



# Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 12:03 PM JST

PDB ID : 7Y8A  
EMDB ID : EMD-33683  
Title : Cryo-EM structure of cryptophyte photosystem I  
Authors : Zhao, L.S.; Zhang, Y.Z.; Liu, L.N.; Li, K.  
Deposited on : 2022-06-23  
Resolution : 2.71 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.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

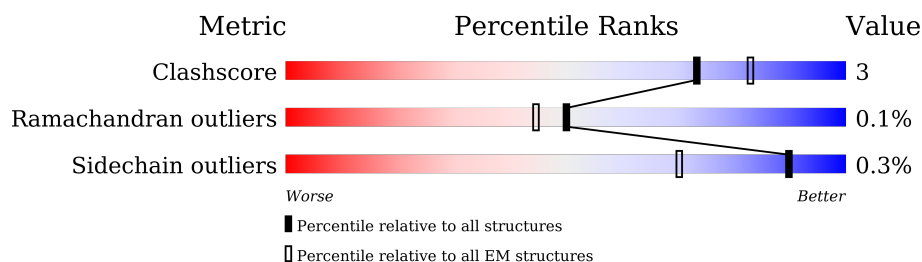
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.71 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1	222	 72%      9%      19%
2	2	216	 70%      7%      22%
3	3	236	 73%      •      24%
4	4	217	 78%      •      19%
5	5	229	 69%      13%      18%
6	6	215	 73%      7%      20%
7	7	230	 70%      7%      23%
8	8	227	 68%      8%      24%

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Mol	Chain	Length	Quality of chain
9	9	220	
10	A	752	
11	B	734	
12	C	81	
13	D	141	
14	E	64	
15	F	183	
16	I	36	
17	J	42	
18	K	87	
19	L	153	
20	M	30	
21	O	154	
22	R	133	
23	X	164	
24	Z	242	
25	a	215	
26	b	218	

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
27	CLA	1	601	X	-	-	-
27	CLA	1	602	X	-	-	-
27	CLA	1	603	X	-	-	-
27	CLA	1	604	X	-	-	-
27	CLA	1	605	X	-	-	-
27	CLA	1	606	X	-	-	-
27	CLA	1	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	1	608	X	-	-	-
27	CLA	1	609	X	-	-	-
27	CLA	1	611	X	-	-	-
27	CLA	1	612	X	-	-	-
27	CLA	1	613	X	-	-	-
27	CLA	2	601	X	-	-	-
27	CLA	2	602	X	-	-	-
27	CLA	2	603	X	-	-	-
27	CLA	2	604	X	-	-	-
27	CLA	2	605	X	-	-	-
27	CLA	2	606	X	-	-	-
27	CLA	2	607	X	-	-	-
27	CLA	2	608	X	-	-	-
27	CLA	2	609	X	-	-	-
27	CLA	2	611	X	-	-	-
27	CLA	2	612	X	-	-	-
27	CLA	3	601	X	-	-	-
27	CLA	3	602	X	-	-	-
27	CLA	3	603	X	-	-	-
27	CLA	3	604	X	-	-	-
27	CLA	3	605	X	-	-	-
27	CLA	3	607	X	-	-	-
27	CLA	3	608	X	-	-	-
27	CLA	3	609	X	-	-	-
27	CLA	3	610	X	-	-	-
27	CLA	3	611	X	-	-	-
27	CLA	3	612	X	-	-	-
27	CLA	4	601	X	-	-	-
27	CLA	4	602	X	-	-	-
27	CLA	4	603	X	-	-	-
27	CLA	4	604	X	-	-	-
27	CLA	4	606	X	-	-	-
27	CLA	4	607	X	-	-	-
27	CLA	4	608	X	-	-	-
27	CLA	4	609	X	-	-	-
27	CLA	4	610	X	-	-	-
27	CLA	4	611	X	-	-	-
27	CLA	5	601	X	-	-	-
27	CLA	5	602	X	-	-	-
27	CLA	5	603	X	-	-	-
27	CLA	5	604	X	-	-	-
27	CLA	5	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	5	606	X	-	-	-
27	CLA	5	607	X	-	-	-
27	CLA	5	608	X	-	-	-
27	CLA	5	609	X	-	-	-
27	CLA	5	611	X	-	-	-
27	CLA	5	612	X	-	-	-
27	CLA	5	613	X	-	-	-
27	CLA	6	601	X	-	-	-
27	CLA	6	602	X	-	-	-
27	CLA	6	603	X	-	-	-
27	CLA	6	604	X	-	-	-
27	CLA	6	605	X	-	-	-
27	CLA	6	606	X	-	-	-
27	CLA	6	607	X	-	-	-
27	CLA	6	608	X	-	-	-
27	CLA	6	609	X	-	-	-
27	CLA	6	611	X	-	-	-
27	CLA	6	612	X	-	-	-
27	CLA	7	302	X	-	-	-
27	CLA	7	303	X	-	-	-
27	CLA	7	304	X	-	-	-
27	CLA	7	305	X	-	-	-
27	CLA	7	306	X	-	-	-
27	CLA	7	308	X	-	-	-
27	CLA	7	309	X	-	-	-
27	CLA	7	310	X	-	-	-
27	CLA	7	312	X	-	-	-
27	CLA	7	313	X	-	-	-
27	CLA	8	601	X	-	-	-
27	CLA	8	602	X	-	-	-
27	CLA	8	603	X	-	-	-
27	CLA	8	604	X	-	-	-
27	CLA	8	605	X	-	-	-
27	CLA	8	606	X	-	-	-
27	CLA	8	607	X	-	-	-
27	CLA	8	608	X	-	-	-
27	CLA	8	615	X	-	-	-
27	CLA	9	601	X	-	-	-
27	CLA	9	602	X	-	-	-
27	CLA	9	603	X	-	-	-
27	CLA	9	604	X	-	-	-
27	CLA	9	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	9	606	X	-	-	-
27	CLA	9	607	X	-	-	-
27	CLA	9	608	X	-	-	-
27	CLA	9	609	X	-	-	-
27	CLA	9	611	X	-	-	-
27	CLA	9	612	X	-	-	-
27	CLA	9	613	X	-	-	-
27	CLA	9	614	X	-	-	-
27	CLA	A	801	X	-	-	-
27	CLA	A	802	X	-	-	-
27	CLA	A	803	X	-	-	-
27	CLA	A	804	X	-	-	-
27	CLA	A	805	X	-	-	-
27	CLA	A	806	X	-	-	-
27	CLA	A	807	X	-	-	-
27	CLA	A	808	X	-	-	-
27	CLA	A	809	X	-	-	-
27	CLA	A	810	X	-	-	-
27	CLA	A	811	X	-	-	-
27	CLA	A	812	X	-	-	-
27	CLA	A	813	X	-	-	-
27	CLA	A	814	X	-	-	-
27	CLA	A	815	X	-	-	-
27	CLA	A	816	X	-	-	-
27	CLA	A	817	X	-	-	-
27	CLA	A	818	X	-	-	-
27	CLA	A	819	X	-	-	-
27	CLA	A	820	X	-	-	-
27	CLA	A	821	X	-	-	-
27	CLA	A	822	X	-	-	-
27	CLA	A	823	X	-	-	-
27	CLA	A	824	X	-	-	-
27	CLA	A	825	X	-	-	-
27	CLA	A	826	X	-	-	-
27	CLA	A	827	X	-	-	-
27	CLA	A	828	X	-	-	-
27	CLA	A	829	X	-	-	-
27	CLA	A	830	X	-	-	-
27	CLA	A	831	X	-	-	-
27	CLA	A	832	X	-	-	-
27	CLA	A	833	X	-	-	-
27	CLA	A	834	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	835	X	-	-	-
27	CLA	A	836	X	-	-	-
27	CLA	A	837	X	-	-	-
27	CLA	A	838	X	-	-	-
27	CLA	A	839	X	-	-	-
27	CLA	A	840	X	-	-	-
27	CLA	A	841	X	-	-	-
27	CLA	A	842	X	-	-	-
27	CLA	A	843	X	-	-	-
27	CLA	A	844	X	-	-	-
27	CLA	B	801	X	-	-	-
27	CLA	B	802	X	-	-	-
27	CLA	B	803	X	-	-	-
27	CLA	B	804	X	-	-	-
27	CLA	B	805	X	-	-	-
27	CLA	B	806	X	-	-	-
27	CLA	B	807	X	-	-	-
27	CLA	B	808	X	-	-	-
27	CLA	B	809	X	-	-	-
27	CLA	B	810	X	-	-	-
27	CLA	B	811	X	-	-	-
27	CLA	B	812	X	-	-	-
27	CLA	B	813	X	-	-	-
27	CLA	B	814	X	-	-	-
27	CLA	B	815	X	-	-	-
27	CLA	B	816	X	-	-	-
27	CLA	B	817	X	-	-	-
27	CLA	B	818	X	-	-	-
27	CLA	B	819	X	-	-	-
27	CLA	B	820	X	-	-	-
27	CLA	B	821	X	-	-	-
27	CLA	B	822	X	-	-	-
27	CLA	B	823	X	-	-	-
27	CLA	B	824	X	-	-	-
27	CLA	B	825	X	-	-	-
27	CLA	B	826	X	-	-	-
27	CLA	B	827	X	-	-	-
27	CLA	B	828	X	-	-	-
27	CLA	B	829	X	-	-	-
27	CLA	B	830	X	-	-	-
27	CLA	B	831	X	-	-	-
27	CLA	B	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	833	X	-	-	-
27	CLA	B	834	X	-	-	-
27	CLA	B	835	X	-	-	-
27	CLA	B	836	X	-	-	-
27	CLA	B	837	X	-	-	-
27	CLA	B	838	X	-	-	-
27	CLA	B	839	X	-	-	-
27	CLA	B	840	X	-	-	-
27	CLA	B	841	X	-	-	-
27	CLA	F	202	X	-	-	-
27	CLA	F	203	X	-	-	-
27	CLA	F	204	X	-	-	-
27	CLA	J	102	X	-	-	-
27	CLA	K	101	X	-	-	-
27	CLA	K	102	X	-	-	-
27	CLA	L	201	X	-	-	-
27	CLA	L	202	X	-	-	-
27	CLA	L	203	X	-	-	-
27	CLA	O	201	X	-	-	-
27	CLA	O	202	X	-	-	-
27	CLA	O	203	X	-	-	-
27	CLA	O	204	X	-	-	-
27	CLA	R	202	X	-	-	-
27	CLA	Z	301	X	-	-	-
27	CLA	Z	304	X	-	-	-
27	CLA	Z	305	X	-	-	-
27	CLA	Z	306	X	-	-	-
27	CLA	Z	310	X	-	-	-
27	CLA	a	601	X	-	-	-
27	CLA	a	602	X	-	-	-
27	CLA	a	603	X	-	-	-
27	CLA	a	604	X	-	-	-
27	CLA	a	605	X	-	-	-
27	CLA	a	606	X	-	-	-
27	CLA	a	607	X	-	-	-
27	CLA	a	608	X	-	-	-
27	CLA	a	610	X	-	-	-
27	CLA	a	611	X	-	-	-
27	CLA	b	601	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	606	X	-	-	-
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 53404 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 ACPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	179	Total	C	N	O	S	0	0
			1338	861	227	242	8		

- Molecule 2 is a protein called ACPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	168	Total	C	N	O	S	0	0
			1320	872	215	230	3		

- Molecule 3 is a protein called ACPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	180	Total	C	N	O	S	0	0
			1362	875	231	246	10		

- Molecule 4 is a protein called ACPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	176	Total	C	N	O	S	0	0
			1366	891	224	245	6		

- Molecule 5 is a protein called ACPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	188	Total	C	N	O	S	0	0
			1403	908	234	253	8		

- Molecule 6 is a protein called ACPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	173	Total	C	N	O	S	0	0
			1305	846	217	232	10		

- Molecule 7 is a protein called ACPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	177	Total	C	N	O	S	0	0
			1337	861	230	238	8		

- Molecule 8 is a protein called ACPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	173	Total	C	N	O	S	0	0
			1298	842	217	235	4		

- Molecule 9 is a protein called ACPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	180	Total	C	N	O	S	0	0
			1349	864	230	243	12		

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	741	Total	C	N	O	S	0	0
			5824	3804	992	1000	28		

- Molecule 11 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	731	Total	C	N	O	S	0	0
			5828	3847	982	984	15		

- Molecule 12 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	80	Total	C	N	O	S	0	0
			591	361	103	115	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	137	Total	C	N	O	S	0	0
			1070	685	184	198	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	E	61	Total	C	N	O	0	0
			491	312	85	94		

- Molecule 15 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	160	Total	C	N	O	S	0	0
			1258	814	214	228	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	33	Total	C	N	O	S	0	0
			258	180	34	42	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	42	Total	C	N	O	S	0	0
			342	232	49	58	3		

- Molecule 18 is a protein called Photosystem I reaction center subunit Psak.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	78	Total	C	N	O	S	0	0
			553	358	90	102	3		

- Molecule 19 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	147	Total	C	N	O	S	0	0
			1119	730	180	207	2		

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	30	Total	C	N	O	S	0	0
			227	152	35	39	1		

- Molecule 21 is a protein called Psao.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	92	Total	C	N	O	S	0	0
			709	481	104	123	1		

- Molecule 22 is a protein called Psar.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	92	Total	C	N	O	S	0	0
			680	439	112	127	2		

- Molecule 23 is a protein called Unk1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	145	Total	C	N	O	S	0	0
			725	435	145	145			

- Molecule 24 is a protein called ACPI-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	153	Total	C	N	O	S	0	0
			1130	721	188	211	10		

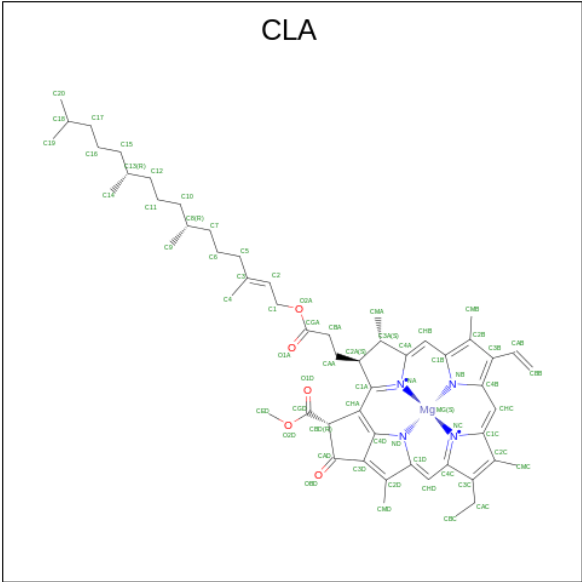
- Molecule 25 is a protein called ACPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		

- Molecule 26 is a protein called ACPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	176	Total	C	N	O	S	0	0
			1368	891	224	244	9		

- Molecule 27 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
27	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	7	1	Total 53	C 43	Mg 1	N 4	O 5	0
27	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	7	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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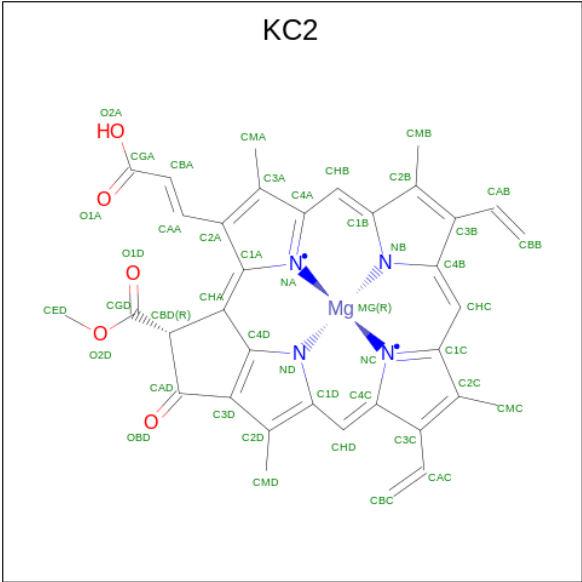
Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0

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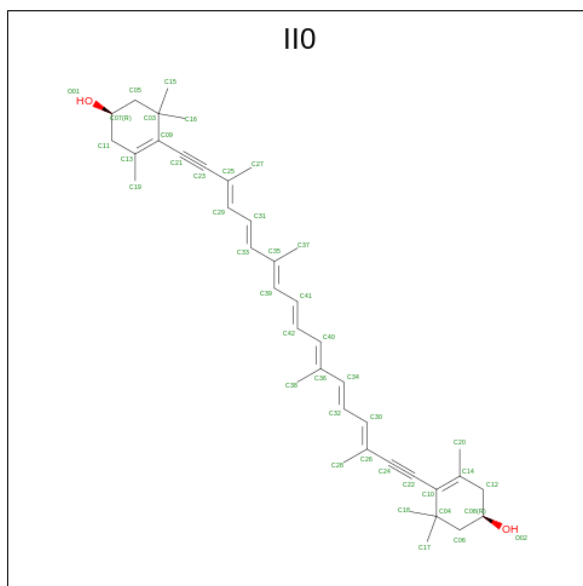
Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 28 is Chlorophyll c2 (three-letter code: KC2) (formula:  $C_{35}H_{28}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (three-letter code: II0) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	9	1	Total	C	O	0
			42	40	2	

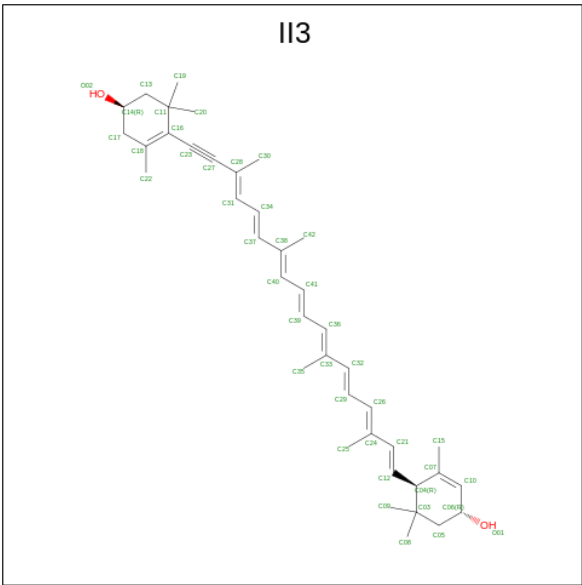
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Mol	Chain	Residues	Atoms			AltConf
29	9	1	Total	C	O	0
			42	40	2	
29	9	1	Total	C	O	0
			42	40	2	
29	9	1	Total	C	O	0
			42	40	2	
29	B	1	Total	C	O	0
			42	40	2	
29	J	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	Z	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	

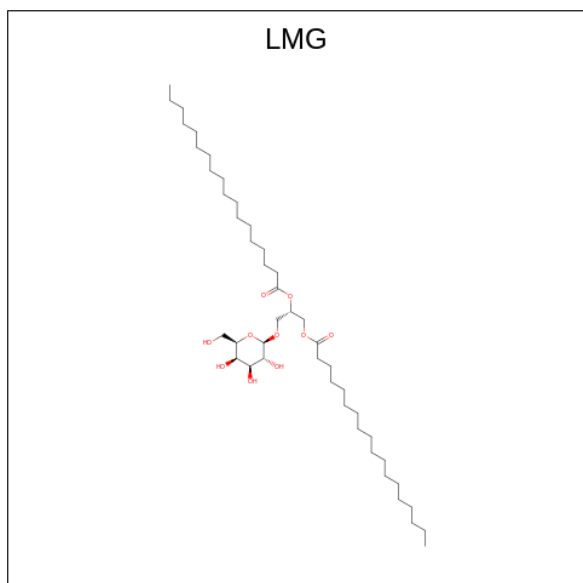
- Molecule 30 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: II3) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			41	40	1	
31	2	1	Total	C	O	0
			41	40	1	
31	5	1	Total	C	O	0
			41	40	1	
31	6	1	Total	C	O	0
			41	40	1	
31	8	1	Total	C	O	0
			41	40	1	
31	9	1	Total	C	O	0
			41	40	1	
31	A	1	Total	C	O	0
			41	40	1	
31	L	1	Total	C	O	0
			41	40	1	
31	Z	1	Total	C	O	0
			41	40	1	
31	a	1	Total	C	O	0
			41	40	1	

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



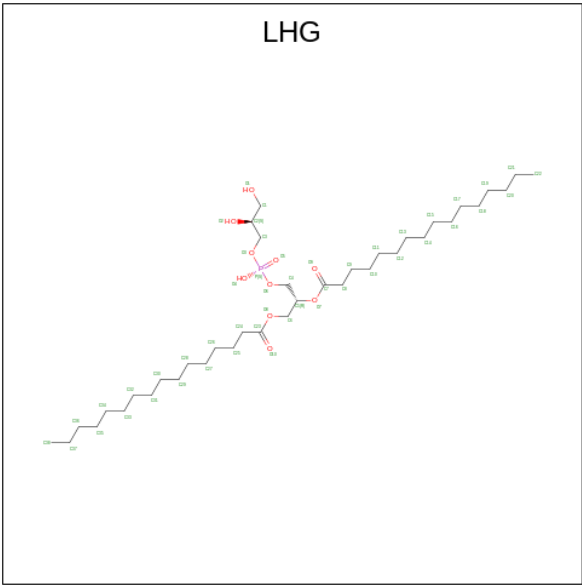
Mol	Chain	Residues	Atoms			AltConf
32	2	1	Total	C	O	0
			36	26	10	

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Mol	Chain	Residues	Atoms			AltConf
32	3	1	Total	C	O	0
			30	20	10	
32	3	1	Total	C	O	0
			32	22	10	
32	6	1	Total	C	O	0
			32	22	10	
32	8	1	Total	C	O	0
			52	42	10	
32	8	1	Total	C	O	0
			51	41	10	
32	F	1	Total	C	O	0
			32	22	10	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



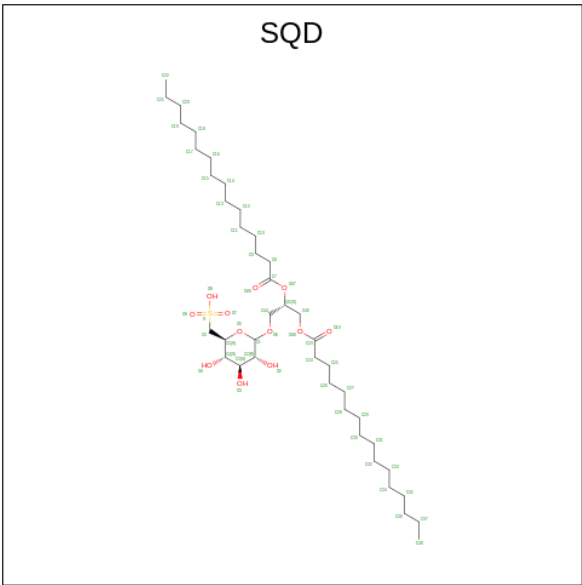
Mol	Chain	Residues	Atoms				AltConf
33	2	1	Total	C	O	P	0
			22	12	9	1	
33	2	1	Total	C	O	P	0
			39	28	10	1	
33	2	1	Total	C	O	P	0
			42	31	10	1	
33	3	1	Total	C	O	P	0
			49	38	10	1	
33	3	1	Total	C	O	P	0
			34	23	10	1	

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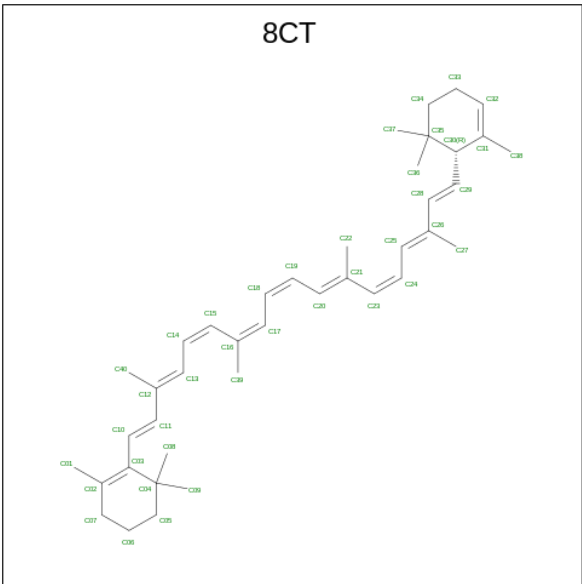
Mol	Chain	Residues	Atoms				AltConf
33	4	1	Total	C	O	P	0
			47	36	10	1	
33	4	1	Total	C	O	P	0
			45	34	10	1	
33	4	1	Total	C	O	P	0
			45	34	10	1	
33	5	1	Total	C	O	P	0
			23	12	10	1	
33	6	1	Total	C	O	P	0
			35	24	10	1	
33	7	1	Total	C	O	P	0
			31	20	10	1	
33	7	1	Total	C	O	P	0
			39	28	10	1	
33	8	1	Total	C	O	P	0
			33	22	10	1	
33	A	1	Total	C	O	P	0
			49	38	10	1	
33	A	1	Total	C	O	P	0
			39	28	10	1	
33	Z	1	Total	C	O	P	0
			46	35	10	1	
33	a	1	Total	C	O	P	0
			49	38	10	1	
33	a	1	Total	C	O	P	0
			29	18	10	1	
33	b	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				AltConf
34	3	1	Total	C	O	S	0
			42	29	12	1	
34	O	1	Total	C	O	S	0
			24	12	11	1	

- Molecule 35 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
35	4	1	Total	C	0
			40	40	

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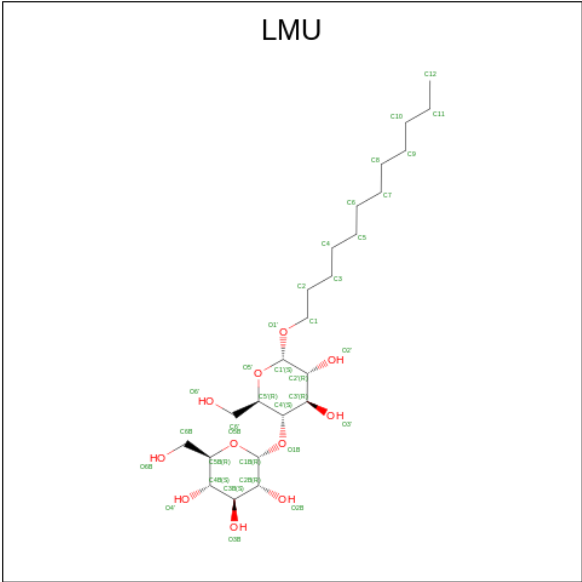
Mol	Chain	Residues	Atoms	AltConf
35	7	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	F	1	Total C 40 40	0
35	I	1	Total C 40 40	0
35	J	1	Total C 40 40	0
35	K	1	Total C 40 40	0
35	L	1	Total C 40 40	0
35	M	1	Total C 40 40	0
35	R	1	Total C 40 40	0
35	R	1	Total C 40 40	0
35	Z	1	Total C 40 40	0

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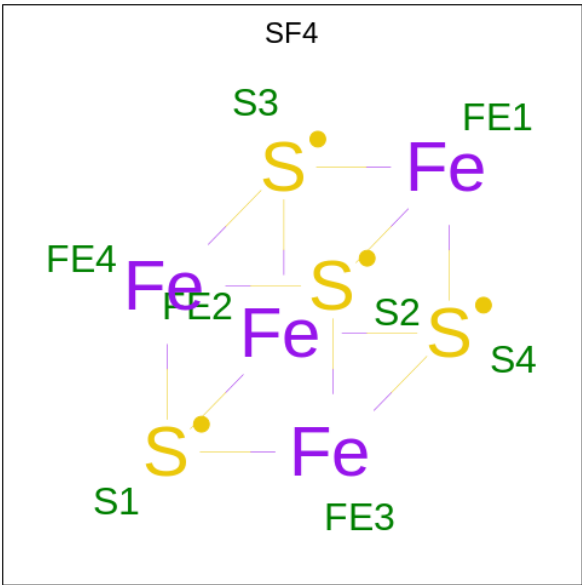
Mol	Chain	Residues	Atoms		AltConf
35	Z	1	Total	C	0
			40	40	
35	b	1	Total	C	0
			40	40	

- Molecule 36 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



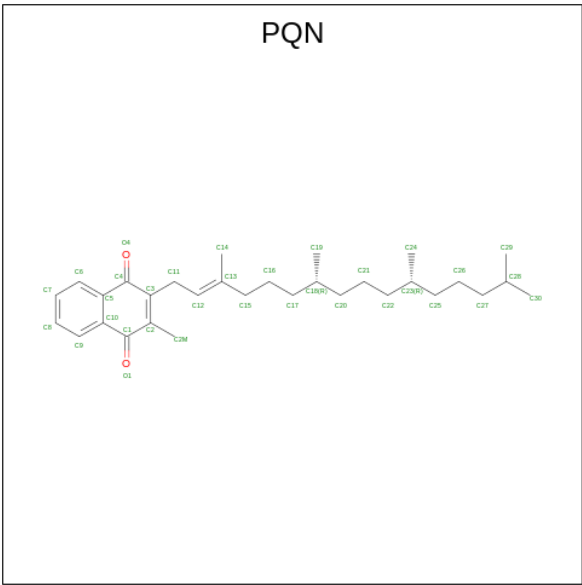
Mol	Chain	Residues	Atoms			AltConf
36	4	1	Total	C	O	0
			35	24	11	
36	7	1	Total	C	O	0
			35	24	11	
36	J	1	Total	C	O	0
			31	20	11	

- Molecule 37 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



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

- Molecule 38 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



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

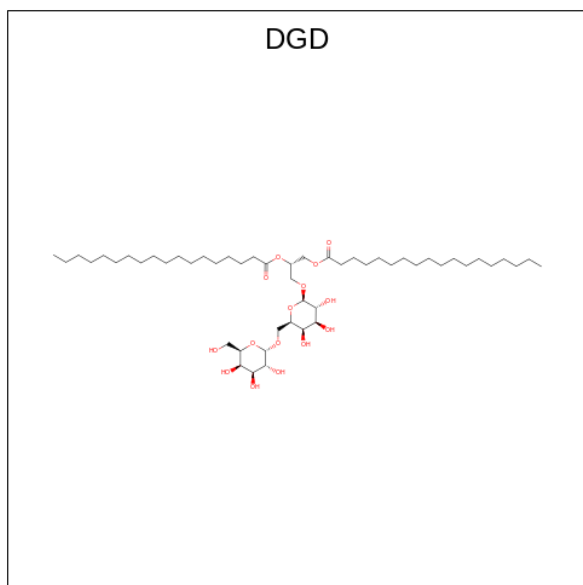
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Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			33	31	2	

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).

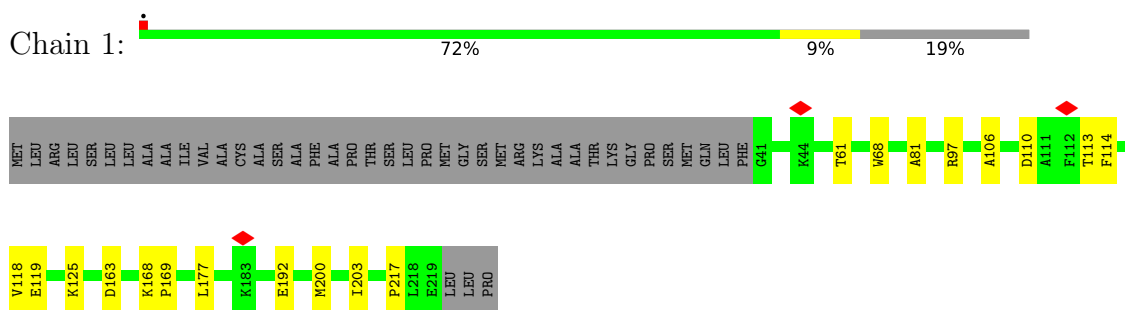


Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			59	44	15	
39	Z	1	Total	C	O	0
			60	45	15	

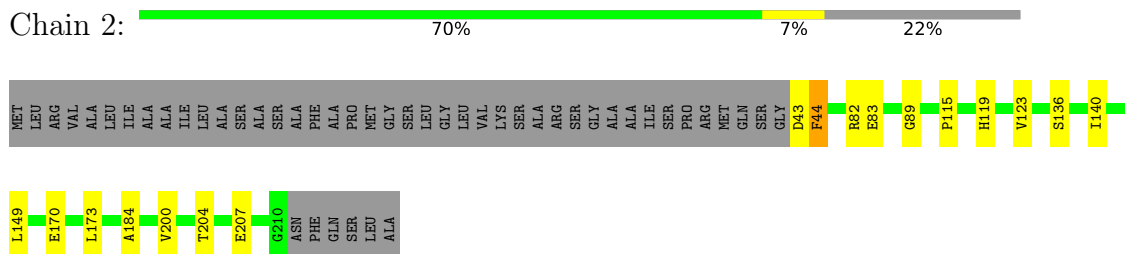
### 3 Residue-property plots

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.

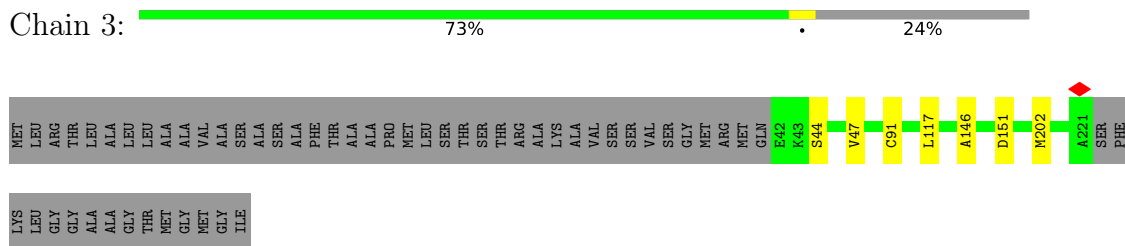
#### • Molecule 1: ACPI-1



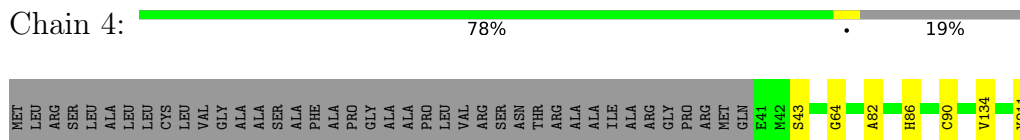
#### • Molecule 2: ACPI-2



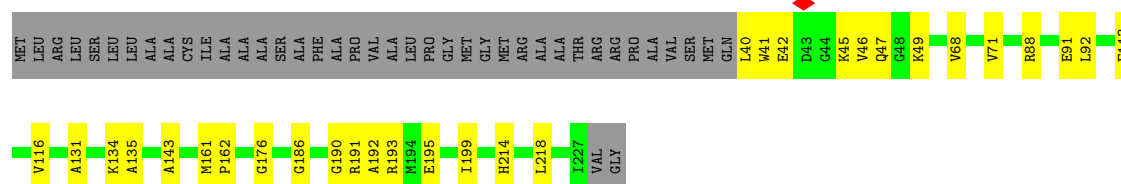
#### • Molecule 3: ACPI-3



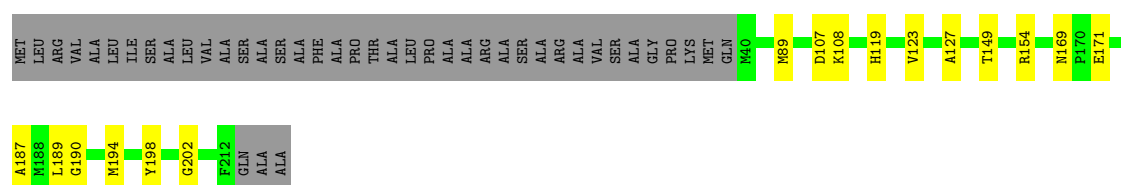
#### • Molecule 4: ACPI-4



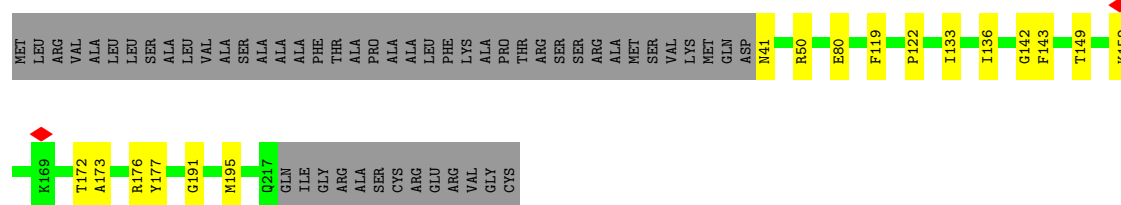
## • Molecule 5: ACPI-5

Chain 5:  69% 13% 18%

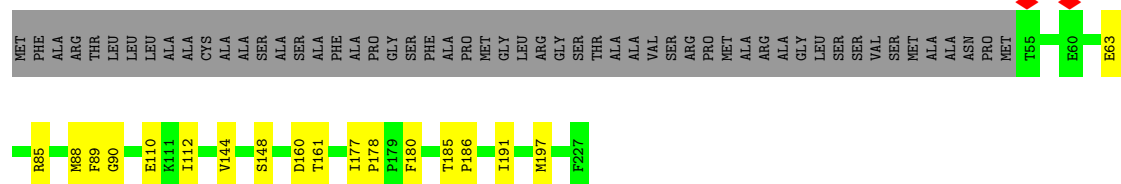
## • Molecule 6: ACPI-6

Chain 6:  73% 7% 20%


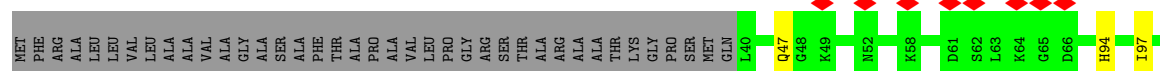
## • Molecule 7: ACPI-7

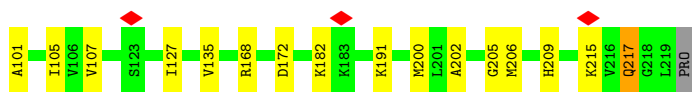
Chain 7:  70% 7% 23%

## • Molecule 8: ACPI-8

Chain 8:  68% 8% 24%

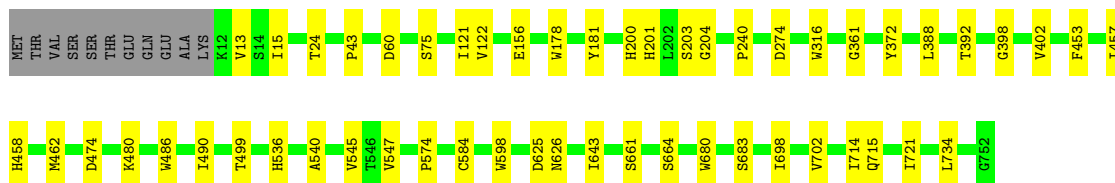
## • Molecule 9: ACPI-12

Chain 9:  5% 73% 8% 18%



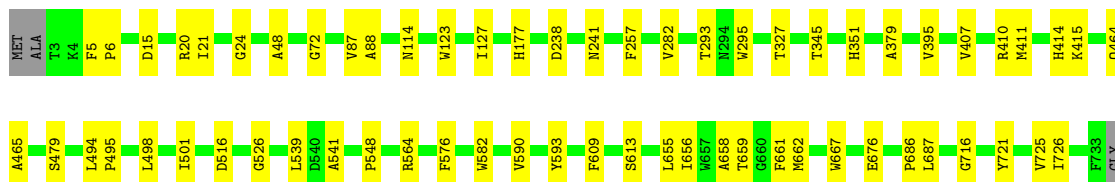
- Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 91% 7% .



- Molecule 11: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 91% 9%



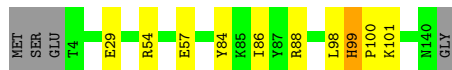
- Molecule 12: Photosystem I iron-sulfur center

Chain C: 86% 11% ..



- Molecule 13: Photosystem I reaction center subunit II

Chain D: 90% 6% . .



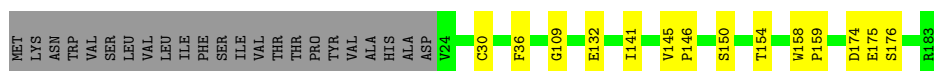
- Molecule 14: Photosystem I reaction center subunit IV

Chain E: 89% 6% 5%



- Molecule 15: Photosystem I reaction center subunit III

Chain F: 80% 8% 13%



• Molecule 16: Photosystem I reaction center subunit VIII

Chain I: 86% 6% 8%



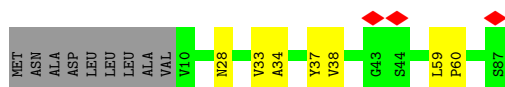
• Molecule 17: Photosystem I reaction center subunit IX

Chain J: 93% 7%



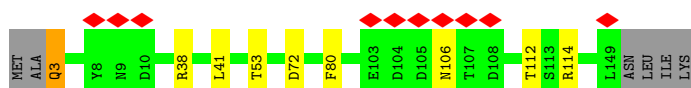
• Molecule 18: Photosystem I reaction center subunit PsaK

Chain K: 82% 8% 10%



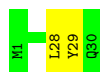
• Molecule 19: Photosystem I reaction center subunit XI

Chain L: 7% 90% 5% . .



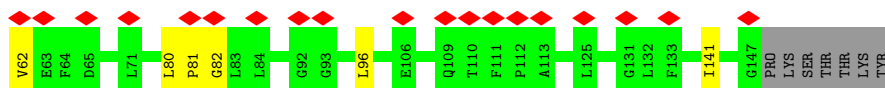
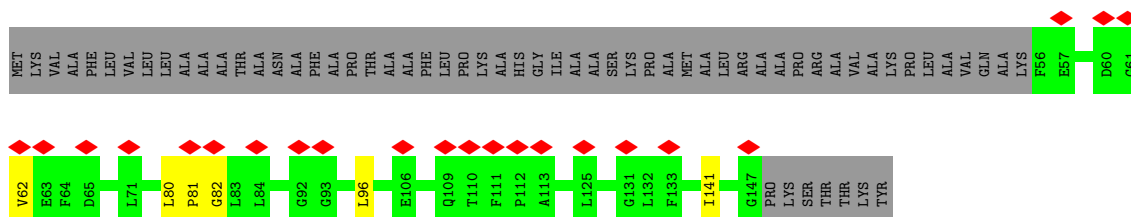
• Molecule 20: Photosystem I reaction center subunit XII

Chain M: 93% 7%

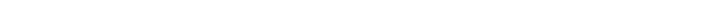


• Molecule 21: PsaO

Chain O: 14% 56% 40%



Chain R:  61% 8% 31%

Chain X: 

Chain Z:  60% 37%

Chain a:  80% 20%

Chain b:  80% 19%

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.988	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, IHT, 8CT, CLA, LMU, PQN, LHG, DGD, SQD, KC2, II3, LMG, II0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.33	0/1371	0.59	0/1854
2	2	0.27	0/1356	0.45	0/1835
3	3	0.26	0/1392	0.47	0/1883
4	4	0.28	0/1406	0.44	0/1900
5	5	0.33	0/1438	0.52	0/1940
6	6	0.27	0/1334	0.46	0/1796
7	7	0.32	0/1373	0.48	0/1858
8	8	0.28	0/1326	0.47	0/1804
9	9	0.27	0/1376	0.46	0/1846
10	A	0.29	0/6019	0.46	0/8204
11	B	0.30	0/6046	0.48	0/8254
12	C	0.30	0/600	0.58	0/812
13	D	0.30	0/1094	0.51	0/1476
14	E	0.33	0/499	0.60	0/677
15	F	0.29	0/1290	0.48	0/1745
16	I	0.29	0/266	0.43	0/362
17	J	0.28	0/353	0.43	0/481
18	K	0.32	0/563	0.45	0/768
19	L	0.35	0/1147	0.54	0/1561
20	M	0.27	0/228	0.41	0/310
21	O	0.29	0/737	0.45	0/1011
22	R	0.31	0/700	0.44	0/963
24	Z	0.29	0/1163	0.47	0/1572
25	a	0.36	0/1299	0.52	0/1747
26	b	0.29	0/1404	0.48	0/1902
All	All	0.30	0/35780	0.48	0/48561

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1338	0	1329	14	0
2	2	1320	0	1309	11	0
3	3	1362	0	1389	5	0
4	4	1366	0	1349	5	0
5	5	1403	0	1398	28	0
6	6	1305	0	1324	9	0
7	7	1337	0	1317	12	0
8	8	1298	0	1322	15	0
9	9	1349	0	1358	17	0
10	A	5824	0	5672	41	0
11	B	5828	0	5626	39	0
12	C	591	0	568	8	0
13	D	1070	0	1076	9	0
14	E	491	0	491	3	0
15	F	1258	0	1266	11	0
16	I	258	0	268	2	0
17	J	342	0	344	2	0
18	K	553	0	581	8	0
19	L	1119	0	1117	5	0
20	M	227	0	257	2	0
21	O	709	0	691	4	0
22	R	680	0	674	6	0
23	X	725	0	151	12	0
24	Z	1130	0	1088	5	0
25	a	1271	0	1280	0	0
26	b	1368	0	1346	0	0
27	1	584	0	476	1	0
27	2	547	0	456	1	0
27	3	625	0	596	0	0
27	4	598	0	597	1	0
27	5	563	0	442	5	0
27	6	581	0	514	2	0
27	7	509	0	431	2	0
27	8	496	0	471	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	9	642	0	539	5	0
27	A	2679	0	2767	28	0
27	B	2471	0	2530	17	0
27	F	160	0	141	0	0
27	J	41	0	29	0	0
27	K	120	0	121	1	0
27	L	161	0	139	1	0
27	O	206	0	176	1	0
27	R	55	0	49	0	0
27	Z	290	0	278	1	0
27	a	580	0	560	0	0
27	b	530	0	525	0	0
28	1	45	0	0	0	0
28	2	45	0	0	0	0
28	3	45	0	0	0	0
28	4	45	0	0	0	0
28	5	45	0	0	0	0
28	6	90	0	0	0	0
28	7	90	0	0	2	0
28	9	45	0	0	1	0
28	Z	45	0	0	0	0
28	a	45	0	0	0	0
28	b	90	0	0	0	0
29	1	168	0	0	0	0
29	2	126	0	0	1	0
29	3	210	0	0	1	0
29	4	168	0	0	1	0
29	5	210	0	0	2	0
29	6	84	0	0	0	0
29	7	210	0	0	0	0
29	8	126	0	0	1	0
29	9	168	0	0	0	0
29	B	42	0	0	0	0
29	J	42	0	0	0	0
29	O	84	0	0	0	0
29	R	42	0	0	0	0
29	Z	42	0	0	0	0
29	a	168	0	0	0	0
29	b	84	0	0	0	0
30	1	42	0	0	0	0
30	b	42	0	0	0	0
31	1	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	2	41	0	0	0	0
31	5	41	0	0	0	0
31	6	41	0	0	0	0
31	8	41	0	0	0	0
31	9	41	0	0	1	0
31	A	41	0	0	1	0
31	L	41	0	0	0	0
31	Z	41	0	0	0	0
31	a	41	0	0	0	0
32	2	36	0	42	0	0
32	3	62	0	64	0	0
32	6	32	0	34	0	0
32	8	103	0	152	0	0
32	F	32	0	34	0	0
33	2	103	0	125	1	0
33	3	83	0	112	0	0
33	4	137	0	190	0	0
33	5	23	0	16	0	0
33	6	35	0	40	0	0
33	7	70	0	83	0	0
33	8	33	0	36	0	0
33	A	88	0	122	0	0
33	Z	46	0	65	0	0
33	a	78	0	102	0	0
33	b	49	0	74	0	0
34	3	42	0	48	0	0
34	O	24	0	18	0	0
35	4	40	0	0	0	0
35	7	40	0	0	0	0
35	A	200	0	0	0	0
35	B	240	0	0	0	0
35	F	40	0	0	0	0
35	I	40	0	0	0	0
35	J	40	0	0	0	0
35	K	40	0	0	0	0
35	L	40	0	0	0	0
35	M	40	0	0	1	0
35	R	80	0	0	0	0
35	Z	80	0	0	0	0
35	b	40	0	0	0	0
36	4	35	0	46	2	0
36	7	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	J	31	0	35	1	0
37	A	8	0	0	0	0
37	C	16	0	0	1	0
38	A	33	0	46	0	0
38	B	33	0	46	0	0
39	B	59	0	79	0	0
39	Z	60	0	78	1	0
All	All	53404	0	48161	285	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (285) 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)
5:5:41:TRP:HB2	5:5:192:ALA:HB1	1.44	0.99
13:D:99:HIS:HB3	13:D:100:PRO:HD3	1.55	0.88
5:5:42:GLU:HB3	5:5:45:LYS:HB2	1.58	0.84
22:R:74:VAL:O	22:R:128:GLN:NE2	2.13	0.81
4:4:43:SER:OG	4:4:64:GLY:O	1.99	0.79
9:9:105:ILE:HG23	9:9:127:ILE:HG21	1.65	0.78
36:J:104:LMU:O5B	36:J:104:LMU:O3'	2.02	0.78
27:A:818:CLA:H61	18:K:59:LEU:HD21	1.63	0.78
16:I:29:TYR:HH	20:M:29:TYR:HH	1.33	0.76
5:5:42:GLU:CB	5:5:45:LYS:HB2	2.17	0.73
15:F:174:ASP:OD2	15:F:176:SER:OG	2.09	0.71
27:A:844:CLA:OBD	27:B:801:CLA:HMB3	1.89	0.70
11:B:609:PHE:O	11:B:613:SER:OG	2.09	0.70
1:1:97:ARG:NH1	1:1:192:GLU:OE2	2.25	0.70
36:4:618:LMU:O5B	36:4:618:LMU:O3'	2.09	0.70
10:A:680:TRP:O	10:A:683:SER:OG	2.11	0.68
9:9:135:VAL:O	39:Z:303:DGD:O2D	2.10	0.67
9:9:107:VAL:HG11	27:9:604:CLA:HBC3	1.77	0.65
10:A:540:ALA:HB1	27:A:836:CLA:HMB3	1.79	0.65
11:B:465:ALA:O	11:B:479:SER:OG	2.15	0.64
1:1:163:ASP:OD2	33:2:619:LHG:O2	2.15	0.63
13:D:88:ARG:HB2	13:D:98:LEU:HD11	1.81	0.63
9:9:168:ARG:NH1	9:9:172:ASP:O	2.31	0.63
11:B:345:THR:HG23	11:B:379:ALA:HB2	1.80	0.62
27:A:801:CLA:HMB3	27:A:840:CLA:OBD	2.00	0.62
15:F:174:ASP:OD1	15:F:175:GLU:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:57:GLU:OE2	13:D:57:GLU:N	2.32	0.61
5:5:88:ARG:NH1	5:5:91:GLU:OE1	2.34	0.61
5:5:40:LEU:HG	5:5:193:ARG:HH11	1.64	0.60
5:5:49:LYS:HA	5:5:49:LYS:HE2	1.82	0.60
2:2:89:GLY:HA3	2:2:184:ALA:HB1	1.83	0.60
5:5:41:TRP:CB	5:5:192:ALA:HB1	2.24	0.60
23:X:81:UNK:O	23:X:82:UNK:C	2.50	0.59
18:K:34:ALA:O	18:K:38:VAL:HG22	2.03	0.59
1:1:110:ASP:OD1	1:1:125:LYS:NZ	2.32	0.58
5:5:42:GLU:HB3	5:5:45:LYS:HE2	1.85	0.58
8:8:197:MET:HE3	27:8:602:CLA:HMC3	1.85	0.58
8:8:144:VAL:O	8:8:148:SER:OG	2.18	0.58
9:9:217:GLN:H	9:9:217:GLN:HE21	1.52	0.57
10:A:547:VAL:HG11	27:A:837:CLA:HMB3	1.86	0.57
5:5:92:LEU:HD13	5:5:176:GLY:HA3	1.85	0.57
1:1:68:TRP:CZ3	1:1:169:PRO:HG3	2.40	0.56
9:9:217:GLN:H	9:9:217:GLN:NE2	2.03	0.56
5:5:68:VAL:HG11	5:5:195:GLU:HB2	1.87	0.56
10:A:200:HIS:CG	27:A:811:CLA:HMC2	2.40	0.56
2:2:83:GLU:OE2	2:2:149:LEU:HD22	2.06	0.56
9:9:97:ILE:HD12	27:9:607:CLA:HMD3	1.86	0.56
10:A:201:HIS:ND1	27:A:823:CLA:OBD	2.38	0.56
5:5:131:ALA:HA	5:5:134:LYS:HG2	1.88	0.56
1:1:61:THR:CG2	1:1:81:ALA:HB2	2.35	0.56
27:B:809:CLA:H2A	27:B:809:CLA:O2A	2.06	0.55
8:8:185:THR:HG23	8:8:186:PRO:HD2	1.87	0.55
6:6:89:MET:HA	6:6:187:ALA:HB1	1.89	0.55
8:8:110:GLU:OE2	8:8:110:GLU:N	2.37	0.55
23:X:95:UNK:C	23:X:97:UNK:H	2.19	0.55
11:B:516:ASP:OD2	11:B:593:TYR:OH	2.22	0.54
7:7:149:THR:HA	7:7:152:LYS:HD2	1.90	0.54
23:X:84:UNK:O	23:X:85:UNK:C	2.54	0.54
9:9:105:ILE:HG23	9:9:127:ILE:CG2	2.37	0.54
5:5:40:LEU:HD12	27:5:609:CLA:HED3	1.90	0.53
13:D:86:ILE:HD12	13:D:99:HIS:HB2	1.90	0.53
1:1:168:LYS:HG3	1:1:169:PRO:HD2	1.91	0.53
27:B:834:CLA:HMB1	27:B:834:CLA:HBB1	1.91	0.53
24:Z:210:GLY:O	24:Z:214:LYS:HG3	2.08	0.52
2:2:115:PRO:O	29:2:614:II0:O01	2.28	0.52
5:5:42:GLU:HB2	5:5:46:VAL:HG22	1.91	0.52
27:B:807:CLA:C1A	27:B:807:CLA:CGA	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:68:TRP:HZ3	1:1:169:PRO:CG	2.23	0.52
8:8:185:THR:CG2	8:8:186:PRO:HD2	2.40	0.52
24:Z:125:GLN:HB2	24:Z:126:PRO:HD3	1.92	0.51
27:A:818:CLA:C6	18:K:59:LEU:HD21	2.38	0.51
13:D:99:HIS:HB3	13:D:100:PRO:CD	2.36	0.51
23:X:76:UNK:O	23:X:78:UNK:N	2.42	0.51
9:9:107:VAL:HG11	27:9:604:CLA:CBC	2.41	0.51
13:D:99:HIS:O	13:D:101:LYS:N	2.43	0.51
5:5:40:LEU:HD13	5:5:46:VAL:HG11	1.93	0.51
5:5:161:MET:N	5:5:162:PRO:CD	2.73	0.51
11:B:410:ARG:O	11:B:414:HIS:ND1	2.37	0.51
22:R:57:TYR:OH	22:R:59:GLU:OE1	2.28	0.51
7:7:133:ILE:HA	7:7:136:ILE:HD12	1.92	0.50
22:R:60:THR:OG1	22:R:62:ALA:O	2.29	0.50
23:X:77:UNK:C	23:X:79:UNK:N	2.68	0.50
10:A:584:CYS:HB2	11:B:667:TRP:HB3	1.93	0.50
12:C:75:ARG:NH1	13:D:29:GLU:OE2	2.45	0.50
15:F:150:SER:O	15:F:154:THR:HG23	2.11	0.50
4:4:82:ALA:O	4:4:86:HIS:ND1	2.44	0.50
10:A:486:TRP:CE2	10:A:490:ILE:HD11	2.47	0.50
11:B:498:LEU:HA	11:B:501:ILE:HG22	1.94	0.50
5:5:71:VAL:HG12	5:5:71:VAL:O	2.12	0.50
10:A:661:SER:O	10:A:664:SER:OG	2.27	0.49
11:B:15:ASP:HB3	11:B:20:ARG:HB2	1.93	0.49
5:5:41:TRP:HA	5:5:47:GLN:HE21	1.76	0.49
12:C:54:CYS:SG	12:C:55:GLU:N	2.85	0.49
22:R:63:PRO:O	22:R:131:ASN:ND2	2.45	0.49
7:7:176:ARG:HG3	7:7:177:TYR:N	2.28	0.49
10:A:388:LEU:O	10:A:392:THR:HG22	2.12	0.49
17:J:8:TYR:HA	17:J:11:THR:HG23	1.95	0.49
7:7:177:TYR:CD1	28:7:311:KC2:O1A	2.66	0.49
10:A:625:ASP:OD1	10:A:625:ASP:O	2.30	0.49
24:Z:149:GLU:OE2	24:Z:158:LYS:NZ	2.46	0.48
10:A:536:HIS:CD2	27:A:836:CLA:HED3	2.48	0.48
7:7:122:PRO:HB3	23:X:3:UNK:HA	1.95	0.48
10:A:625:ASP:O	10:A:626:ASN:CB	2.60	0.48
12:C:61:ASP:OD2	14:E:15:SER:HB2	2.12	0.48
23:X:76:UNK:C	23:X:78:UNK:N	2.77	0.48
10:A:178:TRP:HB2	27:A:809:CLA:HMC3	1.94	0.48
11:B:327:THR:HG21	22:R:47:VAL:HG13	1.96	0.47
23:X:82:UNK:O	23:X:83:UNK:CB	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:819:CLA:OBD	27:A:821:CLA:HMD3	2.14	0.47
5:5:190:GLY:O	5:5:191:ARG:C	2.51	0.47
6:6:127:ALA:HB1	27:6:605:CLA:HMD1	1.96	0.47
9:9:94:HIS:HB3	9:9:200:MET:SD	2.54	0.47
31:A:854:IHT:O01	18:K:38:VAL:HG21	2.13	0.47
11:B:5:PHE:HB3	11:B:6:PRO:HD3	1.96	0.47
27:A:826:CLA:HBB1	27:A:826:CLA:HMB1	1.97	0.47
29:5:620:II0:C30	6:6:189:LEU:HD13	2.45	0.47
7:7:172:THR:HG23	7:7:173:ALA:N	2.30	0.47
10:A:715:GLN:NE2	14:E:43:VAL:O	2.45	0.47
11:B:407:VAL:O	11:B:411:MET:HG2	2.15	0.47
15:F:145:VAL:HG22	15:F:146:PRO:HD3	1.97	0.47
36:7:321:LMU:O5B	36:7:321:LMU:O6'	2.33	0.47
10:A:274:ASP:N	10:A:274:ASP:OD1	2.47	0.47
27:A:810:CLA:H43	27:A:810:CLA:NB	2.30	0.47
5:5:135:ALA:HB3	5:5:143:ALA:HB1	1.97	0.46
19:L:106:ASN:HB3	19:L:112:THR:CG2	2.45	0.46
21:O:141:ILE:HG12	27:O:201:CLA:ND	2.29	0.46
5:5:41:TRP:CG	5:5:41:TRP:O	2.67	0.46
10:A:121:ILE:HG13	10:A:122:VAL:HG13	1.97	0.46
11:B:659:THR:O	11:B:662:MET:HB3	2.16	0.46
23:X:89:UNK:O	23:X:90:UNK:C	2.63	0.46
1:1:177:LEU:N	1:1:177:LEU:HD12	2.31	0.46
5:5:40:LEU:HG	5:5:193:ARG:NH1	2.31	0.46
9:9:191:LYS:NZ	28:9:610:KC2:O2A	2.38	0.46
1:1:114:PHE:N	27:1:604:CLA:OBD	2.42	0.46
7:7:177:TYR:HD1	28:7:311:KC2:O1A	1.99	0.46
10:A:240:PRO:HB2	27:A:812:CLA:HMD1	1.98	0.46
10:A:734:LEU:HD22	27:A:838:CLA:HMA1	1.98	0.46
4:4:211:TYR:OH	27:Z:304:CLA:OBD	2.25	0.46
8:8:148:SER:HB3	27:8:605:CLA:NC	2.31	0.46
2:2:170:GLU:O	2:2:173:LEU:N	2.49	0.46
4:4:134:VAL:HG11	27:4:606:CLA:HMC3	1.97	0.46
10:A:545:VAL:HG11	10:A:598:TRP:CZ2	2.51	0.46
27:A:836:CLA:C1A	27:A:836:CLA:CGA	2.94	0.46
11:B:721:TYR:HB2	27:B:801:CLA:HED2	1.98	0.46
27:B:832:CLA:O1A	27:B:832:CLA:C2	2.64	0.46
3:3:117:LEU:HG	3:3:202:MET:HE3	1.98	0.46
10:A:121:ILE:HG23	10:A:122:VAL:N	2.30	0.46
23:X:77:UNK:O	23:X:81:UNK:N	2.49	0.45
3:3:151:ASP:OD1	3:3:151:ASP:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:14:CYS:SG	12:C:16:GLN:HG2	2.56	0.45
5:5:42:GLU:OE1	5:5:46:VAL:HG13	2.17	0.45
11:B:5:PHE:CE2	11:B:24:GLY:HA3	2.51	0.45
22:R:98:ILE:HB	22:R:99:PRO:HD3	1.99	0.45
29:5:620:II0:C16	27:6:611:CLA:HMD1	2.47	0.45
10:A:156:GLU:OE1	10:A:156:GLU:N	2.49	0.45
27:A:823:CLA:HBB1	27:A:823:CLA:HMB1	1.99	0.45
2:2:119:HIS:O	2:2:123:VAL:HG23	2.17	0.45
11:B:5:PHE:CE2	11:B:21:ILE:HA	2.52	0.45
11:B:88:ALA:N	11:B:114:ASN:O	2.40	0.45
1:1:106:ALA:HB1	1:1:217:PRO:HG3	1.98	0.45
27:7:313:CLA:C1C	27:7:313:CLA:H43	2.46	0.45
8:8:85:ARG:HA	8:8:88:MET:HE3	1.99	0.45
2:2:82:ARG:O	2:2:82:ARG:HD3	2.16	0.44
10:A:474:ASP:OD1	10:A:480:LYS:NZ	2.41	0.44
6:6:107:ASP:OD1	6:6:108:LYS:N	2.51	0.44
9:9:205:GLY:O	9:9:209:HIS:CG	2.70	0.44
10:A:121:ILE:HG23	10:A:122:VAL:H	1.82	0.44
4:4:90:CYS:SG	29:4:613:II0:C39	3.06	0.44
6:6:149:THR:OG1	6:6:154:ARG:NH1	2.50	0.44
9:9:182:LYS:HE2	9:9:182:LYS:HA	1.99	0.44
18:K:59:LEU:O	18:K:60:PRO:C	2.54	0.44
11:B:123:TRP:O	11:B:127:ILE:HG12	2.18	0.44
6:6:198:TYR:O	6:6:202:GLY:N	2.44	0.44
1:1:119:GLU:OE1	1:1:119:GLU:N	2.49	0.44
8:8:160:ASP:OD1	8:8:161:THR:N	2.51	0.44
11:B:351:HIS:CE1	27:B:825:CLA:NB	2.85	0.44
10:A:15:ILE:HD13	27:A:808:CLA:HAA2	2.00	0.44
11:B:5:PHE:HB3	11:B:20:ARG:HH11	1.82	0.44
27:B:816:CLA:O2A	27:B:816:CLA:H42	2.18	0.44
9:9:202:ALA:O	9:9:206:MET:HG3	2.17	0.43
10:A:203:SER:OG	10:A:204:GLY:N	2.51	0.43
10:A:499:THR:HG22	27:A:834:CLA:HED3	1.99	0.43
27:A:810:CLA:H42	27:A:810:CLA:O1A	2.18	0.43
13:D:84:TYR:CE2	13:D:99:HIS:CD2	3.05	0.43
19:L:38:ARG:NH2	19:L:41:LEU:HD11	2.33	0.43
11:B:676:GLU:HG3	12:C:81:TYR:HE2	1.83	0.43
8:8:63:GLU:OE1	8:8:64:SER:N	2.52	0.43
8:8:178:PRO:HG2	8:8:191:ILE:HG13	2.00	0.43
27:B:832:CLA:HMB3	27:B:834:CLA:HED2	2.00	0.43
12:C:17:CYS:SG	12:C:18:VAL:N	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:215:LYS:HB3	9:9:217:GLN:CD	2.39	0.43
11:B:725:VAL:HG12	11:B:726:ILE:N	2.34	0.43
19:L:72:ASP:O	19:L:72:ASP:OD1	2.36	0.43
11:B:395:VAL:CG2	11:B:541:ALA:HB1	2.49	0.43
2:2:200:VAL:HG21	27:2:611:CLA:HMD1	2.01	0.43
8:8:112:ILE:HD12	8:8:112:ILE:N	2.33	0.43
10:A:361:GLY:HA2	10:A:398:GLY:HA2	2.01	0.43
10:A:24:THR:O	10:A:24:THR:HG23	2.18	0.43
5:5:113:PHE:O	5:5:116:VAL:HG12	2.19	0.43
6:6:169:ASN:ND2	6:6:171:GLU:OE1	2.52	0.43
8:8:197:MET:HB3	27:8:602:CLA:HMC3	2.01	0.43
11:B:177:HIS:CG	27:B:812:CLA:HMC2	2.54	0.43
11:B:656:ILE:HG23	11:B:716:GLY:CA	2.49	0.43
12:C:17:CYS:HB3	37:C:102:SF4:S4	2.58	0.43
2:2:204:THR:O	2:2:207:GLU:HG2	2.19	0.42
5:5:41:TRP:HE3	5:5:47:GLN:NE2	2.17	0.42
18:K:28:ASN:ND2	27:K:102:CLA:O1A	2.52	0.42
21:O:82:GLY:O	21:O:96:LEU:N	2.51	0.42
2:2:170:GLU:OE2	2:2:170:GLU:HA	2.19	0.42
3:3:91:CYS:SG	29:3:614:II0:C39	3.08	0.42
15:F:158:TRP:N	15:F:159:PRO:CD	2.82	0.42
24:Z:67:VAL:HG13	24:Z:67:VAL:O	2.20	0.42
10:A:402:VAL:HG11	27:A:824:CLA:HMC3	2.02	0.42
5:5:214:HIS:O	5:5:218:LEU:HD12	2.19	0.42
27:5:604:CLA:CGA	27:5:604:CLA:C1A	2.98	0.42
27:9:606:CLA:HMB3	31:9:619:IHT:C24	2.50	0.42
11:B:48:ALA:HB3	20:M:28:LEU:HD21	2.02	0.42
1:1:200:MET:O	1:1:203:ILE:HG22	2.20	0.42
11:B:548:PRO:HD2	12:C:62:PHE:CE1	2.55	0.42
27:B:802:CLA:CGA	27:B:802:CLA:H3A	2.49	0.42
27:B:840:CLA:HBC3	15:F:109:GLY:CA	2.50	0.42
19:L:3:GLN:O	21:O:62:VAL:HG21	2.19	0.42
5:5:186:GLY:HA3	27:5:608:CLA:HBA2	2.01	0.42
10:A:13:VAL:HG12	27:A:810:CLA:O1D	2.20	0.42
21:O:80:LEU:HB2	21:O:81:PRO:HD3	2.00	0.42
36:4:618:LMU:H3O2	36:4:618:LMU:C5B	2.27	0.42
5:5:218:LEU:HG	27:5:612:CLA:HED2	2.02	0.42
11:B:658:ALA:O	11:B:661:PHE:HB2	2.20	0.42
13:D:54:ARG:NH1	13:D:57:GLU:O	2.52	0.42
15:F:145:VAL:N	15:F:146:PRO:CD	2.83	0.42
18:K:59:LEU:N	18:K:60:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:119:HIS:O	6:6:123:VAL:HG23	2.20	0.42
7:7:142:GLY:O	7:7:143:PHE:HB2	2.19	0.41
9:9:101:ALA:O	9:9:105:ILE:HG13	2.20	0.41
10:A:643:ILE:HG21	27:A:844:CLA:CGA	2.50	0.41
15:F:132:GLU:HA	15:F:132:GLU:OE1	2.20	0.41
10:A:698:ILE:O	10:A:702:VAL:HG23	2.20	0.41
27:B:822:CLA:HMA1	27:B:839:CLA:CGD	2.50	0.41
24:Z:147:GLU:OE2	24:Z:147:GLU:HA	2.21	0.41
7:7:119:PHE:CD1	23:X:81:UNK:CB	3.03	0.41
11:B:494:LEU:N	11:B:495:PRO:HD2	2.35	0.41
27:8:608:CLA:CGA	27:8:608:CLA:C1A	2.98	0.41
11:B:282:VAL:CG2	27:B:815:CLA:HMC3	2.51	0.41
2:2:136:SER:O	2:2:140:ILE:HD13	2.20	0.41
6:6:190:GLY:O	6:6:194:MET:HG3	2.20	0.41
11:B:526:GLY:HA2	11:B:582:TRP:CZ3	2.55	0.41
15:F:30:CYS:SG	15:F:36:PHE:CG	3.13	0.41
8:8:90:GLY:HA3	29:8:610:II0:C14	2.50	0.41
8:8:177:ILE:HD11	8:8:180:PHE:CZ	2.55	0.41
11:B:72:GLY:HA2	11:B:87:VAL:CG2	2.50	0.41
11:B:590:VAL:HG21	27:B:834:CLA:HBB2	2.02	0.41
1:1:113:THR:HG21	1:1:118:VAL:HB	2.03	0.41
3:3:146:ALA:HA	3:3:151:ASP:OD1	2.21	0.41
27:5:608:CLA:H41	27:5:608:CLA:C7	2.51	0.41
27:A:844:CLA:HBA2	11:B:655:LEU:HB2	2.02	0.41
1:1:61:THR:HG22	1:1:81:ALA:HB2	2.03	0.41
10:A:316:TRP:CE2	27:A:818:CLA:O1A	2.74	0.41
10:A:458:HIS:O	10:A:462:MET:HG2	2.21	0.41
10:A:574:PRO:HB3	10:A:721:ILE:HB	2.02	0.41
10:A:584:CYS:CB	11:B:667:TRP:HB3	2.50	0.41
27:A:842:CLA:HED2	17:J:16:LEU:HD22	2.02	0.41
27:A:843:CLA:HAA1	27:B:830:CLA:HMB1	2.02	0.41
35:M:101:8CT:C28	35:M:101:8CT:C38	2.98	0.41
23:X:98:UNK:O	23:X:99:UNK:C	2.69	0.41
7:7:191:GLY:O	7:7:195:MET:HG3	2.20	0.41
10:A:75:SER:OG	10:A:181:TYR:HB2	2.21	0.41
10:A:453:PHE:CZ	10:A:457:ILE:HD11	2.55	0.41
2:2:43:ASP:O	2:2:44:PHE:HB2	2.21	0.40
9:9:200:MET:HE3	27:9:602:CLA:HMC3	2.03	0.40
10:A:43:PRO:HG3	15:F:141:ILE:HG21	2.02	0.40
11:B:464:GLN:NE2	27:B:834:CLA:OBD	2.41	0.40
18:K:33:VAL:O	18:K:37:TYR:HD1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:80:GLU:HG3	27:7:308:CLA:HED2	2.02	0.40
10:A:547:VAL:HG22	27:A:824:CLA:HMC2	2.03	0.40
10:A:714:ILE:HD11	15:F:141:ILE:HG23	2.02	0.40
11:B:415:LYS:HB2	11:B:539:LEU:HD13	2.03	0.40
19:L:53:THR:HG23	27:L:201:CLA:HAB	2.02	0.40
5:5:88:ARG:NH1	5:5:199:ILE:HD12	2.36	0.40
11:B:686:PRO:O	11:B:687:LEU:HB2	2.20	0.40
3:3:44:SER:OG	3:3:47:VAL:O	2.31	0.40
8:8:89:PHE:CG	27:8:605:CLA:HMA1	2.56	0.40
11:B:293:THR:O	11:B:295:TRP:N	2.54	0.40
7:7:41:ASN:O	7:7:50:ARG:N	2.54	0.40
27:8:603:CLA:H43	16:I:17:ILE:HG21	2.02	0.40
11:B:564:ARG:HB3	14:E:45:TYR:HB3	2.03	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	1	177/222 (80%)	167 (94%)	10 (6%)	0	100	100
2	2	166/216 (77%)	162 (98%)	3 (2%)	1 (1%)	22	43
3	3	178/236 (75%)	176 (99%)	2 (1%)	0	100	100
4	4	174/217 (80%)	173 (99%)	1 (1%)	0	100	100
5	5	186/229 (81%)	176 (95%)	10 (5%)	0	100	100
6	6	171/215 (80%)	168 (98%)	3 (2%)	0	100	100
7	7	175/230 (76%)	171 (98%)	4 (2%)	0	100	100
8	8	171/227 (75%)	168 (98%)	3 (2%)	0	100	100
9	9	178/220 (81%)	175 (98%)	3 (2%)	0	100	100
10	A	739/752 (98%)	714 (97%)	25 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	B	729/734 (99%)	708 (97%)	21 (3%)	0	100	100
12	C	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	10	24
13	D	135/141 (96%)	127 (94%)	7 (5%)	1 (1%)	19	40
14	E	59/64 (92%)	59 (100%)	0	0	100	100
15	F	158/183 (86%)	152 (96%)	6 (4%)	0	100	100
16	I	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
17	J	40/42 (95%)	40 (100%)	0	0	100	100
18	K	76/87 (87%)	73 (96%)	3 (4%)	0	100	100
19	L	145/153 (95%)	139 (96%)	6 (4%)	0	100	100
20	M	28/30 (93%)	28 (100%)	0	0	100	100
21	O	90/154 (58%)	88 (98%)	2 (2%)	0	100	100
22	R	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
24	Z	151/242 (62%)	147 (97%)	4 (3%)	0	100	100
25	a	169/215 (79%)	165 (98%)	4 (2%)	0	100	100
26	b	174/218 (80%)	171 (98%)	2 (1%)	1 (1%)	22	43
All	All	4468/5277 (85%)	4338 (97%)	126 (3%)	4 (0%)	50	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	C	62	PHE
2	2	44	PHE
13	D	99	HIS
26	b	172	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	130/163 (80%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	134/167 (80%)	134 (100%)	0	100	100
3	3	145/183 (79%)	145 (100%)	0	100	100
4	4	139/167 (83%)	139 (100%)	0	100	100
5	5	139/166 (84%)	139 (100%)	0	100	100
6	6	134/160 (84%)	134 (100%)	0	100	100
7	7	137/176 (78%)	137 (100%)	0	100	100
8	8	134/169 (79%)	134 (100%)	0	100	100
9	9	138/164 (84%)	136 (99%)	2 (1%)	62	83
10	A	607/617 (98%)	605 (100%)	2 (0%)	91	97
11	B	592/593 (100%)	588 (99%)	4 (1%)	81	92
12	C	66/67 (98%)	66 (100%)	0	100	100
13	D	114/117 (97%)	114 (100%)	0	100	100
14	E	56/59 (95%)	55 (98%)	1 (2%)	54	78
15	F	133/154 (86%)	133 (100%)	0	100	100
16	I	27/29 (93%)	27 (100%)	0	100	100
17	J	38/38 (100%)	38 (100%)	0	100	100
18	K	62/69 (90%)	62 (100%)	0	100	100
19	L	123/128 (96%)	120 (98%)	3 (2%)	44	71
20	M	25/25 (100%)	25 (100%)	0	100	100
21	O	74/115 (64%)	74 (100%)	0	100	100
22	R	74/105 (70%)	74 (100%)	0	100	100
24	Z	117/180 (65%)	117 (100%)	0	100	100
25	a	128/153 (84%)	128 (100%)	0	100	100
26	b	144/173 (83%)	144 (100%)	0	100	100
All	All	3610/4137 (87%)	3598 (100%)	12 (0%)	90	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	9	47	GLN
9	9	217	GLN
10	A	60	ASP
10	A	372	TYR
11	B	238	ASP

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Mol	Chain	Res	Type
11	B	241	ASN
11	B	257	PHE
11	B	576	PHE
14	E	56	ASP
19	L	3	GLN
19	L	80	PHE
19	L	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	207	GLN
9	9	217	GLN
10	A	241	HIS
11	B	266	GLN
13	D	96	GLN
13	D	140	ASN
18	K	28	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

357 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
29	II0	5	614	-	39,43,43	2.66	4 (10%)	50,60,60	1.46	9 (18%)
33	LHG	Z	311	-	45,45,48	0.63	0	48,51,54	1.20	4 (8%)
27	CLA	A	842	-	65,73,73	2.28	8 (12%)	76,113,113	1.41	7 (9%)
27	CLA	3	604	-	65,73,73	2.24	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	B	823	-	65,73,73	2.23	8 (12%)	76,113,113	1.37	9 (11%)
27	CLA	b	611	-	55,63,73	2.41	8 (14%)	64,101,113	1.47	7 (10%)
27	CLA	1	613	-	45,53,73	2.73	8 (17%)	52,89,113	1.71	8 (15%)
27	CLA	6	609	33	41,49,73	2.88	9 (21%)	47,84,113	1.78	7 (14%)
28	KC2	6	613	6	48,53,53	1.52	8 (16%)	54,89,89	1.08	5 (9%)
27	CLA	B	804	-	65,73,73	2.21	8 (12%)	76,113,113	1.40	8 (10%)
27	CLA	B	827	-	65,73,73	2.18	8 (12%)	76,113,113	1.40	7 (9%)
27	CLA	A	813	-	42,50,73	2.81	8 (19%)	48,85,113	1.77	8 (16%)
27	CLA	2	604	2	55,63,73	2.46	8 (14%)	64,101,113	1.52	7 (10%)
27	CLA	2	605	-	60,68,73	2.30	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	2	608	2	60,68,73	2.36	8 (13%)	70,107,113	1.46	9 (12%)
38	PQN	A	850	-	34,34,34	0.35	0	42,45,45	0.72	1 (2%)
29	II0	1	616	-	39,43,43	2.66	4 (10%)	50,60,60	1.48	8 (16%)
27	CLA	1	601	1	45,53,73	2.77	8 (17%)	52,89,113	1.74	8 (15%)
27	CLA	4	609	4	60,68,73	2.33	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	B	809	-	65,73,73	2.24	8 (12%)	76,113,113	1.43	8 (10%)
27	CLA	6	608	6	60,68,73	2.32	8 (13%)	70,107,113	1.46	9 (12%)
27	CLA	A	823	-	65,73,73	2.23	8 (12%)	76,113,113	1.35	7 (9%)
27	CLA	K	102	-	55,63,73	2.47	8 (14%)	64,101,113	1.51	8 (12%)
27	CLA	O	202	-	41,49,73	2.92	9 (21%)	47,84,113	1.83	7 (14%)
27	CLA	9	611	-	41,49,73	2.86	9 (21%)	47,84,113	1.79	8 (17%)
27	CLA	B	813	-	61,69,73	2.28	8 (13%)	71,108,113	1.43	8 (11%)
27	CLA	Z	305	-	50,58,73	2.55	8 (16%)	58,95,113	1.61	8 (13%)
27	CLA	2	612	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	7 (13%)
27	CLA	7	308	7	45,53,73	2.74	8 (17%)	52,89,113	1.70	7 (13%)
27	CLA	L	202	-	60,68,73	2.32	8 (13%)	70,107,113	1.45	7 (10%)
27	CLA	3	608	3	60,68,73	2.36	8 (13%)	70,107,113	1.45	8 (11%)
27	CLA	A	841	-	65,73,73	2.21	8 (12%)	76,113,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	II0	a	612	-	39,43,43	2.72	4 (10%)	50,60,60	1.43	7 (14%)
33	LHG	6	617	27	34,34,48	0.74	1 (2%)	37,40,54	1.19	3 (8%)
27	CLA	Z	306	24	60,68,73	2.32	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	7	303	7	65,73,73	2.27	8 (12%)	76,113,113	1.43	9 (11%)
29	II0	9	618	-	39,43,43	2.67	4 (10%)	50,60,60	1.40	8 (16%)
29	II0	1	617	-	39,43,43	2.70	4 (10%)	50,60,60	1.47	10 (20%)
27	CLA	5	601	5	41,49,73	2.94	9 (21%)	47,84,113	1.89	7 (14%)
33	LHG	3	619	-	48,48,48	0.61	0	51,54,54	1.22	6 (11%)
27	CLA	Z	310	-	65,73,73	2.20	8 (12%)	76,113,113	1.40	7 (9%)
38	PQN	B	842	-	34,34,34	0.35	0	42,45,45	0.59	1 (2%)
27	CLA	5	603	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	8 (15%)
27	CLA	3	612	-	45,53,73	2.68	8 (17%)	52,89,113	1.65	7 (13%)
29	II0	2	614	-	39,43,43	2.66	4 (10%)	50,60,60	1.43	8 (16%)
29	II0	7	301	-	39,43,43	2.72	4 (10%)	50,60,60	1.63	13 (26%)
27	CLA	2	609	-	41,49,73	2.91	9 (21%)	47,84,113	1.81	7 (14%)
27	CLA	5	612	-	45,53,73	2.68	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	8	608	-	65,73,73	2.26	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	B	825	-	65,73,73	2.22	8 (12%)	76,113,113	1.36	9 (11%)
27	CLA	a	607	25	60,68,73	2.33	8 (13%)	70,107,113	1.48	7 (10%)
29	II0	9	616	-	39,43,43	2.68	4 (10%)	50,60,60	1.37	9 (18%)
27	CLA	B	821	-	60,68,73	2.31	8 (13%)	70,107,113	1.49	8 (11%)
27	CLA	9	614	-	41,49,73	2.92	9 (21%)	47,84,113	1.85	8 (17%)
27	CLA	8	602	8	45,53,73	2.70	8 (17%)	52,89,113	1.57	5 (9%)
27	CLA	2	601	2	42,50,73	2.83	8 (19%)	48,85,113	1.81	7 (14%)
29	II0	5	615	-	39,43,43	2.71	4 (10%)	50,60,60	1.48	8 (16%)
27	CLA	A	837	-	65,73,73	2.20	8 (12%)	76,113,113	1.35	7 (9%)
36	LMU	J	104	-	32,32,36	0.46	0	43,43,47	1.03	2 (4%)
27	CLA	2	603	-	50,58,73	2.56	8 (16%)	58,95,113	1.58	7 (12%)
27	CLA	b	601	26	45,53,73	2.70	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	4	607	4	60,68,73	2.34	8 (13%)	70,107,113	1.48	8 (11%)
27	CLA	9	612	-	45,53,73	2.69	8 (17%)	52,89,113	1.63	7 (13%)
27	CLA	3	607	3	60,68,73	2.33	8 (13%)	70,107,113	1.42	7 (10%)
33	LHG	A	851	-	48,48,48	0.59	0	51,54,54	1.17	4 (7%)
29	II0	1	619	-	39,43,43	2.79	4 (10%)	50,60,60	1.54	11 (22%)
29	II0	5	620	-	39,43,43	2.72	4 (10%)	50,60,60	1.51	7 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	A	840	-	55,63,73	2.33	8 (14%)	64,101,113	1.51	5 (7%)
27	CLA	A	808	-	55,63,73	2.45	8 (14%)	64,101,113	1.52	7 (10%)
39	DGD	B	848	-	60,60,67	0.88	2 (3%)	74,74,81	1.34	8 (10%)
27	CLA	3	611	3	50,58,73	2.59	8 (16%)	58,95,113	1.56	7 (12%)
27	CLA	A	834	10	55,63,73	2.43	8 (14%)	64,101,113	1.53	8 (12%)
31	IHT	5	618	-	40,42,42	2.80	5 (12%)	53,58,58	2.24	15 (28%)
28	KC2	b	609	-	48,53,53	1.51	7 (14%)	54,89,89	1.12	5 (9%)
27	CLA	b	607	26	60,68,73	2.36	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	B	803	-	45,53,73	2.68	8 (17%)	52,89,113	1.60	7 (13%)
27	CLA	B	841	-	52,60,73	2.51	8 (15%)	60,97,113	1.57	7 (11%)
27	CLA	B	840	-	65,73,73	2.19	8 (12%)	76,113,113	1.38	7 (9%)
35	8CT	M	101	-	40,41,41	0.15	0	50,56,56	0.80	1 (2%)
30	II3	b	613	-	40,43,43	2.00	3 (7%)	47,60,60	1.66	12 (25%)
27	CLA	9	604	-	55,63,73	2.46	8 (14%)	64,101,113	1.53	7 (10%)
27	CLA	5	611	-	45,53,73	2.71	8 (17%)	52,89,113	1.62	7 (13%)
27	CLA	9	605	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	7 (13%)
35	8CT	F	201	-	40,41,41	0.43	1 (2%)	50,56,56	0.45	0
27	CLA	1	612	-	60,68,73	2.30	8 (13%)	70,107,113	1.40	8 (11%)
27	CLA	Z	304	24	55,63,73	2.43	8 (14%)	64,101,113	1.48	7 (10%)
35	8CT	A	845	-	40,41,41	0.25	0	50,56,56	0.32	0
32	LMG	8	614	-	52,52,55	0.81	2 (3%)	60,60,63	1.30	6 (10%)
27	CLA	a	602	25	55,63,73	2.44	8 (14%)	64,101,113	1.61	10 (15%)
27	CLA	B	814	-	42,50,73	2.79	8 (19%)	48,85,113	1.76	7 (14%)
27	CLA	F	204	15	55,63,73	2.41	8 (14%)	64,101,113	1.48	8 (12%)
27	CLA	5	604	-	55,63,73	2.47	8 (14%)	64,101,113	1.55	7 (10%)
32	LMG	F	205	-	32,32,55	0.85	0	40,40,63	1.29	6 (15%)
27	CLA	6	605	6	55,63,73	2.40	8 (14%)	64,101,113	1.49	8 (12%)
27	CLA	6	601	6	45,53,73	2.69	8 (17%)	52,89,113	1.69	8 (15%)
33	LHG	b	616	-	48,48,48	0.57	1 (2%)	51,54,54	1.16	4 (7%)
27	CLA	1	605	-	41,50,73	2.73	8 (19%)	46,85,113	1.71	6 (13%)
27	CLA	3	605	3	55,63,73	2.44	8 (14%)	64,101,113	1.56	8 (12%)
27	CLA	2	607	2	45,53,73	2.68	8 (17%)	52,89,113	1.70	7 (13%)
27	CLA	A	843	-	65,73,73	2.27	8 (12%)	76,113,113	1.47	6 (7%)
27	CLA	B	833	-	45,53,73	2.64	8 (17%)	52,89,113	1.64	7 (13%)
29	II0	8	612	-	39,43,43	2.70	4 (10%)	50,60,60	1.42	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	B	826	-	65,73,73	2.21	8 (12%)	76,113,113	1.37	7 (9%)
27	CLA	8	615	-	65,73,73	2.27	8 (12%)	76,113,113	1.41	8 (10%)
33	LHG	5	619	-	22,22,48	0.87	1 (4%)	25,28,54	1.30	3 (12%)
27	CLA	4	602	4	59,67,73	2.35	8 (13%)	68,105,113	1.51	7 (10%)
27	CLA	9	613	9	45,53,73	2.70	8 (17%)	52,89,113	1.64	7 (13%)
27	CLA	A	806	10	65,73,73	2.22	8 (12%)	76,113,113	1.35	8 (10%)
27	CLA	9	601	9	45,53,73	2.71	8 (17%)	52,89,113	1.67	8 (15%)
28	KC2	9	610	-	48,53,53	1.51	8 (16%)	54,89,89	1.09	5 (9%)
27	CLA	O	203	-	55,63,73	2.44	8 (14%)	64,101,113	1.50	7 (10%)
27	CLA	B	812	-	65,73,73	2.23	8 (12%)	76,113,113	1.43	8 (10%)
28	KC2	1	610	-	48,53,53	1.55	7 (14%)	54,89,89	1.05	4 (7%)
29	II0	O	206	-	39,43,43	2.72	4 (10%)	50,60,60	1.40	10 (20%)
35	8CT	I	101	-	40,41,41	0.25	0	50,56,56	0.44	0
27	CLA	7	313	-	50,58,73	2.55	8 (16%)	58,95,113	1.62	8 (13%)
27	CLA	B	817	-	60,68,73	2.29	8 (13%)	70,107,113	1.46	7 (10%)
29	II0	O	205	-	39,43,43	2.73	4 (10%)	50,60,60	1.40	6 (12%)
27	CLA	A	833	-	65,73,73	2.25	8 (12%)	76,113,113	1.42	8 (10%)
27	CLA	B	818	-	60,68,73	2.31	8 (13%)	70,107,113	1.49	7 (10%)
27	CLA	B	805	-	65,73,73	2.25	8 (12%)	76,113,113	1.40	7 (9%)
35	8CT	A	853	-	40,41,41	0.24	0	50,56,56	0.60	1 (2%)
35	8CT	Z	308	-	40,41,41	0.16	0	50,56,56	0.30	0
29	II0	b	612	-	39,43,43	2.65	4 (10%)	50,60,60	1.48	7 (14%)
27	CLA	7	302	7	45,53,73	2.70	8 (17%)	52,89,113	1.64	7 (13%)
36	LMU	7	321	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
28	KC2	Z	307	-	48,53,53	1.51	7 (14%)	54,89,89	1.09	5 (9%)
33	LHG	8	613	-	32,32,48	0.76	1 (3%)	35,38,54	1.20	2 (5%)
28	KC2	a	609	-	48,53,53	1.52	8 (16%)	54,89,89	1.06	4 (7%)
27	CLA	A	801	-	65,73,73	2.11	7 (10%)	76,113,113	1.35	9 (11%)
29	II0	R	204	-	39,43,43	2.70	4 (10%)	50,60,60	1.42	10 (20%)
27	CLA	B	816	-	59,67,73	2.34	8 (13%)	68,105,113	1.48	8 (11%)
27	CLA	A	818	-	65,73,73	2.24	8 (12%)	76,113,113	1.43	7 (9%)
29	II0	5	616	-	39,43,43	2.71	4 (10%)	50,60,60	1.48	9 (18%)
27	CLA	8	607	8	41,49,73	2.87	9 (21%)	47,84,113	1.78	8 (17%)
32	LMG	3	618	-	30,30,55	0.96	1 (3%)	38,38,63	1.21	6 (15%)
29	II0	2	613	-	39,43,43	2.75	4 (10%)	50,60,60	1.47	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	A	811	-	65,73,73	2.26	8 (12%)	76,113,113	1.46	5 (6%)
29	II0	4	613	-	39,43,43	2.67	4 (10%)	50,60,60	1.35	7 (14%)
27	CLA	B	832	-	65,73,73	2.22	8 (12%)	76,113,113	1.39	8 (10%)
29	II0	9	615	-	39,43,43	2.66	4 (10%)	50,60,60	1.46	9 (18%)
29	II0	J	101	-	39,43,43	2.71	4 (10%)	50,60,60	1.47	8 (16%)
27	CLA	a	606	25	65,73,73	2.24	8 (12%)	76,113,113	1.36	7 (9%)
27	CLA	9	607	9	65,73,73	2.18	8 (12%)	76,113,113	1.36	8 (10%)
27	CLA	A	817	-	65,73,73	2.23	8 (12%)	76,113,113	1.53	8 (10%)
29	II0	5	617	-	39,43,43	2.69	4 (10%)	50,60,60	1.53	9 (18%)
27	CLA	2	602	2	59,67,73	2.37	8 (13%)	68,105,113	1.62	10 (14%)
29	II0	B	843	-	39,43,43	2.73	4 (10%)	50,60,60	1.40	6 (12%)
28	KC2	6	610	6	48,53,53	1.52	7 (14%)	54,89,89	1.07	4 (7%)
27	CLA	b	604	-	65,73,73	2.26	8 (12%)	76,113,113	1.37	7 (9%)
29	II0	4	614	-	39,43,43	2.67	4 (10%)	50,60,60	1.37	6 (12%)
27	CLA	A	835	-	60,68,73	2.33	8 (13%)	70,107,113	1.43	7 (10%)
33	LHG	3	622	28	33,33,48	0.72	0	36,39,54	1.27	3 (8%)
27	CLA	A	819	-	65,73,73	2.25	8 (12%)	76,113,113	1.42	8 (10%)
27	CLA	3	603	-	60,68,73	2.32	8 (13%)	70,107,113	1.45	7 (10%)
27	CLA	B	839	33	65,73,73	2.26	8 (12%)	76,113,113	1.42	7 (9%)
27	CLA	4	603	-	54,62,73	2.47	8 (14%)	62,99,113	1.58	7 (11%)
31	IHT	2	616	-	40,42,42	2.85	4 (10%)	53,58,58	2.20	16 (30%)
27	CLA	R	202	-	55,63,73	2.43	8 (14%)	64,101,113	1.68	8 (12%)
29	II0	3	613	-	39,43,43	2.68	4 (10%)	50,60,60	1.45	8 (16%)
27	CLA	8	604	-	65,73,73	2.26	8 (12%)	76,113,113	1.42	9 (11%)
27	CLA	L	203	-	50,58,73	2.51	8 (16%)	58,95,113	1.66	9 (15%)
27	CLA	1	607	1	45,53,73	2.74	8 (17%)	52,89,113	1.67	7 (13%)
29	II0	4	615	-	39,43,43	2.68	4 (10%)	50,60,60	1.46	9 (18%)
27	CLA	B	822	-	65,73,73	2.16	8 (12%)	76,113,113	1.41	8 (10%)
27	CLA	7	310	33	41,49,73	2.88	9 (21%)	47,84,113	1.79	7 (14%)
27	CLA	F	202	-	60,68,73	2.34	8 (13%)	70,107,113	1.45	8 (11%)
27	CLA	b	603	-	60,68,73	2.35	8 (13%)	70,107,113	1.47	8 (11%)
27	CLA	A	803	-	65,73,73	2.22	8 (12%)	76,113,113	1.46	8 (10%)
28	KC2	3	606	33	48,53,53	1.51	8 (16%)	54,89,89	1.11	5 (9%)
27	CLA	F	203	-	45,53,73	2.66	8 (17%)	52,89,113	1.65	7 (13%)
27	CLA	B	834	-	55,63,73	2.39	8 (14%)	64,101,113	1.53	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	b	610	26	51,59,73	2.52	8 (15%)	59,96,113	1.62	9 (15%)
31	IHT	A	854	-	40,42,42	2.93	5 (12%)	53,58,58	1.95	17 (32%)
31	IHT	6	616	-	40,42,42	2.81	4 (10%)	53,58,58	2.16	16 (30%)
29	II0	8	610	-	39,43,43	2.75	4 (10%)	50,60,60	1.41	8 (16%)
27	CLA	J	102	-	41,49,73	2.88	9 (21%)	47,84,113	1.81	8 (17%)
37	SF4	A	849	10,11	0,12,12	-	-	-		
27	CLA	6	602	6	65,73,73	2.29	8 (12%)	76,113,113	1.48	7 (9%)
27	CLA	9	603	-	45,53,73	2.72	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	B	824	-	60,68,73	2.31	8 (13%)	70,107,113	1.51	7 (10%)
27	CLA	A	836	-	55,63,73	2.45	8 (14%)	64,101,113	1.52	7 (10%)
27	CLA	5	608	5	60,68,73	2.37	8 (13%)	70,107,113	1.62	8 (11%)
27	CLA	B	802	-	65,73,73	2.23	8 (12%)	76,113,113	1.34	9 (11%)
27	CLA	2	611	-	45,53,73	2.70	8 (17%)	52,89,113	1.65	8 (15%)
27	CLA	A	804	10	65,73,73	2.24	8 (12%)	76,113,113	1.39	8 (10%)
29	II0	6	614	-	39,43,43	2.67	4 (10%)	50,60,60	1.38	7 (14%)
27	CLA	7	304	-	55,63,73	2.46	8 (14%)	64,101,113	1.55	8 (12%)
33	LHG	4	617	27	46,46,48	0.61	0	49,52,54	1.21	6 (12%)
35	8CT	L	205	-	40,41,41	0.16	0	50,56,56	0.38	0
27	CLA	O	204	-	55,63,73	2.49	8 (14%)	64,101,113	1.61	8 (12%)
27	CLA	A	824	-	65,73,73	2.26	8 (12%)	76,113,113	1.40	7 (9%)
35	8CT	B	845	-	40,41,41	0.35	0	50,56,56	0.60	1 (2%)
27	CLA	B	830	-	60,68,73	2.33	8 (13%)	70,107,113	1.49	7 (10%)
27	CLA	a	605	-	55,63,73	2.40	8 (14%)	64,101,113	1.55	8 (12%)
32	LMG	2	617	-	36,36,55	0.85	0	44,44,63	1.23	5 (11%)
28	KC2	b	605	26	48,53,53	1.52	7 (14%)	54,89,89	1.12	5 (9%)
28	KC2	4	605	4	48,53,53	1.55	7 (14%)	54,89,89	1.06	4 (7%)
27	CLA	1	603	-	52,60,73	2.49	8 (15%)	60,97,113	1.56	7 (11%)
27	CLA	A	831	-	65,73,73	2.19	8 (12%)	76,113,113	1.34	7 (9%)
27	CLA	6	612	-	45,53,73	2.66	8 (17%)	52,89,113	1.68	8 (15%)
27	CLA	A	838	-	65,73,73	2.24	8 (12%)	76,113,113	1.36	7 (9%)
27	CLA	9	609	-	41,49,73	2.88	9 (21%)	47,84,113	1.76	8 (17%)
29	II0	a	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.44	11 (22%)
35	8CT	J	103	-	40,41,41	0.17	0	50,56,56	0.38	0
27	CLA	B	838	-	65,73,73	2.26	8 (12%)	76,113,113	1.40	8 (10%)
27	CLA	5	606	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	A	830	-	60,68,73	2.36	8 (13%)	70,107,113	1.48	7 (10%)
27	CLA	1	606	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	8 (15%)
33	LHG	2	620	-	41,41,48	0.65	1 (2%)	44,47,54	1.21	4 (9%)
27	CLA	B	819	-	60,68,73	2.36	8 (13%)	70,107,113	1.52	10 (14%)
27	CLA	8	601	8	45,53,73	2.72	8 (17%)	52,89,113	1.66	7 (13%)
29	II0	4	612	-	39,43,43	2.69	4 (10%)	50,60,60	1.39	6 (12%)
27	CLA	B	810	-	60,68,73	2.30	8 (13%)	70,107,113	1.46	7 (10%)
36	LMU	4	618	-	36,36,36	0.47	0	47,47,47	0.92	2 (4%)
29	II0	1	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.40	6 (12%)
27	CLA	B	806	-	65,73,73	2.17	8 (12%)	76,113,113	1.40	8 (10%)
27	CLA	1	609	-	41,49,73	2.90	9 (21%)	47,84,113	1.80	7 (14%)
29	II0	6	615	-	39,43,43	2.68	4 (10%)	50,60,60	1.41	7 (14%)
35	8CT	K	103	-	40,41,41	0.16	0	50,56,56	0.33	0
29	II0	7	315	-	39,43,43	2.67	4 (10%)	50,60,60	1.51	9 (18%)
27	CLA	A	828	-	65,73,73	2.24	8 (12%)	76,113,113	1.37	7 (9%)
29	II0	3	616	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	6 (12%)
32	LMG	6	618	-	32,32,55	0.98	1 (3%)	40,40,63	1.23	5 (12%)
27	CLA	4	610	-	65,73,73	2.22	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	A	839	-	65,73,73	2.23	8 (12%)	76,113,113	1.44	8 (10%)
35	8CT	B	844	-	40,41,41	0.18	0	50,56,56	0.58	0
27	CLA	6	607	6	55,63,73	2.46	8 (14%)	64,101,113	1.51	7 (10%)
33	LHG	4	619	27	44,44,48	0.64	1 (2%)	47,50,54	1.21	5 (10%)
27	CLA	B	828	-	65,73,73	2.20	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	B	831	-	55,63,73	2.46	8 (14%)	64,101,113	1.57	8 (12%)
27	CLA	4	606	4	60,68,73	2.33	8 (13%)	70,107,113	1.45	8 (11%)
27	CLA	B	820	-	60,68,73	2.36	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	A	809	27	60,68,73	2.33	8 (13%)	70,107,113	1.57	8 (11%)
27	CLA	3	610	-	65,73,73	2.23	8 (12%)	76,113,113	1.42	8 (10%)
32	LMG	8	616	-	51,51,55	0.73	0	59,59,63	1.29	7 (11%)
27	CLA	7	305	7	53,61,73	2.49	8 (15%)	61,98,113	1.57	8 (13%)
27	CLA	A	812	-	55,63,73	2.44	8 (14%)	64,101,113	1.58	9 (14%)
27	CLA	1	608	1	60,68,73	2.36	8 (13%)	70,107,113	1.47	9 (12%)
27	CLA	b	606	26	65,73,73	2.23	8 (12%)	76,113,113	1.36	7 (9%)
27	CLA	A	825	-	65,73,73	2.25	8 (12%)	76,113,113	1.39	8 (10%)
27	CLA	4	604	-	55,63,73	2.44	8 (14%)	64,101,113	1.50	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	3	609	-	65,73,73	2.27	8 (12%)	76,113,113	1.37	7 (9%)
27	CLA	4	601	4	55,63,73	2.41	8 (14%)	64,101,113	1.48	7 (10%)
29	II0	a	614	-	39,43,43	2.74	4 (10%)	50,60,60	1.39	7 (14%)
35	8CT	A	846	-	40,41,41	0.19	0	50,56,56	0.35	0
27	CLA	a	603	-	60,68,73	2.33	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	a	601	25	45,53,73	2.69	8 (17%)	52,89,113	1.66	7 (13%)
31	IHT	9	619	-	40,42,42	2.81	5 (12%)	53,58,58	2.40	14 (26%)
27	CLA	A	820	-	65,73,73	2.24	8 (12%)	76,113,113	1.41	7 (9%)
27	CLA	3	602	3	55,63,73	2.44	8 (14%)	64,101,113	1.55	7 (10%)
27	CLA	A	844	-	65,73,73	2.06	8 (12%)	76,113,113	1.42	9 (11%)
33	LHG	A	852	-	38,38,48	0.70	0	41,44,54	1.26	3 (7%)
29	II0	3	617	-	39,43,43	2.72	4 (10%)	50,60,60	1.39	7 (14%)
27	CLA	8	606	8	55,63,73	2.42	8 (14%)	64,101,113	1.50	8 (12%)
33	LHG	a	618	-	28,28,48	0.82	1 (3%)	31,34,54	1.32	3 (9%)
35	8CT	B	846	-	40,41,41	0.10	0	50,56,56	0.48	0
35	8CT	B	850	-	40,41,41	0.21	0	50,56,56	0.40	0
27	CLA	B	835	-	65,73,73	2.28	8 (12%)	76,113,113	1.52	7 (9%)
33	LHG	4	620	-	44,44,48	0.65	2 (4%)	47,50,54	1.19	4 (8%)
27	CLA	a	611	-	65,73,73	2.19	8 (12%)	76,113,113	1.36	8 (10%)
27	CLA	5	605	5	45,53,73	2.68	8 (17%)	52,89,113	1.66	7 (13%)
39	DGD	Z	303	-	61,61,67	0.94	3 (4%)	75,75,81	1.37	7 (9%)
29	II0	3	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	7 (14%)
27	CLA	4	608	33	65,73,73	2.23	8 (12%)	76,113,113	1.40	8 (10%)
27	CLA	a	610	-	55,63,73	2.46	8 (14%)	64,101,113	1.50	7 (10%)
27	CLA	7	306	7	45,53,73	2.75	8 (17%)	52,89,113	1.65	7 (13%)
27	CLA	B	808	11	65,73,73	2.18	8 (12%)	76,113,113	1.35	8 (10%)
27	CLA	6	611	-	55,63,73	2.44	8 (14%)	64,101,113	1.59	9 (14%)
27	CLA	B	807	-	65,73,73	2.20	8 (12%)	76,113,113	1.34	8 (10%)
28	KC2	7	307	-	48,53,53	1.55	7 (14%)	54,89,89	1.12	5 (9%)
29	II0	b	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.45	8 (16%)
27	CLA	A	810	-	65,73,73	2.24	8 (12%)	76,113,113	1.38	9 (11%)
29	II0	2	615	-	39,43,43	2.72	4 (10%)	50,60,60	1.50	10 (20%)
27	CLA	B	837	-	65,73,73	2.24	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	1	611	-	45,53,73	2.75	8 (17%)	52,89,113	1.68	7 (13%)
31	IHT	1	618	-	40,42,42	2.83	5 (12%)	53,58,58	2.05	14 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	II0	8	611	-	39,43,43	2.73	4 (10%)	50,60,60	1.32	6 (12%)
35	8CT	B	849	-	40,41,41	0.33	0	50,56,56	0.72	1 (2%)
27	CLA	5	607	5	45,53,73	2.68	8 (17%)	52,89,113	1.65	7 (13%)
27	CLA	8	605	8	50,58,73	2.53	8 (16%)	58,95,113	1.62	9 (15%)
27	CLA	a	608	-	60,68,73	2.34	8 (13%)	70,107,113	1.49	9 (12%)
27	CLA	4	611	-	65,73,73	2.21	8 (12%)	76,113,113	1.38	8 (10%)
27	CLA	6	604	-	60,68,73	2.35	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	O	201	-	55,63,73	2.43	8 (14%)	64,101,113	1.54	10 (15%)
29	II0	7	317	-	39,43,43	2.71	4 (10%)	50,60,60	1.53	9 (18%)
37	SF4	C	102	12	0,12,12	-	-	-	-	-
35	8CT	R	201	-	40,41,41	0.20	0	50,56,56	0.41	0
35	8CT	Z	309	-	40,41,41	0.23	0	50,56,56	0.63	1 (2%)
27	CLA	L	201	19	51,59,73	2.53	8 (15%)	59,96,113	1.58	7 (11%)
27	CLA	B	829	-	45,53,73	2.70	8 (17%)	52,89,113	1.76	8 (15%)
35	8CT	R	203	-	40,41,41	0.16	0	50,56,56	0.46	1 (2%)
27	CLA	3	601	3	45,53,73	2.71	8 (17%)	52,89,113	1.62	7 (13%)
28	KC2	5	610	5	48,53,53	1.52	7 (14%)	54,89,89	1.06	5 (9%)
27	CLA	A	821	-	55,63,73	2.42	8 (14%)	64,101,113	1.58	7 (10%)
35	8CT	4	616	-	40,41,41	0.18	0	50,56,56	0.31	0
35	8CT	b	615	-	40,41,41	0.22	0	50,56,56	0.30	0
27	CLA	7	312	-	55,63,73	2.44	8 (14%)	64,101,113	1.52	7 (10%)
27	CLA	B	811	-	55,63,73	2.44	8 (14%)	64,101,113	1.55	7 (10%)
35	8CT	7	318	-	40,41,41	0.41	1 (2%)	50,56,56	0.59	0
27	CLA	7	309	7	55,63,73	2.43	8 (14%)	64,101,113	1.57	9 (14%)
29	II0	Z	312	-	39,43,43	2.67	4 (10%)	50,60,60	1.39	8 (16%)
35	8CT	A	848	-	40,41,41	0.37	0	50,56,56	0.56	0
30	II3	1	615	-	40,43,43	2.03	3 (7%)	47,60,60	1.57	9 (19%)
27	CLA	B	836	-	47,55,73	2.58	8 (17%)	54,91,113	1.62	7 (12%)
28	KC2	7	311	7	48,53,53	1.51	8 (16%)	54,89,89	1.10	4 (7%)
34	SQD	O	207	-	23,24,54	1.57	4 (17%)	31,34,65	1.39	4 (12%)
27	CLA	A	822	-	65,73,73	2.26	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	2	606	-	45,53,73	2.69	8 (17%)	52,89,113	1.64	7 (13%)
31	IHT	8	609	-	40,42,42	2.80	4 (10%)	53,58,58	2.33	16 (30%)
33	LHG	2	618	-	21,21,48	0.75	0	23,26,54	1.25	2 (8%)
37	SF4	C	101	12	0,12,12	-	-	-	-	-
33	LHG	a	617	-	48,48,48	0.60	1 (2%)	51,54,54	1.20	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	IHT	a	616	-	40,42,42	2.81	4 (10%)	53,58,58	2.33	17 (32%)
35	8CT	A	847	-	40,41,41	0.23	0	50,56,56	0.77	1 (2%)
27	CLA	9	606	-	64,72,73	2.21	8 (12%)	74,111,113	1.41	9 (12%)
27	CLA	5	613	5	41,49,73	2.90	9 (21%)	47,84,113	1.76	8 (17%)
29	II0	3	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.37	8 (16%)
27	CLA	6	603	-	45,53,73	2.69	8 (17%)	52,89,113	1.70	7 (13%)
27	CLA	b	608	-	65,73,73	2.25	8 (12%)	76,113,113	1.38	8 (10%)
31	IHT	L	204	-	40,42,42	2.83	4 (10%)	53,58,58	2.23	16 (30%)
27	CLA	5	609	-	41,49,73	2.90	9 (21%)	47,84,113	1.77	7 (14%)
29	II0	7	314	-	39,43,43	2.68	4 (10%)	50,60,60	1.43	8 (16%)
33	LHG	2	619	-	38,38,48	0.69	1 (2%)	41,44,54	1.25	4 (9%)
28	KC2	2	610	-	48,53,53	1.53	7 (14%)	54,89,89	1.07	5 (9%)
27	CLA	1	602	1	59,67,73	2.37	8 (13%)	68,105,113	1.49	8 (11%)
35	8CT	B	847	-	40,41,41	0.16	0	50,56,56	0.46	0
27	CLA	9	602	9	55,63,73	2.45	8 (14%)	64,101,113	1.57	8 (12%)
27	CLA	1	604	1	45,53,73	2.72	8 (17%)	52,89,113	1.64	7 (13%)
27	CLA	K	101	-	65,73,73	2.24	8 (12%)	76,113,113	1.34	7 (9%)
27	CLA	8	603	-	65,73,73	2.27	8 (12%)	76,113,113	1.40	7 (9%)
27	CLA	Z	301	-	60,68,73	2.39	8 (13%)	70,107,113	1.46	7 (10%)
29	II0	9	617	-	39,43,43	2.71	4 (10%)	50,60,60	1.46	8 (16%)
31	IHT	Z	302	-	40,42,42	2.84	4 (10%)	53,58,58	2.12	14 (26%)
33	LHG	7	320	27	38,38,48	0.65	0	41,44,54	1.17	3 (7%)
27	CLA	A	814	-	45,53,73	2.71	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	9	608	9	55,63,73	2.43	8 (14%)	64,101,113	1.54	8 (12%)
27	CLA	B	801	-	65,73,73	2.12	8 (12%)	76,113,113	1.33	8 (10%)
27	CLA	B	815	-	65,73,73	2.28	8 (12%)	76,113,113	1.43	8 (10%)
27	CLA	a	604	-	60,68,73	2.37	8 (13%)	70,107,113	1.48	6 (8%)
27	CLA	A	832	-	65,73,73	2.23	8 (12%)	76,113,113	1.36	7 (9%)
29	II0	7	316	-	39,43,43	2.73	4 (10%)	50,60,60	1.45	8 (16%)
27	CLA	5	602	5	55,63,73	2.46	8 (14%)	64,101,113	1.53	7 (10%)
27	CLA	A	807	10	50,58,73	2.56	8 (16%)	58,95,113	1.62	8 (13%)
32	LMG	3	620	-	32,32,55	0.91	0	40,40,63	1.28	6 (15%)
29	II0	a	613	-	39,43,43	2.68	4 (10%)	50,60,60	1.43	8 (16%)
27	CLA	A	829	-	50,58,73	2.55	8 (16%)	58,95,113	1.66	7 (12%)
27	CLA	A	805	-	50,58,73	2.57	8 (16%)	58,95,113	1.62	7 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LHG	7	319	-	30,30,48	0.75	1 (3%)	33,36,54	1.20	3 (9%)
27	CLA	b	602	26	64,72,73	2.29	8 (12%)	74,111,113	1.48	9 (12%)
27	CLA	A	827	-	65,73,73	2.14	8 (12%)	76,113,113	1.38	8 (10%)
27	CLA	A	815	-	62,70,73	2.31	8 (12%)	72,109,113	1.42	7 (9%)
27	CLA	A	826	-	65,73,73	2.13	8 (12%)	76,113,113	1.35	8 (10%)
27	CLA	A	816	-	60,68,73	2.30	8 (13%)	70,107,113	1.47	7 (10%)
34	SQD	3	621	-	41,42,54	1.33	4 (9%)	50,53,65	1.09	3 (6%)
27	CLA	6	606	-	55,63,73	2.45	8 (14%)	64,101,113	1.59	9 (14%)
27	CLA	A	802	27	55,63,73	2.41	8 (14%)	64,101,113	1.50	7 (10%)

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
29	II0	5	614	-	-	2/21/67/67	0/2/2/2
33	LHG	Z	311	-	-	23/50/50/53	-
27	CLA	A	842	-	1/1/15/20	6/37/115/115	-
27	CLA	3	604	-	1/1/15/20	3/37/115/115	-
27	CLA	B	823	-	1/1/15/20	10/37/115/115	-
27	CLA	b	611	-	1/1/13/20	4/25/103/115	-
27	CLA	1	613	-	1/1/11/20	3/13/91/115	-
27	CLA	6	609	33	1/1/10/20	0/8/86/115	-
28	KC2	6	613	6	-	9/15/71/71	-
27	CLA	B	804	-	1/1/15/20	10/37/115/115	-
27	CLA	B	827	-	1/1/15/20	6/37/115/115	-
27	CLA	A	813	-	1/1/10/20	1/10/88/115	-
27	CLA	2	604	2	1/1/13/20	1/25/103/115	-
27	CLA	2	605	-	1/1/14/20	4/31/109/115	-
27	CLA	2	608	2	1/1/14/20	6/31/109/115	-
38	PQN	A	850	-	-	10/23/43/43	0/2/2/2
29	II0	1	616	-	-	2/21/67/67	0/2/2/2
27	CLA	1	601	1	1/1/11/20	3/13/91/115	-
27	CLA	4	609	4	1/1/14/20	4/31/109/115	-
27	CLA	B	809	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	6	608	6	1/1/14/20	5/31/109/115	-
27	CLA	A	823	-	1/1/15/20	10/37/115/115	-
27	CLA	K	102	-	1/1/13/20	3/25/103/115	-
27	CLA	O	202	-	1/1/10/20	2/8/86/115	-
27	CLA	9	611	-	1/1/10/20	3/8/86/115	-
27	CLA	B	813	-	1/1/14/20	11/33/111/115	-
27	CLA	Z	305	-	1/1/12/20	1/19/97/115	-
27	CLA	2	612	-	1/1/11/20	3/13/91/115	-
27	CLA	7	308	7	1/1/11/20	1/13/91/115	-
27	CLA	L	202	-	1/1/14/20	9/31/109/115	-
27	CLA	3	608	3	1/1/14/20	2/31/109/115	-
27	CLA	A	841	-	1/1/15/20	5/37/115/115	-
29	II0	a	612	-	-	2/21/67/67	0/2/2/2
33	LHG	6	617	27	-	16/39/39/53	-
27	CLA	Z	306	24	1/1/14/20	11/31/109/115	-
27	CLA	7	303	7	1/1/15/20	7/37/115/115	-
29	II0	9	618	-	-	2/21/67/67	0/2/2/2
29	II0	1	617	-	-	2/21/67/67	0/2/2/2
27	CLA	5	601	5	1/1/10/20	0/8/86/115	-
33	LHG	3	619	-	-	23/53/53/53	-
27	CLA	Z	310	-	1/1/15/20	5/37/115/115	-
38	PQN	B	842	-	-	5/23/43/43	0/2/2/2
27	CLA	5	603	-	1/1/11/20	3/13/91/115	-
27	CLA	3	612	-	1/1/11/20	2/13/91/115	-
29	II0	2	614	-	-	0/21/67/67	0/2/2/2
29	II0	7	301	-	-	2/21/67/67	0/2/2/2
27	CLA	2	609	-	1/1/10/20	0/8/86/115	-
27	CLA	5	612	-	1/1/11/20	3/13/91/115	-
27	CLA	8	608	-	1/1/15/20	4/37/115/115	-
27	CLA	B	825	-	1/1/15/20	2/37/115/115	-
27	CLA	a	607	25	1/1/14/20	3/31/109/115	-
29	II0	9	616	-	-	2/21/67/67	0/2/2/2
27	CLA	B	821	-	1/1/14/20	9/31/109/115	-
27	CLA	9	614	-	1/1/10/20	1/8/86/115	-
27	CLA	8	602	8	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	2	601	2	1/1/10/20	3/10/88/115	-
29	II0	5	615	-	-	1/21/67/67	0/2/2/2
27	CLA	A	837	-	1/1/15/20	7/37/115/115	-
36	LMU	J	104	-	-	9/17/57/61	0/2/2/2
27	CLA	2	603	-	1/1/12/20	4/19/97/115	-
27	CLA	b	601	26	1/1/11/20	3/13/91/115	-
27	CLA	4	607	4	1/1/14/20	5/31/109/115	-
27	CLA	9	612	-	1/1/11/20	2/13/91/115	-
27	CLA	3	607	3	1/1/14/20	4/31/109/115	-
33	LHG	A	851	-	-	22/53/53/53	-
29	II0	1	619	-	-	1/21/67/67	0/2/2/2
29	II0	5	620	-	-	1/21/67/67	0/2/2/2
27	CLA	A	840	-	1/1/13/20	3/25/103/115	-
27	CLA	A	808	-	1/1/13/20	2/25/103/115	-
39	DGD	B	848	-	-	15/48/88/95	0/2/2/2
27	CLA	3	611	3	1/1/12/20	2/19/97/115	-
27	CLA	A	834	10	1/1/13/20	7/25/103/115	-
31	IHT	5	618	-	-	1/25/65/65	0/2/2/2
28	KC2	b	609	-	-	2/15/71/71	-
27	CLA	b	607	26	1/1/14/20	5/31/109/115	-
27	CLA	B	803	-	1/1/11/20	3/13/91/115	-
27	CLA	B	841	-	1/1/12/20	5/22/100/115	-
27	CLA	B	840	-	1/1/15/20	1/37/115/115	-
35	8CT	M	101	-	-	5/29/63/63	0/2/2/2
30	II3	b	613	-	-	1/25/67/67	0/2/2/2
27	CLA	9	604	-	1/1/13/20	1/25/103/115	-
27	CLA	5	611	-	1/1/11/20	6/13/91/115	-
27	CLA	9	605	-	1/1/11/20	2/13/91/115	-
35	8CT	F	201	-	-	4/29/63/63	0/2/2/2
27	CLA	1	612	-	1/1/14/20	6/31/109/115	-
27	CLA	Z	304	24	1/1/13/20	2/25/103/115	-
35	8CT	A	845	-	-	1/29/63/63	0/2/2/2
32	LMG	8	614	-	-	23/47/67/70	0/1/1/1
27	CLA	a	602	25	1/1/13/20	9/25/103/115	-
27	CLA	B	814	-	1/1/10/20	4/10/88/115	-
27	CLA	F	204	15	1/1/13/20	4/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	5	604	-	1/1/13/20	9/25/103/115	-
32	LMG	F	205	-	-	11/27/47/70	0/1/1/1
27	CLA	6	605	6	1/1/13/20	5/25/103/115	-
27	CLA	6	601	6	1/1/11/20	2/13/91/115	-
33	LHG	b	616	-	-	25/53/53/53	-
27	CLA	1	605	-	1/1/10/20	1/9/87/115	-
27	CLA	3	605	3	1/1/13/20	2/25/103/115	-
27	CLA	2	607	2	1/1/11/20	0/13/91/115	-
27	CLA	A	843	-	1/1/15/20	10/37/115/115	-
27	CLA	B	833	-	1/1/11/20	1/13/91/115	-
29	II0	8	612	-	-	1/21/67/67	0/2/2/2
27	CLA	B	826	-	1/1/15/20	11/37/115/115	-
27	CLA	8	615	-	1/1/15/20	5/37/115/115	-
33	LHG	5	619	-	-	14/26/26/53	-
27	CLA	4	602	4	1/1/13/20	2/30/108/115	-
27	CLA	9	613	9	1/1/11/20	1/13/91/115	-
27	CLA	A	806	10	1/1/15/20	7/37/115/115	-
27	CLA	9	601	9	1/1/11/20	5/13/91/115	-
28	KC2	9	610	-	-	6/15/71/71	-
27	CLA	O	203	-	1/1/13/20	4/25/103/115	-
27	CLA	B	812	-	1/1/15/20	13/37/115/115	-
28	KC2	1	610	-	-	7/15/71/71	-
29	II0	O	206	-	-	1/21/67/67	0/2/2/2
35	8CT	I	101	-	-	3/29/63/63	0/2/2/2
27	CLA	7	313	-	1/1/12/20	6/19/97/115	-
27	CLA	B	817	-	1/1/14/20	1/31/109/115	-
29	II0	O	205	-	-	2/21/67/67	0/2/2/2
27	CLA	A	833	-	1/1/15/20	4/37/115/115	-
27	CLA	B	818	-	1/1/14/20	1/31/109/115	-
27	CLA	B	805	-	1/1/15/20	10/37/115/115	-
35	8CT	A	853	-	-	6/29/63/63	0/2/2/2
35	8CT	Z	308	-	-	6/29/63/63	0/2/2/2
29	II0	b	612	-	-	1/21/67/67	0/2/2/2
27	CLA	7	302	7	1/1/11/20	0/13/91/115	-
36	LMU	7	321	-	-	8/21/61/61	0/2/2/2
28	KC2	Z	307	-	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	8	613	-	-	21/37/37/53	-
28	KC2	a	609	-	-	3/15/71/71	-
27	CLA	A	801	-	1/1/15/20	8/37/115/115	-
29	II0	R	204	-	-	2/21/67/67	0/2/2/2
27	CLA	B	816	-	1/1/13/20	12/30/108/115	-
27	CLA	A	818	-	1/1/15/20	7/37/115/115	-
29	II0	5	616	-	-	1/21/67/67	0/2/2/2
27	CLA	8	607	8	1/1/10/20	1/8/86/115	-
32	LMG	3	618	-	-	9/25/45/70	0/1/1/1
29	II0	2	613	-	-	1/21/67/67	0/2/2/2
27	CLA	A	811	-	1/1/15/20	12/37/115/115	-
29	II0	4	613	-	-	1/21/67/67	0/2/2/2
27	CLA	B	832	-	1/1/15/20	15/37/115/115	-
29	II0	9	615	-	-	1/21/67/67	0/2/2/2
29	II0	J	101	-	-	1/21/67/67	0/2/2/2
27	CLA	a	606	25	1/1/15/20	4/37/115/115	-
27	CLA	9	607	9	1/1/15/20	10/37/115/115	-
27	CLA	A	817	-	1/1/15/20	13/37/115/115	-
29	II0	5	617	-	-	2/21/67/67	0/2/2/2
27	CLA	2	602	2	1/1/13/20	12/30/108/115	-
29	II0	B	843	-	-	2/21/67/67	0/2/2/2
28	KC2	6	610	6	-	6/15/71/71	-
27	CLA	b	604	-	1/1/15/20	16/37/115/115	-
29	II0	4	614	-	-	2/21/67/67	0/2/2/2
27	CLA	A	835	-	1/1/14/20	6/31/109/115	-
33	LHG	3	622	28	-	13/38/38/53	-
27	CLA	A	819	-	1/1/15/20	5/37/115/115	-
27	CLA	3	603	-	1/1/14/20	3/31/109/115	-
27	CLA	B	839	33	1/1/15/20	5/37/115/115	-
27	CLA	4	603	-	1/1/12/20	5/24/102/115	-
31	IHT	2	616	-	-	2/25/65/65	0/2/2/2
27	CLA	R	202	-	1/1/13/20	10/25/103/115	-
29	II0	3	613	-	-	2/21/67/67	0/2/2/2
27	CLA	8	604	-	1/1/15/20	4/37/115/115	-
27	CLA	L	203	-	1/1/12/20	5/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	1	607	1	1/1/11/20	0/13/91/115	-
29	II0	4	615	-	-	0/21/67/67	0/2/2/2
27	CLA	B	822	-	1/1/15/20	7/37/115/115	-
27	CLA	7	310	33	1/1/10/20	0/8/86/115	-
27	CLA	F	202	-	1/1/14/20	10/31/109/115	-
27	CLA	b	603	-	1/1/14/20	7/31/109/115	-
27	CLA	A	803	-	1/1/15/20	8/37/115/115	-
28	KC2	3	606	33	-	8/15/71/71	-
27	CLA	F	203	-	1/1/11/20	3/13/91/115	-
27	CLA	B	834	-	1/1/13/20	2/25/103/115	-
27	CLA	b	610	26	1/1/12/20	9/21/99/115	-
31	IHT	A	854	-	-	2/25/65/65	0/2/2/2
31	IHT	6	616	-	-	3/25/65/65	0/2/2/2
29	II0	8	610	-	-	2/21/67/67	0/2/2/2
27	CLA	J	102	-	1/1/10/20	1/8/86/115	-
37	SF4	A	849	10,11	-	-	0/6/5/5
27	CLA	6	602	6	1/1/15/20	7/37/115/115	-
27	CLA	9	603	-	1/1/11/20	5/13/91/115	-
27	CLA	B	824	-	1/1/14/20	5/31/109/115	-
27	CLA	A	836	-	1/1/13/20	1/25/103/115	-
27	CLA	5	608	5	1/1/14/20	10/31/109/115	-
27	CLA	B	802	-	1/1/15/20	8/37/115/115	-
27	CLA	2	611	-	1/1/11/20	2/13/91/115	-
27	CLA	A	804	10	1/1/15/20	16/37/115/115	-
29	II0	6	614	-	-	1/21/67/67	0/2/2/2
27	CLA	7	304	-	1/1/13/20	1/25/103/115	-
33	LHG	4	617	27	-	18/51/51/53	-
35	8CT	L	205	-	-	2/29/63/63	0/2/2/2
27	CLA	O	204	-	1/1/13/20	8/25/103/115	-
27	CLA	A	824	-	1/1/15/20	3/37/115/115	-
35	8CT	B	845	-	-	8/29/63/63	0/2/2/2
27	CLA	B	830	-	1/1/14/20	0/31/109/115	-
27	CLA	a	605	-	1/1/13/20	10/25/103/115	-
32	LMG	2	617	-	-	8/31/51/70	0/1/1/1
28	KC2	b	605	26	-	7/15/71/71	-
28	KC2	4	605	4	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	1	603	-	1/1/12/20	4/22/100/115	-
27	CLA	A	831	-	1/1/15/20	11/37/115/115	-
27	CLA	6	612	-	1/1/11/20	2/13/91/115	-
27	CLA	A	838	-	1/1/15/20	3/37/115/115	-
27	CLA	9	609	-	1/1/10/20	3/8/86/115	-
29	II0	a	615	-	-	1/21/67/67	0/2/2/2
35	8CT	J	103	-	-	7/29/63/63	0/2/2/2
27	CLA	B	838	-	1/1/15/20	5/37/115/115	-
27	CLA	5	606	-	1/1/11/20	5/13/91/115	-
27	CLA	A	830	-	1/1/14/20	4/31/109/115	-
27	CLA	1	606	-	1/1/11/20	0/13/91/115	-
33	LHG	2	620	-	-	17/46/46/53	-
27	CLA	B	819	-	1/1/14/20	8/31/109/115	-
27	CLA	8	601	8	1/1/11/20	3/13/91/115	-
29	II0	4	612	-	-	2/21/67/67	0/2/2/2
27	CLA	B	810	-	1/1/14/20	4/31/109/115	-
36	LMU	4	618	-	-	11/21/61/61	0/2/2/2
29	II0	1	614	-	-	2/21/67/67	0/2/2/2
27	CLA	B	806	-	1/1/15/20	4/37/115/115	-
27	CLA	1	609	-	1/1/10/20	1/8/86/115	-
29	II0	6	615	-	-	1/21/67/67	0/2/2/2
35	8CT	K	103	-	-	3/29/63/63	0/2/2/2
29	II0	7	315	-	-	1/21/67/67	0/2/2/2
27	CLA	A	828	-	1/1/15/20	7/37/115/115	-
29	II0	3	616	-	-	2/21/67/67	0/2/2/2
32	LMG	6	618	-	-	5/27/47/70	0/1/1/1
27	CLA	4	610	-	1/1/15/20	7/37/115/115	-
27	CLA	A	839	-	1/1/15/20	13/37/115/115	-
35	8CT	B	844	-	-	3/29/63/63	0/2/2/2
27	CLA	6	607	6	1/1/13/20	2/25/103/115	-
33	LHG	4	619	27	-	20/49/49/53	-
27	CLA	B	828	-	1/1/15/20	9/37/115/115	-
27	CLA	B	831	-	1/1/13/20	8/25/103/115	-
27	CLA	4	606	4	1/1/14/20	4/31/109/115	-
27	CLA	B	820	-	1/1/14/20	8/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	809	27	1/1/14/20	3/31/109/115	-
27	CLA	3	610	-	1/1/15/20	8/37/115/115	-
32	LMG	8	616	-	-	24/46/66/70	0/1/1/1
27	CLA	7	305	7	1/1/12/20	6/23/101/115	-
27	CLA	A	812	-	1/1/13/20	3/25/103/115	-
27	CLA	1	608	1	1/1/14/20	3/31/109/115	-
27	CLA	b	606	26	1/1/15/20	4/37/115/115	-
27	CLA	A	825	-	1/1/15/20	7/37/115/115	-
27	CLA	4	604	-	1/1/13/20	9/25/103/115	-
27	CLA	3	609	-	1/1/15/20	0/37/115/115	-
27	CLA	4	601	4	1/1/13/20	5/25/103/115	-
29	II0	a	614	-	-	2/21/67/67	0/2/2/2
35	8CT	A	846	-	-	3/29/63/63	0/2/2/2
27	CLA	a	603	-	1/1/14/20	5/31/109/115	-
27	CLA	a	601	25	1/1/11/20	6/13/91/115	-
31	IHT	9	619	-	-	3/25/65/65	0/2/2/2
27	CLA	A	820	-	1/1/15/20	8/37/115/115	-
27	CLA	3	602	3	1/1/13/20	2/25/103/115	-
27	CLA	A	844	-	1/1/15/20	6/37/115/115	-
33	LHG	A	852	-	-	20/43/43/53	-
29	II0	3	617	-	-	2/21/67/67	0/2/2/2
27	CLA	8	606	8	1/1/13/20	3/25/103/115	-
33	LHG	a	618	-	-	16/33/33/53	-
35	8CT	B	846	-	-	8/29/63/63	0/2/2/2
35	8CT	B	850	-	-	9/29/63/63	0/2/2/2
27	CLA	B	835	-	1/1/15/20	9/37/115/115	-
33	LHG	4	620	-	-	17/49/49/53	-
27	CLA	a	611	-	1/1/15/20	5/37/115/115	-
27	CLA	5	605	5	1/1/11/20	2/13/91/115	-
39	DGD	Z	303	-	-	27/49/89/95	0/2/2/2
29	II0	3	614	-	-	0/21/67/67	0/2/2/2
27	CLA	4	608	33	1/1/15/20	2/37/115/115	-
27	CLA	a	610	-	1/1/13/20	6/25/103/115	-
27	CLA	7	306	7	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	808	11	1/1/15/20	8/37/115/115	-
27	CLA	6	611	-	1/1/13/20	4/25/103/115	-
27	CLA	B	807	-	1/1/15/20	9/37/115/115	-
28	KC2	7	307	-	-	6/15/71/71	-
29	II0	b	614	-	-	0/21/67/67	0/2/2/2
27	CLA	A	810	-	1/1/15/20	16/37/115/115	-
29	II0	2	615	-	-	2/21/67/67	0/2/2/2
27	CLA	B	837	-	1/1/15/20	3/37/115/115	-
27	CLA	1	611	-	1/1/11/20	3/13/91/115	-
31	IHT	1	618	-	-	2/25/65/65	0/2/2/2
29	II0	8	611	-	-	2/21/67/67	0/2/2/2
35	8CT	B	849	-	-	4/29/63/63	0/2/2/2
27	CLA	5	607	5	1/1/11/20	0/13/91/115	-
27	CLA	8	605	8	1/1/12/20	3/19/97/115	-
27	CLA	a	608	-	1/1/14/20	7/31/109/115	-
27	CLA	4	611	-	1/1/15/20	9/37/115/115	-
27	CLA	6	604	-	1/1/14/20	6/31/109/115	-
27	CLA	O	201	-	1/1/13/20	3/25/103/115	-
29	II0	7	317	-	-	1/21/67/67	0/2/2/2
37	SF4	C	102	12	-	-	0/6/5/5
35	8CT	R	201	-	-	7/29/63/63	0/2/2/2
35	8CT	Z	309	-	-	6/29/63/63	0/2/2/2
27	CLA	L	201	19	1/1/12/20	1/21/99/115	-
27	CLA	B	829	-	1/1/11/20	0/13/91/115	-
35	8CT	R	203	-	-	4/29/63/63	0/2/2/2
27	CLA	3	601	3	1/1/11/20	4/13/91/115	-
28	KC2	5	610	5	-	4/15/71/71	-
27	CLA	A	821	-	1/1/13/20	2/25/103/115	-
35	8CT	4	616	-	-	5/29/63/63	0/2/2/2
35	8CT	b	615	-	-	6/29/63/63	0/2/2/2
27	CLA	7	312	-	1/1/13/20	5/25/103/115	-
27	CLA	B	811	-	1/1/13/20	6/25/103/115	-
35	8CT	7	318	-	-	9/29/63/63	0/2/2/2
27	CLA	7	309	7	1/1/13/20	7/25/103/115	-
29	II0	Z	312	-	-	1/21/67/67	0/2/2/2
35	8CT	A	848	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	II3	1	615	-	-	1/25/67/67	0/2/2/2
27	CLA	B	836	-	1/1/11/20	1/16/94/115	-
28	KC2	7	311	7	-	7/15/71/71	-
34	SQD	O	207	-	-	7/18/38/69	0/1/1/1
27	CLA	A	822	-	1/1/15/20	8/37/115/115	-
27	CLA	2	606	-	1/1/11/20	2/13/91/115	-
31	IHT	8	609	-	-	1/25/65/65	0/2/2/2
33	LHG	2	618	-	-	9/24/24/53	-
37	SF4	C	101	12	-	-	0/6/5/5
33	LHG	a	617	-	-	25/53/53/53	-
31	IHT	a	616	-	-	6/25/65/65	0/2/2/2
35	8CT	A	847	-	-	9/29/63/63	0/2/2/2
27	CLA	9	606	-	1/1/14/20	10/36/114/115	-
27	CLA	5	613	5	1/1/10/20	1/8/86/115	-
29	II0	3	615	-	-	1/21/67/67	0/2/2/2
27	CLA	6	603	-	1/1/11/20	5/13/91/115	-
27	CLA	b	608	-	1/1/15/20	7/37/115/115	-
31	IHT	L	204	-	-	2/25/65/65	0/2/2/2
27	CLA	5	609	-	1/1/10/20	0/8/86/115	-
29	II0	7	314	-	-	0/21/67/67	0/2/2/2
33	LHG	2	619	-	-	17/43/43/53	-
28	KC2	2	610	-	-	6/15/71/71	-
27	CLA	1	602	1	1/1/13/20	6/30/108/115	-
35	8CT	B	847	-	-	4/29/63/63	0/2/2/2
27	CLA	9	602	9	1/1/13/20	7/25/103/115	-
27	CLA	1	604	1	1/1/11/20	1/13/91/115	-
27	CLA	K	101	-	1/1/15/20	6/37/115/115	-
27	CLA	8	603	-	1/1/15/20	8/37/115/115	-
27	CLA	Z	301	-	1/1/14/20	11/31/109/115	-
29	II0	9	617	-	-	2/21/67/67	0/2/2/2
31	IHT	Z	302	-	-	2/25/65/65	0/2/2/2
33	LHG	7	320	27	-	20/43/43/53	-
27	CLA	A	814	-	1/1/11/20	5/13/91/115	-
27	CLA	9	608	9	1/1/13/20	9/25/103/115	-
27	CLA	B	801	-	1/1/15/20	5/37/115/115	-
27	CLA	B	815	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	604	-	1/1/14/20	9/31/109/115	-
27	CLA	A	832	-	1/1/15/20	6/37/115/115	-
29	II0	7	316	-	-	2/21/67/67	0/2/2/2
27	CLA	5	602	5	1/1/13/20	4/25/103/115	-
27	CLA	A	807	10	1/1/12/20	2/19/97/115	-
32	LMG	3	620	-	-	11/27/47/70	0/1/1/1
29	II0	a	613	-	-	2/21/67/67	0/2/2/2
27	CLA	A	829	-	1/1/12/20	4/19/97/115	-
27	CLA	A	805	-	1/1/12/20	1/19/97/115	-
33	LHG	7	319	-	-	9/35/35/53	-
27	CLA	b	602	26	1/1/14/20	14/36/114/115	-
27	CLA	A	827	-	1/1/15/20	5/37/115/115	-
27	CLA	A	815	-	1/1/14/20	1/34/112/115	-
27	CLA	A	826	-	1/1/15/20	5/37/115/115	-
27	CLA	A	816	-	1/1/14/20	7/31/109/115	-
34	SQD	3	621	-	-	14/37/57/69	0/1/1/1
27	CLA	6	606	-	1/1/13/20	8/25/103/115	-
27	CLA	A	802	27	1/1/13/20	3/25/103/115	-

All (2160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	601	CLA	C1B-NB	10.96	1.45	1.35
27	5	608	CLA	C1B-NB	10.93	1.45	1.35
27	5	601	CLA	C1B-NB	10.92	1.45	1.35
27	A	811	CLA	C1B-NB	10.91	1.44	1.35
27	O	204	CLA	C1B-NB	10.88	1.44	1.35
27	B	815	CLA	C1B-NB	10.86	1.44	1.35
27	O	202	CLA	C1B-NB	10.86	1.44	1.35
27	a	604	CLA	C1B-NB	10.84	1.44	1.35
27	1	611	CLA	C1B-NB	10.83	1.44	1.35
27	6	602	CLA	C1B-NB	10.83	1.44	1.35
27	Z	301	CLA	C1B-NB	10.83	1.44	1.35
27	7	306	CLA	C1B-NB	10.82	1.44	1.35
27	3	609	CLA	C1B-NB	10.81	1.44	1.35
27	1	609	CLA	C1B-NB	10.81	1.44	1.35
27	3	611	CLA	C1B-NB	10.79	1.44	1.35
27	9	614	CLA	C1B-NB	10.79	1.44	1.35
27	1	607	CLA	C1B-NB	10.78	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	835	CLA	C1B-NB	10.78	1.44	1.35
27	J	102	CLA	C1B-NB	10.78	1.44	1.35
27	2	602	CLA	C1B-NB	10.77	1.44	1.35
27	1	608	CLA	C1B-NB	10.76	1.44	1.35
27	5	609	CLA	C1B-NB	10.76	1.44	1.35
27	7	308	CLA	C1B-NB	10.75	1.44	1.35
27	8	615	CLA	C1B-NB	10.75	1.44	1.35
27	8	608	CLA	C1B-NB	10.75	1.44	1.35
27	2	601	CLA	C1B-NB	10.74	1.44	1.35
27	9	601	CLA	C1B-NB	10.73	1.44	1.35
27	A	830	CLA	C1B-NB	10.72	1.44	1.35
27	A	822	CLA	C1B-NB	10.72	1.44	1.35
27	B	819	CLA	C1B-NB	10.71	1.44	1.35
27	6	607	CLA	C1B-NB	10.71	1.44	1.35
27	2	609	CLA	C1B-NB	10.71	1.44	1.35
27	7	310	CLA	C1B-NB	10.71	1.44	1.35
27	7	303	CLA	C1B-NB	10.71	1.44	1.35
27	8	601	CLA	C1B-NB	10.71	1.44	1.35
27	8	603	CLA	C1B-NB	10.70	1.44	1.35
27	A	842	CLA	C1B-NB	10.70	1.44	1.35
27	3	608	CLA	C1B-NB	10.70	1.44	1.35
27	5	604	CLA	C1B-NB	10.70	1.44	1.35
27	a	606	CLA	C1B-NB	10.70	1.44	1.35
27	7	305	CLA	C1B-NB	10.69	1.44	1.35
27	9	604	CLA	C1B-NB	10.69	1.44	1.35
27	3	601	CLA	C1B-NB	10.69	1.44	1.35
27	6	601	CLA	C1B-NB	10.69	1.44	1.35
27	A	808	CLA	C1B-NB	10.68	1.44	1.35
27	B	841	CLA	C1B-NB	10.67	1.44	1.35
27	B	838	CLA	C1B-NB	10.66	1.44	1.35
27	B	812	CLA	C1B-NB	10.66	1.44	1.35
27	8	607	CLA	C1B-NB	10.66	1.44	1.35
27	a	608	CLA	C1B-NB	10.66	1.44	1.35
27	2	606	CLA	C1B-NB	10.65	1.44	1.35
27	6	611	CLA	C1B-NB	10.65	1.44	1.35
27	a	607	CLA	C1B-NB	10.65	1.44	1.35
27	A	824	CLA	C1B-NB	10.65	1.44	1.35
27	A	836	CLA	C1B-NB	10.64	1.44	1.35
27	B	829	CLA	C1B-NB	10.64	1.44	1.35
27	b	608	CLA	C1B-NB	10.64	1.44	1.35
27	B	811	CLA	C1B-NB	10.64	1.44	1.35
27	4	602	CLA	C1B-NB	10.63	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	602	CLA	C1B-NB	10.63	1.44	1.35
27	A	805	CLA	C1B-NB	10.63	1.44	1.35
27	7	304	CLA	C1B-NB	10.63	1.44	1.35
27	6	604	CLA	C1B-NB	10.63	1.44	1.35
27	A	815	CLA	C1B-NB	10.63	1.44	1.35
27	9	603	CLA	C1B-NB	10.62	1.44	1.35
27	6	606	CLA	C1B-NB	10.60	1.44	1.35
27	6	609	CLA	C1B-NB	10.60	1.44	1.35
27	B	805	CLA	C1B-NB	10.60	1.44	1.35
27	A	819	CLA	C1B-NB	10.60	1.44	1.35
27	F	202	CLA	C1B-NB	10.60	1.44	1.35
27	1	602	CLA	C1B-NB	10.59	1.44	1.35
27	b	601	CLA	C1B-NB	10.59	1.44	1.35
27	4	608	CLA	C1B-NB	10.59	1.44	1.35
27	A	843	CLA	C1B-NB	10.59	1.44	1.35
27	3	607	CLA	C1B-NB	10.58	1.44	1.35
27	4	607	CLA	C1B-NB	10.58	1.44	1.35
27	a	602	CLA	C1B-NB	10.58	1.44	1.35
27	b	607	CLA	C1B-NB	10.58	1.44	1.35
27	5	602	CLA	C1B-NB	10.58	1.44	1.35
27	B	839	CLA	C1B-NB	10.58	1.44	1.35
27	2	608	CLA	C1B-NB	10.58	1.44	1.35
27	8	602	CLA	C1B-NB	10.57	1.44	1.35
27	1	604	CLA	C1B-NB	10.57	1.44	1.35
27	2	604	CLA	C1B-NB	10.57	1.44	1.35
27	4	603	CLA	C1B-NB	10.57	1.44	1.35
27	b	606	CLA	C1B-NB	10.57	1.44	1.35
27	5	611	CLA	C1B-NB	10.57	1.44	1.35
27	K	102	CLA	C1B-NB	10.57	1.44	1.35
27	L	201	CLA	C1B-NB	10.56	1.44	1.35
27	A	813	CLA	C1B-NB	10.56	1.44	1.35
27	3	602	CLA	C1B-NB	10.56	1.44	1.35
27	9	609	CLA	C1B-NB	10.56	1.44	1.35
27	A	838	CLA	C1B-NB	10.56	1.44	1.35
27	Z	304	CLA	C1B-NB	10.56	1.44	1.35
27	b	604	CLA	C1B-NB	10.55	1.44	1.35
27	B	802	CLA	C1B-NB	10.55	1.44	1.35
27	B	820	CLA	C1B-NB	10.55	1.44	1.35
27	B	831	CLA	C1B-NB	10.55	1.44	1.35
27	A	814	CLA	C1B-NB	10.55	1.44	1.35
27	1	613	CLA	C1B-NB	10.55	1.44	1.35
27	a	610	CLA	C1B-NB	10.54	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	829	CLA	C1B-NB	10.54	1.44	1.35
27	a	601	CLA	C1B-NB	10.54	1.44	1.35
27	7	312	CLA	C1B-NB	10.54	1.44	1.35
27	A	821	CLA	C1B-NB	10.54	1.44	1.35
27	4	601	CLA	C1B-NB	10.53	1.44	1.35
27	B	816	CLA	C1B-NB	10.52	1.44	1.35
27	3	605	CLA	C1B-NB	10.52	1.44	1.35
27	9	608	CLA	C1B-NB	10.52	1.44	1.35
27	b	603	CLA	C1B-NB	10.52	1.44	1.35
27	3	604	CLA	C1B-NB	10.51	1.44	1.35
27	7	309	CLA	C1B-NB	10.51	1.44	1.35
27	5	613	CLA	C1B-NB	10.51	1.44	1.35
27	Z	306	CLA	C1B-NB	10.51	1.44	1.35
27	a	603	CLA	C1B-NB	10.50	1.44	1.35
27	9	602	CLA	C1B-NB	10.50	1.44	1.35
27	1	603	CLA	C1B-NB	10.50	1.44	1.35
27	A	825	CLA	C1B-NB	10.50	1.44	1.35
27	5	606	CLA	C1B-NB	10.50	1.44	1.35
27	B	814	CLA	C1B-NB	10.50	1.44	1.35
27	A	818	CLA	C1B-NB	10.49	1.44	1.35
27	A	835	CLA	C1B-NB	10.49	1.44	1.35
27	B	830	CLA	C1B-NB	10.48	1.44	1.35
27	5	605	CLA	C1B-NB	10.48	1.44	1.35
27	9	611	CLA	C1B-NB	10.47	1.44	1.35
27	6	612	CLA	C1B-NB	10.47	1.44	1.35
27	7	302	CLA	C1B-NB	10.47	1.44	1.35
27	9	605	CLA	C1B-NB	10.46	1.44	1.35
27	B	821	CLA	C1B-NB	10.46	1.44	1.35
27	O	203	CLA	C1B-NB	10.46	1.44	1.35
27	2	603	CLA	C1B-NB	10.46	1.44	1.35
27	2	611	CLA	C1B-NB	10.46	1.44	1.35
27	A	834	CLA	C1B-NB	10.45	1.44	1.35
27	F	204	CLA	C1B-NB	10.45	1.44	1.35
27	Z	305	CLA	C1B-NB	10.45	1.44	1.35
27	5	612	CLA	C1B-NB	10.44	1.44	1.35
27	3	603	CLA	C1B-NB	10.44	1.44	1.35
27	8	604	CLA	C1B-NB	10.44	1.44	1.35
27	A	807	CLA	C1B-NB	10.44	1.44	1.35
27	A	810	CLA	C1B-NB	10.43	1.44	1.35
27	O	201	CLA	C1B-NB	10.43	1.44	1.35
27	2	607	CLA	C1B-NB	10.43	1.44	1.35
27	1	606	CLA	C1B-NB	10.43	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	604	CLA	C1B-NB	10.43	1.44	1.35
27	4	609	CLA	C1B-NB	10.43	1.44	1.35
27	A	820	CLA	C1B-NB	10.43	1.44	1.35
27	B	804	CLA	C1B-NB	10.43	1.44	1.35
27	2	612	CLA	C1B-NB	10.42	1.44	1.35
27	A	803	CLA	C1B-NB	10.42	1.44	1.35
27	3	610	CLA	C1B-NB	10.42	1.44	1.35
27	7	313	CLA	C1B-NB	10.42	1.44	1.35
27	A	806	CLA	C1B-NB	10.42	1.44	1.35
27	5	603	CLA	C1B-NB	10.41	1.44	1.35
27	A	802	CLA	C1B-NB	10.41	1.44	1.35
27	9	613	CLA	C1B-NB	10.41	1.44	1.35
27	9	612	CLA	C1B-NB	10.41	1.44	1.35
27	A	804	CLA	C1B-NB	10.41	1.44	1.35
27	B	809	CLA	C1B-NB	10.41	1.44	1.35
27	1	612	CLA	C1B-NB	10.40	1.44	1.35
27	4	606	CLA	C1B-NB	10.40	1.44	1.35
27	K	101	CLA	C1B-NB	10.40	1.44	1.35
27	A	812	CLA	C1B-NB	10.40	1.44	1.35
27	A	816	CLA	C1B-NB	10.40	1.44	1.35
27	A	809	CLA	C1B-NB	10.39	1.44	1.35
27	A	832	CLA	C1B-NB	10.38	1.44	1.35
27	a	605	CLA	C1B-NB	10.38	1.44	1.35
27	4	610	CLA	C1B-NB	10.38	1.44	1.35
27	B	837	CLA	C1B-NB	10.37	1.44	1.35
27	2	605	CLA	C1B-NB	10.36	1.44	1.35
27	A	833	CLA	C1B-NB	10.36	1.44	1.35
27	b	610	CLA	C1B-NB	10.36	1.44	1.35
27	A	839	CLA	C1B-NB	10.36	1.44	1.35
27	3	612	CLA	C1B-NB	10.35	1.44	1.35
27	5	607	CLA	C1B-NB	10.34	1.44	1.35
27	R	202	CLA	C1B-NB	10.33	1.44	1.35
27	A	841	CLA	C1B-NB	10.33	1.44	1.35
27	B	803	CLA	C1B-NB	10.33	1.44	1.35
27	6	605	CLA	C1B-NB	10.32	1.44	1.35
27	B	818	CLA	C1B-NB	10.32	1.44	1.35
27	6	603	CLA	C1B-NB	10.31	1.44	1.35
27	A	817	CLA	C1B-NB	10.30	1.44	1.35
27	b	611	CLA	C1B-NB	10.28	1.44	1.35
27	L	202	CLA	C1B-NB	10.27	1.44	1.35
27	B	817	CLA	C1B-NB	10.27	1.44	1.35
27	6	608	CLA	C1B-NB	10.26	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	203	CLA	C1B-NB	10.26	1.44	1.35
27	F	203	CLA	C1B-NB	10.24	1.44	1.35
27	9	607	CLA	C1B-NB	10.24	1.44	1.35
27	B	826	CLA	C1B-NB	10.24	1.44	1.35
27	4	611	CLA	C1B-NB	10.23	1.44	1.35
27	B	836	CLA	C1B-NB	10.23	1.44	1.35
27	B	825	CLA	C1B-NB	10.23	1.44	1.35
27	8	606	CLA	C1B-NB	10.22	1.44	1.35
27	B	832	CLA	C1B-NB	10.22	1.44	1.35
31	A	854	IHT	C10-C07	10.21	1.52	1.34
27	B	833	CLA	C1B-NB	10.20	1.44	1.35
27	a	611	CLA	C1B-NB	10.20	1.44	1.35
27	B	840	CLA	C1B-NB	10.19	1.44	1.35
27	A	828	CLA	C1B-NB	10.18	1.44	1.35
27	A	823	CLA	C1B-NB	10.17	1.44	1.35
27	B	823	CLA	C1B-NB	10.17	1.44	1.35
27	1	605	CLA	C1B-NB	10.16	1.44	1.35
27	B	813	CLA	C1B-NB	10.15	1.44	1.35
27	8	605	CLA	C1B-NB	10.15	1.44	1.35
27	9	606	CLA	C1B-NB	10.15	1.44	1.35
27	B	807	CLA	C1B-NB	10.15	1.44	1.35
27	A	837	CLA	C1B-NB	10.14	1.44	1.35
27	B	828	CLA	C1B-NB	10.14	1.44	1.35
27	Z	310	CLA	C1B-NB	10.11	1.44	1.35
27	B	810	CLA	C1B-NB	10.11	1.44	1.35
27	B	834	CLA	C1B-NB	10.09	1.44	1.35
27	B	824	CLA	C1B-NB	10.05	1.44	1.35
27	A	840	CLA	C1B-NB	10.05	1.44	1.35
27	A	831	CLA	C1B-NB	10.04	1.44	1.35
27	B	822	CLA	C1B-NB	9.95	1.44	1.35
27	B	808	CLA	C1B-NB	9.95	1.44	1.35
27	B	827	CLA	C1B-NB	9.90	1.44	1.35
31	1	618	IHT	C10-C07	9.86	1.51	1.34
27	B	806	CLA	C1B-NB	9.80	1.44	1.35
27	A	801	CLA	C1B-NB	9.72	1.43	1.35
31	Z	302	IHT	C10-C07	9.71	1.51	1.34
27	A	826	CLA	C1B-NB	9.65	1.43	1.35
27	B	801	CLA	C1B-NB	9.62	1.43	1.35
27	A	827	CLA	C1B-NB	9.57	1.43	1.35
31	5	618	IHT	C10-C07	9.53	1.50	1.34
31	6	616	IHT	C10-C07	9.51	1.50	1.34
27	A	844	CLA	C1B-NB	9.48	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	204	IHT	C10-C07	9.44	1.50	1.34
31	2	616	IHT	C10-C07	9.26	1.50	1.34
31	a	616	IHT	C10-C07	9.26	1.50	1.34
27	Z	301	CLA	C4B-NB	9.08	1.43	1.35
31	9	619	IHT	C10-C07	9.06	1.50	1.34
31	8	609	IHT	C10-C07	9.06	1.50	1.34
27	A	842	CLA	C4B-NB	9.03	1.43	1.35
27	1	608	CLA	C4B-NB	9.02	1.43	1.35
27	b	602	CLA	C4B-NB	8.99	1.43	1.35
31	A	854	IHT	C24-C26	-8.97	1.25	1.42
27	2	608	CLA	C4B-NB	8.96	1.43	1.35
29	1	619	II0	C24-C26	-8.95	1.25	1.42
27	A	810	CLA	C4B-NB	8.92	1.43	1.35
31	L	204	IHT	C24-C26	-8.88	1.25	1.42
27	9	611	CLA	C4B-NB	8.88	1.43	1.35
29	8	611	II0	C23-C25	-8.87	1.25	1.42
27	1	607	CLA	C4B-NB	8.85	1.43	1.35
27	5	613	CLA	C4B-NB	8.85	1.43	1.35
27	1	602	CLA	C4B-NB	8.85	1.43	1.35
27	O	204	CLA	C4B-NB	8.85	1.43	1.35
27	7	303	CLA	C4B-NB	8.84	1.43	1.35
27	b	607	CLA	C4B-NB	8.84	1.43	1.35
27	6	602	CLA	C4B-NB	8.83	1.43	1.35
27	O	202	CLA	C4B-NB	8.83	1.43	1.35
29	a	614	II0	C23-C25	-8.83	1.25	1.42
31	2	616	IHT	C09-C10	-8.83	1.33	1.51
27	a	610	CLA	C4B-NB	8.82	1.43	1.35
27	6	607	CLA	C4B-NB	8.82	1.43	1.35
27	7	306	CLA	C4B-NB	8.82	1.43	1.35
31	2	616	IHT	C24-C26	-8.81	1.25	1.42
27	5	609	CLA	C4B-NB	8.81	1.43	1.35
27	1	611	CLA	C4B-NB	8.81	1.43	1.35
27	7	308	CLA	C4B-NB	8.80	1.43	1.35
27	B	819	CLA	C4B-NB	8.80	1.43	1.35
31	6	616	IHT	C24-C26	-8.80	1.25	1.42
29	2	613	II0	C24-C26	-8.80	1.25	1.42
31	9	619	IHT	C09-C10	-8.79	1.33	1.51
27	B	820	CLA	C4B-NB	8.78	1.43	1.35
27	A	830	CLA	C4B-NB	8.78	1.43	1.35
27	b	603	CLA	C4B-NB	8.78	1.43	1.35
27	B	813	CLA	C4B-NB	8.77	1.43	1.35
27	2	609	CLA	C4B-NB	8.77	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	610	II0	C24-C26	-8.77	1.25	1.42
29	O	205	II0	C23-C25	-8.77	1.25	1.42
27	2	604	CLA	C4B-NB	8.76	1.43	1.35
27	3	609	CLA	C4B-NB	8.76	1.43	1.35
27	K	101	CLA	C4B-NB	8.76	1.43	1.35
27	9	608	CLA	C4B-NB	8.76	1.43	1.35
29	8	610	II0	C23-C25	-8.76	1.25	1.42
27	1	601	CLA	C4B-NB	8.75	1.43	1.35
27	A	836	CLA	C4B-NB	8.75	1.43	1.35
27	9	609	CLA	C4B-NB	8.75	1.43	1.35
29	2	613	II0	C23-C25	-8.75	1.25	1.42
27	3	608	CLA	C4B-NB	8.75	1.43	1.35
27	A	839	CLA	C4B-NB	8.75	1.43	1.35
29	7	301	II0	C24-C26	-8.74	1.25	1.42
27	A	833	CLA	C4B-NB	8.74	1.43	1.35
29	a	615	II0	C23-C25	-8.74	1.25	1.42
27	b	604	CLA	C4B-NB	8.74	1.43	1.35
29	J	101	II0	C23-C25	-8.74	1.25	1.42
29	1	617	II0	C24-C26	-8.74	1.25	1.42
27	8	601	CLA	C4B-NB	8.74	1.43	1.35
27	O	203	CLA	C4B-NB	8.73	1.43	1.35
27	4	607	CLA	C4B-NB	8.73	1.43	1.35
27	5	608	CLA	C4B-NB	8.73	1.43	1.35
29	5	615	II0	C24-C26	-8.73	1.25	1.42
27	9	612	CLA	C4B-NB	8.73	1.43	1.35
27	3	604	CLA	C4B-NB	8.72	1.43	1.35
27	Z	305	CLA	C4B-NB	8.72	1.43	1.35
27	8	608	CLA	C4B-NB	8.72	1.43	1.35
29	3	617	II0	C23-C25	-8.72	1.25	1.42
27	7	302	CLA	C4B-NB	8.72	1.43	1.35
27	8	607	CLA	C4B-NB	8.72	1.43	1.35
27	9	601	CLA	C4B-NB	8.72	1.43	1.35
29	7	316	II0	C23-C25	-8.72	1.25	1.42
27	B	841	CLA	C4B-NB	8.72	1.43	1.35
31	8	609	IHT	C24-C26	-8.72	1.25	1.42
27	8	604	CLA	C4B-NB	8.72	1.43	1.35
27	B	831	CLA	C4B-NB	8.72	1.43	1.35
29	O	205	II0	C24-C26	-8.72	1.25	1.42
27	6	604	CLA	C4B-NB	8.72	1.43	1.35
27	A	805	CLA	C4B-NB	8.71	1.43	1.35
31	8	609	IHT	C09-C10	-8.71	1.33	1.51
27	O	201	CLA	C4B-NB	8.71	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	843	II0	C24-C26	-8.71	1.25	1.42
27	4	604	CLA	C4B-NB	8.71	1.43	1.35
27	2	611	CLA	C4B-NB	8.71	1.43	1.35
31	a	616	IHT	C24-C26	-8.70	1.25	1.42
27	A	838	CLA	C4B-NB	8.70	1.43	1.35
27	8	603	CLA	C4B-NB	8.70	1.43	1.35
27	9	614	CLA	C4B-NB	8.70	1.43	1.35
27	5	601	CLA	C4B-NB	8.70	1.43	1.35
30	1	615	II3	C27-C28	-8.70	1.25	1.42
27	5	611	CLA	C4B-NB	8.70	1.43	1.35
27	A	822	CLA	C4B-NB	8.69	1.43	1.35
31	1	618	IHT	C24-C26	-8.69	1.25	1.42
29	a	612	II0	C24-C26	-8.69	1.25	1.42
27	B	838	CLA	C4B-NB	8.69	1.43	1.35
29	2	615	II0	C23-C25	-8.69	1.25	1.42
27	5	602	CLA	C4B-NB	8.69	1.43	1.35
27	B	823	CLA	C4B-NB	8.69	1.43	1.35
29	5	620	II0	C23-C25	-8.68	1.25	1.42
29	a	613	II0	C23-C25	-8.68	1.25	1.42
27	8	615	CLA	C4B-NB	8.68	1.42	1.35
27	9	613	CLA	C4B-NB	8.68	1.42	1.35
29	B	843	II0	C23-C25	-8.67	1.25	1.42
27	1	609	CLA	C4B-NB	8.67	1.42	1.35
29	3	617	II0	C24-C26	-8.67	1.25	1.42
27	5	607	CLA	C4B-NB	8.67	1.42	1.35
29	7	317	II0	C24-C26	-8.67	1.25	1.42
29	3	614	II0	C24-C26	-8.67	1.25	1.42
27	K	102	CLA	C4B-NB	8.67	1.42	1.35
29	1	619	II0	C23-C25	-8.66	1.25	1.42
27	B	839	CLA	C4B-NB	8.66	1.42	1.35
29	a	614	II0	C24-C26	-8.66	1.25	1.42
31	Z	302	IHT	C24-C26	-8.66	1.25	1.42
27	2	612	CLA	C4B-NB	8.66	1.42	1.35
27	A	813	CLA	C4B-NB	8.66	1.42	1.35
27	1	606	CLA	C4B-NB	8.65	1.42	1.35
29	5	616	II0	C23-C25	-8.65	1.25	1.42
27	A	825	CLA	C4B-NB	8.65	1.42	1.35
29	1	614	II0	C23-C25	-8.65	1.25	1.42
27	b	608	CLA	C4B-NB	8.65	1.42	1.35
27	2	602	CLA	C4B-NB	8.65	1.42	1.35
27	6	611	CLA	C4B-NB	8.65	1.42	1.35
27	9	605	CLA	C4B-NB	8.65	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3	616	II0	C24-C26	-8.65	1.25	1.42
29	O	206	II0	C24-C26	-8.65	1.25	1.42
27	4	609	CLA	C4B-NB	8.65	1.42	1.35
27	9	602	CLA	C4B-NB	8.65	1.42	1.35
27	A	835	CLA	C4B-NB	8.65	1.42	1.35
27	B	803	CLA	C4B-NB	8.64	1.42	1.35
27	B	815	CLA	C4B-NB	8.64	1.42	1.35
27	3	605	CLA	C4B-NB	8.64	1.42	1.35
29	7	317	II0	C23-C25	-8.64	1.25	1.42
27	A	802	CLA	C4B-NB	8.64	1.42	1.35
27	A	808	CLA	C4B-NB	8.64	1.42	1.35
27	A	843	CLA	C4B-NB	8.64	1.42	1.35
27	2	601	CLA	C4B-NB	8.64	1.42	1.35
27	3	611	CLA	C4B-NB	8.64	1.42	1.35
29	1	616	II0	C24-C26	-8.63	1.25	1.42
31	A	854	IHT	C09-C10	-8.63	1.34	1.51
27	A	812	CLA	C4B-NB	8.63	1.42	1.35
27	7	304	CLA	C4B-NB	8.63	1.42	1.35
29	4	615	II0	C24-C26	-8.63	1.25	1.42
29	6	614	II0	C23-C25	-8.63	1.25	1.42
29	5	620	II0	C24-C26	-8.62	1.26	1.42
29	R	204	II0	C24-C26	-8.62	1.26	1.42
29	7	316	II0	C24-C26	-8.62	1.26	1.42
31	5	618	IHT	C24-C26	-8.62	1.26	1.42
29	O	206	II0	C23-C25	-8.62	1.26	1.42
27	3	602	CLA	C4B-NB	8.62	1.42	1.35
27	4	602	CLA	C4B-NB	8.62	1.42	1.35
30	b	613	II3	C27-C28	-8.62	1.26	1.42
29	b	614	II0	C24-C26	-8.61	1.26	1.42
29	9	617	II0	C23-C25	-8.61	1.26	1.42
27	3	601	CLA	C4B-NB	8.61	1.42	1.35
29	9	616	II0	C23-C25	-8.61	1.26	1.42
31	9	619	IHT	C24-C26	-8.61	1.26	1.42
27	a	604	CLA	C4B-NB	8.61	1.42	1.35
27	3	612	CLA	C4B-NB	8.61	1.42	1.35
27	b	611	CLA	C4B-NB	8.60	1.42	1.35
27	A	804	CLA	C4B-NB	8.60	1.42	1.35
27	a	608	CLA	C4B-NB	8.60	1.42	1.35
27	B	835	CLA	C4B-NB	8.59	1.42	1.35
29	9	618	II0	C23-C25	-8.59	1.26	1.42
27	7	309	CLA	C4B-NB	8.59	1.42	1.35
29	8	612	II0	C24-C26	-8.59	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	602	CLA	C4B-NB	8.58	1.42	1.35
27	3	607	CLA	C4B-NB	8.58	1.42	1.35
27	A	834	CLA	C4B-NB	8.58	1.42	1.35
27	5	612	CLA	C4B-NB	8.58	1.42	1.35
29	6	615	II0	C24-C26	-8.58	1.26	1.42
27	5	604	CLA	C4B-NB	8.58	1.42	1.35
29	7	314	II0	C24-C26	-8.58	1.26	1.42
27	9	604	CLA	C4B-NB	8.57	1.42	1.35
27	7	312	CLA	C4B-NB	8.57	1.42	1.35
29	Z	312	II0	C23-C25	-8.57	1.26	1.42
29	7	301	II0	C23-C25	-8.57	1.26	1.42
29	9	617	II0	C24-C26	-8.57	1.26	1.42
29	2	615	II0	C24-C26	-8.57	1.26	1.42
27	A	806	CLA	C4B-NB	8.57	1.42	1.35
27	A	807	CLA	C4B-NB	8.57	1.42	1.35
27	b	601	CLA	C4B-NB	8.56	1.42	1.35
27	2	603	CLA	C4B-NB	8.56	1.42	1.35
27	A	814	CLA	C4B-NB	8.56	1.42	1.35
27	A	819	CLA	C4B-NB	8.56	1.42	1.35
27	B	805	CLA	C4B-NB	8.56	1.42	1.35
29	8	612	II0	C23-C25	-8.56	1.26	1.42
29	J	101	II0	C24-C26	-8.56	1.26	1.42
27	4	603	CLA	C4B-NB	8.56	1.42	1.35
29	7	315	II0	C23-C25	-8.56	1.26	1.42
29	R	204	II0	C23-C25	-8.56	1.26	1.42
27	Z	304	CLA	C4B-NB	8.56	1.42	1.35
29	a	612	II0	C23-C25	-8.56	1.26	1.42
27	F	202	CLA	C4B-NB	8.56	1.42	1.35
27	7	313	CLA	C4B-NB	8.56	1.42	1.35
27	b	610	CLA	C4B-NB	8.55	1.42	1.35
29	3	613	II0	C23-C25	-8.55	1.26	1.42
27	A	829	CLA	C4B-NB	8.55	1.42	1.35
27	A	828	CLA	C4B-NB	8.55	1.42	1.35
29	5	614	II0	C24-C26	-8.55	1.26	1.42
27	A	823	CLA	C4B-NB	8.54	1.42	1.35
27	B	818	CLA	C4B-NB	8.54	1.42	1.35
27	3	603	CLA	C4B-NB	8.54	1.42	1.35
27	L	201	CLA	C4B-NB	8.54	1.42	1.35
27	2	606	CLA	C4B-NB	8.54	1.42	1.35
29	1	614	II0	C24-C26	-8.54	1.26	1.42
29	5	616	II0	C24-C26	-8.54	1.26	1.42
27	a	601	CLA	C4B-NB	8.54	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	602	CLA	C4B-NB	8.53	1.42	1.35
27	7	305	CLA	C4B-NB	8.53	1.42	1.35
27	9	603	CLA	C4B-NB	8.53	1.42	1.35
27	A	820	CLA	C4B-NB	8.53	1.42	1.35
29	4	612	II0	C24-C26	-8.53	1.26	1.42
27	4	610	CLA	C4B-NB	8.53	1.42	1.35
27	2	607	CLA	C4B-NB	8.53	1.42	1.35
27	A	815	CLA	C4B-NB	8.53	1.42	1.35
27	Z	310	CLA	C4B-NB	8.53	1.42	1.35
29	3	615	II0	C23-C25	-8.52	1.26	1.42
29	9	618	II0	C24-C26	-8.52	1.26	1.42
29	3	615	II0	C24-C26	-8.52	1.26	1.42
29	4	612	II0	C23-C25	-8.52	1.26	1.42
27	1	612	CLA	C4B-NB	8.52	1.42	1.35
29	4	614	II0	C23-C25	-8.52	1.26	1.42
27	1	603	CLA	C4B-NB	8.52	1.42	1.35
29	5	617	II0	C24-C26	-8.51	1.26	1.42
27	6	609	CLA	C4B-NB	8.51	1.42	1.35
27	B	817	CLA	C4B-NB	8.51	1.42	1.35
27	B	810	CLA	C4B-NB	8.51	1.42	1.35
27	1	613	CLA	C4B-NB	8.51	1.42	1.35
31	Z	302	IHT	C09-C10	-8.51	1.34	1.51
27	7	310	CLA	C4B-NB	8.50	1.42	1.35
27	a	611	CLA	C4B-NB	8.50	1.42	1.35
29	8	611	II0	C24-C26	-8.50	1.26	1.42
27	6	608	CLA	C4B-NB	8.50	1.42	1.35
27	A	837	CLA	C4B-NB	8.50	1.42	1.35
29	3	614	II0	C23-C25	-8.50	1.26	1.42
29	5	615	II0	C23-C25	-8.50	1.26	1.42
27	B	814	CLA	C4B-NB	8.49	1.42	1.35
29	4	613	II0	C24-C26	-8.49	1.26	1.42
27	B	811	CLA	C4B-NB	8.49	1.42	1.35
29	7	315	II0	C24-C26	-8.49	1.26	1.42
27	6	606	CLA	C4B-NB	8.49	1.42	1.35
29	6	615	II0	C23-C25	-8.49	1.26	1.42
29	1	617	II0	C23-C25	-8.49	1.26	1.42
27	5	606	CLA	C4B-NB	8.49	1.42	1.35
27	A	817	CLA	C4B-NB	8.49	1.42	1.35
27	a	603	CLA	C4B-NB	8.49	1.42	1.35
29	3	616	II0	C23-C25	-8.49	1.26	1.42
27	3	610	CLA	C4B-NB	8.49	1.42	1.35
29	b	614	II0	C23-C25	-8.48	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	601	CLA	C4B-NB	8.48	1.42	1.35
27	B	825	CLA	C4B-NB	8.48	1.42	1.35
27	8	606	CLA	C4B-NB	8.48	1.42	1.35
27	A	832	CLA	C4B-NB	8.48	1.42	1.35
27	B	807	CLA	C4B-NB	8.48	1.42	1.35
29	2	614	II0	C24-C26	-8.48	1.26	1.42
27	a	606	CLA	C4B-NB	8.48	1.42	1.35
29	3	613	II0	C24-C26	-8.48	1.26	1.42
27	A	811	CLA	C4B-NB	8.47	1.42	1.35
27	B	812	CLA	C4B-NB	8.47	1.42	1.35
27	5	605	CLA	C4B-NB	8.47	1.42	1.35
27	F	204	CLA	C4B-NB	8.47	1.42	1.35
29	4	614	II0	C24-C26	-8.47	1.26	1.42
27	4	611	CLA	C4B-NB	8.46	1.42	1.35
27	B	826	CLA	C4B-NB	8.46	1.42	1.35
27	B	837	CLA	C4B-NB	8.46	1.42	1.35
31	a	616	IHT	C09-C10	-8.46	1.34	1.51
27	B	834	CLA	C4B-NB	8.46	1.42	1.35
29	a	615	II0	C24-C26	-8.46	1.26	1.42
27	4	606	CLA	C4B-NB	8.46	1.42	1.35
27	5	603	CLA	C4B-NB	8.46	1.42	1.35
27	A	816	CLA	C4B-NB	8.46	1.42	1.35
27	L	203	CLA	C4B-NB	8.45	1.42	1.35
29	b	612	II0	C24-C26	-8.45	1.26	1.42
29	4	615	II0	C23-C25	-8.45	1.26	1.42
29	5	617	II0	C23-C25	-8.44	1.26	1.42
27	B	821	CLA	C4B-NB	8.44	1.42	1.35
27	Z	306	CLA	C4B-NB	8.44	1.42	1.35
27	a	607	CLA	C4B-NB	8.44	1.42	1.35
27	A	818	CLA	C4B-NB	8.44	1.42	1.35
29	9	615	II0	C23-C25	-8.44	1.26	1.42
27	8	605	CLA	C4B-NB	8.44	1.42	1.35
27	1	604	CLA	C4B-NB	8.44	1.42	1.35
27	a	605	CLA	C4B-NB	8.43	1.42	1.35
27	A	824	CLA	C4B-NB	8.43	1.42	1.35
29	9	616	II0	C24-C26	-8.43	1.26	1.42
27	B	808	CLA	C4B-NB	8.42	1.42	1.35
29	a	613	II0	C24-C26	-8.42	1.26	1.42
29	9	615	II0	C24-C26	-8.42	1.26	1.42
27	B	832	CLA	C4B-NB	8.42	1.42	1.35
29	4	613	II0	C23-C25	-8.42	1.26	1.42
27	4	608	CLA	C4B-NB	8.42	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	824	CLA	C4B-NB	8.41	1.42	1.35
31	L	204	IHT	C09-C10	-8.41	1.34	1.51
27	A	803	CLA	C4B-NB	8.41	1.42	1.35
27	B	806	CLA	C4B-NB	8.41	1.42	1.35
27	4	601	CLA	C4B-NB	8.40	1.42	1.35
27	b	606	CLA	C4B-NB	8.39	1.42	1.35
29	6	614	II0	C24-C26	-8.39	1.26	1.42
27	6	612	CLA	C4B-NB	8.39	1.42	1.35
27	B	830	CLA	C4B-NB	8.39	1.42	1.35
29	b	612	II0	C23-C25	-8.39	1.26	1.42
27	B	816	CLA	C4B-NB	8.39	1.42	1.35
29	7	314	II0	C23-C25	-8.38	1.26	1.42
27	9	606	CLA	C4B-NB	8.37	1.42	1.35
27	B	836	CLA	C4B-NB	8.36	1.42	1.35
27	B	809	CLA	C4B-NB	8.36	1.42	1.35
27	A	821	CLA	C4B-NB	8.35	1.42	1.35
27	R	202	CLA	C4B-NB	8.35	1.42	1.35
27	6	605	CLA	C4B-NB	8.35	1.42	1.35
29	5	614	II0	C23-C25	-8.35	1.26	1.42
27	2	605	CLA	C4B-NB	8.35	1.42	1.35
27	J	102	CLA	C4B-NB	8.35	1.42	1.35
27	L	202	CLA	C4B-NB	8.35	1.42	1.35
27	B	804	CLA	C4B-NB	8.34	1.42	1.35
29	1	616	II0	C23-C25	-8.34	1.26	1.42
27	A	831	CLA	C4B-NB	8.33	1.42	1.35
29	2	614	II0	C23-C25	-8.33	1.26	1.42
27	B	829	CLA	C4B-NB	8.32	1.42	1.35
29	Z	312	II0	C24-C26	-8.31	1.26	1.42
27	F	203	CLA	C4B-NB	8.30	1.42	1.35
27	B	827	CLA	C4B-NB	8.27	1.42	1.35
27	B	828	CLA	C4B-NB	8.26	1.42	1.35
27	6	603	CLA	C4B-NB	8.25	1.42	1.35
27	9	607	CLA	C4B-NB	8.24	1.42	1.35
27	B	833	CLA	C4B-NB	8.23	1.42	1.35
27	B	840	CLA	C4B-NB	8.22	1.42	1.35
31	5	618	IHT	C09-C10	-8.20	1.34	1.51
27	A	841	CLA	C4B-NB	8.18	1.42	1.35
27	A	809	CLA	C4B-NB	8.16	1.42	1.35
27	1	605	CLA	C4B-NB	8.15	1.42	1.35
31	1	618	IHT	C09-C10	-8.13	1.35	1.51
31	6	616	IHT	C09-C10	-8.12	1.35	1.51
27	A	827	CLA	C4B-NB	8.12	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	802	CLA	C4B-NB	8.10	1.42	1.35
29	1	619	II0	C22-C10	-8.07	1.25	1.42
27	B	822	CLA	C4B-NB	8.05	1.42	1.35
31	A	854	IHT	C21-C11	-8.01	1.25	1.42
31	2	616	IHT	C21-C11	-7.97	1.25	1.42
29	8	611	II0	C21-C09	-7.97	1.25	1.42
27	B	801	CLA	C4B-NB	7.96	1.42	1.35
29	1	617	II0	C22-C10	-7.96	1.25	1.42
31	6	616	IHT	C21-C11	-7.95	1.25	1.42
29	a	614	II0	C21-C09	-7.94	1.25	1.42
29	B	843	II0	C22-C10	-7.92	1.25	1.42
29	7	301	II0	C22-C10	-7.92	1.25	1.42
31	L	204	IHT	C21-C11	-7.92	1.25	1.42
29	2	613	II0	C22-C10	-7.91	1.25	1.42
29	2	613	II0	C21-C09	-7.90	1.25	1.42
27	A	826	CLA	C4B-NB	7.89	1.42	1.35
29	a	615	II0	C21-C09	-7.89	1.25	1.42
29	O	205	II0	C21-C09	-7.89	1.25	1.42
29	8	610	II0	C22-C10	-7.88	1.25	1.42
31	a	616	IHT	C21-C11	-7.88	1.25	1.42
29	J	101	II0	C22-C10	-7.87	1.25	1.42
29	a	612	II0	C22-C10	-7.87	1.25	1.42
30	1	615	II3	C23-C16	-7.87	1.25	1.42
29	7	316	II0	C22-C10	-7.87	1.25	1.42
29	7	316	II0	C21-C09	-7.86	1.25	1.42
29	3	615	II0	C21-C09	-7.85	1.26	1.42
29	a	614	II0	C22-C10	-7.85	1.26	1.42
31	Z	302	IHT	C21-C11	-7.85	1.26	1.42
31	1	618	IHT	C21-C11	-7.85	1.26	1.42
29	B	843	II0	C21-C09	-7.85	1.26	1.42
31	8	609	IHT	C21-C11	-7.84	1.26	1.42
29	O	205	II0	C22-C10	-7.83	1.26	1.42
29	3	616	II0	C22-C10	-7.83	1.26	1.42
29	8	612	II0	C22-C10	-7.83	1.26	1.42
29	J	101	II0	C21-C09	-7.83	1.26	1.42
29	1	619	II0	C21-C09	-7.83	1.26	1.42
29	3	617	II0	C22-C10	-7.83	1.26	1.42
29	2	615	II0	C21-C09	-7.82	1.26	1.42
29	a	613	II0	C21-C09	-7.82	1.26	1.42
29	1	614	II0	C21-C09	-7.82	1.26	1.42
29	7	317	II0	C22-C10	-7.82	1.26	1.42
29	8	610	II0	C21-C09	-7.82	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	615	II0	C22-C10	-7.81	1.26	1.42
29	9	617	II0	C22-C10	-7.81	1.26	1.42
29	5	615	II0	C22-C10	-7.81	1.26	1.42
29	1	614	II0	C22-C10	-7.80	1.26	1.42
29	7	317	II0	C21-C09	-7.80	1.26	1.42
29	b	614	II0	C22-C10	-7.80	1.26	1.42
29	5	620	II0	C21-C09	-7.80	1.26	1.42
29	5	620	II0	C22-C10	-7.80	1.26	1.42
29	O	206	II0	C22-C10	-7.80	1.26	1.42
29	R	204	II0	C22-C10	-7.79	1.26	1.42
29	3	614	II0	C22-C10	-7.79	1.26	1.42
29	O	206	II0	C21-C09	-7.79	1.26	1.42
29	5	617	II0	C22-C10	-7.78	1.26	1.42
31	5	618	IHT	C21-C11	-7.78	1.26	1.42
27	A	801	CLA	C4B-NB	7.78	1.42	1.35
30	b	613	II3	C23-C16	-7.78	1.26	1.42
29	5	614	II0	C22-C10	-7.78	1.26	1.42
29	1	616	II0	C22-C10	-7.77	1.26	1.42
29	6	614	II0	C21-C09	-7.77	1.26	1.42
31	9	619	IHT	C21-C11	-7.76	1.26	1.42
29	3	615	II0	C22-C10	-7.76	1.26	1.42
29	4	612	II0	C22-C10	-7.76	1.26	1.42
29	Z	312	II0	C21-C09	-7.76	1.26	1.42
29	9	616	II0	C21-C09	-7.76	1.26	1.42
29	3	617	II0	C21-C09	-7.75	1.26	1.42
29	7	314	II0	C22-C10	-7.75	1.26	1.42
29	7	301	II0	C21-C09	-7.74	1.26	1.42
29	a	612	II0	C21-C09	-7.74	1.26	1.42
29	2	615	II0	C22-C10	-7.74	1.26	1.42
29	8	611	II0	C22-C10	-7.74	1.26	1.42
29	9	618	II0	C21-C09	-7.74	1.26	1.42
29	4	614	II0	C21-C09	-7.74	1.26	1.42
29	2	614	II0	C22-C10	-7.73	1.26	1.42
29	6	615	II0	C22-C10	-7.73	1.26	1.42
29	9	617	II0	C21-C09	-7.73	1.26	1.42
29	5	616	II0	C22-C10	-7.72	1.26	1.42
29	3	613	II0	C21-C09	-7.72	1.26	1.42
29	4	614	II0	C22-C10	-7.72	1.26	1.42
29	7	315	II0	C21-C09	-7.72	1.26	1.42
29	4	613	II0	C22-C10	-7.72	1.26	1.42
29	3	614	II0	C21-C09	-7.71	1.26	1.42
29	R	204	II0	C21-C09	-7.71	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	807	CLA	C1D-ND	7.71	1.47	1.37
29	b	614	II0	C21-C09	-7.71	1.26	1.42
27	8	606	CLA	C1D-ND	7.71	1.47	1.37
29	8	612	II0	C21-C09	-7.71	1.26	1.42
29	3	613	II0	C22-C10	-7.71	1.26	1.42
27	B	823	CLA	C1D-ND	7.70	1.47	1.37
29	5	617	II0	C21-C09	-7.70	1.26	1.42
27	A	828	CLA	C1D-ND	7.69	1.47	1.37
29	9	615	II0	C21-C09	-7.69	1.26	1.42
29	4	612	II0	C21-C09	-7.68	1.26	1.42
27	1	604	CLA	C1D-ND	7.67	1.47	1.37
29	5	616	II0	C21-C09	-7.67	1.26	1.42
29	6	615	II0	C21-C09	-7.67	1.26	1.42
27	9	613	CLA	C1D-ND	7.67	1.47	1.37
27	Z	301	CLA	C1D-ND	7.67	1.47	1.37
29	3	616	II0	C21-C09	-7.67	1.26	1.42
29	7	315	II0	C22-C10	-7.66	1.26	1.42
27	B	837	CLA	C1D-ND	7.65	1.47	1.37
27	1	613	CLA	C1D-ND	7.65	1.47	1.37
29	4	613	II0	C21-C09	-7.65	1.26	1.42
27	7	306	CLA	C1D-ND	7.64	1.47	1.37
29	5	615	II0	C21-C09	-7.64	1.26	1.42
29	1	617	II0	C21-C09	-7.64	1.26	1.42
29	9	618	II0	C22-C10	-7.64	1.26	1.42
29	9	616	II0	C22-C10	-7.64	1.26	1.42
29	9	615	II0	C22-C10	-7.64	1.26	1.42
27	4	609	CLA	C1D-ND	7.64	1.47	1.37
27	B	820	CLA	C1D-ND	7.64	1.47	1.37
27	A	840	CLA	C4B-NB	7.63	1.42	1.35
27	K	102	CLA	C1D-ND	7.63	1.47	1.37
29	a	615	II0	C22-C10	-7.63	1.26	1.42
27	9	609	CLA	C1D-ND	7.63	1.47	1.37
29	4	615	II0	C21-C09	-7.62	1.26	1.42
29	b	612	II0	C21-C09	-7.62	1.26	1.42
27	5	613	CLA	C1D-ND	7.62	1.47	1.37
27	8	604	CLA	C1D-ND	7.62	1.47	1.37
29	b	612	II0	C22-C10	-7.62	1.26	1.42
27	3	609	CLA	C1D-ND	7.61	1.47	1.37
29	2	614	II0	C21-C09	-7.61	1.26	1.42
29	7	314	II0	C21-C09	-7.61	1.26	1.42
27	5	611	CLA	C1D-ND	7.61	1.47	1.37
27	8	601	CLA	C1D-ND	7.60	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	302	CLA	C1D-ND	7.59	1.47	1.37
29	1	616	II0	C21-C09	-7.59	1.26	1.42
29	a	613	II0	C22-C10	-7.58	1.26	1.42
29	5	614	II0	C21-C09	-7.58	1.26	1.42
29	Z	312	II0	C22-C10	-7.58	1.26	1.42
27	5	601	CLA	C1D-ND	7.57	1.47	1.37
27	A	823	CLA	C1D-ND	7.57	1.47	1.37
27	b	608	CLA	C1D-ND	7.57	1.47	1.37
27	O	203	CLA	C1D-ND	7.56	1.47	1.37
27	5	604	CLA	C1D-ND	7.55	1.47	1.37
27	5	609	CLA	C1D-ND	7.55	1.47	1.37
27	b	604	CLA	C1D-ND	7.55	1.47	1.37
27	A	842	CLA	C1D-ND	7.55	1.47	1.37
27	6	609	CLA	C1D-ND	7.54	1.47	1.37
27	a	610	CLA	C1D-ND	7.54	1.47	1.37
27	3	611	CLA	C1D-ND	7.53	1.47	1.37
27	7	304	CLA	C1D-ND	7.52	1.47	1.37
27	2	604	CLA	C1D-ND	7.52	1.47	1.37
27	A	832	CLA	C1D-ND	7.52	1.47	1.37
27	F	203	CLA	C1D-ND	7.52	1.47	1.37
29	6	614	II0	C22-C10	-7.52	1.26	1.42
27	1	609	CLA	C1D-ND	7.51	1.47	1.37
27	9	601	CLA	C1D-ND	7.51	1.47	1.37
27	F	204	CLA	C1D-ND	7.51	1.47	1.37
27	J	102	CLA	C1D-ND	7.51	1.47	1.37
27	7	312	CLA	C1D-ND	7.51	1.47	1.37
27	3	612	CLA	C1D-ND	7.51	1.47	1.37
27	9	604	CLA	C1D-ND	7.51	1.47	1.37
27	2	612	CLA	C1D-ND	7.51	1.47	1.37
27	6	604	CLA	C1D-ND	7.51	1.47	1.37
27	7	310	CLA	C1D-ND	7.50	1.47	1.37
27	a	608	CLA	C1D-ND	7.50	1.47	1.37
27	9	603	CLA	C1D-ND	7.49	1.47	1.37
27	9	614	CLA	C1D-ND	7.49	1.47	1.37
27	8	607	CLA	C1D-ND	7.49	1.47	1.37
27	A	813	CLA	C1D-ND	7.49	1.47	1.37
27	b	601	CLA	C1D-ND	7.48	1.47	1.37
27	4	603	CLA	C1D-ND	7.47	1.47	1.37
27	A	835	CLA	C1D-ND	7.47	1.47	1.37
27	K	101	CLA	C1D-ND	7.46	1.47	1.37
27	3	601	CLA	C1D-ND	7.45	1.46	1.37
27	A	830	CLA	C1D-ND	7.45	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	204	CLA	C1D-ND	7.45	1.46	1.37
27	A	836	CLA	C1D-ND	7.45	1.46	1.37
27	F	202	CLA	C1D-ND	7.44	1.46	1.37
27	2	611	CLA	C1D-ND	7.44	1.46	1.37
27	A	814	CLA	C1D-ND	7.44	1.46	1.37
27	B	809	CLA	C1D-ND	7.43	1.46	1.37
27	B	838	CLA	C1D-ND	7.43	1.46	1.37
27	1	611	CLA	C1D-ND	7.42	1.46	1.37
27	5	603	CLA	C1D-ND	7.42	1.46	1.37
27	b	610	CLA	C1D-ND	7.42	1.46	1.37
27	B	839	CLA	C1D-ND	7.41	1.46	1.37
27	1	606	CLA	C1D-ND	7.41	1.46	1.37
27	B	805	CLA	C1D-ND	7.41	1.46	1.37
27	a	601	CLA	C1D-ND	7.41	1.46	1.37
27	4	606	CLA	C1D-ND	7.41	1.46	1.37
27	2	609	CLA	C1D-ND	7.41	1.46	1.37
27	B	810	CLA	C1D-ND	7.41	1.46	1.37
27	A	805	CLA	C1D-ND	7.40	1.46	1.37
27	A	837	CLA	C1D-ND	7.40	1.46	1.37
27	4	601	CLA	C1D-ND	7.40	1.46	1.37
27	A	824	CLA	C1D-ND	7.40	1.46	1.37
27	O	202	CLA	C1D-ND	7.40	1.46	1.37
27	B	825	CLA	C1D-ND	7.40	1.46	1.37
27	4	604	CLA	C1D-ND	7.39	1.46	1.37
27	b	603	CLA	C1D-ND	7.39	1.46	1.37
27	6	601	CLA	C1D-ND	7.39	1.46	1.37
27	A	804	CLA	C1D-ND	7.39	1.46	1.37
27	Z	305	CLA	C1D-ND	7.39	1.46	1.37
27	3	608	CLA	C1D-ND	7.39	1.46	1.37
27	4	610	CLA	C1D-ND	7.38	1.46	1.37
27	8	608	CLA	C1D-ND	7.38	1.46	1.37
27	A	834	CLA	C1D-ND	7.38	1.46	1.37
27	1	612	CLA	C1D-ND	7.38	1.46	1.37
27	3	604	CLA	C1D-ND	7.38	1.46	1.37
27	7	305	CLA	C1D-ND	7.38	1.46	1.37
27	B	819	CLA	C1D-ND	7.37	1.46	1.37
27	4	611	CLA	C1D-ND	7.37	1.46	1.37
27	5	612	CLA	C1D-ND	7.37	1.46	1.37
27	A	833	CLA	C1D-ND	7.37	1.46	1.37
27	3	610	CLA	C1D-ND	7.37	1.46	1.37
27	1	607	CLA	C1D-ND	7.37	1.46	1.37
27	b	607	CLA	C1D-ND	7.37	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	601	CLA	C1D-ND	7.37	1.46	1.37
27	A	825	CLA	C1D-ND	7.37	1.46	1.37
27	2	603	CLA	C1D-ND	7.36	1.46	1.37
27	5	606	CLA	C1D-ND	7.36	1.46	1.37
27	2	608	CLA	C1D-ND	7.36	1.46	1.37
27	a	603	CLA	C1D-ND	7.36	1.46	1.37
27	6	607	CLA	C1D-ND	7.35	1.46	1.37
27	8	603	CLA	C1D-ND	7.35	1.46	1.37
27	B	830	CLA	C1D-ND	7.35	1.46	1.37
27	6	603	CLA	C1D-ND	7.35	1.46	1.37
27	6	606	CLA	C1D-ND	7.35	1.46	1.37
27	1	601	CLA	C1D-ND	7.34	1.46	1.37
27	8	615	CLA	C1D-ND	7.34	1.46	1.37
27	a	604	CLA	C1D-ND	7.34	1.46	1.37
27	4	608	CLA	C1D-ND	7.34	1.46	1.37
27	9	612	CLA	C1D-ND	7.34	1.46	1.37
27	L	203	CLA	C1D-ND	7.34	1.46	1.37
27	Z	304	CLA	C1D-ND	7.34	1.46	1.37
27	5	602	CLA	C1D-ND	7.33	1.46	1.37
27	B	833	CLA	C1D-ND	7.33	1.46	1.37
27	4	607	CLA	C1D-ND	7.33	1.46	1.37
27	2	606	CLA	C1D-ND	7.33	1.46	1.37
27	A	822	CLA	C1D-ND	7.33	1.46	1.37
27	A	810	CLA	C1D-ND	7.33	1.46	1.37
27	Z	306	CLA	C1D-ND	7.32	1.46	1.37
27	Z	310	CLA	C1D-ND	7.32	1.46	1.37
27	A	831	CLA	C1D-ND	7.32	1.46	1.37
27	b	611	CLA	C1D-ND	7.32	1.46	1.37
27	A	819	CLA	C1D-ND	7.31	1.46	1.37
27	B	816	CLA	C1D-ND	7.31	1.46	1.37
27	B	803	CLA	C1D-ND	7.31	1.46	1.37
27	B	815	CLA	C1D-ND	7.31	1.46	1.37
27	A	820	CLA	C1D-ND	7.30	1.46	1.37
27	L	201	CLA	C1D-ND	7.30	1.46	1.37
27	B	834	CLA	C1D-ND	7.30	1.46	1.37
27	1	602	CLA	C1D-ND	7.29	1.46	1.37
27	B	829	CLA	C1D-ND	7.29	1.46	1.37
27	B	811	CLA	C1D-ND	7.29	1.46	1.37
27	1	608	CLA	C1D-ND	7.28	1.46	1.37
27	B	812	CLA	C1D-ND	7.28	1.46	1.37
27	5	608	CLA	C1D-ND	7.28	1.46	1.37
27	B	832	CLA	C1D-ND	7.28	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	841	CLA	C1D-ND	7.28	1.46	1.37
27	7	313	CLA	C1D-ND	7.28	1.46	1.37
27	A	818	CLA	C1D-ND	7.28	1.46	1.37
27	A	815	CLA	C1D-ND	7.27	1.46	1.37
27	3	603	CLA	C1D-ND	7.27	1.46	1.37
27	6	612	CLA	C1D-ND	7.27	1.46	1.37
27	A	829	CLA	C1D-ND	7.26	1.46	1.37
27	9	611	CLA	C1D-ND	7.26	1.46	1.37
27	7	308	CLA	C1D-ND	7.26	1.46	1.37
27	B	804	CLA	C1D-ND	7.25	1.46	1.37
27	A	811	CLA	C1D-ND	7.25	1.46	1.37
27	B	802	CLA	C1D-ND	7.25	1.46	1.37
27	B	828	CLA	C1D-ND	7.25	1.46	1.37
27	A	808	CLA	C1D-ND	7.25	1.46	1.37
27	B	814	CLA	C1D-ND	7.24	1.46	1.37
27	A	844	CLA	C4B-NB	7.24	1.41	1.35
27	A	803	CLA	C1D-ND	7.24	1.46	1.37
27	1	603	CLA	C1D-ND	7.24	1.46	1.37
27	2	602	CLA	C1D-ND	7.24	1.46	1.37
27	7	309	CLA	C1D-ND	7.23	1.46	1.37
27	A	827	CLA	C1D-ND	7.23	1.46	1.37
27	A	802	CLA	C1D-ND	7.23	1.46	1.37
27	5	607	CLA	C1D-ND	7.21	1.46	1.37
27	6	608	CLA	C1D-ND	7.21	1.46	1.37
27	A	812	CLA	C1D-ND	7.21	1.46	1.37
27	b	606	CLA	C1D-ND	7.21	1.46	1.37
27	2	607	CLA	C1D-ND	7.21	1.46	1.37
27	9	605	CLA	C1D-ND	7.20	1.46	1.37
27	B	821	CLA	C1D-ND	7.20	1.46	1.37
27	B	831	CLA	C1D-ND	7.20	1.46	1.37
27	3	607	CLA	C1D-ND	7.20	1.46	1.37
27	L	202	CLA	C1D-ND	7.20	1.46	1.37
27	A	821	CLA	C1D-ND	7.20	1.46	1.37
27	A	838	CLA	C1D-ND	7.19	1.46	1.37
27	B	840	CLA	C1D-ND	7.19	1.46	1.37
27	B	836	CLA	C1D-ND	7.19	1.46	1.37
27	9	608	CLA	C1D-ND	7.18	1.46	1.37
27	a	602	CLA	C1D-ND	7.18	1.46	1.37
27	B	808	CLA	C1D-ND	7.18	1.46	1.37
27	b	602	CLA	C1D-ND	7.18	1.46	1.37
27	9	606	CLA	C1D-ND	7.18	1.46	1.37
27	A	816	CLA	C1D-ND	7.18	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	839	CLA	C1D-ND	7.17	1.46	1.37
27	B	813	CLA	C1D-ND	7.17	1.46	1.37
27	7	303	CLA	C1D-ND	7.17	1.46	1.37
27	B	817	CLA	C1D-ND	7.16	1.46	1.37
27	B	827	CLA	C1D-ND	7.15	1.46	1.37
27	B	835	CLA	C1D-ND	7.15	1.46	1.37
27	B	826	CLA	C1D-ND	7.15	1.46	1.37
27	6	611	CLA	C1D-ND	7.14	1.46	1.37
27	6	602	CLA	C1D-ND	7.14	1.46	1.37
27	3	605	CLA	C1D-ND	7.13	1.46	1.37
27	a	606	CLA	C1D-ND	7.12	1.46	1.37
27	8	605	CLA	C1D-ND	7.11	1.46	1.37
27	9	602	CLA	C1D-ND	7.11	1.46	1.37
27	a	611	CLA	C1D-ND	7.10	1.46	1.37
27	a	607	CLA	C1D-ND	7.10	1.46	1.37
27	A	843	CLA	C1D-ND	7.08	1.46	1.37
27	B	806	CLA	C1D-ND	7.08	1.46	1.37
27	8	602	CLA	C1D-ND	7.08	1.46	1.37
27	B	818	CLA	C1D-ND	7.08	1.46	1.37
27	2	605	CLA	C1D-ND	7.07	1.46	1.37
27	a	605	CLA	C1D-ND	7.07	1.46	1.37
27	5	605	CLA	C1D-ND	7.06	1.46	1.37
27	6	605	CLA	C1D-ND	7.06	1.46	1.37
27	4	602	CLA	C1D-ND	7.06	1.46	1.37
27	B	824	CLA	C1D-ND	7.03	1.46	1.37
27	B	822	CLA	C1D-ND	6.99	1.46	1.37
27	A	806	CLA	C1D-ND	6.99	1.46	1.37
27	R	202	CLA	C1D-ND	6.98	1.46	1.37
27	3	602	CLA	C1D-ND	6.97	1.46	1.37
27	A	809	CLA	C1D-ND	6.96	1.46	1.37
27	9	607	CLA	C1D-ND	6.94	1.46	1.37
27	A	817	CLA	C1D-ND	6.93	1.46	1.37
27	A	826	CLA	C1D-ND	6.92	1.46	1.37
27	O	201	CLA	C1D-ND	6.92	1.46	1.37
27	B	807	CLA	C1D-ND	6.83	1.46	1.37
27	1	605	CLA	C1D-ND	6.80	1.46	1.37
27	A	841	CLA	C1D-ND	6.76	1.46	1.37
27	B	801	CLA	C1D-ND	6.57	1.45	1.37
27	A	840	CLA	C1D-ND	6.55	1.45	1.37
27	A	844	CLA	C1D-ND	6.50	1.45	1.37
27	A	801	CLA	MG-ND	-6.38	1.93	2.05
28	a	609	KC2	C4B-NB	6.18	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	801	CLA	C1D-ND	6.14	1.45	1.37
27	A	844	CLA	MG-ND	-6.10	1.93	2.05
28	1	610	KC2	C4B-NB	5.94	1.45	1.37
28	b	605	KC2	C4B-NB	5.91	1.45	1.37
27	1	605	CLA	MG-ND	-5.89	1.94	2.05
28	6	610	KC2	C4B-NB	5.89	1.45	1.37
28	4	605	KC2	C4B-NB	5.88	1.45	1.37
28	9	610	KC2	C4B-NB	5.86	1.45	1.37
27	A	826	CLA	MG-ND	-5.85	1.94	2.05
27	A	840	CLA	MG-ND	-5.85	1.94	2.05
27	B	801	CLA	MG-ND	-5.84	1.94	2.05
28	7	307	KC2	C4B-NB	5.83	1.44	1.37
27	B	802	CLA	MG-ND	-5.79	1.94	2.05
27	A	809	CLA	MG-NA	-5.77	1.92	2.06
28	6	613	KC2	C4B-NB	5.70	1.44	1.37
27	8	605	CLA	MG-NA	-5.70	1.92	2.06
28	5	610	KC2	C4B-NB	5.70	1.44	1.37
28	Z	307	KC2	C4B-NB	5.68	1.44	1.37
28	7	311	KC2	C4B-NB	5.67	1.44	1.37
27	8	602	CLA	MG-ND	-5.66	1.94	2.05
27	9	607	CLA	MG-ND	-5.66	1.94	2.05
28	2	610	KC2	C4B-NB	5.65	1.44	1.37
27	B	822	CLA	MG-ND	-5.64	1.94	2.05
28	b	609	KC2	C4B-NB	5.63	1.44	1.37
27	a	606	CLA	MG-ND	-5.62	1.94	2.05
28	3	606	KC2	C4B-NB	5.60	1.44	1.37
27	A	809	CLA	MG-ND	-5.59	1.94	2.05
27	2	605	CLA	MG-ND	-5.59	1.94	2.05
27	A	841	CLA	MG-NA	-5.58	1.93	2.06
27	B	839	CLA	MG-ND	-5.57	1.94	2.05
27	R	202	CLA	MG-NA	-5.57	1.93	2.06
27	5	605	CLA	MG-ND	-5.57	1.94	2.05
27	b	606	CLA	MG-ND	-5.56	1.94	2.05
27	A	827	CLA	MG-ND	-5.55	1.94	2.05
27	L	202	CLA	MG-NA	-5.55	1.93	2.06
27	A	806	CLA	MG-ND	-5.55	1.94	2.05
27	6	603	CLA	MG-ND	-5.55	1.94	2.05
27	A	843	CLA	MG-NA	-5.54	1.93	2.06
27	B	833	CLA	MG-ND	-5.53	1.94	2.05
27	R	202	CLA	MG-ND	-5.53	1.94	2.05
27	A	841	CLA	MG-ND	-5.52	1.94	2.05
27	B	808	CLA	MG-ND	-5.52	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	605	CLA	MG-ND	-5.52	1.94	2.05
27	A	812	CLA	MG-ND	-5.52	1.94	2.05
27	B	835	CLA	MG-NA	-5.51	1.93	2.06
27	B	827	CLA	MG-ND	-5.50	1.94	2.05
27	6	602	CLA	MG-ND	-5.50	1.94	2.05
27	B	826	CLA	MG-ND	-5.50	1.94	2.05
27	B	824	CLA	MG-NA	-5.50	1.93	2.06
27	A	815	CLA	MG-ND	-5.49	1.94	2.05
27	B	832	CLA	MG-ND	-5.49	1.94	2.05
27	1	601	CLA	MG-NA	-5.49	1.93	2.06
27	4	611	CLA	MG-ND	-5.48	1.94	2.05
27	A	831	CLA	MG-ND	-5.48	1.94	2.05
27	B	813	CLA	MG-ND	-5.48	1.94	2.05
27	B	824	CLA	MG-ND	-5.48	1.94	2.05
27	B	814	CLA	MG-NA	-5.47	1.93	2.06
27	4	606	CLA	MG-ND	-5.47	1.94	2.05
27	A	839	CLA	MG-ND	-5.47	1.95	2.05
27	a	605	CLA	MG-ND	-5.46	1.95	2.05
27	L	201	CLA	MG-ND	-5.46	1.95	2.05
27	A	820	CLA	MG-ND	-5.46	1.95	2.05
27	7	313	CLA	MG-ND	-5.46	1.95	2.05
27	2	607	CLA	MG-ND	-5.45	1.95	2.05
27	B	809	CLA	MG-ND	-5.44	1.95	2.05
27	a	603	CLA	MG-ND	-5.44	1.95	2.05
27	9	602	CLA	MG-ND	-5.43	1.95	2.05
27	1	601	CLA	MG-ND	-5.42	1.95	2.05
27	A	829	CLA	MG-ND	-5.42	1.95	2.05
27	a	611	CLA	MG-ND	-5.42	1.95	2.05
27	4	608	CLA	MG-ND	-5.42	1.95	2.05
27	B	835	CLA	MG-ND	-5.41	1.95	2.05
27	5	604	CLA	MG-NA	-5.41	1.93	2.06
27	A	817	CLA	MG-NA	-5.41	1.93	2.06
27	F	203	CLA	MG-ND	-5.41	1.95	2.05
27	A	838	CLA	MG-ND	-5.41	1.95	2.05
27	9	614	CLA	MG-ND	-5.41	1.95	2.05
27	6	609	CLA	MG-ND	-5.40	1.95	2.05
27	6	611	CLA	MG-ND	-5.39	1.95	2.05
27	B	823	CLA	MG-ND	-5.39	1.95	2.05
27	6	612	CLA	MG-ND	-5.39	1.95	2.05
27	1	612	CLA	MG-ND	-5.39	1.95	2.05
27	O	202	CLA	MG-NA	-5.38	1.93	2.06
27	1	613	CLA	MG-ND	-5.38	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	818	CLA	MG-ND	-5.38	1.95	2.05
27	O	202	CLA	MG-ND	-5.38	1.95	2.05
27	A	817	CLA	MG-ND	-5.38	1.95	2.05
27	B	817	CLA	MG-ND	-5.38	1.95	2.05
27	9	605	CLA	MG-ND	-5.38	1.95	2.05
27	B	836	CLA	MG-ND	-5.38	1.95	2.05
27	a	607	CLA	MG-ND	-5.38	1.95	2.05
27	5	606	CLA	MG-ND	-5.38	1.95	2.05
27	2	606	CLA	MG-ND	-5.37	1.95	2.05
27	B	815	CLA	MG-NA	-5.37	1.93	2.06
27	9	612	CLA	MG-ND	-5.37	1.95	2.05
27	2	601	CLA	MG-ND	-5.37	1.95	2.05
27	A	810	CLA	MG-ND	-5.37	1.95	2.05
27	5	601	CLA	MG-ND	-5.37	1.95	2.05
27	7	310	CLA	MG-ND	-5.36	1.95	2.05
27	A	843	CLA	MG-ND	-5.36	1.95	2.05
27	B	805	CLA	MG-ND	-5.36	1.95	2.05
27	4	601	CLA	MG-ND	-5.36	1.95	2.05
27	1	603	CLA	MG-ND	-5.36	1.95	2.05
27	5	613	CLA	MG-ND	-5.36	1.95	2.05
27	9	611	CLA	MG-ND	-5.36	1.95	2.05
27	2	611	CLA	MG-ND	-5.36	1.95	2.05
27	A	804	CLA	MG-ND	-5.35	1.95	2.05
27	B	831	CLA	MG-NA	-5.35	1.93	2.06
27	6	606	CLA	MG-ND	-5.35	1.95	2.05
27	5	612	CLA	MG-ND	-5.35	1.95	2.05
27	b	608	CLA	MG-ND	-5.35	1.95	2.05
27	9	614	CLA	MG-NA	-5.35	1.93	2.06
27	9	613	CLA	MG-ND	-5.35	1.95	2.05
27	B	825	CLA	MG-ND	-5.35	1.95	2.05
27	O	204	CLA	MG-NA	-5.35	1.93	2.06
27	9	603	CLA	MG-ND	-5.35	1.95	2.05
27	B	812	CLA	MG-ND	-5.34	1.95	2.05
27	7	308	CLA	MG-ND	-5.34	1.95	2.05
27	Z	305	CLA	MG-ND	-5.34	1.95	2.05
27	1	604	CLA	MG-ND	-5.34	1.95	2.05
27	B	816	CLA	MG-ND	-5.34	1.95	2.05
27	B	830	CLA	MG-ND	-5.34	1.95	2.05
27	A	823	CLA	MG-ND	-5.34	1.95	2.05
27	K	101	CLA	MG-ND	-5.34	1.95	2.05
27	1	611	CLA	MG-ND	-5.34	1.95	2.05
27	8	604	CLA	MG-ND	-5.34	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	607	CLA	MG-ND	-5.34	1.95	2.05
27	5	603	CLA	MG-ND	-5.33	1.95	2.05
27	a	608	CLA	MG-ND	-5.33	1.95	2.05
27	1	607	CLA	MG-ND	-5.33	1.95	2.05
27	5	607	CLA	MG-ND	-5.33	1.95	2.05
27	B	814	CLA	MG-ND	-5.33	1.95	2.05
27	B	829	CLA	MG-ND	-5.33	1.95	2.05
27	6	609	CLA	MG-NA	-5.33	1.93	2.06
27	8	615	CLA	MG-ND	-5.33	1.95	2.05
27	6	606	CLA	MG-NA	-5.33	1.93	2.06
27	B	807	CLA	MG-ND	-5.33	1.95	2.05
27	1	606	CLA	MG-ND	-5.32	1.95	2.05
27	2	601	CLA	MG-NA	-5.32	1.93	2.06
27	Z	306	CLA	MG-ND	-5.32	1.95	2.05
27	B	810	CLA	MG-ND	-5.32	1.95	2.05
27	A	824	CLA	MG-NA	-5.32	1.93	2.06
27	B	821	CLA	MG-ND	-5.32	1.95	2.05
27	6	602	CLA	MG-NA	-5.32	1.93	2.06
27	A	821	CLA	MG-ND	-5.32	1.95	2.05
27	9	606	CLA	MG-ND	-5.32	1.95	2.05
27	3	604	CLA	MG-ND	-5.31	1.95	2.05
27	1	609	CLA	MG-ND	-5.31	1.95	2.05
27	B	829	CLA	MG-NA	-5.31	1.93	2.06
27	2	603	CLA	MG-ND	-5.31	1.95	2.05
27	a	601	CLA	MG-ND	-5.30	1.95	2.05
27	A	808	CLA	MG-ND	-5.30	1.95	2.05
27	F	202	CLA	MG-ND	-5.30	1.95	2.05
27	B	806	CLA	MG-ND	-5.30	1.95	2.05
27	5	601	CLA	MG-NA	-5.30	1.93	2.06
27	7	312	CLA	MG-ND	-5.30	1.95	2.05
27	b	611	CLA	MG-ND	-5.30	1.95	2.05
27	7	306	CLA	MG-ND	-5.30	1.95	2.05
27	2	612	CLA	MG-ND	-5.30	1.95	2.05
27	B	807	CLA	MG-NA	-5.30	1.93	2.06
27	3	603	CLA	MG-ND	-5.30	1.95	2.05
27	K	102	CLA	MG-NA	-5.30	1.93	2.06
27	6	607	CLA	MG-ND	-5.30	1.95	2.05
27	4	610	CLA	MG-ND	-5.29	1.95	2.05
27	F	204	CLA	MG-ND	-5.29	1.95	2.05
27	B	815	CLA	MG-ND	-5.29	1.95	2.05
27	A	807	CLA	MG-ND	-5.28	1.95	2.05
27	5	609	CLA	MG-ND	-5.28	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	822	CLA	MG-ND	-5.28	1.95	2.05
27	9	608	CLA	MG-ND	-5.28	1.95	2.05
27	B	803	CLA	MG-ND	-5.28	1.95	2.05
27	3	608	CLA	MG-ND	-5.28	1.95	2.05
27	7	303	CLA	MG-ND	-5.28	1.95	2.05
27	b	601	CLA	MG-ND	-5.28	1.95	2.05
27	A	811	CLA	MG-ND	-5.28	1.95	2.05
27	B	820	CLA	MG-ND	-5.28	1.95	2.05
27	2	609	CLA	MG-NA	-5.27	1.93	2.06
27	A	802	CLA	MG-ND	-5.27	1.95	2.05
27	6	601	CLA	MG-ND	-5.27	1.95	2.05
27	6	603	CLA	MG-NA	-5.27	1.93	2.06
27	A	830	CLA	MG-ND	-5.26	1.95	2.05
27	B	828	CLA	MG-ND	-5.26	1.95	2.05
27	1	602	CLA	MG-ND	-5.26	1.95	2.05
27	A	819	CLA	MG-ND	-5.26	1.95	2.05
27	B	811	CLA	MG-ND	-5.26	1.95	2.05
27	O	201	CLA	MG-ND	-5.26	1.95	2.05
27	3	605	CLA	MG-ND	-5.26	1.95	2.05
27	7	305	CLA	MG-ND	-5.26	1.95	2.05
27	A	825	CLA	MG-ND	-5.26	1.95	2.05
27	L	203	CLA	MG-ND	-5.26	1.95	2.05
27	b	602	CLA	MG-ND	-5.26	1.95	2.05
27	9	601	CLA	MG-ND	-5.26	1.95	2.05
27	8	608	CLA	MG-ND	-5.26	1.95	2.05
27	6	608	CLA	MG-ND	-5.26	1.95	2.05
27	Z	310	CLA	MG-ND	-5.26	1.95	2.05
27	7	302	CLA	MG-ND	-5.25	1.95	2.05
27	4	604	CLA	MG-ND	-5.25	1.95	2.05
27	a	602	CLA	MG-ND	-5.25	1.95	2.05
27	A	832	CLA	MG-ND	-5.25	1.95	2.05
27	8	603	CLA	MG-NA	-5.25	1.93	2.06
27	7	309	CLA	MG-ND	-5.25	1.95	2.05
27	A	816	CLA	MG-ND	-5.25	1.95	2.05
27	O	201	CLA	MG-NA	-5.25	1.93	2.06
27	5	602	CLA	MG-NA	-5.24	1.93	2.06
27	3	611	CLA	MG-ND	-5.24	1.95	2.05
27	Z	304	CLA	MG-ND	-5.24	1.95	2.05
27	B	832	CLA	MG-NA	-5.24	1.93	2.06
27	3	602	CLA	MG-ND	-5.24	1.95	2.05
27	A	813	CLA	MG-ND	-5.24	1.95	2.05
27	3	610	CLA	MG-NA	-5.24	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	609	CLA	MG-ND	-5.24	1.95	2.05
27	2	603	CLA	MG-NA	-5.24	1.93	2.06
27	3	601	CLA	MG-ND	-5.24	1.95	2.05
27	A	837	CLA	MG-ND	-5.23	1.95	2.05
27	B	837	CLA	MG-ND	-5.23	1.95	2.05
27	A	819	CLA	MG-NA	-5.23	1.93	2.06
27	A	818	CLA	MG-NA	-5.23	1.93	2.06
27	A	828	CLA	MG-ND	-5.23	1.95	2.05
27	3	609	CLA	MG-ND	-5.23	1.95	2.05
27	3	612	CLA	MG-ND	-5.23	1.95	2.05
27	b	607	CLA	MG-ND	-5.22	1.95	2.05
27	4	607	CLA	MG-ND	-5.22	1.95	2.05
27	a	604	CLA	MG-ND	-5.22	1.95	2.05
27	A	833	CLA	MG-ND	-5.22	1.95	2.05
27	a	602	CLA	MG-NA	-5.22	1.93	2.06
27	A	803	CLA	MG-NA	-5.22	1.93	2.06
27	A	814	CLA	MG-NA	-5.22	1.93	2.06
27	5	611	CLA	MG-ND	-5.22	1.95	2.05
27	b	604	CLA	MG-ND	-5.22	1.95	2.05
27	B	840	CLA	MG-ND	-5.21	1.95	2.05
27	b	610	CLA	MG-ND	-5.21	1.95	2.05
27	b	610	CLA	MG-NA	-5.21	1.93	2.06
27	a	604	CLA	MG-NA	-5.21	1.93	2.06
27	8	601	CLA	MG-ND	-5.20	1.95	2.05
27	4	602	CLA	MG-ND	-5.20	1.95	2.05
27	9	609	CLA	MG-ND	-5.20	1.95	2.05
27	J	102	CLA	MG-ND	-5.20	1.95	2.05
27	B	838	CLA	MG-ND	-5.20	1.95	2.05
27	8	605	CLA	MG-ND	-5.20	1.95	2.05
27	4	609	CLA	MG-ND	-5.19	1.95	2.05
27	7	304	CLA	MG-NA	-5.19	1.93	2.06
27	7	310	CLA	MG-NA	-5.19	1.93	2.06
27	A	818	CLA	MG-ND	-5.19	1.95	2.05
27	b	603	CLA	MG-ND	-5.19	1.95	2.05
27	3	605	CLA	MG-NA	-5.19	1.93	2.06
27	9	602	CLA	MG-NA	-5.19	1.93	2.06
27	A	836	CLA	MG-ND	-5.19	1.95	2.05
27	O	204	CLA	MG-ND	-5.19	1.95	2.05
27	A	815	CLA	MG-NA	-5.19	1.93	2.06
27	B	819	CLA	MG-ND	-5.19	1.95	2.05
27	7	313	CLA	MG-NA	-5.19	1.93	2.06
27	3	602	CLA	MG-NA	-5.19	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	603	CLA	MG-ND	-5.19	1.95	2.05
27	A	833	CLA	MG-NA	-5.19	1.94	2.06
27	A	824	CLA	MG-ND	-5.19	1.95	2.05
27	8	606	CLA	MG-ND	-5.18	1.95	2.05
27	6	608	CLA	MG-NA	-5.18	1.94	2.06
27	1	604	CLA	MG-NA	-5.18	1.94	2.06
27	B	838	CLA	MG-NA	-5.18	1.94	2.06
27	6	604	CLA	MG-ND	-5.18	1.95	2.05
27	2	602	CLA	MG-ND	-5.18	1.95	2.05
27	4	603	CLA	MG-ND	-5.17	1.95	2.05
27	A	814	CLA	MG-ND	-5.17	1.95	2.05
27	B	809	CLA	MG-NA	-5.17	1.94	2.06
27	5	602	CLA	MG-ND	-5.16	1.95	2.05
27	B	804	CLA	MG-ND	-5.16	1.95	2.05
27	B	827	CLA	MG-NA	-5.16	1.94	2.06
27	9	604	CLA	MG-ND	-5.16	1.95	2.05
27	1	613	CLA	MG-NA	-5.16	1.94	2.06
27	K	102	CLA	MG-ND	-5.15	1.95	2.05
27	O	203	CLA	MG-ND	-5.15	1.95	2.05
27	8	615	CLA	MG-NA	-5.14	1.94	2.06
27	9	604	CLA	MG-NA	-5.14	1.94	2.06
27	B	819	CLA	MG-NA	-5.14	1.94	2.06
27	B	830	CLA	MG-NA	-5.14	1.94	2.06
27	A	834	CLA	MG-NA	-5.14	1.94	2.06
27	B	828	CLA	MG-NA	-5.14	1.94	2.06
27	A	803	CLA	MG-ND	-5.14	1.95	2.05
27	5	603	CLA	MG-NA	-5.14	1.94	2.06
27	A	835	CLA	MG-ND	-5.14	1.95	2.05
27	A	805	CLA	MG-ND	-5.14	1.95	2.05
27	B	818	CLA	MG-NA	-5.14	1.94	2.06
27	a	610	CLA	MG-NA	-5.14	1.94	2.06
27	3	611	CLA	MG-NA	-5.14	1.94	2.06
27	1	608	CLA	MG-ND	-5.14	1.95	2.05
27	7	304	CLA	MG-ND	-5.14	1.95	2.05
27	B	834	CLA	MG-ND	-5.14	1.95	2.05
27	7	308	CLA	MG-NA	-5.13	1.94	2.06
27	5	604	CLA	MG-ND	-5.13	1.95	2.05
27	5	606	CLA	MG-NA	-5.13	1.94	2.06
27	A	812	CLA	MG-NA	-5.13	1.94	2.06
27	A	828	CLA	MG-NA	-5.13	1.94	2.06
27	B	831	CLA	MG-ND	-5.12	1.95	2.05
27	5	608	CLA	MG-ND	-5.12	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	611	CLA	MG-NA	-5.12	1.94	2.06
27	A	842	CLA	MG-ND	-5.12	1.95	2.05
27	9	603	CLA	MG-NA	-5.12	1.94	2.06
27	B	841	CLA	MG-ND	-5.12	1.95	2.05
27	B	834	CLA	MG-NA	-5.12	1.94	2.06
27	J	102	CLA	MG-NA	-5.12	1.94	2.06
27	L	202	CLA	MG-ND	-5.12	1.95	2.05
27	Z	301	CLA	MG-ND	-5.12	1.95	2.05
27	2	608	CLA	MG-ND	-5.11	1.95	2.05
27	a	610	CLA	MG-ND	-5.11	1.95	2.05
27	8	607	CLA	MG-ND	-5.11	1.95	2.05
27	A	813	CLA	MG-NA	-5.11	1.94	2.06
27	B	811	CLA	MG-NA	-5.11	1.94	2.06
27	b	602	CLA	MG-NA	-5.11	1.94	2.06
27	A	808	CLA	MG-NA	-5.11	1.94	2.06
27	2	602	CLA	MG-NA	-5.10	1.94	2.06
27	2	605	CLA	MG-NA	-5.10	1.94	2.06
27	6	605	CLA	MG-NA	-5.09	1.94	2.06
27	2	604	CLA	MG-ND	-5.09	1.95	2.05
27	b	607	CLA	MG-NA	-5.08	1.94	2.06
27	4	602	CLA	MG-NA	-5.08	1.94	2.06
27	A	821	CLA	MG-NA	-5.08	1.94	2.06
27	A	822	CLA	MG-NA	-5.08	1.94	2.06
27	b	604	CLA	MG-NA	-5.08	1.94	2.06
27	B	802	CLA	MG-NA	-5.07	1.94	2.06
27	8	608	CLA	MG-NA	-5.07	1.94	2.06
27	5	605	CLA	MG-NA	-5.06	1.94	2.06
27	B	803	CLA	MG-NA	-5.06	1.94	2.06
27	3	603	CLA	MG-NA	-5.06	1.94	2.06
27	4	603	CLA	MG-NA	-5.06	1.94	2.06
27	A	806	CLA	MG-NA	-5.06	1.94	2.06
27	3	607	CLA	MG-NA	-5.05	1.94	2.06
27	a	607	CLA	MG-NA	-5.05	1.94	2.06
27	F	202	CLA	MG-NA	-5.05	1.94	2.06
27	b	603	CLA	MG-NA	-5.05	1.94	2.06
27	8	602	CLA	MG-NA	-5.04	1.94	2.06
27	A	820	CLA	MG-NA	-5.04	1.94	2.06
27	Z	304	CLA	MG-NA	-5.04	1.94	2.06
27	1	607	CLA	MG-NA	-5.03	1.94	2.06
27	9	605	CLA	MG-NA	-5.03	1.94	2.06
27	1	603	CLA	MG-NA	-5.03	1.94	2.06
27	7	309	CLA	MG-NA	-5.03	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	605	CLA	MG-NA	-5.03	1.94	2.06
27	B	837	CLA	MG-NA	-5.03	1.94	2.06
27	A	804	CLA	MG-NA	-5.03	1.94	2.06
27	7	303	CLA	MG-NA	-5.02	1.94	2.06
27	9	609	CLA	MG-NA	-5.02	1.94	2.06
27	B	822	CLA	MG-NA	-5.02	1.94	2.06
27	3	610	CLA	MG-ND	-5.01	1.95	2.05
27	7	306	CLA	MG-NA	-5.01	1.94	2.06
27	A	834	CLA	MG-ND	-5.01	1.95	2.05
27	1	609	CLA	MG-NA	-5.01	1.94	2.06
27	B	839	CLA	MG-NA	-5.01	1.94	2.06
27	A	839	CLA	MG-NA	-5.01	1.94	2.06
27	3	601	CLA	MG-NA	-5.01	1.94	2.06
27	b	611	CLA	MG-NA	-5.01	1.94	2.06
27	2	604	CLA	MG-NA	-5.00	1.94	2.06
27	A	825	CLA	MG-NA	-5.00	1.94	2.06
27	Z	306	CLA	MG-NA	-5.00	1.94	2.06
27	B	833	CLA	MG-NA	-5.00	1.94	2.06
27	4	604	CLA	MG-NA	-5.00	1.94	2.06
27	1	606	CLA	MG-NA	-5.00	1.94	2.06
27	7	312	CLA	MG-NA	-5.00	1.94	2.06
27	4	606	CLA	MG-NA	-5.00	1.94	2.06
27	9	606	CLA	MG-NA	-5.00	1.94	2.06
27	b	601	CLA	MG-NA	-5.00	1.94	2.06
27	A	805	CLA	MG-NA	-5.00	1.94	2.06
27	L	201	CLA	MG-NA	-5.00	1.94	2.06
27	A	831	CLA	MG-NA	-5.00	1.94	2.06
27	6	604	CLA	MG-NA	-5.00	1.94	2.06
27	B	804	CLA	MG-NA	-4.99	1.94	2.06
27	a	601	CLA	MG-NA	-4.99	1.94	2.06
27	5	609	CLA	MG-NA	-4.99	1.94	2.06
27	3	608	CLA	MG-NA	-4.99	1.94	2.06
27	B	821	CLA	MG-NA	-4.99	1.94	2.06
27	B	810	CLA	MG-NA	-4.98	1.94	2.06
27	5	608	CLA	MG-NA	-4.98	1.94	2.06
27	Z	310	CLA	MG-NA	-4.98	1.94	2.06
27	A	832	CLA	MG-NA	-4.98	1.94	2.06
27	B	806	CLA	MG-NA	-4.98	1.94	2.06
27	B	840	CLA	MG-NA	-4.98	1.94	2.06
27	O	203	CLA	MG-NA	-4.98	1.94	2.06
27	9	611	CLA	MG-NA	-4.98	1.94	2.06
27	2	607	CLA	MG-NA	-4.98	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	801	CLA	MG-NA	-4.97	1.94	2.06
27	5	612	CLA	MG-NA	-4.96	1.94	2.06
27	A	842	CLA	MG-NA	-4.96	1.94	2.06
27	b	606	CLA	MG-NA	-4.96	1.94	2.06
27	A	838	CLA	MG-NA	-4.96	1.94	2.06
27	a	606	CLA	MG-NA	-4.96	1.94	2.06
27	A	816	CLA	MG-NA	-4.96	1.94	2.06
27	2	611	CLA	MG-NA	-4.95	1.94	2.06
27	5	607	CLA	MG-NA	-4.95	1.94	2.06
27	B	812	CLA	MG-NA	-4.95	1.94	2.06
27	7	305	CLA	MG-NA	-4.95	1.94	2.06
27	B	825	CLA	MG-NA	-4.95	1.94	2.06
27	2	608	CLA	MG-NA	-4.94	1.94	2.06
27	A	830	CLA	MG-NA	-4.94	1.94	2.06
27	A	811	CLA	MG-NA	-4.93	1.94	2.06
27	3	612	CLA	MG-NA	-4.93	1.94	2.06
27	A	840	CLA	MG-NA	-4.93	1.94	2.06
27	3	609	CLA	MG-NA	-4.93	1.94	2.06
27	5	613	CLA	MG-NA	-4.93	1.94	2.06
27	6	611	CLA	MG-NA	-4.92	1.94	2.06
27	1	602	CLA	MG-NA	-4.92	1.94	2.06
27	8	606	CLA	MG-NA	-4.92	1.94	2.06
27	B	816	CLA	MG-NA	-4.92	1.94	2.06
27	4	601	CLA	MG-NA	-4.92	1.94	2.06
27	B	805	CLA	MG-NA	-4.92	1.94	2.06
27	A	807	CLA	MG-NA	-4.92	1.94	2.06
27	F	203	CLA	MG-NA	-4.91	1.94	2.06
27	6	612	CLA	MG-NA	-4.91	1.94	2.06
27	6	601	CLA	MG-NA	-4.91	1.94	2.06
27	4	607	CLA	MG-NA	-4.91	1.94	2.06
27	A	836	CLA	MG-NA	-4.91	1.94	2.06
27	A	829	CLA	MG-NA	-4.91	1.94	2.06
27	2	606	CLA	MG-NA	-4.90	1.94	2.06
27	9	601	CLA	MG-NA	-4.90	1.94	2.06
27	2	612	CLA	MG-NA	-4.89	1.94	2.06
27	B	808	CLA	MG-NA	-4.89	1.94	2.06
27	A	802	CLA	MG-NA	-4.89	1.94	2.06
27	Z	301	CLA	MG-NA	-4.88	1.94	2.06
27	4	609	CLA	MG-NA	-4.88	1.94	2.06
27	B	826	CLA	MG-NA	-4.88	1.94	2.06
27	9	612	CLA	MG-NA	-4.88	1.94	2.06
27	L	203	CLA	MG-NA	-4.88	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	607	CLA	MG-NA	-4.88	1.94	2.06
27	4	608	CLA	MG-NA	-4.88	1.94	2.06
27	A	823	CLA	MG-NA	-4.88	1.94	2.06
27	B	841	CLA	MG-NA	-4.88	1.94	2.06
27	9	608	CLA	MG-NA	-4.87	1.94	2.06
27	3	604	CLA	MG-NA	-4.87	1.94	2.06
27	4	610	CLA	MG-NA	-4.87	1.94	2.06
27	8	601	CLA	MG-NA	-4.87	1.94	2.06
27	A	835	CLA	MG-NA	-4.86	1.94	2.06
27	5	611	CLA	MG-NA	-4.86	1.94	2.06
27	6	607	CLA	MG-NA	-4.85	1.94	2.06
27	4	611	CLA	MG-NA	-4.85	1.94	2.06
27	K	101	CLA	MG-NA	-4.84	1.94	2.06
27	B	836	CLA	MG-NA	-4.84	1.94	2.06
27	A	826	CLA	MG-NA	-4.84	1.94	2.06
27	B	820	CLA	MG-NA	-4.84	1.94	2.06
27	a	603	CLA	MG-NA	-4.84	1.94	2.06
27	7	302	CLA	MG-NA	-4.83	1.94	2.06
27	9	607	CLA	MG-NA	-4.83	1.94	2.06
27	a	611	CLA	MG-NA	-4.83	1.94	2.06
27	A	801	CLA	MG-NA	-4.83	1.94	2.06
27	1	605	CLA	MG-NA	-4.82	1.94	2.06
27	8	604	CLA	MG-NA	-4.82	1.94	2.06
27	B	817	CLA	MG-NA	-4.81	1.94	2.06
27	A	837	CLA	MG-NA	-4.81	1.94	2.06
27	A	827	CLA	MG-NA	-4.80	1.94	2.06
27	Z	305	CLA	MG-NA	-4.78	1.94	2.06
27	b	608	CLA	MG-NA	-4.78	1.94	2.06
27	9	613	CLA	MG-NA	-4.77	1.94	2.06
27	1	608	CLA	MG-NA	-4.77	1.94	2.06
27	a	608	CLA	MG-NA	-4.76	1.95	2.06
27	F	204	CLA	MG-NA	-4.73	1.95	2.06
27	1	612	CLA	MG-NA	-4.73	1.95	2.06
27	B	813	CLA	MG-NA	-4.73	1.95	2.06
34	O	207	SQD	O8-S	4.67	1.64	1.47
27	B	823	CLA	MG-NA	-4.66	1.95	2.06
27	A	810	CLA	MG-NA	-4.62	1.95	2.06
34	3	621	SQD	O8-S	4.61	1.63	1.47
27	A	844	CLA	MG-NA	-4.60	1.95	2.06
34	3	621	SQD	O48-C23	4.23	1.45	1.33
28	7	307	KC2	C3D-C4D	4.15	1.44	1.40
34	O	207	SQD	O47-C7	4.11	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	3	621	SQD	O47-C7	4.07	1.45	1.34
28	4	605	KC2	C1B-NB	3.96	1.42	1.37
28	7	311	KC2	C4C-NC	3.92	1.43	1.37
28	2	610	KC2	C1B-NB	3.91	1.42	1.37
28	5	610	KC2	C1B-NB	3.91	1.42	1.37
27	A	841	CLA	MG-NC	-3.90	1.97	2.06
28	1	610	KC2	C4C-NC	3.88	1.43	1.37
27	A	809	CLA	MG-NC	-3.88	1.97	2.06
28	b	609	KC2	C4C-NC	3.86	1.43	1.37
28	b	605	KC2	C3D-C4D	3.86	1.43	1.40
27	L	202	CLA	MG-NC	-3.85	1.97	2.06
27	B	831	CLA	MG-NC	-3.84	1.97	2.06
28	2	610	KC2	C3D-C4D	3.83	1.43	1.40
28	7	307	KC2	C4C-NC	3.83	1.43	1.37
27	6	603	CLA	MG-NC	-3.83	1.97	2.06
27	5	604	CLA	MG-NC	-3.83	1.97	2.06
28	b	609	KC2	C3D-C4D	3.81	1.43	1.40
28	5	610	KC2	C4C-NC	3.81	1.43	1.37
28	2	610	KC2	C4C-NC	3.80	1.43	1.37
27	K	102	CLA	MG-NC	-3.78	1.97	2.06
28	3	606	KC2	C4C-NC	3.78	1.43	1.37
28	1	610	KC2	C1B-NB	3.77	1.42	1.37
28	6	613	KC2	C4C-NC	3.77	1.43	1.37
27	O	201	CLA	MG-NC	-3.77	1.97	2.06
28	3	606	KC2	C3D-C4D	3.76	1.43	1.40
28	Z	307	KC2	C3D-C4D	3.76	1.43	1.40
27	8	605	CLA	MG-NC	-3.75	1.97	2.06
27	A	817	CLA	MG-NC	-3.75	1.97	2.06
28	6	610	KC2	C1B-NB	3.75	1.42	1.37
28	6	613	KC2	C1B-NB	3.75	1.42	1.37
27	1	601	CLA	MG-NC	-3.74	1.97	2.06
27	2	609	CLA	MG-NC	-3.74	1.97	2.06
27	1	613	CLA	MG-NC	-3.73	1.97	2.06
27	A	843	CLA	MG-NC	-3.73	1.97	2.06
27	5	601	CLA	MG-NC	-3.73	1.97	2.06
27	6	608	CLA	MG-NC	-3.73	1.97	2.06
27	A	814	CLA	MG-NC	-3.72	1.97	2.06
27	B	829	CLA	MG-NC	-3.72	1.97	2.06
27	7	304	CLA	MG-NC	-3.71	1.97	2.06
27	B	814	CLA	MG-NC	-3.71	1.97	2.06
27	b	602	CLA	MG-NC	-3.71	1.97	2.06
27	B	815	CLA	MG-NC	-3.70	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	610	KC2	C3D-C4D	3.70	1.43	1.40
28	6	610	KC2	C4C-NC	3.70	1.43	1.37
27	9	602	CLA	MG-NC	-3.69	1.97	2.06
28	9	610	KC2	C1B-NB	3.68	1.42	1.37
27	B	824	CLA	MG-NC	-3.68	1.97	2.06
27	1	604	CLA	MG-NC	-3.68	1.97	2.06
27	O	202	CLA	MG-NC	-3.67	1.97	2.06
27	O	204	CLA	MG-NC	-3.67	1.97	2.06
28	4	605	KC2	C4C-NC	3.67	1.43	1.37
28	b	609	KC2	C1B-NB	3.67	1.42	1.37
27	A	828	CLA	MG-NC	-3.67	1.97	2.06
27	9	614	CLA	MG-NC	-3.67	1.97	2.06
28	a	609	KC2	C1B-NB	3.67	1.42	1.37
27	A	824	CLA	MG-NC	-3.66	1.97	2.06
27	A	818	CLA	MG-NC	-3.66	1.97	2.06
27	R	202	CLA	MG-NC	-3.66	1.97	2.06
27	J	102	CLA	C3A-C2A	-3.66	1.51	1.54
28	4	605	KC2	C3D-C4D	3.65	1.43	1.40
27	a	604	CLA	MG-NC	-3.65	1.97	2.06
27	A	801	CLA	MG-NC	-3.65	1.97	2.06
27	6	609	CLA	MG-NC	-3.65	1.97	2.06
27	A	834	CLA	MG-NC	-3.65	1.97	2.06
27	2	602	CLA	MG-NC	-3.65	1.97	2.06
27	B	802	CLA	MG-NC	-3.65	1.97	2.06
27	B	828	CLA	MG-NC	-3.65	1.97	2.06
27	6	606	CLA	MG-NC	-3.64	1.97	2.06
27	A	803	CLA	MG-NC	-3.64	1.97	2.06
27	A	833	CLA	MG-NC	-3.63	1.97	2.06
27	2	604	CLA	MG-NC	-3.63	1.97	2.06
27	3	602	CLA	MG-NC	-3.63	1.97	2.06
28	7	311	KC2	C3D-C4D	3.63	1.43	1.40
28	3	606	KC2	C1B-NB	3.63	1.42	1.37
27	3	610	CLA	MG-NC	-3.62	1.97	2.06
28	a	609	KC2	C4C-NC	3.62	1.43	1.37
27	A	842	CLA	MG-NC	-3.62	1.97	2.06
27	1	611	CLA	MG-NC	-3.62	1.97	2.06
28	Z	307	KC2	C1B-NB	3.62	1.42	1.37
27	5	602	CLA	MG-NC	-3.62	1.97	2.06
28	9	610	KC2	C4C-NC	3.62	1.43	1.37
27	2	601	CLA	MG-NC	-3.61	1.97	2.06
28	Z	307	KC2	C4C-NC	3.61	1.43	1.37
27	2	603	CLA	MG-NC	-3.61	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	835	CLA	MG-NC	-3.61	1.97	2.06
27	7	308	CLA	MG-NC	-3.60	1.97	2.06
27	B	834	CLA	MG-NC	-3.60	1.97	2.06
27	b	610	CLA	MG-NC	-3.60	1.97	2.06
27	B	830	CLA	MG-NC	-3.60	1.97	2.06
27	9	603	CLA	MG-NC	-3.59	1.97	2.06
27	B	819	CLA	MG-NC	-3.59	1.97	2.06
28	6	610	KC2	C3D-C4D	3.59	1.43	1.40
27	4	603	CLA	MG-NC	-3.59	1.97	2.06
27	8	603	CLA	MG-NC	-3.59	1.97	2.06
27	B	838	CLA	MG-NC	-3.59	1.97	2.06
27	A	819	CLA	MG-NC	-3.58	1.97	2.06
27	5	606	CLA	MG-NC	-3.58	1.97	2.06
28	b	605	KC2	C1B-NB	3.58	1.42	1.37
27	5	603	CLA	MG-NC	-3.58	1.97	2.06
27	5	608	CLA	MG-NC	-3.58	1.97	2.06
27	A	823	CLA	MG-NC	-3.57	1.97	2.06
28	7	311	KC2	C1B-NB	3.57	1.42	1.37
27	3	611	CLA	MG-NC	-3.57	1.97	2.06
28	7	307	KC2	C1B-NB	3.57	1.42	1.37
27	9	604	CLA	MG-NC	-3.56	1.97	2.06
27	A	815	CLA	MG-NC	-3.56	1.97	2.06
27	B	818	CLA	MG-NC	-3.56	1.97	2.06
27	8	606	CLA	MG-NC	-3.56	1.97	2.06
27	7	310	CLA	MG-NC	-3.56	1.97	2.06
28	5	610	KC2	C3D-C4D	3.55	1.43	1.40
27	3	605	CLA	MG-NC	-3.55	1.97	2.06
27	1	606	CLA	MG-NC	-3.55	1.97	2.06
27	B	827	CLA	MG-NC	-3.55	1.97	2.06
27	B	804	CLA	MG-NC	-3.55	1.97	2.06
27	B	837	CLA	MG-NC	-3.54	1.97	2.06
27	B	809	CLA	MG-NC	-3.54	1.97	2.06
27	a	602	CLA	MG-NC	-3.54	1.97	2.06
27	6	604	CLA	MG-NC	-3.54	1.97	2.06
27	A	820	CLA	MG-NC	-3.54	1.97	2.06
27	b	607	CLA	MG-NC	-3.54	1.97	2.06
27	7	306	CLA	MG-NC	-3.54	1.97	2.06
27	7	313	CLA	MG-NC	-3.54	1.97	2.06
27	B	807	CLA	MG-NC	-3.54	1.97	2.06
27	a	610	CLA	MG-NC	-3.53	1.97	2.06
27	B	832	CLA	MG-NC	-3.53	1.97	2.06
27	9	609	CLA	MG-NC	-3.53	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	9	611	CLA	MG-NC	-3.53	1.97	2.06
27	A	808	CLA	MG-NC	-3.53	1.97	2.06
27	2	608	CLA	MG-NC	-3.53	1.97	2.06
27	1	603	CLA	MG-NC	-3.53	1.97	2.06
28	6	613	KC2	C3D-C4D	3.53	1.43	1.40
27	5	609	CLA	MG-NC	-3.53	1.97	2.06
27	8	607	CLA	MG-NC	-3.53	1.97	2.06
27	5	613	CLA	C3A-C2A	-3.52	1.51	1.54
27	8	615	CLA	MG-NC	-3.52	1.97	2.06
27	2	611	CLA	MG-NC	-3.52	1.97	2.06
27	8	602	CLA	MG-NC	-3.51	1.97	2.06
27	A	812	CLA	MG-NC	-3.51	1.97	2.06
28	9	610	KC2	C3D-C4D	3.51	1.43	1.40
27	J	102	CLA	MG-NC	-3.51	1.97	2.06
27	3	603	CLA	MG-NC	-3.51	1.97	2.06
27	B	806	CLA	MG-NC	-3.50	1.97	2.06
27	A	813	CLA	MG-NC	-3.50	1.98	2.06
27	B	840	CLA	MG-NC	-3.49	1.98	2.06
27	Z	301	CLA	MG-NC	-3.49	1.98	2.06
27	B	839	CLA	MG-NC	-3.49	1.98	2.06
27	B	811	CLA	MG-NC	-3.49	1.98	2.06
27	A	825	CLA	MG-NC	-3.48	1.98	2.06
27	1	609	CLA	MG-NC	-3.48	1.98	2.06
27	A	822	CLA	MG-NC	-3.48	1.98	2.06
27	b	601	CLA	MG-NC	-3.48	1.98	2.06
27	9	605	CLA	MG-NC	-3.48	1.98	2.06
27	7	305	CLA	MG-NC	-3.48	1.98	2.06
27	2	607	CLA	MG-NC	-3.48	1.98	2.06
27	6	602	CLA	MG-NC	-3.47	1.98	2.06
27	7	303	CLA	MG-NC	-3.47	1.98	2.06
27	4	602	CLA	MG-NC	-3.47	1.98	2.06
27	4	606	CLA	MG-NC	-3.47	1.98	2.06
27	A	821	CLA	MG-NC	-3.47	1.98	2.06
27	F	202	CLA	MG-NC	-3.47	1.98	2.06
27	1	607	CLA	MG-NC	-3.46	1.98	2.06
27	A	839	CLA	MG-NC	-3.46	1.98	2.06
27	a	603	CLA	MG-NC	-3.46	1.98	2.06
27	B	841	CLA	MG-NC	-3.46	1.98	2.06
27	b	611	CLA	MG-NC	-3.46	1.98	2.06
27	7	302	CLA	MG-NC	-3.46	1.98	2.06
27	b	603	CLA	MG-NC	-3.46	1.98	2.06
27	L	201	CLA	MG-NC	-3.45	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	807	CLA	MG-NC	-3.45	1.98	2.06
27	6	611	CLA	MG-NC	-3.45	1.98	2.06
27	B	803	CLA	MG-NC	-3.45	1.98	2.06
27	Z	304	CLA	MG-NC	-3.45	1.98	2.06
27	5	605	CLA	MG-NC	-3.45	1.98	2.06
27	B	820	CLA	MG-NC	-3.44	1.98	2.06
27	B	822	CLA	MG-NC	-3.44	1.98	2.06
27	3	607	CLA	MG-NC	-3.44	1.98	2.06
27	7	309	CLA	MG-NC	-3.44	1.98	2.06
27	A	836	CLA	MG-NC	-3.44	1.98	2.06
27	9	612	CLA	MG-NC	-3.43	1.98	2.06
27	A	816	CLA	MG-NC	-3.43	1.98	2.06
27	5	613	CLA	MG-NC	-3.43	1.98	2.06
27	5	607	CLA	MG-NC	-3.43	1.98	2.06
27	K	101	CLA	MG-NC	-3.43	1.98	2.06
27	5	612	CLA	MG-NC	-3.42	1.98	2.06
27	A	830	CLA	MG-NC	-3.42	1.98	2.06
27	O	203	CLA	MG-NC	-3.42	1.98	2.06
27	b	604	CLA	MG-NC	-3.42	1.98	2.06
27	4	609	CLA	MG-NC	-3.42	1.98	2.06
27	4	607	CLA	MG-NC	-3.42	1.98	2.06
27	A	805	CLA	MG-NC	-3.42	1.98	2.06
27	a	605	CLA	MG-NC	-3.42	1.98	2.06
27	7	312	CLA	MG-NC	-3.42	1.98	2.06
27	8	608	CLA	MG-NC	-3.42	1.98	2.06
27	9	613	CLA	MG-NC	-3.41	1.98	2.06
27	a	601	CLA	MG-NC	-3.41	1.98	2.06
27	A	810	CLA	MG-NC	-3.41	1.98	2.06
27	4	604	CLA	MG-NC	-3.41	1.98	2.06
27	A	829	CLA	MG-NC	-3.41	1.98	2.06
28	a	609	KC2	C3D-C4D	3.41	1.43	1.40
27	B	805	CLA	MG-NC	-3.41	1.98	2.06
27	8	601	CLA	MG-NC	-3.41	1.98	2.06
27	A	811	CLA	MG-NC	-3.41	1.98	2.06
28	b	605	KC2	C4C-NC	3.40	1.42	1.37
27	9	608	CLA	MG-NC	-3.40	1.98	2.06
27	3	601	CLA	MG-NC	-3.39	1.98	2.06
27	2	606	CLA	MG-NC	-3.39	1.98	2.06
27	A	837	CLA	MG-NC	-3.39	1.98	2.06
27	B	810	CLA	MG-NC	-3.39	1.98	2.06
27	9	606	CLA	MG-NC	-3.39	1.98	2.06
27	a	607	CLA	MG-NC	-3.38	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	821	CLA	MG-NC	-3.38	1.98	2.06
27	A	804	CLA	MG-NC	-3.38	1.98	2.06
27	1	602	CLA	MG-NC	-3.38	1.98	2.06
27	A	806	CLA	MG-NC	-3.38	1.98	2.06
27	A	840	CLA	MG-NC	-3.38	1.98	2.06
27	B	823	CLA	MG-NC	-3.37	1.98	2.06
27	2	605	CLA	MG-NC	-3.37	1.98	2.06
27	L	203	CLA	MG-NC	-3.37	1.98	2.06
27	3	604	CLA	MG-NC	-3.37	1.98	2.06
27	B	836	CLA	MG-NC	-3.36	1.98	2.06
27	3	608	CLA	MG-NC	-3.36	1.98	2.06
27	8	604	CLA	MG-NC	-3.36	1.98	2.06
27	2	612	CLA	MG-NC	-3.36	1.98	2.06
27	6	612	CLA	MG-NC	-3.36	1.98	2.06
27	B	826	CLA	MG-NC	-3.36	1.98	2.06
27	A	832	CLA	MG-NC	-3.35	1.98	2.06
27	A	835	CLA	MG-NC	-3.35	1.98	2.06
27	Z	306	CLA	MG-NC	-3.35	1.98	2.06
27	Z	310	CLA	MG-NC	-3.34	1.98	2.06
27	B	801	CLA	MG-NC	-3.34	1.98	2.06
27	1	608	CLA	MG-NC	-3.34	1.98	2.06
27	F	203	CLA	MG-NC	-3.34	1.98	2.06
27	b	606	CLA	MG-NC	-3.33	1.98	2.06
27	3	609	CLA	MG-NC	-3.33	1.98	2.06
27	B	816	CLA	MG-NC	-3.33	1.98	2.06
27	5	611	CLA	MG-NC	-3.33	1.98	2.06
27	6	601	CLA	MG-NC	-3.32	1.98	2.06
27	4	608	CLA	MG-NC	-3.32	1.98	2.06
27	3	612	CLA	MG-NC	-3.32	1.98	2.06
27	B	817	CLA	MG-NC	-3.32	1.98	2.06
27	A	838	CLA	MG-NC	-3.31	1.98	2.06
27	6	605	CLA	MG-NC	-3.30	1.98	2.06
27	1	609	CLA	C3A-C2A	-3.30	1.51	1.54
27	5	601	CLA	C3A-C2A	-3.30	1.51	1.54
27	6	607	CLA	MG-NC	-3.30	1.98	2.06
27	B	825	CLA	MG-NC	-3.29	1.98	2.06
27	A	802	CLA	MG-NC	-3.29	1.98	2.06
27	b	608	CLA	MG-NC	-3.29	1.98	2.06
27	a	611	CLA	MG-NC	-3.29	1.98	2.06
27	A	826	CLA	MG-NC	-3.28	1.98	2.06
27	A	827	CLA	MG-NC	-3.28	1.98	2.06
27	F	204	CLA	MG-NC	-3.28	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	9	601	CLA	MG-NC	-3.28	1.98	2.06
27	A	831	CLA	MG-NC	-3.28	1.98	2.06
27	4	610	CLA	MG-NC	-3.27	1.98	2.06
27	a	608	CLA	MG-NC	-3.26	1.98	2.06
27	B	812	CLA	MG-NC	-3.26	1.98	2.06
27	B	833	CLA	MG-NC	-3.25	1.98	2.06
27	Z	305	CLA	MG-NC	-3.25	1.98	2.06
27	4	611	CLA	MG-NC	-3.24	1.98	2.06
27	B	808	CLA	MG-NC	-3.24	1.98	2.06
27	4	601	CLA	MG-NC	-3.23	1.98	2.06
27	9	607	CLA	MG-NC	-3.22	1.98	2.06
28	6	613	KC2	C1D-ND	3.21	1.38	1.35
27	a	606	CLA	MG-NC	-3.20	1.98	2.06
28	3	606	KC2	C1D-ND	3.20	1.38	1.35
27	1	612	CLA	MG-NC	-3.19	1.98	2.06
28	5	610	KC2	C1D-ND	3.18	1.38	1.35
27	B	813	CLA	MG-NC	-3.17	1.98	2.06
28	Z	307	KC2	C1D-ND	3.14	1.38	1.35
27	9	614	CLA	C3A-C2A	-3.14	1.51	1.54
28	9	610	KC2	C1D-ND	3.14	1.38	1.35
28	1	610	KC2	C1D-ND	3.13	1.38	1.35
28	7	307	KC2	C1D-ND	3.13	1.38	1.35
27	1	605	CLA	MG-NC	-3.13	1.98	2.06
28	b	605	KC2	C1D-ND	3.12	1.38	1.35
27	2	609	CLA	C3A-C2A	-3.12	1.51	1.54
27	A	844	CLA	MG-NC	-3.10	1.98	2.06
28	4	605	KC2	C1D-ND	3.10	1.38	1.35
28	6	610	KC2	C1D-ND	3.09	1.38	1.35
28	7	311	KC2	C1D-ND	3.08	1.38	1.35
27	8	607	CLA	C3A-C2A	-3.08	1.51	1.54
28	a	609	KC2	C1D-ND	3.07	1.37	1.35
28	2	610	KC2	C1D-ND	3.06	1.37	1.35
27	5	609	CLA	C3A-C2A	-3.06	1.51	1.54
28	b	609	KC2	C1D-ND	3.04	1.37	1.35
27	7	310	CLA	C3A-C2A	-3.01	1.51	1.54
34	3	621	SQD	C6-S	-2.94	1.66	1.77
27	9	609	CLA	C3A-C2A	-2.93	1.51	1.54
28	b	609	KC2	C3D-C2D	2.82	1.44	1.39
27	O	202	CLA	C3A-C2A	-2.79	1.51	1.54
27	6	609	CLA	C3A-C2A	-2.79	1.51	1.54
28	Z	307	KC2	C3D-C2D	2.78	1.44	1.39
28	a	609	KC2	C3D-C2D	2.78	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	4	605	KC2	C3D-C2D	2.78	1.44	1.39
28	7	307	KC2	C3D-C2D	2.77	1.44	1.39
28	1	610	KC2	C3D-C2D	2.77	1.44	1.39
28	6	613	KC2	C3D-C2D	2.76	1.44	1.39
28	2	610	KC2	C3D-C2D	2.75	1.44	1.39
28	b	605	KC2	C3D-C2D	2.75	1.44	1.39
27	9	611	CLA	C3A-C2A	-2.74	1.52	1.54
28	7	311	KC2	C3D-C2D	2.74	1.44	1.39
28	9	610	KC2	C3D-C2D	2.73	1.44	1.39
34	O	207	SQD	C6-S	-2.72	1.67	1.77
28	3	606	KC2	C3D-C2D	2.71	1.44	1.39
28	5	610	KC2	C3D-C2D	2.69	1.44	1.39
28	6	610	KC2	C3D-C2D	2.68	1.44	1.39
28	1	610	KC2	C4D-CHA	-2.57	1.41	1.45
28	4	605	KC2	C4D-CHA	-2.56	1.41	1.45
32	6	618	LMG	C4-C5	2.50	1.58	1.53
39	Z	303	DGD	O2G-C2G	-2.47	1.40	1.46
39	Z	303	DGD	O1G-C1G	-2.47	1.39	1.45
35	F	201	8CT	C35-C30	2.45	1.63	1.56
30	b	613	II3	C05-C03	-2.43	1.51	1.54
28	2	610	KC2	C4D-CHA	-2.40	1.42	1.45
34	O	207	SQD	O6-C1	2.38	1.44	1.40
28	5	610	KC2	C4D-CHA	-2.36	1.42	1.45
27	A	844	CLA	C3D-C4D	-2.36	1.38	1.44
28	7	307	KC2	C4D-ND	2.35	1.37	1.35
27	B	839	CLA	C1D-C2D	-2.32	1.40	1.45
27	1	605	CLA	C1D-C2D	-2.30	1.40	1.45
27	B	813	CLA	C1D-C2D	-2.30	1.40	1.45
27	a	603	CLA	C1D-C2D	-2.30	1.40	1.45
27	8	604	CLA	C1D-C2D	-2.30	1.40	1.45
28	Z	307	KC2	C4D-CHA	-2.30	1.42	1.45
27	1	602	CLA	C1D-C2D	-2.29	1.40	1.45
27	b	606	CLA	C1D-C2D	-2.28	1.40	1.45
27	K	101	CLA	C1D-C2D	-2.28	1.40	1.45
27	6	608	CLA	C1D-C2D	-2.27	1.40	1.45
27	B	823	CLA	C1D-C2D	-2.27	1.40	1.45
27	A	823	CLA	C1D-C2D	-2.27	1.40	1.45
35	7	318	8CT	C35-C30	2.27	1.62	1.56
27	A	810	CLA	C1D-C2D	-2.27	1.40	1.45
27	3	602	CLA	C1D-C2D	-2.27	1.40	1.45
27	A	840	CLA	C3D-C4D	-2.26	1.39	1.44
27	b	602	CLA	C1D-C2D	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	804	CLA	C1D-C2D	-2.26	1.40	1.45
27	A	801	CLA	C1D-C2D	-2.26	1.40	1.45
33	6	617	LHG	O7-C5	-2.26	1.41	1.46
27	A	841	CLA	C1D-C2D	-2.26	1.40	1.45
27	6	602	CLA	C1D-C2D	-2.25	1.40	1.45
27	B	805	CLA	C1D-C2D	-2.25	1.40	1.45
27	A	825	CLA	C1D-C2D	-2.25	1.40	1.45
27	B	807	CLA	C1D-C2D	-2.25	1.40	1.45
27	a	608	CLA	C1D-C2D	-2.24	1.40	1.45
27	8	602	CLA	C1D-C2D	-2.24	1.40	1.45
27	9	607	CLA	C1D-C2D	-2.24	1.40	1.45
27	A	815	CLA	C1D-C2D	-2.24	1.40	1.45
27	6	611	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	607	CLA	C1D-C2D	-2.24	1.40	1.45
27	F	204	CLA	C1D-C2D	-2.24	1.40	1.45
27	B	836	CLA	C1D-C2D	-2.24	1.40	1.45
33	8	613	LHG	O7-C5	-2.24	1.41	1.46
27	A	820	CLA	C1D-C2D	-2.24	1.40	1.45
39	Z	303	DGD	O6D-C5D	-2.23	1.38	1.44
27	A	828	CLA	C1D-C2D	-2.23	1.40	1.45
27	R	202	CLA	C1D-C2D	-2.23	1.40	1.45
27	4	606	CLA	C1D-C2D	-2.23	1.40	1.45
27	B	833	CLA	C1D-C2D	-2.23	1.40	1.45
27	5	603	CLA	C1D-C2D	-2.23	1.40	1.45
27	9	602	CLA	C1D-C2D	-2.23	1.40	1.45
27	3	603	CLA	C1D-C2D	-2.23	1.40	1.45
27	9	613	CLA	C1D-C2D	-2.23	1.40	1.45
27	3	601	CLA	C1D-C2D	-2.23	1.40	1.45
27	A	806	CLA	C1D-C2D	-2.23	1.40	1.45
27	B	809	CLA	C1D-C2D	-2.23	1.40	1.45
27	B	815	CLA	C1D-C2D	-2.22	1.40	1.45
27	B	802	CLA	C1D-C2D	-2.22	1.40	1.45
27	B	829	CLA	C3D-C4D	-2.22	1.39	1.44
27	A	824	CLA	C3D-C4D	-2.22	1.39	1.44
27	A	826	CLA	C1D-C2D	-2.22	1.40	1.45
27	A	817	CLA	C3D-C4D	-2.22	1.39	1.44
27	L	203	CLA	C1D-C2D	-2.22	1.40	1.45
27	1	604	CLA	C1D-C2D	-2.22	1.40	1.45
27	A	827	CLA	C1D-C2D	-2.22	1.40	1.45
27	B	835	CLA	C1D-C2D	-2.22	1.40	1.45
27	5	613	CLA	C1D-C2D	-2.22	1.40	1.45
27	b	607	CLA	C1D-C2D	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	605	CLA	C1D-C2D	-2.22	1.40	1.45
27	6	603	CLA	C3D-C4D	-2.22	1.39	1.44
27	A	836	CLA	C3D-C4D	-2.22	1.39	1.44
27	7	303	CLA	C1D-C2D	-2.22	1.41	1.45
27	B	832	CLA	C1D-C2D	-2.22	1.41	1.45
27	A	812	CLA	C1D-C2D	-2.22	1.41	1.45
27	b	604	CLA	C1D-C2D	-2.21	1.41	1.45
27	B	825	CLA	C1D-C2D	-2.21	1.41	1.45
27	3	611	CLA	C1D-C2D	-2.21	1.41	1.45
27	A	835	CLA	C1D-C2D	-2.21	1.41	1.45
27	3	612	CLA	C1D-C2D	-2.21	1.41	1.45
27	4	610	CLA	C1D-C2D	-2.21	1.41	1.45
27	B	824	CLA	C1D-C2D	-2.21	1.41	1.45
27	3	607	CLA	C1D-C2D	-2.21	1.41	1.45
27	4	602	CLA	C1D-C2D	-2.21	1.41	1.45
28	3	606	KC2	C4D-ND	2.21	1.37	1.35
28	6	613	KC2	C4D-ND	2.21	1.37	1.35
27	A	832	CLA	C1D-C2D	-2.21	1.41	1.45
27	B	813	CLA	C3D-C4D	-2.21	1.39	1.44
27	9	603	CLA	C1D-C2D	-2.21	1.41	1.45
27	B	801	CLA	C1D-C2D	-2.21	1.41	1.45
27	5	609	CLA	C1D-C2D	-2.21	1.41	1.45
27	A	839	CLA	C1D-C2D	-2.21	1.41	1.45
27	4	609	CLA	C1D-C2D	-2.21	1.41	1.45
27	7	303	CLA	C3D-C4D	-2.21	1.39	1.44
30	1	615	II3	C05-C03	-2.21	1.51	1.54
27	5	602	CLA	C1D-C2D	-2.20	1.41	1.45
27	B	826	CLA	C1D-C2D	-2.20	1.41	1.45
27	Z	304	CLA	C1D-C2D	-2.20	1.41	1.45
27	A	829	CLA	C1D-C2D	-2.20	1.41	1.45
27	b	603	CLA	C1D-C2D	-2.20	1.41	1.45
27	9	601	CLA	C1D-C2D	-2.20	1.41	1.45
27	A	831	CLA	C1D-C2D	-2.20	1.41	1.45
27	F	203	CLA	C1D-C2D	-2.20	1.41	1.45
27	4	608	CLA	C1D-C2D	-2.20	1.41	1.45
27	9	608	CLA	C1D-C2D	-2.20	1.41	1.45
27	a	606	CLA	C1D-C2D	-2.20	1.41	1.45
27	A	836	CLA	C1D-C2D	-2.20	1.41	1.45
27	2	611	CLA	C1D-C2D	-2.20	1.41	1.45
27	6	603	CLA	C1D-C2D	-2.20	1.41	1.45
27	b	608	CLA	C1D-C2D	-2.20	1.41	1.45
27	B	815	CLA	C3D-C4D	-2.20	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	302	CLA	C1D-C2D	-2.20	1.41	1.45
27	7	312	CLA	C1D-C2D	-2.20	1.41	1.45
27	9	611	CLA	C1D-C2D	-2.20	1.41	1.45
27	A	834	CLA	C1D-C2D	-2.20	1.41	1.45
27	9	612	CLA	C1D-C2D	-2.20	1.41	1.45
27	A	838	CLA	C1D-C2D	-2.20	1.41	1.45
27	B	818	CLA	C3D-C4D	-2.19	1.39	1.44
27	1	613	CLA	C1D-C2D	-2.19	1.41	1.45
28	9	610	KC2	C4D-CHA	-2.19	1.42	1.45
27	A	821	CLA	C3D-C4D	-2.19	1.39	1.44
27	A	815	CLA	C3D-C4D	-2.19	1.39	1.44
27	B	821	CLA	C3D-C4D	-2.19	1.39	1.44
27	8	607	CLA	C1D-C2D	-2.19	1.41	1.45
27	A	819	CLA	C3D-C4D	-2.19	1.39	1.44
27	A	829	CLA	C3D-C4D	-2.19	1.39	1.44
27	a	602	CLA	C1D-C2D	-2.19	1.41	1.45
31	A	854	IHT	C18-C07	2.19	1.52	1.45
27	K	102	CLA	C1D-C2D	-2.19	1.41	1.45
27	b	610	CLA	C1D-C2D	-2.19	1.41	1.45
27	A	802	CLA	C3D-C4D	-2.19	1.39	1.44
27	a	605	CLA	C3D-C4D	-2.19	1.39	1.44
27	3	609	CLA	C1D-C2D	-2.19	1.41	1.45
27	7	308	CLA	C1D-C2D	-2.19	1.41	1.45
27	2	602	CLA	C3D-C4D	-2.19	1.39	1.44
27	B	816	CLA	C1D-C2D	-2.19	1.41	1.45
27	F	202	CLA	C1D-C2D	-2.19	1.41	1.45
27	4	611	CLA	C1D-C2D	-2.19	1.41	1.45
27	5	605	CLA	C1D-C2D	-2.19	1.41	1.45
27	1	605	CLA	C3D-C4D	-2.18	1.39	1.44
27	B	837	CLA	C3D-C4D	-2.18	1.39	1.44
27	A	837	CLA	C1D-C2D	-2.18	1.41	1.45
27	A	809	CLA	C3D-C4D	-2.18	1.39	1.44
27	A	843	CLA	C1D-C2D	-2.18	1.41	1.45
27	B	812	CLA	C1D-C2D	-2.18	1.41	1.45
27	B	820	CLA	C1D-C2D	-2.18	1.41	1.45
27	a	604	CLA	C3D-C4D	-2.18	1.39	1.44
27	3	604	CLA	C1D-C2D	-2.18	1.41	1.45
27	3	608	CLA	C1D-C2D	-2.18	1.41	1.45
27	B	818	CLA	C1D-C2D	-2.18	1.41	1.45
28	7	311	KC2	C4D-ND	2.18	1.37	1.35
32	8	614	LMG	O6-C5	-2.18	1.39	1.44
27	B	826	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	839	CLA	C3D-C4D	-2.18	1.39	1.44
27	B	840	CLA	C3D-C4D	-2.18	1.39	1.44
27	1	612	CLA	C1D-C2D	-2.18	1.41	1.45
27	A	842	CLA	C1D-C2D	-2.18	1.41	1.45
27	B	803	CLA	C1D-C2D	-2.18	1.41	1.45
27	B	817	CLA	C3D-C4D	-2.18	1.39	1.44
27	B	822	CLA	C3D-C4D	-2.18	1.39	1.44
27	4	602	CLA	C3D-C4D	-2.18	1.39	1.44
27	B	828	CLA	C1D-C2D	-2.18	1.41	1.45
27	B	810	CLA	C1D-C2D	-2.18	1.41	1.45
27	O	203	CLA	C1D-C2D	-2.18	1.41	1.45
27	b	611	CLA	C1D-C2D	-2.18	1.41	1.45
27	4	604	CLA	C1D-C2D	-2.18	1.41	1.45
27	L	202	CLA	C1D-C2D	-2.18	1.41	1.45
27	6	611	CLA	C3D-C4D	-2.18	1.39	1.44
27	a	611	CLA	C1D-C2D	-2.18	1.41	1.45
27	7	313	CLA	C1D-C2D	-2.18	1.41	1.45
27	A	824	CLA	C1D-C2D	-2.18	1.41	1.45
27	A	839	CLA	C3D-C4D	-2.18	1.39	1.44
27	6	607	CLA	C1D-C2D	-2.17	1.41	1.45
27	5	611	CLA	C1D-C2D	-2.17	1.41	1.45
27	B	822	CLA	C1D-C2D	-2.17	1.41	1.45
27	B	838	CLA	C1D-C2D	-2.17	1.41	1.45
27	O	201	CLA	C1D-C2D	-2.17	1.41	1.45
27	B	836	CLA	C3D-C4D	-2.17	1.39	1.44
27	a	604	CLA	C1D-C2D	-2.17	1.41	1.45
27	B	808	CLA	C3D-C4D	-2.17	1.39	1.44
27	A	838	CLA	C3D-C4D	-2.17	1.39	1.44
27	B	808	CLA	C1D-C2D	-2.17	1.41	1.45
27	B	817	CLA	C1D-C2D	-2.17	1.41	1.45
27	1	611	CLA	C1D-C2D	-2.17	1.41	1.45
27	4	607	CLA	C1D-C2D	-2.17	1.41	1.45
33	4	619	LHG	O7-C5	-2.17	1.41	1.46
27	1	609	CLA	C1D-C2D	-2.17	1.41	1.45
27	2	602	CLA	C1D-C2D	-2.17	1.41	1.45
27	6	602	CLA	C3D-C4D	-2.17	1.39	1.44
27	Z	305	CLA	C3D-C4D	-2.17	1.39	1.44
27	8	606	CLA	C1D-C2D	-2.16	1.41	1.45
27	9	606	CLA	C3D-C4D	-2.16	1.39	1.44
27	A	816	CLA	C3D-C4D	-2.16	1.39	1.44
27	A	830	CLA	C1D-C2D	-2.16	1.41	1.45
27	L	201	CLA	C1D-C2D	-2.16	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	9	605	CLA	C1D-C2D	-2.16	1.41	1.45
27	A	813	CLA	C3D-C4D	-2.16	1.39	1.44
27	7	309	CLA	C1D-C2D	-2.16	1.41	1.45
27	7	306	CLA	C1D-C2D	-2.16	1.41	1.45
27	Z	301	CLA	C1D-C2D	-2.16	1.41	1.45
27	2	603	CLA	C1D-C2D	-2.16	1.41	1.45
27	B	834	CLA	C1D-C2D	-2.16	1.41	1.45
27	2	609	CLA	C1D-C2D	-2.16	1.41	1.45
27	2	605	CLA	C1D-C2D	-2.16	1.41	1.45
27	2	608	CLA	C1D-C2D	-2.16	1.41	1.45
27	5	612	CLA	C1D-C2D	-2.16	1.41	1.45
27	9	609	CLA	C1D-C2D	-2.16	1.41	1.45
27	2	605	CLA	C3D-C4D	-2.16	1.39	1.44
27	5	612	CLA	C3D-C4D	-2.16	1.39	1.44
27	5	606	CLA	C1D-C2D	-2.16	1.41	1.45
27	A	816	CLA	C1D-C2D	-2.16	1.41	1.45
27	4	603	CLA	C1D-C2D	-2.16	1.41	1.45
27	4	610	CLA	C3D-C4D	-2.16	1.39	1.44
27	B	831	CLA	C1D-C2D	-2.16	1.41	1.45
27	8	608	CLA	C1D-C2D	-2.16	1.41	1.45
27	4	607	CLA	C3D-C4D	-2.16	1.39	1.44
27	3	611	CLA	C3D-C4D	-2.16	1.39	1.44
27	A	830	CLA	C3D-C4D	-2.16	1.39	1.44
27	5	606	CLA	C3D-C4D	-2.15	1.39	1.44
27	A	820	CLA	C3D-C4D	-2.15	1.39	1.44
27	8	601	CLA	C1D-C2D	-2.15	1.41	1.45
27	A	809	CLA	C1D-C2D	-2.15	1.41	1.45
27	3	607	CLA	C3D-C4D	-2.15	1.39	1.44
27	a	606	CLA	C3D-C4D	-2.15	1.39	1.44
27	5	607	CLA	C1D-C2D	-2.15	1.41	1.45
27	6	601	CLA	C1D-C2D	-2.15	1.41	1.45
27	A	811	CLA	C3D-C4D	-2.15	1.39	1.44
27	a	603	CLA	C3D-C4D	-2.15	1.39	1.44
27	A	841	CLA	C3D-C4D	-2.15	1.39	1.44
27	b	607	CLA	C3D-C4D	-2.15	1.39	1.44
27	6	606	CLA	C1D-C2D	-2.15	1.41	1.45
27	A	818	CLA	C3D-C4D	-2.15	1.39	1.44
27	9	614	CLA	C1D-C2D	-2.15	1.41	1.45
27	A	808	CLA	C1D-C2D	-2.15	1.41	1.45
27	Z	305	CLA	C1D-C2D	-2.15	1.41	1.45
27	B	824	CLA	C3D-C4D	-2.15	1.39	1.44
27	a	602	CLA	C3D-C4D	-2.15	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	822	CLA	C1D-C2D	-2.15	1.41	1.45
27	B	806	CLA	C1D-C2D	-2.15	1.41	1.45
27	Z	306	CLA	C1D-C2D	-2.15	1.41	1.45
27	A	833	CLA	C1D-C2D	-2.15	1.41	1.45
27	3	608	CLA	C3D-C4D	-2.15	1.39	1.44
27	A	807	CLA	C1D-C2D	-2.15	1.41	1.45
27	8	607	CLA	C3D-C4D	-2.15	1.39	1.44
27	6	609	CLA	C1D-C2D	-2.15	1.41	1.45
27	6	608	CLA	C3D-C4D	-2.15	1.39	1.44
27	8	603	CLA	C3D-C4D	-2.15	1.39	1.44
27	9	611	CLA	C3D-C4D	-2.15	1.39	1.44
27	B	827	CLA	C1D-C2D	-2.15	1.41	1.45
27	A	803	CLA	C3D-C4D	-2.15	1.39	1.44
27	B	821	CLA	C1D-C2D	-2.15	1.41	1.45
27	Z	306	CLA	C3D-C4D	-2.15	1.39	1.44
27	B	814	CLA	C1D-C2D	-2.15	1.41	1.45
27	O	202	CLA	C1D-C2D	-2.15	1.41	1.45
28	6	613	KC2	C4D-CHA	-2.15	1.42	1.45
27	8	615	CLA	C3D-C4D	-2.15	1.39	1.44
27	4	609	CLA	C3D-C4D	-2.15	1.39	1.44
27	1	604	CLA	C3D-C4D	-2.15	1.39	1.44
27	6	606	CLA	C3D-C4D	-2.15	1.39	1.44
27	5	603	CLA	C3D-C4D	-2.15	1.39	1.44
27	7	310	CLA	C1D-C2D	-2.15	1.41	1.45
27	1	606	CLA	C1D-C2D	-2.14	1.41	1.45
27	2	612	CLA	C3D-C4D	-2.14	1.39	1.44
27	A	814	CLA	C1D-C2D	-2.14	1.41	1.45
27	5	601	CLA	C3D-C4D	-2.14	1.39	1.44
27	5	604	CLA	C1D-C2D	-2.14	1.41	1.45
27	7	304	CLA	C1D-C2D	-2.14	1.41	1.45
27	B	830	CLA	C3D-C4D	-2.14	1.39	1.44
27	a	601	CLA	C1D-C2D	-2.14	1.41	1.45
27	3	612	CLA	C3D-C4D	-2.14	1.39	1.44
27	A	826	CLA	C3D-C4D	-2.14	1.39	1.44
27	A	831	CLA	C3D-C4D	-2.14	1.39	1.44
33	4	620	LHG	O7-C5	-2.14	1.41	1.46
27	3	602	CLA	C3D-C4D	-2.14	1.39	1.44
27	B	804	CLA	C1D-C2D	-2.14	1.41	1.45
27	B	827	CLA	C3D-C4D	-2.14	1.39	1.44
28	6	610	KC2	C4D-CHA	-2.14	1.42	1.45
27	1	603	CLA	C1D-C2D	-2.14	1.41	1.45
27	A	802	CLA	C1D-C2D	-2.14	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	807	CLA	C3D-C4D	-2.14	1.39	1.44
27	1	608	CLA	C1D-C2D	-2.14	1.41	1.45
27	8	605	CLA	C1D-C2D	-2.14	1.41	1.45
27	A	814	CLA	C3D-C4D	-2.14	1.39	1.44
27	B	831	CLA	C3D-C4D	-2.14	1.39	1.44
27	B	833	CLA	C3D-C4D	-2.14	1.39	1.44
27	8	615	CLA	C1D-C2D	-2.14	1.41	1.45
27	2	608	CLA	C3D-C4D	-2.14	1.39	1.44
27	B	835	CLA	C3D-C4D	-2.14	1.39	1.44
27	L	202	CLA	C3D-C4D	-2.14	1.39	1.44
27	a	607	CLA	C3D-C4D	-2.14	1.39	1.44
27	A	840	CLA	C1D-C2D	-2.14	1.41	1.45
27	b	610	CLA	C3D-C4D	-2.14	1.39	1.44
27	5	608	CLA	C3D-C4D	-2.14	1.39	1.44
27	9	605	CLA	C3D-C4D	-2.14	1.39	1.44
27	A	833	CLA	C3D-C4D	-2.14	1.39	1.44
28	b	609	KC2	C4D-CHA	-2.14	1.42	1.45
27	2	612	CLA	C1D-C2D	-2.14	1.41	1.45
27	2	604	CLA	C3D-C4D	-2.14	1.39	1.44
27	A	827	CLA	C3D-C4D	-2.14	1.39	1.44
27	B	832	CLA	C3D-C4D	-2.14	1.39	1.44
27	2	609	CLA	C3D-C4D	-2.14	1.39	1.44
27	b	606	CLA	C3D-C4D	-2.14	1.39	1.44
27	1	607	CLA	C1D-C2D	-2.14	1.41	1.45
27	3	604	CLA	C3D-C4D	-2.14	1.39	1.44
27	4	603	CLA	C3D-C4D	-2.13	1.39	1.44
27	R	202	CLA	C3D-C4D	-2.13	1.39	1.44
27	b	603	CLA	C3D-C4D	-2.13	1.39	1.44
27	A	819	CLA	C1D-C2D	-2.13	1.41	1.45
27	9	602	CLA	C3D-C4D	-2.13	1.39	1.44
27	7	305	CLA	C1D-C2D	-2.13	1.41	1.45
27	b	602	CLA	C3D-C4D	-2.13	1.39	1.44
27	2	604	CLA	C1D-C2D	-2.13	1.41	1.45
27	F	203	CLA	C3D-C4D	-2.13	1.39	1.44
27	3	605	CLA	C3D-C4D	-2.13	1.39	1.44
27	a	610	CLA	C3D-C4D	-2.13	1.39	1.44
27	A	813	CLA	C1D-C2D	-2.13	1.41	1.45
27	A	817	CLA	C1D-C2D	-2.13	1.41	1.45
27	b	601	CLA	C1D-C2D	-2.13	1.41	1.45
27	6	605	CLA	C3D-C4D	-2.13	1.39	1.44
27	A	843	CLA	C3D-C4D	-2.13	1.39	1.44
27	B	820	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	9	610	KC2	C4D-ND	2.13	1.37	1.35
27	A	805	CLA	C3D-C4D	-2.13	1.39	1.44
27	6	604	CLA	C1D-C2D	-2.13	1.41	1.45
27	B	819	CLA	C1D-C2D	-2.13	1.41	1.45
27	B	840	CLA	C1D-C2D	-2.13	1.41	1.45
27	1	608	CLA	C3D-C4D	-2.13	1.39	1.44
27	F	202	CLA	C3D-C4D	-2.13	1.39	1.44
27	L	203	CLA	C3D-C4D	-2.13	1.39	1.44
27	O	201	CLA	C3D-C4D	-2.13	1.39	1.44
27	a	610	CLA	C1D-C2D	-2.13	1.41	1.45
27	6	601	CLA	C3D-C4D	-2.13	1.39	1.44
27	B	816	CLA	C3D-C4D	-2.13	1.39	1.44
27	B	811	CLA	C3D-C4D	-2.13	1.39	1.44
27	Z	304	CLA	C3D-C4D	-2.13	1.39	1.44
27	B	819	CLA	C3D-C4D	-2.13	1.39	1.44
27	J	102	CLA	C1D-C2D	-2.13	1.41	1.45
27	8	601	CLA	C3D-C4D	-2.13	1.39	1.44
27	3	610	CLA	C1D-C2D	-2.13	1.41	1.45
27	3	610	CLA	C3D-C4D	-2.12	1.39	1.44
27	B	838	CLA	C3D-C4D	-2.12	1.39	1.44
27	B	837	CLA	C1D-C2D	-2.12	1.41	1.45
27	Z	310	CLA	C3D-C4D	-2.12	1.39	1.44
27	A	811	CLA	C1D-C2D	-2.12	1.41	1.45
27	4	611	CLA	C3D-C4D	-2.12	1.39	1.44
27	B	828	CLA	C3D-C4D	-2.12	1.39	1.44
27	9	606	CLA	C1D-C2D	-2.12	1.41	1.45
27	B	830	CLA	C1D-C2D	-2.12	1.41	1.45
27	5	604	CLA	C3D-C4D	-2.12	1.39	1.44
27	J	102	CLA	C3D-C4D	-2.12	1.39	1.44
27	8	603	CLA	C1D-C2D	-2.12	1.41	1.45
27	1	602	CLA	C3D-C4D	-2.12	1.39	1.44
27	5	609	CLA	C3D-C4D	-2.12	1.39	1.44
27	4	604	CLA	C3D-C4D	-2.12	1.39	1.44
27	5	602	CLA	C3D-C4D	-2.12	1.39	1.44
27	b	604	CLA	C3D-C4D	-2.12	1.39	1.44
27	7	310	CLA	C3D-C4D	-2.12	1.39	1.44
27	1	603	CLA	C3D-C4D	-2.12	1.39	1.44
27	2	606	CLA	C1D-C2D	-2.12	1.41	1.45
27	6	609	CLA	C3D-C4D	-2.12	1.39	1.44
27	9	604	CLA	C1D-C2D	-2.12	1.41	1.45
27	3	605	CLA	C1D-C2D	-2.12	1.41	1.45
28	a	609	KC2	C4D-CHA	-2.12	1.42	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	612	CLA	C1D-C2D	-2.12	1.41	1.45
27	A	803	CLA	C1D-C2D	-2.12	1.41	1.45
27	7	304	CLA	C3D-C4D	-2.12	1.39	1.44
27	A	818	CLA	C1D-C2D	-2.12	1.41	1.45
27	7	312	CLA	C3D-C4D	-2.12	1.39	1.44
27	K	102	CLA	C3D-C4D	-2.12	1.39	1.44
27	A	844	CLA	C1D-C2D	-2.12	1.41	1.45
27	4	601	CLA	C1D-C2D	-2.11	1.41	1.45
27	B	841	CLA	C1D-C2D	-2.11	1.41	1.45
27	1	611	CLA	C3D-C4D	-2.11	1.39	1.44
27	2	607	CLA	C3D-C4D	-2.11	1.39	1.44
27	4	606	CLA	C3D-C4D	-2.11	1.39	1.44
27	8	608	CLA	C3D-C4D	-2.11	1.39	1.44
31	5	618	IHT	C18-C07	2.11	1.52	1.45
27	6	612	CLA	C3D-C4D	-2.11	1.39	1.44
27	A	807	CLA	C3D-C4D	-2.11	1.39	1.44
27	4	601	CLA	C3D-C4D	-2.11	1.39	1.44
27	Z	310	CLA	C1D-C2D	-2.11	1.41	1.45
27	a	605	CLA	C1D-C2D	-2.11	1.41	1.45
27	5	605	CLA	C3D-C4D	-2.11	1.39	1.44
27	O	204	CLA	C1D-C2D	-2.11	1.41	1.45
27	B	806	CLA	C3D-C4D	-2.11	1.39	1.44
28	7	311	KC2	C4D-CHA	-2.11	1.42	1.45
27	1	601	CLA	C1D-C2D	-2.11	1.41	1.45
27	2	601	CLA	C1D-C2D	-2.11	1.41	1.45
27	1	606	CLA	C3D-C4D	-2.11	1.39	1.44
27	2	601	CLA	C3D-C4D	-2.11	1.39	1.44
27	O	204	CLA	C3D-C4D	-2.11	1.39	1.44
27	A	828	CLA	C3D-C4D	-2.11	1.39	1.44
27	7	305	CLA	C3D-C4D	-2.11	1.39	1.44
27	9	603	CLA	C3D-C4D	-2.11	1.39	1.44
27	A	822	CLA	C3D-C4D	-2.11	1.39	1.44
27	1	612	CLA	C3D-C4D	-2.11	1.39	1.44
27	A	812	CLA	C3D-C4D	-2.11	1.39	1.44
27	B	805	CLA	C3D-C4D	-2.11	1.39	1.44
27	5	607	CLA	C3D-C4D	-2.10	1.39	1.44
27	9	604	CLA	C3D-C4D	-2.10	1.39	1.44
27	9	608	CLA	C3D-C4D	-2.10	1.39	1.44
27	7	308	CLA	C3D-C4D	-2.10	1.39	1.44
27	A	832	CLA	C3D-C4D	-2.10	1.39	1.44
27	4	608	CLA	C3D-C4D	-2.10	1.39	1.44
27	A	808	CLA	C3D-C4D	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	9	607	CLA	C3D-C4D	-2.10	1.39	1.44
27	B	825	CLA	C3D-C4D	-2.10	1.39	1.44
27	5	613	CLA	C3D-C4D	-2.10	1.39	1.44
27	B	801	CLA	C3D-C4D	-2.10	1.39	1.44
27	a	611	CLA	C3D-C4D	-2.10	1.39	1.44
27	A	821	CLA	C1D-C2D	-2.10	1.41	1.45
27	L	201	CLA	C3D-C4D	-2.10	1.39	1.44
27	b	601	CLA	C3D-C4D	-2.10	1.39	1.44
27	B	811	CLA	C1D-C2D	-2.10	1.41	1.45
27	7	313	CLA	C3D-C4D	-2.10	1.39	1.44
27	A	804	CLA	C3D-C4D	-2.10	1.39	1.44
39	B	848	DGD	O1G-C1G	-2.10	1.40	1.45
27	2	607	CLA	C1D-C2D	-2.10	1.41	1.45
27	A	806	CLA	C3D-C4D	-2.10	1.39	1.44
27	B	812	CLA	C3D-C4D	-2.10	1.39	1.44
27	5	608	CLA	C1D-C2D	-2.10	1.41	1.45
27	A	834	CLA	C3D-C4D	-2.10	1.39	1.44
28	3	606	KC2	C4D-CHA	-2.10	1.42	1.45
27	B	834	CLA	C3D-C4D	-2.10	1.39	1.44
27	3	601	CLA	C3D-C4D	-2.10	1.39	1.44
27	1	601	CLA	C3D-C4D	-2.10	1.39	1.44
27	7	309	CLA	C3D-C4D	-2.10	1.39	1.44
27	2	603	CLA	C3D-C4D	-2.09	1.39	1.44
27	O	203	CLA	C3D-C4D	-2.09	1.39	1.44
27	B	810	CLA	C3D-C4D	-2.09	1.39	1.44
27	O	202	CLA	C3D-C4D	-2.09	1.39	1.44
27	2	606	CLA	C3D-C4D	-2.09	1.39	1.44
27	7	306	CLA	C3D-C4D	-2.09	1.39	1.44
27	9	609	CLA	C3D-C4D	-2.09	1.39	1.44
27	A	842	CLA	C3D-C4D	-2.09	1.39	1.44
27	K	101	CLA	C3D-C4D	-2.09	1.39	1.44
27	9	601	CLA	C3D-C4D	-2.09	1.39	1.44
27	6	604	CLA	C3D-C4D	-2.09	1.39	1.44
27	B	814	CLA	C3D-C4D	-2.09	1.39	1.44
27	B	804	CLA	C3D-C4D	-2.09	1.39	1.44
27	6	607	CLA	C3D-C4D	-2.09	1.39	1.44
27	9	612	CLA	C3D-C4D	-2.09	1.39	1.44
27	A	805	CLA	C1D-C2D	-2.09	1.41	1.45
27	3	609	CLA	C3D-C4D	-2.09	1.39	1.44
27	B	809	CLA	C3D-C4D	-2.08	1.39	1.44
27	A	835	CLA	C3D-C4D	-2.08	1.39	1.44
27	1	609	CLA	C3D-C4D	-2.08	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	613	CLA	C3D-C4D	-2.08	1.39	1.44
27	A	825	CLA	C3D-C4D	-2.08	1.39	1.44
27	7	302	CLA	C3D-C4D	-2.08	1.39	1.44
27	8	602	CLA	C3D-C4D	-2.08	1.39	1.44
27	8	606	CLA	C3D-C4D	-2.08	1.39	1.44
27	a	608	CLA	C3D-C4D	-2.08	1.39	1.44
27	9	614	CLA	C3D-C4D	-2.08	1.39	1.44
27	3	603	CLA	C3D-C4D	-2.07	1.39	1.44
27	8	605	CLA	C3D-C4D	-2.07	1.39	1.44
27	B	803	CLA	C3D-C4D	-2.07	1.39	1.44
27	Z	301	CLA	C3D-C4D	-2.07	1.39	1.44
27	a	601	CLA	C3D-C4D	-2.06	1.39	1.44
27	1	607	CLA	C3D-C4D	-2.06	1.39	1.44
33	a	617	LHG	O7-C5	-2.06	1.41	1.46
27	b	611	CLA	C3D-C4D	-2.06	1.39	1.44
39	B	848	DGD	O2G-C2G	-2.06	1.41	1.46
27	A	837	CLA	C3D-C4D	-2.06	1.39	1.44
28	b	605	KC2	C4D-ND	2.06	1.37	1.35
27	5	601	CLA	C1D-C2D	-2.05	1.41	1.45
27	2	611	CLA	C3D-C4D	-2.05	1.39	1.44
33	7	319	LHG	O7-C5	-2.05	1.41	1.46
27	B	841	CLA	C3D-C4D	-2.05	1.39	1.44
27	b	608	CLA	C3D-C4D	-2.05	1.39	1.44
33	2	619	LHG	O7-C5	-2.05	1.41	1.46
27	8	604	CLA	C3D-C4D	-2.05	1.39	1.44
27	A	823	CLA	C3D-C4D	-2.04	1.39	1.44
31	9	619	IHT	C18-C07	2.04	1.52	1.45
27	B	829	CLA	C1D-C2D	-2.04	1.41	1.45
27	9	613	CLA	C3D-C4D	-2.04	1.39	1.44
27	B	823	CLA	C3D-C4D	-2.04	1.39	1.44
28	a	609	KC2	C4D-ND	2.04	1.37	1.35
33	5	619	LHG	O7-C5	-2.03	1.41	1.46
27	5	611	CLA	C3D-C4D	-2.03	1.39	1.44
32	3	618	LMG	O7-C8	-2.03	1.41	1.46
27	A	810	CLA	C3D-C4D	-2.03	1.39	1.44
27	F	204	CLA	C3D-C4D	-2.03	1.39	1.44
32	8	614	LMG	O7-C8	-2.02	1.41	1.46
27	B	802	CLA	C3D-C4D	-2.02	1.39	1.44
33	4	620	LHG	P-O6	2.02	1.67	1.59
33	2	620	LHG	O7-C5	-2.01	1.41	1.46
31	1	618	IHT	C18-C07	2.01	1.52	1.45
33	b	616	LHG	P-O6	2.00	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	618	LHG	P-O6	2.00	1.67	1.59

All (2443) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	609	IHT	C02-C07-C10	-10.15	108.32	122.61
31	9	619	IHT	C02-C07-C10	-10.12	108.35	122.61
31	L	204	IHT	C02-C07-C10	-9.21	109.64	122.61
31	5	618	IHT	C02-C07-C10	-8.96	110.00	122.61
31	6	616	IHT	C02-C07-C10	-8.07	111.24	122.61
31	2	616	IHT	C02-C07-C10	-7.88	111.51	122.61
31	a	616	IHT	C02-C07-C10	-7.80	111.63	122.61
31	Z	302	IHT	C18-C07-C10	-6.92	104.69	121.46
31	1	618	IHT	C02-C07-C10	-6.90	112.89	122.61
27	B	835	CLA	C4A-NA-C1A	-6.90	103.60	106.71
27	A	843	CLA	C4A-NA-C1A	-6.81	103.64	106.71
27	B	824	CLA	C4A-NA-C1A	-6.54	103.77	106.71
27	6	602	CLA	C4A-NA-C1A	-6.51	103.78	106.71
27	A	809	CLA	C4A-NA-C1A	-6.51	103.78	106.71
27	A	812	CLA	C4A-NA-C1A	-6.47	103.80	106.71
27	5	608	CLA	C1D-ND-C4D	-6.45	101.75	106.33
27	A	817	CLA	C4A-NA-C1A	-6.43	103.81	106.71
27	9	614	CLA	C4A-NA-C1A	-6.40	103.83	106.71
27	R	202	CLA	C4A-NA-C1A	-6.40	103.83	106.71
27	A	814	CLA	C1D-ND-C4D	-6.31	101.85	106.33
27	A	811	CLA	C4A-NA-C1A	-6.31	103.87	106.71
27	5	601	CLA	C1D-ND-C4D	-6.31	101.85	106.33
27	5	604	CLA	C1D-ND-C4D	-6.30	101.86	106.33
27	a	604	CLA	C1D-ND-C4D	-6.30	101.86	106.33
27	O	204	CLA	C1D-ND-C4D	-6.30	101.86	106.33
27	5	601	CLA	C4A-NA-C1A	-6.28	103.88	106.71
27	7	303	CLA	C1D-ND-C4D	-6.28	101.87	106.33
27	A	836	CLA	C1D-ND-C4D	-6.26	101.89	106.33
27	B	829	CLA	C1D-ND-C4D	-6.26	101.89	106.33
27	8	601	CLA	C1D-ND-C4D	-6.26	101.89	106.33
27	9	604	CLA	C1D-ND-C4D	-6.25	101.89	106.33
27	8	603	CLA	C1D-ND-C4D	-6.25	101.90	106.33
27	K	102	CLA	C1D-ND-C4D	-6.25	101.90	106.33
27	A	821	CLA	C1D-ND-C4D	-6.24	101.90	106.33
27	A	813	CLA	C1D-ND-C4D	-6.23	101.91	106.33
27	9	609	CLA	C1D-ND-C4D	-6.23	101.91	106.33
27	b	607	CLA	C1D-ND-C4D	-6.22	101.92	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	608	CLA	C1D-ND-C4D	-6.21	101.92	106.33
27	a	610	CLA	C1D-ND-C4D	-6.21	101.93	106.33
27	9	611	CLA	C1D-ND-C4D	-6.20	101.93	106.33
27	6	601	CLA	C1D-ND-C4D	-6.20	101.93	106.33
27	7	304	CLA	C1D-ND-C4D	-6.20	101.93	106.33
27	2	602	CLA	C1D-ND-C4D	-6.20	101.93	106.33
27	Z	301	CLA	C1D-ND-C4D	-6.19	101.94	106.33
27	B	834	CLA	C1D-ND-C4D	-6.19	101.94	106.33
27	A	811	CLA	C1D-ND-C4D	-6.19	101.94	106.33
27	B	829	CLA	C4A-NA-C1A	-6.19	103.92	106.71
27	4	609	CLA	C1D-ND-C4D	-6.19	101.94	106.33
27	A	818	CLA	C1D-ND-C4D	-6.19	101.94	106.33
27	1	601	CLA	C4A-NA-C1A	-6.18	103.93	106.71
27	2	601	CLA	C4A-NA-C1A	-6.18	103.93	106.71
27	A	824	CLA	C1D-ND-C4D	-6.18	101.94	106.33
27	2	608	CLA	C1D-ND-C4D	-6.18	101.95	106.33
27	B	839	CLA	C1D-ND-C4D	-6.18	101.95	106.33
27	A	834	CLA	C1D-ND-C4D	-6.18	101.95	106.33
27	8	607	CLA	C1D-ND-C4D	-6.17	101.95	106.33
27	O	202	CLA	C4A-NA-C1A	-6.17	103.93	106.71
27	A	805	CLA	C1D-ND-C4D	-6.17	101.95	106.33
27	2	604	CLA	C1D-ND-C4D	-6.17	101.95	106.33
27	4	603	CLA	C1D-ND-C4D	-6.17	101.95	106.33
27	9	602	CLA	C1D-ND-C4D	-6.17	101.95	106.33
27	4	602	CLA	C1D-ND-C4D	-6.17	101.95	106.33
27	A	830	CLA	C1D-ND-C4D	-6.16	101.96	106.33
27	Z	304	CLA	C1D-ND-C4D	-6.16	101.96	106.33
27	B	812	CLA	C1D-ND-C4D	-6.16	101.96	106.33
27	3	610	CLA	C1D-ND-C4D	-6.15	101.96	106.33
27	4	607	CLA	C1D-ND-C4D	-6.15	101.96	106.33
27	3	605	CLA	C1D-ND-C4D	-6.15	101.97	106.33
27	3	609	CLA	C1D-ND-C4D	-6.15	101.97	106.33
27	A	829	CLA	C1D-ND-C4D	-6.15	101.97	106.33
27	A	815	CLA	C1D-ND-C4D	-6.15	101.97	106.33
27	3	612	CLA	C1D-ND-C4D	-6.15	101.97	106.33
27	A	819	CLA	C1D-ND-C4D	-6.14	101.97	106.33
27	B	837	CLA	C1D-ND-C4D	-6.14	101.97	106.33
27	1	604	CLA	C1D-ND-C4D	-6.14	101.97	106.33
27	1	611	CLA	C1D-ND-C4D	-6.14	101.97	106.33
27	A	842	CLA	C1D-ND-C4D	-6.14	101.97	106.33
27	3	604	CLA	C1D-ND-C4D	-6.14	101.97	106.33
27	L	203	CLA	C1D-ND-C4D	-6.14	101.97	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	612	CLA	C1D-ND-C4D	-6.14	101.98	106.33
27	O	203	CLA	C1D-ND-C4D	-6.14	101.98	106.33
31	A	854	IHT	C02-C07-C10	-6.14	113.97	122.61
27	3	608	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	L	202	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	A	803	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	3	611	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	5	603	CLA	C1D-ND-C4D	-6.13	101.98	106.33
27	1	609	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	3	602	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	9	603	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	7	306	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	1	606	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	8	606	CLA	C1D-ND-C4D	-6.12	101.99	106.33
27	A	807	CLA	C1D-ND-C4D	-6.11	101.99	106.33
27	J	102	CLA	C1D-ND-C4D	-6.11	101.99	106.33
27	7	312	CLA	C1D-ND-C4D	-6.11	101.99	106.33
27	B	838	CLA	C1D-ND-C4D	-6.11	101.99	106.33
27	A	833	CLA	C1D-ND-C4D	-6.11	102.00	106.33
27	b	601	CLA	C1D-ND-C4D	-6.11	102.00	106.33
27	2	609	CLA	C1D-ND-C4D	-6.11	102.00	106.33
27	b	610	CLA	C1D-ND-C4D	-6.10	102.00	106.33
27	6	603	CLA	C1D-ND-C4D	-6.10	102.00	106.33
27	6	608	CLA	C1D-ND-C4D	-6.09	102.01	106.33
27	8	608	CLA	C1D-ND-C4D	-6.09	102.01	106.33
27	a	607	CLA	C1D-ND-C4D	-6.09	102.01	106.33
27	3	605	CLA	C4A-NA-C1A	-6.09	103.97	106.71
27	1	613	CLA	C1D-ND-C4D	-6.09	102.01	106.33
27	A	820	CLA	C1D-ND-C4D	-6.09	102.01	106.33
27	B	811	CLA	C1D-ND-C4D	-6.09	102.01	106.33
27	A	825	CLA	C1D-ND-C4D	-6.08	102.02	106.33
27	A	835	CLA	C1D-ND-C4D	-6.08	102.02	106.33
27	B	815	CLA	C1D-ND-C4D	-6.08	102.02	106.33
27	9	601	CLA	C1D-ND-C4D	-6.08	102.02	106.33
27	5	602	CLA	C1D-ND-C4D	-6.07	102.02	106.33
27	7	305	CLA	C1D-ND-C4D	-6.07	102.03	106.33
27	A	839	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	B	830	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	5	609	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	9	614	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	Z	306	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	1	602	CLA	C1D-ND-C4D	-6.06	102.03	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	610	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	b	603	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	b	604	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	6	604	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	6	611	CLA	C1D-ND-C4D	-6.06	102.03	106.33
27	2	603	CLA	C1D-ND-C4D	-6.05	102.03	106.33
27	2	612	CLA	C1D-ND-C4D	-6.05	102.03	106.33
27	b	602	CLA	C1D-ND-C4D	-6.05	102.03	106.33
27	4	601	CLA	C1D-ND-C4D	-6.05	102.04	106.33
27	5	613	CLA	C1D-ND-C4D	-6.05	102.04	106.33
27	B	821	CLA	C1D-ND-C4D	-6.04	102.04	106.33
27	a	602	CLA	C1D-ND-C4D	-6.04	102.04	106.33
27	2	601	CLA	C1D-ND-C4D	-6.04	102.04	106.33
27	4	604	CLA	C1D-ND-C4D	-6.04	102.04	106.33
27	8	615	CLA	C1D-ND-C4D	-6.04	102.04	106.33
27	a	605	CLA	C1D-ND-C4D	-6.04	102.04	106.33
27	B	831	CLA	C1D-ND-C4D	-6.04	102.05	106.33
27	A	828	CLA	C1D-ND-C4D	-6.04	102.05	106.33
27	9	608	CLA	C1D-ND-C4D	-6.04	102.05	106.33
27	7	302	CLA	C1D-ND-C4D	-6.03	102.05	106.33
27	7	309	CLA	C1D-ND-C4D	-6.03	102.05	106.33
27	a	601	CLA	C1D-ND-C4D	-6.03	102.05	106.33
27	A	816	CLA	C1D-ND-C4D	-6.03	102.05	106.33
27	A	821	CLA	C4A-NA-C1A	-6.03	104.00	106.71
27	A	808	CLA	C1D-ND-C4D	-6.03	102.05	106.33
27	6	606	CLA	C1D-ND-C4D	-6.02	102.06	106.33
27	A	822	CLA	C1D-ND-C4D	-6.02	102.06	106.33
27	5	606	CLA	C1D-ND-C4D	-6.01	102.06	106.33
27	Z	305	CLA	C1D-ND-C4D	-6.01	102.06	106.33
27	7	310	CLA	C1D-ND-C4D	-6.01	102.06	106.33
27	B	819	CLA	C1D-ND-C4D	-6.01	102.07	106.33
27	B	820	CLA	C1D-ND-C4D	-6.01	102.07	106.33
27	7	308	CLA	C1D-ND-C4D	-6.00	102.07	106.33
27	B	818	CLA	C1D-ND-C4D	-6.00	102.07	106.33
27	9	606	CLA	C1D-ND-C4D	-6.00	102.07	106.33
27	4	608	CLA	C1D-ND-C4D	-6.00	102.07	106.33
27	Z	310	CLA	C1D-ND-C4D	-6.00	102.08	106.33
31	a	616	IHT	C41-C38-C35	-6.00	118.75	127.31
27	A	838	CLA	C1D-ND-C4D	-5.99	102.08	106.33
27	B	828	CLA	C1D-ND-C4D	-5.99	102.08	106.33
27	3	601	CLA	C1D-ND-C4D	-5.99	102.08	106.33
27	A	837	CLA	C1D-ND-C4D	-5.99	102.08	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	840	CLA	C1D-ND-C4D	-5.99	102.08	106.33
27	a	603	CLA	C1D-ND-C4D	-5.98	102.08	106.33
27	9	613	CLA	C1D-ND-C4D	-5.98	102.09	106.33
27	B	833	CLA	C1D-ND-C4D	-5.98	102.09	106.33
27	F	203	CLA	C1D-ND-C4D	-5.98	102.09	106.33
27	6	606	CLA	C4A-NA-C1A	-5.98	104.02	106.71
27	B	813	CLA	C1D-ND-C4D	-5.98	102.09	106.33
27	1	601	CLA	C1D-ND-C4D	-5.98	102.09	106.33
27	B	823	CLA	C1D-ND-C4D	-5.98	102.09	106.33
27	F	202	CLA	C1D-ND-C4D	-5.97	102.09	106.33
27	1	603	CLA	C1D-ND-C4D	-5.97	102.09	106.33
27	5	611	CLA	C1D-ND-C4D	-5.97	102.09	106.33
27	6	602	CLA	C1D-ND-C4D	-5.97	102.09	106.33
27	3	603	CLA	C1D-ND-C4D	-5.97	102.09	106.33
27	B	810	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	a	608	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	K	101	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	6	607	CLA	C1D-ND-C4D	-5.96	102.10	106.33
27	9	605	CLA	C1D-ND-C4D	-5.94	102.12	106.33
27	A	802	CLA	C1D-ND-C4D	-5.94	102.12	106.33
27	B	841	CLA	C1D-ND-C4D	-5.94	102.12	106.33
27	2	607	CLA	C1D-ND-C4D	-5.94	102.12	106.33
27	B	817	CLA	C1D-ND-C4D	-5.93	102.12	106.33
27	4	606	CLA	C1D-ND-C4D	-5.93	102.12	106.33
27	6	609	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	B	804	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	4	611	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	B	832	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	A	832	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	B	816	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	B	814	CLA	C1D-ND-C4D	-5.92	102.13	106.33
27	5	607	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	3	607	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	B	805	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	B	822	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	1	607	CLA	C1D-ND-C4D	-5.91	102.14	106.33
27	O	202	CLA	C1D-ND-C4D	-5.90	102.14	106.33
27	2	606	CLA	C1D-ND-C4D	-5.90	102.14	106.33
27	9	612	CLA	C1D-ND-C4D	-5.90	102.15	106.33
27	A	803	CLA	C4A-NA-C1A	-5.89	104.06	106.71
27	b	608	CLA	C1D-ND-C4D	-5.89	102.15	106.33
27	A	817	CLA	C1D-ND-C4D	-5.88	102.16	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	836	CLA	C1D-ND-C4D	-5.87	102.16	106.33
27	A	804	CLA	C1D-ND-C4D	-5.85	102.18	106.33
27	2	605	CLA	C1D-ND-C4D	-5.85	102.18	106.33
27	5	605	CLA	C1D-ND-C4D	-5.85	102.18	106.33
27	F	204	CLA	C1D-ND-C4D	-5.85	102.18	106.33
27	b	611	CLA	C1D-ND-C4D	-5.85	102.18	106.33
27	B	826	CLA	C1D-ND-C4D	-5.84	102.18	106.33
27	6	612	CLA	C1D-ND-C4D	-5.84	102.19	106.33
27	1	605	CLA	C1D-ND-C4D	-5.84	102.19	106.33
27	A	829	CLA	C4A-NA-C1A	-5.84	104.08	106.71
27	B	825	CLA	C1D-ND-C4D	-5.83	102.19	106.33
27	2	607	CLA	C4A-NA-C1A	-5.83	104.08	106.71
27	A	809	CLA	C1D-ND-C4D	-5.83	102.19	106.33
27	O	201	CLA	C1D-ND-C4D	-5.83	102.19	106.33
27	A	823	CLA	C1D-ND-C4D	-5.82	102.20	106.33
27	B	808	CLA	C1D-ND-C4D	-5.82	102.20	106.33
27	7	313	CLA	C1D-ND-C4D	-5.82	102.20	106.33
27	B	830	CLA	C4A-NA-C1A	-5.81	104.09	106.71
27	1	613	CLA	C4A-NA-C1A	-5.81	104.09	106.71
27	A	831	CLA	C1D-ND-C4D	-5.81	102.21	106.33
27	b	606	CLA	C1D-ND-C4D	-5.81	102.21	106.33
27	2	611	CLA	C1D-ND-C4D	-5.80	102.22	106.33
27	A	840	CLA	C1D-ND-C4D	-5.80	102.22	106.33
31	Z	302	IHT	C02-C07-C10	-5.80	114.45	122.61
27	B	809	CLA	C1D-ND-C4D	-5.80	102.22	106.33
27	L	201	CLA	C1D-ND-C4D	-5.80	102.22	106.33
27	6	605	CLA	C1D-ND-C4D	-5.79	102.22	106.33
27	B	835	CLA	C1D-ND-C4D	-5.78	102.23	106.33
27	B	827	CLA	C1D-ND-C4D	-5.77	102.23	106.33
27	B	803	CLA	C1D-ND-C4D	-5.77	102.24	106.33
27	B	809	CLA	C4A-NA-C1A	-5.76	104.11	106.71
27	A	844	CLA	C1D-ND-C4D	-5.76	102.24	106.33
27	1	612	CLA	C1D-ND-C4D	-5.76	102.24	106.33
27	B	806	CLA	C1D-ND-C4D	-5.76	102.25	106.33
27	a	611	CLA	C1D-ND-C4D	-5.75	102.25	106.33
27	7	308	CLA	C4A-NA-C1A	-5.75	104.12	106.71
27	7	313	CLA	C4A-NA-C1A	-5.75	104.12	106.71
27	a	606	CLA	C1D-ND-C4D	-5.75	102.25	106.33
27	B	815	CLA	C4A-NA-C1A	-5.74	104.12	106.71
27	A	827	CLA	C1D-ND-C4D	-5.74	102.26	106.33
27	3	602	CLA	C4A-NA-C1A	-5.74	104.13	106.71
27	A	840	CLA	C4A-NA-C1A	-5.72	104.13	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	9	605	CLA	C4A-NA-C1A	-5.71	104.14	106.71
27	8	605	CLA	C1D-ND-C4D	-5.70	102.28	106.33
27	A	810	CLA	C1D-ND-C4D	-5.70	102.28	106.33
27	1	609	CLA	C4A-NA-C1A	-5.69	104.15	106.71
27	7	310	CLA	C4A-NA-C1A	-5.69	104.15	106.71
27	B	827	CLA	C4A-NA-C1A	-5.69	104.15	106.71
27	2	609	CLA	C4A-NA-C1A	-5.68	104.15	106.71
27	4	602	CLA	C4A-NA-C1A	-5.68	104.15	106.71
27	a	607	CLA	C4A-NA-C1A	-5.67	104.16	106.71
27	B	824	CLA	C1D-ND-C4D	-5.67	102.31	106.33
27	B	811	CLA	C4A-NA-C1A	-5.67	104.16	106.71
27	A	812	CLA	C1D-ND-C4D	-5.66	102.31	106.33
27	8	604	CLA	C1D-ND-C4D	-5.65	102.32	106.33
27	a	606	CLA	C4A-NA-C1A	-5.63	104.18	106.71
27	B	819	CLA	C4A-NA-C1A	-5.63	104.18	106.71
27	R	202	CLA	C1D-ND-C4D	-5.62	102.34	106.33
27	B	810	CLA	C4A-NA-C1A	-5.62	104.18	106.71
27	A	843	CLA	C1D-ND-C4D	-5.62	102.34	106.33
27	9	607	CLA	C1D-ND-C4D	-5.62	102.34	106.33
27	A	830	CLA	C4A-NA-C1A	-5.61	104.18	106.71
27	2	602	CLA	C4A-NA-C1A	-5.60	104.19	106.71
27	B	821	CLA	C4A-NA-C1A	-5.60	104.19	106.71
27	1	607	CLA	C4A-NA-C1A	-5.59	104.19	106.71
27	a	602	CLA	C4A-NA-C1A	-5.59	104.19	106.71
27	8	602	CLA	C1D-ND-C4D	-5.58	102.37	106.33
27	B	812	CLA	C4A-NA-C1A	-5.58	104.20	106.71
27	A	841	CLA	C1D-ND-C4D	-5.57	102.38	106.33
27	A	842	CLA	C4A-NA-C1A	-5.57	104.20	106.71
27	B	839	CLA	C4A-NA-C1A	-5.57	104.20	106.71
27	A	801	CLA	CHD-C1D-ND	-5.56	119.34	124.45
27	6	609	CLA	C4A-NA-C1A	-5.56	104.21	106.71
27	B	807	CLA	C1D-ND-C4D	-5.56	102.39	106.33
27	9	602	CLA	C4A-NA-C1A	-5.55	104.21	106.71
27	Z	306	CLA	C4A-NA-C1A	-5.55	104.21	106.71
27	B	818	CLA	C4A-NA-C1A	-5.53	104.22	106.71
27	a	604	CLA	C4A-NA-C1A	-5.53	104.22	106.71
27	5	605	CLA	C4A-NA-C1A	-5.52	104.22	106.71
27	A	806	CLA	C4A-NA-C1A	-5.52	104.22	106.71
27	A	806	CLA	C1D-ND-C4D	-5.52	102.42	106.33
27	6	604	CLA	C4A-NA-C1A	-5.51	104.23	106.71
27	J	102	CLA	C4A-NA-C1A	-5.49	104.24	106.71
27	7	305	CLA	C4A-NA-C1A	-5.49	104.24	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	604	CLA	C4A-NA-C1A	-5.47	104.25	106.71
27	6	603	CLA	C4A-NA-C1A	-5.47	104.25	106.71
27	L	201	CLA	C4A-NA-C1A	-5.44	104.26	106.71
27	B	817	CLA	C4A-NA-C1A	-5.44	104.26	106.71
27	A	822	CLA	C4A-NA-C1A	-5.43	104.26	106.71
27	b	602	CLA	C4A-NA-C1A	-5.43	104.26	106.71
27	6	611	CLA	C4A-NA-C1A	-5.41	104.27	106.71
27	B	814	CLA	C4A-NA-C1A	-5.41	104.27	106.71
27	1	603	CLA	C4A-NA-C1A	-5.41	104.28	106.71
27	5	606	CLA	C4A-NA-C1A	-5.40	104.28	106.71
27	8	604	CLA	C4A-NA-C1A	-5.40	104.28	106.71
27	5	608	CLA	C4A-NA-C1A	-5.39	104.28	106.71
27	4	603	CLA	C4A-NA-C1A	-5.38	104.29	106.71
27	3	603	CLA	C4A-NA-C1A	-5.36	104.30	106.71
27	2	605	CLA	C4A-NA-C1A	-5.36	104.30	106.71
27	A	809	CLA	CHD-C1D-ND	-5.36	119.53	124.45
27	A	805	CLA	C4A-NA-C1A	-5.35	104.30	106.71
27	A	826	CLA	C1D-ND-C4D	-5.35	102.54	106.33
27	7	303	CLA	C4A-NA-C1A	-5.34	104.30	106.71
27	A	820	CLA	C4A-NA-C1A	-5.34	104.30	106.71
27	1	606	CLA	C4A-NA-C1A	-5.34	104.31	106.71
27	A	818	CLA	C4A-NA-C1A	-5.33	104.31	106.71
27	O	204	CLA	C4A-NA-C1A	-5.33	104.31	106.71
27	b	603	CLA	C4A-NA-C1A	-5.33	104.31	106.71
27	9	608	CLA	C4A-NA-C1A	-5.32	104.31	106.71
27	1	611	CLA	C4A-NA-C1A	-5.31	104.32	106.71
27	2	604	CLA	C4A-NA-C1A	-5.31	104.32	106.71
27	8	615	CLA	C4A-NA-C1A	-5.31	104.32	106.71
27	B	816	CLA	C4A-NA-C1A	-5.30	104.32	106.71
27	9	603	CLA	C4A-NA-C1A	-5.28	104.33	106.71
35	M	101	8CT	C30-C31-C32	-5.28	114.97	121.47
27	A	839	CLA	C4A-NA-C1A	-5.28	104.33	106.71
27	4	611	CLA	C4A-NA-C1A	-5.28	104.33	106.71
27	A	819	CLA	C4A-NA-C1A	-5.26	104.34	106.71
27	A	826	CLA	C4A-NA-C1A	-5.26	104.34	106.71
27	A	813	CLA	C4A-NA-C1A	-5.25	104.34	106.71
27	8	605	CLA	CHD-C1D-ND	-5.25	119.63	124.45
27	B	831	CLA	CHD-C1D-ND	-5.25	119.63	124.45
27	6	601	CLA	C4A-NA-C1A	-5.25	104.35	106.71
27	A	814	CLA	CHD-C1D-ND	-5.25	119.63	124.45
27	A	808	CLA	C4A-NA-C1A	-5.24	104.35	106.71
27	6	612	CLA	C4A-NA-C1A	-5.24	104.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	9	601	CLA	C4A-NA-C1A	-5.23	104.35	106.71
31	9	619	IHT	C30-C27-C23	-5.23	119.85	127.31
27	2	611	CLA	C4A-NA-C1A	-5.22	104.36	106.71
27	2	612	CLA	C4A-NA-C1A	-5.22	104.36	106.71
27	A	833	CLA	C4A-NA-C1A	-5.22	104.36	106.71
27	A	844	CLA	C4A-NA-C1A	-5.22	104.36	106.71
27	5	601	CLA	CHD-C1D-ND	-5.22	119.66	124.45
27	B	802	CLA	C1D-ND-C4D	-5.22	102.63	106.33
27	3	607	CLA	C4A-NA-C1A	-5.22	104.36	106.71
27	B	829	CLA	CHD-C1D-ND	-5.22	119.66	124.45
27	6	608	CLA	C4A-NA-C1A	-5.21	104.36	106.71
27	B	806	CLA	C4A-NA-C1A	-5.21	104.36	106.71
27	B	805	CLA	C4A-NA-C1A	-5.20	104.37	106.71
27	A	841	CLA	C4A-NA-C1A	-5.19	104.37	106.71
27	A	803	CLA	CHD-C1D-ND	-5.18	119.69	124.45
27	A	818	CLA	CHD-C1D-ND	-5.18	119.69	124.45
27	B	801	CLA	C1D-ND-C4D	-5.18	102.66	106.33
27	A	821	CLA	CHD-C1D-ND	-5.18	119.70	124.45
27	F	202	CLA	CHD-C1D-ND	-5.18	119.70	124.45
27	B	838	CLA	C4A-NA-C1A	-5.17	104.38	106.71
27	8	603	CLA	C4A-NA-C1A	-5.17	104.38	106.71
27	A	805	CLA	CHD-C1D-ND	-5.17	119.70	124.45
27	O	201	CLA	CHD-C1D-ND	-5.17	119.70	124.45
27	9	604	CLA	C4A-NA-C1A	-5.17	104.38	106.71
27	B	832	CLA	C4A-NA-C1A	-5.16	104.39	106.71
27	A	824	CLA	C4A-NA-C1A	-5.16	104.39	106.71
27	B	802	CLA	CHD-C1D-ND	-5.15	119.72	124.45
27	5	612	CLA	C4A-NA-C1A	-5.15	104.39	106.71
27	4	603	CLA	CHD-C1D-ND	-5.15	119.72	124.45
27	5	602	CLA	C4A-NA-C1A	-5.15	104.39	106.71
27	8	608	CLA	C4A-NA-C1A	-5.15	104.39	106.71
27	3	608	CLA	C4A-NA-C1A	-5.15	104.39	106.71
27	4	607	CLA	C4A-NA-C1A	-5.15	104.39	106.71
27	a	605	CLA	CHD-C1D-ND	-5.15	119.72	124.45
27	L	203	CLA	C4A-NA-C1A	-5.14	104.39	106.71
27	5	608	CLA	CHD-C1D-ND	-5.14	119.73	124.45
27	B	830	CLA	CHD-C1D-ND	-5.14	119.73	124.45
27	B	807	CLA	C4A-NA-C1A	-5.14	104.40	106.71
27	A	804	CLA	C4A-NA-C1A	-5.13	104.40	106.71
27	A	824	CLA	CHD-C1D-ND	-5.13	119.74	124.45
31	a	616	IHT	C18-C07-C10	-5.13	109.04	121.46
27	2	606	CLA	C4A-NA-C1A	-5.13	104.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	310	CLA	C4A-NA-C1A	-5.12	104.40	106.71
27	b	608	CLA	C4A-NA-C1A	-5.12	104.40	106.71
27	8	606	CLA	CHD-C1D-ND	-5.12	119.75	124.45
27	Z	305	CLA	C4A-NA-C1A	-5.12	104.41	106.71
27	B	837	CLA	CHD-C1D-ND	-5.12	119.75	124.45
27	2	604	CLA	CHD-C1D-ND	-5.11	119.75	124.45
27	A	834	CLA	CHD-C1D-ND	-5.11	119.76	124.45
27	L	202	CLA	CHD-C1D-ND	-5.11	119.76	124.45
27	B	804	CLA	C4A-NA-C1A	-5.11	104.41	106.71
27	O	201	CLA	C4A-NA-C1A	-5.11	104.41	106.71
27	B	814	CLA	CHD-C1D-ND	-5.11	119.76	124.45
27	6	607	CLA	C4A-NA-C1A	-5.10	104.41	106.71
27	A	827	CLA	C4A-NA-C1A	-5.10	104.41	106.71
27	A	840	CLA	CHD-C1D-ND	-5.10	119.76	124.45
27	2	607	CLA	CHD-C1D-ND	-5.10	119.76	124.45
27	B	828	CLA	CHD-C1D-ND	-5.10	119.76	124.45
27	3	610	CLA	CHD-C1D-ND	-5.10	119.77	124.45
27	5	612	CLA	CHD-C1D-ND	-5.10	119.77	124.45
27	B	832	CLA	CHD-C1D-ND	-5.10	119.77	124.45
27	7	308	CLA	CHD-C1D-ND	-5.10	119.77	124.45
27	6	605	CLA	C4A-NA-C1A	-5.10	104.42	106.71
27	5	609	CLA	C4A-NA-C1A	-5.09	104.42	106.71
27	A	817	CLA	CHD-C1D-ND	-5.09	119.77	124.45
27	A	827	CLA	CHD-C1D-ND	-5.09	119.77	124.45
27	A	844	CLA	CHD-C1D-ND	-5.09	119.78	124.45
27	6	603	CLA	CHD-C1D-ND	-5.09	119.78	124.45
27	3	604	CLA	C4A-NA-C1A	-5.09	104.42	106.71
27	B	827	CLA	CHD-C1D-ND	-5.08	119.78	124.45
27	9	604	CLA	CHD-C1D-ND	-5.08	119.79	124.45
27	9	606	CLA	C4A-NA-C1A	-5.08	104.42	106.71
27	b	607	CLA	C4A-NA-C1A	-5.08	104.42	106.71
27	4	608	CLA	C4A-NA-C1A	-5.07	104.43	106.71
27	1	602	CLA	C4A-NA-C1A	-5.07	104.43	106.71
27	7	304	CLA	CHD-C1D-ND	-5.07	119.80	124.45
27	9	605	CLA	CHD-C1D-ND	-5.06	119.80	124.45
27	2	608	CLA	C4A-NA-C1A	-5.06	104.43	106.71
27	B	834	CLA	C4A-NA-C1A	-5.06	104.43	106.71
27	4	601	CLA	C4A-NA-C1A	-5.06	104.43	106.71
27	5	607	CLA	C4A-NA-C1A	-5.06	104.43	106.71
27	b	601	CLA	CHD-C1D-ND	-5.06	119.81	124.45
27	9	611	CLA	C4A-NA-C1A	-5.05	104.43	106.71
27	A	833	CLA	CHD-C1D-ND	-5.05	119.81	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	609	CLA	CHD-C1D-ND	-5.05	119.81	124.45
27	8	605	CLA	C4A-NA-C1A	-5.05	104.44	106.71
27	O	202	CLA	CHD-C1D-ND	-5.05	119.82	124.45
27	O	204	CLA	CHD-C1D-ND	-5.05	119.82	124.45
27	1	601	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	B	818	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	3	605	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	B	817	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	9	607	CLA	C4A-NA-C1A	-5.04	104.44	106.71
27	1	608	CLA	C4A-NA-C1A	-5.04	104.44	106.71
27	B	840	CLA	CHD-C1D-ND	-5.04	119.82	124.45
27	A	815	CLA	C4A-NA-C1A	-5.04	104.44	106.71
27	a	603	CLA	C4A-NA-C1A	-5.04	104.44	106.71
31	5	618	IHT	C06-C09-C10	5.04	123.07	114.08
27	5	602	CLA	CHD-C1D-ND	-5.04	119.83	124.45
27	B	811	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	A	843	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	A	841	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	B	803	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	B	802	CLA	C4A-NA-C1A	-5.03	104.45	106.71
27	2	602	CLA	CHD-C1D-ND	-5.03	119.83	124.45
27	J	102	CLA	CHD-C1D-ND	-5.02	119.84	124.45
27	b	601	CLA	C4A-NA-C1A	-5.02	104.45	106.71
27	a	611	CLA	C4A-NA-C1A	-5.02	104.45	106.71
27	b	611	CLA	C4A-NA-C1A	-5.02	104.45	106.71
27	A	819	CLA	CHD-C1D-ND	-5.02	119.84	124.45
27	a	605	CLA	C4A-NA-C1A	-5.02	104.45	106.71
27	8	615	CLA	CHD-C1D-ND	-5.02	119.84	124.45
27	5	604	CLA	CHD-C1D-ND	-5.02	119.84	124.45
27	A	813	CLA	CHD-C1D-ND	-5.01	119.85	124.45
27	b	610	CLA	CHD-C1D-ND	-5.01	119.85	124.45
27	5	613	CLA	C4A-NA-C1A	-5.01	104.45	106.71
27	B	826	CLA	CHD-C1D-ND	-5.01	119.85	124.45
27	8	603	CLA	CHD-C1D-ND	-5.01	119.85	124.45
27	A	811	CLA	CHD-C1D-ND	-5.01	119.85	124.45
27	6	606	CLA	CHD-C1D-ND	-5.01	119.85	124.45
27	A	836	CLA	CHD-C1D-ND	-5.01	119.85	124.45
27	3	603	CLA	CHD-C1D-ND	-5.00	119.86	124.45
31	Z	302	IHT	C19-C10-C07	-5.00	118.91	124.53
27	8	608	CLA	CHD-C1D-ND	-5.00	119.86	124.45
27	a	610	CLA	CHD-C1D-ND	-5.00	119.86	124.45
27	A	828	CLA	CHD-C1D-ND	-4.99	119.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	603	CLA	CHD-C1D-ND	-4.99	119.86	124.45
27	6	604	CLA	CHD-C1D-ND	-4.99	119.87	124.45
27	A	825	CLA	CHD-C1D-ND	-4.99	119.87	124.45
27	B	806	CLA	CHD-C1D-ND	-4.99	119.87	124.45
27	2	612	CLA	CHD-C1D-ND	-4.99	119.87	124.45
27	8	601	CLA	CHD-C1D-ND	-4.99	119.87	124.45
27	A	837	CLA	CHD-C1D-ND	-4.98	119.88	124.45
35	A	847	8CT	C30-C31-C32	-4.98	115.34	121.47
27	F	202	CLA	C4A-NA-C1A	-4.97	104.47	106.71
27	a	604	CLA	CHD-C1D-ND	-4.97	119.88	124.45
27	Z	301	CLA	CHD-C1D-ND	-4.97	119.89	124.45
27	2	603	CLA	CHD-C1D-ND	-4.97	119.89	124.45
27	B	824	CLA	CHD-C1D-ND	-4.97	119.89	124.45
27	7	304	CLA	C4A-NA-C1A	-4.97	104.47	106.71
27	B	822	CLA	CHD-C1D-ND	-4.97	119.89	124.45
27	2	608	CLA	CHD-C1D-ND	-4.97	119.89	124.45
27	9	606	CLA	CHD-C1D-ND	-4.96	119.89	124.45
27	A	829	CLA	CHD-C1D-ND	-4.96	119.89	124.45
27	b	611	CLA	CHD-C1D-ND	-4.96	119.89	124.45
27	2	605	CLA	CHD-C1D-ND	-4.96	119.90	124.45
27	4	606	CLA	CHD-C1D-ND	-4.96	119.90	124.45
27	b	603	CLA	CHD-C1D-ND	-4.96	119.90	124.45
27	7	313	CLA	CHD-C1D-ND	-4.96	119.90	124.45
27	A	832	CLA	CHD-C1D-ND	-4.96	119.90	124.45
27	B	841	CLA	CHD-C1D-ND	-4.96	119.90	124.45
27	2	601	CLA	CHD-C1D-ND	-4.96	119.90	124.45
27	A	825	CLA	C4A-NA-C1A	-4.96	104.48	106.71
27	B	819	CLA	CHD-C1D-ND	-4.95	119.90	124.45
27	A	808	CLA	CHD-C1D-ND	-4.95	119.90	124.45
27	1	606	CLA	CHD-C1D-ND	-4.95	119.91	124.45
27	9	612	CLA	CHD-C1D-ND	-4.95	119.91	124.45
27	Z	306	CLA	CHD-C1D-ND	-4.95	119.91	124.45
27	F	203	CLA	CHD-C1D-ND	-4.95	119.91	124.45
31	L	204	IHT	C06-C09-C10	4.95	122.91	114.08
27	b	610	CLA	C4A-NA-C1A	-4.94	104.48	106.71
27	3	602	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	4	606	CLA	C4A-NA-C1A	-4.94	104.48	106.71
27	7	306	CLA	C4A-NA-C1A	-4.94	104.48	106.71
27	A	839	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	B	810	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	B	838	CLA	CHD-C1D-ND	-4.94	119.91	124.45
27	A	816	CLA	CHD-C1D-ND	-4.94	119.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	804	CLA	CHD-C1D-ND	-4.94	119.92	124.45
27	B	836	CLA	CHD-C1D-ND	-4.94	119.92	124.45
27	A	830	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	B	816	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	a	602	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	b	607	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	1	608	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	B	834	CLA	CHD-C1D-ND	-4.93	119.92	124.45
27	1	607	CLA	CHD-C1D-ND	-4.93	119.93	124.45
27	5	609	CLA	CHD-C1D-ND	-4.93	119.93	124.45
27	B	815	CLA	CHD-C1D-ND	-4.93	119.93	124.45
27	A	802	CLA	CHD-C1D-ND	-4.92	119.93	124.45
27	A	826	CLA	CHD-C1D-ND	-4.92	119.93	124.45
27	7	309	CLA	C4A-NA-C1A	-4.92	104.49	106.71
27	8	607	CLA	CHD-C1D-ND	-4.92	119.93	124.45
27	B	801	CLA	C4A-NA-C1A	-4.92	104.49	106.71
27	4	607	CLA	CHD-C1D-ND	-4.92	119.93	124.45
31	1	618	IHT	C06-C09-C10	4.92	122.86	114.08
27	4	611	CLA	CHD-C1D-ND	-4.92	119.94	124.45
27	9	603	CLA	CHD-C1D-ND	-4.92	119.94	124.45
27	Z	305	CLA	CHD-C1D-ND	-4.92	119.94	124.45
27	A	807	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	K	102	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	4	604	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	5	605	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	9	614	CLA	CHD-C1D-ND	-4.91	119.94	124.45
31	9	619	IHT	C18-C07-C10	-4.91	109.57	121.46
27	7	302	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	1	613	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	7	305	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	b	602	CLA	CHD-C1D-ND	-4.91	119.94	124.45
27	4	608	CLA	CHD-C1D-ND	-4.91	119.95	124.45
27	6	601	CLA	CHD-C1D-ND	-4.91	119.95	124.45
27	B	801	CLA	CHD-C1D-ND	-4.90	119.95	124.45
27	6	609	CLA	CHD-C1D-ND	-4.90	119.95	124.45
27	4	602	CLA	CHD-C1D-ND	-4.90	119.95	124.45
27	A	820	CLA	CHD-C1D-ND	-4.90	119.95	124.45
27	Z	310	CLA	CHD-C1D-ND	-4.90	119.95	124.45
27	B	841	CLA	C4A-NA-C1A	-4.90	104.50	106.71
27	a	608	CLA	C4A-NA-C1A	-4.90	104.50	106.71
27	5	607	CLA	CHD-C1D-ND	-4.90	119.95	124.45
27	a	601	CLA	CHD-C1D-ND	-4.90	119.95	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	812	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	A	802	CLA	C4A-NA-C1A	-4.89	104.51	106.71
27	3	610	CLA	C4A-NA-C1A	-4.89	104.51	106.71
27	5	603	CLA	C4A-NA-C1A	-4.89	104.51	106.71
27	B	826	CLA	C4A-NA-C1A	-4.89	104.51	106.71
27	B	809	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	3	607	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	6	607	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	B	820	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	7	312	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	2	606	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	9	602	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	b	608	CLA	CHD-C1D-ND	-4.89	119.96	124.45
27	O	203	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	4	609	CLA	C4A-NA-C1A	-4.88	104.51	106.71
27	5	613	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	6	612	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	B	835	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	5	606	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	2	611	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	B	808	CLA	CHD-C1D-ND	-4.88	119.97	124.45
27	A	838	CLA	C4A-NA-C1A	-4.87	104.52	106.71
27	3	612	CLA	CHD-C1D-ND	-4.87	119.98	124.45
27	B	805	CLA	CHD-C1D-ND	-4.87	119.98	124.45
27	B	833	CLA	CHD-C1D-ND	-4.87	119.98	124.45
27	2	603	CLA	C4A-NA-C1A	-4.87	104.52	106.71
31	6	616	IHT	C06-C09-C10	4.87	122.77	114.08
27	A	842	CLA	CHD-C1D-ND	-4.86	119.98	124.45
27	1	612	CLA	CHD-C1D-ND	-4.86	119.99	124.45
27	A	835	CLA	CHD-C1D-ND	-4.86	119.99	124.45
27	a	611	CLA	CHD-C1D-ND	-4.86	119.99	124.45
27	1	611	CLA	CHD-C1D-ND	-4.86	119.99	124.45
27	7	309	CLA	CHD-C1D-ND	-4.85	119.99	124.45
27	9	611	CLA	CHD-C1D-ND	-4.85	119.99	124.45
27	B	820	CLA	C4A-NA-C1A	-4.85	104.53	106.71
27	a	601	CLA	C4A-NA-C1A	-4.85	104.53	106.71
27	1	603	CLA	CHD-C1D-ND	-4.85	120.00	124.45
27	1	609	CLA	CHD-C1D-ND	-4.85	120.00	124.45
27	9	609	CLA	CHD-C1D-ND	-4.84	120.00	124.45
27	7	306	CLA	CHD-C1D-ND	-4.84	120.00	124.45
27	L	201	CLA	CHD-C1D-ND	-4.84	120.01	124.45
27	a	603	CLA	CHD-C1D-ND	-4.84	120.01	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	101	CLA	C4A-NA-C1A	-4.84	104.53	106.71
27	A	815	CLA	CHD-C1D-ND	-4.83	120.01	124.45
27	3	611	CLA	CHD-C1D-ND	-4.83	120.01	124.45
27	B	836	CLA	C4A-NA-C1A	-4.83	104.53	106.71
27	4	610	CLA	C4A-NA-C1A	-4.83	104.53	106.71
27	3	609	CLA	C4A-NA-C1A	-4.83	104.54	106.71
27	A	810	CLA	CHD-C1D-ND	-4.82	120.02	124.45
27	A	822	CLA	CHD-C1D-ND	-4.82	120.02	124.45
27	B	825	CLA	CHD-C1D-ND	-4.82	120.02	124.45
27	7	310	CLA	CHD-C1D-ND	-4.82	120.03	124.45
27	3	608	CLA	CHD-C1D-ND	-4.81	120.03	124.45
27	B	822	CLA	C4A-NA-C1A	-4.81	104.54	106.71
27	O	203	CLA	C4A-NA-C1A	-4.81	104.54	106.71
27	R	202	CLA	CHD-C1D-ND	-4.81	120.03	124.45
31	6	616	IHT	C19-C10-C07	-4.81	119.13	124.53
27	1	604	CLA	CHD-C1D-ND	-4.80	120.04	124.45
27	b	606	CLA	CHD-C1D-ND	-4.80	120.04	124.45
27	3	609	CLA	CHD-C1D-ND	-4.80	120.04	124.45
27	6	605	CLA	CHD-C1D-ND	-4.80	120.04	124.45
27	Z	304	CLA	CHD-C1D-ND	-4.80	120.04	124.45
27	B	833	CLA	C4A-NA-C1A	-4.80	104.55	106.71
27	4	610	CLA	CHD-C1D-ND	-4.80	120.05	124.45
27	7	303	CLA	CHD-C1D-ND	-4.79	120.05	124.45
27	8	602	CLA	CHD-C1D-ND	-4.79	120.05	124.45
27	8	607	CLA	C4A-NA-C1A	-4.79	104.55	106.71
27	1	605	CLA	C4A-NA-C1A	-4.79	104.55	106.71
27	6	611	CLA	CHD-C1D-ND	-4.79	120.06	124.45
27	L	203	CLA	CHD-C1D-ND	-4.78	120.06	124.45
27	7	312	CLA	C4A-NA-C1A	-4.78	104.56	106.71
27	B	840	CLA	C4A-NA-C1A	-4.78	104.56	106.71
27	9	609	CLA	C4A-NA-C1A	-4.78	104.56	106.71
27	4	609	CLA	CHD-C1D-ND	-4.78	120.06	124.45
27	B	837	CLA	C4A-NA-C1A	-4.78	104.56	106.71
27	A	804	CLA	CHD-C1D-ND	-4.77	120.07	124.45
27	4	604	CLA	C4A-NA-C1A	-4.77	104.56	106.71
27	9	613	CLA	CHD-C1D-ND	-4.77	120.07	124.45
27	B	821	CLA	CHD-C1D-ND	-4.77	120.07	124.45
27	6	602	CLA	CHD-C1D-ND	-4.77	120.07	124.45
27	a	607	CLA	CHD-C1D-ND	-4.77	120.08	124.45
27	F	203	CLA	C4A-NA-C1A	-4.76	104.56	106.71
27	B	812	CLA	CHD-C1D-ND	-4.76	120.08	124.45
27	1	604	CLA	C4A-NA-C1A	-4.76	104.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	601	CLA	C4A-NA-C1A	-4.76	104.57	106.71
31	8	609	IHT	C18-C07-C10	-4.76	109.94	121.46
27	Z	301	CLA	C4A-NA-C1A	-4.76	104.57	106.71
27	3	604	CLA	CHD-C1D-ND	-4.75	120.08	124.45
27	3	601	CLA	CHD-C1D-ND	-4.75	120.09	124.45
27	A	838	CLA	CHD-C1D-ND	-4.75	120.09	124.45
27	6	608	CLA	CHD-C1D-ND	-4.75	120.09	124.45
27	F	204	CLA	C4A-NA-C1A	-4.74	104.57	106.71
27	5	611	CLA	CHD-C1D-ND	-4.74	120.10	124.45
27	B	831	CLA	C4A-NA-C1A	-4.74	104.58	106.71
27	1	602	CLA	CHD-C1D-ND	-4.73	120.10	124.45
27	3	611	CLA	C4A-NA-C1A	-4.72	104.58	106.71
27	B	828	CLA	C4A-NA-C1A	-4.72	104.58	106.71
27	A	806	CLA	CHD-C1D-ND	-4.72	120.12	124.45
27	B	839	CLA	CHD-C1D-ND	-4.71	120.13	124.45
27	4	601	CLA	CHD-C1D-ND	-4.71	120.13	124.45
27	L	202	CLA	C4A-NA-C1A	-4.70	104.59	106.71
27	A	831	CLA	C4A-NA-C1A	-4.70	104.59	106.71
27	A	823	CLA	C4A-NA-C1A	-4.69	104.60	106.71
27	a	610	CLA	C4A-NA-C1A	-4.69	104.60	106.71
27	9	608	CLA	CHD-C1D-ND	-4.69	120.14	124.45
27	9	607	CLA	CHD-C1D-ND	-4.69	120.15	124.45
27	5	611	CLA	C4A-NA-C1A	-4.69	104.60	106.71
27	9	613	CLA	C4A-NA-C1A	-4.69	104.60	106.71
27	A	816	CLA	C4A-NA-C1A	-4.69	104.60	106.71
27	A	831	CLA	CHD-C1D-ND	-4.68	120.15	124.45
27	9	601	CLA	CHD-C1D-ND	-4.68	120.15	124.45
27	8	602	CLA	C4A-NA-C1A	-4.68	104.60	106.71
27	a	608	CLA	CHD-C1D-ND	-4.67	120.17	124.45
27	B	823	CLA	CHD-C1D-ND	-4.66	120.17	124.45
27	A	823	CLA	CHD-C1D-ND	-4.66	120.17	124.45
27	B	807	CLA	CHD-C1D-ND	-4.66	120.17	124.45
27	b	606	CLA	C4A-NA-C1A	-4.66	104.61	106.71
27	Z	304	CLA	C4A-NA-C1A	-4.66	104.61	106.71
27	A	807	CLA	C4A-NA-C1A	-4.65	104.61	106.71
27	A	836	CLA	C4A-NA-C1A	-4.64	104.62	106.71
27	K	102	CLA	C4A-NA-C1A	-4.64	104.62	106.71
27	K	101	CLA	CHD-C1D-ND	-4.63	120.20	124.45
27	A	832	CLA	C4A-NA-C1A	-4.63	104.62	106.71
27	F	204	CLA	CHD-C1D-ND	-4.62	120.20	124.45
27	A	810	CLA	C4A-NA-C1A	-4.62	104.63	106.71
27	b	604	CLA	CHD-C1D-ND	-4.62	120.21	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	9	612	CLA	C4A-NA-C1A	-4.61	104.63	106.71
27	8	604	CLA	CHD-C1D-ND	-4.61	120.22	124.45
27	8	601	CLA	C4A-NA-C1A	-4.59	104.64	106.71
31	2	616	IHT	C18-C07-C10	-4.58	110.37	121.46
27	A	835	CLA	C4A-NA-C1A	-4.58	104.65	106.71
27	B	808	CLA	C4A-NA-C1A	-4.58	104.65	106.71
27	7	302	CLA	C4A-NA-C1A	-4.56	104.66	106.71
27	B	825	CLA	C4A-NA-C1A	-4.54	104.66	106.71
27	a	606	CLA	CHD-C1D-ND	-4.54	120.28	124.45
27	A	828	CLA	C4A-NA-C1A	-4.54	104.67	106.71
27	A	814	CLA	C4A-NA-C1A	-4.53	104.67	106.71
27	B	823	CLA	C4A-NA-C1A	-4.51	104.68	106.71
31	a	616	IHT	C19-C10-C07	-4.49	119.48	124.53
27	B	813	CLA	CHD-C1D-ND	-4.49	120.33	124.45
27	3	612	CLA	C4A-NA-C1A	-4.47	104.70	106.71
27	1	605	CLA	CHD-C1D-ND	-4.46	120.36	124.45
31	1	618	IHT	C19-C10-C07	-4.44	119.55	124.53
27	b	604	CLA	C4A-NA-C1A	-4.39	104.73	106.71
27	A	834	CLA	C4A-NA-C1A	-4.38	104.74	106.71
27	A	801	CLA	C4A-NA-C1A	-4.38	104.74	106.71
31	6	616	IHT	C18-C07-C10	-4.37	110.88	121.46
27	1	612	CLA	C4A-NA-C1A	-4.30	104.77	106.71
27	5	608	CLA	C1-C2-C3	-4.28	118.64	126.04
29	1	616	II0	C42-C40-C36	-4.24	121.26	127.31
27	A	801	CLA	C1D-ND-C4D	-4.23	103.33	106.33
33	5	619	LHG	O4-P-O5	4.23	133.13	112.24
27	8	606	CLA	C4A-NA-C1A	-4.21	104.81	106.71
33	2	620	LHG	O4-P-O5	4.20	133.02	112.24
33	4	617	LHG	O4-P-O5	4.20	133.01	112.24
33	2	618	LHG	O4-P-O5	4.20	133.00	112.24
33	a	618	LHG	O4-P-O5	4.20	132.98	112.24
27	B	803	CLA	C4A-NA-C1A	-4.19	104.82	106.71
33	7	319	LHG	O4-P-O5	4.19	132.94	112.24
33	2	619	LHG	O4-P-O5	4.19	132.94	112.24
33	3	619	LHG	O4-P-O5	4.19	132.93	112.24
33	A	852	LHG	O4-P-O5	4.18	132.93	112.24
33	7	320	LHG	O4-P-O5	4.18	132.92	112.24
33	A	851	LHG	O4-P-O5	4.18	132.91	112.24
33	6	617	LHG	O4-P-O5	4.18	132.89	112.24
33	4	619	LHG	O4-P-O5	4.17	132.88	112.24
33	a	617	LHG	O4-P-O5	4.17	132.88	112.24
33	8	613	LHG	O4-P-O5	4.17	132.86	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	4	620	LHG	O4-P-O5	4.16	132.83	112.24
33	Z	311	LHG	O4-P-O5	4.16	132.83	112.24
33	3	622	LHG	O4-P-O5	4.16	132.81	112.24
33	b	616	LHG	O4-P-O5	4.15	132.75	112.24
27	R	202	CLA	C1-C2-C3	-4.15	118.87	126.04
31	9	619	IHT	C19-C10-C09	4.14	121.57	113.62
39	Z	303	DGD	O3G-C3G-C2G	-4.12	100.96	110.90
31	8	609	IHT	C09-C10-C07	-4.09	116.79	122.73
31	5	618	IHT	C18-C07-C10	-4.08	111.57	121.46
35	B	849	8CT	C30-C31-C32	-4.04	116.50	121.47
31	8	609	IHT	C19-C10-C09	4.03	121.36	113.62
29	3	614	II0	C42-C40-C36	-4.02	121.57	127.31
35	Z	309	8CT	C30-C31-C32	-4.00	116.54	121.47
27	B	813	CLA	C4A-NA-C1A	-3.97	104.92	106.71
31	A	854	IHT	C30-C27-C23	-3.96	121.66	127.31
29	7	317	II0	C42-C40-C36	-3.94	121.69	127.31
29	5	615	II0	C42-C40-C36	-3.93	121.70	127.31
31	9	619	IHT	C09-C10-C07	-3.93	117.03	122.73
29	8	612	II0	C20-C14-C10	-3.92	119.03	124.35
31	2	616	IHT	C19-C10-C09	3.91	121.13	113.62
27	A	837	CLA	C4A-NA-C1A	-3.91	104.95	106.71
29	B	843	II0	C42-C40-C36	-3.91	121.73	127.31
29	9	617	II0	C42-C40-C36	-3.90	121.75	127.31
31	A	854	IHT	C40-C37-C33	-3.90	121.75	127.31
29	4	613	II0	C42-C40-C36	-3.89	121.76	127.31
31	2	616	IHT	C09-C10-C07	-3.88	117.09	122.73
29	8	610	II0	C20-C14-C10	-3.88	119.07	124.35
30	b	613	II3	C25-C24-C21	3.88	124.19	118.08
31	9	619	IHT	C36-C33-C37	-3.88	117.49	122.92
29	7	314	II0	C42-C40-C36	-3.86	121.80	127.31
29	5	617	II0	C20-C14-C10	-3.85	119.12	124.35
29	b	614	II0	C20-C14-C10	-3.85	119.12	124.35
31	L	204	IHT	C25-C23-C22	3.84	124.13	118.08
29	1	619	II0	C42-C40-C36	-3.84	121.83	127.31
29	2	614	II0	C42-C40-C36	-3.84	121.83	127.31
31	Z	302	IHT	C30-C27-C23	-3.78	121.92	127.31
29	b	612	II0	C42-C40-C36	-3.77	121.93	127.31
31	2	616	IHT	C25-C23-C22	3.75	123.99	118.08
29	O	205	II0	C42-C40-C36	-3.75	121.96	127.31
29	6	615	II0	C42-C40-C36	-3.73	121.98	127.31
31	1	618	IHT	C30-C27-C23	-3.72	122.00	127.31
29	8	612	II0	C38-C36-C34	3.72	123.94	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	619	IHT	C22-C23-C27	3.72	124.65	118.94
31	8	609	IHT	C36-C33-C32	3.72	123.93	118.08
31	5	618	IHT	C19-C10-C07	-3.71	120.36	124.53
29	2	613	II0	C20-C14-C10	-3.71	119.31	124.35
31	1	618	IHT	C18-C07-C10	-3.71	112.47	121.46
29	a	612	II0	C42-C40-C36	-3.70	122.03	127.31
29	5	617	II0	C03-C09-C13	-3.70	117.41	122.63
29	7	317	II0	C20-C14-C10	-3.69	119.34	124.35
29	5	614	II0	C42-C40-C36	-3.68	122.06	127.31
31	L	204	IHT	C36-C33-C32	3.67	123.86	118.08
29	7	301	II0	C38-C36-C34	3.66	123.84	118.08
29	1	614	II0	C20-C14-C10	-3.64	119.41	124.35
31	9	619	IHT	C40-C37-C33	-3.63	122.13	127.31
29	4	615	II0	C20-C14-C10	-3.62	119.43	124.35
29	B	843	II0	C20-C14-C10	-3.62	119.43	124.35
29	7	301	II0	C42-C40-C36	-3.61	122.15	127.31
29	Z	312	II0	C38-C36-C34	3.61	123.76	118.08
30	1	615	II3	C25-C24-C21	3.60	123.75	118.08
29	3	617	II0	C20-C14-C10	-3.59	119.47	124.35
29	3	616	II0	C20-C14-C10	-3.59	119.47	124.35
29	a	613	II0	C38-C36-C34	3.58	123.72	118.08
31	8	609	IHT	C25-C23-C22	3.58	123.72	118.08
29	a	612	II0	C20-C14-C10	-3.57	119.50	124.35
31	9	619	IHT	C22-C18-C07	-3.56	117.19	127.20
29	5	620	II0	C19-C13-C11	3.55	120.93	114.36
31	a	616	IHT	C20-C15-C11	-3.55	119.53	124.35
29	a	614	II0	C38-C36-C34	3.55	123.67	118.08
29	O	205	II0	C20-C14-C10	-3.55	119.53	124.35
29	1	614	II0	C38-C36-C34	3.54	123.66	118.08
29	4	614	II0	C20-C14-C10	-3.54	119.53	124.35
27	B	831	CLA	C1-C2-C3	-3.53	119.93	126.04
29	4	612	II0	C20-C14-C10	-3.52	119.56	124.35
29	5	620	II0	C20-C14-C10	-3.52	119.56	124.35
29	7	301	II0	C20-C14-C10	-3.52	119.57	124.35
29	3	614	II0	C20-C14-C10	-3.52	119.57	124.35
31	2	616	IHT	C36-C33-C32	3.51	123.61	118.08
29	Z	312	II0	C20-C14-C10	-3.51	119.58	124.35
29	7	316	II0	C20-C14-C10	-3.50	119.59	124.35
31	5	618	IHT	C30-C27-C23	-3.50	122.31	127.31
27	L	203	CLA	C1-C2-C3	-3.50	121.09	126.75
27	a	608	CLA	C1-C2-C3	-3.50	120.00	126.04
29	5	617	II0	C42-C40-C36	-3.49	122.32	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	618	IHT	C36-C33-C32	3.49	123.58	118.08
29	5	620	II0	C03-C09-C13	-3.49	117.71	122.63
29	7	315	II0	C42-C40-C36	-3.49	122.33	127.31
29	3	615	II0	C38-C36-C34	3.47	123.55	118.08
30	b	613	II3	C39-C36-C33	-3.47	122.36	127.31
29	3	613	II0	C20-C14-C10	-3.46	119.65	124.35
29	3	616	II0	C42-C40-C36	-3.45	122.39	127.31
31	a	616	IHT	C22-C18-C07	-3.45	117.52	127.20
29	R	204	II0	C41-C42-C40	-3.44	116.42	123.47
31	Z	302	IHT	C40-C37-C33	-3.44	122.40	127.31
29	J	101	II0	C38-C36-C34	3.44	123.50	118.08
31	a	616	IHT	C06-C09-C10	3.43	120.20	114.08
29	b	614	II0	C38-C36-C34	3.43	123.48	118.08
29	2	615	II0	C42-C40-C36	-3.43	122.42	127.31
29	9	618	II0	C38-C36-C34	3.43	123.47	118.08
31	A	854	IHT	C36-C33-C32	3.42	123.47	118.08
29	b	612	II0	C20-C14-C10	-3.42	119.70	124.35
29	9	615	II0	C42-C40-C36	-3.42	122.43	127.31
29	R	204	II0	C20-C14-C10	-3.41	119.71	124.35
31	L	204	IHT	C18-C07-C10	-3.41	113.21	121.46
29	a	615	II0	C20-C14-C10	-3.40	119.72	124.35
29	1	617	II0	C20-C14-C10	-3.40	119.73	124.35
39	Z	303	DGD	O6D-C1D-O3G	-3.39	101.95	109.97
29	1	619	II0	C38-C36-C34	3.38	123.41	118.08
29	9	616	II0	C38-C36-C34	3.38	123.40	118.08
29	O	206	II0	C20-C14-C10	-3.37	119.77	124.35
31	8	609	IHT	C22-C18-C07	-3.37	117.73	127.20
29	1	619	II0	C20-C14-C10	-3.36	119.78	124.35
29	4	612	II0	C38-C36-C34	3.36	123.37	118.08
34	3	621	SQD	O47-C7-C8	3.36	118.74	111.50
31	A	854	IHT	C25-C23-C22	3.36	123.36	118.08
29	6	614	II0	C38-C36-C34	3.35	123.36	118.08
29	5	616	II0	C38-C36-C34	3.35	123.36	118.08
31	5	618	IHT	C25-C23-C22	3.35	123.35	118.08
31	6	616	IHT	C25-C23-C22	3.35	123.35	118.08
29	2	615	II0	C20-C14-C10	-3.35	119.80	124.35
29	2	615	II0	C38-C36-C34	3.34	123.34	118.08
32	8	616	LMG	O6-C1-O1	-3.34	102.07	109.97
30	b	613	II3	C35-C33-C32	3.34	123.33	118.08
30	1	615	II3	C39-C36-C33	-3.33	122.56	127.31
29	3	613	II0	C38-C36-C34	3.32	123.31	118.08
34	O	207	SQD	O8-S-C6	3.32	111.03	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	613	II0	C38-C36-C34	3.31	123.30	118.08
29	1	617	II0	C42-C40-C36	-3.31	122.58	127.31
29	9	616	II0	C20-C14-C10	-3.31	119.86	124.35
29	4	615	II0	C42-C40-C36	-3.30	122.60	127.31
29	a	614	II0	C20-C14-C10	-3.30	119.86	124.35
31	6	616	IHT	C22-C18-C07	-3.29	117.96	127.20
29	3	613	II0	C42-C40-C36	-3.29	122.62	127.31
31	1	618	IHT	C36-C33-C32	3.28	123.25	118.08
29	7	315	II0	C20-C14-C10	-3.28	119.89	124.35
29	4	615	II0	C38-C36-C34	3.28	123.25	118.08
29	J	101	II0	C20-C14-C10	-3.28	119.89	124.35
30	1	615	II3	C35-C33-C32	3.28	123.25	118.08
29	3	616	II0	C38-C36-C34	3.27	123.24	118.08
29	5	615	II0	C20-C14-C12	3.27	120.41	114.36
29	a	613	II0	C20-C14-C10	-3.26	119.92	124.35
29	4	614	II0	C38-C36-C34	3.26	123.21	118.08
29	2	615	II0	C03-C09-C13	-3.25	118.04	122.63
29	8	611	II0	C20-C14-C10	-3.25	119.93	124.35
31	2	616	IHT	C41-C40-C37	-3.25	116.82	123.47
27	b	602	CLA	C1-C2-C3	-3.24	120.43	126.04
31	1	618	IHT	C25-C23-C22	3.23	123.17	118.08
29	b	614	II0	C42-C40-C36	-3.23	122.70	127.31
29	3	614	II0	C42-C41-C39	-3.23	116.86	123.47
29	7	316	II0	C42-C40-C36	-3.23	122.70	127.31
29	8	612	II0	C41-C42-C40	-3.23	116.86	123.47
31	Z	302	IHT	C25-C23-C22	3.22	123.15	118.08
29	9	615	II0	C20-C14-C12	3.22	120.32	114.36
29	5	614	II0	C20-C14-C10	-3.22	119.98	124.35
29	9	617	II0	C20-C14-C10	-3.21	119.98	124.35
39	B	848	DGD	O3G-C3G-C2G	-3.21	103.15	110.90
27	5	608	CLA	C3D-C4D-ND	3.21	115.44	110.24
29	5	616	II0	C20-C14-C10	-3.21	119.99	124.35
29	5	617	II0	C38-C36-C34	3.21	123.13	118.08
29	1	619	II0	C20-C14-C12	3.20	120.28	114.36
31	1	618	IHT	C40-C37-C33	-3.19	122.75	127.31
31	2	616	IHT	C30-C27-C23	-3.19	122.75	127.31
31	2	616	IHT	C22-C18-C07	-3.19	118.23	127.20
29	7	315	II0	C38-C36-C34	3.18	123.09	118.08
29	4	613	II0	C20-C14-C10	-3.18	120.03	124.35
31	a	616	IHT	C40-C37-C33	-3.18	122.77	127.31
29	3	613	II0	C19-C13-C09	-3.18	120.03	124.35
29	2	614	II0	C20-C14-C10	-3.18	120.03	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	616	II0	C42-C40-C36	-3.18	122.77	127.31
29	5	617	II0	C19-C13-C11	3.18	120.24	114.36
27	2	602	CLA	C1-C2-C3	-3.17	120.56	126.04
29	1	616	II0	C20-C14-C10	-3.16	120.05	124.35
29	9	618	II0	C42-C40-C36	-3.16	122.80	127.31
29	7	314	II0	C20-C14-C10	-3.15	120.07	124.35
29	6	615	II0	C38-C36-C34	3.15	123.03	118.08
29	5	620	II0	C38-C36-C34	3.14	123.03	118.08
27	A	807	CLA	C1-C2-C3	-3.14	121.68	126.75
29	O	206	II0	C42-C40-C36	-3.13	122.84	127.31
27	6	611	CLA	C1-C2-C3	-3.13	120.63	126.04
29	9	615	II0	C38-C36-C34	3.13	123.01	118.08
29	2	613	II0	C19-C13-C09	-3.13	120.10	124.35
29	7	316	II0	C38-C36-C34	3.13	123.00	118.08
31	a	616	IHT	C31-C34-C35	-3.13	117.63	126.42
29	7	314	II0	C38-C36-C34	3.13	123.00	118.08
29	5	620	II0	C42-C40-C36	-3.12	122.85	127.31
29	B	843	II0	C38-C36-C34	3.12	123.00	118.08
29	2	613	II0	C41-C42-C40	-3.12	117.08	123.47
34	O	207	SQD	O47-C7-C8	3.11	119.48	110.80
31	9	619	IHT	C36-C33-C32	3.11	122.98	118.08
27	7	309	CLA	C1-C2-C3	-3.11	120.67	126.04
30	b	613	II3	C21-C24-C26	-3.11	114.17	118.94
29	O	205	II0	C38-C36-C34	3.10	122.95	118.08
29	3	614	II0	C38-C36-C34	3.09	122.95	118.08
29	2	614	II0	C38-C36-C40	-3.09	118.59	122.92
27	A	821	CLA	C3D-C4D-ND	3.09	115.24	110.24
27	5	604	CLA	C3D-C4D-ND	3.09	115.24	110.24
29	8	611	II0	C38-C36-C34	3.09	122.95	118.08
27	8	603	CLA	C3D-C4D-ND	3.09	115.24	110.24
27	B	806	CLA	C1-C2-C3	-3.09	120.70	126.04
31	L	204	IHT	C30-C27-C23	-3.09	122.90	127.31
29	1	617	II0	C38-C36-C34	3.09	122.94	118.08
31	8	609	IHT	C41-C40-C37	-3.08	117.16	123.47
29	b	612	II0	C38-C36-C40	-3.08	118.61	122.92
29	7	317	II0	C38-C36-C34	3.08	122.93	118.08
27	7	303	CLA	C3D-C4D-ND	3.08	115.22	110.24
27	4	602	CLA	C3D-C4D-ND	3.08	115.22	110.24
29	3	615	II0	C20-C14-C12	3.08	120.05	114.36
31	a	616	IHT	C19-C10-C09	3.08	119.52	113.62
27	B	829	CLA	C3D-C4D-ND	3.07	115.21	110.24
27	2	602	CLA	C3D-C4D-ND	3.07	115.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	9	617	II0	C38-C36-C34	3.07	122.92	118.08
29	3	615	II0	C04-C10-C14	-3.07	118.30	122.63
27	A	811	CLA	C3D-C4D-ND	3.07	115.21	110.24
27	a	604	CLA	C3D-C4D-ND	3.07	115.21	110.24
27	A	844	CLA	C3D-C4D-ND	3.07	115.20	110.24
29	a	612	II0	C19-C13-C09	-3.07	120.18	124.35
29	7	301	II0	C07-C11-C13	-3.06	105.75	111.85
29	9	616	II0	C42-C40-C36	-3.06	122.94	127.31
29	a	612	II0	C38-C36-C34	3.06	122.90	118.08
27	A	813	CLA	C3D-C4D-ND	3.06	115.19	110.24
29	5	615	II0	C20-C14-C10	-3.06	120.19	124.35
27	5	601	CLA	C3D-C4D-ND	3.05	115.17	110.24
27	A	818	CLA	C3D-C4D-ND	3.05	115.17	110.24
29	9	617	II0	C38-C36-C40	-3.05	118.66	122.92
29	5	614	II0	C38-C36-C34	3.04	122.87	118.08
29	8	610	II0	C41-C42-C40	-3.04	117.24	123.47
29	9	617	II0	C20-C14-C12	3.04	119.99	114.36
27	A	814	CLA	C3D-C4D-ND	3.04	115.15	110.24
27	B	812	CLA	C3D-C4D-ND	3.03	115.14	110.24
27	9	604	CLA	C3D-C4D-ND	3.03	115.14	110.24
27	O	204	CLA	CAA-C2A-C1A	-3.03	102.05	111.97
27	O	204	CLA	C3D-C4D-ND	3.03	115.14	110.24
27	B	830	CLA	C3D-C4D-ND	3.03	115.13	110.24
27	3	602	CLA	C3D-C4D-ND	3.02	115.13	110.24
31	L	204	IHT	C41-C40-C37	-3.02	117.29	123.47
29	b	614	II0	C03-C09-C13	-3.02	118.37	122.63
31	6	616	IHT	C36-C33-C32	3.02	122.83	118.08
29	1	619	II0	C03-C09-C13	-3.02	118.37	122.63
27	B	811	CLA	C3D-C4D-ND	3.02	115.12	110.24
32	8	614	LMG	O6-C1-O1	-3.02	102.83	109.97
27	Z	306	CLA	C3D-C4D-ND	3.02	115.11	110.24
27	A	815	CLA	C3D-C4D-ND	3.01	115.11	110.24
29	3	617	II0	C38-C36-C34	3.01	122.82	118.08
27	A	803	CLA	C3D-C4D-ND	3.01	115.11	110.24
27	L	202	CLA	C3D-C4D-ND	3.01	115.11	110.24
39	B	848	DGD	O6D-C1D-O3G	-3.01	102.85	109.97
27	A	840	CLA	C3D-C4D-ND	3.01	115.10	110.24
29	4	614	II0	C42-C40-C36	-3.00	123.02	127.31
27	A	829	CLA	C3D-C4D-ND	3.00	115.09	110.24
27	1	608	CLA	C3D-C4D-ND	3.00	115.09	110.24
27	3	605	CLA	C3D-C4D-ND	3.00	115.09	110.24
29	2	614	II0	C38-C36-C34	3.00	122.80	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	610	CLA	C3D-C4D-ND	3.00	115.09	110.24
30	b	613	II3	C03-C04-C12	-3.00	108.91	112.70
29	5	615	II0	C38-C36-C34	3.00	122.80	118.08
27	4	603	CLA	C3D-C4D-ND	3.00	115.09	110.24
31	L	204	IHT	C40-C37-C33	-3.00	123.03	127.31
27	4	607	CLA	C3D-C4D-ND	3.00	115.08	110.24
27	2	601	CLA	C3D-C4D-ND	2.99	115.07	110.24
27	B	834	CLA	C3D-C4D-ND	2.99	115.07	110.24
31	A	854	IHT	C09-C10-C07	-2.99	118.40	122.73
27	A	824	CLA	C3D-C4D-ND	2.98	115.07	110.24
27	6	608	CLA	C3D-C4D-ND	2.98	115.06	110.24
27	6	601	CLA	C3D-C4D-ND	2.98	115.06	110.24
27	1	611	CLA	C3D-C4D-ND	2.98	115.05	110.24
27	A	816	CLA	C3D-C4D-ND	2.98	115.05	110.24
27	9	611	CLA	C3D-C4D-ND	2.98	115.05	110.24
27	A	819	CLA	C3D-C4D-ND	2.97	115.05	110.24
27	9	602	CLA	C3D-C4D-ND	2.97	115.05	110.24
29	7	316	II0	C03-C09-C13	-2.97	118.44	122.63
27	a	605	CLA	C3D-C4D-ND	2.97	115.05	110.24
27	A	817	CLA	C3D-C4D-ND	2.97	115.04	110.24
27	A	827	CLA	C2C-C1C-NC	2.97	112.75	109.97
27	a	607	CLA	C3D-C4D-ND	2.97	115.04	110.24
31	5	618	IHT	C40-C37-C33	-2.97	123.08	127.31
29	J	101	II0	C42-C40-C36	-2.97	123.08	127.31
27	b	607	CLA	C3D-C4D-ND	2.96	115.03	110.24
27	2	608	CLA	C3D-C4D-ND	2.96	115.03	110.24
29	8	611	II0	C42-C40-C36	-2.96	123.08	127.31
27	A	839	CLA	C3D-C4D-ND	2.96	115.03	110.24
27	1	609	CLA	C3D-C4D-ND	2.96	115.03	110.24
27	7	304	CLA	C3D-C4D-ND	2.96	115.02	110.24
27	B	821	CLA	C3D-C4D-ND	2.96	115.02	110.24
27	K	102	CLA	C3D-C4D-ND	2.96	115.02	110.24
27	B	818	CLA	C3D-C4D-ND	2.96	115.02	110.24
27	9	609	CLA	C3D-C4D-ND	2.95	115.01	110.24
27	3	608	CLA	C3D-C4D-ND	2.95	115.01	110.24
29	3	616	II0	C05-C07-C11	-2.95	106.26	110.30
27	a	602	CLA	C3D-C4D-ND	2.95	115.01	110.24
27	9	614	CLA	C3D-C4D-ND	2.95	115.01	110.24
27	A	836	CLA	C3D-C4D-ND	2.95	115.01	110.24
29	4	612	II0	C03-C09-C13	-2.95	118.47	122.63
27	5	606	CLA	C3D-C4D-ND	2.95	115.01	110.24
27	B	822	CLA	C2C-C1C-NC	2.95	112.73	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	604	CLA	C3D-C4D-ND	2.95	115.00	110.24
27	7	305	CLA	C3D-C4D-ND	2.95	115.00	110.24
27	Z	304	CLA	C3D-C4D-ND	2.95	115.00	110.24
27	3	604	CLA	C3D-C4D-ND	2.95	115.00	110.24
27	6	603	CLA	C3D-C4D-ND	2.94	115.00	110.24
29	5	615	II0	C38-C36-C40	-2.94	118.80	122.92
32	6	618	LMG	O6-C1-O1	-2.94	103.00	109.97
29	O	206	II0	C38-C36-C34	2.94	122.71	118.08
27	6	611	CLA	C3D-C4D-ND	2.94	115.00	110.24
27	A	801	CLA	CHA-C1A-NA	-2.94	119.66	126.40
27	a	610	CLA	C3D-C4D-ND	2.94	115.00	110.24
27	A	842	CLA	C3D-C4D-ND	2.94	114.99	110.24
27	2	603	CLA	C3D-C4D-ND	2.94	114.99	110.24
27	8	601	CLA	C3D-C4D-ND	2.94	114.99	110.24
27	B	836	CLA	C2C-C1C-NC	2.94	112.72	109.97
27	a	601	CLA	C3D-C4D-ND	2.94	114.99	110.24
27	9	608	CLA	C3D-C4D-ND	2.94	114.99	110.24
27	2	607	CLA	C3D-C4D-ND	2.93	114.98	110.24
27	4	601	CLA	C3D-C4D-ND	2.93	114.98	110.24
27	B	815	CLA	C3D-C4D-ND	2.93	114.98	110.24
27	8	608	CLA	C3D-C4D-ND	2.93	114.98	110.24
29	b	612	II0	C38-C36-C34	2.93	122.69	118.08
27	B	817	CLA	C3D-C4D-ND	2.93	114.98	110.24
27	B	828	CLA	C3D-C4D-ND	2.93	114.98	110.24
27	7	309	CLA	C3D-C4D-ND	2.93	114.98	110.24
27	A	805	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	A	834	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	1	603	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	7	308	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	b	601	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	1	605	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	9	603	CLA	C3D-C4D-ND	2.93	114.97	110.24
27	2	609	CLA	C3D-C4D-ND	2.93	114.97	110.24
33	7	320	LHG	O8-C23-C24	2.93	121.09	111.91
27	6	602	CLA	C3D-C4D-ND	2.92	114.97	110.24
27	B	841	CLA	C3D-C4D-ND	2.92	114.97	110.24
27	L	203	CLA	C3D-C4D-ND	2.92	114.97	110.24
27	J	102	CLA	C3D-C4D-ND	2.92	114.96	110.24
27	B	839	CLA	C3D-C4D-ND	2.92	114.96	110.24
27	1	602	CLA	C3D-C4D-ND	2.92	114.96	110.24
27	A	820	CLA	C3D-C4D-ND	2.92	114.95	110.24
27	B	838	CLA	C3D-C4D-ND	2.92	114.95	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	810	CLA	C3D-C4D-ND	2.91	114.95	110.24
27	A	830	CLA	C3D-C4D-ND	2.91	114.95	110.24
27	B	822	CLA	C3D-C4D-ND	2.91	114.95	110.24
27	B	837	CLA	C3D-C4D-ND	2.91	114.95	110.24
29	5	614	II0	C06-C08-C12	-2.91	106.32	110.30
29	9	618	II0	C41-C39-C35	-2.91	123.16	127.31
31	L	204	IHT	C22-C18-C07	-2.91	119.03	127.20
27	A	833	CLA	C3D-C4D-ND	2.91	114.94	110.24
27	b	610	CLA	C3D-C4D-ND	2.91	114.94	110.24
27	9	606	CLA	C3D-C4D-ND	2.91	114.94	110.24
27	A	822	CLA	C3D-C4D-ND	2.91	114.94	110.24
31	Z	302	IHT	C06-C09-C10	2.91	119.27	114.08
27	5	602	CLA	C3D-C4D-ND	2.91	114.94	110.24
27	A	838	CLA	C3D-C4D-ND	2.91	114.94	110.24
29	a	613	II0	C42-C40-C36	-2.91	123.16	127.31
27	6	606	CLA	C3D-C4D-ND	2.90	114.94	110.24
27	A	808	CLA	C3D-C4D-ND	2.90	114.93	110.24
27	7	310	CLA	C3D-C4D-ND	2.90	114.93	110.24
27	9	605	CLA	C3D-C4D-ND	2.90	114.93	110.24
27	B	819	CLA	C3D-C4D-ND	2.90	114.93	110.24
31	a	616	IHT	C41-C40-C37	-2.90	117.53	123.47
27	b	602	CLA	C3D-C4D-ND	2.90	114.93	110.24
27	B	831	CLA	C3D-C4D-ND	2.90	114.93	110.24
27	O	203	CLA	C3D-C4D-ND	2.90	114.92	110.24
27	2	612	CLA	C3D-C4D-ND	2.90	114.92	110.24
27	8	607	CLA	C3D-C4D-ND	2.90	114.92	110.24
27	1	606	CLA	C3D-C4D-ND	2.90	114.92	110.24
27	8	615	CLA	C3D-C4D-ND	2.89	114.92	110.24
29	6	614	II0	C41-C42-C40	-2.89	117.55	123.47
27	Z	305	CLA	C3D-C4D-ND	2.89	114.92	110.24
33	3	622	LHG	O8-C23-C24	2.89	120.98	111.91
27	6	604	CLA	C3D-C4D-ND	2.89	114.92	110.24
27	3	609	CLA	C3D-C4D-ND	2.89	114.91	110.24
27	A	802	CLA	C3D-C4D-ND	2.89	114.91	110.24
27	1	613	CLA	C3D-C4D-ND	2.89	114.91	110.24
27	3	611	CLA	C3D-C4D-ND	2.89	114.91	110.24
29	4	615	II0	C03-C09-C13	-2.89	118.56	122.63
27	5	603	CLA	C3D-C4D-ND	2.89	114.91	110.24
27	5	612	CLA	C3D-C4D-ND	2.89	114.91	110.24
39	Z	303	DGD	O5D-C6D-C5D	-2.88	103.71	109.05
29	3	617	II0	C42-C40-C36	-2.88	123.19	127.31
27	Z	301	CLA	C3D-C4D-ND	2.88	114.90	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	201	CLA	C3D-C4D-ND	2.88	114.90	110.24
27	3	612	CLA	C3D-C4D-ND	2.88	114.90	110.24
27	9	601	CLA	C3D-C4D-ND	2.88	114.90	110.24
27	F	204	CLA	C2C-C1C-NC	2.88	112.67	109.97
36	4	618	LMU	C1B-O5B-C5B	2.88	119.34	113.69
27	1	601	CLA	C3D-C4D-ND	2.88	114.89	110.24
29	1	616	II0	C42-C41-C39	-2.88	117.58	123.47
27	2	606	CLA	C3D-C4D-ND	2.88	114.89	110.24
27	B	840	CLA	C3D-C4D-ND	2.88	114.89	110.24
29	9	618	II0	C41-C42-C40	-2.88	117.58	123.47
27	A	835	CLA	C3D-C4D-ND	2.88	114.89	110.24
27	b	603	CLA	C3D-C4D-ND	2.87	114.89	110.24
27	7	306	CLA	C3D-C4D-ND	2.87	114.89	110.24
27	B	814	CLA	C3D-C4D-ND	2.87	114.88	110.24
27	B	804	CLA	C3D-C4D-ND	2.87	114.88	110.24
27	Z	305	CLA	C1-C2-C3	-2.87	122.11	126.75
27	4	604	CLA	C3D-C4D-ND	2.87	114.88	110.24
27	1	604	CLA	C3D-C4D-ND	2.87	114.88	110.24
29	7	301	II0	C19-C13-C11	2.87	119.67	114.36
27	5	607	CLA	C3D-C4D-ND	2.87	114.88	110.24
27	B	827	CLA	C3D-C4D-ND	2.87	114.88	110.24
27	4	608	CLA	C3D-C4D-ND	2.87	114.87	110.24
31	A	854	IHT	C06-C09-C10	2.87	119.19	114.08
27	A	809	CLA	C3D-C4D-ND	2.86	114.87	110.24
27	6	607	CLA	C3D-C4D-ND	2.86	114.87	110.24
29	2	615	II0	C20-C14-C12	2.86	119.66	114.36
30	1	615	II3	C29-C26-C24	-2.86	123.22	127.31
27	1	607	CLA	C3D-C4D-ND	2.86	114.87	110.24
38	A	850	PQN	C11-C3-C4	-2.86	115.44	118.50
29	a	613	II0	C41-C39-C35	-2.86	123.23	127.31
29	1	616	II0	C38-C36-C40	-2.86	118.92	122.92
27	Z	310	CLA	C3D-C4D-ND	2.86	114.86	110.24
29	4	613	II0	C38-C36-C40	-2.86	118.92	122.92
27	2	605	CLA	C3D-C4D-ND	2.86	114.86	110.24
27	O	202	CLA	C3D-C4D-ND	2.86	114.86	110.24
29	J	101	II0	C06-C08-C12	-2.86	106.39	110.30
27	6	612	CLA	C3D-C4D-ND	2.85	114.86	110.24
27	F	202	CLA	C3D-C4D-ND	2.85	114.85	110.24
27	a	606	CLA	C3D-C4D-ND	2.85	114.85	110.24
27	7	312	CLA	C3D-C4D-ND	2.85	114.85	110.24
33	6	617	LHG	O8-C23-C24	2.85	120.85	111.91
27	3	601	CLA	C3D-C4D-ND	2.85	114.85	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	826	CLA	C3D-C4D-ND	2.85	114.84	110.24
27	A	825	CLA	C3D-C4D-ND	2.85	114.84	110.24
27	5	609	CLA	C3D-C4D-ND	2.85	114.84	110.24
27	B	833	CLA	C3D-C4D-ND	2.85	114.84	110.24
29	a	615	II0	C42-C40-C36	-2.84	123.25	127.31
34	3	621	SQD	O48-C23-C24	2.84	120.83	111.91
29	R	204	II0	C38-C36-C34	2.84	122.55	118.08
29	7	317	II0	C42-C41-C39	-2.84	117.66	123.47
29	4	613	II0	C42-C41-C39	-2.84	117.66	123.47
27	4	609	CLA	C3D-C4D-ND	2.84	114.83	110.24
27	A	807	CLA	C3D-C4D-ND	2.84	114.83	110.24
29	a	614	II0	C41-C42-C40	-2.84	117.66	123.47
27	B	816	CLA	C3D-C4D-ND	2.84	114.83	110.24
27	L	201	CLA	C3D-C4D-ND	2.84	114.83	110.24
30	1	615	II3	C22-C18-C16	-2.83	120.50	124.35
27	4	610	CLA	C3D-C4D-ND	2.83	114.82	110.24
27	B	836	CLA	C3D-C4D-ND	2.83	114.81	110.24
29	9	617	II0	C04-C10-C14	-2.83	118.64	122.63
32	F	205	LMG	O6-C1-O1	-2.83	103.28	109.97
27	B	806	CLA	C3D-C4D-ND	2.82	114.81	110.24
39	B	848	DGD	O5D-C6D-C5D	-2.82	103.83	109.05
27	F	203	CLA	C3D-C4D-ND	2.82	114.80	110.24
32	2	617	LMG	O6-C1-O1	-2.82	103.30	109.97
27	6	609	CLA	C3D-C4D-ND	2.82	114.80	110.24
29	a	614	II0	C42-C40-C36	-2.82	123.29	127.31
27	1	605	CLA	C2C-C1C-NC	2.82	112.61	109.97
29	R	204	II0	C41-C39-C35	-2.82	123.29	127.31
27	B	832	CLA	C3D-C4D-ND	2.82	114.79	110.24
27	3	612	CLA	C2C-C1C-NC	2.81	112.61	109.97
27	3	607	CLA	C3D-C4D-ND	2.81	114.79	110.24
27	5	605	CLA	C3D-C4D-ND	2.81	114.79	110.24
31	6	616	IHT	C40-C37-C33	-2.81	123.30	127.31
29	8	610	II0	C19-C13-C11	2.81	119.56	114.36
27	3	603	CLA	C3D-C4D-ND	2.81	114.78	110.24
27	4	611	CLA	C3D-C4D-ND	2.81	114.78	110.24
27	6	605	CLA	C3D-C4D-ND	2.81	114.78	110.24
27	B	808	CLA	C3D-C4D-ND	2.81	114.78	110.24
27	4	606	CLA	C3D-C4D-ND	2.81	114.78	110.24
27	8	606	CLA	C3D-C4D-ND	2.81	114.78	110.24
31	2	616	IHT	C41-C38-C35	-2.81	123.30	127.31
27	A	828	CLA	C3D-C4D-ND	2.81	114.78	110.24
27	A	841	CLA	C3D-C4D-ND	2.81	114.78	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	604	CLA	C3D-C4D-ND	2.81	114.78	110.24
29	4	613	II0	C38-C36-C34	2.80	122.50	118.08
27	B	820	CLA	C3D-C4D-ND	2.80	114.77	110.24
33	4	619	LHG	O8-C23-C24	2.80	120.71	111.91
31	2	616	IHT	C03-C11-C15	-2.80	118.68	122.63
29	5	617	II0	C38-C36-C40	-2.80	119.00	122.92
33	a	618	LHG	O8-C23-C24	2.80	120.69	111.91
27	a	608	CLA	C3D-C4D-ND	2.80	114.76	110.24
31	2	616	IHT	C40-C37-C33	-2.80	123.32	127.31
29	b	612	II0	C05-C07-C11	-2.79	106.48	110.30
27	7	302	CLA	C3D-C4D-ND	2.79	114.75	110.24
27	9	613	CLA	C3D-C4D-ND	2.79	114.75	110.24
27	K	101	CLA	C3D-C4D-ND	2.79	114.75	110.24
27	B	835	CLA	C1-C2-C3	-2.79	121.22	126.04
29	5	617	II0	C19-C13-C09	-2.79	120.56	124.35
27	L	201	CLA	C2C-C1C-NC	2.79	112.58	109.97
27	7	313	CLA	C3D-C4D-ND	2.79	114.75	110.24
29	Z	312	II0	C42-C40-C36	-2.79	123.33	127.31
27	9	612	CLA	C3D-C4D-ND	2.79	114.75	110.24
29	7	314	II0	C38-C36-C40	-2.79	119.02	122.92
27	a	603	CLA	C3D-C4D-ND	2.79	114.75	110.24
27	A	837	CLA	C3D-C4D-ND	2.79	114.74	110.24
31	5	618	IHT	C25-C23-C27	-2.78	119.02	122.92
28	a	609	KC2	CHB-C1B-NB	2.78	127.01	124.45
29	9	618	II0	C19-C13-C09	-2.78	120.57	124.35
27	B	803	CLA	C3D-C4D-ND	2.78	114.74	110.24
27	b	606	CLA	C3D-C4D-ND	2.78	114.73	110.24
27	A	820	CLA	C2C-C1C-NC	2.78	112.58	109.97
27	9	607	CLA	C3D-C4D-ND	2.78	114.73	110.24
27	a	611	CLA	C3D-C4D-ND	2.78	114.73	110.24
31	9	619	IHT	C19-C10-C07	-2.78	121.41	124.53
31	A	854	IHT	C36-C33-C37	-2.78	119.03	122.92
29	8	612	II0	C19-C13-C09	-2.78	120.58	124.35
28	4	605	KC2	CHB-C1B-NB	2.78	127.01	124.45
27	8	606	CLA	C2C-C1C-NC	2.78	112.57	109.97
27	b	608	CLA	C3D-C4D-ND	2.77	114.72	110.24
27	B	824	CLA	C3D-C4D-ND	2.77	114.72	110.24
31	L	204	IHT	C19-C10-C09	2.77	118.94	113.62
27	A	835	CLA	C2C-C1C-NC	2.77	112.57	109.97
27	8	605	CLA	C3D-C4D-ND	2.77	114.71	110.24
38	B	842	PQN	C11-C3-C4	-2.77	115.54	118.50
27	5	606	CLA	C2C-C1C-NC	2.76	112.56	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	613	II0	C42-C40-C36	-2.76	123.37	127.31
31	Z	302	IHT	C19-C10-C09	2.76	118.92	113.62
29	5	615	II0	C42-C41-C39	-2.76	117.82	123.47
27	5	613	CLA	C3D-C4D-ND	2.76	114.70	110.24
29	6	615	II0	C42-C41-C39	-2.76	117.82	123.47
27	B	807	CLA	C3D-C4D-ND	2.76	114.70	110.24
27	A	804	CLA	C3D-C4D-ND	2.76	114.70	110.24
29	5	614	II0	C38-C36-C40	-2.76	119.06	122.92
27	A	810	CLA	O2A-C1-C2	2.76	115.88	108.64
29	1	616	II0	C38-C36-C34	2.75	122.42	118.08
27	5	611	CLA	C3D-C4D-ND	2.75	114.69	110.24
28	6	610	KC2	CHB-C1B-NB	2.75	126.98	124.45
31	Z	302	IHT	C22-C18-C07	-2.75	119.47	127.20
27	1	602	CLA	C1-C2-C3	-2.75	121.28	126.04
31	5	618	IHT	C41-C40-C37	-2.75	117.84	123.47
27	B	823	CLA	C1-C2-C3	-2.75	121.29	126.04
29	4	612	II0	C42-C40-C36	-2.75	123.39	127.31
27	R	202	CLA	C3D-C4D-ND	2.75	114.69	110.24
27	A	831	CLA	C3D-C4D-ND	2.75	114.68	110.24
27	2	611	CLA	C3D-C4D-ND	2.75	114.68	110.24
27	F	203	CLA	C2C-C1C-NC	2.75	112.54	109.97
28	1	610	KC2	CHB-C1B-NB	2.74	126.98	124.45
27	b	611	CLA	C3D-C4D-ND	2.74	114.67	110.24
27	B	813	CLA	C3D-C4D-ND	2.74	114.67	110.24
27	B	825	CLA	C3D-C4D-ND	2.74	114.67	110.24
27	A	812	CLA	C3D-C4D-ND	2.74	114.67	110.24
27	A	832	CLA	C3D-C4D-ND	2.74	114.67	110.24
27	4	609	CLA	C2C-C1C-NC	2.74	112.54	109.97
29	a	612	II0	C42-C41-C39	-2.74	117.87	123.47
27	B	835	CLA	C3D-C4D-ND	2.73	114.66	110.24
33	3	619	LHG	O8-C23-C24	2.73	120.47	111.91
27	A	827	CLA	C3D-C4D-ND	2.73	114.65	110.24
27	5	603	CLA	C2C-C1C-NC	2.73	112.53	109.97
27	B	821	CLA	C1-C2-C3	-2.73	121.33	126.04
27	B	805	CLA	C3D-C4D-ND	2.72	114.64	110.24
31	A	854	IHT	C04-C02-C07	2.72	114.67	110.48
27	B	828	CLA	C2C-C1C-NC	2.72	112.52	109.97
27	A	843	CLA	C3D-C4D-ND	2.72	114.64	110.24
27	A	817	CLA	CAA-C2A-C1A	-2.72	103.07	111.97
27	B	833	CLA	C2C-C1C-NC	2.72	112.52	109.97
31	5	618	IHT	C19-C10-C09	2.71	118.83	113.62
27	A	816	CLA	C2C-C1C-NC	2.71	112.51	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	619	II0	C04-C10-C14	-2.71	118.80	122.63
29	9	617	II0	C42-C41-C39	-2.71	117.92	123.47
27	A	807	CLA	C2C-C1C-NC	2.71	112.51	109.97
27	a	601	CLA	C2C-C1C-NC	2.71	112.51	109.97
27	B	820	CLA	C2C-C1C-NC	2.71	112.51	109.97
27	a	602	CLA	CAA-C2A-C1A	-2.71	103.10	111.97
27	B	823	CLA	C3D-C4D-ND	2.71	114.62	110.24
33	A	851	LHG	O8-C23-C24	2.71	120.41	111.91
31	A	854	IHT	C02-C07-C18	-2.70	108.13	115.78
31	A	854	IHT	C25-C23-C27	-2.70	119.14	122.92
31	5	618	IHT	C04-C02-C07	-2.70	106.33	110.48
27	8	601	CLA	C2C-C1C-NC	2.70	112.50	109.97
28	7	311	KC2	CHB-C1B-NB	2.70	126.93	124.45
29	1	614	II0	C41-C42-C40	-2.70	117.95	123.47
29	2	615	II0	C04-C10-C14	-2.69	118.84	122.63
27	B	840	CLA	C2C-C1C-NC	2.69	112.49	109.97
27	A	806	CLA	C3D-C4D-ND	2.69	114.59	110.24
29	1	617	II0	C41-C39-C35	-2.69	123.47	127.31
29	1	617	II0	C41-C42-C40	-2.69	117.97	123.47
27	3	610	CLA	C2C-C1C-NC	2.69	112.49	109.97
27	9	606	CLA	C2C-C1C-NC	2.69	112.49	109.97
29	4	612	II0	C41-C42-C40	-2.69	117.97	123.47
29	J	101	II0	C41-C39-C35	-2.69	123.48	127.31
27	1	612	CLA	C2C-C1C-NC	2.68	112.49	109.97
29	7	315	II0	C38-C36-C40	-2.68	119.17	122.92
29	7	314	II0	C20-C14-C12	2.68	119.32	114.36
27	A	823	CLA	C2C-C1C-NC	2.68	112.48	109.97
27	b	610	CLA	C1-C2-C3	-2.68	121.41	126.04
29	3	615	II0	C41-C42-C40	-2.68	117.99	123.47
29	3	614	II0	C38-C36-C40	-2.67	119.18	122.92
29	8	610	II0	C41-C39-C35	-2.67	123.49	127.31
28	Z	307	KC2	CHB-C1B-NB	2.67	126.91	124.45
27	9	613	CLA	C2C-C1C-NC	2.67	112.47	109.97
27	B	809	CLA	C3D-C4D-ND	2.67	114.56	110.24
27	A	837	CLA	C2C-C1C-NC	2.67	112.47	109.97
27	6	601	CLA	C2C-C1C-NC	2.67	112.47	109.97
29	7	316	II0	C19-C13-C11	2.67	119.30	114.36
29	J	101	II0	C20-C14-C12	2.67	119.30	114.36
27	B	816	CLA	C2C-C1C-NC	2.67	112.47	109.97
29	B	843	II0	C42-C41-C39	-2.67	118.01	123.47
27	1	612	CLA	C3D-C4D-ND	2.67	114.55	110.24
27	1	606	CLA	C2C-C1C-NC	2.67	112.47	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	3	606	KC2	CHB-C1B-NB	2.66	126.90	124.45
27	F	204	CLA	C3D-C4D-ND	2.66	114.55	110.24
27	7	302	CLA	C2C-C1C-NC	2.66	112.47	109.97
27	A	831	CLA	C2C-C1C-NC	2.66	112.47	109.97
33	8	613	LHG	O8-C23-C24	2.66	120.26	111.91
27	A	839	CLA	O2A-C1-C2	-2.66	101.64	108.64
29	8	612	II0	C41-C39-C35	-2.66	123.52	127.31
33	2	619	LHG	O8-C23-C24	2.65	120.24	111.91
27	4	607	CLA	C1-C2-C3	-2.65	121.45	126.04
31	6	616	IHT	C19-C10-C09	2.65	118.71	113.62
27	A	826	CLA	C3D-C4D-ND	2.65	114.53	110.24
29	a	615	II0	C20-C14-C12	2.65	119.26	114.36
28	6	613	KC2	CHB-C1B-NB	2.65	126.89	124.45
28	5	610	KC2	CHB-C1B-NB	2.64	126.88	124.45
27	7	312	CLA	C2C-C1C-NC	2.64	112.45	109.97
27	b	608	CLA	C2C-C1C-NC	2.64	112.45	109.97
29	5	616	II0	C19-C13-C11	2.64	119.25	114.36
27	b	601	CLA	C2C-C1C-NC	2.64	112.45	109.97
29	3	615	II0	C20-C14-C10	-2.64	120.76	124.35
27	8	602	CLA	C3D-C4D-ND	2.64	114.50	110.24
27	a	605	CLA	C2C-C1C-NC	2.64	112.44	109.97
29	8	610	II0	C19-C13-C09	-2.63	120.77	124.35
27	8	607	CLA	C2C-C1C-NC	2.63	112.44	109.97
27	A	833	CLA	C2C-C1C-NC	2.63	112.44	109.97
29	1	617	II0	C06-C08-C12	-2.63	106.70	110.30
31	6	616	IHT	C41-C40-C37	-2.63	118.09	123.47
27	4	608	CLA	C2C-C1C-NC	2.63	112.43	109.97
29	8	612	II0	C42-C40-C36	-2.63	123.56	127.31
27	2	612	CLA	C2C-C1C-NC	2.62	112.43	109.97
27	B	808	CLA	C2C-C1C-NC	2.62	112.43	109.97
29	7	314	II0	C04-C10-C14	-2.62	118.93	122.63
27	B	827	CLA	C2C-C1C-NC	2.62	112.43	109.97
31	L	204	IHT	C19-C10-C07	-2.62	121.59	124.53
27	B	801	CLA	C3D-C4D-ND	2.62	114.47	110.24
27	4	604	CLA	C2C-C1C-NC	2.62	112.42	109.97
29	5	614	II0	C42-C41-C39	-2.61	118.12	123.47
27	K	101	CLA	C2C-C1C-NC	2.61	112.42	109.97
27	5	611	CLA	C2C-C1C-NC	2.61	112.42	109.97
31	2	616	IHT	C20-C15-C12	2.61	119.19	114.36
28	b	605	KC2	CHB-C1B-NB	2.61	126.85	124.45
28	2	610	KC2	CHB-C1B-NB	2.61	126.85	124.45
27	6	606	CLA	C2C-C1C-NC	2.61	112.41	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	306	CLA	C2C-C1C-NC	2.60	112.41	109.97
34	3	621	SQD	O8-S-C6	2.60	109.89	105.74
27	B	812	CLA	C1-C2-C3	-2.60	121.54	126.04
27	8	605	CLA	C1-C2-C3	-2.60	122.54	126.75
27	B	825	CLA	C2C-C1C-NC	2.60	112.41	109.97
31	Z	302	IHT	C40-C41-C38	-2.60	118.14	123.47
27	A	823	CLA	C3D-C4D-ND	2.60	114.45	110.24
33	a	618	LHG	C11-C10-C9	-2.60	101.22	114.42
28	b	609	KC2	CHB-C1B-NB	2.60	126.84	124.45
27	B	811	CLA	C2C-C1C-NC	2.60	112.41	109.97
29	6	615	II0	C20-C14-C10	-2.60	120.82	124.35
27	A	836	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	Z	312	II0	C41-C42-C40	-2.59	118.16	123.47
33	2	620	LHG	C11-C10-C9	-2.59	101.27	114.42
31	5	618	IHT	C13-C02-C07	2.59	114.50	110.30
33	Z	311	LHG	O8-C23-C24	2.59	120.02	111.91
27	2	611	CLA	C2C-C1C-NC	2.59	112.39	109.97
27	5	609	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	b	612	II0	C06-C08-C12	-2.58	106.77	110.30
27	4	606	CLA	C2C-C1C-NC	2.58	112.39	109.97
27	6	611	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	8	610	II0	C38-C36-C34	2.58	122.14	118.08
27	9	601	CLA	C2C-C1C-NC	2.58	112.39	109.97
29	5	615	II0	C04-C10-C14	-2.58	119.00	122.63
27	A	842	CLA	C2C-C1C-NC	2.58	112.39	109.97
27	b	603	CLA	C2C-C1C-NC	2.57	112.38	109.97
28	3	606	KC2	C4C-C3C-C2C	2.57	109.16	107.11
27	1	611	CLA	C2C-C1C-NC	2.57	112.38	109.97
27	A	818	CLA	C2C-C1C-NC	2.57	112.38	109.97
27	a	603	CLA	C2C-C1C-NC	2.57	112.38	109.97
29	4	614	II0	C20-C14-C12	2.57	119.12	114.36
27	3	604	CLA	C2C-C1C-NC	2.57	112.38	109.97
27	4	610	CLA	C2C-C1C-NC	2.57	112.38	109.97
32	3	618	LMG	O6-C1-O1	-2.57	103.90	109.97
29	1	614	II0	C42-C40-C36	-2.56	123.65	127.31
29	5	616	II0	C19-C13-C09	-2.56	120.87	124.35
27	A	834	CLA	C2C-C1C-NC	2.56	112.37	109.97
31	8	609	IHT	C40-C37-C33	-2.56	123.66	127.31
39	Z	303	DGD	C3G-C2G-C1G	-2.56	105.74	111.79
29	2	614	II0	C06-C08-C12	-2.55	106.81	110.30
29	J	101	II0	C41-C42-C40	-2.55	118.24	123.47
29	7	317	II0	C19-C13-C09	-2.55	120.88	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	815	CLA	C2C-C1C-NC	2.55	112.36	109.97
27	1	602	CLA	C2C-C1C-NC	2.55	112.36	109.97
27	B	813	CLA	C2C-C1C-NC	2.55	112.36	109.97
29	a	613	II0	C41-C42-C40	-2.54	118.27	123.47
27	3	601	CLA	C2C-C1C-NC	2.54	112.35	109.97
27	A	813	CLA	C2C-C1C-NC	2.54	112.35	109.97
28	7	307	KC2	CHB-C1B-NB	2.54	126.79	124.45
29	6	614	II0	C20-C14-C12	2.54	119.06	114.36
29	7	301	II0	C41-C39-C35	-2.54	123.69	127.31
27	B	834	CLA	C2C-C1C-NC	2.54	112.35	109.97
29	b	612	II0	C42-C41-C39	-2.53	118.28	123.47
27	A	804	CLA	C2C-C1C-NC	2.53	112.34	109.97
27	B	806	CLA	C2C-C1C-NC	2.53	112.34	109.97
29	9	615	II0	C38-C36-C40	-2.53	119.38	122.92
27	O	204	CLA	C2C-C1C-NC	2.53	112.34	109.97
30	b	613	II3	C29-C26-C24	-2.53	123.70	127.31
29	J	101	II0	C38-C36-C40	-2.53	119.38	122.92
27	A	828	CLA	C2C-C1C-NC	2.53	112.34	109.97
29	7	317	II0	C38-C36-C40	-2.53	119.38	122.92
32	3	620	LMG	O6-C1-O1	-2.53	103.99	109.97
28	9	610	KC2	CHB-C1B-NB	2.52	126.77	124.45
27	A	810	CLA	C3D-C4D-ND	2.52	114.32	110.24
27	A	814	CLA	C2C-C1C-NC	2.52	112.33	109.97
31	Z	302	IHT	C04-C06-C09	-2.52	105.74	111.38
33	b	616	LHG	O8-C23-C24	2.52	119.82	111.91
29	7	315	II0	C16-C03-C09	-2.52	106.46	110.47
33	5	619	LHG	O8-C23-C24	2.52	119.81	111.91
27	a	608	CLA	C2C-C1C-NC	2.52	112.33	109.97
29	6	615	II0	C05-C07-C11	-2.52	106.86	110.30
27	A	803	CLA	C2C-C1C-NC	2.52	112.33	109.97
29	7	301	II0	C38-C36-C40	-2.51	119.40	122.92
27	b	606	CLA	C2C-C1C-NC	2.51	112.33	109.97
33	4	620	LHG	O8-C23-C24	2.51	119.79	111.91
27	6	612	CLA	C2C-C1C-NC	2.51	112.33	109.97
31	1	618	IHT	C36-C33-C37	-2.51	119.41	122.92
29	3	617	II0	C20-C14-C12	2.50	118.99	114.36
27	B	802	CLA	C3D-C4D-ND	2.50	114.29	110.24
27	7	304	CLA	C2C-C1C-NC	2.50	112.32	109.97
27	L	203	CLA	C2C-C1C-NC	2.50	112.32	109.97
31	5	618	IHT	C36-C33-C37	-2.50	119.42	122.92
29	a	615	II0	C41-C42-C40	-2.50	118.35	123.47
30	b	613	II3	C39-C41-C40	-2.50	118.35	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	9	616	II0	C38-C36-C40	-2.50	119.42	122.92
29	5	616	II0	C20-C14-C12	2.50	118.99	114.36
27	9	611	CLA	C2C-C1C-NC	2.50	112.31	109.97
27	L	202	CLA	C2C-C1C-NC	2.50	112.31	109.97
27	A	804	CLA	C1-C2-C3	-2.50	121.72	126.04
29	7	314	II0	C42-C41-C39	-2.50	118.36	123.47
27	8	604	CLA	C2C-C1C-NC	2.50	112.31	109.97
28	6	610	KC2	CHD-C4C-NC	2.50	127.99	124.20
29	3	615	II0	C42-C40-C36	-2.49	123.75	127.31
27	2	609	CLA	C2C-C1C-NC	2.49	112.31	109.97
27	O	203	CLA	C2C-C1C-NC	2.49	112.31	109.97
27	7	313	CLA	C2C-C1C-NC	2.49	112.30	109.97
27	7	303	CLA	C1-C2-C3	-2.49	121.74	126.04
29	O	205	II0	C38-C36-C40	-2.48	119.44	122.92
27	5	601	CLA	C2C-C1C-NC	2.48	112.30	109.97
28	9	610	KC2	CHD-C4C-NC	2.48	127.97	124.20
29	2	614	II0	C42-C41-C39	-2.48	118.39	123.47
29	5	620	II0	C20-C14-C12	2.48	118.95	114.36
31	8	609	IHT	C32-C33-C37	-2.48	115.14	118.94
29	O	205	II0	C42-C41-C39	-2.48	118.40	123.47
27	8	604	CLA	C3D-C4D-ND	2.48	114.24	110.24
27	9	608	CLA	C1-C2-C3	-2.47	121.76	126.04
32	8	614	LMG	O1-C7-C8	-2.47	104.93	110.90
27	2	603	CLA	C2C-C1C-NC	2.47	112.29	109.97
29	2	613	II0	C41-C39-C35	-2.47	123.78	127.31
33	7	319	LHG	O8-C23-C24	2.47	119.67	111.91
27	6	603	CLA	C2C-C1C-NC	2.47	112.29	109.97
27	B	817	CLA	C2C-C1C-NC	2.47	112.29	109.97
27	B	832	CLA	C2C-C1C-NC	2.47	112.29	109.97
27	O	201	CLA	C1-C2-C3	-2.47	121.77	126.04
27	B	814	CLA	C2C-C1C-NC	2.46	112.28	109.97
27	A	838	CLA	C2C-C1C-NC	2.46	112.28	109.97
29	6	615	II0	C38-C36-C40	-2.46	119.47	122.92
27	1	608	CLA	C1-C2-C3	-2.46	121.79	126.04
33	4	617	LHG	O8-C23-C24	2.46	119.63	111.91
27	5	613	CLA	C2C-C1C-NC	2.46	112.28	109.97
27	B	810	CLA	C2C-C1C-NC	2.46	112.28	109.97
29	9	615	II0	C08-C12-C14	-2.46	106.96	111.85
27	B	809	CLA	C2C-C1C-NC	2.46	112.27	109.97
29	1	616	II0	C06-C08-C12	-2.46	106.94	110.30
29	6	614	II0	C42-C40-C36	-2.46	123.80	127.31
31	9	619	IHT	C41-C38-C35	-2.46	123.80	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	826	CLA	C2C-C1C-NC	2.46	112.27	109.97
27	B	837	CLA	C2C-C1C-NC	2.46	112.27	109.97
27	4	606	CLA	C1-C2-C3	-2.46	121.80	126.04
31	Z	302	IHT	C36-C33-C32	2.45	121.94	118.08
27	6	609	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	5	614	II0	C20-C14-C12	2.45	118.89	114.36
31	2	616	IHT	C19-C10-C07	-2.45	121.78	124.53
33	a	617	LHG	O8-C23-C24	2.45	119.59	111.91
29	3	613	II0	C38-C36-C40	-2.45	119.50	122.92
27	A	829	CLA	C2C-C1C-NC	2.44	112.26	109.97
27	4	601	CLA	C2C-C1C-NC	2.44	112.26	109.97
27	B	823	CLA	C2C-C1C-NC	2.44	112.26	109.97
29	7	316	II0	C41-C39-C35	-2.44	123.83	127.31
27	1	609	CLA	C2C-C1C-NC	2.44	112.26	109.97
27	4	603	CLA	C2C-C1C-NC	2.44	112.26	109.97
29	R	204	II0	C19-C13-C09	-2.44	121.03	124.35
28	a	609	KC2	CHD-C4C-NC	2.44	127.90	124.20
31	5	618	IHT	C41-C38-C35	-2.44	123.83	127.31
32	F	205	LMG	O1-C1-C2	-2.44	104.50	108.30
31	6	616	IHT	C30-C27-C23	-2.44	123.83	127.31
29	Z	312	II0	C20-C14-C12	2.44	118.87	114.36
27	9	612	CLA	C2C-C1C-NC	2.44	112.25	109.97
27	Z	305	CLA	C2C-C1C-NC	2.43	112.25	109.97
29	5	620	II0	C19-C13-C09	-2.43	121.04	124.35
31	a	616	IHT	C20-C15-C12	2.43	118.86	114.36
27	5	612	CLA	C2C-C1C-NC	2.43	112.25	109.97
27	A	812	CLA	C1-C2-C3	-2.43	121.84	126.04
29	1	619	II0	C38-C36-C40	-2.43	119.52	122.92
27	3	609	CLA	C2C-C1C-NC	2.43	112.25	109.97
28	Z	307	KC2	CHD-C4C-NC	2.43	127.89	124.20
27	A	801	CLA	CHD-C1D-C2D	2.43	130.57	125.48
31	8	609	IHT	C30-C27-C23	-2.43	123.84	127.31
27	6	605	CLA	C2C-C1C-NC	2.43	112.25	109.97
29	b	614	II0	C41-C42-C40	-2.43	118.50	123.47
29	4	614	II0	C38-C36-C40	-2.43	119.52	122.92
27	A	808	CLA	C2C-C1C-NC	2.43	112.25	109.97
27	1	613	CLA	C2C-C1C-NC	2.43	112.24	109.97
33	3	619	LHG	C11-C10-C9	-2.42	102.11	114.42
27	B	818	CLA	C2C-C1C-NC	2.42	112.24	109.97
29	1	616	II0	C05-C07-C11	-2.42	106.99	110.30
27	F	204	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
27	A	805	CLA	C2C-C1C-NC	2.42	112.24	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	J	104	LMU	C3'-C4'-C5'	-2.42	105.38	110.93
27	A	806	CLA	C2C-C1C-NC	2.42	112.24	109.97
27	A	832	CLA	C2C-C1C-NC	2.42	112.24	109.97
27	7	310	CLA	C2C-C1C-NC	2.42	112.24	109.97
29	6	614	II0	C41-C39-C35	-2.42	123.86	127.31
29	9	615	II0	C42-C41-C39	-2.41	118.53	123.47
27	9	603	CLA	C2C-C1C-NC	2.41	112.23	109.97
27	5	606	CLA	CHC-C1C-C2C	-2.41	120.05	126.72
27	9	609	CLA	C2C-C1C-NC	2.41	112.23	109.97
27	B	841	CLA	C2C-C1C-NC	2.41	112.23	109.97
27	A	825	CLA	C2C-C1C-NC	2.41	112.23	109.97
33	2	620	LHG	O8-C23-C24	2.41	119.46	111.91
27	b	604	CLA	C2C-C1C-NC	2.41	112.23	109.97
27	B	803	CLA	C2C-C1C-NC	2.40	112.22	109.97
28	3	606	KC2	CHC-C4B-NB	2.40	126.66	124.45
28	b	609	KC2	CHB-C4A-NA	2.40	127.99	124.20
29	O	206	II0	C03-C09-C13	-2.40	119.24	122.63
32	3	620	LMG	O1-C7-C8	-2.40	105.11	110.90
27	B	804	CLA	C2C-C1C-NC	2.40	112.22	109.97
29	9	615	II0	C20-C14-C10	-2.40	121.09	124.35
27	4	607	CLA	C2C-C1C-NC	2.39	112.22	109.97
27	4	611	CLA	C2C-C1C-NC	2.39	112.22	109.97
29	b	614	II0	C38-C36-C40	-2.39	119.57	122.92
32	F	205	LMG	O1-C7-C8	-2.39	105.13	110.90
31	a	616	IHT	C30-C27-C23	-2.39	123.90	127.31
27	6	601	CLA	CHC-C1C-C2C	-2.39	120.11	126.72
27	b	607	CLA	C2C-C1C-NC	2.39	112.21	109.97
29	7	301	II0	C41-C42-C40	-2.39	118.59	123.47
29	1	617	II0	C19-C13-C09	-2.39	121.11	124.35
27	A	807	CLA	CHC-C1C-C2C	-2.38	120.12	126.72
31	8	609	IHT	C19-C10-C07	-2.38	121.85	124.53
27	a	606	CLA	C2C-C1C-NC	2.38	112.20	109.97
29	O	206	II0	C41-C42-C40	-2.38	118.59	123.47
29	5	616	II0	C41-C42-C40	-2.38	118.59	123.47
27	6	607	CLA	C2C-C1C-NC	2.38	112.20	109.97
27	B	816	CLA	C1-C2-C3	-2.38	121.92	126.04
27	5	607	CLA	C2C-C1C-NC	2.38	112.20	109.97
27	8	608	CLA	C2C-C1C-NC	2.38	112.20	109.97
27	A	810	CLA	C2C-C1C-NC	2.38	112.20	109.97
27	4	609	CLA	CHC-C1C-C2C	-2.38	120.15	126.72
31	a	616	IHT	C27-C30-C32	-2.38	115.80	123.22
27	5	605	CLA	C2C-C1C-NC	2.38	112.20	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	O	206	II0	C05-C07-C11	2.38	113.56	110.30
27	A	827	CLA	CHC-C1C-C2C	-2.38	120.15	126.72
27	B	838	CLA	C2C-C1C-NC	2.37	112.20	109.97
27	J	102	CLA	C2C-C1C-NC	2.37	112.20	109.97
29	9	618	II0	C20-C14-C10	-2.37	121.12	124.35
31	L	204	IHT	C41-C38-C35	-2.37	123.92	127.31
30	b	613	II3	C26-C29-C32	-2.37	115.81	123.22
27	B	807	CLA	C2C-C1C-NC	2.37	112.19	109.97
27	1	603	CLA	C2C-C1C-NC	2.37	112.19	109.97
27	A	830	CLA	C2C-C1C-NC	2.37	112.19	109.97
27	7	303	CLA	C2C-C1C-NC	2.37	112.19	109.97
29	B	843	II0	C38-C36-C40	-2.37	119.61	122.92
27	A	822	CLA	C2C-C1C-NC	2.37	112.19	109.97
27	A	826	CLA	C2C-C1C-NC	2.37	112.19	109.97
29	2	613	II0	C06-C08-C12	-2.37	107.07	110.30
29	9	616	II0	C41-C42-C40	-2.37	118.63	123.47
27	9	601	CLA	CHC-C1C-C2C	-2.36	120.18	126.72
27	9	604	CLA	C2C-C1C-NC	2.36	112.19	109.97
29	a	613	II0	C05-C07-C11	-2.36	107.07	110.30
27	6	604	CLA	C2C-C1C-NC	2.36	112.19	109.97
29	7	314	II0	C05-C07-C11	-2.36	107.07	110.30
27	B	822	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
29	6	614	II0	C04-C10-C14	-2.36	119.30	122.63
27	B	834	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
28	a	609	KC2	CHB-C4A-NA	2.36	127.92	124.20
27	O	201	CLA	C2C-C1C-NC	2.36	112.18	109.97
27	A	839	CLA	C2C-C1C-NC	2.36	112.18	109.97
33	A	852	LHG	C11-C10-C9	-2.35	102.47	114.42
27	7	305	CLA	C2C-C1C-NC	2.35	112.18	109.97
28	4	605	KC2	CHD-C4C-NC	2.35	127.78	124.20
27	9	605	CLA	C2C-C1C-NC	2.35	112.18	109.97
27	B	825	CLA	C1-C2-C3	-2.35	121.97	126.04
27	Z	304	CLA	C2C-C1C-NC	2.35	112.17	109.97
27	9	614	CLA	C2C-C1C-NC	2.35	112.17	109.97
28	9	610	KC2	CHB-C4A-NA	2.35	127.91	124.20
27	5	602	CLA	C2C-C1C-NC	2.35	112.17	109.97
27	1	606	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
29	9	616	II0	C19-C13-C09	-2.34	121.16	124.35
27	3	612	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
29	7	317	II0	C33-C35-C39	-2.34	115.35	118.94
29	O	206	II0	C06-C08-C12	-2.34	107.10	110.30
27	A	809	CLA	CHD-C1D-C2D	2.34	130.39	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	605	CLA	C1-C2-C3	-2.34	122.00	126.04
29	4	612	II0	C41-C39-C35	-2.34	123.97	127.31
39	B	848	DGD	CDB-CCB-CBB	-2.34	102.56	114.42
27	F	203	CLA	CHC-C1C-C2C	-2.34	120.26	126.72
28	6	613	KC2	CHC-C4B-NB	2.34	126.60	124.45
29	7	315	II0	C05-C07-C11	-2.33	107.11	110.30
27	A	842	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
27	5	601	CLA	CHD-C1D-C2D	2.33	130.38	125.48
27	a	608	CLA	O2A-C1-C2	2.33	114.77	108.64
27	A	819	CLA	C2C-C1C-NC	2.33	112.16	109.97
27	9	606	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
29	2	615	II0	C38-C36-C40	-2.33	119.66	122.92
31	1	618	IHT	C25-C23-C27	-2.33	119.66	122.92
27	1	605	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
33	A	852	LHG	O8-C23-C24	2.33	119.23	111.91
27	L	203	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
27	7	302	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
27	B	819	CLA	CBA-CAA-C2A	2.33	120.74	113.86
27	b	611	CLA	C2C-C1C-NC	2.33	112.16	109.97
28	2	610	KC2	CHC-C4B-NB	2.33	126.59	124.45
27	a	601	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
31	8	609	IHT	C06-C09-C10	2.33	118.24	114.08
27	L	201	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
33	2	619	LHG	C11-C10-C9	-2.33	102.61	114.42
29	a	615	II0	C38-C36-C34	2.33	121.74	118.08
27	A	835	CLA	CHC-C1C-C2C	-2.32	120.29	126.72
29	7	301	II0	C03-C09-C13	-2.32	119.35	122.63
27	4	602	CLA	C2C-C1C-NC	2.32	112.15	109.97
29	5	615	II0	C19-C13-C09	-2.32	121.19	124.35
28	b	605	KC2	CHD-C4C-NC	2.32	127.72	124.20
27	6	606	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
29	7	315	II0	C06-C08-C12	-2.32	107.13	110.30
29	a	614	II0	C05-C07-C11	-2.32	107.13	110.30
27	2	601	CLA	C2C-C1C-NC	2.32	112.14	109.97
27	b	610	CLA	C2C-C1C-NC	2.32	112.14	109.97
27	A	816	CLA	CHC-C1C-C2C	-2.32	120.32	126.72
30	b	613	II3	C37-C38-C40	-2.31	115.39	118.94
29	2	615	II0	C19-C13-C11	2.31	118.64	114.36
27	3	602	CLA	C2C-C1C-NC	2.31	112.14	109.97
27	1	612	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
33	5	619	LHG	C5-O7-C7	-2.31	113.59	117.90
35	A	853	8CT	C07-C02-C03	-2.31	119.38	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	608	CLA	C1-C2-C3	-2.31	122.05	126.04
27	B	828	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
27	B	839	CLA	C2C-C1C-NC	2.31	112.14	109.97
27	B	840	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
29	a	615	II0	C05-C07-C11	-2.31	107.14	110.30
27	Z	306	CLA	C2C-C1C-NC	2.31	112.13	109.97
31	1	618	IHT	C19-C10-C09	2.31	118.05	113.62
27	8	605	CLA	CHD-C1D-C2D	2.31	130.32	125.48
31	1	618	IHT	C41-C40-C37	-2.31	118.75	123.47
27	B	804	CLA	CAA-C2A-C1A	-2.31	104.42	111.97
27	B	836	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
29	4	615	II0	C41-C42-C40	-2.31	118.75	123.47
27	A	833	CLA	CHC-C1C-C2C	-2.30	120.35	126.72
29	b	614	II0	C19-C13-C11	2.30	118.62	114.36
27	B	829	CLA	C2C-C1C-NC	2.30	112.13	109.97
27	a	602	CLA	CAA-C2A-C3A	2.30	119.08	112.78
29	7	301	II0	C20-C14-C12	2.30	118.62	114.36
27	5	611	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
29	3	613	II0	C42-C41-C39	-2.30	118.76	123.47
27	3	611	CLA	C2C-C1C-NC	2.30	112.13	109.97
29	O	206	II0	C41-C39-C35	-2.30	124.03	127.31
28	7	307	KC2	CHB-C4A-NA	2.30	127.82	124.20
28	Z	307	KC2	C4C-C3C-C2C	2.30	108.94	107.11
29	a	612	II0	C38-C36-C40	-2.30	119.71	122.92
27	1	609	CLA	CHC-C1C-C2C	-2.30	120.37	126.72
27	Z	310	CLA	C2C-C1C-NC	2.30	112.12	109.97
29	1	619	II0	C19-C13-C11	2.30	118.61	114.36
27	A	810	CLA	CHA-C1A-NA	-2.29	121.14	126.40
27	5	609	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
27	1	601	CLA	C2C-C1C-NC	2.29	112.12	109.97
29	2	613	II0	C20-C14-C12	2.29	118.60	114.36
27	3	607	CLA	C2C-C1C-NC	2.29	112.12	109.97
27	4	608	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
28	3	606	KC2	CHD-C4C-NC	2.29	127.68	124.20
29	7	316	II0	C20-C14-C12	2.29	118.60	114.36
27	2	606	CLA	C2C-C1C-NC	2.29	112.12	109.97
31	6	616	IHT	C04-C02-C07	-2.29	106.95	110.48
27	A	844	CLA	CHD-C1D-C2D	2.29	130.28	125.48
27	A	821	CLA	C2C-C1C-NC	2.29	112.12	109.97
27	B	802	CLA	CHD-C1D-C2D	2.29	130.28	125.48
29	a	614	II0	C41-C39-C35	-2.29	124.05	127.31
27	6	609	CLA	CHC-C1C-C2C	-2.29	120.39	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	601	CLA	CHC-C1C-C2C	-2.29	120.40	126.72
27	A	844	CLA	C2C-C1C-NC	2.29	112.11	109.97
27	B	830	CLA	C2C-C1C-NC	2.28	112.11	109.97
29	8	611	II0	C41-C42-C40	-2.28	118.80	123.47
27	B	821	CLA	C2C-C1C-NC	2.28	112.11	109.97
27	a	610	CLA	C2C-C1C-NC	2.28	112.11	109.97
34	O	207	SQD	C45-O47-C7	-2.28	112.17	117.79
27	4	610	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
27	1	607	CLA	C2C-C1C-NC	2.28	112.11	109.97
27	B	811	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
27	b	608	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
29	9	616	II0	C20-C14-C12	2.28	118.58	114.36
31	8	609	IHT	C41-C38-C35	-2.28	124.06	127.31
28	4	605	KC2	CHC-C4B-NB	2.28	126.55	124.45
27	8	601	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
27	A	802	CLA	C2C-C1C-NC	2.28	112.11	109.97
29	3	616	II0	C42-C41-C39	-2.28	118.81	123.47
27	A	822	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
27	7	306	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
27	A	828	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
27	2	611	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
27	A	803	CLA	CHD-C1D-C2D	2.28	130.25	125.48
27	A	837	CLA	CHC-C1C-C2C	-2.28	120.43	126.72
27	B	801	CLA	C2C-C1C-NC	2.28	112.10	109.97
27	a	605	CLA	CHD-C1D-C2D	2.28	130.25	125.48
27	2	603	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
27	3	610	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
27	A	823	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
29	7	317	II0	C20-C14-C12	2.27	118.57	114.36
32	8	616	LMG	O3-C3-C2	-2.27	105.09	110.35
27	A	805	CLA	CHD-C1D-C2D	2.27	130.25	125.48
30	1	615	II3	C39-C41-C40	-2.27	118.82	123.47
27	A	801	CLA	C2C-C1C-NC	2.27	112.10	109.97
28	b	605	KC2	C4C-C3C-C2C	2.27	108.92	107.11
32	2	617	LMG	O2-C2-C1	-2.27	104.53	110.05
27	5	603	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
27	K	102	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
27	9	606	CLA	CAA-C2A-C1A	-2.27	104.53	111.97
27	8	603	CLA	C2C-C1C-NC	2.27	112.10	109.97
27	B	829	CLA	CHD-C1D-C2D	2.27	130.24	125.48
27	5	601	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
27	9	613	CLA	CHC-C1C-C2C	-2.27	120.44	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	605	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
31	8	609	IHT	C27-C30-C32	-2.27	116.13	123.22
27	2	607	CLA	C2C-C1C-NC	2.27	112.10	109.97
27	B	812	CLA	C2C-C1C-NC	2.27	112.10	109.97
29	4	615	II0	C19-C13-C11	2.27	118.56	114.36
27	B	820	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
29	6	615	II0	C20-C14-C12	2.27	118.56	114.36
27	A	815	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
29	R	204	II0	C34-C36-C40	-2.27	115.46	118.94
27	B	806	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
27	A	834	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
28	1	610	KC2	CHD-C4C-NC	2.27	127.64	124.20
27	3	604	CLA	CHC-C1C-C2C	-2.27	120.46	126.72
31	6	616	IHT	C41-C38-C35	-2.26	124.08	127.31
33	2	618	LHG	O8-C23-C24	2.26	119.01	111.91
29	7	315	II0	C42-C41-C39	-2.26	118.84	123.47
32	6	618	LMG	O2-C2-C1	-2.26	104.55	110.05
27	4	601	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
27	A	821	CLA	CHD-C1D-C2D	2.26	130.23	125.48
27	2	612	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
29	3	614	II0	C33-C35-C39	-2.26	115.47	118.94
33	3	619	LHG	C18-C17-C16	-2.26	102.94	114.42
27	b	603	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
28	6	610	KC2	CHC-C4B-NB	2.26	126.53	124.45
27	B	827	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
27	B	831	CLA	CHD-C1D-C2D	2.26	130.22	125.48
28	9	610	KC2	C4C-C3C-C2C	2.26	108.91	107.11
27	B	830	CLA	CHD-C1D-C2D	2.26	130.22	125.48
32	2	617	LMG	O3-C3-C2	-2.26	105.13	110.35
27	9	609	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
32	8	614	LMG	O2-C2-C1	-2.26	104.56	110.05
27	6	611	CLA	CHC-C1C-C2C	-2.26	120.48	126.72
27	O	204	CLA	CHC-C1C-C2C	-2.26	120.48	126.72
31	A	854	IHT	C18-C07-C10	-2.26	116.00	121.46
29	3	615	II0	C41-C39-C35	-2.25	124.09	127.31
27	8	604	CLA	CHC-C1C-C2C	-2.25	120.48	126.72
27	A	818	CLA	CHC-C1C-C2C	-2.25	120.48	126.72
27	7	310	CLA	CHC-C1C-C2C	-2.25	120.49	126.72
27	B	807	CLA	CHC-C1C-C2C	-2.25	120.49	126.72
29	6	614	II0	C05-C07-C11	-2.25	107.22	110.30
29	9	618	II0	C06-C08-C12	-2.25	107.22	110.30
28	b	609	KC2	CHC-C4B-NB	2.25	126.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	802	CLA	CHA-C1A-NA	-2.25	121.24	126.40
27	B	823	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
27	A	814	CLA	CHD-C1D-C2D	2.25	130.20	125.48
27	1	608	CLA	C2C-C1C-NC	2.25	112.08	109.97
27	B	829	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
27	O	201	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
27	B	822	CLA	O2A-C1-C2	-2.25	102.72	108.64
31	L	204	IHT	C09-C10-C07	-2.25	119.47	122.73
27	8	606	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
31	L	204	IHT	C22-C23-C27	-2.25	115.49	118.94
27	1	611	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
27	a	608	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
27	B	837	CLA	CHD-C1D-C2D	2.25	130.20	125.48
27	6	612	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
27	A	818	CLA	CHD-C1D-C2D	2.25	130.19	125.48
29	2	615	II0	C41-C42-C40	-2.25	118.87	123.47
27	1	604	CLA	C2C-C1C-NC	2.25	112.08	109.97
27	8	615	CLA	C2C-C1C-NC	2.25	112.08	109.97
27	5	613	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
27	B	838	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
30	1	615	II3	C21-C24-C26	-2.25	115.49	118.94
29	1	614	II0	C41-C39-C35	-2.25	124.11	127.31
27	2	606	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
27	A	820	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
27	A	836	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
28	b	605	KC2	CHC-C4B-NB	2.24	126.52	124.45
29	4	614	II0	C41-C42-C40	-2.24	118.88	123.47
27	1	603	CLA	CHC-C1C-C2C	-2.24	120.51	126.72
27	K	101	CLA	CHC-C1C-C2C	-2.24	120.51	126.72
28	6	613	KC2	CHB-C4A-NA	2.24	127.74	124.20
28	b	605	KC2	CHB-C4A-NA	2.24	127.74	124.20
27	4	603	CLA	CHD-C1D-C2D	2.24	130.19	125.48
32	8	614	LMG	O3-C3-C2	-2.24	105.16	110.35
27	4	603	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
27	A	803	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
27	A	817	CLA	CHD-C1D-C2D	2.24	130.18	125.48
27	A	804	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
27	A	831	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
27	A	840	CLA	CHD-C1D-C2D	2.24	130.18	125.48
27	B	819	CLA	C2C-C1C-NC	2.24	112.07	109.97
29	O	205	II0	C20-C14-C12	2.24	118.51	114.36
27	5	612	CLA	CHD-C1D-C2D	2.24	130.18	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	304	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
27	9	605	CLA	CHD-C1D-C2D	2.24	130.18	125.48
27	F	202	CLA	C2C-C1C-NC	2.24	112.07	109.97
27	A	827	CLA	CHD-C1D-C2D	2.24	130.18	125.48
31	L	204	IHT	C32-C33-C37	-2.24	115.51	118.94
27	9	604	CLA	CHD-C1D-C2D	2.24	130.18	125.48
29	a	613	II0	C38-C36-C40	-2.24	119.79	122.92
27	1	613	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
27	B	827	CLA	CHD-C1D-C2D	2.24	130.17	125.48
28	7	307	KC2	CHC-C4B-NB	2.24	126.51	124.45
27	O	202	CLA	CHD-C1D-C2D	2.24	130.17	125.48
31	a	616	IHT	C05-C08-C12	-2.24	107.24	110.30
29	2	615	II0	C41-C39-C35	-2.24	124.12	127.31
27	B	833	CLA	CHC-C1C-C2C	-2.24	120.54	126.72
27	6	607	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
27	9	612	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
27	B	825	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
27	9	611	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
27	7	308	CLA	CHD-C1D-C2D	2.23	130.16	125.48
27	2	607	CLA	CHD-C1D-C2D	2.23	130.16	125.48
27	9	608	CLA	C2C-C1C-NC	2.23	112.06	109.97
27	Z	301	CLA	C2C-C1C-NC	2.23	112.06	109.97
27	6	603	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
27	7	312	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
27	9	603	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
27	A	809	CLA	C3A-C2A-C1A	-2.23	98.00	101.34
27	A	824	CLA	CHD-C1D-C2D	2.23	130.16	125.48
27	A	814	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
29	3	617	II0	C41-C42-C40	-2.23	118.91	123.47
31	a	616	IHT	C18-C22-C23	-2.23	122.87	126.23
27	3	610	CLA	CHD-C1D-C2D	2.23	130.16	125.48
27	B	817	CLA	CHD-C1D-C2D	2.23	130.16	125.48
28	7	311	KC2	CHB-C4A-NA	2.23	127.72	124.20
27	A	829	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
27	2	604	CLA	CHD-C1D-C2D	2.23	130.15	125.48
27	B	818	CLA	CHD-C1D-C2D	2.23	130.15	125.48
31	Z	302	IHT	C25-C23-C27	-2.23	119.80	122.92
27	B	832	CLA	CHD-C1D-C2D	2.23	130.15	125.48
27	Z	305	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
29	5	617	II0	C41-C42-C40	-2.23	118.92	123.47
29	Z	312	II0	C38-C36-C40	-2.23	119.81	122.92
33	3	622	LHG	C11-C10-C9	-2.22	103.13	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	6	616	IHT	C22-C23-C27	-2.22	115.53	118.94
27	a	611	CLA	C2C-C1C-NC	2.22	112.06	109.97
27	B	810	CLA	CHC-C1C-C2C	-2.22	120.57	126.72
27	A	843	CLA	CHD-C1D-C2D	2.22	130.15	125.48
32	8	616	LMG	O1-C7-C8	-2.22	105.53	110.90
27	3	609	CLA	CHC-C1C-C2C	-2.22	120.57	126.72
27	A	838	CLA	CHC-C1C-C2C	-2.22	120.57	126.72
27	9	614	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	B	803	CLA	CHD-C1D-C2D	2.22	130.14	125.48
27	F	202	CLA	CHD-C1D-C2D	2.22	130.14	125.48
27	B	816	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	B	841	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	O	201	CLA	CHD-C1D-C2D	2.22	130.14	125.48
27	8	607	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	B	837	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	A	841	CLA	CAA-C2A-C1A	-2.22	104.70	111.97
28	a	609	KC2	C4C-C3C-C2C	2.22	108.88	107.11
27	A	839	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	2	604	CLA	C2C-C1C-NC	2.22	112.05	109.97
27	3	601	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	A	813	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	O	203	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
28	2	610	KC2	CHD-C4C-NC	2.22	127.57	124.20
28	6	613	KC2	CHD-C4C-NC	2.22	127.57	124.20
32	3	620	LMG	O3-C3-C2	-2.22	105.22	110.35
27	A	803	CLA	CAA-C2A-C1A	-2.22	104.70	111.97
27	2	607	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
27	7	304	CLA	CHD-C1D-C2D	2.22	130.13	125.48
27	B	814	CLA	CHD-C1D-C2D	2.22	130.13	125.48
27	J	102	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
31	9	619	IHT	C20-C15-C11	-2.22	121.33	124.35
27	2	609	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
33	3	619	LHG	C20-C19-C18	-2.22	103.17	114.42
27	4	604	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
27	7	309	CLA	C2C-C1C-NC	2.22	112.05	109.97
27	3	605	CLA	CHD-C1D-C2D	2.22	130.13	125.48
31	8	609	IHT	C22-C23-C27	-2.22	115.54	118.94
27	1	601	CLA	CHD-C1D-C2D	2.22	130.13	125.48
27	B	801	CLA	CHD-C1D-C2D	2.22	130.13	125.48
27	O	204	CLA	CHD-C1D-C2D	2.22	130.13	125.48
29	1	616	II0	C20-C14-C12	2.22	118.46	114.36
31	A	854	IHT	C40-C41-C38	-2.21	118.94	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	812	CLA	CHA-C1A-NA	-2.21	121.33	126.40
27	b	604	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
27	A	808	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
27	8	606	CLA	CHD-C1D-C2D	2.21	130.12	125.48
27	8	603	CLA	CHD-C1D-C2D	2.21	130.12	125.48
27	1	607	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
30	b	613	II3	C32-C33-C36	-2.21	115.55	118.94
27	B	824	CLA	C2C-C1C-NC	2.21	112.05	109.97
27	a	603	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
29	1	614	II0	C05-C07-C11	-2.21	107.28	110.30
29	1	617	II0	C20-C14-C12	2.21	118.45	114.36
27	B	818	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
27	5	608	CLA	CHD-C1D-C2D	2.21	130.12	125.48
27	B	813	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
27	2	612	CLA	CHD-C1D-C2D	2.21	130.12	125.48
27	3	603	CLA	C2C-C1C-NC	2.21	112.04	109.97
27	9	607	CLA	C2C-C1C-NC	2.21	112.04	109.97
27	6	603	CLA	CHD-C1D-C2D	2.21	130.12	125.48
27	B	808	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
27	A	826	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	J	102	CLA	CAA-C2A-C1A	-2.21	106.35	111.81
27	b	611	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
27	A	834	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	2	602	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	A	829	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	8	615	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
33	A	851	LHG	C11-C10-C9	-2.21	103.21	114.42
27	Z	310	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
31	A	854	IHT	C41-C38-C35	-2.21	124.16	127.31
29	8	610	II0	C42-C40-C36	-2.21	124.16	127.31
33	b	616	LHG	C20-C19-C18	-2.21	103.22	114.42
27	A	810	CLA	CHC-C1C-C2C	-2.21	120.62	126.72
27	6	606	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	2	601	CLA	CHC-C1C-C2C	-2.21	120.62	126.72
27	Z	306	CLA	CHC-C1C-C2C	-2.21	120.62	126.72
27	2	609	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	B	811	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	J	102	CLA	CHD-C1D-C2D	2.21	130.11	125.48
27	A	844	CLA	CBA-CAA-C2A	2.21	120.37	113.86
27	B	801	CLA	CHA-C1A-NA	-2.20	121.35	126.40
27	L	202	CLA	CHD-C1D-C2D	2.20	130.10	125.48
27	B	819	CLA	CHC-C1C-C2C	-2.20	120.62	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Z	312	II0	C41-C39-C35	-2.20	124.17	127.31
30	b	613	II3	C31-C34-C37	-2.20	116.34	123.22
27	A	819	CLA	CHD-C1D-C2D	2.20	130.10	125.48
27	B	840	CLA	CHD-C1D-C2D	2.20	130.10	125.48
27	5	604	CLA	CHD-C1D-C2D	2.20	130.09	125.48
27	2	605	CLA	C2C-C1C-NC	2.20	112.03	109.97
27	Z	306	CLA	CHD-C1D-C2D	2.20	130.09	125.48
27	A	830	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
27	8	608	CLA	CHD-C1D-C2D	2.20	130.09	125.48
27	B	806	CLA	CHD-C1D-C2D	2.20	130.09	125.48
29	8	611	II0	C06-C08-C12	-2.20	107.29	110.30
27	A	833	CLA	CHD-C1D-C2D	2.20	130.09	125.48
27	B	824	CLA	CHD-C1D-C2D	2.20	130.09	125.48
27	A	841	CLA	CHD-C1D-C2D	2.20	130.09	125.48
27	1	602	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
27	A	821	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
27	b	601	CLA	CHD-C1D-C2D	2.20	130.09	125.48
29	5	614	II0	C05-C07-C11	-2.20	107.30	110.30
39	Z	303	DGD	CAB-C9B-C8B	-2.20	103.28	114.42
27	A	817	CLA	C2C-C1C-NC	2.20	112.03	109.97
27	B	828	CLA	CHD-C1D-C2D	2.20	130.09	125.48
27	B	821	CLA	CHC-C1C-C2C	-2.19	120.65	126.72
27	A	844	CLA	CHA-C1A-NA	-2.19	121.37	126.40
27	B	813	CLA	CBA-CAA-C2A	2.19	120.34	113.86
27	B	814	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
27	B	826	CLA	CHD-C1D-C2D	2.19	130.08	125.48
32	6	618	LMG	O3-C3-C2	-2.19	105.28	110.35
27	A	813	CLA	CHD-C1D-C2D	2.19	130.08	125.48
32	3	618	LMG	O3-C3-C2	-2.19	105.28	110.35
32	F	205	LMG	O2-C2-C1	-2.19	104.72	110.05
27	1	601	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
29	8	611	II0	C38-C36-C40	-2.19	119.85	122.92
29	9	617	II0	C19-C13-C09	-2.19	121.37	124.35
32	3	620	LMG	O1-C1-C2	-2.19	104.88	108.30
27	5	612	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
27	B	822	CLA	CHD-C1D-C2D	2.19	130.07	125.48
27	B	810	CLA	CHD-C1D-C2D	2.19	130.07	125.48
27	6	604	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
27	3	610	CLA	C1-C2-C3	-2.19	122.26	126.04
27	7	313	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
27	A	837	CLA	CHD-C1D-C2D	2.19	130.07	125.48
32	6	618	LMG	O1-C7-C8	-2.19	105.62	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	605	CLA	CHD-C1D-C2D	2.19	130.07	125.48
33	A	851	LHG	C20-C19-C18	-2.19	103.32	114.42
27	B	803	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
27	4	611	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
27	2	601	CLA	CHD-C1D-C2D	2.19	130.06	125.48
27	A	839	CLA	CHD-C1D-C2D	2.19	130.06	125.48
27	2	608	CLA	C1-C2-C3	-2.19	122.26	126.04
27	5	602	CLA	CHD-C1D-C2D	2.19	130.06	125.48
27	A	811	CLA	CHD-C1D-C2D	2.19	130.06	125.48
29	3	613	II0	C19-C13-C11	2.19	118.40	114.36
27	B	841	CLA	CHD-C1D-C2D	2.18	130.06	125.48
27	9	604	CLA	CHC-C1C-C2C	-2.18	120.68	126.72
27	6	604	CLA	CHD-C1D-C2D	2.18	130.06	125.48
33	4	620	LHG	C27-C26-C25	-2.18	103.34	114.42
27	6	605	CLA	CHC-C1C-C2C	-2.18	120.68	126.72
27	2	605	CLA	CHC-C1C-C2C	-2.18	120.68	126.72
27	4	606	CLA	CHC-C1C-C2C	-2.18	120.68	126.72
27	7	305	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
27	9	606	CLA	CHD-C1D-C2D	2.18	130.06	125.48
27	B	802	CLA	C2C-C1C-NC	2.18	112.02	109.97
27	b	606	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
28	1	610	KC2	C4C-C3C-C2C	2.18	108.85	107.11
27	5	607	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
28	5	610	KC2	CHC-C4B-NB	2.18	126.46	124.45
27	B	817	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
32	2	617	LMG	O1-C7-C8	-2.18	105.64	110.90
28	4	605	KC2	C4C-C3C-C2C	2.18	108.84	107.11
29	4	615	II0	C38-C36-C40	-2.18	119.87	122.92
29	R	204	II0	C06-C08-C12	-2.18	107.32	110.30
29	3	617	II0	C41-C39-C35	-2.18	124.20	127.31
29	9	615	II0	C05-C07-C11	-2.18	107.32	110.30
27	8	615	CLA	CHD-C1D-C2D	2.18	130.04	125.48
27	A	802	CLA	CHD-C1D-C2D	2.18	130.04	125.48
27	A	816	CLA	CHD-C1D-C2D	2.18	130.04	125.48
27	B	836	CLA	CHD-C1D-C2D	2.18	130.04	125.48
27	B	838	CLA	CHD-C1D-C2D	2.18	130.04	125.48
27	Z	301	CLA	CHD-C1D-C2D	2.18	130.04	125.48
27	b	610	CLA	CHD-C1D-C2D	2.18	130.04	125.48
27	9	607	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
27	4	606	CLA	CHD-C1D-C2D	2.18	130.04	125.48
31	A	854	IHT	C19-C10-C09	2.17	117.79	113.62
27	A	832	CLA	CHD-C1D-C2D	2.17	130.04	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1	618	IHT	C41-C38-C35	-2.17	124.21	127.31
27	L	202	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
27	3	603	CLA	CHD-C1D-C2D	2.17	130.04	125.48
27	B	808	CLA	CHD-C1D-C2D	2.17	130.04	125.48
27	6	612	CLA	CAA-C2A-C1A	-2.17	104.85	111.97
27	1	606	CLA	CHD-C1D-C2D	2.17	130.04	125.48
27	9	612	CLA	CHD-C1D-C2D	2.17	130.04	125.48
27	Z	305	CLA	CHD-C1D-C2D	2.17	130.04	125.48
28	Z	307	KC2	CHC-C4B-NB	2.17	126.45	124.45
27	9	614	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	B	804	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
27	B	805	CLA	C2C-C1C-NC	2.17	112.01	109.97
29	a	615	II0	C42-C41-C39	-2.17	119.03	123.47
27	Z	310	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	A	832	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
27	a	610	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	b	603	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	1	604	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
27	A	825	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
27	4	611	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	A	836	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	a	606	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
27	9	609	CLA	CAA-C2A-C1A	-2.17	106.45	111.81
27	a	602	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	9	605	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
27	A	828	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	A	819	CLA	CHC-C1C-C2C	-2.17	120.73	126.72
27	7	302	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	B	819	CLA	CHD-C1D-C2D	2.17	130.03	125.48
27	B	809	CLA	CHC-C1C-C2C	-2.17	120.73	126.72
27	7	313	CLA	CHD-C1D-C2D	2.17	130.02	125.48
27	9	602	CLA	C2C-C1C-NC	2.17	112.00	109.97
27	K	102	CLA	C2C-C1C-NC	2.17	112.00	109.97
27	2	604	CLA	CHC-C1C-C2C	-2.17	120.73	126.72
27	8	603	CLA	CHC-C1C-C2C	-2.17	120.73	126.72
27	A	812	CLA	CHD-C1D-C2D	2.16	130.02	125.48
27	1	613	CLA	CHD-C1D-C2D	2.16	130.02	125.48
32	8	616	LMG	C42-C41-C40	-2.16	103.44	114.42
29	5	614	II0	C19-C13-C09	-2.16	121.41	124.35
27	K	102	CLA	CHC-C1C-NC	2.16	127.48	124.20
27	3	603	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
27	B	816	CLA	CHD-C1D-C2D	2.16	130.02	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	607	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
27	B	804	CLA	CHD-C1D-C2D	2.16	130.02	125.48
28	5	610	KC2	CHD-C4C-NC	2.16	127.48	124.20
33	a	617	LHG	C11-C10-C9	-2.16	103.45	114.42
27	3	611	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
27	1	607	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	2	603	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	6	609	CLA	CHD-C1D-C2D	2.16	130.01	125.48
29	R	204	II0	C03-C09-C13	-2.16	119.58	122.63
27	5	603	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	8	604	CLA	CHA-C1A-NA	-2.16	121.45	126.40
27	3	602	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
27	2	611	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	5	605	CLA	CHD-C1D-C2D	2.16	130.01	125.48
30	b	613	II3	C41-C39-C36	-2.16	119.05	123.47
28	2	610	KC2	C4C-C3C-C2C	2.16	108.83	107.11
27	2	606	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	5	606	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	A	807	CLA	CHD-C1D-C2D	2.16	130.01	125.48
27	L	201	CLA	CHD-C1D-C2D	2.16	130.01	125.48
33	Z	311	LHG	C11-C10-C9	-2.16	103.47	114.42
27	8	615	CLA	C1-C2-C3	-2.16	122.31	126.04
27	A	806	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
27	6	601	CLA	CHD-C1D-C2D	2.16	130.00	125.48
27	A	808	CLA	CHD-C1D-C2D	2.16	130.00	125.48
27	A	805	CLA	CHC-C1C-C2C	-2.16	120.76	126.72
33	4	620	LHG	C11-C10-C9	-2.16	103.48	114.42
27	8	604	CLA	C1-C2-C3	-2.16	122.31	126.04
27	A	825	CLA	CHD-C1D-C2D	2.16	130.00	125.48
27	A	830	CLA	CHD-C1D-C2D	2.16	130.00	125.48
27	b	608	CLA	CHD-C1D-C2D	2.16	130.00	125.48
27	7	308	CLA	C2C-C1C-NC	2.16	111.99	109.97
27	B	830	CLA	CHC-C1C-C2C	-2.16	120.76	126.72
27	B	820	CLA	CHD-C1D-C2D	2.16	130.00	125.48
31	1	618	IHT	C02-C07-C18	-2.15	109.68	115.78
28	9	610	KC2	CHC-C4B-NB	2.15	126.43	124.45
27	F	203	CLA	CHD-C1D-C2D	2.15	130.00	125.48
27	O	203	CLA	CHD-C1D-C2D	2.15	130.00	125.48
27	2	602	CLA	C2C-C1C-NC	2.15	111.99	109.97
27	7	305	CLA	CHD-C1D-C2D	2.15	130.00	125.48
27	B	833	CLA	CHD-C1D-C2D	2.15	130.00	125.48
32	F	205	LMG	C3-C4-C5	-2.15	106.40	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	612	CLA	CHD-C1D-C2D	2.15	129.99	125.48
27	6	602	CLA	C2C-C1C-NC	2.15	111.99	109.97
29	9	616	II0	C06-C08-C12	-2.15	107.36	110.30
27	5	607	CLA	CHD-C1D-C2D	2.15	129.99	125.48
31	Z	302	IHT	C05-C08-C12	-2.15	107.36	110.30
27	5	613	CLA	CHD-C1D-C2D	2.15	129.99	125.48
27	5	604	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
27	A	826	CLA	CHA-C1A-NA	-2.15	121.47	126.40
27	8	601	CLA	CHD-C1D-C2D	2.15	129.99	125.48
27	b	611	CLA	CHD-C1D-C2D	2.15	129.99	125.48
27	b	607	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
27	3	607	CLA	CHD-C1D-C2D	2.15	129.99	125.48
29	a	615	II0	C41-C39-C35	-2.15	124.24	127.31
29	R	204	II0	C20-C14-C12	2.15	118.33	114.36
27	B	832	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
27	2	602	CLA	CAA-C2A-C3A	2.15	118.66	112.78
28	6	610	KC2	C4C-C3C-C2C	2.15	108.82	107.11
27	8	607	CLA	CHD-C1D-C2D	2.15	129.98	125.48
27	B	815	CLA	CHD-C1D-C2D	2.15	129.98	125.48
30	1	615	II3	C41-C39-C36	-2.15	119.08	123.47
27	a	604	CLA	CHD-C1D-C2D	2.15	129.98	125.48
27	3	607	CLA	CHC-C1C-C2C	-2.15	120.79	126.72
27	A	817	CLA	CHC-C1C-C2C	-2.15	120.79	126.72
27	B	835	CLA	CHD-C1D-C2D	2.15	129.98	125.48
29	7	317	II0	C29-C31-C33	-2.15	116.52	123.22
33	b	616	LHG	C11-C10-C9	-2.14	103.54	114.42
27	Z	301	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
27	6	607	CLA	CHD-C1D-C2D	2.14	129.98	125.48
27	B	826	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
27	a	611	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
33	4	619	LHG	C18-C17-C16	-2.14	103.54	114.42
27	B	809	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	7	308	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
29	7	301	II0	C32-C30-C26	-2.14	120.36	126.58
27	A	802	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
27	a	601	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	b	610	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
28	b	609	KC2	C4C-C3C-C2C	2.14	108.81	107.11
29	1	619	II0	C41-C39-C35	-2.14	124.25	127.31
33	4	617	LHG	C11-C10-C9	-2.14	103.56	114.42
27	9	603	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	B	839	CLA	CHC-C1C-C2C	-2.14	120.80	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	602	CLA	CHD-C1D-C2D	2.14	129.97	125.48
27	8	608	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
27	A	812	CLA	C2C-C1C-NC	2.14	111.97	109.97
27	4	607	CLA	CHD-C1D-C2D	2.14	129.96	125.48
29	5	617	II0	C41-C39-C35	-2.14	124.26	127.31
27	A	815	CLA	CHD-C1D-C2D	2.14	129.96	125.48
28	5	610	KC2	C4C-C3C-C2C	2.14	108.81	107.11
27	A	801	CLA	C4D-CHA-C1A	-2.14	118.65	121.25
27	B	834	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	K	102	CLA	CHD-C1D-C2D	2.14	129.96	125.48
29	a	612	II0	C20-C14-C12	2.14	118.31	114.36
35	R	203	8CT	C30-C31-C32	-2.14	118.84	121.47
28	7	307	KC2	C4C-C3C-C2C	2.14	108.81	107.11
27	1	613	CLA	CHA-C1A-NA	-2.14	121.51	126.40
27	A	842	CLA	CHD-C1D-C2D	2.14	129.96	125.48
27	B	802	CLA	CHB-C4A-NA	2.14	127.47	124.51
29	9	616	II0	C41-C39-C35	-2.13	124.26	127.31
27	3	602	CLA	CHD-C1D-C2D	2.13	129.96	125.48
27	B	815	CLA	CHC-C1C-C2C	-2.13	120.82	126.72
32	3	618	LMG	O2-C2-C1	-2.13	104.86	110.05
27	3	605	CLA	CHC-C1C-C2C	-2.13	120.82	126.72
27	7	310	CLA	CHD-C1D-C2D	2.13	129.96	125.48
27	5	602	CLA	CHC-C1C-C2C	-2.13	120.82	126.72
27	7	303	CLA	CHC-C1C-C2C	-2.13	120.82	126.72
28	2	610	KC2	CHB-C4A-NA	2.13	127.56	124.20
27	1	611	CLA	CHD-C1D-C2D	2.13	129.95	125.48
27	a	610	CLA	CHC-C1C-C2C	-2.13	120.82	126.72
27	R	202	CLA	CHB-C4A-NA	2.13	127.46	124.51
27	7	305	CLA	C1-C2-C3	-2.13	122.36	126.04
27	8	605	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
28	7	311	KC2	CHD-C4C-NC	2.13	127.44	124.20
27	5	605	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
27	A	819	CLA	C1-C2-C3	-2.13	122.36	126.04
27	a	611	CLA	CHD-C1D-C2D	2.13	129.95	125.48
27	5	609	CLA	CHD-C1D-C2D	2.13	129.95	125.48
27	1	612	CLA	C1-C2-C3	-2.13	122.36	126.04
27	A	841	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
27	O	202	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
27	B	805	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
28	6	613	KC2	C4C-C3C-C2C	2.13	108.81	107.11
27	A	809	CLA	C2C-C1C-NC	2.13	111.97	109.97
33	4	617	LHG	C20-C19-C18	-2.13	103.62	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	J	104	LMU	O5'-C1'-C2'	2.13	114.85	110.35
27	1	612	CLA	CHD-C1D-C2D	2.13	129.94	125.48
27	2	608	CLA	CHD-C1D-C2D	2.13	129.94	125.48
27	4	604	CLA	CHD-C1D-C2D	2.13	129.94	125.48
27	8	605	CLA	C2C-C1C-NC	2.13	111.97	109.97
27	b	602	CLA	CHD-C1D-C2D	2.13	129.94	125.48
33	4	619	LHG	C27-C26-C25	-2.13	103.63	114.42
36	4	618	LMU	C4B-C3B-C2B	-2.13	107.11	110.82
27	7	312	CLA	CHD-C1D-C2D	2.13	129.94	125.48
27	3	611	CLA	CHD-C1D-C2D	2.13	129.94	125.48
27	A	822	CLA	CHD-C1D-C2D	2.12	129.94	125.48
27	A	824	CLA	C2C-C1C-NC	2.12	111.96	109.97
27	1	608	CLA	CHD-C1D-C2D	2.12	129.94	125.48
27	6	605	CLA	CHD-C1D-C2D	2.12	129.93	125.48
27	6	608	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
27	8	602	CLA	CHD-C1D-C2D	2.12	129.93	125.48
27	a	602	CLA	CBA-CAA-C2A	2.12	120.12	113.86
27	4	608	CLA	C1-C2-C3	-2.12	122.38	126.04
27	3	612	CLA	CHD-C1D-C2D	2.12	129.92	125.48
27	B	812	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
27	4	608	CLA	CHD-C1D-C2D	2.12	129.92	125.48
27	6	602	CLA	CHA-C1A-NA	-2.12	121.55	126.40
33	4	619	LHG	C11-C10-C9	-2.12	103.68	114.42
28	1	610	KC2	CHC-C4B-NB	2.12	126.40	124.45
27	7	306	CLA	CHD-C1D-C2D	2.12	129.92	125.48
32	6	618	LMG	O1-C1-C2	-2.12	105.00	108.30
27	A	801	CLA	C3D-C4D-ND	2.12	113.66	110.24
27	A	820	CLA	CHD-C1D-C2D	2.11	129.92	125.48
27	b	602	CLA	C2C-C1C-NC	2.11	111.95	109.97
27	B	802	CLA	CHC-C1C-C2C	-2.11	120.87	126.72
27	1	609	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	B	821	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	9	602	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	O	202	CLA	C2C-C1C-NC	2.11	111.95	109.97
27	7	309	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	Z	304	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
27	A	835	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	b	607	CLA	CHD-C1D-C2D	2.11	129.91	125.48
27	b	606	CLA	CHD-C1D-C2D	2.11	129.91	125.48
28	b	609	KC2	CHD-C4C-NC	2.11	127.41	124.20
29	2	614	II0	C20-C14-C12	2.11	118.27	114.36
27	a	605	CLA	CAA-C2A-C1A	-2.11	105.06	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	825	CLA	CHD-C1D-C2D	2.11	129.90	125.48
33	2	619	LHG	C27-C26-C25	-2.11	103.72	114.42
34	O	207	SQD	O7-S-C6	2.11	109.44	106.94
27	R	202	CLA	CHD-C1D-C2D	2.11	129.90	125.48
27	B	831	CLA	C2C-C1C-NC	2.11	111.95	109.97
27	4	602	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
27	1	604	CLA	CHD-C1D-C2D	2.11	129.90	125.48
27	4	610	CLA	CHD-C1D-C2D	2.11	129.90	125.48
27	1	603	CLA	CHD-C1D-C2D	2.10	129.89	125.48
31	L	204	IHT	C27-C30-C32	-2.10	116.65	123.22
27	5	604	CLA	C2C-C1C-NC	2.10	111.94	109.97
27	B	824	CLA	CHC-C1C-C2C	-2.10	120.91	126.72
33	a	617	LHG	C20-C19-C18	-2.10	103.76	114.42
27	Z	304	CLA	CHD-C1D-C2D	2.10	129.89	125.48
27	6	602	CLA	CHD-C1D-C2D	2.10	129.89	125.48
27	A	806	CLA	CHD-C1D-C2D	2.10	129.89	125.48
39	Z	303	DGD	C4E-C3E-C2E	-2.10	107.16	110.82
27	B	831	CLA	CHC-C1C-C2C	-2.10	120.91	126.72
27	9	611	CLA	CHD-C1D-C2D	2.10	129.88	125.48
27	a	603	CLA	CHD-C1D-C2D	2.10	129.88	125.48
27	B	805	CLA	CHD-C1D-C2D	2.10	129.88	125.48
27	3	608	CLA	C2C-C1C-NC	2.10	111.94	109.97
32	2	617	LMG	O1-C1-C2	-2.10	105.03	108.30
27	A	812	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
27	4	601	CLA	CHD-C1D-C2D	2.10	129.88	125.48
27	9	609	CLA	CHD-C1D-C2D	2.10	129.88	125.48
33	Z	311	LHG	C27-C26-C25	-2.10	103.78	114.42
27	6	611	CLA	CHD-C1D-C2D	2.10	129.88	125.48
28	Z	307	KC2	CHB-C4A-NA	2.10	127.51	124.20
30	1	615	II3	C15-C07-C10	-2.10	119.08	123.56
27	9	613	CLA	CHD-C1D-C2D	2.09	129.87	125.48
27	A	843	CLA	CHA-C1A-NA	-2.09	121.60	126.40
27	2	602	CLA	CAA-C2A-C1A	-2.09	105.12	111.97
27	9	608	CLA	CHC-C1C-C2C	-2.09	120.93	126.72
27	3	609	CLA	CHD-C1D-C2D	2.09	129.87	125.48
27	A	813	CLA	CAA-C2A-C1A	-2.09	107.51	112.14
27	F	202	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
27	9	611	CLA	CAA-C2A-C1A	-2.09	106.65	111.81
27	5	608	CLA	C2C-C1C-NC	2.09	111.93	109.97
27	B	812	CLA	CHD-C1D-C2D	2.09	129.86	125.48
31	a	616	IHT	C39-C35-C38	-2.09	120.00	122.92
27	5	603	CLA	CAA-C2A-C1A	-2.09	105.14	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	617	II0	C05-C07-C11	-2.09	107.45	110.30
29	4	613	II0	C06-C08-C12	-2.09	107.45	110.30
27	L	203	CLA	CHC-C1C-NC	2.09	127.37	124.20
32	3	618	LMG	C1-O6-C5	-2.09	109.59	113.69
27	3	604	CLA	CHD-C1D-C2D	2.08	129.85	125.48
27	A	804	CLA	CHD-C1D-C2D	2.08	129.85	125.48
29	7	315	II0	C07-C11-C13	-2.08	107.70	111.85
27	L	203	CLA	CHD-C1D-C2D	2.08	129.85	125.48
29	8	612	II0	C38-C36-C40	-2.08	120.00	122.92
27	4	609	CLA	CHD-C1D-C2D	2.08	129.85	125.48
27	A	810	CLA	CHD-C1D-C2D	2.08	129.85	125.48
27	7	304	CLA	C1-C2-C3	-2.08	122.44	126.04
27	B	801	CLA	CHC-C1C-C2C	-2.08	120.96	126.72
27	A	838	CLA	CHD-C1D-C2D	2.08	129.85	125.48
27	9	601	CLA	CHC-C1C-NC	2.08	127.36	124.20
27	5	613	CLA	CAA-C2A-C3A	-2.08	111.24	116.10
27	7	309	CLA	CHB-C4A-NA	2.08	127.39	124.51
29	b	614	II0	C41-C39-C35	-2.08	124.34	127.31
27	a	604	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
27	5	606	CLA	CHC-C1C-NC	2.08	127.36	124.20
27	A	831	CLA	CHD-C1D-C2D	2.08	129.84	125.48
29	a	615	II0	C06-C04-C10	2.08	113.83	109.62
27	2	608	CLA	C2C-C1C-NC	2.08	111.92	109.97
27	B	819	CLA	CAA-C2A-C3A	2.08	118.47	112.78
27	3	608	CLA	CHD-C1D-C2D	2.08	129.84	125.48
27	7	309	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
27	7	303	CLA	CHD-C1D-C2D	2.08	129.84	125.48
29	3	616	II0	C38-C36-C40	-2.08	120.01	122.92
29	1	619	II0	C41-C42-C40	-2.08	119.22	123.47
27	1	602	CLA	CHD-C1D-C2D	2.08	129.83	125.48
27	a	607	CLA	CHD-C1D-C2D	2.07	129.83	125.48
27	2	602	CLA	CHC-C1C-C2C	-2.07	120.98	126.72
27	9	607	CLA	C1-C2-C3	-2.07	122.45	126.04
27	6	608	CLA	CHD-C1D-C2D	2.07	129.83	125.48
27	2	608	CLA	CHD-C4C-C3C	-2.07	121.79	124.84
27	7	303	CLA	CHD-C4C-C3C	-2.07	121.79	124.84
27	5	611	CLA	CHD-C1D-C2D	2.07	129.83	125.48
27	3	601	CLA	CHD-C1D-C2D	2.07	129.83	125.48
27	b	602	CLA	CHA-C1A-NA	-2.07	121.65	126.40
29	7	301	II0	C06-C08-C12	-2.07	107.47	110.30
27	6	601	CLA	CHC-C1C-NC	2.07	127.35	124.20
27	5	608	CLA	CHD-C4C-C3C	-2.07	121.80	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	841	CLA	C2C-C1C-NC	2.07	111.91	109.97
32	3	618	LMG	O7-C10-O9	-2.07	118.70	123.70
27	9	601	CLA	CHD-C1D-C2D	2.07	129.82	125.48
27	b	610	CLA	O2A-C1-C2	2.07	114.07	108.64
31	A	854	IHT	C41-C40-C37	-2.07	119.24	123.47
33	4	617	LHG	C27-C26-C25	-2.07	103.93	114.42
31	6	616	IHT	C27-C30-C32	-2.07	116.77	123.22
33	3	619	LHG	C27-C26-C25	-2.06	103.94	114.42
29	7	316	II0	C41-C42-C40	-2.06	119.25	123.47
39	B	848	DGD	O6E-C1E-O5D	-2.06	105.09	109.97
27	9	607	CLA	CHD-C1D-C2D	2.06	129.81	125.48
29	B	843	II0	C20-C14-C12	2.06	118.18	114.36
27	F	202	CLA	C1-C2-C3	-2.06	122.48	126.04
29	Z	312	II0	C06-C08-C12	-2.06	107.48	110.30
28	7	311	KC2	C4C-C3C-C2C	2.06	108.75	107.11
28	7	307	KC2	CHD-C4C-NC	2.06	127.33	124.20
27	a	602	CLA	C2C-C1C-NC	2.06	111.90	109.97
27	B	808	CLA	C1-C2-C3	-2.06	122.48	126.04
32	3	620	LMG	O7-C10-O9	-2.06	118.73	123.70
27	1	601	CLA	CHA-C1A-NA	-2.06	121.69	126.40
35	B	845	8CT	C30-C31-C32	-2.06	118.94	121.47
27	6	606	CLA	C1-C2-C3	-2.06	122.49	126.04
29	R	204	II0	C31-C33-C35	-2.06	120.64	126.42
27	B	807	CLA	CHD-C1D-C2D	2.05	129.79	125.48
27	B	809	CLA	CHA-C1A-NA	-2.05	121.69	126.40
27	a	607	CLA	CMC-C2C-C1C	2.05	128.17	125.04
27	9	608	CLA	CHD-C1D-C2D	2.05	129.79	125.48
29	1	619	II0	C42-C41-C39	-2.05	119.27	123.47
32	F	205	LMG	O3-C3-C2	-2.05	105.60	110.35
27	B	839	CLA	CHD-C1D-C2D	2.05	129.78	125.48
29	a	614	II0	C34-C36-C40	-2.05	115.79	118.94
39	B	848	DGD	C4E-C3E-C2E	-2.05	107.24	110.82
27	B	835	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
29	5	616	II0	C28-C26-C24	2.05	120.90	116.84
27	R	202	CLA	CHA-C1A-NA	-2.05	121.70	126.40
36	7	321	LMU	C2'-C3'-C4'	2.05	114.36	109.68
27	1	608	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
29	a	615	II0	C08-C12-C14	-2.05	107.77	111.85
27	B	829	CLA	CHC-C1C-NC	2.05	127.31	124.20
33	a	617	LHG	C27-C26-C25	-2.05	104.03	114.42
29	1	617	II0	C38-C36-C40	-2.05	120.06	122.92
28	5	610	KC2	CHB-C4A-NA	2.05	127.43	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	4	617	LHG	C15-C14-C13	-2.05	104.04	114.42
27	A	833	CLA	CHB-C4A-NA	2.05	127.34	124.51
27	9	602	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
27	B	813	CLA	CHB-C4A-NA	2.05	127.34	124.51
32	8	616	LMG	O2-C2-C1	-2.04	105.08	110.05
32	8	614	LMG	C1-O6-C5	-2.04	109.68	113.69
39	B	848	DGD	O2D-C2D-C1D	-2.04	105.09	110.05
27	6	608	CLA	C2C-C1C-NC	2.04	111.88	109.97
27	a	608	CLA	CHD-C1D-C2D	2.04	129.76	125.48
27	b	602	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
33	7	320	LHG	C27-C26-C25	-2.04	104.08	114.42
27	3	608	CLA	C1-C2-C3	-2.04	122.52	126.04
29	7	301	II0	C42-C41-C39	-2.04	119.30	123.47
27	O	201	CLA	CHB-C4A-NA	2.04	127.33	124.51
29	3	615	II0	C38-C36-C40	-2.04	120.07	122.92
29	5	616	II0	C38-C36-C40	-2.04	120.07	122.92
27	F	204	CLA	CHC-C1C-NC	2.04	127.29	124.20
27	K	101	CLA	CHD-C1D-C2D	2.04	129.75	125.48
27	A	844	CLA	CHC-C1C-C2C	-2.04	121.09	126.72
27	8	607	CLA	CAA-C2A-C1A	-2.04	106.78	111.81
27	A	823	CLA	CHD-C1D-C2D	2.03	129.75	125.48
31	9	619	IHT	C25-C23-C22	-2.03	114.87	118.08
28	3	606	KC2	CHB-C4A-NA	2.03	127.41	124.20
39	Z	303	DGD	O2D-C2D-C1D	-2.03	105.11	110.05
27	7	313	CLA	CHA-C1A-NA	-2.03	121.74	126.40
27	F	204	CLA	CHD-C1D-C2D	2.03	129.74	125.48
31	6	616	IHT	C02-C07-C18	-2.03	110.03	115.78
27	3	605	CLA	C2C-C1C-NC	2.03	111.88	109.97
27	A	826	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
33	2	620	LHG	C27-C26-C25	-2.03	104.11	114.42
27	3	608	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
27	B	819	CLA	CHC-C1C-NC	2.03	127.28	124.20
29	a	615	II0	C34-C36-C40	-2.03	115.83	118.94
27	B	838	CLA	CHC-C1C-NC	2.03	127.28	124.20
27	8	605	CLA	CHB-C4A-NA	2.03	127.32	124.51
27	b	603	CLA	CHB-C4A-NA	2.03	127.32	124.51
27	B	832	CLA	CHA-C1A-NA	-2.03	121.75	126.40
29	3	614	II0	C19-C13-C09	-2.03	121.59	124.35
33	7	319	LHG	C27-C26-C25	-2.03	104.13	114.42
32	8	616	LMG	C38-C37-C36	-2.03	104.13	114.42
29	8	610	II0	C03-C09-C13	-2.03	119.77	122.63
32	3	620	LMG	O2-C2-C1	-2.03	105.12	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	825	CLA	CHB-C4A-NA	2.03	127.31	124.51
27	A	827	CLA	CHA-C1A-NA	-2.03	121.76	126.40
39	B	848	DGD	C1D-C2D-C3D	-2.03	105.78	110.00
27	4	611	CLA	CHA-C1A-NA	-2.03	121.76	126.40
27	b	604	CLA	CHD-C1D-C2D	2.03	129.73	125.48
27	B	823	CLA	CHA-C1A-NA	-2.03	121.76	126.40
27	A	834	CLA	CBA-CAA-C2A	2.03	119.84	113.86
29	3	617	II0	C06-C08-C12	-2.03	107.53	110.30
27	A	806	CLA	CHA-C1A-NA	-2.03	121.76	126.40
27	6	611	CLA	CHD-C4C-C3C	-2.02	121.86	124.84
27	2	608	CLA	CHC-C1C-C2C	-2.02	121.12	126.72
27	9	602	CLA	CHC-C1C-C2C	-2.02	121.12	126.72
27	B	823	CLA	CHD-C1D-C2D	2.02	129.72	125.48
27	a	606	CLA	CHD-C1D-C2D	2.02	129.72	125.48
29	4	615	II0	C19-C13-C09	-2.02	121.60	124.35
27	B	807	CLA	CHC-C1C-NC	2.02	127.27	124.20
32	3	618	LMG	O1-C7-C8	-2.02	106.02	110.90
29	9	615	II0	C06-C04-C10	2.02	113.72	109.62
27	1	606	CLA	CHC-C1C-NC	2.02	127.27	124.20
29	4	615	II0	C41-C39-C35	-2.02	124.42	127.31
27	8	604	CLA	CHD-C1D-C2D	2.02	129.72	125.48
27	B	815	CLA	C1-C2-C3	-2.02	122.55	126.04
27	9	614	CLA	CHA-C1A-NA	-2.02	121.77	126.40
27	A	809	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
27	8	606	CLA	O2A-C1-C2	2.02	113.94	108.64
32	8	614	LMG	C38-C37-C36	-2.02	104.17	114.42
29	2	614	II0	C05-C07-C11	-2.02	107.54	110.30
29	3	613	II0	C05-C07-C11	-2.02	107.54	110.30
29	O	206	II0	C20-C14-C12	2.02	118.09	114.36
27	A	825	CLA	CHD-C4C-C3C	-2.02	121.88	124.84
27	O	201	CLA	CHC-C1C-NC	2.01	127.26	124.20
27	1	608	CLA	CHD-C4C-C3C	-2.01	121.88	124.84
27	6	608	CLA	CHC-C1C-NC	2.01	127.26	124.20
27	A	801	CLA	CHC-C1C-C2C	-2.01	121.15	126.72
29	9	618	II0	C38-C36-C40	-2.01	120.11	122.92
29	O	206	II0	C38-C36-C40	-2.01	120.11	122.92
31	A	854	IHT	C31-C34-C35	-2.01	120.77	126.42
31	2	616	IHT	C22-C23-C27	-2.01	115.86	118.94
27	B	815	CLA	C2C-C1C-NC	2.01	111.86	109.97
31	2	616	IHT	C31-C34-C35	-2.01	120.77	126.42
27	6	606	CLA	CAA-C2A-C1A	-2.01	105.39	111.97
27	A	824	CLA	CHC-C1C-C2C	-2.01	121.17	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	602	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
29	4	613	II0	C05-C07-C11	-2.01	107.56	110.30
29	a	613	II0	C06-C08-C12	-2.01	107.56	110.30
32	8	616	LMG	C3-C4-C5	-2.01	106.66	110.24
33	6	617	LHG	C5-O7-C7	-2.00	112.86	117.79
27	9	606	CLA	CHC-C1C-NC	2.00	127.24	124.20
27	b	608	CLA	CHA-C1A-NA	-2.00	121.81	126.40
27	2	611	CLA	CHA-C1A-NA	-2.00	121.81	126.40
27	B	834	CLA	CHC-C1C-NC	2.00	127.24	124.20
27	3	605	CLA	CHC-C1C-NC	2.00	127.24	124.20
27	a	611	CLA	CHA-C1A-NA	-2.00	121.82	126.40
27	a	607	CLA	CHD-C4C-C3C	-2.00	121.90	124.84

All (222) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	1	601	CLA	ND
27	1	602	CLA	ND
27	1	603	CLA	ND
27	1	604	CLA	ND
27	1	605	CLA	ND
27	1	606	CLA	ND
27	1	607	CLA	ND
27	1	608	CLA	ND
27	1	609	CLA	ND
27	1	611	CLA	ND
27	1	612	CLA	ND
27	1	613	CLA	ND
27	2	601	CLA	ND
27	2	602	CLA	ND
27	2	603	CLA	ND
27	2	604	CLA	ND
27	2	605	CLA	ND
27	2	606	CLA	ND
27	2	607	CLA	ND
27	2	608	CLA	ND
27	2	609	CLA	ND
27	2	611	CLA	ND
27	2	612	CLA	ND
27	3	601	CLA	ND
27	3	602	CLA	ND
27	3	603	CLA	ND

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Mol	Chain	Res	Type	Atom
27	3	604	CLA	ND
27	3	605	CLA	ND
27	3	607	CLA	ND
27	3	608	CLA	ND
27	3	609	CLA	ND
27	3	610	CLA	ND
27	3	611	CLA	ND
27	3	612	CLA	ND
27	4	601	CLA	ND
27	4	602	CLA	ND
27	4	603	CLA	ND
27	4	604	CLA	ND
27	4	606	CLA	ND
27	4	607	CLA	ND
27	4	608	CLA	ND
27	4	609	CLA	ND
27	4	610	CLA	ND
27	4	611	CLA	ND
27	5	601	CLA	ND
27	5	602	CLA	ND
27	5	603	CLA	ND
27	5	604	CLA	ND
27	5	605	CLA	ND
27	5	606	CLA	ND
27	5	607	CLA	ND
27	5	608	CLA	ND
27	5	609	CLA	ND
27	5	611	CLA	ND
27	5	612	CLA	ND
27	5	613	CLA	ND
27	6	601	CLA	ND
27	6	602	CLA	ND
27	6	603	CLA	ND
27	6	604	CLA	ND
27	6	605	CLA	ND
27	6	606	CLA	ND
27	6	607	CLA	ND
27	6	608	CLA	ND
27	6	609	CLA	ND
27	6	611	CLA	ND
27	6	612	CLA	ND
27	7	302	CLA	ND

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Mol	Chain	Res	Type	Atom
27	7	303	CLA	ND
27	7	304	CLA	ND
27	7	305	CLA	ND
27	7	306	CLA	ND
27	7	308	CLA	ND
27	7	309	CLA	ND
27	7	310	CLA	ND
27	7	312	CLA	ND
27	7	313	CLA	ND
27	8	601	CLA	ND
27	8	602	CLA	ND
27	8	603	CLA	ND
27	8	604	CLA	ND
27	8	605	CLA	ND
27	8	606	CLA	ND
27	8	607	CLA	ND
27	8	608	CLA	ND
27	8	615	CLA	ND
27	9	601	CLA	ND
27	9	602	CLA	ND
27	9	603	CLA	ND
27	9	604	CLA	ND
27	9	605	CLA	ND
27	9	606	CLA	ND
27	9	607	CLA	ND
27	9	608	CLA	ND
27	9	609	CLA	ND
27	9	611	CLA	ND
27	9	612	CLA	ND
27	9	613	CLA	ND
27	9	614	CLA	ND
27	A	801	CLA	ND
27	A	802	CLA	ND
27	A	803	CLA	ND
27	A	804	CLA	ND
27	A	805	CLA	ND
27	A	806	CLA	ND
27	A	807	CLA	ND
27	A	808	CLA	ND
27	A	809	CLA	ND
27	A	810	CLA	ND
27	A	811	CLA	ND

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Mol	Chain	Res	Type	Atom
27	A	812	CLA	ND
27	A	813	CLA	ND
27	A	814	CLA	ND
27	A	815	CLA	ND
27	A	816	CLA	ND
27	A	817	CLA	ND
27	A	818	CLA	ND
27	A	819	CLA	ND
27	A	820	CLA	ND
27	A	821	CLA	ND
27	A	822	CLA	ND
27	A	823	CLA	ND
27	A	824	CLA	ND
27	A	825	CLA	ND
27	A	826	CLA	ND
27	A	827	CLA	ND
27	A	828	CLA	ND
27	A	829	CLA	ND
27	A	830	CLA	ND
27	A	831	CLA	ND
27	A	832	CLA	ND
27	A	833	CLA	ND
27	A	834	CLA	ND
27	A	835	CLA	ND
27	A	836	CLA	ND
27	A	837	CLA	ND
27	A	838	CLA	ND
27	A	839	CLA	ND
27	A	840	CLA	ND
27	A	841	CLA	ND
27	A	842	CLA	ND
27	A	843	CLA	ND
27	A	844	CLA	ND
27	B	801	CLA	ND
27	B	802	CLA	ND
27	B	803	CLA	ND
27	B	804	CLA	ND
27	B	805	CLA	ND
27	B	806	CLA	ND
27	B	807	CLA	ND
27	B	808	CLA	ND
27	B	809	CLA	ND

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Mol	Chain	Res	Type	Atom
27	B	810	CLA	ND
27	B	811	CLA	ND
27	B	812	CLA	ND
27	B	813	CLA	ND
27	B	814	CLA	ND
27	B	815	CLA	ND
27	B	816	CLA	ND
27	B	817	CLA	ND
27	B	818	CLA	ND
27	B	819	CLA	ND
27	B	820	CLA	ND
27	B	821	CLA	ND
27	B	822	CLA	ND
27	B	823	CLA	ND
27	B	824	CLA	ND
27	B	825	CLA	ND
27	B	826	CLA	ND
27	B	827	CLA	ND
27	B	828	CLA	ND
27	B	829	CLA	ND
27	B	830	CLA	ND
27	B	831	CLA	ND
27	B	832	CLA	ND
27	B	833	CLA	ND
27	B	834	CLA	ND
27	B	835	CLA	ND
27	B	836	CLA	ND
27	B	837	CLA	ND
27	B	838	CLA	ND
27	B	839	CLA	ND
27	B	840	CLA	ND
27	B	841	CLA	ND
27	F	202	CLA	ND
27	F	203	CLA	ND
27	F	204	CLA	ND
27	J	102	CLA	ND
27	K	101	CLA	ND
27	K	102	CLA	ND
27	L	201	CLA	ND
27	L	202	CLA	ND
27	L	203	CLA	ND
27	O	201	CLA	ND

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Mol	Chain	Res	Type	Atom
27	O	202	CLA	ND
27	O	203	CLA	ND
27	O	204	CLA	ND
27	R	202	CLA	ND
27	Z	301	CLA	ND
27	Z	304	CLA	ND
27	Z	305	CLA	ND
27	Z	306	CLA	ND
27	Z	310	CLA	ND
27	a	601	CLA	ND
27	a	602	CLA	ND
27	a	603	CLA	ND
27	a	604	CLA	ND
27	a	605	CLA	ND
27	a	606	CLA	ND
27	a	607	CLA	ND
27	a	608	CLA	ND
27	a	610	CLA	ND
27	a	611	CLA	ND
27	b	601	CLA	ND
27	b	602	CLA	ND
27	b	603	CLA	ND
27	b	604	CLA	ND
27	b	606	CLA	ND
27	b	607	CLA	ND
27	b	608	CLA	ND
27	b	610	CLA	ND
27	b	611	CLA	ND

All (1972) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	1	603	CLA	C1A-C2A-CAA-CBA
27	2	601	CLA	C3A-C2A-CAA-CBA
27	2	601	CLA	CHA-CBD-CGD-O1D
27	2	601	CLA	CHA-CBD-CGD-O2D
27	2	602	CLA	C3A-C2A-CAA-CBA
27	2	602	CLA	CHA-CBD-CGD-O1D
27	2	602	CLA	CHA-CBD-CGD-O2D
27	2	603	CLA	C1A-C2A-CAA-CBA
27	2	608	CLA	CHA-CBD-CGD-O1D
27	2	608	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	2	611	CLA	CHA-CBD-CGD-O1D
27	2	611	CLA	CHA-CBD-CGD-O2D
27	3	602	CLA	CHA-CBD-CGD-O1D
27	3	602	CLA	CHA-CBD-CGD-O2D
27	3	612	CLA	CHA-CBD-CGD-O1D
27	4	604	CLA	CHA-CBD-CGD-O1D
27	4	604	CLA	CHA-CBD-CGD-O2D
27	4	604	CLA	CAD-CBD-CGD-O1D
27	4	608	CLA	O2A-C1-C2-C3
27	5	602	CLA	CHA-CBD-CGD-O1D
27	5	602	CLA	CHA-CBD-CGD-O2D
27	5	605	CLA	CHA-CBD-CGD-O1D
27	5	605	CLA	CHA-CBD-CGD-O2D
27	5	606	CLA	C1A-C2A-CAA-CBA
27	5	606	CLA	C3A-C2A-CAA-CBA
27	5	608	CLA	C3A-C2A-CAA-CBA
27	5	611	CLA	CAD-CBD-CGD-O1D
27	5	611	CLA	CAD-CBD-CGD-O2D
27	6	602	CLA	CHA-CBD-CGD-O1D
27	6	602	CLA	CHA-CBD-CGD-O2D
27	6	606	CLA	C1A-C2A-CAA-CBA
27	6	606	CLA	CHA-CBD-CGD-O1D
27	6	606	CLA	CHA-CBD-CGD-O2D
27	6	606	CLA	O2A-C1-C2-C3
27	6	612	CLA	C1A-C2A-CAA-CBA
27	6	612	CLA	C3A-C2A-CAA-CBA
27	7	303	CLA	CHA-CBD-CGD-O1D
27	7	303	CLA	CHA-CBD-CGD-O2D
27	7	309	CLA	C3A-C2A-CAA-CBA
27	7	313	CLA	C1A-C2A-CAA-CBA
27	7	313	CLA	C3A-C2A-CAA-CBA
27	9	602	CLA	C3A-C2A-CAA-CBA
27	9	608	CLA	C1A-C2A-CAA-CBA
27	9	608	CLA	C3A-C2A-CAA-CBA
27	9	608	CLA	C4-C3-C5-C6
27	9	609	CLA	CHA-CBD-CGD-O1D
27	9	609	CLA	CHA-CBD-CGD-O2D
27	A	802	CLA	C1A-C2A-CAA-CBA
27	A	802	CLA	C3A-C2A-CAA-CBA
27	A	803	CLA	CHA-CBD-CGD-O1D
27	A	803	CLA	CHA-CBD-CGD-O2D
27	A	803	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	A	803	CLA	CAD-CBD-CGD-O2D
27	A	810	CLA	C1A-C2A-CAA-CBA
27	A	810	CLA	C3A-C2A-CAA-CBA
27	A	810	CLA	CHA-CBD-CGD-O1D
27	A	810	CLA	CHA-CBD-CGD-O2D
27	A	810	CLA	CAD-CBD-CGD-O1D
27	A	810	CLA	CAD-CBD-CGD-O2D
27	A	814	CLA	CHA-CBD-CGD-O1D
27	A	814	CLA	CHA-CBD-CGD-O2D
27	A	816	CLA	C3A-C2A-CAA-CBA
27	A	817	CLA	C3A-C2A-CAA-CBA
27	A	817	CLA	CHA-CBD-CGD-O1D
27	A	817	CLA	CHA-CBD-CGD-O2D
27	A	818	CLA	C6-C7-C8-C10
27	A	821	CLA	C1A-C2A-CAA-CBA
27	A	822	CLA	CHA-CBD-CGD-O1D
27	A	822	CLA	CHA-CBD-CGD-O2D
27	A	825	CLA	CHA-CBD-CGD-O1D
27	A	825	CLA	CHA-CBD-CGD-O2D
27	A	832	CLA	CHA-CBD-CGD-O1D
27	A	832	CLA	CHA-CBD-CGD-O2D
27	A	834	CLA	C1A-C2A-CAA-CBA
27	A	834	CLA	CHA-CBD-CGD-O1D
27	A	834	CLA	CHA-CBD-CGD-O2D
27	A	835	CLA	C1A-C2A-CAA-CBA
27	A	835	CLA	C3A-C2A-CAA-CBA
27	A	837	CLA	C1A-C2A-CAA-CBA
27	A	837	CLA	C3A-C2A-CAA-CBA
27	A	837	CLA	CHA-CBD-CGD-O1D
27	A	837	CLA	CHA-CBD-CGD-O2D
27	A	843	CLA	CHA-CBD-CGD-O1D
27	A	843	CLA	CHA-CBD-CGD-O2D
27	A	844	CLA	C3A-C2A-CAA-CBA
27	B	804	CLA	C1A-C2A-CAA-CBA
27	B	808	CLA	C1A-C2A-CAA-CBA
27	B	809	CLA	C1A-C2A-CAA-CBA
27	B	809	CLA	C2-C3-C5-C6
27	B	809	CLA	C4-C3-C5-C6
27	B	813	CLA	C1A-C2A-CAA-CBA
27	B	813	CLA	C3A-C2A-CAA-CBA
27	B	813	CLA	CAD-CBD-CGD-O2D
27	B	813	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	B	813	CLA	C4-C3-C5-C6
27	B	814	CLA	C1A-C2A-CAA-CBA
27	B	814	CLA	C3A-C2A-CAA-CBA
27	B	816	CLA	O2A-C1-C2-C3
27	B	819	CLA	C1A-C2A-CAA-CBA
27	B	819	CLA	C3A-C2A-CAA-CBA
27	B	822	CLA	CHA-CBD-CGD-O1D
27	B	822	CLA	CHA-CBD-CGD-O2D
27	B	824	CLA	CHA-CBD-CGD-O1D
27	B	824	CLA	CHA-CBD-CGD-O2D
27	B	828	CLA	CHA-CBD-CGD-O1D
27	B	828	CLA	CHA-CBD-CGD-O2D
27	B	828	CLA	CAD-CBD-CGD-O1D
27	B	831	CLA	C1A-C2A-CAA-CBA
27	B	831	CLA	C3A-C2A-CAA-CBA
27	B	832	CLA	C1A-C2A-CAA-CBA
27	F	204	CLA	CHA-CBD-CGD-O1D
27	F	204	CLA	CHA-CBD-CGD-O2D
27	K	102	CLA	O2A-C1-C2-C3
27	O	204	CLA	C1A-C2A-CAA-CBA
27	O	204	CLA	CHA-CBD-CGD-O1D
27	O	204	CLA	CHA-CBD-CGD-O2D
27	a	602	CLA	C3A-C2A-CAA-CBA
27	a	605	CLA	C1A-C2A-CAA-CBA
27	a	605	CLA	C3A-C2A-CAA-CBA
27	a	605	CLA	C4-C3-C5-C6
27	a	610	CLA	C2-C3-C5-C6
27	a	610	CLA	C4-C3-C5-C6
27	b	602	CLA	C1A-C2A-CAA-CBA
27	b	602	CLA	C3A-C2A-CAA-CBA
27	b	602	CLA	CHA-CBD-CGD-O1D
27	b	602	CLA	CHA-CBD-CGD-O2D
27	b	604	CLA	CHA-CBD-CGD-O1D
27	b	604	CLA	CHA-CBD-CGD-O2D
27	b	606	CLA	C1A-C2A-CAA-CBA
27	b	606	CLA	C3A-C2A-CAA-CBA
27	b	607	CLA	CHA-CBD-CGD-O1D
27	b	607	CLA	CHA-CBD-CGD-O2D
27	b	610	CLA	C2-C3-C5-C6
28	1	610	KC2	C1A-C2A-CAA-CBA
28	3	606	KC2	C1A-C2A-CAA-CBA
28	3	606	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	3	606	KC2	CHA-CBD-CGD-O1D
28	3	606	KC2	CHA-CBD-CGD-O2D
28	4	605	KC2	C2B-C3B-CAB-CBB
28	4	605	KC2	C4B-C3B-CAB-CBB
28	7	307	KC2	C2B-C3B-CAB-CBB
28	7	307	KC2	C4B-C3B-CAB-CBB
28	7	307	KC2	CAA-CBA-CGA-O1A
28	7	307	KC2	CAA-CBA-CGA-O2A
28	7	311	KC2	C1A-C2A-CAA-CBA
28	7	311	KC2	C3A-C2A-CAA-CBA
28	9	610	KC2	CHA-CBD-CGD-O1D
28	9	610	KC2	CHA-CBD-CGD-O2D
28	b	605	KC2	C1A-C2A-CAA-CBA
28	b	605	KC2	C3A-C2A-CAA-CBA
28	b	605	KC2	C2B-C3B-CAB-CBB
28	b	605	KC2	C4B-C3B-CAB-CBB
29	1	616	II0	C10-C22-C24-C26
29	2	613	II0	C09-C21-C23-C25
29	3	613	II0	C10-C22-C24-C26
29	4	614	II0	C09-C21-C23-C25
29	4	614	II0	C10-C22-C24-C26
29	6	615	II0	C09-C21-C23-C25
29	7	315	II0	C09-C21-C23-C25
29	8	612	II0	C09-C21-C23-C25
29	9	615	II0	C10-C22-C24-C26
29	9	618	II0	C09-C21-C23-C25
29	9	618	II0	C10-C22-C24-C26
29	O	205	II0	C10-C22-C24-C26
30	b	613	II3	C16-C23-C27-C28
31	5	618	IHT	C02-C07-C18-C22
31	6	616	IHT	C11-C21-C24-C26
31	9	619	IHT	C18-C22-C23-C25
31	9	619	IHT	C18-C22-C23-C27
31	A	854	IHT	C02-C07-C18-C22
31	Z	302	IHT	C10-C07-C18-C22
31	a	616	IHT	C10-C07-C18-C22
31	a	616	IHT	C31-C34-C35-C38
31	a	616	IHT	C31-C34-C35-C39
32	3	618	LMG	O6-C1-O1-C7
32	8	616	LMG	O6-C1-O1-C7
33	2	618	LHG	O2-C2-C3-O3
33	2	618	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
33	2	619	LHG	C4-O6-P-O5
33	2	620	LHG	C3-O3-P-O5
33	2	620	LHG	C4-O6-P-O4
33	2	620	LHG	O7-C5-C6-O8
33	3	619	LHG	O6-C4-C5-O7
33	3	619	LHG	O9-C7-O7-C5
33	3	619	LHG	C8-C7-O7-C5
33	3	622	LHG	O1-C1-C2-C3
33	3	622	LHG	C8-C7-O7-C5
33	4	617	LHG	O7-C5-C6-O8
33	4	619	LHG	O1-C1-C2-C3
33	4	619	LHG	O9-C7-O7-C5
33	4	619	LHG	C8-C7-O7-C5
33	4	620	LHG	C4-O6-P-O5
33	4	620	LHG	C8-C7-O7-C5
33	5	619	LHG	C1-C2-C3-O3
33	5	619	LHG	C3-O3-P-O4
33	5	619	LHG	C3-O3-P-O5
33	5	619	LHG	C3-O3-P-O6
33	5	619	LHG	C8-C7-O7-C5
33	7	320	LHG	C3-O3-P-O4
33	7	320	LHG	C8-C7-O7-C5
33	8	613	LHG	O1-C1-C2-C3
33	8	613	LHG	O2-C2-C3-O3
33	8	613	LHG	C3-O3-P-O4
33	8	613	LHG	O7-C5-C6-O8
33	A	851	LHG	C1-C2-C3-O3
33	A	851	LHG	O2-C2-C3-O3
33	A	851	LHG	C3-O3-P-O4
33	A	852	LHG	O1-C1-C2-C3
33	A	852	LHG	C3-O3-P-O5
33	A	852	LHG	C4-O6-P-O5
33	Z	311	LHG	C1-C2-C3-O3
33	Z	311	LHG	C3-O3-P-O4
33	Z	311	LHG	C3-O3-P-O5
33	Z	311	LHG	O7-C5-C6-O8
33	Z	311	LHG	O9-C7-O7-C5
33	Z	311	LHG	C8-C7-O7-C5
33	a	617	LHG	O1-C1-C2-C3
33	a	617	LHG	C4-O6-P-O4
33	a	617	LHG	C4-O6-P-O5
33	a	617	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
33	a	618	LHG	O1-C1-C2-C3
33	b	616	LHG	C3-O3-P-O4
34	3	621	SQD	O5-C5-C6-S
34	O	207	SQD	O5-C5-C6-S
34	O	207	SQD	C5-C6-S-O7
34	O	207	SQD	C5-C6-S-O8
34	O	207	SQD	C5-C6-S-O9
35	4	616	8CT	C02-C03-C10-C11
35	4	616	8CT	C04-C03-C10-C11
35	4	616	8CT	C28-C29-C30-C31
35	4	616	8CT	C28-C29-C30-C35
35	7	318	8CT	C03-C10-C11-C12
35	7	318	8CT	C13-C14-C15-C16
35	7	318	8CT	C25-C26-C28-C29
35	7	318	8CT	C27-C26-C28-C29
35	7	318	8CT	C28-C29-C30-C35
35	A	845	8CT	C21-C23-C24-C25
35	A	846	8CT	C28-C29-C30-C35
35	A	847	8CT	C03-C10-C11-C12
35	A	847	8CT	C28-C29-C30-C31
35	A	847	8CT	C28-C29-C30-C35
35	A	853	8CT	C03-C10-C11-C12
35	A	853	8CT	C28-C29-C30-C31
35	B	844	8CT	C28-C29-C30-C31
35	B	844	8CT	C28-C29-C30-C35
35	B	845	8CT	C28-C29-C30-C31
35	B	845	8CT	C28-C29-C30-C35
35	B	846	8CT	C28-C29-C30-C31
35	B	846	8CT	C28-C29-C30-C35
35	B	847	8CT	C28-C29-C30-C31
35	B	849	8CT	C03-C10-C11-C12
35	B	849	8CT	C28-C29-C30-C35
35	B	850	8CT	C21-C23-C24-C25
35	B	850	8CT	C28-C29-C30-C35
35	F	201	8CT	C28-C29-C30-C31
35	F	201	8CT	C28-C29-C30-C35
35	J	103	8CT	C16-C17-C18-C19
35	J	103	8CT	C28-C29-C30-C35
35	K	103	8CT	C28-C29-C30-C35
35	L	205	8CT	C28-C29-C30-C31
35	L	205	8CT	C28-C29-C30-C35
35	M	101	8CT	C03-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	M	101	8CT	C18-C19-C20-C21
35	M	101	8CT	C28-C29-C30-C31
35	M	101	8CT	C28-C29-C30-C35
35	R	201	8CT	C10-C11-C12-C13
35	R	201	8CT	C10-C11-C12-C40
35	R	203	8CT	C03-C10-C11-C12
35	Z	309	8CT	C21-C23-C24-C25
35	Z	309	8CT	C28-C29-C30-C35
35	b	615	8CT	C28-C29-C30-C35
36	4	618	LMU	O5B-C1B-O1B-C4'
36	4	618	LMU	C2'-C1'-O1'-C1
36	4	618	LMU	O5'-C1'-O1'-C1
36	4	618	LMU	C2-C1-O1'-C1'
38	A	850	PQN	C16-C17-C18-C19
39	B	848	DGD	O1B-C1B-O2G-C2G
33	2	619	LHG	O10-C23-O8-C6
33	4	620	LHG	O10-C23-O8-C6
33	8	613	LHG	O10-C23-O8-C6
36	J	104	LMU	O5B-C1B-O1B-C4'
33	2	619	LHG	C24-C23-O8-C6
33	5	619	LHG	O10-C23-O8-C6
33	a	618	LHG	O10-C23-O8-C6
28	4	605	KC2	CAA-CBA-CGA-O2A
32	3	620	LMG	C4-C5-C6-O5
33	3	622	LHG	O9-C7-O7-C5
33	6	617	LHG	O9-C7-O7-C5
33	7	320	LHG	O9-C7-O7-C5
33	8	613	LHG	O9-C7-O7-C5
33	a	617	LHG	O9-C7-O7-C5
33	a	618	LHG	O9-C7-O7-C5
33	b	616	LHG	O9-C7-O7-C5
27	4	604	CLA	C3-C5-C6-C7
27	4	607	CLA	C3-C5-C6-C7
27	4	611	CLA	C3-C5-C6-C7
27	5	604	CLA	C3-C5-C6-C7
27	A	804	CLA	C3-C5-C6-C7
27	A	806	CLA	C3-C5-C6-C7
27	A	819	CLA	C3-C5-C6-C7
27	A	823	CLA	C3-C5-C6-C7
27	A	831	CLA	C3-C5-C6-C7
27	B	811	CLA	C3-C5-C6-C7
27	B	820	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	B	832	CLA	C3-C5-C6-C7
27	F	202	CLA	C3-C5-C6-C7
27	Z	306	CLA	C3-C5-C6-C7
33	4	620	LHG	C24-C23-O8-C6
32	3	618	LMG	C11-C10-O7-C8
33	6	617	LHG	C8-C7-O7-C5
33	a	618	LHG	C8-C7-O7-C5
39	B	848	DGD	C2B-C1B-O2G-C2G
28	2	610	KC2	CAA-CBA-CGA-O1A
28	2	610	KC2	CAA-CBA-CGA-O2A
28	7	311	KC2	CAA-CBA-CGA-O1A
28	7	311	KC2	CAA-CBA-CGA-O2A
28	9	610	KC2	CAA-CBA-CGA-O1A
28	9	610	KC2	CAA-CBA-CGA-O2A
27	9	608	CLA	C2-C3-C5-C6
27	a	605	CLA	C2-C3-C5-C6
27	A	827	CLA	C2A-CAA-CBA-CGA
27	A	839	CLA	C2A-CAA-CBA-CGA
27	B	808	CLA	C2A-CAA-CBA-CGA
27	B	837	CLA	C2A-CAA-CBA-CGA
27	a	602	CLA	C2A-CAA-CBA-CGA
27	6	611	CLA	C3-C5-C6-C7
27	B	807	CLA	C3-C5-C6-C7
27	K	102	CLA	C3-C5-C6-C7
27	a	608	CLA	CBA-CGA-O2A-C1
33	5	619	LHG	C24-C23-O8-C6
33	8	613	LHG	C24-C23-O8-C6
33	a	618	LHG	C24-C23-O8-C6
32	3	618	LMG	C4-C5-C6-O5
33	4	620	LHG	O9-C7-O7-C5
33	5	619	LHG	O2-C2-C3-O3
33	7	320	LHG	O2-C2-C3-O3
32	8	616	LMG	C11-C10-O7-C8
33	A	852	LHG	C8-C7-O7-C5
32	3	620	LMG	O6-C5-C6-O5
33	b	616	LHG	C11-C12-C13-C14
39	Z	303	DGD	O6E-C5E-C6E-O5E
27	9	606	CLA	C3-C5-C6-C7
28	4	605	KC2	CAA-CBA-CGA-O1A
36	4	618	LMU	C4-C5-C6-C7
33	5	619	LHG	O9-C7-O7-C5
27	4	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	834	CLA	C4-C3-C5-C6
27	B	831	CLA	C4-C3-C5-C6
27	a	602	CLA	C4-C3-C5-C6
27	4	603	CLA	C2-C3-C5-C6
27	A	834	CLA	C2-C3-C5-C6
27	B	831	CLA	C2-C3-C5-C6
27	a	602	CLA	C2-C3-C5-C6
27	B	803	CLA	C2A-CAA-CBA-CGA
27	B	819	CLA	C2A-CAA-CBA-CGA
32	3	618	LMG	O6-C5-C6-O5
32	F	205	LMG	O6-C5-C6-O5
27	a	608	CLA	O1A-CGA-O2A-C1
27	B	826	CLA	C3-C5-C6-C7
33	4	617	LHG	C24-C23-O8-C6
33	Z	311	LHG	C24-C23-O8-C6
39	Z	303	DGD	C4E-C5E-C6E-O5E
27	4	610	CLA	C3-C5-C6-C7
27	A	811	CLA	C3-C5-C6-C7
27	A	810	CLA	CBA-CGA-O2A-C1
27	A	839	CLA	CBA-CGA-O2A-C1
32	3	620	LMG	C29-C28-O8-C9
33	7	320	LHG	C23-C24-C25-C26
33	Z	311	LHG	C23-C24-C25-C26
28	b	609	KC2	CAA-CBA-CGA-O1A
28	b	609	KC2	CAA-CBA-CGA-O2A
27	2	608	CLA	C8-C10-C11-C12
27	B	826	CLA	C10-C11-C12-C13
33	7	319	LHG	O2-C2-C3-O3
33	Z	311	LHG	O2-C2-C3-O3
32	8	616	LMG	C2-C1-O1-C7
27	1	612	CLA	C6-C7-C8-C9
27	9	606	CLA	C6-C7-C8-C9
27	A	806	CLA	C14-C13-C15-C16
27	A	822	CLA	C14-C13-C15-C16
27	A	824	CLA	C6-C7-C8-C9
27	A	833	CLA	C11-C10-C8-C9
27	B	816	CLA	C11-C10-C8-C9
27	B	839	CLA	C11-C10-C8-C9
27	L	202	CLA	C11-C10-C8-C9
27	a	608	CLA	C11-C10-C8-C9
27	b	604	CLA	C6-C7-C8-C9
32	F	205	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
32	F	205	LMG	C10-C11-C12-C13
33	a	617	LHG	C23-C24-C25-C26
33	b	616	LHG	C23-C24-C25-C26
27	4	611	CLA	C5-C6-C7-C8
27	5	608	CLA	C5-C6-C7-C8
27	A	839	CLA	C15-C16-C17-C18
27	A	842	CLA	C10-C11-C12-C13
27	B	832	CLA	C13-C15-C16-C17
27	B	837	CLA	C5-C6-C7-C8
27	a	603	CLA	C5-C6-C7-C8
27	8	606	CLA	CBA-CGA-O2A-C1
27	B	809	CLA	CBA-CGA-O2A-C1
27	9	606	CLA	C10-C11-C12-C13
27	A	818	CLA	C8-C10-C11-C12
27	B	807	CLA	C8-C10-C11-C12
27	B	817	CLA	C10-C11-C12-C13
27	B	838	CLA	C13-C15-C16-C17
27	Z	306	CLA	C10-C11-C12-C13
27	A	806	CLA	C8-C10-C11-C12
27	B	802	CLA	C5-C6-C7-C8
27	B	813	CLA	C5-C6-C7-C8
27	B	815	CLA	C8-C10-C11-C12
27	B	821	CLA	C8-C10-C11-C12
27	K	101	CLA	C5-C6-C7-C8
38	B	842	PQN	C25-C26-C27-C28
32	2	617	LMG	C28-C29-C30-C31
33	A	851	LHG	C7-C8-C9-C10
33	A	852	LHG	C23-C24-C25-C26
27	A	826	CLA	C8-C10-C11-C12
27	A	837	CLA	C5-C6-C7-C8
27	A	839	CLA	C13-C15-C16-C17
27	A	835	CLA	C3-C5-C6-C7
27	b	610	CLA	CBA-CGA-O2A-C1
32	2	617	LMG	C29-C28-O8-C9
27	B	832	CLA	C2-C1-O2A-CGA
36	4	618	LMU	C5'-C4'-O1B-C1B
27	B	812	CLA	C5-C6-C7-C8
27	B	831	CLA	C5-C6-C7-C8
27	B	839	CLA	C10-C11-C12-C13
33	8	613	LHG	C8-C7-O7-C5
34	3	621	SQD	C8-C7-O47-C45
27	4	608	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	B	809	CLA	C8-C10-C11-C12
27	9	606	CLA	C6-C7-C8-C10
27	A	839	CLA	C6-C7-C8-C10
27	B	805	CLA	C6-C7-C8-C10
27	B	832	CLA	C12-C13-C15-C16
27	A	841	CLA	C3-C5-C6-C7
31	a	616	IHT	C26-C29-C31-C34
35	R	201	8CT	C12-C13-C14-C15
27	3	610	CLA	C2A-CAA-CBA-CGA
27	A	809	CLA	C2A-CAA-CBA-CGA
27	A	838	CLA	C2A-CAA-CBA-CGA
28	6	613	KC2	CAA-CBA-CGA-O1A
27	F	202	CLA	C8-C10-C11-C12
35	7	318	8CT	C21-C23-C24-C25
35	A	846	8CT	C21-C23-C24-C25
35	A	847	8CT	C21-C23-C24-C25
35	A	848	8CT	C21-C23-C24-C25
35	B	846	8CT	C21-C23-C24-C25
35	B	847	8CT	C21-C23-C24-C25
35	I	101	8CT	C21-C23-C24-C25
35	J	103	8CT	C21-C23-C24-C25
35	M	101	8CT	C21-C23-C24-C25
35	R	201	8CT	C13-C14-C15-C16
35	R	203	8CT	C21-C23-C24-C25
35	b	615	8CT	C21-C23-C24-C25
33	2	619	LHG	O2-C2-C3-O3
33	3	622	LHG	O2-C2-C3-O3
38	A	850	PQN	C13-C15-C16-C17
27	A	810	CLA	C5-C6-C7-C8
27	A	837	CLA	C10-C11-C12-C13
33	7	319	LHG	C24-C23-O8-C6
27	A	810	CLA	O1A-CGA-O2A-C1
27	A	839	CLA	O1A-CGA-O2A-C1
27	4	610	CLA	C5-C6-C7-C8
27	6	602	CLA	C8-C10-C11-C12
27	A	831	CLA	C13-C15-C16-C17
27	A	841	CLA	C15-C16-C17-C18
27	B	805	CLA	C5-C6-C7-C8
27	B	805	CLA	C15-C16-C17-C18
28	6	613	KC2	CAA-CBA-CGA-O2A
33	b	616	LHG	C8-C7-O7-C5
27	3	603	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	A	823	CLA	C15-C16-C17-C18
27	B	812	CLA	C13-C15-C16-C17
27	K	101	CLA	C13-C15-C16-C17
33	2	618	LHG	C4-O6-P-O3
33	2	619	LHG	C4-O6-P-O3
33	3	619	LHG	C3-O3-P-O6
33	7	320	LHG	C3-O3-P-O6
33	8	613	LHG	C3-O3-P-O6
33	A	851	LHG	C3-O3-P-O6
33	A	852	LHG	C3-O3-P-O6
33	Z	311	LHG	C3-O3-P-O6
33	a	617	LHG	C4-O6-P-O3
33	a	618	LHG	C3-O3-P-O6
33	b	616	LHG	C3-O3-P-O6
27	a	611	CLA	C3-C5-C6-C7
27	B	832	CLA	CBA-CGA-O2A-C1
33	2	618	LHG	C1-C2-C3-O3
33	2	619	LHG	C1-C2-C3-O3
33	3	622	LHG	C1-C2-C3-O3
33	7	320	LHG	C1-C2-C3-O3
33	8	613	LHG	C1-C2-C3-O3
34	3	621	SQD	O49-C7-O47-C45
27	4	610	CLA	C4-C3-C5-C6
27	B	812	CLA	C4-C3-C5-C6
27	A	828	CLA	C5-C6-C7-C8
27	8	602	CLA	C2A-CAA-CBA-CGA
27	A	834	CLA	C2A-CAA-CBA-CGA
27	a	603	CLA	C2A-CAA-CBA-CGA
27	B	815	CLA	C16-C17-C18-C19
28	b	605	KC2	CAA-CBA-CGA-O2A
33	a	617	LHG	C24-C23-O8-C6
27	B	823	CLA	C8-C10-C11-C12
32	8	614	LMG	C31-C32-C33-C34
33	4	620	LHG	C31-C32-C33-C34
32	3	620	LMG	C11-C10-O7-C8
33	2	620	LHG	C8-C7-O7-C5
32	8	614	LMG	C32-C33-C34-C35
33	6	617	LHG	C24-C25-C26-C27
33	7	320	LHG	C27-C28-C29-C30
33	A	851	LHG	C13-C14-C15-C16
33	A	851	LHG	C31-C32-C33-C34
33	A	852	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	b	616	LHG	C33-C34-C35-C36
34	3	621	SQD	C26-C27-C28-C29
39	Z	303	DGD	C3B-C4B-C5B-C6B
27	A	831	CLA	C16-C17-C18-C19
27	Z	306	CLA	C11-C12-C13-C14
32	3	620	LMG	C31-C32-C33-C34
33	2	620	LHG	C32-C33-C34-C35
33	7	320	LHG	C29-C30-C31-C32
33	7	320	LHG	C31-C32-C33-C34
33	a	617	LHG	C28-C29-C30-C31
27	a	607	CLA	C5-C6-C7-C8
32	8	614	LMG	C34-C35-C36-C37
32	8	614	LMG	C38-C39-C40-C41
33	3	622	LHG	C11-C10-C9-C8
33	A	851	LHG	C24-C25-C26-C27
36	7	321	LMU	C3-C4-C5-C6
32	2	617	LMG	C30-C31-C32-C33
32	8	616	LMG	C19-C20-C21-C22
39	B	848	DGD	C2A-C3A-C4A-C5A
39	B	848	DGD	C5A-C6A-C7A-C8A
33	4	620	LHG	O2-C2-C3-O3
33	7	320	LHG	C24-C25-C26-C27
34	3	621	SQD	C28-C29-C30-C31
33	2	619	LHG	C23-C24-C25-C26
36	J	104	LMU	C2'-C1'-O1'-C1
27	B	816	CLA	CBA-CGA-O2A-C1
33	2	620	LHG	C24-C23-O8-C6
34	3	621	SQD	C11-C10-C9-C8
39	Z	303	DGD	O1A-C1A-O1G-C1G
27	4	606	CLA	C11-C12-C13-C15
27	9	608	CLA	C6-C7-C8-C9
27	a	606	CLA	C16-C17-C18-C20
27	a	610	CLA	C6-C7-C8-C9
27	b	604	CLA	C16-C17-C18-C20
33	7	320	LHG	C33-C34-C35-C36
33	A	851	LHG	C25-C26-C27-C28
33	a	617	LHG	C17-C18-C19-C20
27	B	834	CLA	C2-C3-C5-C6
27	9	607	CLA	C11-C10-C8-C9
27	A	801	CLA	C14-C13-C15-C16
27	A	804	CLA	C14-C13-C15-C16
27	A	806	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	A	816	CLA	C6-C7-C8-C9
27	A	818	CLA	C6-C7-C8-C9
27	A	843	CLA	C11-C10-C8-C9
27	B	828	CLA	C6-C7-C8-C9
27	b	603	CLA	C6-C7-C8-C9
32	F	205	LMG	C28-C29-C30-C31
33	2	620	LHG	C23-C24-C25-C26
27	4	603	CLA	C5-C6-C7-C8
33	2	619	LHG	C24-C25-C26-C27
33	2	620	LHG	C28-C29-C30-C31
33	b	616	LHG	C31-C32-C33-C34
27	8	604	CLA	C5-C6-C7-C8
27	1	603	CLA	C2A-CAA-CBA-CGA
27	6	606	CLA	C2A-CAA-CBA-CGA
27	A	829	CLA	C2A-CAA-CBA-CGA
33	2	620	LHG	C34-C35-C36-C37
39	B	848	DGD	C2B-C3B-C4B-C5B
33	b	616	LHG	O1-C1-C2-C3
27	9	608	CLA	C3-C5-C6-C7
32	3	618	LMG	O9-C10-O7-C8
33	A	852	LHG	O9-C7-O7-C5
27	A	817	CLA	C5-C6-C7-C8
32	3	618	LMG	C28-C29-C30-C31
33	3	619	LHG	C18-C19-C20-C21
33	3	619	LHG	C31-C32-C33-C34
33	4	619	LHG	C26-C27-C28-C29
33	7	319	LHG	C28-C29-C30-C31
33	Z	311	LHG	C11-C12-C13-C14
33	a	617	LHG	C25-C26-C27-C28
36	4	618	LMU	C3'-C4'-O1B-C1B
27	4	604	CLA	C6-C7-C8-C9
27	7	303	CLA	C16-C17-C18-C19
27	7	303	CLA	C16-C17-C18-C20
27	A	810	CLA	C16-C17-C18-C19
27	A	810	CLA	C16-C17-C18-C20
27	Z	301	CLA	C11-C12-C13-C14
27	Z	301	CLA	C11-C12-C13-C15
27	B	807	CLA	C15-C16-C17-C18
27	b	602	CLA	C15-C16-C17-C18
33	4	619	LHG	C31-C32-C33-C34
33	8	613	LHG	C27-C28-C29-C30
39	Z	303	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
32	8	616	LMG	C37-C38-C39-C40
33	2	619	LHG	C27-C28-C29-C30
33	A	851	LHG	C14-C15-C16-C17
33	Z	311	LHG	C33-C34-C35-C36
33	b	616	LHG	C11-C10-C9-C8
32	8	614	LMG	C10-C11-C12-C13
28	b	605	KC2	CAA-CBA-CGA-O1A
33	4	619	LHG	C14-C15-C16-C17
27	3	608	CLA	C3-C5-C6-C7
27	A	820	CLA	C3-C5-C6-C7
27	Z	301	CLA	CBA-CGA-O2A-C1
39	Z	303	DGD	C9B-CAB-CBB-CCB
27	1	603	CLA	C3A-C2A-CAA-CBA
27	2	603	CLA	C3A-C2A-CAA-CBA
27	6	603	CLA	C3A-C2A-CAA-CBA
27	6	605	CLA	C3A-C2A-CAA-CBA
27	6	606	CLA	C3A-C2A-CAA-CBA
27	A	804	CLA	C3A-C2A-CAA-CBA
27	A	831	CLA	C3A-C2A-CAA-CBA
27	A	834	CLA	C3A-C2A-CAA-CBA
27	A	842	CLA	C3A-C2A-CAA-CBA
27	B	808	CLA	C3A-C2A-CAA-CBA
27	B	832	CLA	C3A-C2A-CAA-CBA
27	F	202	CLA	C3A-C2A-CAA-CBA
27	F	203	CLA	C3A-C2A-CAA-CBA
27	6	608	CLA	C8-C10-C11-C12
27	a	603	CLA	C10-C11-C12-C13
27	4	604	CLA	C6-C7-C8-C10
27	4	611	CLA	C16-C17-C18-C19
27	9	602	CLA	C6-C7-C8-C9
27	A	831	CLA	C16-C17-C18-C20
33	4	619	LHG	C29-C30-C31-C32
27	B	822	CLA	C3-C5-C6-C7
36	7	321	LMU	C7-C8-C9-C10
27	8	606	CLA	O1A-CGA-O2A-C1
27	B	809	CLA	O1A-CGA-O2A-C1
27	A	817	CLA	C4-C3-C5-C6
27	B	821	CLA	C4-C3-C5-C6
27	B	822	CLA	C4-C3-C5-C6
27	B	823	CLA	C4-C3-C5-C6
27	B	827	CLA	C4-C3-C5-C6
27	Z	310	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	817	CLA	CBA-CGA-O2A-C1
27	L	203	CLA	CBA-CGA-O2A-C1
27	4	610	CLA	C2-C3-C5-C6
27	9	607	CLA	C2-C3-C5-C6
27	A	817	CLA	C2-C3-C5-C6
27	B	805	CLA	C2-C3-C5-C6
27	B	821	CLA	C2-C3-C5-C6
27	B	823	CLA	C2-C3-C5-C6
27	B	827	CLA	C2-C3-C5-C6
34	O	207	SQD	C8-C7-O47-C45
27	A	842	CLA	C2A-CAA-CBA-CGA
33	3	622	LHG	O1-C1-C2-O2
33	4	619	LHG	O1-C1-C2-O2
33	8	613	LHG	O1-C1-C2-O2
33	A	852	LHG	O1-C1-C2-O2
33	a	617	LHG	O1-C1-C2-O2
33	a	618	LHG	O1-C1-C2-O2
33	b	616	LHG	C16-C17-C18-C19
27	b	610	CLA	O1A-CGA-O2A-C1
33	4	620	LHG	C9-C10-C11-C12
33	3	619	LHG	C9-C10-C11-C12
39	Z	303	DGD	C2B-C3B-C4B-C5B
27	A	825	CLA	C10-C11-C12-C13
33	4	620	LHG	C1-C2-C3-O3
32	8	616	LMG	O9-C10-O7-C8
33	2	620	LHG	O9-C7-O7-C5
34	O	207	SQD	O49-C7-O47-C45
27	a	608	CLA	C2-C1-O2A-CGA
33	6	617	LHG	C26-C27-C28-C29
32	2	617	LMG	C13-C14-C15-C16
32	8	616	LMG	C13-C14-C15-C16
31	1	618	IHT	C02-C07-C18-C22
31	2	616	IHT	C10-C07-C18-C22
31	6	616	IHT	C02-C07-C18-C22
31	8	609	IHT	C10-C07-C18-C22
31	9	619	IHT	C10-C07-C18-C22
31	L	204	IHT	C02-C07-C18-C22
35	7	318	8CT	C02-C03-C10-C11
35	7	318	8CT	C04-C03-C10-C11
35	A	847	8CT	C02-C03-C10-C11
35	A	847	8CT	C04-C03-C10-C11
35	B	846	8CT	C02-C03-C10-C11

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Mol	Chain	Res	Type	Atoms
35	B	846	8CT	C04-C03-C10-C11
35	B	850	8CT	C02-C03-C10-C11
35	B	850	8CT	C04-C03-C10-C11
35	J	103	8CT	C02-C03-C10-C11
35	J	103	8CT	C04-C03-C10-C11
35	Z	309	8CT	C02-C03-C10-C11
35	Z	309	8CT	C04-C03-C10-C11
27	1	605	CLA	C2A-CAA-CBA-CGA
32	8	614	LMG	C13-C14-C15-C16
33	8	613	LHG	C25-C26-C27-C28
33	2	618	LHG	C24-C23-O8-C6
27	A	801	CLA	C15-C16-C17-C18
27	A	821	CLA	C5-C6-C7-C8
27	K	101	CLA	C8-C10-C11-C12
33	a	618	LHG	C23-C24-C25-C26
33	2	619	LHG	C15-C16-C17-C18
27	A	830	CLA	C5-C6-C7-C8
27	B	828	CLA	C10-C11-C12-C13
38	A	850	PQN	C25-C26-C27-C28
27	5	604	CLA	C4-C3-C5-C6
27	6	606	CLA	C4-C3-C5-C6
27	B	805	CLA	C4-C3-C5-C6
27	B	834	CLA	C4-C3-C5-C6
27	O	204	CLA	C4-C3-C5-C6
27	1	612	CLA	C6-C7-C8-C10
27	2	605	CLA	C11-C10-C8-C7
27	5	608	CLA	C11-C10-C8-C7
27	6	604	CLA	C11-C10-C8-C7
27	6	606	CLA	C2-C3-C5-C6
27	8	615	CLA	C11-C12-C13-C15
27	A	811	CLA	C12-C13-C15-C16
27	A	816	CLA	C6-C7-C8-C10
27	A	825	CLA	C12-C13-C15-C16
27	A	839	CLA	C11-C12-C13-C15
27	B	801	CLA	C6-C7-C8-C10
27	B	807	CLA	C6-C7-C8-C10
27	B	812	CLA	C2-C3-C5-C6
27	B	820	CLA	C11-C10-C8-C7
27	B	822	CLA	C2-C3-C5-C6
27	B	828	CLA	C6-C7-C8-C10
27	Z	306	CLA	C6-C7-C8-C10
27	Z	310	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	b	603	CLA	C6-C7-C8-C10
32	8	616	LMG	C32-C33-C34-C35
27	B	801	CLA	C13-C15-C16-C17
27	B	823	CLA	C15-C16-C17-C18
35	J	103	8CT	C18-C19-C20-C21
27	a	610	CLA	C6-C7-C8-C10
33	8	613	LHG	C23-C24-C25-C26
39	B	848	DGD	C1B-C2B-C3B-C4B
32	8	614	LMG	C15-C16-C17-C18
39	Z	303	DGD	C8A-C9A-CAA-CBA
27	A	840	CLA	C2A-CAA-CBA-CGA
27	B	835	CLA	C2A-CAA-CBA-CGA
27	A	804	CLA	C13-C15-C16-C17
32	8	614	LMG	C37-C38-C39-C40
33	4	620	LHG	C26-C27-C28-C29
33	4	617	LHG	C7-C8-C9-C10
27	A	835	CLA	C5-C6-C7-C8
28	1	610	KC2	C2B-C3B-CAB-CBB
28	2	610	KC2	C2C-C3C-CAC-CBC
28	3	606	KC2	C2C-C3C-CAC-CBC
28	6	610	KC2	C2C-C3C-CAC-CBC
28	6	613	KC2	C2C-C3C-CAC-CBC
28	7	307	KC2	C2C-C3C-CAC-CBC
36	7	321	LMU	C1-C2-C3-C4
27	A	844	CLA	C16-C17-C18-C19
27	B	826	CLA	C16-C17-C18-C20
33	4	619	LHG	C15-C16-C17-C18
33	a	617	LHG	C13-C14-C15-C16
32	8	616	LMG	C10-C11-C12-C13
32	F	205	LMG	C11-C10-O7-C8
39	Z	303	DGD	C2B-C1B-O2G-C2G
33	6	617	LHG	O6-C4-C5-O7
35	4	616	8CT	C21-C23-C24-C25
32	8	616	LMG	C11-C12-C13-C14
33	4	617	LHG	C18-C19-C20-C21
28	1	610	KC2	C4B-C3B-CAB-CBB
28	3	606	KC2	C4C-C3C-CAC-CBC
28	6	610	KC2	C4C-C3C-CAC-CBC
28	6	613	KC2	C4C-C3C-CAC-CBC
27	L	202	CLA	C5-C6-C7-C8
33	4	617	LHG	C9-C10-C11-C12
27	5	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	A	811	CLA	C13-C15-C16-C17
33	5	619	LHG	O7-C5-C6-O8
33	a	617	LHG	C31-C32-C33-C34
27	B	832	CLA	O1A-CGA-O2A-C1
32	3	620	LMG	O10-C28-O8-C9
27	b	604	CLA	C16-C17-C18-C19
32	8	614	LMG	C11-C12-C13-C14
27	8	615	CLA	C15-C16-C17-C18
27	A	818	CLA	C13-C15-C16-C17
27	A	820	CLA	C15-C16-C17-C18
27	A	831	CLA	C5-C6-C7-C8
27	B	801	CLA	C5-C6-C7-C8
27	9	607	CLA	C4-C3-C5-C6
27	4	604	CLA	C2-C3-C5-C6
27	5	604	CLA	C2-C3-C5-C6
27	9	606	CLA	C2-C3-C5-C6
29	1	614	II0	C09-C21-C23-C25
29	1	616	II0	C09-C21-C23-C25
29	1	617	II0	C09-C21-C23-C25
29	1	617	II0	C10-C22-C24-C26
29	2	615	II0	C10-C22-C24-C26
29	3	616	II0	C09-C21-C23-C25
29	4	613	II0	C09-C21-C23-C25
29	5	614	II0	C10-C22-C24-C26
29	5	616	II0	C10-C22-C24-C26
29	5	617	II0	C09-C21-C23-C25
29	5	617	II0	C10-C22-C24-C26
29	6	614	II0	C09-C21-C23-C25
29	7	316	II0	C09-C21-C23-C25
29	7	316	II0	C10-C22-C24-C26
29	8	610	II0	C09-C21-C23-C25
29	8	611	II0	C09-C21-C23-C25
29	8	611	II0	C10-C22-C24-C26
29	9	616	II0	C09-C21-C23-C25
29	9	617	II0	C09-C21-C23-C25
29	9	617	II0	C10-C22-C24-C26
29	B	843	II0	C10-C22-C24-C26
29	O	205	II0	C09-C21-C23-C25
29	O	206	II0	C09-C21-C23-C25
29	R	204	II0	C09-C21-C23-C25
29	Z	312	II0	C09-C21-C23-C25
29	a	612	II0	C09-C21-C23-C25

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Mol	Chain	Res	Type	Atoms
29	a	612	II0	C10-C22-C24-C26
29	a	613	II0	C09-C21-C23-C25
29	a	614	II0	C10-C22-C24-C26
29	b	612	II0	C10-C22-C24-C26
31	1	618	IHT	C11-C21-C24-C26
31	2	616	IHT	C11-C21-C24-C26
31	L	204	IHT	C11-C21-C24-C26
27	2	605	CLA	C11-C10-C8-C9
27	8	615	CLA	C11-C12-C13-C14
27	A	823	CLA	C11-C12-C13-C14
27	A	839	CLA	C11-C12-C13-C14
27	B	801	CLA	C6-C7-C8-C9
27	B	805	CLA	C6-C7-C8-C9
27	B	832	CLA	C14-C13-C15-C16
27	Z	306	CLA	C6-C7-C8-C9
36	4	618	LMU	O1'-C1-C2-C3
27	Z	301	CLA	C2A-CAA-CBA-CGA
27	a	604	CLA	C8-C10-C11-C12
27	2	602	CLA	C1A-C2A-CAA-CBA
27	2	612	CLA	C1A-C2A-CAA-CBA
27	4	601	CLA	C1A-C2A-CAA-CBA
27	5	608	CLA	C1A-C2A-CAA-CBA
27	5	612	CLA	C1A-C2A-CAA-CBA
27	6	603	CLA	C1A-C2A-CAA-CBA
27	6	611	CLA	C1A-C2A-CAA-CBA
27	7	309	CLA	C1A-C2A-CAA-CBA
27	8	603	CLA	C1A-C2A-CAA-CBA
27	9	602	CLA	C1A-C2A-CAA-CBA
27	A	804	CLA	C1A-C2A-CAA-CBA
27	A	816	CLA	C1A-C2A-CAA-CBA
27	A	817	CLA	C1A-C2A-CAA-CBA
27	A	822	CLA	C1A-C2A-CAA-CBA
27	A	828	CLA	C1A-C2A-CAA-CBA
27	A	831	CLA	C1A-C2A-CAA-CBA
27	A	842	CLA	C1A-C2A-CAA-CBA
27	A	844	CLA	C1A-C2A-CAA-CBA
27	B	815	CLA	C1A-C2A-CAA-CBA
27	B	827	CLA	C1A-C2A-CAA-CBA
27	F	202	CLA	C1A-C2A-CAA-CBA
27	F	203	CLA	C1A-C2A-CAA-CBA
27	L	203	CLA	C1A-C2A-CAA-CBA
27	Z	306	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	a	602	CLA	C1A-C2A-CAA-CBA
27	a	610	CLA	C1A-C2A-CAA-CBA
27	a	611	CLA	C1A-C2A-CAA-CBA
27	b	610	CLA	C1A-C2A-CAA-CBA
27	3	607	CLA	C11-C12-C13-C15
27	9	608	CLA	C6-C7-C8-C10
27	R	202	CLA	C6-C7-C8-C9
27	Z	306	CLA	C11-C12-C13-C15
32	6	618	LMG	C11-C10-O7-C8
32	8	616	LMG	C38-C39-C40-C41
39	Z	303	DGD	C2A-C3A-C4A-C5A
35	B	845	8CT	C18-C19-C20-C21
35	B	850	8CT	C16-C17-C18-C19
27	8	603	CLA	C8-C10-C11-C12
33	A	851	LHG	C4-O6-P-O3
33	a	618	LHG	C4-O6-P-O3
36	7	321	LMU	O5'-C5'-C6'-O6'
27	B	816	CLA	C3-C5-C6-C7
33	3	619	LHG	O6-C4-C5-C6
33	A	852	LHG	O6-C4-C5-C6
33	A	851	LHG	C28-C29-C30-C31
39	B	848	DGD	CEB-CFB-CGB-CHB
27	A	817	CLA	C13-C15-C16-C17
27	a	606	CLA	C16-C17-C18-C19
33	4	619	LHG	C10-C11-C12-C13
27	A	832	CLA	C15-C16-C17-C18
32	8	614	LMG	C28-C29-C30-C31
27	9	606	CLA	C4-C3-C5-C6
32	8	616	LMG	C18-C19-C20-C21
33	3	619	LHG	C29-C30-C31-C32
33	Z	311	LHG	O10-C23-O8-C6
27	A	820	CLA	C8-C10-C11-C12
27	B	822	CLA	C10-C11-C12-C13
27	b	611	CLA	C5-C6-C7-C8
27	7	309	CLA	C2A-CAA-CBA-CGA
27	9	607	CLA	C2A-CAA-CBA-CGA
27	B	815	CLA	C16-C17-C18-C20
27	B	820	CLA	C11-C12-C13-C14
32	3	620	LMG	C7-C8-C9-O8
32	F	205	LMG	O1-C7-C8-C9
33	2	620	LHG	C4-C5-C6-O8
33	4	617	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
33	4	619	LHG	C4-C5-C6-O8
33	6	617	LHG	C4-C5-C6-O8
33	Z	311	LHG	C4-C5-C6-O8
33	a	618	LHG	C4-C5-C6-O8
34	3	621	SQD	O6-C44-C45-C46
39	B	848	DGD	O1G-C1G-C2G-C3G
28	1	610	KC2	CAA-CBA-CGA-O1A
28	6	610	KC2	CAA-CBA-CGA-O1A
27	B	804	CLA	C10-C11-C12-C13
33	6	617	LHG	C28-C29-C30-C31
39	B	848	DGD	O1A-C1A-O1G-C1G
39	Z	303	DGD	C2G-C3G-O3G-C1D
33	7	320	LHG	C35-C36-C37-C38
33	Z	311	LHG	C35-C36-C37-C38
34	3	621	SQD	C30-C31-C32-C33
36	7	321	LMU	C2-C3-C4-C5
27	B	816	CLA	O1A-CGA-O2A-C1
27	9	606	CLA	C16-C17-C18-C19
39	Z	303	DGD	C6A-C7A-C8A-C9A
33	6	617	LHG	C7-C8-C9-C10
27	A	836	CLA	C5-C6-C7-C8
27	3	610	CLA	C4-C3-C5-C6
27	4	604	CLA	C4-C3-C5-C6
27	6	605	CLA	C4-C3-C5-C6
27	7	305	CLA	C4-C3-C5-C6
39	Z	303	DGD	C5B-C6B-C7B-C8B
27	Z	301	CLA	O1A-CGA-O2A-C1
27	O	204	CLA	C2-C3-C5-C6
28	2	610	KC2	C2A-CAA-CBA-CGA
28	6	610	KC2	C2A-CAA-CBA-CGA
27	4	611	CLA	CBA-CGA-O2A-C1
33	3	619	LHG	C24-C23-O8-C6
39	Z	303	DGD	C2A-C1A-O1G-C1G
36	J	104	LMU	O5B-C5B-C6B-O6B
33	b	616	LHG	C28-C29-C30-C31
27	A	828	CLA	C15-C16-C17-C18
33	A	852	LHG	C9-C10-C11-C12
33	b	616	LHG	C6-C5-O7-C7
36	4	618	LMU	O5'-C5'-C6'-O6'
27	7	309	CLA	C5-C6-C7-C8
27	B	841	CLA	C2-C1-O2A-CGA
33	a	617	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
36	7	321	LMU	C5-C6-C7-C8
27	B	828	CLA	CBA-CGA-O2A-C1
27	b	608	CLA	CBA-CGA-O2A-C1
33	4	617	LHG	O10-C23-O8-C6
33	7	320	LHG	O6-C4-C5-O7
33	8	613	LHG	O6-C4-C5-O7
33	A	852	LHG	O6-C4-C5-O7
27	B	826	CLA	C16-C17-C18-C19
27	4	602	CLA	C10-C11-C12-C13
27	7	312	CLA	C5-C6-C7-C8
28	1	610	KC2	CAA-CBA-CGA-O2A
28	6	610	KC2	CAA-CBA-CGA-O2A
27	B	822	CLA	C8-C10-C11-C12
34	O	207	SQD	C2-C1-O6-C44
32	8	616	LMG	O8-C28-C29-C30
32	F	205	LMG	O1-C7-C8-O7
33	4	617	LHG	C11-C12-C13-C14
33	Z	311	LHG	C30-C31-C32-C33
33	4	617	LHG	C24-C25-C26-C27
27	A	819	CLA	C4-C3-C5-C6
27	b	604	CLA	C4-C3-C5-C6
32	8	614	LMG	C23-C24-C25-C26
27	3	610	CLA	C2-C3-C5-C6
27	6	608	CLA	C11-C10-C8-C7
27	7	305	CLA	C2-C3-C5-C6
27	A	819	CLA	C2-C3-C5-C6
27	A	825	CLA	C6-C7-C8-C10
27	A	826	CLA	C11-C10-C8-C7
27	A	833	CLA	C11-C12-C13-C15
27	A	843	CLA	C11-C10-C8-C7
27	B	805	CLA	C11-C12-C13-C15
27	B	808	CLA	C11-C12-C13-C15
27	B	816	CLA	C11-C10-C8-C7
27	B	835	CLA	C12-C13-C15-C16
27	Z	301	CLA	C11-C10-C8-C7
27	a	608	CLA	C11-C10-C8-C7
27	b	602	CLA	C6-C7-C8-C10
27	b	604	CLA	C6-C7-C8-C10
27	b	608	CLA	C11-C10-C8-C7
27	B	816	CLA	C10-C11-C12-C13
27	5	608	CLA	C11-C10-C8-C9
27	6	604	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
27	A	811	CLA	C14-C13-C15-C16
27	A	835	CLA	C11-C10-C8-C9
27	A	839	CLA	C6-C7-C8-C9
27	B	807	CLA	C6-C7-C8-C9
27	B	808	CLA	C11-C12-C13-C14
27	B	821	CLA	C6-C7-C8-C9
27	B	835	CLA	C11-C10-C8-C9
27	L	202	CLA	C6-C7-C8-C9
27	Z	301	CLA	C11-C10-C8-C9
27	b	604	CLA	C11-C10-C8-C9
33	6	617	LHG	C27-C28-C29-C30
33	A	851	LHG	C34-C35-C36-C37
27	A	806	CLA	C10-C11-C12-C13
27	A	817	CLA	O1A-CGA-O2A-C1
27	L	203	CLA	O1A-CGA-O2A-C1
27	F	204	CLA	C6-C7-C8-C9
32	3	618	LMG	C11-C12-C13-C14
33	8	613	LHG	C24-C25-C26-C27
32	8	616	LMG	C16-C17-C18-C19
32	F	205	LMG	C11-C12-C13-C14
33	4	620	LHG	C28-C29-C30-C31
33	b	616	LHG	C24-C23-O8-C6
33	4	617	LHG	C31-C32-C33-C34
27	4	611	CLA	C16-C17-C18-C20
27	B	828	CLA	C8-C10-C11-C12
33	3	622	LHG	O6-C4-C5-C6
33	6	617	LHG	O6-C4-C5-C6
33	8	613	LHG	O6-C4-C5-C6
33	b	616	LHG	O6-C4-C5-C6
27	b	604	CLA	C3-C5-C6-C7
33	4	620	LHG	C23-C24-C25-C26
27	B	813	CLA	C8-C10-C11-C12
38	B	842	PQN	C15-C16-C17-C18
27	A	810	CLA	C4-C3-C5-C6
27	6	605	CLA	C2-C3-C5-C6
27	A	810	CLA	C2-C3-C5-C6
27	b	604	CLA	C2-C3-C5-C6
33	7	320	LHG	C7-C8-C9-C10
39	Z	303	DGD	CAB-CBB-CCB-CDB
27	B	839	CLA	C13-C15-C16-C17
27	b	602	CLA	C8-C10-C11-C12
27	5	608	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	4	606	CLA	C11-C12-C13-C14
27	A	809	CLA	C3A-C2A-CAA-CBA
27	B	804	CLA	C3A-C2A-CAA-CBA
27	O	204	CLA	C3A-C2A-CAA-CBA
27	a	611	CLA	C3A-C2A-CAA-CBA
32	8	614	LMG	C29-C30-C31-C32
33	3	619	LHG	C11-C12-C13-C14
27	B	827	CLA	C5-C6-C7-C8
39	B	848	DGD	C8A-C9A-CAA-CBA
27	7	313	CLA	CBA-CGA-O2A-C1
27	A	823	CLA	CBA-CGA-O2A-C1
32	8	614	LMG	C33-C34-C35-C36
33	4	619	LHG	C27-C28-C29-C30
27	B	841	CLA	C3-C5-C6-C7
27	A	818	CLA	C10-C11-C12-C13
27	A	827	CLA	C5-C6-C7-C8
33	3	619	LHG	C4-C5-C6-O8
33	5	619	LHG	C4-C5-C6-O8
33	4	619	LHG	C18-C19-C20-C21
27	1	602	CLA	C10-C11-C12-C13
33	A	852	LHG	C4-O6-P-O3
27	B	801	CLA	C3-C5-C6-C7
27	O	203	CLA	C3-C5-C6-C7
27	B	816	CLA	C2A-CAA-CBA-CGA
27	3	607	CLA	C5-C6-C7-C8
39	Z	303	DGD	C7A-C8A-C9A-CAA
33	a	617	LHG	O6-C4-C5-O7
27	A	844	CLA	CBA-CGA-O2A-C1
33	A	852	LHG	C24-C23-O8-C6
34	3	621	SQD	C11-C12-C13-C14
27	4	601	CLA	C2C-C3C-CAC-CBC
32	8	614	LMG	C24-C25-C26-C27
27	B	816	CLA	C11-C12-C13-C14
27	A	817	CLA	C3-C5-C6-C7
27	A	833	CLA	C3-C5-C6-C7
33	4	619	LHG	O7-C5-C6-O8
33	A	851	LHG	O7-C5-C6-O8
33	4	617	LHG	C33-C34-C35-C36
27	1	612	CLA	C11-C12-C13-C15
27	B	820	CLA	C11-C12-C13-C15
27	R	202	CLA	C6-C7-C8-C10
32	8	614	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
27	A	804	CLA	C10-C11-C12-C13
33	7	319	LHG	C1-C2-C3-O3
33	3	619	LHG	C34-C35-C36-C37
32	3	620	LMG	O9-C10-O7-C8
27	4	611	CLA	C2-C1-O2A-CGA
27	A	807	CLA	C2-C1-O2A-CGA
27	B	838	CLA	C2-C1-O2A-CGA
27	Z	304	CLA	C2-C1-O2A-CGA
27	a	610	CLA	C2-C1-O2A-CGA
27	b	607	CLA	C2-C1-O2A-CGA
33	7	319	LHG	O10-C23-O8-C6
27	B	806	CLA	C13-C15-C16-C17
27	6	608	CLA	C11-C10-C8-C9
27	A	820	CLA	C6-C7-C8-C9
27	A	826	CLA	C11-C10-C8-C9
27	B	802	CLA	C11-C10-C8-C9
27	B	835	CLA	C14-C13-C15-C16
27	F	202	CLA	C11-C10-C8-C9
27	a	604	CLA	C6-C7-C8-C9
33	b	616	LHG	C26-C27-C28-C29
33	A	852	LHG	C10-C11-C12-C13
39	Z	303	DGD	CCA-CDA-CEA-CFA
27	b	610	CLA	C4-C3-C5-C6
28	6	610	KC2	C1A-C2A-CAA-CBA
33	2	619	LHG	C2-C3-O3-P
33	3	622	LHG	C2-C3-O3-P
27	3	607	CLA	C11-C12-C13-C14
27	6	607	CLA	C6-C7-C8-C10
27	9	602	CLA	C6-C7-C8-C10
31	6	616	IHT	C10-C07-C18-C22
35	Z	308	8CT	C02-C03-C10-C11
35	Z	308	8CT	C04-C03-C10-C11
35	b	615	8CT	C04-C03-C10-C11
27	2	605	CLA	C8-C10-C11-C12
32	6	618	LMG	C29-C30-C31-C32
33	3	619	LHG	C27-C28-C29-C30
33	b	616	LHG	C19-C20-C21-C22
27	K	101	CLA	C10-C11-C12-C13
27	A	844	CLA	C16-C17-C18-C20
27	4	601	CLA	C5-C6-C7-C8
27	A	812	CLA	C5-C6-C7-C8
33	2	619	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	7	320	LHG	O6-C4-C5-C6
27	6	602	CLA	C11-C10-C8-C7
27	A	801	CLA	C12-C13-C15-C16
27	A	804	CLA	C11-C12-C13-C15
27	A	822	CLA	C12-C13-C15-C16
27	A	823	CLA	C11-C10-C8-C7
27	B	802	CLA	C11-C12-C13-C15
27	B	821	CLA	C6-C7-C8-C10
27	B	823	CLA	C6-C7-C8-C10
27	B	835	CLA	C11-C10-C8-C7
27	L	202	CLA	C6-C7-C8-C10
27	a	604	CLA	C6-C7-C8-C10
27	b	602	CLA	C11-C12-C13-C15
38	A	850	PQN	C16-C17-C18-C20
38	A	850	PQN	C22-C23-C25-C26
38	B	842	PQN	C21-C22-C23-C25
35	A	847	8CT	C18-C19-C20-C21
35	A	847	8CT	C23-C24-C25-C26
35	B	845	8CT	C23-C24-C25-C26
35	B	846	8CT	C18-C19-C20-C21
27	F	204	CLA	C6-C7-C8-C10
36	J	104	LMU	C5'-C4'-O1B-C1B
27	A	829	CLA	CBA-CGA-O2A-C1
27	9	601	CLA	C2C-C3C-CAC-CBC
27	A	843	CLA	C2A-CAA-CBA-CGA
33	4	617	LHG	C15-C16-C17-C18
27	1	602	CLA	C3-C5-C6-C7
33	4	620	LHG	C10-C11-C12-C13
27	3	608	CLA	C5-C6-C7-C8
27	A	816	CLA	C5-C6-C7-C8
27	b	604	CLA	C15-C16-C17-C18
27	A	801	CLA	CAA-CBA-CGA-O2A
27	1	603	CLA	CAD-CBD-CGD-O2D
27	1	613	CLA	CAD-CBD-CGD-O2D
27	4	604	CLA	CAD-CBD-CGD-O2D
27	6	608	CLA	CAD-CBD-CGD-O2D
27	7	312	CLA	CAD-CBD-CGD-O2D
27	8	615	CLA	CAD-CBD-CGD-O2D
27	9	601	CLA	CAD-CBD-CGD-O2D
27	9	614	CLA	CAD-CBD-CGD-O2D
27	A	805	CLA	CAD-CBD-CGD-O2D
27	A	823	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	A	828	CLA	CAD-CBD-CGD-O2D
27	A	838	CLA	CAD-CBD-CGD-O2D
27	A	840	CLA	CAD-CBD-CGD-O2D
27	B	806	CLA	CAD-CBD-CGD-O2D
27	B	831	CLA	CAD-CBD-CGD-O2D
27	B	832	CLA	CAD-CBD-CGD-O2D
27	B	836	CLA	CAD-CBD-CGD-O2D
27	B	837	CLA	CAD-CBD-CGD-O2D
27	L	201	CLA	CAD-CBD-CGD-O2D
27	Z	301	CLA	CAD-CBD-CGD-O2D
27	Z	306	CLA	CAD-CBD-CGD-O2D
27	a	602	CLA	CAD-CBD-CGD-O2D
27	b	601	CLA	CAD-CBD-CGD-O2D
27	b	610	CLA	CAD-CBD-CGD-O2D
28	2	610	KC2	CAD-CBD-CGD-O2D
28	3	606	KC2	C2B-C3B-CAB-CBB
28	4	605	KC2	C2C-C3C-CAC-CBC
28	7	307	KC2	CAD-CBD-CGD-O2D
28	Z	307	KC2	C2C-C3C-CAC-CBC
28	b	605	KC2	CAD-CBD-CGD-O2D
27	8	608	CLA	C10-C11-C12-C13
27	A	825	CLA	C5-C6-C7-C8
27	B	826	CLA	C8-C10-C11-C12
27	2	602	CLA	CBA-CGA-O2A-C1
27	A	804	CLA	C4-C3-C5-C6
27	L	202	CLA	C4-C3-C5-C6
36	J	104	LMU	O5'-C1'-O1'-C1
33	7	320	LHG	C4-C5-C6-O8
39	Z	303	DGD	C1G-C2G-C3G-O3G
27	B	828	CLA	O1A-CGA-O2A-C1
33	2	619	LHG	O6-C4-C5-O7
27	A	843	CLA	C8-C10-C11-C12
27	Z	306	CLA	C5-C6-C7-C8
28	Z	307	KC2	CAA-CBA-CGA-O1A
27	8	608	CLA	C16-C17-C18-C19
27	1	613	CLA	CHA-CBD-CGD-O1D
27	2	612	CLA	CHA-CBD-CGD-O1D
27	3	604	CLA	CHA-CBD-CGD-O1D
27	3	604	CLA	CHA-CBD-CGD-O2D
27	3	612	CLA	CHA-CBD-CGD-O2D
27	5	604	CLA	CHA-CBD-CGD-O1D
27	5	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	5	612	CLA	CHA-CBD-CGD-O2D
27	7	305	CLA	CHA-CBD-CGD-O1D
27	7	313	CLA	CHA-CBD-CGD-O1D
27	9	611	CLA	CHA-CBD-CGD-O1D
27	9	611	CLA	CHA-CBD-CGD-O2D
27	A	804	CLA	CHA-CBD-CGD-O1D
27	A	806	CLA	CHA-CBD-CGD-O1D
27	A	806	CLA	CHA-CBD-CGD-O2D
27	B	807	CLA	CHA-CBD-CGD-O1D
27	B	807	CLA	CHA-CBD-CGD-O2D
27	B	814	CLA	CHA-CBD-CGD-O2D
27	R	202	CLA	CHA-CBD-CGD-O1D
27	R	202	CLA	CHA-CBD-CGD-O2D
28	6	613	KC2	CHA-CBD-CGD-O1D
28	6	613	KC2	CHA-CBD-CGD-O2D
28	a	609	KC2	CHA-CBD-CGD-O1D
28	a	609	KC2	CHA-CBD-CGD-O2D
27	A	816	CLA	CAA-CBA-CGA-O2A
32	8	614	LMG	C18-C19-C20-C21
32	8	616	LMG	C29-C30-C31-C32
33	2	620	LHG	C30-C31-C32-C33
27	3	605	CLA	C3-C5-C6-C7
27	B	813	CLA	C3-C5-C6-C7
27	4	611	CLA	O1A-CGA-O2A-C1
27	b	608	CLA	O1A-CGA-O2A-C1
33	3	619	LHG	O10-C23-O8-C6
32	8	616	LMG	C34-C35-C36-C37
33	3	619	LHG	O7-C5-C6-O8
33	6	617	LHG	O7-C5-C6-O8
34	3	621	SQD	O6-C44-C45-O47
39	B	848	DGD	O1G-C1G-C2G-O2G
39	Z	303	DGD	O2G-C2G-C3G-O3G
28	Z	307	KC2	CAA-CBA-CGA-O2A
27	B	802	CLA	C10-C11-C12-C13
32	2	617	LMG	O10-C28-O8-C9
27	B	818	CLA	C11-C12-C13-C14
33	5	619	LHG	O1-C1-C2-O2
33	7	320	LHG	C11-C10-C9-C8
39	B	848	DGD	C3B-C4B-C5B-C6B
39	Z	303	DGD	C8B-C9B-CAB-CBB
27	4	607	CLA	C4-C3-C5-C6
36	7	321	LMU	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	B	807	CLA	C2-C3-C5-C6
29	1	614	II0	C10-C22-C24-C26
29	1	619	II0	C10-C22-C24-C26
29	2	615	II0	C09-C21-C23-C25
29	3	613	II0	C09-C21-C23-C25
29	3	615	II0	C10-C22-C24-C26
29	3	616	II0	C10-C22-C24-C26
29	3	617	II0	C09-C21-C23-C25
29	4	612	II0	C09-C21-C23-C25
29	4	612	II0	C10-C22-C24-C26
29	5	614	II0	C09-C21-C23-C25
29	5	615	II0	C10-C22-C24-C26
29	5	620	II0	C10-C22-C24-C26
29	7	301	II0	C09-C21-C23-C25
29	7	301	II0	C10-C22-C24-C26
29	8	610	II0	C10-C22-C24-C26
29	9	616	II0	C10-C22-C24-C26
29	B	843	II0	C09-C21-C23-C25
29	J	101	II0	C09-C21-C23-C25
29	R	204	II0	C10-C22-C24-C26
29	a	613	II0	C10-C22-C24-C26
29	a	614	II0	C09-C21-C23-C25
29	a	615	II0	C10-C22-C24-C26
30	1	615	II3	C16-C23-C27-C28
31	Z	302	IHT	C11-C21-C24-C26
27	b	607	CLA	C5-C6-C7-C8
27	A	804	CLA	C11-C12-C13-C14
27	B	802	CLA	C11-C12-C13-C14
27	B	804	CLA	C11-C10-C8-C9
27	Z	310	CLA	C14-C13-C15-C16
27	b	602	CLA	C11-C12-C13-C14
38	B	842	PQN	C21-C22-C23-C24
27	B	823	CLA	C3-C5-C6-C7
34	3	621	SQD	O47-C7-C8-C9
27	A	801	CLA	C5-C6-C7-C8
27	3	611	CLA	C1A-C2A-CAA-CBA
27	6	602	CLA	C1A-C2A-CAA-CBA
27	6	605	CLA	C1A-C2A-CAA-CBA
27	A	809	CLA	C1A-C2A-CAA-CBA
27	A	814	CLA	C1A-C2A-CAA-CBA
27	B	811	CLA	C1A-C2A-CAA-CBA
27	B	826	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	a	601	CLA	C1A-C2A-CAA-CBA
33	2	619	LHG	C7-C8-C9-C10
27	a	605	CLA	CBA-CGA-O2A-C1
35	B	845	8CT	C16-C17-C18-C19
33	4	620	LHG	C3-O3-P-O6
33	a	617	LHG	C3-O3-P-O6
27	4	601	CLA	C4C-C3C-CAC-CBC
27	B	807	CLA	C4-C3-C5-C6
27	6	608	CLA	C3-C5-C6-C7
32	3	618	LMG	O10-C28-O8-C9
33	2	618	LHG	C3-O3-P-O4
33	2	618	LHG	C4-O6-P-O4
33	3	619	LHG	C3-O3-P-O5
33	4	620	LHG	C3-O3-P-O4
33	A	851	LHG	C4-O6-P-O4
33	A	852	LHG	C3-O3-P-O4
33	a	617	LHG	C3-O3-P-O4
33	a	618	LHG	C3-O3-P-O5
33	a	618	LHG	C4-O6-P-O4
33	b	616	LHG	C3-O3-P-O5
38	B	842	PQN	C26-C27-C28-C30
33	A	852	LHG	C7-C8-C9-C10
39	Z	303	DGD	C1B-C2B-C3B-C4B
33	A	851	LHG	C19-C20-C21-C22
33	6	617	LHG	C32-C33-C34-C35
33	A	851	LHG	C27-C28-C29-C30
27	B	812	CLA	C2C-C3C-CAC-CBC
33	a	618	LHG	C24-C25-C26-C27
27	3	604	CLA	CAD-CBD-CGD-O1D
27	3	610	CLA	CAD-CBD-CGD-O1D
27	5	604	CLA	CAD-CBD-CGD-O1D
27	5	613	CLA	CAD-CBD-CGD-O1D
27	6	604	CLA	CAD-CBD-CGD-O1D
27	7	305	CLA	CAD-CBD-CGD-O1D
27	8	607	CLA	CAD-CBD-CGD-O1D
27	9	611	CLA	CAD-CBD-CGD-O1D
27	B	813	CLA	CAD-CBD-CGD-O1D
27	R	202	CLA	CAD-CBD-CGD-O1D
28	1	610	KC2	CAD-CBD-CGD-O1D
28	6	613	KC2	CAD-CBD-CGD-O1D
34	3	621	SQD	C5-C6-S-O7
38	A	850	PQN	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
33	a	617	LHG	C29-C30-C31-C32
32	2	617	LMG	C4-C5-C6-O5
33	4	617	LHG	C12-C13-C14-C15
33	4	620	LHG	C34-C35-C36-C37
33	A	852	LHG	C11-C12-C13-C14
36	4	618	LMU	C7-C8-C9-C10
27	A	822	CLA	C4-C3-C5-C6
27	7	303	CLA	C12-C13-C15-C16
27	8	603	CLA	C11-C10-C8-C7
27	8	608	CLA	C11-C10-C8-C7
27	A	824	CLA	C6-C7-C8-C10
27	A	828	CLA	C11-C12-C13-C15
27	B	804	CLA	C11-C12-C13-C15
27	B	809	CLA	C3A-C2A-CAA-CBA
27	B	815	CLA	C12-C13-C15-C16
27	B	826	CLA	C11-C12-C13-C15
27	B	832	CLA	C6-C7-C8-C10
27	B	835	CLA	C3A-C2A-CAA-CBA
27	b	602	CLA	C11-C10-C8-C7
33	3	622	LHG	O6-C4-C5-O7
33	b	616	LHG	O6-C4-C5-O7
35	7	318	8CT	C28-C29-C30-C31
35	A	846	8CT	C28-C29-C30-C31
35	B	850	8CT	C28-C29-C30-C31
35	I	101	8CT	C28-C29-C30-C31
35	J	103	8CT	C28-C29-C30-C31
35	K	103	8CT	C28-C29-C30-C31
35	R	201	8CT	C28-C29-C30-C31
35	R	203	8CT	C28-C29-C30-C31
35	Z	309	8CT	C28-C29-C30-C31
35	b	615	8CT	C28-C29-C30-C31
32	2	617	LMG	O6-C5-C6-O5
32	8	616	LMG	C12-C13-C14-C15
33	2	619	LHG	C12-C13-C14-C15
33	4	619	LHG	C13-C14-C15-C16
27	a	608	CLA	C2C-C3C-CAC-CBC
32	F	205	LMG	C30-C31-C32-C33
27	A	823	CLA	O1A-CGA-O2A-C1
27	9	613	CLA	C2A-CAA-CBA-CGA
27	A	803	CLA	C16-C17-C18-C19
32	8	614	LMG	C36-C37-C38-C39
27	B	804	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	8	613	LHG	C4-C5-C6-O8
33	a	617	LHG	C4-C5-C6-O8
32	8	616	LMG	O1-C7-C8-O7
33	a	617	LHG	O7-C5-C6-O8
33	a	618	LHG	O7-C5-C6-O8
36	J	104	LMU	C3'-C4'-O1B-C1B
32	8	616	LMG	C31-C32-C33-C34
27	7	313	CLA	O1A-CGA-O2A-C1
27	B	820	CLA	C5-C6-C7-C8
27	3	607	CLA	C3-C5-C6-C7
27	b	608	CLA	C3-C5-C6-C7
27	B	810	CLA	C4-C3-C5-C6
27	5	608	CLA	CBA-CGA-O2A-C1
27	4	610	CLA	C11-C12-C13-C14
27	7	303	CLA	C14-C13-C15-C16
27	8	608	CLA	C11-C10-C8-C9
27	A	811	CLA	C11-C10-C8-C9
27	A	826	CLA	C14-C13-C15-C16
27	B	812	CLA	C6-C7-C8-C9
27	B	815	CLA	C14-C13-C15-C16
27	B	823	CLA	C6-C7-C8-C9
27	B	826	CLA	C11-C12-C13-C14
27	B	832	CLA	C6-C7-C8-C9
27	b	602	CLA	C11-C10-C8-C9
27	b	606	CLA	C11-C10-C8-C9
38	A	850	PQN	C24-C23-C25-C26
27	B	841	CLA	CBD-CGD-O2D-CED
33	3	619	LHG	C19-C20-C21-C22
27	B	839	CLA	C16-C17-C18-C19
33	b	616	LHG	C14-C15-C16-C17
33	A	851	LHG	C33-C34-C35-C36
27	1	612	CLA	C11-C12-C13-C14
27	6	605	CLA	CAA-CBA-CGA-O2A
34	3	621	SQD	C29-C30-C31-C32
36	7	321	LMU	C6-C7-C8-C9
27	L	202	CLA	C2-C3-C5-C6
27	b	602	CLA	C5-C6-C7-C8
27	B	823	CLA	C13-C15-C16-C17
27	2	605	CLA	CAA-CBA-CGA-O2A
33	4	617	LHG	C16-C17-C18-C19
27	A	811	CLA	C10-C11-C12-C13
33	7	320	LHG	C6-C5-O7-C7

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Mol	Chain	Res	Type	Atoms
27	6	603	CLA	C2A-CAA-CBA-CGA
27	7	312	CLA	C2-C1-O2A-CGA
27	8	605	CLA	C2-C1-O2A-CGA
27	B	826	CLA	C2-C1-O2A-CGA
27	b	610	CLA	C2-C1-O2A-CGA
33	Z	311	LHG	C15-C16-C17-C18
33	a	617	LHG	O10-C23-O8-C6
27	b	602	CLA	C3-C5-C6-C7
33	7	319	LHG	C27-C28-C29-C30
27	B	831	CLA	CBA-CGA-O2A-C1
35	I	101	8CT	C18-C19-C20-C21
27	8	606	CLA	C6-C7-C8-C9
27	F	202	CLA	C4-C3-C5-C6
35	R	201	8CT	C02-C03-C10-C11
35	R	201	8CT	C04-C03-C10-C11
27	A	822	CLA	C2-C3-C5-C6
27	B	812	CLA	C4C-C3C-CAC-CBC
36	4	618	LMU	C6-C7-C8-C9
32	3	620	LMG	O7-C8-C9-O8
33	7	320	LHG	O7-C5-C6-O8
39	Z	303	DGD	CBA-CCA-CDA-CEA
33	2	618	LHG	C3-O3-P-O6
33	2	619	LHG	C3-O3-P-O6
33	2	620	LHG	C3-O3-P-O6
33	4	619	LHG	C4-O6-P-O3
33	3	619	LHG	C10-C11-C12-C13
39	Z	303	DGD	CDA-CEA-CFA-CGA
32	8	614	LMG	C30-C31-C32-C33
32	8	614	LMG	C8-C9-O8-C28
32	3	620	LMG	C10-C11-C12-C13
39	Z	303	DGD	O1G-C1G-C2G-C3G
27	A	810	CLA	CBD-CGD-O2D-CED
27	4	607	CLA	C2-C3-C5-C6
27	B	838	CLA	C6-C7-C8-C10
27	L	203	CLA	C2C-C3C-CAC-CBC
33	3	619	LHG	C15-C16-C17-C18
27	6	602	CLA	C11-C10-C8-C9
27	A	823	CLA	C11-C10-C8-C9
27	A	825	CLA	C6-C7-C8-C9
27	B	824	CLA	C11-C10-C8-C9
27	b	602	CLA	C6-C7-C8-C9
27	b	608	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
27	2	608	CLA	C10-C11-C12-C13
35	A	847	8CT	C16-C17-C18-C19
35	A	853	8CT	C12-C13-C14-C15
35	A	853	8CT	C16-C17-C18-C19
27	6	607	CLA	C6-C7-C8-C9
27	b	603	CLA	C2A-CAA-CBA-CGA
27	4	603	CLA	C6-C7-C8-C9
33	5	619	LHG	C5-C4-O6-P
27	A	823	CLA	C8-C10-C11-C12
36	J	104	LMU	C2B-C1B-O1B-C4'
27	a	606	CLA	C4-C3-C5-C6
27	A	829	CLA	O1A-CGA-O2A-C1
33	b	616	LHG	O1-C1-C2-O2
27	B	810	CLA	C2-C3-C5-C6
28	7	311	KC2	C2C-C3C-CAC-CBC
27	8	602	CLA	CAA-CBA-CGA-O2A
33	4	617	LHG	C32-C33-C34-C35
27	A	844	CLA	O1A-CGA-O2A-C1
27	A	840	CLA	C6-C7-C8-C10
27	4	607	CLA	C5-C6-C7-C8
35	B	846	8CT	C16-C17-C18-C19
35	Z	308	8CT	C16-C17-C18-C19
27	B	808	CLA	C5-C6-C7-C8
27	B	819	CLA	C5-C6-C7-C8
27	6	603	CLA	CAA-CBA-CGA-O2A
27	8	601	CLA	CAA-CBA-CGA-O2A
27	2	602	CLA	O1A-CGA-O2A-C1
27	3	603	CLA	C11-C12-C13-C14
27	5	604	CLA	C6-C7-C8-C10
28	2	610	KC2	C4C-C3C-CAC-CBC
28	4	605	KC2	C4C-C3C-CAC-CBC
28	9	610	KC2	C4C-C3C-CAC-CBC
28	Z	307	KC2	C4B-C3B-CAB-CBB
36	J	104	LMU	C3-C4-C5-C6
27	R	202	CLA	C4-C3-C5-C6
27	8	604	CLA	C2-C3-C5-C6
27	4	606	CLA	C2-C1-O2A-CGA
27	A	823	CLA	C2-C1-O2A-CGA
27	A	832	CLA	C2-C1-O2A-CGA
27	a	602	CLA	C2-C1-O2A-CGA
27	5	611	CLA	CAA-CBA-CGA-O1A
27	6	603	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	2	602	CLA	C2A-CAA-CBA-CGA
39	B	848	DGD	O2G-C2G-C3G-O3G
33	8	613	LHG	C5-C4-O6-P
27	A	808	CLA	C3A-C2A-CAA-CBA
27	A	811	CLA	C3A-C2A-CAA-CBA
27	A	812	CLA	C3A-C2A-CAA-CBA
27	A	843	CLA	C3A-C2A-CAA-CBA
27	A	837	CLA	C16-C17-C18-C20
32	6	618	LMG	O8-C28-C29-C30
33	6	617	LHG	C24-C23-O8-C6
27	A	820	CLA	C10-C11-C12-C13
32	8	616	LMG	C40-C41-C42-C43
27	8	601	CLA	CAA-CBA-CGA-O1A
27	2	602	CLA	C4-C3-C5-C6
27	8	604	CLA	C4-C3-C5-C6
27	A	804	CLA	C2-C3-C5-C6
29	3	617	II0	C10-C22-C24-C26
29	7	317	II0	C09-C21-C23-C25
31	A	854	IHT	C11-C21-C24-C26
27	3	605	CLA	CAA-CBA-CGA-O2A
27	6	602	CLA	C14-C13-C15-C16
27	8	603	CLA	C11-C12-C13-C14
27	A	804	CLA	C6-C7-C8-C9
27	A	819	CLA	C11-C10-C8-C9
27	A	831	CLA	C11-C12-C13-C14
27	8	603	CLA	CBA-CGA-O2A-C1
33	b	616	LHG	C18-C19-C20-C21
35	A	853	8CT	C39-C16-C17-C18
35	B	845	8CT	C40-C12-C13-C14
35	B	847	8CT	C28-C29-C30-C35
35	B	850	8CT	C40-C12-C13-C14
27	B	805	CLA	C3-C5-C6-C7
27	a	601	CLA	CAA-CBA-CGA-O1A
27	2	603	CLA	C2A-CAA-CBA-CGA
27	9	601	CLA	C4C-C3C-CAC-CBC
32	6	618	LMG	C32-C33-C34-C35
27	8	615	CLA	O2A-C1-C2-C3
27	B	823	CLA	O2A-C1-C2-C3
27	1	611	CLA	CAA-CBA-CGA-O1A
27	9	612	CLA	CAA-CBA-CGA-O1A
31	a	616	IHT	C18-C22-C23-C25
27	5	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	7	312	CLA	C1A-C2A-CAA-CBA
27	8	601	CLA	C1A-C2A-CAA-CBA
27	A	811	CLA	C1A-C2A-CAA-CBA
27	A	830	CLA	C1A-C2A-CAA-CBA
27	B	841	CLA	C1A-C2A-CAA-CBA
27	O	203	CLA	C1A-C2A-CAA-CBA
27	2	602	CLA	C6-C7-C8-C10
27	9	607	CLA	C11-C10-C8-C7
27	A	804	CLA	C12-C13-C15-C16
27	A	828	CLA	C11-C10-C8-C7
27	B	838	CLA	C11-C12-C13-C15
27	K	101	CLA	C6-C7-C8-C10
27	Z	301	CLA	C6-C7-C8-C10
27	a	604	CLA	C11-C10-C8-C7
27	b	604	CLA	C11-C12-C13-C15
38	A	850	PQN	C17-C18-C20-C21
27	A	801	CLA	C3-C5-C6-C7
27	A	830	CLA	C3-C5-C6-C7
27	5	606	CLA	CAA-CBA-CGA-O1A
27	5	606	CLA	CAA-CBA-CGA-O2A
39	B	848	DGD	C9B-CAB-CBB-CCB
35	R	203	8CT	C16-C17-C18-C19
27	L	203	CLA	C4C-C3C-CAC-CBC
32	8	616	LMG	C42-C43-C44-C45
27	9	601	CLA	CAA-CBA-CGA-O1A
27	9	601	CLA	CAA-CBA-CGA-O2A
27	B	803	CLA	CAA-CBA-CGA-O2A
27	b	601	CLA	CAA-CBA-CGA-O2A
32	2	617	LMG	C15-C16-C17-C18
27	7	304	CLA	C6-C7-C8-C9
27	1	608	CLA	C3-C5-C6-C7
33	8	613	LHG	C2-C3-O3-P
27	1	604	CLA	C2A-CAA-CBA-CGA
27	9	603	CLA	C2A-CAA-CBA-CGA
27	a	604	CLA	C2A-CAA-CBA-CGA
27	A	827	CLA	C13-C15-C16-C17
27	5	603	CLA	CAA-CBA-CGA-O1A
27	5	611	CLA	CAA-CBA-CGA-O2A
28	1	610	KC2	C3A-C2A-CAA-CBA
27	5	603	CLA	CAA-CBA-CGA-O2A
27	8	602	CLA	CAA-CBA-CGA-O1A
27	A	814	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	R	202	CLA	C2-C3-C5-C6
27	A	814	CLA	CAA-CBA-CGA-O1A
27	B	803	CLA	CAA-CBA-CGA-O1A
27	B	806	CLA	C15-C16-C17-C18
33	A	851	LHG	C23-C24-C25-C26
35	A	853	8CT	C15-C16-C17-C18
35	B	845	8CT	C11-C12-C13-C14
35	B	850	8CT	C11-C12-C13-C14
33	4	619	LHG	C17-C18-C19-C20
27	B	841	CLA	CBA-CGA-O2A-C1
33	2	618	LHG	O7-C5-C6-O8
35	B	844	8CT	C12-C13-C14-C15
35	K	103	8CT	C16-C17-C18-C19
35	Z	308	8CT	C23-C24-C25-C26
35	b	615	8CT	C12-C13-C14-C15
33	6	617	LHG	C30-C31-C32-C33
27	R	202	CLA	CAA-CBA-CGA-O2A
27	8	603	CLA	C4-C3-C5-C6
27	A	827	CLA	C4-C3-C5-C6
27	A	843	CLA	C4-C3-C5-C6
27	B	811	CLA	C4-C3-C5-C6
27	B	811	CLA	C2-C1-O2A-CGA
27	B	816	CLA	C2-C1-O2A-CGA
27	F	202	CLA	C2-C1-O2A-CGA
27	O	204	CLA	C2-C1-O2A-CGA
27	a	606	CLA	C2-C3-C5-C6
27	7	305	CLA	C5-C6-C7-C8
27	a	605	CLA	O1A-CGA-O2A-C1
27	A	832	CLA	C11-C10-C8-C9
27	9	612	CLA	CAA-CBA-CGA-O2A
27	b	601	CLA	CAA-CBA-CGA-O1A
35	B	847	8CT	C04-C03-C10-C11
35	b	615	8CT	C02-C03-C10-C11
33	A	851	LHG	C11-C10-C9-C8
33	5	619	LHG	O1-C1-C2-C3
33	3	619	LHG	C30-C31-C32-C33
35	B	845	8CT	C12-C13-C14-C15
35	B	850	8CT	C12-C13-C14-C15
35	F	201	8CT	C18-C19-C20-C21
39	B	848	DGD	C2A-C1A-O1G-C1G
27	6	601	CLA	C2C-C3C-CAC-CBC
27	6	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	9	602	CLA	C4-C3-C5-C6
27	B	816	CLA	C4-C3-C5-C6
27	A	803	CLA	C16-C17-C18-C20
27	B	827	CLA	C13-C15-C16-C17
27	F	202	CLA	C10-C11-C12-C13
27	F	202	CLA	C2-C3-C5-C6
32	8	614	LMG	C12-C13-C14-C15
27	A	832	CLA	C13-C15-C16-C17
27	a	601	CLA	CAA-CBA-CGA-O2A
33	A	852	LHG	C14-C15-C16-C17
27	B	827	CLA	C16-C17-C18-C19
27	L	202	CLA	C11-C12-C13-C15
27	A	839	CLA	C3-C5-C6-C7
33	3	622	LHG	C11-C12-C13-C14
27	4	611	CLA	C15-C16-C17-C18
27	Z	306	CLA	C2A-CAA-CBA-CGA
27	8	603	CLA	C2-C3-C5-C6
27	A	817	CLA	C6-C7-C8-C10
27	A	831	CLA	C11-C12-C13-C15
27	B	802	CLA	C11-C10-C8-C7
27	F	202	CLA	C11-C10-C8-C7
27	A	830	CLA	CBA-CGA-O2A-C1
27	B	811	CLA	CBA-CGA-O2A-C1
27	B	824	CLA	C10-C11-C12-C13
33	6	617	LHG	C31-C32-C33-C34
35	Z	309	8CT	C18-C19-C20-C21
28	5	610	KC2	CAA-CBA-CGA-O2A
39	Z	303	DGD	O1G-C1G-C2G-O2G
27	O	204	CLA	CBA-CGA-O2A-C1
32	6	618	LMG	C30-C31-C32-C33
33	Z	311	LHG	C25-C26-C27-C28
27	A	804	CLA	CAA-CBA-CGA-O2A
27	b	610	CLA	CAA-CBA-CGA-O2A
28	5	610	KC2	CAA-CBA-CGA-O1A
32	8	614	LMG	C11-C10-O7-C8
27	7	306	CLA	CAA-CBA-CGA-O2A
33	2	619	LHG	C11-C10-C9-C8
27	b	603	CLA	C4-C3-C5-C6
38	A	850	PQN	C18-C20-C21-C22
27	5	608	CLA	O1A-CGA-O2A-C1
33	4	619	LHG	C3-O3-P-O6
27	A	827	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	B	811	CLA	C2-C3-C5-C6
27	3	610	CLA	C6-C7-C8-C9
27	8	603	CLA	C11-C10-C8-C9
27	A	828	CLA	C11-C12-C13-C14
27	A	831	CLA	C14-C13-C15-C16
27	A	833	CLA	C11-C12-C13-C14
27	A	839	CLA	C11-C10-C8-C9
27	B	804	CLA	C11-C12-C13-C14
27	B	806	CLA	C11-C12-C13-C14
27	b	604	CLA	C14-C13-C15-C16
27	4	601	CLA	C3-C5-C6-C7
27	B	831	CLA	O1A-CGA-O2A-C1
27	2	602	CLA	CAA-CBA-CGA-O2A
27	B	802	CLA	CAA-CBA-CGA-O2A
27	B	832	CLA	CAA-CBA-CGA-O2A
27	1	601	CLA	CAD-CBD-CGD-O2D
27	1	609	CLA	CAD-CBD-CGD-O2D
27	1	611	CLA	CAD-CBD-CGD-O2D
27	2	603	CLA	CAD-CBD-CGD-O2D
27	3	611	CLA	CAD-CBD-CGD-O2D
27	4	609	CLA	CAD-CBD-CGD-O2D
27	5	603	CLA	CAD-CBD-CGD-O2D
27	5	606	CLA	CAD-CBD-CGD-O2D
27	6	611	CLA	CAD-CBD-CGD-O2D
27	9	607	CLA	CAD-CBD-CGD-O2D
27	A	802	CLA	CAD-CBD-CGD-O2D
27	A	804	CLA	CAD-CBD-CGD-O2D
27	A	807	CLA	CAD-CBD-CGD-O2D
27	A	811	CLA	CAD-CBD-CGD-O2D
27	A	812	CLA	CAD-CBD-CGD-O2D
27	A	813	CLA	CAD-CBD-CGD-O2D
27	A	824	CLA	CAD-CBD-CGD-O2D
27	A	829	CLA	CAD-CBD-CGD-O2D
27	A	831	CLA	CAD-CBD-CGD-O2D
27	A	835	CLA	CAD-CBD-CGD-O2D
27	B	810	CLA	CAD-CBD-CGD-O2D
27	B	815	CLA	CAD-CBD-CGD-O2D
27	B	821	CLA	CAD-CBD-CGD-O2D
27	B	825	CLA	CAD-CBD-CGD-O2D
27	B	833	CLA	CAD-CBD-CGD-O2D
27	B	840	CLA	CAD-CBD-CGD-O2D
27	J	102	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	K	102	CLA	CAD-CBD-CGD-O2D
27	O	203	CLA	CAD-CBD-CGD-O2D
27	Z	304	CLA	CAD-CBD-CGD-O2D
27	a	604	CLA	CAD-CBD-CGD-O2D
27	a	605	CLA	CAD-CBD-CGD-O2D
27	b	603	CLA	CAD-CBD-CGD-O2D
28	6	613	KC2	C2B-C3B-CAB-CBB
28	9	610	KC2	C2C-C3C-CAC-CBC
32	F	205	LMG	C9-C8-O7-C10
27	Z	301	CLA	C8-C10-C11-C12
27	b	608	CLA	C8-C10-C11-C12
27	F	203	CLA	C2A-CAA-CBA-CGA
27	9	607	CLA	C3-C5-C6-C7
33	4	617	LHG	C19-C20-C21-C22
27	B	821	CLA	C2-C1-O2A-CGA
27	a	605	CLA	C2-C1-O2A-CGA
27	1	611	CLA	CAA-CBA-CGA-O2A
27	9	603	CLA	CAA-CBA-CGA-O2A
33	4	620	LHG	C32-C33-C34-C35
27	3	610	CLA	CAA-CBA-CGA-O2A
27	B	809	CLA	CAA-CBA-CGA-O2A
27	B	813	CLA	CAA-CBA-CGA-O2A
27	a	604	CLA	CAA-CBA-CGA-O2A
33	Z	311	LHG	O7-C7-C8-C9
27	5	602	CLA	C4-C3-C5-C6
38	A	850	PQN	C14-C13-C15-C16
27	7	306	CLA	CAA-CBA-CGA-O1A
27	A	843	CLA	C2-C3-C5-C6
27	B	815	CLA	C2-C3-C5-C6
27	B	812	CLA	CAA-CBA-CGA-O2A
27	B	819	CLA	CAA-CBA-CGA-O2A
32	8	616	LMG	C41-C42-C43-C44
33	A	851	LHG	C4-C5-C6-O8
27	4	609	CLA	CAA-CBA-CGA-O2A
27	A	803	CLA	CAA-CBA-CGA-O2A
27	A	839	CLA	CAA-CBA-CGA-O2A
27	3	601	CLA	CAA-CBA-CGA-O1A
27	1	612	CLA	O2A-C1-C2-C3
27	4	606	CLA	O2A-C1-C2-C3
27	7	312	CLA	O2A-C1-C2-C3
27	8	605	CLA	O2A-C1-C2-C3
27	O	201	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	Z	305	CLA	O2A-C1-C2-C3
28	3	606	KC2	C4B-C3B-CAB-CBB
28	6	613	KC2	C4B-C3B-CAB-CBB
28	Z	307	KC2	C4C-C3C-CAC-CBC
28	a	609	KC2	C4C-C3C-CAC-CBC
33	Z	311	LHG	C9-C10-C11-C12
33	Z	311	LHG	C26-C27-C28-C29
27	7	309	CLA	CAA-CBA-CGA-O2A
33	4	617	LHG	C11-C10-C9-C8
27	1	602	CLA	CHA-CBD-CGD-O1D
27	1	602	CLA	CHA-CBD-CGD-O2D
27	1	613	CLA	CHA-CBD-CGD-O2D
27	2	606	CLA	CHA-CBD-CGD-O1D
27	2	606	CLA	CHA-CBD-CGD-O2D
27	2	612	CLA	CHA-CBD-CGD-O2D
27	3	601	CLA	CHA-CBD-CGD-O1D
27	3	601	CLA	CHA-CBD-CGD-O2D
27	3	610	CLA	CHA-CBD-CGD-O1D
27	4	602	CLA	CHA-CBD-CGD-O1D
27	4	607	CLA	CHA-CBD-CGD-O2D
27	4	611	CLA	CHA-CBD-CGD-O1D
27	5	608	CLA	CHA-CBD-CGD-O2D
27	5	611	CLA	CHA-CBD-CGD-O1D
27	5	611	CLA	CHA-CBD-CGD-O2D
27	6	604	CLA	CHA-CBD-CGD-O1D
27	7	305	CLA	CHA-CBD-CGD-O2D
27	7	306	CLA	CHA-CBD-CGD-O1D
27	7	306	CLA	CHA-CBD-CGD-O2D
27	7	309	CLA	CHA-CBD-CGD-O2D
27	7	313	CLA	CHA-CBD-CGD-O2D
27	9	602	CLA	CHA-CBD-CGD-O1D
27	9	603	CLA	CHA-CBD-CGD-O1D
27	9	603	CLA	CHA-CBD-CGD-O2D
27	9	606	CLA	CHA-CBD-CGD-O1D
27	9	606	CLA	CHA-CBD-CGD-O2D
27	9	608	CLA	CHA-CBD-CGD-O1D
27	9	608	CLA	CHA-CBD-CGD-O2D
27	A	819	CLA	CHA-CBD-CGD-O2D
27	A	820	CLA	CHA-CBD-CGD-O1D
27	A	820	CLA	CHA-CBD-CGD-O2D
27	A	841	CLA	CHA-CBD-CGD-O2D
27	A	842	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	A	842	CLA	CHA-CBD-CGD-O2D
27	B	814	CLA	CHA-CBD-CGD-O1D
27	B	820	CLA	CHA-CBD-CGD-O1D
27	B	820	CLA	CHA-CBD-CGD-O2D
27	O	202	CLA	CHA-CBD-CGD-O1D
27	O	202	CLA	CHA-CBD-CGD-O2D
27	Z	310	CLA	CHA-CBD-CGD-O1D
27	Z	310	CLA	CHA-CBD-CGD-O2D
27	a	601	CLA	CHA-CBD-CGD-O1D
27	a	601	CLA	CHA-CBD-CGD-O2D
27	a	607	CLA	CHA-CBD-CGD-O1D
27	a	607	CLA	CHA-CBD-CGD-O2D
27	b	611	CLA	CHA-CBD-CGD-O1D
27	b	611	CLA	CHA-CBD-CGD-O2D
28	5	610	KC2	CHA-CBD-CGD-O1D
28	5	610	KC2	CHA-CBD-CGD-O2D
28	7	311	KC2	CHA-CBD-CGD-O1D
28	7	311	KC2	CHA-CBD-CGD-O2D
28	Z	307	KC2	CHA-CBD-CGD-O1D
28	Z	307	KC2	CHA-CBD-CGD-O2D
27	9	603	CLA	CAA-CBA-CGA-O1A
33	a	617	LHG	O7-C7-C8-C9
27	a	608	CLA	C4C-C3C-CAC-CBC
27	B	816	CLA	C2-C3-C5-C6
33	2	620	LHG	O6-C4-C5-C6
27	4	610	CLA	C13-C15-C16-C17
27	a	602	CLA	CAA-CBA-CGA-O2A
27	b	603	CLA	CAA-CBA-CGA-O2A
27	8	604	CLA	C15-C16-C17-C18
27	9	607	CLA	C4C-C3C-CAC-CBC
27	B	808	CLA	CAA-CBA-CGA-O2A
32	8	614	LMG	O7-C10-C11-C12
27	4	609	CLA	C2A-CAA-CBA-CGA
27	6	604	CLA	C2A-CAA-CBA-CGA
27	3	601	CLA	CAA-CBA-CGA-O2A
27	B	805	CLA	CAA-CBA-CGA-O2A
27	Z	306	CLA	CAA-CBA-CGA-O2A
27	4	610	CLA	C11-C12-C13-C15
27	9	607	CLA	C6-C7-C8-C10
27	B	804	CLA	C11-C10-C8-C7
27	B	812	CLA	C6-C7-C8-C10
27	a	603	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
27	b	606	CLA	C11-C10-C8-C7
33	3	622	LHG	O7-C7-C8-C9
33	7	319	LHG	O7-C7-C8-C9
27	9	605	CLA	CAA-CBA-CGA-O1A
27	A	801	CLA	C11-C12-C13-C14
27	A	810	CLA	C11-C12-C13-C14
27	K	101	CLA	C6-C7-C8-C9
27	a	604	CLA	C11-C10-C8-C9
33	a	618	LHG	C5-C6-O8-C23
27	A	841	CLA	C8-C10-C11-C12
27	A	843	CLA	CBA-CGA-O2A-C1
27	3	610	CLA	CAA-CBA-CGA-O1A
34	3	621	SQD	C5-C6-S-O8
33	2	620	LHG	O10-C23-O8-C6
27	B	821	CLA	CAA-CBA-CGA-O2A
27	a	605	CLA	CAA-CBA-CGA-O2A
32	3	618	LMG	O7-C10-C11-C12
33	b	616	LHG	C17-C18-C19-C20
27	2	602	CLA	CAA-CBA-CGA-O1A
27	B	832	CLA	CAA-CBA-CGA-O1A
33	2	620	LHG	C24-C25-C26-C27
27	B	815	CLA	C4-C3-C5-C6
27	A	811	CLA	CAA-CBA-CGA-O2A
27	2	602	CLA	C11-C12-C13-C14
27	a	604	CLA	CAA-CBA-CGA-O1A
31	a	616	IHT	C18-C22-C23-C27
27	1	612	CLA	C8-C10-C11-C12
27	1	601	CLA	C1A-C2A-CAA-CBA
27	A	808	CLA	C1A-C2A-CAA-CBA
27	B	812	CLA	C1A-C2A-CAA-CBA
27	B	825	CLA	C1A-C2A-CAA-CBA
27	B	835	CLA	C1A-C2A-CAA-CBA
27	R	202	CLA	C1A-C2A-CAA-CBA
27	A	838	CLA	C16-C17-C18-C19
27	B	808	CLA	CAA-CBA-CGA-O1A
27	B	813	CLA	CAA-CBA-CGA-O1A
27	6	611	CLA	C2-C1-O2A-CGA
27	O	203	CLA	C5-C6-C7-C8
27	A	803	CLA	CAA-CBA-CGA-O1A
27	A	804	CLA	CAA-CBA-CGA-O1A
27	B	802	CLA	CAA-CBA-CGA-O1A
27	B	821	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	8	616	LMG	O10-C28-C29-C30
27	B	810	CLA	C8-C10-C11-C12
27	2	604	CLA	C2A-CAA-CBA-CGA
33	2	620	LHG	C4-O6-P-O3
33	b	616	LHG	C13-C14-C15-C16
27	3	603	CLA	C11-C12-C13-C15
27	B	812	CLA	CAA-CBA-CGA-O1A
27	a	602	CLA	CAA-CBA-CGA-O1A
33	Z	311	LHG	O9-C7-C8-C9
27	7	308	CLA	CAA-CBA-CGA-O2A
27	7	309	CLA	CAA-CBA-CGA-O1A
33	4	619	LHG	C3-O3-P-O5
33	4	619	LHG	C4-O6-P-O5
33	A	851	LHG	C4-O6-P-O5
33	A	852	LHG	C4-O6-P-O4
33	a	618	LHG	C4-O6-P-O5
27	6	601	CLA	C4C-C3C-CAC-CBC
27	A	839	CLA	CAA-CBA-CGA-O1A
27	b	610	CLA	CAA-CBA-CGA-O1A
39	Z	303	DGD	O1B-C1B-C2B-C3B
33	a	617	LHG	O6-C4-C5-C6
33	Z	311	LHG	C13-C14-C15-C16
27	4	609	CLA	CAA-CBA-CGA-O1A
32	8	614	LMG	O9-C10-C11-C12
33	3	622	LHG	C13-C14-C15-C16
27	b	607	CLA	CAA-CBA-CGA-O2A
27	A	822	CLA	C5-C6-C7-C8
35	F	201	8CT	C13-C14-C15-C16
27	9	604	CLA	C2A-CAA-CBA-CGA
27	A	801	CLA	CAA-CBA-CGA-O1A
32	3	620	LMG	C30-C31-C32-C33
27	O	201	CLA	CAA-CBA-CGA-O2A
27	A	816	CLA	CAA-CBA-CGA-O1A
33	a	617	LHG	O9-C7-C8-C9
33	3	619	LHG	C14-C15-C16-C17
27	A	811	CLA	CAD-CBD-CGD-O1D
27	A	818	CLA	CAD-CBD-CGD-O1D
27	B	804	CLA	CAD-CBD-CGD-O1D
27	B	812	CLA	CAD-CBD-CGD-O1D
27	B	819	CLA	CAD-CBD-CGD-O1D
27	B	839	CLA	CAD-CBD-CGD-O1D
27	L	202	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	a	601	CLA	CAD-CBD-CGD-O1D
28	4	605	KC2	CAD-CBD-CGD-O1D
27	B	819	CLA	CAA-CBA-CGA-O1A
33	7	319	LHG	O9-C7-C8-C9
33	8	613	LHG	C9-C10-C11-C12
33	b	616	LHG	C32-C33-C34-C35
33	6	617	LHG	O7-C7-C8-C9
27	A	817	CLA	C6-C7-C8-C9
27	B	804	CLA	C6-C7-C8-C9
27	B	823	CLA	C14-C13-C15-C16
27	B	838	CLA	C6-C7-C8-C9
27	Z	301	CLA	C6-C7-C8-C9
33	4	617	LHG	C17-C18-C19-C20
27	B	835	CLA	C13-C15-C16-C17
27	b	603	CLA	CAA-CBA-CGA-O1A
27	1	608	CLA	CAA-CBA-CGA-O2A
27	9	606	CLA	C13-C15-C16-C17
27	9	605	CLA	CAA-CBA-CGA-O2A
27	9	609	CLA	C2C-C3C-CAC-CBC
27	B	826	CLA	C15-C16-C17-C18
27	8	605	CLA	C2A-CAA-CBA-CGA
27	A	815	CLA	C2A-CAA-CBA-CGA
27	b	611	CLA	C2A-CAA-CBA-CGA
27	4	603	CLA	CAA-CBA-CGA-O2A
27	a	611	CLA	CAA-CBA-CGA-O2A
27	b	604	CLA	CAA-CBA-CGA-O2A
27	b	604	CLA	C5-C6-C7-C8
33	7	319	LHG	O10-C23-C24-C25
27	1	602	CLA	C11-C12-C13-C14
27	A	841	CLA	C4-C3-C5-C6
27	b	608	CLA	C4-C3-C5-C6
27	B	812	CLA	C8-C10-C11-C12
27	1	601	CLA	C3A-C2A-CAA-CBA
27	5	608	CLA	C6-C7-C8-C10
27	9	602	CLA	C2-C3-C5-C6
27	A	810	CLA	C11-C10-C8-C7
27	A	826	CLA	C12-C13-C15-C16
27	B	819	CLA	C11-C10-C8-C7
27	B	824	CLA	C11-C10-C8-C7
27	B	826	CLA	C6-C7-C8-C10
27	R	202	CLA	C3A-C2A-CAA-CBA
27	a	603	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
35	B	849	8CT	C28-C29-C30-C31
35	Z	308	8CT	C28-C29-C30-C31
27	O	201	CLA	CAA-CBA-CGA-O1A
32	F	205	LMG	O10-C28-C29-C30
27	B	835	CLA	CAA-CBA-CGA-O2A
33	3	619	LHG	O7-C7-C8-C9
27	5	604	CLA	CBD-CGD-O2D-CED
27	9	607	CLA	C13-C15-C16-C17
27	B	805	CLA	CAA-CBA-CGA-O1A
35	B	846	8CT	C23-C24-C25-C26
35	B	849	8CT	C12-C13-C14-C15
35	Z	308	8CT	C18-C19-C20-C21
27	5	604	CLA	C6-C7-C8-C9
36	J	104	LMU	C2-C1-O1'-C1'
27	2	608	CLA	CAA-CBA-CGA-O2A
27	7	303	CLA	CAA-CBA-CGA-O2A
32	8	616	LMG	C14-C15-C16-C17
27	B	832	CLA	C5-C6-C7-C8
27	A	811	CLA	CAA-CBA-CGA-O1A
27	b	604	CLA	CAA-CBA-CGA-O1A
27	B	820	CLA	CBA-CGA-O2A-C1
27	1	602	CLA	CAA-CBA-CGA-O2A
27	A	818	CLA	CAA-CBA-CGA-O2A
27	1	608	CLA	CAA-CBA-CGA-O1A
27	2	608	CLA	CAA-CBA-CGA-O1A
27	a	605	CLA	CAA-CBA-CGA-O1A
27	a	611	CLA	CAA-CBA-CGA-O1A
27	A	820	CLA	C13-C15-C16-C17
39	Z	303	DGD	C5A-C6A-C7A-C8A
27	L	202	CLA	C3-C5-C6-C7

There are no ring outliers.

73 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	842	CLA	1	0
27	B	809	CLA	1	0
27	A	823	CLA	2	0
27	K	102	CLA	1	0
27	7	308	CLA	1	0
29	2	614	II0	1	0
27	5	612	CLA	1	0

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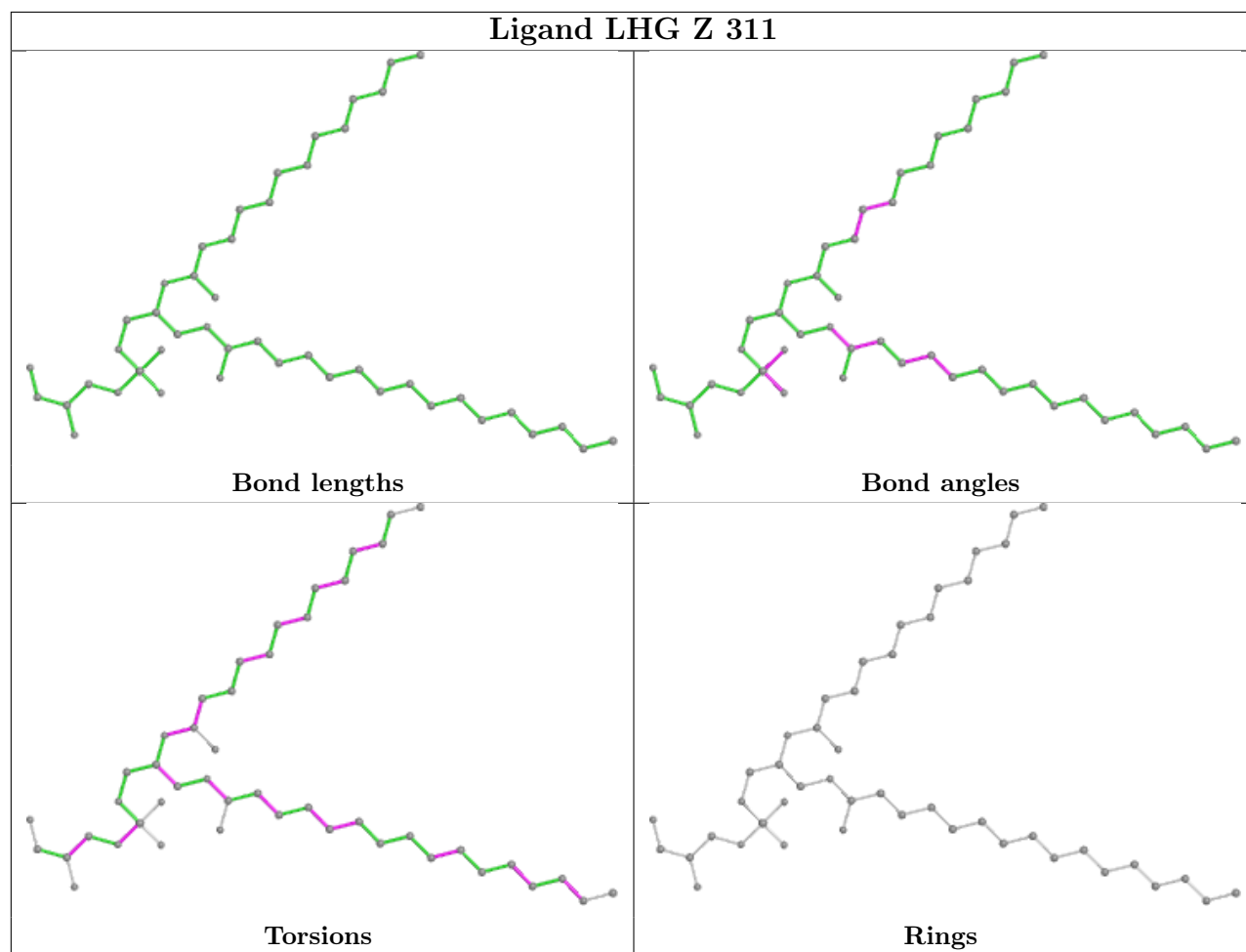
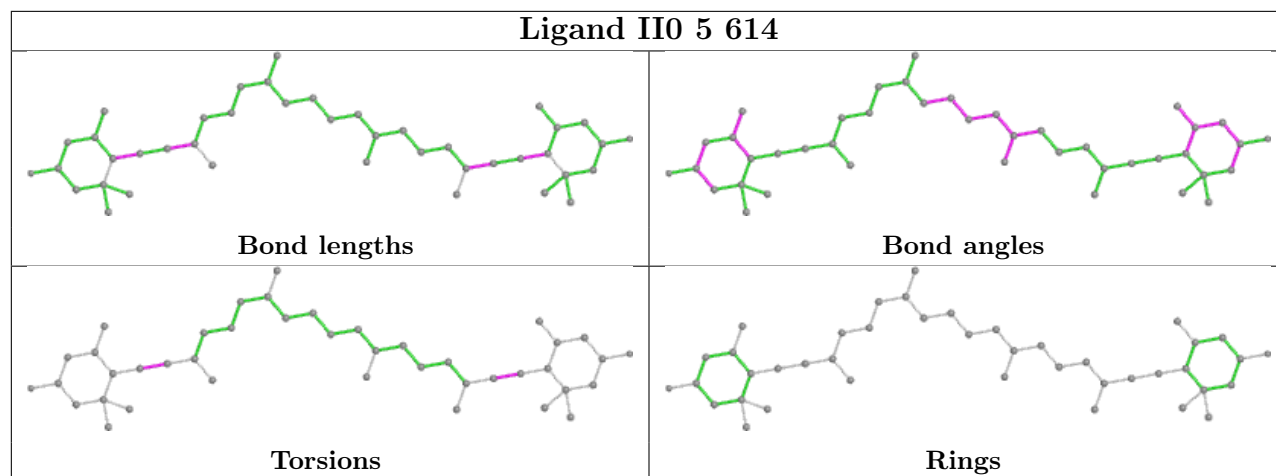
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	8	608	CLA	1	0
27	B	825	CLA	1	0
27	8	602	CLA	2	0
27	A	837	CLA	1	0
36	J	104	LMU	1	0
29	5	620	II0	2	0
27	A	840	CLA	1	0
27	A	808	CLA	1	0
27	A	834	CLA	1	0
27	B	840	CLA	1	0
35	M	101	8CT	1	0
27	9	604	CLA	2	0
27	Z	304	CLA	1	0
27	5	604	CLA	1	0
27	6	605	CLA	1	0
27	A	843	CLA	1	0
28	9	610	KC2	1	0
27	B	812	CLA	1	0
27	7	313	CLA	1	0
36	7	321	LMU	1	0
27	A	801	CLA	1	0
27	B	816	CLA	1	0
27	A	818	CLA	3	0
27	A	811	CLA	1	0
29	4	613	II0	1	0
27	B	832	CLA	2	0
27	9	607	CLA	1	0
27	A	819	CLA	1	0
27	B	839	CLA	1	0
27	B	822	CLA	1	0
27	B	834	CLA	4	0
31	A	854	IHT	1	0
29	8	610	II0	1	0
27	A	836	CLA	3	0
27	5	608	CLA	2	0
27	B	802	CLA	1	0
27	2	611	CLA	1	0
27	A	824	CLA	2	0
27	B	830	CLA	1	0
27	A	838	CLA	1	0
36	4	618	LMU	2	0
27	4	606	CLA	1	0

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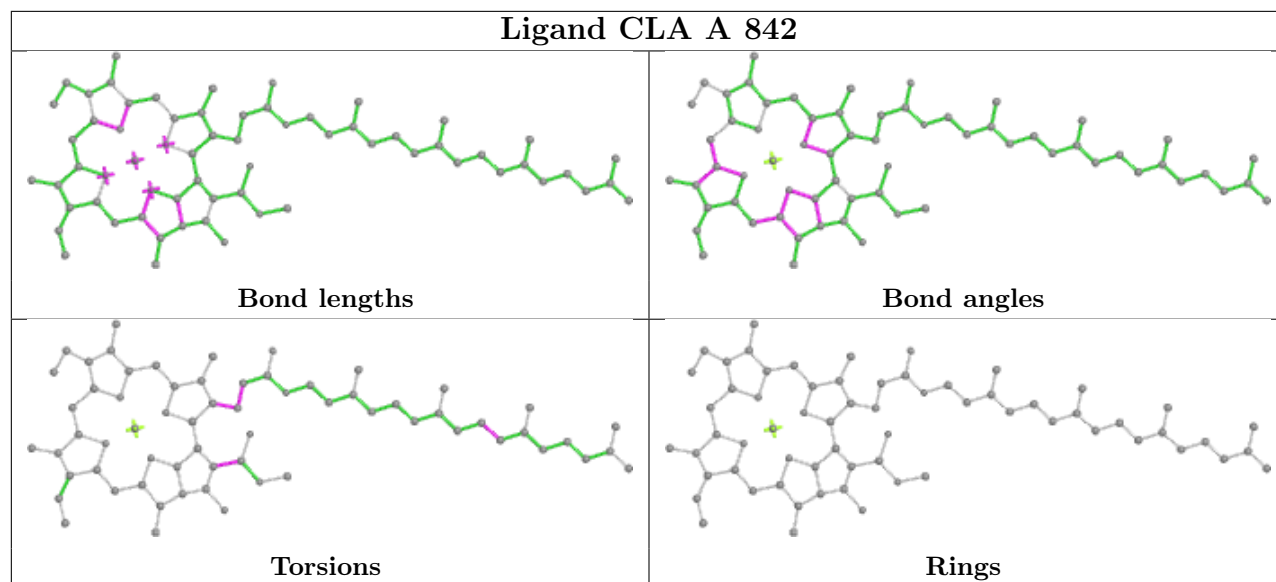
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	809	CLA	1	0
27	A	812	CLA	1	0
31	9	619	IHT	1	0
27	A	844	CLA	3	0
39	Z	303	DGD	1	0
29	3	614	II0	1	0
27	6	611	CLA	1	0
27	B	807	CLA	1	0
27	A	810	CLA	3	0
27	8	605	CLA	2	0
27	O	201	CLA	1	0
37	C	102	SF4	1	0
27	L	201	CLA	1	0
27	A	821	CLA	1	0
28	7	311	KC2	2	0
27	9	606	CLA	1	0
27	5	609	CLA	1	0
33	2	619	LHG	1	0
27	9	602	CLA	1	0
27	1	604	CLA	1	0
27	8	603	CLA	1	0
27	B	801	CLA	2	0
27	B	815	CLA	1	0
27	A	826	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.

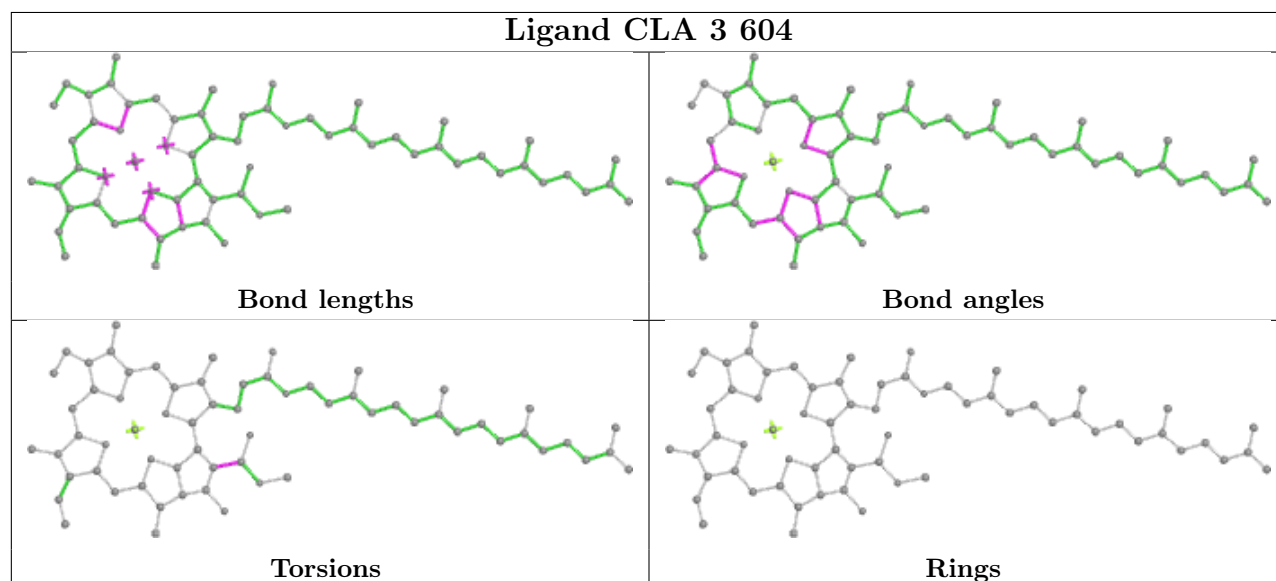




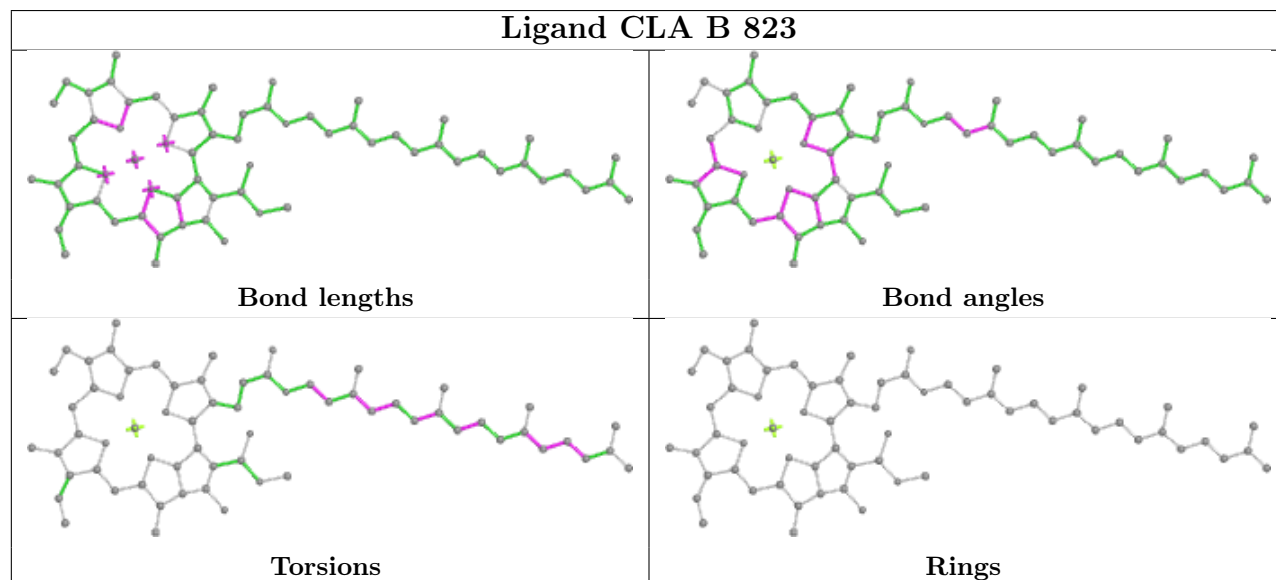
## Ligand CLA A 842

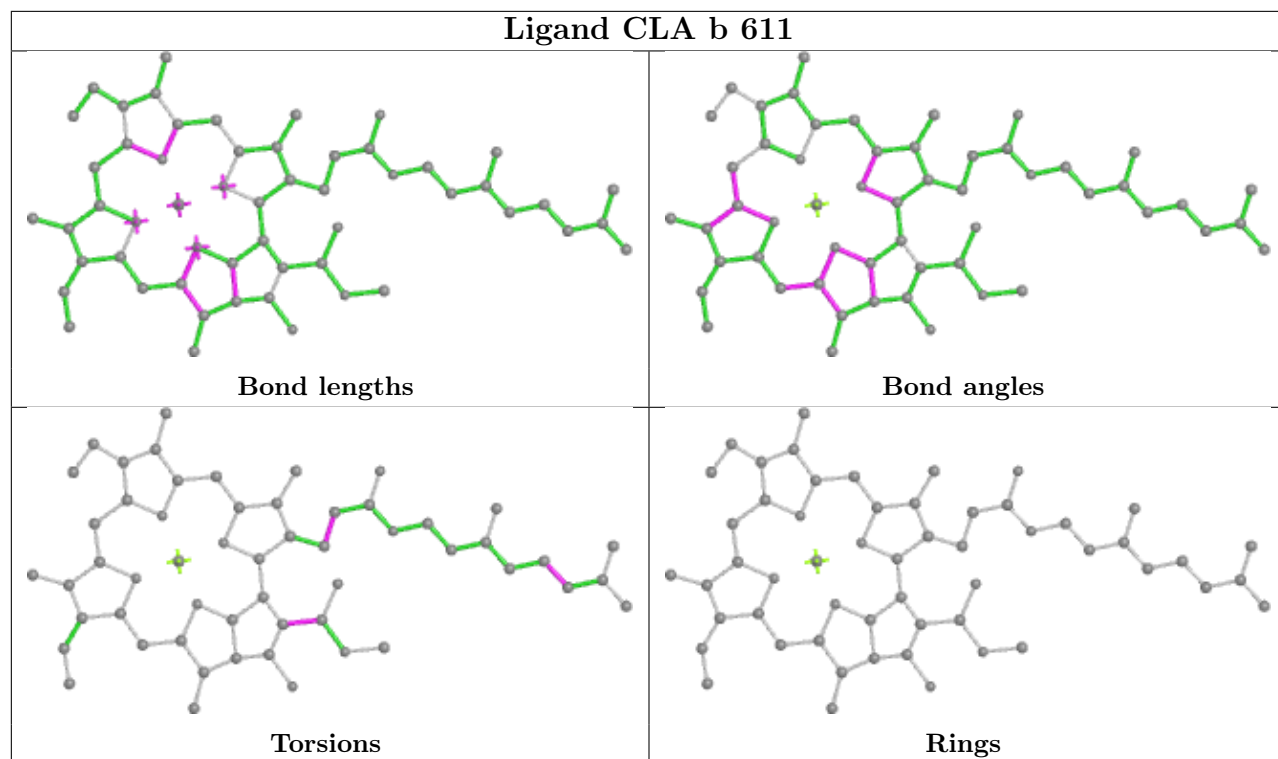


## Ligand CLA 3 604

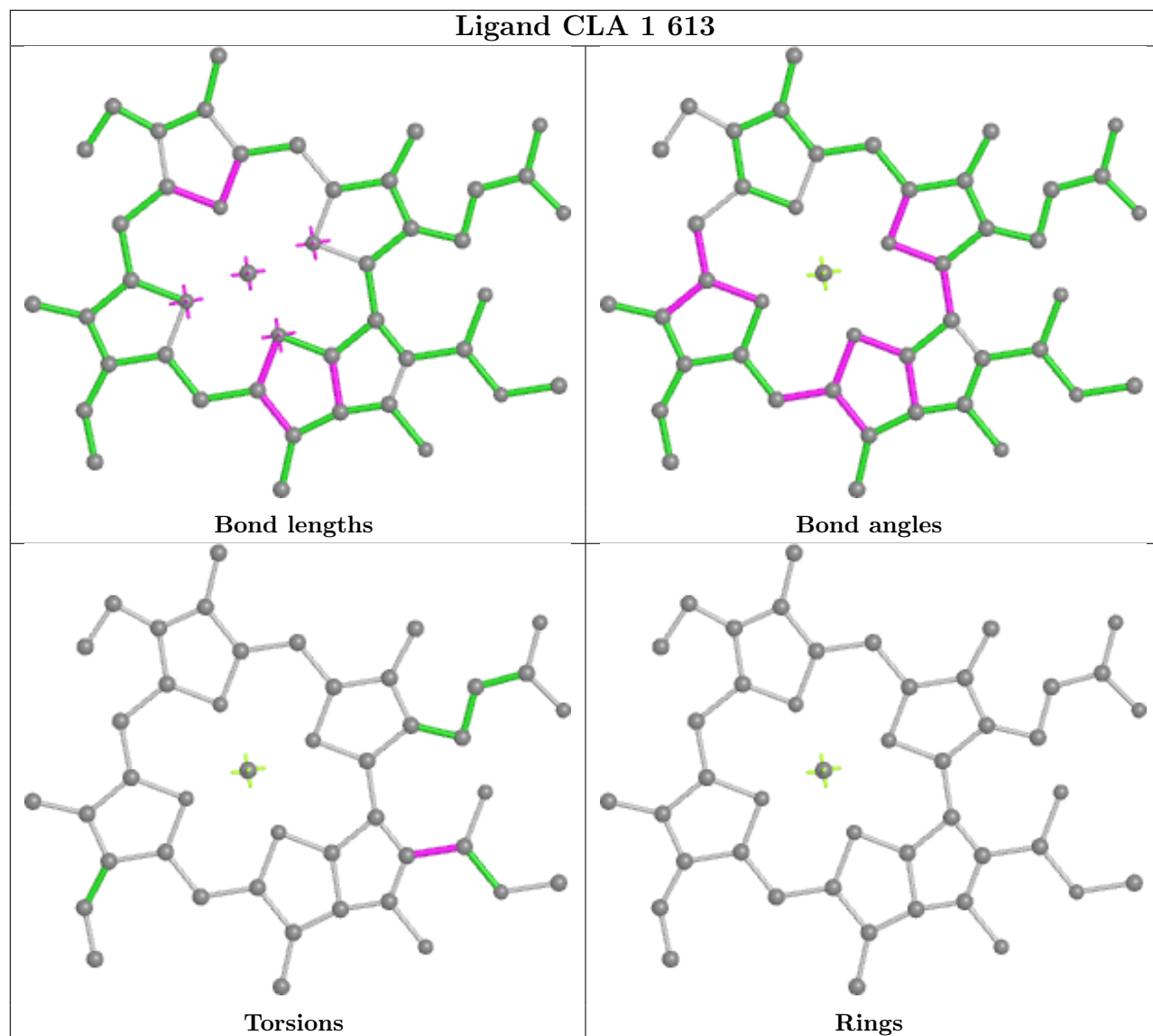


## Ligand CLA B 823

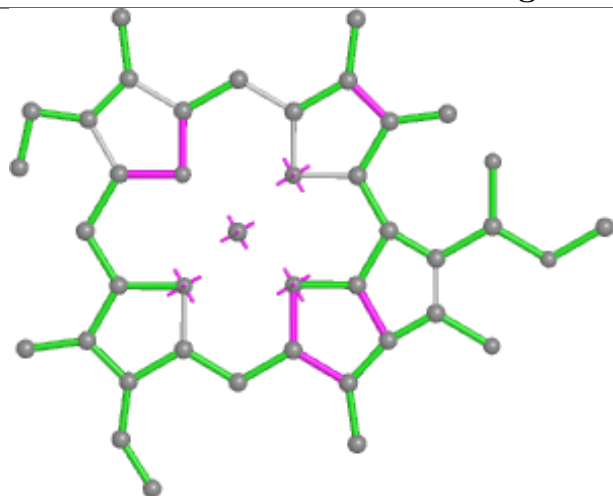




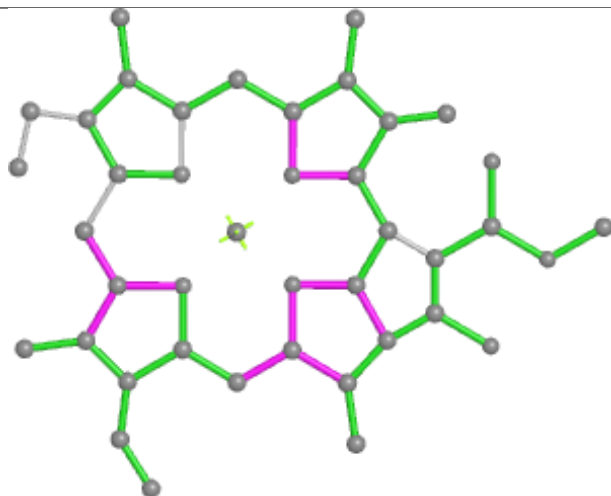
## Ligand CLA 1 613



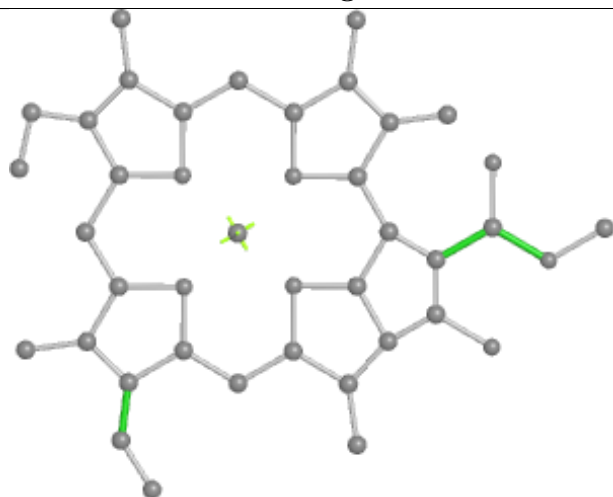
## Ligand CLA 6 609



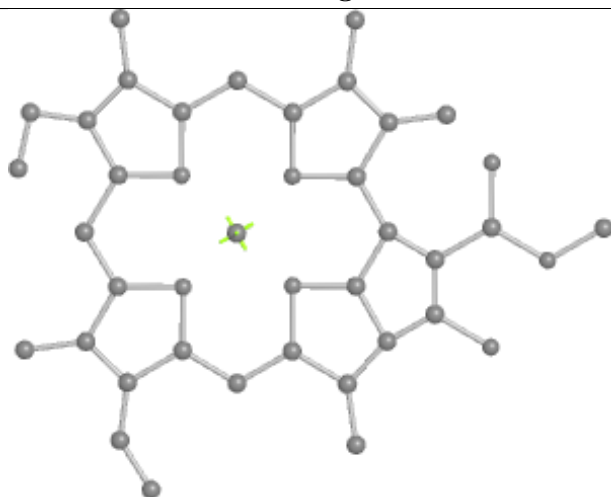
Bond lengths



Bond angles

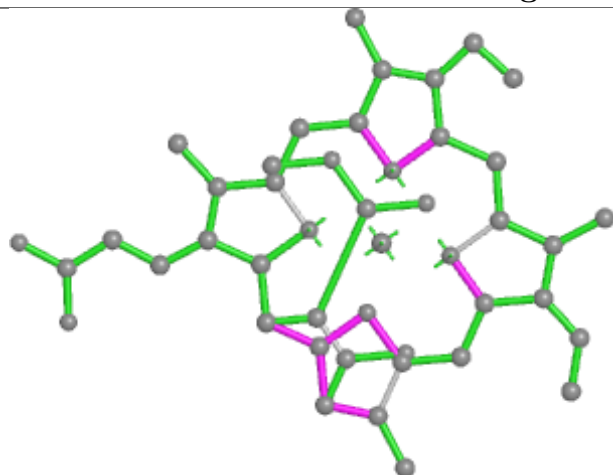


Torsions

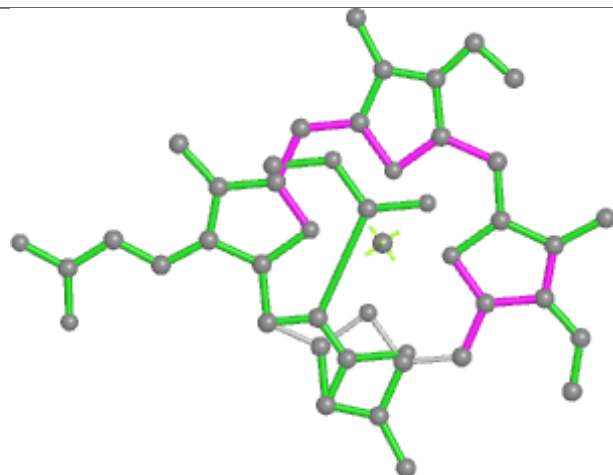


Rings

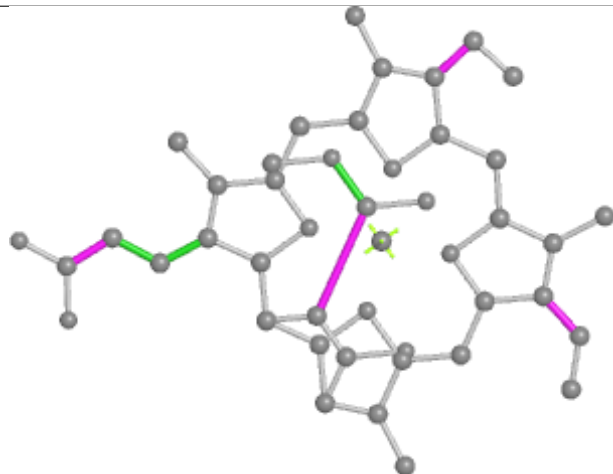
## Ligand KC2 6 613



Bond lengths



Bond angles

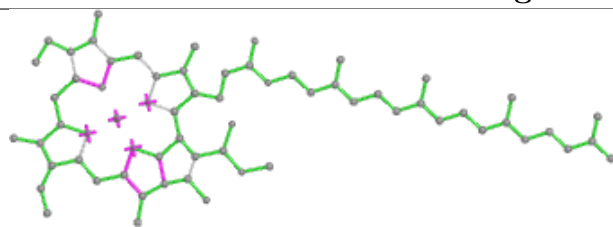


Torsions

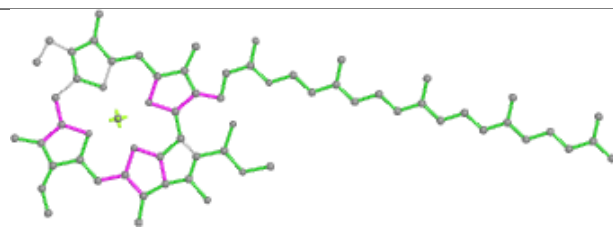


Rings

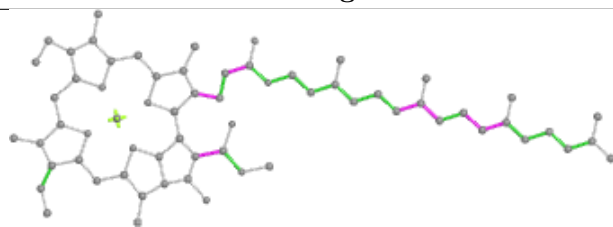
## Ligand CLA B 804



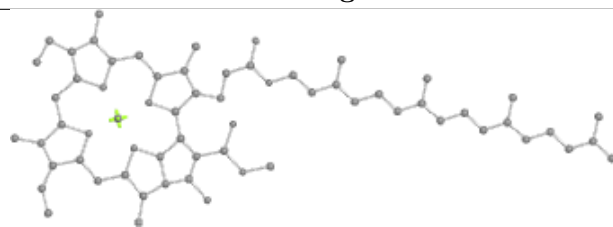
Bond lengths



Bond angles

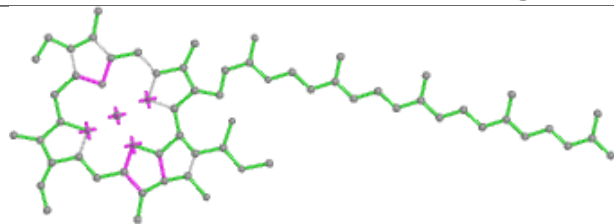


Torsions

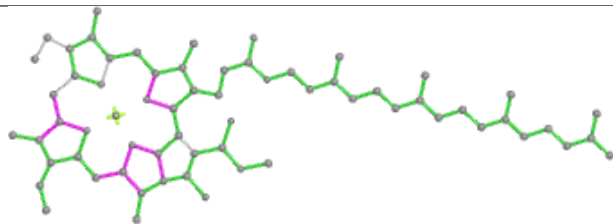


Rings

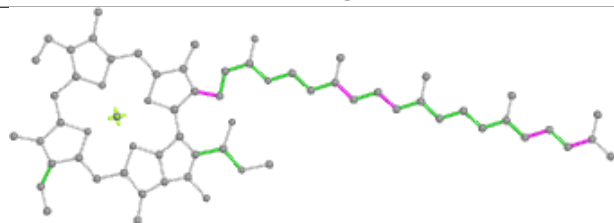
## Ligand CLA B 827



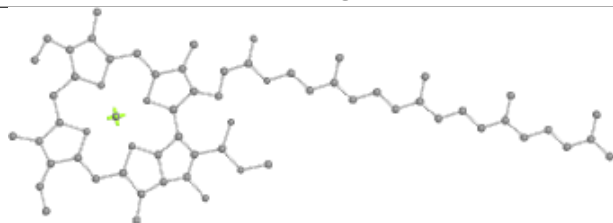
Bond lengths



Bond angles

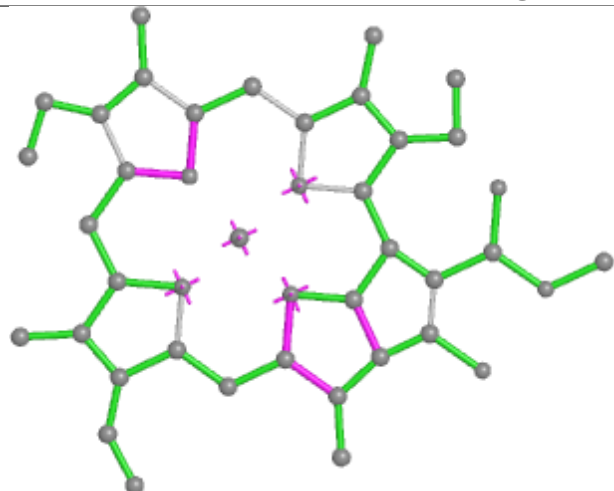


Torsions

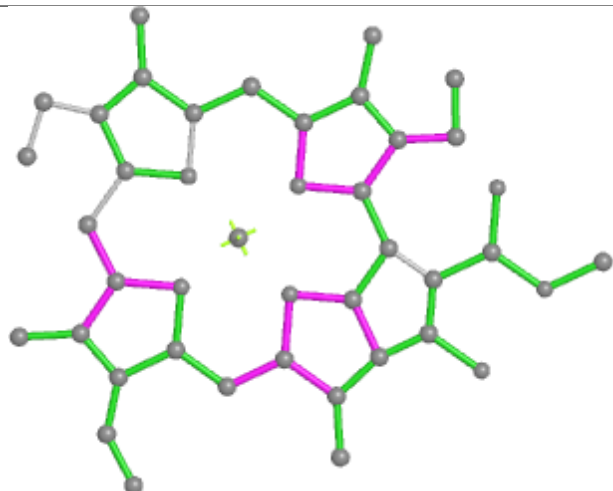


Rings

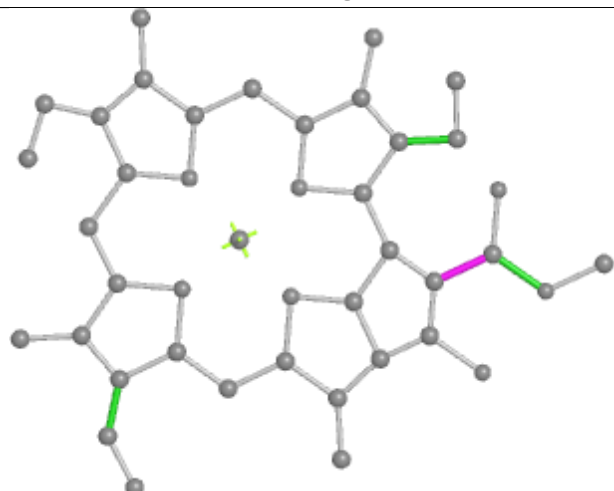
## Ligand CLA A 813



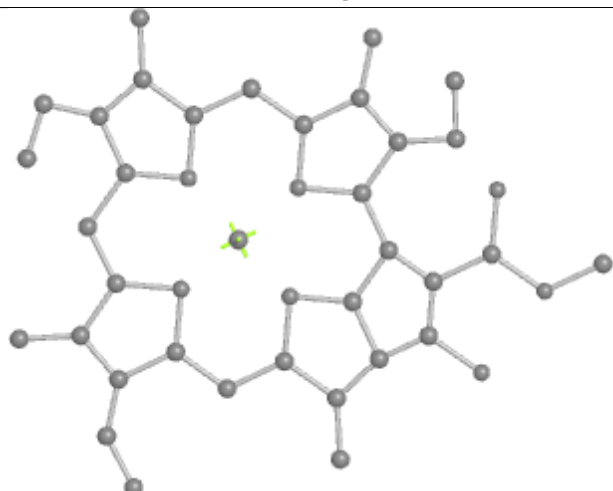
Bond lengths



Bond angles

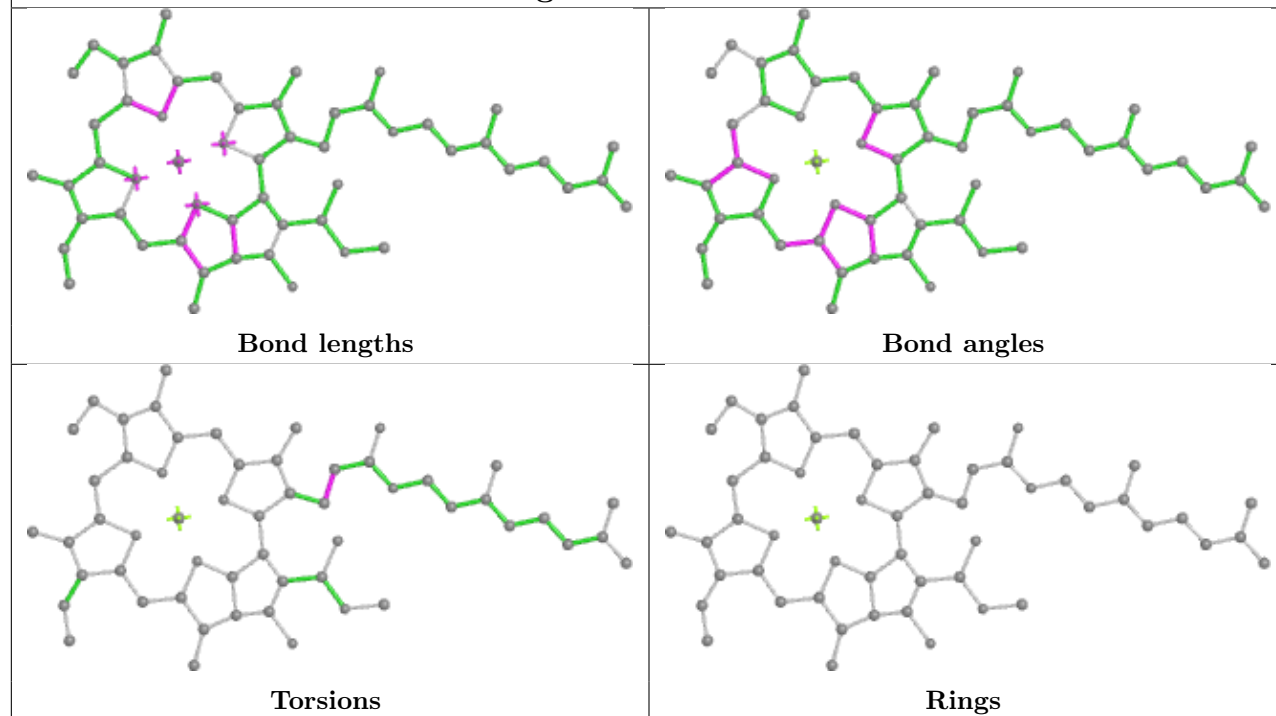


Torsions

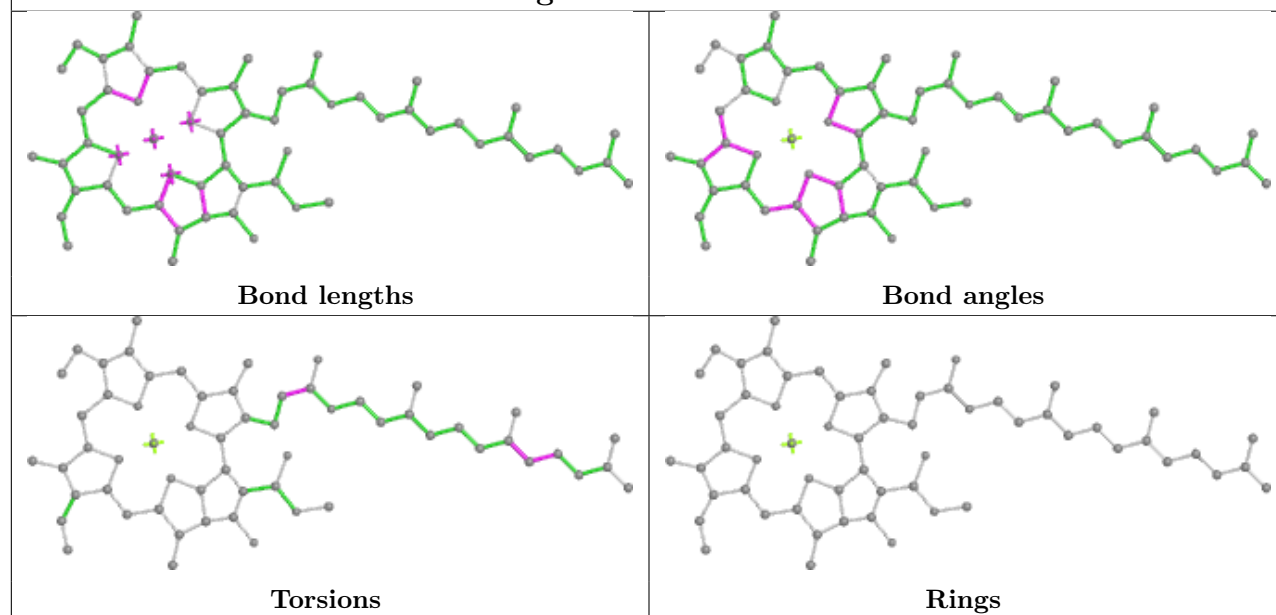


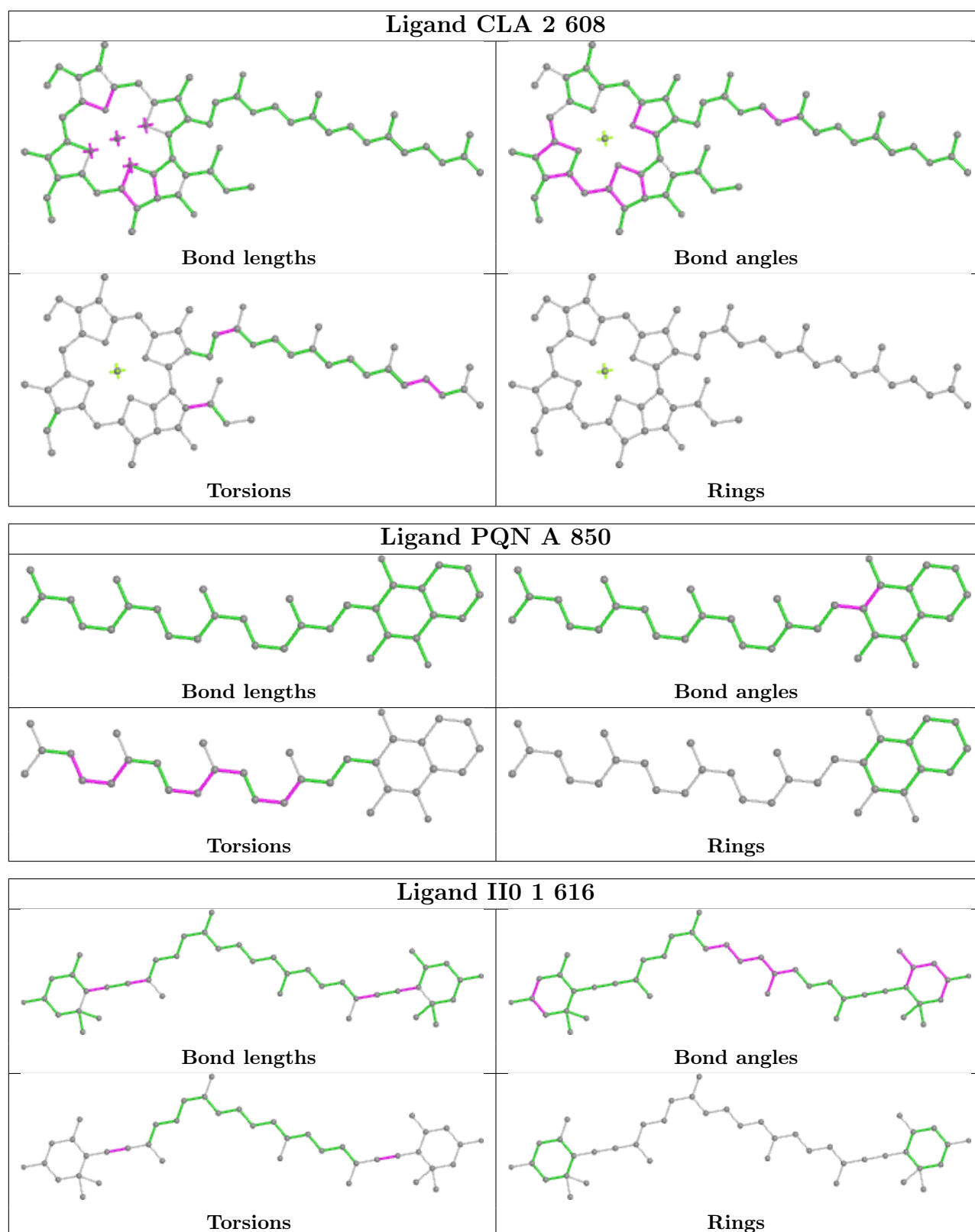
Rings

## Ligand CLA 2 604



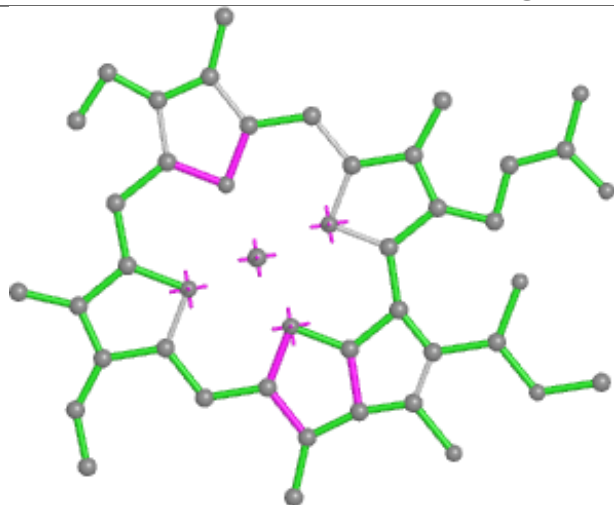
## Ligand CLA 2 605



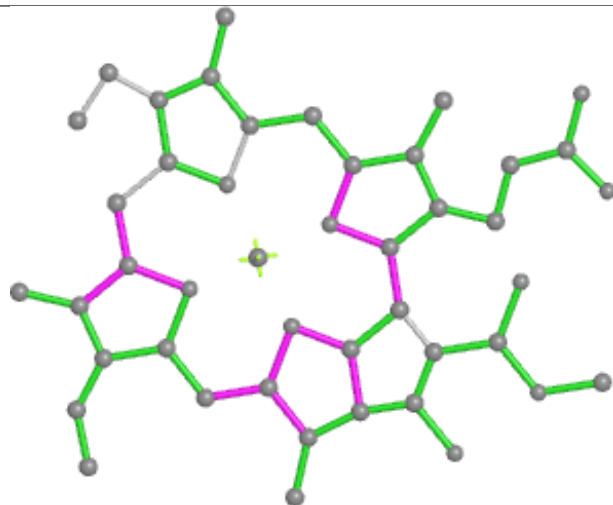




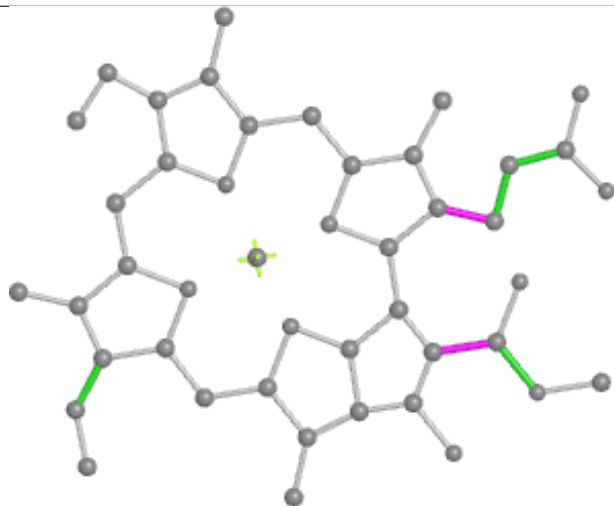
## Ligand CLA 1 601



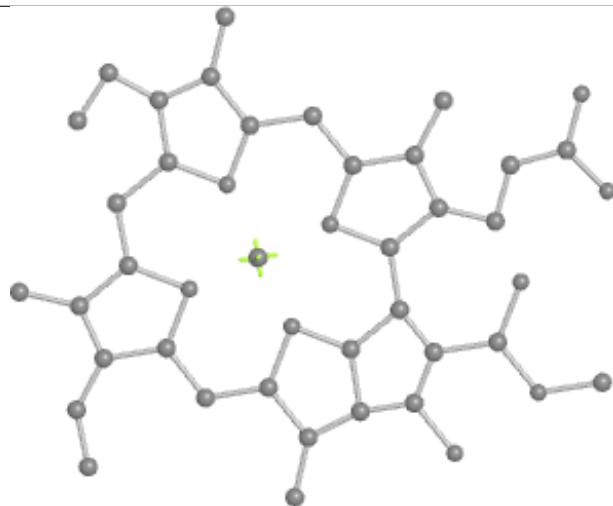
Bond lengths



Bond angles

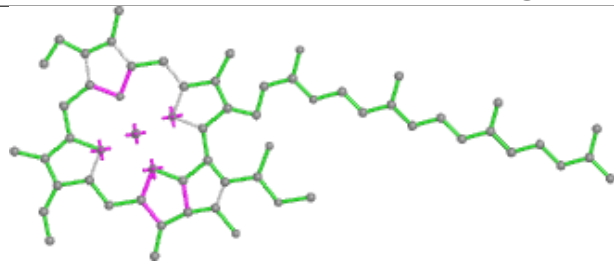


Torsions

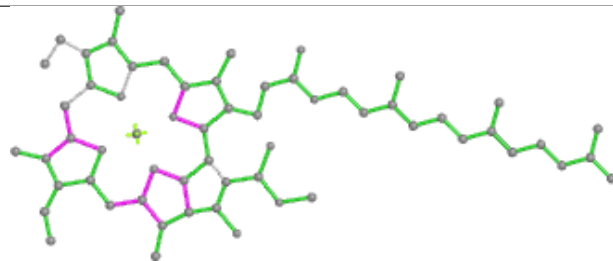


Rings

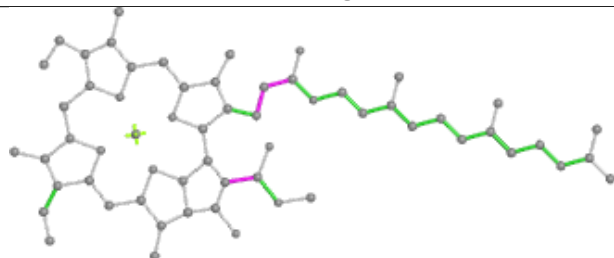
## Ligand CLA 4 609



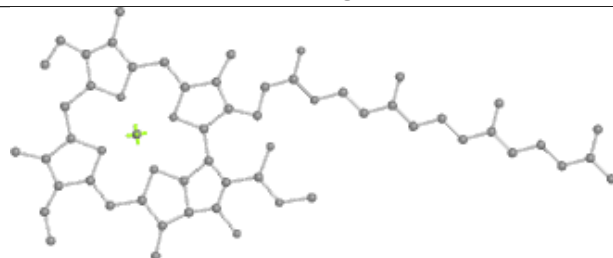
Bond lengths



Bond angles

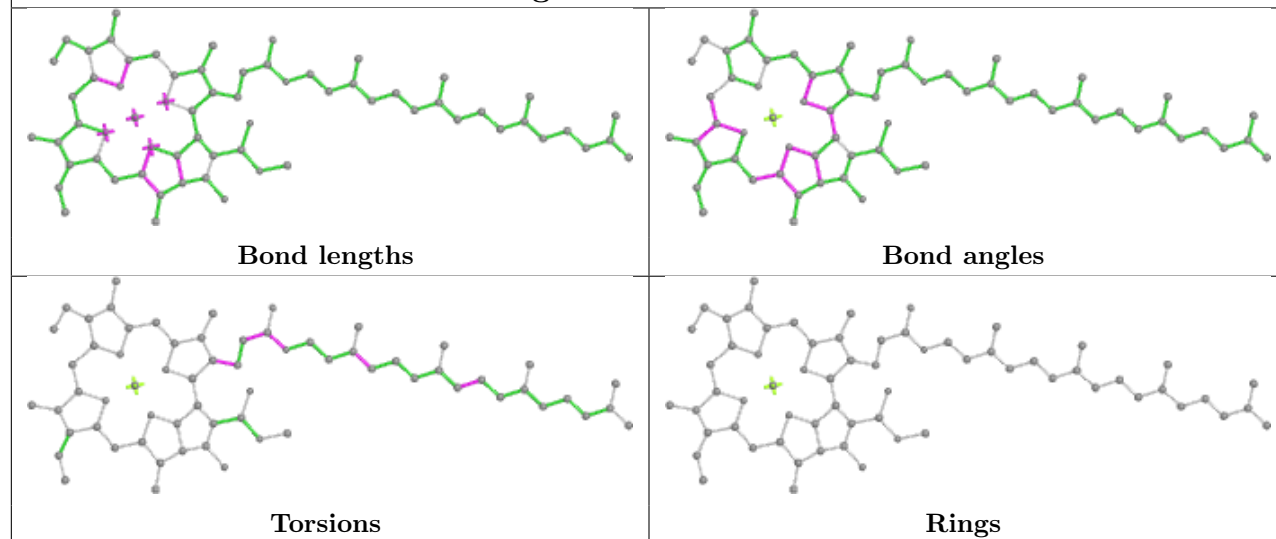


Torsions

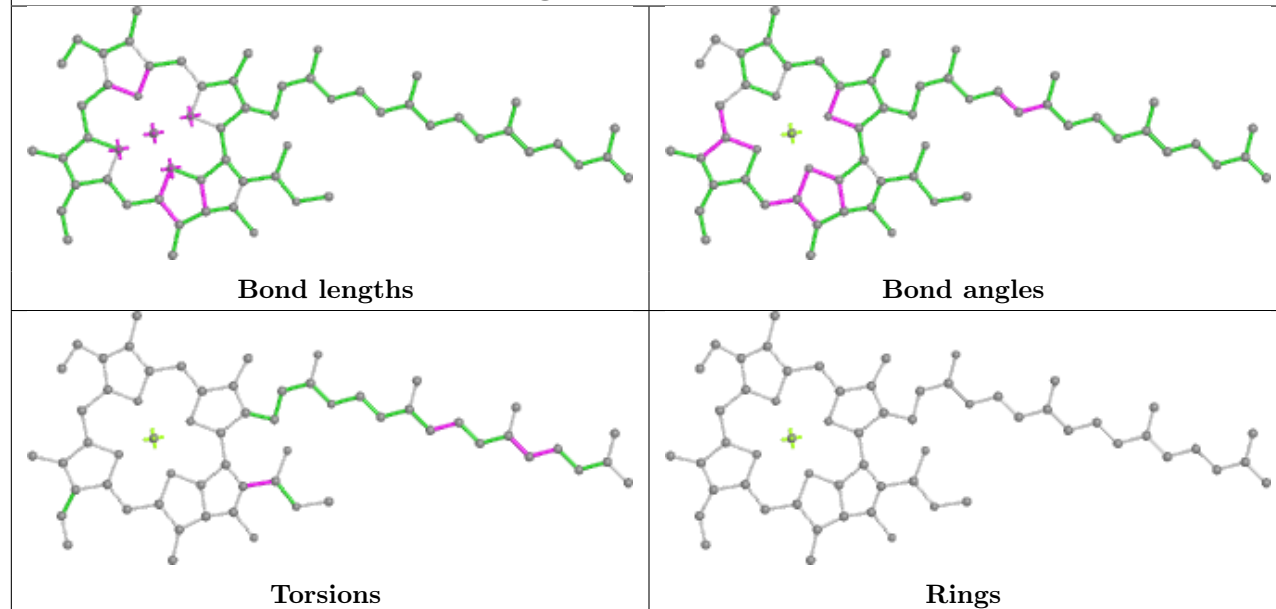


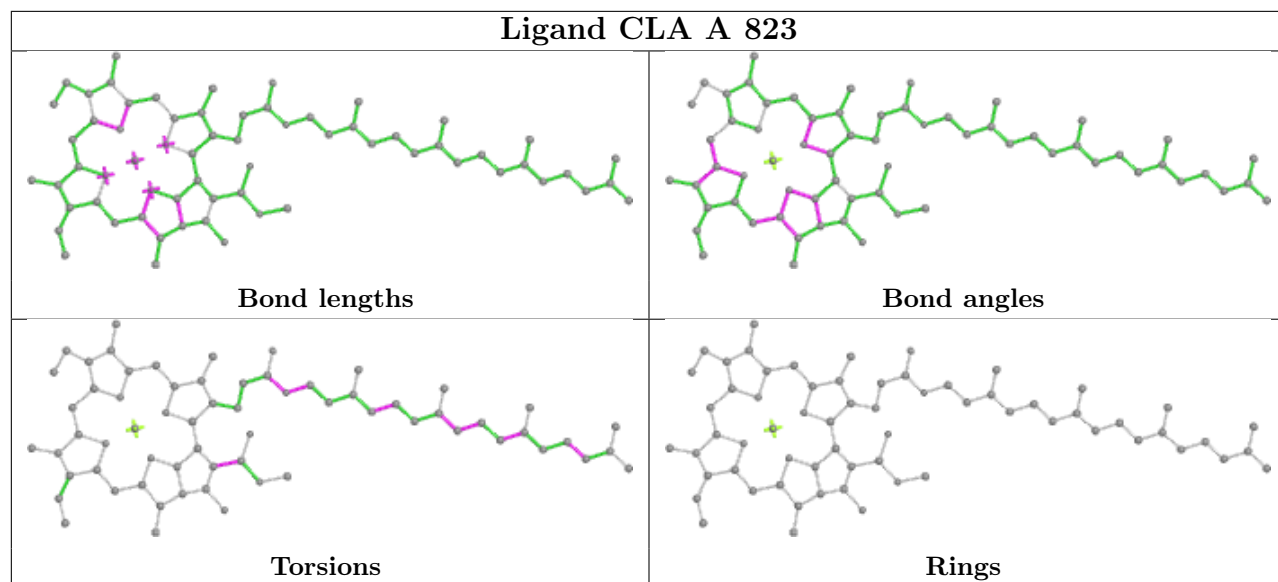
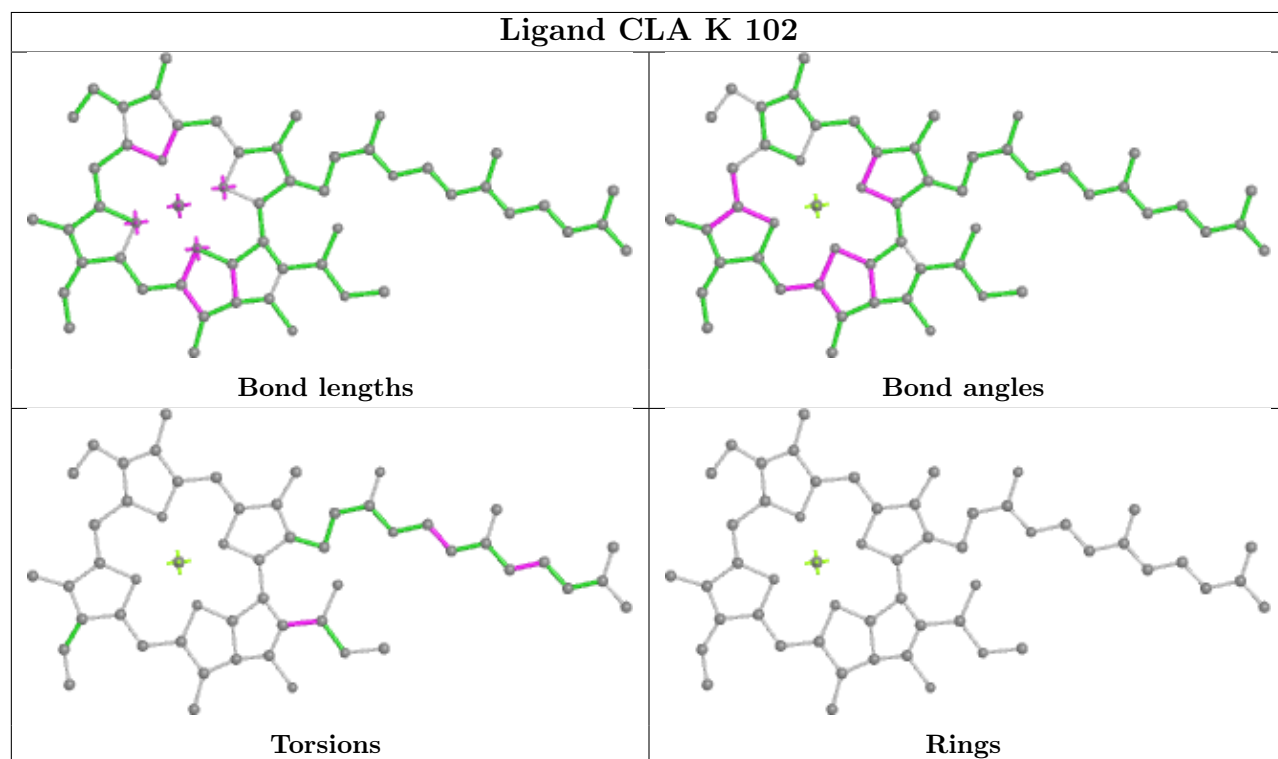
Rings

## Ligand CLA B 809

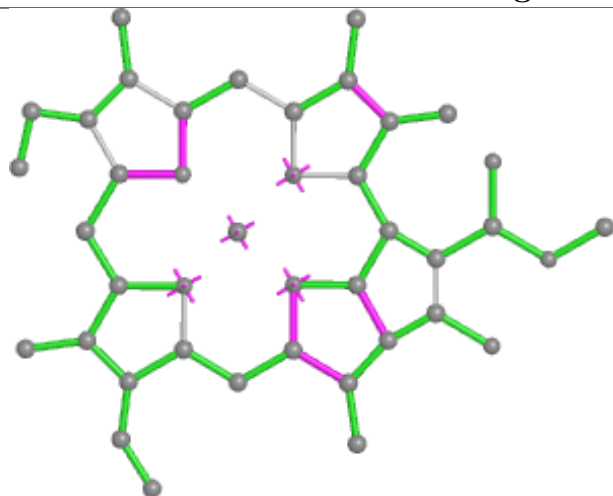


## Ligand CLA 6 608

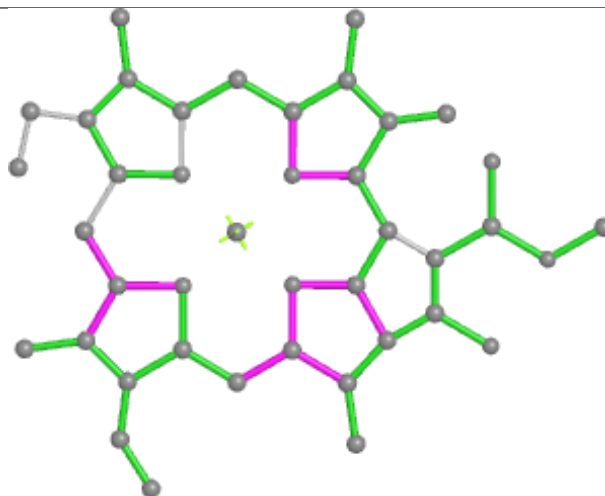


**Ligand CLA A 823****Ligand CLA K 102**

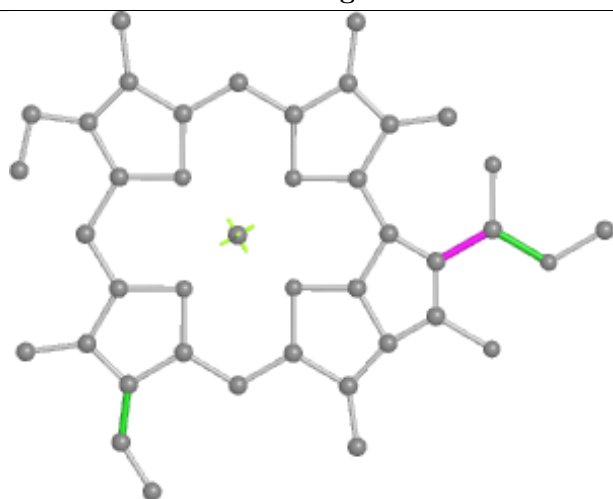
## Ligand CLA O 202



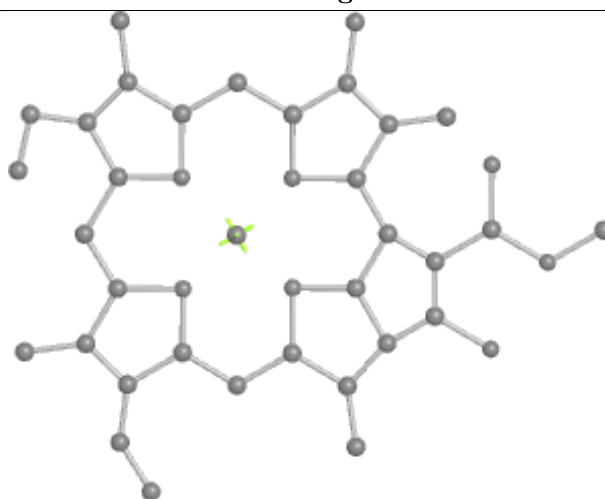
Bond lengths



Bond angles

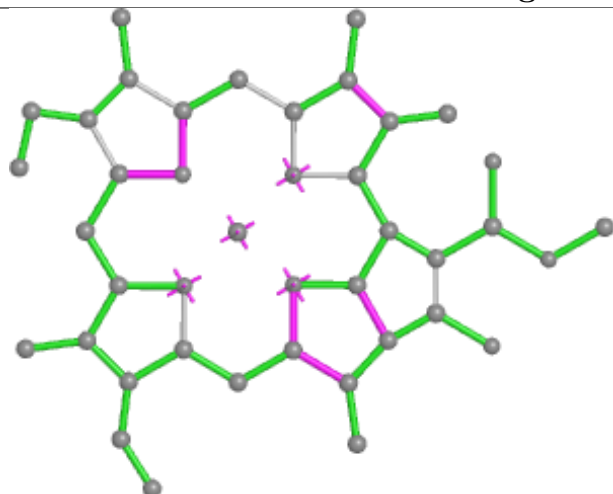


Torsions

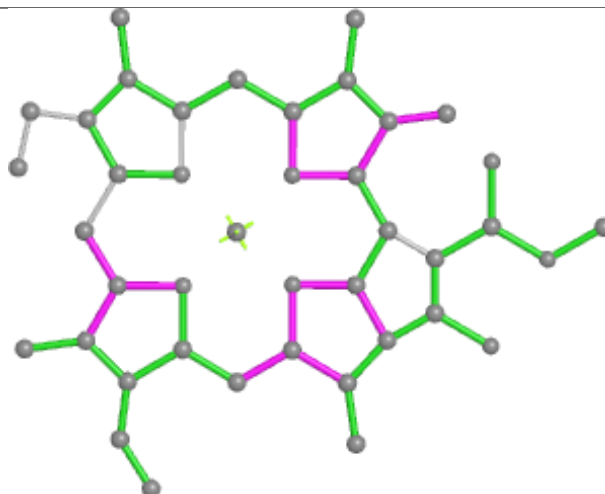


Rings

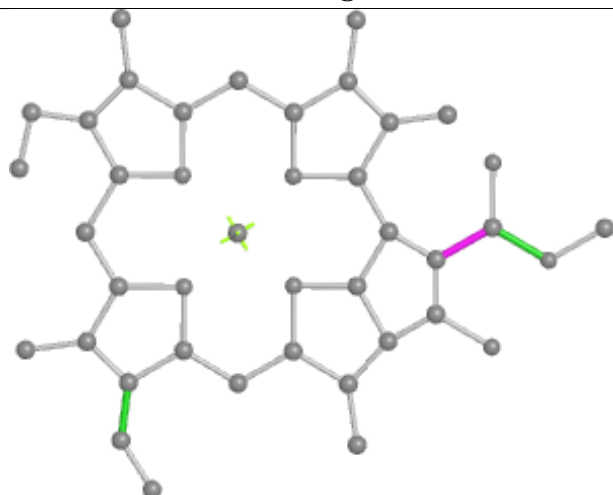
## Ligand CLA 9 611



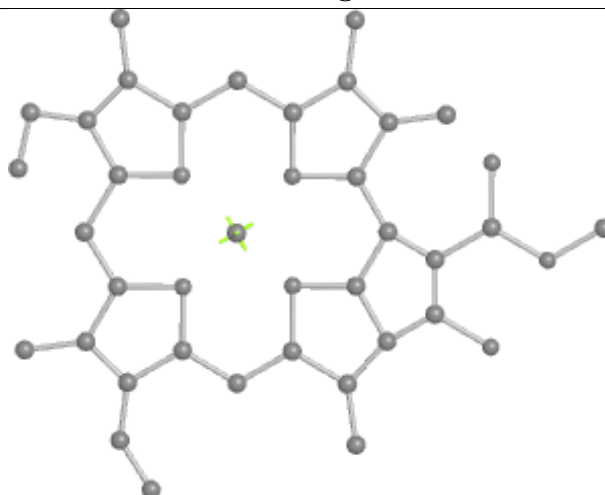
Bond lengths



Bond angles

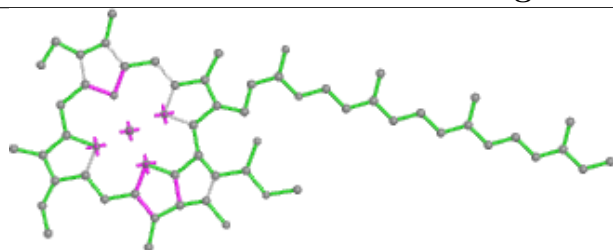


Torsions

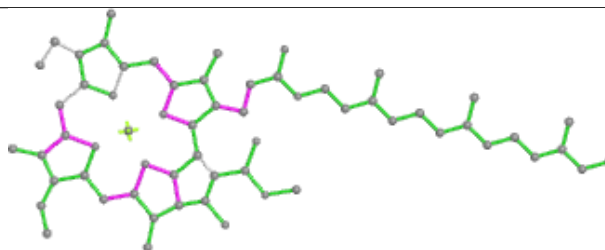


Rings

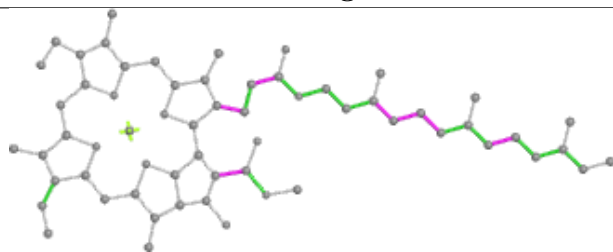
## Ligand CLA B 813



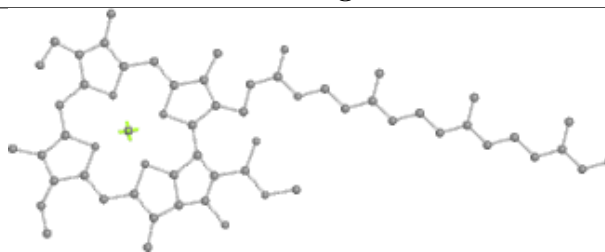
Bond lengths



Bond angles

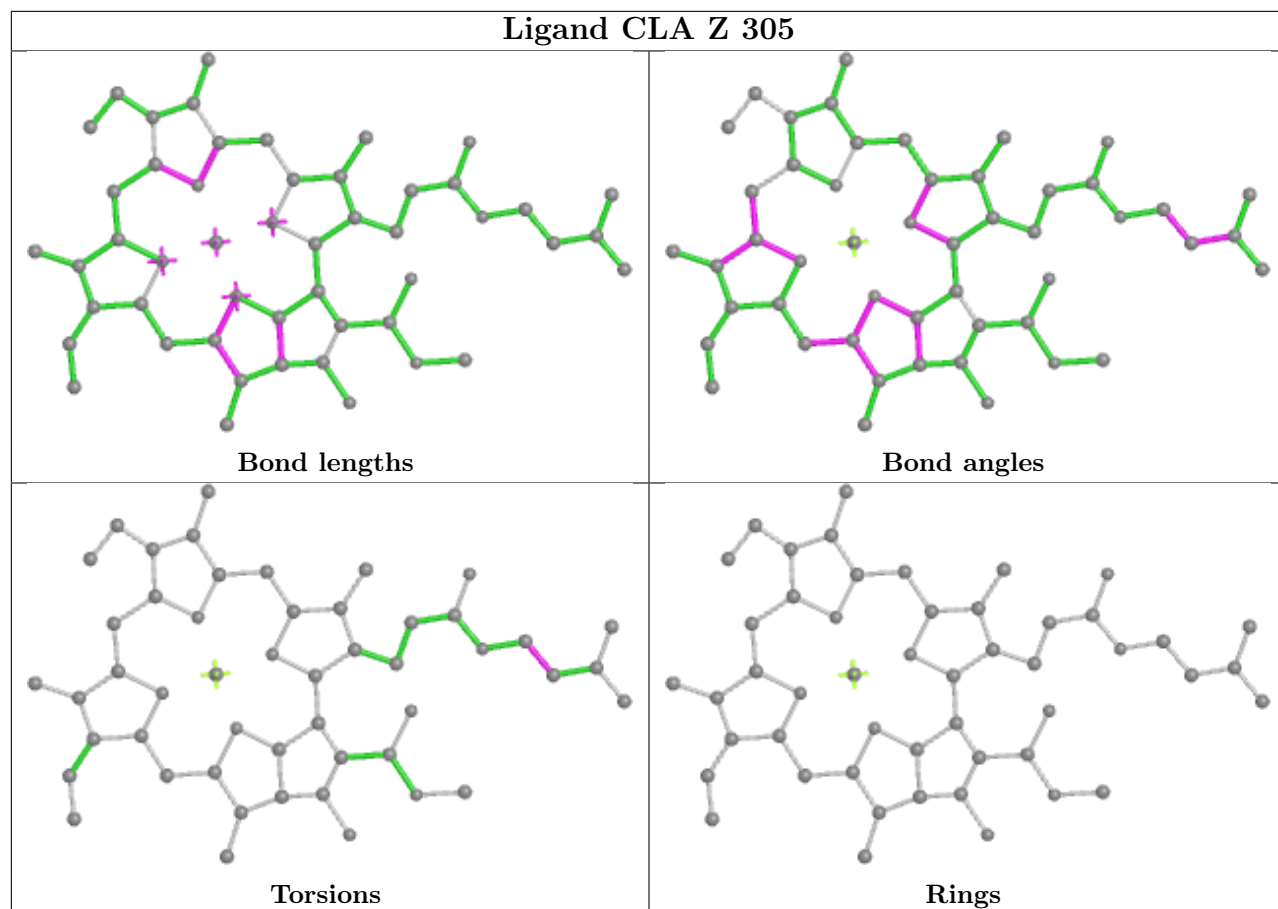


Torsions

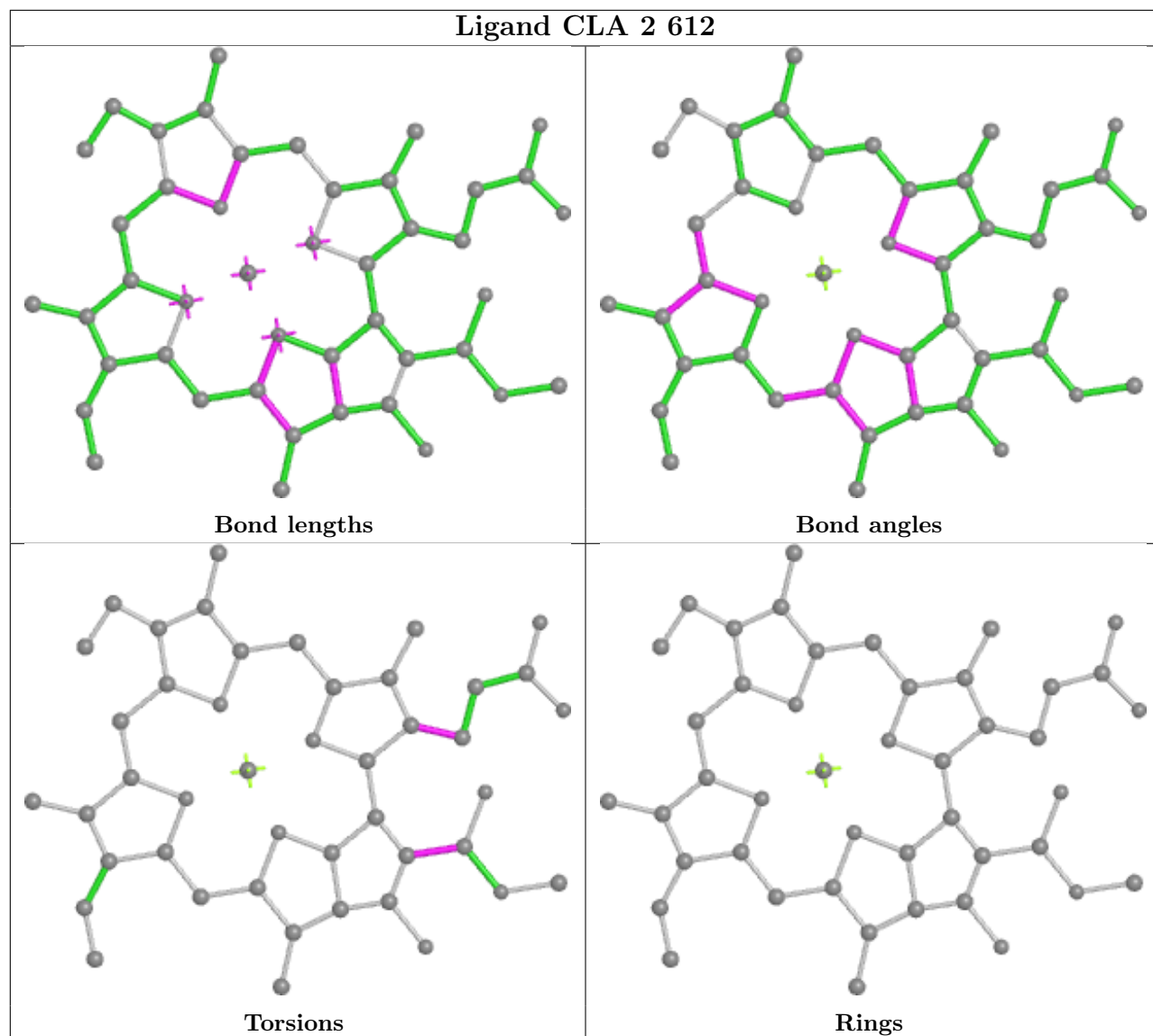


Rings

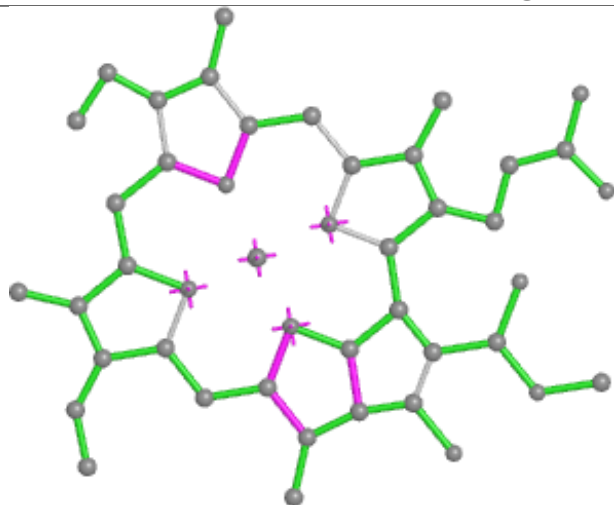
## Ligand CLA Z 305



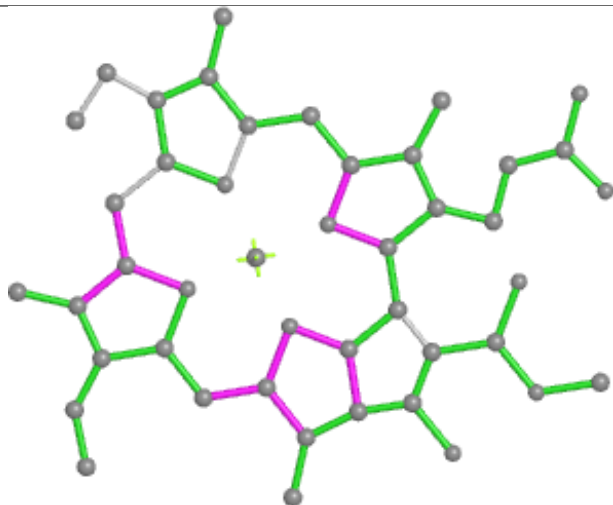
## Ligand CLA 2 612



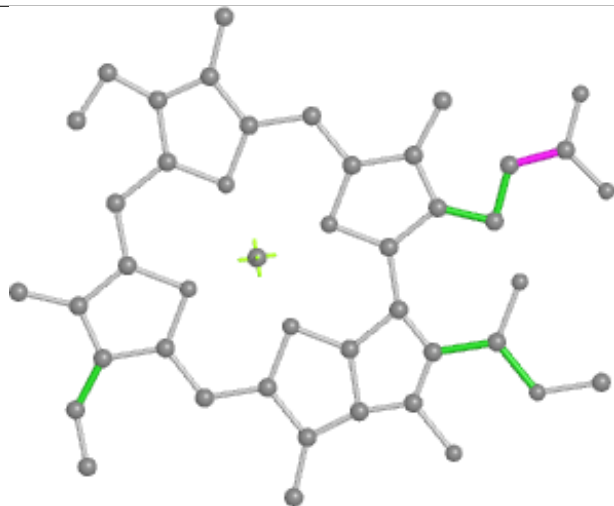
## Ligand CLA 7 308



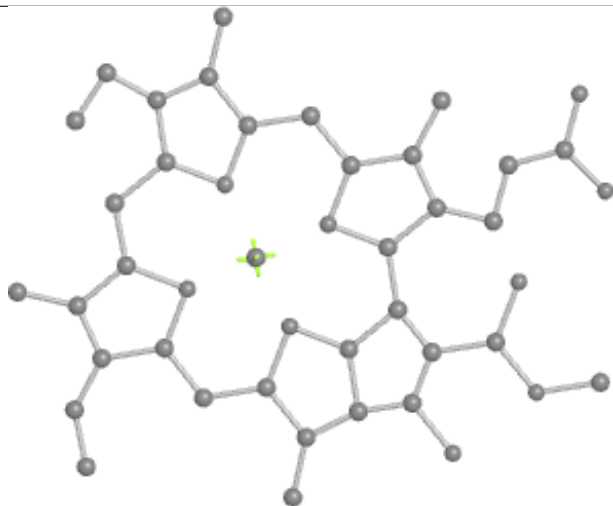
Bond lengths



Bond angles

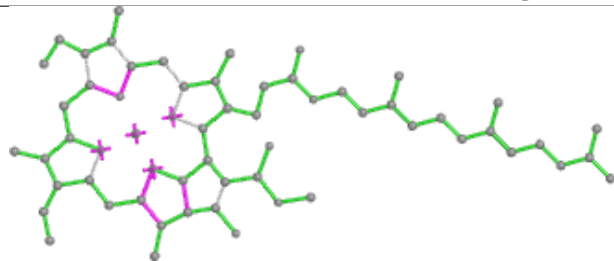


Torsions

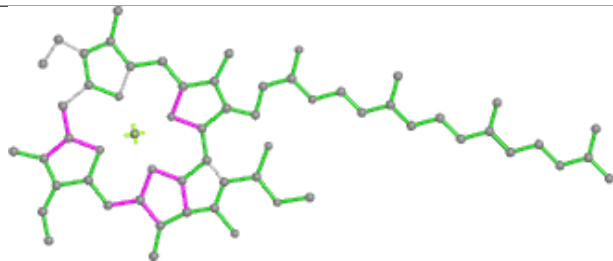


Rings

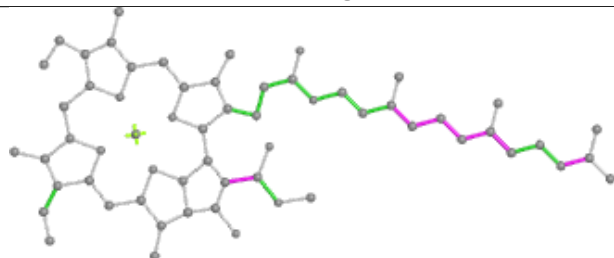
## Ligand CLA L 202



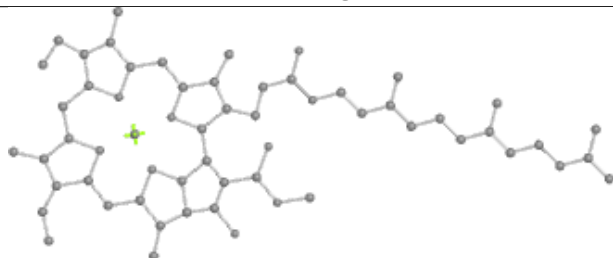
Bond lengths



Bond angles



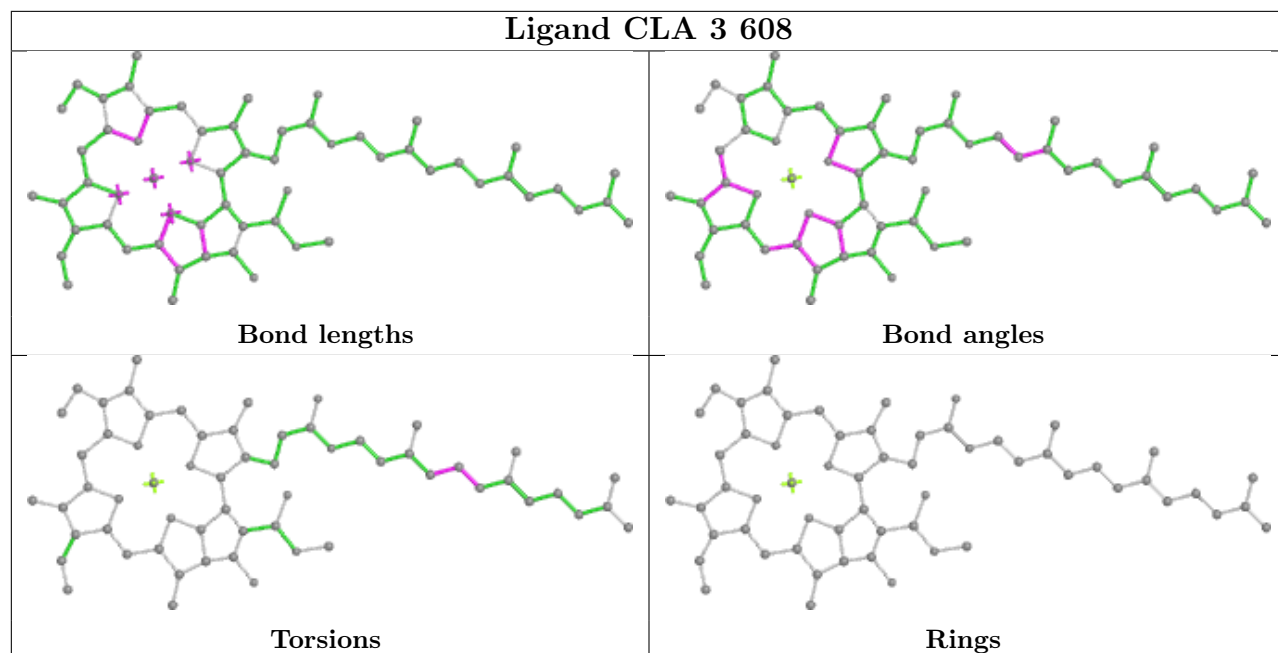
Torsions



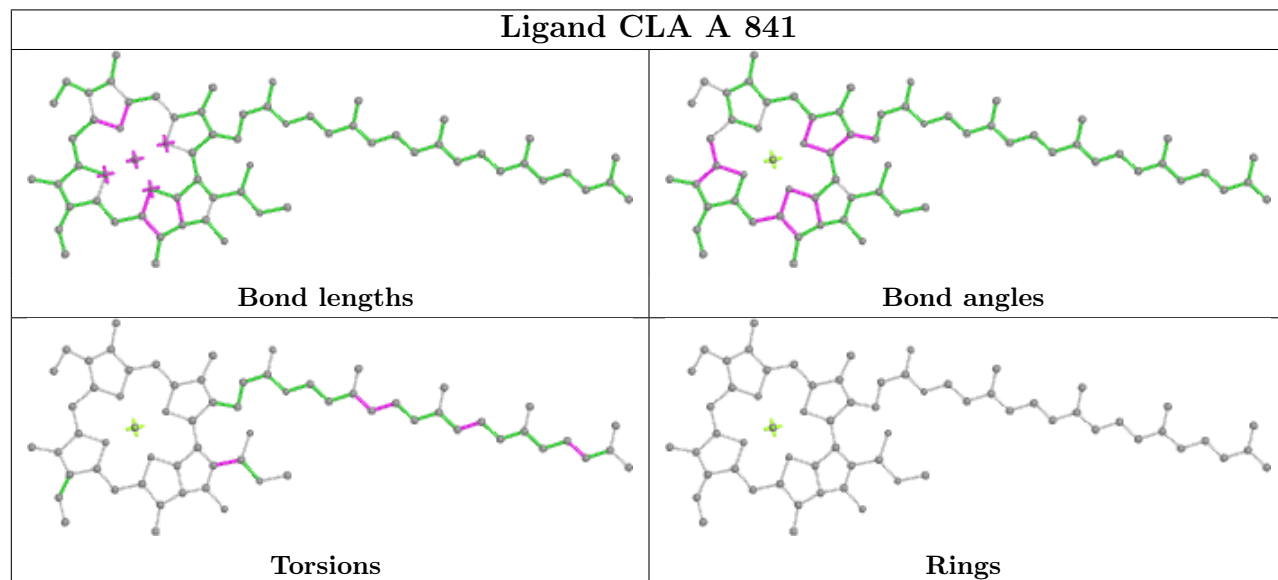
Rings



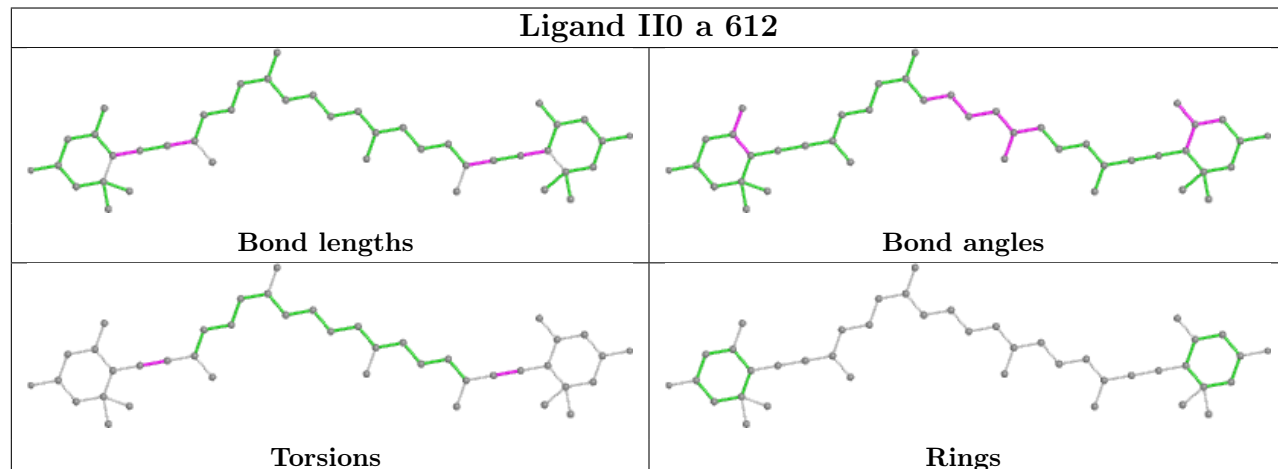
## Ligand CLA 3 608

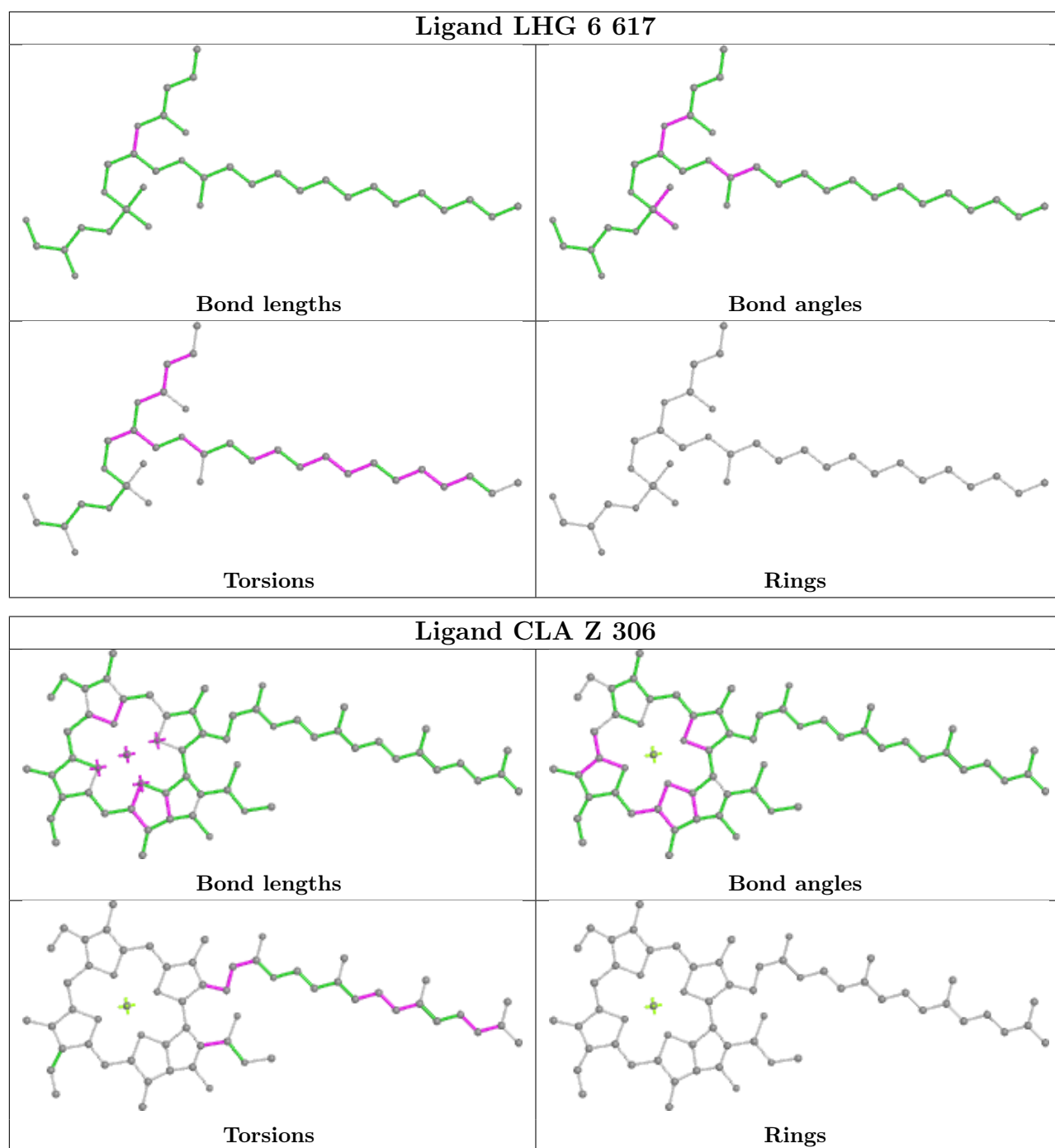


## Ligand CLA A 841

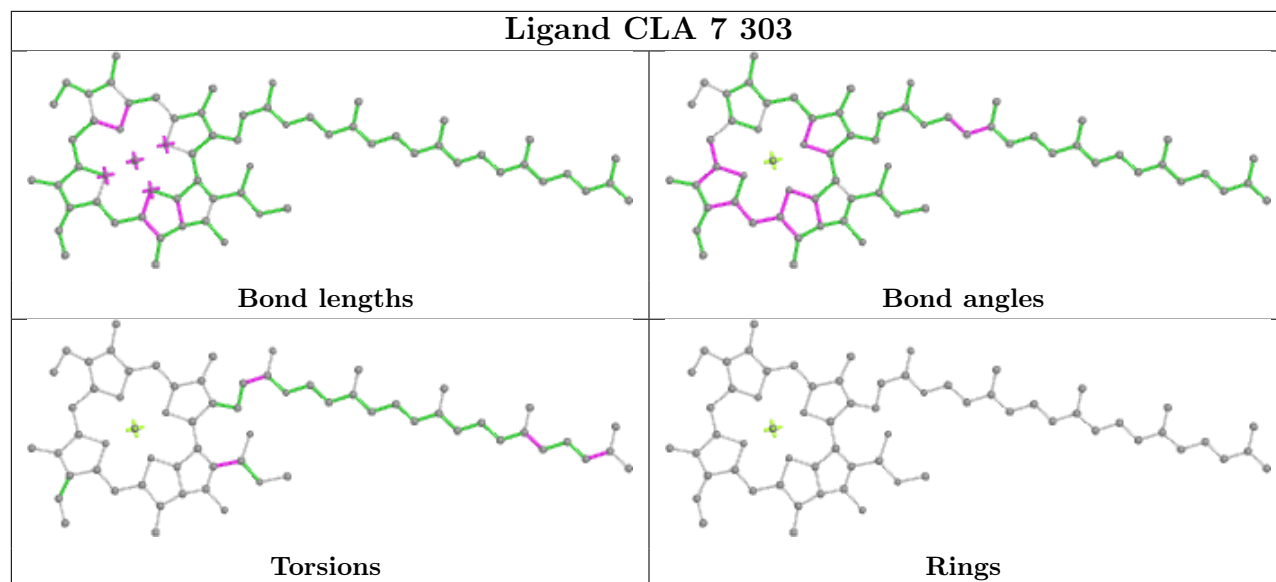


## Ligand II0 a 612

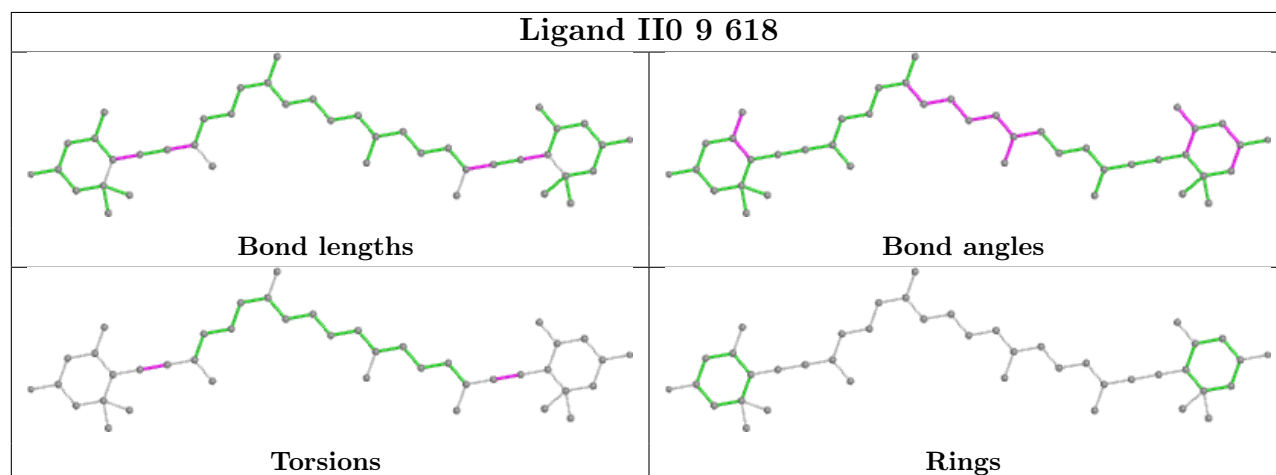




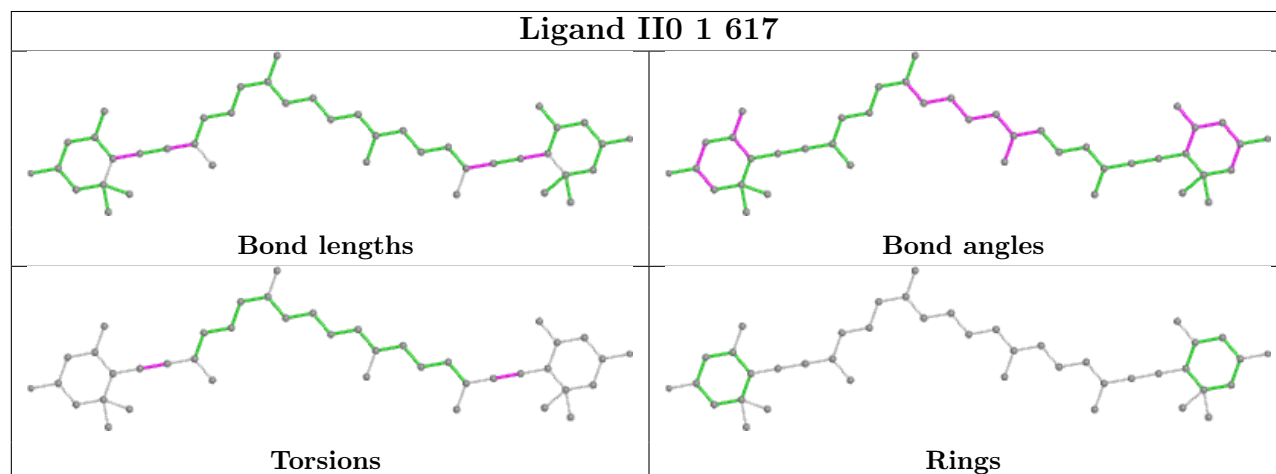
## Ligand CLA 7 303



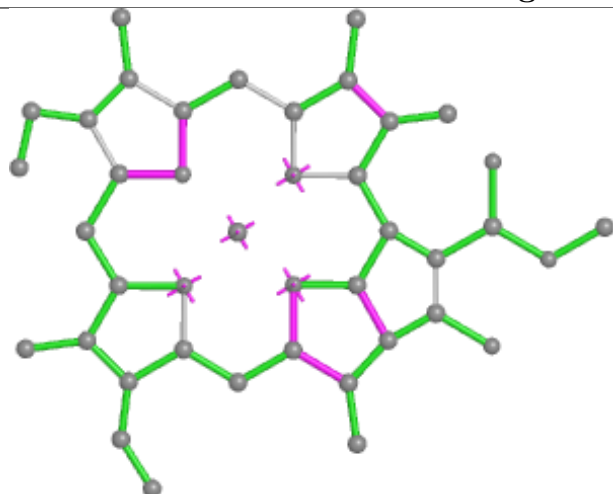
## Ligand II0 9 618



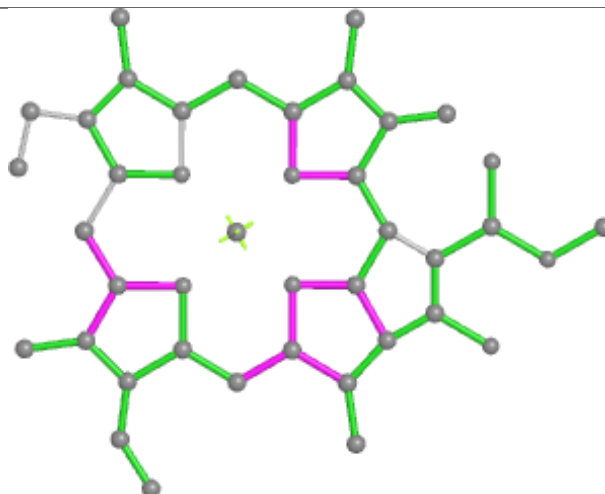
## Ligand II0 1 617



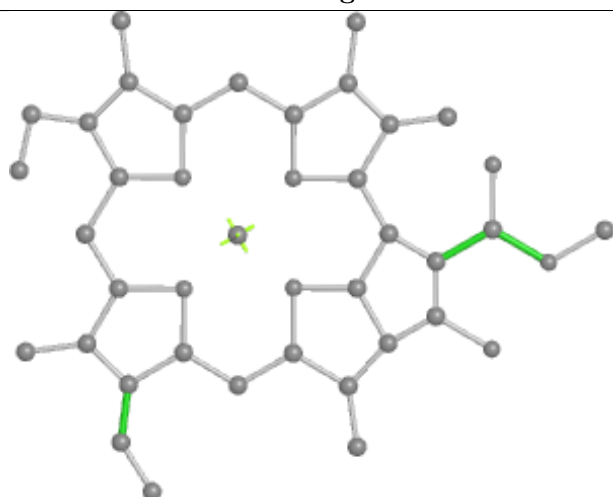
## Ligand CLA 5 601



Bond lengths



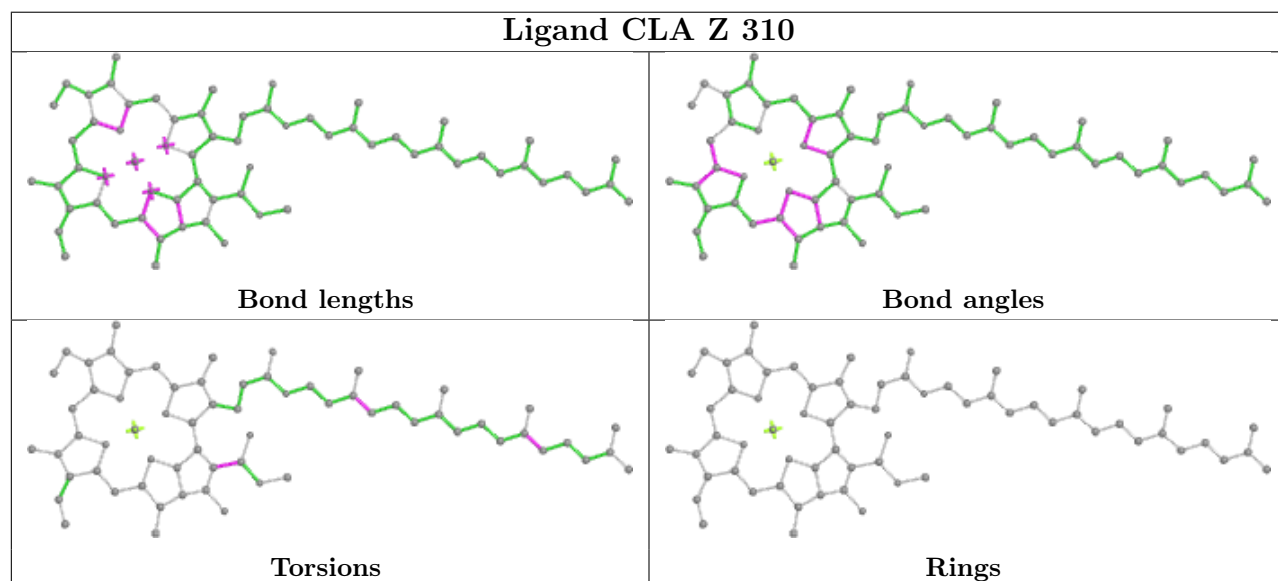
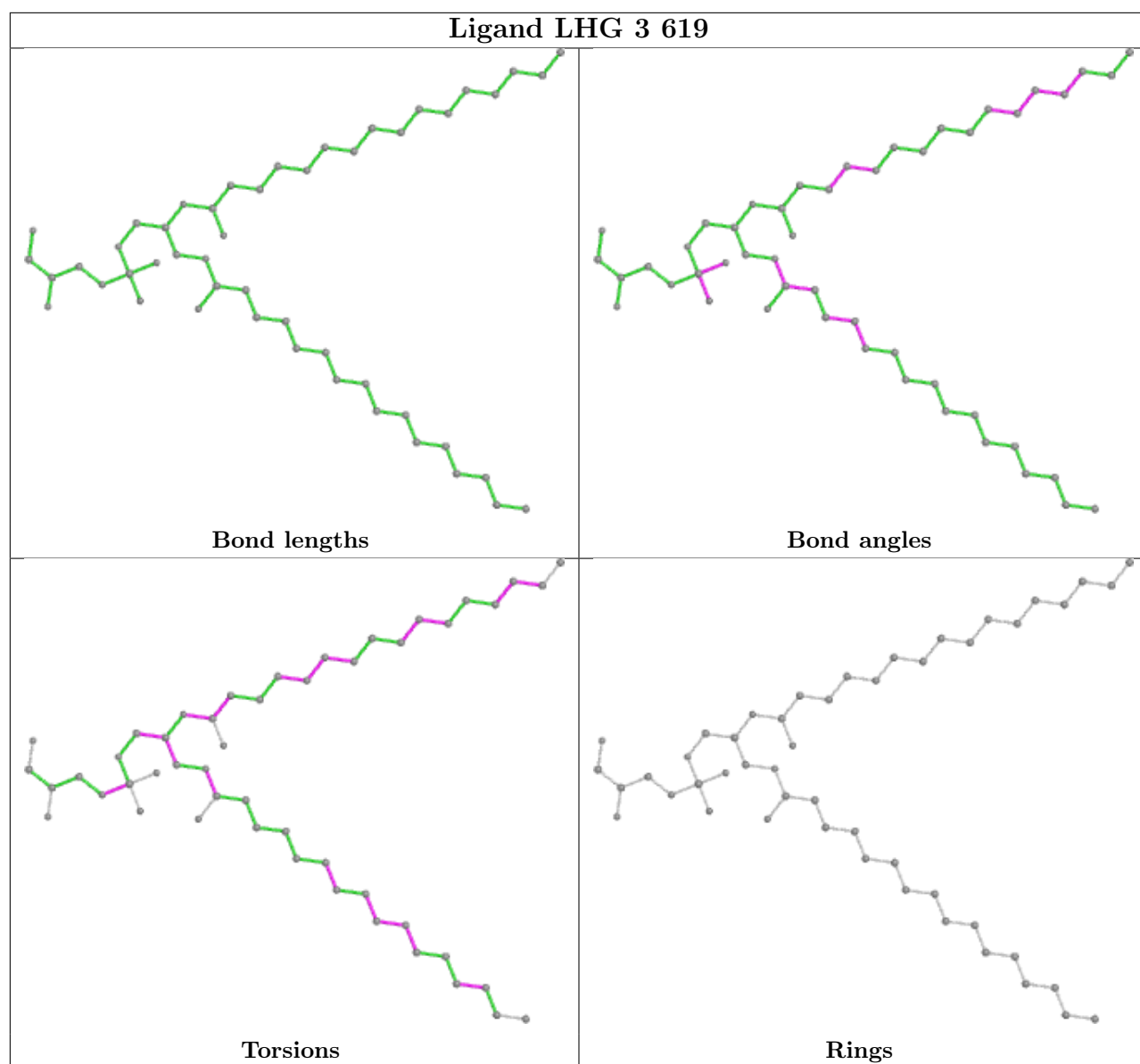
Bond angles

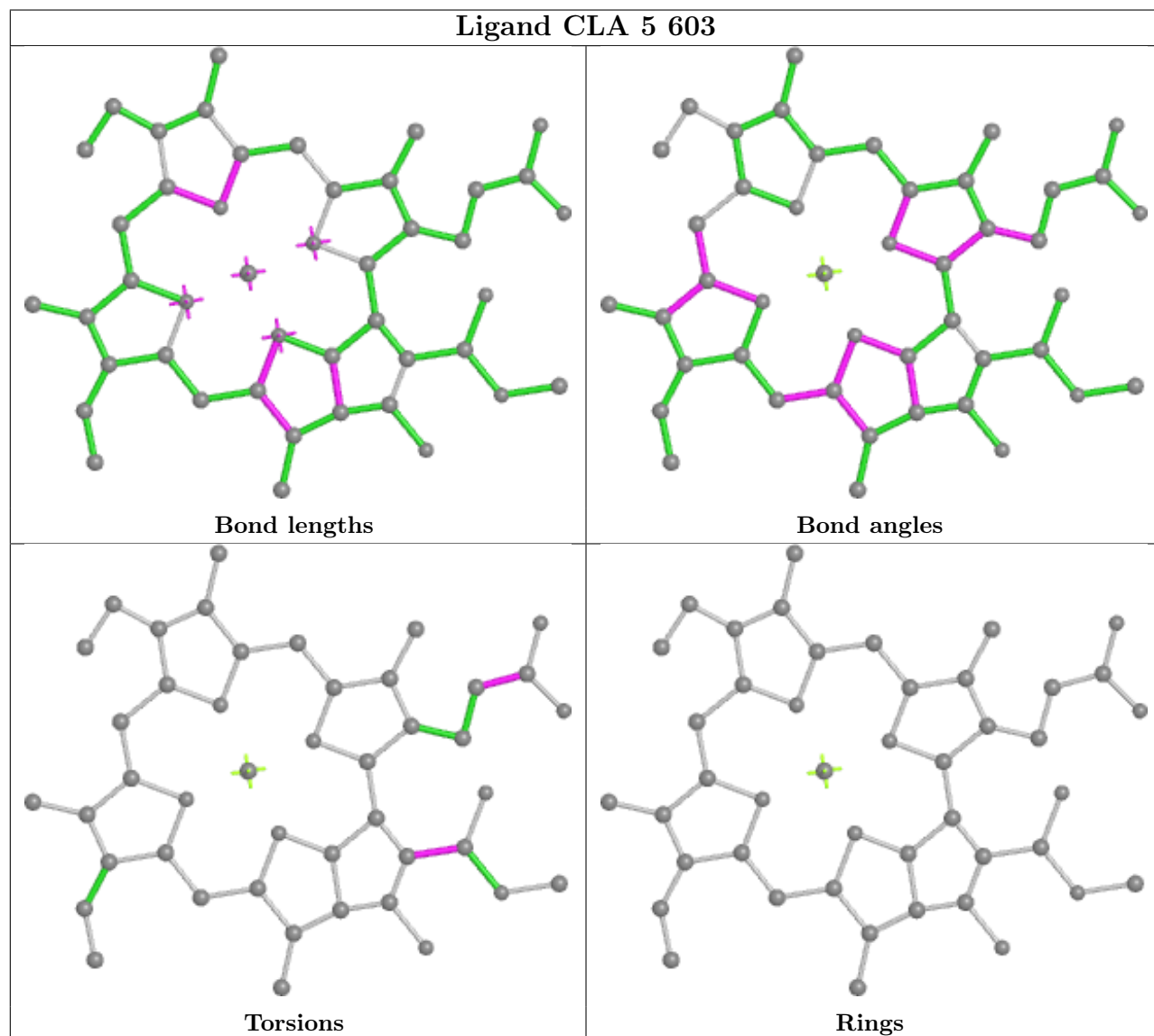
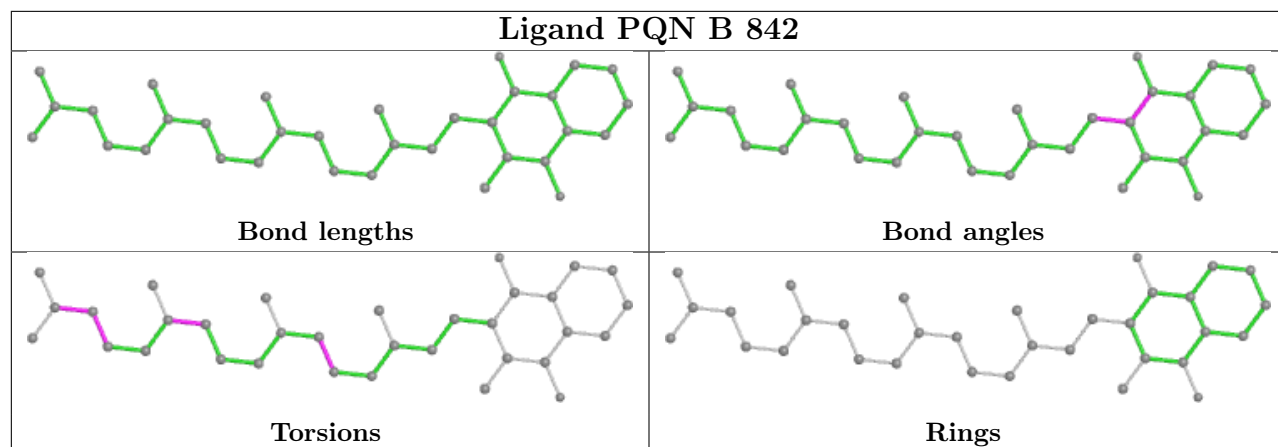


Torsions

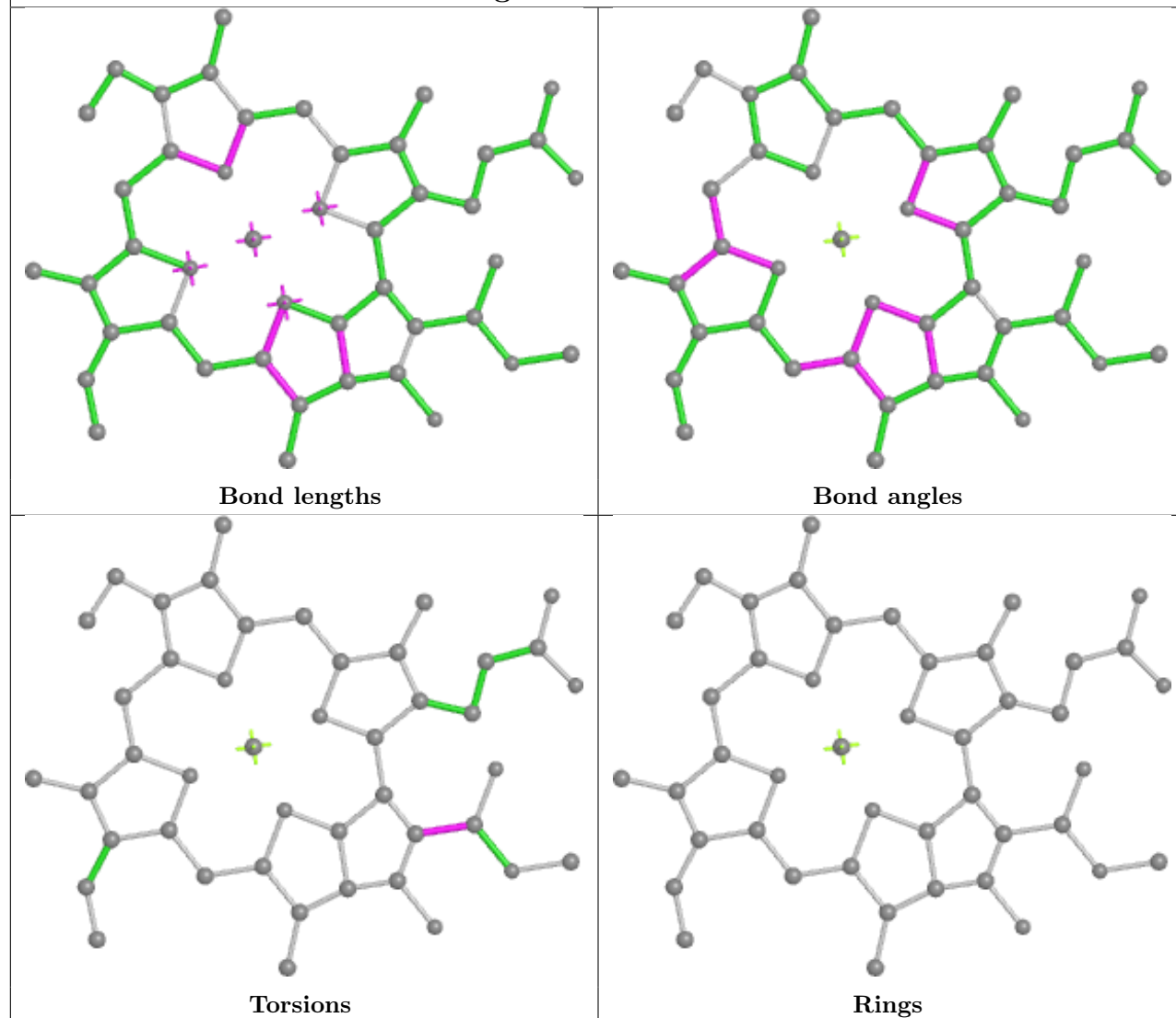


Rings

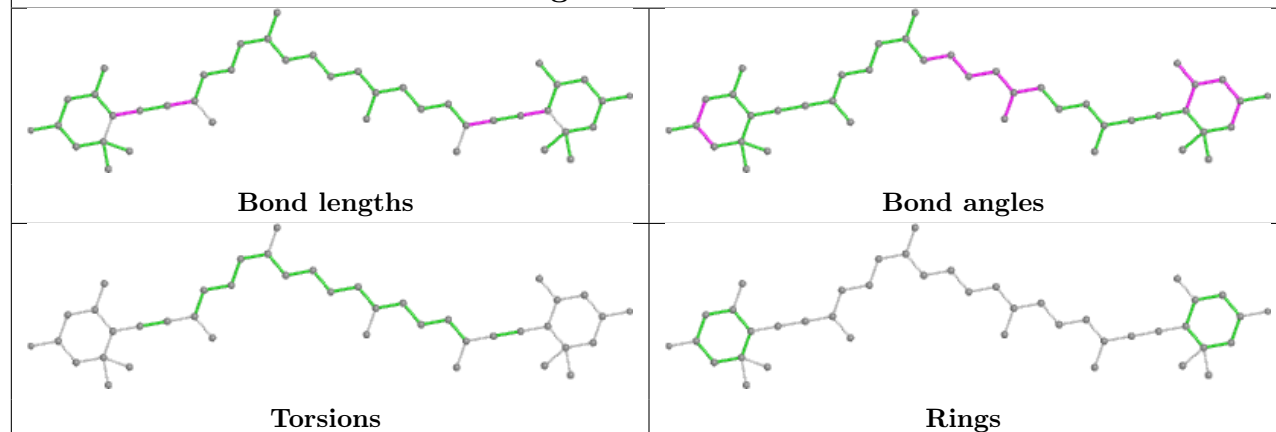




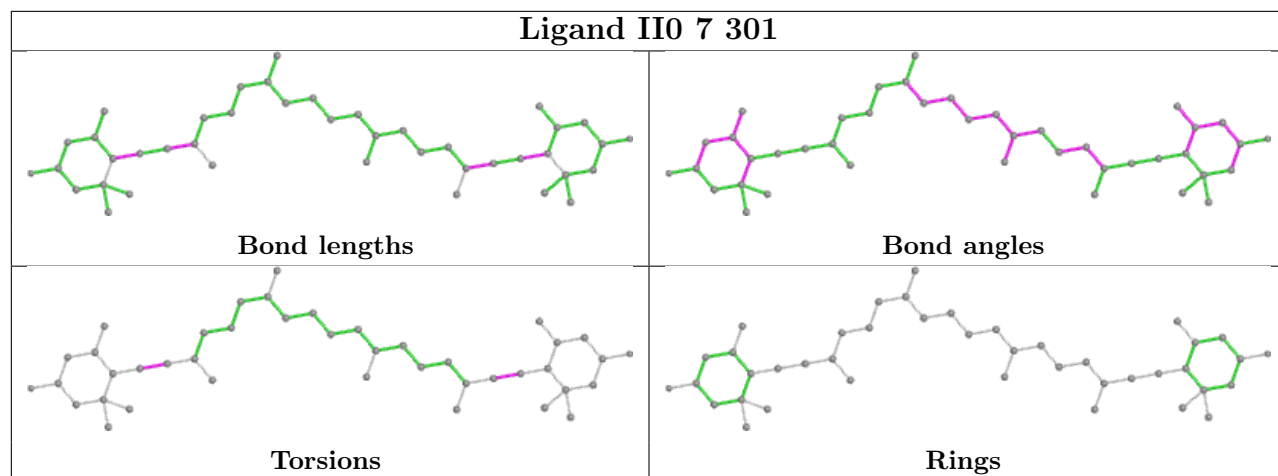
## Ligand CLA 3 612



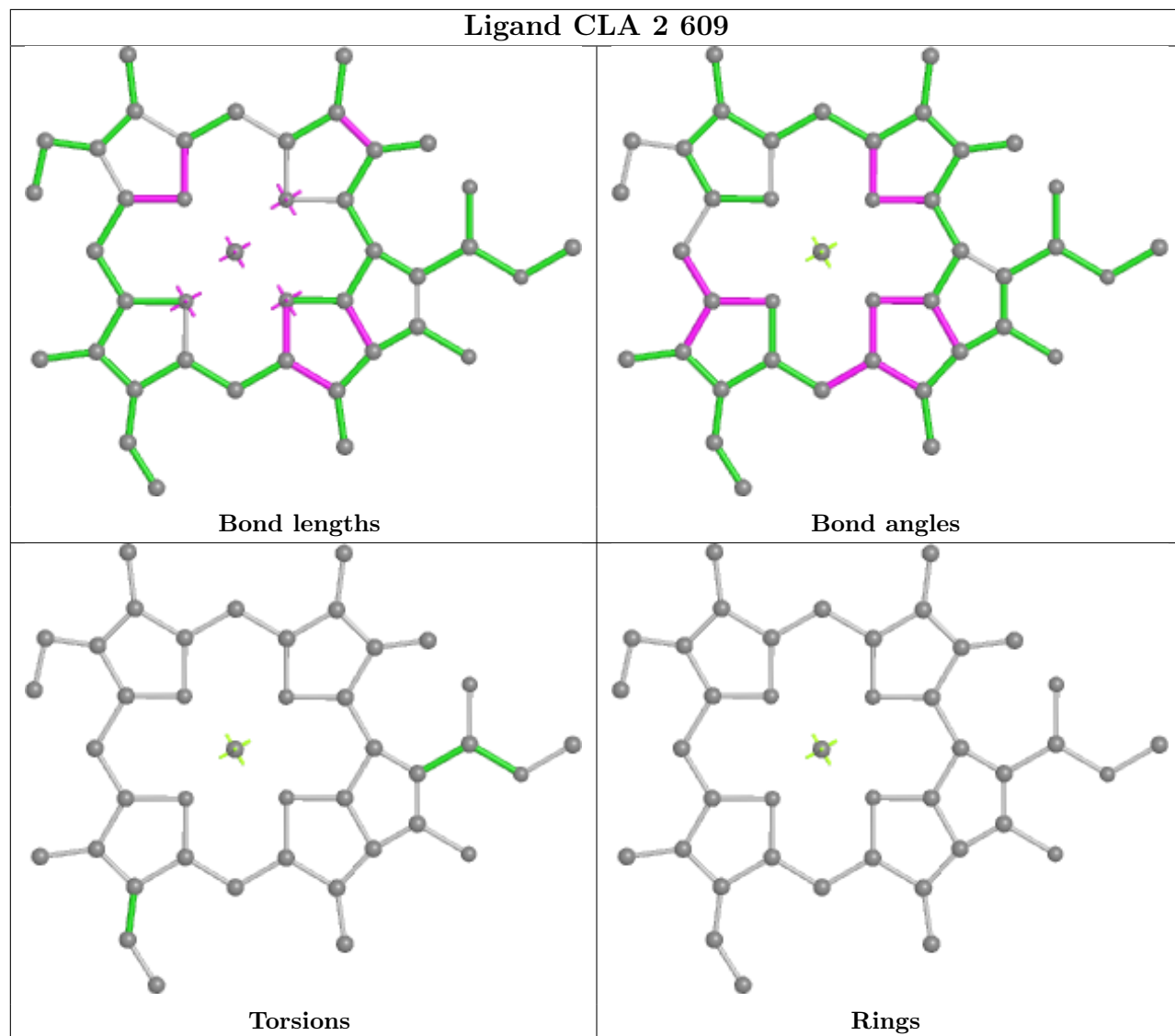
## Ligand II0 2 614



## Ligand II0 7 301

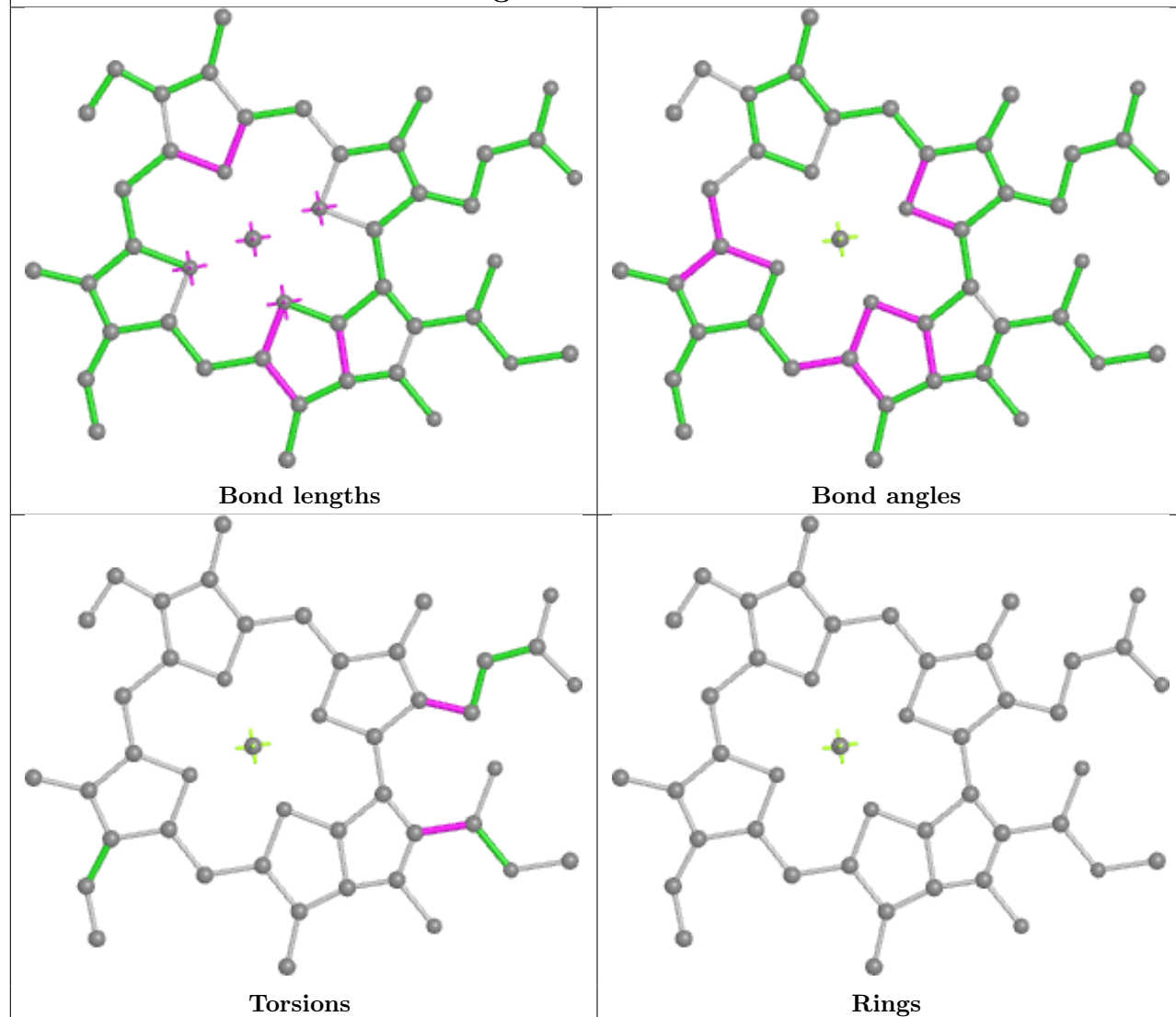


## Ligand CLA 2 609

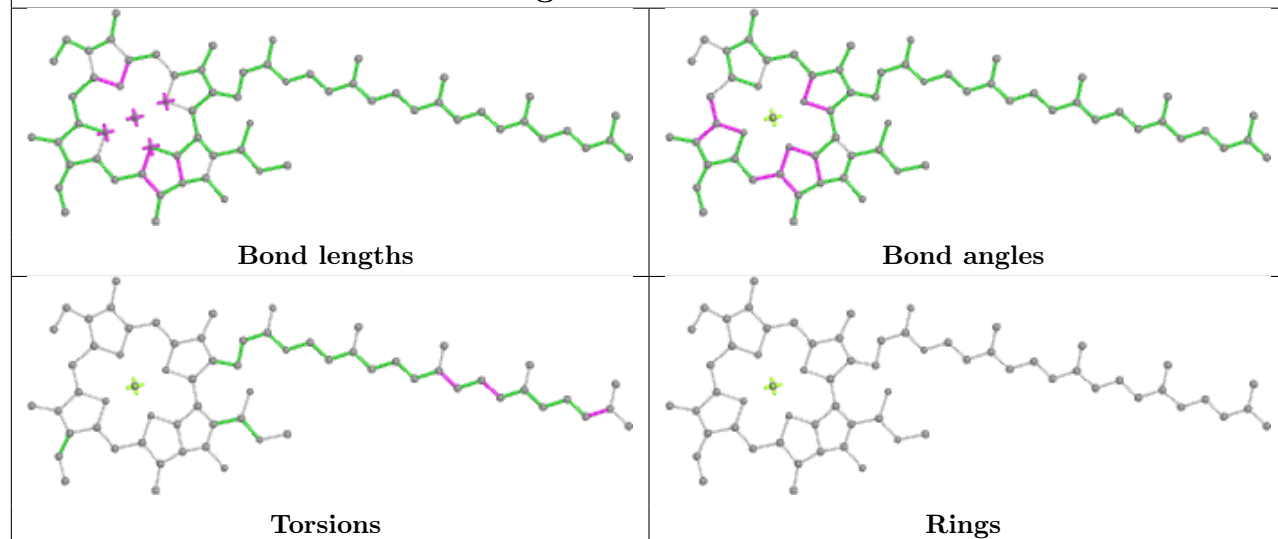




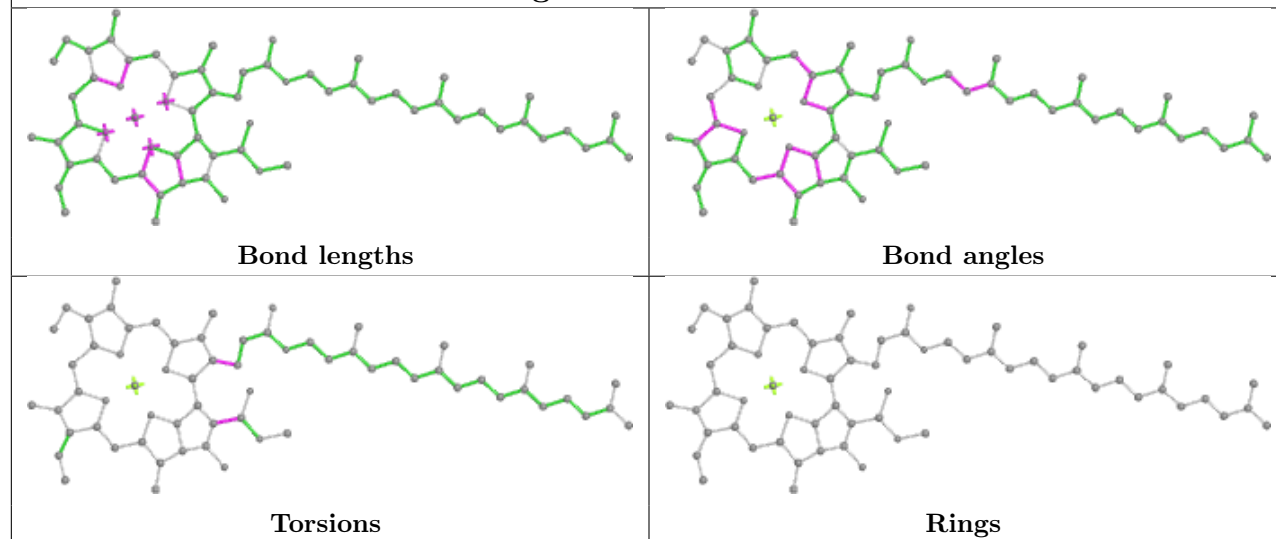
## Ligand CLA 5 612



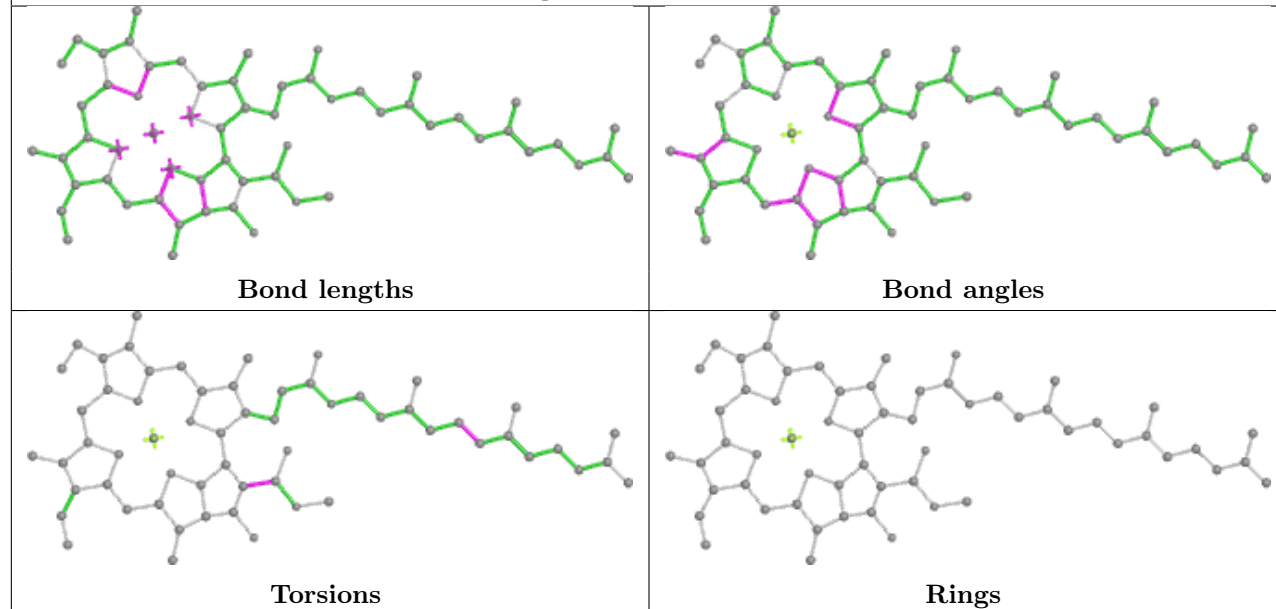
## Ligand CLA 8 608



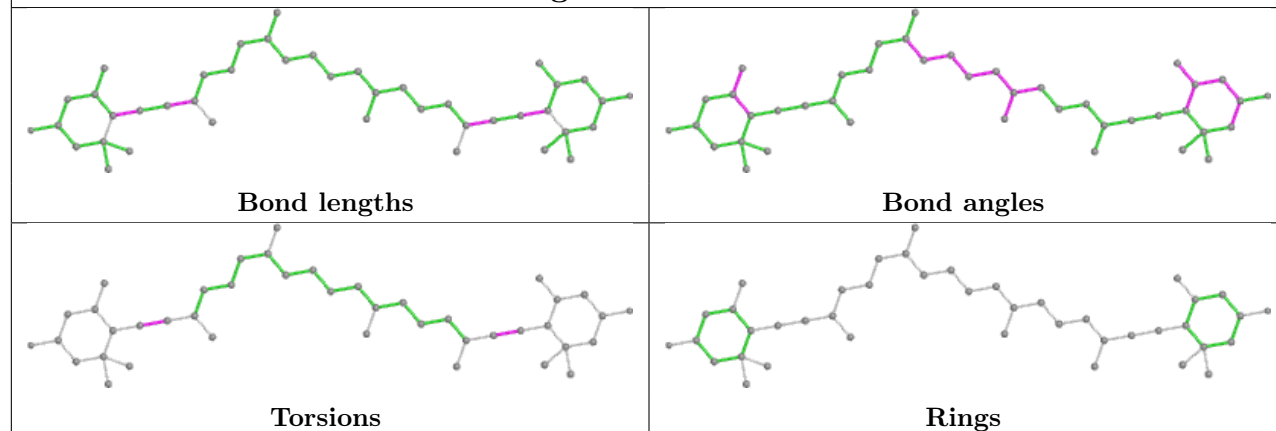
## Ligand CLA B 825



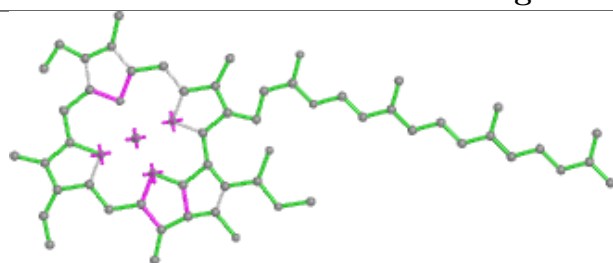
## Ligand CLA a 607



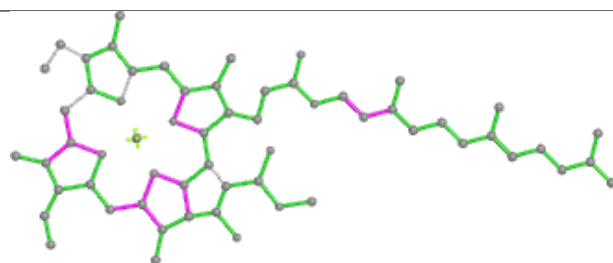
## Ligand II0 9 616



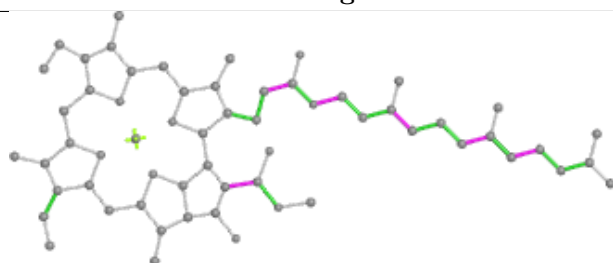
## Ligand CLA B 821



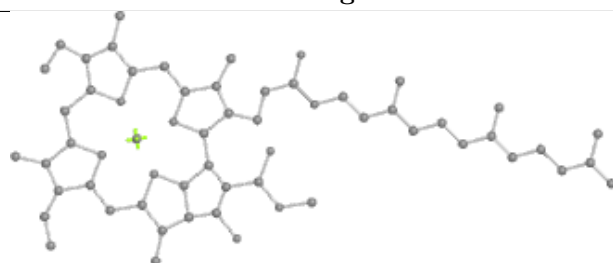
Bond lengths



Bond angles

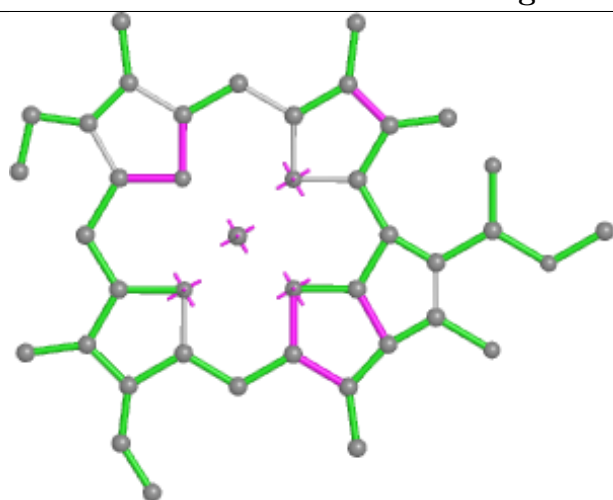


Torsions

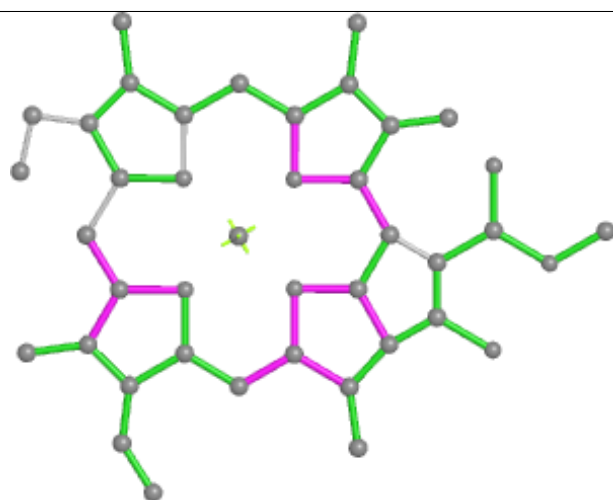


Rings

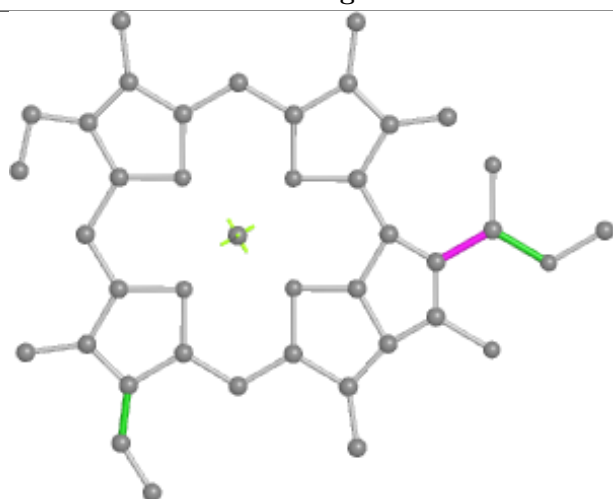
## Ligand CLA 9 614



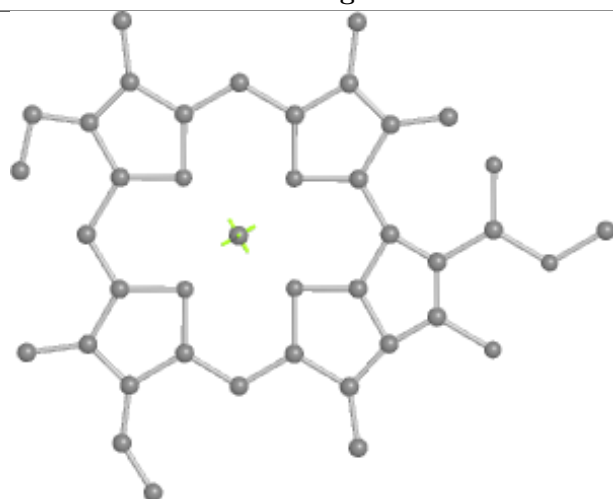
Bond lengths



Bond angles

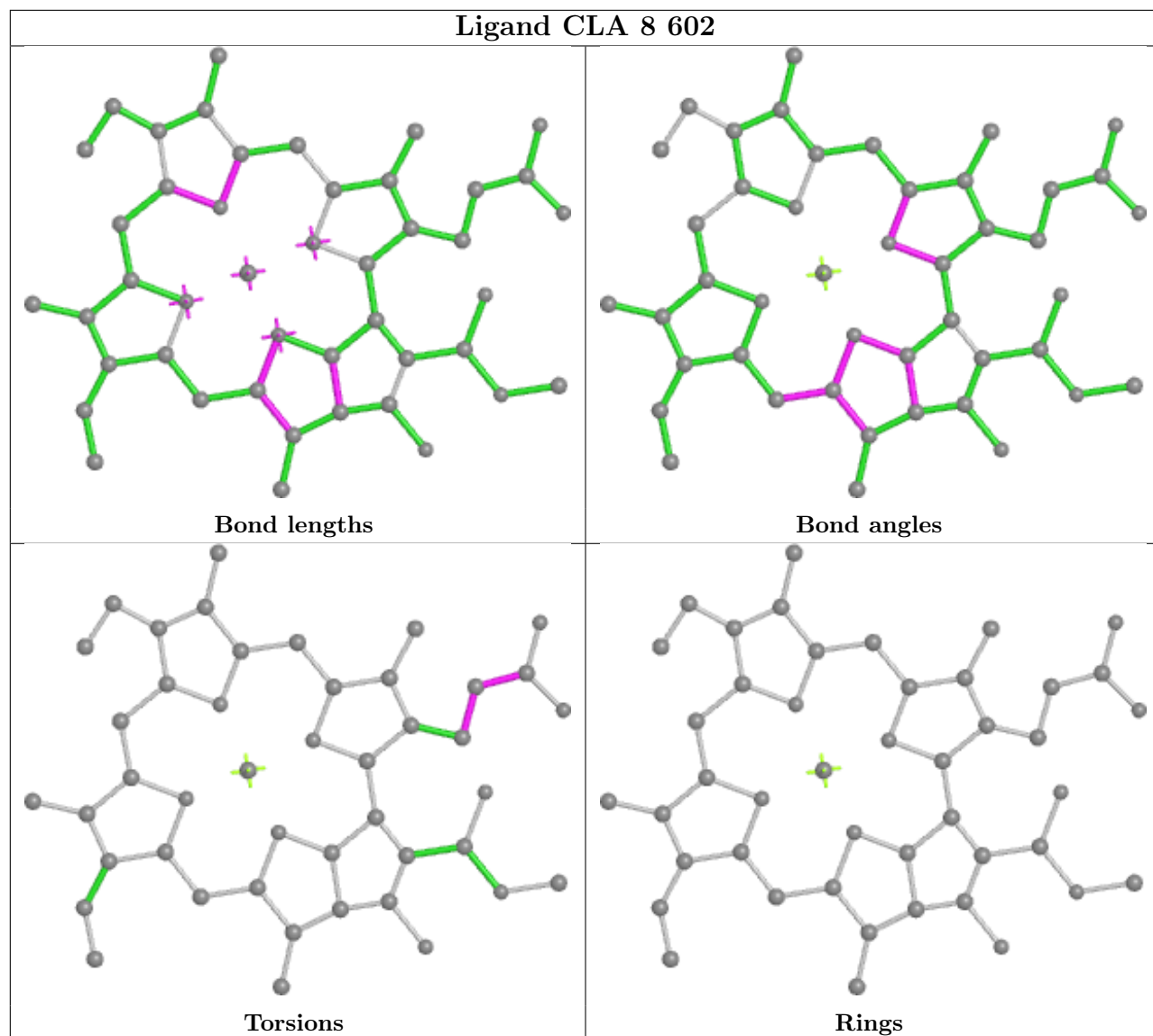


Torsions

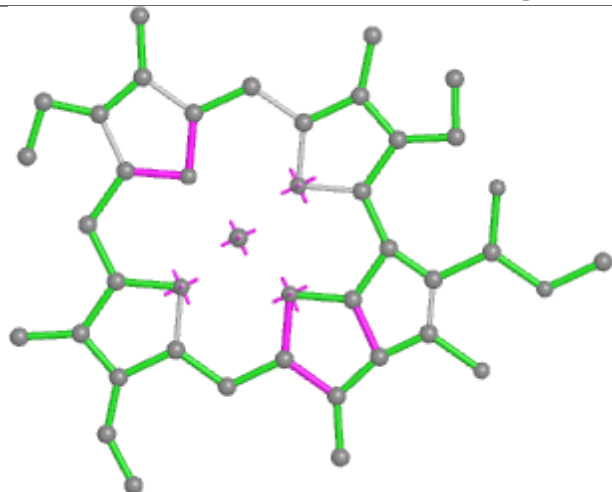


Rings

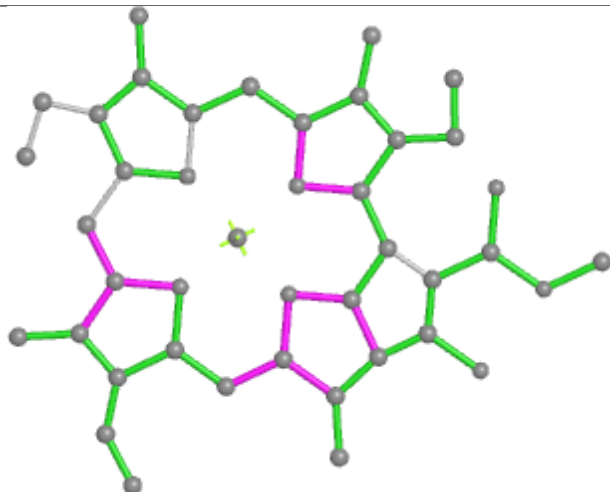
## Ligand CLA 8 602



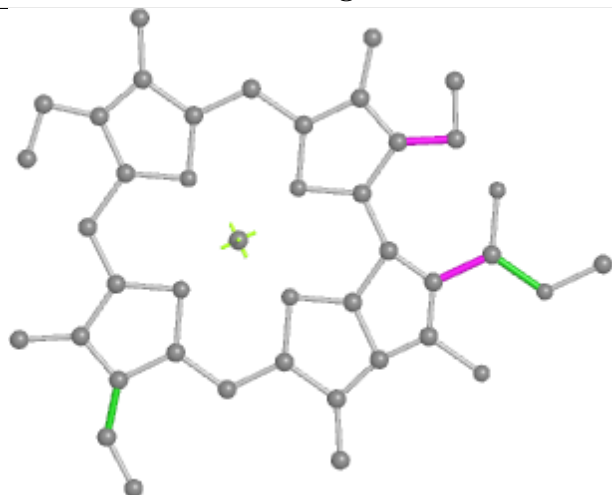
## Ligand CLA 2 601



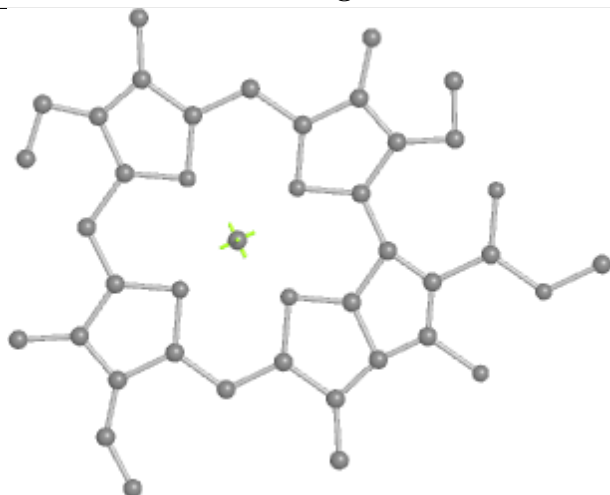
Bond lengths



Bond angles

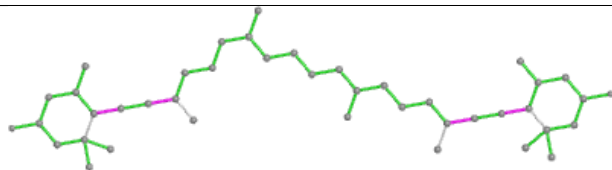


Torsions

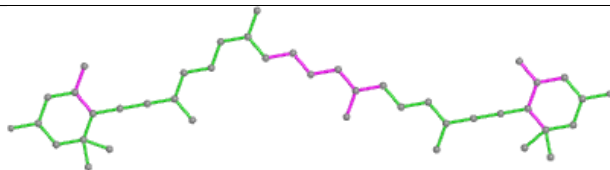


Rings

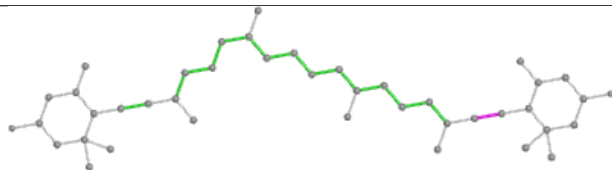
## Ligand II0 5 615



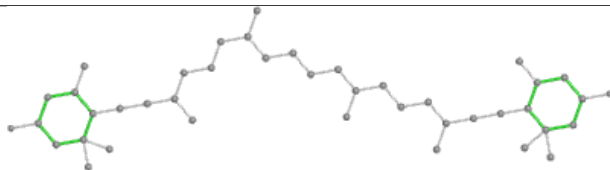
Bond lengths



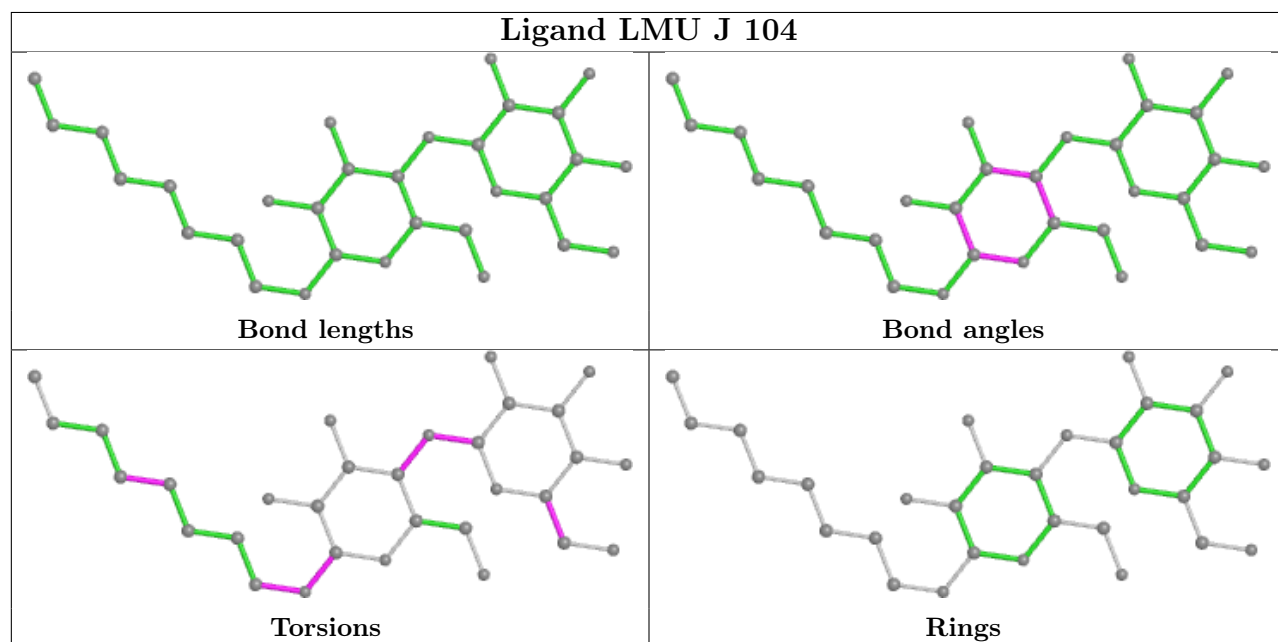
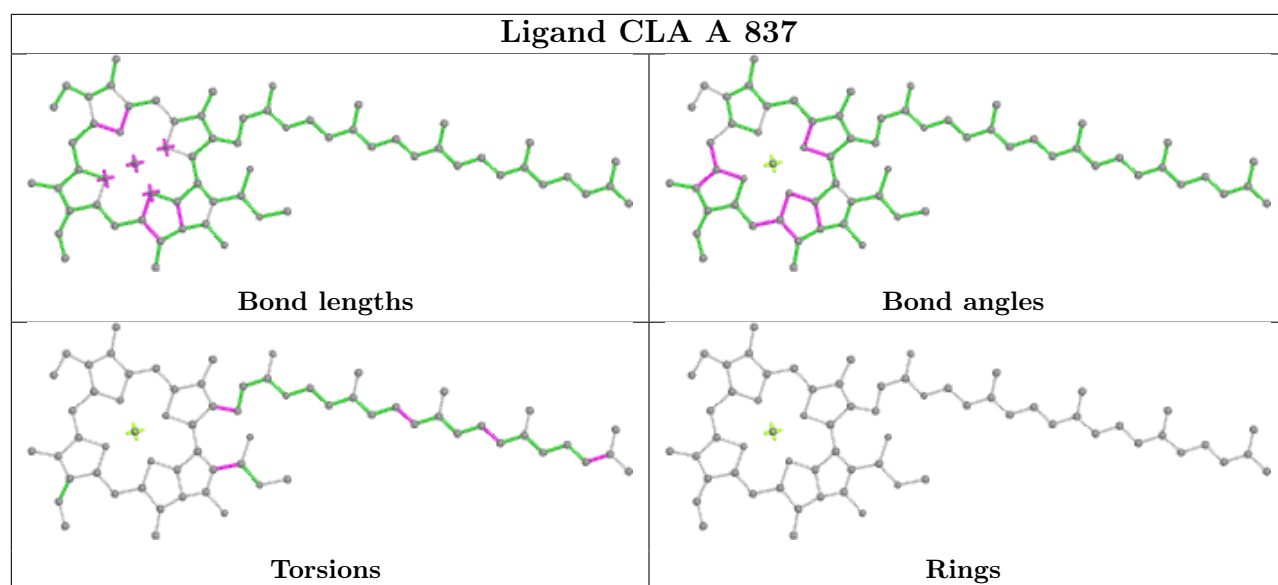
Bond angles



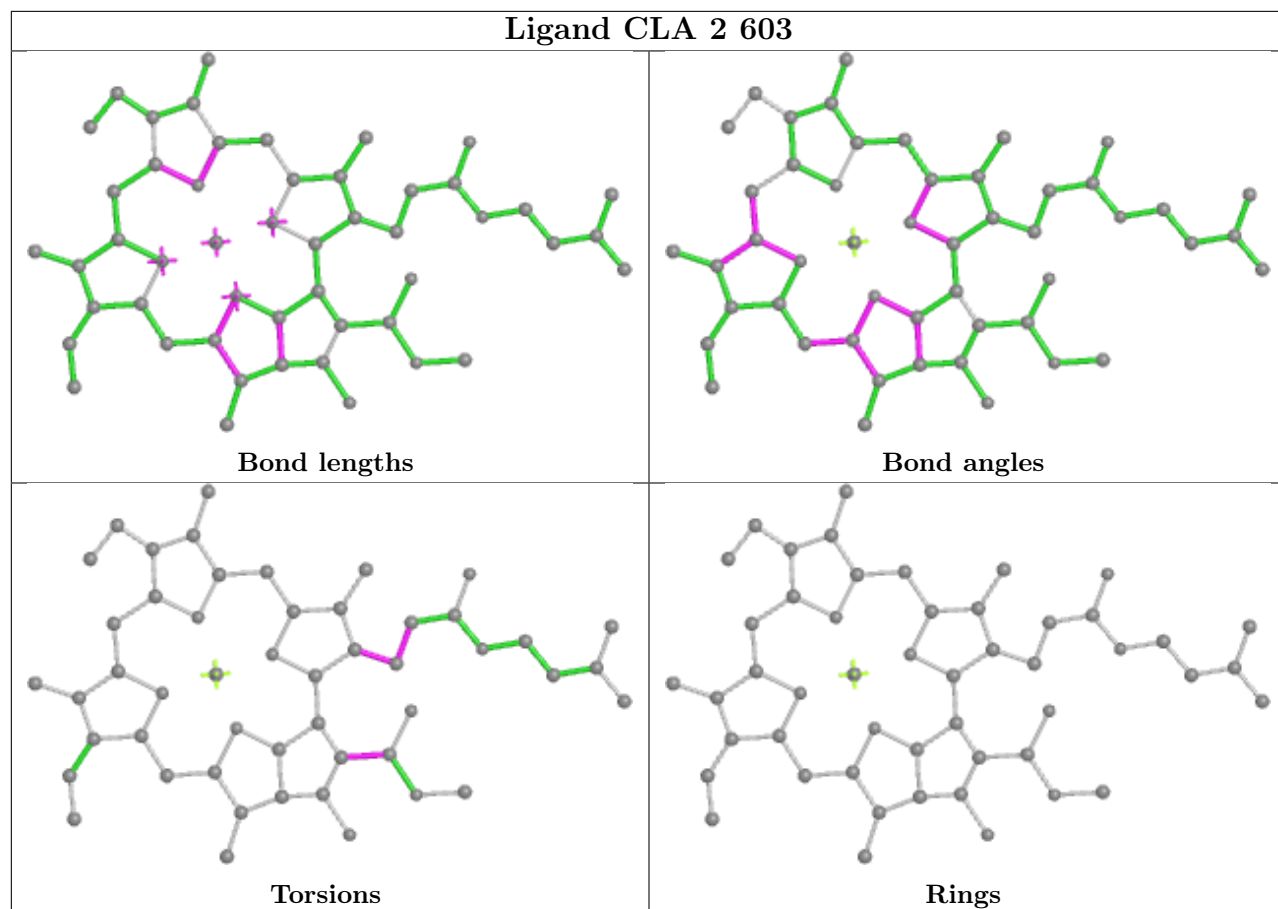
Torsions



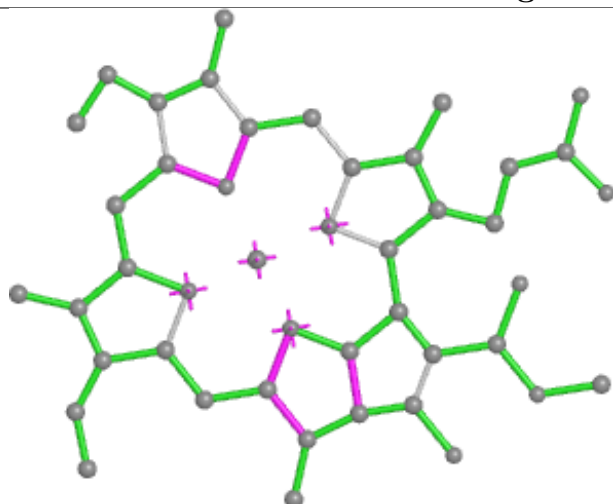
Rings



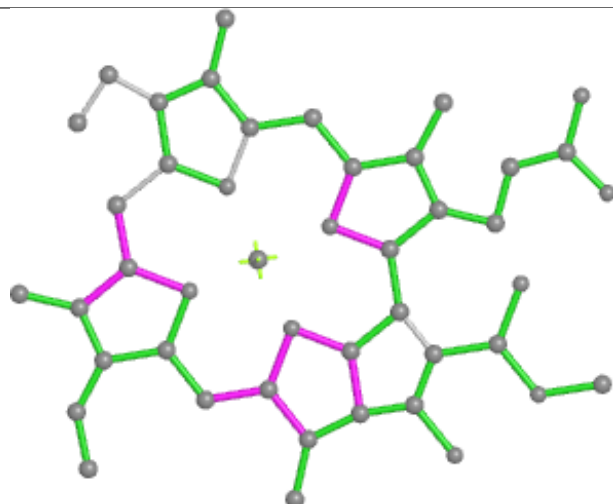
## Ligand CLA 2 603



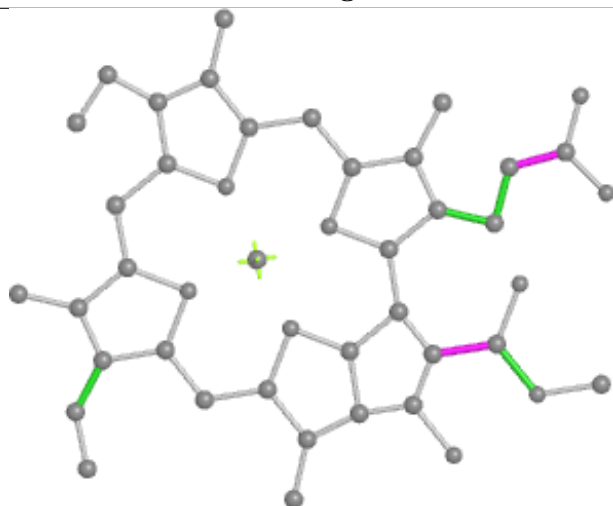
## Ligand CLA b 601



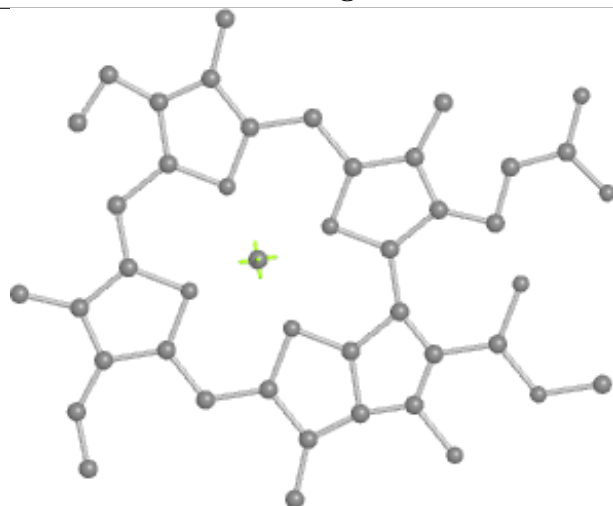
Bond lengths



Bond angles

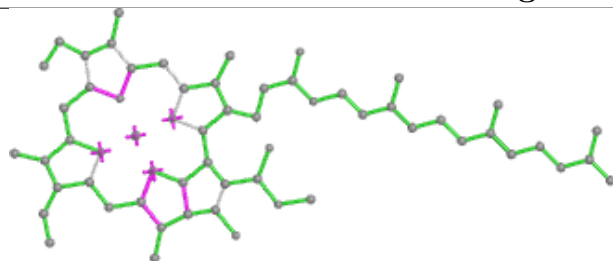


Torsions

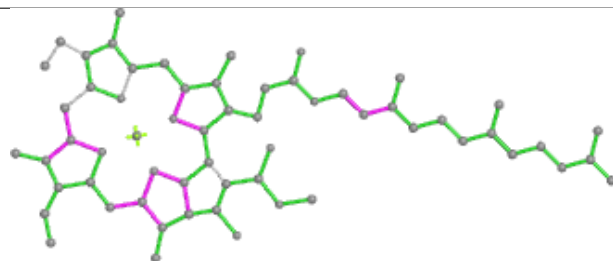


Rings

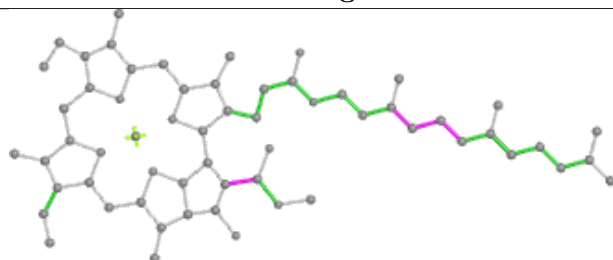
## Ligand CLA 4 607



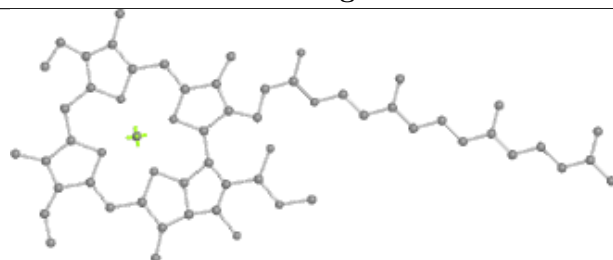
Bond lengths



Bond angles



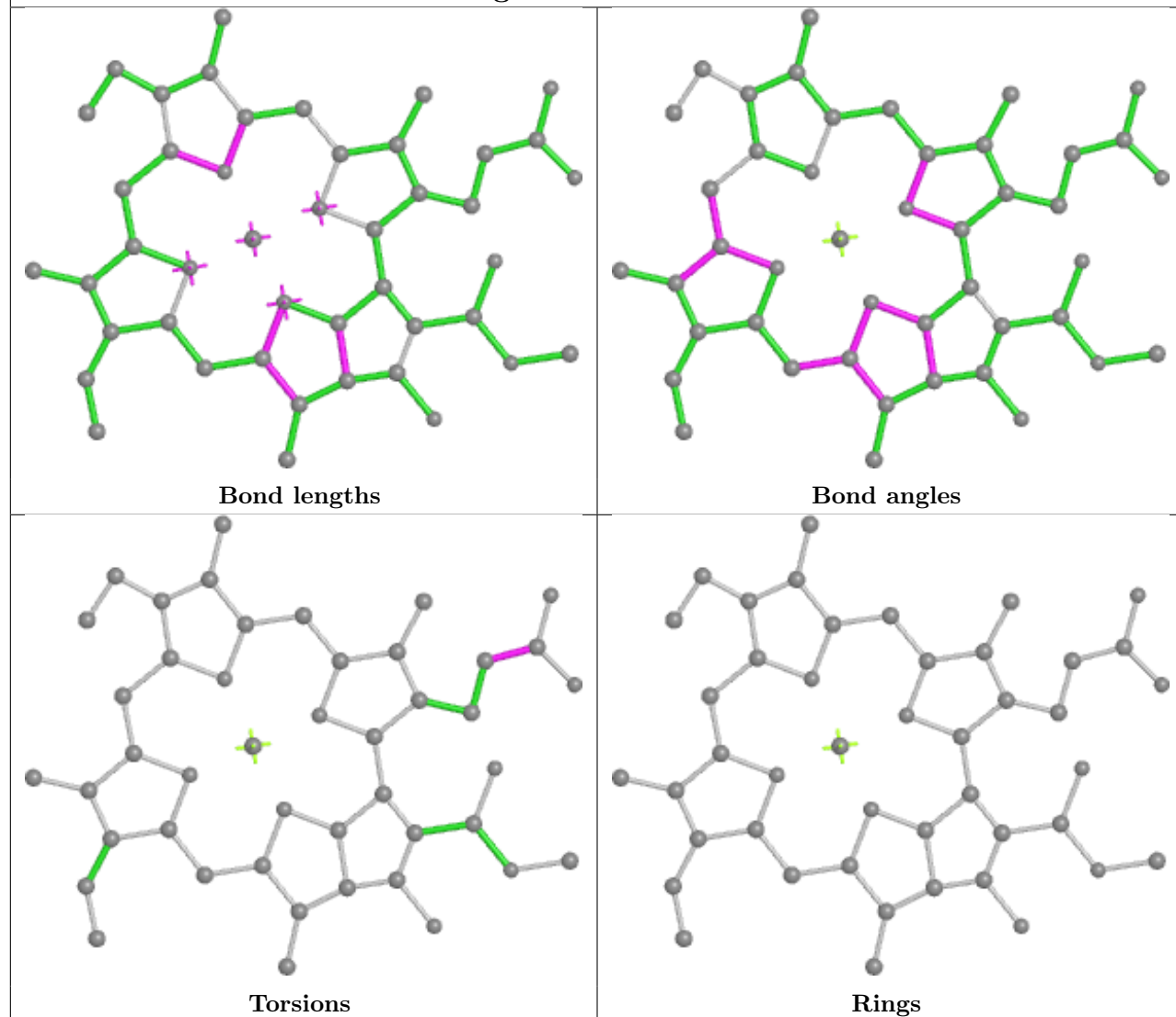
Torsions



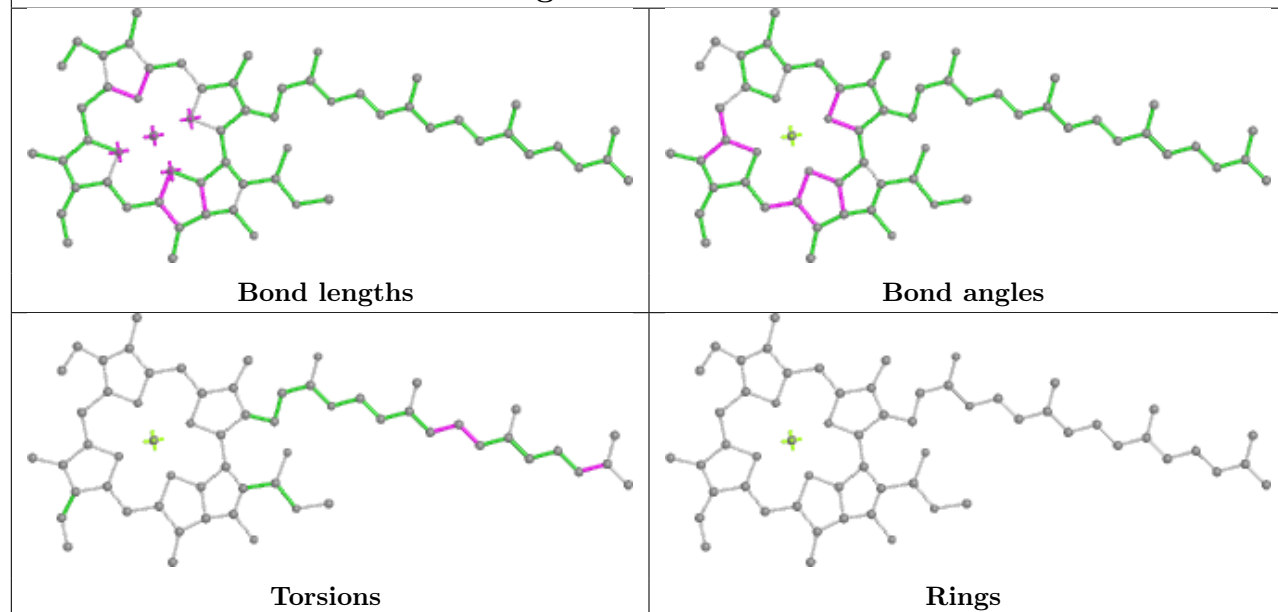
Rings

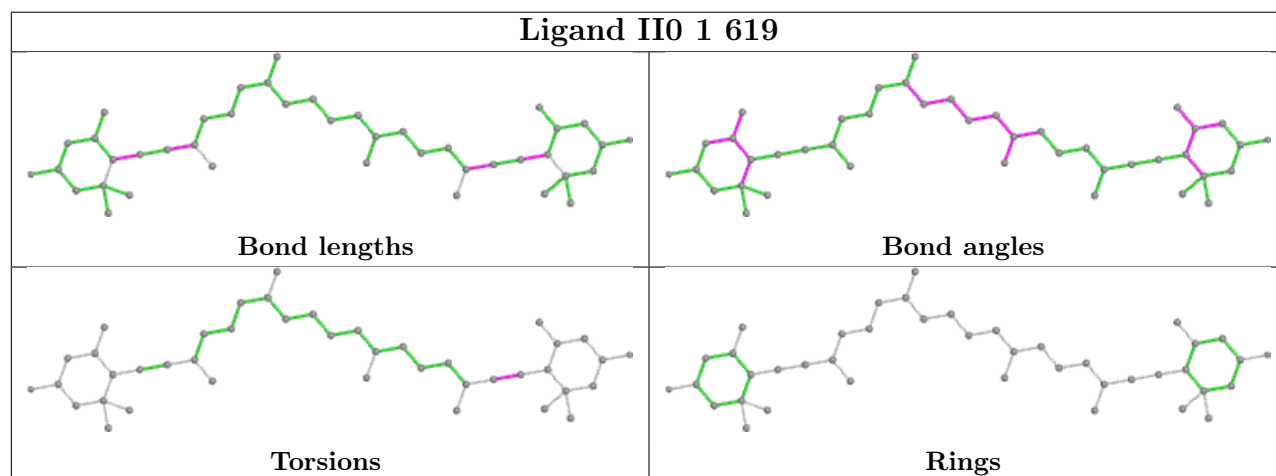
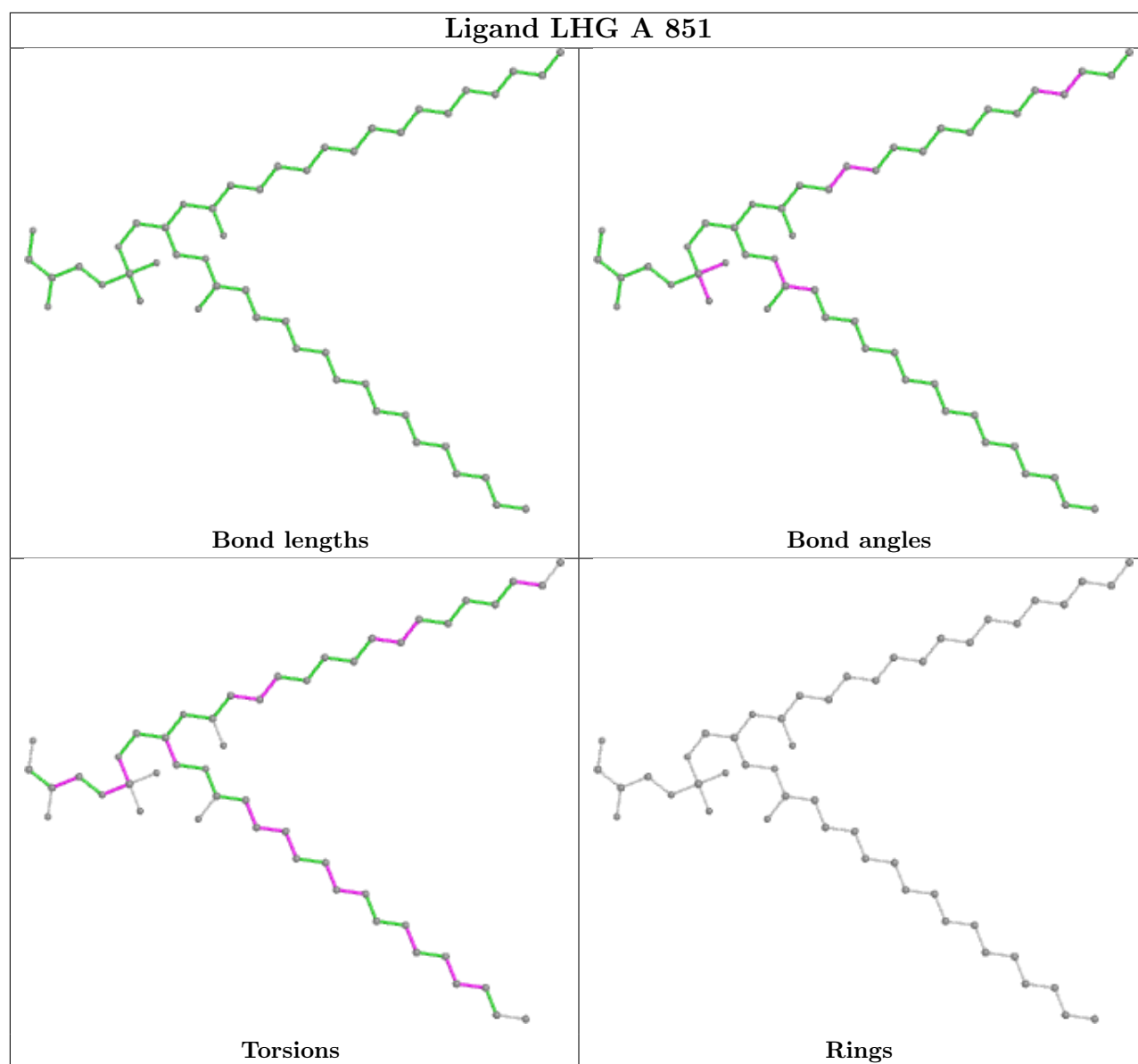


## Ligand CLA 9 612

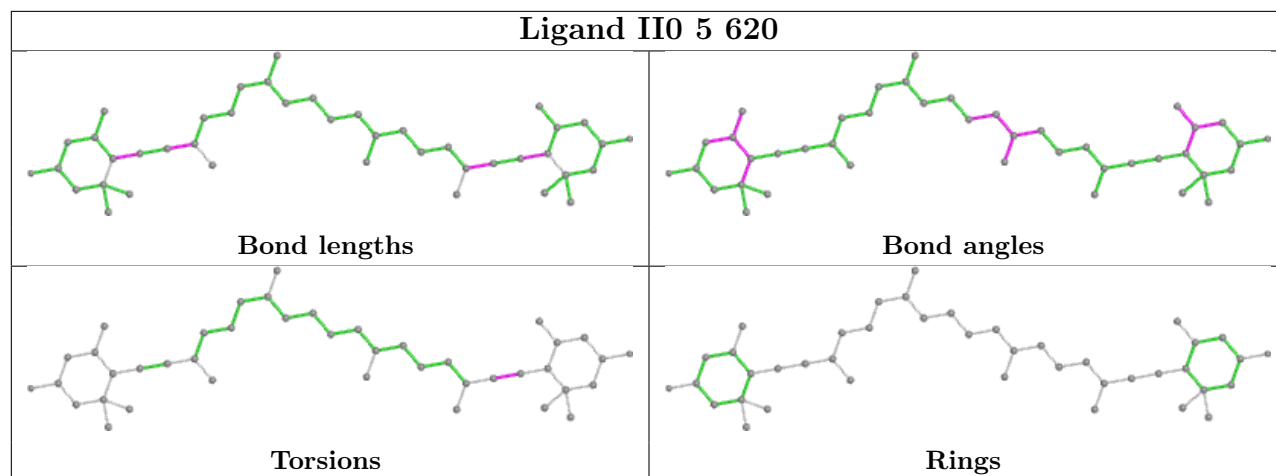


## Ligand CLA 3 607

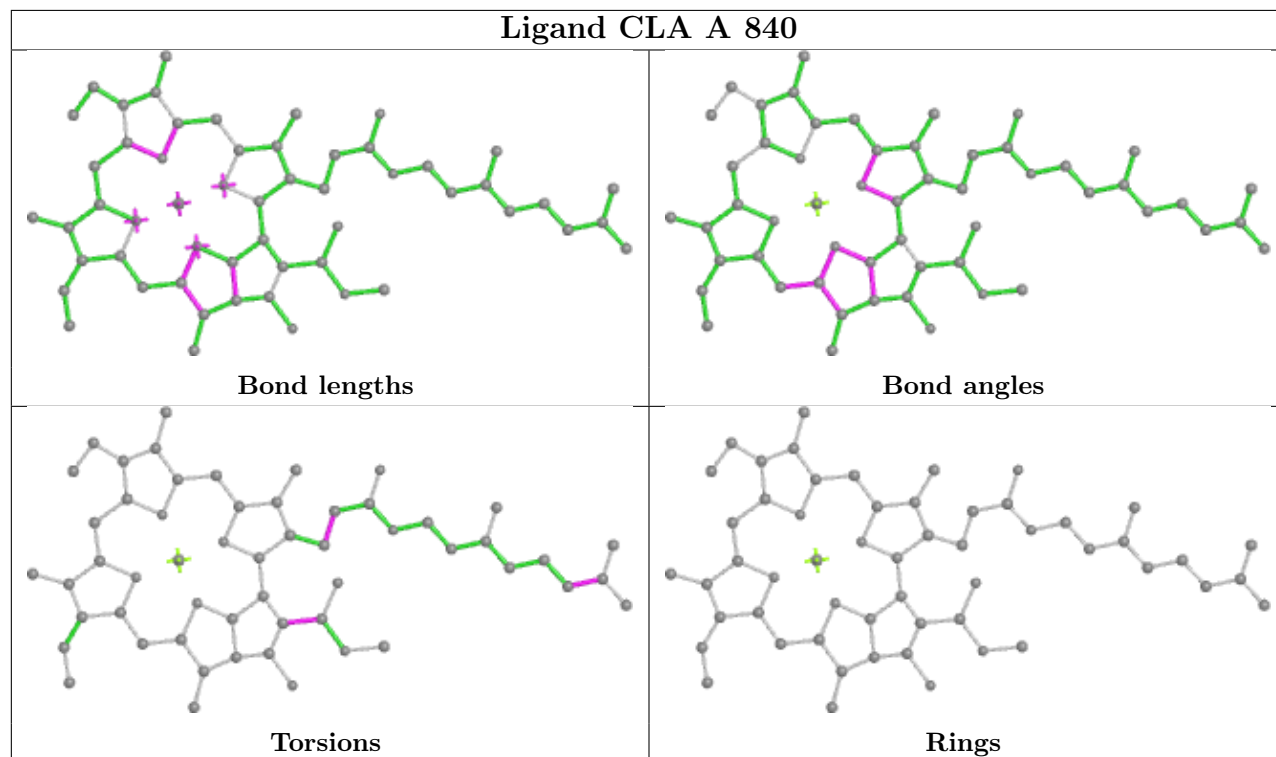


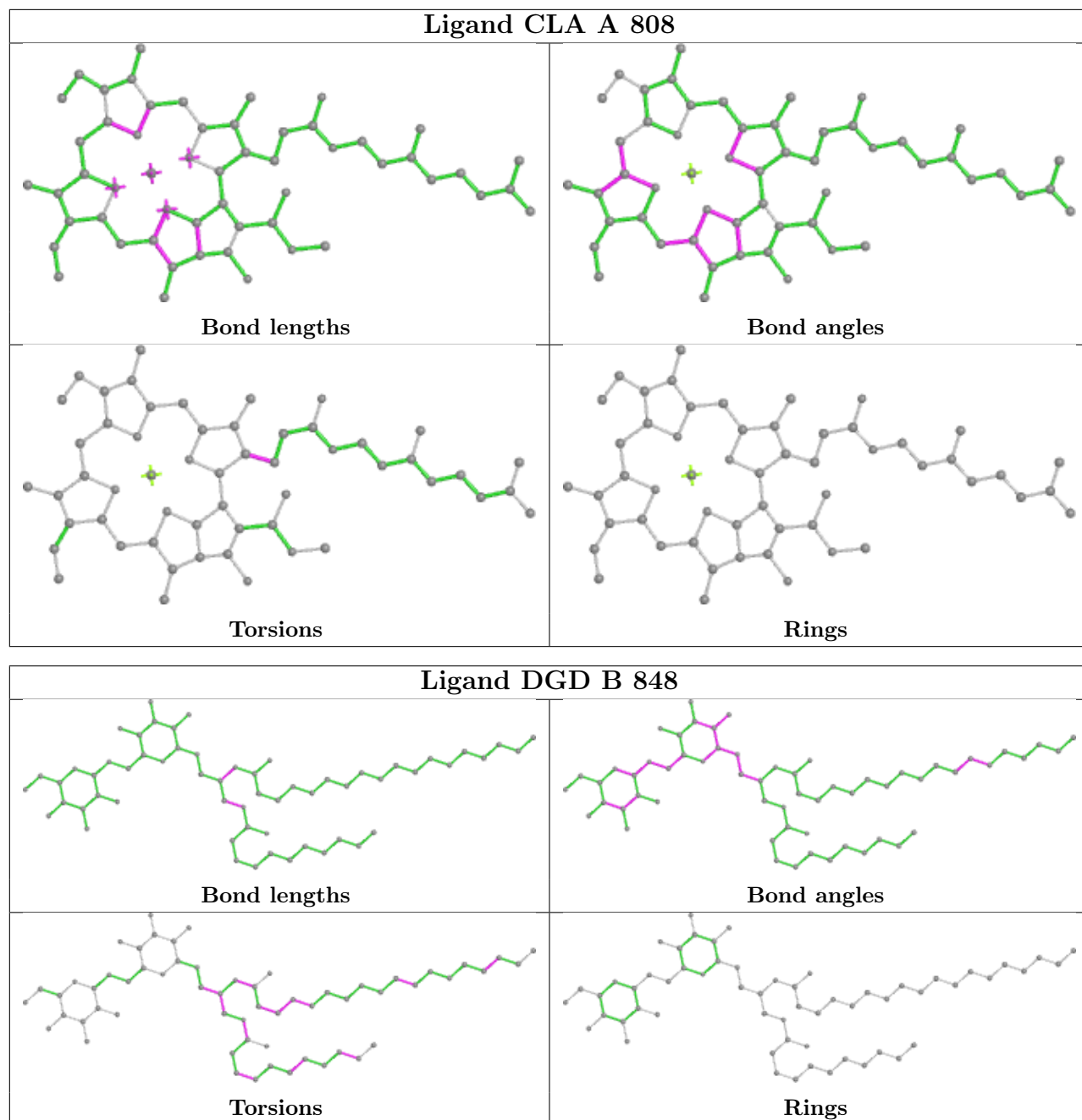


## Ligand II0 5 620

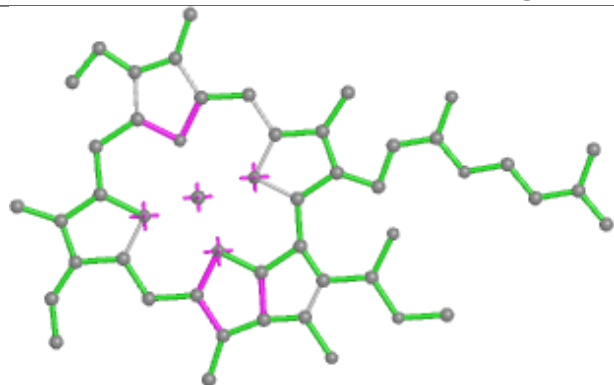


## Ligand CLA A 840

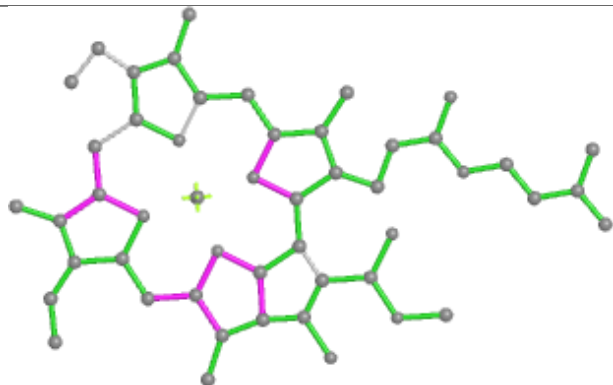




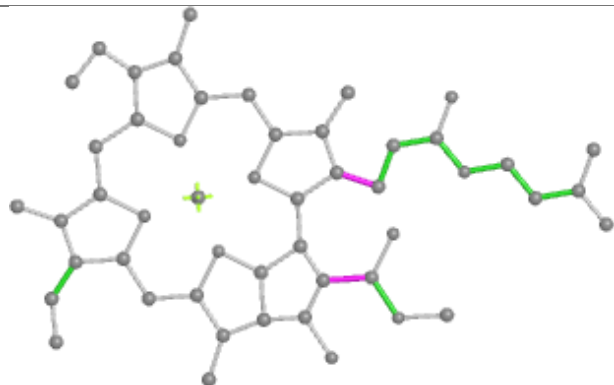
## Ligand CLA 3 611



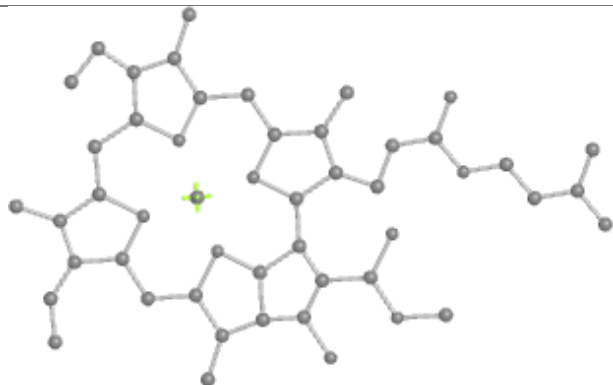
Bond lengths



Bond angles

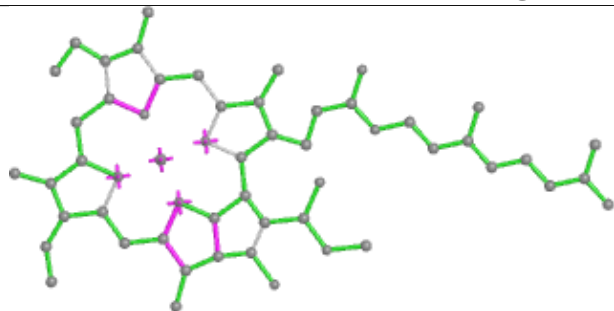


Torsions

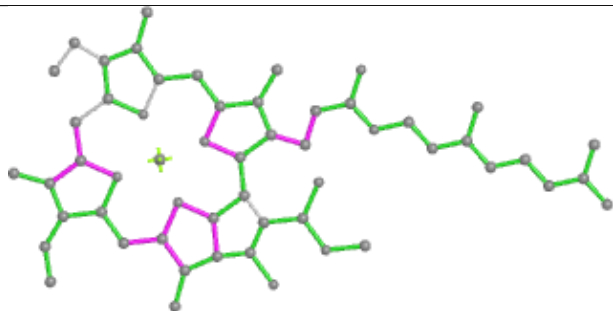


Rings

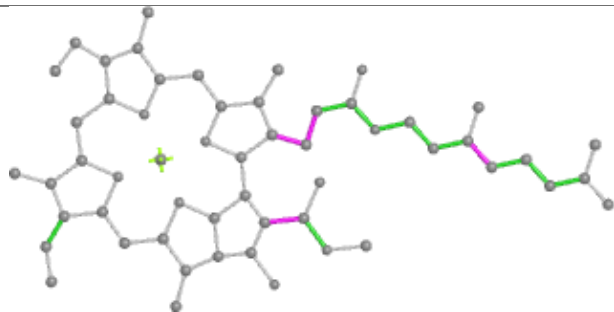
## Ligand CLA A 834



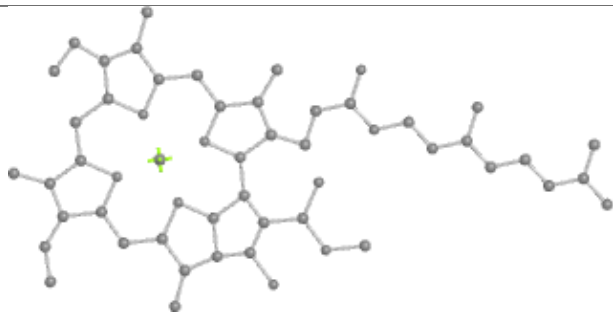
Bond lengths



Bond angles

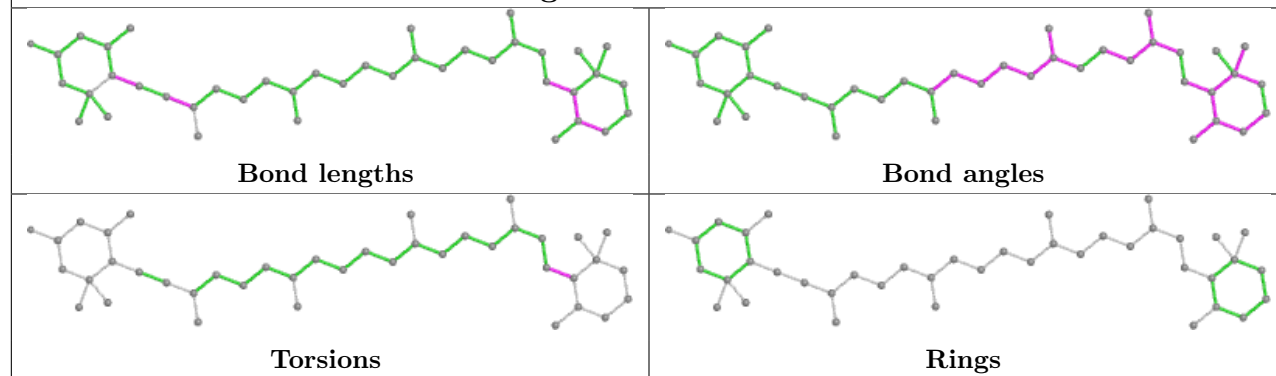


Torsions

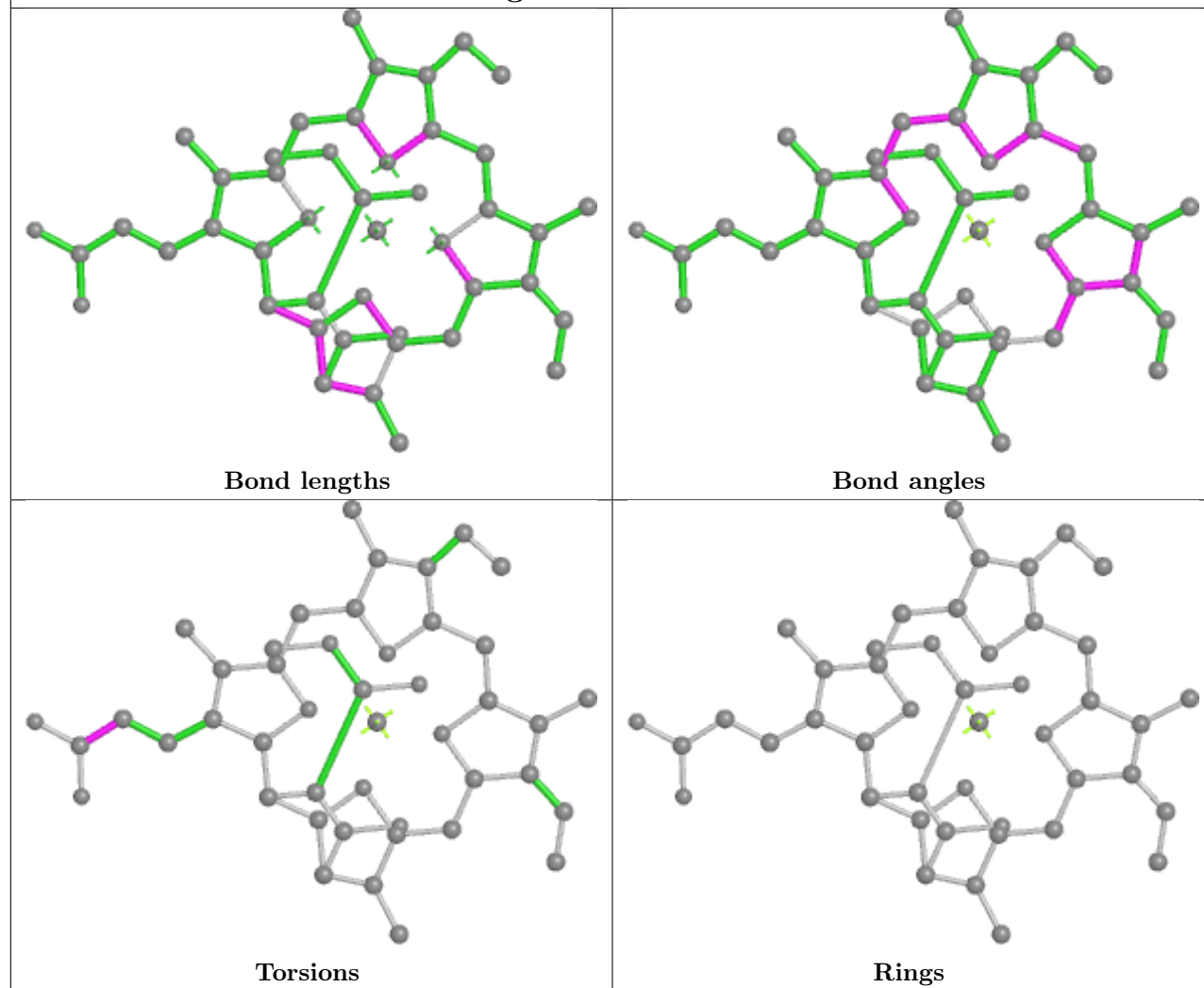


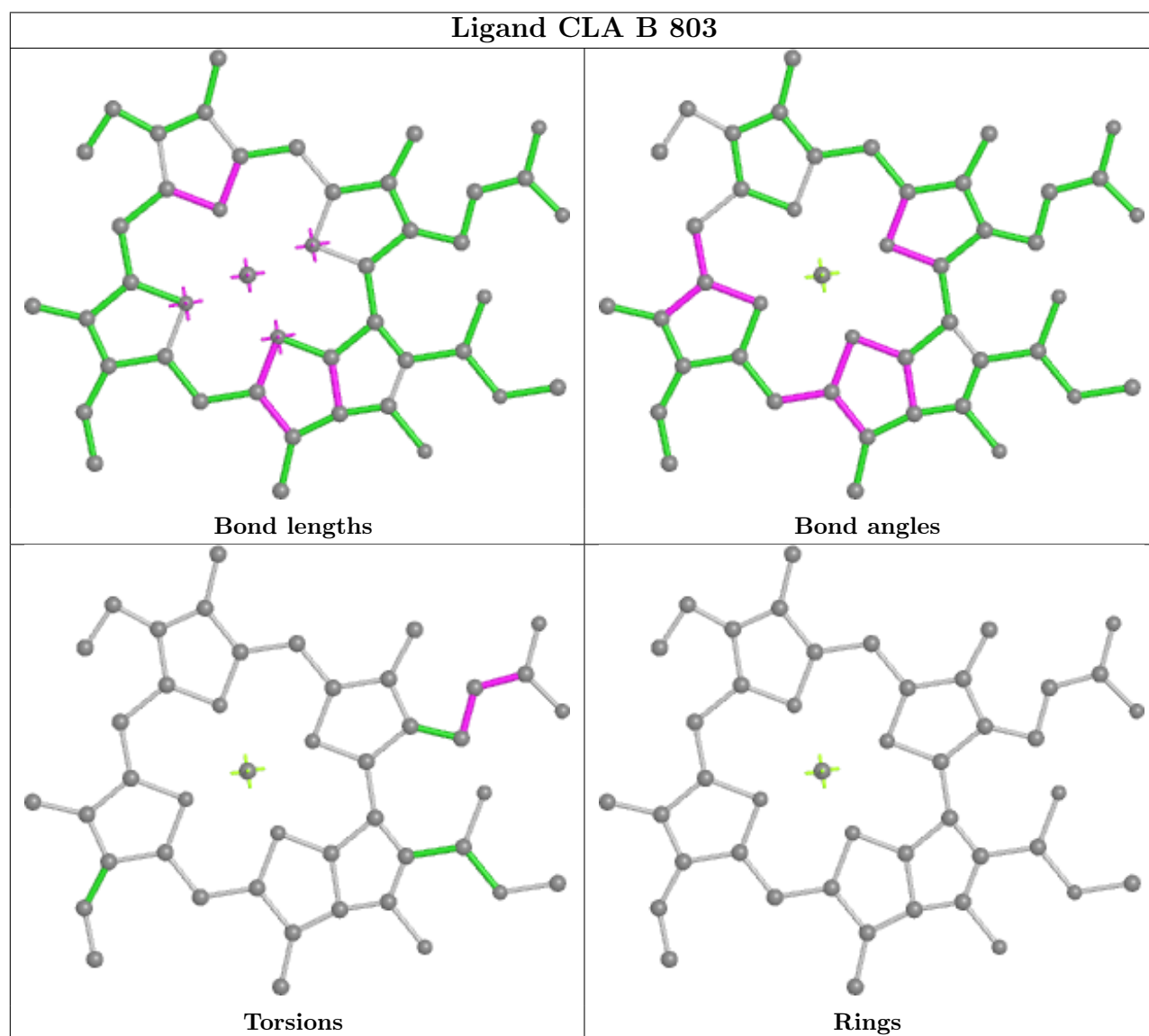
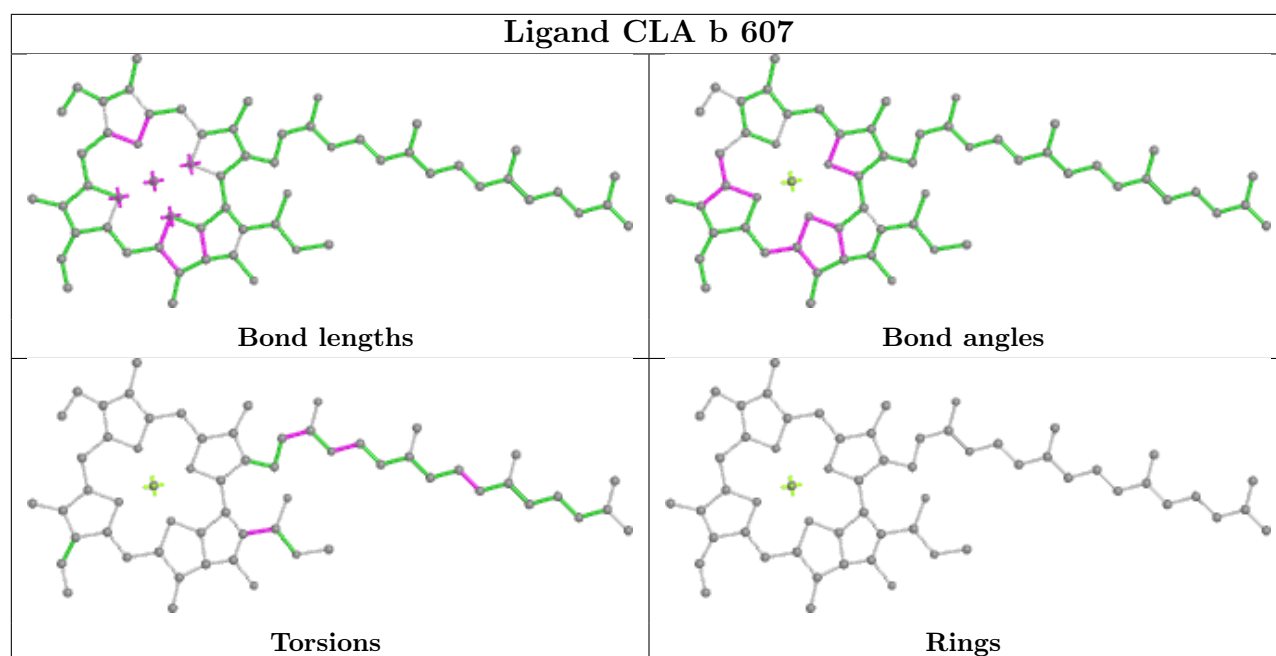
Rings

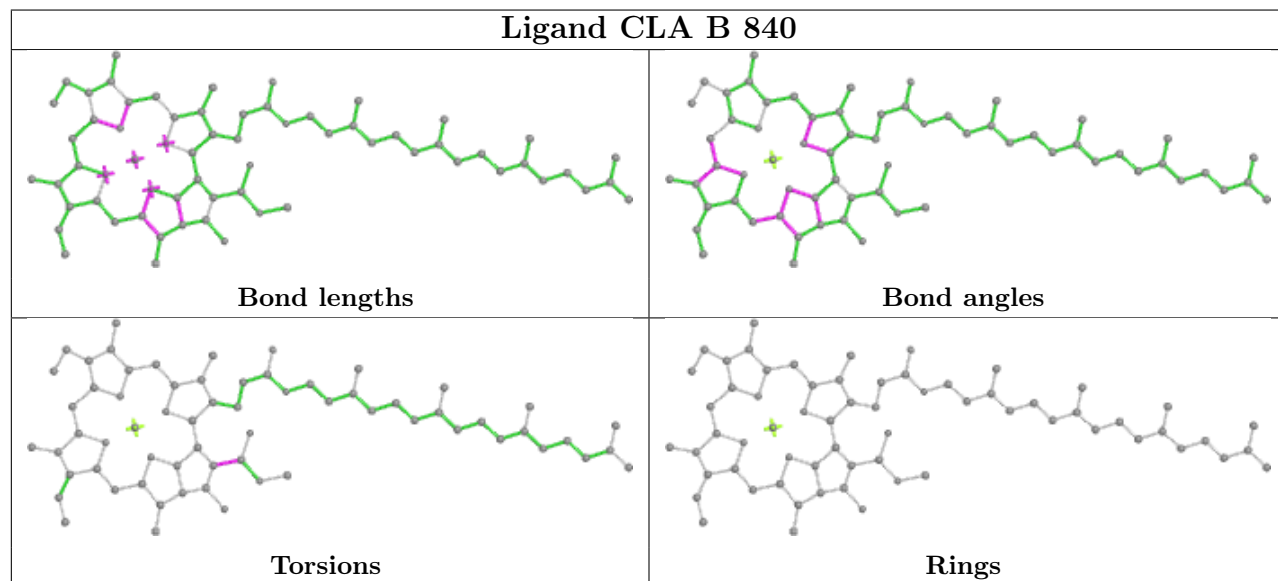
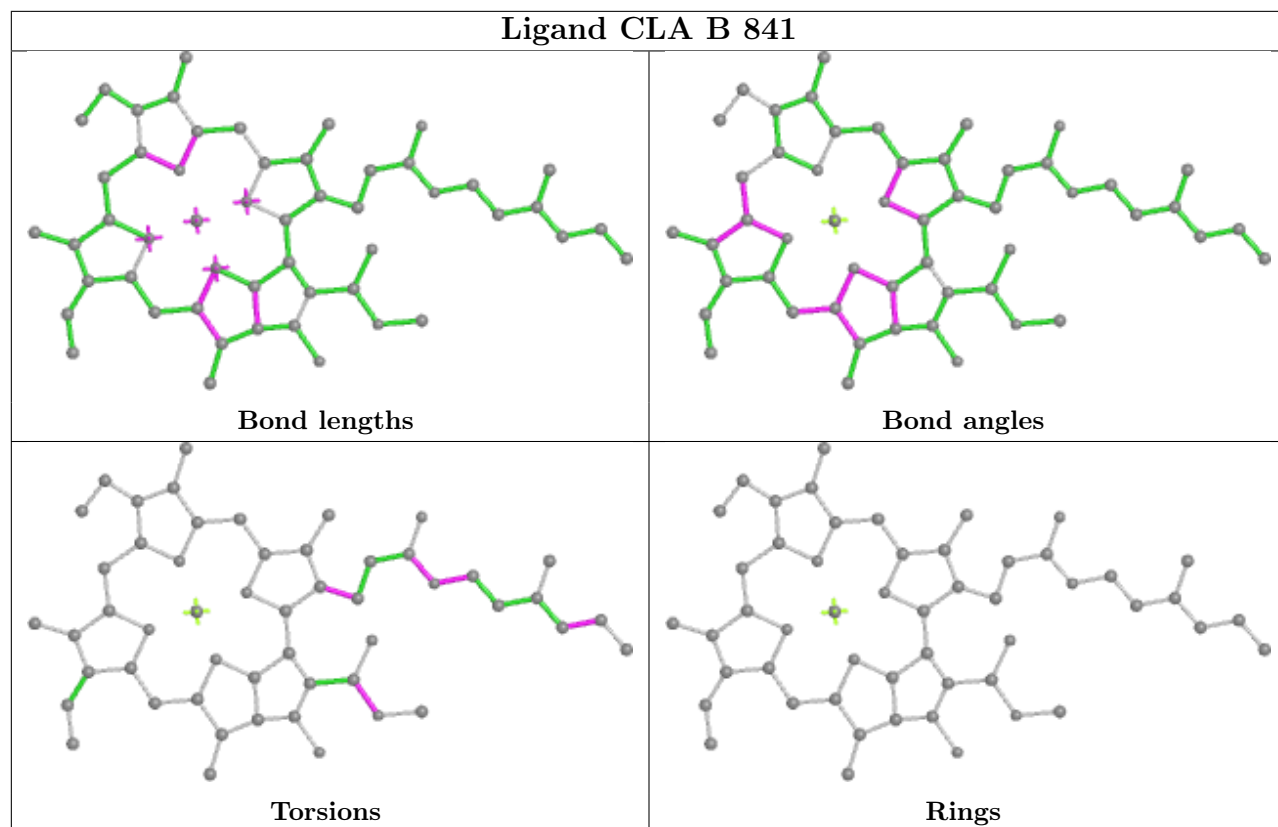
## Ligand IHT 5 618



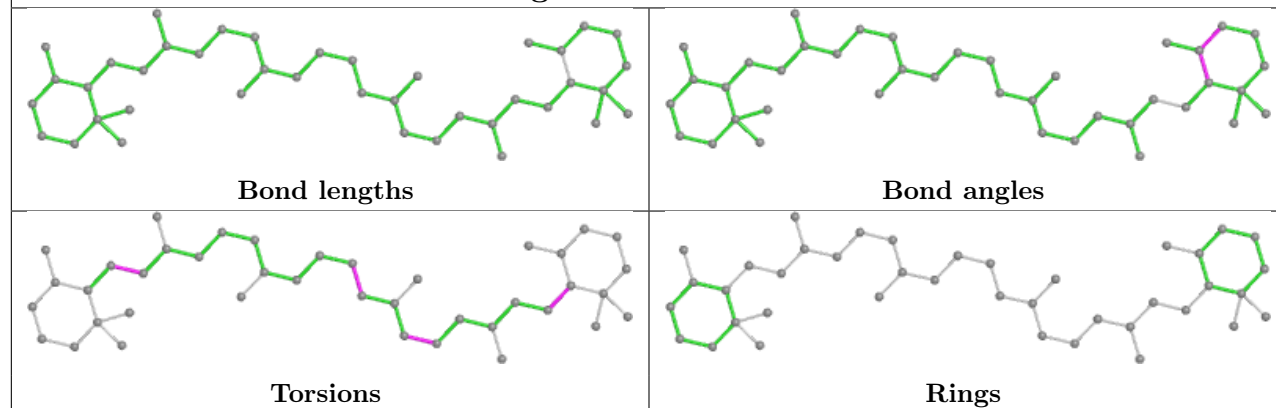
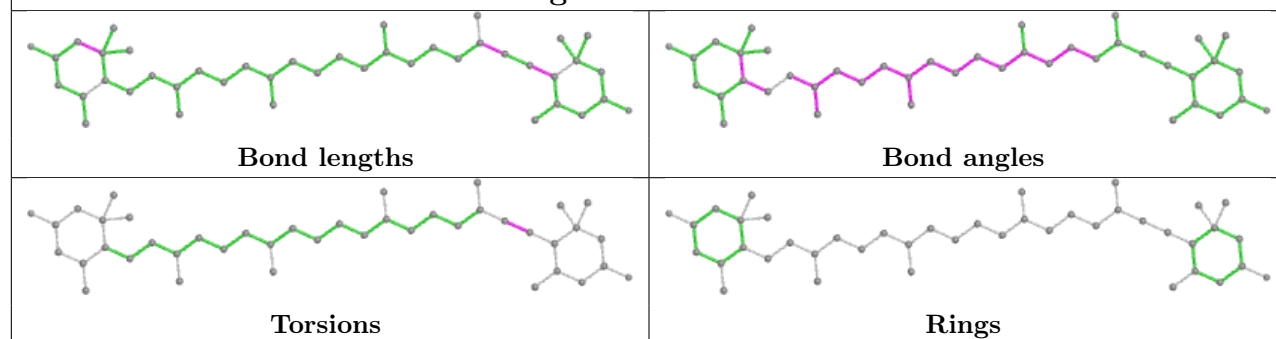
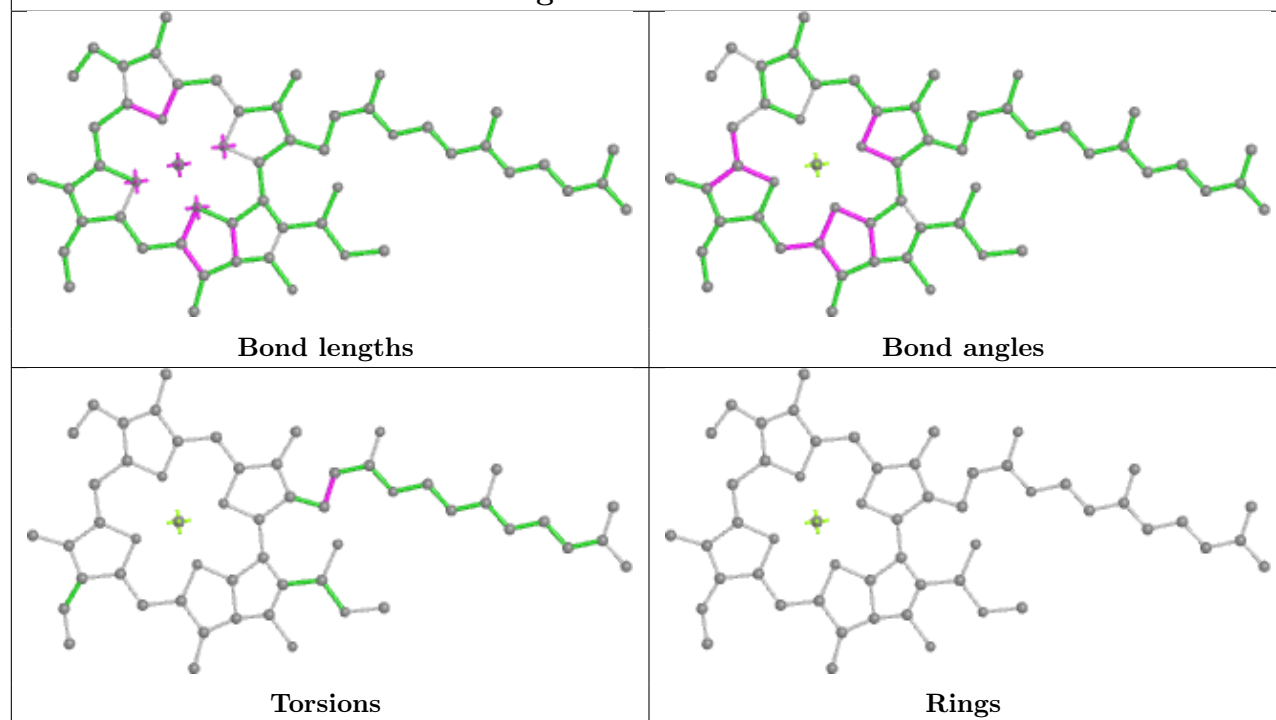
## Ligand KC2 b 609



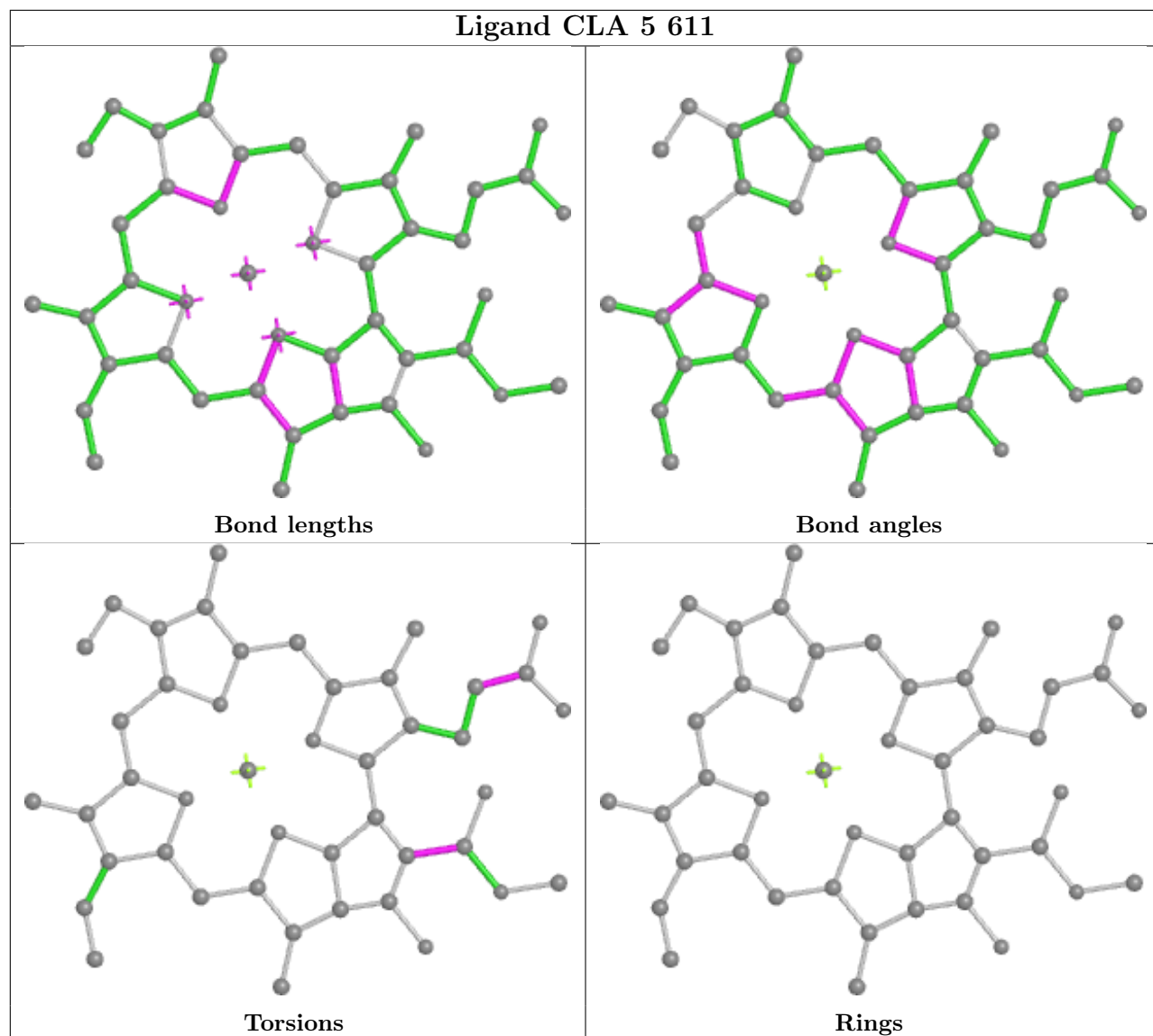




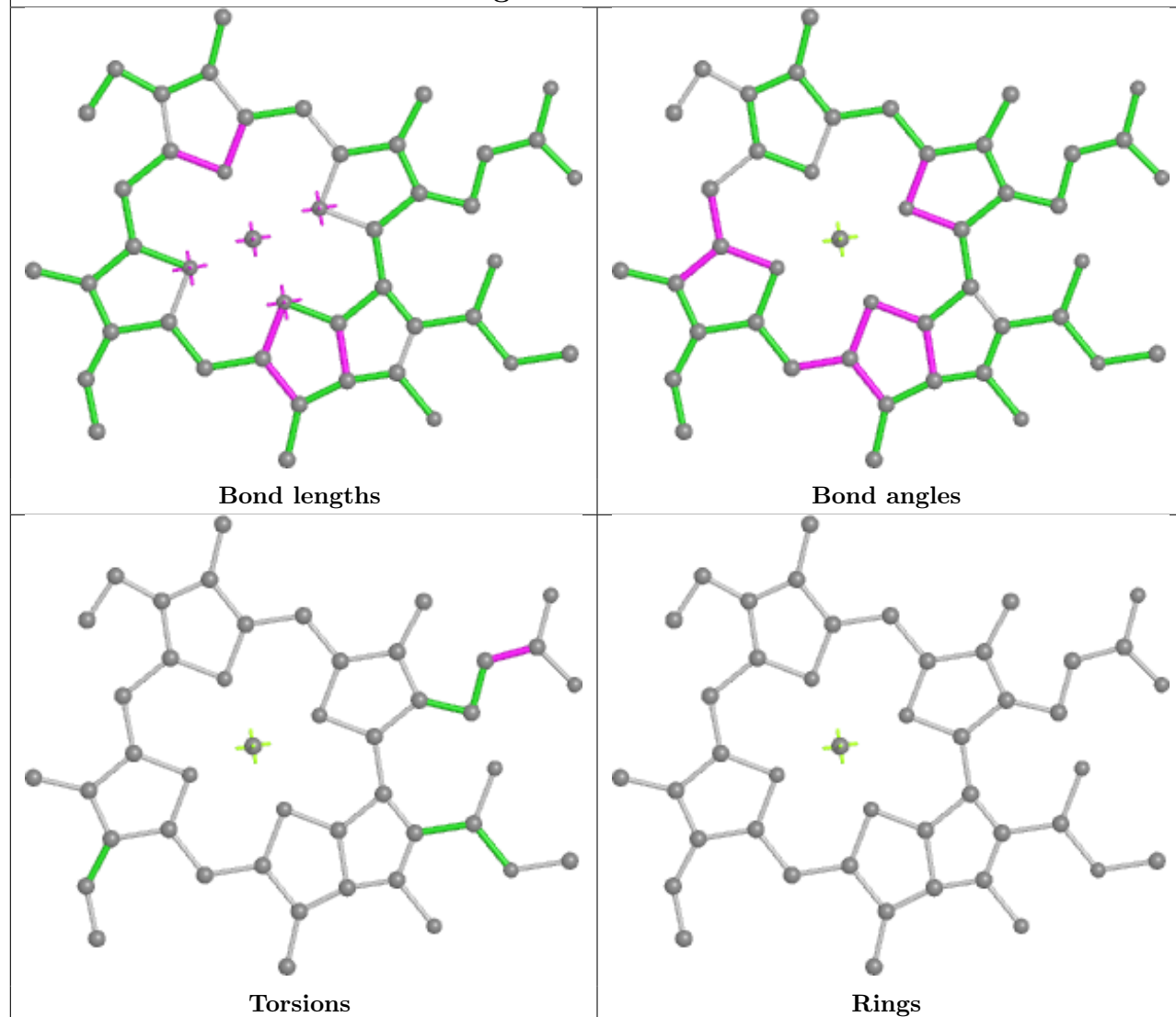


**Ligand 8CT M 101****Ligand II3 b 613****Ligand CLA 9 604**

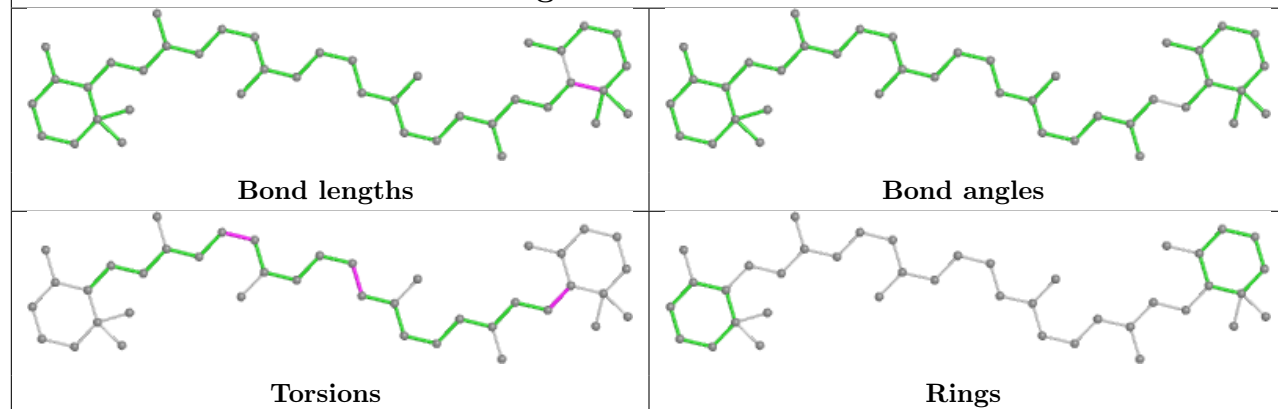
## Ligand CLA 5 611



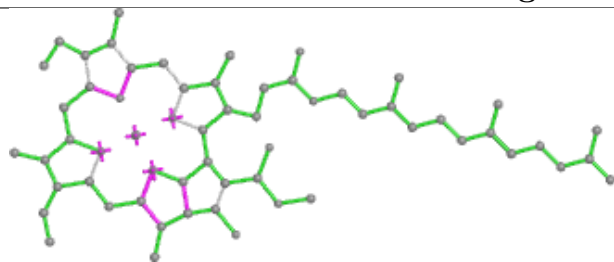
## Ligand CLA 9 605



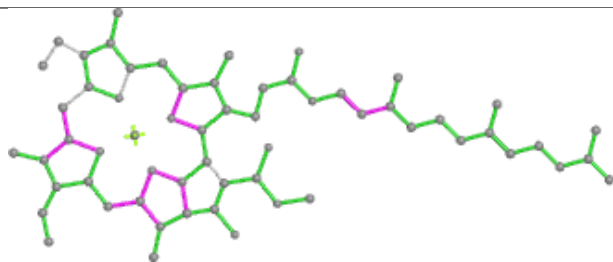
## Ligand 8CT F 201



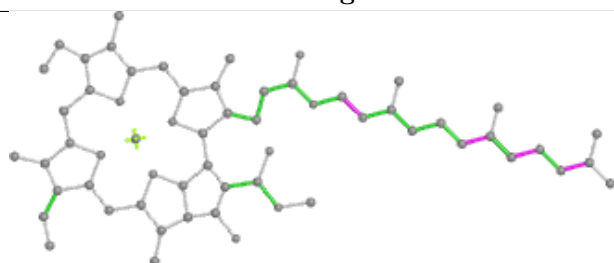
## Ligand CLA 1 612



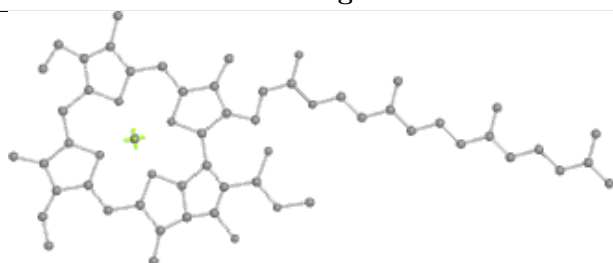
Bond lengths



Bond angles

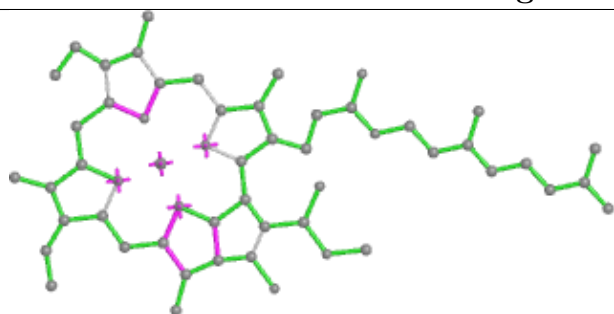


Torsions

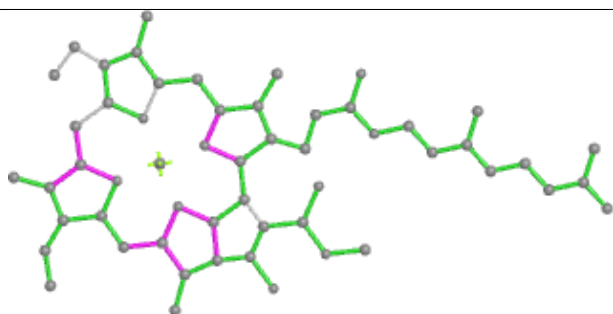


Rings

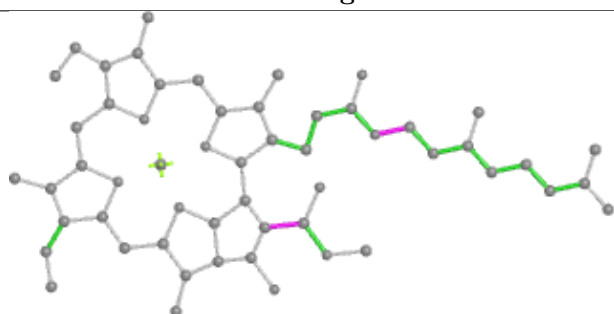
## Ligand CLA Z 304



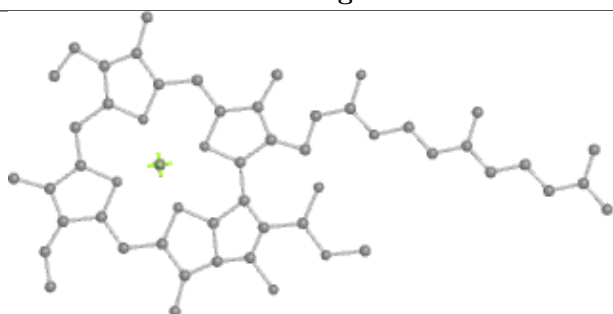
Bond lengths



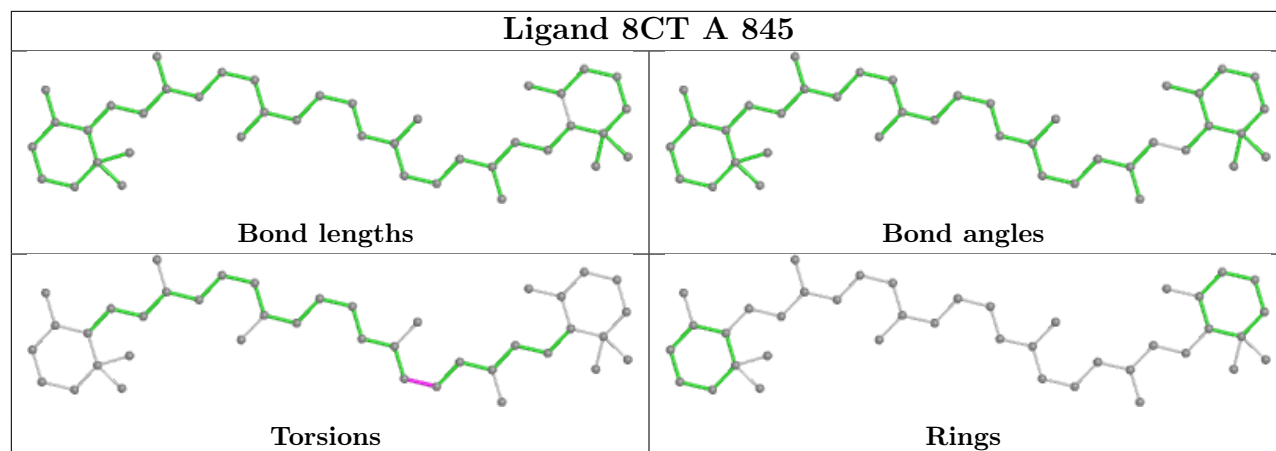
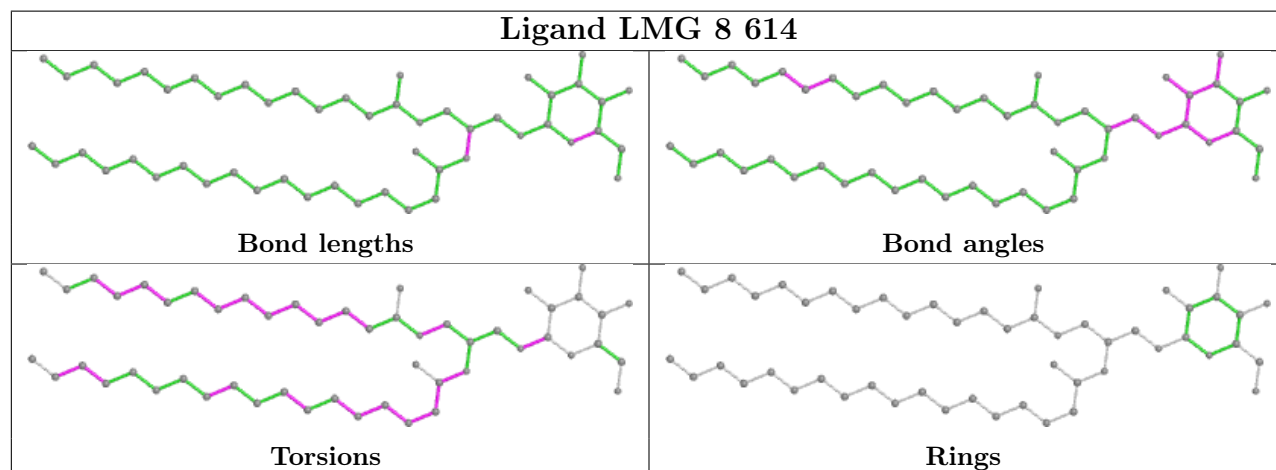
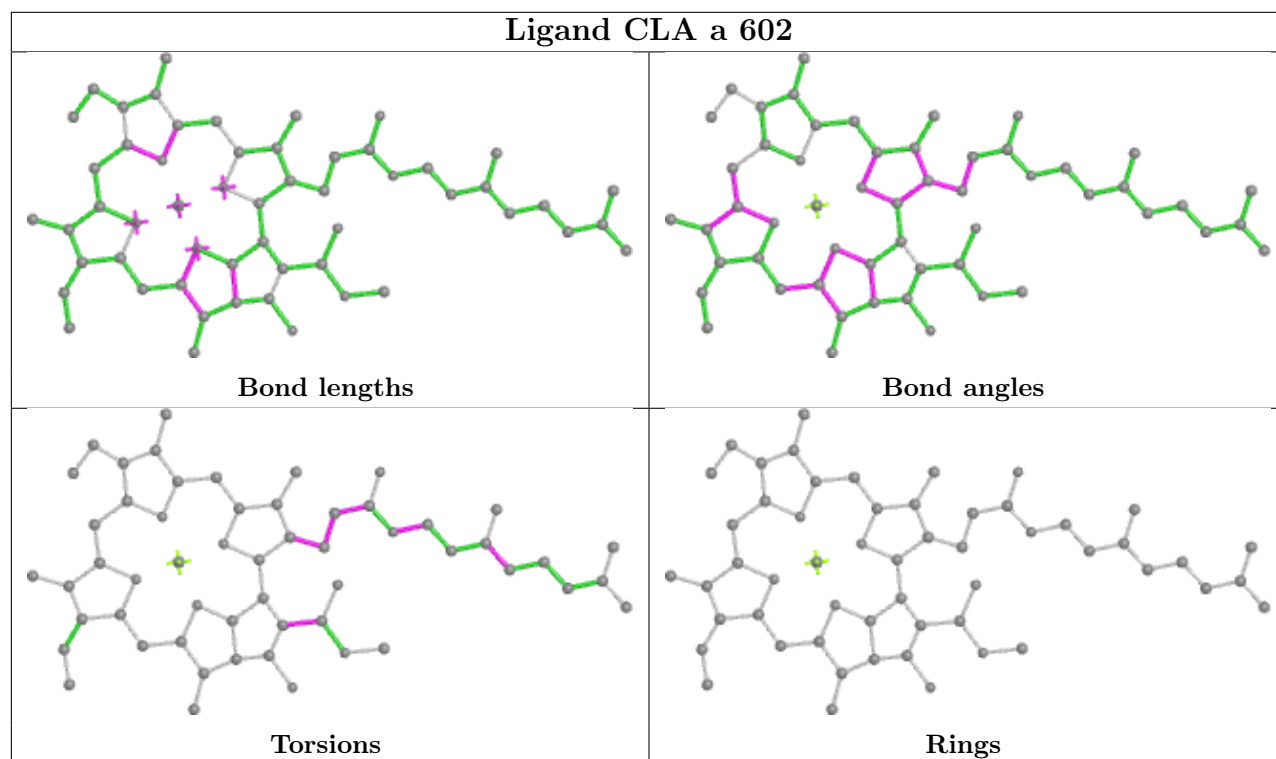
Bond angles



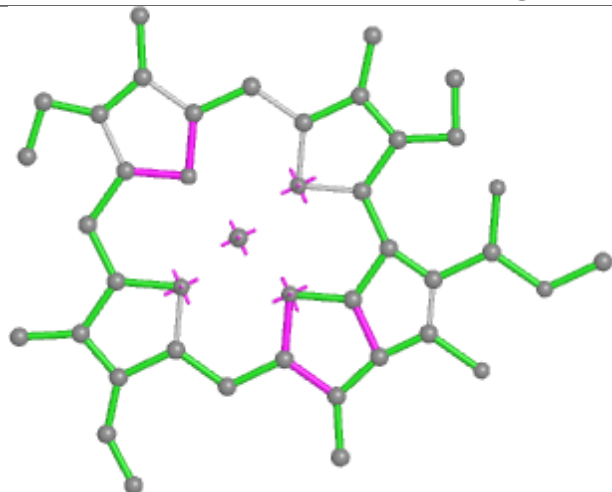
Torsions



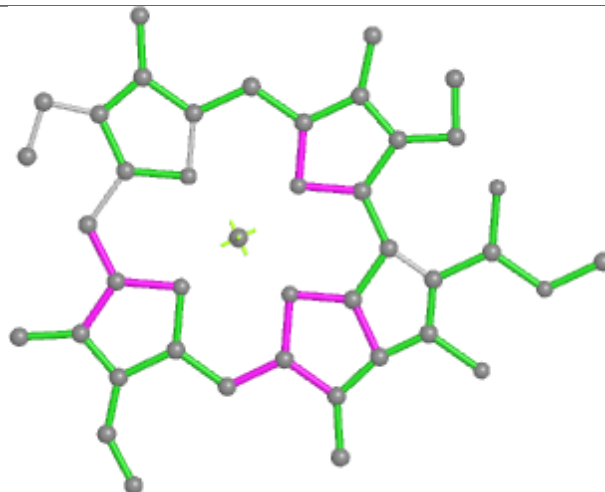
Rings

**Ligand 8CT A 845****Ligand LMG 8 614****Ligand CLA a 602**

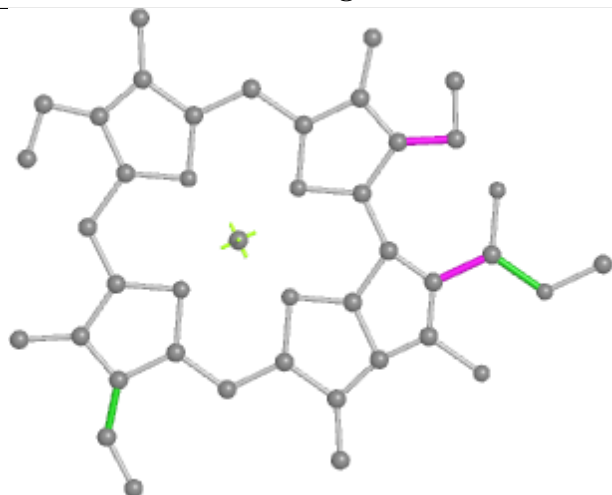
## Ligand CLA B 814



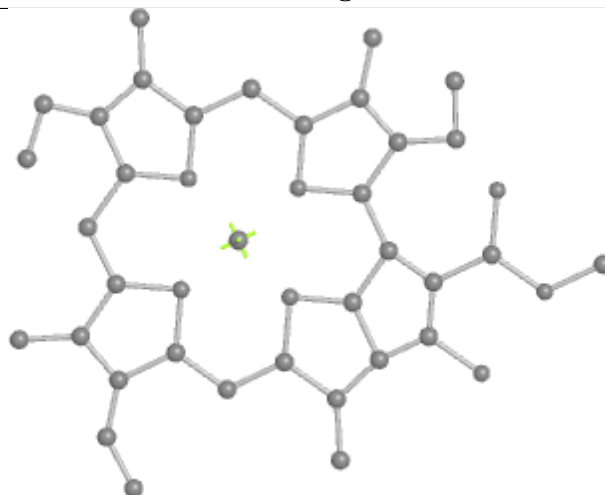
Bond lengths



Bond angles

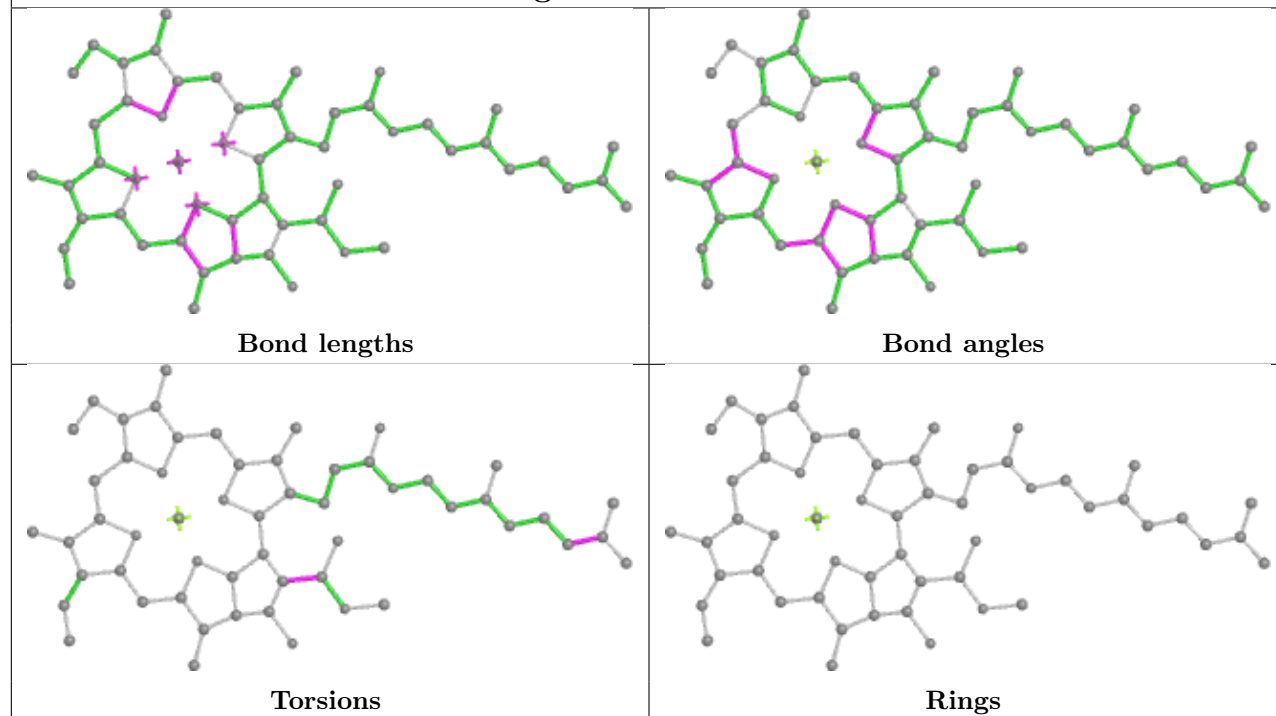


Torsions

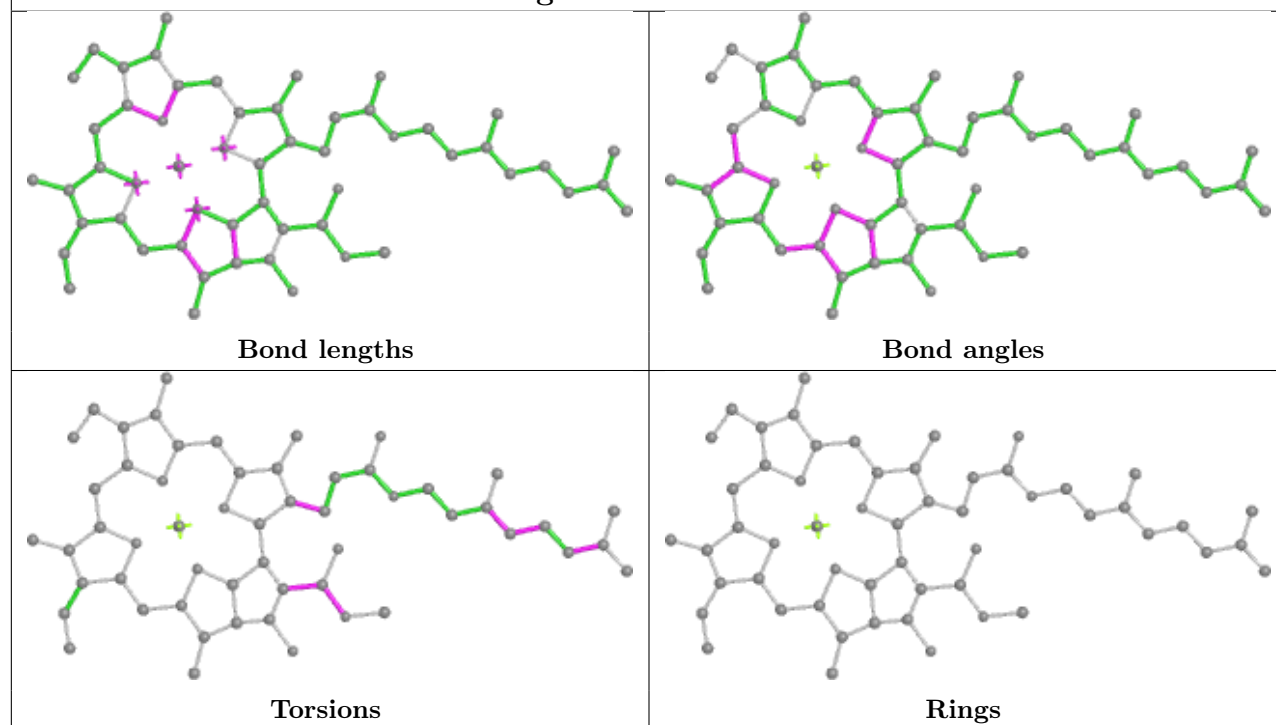


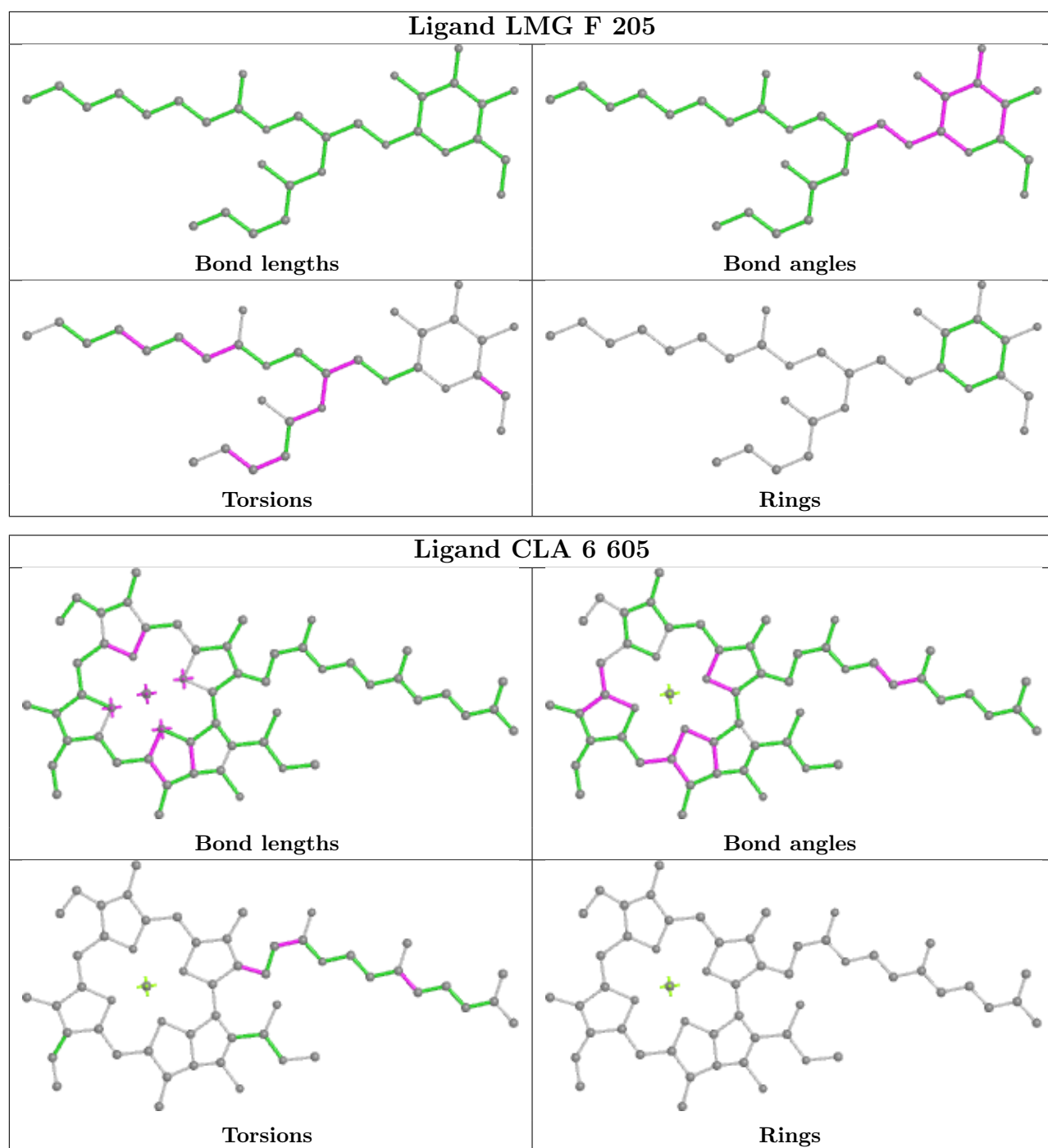
Rings

## Ligand CLA F 204



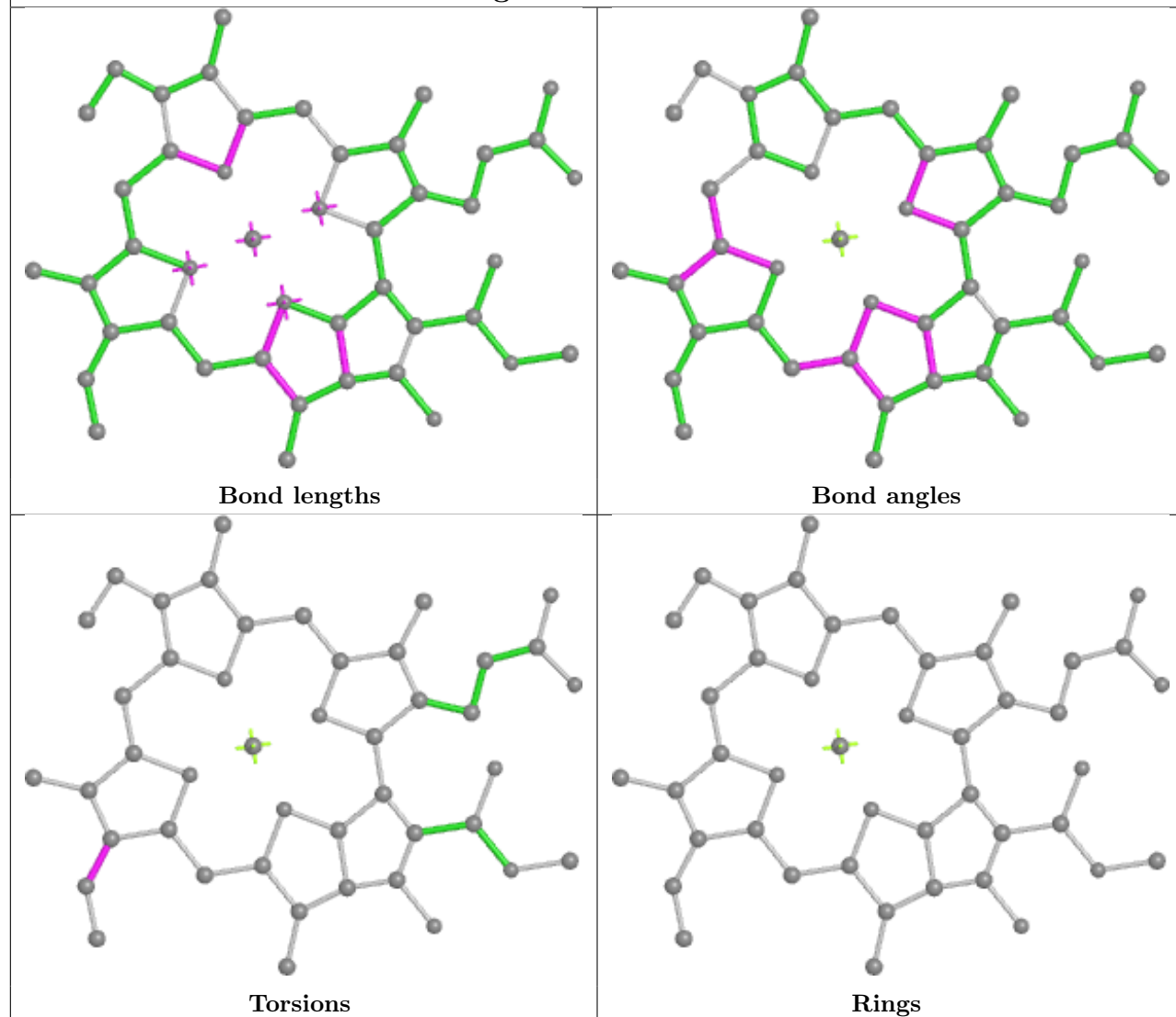
## Ligand CLA 5 604

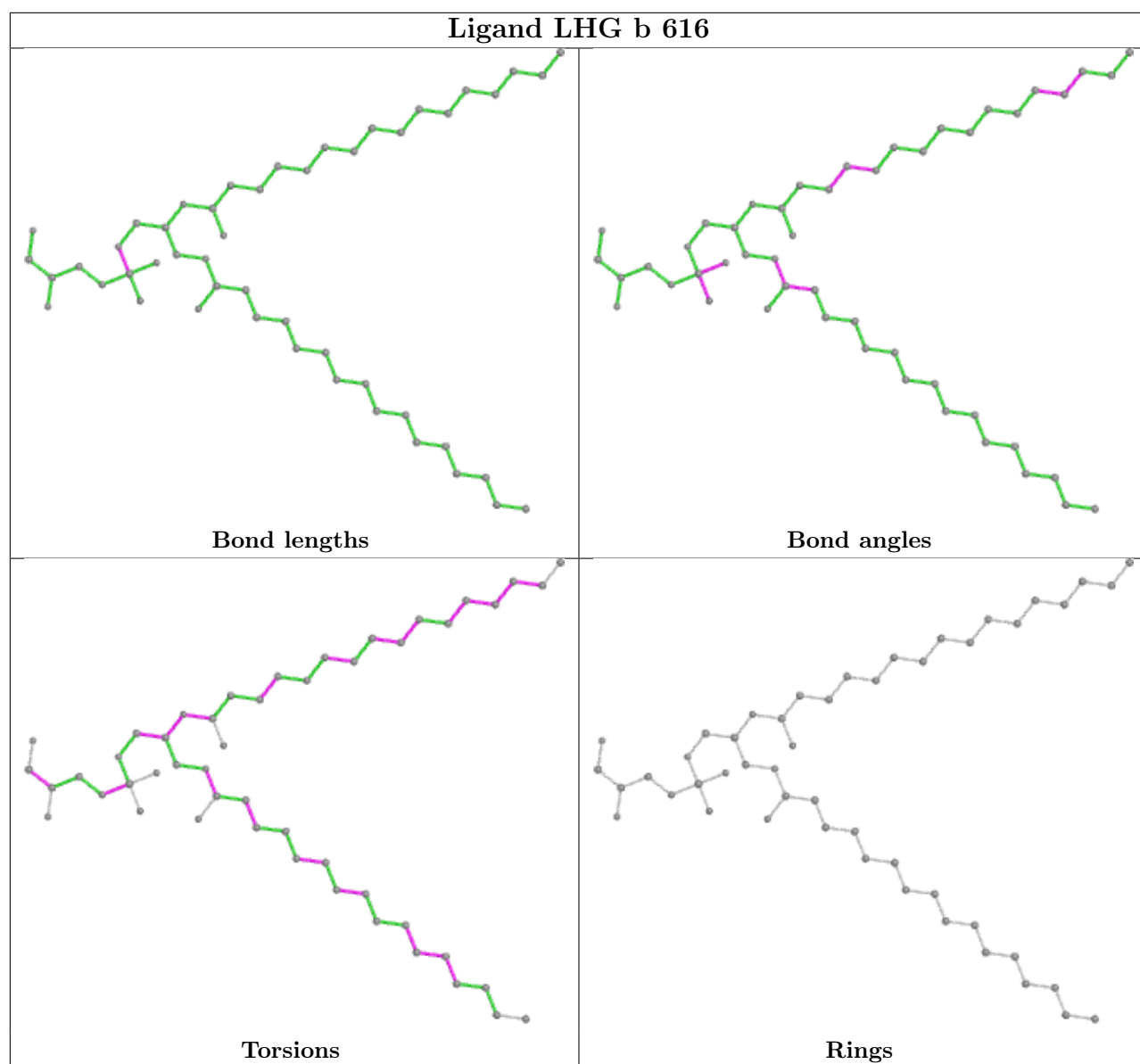




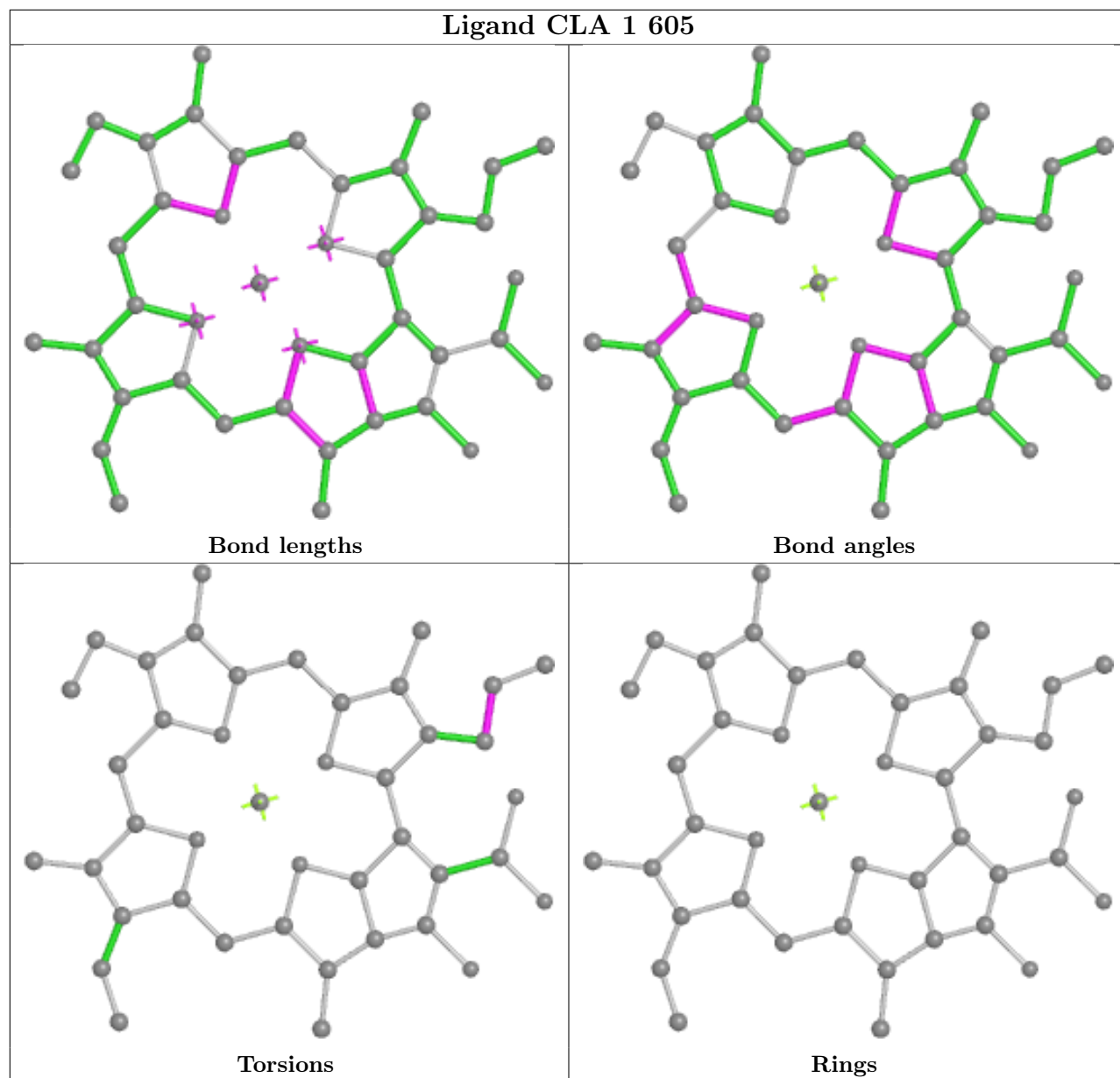


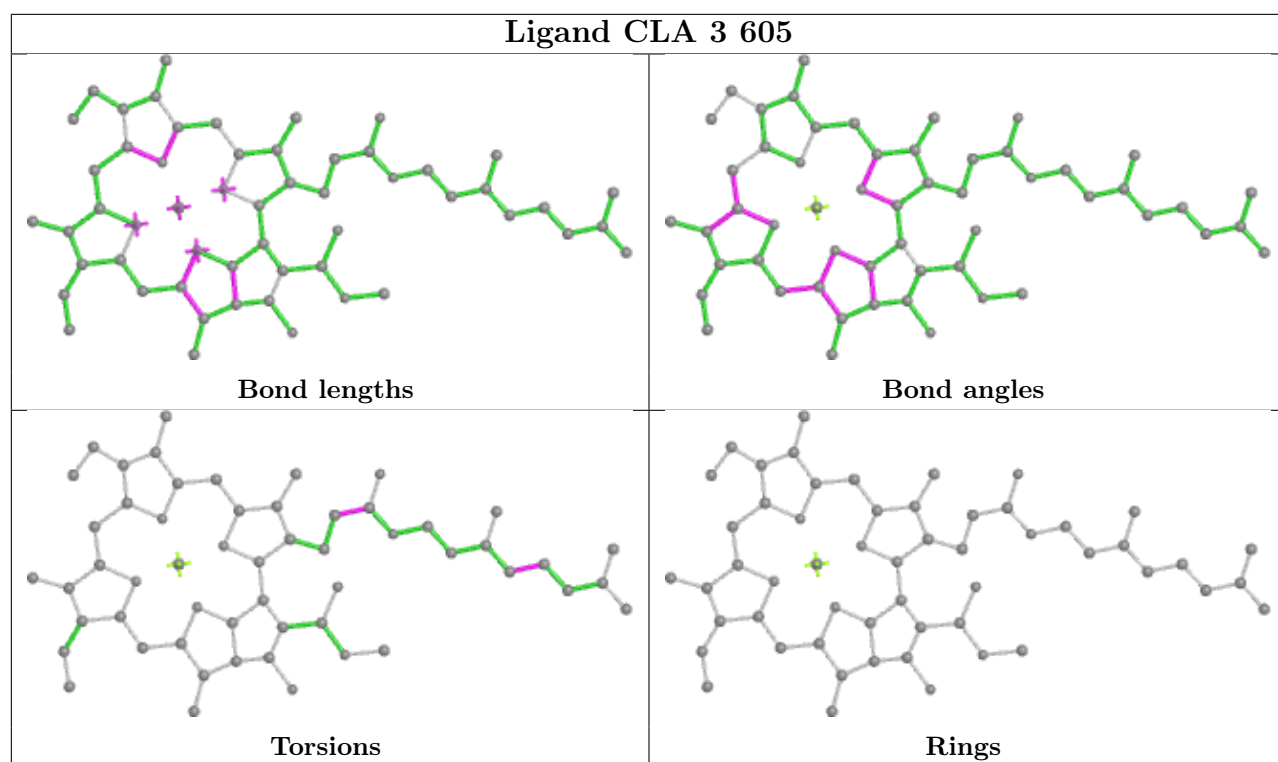
## Ligand CLA 6 601



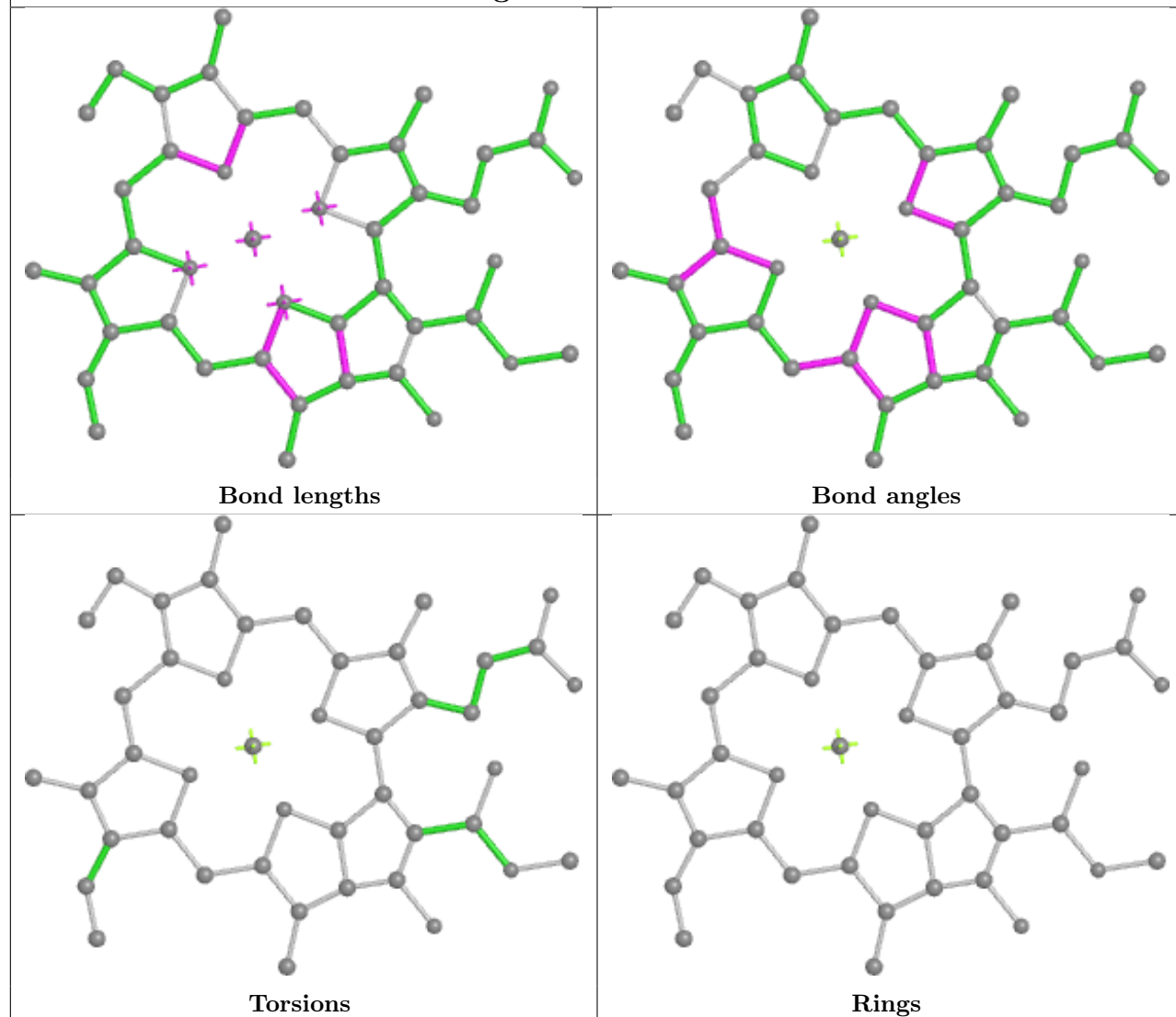


## Ligand CLA 1 605

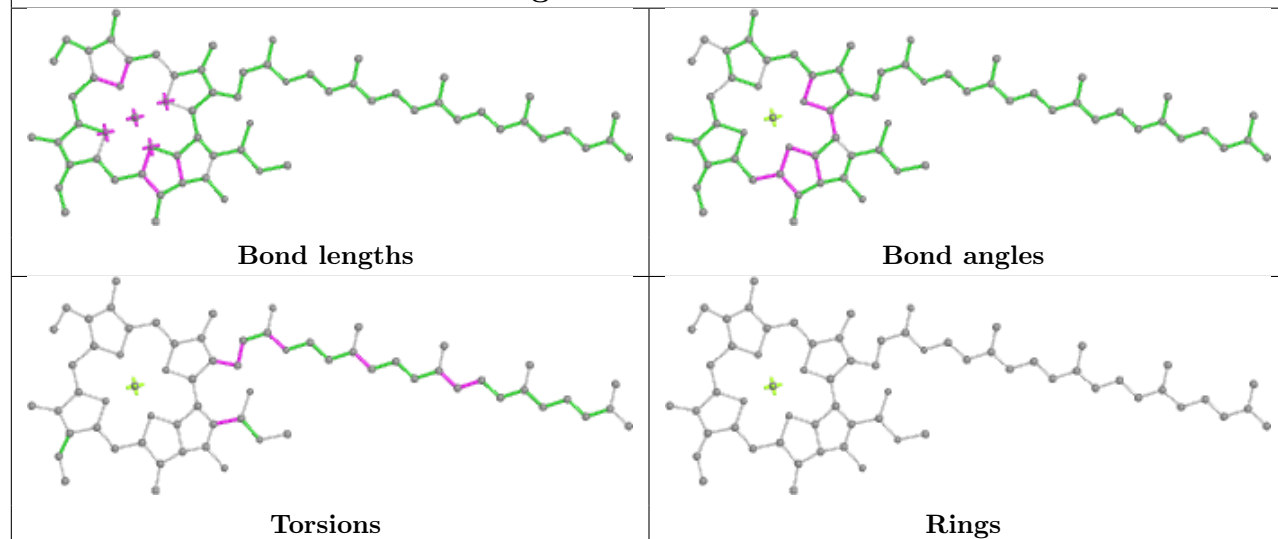




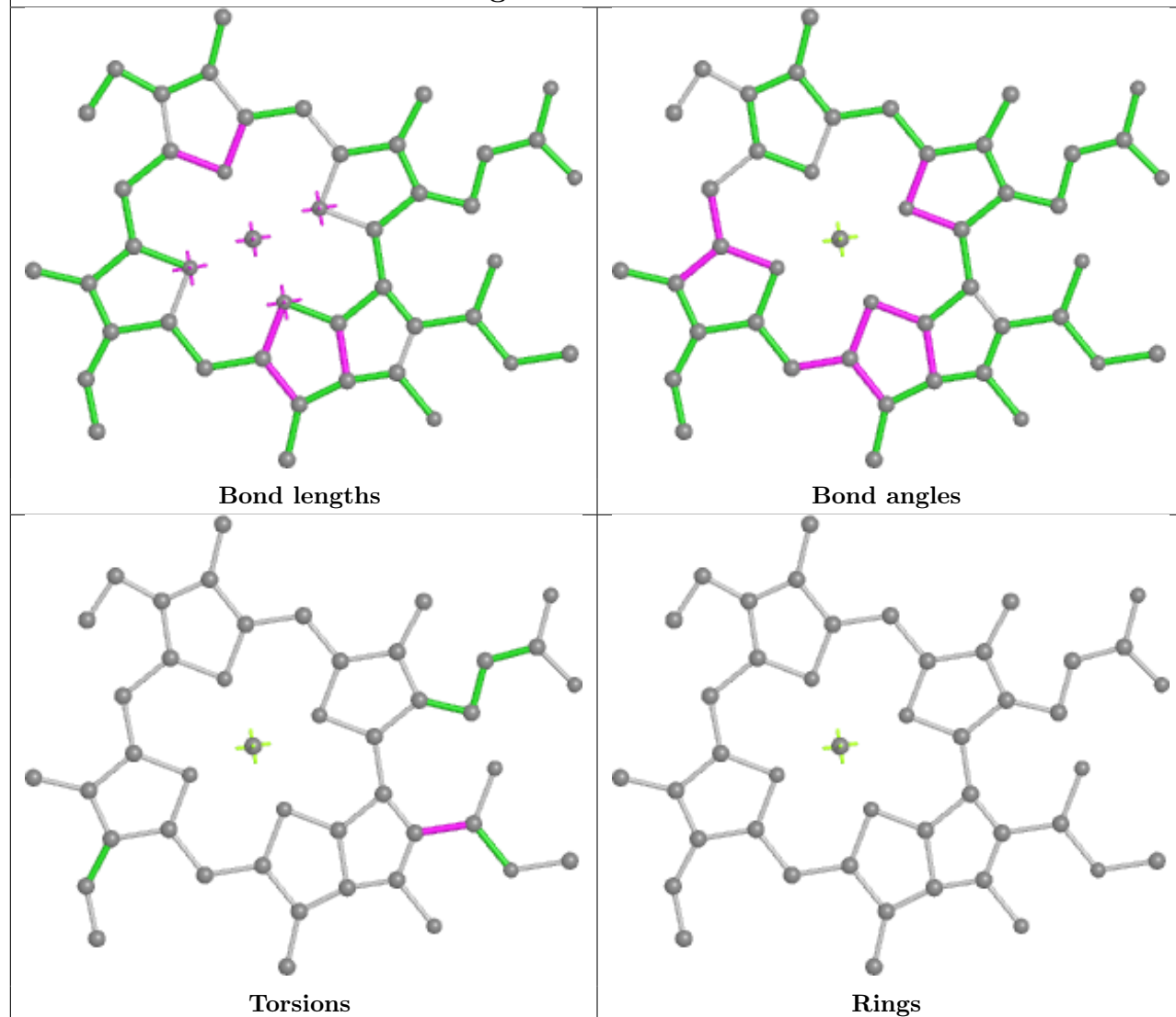
## Ligand CLA 2 607



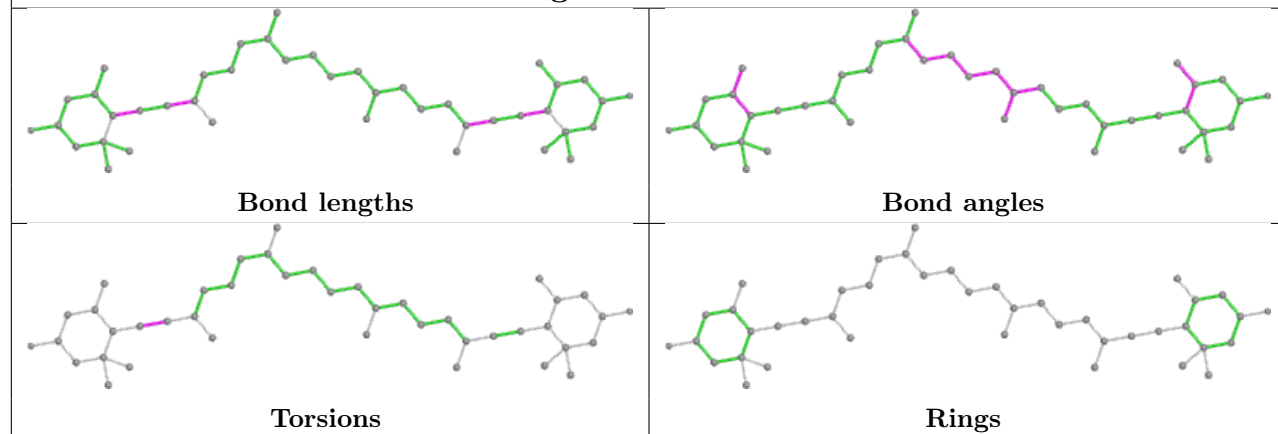
## Ligand CLA A 843

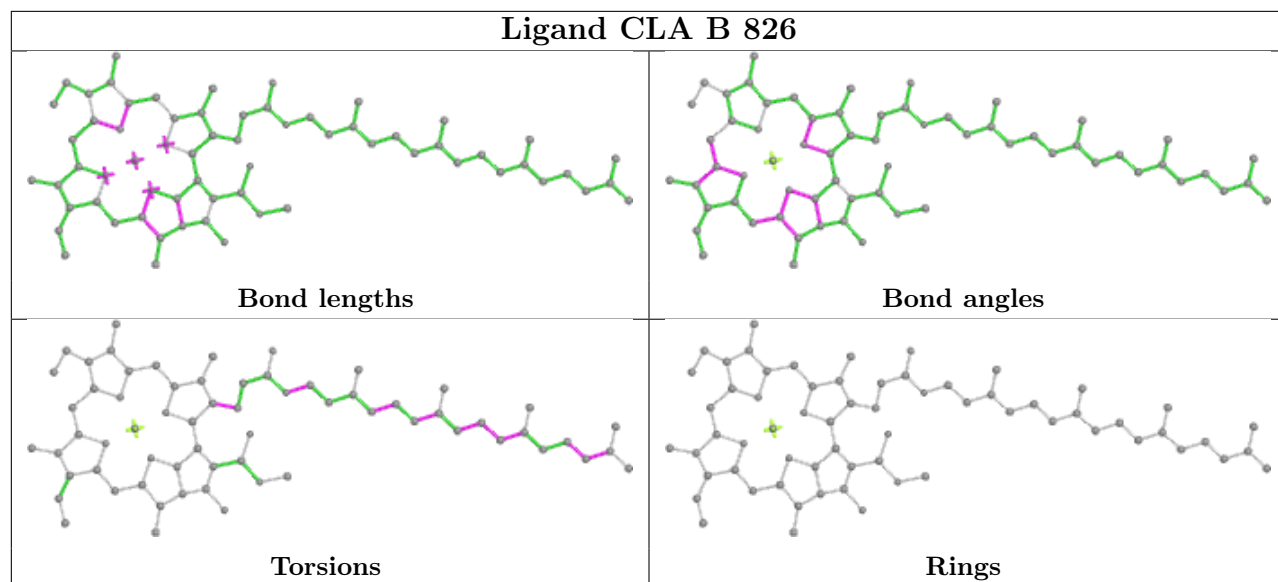
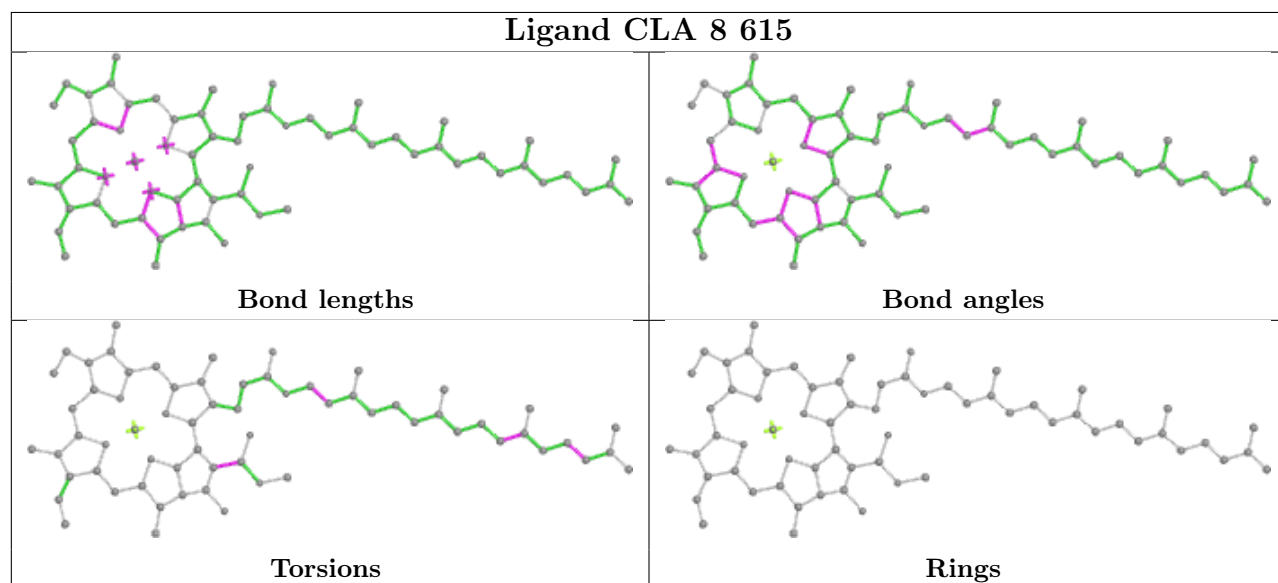


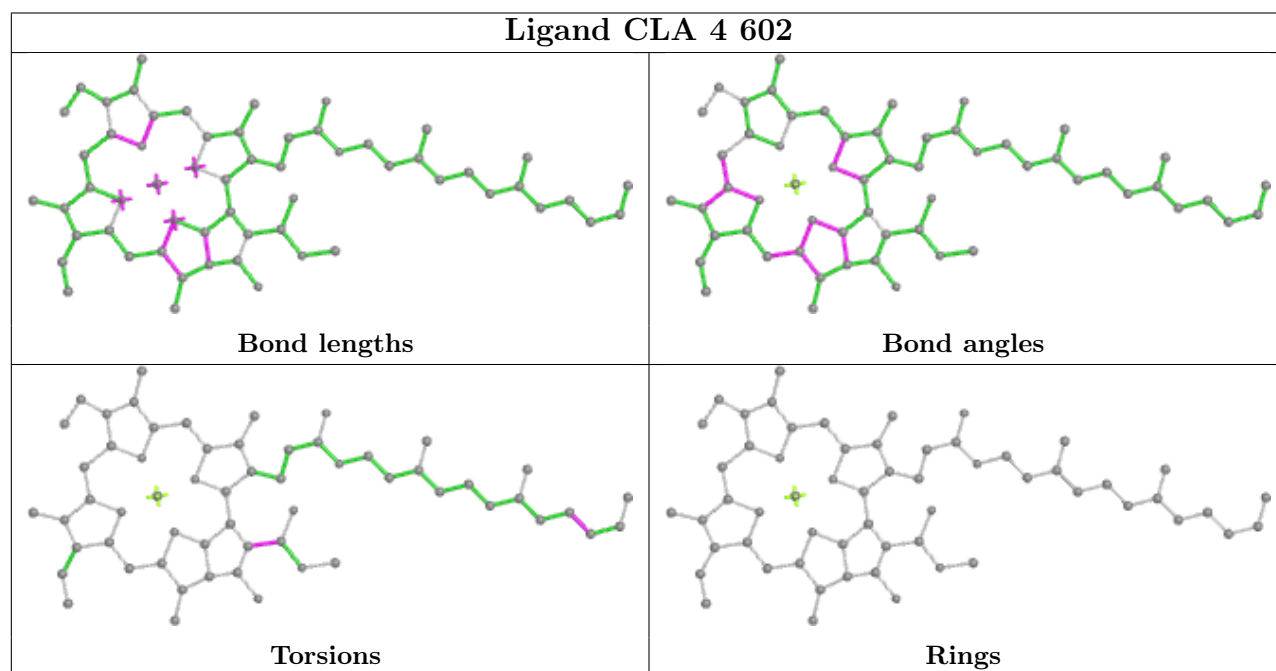
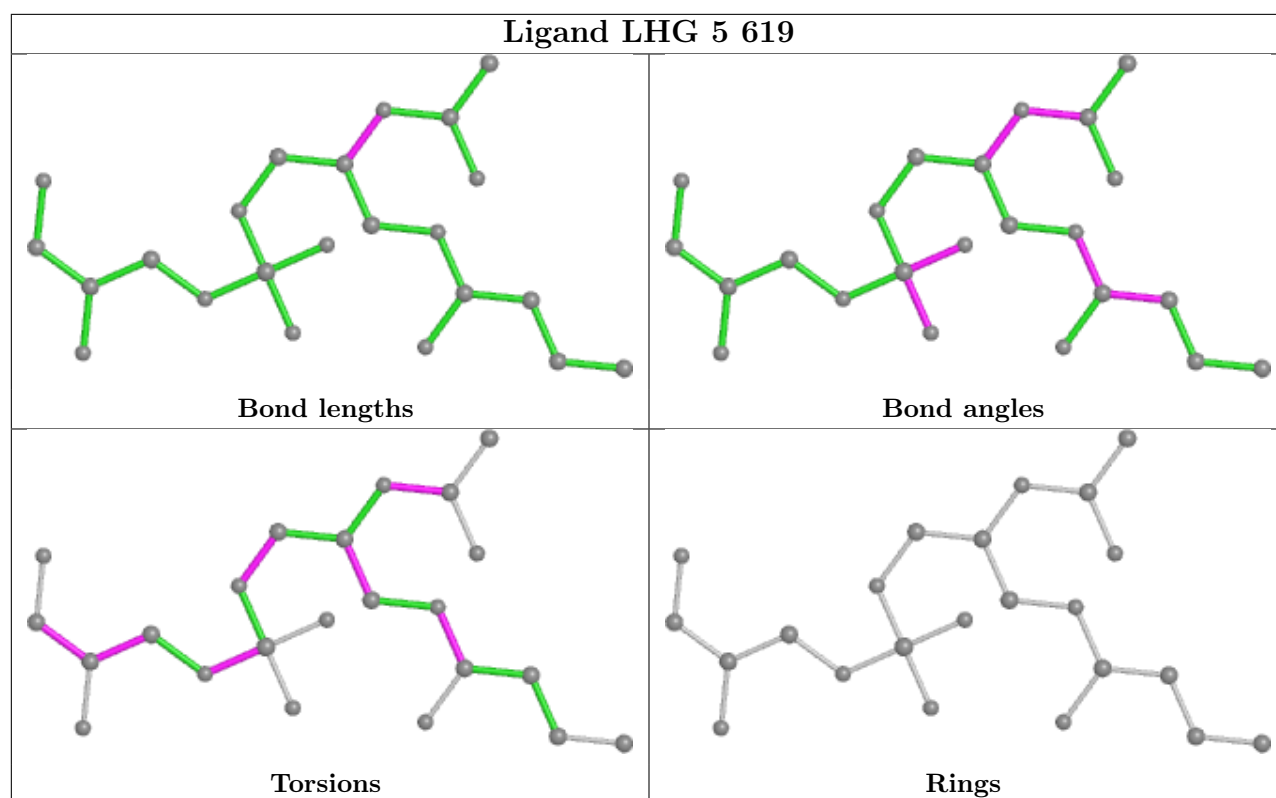
## Ligand CLA B 833



## Ligand II0 8 612

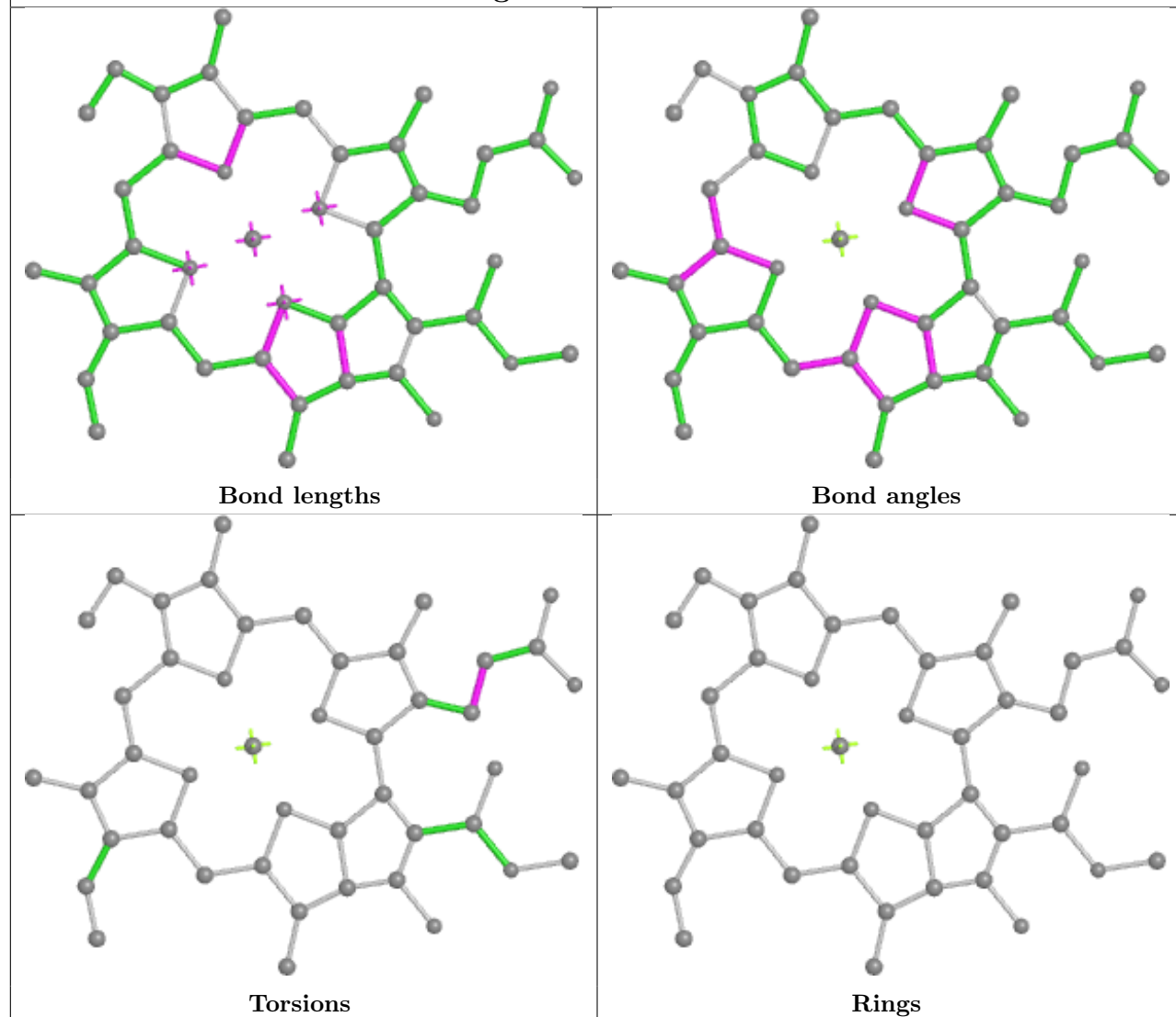


**Ligand CLA B 826****Ligand CLA 8 615**

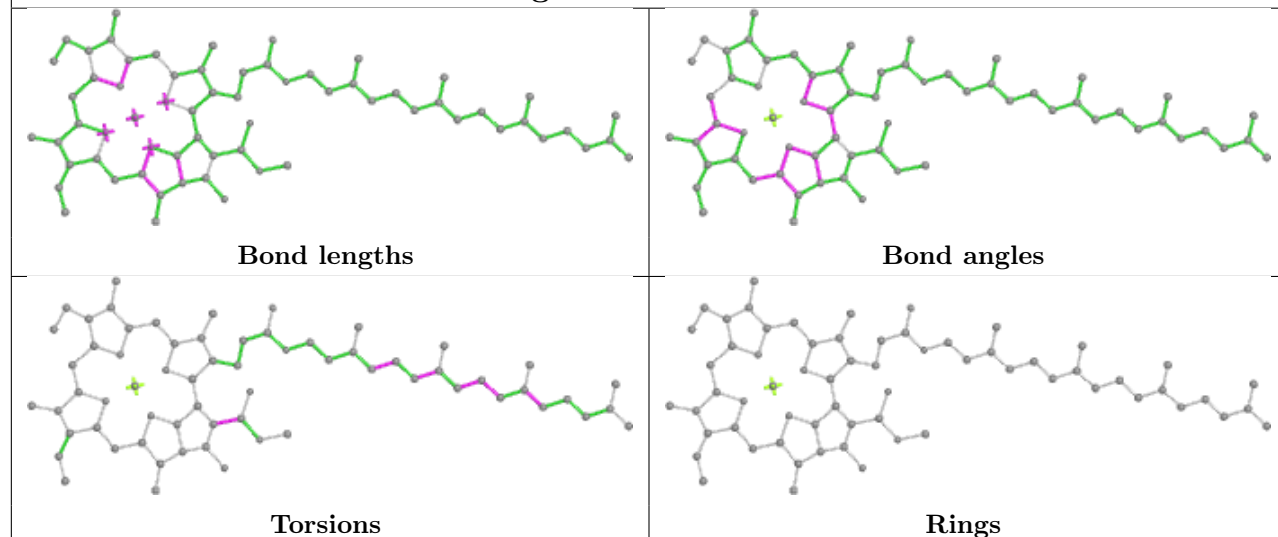




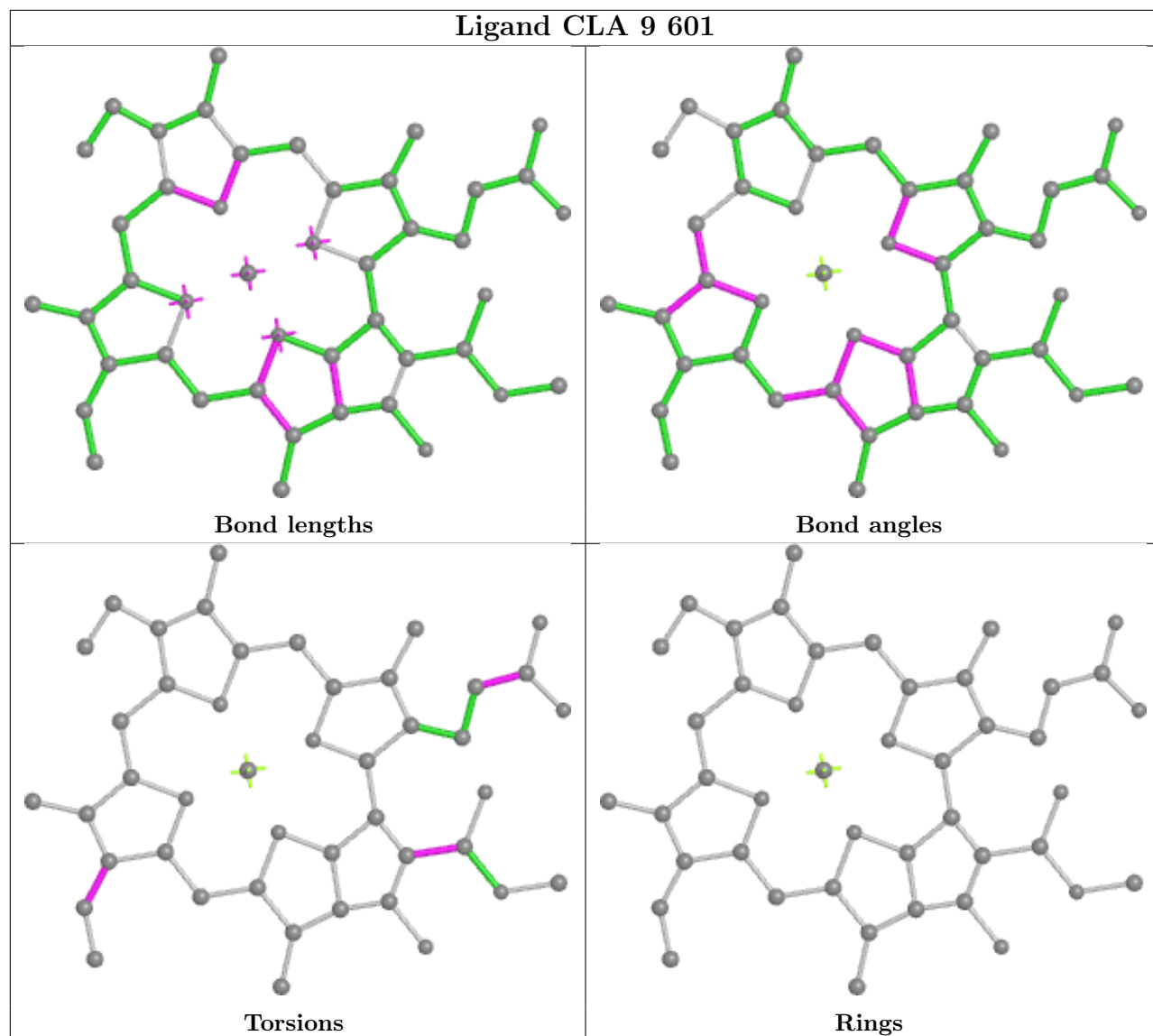
## Ligand CLA 9 613



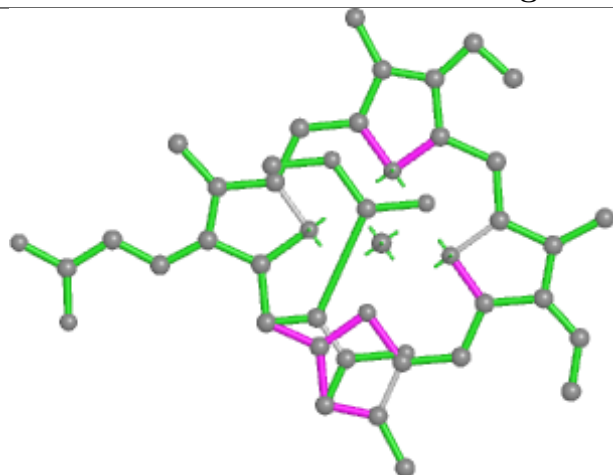
## Ligand CLA A 806



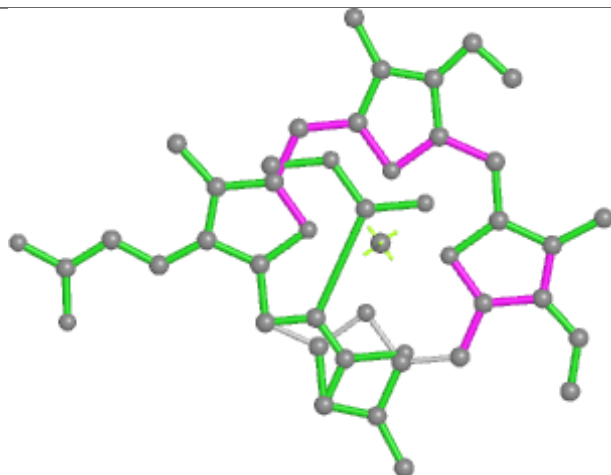
## Ligand CLA 9 601



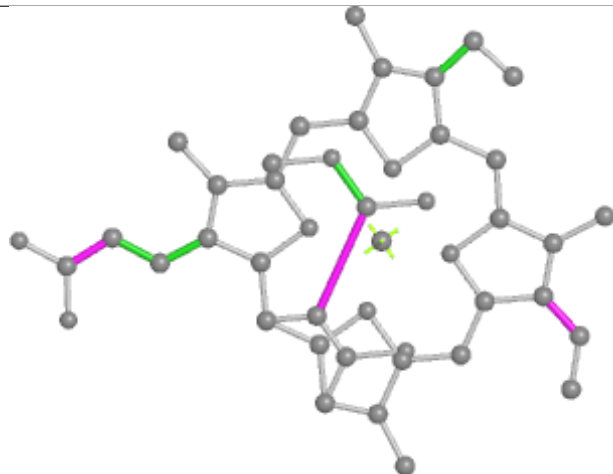
## Ligand KC2 9 610



Bond lengths



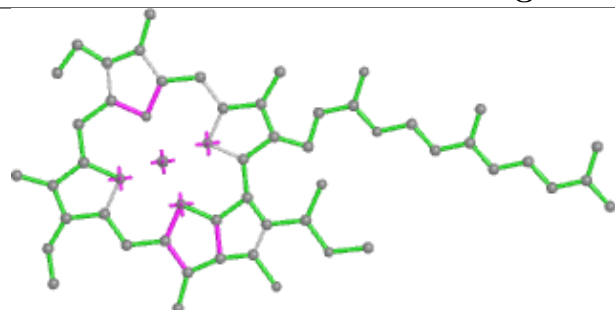
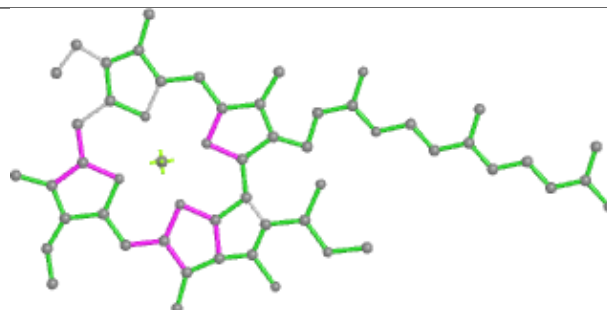
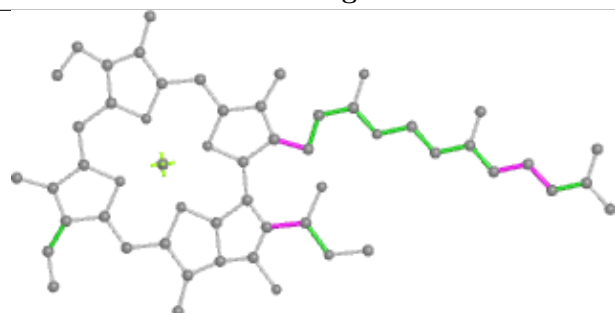
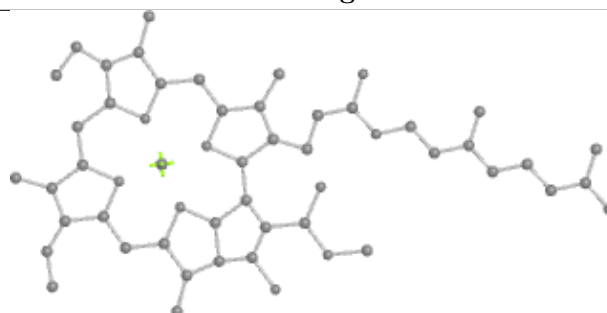
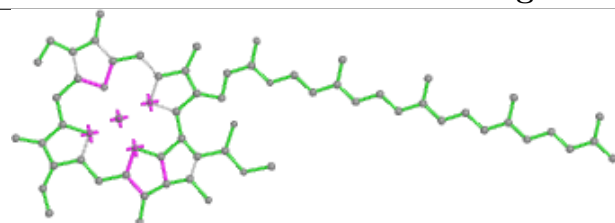
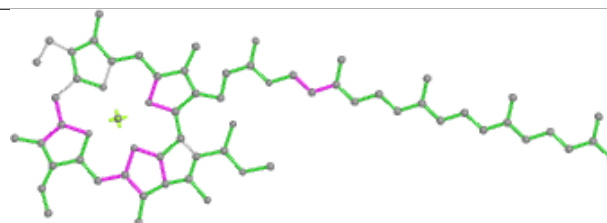
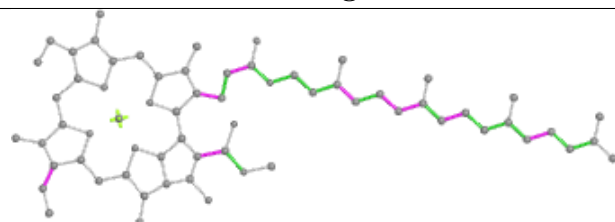
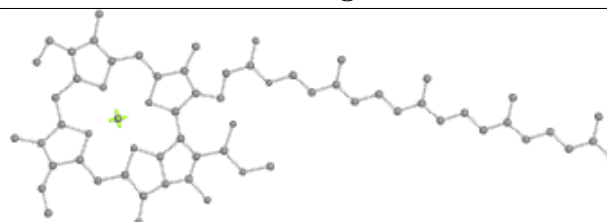
Bond angles



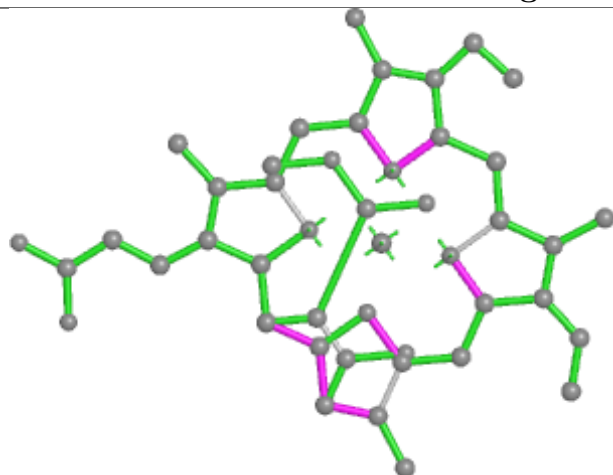
Torsions



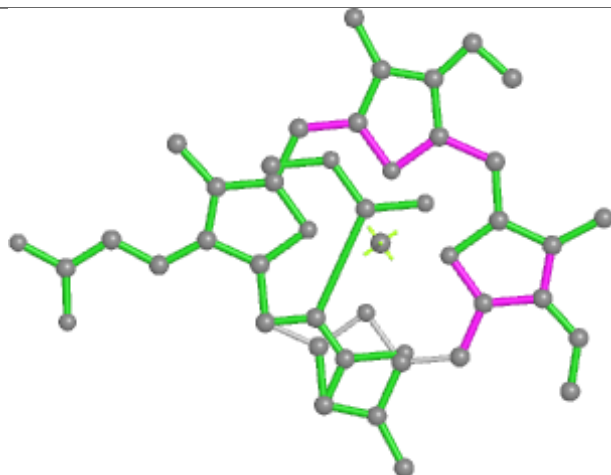
Rings

**Ligand CLA O 203****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 812****Bond lengths****Bond angles****Torsions****Rings**

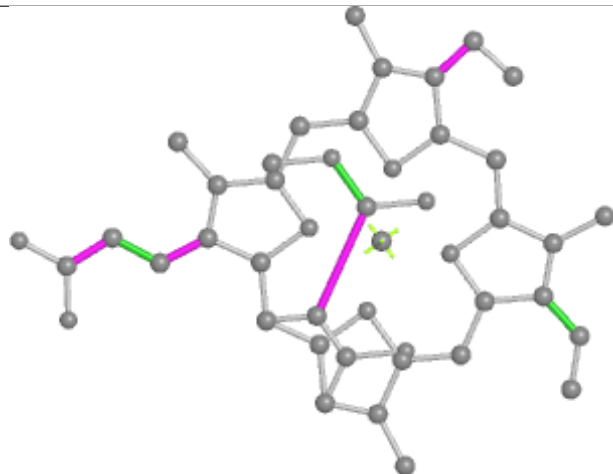
## Ligand KC2 1 610



Bond lengths



Bond angles

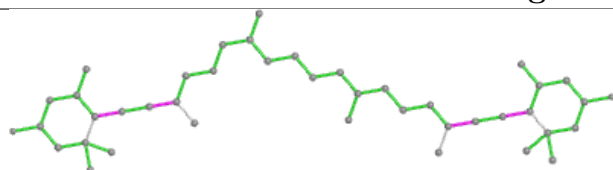


Torsions

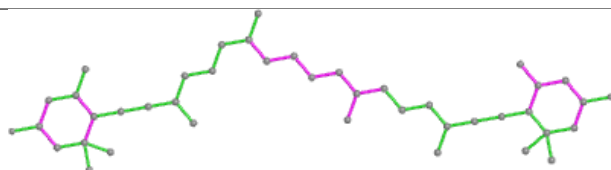


Rings

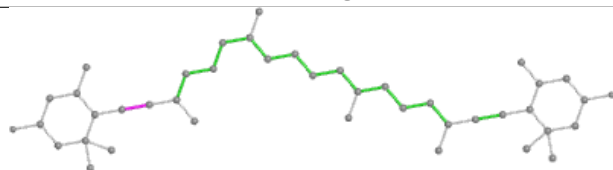
## Ligand II0 O 206



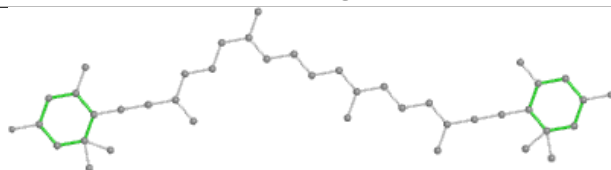
Bond lengths



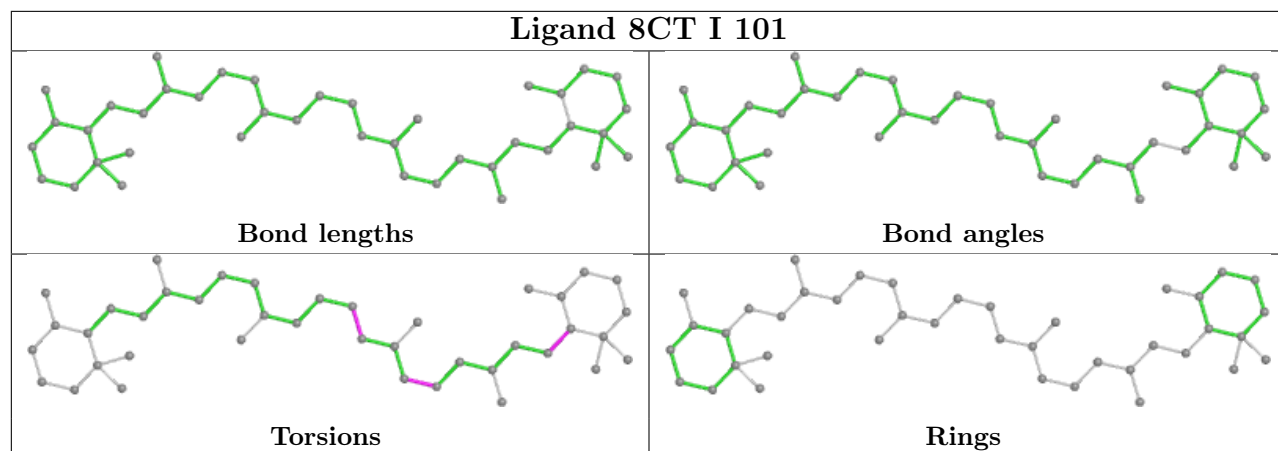
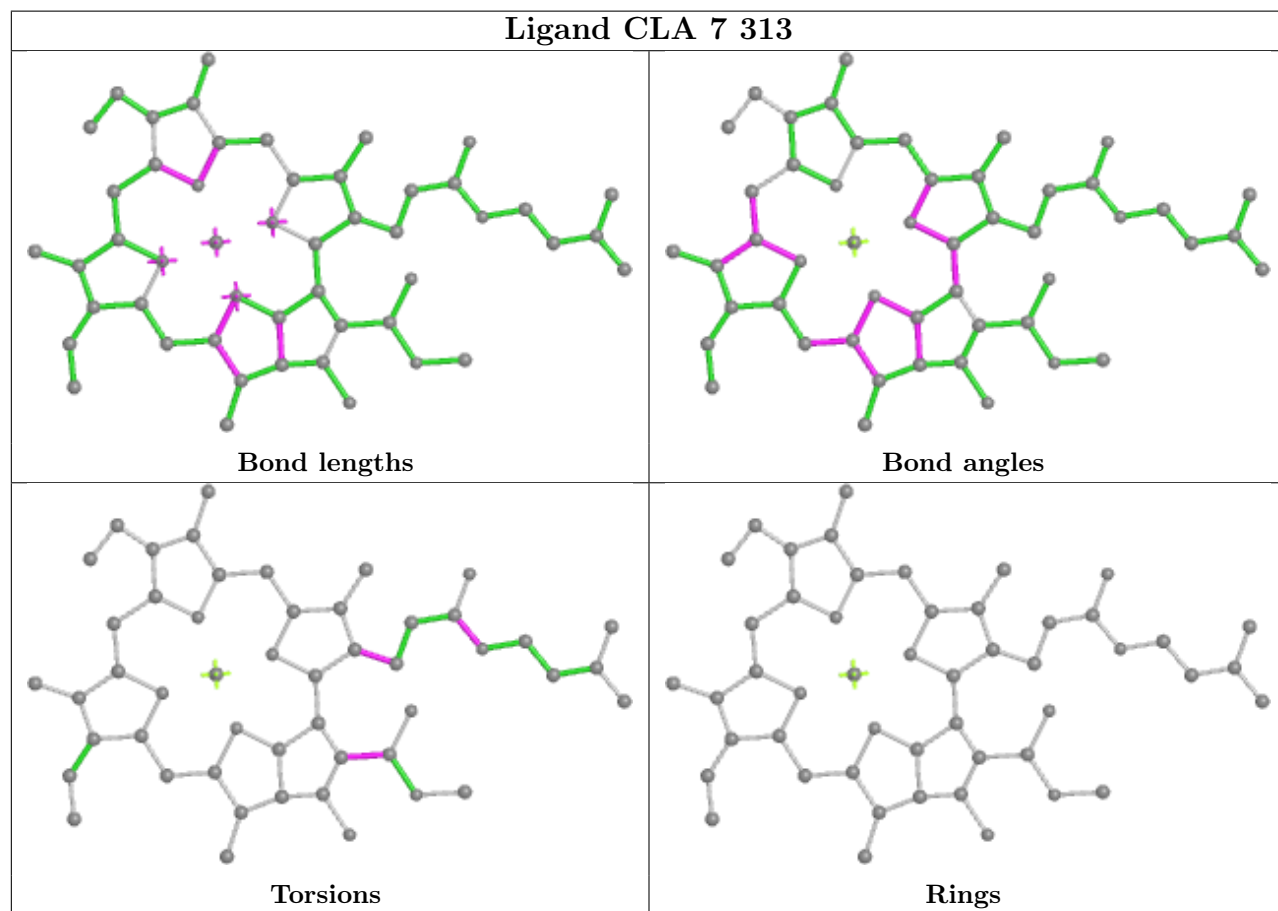
Bond angles



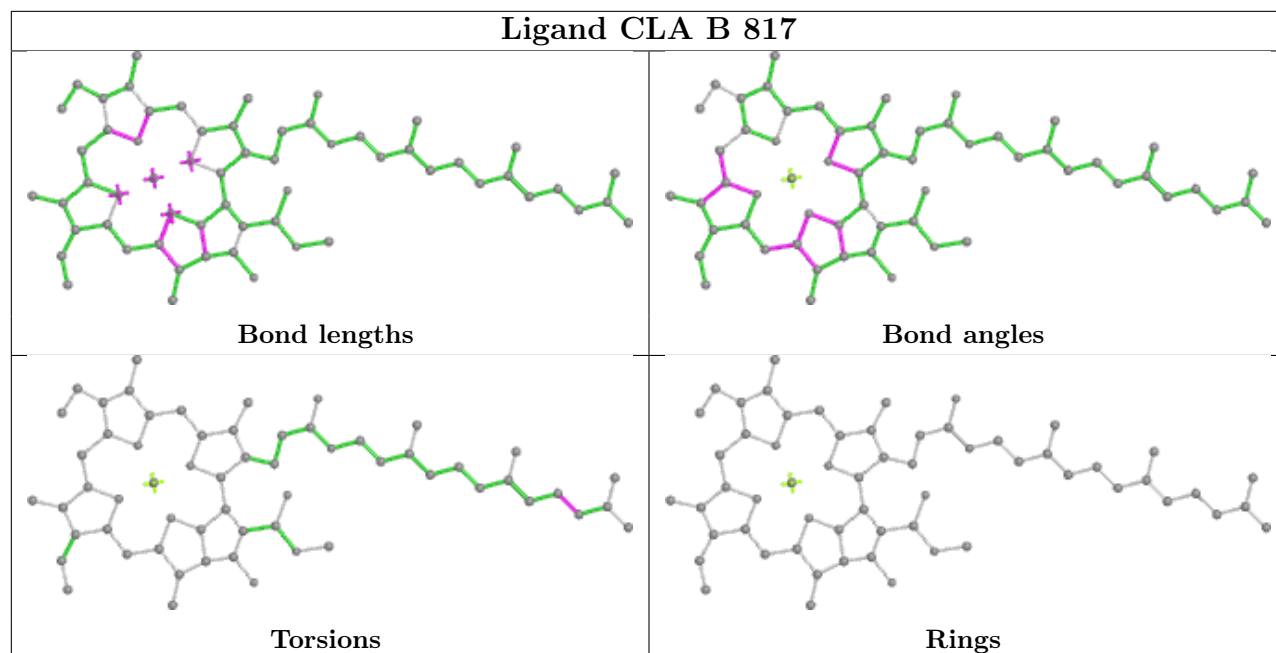
Torsions



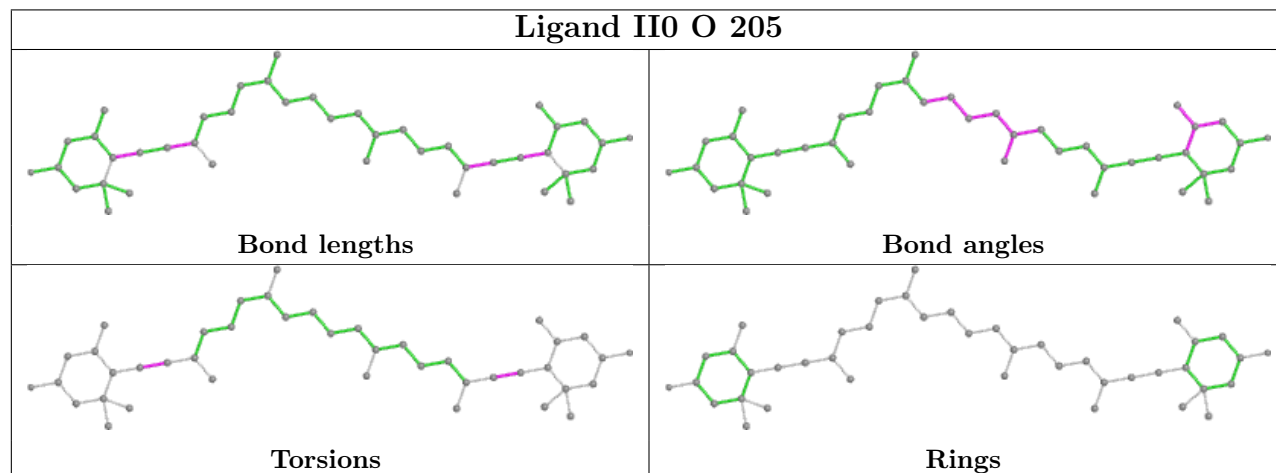
Rings

**Ligand 8CT I 101****Ligand CLA 7 313**

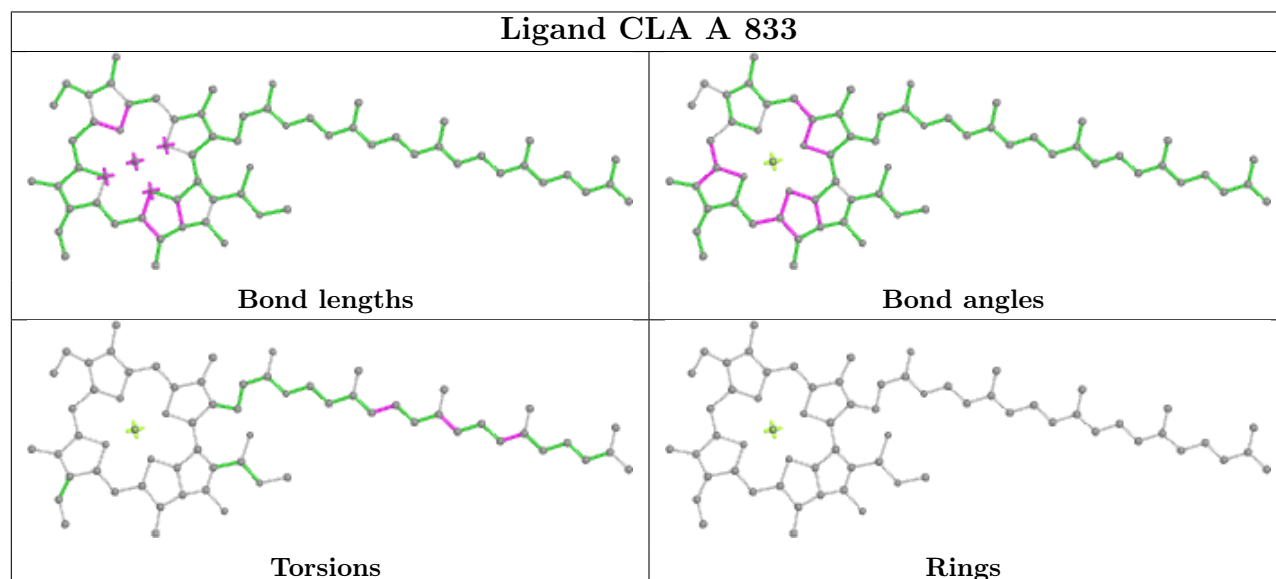
## Ligand CLA B 817

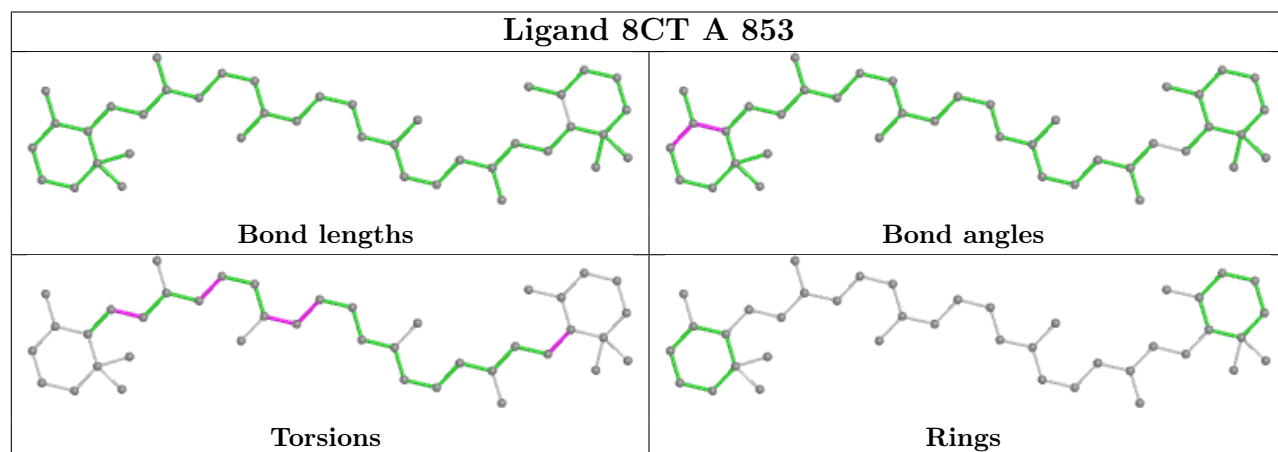
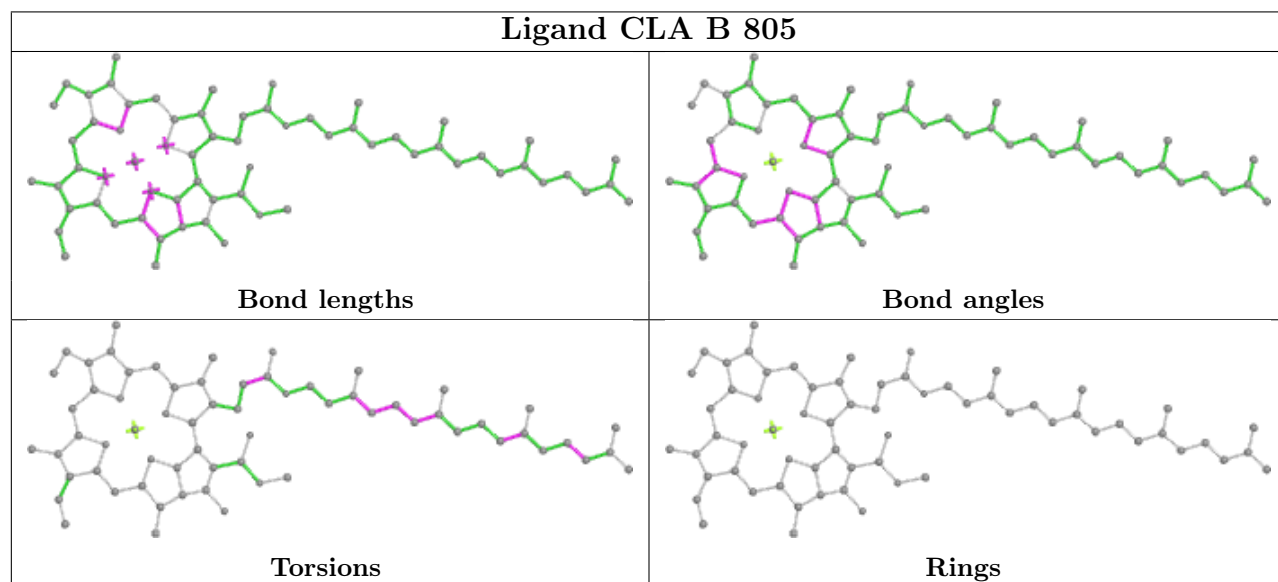
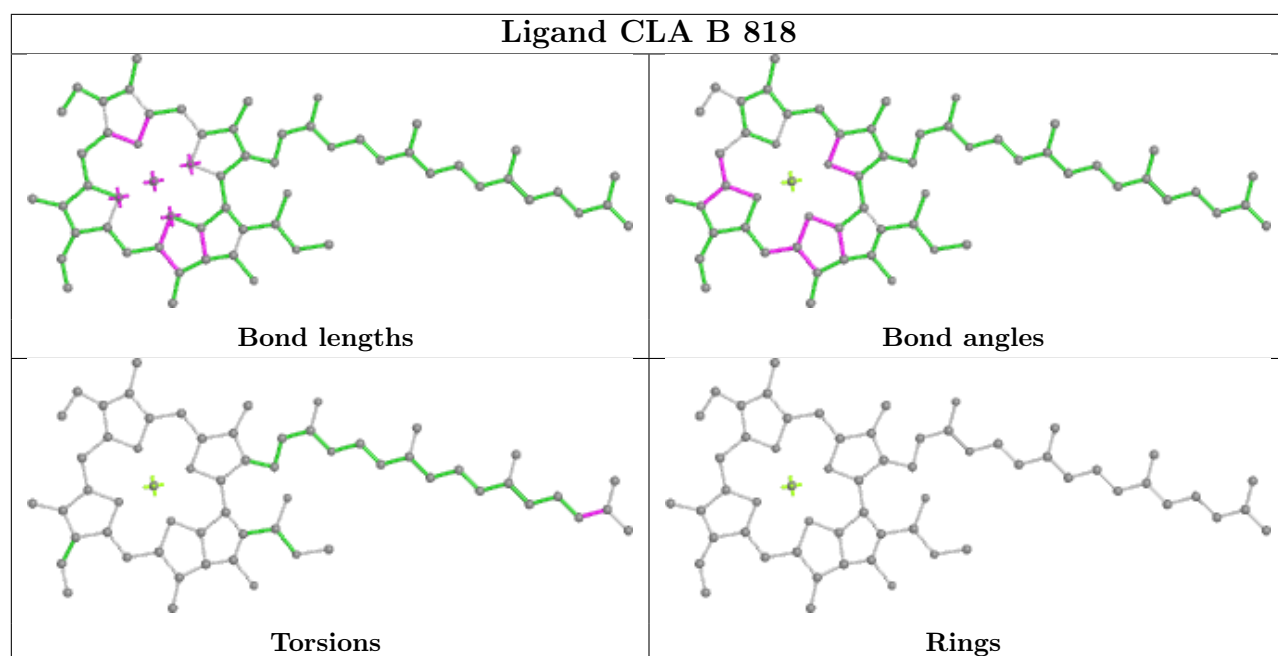


## Ligand II0 O 205

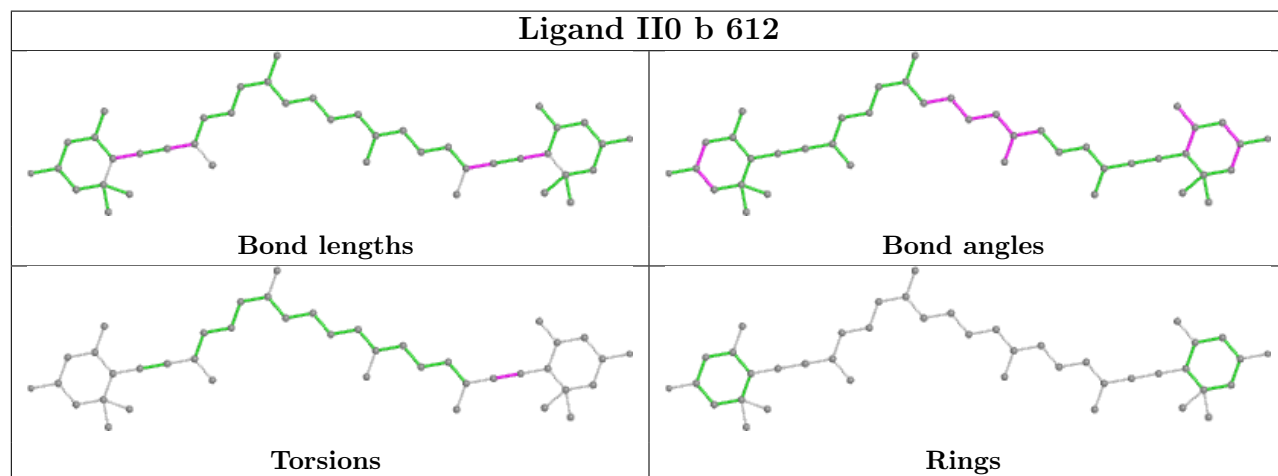
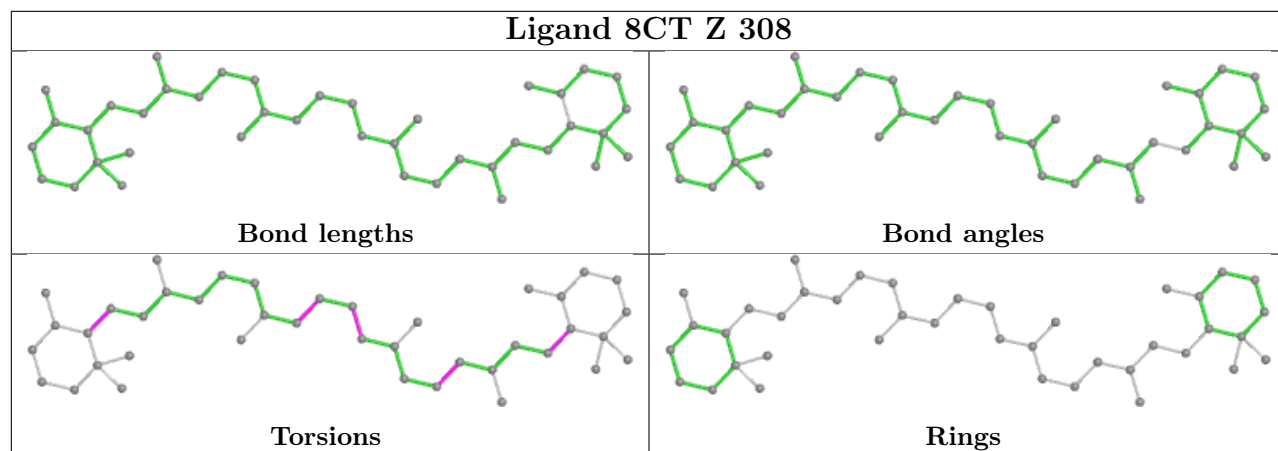


## Ligand CLA A 833

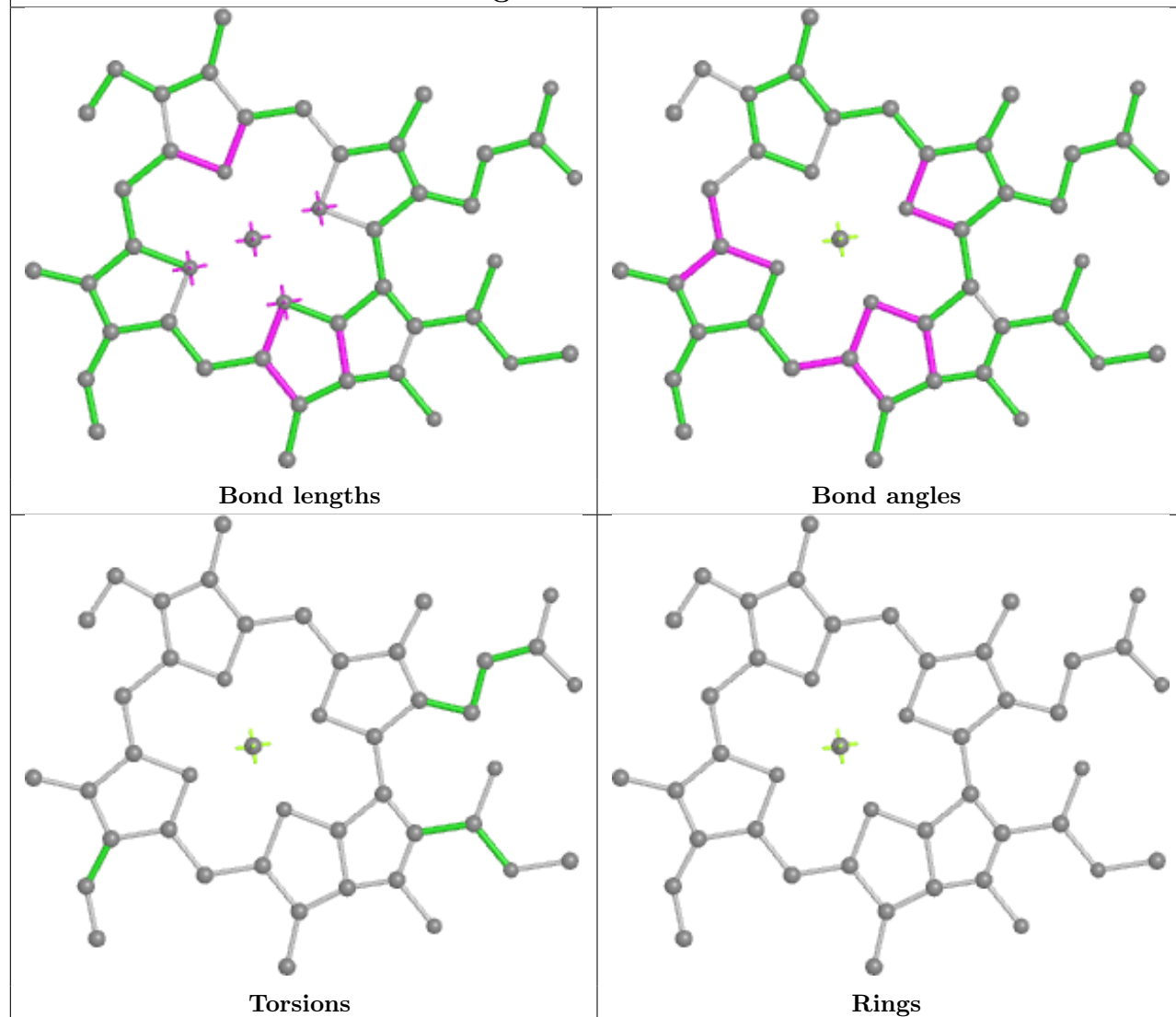




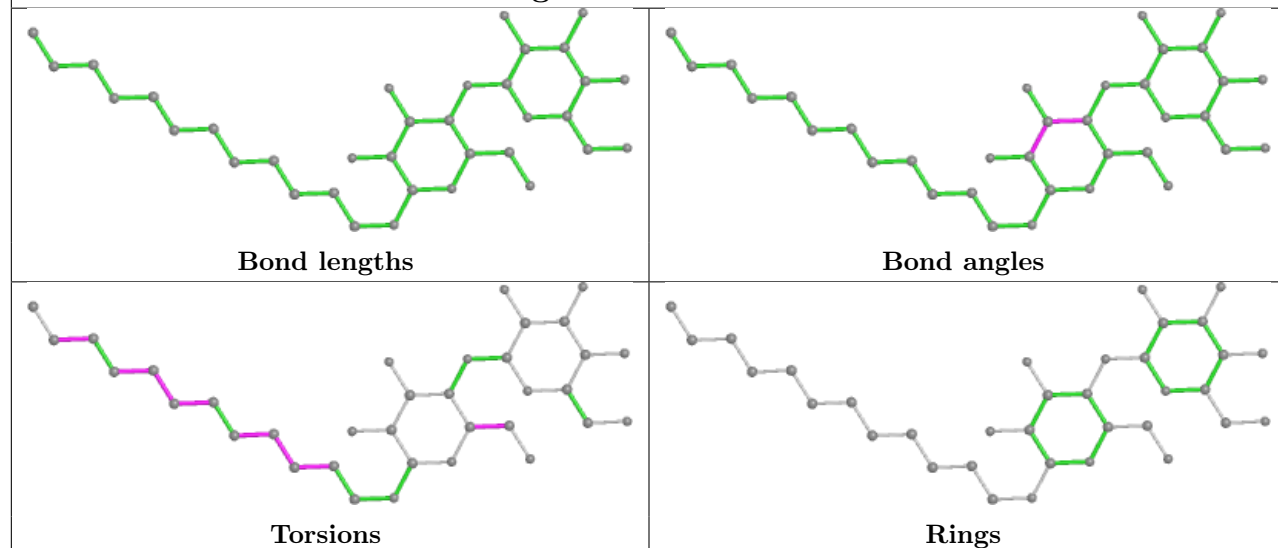




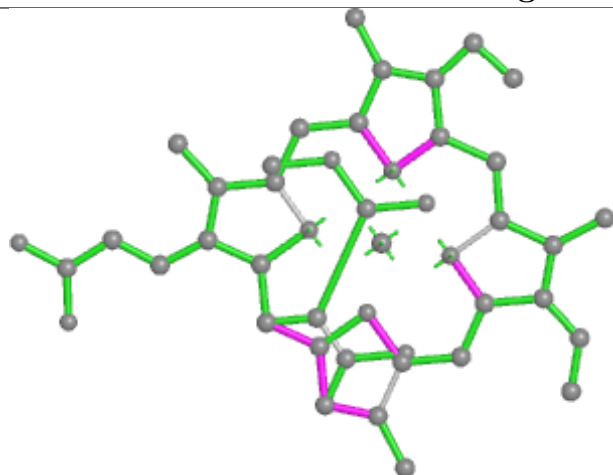
## Ligand CLA 7 302



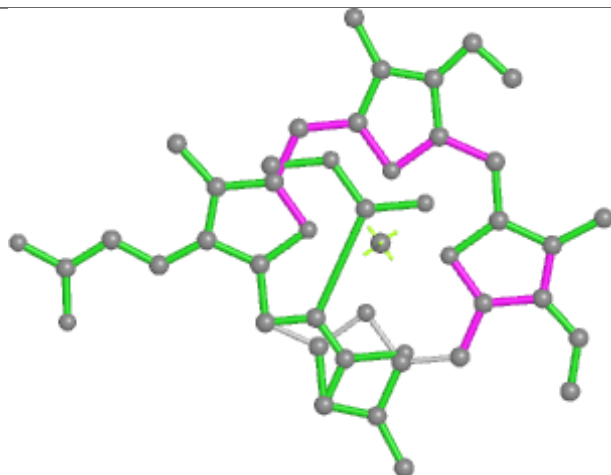
## Ligand LMU 7 321



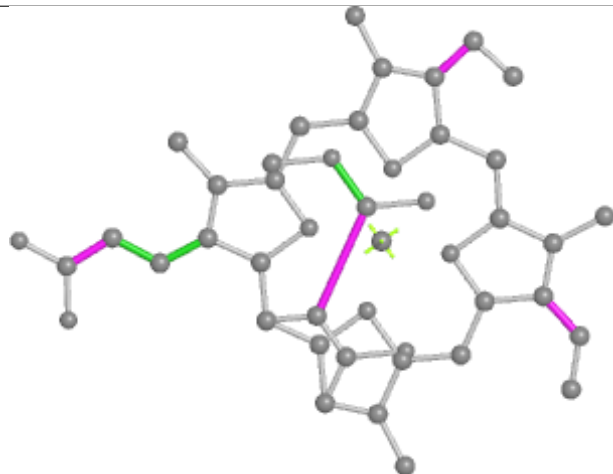
## Ligand KC2 Z 307



Bond lengths



Bond angles

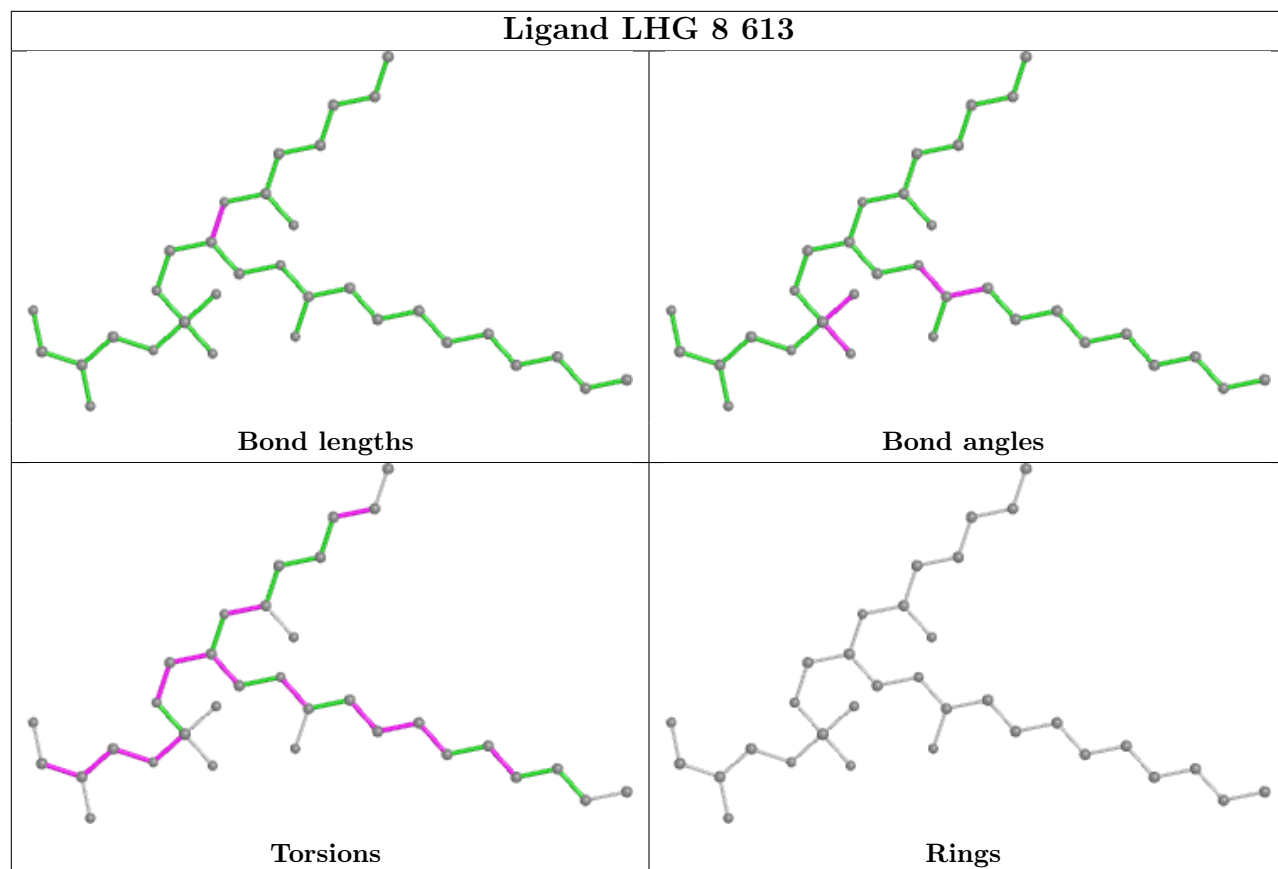


Torsions

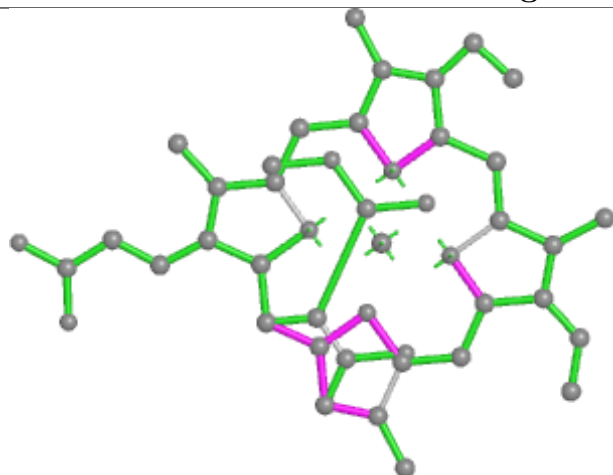


Rings

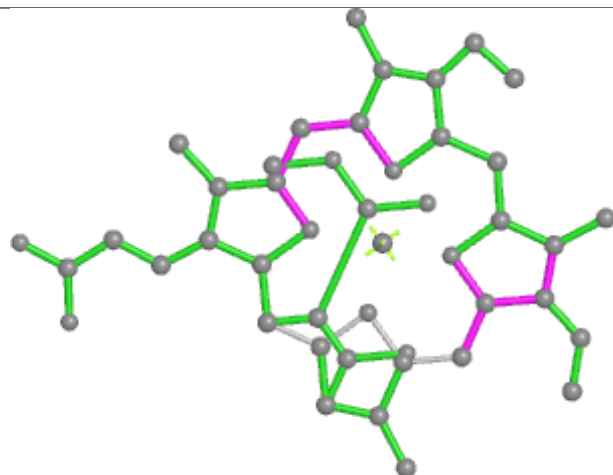
## Ligand LHG 8 613



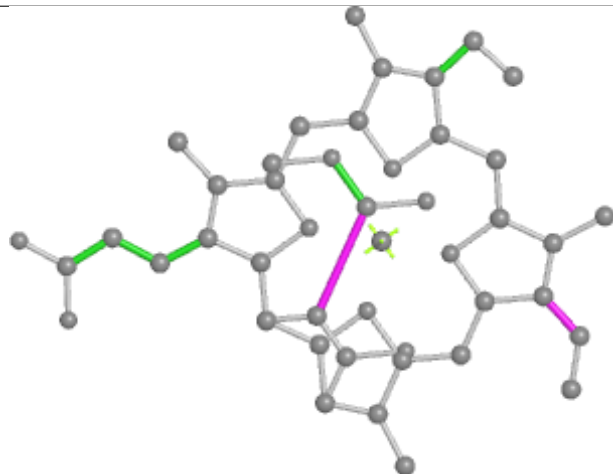
## Ligand KC2 a 609



Bond lengths



Bond angles

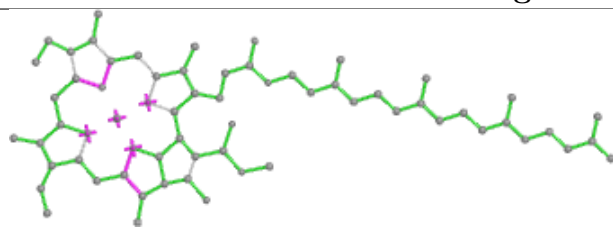


Torsions

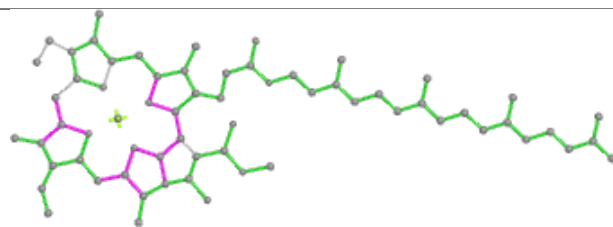


Rings

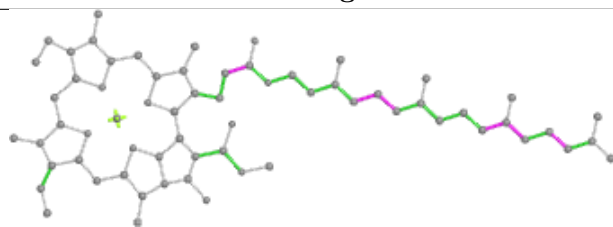
## Ligand CLA A 801



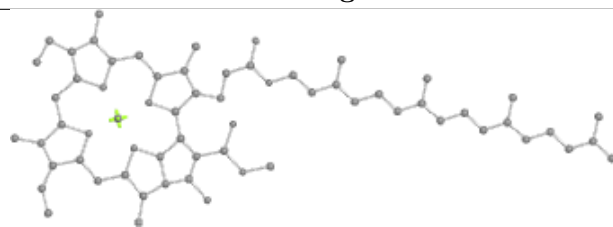
Bond lengths



Bond angles

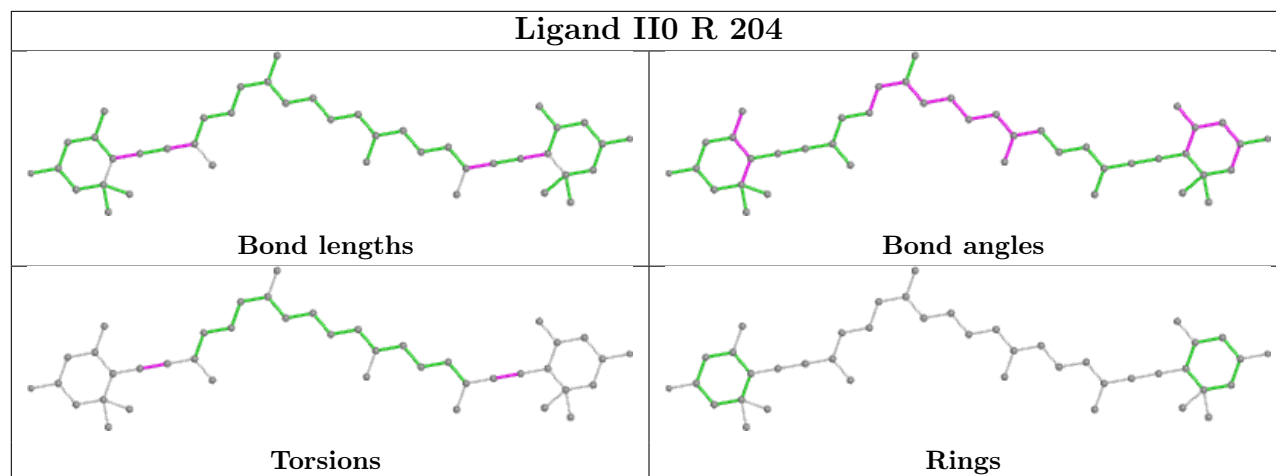


Torsions

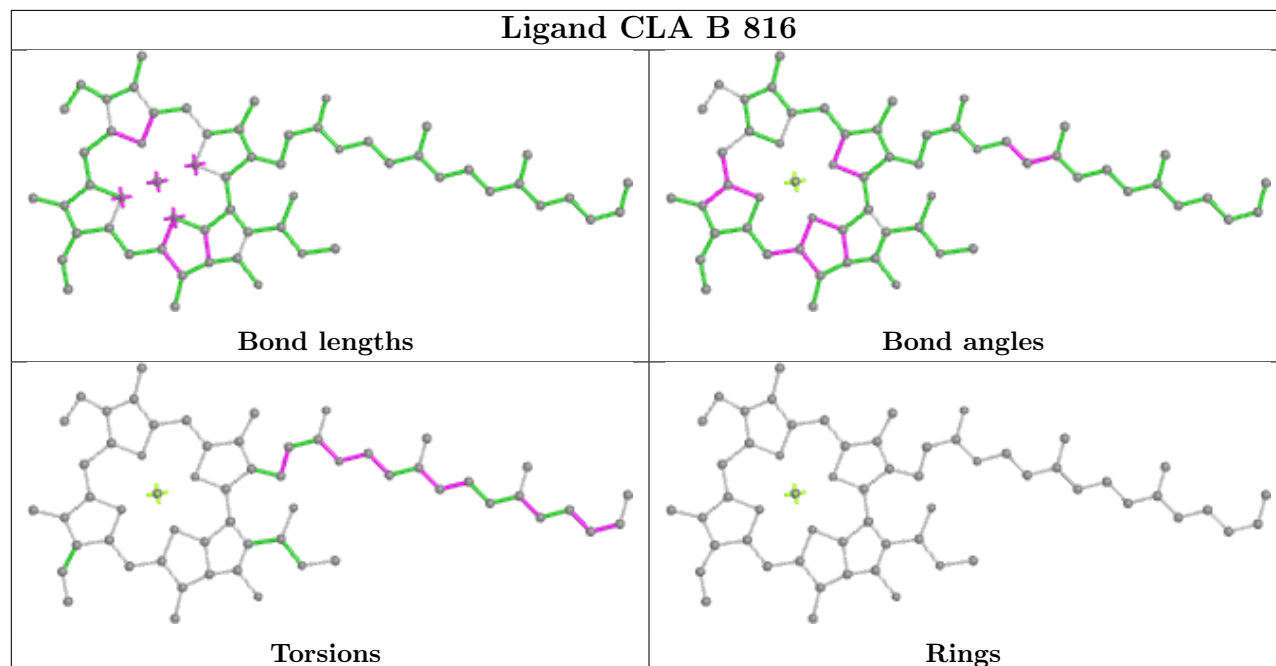


Rings

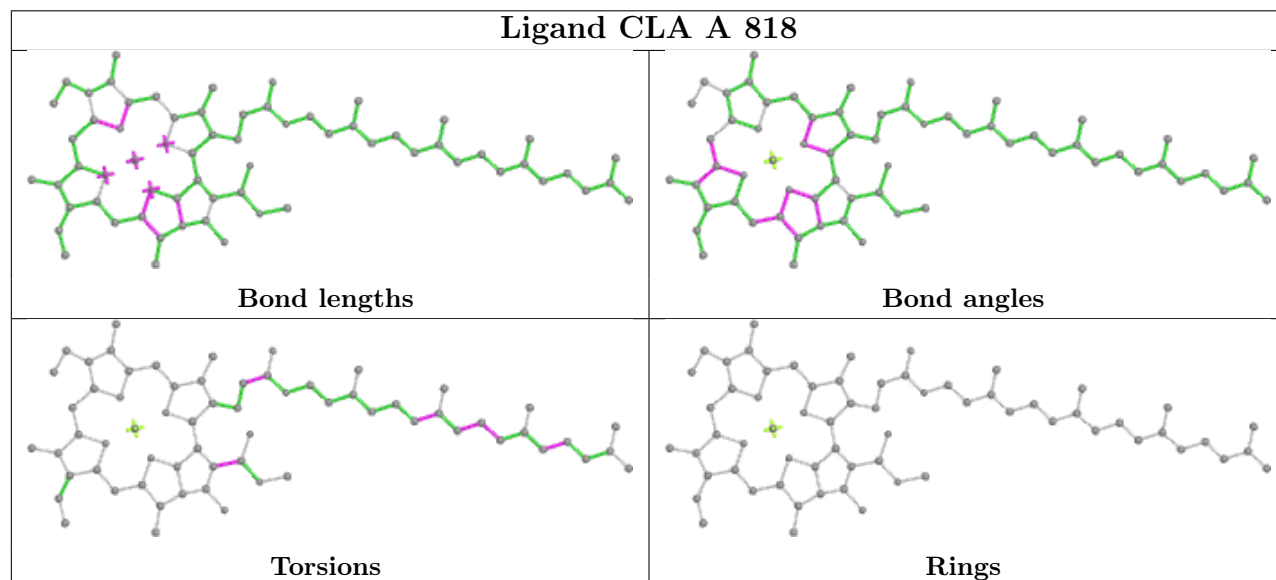
## Ligand II0 R 204



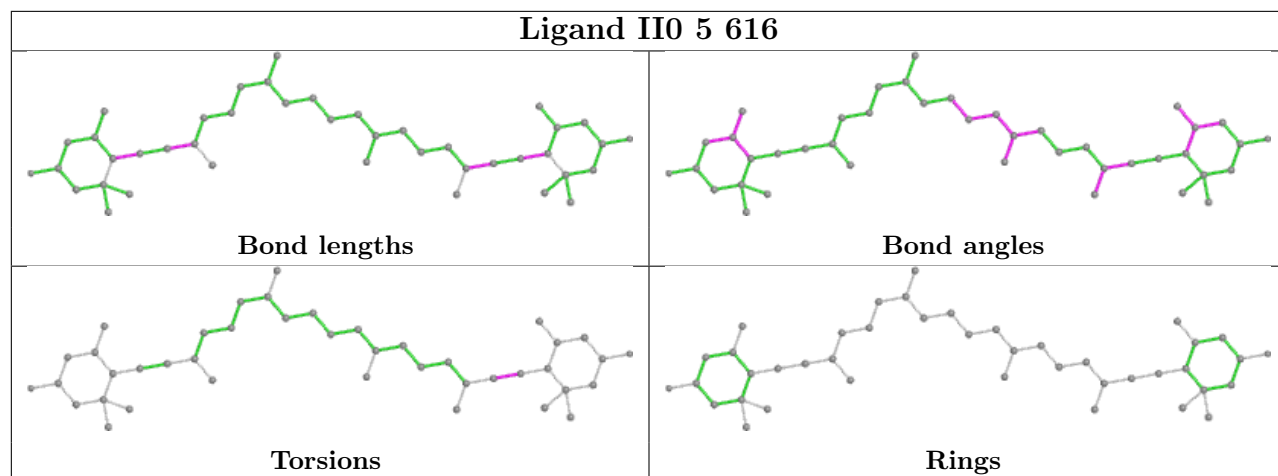
## Ligand CLA B 816



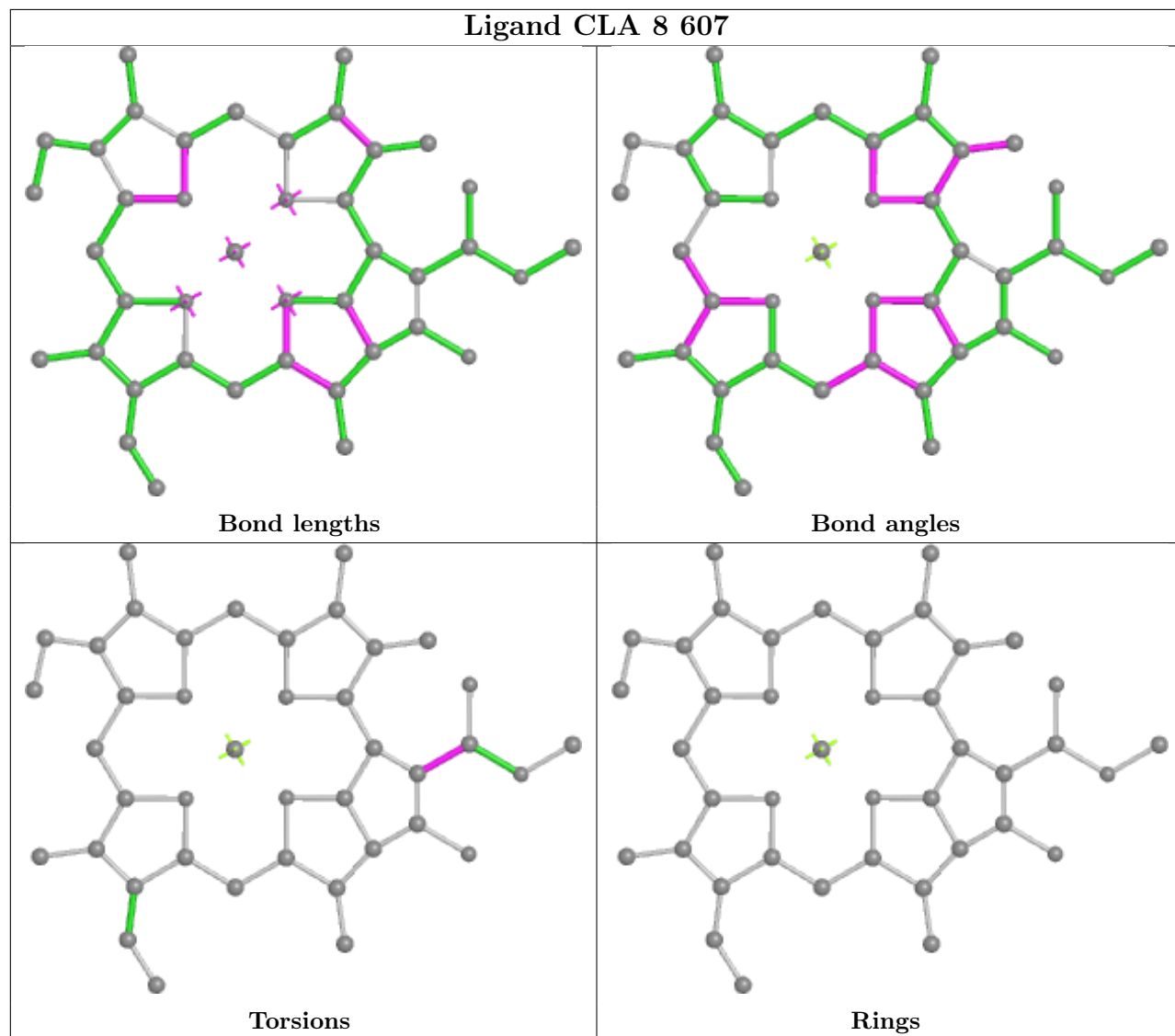
## Ligand CLA A 818

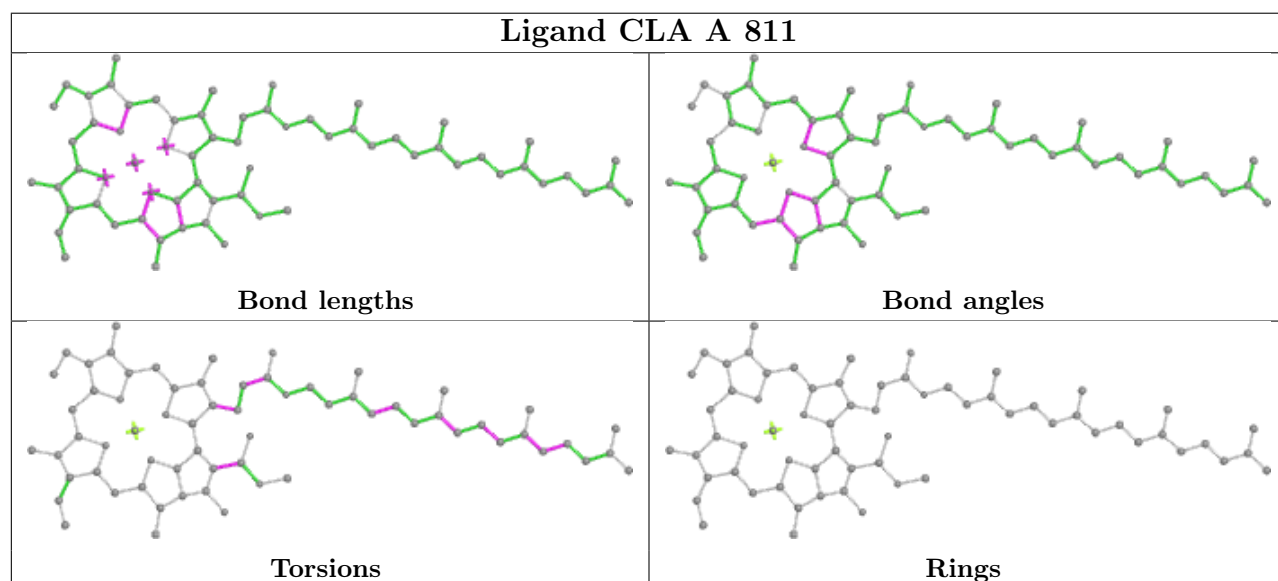
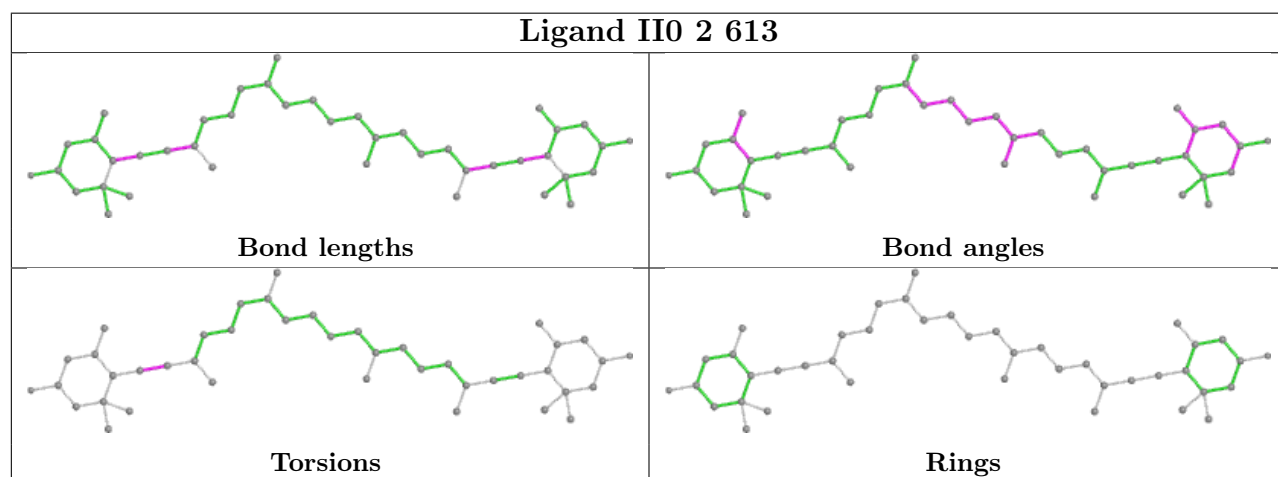
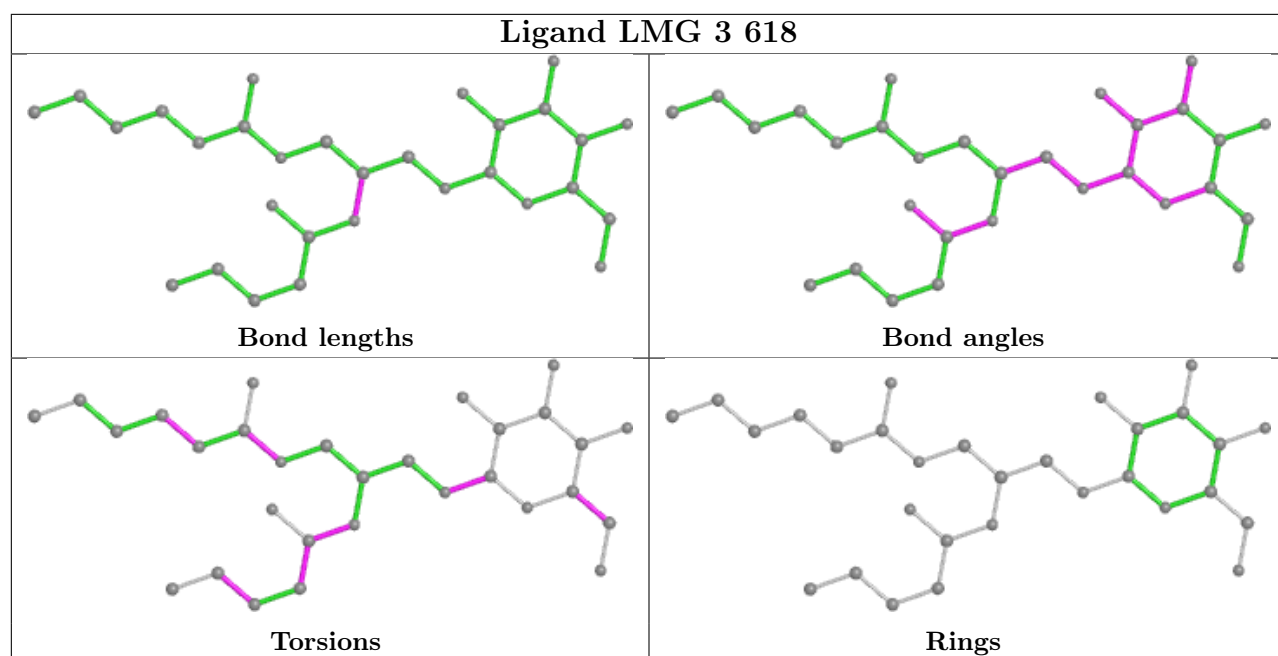


## Ligand II0 5 616

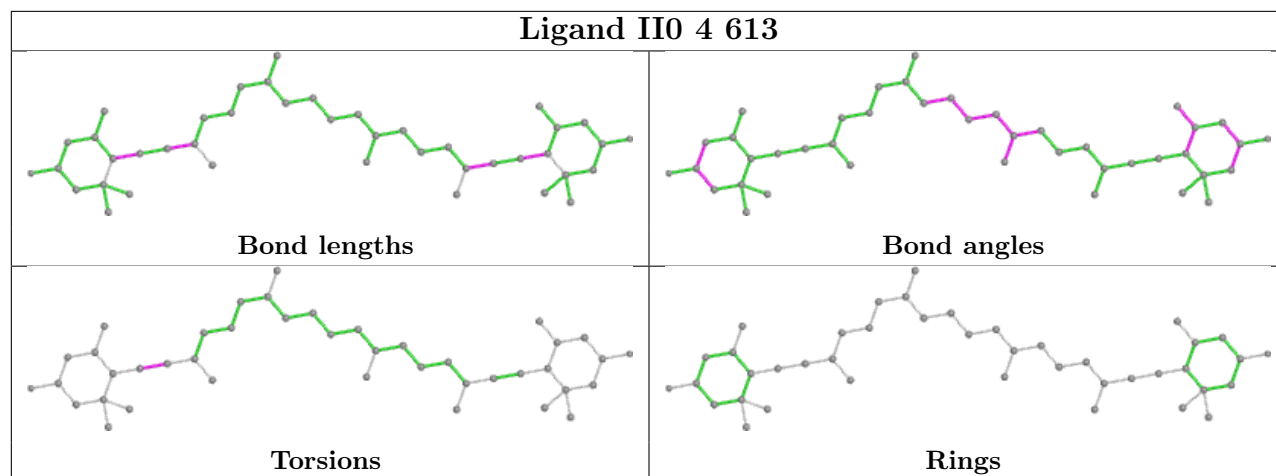
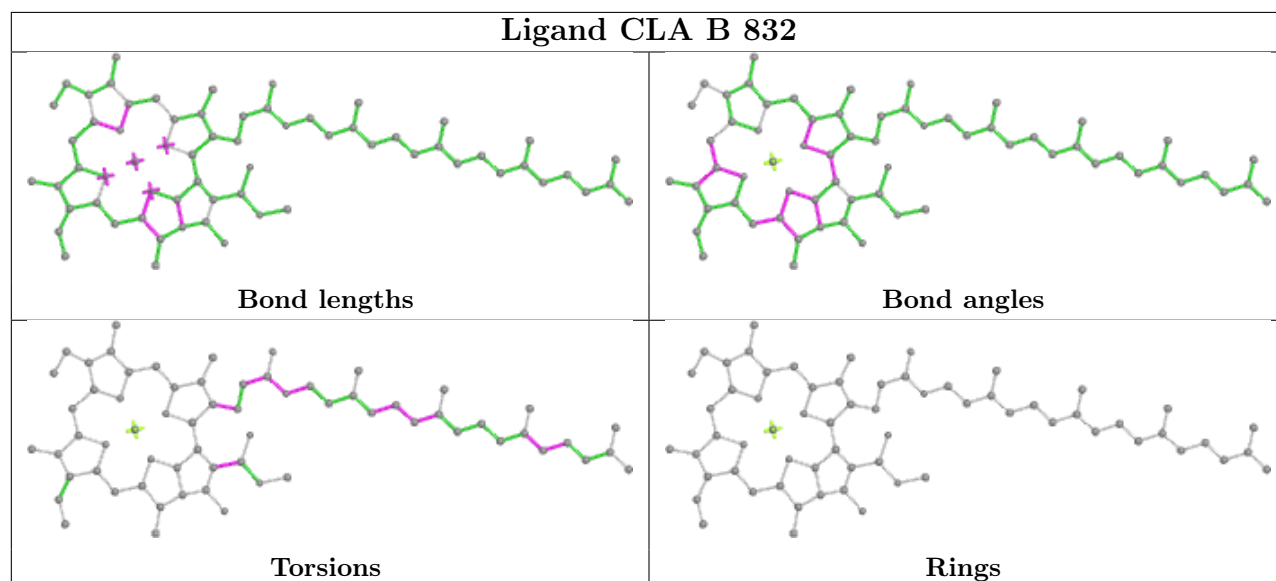
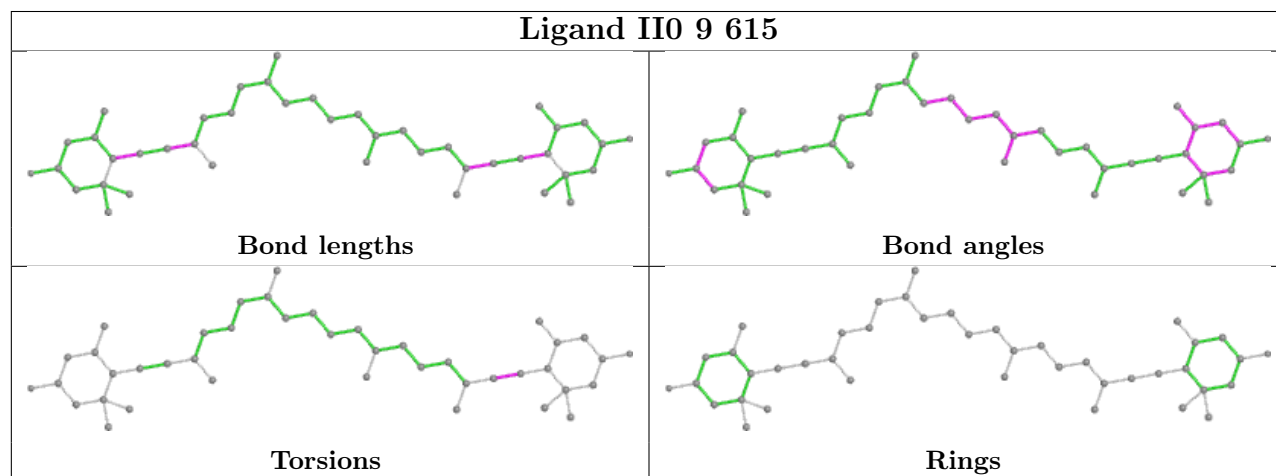


## Ligand CLA 8 607

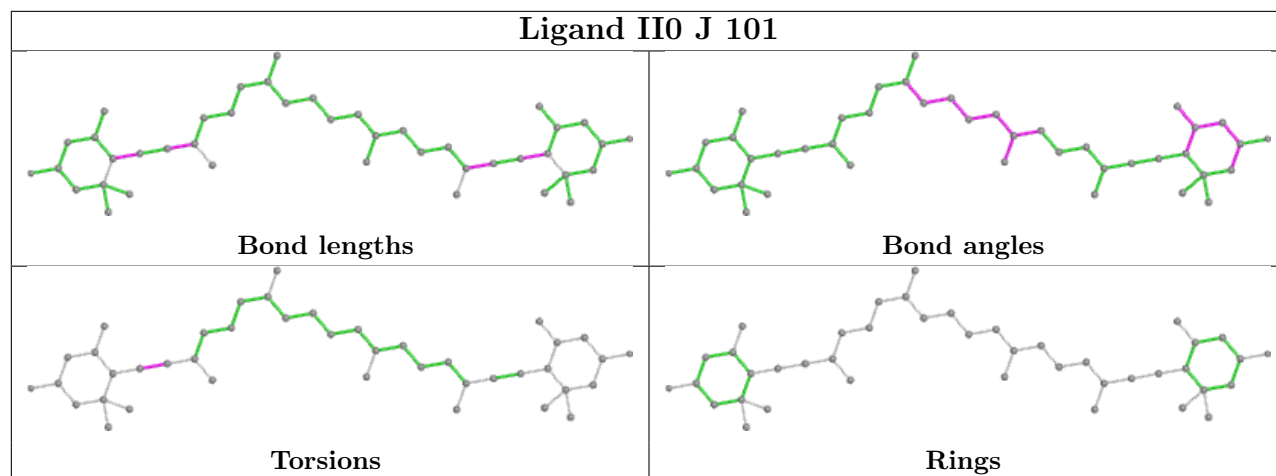




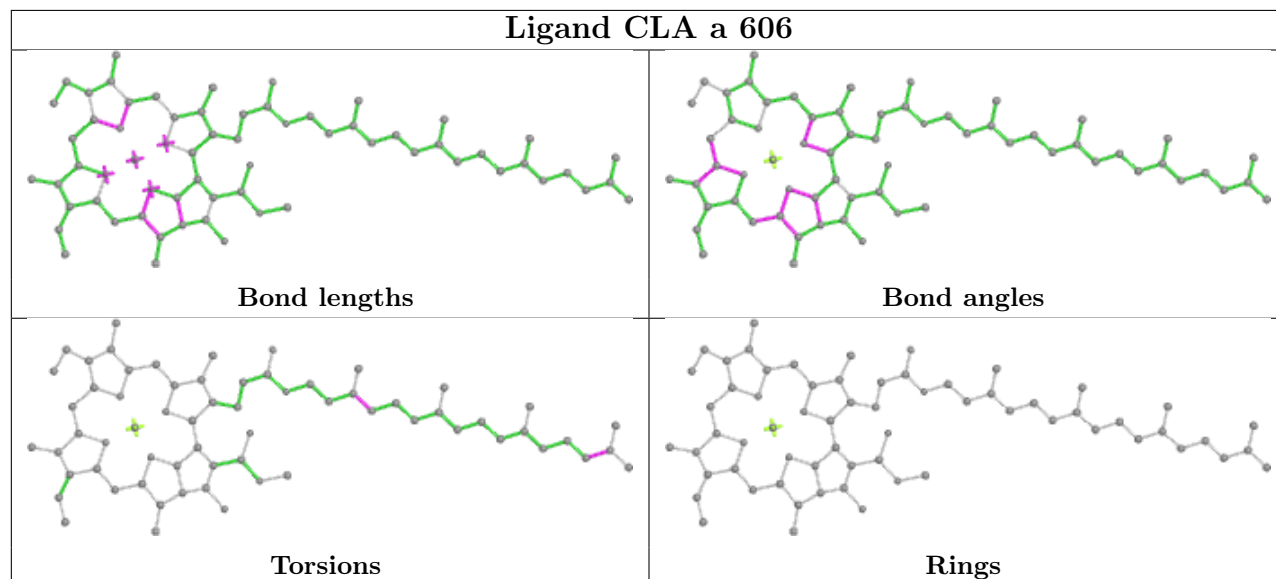


**Ligand II0 4 613****Ligand CLA B 832****Ligand II0 9 615**

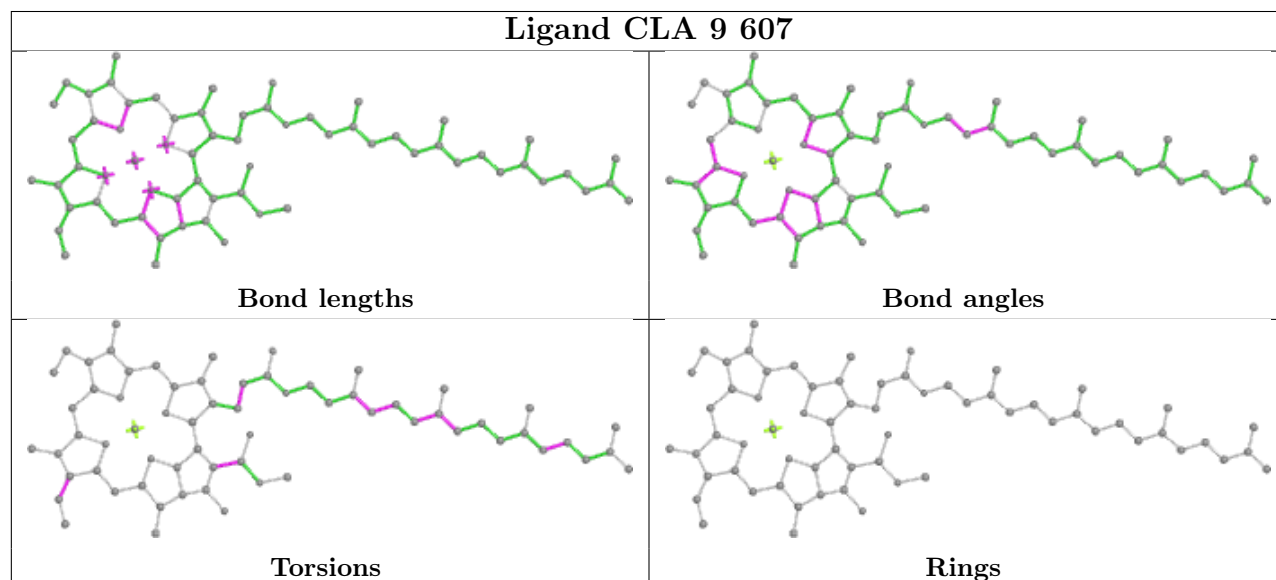
## Ligand II0 J 101



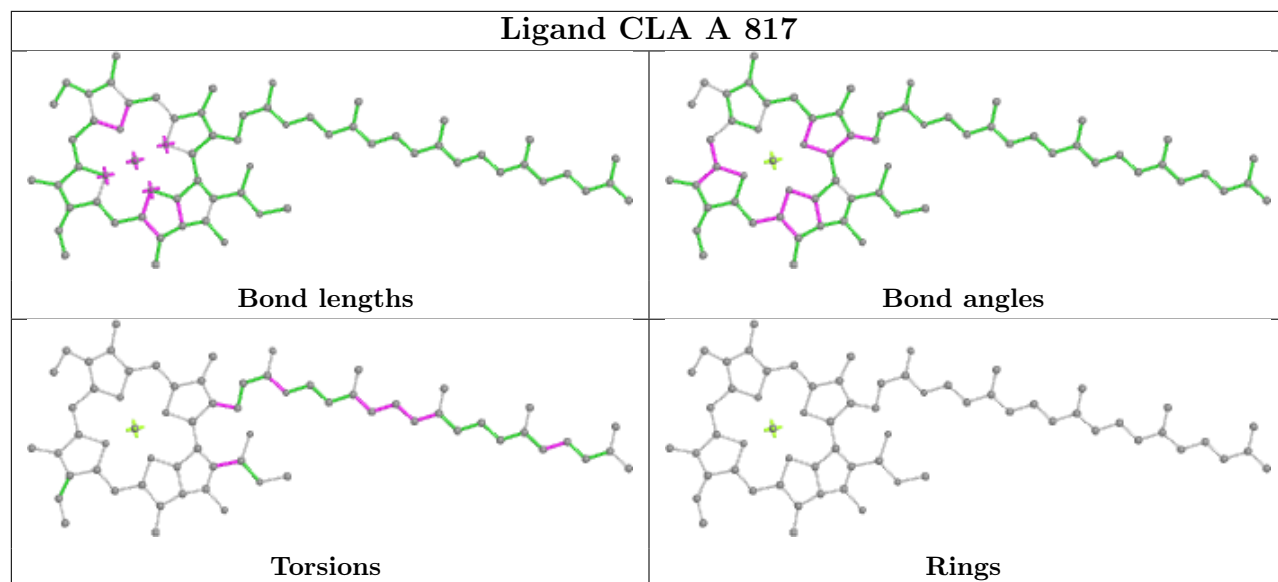
## Ligand CLA a 606



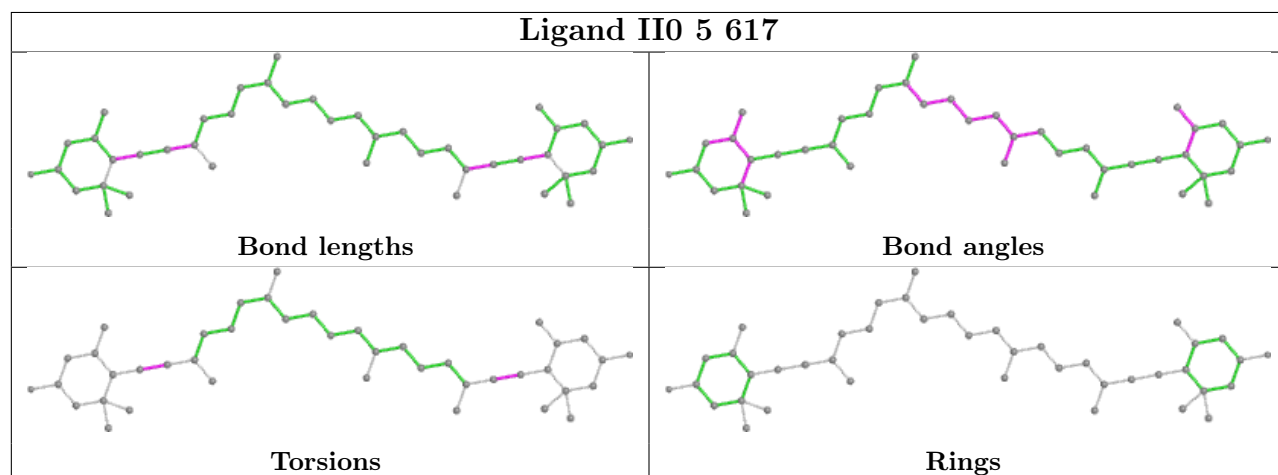
## Ligand CLA 9 607



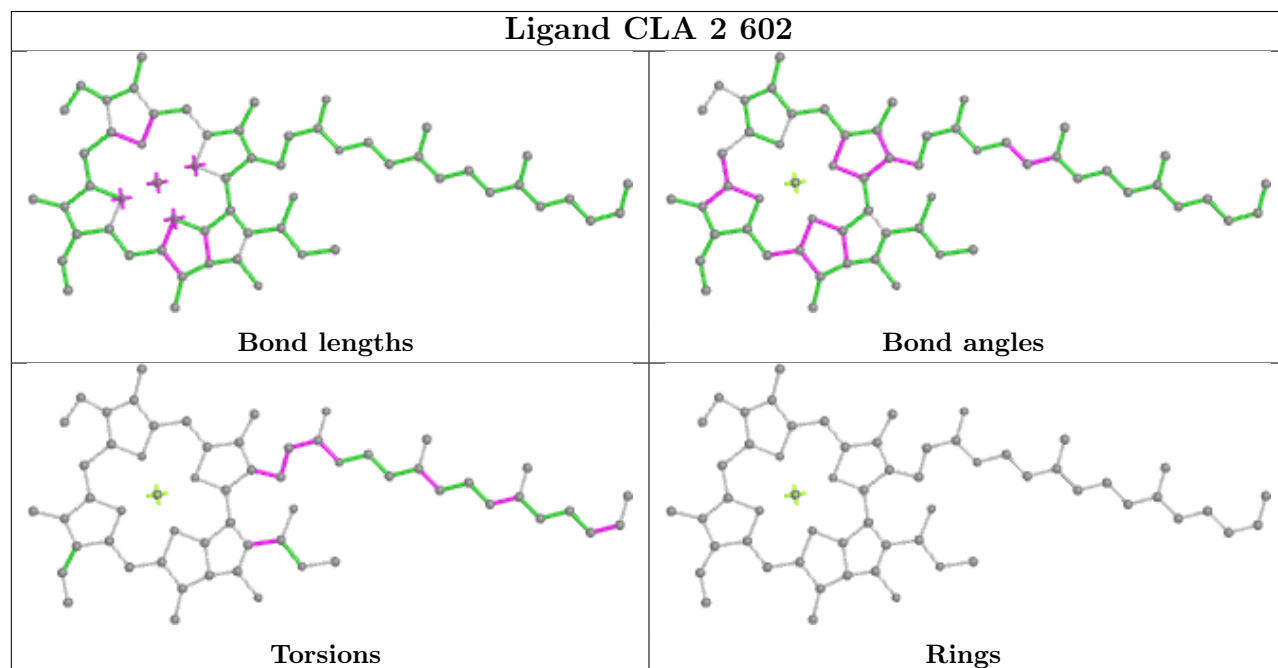
## Ligand CLA A 817



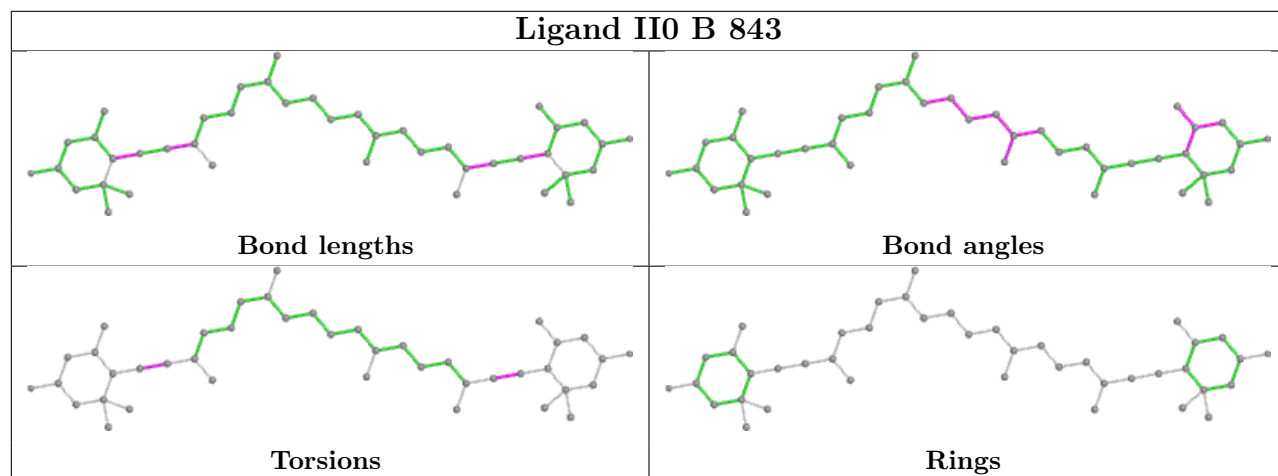
## Ligand II0 5 617



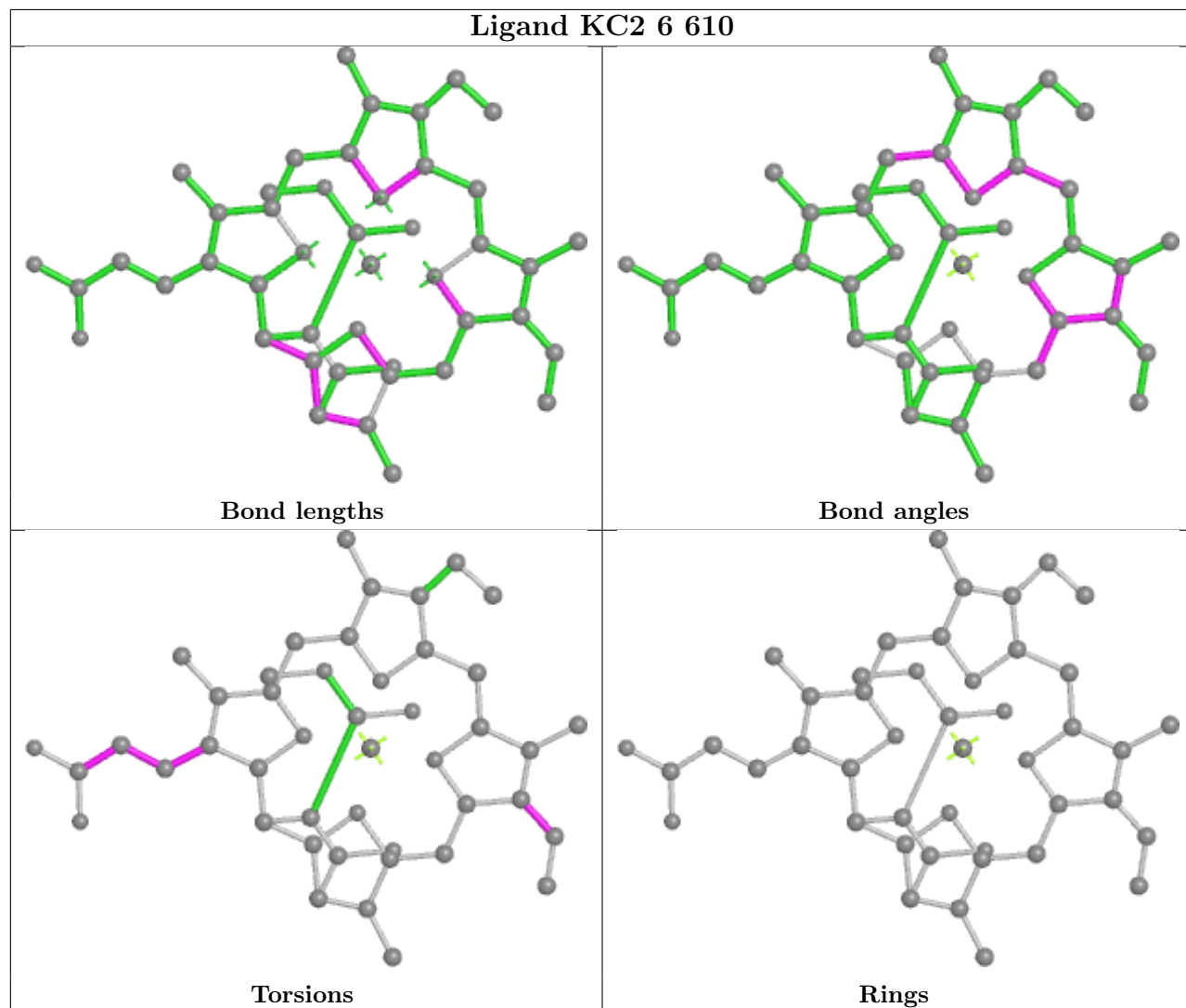
## Ligand CLA 2 602



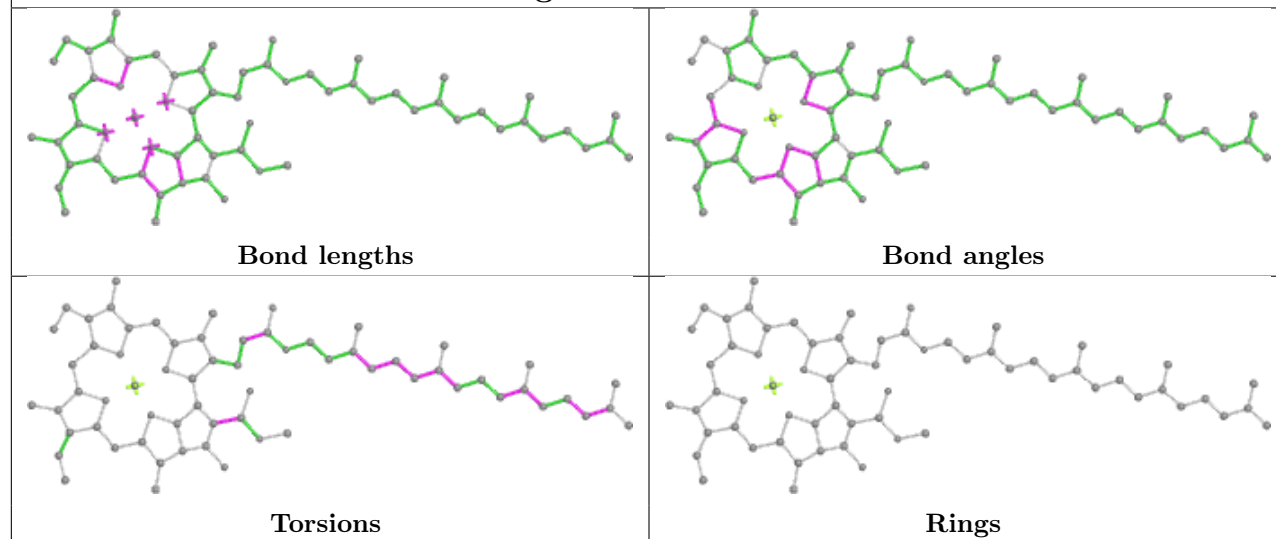
## Ligand II0 B 843



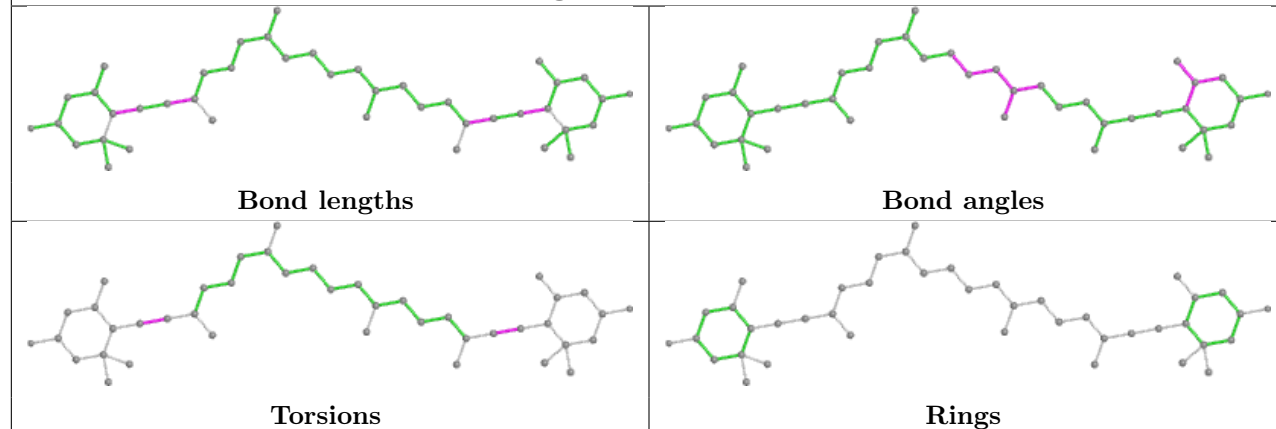
## Ligand KC2 6 610



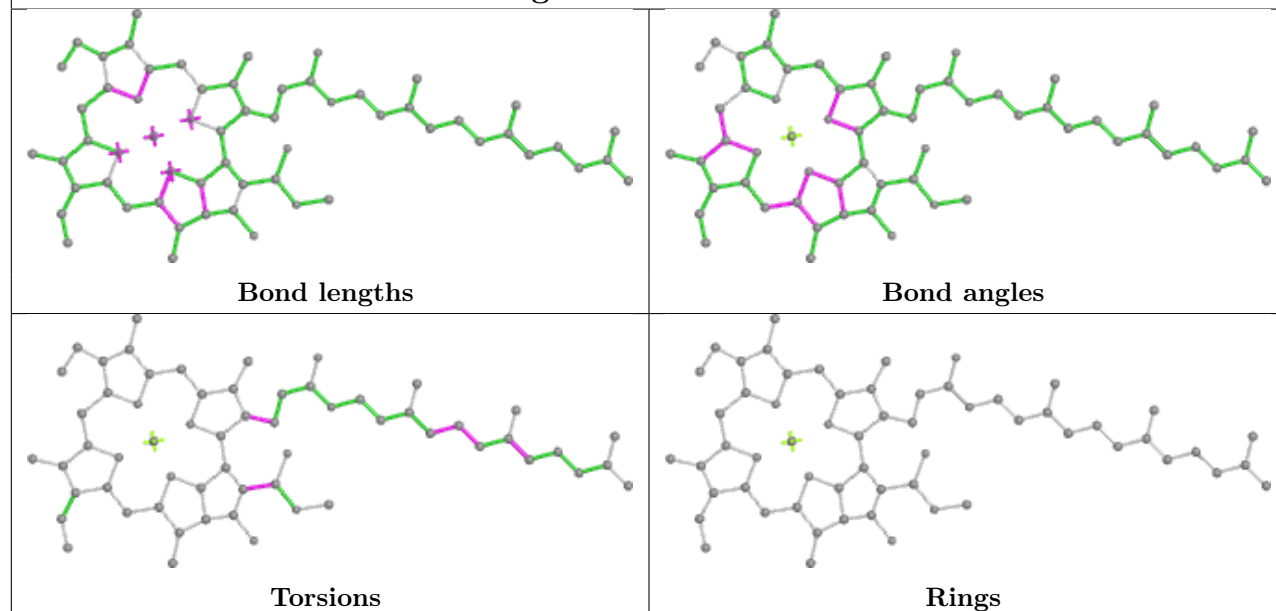
## Ligand CLA b 604

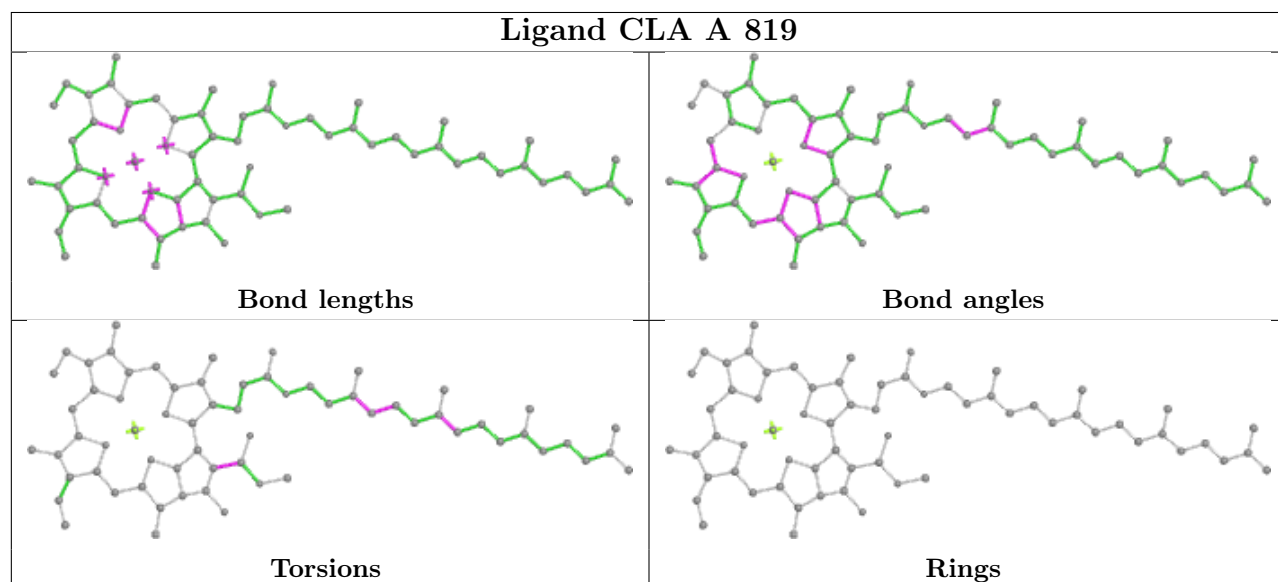
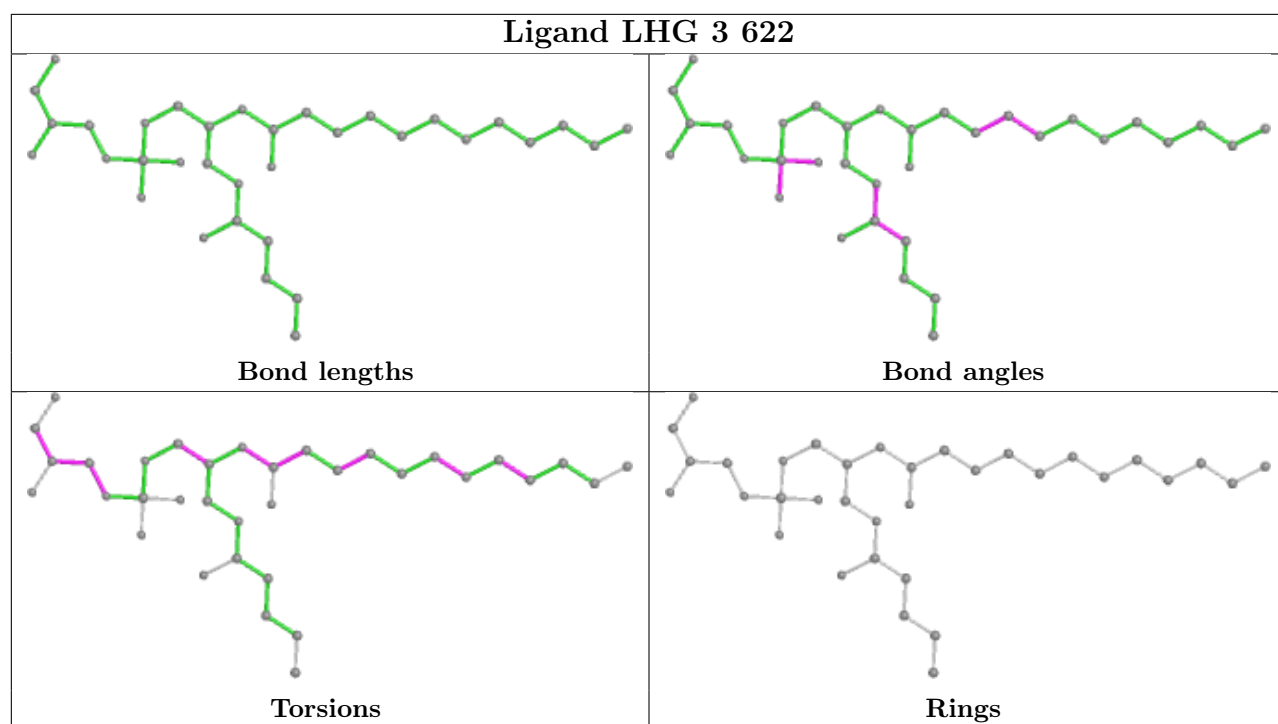


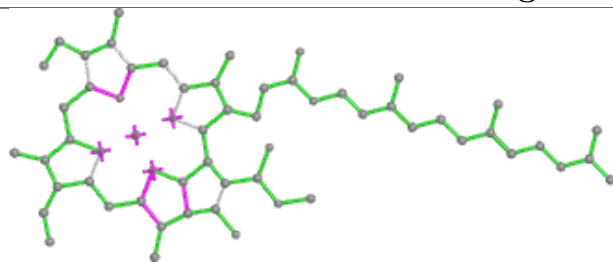
## Ligand II0 4 614



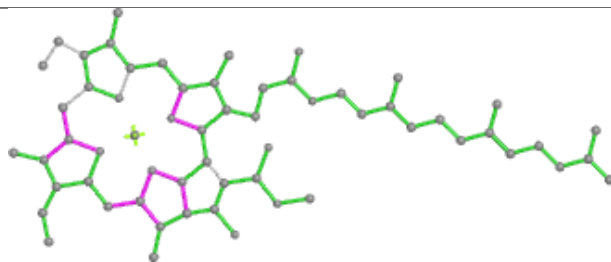
## Ligand CLA A 835



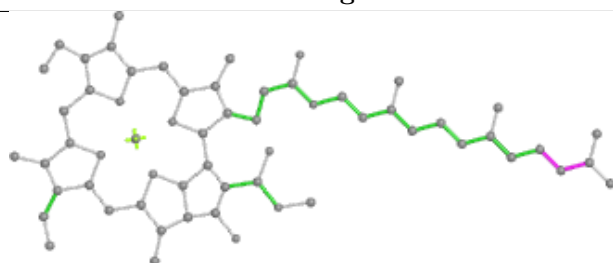


**Ligand CLA 3 603**

Bond lengths



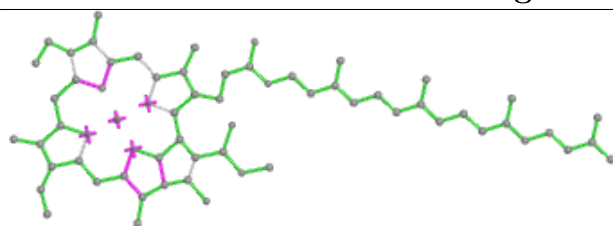
Bond angles



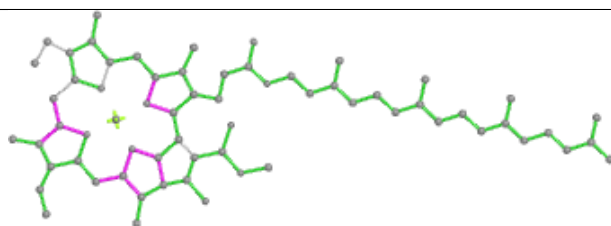
Torsions



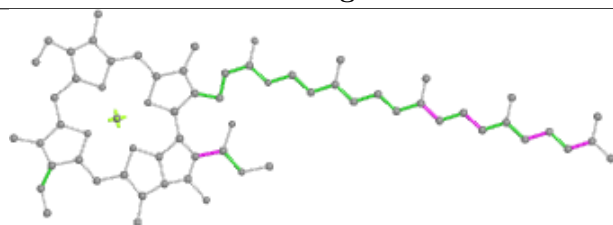
Rings

**Ligand CLA B 839**

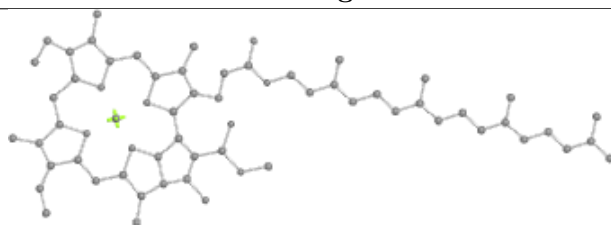
Bond lengths



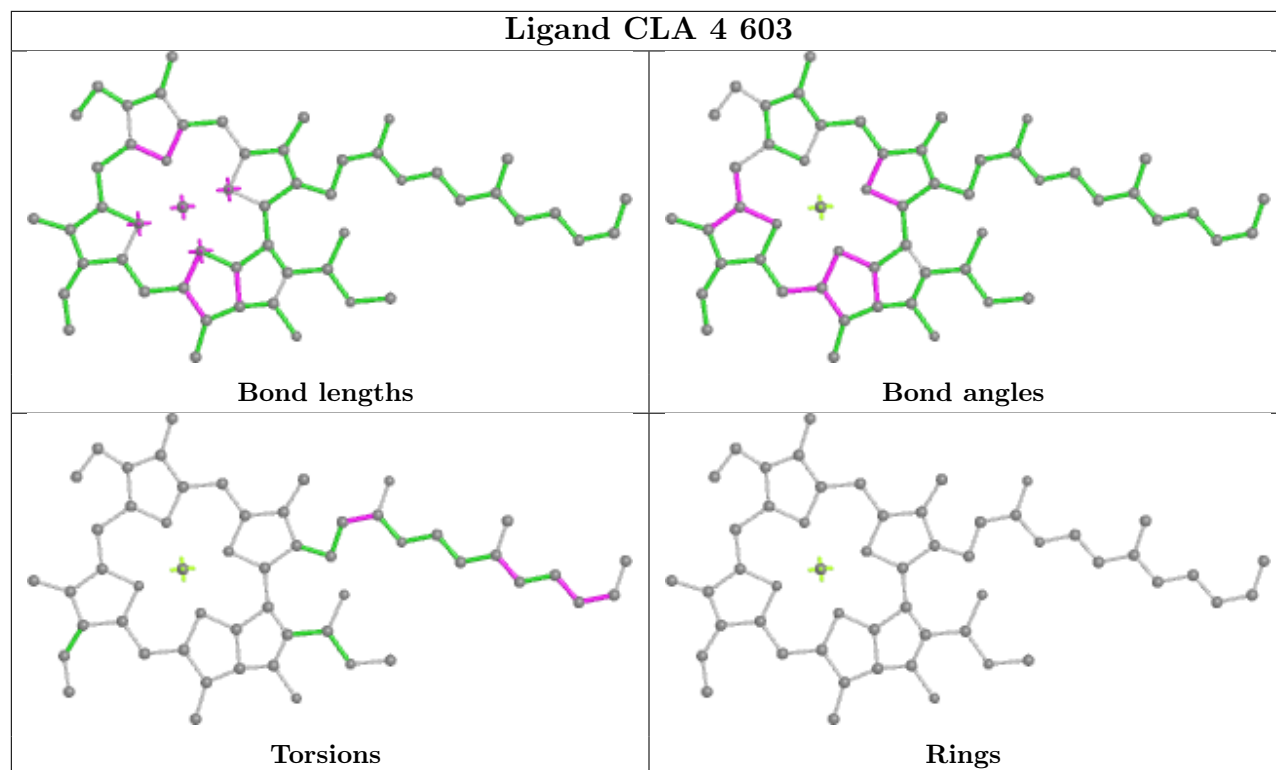
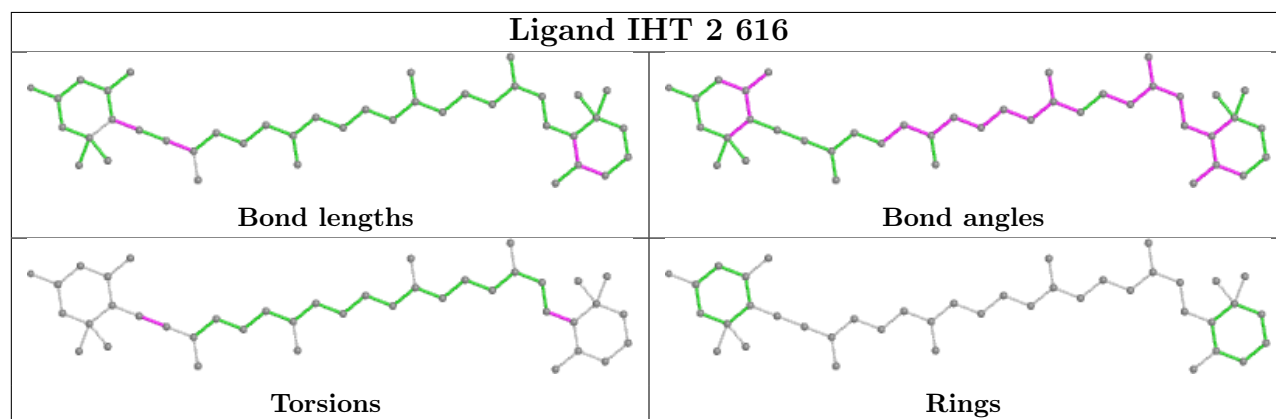
Bond angles



Torsions

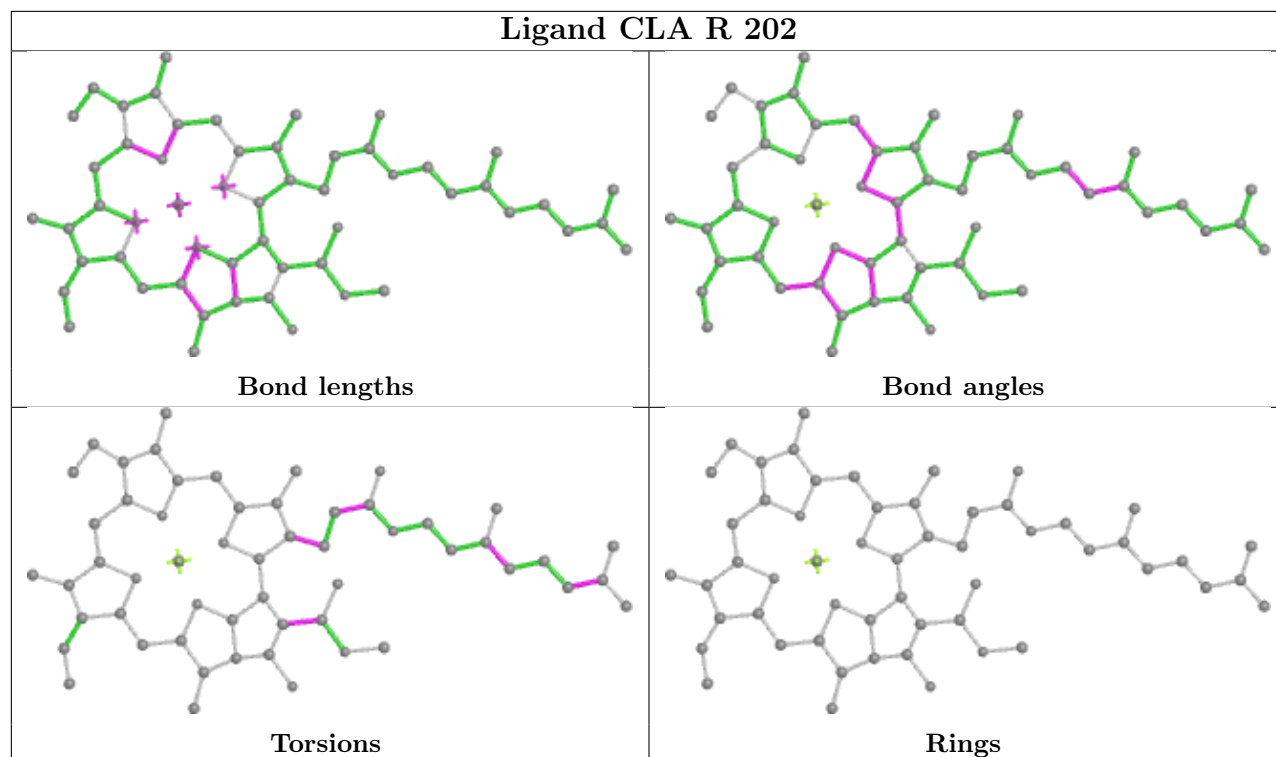


Rings

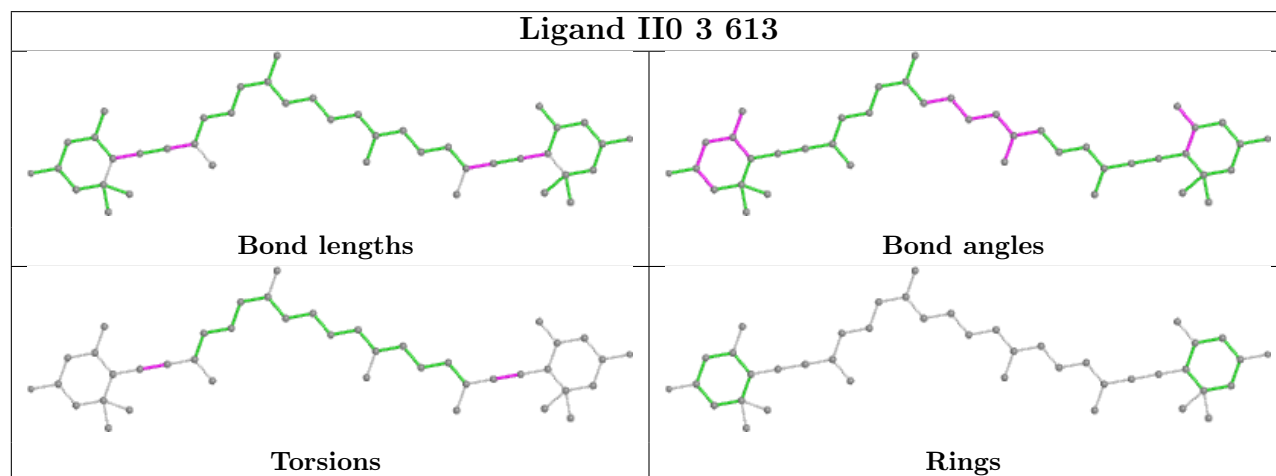
**Ligand CLA 4 603****Ligand IHT 2 616**



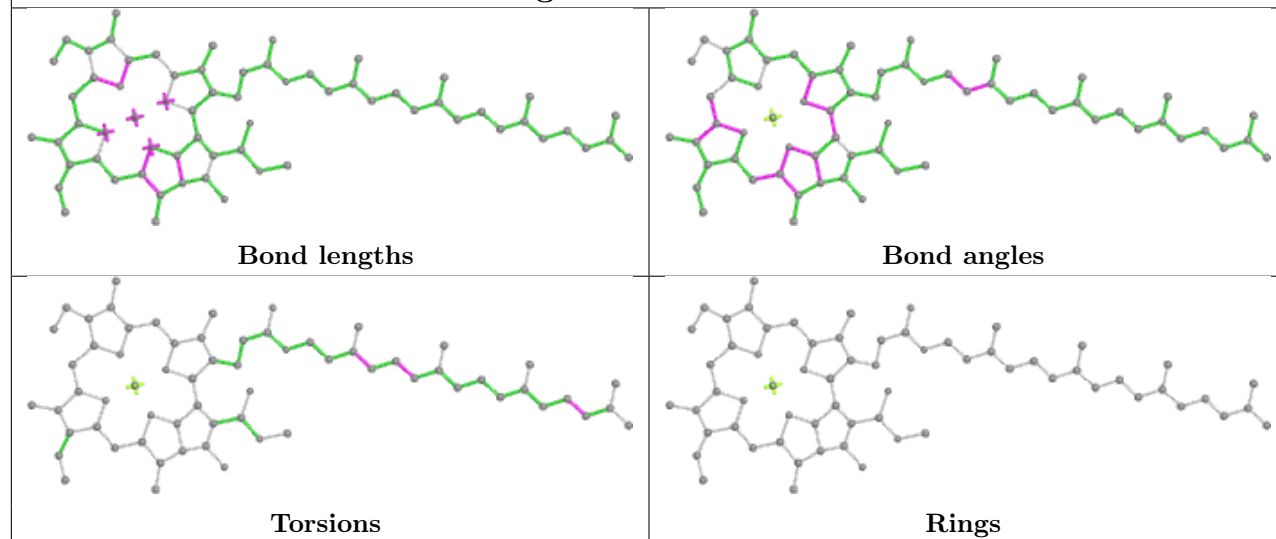
## Ligand CLA R 202



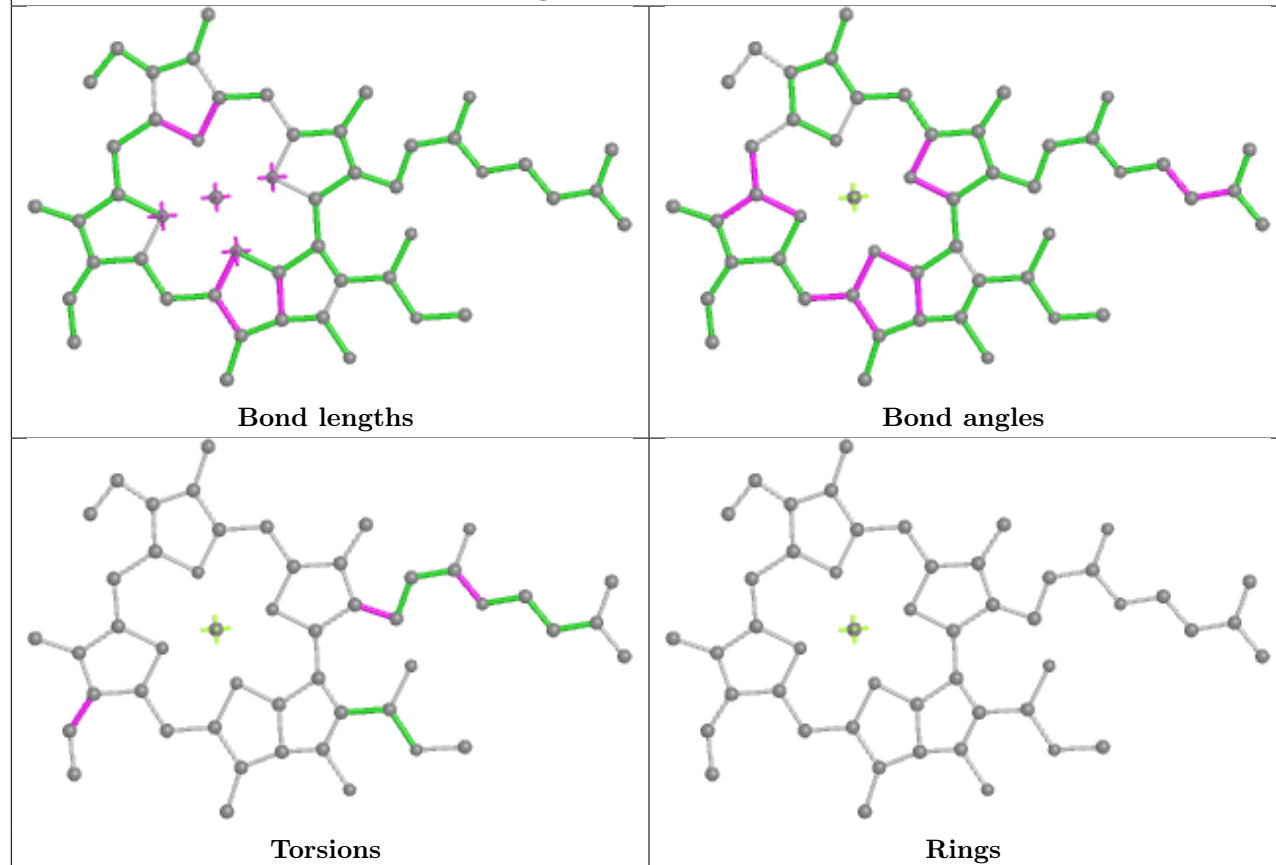
## Ligand II0 3 613



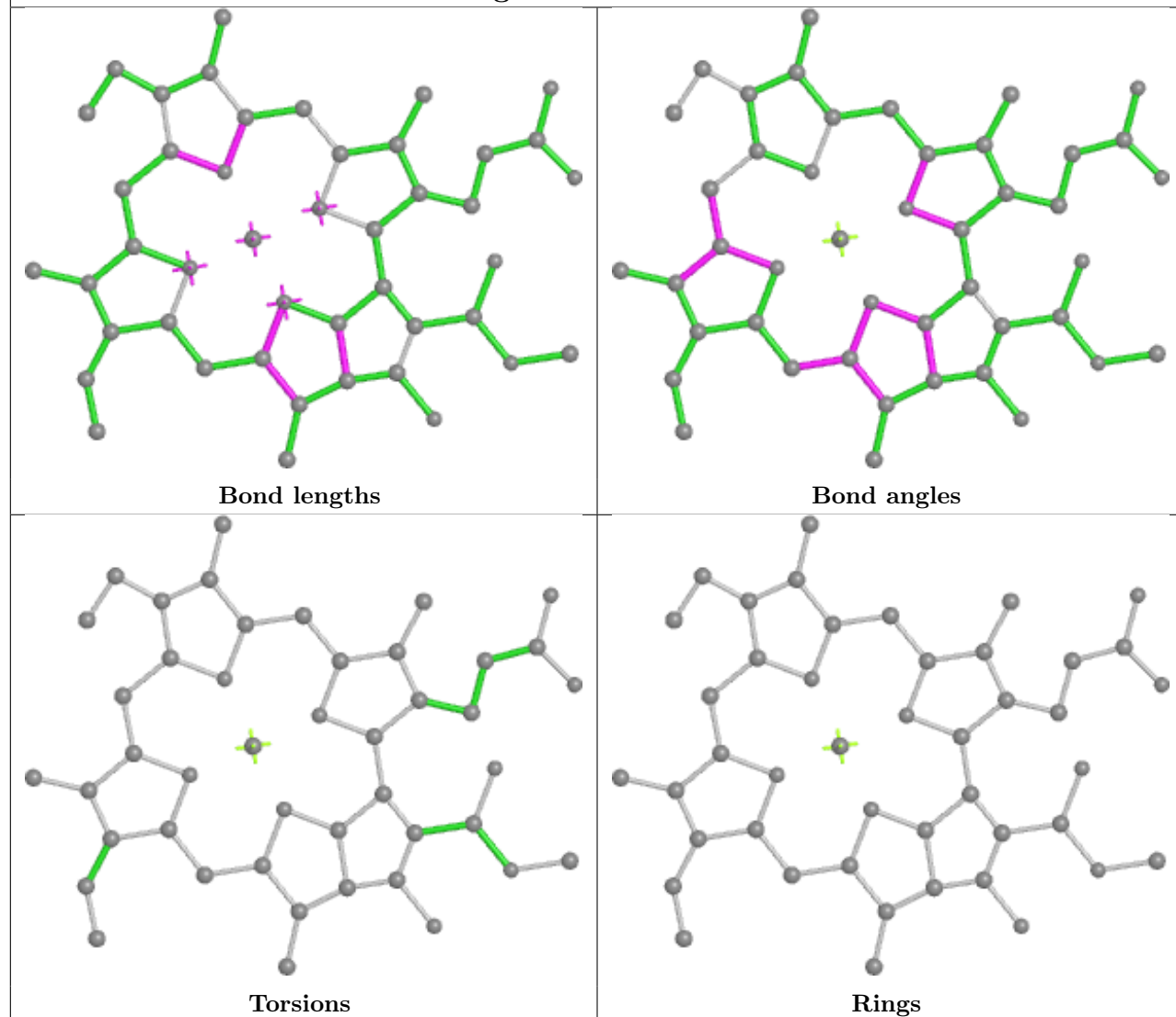
## Ligand CLA 8 604



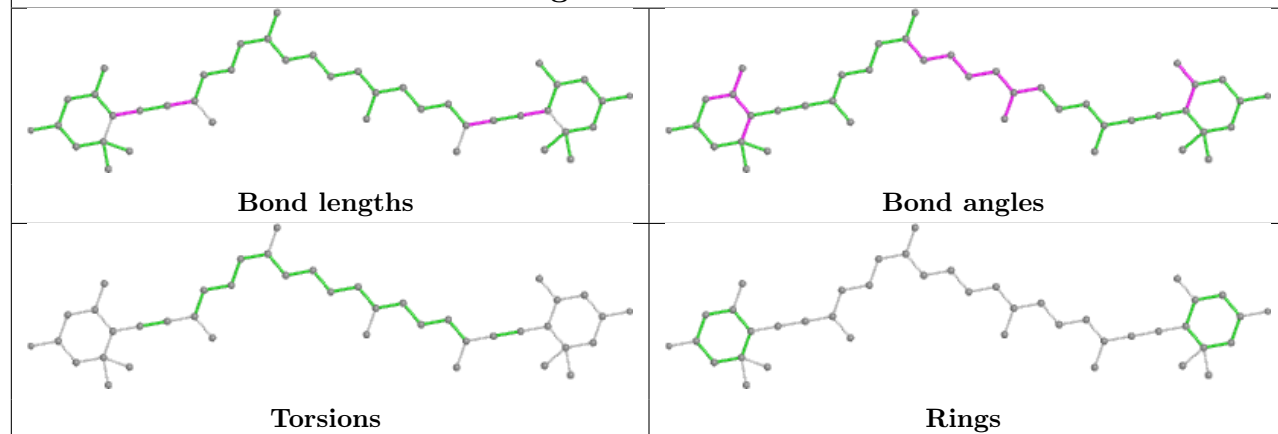
## Ligand CLA L 203



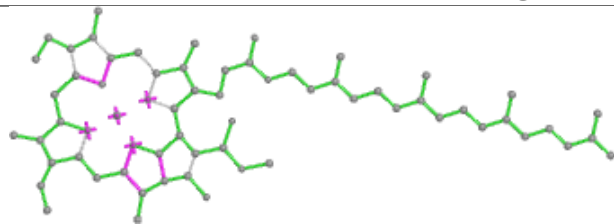
## Ligand CLA 1 607



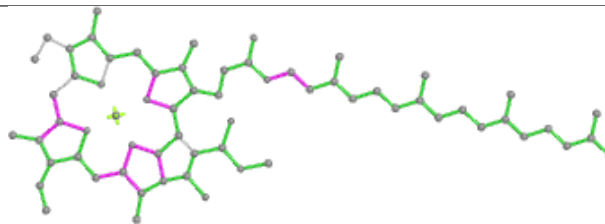
## Ligand II0 4 615



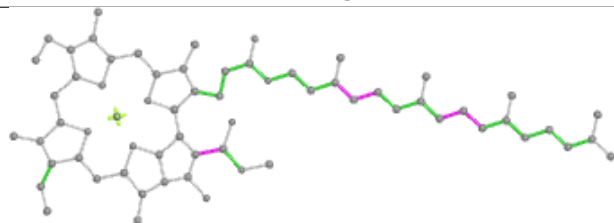
## Ligand CLA B 822



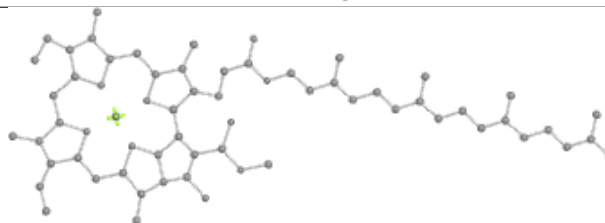
Bond lengths



Bond angles

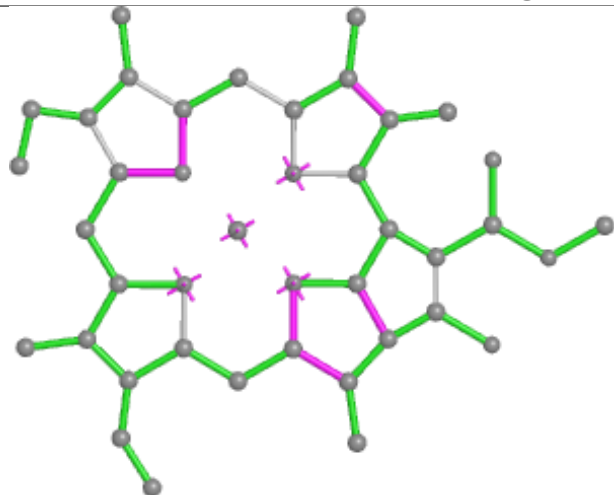


Torsions

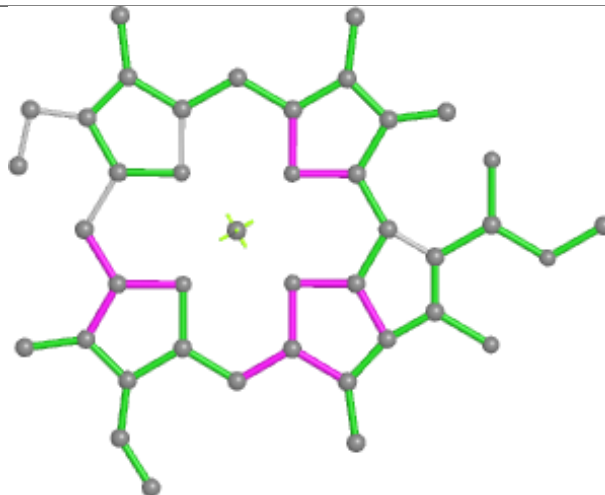


Rings

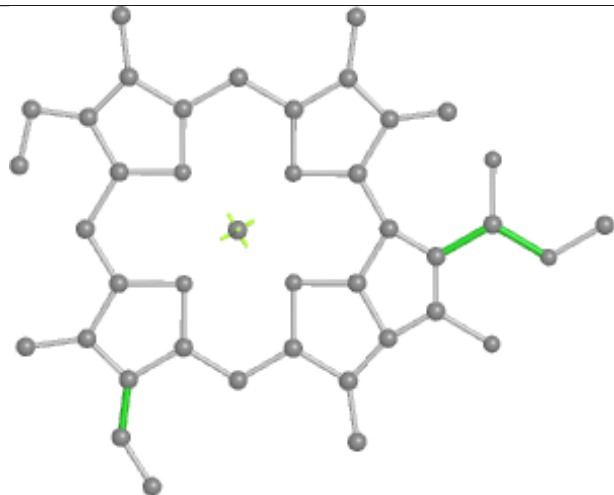
## Ligand CLA 7 310



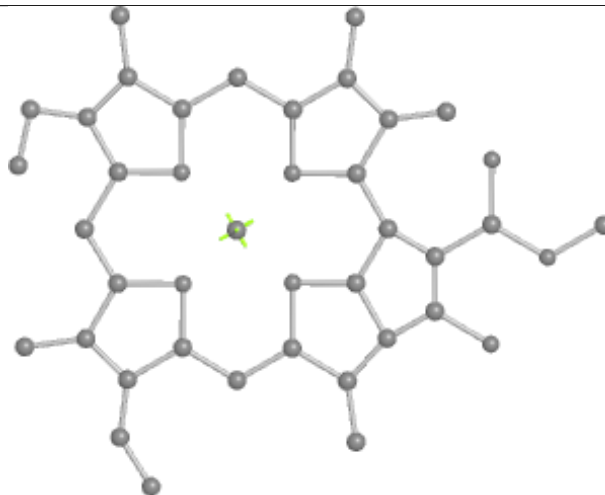
Bond lengths



Bond angles

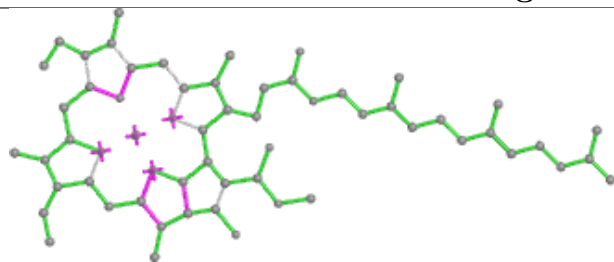


Torsions

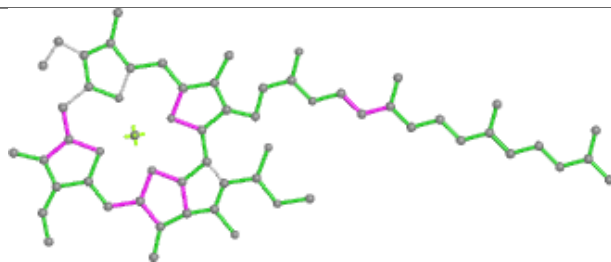


Rings

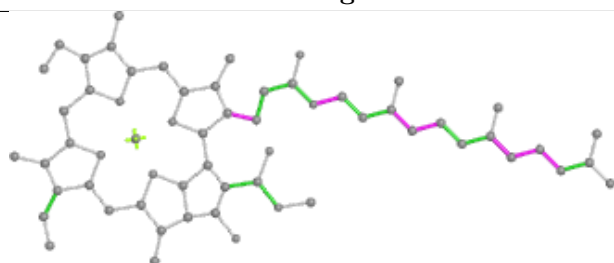
## Ligand CLA F 202



Bond lengths



Bond angles

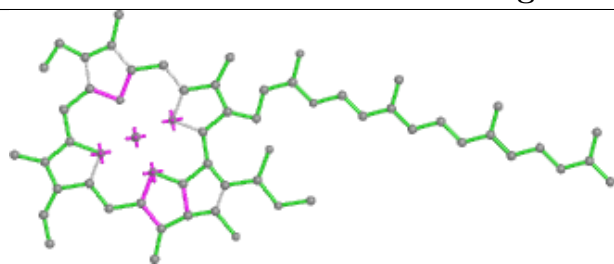


Torsions

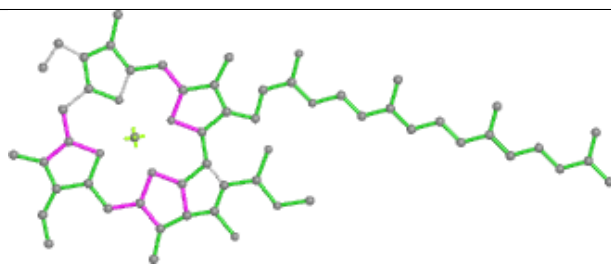


Rings

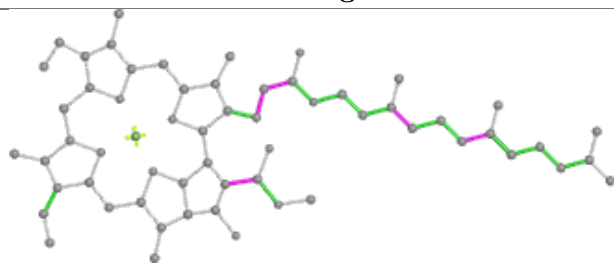
## Ligand CLA b 603



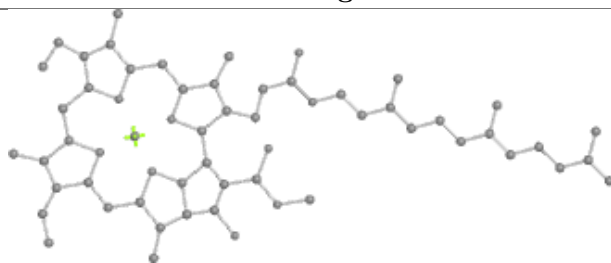
Bond lengths



Bond angles

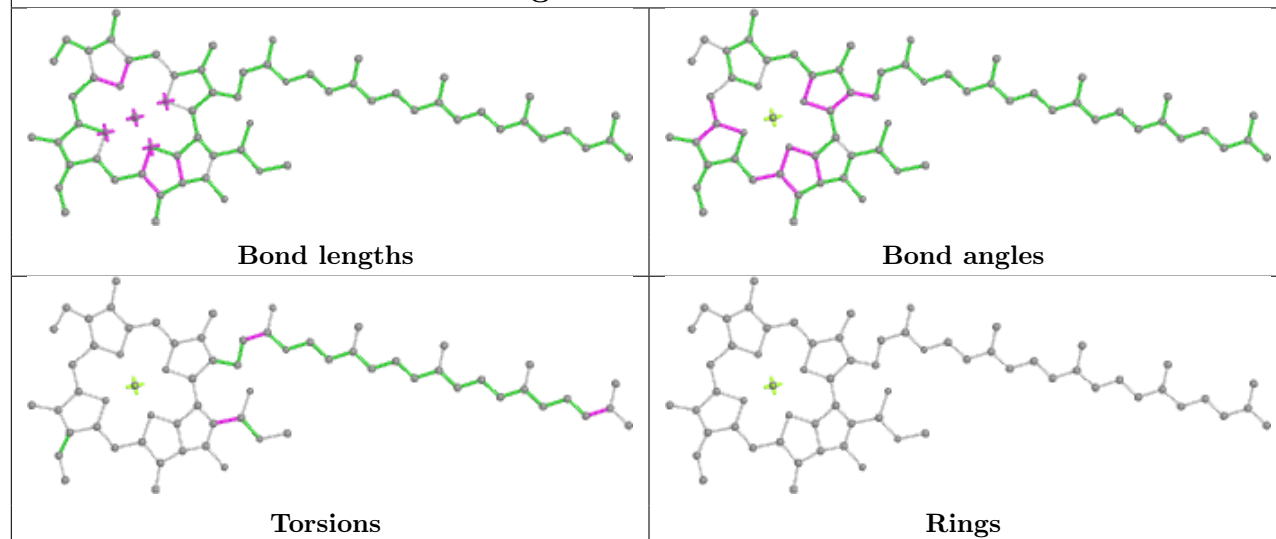


Torsions

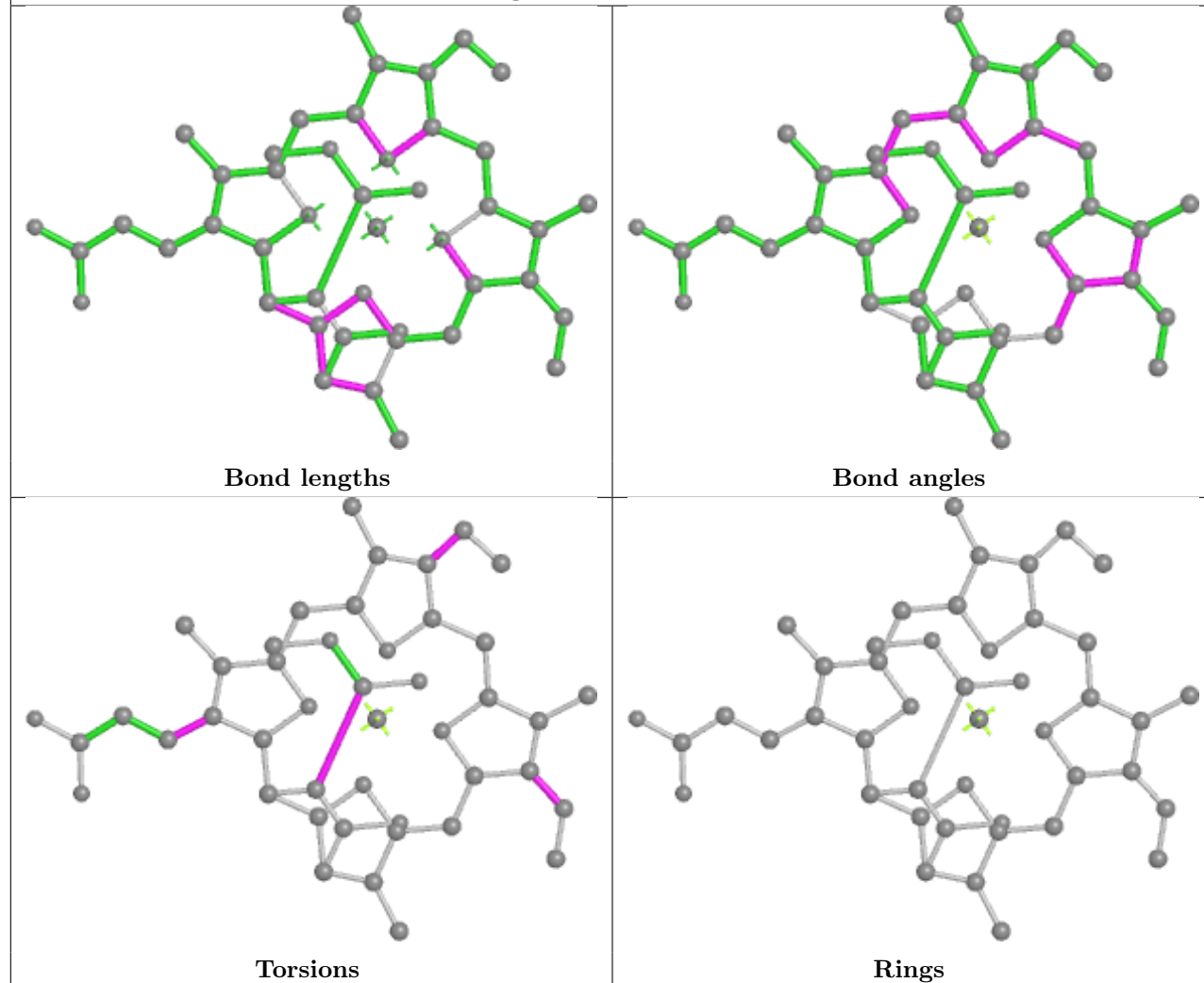


Rings

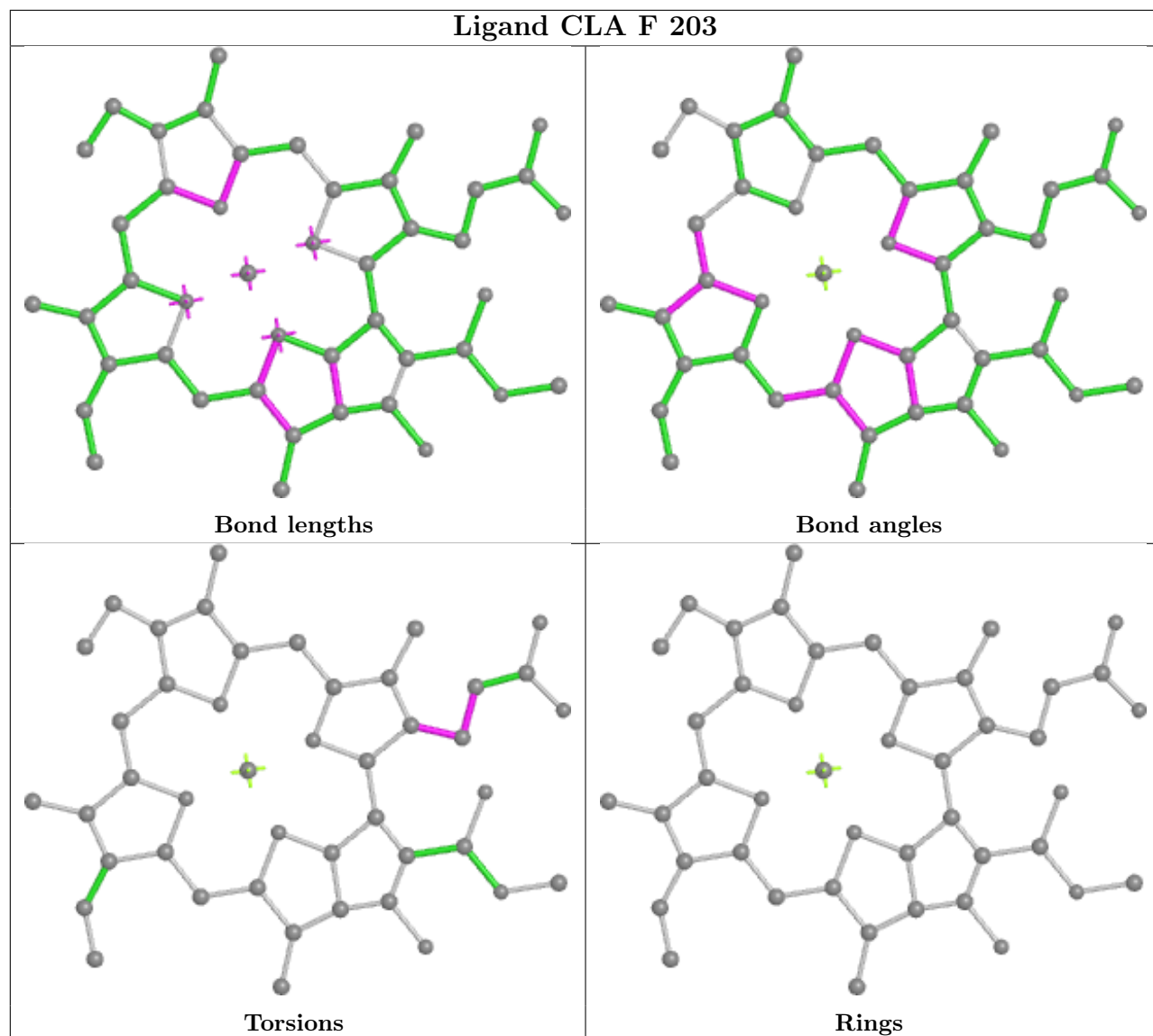
## Ligand CLA A 803



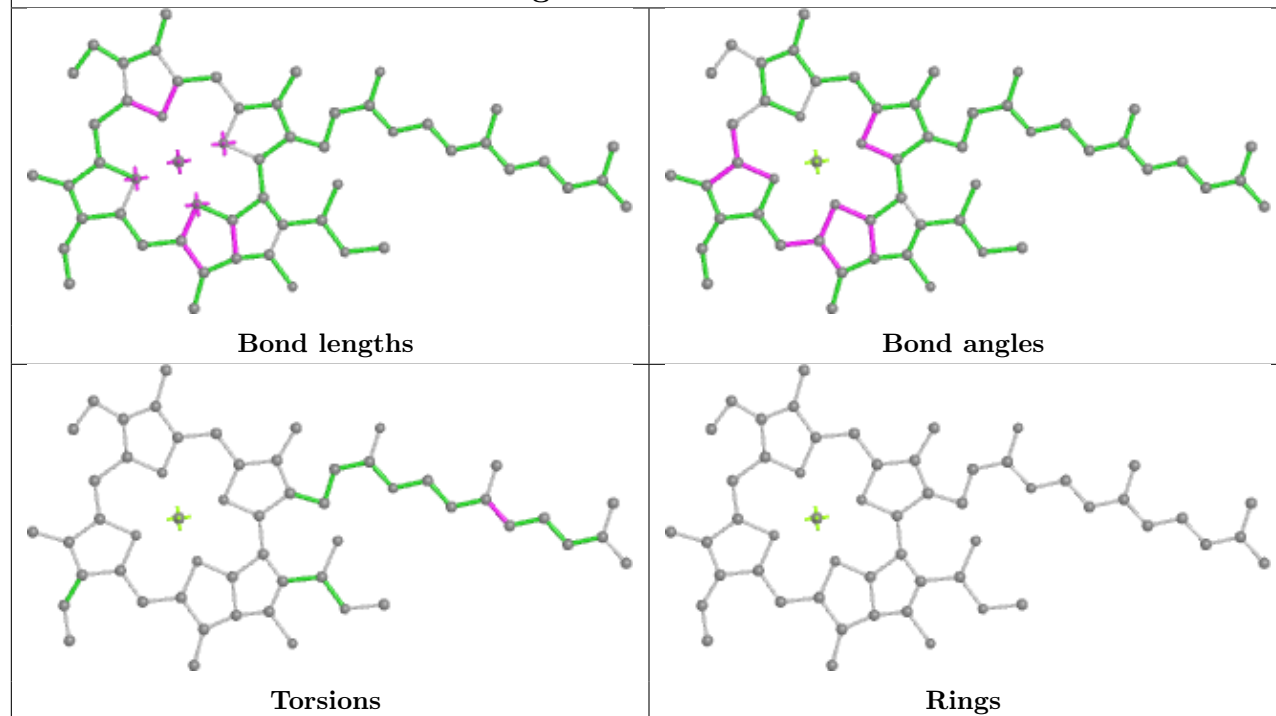
## Ligand KC2 3 606



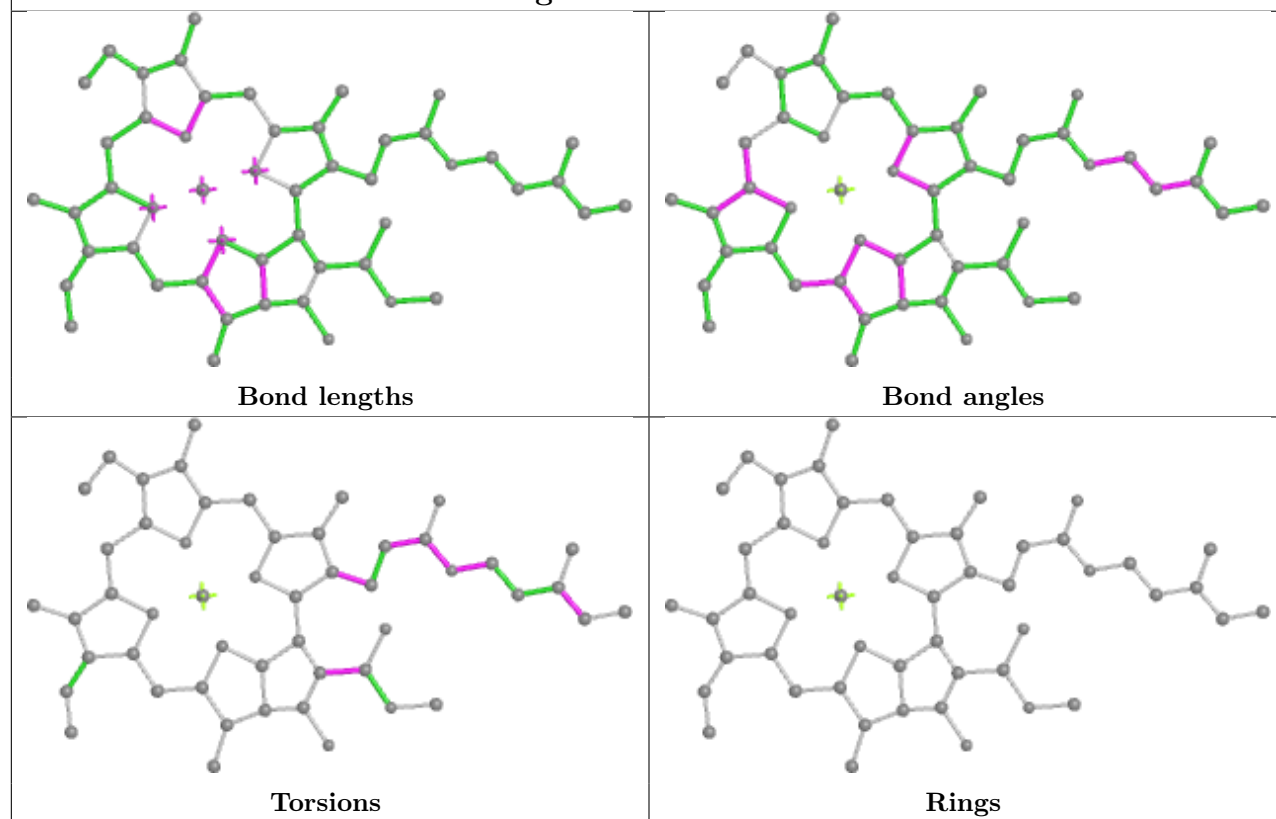
## Ligand CLA F 203



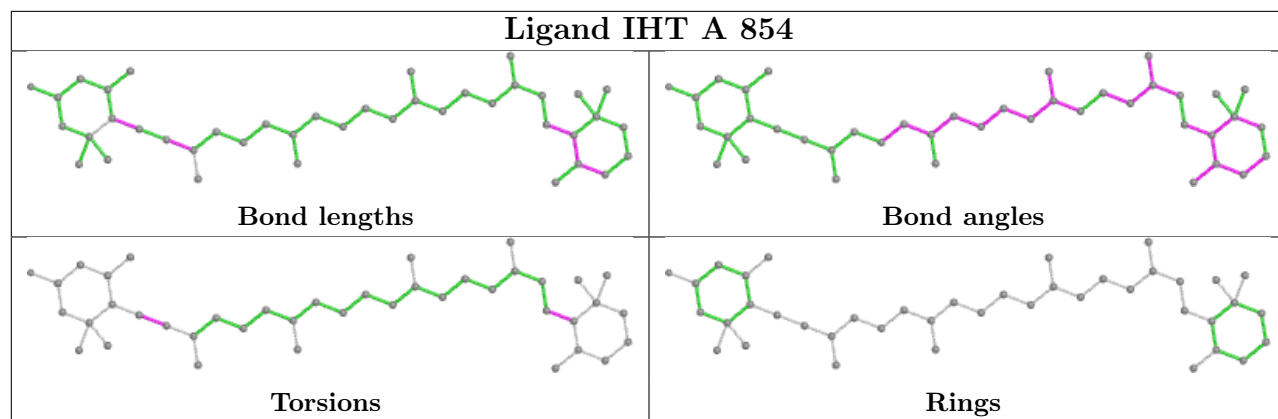
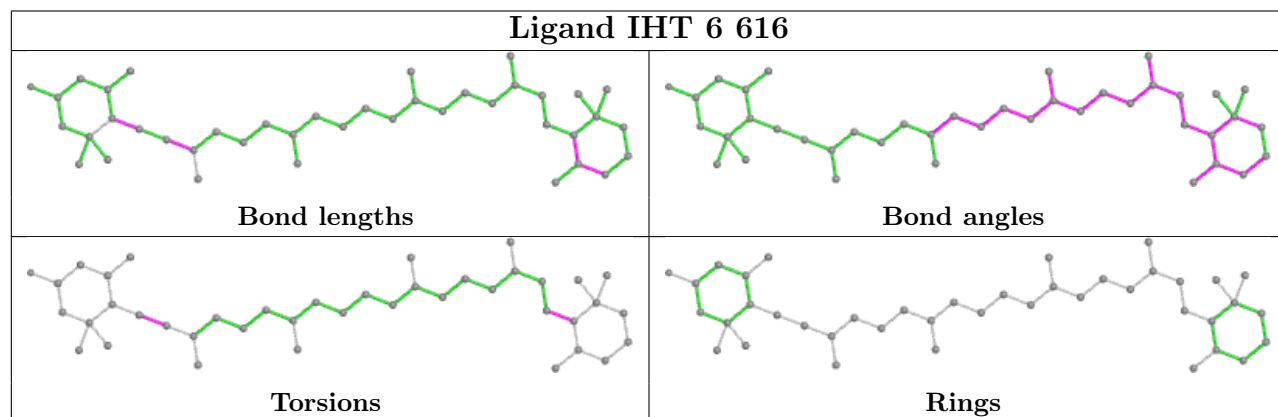
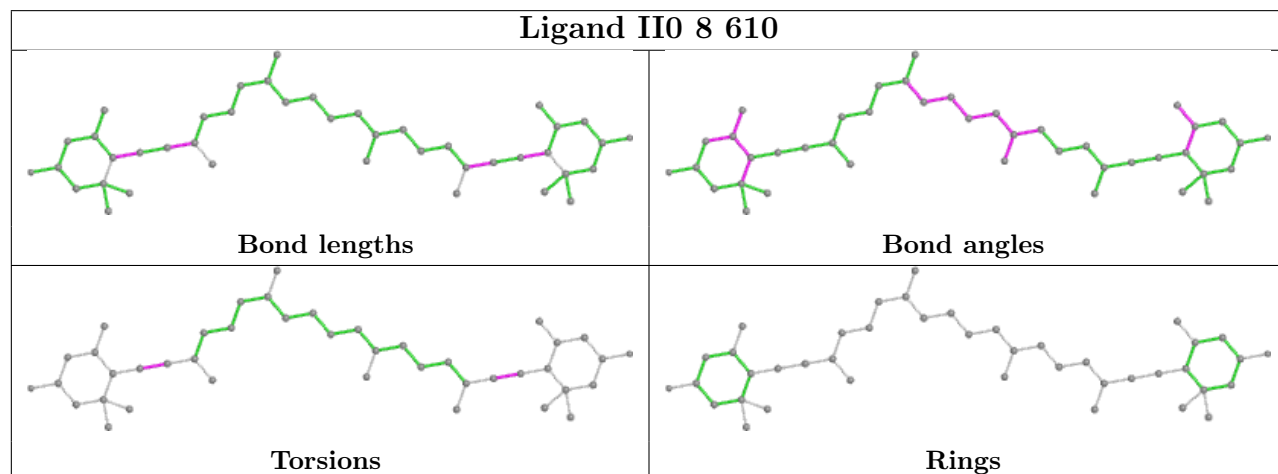
## Ligand CLA B 834



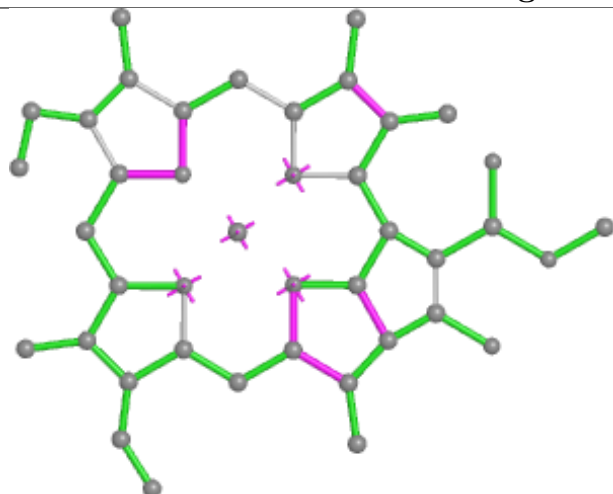
## Ligand CLA b 610



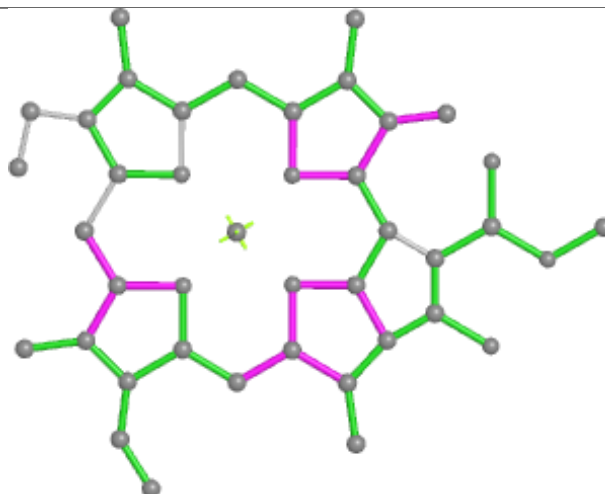


**Ligand IHT A 854****Ligand IHT 6 616****Ligand II0 8 610**

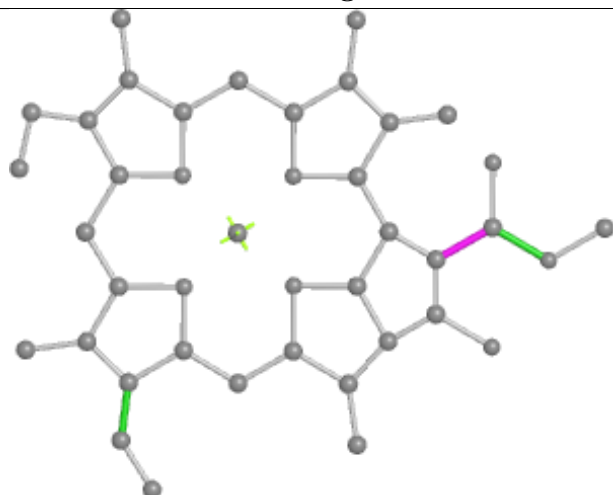
## Ligand CLA J 102



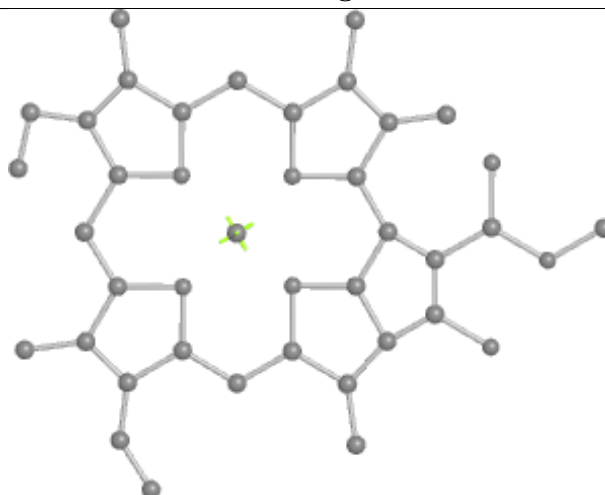
Bond lengths



Bond angles

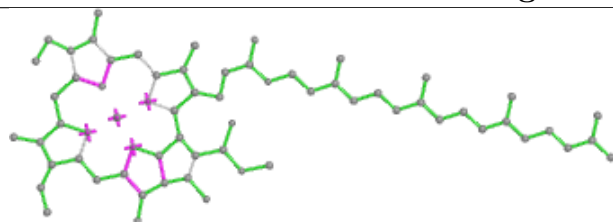


Torsions

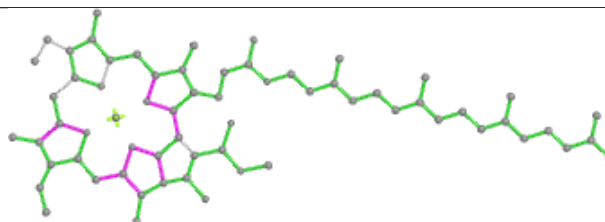


Rings

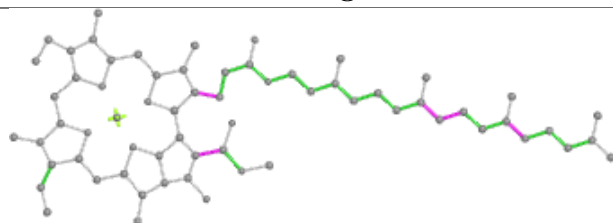
## Ligand CLA 6 602



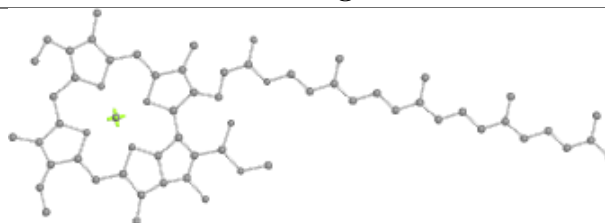
Bond lengths



Bond angles

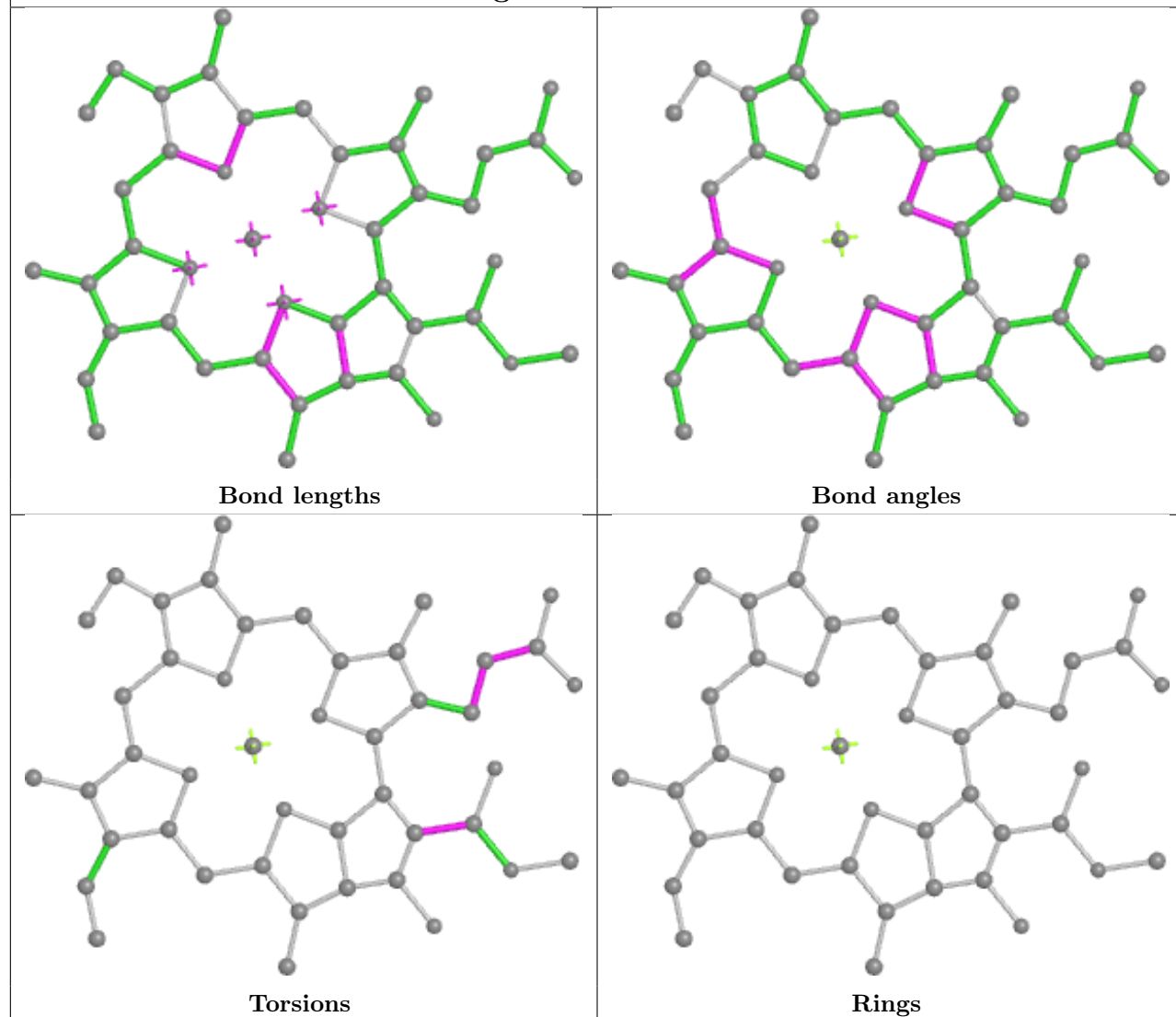


Torsions

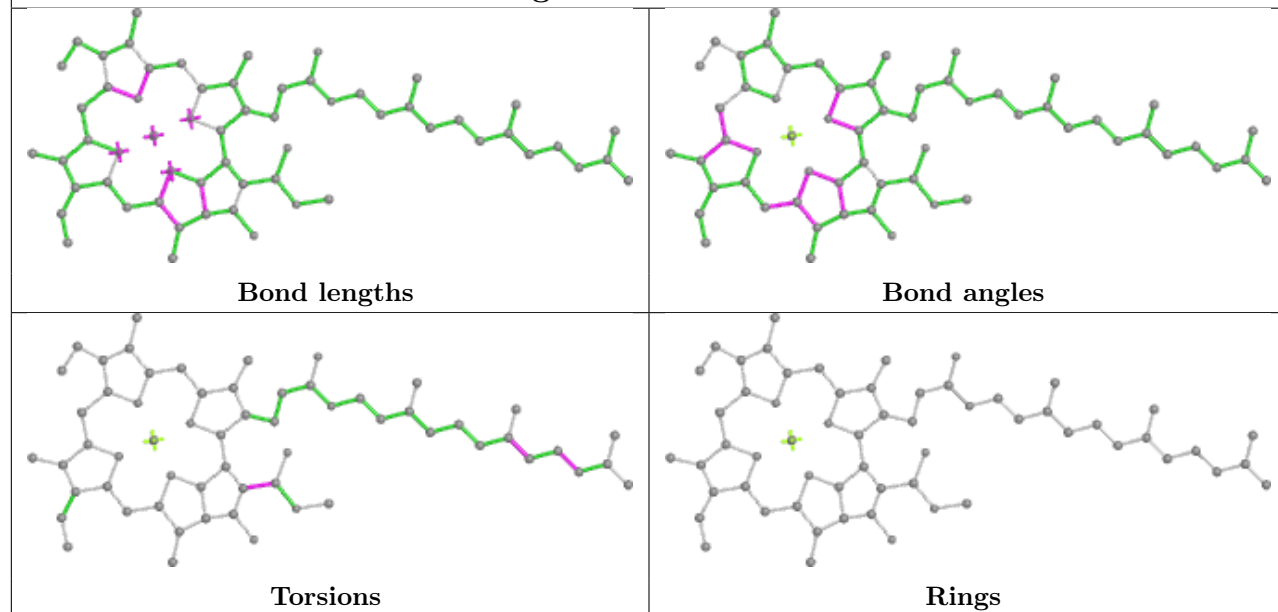


Rings

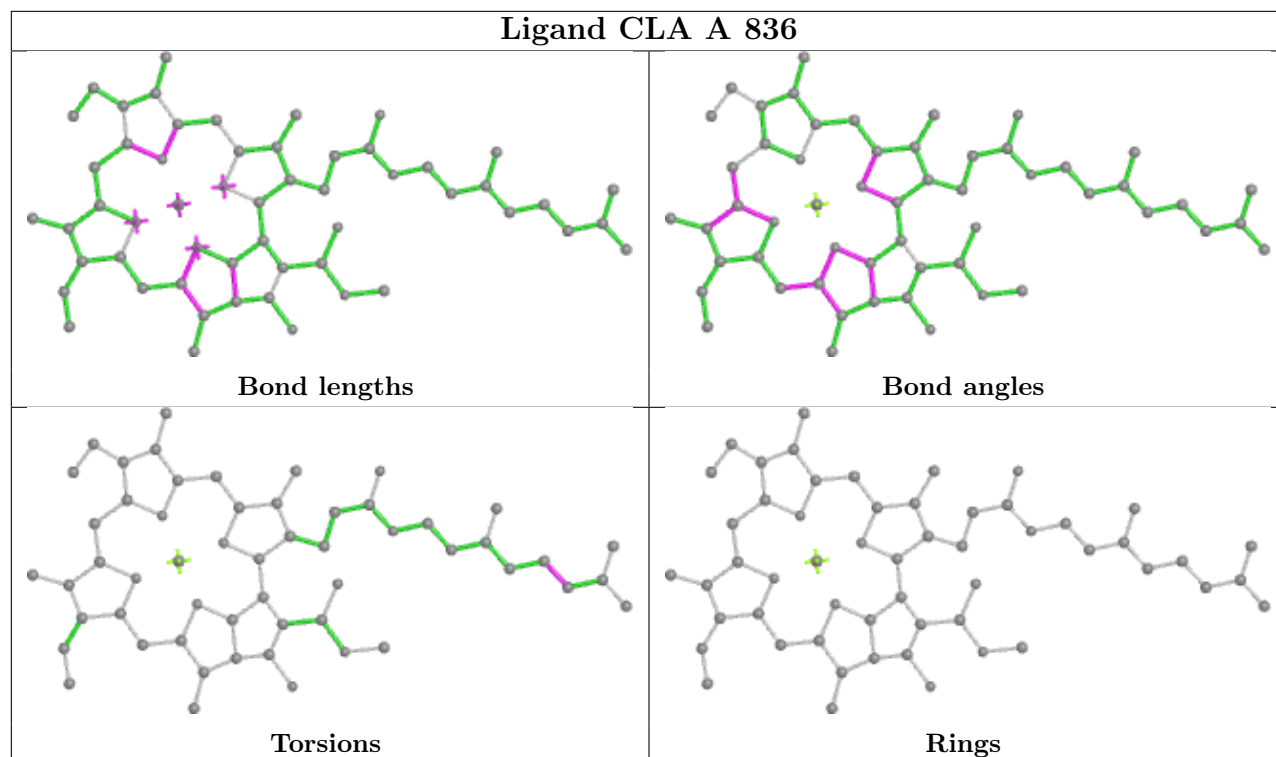
## Ligand CLA 9 603



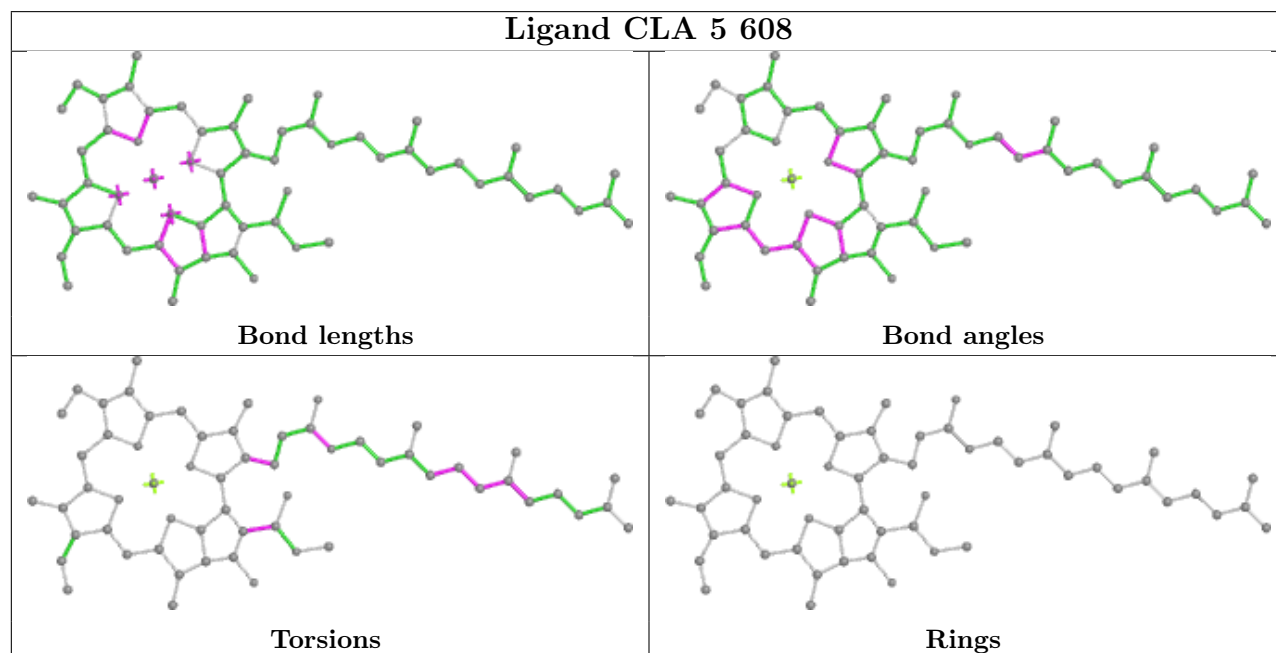
## Ligand CLA B 824



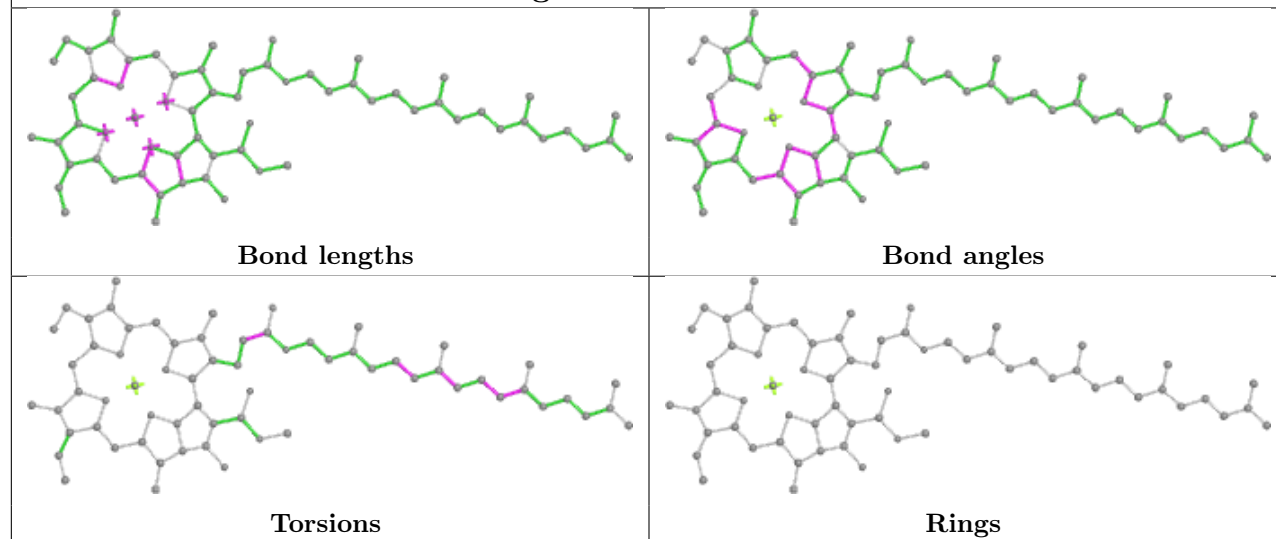
## Ligand CLA A 836



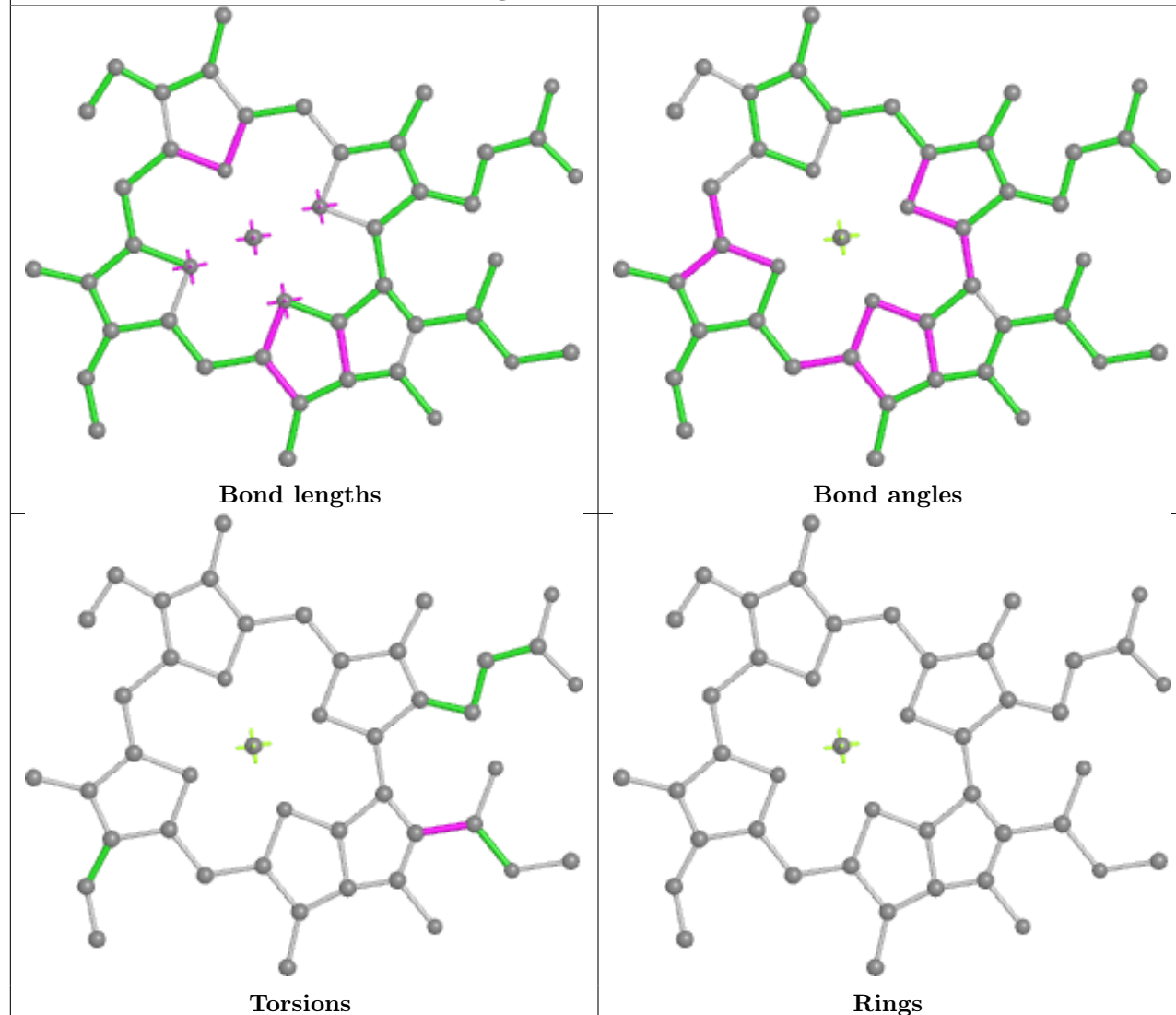
## Ligand CLA 5 608

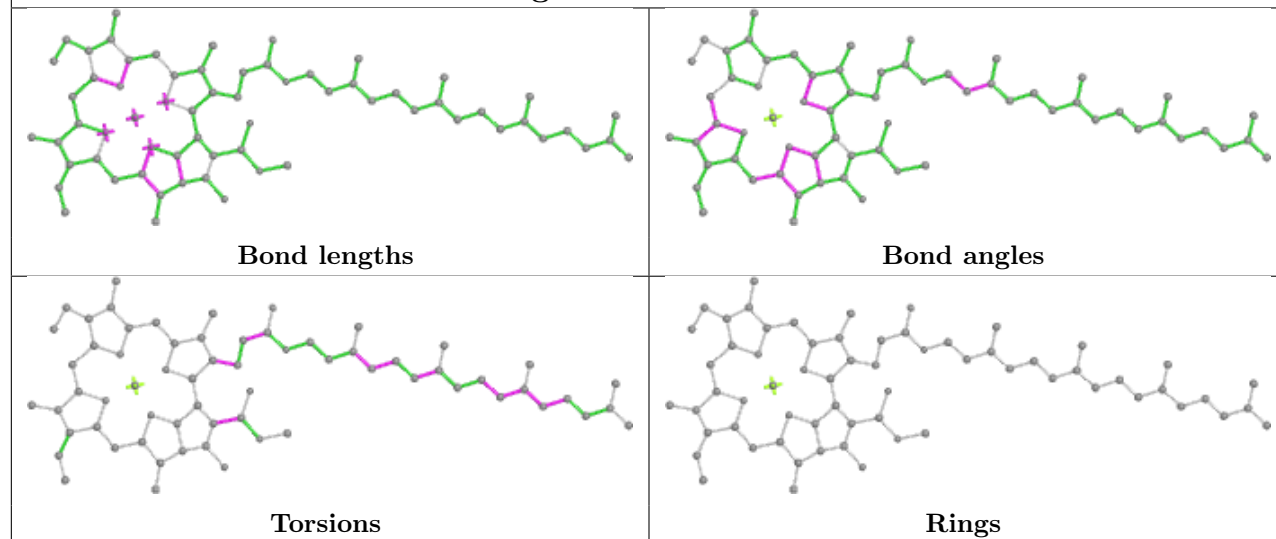
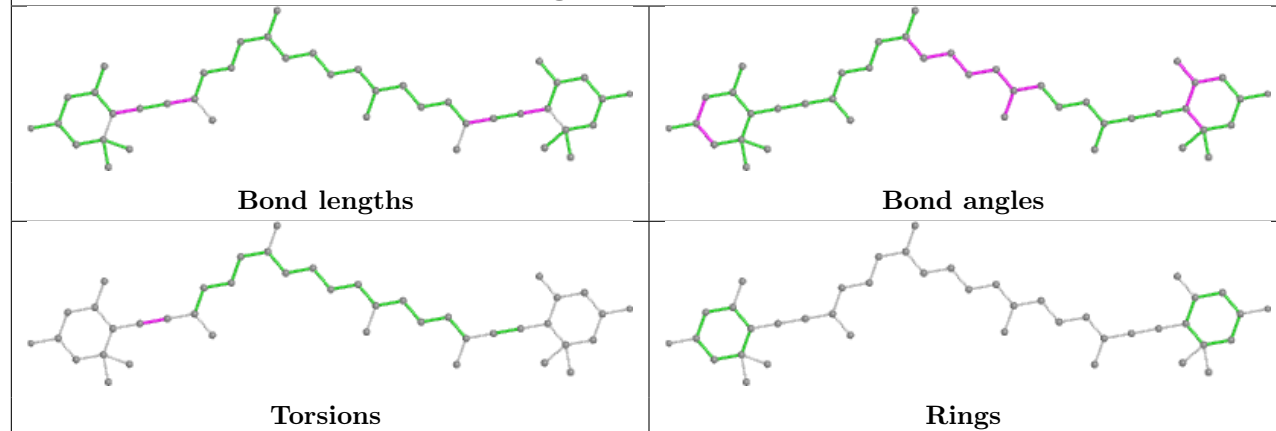


## Ligand CLA B 802

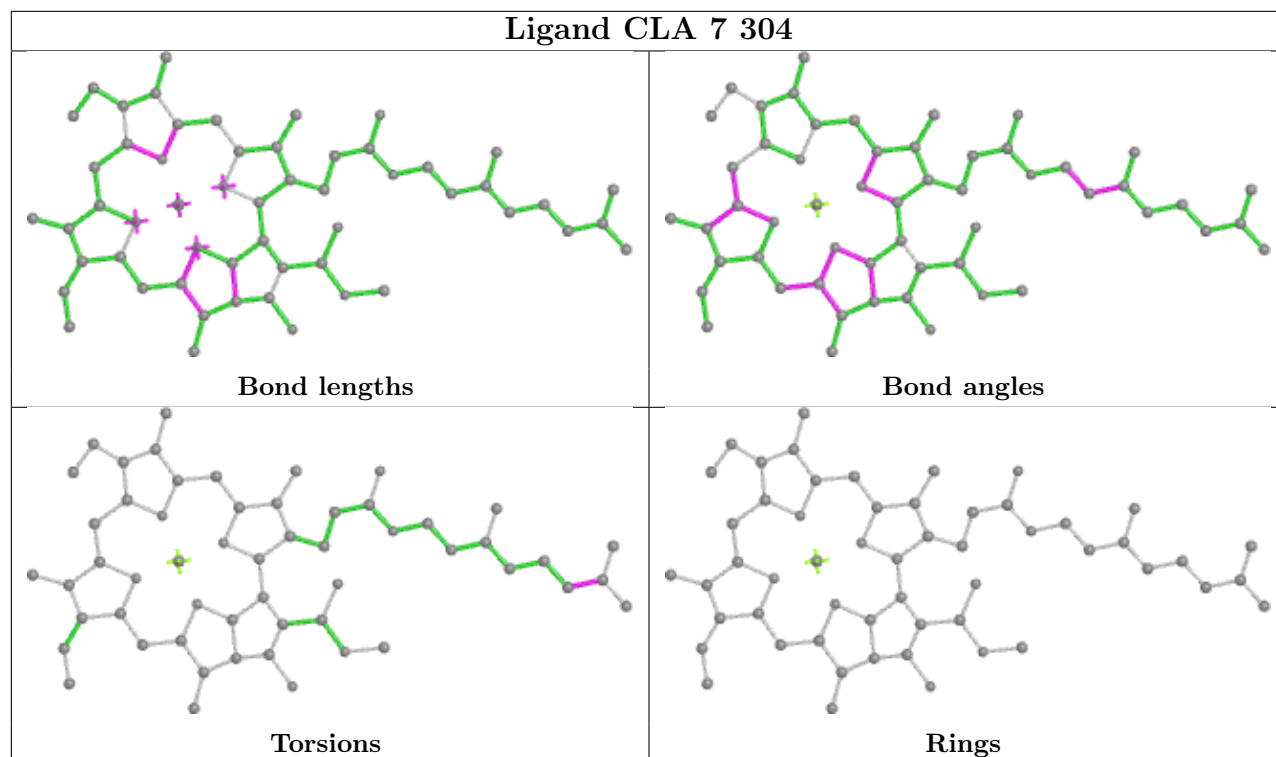


## Ligand CLA 2 611

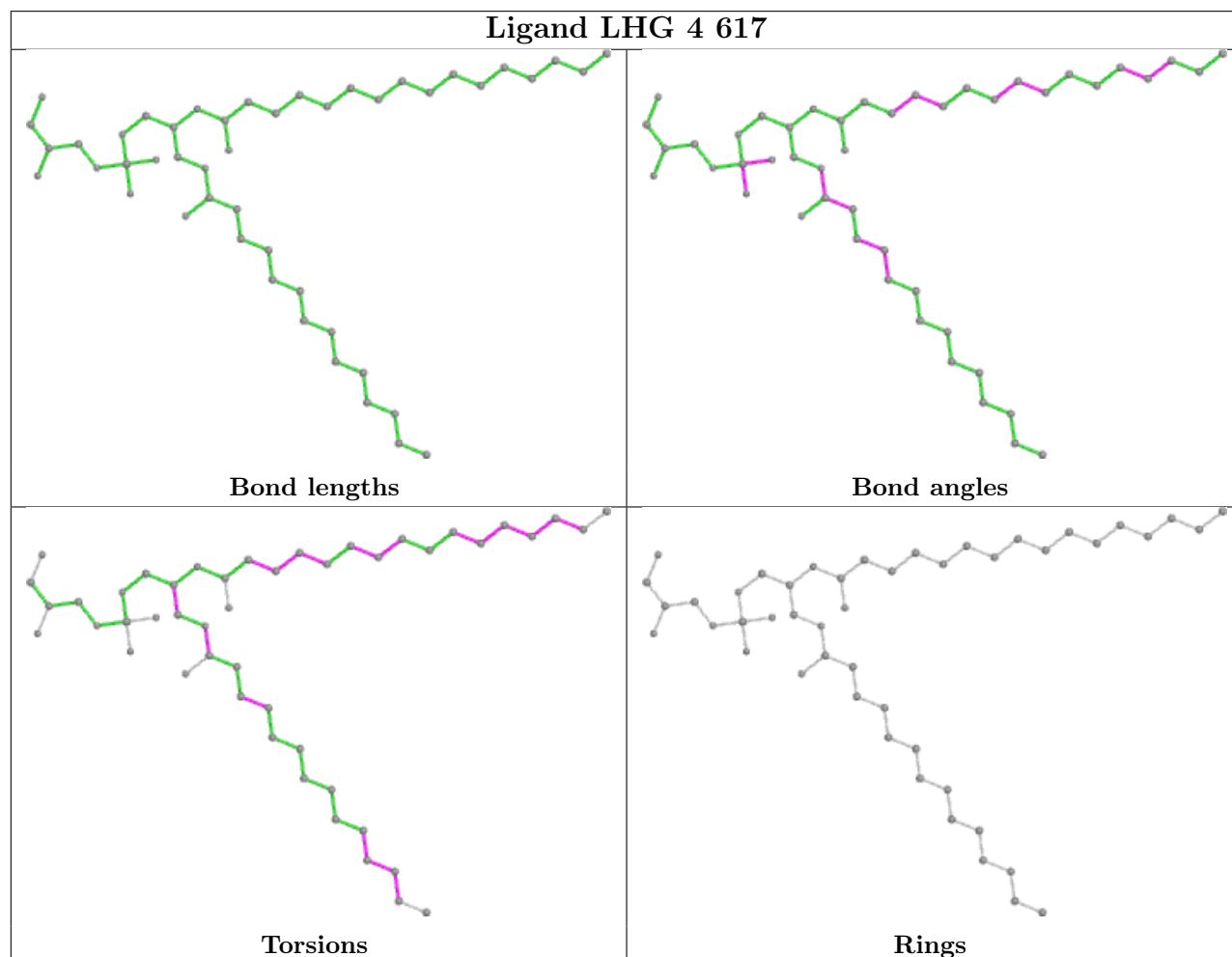


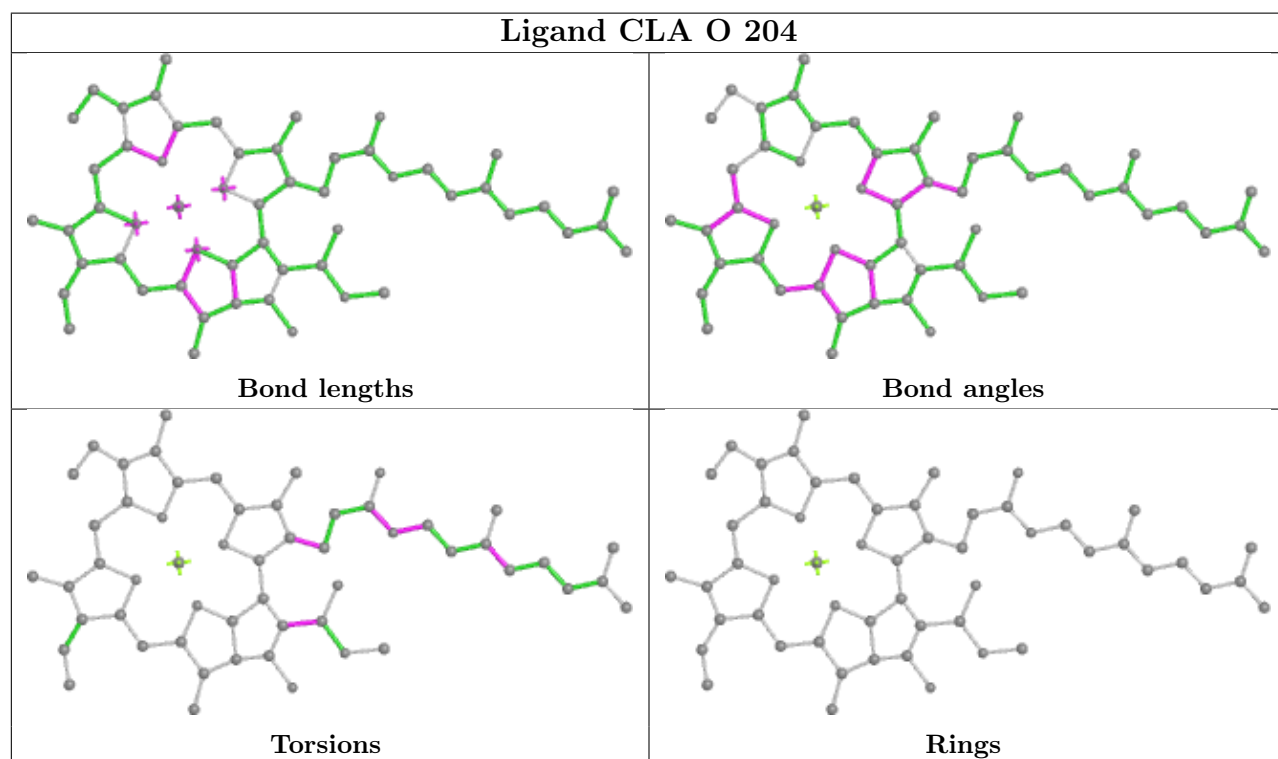
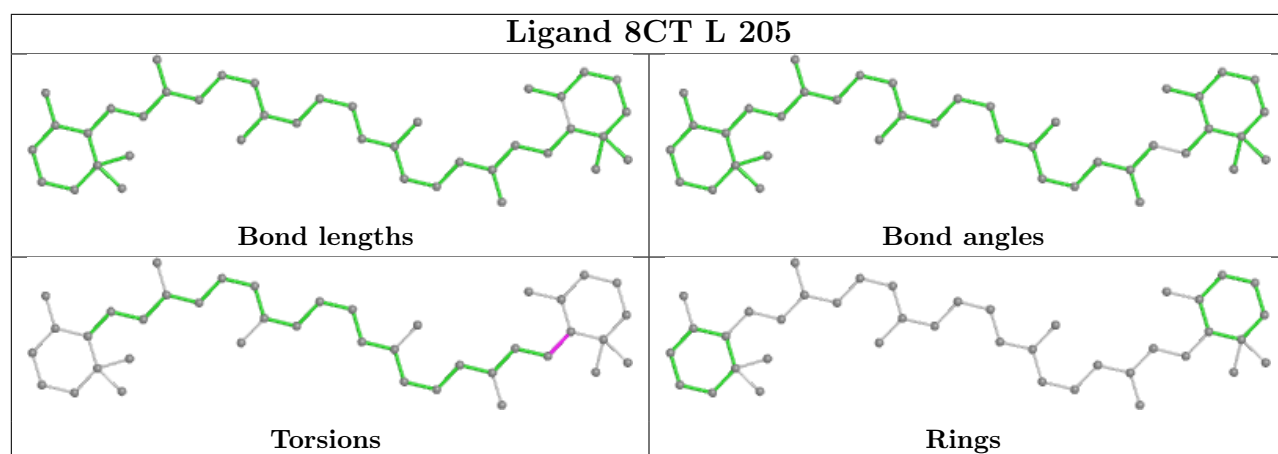
**Ligand CLA A 804****Ligand II0 6 614**

## Ligand CLA 7 304



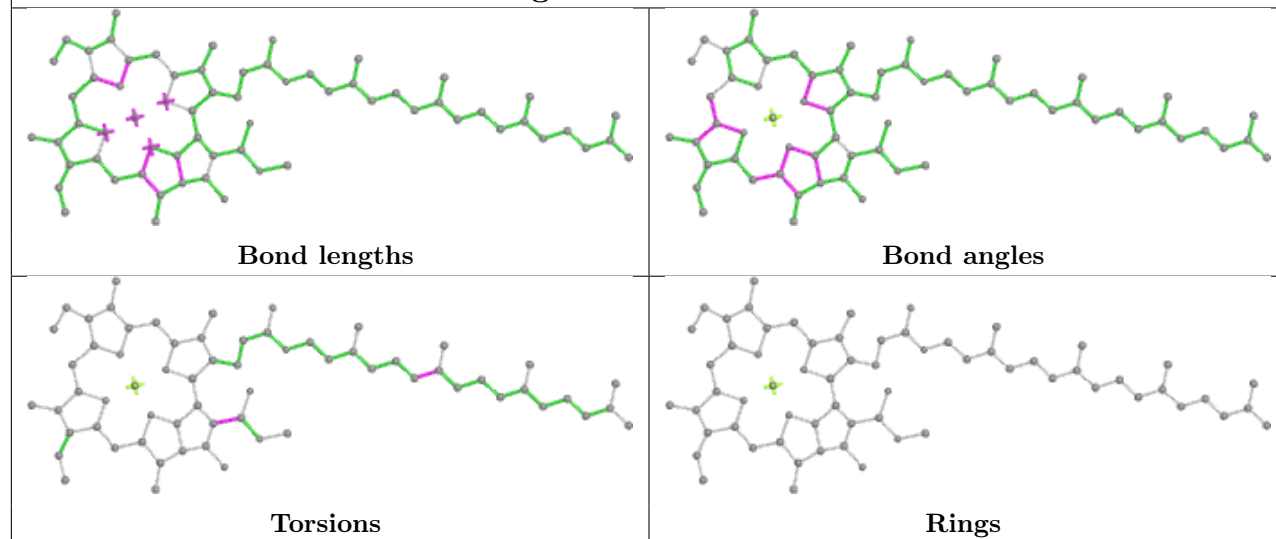
## Ligand LHG 4 617



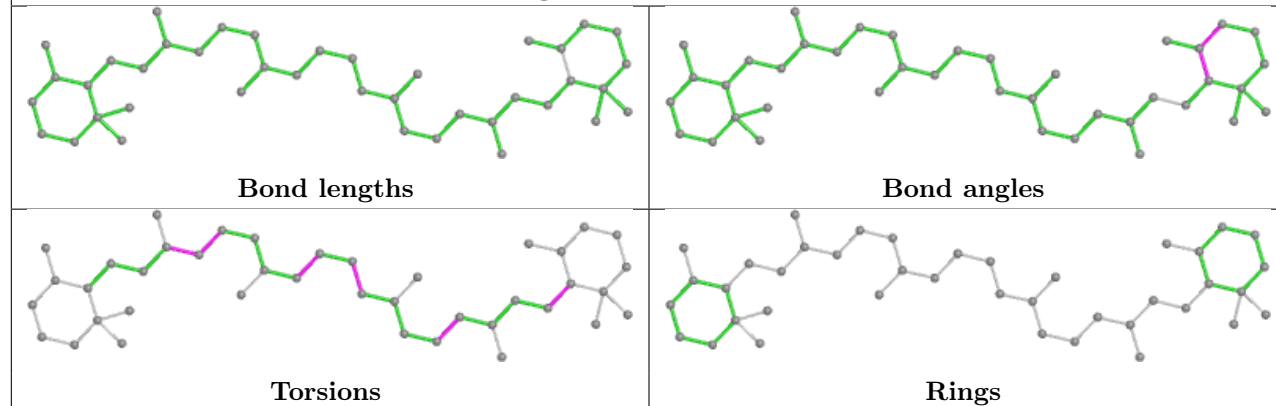




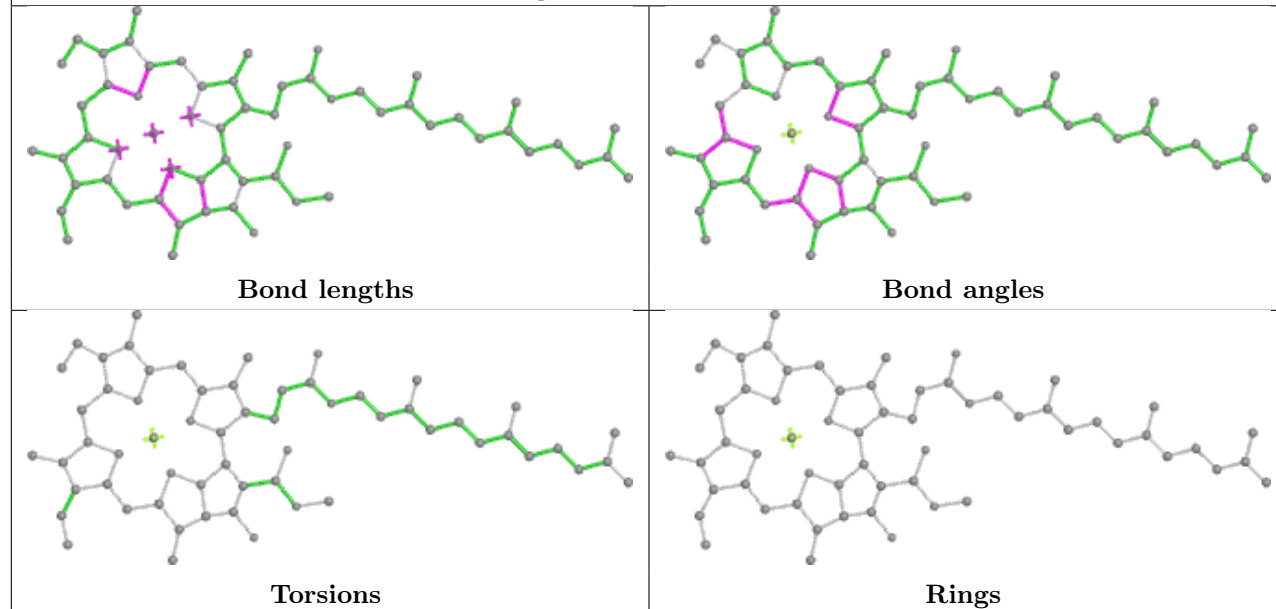
## Ligand CLA A 824



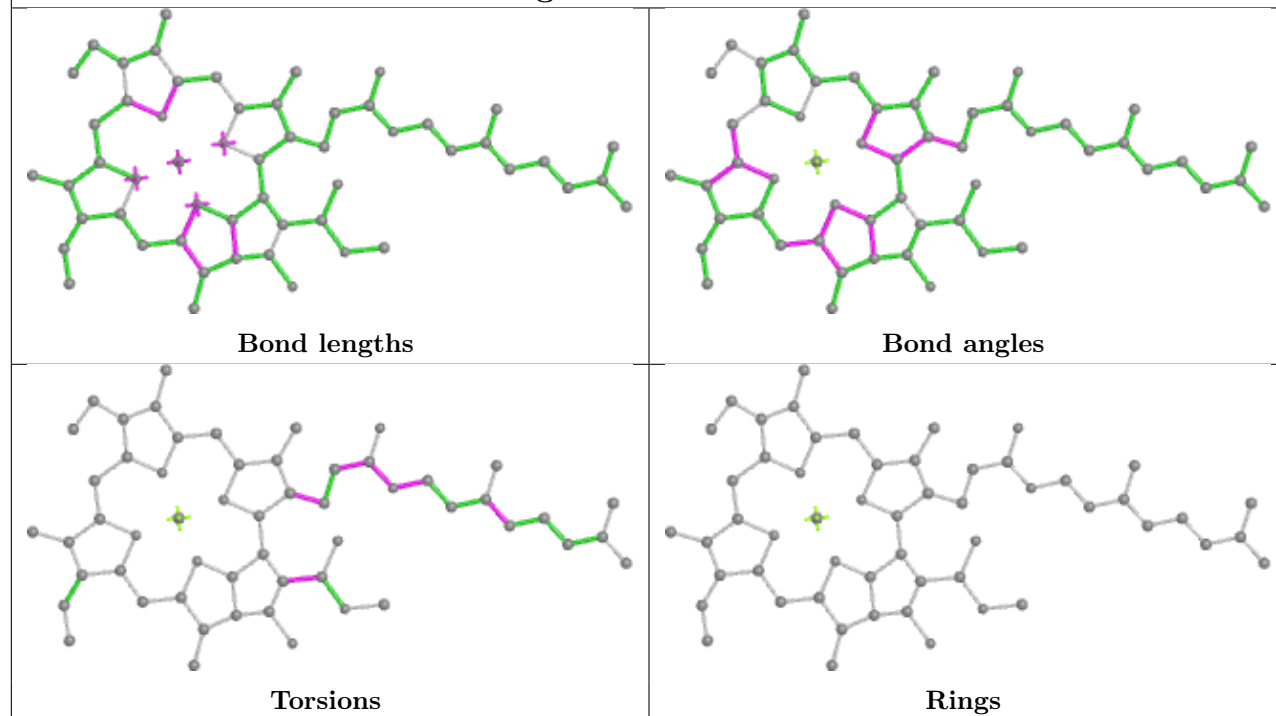
## Ligand 8CT B 845



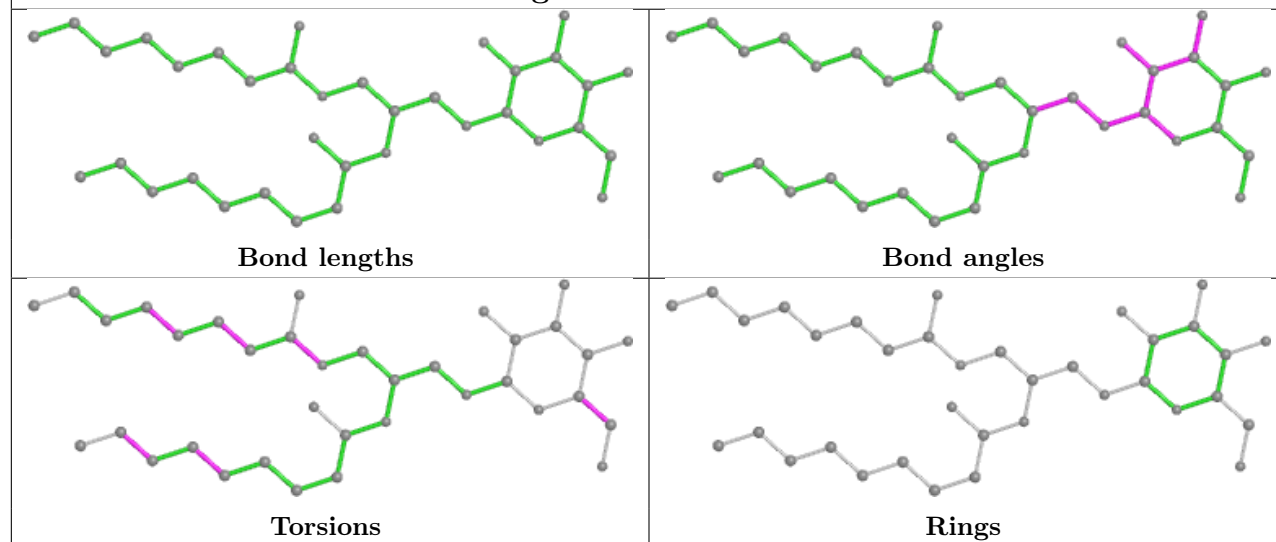
## Ligand CLA B 830



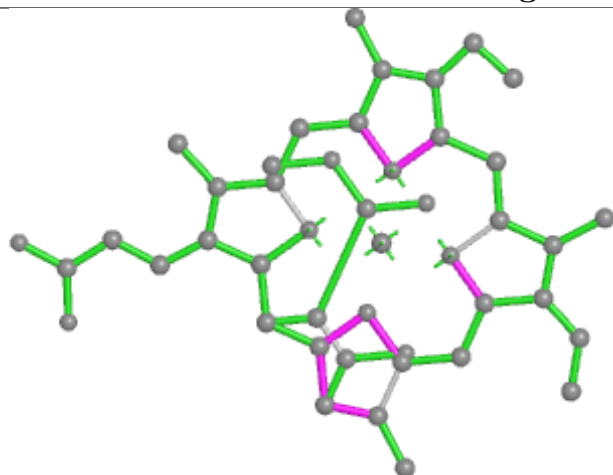
## Ligand CLA a 605



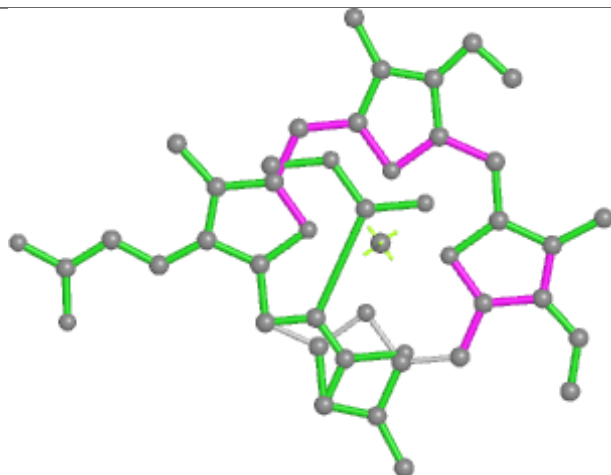
## Ligand LMG 2 617



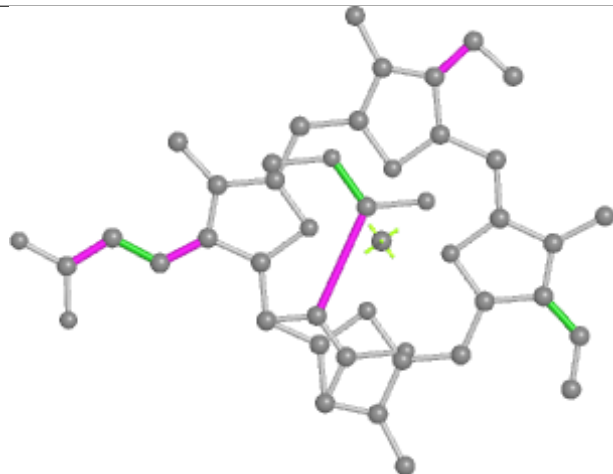
## Ligand KC2 b 605



Bond lengths



Bond angles

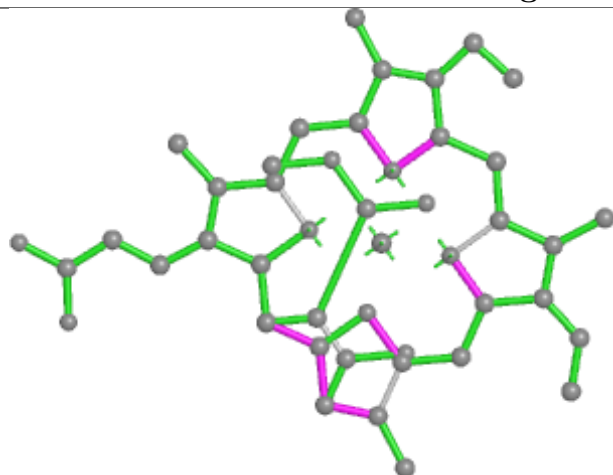


Torsions

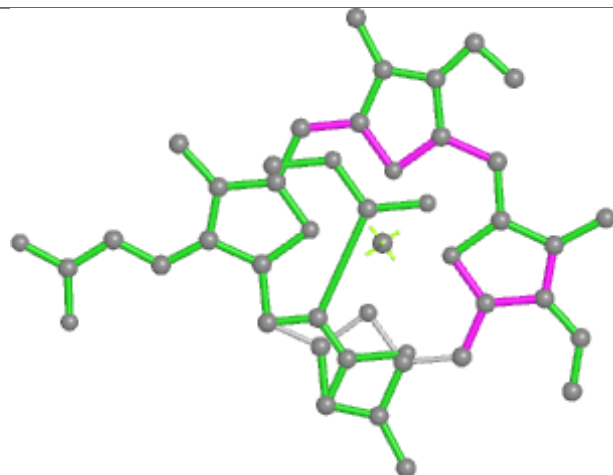


Rings

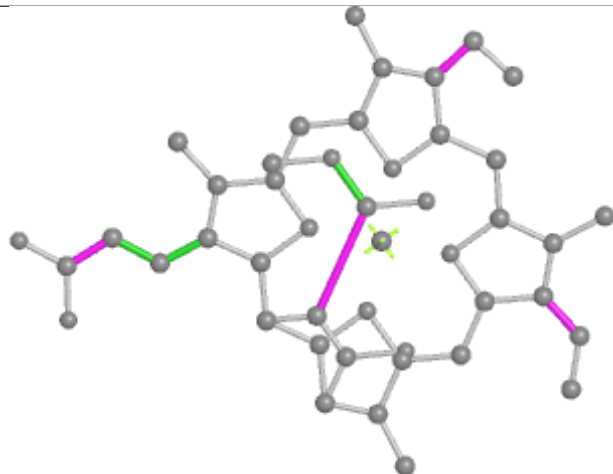
## Ligand KC2 4 605



Bond lengths



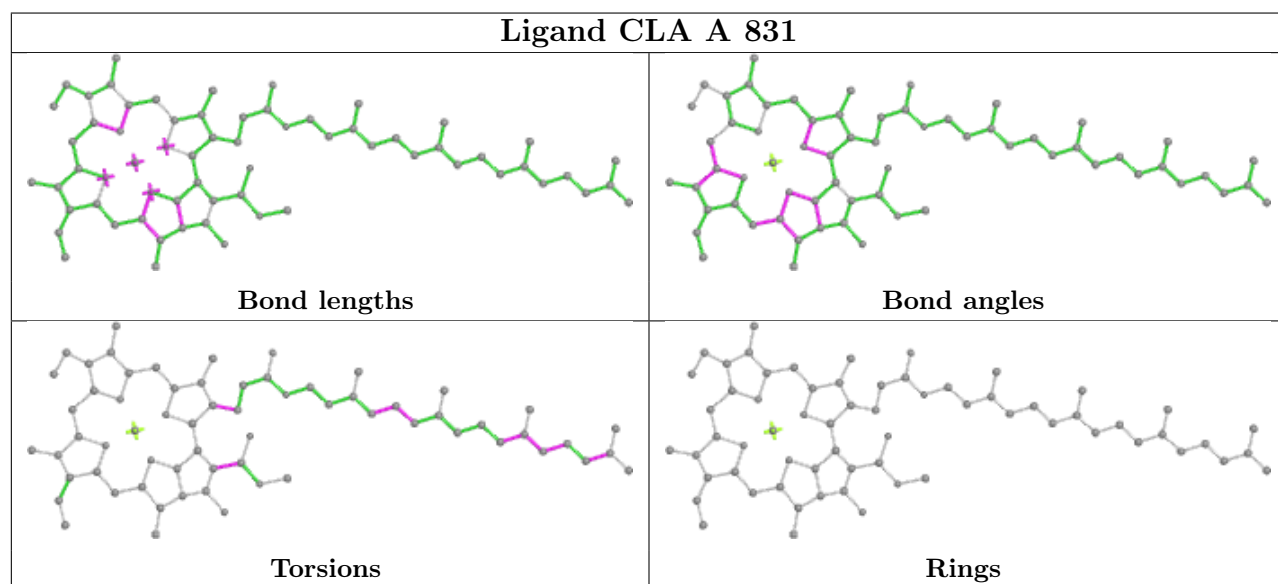
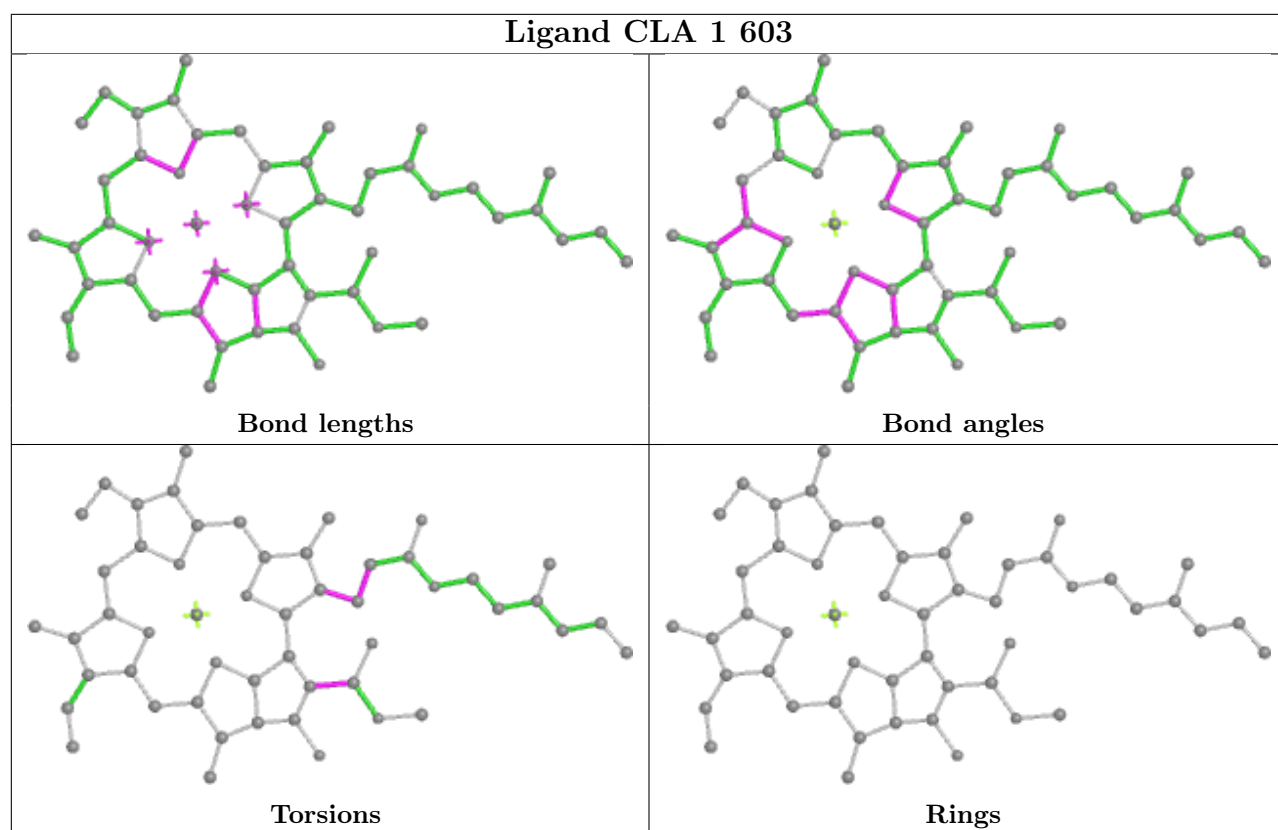
Bond angles



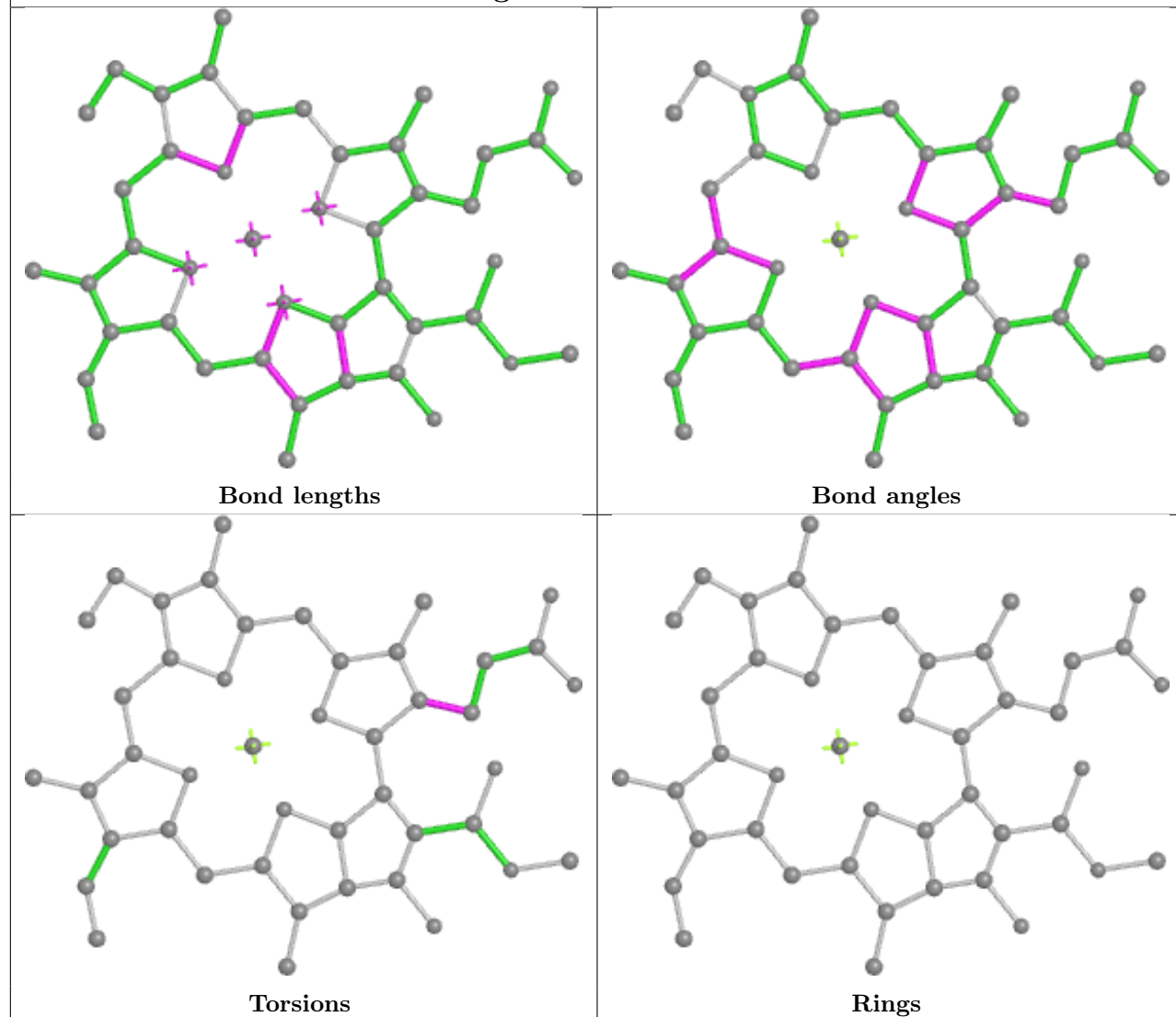
Torsions



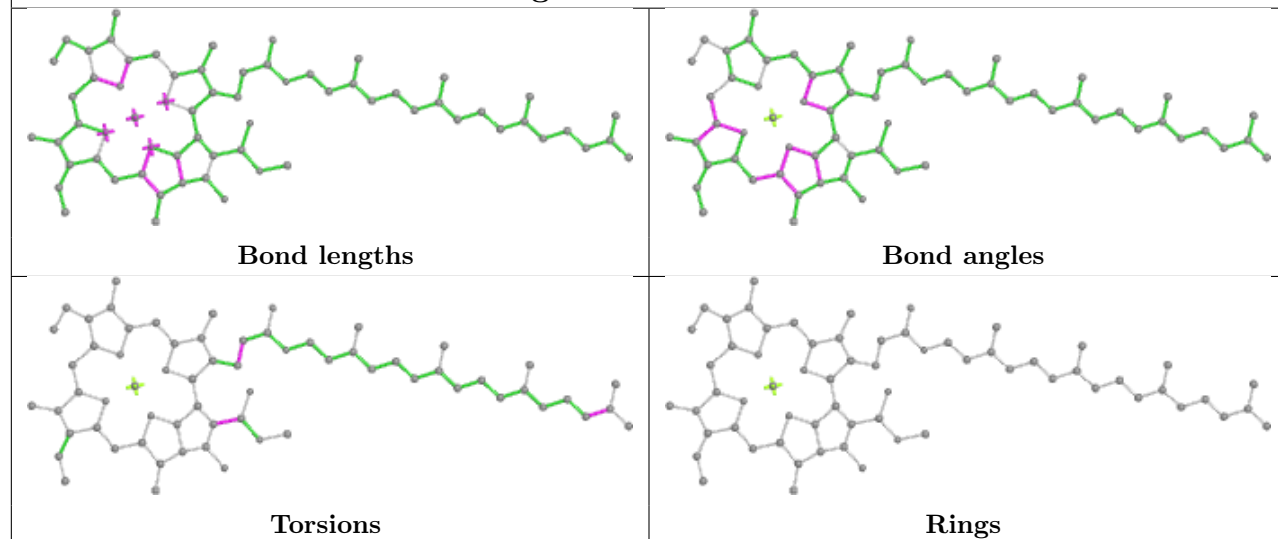
Rings



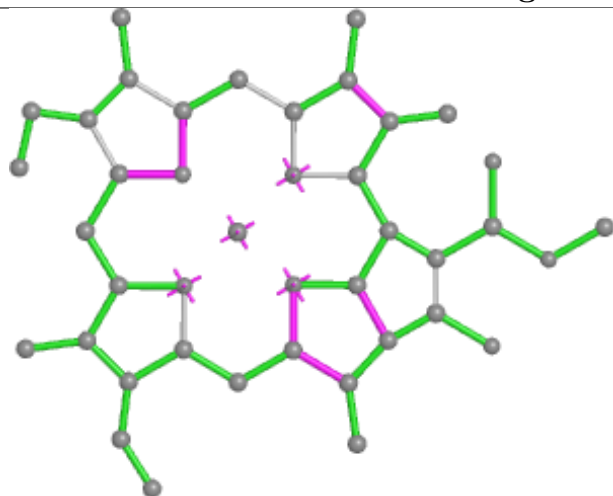
## Ligand CLA 6 612



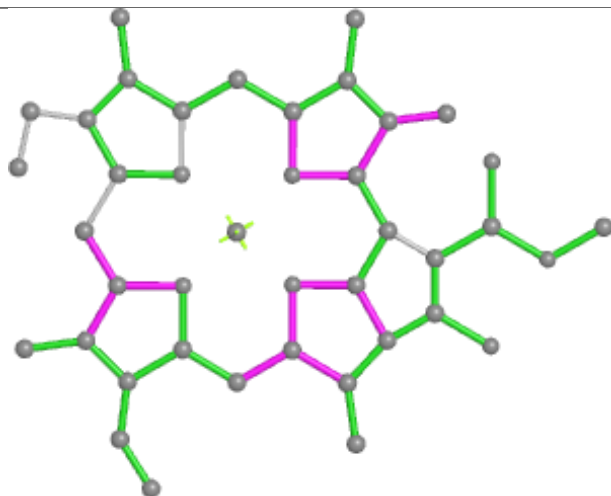
## Ligand CLA A 838



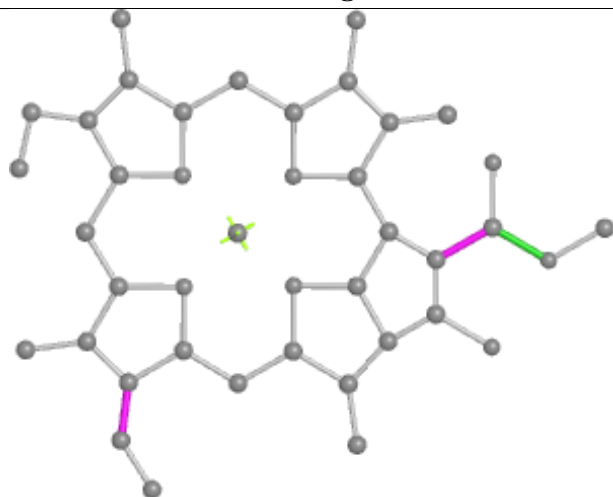
## Ligand CLA 9 609



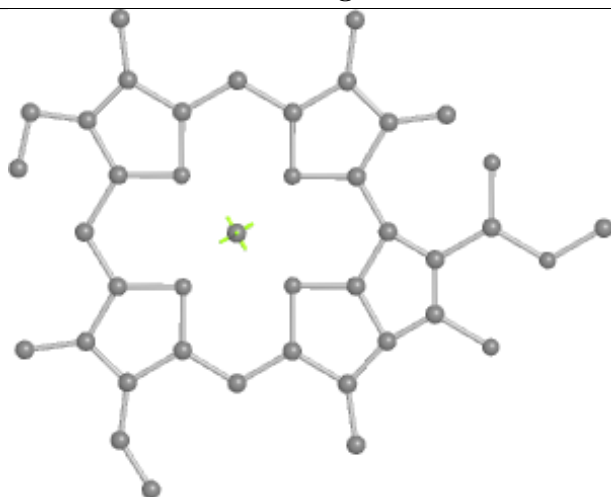
Bond lengths



Bond angles

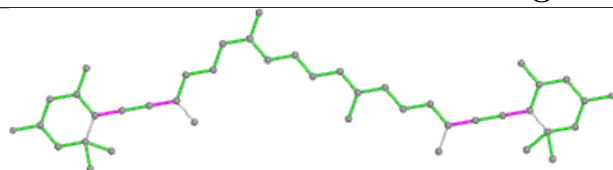


Torsions

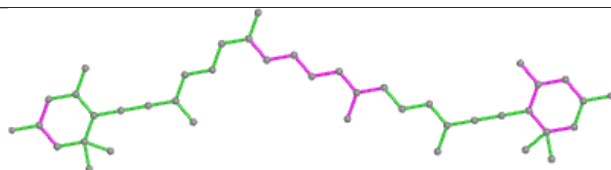


Rings

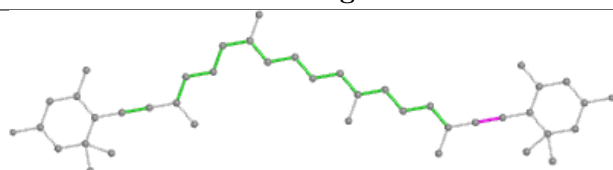
## Ligand II0 a 615



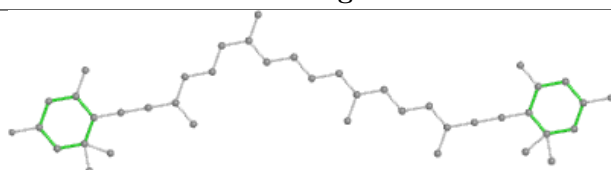
Bond lengths



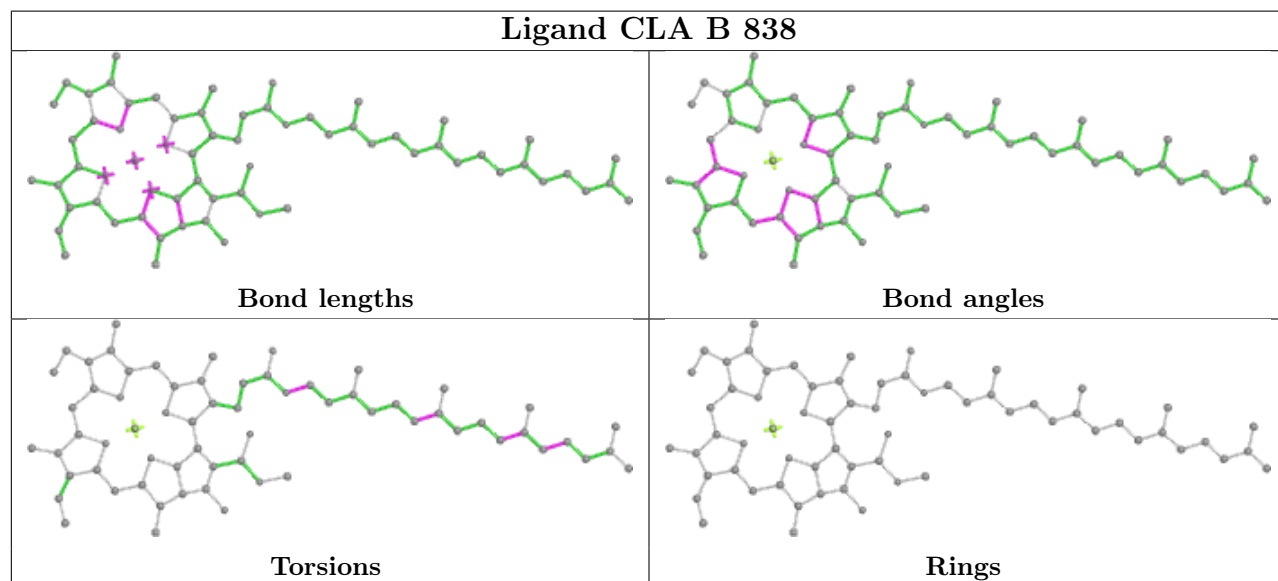
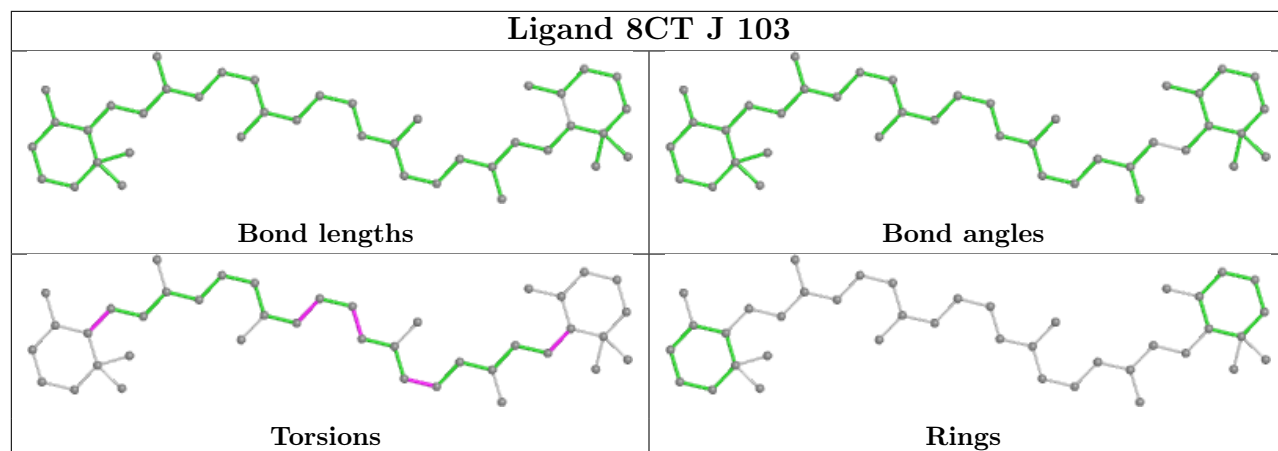
Bond angles



Torsions

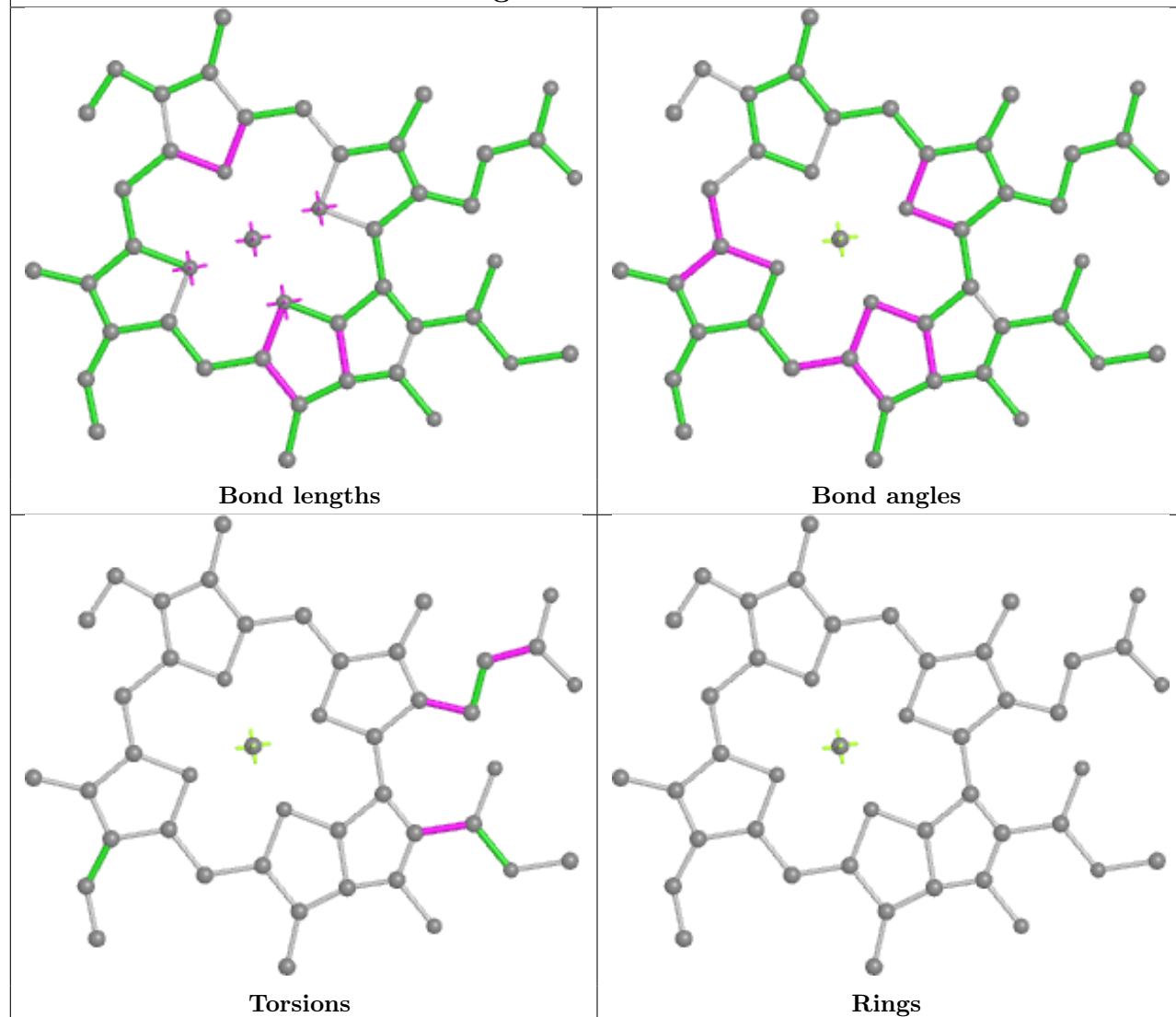


Rings

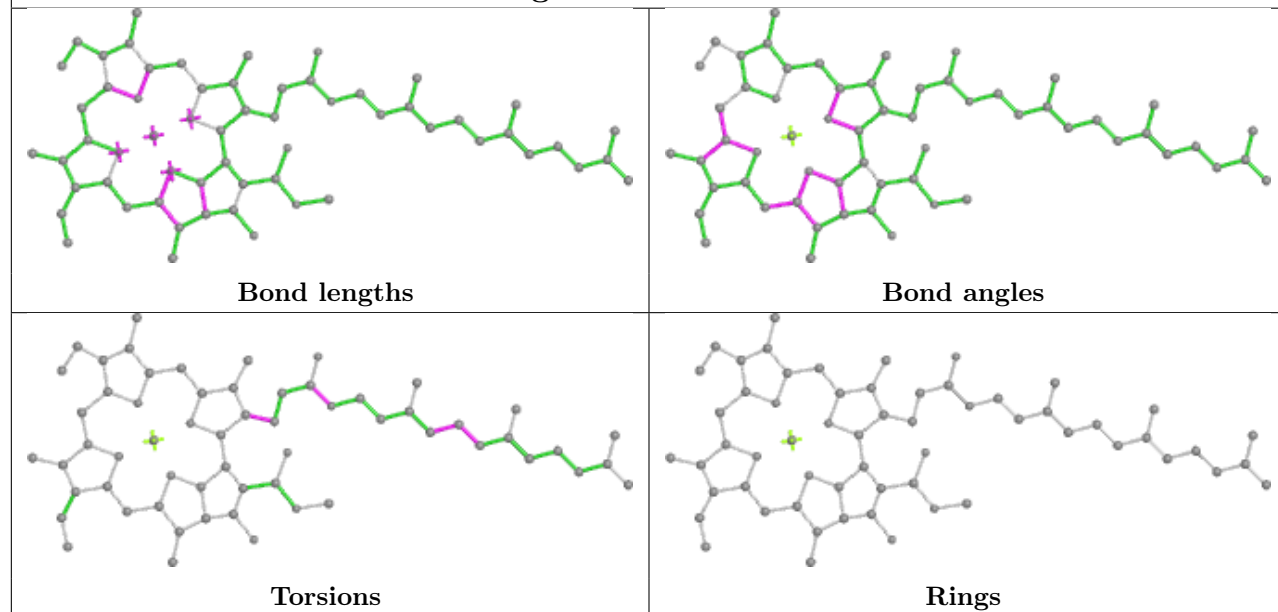




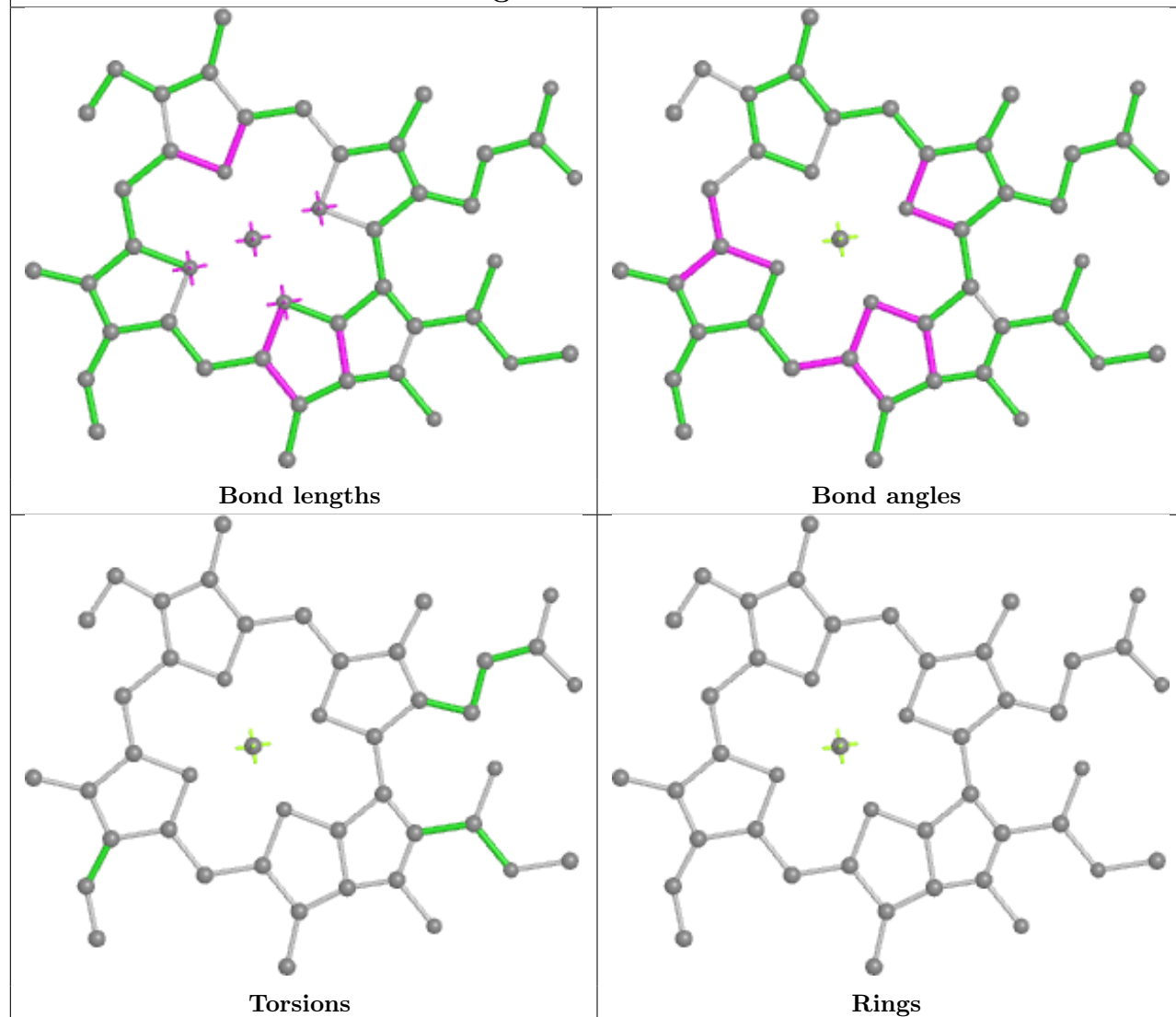
## Ligand CLA 5 606



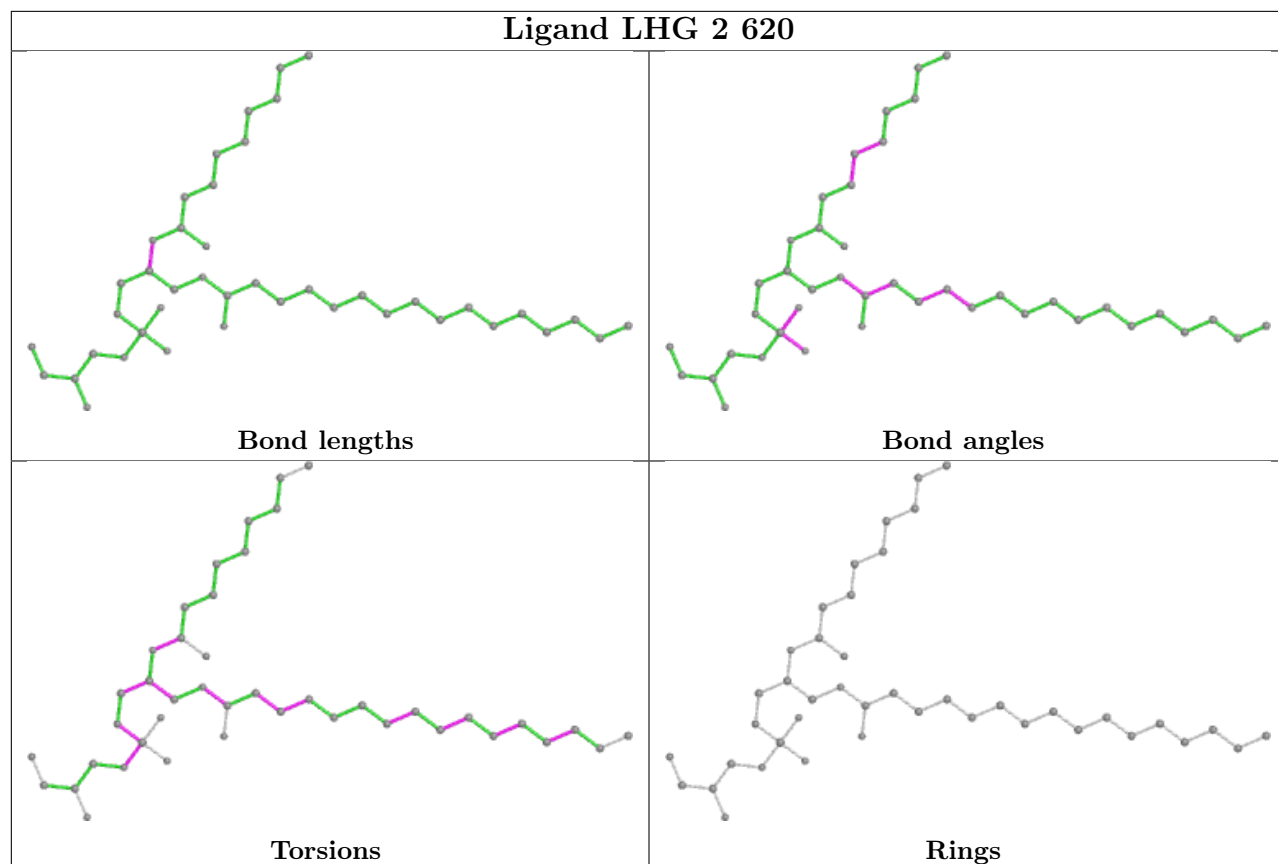
## Ligand CLA A 830



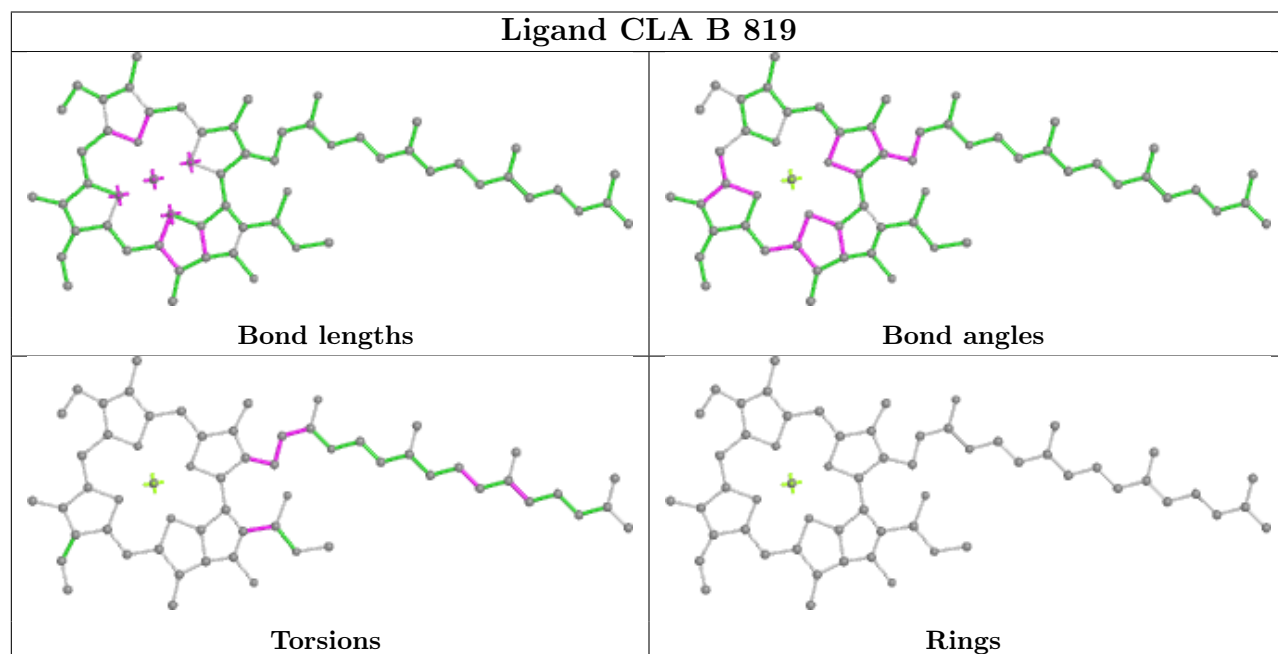
## Ligand CLA 1 606



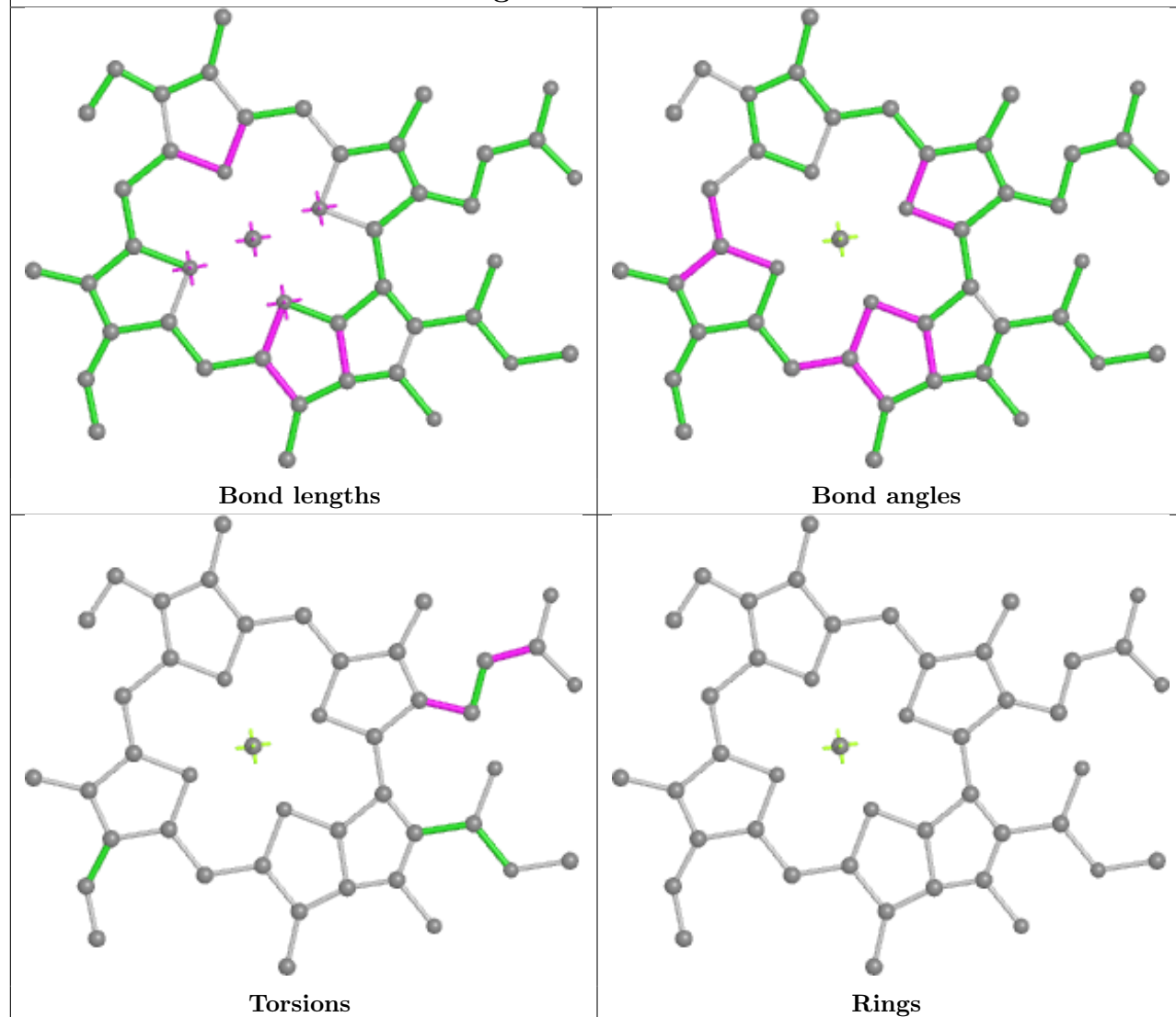
## Ligand LHG 2 620



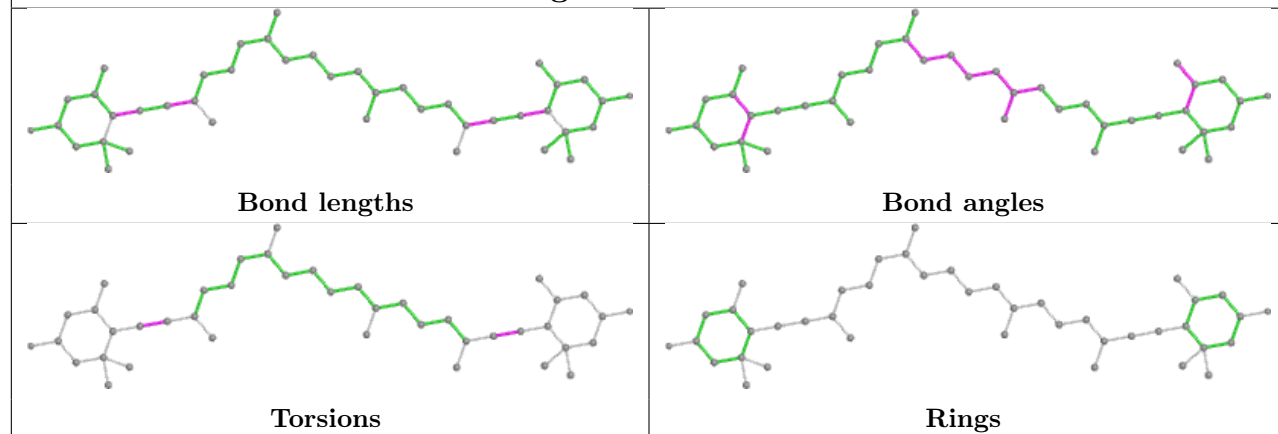
## Ligand CLA B 819

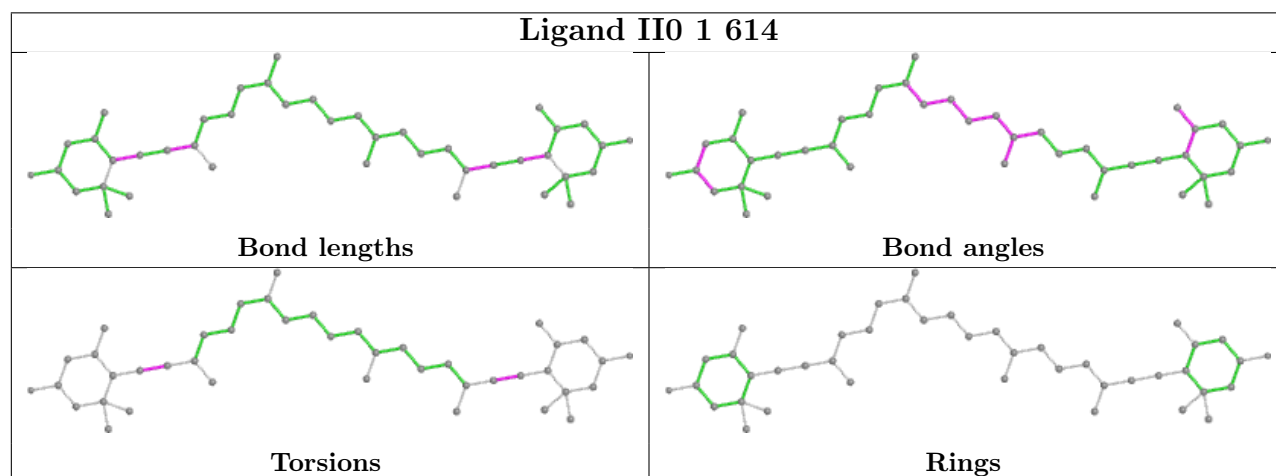
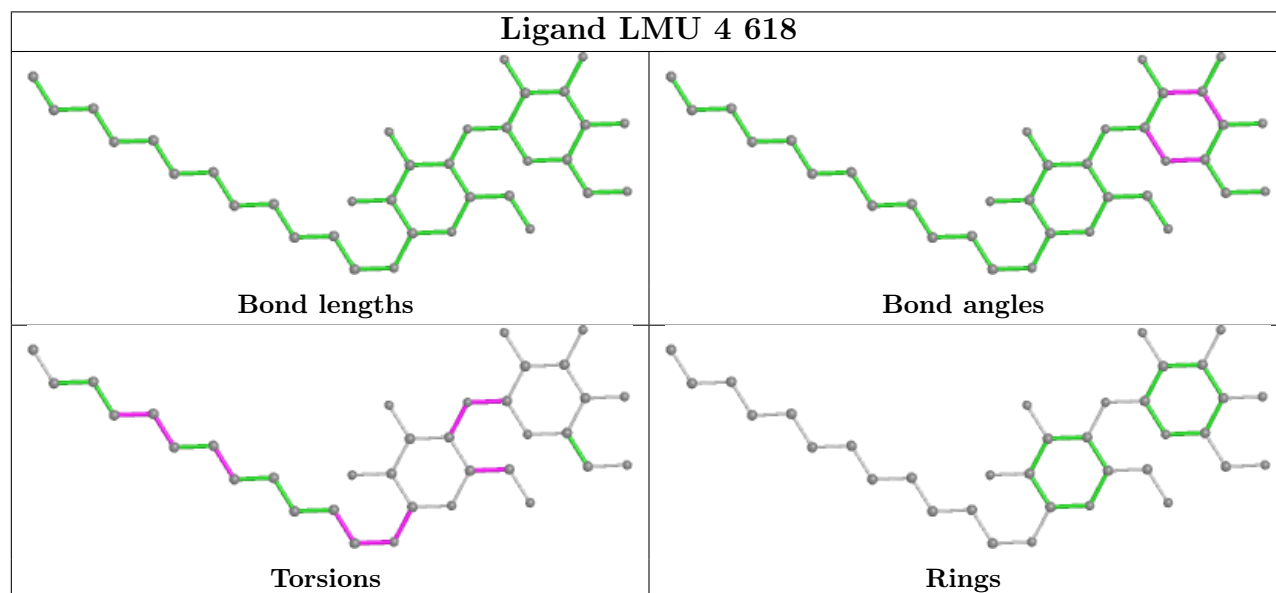
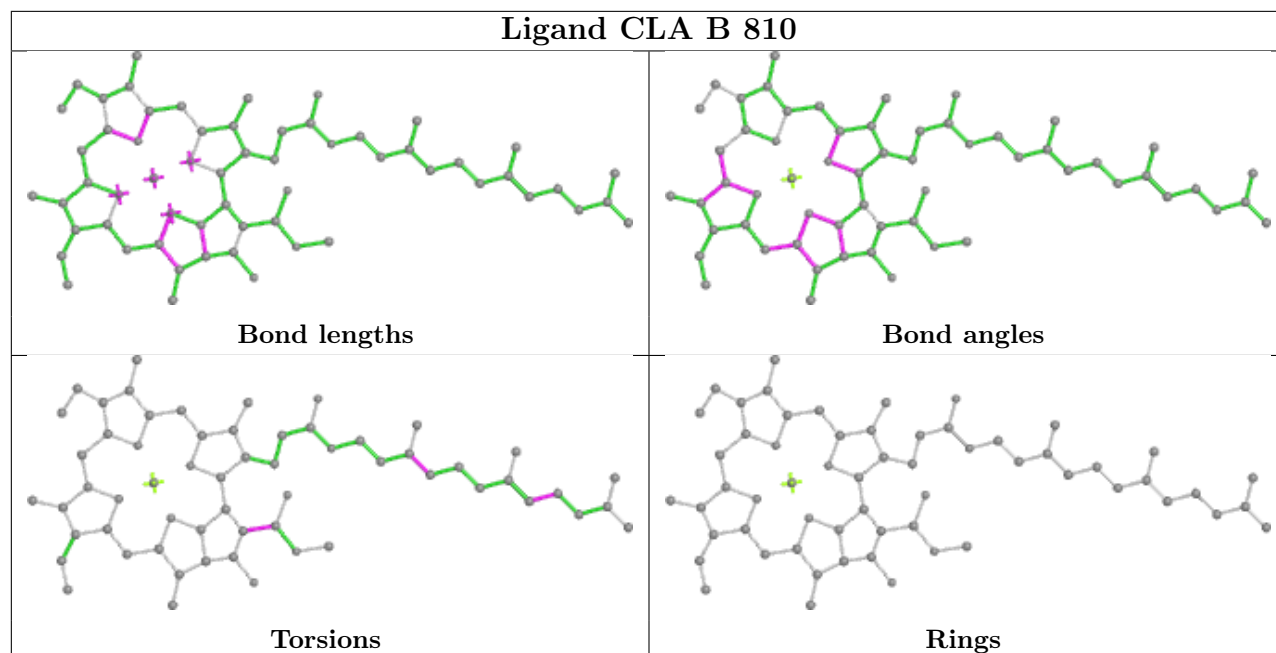


## Ligand CLA 8 601

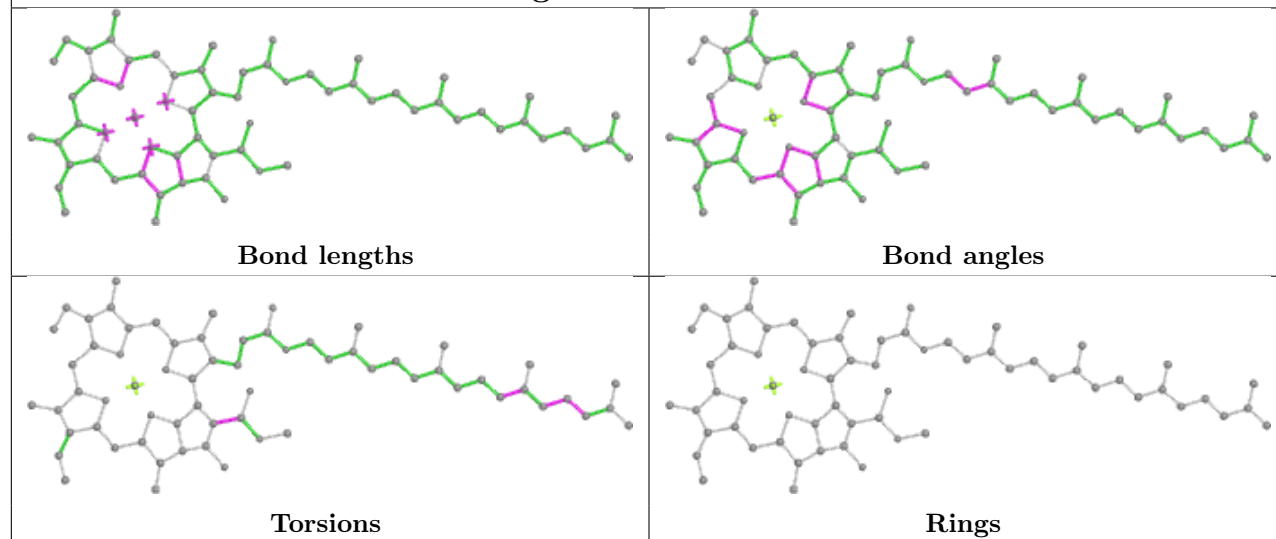


## Ligand II0 4 612

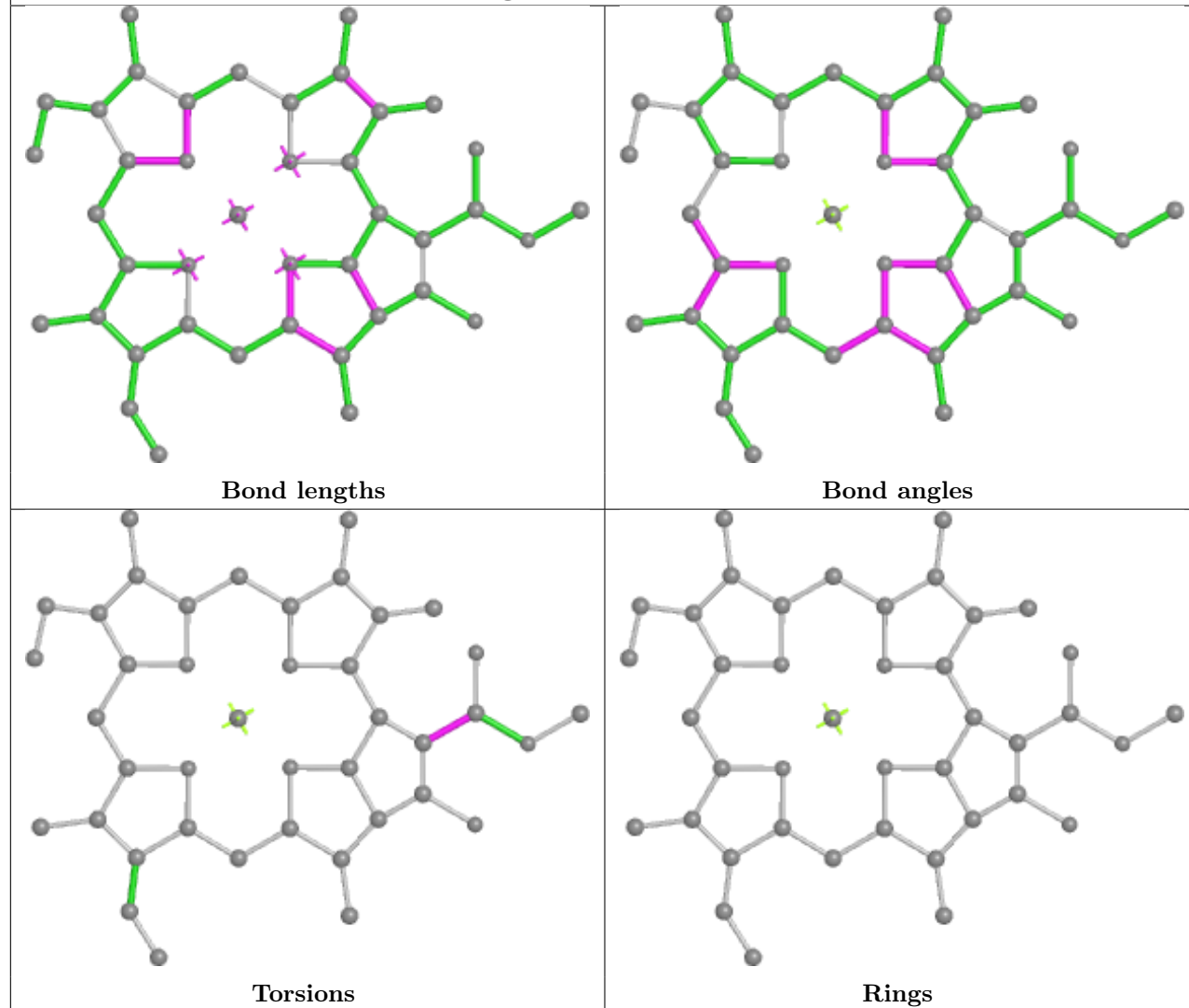


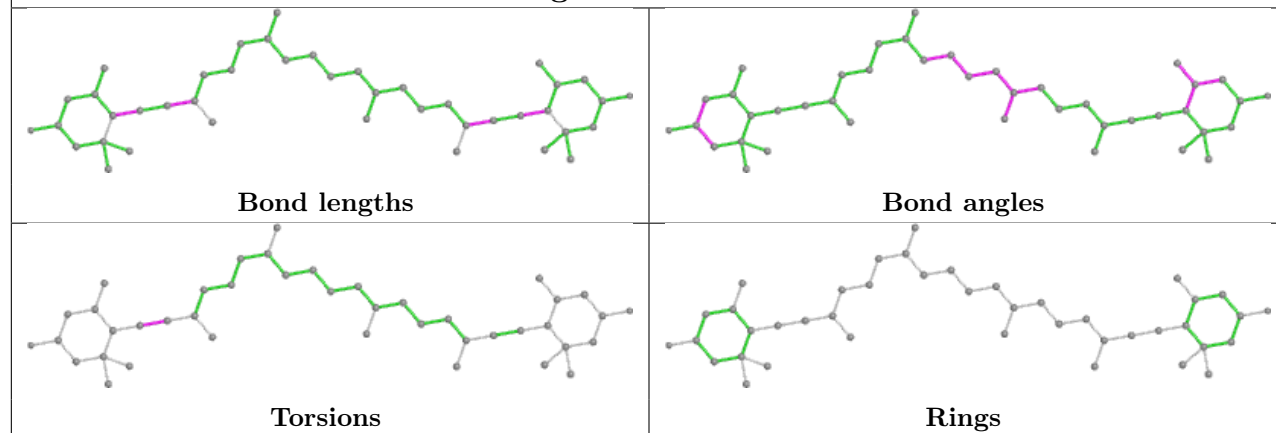
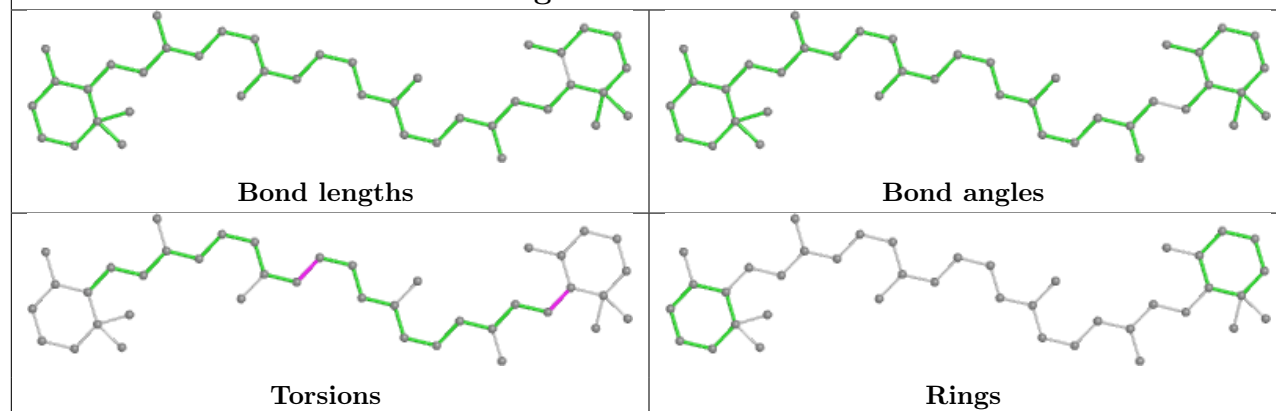
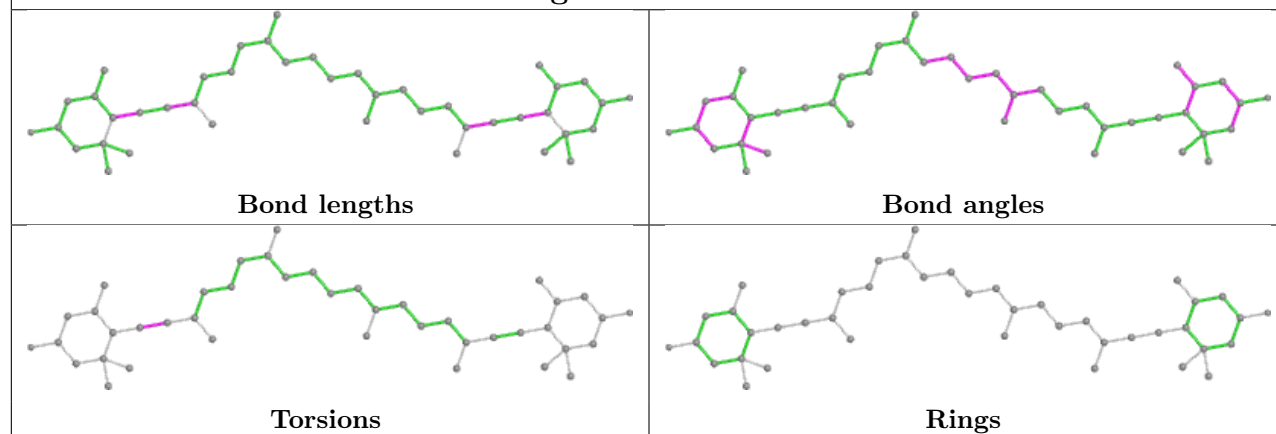


## Ligand CLA B 806

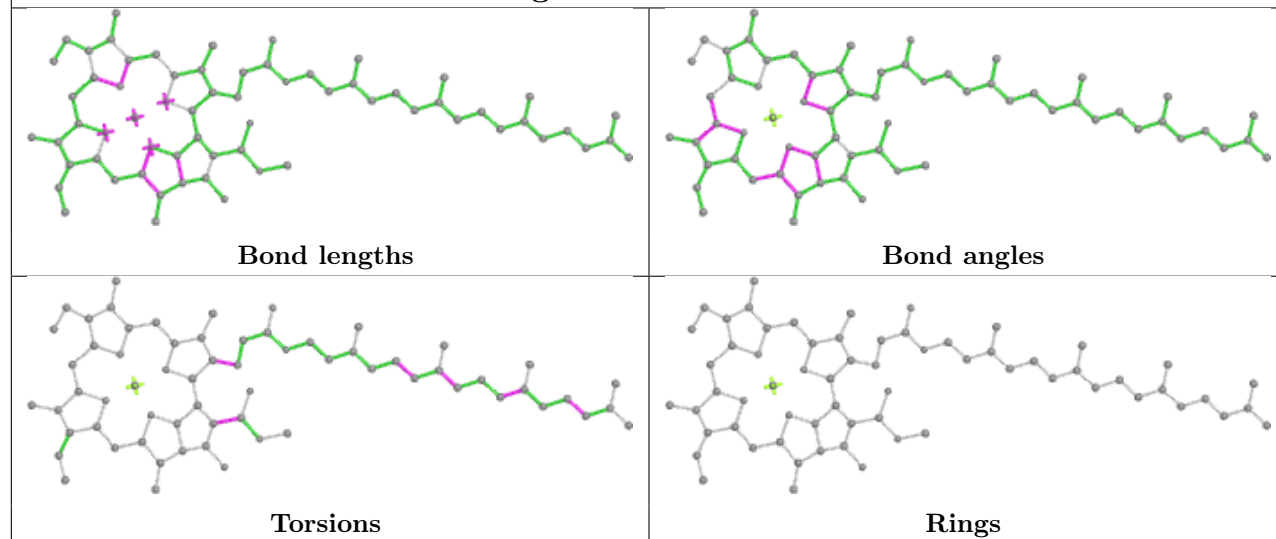


## Ligand CLA 1 609

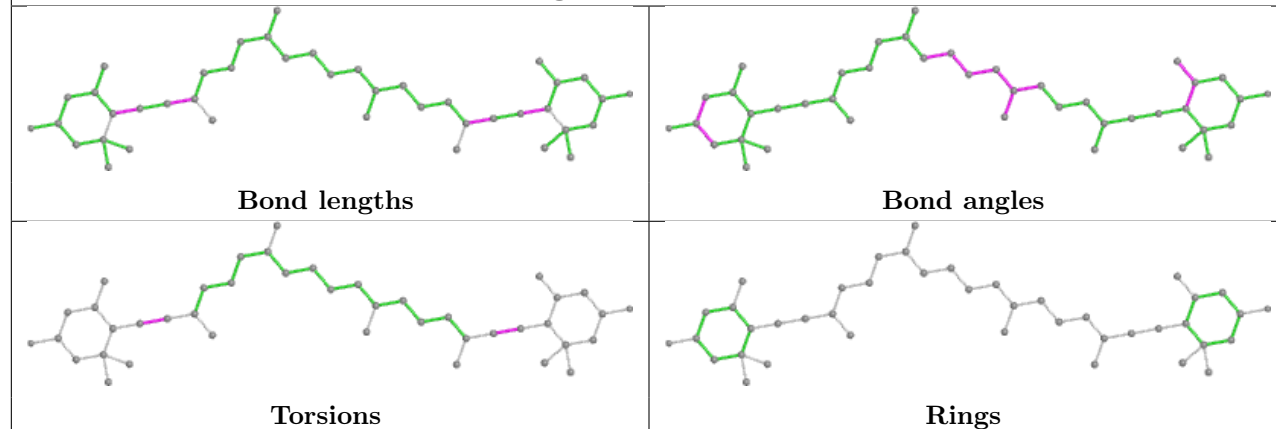


**Ligand II0 6 615****Ligand 8CT K 103****Ligand II0 7 315**

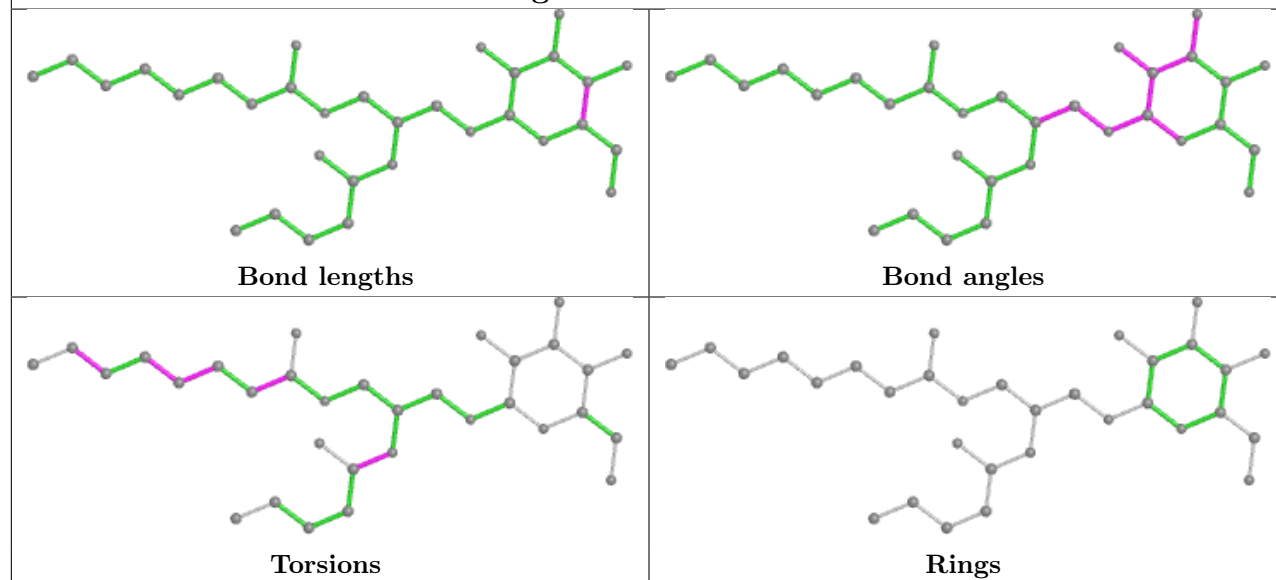
## Ligand CLA A 828



## Ligand II0 3 616

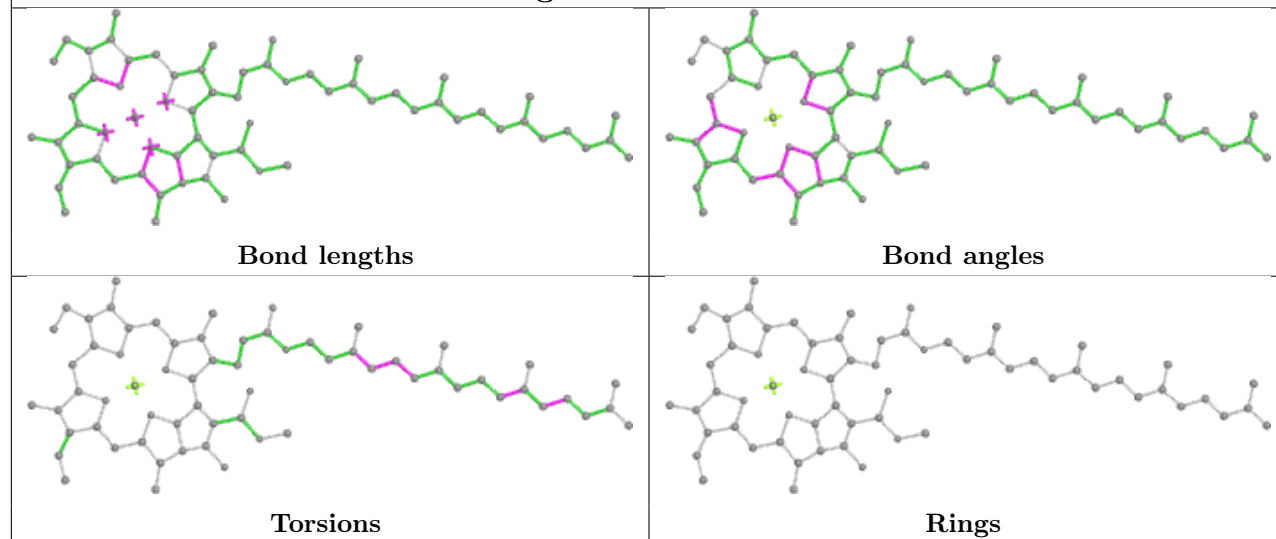


## Ligand LMG 6 618

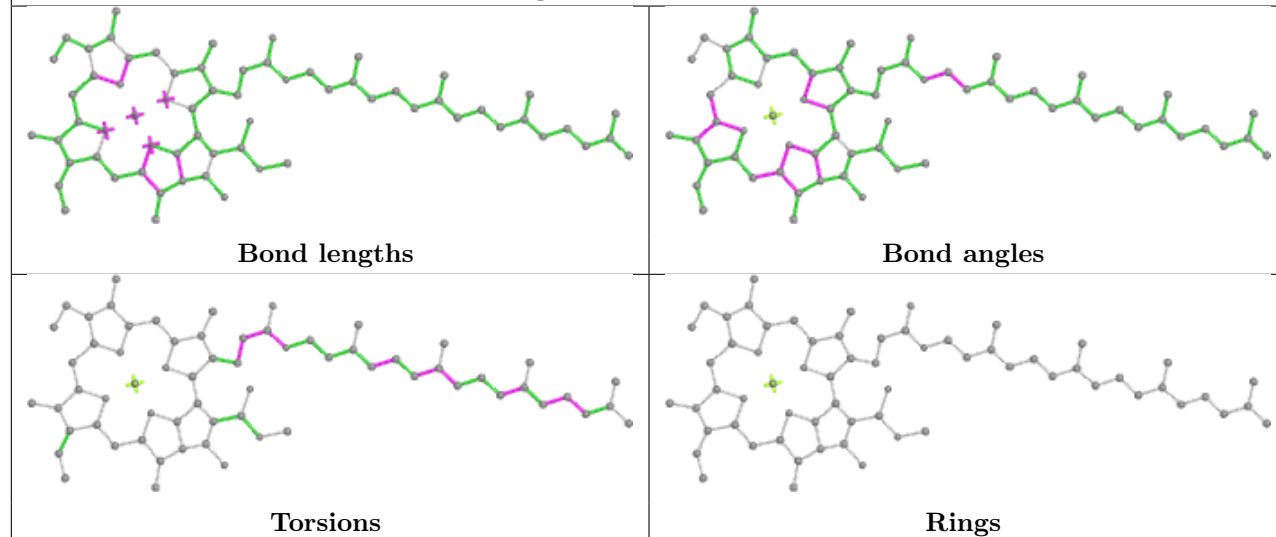




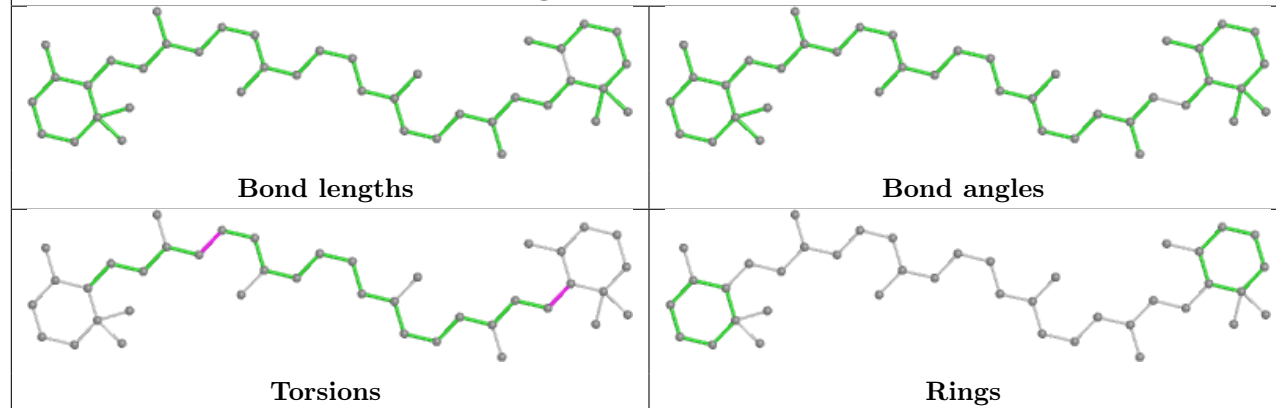
## Ligand CLA 4 610



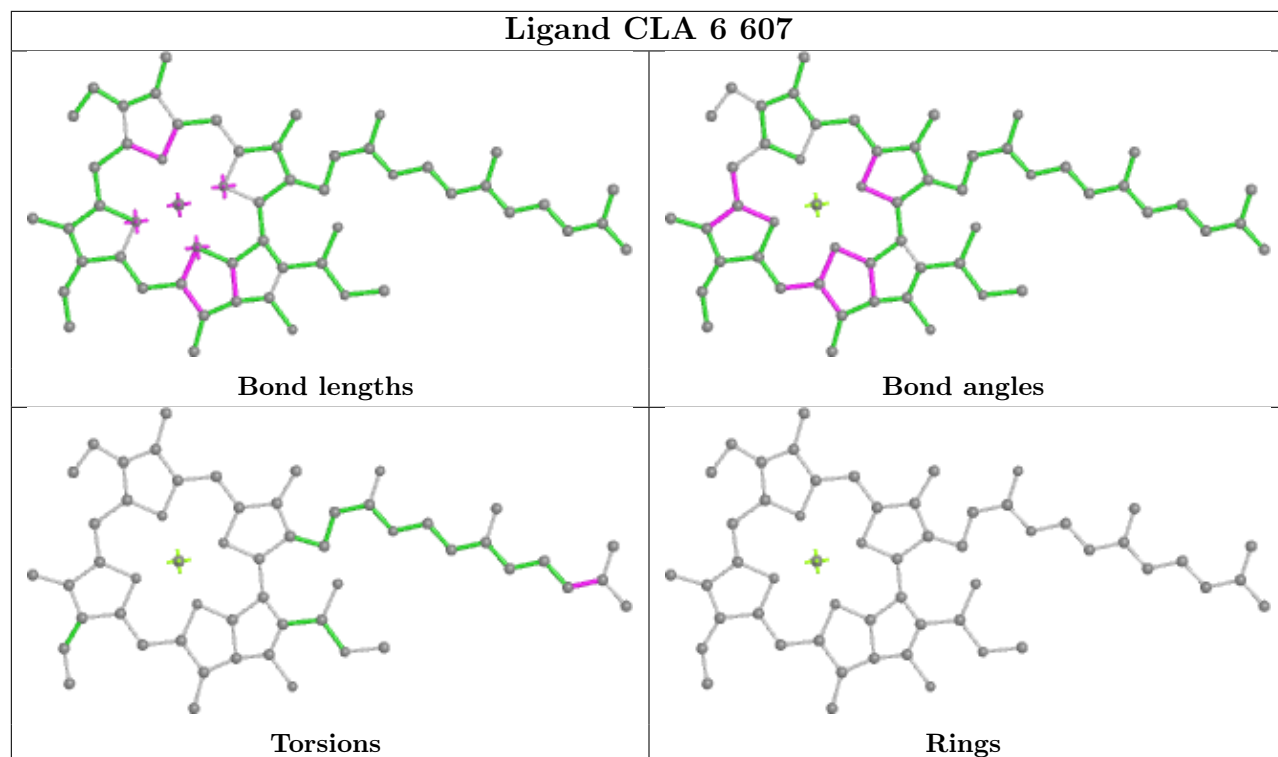
## Ligand CLA A 839



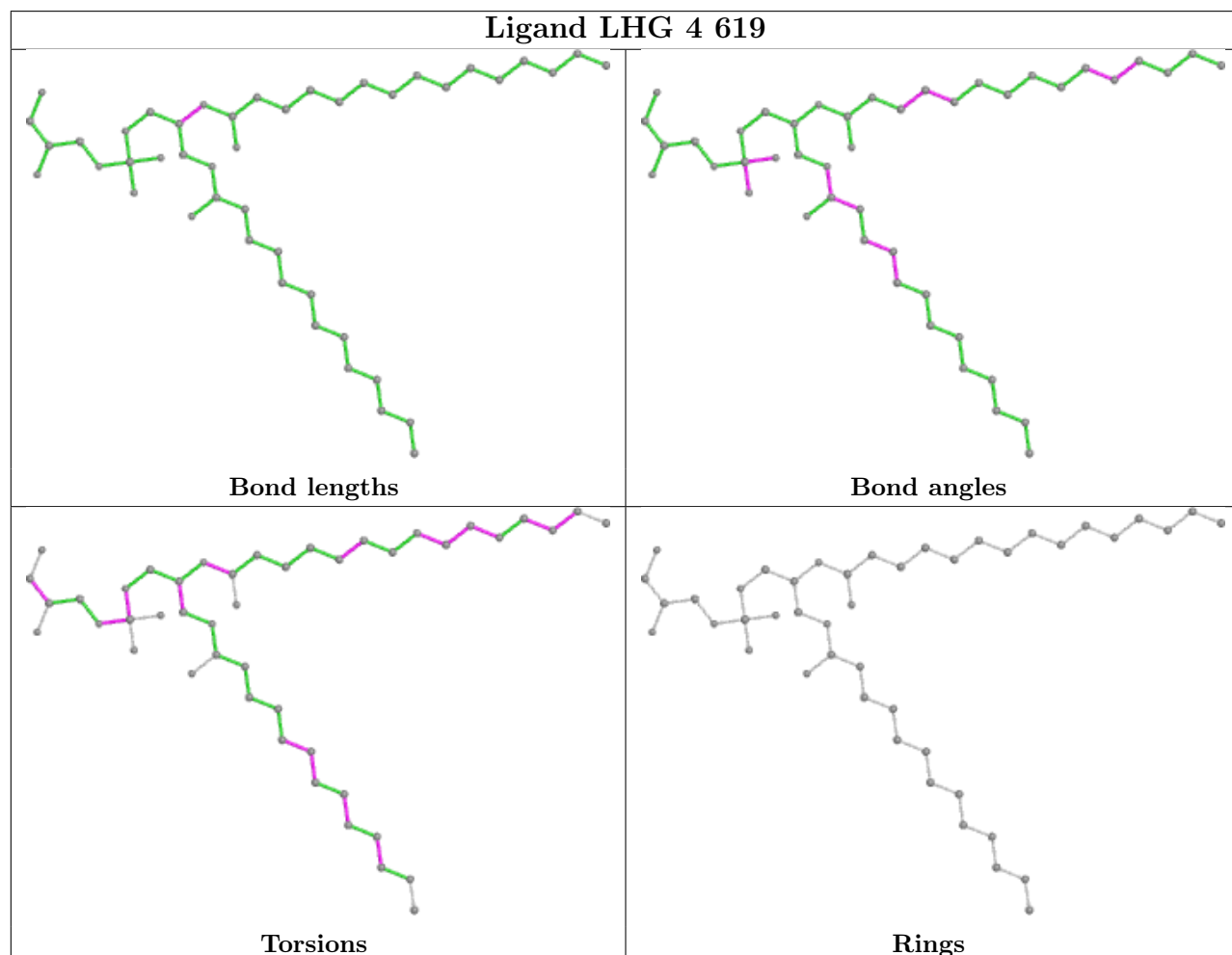
## Ligand 8CT B 844



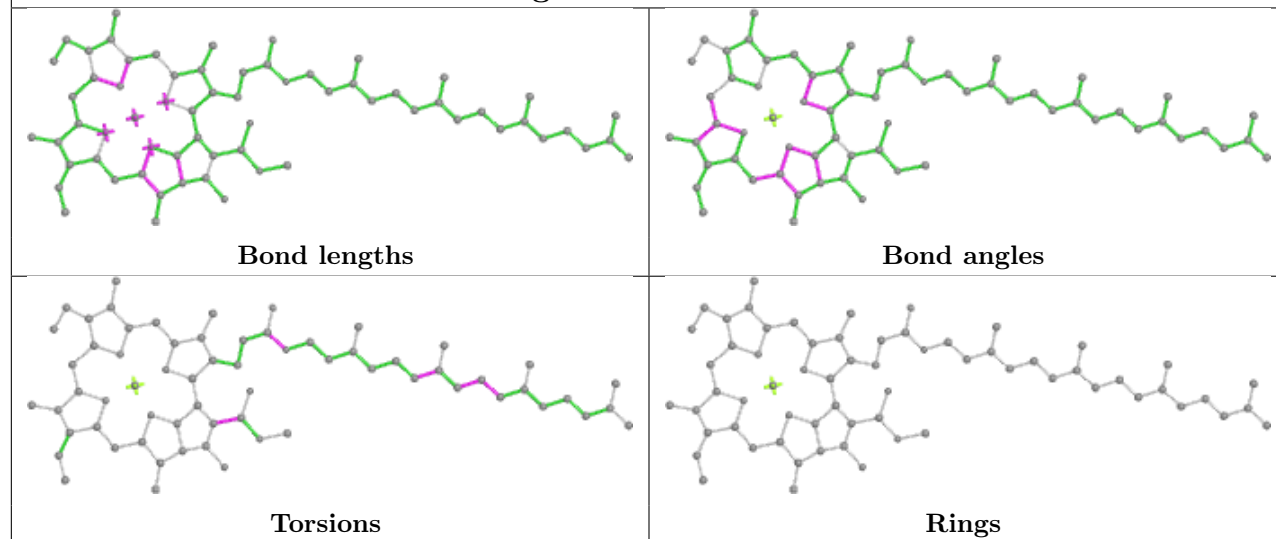
## Ligand CLA 6 607



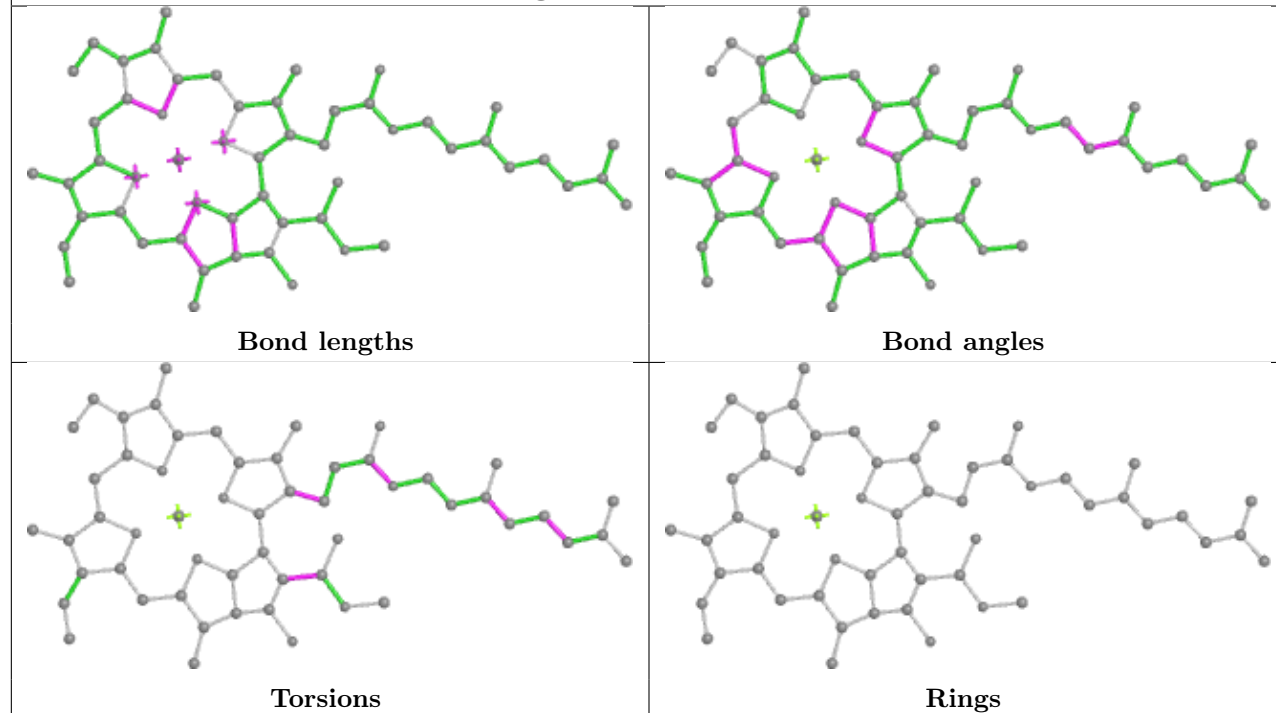
## Ligand LHG 4 619

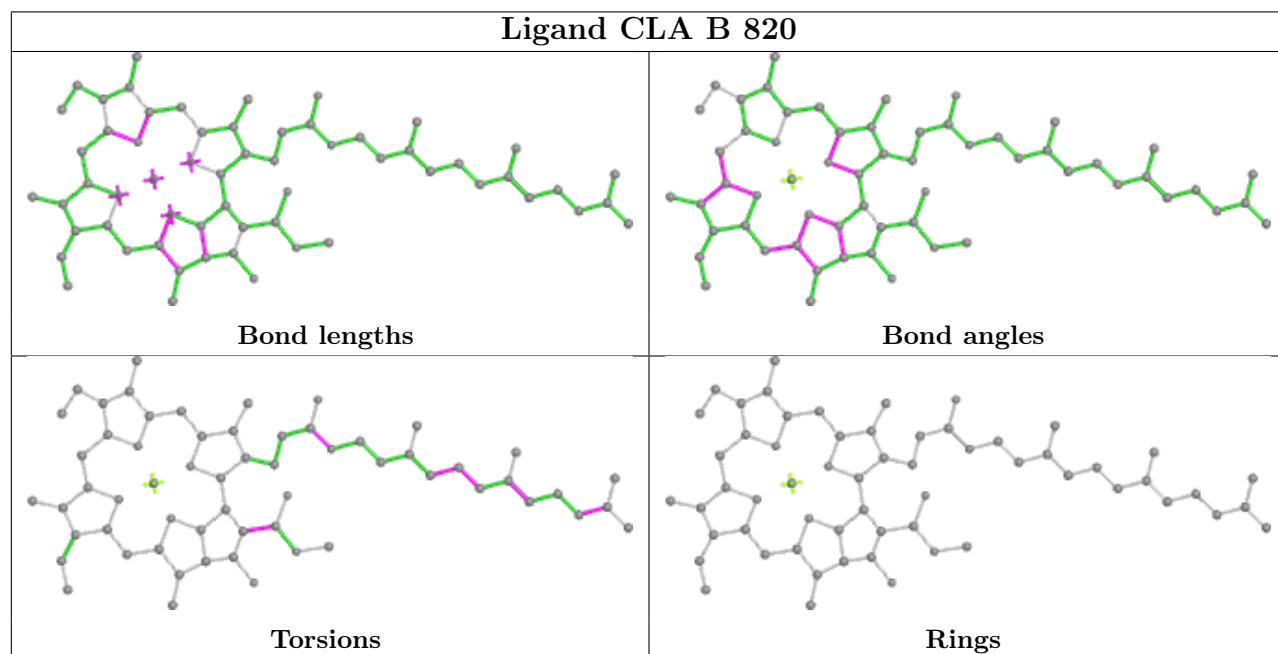
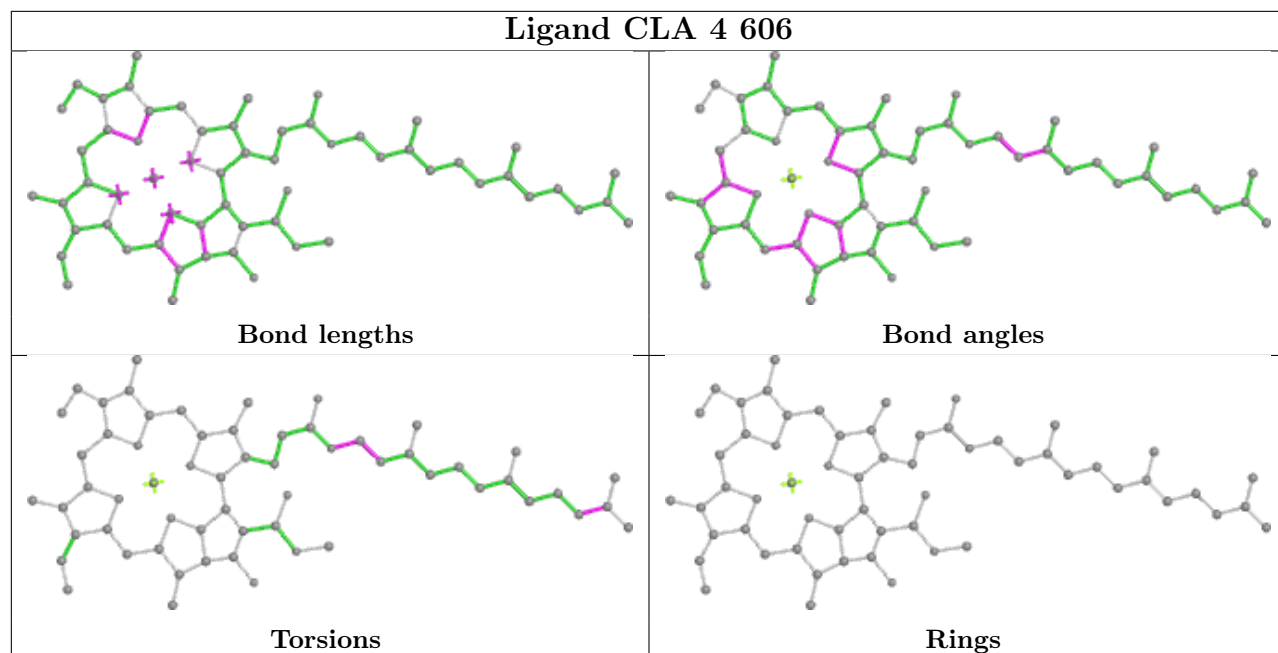


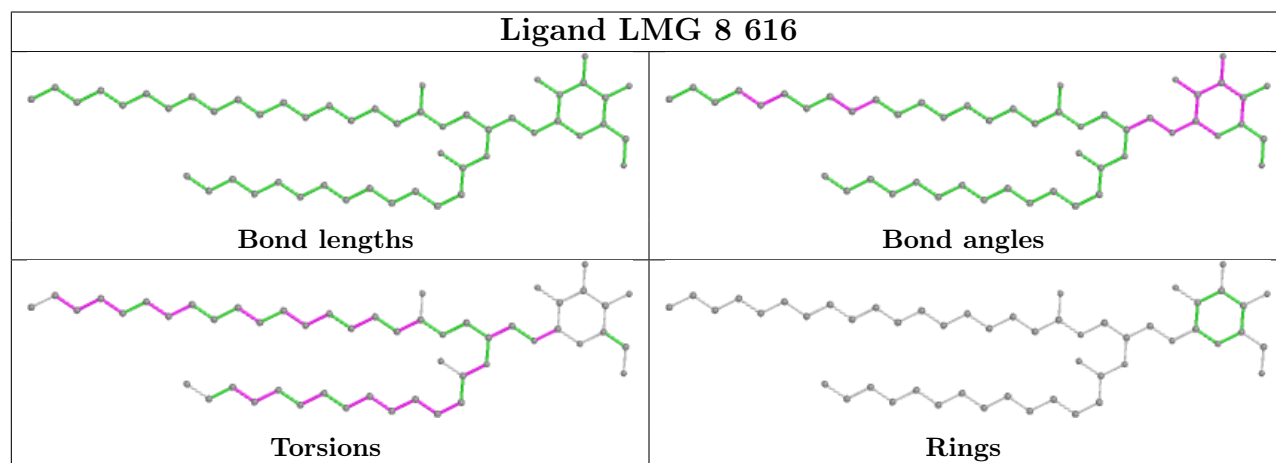
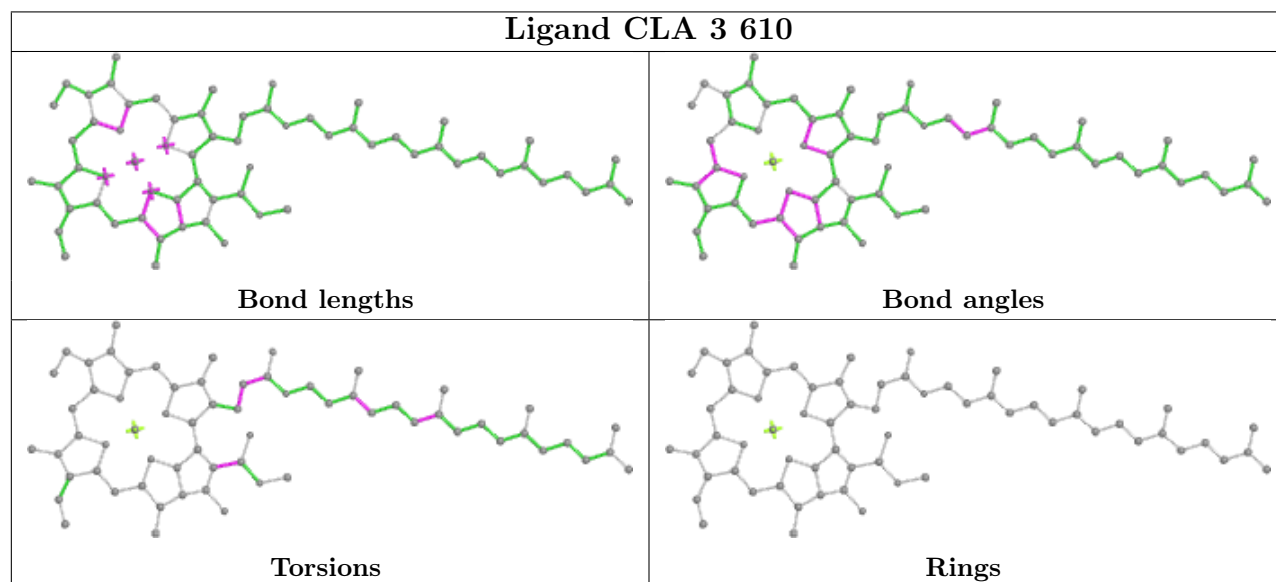
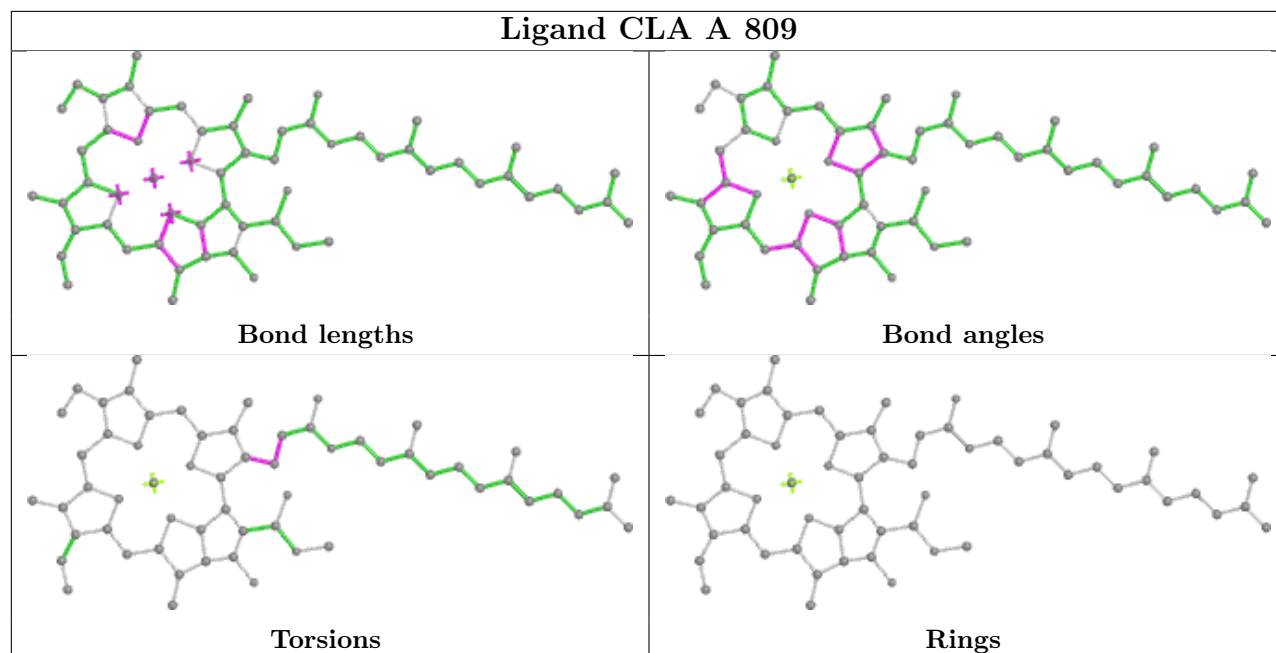
## Ligand CLA B 828



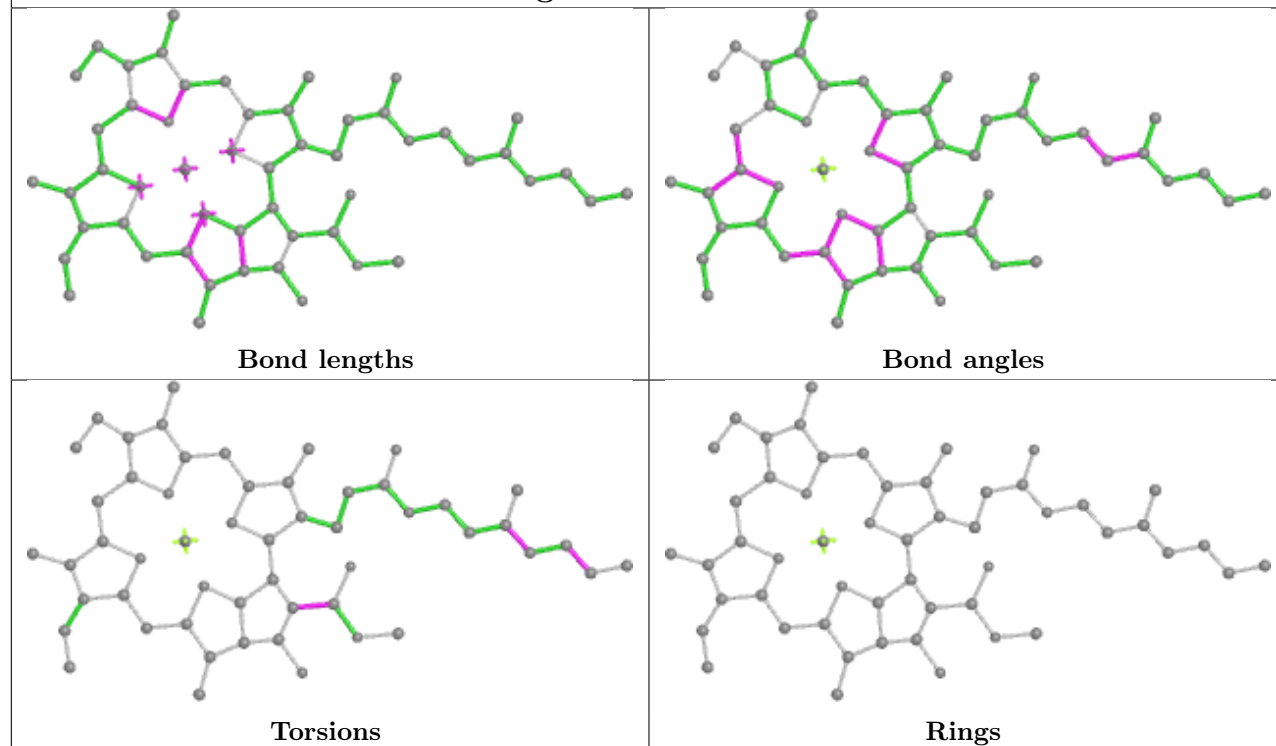
## Ligand CLA B 831



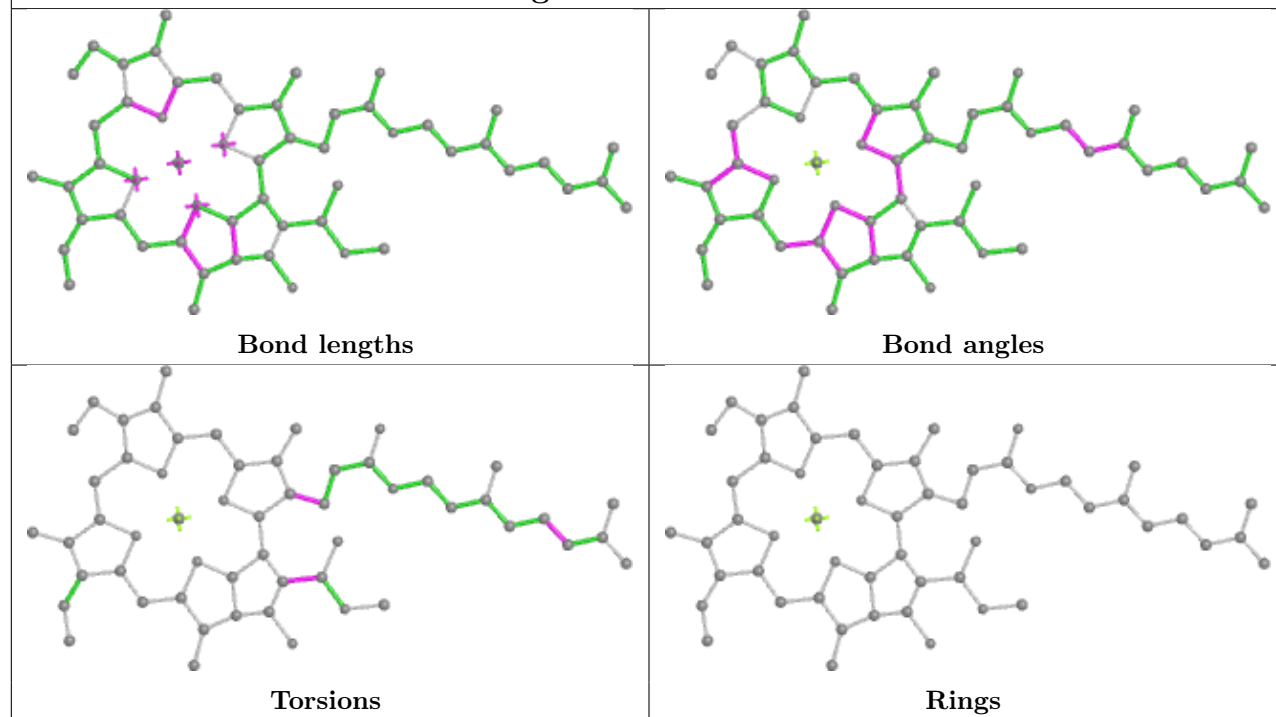


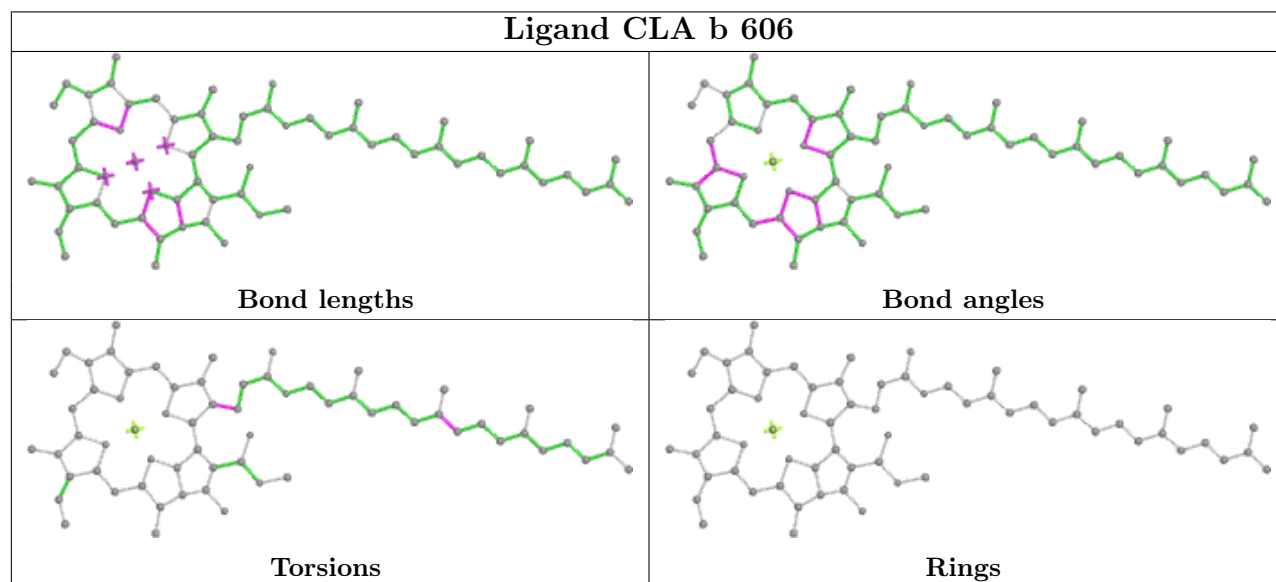
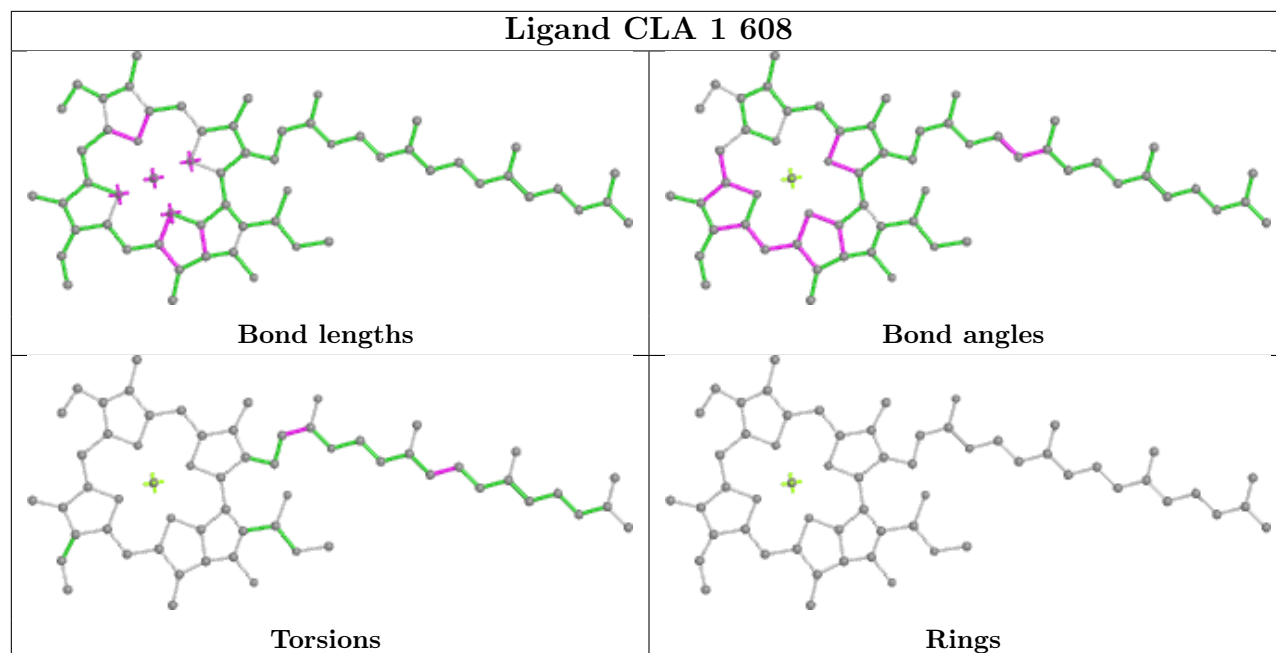


## Ligand CLA 7 305

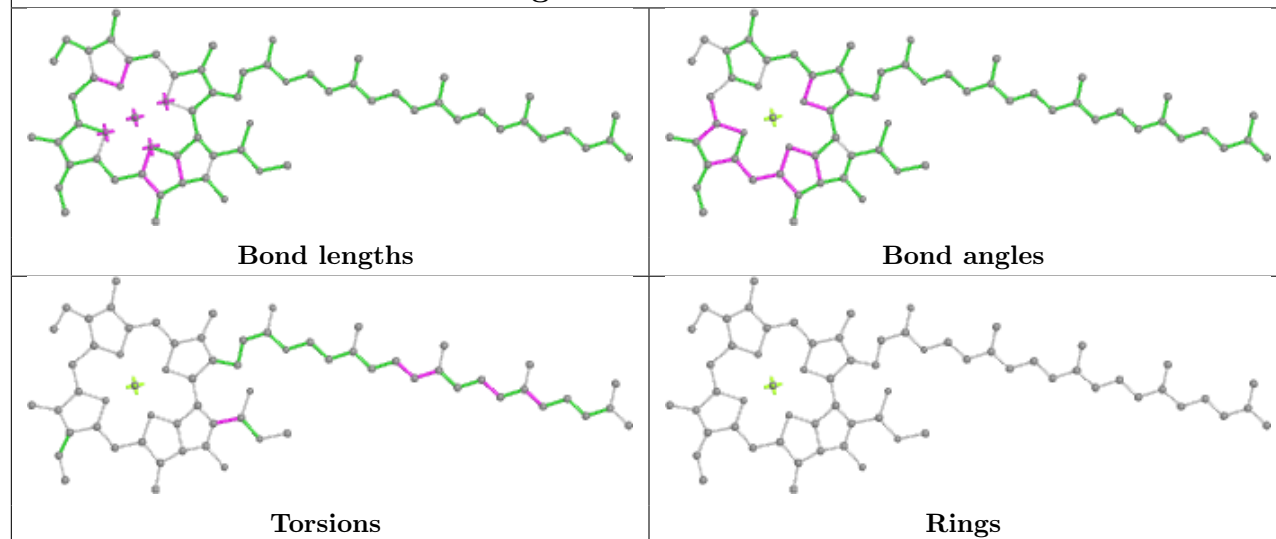


## Ligand CLA A 812

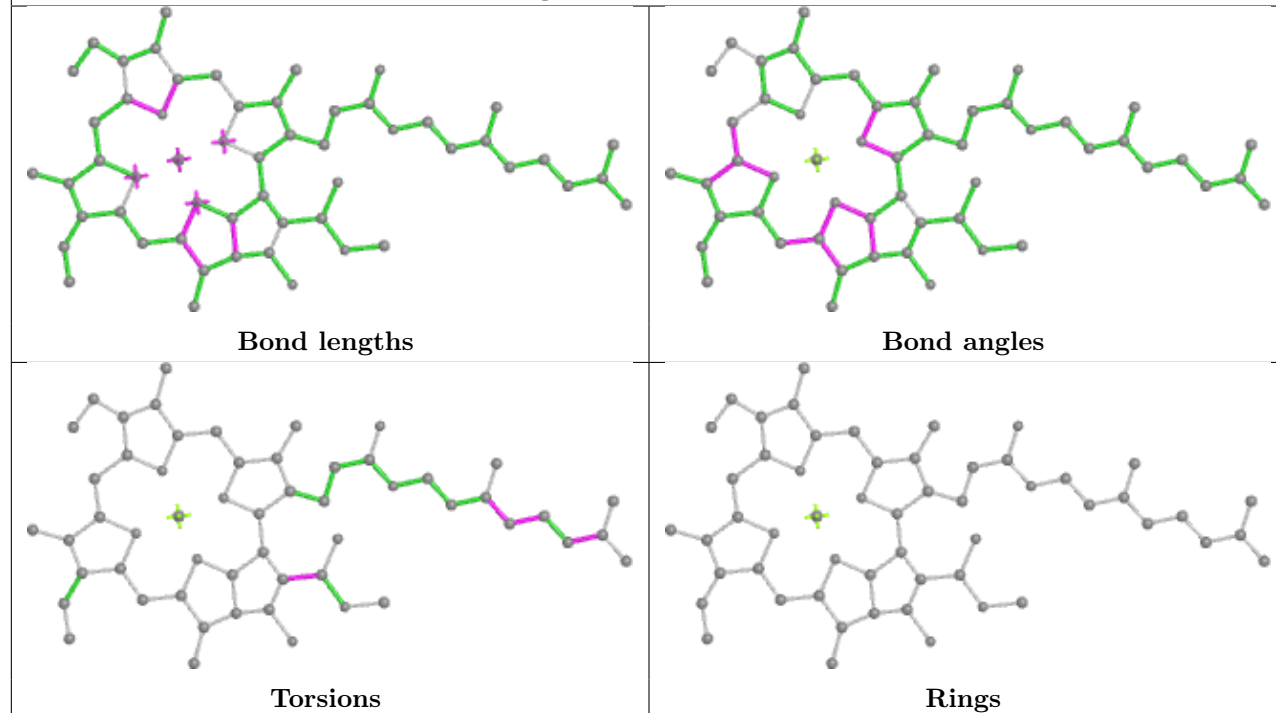




## Ligand CLA A 825

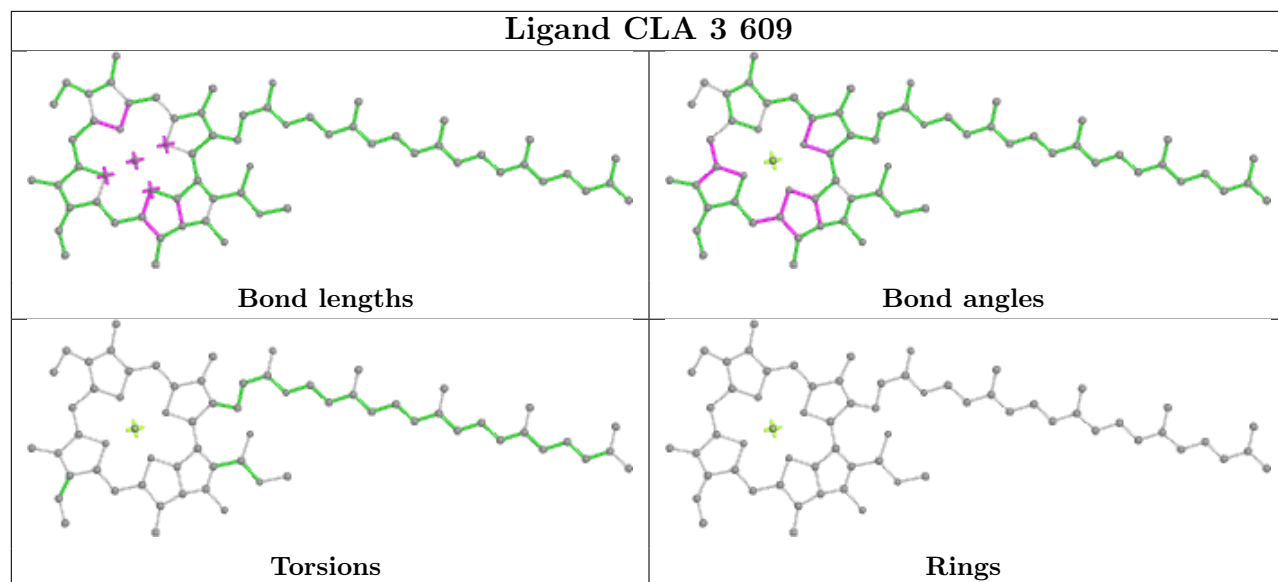


## Ligand CLA 4 604

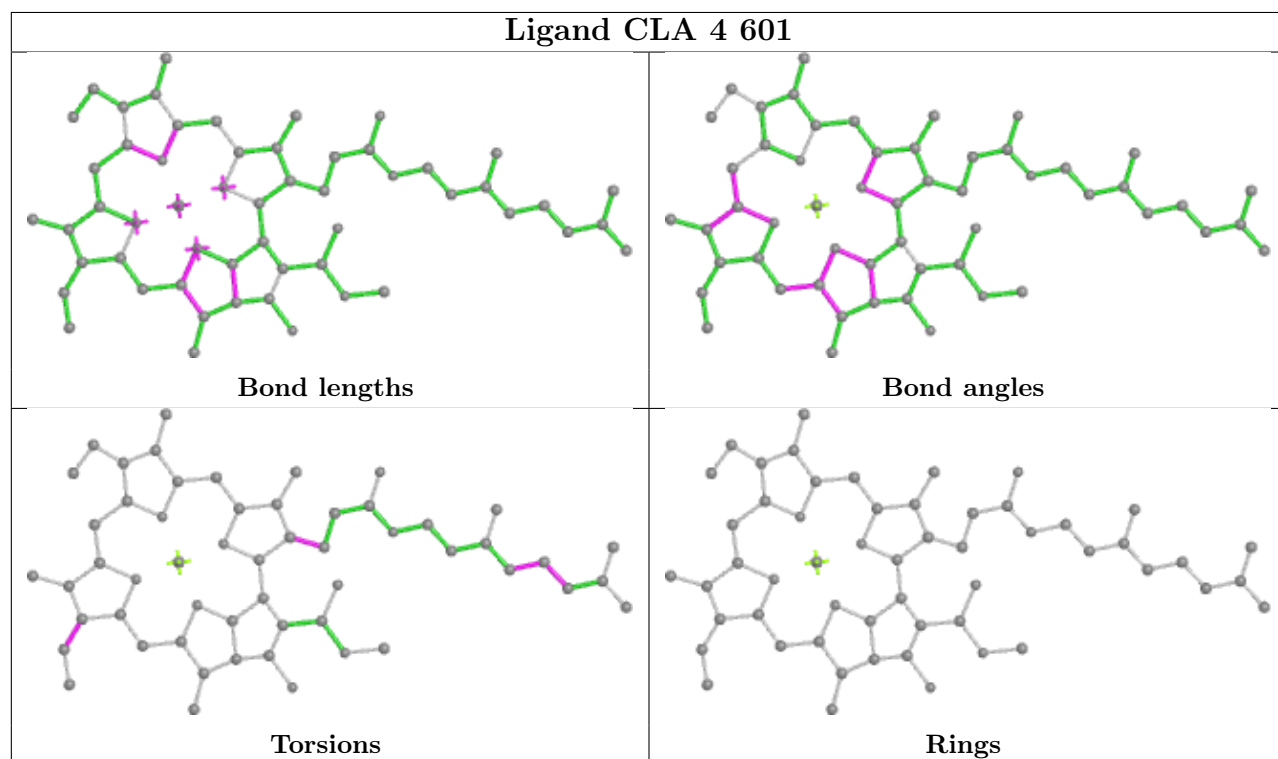




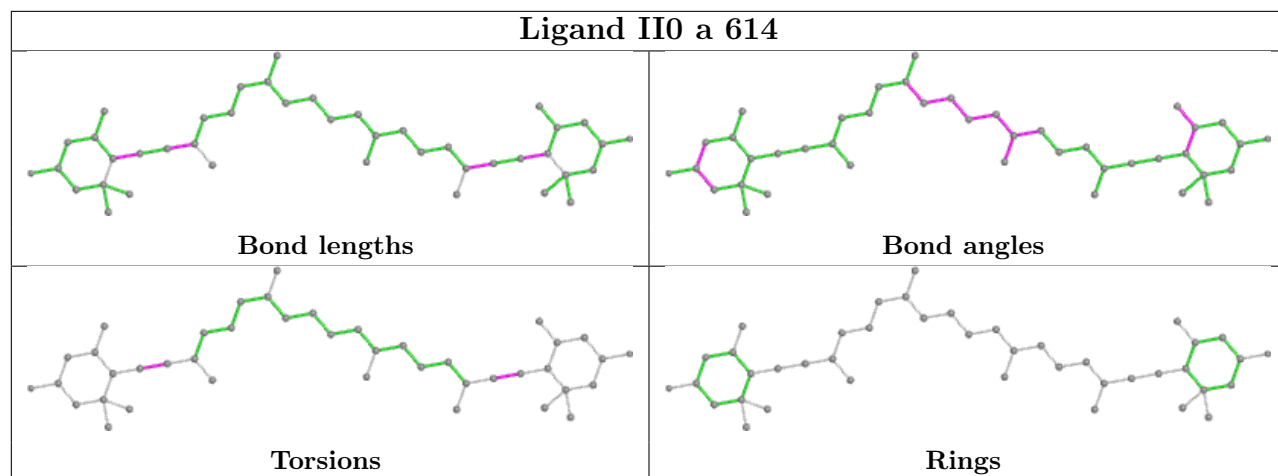
## Ligand CLA 3 609



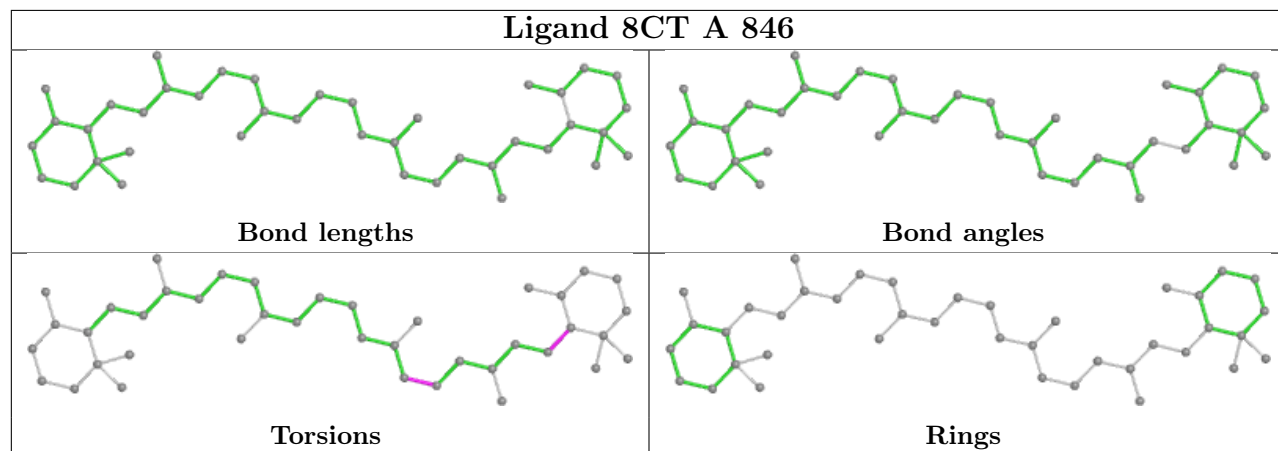
## Ligand CLA 4 601



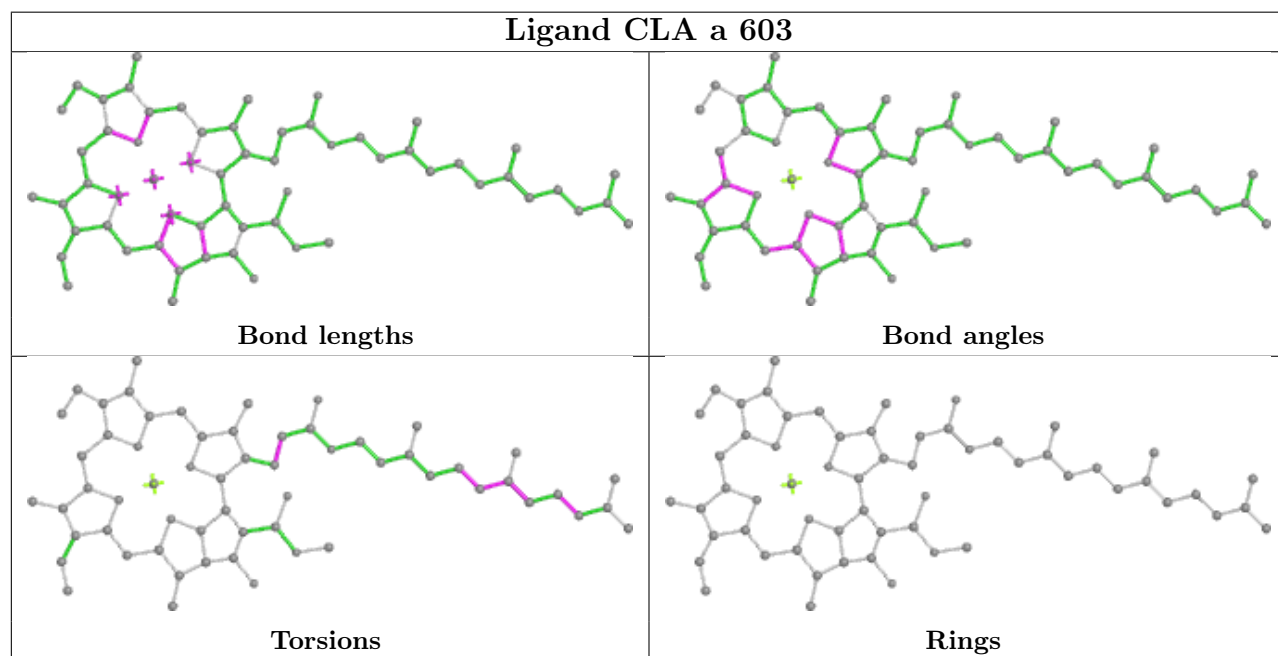
## Ligand II0 a 614



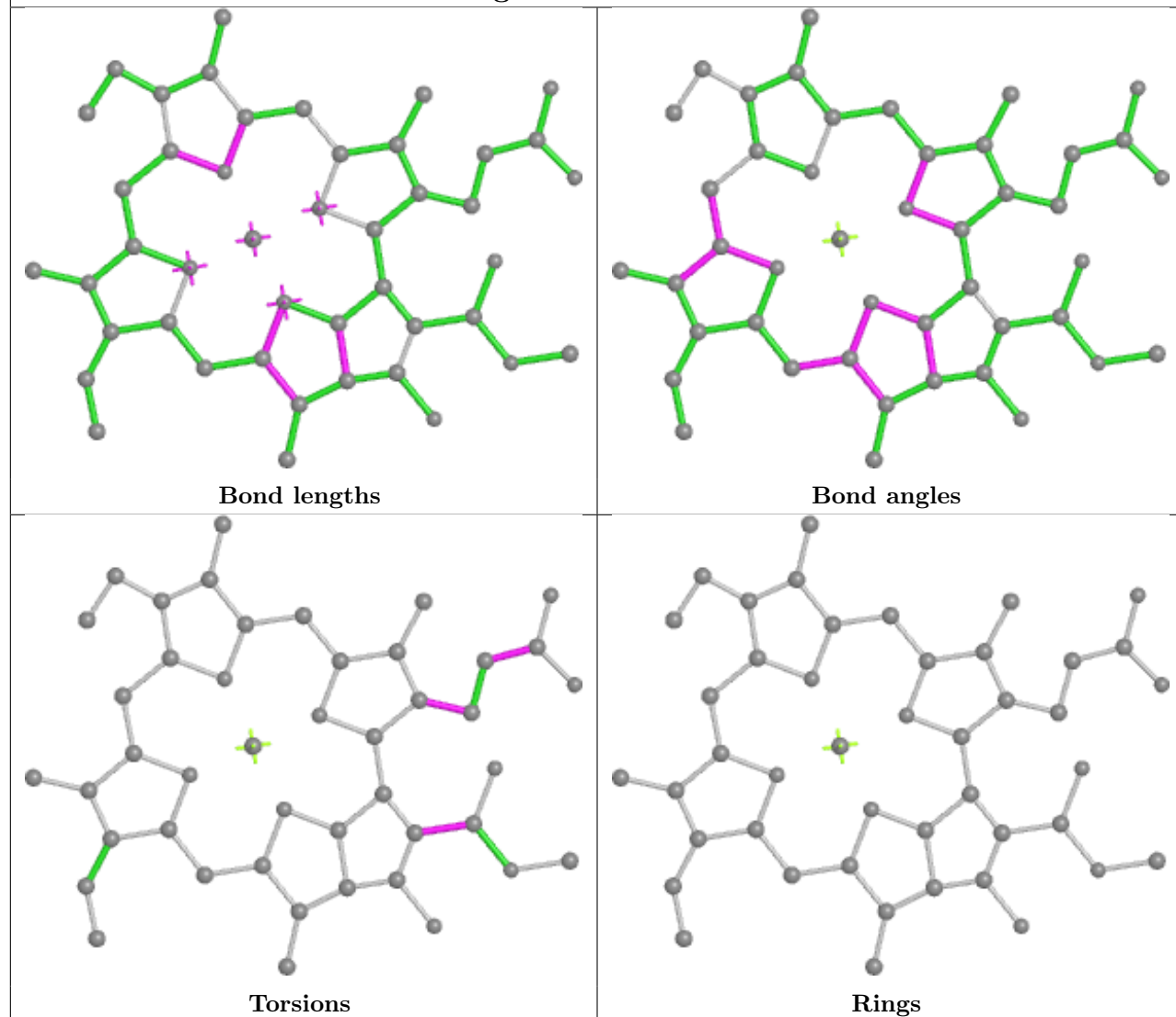
## Ligand 8CT A 846



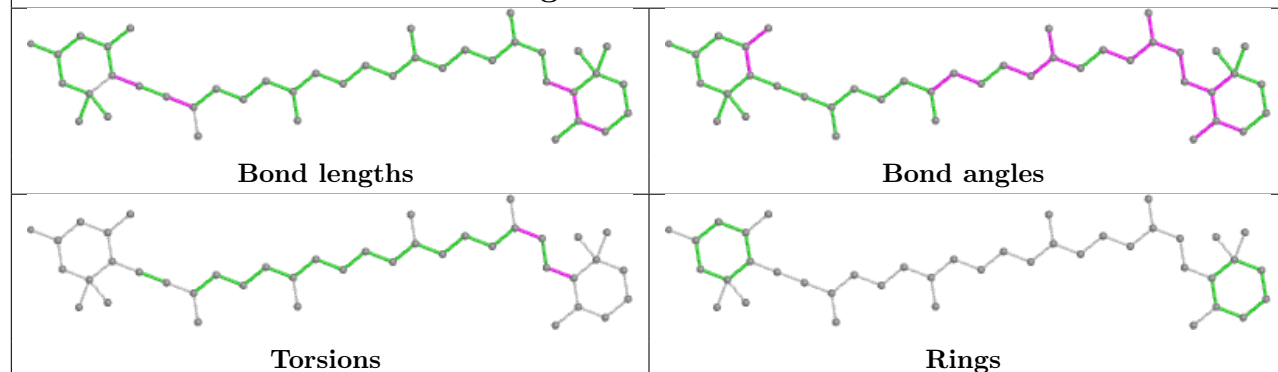
## Ligand CLA a 603



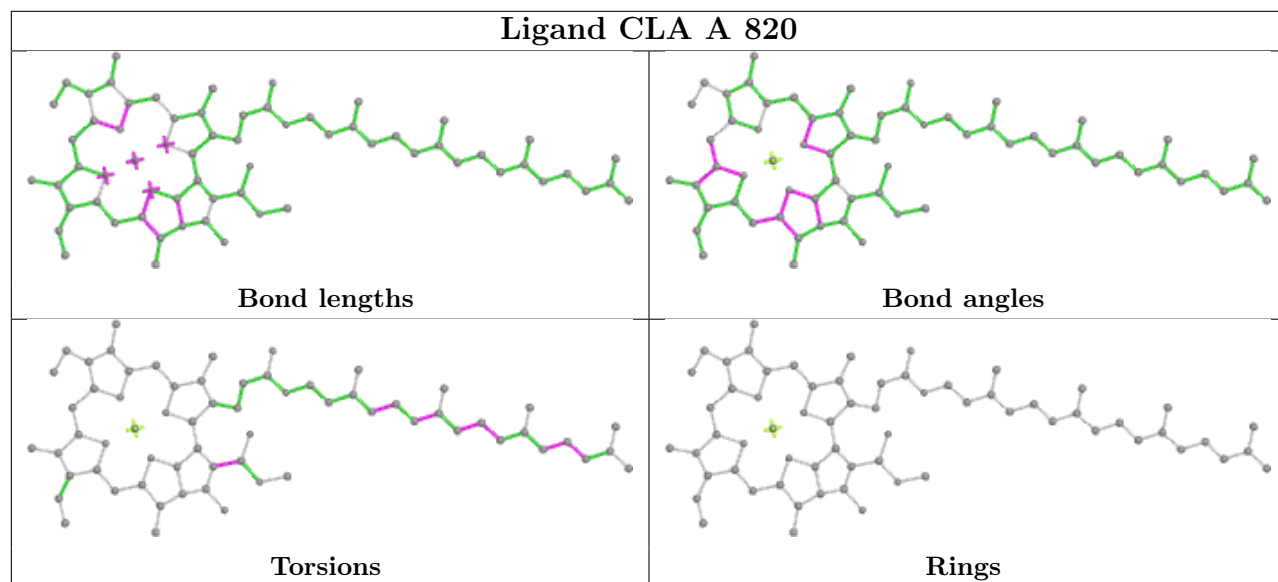
## Ligand CLA a 601



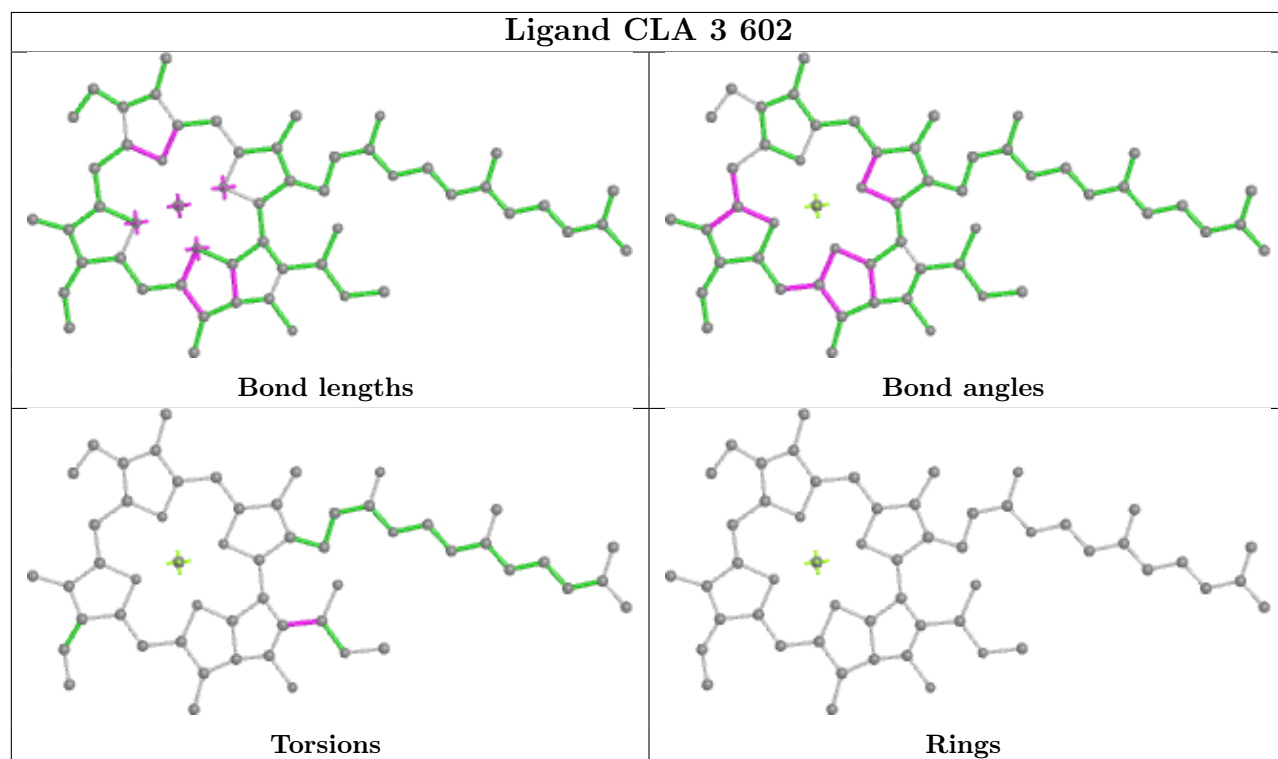
## Ligand IHT 9 619



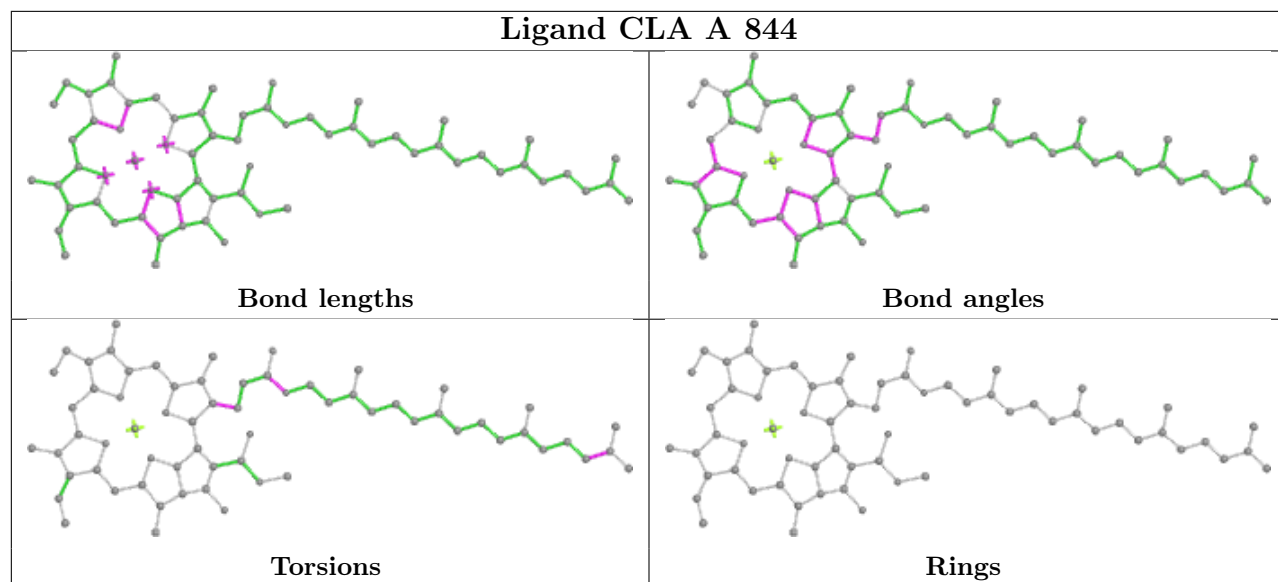
## Ligand CLA A 820



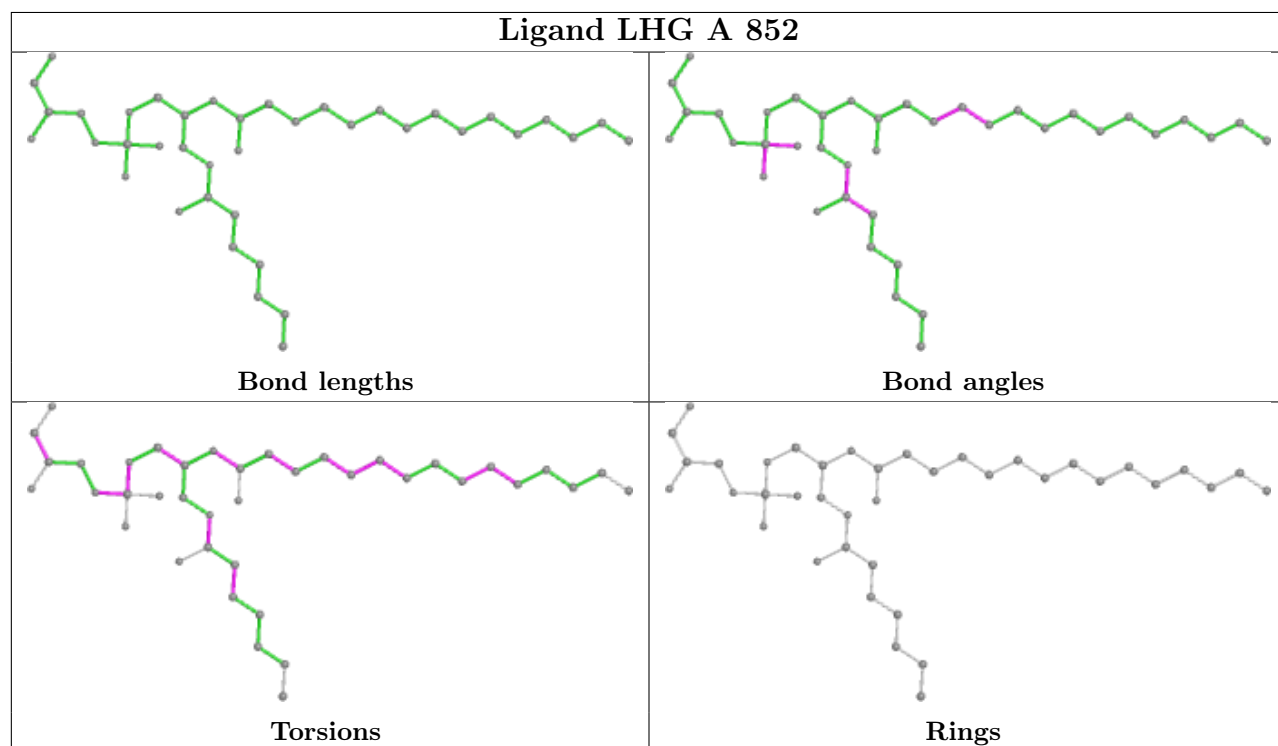
## Ligand CLA 3 602

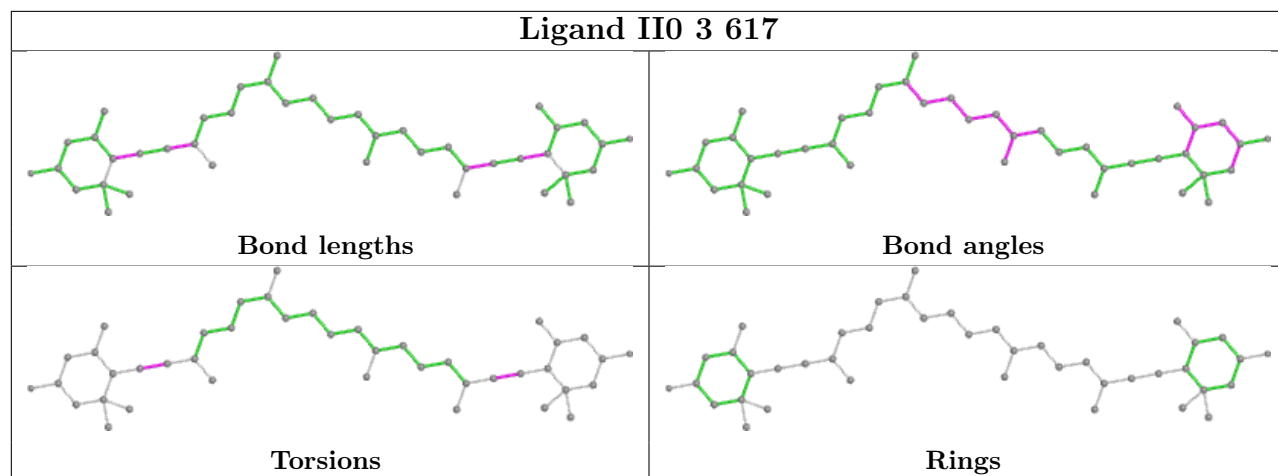
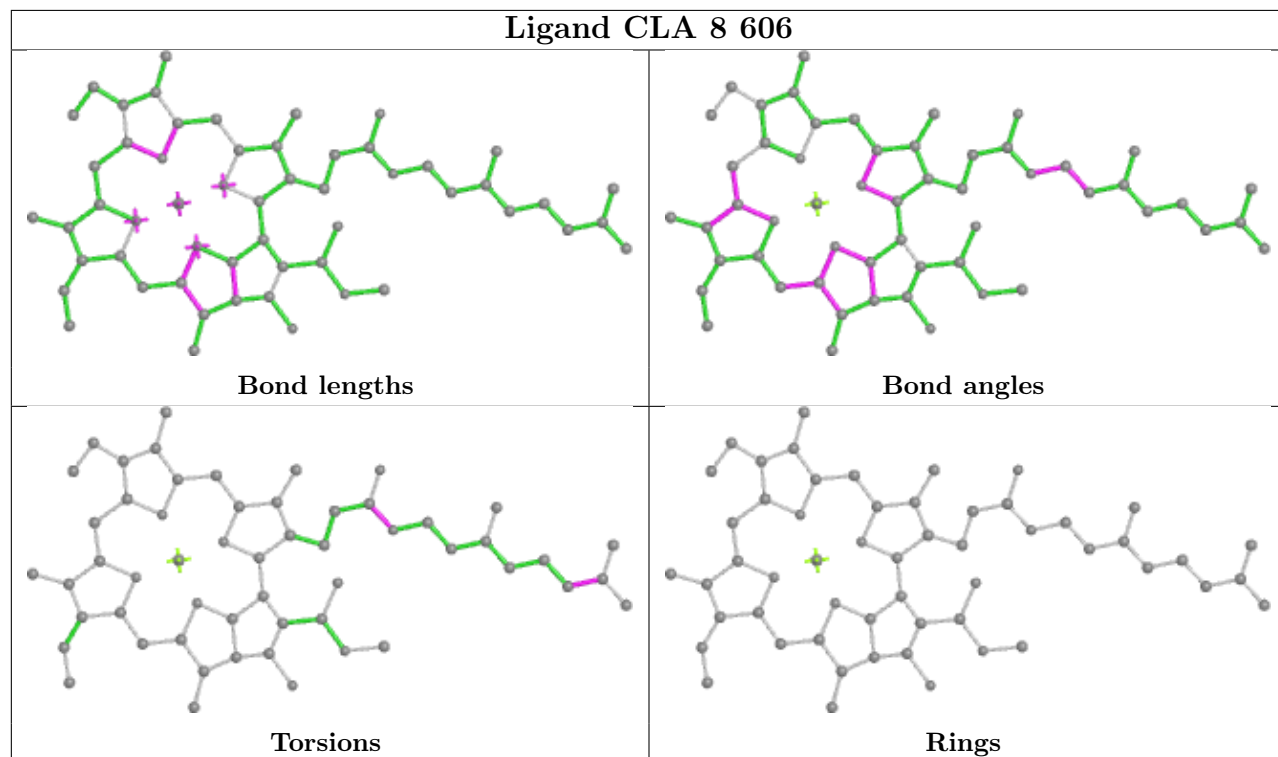


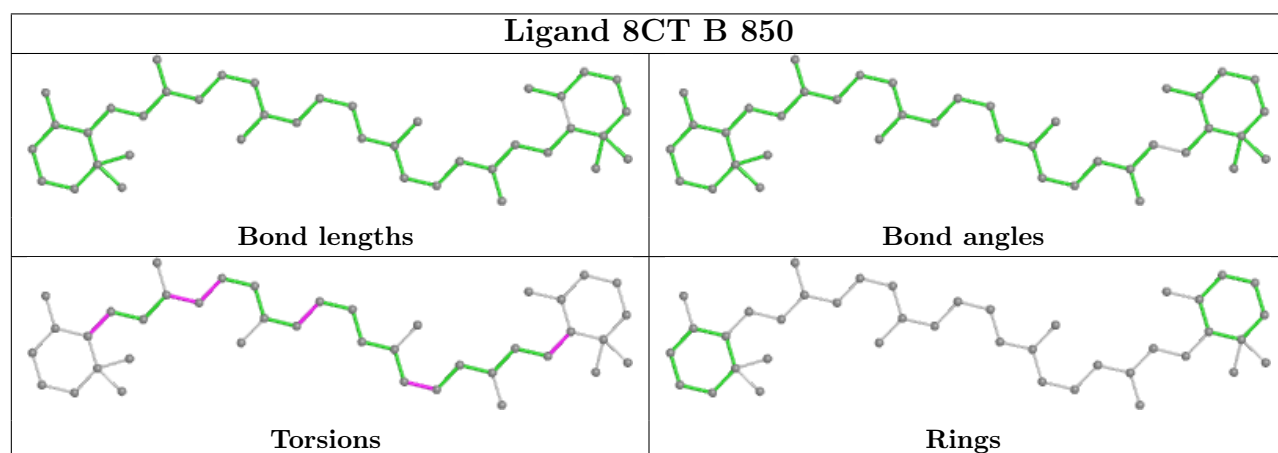
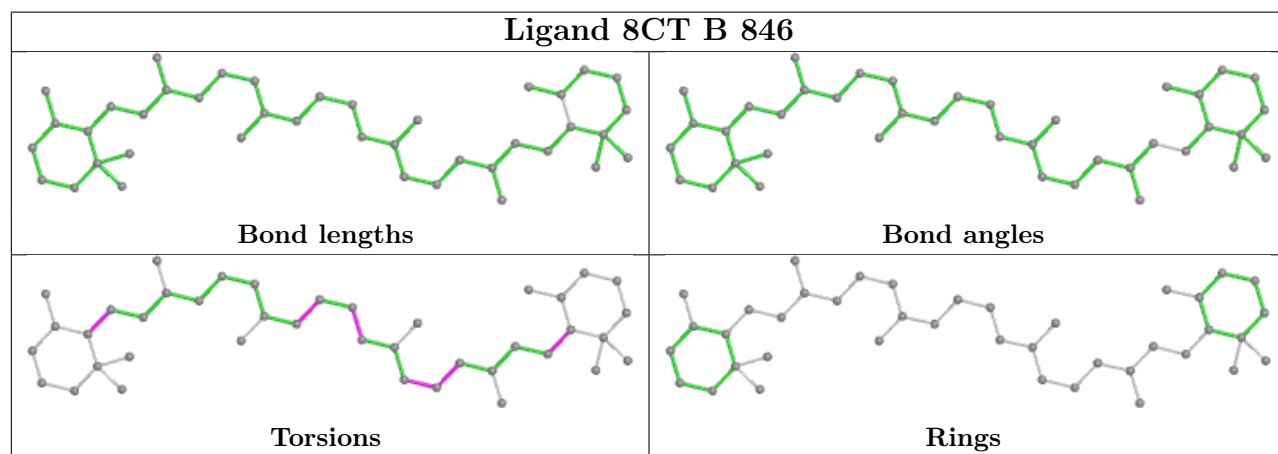
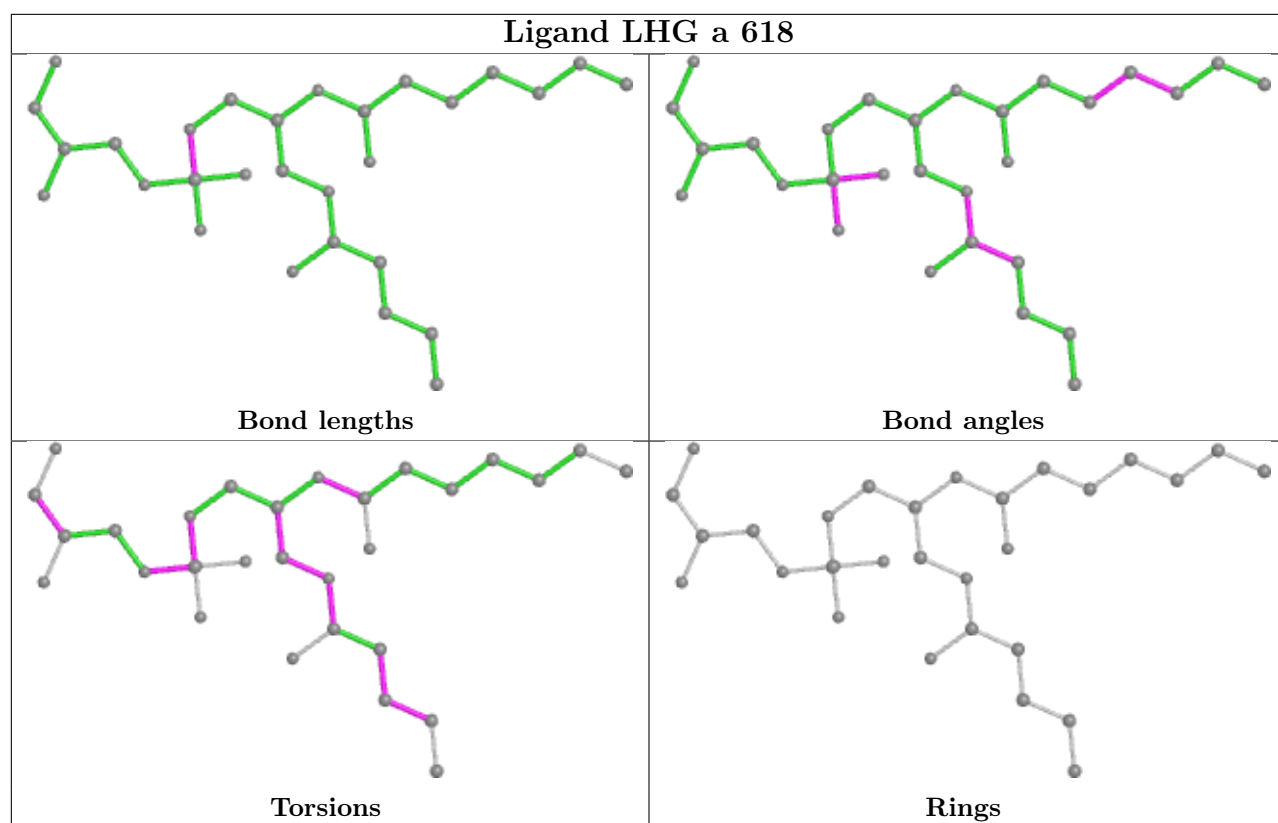
## Ligand CLA A 844

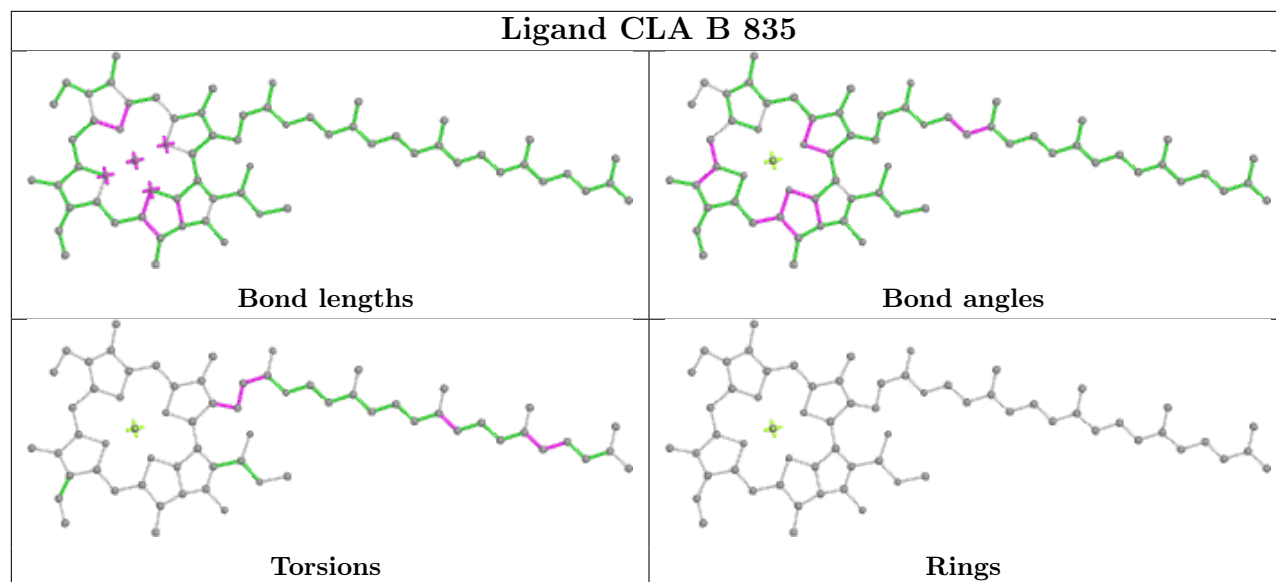
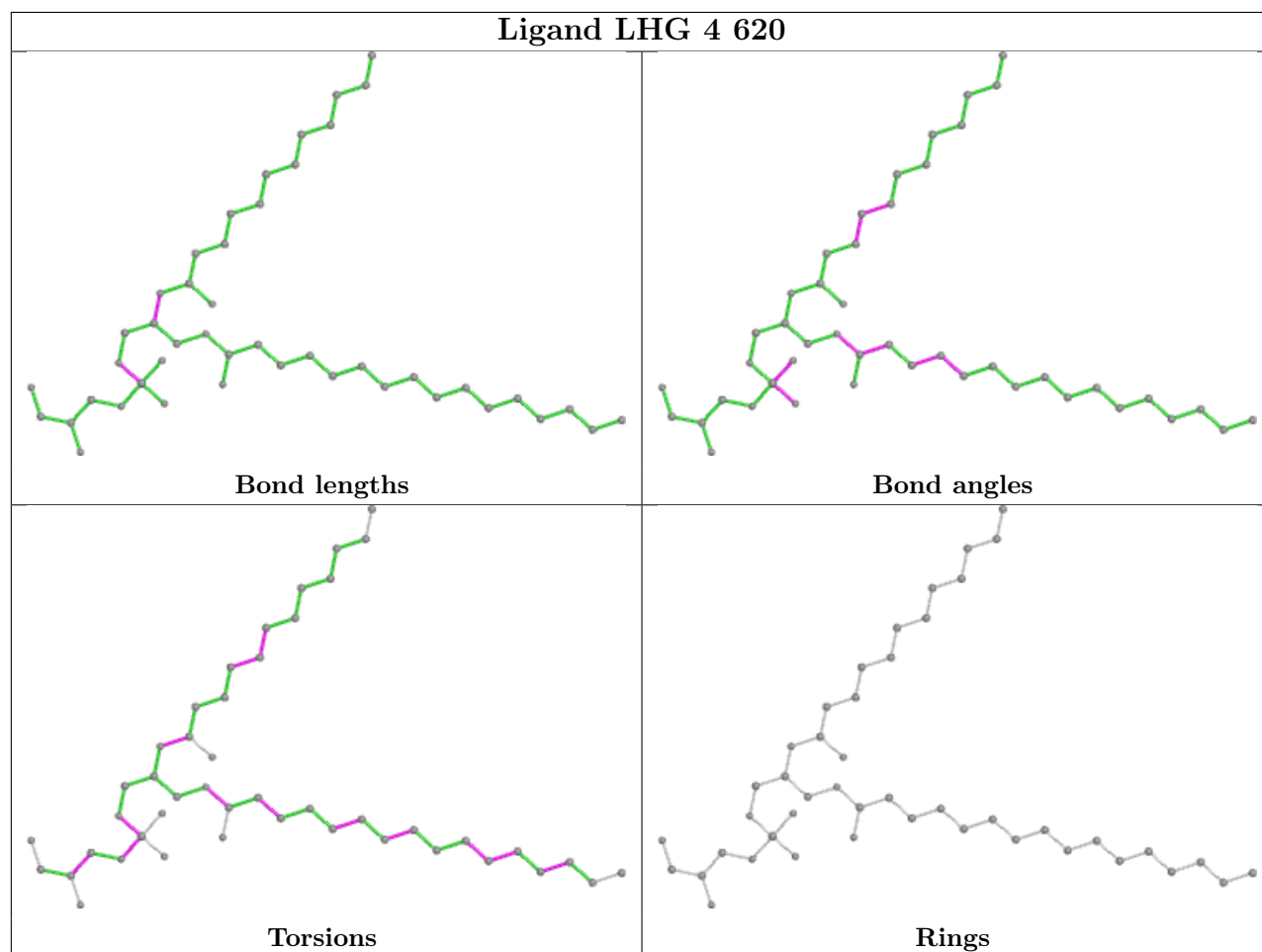


## Ligand LHG A 852



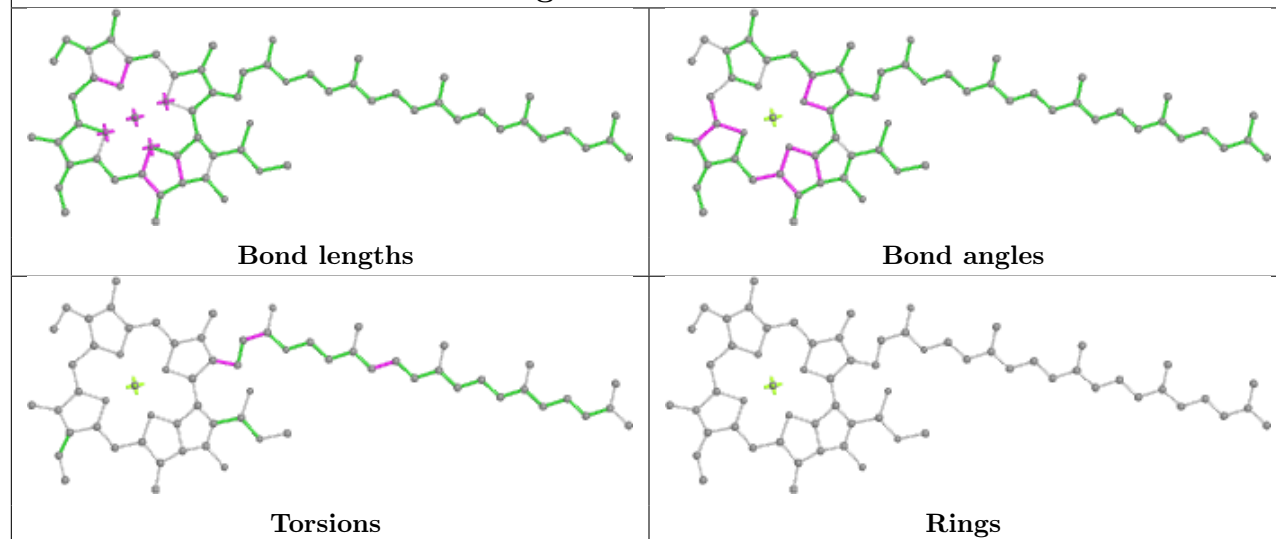
**Ligand II0 3 617****Ligand CLA 8 606**



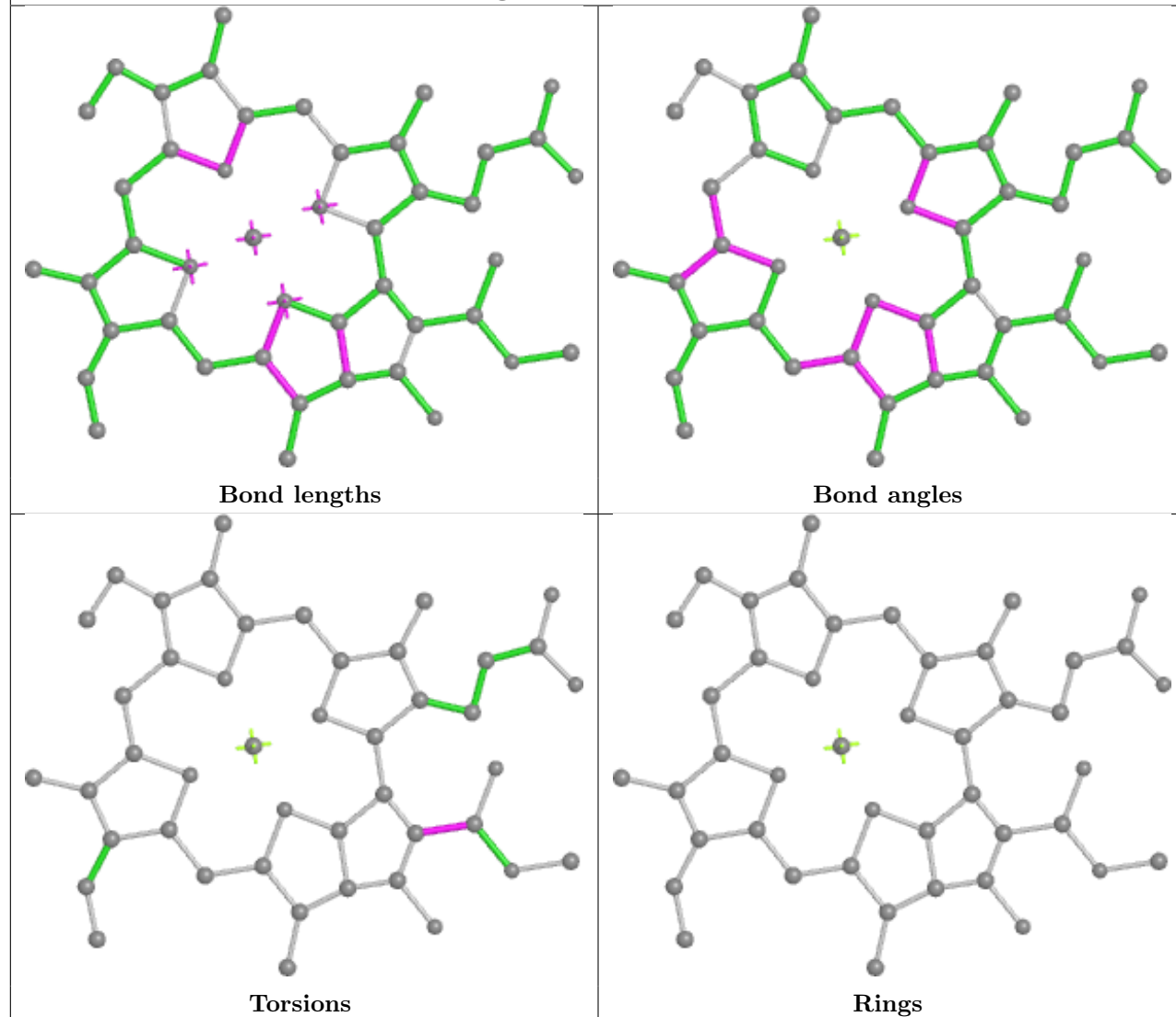
**Ligand CLA B 835****Ligand LHG 4 620**

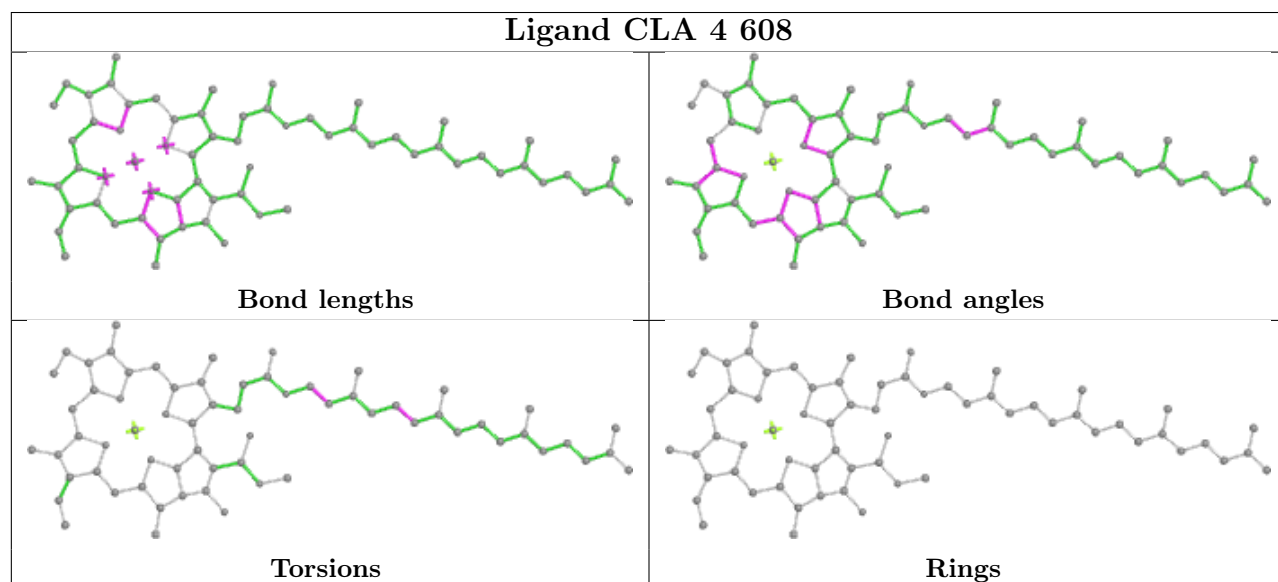
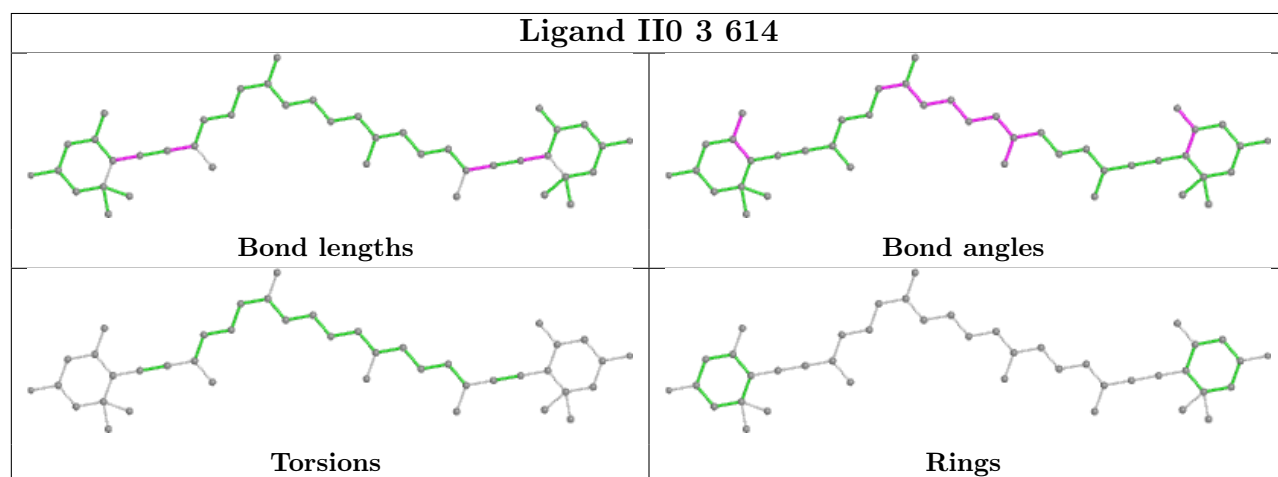
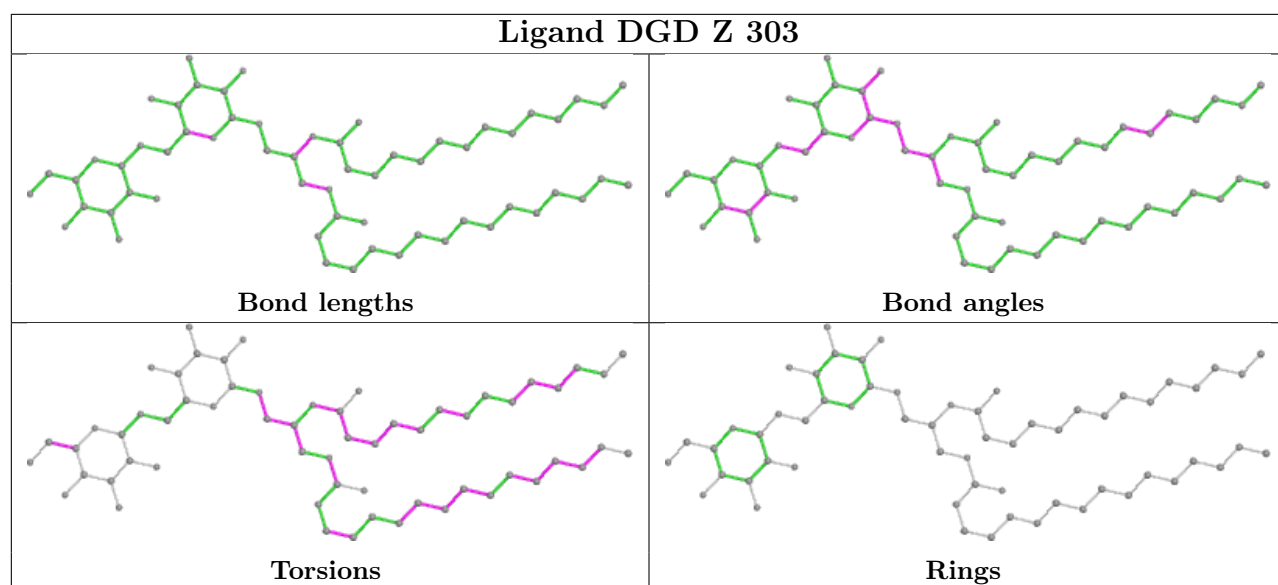


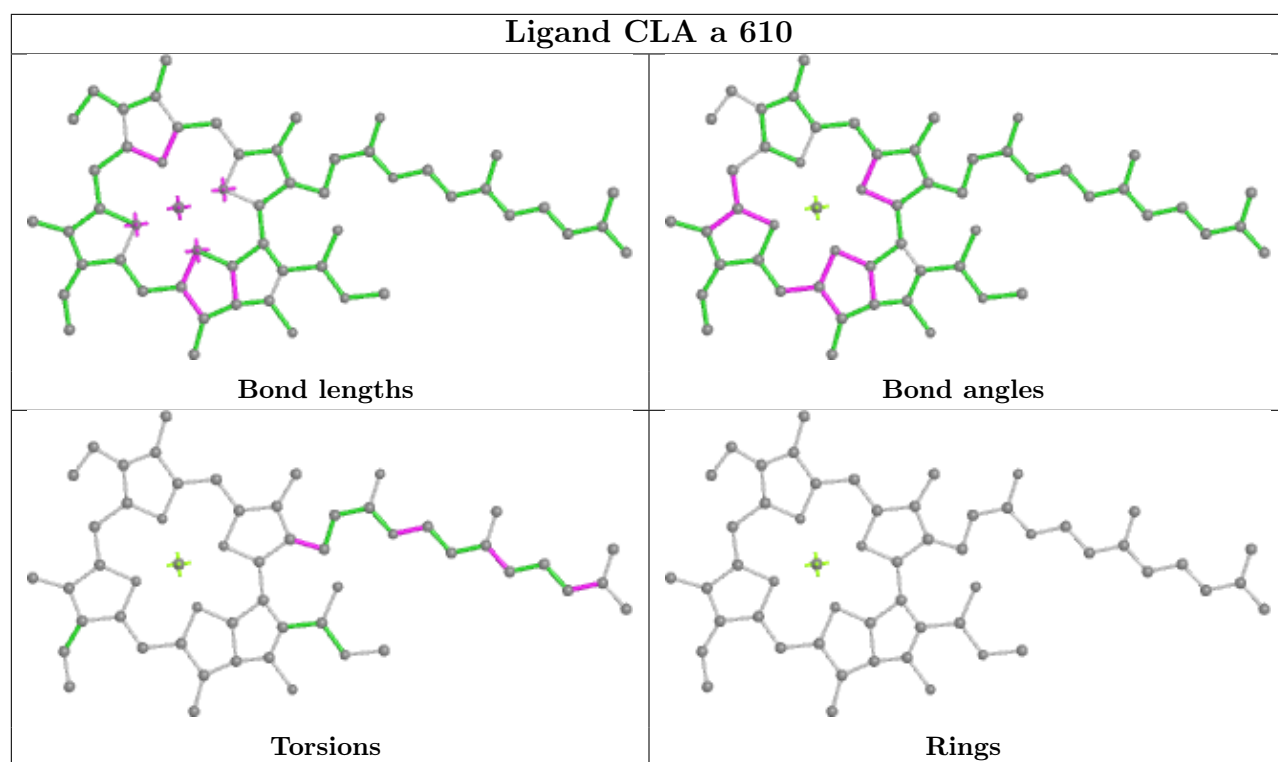
## Ligand CLA a 611



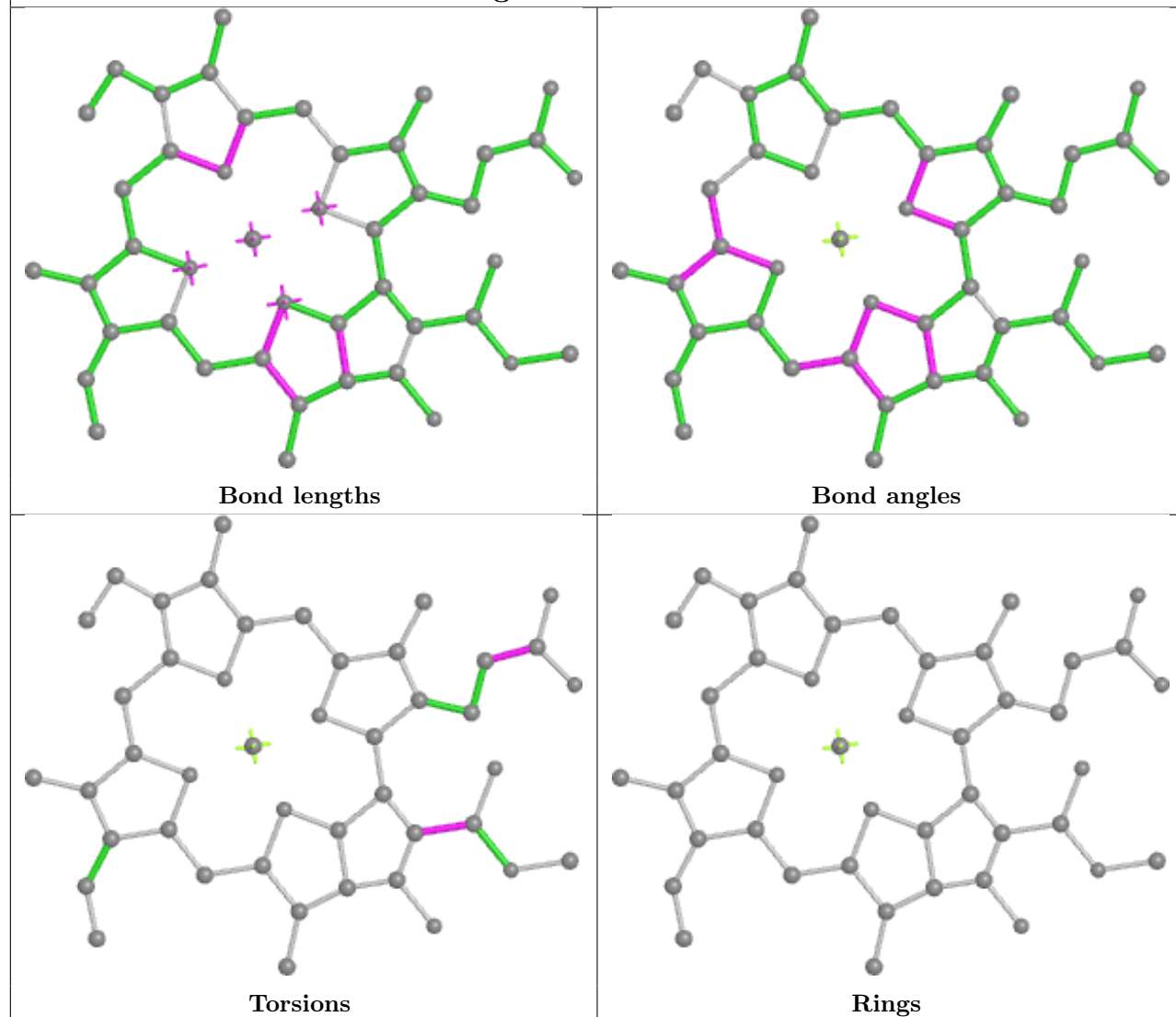
## Ligand CLA 5 605



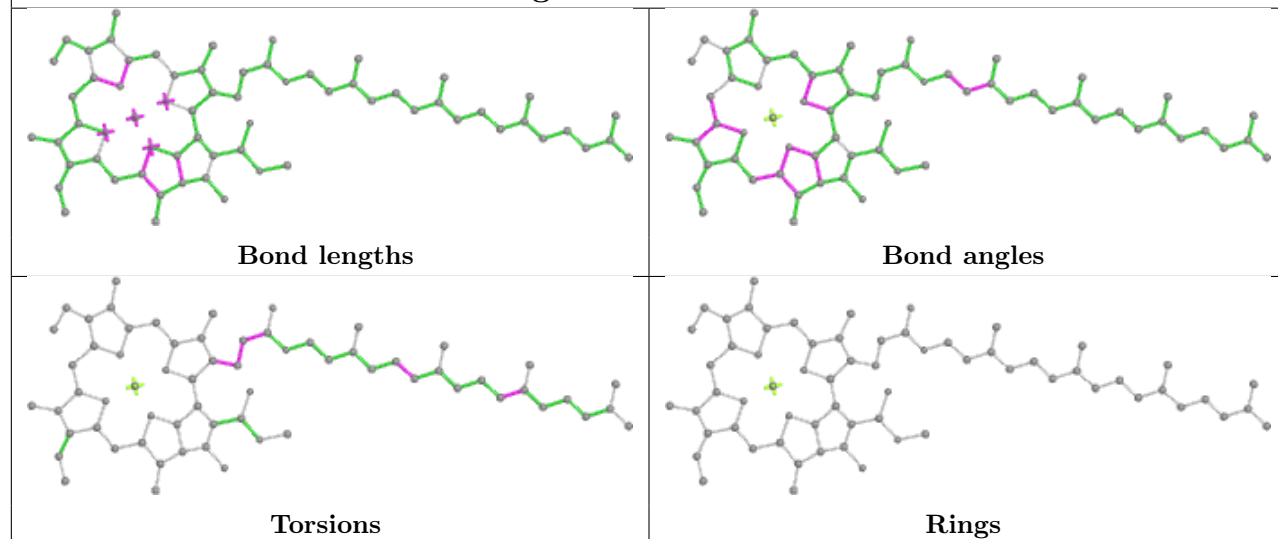


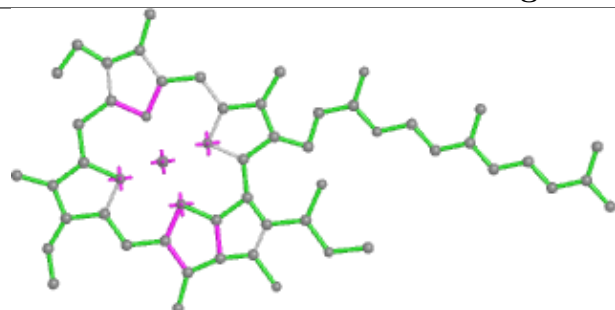


## Ligand CLA 7 306

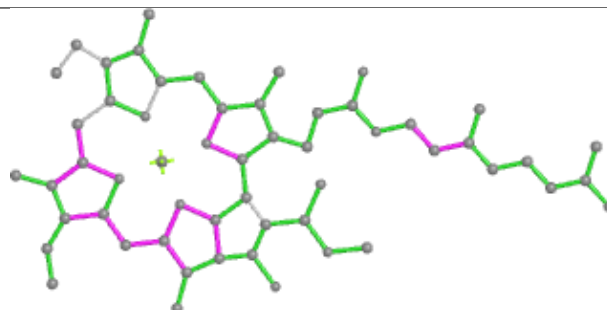


## Ligand CLA B 808

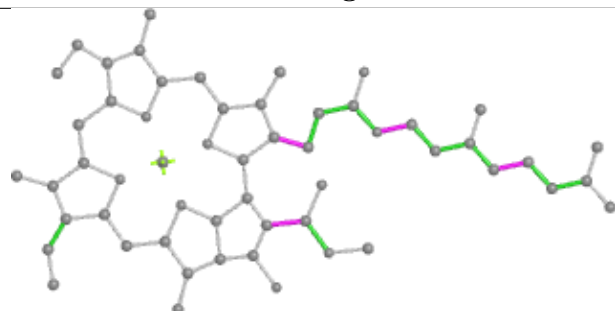


**Ligand CLA 6 611**

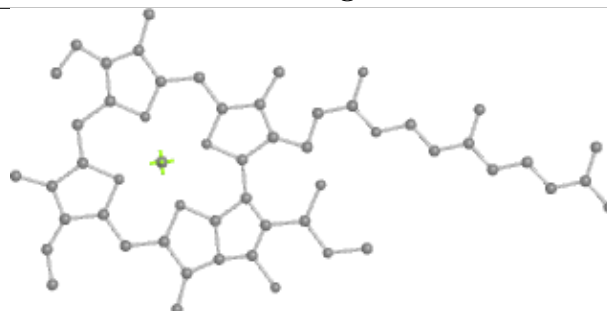
Bond lengths



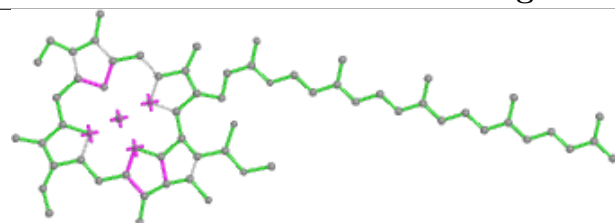
Bond angles



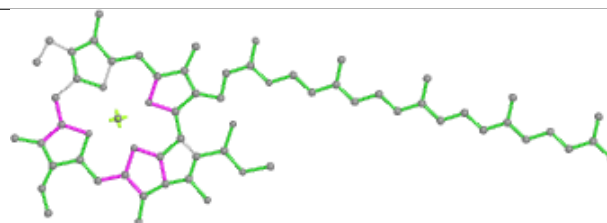
Torsions



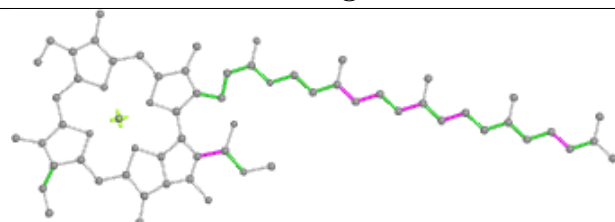
Rings

**Ligand CLA B 807**

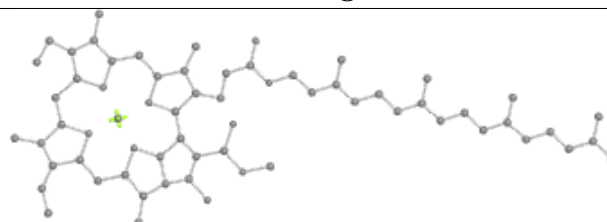
Bond lengths



Bond angles

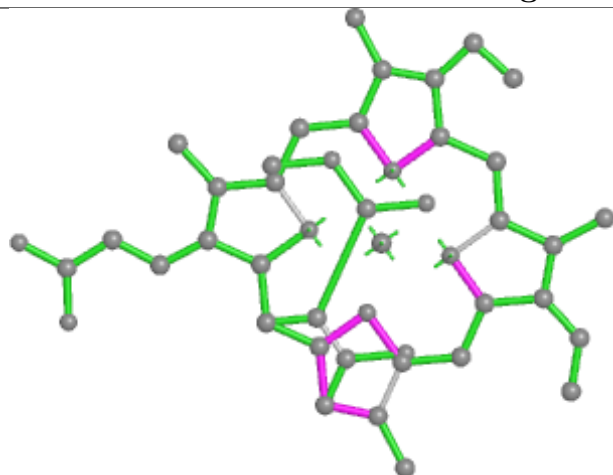


Torsions

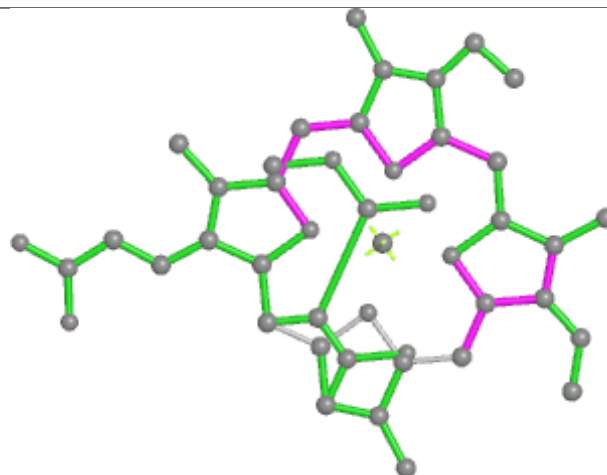


Rings

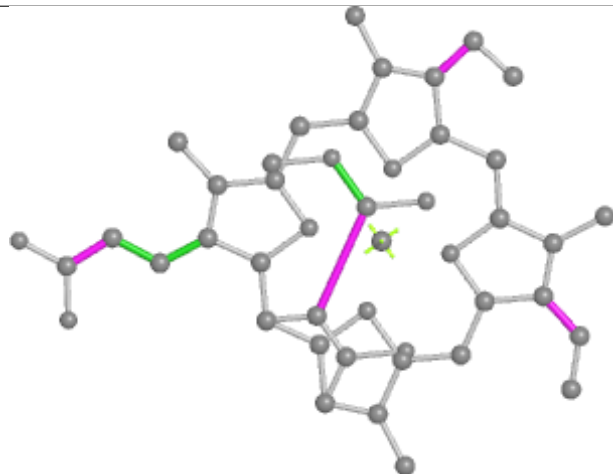
## Ligand KC2 7 307



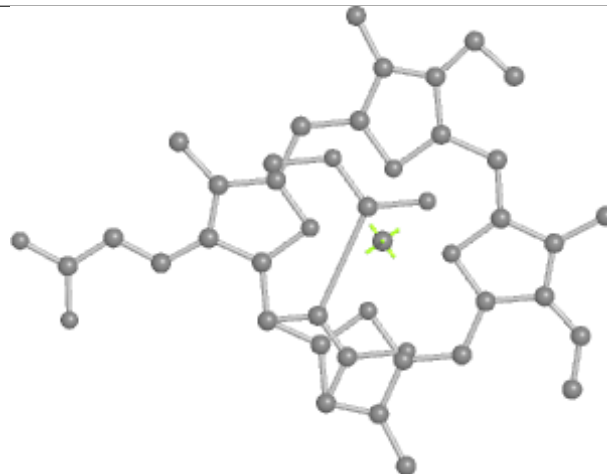
Bond lengths



Bond angles

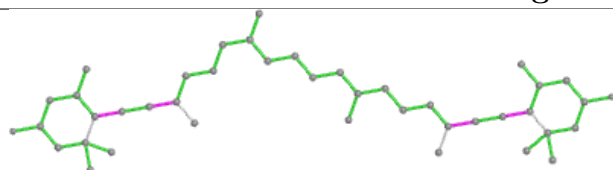


Torsions

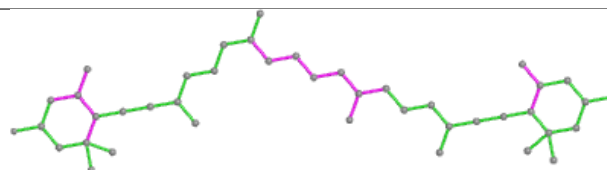


Rings

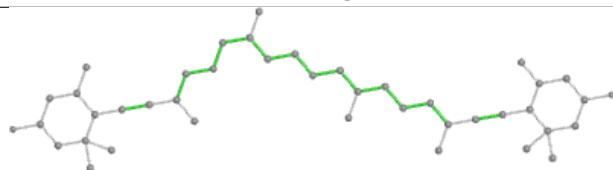
## Ligand II0 b 614



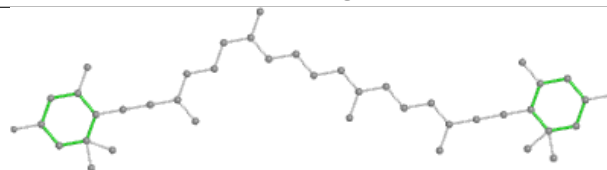
Bond lengths



Bond angles

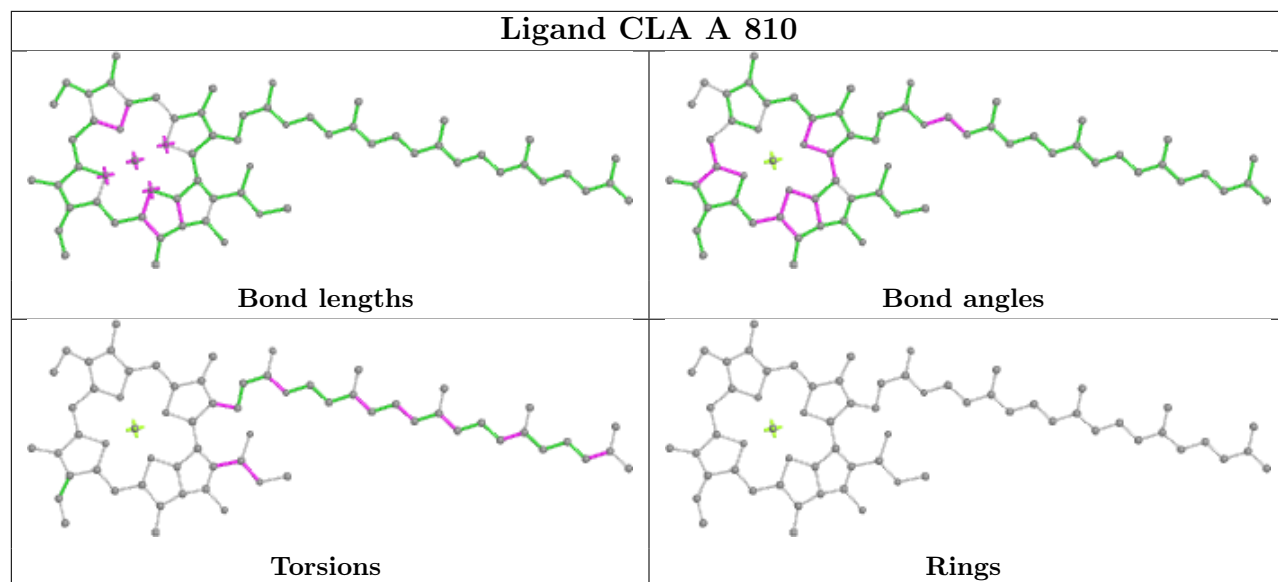


Torsions

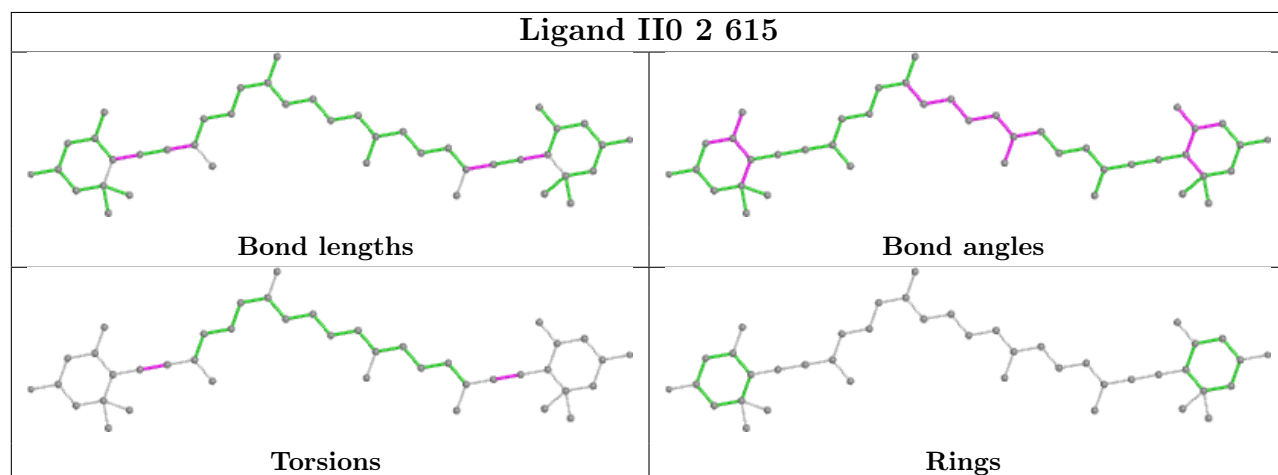


Rings

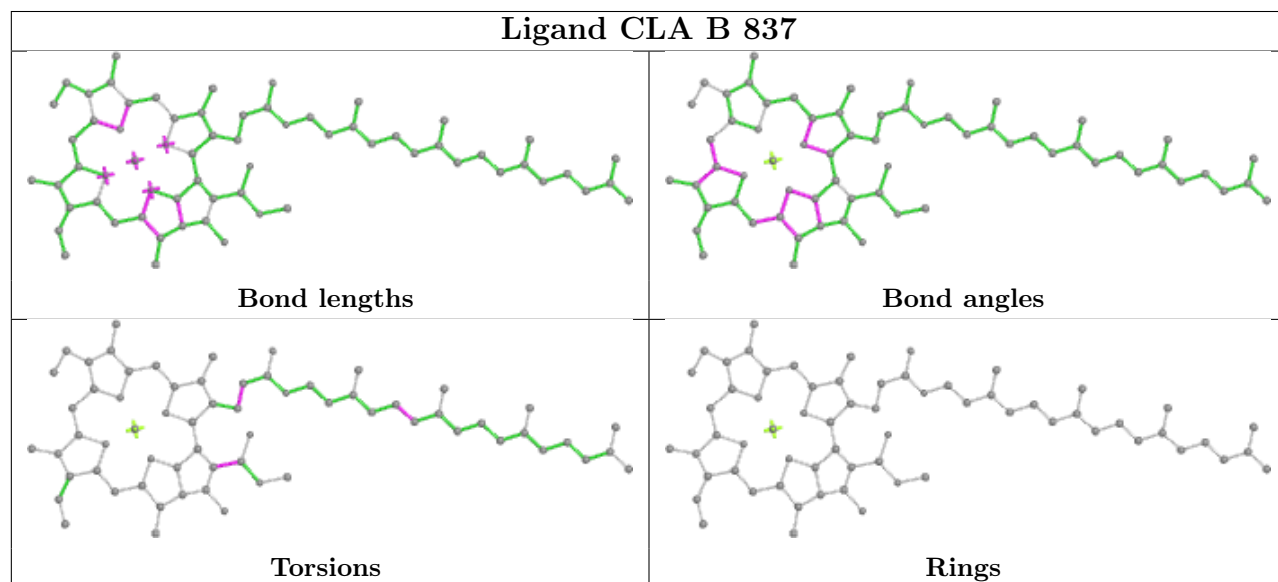
## Ligand CLA A 810



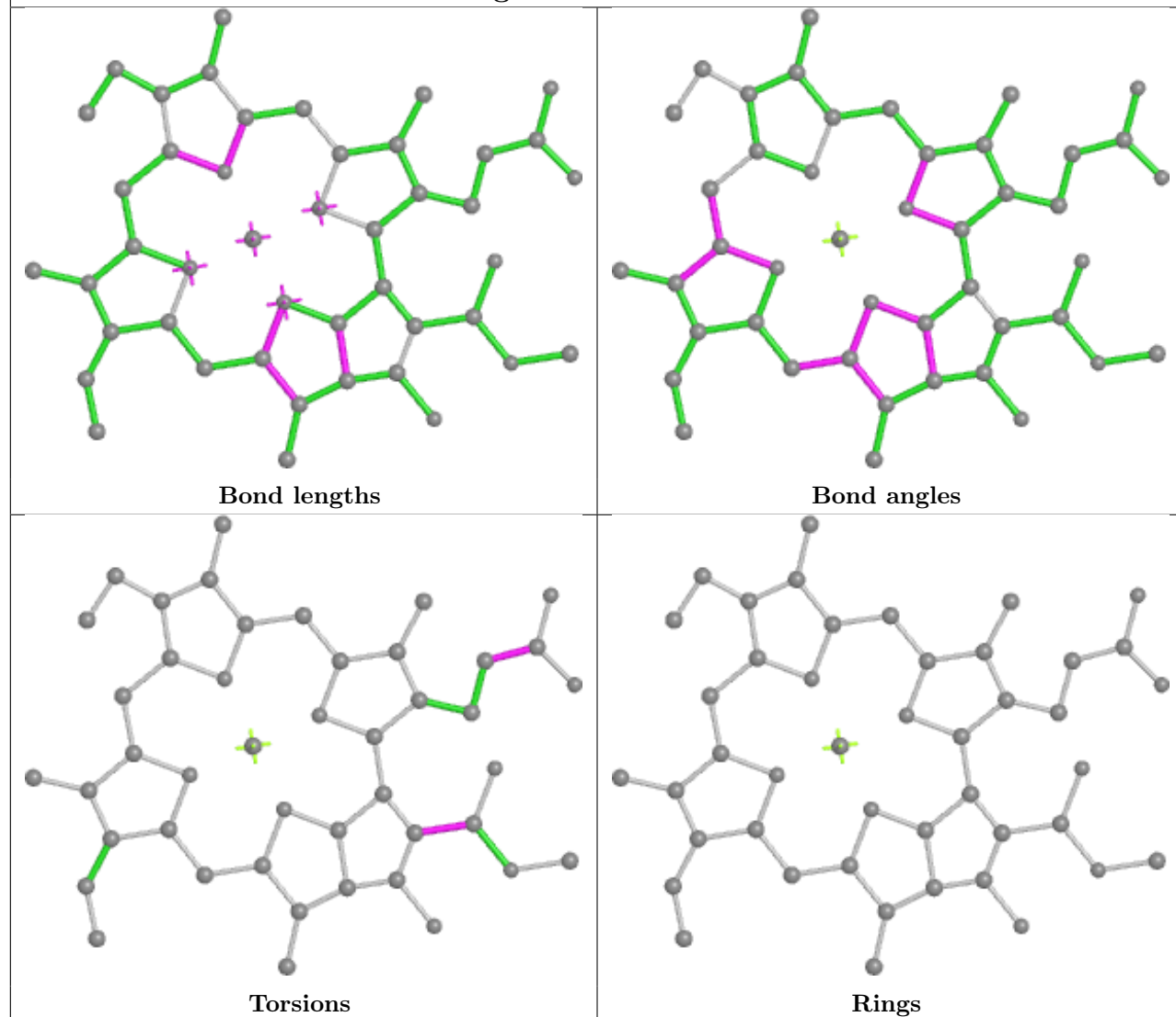
## Ligand II0 2 615



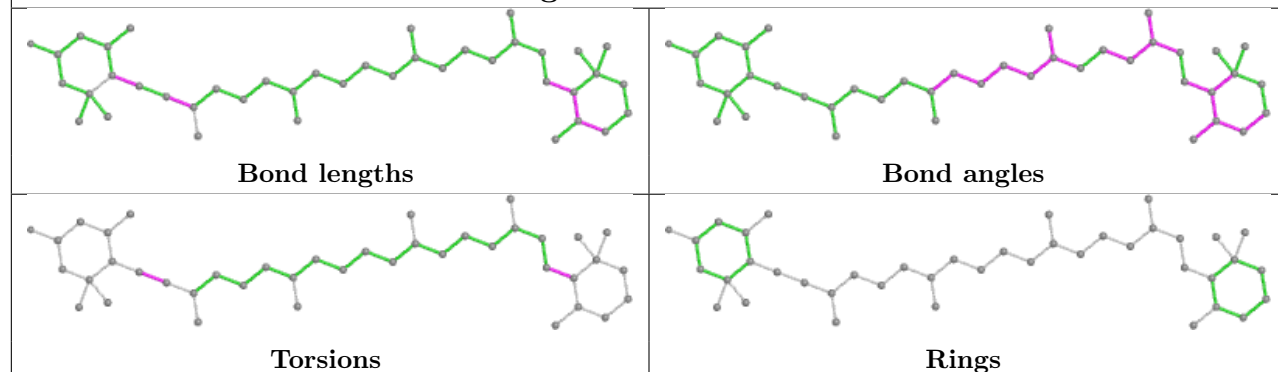
## Ligand CLA B 837



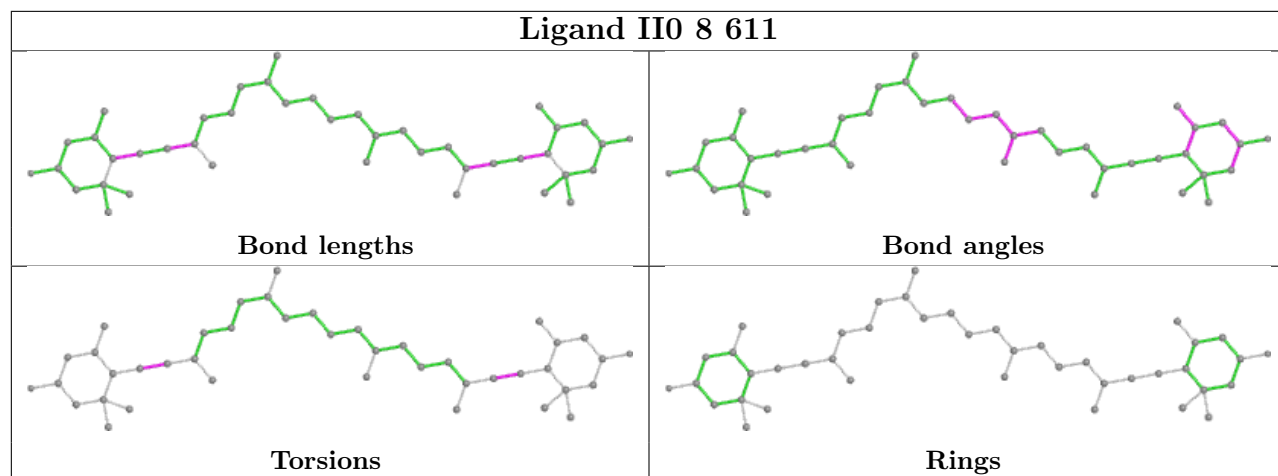
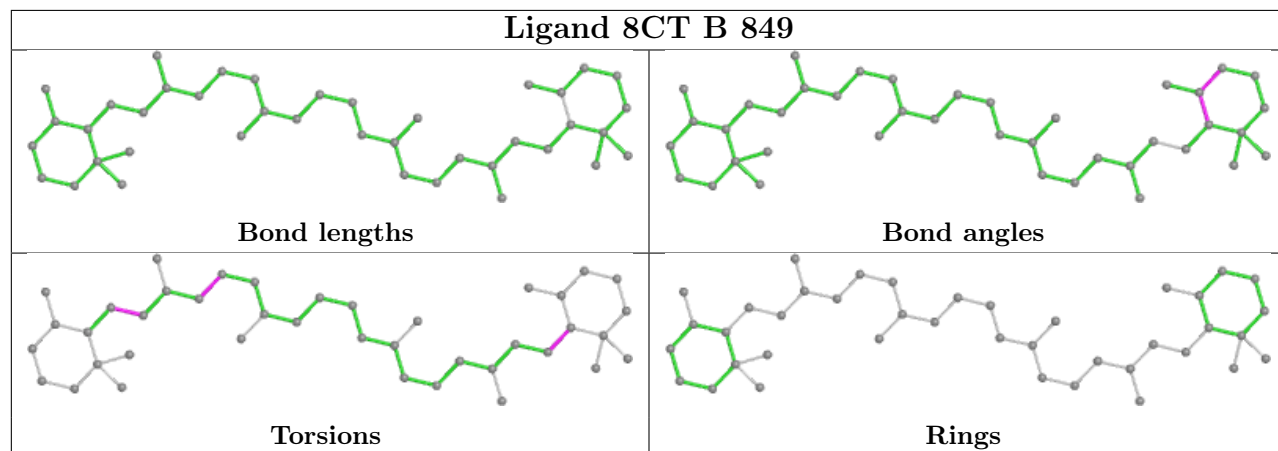
## Ligand CLA 1 611



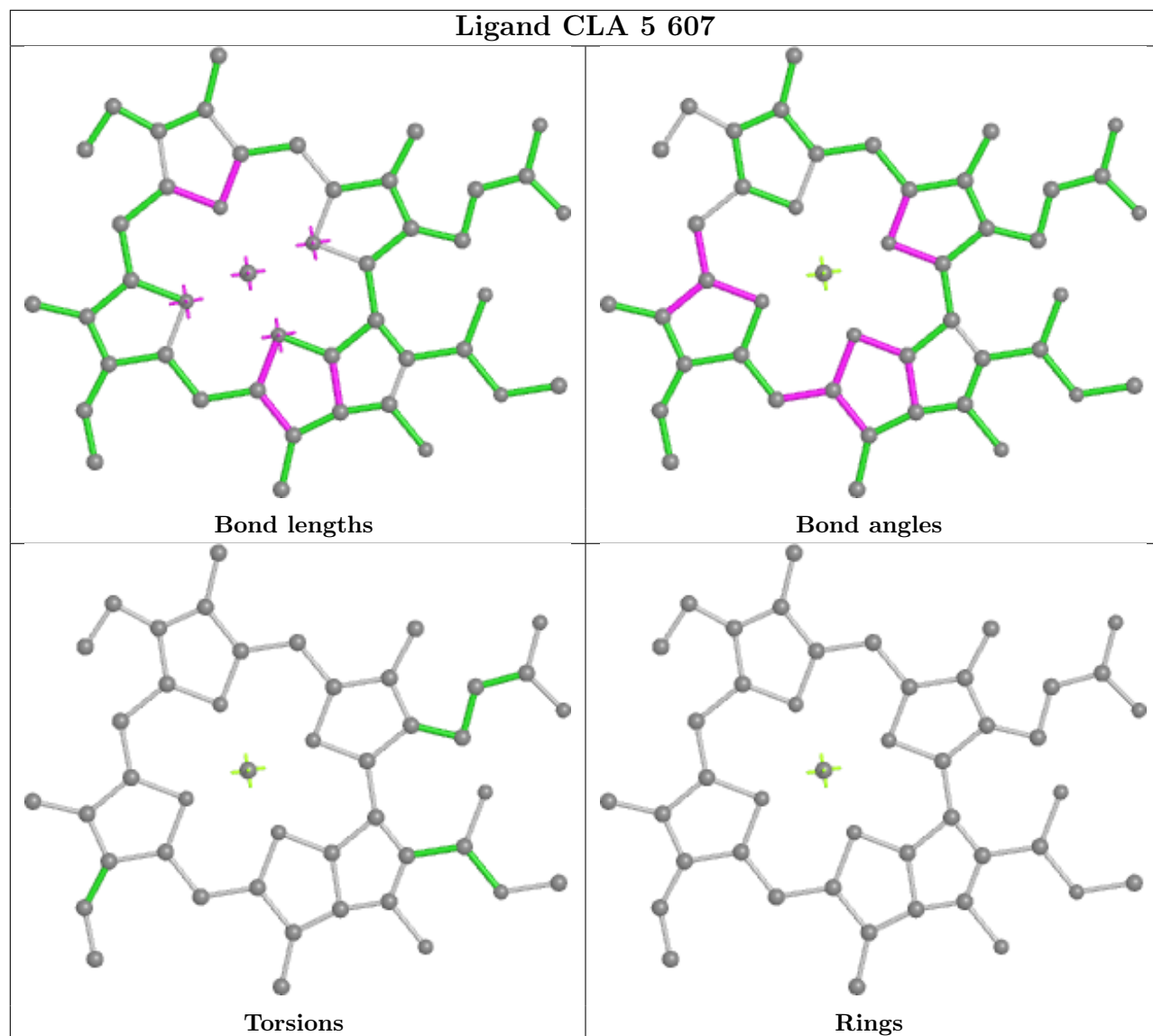
## Ligand IHT 1 618



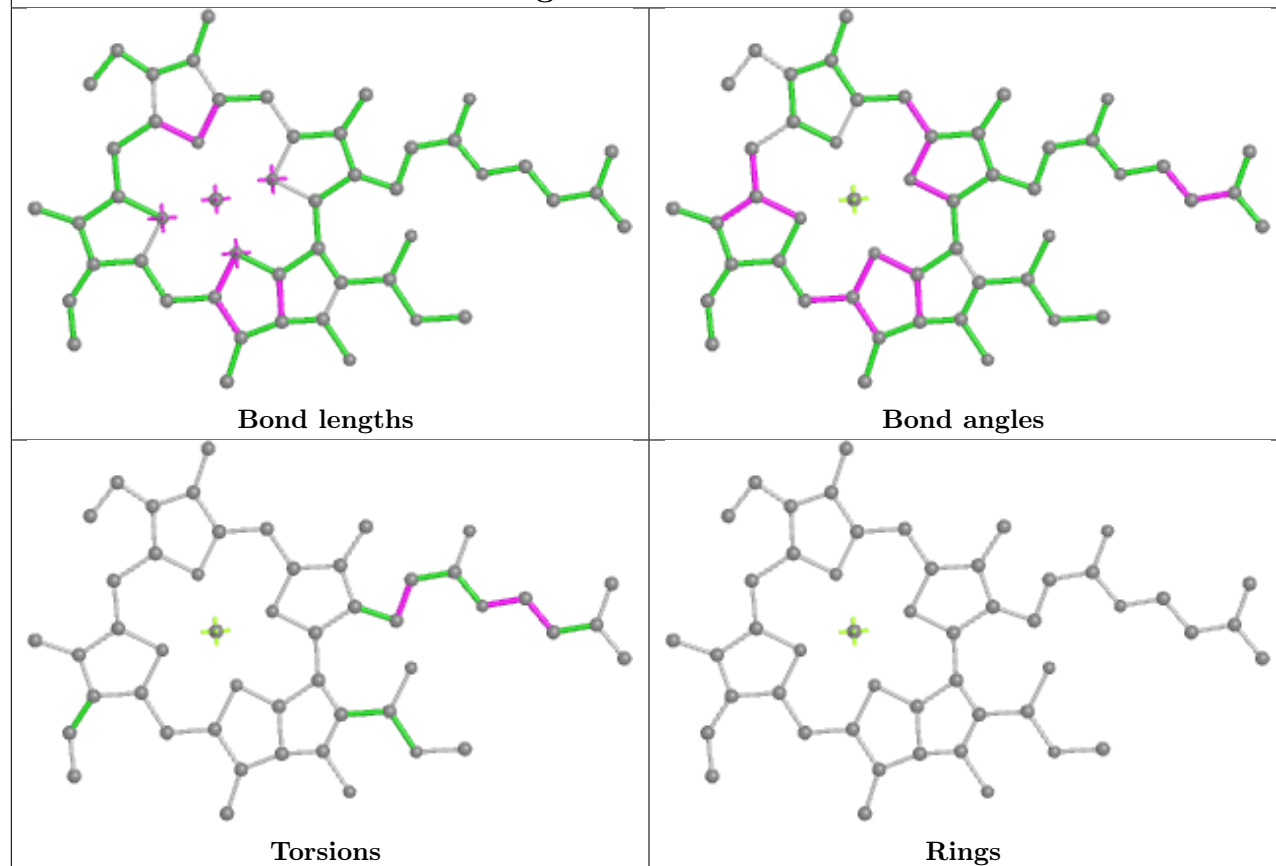


**Ligand II0 8 611****Ligand 8CT B 849**

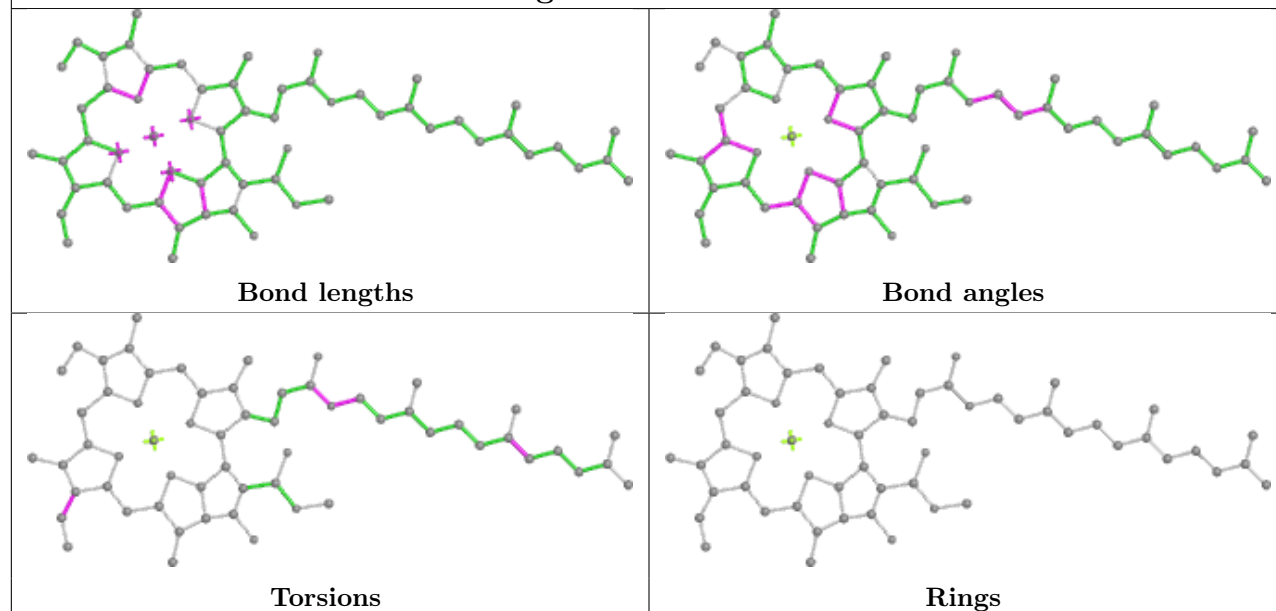
## Ligand CLA 5 607

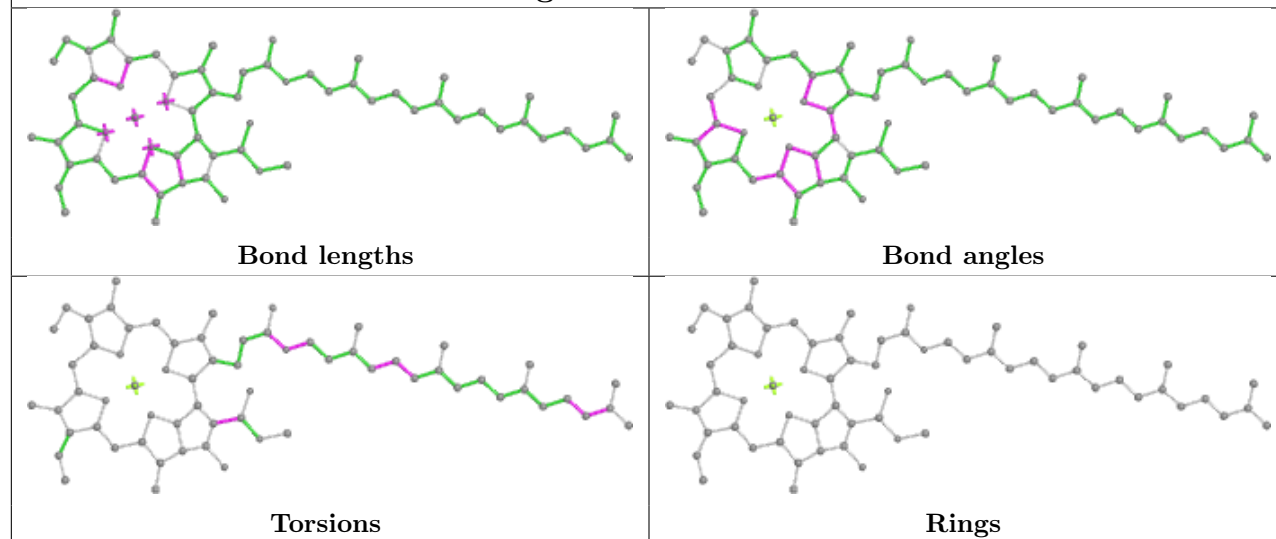
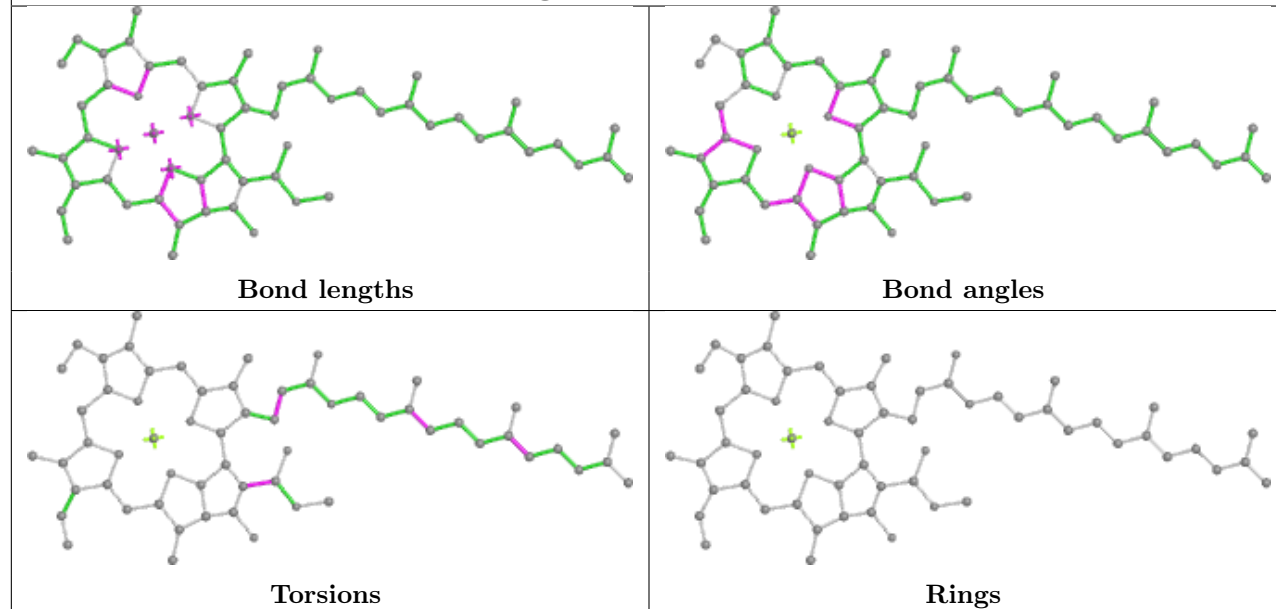


## Ligand CLA 8 605

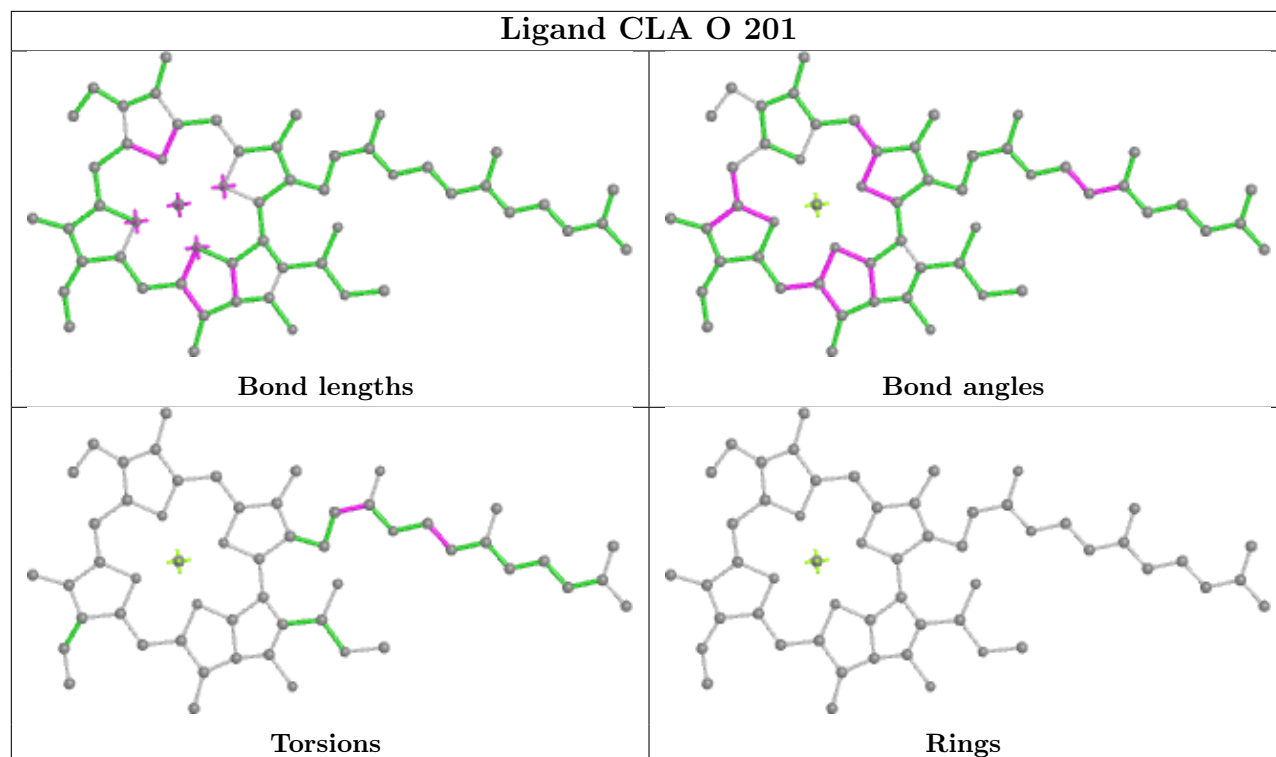


## Ligand CLA a 608

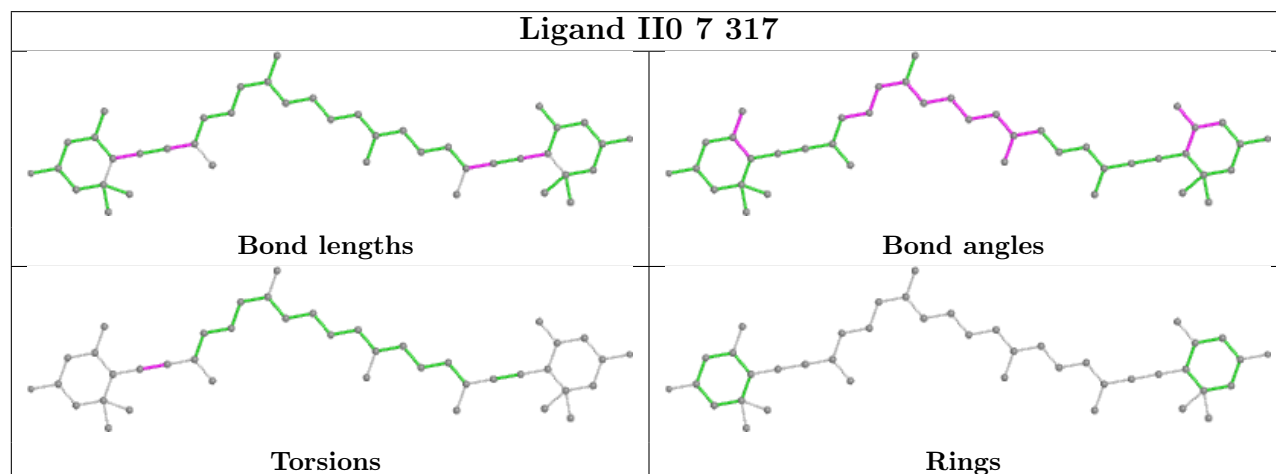


**Ligand CLA 4 611****Ligand CLA 6 604**

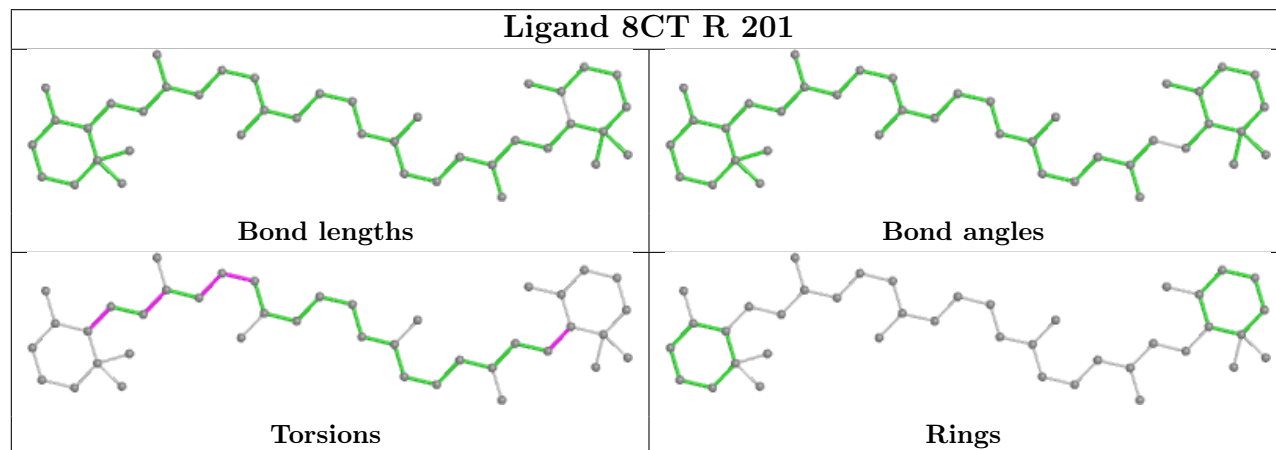
## Ligand CLA O 201



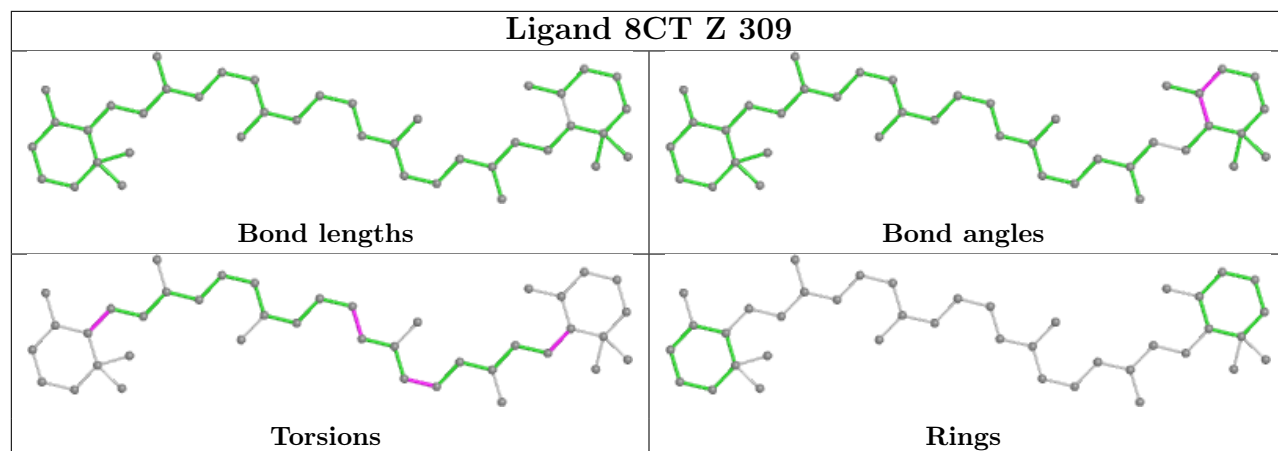
## Ligand II0 7 317



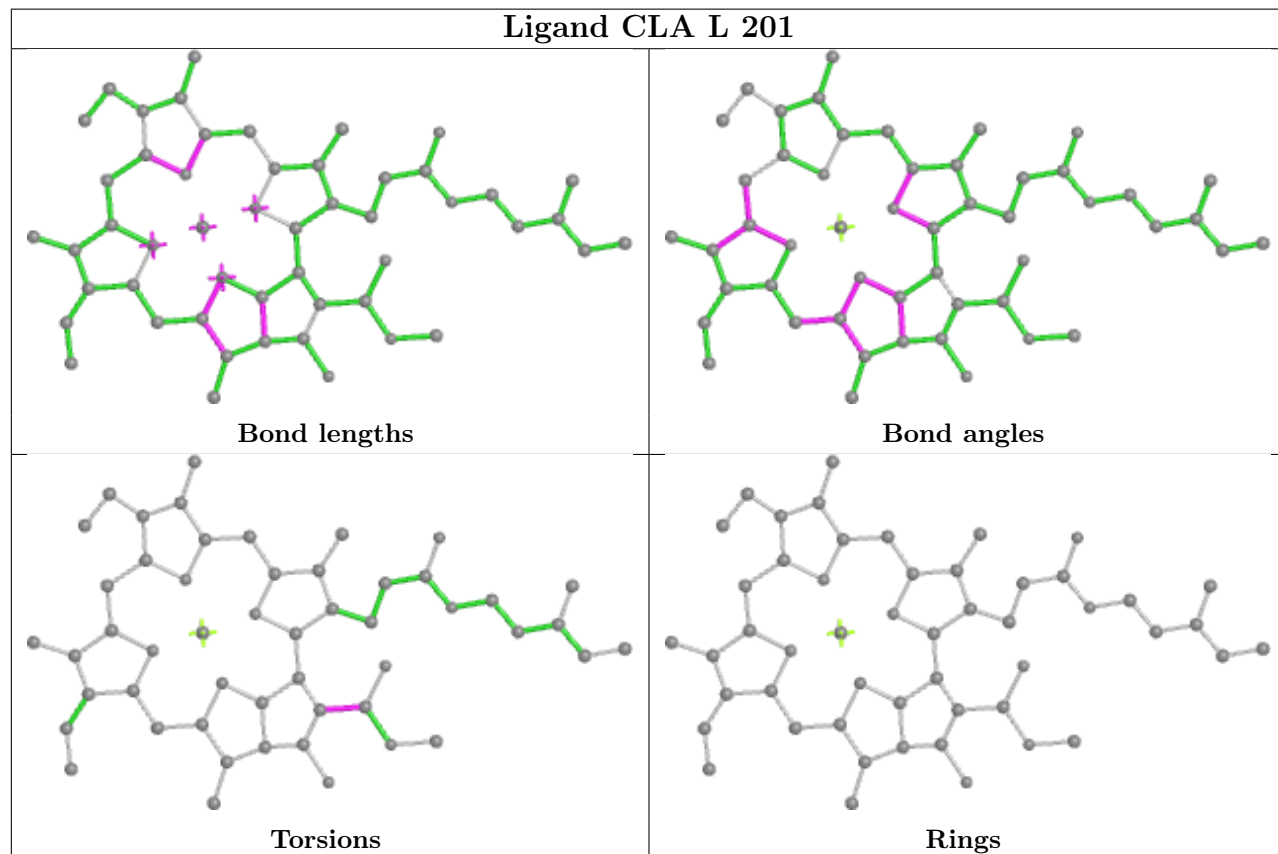
## Ligand 8CT R 201



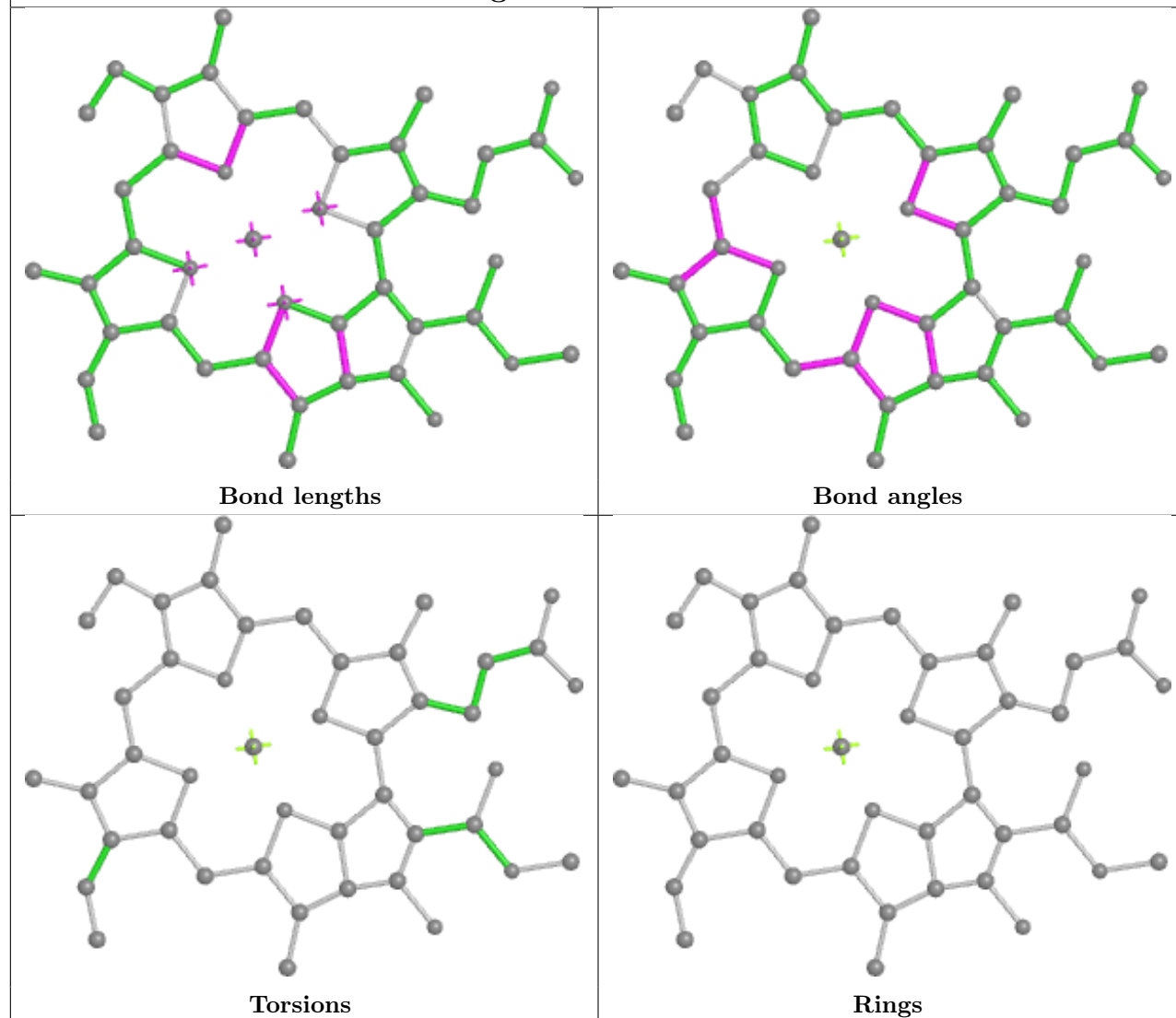
## Ligand 8CT Z 309



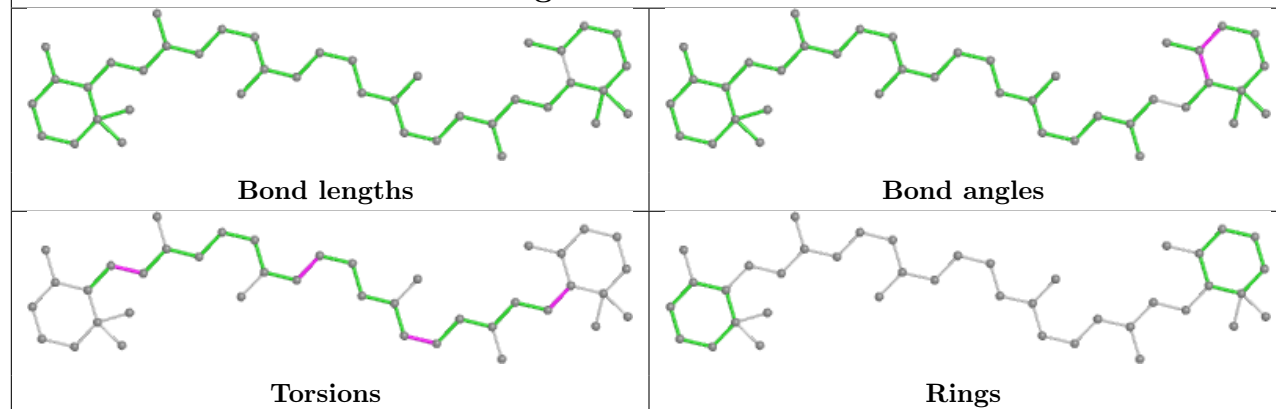
## Ligand CLA L 201



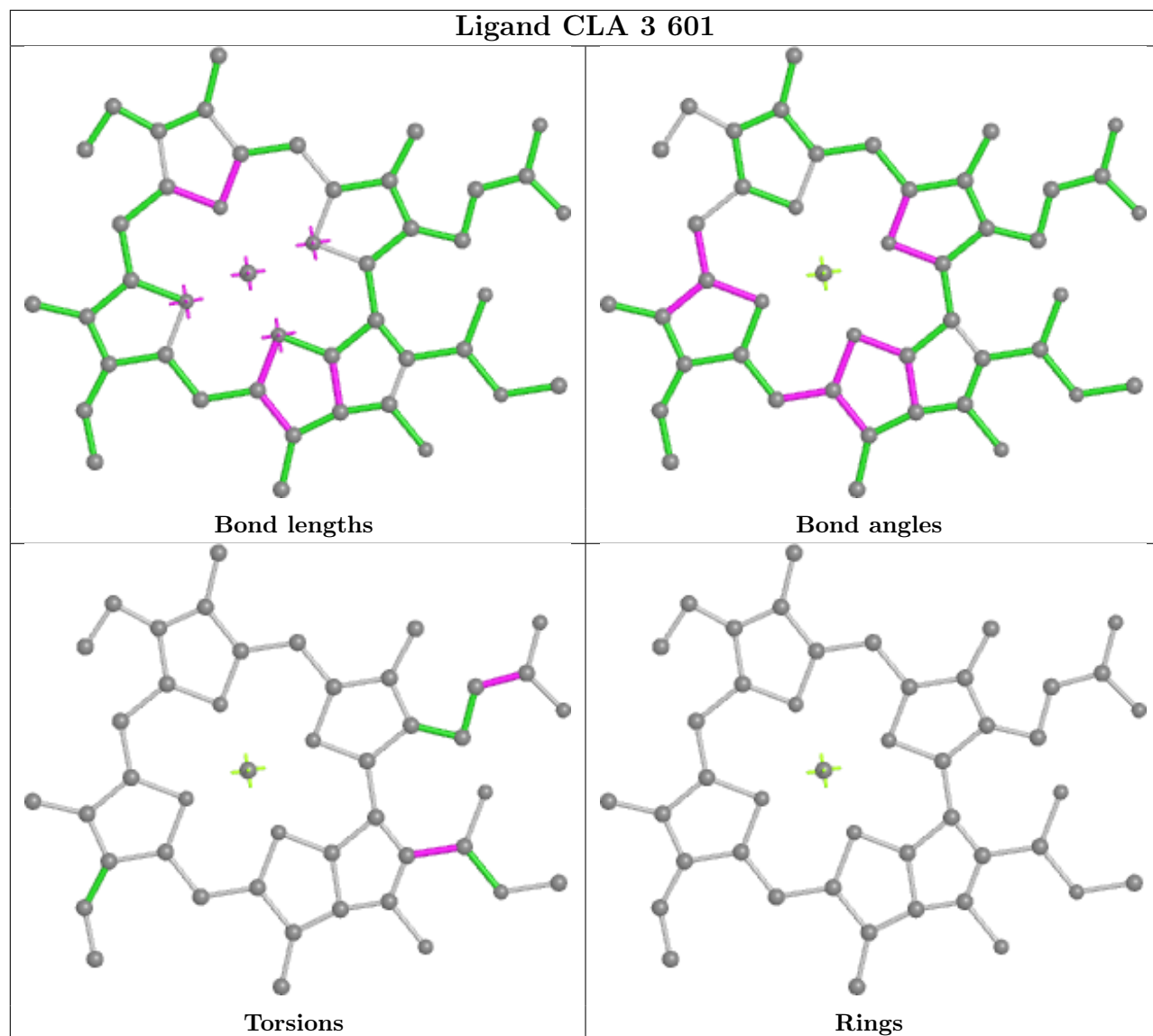
## Ligand CLA B 829



## Ligand 8CT R 203

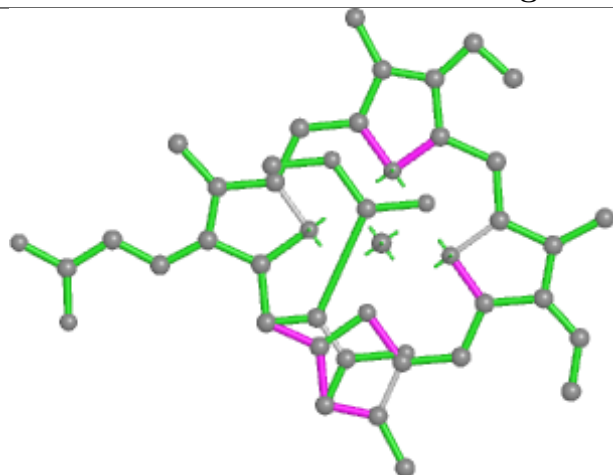


## Ligand CLA 3 601

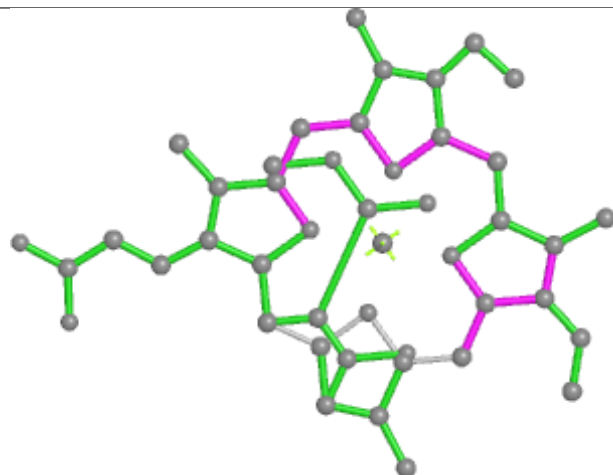




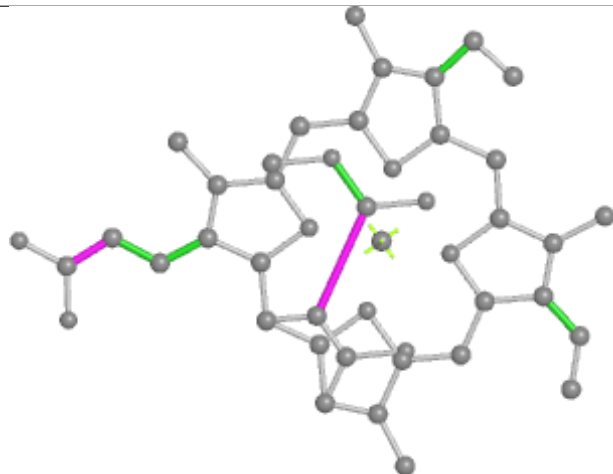
## Ligand KC2 5 610



Bond lengths



Bond angles

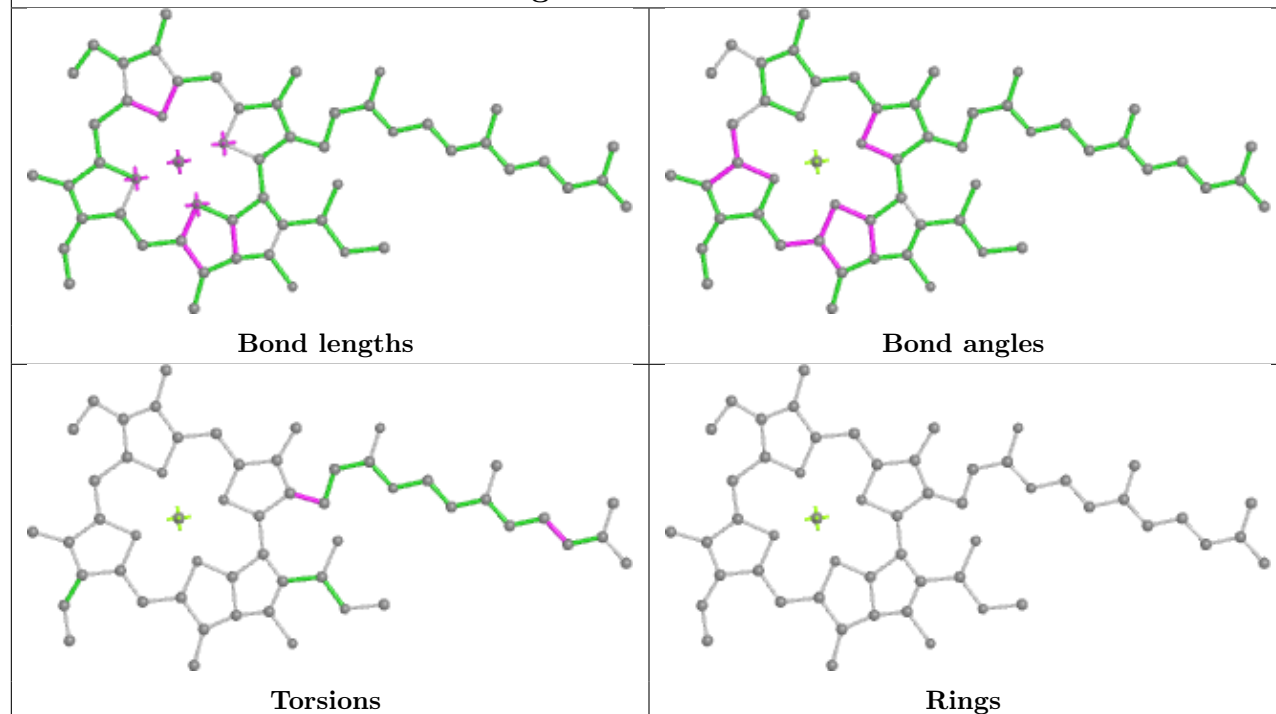


Torsions

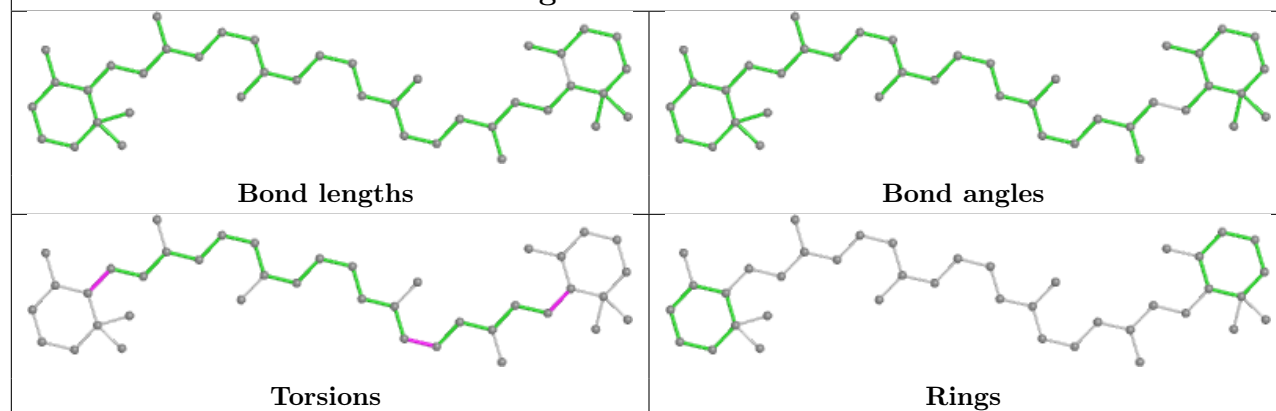


Rings

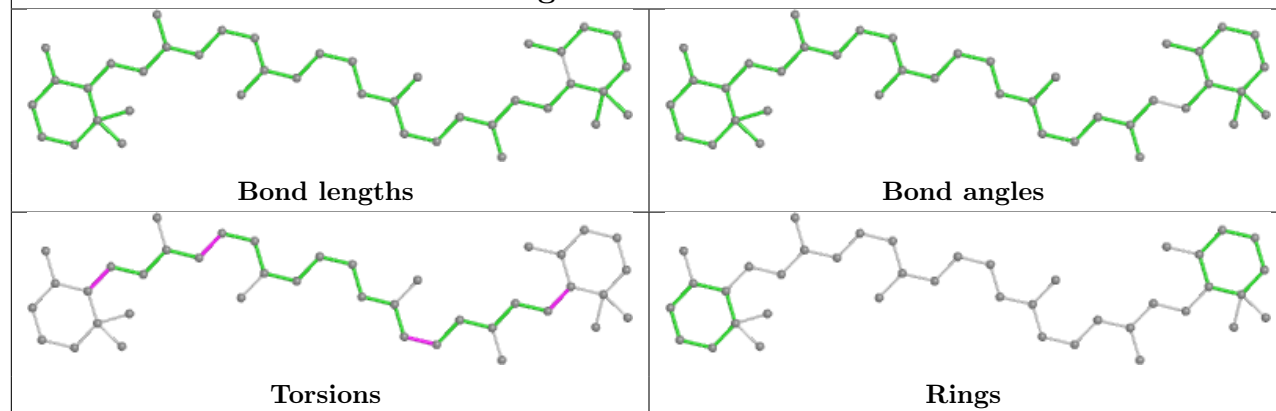
## Ligand CLA A 821



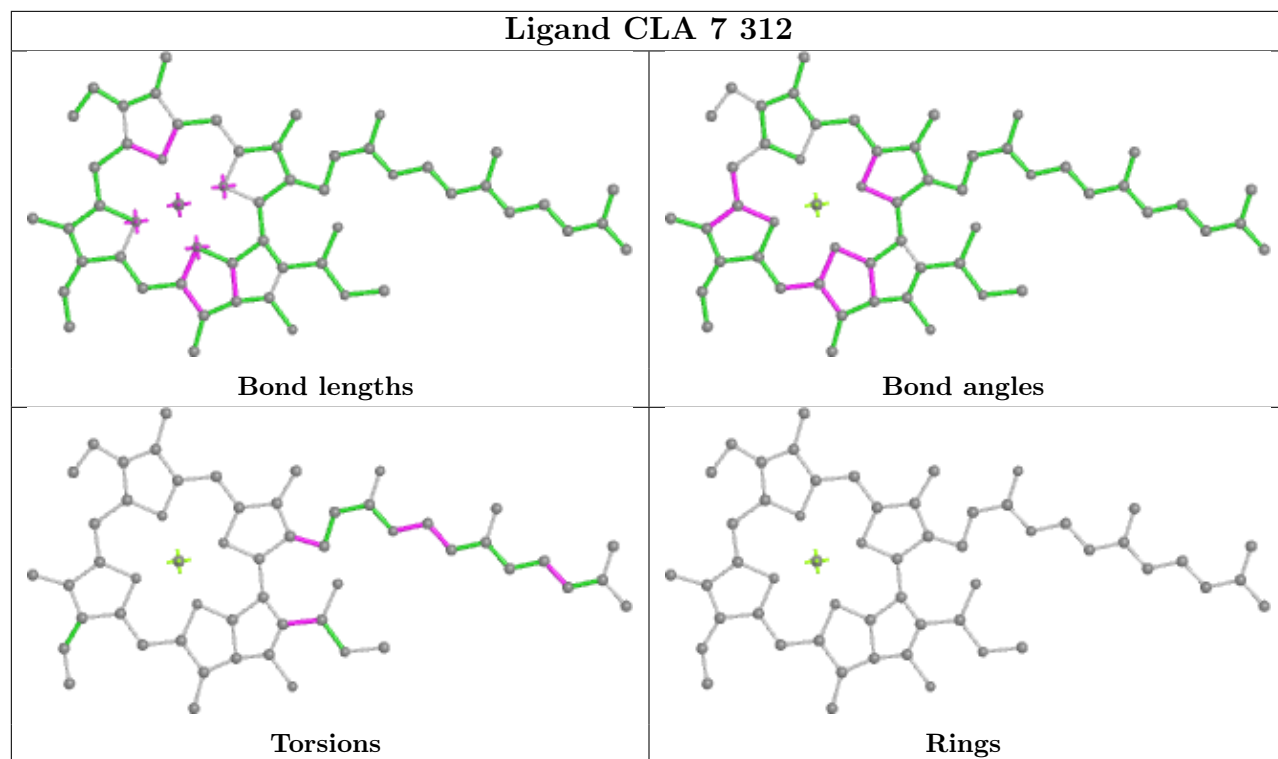
## Ligand 8CT 4 616



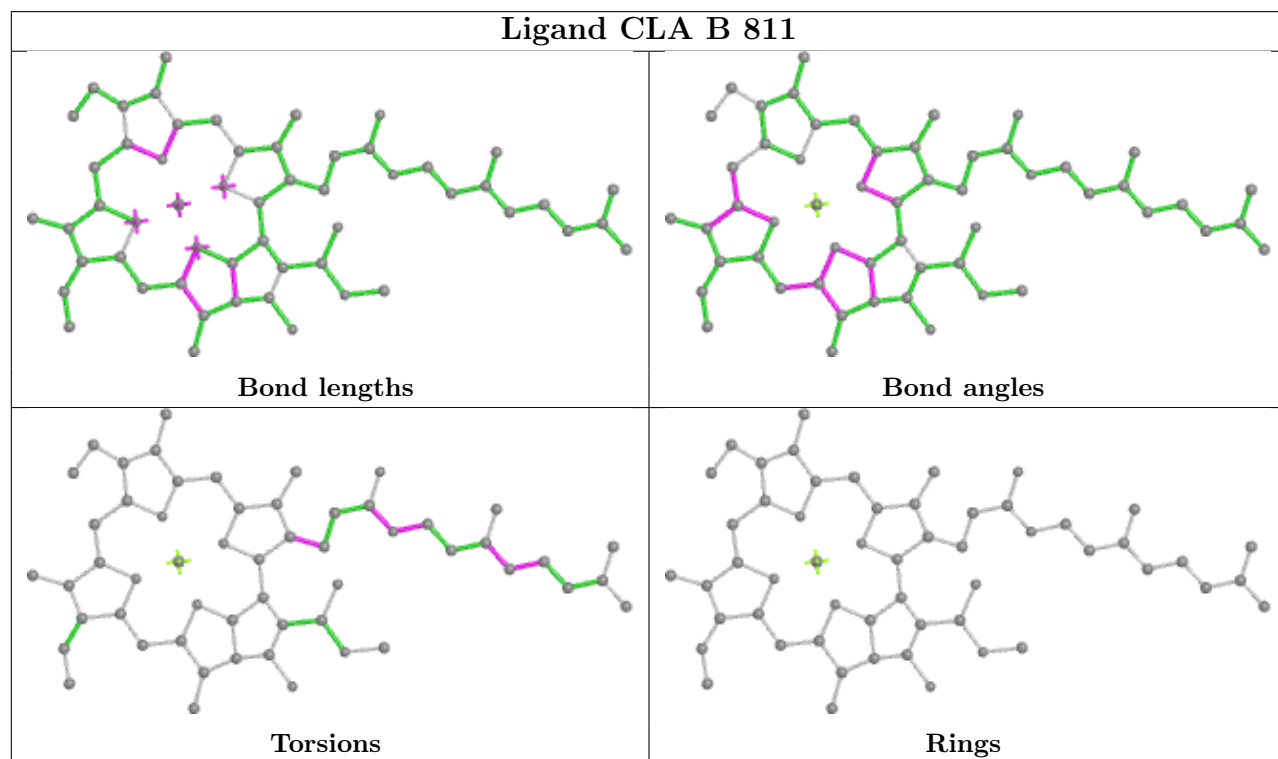
## Ligand 8CT b 615



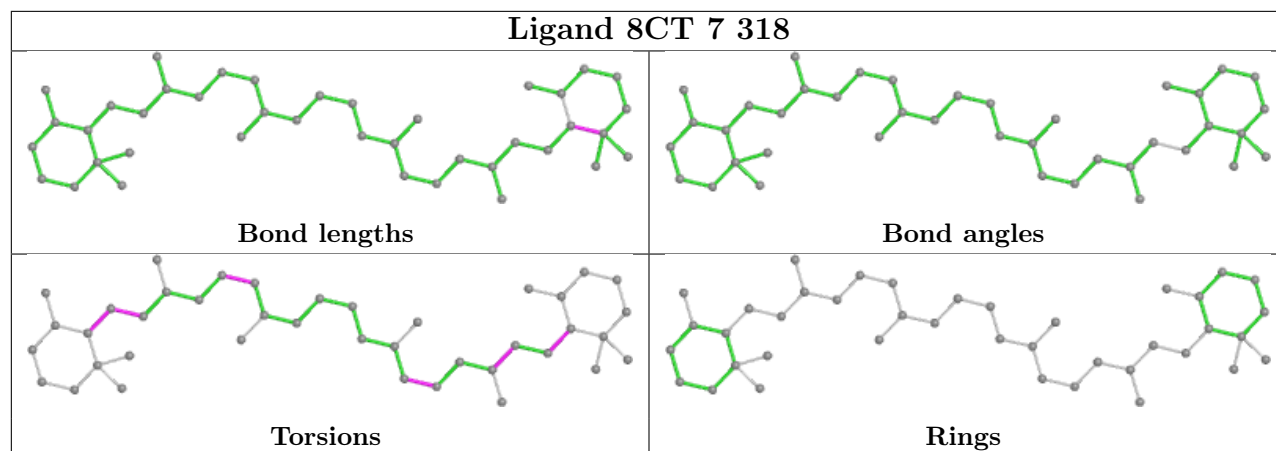
## Ligand CLA 7 312



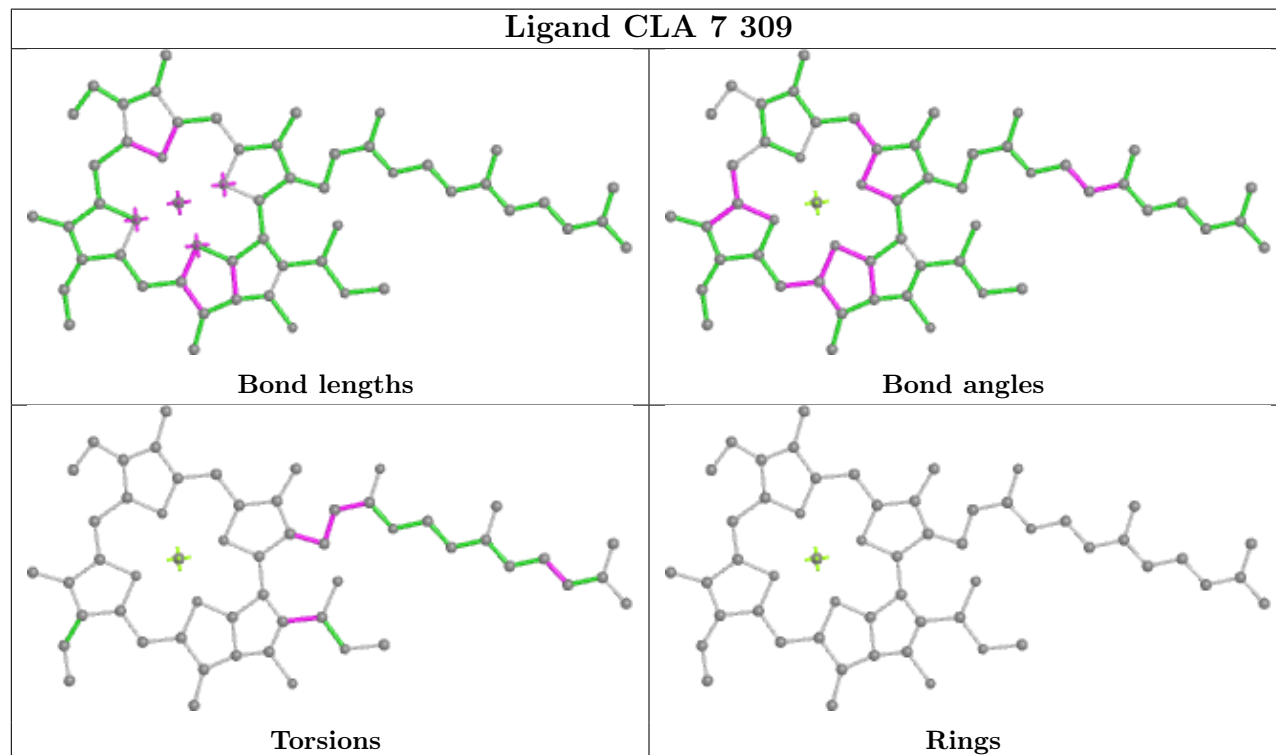
## Ligand CLA B 811



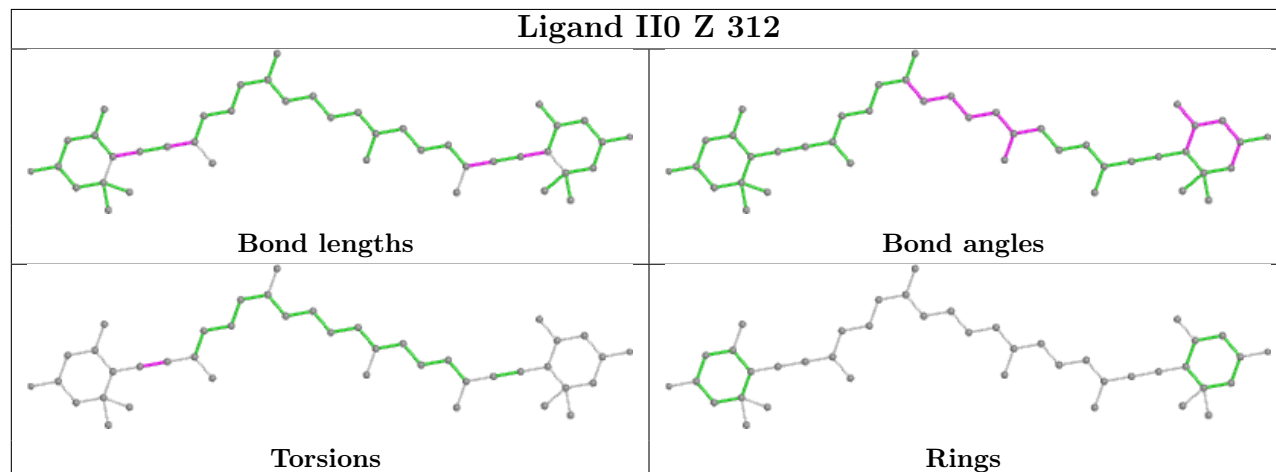
## Ligand 8CT 7 318

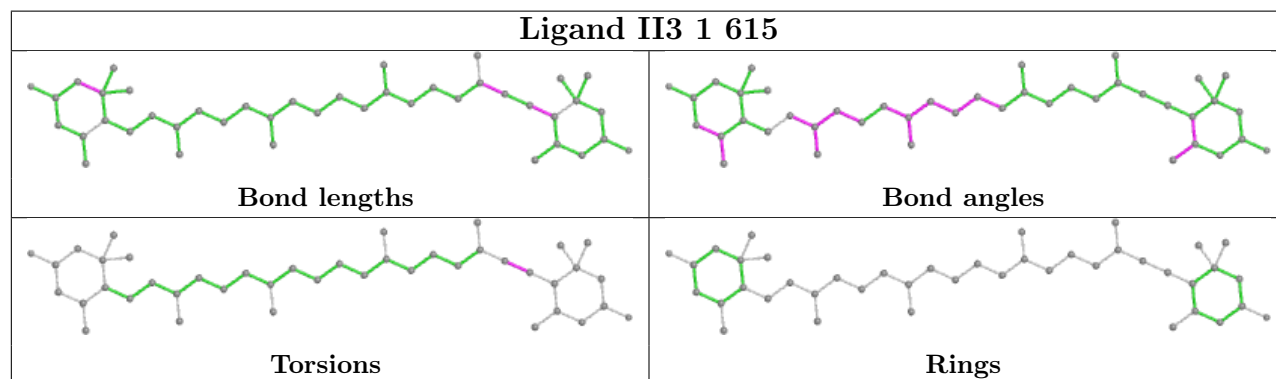
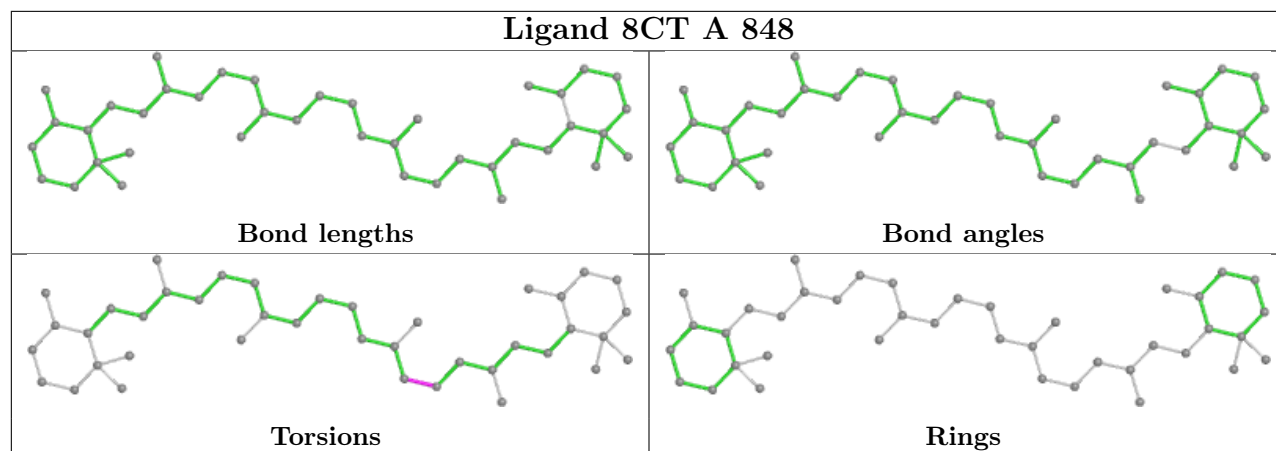


## Ligand CLA 7 309

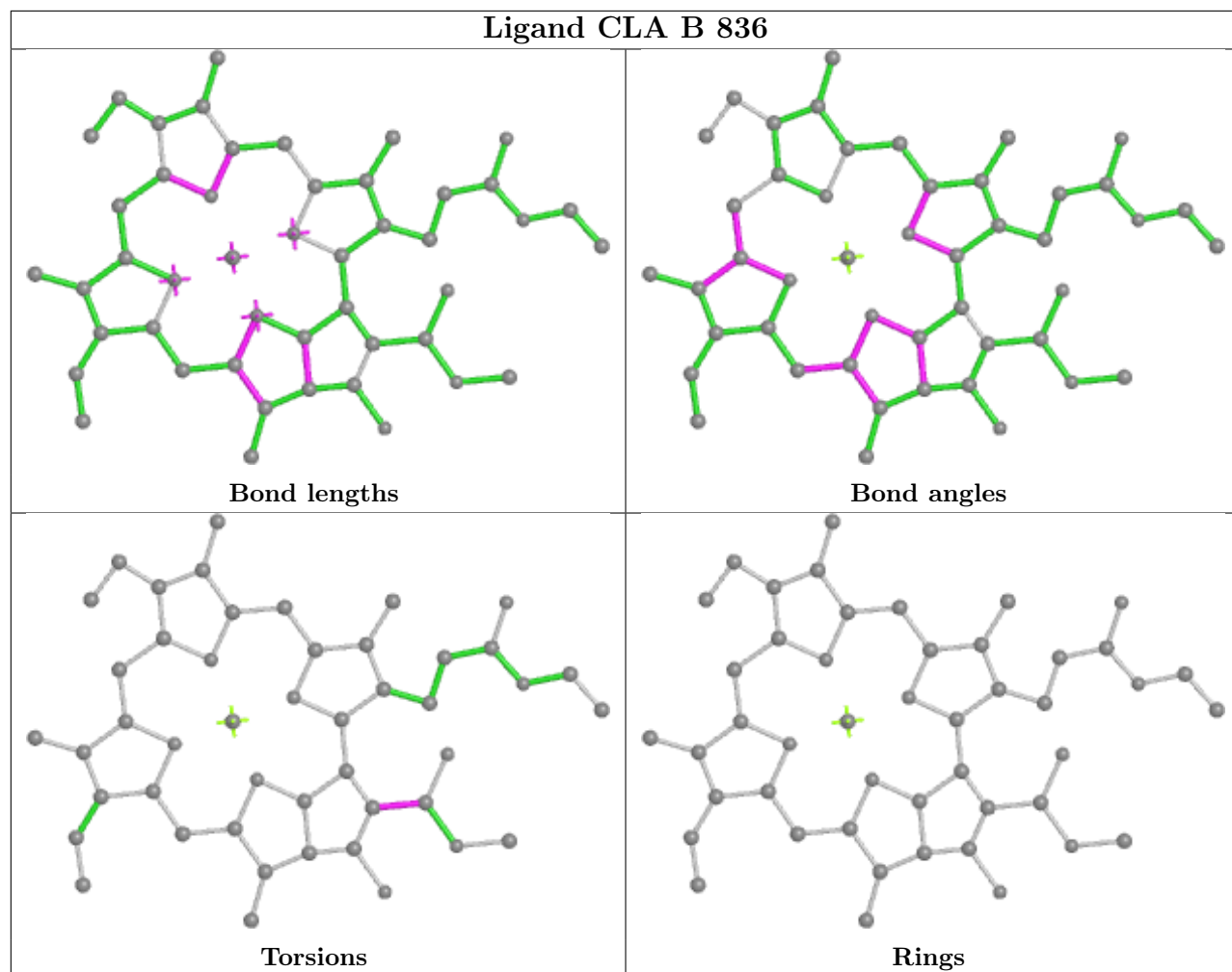


## Ligand II0 Z 312

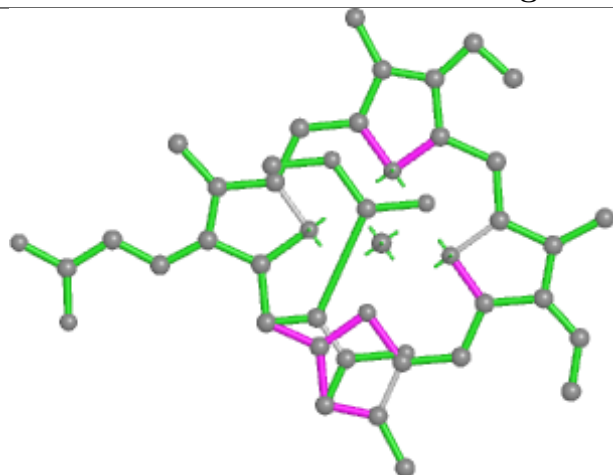




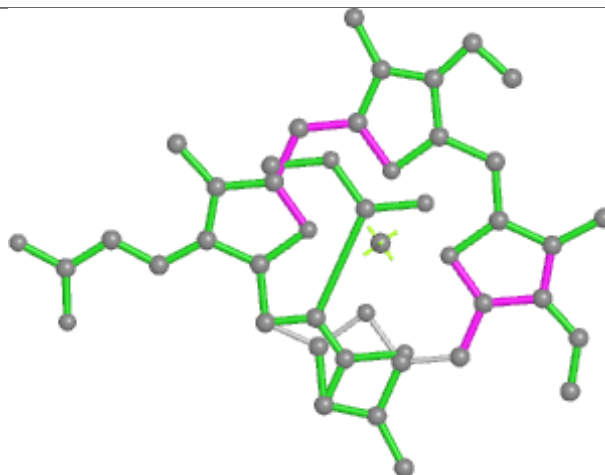
## Ligand CLA B 836



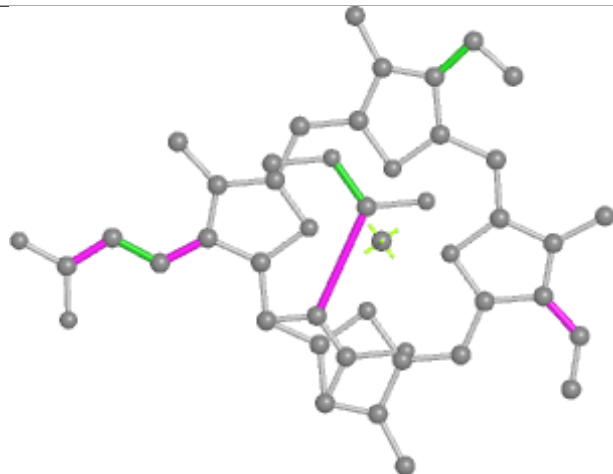
## Ligand KC2 7 311



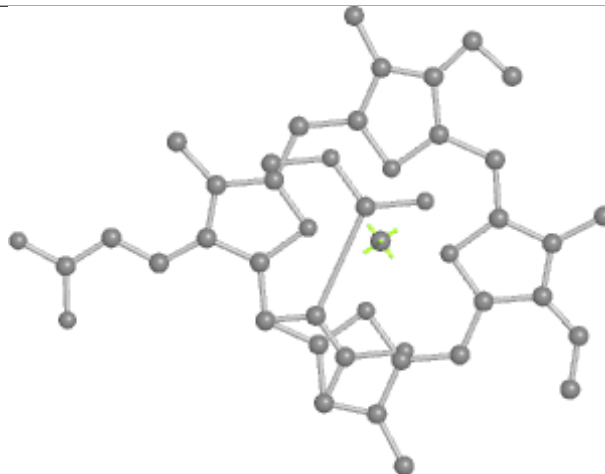
Bond lengths



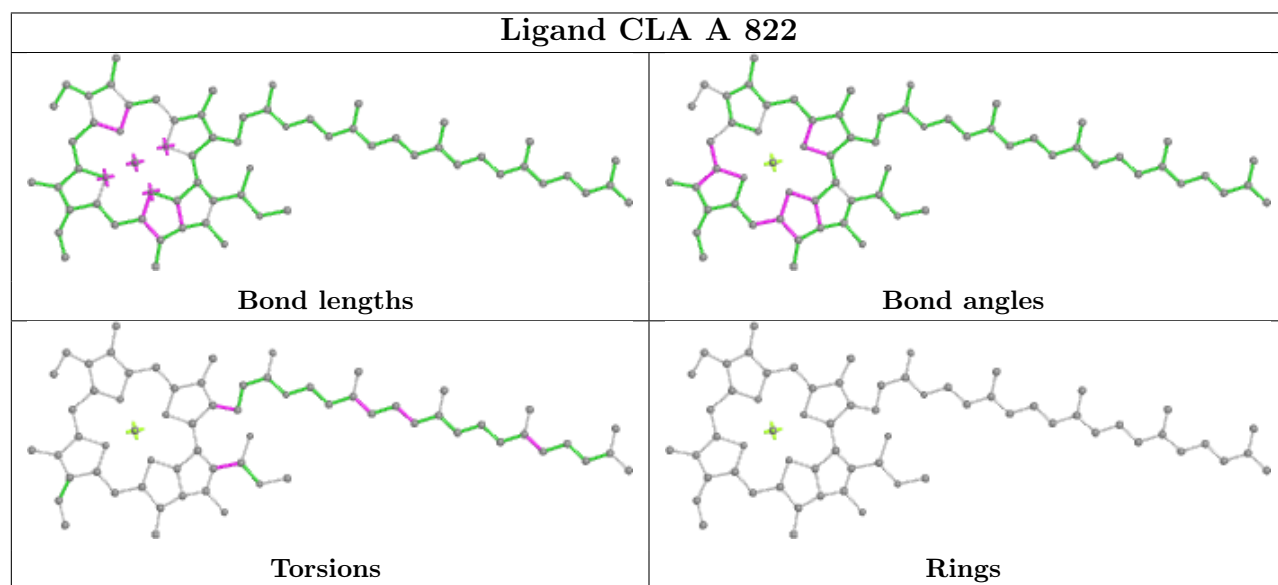
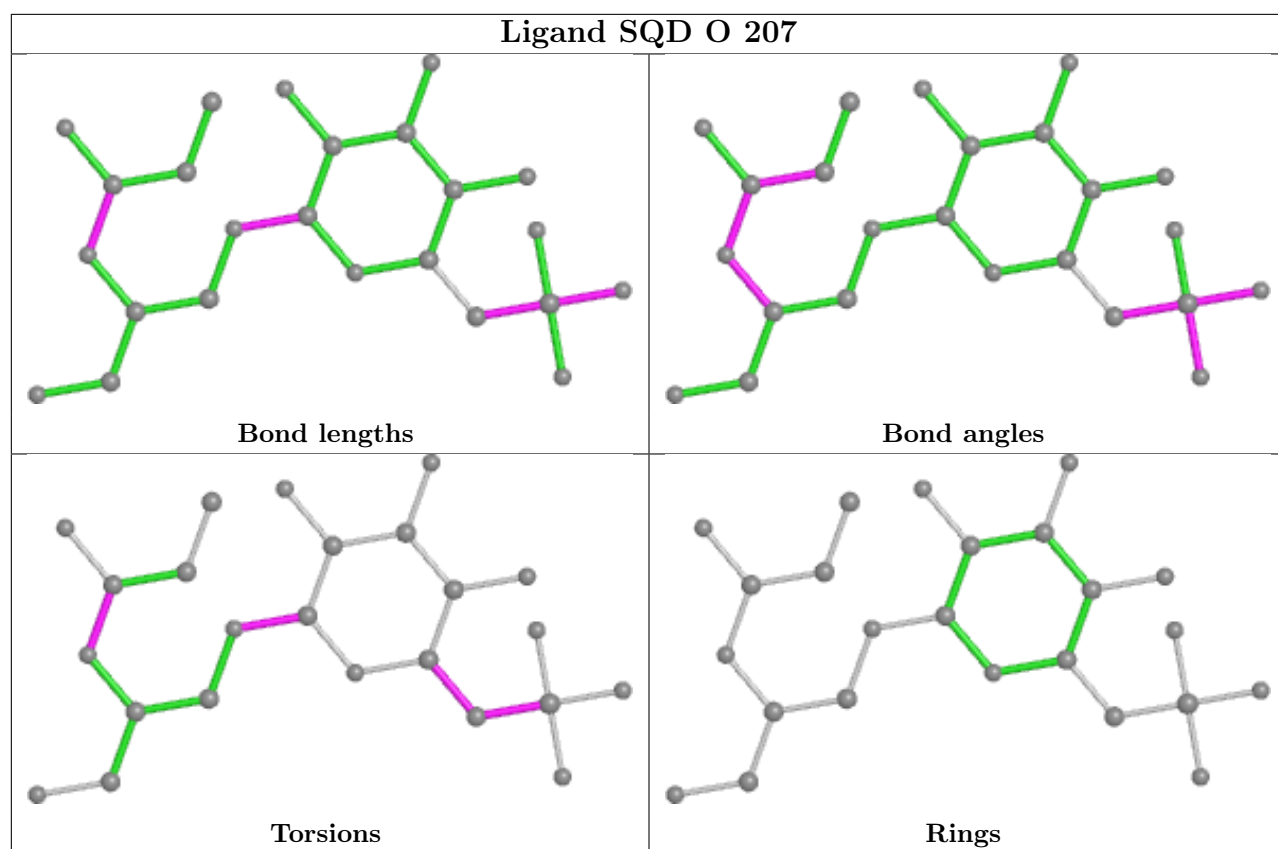
Bond angles



Torsions

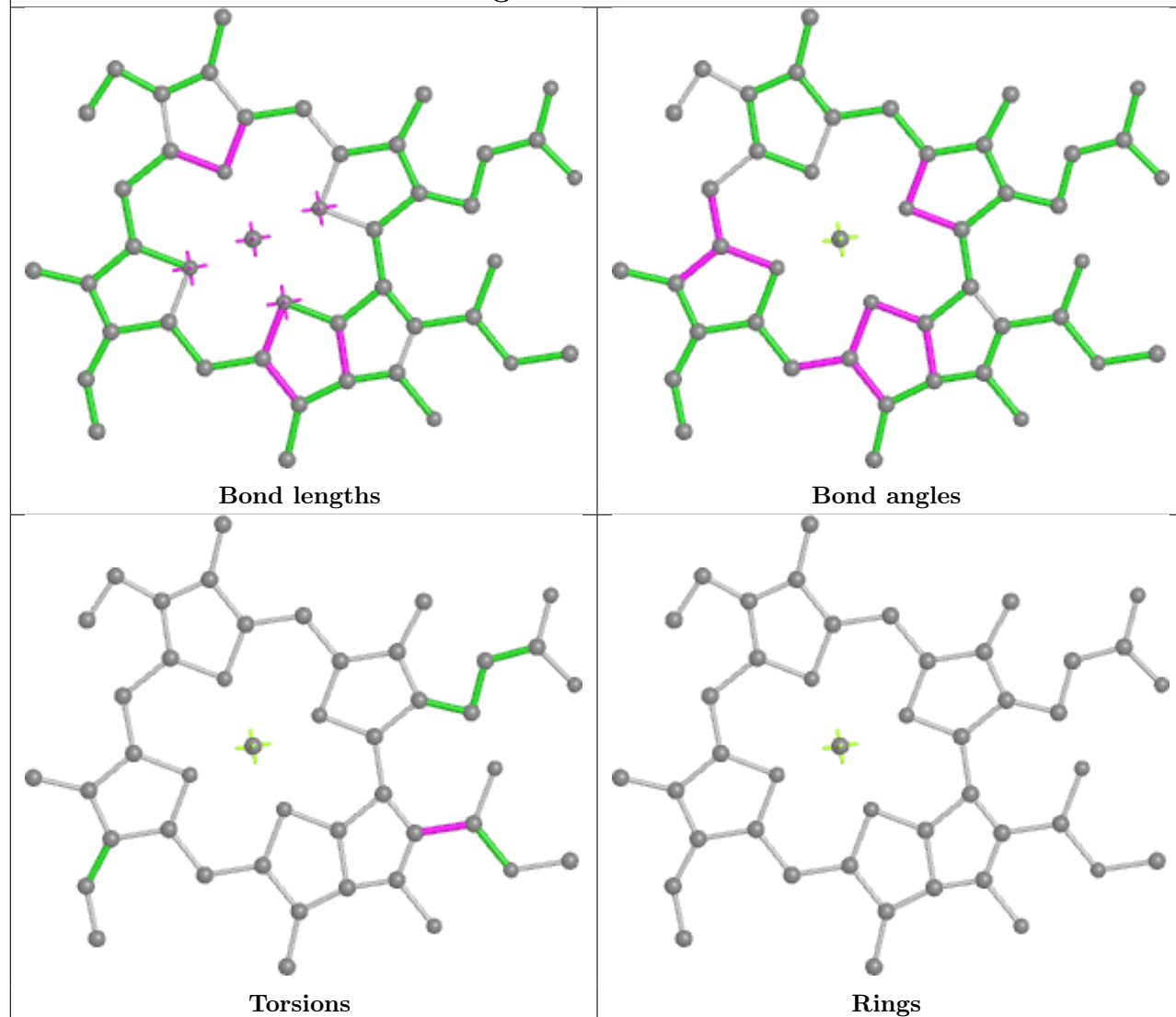


Rings

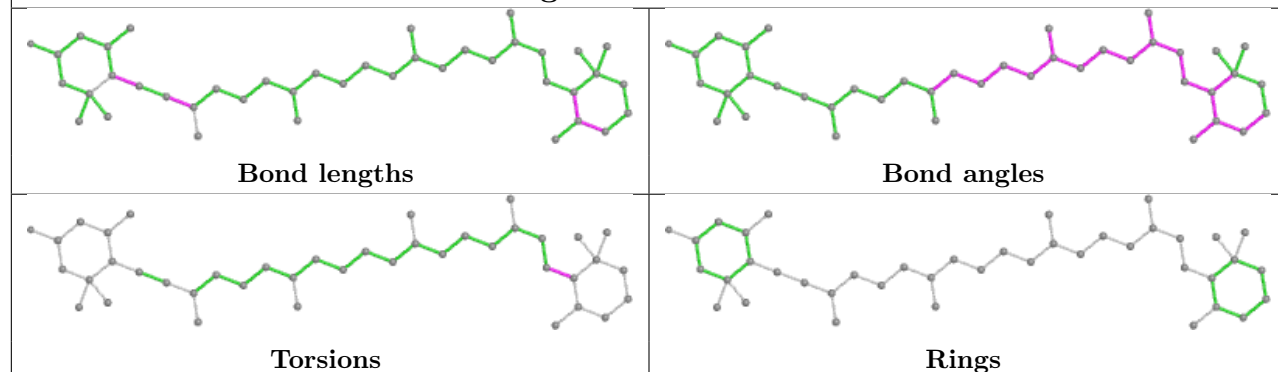


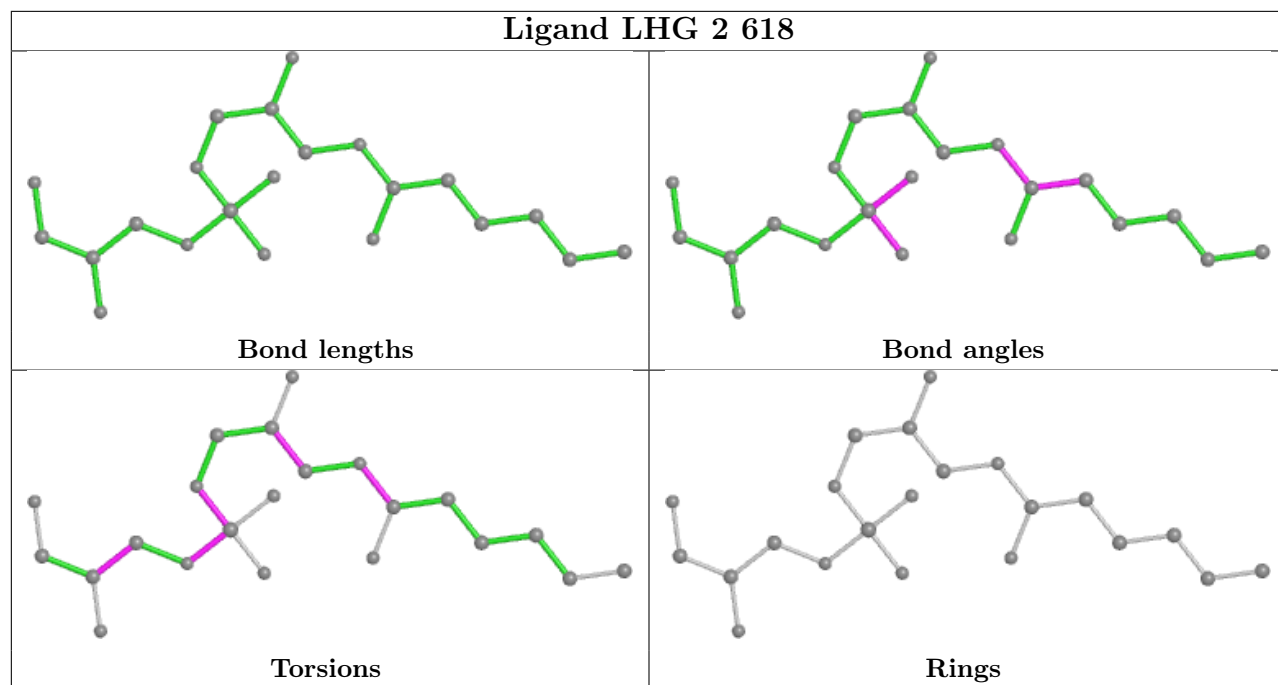


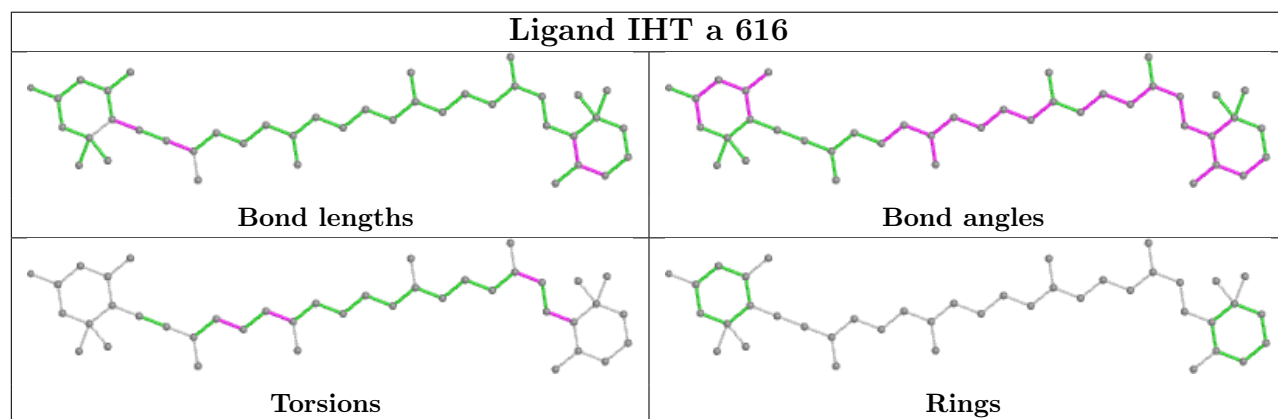
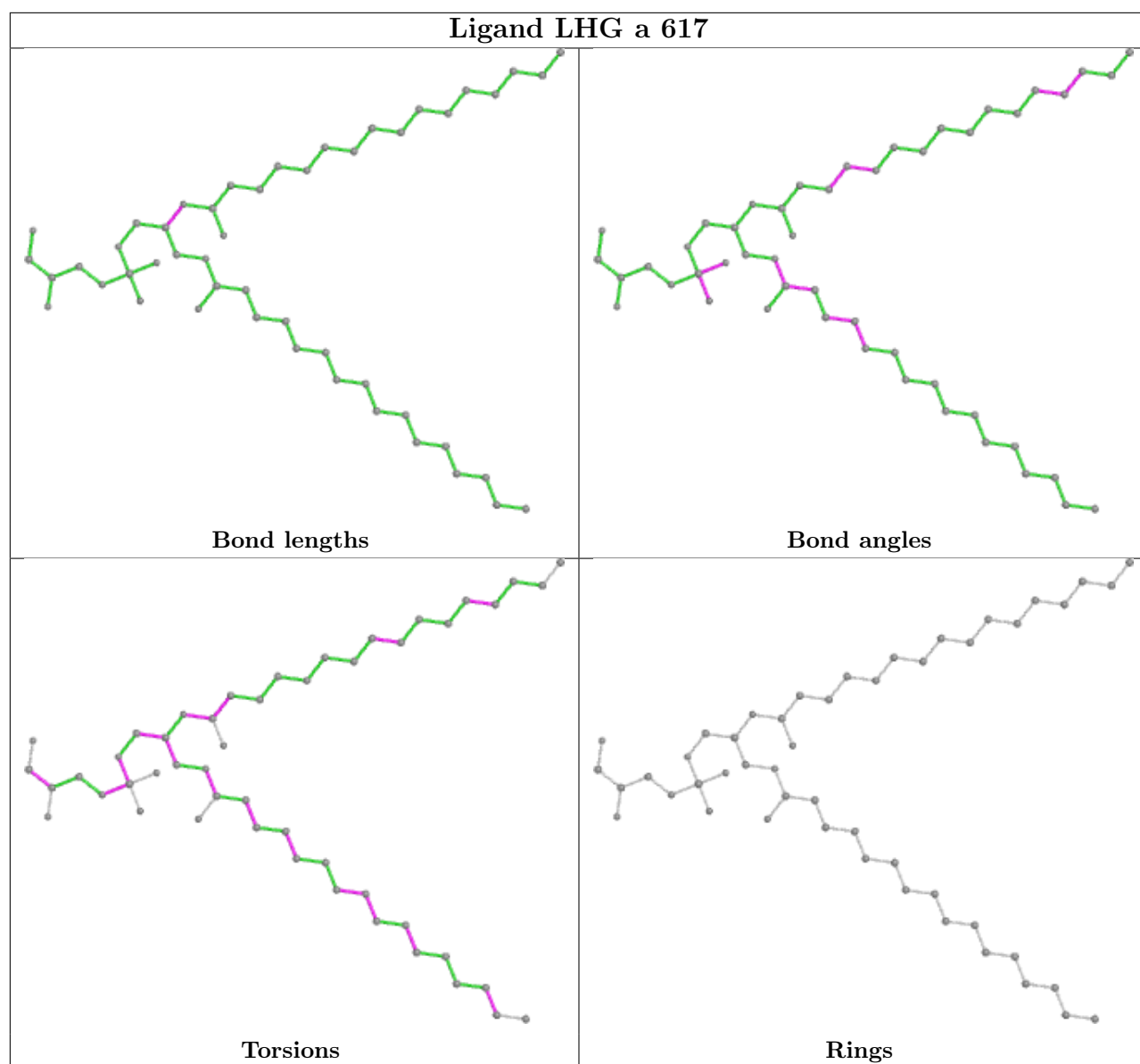
## Ligand CLA 2 606

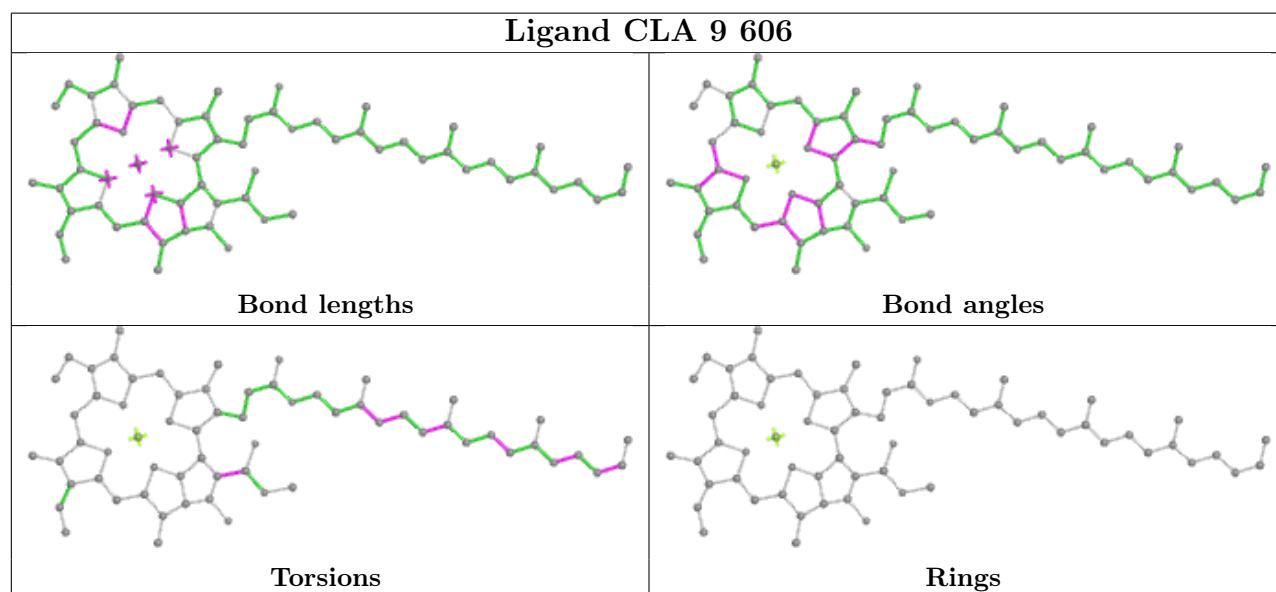
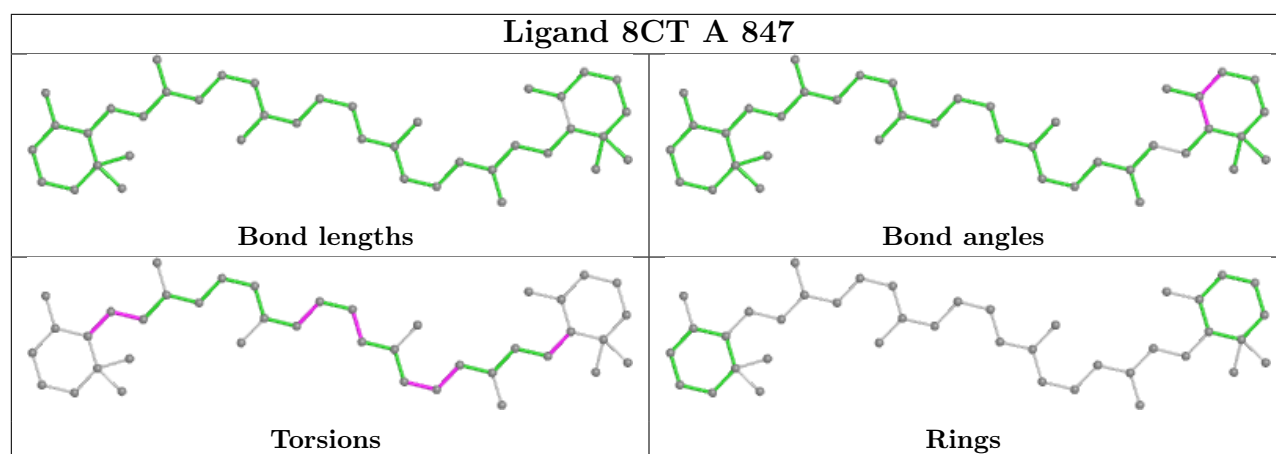


## Ligand IHT 8 609

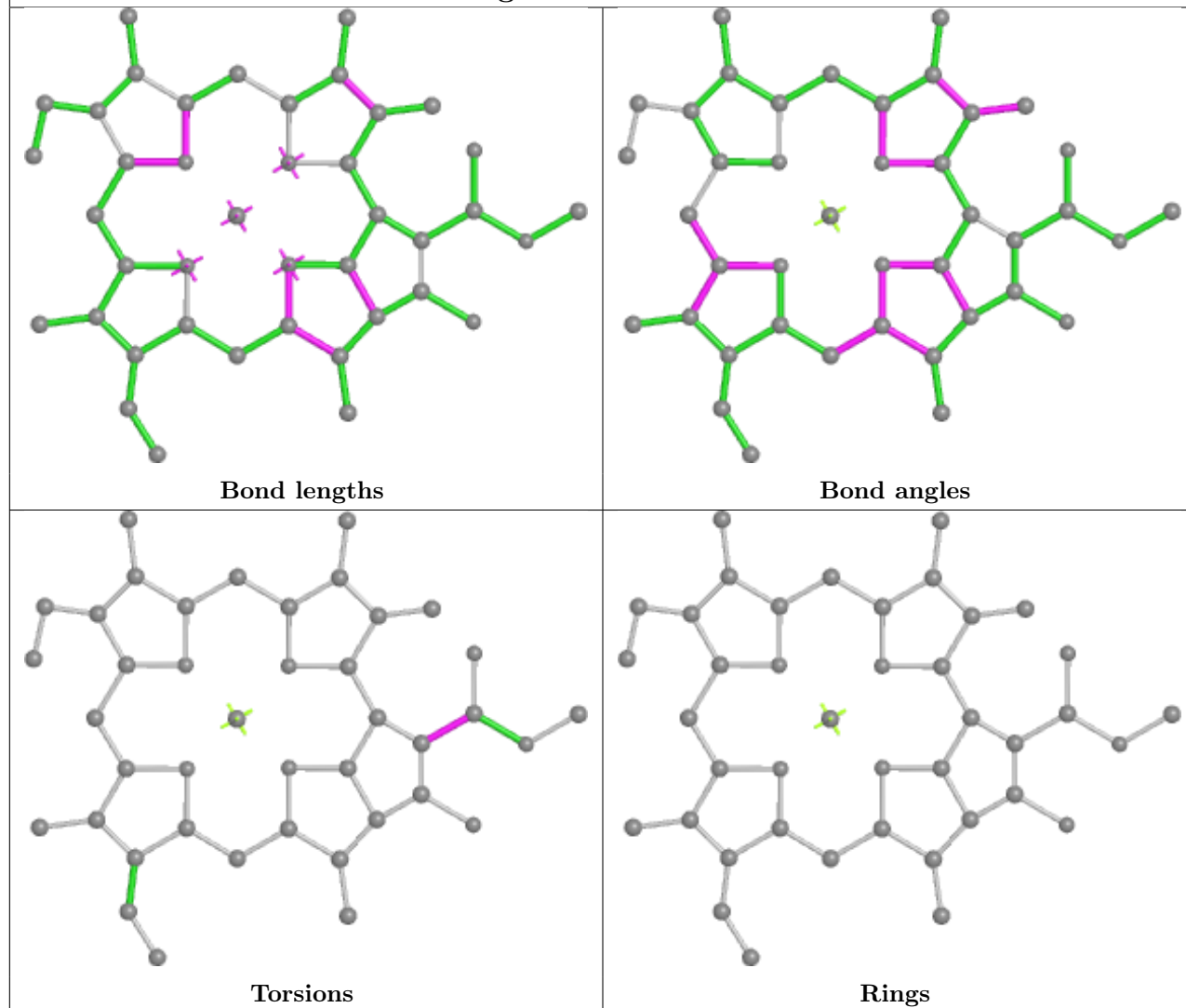




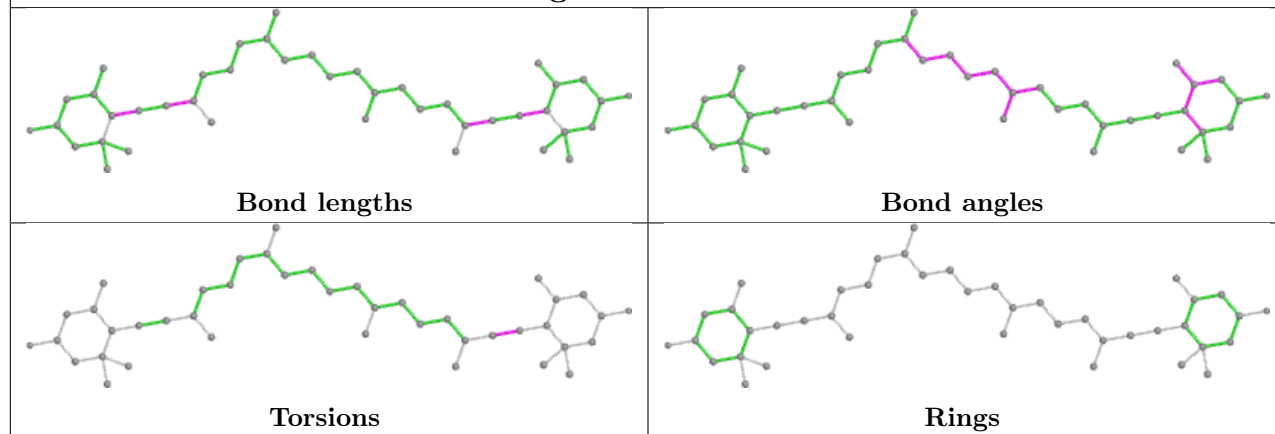




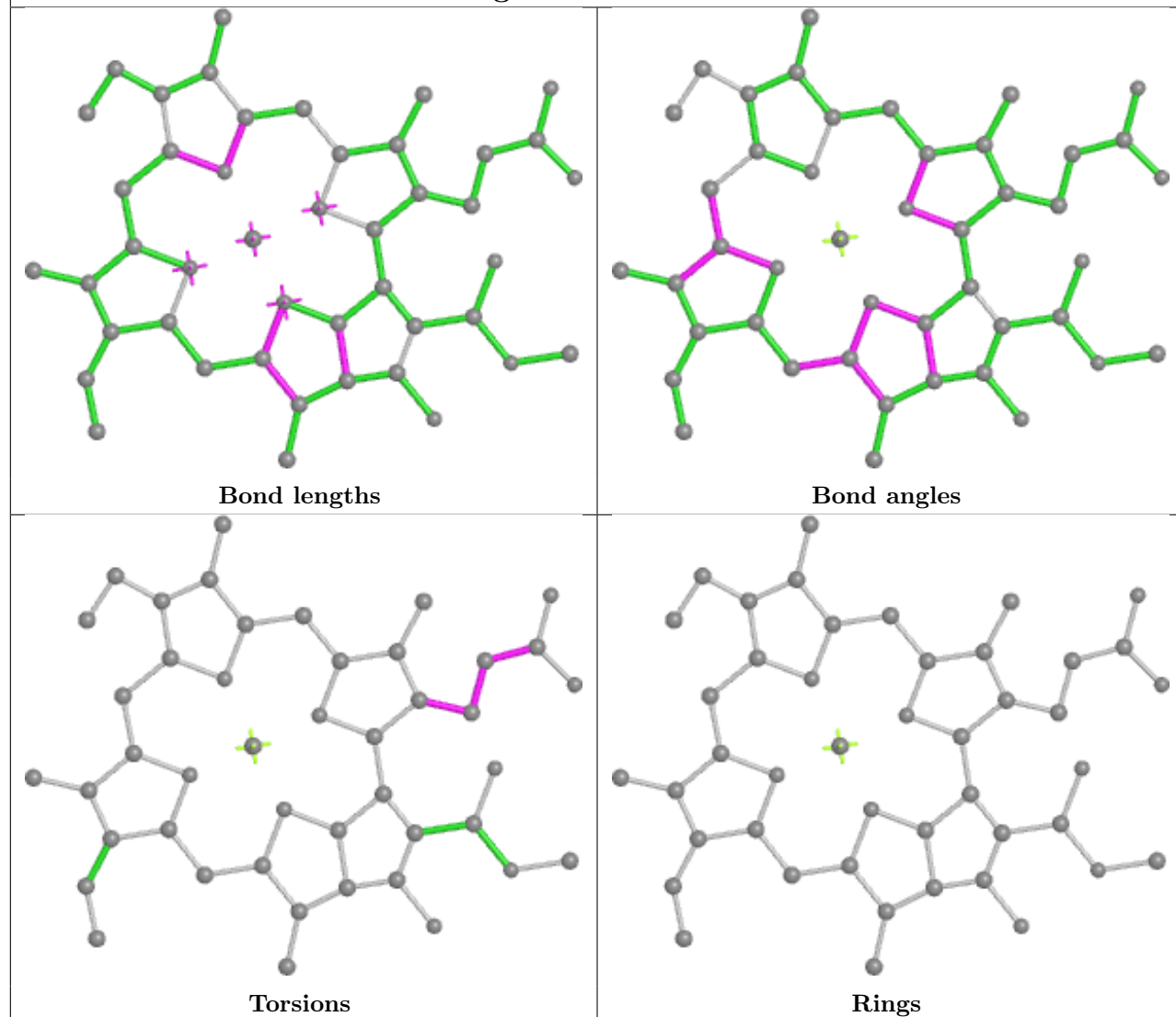
## Ligand CLA 5 613



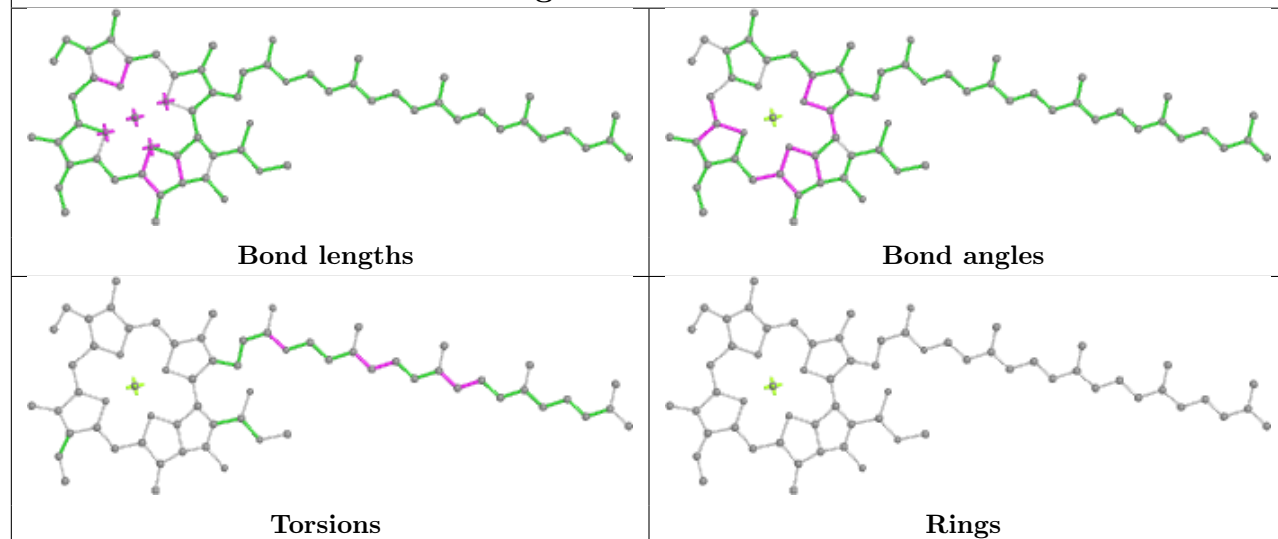
## Ligand II0 3 615



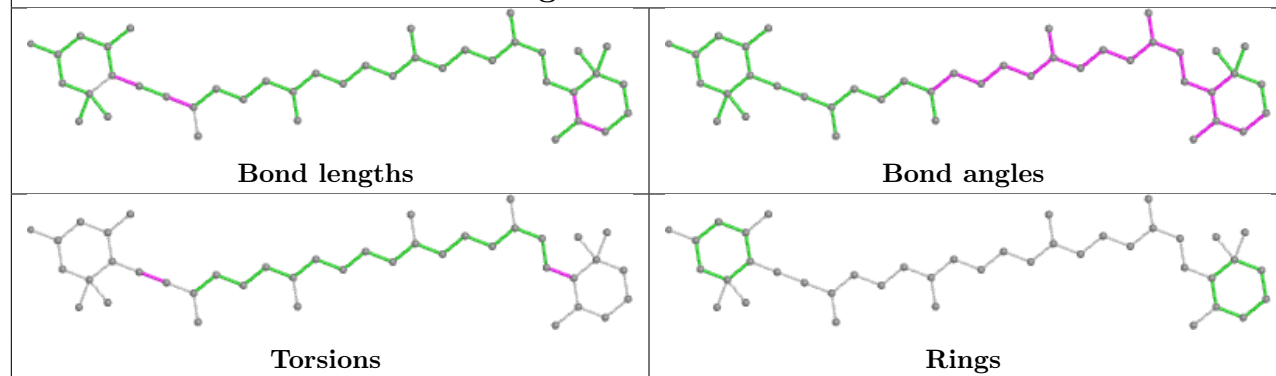
## Ligand CLA 6 603



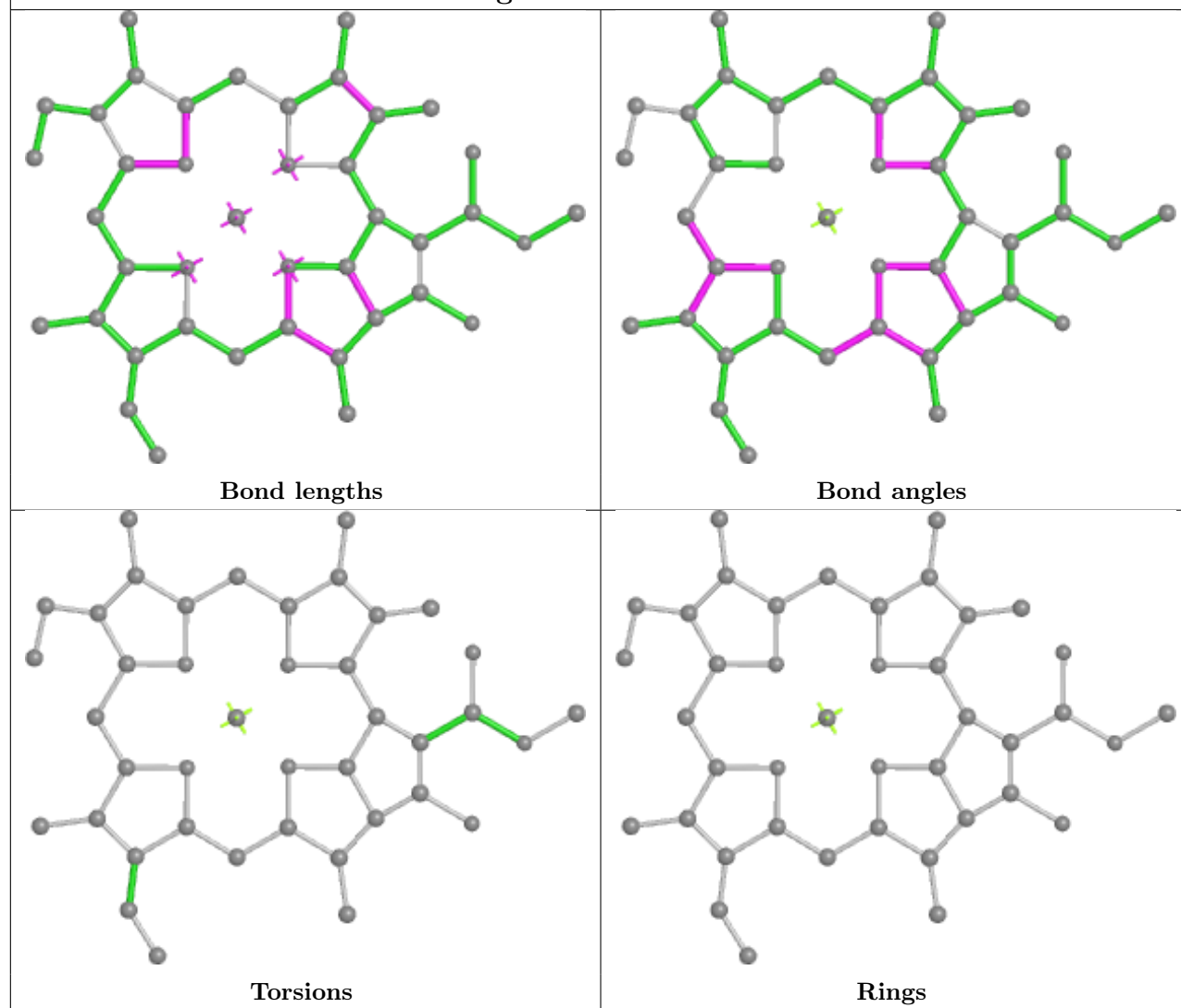
## Ligand CLA b 608



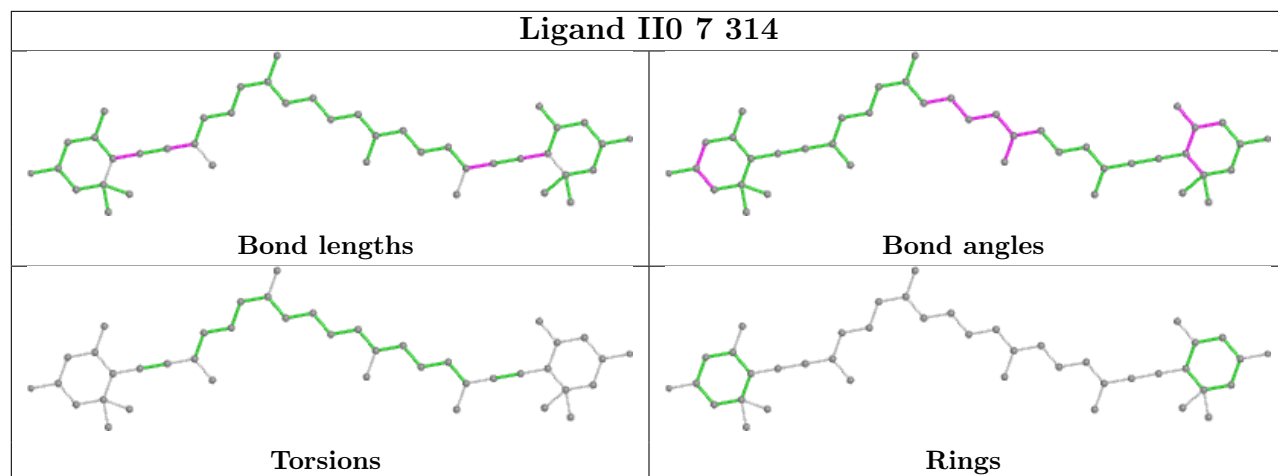
## Ligand IHT L 204



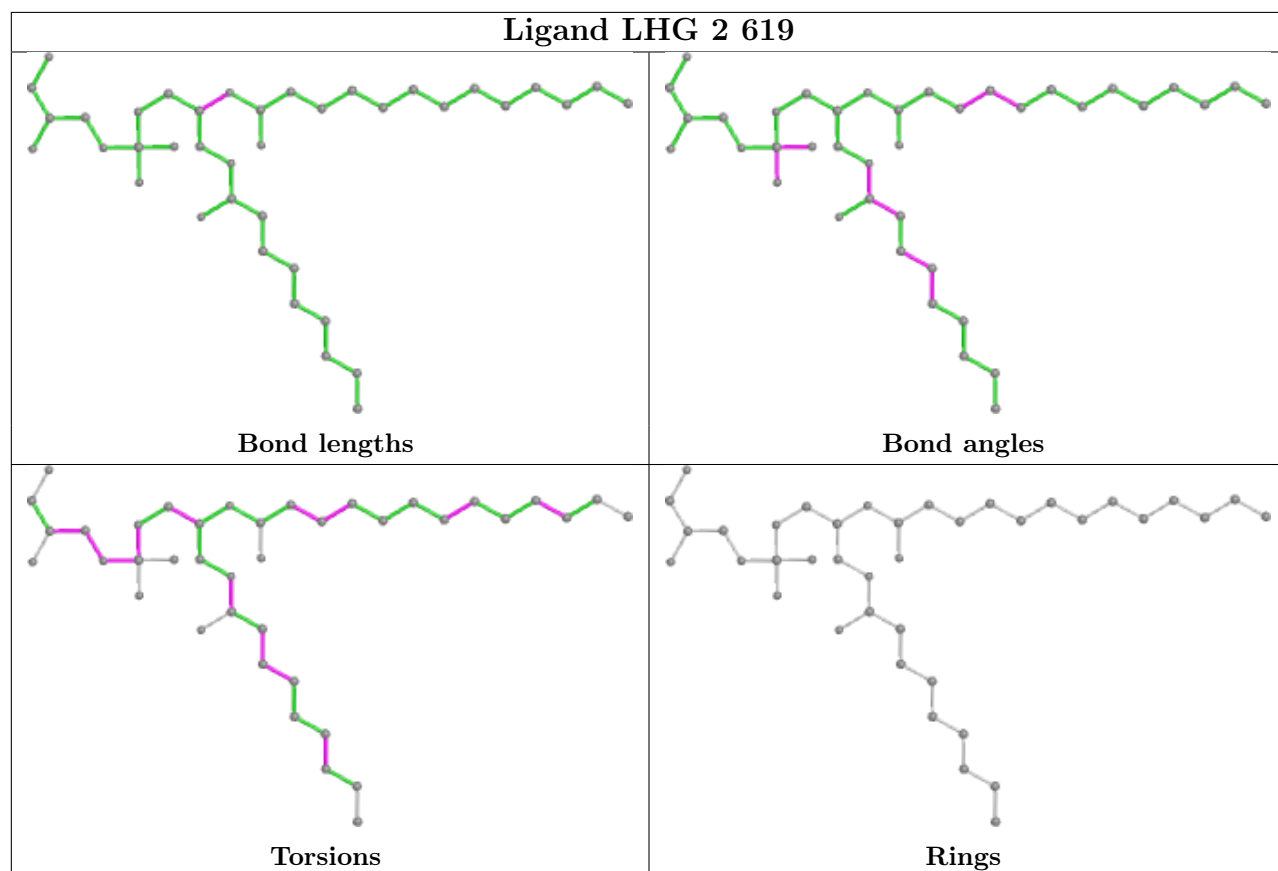
## Ligand CLA 5 609



## Ligand II0 7 314

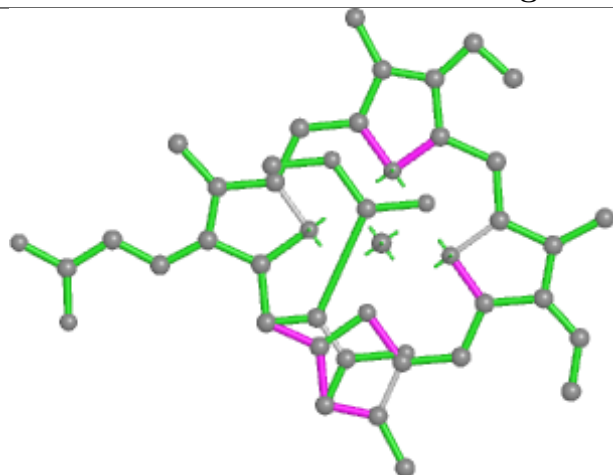


## Ligand LHG 2 619

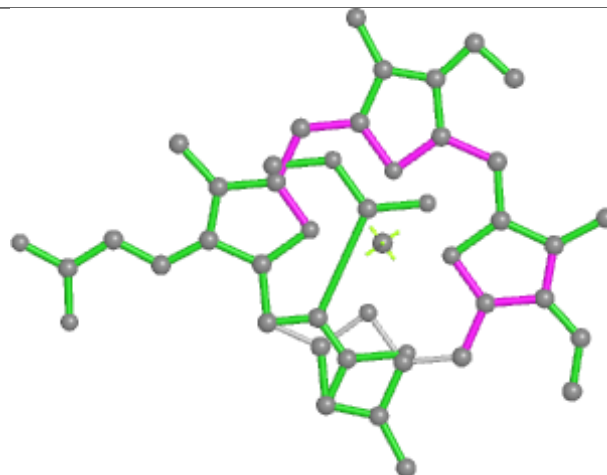




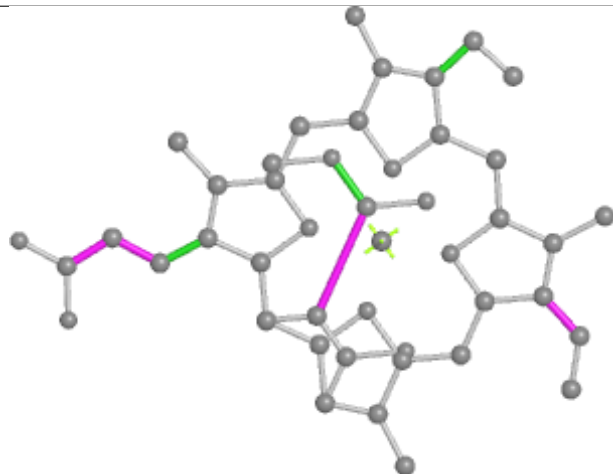
## Ligand KC2 2 610



Bond lengths



Bond angles

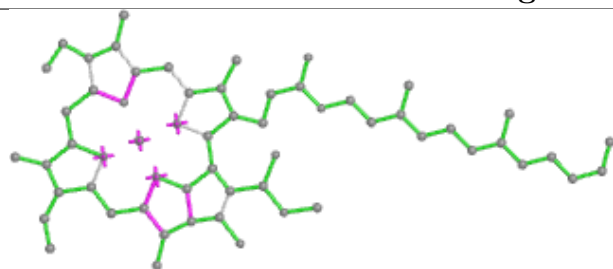


Torsions

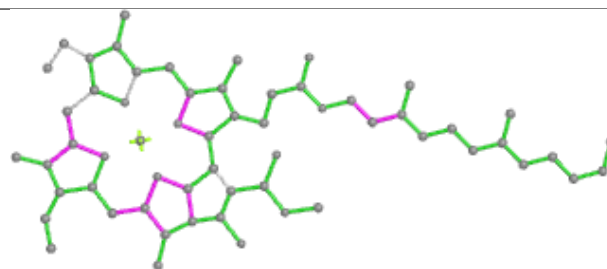


Rings

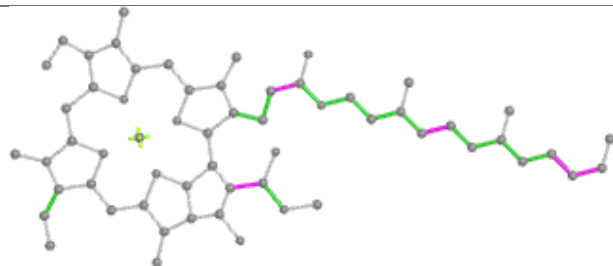
## Ligand CLA 1 602



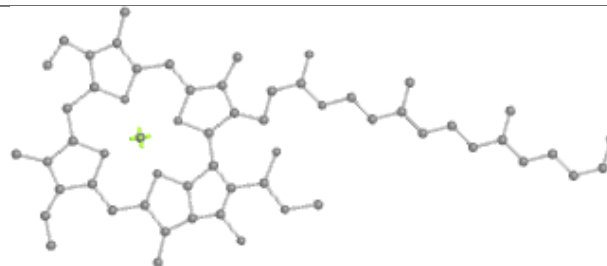
Bond lengths



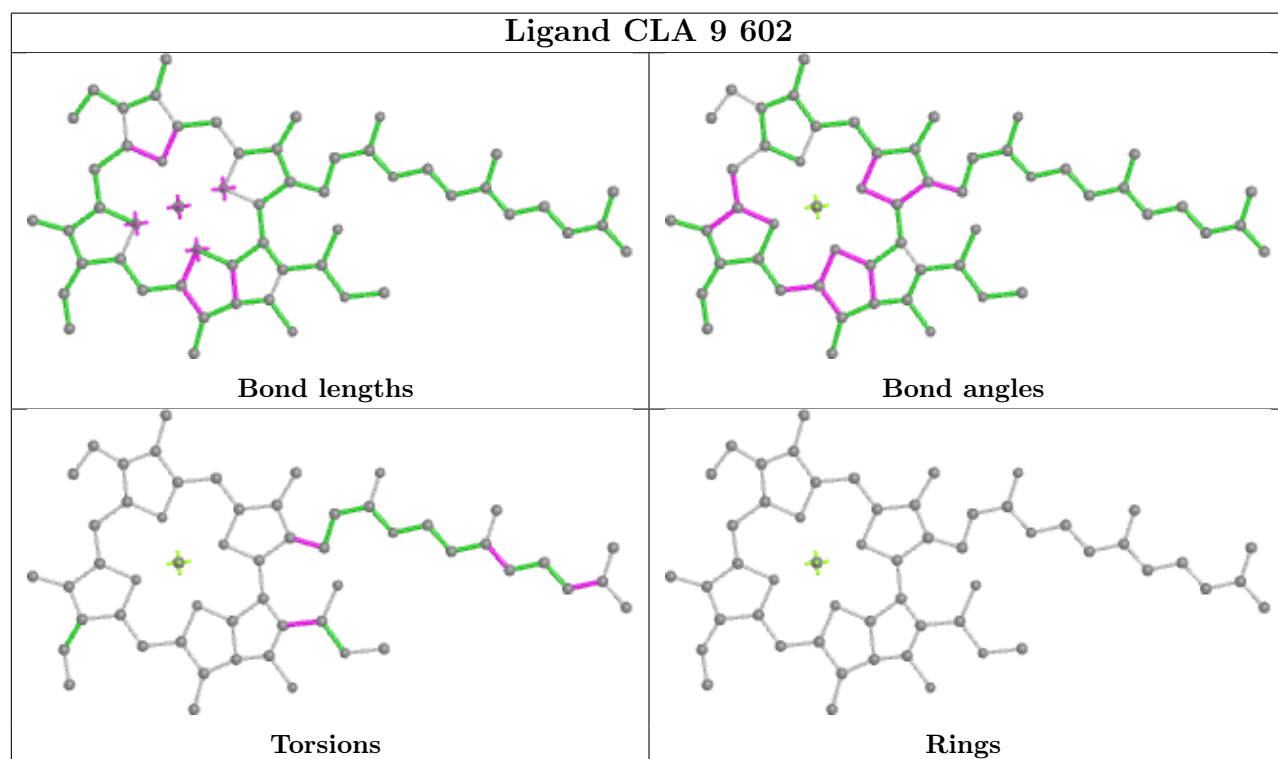
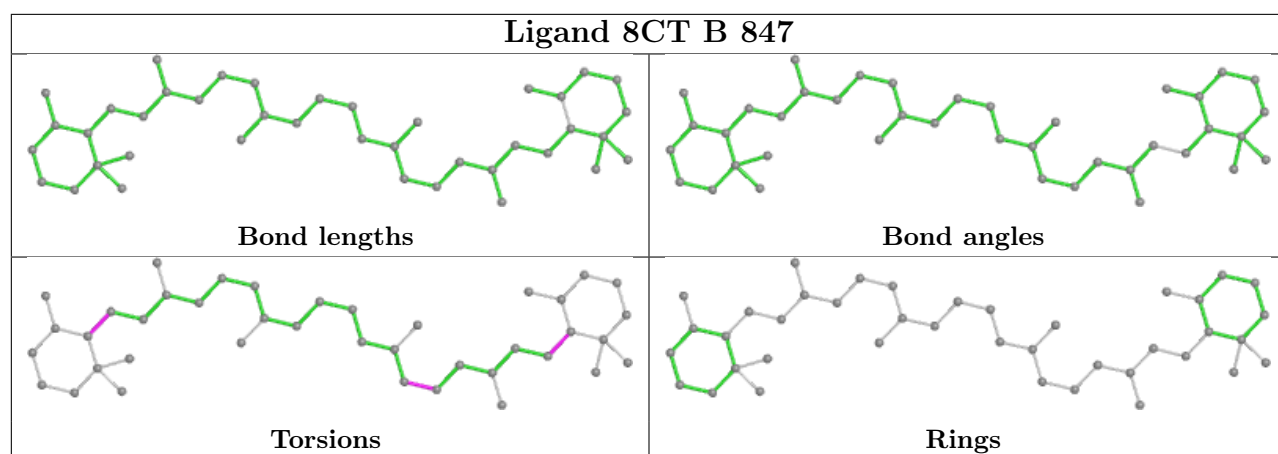
Bond angles



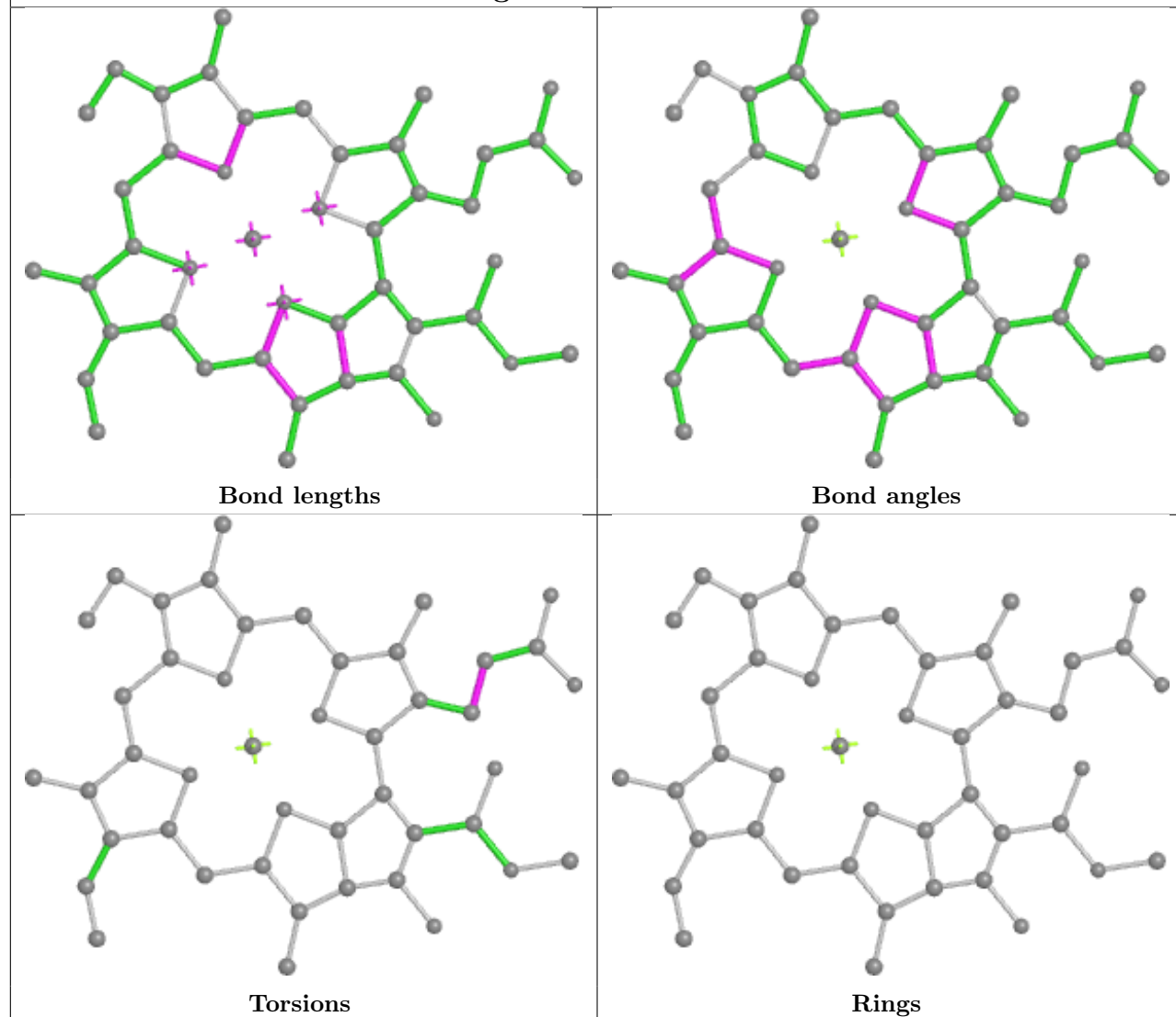
Torsions



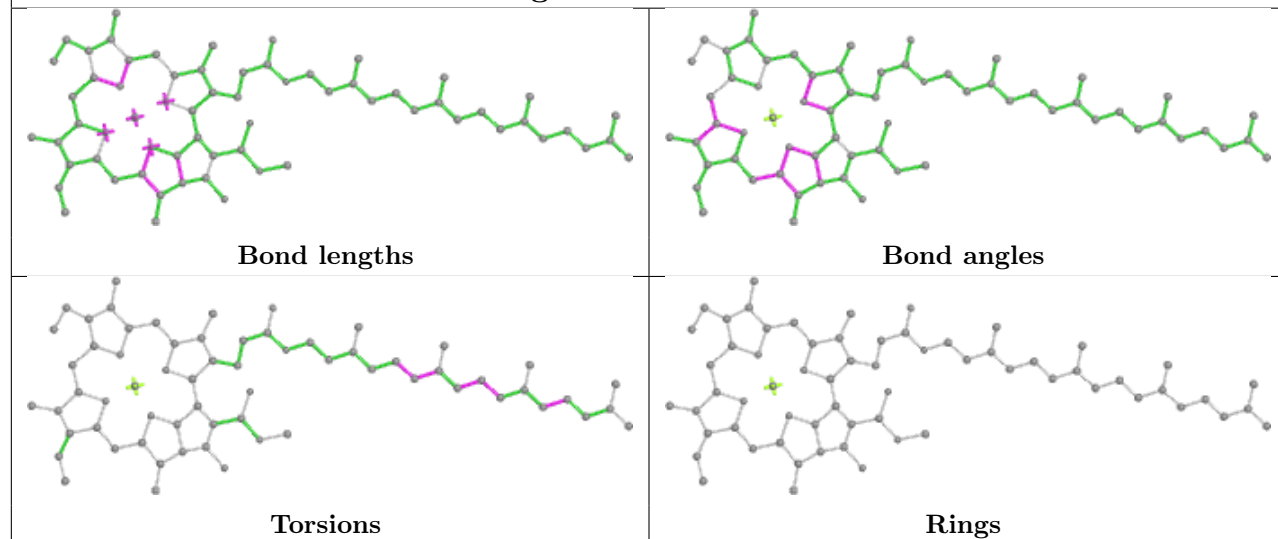
Rings



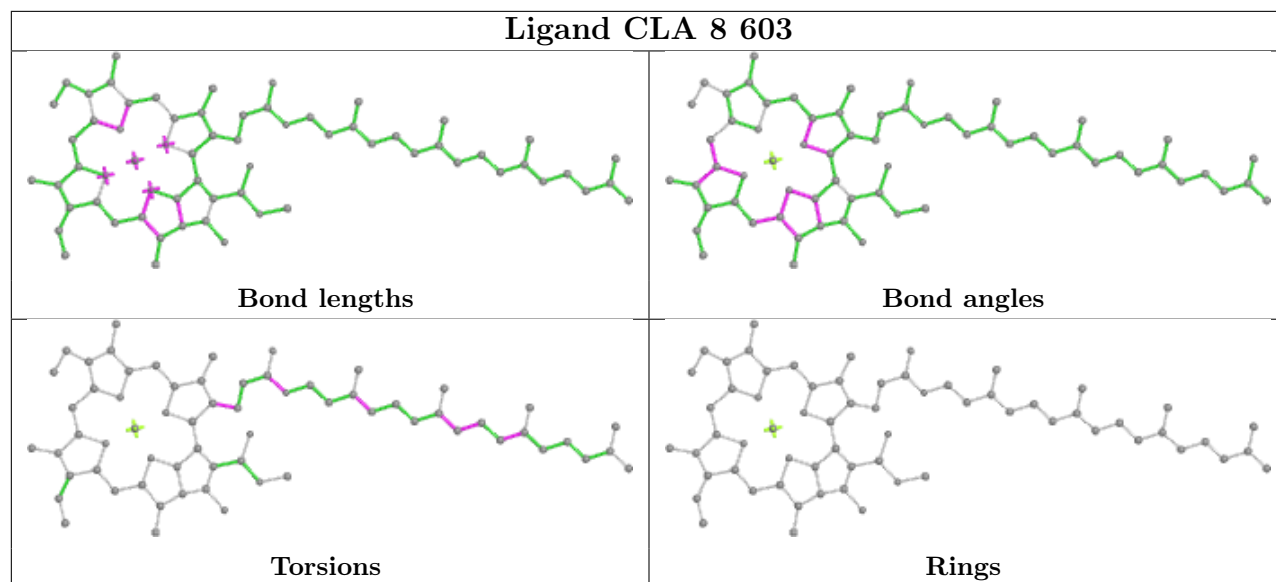
## Ligand CLA 1 604



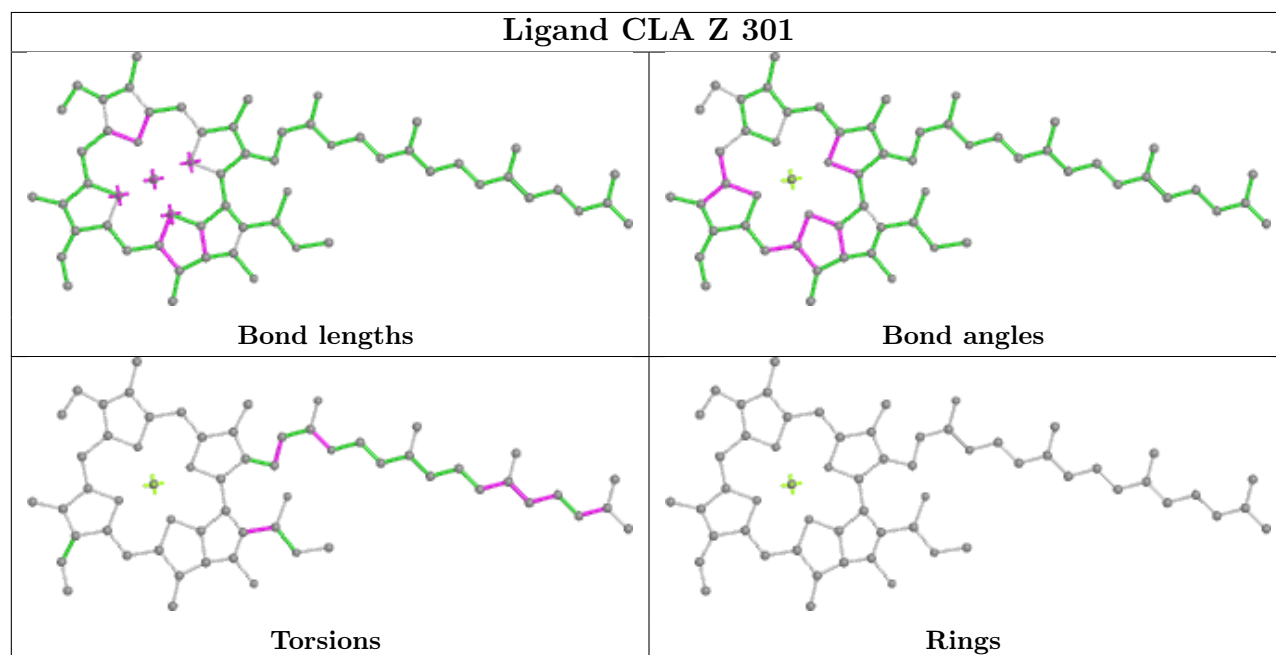
## Ligand CLA K 101



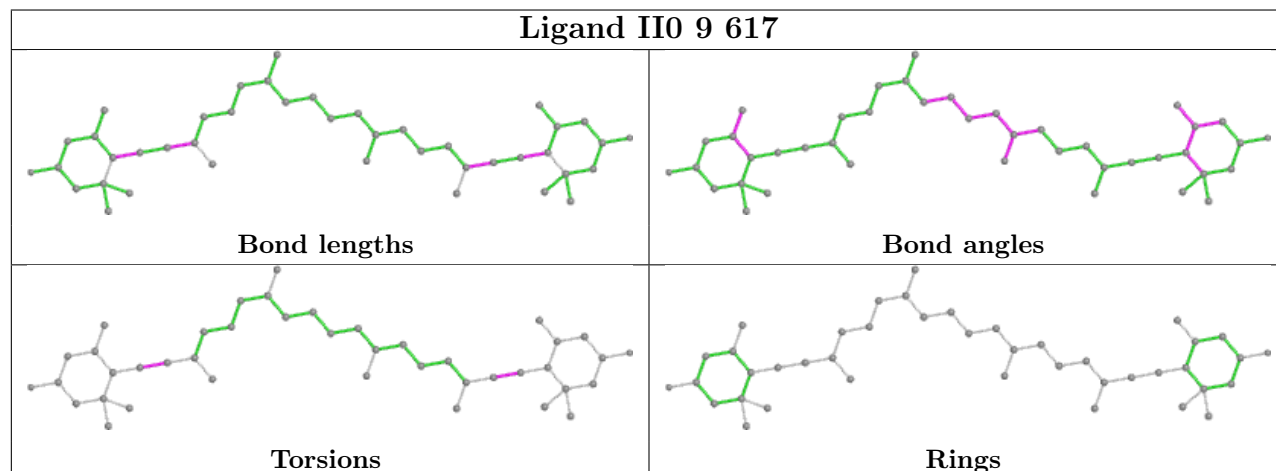
## Ligand CLA 8 603

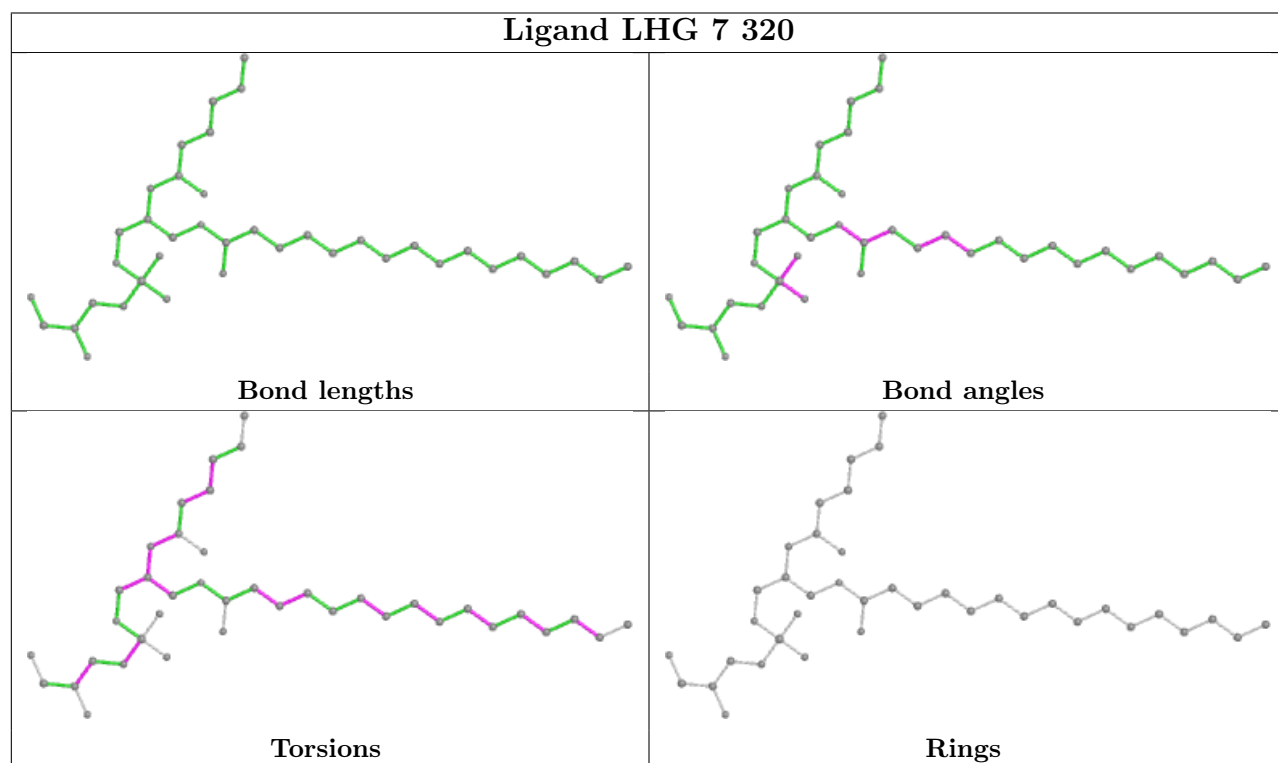
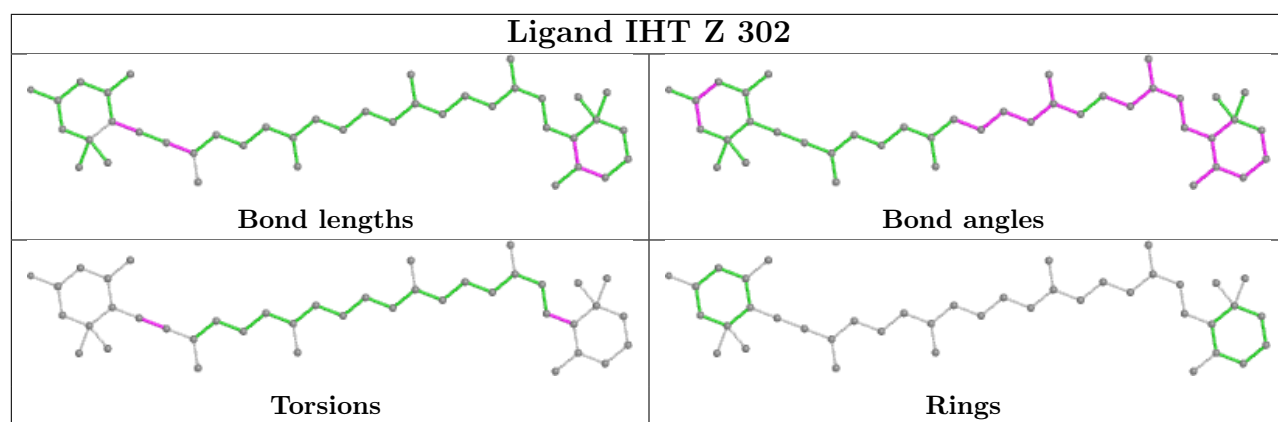


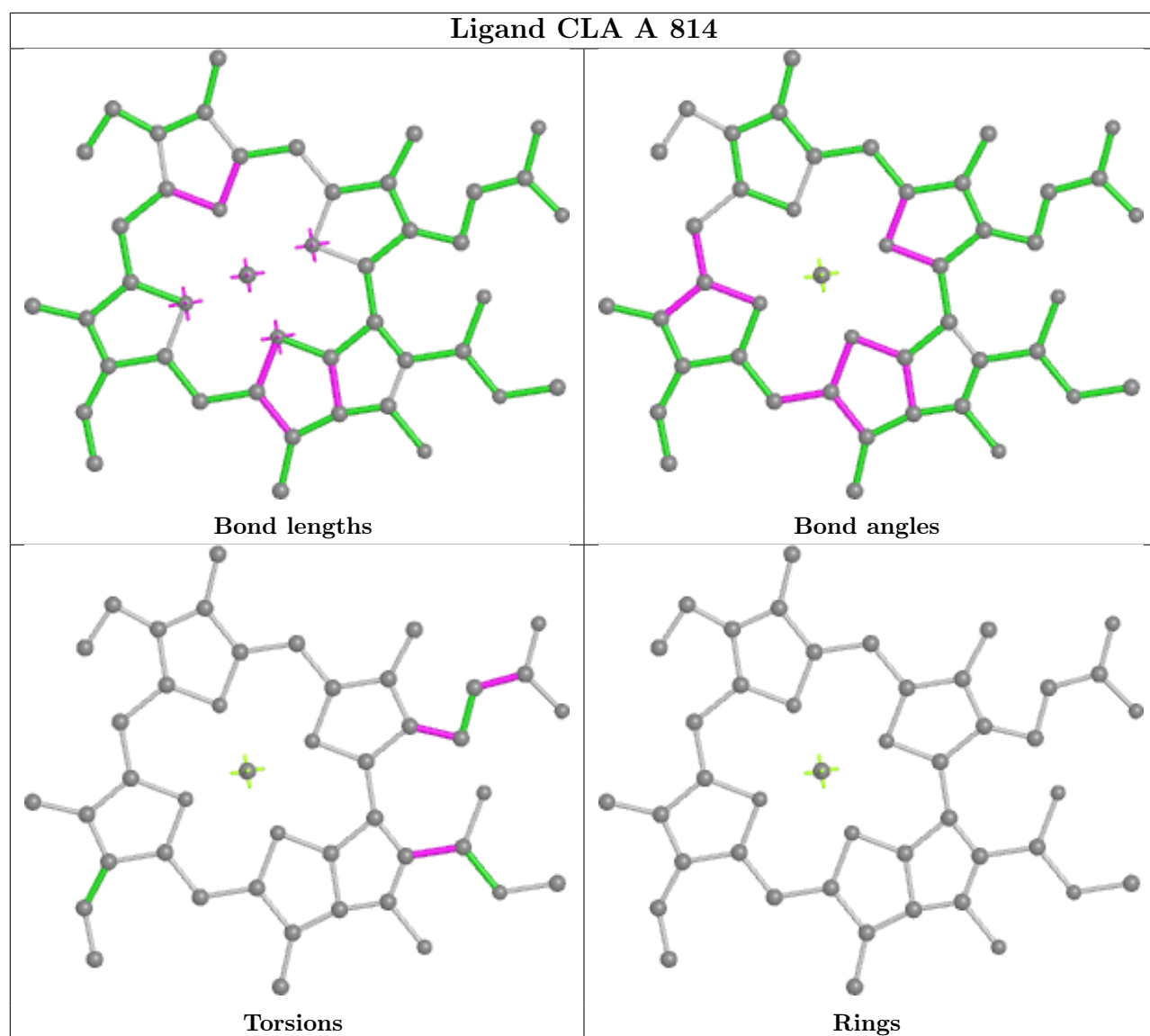
## Ligand CLA Z 301

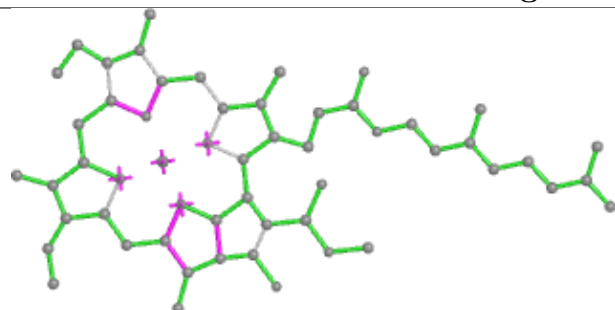


## Ligand II0 9 617

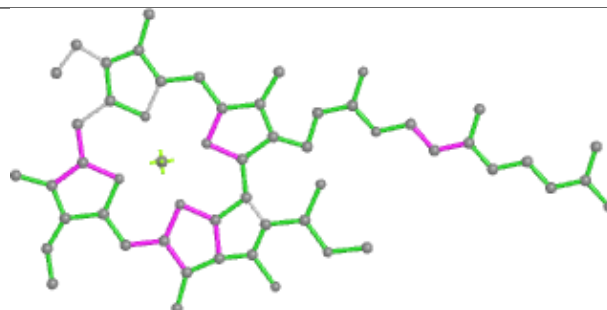




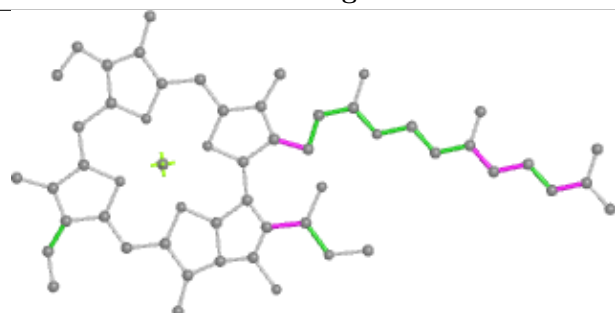


**Ligand CLA 9 608**

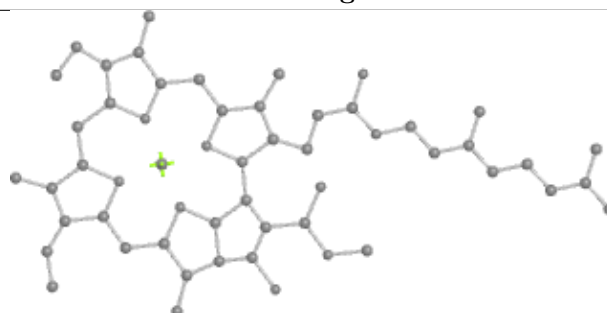
Bond lengths



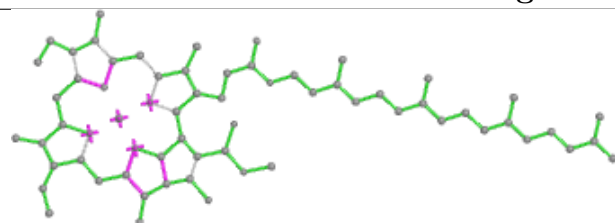
Bond angles



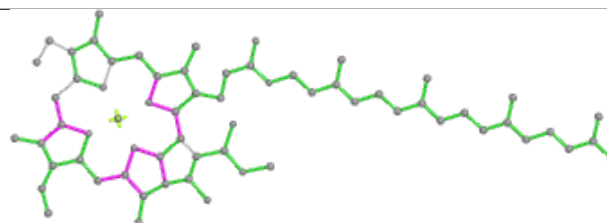
Torsions



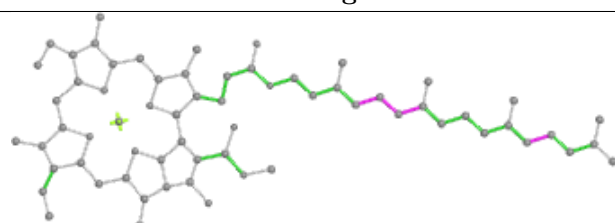
Rings

**Ligand CLA B 801**

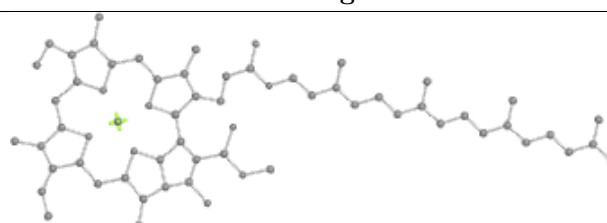
Bond lengths



Bond angles

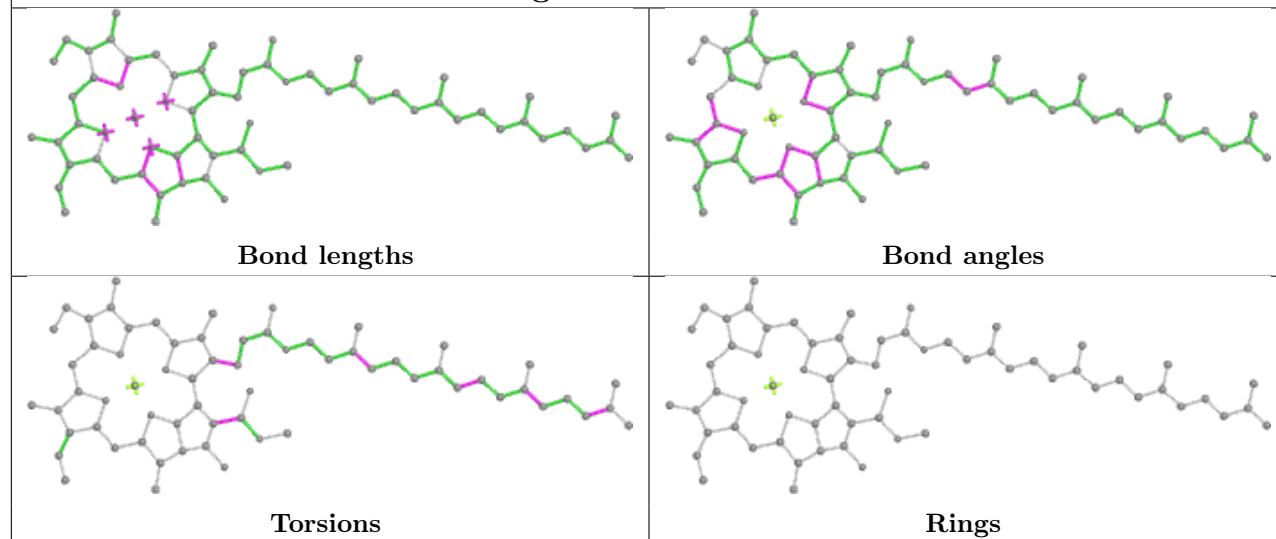


Torsions

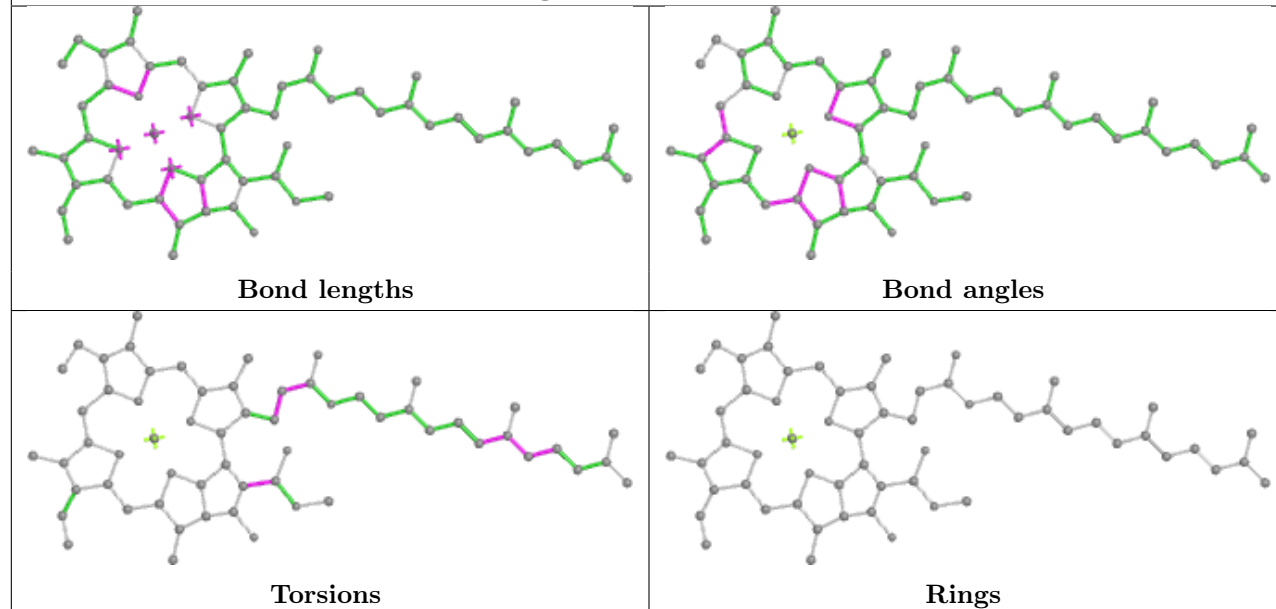


Rings

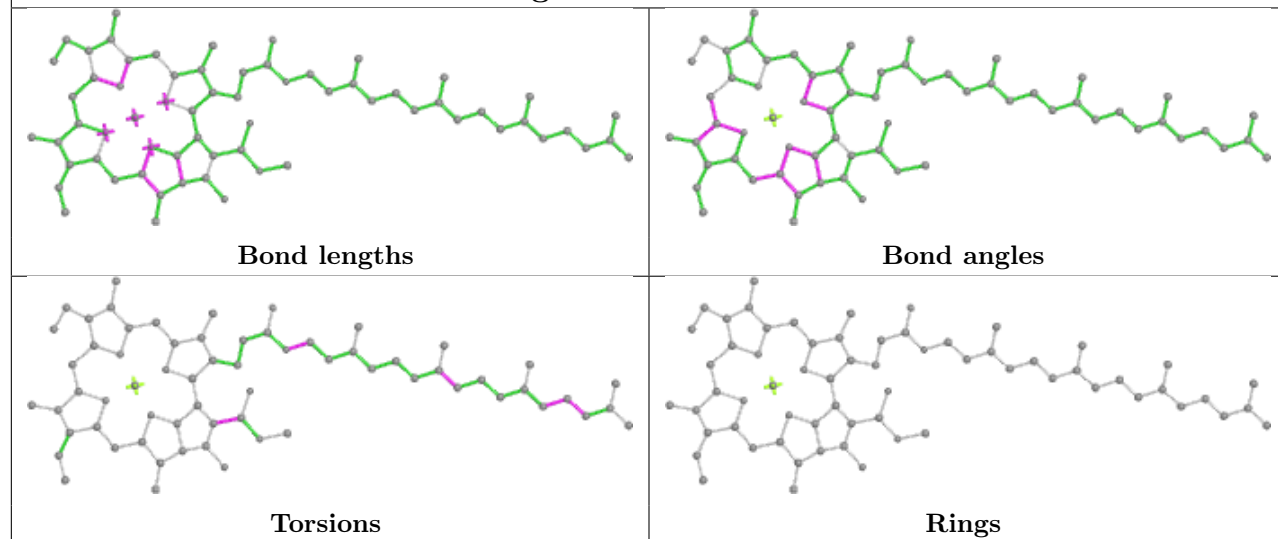
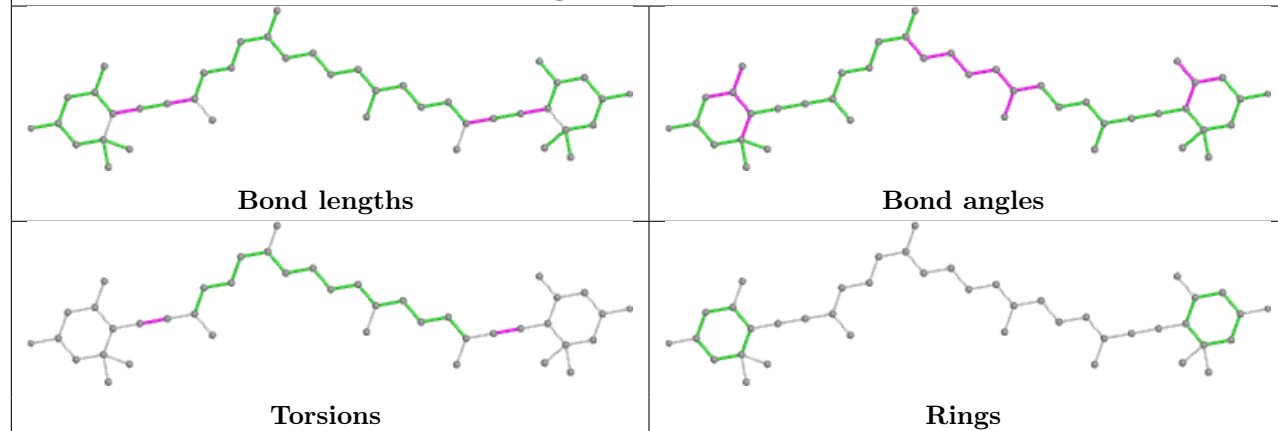
## Ligand CLA B 815



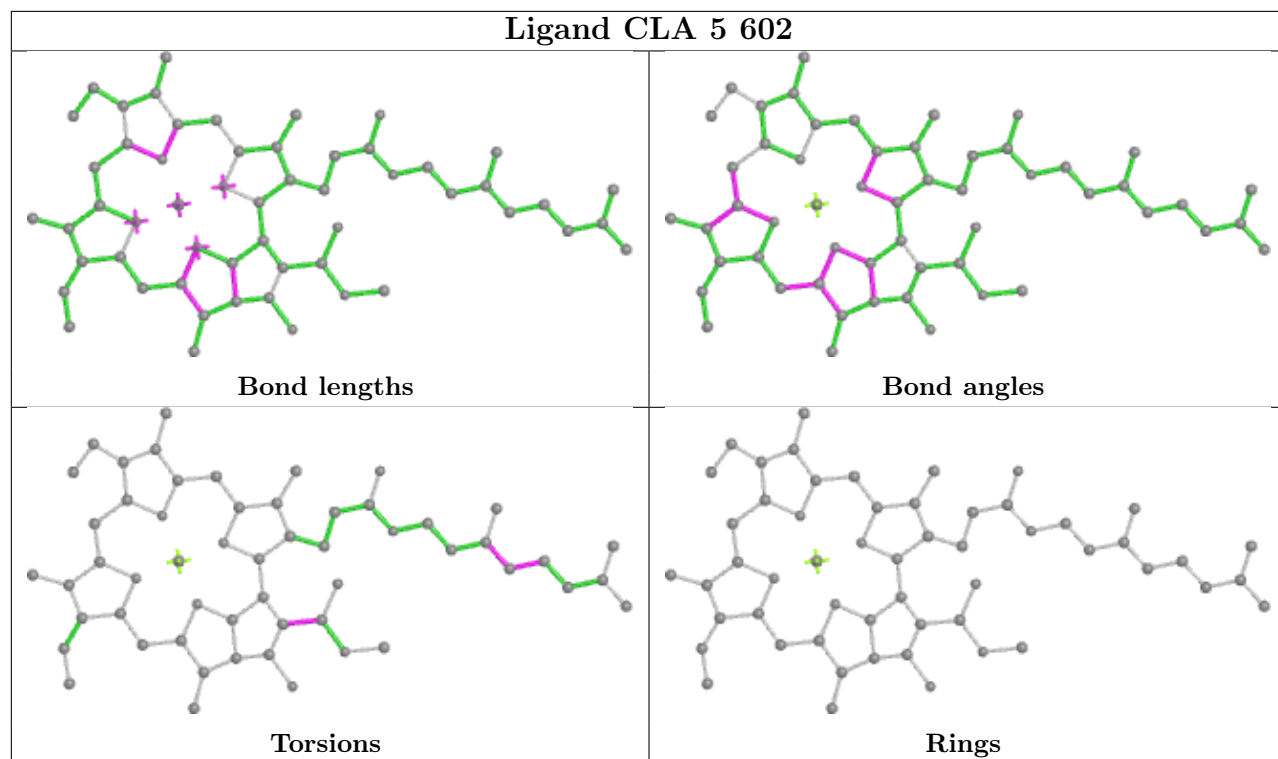
## Ligand CLA a 604



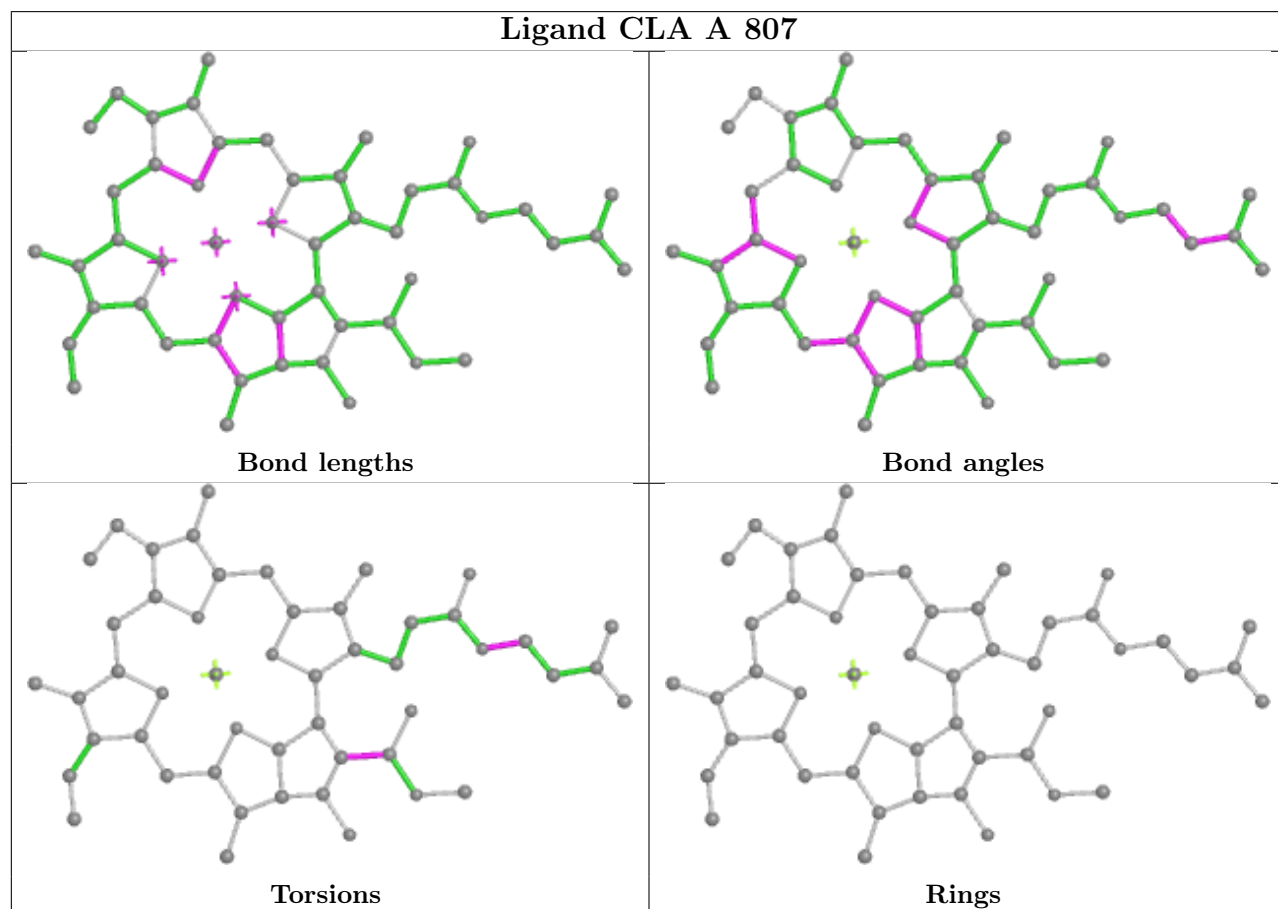


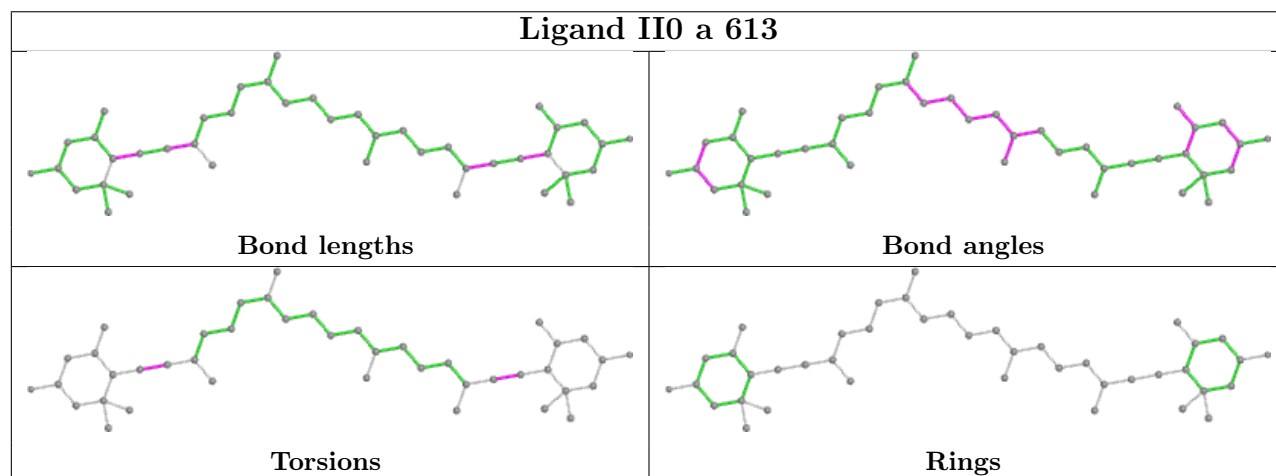
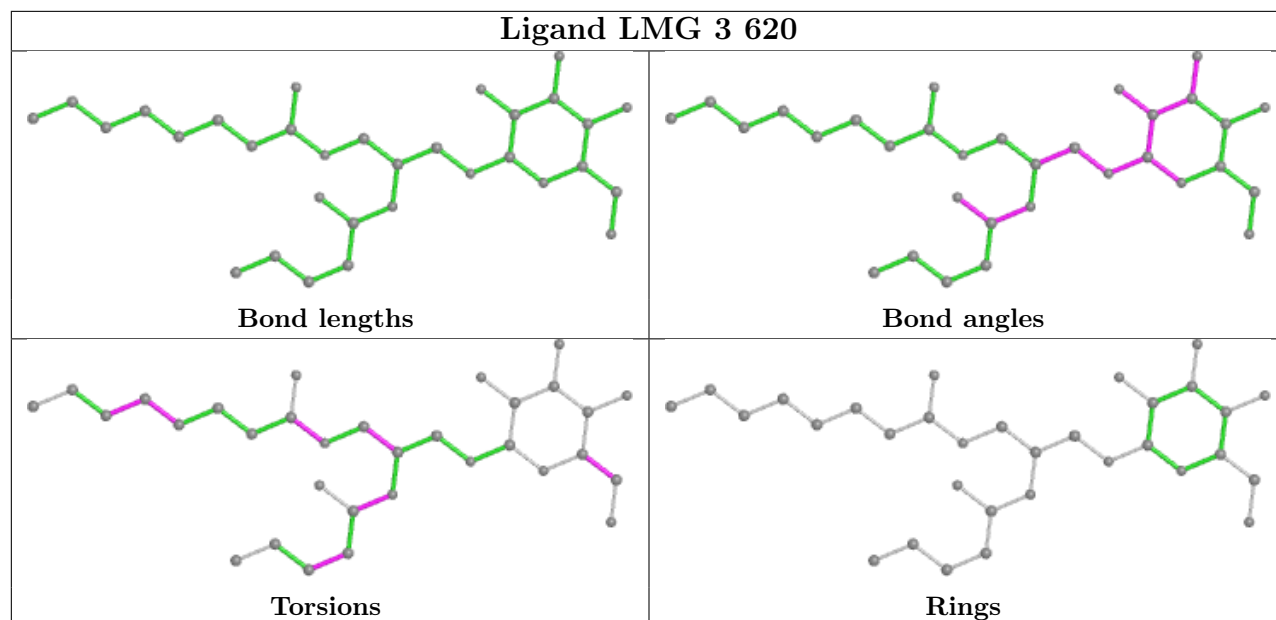
**Ligand CLA A 832****Ligand II0 7 316**

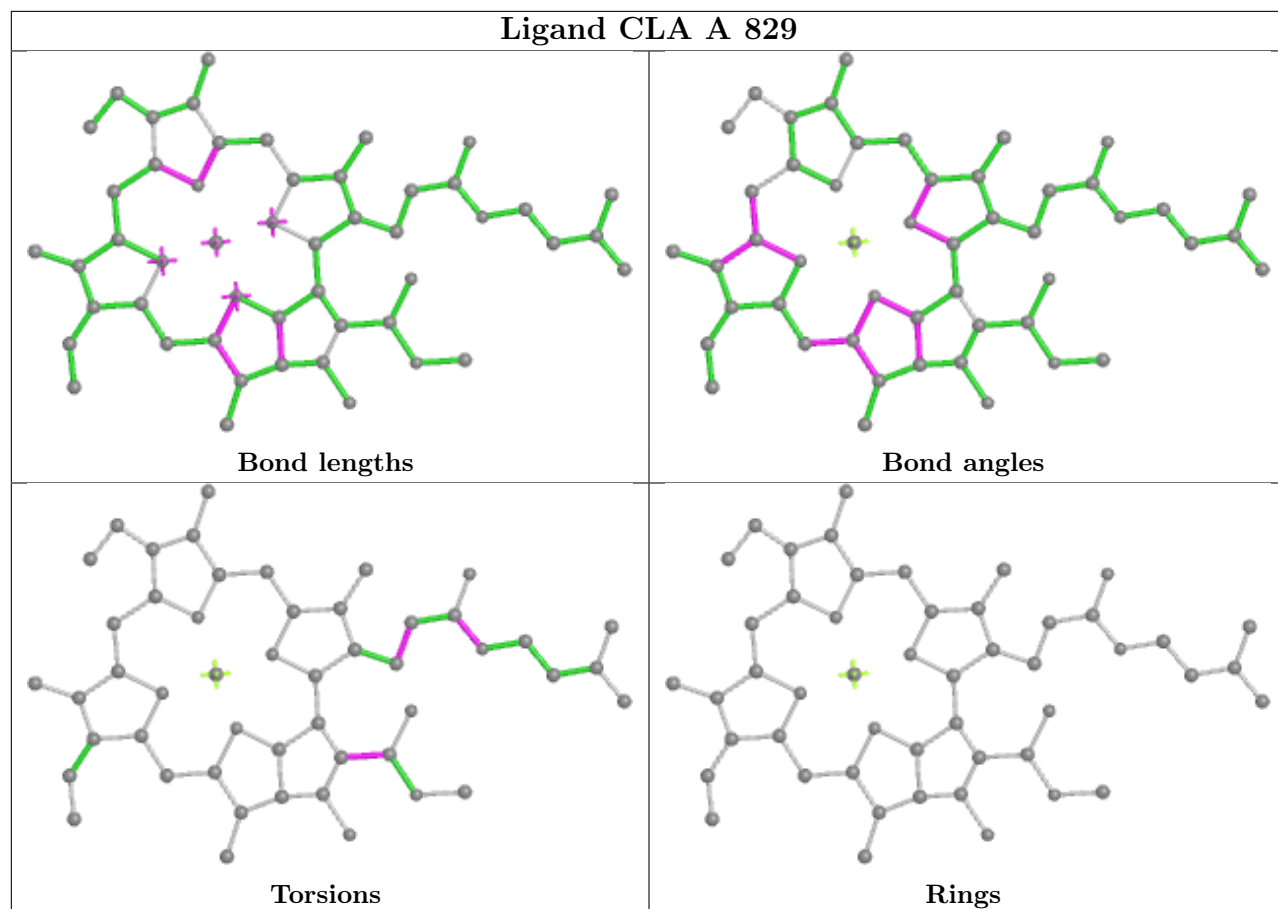
## Ligand CLA 5 602



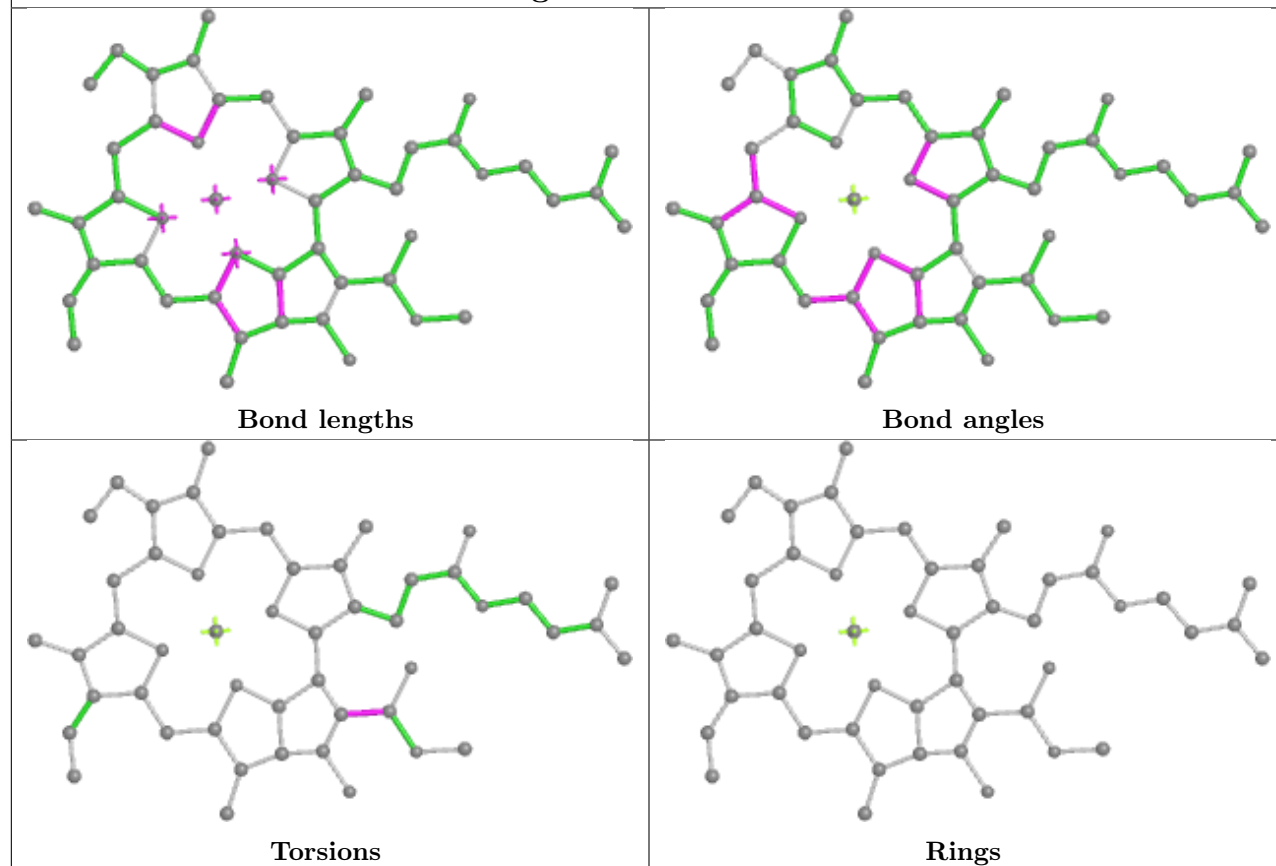
## Ligand CLA A 807



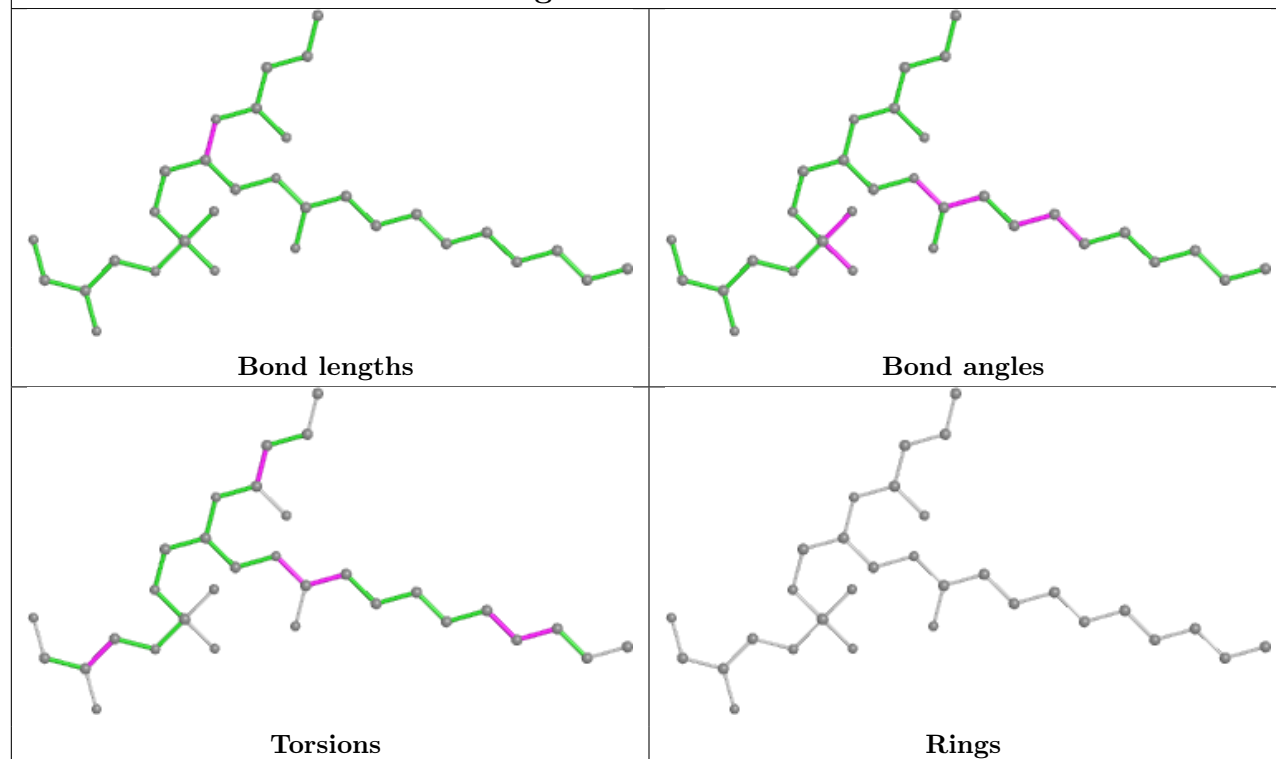


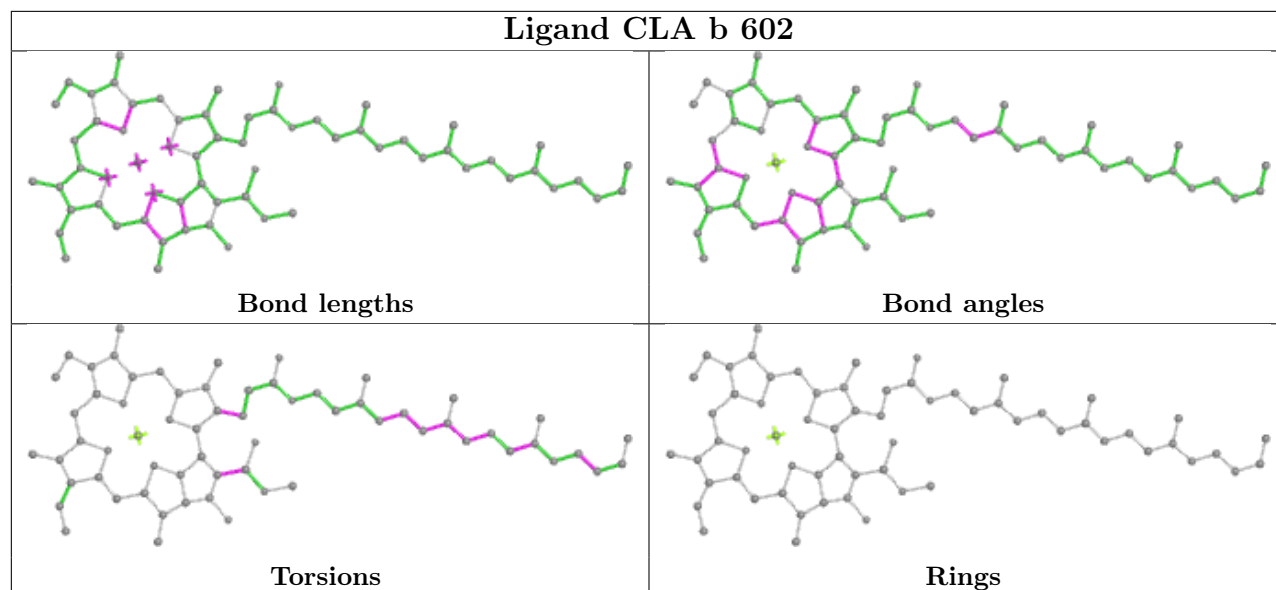
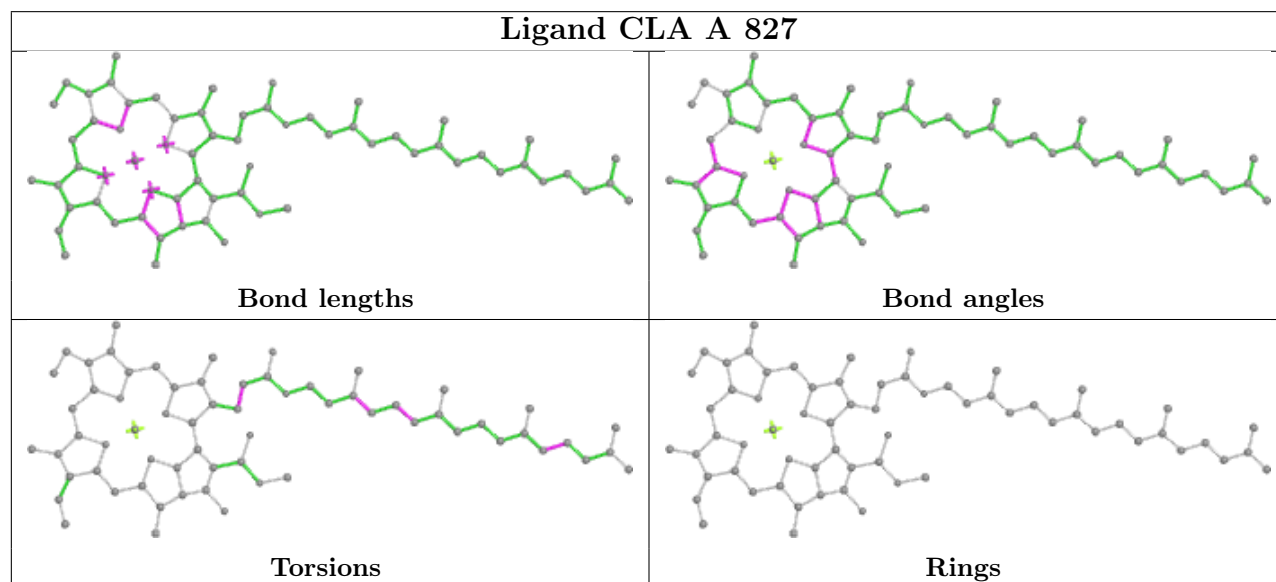


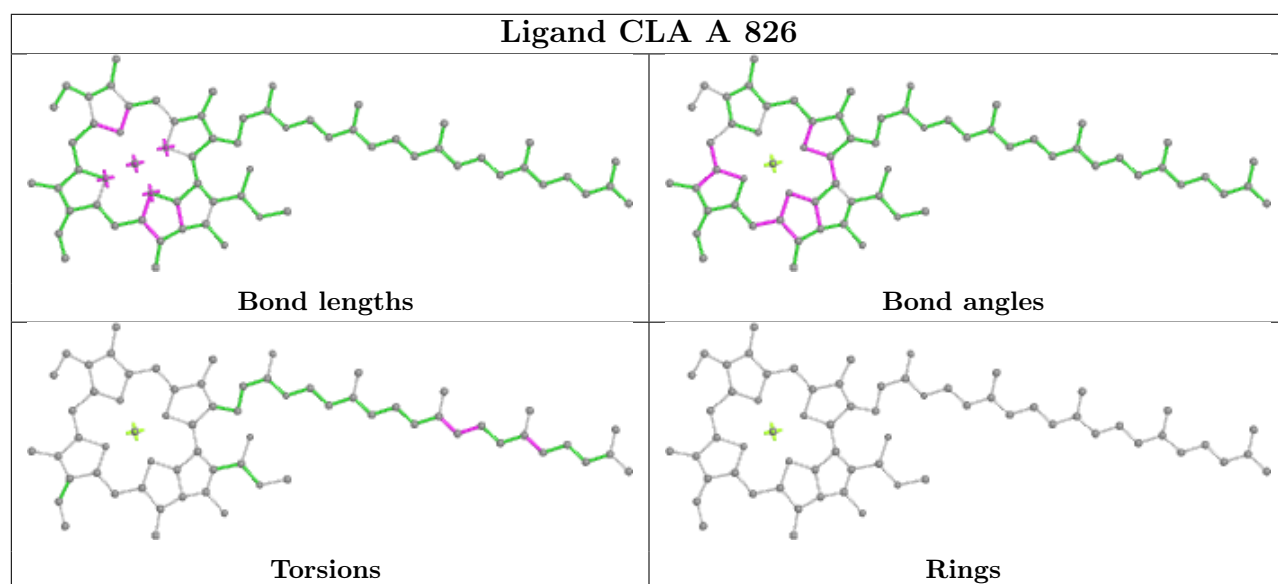
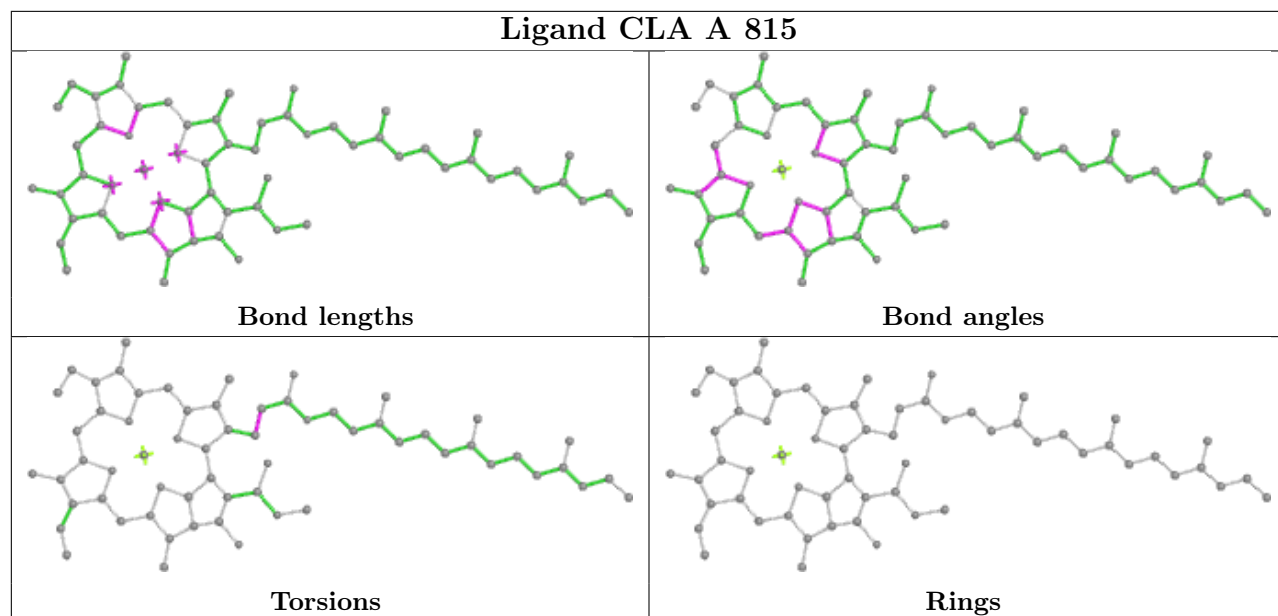
## Ligand CLA A 805

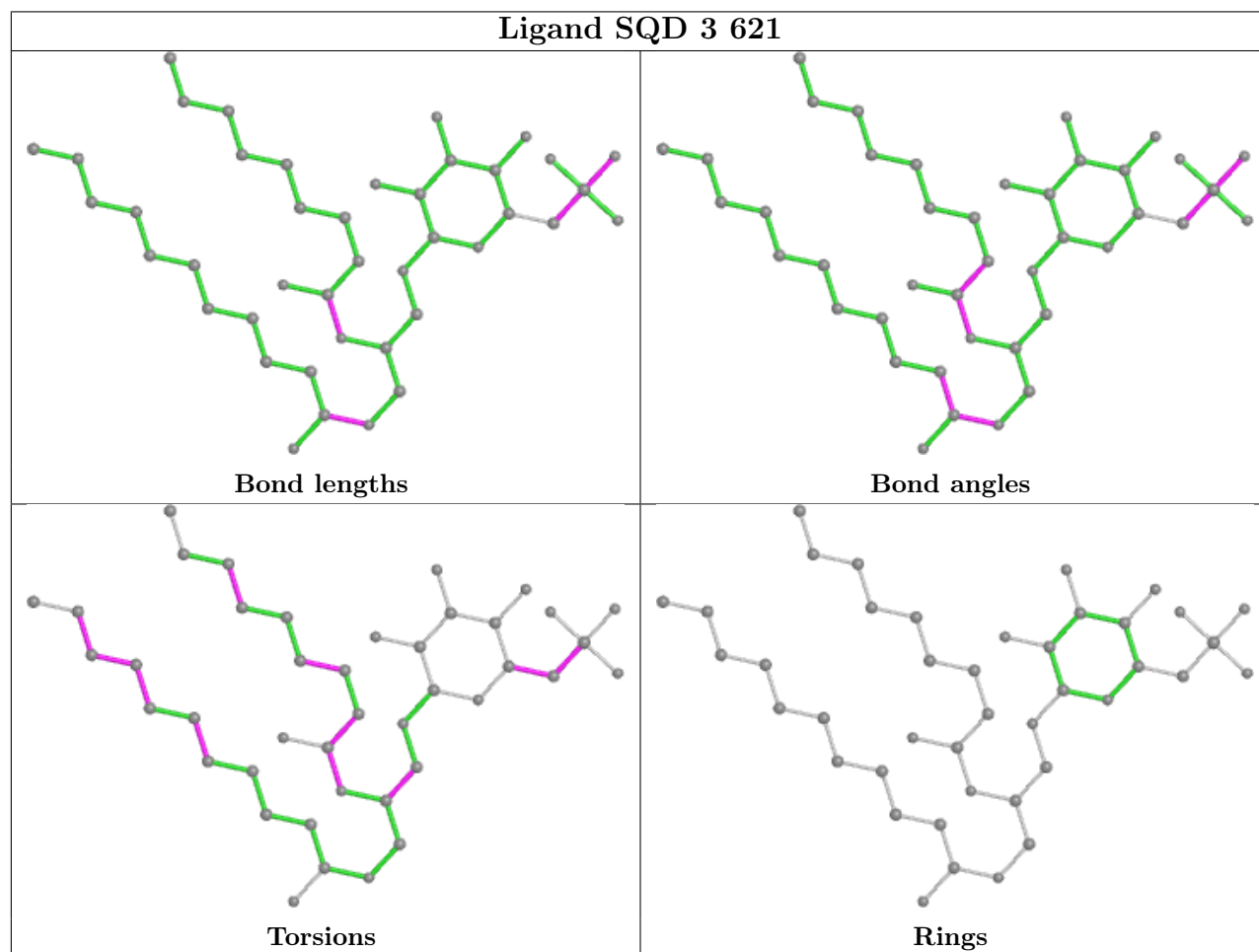
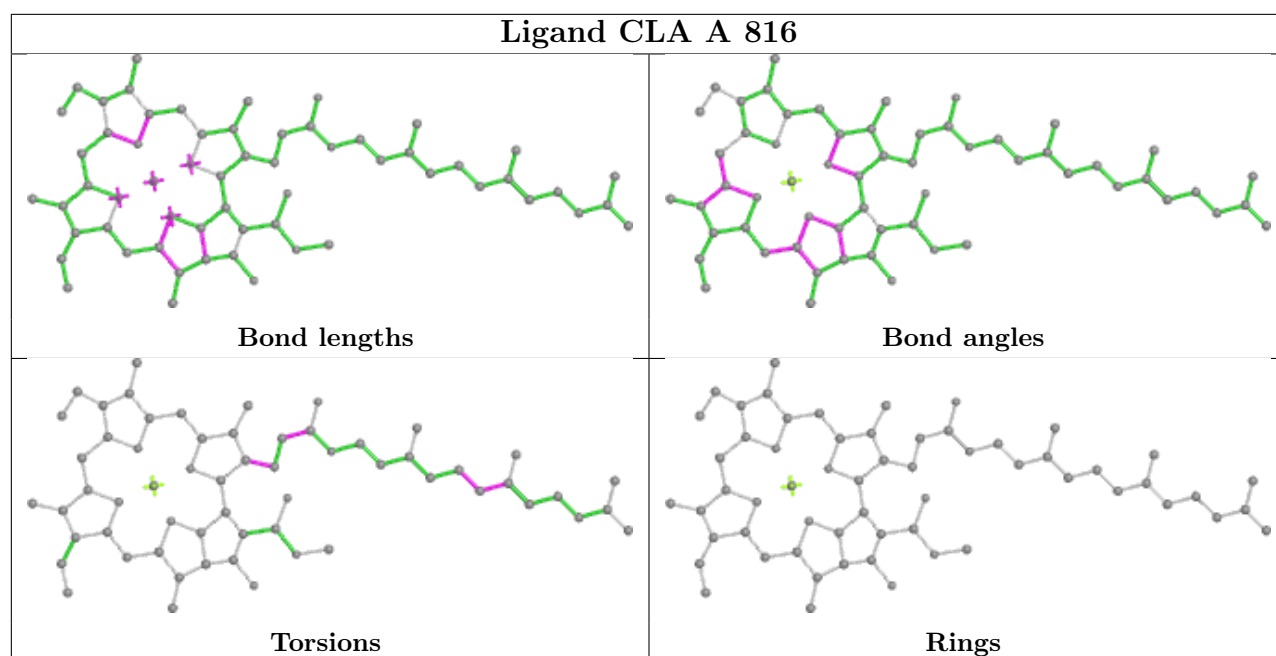


## Ligand LHG 7 319

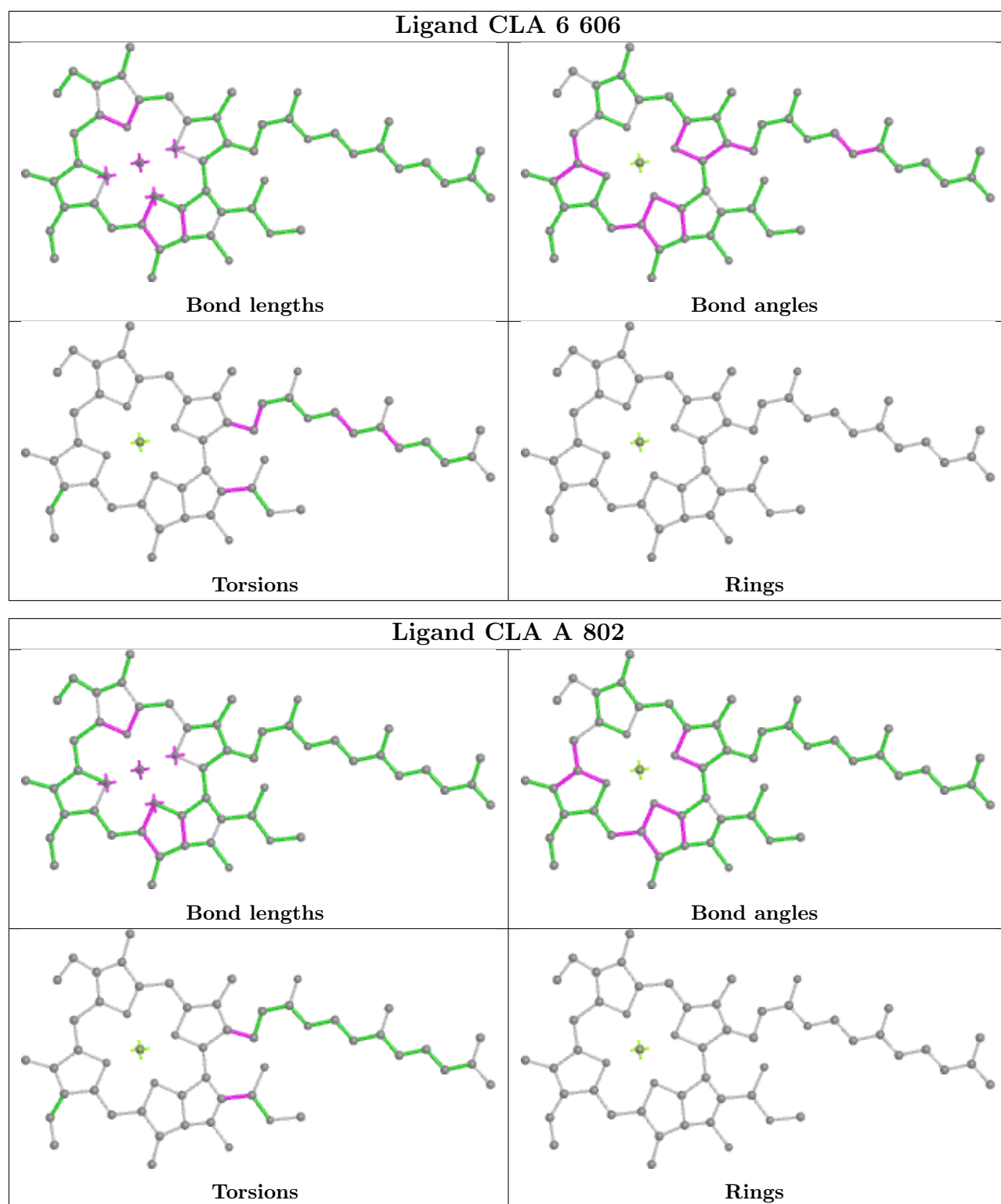


**Ligand CLA b 602****Ligand CLA A 827**









## 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.

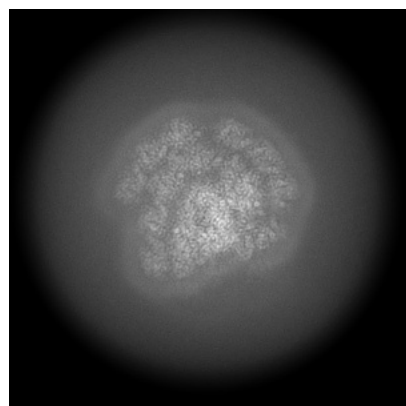
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33683. These allow visual inspection of the internal detail of the map and identification of artifacts.

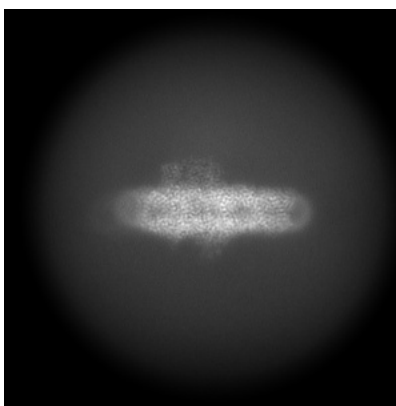
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

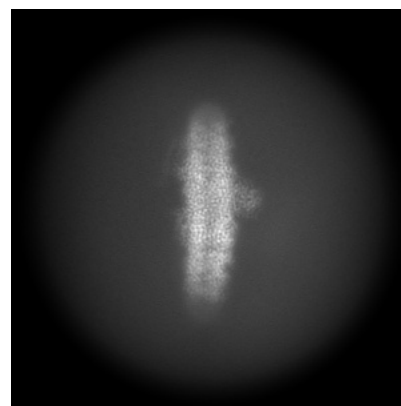
#### 6.1.1 Primary map



X

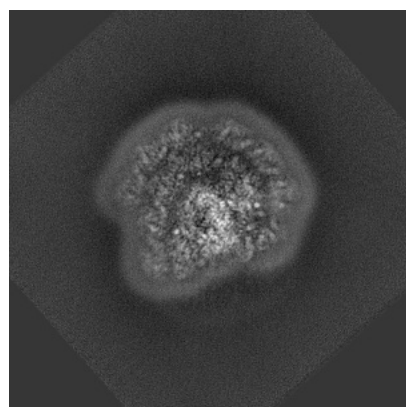


Y

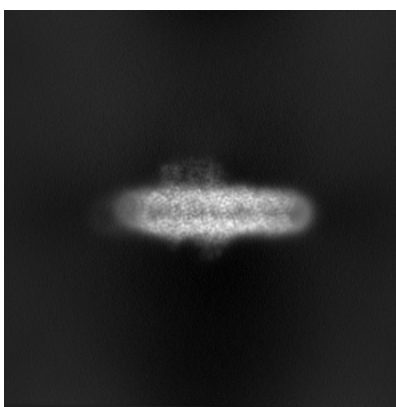


Z

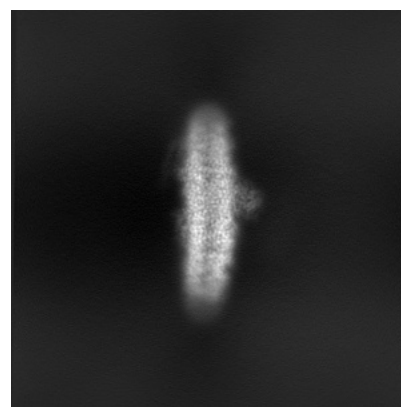
#### 6.1.2 Raw map



X



Y

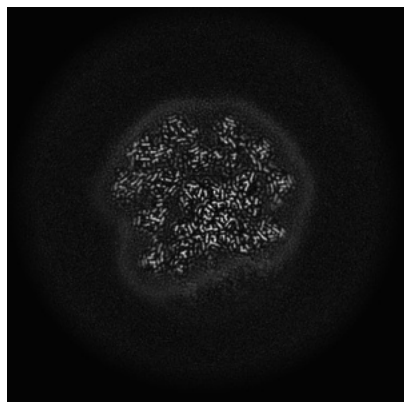


Z

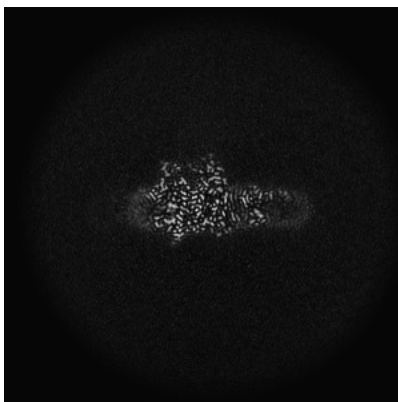
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

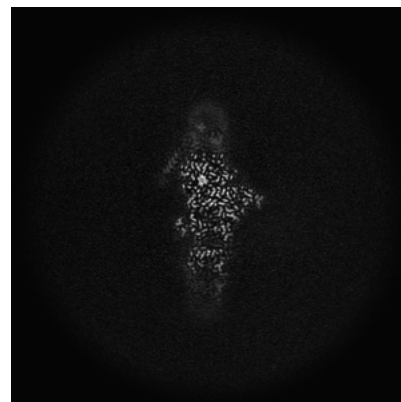
### 6.2.1 Primary map



X Index: 200

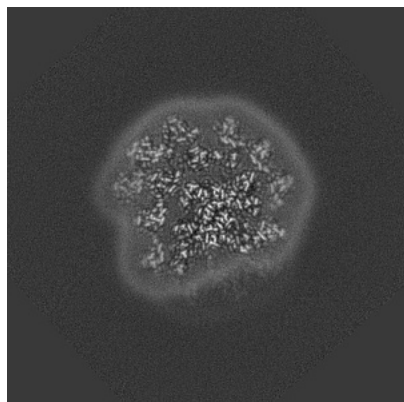


Y Index: 200

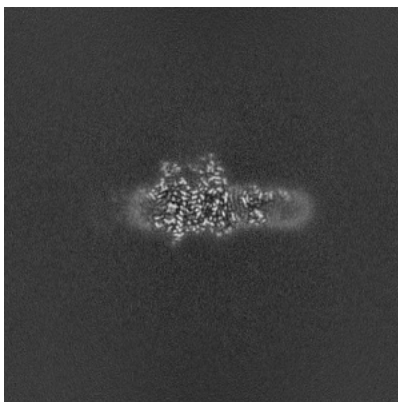


Z Index: 200

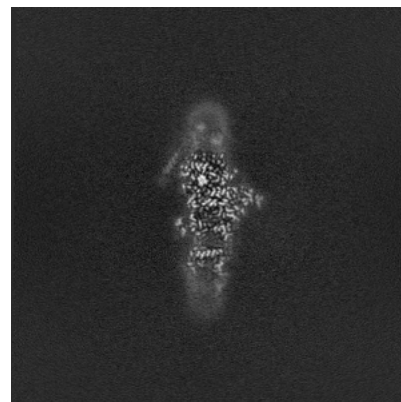
### 6.2.2 Raw map



X Index: 200



Y Index: 200

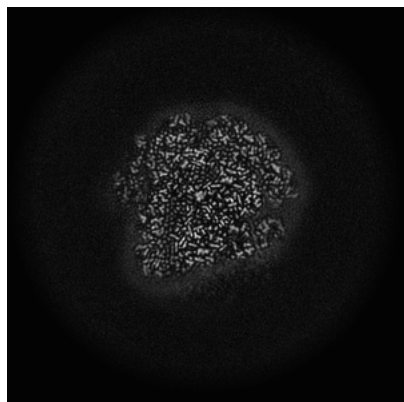


Z Index: 200

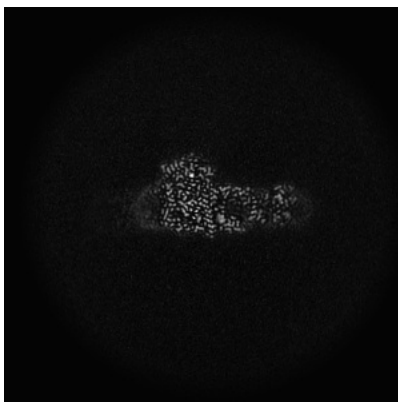
The images above show central slices of the map in three orthogonal directions.

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

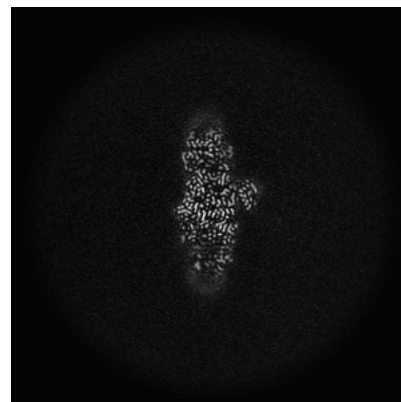
### 6.3.1 Primary map



X Index: 210

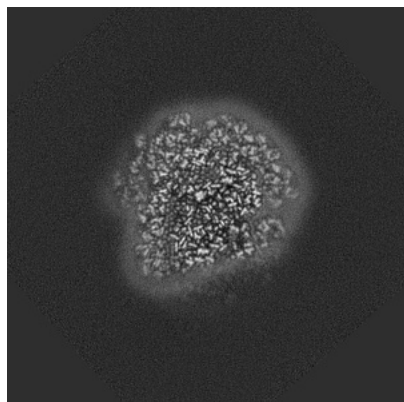


Y Index: 212

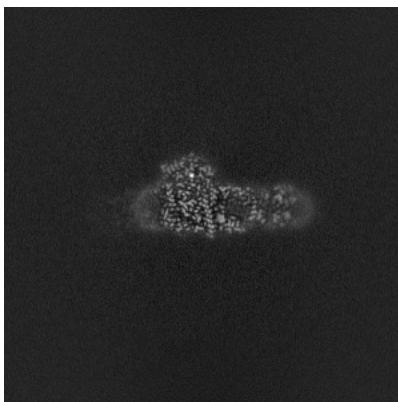


Z Index: 174

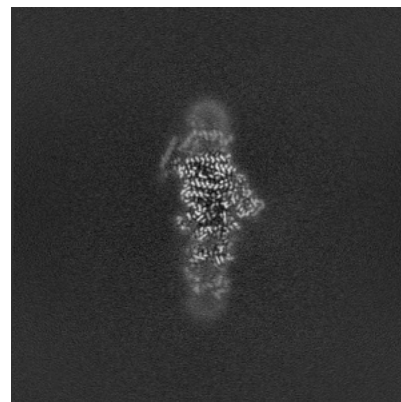
### 6.3.2 Raw map



X Index: 210



Y Index: 212

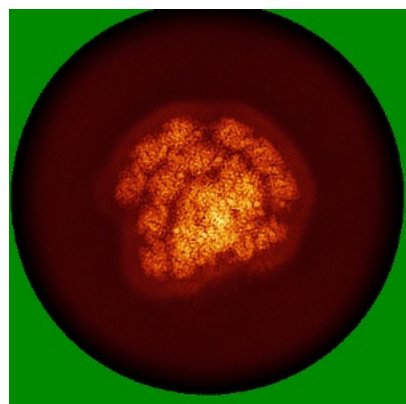


Z Index: 206

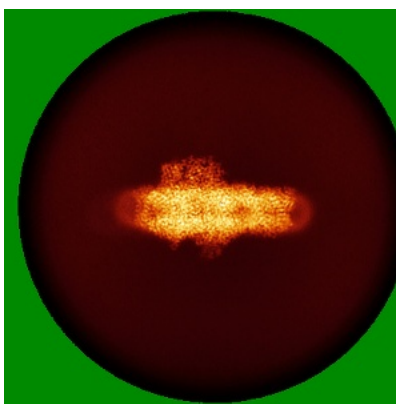
The images above show the largest variance slices of the map in three orthogonal directions.

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

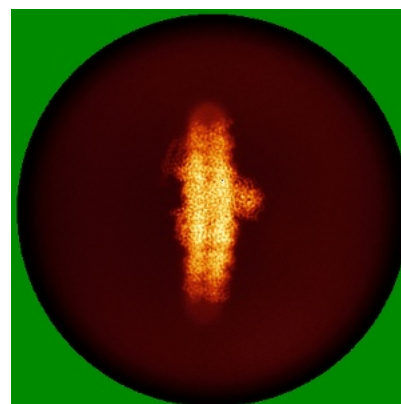
### 6.4.1 Primary map



X

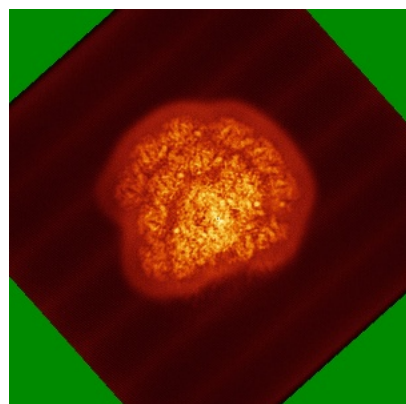


Y

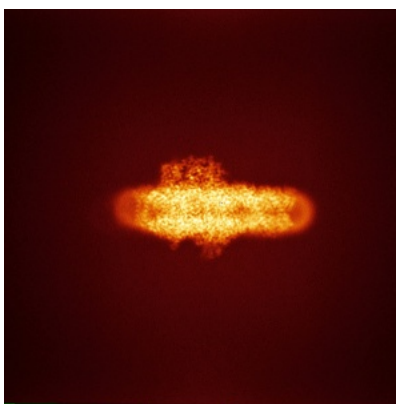


Z

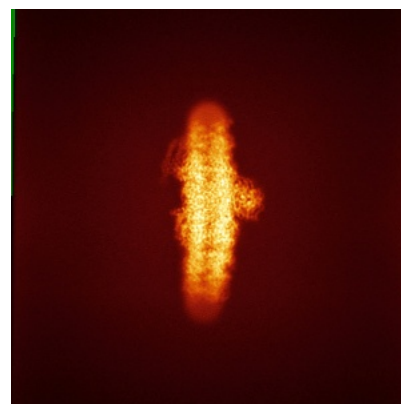
### 6.4.2 Raw map



X



Y



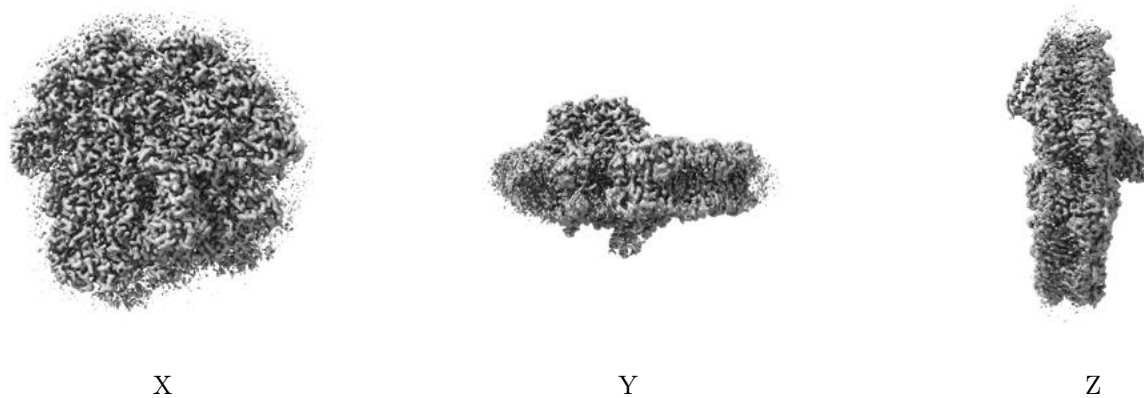
Z

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



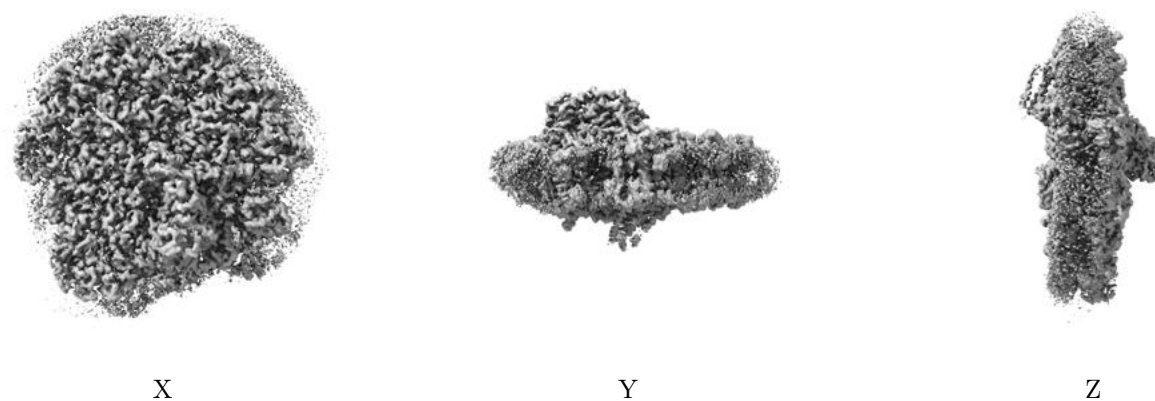
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

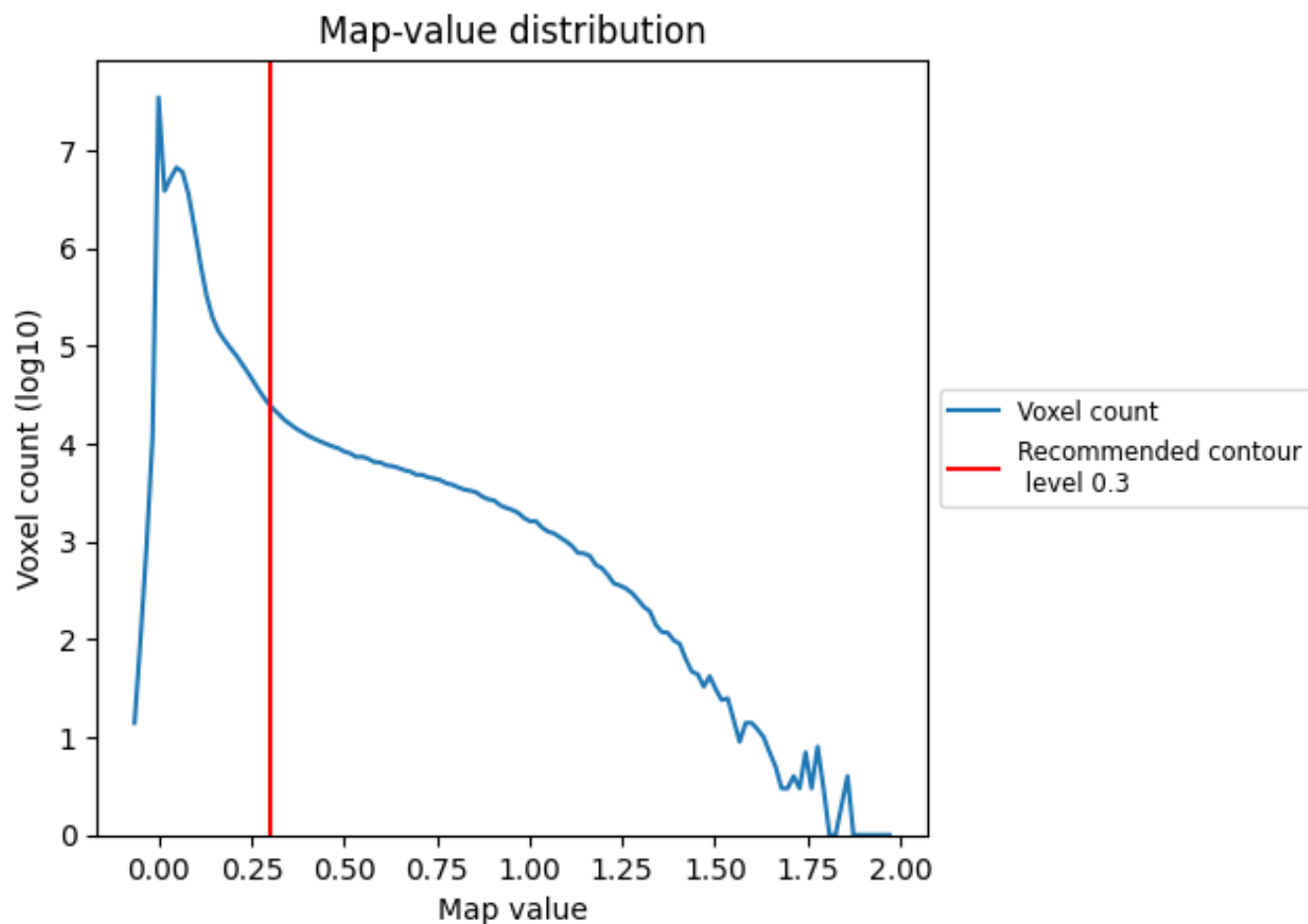
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

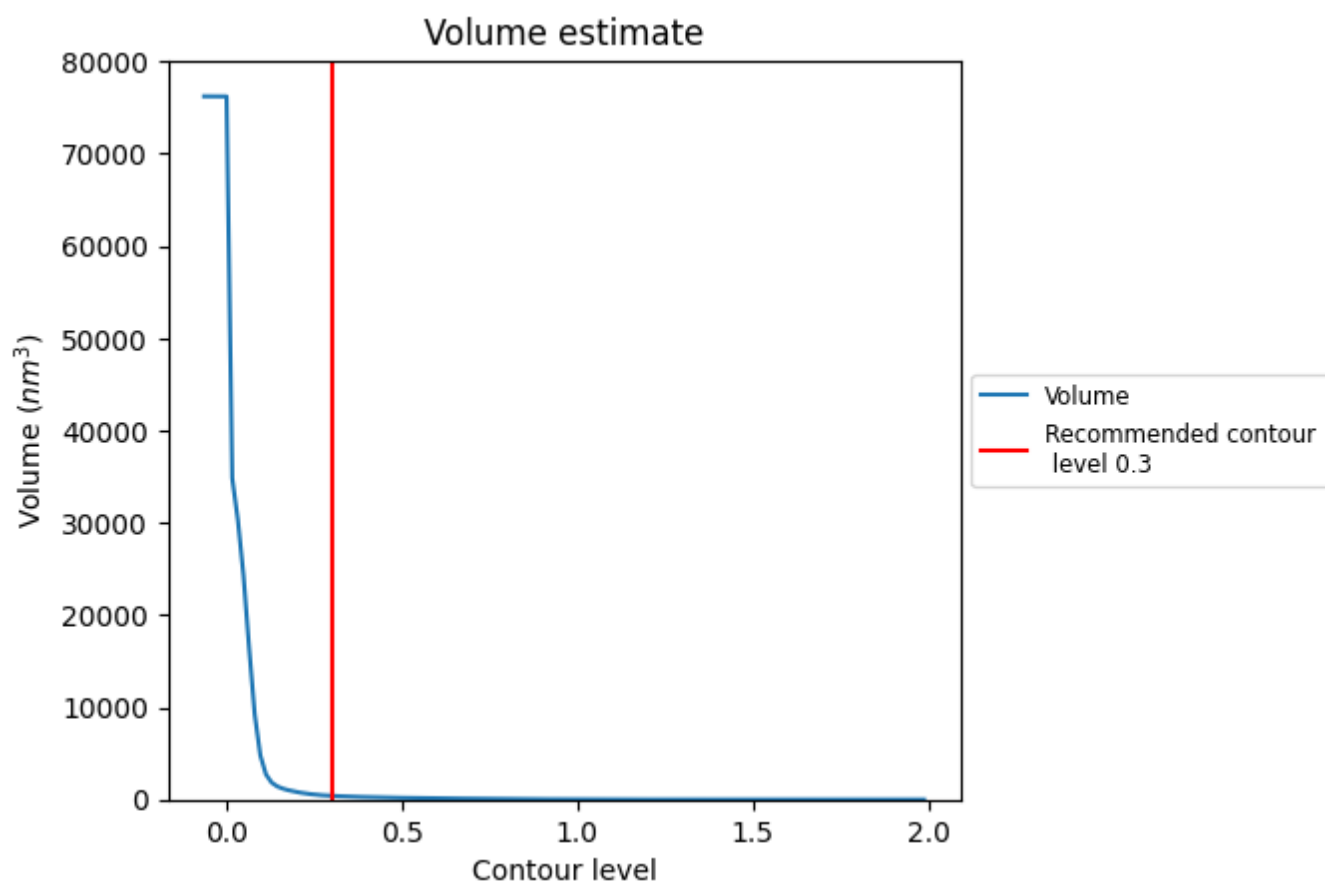
### 7.1 Map-value distribution [i](#)



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.



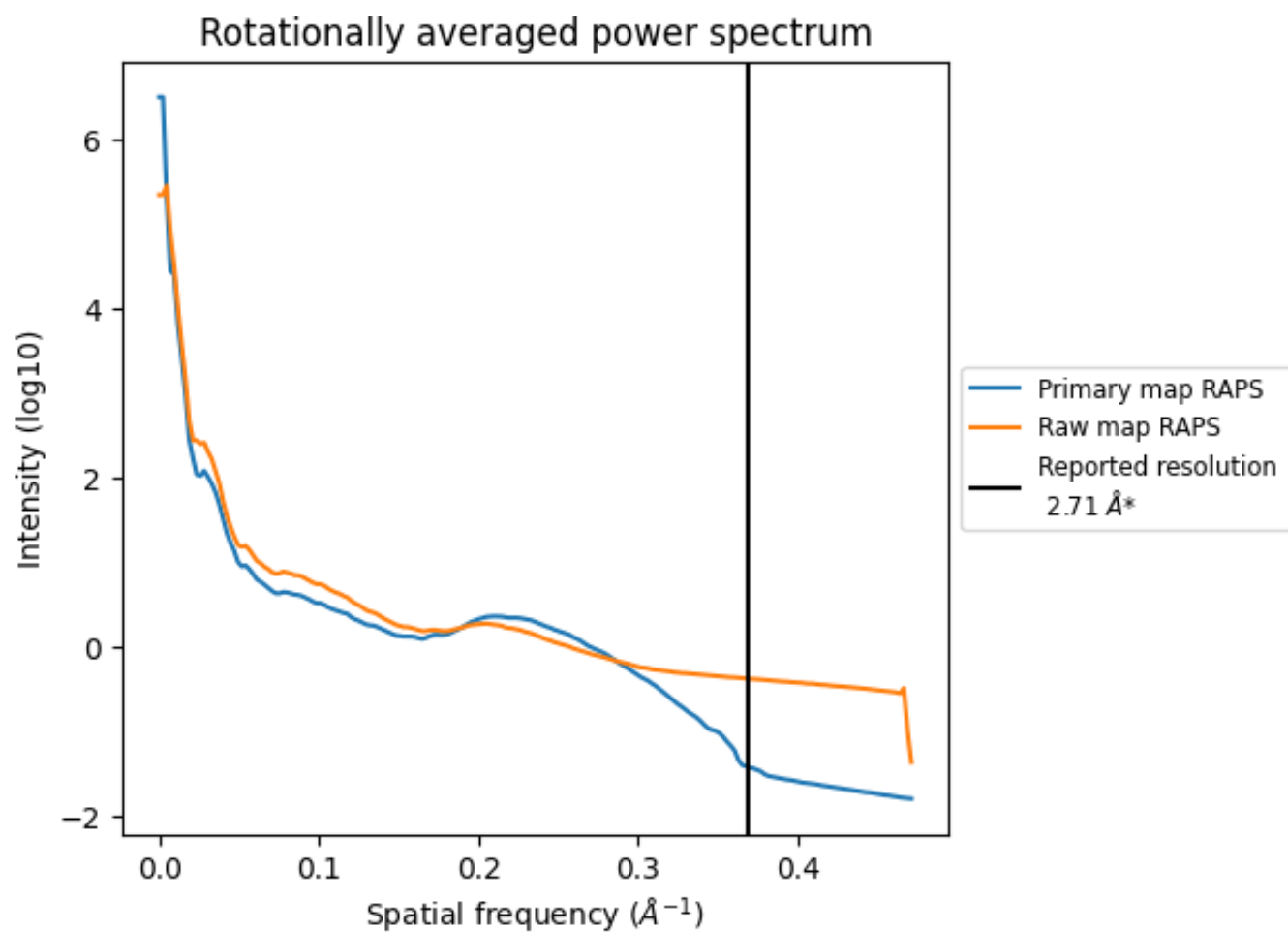
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 402 nm<sup>3</sup>; this corresponds to an approximate mass of 363 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 ⓘ

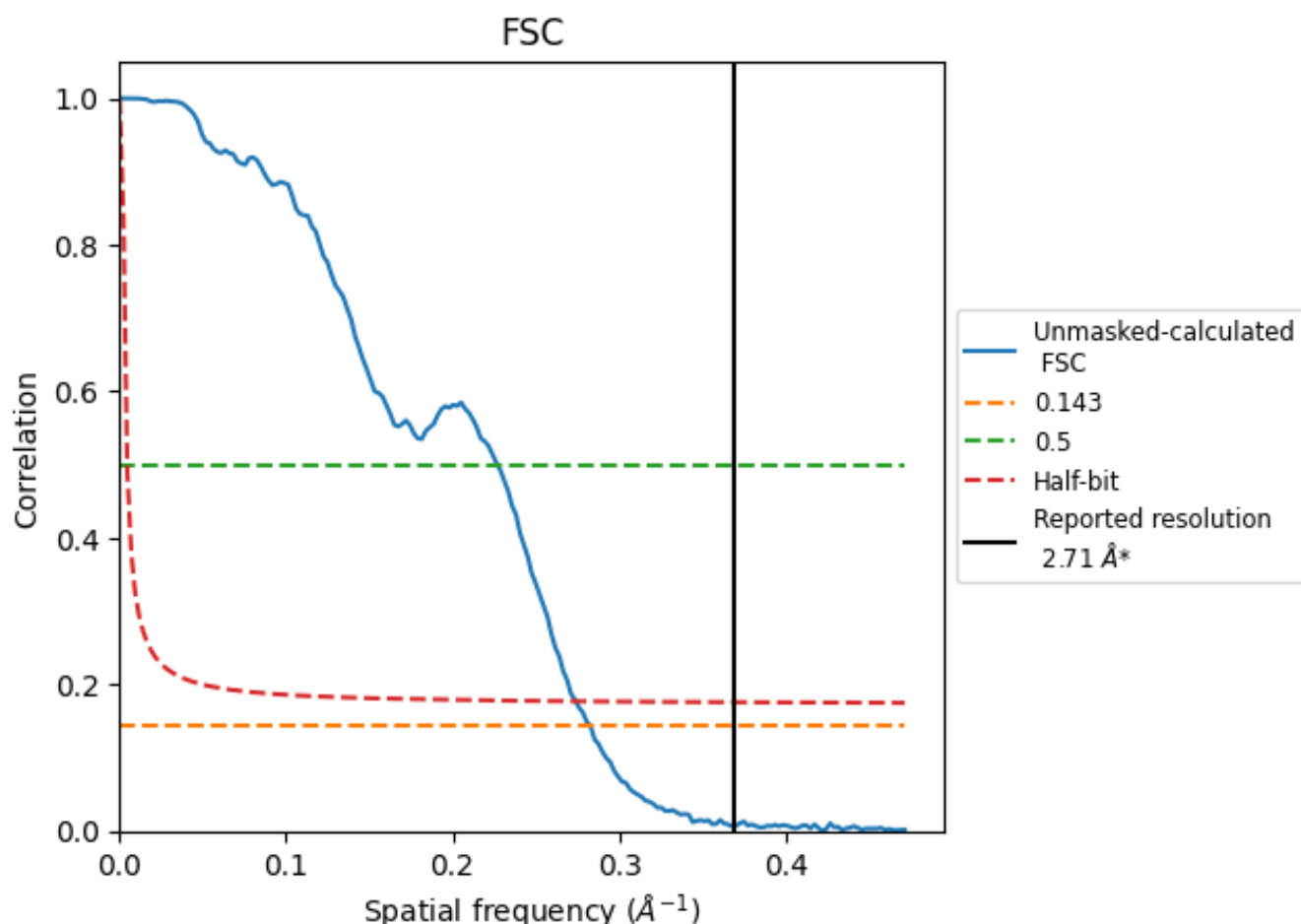


\*Reported resolution corresponds to spatial frequency of 0.369  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.369  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

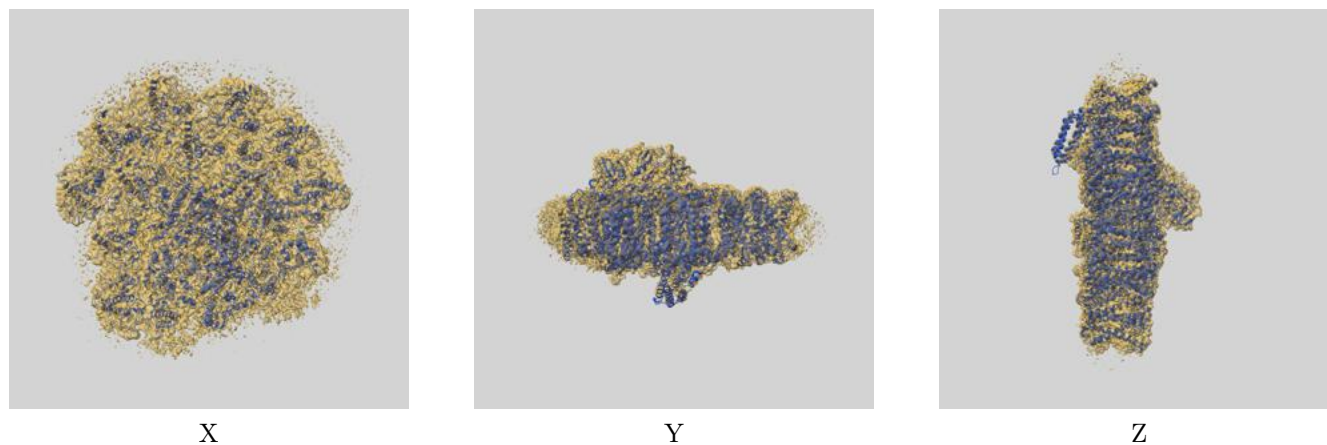
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.41	3.65

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 2.71 by more than 10 %

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

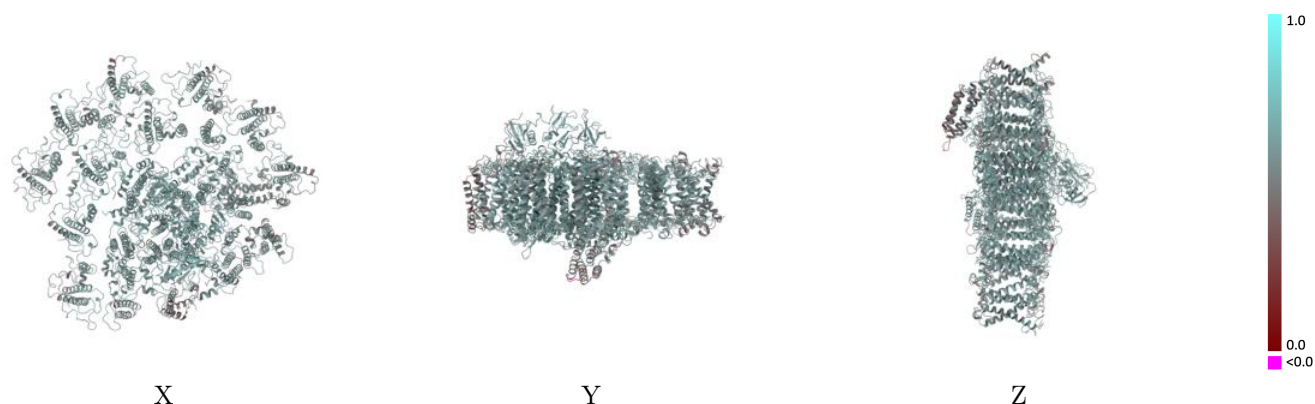
This section contains information regarding the fit between EMDB map EMD-33683 and PDB model 7Y8A. Per-residue inclusion information can be found in [section 3](#) on [page 38](#).

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



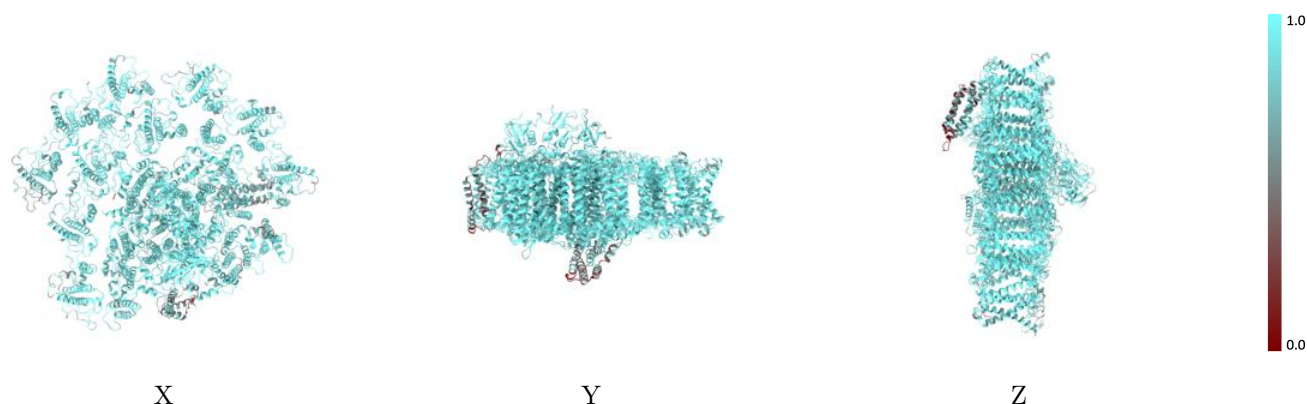
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



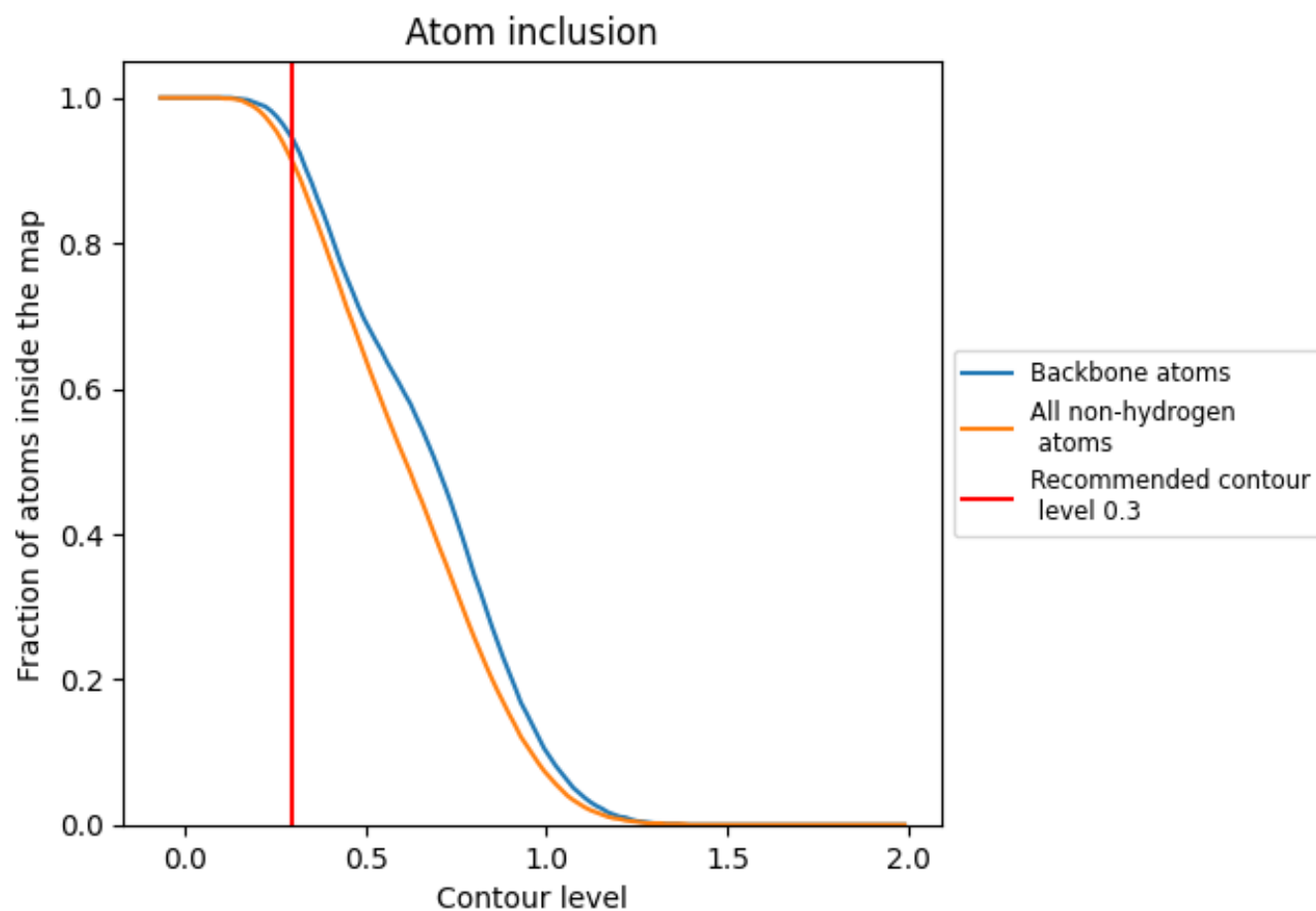
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9110	 0.5810
1	 0.8440	 0.5270
2	 0.9210	 0.5810
3	 0.9450	 0.6080
4	 0.9400	 0.5980
5	 0.8730	 0.5370
6	 0.9080	 0.5580
7	 0.8780	 0.5340
8	 0.8870	 0.5560
9	 0.7800	 0.5420
A	 0.9690	 0.6140
B	 0.9730	 0.6220
C	 0.9680	 0.6020
D	 0.9470	 0.5840
E	 0.8740	 0.5850
F	 0.9230	 0.5960
I	 0.9760	 0.6120
J	 0.9610	 0.6110
K	 0.8740	 0.5370
L	 0.8760	 0.5640
M	 0.9430	 0.5940
O	 0.5870	 0.4700
R	 0.9360	 0.5890
X	 0.5590	 0.4670
Z	 0.8960	 0.5790
a	 0.9040	 0.5640
b	 0.9200	 0.5640

