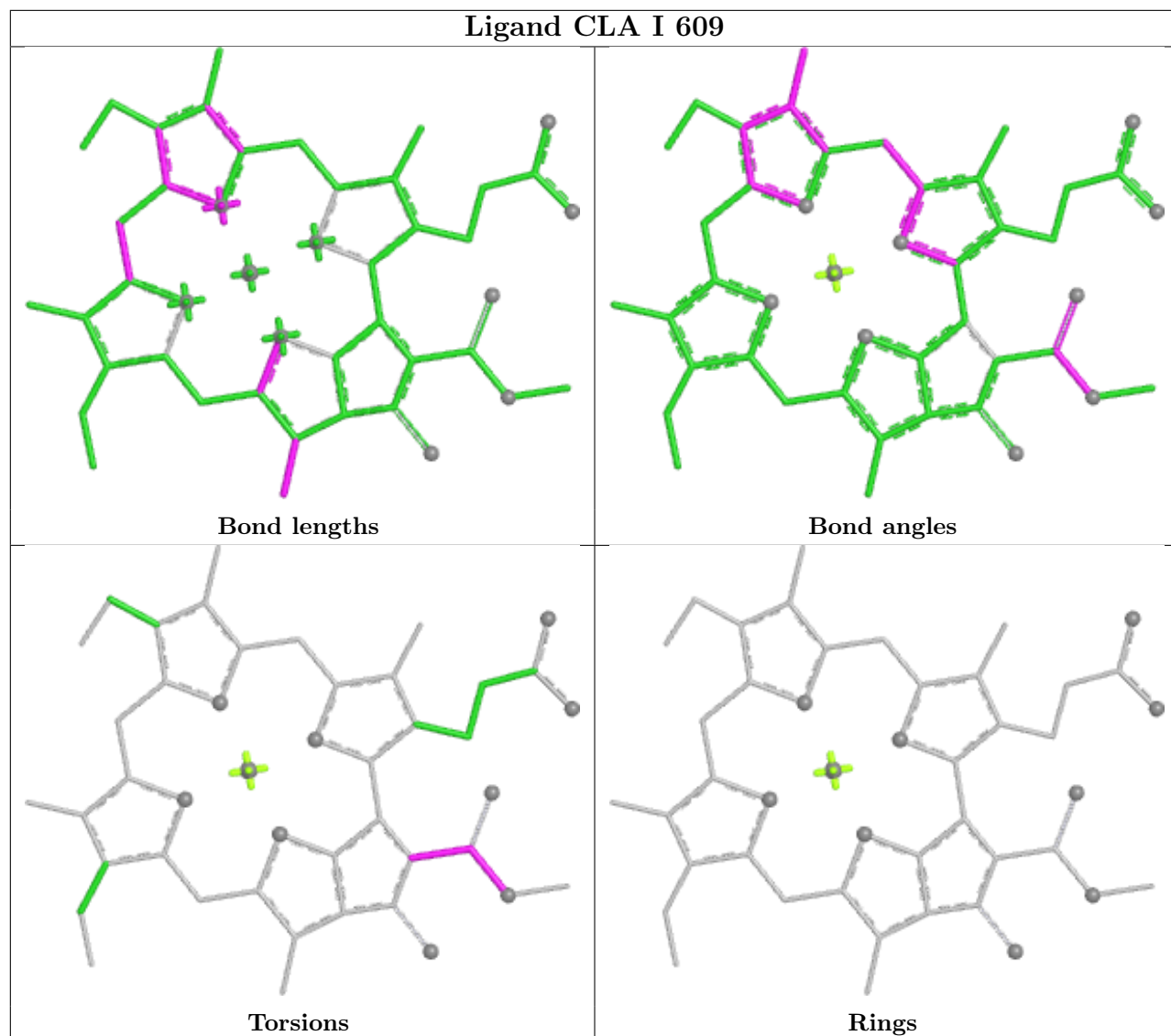




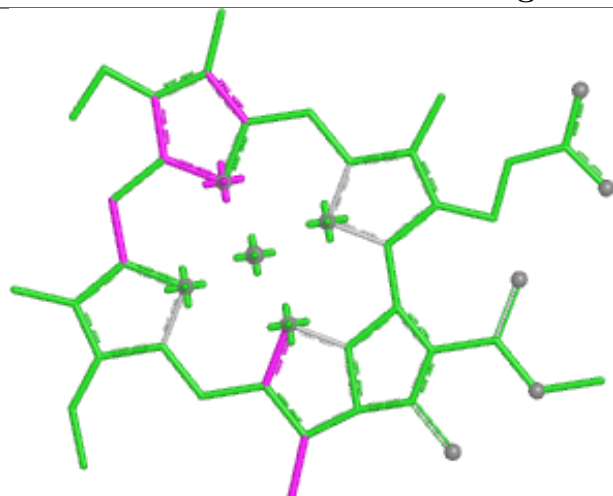




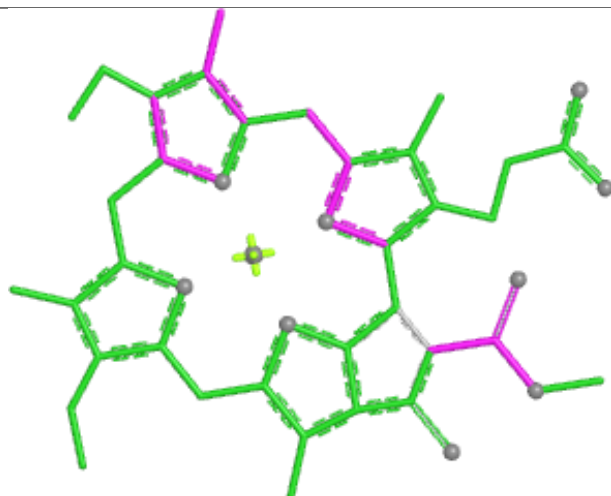
## Ligand CLA I 609



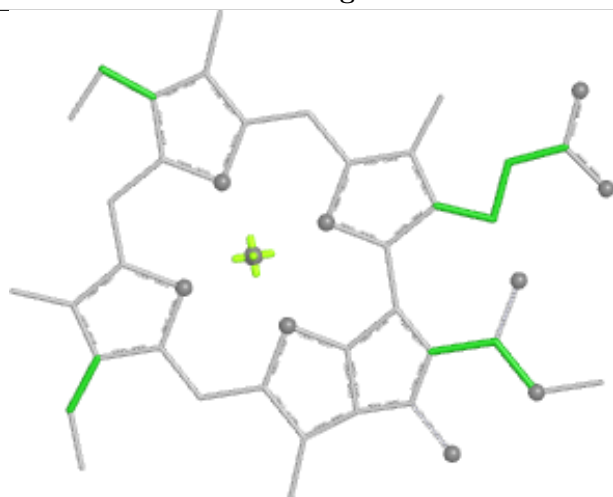
## Ligand CLA S 614



Bond lengths



Bond angles

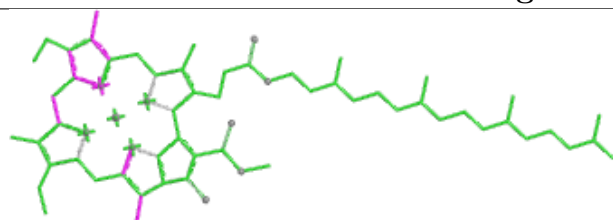


Torsions

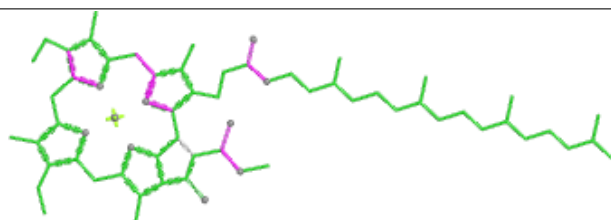


Rings

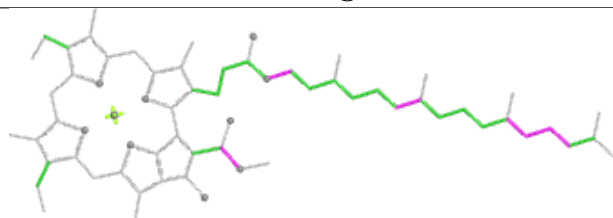
## Ligand CLA L 406



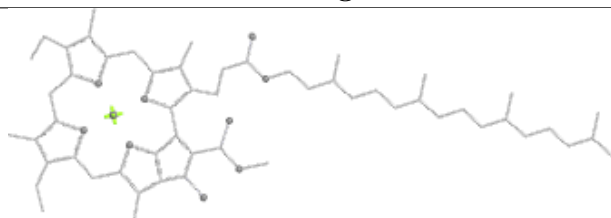
Bond lengths



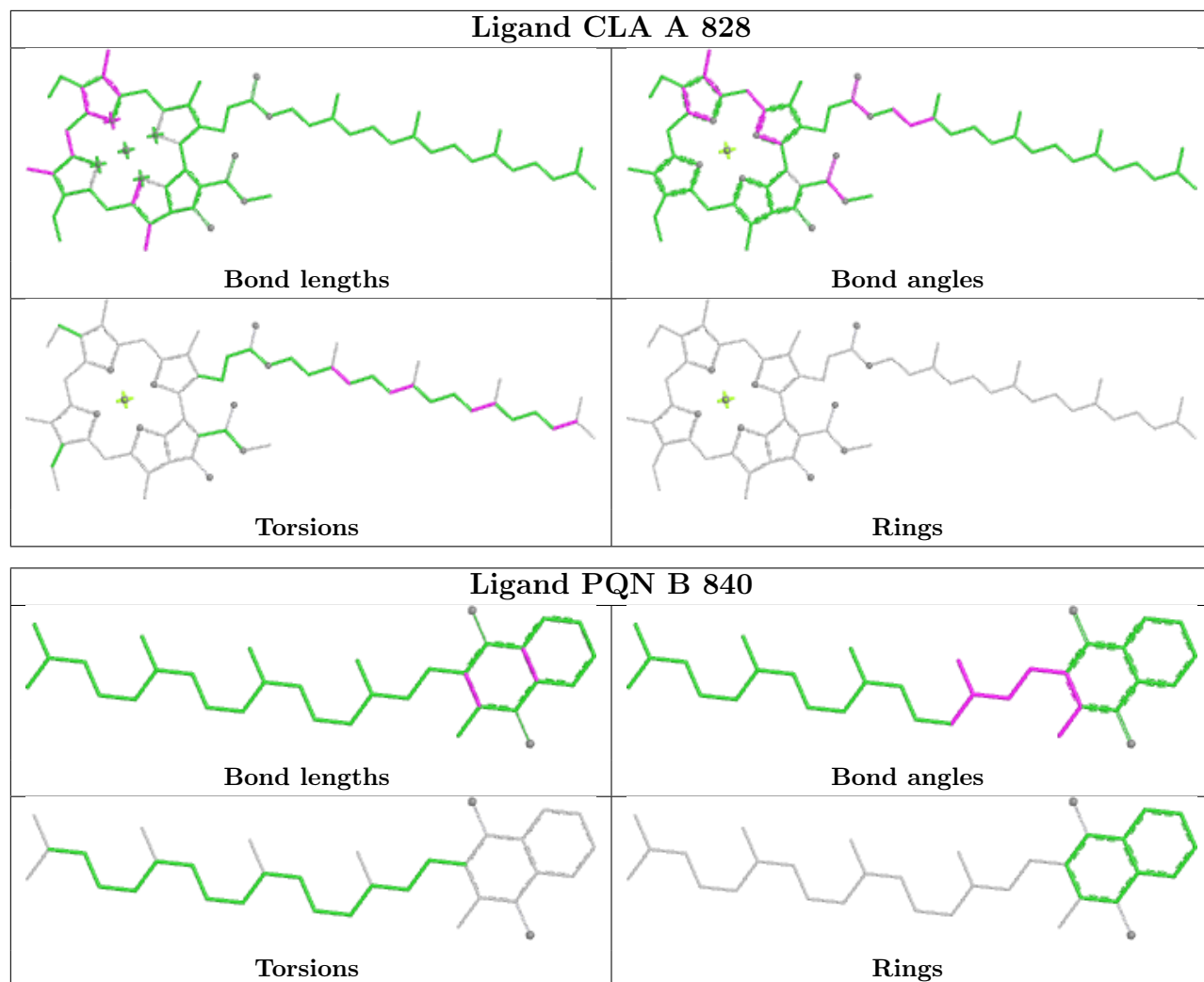
Bond angles



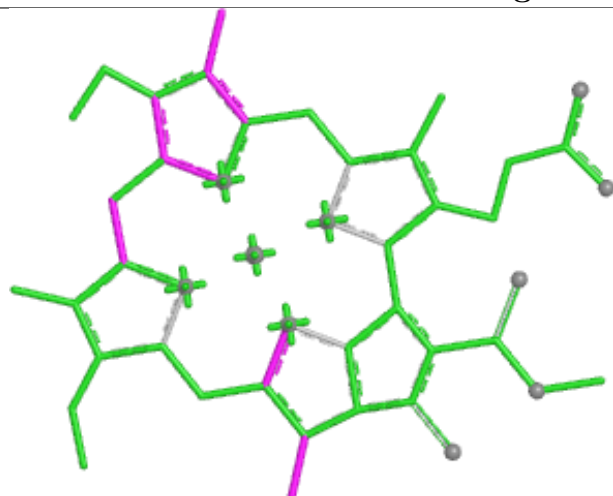
Torsions



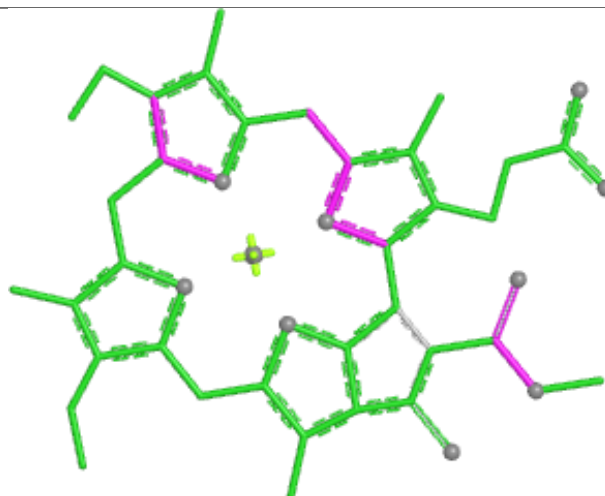
Rings



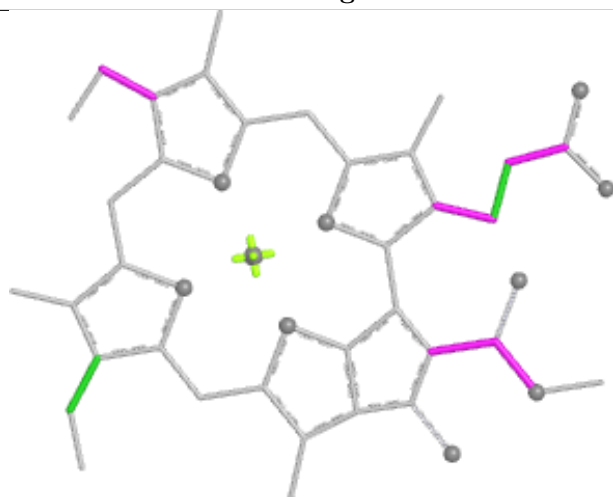
## Ligand CLA V 613



Bond lengths



Bond angles

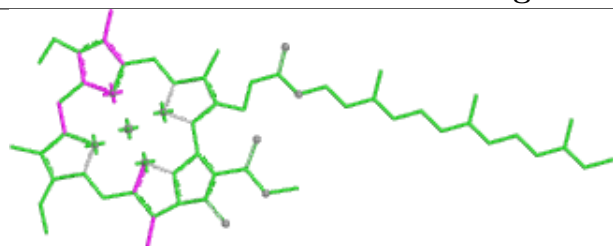


Torsions

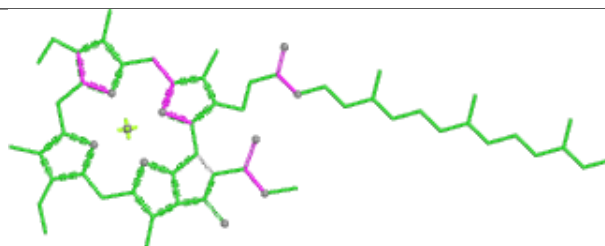


Rings

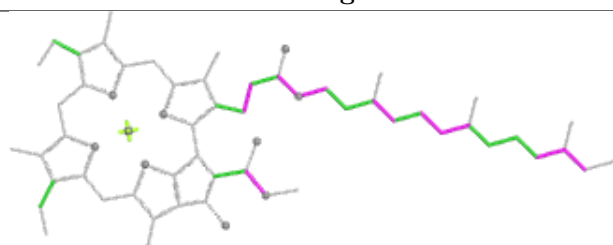
## Ligand CLA U 414



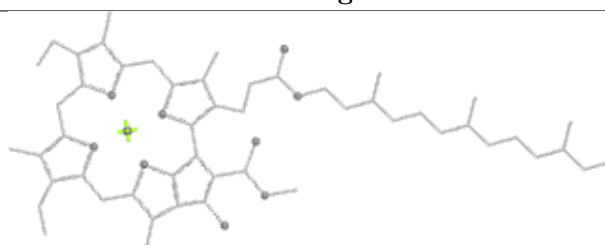
Bond lengths



Bond angles

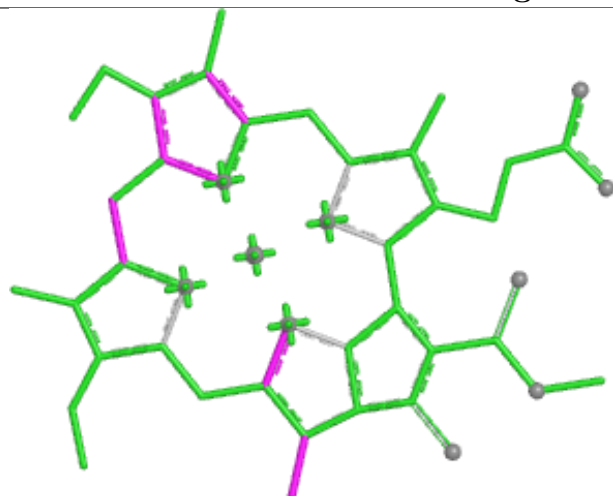


Torsions

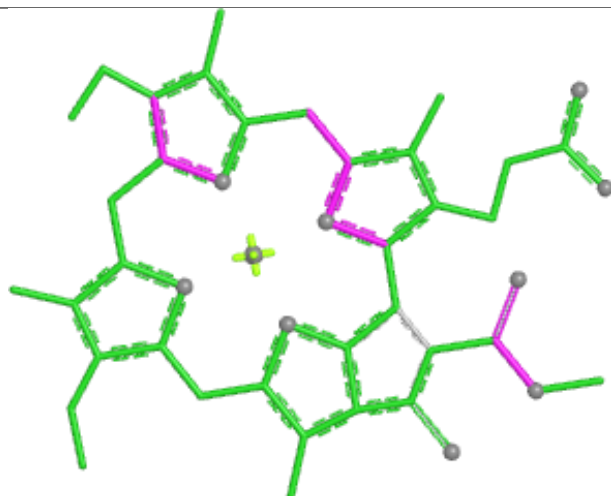


Rings

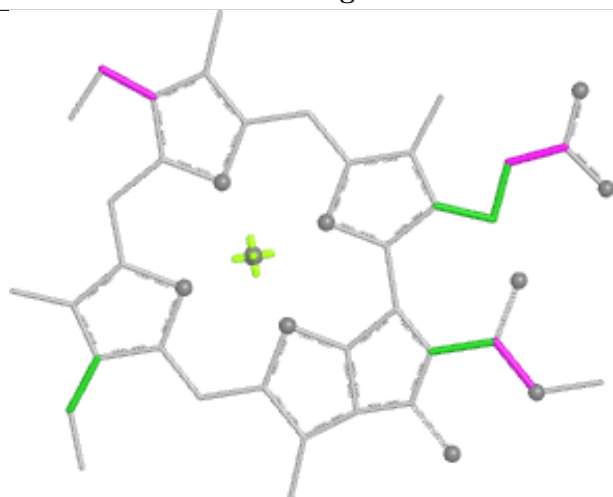
## Ligand CLA V 601



Bond lengths



Bond angles

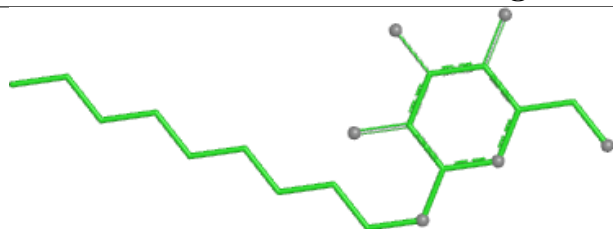


Torsions

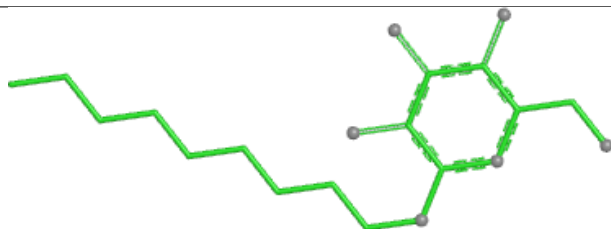


Rings

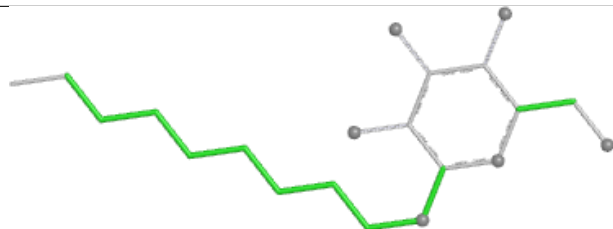
## Ligand LMU A 856



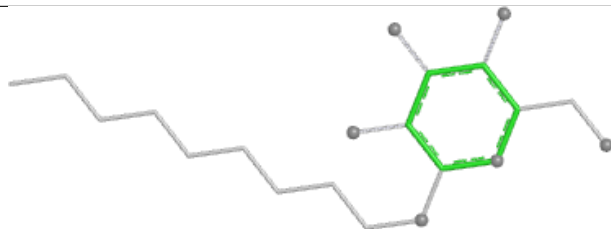
Bond lengths



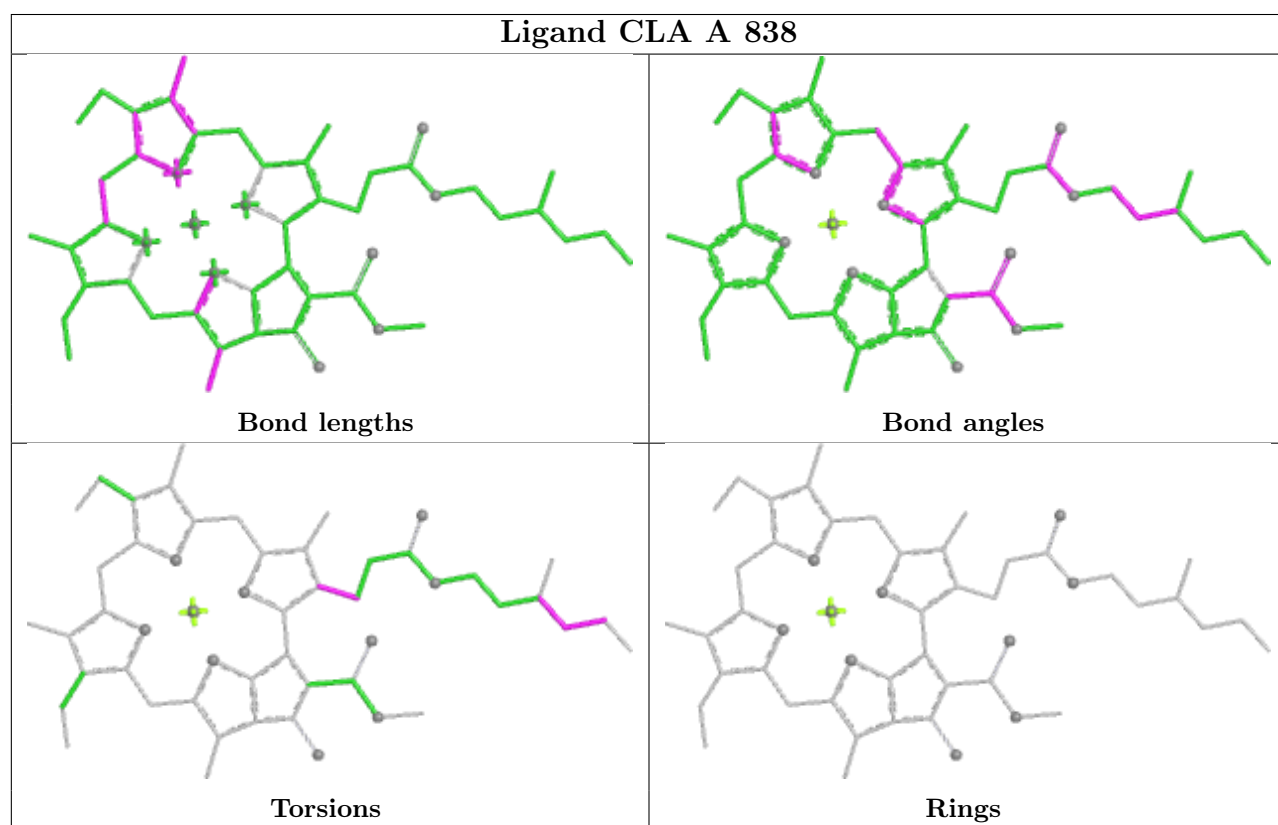
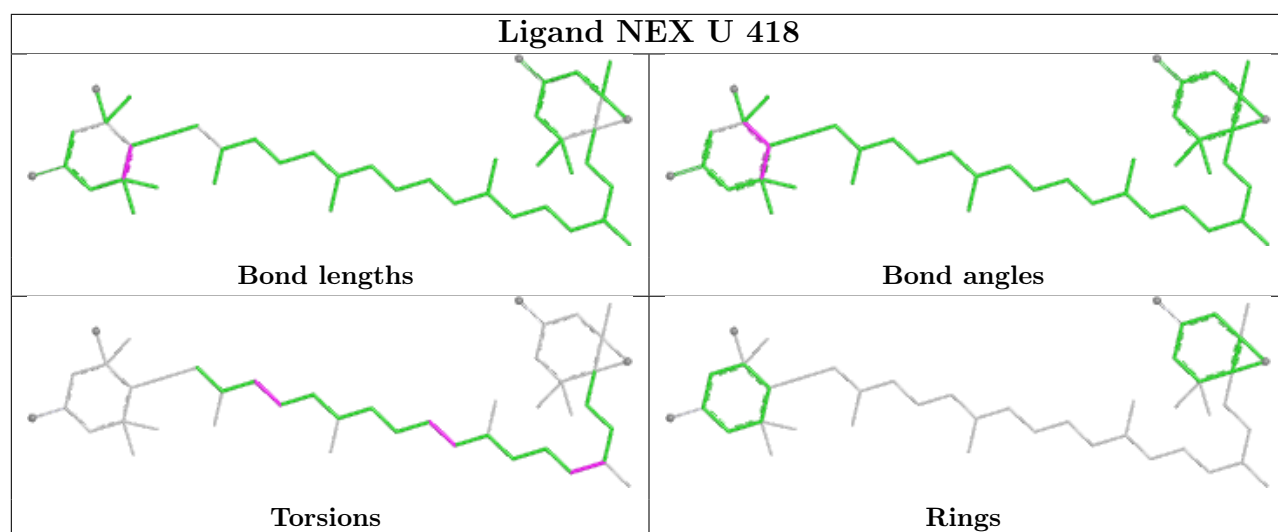
Bond angles

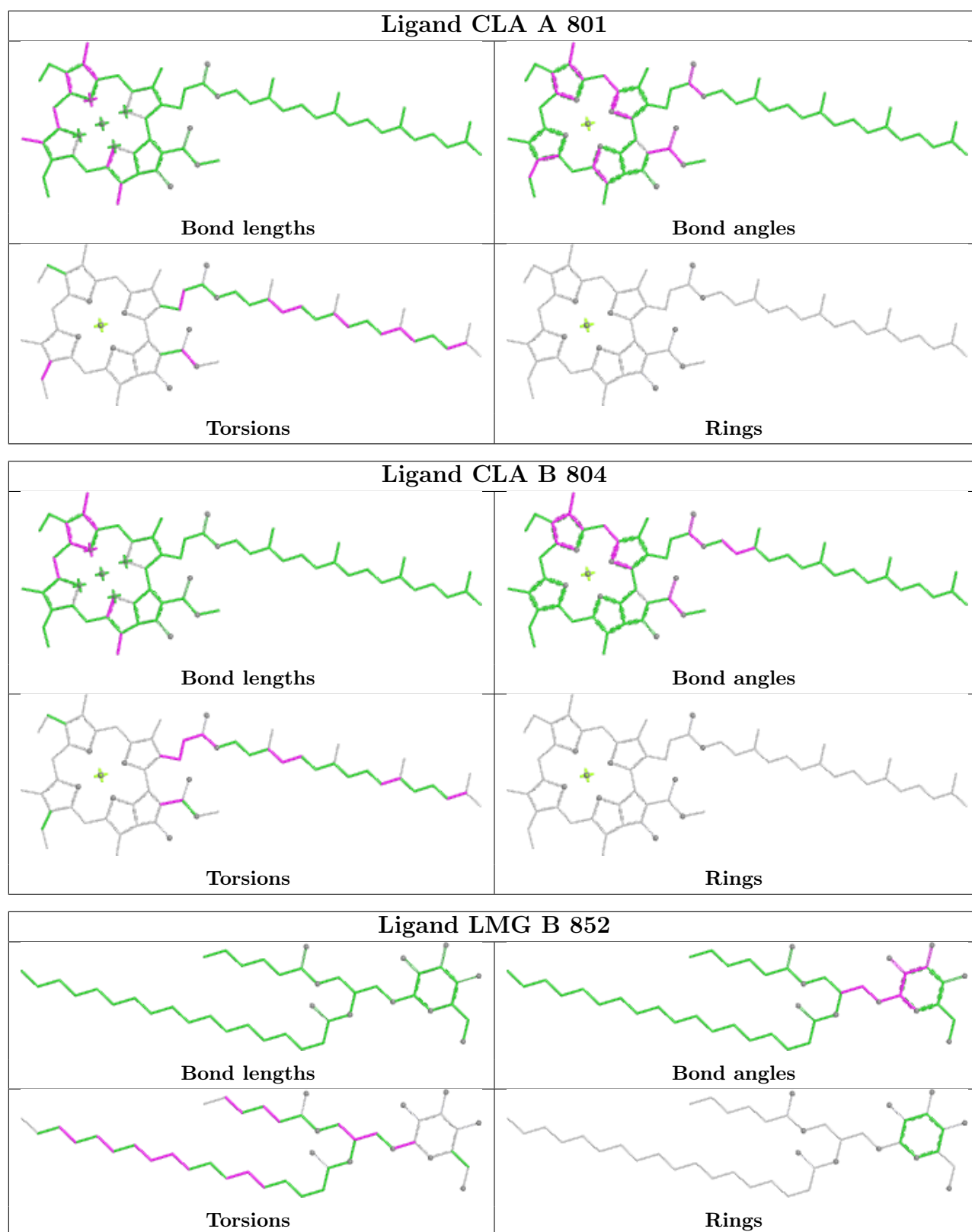


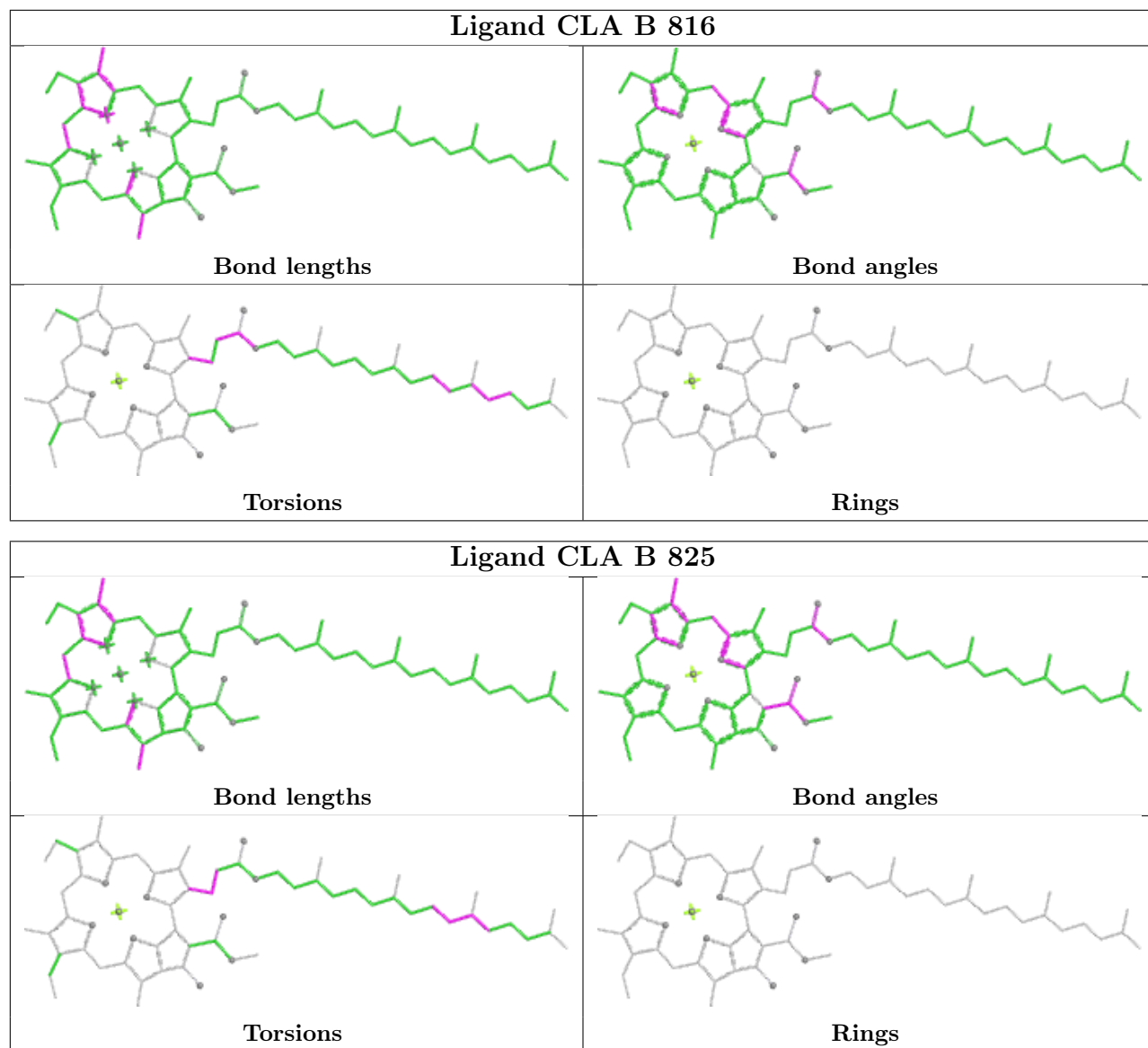
Torsions



Rings

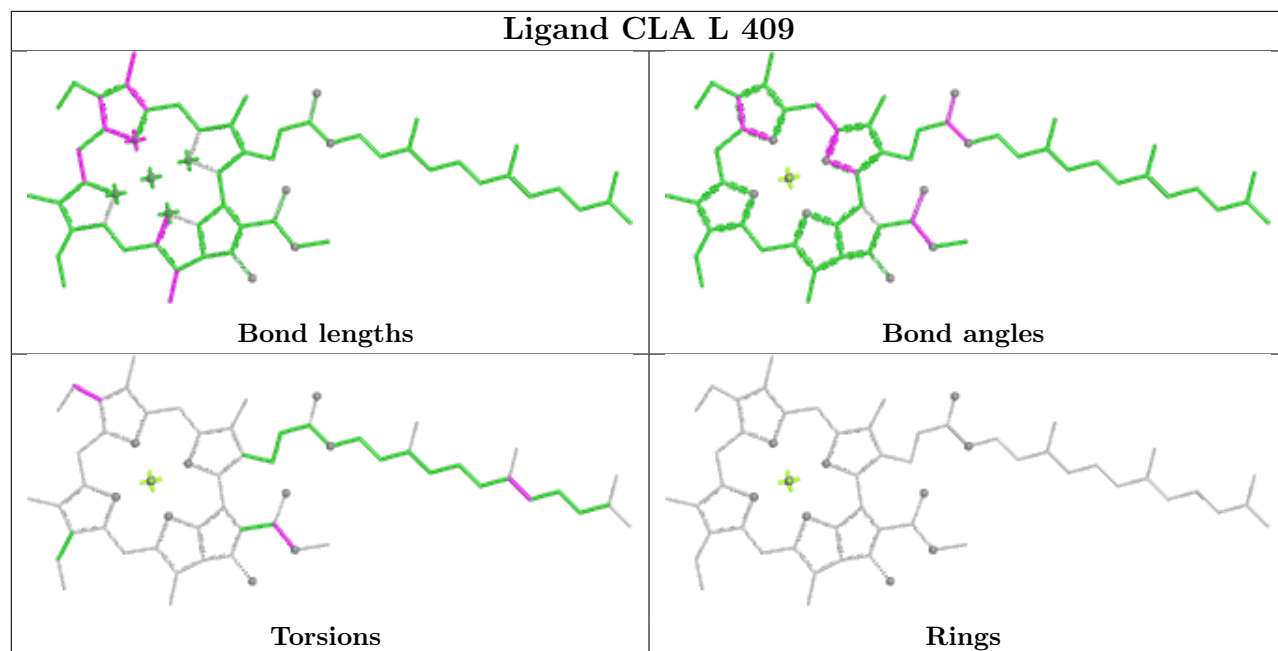




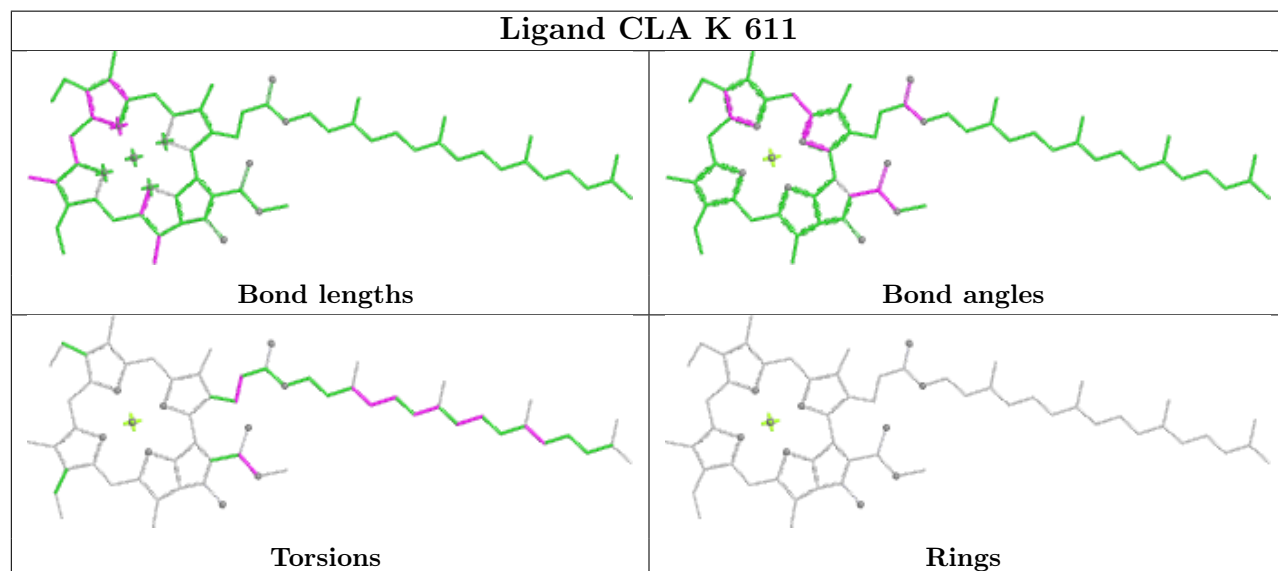


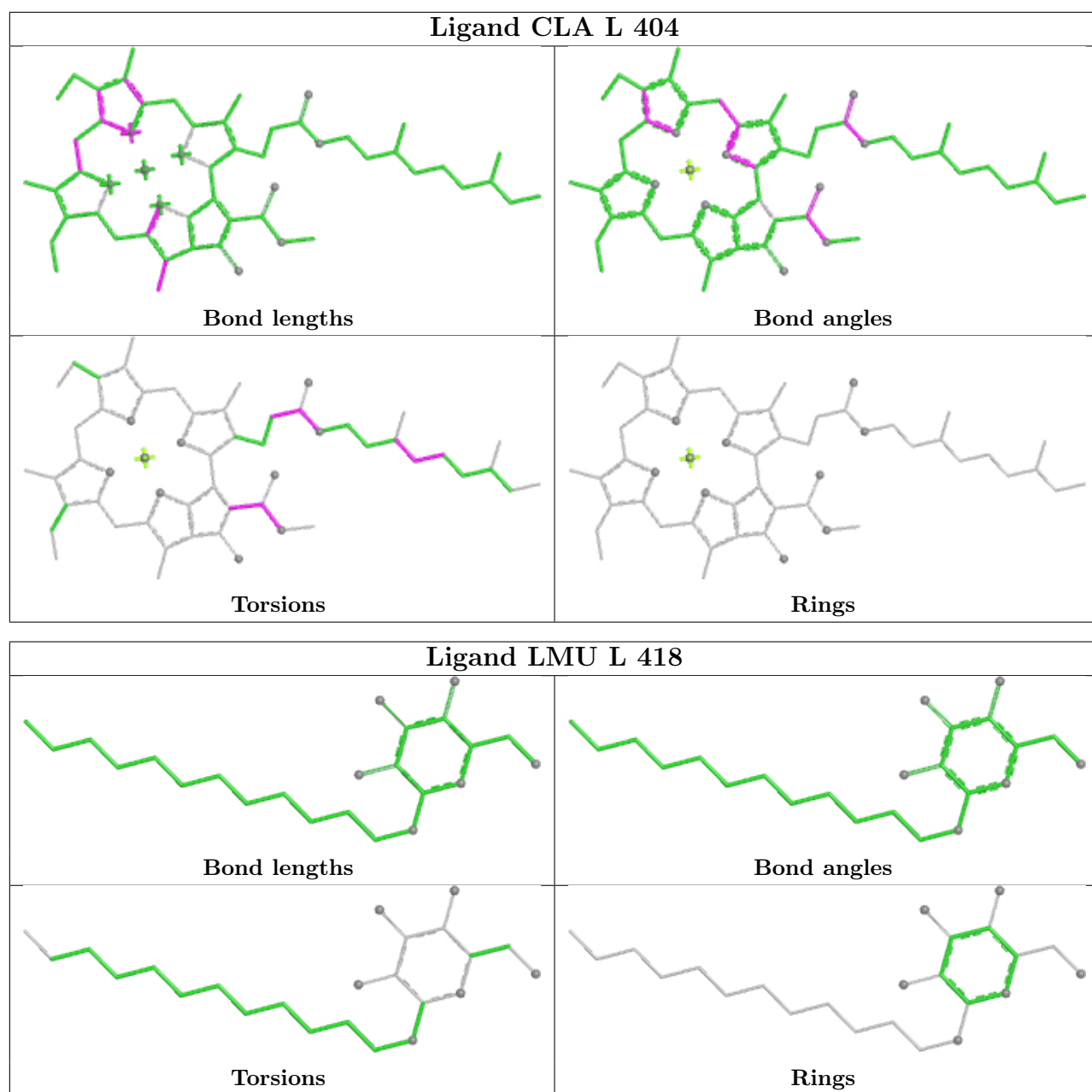


## Ligand CLA L 409

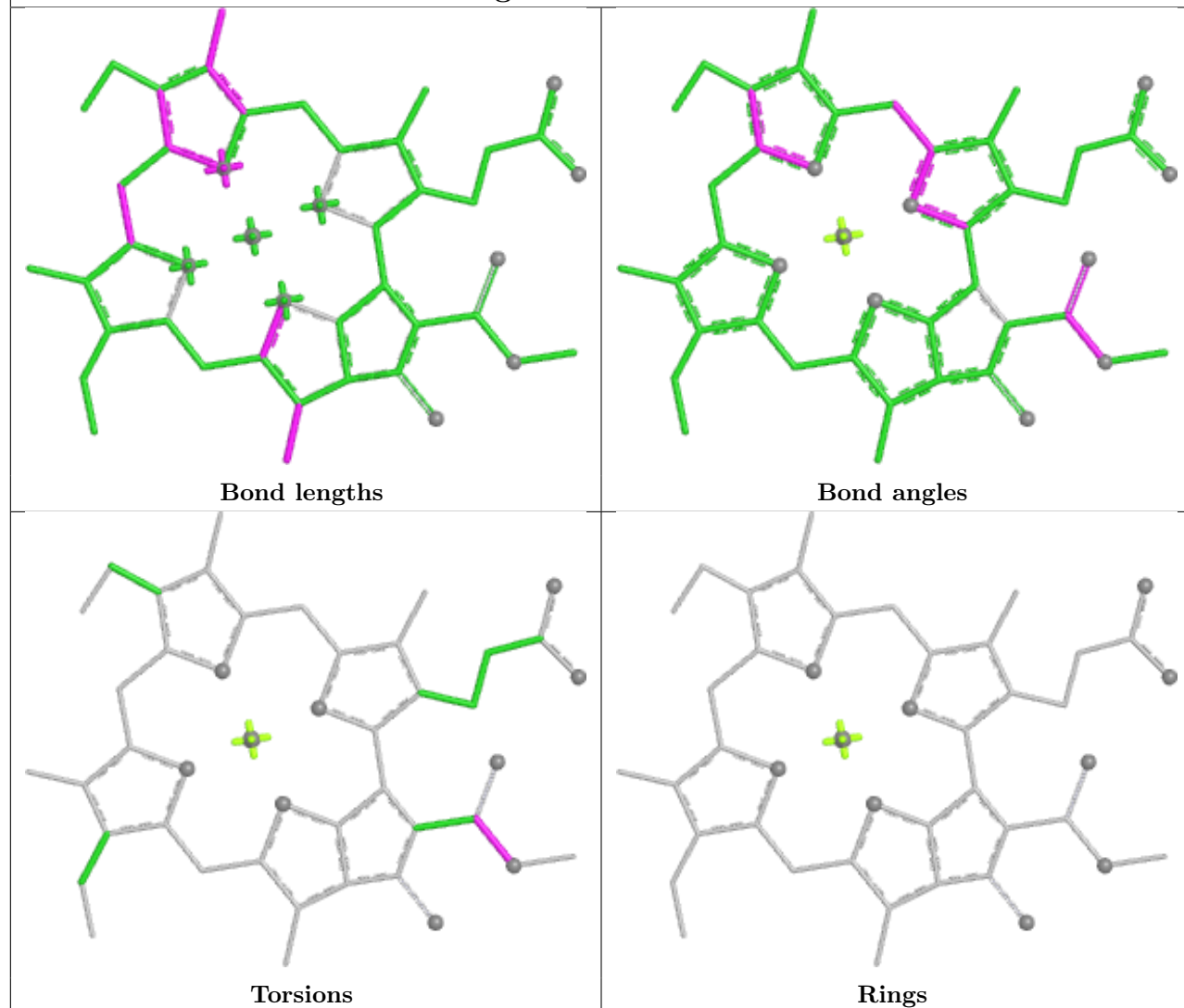


## Ligand CLA K 611

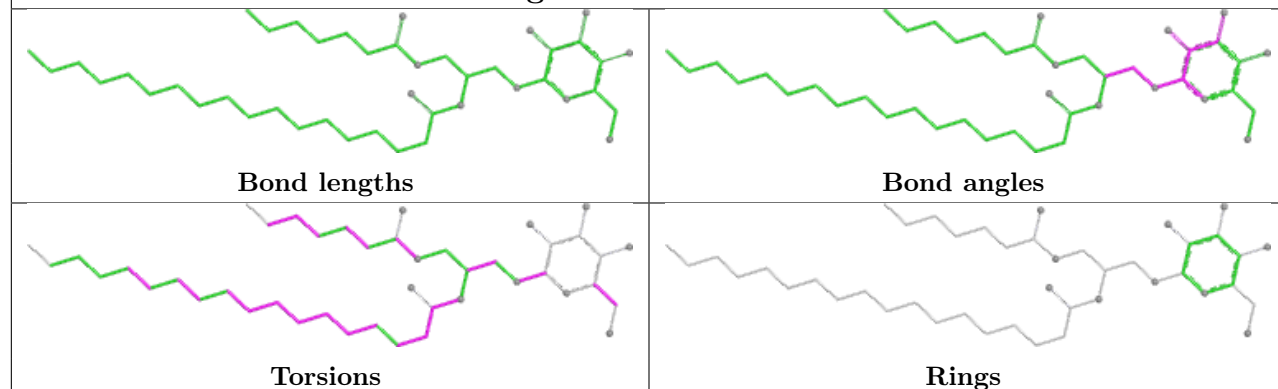




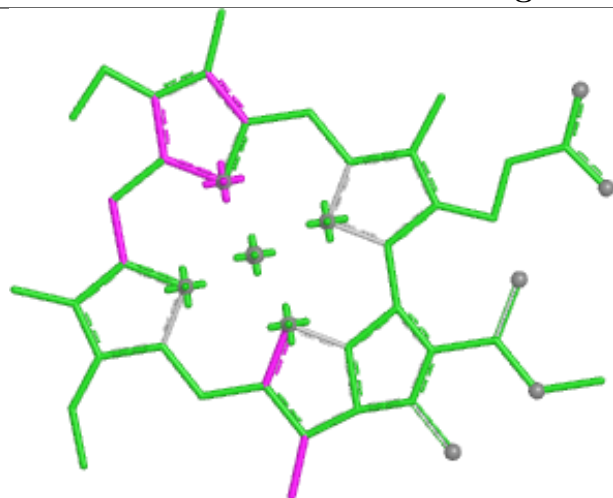
## Ligand CLA L 405



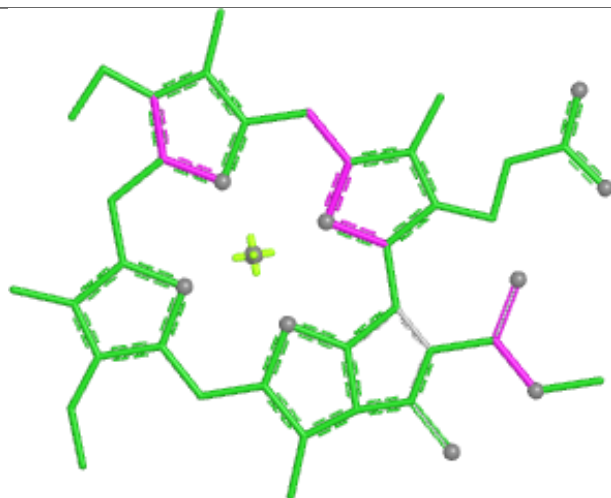
## Ligand LMG N 615



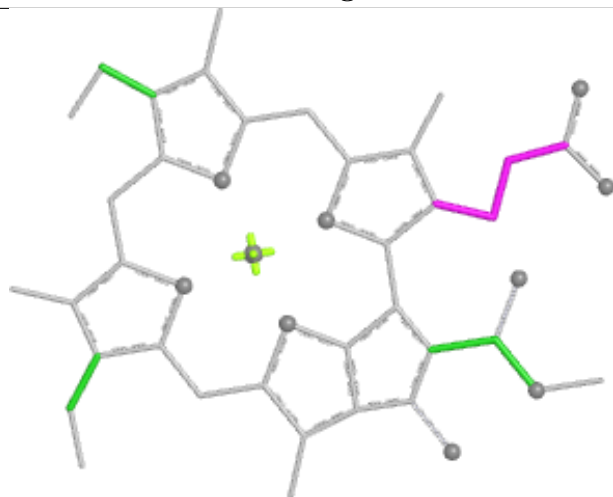
## Ligand CLA P 605



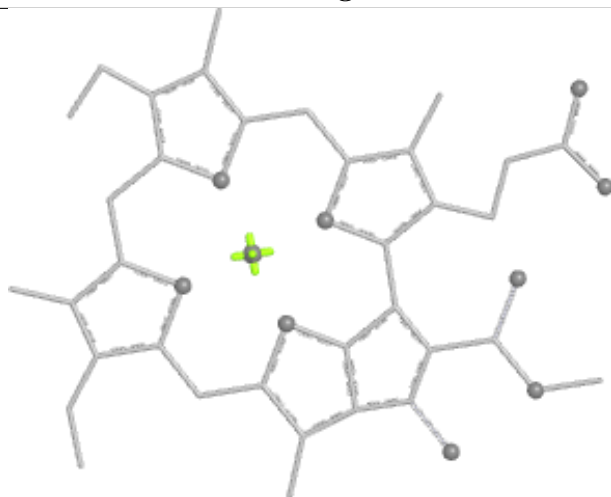
Bond lengths



Bond angles

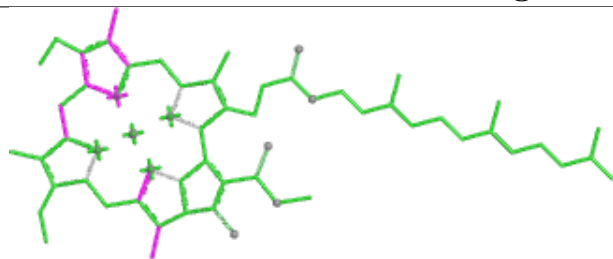


Torsions

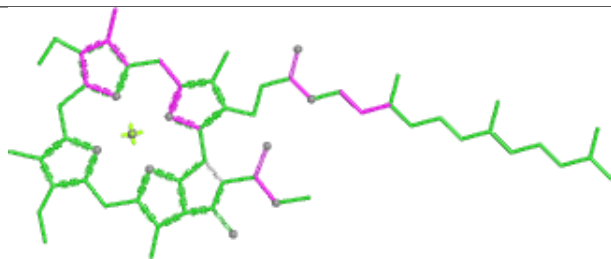


Rings

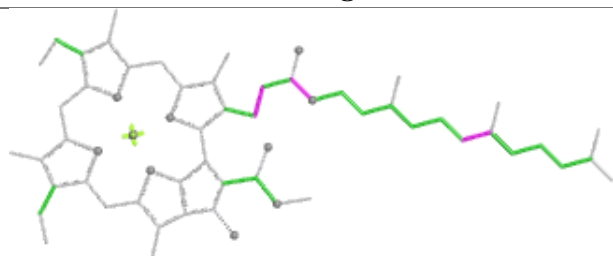
## Ligand CLA G 602



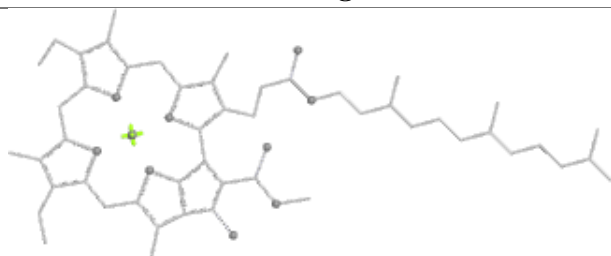
Bond lengths



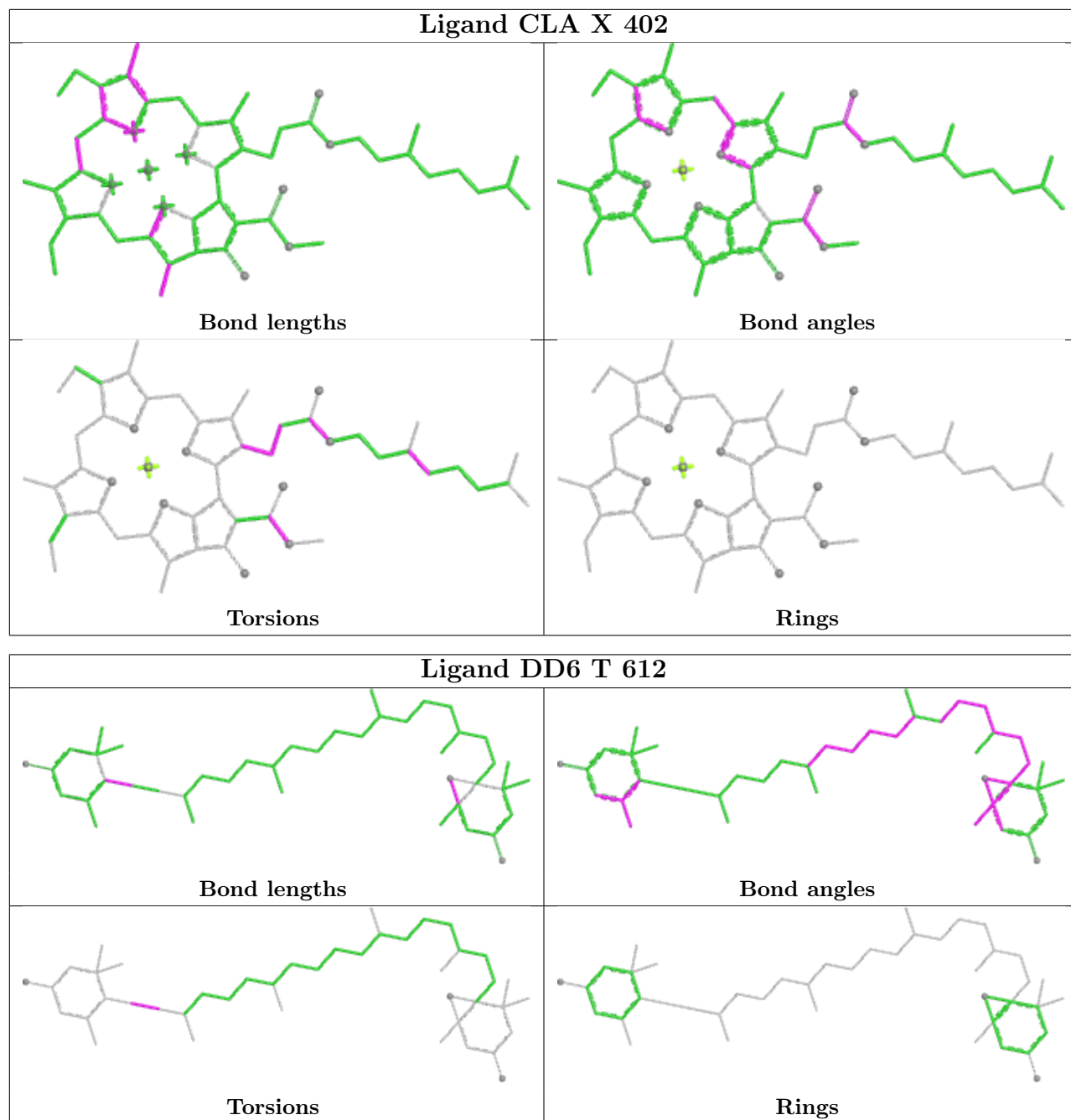
Bond angles



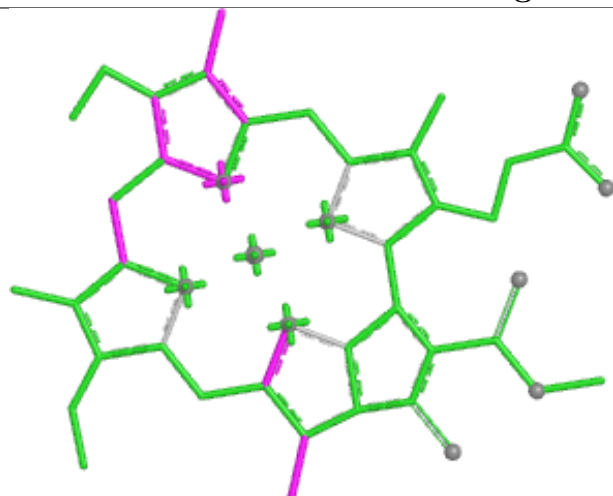
Torsions



Rings



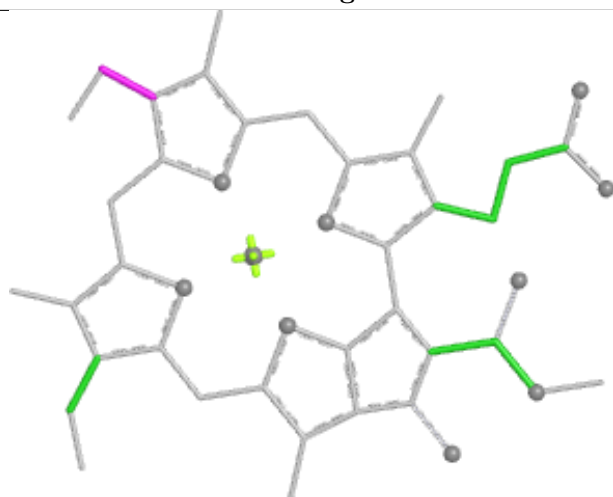
## Ligand CLA B 837



Bond lengths



Bond angles

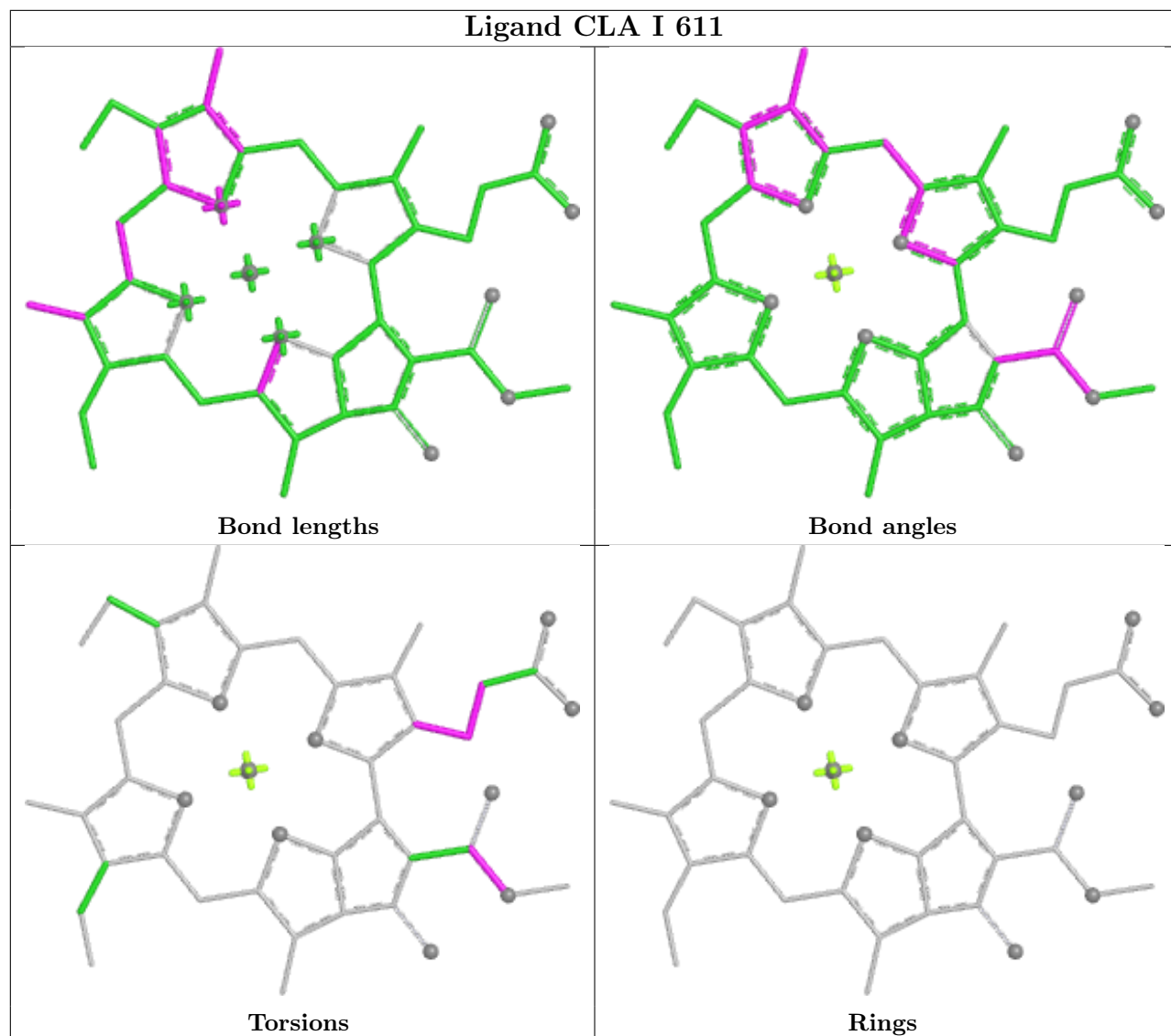


Torsions

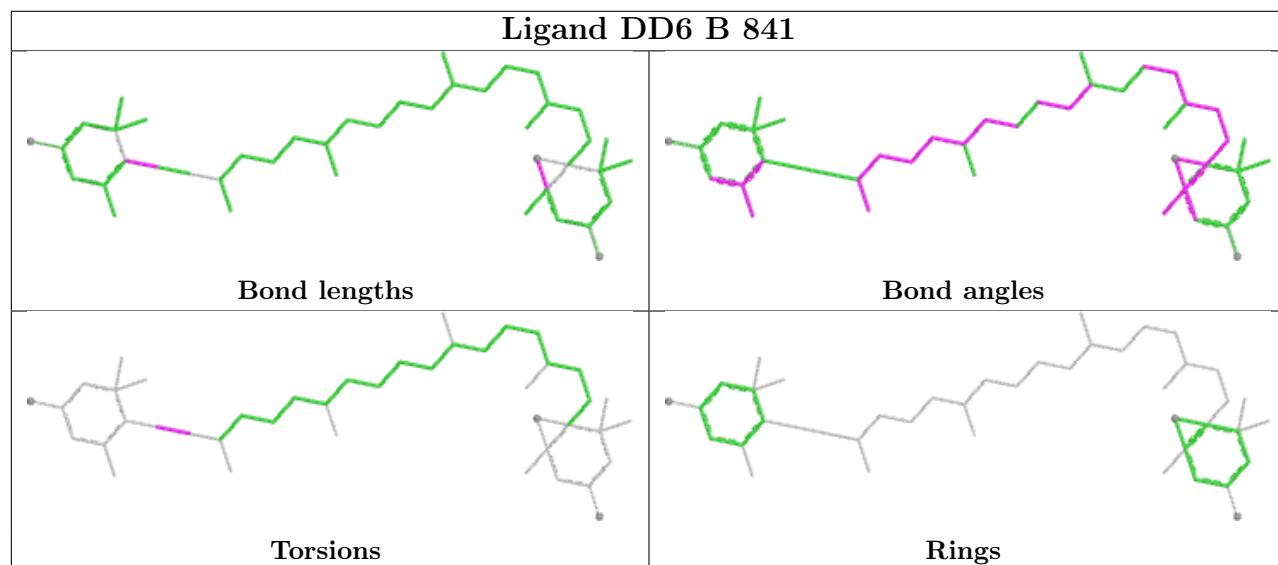


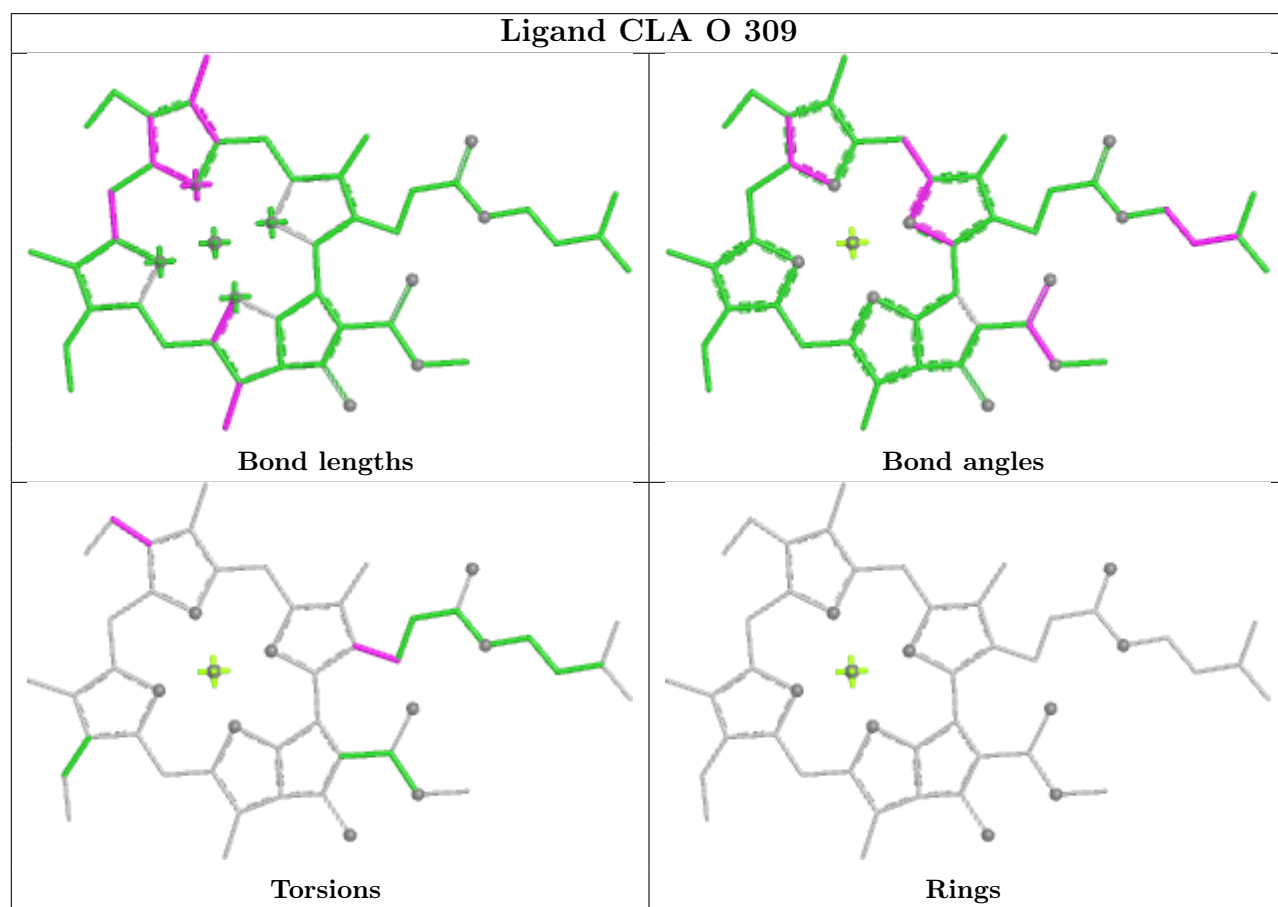
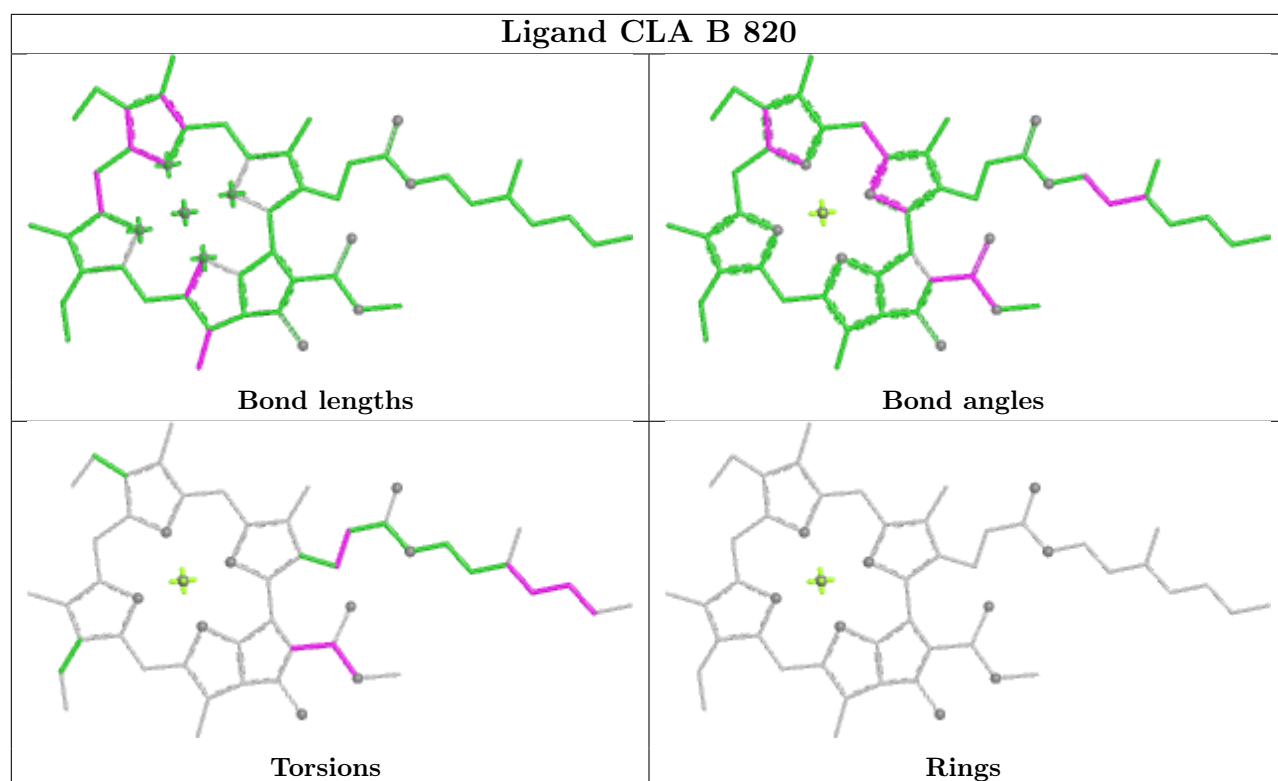
Rings

## Ligand CLA I 611

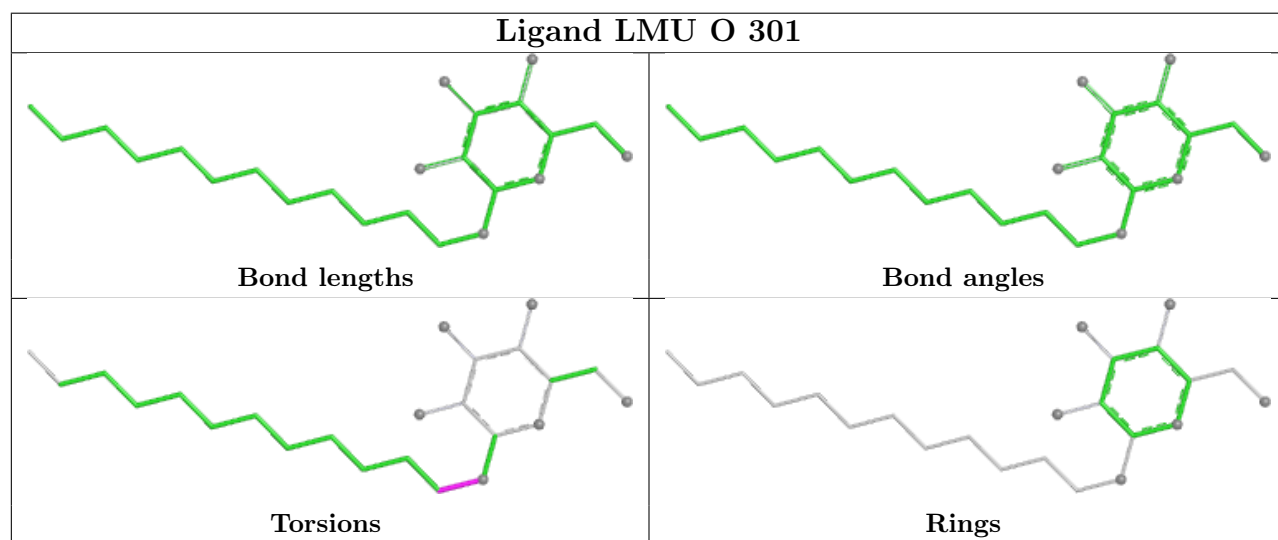
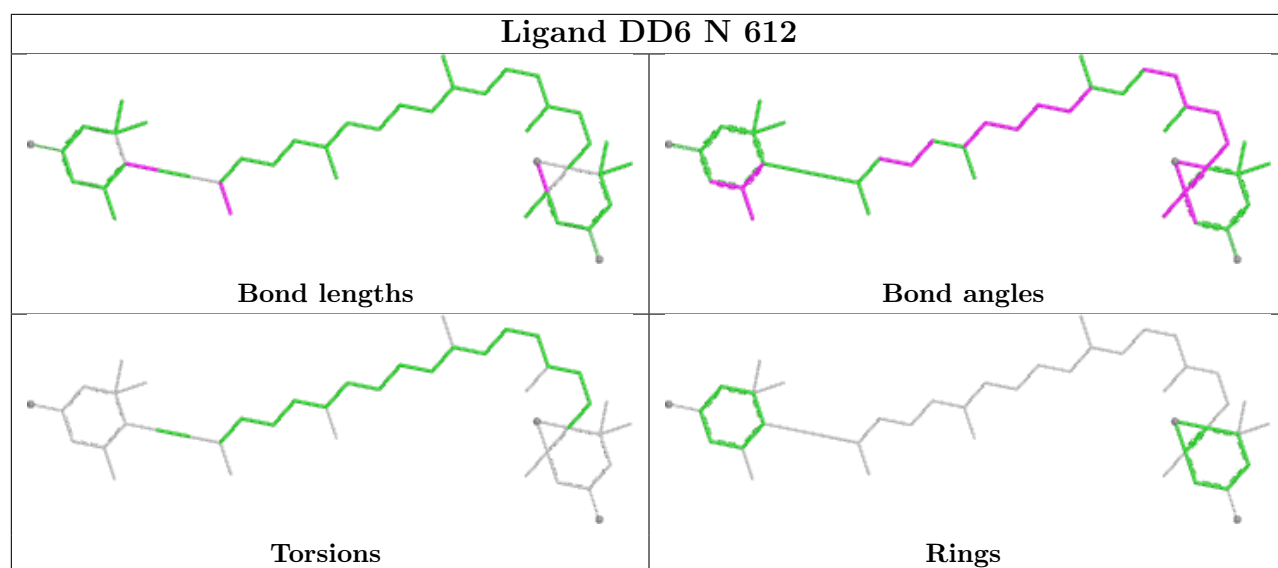


## Ligand DD6 B 841

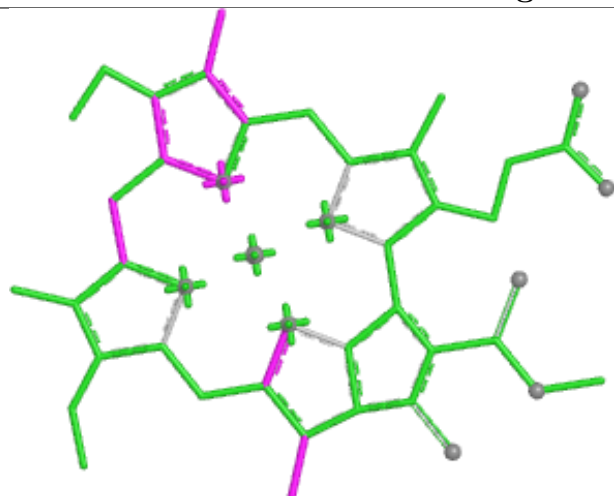




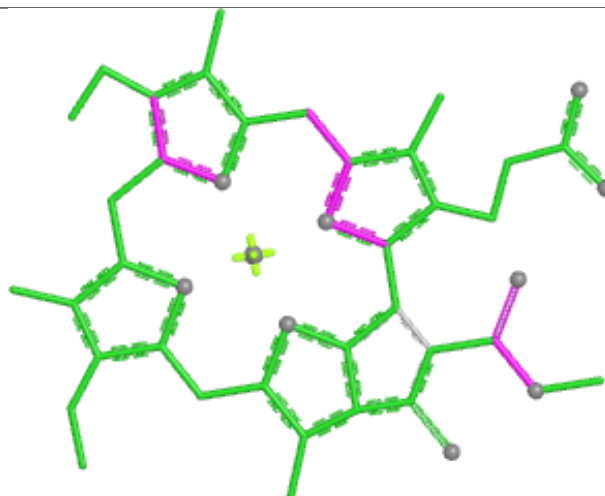




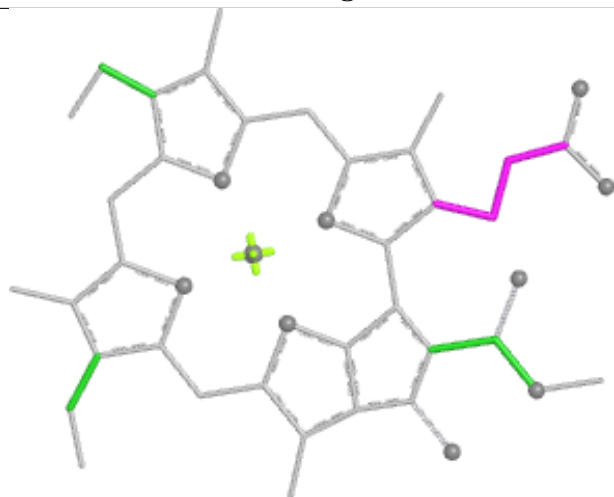
## Ligand CLA L 412



Bond lengths



Bond angles

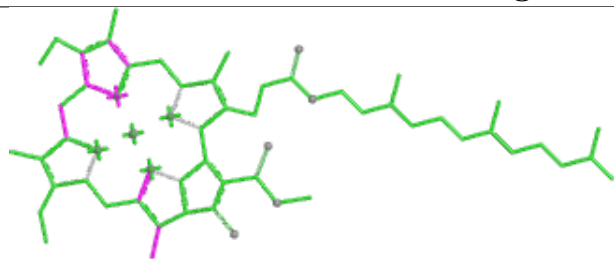


Torsions

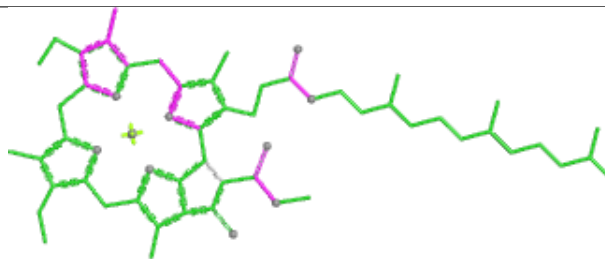


Rings

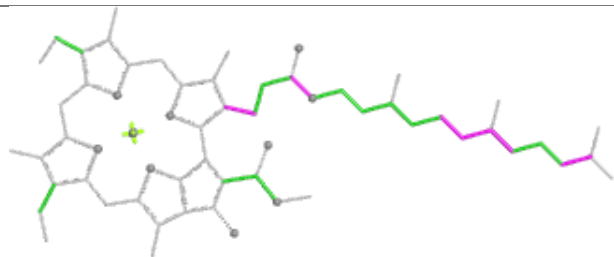
## Ligand CLA H 305



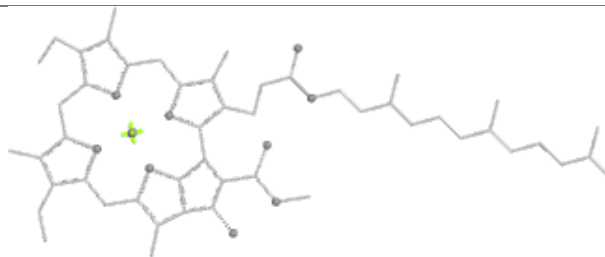
Bond lengths



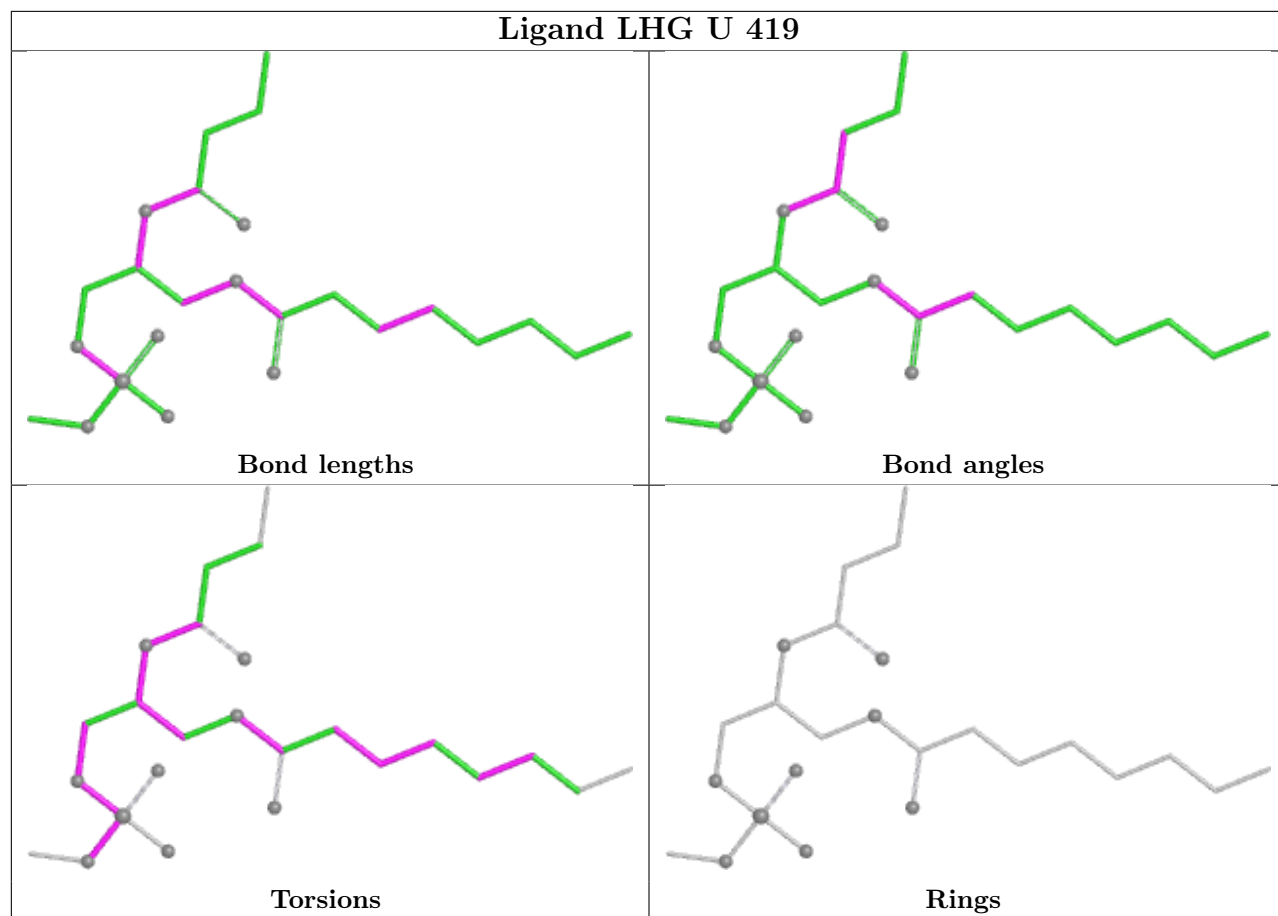
Bond angles



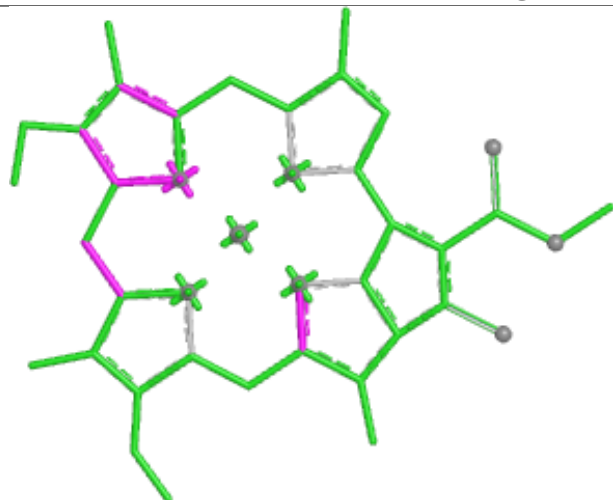
Torsions



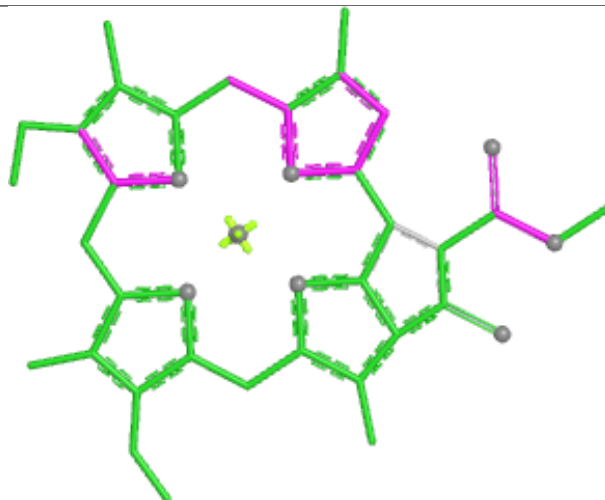
Rings



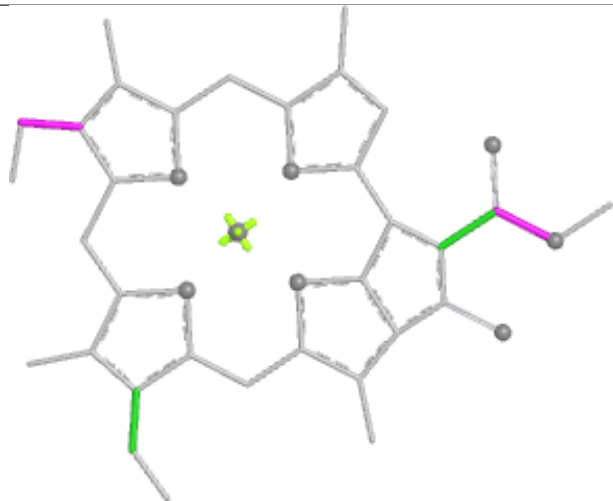
## Ligand CLA N 611



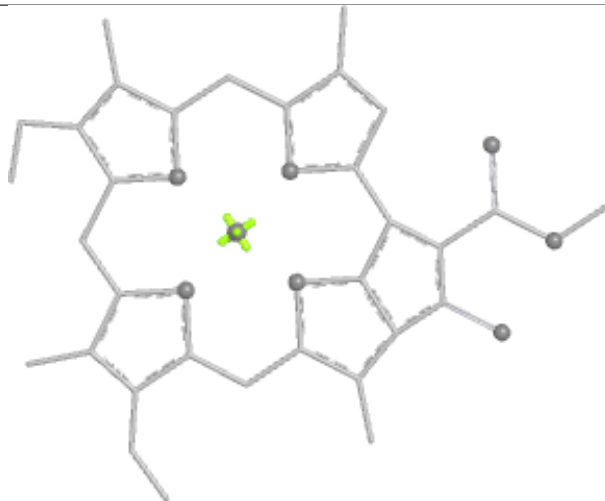
Bond lengths



Bond angles

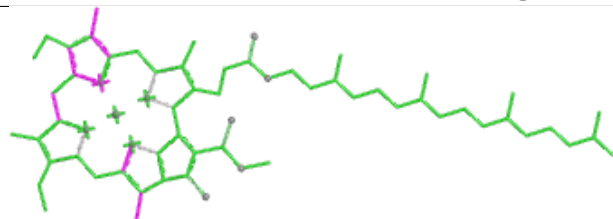


Torsions

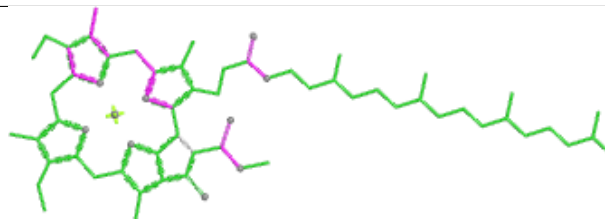


Rings

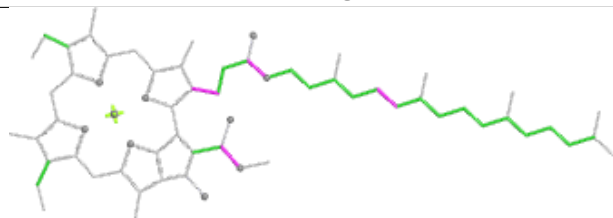
## Ligand CLA B 827



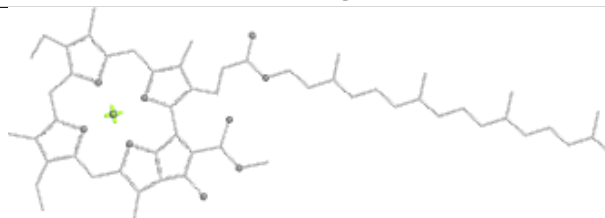
Bond lengths



Bond angles

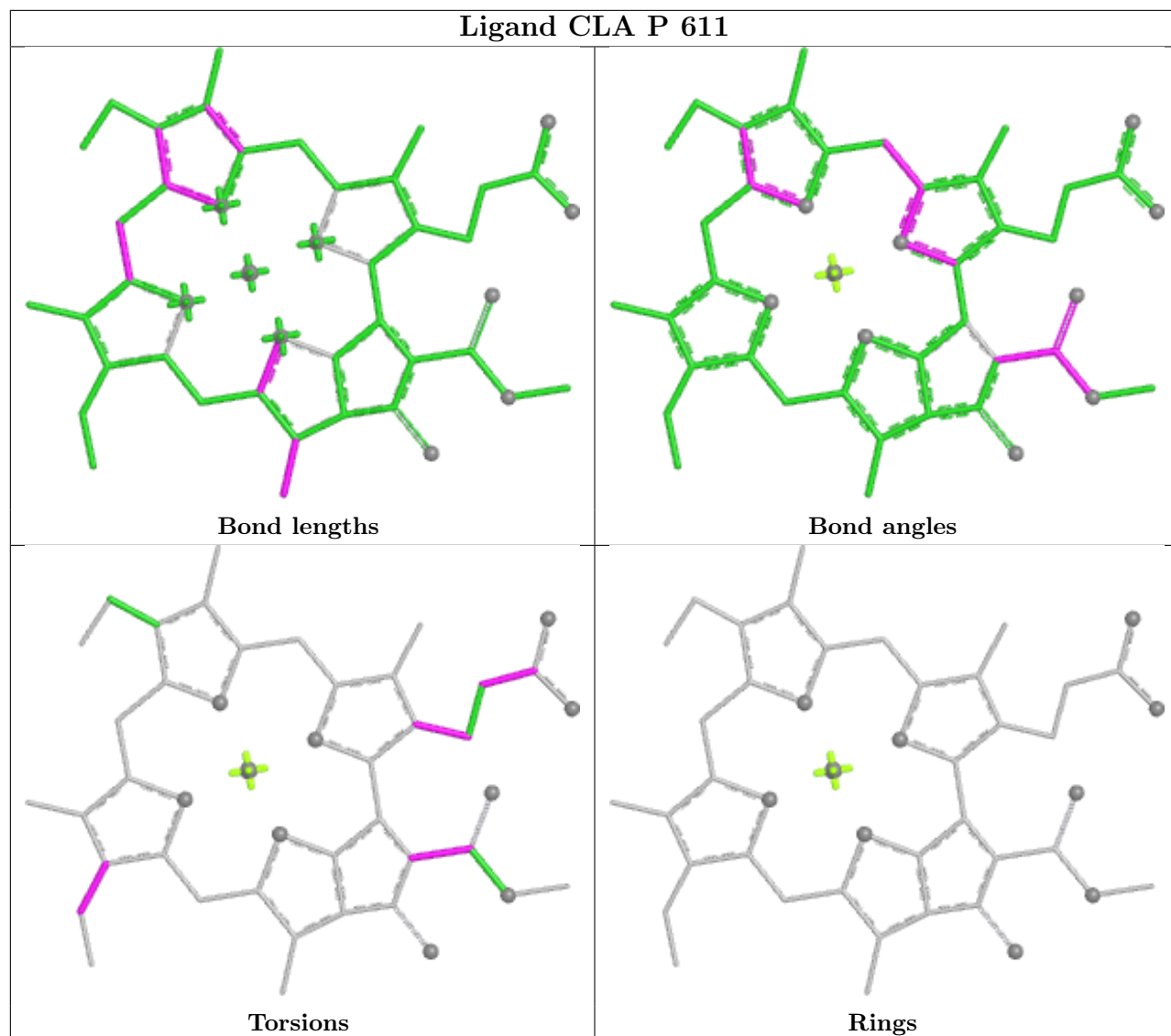


Torsions

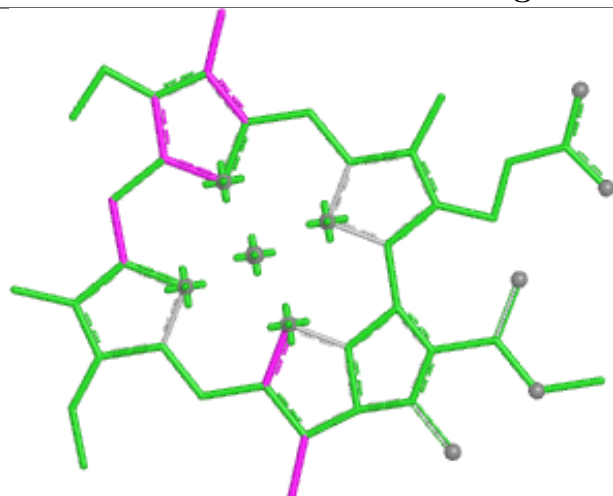


Rings

## Ligand CLA P 611



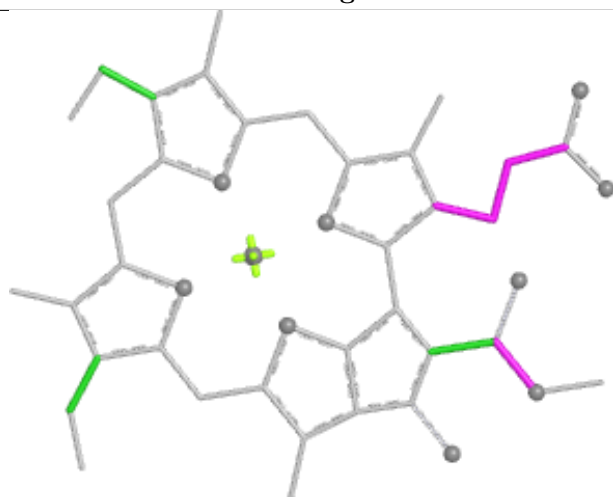
## Ligand CLA A 823



Bond lengths



Bond angles

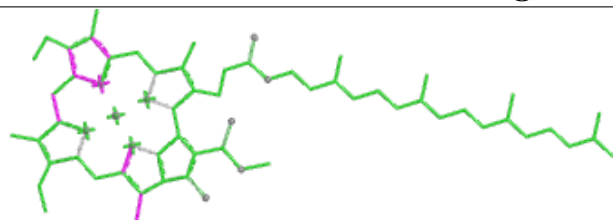


Torsions

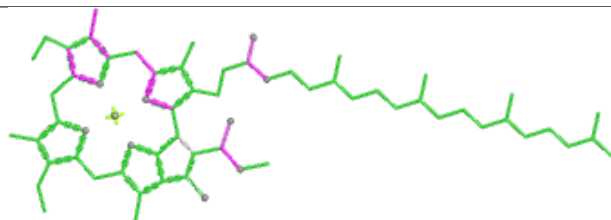


Rings

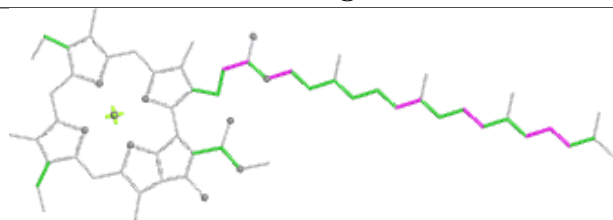
## Ligand CLA N 603



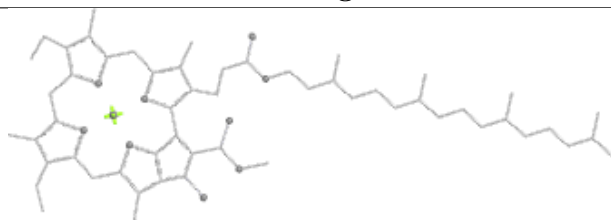
Bond lengths



Bond angles

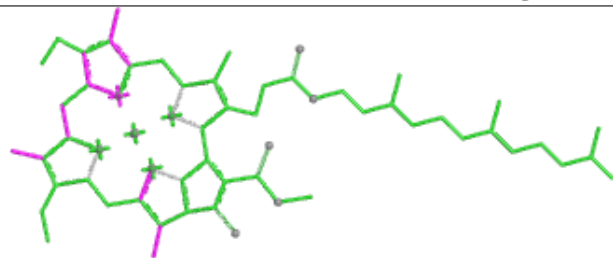


Torsions

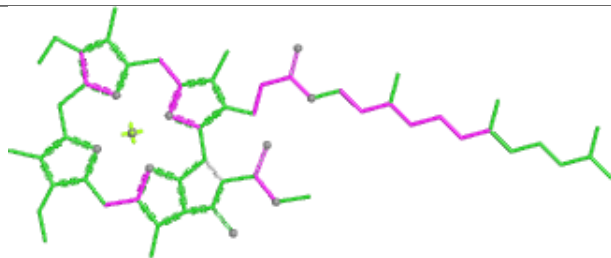


Rings

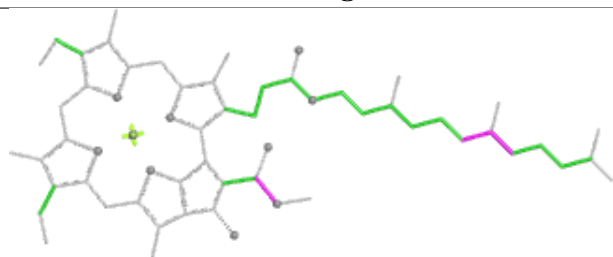
## Ligand CLA L 408



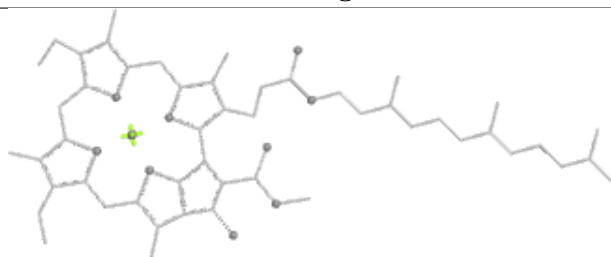
Bond lengths



Bond angles

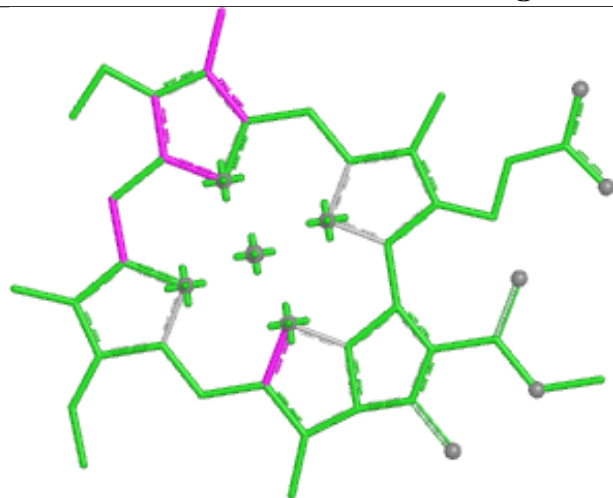


Torsions

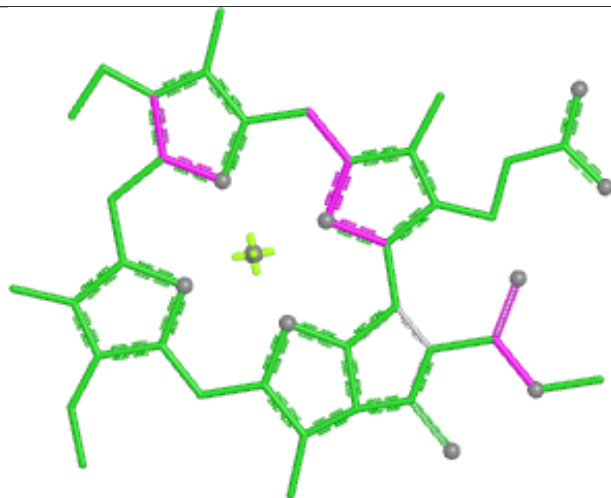


Rings

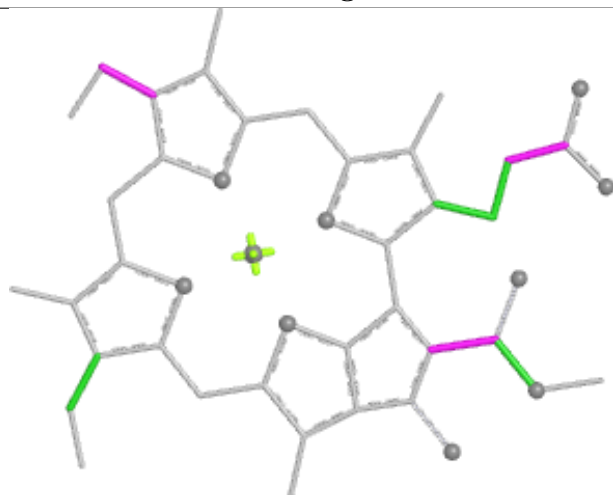
## Ligand CLA P 603



Bond lengths



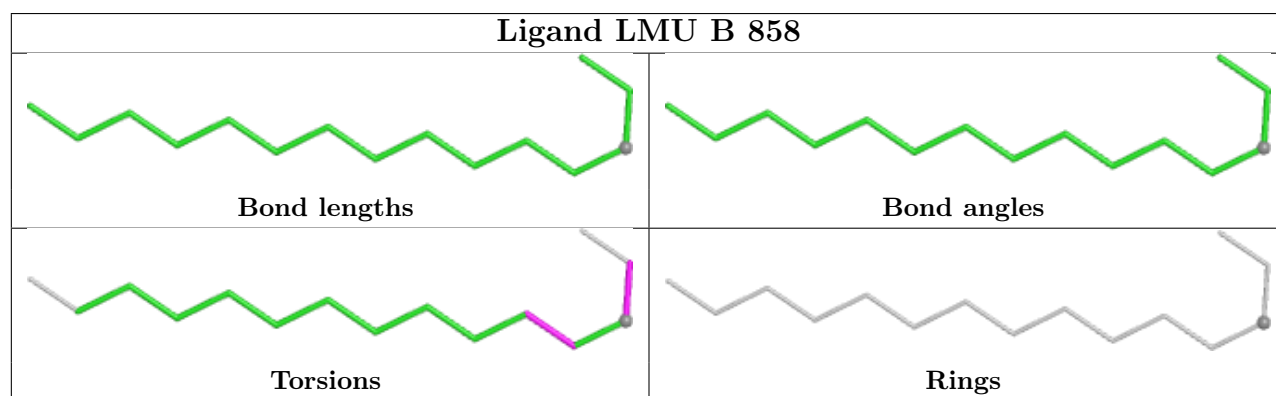
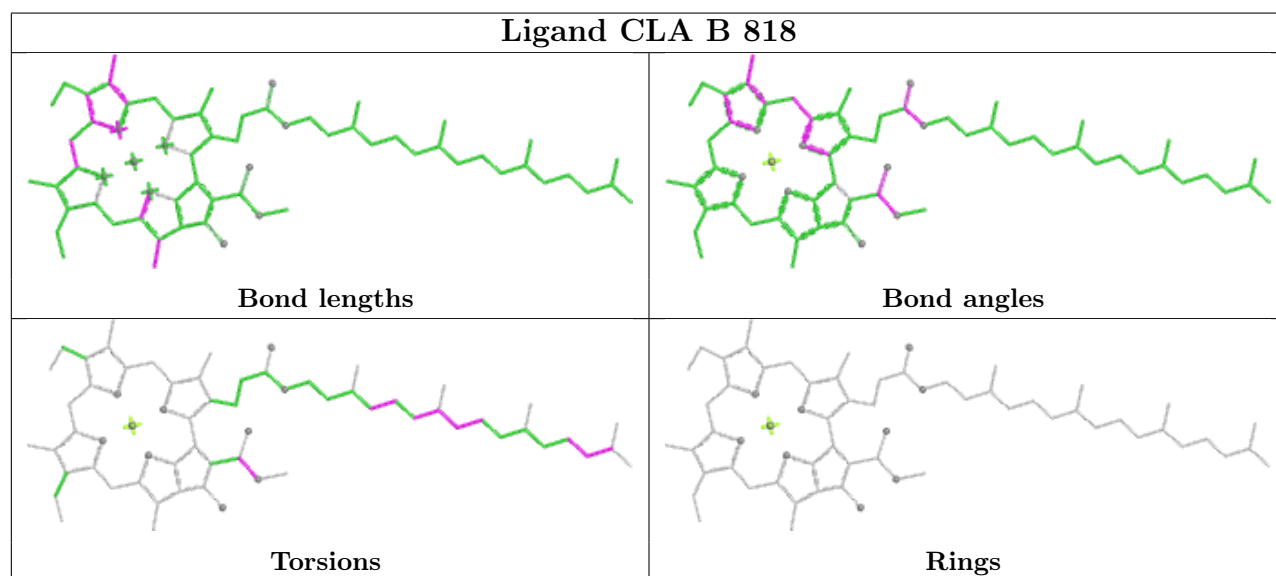
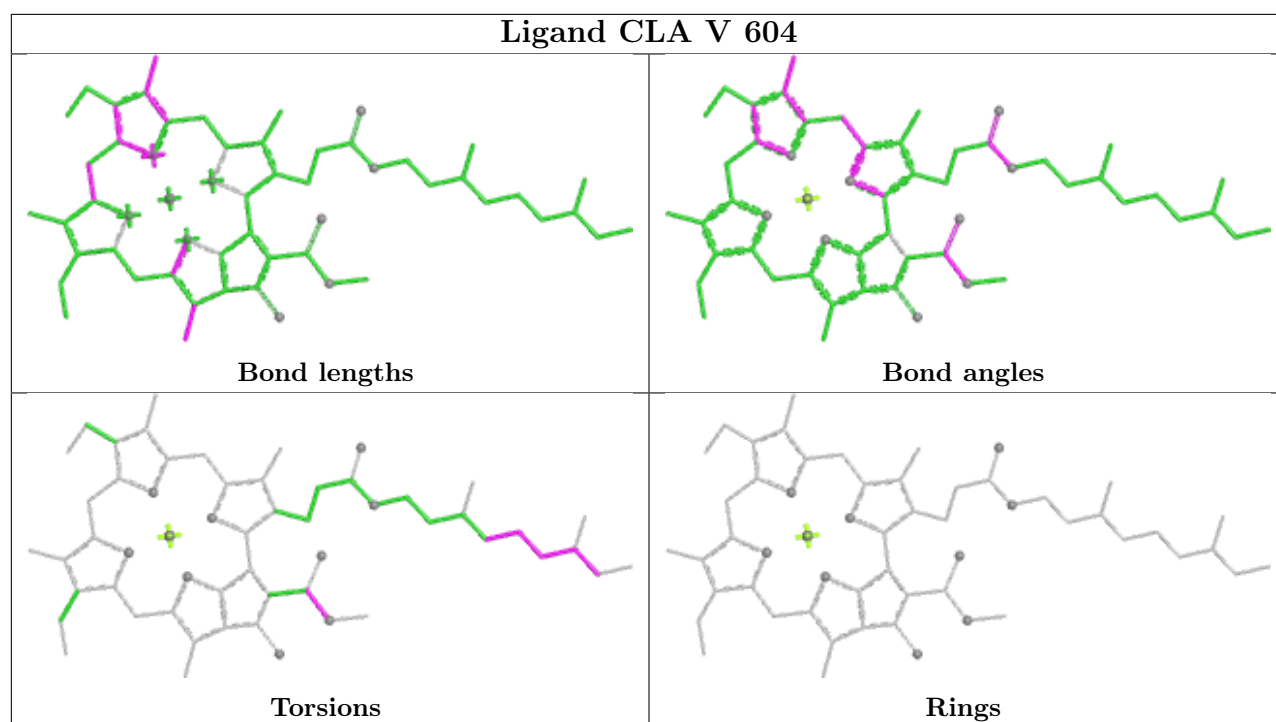
Bond angles



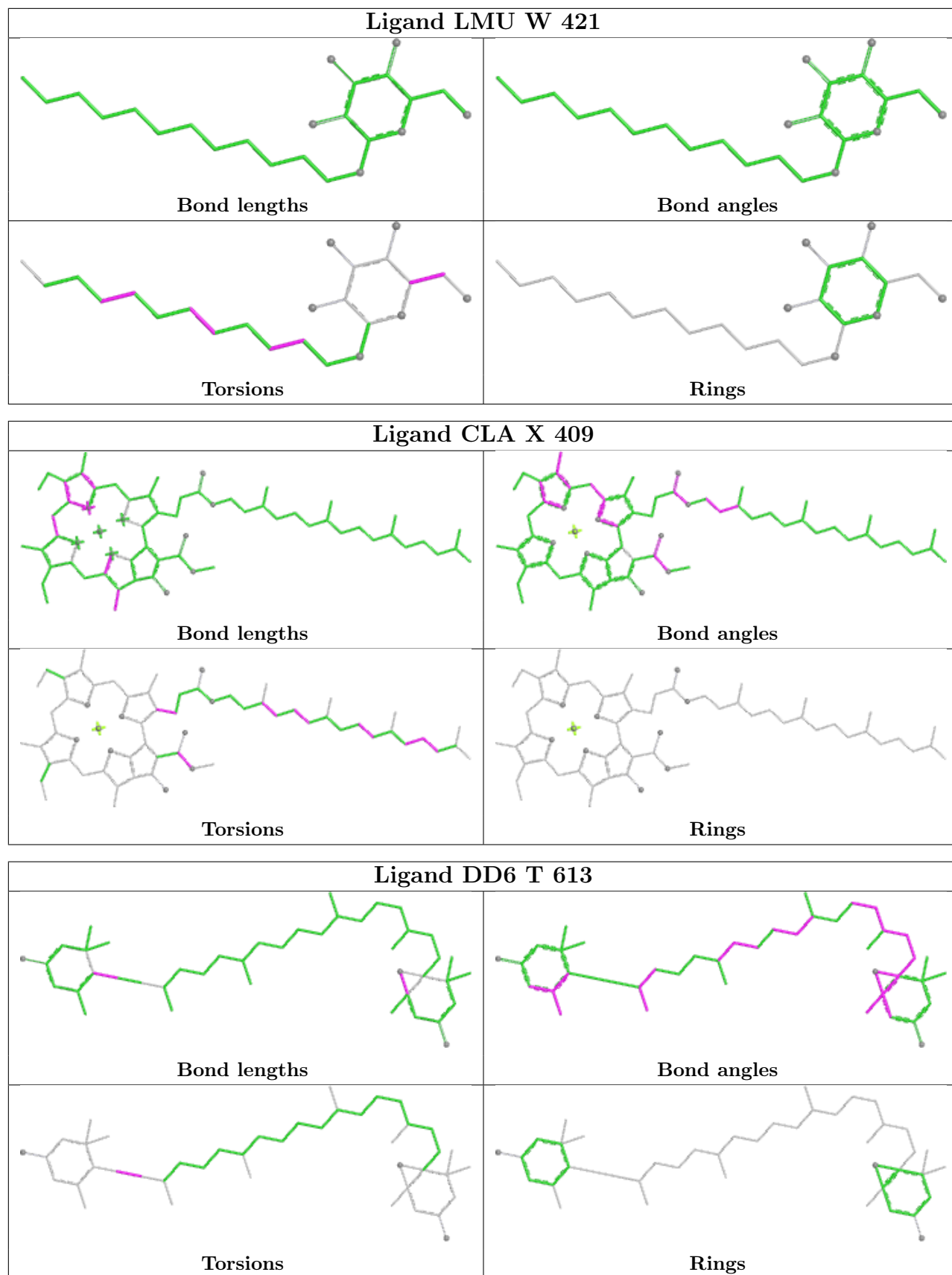
Torsions

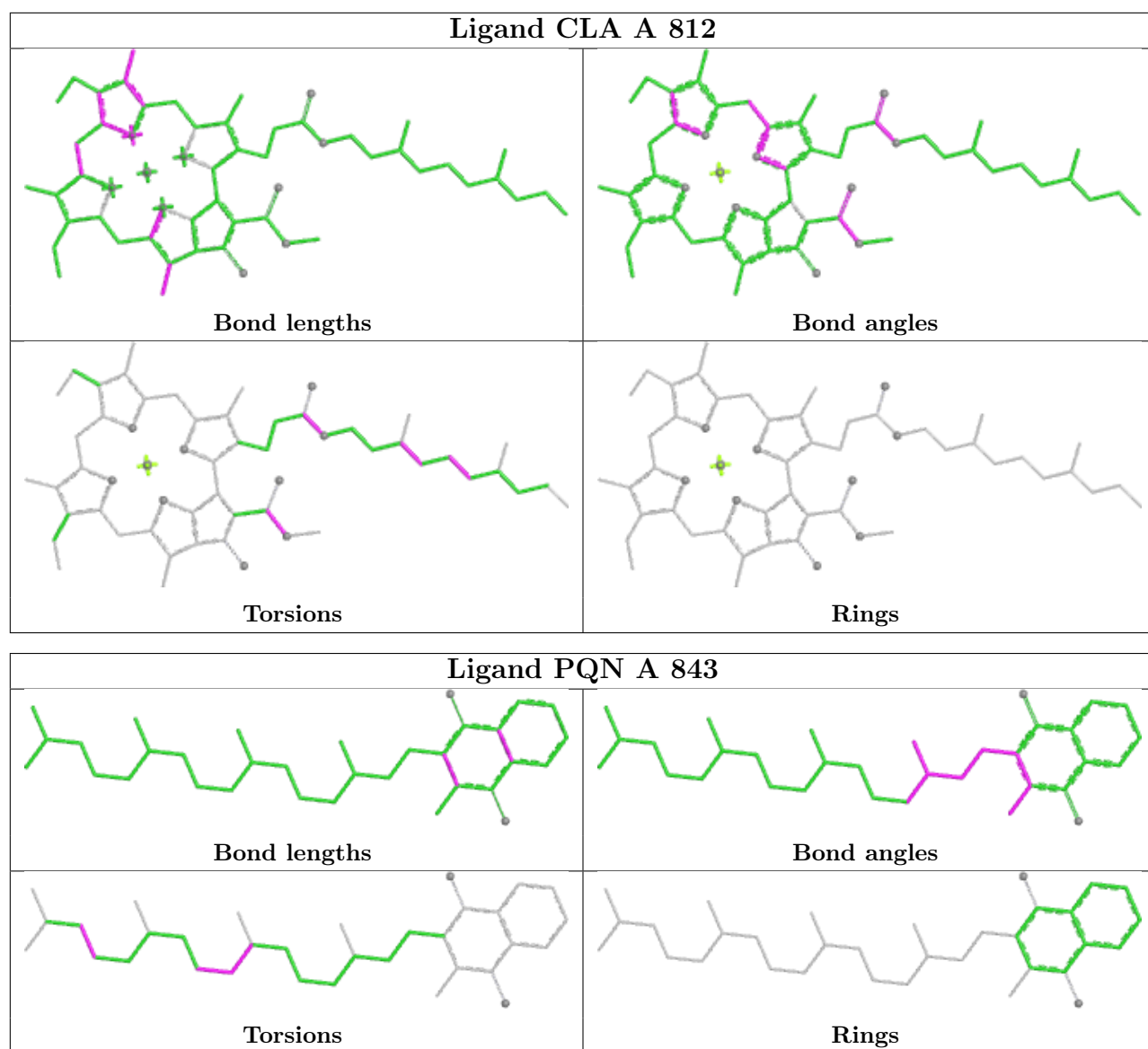


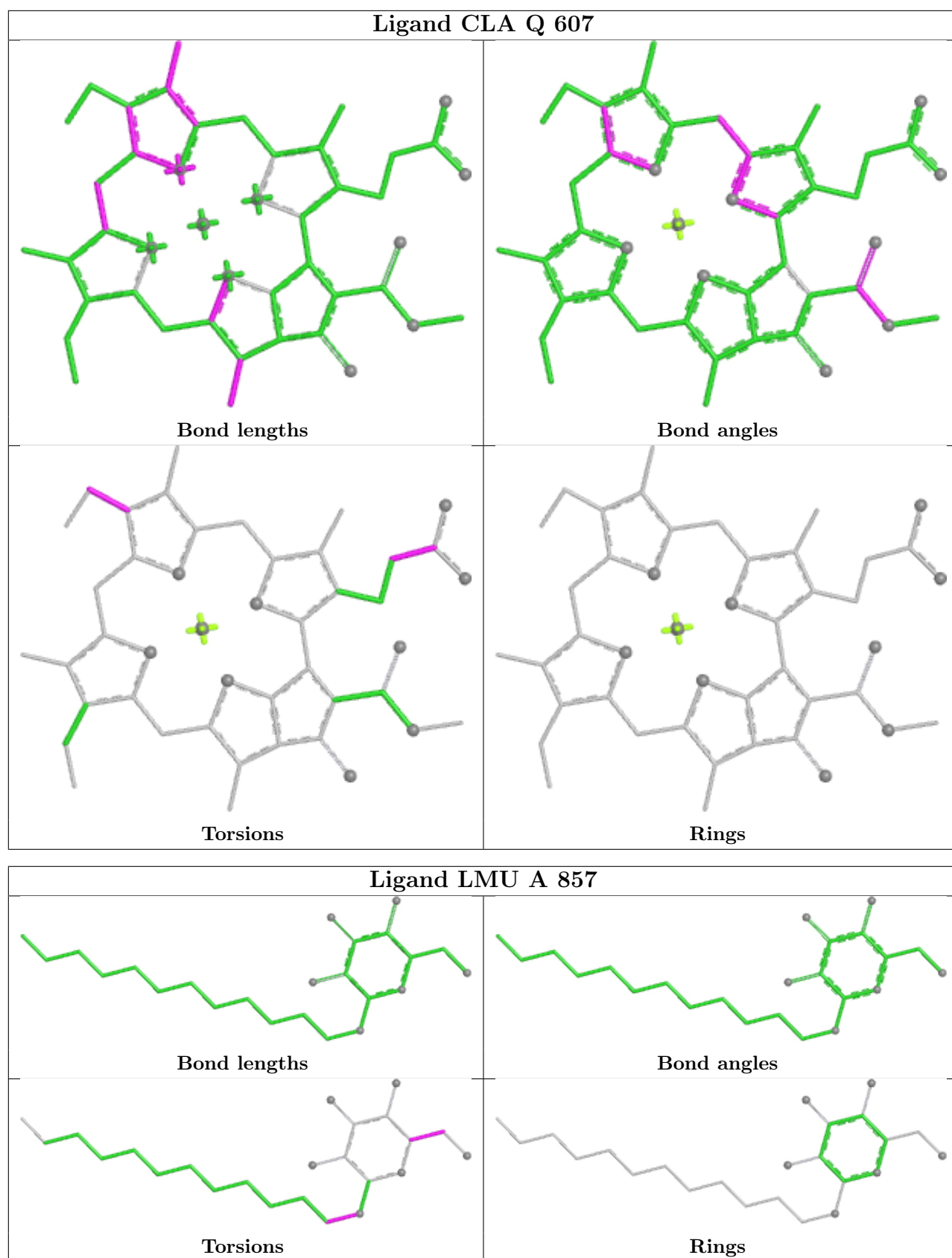
Rings

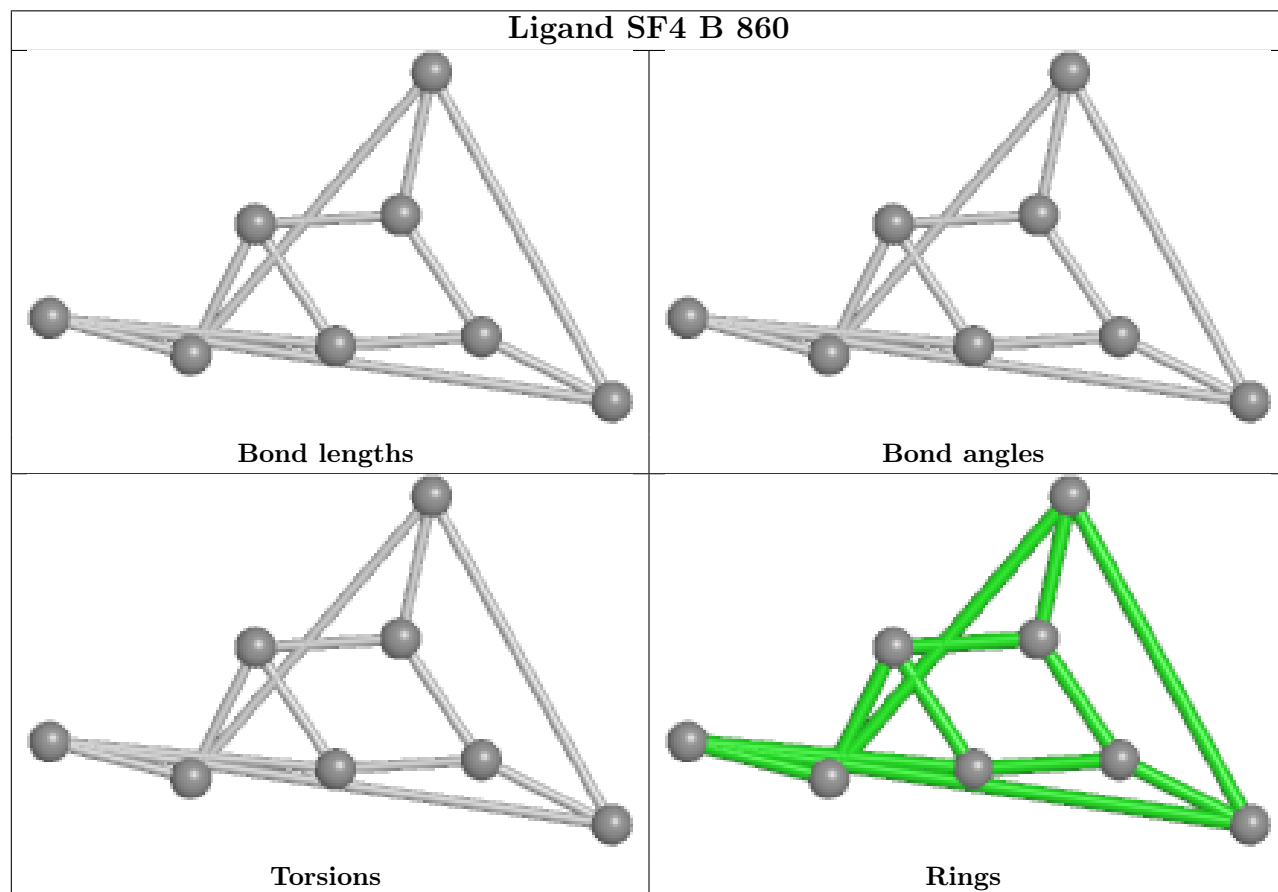
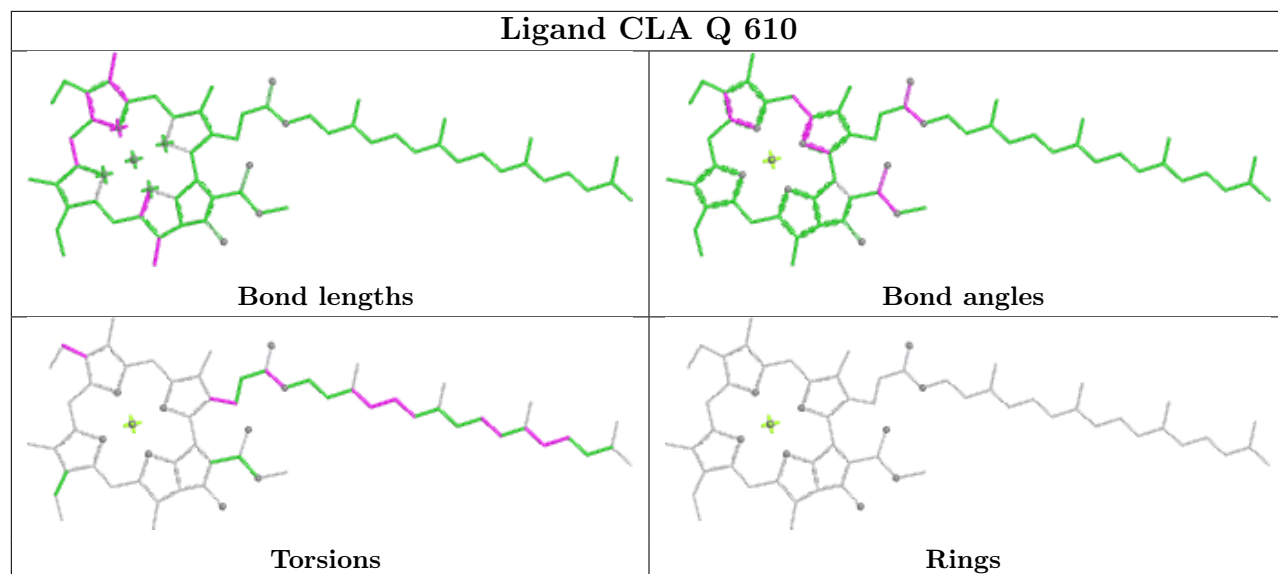


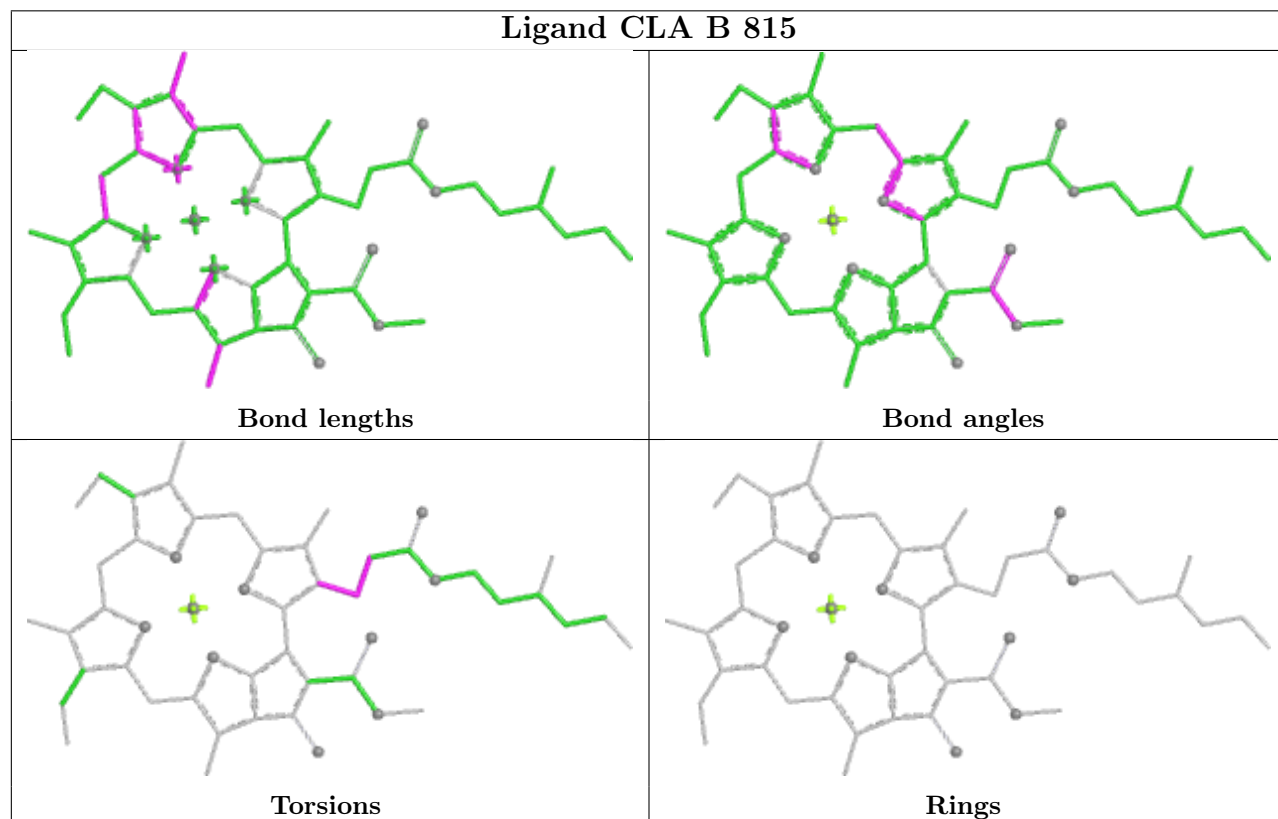
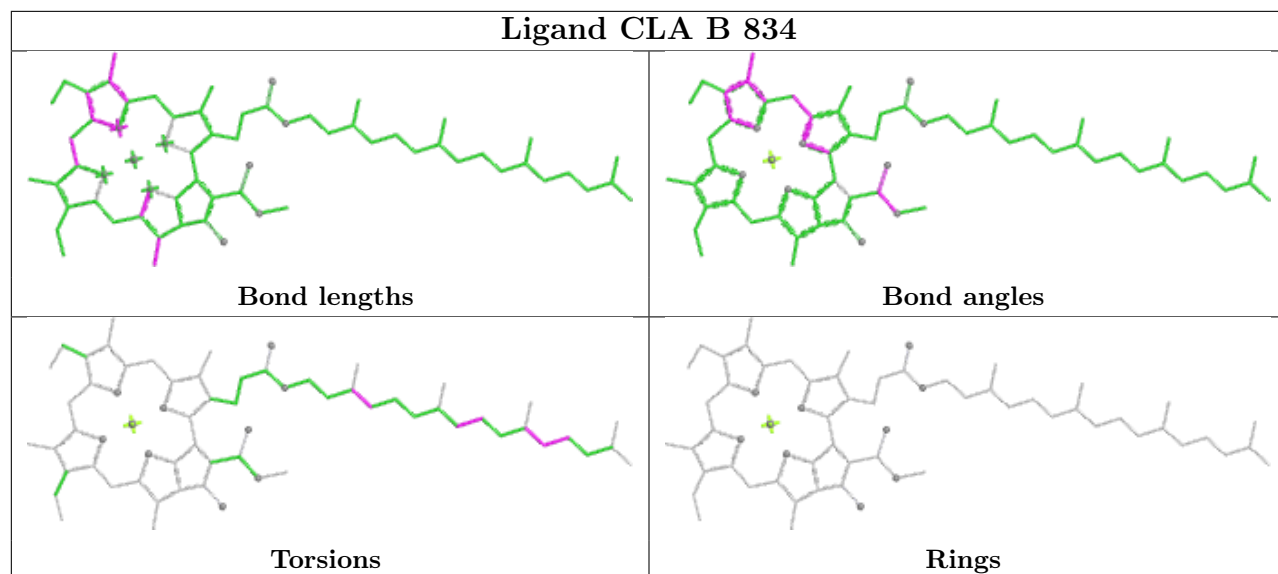


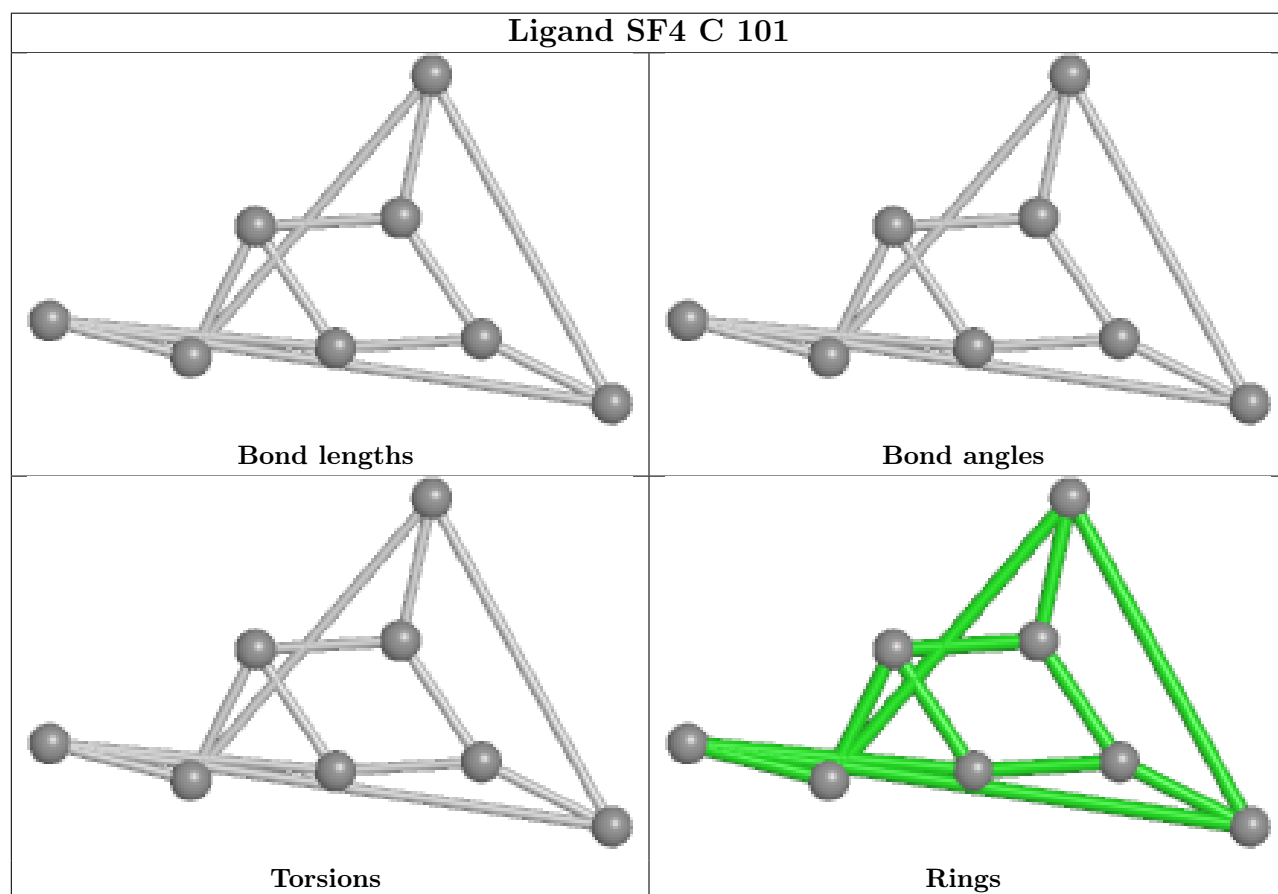
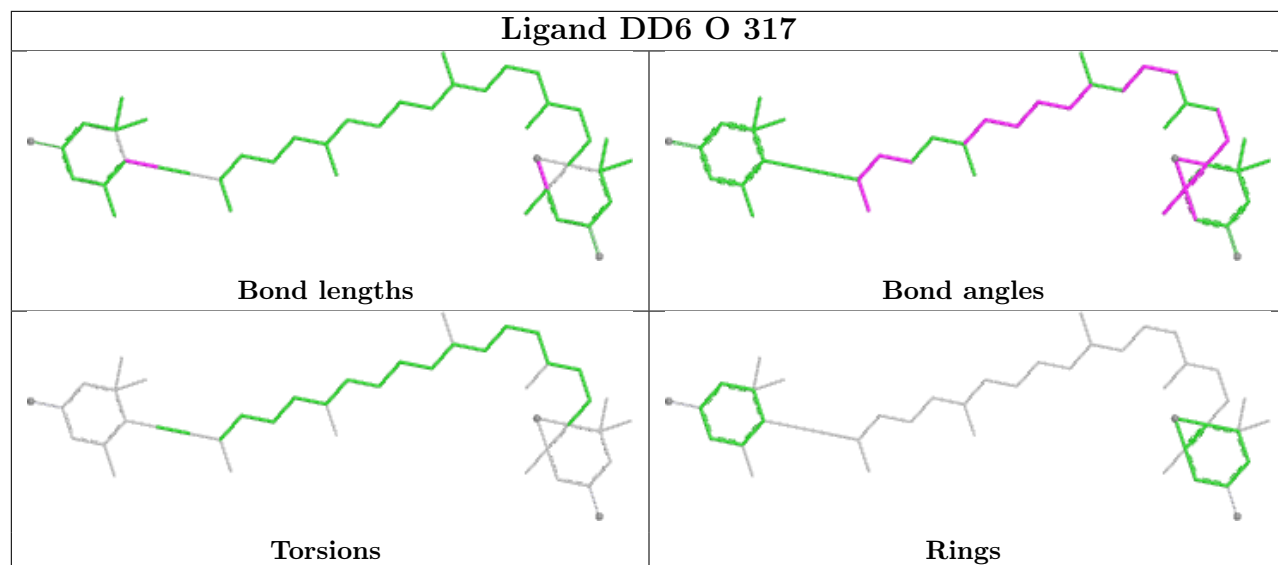


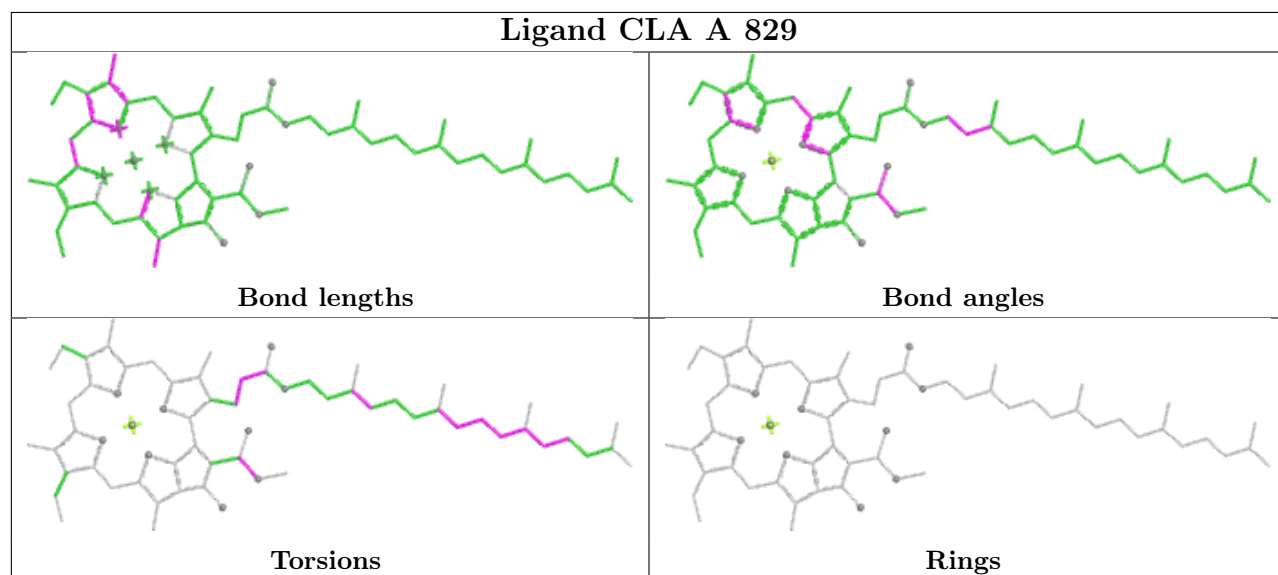
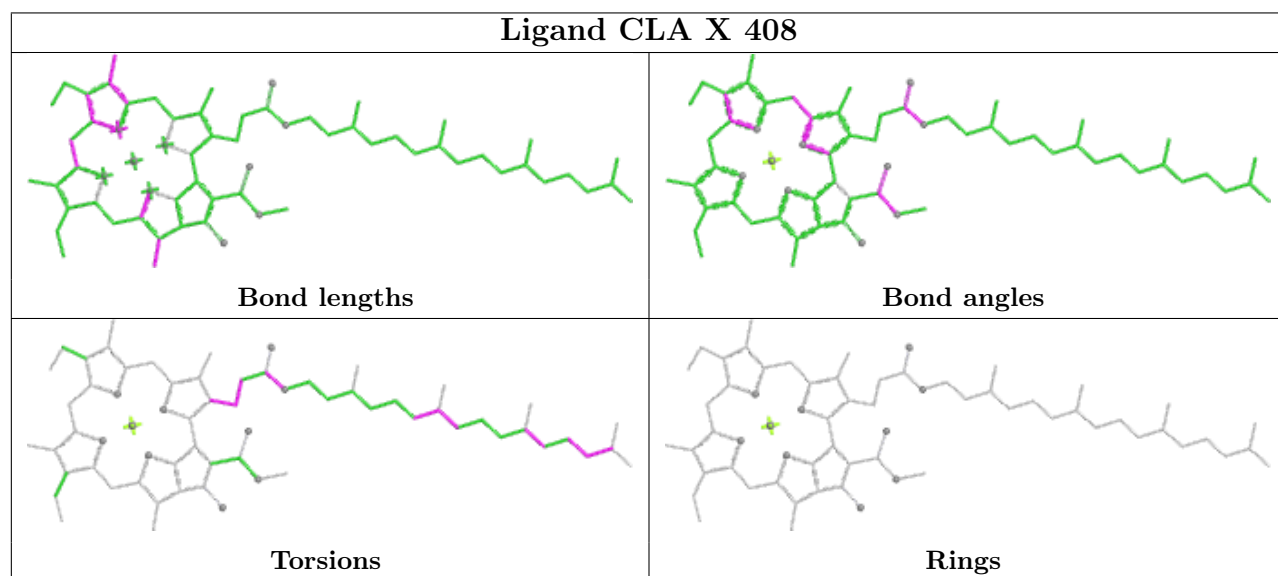
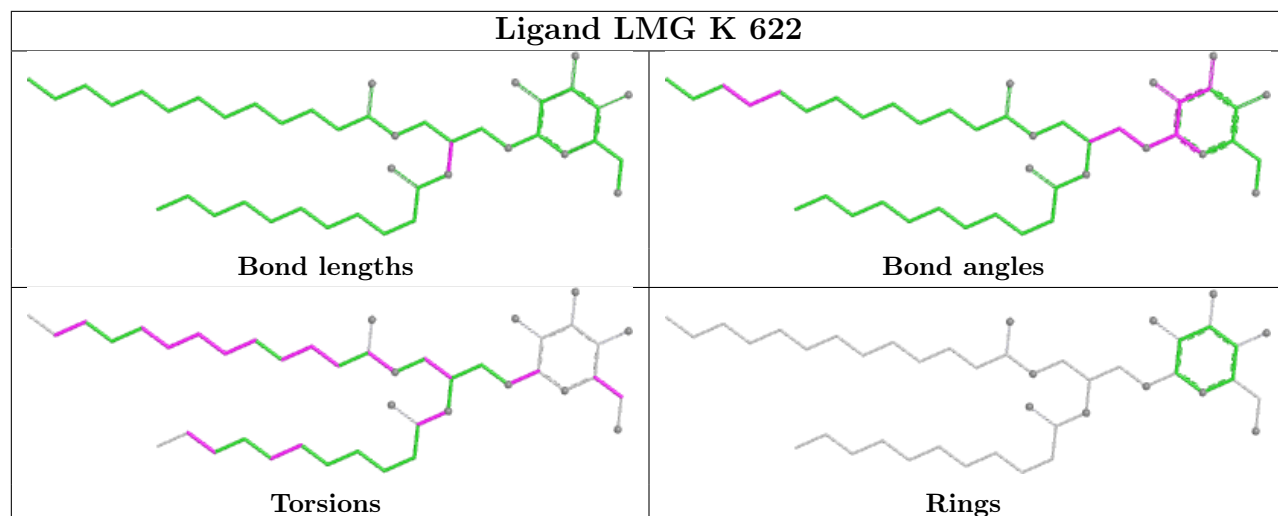


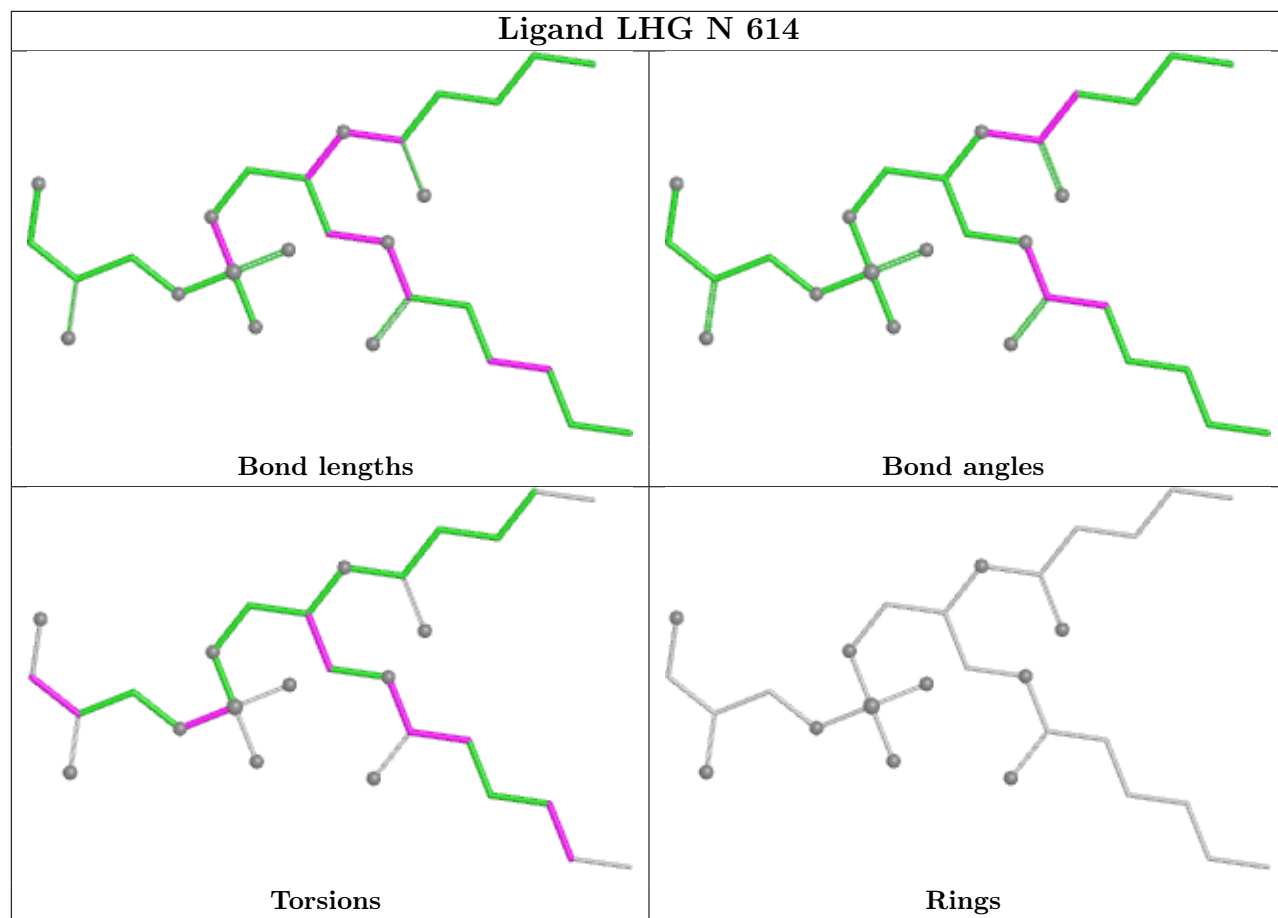




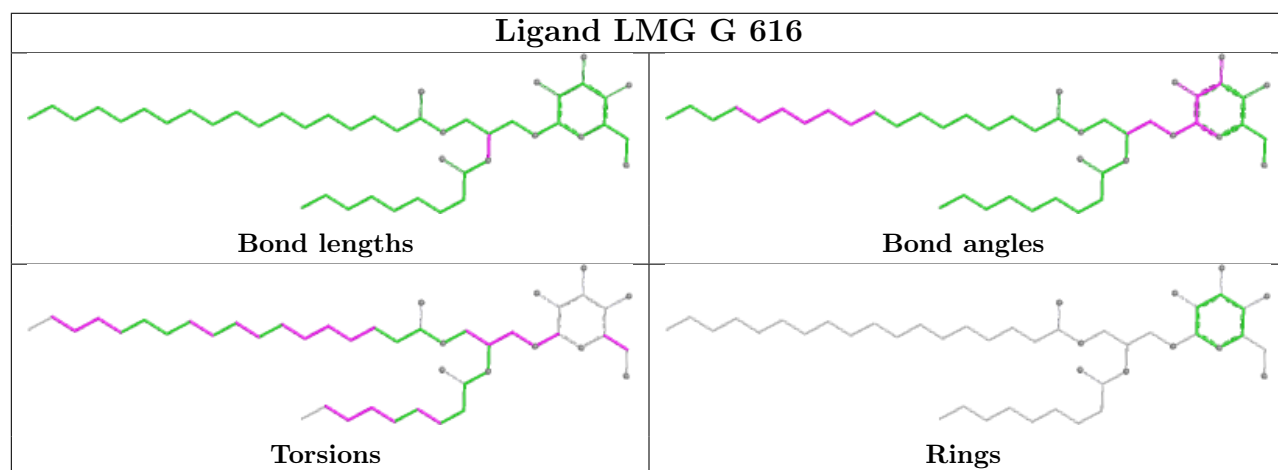
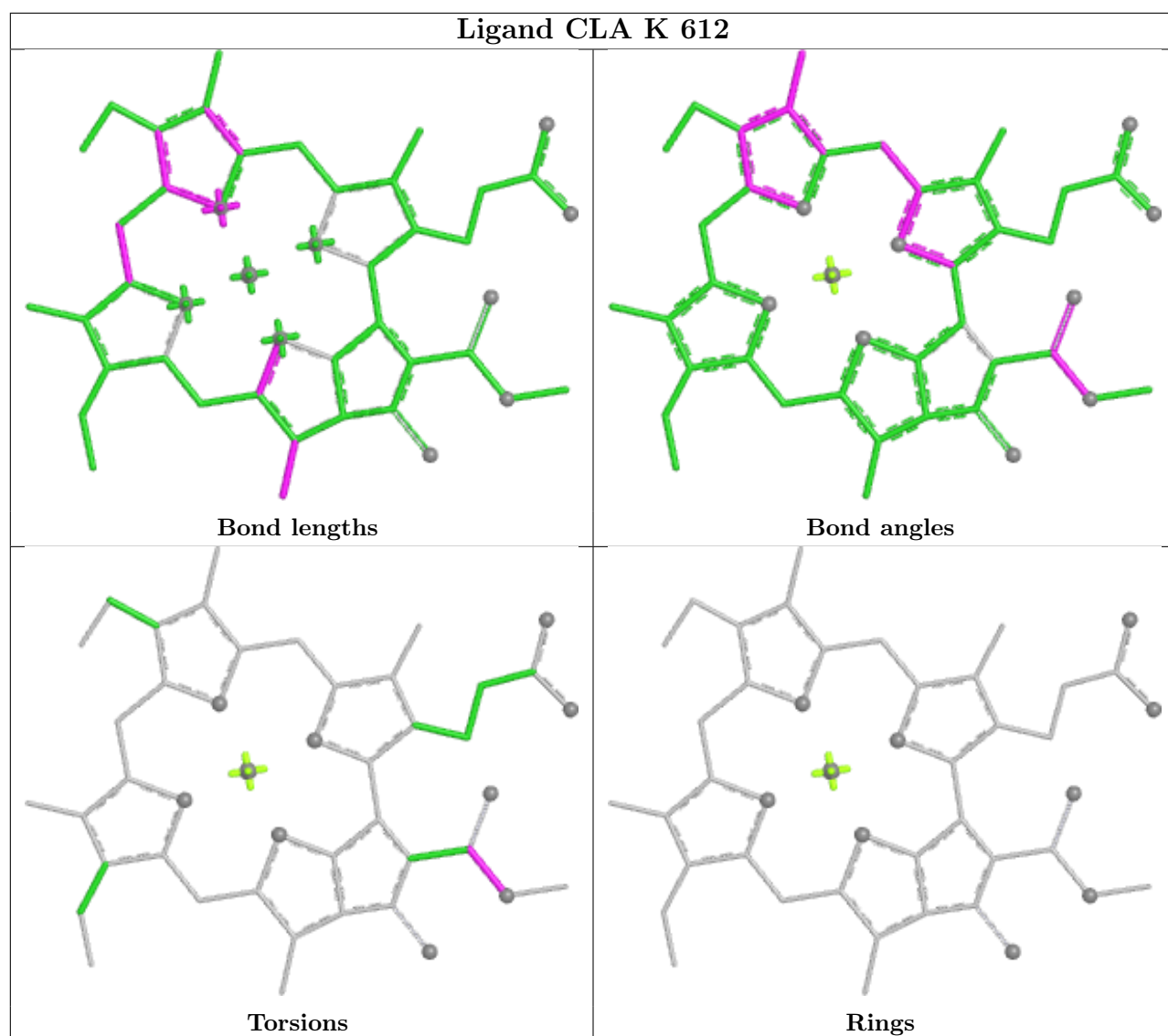


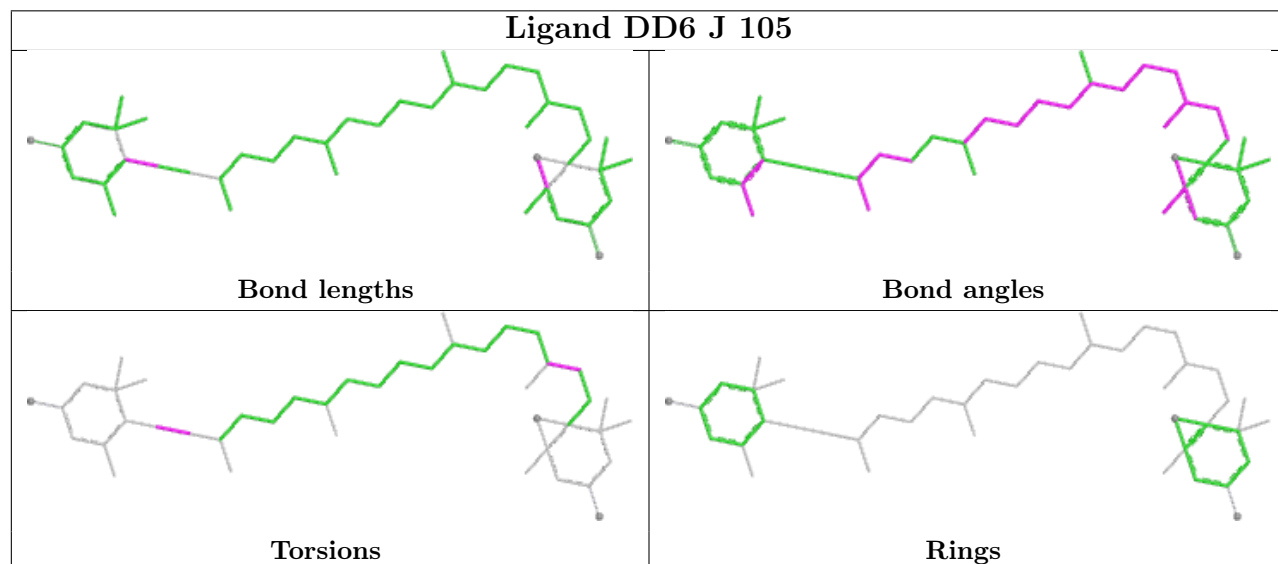
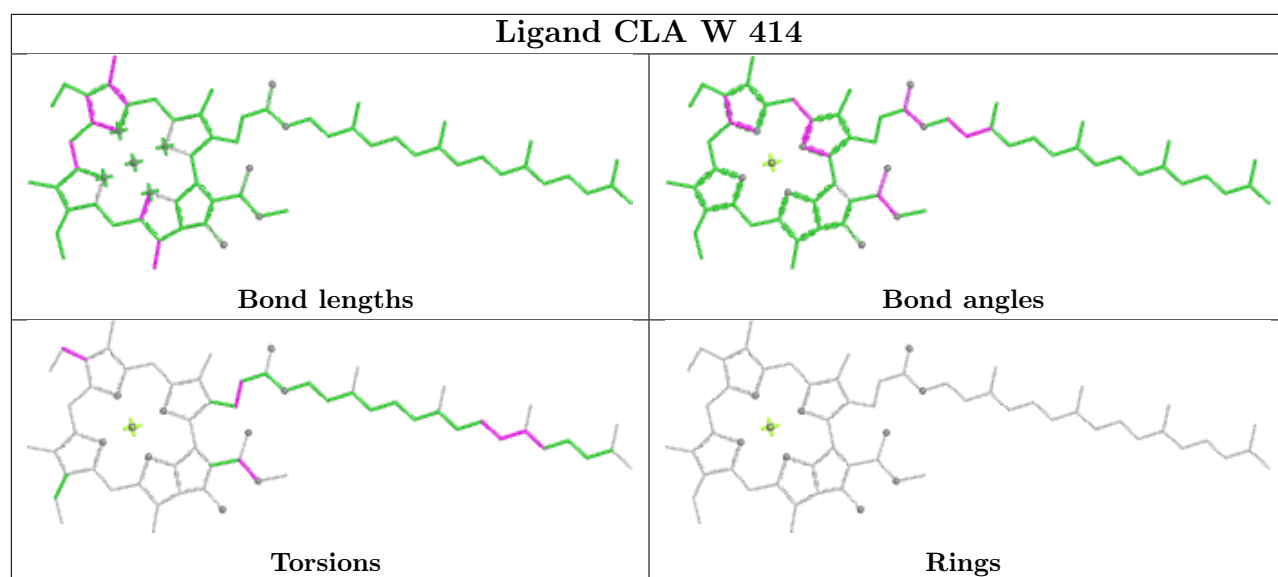


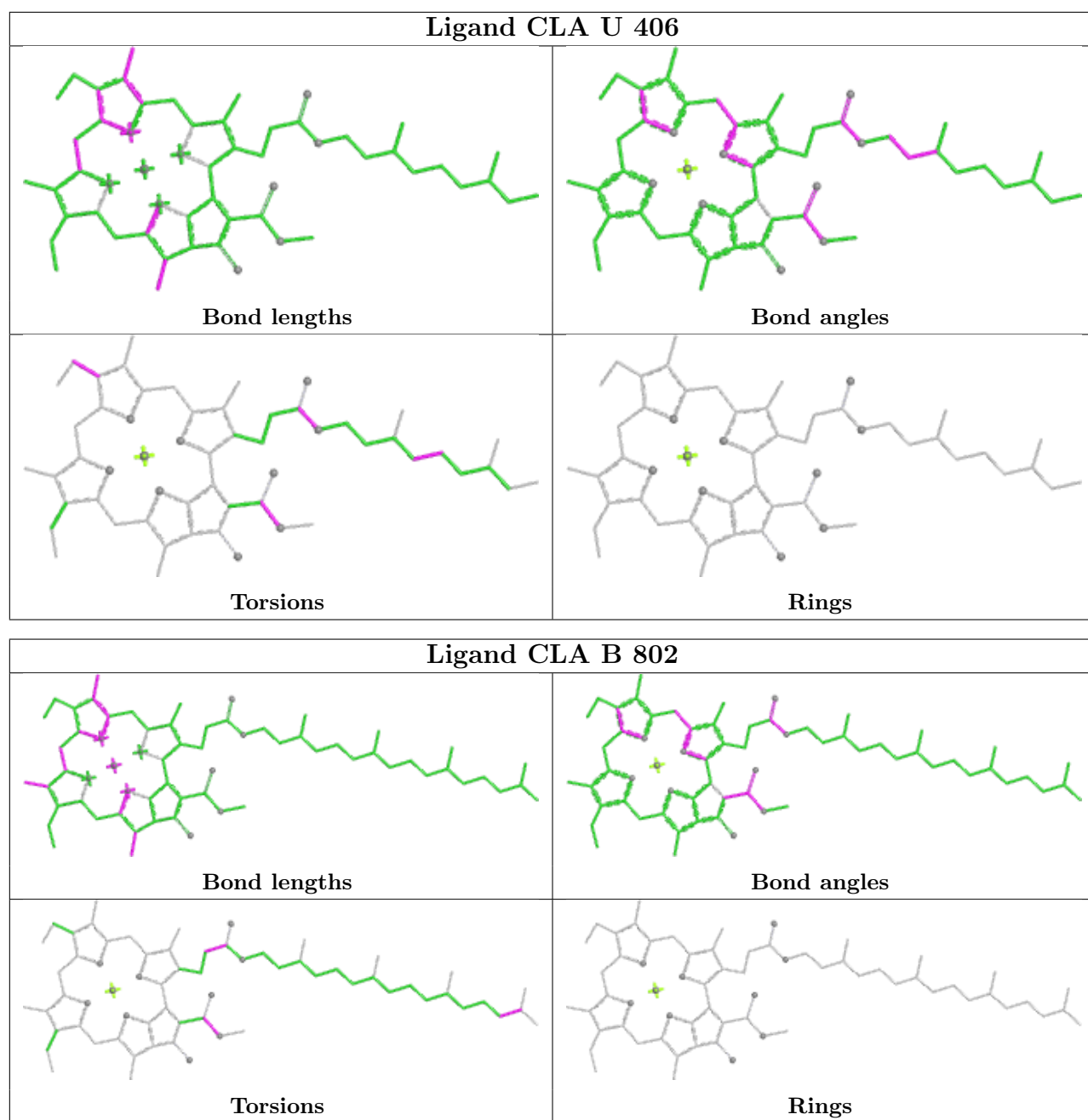


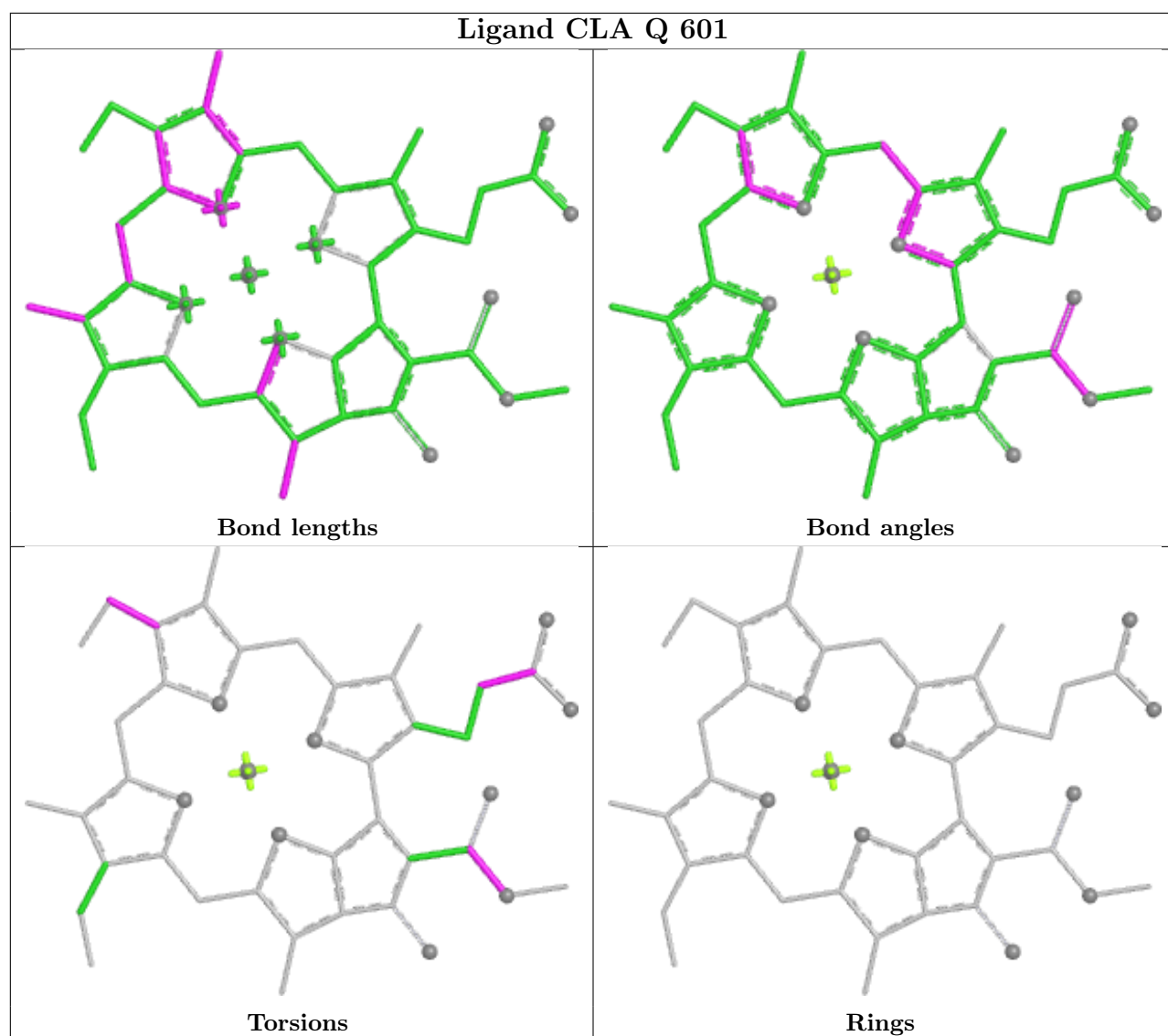


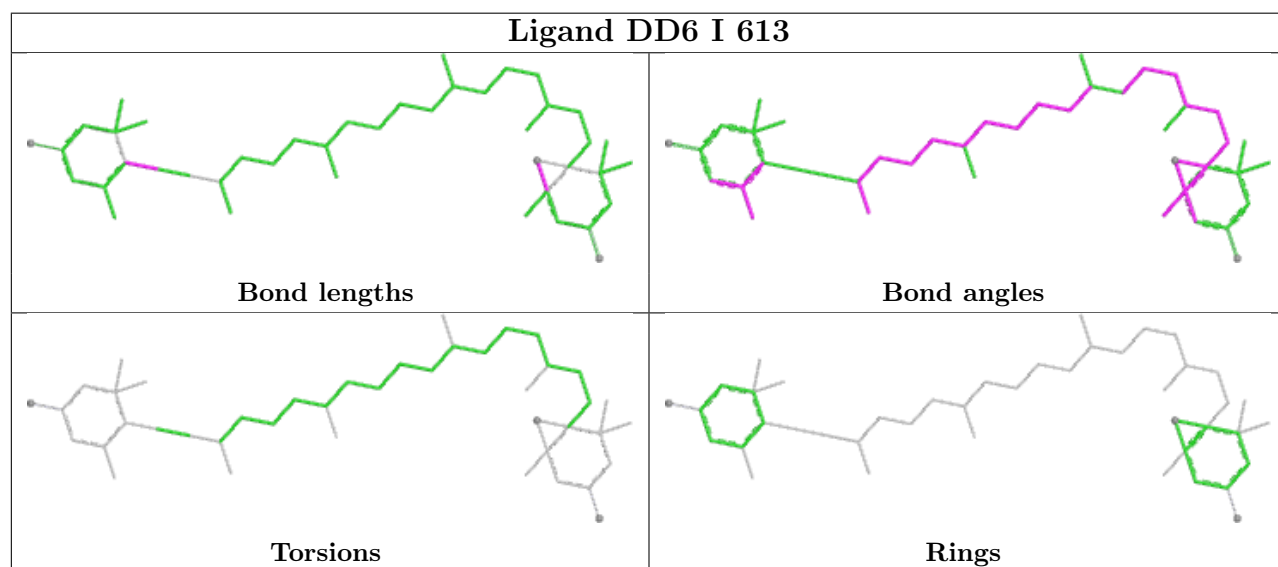
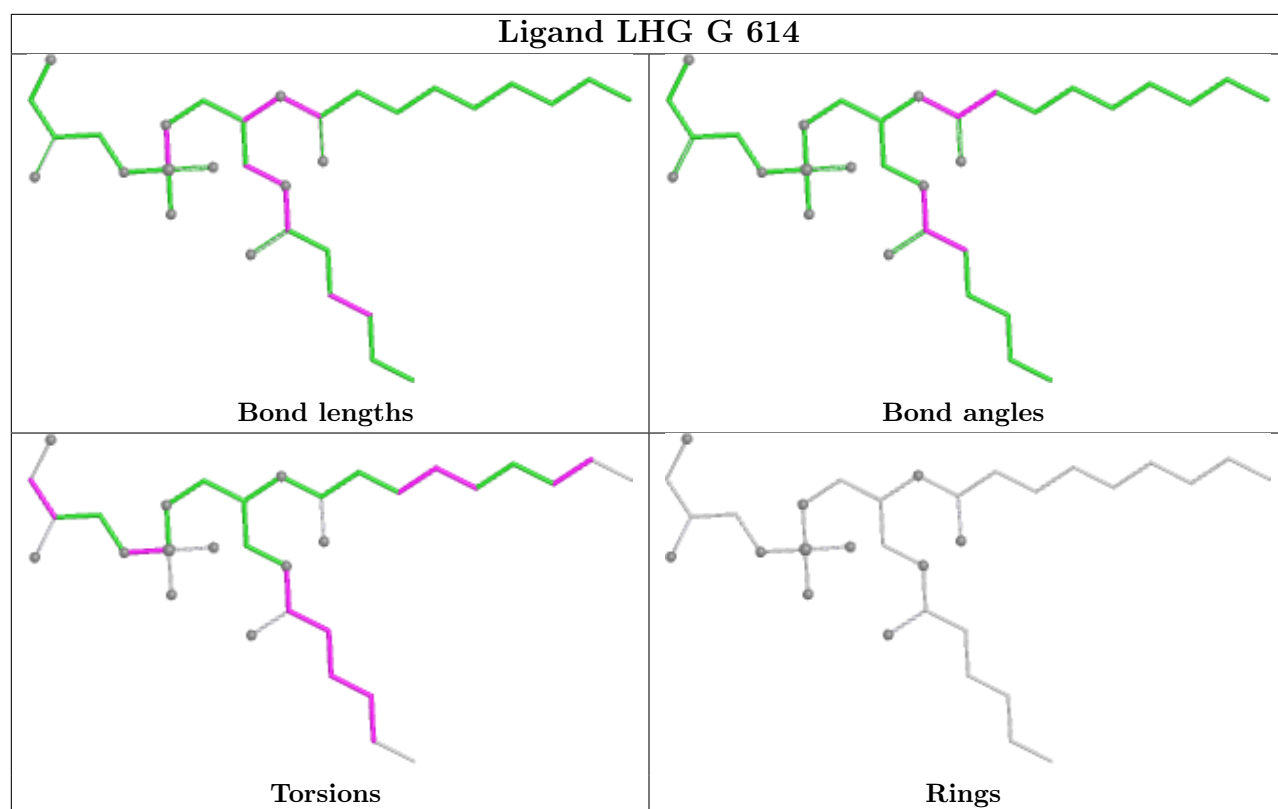


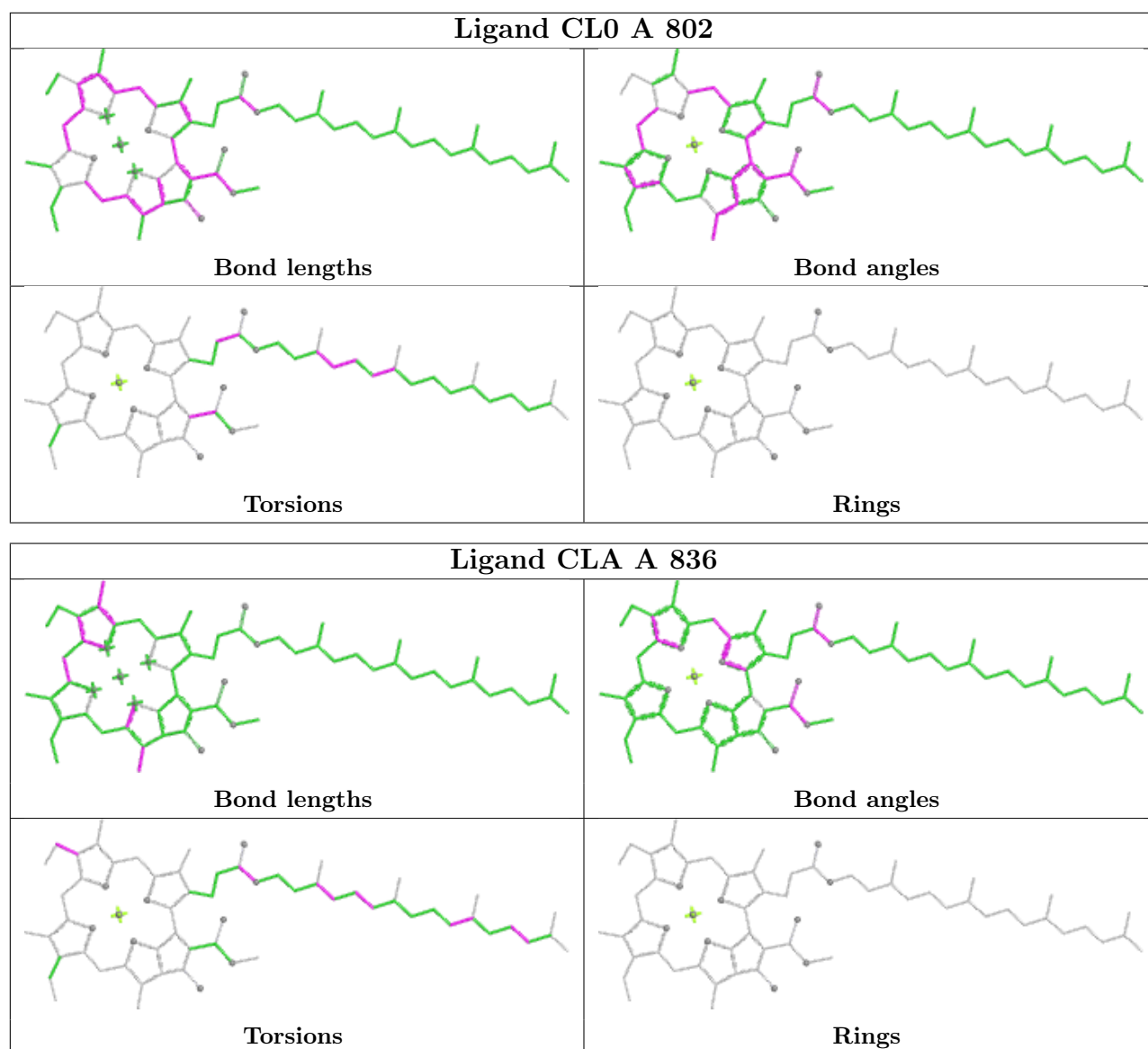


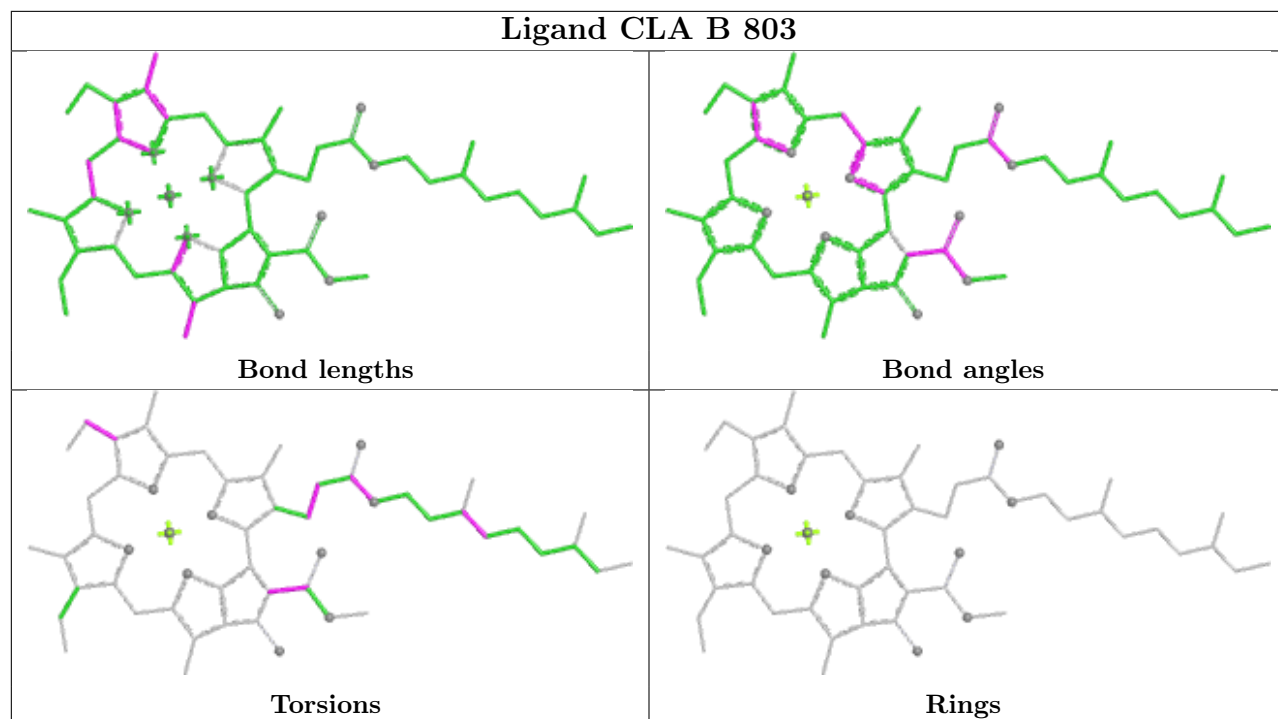




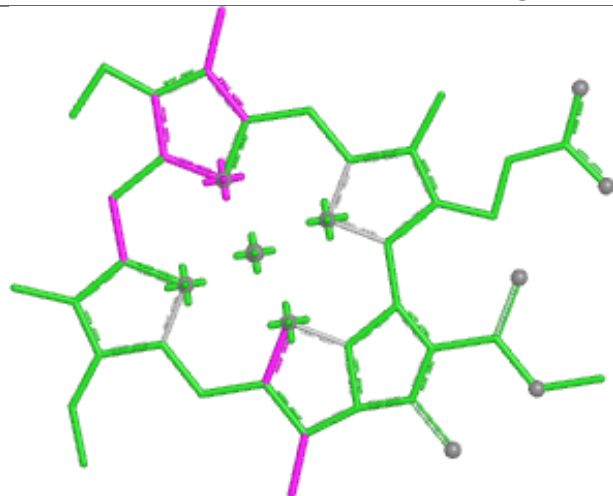




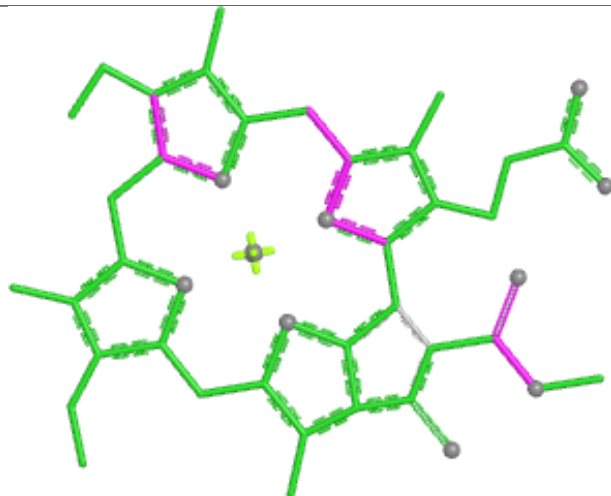




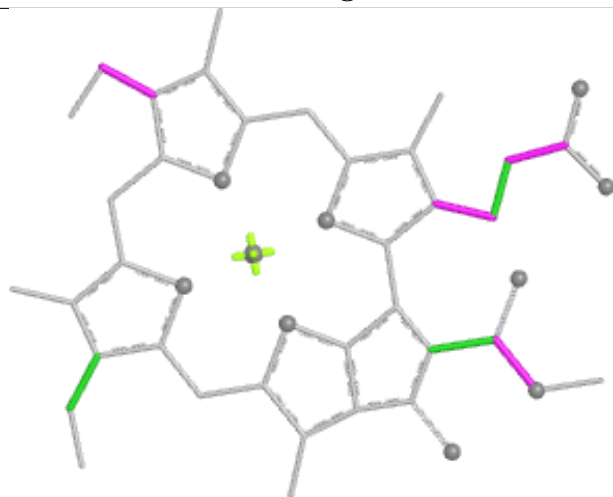
## Ligand CLA X 419



Bond lengths



Bond angles

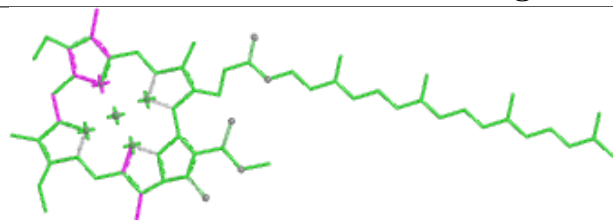


Torsions

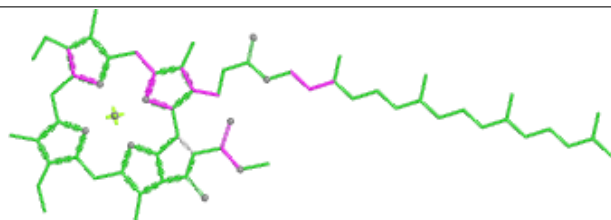


Rings

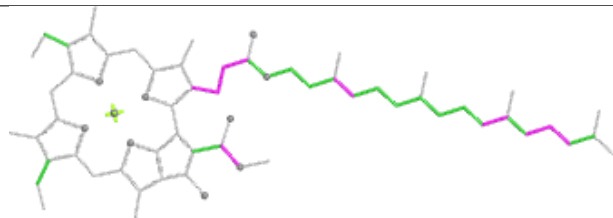
## Ligand CLA A 830



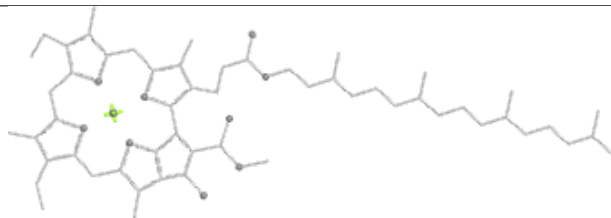
Bond lengths



Bond angles

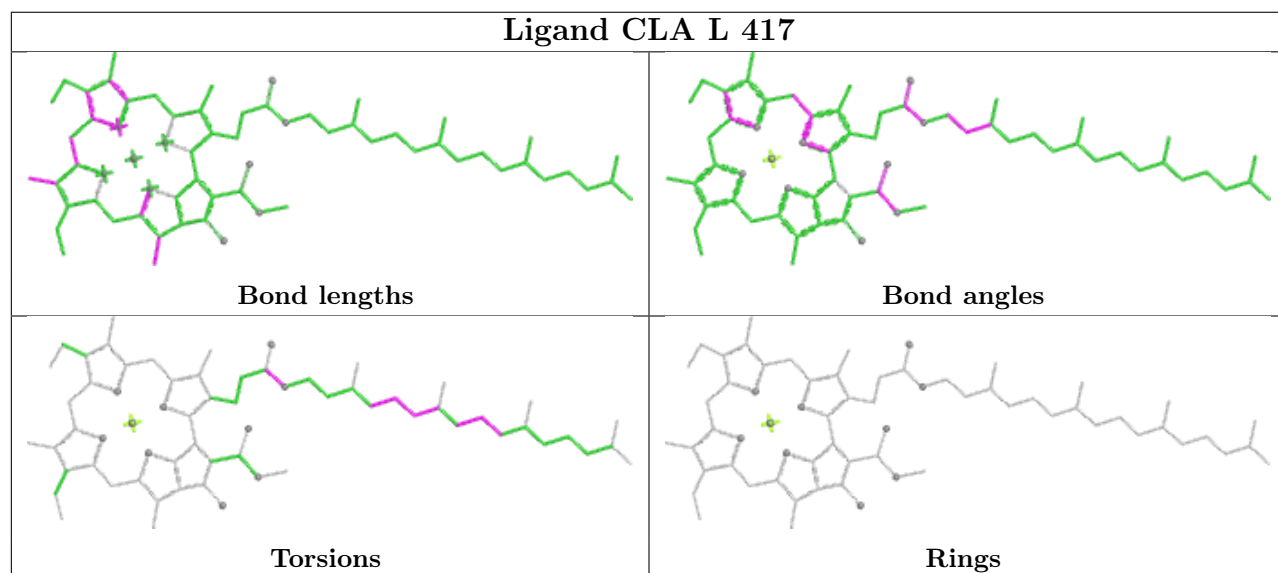
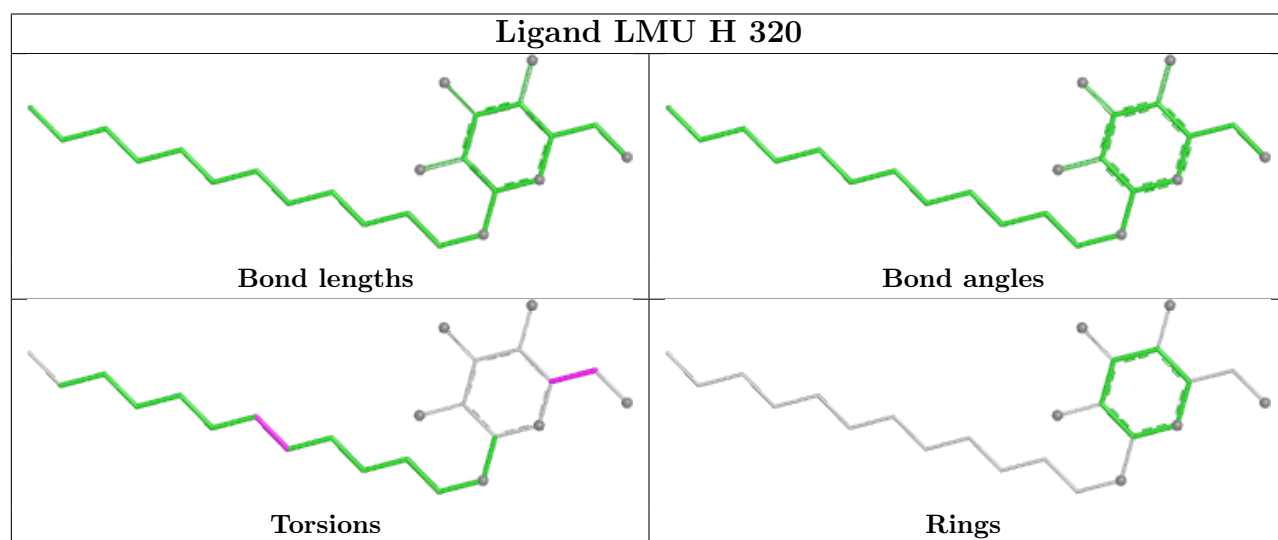
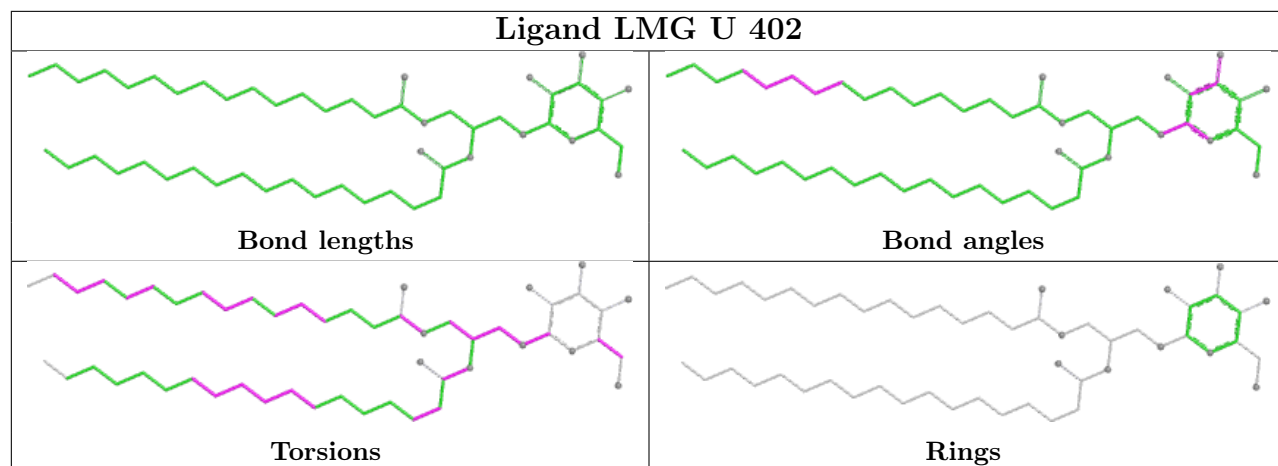


Torsions

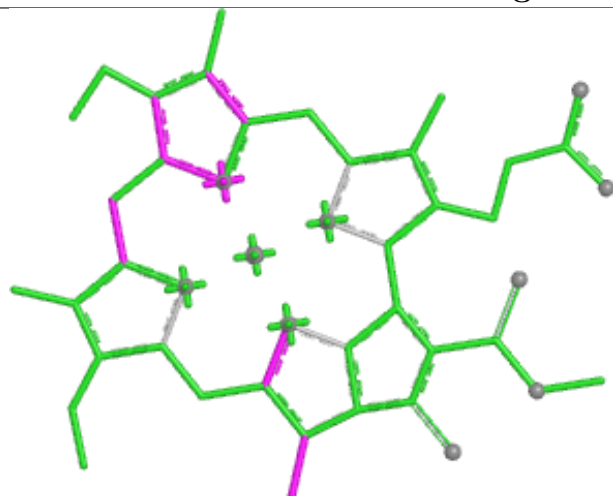


Rings

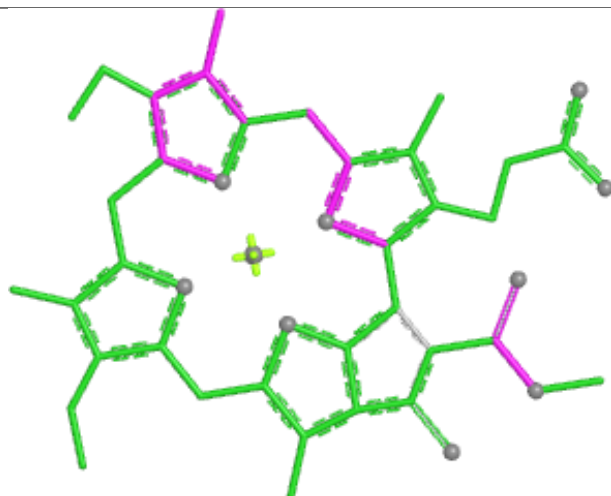




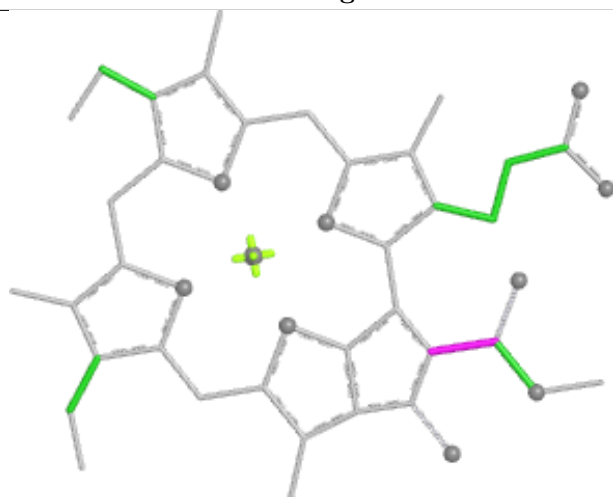
## Ligand CLA N 605



Bond lengths



Bond angles

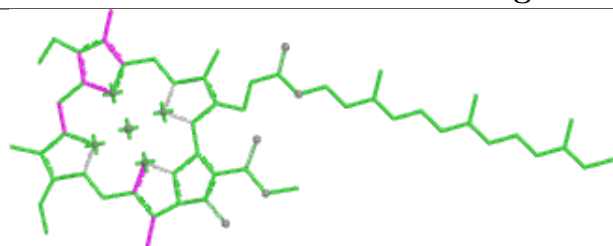


Torsions

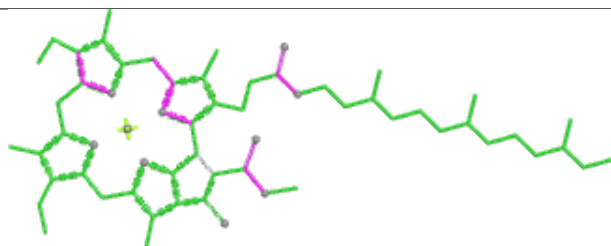


Rings

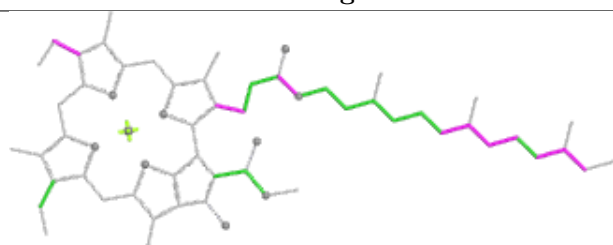
## Ligand CLA A 825



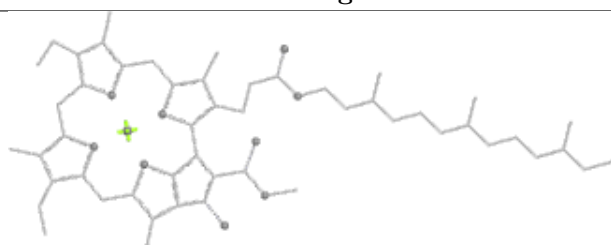
Bond lengths



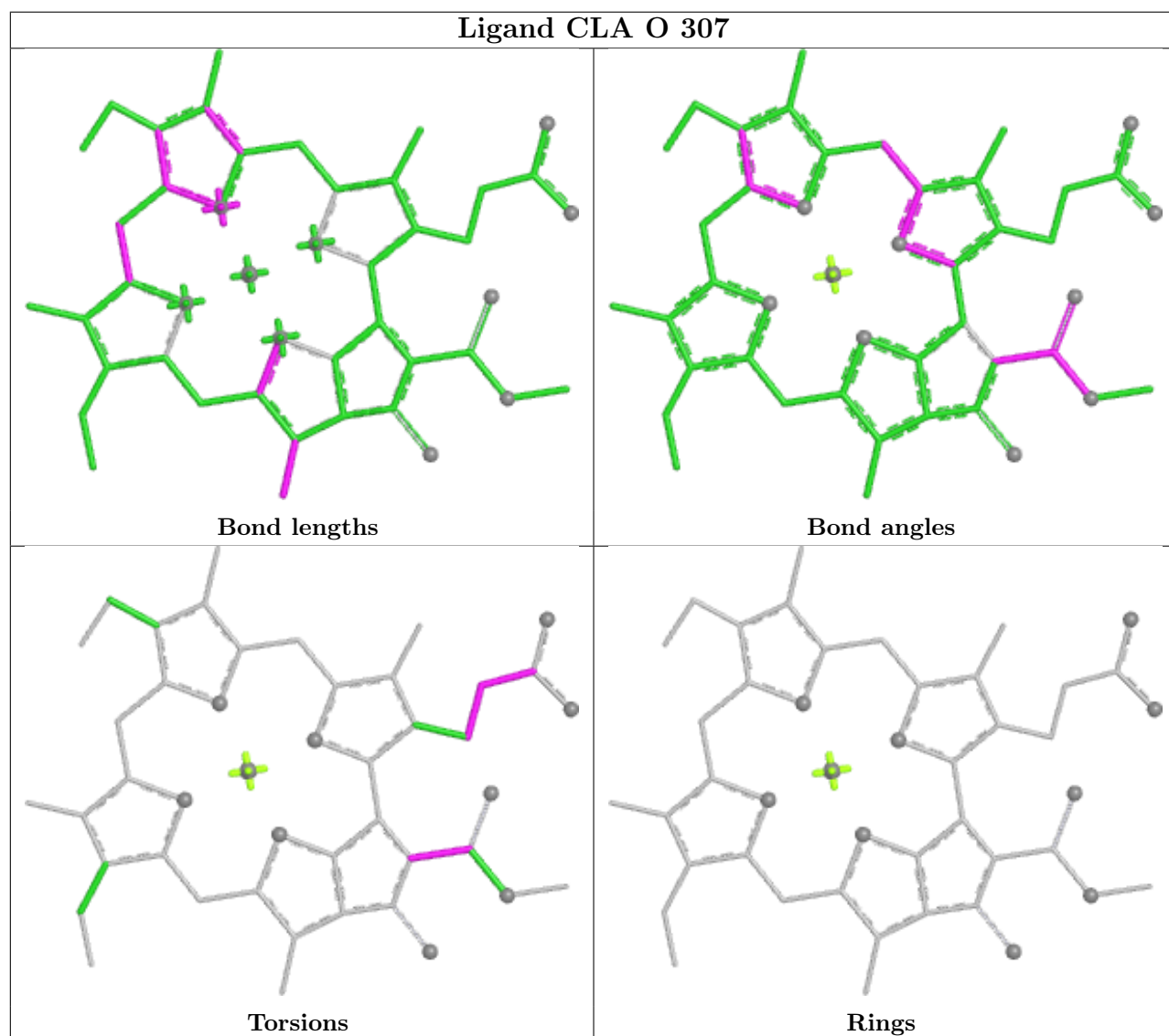
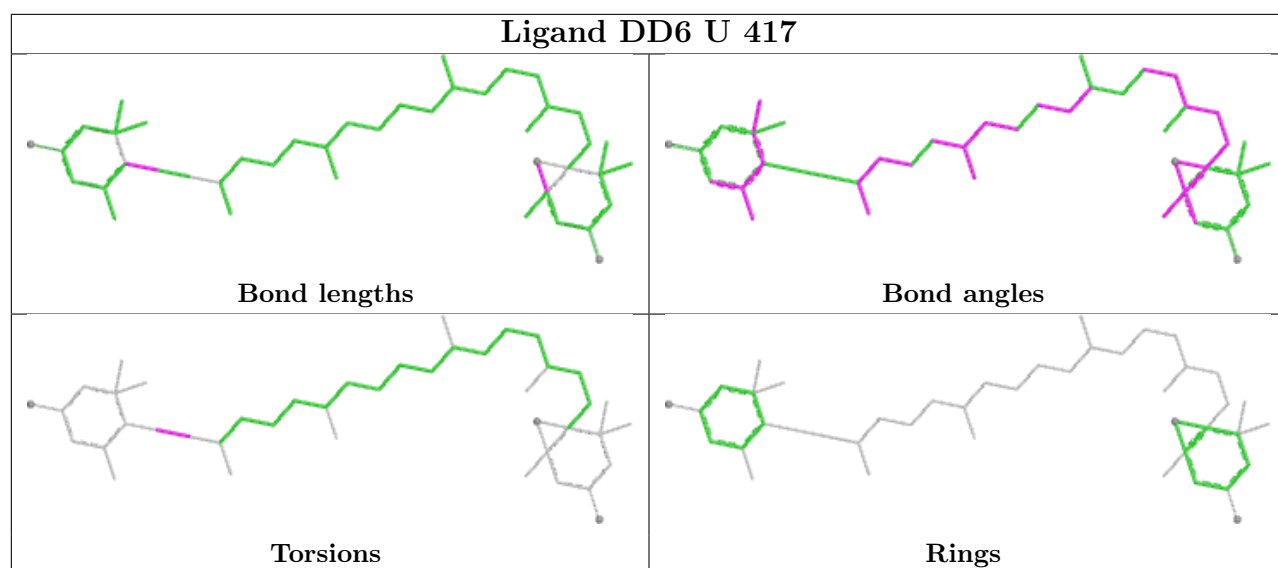
Bond angles

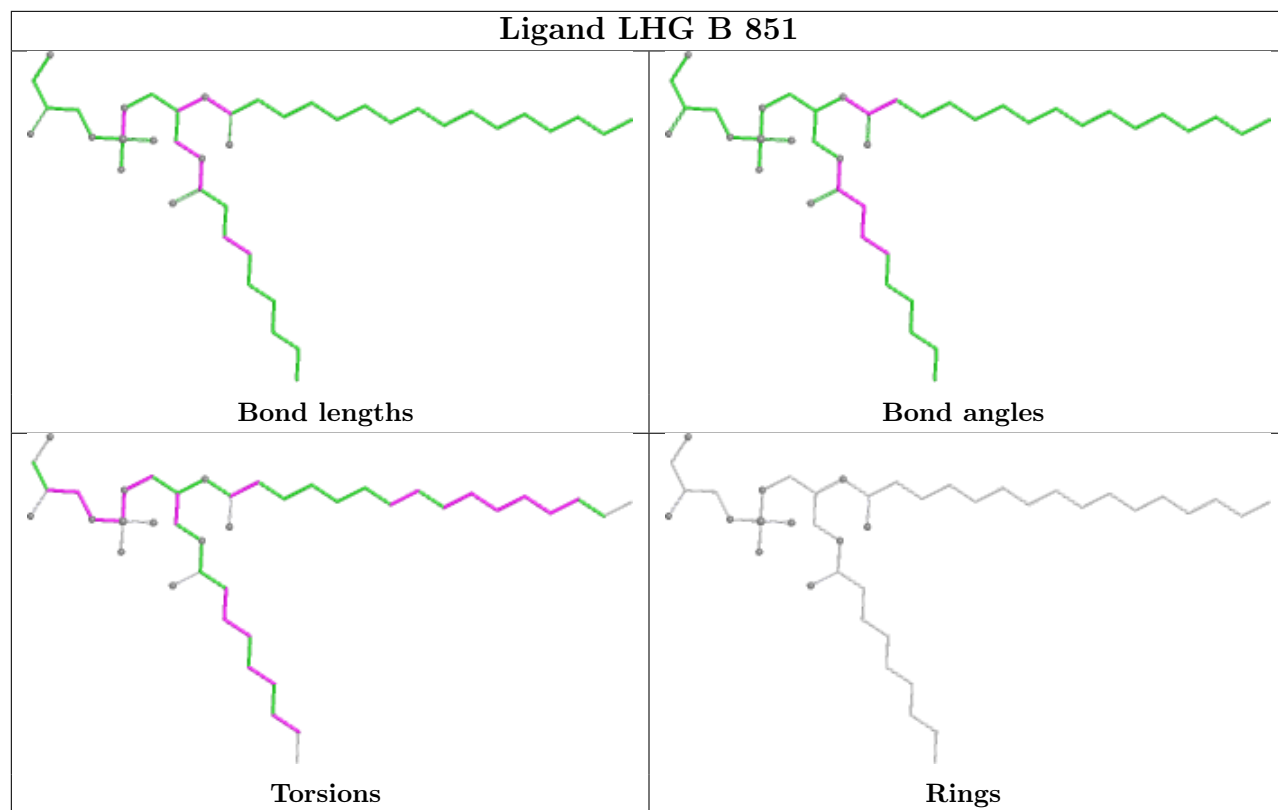


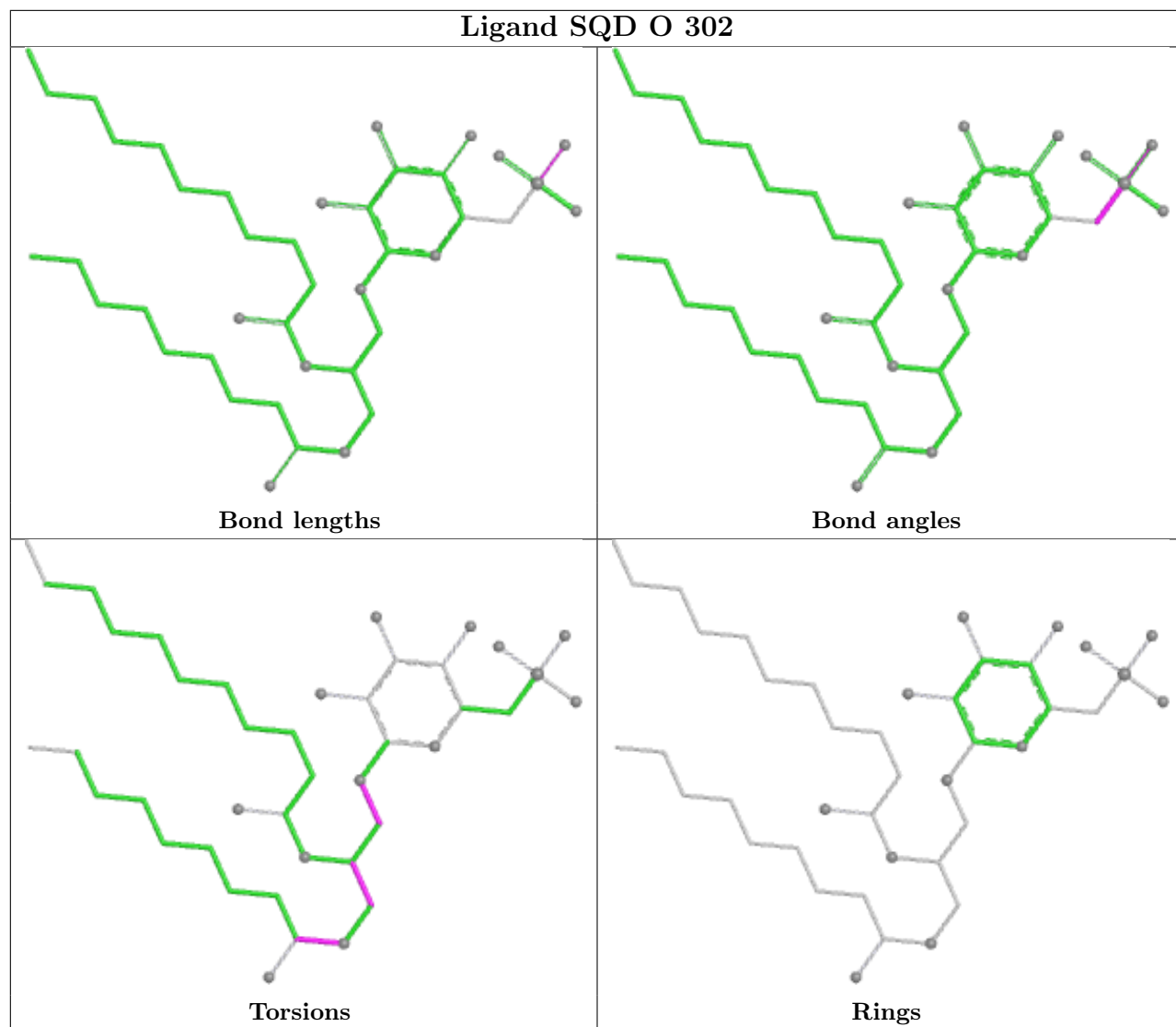
Torsions



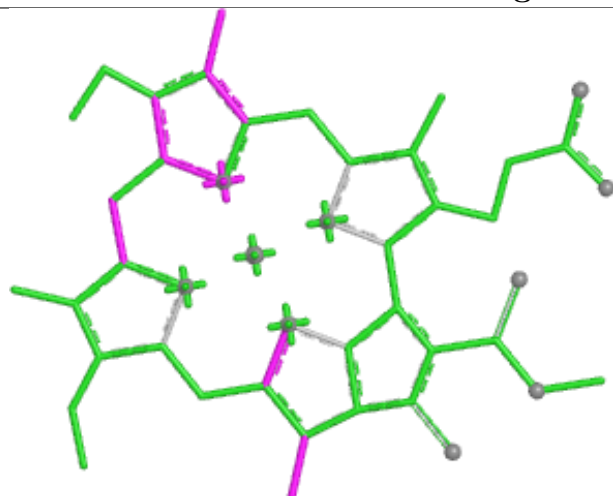
Rings







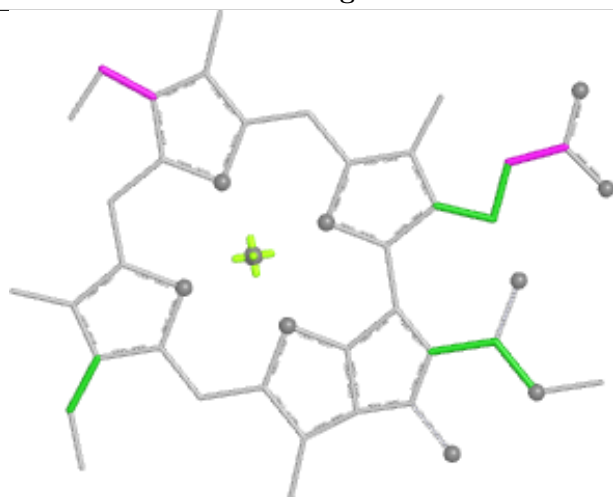
## Ligand CLA A 834



Bond lengths



Bond angles

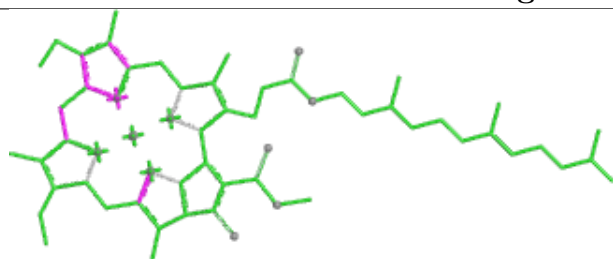


Torsions

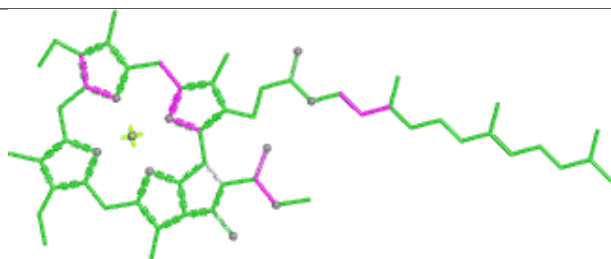


Rings

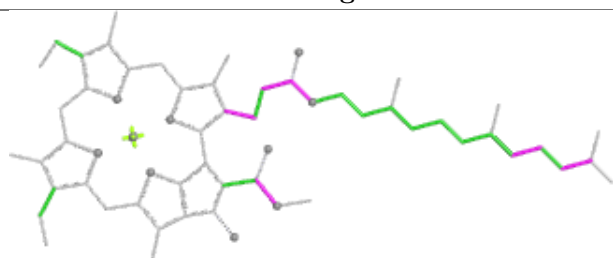
## Ligand CLA S 607



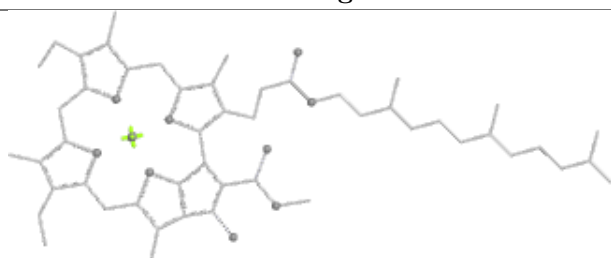
Bond lengths



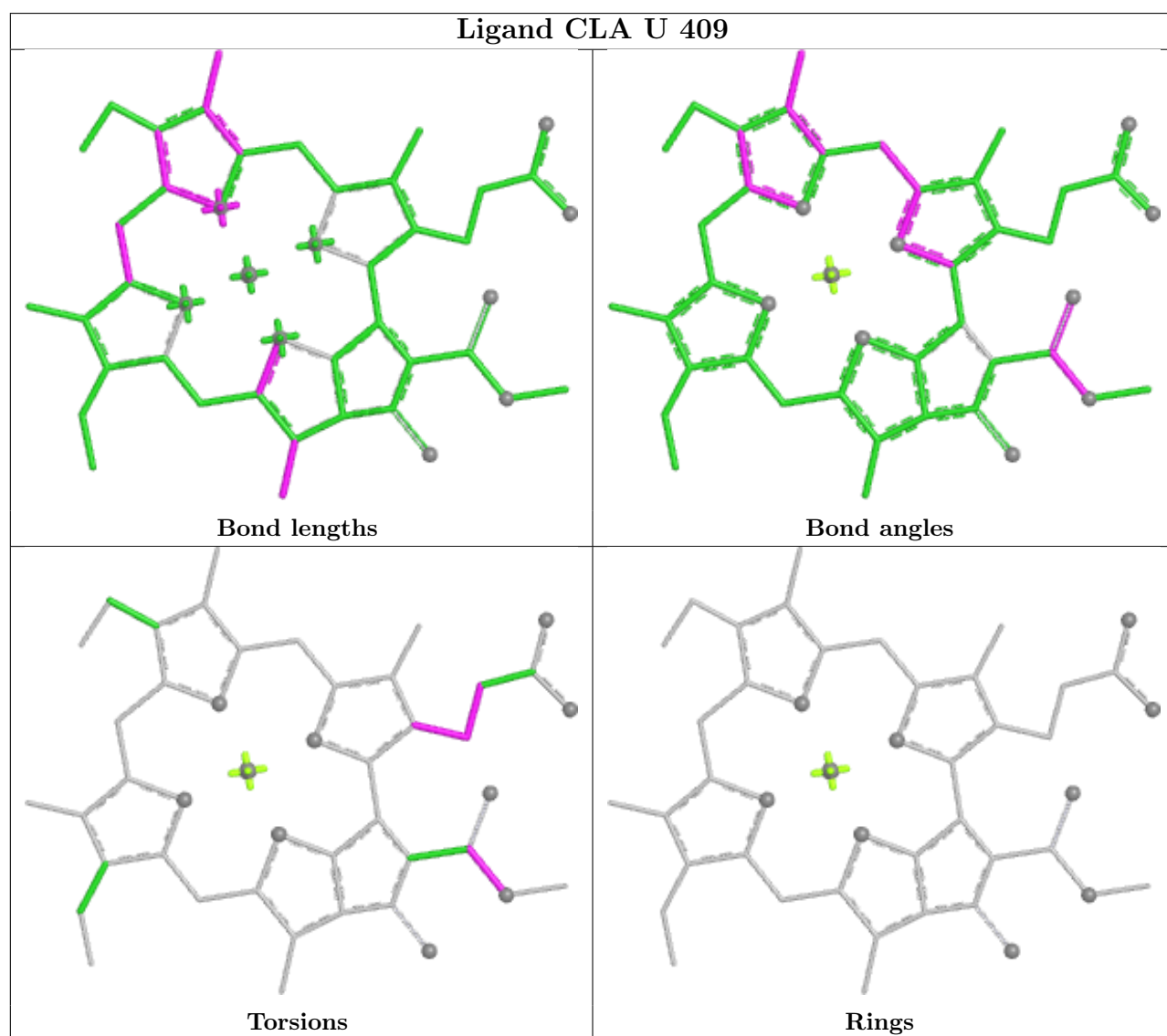
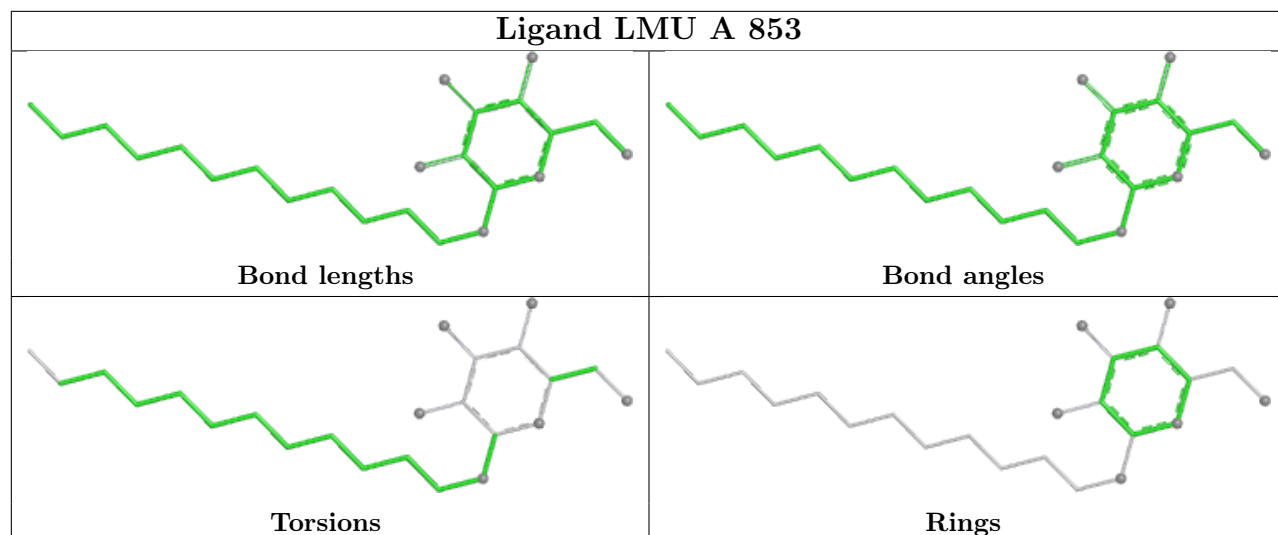
Bond angles

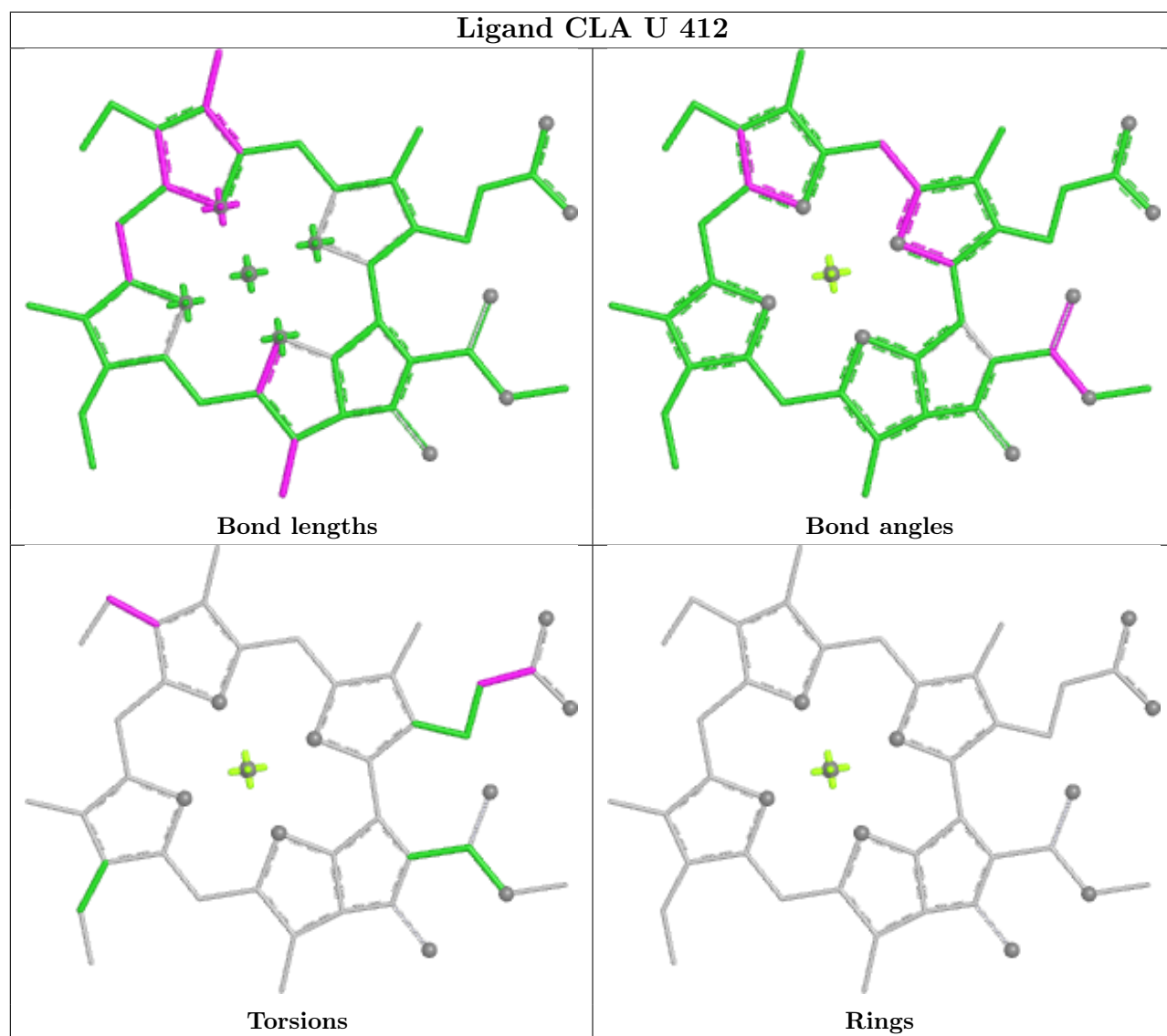
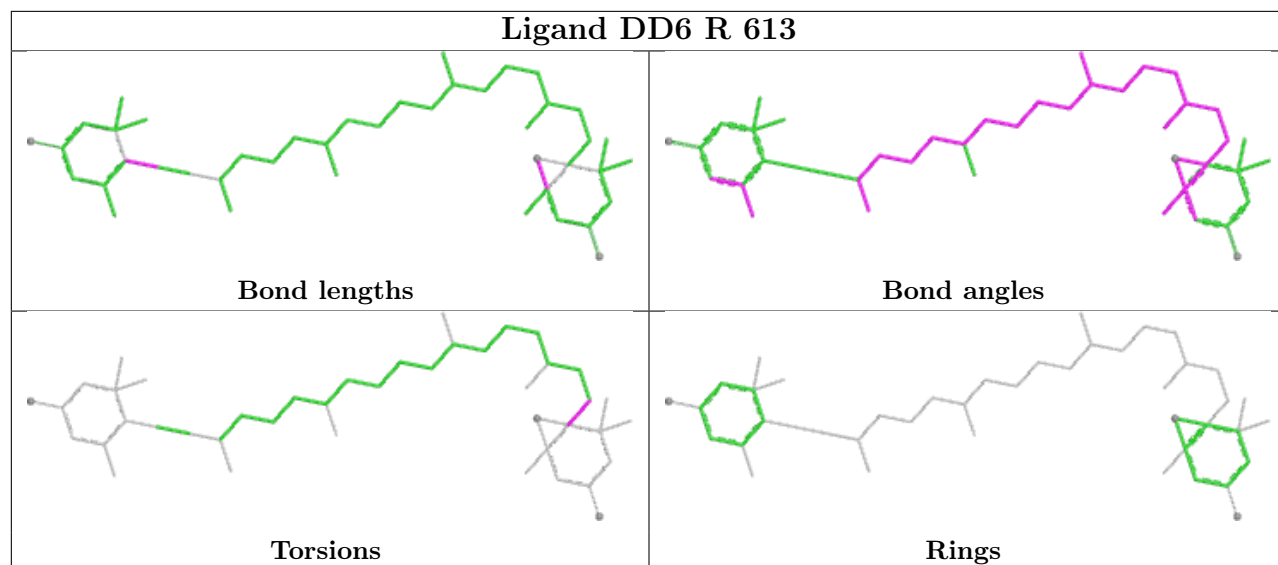


Torsions



Rings







## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

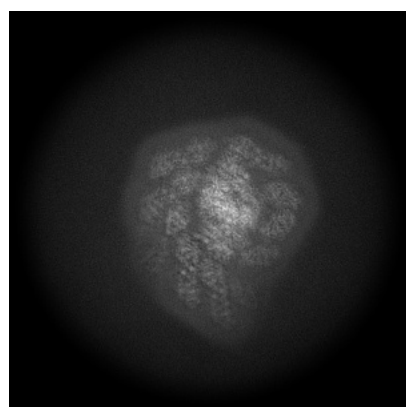
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63994. These allow visual inspection of the internal detail of the map and identification of artifacts.

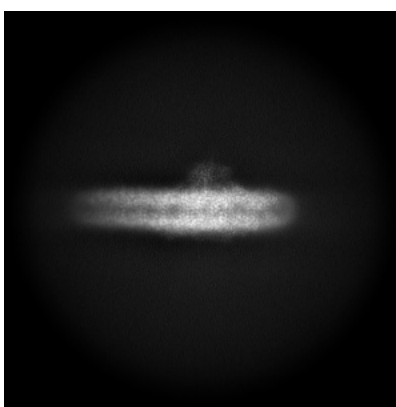
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

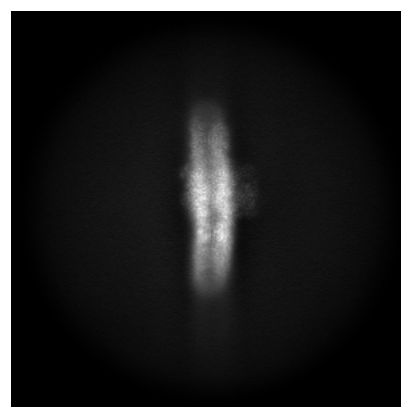
#### 6.1.1 Primary map



X



Y

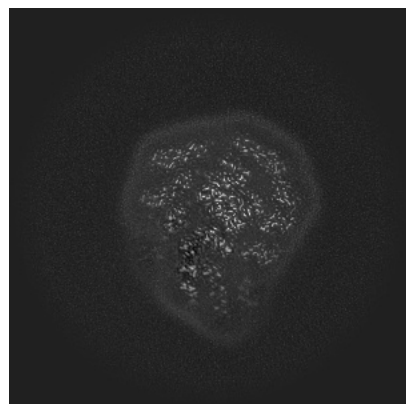


Z

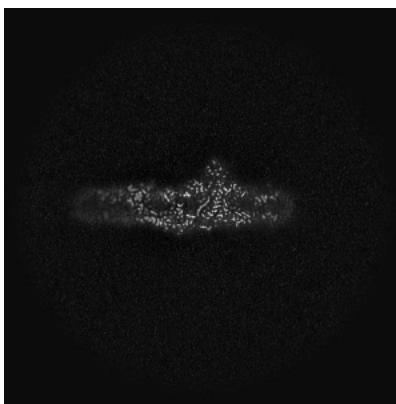
The images above show the map projected in three orthogonal directions.

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

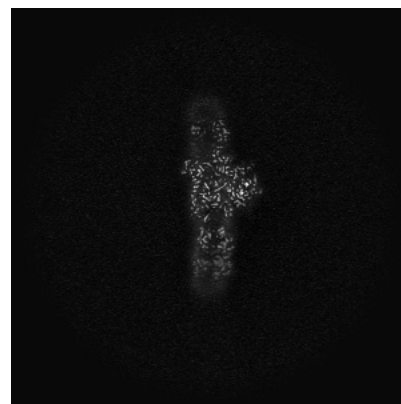
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

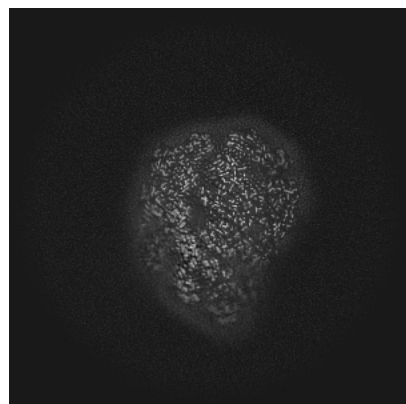


Z Index: 256

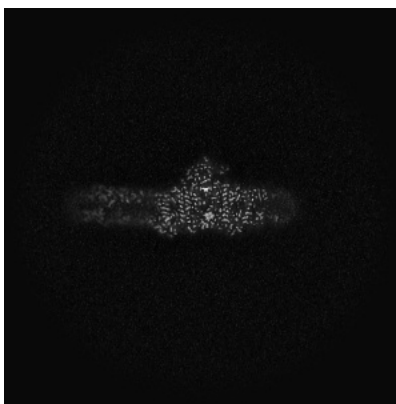
The images above show central slices of the map in three orthogonal directions.

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

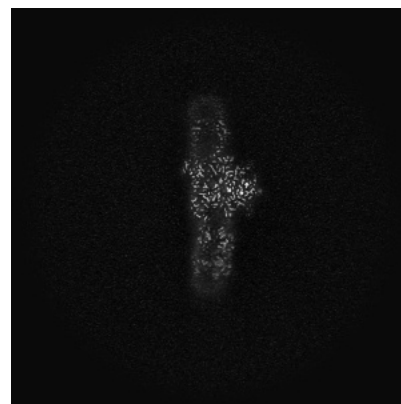
### 6.3.1 Primary map



X Index: 270



Y Index: 278

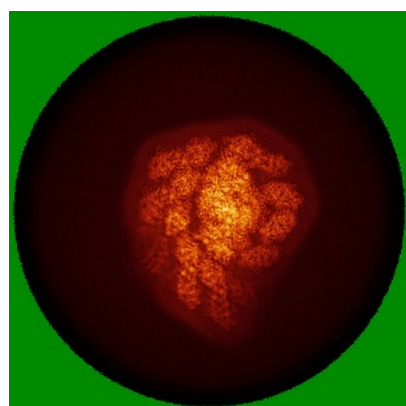


Z Index: 257

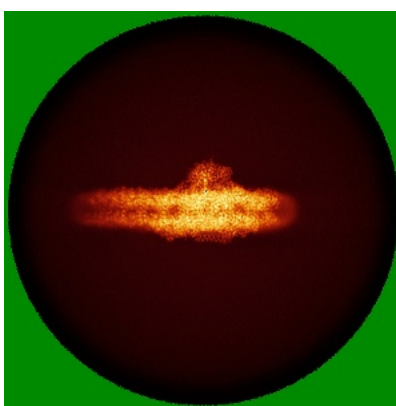
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

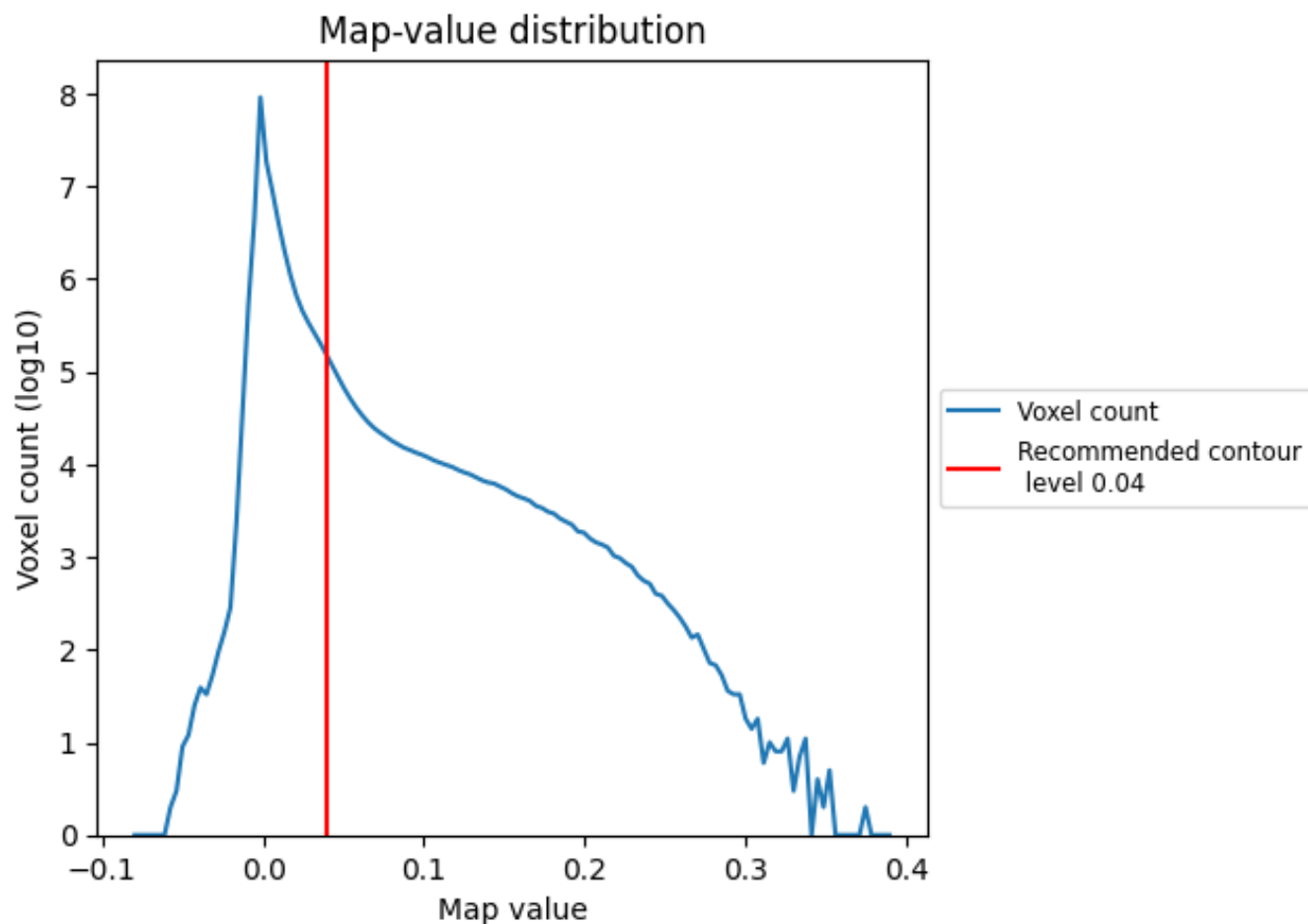
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

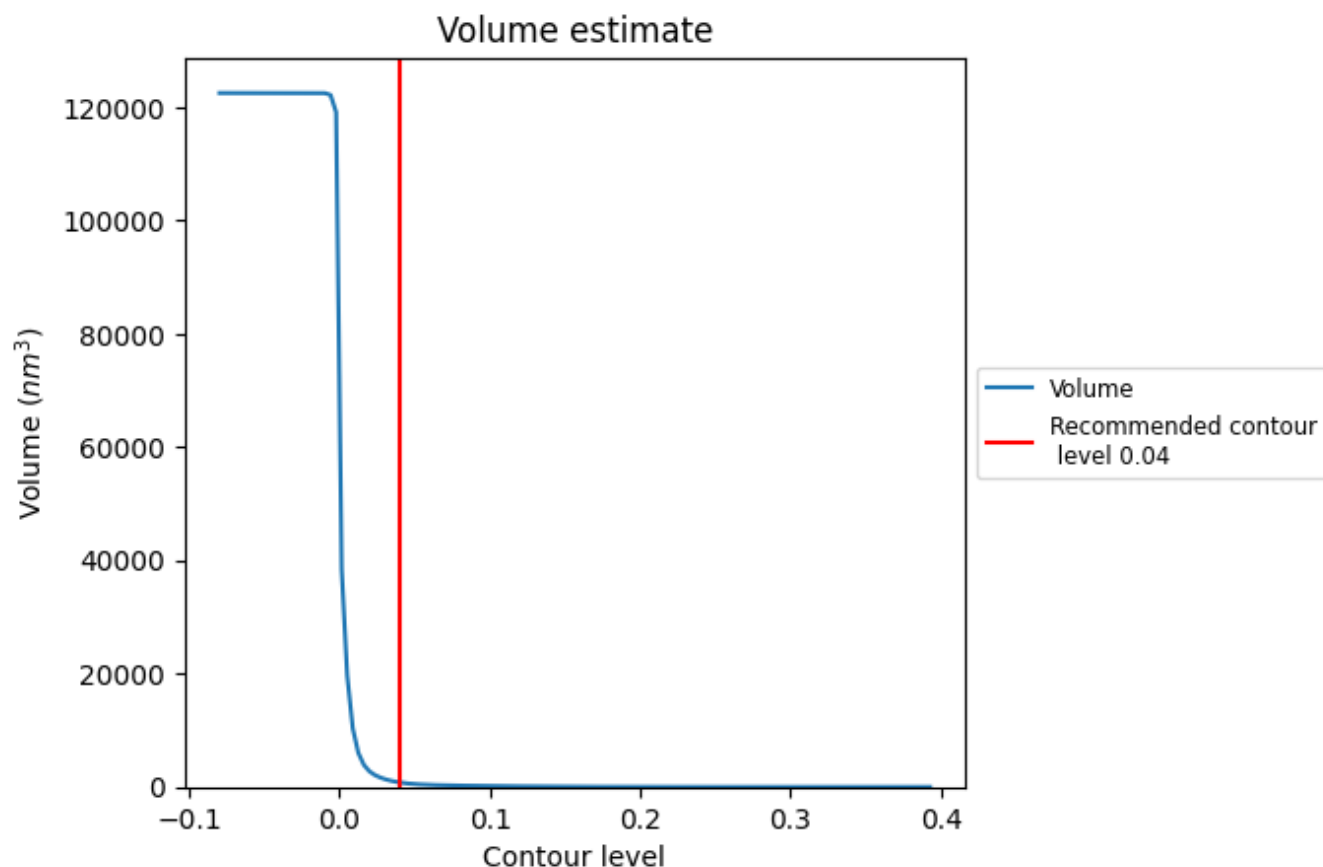
This section contains the results of statistical analysis of the map.

### 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.

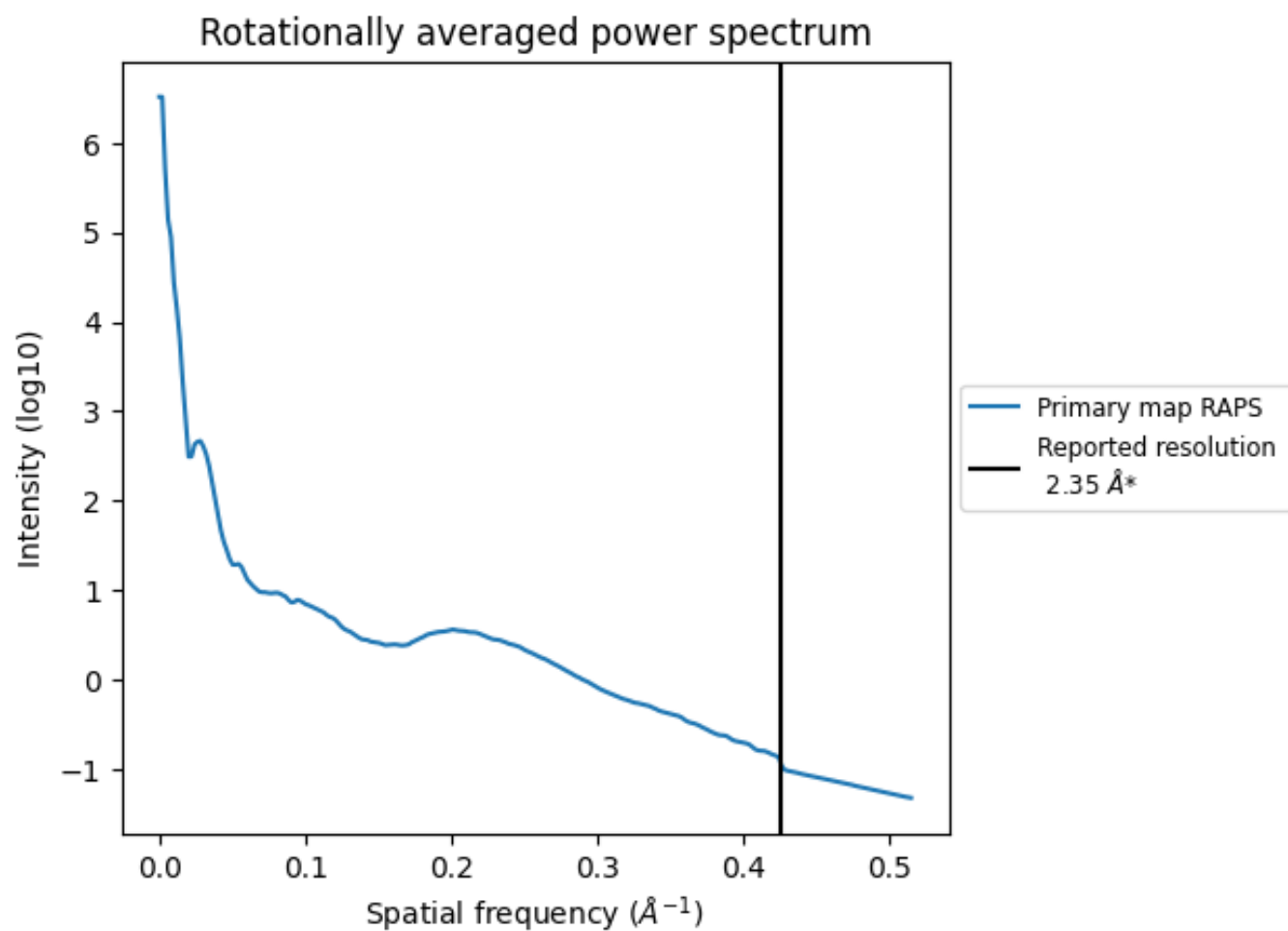
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 801  $\text{nm}^3$ ; this corresponds to an approximate mass of 724 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 ⓘ

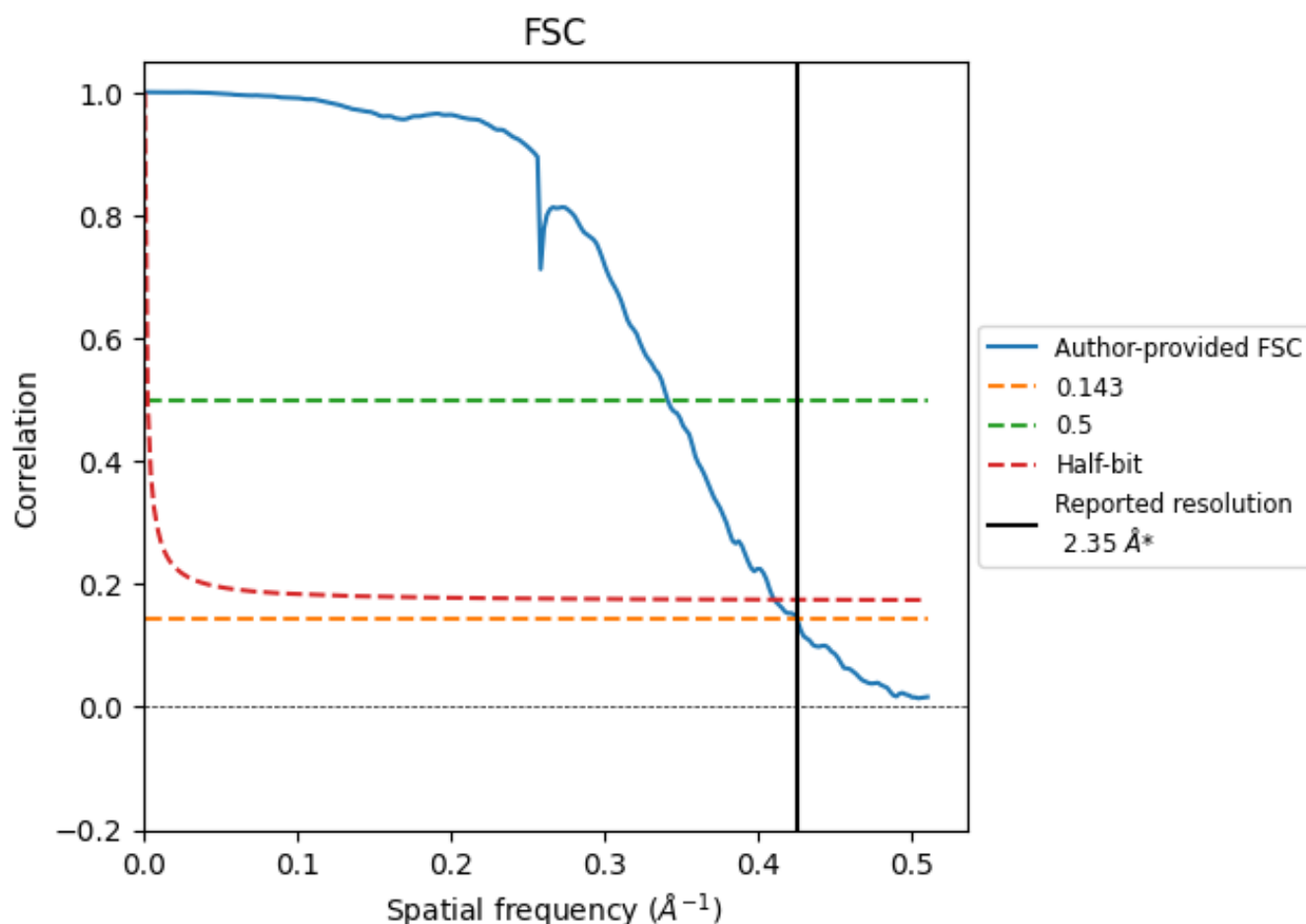


\*Reported resolution corresponds to spatial frequency of 0.426 Å<sup>-1</sup>

## 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 0.426  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

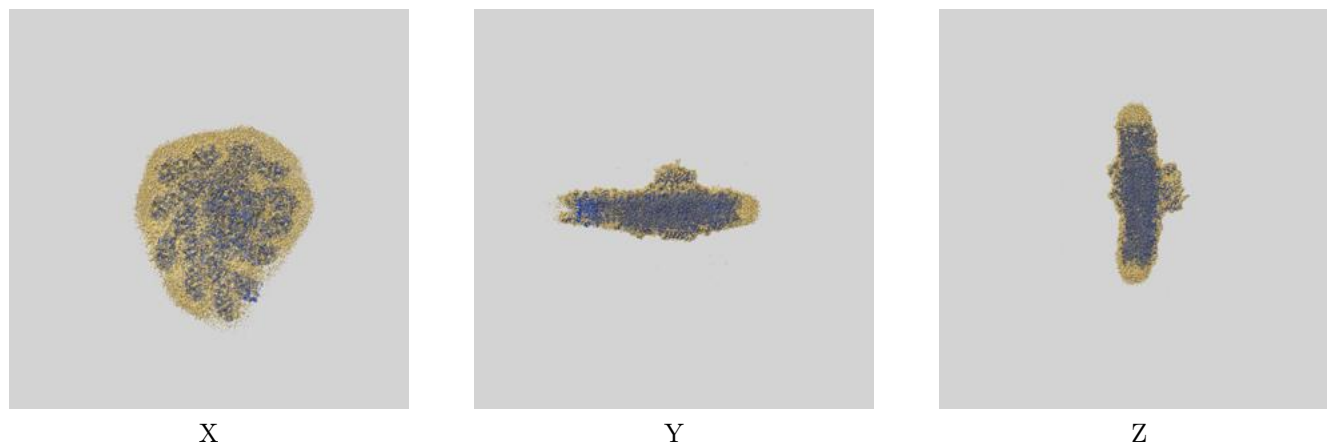
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.35	2.93	2.43
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

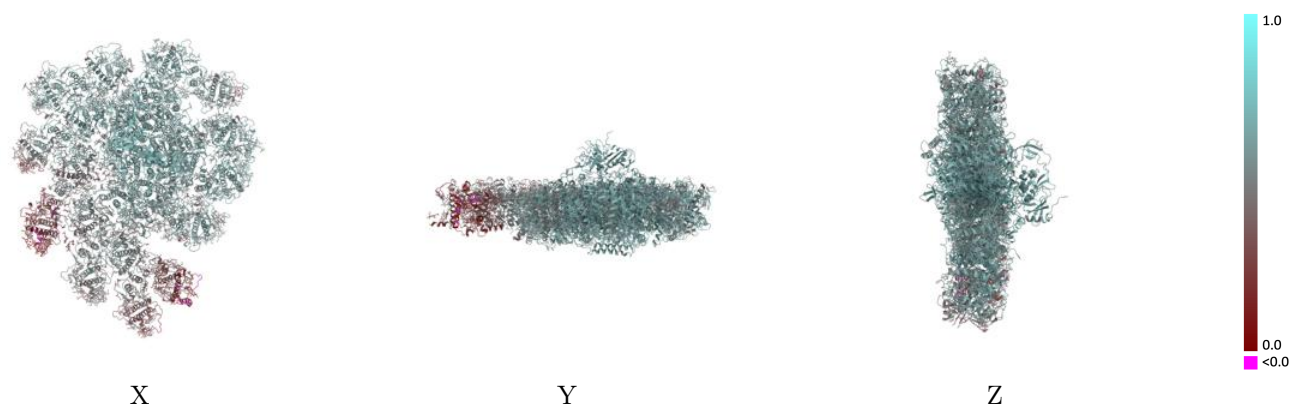
This section contains information regarding the fit between EMDB map EMD-63994 and PDB model 9UAS. Per-residue inclusion information can be found in section [3](#) on page [42](#).

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



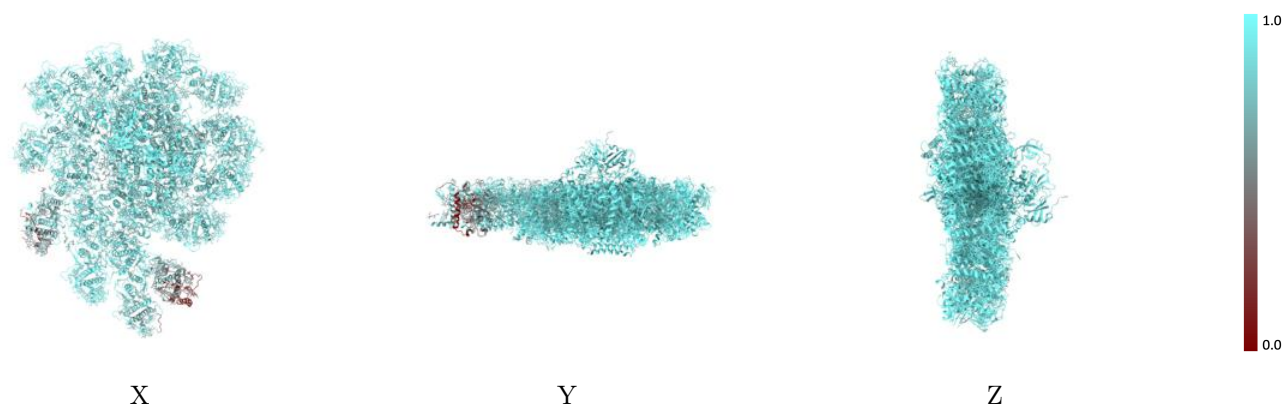
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



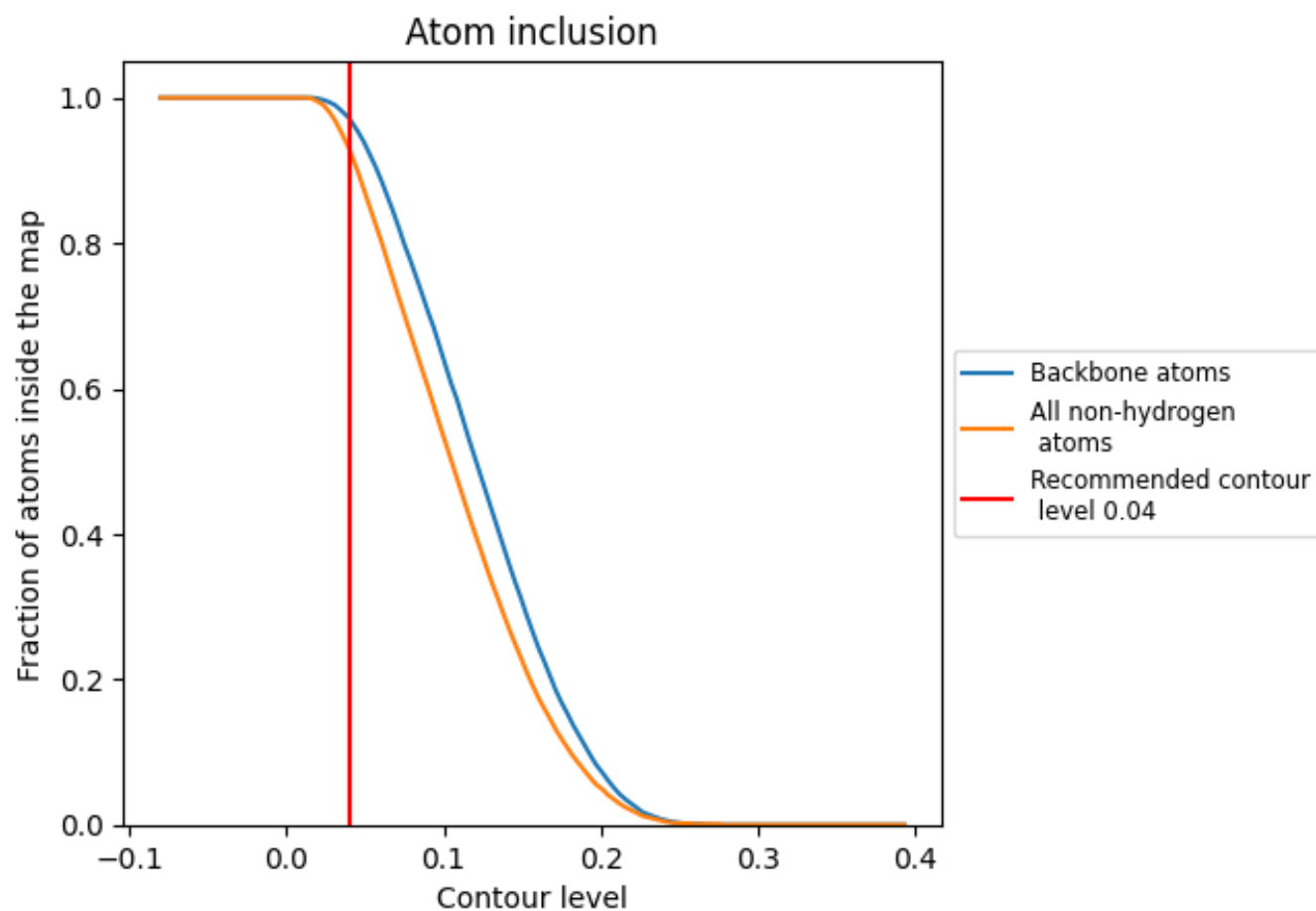
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.5550
A	 0.9840	 0.6580
B	 0.9780	 0.6190
C	 0.9970	 0.6770
D	 0.9510	 0.6400
E	 0.9560	 0.6350
F	 0.9620	 0.6150
G	 0.9560	 0.5620
H	 0.9670	 0.5870
I	 0.9400	 0.4830
J	 0.9420	 0.6280
K	 0.9690	 0.6110
L	 0.9710	 0.5060
M	 0.9840	 0.5760
N	 0.9490	 0.4660
O	 0.9660	 0.4920
P	 0.7790	 0.3540
Q	 0.9570	 0.5030
R	 0.4970	 0.2490
S	 0.9380	 0.5600
T	 0.9500	 0.6030
U	 0.9200	 0.5570
V	 0.6770	 0.2230
W	 0.9550	 0.6060
X	 0.9420	 0.6030

