



## Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 12:41 PM JST

PDB ID : 8ZEH / pdb\_00008zeh  
EMDB ID : EMD-60032  
Title : PSI-FCPI-L in Thalassiosira pseudonana  
Authors : Feng, Y.; Li, Z.; Wang, W.; Shen, J.R.  
Deposited on : 2024-05-06  
Resolution : 2.78 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:

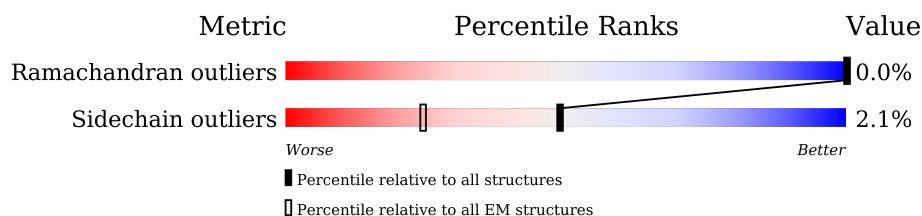
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 2.78 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.



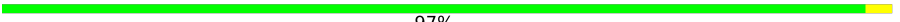
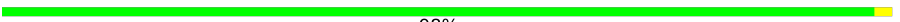






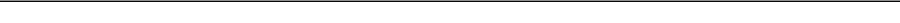

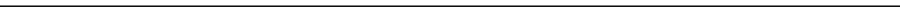


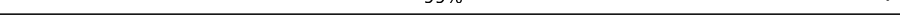
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	148	99% .
2	B	165	95% 5% .
3	C	170	98% .
4	E	185	100%
5	F	170	96% . .
6	G	174	99% .
7	H	168	100%
8	I	172	98% .
9	J	183	96% .

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Mol	Chain	Length	Quality of chain
10	K	176	 97%
11	L	217	 98%
12	M	171	 98%
13	a	743	 99%
14	d	132	 98%
15	e	62	 95% 5%
16	f	160	 99%
17	g	131	 97%
18	i	33	 100%
19	j	40	 92% 8%
20	l	146	 99%
21	m	29	 100%
22	r	89	 99%
23	D	164	 98%
24	b	732	 99%
25	c	80	 100%

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	A	203	X	-	-	-
27	CLA	A	204	X	-	-	-
27	CLA	A	205	X	-	-	-
27	CLA	A	206	X	-	-	-
27	CLA	A	207	X	-	-	-
27	CLA	A	208	X	-	-	-
27	CLA	A	210	X	-	-	-
27	CLA	A	211	X	-	-	-
27	CLA	B	306	X	-	-	-
27	CLA	B	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	308	X	-	-	-
27	CLA	B	309	X	-	-	-
27	CLA	B	310	X	-	-	-
27	CLA	B	311	X	-	-	-
27	CLA	B	312	X	-	-	-
27	CLA	B	314	X	-	-	-
27	CLA	C	306	X	-	-	-
27	CLA	C	307	X	-	-	-
27	CLA	C	309	X	-	-	-
27	CLA	C	310	X	-	-	-
27	CLA	C	311	X	-	-	-
27	CLA	C	312	X	-	-	-
27	CLA	C	314	X	-	-	-
27	CLA	C	315	X	-	-	-
27	CLA	C	316	X	-	-	-
27	CLA	C	317	X	-	-	-
27	CLA	C	318	X	-	-	-
27	CLA	D	207	X	-	-	-
27	CLA	D	208	X	-	-	-
27	CLA	D	209	X	-	-	-
27	CLA	D	210	X	-	-	-
27	CLA	D	211	X	-	-	-
27	CLA	D	212	X	-	-	-
27	CLA	D	213	X	-	-	-
27	CLA	D	214	X	-	-	-
27	CLA	D	215	X	-	-	-
27	CLA	D	216	X	-	-	-
27	CLA	D	217	X	-	-	-
27	CLA	E	308	X	-	-	-
27	CLA	E	309	X	-	-	-
27	CLA	E	310	X	-	-	-
27	CLA	E	311	X	-	-	-
27	CLA	E	312	X	-	-	-
27	CLA	E	313	X	-	-	-
27	CLA	E	314	X	-	-	-
27	CLA	E	315	X	-	-	-
27	CLA	F	305	X	-	-	-
27	CLA	F	306	X	-	-	-
27	CLA	F	307	X	-	-	-
27	CLA	F	308	X	-	-	-
27	CLA	F	309	X	-	-	-
27	CLA	F	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	F	311	X	-	-	-
27	CLA	F	313	X	-	-	-
27	CLA	F	314	X	-	-	-
27	CLA	F	315	X	-	-	-
27	CLA	F	316	X	-	-	-
27	CLA	F	317	X	-	-	-
27	CLA	G	306	X	-	-	-
27	CLA	G	307	X	-	-	-
27	CLA	G	308	X	-	-	-
27	CLA	G	309	X	-	-	-
27	CLA	G	310	X	-	-	-
27	CLA	G	311	X	-	-	-
27	CLA	G	312	X	-	-	-
27	CLA	G	314	X	-	-	-
27	CLA	G	315	X	-	-	-
27	CLA	G	316	X	-	-	-
27	CLA	G	317	X	-	-	-
27	CLA	H	204	X	-	-	-
27	CLA	H	205	X	-	-	-
27	CLA	H	206	X	-	-	-
27	CLA	H	207	X	-	-	-
27	CLA	H	208	X	-	-	-
27	CLA	H	209	X	-	-	-
27	CLA	H	210	X	-	-	-
27	CLA	H	212	X	-	-	-
27	CLA	H	213	X	-	-	-
27	CLA	H	214	X	-	-	-
27	CLA	I	305	X	-	-	-
27	CLA	I	306	X	-	-	-
27	CLA	I	307	X	-	-	-
27	CLA	I	308	X	-	-	-
27	CLA	I	309	X	-	-	-
27	CLA	I	310	X	-	-	-
27	CLA	I	311	X	-	-	-
27	CLA	I	313	X	-	-	-
27	CLA	I	314	X	-	-	-
27	CLA	I	315	X	-	-	-
27	CLA	I	316	X	-	-	-
27	CLA	I	317	X	-	-	-
27	CLA	J	307	X	-	-	-
27	CLA	J	308	X	-	-	-
27	CLA	J	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	J	310	X	-	-	-
27	CLA	J	311	X	-	-	-
27	CLA	J	312	X	-	-	-
27	CLA	J	313	X	-	-	-
27	CLA	J	314	X	-	-	-
27	CLA	J	315	X	-	-	-
27	CLA	K	309	X	-	-	-
27	CLA	K	310	X	-	-	-
27	CLA	K	311	X	-	-	-
27	CLA	K	312	X	-	-	-
27	CLA	K	313	X	-	-	-
27	CLA	K	314	X	-	-	-
27	CLA	K	316	X	-	-	-
27	CLA	K	317	X	-	-	-
27	CLA	K	318	X	-	-	-
27	CLA	K	319	X	-	-	-
27	CLA	L	307	X	-	-	-
27	CLA	L	308	X	-	-	-
27	CLA	L	309	X	-	-	-
27	CLA	L	310	X	-	-	-
27	CLA	L	311	X	-	-	-
27	CLA	L	312	X	-	-	-
27	CLA	L	313	X	-	-	-
27	CLA	L	315	X	-	-	-
27	CLA	L	316	X	-	-	-
27	CLA	L	317	X	-	-	-
27	CLA	L	318	X	-	-	-
27	CLA	L	319	X	-	-	-
27	CLA	L	321	X	-	-	-
27	CLA	M	307	X	-	-	-
27	CLA	M	308	X	-	-	-
27	CLA	M	309	X	-	-	-
27	CLA	M	310	X	-	-	-
27	CLA	M	311	X	-	-	-
27	CLA	M	312	X	-	-	-
27	CLA	M	313	X	-	-	-
27	CLA	M	315	X	-	-	-
27	CLA	M	316	X	-	-	-
27	CLA	M	318	X	-	-	-
27	CLA	M	319	X	-	-	-
27	CLA	a	803	X	-	-	-
27	CLA	a	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	832	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	a	845	X	-	-	-
27	CLA	a	846	X	-	-	-
27	CLA	a	848	X	-	-	-
27	CLA	a	849	X	-	-	-
27	CLA	a	850	X	-	-	-
27	CLA	a	854	X	-	-	-
27	CLA	a	855	X	-	-	-
27	CLA	a	856	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	801	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	838	X	-	-	-
27	CLA	b	839	X	-	-	-
27	CLA	b	841	X	-	-	-
27	CLA	b	842	X	-	-	-
27	CLA	b	843	X	-	-	-
27	CLA	b	844	X	-	-	-
27	CLA	b	845	X	-	-	-
27	CLA	b	846	X	-	-	-
27	CLA	b	847	X	-	-	-
27	CLA	b	849	X	-	-	-
27	CLA	b	850	X	-	-	-
27	CLA	f	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	f	302	X	-	-	-
27	CLA	f	303	X	-	-	-
27	CLA	i	101	X	-	-	-
27	CLA	j	104	X	-	-	-
27	CLA	l	203	X	-	-	-
27	CLA	l	204	X	-	-	-
27	CLA	l	206	X	-	-	-
27	CLA	r	201	X	-	-	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 54849 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 Tp-Lhcr18.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	148	Total	C	N	O	S	0	0
			1172	760	194	212	6		

- Molecule 2 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	165	Total	C	N	O	S	0	0
			1285	833	204	240	8		

- Molecule 3 is a protein called Fucoxanthin chl a/c light-harvesting protein, major type.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	170	Total	C	N	O	S	0	0
			1302	841	213	240	8		

- Molecule 4 is a protein called Tp-RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	185	Total	C	N	O	S	0	0
			1413	902	235	262	14		

- Molecule 5 is a protein called Tp-Lhcr20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	170	Total	C	N	O	S	0	0
			1299	830	221	236	12		

- Molecule 6 is a protein called Fucoxanthin chl a/c light-harvesting protein, lhcr type.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	174	Total	C	N	O	S	0	0
			1320	837	218	250	15		

- Molecule 7 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	168	Total	C	N	O	S	0	0
			1300	834	214	242	10		

- Molecule 8 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	172	Total	C	N	O	S	0	0
			1315	850	212	243	10		

- Molecule 9 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	183	Total	C	N	O	S	0	0
			1389	887	233	258	11		

- Molecule 10 is a protein called Fucoxanthin chlorophyll a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	176	Total	C	N	O	S	0	0
			1332	853	223	242	14		

- Molecule 11 is a protein called Fucoxanthin chlorophyll a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	217	Total	C	N	O	S	0	0
			1669	1074	274	306	15		

- Molecule 12 is a protein called Fucoxanthin chlorophyll a/c light-harvesting protein, lhcr type.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	171	Total	C	N	O	S	0	0
			1308	847	214	237	10		

- Molecule 13 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	743	Total	C	N	O	S	0	0
			5852	3822	992	1009	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	132	Total	C	N	O	S	0	0
			1040	665	177	195	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	62	Total	C	N	O	S	0	0
			503	317	89	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	160	Total	C	N	O	S	0	0
			1242	795	211	233	3		

- Molecule 17 is a protein called Photosystem I reaction center subunit Psa29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	131	Total	C	N	O	S	0	0
			981	619	154	204	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	i	33	Total	C	N	O	S	0	0
			256	177	34	44	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	j	40	Total	C	N	O	S	0	0
			332	224	48	57	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	146	Total	C	N	O	S	0	0
			1095	722	178	193	2		

- Molecule 21 is a protein called Photosystem I reaction center subunit XII.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	29	Total	C	N	O	S	0	0
			220	147	33	38	2		

- Molecule 22 is a protein called Tp-PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	89	Total	C	N	O	S	0	0
			683	443	112	121	7		

- Molecule 23 is a protein called Pt17531-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	164	Total	C	N	O	S	0	0
			1271	819	208	234	10		

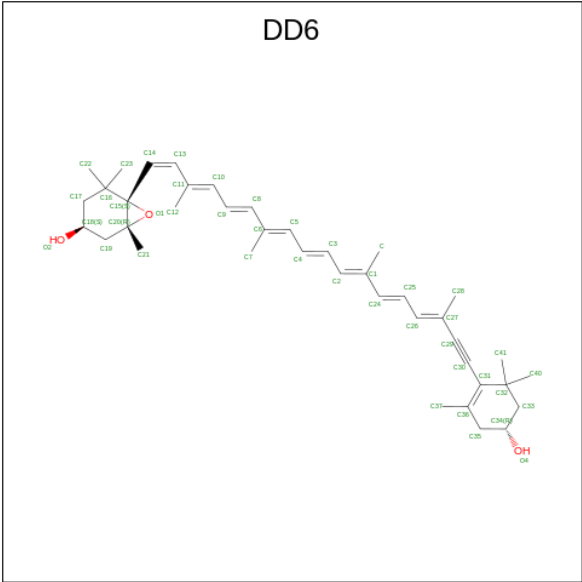
- Molecule 24 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	732	Total	C	N	O	S	0	0
			5824	3827	982	996	19		

- Molecule 25 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	80	Total	C	N	O	S	0	0
			599	368	103	118	10		

- Molecule 26 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



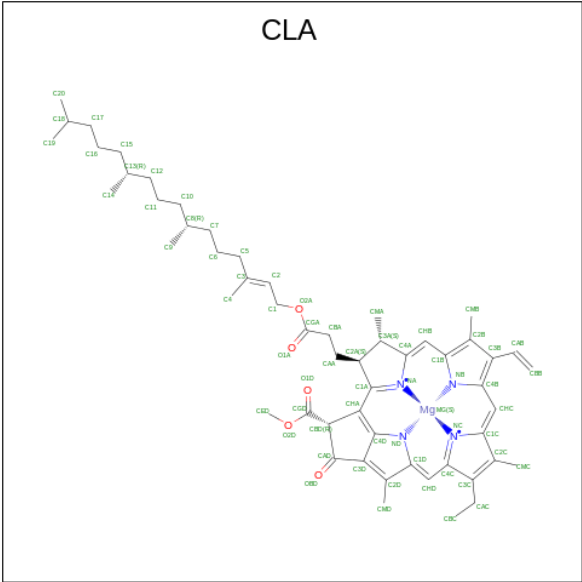
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			43	40	3	
26	A	1	Total	C	O	0
			43	40	3	
26	B	1	Total	C	O	0
			43	40	3	
26	C	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	E	1	Total	C	O	0
			43	40	3	
26	F	1	Total	C	O	0
			43	40	3	
26	F	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
26	H	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	J	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	L	1	Total	C	O	0
			43	40	3	
26	L	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	D	1	Total	C	O	0
			43	40	3	

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



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			61	51	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
			46	36	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
			54	44	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	B	1	Total	C	Mg	N	O	0
			57	49	1	4	3	
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
			46	36	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 41	C 33	Mg 1	N 4	O 3	0
27	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	F	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	F	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	F	1	Total 46	C 36	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 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	F	1	Total 58	C 48	Mg 1	N 4	O 5	0
27	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	G	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	G	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
27	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	I	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	L	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	L	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	L	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	L	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	M	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	M	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	M	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	M	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	M	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	M	1	Total	C	Mg	N	O	0
			46	36	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	
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
			62	52	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
			45	35	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
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			51	41	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
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			51	41	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
			52	42	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
			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	

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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	a	1	Total 56	C 46	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	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	i	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	j	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	l	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	D	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	D	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	D	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	D	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	D	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
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
			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
			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
			60	50	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			59	49	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
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 55	C 45	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 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 50	C 40	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 58	C 48	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 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 47	C 37	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 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 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

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Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 62	C 52	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 54	C 44	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

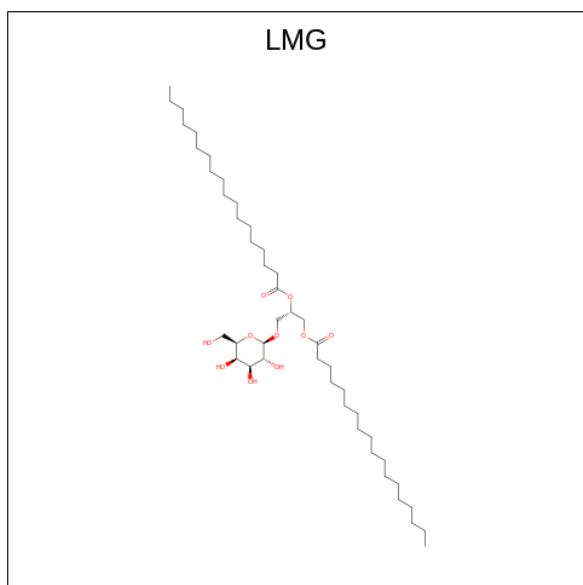
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Mol	Chain	Residues	Atoms					AltConf
28	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			51	41	10	
29	A	1	Total	C	O	0
			41	31	10	

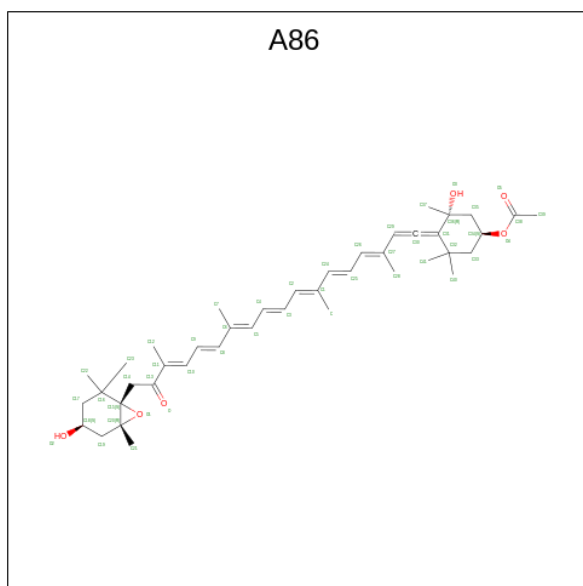
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Mol	Chain	Residues	Atoms			AltConf
29	C	1	Total	C	O	0
			31	21	10	
29	C	1	Total	C	O	0
			44	34	10	
29	E	1	Total	C	O	0
			43	33	10	
29	I	1	Total	C	O	0
			37	27	10	
29	J	1	Total	C	O	0
			51	41	10	
29	L	1	Total	C	O	0
			46	36	10	
29	M	1	Total	C	O	0
			42	32	10	
29	a	1	Total	C	O	0
			33	23	10	
29	j	1	Total	C	O	0
			37	27	10	
29	l	1	Total	C	O	0
			40	30	10	
29	D	1	Total	C	O	0
			46	36	10	

- Molecule 30 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula:  $C_{42}H_{58}O_6$ ) (labeled as "Ligand of Interest" by depositor).



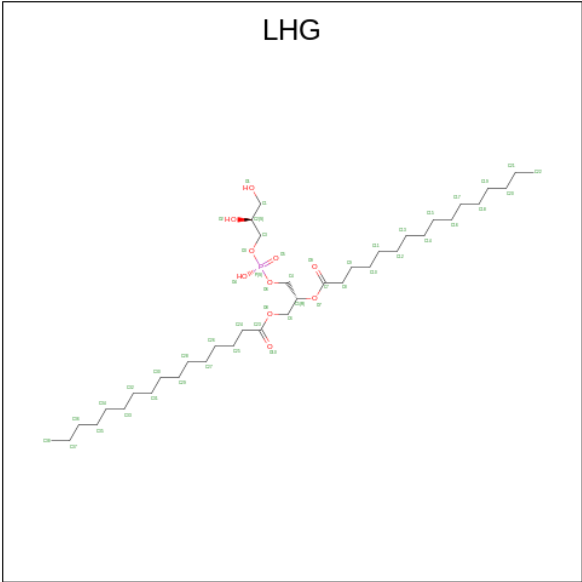
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	B	1	Total	C	O	0
			48	42	6	
30	C	1	Total	C	O	0
			48	42	6	
30	C	1	Total	C	O	0
			48	42	6	
30	C	1	Total	C	O	0
			48	42	6	
30	E	1	Total	C	O	0
			48	42	6	
30	F	1	Total	C	O	0
			48	42	6	
30	F	1	Total	C	O	0
			48	42	6	
30	G	1	Total	C	O	0
			48	42	6	
30	H	1	Total	C	O	0
			48	42	6	
30	H	1	Total	C	O	0
			48	42	6	
30	I	1	Total	C	O	0
			48	42	6	
30	I	1	Total	C	O	0
			48	42	6	
30	J	1	Total	C	O	0
			48	42	6	
30	J	1	Total	C	O	0
			48	42	6	
30	J	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
30	K	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	
30	K	1	Total	C	O	0
			48	42	6	
30	L	1	Total	C	O	0
			48	42	6	
30	L	1	Total	C	O	0
			48	42	6	
30	L	1	Total	C	O	0
			48	42	6	
30	L	1	Total	C	O	0
			48	42	6	
30	M	1	Total	C	O	0
			48	42	6	
30	M	1	Total	C	O	0
			48	42	6	
30	M	1	Total	C	O	0
			48	42	6	
30	m	1	Total	C	O	0
			48	42	6	
30	r	1	Total	C	O	0
			48	42	6	
30	D	1	Total	C	O	0
			48	42	6	
30	D	1	Total	C	O	0
			48	42	6	
30	D	1	Total	C	O	0
			48	42	6	
30	b	1	Total	C	O	0
			48	42	6	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



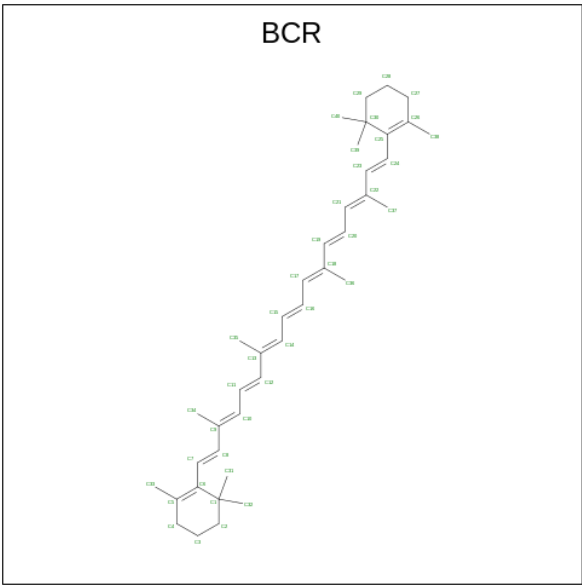
Mol	Chain	Residues	Atoms				AltConf
31	B	1	Total	C	O	P	0
			42	31	10	1	
31	E	1	Total	C	O	P	0
			42	31	10	1	
31	E	1	Total	C	O	P	0
			49	38	10	1	
31	H	1	Total	C	O	P	0
			35	24	10	1	
31	I	1	Total	C	O	P	0
			35	24	10	1	
31	K	1	Total	C	O	P	0
			33	24	8	1	
31	M	1	Total	C	O	P	0
			47	36	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			27	16	10	1	
31	a	1	Total	C	O	P	0
			33	22	10	1	
31	j	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
31	b	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 32 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



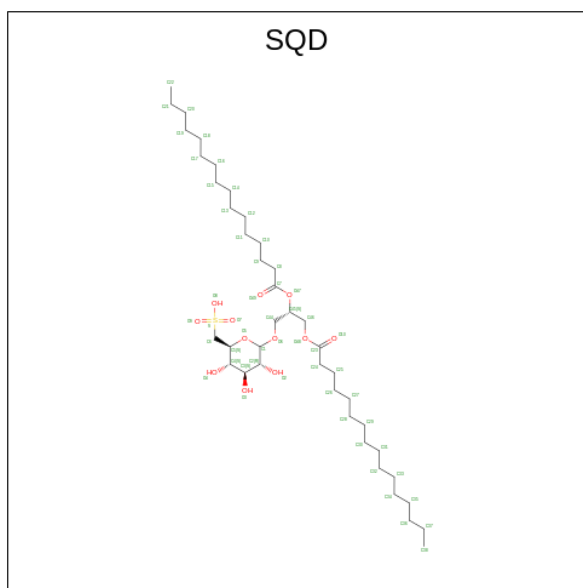
Mol	Chain	Residues	Atoms		AltConf
32	E	1	Total	C	0
			40	40	
32	E	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	f	1	Total	C	0
			40	40	
32	f	1	Total	C	0
			40	40	
32	i	1	Total	C	0
			40	40	

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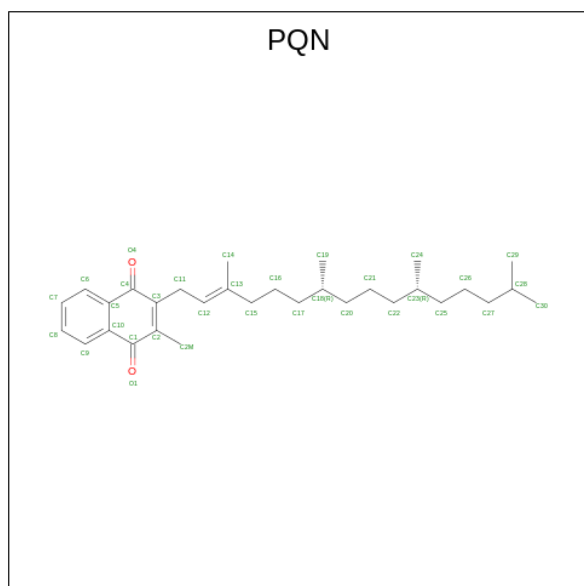
Mol	Chain	Residues	Atoms	AltConf
32	i	1	Total C 40 40	0
32	j	1	Total C 40 40	0
32	j	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	m	1	Total C 40 40	0
32	r	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



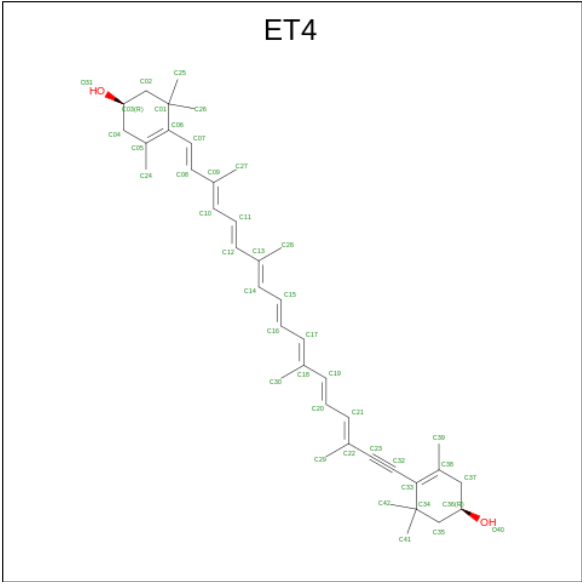
Mol	Chain	Residues	Atoms				AltConf
33	J	1	Total	C	O	S	0
			33	23	9	1	

- Molecule 34 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



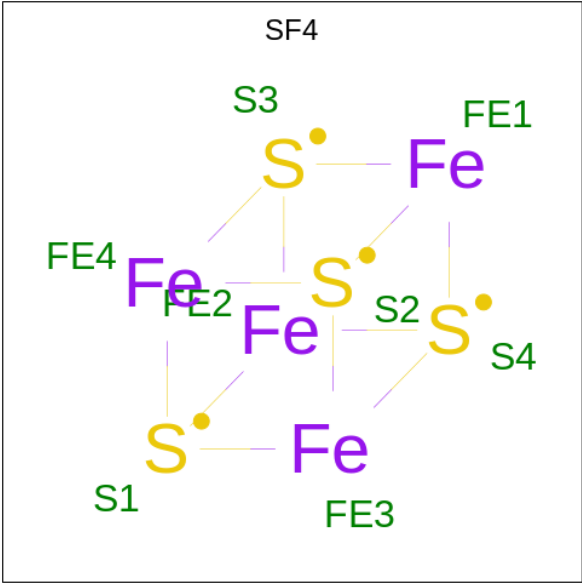
Mol	Chain	Residues	Atoms				AltConf
34	a	1	Total	C	O		0
			33	31	2		
34	b	1	Total	C	O		0
			33	31	2		

- Molecule 35 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},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-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula:  $C_{40}H_{54}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			42	40	2	

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	b	1	Total	Fe	S	0
			8	4	4	
36	c	1	Total	Fe	S	0
			8	4	4	

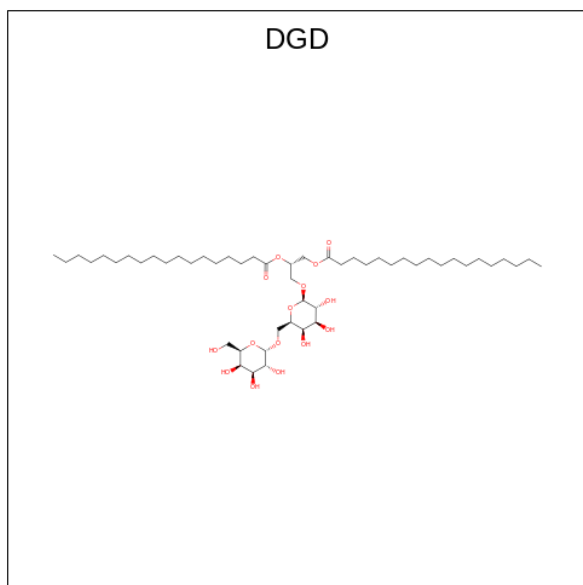
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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
36	c	1	8	4	4	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	b	1	60	45	15	0

### 3 Residue-property plots

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

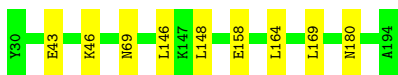
- Molecule 1: Tp-Lhcr18

Chain A:  99%



- Molecule 2: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

Chain B:  95% 5%



- Molecule 3: Fucoxanthin chl a/c light-harvesting protein, major type

Chain C:  98%



- Molecule 4: Tp-RedCAP

Chain E:  100%

There are no outlier residues recorded for this chain.

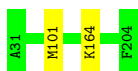
- Molecule 5: Tp-Lhcr20

Chain F:  96%



- Molecule 6: Fucoxanthin chl a/c light-harvesting protein, lhcr type

Chain G:  99%



- Molecule 7: Fucoxanthin chl a/c light-harvesting protein

Chain H: 100%

There are no outlier residues recorded for this chain.

- Molecule 8: Fucoxanthin chl a/c light-harvesting protein

Chain I: 98%



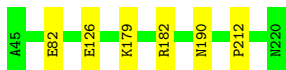
- Molecule 9: Fucoxanthin chl a/c light-harvesting protein

Chain J: 96%



- Molecule 10: Fucoxanthin chlorophyll a/c light-harvesting protein

Chain K: 97%



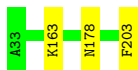
- Molecule 11: Fucoxanthin chlorophyll a/c light-harvesting protein

Chain L: 98%



- Molecule 12: Fucoxanthin chlorophyll a/c light-harvesting protein, lhcr type

Chain M: 98%



- Molecule 13: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 99%



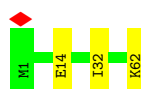
- Molecule 14: Photosystem I reaction center subunit II

Chain d: 98%



- Molecule 15: Photosystem I reaction center subunit IV

Chain e: 95%



- Molecule 16: Photosystem I reaction center subunit III

Chain f: 99%



- Molecule 17: Photosystem I reaction center subunit Psa29

Chain g: 97%



- Molecule 18: Photosystem I reaction center subunit VIII

Chain i: 100%

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem I reaction center subunit IX

Chain j: 92%



- Molecule 20: Photosystem I reaction center subunit XI

Chain l: 99%



- Molecule 21: Photosystem I reaction center subunit XII

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: Tp-PsaR

Chain r:  99%



- Molecule 23: Pt17531-like protein

Chain D:  98%



- Molecule 24: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  99%



- Molecule 25: Photosystem I iron-sulfur center

Chain c:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129097	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.719	Depositor
Minimum map value	-0.472	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.088	Depositor
Map size ( $\text{\AA}$ )	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	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: BCR, SF4, CLA, DD6, LHG, PQN, SQD, LMG, DGD, ET4, KC1, A86

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/1206	0.42	0/1637
2	B	0.34	0/1324	0.39	0/1804
3	C	0.33	0/1339	0.40	0/1813
4	E	0.33	0/1450	0.40	0/1974
5	F	0.33	0/1330	0.42	0/1794
6	G	0.32	0/1348	0.41	0/1815
7	H	0.33	0/1334	0.41	0/1809
8	I	0.35	0/1348	0.43	0/1820
9	J	0.33	0/1426	0.39	0/1931
10	K	0.34	0/1368	0.39	0/1845
11	L	0.29	0/1716	0.39	0/2327
12	M	0.33	0/1345	0.41	0/1823
13	a	0.34	0/6049	0.41	0/8234
14	d	0.32	0/1067	0.41	0/1441
15	e	0.31	0/511	0.40	0/690
16	f	0.33	0/1271	0.42	0/1727
17	g	0.29	0/1003	0.41	0/1354
18	i	0.32	0/264	0.40	0/360
19	j	0.34	0/342	0.50	0/463
20	l	0.35	0/1123	0.44	0/1523
21	m	0.35	0/222	0.38	0/300
22	r	0.31	0/704	0.37	0/957
23	D	0.32	0/1304	0.39	0/1771
24	b	0.33	0/6034	0.41	0/8236
25	c	0.33	0/609	0.44	0/826
All	All	0.33	0/37037	0.41	0/50274

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
14	d	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	d	96	HIS	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
2	B	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
3	C	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
4	E	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
5	F	168/170 (99%)	152 (90%)	15 (9%)	1 (1%)	22	48
6	G	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
7	H	166/168 (99%)	162 (98%)	4 (2%)	0	100	100
8	I	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
9	J	181/183 (99%)	172 (95%)	9 (5%)	0	100	100
10	K	174/176 (99%)	172 (99%)	1 (1%)	1 (1%)	22	48
11	L	215/217 (99%)	211 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
13	a	741/743 (100%)	723 (98%)	18 (2%)	0	100	100
14	d	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
15	e	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
16	f	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
17	g	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
18	i	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
19	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
20	l	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
21	m	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
22	r	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
23	D	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
24	b	730/732 (100%)	713 (98%)	17 (2%)	0	100	100
25	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
All	All	4590/4640 (99%)	4449 (97%)	139 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	192	MET
10	K	212	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	A	122/122 (100%)	121 (99%)	1 (1%)	79	92
2	B	133/133 (100%)	124 (93%)	9 (7%)	13	34
3	C	129/130 (99%)	126 (98%)	3 (2%)	45	75
4	E	144/144 (100%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	133/133 (100%)	127 (96%)	6 (4%)	23	52
6	G	139/139 (100%)	137 (99%)	2 (1%)	62	85
7	H	136/136 (100%)	136 (100%)	0	100	100
8	I	136/136 (100%)	133 (98%)	3 (2%)	47	76
9	J	139/139 (100%)	131 (94%)	8 (6%)	17	42
10	K	134/134 (100%)	129 (96%)	5 (4%)	29	60
11	L	173/173 (100%)	168 (97%)	5 (3%)	37	68
12	M	133/133 (100%)	130 (98%)	3 (2%)	45	75
13	a	603/603 (100%)	597 (99%)	6 (1%)	73	89
14	d	111/111 (100%)	110 (99%)	1 (1%)	75	91
15	e	55/55 (100%)	52 (94%)	3 (6%)	18	44
16	f	132/132 (100%)	130 (98%)	2 (2%)	60	84
17	g	98/98 (100%)	94 (96%)	4 (4%)	26	56
18	i	28/28 (100%)	28 (100%)	0	100	100
19	j	36/36 (100%)	33 (92%)	3 (8%)	9	26
20	l	113/113 (100%)	112 (99%)	1 (1%)	75	91
21	m	22/22 (100%)	22 (100%)	0	100	100
22	r	72/72 (100%)	71 (99%)	1 (1%)	62	85
23	D	128/128 (100%)	124 (97%)	4 (3%)	35	66
24	b	597/597 (100%)	589 (99%)	8 (1%)	65	86
25	c	69/69 (100%)	69 (100%)	0	100	100
All	All	3715/3716 (100%)	3637 (98%)	78 (2%)	49	77

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
2	B	43	GLU
2	B	46	LYS
2	B	69	ASN
2	B	146	LEU
2	B	148	LEU
2	B	158	GLU
2	B	164	LEU
2	B	169	LEU

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Mol	Chain	Res	Type
2	B	180	ASN
3	C	68	LEU
3	C	103	VAL
3	C	201	ASN
5	F	45	MET
5	F	96	GLU
5	F	107	PHE
5	F	127	GLN
5	F	166	LYS
5	F	192	MET
6	G	101	MET
6	G	164	LYS
8	I	144	GLU
8	I	171	MET
8	I	179	CYS
9	J	65	ILE
9	J	111	LYS
9	J	168	LYS
9	J	175	LYS
9	J	176	MET
9	J	177	GLN
9	J	179	LYS
9	J	183	ASN
10	K	82	GLU
10	K	126	GLU
10	K	179	LYS
10	K	182	ARG
10	K	190	ASN
11	L	94	GLU
11	L	185	ARG
11	L	201	LYS
11	L	206	ILE
11	L	216	ASN
12	M	163	LYS
12	M	178	ASN
12	M	203	PHE
13	a	24	THR
13	a	80	GLN
13	a	198	MET
13	a	225	ASN
13	a	278	PHE
13	a	435	ASP

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Mol	Chain	Res	Type
14	d	53	ASN
15	e	14	GLU
15	e	32	ILE
15	e	62	LYS
16	f	139	SER
16	f	178	GLU
17	g	91	TYR
17	g	152	GLU
17	g	158	LEU
17	g	173	LYS
19	j	2	ASN
19	j	25	PHE
19	j	37	LEU
20	l	105	LYS
22	r	113	TYR
23	D	71	ASN
23	D	85	ASN
23	D	96	GLU
23	D	108	LEU
24	b	54	LEU
24	b	112	VAL
24	b	115	THR
24	b	242	VAL
24	b	245	THR
24	b	256	PHE
24	b	515	ASP
24	b	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	18	ASN
1	A	94	HIS
1	A	148	ASN
2	B	52	ASN
2	B	69	ASN
2	B	180	ASN
2	B	181	HIS
3	C	52	ASN
3	C	201	ASN
4	E	213	ASN

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Mol	Chain	Res	Type
5	F	48	ASN
5	F	72	ASN
5	F	155	ASN
5	F	201	HIS
6	G	53	ASN
6	G	91	GLN
6	G	162	GLN
6	G	181	ASN
7	H	91	GLN
7	H	185	GLN
8	I	45	ASN
8	I	112	HIS
8	I	123	GLN
9	J	122	ASN
9	J	183	ASN
10	K	47	ASN
10	K	76	ASN
10	K	220	ASN
11	L	183	ASN
11	L	215	GLN
11	L	216	ASN
12	M	145	GLN
12	M	178	ASN
12	M	192	GLN
13	a	12	ASN
13	a	14	GLN
13	a	134	ASN
13	a	321	ASN
13	a	421	ASN
13	a	478	GLN
13	a	489	ASN
13	a	501	ASN
14	d	53	ASN
14	d	114	ASN
16	f	55	GLN
16	f	171	ASN
19	j	2	ASN
20	l	9	ASN
20	l	33	ASN
23	D	71	ASN
23	D	85	ASN
23	D	179	GLN

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Mol	Chain	Res	Type
24	b	10	GLN
24	b	34	HIS
24	b	89	HIS
24	b	113	ASN
24	b	330	HIS
24	b	451	GLN
24	b	472	GLN
24	b	474	ASN
24	b	626	ASN
24	b	688	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 ⓘ

366 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	$\# Z  > 2$
27	CLA	F	311	5	60,68,73	1.55	7 (11%)	70,107,113	1.40	7 (10%)
32	BCR	b	837	-	41,41,41	0.74	0	56,56,56	2.00	18 (32%)
27	CLA	a	811	13,27	62,70,73	1.51	6 (9%)	72,109,113	1.39	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	E	309	4	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
30	A86	K	307	-	44,50,50	1.33	5 (11%)	51,76,76	2.31	15 (29%)
31	LHG	K	320	-	32,32,48	1.27	7 (21%)	36,37,54	1.15	2 (5%)
26	DD6	G	301	-	39,45,45	2.01	3 (7%)	52,67,67	1.84	12 (23%)
27	CLA	a	855	13	65,73,73	1.45	6 (9%)	76,113,113	1.45	7 (9%)
26	DD6	M	304	-	39,45,45	2.27	6 (15%)	52,67,67	2.72	12 (23%)
30	A86	M	305	-	44,50,50	1.29	4 (9%)	51,76,76	2.14	14 (27%)
27	CLA	D	214	23	56,64,73	1.59	7 (12%)	65,102,113	1.52	7 (10%)
27	CLA	M	319	12	46,54,73	1.72	9 (19%)	53,90,113	1.50	7 (13%)
31	LHG	a	834	27	26,26,48	1.28	5 (19%)	29,32,54	1.20	2 (6%)
26	DD6	K	303	-	39,45,45	2.31	7 (17%)	52,67,67	2.80	20 (38%)
27	CLA	B	310	2	46,54,73	1.77	6 (13%)	53,90,113	1.54	6 (11%)
27	CLA	b	812	24	60,68,73	1.49	10 (16%)	70,107,113	1.51	8 (11%)
27	CLA	b	824	24	58,66,73	1.56	6 (10%)	67,104,113	1.48	8 (11%)
27	CLA	D	209	23	49,57,73	1.71	7 (14%)	55,93,113	1.56	7 (12%)
30	A86	J	316	-	44,50,50	1.35	5 (11%)	51,76,76	3.63	25 (49%)
27	CLA	L	318	11	41,50,73	1.77	8 (19%)	46,85,113	1.63	6 (13%)
30	A86	K	301	-	44,50,50	1.26	3 (6%)	51,76,76	2.19	17 (33%)
28	KC1	F	312	5	48,53,53	1.51	7 (14%)	55,89,89	1.87	8 (14%)
27	CLA	L	319	-	45,53,73	1.76	9 (20%)	52,89,113	1.68	8 (15%)
27	CLA	M	318	12	46,54,73	1.73	10 (21%)	53,90,113	1.58	7 (13%)
31	LHG	E	318	-	48,48,48	1.11	6 (12%)	51,54,54	1.03	3 (5%)
27	CLA	J	307	9	65,73,73	1.46	9 (13%)	76,113,113	1.42	8 (10%)
30	A86	M	302	-	44,50,50	1.51	8 (18%)	51,76,76	3.16	24 (47%)
27	CLA	a	821	13	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
27	CLA	b	845	24	62,70,73	1.50	6 (9%)	72,109,113	1.44	6 (8%)
27	CLA	C	318	3	42,50,73	1.78	10 (23%)	48,85,113	1.60	6 (12%)
32	BCR	l	202	-	41,41,41	0.99	2 (4%)	56,56,56	2.04	16 (28%)
26	DD6	F	303	-	39,45,45	2.04	3 (7%)	52,67,67	2.00	14 (26%)
27	CLA	M	311	-	46,54,73	1.72	10 (21%)	53,90,113	1.63	8 (15%)
29	LMG	L	323	-	46,46,55	1.98	6 (13%)	54,54,63	2.19	8 (14%)
30	A86	K	306	-	44,50,50	1.34	5 (11%)	51,76,76	2.31	19 (37%)
27	CLA	a	828	13	65,73,73	1.52	7 (10%)	76,113,113	1.39	7 (9%)
32	BCR	f	305	-	41,41,41	0.94	1 (2%)	56,56,56	1.94	18 (32%)
30	A86	M	303	-	44,50,50	1.43	5 (11%)	51,76,76	3.79	23 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	b	805	24	45,53,73	1.74	12 (26%)	52,89,113	1.69	8 (15%)
28	KC1	I	312	8	48,53,53	1.78	7 (14%)	55,89,89	1.87	10 (18%)
30	A86	r	202	-	44,50,50	1.51	8 (18%)	51,76,76	3.78	27 (52%)
27	CLA	L	315	11	41,49,73	1.81	10 (24%)	47,84,113	1.56	6 (12%)
27	CLA	D	212	23	42,50,73	1.80	6 (14%)	48,85,113	1.58	6 (12%)
27	CLA	a	820	13	51,59,73	1.64	11 (21%)	59,96,113	1.69	7 (11%)
30	A86	B	302	-	44,50,50	1.61	9 (20%)	51,76,76	3.40	23 (45%)
27	CLA	F	308	-	62,70,73	1.52	6 (9%)	72,109,113	1.42	8 (11%)
27	CLA	D	217	-	41,49,73	1.80	6 (14%)	47,84,113	1.65	8 (17%)
27	CLA	M	315	12	41,49,73	1.83	6 (14%)	47,84,113	1.71	7 (14%)
27	CLA	K	313	10	52,60,73	1.60	9 (17%)	60,97,113	1.63	9 (15%)
27	CLA	D	211	23	46,54,73	1.75	7 (15%)	53,90,113	1.54	6 (11%)
30	A86	m	101	-	44,50,50	1.35	4 (9%)	51,76,76	3.28	25 (49%)
27	CLA	B	312	2	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
30	A86	D	203	-	44,50,50	1.34	4 (9%)	51,76,76	3.59	21 (41%)
27	CLA	b	826	-	45,53,73	1.80	6 (13%)	52,89,113	1.58	7 (13%)
31	LHG	E	316	-	41,41,48	1.00	2 (4%)	44,47,54	1.21	4 (9%)
27	CLA	a	817	13	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
27	CLA	G	311	6	56,64,73	1.57	6 (10%)	65,102,113	1.44	7 (10%)
27	CLA	H	212	7	65,73,73	1.45	11 (16%)	76,113,113	1.53	9 (11%)
27	CLA	K	318	10	46,54,73	1.70	9 (19%)	53,90,113	1.60	8 (15%)
31	LHG	a	801	-	48,48,48	1.10	5 (10%)	51,54,54	0.97	2 (3%)
27	CLA	G	306	-	46,54,73	1.75	6 (13%)	53,90,113	1.57	6 (11%)
27	CLA	F	313	-	41,49,73	1.80	6 (14%)	47,84,113	1.72	8 (17%)
36	SF4	b	802	24	0,12,12	-	-	-	-	-
27	CLA	B	309	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
27	CLA	D	216	23	46,54,73	1.70	10 (21%)	53,90,113	1.55	7 (13%)
27	CLA	b	839	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
27	CLA	b	813	24	59,67,73	1.53	6 (10%)	68,105,113	1.47	7 (10%)
26	DD6	E	307	-	39,45,45	1.99	3 (7%)	52,67,67	1.79	13 (25%)
27	CLA	b	850	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	7 (9%)
27	CLA	B	311	2	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
27	CLA	b	829	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	8 (10%)
27	CLA	H	205	7	65,73,73	1.44	10 (15%)	76,113,113	1.40	9 (11%)
27	CLA	D	208	23	65,73,73	1.48	10 (15%)	76,113,113	1.52	11 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	b	803	24	65,73,73	1.47	6 (9%)	76,113,113	1.39	6 (7%)
27	CLA	E	314	4	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
27	CLA	J	308	9	56,64,73	1.61	6 (10%)	65,102,113	1.45	7 (10%)
27	CLA	L	321	11	45,53,73	1.78	10 (22%)	52,89,113	1.59	8 (15%)
31	LHG	a	802	-	48,48,48	1.07	5 (10%)	51,54,54	0.93	2 (3%)
26	DD6	J	302	-	39,45,45	2.07	2 (5%)	52,67,67	2.34	17 (32%)
32	BCR	m	102	-	41,41,41	0.67	0	56,56,56	2.14	16 (28%)
27	CLA	M	310	-	59,67,73	1.51	10 (16%)	68,105,113	1.44	7 (10%)
27	CLA	A	207	1	65,73,73	1.42	9 (13%)	76,113,113	1.41	8 (10%)
27	CLA	a	809	13	65,73,73	1.47	11 (16%)	76,113,113	1.56	11 (14%)
27	CLA	G	309	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
27	CLA	b	838	24	60,68,73	1.52	10 (16%)	70,107,113	1.55	8 (11%)
36	SF4	c	102	25	0,12,12	-	-	-	-	-
27	CLA	a	812	13	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
26	DD6	G	303	-	39,45,45	2.01	3 (7%)	52,67,67	1.82	14 (26%)
27	CLA	f	302	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
27	CLA	H	204	-	54,62,73	1.61	10 (18%)	62,99,113	1.61	6 (9%)
32	BCR	a	835	-	41,41,41	0.93	1 (2%)	56,56,56	1.93	20 (35%)
27	CLA	b	815	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
27	CLA	J	312	9	65,73,73	1.46	10 (15%)	76,113,113	1.41	7 (9%)
27	CLA	a	841	13	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
28	KC1	H	211	7	48,53,53	1.82	8 (16%)	55,89,89	1.95	11 (20%)
27	CLA	b	830	24	65,73,73	1.47	10 (15%)	76,113,113	1.52	10 (13%)
28	KC1	G	313	6	48,53,53	1.52	7 (14%)	55,89,89	1.86	10 (18%)
27	CLA	J	315	9	49,57,73	1.63	10 (20%)	55,93,113	1.52	7 (12%)
27	CLA	b	842	24	65,73,73	1.49	6 (9%)	76,113,113	1.41	7 (9%)
30	A86	B	305	-	44,50,50	1.50	6 (13%)	51,76,76	3.14	26 (50%)
27	CLA	B	307	2	65,73,73	1.49	7 (10%)	76,113,113	1.37	7 (9%)
30	A86	C	304	-	44,50,50	1.44	5 (11%)	51,76,76	2.68	16 (31%)
27	CLA	a	818	13	45,53,73	1.80	6 (13%)	52,89,113	1.58	6 (11%)
30	A86	K	302	-	44,50,50	1.28	4 (9%)	51,76,76	2.59	19 (37%)
28	KC1	C	308	3	48,53,53	1.51	7 (14%)	55,89,89	1.92	10 (18%)
27	CLA	H	209	-	60,68,73	1.46	10 (16%)	70,107,113	1.59	9 (12%)
30	A86	H	201	-	44,50,50	1.61	9 (20%)	51,76,76	3.40	23 (45%)
32	BCR	a	853	-	41,41,41	0.71	0	56,56,56	2.15	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	A86	A	213	-	44,50,50	1.31	5 (11%)	51,76,76	2.26	18 (35%)
27	CLA	H	208	7	46,54,73	1.76	6 (13%)	53,90,113	1.57	6 (11%)
27	CLA	E	312	4	55,63,73	1.60	6 (10%)	64,101,113	1.51	7 (10%)
30	A86	L	306	-	44,50,50	1.26	3 (6%)	51,76,76	2.15	14 (27%)
27	CLA	I	317	-	46,54,73	1.72	7 (15%)	53,90,113	1.58	6 (11%)
27	CLA	D	210	-	56,64,73	1.57	10 (17%)	65,102,113	1.54	9 (13%)
27	CLA	C	311	3	60,68,73	1.55	9 (15%)	70,107,113	1.45	9 (12%)
29	LMG	J	317	-	51,51,55	1.41	6 (11%)	59,59,63	1.27	7 (11%)
27	CLA	H	213	7	65,73,73	1.44	11 (16%)	76,113,113	1.50	10 (13%)
30	A86	K	305	-	44,50,50	1.28	5 (11%)	51,76,76	2.17	16 (31%)
27	CLA	C	317	-	42,50,73	1.81	10 (23%)	48,85,113	1.69	8 (16%)
30	A86	B	301	-	44,50,50	1.30	4 (9%)	51,76,76	2.80	18 (35%)
27	CLA	a	830	13	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
27	CLA	a	825	13	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
36	SF4	c	101	25	0,12,12	-	-	-	-	-
32	BCR	E	305	-	41,41,41	0.72	0	56,56,56	2.02	16 (28%)
27	CLA	I	316	8	45,53,73	1.71	9 (20%)	52,89,113	1.56	6 (11%)
27	CLA	F	315	5	58,66,73	1.59	6 (10%)	67,104,113	1.41	9 (13%)
29	LMG	M	321	-	42,42,55	1.57	6 (14%)	50,50,63	1.38	5 (10%)
27	CLA	F	309	5	46,54,73	1.68	10 (21%)	53,90,113	1.58	6 (11%)
27	CLA	b	810	24	55,63,73	1.62	7 (12%)	64,101,113	1.47	6 (9%)
27	CLA	A	210	1	46,54,73	1.73	9 (19%)	53,90,113	1.58	7 (13%)
27	CLA	a	813	13	50,58,73	1.65	6 (12%)	58,95,113	1.62	7 (12%)
27	CLA	a	805	13	65,73,73	1.44	11 (16%)	76,113,113	1.59	10 (13%)
27	CLA	K	311	-	52,60,73	1.61	10 (19%)	60,97,113	1.58	9 (15%)
27	CLA	J	309	-	65,73,73	1.45	11 (16%)	76,113,113	1.43	8 (10%)
27	CLA	b	816	24	46,54,73	1.73	6 (13%)	53,90,113	1.62	6 (11%)
27	CLA	b	827	24	60,68,73	1.51	6 (10%)	70,107,113	1.53	7 (10%)
27	CLA	a	838	13	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)
27	CLA	b	820	24	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
27	CLA	l	204	20	65,73,73	1.45	11 (16%)	76,113,113	1.56	9 (11%)
27	CLA	C	310	3	46,54,73	1.66	7 (15%)	53,90,113	1.55	7 (13%)
27	CLA	G	314	-	41,49,73	1.83	5 (12%)	47,84,113	1.70	7 (14%)
32	BCR	b	840	-	41,41,41	1.02	2 (4%)	56,56,56	2.04	21 (37%)
27	CLA	J	314	-	65,73,73	1.46	9 (13%)	76,113,113	1.38	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	b	822	24	50,58,73	1.69	6 (12%)	58,95,113	1.50	8 (13%)
27	CLA	K	316	10	65,73,73	1.45	11 (16%)	76,113,113	1.50	10 (13%)
29	LMG	D	202	-	46,46,55	1.83	5 (10%)	54,54,63	1.36	5 (9%)
27	CLA	G	312	6	61,69,73	1.52	6 (9%)	71,108,113	1.43	7 (9%)
31	LHG	B	315	-	41,41,48	0.98	2 (4%)	44,47,54	1.08	3 (6%)
27	CLA	f	303	16	45,53,73	1.77	6 (13%)	52,89,113	1.60	6 (11%)
27	CLA	I	310	8	47,55,73	1.73	5 (10%)	54,91,113	1.53	7 (12%)
27	CLA	A	205	1	65,73,73	1.43	9 (13%)	76,113,113	1.42	9 (11%)
27	CLA	B	306	2	58,65,73	1.53	9 (15%)	67,102,113	1.38	5 (7%)
27	CLA	I	306	8	65,73,73	1.47	7 (10%)	76,113,113	1.36	7 (9%)
34	PQN	a	831	-	34,34,34	1.59	2 (5%)	42,45,45	1.06	2 (4%)
27	CLA	b	849	24	54,62,73	1.61	6 (11%)	62,99,113	1.44	6 (9%)
27	CLA	a	824	13	50,58,73	1.68	6 (12%)	58,95,113	1.56	8 (13%)
27	CLA	B	308	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
27	CLA	a	804	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
27	CLA	b	819	24	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
27	CLA	I	315	-	55,63,73	1.56	10 (18%)	64,101,113	1.52	8 (12%)
27	CLA	C	307	3	65,73,73	1.44	10 (15%)	76,113,113	1.45	9 (11%)
26	DD6	A	201	-	39,45,45	2.18	4 (10%)	52,67,67	2.03	15 (28%)
32	BCR	i	103	-	41,41,41	0.70	0	56,56,56	2.04	13 (23%)
27	CLA	F	306	5	55,63,73	1.62	6 (10%)	64,101,113	1.43	9 (14%)
27	CLA	F	314	5	47,55,73	1.75	6 (12%)	54,91,113	1.55	7 (12%)
32	BCR	l	205	-	41,41,41	0.86	0	56,56,56	2.07	15 (26%)
27	CLA	I	309	8	46,54,73	1.74	9 (19%)	53,90,113	1.61	7 (13%)
27	CLA	a	844	-	65,73,73	1.43	11 (16%)	76,113,113	1.50	9 (11%)
28	KC1	L	314	-	48,53,53	1.71	7 (14%)	55,89,89	1.92	12 (21%)
27	CLA	l	203	20	49,57,73	1.66	9 (18%)	55,93,113	1.62	8 (14%)
30	A86	E	301	-	44,50,50	1.45	6 (13%)	51,76,76	2.82	22 (43%)
27	CLA	l	206	-	45,53,73	1.75	6 (13%)	52,89,113	1.63	6 (11%)
27	CLA	b	801	-	65,73,73	1.48	12 (18%)	76,113,113	1.57	8 (10%)
27	CLA	I	305	-	45,53,73	1.74	9 (20%)	52,89,113	1.58	8 (15%)
27	CLA	b	828	24	47,55,73	1.76	7 (14%)	54,91,113	1.55	7 (12%)
32	BCR	b	833	-	41,41,41	0.71	0	56,56,56	1.92	14 (25%)
27	CLA	b	846	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	8 (10%)
27	CLA	a	803	13	65,73,73	1.53	11 (16%)	76,113,113	1.44	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	a	823	13	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)
30	A86	D	204	-	44,50,50	1.54	8 (18%)	51,76,76	3.73	22 (43%)
26	DD6	D	205	-	39,45,45	2.22	7 (17%)	52,67,67	3.22	26 (50%)
27	CLA	a	814	-	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
31	LHG	a	837	-	32,32,48	1.28	5 (15%)	35,38,54	1.17	2 (5%)
30	A86	K	304	27	44,50,50	1.26	3 (6%)	51,76,76	2.32	14 (27%)
37	DGD	b	835	-	61,61,67	0.85	2 (3%)	75,75,81	1.10	4 (5%)
29	LMG	j	103	-	37,37,55	1.58	5 (13%)	45,45,63	3.61	8 (17%)
32	BCR	f	304	-	41,41,41	0.73	0	56,56,56	1.96	16 (28%)
26	DD6	C	303	-	39,45,45	2.20	5 (12%)	52,67,67	2.32	18 (34%)
27	CLA	E	313	4	45,53,73	1.76	11 (24%)	52,89,113	1.62	9 (17%)
27	CLA	L	316	11	56,64,73	1.55	9 (16%)	65,102,113	1.54	8 (12%)
26	DD6	G	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.86	14 (26%)
27	CLA	H	207	7	65,73,73	1.45	10 (15%)	76,113,113	1.51	9 (11%)
27	CLA	a	822	13	65,73,73	1.48	6 (9%)	76,113,113	1.42	8 (10%)
28	KC1	L	322	28	48,53,53	1.82	8 (16%)	55,89,89	1.98	11 (20%)
27	CLA	J	313	-	46,54,73	1.71	10 (21%)	53,90,113	1.58	6 (11%)
29	LMG	a	852	-	33,33,55	1.62	5 (15%)	41,41,63	3.62	8 (19%)
32	BCR	r	203	-	41,41,41	0.70	0	56,56,56	1.76	15 (26%)
27	CLA	a	849	13	65,73,73	1.48	6 (9%)	76,113,113	1.40	6 (7%)
26	DD6	L	303	-	39,45,45	2.24	6 (15%)	52,67,67	2.12	17 (32%)
27	CLA	a	816	13	65,73,73	1.49	7 (10%)	76,113,113	1.37	8 (10%)
26	DD6	I	304	-	39,45,45	2.34	7 (17%)	52,67,67	2.48	18 (34%)
27	CLA	b	843	24	65,73,73	1.48	6 (9%)	76,113,113	1.40	8 (10%)
30	A86	I	303	-	44,50,50	1.44	5 (11%)	51,76,76	3.08	24 (47%)
27	CLA	D	213	23	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
27	CLA	a	810	13	65,73,73	1.49	8 (12%)	76,113,113	1.38	7 (9%)
26	DD6	A	202	-	39,45,45	2.33	6 (15%)	52,67,67	2.70	17 (32%)
31	LHG	b	836	27	48,48,48	1.10	3 (6%)	51,54,54	1.03	3 (5%)
28	KC1	C	313	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
27	CLA	a	845	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	7 (9%)
27	CLA	G	317	6	49,57,73	1.71	5 (10%)	55,93,113	1.56	7 (12%)
26	DD6	L	301	-	39,45,45	2.04	2 (5%)	52,67,67	2.17	18 (34%)
27	CLA	a	854	13	55,63,73	1.60	6 (10%)	64,101,113	1.50	7 (10%)
26	DD6	E	302	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	C	314	3	41,49,73	1.79	10 (24%)	47,84,113	1.64	8 (17%)
26	DD6	M	301	-	39,45,45	2.11	2 (5%)	52,67,67	2.00	15 (28%)
27	CLA	M	313	12	65,73,73	1.45	10 (15%)	76,113,113	1.61	13 (17%)
30	A86	D	206	-	44,50,50	1.46	6 (13%)	51,76,76	3.10	21 (41%)
33	SQD	J	318	-	31,32,54	3.14	8 (25%)	34,36,65	2.92	9 (26%)
27	CLA	I	314	8	49,57,73	1.68	10 (20%)	55,93,113	1.47	7 (12%)
27	CLA	a	848	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	8 (10%)
27	CLA	L	313	11	65,73,73	1.43	10 (15%)	76,113,113	1.45	8 (10%)
29	LMG	C	301	-	31,31,55	1.61	6 (19%)	39,39,63	3.02	7 (17%)
28	KC1	A	209	-	48,53,53	1.60	7 (14%)	55,89,89	1.85	11 (20%)
27	CLA	K	310	10	56,64,73	1.57	10 (17%)	65,102,113	1.61	10 (15%)
27	CLA	b	804	24	65,73,73	1.46	12 (18%)	76,113,113	1.41	9 (11%)
27	CLA	F	317	-	47,55,73	1.64	6 (12%)	54,91,113	1.56	6 (11%)
31	LHG	I	318	-	34,34,48	1.29	5 (14%)	37,40,54	1.13	2 (5%)
30	A86	C	302	-	44,50,50	1.50	6 (13%)	51,76,76	2.99	22 (43%)
27	CLA	K	314	30,10	65,73,73	1.56	8 (12%)	76,113,113	1.82	16 (21%)
27	CLA	A	203	1	61,69,73	1.52	6 (9%)	71,108,113	1.43	6 (8%)
27	CLA	C	312	3	61,69,73	1.52	10 (16%)	71,108,113	1.47	7 (9%)
30	A86	b	848	-	44,50,50	1.42	6 (13%)	51,76,76	2.22	13 (25%)
28	KC1	K	315	10	48,53,53	1.78	8 (16%)	55,89,89	1.87	10 (18%)
26	DD6	B	303	-	39,45,45	2.32	6 (15%)	52,67,67	2.91	20 (38%)
27	CLA	a	839	13	60,68,73	1.53	12 (20%)	70,107,113	1.62	10 (14%)
28	KC1	M	314	-	48,53,53	1.79	8 (16%)	55,89,89	2.03	13 (23%)
27	CLA	A	211	-	39,48,73	1.78	10 (25%)	45,82,113	1.73	8 (17%)
27	CLA	C	315	3	42,50,73	1.84	5 (11%)	48,85,113	1.59	6 (12%)
27	CLA	H	214	7	45,53,73	1.77	5 (11%)	52,89,113	1.61	6 (11%)
27	CLA	a	850	13	56,64,73	1.59	6 (10%)	65,102,113	1.46	6 (9%)
28	KC1	L	320	28	48,53,53	1.51	7 (14%)	55,89,89	1.87	11 (20%)
26	DD6	E	306	-	39,45,45	2.13	3 (7%)	52,67,67	3.02	23 (44%)
27	CLA	F	316	-	41,49,73	1.87	5 (12%)	47,84,113	1.58	9 (19%)
27	CLA	G	307	6	56,64,73	1.59	7 (12%)	65,102,113	1.50	8 (12%)
27	CLA	i	101	-	60,68,73	1.54	6 (10%)	70,107,113	1.42	9 (12%)
32	BCR	b	834	-	41,41,41	0.71	0	56,56,56	3.24	21 (37%)
27	CLA	A	206	1	46,54,73	1.74	5 (10%)	53,90,113	1.54	6 (11%)
31	LHG	a	833	-	48,48,48	1.11	3 (6%)	51,54,54	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	b	831	31	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
27	CLA	b	823	24	65,73,73	1.48	6 (9%)	76,113,113	1.44	6 (7%)
31	LHG	H	215	-	34,34,48	1.12	3 (8%)	37,40,54	0.97	2 (5%)
28	KC1	K	308	-	48,53,53	1.70	7 (14%)	55,89,89	1.99	13 (23%)
30	A86	L	304	-	44,50,50	1.23	4 (9%)	51,76,76	2.46	17 (33%)
27	CLA	b	817	24	55,63,73	1.61	6 (10%)	64,101,113	1.46	7 (10%)
26	DD6	M	306	-	39,45,45	2.36	7 (17%)	52,67,67	2.84	15 (28%)
32	BCR	a	851	-	41,41,41	1.03	2 (4%)	56,56,56	1.82	13 (23%)
27	CLA	I	313	8	41,49,73	1.77	10 (24%)	47,84,113	1.71	9 (19%)
29	LMG	l	201	-	40,40,55	1.23	4 (10%)	48,48,63	1.76	4 (8%)
29	LMG	C	319	27	44,44,55	1.31	7 (15%)	52,52,63	1.86	4 (7%)
27	CLA	b	806	24	65,73,73	1.48	6 (9%)	76,113,113	1.45	6 (7%)
27	CLA	K	317	10	41,49,73	1.81	10 (24%)	47,84,113	1.77	8 (17%)
27	CLA	a	856	-	65,73,73	1.45	11 (16%)	76,113,113	1.54	10 (13%)
27	CLA	F	305	5	61,69,73	1.56	6 (9%)	71,108,113	1.39	7 (9%)
34	PQN	b	832	-	34,34,34	1.58	2 (5%)	42,45,45	1.18	3 (7%)
30	A86	I	301	-	44,50,50	1.44	6 (13%)	51,76,76	2.96	22 (43%)
27	CLA	b	818	24	60,68,73	1.54	7 (11%)	70,107,113	1.41	7 (10%)
32	BCR	E	304	-	41,41,41	0.68	0	56,56,56	1.87	17 (30%)
27	CLA	L	307	-	54,62,73	1.58	10 (18%)	62,99,113	1.49	6 (9%)
29	LMG	I	319	-	37,37,55	2.10	6 (16%)	45,45,63	2.70	4 (8%)
27	CLA	F	310	5	60,68,73	1.55	6 (10%)	70,107,113	1.41	7 (10%)
27	CLA	D	215	-	41,49,73	1.84	6 (14%)	47,84,113	1.67	7 (14%)
26	DD6	H	202	-	39,45,45	2.47	11 (28%)	52,67,67	2.56	20 (38%)
27	CLA	b	807	24	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
27	CLA	a	832	31	52,60,73	1.66	7 (13%)	60,97,113	1.53	7 (11%)
27	CLA	M	307	29	61,69,73	1.47	10 (16%)	71,108,113	1.51	8 (11%)
32	BCR	a	836	-	41,41,41	0.73	0	56,56,56	1.96	14 (25%)
30	A86	B	304	-	44,50,50	1.53	7 (15%)	51,76,76	2.80	18 (35%)
26	DD6	E	303	-	39,45,45	2.53	8 (20%)	52,67,67	3.41	16 (30%)
26	DD6	G	305	-	39,45,45	1.95	3 (7%)	52,67,67	1.92	14 (26%)
27	CLA	B	314	2	41,49,73	1.84	10 (24%)	47,84,113	1.62	8 (17%)
27	CLA	D	207	-	61,69,73	1.52	10 (16%)	71,108,113	1.48	8 (11%)
27	CLA	C	309	-	62,70,73	1.48	10 (16%)	72,109,113	1.59	10 (13%)
30	A86	L	305	-	44,50,50	1.26	3 (6%)	51,76,76	2.01	12 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	DD6	J	305	-	39,45,45	2.21	5 (12%)	52,67,67	2.78	15 (28%)
27	CLA	J	311	9	65,73,73	1.46	9 (13%)	76,113,113	1.37	7 (9%)
27	CLA	a	840	13	65,73,73	1.49	6 (9%)	76,113,113	1.44	7 (9%)
30	A86	L	302	-	44,50,50	1.26	3 (6%)	51,76,76	2.67	16 (31%)
27	CLA	K	312	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	9 (11%)
27	CLA	b	825	-	65,73,73	1.48	10 (15%)	76,113,113	1.57	8 (10%)
27	CLA	I	308	-	65,73,73	1.42	9 (13%)	76,113,113	1.40	8 (10%)
27	CLA	b	808	24	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
27	CLA	A	208	1	54,62,73	1.62	10 (18%)	62,99,113	1.51	7 (11%)
29	LMG	E	317	-	43,43,55	2.06	7 (16%)	51,51,63	1.98	7 (13%)
27	CLA	J	310	9	46,54,73	1.69	8 (17%)	53,90,113	1.53	8 (15%)
32	BCR	j	101	-	41,41,41	0.70	0	56,56,56	2.06	14 (25%)
30	A86	J	301	-	44,50,50	1.36	5 (11%)	51,76,76	2.94	21 (41%)
28	KC1	B	313	-	48,53,53	1.72	8 (16%)	55,89,89	1.98	10 (18%)
27	CLA	a	829	13	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
27	CLA	f	301	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
31	LHG	D	201	-	48,48,48	1.07	4 (8%)	51,54,54	1.03	2 (3%)
27	CLA	L	317	11	45,53,73	1.76	6 (13%)	52,89,113	1.58	6 (11%)
27	CLA	L	311	11	39,48,73	1.83	8 (20%)	45,82,113	1.67	8 (17%)
27	CLA	r	201	22	45,53,73	1.77	6 (13%)	52,89,113	1.58	7 (13%)
26	DD6	J	303	-	39,45,45	2.10	3 (7%)	52,67,67	2.19	14 (26%)
27	CLA	M	317	-	45,53,73	1.72	9 (20%)	52,89,113	1.64	10 (19%)
26	DD6	I	302	-	39,45,45	1.99	3 (7%)	52,67,67	1.75	13 (25%)
27	CLA	M	308	12	60,68,73	1.51	10 (16%)	70,107,113	1.45	9 (12%)
27	CLA	a	806	13,27	55,63,73	1.65	6 (10%)	64,101,113	1.49	8 (12%)
27	CLA	G	316	6	55,63,73	1.63	6 (10%)	64,101,113	1.44	8 (12%)
27	CLA	G	315	6	42,50,73	1.82	6 (14%)	48,85,113	1.61	6 (12%)
27	CLA	a	815	13	65,73,73	1.44	10 (15%)	76,113,113	1.57	12 (15%)
27	CLA	E	311	4	65,73,73	1.47	11 (16%)	76,113,113	1.44	9 (11%)
27	CLA	K	309	10	65,73,73	1.43	10 (15%)	76,113,113	1.47	7 (9%)
27	CLA	M	316	12	54,62,73	1.65	11 (20%)	62,99,113	1.69	11 (17%)
32	BCR	a	847	-	41,41,41	0.97	2 (4%)	56,56,56	1.95	19 (33%)
30	A86	H	203	-	44,50,50	1.46	5 (11%)	51,76,76	2.90	24 (47%)
27	CLA	a	808	13	65,73,73	1.46	6 (9%)	76,113,113	1.39	6 (7%)
30	A86	F	301	-	44,50,50	1.26	4 (9%)	51,76,76	2.69	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LHG	j	102	-	48,48,48	1.10	6 (12%)	51,54,54	0.92	2 (3%)
27	CLA	E	315	-	56,64,73	1.56	6 (10%)	65,102,113	1.52	6 (9%)
30	A86	G	302	-	44,50,50	1.54	6 (13%)	51,76,76	3.69	28 (54%)
32	BCR	i	102	-	41,41,41	0.76	0	56,56,56	1.94	17 (30%)
27	CLA	K	319	10	46,54,73	1.67	10 (21%)	53,90,113	1.52	6 (11%)
27	CLA	b	847	24	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
27	CLA	L	308	11	65,73,73	1.44	10 (15%)	76,113,113	1.40	11 (14%)
35	ET4	l	207	-	41,43,43	1.46	6 (14%)	54,60,60	2.27	19 (35%)
27	CLA	H	206	7	65,73,73	1.43	11 (16%)	76,113,113	1.62	13 (17%)
27	CLA	j	104	19	41,49,73	1.84	6 (14%)	47,84,113	1.67	7 (14%)
31	LHG	M	320	-	46,46,48	1.10	4 (8%)	49,52,54	1.05	3 (6%)
30	A86	F	304	-	44,50,50	1.26	4 (9%)	51,76,76	2.70	20 (39%)
27	CLA	I	307	8	55,63,73	1.56	10 (18%)	64,101,113	1.54	7 (10%)
27	CLA	C	306	29	45,53,73	1.78	6 (13%)	52,89,113	1.59	6 (11%)
27	CLA	H	210	7	57,65,73	1.53	10 (17%)	66,103,113	1.50	7 (10%)
30	A86	J	304	-	44,50,50	1.34	5 (11%)	51,76,76	2.88	21 (41%)
30	A86	C	305	-	44,50,50	1.52	6 (13%)	51,76,76	3.11	24 (47%)
27	CLA	a	819	13	49,57,73	1.70	6 (12%)	55,93,113	1.58	7 (12%)
27	CLA	a	846	13	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
27	CLA	L	310	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	8 (10%)
27	CLA	E	308	4	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
27	CLA	G	310	6	46,54,73	1.76	5 (10%)	53,90,113	1.54	6 (11%)
26	DD6	F	302	-	39,45,45	2.03	2 (5%)	52,67,67	1.99	11 (21%)
27	CLA	b	841	24	61,69,73	1.52	7 (11%)	71,108,113	1.46	8 (11%)
27	CLA	M	309	12	65,73,73	1.44	10 (15%)	76,113,113	1.48	9 (11%)
27	CLA	C	316	3	41,49,73	1.81	10 (24%)	47,84,113	1.68	9 (19%)
27	CLA	b	811	24	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
29	LMG	A	214	27	41,41,55	1.76	7 (17%)	49,49,63	1.59	5 (10%)
27	CLA	a	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	9 (11%)
27	CLA	L	312	11	56,64,73	1.54	9 (16%)	65,102,113	1.47	8 (12%)
27	CLA	F	307	5	59,67,73	1.57	6 (10%)	68,105,113	1.44	6 (8%)
27	CLA	b	814	24	55,63,73	1.61	7 (12%)	64,101,113	1.49	6 (9%)
29	LMG	A	212	-	51,51,55	1.14	5 (9%)	59,59,63	1.58	5 (8%)
27	CLA	b	821	24	65,73,73	1.44	11 (16%)	76,113,113	1.59	9 (11%)
27	CLA	a	826	13	51,59,73	1.64	7 (13%)	59,96,113	1.56	7 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	M	312	12	46,54,73	1.70	10 (21%)	53,90,113	1.65	10 (18%)
32	BCR	j	105	-	41,41,41	0.73	0	56,56,56	2.09	13 (23%)
27	CLA	a	827	13	60,68,73	1.56	11 (18%)	70,107,113	1.55	9 (12%)
27	CLA	G	308	6	54,62,73	1.63	6 (11%)	62,99,113	1.49	7 (11%)
27	CLA	I	311	8	65,73,73	1.39	11 (16%)	76,113,113	1.57	11 (14%)
27	CLA	a	843	-	65,73,73	1.47	10 (15%)	76,113,113	1.47	8 (10%)
27	CLA	E	310	4	46,54,73	1.75	6 (13%)	53,90,113	1.53	7 (13%)
27	CLA	L	309	11	65,73,73	1.48	8 (12%)	76,113,113	1.42	9 (11%)
27	CLA	A	204	1	65,73,73	1.45	10 (15%)	76,113,113	1.50	8 (10%)
28	KC1	J	306	-	48,53,53	1.71	7 (14%)	55,89,89	1.95	12 (21%)
27	CLA	b	809	24	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
27	CLA	b	844	24	65,73,73	1.45	10 (15%)	76,113,113	1.46	7 (9%)
27	CLA	a	807	13	65,73,73	1.45	7 (10%)	76,113,113	1.47	6 (7%)

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
27	CLA	F	311	5	1/1/14/20	13/31/109/115	-
32	BCR	b	837	-	-	5/29/63/63	0/2/2/2
27	CLA	a	811	13,27	1/1/14/20	12/34/112/115	-
27	CLA	E	309	4	1/1/15/20	12/37/115/115	-
30	A86	K	307	-	-	3/34/90/90	1/3/3/3
31	LHG	K	320	-	-	24/34/34/53	-
26	DD6	G	301	-	-	3/26/80/80	0/3/3/3
27	CLA	a	855	13	1/1/15/20	13/37/115/115	-
26	DD6	M	304	-	-	0/26/80/80	0/3/3/3
30	A86	M	305	-	-	6/34/90/90	0/3/3/3
27	CLA	D	214	23	1/1/13/20	9/27/105/115	-
27	CLA	M	319	12	1/1/11/20	7/15/93/115	-
31	LHG	a	834	27	-	12/31/31/53	-
26	DD6	K	303	-	-	6/26/80/80	0/3/3/3
27	CLA	B	310	2	1/1/11/20	4/15/93/115	-
27	CLA	b	812	24	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	824	24	1/1/13/20	11/29/107/115	-
27	CLA	D	209	23	1/1/11/20	9/18/96/115	-
30	A86	J	316	-	-	15/34/90/90	0/3/3/3
27	CLA	L	318	11	1/1/10/20	1/9/87/115	-
30	A86	K	301	-	-	9/34/90/90	0/3/3/3
28	KC1	F	312	5	-	5/15/71/71	-
27	CLA	L	319	-	1/1/11/20	4/13/91/115	-
27	CLA	M	318	12	1/1/11/20	11/15/93/115	-
31	LHG	E	318	-	-	35/53/53/53	-
27	CLA	J	307	9	1/1/15/20	10/37/115/115	-
30	A86	M	302	-	-	5/34/90/90	0/3/3/3
27	CLA	a	821	13	1/1/15/20	4/37/115/115	-
27	CLA	b	845	24	1/1/14/20	10/34/112/115	-
27	CLA	C	318	3	1/1/10/20	5/10/88/115	-
32	BCR	l	202	-	-	6/29/63/63	0/2/2/2
26	DD6	F	303	-	-	5/26/80/80	0/3/3/3
27	CLA	M	311	-	1/1/11/20	7/15/93/115	-
29	LMG	L	323	-	-	23/41/61/70	0/1/1/1
30	A86	K	306	-	-	5/34/90/90	0/3/3/3
27	CLA	a	828	13	1/1/15/20	12/37/115/115	-
32	BCR	f	305	-	-	9/29/63/63	0/2/2/2
30	A86	M	303	-	-	11/34/90/90	0/3/3/3
27	CLA	b	805	24	1/1/11/20	3/13/91/115	-
28	KC1	I	312	8	-	6/15/71/71	-
30	A86	r	202	-	-	5/34/90/90	0/3/3/3
27	CLA	L	315	11	1/1/10/20	6/8/86/115	-
27	CLA	D	212	23	1/1/10/20	1/10/88/115	-
27	CLA	a	820	13	1/1/12/20	5/21/99/115	-
30	A86	B	302	-	-	5/34/90/90	0/3/3/3
27	CLA	F	308	-	1/1/14/20	9/34/112/115	-
27	CLA	D	217	-	1/1/10/20	5/8/86/115	-
27	CLA	M	315	12	1/1/10/20	2/8/86/115	-
27	CLA	K	313	10	1/1/12/20	9/22/100/115	-
27	CLA	D	211	23	1/1/11/20	9/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	A86	m	101	-	-	7/34/90/90	0/3/3/3
27	CLA	B	312	2	1/1/15/20	11/37/115/115	-
30	A86	D	203	-	-	10/34/90/90	0/3/3/3
27	CLA	b	826	-	1/1/11/20	4/13/91/115	-
31	LHG	E	316	-	-	6/46/46/53	-
27	CLA	a	817	13	1/1/15/20	15/37/115/115	-
27	CLA	G	311	6	1/1/13/20	8/27/105/115	-
27	CLA	H	212	7	1/1/15/20	18/37/115/115	-
27	CLA	K	318	10	1/1/11/20	6/15/93/115	-
31	LHG	a	801	-	-	28/53/53/53	-
27	CLA	G	306	-	1/1/11/20	8/15/93/115	-
27	CLA	F	313	-	1/1/10/20	2/8/86/115	-
36	SF4	b	802	24	-	-	0/6/5/5
27	CLA	B	309	-	1/1/15/20	12/37/115/115	-
27	CLA	D	216	23	1/1/11/20	5/15/93/115	-
27	CLA	b	839	-	1/1/15/20	5/37/115/115	-
27	CLA	b	813	24	1/1/13/20	9/30/108/115	-
26	DD6	E	307	-	-	1/26/80/80	0/3/3/3
27	CLA	b	850	-	1/1/15/20	14/37/115/115	-
27	CLA	B	311	2	1/1/15/20	11/37/115/115	-
27	CLA	b	829	-	1/1/15/20	9/37/115/115	-
27	CLA	H	205	7	1/1/15/20	12/37/115/115	-
27	CLA	D	208	23	1/1/15/20	13/37/115/115	-
27	CLA	b	803	24	1/1/15/20	12/37/115/115	-
27	CLA	E	314	4	1/1/15/20	10/37/115/115	-
27	CLA	J	308	9	1/1/13/20	7/27/105/115	-
27	CLA	L	321	11	1/1/11/20	6/13/91/115	-
31	LHG	a	802	-	-	33/53/53/53	-
26	DD6	J	302	-	-	10/26/80/80	0/3/3/3
32	BCR	m	102	-	-	7/29/63/63	0/2/2/2
27	CLA	M	310	-	1/1/13/20	14/30/108/115	-
27	CLA	A	207	1	1/1/15/20	18/37/115/115	-
27	CLA	a	809	13	1/1/15/20	9/37/115/115	-
27	CLA	G	309	-	1/1/15/20	26/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	838	24	1/1/14/20	14/31/109/115	-
36	SF4	c	102	25	-	-	0/6/5/5
27	CLA	a	812	13	1/1/15/20	7/37/115/115	-
26	DD6	G	303	-	-	0/26/80/80	0/3/3/3
27	CLA	f	302	-	1/1/15/20	10/37/115/115	-
27	CLA	H	204	-	1/1/12/20	10/24/102/115	-
32	BCR	a	835	-	-	0/29/63/63	0/2/2/2
27	CLA	b	815	-	1/1/15/20	11/37/115/115	-
27	CLA	J	312	9	1/1/15/20	17/37/115/115	-
27	CLA	a	841	13	1/1/15/20	9/37/115/115	-
28	KC1	H	211	7	-	9/15/71/71	-
27	CLA	b	830	24	1/1/15/20	14/37/115/115	-
28	KC1	G	313	6	-	5/15/71/71	-
27	CLA	J	315	9	1/1/11/20	11/18/96/115	-
27	CLA	b	842	24	1/1/15/20	9/37/115/115	-
30	A86	B	305	-	-	4/34/90/90	0/3/3/3
27	CLA	B	307	2	1/1/15/20	7/37/115/115	-
30	A86	C	304	-	-	3/34/90/90	0/3/3/3
27	CLA	a	818	13	1/1/11/20	7/13/91/115	-
30	A86	K	302	-	-	8/34/90/90	0/3/3/3
28	KC1	C	308	3	-	7/15/71/71	-
27	CLA	H	209	-	1/1/14/20	9/31/109/115	-
30	A86	H	201	-	-	5/34/90/90	0/3/3/3
32	BCR	a	853	-	-	8/29/63/63	0/2/2/2
30	A86	A	213	-	-	4/34/90/90	0/3/3/3
27	CLA	H	208	7	1/1/11/20	8/15/93/115	-
27	CLA	E	312	4	1/1/13/20	9/25/103/115	-
30	A86	L	306	-	-	6/34/90/90	0/3/3/3
27	CLA	I	317	-	1/1/11/20	7/15/93/115	-
27	CLA	D	210	-	1/1/13/20	6/27/105/115	-
27	CLA	C	311	3	1/1/14/20	12/31/109/115	-
29	LMG	J	317	-	-	26/46/66/70	0/1/1/1
27	CLA	H	213	7	1/1/15/20	15/37/115/115	-
30	A86	K	305	-	-	3/34/90/90	0/3/3/3
27	CLA	C	317	-	1/1/10/20	8/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	A86	B	301	-	-	12/34/90/90	0/3/3/3
27	CLA	a	830	13	1/1/15/20	11/37/115/115	-
27	CLA	a	825	13	1/1/11/20	9/13/91/115	-
36	SF4	c	101	25	-	-	0/6/5/5
32	BCR	E	305	-	-	0/29/63/63	0/2/2/2
27	CLA	I	316	8	1/1/11/20	4/13/91/115	-
27	CLA	F	315	5	1/1/13/20	16/29/107/115	-
29	LMG	M	321	-	-	15/37/57/70	0/1/1/1
27	CLA	F	309	5	1/1/11/20	2/15/93/115	-
27	CLA	b	810	24	1/1/13/20	3/25/103/115	-
27	CLA	A	210	1	1/1/11/20	4/15/93/115	-
27	CLA	a	813	13	1/1/12/20	8/19/97/115	-
27	CLA	a	805	13	1/1/15/20	13/37/115/115	-
27	CLA	K	311	-	1/1/12/20	13/22/100/115	-
27	CLA	J	309	-	1/1/15/20	21/37/115/115	-
27	CLA	b	816	24	1/1/11/20	5/15/93/115	-
27	CLA	b	827	24	1/1/14/20	8/31/109/115	-
27	CLA	a	838	13	1/1/15/20	13/37/115/115	-
27	CLA	b	820	24	1/1/15/20	14/37/115/115	-
27	CLA	l	204	20	1/1/15/20	16/37/115/115	-
27	CLA	C	310	3	1/1/11/20	6/15/93/115	-
27	CLA	G	314	-	1/1/10/20	3/8/86/115	-
32	BCR	b	840	-	-	6/29/63/63	0/2/2/2
27	CLA	J	314	-	1/1/15/20	15/37/115/115	-
27	CLA	b	822	24	1/1/12/20	8/19/97/115	-
27	CLA	K	316	10	1/1/15/20	18/37/115/115	-
29	LMG	D	202	-	-	17/41/61/70	0/1/1/1
27	CLA	G	312	6	1/1/14/20	12/33/111/115	-
31	LHG	B	315	-	-	25/46/46/53	-
27	CLA	f	303	16	1/1/11/20	3/13/91/115	-
27	CLA	I	310	8	1/1/11/20	7/16/94/115	-
27	CLA	A	205	1	1/1/15/20	21/37/115/115	-
27	CLA	B	306	2	1/1/12/20	17/27/101/115	-
27	CLA	I	306	8	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PQN	a	831	-	-	2/23/43/43	0/2/2/2
27	CLA	b	849	24	1/1/12/20	8/24/102/115	-
27	CLA	a	824	13	1/1/12/20	5/19/97/115	-
27	CLA	B	308	2	1/1/15/20	11/37/115/115	-
27	CLA	a	804	-	1/1/15/20	10/37/115/115	-
27	CLA	b	819	24	1/1/15/20	9/37/115/115	-
27	CLA	I	315	-	1/1/13/20	11/25/103/115	-
27	CLA	C	307	3	1/1/15/20	7/37/115/115	-
26	DD6	A	201	-	-	7/26/80/80	0/3/3/3
32	BCR	i	103	-	-	4/29/63/63	0/2/2/2
27	CLA	F	306	5	1/1/13/20	10/25/103/115	-
27	CLA	F	314	5	1/1/11/20	3/16/94/115	-
32	BCR	l	205	-	-	8/29/63/63	0/2/2/2
27	CLA	I	309	8	1/1/11/20	8/15/93/115	-
27	CLA	a	844	-	1/1/15/20	10/37/115/115	-
28	KC1	L	314	-	-	11/15/71/71	-
27	CLA	l	203	20	1/1/11/20	8/18/96/115	-
30	A86	E	301	-	-	5/34/90/90	0/3/3/3
27	CLA	l	206	-	1/1/11/20	4/13/91/115	-
27	CLA	b	801	-	1/1/15/20	9/37/115/115	-
27	CLA	I	305	-	1/1/11/20	5/13/91/115	-
27	CLA	b	828	24	1/1/11/20	5/16/94/115	-
32	BCR	b	833	-	-	0/29/63/63	0/2/2/2
27	CLA	b	846	-	1/1/15/20	12/37/115/115	-
27	CLA	a	803	13	1/1/15/20	15/37/115/115	-
27	CLA	a	823	13	1/1/15/20	10/37/115/115	-
30	A86	D	204	-	-	4/34/90/90	0/3/3/3
26	DD6	D	205	-	-	3/26/80/80	0/3/3/3
27	CLA	a	814	-	1/1/11/20	4/13/91/115	-
31	LHG	a	837	-	-	20/36/36/53	-
30	A86	K	304	27	-	3/34/90/90	0/3/3/3
37	DGD	b	835	-	-	27/49/89/95	0/2/2/2
29	LMG	j	103	-	-	16/32/52/70	0/1/1/1
32	BCR	f	304	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	C	303	-	-	5/26/80/80	0/3/3/3
27	CLA	E	313	4	1/1/11/20	3/13/91/115	-
27	CLA	L	316	11	1/1/13/20	17/27/105/115	-
26	DD6	G	304	-	-	0/26/80/80	0/3/3/3
27	CLA	H	207	7	1/1/15/20	10/37/115/115	-
27	CLA	a	822	13	1/1/15/20	9/37/115/115	-
28	KC1	L	322	28	-	8/15/71/71	-
27	CLA	J	313	-	1/1/11/20	10/15/93/115	-
29	LMG	a	852	-	-	16/28/48/70	0/1/1/1
32	BCR	r	203	-	-	4/29/63/63	0/2/2/2
27	CLA	a	849	13	1/1/15/20	13/37/115/115	-
26	DD6	L	303	-	-	0/26/80/80	0/3/3/3
27	CLA	a	816	13	1/1/15/20	7/37/115/115	-
26	DD6	I	304	-	-	3/26/80/80	0/3/3/3
27	CLA	b	843	24	1/1/15/20	14/37/115/115	-
30	A86	I	303	-	-	5/34/90/90	0/3/3/3
27	CLA	D	213	23	1/1/15/20	8/37/115/115	-
27	CLA	a	810	13	1/1/15/20	10/37/115/115	-
26	DD6	A	202	-	-	3/26/80/80	0/3/3/3
31	LHG	b	836	27	-	32/53/53/53	-
28	KC1	C	313	-	-	7/15/71/71	-
27	CLA	a	845	-	1/1/15/20	12/37/115/115	-
27	CLA	G	317	6	1/1/11/20	7/18/96/115	-
26	DD6	L	301	-	-	8/26/80/80	0/3/3/3
27	CLA	a	854	13	1/1/13/20	10/25/103/115	-
26	DD6	E	302	-	-	3/26/80/80	0/3/3/3
27	CLA	C	314	3	1/1/10/20	4/8/86/115	-
26	DD6	M	301	-	-	2/26/80/80	0/3/3/3
27	CLA	M	313	12	1/1/15/20	21/37/115/115	-
30	A86	D	206	-	-	6/34/90/90	0/3/3/3
33	SQD	J	318	-	-	18/33/33/69	-
27	CLA	I	314	8	1/1/11/20	7/18/96/115	-
27	CLA	a	848	-	1/1/15/20	8/37/115/115	-
27	CLA	L	313	11	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	C	301	-	-	14/26/46/70	0/1/1/1
28	KC1	A	209	-	-	9/15/71/71	-
27	CLA	K	310	10	1/1/13/20	16/27/105/115	-
27	CLA	b	804	24	1/1/15/20	16/37/115/115	-
27	CLA	F	317	-	1/1/11/20	8/16/94/115	-
31	LHG	I	318	-	-	15/39/39/53	-
30	A86	C	302	-	-	5/34/90/90	0/3/3/3
27	CLA	K	314	30,10	1/1/15/20	20/37/115/115	-
27	CLA	A	203	1	1/1/14/20	3/33/111/115	-
27	CLA	C	312	3	1/1/14/20	10/33/111/115	-
30	A86	b	848	-	-	16/34/90/90	0/3/3/3
28	KC1	K	315	10	-	5/15/71/71	-
26	DD6	B	303	-	-	0/26/80/80	0/3/3/3
27	CLA	a	839	13	1/1/14/20	14/31/109/115	-
28	KC1	M	314	-	-	7/15/71/71	-
27	CLA	A	211	-	1/1/9/20	4/8/82/115	-
27	CLA	C	315	3	1/1/10/20	4/10/88/115	-
27	CLA	H	214	7	1/1/11/20	4/13/91/115	-
27	CLA	a	850	13	1/1/13/20	9/27/105/115	-
28	KC1	L	320	28	-	6/15/71/71	-
27	CLA	F	316	-	1/1/10/20	4/8/86/115	-
26	DD6	E	306	-	-	10/26/80/80	0/3/3/3
27	CLA	G	307	6	1/1/13/20	6/27/105/115	-
27	CLA	i	101	-	1/1/14/20	11/31/109/115	-
32	BCR	b	834	-	-	6/29/63/63	0/2/2/2
27	CLA	A	206	1	1/1/11/20	4/15/93/115	-
31	LHG	a	833	-	-	26/53/53/53	-
27	CLA	b	831	31	1/1/15/20	7/37/115/115	-
27	CLA	b	823	24	1/1/15/20	18/37/115/115	-
31	LHG	H	215	-	-	19/38/38/53	-
28	KC1	K	308	-	-	8/15/71/71	-
30	A86	L	304	-	-	6/34/90/90	0/3/3/3
27	CLA	b	817	24	1/1/13/20	3/25/103/115	-
26	DD6	M	306	-	-	2/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	a	851	-	-	4/29/63/63	0/2/2/2
27	CLA	I	313	8	1/1/10/20	8/8/86/115	-
29	LMG	l	201	-	-	16/35/55/70	0/1/1/1
29	LMG	C	319	27	-	19/39/59/70	0/1/1/1
27	CLA	b	806	24	1/1/15/20	13/37/115/115	-
27	CLA	K	317	10	1/1/10/20	5/8/86/115	-
27	CLA	a	856	-	1/1/15/20	16/37/115/115	-
27	CLA	F	305	5	1/1/14/20	12/33/111/115	-
34	PQN	b	832	-	-	3/23/43/43	0/2/2/2
30	A86	I	301	-	-	10/34/90/90	0/3/3/3
27	CLA	b	818	24	1/1/14/20	17/31/109/115	-
32	BCR	E	304	-	-	2/29/63/63	0/2/2/2
27	CLA	L	307	-	1/1/12/20	14/24/102/115	-
29	LMG	I	319	-	-	13/32/52/70	0/1/1/1
27	CLA	F	310	5	1/1/14/20	12/31/109/115	-
27	CLA	D	215	-	1/1/10/20	2/8/86/115	-
26	DD6	H	202	-	-	3/26/80/80	0/3/3/3
27	CLA	b	807	24	1/1/15/20	17/37/115/115	-
27	CLA	a	832	31	1/1/12/20	6/22/100/115	-
27	CLA	M	307	29	1/1/14/20	11/33/111/115	-
32	BCR	a	836	-	-	4/29/63/63	0/2/2/2
30	A86	B	304	-	-	3/34/90/90	0/3/3/3
26	DD6	E	303	-	-	6/26/80/80	0/3/3/3
26	DD6	G	305	-	-	2/26/80/80	0/3/3/3
27	CLA	B	314	2	1/1/10/20	2/8/86/115	-
27	CLA	D	207	-	1/1/14/20	10/33/111/115	-
27	CLA	C	309	-	1/1/14/20	12/34/112/115	-
30	A86	L	305	-	-	7/34/90/90	0/3/3/3
26	DD6	J	305	-	-	2/26/80/80	0/3/3/3
27	CLA	J	311	9	1/1/15/20	14/37/115/115	-
27	CLA	a	840	13	1/1/15/20	12/37/115/115	-
30	A86	L	302	-	-	8/34/90/90	0/3/3/3
27	CLA	K	312	-	1/1/15/20	23/37/115/115	-
27	CLA	b	825	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	I	308	-	1/1/15/20	13/37/115/115	-
27	CLA	b	808	24	1/1/15/20	10/37/115/115	-
27	CLA	A	208	1	1/1/12/20	10/24/102/115	-
29	LMG	E	317	-	-	21/38/58/70	0/1/1/1
27	CLA	J	310	9	1/1/11/20	9/15/93/115	-
32	BCR	j	101	-	-	4/29/63/63	0/2/2/2
30	A86	J	301	-	-	7/34/90/90	0/3/3/3
28	KC1	B	313	-	-	8/15/71/71	-
27	CLA	a	829	13	1/1/15/20	10/37/115/115	-
27	CLA	f	301	-	1/1/15/20	10/37/115/115	-
31	LHG	D	201	-	-	32/53/53/53	-
27	CLA	L	317	11	1/1/11/20	5/13/91/115	-
27	CLA	L	311	11	1/1/9/20	6/8/82/115	-
27	CLA	r	201	22	1/1/11/20	12/13/91/115	-
26	DD6	J	303	-	-	4/26/80/80	0/3/3/3
27	CLA	M	317	-	-	7/13/91/115	-
26	DD6	I	302	-	-	1/26/80/80	0/3/3/3
27	CLA	M	308	12	1/1/14/20	13/31/109/115	-
27	CLA	a	806	13,27	1/1/13/20	6/25/103/115	-
27	CLA	G	316	6	1/1/13/20	7/25/103/115	-
27	CLA	G	315	6	1/1/10/20	4/10/88/115	-
27	CLA	a	815	13	1/1/15/20	24/37/115/115	-
27	CLA	E	311	4	1/1/15/20	11/37/115/115	-
27	CLA	K	309	10	1/1/15/20	17/37/115/115	-
27	CLA	M	316	12	1/1/12/20	8/24/102/115	-
32	BCR	a	847	-	-	2/29/63/63	0/2/2/2
30	A86	H	203	-	-	4/34/90/90	0/3/3/3
27	CLA	a	808	13	1/1/15/20	13/37/115/115	-
30	A86	F	301	-	-	9/34/90/90	0/3/3/3
31	LHG	j	102	-	-	20/53/53/53	-
27	CLA	E	315	-	1/1/13/20	7/27/105/115	-
30	A86	G	302	-	-	14/34/90/90	0/3/3/3
32	BCR	i	102	-	-	0/29/63/63	0/2/2/2
27	CLA	K	319	10	1/1/11/20	7/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	847	24	1/1/15/20	12/37/115/115	-
27	CLA	L	308	11	1/1/15/20	10/37/115/115	-
35	ET4	l	207	-	-	3/25/67/67	0/2/2/2
27	CLA	H	206	7	1/1/15/20	15/37/115/115	-
27	CLA	j	104	19	1/1/10/20	2/8/86/115	-
31	LHG	M	320	-	-	30/51/51/53	-
30	A86	F	304	-	-	5/34/90/90	0/3/3/3
27	CLA	I	307	8	1/1/13/20	8/25/103/115	-
27	CLA	C	306	29	1/1/11/20	4/13/91/115	-
27	CLA	H	210	7	1/1/13/20	8/28/106/115	-
30	A86	J	304	-	-	4/34/90/90	0/3/3/3
30	A86	C	305	-	-	4/34/90/90	0/3/3/3
27	CLA	a	819	13	1/1/11/20	10/18/96/115	-
27	CLA	a	846	13	1/1/15/20	17/37/115/115	-
27	CLA	L	310	-	1/1/15/20	15/37/115/115	-
27	CLA	E	308	4	1/1/15/20	14/37/115/115	-
27	CLA	G	310	6	1/1/11/20	6/15/93/115	-
26	DD6	F	302	-	-	1/26/80/80	0/3/3/3
27	CLA	b	841	24	1/1/14/20	10/33/111/115	-
27	CLA	M	309	12	1/1/15/20	13/37/115/115	-
27	CLA	C	316	3	1/1/10/20	3/8/86/115	-
27	CLA	b	811	24	1/1/15/20	10/37/115/115	-
29	LMG	A	214	27	-	28/36/56/70	0/1/1/1
27	CLA	a	842	-	1/1/15/20	13/37/115/115	-
27	CLA	L	312	11	1/1/13/20	8/27/105/115	-
27	CLA	F	307	5	1/1/13/20	9/30/108/115	-
27	CLA	b	814	24	1/1/13/20	12/25/103/115	-
29	LMG	A	212	-	-	24/46/66/70	0/1/1/1
27	CLA	b	821	24	1/1/15/20	17/37/115/115	-
27	CLA	a	826	13	1/1/12/20	10/21/99/115	-
27	CLA	M	312	12	1/1/11/20	7/15/93/115	-
32	BCR	j	105	-	-	5/29/63/63	0/2/2/2
27	CLA	a	827	13	1/1/14/20	14/31/109/115	-
27	CLA	G	308	6	1/1/12/20	9/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	I	311	8	1/1/15/20	21/37/115/115	-
27	CLA	a	843	-	1/1/15/20	21/37/115/115	-
27	CLA	E	310	4	1/1/11/20	6/15/93/115	-
27	CLA	L	309	11	1/1/15/20	17/37/115/115	-
27	CLA	A	204	1	1/1/15/20	17/37/115/115	-
28	KC1	J	306	-	-	6/15/71/71	-
27	CLA	b	809	24	1/1/15/20	10/37/115/115	-
27	CLA	b	844	24	1/1/15/20	17/37/115/115	-
27	CLA	a	807	13	1/1/15/20	15/37/115/115	-

All (2405) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	318	SQD	C6-S	-12.45	1.59	1.77
29	L	323	LMG	O6-C1	10.89	1.69	1.41
29	E	317	LMG	O2-C2	-10.76	1.17	1.43
29	I	319	LMG	O2-C2	-10.03	1.19	1.43
29	D	202	LMG	O2-C2	-9.32	1.21	1.43
26	H	202	DD6	C29-C27	-9.17	1.24	1.42
26	C	303	DD6	C29-C27	-9.14	1.25	1.42
26	A	201	DD6	C29-C27	-9.12	1.25	1.42
26	E	303	DD6	C29-C27	-9.06	1.25	1.42
26	I	304	DD6	C29-C27	-8.97	1.25	1.42
26	A	202	DD6	C29-C27	-8.88	1.25	1.42
26	E	306	DD6	C29-C27	-8.87	1.25	1.42
26	M	306	DD6	C29-C27	-8.81	1.25	1.42
26	J	302	DD6	C29-C27	-8.79	1.25	1.42
26	M	301	DD6	C29-C27	-8.73	1.25	1.42
26	G	304	DD6	C29-C27	-8.71	1.25	1.42
26	G	301	DD6	C29-C27	-8.67	1.25	1.42
26	F	302	DD6	C29-C27	-8.66	1.25	1.42
26	L	301	DD6	C29-C27	-8.64	1.25	1.42
26	G	303	DD6	C29-C27	-8.64	1.25	1.42
26	E	302	DD6	C29-C27	-8.63	1.25	1.42
26	E	307	DD6	C29-C27	-8.61	1.26	1.42
26	F	303	DD6	C29-C27	-8.60	1.26	1.42
26	J	303	DD6	C29-C27	-8.58	1.26	1.42
26	J	305	DD6	C29-C27	-8.55	1.26	1.42
26	L	303	DD6	C29-C27	-8.49	1.26	1.42
26	I	302	DD6	C29-C27	-8.40	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	303	DD6	C29-C27	-8.35	1.26	1.42
26	A	202	DD6	C30-C31	-8.33	1.24	1.42
26	A	201	DD6	C30-C31	-8.29	1.25	1.42
26	E	306	DD6	C30-C31	-8.29	1.25	1.42
26	E	303	DD6	C30-C31	-8.28	1.25	1.42
26	M	304	DD6	C29-C27	-8.27	1.26	1.42
26	C	303	DD6	C30-C31	-8.25	1.25	1.42
26	B	303	DD6	C29-C27	-8.21	1.26	1.42
26	G	305	DD6	C29-C27	-8.11	1.26	1.42
26	I	304	DD6	C30-C31	-8.09	1.25	1.42
26	J	302	DD6	C30-C31	-7.99	1.25	1.42
26	J	305	DD6	C30-C31	-7.97	1.25	1.42
26	M	306	DD6	C30-C31	-7.96	1.25	1.42
26	F	303	DD6	C30-C31	-7.95	1.25	1.42
26	M	301	DD6	C30-C31	-7.95	1.25	1.42
28	L	322	KC1	C4D-CHA	-7.94	1.35	1.45
26	M	304	DD6	C30-C31	-7.93	1.25	1.42
28	K	315	KC1	C4D-CHA	-7.91	1.35	1.45
26	L	301	DD6	C30-C31	-7.91	1.25	1.42
26	J	303	DD6	C30-C31	-7.91	1.25	1.42
26	D	205	DD6	C29-C27	-7.88	1.27	1.42
26	L	303	DD6	C30-C31	-7.87	1.25	1.42
26	B	303	DD6	C30-C31	-7.84	1.26	1.42
26	F	302	DD6	C30-C31	-7.83	1.26	1.42
26	H	202	DD6	C30-C31	-7.82	1.26	1.42
26	G	304	DD6	C30-C31	-7.82	1.26	1.42
27	a	806	CLA	C4B-NB	7.81	1.42	1.35
26	G	303	DD6	C30-C31	-7.77	1.26	1.42
26	G	305	DD6	C30-C31	-7.77	1.26	1.42
27	a	828	CLA	C4B-NB	7.77	1.42	1.35
26	I	302	DD6	C30-C31	-7.77	1.26	1.42
29	A	214	LMG	O2-C2	-7.76	1.24	1.43
26	G	301	DD6	C30-C31	-7.75	1.26	1.42
26	E	302	DD6	C30-C31	-7.71	1.26	1.42
28	I	312	KC1	C4D-CHA	-7.70	1.35	1.45
34	a	831	PQN	C3-C2	7.69	1.49	1.35
26	E	307	DD6	C30-C31	-7.68	1.26	1.42
27	F	305	CLA	C4B-NB	7.64	1.42	1.35
27	G	316	CLA	C4B-NB	7.62	1.42	1.35
27	b	828	CLA	C4B-NB	7.62	1.42	1.35
27	B	311	CLA	C4B-NB	7.56	1.42	1.35
27	a	818	CLA	C4B-NB	7.56	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	832	PQN	C3-C2	7.56	1.49	1.35
27	C	315	CLA	C4B-NB	7.56	1.42	1.35
26	K	303	DD6	C30-C31	-7.54	1.26	1.42
28	H	211	KC1	C4D-CHA	-7.53	1.35	1.45
27	b	826	CLA	C4B-NB	7.53	1.41	1.35
27	F	316	CLA	C4B-NB	7.53	1.41	1.35
27	b	823	CLA	C4B-NB	7.51	1.41	1.35
27	G	317	CLA	C4B-NB	7.51	1.41	1.35
27	b	842	CLA	C4B-NB	7.51	1.41	1.35
27	a	840	CLA	C4B-NB	7.51	1.41	1.35
27	B	310	CLA	C4B-NB	7.51	1.41	1.35
27	J	308	CLA	C4B-NB	7.50	1.41	1.35
27	F	307	CLA	C4B-NB	7.49	1.41	1.35
27	j	104	CLA	C4B-NB	7.48	1.41	1.35
28	L	314	KC1	C4D-CHA	-7.48	1.35	1.45
27	F	315	CLA	C4B-NB	7.47	1.41	1.35
27	a	829	CLA	C4B-NB	7.47	1.41	1.35
27	b	822	CLA	C4B-NB	7.47	1.41	1.35
27	a	823	CLA	C4B-NB	7.46	1.41	1.35
27	H	208	CLA	C4B-NB	7.46	1.41	1.35
28	M	314	KC1	C4D-CHA	-7.46	1.35	1.45
27	F	314	CLA	C4B-NB	7.45	1.41	1.35
27	G	310	CLA	C4B-NB	7.45	1.41	1.35
27	F	311	CLA	C4B-NB	7.44	1.41	1.35
27	G	315	CLA	C4B-NB	7.44	1.41	1.35
27	a	814	CLA	C4B-NB	7.44	1.41	1.35
27	D	215	CLA	C4B-NB	7.44	1.41	1.35
27	F	310	CLA	C4B-NB	7.43	1.41	1.35
27	b	817	CLA	C4B-NB	7.43	1.41	1.35
27	G	308	CLA	C4B-NB	7.42	1.41	1.35
27	a	825	CLA	C4B-NB	7.42	1.41	1.35
27	E	309	CLA	C4B-NB	7.42	1.41	1.35
27	a	810	CLA	C4B-NB	7.42	1.41	1.35
27	b	806	CLA	C4B-NB	7.41	1.41	1.35
27	a	816	CLA	C4B-NB	7.41	1.41	1.35
27	C	306	CLA	C4B-NB	7.40	1.41	1.35
27	D	209	CLA	C4B-NB	7.40	1.41	1.35
27	b	810	CLA	C4B-NB	7.40	1.41	1.35
28	J	306	KC1	C4D-CHA	-7.40	1.35	1.45
27	b	829	CLA	C4B-NB	7.40	1.41	1.35
27	b	850	CLA	C4B-NB	7.40	1.41	1.35
27	F	306	CLA	C4B-NB	7.39	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	830	CLA	C4B-NB	7.39	1.41	1.35
27	D	214	CLA	C4B-NB	7.38	1.41	1.35
27	a	822	CLA	C4B-NB	7.38	1.41	1.35
27	b	847	CLA	C4B-NB	7.37	1.41	1.35
27	D	211	CLA	C4B-NB	7.36	1.41	1.35
27	E	310	CLA	C4B-NB	7.36	1.41	1.35
27	H	214	CLA	C4B-NB	7.35	1.41	1.35
27	b	809	CLA	C4B-NB	7.35	1.41	1.35
27	f	302	CLA	C4B-NB	7.35	1.41	1.35
27	b	824	CLA	C4B-NB	7.35	1.41	1.35
27	b	849	CLA	C4B-NB	7.35	1.41	1.35
28	K	308	KC1	C4D-CHA	-7.34	1.35	1.45
27	a	819	CLA	C4B-NB	7.34	1.41	1.35
27	M	315	CLA	C4B-NB	7.34	1.41	1.35
27	G	306	CLA	C4B-NB	7.34	1.41	1.35
27	a	854	CLA	C4B-NB	7.33	1.41	1.35
27	b	807	CLA	C4B-NB	7.32	1.41	1.35
27	b	803	CLA	C4B-NB	7.32	1.41	1.35
27	b	845	CLA	C4B-NB	7.32	1.41	1.35
28	B	313	KC1	C4D-CHA	-7.32	1.35	1.45
27	I	310	CLA	C4B-NB	7.31	1.41	1.35
27	B	307	CLA	C4B-NB	7.31	1.41	1.35
27	a	832	CLA	C4B-NB	7.31	1.41	1.35
27	G	312	CLA	C4B-NB	7.31	1.41	1.35
27	E	314	CLA	C4B-NB	7.31	1.41	1.35
27	a	850	CLA	C4B-NB	7.30	1.41	1.35
27	A	206	CLA	C4B-NB	7.30	1.41	1.35
27	E	312	CLA	C4B-NB	7.30	1.41	1.35
27	b	819	CLA	C4B-NB	7.30	1.41	1.35
27	F	308	CLA	C4B-NB	7.30	1.41	1.35
27	b	811	CLA	C4B-NB	7.30	1.41	1.35
27	a	849	CLA	C4B-NB	7.29	1.41	1.35
27	a	811	CLA	C4B-NB	7.29	1.41	1.35
27	b	818	CLA	C4B-NB	7.29	1.41	1.35
27	G	314	CLA	C4B-NB	7.29	1.41	1.35
27	G	307	CLA	C4B-NB	7.29	1.41	1.35
27	b	815	CLA	C4B-NB	7.28	1.41	1.35
27	D	212	CLA	C4B-NB	7.28	1.41	1.35
27	b	841	CLA	C4B-NB	7.28	1.41	1.35
27	E	308	CLA	C4B-NB	7.28	1.41	1.35
27	I	306	CLA	C4B-NB	7.27	1.41	1.35
27	a	812	CLA	C4B-NB	7.27	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	807	CLA	C4B-NB	7.26	1.41	1.35
27	B	308	CLA	C4B-NB	7.26	1.41	1.35
27	b	808	CLA	C4B-NB	7.26	1.41	1.35
27	i	101	CLA	C4B-NB	7.26	1.41	1.35
27	D	213	CLA	C4B-NB	7.26	1.41	1.35
27	a	817	CLA	C4B-NB	7.25	1.41	1.35
27	b	843	CLA	C4B-NB	7.25	1.41	1.35
27	f	301	CLA	C4B-NB	7.25	1.41	1.35
27	a	838	CLA	C4B-NB	7.25	1.41	1.35
27	a	824	CLA	C4B-NB	7.24	1.41	1.35
27	G	309	CLA	C4B-NB	7.24	1.41	1.35
27	b	831	CLA	C4B-NB	7.23	1.41	1.35
27	A	203	CLA	C4B-NB	7.23	1.41	1.35
27	b	816	CLA	C4B-NB	7.22	1.41	1.35
27	f	303	CLA	C4B-NB	7.22	1.41	1.35
27	b	820	CLA	C4B-NB	7.22	1.41	1.35
27	a	804	CLA	C4B-NB	7.20	1.41	1.35
27	a	848	CLA	C4B-NB	7.19	1.41	1.35
27	b	846	CLA	C4B-NB	7.19	1.41	1.35
27	a	846	CLA	C4B-NB	7.19	1.41	1.35
27	l	206	CLA	C4B-NB	7.18	1.41	1.35
27	b	839	CLA	C4B-NB	7.18	1.41	1.35
27	r	201	CLA	C4B-NB	7.18	1.41	1.35
27	E	315	CLA	C4B-NB	7.18	1.41	1.35
27	L	317	CLA	C4B-NB	7.18	1.41	1.35
27	a	821	CLA	C4B-NB	7.17	1.41	1.35
27	b	814	CLA	C4B-NB	7.17	1.41	1.35
27	b	813	CLA	C4B-NB	7.16	1.41	1.35
27	a	845	CLA	C4B-NB	7.16	1.41	1.35
27	I	317	CLA	C4B-NB	7.16	1.41	1.35
27	a	808	CLA	C4B-NB	7.14	1.41	1.35
27	B	312	CLA	C4B-NB	7.12	1.41	1.35
27	a	841	CLA	C4B-NB	7.12	1.41	1.35
27	a	813	CLA	C4B-NB	7.11	1.41	1.35
27	a	855	CLA	C4B-NB	7.11	1.41	1.35
27	B	309	CLA	C4B-NB	7.09	1.41	1.35
27	b	827	CLA	C4B-NB	7.07	1.41	1.35
27	a	826	CLA	C4B-NB	7.06	1.41	1.35
27	F	313	CLA	C4B-NB	7.05	1.41	1.35
27	L	319	CLA	C4B-NB	7.01	1.41	1.35
26	D	205	DD6	C30-C31	-7.00	1.27	1.42
27	K	314	CLA	C4B-NB	6.99	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	G	311	CLA	C4B-NB	6.99	1.41	1.35
27	I	309	CLA	C4B-NB	6.97	1.41	1.35
28	A	209	KC1	C4D-CHA	-6.96	1.36	1.45
27	B	314	CLA	C4B-NB	6.93	1.41	1.35
27	J	314	CLA	C4B-NB	6.92	1.41	1.35
27	D	217	CLA	C4B-NB	6.89	1.41	1.35
27	B	306	CLA	C4B-NB	6.84	1.41	1.35
27	J	313	CLA	C4B-NB	6.84	1.41	1.35
27	L	311	CLA	C4B-NB	6.83	1.41	1.35
27	L	309	CLA	C4B-NB	6.82	1.41	1.35
33	J	318	SQD	O9-S	6.78	1.65	1.45
27	J	311	CLA	C4B-NB	6.78	1.41	1.35
27	L	321	CLA	C4B-NB	6.76	1.41	1.35
27	M	319	CLA	C4B-NB	6.76	1.41	1.35
27	L	310	CLA	C4B-NB	6.75	1.41	1.35
27	K	318	CLA	C4B-NB	6.75	1.41	1.35
27	J	312	CLA	C4B-NB	6.73	1.41	1.35
27	A	210	CLA	C4B-NB	6.73	1.41	1.35
27	C	311	CLA	C4B-NB	6.72	1.41	1.35
27	J	307	CLA	C4B-NB	6.72	1.41	1.35
28	C	313	KC1	C4D-CHA	-6.69	1.36	1.45
27	L	307	CLA	C4B-NB	6.67	1.41	1.35
28	L	320	KC1	C4D-CHA	-6.65	1.36	1.45
28	G	313	KC1	C4D-CHA	-6.64	1.36	1.45
27	L	315	CLA	C4B-NB	6.62	1.41	1.35
28	F	312	KC1	C4D-CHA	-6.59	1.36	1.45
27	H	204	CLA	C4B-NB	6.58	1.41	1.35
27	L	316	CLA	C4B-NB	6.57	1.41	1.35
27	J	309	CLA	C4B-NB	6.57	1.41	1.35
27	C	316	CLA	C4B-NB	6.56	1.41	1.35
27	A	208	CLA	C4B-NB	6.55	1.41	1.35
27	K	310	CLA	C4B-NB	6.54	1.41	1.35
27	a	827	CLA	C4B-NB	6.54	1.41	1.35
27	M	318	CLA	C4B-NB	6.53	1.41	1.35
27	L	308	CLA	C4B-NB	6.52	1.41	1.35
28	C	308	KC1	C4D-CHA	-6.51	1.36	1.45
27	M	311	CLA	C4B-NB	6.49	1.41	1.35
27	L	313	CLA	C4B-NB	6.47	1.41	1.35
27	L	318	CLA	C4B-NB	6.46	1.41	1.35
27	F	317	CLA	C4B-NB	6.46	1.41	1.35
27	A	204	CLA	C4B-NB	6.46	1.41	1.35
27	D	207	CLA	C4B-NB	6.41	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	310	CLA	C4B-NB	6.41	1.40	1.35
29	M	321	LMG	O2-C2	6.40	1.58	1.43
27	I	305	CLA	C4B-NB	6.39	1.40	1.35
27	E	313	CLA	C4B-NB	6.38	1.40	1.35
27	C	309	CLA	C4B-NB	6.38	1.40	1.35
27	A	205	CLA	C4B-NB	6.38	1.40	1.35
27	A	211	CLA	C4B-NB	6.37	1.40	1.35
27	J	315	CLA	C4B-NB	6.36	1.40	1.35
27	K	317	CLA	C4B-NB	6.35	1.40	1.35
27	H	207	CLA	C4B-NB	6.35	1.40	1.35
27	I	314	CLA	C4B-NB	6.34	1.40	1.35
27	L	312	CLA	C4B-NB	6.33	1.40	1.35
27	D	210	CLA	C4B-NB	6.32	1.40	1.35
27	C	314	CLA	C4B-NB	6.31	1.40	1.35
27	I	315	CLA	C4B-NB	6.31	1.40	1.35
27	J	310	CLA	C4B-NB	6.31	1.40	1.35
27	H	212	CLA	C4B-NB	6.29	1.40	1.35
27	I	313	CLA	C4B-NB	6.27	1.40	1.35
27	I	308	CLA	C4B-NB	6.26	1.40	1.35
27	F	309	CLA	C4B-NB	6.25	1.40	1.35
27	M	316	CLA	C4B-NB	6.24	1.40	1.35
27	a	843	CLA	C4B-NB	6.22	1.40	1.35
27	K	311	CLA	C4B-NB	6.21	1.40	1.35
27	I	316	CLA	C4B-NB	6.20	1.40	1.35
27	C	312	CLA	C4B-NB	6.20	1.40	1.35
27	K	312	CLA	C4B-NB	6.20	1.40	1.35
27	D	208	CLA	C4B-NB	6.20	1.40	1.35
27	K	316	CLA	C4B-NB	6.17	1.40	1.35
27	b	801	CLA	C4B-NB	6.17	1.40	1.35
29	J	317	LMG	O2-C2	-6.13	1.28	1.43
27	D	216	CLA	C4B-NB	6.12	1.40	1.35
27	I	307	CLA	C4B-NB	6.11	1.40	1.35
33	J	318	SQD	O47-C45	-6.08	1.39	1.46
27	l	203	CLA	C4B-NB	6.08	1.40	1.35
27	C	318	CLA	C4B-NB	6.05	1.40	1.35
27	K	313	CLA	C4B-NB	6.04	1.40	1.35
27	a	842	CLA	C4B-NB	6.04	1.40	1.35
27	a	815	CLA	C4B-NB	6.03	1.40	1.35
27	b	838	CLA	C4B-NB	6.03	1.40	1.35
27	A	207	CLA	C4B-NB	5.99	1.40	1.35
27	M	310	CLA	C4B-NB	5.99	1.40	1.35
27	a	820	CLA	C4B-NB	5.98	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	317	CLA	C4B-NB	5.98	1.40	1.35
27	H	213	CLA	C4B-NB	5.97	1.40	1.35
27	b	844	CLA	C4B-NB	5.96	1.40	1.35
27	b	825	CLA	C4B-NB	5.96	1.40	1.35
27	b	830	CLA	C4B-NB	5.96	1.40	1.35
29	j	103	LMG	O2-C2	-5.95	1.29	1.43
27	M	312	CLA	C4B-NB	5.94	1.40	1.35
27	M	307	CLA	C4B-NB	5.93	1.40	1.35
29	a	852	LMG	O2-C2	-5.93	1.29	1.43
27	M	308	CLA	C4B-NB	5.93	1.40	1.35
27	M	309	CLA	C4B-NB	5.92	1.40	1.35
27	K	309	CLA	C4B-NB	5.90	1.40	1.35
27	M	313	CLA	C4B-NB	5.86	1.40	1.35
27	a	809	CLA	C4B-NB	5.85	1.40	1.35
27	l	204	CLA	C4B-NB	5.85	1.40	1.35
27	H	210	CLA	C4B-NB	5.77	1.40	1.35
27	b	805	CLA	C4B-NB	5.77	1.40	1.35
27	a	805	CLA	C4B-NB	5.77	1.40	1.35
27	H	209	CLA	C4B-NB	5.70	1.40	1.35
27	H	206	CLA	C4B-NB	5.68	1.40	1.35
27	a	844	CLA	C4B-NB	5.66	1.40	1.35
27	b	821	CLA	C4B-NB	5.64	1.40	1.35
27	a	839	CLA	C4B-NB	5.64	1.40	1.35
27	C	307	CLA	C4B-NB	5.64	1.40	1.35
27	K	319	CLA	C4B-NB	5.61	1.40	1.35
27	a	803	CLA	C4B-NB	5.58	1.40	1.35
27	H	205	CLA	C4B-NB	5.57	1.40	1.35
27	E	311	CLA	C4B-NB	5.54	1.40	1.35
27	b	812	CLA	C4B-NB	5.54	1.40	1.35
27	a	856	CLA	C4B-NB	5.49	1.40	1.35
27	C	317	CLA	C4B-NB	5.45	1.40	1.35
28	L	322	KC1	MG-NB	-5.27	1.95	2.05
28	H	211	KC1	MG-NB	-5.18	1.95	2.05
28	I	312	KC1	MG-NB	-5.14	1.95	2.05
28	J	306	KC1	MG-NB	-5.13	1.95	2.05
27	b	804	CLA	C4B-NB	5.13	1.39	1.35
28	M	314	KC1	MG-NB	-5.08	1.95	2.05
28	B	313	KC1	MG-NB	-5.07	1.95	2.05
30	b	848	A86	O4-C38	5.04	1.46	1.35
28	L	314	KC1	MG-NB	-5.04	1.95	2.05
28	K	315	KC1	MG-NB	-5.03	1.95	2.05
28	A	209	KC1	MG-NB	-5.02	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	K	308	KC1	MG-NB	-4.95	1.96	2.05
33	J	318	SQD	O8-S	4.95	1.65	1.47
29	C	301	LMG	O2-C2	4.84	1.54	1.43
30	B	301	A86	O4-C38	4.80	1.46	1.35
30	G	302	A86	O4-C38	4.80	1.46	1.35
27	a	803	CLA	C4D-ND	-4.76	1.31	1.37
27	C	317	CLA	C4D-ND	-4.75	1.31	1.37
34	b	832	PQN	C10-C5	4.74	1.48	1.40
34	a	831	PQN	C10-C5	4.74	1.48	1.40
27	K	314	CLA	C4D-ND	-4.71	1.31	1.37
30	L	306	A86	O4-C38	4.71	1.45	1.35
28	C	308	KC1	MG-NB	-4.71	1.96	2.05
30	m	101	A86	O4-C38	4.69	1.45	1.35
30	L	305	A86	O4-C38	4.67	1.45	1.35
30	E	301	A86	O4-C38	4.66	1.45	1.35
28	G	313	KC1	MG-NB	-4.66	1.96	2.05
28	F	312	KC1	MG-NB	-4.65	1.96	2.05
30	F	301	A86	O4-C38	4.64	1.45	1.35
28	L	320	KC1	MG-NB	-4.64	1.96	2.05
30	K	306	A86	O4-C38	4.64	1.45	1.35
27	I	311	CLA	C4B-NB	4.64	1.39	1.35
30	L	304	A86	O4-C38	4.63	1.45	1.35
30	F	304	A86	O4-C38	4.63	1.45	1.35
28	C	313	KC1	MG-NB	-4.62	1.96	2.05
30	K	302	A86	O4-C38	4.62	1.45	1.35
30	A	213	A86	O4-C38	4.61	1.45	1.35
30	K	301	A86	O4-C38	4.59	1.45	1.35
30	K	307	A86	O4-C38	4.59	1.45	1.35
30	L	302	A86	O4-C38	4.58	1.45	1.35
30	M	305	A86	O4-C38	4.56	1.45	1.35
30	K	304	A86	O4-C38	4.54	1.45	1.35
30	D	203	A86	O4-C38	4.54	1.45	1.35
30	J	316	A86	O4-C38	4.53	1.45	1.35
30	C	305	A86	O4-C38	4.52	1.45	1.35
30	I	301	A86	O4-C38	4.49	1.45	1.35
30	M	302	A86	O4-C38	4.48	1.45	1.35
30	H	203	A86	O4-C38	4.47	1.45	1.35
30	J	304	A86	O4-C38	4.43	1.45	1.35
30	G	302	A86	C32-C31	-4.43	1.47	1.54
30	B	304	A86	O4-C38	4.38	1.45	1.35
30	K	305	A86	O4-C38	4.37	1.45	1.35
30	I	303	A86	O4-C38	4.36	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	303	A86	O4-C38	4.36	1.45	1.35
30	D	204	A86	O4-C38	4.35	1.45	1.35
33	J	318	SQD	O49-C7	4.32	1.40	1.22
30	I	303	A86	C30-C29	-4.25	1.24	1.32
30	D	206	A86	O4-C38	4.25	1.44	1.35
27	I	311	CLA	C4D-ND	-4.24	1.31	1.37
30	J	301	A86	O4-C38	4.24	1.44	1.35
30	C	302	A86	O4-C38	4.23	1.44	1.35
31	B	315	LHG	O8-C23	4.21	1.45	1.33
31	E	316	LHG	O8-C23	4.18	1.45	1.33
30	C	302	A86	C30-C29	-4.18	1.25	1.32
27	K	319	CLA	C4D-ND	-4.17	1.32	1.37
30	H	201	A86	O4-C38	4.16	1.44	1.35
27	b	805	CLA	C4D-ND	-4.15	1.32	1.37
30	J	301	A86	C30-C29	-4.15	1.25	1.32
27	a	820	CLA	C4D-ND	-4.14	1.32	1.37
27	b	825	CLA	C4D-ND	-4.14	1.32	1.37
30	B	302	A86	O4-C38	4.12	1.44	1.35
30	B	302	A86	C30-C29	-4.12	1.25	1.32
27	H	205	CLA	C4D-ND	-4.12	1.32	1.37
30	C	304	A86	C30-C29	-4.12	1.25	1.32
37	b	835	DGD	O1G-C1A	4.10	1.45	1.33
35	l	207	ET4	C08-C07	4.09	1.45	1.33
30	r	202	A86	C30-C29	-4.08	1.25	1.32
27	l	204	CLA	C4D-ND	-4.07	1.32	1.37
30	H	201	A86	C30-C29	-4.07	1.25	1.32
30	C	304	A86	O4-C38	4.06	1.44	1.35
31	E	316	LHG	O7-C7	4.06	1.45	1.34
27	b	812	CLA	C4D-ND	-4.06	1.32	1.37
27	a	839	CLA	C4D-ND	-4.05	1.32	1.37
30	D	204	A86	C30-C29	-4.04	1.25	1.32
30	J	316	A86	C30-C29	-4.03	1.25	1.32
30	K	306	A86	C30-C29	-4.03	1.25	1.32
30	E	301	A86	C30-C29	-4.02	1.25	1.32
27	b	843	CLA	C1D-ND	4.01	1.42	1.37
30	r	202	A86	O4-C38	4.01	1.44	1.35
27	a	842	CLA	C4D-ND	-4.01	1.32	1.37
27	b	838	CLA	C4D-ND	-4.00	1.32	1.37
30	B	305	A86	O4-C38	4.00	1.44	1.35
27	H	213	CLA	C4D-ND	-3.99	1.32	1.37
27	a	809	CLA	C4D-ND	-3.99	1.32	1.37
27	a	840	CLA	C1D-ND	3.98	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	207	CLA	C4D-ND	-3.98	1.32	1.37
27	K	312	CLA	C4D-ND	-3.97	1.32	1.37
37	b	835	DGD	O2G-C1B	3.97	1.45	1.34
27	C	318	CLA	C4D-ND	-3.97	1.32	1.37
27	D	208	CLA	C4D-ND	-3.96	1.32	1.37
30	M	302	A86	C30-C29	-3.96	1.25	1.32
27	D	216	CLA	C4D-ND	-3.94	1.32	1.37
27	H	210	CLA	C4D-ND	-3.94	1.32	1.37
27	b	844	CLA	C4D-ND	-3.93	1.32	1.37
30	J	304	A86	C30-C29	-3.93	1.25	1.32
27	F	314	CLA	C1D-ND	3.93	1.42	1.37
27	a	856	CLA	C4D-ND	-3.93	1.32	1.37
30	C	305	A86	C30-C29	-3.93	1.25	1.32
30	M	305	A86	C30-C29	-3.92	1.25	1.32
27	a	828	CLA	C1D-ND	3.92	1.42	1.37
27	b	819	CLA	C1D-ND	3.92	1.42	1.37
27	C	307	CLA	C4D-ND	-3.92	1.32	1.37
27	b	842	CLA	C1D-ND	3.92	1.42	1.37
30	H	203	A86	C30-C29	-3.92	1.25	1.32
27	a	805	CLA	C4D-ND	-3.92	1.32	1.37
27	A	210	CLA	C4D-ND	-3.92	1.32	1.37
27	F	305	CLA	C1D-ND	3.91	1.42	1.37
27	b	821	CLA	C4D-ND	-3.91	1.32	1.37
30	B	305	A86	C30-C29	-3.91	1.25	1.32
30	D	206	A86	C30-C29	-3.91	1.25	1.32
27	a	846	CLA	C1D-ND	3.91	1.42	1.37
27	a	816	CLA	C1D-ND	3.90	1.42	1.37
27	b	830	CLA	C4D-ND	-3.89	1.32	1.37
27	F	310	CLA	C1D-ND	3.89	1.42	1.37
27	E	311	CLA	C4D-ND	-3.89	1.32	1.37
27	M	316	CLA	C4D-ND	-3.89	1.32	1.37
27	K	309	CLA	C4D-ND	-3.88	1.32	1.37
27	l	203	CLA	C4D-ND	-3.88	1.32	1.37
27	a	827	CLA	C4D-ND	-3.87	1.32	1.37
27	M	308	CLA	C4D-ND	-3.87	1.32	1.37
27	G	310	CLA	C1D-ND	3.87	1.42	1.37
30	B	304	A86	C30-C29	-3.87	1.25	1.32
30	L	305	A86	C30-C29	-3.87	1.25	1.32
27	D	211	CLA	C1D-ND	3.87	1.42	1.37
27	G	314	CLA	C1D-ND	3.86	1.42	1.37
27	b	804	CLA	C4D-ND	-3.86	1.32	1.37
27	M	312	CLA	C4D-ND	-3.86	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	307	CLA	C1D-ND	3.85	1.42	1.37
27	b	810	CLA	C1D-ND	3.85	1.42	1.37
26	E	303	DD6	C21-C20	-3.85	1.45	1.51
27	L	315	CLA	C4D-ND	-3.85	1.32	1.37
27	a	819	CLA	C1D-ND	3.85	1.42	1.37
27	a	826	CLA	C1D-ND	3.85	1.42	1.37
27	F	315	CLA	C1D-ND	3.84	1.42	1.37
27	C	315	CLA	C1D-ND	3.83	1.42	1.37
27	G	315	CLA	C1D-ND	3.83	1.42	1.37
27	C	312	CLA	C4D-ND	-3.83	1.32	1.37
27	f	303	CLA	C1D-ND	3.82	1.42	1.37
27	b	816	CLA	C1D-ND	3.82	1.42	1.37
27	a	823	CLA	C1D-ND	3.82	1.42	1.37
27	b	826	CLA	C1D-ND	3.82	1.42	1.37
27	b	807	CLA	C1D-ND	3.82	1.42	1.37
27	a	815	CLA	C4D-ND	-3.82	1.32	1.37
27	A	208	CLA	C4D-ND	-3.81	1.32	1.37
30	K	305	A86	C30-C29	-3.81	1.25	1.32
27	J	308	CLA	C1D-ND	3.81	1.42	1.37
27	C	311	CLA	C4D-ND	-3.81	1.32	1.37
27	M	315	CLA	C1D-ND	3.81	1.42	1.37
27	a	813	CLA	C1D-ND	3.80	1.42	1.37
27	C	314	CLA	C4D-ND	-3.80	1.32	1.37
27	a	843	CLA	C4D-ND	-3.80	1.32	1.37
27	H	206	CLA	C4D-ND	-3.80	1.32	1.37
27	A	203	CLA	C1D-ND	3.80	1.42	1.37
27	A	206	CLA	C1D-ND	3.80	1.42	1.37
31	B	315	LHG	O7-C7	3.80	1.45	1.34
27	a	808	CLA	C1D-ND	3.80	1.42	1.37
27	a	854	CLA	C1D-ND	3.80	1.42	1.37
27	B	312	CLA	C1D-ND	3.79	1.42	1.37
27	C	306	CLA	C1D-ND	3.79	1.42	1.37
27	a	832	CLA	C1D-ND	3.79	1.42	1.37
27	a	850	CLA	C1D-ND	3.79	1.42	1.37
27	E	312	CLA	C1D-ND	3.79	1.42	1.37
27	M	309	CLA	C4D-ND	-3.79	1.32	1.37
27	G	308	CLA	C1D-ND	3.79	1.42	1.37
27	b	839	CLA	C1D-ND	3.79	1.42	1.37
27	F	311	CLA	C1D-ND	3.79	1.42	1.37
27	b	806	CLA	C1D-ND	3.79	1.42	1.37
27	D	215	CLA	C1D-ND	3.79	1.42	1.37
27	b	824	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	307	CLA	C4D-ND	-3.78	1.32	1.37
27	I	313	CLA	C4D-ND	-3.78	1.32	1.37
27	a	821	CLA	C1D-ND	3.78	1.42	1.37
27	a	855	CLA	C1D-ND	3.78	1.42	1.37
27	M	313	CLA	C4D-ND	-3.78	1.32	1.37
27	b	847	CLA	C1D-ND	3.78	1.42	1.37
27	G	306	CLA	C1D-ND	3.77	1.42	1.37
27	H	208	CLA	C1D-ND	3.77	1.42	1.37
27	r	201	CLA	C1D-ND	3.77	1.42	1.37
27	j	104	CLA	C1D-ND	3.77	1.42	1.37
27	M	310	CLA	C4D-ND	-3.77	1.32	1.37
27	G	317	CLA	C1D-ND	3.77	1.42	1.37
27	a	825	CLA	C1D-ND	3.77	1.42	1.37
27	B	308	CLA	C1D-ND	3.77	1.42	1.37
27	J	309	CLA	C4D-ND	-3.77	1.32	1.37
27	a	818	CLA	C1D-ND	3.77	1.42	1.37
30	A	213	A86	C30-C29	-3.77	1.25	1.32
30	K	302	A86	C30-C29	-3.77	1.25	1.32
27	b	814	CLA	C1D-ND	3.77	1.42	1.37
27	G	311	CLA	C1D-ND	3.77	1.42	1.37
28	I	312	KC1	C4B-NB	-3.77	1.33	1.37
27	G	307	CLA	C1D-ND	3.76	1.42	1.37
27	b	803	CLA	C1D-ND	3.76	1.42	1.37
27	b	828	CLA	C1D-ND	3.76	1.42	1.37
27	a	844	CLA	C4D-ND	-3.76	1.32	1.37
27	a	845	CLA	C1D-ND	3.76	1.42	1.37
27	a	849	CLA	C1D-ND	3.76	1.42	1.37
27	I	310	CLA	C1D-ND	3.76	1.42	1.37
27	a	830	CLA	C1D-ND	3.76	1.42	1.37
30	K	301	A86	C30-C29	-3.75	1.25	1.32
27	b	801	CLA	C4D-ND	-3.75	1.32	1.37
27	D	209	CLA	C1D-ND	3.75	1.42	1.37
30	L	302	A86	C30-C29	-3.75	1.25	1.32
27	b	827	CLA	C1D-ND	3.74	1.42	1.37
27	a	814	CLA	C1D-ND	3.74	1.42	1.37
27	a	824	CLA	C1D-ND	3.74	1.42	1.37
27	E	310	CLA	C1D-ND	3.74	1.42	1.37
27	H	214	CLA	C1D-ND	3.74	1.42	1.37
27	D	214	CLA	C1D-ND	3.74	1.42	1.37
27	E	308	CLA	C1D-ND	3.74	1.42	1.37
27	F	313	CLA	C1D-ND	3.74	1.42	1.37
27	H	212	CLA	C4D-ND	-3.74	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	309	CLA	C1D-ND	3.74	1.42	1.37
27	G	312	CLA	C1D-ND	3.74	1.42	1.37
30	K	307	A86	C30-C29	-3.74	1.25	1.32
26	B	303	DD6	C-C1	-3.74	1.43	1.50
27	b	845	CLA	C1D-ND	3.74	1.42	1.37
27	b	813	CLA	C1D-ND	3.74	1.42	1.37
27	G	309	CLA	C1D-ND	3.73	1.42	1.37
27	F	316	CLA	C1D-ND	3.73	1.42	1.37
27	a	806	CLA	C1D-ND	3.73	1.42	1.37
27	b	808	CLA	C1D-ND	3.73	1.42	1.37
27	L	317	CLA	C1D-ND	3.73	1.42	1.37
27	a	817	CLA	C1D-ND	3.73	1.42	1.37
27	b	846	CLA	C1D-ND	3.73	1.42	1.37
30	I	301	A86	C30-C29	-3.73	1.25	1.32
27	a	811	CLA	C1D-ND	3.73	1.42	1.37
27	a	829	CLA	C1D-ND	3.73	1.42	1.37
27	b	811	CLA	C1D-ND	3.73	1.42	1.37
28	H	211	KC1	C4B-NB	-3.72	1.33	1.37
27	J	310	CLA	C4D-ND	-3.72	1.32	1.37
27	F	306	CLA	C1D-ND	3.72	1.42	1.37
27	a	812	CLA	C1D-ND	3.72	1.42	1.37
27	A	204	CLA	C4D-ND	-3.72	1.32	1.37
30	F	304	A86	C30-C29	-3.72	1.25	1.32
27	E	313	CLA	C4D-ND	-3.71	1.32	1.37
27	b	820	CLA	C1D-ND	3.71	1.42	1.37
27	B	310	CLA	C1D-ND	3.71	1.42	1.37
27	K	311	CLA	C4D-ND	-3.70	1.32	1.37
27	K	310	CLA	C4D-ND	-3.70	1.32	1.37
27	B	309	CLA	C1D-ND	3.70	1.42	1.37
27	H	204	CLA	C4D-ND	-3.70	1.32	1.37
27	I	308	CLA	C4D-ND	-3.70	1.32	1.37
27	F	308	CLA	C1D-ND	3.69	1.42	1.37
27	K	317	CLA	C4D-ND	-3.69	1.32	1.37
27	D	213	CLA	C1D-ND	3.69	1.42	1.37
27	b	817	CLA	C1D-ND	3.69	1.42	1.37
27	a	822	CLA	C1D-ND	3.69	1.42	1.37
27	l	206	CLA	C1D-ND	3.68	1.42	1.37
27	M	307	CLA	C4D-ND	-3.68	1.32	1.37
27	G	316	CLA	C1D-ND	3.68	1.42	1.37
27	b	818	CLA	C1D-ND	3.68	1.42	1.37
27	b	841	CLA	C1D-ND	3.68	1.42	1.37
27	B	307	CLA	C1D-ND	3.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	848	CLA	C1D-ND	3.67	1.42	1.37
27	L	309	CLA	C4D-ND	-3.67	1.32	1.37
27	f	301	CLA	C1D-ND	3.67	1.42	1.37
30	b	848	A86	C30-C29	-3.66	1.25	1.32
27	f	302	CLA	C1D-ND	3.66	1.42	1.37
27	b	815	CLA	C1D-ND	3.66	1.42	1.37
27	b	809	CLA	C1D-ND	3.66	1.42	1.37
27	H	209	CLA	C4D-ND	-3.66	1.32	1.37
30	K	304	A86	C30-C29	-3.66	1.25	1.32
27	a	810	CLA	C1D-ND	3.66	1.42	1.37
27	I	314	CLA	C4D-ND	-3.65	1.32	1.37
27	L	316	CLA	C4D-ND	-3.65	1.32	1.37
27	I	305	CLA	C4D-ND	-3.65	1.32	1.37
27	K	313	CLA	C4D-ND	-3.65	1.32	1.37
27	A	205	CLA	C4D-ND	-3.65	1.32	1.37
27	E	314	CLA	C1D-ND	3.64	1.42	1.37
30	G	302	A86	C30-C29	-3.64	1.25	1.32
27	I	306	CLA	C1D-ND	3.64	1.42	1.37
27	b	829	CLA	C1D-ND	3.64	1.42	1.37
27	a	807	CLA	C1D-ND	3.64	1.42	1.37
27	B	314	CLA	C4D-ND	-3.64	1.32	1.37
29	C	319	LMG	O2-C2	-3.63	1.34	1.43
26	K	303	DD6	C-C1	-3.62	1.43	1.50
27	i	101	CLA	C1D-ND	3.61	1.42	1.37
27	b	850	CLA	C1D-ND	3.61	1.42	1.37
27	a	841	CLA	C1D-ND	3.60	1.42	1.37
27	A	207	CLA	C4D-ND	-3.60	1.32	1.37
26	H	202	DD6	C-C1	-3.60	1.43	1.50
27	b	823	CLA	C1D-ND	3.60	1.42	1.37
27	I	316	CLA	C4D-ND	-3.60	1.32	1.37
27	B	311	CLA	C1D-ND	3.60	1.42	1.37
27	D	212	CLA	C1D-ND	3.59	1.42	1.37
27	M	318	CLA	C4D-ND	-3.59	1.32	1.37
27	E	315	CLA	C1D-ND	3.59	1.42	1.37
27	b	849	CLA	C1D-ND	3.59	1.42	1.37
27	L	313	CLA	C4D-ND	-3.59	1.32	1.37
27	b	831	CLA	C1D-ND	3.59	1.42	1.37
27	a	838	CLA	C1D-ND	3.58	1.42	1.37
27	L	318	CLA	C4D-ND	-3.58	1.32	1.37
27	D	210	CLA	C4D-ND	-3.57	1.32	1.37
30	B	301	A86	C30-C29	-3.57	1.26	1.32
27	M	317	CLA	C4D-ND	-3.57	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	315	CLA	C4D-ND	-3.57	1.32	1.37
30	L	306	A86	C30-C29	-3.55	1.26	1.32
27	A	211	CLA	C4D-ND	-3.55	1.32	1.37
27	K	318	CLA	C4D-ND	-3.54	1.32	1.37
27	I	309	CLA	C4D-ND	-3.54	1.32	1.37
27	M	311	CLA	C4D-ND	-3.53	1.32	1.37
28	M	314	KC1	C4B-NB	-3.53	1.33	1.37
27	D	217	CLA	C4D-ND	-3.53	1.32	1.37
27	I	317	CLA	C4D-ND	-3.53	1.32	1.37
30	D	203	A86	O1-C20	-3.52	1.41	1.46
28	L	322	KC1	C4B-NB	-3.50	1.33	1.37
27	b	822	CLA	C1D-ND	3.50	1.42	1.37
27	a	804	CLA	C1D-ND	3.49	1.42	1.37
27	C	309	CLA	C4D-ND	-3.49	1.32	1.37
27	J	307	CLA	C4D-ND	-3.49	1.32	1.37
30	L	304	A86	C30-C29	-3.48	1.26	1.32
27	L	308	CLA	C4D-ND	-3.48	1.32	1.37
27	L	321	CLA	C4D-ND	-3.48	1.32	1.37
26	E	303	DD6	C19-C18	-3.48	1.47	1.52
29	D	202	LMG	O6-C1	3.48	1.50	1.41
27	C	310	CLA	C4D-ND	-3.47	1.32	1.37
27	M	319	CLA	C1D-ND	3.47	1.42	1.37
27	K	316	CLA	C4D-ND	-3.47	1.32	1.37
27	J	315	CLA	C4D-ND	-3.46	1.32	1.37
27	L	311	CLA	C1D-ND	3.45	1.42	1.37
27	F	309	CLA	C4D-ND	-3.44	1.33	1.37
28	H	211	KC1	CBA-CGA	-3.44	1.40	1.48
27	J	313	CLA	C4D-ND	-3.44	1.33	1.37
30	M	303	A86	O1-C20	-3.43	1.41	1.46
27	H	207	CLA	C4D-ND	-3.43	1.33	1.37
27	L	311	CLA	C4D-ND	-3.43	1.33	1.37
27	M	319	CLA	C4D-ND	-3.43	1.33	1.37
30	D	203	A86	C30-C29	-3.43	1.26	1.32
28	J	306	KC1	C4B-NB	-3.42	1.33	1.37
27	L	310	CLA	C4D-ND	-3.42	1.33	1.37
29	I	201	LMG	O6-C1	3.41	1.50	1.41
30	M	303	A86	C30-C29	-3.41	1.26	1.32
27	C	316	CLA	C4D-ND	-3.41	1.33	1.37
27	J	311	CLA	C4D-ND	-3.41	1.33	1.37
27	J	314	CLA	C1D-ND	3.40	1.42	1.37
27	F	317	CLA	C1D-ND	3.40	1.42	1.37
27	M	318	CLA	C1D-ND	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	j	103	LMG	O6-C1	3.40	1.50	1.41
27	D	217	CLA	C1D-ND	3.39	1.41	1.37
27	M	311	CLA	C1D-ND	3.38	1.41	1.37
27	L	312	CLA	C4D-ND	-3.37	1.33	1.37
28	I	312	KC1	CBA-CGA	-3.37	1.40	1.48
27	B	314	CLA	C1D-ND	3.37	1.41	1.37
28	K	315	KC1	C4B-NB	-3.37	1.33	1.37
30	B	302	A86	O1-C20	-3.37	1.41	1.46
26	E	303	DD6	C36-C31	-3.36	1.31	1.34
27	L	307	CLA	C4D-ND	-3.36	1.33	1.37
27	F	309	CLA	C1D-ND	3.36	1.41	1.37
27	L	310	CLA	C1D-ND	3.35	1.41	1.37
27	J	314	CLA	C4D-ND	-3.35	1.33	1.37
27	J	312	CLA	C4D-ND	-3.35	1.33	1.37
28	B	313	KC1	C4B-NB	-3.34	1.33	1.37
28	K	315	KC1	CBA-CGA	-3.33	1.40	1.48
27	J	315	CLA	C1D-ND	3.33	1.41	1.37
30	F	301	A86	C30-C29	-3.32	1.26	1.32
28	L	314	KC1	CBA-CGA	-3.31	1.40	1.48
27	A	205	CLA	C1D-ND	3.31	1.41	1.37
29	E	317	LMG	O6-C1	3.31	1.50	1.41
27	L	319	CLA	C4D-ND	-3.31	1.33	1.37
30	m	101	A86	C30-C29	-3.31	1.26	1.32
27	J	307	CLA	C1D-ND	3.30	1.41	1.37
27	a	806	CLA	CHC-C1C	3.30	1.43	1.35
27	B	306	CLA	C4D-ND	-3.30	1.33	1.37
27	L	307	CLA	C1D-ND	3.30	1.41	1.37
27	b	801	CLA	CMB-C2B	-3.29	1.44	1.51
27	b	814	CLA	C4D-ND	-3.27	1.33	1.37
28	L	322	KC1	CBA-CGA	-3.27	1.40	1.48
30	C	302	A86	O1-C20	-3.27	1.41	1.46
30	H	201	A86	O1-C20	-3.27	1.41	1.46
27	L	319	CLA	C1D-ND	3.27	1.41	1.37
27	J	310	CLA	C1D-ND	3.27	1.41	1.37
30	D	206	A86	O1-C20	-3.26	1.41	1.46
27	C	310	CLA	C1D-ND	3.26	1.41	1.37
27	I	305	CLA	C1D-ND	3.23	1.41	1.37
30	H	201	A86	C32-C31	-3.23	1.49	1.54
27	I	313	CLA	C1D-ND	3.23	1.41	1.37
27	D	213	CLA	CHC-C1C	3.23	1.43	1.35
28	K	308	KC1	C4B-NB	-3.23	1.33	1.37
27	A	211	CLA	C1D-ND	3.22	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	214	LMG	O1-C1	-3.22	1.34	1.40
27	L	318	CLA	C1D-ND	3.21	1.41	1.37
27	I	316	CLA	C1D-ND	3.21	1.41	1.37
28	L	314	KC1	C4B-NB	-3.21	1.33	1.37
27	L	321	CLA	C1D-ND	3.20	1.41	1.37
27	J	313	CLA	C1D-ND	3.20	1.41	1.37
27	K	316	CLA	C1D-ND	3.20	1.41	1.37
27	E	308	CLA	CHC-C1C	3.20	1.43	1.35
29	M	321	LMG	O6-C1	3.20	1.50	1.41
27	F	317	CLA	C4D-ND	-3.19	1.33	1.37
27	F	306	CLA	CHC-C1C	3.19	1.43	1.35
26	M	306	DD6	C36-C31	-3.19	1.31	1.34
30	C	305	A86	C32-C31	-3.19	1.49	1.54
27	C	316	CLA	C1D-ND	3.18	1.41	1.37
27	a	817	CLA	CHC-C1C	3.18	1.43	1.35
27	b	842	CLA	CHC-C1C	3.18	1.43	1.35
27	a	854	CLA	CHC-C1C	3.18	1.43	1.35
27	b	815	CLA	CHC-C1C	3.18	1.43	1.35
28	H	211	KC1	C4A-C3A	-3.17	1.38	1.44
27	H	204	CLA	C1D-ND	3.17	1.41	1.37
27	a	840	CLA	CHC-C1C	3.17	1.43	1.35
28	B	313	KC1	CBA-CGA	-3.17	1.41	1.48
30	B	302	A86	C32-C31	-3.17	1.49	1.54
27	I	306	CLA	CHC-C1C	3.17	1.43	1.35
28	H	211	KC1	C1B-NB	-3.16	1.33	1.37
27	F	305	CLA	CHC-C1C	3.16	1.43	1.35
27	b	829	CLA	CHC-C1C	3.16	1.43	1.35
30	B	305	A86	C32-C31	-3.16	1.49	1.54
27	b	823	CLA	CHC-C1C	3.16	1.43	1.35
27	B	307	CLA	CHC-C1C	3.16	1.43	1.35
27	F	310	CLA	CHC-C1C	3.15	1.43	1.35
27	l	206	CLA	CHC-C1C	3.15	1.43	1.35
26	D	205	DD6	C36-C31	-3.15	1.31	1.34
27	b	827	CLA	CHC-C1C	3.15	1.43	1.35
27	D	212	CLA	CHC-C1C	3.15	1.43	1.35
30	B	304	A86	O1-C20	-3.14	1.41	1.46
27	I	310	CLA	CHC-C1C	3.14	1.43	1.35
27	D	210	CLA	C1D-ND	3.14	1.41	1.37
27	G	314	CLA	CHC-C1C	3.14	1.43	1.35
27	I	314	CLA	C1D-ND	3.14	1.41	1.37
27	M	310	CLA	C1D-ND	3.14	1.41	1.37
29	C	301	LMG	O6-C1	3.13	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	306	CLA	C4D-ND	-3.13	1.33	1.37
27	a	812	CLA	CHC-C1C	3.13	1.43	1.35
27	a	821	CLA	CHC-C1C	3.13	1.43	1.35
27	B	306	CLA	C1D-ND	3.13	1.41	1.37
27	I	309	CLA	C1D-ND	3.13	1.41	1.37
27	I	317	CLA	C1D-ND	3.13	1.41	1.37
27	i	101	CLA	CHC-C1C	3.12	1.43	1.35
27	M	315	CLA	CHC-C1C	3.12	1.43	1.35
28	M	314	KC1	CBA-CGA	-3.12	1.41	1.48
27	F	306	CLA	C4D-ND	-3.12	1.33	1.37
27	D	214	CLA	CHC-C1C	3.12	1.43	1.35
27	J	308	CLA	CHC-C1C	3.12	1.43	1.35
27	l	203	CLA	CMB-C2B	-3.12	1.45	1.51
29	I	319	LMG	O6-C1	3.12	1.49	1.41
27	a	855	CLA	CHC-C1C	3.12	1.43	1.35
27	a	848	CLA	CHC-C1C	3.12	1.43	1.35
27	b	811	CLA	CHC-C1C	3.12	1.43	1.35
27	a	824	CLA	CHC-C1C	3.12	1.43	1.35
27	j	104	CLA	CHC-C1C	3.12	1.43	1.35
29	J	317	LMG	O6-C1	3.11	1.49	1.41
27	E	309	CLA	CHC-C1C	3.11	1.42	1.35
27	E	312	CLA	CHC-C1C	3.11	1.42	1.35
27	A	208	CLA	C1D-ND	3.11	1.41	1.37
27	F	316	CLA	CHC-C1C	3.11	1.42	1.35
27	a	804	CLA	C4D-ND	-3.11	1.33	1.37
27	a	816	CLA	CHC-C1C	3.11	1.42	1.35
27	C	306	CLA	CHC-C1C	3.11	1.42	1.35
27	E	314	CLA	CHC-C1C	3.11	1.42	1.35
27	D	209	CLA	CHC-C1C	3.11	1.42	1.35
27	F	311	CLA	CHC-C1C	3.11	1.42	1.35
27	a	821	CLA	C4D-ND	-3.11	1.33	1.37
27	b	831	CLA	CHC-C1C	3.11	1.42	1.35
27	C	315	CLA	CHC-C1C	3.10	1.42	1.35
27	b	813	CLA	CHC-C1C	3.10	1.42	1.35
27	A	206	CLA	CHC-C1C	3.10	1.42	1.35
27	H	208	CLA	CHC-C1C	3.10	1.42	1.35
27	a	828	CLA	CHC-C1C	3.10	1.42	1.35
27	F	315	CLA	CHC-C1C	3.10	1.42	1.35
27	a	849	CLA	CHC-C1C	3.10	1.42	1.35
27	a	841	CLA	CHC-C1C	3.10	1.42	1.35
27	b	806	CLA	CHC-C1C	3.10	1.42	1.35
27	G	316	CLA	CHC-C1C	3.10	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	301	CLA	CHC-C1C	3.10	1.42	1.35
27	G	306	CLA	CHC-C1C	3.10	1.42	1.35
27	b	804	CLA	C3B-C2B	-3.10	1.36	1.40
27	H	214	CLA	CHC-C1C	3.10	1.42	1.35
27	r	201	CLA	CHC-C1C	3.09	1.42	1.35
27	a	808	CLA	CHC-C1C	3.09	1.42	1.35
27	b	807	CLA	C4D-ND	-3.09	1.33	1.37
27	E	310	CLA	CHC-C1C	3.09	1.42	1.35
27	b	818	CLA	CHC-C1C	3.09	1.42	1.35
27	a	818	CLA	CHC-C1C	3.09	1.42	1.35
27	a	814	CLA	CHC-C1C	3.09	1.42	1.35
27	b	819	CLA	CHC-C1C	3.09	1.42	1.35
27	b	849	CLA	CHC-C1C	3.09	1.42	1.35
27	a	804	CLA	CHC-C1C	3.09	1.42	1.35
27	b	810	CLA	CHC-C1C	3.09	1.42	1.35
27	B	310	CLA	CHC-C1C	3.09	1.42	1.35
27	D	211	CLA	CHC-C1C	3.09	1.42	1.35
27	a	839	CLA	CMB-C2B	-3.09	1.45	1.51
27	a	856	CLA	CMB-C2B	-3.09	1.45	1.51
27	b	824	CLA	CHC-C1C	3.09	1.42	1.35
27	b	846	CLA	CHC-C1C	3.09	1.42	1.35
27	a	827	CLA	CMB-C2B	-3.09	1.45	1.51
27	r	201	CLA	C4D-ND	-3.09	1.33	1.37
27	a	829	CLA	CHC-C1C	3.09	1.42	1.35
27	F	307	CLA	CHC-C1C	3.09	1.42	1.35
27	b	808	CLA	CHC-C1C	3.09	1.42	1.35
27	G	315	CLA	CHC-C1C	3.08	1.42	1.35
26	M	306	DD6	C-C1	-3.08	1.44	1.50
27	b	820	CLA	CHC-C1C	3.08	1.42	1.35
27	b	826	CLA	CHC-C1C	3.08	1.42	1.35
27	a	845	CLA	CHC-C1C	3.08	1.42	1.35
27	b	821	CLA	CMB-C2B	-3.08	1.45	1.51
27	G	317	CLA	CHC-C1C	3.08	1.42	1.35
27	B	312	CLA	CHC-C1C	3.08	1.42	1.35
27	b	845	CLA	CHC-C1C	3.08	1.42	1.35
27	F	314	CLA	CHC-C1C	3.08	1.42	1.35
27	G	308	CLA	CHC-C1C	3.08	1.42	1.35
27	b	838	CLA	CMB-C2B	-3.08	1.45	1.51
27	b	827	CLA	C4D-ND	-3.08	1.33	1.37
27	a	825	CLA	CHC-C1C	3.08	1.42	1.35
27	L	308	CLA	C1D-ND	3.08	1.41	1.37
27	a	811	CLA	CHC-C1C	3.08	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	201	LHG	C26-C25	-3.08	1.34	1.51
27	G	310	CLA	CHC-C1C	3.07	1.42	1.35
27	A	207	CLA	C1D-ND	3.07	1.41	1.37
27	C	314	CLA	C1D-ND	3.07	1.41	1.37
27	A	203	CLA	CHC-C1C	3.07	1.42	1.35
27	D	215	CLA	CHC-C1C	3.07	1.42	1.35
27	B	308	CLA	CHC-C1C	3.07	1.42	1.35
27	G	312	CLA	CHC-C1C	3.07	1.42	1.35
27	D	216	CLA	C1D-ND	3.07	1.41	1.37
27	B	311	CLA	CHC-C1C	3.07	1.42	1.35
27	G	309	CLA	CHC-C1C	3.07	1.42	1.35
27	J	311	CLA	CHC-C1C	3.07	1.42	1.35
27	G	307	CLA	C4D-ND	-3.07	1.33	1.37
30	H	203	A86	O1-C20	-3.07	1.41	1.46
27	C	307	CLA	C1D-ND	3.07	1.41	1.37
27	b	843	CLA	CHC-C1C	3.07	1.42	1.35
27	K	318	CLA	C1D-ND	3.06	1.41	1.37
27	a	848	CLA	C4D-ND	-3.06	1.33	1.37
27	L	316	CLA	C1D-ND	3.06	1.41	1.37
27	a	810	CLA	CHC-C1C	3.06	1.42	1.35
27	L	309	CLA	C1D-ND	3.06	1.41	1.37
27	a	826	CLA	CHC-C1C	3.06	1.42	1.35
27	a	832	CLA	CHC-C1C	3.06	1.42	1.35
27	b	816	CLA	CHC-C1C	3.06	1.42	1.35
27	b	850	CLA	CHC-C1C	3.06	1.42	1.35
27	a	819	CLA	CHC-C1C	3.06	1.42	1.35
27	b	847	CLA	CHC-C1C	3.06	1.42	1.35
27	b	803	CLA	CHC-C1C	3.06	1.42	1.35
27	G	311	CLA	CHC-C1C	3.05	1.42	1.35
30	G	302	A86	O1-C20	-3.05	1.41	1.46
27	f	303	CLA	CHC-C1C	3.05	1.42	1.35
27	b	803	CLA	C4D-ND	-3.05	1.33	1.37
27	I	317	CLA	CHC-C1C	3.05	1.42	1.35
30	C	304	A86	O1-C20	-3.05	1.41	1.46
27	a	842	CLA	CMB-C2B	-3.05	1.45	1.51
27	I	307	CLA	C1D-ND	3.05	1.41	1.37
27	F	308	CLA	CHC-C1C	3.04	1.42	1.35
27	b	807	CLA	CHC-C1C	3.04	1.42	1.35
27	B	307	CLA	C4D-ND	-3.04	1.33	1.37
27	a	830	CLA	CHC-C1C	3.04	1.42	1.35
27	a	838	CLA	CHC-C1C	3.04	1.42	1.35
27	F	316	CLA	C4D-ND	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	J	309	CLA	C1D-ND	3.04	1.41	1.37
29	E	317	LMG	O1-C1	-3.04	1.35	1.40
27	a	823	CLA	CHC-C1C	3.04	1.42	1.35
29	C	301	LMG	O8-C28	3.04	1.42	1.33
28	K	308	KC1	CBA-CGA	-3.04	1.41	1.48
27	b	839	CLA	CHC-C1C	3.04	1.42	1.35
27	a	850	CLA	CHC-C1C	3.03	1.42	1.35
27	b	822	CLA	CHC-C1C	3.03	1.42	1.35
27	K	309	CLA	C1D-ND	3.03	1.41	1.37
27	B	312	CLA	C4D-ND	-3.03	1.33	1.37
27	b	818	CLA	C4D-ND	-3.03	1.33	1.37
27	b	828	CLA	CHC-C1C	3.03	1.42	1.35
27	a	819	CLA	C4D-ND	-3.03	1.33	1.37
29	A	212	LMG	O6-C1	3.03	1.49	1.41
27	a	827	CLA	C3B-C2B	-3.03	1.36	1.40
27	K	313	CLA	C1D-ND	3.03	1.41	1.37
27	a	807	CLA	CHC-C1C	3.03	1.42	1.35
27	G	307	CLA	CHC-C1C	3.03	1.42	1.35
27	f	301	CLA	C4D-ND	-3.03	1.33	1.37
27	b	847	CLA	C4D-ND	-3.02	1.33	1.37
27	b	816	CLA	C4D-ND	-3.02	1.33	1.37
27	a	813	CLA	CHC-C1C	3.02	1.42	1.35
27	I	315	CLA	C1D-ND	3.02	1.41	1.37
27	H	206	CLA	C1D-ND	3.02	1.41	1.37
27	E	315	CLA	CHC-C1C	3.02	1.42	1.35
27	D	213	CLA	C4D-ND	-3.02	1.33	1.37
27	C	311	CLA	C1D-ND	3.02	1.41	1.37
28	J	306	KC1	CBA-CGA	-3.02	1.41	1.48
27	F	313	CLA	CHC-C1C	3.02	1.42	1.35
27	F	313	CLA	C4D-ND	-3.01	1.33	1.37
27	I	310	CLA	C4D-ND	-3.01	1.33	1.37
27	L	317	CLA	CHC-C1C	3.01	1.42	1.35
27	i	101	CLA	C4D-ND	-3.01	1.33	1.37
27	b	831	CLA	C4D-ND	-3.01	1.33	1.37
27	H	207	CLA	C1D-ND	3.01	1.41	1.37
27	f	302	CLA	CHC-C1C	3.01	1.42	1.35
26	E	303	DD6	O1-C20	-3.01	1.41	1.46
28	L	322	KC1	C1B-NB	-3.01	1.34	1.37
27	F	308	CLA	C4D-ND	-3.01	1.33	1.37
27	G	311	CLA	C4D-ND	-3.01	1.33	1.37
27	b	808	CLA	C4D-ND	-3.00	1.33	1.37
27	b	830	CLA	CMB-C2B	-3.00	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	314	CLA	CHC-C1C	3.00	1.42	1.35
27	b	844	CLA	CMB-C2B	-3.00	1.45	1.51
27	M	313	CLA	C1D-ND	3.00	1.41	1.37
27	K	312	CLA	C1D-ND	3.00	1.41	1.37
27	J	311	CLA	C1D-ND	3.00	1.41	1.37
27	b	815	CLA	C4D-ND	-3.00	1.33	1.37
27	b	829	CLA	C4D-ND	-3.00	1.33	1.37
28	B	313	KC1	C1B-NB	-3.00	1.34	1.37
27	F	315	CLA	C4D-ND	-3.00	1.33	1.37
27	a	846	CLA	CHC-C1C	3.00	1.42	1.35
27	b	809	CLA	CHC-C1C	3.00	1.42	1.35
27	C	309	CLA	C1D-ND	3.00	1.41	1.37
28	M	314	KC1	C1B-NB	-3.00	1.34	1.37
27	a	844	CLA	CMB-C2B	-3.00	1.45	1.51
27	l	204	CLA	CMB-C2B	-3.00	1.45	1.51
27	b	841	CLA	CHC-C1C	3.00	1.42	1.35
27	B	309	CLA	CHC-C1C	3.00	1.42	1.35
27	G	309	CLA	C4D-ND	-2.99	1.33	1.37
27	a	810	CLA	C4D-ND	-2.99	1.33	1.37
27	b	817	CLA	CHC-C1C	2.99	1.42	1.35
27	I	305	CLA	CHC-C1C	2.99	1.42	1.35
27	a	808	CLA	C4D-ND	-2.99	1.33	1.37
27	B	314	CLA	CHC-C1C	2.99	1.42	1.35
33	J	318	SQD	O47-C7	2.99	1.40	1.33
27	D	208	CLA	CHC-C1C	2.99	1.42	1.35
27	a	826	CLA	C4D-ND	-2.99	1.33	1.37
27	D	214	CLA	C4D-ND	-2.99	1.33	1.37
27	b	850	CLA	C4D-ND	-2.99	1.33	1.37
27	L	318	CLA	CHC-C1C	2.99	1.42	1.35
27	C	312	CLA	CHC-C1C	2.99	1.42	1.35
27	B	309	CLA	C4D-ND	-2.98	1.33	1.37
27	f	303	CLA	C4D-ND	-2.98	1.33	1.37
27	b	846	CLA	C4D-ND	-2.98	1.33	1.37
26	H	202	DD6	O1-C20	-2.98	1.41	1.46
27	H	208	CLA	C4D-ND	-2.98	1.33	1.37
27	K	317	CLA	C1D-ND	2.98	1.41	1.37
27	K	316	CLA	CHC-C1C	2.98	1.42	1.35
27	E	315	CLA	C4D-ND	-2.98	1.33	1.37
27	A	207	CLA	CHC-C1C	2.98	1.42	1.35
26	B	303	DD6	O1-C20	-2.98	1.41	1.46
27	C	314	CLA	CHC-C1C	2.98	1.42	1.35
27	a	809	CLA	CMB-C2B	-2.98	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	313	CLA	CHC-C1C	2.98	1.42	1.35
27	b	805	CLA	CMB-C2B	-2.97	1.45	1.51
27	B	311	CLA	C4D-ND	-2.97	1.33	1.37
27	L	315	CLA	CHC-C1C	2.97	1.42	1.35
30	M	302	A86	O1-C20	-2.97	1.42	1.46
27	M	316	CLA	C1D-ND	2.97	1.41	1.37
31	M	320	LHG	C26-C25	-2.97	1.34	1.51
26	I	304	DD6	C-C1	-2.97	1.44	1.50
27	M	317	CLA	C1D-ND	2.97	1.41	1.37
27	A	203	CLA	C4D-ND	-2.97	1.33	1.37
27	L	313	CLA	CHC-C1C	2.97	1.42	1.35
27	J	313	CLA	CHC-C1C	2.97	1.42	1.35
27	A	208	CLA	CHC-C1C	2.97	1.42	1.35
27	G	316	CLA	C4D-ND	-2.97	1.33	1.37
31	a	801	LHG	C26-C25	-2.97	1.34	1.51
27	a	825	CLA	C4D-ND	-2.97	1.33	1.37
27	L	309	CLA	CHC-C1C	2.96	1.42	1.35
27	M	309	CLA	C1D-ND	2.96	1.41	1.37
27	a	803	CLA	CMB-C2B	-2.96	1.45	1.51
27	C	316	CLA	CHC-C1C	2.96	1.42	1.35
27	C	312	CLA	C1D-ND	2.96	1.41	1.37
27	a	845	CLA	C4D-ND	-2.96	1.33	1.37
31	b	836	LHG	O8-C6	-2.96	1.38	1.45
30	m	101	A86	O1-C20	-2.96	1.42	1.46
27	E	308	CLA	C4D-ND	-2.96	1.33	1.37
27	E	309	CLA	C4D-ND	-2.96	1.33	1.37
29	D	202	LMG	O8-C28	2.96	1.42	1.33
27	L	307	CLA	CHC-C1C	2.96	1.42	1.35
29	A	212	LMG	O8-C28	2.96	1.42	1.33
27	J	312	CLA	CMB-C2B	-2.96	1.45	1.51
27	I	308	CLA	CHC-C1C	2.96	1.42	1.35
27	a	841	CLA	C4D-ND	-2.96	1.33	1.37
27	a	815	CLA	C1D-ND	2.96	1.41	1.37
29	I	319	LMG	O1-C1	-2.95	1.35	1.40
27	L	312	CLA	C1D-ND	2.95	1.41	1.37
30	B	305	A86	O1-C20	-2.95	1.42	1.46
27	a	818	CLA	C4D-ND	-2.95	1.33	1.37
27	E	311	CLA	C1D-ND	2.95	1.41	1.37
27	E	312	CLA	C4D-ND	-2.95	1.33	1.37
27	a	822	CLA	CHC-C1C	2.95	1.42	1.35
27	l	206	CLA	C4D-ND	-2.95	1.33	1.37
27	F	311	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	306	CLA	C4D-ND	-2.95	1.33	1.37
27	a	843	CLA	CMB-C2B	-2.95	1.45	1.51
27	b	826	CLA	C4D-ND	-2.95	1.33	1.37
28	A	209	KC1	C4B-NB	-2.95	1.34	1.37
28	J	306	KC1	C1B-NB	-2.95	1.34	1.37
27	b	820	CLA	C4D-ND	-2.94	1.33	1.37
27	b	823	CLA	C4D-ND	-2.94	1.33	1.37
27	C	311	CLA	CHC-C1C	2.94	1.42	1.35
27	D	210	CLA	CMB-C2B	-2.94	1.45	1.51
27	a	814	CLA	C4D-ND	-2.94	1.33	1.37
29	M	321	LMG	O1-C1	-2.94	1.35	1.40
27	M	311	CLA	CMB-C2B	-2.94	1.45	1.51
27	a	803	CLA	C1D-ND	2.94	1.41	1.37
27	C	315	CLA	C4D-ND	-2.94	1.33	1.37
27	a	846	CLA	C4D-ND	-2.94	1.33	1.37
27	I	309	CLA	CHC-C1C	2.94	1.42	1.35
27	l	203	CLA	C1D-ND	2.94	1.41	1.37
27	a	843	CLA	CHC-C1C	2.93	1.42	1.35
27	L	316	CLA	CHC-C1C	2.93	1.42	1.35
27	J	307	CLA	CHC-C1C	2.93	1.42	1.35
27	a	806	CLA	C4D-ND	-2.93	1.33	1.37
27	a	832	CLA	C4D-ND	-2.93	1.33	1.37
27	M	309	CLA	CHC-C1C	2.93	1.42	1.35
27	b	825	CLA	CMB-C2B	-2.93	1.45	1.51
27	D	208	CLA	CMB-C2B	-2.93	1.45	1.51
27	a	812	CLA	C4D-ND	-2.93	1.33	1.37
30	r	202	A86	O1-C20	-2.93	1.42	1.46
27	C	311	CLA	CMB-C2B	-2.93	1.45	1.51
27	M	307	CLA	CMB-C2B	-2.93	1.45	1.51
27	H	210	CLA	CHC-C1C	2.93	1.42	1.35
27	B	310	CLA	C4D-ND	-2.93	1.33	1.37
27	a	807	CLA	C4D-ND	-2.93	1.33	1.37
27	a	855	CLA	C4D-ND	-2.93	1.33	1.37
27	b	822	CLA	C4D-ND	-2.92	1.33	1.37
27	j	104	CLA	C4D-ND	-2.92	1.33	1.37
27	G	317	CLA	C4D-ND	-2.92	1.33	1.37
27	A	210	CLA	C1D-ND	2.92	1.41	1.37
27	D	207	CLA	CMB-C2B	-2.92	1.45	1.51
30	H	203	A86	C32-C31	-2.92	1.49	1.54
27	a	838	CLA	C4D-ND	-2.92	1.33	1.37
27	I	313	CLA	CHC-C1C	2.92	1.42	1.35
27	a	849	CLA	C4D-ND	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	828	CLA	C4D-ND	-2.92	1.33	1.37
29	A	214	LMG	O6-C1	2.92	1.49	1.41
27	D	209	CLA	C4D-ND	-2.92	1.33	1.37
27	J	310	CLA	CHC-C1C	2.92	1.42	1.35
27	b	841	CLA	C4D-ND	-2.92	1.33	1.37
30	M	302	A86	C32-C31	-2.92	1.49	1.54
27	H	204	CLA	CHC-C1C	2.92	1.42	1.35
30	B	302	A86	C2-C1	-2.92	1.31	1.35
27	A	206	CLA	C4D-ND	-2.92	1.33	1.37
27	a	817	CLA	C4D-ND	-2.92	1.33	1.37
27	b	814	CLA	CHC-C1C	2.92	1.42	1.35
30	H	201	A86	C2-C1	-2.92	1.31	1.35
27	M	310	CLA	CHC-C1C	2.91	1.42	1.35
29	l	201	LMG	O8-C28	2.91	1.41	1.33
27	E	311	CLA	CHC-C1C	2.91	1.42	1.35
27	L	310	CLA	CHC-C1C	2.91	1.42	1.35
27	H	214	CLA	C4D-ND	-2.91	1.33	1.37
27	K	317	CLA	CHC-C1C	2.91	1.42	1.35
27	D	207	CLA	CHC-C1C	2.91	1.42	1.35
27	L	315	CLA	C1D-ND	2.91	1.41	1.37
27	L	311	CLA	CHC-C1C	2.91	1.42	1.35
27	L	321	CLA	CHC-C1C	2.91	1.42	1.35
28	K	315	KC1	C1B-NB	-2.91	1.34	1.37
28	C	313	KC1	CBA-CGA	-2.91	1.41	1.48
27	L	312	CLA	CHC-C1C	2.91	1.42	1.35
27	J	312	CLA	CHC-C1C	2.91	1.42	1.35
27	a	823	CLA	C4D-ND	-2.91	1.33	1.37
27	b	805	CLA	C1D-ND	2.91	1.41	1.37
27	K	311	CLA	CMB-C2B	-2.91	1.45	1.51
27	E	314	CLA	C4D-ND	-2.91	1.33	1.37
27	D	211	CLA	C4D-ND	-2.91	1.33	1.37
27	b	806	CLA	C4D-ND	-2.91	1.33	1.37
27	L	308	CLA	CHC-C1C	2.90	1.42	1.35
27	H	213	CLA	CMB-C2B	-2.90	1.45	1.51
27	C	312	CLA	CMB-C2B	-2.90	1.45	1.51
27	B	308	CLA	C4D-ND	-2.90	1.33	1.37
28	L	314	KC1	C4A-C3A	-2.90	1.39	1.44
27	H	206	CLA	CMB-C2B	-2.90	1.45	1.51
27	b	804	CLA	CMB-C2B	-2.90	1.45	1.51
27	b	839	CLA	C4D-ND	-2.90	1.33	1.37
27	D	212	CLA	C4D-ND	-2.90	1.33	1.37
31	E	318	LHG	C26-C25	-2.90	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	317	CLA	CMB-C2B	-2.90	1.45	1.51
27	D	217	CLA	CHC-C1C	2.90	1.42	1.35
27	H	205	CLA	CMB-C2B	-2.90	1.45	1.51
31	b	836	LHG	C26-C25	-2.90	1.35	1.51
27	A	204	CLA	CHC-C1C	2.90	1.42	1.35
27	G	314	CLA	C4D-ND	-2.90	1.33	1.37
27	G	315	CLA	C4D-ND	-2.90	1.33	1.37
27	a	844	CLA	C1D-ND	2.90	1.41	1.37
31	a	833	LHG	C26-C25	-2.89	1.35	1.51
27	a	824	CLA	C4D-ND	-2.89	1.33	1.37
27	a	805	CLA	CMB-C2B	-2.89	1.45	1.51
27	M	315	CLA	C4D-ND	-2.89	1.33	1.37
27	b	843	CLA	C4D-ND	-2.89	1.33	1.37
27	f	302	CLA	C4D-ND	-2.89	1.33	1.37
27	a	809	CLA	C1D-ND	2.89	1.41	1.37
27	C	307	CLA	CHC-C1C	2.89	1.42	1.35
27	b	810	CLA	C4D-ND	-2.89	1.33	1.37
27	A	211	CLA	CHC-C1C	2.89	1.42	1.35
27	A	207	CLA	CMB-C2B	-2.89	1.45	1.51
30	C	305	A86	O1-C20	-2.89	1.42	1.46
30	I	303	A86	C32-C31	-2.89	1.49	1.54
27	M	308	CLA	C1D-ND	2.89	1.41	1.37
27	K	313	CLA	CMB-C2B	-2.89	1.45	1.51
27	K	311	CLA	C1D-ND	2.89	1.41	1.37
27	G	310	CLA	C4D-ND	-2.89	1.33	1.37
27	L	319	CLA	CHC-C1C	2.89	1.42	1.35
27	E	311	CLA	CMB-C2B	-2.89	1.45	1.51
27	b	812	CLA	CMB-C2B	-2.89	1.45	1.51
27	A	205	CLA	CHC-C1C	2.89	1.42	1.35
27	M	312	CLA	CHC-C1C	2.89	1.42	1.35
27	b	838	CLA	CHC-C1C	2.89	1.42	1.35
27	a	829	CLA	C4D-ND	-2.89	1.33	1.37
27	G	312	CLA	C4D-ND	-2.88	1.33	1.37
27	L	313	CLA	C1D-ND	2.88	1.41	1.37
30	D	204	A86	O1-C20	-2.88	1.42	1.46
27	M	307	CLA	CHC-C1C	2.88	1.42	1.35
27	a	816	CLA	C4D-ND	-2.88	1.33	1.37
27	J	314	CLA	CHC-C1C	2.88	1.42	1.35
27	K	314	CLA	C3B-C2B	-2.88	1.36	1.40
27	C	312	CLA	C3B-C2B	-2.88	1.36	1.40
27	b	801	CLA	C3B-C2B	-2.88	1.36	1.40
27	M	313	CLA	CHC-C1C	2.88	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	822	CLA	C4D-ND	-2.88	1.33	1.37
27	a	813	CLA	C4D-ND	-2.87	1.33	1.37
27	F	314	CLA	C4D-ND	-2.87	1.33	1.37
27	b	849	CLA	C4D-ND	-2.87	1.33	1.37
27	a	815	CLA	CHC-C1C	2.87	1.42	1.35
27	G	306	CLA	C4D-ND	-2.87	1.33	1.37
27	b	811	CLA	C4D-ND	-2.87	1.33	1.37
27	b	845	CLA	C4D-ND	-2.87	1.33	1.37
27	b	838	CLA	C1D-ND	2.87	1.41	1.37
27	H	212	CLA	CHC-C1C	2.87	1.42	1.35
27	a	811	CLA	C4D-ND	-2.87	1.33	1.37
31	a	802	LHG	C26-C25	-2.87	1.35	1.51
27	b	813	CLA	C4D-ND	-2.87	1.33	1.37
28	M	314	KC1	C4A-C3A	-2.87	1.39	1.44
27	K	309	CLA	CMB-C2B	-2.87	1.45	1.51
27	b	809	CLA	C4D-ND	-2.86	1.33	1.37
27	C	318	CLA	CHC-C1C	2.86	1.42	1.35
26	D	205	DD6	C17-C16	-2.86	1.50	1.54
26	A	202	DD6	C-C1	-2.86	1.45	1.50
28	K	308	KC1	C1B-NB	-2.86	1.34	1.37
29	L	323	LMG	O2-C2	-2.86	1.36	1.43
29	L	323	LMG	O8-C28	2.86	1.41	1.33
27	I	308	CLA	C1D-ND	2.86	1.41	1.37
27	a	828	CLA	C4D-ND	-2.86	1.33	1.37
27	K	319	CLA	CHC-C1C	2.86	1.42	1.35
31	a	837	LHG	C26-C25	-2.86	1.35	1.51
27	a	820	CLA	CMB-C2B	-2.86	1.45	1.51
27	M	317	CLA	CHC-C1C	2.86	1.42	1.35
27	b	819	CLA	C4D-ND	-2.86	1.33	1.37
27	L	313	CLA	CMB-C2B	-2.86	1.45	1.51
27	a	842	CLA	C3B-C2B	-2.86	1.36	1.40
29	C	319	LMG	O1-C1	-2.86	1.35	1.40
27	l	203	CLA	CHC-C1C	2.85	1.42	1.35
27	L	317	CLA	C4D-ND	-2.85	1.33	1.37
30	I	301	A86	C32-C31	-2.85	1.49	1.54
27	F	310	CLA	C4D-ND	-2.85	1.33	1.37
27	a	830	CLA	C4D-ND	-2.85	1.33	1.37
27	J	309	CLA	CMB-C2B	-2.85	1.45	1.51
27	J	308	CLA	C4D-ND	-2.85	1.33	1.37
31	I	318	LHG	C26-C25	-2.85	1.35	1.51
27	K	313	CLA	CHC-C1C	2.85	1.42	1.35
26	B	303	DD6	C17-C16	-2.85	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	318	CLA	CMB-C2B	-2.85	1.45	1.51
27	K	314	CLA	CMB-C2B	-2.85	1.45	1.51
27	I	311	CLA	CHC-C1C	2.85	1.42	1.35
27	K	310	CLA	C1D-ND	2.85	1.41	1.37
29	a	852	LMG	O6-C1	2.84	1.49	1.41
27	b	824	CLA	C4D-ND	-2.84	1.33	1.37
26	I	304	DD6	C36-C31	-2.84	1.31	1.34
27	J	312	CLA	C1D-ND	2.84	1.41	1.37
27	C	309	CLA	CMB-C2B	-2.84	1.45	1.51
27	K	319	CLA	C1D-ND	2.84	1.41	1.37
27	a	850	CLA	C4D-ND	-2.84	1.33	1.37
27	K	312	CLA	CMB-C2B	-2.84	1.45	1.51
26	M	304	DD6	C17-C16	-2.84	1.50	1.54
27	M	309	CLA	CMB-C2B	-2.84	1.45	1.51
27	b	830	CLA	C3B-C2B	-2.83	1.36	1.40
27	K	318	CLA	CHC-C1C	2.83	1.42	1.35
30	E	301	A86	O1-C20	-2.83	1.42	1.46
27	K	317	CLA	CMB-C2B	-2.83	1.45	1.51
27	D	216	CLA	CHC-C1C	2.83	1.42	1.35
27	a	803	CLA	C3B-C2B	-2.83	1.36	1.40
27	M	316	CLA	CMB-C2B	-2.83	1.45	1.51
27	b	842	CLA	C4D-ND	-2.83	1.33	1.37
27	K	312	CLA	CHC-C1C	2.83	1.42	1.35
28	I	312	KC1	C1B-NB	-2.82	1.34	1.37
27	K	310	CLA	CHC-C1C	2.82	1.42	1.35
27	a	842	CLA	C1D-ND	2.82	1.41	1.37
28	A	209	KC1	CBA-CGA	-2.82	1.42	1.48
27	I	307	CLA	CMB-C2B	-2.82	1.45	1.51
27	b	805	CLA	CHC-C1C	2.82	1.42	1.35
26	C	303	DD6	C36-C31	-2.82	1.31	1.34
27	D	215	CLA	C4D-ND	-2.81	1.33	1.37
27	C	318	CLA	CMB-C2B	-2.81	1.45	1.51
28	B	313	KC1	C4A-C3A	-2.81	1.39	1.44
27	M	312	CLA	CMB-C2B	-2.81	1.45	1.51
27	b	830	CLA	C1D-ND	2.81	1.41	1.37
27	A	204	CLA	C1D-ND	2.81	1.41	1.37
27	M	319	CLA	CHC-C1C	2.81	1.42	1.35
27	a	854	CLA	C4D-ND	-2.81	1.33	1.37
31	j	102	LHG	C26-C25	-2.81	1.35	1.51
26	D	205	DD6	O1-C20	-2.81	1.42	1.46
29	D	202	LMG	O1-C1	-2.81	1.35	1.40
27	K	316	CLA	CMB-C2B	-2.81	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	320	KC1	CBA-CGA	-2.81	1.42	1.48
27	C	307	CLA	CMB-C2B	-2.80	1.45	1.51
27	J	307	CLA	CMB-C2B	-2.80	1.45	1.51
27	A	208	CLA	CMB-C2B	-2.80	1.45	1.51
28	G	313	KC1	CBA-CGA	-2.80	1.42	1.48
27	A	210	CLA	CMB-C2B	-2.80	1.45	1.51
27	K	309	CLA	CHC-C1C	2.80	1.42	1.35
27	K	317	CLA	C3B-C2B	-2.80	1.36	1.40
27	D	210	CLA	CHC-C1C	2.80	1.42	1.35
27	M	313	CLA	CMB-C2B	-2.80	1.45	1.51
27	F	305	CLA	C4D-ND	-2.80	1.33	1.37
29	j	103	LMG	O8-C28	2.79	1.41	1.33
30	H	201	A86	C-C1	-2.79	1.45	1.50
27	b	821	CLA	C1D-ND	2.79	1.41	1.37
27	b	844	CLA	CHC-C1C	2.79	1.42	1.35
30	D	204	A86	C32-C31	-2.79	1.49	1.54
27	L	321	CLA	CMB-C2B	-2.79	1.45	1.51
27	M	311	CLA	CHC-C1C	2.79	1.42	1.35
28	C	313	KC1	C4B-NB	-2.79	1.34	1.37
27	H	204	CLA	CMB-C2B	-2.79	1.45	1.51
27	F	307	CLA	C4D-ND	-2.79	1.33	1.37
27	a	842	CLA	CHC-C1C	2.79	1.42	1.35
27	a	820	CLA	C1D-ND	2.79	1.41	1.37
27	F	317	CLA	CHC-C1C	2.79	1.42	1.35
27	M	318	CLA	CHC-C1C	2.79	1.42	1.35
27	G	308	CLA	C4D-ND	-2.79	1.33	1.37
27	C	310	CLA	CHC-C1C	2.79	1.42	1.35
27	J	315	CLA	CHC-C1C	2.79	1.42	1.35
31	a	833	LHG	O8-C6	-2.79	1.38	1.45
27	E	310	CLA	C4D-ND	-2.79	1.33	1.37
27	a	805	CLA	C1D-ND	2.79	1.41	1.37
27	E	313	CLA	C1D-ND	2.78	1.41	1.37
28	K	308	KC1	C4A-C3A	-2.78	1.39	1.44
27	a	839	CLA	C1D-ND	2.78	1.41	1.37
27	M	308	CLA	CMB-C2B	-2.78	1.45	1.51
27	b	825	CLA	CMD-C2D	-2.78	1.44	1.50
27	B	306	CLA	CHC-C1C	2.78	1.42	1.35
30	B	302	A86	C-C1	-2.78	1.45	1.50
27	H	210	CLA	C1D-ND	2.78	1.41	1.37
27	C	314	CLA	CMB-C2B	-2.78	1.45	1.51
27	K	311	CLA	CHC-C1C	2.78	1.42	1.35
27	M	312	CLA	C1D-ND	2.77	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	312	KC1	CBA-CGA	-2.77	1.42	1.48
27	J	315	CLA	CMB-C2B	-2.77	1.45	1.51
27	C	317	CLA	CHC-C1C	2.77	1.42	1.35
26	A	202	DD6	C36-C31	-2.77	1.31	1.34
30	J	301	A86	O1-C20	-2.77	1.42	1.46
27	M	317	CLA	C3B-C2B	-2.77	1.36	1.40
27	D	208	CLA	C3B-C2B	-2.77	1.36	1.40
27	a	840	CLA	C4D-ND	-2.77	1.33	1.37
27	H	212	CLA	CMB-C2B	-2.77	1.45	1.51
27	I	307	CLA	CHC-C1C	2.77	1.42	1.35
27	H	207	CLA	CMB-C2B	-2.76	1.45	1.51
29	D	202	LMG	O7-C8	-2.76	1.39	1.46
27	H	205	CLA	C1D-ND	2.76	1.41	1.37
26	H	202	DD6	C36-C31	-2.76	1.31	1.34
27	a	822	CLA	CMB-C2B	-2.76	1.45	1.51
27	a	809	CLA	CHC-C1C	2.76	1.42	1.35
27	K	310	CLA	CMB-C2B	-2.76	1.45	1.51
27	C	309	CLA	CHC-C1C	2.76	1.42	1.35
27	b	817	CLA	C4D-ND	-2.76	1.33	1.37
27	D	216	CLA	CMB-C2B	-2.76	1.45	1.51
27	I	315	CLA	CMB-C2B	-2.76	1.45	1.51
27	M	319	CLA	CMB-C2B	-2.76	1.45	1.51
27	I	311	CLA	CMB-C2B	-2.76	1.45	1.51
32	a	851	BCR	C30-C25	-2.75	1.50	1.53
27	E	313	CLA	CMB-C2B	-2.75	1.45	1.51
27	a	827	CLA	CHC-C1C	2.75	1.42	1.35
27	b	825	CLA	C1D-ND	2.75	1.41	1.37
28	F	312	KC1	C4B-NB	-2.75	1.34	1.37
27	I	308	CLA	CMB-C2B	-2.75	1.45	1.51
29	A	214	LMG	O8-C28	2.75	1.41	1.33
27	a	843	CLA	C1D-ND	2.75	1.41	1.37
27	L	312	CLA	CMB-C2B	-2.75	1.45	1.51
27	b	838	CLA	C3B-C2B	-2.74	1.36	1.40
27	L	310	CLA	CMB-C2B	-2.74	1.45	1.51
35	l	207	ET4	C37-C38	-2.74	1.46	1.51
27	a	856	CLA	CHC-C1C	2.74	1.42	1.35
28	G	313	KC1	C4B-NB	-2.74	1.34	1.37
27	I	315	CLA	CHC-C1C	2.74	1.42	1.35
27	C	316	CLA	CMB-C2B	-2.74	1.46	1.51
26	D	205	DD6	C-C1	-2.73	1.45	1.50
26	K	303	DD6	C17-C16	-2.73	1.50	1.54
27	M	316	CLA	C3B-C2B	-2.73	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	308	KC1	CBA-CGA	-2.73	1.42	1.48
27	a	815	CLA	CMB-C2B	-2.73	1.46	1.51
27	A	204	CLA	CMB-C2B	-2.73	1.46	1.51
27	b	812	CLA	CHC-C1C	2.73	1.42	1.35
27	b	809	CLA	CMB-C2B	-2.73	1.46	1.51
27	H	209	CLA	CMB-C2B	-2.73	1.46	1.51
27	H	213	CLA	C1D-ND	2.73	1.41	1.37
27	I	314	CLA	CMB-C2B	-2.73	1.46	1.51
27	H	205	CLA	CHC-C1C	2.72	1.42	1.35
27	H	210	CLA	CMB-C2B	-2.72	1.46	1.51
27	H	212	CLA	C1D-ND	2.72	1.41	1.37
27	L	307	CLA	CMB-C2B	-2.72	1.46	1.51
27	L	308	CLA	CMB-C2B	-2.72	1.46	1.51
28	L	320	KC1	C4B-NB	-2.72	1.34	1.37
29	J	317	LMG	O1-C1	-2.72	1.35	1.40
27	A	210	CLA	CHC-C1C	2.72	1.41	1.35
27	H	209	CLA	C1D-ND	2.72	1.41	1.37
27	H	207	CLA	CHC-C1C	2.72	1.41	1.35
28	C	308	KC1	C4B-NB	-2.72	1.34	1.37
27	L	318	CLA	CMB-C2B	-2.71	1.46	1.51
27	I	316	CLA	CMB-C2B	-2.71	1.46	1.51
27	M	308	CLA	CHC-C1C	2.71	1.41	1.35
27	a	820	CLA	CHC-C1C	2.71	1.41	1.35
27	K	314	CLA	CHC-C1C	2.71	1.41	1.35
27	a	839	CLA	CHC-C1C	2.70	1.41	1.35
27	I	313	CLA	CMB-C2B	-2.70	1.46	1.51
27	I	314	CLA	C3B-C2B	-2.70	1.36	1.40
26	K	303	DD6	C21-C20	-2.70	1.47	1.51
27	b	830	CLA	CHC-C1C	2.70	1.41	1.35
28	L	314	KC1	C1B-NB	-2.70	1.34	1.37
27	a	803	CLA	CHC-C1C	2.69	1.41	1.35
27	M	316	CLA	CHC-C1C	2.69	1.41	1.35
27	J	309	CLA	CHC-C1C	2.69	1.41	1.35
27	M	310	CLA	CMD-C2D	-2.69	1.45	1.50
27	C	318	CLA	CMD-C2D	-2.69	1.45	1.50
27	b	801	CLA	CHC-C1C	2.69	1.41	1.35
27	L	315	CLA	CMB-C2B	-2.69	1.46	1.51
30	I	303	A86	O1-C20	-2.69	1.42	1.46
27	L	309	CLA	CMB-C2B	-2.69	1.46	1.51
27	b	812	CLA	C3B-C2B	-2.68	1.36	1.40
31	a	801	LHG	O8-C6	-2.68	1.39	1.45
27	b	804	CLA	C3B-CAB	-2.68	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	313	CLA	C3B-C2B	-2.68	1.36	1.40
27	l	204	CLA	CHC-C1C	2.68	1.41	1.35
27	E	311	CLA	C3B-C2B	-2.68	1.36	1.40
27	M	310	CLA	CMB-C2B	-2.68	1.46	1.51
29	I	319	LMG	O8-C28	2.67	1.41	1.33
27	C	318	CLA	C3B-C2B	-2.67	1.36	1.40
27	b	821	CLA	CMD-C2D	-2.67	1.45	1.50
27	b	825	CLA	CHC-C1C	2.67	1.41	1.35
27	D	207	CLA	C1D-ND	2.67	1.41	1.37
27	C	317	CLA	C3B-CAB	-2.67	1.42	1.47
32	a	851	BCR	C1-C6	-2.66	1.50	1.53
27	M	318	CLA	C3B-C2B	-2.66	1.36	1.40
27	A	211	CLA	CMB-C2B	-2.66	1.46	1.51
27	b	801	CLA	C1D-ND	2.66	1.41	1.37
27	b	804	CLA	CMD-C2D	-2.66	1.45	1.50
27	a	805	CLA	CHC-C1C	2.66	1.41	1.35
27	D	208	CLA	C1D-ND	2.66	1.41	1.37
27	B	314	CLA	CMB-C2B	-2.66	1.46	1.51
27	b	844	CLA	C1D-ND	2.65	1.41	1.37
30	L	302	A86	O1-C20	-2.65	1.42	1.46
27	J	313	CLA	CMB-C2B	-2.65	1.46	1.51
27	J	314	CLA	CMB-C2B	-2.65	1.46	1.51
27	b	812	CLA	CMC-C2C	-2.65	1.45	1.50
27	b	850	CLA	CMB-C2B	-2.64	1.46	1.51
30	C	302	A86	C32-C31	-2.64	1.50	1.54
27	L	316	CLA	CMB-C2B	-2.64	1.46	1.51
27	K	319	CLA	CMB-C2B	-2.64	1.46	1.51
27	M	316	CLA	CAA-C2A	-2.64	1.49	1.54
27	F	309	CLA	CMD-C2D	-2.64	1.45	1.50
27	I	309	CLA	CMB-C2B	-2.64	1.46	1.51
27	C	318	CLA	C3B-CAB	-2.64	1.42	1.47
27	a	844	CLA	CHC-C1C	2.63	1.41	1.35
27	b	804	CLA	C1D-ND	2.63	1.41	1.37
27	b	804	CLA	MG-ND	-2.63	2.00	2.05
27	M	317	CLA	CMB-C2B	-2.63	1.46	1.51
27	b	821	CLA	C3B-C2B	-2.63	1.36	1.40
27	a	803	CLA	CMD-C2D	-2.63	1.45	1.50
27	a	856	CLA	C3B-C2B	-2.63	1.36	1.40
26	M	306	DD6	C17-C16	-2.63	1.50	1.54
29	C	319	LMG	O6-C1	2.63	1.48	1.41
31	D	201	LHG	O8-C6	-2.62	1.39	1.45
29	C	319	LMG	O8-C28	2.62	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	319	CLA	CMB-C2B	-2.62	1.46	1.51
28	A	209	KC1	C1B-NB	-2.62	1.34	1.37
27	C	317	CLA	CMD-C2D	-2.62	1.45	1.50
27	H	207	CLA	C3B-C2B	-2.62	1.36	1.40
32	b	840	BCR	C30-C25	-2.61	1.50	1.53
27	H	213	CLA	CHC-C1C	2.61	1.41	1.35
29	E	317	LMG	O8-C28	2.61	1.41	1.33
27	A	205	CLA	CMB-C2B	-2.61	1.46	1.51
30	J	316	A86	O1-C20	-2.60	1.42	1.46
29	A	212	LMG	O7-C10	2.60	1.41	1.34
29	L	323	LMG	O7-C10	2.60	1.41	1.34
27	M	307	CLA	C3B-C2B	-2.60	1.36	1.40
27	b	814	CLA	CMB-C2B	-2.59	1.46	1.51
28	K	315	KC1	C4A-C3A	-2.59	1.39	1.44
27	E	311	CLA	CMD-C2D	-2.59	1.45	1.50
27	b	821	CLA	CHC-C1C	2.59	1.41	1.35
27	a	839	CLA	C3B-C2B	-2.59	1.36	1.40
27	C	318	CLA	C1D-ND	2.59	1.41	1.37
27	a	803	CLA	C3B-CAB	-2.59	1.42	1.47
27	M	307	CLA	C1D-ND	2.58	1.41	1.37
29	M	321	LMG	O8-C28	2.58	1.40	1.33
30	D	204	A86	C13-C11	-2.58	1.44	1.49
27	I	316	CLA	CHC-C1C	2.58	1.41	1.35
31	H	215	LHG	O8-C6	-2.58	1.39	1.45
30	D	204	A86	C2-C1	-2.58	1.32	1.35
27	A	208	CLA	C3B-C2B	-2.58	1.36	1.40
27	b	829	CLA	CMB-C2B	-2.58	1.46	1.51
27	a	839	CLA	CMD-C2D	-2.58	1.45	1.50
27	C	317	CLA	C3B-C2B	-2.58	1.36	1.40
27	a	817	CLA	CMB-C2B	-2.58	1.46	1.51
30	D	203	A86	C13-C11	-2.58	1.44	1.49
27	K	318	CLA	CMB-C2B	-2.58	1.46	1.51
27	H	209	CLA	CHC-C1C	2.58	1.41	1.35
27	M	317	CLA	CMD-C2D	-2.58	1.45	1.50
27	F	309	CLA	CMB-C2B	-2.58	1.46	1.51
27	l	204	CLA	C3B-C2B	-2.57	1.36	1.40
29	j	103	LMG	O7-C8	-2.57	1.40	1.46
30	B	304	A86	C32-C31	-2.57	1.50	1.54
27	D	217	CLA	CMB-C2B	-2.57	1.46	1.51
27	b	830	CLA	CMD-C2D	-2.57	1.45	1.50
27	a	804	CLA	CMB-C2B	-2.57	1.46	1.51
27	I	305	CLA	CMB-C2B	-2.57	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	306	CLA	CMB-C2B	-2.57	1.46	1.51
27	a	856	CLA	C3B-CAB	-2.57	1.42	1.47
30	M	305	A86	O1-C20	-2.57	1.42	1.46
30	I	301	A86	O1-C20	-2.57	1.42	1.46
31	a	837	LHG	O8-C6	-2.57	1.39	1.45
27	a	820	CLA	CMD-C2D	-2.57	1.45	1.50
27	E	311	CLA	C3B-CAB	-2.56	1.42	1.47
27	J	311	CLA	CMB-C2B	-2.56	1.46	1.51
27	a	827	CLA	C1D-ND	2.56	1.40	1.37
27	M	313	CLA	C3B-C2B	-2.56	1.36	1.40
30	C	302	A86	C13-C11	-2.56	1.44	1.49
27	l	203	CLA	CMD-C2D	-2.56	1.45	1.50
27	a	839	CLA	CMC-C2C	-2.56	1.45	1.50
27	K	317	CLA	C3B-CAB	-2.56	1.42	1.47
30	E	301	A86	C32-C31	-2.55	1.50	1.54
27	b	805	CLA	C3B-C2B	-2.55	1.36	1.40
30	K	307	A86	O1-C20	-2.55	1.42	1.46
27	a	815	CLA	C3B-C2B	-2.55	1.36	1.40
27	a	843	CLA	CMD-C2D	-2.55	1.45	1.50
27	b	812	CLA	C1D-ND	2.55	1.40	1.37
26	M	306	DD6	O1-C20	-2.55	1.42	1.46
30	J	304	A86	C32-C31	-2.55	1.50	1.54
27	E	314	CLA	CMB-C2B	-2.55	1.46	1.51
27	a	814	CLA	CMB-C2B	-2.55	1.46	1.51
27	C	310	CLA	CMB-C2B	-2.55	1.46	1.51
30	F	301	A86	C13-C11	-2.54	1.44	1.49
27	K	311	CLA	C3B-C2B	-2.54	1.36	1.40
27	H	206	CLA	CHC-C1C	2.54	1.41	1.35
31	I	318	LHG	O8-C6	-2.54	1.39	1.45
30	J	304	A86	O1-C20	-2.54	1.42	1.46
27	a	809	CLA	CAA-C2A	-2.54	1.49	1.54
27	M	316	CLA	C3B-CAB	-2.54	1.42	1.47
26	E	303	DD6	C-C1	-2.54	1.45	1.50
27	C	311	CLA	C3B-C2B	-2.54	1.36	1.40
27	A	211	CLA	CMD-C2D	-2.54	1.45	1.50
27	M	307	CLA	CMD-C2D	-2.53	1.45	1.50
27	C	317	CLA	C1D-ND	2.53	1.40	1.37
31	E	318	LHG	O8-C6	-2.53	1.39	1.45
27	b	817	CLA	CMB-C2B	-2.53	1.46	1.51
28	I	312	KC1	C4A-C3A	-2.53	1.39	1.44
27	b	821	CLA	C3B-CAB	-2.53	1.42	1.47
27	l	203	CLA	C3B-C2B	-2.53	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	305	DD6	O1-C20	-2.53	1.42	1.46
27	a	809	CLA	C3B-C2B	-2.53	1.36	1.40
30	b	848	A86	C32-C31	-2.53	1.50	1.54
27	B	307	CLA	CMB-C2B	-2.53	1.46	1.51
27	a	839	CLA	MG-ND	-2.53	2.00	2.05
30	r	202	A86	C32-C31	-2.52	1.50	1.54
27	J	312	CLA	C3B-C2B	-2.52	1.36	1.40
27	B	306	CLA	CBD-CAD	2.52	1.57	1.51
27	G	311	CLA	CMB-C2B	-2.52	1.46	1.51
29	J	317	LMG	O8-C28	2.52	1.40	1.33
27	H	210	CLA	CMC-C2C	-2.52	1.45	1.50
31	I	318	LHG	O7-C5	-2.52	1.40	1.46
27	a	841	CLA	CMB-C2B	-2.52	1.46	1.51
27	a	844	CLA	CMD-C2D	-2.52	1.45	1.50
30	K	305	A86	O1-C20	-2.52	1.42	1.46
27	b	822	CLA	CMB-C2B	-2.52	1.46	1.51
27	D	208	CLA	CMC-C2C	-2.52	1.45	1.50
27	F	317	CLA	CMB-C2B	-2.52	1.46	1.51
27	b	815	CLA	CMB-C2B	-2.52	1.46	1.51
27	L	317	CLA	CMB-C2B	-2.52	1.46	1.51
27	D	212	CLA	CMB-C2B	-2.51	1.46	1.51
28	J	306	KC1	C4A-C3A	-2.51	1.39	1.44
27	C	309	CLA	C3B-C2B	-2.51	1.36	1.40
27	a	824	CLA	CMB-C2B	-2.51	1.46	1.51
31	a	833	LHG	O7-C5	-2.51	1.40	1.46
27	I	314	CLA	C3B-CAB	-2.51	1.42	1.47
27	b	801	CLA	CMC-C2C	-2.51	1.45	1.50
27	E	309	CLA	CMB-C2B	-2.51	1.46	1.51
27	b	810	CLA	CMB-C2B	-2.51	1.46	1.51
27	b	828	CLA	CMB-C2B	-2.51	1.46	1.51
27	D	207	CLA	C3B-C2B	-2.51	1.36	1.40
27	M	317	CLA	C3B-CAB	-2.51	1.42	1.47
27	a	821	CLA	CMB-C2B	-2.51	1.46	1.51
28	C	308	KC1	C1B-NB	-2.51	1.34	1.37
27	b	843	CLA	CMB-C2B	-2.51	1.46	1.51
27	M	309	CLA	CMD-C2D	-2.51	1.45	1.50
27	H	205	CLA	C3B-C2B	-2.51	1.36	1.40
27	a	823	CLA	CMB-C2B	-2.51	1.46	1.51
27	b	826	CLA	CMB-C2B	-2.51	1.46	1.51
30	K	306	A86	O1-C20	-2.50	1.42	1.46
27	a	842	CLA	CMD-C2D	-2.50	1.45	1.50
27	F	316	CLA	CMB-C2B	-2.50	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	843	CLA	C3B-C2B	-2.50	1.36	1.40
27	B	311	CLA	CMB-C2B	-2.50	1.46	1.51
27	a	828	CLA	CMB-C2B	-2.50	1.46	1.51
32	b	840	BCR	C1-C6	-2.50	1.50	1.53
27	K	319	CLA	C3B-CAB	-2.50	1.42	1.47
27	a	854	CLA	CMB-C2B	-2.50	1.46	1.51
27	b	849	CLA	CMB-C2B	-2.50	1.46	1.51
27	b	846	CLA	CMB-C2B	-2.49	1.46	1.51
30	C	304	A86	C13-C11	-2.49	1.44	1.49
26	L	303	DD6	C36-C31	-2.49	1.32	1.34
31	K	320	LHG	O8-C6	-2.49	1.39	1.45
27	I	307	CLA	CMD-C2D	-2.49	1.45	1.50
27	b	812	CLA	CMD-C2D	-2.49	1.45	1.50
27	H	209	CLA	CMD-C2D	-2.49	1.45	1.50
27	a	810	CLA	CMB-C2B	-2.49	1.46	1.51
27	a	850	CLA	CMB-C2B	-2.49	1.46	1.51
27	b	845	CLA	CMB-C2B	-2.49	1.46	1.51
27	B	309	CLA	CMB-C2B	-2.49	1.46	1.51
27	F	309	CLA	CHC-C1C	2.49	1.41	1.35
27	E	311	CLA	MG-ND	-2.49	2.00	2.05
27	H	210	CLA	C3B-CAB	-2.49	1.42	1.47
26	L	303	DD6	C21-C20	-2.49	1.47	1.51
27	D	213	CLA	CMB-C2B	-2.49	1.46	1.51
27	b	841	CLA	CMB-C2B	-2.49	1.46	1.51
30	F	301	A86	O1-C20	-2.49	1.42	1.46
27	G	317	CLA	CMB-C2B	-2.49	1.46	1.51
27	a	843	CLA	CMC-C2C	-2.48	1.45	1.50
27	F	308	CLA	CMB-C2B	-2.48	1.46	1.51
27	G	306	CLA	CMB-C2B	-2.48	1.46	1.51
27	i	101	CLA	CMB-C2B	-2.48	1.46	1.51
27	l	204	CLA	C1D-ND	2.48	1.40	1.37
27	a	846	CLA	CMB-C2B	-2.48	1.46	1.51
29	a	852	LMG	O8-C28	2.48	1.40	1.33
27	M	315	CLA	CMB-C2B	-2.48	1.46	1.51
27	D	216	CLA	CMD-C2D	-2.48	1.45	1.50
27	b	824	CLA	CMB-C2B	-2.48	1.46	1.51
27	a	856	CLA	CMC-C2C	-2.48	1.45	1.50
27	b	825	CLA	CMC-C2C	-2.48	1.45	1.50
27	b	806	CLA	CMB-C2B	-2.48	1.46	1.51
27	C	317	CLA	MG-ND	-2.47	2.00	2.05
27	B	310	CLA	CMB-C2B	-2.47	1.46	1.51
27	a	825	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	G	310	CLA	CMB-C2B	-2.47	1.46	1.51
27	a	815	CLA	CMD-C2D	-2.47	1.45	1.50
27	M	313	CLA	C3B-CAB	-2.47	1.42	1.47
27	b	830	CLA	CMC-C2C	-2.47	1.45	1.50
29	E	317	LMG	O7-C8	-2.47	1.40	1.46
27	I	317	CLA	CMB-C2B	-2.47	1.46	1.51
27	C	306	CLA	CMB-C2B	-2.47	1.46	1.51
27	H	205	CLA	C3B-CAB	-2.47	1.42	1.47
27	l	204	CLA	CMC-C2C	-2.47	1.45	1.50
27	M	309	CLA	C3B-C2B	-2.47	1.36	1.40
27	F	315	CLA	CMB-C2B	-2.47	1.46	1.51
30	K	302	A86	O1-C20	-2.47	1.42	1.46
27	B	312	CLA	CMB-C2B	-2.47	1.46	1.51
27	b	847	CLA	CMB-C2B	-2.47	1.46	1.51
27	G	312	CLA	CMB-C2B	-2.47	1.46	1.51
27	a	816	CLA	CMB-C2B	-2.46	1.46	1.51
27	b	804	CLA	CHC-C1C	2.46	1.41	1.35
27	b	818	CLA	CMB-C2B	-2.46	1.46	1.51
30	b	848	A86	O1-C20	-2.46	1.42	1.46
27	J	310	CLA	CMB-C2B	-2.46	1.46	1.51
27	H	210	CLA	CMD-C2D	-2.46	1.45	1.50
27	b	807	CLA	CMB-C2B	-2.46	1.46	1.51
27	b	844	CLA	CMD-C2D	-2.46	1.45	1.50
27	b	812	CLA	C3B-CAB	-2.46	1.42	1.47
27	b	801	CLA	CMD-C2D	-2.46	1.45	1.50
27	D	215	CLA	CMB-C2B	-2.46	1.46	1.51
27	a	842	CLA	CMC-C2C	-2.46	1.45	1.50
27	l	204	CLA	CMD-C2D	-2.46	1.45	1.50
27	E	310	CLA	CMB-C2B	-2.46	1.46	1.51
27	b	811	CLA	CMB-C2B	-2.46	1.46	1.51
27	C	309	CLA	CMD-C2D	-2.46	1.45	1.50
30	C	304	A86	C32-C31	-2.46	1.50	1.54
27	a	805	CLA	C3B-C2B	-2.46	1.37	1.40
27	a	818	CLA	CMB-C2B	-2.46	1.46	1.51
27	E	313	CLA	CMD-C2D	-2.45	1.45	1.50
27	b	813	CLA	CMB-C2B	-2.45	1.46	1.51
27	C	314	CLA	C3B-C2B	-2.45	1.37	1.40
27	F	313	CLA	CMB-C2B	-2.45	1.46	1.51
27	b	820	CLA	CMB-C2B	-2.45	1.46	1.51
27	F	311	CLA	CMB-C2B	-2.45	1.46	1.51
26	H	202	DD6	C17-C16	-2.45	1.50	1.54
27	a	827	CLA	CMD-C2D	-2.45	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	802	LHG	O8-C6	-2.45	1.39	1.45
27	H	208	CLA	CMB-C2B	-2.45	1.46	1.51
27	a	832	CLA	CMB-C2B	-2.45	1.46	1.51
27	b	839	CLA	CMB-C2B	-2.45	1.46	1.51
27	b	804	CLA	CMC-C2C	-2.45	1.45	1.50
27	D	209	CLA	CMB-C2B	-2.45	1.46	1.51
27	b	819	CLA	CMB-C2B	-2.45	1.46	1.51
27	K	319	CLA	CMD-C2D	-2.45	1.45	1.50
27	L	312	CLA	CMD-C2D	-2.45	1.45	1.50
31	K	320	LHG	P-O3	2.45	1.64	1.54
27	a	807	CLA	CMB-C2B	-2.45	1.46	1.51
27	K	317	CLA	CMD-C2D	-2.45	1.45	1.50
27	C	314	CLA	CMD-C2D	-2.45	1.45	1.50
27	a	811	CLA	CMB-C2B	-2.44	1.46	1.51
31	M	320	LHG	O7-C5	-2.44	1.40	1.46
27	a	805	CLA	CMD-C2D	-2.44	1.45	1.50
27	H	214	CLA	CMB-C2B	-2.44	1.46	1.51
27	M	308	CLA	C3B-C2B	-2.44	1.37	1.40
27	j	104	CLA	CMB-C2B	-2.44	1.46	1.51
30	M	303	A86	C32-C31	-2.44	1.50	1.54
27	C	316	CLA	CMD-C2D	-2.44	1.45	1.50
27	M	308	CLA	CMD-C2D	-2.44	1.45	1.50
28	L	322	KC1	C4A-C3A	-2.44	1.39	1.44
29	C	319	LMG	O7-C10	2.44	1.41	1.34
27	A	203	CLA	CMB-C2B	-2.44	1.46	1.51
27	a	812	CLA	CMB-C2B	-2.44	1.46	1.51
26	K	303	DD6	O1-C20	-2.44	1.42	1.46
27	f	302	CLA	CMB-C2B	-2.44	1.46	1.51
27	D	211	CLA	CMB-C2B	-2.44	1.46	1.51
31	b	836	LHG	O7-C5	-2.44	1.40	1.46
27	M	308	CLA	C3B-CAB	-2.44	1.43	1.47
27	a	849	CLA	CMB-C2B	-2.44	1.46	1.51
27	f	303	CLA	CMB-C2B	-2.44	1.46	1.51
27	M	312	CLA	CMD-C2D	-2.44	1.45	1.50
27	b	844	CLA	C3B-C2B	-2.44	1.37	1.40
27	b	838	CLA	CMD-C2D	-2.44	1.45	1.50
27	D	210	CLA	C3B-C2B	-2.44	1.37	1.40
27	E	312	CLA	CMB-C2B	-2.44	1.46	1.51
27	a	813	CLA	CMB-C2B	-2.44	1.46	1.51
27	C	316	CLA	C3B-C2B	-2.44	1.37	1.40
26	H	202	DD6	C19-C18	-2.43	1.48	1.52
27	J	308	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	r	201	CLA	CMB-C2B	-2.43	1.46	1.51
27	K	316	CLA	CMD-C2D	-2.43	1.45	1.50
27	M	310	CLA	C3B-C2B	-2.43	1.37	1.40
27	a	809	CLA	CMD-C2D	-2.43	1.45	1.50
27	I	311	CLA	C1D-ND	2.43	1.40	1.37
27	a	829	CLA	CMB-C2B	-2.43	1.46	1.51
27	I	316	CLA	MG-ND	-2.43	2.01	2.05
27	l	206	CLA	CMB-C2B	-2.43	1.46	1.51
29	M	321	LMG	O7-C8	-2.43	1.40	1.46
29	l	201	LMG	O7-C8	-2.43	1.40	1.46
27	b	831	CLA	CMB-C2B	-2.43	1.46	1.51
27	F	306	CLA	CMB-C2B	-2.43	1.46	1.51
27	a	830	CLA	CMB-C2B	-2.43	1.46	1.51
27	a	848	CLA	CMB-C2B	-2.43	1.46	1.51
31	a	837	LHG	O7-C5	-2.43	1.40	1.46
27	M	316	CLA	CMD-C2D	-2.42	1.45	1.50
27	G	308	CLA	CMB-C2B	-2.42	1.46	1.51
35	l	207	ET4	C19-C18	2.42	1.51	1.45
27	H	206	CLA	CMC-C2C	-2.42	1.45	1.50
27	a	839	CLA	C3B-CAB	-2.42	1.43	1.47
27	b	816	CLA	CMB-C2B	-2.42	1.46	1.51
27	B	308	CLA	CMB-C2B	-2.42	1.46	1.51
27	C	307	CLA	C3B-CAB	-2.42	1.43	1.47
29	C	301	LMG	O7-C10	2.42	1.41	1.34
29	A	212	LMG	O7-C8	-2.42	1.40	1.46
27	a	819	CLA	CMB-C2B	-2.42	1.46	1.51
27	J	311	CLA	CMD-C2D	-2.42	1.45	1.50
26	L	303	DD6	O1-C20	-2.42	1.42	1.46
29	I	319	LMG	O7-C8	-2.42	1.40	1.46
27	a	803	CLA	MG-ND	-2.42	2.01	2.05
27	b	844	CLA	CMC-C2C	-2.42	1.45	1.50
27	K	319	CLA	MG-ND	-2.42	2.01	2.05
27	a	806	CLA	CMB-C2B	-2.42	1.46	1.51
27	D	216	CLA	CMC-C2C	-2.42	1.45	1.50
27	A	206	CLA	CMB-C2B	-2.42	1.46	1.51
27	a	855	CLA	CMB-C2B	-2.42	1.46	1.51
27	a	809	CLA	CMC-C2C	-2.42	1.45	1.50
27	I	311	CLA	C3B-C2B	-2.42	1.37	1.40
26	J	305	DD6	C-C1	-2.42	1.45	1.50
27	a	815	CLA	CMC-C2C	-2.42	1.45	1.50
27	b	803	CLA	CMB-C2B	-2.42	1.46	1.51
27	b	808	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	207	CLA	C3B-CAB	-2.42	1.43	1.47
27	a	827	CLA	CMC-C2C	-2.41	1.45	1.50
31	M	320	LHG	O8-C6	-2.41	1.39	1.45
30	D	206	A86	C32-C31	-2.41	1.50	1.54
27	G	309	CLA	CMB-C2B	-2.41	1.46	1.51
31	E	318	LHG	O7-C5	-2.41	1.40	1.46
27	C	315	CLA	CMB-C2B	-2.41	1.46	1.51
27	b	801	CLA	C3B-CAB	-2.41	1.43	1.47
27	A	204	CLA	CMD-C2D	-2.41	1.45	1.50
27	b	805	CLA	CMC-C2C	-2.41	1.45	1.50
27	F	314	CLA	CMB-C2B	-2.41	1.46	1.51
27	D	207	CLA	CMD-C2D	-2.41	1.45	1.50
27	F	310	CLA	CMB-C2B	-2.41	1.46	1.51
27	M	318	CLA	C3B-CAB	-2.41	1.43	1.47
27	a	838	CLA	CMB-C2B	-2.41	1.46	1.51
27	H	210	CLA	C3B-C2B	-2.41	1.37	1.40
30	b	848	A86	C17-C16	-2.41	1.50	1.54
27	I	306	CLA	CMB-C2B	-2.41	1.46	1.51
27	a	808	CLA	CMB-C2B	-2.41	1.46	1.51
26	I	304	DD6	C21-C20	-2.41	1.48	1.51
27	H	204	CLA	CMD-C2D	-2.41	1.45	1.50
27	I	311	CLA	CMC-C2C	-2.41	1.45	1.50
27	I	311	CLA	CMD-C2D	-2.41	1.45	1.50
27	D	214	CLA	CMB-C2B	-2.41	1.46	1.51
27	K	310	CLA	CMD-C2D	-2.41	1.45	1.50
27	b	825	CLA	MG-ND	-2.41	2.01	2.05
27	D	210	CLA	CMD-C2D	-2.41	1.45	1.50
27	K	314	CLA	CMD-C2D	-2.40	1.45	1.50
27	a	805	CLA	CMC-C2C	-2.40	1.45	1.50
27	D	208	CLA	C3B-CAB	-2.40	1.43	1.47
27	H	206	CLA	CMD-C2D	-2.40	1.45	1.50
30	B	301	A86	O1-C20	-2.40	1.42	1.46
27	K	312	CLA	CMD-C2D	-2.40	1.45	1.50
27	b	842	CLA	CMB-C2B	-2.40	1.46	1.51
27	a	842	CLA	C3B-CAB	-2.40	1.43	1.47
27	G	315	CLA	CMB-C2B	-2.40	1.46	1.51
27	H	207	CLA	CMD-C2D	-2.40	1.45	1.50
29	J	317	LMG	O7-C10	2.40	1.41	1.34
27	L	311	CLA	CMB-C2B	-2.40	1.46	1.51
27	H	209	CLA	CMC-C2C	-2.39	1.45	1.50
29	C	319	LMG	O7-C8	-2.39	1.40	1.46
27	G	314	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	207	CLA	C3B-C2B	-2.39	1.37	1.40
28	L	320	KC1	C1B-NB	-2.39	1.34	1.37
27	G	316	CLA	CMB-C2B	-2.39	1.46	1.51
27	b	827	CLA	CMB-C2B	-2.39	1.46	1.51
29	L	323	LMG	O1-C1	-2.39	1.36	1.40
27	a	856	CLA	CMD-C2D	-2.39	1.45	1.50
27	G	307	CLA	CMB-C2B	-2.39	1.46	1.51
27	H	205	CLA	CMD-C2D	-2.39	1.45	1.50
27	C	307	CLA	CMC-C2C	-2.39	1.45	1.50
27	K	311	CLA	CMC-C2C	-2.39	1.45	1.50
27	a	826	CLA	CMB-C2B	-2.39	1.46	1.51
27	a	856	CLA	C1D-ND	2.39	1.40	1.37
30	M	302	A86	C2-C1	-2.39	1.32	1.35
30	K	301	A86	O1-C20	-2.39	1.42	1.46
27	L	309	CLA	C3B-C2B	-2.38	1.37	1.40
28	A	209	KC1	CHD-C4C	2.38	1.41	1.35
26	E	303	DD6	C17-C16	-2.38	1.50	1.54
27	D	208	CLA	CMD-C2D	-2.38	1.45	1.50
27	F	307	CLA	CMB-C2B	-2.38	1.46	1.51
27	b	823	CLA	CMB-C2B	-2.38	1.46	1.51
27	D	216	CLA	C3B-C2B	-2.38	1.37	1.40
27	f	301	CLA	CMB-C2B	-2.38	1.46	1.51
27	F	305	CLA	CMB-C2B	-2.38	1.46	1.51
27	H	207	CLA	CMC-C2C	-2.38	1.45	1.50
26	M	304	DD6	O1-C20	-2.38	1.42	1.46
27	I	305	CLA	C3B-CAB	-2.38	1.43	1.47
28	C	313	KC1	C4A-C3A	-2.38	1.40	1.44
27	I	315	CLA	C3B-C2B	-2.38	1.37	1.40
27	D	210	CLA	C3B-CAB	-2.38	1.43	1.47
27	L	321	CLA	C3B-C2B	-2.38	1.37	1.40
29	a	852	LMG	O7-C10	2.37	1.41	1.34
27	I	310	CLA	CMB-C2B	-2.37	1.46	1.51
27	J	307	CLA	CMD-C2D	-2.37	1.45	1.50
27	K	313	CLA	C3B-C2B	-2.37	1.37	1.40
27	b	814	CLA	CMC-C2C	-2.37	1.45	1.50
27	a	840	CLA	CMB-C2B	-2.37	1.46	1.51
27	E	315	CLA	CMB-C2B	-2.37	1.46	1.51
30	J	304	A86	O1-C15	-2.37	1.41	1.45
27	C	316	CLA	C3B-CAB	-2.37	1.43	1.47
27	E	308	CLA	CMB-C2B	-2.37	1.46	1.51
29	J	317	LMG	O7-C8	-2.37	1.40	1.46
27	H	206	CLA	C3B-CAB	-2.37	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	309	CLA	CMC-C2C	-2.37	1.45	1.50
27	J	312	CLA	C3B-CAB	-2.37	1.43	1.47
30	J	301	A86	C32-C31	-2.37	1.50	1.54
28	C	313	KC1	C1B-NB	-2.37	1.34	1.37
27	a	844	CLA	MG-ND	-2.37	2.01	2.05
27	I	307	CLA	C3B-C2B	-2.37	1.37	1.40
27	l	204	CLA	C3B-CAB	-2.37	1.43	1.47
27	C	312	CLA	CMD-C2D	-2.36	1.45	1.50
27	C	312	CLA	C3B-CAB	-2.36	1.43	1.47
33	J	318	SQD	O48-C23	2.36	1.40	1.33
27	a	842	CLA	MG-ND	-2.36	2.01	2.05
31	a	834	LHG	O8-C6	-2.36	1.39	1.45
30	K	304	A86	O1-C20	-2.36	1.42	1.46
27	K	313	CLA	C3B-CAB	-2.36	1.43	1.47
30	D	204	A86	C17-C16	-2.36	1.50	1.54
30	B	304	A86	C-C1	-2.36	1.46	1.50
27	M	312	CLA	C3B-CAB	-2.36	1.43	1.47
27	b	844	CLA	MG-ND	-2.36	2.01	2.05
27	H	213	CLA	CMD-C2D	-2.36	1.45	1.50
27	D	207	CLA	CMC-C2C	-2.36	1.45	1.50
28	C	313	KC1	CHD-C4C	2.36	1.41	1.35
27	I	305	CLA	C3B-C2B	-2.36	1.37	1.40
27	M	312	CLA	C3B-C2B	-2.36	1.37	1.40
27	a	856	CLA	MG-ND	-2.35	2.01	2.05
27	I	311	CLA	MG-ND	-2.35	2.01	2.05
27	a	843	CLA	MG-ND	-2.35	2.01	2.05
30	L	304	A86	O1-C20	-2.35	1.42	1.46
27	K	309	CLA	CMC-C2C	-2.35	1.45	1.50
27	J	310	CLA	C3B-CAB	-2.35	1.43	1.47
26	H	202	DD6	C35-C36	-2.35	1.47	1.51
31	a	837	LHG	O7-C7	2.35	1.40	1.35
27	l	203	CLA	CMC-C2C	-2.35	1.45	1.50
28	G	313	KC1	C1B-NB	-2.35	1.34	1.37
27	a	845	CLA	CMB-C2B	-2.35	1.46	1.51
27	B	314	CLA	MG-ND	-2.35	2.01	2.05
27	K	309	CLA	CMD-C2D	-2.35	1.45	1.50
35	l	207	ET4	C04-C05	-2.35	1.47	1.51
28	M	314	KC1	CHD-C4C	2.35	1.41	1.35
27	l	203	CLA	MG-ND	-2.34	2.01	2.05
32	l	202	BCR	C30-C25	-2.34	1.50	1.53
26	B	303	DD6	C36-C31	-2.34	1.32	1.34
32	a	835	BCR	C1-C6	-2.34	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	820	CLA	CMC-C2C	-2.34	1.45	1.50
27	L	315	CLA	C3B-C2B	-2.34	1.37	1.40
32	a	847	BCR	C1-C6	-2.34	1.50	1.53
27	b	805	CLA	CMD-C2D	-2.34	1.45	1.50
27	a	820	CLA	MG-ND	-2.34	2.01	2.05
30	K	307	A86	C32-C31	-2.34	1.50	1.54
27	M	309	CLA	CMC-C2C	-2.34	1.45	1.50
27	M	310	CLA	C3B-CAB	-2.34	1.43	1.47
27	K	310	CLA	CMC-C2C	-2.34	1.45	1.50
27	b	838	CLA	CMC-C2C	-2.34	1.45	1.50
31	a	837	LHG	O8-C23	2.34	1.40	1.33
29	C	301	LMG	O7-C8	-2.34	1.40	1.46
26	H	202	DD6	C21-C20	-2.33	1.48	1.51
29	M	321	LMG	O7-C10	2.33	1.40	1.34
27	b	801	CLA	MG-ND	-2.33	2.01	2.05
27	L	309	CLA	CMD-C2D	-2.33	1.45	1.50
29	A	214	LMG	O7-C10	2.33	1.40	1.34
30	b	848	A86	C13-C11	-2.33	1.45	1.49
31	j	102	LHG	O8-C23	2.33	1.40	1.33
27	a	844	CLA	C3B-CAB	-2.33	1.43	1.47
27	J	315	CLA	C3B-C2B	-2.33	1.37	1.40
27	H	213	CLA	CMC-C2C	-2.33	1.45	1.50
27	A	207	CLA	C3B-CAB	-2.33	1.43	1.47
30	K	306	A86	C32-C31	-2.33	1.50	1.54
27	L	321	CLA	CMD-C2D	-2.33	1.45	1.50
27	M	313	CLA	CMC-C2C	-2.33	1.45	1.50
27	C	314	CLA	CMC-C2C	-2.33	1.45	1.50
27	E	313	CLA	C3B-CAB	-2.33	1.43	1.47
27	a	805	CLA	C3B-CAB	-2.33	1.43	1.47
30	J	316	A86	C32-C31	-2.33	1.50	1.54
27	K	312	CLA	MG-ND	-2.32	2.01	2.05
27	H	207	CLA	C3B-CAB	-2.32	1.43	1.47
27	b	825	CLA	C3B-CAB	-2.32	1.43	1.47
27	H	205	CLA	CMC-C2C	-2.32	1.45	1.50
27	a	803	CLA	CMC-C2C	-2.32	1.45	1.50
27	J	309	CLA	CMC-C2C	-2.32	1.45	1.50
27	M	311	CLA	CMD-C2D	-2.32	1.45	1.50
31	H	215	LHG	O7-C7	2.32	1.40	1.34
28	C	308	KC1	CHD-C4C	2.32	1.40	1.35
31	j	102	LHG	O8-C6	-2.32	1.39	1.45
27	A	205	CLA	CMD-C2D	-2.32	1.45	1.50
27	M	319	CLA	C3B-C2B	-2.31	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	216	CLA	C3B-CAB	-2.31	1.43	1.47
27	E	311	CLA	CMC-C2C	-2.31	1.45	1.50
32	a	847	BCR	C30-C25	-2.31	1.50	1.53
27	K	313	CLA	CMD-C2D	-2.31	1.45	1.50
30	F	304	A86	O1-C20	-2.31	1.42	1.46
27	K	309	CLA	C3B-C2B	-2.31	1.37	1.40
27	K	312	CLA	C3B-C2B	-2.31	1.37	1.40
27	M	308	CLA	CMC-C2C	-2.31	1.45	1.50
31	D	201	LHG	O7-C5	-2.31	1.40	1.46
28	F	312	KC1	C1B-NB	-2.31	1.34	1.37
27	K	319	CLA	C3B-C2B	-2.31	1.37	1.40
27	M	311	CLA	MG-ND	-2.31	2.01	2.05
30	C	305	A86	C17-C16	-2.30	1.50	1.54
27	A	208	CLA	C3B-CAB	-2.30	1.43	1.47
27	M	308	CLA	MG-ND	-2.30	2.01	2.05
27	D	210	CLA	CMC-C2C	-2.30	1.45	1.50
27	L	315	CLA	C3B-CAB	-2.30	1.43	1.47
27	M	316	CLA	MG-ND	-2.30	2.01	2.05
27	L	308	CLA	CMD-C2D	-2.30	1.45	1.50
31	a	801	LHG	O7-C5	-2.30	1.40	1.46
30	H	201	A86	C17-C16	-2.30	1.50	1.54
27	C	312	CLA	CMC-C2C	-2.30	1.45	1.50
27	C	309	CLA	C3B-CAB	-2.30	1.43	1.47
27	I	314	CLA	CMC-C2C	-2.30	1.45	1.50
27	H	212	CLA	C3B-C2B	-2.30	1.37	1.40
27	K	314	CLA	CMC-C2C	-2.30	1.45	1.50
30	r	202	A86	C-C1	-2.30	1.46	1.50
27	H	209	CLA	MG-ND	-2.30	2.01	2.05
27	H	206	CLA	C3B-C2B	-2.30	1.37	1.40
31	a	834	LHG	O7-C7	2.30	1.40	1.34
31	j	102	LHG	O7-C7	2.30	1.40	1.34
27	a	815	CLA	C3B-CAB	-2.29	1.43	1.47
30	A	213	A86	O1-C20	-2.29	1.42	1.46
27	K	311	CLA	CMD-C2D	-2.29	1.45	1.50
31	a	834	LHG	O8-C23	2.29	1.40	1.33
27	J	307	CLA	C3B-C2B	-2.29	1.37	1.40
27	M	309	CLA	C3B-CAB	-2.29	1.43	1.47
27	a	844	CLA	CMC-C2C	-2.29	1.45	1.50
29	I	319	LMG	O7-C10	2.29	1.40	1.34
26	A	202	DD6	O1-C20	-2.29	1.42	1.46
27	A	204	CLA	CMC-C2C	-2.29	1.45	1.50
30	J	316	A86	C13-C11	-2.29	1.45	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	310	CLA	CMC-C2C	-2.29	1.45	1.50
26	I	304	DD6	O1-C20	-2.29	1.42	1.46
27	b	830	CLA	C3B-CAB	-2.29	1.43	1.47
27	I	307	CLA	CMC-C2C	-2.29	1.46	1.50
27	M	318	CLA	CMD-C2D	-2.29	1.46	1.50
30	K	307	A86	C13-C11	-2.29	1.45	1.49
28	L	320	KC1	CHD-C4C	2.28	1.40	1.35
27	E	315	CLA	CMD-C2D	-2.28	1.46	1.50
27	H	212	CLA	CMD-C2D	-2.28	1.46	1.50
28	A	209	KC1	C4A-C3A	-2.28	1.40	1.44
27	K	312	CLA	C3B-CAB	-2.28	1.43	1.47
27	b	822	CLA	CMD-C2D	-2.28	1.46	1.50
28	F	312	KC1	CHD-C4C	2.28	1.40	1.35
27	I	315	CLA	CMD-C2D	-2.28	1.46	1.50
27	b	825	CLA	C3B-C2B	-2.28	1.37	1.40
27	b	850	CLA	CMD-C2D	-2.28	1.46	1.50
28	G	313	KC1	CHD-C4C	2.28	1.40	1.35
27	J	311	CLA	CMC-C2C	-2.28	1.46	1.50
27	K	309	CLA	C3B-CAB	-2.28	1.43	1.47
27	I	309	CLA	CMD-C2D	-2.28	1.46	1.50
27	C	318	CLA	MG-ND	-2.28	2.01	2.05
27	b	838	CLA	C3B-CAB	-2.28	1.43	1.47
31	K	320	LHG	C26-C25	-2.28	1.35	1.51
27	M	307	CLA	C3B-CAB	-2.27	1.43	1.47
32	l	202	BCR	C1-C6	-2.27	1.50	1.53
27	J	312	CLA	CMC-C2C	-2.27	1.46	1.50
27	E	313	CLA	CMC-C2C	-2.27	1.46	1.50
27	A	207	CLA	CMD-C2D	-2.27	1.46	1.50
27	A	208	CLA	CMD-C2D	-2.27	1.46	1.50
27	K	312	CLA	CMC-C2C	-2.27	1.46	1.50
27	K	311	CLA	C3B-CAB	-2.27	1.43	1.47
31	a	802	LHG	O7-C5	-2.27	1.40	1.46
28	H	211	KC1	C1B-C2B	-2.27	1.40	1.45
27	B	310	CLA	CMD-C2D	-2.27	1.46	1.50
26	J	305	DD6	C36-C31	-2.27	1.32	1.34
27	H	205	CLA	MG-ND	-2.27	2.01	2.05
27	b	838	CLA	MG-ND	-2.27	2.01	2.05
27	A	208	CLA	CMC-C2C	-2.27	1.46	1.50
27	H	209	CLA	C3B-CAB	-2.27	1.43	1.47
30	B	302	A86	C17-C16	-2.27	1.51	1.54
27	M	311	CLA	CMC-C2C	-2.27	1.46	1.50
31	K	320	LHG	O7-C5	-2.26	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	827	CLA	C3B-CAB	-2.26	1.43	1.47
27	F	309	CLA	MG-ND	-2.26	2.01	2.05
26	E	306	DD6	C36-C31	-2.26	1.32	1.34
27	I	308	CLA	CMD-C2D	-2.26	1.46	1.50
27	I	316	CLA	C3B-C2B	-2.26	1.37	1.40
27	A	207	CLA	CMC-C2C	-2.26	1.46	1.50
27	C	307	CLA	MG-ND	-2.26	2.01	2.05
27	M	312	CLA	CAA-C2A	-2.26	1.49	1.54
27	I	313	CLA	CMD-C2D	-2.26	1.46	1.50
27	K	316	CLA	C3B-C2B	-2.26	1.37	1.40
30	L	306	A86	O1-C20	-2.26	1.43	1.46
27	C	316	CLA	CMC-C2C	-2.26	1.46	1.50
27	B	314	CLA	C3B-CAB	-2.26	1.43	1.47
27	H	210	CLA	MG-ND	-2.26	2.01	2.05
27	E	311	CLA	CAA-C2A	-2.26	1.49	1.54
27	M	313	CLA	CMD-C2D	-2.26	1.46	1.50
30	A	213	A86	C32-C31	-2.26	1.50	1.54
27	L	315	CLA	CMC-C2C	-2.25	1.46	1.50
27	C	314	CLA	C3B-CAB	-2.25	1.43	1.47
27	I	305	CLA	CMD-C2D	-2.25	1.46	1.50
27	A	210	CLA	CMD-C2D	-2.25	1.46	1.50
31	K	320	LHG	O8-C23	2.25	1.39	1.33
30	B	301	A86	C13-C11	-2.25	1.45	1.49
27	K	318	CLA	CMD-C2D	-2.25	1.46	1.50
30	L	305	A86	O1-C20	-2.25	1.43	1.46
27	I	317	CLA	CMC-C2C	-2.25	1.46	1.50
27	A	204	CLA	C3B-C2B	-2.25	1.37	1.40
30	C	305	A86	C13-C11	-2.25	1.45	1.49
29	C	301	LMG	O1-C1	-2.25	1.36	1.40
27	H	213	CLA	C3B-CAB	-2.25	1.43	1.47
27	H	212	CLA	CMC-C2C	-2.25	1.46	1.50
27	a	820	CLA	C3B-CAB	-2.24	1.43	1.47
27	M	307	CLA	MG-ND	-2.24	2.01	2.05
27	D	207	CLA	MG-ND	-2.24	2.01	2.05
29	A	214	LMG	O7-C8	-2.24	1.41	1.46
27	A	210	CLA	CMC-C2C	-2.24	1.46	1.50
27	I	309	CLA	CMC-C2C	-2.24	1.46	1.50
27	K	316	CLA	C3B-CAB	-2.24	1.43	1.47
27	M	307	CLA	CMC-C2C	-2.24	1.46	1.50
26	M	304	DD6	C36-C31	-2.24	1.32	1.34
27	b	805	CLA	MG-ND	-2.24	2.01	2.05
30	I	301	A86	C13-C11	-2.23	1.45	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	313	CLA	CMD-C2D	-2.23	1.46	1.50
27	M	316	CLA	CMC-C2C	-2.23	1.46	1.50
27	a	809	CLA	C3B-CAB	-2.23	1.43	1.47
27	I	315	CLA	CMC-C2C	-2.23	1.46	1.50
27	J	312	CLA	CMD-C2D	-2.23	1.46	1.50
27	K	316	CLA	CMC-C2C	-2.23	1.46	1.50
27	a	844	CLA	C3B-C2B	-2.23	1.37	1.40
30	B	304	A86	C2-C1	-2.23	1.32	1.35
27	A	204	CLA	C3B-CAB	-2.23	1.43	1.47
27	a	843	CLA	C3B-CAB	-2.23	1.43	1.47
27	b	805	CLA	C3B-CAB	-2.23	1.43	1.47
27	J	314	CLA	C3B-C2B	-2.23	1.37	1.40
27	J	307	CLA	CMC-C2C	-2.23	1.46	1.50
27	C	307	CLA	CMD-C2D	-2.23	1.46	1.50
31	a	802	LHG	O7-C7	2.23	1.40	1.34
27	J	312	CLA	MG-ND	-2.23	2.01	2.05
27	J	309	CLA	C3B-C2B	-2.23	1.37	1.40
27	I	308	CLA	CMC-C2C	-2.23	1.46	1.50
27	b	812	CLA	MG-ND	-2.23	2.01	2.05
27	I	314	CLA	CMD-C2D	-2.23	1.46	1.50
27	C	307	CLA	C3B-C2B	-2.23	1.37	1.40
27	M	317	CLA	CMC-C2C	-2.23	1.46	1.50
27	M	319	CLA	CMC-C2C	-2.23	1.46	1.50
27	I	307	CLA	C3B-CAB	-2.22	1.43	1.47
27	H	206	CLA	MG-ND	-2.22	2.01	2.05
27	L	316	CLA	CMD-C2D	-2.22	1.46	1.50
27	I	309	CLA	C3B-C2B	-2.22	1.37	1.40
27	I	316	CLA	CMD-C2D	-2.22	1.46	1.50
27	L	315	CLA	CMD-C2D	-2.22	1.46	1.50
27	b	821	CLA	CMC-C2C	-2.22	1.46	1.50
26	I	304	DD6	C19-C18	-2.22	1.49	1.52
27	H	204	CLA	CMC-C2C	-2.22	1.46	1.50
28	J	306	KC1	CHD-C4C	2.22	1.40	1.35
27	M	311	CLA	C3B-C2B	-2.22	1.37	1.40
27	b	849	CLA	CMD-C2D	-2.21	1.46	1.50
27	I	307	CLA	MG-ND	-2.21	2.01	2.05
27	A	210	CLA	C3B-C2B	-2.21	1.37	1.40
27	A	210	CLA	C3B-CAB	-2.21	1.43	1.47
27	L	310	CLA	C3B-CAB	-2.21	1.43	1.47
27	C	311	CLA	CMC-C2C	-2.21	1.46	1.50
27	b	804	CLA	C4B-CHC	-2.21	1.34	1.41
26	G	303	DD6	O1-C20	-2.21	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	313	KC1	C1B-C2B	-2.21	1.41	1.45
32	f	305	BCR	C1-C6	-2.21	1.50	1.53
28	L	314	KC1	CHD-C4C	2.21	1.40	1.35
27	L	315	CLA	MG-ND	-2.21	2.01	2.05
27	H	213	CLA	MG-ND	-2.21	2.01	2.05
31	a	834	LHG	O7-C5	-2.21	1.41	1.46
27	J	313	CLA	CMD-C2D	-2.21	1.46	1.50
27	L	319	CLA	CMD-C2D	-2.21	1.46	1.50
30	I	303	A86	C13-C11	-2.21	1.45	1.49
28	K	308	KC1	CHD-C4C	2.21	1.40	1.35
26	G	304	DD6	O1-C20	-2.20	1.43	1.46
27	L	310	CLA	CMD-C2D	-2.20	1.46	1.50
27	M	318	CLA	CMC-C2C	-2.20	1.46	1.50
27	L	321	CLA	C3B-CAB	-2.20	1.43	1.47
27	a	810	CLA	CMD-C2D	-2.20	1.46	1.50
30	A	213	A86	C13-C11	-2.20	1.45	1.49
26	M	304	DD6	C-C1	-2.20	1.46	1.50
27	L	319	CLA	CMC-C2C	-2.20	1.46	1.50
27	M	310	CLA	MG-ND	-2.19	2.01	2.05
27	K	317	CLA	CMC-C2C	-2.19	1.46	1.50
27	E	308	CLA	CMC-C2C	-2.19	1.46	1.50
27	H	212	CLA	C3B-CAB	-2.19	1.43	1.47
27	C	311	CLA	CMD-C2D	-2.19	1.46	1.50
29	j	103	LMG	O7-C10	2.19	1.40	1.34
27	L	318	CLA	CMD-C2D	-2.19	1.46	1.50
27	J	311	CLA	C3B-C2B	-2.19	1.37	1.40
28	B	313	KC1	CHD-C4C	2.19	1.40	1.35
27	b	804	CLA	CAA-C2A	-2.19	1.50	1.54
27	K	318	CLA	C3B-CAB	-2.19	1.43	1.47
27	L	307	CLA	CMD-C2D	-2.19	1.46	1.50
27	I	313	CLA	C3B-CAB	-2.19	1.43	1.47
27	I	311	CLA	C4B-CHC	-2.19	1.34	1.41
27	a	827	CLA	MG-ND	-2.19	2.01	2.05
31	I	318	LHG	O8-C23	2.19	1.39	1.33
27	C	318	CLA	CMC-C2C	-2.19	1.46	1.50
31	K	320	LHG	P-O6	2.18	1.67	1.60
28	M	314	KC1	C1B-C2B	-2.18	1.41	1.45
27	I	314	CLA	MG-ND	-2.18	2.01	2.05
27	I	317	CLA	CMD-C2D	-2.18	1.46	1.50
27	K	310	CLA	C3B-C2B	-2.18	1.37	1.40
27	J	310	CLA	MG-ND	-2.18	2.01	2.05
27	J	307	CLA	C3B-CAB	-2.18	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	311	CLA	C3B-CAB	-2.18	1.43	1.47
27	I	206	CLA	CMD-C2D	-2.18	1.46	1.50
26	A	201	DD6	C17-C16	-2.18	1.51	1.54
27	I	308	CLA	C3B-C2B	-2.18	1.37	1.40
27	a	805	CLA	CAA-C2A	-2.18	1.50	1.54
27	a	838	CLA	CMD-C2D	-2.17	1.46	1.50
27	a	820	CLA	C3B-C2B	-2.17	1.37	1.40
28	L	320	KC1	C4A-C3A	-2.17	1.40	1.44
27	I	311	CLA	C3B-CAB	-2.17	1.43	1.47
31	I	318	LHG	O7-C7	2.17	1.40	1.34
27	M	312	CLA	CMC-C2C	-2.17	1.46	1.50
27	J	313	CLA	CMC-C2C	-2.17	1.46	1.50
27	J	309	CLA	CMD-C2D	-2.17	1.46	1.50
27	J	311	CLA	C3B-CAB	-2.17	1.43	1.47
27	L	321	CLA	CMC-C2C	-2.17	1.46	1.50
27	D	217	CLA	CMD-C2D	-2.17	1.46	1.50
26	I	302	DD6	O1-C20	-2.17	1.43	1.46
27	B	306	CLA	MG-ND	-2.17	2.01	2.05
27	L	311	CLA	CMC-C2C	-2.17	1.46	1.50
31	a	801	LHG	O7-C7	2.17	1.40	1.34
27	K	318	CLA	C3B-C2B	-2.17	1.37	1.40
27	F	317	CLA	CMD-C2D	-2.17	1.46	1.50
27	A	205	CLA	CMC-C2C	-2.17	1.46	1.50
27	M	311	CLA	C3B-CAB	-2.17	1.43	1.47
27	a	832	CLA	CMC-C2C	-2.17	1.46	1.50
27	b	821	CLA	C4B-CHC	-2.16	1.35	1.41
29	C	319	LMG	C3-C2	-2.16	1.46	1.52
27	H	207	CLA	MG-ND	-2.16	2.01	2.05
27	b	830	CLA	MG-ND	-2.16	2.01	2.05
27	L	312	CLA	C3B-C2B	-2.16	1.37	1.40
27	a	807	CLA	CMD-C2D	-2.16	1.46	1.50
27	I	204	CLA	MG-ND	-2.16	2.01	2.05
28	F	312	KC1	C4A-C3A	-2.16	1.40	1.44
27	A	204	CLA	MG-ND	-2.16	2.01	2.05
27	H	212	CLA	MG-ND	-2.16	2.01	2.05
30	F	304	A86	C32-C31	-2.16	1.50	1.54
27	K	318	CLA	CMC-C2C	-2.16	1.46	1.50
27	L	310	CLA	CMC-C2C	-2.16	1.46	1.50
27	a	823	CLA	C3B-C2B	-2.16	1.37	1.40
27	K	309	CLA	MG-ND	-2.16	2.01	2.05
27	b	821	CLA	MG-ND	-2.16	2.01	2.05
28	K	315	KC1	CHD-C4C	2.16	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	821	CLA	CMC-C2C	-2.16	1.46	1.50
35	l	207	ET4	C35-C36	-2.15	1.49	1.52
27	A	205	CLA	C3B-CAB	-2.15	1.43	1.47
27	b	844	CLA	C3B-CAB	-2.15	1.43	1.47
28	G	313	KC1	C4A-C3A	-2.15	1.40	1.44
27	C	317	CLA	CMC-C2C	-2.15	1.46	1.50
26	H	202	DD6	C40-C32	-2.15	1.49	1.53
27	B	314	CLA	CMD-C2D	-2.15	1.46	1.50
27	A	211	CLA	MG-ND	-2.15	2.01	2.05
27	I	305	CLA	CMC-C2C	-2.15	1.46	1.50
27	M	309	CLA	MG-ND	-2.15	2.01	2.05
27	J	314	CLA	CMD-C2D	-2.15	1.46	1.50
27	a	809	CLA	MG-ND	-2.15	2.01	2.05
30	M	305	A86	C32-C31	-2.15	1.50	1.54
27	L	309	CLA	CMC-C2C	-2.15	1.46	1.50
27	K	313	CLA	CMC-C2C	-2.15	1.46	1.50
27	L	318	CLA	CMC-C2C	-2.15	1.46	1.50
27	A	211	CLA	C3B-CAB	-2.15	1.43	1.47
31	j	102	LHG	O7-C5	-2.15	1.41	1.46
27	J	309	CLA	MG-ND	-2.15	2.01	2.05
27	L	307	CLA	MG-ND	-2.15	2.01	2.05
31	K	320	LHG	O7-C7	2.15	1.40	1.34
27	L	310	CLA	C3B-C2B	-2.14	1.37	1.40
28	C	308	KC1	C4A-C3A	-2.14	1.40	1.44
27	E	313	CLA	MG-ND	-2.14	2.01	2.05
27	H	204	CLA	C3B-C2B	-2.14	1.37	1.40
27	H	209	CLA	C4B-CHC	-2.14	1.35	1.41
27	I	308	CLA	C3B-CAB	-2.14	1.43	1.47
30	B	304	A86	C5-C6	-2.14	1.32	1.35
30	E	301	A86	C13-C11	-2.14	1.45	1.49
27	J	313	CLA	C3B-CAB	-2.14	1.43	1.47
27	b	841	CLA	CMD-C2D	-2.14	1.46	1.50
27	L	313	CLA	CMC-C2C	-2.14	1.46	1.50
30	L	304	A86	C32-C31	-2.14	1.51	1.54
27	I	315	CLA	C3B-CAB	-2.14	1.43	1.47
27	L	316	CLA	C3B-C2B	-2.14	1.37	1.40
27	K	310	CLA	C3B-CAB	-2.14	1.43	1.47
27	H	204	CLA	MG-ND	-2.14	2.01	2.05
27	M	313	CLA	MG-ND	-2.14	2.01	2.05
27	C	310	CLA	CMD-C2D	-2.13	1.46	1.50
31	E	318	LHG	P-O6	2.13	1.67	1.59
27	b	805	CLA	CAA-C2A	-2.13	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	302	A86	O1-C15	-2.13	1.41	1.45
27	L	312	CLA	CMC-C2C	-2.13	1.46	1.50
27	C	314	CLA	MG-ND	-2.13	2.01	2.05
27	I	315	CLA	MG-ND	-2.13	2.01	2.05
27	J	315	CLA	MG-ND	-2.13	2.01	2.05
27	I	313	CLA	CMC-C2C	-2.13	1.46	1.50
31	E	318	LHG	O7-C7	2.13	1.40	1.34
27	E	309	CLA	CMD-C2D	-2.13	1.46	1.50
28	I	312	KC1	CHD-C4C	2.13	1.40	1.35
27	L	308	CLA	MG-ND	-2.13	2.01	2.05
27	D	216	CLA	MG-ND	-2.13	2.01	2.05
29	L	323	LMG	O7-C8	-2.13	1.41	1.46
27	b	841	CLA	CMC-C2C	-2.13	1.46	1.50
27	C	309	CLA	MG-ND	-2.13	2.01	2.05
26	G	305	DD6	O1-C20	-2.12	1.43	1.46
30	M	302	A86	C-C1	-2.12	1.46	1.50
29	a	852	LMG	O7-C8	-2.12	1.41	1.46
27	B	306	CLA	CMC-C2C	-2.12	1.46	1.50
29	E	317	LMG	O1-C7	-2.12	1.39	1.43
27	M	319	CLA	C3B-CAB	-2.12	1.43	1.47
29	A	214	LMG	O1-C7	-2.12	1.39	1.43
27	L	313	CLA	MG-ND	-2.12	2.01	2.05
27	b	829	CLA	CMD-C2D	-2.12	1.46	1.50
30	B	302	A86	C26-C27	-2.12	1.33	1.35
26	E	307	DD6	O1-C20	-2.12	1.43	1.46
30	J	301	A86	C17-C16	-2.12	1.51	1.54
27	a	815	CLA	MG-ND	-2.12	2.01	2.05
27	a	811	CLA	CMD-C2D	-2.11	1.46	1.50
27	K	310	CLA	MG-ND	-2.11	2.01	2.05
27	D	208	CLA	MG-ND	-2.11	2.01	2.05
27	D	210	CLA	MG-ND	-2.11	2.01	2.05
27	a	824	CLA	CMD-C2D	-2.11	1.46	1.50
30	r	202	A86	O4-C34	-2.11	1.41	1.46
27	I	316	CLA	CMC-C2C	-2.11	1.46	1.50
27	F	313	CLA	CMD-C2D	-2.11	1.46	1.50
27	a	822	CLA	CMD-C2D	-2.11	1.46	1.50
27	B	309	CLA	CMD-C2D	-2.11	1.46	1.50
30	K	305	A86	C32-C31	-2.11	1.51	1.54
30	G	302	A86	O1-C15	-2.11	1.42	1.45
27	L	311	CLA	CMD-C2D	-2.11	1.46	1.50
27	D	213	CLA	CMC-C2C	-2.11	1.46	1.50
27	J	315	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	207	ET4	C12-C13	2.11	1.50	1.45
27	D	209	CLA	CMD-C2D	-2.11	1.46	1.50
30	K	306	A86	C13-C11	-2.11	1.45	1.49
27	a	839	CLA	CAA-C2A	-2.10	1.50	1.54
31	E	318	LHG	O8-C23	2.10	1.39	1.33
27	a	839	CLA	C4B-CHC	-2.10	1.35	1.41
27	B	314	CLA	CMC-C2C	-2.10	1.46	1.50
27	b	811	CLA	CMC-C2C	-2.10	1.46	1.50
27	D	214	CLA	CMC-C2C	-2.10	1.46	1.50
27	L	316	CLA	CMC-C2C	-2.10	1.46	1.50
27	a	805	CLA	MG-ND	-2.10	2.01	2.05
30	D	206	A86	O4-C34	-2.10	1.41	1.46
27	a	804	CLA	CMD-C2D	-2.10	1.46	1.50
27	L	308	CLA	C3B-CAB	-2.10	1.43	1.47
28	L	322	KC1	CHD-C4C	2.10	1.40	1.35
27	L	308	CLA	C3B-C2B	-2.10	1.37	1.40
30	H	201	A86	C26-C27	-2.10	1.33	1.35
27	K	314	CLA	C3B-CAB	-2.10	1.43	1.47
27	J	309	CLA	C3B-CAB	-2.10	1.43	1.47
27	H	212	CLA	CAA-C2A	-2.10	1.50	1.54
26	A	202	DD6	C17-C16	-2.10	1.51	1.54
30	I	301	A86	C2-C1	-2.10	1.33	1.35
26	H	202	DD6	C41-C32	-2.10	1.49	1.53
27	i	101	CLA	CMD-C2D	-2.10	1.46	1.50
27	B	314	CLA	C3B-C2B	-2.09	1.37	1.40
27	b	831	CLA	CMD-C2D	-2.09	1.46	1.50
31	H	215	LHG	P-O6	2.09	1.67	1.59
27	A	208	CLA	MG-ND	-2.09	2.01	2.05
27	B	308	CLA	CMD-C2D	-2.09	1.46	1.50
27	A	205	CLA	MG-ND	-2.09	2.01	2.05
27	K	317	CLA	MG-ND	-2.09	2.01	2.05
33	J	318	SQD	O48-C46	-2.09	1.40	1.45
27	L	318	CLA	MG-ND	-2.09	2.01	2.05
27	A	211	CLA	C3B-C2B	-2.09	1.37	1.40
30	B	305	A86	C17-C16	-2.09	1.51	1.54
29	E	317	LMG	O7-C10	2.09	1.40	1.34
30	G	302	A86	C-C1	-2.09	1.46	1.50
27	b	846	CLA	CMD-C2D	-2.09	1.46	1.50
31	j	102	LHG	P-O6	2.09	1.67	1.59
26	C	303	DD6	C2-C1	-2.09	1.33	1.35
30	D	204	A86	C-C1	-2.09	1.46	1.50
27	C	310	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L	317	CLA	CMD-C2D	-2.09	1.46	1.50
27	b	847	CLA	CMD-C2D	-2.08	1.46	1.50
27	a	846	CLA	CMD-C2D	-2.08	1.46	1.50
29	A	212	LMG	O1-C1	-2.08	1.36	1.40
27	D	212	CLA	CMD-C2D	-2.08	1.46	1.50
27	H	213	CLA	C3B-C2B	-2.08	1.37	1.40
27	b	806	CLA	CMD-C2D	-2.08	1.46	1.50
27	a	817	CLA	CMD-C2D	-2.08	1.46	1.50
27	j	104	CLA	CMD-C2D	-2.08	1.46	1.50
27	M	318	CLA	MG-ND	-2.08	2.01	2.05
26	M	306	DD6	C35-C36	-2.08	1.47	1.51
27	E	310	CLA	CMD-C2D	-2.08	1.46	1.50
27	f	301	CLA	CMD-C2D	-2.08	1.46	1.50
30	B	302	A86	O1-C15	-2.08	1.42	1.45
31	D	201	LHG	O7-C7	2.08	1.40	1.34
27	a	803	CLA	CAA-C2A	-2.08	1.50	1.54
27	M	319	CLA	CMD-C2D	-2.08	1.46	1.50
27	K	311	CLA	MG-ND	-2.08	2.01	2.05
27	H	213	CLA	C4B-CHC	-2.08	1.35	1.41
27	J	314	CLA	C3B-CAB	-2.08	1.43	1.47
27	K	319	CLA	CMC-C2C	-2.08	1.46	1.50
27	L	307	CLA	C3B-C2B	-2.07	1.37	1.40
27	L	307	CLA	CMC-C2C	-2.07	1.46	1.50
27	J	314	CLA	CMC-C2C	-2.07	1.46	1.50
27	L	311	CLA	C3B-CAB	-2.07	1.43	1.47
27	a	855	CLA	CMD-C2D	-2.07	1.46	1.50
26	K	303	DD6	C36-C31	-2.07	1.32	1.34
27	b	811	CLA	CMD-C2D	-2.07	1.46	1.50
26	L	303	DD6	C19-C18	-2.07	1.49	1.52
26	G	301	DD6	O1-C20	-2.07	1.43	1.46
27	B	311	CLA	CMD-C2D	-2.07	1.46	1.50
27	I	313	CLA	C3B-C2B	-2.07	1.37	1.40
27	A	203	CLA	CMD-C2D	-2.07	1.46	1.50
27	H	204	CLA	C3B-CAB	-2.07	1.43	1.47
27	b	828	CLA	C3B-C2B	-2.07	1.37	1.40
27	a	845	CLA	CMD-C2D	-2.07	1.46	1.50
27	F	309	CLA	C3B-CAB	-2.07	1.43	1.47
27	b	817	CLA	CMD-C2D	-2.07	1.46	1.50
27	L	316	CLA	C3B-CAB	-2.07	1.43	1.47
27	b	810	CLA	CMD-C2D	-2.07	1.46	1.50
27	J	310	CLA	CMD-C2D	-2.06	1.46	1.50
27	b	820	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	306	CLA	CMD-C2D	-2.06	1.46	1.50
27	b	808	CLA	CMD-C2D	-2.06	1.46	1.50
31	a	802	LHG	O8-C23	2.06	1.39	1.33
27	b	801	CLA	C4B-CHC	-2.06	1.35	1.41
27	F	311	CLA	CMD-C2D	-2.06	1.46	1.50
27	D	213	CLA	CMD-C2D	-2.06	1.46	1.50
27	b	818	CLA	CMC-C2C	-2.06	1.46	1.50
27	A	211	CLA	CMC-C2C	-2.06	1.46	1.50
27	b	809	CLA	CMD-C2D	-2.06	1.46	1.50
27	b	819	CLA	CMD-C2D	-2.06	1.46	1.50
27	b	842	CLA	CMD-C2D	-2.06	1.46	1.50
27	a	854	CLA	CMD-C2D	-2.06	1.46	1.50
27	b	819	CLA	CMC-C2C	-2.06	1.46	1.50
31	a	834	LHG	P-O6	2.06	1.67	1.59
30	r	202	A86	O1-C15	-2.06	1.42	1.45
31	M	320	LHG	O8-C23	2.06	1.39	1.33
27	b	839	CLA	CMD-C2D	-2.06	1.46	1.50
31	a	801	LHG	P-O6	2.06	1.67	1.59
27	J	315	CLA	C3B-CAB	-2.06	1.43	1.47
27	L	319	CLA	MG-ND	-2.06	2.01	2.05
27	E	312	CLA	CMD-C2D	-2.06	1.46	1.50
27	a	849	CLA	CMD-C2D	-2.06	1.46	1.50
27	a	819	CLA	CMD-C2D	-2.06	1.46	1.50
27	F	314	CLA	CMD-C2D	-2.06	1.46	1.50
27	a	827	CLA	CAC-C3C	-2.06	1.45	1.51
27	b	803	CLA	CMD-C2D	-2.06	1.46	1.50
27	F	306	CLA	CMD-C2D	-2.05	1.46	1.50
27	a	816	CLA	CMD-C2D	-2.05	1.46	1.50
27	F	310	CLA	CMD-C2D	-2.05	1.46	1.50
27	a	828	CLA	C3B-C2B	-2.05	1.37	1.40
27	f	302	CLA	CMD-C2D	-2.05	1.46	1.50
27	C	316	CLA	MG-ND	-2.05	2.01	2.05
27	L	307	CLA	C3B-CAB	-2.05	1.43	1.47
27	G	307	CLA	CMC-C2C	-2.05	1.46	1.50
27	a	808	CLA	CMD-C2D	-2.05	1.46	1.50
27	b	807	CLA	CMD-C2D	-2.05	1.46	1.50
30	K	305	A86	C13-C11	-2.05	1.45	1.49
27	a	850	CLA	CMD-C2D	-2.05	1.46	1.50
27	E	313	CLA	CAA-C2A	-2.05	1.50	1.54
27	H	208	CLA	CMD-C2D	-2.05	1.46	1.50
27	b	828	CLA	CMD-C2D	-2.05	1.46	1.50
27	b	845	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	826	CLA	CMD-C2D	-2.05	1.46	1.50
27	b	827	CLA	CMD-C2D	-2.05	1.46	1.50
27	I	313	CLA	MG-ND	-2.05	2.01	2.05
27	L	319	CLA	C3B-CAB	-2.05	1.43	1.47
27	a	830	CLA	CMD-C2D	-2.05	1.46	1.50
27	a	844	CLA	C4B-CHC	-2.05	1.35	1.41
27	G	311	CLA	CMD-C2D	-2.05	1.46	1.50
27	a	814	CLA	CMD-C2D	-2.05	1.46	1.50
27	F	309	CLA	C4B-CHC	-2.04	1.35	1.41
27	B	307	CLA	CMC-C2C	-2.04	1.46	1.50
30	H	203	A86	C13-C11	-2.04	1.45	1.49
27	E	308	CLA	CMD-C2D	-2.04	1.46	1.50
30	K	302	A86	C13-C11	-2.04	1.45	1.49
27	F	311	CLA	CMC-C2C	-2.04	1.46	1.50
27	a	812	CLA	CMD-C2D	-2.04	1.46	1.50
27	b	818	CLA	CMD-C2D	-2.04	1.46	1.50
27	f	303	CLA	CMD-C2D	-2.04	1.46	1.50
27	b	823	CLA	CMD-C2D	-2.04	1.46	1.50
29	l	201	LMG	O7-C10	2.04	1.40	1.34
27	C	312	CLA	MG-ND	-2.04	2.01	2.05
27	a	829	CLA	CMD-C2D	-2.04	1.46	1.50
27	a	840	CLA	CMD-C2D	-2.04	1.46	1.50
27	D	211	CLA	CMD-C2D	-2.04	1.46	1.50
30	M	302	A86	C13-C11	-2.04	1.45	1.49
27	I	306	CLA	CMD-C2D	-2.04	1.46	1.50
26	C	303	DD6	C17-C16	-2.04	1.51	1.54
27	G	309	CLA	CMD-C2D	-2.04	1.46	1.50
27	a	818	CLA	CMD-C2D	-2.04	1.46	1.50
26	J	303	DD6	O1-C20	-2.04	1.43	1.46
30	M	302	A86	O1-C15	-2.04	1.42	1.45
27	a	820	CLA	C4B-CHC	-2.04	1.35	1.41
26	F	303	DD6	O1-C20	-2.04	1.43	1.46
27	L	321	CLA	MG-ND	-2.04	2.01	2.05
27	a	812	CLA	CMC-C2C	-2.04	1.46	1.50
27	b	816	CLA	CMD-C2D	-2.04	1.46	1.50
27	G	308	CLA	CMD-C2D	-2.04	1.46	1.50
27	J	315	CLA	CMC-C2C	-2.04	1.46	1.50
27	a	807	CLA	CMC-C2C	-2.03	1.46	1.50
27	l	204	CLA	C4B-CHC	-2.03	1.35	1.41
27	a	806	CLA	CMD-C2D	-2.03	1.46	1.50
28	H	211	KC1	CHD-C4C	2.03	1.40	1.35
28	L	322	KC1	C1B-C2B	-2.03	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	201	DD6	C36-C31	-2.03	1.32	1.34
27	b	815	CLA	CMD-C2D	-2.03	1.46	1.50
27	K	316	CLA	CAA-C2A	-2.03	1.50	1.54
27	a	832	CLA	CMD-C2D	-2.03	1.46	1.50
30	D	206	A86	O1-C15	-2.03	1.42	1.45
27	K	316	CLA	MG-ND	-2.03	2.01	2.05
27	L	313	CLA	C3B-CAB	-2.03	1.43	1.47
27	G	316	CLA	CMD-C2D	-2.03	1.46	1.50
27	a	841	CLA	CMD-C2D	-2.03	1.46	1.50
27	L	308	CLA	CMC-C2C	-2.03	1.46	1.50
27	a	821	CLA	CMD-C2D	-2.03	1.46	1.50
27	a	856	CLA	C4B-CHC	-2.03	1.35	1.41
27	b	805	CLA	C4B-CHC	-2.03	1.35	1.41
27	D	215	CLA	CMD-C2D	-2.03	1.46	1.50
27	b	813	CLA	CMD-C2D	-2.03	1.46	1.50
27	b	824	CLA	CMD-C2D	-2.02	1.46	1.50
27	F	315	CLA	CMD-C2D	-2.02	1.46	1.50
27	J	309	CLA	C4B-CHC	-2.02	1.35	1.41
27	G	306	CLA	CMD-C2D	-2.02	1.46	1.50
27	a	810	CLA	CMC-C2C	-2.02	1.46	1.50
27	a	813	CLA	CMD-C2D	-2.02	1.46	1.50
30	E	301	A86	C17-C16	-2.02	1.51	1.54
27	L	313	CLA	C3B-C2B	-2.02	1.37	1.40
30	B	305	A86	C-C1	-2.02	1.46	1.50
27	G	307	CLA	CMD-C2D	-2.02	1.46	1.50
30	M	303	A86	C13-C11	-2.02	1.45	1.49
27	a	816	CLA	CMC-C2C	-2.02	1.46	1.50
27	B	307	CLA	CMD-C2D	-2.02	1.46	1.50
27	a	828	CLA	CMD-C2D	-2.02	1.46	1.50
27	J	313	CLA	C3B-C2B	-2.02	1.37	1.40
27	F	309	CLA	C3B-C2B	-2.01	1.37	1.40
27	G	315	CLA	CMD-C2D	-2.01	1.46	1.50
27	G	312	CLA	CMD-C2D	-2.01	1.46	1.50
26	D	205	DD6	C37-C36	-2.01	1.47	1.50
27	D	209	CLA	CMC-C2C	-2.01	1.46	1.50
27	r	201	CLA	CMD-C2D	-2.01	1.46	1.50
27	D	214	CLA	CMD-C2D	-2.01	1.46	1.50
27	b	814	CLA	CMD-C2D	-2.01	1.46	1.50
27	b	826	CLA	CMD-C2D	-2.01	1.46	1.50
27	L	312	CLA	MG-ND	-2.01	2.01	2.05
30	r	202	A86	C2-C1	-2.01	1.33	1.35
27	b	801	CLA	CAC-C3C	-2.01	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	314	CLA	CMD-C2D	-2.01	1.46	1.50
30	m	101	A86	C32-C31	-2.01	1.51	1.54
27	a	848	CLA	CMD-C2D	-2.01	1.46	1.50
27	D	211	CLA	CMC-C2C	-2.01	1.46	1.50
27	F	308	CLA	CMC-C2C	-2.01	1.46	1.50
27	J	308	CLA	CMD-C2D	-2.01	1.46	1.50
27	b	843	CLA	CMD-C2D	-2.01	1.46	1.50
27	b	820	CLA	CMC-C2C	-2.01	1.46	1.50
27	a	810	CLA	C3B-C2B	-2.01	1.37	1.40
28	K	315	KC1	C1B-C2B	-2.01	1.41	1.45
27	F	305	CLA	CMD-C2D	-2.01	1.46	1.50
27	F	307	CLA	CMD-C2D	-2.01	1.46	1.50
27	H	206	CLA	C4B-CHC	-2.00	1.35	1.41
27	M	315	CLA	CMD-C2D	-2.00	1.46	1.50
27	J	313	CLA	MG-ND	-2.00	2.01	2.05
27	I	309	CLA	C3B-CAB	-2.00	1.43	1.47
27	I	306	CLA	CMC-C2C	-2.00	1.46	1.50
27	b	839	CLA	CMC-C2C	-2.00	1.46	1.50
27	B	312	CLA	CMD-C2D	-2.00	1.46	1.50
27	f	302	CLA	CMC-C2C	-2.00	1.46	1.50
27	C	306	CLA	CMD-C2D	-2.00	1.46	1.50
27	a	826	CLA	CMC-C2C	-2.00	1.46	1.50
27	a	825	CLA	CMD-C2D	-2.00	1.46	1.50
26	E	302	DD6	O1-C20	-2.00	1.43	1.46
27	b	810	CLA	CMC-C2C	-2.00	1.46	1.50
30	H	201	A86	O1-C15	-2.00	1.42	1.45

All (3596) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j	103	LMG	O2-C2-C1	-21.31	58.28	110.05
29	a	852	LMG	O2-C2-C1	-18.82	64.32	110.05
26	E	303	DD6	C21-C20-C15	-16.15	95.19	122.26
30	r	202	A86	O1-C20-C19	-15.67	101.61	113.38
29	C	301	LMG	O2-C2-C1	15.26	147.12	110.05
30	M	303	A86	O1-C20-C19	-15.19	101.97	113.38
29	I	319	LMG	O2-C2-C3	-14.80	76.13	110.35
32	b	834	BCR	C32-C1-C6	-14.10	87.43	110.30
30	D	203	A86	O1-C20-C19	-13.72	103.08	113.38
30	D	204	A86	C3-C4-C5	-12.09	98.71	123.47
30	C	304	A86	O1-C20-C19	-11.95	104.41	113.38
26	M	304	DD6	C21-C20-C15	-11.87	102.37	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	H	201	A86	O1-C20-C19	-11.85	104.48	113.38
30	B	302	A86	O1-C20-C19	-11.80	104.52	113.38
30	L	302	A86	O1-C20-C19	-11.47	104.76	113.38
26	B	303	DD6	C21-C20-C15	-11.34	103.25	122.26
30	D	203	A86	C25-C26-C27	-11.17	111.37	127.31
26	M	306	DD6	C21-C20-C15	-11.01	103.80	122.26
30	D	206	A86	O1-C20-C19	-10.92	105.18	113.38
30	G	302	A86	C40-C32-C31	-10.80	100.81	110.47
33	J	318	SQD	O47-C7-O49	-10.77	111.86	125.57
30	J	316	A86	C3-C2-C1	-10.70	112.03	127.31
26	D	205	DD6	C21-C20-C15	-10.69	104.34	122.26
30	F	301	A86	O1-C20-C19	-10.64	105.39	113.38
30	C	305	A86	O1-C20-C19	-10.46	105.53	113.38
29	C	319	LMG	O2-C2-C3	-10.40	86.30	110.35
30	J	301	A86	O1-C20-C19	-10.31	105.64	113.38
30	M	302	A86	O1-C20-C19	-10.28	105.66	113.38
29	L	323	LMG	O2-C2-C1	10.12	134.63	110.05
30	m	101	A86	O1-C20-C19	-10.03	105.84	113.38
26	J	305	DD6	C21-C20-C15	-9.97	105.55	122.26
30	H	203	A86	O1-C20-C19	-9.91	105.94	113.38
30	I	303	A86	O1-C20-C19	-9.71	106.09	113.38
30	B	302	A86	C3-C4-C5	-9.56	103.89	123.47
30	H	201	A86	C3-C4-C5	-9.55	103.90	123.47
30	C	305	A86	C3-C4-C5	-9.39	104.24	123.47
26	E	306	DD6	C14-C13-C11	-9.38	110.97	125.53
29	l	201	LMG	O2-C2-C1	9.37	132.81	110.05
30	E	301	A86	O1-C20-C19	-9.25	106.43	113.38
30	B	301	A86	O1-C20-C19	-9.22	106.45	113.38
29	A	212	LMG	O2-C2-C3	9.15	131.51	110.35
30	B	304	A86	C3-C4-C5	-9.07	104.89	123.47
30	D	204	A86	C4-C3-C2	9.04	142.00	123.47
30	m	101	A86	C24-C1-C2	9.00	132.75	118.94
30	J	316	A86	O1-C20-C19	-8.97	106.64	113.38
26	E	303	DD6	O1-C20-C19	8.81	120.00	113.38
30	J	304	A86	O1-C20-C19	-8.77	106.79	113.38
26	A	202	DD6	O1-C20-C19	-8.76	106.81	113.38
26	E	306	DD6	C3-C2-C1	-8.71	114.87	127.31
30	G	302	A86	O1-C20-C21	-8.69	104.65	115.06
32	b	834	BCR	C32-C1-C31	-8.63	82.04	108.53
30	K	304	A86	O1-C20-C19	-8.60	106.92	113.38
30	C	302	A86	C3-C4-C5	-8.58	105.90	123.47
30	I	301	A86	O1-C20-C19	-8.56	106.95	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	302	A86	O1-C20-C19	-8.52	106.98	113.38
30	J	316	A86	C25-C26-C27	-8.34	115.40	127.31
29	E	317	LMG	O2-C2-C3	-8.34	91.06	110.35
30	B	305	A86	C3-C4-C5	-8.29	106.48	123.47
30	H	201	A86	C4-C3-C2	8.20	140.27	123.47
30	B	302	A86	C4-C3-C2	8.19	140.24	123.47
30	B	305	A86	O1-C20-C19	-8.18	107.24	113.38
26	B	303	DD6	C21-C20-C19	8.14	123.44	114.28
30	D	204	A86	O1-C20-C19	-8.11	107.29	113.38
30	D	204	A86	C3-C2-C1	8.10	138.88	127.31
30	M	302	A86	C3-C4-C5	-8.04	107.01	123.47
30	M	303	A86	O1-C15-C14	-7.90	97.35	113.21
26	D	205	DD6	C8-C6-C5	7.88	131.04	118.94
29	E	317	LMG	O2-C2-C1	-7.79	91.11	110.05
26	K	303	DD6	C21-C20-C15	-7.77	109.23	122.26
30	I	301	A86	C3-C4-C5	-7.76	107.58	123.47
30	G	302	A86	C41-C32-C31	-7.68	103.59	110.47
26	J	305	DD6	C21-C20-C19	7.61	122.84	114.28
27	a	856	CLA	C4A-NA-C1A	7.61	110.13	106.71
29	A	214	LMG	O2-C2-C1	-7.57	91.66	110.05
27	b	830	CLA	C4A-NA-C1A	7.55	110.10	106.71
30	H	203	A86	C3-C4-C5	-7.54	108.02	123.47
30	D	203	A86	O1-C15-C14	-7.54	98.08	113.21
26	M	304	DD6	O1-C20-C21	7.51	124.06	115.06
30	I	303	A86	C3-C4-C5	-7.51	108.09	123.47
27	a	839	CLA	C4A-NA-C1A	7.51	110.08	106.71
27	L	313	CLA	C4A-NA-C1A	7.48	110.07	106.71
27	H	204	CLA	C4A-NA-C1A	7.47	110.06	106.71
27	b	806	CLA	C4A-NA-C1A	7.46	110.06	106.71
27	I	311	CLA	C4A-NA-C1A	7.44	110.05	106.71
27	a	807	CLA	C4A-NA-C1A	7.44	110.05	106.71
27	b	821	CLA	C4A-NA-C1A	7.43	110.05	106.71
29	I	319	LMG	O2-C2-C1	-7.41	92.05	110.05
27	H	209	CLA	C4A-NA-C1A	7.40	110.03	106.71
30	E	301	A86	C3-C4-C5	-7.39	108.34	123.47
27	M	311	CLA	C4A-NA-C1A	7.34	110.01	106.71
30	F	304	A86	C3-C4-C5	-7.33	108.47	123.47
27	a	809	CLA	C4A-NA-C1A	7.32	110.00	106.71
27	a	805	CLA	C4A-NA-C1A	7.27	109.97	106.71
28	M	314	KC1	CHB-C1B-NB	7.25	131.12	124.45
27	M	313	CLA	C4A-NA-C1A	7.24	109.96	106.71
27	b	825	CLA	C4A-NA-C1A	7.24	109.96	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	202	DD6	C21-C20-C19	7.22	122.40	114.28
27	K	309	CLA	C4A-NA-C1A	7.20	109.94	106.71
27	a	829	CLA	C4A-NA-C1A	7.20	109.94	106.71
27	b	804	CLA	C4A-NA-C1A	7.19	109.94	106.71
27	C	309	CLA	C4A-NA-C1A	7.18	109.93	106.71
30	D	204	A86	C4-C5-C6	7.16	137.53	127.31
26	H	202	DD6	C24-C1-C2	7.15	129.92	118.94
28	B	313	KC1	CHB-C1B-NB	7.14	131.02	124.45
30	J	301	A86	C3-C4-C5	-7.12	108.89	123.47
27	a	828	CLA	C4A-NA-C1A	7.12	109.91	106.71
27	D	210	CLA	C4A-NA-C1A	7.12	109.91	106.71
26	D	205	DD6	O1-C20-C21	7.11	123.57	115.06
27	b	841	CLA	C4A-NA-C1A	7.10	109.90	106.71
27	a	820	CLA	C4A-NA-C1A	7.09	109.89	106.71
30	F	304	A86	C17-C16-C15	7.09	116.40	109.16
30	B	301	A86	C25-C26-C27	-7.08	117.21	127.31
30	D	204	A86	O1-C20-C21	-7.08	106.58	115.06
28	K	315	KC1	CHB-C1B-NB	7.07	130.95	124.45
28	H	211	KC1	CHB-C1B-NB	7.04	130.93	124.45
27	b	816	CLA	C4A-NA-C1A	7.04	109.87	106.71
26	J	305	DD6	O1-C20-C21	7.03	123.48	115.06
27	A	204	CLA	C4A-NA-C1A	7.03	109.87	106.71
27	H	206	CLA	C4A-NA-C1A	7.03	109.87	106.71
26	M	306	DD6	C21-C20-C19	7.03	122.19	114.28
27	a	813	CLA	C4A-NA-C1A	7.02	109.86	106.71
33	J	318	SQD	O8-S-C6	7.02	117.12	105.77
27	E	312	CLA	C4A-NA-C1A	7.01	109.86	106.71
30	J	316	A86	C24-C1-C2	7.00	129.69	118.94
27	a	824	CLA	C4A-NA-C1A	7.00	109.85	106.71
27	B	309	CLA	C4A-NA-C1A	6.99	109.85	106.71
30	M	303	A86	C3-C2-C1	-6.99	117.33	127.31
27	b	805	CLA	C4A-NA-C1A	6.98	109.84	106.71
27	a	822	CLA	C4A-NA-C1A	6.98	109.84	106.71
27	L	319	CLA	C4A-NA-C1A	6.97	109.84	106.71
30	r	202	A86	C34-O4-C38	-6.95	104.94	117.90
27	b	803	CLA	C4A-NA-C1A	6.94	109.83	106.71
30	K	306	A86	O1-C20-C19	-6.94	108.17	113.38
27	I	309	CLA	C4A-NA-C1A	6.94	109.82	106.71
27	F	308	CLA	C4A-NA-C1A	6.93	109.82	106.71
27	I	315	CLA	C4A-NA-C1A	6.93	109.82	106.71
27	K	313	CLA	C4A-NA-C1A	6.90	109.81	106.71
28	L	322	KC1	CHB-C1B-NB	6.90	130.79	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	845	CLA	C4A-NA-C1A	6.90	109.81	106.71
27	a	841	CLA	C4A-NA-C1A	6.90	109.81	106.71
27	H	212	CLA	C4A-NA-C1A	6.89	109.80	106.71
30	M	305	A86	O1-C20-C19	-6.88	108.21	113.38
27	E	315	CLA	C4A-NA-C1A	6.88	109.80	106.71
27	b	823	CLA	C4A-NA-C1A	6.87	109.79	106.71
27	b	817	CLA	C4A-NA-C1A	6.85	109.79	106.71
27	a	815	CLA	C4A-NA-C1A	6.85	109.78	106.71
30	L	304	A86	C25-C26-C27	-6.85	117.54	127.31
30	B	302	A86	C3-C2-C1	6.85	137.08	127.31
27	I	316	CLA	C4A-NA-C1A	6.84	109.78	106.71
27	F	317	CLA	C4A-NA-C1A	6.84	109.78	106.71
27	b	839	CLA	C4A-NA-C1A	6.83	109.78	106.71
27	C	317	CLA	C4A-NA-C1A	6.83	109.78	106.71
27	b	810	CLA	C4A-NA-C1A	6.83	109.78	106.71
27	K	312	CLA	C4A-NA-C1A	6.82	109.77	106.71
27	b	828	CLA	C4A-NA-C1A	6.82	109.77	106.71
27	a	821	CLA	C4A-NA-C1A	6.81	109.77	106.71
27	G	307	CLA	C4A-NA-C1A	6.81	109.77	106.71
27	J	307	CLA	C4A-NA-C1A	6.81	109.77	106.71
27	D	214	CLA	C4A-NA-C1A	6.81	109.77	106.71
27	b	850	CLA	C4A-NA-C1A	6.81	109.77	106.71
26	J	302	DD6	C21-C20-C19	6.81	121.94	114.28
30	H	201	A86	C3-C2-C1	6.81	137.02	127.31
29	a	852	LMG	O1-C1-C2	6.80	118.92	108.30
27	a	826	CLA	C4A-NA-C1A	6.80	109.76	106.71
27	H	207	CLA	C4A-NA-C1A	6.80	109.76	106.71
27	A	207	CLA	C4A-NA-C1A	6.80	109.76	106.71
27	b	814	CLA	C4A-NA-C1A	6.78	109.76	106.71
30	M	302	A86	C4-C3-C2	6.78	137.36	123.47
28	K	308	KC1	CHB-C1B-NB	6.78	130.69	124.45
27	M	318	CLA	C4A-NA-C1A	6.78	109.75	106.71
27	a	832	CLA	C4A-NA-C1A	6.77	109.75	106.71
27	B	312	CLA	C4A-NA-C1A	6.77	109.75	106.71
27	a	830	CLA	C4A-NA-C1A	6.77	109.75	106.71
27	b	818	CLA	C4A-NA-C1A	6.77	109.75	106.71
30	B	305	A86	C41-C32-C31	-6.77	104.42	110.47
27	a	810	CLA	C4A-NA-C1A	6.77	109.75	106.71
27	a	814	CLA	C4A-NA-C1A	6.76	109.75	106.71
27	G	306	CLA	C4A-NA-C1A	6.76	109.75	106.71
32	b	834	BCR	C31-C1-C6	6.76	121.26	110.30
30	J	316	A86	C3-C4-C5	-6.75	109.65	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	301	CLA	C4A-NA-C1A	6.75	109.74	106.71
27	b	843	CLA	C4A-NA-C1A	6.75	109.74	106.71
27	A	203	CLA	C4A-NA-C1A	6.74	109.73	106.71
30	K	302	A86	O1-C20-C19	-6.74	108.32	113.38
28	L	314	KC1	CHB-C1B-NB	6.73	130.64	124.45
27	B	310	CLA	C4A-NA-C1A	6.73	109.73	106.71
27	F	310	CLA	C4A-NA-C1A	6.73	109.73	106.71
27	M	307	CLA	C4A-NA-C1A	6.72	109.73	106.71
27	b	819	CLA	C4A-NA-C1A	6.71	109.72	106.71
27	a	842	CLA	C4A-NA-C1A	6.71	109.72	106.71
27	G	312	CLA	C4A-NA-C1A	6.71	109.72	106.71
27	a	827	CLA	C4A-NA-C1A	6.70	109.72	106.71
27	j	104	CLA	C4A-NA-C1A	6.70	109.72	106.71
27	C	306	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	K	316	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	B	307	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	G	317	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	H	214	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	b	812	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	D	209	CLA	C4A-NA-C1A	6.68	109.71	106.71
27	I	307	CLA	C4A-NA-C1A	6.67	109.70	106.71
30	C	304	A86	C3-C2-C1	-6.66	117.80	127.31
27	B	308	CLA	C4A-NA-C1A	6.66	109.70	106.71
27	I	313	CLA	C4A-NA-C1A	6.66	109.70	106.71
27	J	313	CLA	C4A-NA-C1A	6.66	109.70	106.71
30	G	302	A86	C24-C1-C2	6.66	129.16	118.94
27	M	315	CLA	C4A-NA-C1A	6.66	109.70	106.71
27	F	311	CLA	C4A-NA-C1A	6.65	109.70	106.71
27	J	312	CLA	C4A-NA-C1A	6.65	109.70	106.71
27	G	311	CLA	C4A-NA-C1A	6.65	109.69	106.71
27	G	314	CLA	C4A-NA-C1A	6.65	109.69	106.71
30	b	848	A86	C3-C2-C1	-6.64	117.83	127.31
27	H	210	CLA	C4A-NA-C1A	6.63	109.69	106.71
27	b	846	CLA	C4A-NA-C1A	6.63	109.69	106.71
27	K	317	CLA	C4A-NA-C1A	6.63	109.69	106.71
27	G	315	CLA	C4A-NA-C1A	6.62	109.68	106.71
27	f	303	CLA	C4A-NA-C1A	6.62	109.68	106.71
27	b	813	CLA	C4A-NA-C1A	6.62	109.68	106.71
27	D	211	CLA	C4A-NA-C1A	6.62	109.68	106.71
27	a	819	CLA	C4A-NA-C1A	6.62	109.68	106.71
27	b	824	CLA	C4A-NA-C1A	6.62	109.68	106.71
27	b	844	CLA	C4A-NA-C1A	6.60	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	838	CLA	C4A-NA-C1A	6.60	109.67	106.71
30	B	304	A86	C4-C3-C2	6.60	136.99	123.47
27	C	310	CLA	C4A-NA-C1A	6.59	109.67	106.71
27	a	812	CLA	C4A-NA-C1A	6.59	109.67	106.71
27	a	845	CLA	C4A-NA-C1A	6.59	109.67	106.71
27	l	204	CLA	C4A-NA-C1A	6.59	109.67	106.71
27	a	818	CLA	C4A-NA-C1A	6.59	109.67	106.71
27	F	305	CLA	C4A-NA-C1A	6.58	109.67	106.71
26	H	202	DD6	C21-C20-C19	6.58	121.68	114.28
27	b	808	CLA	C4A-NA-C1A	6.58	109.66	106.71
27	b	831	CLA	C4A-NA-C1A	6.58	109.66	106.71
27	J	309	CLA	C4A-NA-C1A	6.58	109.66	106.71
27	J	314	CLA	C4A-NA-C1A	6.57	109.66	106.71
27	b	809	CLA	C4A-NA-C1A	6.57	109.66	106.71
27	C	318	CLA	C4A-NA-C1A	6.57	109.66	106.71
27	K	318	CLA	C4A-NA-C1A	6.57	109.66	106.71
27	G	310	CLA	C4A-NA-C1A	6.57	109.66	106.71
27	b	811	CLA	C4A-NA-C1A	6.56	109.66	106.71
28	I	312	KC1	CHC-C4B-NB	6.56	130.48	124.45
27	G	309	CLA	C4A-NA-C1A	6.56	109.65	106.71
27	B	306	CLA	C4A-NA-C1A	6.55	109.65	106.71
27	M	317	CLA	C4A-NA-C1A	6.55	109.65	106.71
26	I	304	DD6	C21-C20-C15	-6.54	111.29	122.26
27	b	822	CLA	C4A-NA-C1A	6.54	109.65	106.71
27	a	840	CLA	C4A-NA-C1A	6.54	109.65	106.71
28	F	312	KC1	CHB-C1B-NB	6.54	130.46	124.45
30	J	304	A86	C17-C16-C15	6.54	115.83	109.16
27	a	849	CLA	C4A-NA-C1A	6.53	109.64	106.71
28	A	209	KC1	CHC-C4B-NB	6.53	130.45	124.45
26	A	202	DD6	C21-C20-C15	-6.52	111.33	122.26
27	a	816	CLA	C4A-NA-C1A	6.51	109.64	106.71
27	F	314	CLA	C4A-NA-C1A	6.51	109.63	106.71
27	b	826	CLA	C4A-NA-C1A	6.51	109.63	106.71
27	A	211	CLA	C4A-NA-C1A	6.51	109.63	106.71
27	E	309	CLA	C4A-NA-C1A	6.50	109.63	106.71
27	b	807	CLA	C4A-NA-C1A	6.50	109.63	106.71
30	J	304	A86	C3-C4-C5	-6.50	110.16	123.47
30	K	307	A86	C3-C2-C1	-6.50	118.04	127.31
27	a	846	CLA	C4A-NA-C1A	6.49	109.63	106.71
28	C	308	KC1	CHB-C1B-NB	6.49	130.42	124.45
27	F	307	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	C	301	LMG	O2-C2-C3	-6.49	95.34	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	206	A86	C3-C4-C5	-6.49	110.18	123.47
30	D	206	A86	C4-C3-C2	6.49	136.76	123.47
27	a	854	CLA	C4A-NA-C1A	6.49	109.62	106.71
27	D	208	CLA	C4A-NA-C1A	6.48	109.62	106.71
30	D	206	A86	C3-C2-C1	6.48	136.56	127.31
27	A	206	CLA	C4A-NA-C1A	6.48	109.62	106.71
27	E	308	CLA	C4A-NA-C1A	6.48	109.62	106.71
27	B	311	CLA	C4A-NA-C1A	6.47	109.62	106.71
27	G	316	CLA	C4A-NA-C1A	6.47	109.62	106.71
27	a	803	CLA	C4A-NA-C1A	6.47	109.61	106.71
28	J	306	KC1	CHC-C4B-NB	6.47	130.40	124.45
27	a	825	CLA	C4A-NA-C1A	6.46	109.61	106.71
27	D	215	CLA	C4A-NA-C1A	6.46	109.61	106.71
27	F	313	CLA	C4A-NA-C1A	6.46	109.61	106.71
27	a	811	CLA	C4A-NA-C1A	6.45	109.61	106.71
26	M	304	DD6	C21-C20-C19	6.45	121.54	114.28
27	A	208	CLA	C4A-NA-C1A	6.45	109.61	106.71
28	C	313	KC1	CHB-C1B-NB	6.45	130.38	124.45
27	D	213	CLA	C4A-NA-C1A	6.45	109.60	106.71
27	A	210	CLA	C4A-NA-C1A	6.44	109.60	106.71
27	L	316	CLA	C4A-NA-C1A	6.44	109.60	106.71
27	r	201	CLA	C4A-NA-C1A	6.44	109.60	106.71
28	J	306	KC1	CHB-C1B-NB	6.44	130.37	124.45
30	B	301	A86	C3-C2-C1	-6.44	118.12	127.31
28	C	308	KC1	CHC-C4B-NB	6.44	130.37	124.45
27	a	808	CLA	C4A-NA-C1A	6.44	109.60	106.71
28	L	320	KC1	CHC-C4B-NB	6.44	130.37	124.45
27	H	208	CLA	C4A-NA-C1A	6.43	109.60	106.71
28	L	322	KC1	CHC-C4B-NB	6.43	130.36	124.45
27	a	850	CLA	C4A-NA-C1A	6.42	109.59	106.71
27	C	307	CLA	C4A-NA-C1A	6.41	109.59	106.71
27	C	311	CLA	C4A-NA-C1A	6.41	109.59	106.71
27	b	820	CLA	C4A-NA-C1A	6.41	109.59	106.71
27	a	823	CLA	C4A-NA-C1A	6.41	109.59	106.71
27	a	855	CLA	C4A-NA-C1A	6.41	109.59	106.71
27	l	206	CLA	C4A-NA-C1A	6.41	109.59	106.71
27	F	306	CLA	C4A-NA-C1A	6.40	109.58	106.71
27	E	314	CLA	C4A-NA-C1A	6.40	109.58	106.71
30	A	213	A86	O1-C20-C19	-6.39	108.58	113.38
27	E	311	CLA	C4A-NA-C1A	6.39	109.58	106.71
27	b	801	CLA	C4A-NA-C1A	6.39	109.58	106.71
27	b	842	CLA	C4A-NA-C1A	6.39	109.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	313	KC1	CHB-C1B-NB	6.39	130.33	124.45
26	B	303	DD6	C24-C1-C2	6.39	128.75	118.94
29	a	852	LMG	O6-C1-O1	-6.39	94.85	109.97
27	C	312	CLA	C4A-NA-C1A	6.38	109.58	106.71
27	b	838	CLA	C4A-NA-C1A	6.38	109.57	106.71
26	J	303	DD6	C4-C5-C6	-6.38	118.21	127.31
27	a	848	CLA	C4A-NA-C1A	6.37	109.57	106.71
30	M	303	A86	C17-C16-C15	6.37	115.66	109.16
30	B	305	A86	C4-C3-C2	6.37	136.52	123.47
30	G	302	A86	O1-C20-C19	-6.36	108.61	113.38
27	L	307	CLA	C4A-NA-C1A	6.35	109.56	106.71
27	K	310	CLA	C4A-NA-C1A	6.35	109.56	106.71
27	F	309	CLA	C4A-NA-C1A	6.34	109.56	106.71
27	a	806	CLA	C4A-NA-C1A	6.34	109.56	106.71
27	L	317	CLA	C4A-NA-C1A	6.34	109.56	106.71
27	D	212	CLA	C4A-NA-C1A	6.34	109.56	106.71
30	K	307	A86	O1-C20-C19	-6.33	108.62	113.38
26	K	303	DD6	C24-C1-C2	6.33	128.66	118.94
27	I	310	CLA	C4A-NA-C1A	6.33	109.55	106.71
27	M	316	CLA	C4A-NA-C1A	6.33	109.55	106.71
27	a	804	CLA	C4A-NA-C1A	6.33	109.55	106.71
27	F	315	CLA	C4A-NA-C1A	6.32	109.55	106.71
30	r	202	A86	C25-C24-C1	-6.32	108.65	126.42
26	K	303	DD6	C21-C20-C19	6.32	121.39	114.28
27	C	315	CLA	C4A-NA-C1A	6.32	109.55	106.71
27	b	815	CLA	C4A-NA-C1A	6.32	109.55	106.71
30	r	202	A86	O1-C15-C14	-6.32	100.53	113.21
28	L	320	KC1	CHB-C1B-NB	6.30	130.25	124.45
27	J	315	CLA	C4A-NA-C1A	6.30	109.54	106.71
28	H	211	KC1	CHC-C4B-NB	6.30	130.24	124.45
27	A	205	CLA	C4A-NA-C1A	6.30	109.54	106.71
27	I	306	CLA	C4A-NA-C1A	6.30	109.54	106.71
27	b	847	CLA	C4A-NA-C1A	6.30	109.54	106.71
30	L	302	A86	C34-O4-C38	-6.30	106.16	117.90
27	I	317	CLA	C4A-NA-C1A	6.29	109.54	106.71
27	M	309	CLA	C4A-NA-C1A	6.29	109.53	106.71
27	b	849	CLA	C4A-NA-C1A	6.29	109.53	106.71
30	C	305	A86	C4-C3-C2	6.28	136.34	123.47
27	D	217	CLA	C4A-NA-C1A	6.28	109.53	106.71
27	E	313	CLA	C4A-NA-C1A	6.28	109.53	106.71
27	E	310	CLA	C4A-NA-C1A	6.28	109.53	106.71
27	b	829	CLA	C4A-NA-C1A	6.27	109.52	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I	312	KC1	CHB-C1B-NB	6.26	130.21	124.45
30	I	301	A86	C4-C3-C2	6.25	136.28	123.47
30	r	202	A86	C3-C4-C5	-6.24	110.69	123.47
27	L	312	CLA	C4A-NA-C1A	6.24	109.51	106.71
27	M	310	CLA	C4A-NA-C1A	6.24	109.51	106.71
27	b	827	CLA	C4A-NA-C1A	6.22	109.50	106.71
26	E	306	DD6	C24-C1-C2	6.22	128.49	118.94
30	D	204	A86	C8-C6-C5	6.21	128.47	118.94
28	F	312	KC1	CHC-C4B-NB	6.21	130.16	124.45
27	L	309	CLA	C4A-NA-C1A	6.21	109.50	106.71
27	l	203	CLA	C4A-NA-C1A	6.20	109.50	106.71
27	L	311	CLA	C4A-NA-C1A	6.20	109.49	106.71
28	L	314	KC1	CHC-C4B-NB	6.19	130.15	124.45
27	f	302	CLA	C4A-NA-C1A	6.19	109.49	106.71
26	E	303	DD6	C4-C5-C6	-6.17	118.50	127.31
30	J	316	A86	C4-C3-C2	6.16	136.09	123.47
27	G	308	CLA	C4A-NA-C1A	6.14	109.47	106.71
27	L	315	CLA	C4A-NA-C1A	6.14	109.47	106.71
26	D	205	DD6	C21-C20-C19	6.14	121.19	114.28
27	L	321	CLA	C4A-NA-C1A	6.14	109.47	106.71
26	I	304	DD6	C24-C1-C2	6.14	128.36	118.94
29	L	323	LMG	O1-C1-C2	6.14	117.89	108.30
27	F	316	CLA	C4A-NA-C1A	6.14	109.47	106.71
27	J	308	CLA	C4A-NA-C1A	6.14	109.47	106.71
30	G	302	A86	C9-C10-C11	-6.13	108.59	126.61
32	l	202	BCR	C7-C8-C9	-6.13	116.98	126.23
27	i	101	CLA	C4A-NA-C1A	6.12	109.46	106.71
27	K	311	CLA	C4A-NA-C1A	6.12	109.46	106.71
28	G	313	KC1	CHC-C4B-NB	6.12	130.08	124.45
26	H	202	DD6	C21-C20-C15	-6.11	112.01	122.26
30	B	304	A86	O1-C20-C19	-6.11	108.79	113.38
27	a	844	CLA	C4A-NA-C1A	6.11	109.45	106.71
27	M	312	CLA	C4A-NA-C1A	6.10	109.45	106.71
27	D	207	CLA	C4A-NA-C1A	6.10	109.45	106.71
28	C	313	KC1	CHC-C4B-NB	6.09	130.05	124.45
32	j	105	BCR	C24-C23-C22	-6.09	117.03	126.23
27	M	308	CLA	C4A-NA-C1A	6.09	109.44	106.71
27	D	216	CLA	C4A-NA-C1A	6.08	109.44	106.71
32	b	837	BCR	C16-C17-C18	-6.08	118.64	127.31
26	L	303	DD6	C21-C20-C15	-6.08	112.08	122.26
32	a	853	BCR	C15-C14-C13	-6.07	118.65	127.31
27	I	308	CLA	C4A-NA-C1A	6.07	109.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	319	CLA	C4A-NA-C1A	6.06	109.43	106.71
26	E	306	DD6	C13-C11-C10	6.06	128.24	118.94
27	I	305	CLA	C4A-NA-C1A	6.05	109.43	106.71
27	L	310	CLA	C4A-NA-C1A	6.05	109.43	106.71
30	C	302	A86	C4-C3-C2	6.04	135.86	123.47
26	K	303	DD6	C-C1-C2	-6.04	114.46	122.92
26	J	302	DD6	C3-C2-C1	-6.04	118.69	127.31
27	a	817	CLA	C4A-NA-C1A	6.04	109.42	106.71
27	K	314	CLA	C1D-ND-C4D	6.04	110.62	106.33
26	M	306	DD6	C24-C1-C2	6.03	128.20	118.94
30	M	303	A86	C33-C32-C31	6.00	115.04	109.21
26	I	304	DD6	C21-C20-C19	6.00	121.03	114.28
26	E	306	DD6	C21-C20-C19	6.00	121.03	114.28
30	M	303	A86	C25-C24-C1	-5.99	109.59	126.42
30	D	204	A86	C9-C8-C6	-5.96	109.69	126.42
27	H	205	CLA	C4A-NA-C1A	5.95	109.38	106.71
28	K	308	KC1	CHC-C4B-NB	5.95	129.92	124.45
26	A	202	DD6	C24-C1-C2	5.95	128.07	118.94
26	I	304	DD6	C3-C2-C1	-5.94	118.83	127.31
30	B	305	A86	O1-C20-C21	-5.94	107.94	115.06
26	H	202	DD6	C-C1-C2	-5.92	114.63	122.92
30	K	305	A86	O1-C20-C19	-5.92	108.93	113.38
30	J	301	A86	C4-C3-C2	5.92	135.60	123.47
30	I	301	A86	C3-C2-C1	5.91	135.75	127.31
32	m	102	BCR	C7-C8-C9	-5.91	117.31	126.23
28	M	314	KC1	CHC-C4B-NB	5.91	129.88	124.45
32	l	205	BCR	C11-C10-C9	-5.89	118.90	127.31
27	C	314	CLA	C4A-NA-C1A	5.88	109.35	106.71
27	L	308	CLA	C4A-NA-C1A	5.88	109.35	106.71
27	H	213	CLA	C4A-NA-C1A	5.87	109.34	106.71
27	a	843	CLA	C4A-NA-C1A	5.86	109.34	106.71
30	H	203	A86	O1-C20-C21	-5.86	108.04	115.06
32	a	836	BCR	C24-C23-C22	-5.85	117.39	126.23
27	L	318	CLA	C4A-NA-C1A	5.85	109.34	106.71
30	r	202	A86	C9-C10-C11	-5.85	109.42	126.61
30	m	101	A86	C17-C16-C15	5.83	115.11	109.16
30	B	304	A86	C17-C16-C15	5.81	115.09	109.16
30	M	303	A86	C24-C1-C2	5.81	127.85	118.94
26	M	306	DD6	O1-C20-C21	5.80	122.01	115.06
27	C	316	CLA	C4A-NA-C1A	5.77	109.30	106.71
26	C	303	DD6	C3-C2-C1	-5.76	119.09	127.31
26	M	306	DD6	C-C1-C2	-5.75	114.86	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	303	DD6	O1-C20-C21	5.73	121.93	115.06
30	C	302	A86	C9-C10-C11	-5.73	109.77	126.61
30	B	302	A86	C9-C10-C11	-5.72	109.78	126.61
27	J	310	CLA	C4A-NA-C1A	5.72	109.28	106.71
30	H	201	A86	C9-C10-C11	-5.70	109.85	126.61
32	b	840	BCR	C11-C10-C9	-5.68	119.20	127.31
30	G	302	A86	C9-C8-C6	5.67	142.34	126.42
30	F	301	A86	C3-C2-C1	-5.67	119.22	127.31
27	I	314	CLA	C4A-NA-C1A	5.66	109.25	106.71
28	A	209	KC1	CHB-C1B-NB	5.64	129.64	124.45
26	J	303	DD6	C3-C2-C1	-5.64	119.26	127.31
30	H	203	A86	C4-C3-C2	5.62	134.99	123.47
30	K	305	A86	C3-C2-C1	-5.62	119.29	127.31
30	D	203	A86	C9-C10-C11	-5.61	110.11	126.61
27	B	314	CLA	C4A-NA-C1A	5.60	109.22	106.71
30	C	302	A86	O1-C20-C21	-5.60	108.35	115.06
30	b	848	A86	C4-C5-C6	-5.59	119.33	127.31
27	K	314	CLA	C2D-C1D-ND	-5.59	105.98	110.10
26	L	301	DD6	C4-C5-C6	-5.59	119.33	127.31
30	F	304	A86	C4-C3-C2	5.58	134.91	123.47
26	A	201	DD6	C4-C5-C6	-5.58	119.35	127.31
30	H	201	A86	O1-C20-C21	-5.57	108.38	115.06
30	J	316	A86	C34-O4-C38	-5.56	107.53	117.90
29	a	852	LMG	O2-C2-C3	5.56	123.21	110.35
30	I	303	A86	C9-C10-C11	-5.56	110.28	126.61
30	M	302	A86	O1-C20-C21	-5.55	108.40	115.06
30	B	302	A86	O1-C20-C21	-5.55	108.41	115.06
30	m	101	A86	C7-C6-C5	-5.55	115.15	122.92
32	j	105	BCR	C20-C21-C22	-5.53	119.42	127.31
32	l	205	BCR	C28-C27-C26	-5.53	104.20	114.08
28	B	313	KC1	CHC-C4B-NB	5.53	129.53	124.45
30	J	301	A86	C3-C2-C1	5.53	135.20	127.31
28	K	315	KC1	CHC-C4B-NB	5.53	129.53	124.45
27	J	311	CLA	C4A-NA-C1A	5.52	109.19	106.71
26	F	303	DD6	C4-C5-C6	-5.52	119.43	127.31
30	G	302	A86	C17-C16-C15	5.52	114.79	109.16
30	M	303	A86	C4-C5-C6	-5.51	119.44	127.31
30	D	206	A86	O1-C20-C21	-5.51	108.45	115.06
30	K	301	A86	O1-C20-C19	-5.51	109.24	113.38
27	K	319	CLA	C4A-NA-C1A	5.49	109.18	106.71
35	l	207	ET4	C29-C22-C23	5.48	127.69	116.84
28	K	308	KC1	O2D-CGD-CBD	5.48	121.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	G	302	A86	C10-C9-C8	5.47	140.29	123.22
30	I	303	A86	C4-C3-C2	5.46	134.66	123.47
32	b	834	BCR	C11-C10-C9	-5.46	119.52	127.31
26	L	301	DD6	C9-C10-C11	-5.45	119.53	127.31
30	L	306	A86	O1-C20-C19	-5.45	109.29	113.38
30	K	302	A86	C4-C5-C6	-5.45	119.54	127.31
30	B	304	A86	C9-C10-C11	-5.44	110.63	126.61
32	j	101	BCR	C24-C23-C22	-5.43	118.03	126.23
33	J	318	SQD	O8-S-O7	5.43	124.53	111.27
26	K	303	DD6	C3-C2-C1	-5.41	119.59	127.31
32	E	305	BCR	C16-C17-C18	-5.40	119.61	127.31
35	l	207	ET4	C19-C18-C17	5.38	127.20	118.94
30	D	203	A86	O1-C20-C21	-5.38	108.61	115.06
30	D	206	A86	C34-O4-C38	-5.37	107.89	117.90
26	F	302	DD6	C21-C20-C19	5.37	120.32	114.28
30	K	305	A86	C4-C5-C6	-5.36	119.66	127.31
30	L	304	A86	O1-C20-C19	-5.36	109.36	113.38
26	J	305	DD6	C4-C5-C6	-5.36	119.66	127.31
30	K	306	A86	C4-C5-C6	-5.36	119.67	127.31
30	m	101	A86	C25-C24-C1	-5.36	111.37	126.42
30	B	305	A86	C9-C10-C11	-5.36	110.87	126.61
30	L	306	A86	C4-C5-C6	-5.35	119.67	127.31
30	J	301	A86	O1-C20-C21	-5.34	108.66	115.06
30	r	202	A86	C4-C3-C2	5.32	134.37	123.47
29	j	103	LMG	O6-C1-O1	-5.32	97.38	109.97
30	E	301	A86	C4-C3-C2	5.32	134.37	123.47
30	K	306	A86	C3-C2-C1	-5.31	119.72	127.31
33	J	318	SQD	O8-S-O9	-5.31	98.30	111.27
30	M	303	A86	C-C1-C2	-5.30	115.50	122.92
32	i	103	BCR	C24-C23-C22	-5.30	118.22	126.23
26	F	303	DD6	C9-C10-C11	-5.30	119.75	127.31
30	M	302	A86	C3-C2-C1	5.29	134.86	127.31
32	m	102	BCR	C16-C17-C18	-5.29	119.77	127.31
32	b	833	BCR	C16-C17-C18	-5.27	119.79	127.31
32	b	834	BCR	C32-C1-C2	-5.26	87.87	108.91
26	J	302	DD6	C4-C5-C6	-5.26	119.81	127.31
30	D	203	A86	C17-C16-C15	5.25	114.52	109.16
30	I	303	A86	C3-C2-C1	5.25	134.80	127.31
30	m	101	A86	C-C1-C2	-5.25	115.58	122.92
30	E	301	A86	C9-C10-C11	-5.24	111.20	126.61
26	K	303	DD6	C9-C10-C11	-5.23	119.85	127.31
35	l	207	ET4	C30-C18-C17	-5.21	115.63	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	303	DD6	C21-C20-C19	5.20	120.13	114.28
30	F	301	A86	C25-C26-C27	-5.20	119.89	127.31
30	J	316	A86	C-C1-C2	-5.20	115.64	122.92
30	C	305	A86	C9-C10-C11	-5.20	111.32	126.61
26	D	205	DD6	C3-C2-C1	-5.19	119.91	127.31
26	M	306	DD6	C3-C2-C1	-5.18	119.92	127.31
26	E	303	DD6	O1-C20-C21	5.18	121.26	115.06
26	D	205	DD6	C7-C6-C5	-5.18	115.67	122.92
30	b	848	A86	O1-C20-C21	-5.18	108.86	115.06
30	F	304	A86	C9-C10-C11	-5.17	111.40	126.61
28	L	322	KC1	O2D-CGD-CBD	5.17	120.46	111.27
30	E	301	A86	O1-C20-C21	-5.16	108.88	115.06
26	G	304	DD6	C3-C2-C1	-5.15	119.97	127.31
30	r	202	A86	C17-C16-C15	5.14	114.41	109.16
32	b	834	BCR	C15-C14-C13	-5.14	119.98	127.31
30	B	301	A86	O1-C15-C14	-5.13	102.91	113.21
30	L	306	A86	O1-C20-C21	-5.13	108.91	115.06
26	M	301	DD6	C21-C20-C19	5.13	120.05	114.28
30	r	202	A86	O1-C20-C21	-5.12	108.92	115.06
32	j	101	BCR	C20-C21-C22	-5.11	120.01	127.31
30	L	302	A86	C17-C16-C15	5.11	114.38	109.16
30	K	302	A86	C3-C2-C1	-5.11	120.02	127.31
30	J	304	A86	C4-C3-C2	5.11	133.93	123.47
30	M	305	A86	O1-C20-C21	-5.10	108.95	115.06
32	l	202	BCR	C33-C5-C6	-5.09	118.81	124.53
30	L	305	A86	O1-C20-C19	-5.09	109.56	113.38
30	M	303	A86	O1-C20-C21	-5.07	108.98	115.06
32	f	304	BCR	C15-C14-C13	-5.07	120.08	127.31
29	D	202	LMG	O2-C2-C1	5.06	122.34	110.05
29	L	323	LMG	C1-O6-C5	5.06	123.62	113.69
26	M	301	DD6	C3-C2-C1	-5.05	120.10	127.31
26	G	305	DD6	C3-C2-C1	-5.05	120.11	127.31
32	f	305	BCR	C24-C23-C22	-5.05	118.61	126.23
30	B	301	A86	O1-C20-C21	-5.04	109.01	115.06
26	L	301	DD6	C3-C2-C1	-5.04	120.12	127.31
30	K	301	A86	C36-C31-C32	5.04	124.69	119.70
26	K	303	DD6	C4-C5-C6	-5.03	120.13	127.31
30	K	302	A86	O1-C20-C21	-5.01	109.06	115.06
28	B	313	KC1	O2D-CGD-CBD	5.00	120.16	111.27
30	J	316	A86	O1-C20-C21	-5.00	109.06	115.06
26	B	303	DD6	O1-C20-C21	4.99	121.04	115.06
30	G	302	A86	C3-C4-C5	-4.98	113.27	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	302	DD6	C4-C5-C6	-4.98	120.20	127.31
30	B	304	A86	O1-C20-C21	-4.98	109.09	115.06
30	H	203	A86	C9-C10-C11	-4.97	112.00	126.61
32	b	834	BCR	C33-C5-C6	-4.95	118.97	124.53
30	D	204	A86	C7-C6-C5	-4.95	116.00	122.92
32	a	836	BCR	C20-C21-C22	-4.95	120.25	127.31
26	M	304	DD6	C-C1-C2	-4.94	116.00	122.92
30	K	302	A86	C36-C31-C32	4.94	124.60	119.70
30	F	301	A86	C4-C5-C6	-4.93	120.27	127.31
30	m	101	A86	O1-C20-C21	-4.93	109.15	115.06
30	J	304	A86	C9-C10-C11	-4.92	112.14	126.61
32	m	102	BCR	C3-C4-C5	-4.92	105.29	114.08
32	i	103	BCR	C15-C14-C13	-4.90	120.31	127.31
27	b	827	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
26	G	303	DD6	C3-C2-C1	-4.90	120.32	127.31
30	K	304	A86	C3-C2-C1	-4.90	120.32	127.31
26	G	305	DD6	C21-C20-C19	4.89	119.79	114.28
35	l	207	ET4	C24-C05-C06	-4.88	119.05	124.53
30	r	202	A86	C35-C34-C33	4.88	118.39	109.88
30	K	302	A86	C17-C16-C15	4.88	114.14	109.16
30	B	302	A86	O4-C38-C39	4.88	120.07	111.09
32	l	202	BCR	C38-C26-C25	-4.88	119.05	124.53
26	C	303	DD6	C4-C5-C6	-4.87	120.36	127.31
30	H	201	A86	O4-C38-C39	4.87	120.05	111.09
30	K	301	A86	O4-C38-C39	4.87	120.04	111.09
30	D	206	A86	C9-C10-C11	-4.86	112.32	126.61
30	F	304	A86	O4-C38-C39	4.86	120.02	111.09
30	M	302	A86	C33-C32-C31	4.86	113.93	109.21
30	C	305	A86	O4-C38-C39	4.85	120.02	111.09
30	F	301	A86	O1-C20-C21	-4.85	109.24	115.06
30	A	213	A86	C25-C26-C27	-4.84	120.40	127.31
28	G	313	KC1	O2D-CGD-CBD	4.84	119.86	111.27
26	G	304	DD6	C21-C20-C19	4.83	119.72	114.28
30	A	213	A86	C3-C2-C1	-4.83	120.42	127.31
26	E	303	DD6	C-C1-C2	-4.82	116.17	122.92
30	m	101	A86	C33-C32-C31	4.82	113.90	109.21
30	b	848	A86	O1-C20-C19	-4.82	109.76	113.38
26	F	303	DD6	C21-C20-C19	4.82	119.70	114.28
28	J	306	KC1	O2D-CGD-CBD	4.81	119.82	111.27
26	E	306	DD6	C7-C6-C5	-4.81	116.19	122.92
33	J	318	SQD	O9-S-C6	-4.81	101.12	106.92
37	b	835	DGD	O2G-C1B-C2B	4.81	121.86	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	306	DD6	C34-C35-C36	-4.80	102.29	111.85
29	j	103	LMG	O1-C1-C2	4.80	115.79	108.30
32	E	305	BCR	C20-C21-C22	-4.79	120.47	127.31
30	K	305	A86	O1-C20-C21	-4.78	109.32	115.06
26	L	301	DD6	C21-C20-C19	4.78	119.66	114.28
28	C	308	KC1	O2D-CGD-CBD	4.78	119.77	111.27
30	L	304	A86	O1-C20-C21	-4.77	109.34	115.06
32	a	853	BCR	C16-C17-C18	-4.77	120.50	127.31
30	B	305	A86	C33-C32-C31	4.76	113.84	109.21
30	L	305	A86	O4-C38-C39	4.76	119.85	111.09
30	K	306	A86	O1-C20-C21	-4.76	109.36	115.06
30	L	302	A86	O1-C20-C21	-4.76	109.36	115.06
30	L	304	A86	O4-C38-C39	4.76	119.84	111.09
26	G	301	DD6	C21-C20-C19	4.76	119.63	114.28
30	M	302	A86	O4-C38-C39	4.76	119.84	111.09
30	F	304	A86	O1-C20-C21	-4.75	109.37	115.06
28	C	313	KC1	O2D-CGD-CBD	4.74	119.70	111.27
28	F	312	KC1	O2D-CGD-CBD	4.74	119.69	111.27
30	L	306	A86	C3-C2-C1	-4.74	120.55	127.31
30	G	302	A86	C4-C3-C2	4.74	133.18	123.47
26	A	202	DD6	C4-C5-C6	-4.74	120.55	127.31
30	A	213	A86	O4-C38-C39	4.74	119.80	111.09
30	F	301	A86	O4-C38-C39	4.73	119.80	111.09
30	F	301	A86	O1-C15-C14	-4.73	103.73	113.21
30	A	213	A86	C4-C5-C6	-4.72	120.57	127.31
30	G	302	A86	C33-C32-C31	4.72	113.80	109.21
30	L	305	A86	O1-C20-C21	-4.72	109.40	115.06
26	E	302	DD6	C21-C20-C19	4.72	119.59	114.28
30	L	304	A86	C25-C24-C1	-4.71	113.17	126.42
30	J	316	A86	C26-C25-C24	-4.71	108.53	123.22
27	a	855	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
30	C	302	A86	O4-C38-C39	4.69	119.73	111.09
30	I	301	A86	O4-C38-C39	4.69	119.71	111.09
32	a	851	BCR	C33-C5-C6	-4.68	119.27	124.53
30	C	305	A86	O1-C20-C21	-4.68	109.45	115.06
29	j	103	LMG	O2-C2-C3	4.68	121.16	110.35
30	J	316	A86	C9-C10-C11	-4.67	112.87	126.61
30	m	101	A86	C25-C26-C27	-4.67	120.64	127.31
30	J	304	A86	O1-C20-C21	-4.67	109.46	115.06
32	i	102	BCR	C20-C21-C22	-4.67	120.65	127.31
31	M	320	LHG	O7-C7-C8	4.67	121.56	111.50
26	F	302	DD6	C9-C10-C11	-4.67	120.65	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	837	LHG	O7-C7-C8	4.66	119.67	111.09
26	G	303	DD6	C21-C20-C19	4.66	119.53	114.28
27	K	314	CLA	C4A-NA-C1A	4.66	108.80	106.71
30	K	307	A86	C4-C5-C6	-4.66	120.66	127.31
26	D	205	DD6	C32-C31-C36	-4.66	116.06	122.63
26	A	201	DD6	C3-C2-C1	-4.66	120.67	127.31
30	D	204	A86	O4-C38-C39	4.65	119.65	111.09
30	G	302	A86	C-C1-C2	-4.65	116.41	122.92
32	a	853	BCR	C7-C8-C9	-4.65	119.22	126.23
30	L	305	A86	C4-C5-C6	-4.64	120.69	127.31
30	H	203	A86	C3-C2-C1	4.63	133.91	127.31
30	J	301	A86	O4-C38-C39	4.63	119.60	111.09
30	M	303	A86	C41-C32-C31	-4.61	106.34	110.47
26	E	302	DD6	C9-C10-C11	-4.61	120.73	127.31
32	b	840	BCR	C38-C26-C25	-4.60	119.36	124.53
26	I	304	DD6	C-C1-C2	-4.60	116.48	122.92
26	G	301	DD6	C3-C2-C1	-4.60	120.75	127.31
28	L	320	KC1	O2D-CGD-CBD	4.60	119.43	111.27
32	i	102	BCR	C16-C17-C18	-4.59	120.77	127.31
32	a	836	BCR	C16-C17-C18	-4.58	120.78	127.31
26	E	303	DD6	C24-C1-C2	4.57	125.96	118.94
28	M	314	KC1	O2D-CGD-CBD	4.57	119.39	111.27
29	J	317	LMG	O7-C10-C11	4.56	121.33	111.50
30	C	304	A86	C-C1-C2	-4.56	116.54	122.92
30	I	301	A86	C9-C10-C11	-4.56	113.21	126.61
30	K	306	A86	O4-C38-C39	4.56	119.47	111.09
30	M	305	A86	C4-C5-C6	-4.55	120.81	127.31
30	D	203	A86	C8-C6-C5	-4.55	111.96	118.94
27	b	823	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
32	a	851	BCR	C24-C23-C22	-4.55	119.36	126.23
30	B	305	A86	O4-C38-C39	4.54	119.44	111.09
26	E	303	DD6	C3-C2-C1	-4.54	120.84	127.31
27	a	845	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
29	C	301	LMG	C3-C4-C5	4.53	118.32	110.24
32	j	105	BCR	C16-C17-C18	-4.53	120.84	127.31
30	K	307	A86	O1-C20-C21	-4.53	109.63	115.06
30	B	301	A86	O4-C38-C39	4.52	119.41	111.09
32	E	304	BCR	C15-C14-C13	-4.52	120.86	127.31
30	L	305	A86	C3-C2-C1	-4.51	120.87	127.31
30	E	301	A86	O4-C38-C39	4.51	119.39	111.09
30	I	301	A86	O1-C20-C21	-4.50	109.67	115.06
32	a	847	BCR	C33-C5-C6	-4.50	119.48	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	213	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
26	E	302	DD6	C3-C2-C1	-4.49	120.90	127.31
30	L	304	A86	C24-C1-C2	4.48	125.82	118.94
26	A	201	DD6	C21-C20-C19	4.48	119.32	114.28
30	J	301	A86	C9-C10-C11	-4.47	113.46	126.61
30	G	302	A86	O4-C38-C39	4.46	119.30	111.09
30	m	101	A86	O4-C38-C39	4.46	119.30	111.09
27	b	815	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
29	M	321	LMG	O2-C2-C1	4.46	120.88	110.05
27	E	315	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
30	J	301	A86	C34-O4-C38	-4.46	109.59	117.90
26	E	306	DD6	C12-C11-C10	-4.46	116.68	122.92
26	J	302	DD6	O1-C20-C19	-4.46	110.03	113.38
30	M	305	A86	C3-C2-C1	-4.45	120.95	127.31
30	D	203	A86	O4-C38-C39	4.45	119.28	111.09
32	f	304	BCR	C11-C10-C9	-4.45	120.96	127.31
30	K	307	A86	O4-C38-C39	4.45	119.27	111.09
30	L	306	A86	O4-C38-C39	4.45	119.27	111.09
35	l	207	ET4	C27-C09-C10	-4.43	116.71	122.92
27	b	821	CLA	O2D-CGD-O1D	-4.43	115.18	123.84
30	K	302	A86	O4-C38-C39	4.43	119.24	111.09
26	J	305	DD6	C20-C19-C18	-4.42	104.00	112.75
26	E	307	DD6	C21-C20-C19	4.42	119.25	114.28
30	K	301	A86	O1-C20-C21	-4.41	109.77	115.06
30	r	202	A86	C25-C26-C27	4.41	133.61	127.31
29	j	103	LMG	O7-C10-C11	4.41	121.01	111.50
31	E	316	LHG	O7-C7-C8	4.41	121.01	111.50
27	a	840	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
31	I	318	LHG	O7-C7-C8	4.40	120.98	111.50
32	a	853	BCR	C20-C21-C22	-4.39	121.04	127.31
30	B	305	A86	C35-C34-C33	4.39	117.54	109.88
30	I	301	A86	C41-C32-C31	-4.39	106.55	110.47
32	m	102	BCR	C20-C21-C22	-4.38	121.06	127.31
30	E	301	A86	C17-C16-C15	4.37	113.62	109.16
27	a	805	CLA	O2D-CGD-O1D	-4.37	115.30	123.84
30	J	316	A86	O4-C38-C39	4.36	119.11	111.09
26	C	303	DD6	C25-C26-C27	-4.36	113.92	126.58
31	b	836	LHG	O7-C7-C8	4.36	120.89	111.50
27	M	316	CLA	CAA-C2A-C3A	-4.35	100.85	112.78
26	J	305	DD6	C24-C1-C2	4.35	125.62	118.94
31	a	801	LHG	O7-C7-C8	4.35	120.87	111.50
30	L	304	A86	C9-C8-C6	-4.34	114.22	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	202	DD6	C32-C31-C36	-4.34	116.50	122.63
27	L	318	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
30	D	203	A86	C34-O4-C38	-4.33	109.82	117.90
30	M	305	A86	O4-C38-C39	4.33	119.06	111.09
26	I	302	DD6	C21-C20-C19	4.33	119.15	114.28
27	b	801	CLA	O2D-CGD-O1D	-4.33	115.38	123.84
32	l	205	BCR	C24-C23-C22	-4.33	119.70	126.23
26	A	202	DD6	C-C1-C24	-4.33	111.26	118.08
26	C	303	DD6	C21-C20-C19	4.32	119.14	114.28
26	E	302	DD6	C14-C13-C11	-4.31	118.84	125.53
30	M	302	A86	C17-C16-C15	4.31	113.56	109.16
30	J	304	A86	O4-C38-C39	4.31	119.02	111.09
30	M	302	A86	C9-C10-C11	-4.31	113.94	126.61
28	K	315	KC1	O2D-CGD-CBD	4.30	118.91	111.27
30	B	304	A86	C3-C2-C1	4.30	133.45	127.31
30	F	304	A86	C8-C6-C5	-4.30	112.35	118.94
32	i	102	BCR	C24-C23-C22	-4.30	119.75	126.23
30	L	302	A86	O4-C38-C39	4.29	118.99	111.09
31	D	201	LHG	O7-C7-C8	4.29	120.75	111.50
32	a	836	BCR	C15-C14-C13	-4.29	121.19	127.31
27	b	844	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
26	D	205	DD6	C34-C35-C36	-4.29	103.31	111.85
31	K	320	LHG	O7-C7-C8	4.28	120.73	111.50
30	H	203	A86	O4-C38-C39	4.28	118.96	111.09
30	B	304	A86	O4-C38-C39	4.27	118.95	111.09
29	D	202	LMG	O7-C10-C11	4.27	120.71	111.50
32	a	835	BCR	C28-C27-C26	-4.27	106.45	114.08
30	K	304	A86	O4-C38-C39	4.27	118.94	111.09
30	I	303	A86	O4-C38-C39	4.26	118.93	111.09
29	C	319	LMG	O7-C10-C11	4.26	120.68	111.50
27	a	807	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
30	C	305	A86	C3-C2-C1	4.26	133.39	127.31
30	K	302	A86	C9-C8-C6	-4.25	114.48	126.42
26	A	202	DD6	C41-C32-C31	-4.25	103.72	110.47
32	j	101	BCR	C15-C14-C13	-4.24	121.25	127.31
30	r	202	A86	C24-C1-C2	4.24	125.44	118.94
27	l	206	CLA	CMB-C2B-C1B	-4.23	121.95	128.46
32	f	305	BCR	C33-C5-C6	-4.23	119.78	124.53
30	J	316	A86	C41-C32-C31	-4.22	106.70	110.47
30	M	303	A86	O4-C38-C39	4.22	118.84	111.09
29	a	852	LMG	O7-C10-C11	4.21	120.58	111.50
30	K	301	A86	C4-C5-C6	-4.21	121.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	103	BCR	C11-C10-C9	-4.21	121.31	127.31
26	C	303	DD6	C3-C4-C5	-4.20	114.86	123.47
30	K	304	A86	C25-C26-C27	-4.20	121.31	127.31
32	r	203	BCR	C3-C4-C5	-4.20	106.58	114.08
32	b	833	BCR	C20-C21-C22	-4.20	121.32	127.31
27	l	203	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
27	l	204	CLA	O2D-CGD-O1D	-4.19	115.65	123.84
30	J	304	A86	C3-C2-C1	4.19	133.29	127.31
26	J	302	DD6	C9-C10-C11	-4.19	121.33	127.31
27	a	817	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
30	D	206	A86	O4-C38-C39	4.18	118.78	111.09
30	J	301	A86	C26-C25-C24	-4.18	110.17	123.22
30	I	303	A86	C26-C25-C24	-4.18	110.17	123.22
32	f	305	BCR	C20-C21-C22	-4.17	121.35	127.31
27	E	308	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
27	b	827	CLA	CMB-C2B-C3B	4.17	132.48	124.68
30	K	301	A86	C34-O4-C38	-4.17	110.12	117.90
30	A	213	A86	O1-C20-C21	-4.17	110.06	115.06
29	L	323	LMG	O7-C10-C11	4.16	120.48	111.50
27	b	838	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
30	B	305	A86	C3-C2-C1	4.15	133.24	127.31
27	b	825	CLA	C1-C2-C3	-4.15	118.86	126.04
26	F	303	DD6	C3-C2-C1	-4.15	121.39	127.31
30	K	304	A86	C4-C5-C6	-4.15	121.39	127.31
27	f	301	CLA	CMB-C2B-C1B	-4.14	122.09	128.46
30	C	304	A86	O1-C20-C21	-4.14	110.10	115.06
30	I	303	A86	C41-C32-C31	-4.14	106.77	110.47
26	E	302	DD6	C4-C5-C6	-4.14	121.41	127.31
31	a	834	LHG	O7-C7-C8	4.14	120.41	111.50
27	C	307	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
26	I	302	DD6	C3-C2-C1	-4.13	121.41	127.31
30	K	305	A86	O4-C38-C39	4.13	118.68	111.09
30	D	206	A86	O1-C15-C14	-4.12	104.94	113.21
26	C	303	DD6	C37-C36-C35	4.12	121.98	114.36
26	E	303	DD6	O2-C18-C19	-4.12	101.62	109.80
28	H	211	KC1	O2D-CGD-CBD	4.11	118.58	111.27
33	J	318	SQD	O9-S-O7	-4.11	99.72	113.95
26	H	202	DD6	C34-C35-C36	-4.11	103.66	111.85
27	a	820	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
30	K	307	A86	C25-C26-C27	-4.11	121.45	127.31
27	b	829	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
31	E	318	LHG	O7-C7-C8	4.10	120.34	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	826	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
27	H	206	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
27	b	842	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
32	E	305	BCR	C24-C23-C22	-4.09	120.05	126.23
27	H	212	CLA	C1-C2-C3	-4.09	118.97	126.04
32	j	101	BCR	C11-C10-C9	-4.09	121.48	127.31
30	I	303	A86	C10-C9-C8	4.08	135.96	123.22
27	M	313	CLA	CAA-CBA-CGA	-4.08	101.33	113.25
26	J	303	DD6	C37-C36-C31	-4.08	118.81	124.35
30	b	848	A86	O4-C38-C39	4.07	118.58	111.09
27	a	806	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
27	b	813	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
32	i	103	BCR	C20-C21-C22	-4.07	121.50	127.31
30	m	101	A86	C-C1-C24	-4.07	111.67	118.08
32	b	834	BCR	C24-C23-C22	-4.07	120.09	126.23
30	r	202	A86	C10-C9-C8	4.06	135.90	123.22
26	M	304	DD6	C3-C2-C1	-4.05	121.53	127.31
30	C	304	A86	C4-C5-C6	-4.05	121.54	127.31
32	m	102	BCR	C24-C23-C22	-4.04	120.12	126.23
27	K	311	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
26	B	303	DD6	C14-C13-C11	-4.04	119.26	125.53
29	A	212	LMG	O7-C10-C11	4.04	120.21	111.50
32	b	834	BCR	C38-C26-C25	-4.04	119.99	124.53
30	K	304	A86	C34-O4-C38	-4.04	110.37	117.90
26	J	302	DD6	C15-C14-C13	-4.04	117.46	125.99
28	L	314	KC1	O2D-CGD-CBD	4.03	118.44	111.27
30	J	304	A86	C10-C9-C8	4.03	135.80	123.22
31	j	102	LHG	O7-C7-C8	4.03	120.19	111.50
30	I	303	A86	O1-C20-C21	-4.03	110.23	115.06
32	a	835	BCR	C16-C17-C18	-4.02	121.57	127.31
30	C	304	A86	O4-C38-C39	4.02	118.49	111.09
26	D	205	DD6	C24-C1-C2	4.02	125.10	118.94
29	C	301	LMG	O7-C10-C11	4.02	120.16	111.50
29	M	321	LMG	O2-C2-C3	4.01	119.62	110.35
27	D	214	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
31	H	215	LHG	O7-C7-C8	4.01	120.14	111.50
27	K	309	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
27	a	822	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
26	B	303	DD6	C-C1-C2	-4.01	117.31	122.92
27	a	843	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
32	b	833	BCR	C28-C27-C26	-4.00	106.93	114.08
27	b	825	CLA	CMB-C2B-C1B	-4.00	122.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	855	CLA	CMB-C2B-C3B	4.00	132.16	124.68
26	G	301	DD6	C4-C5-C6	-4.00	121.61	127.31
30	J	304	A86	O1-C15-C14	-3.99	105.19	113.21
32	f	304	BCR	C7-C8-C9	-3.99	120.21	126.23
29	M	321	LMG	O7-C10-C11	3.99	120.10	111.50
27	a	813	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
26	A	201	DD6	C15-C14-C13	-3.99	117.56	125.99
30	C	302	A86	C17-C16-C15	3.98	113.23	109.16
26	M	301	DD6	C4-C5-C6	-3.98	121.63	127.31
32	i	103	BCR	C7-C8-C9	-3.98	120.22	126.23
26	J	305	DD6	C37-C36-C31	-3.97	118.95	124.35
28	A	209	KC1	O2D-CGD-CBD	3.97	118.33	111.27
30	M	302	A86	C41-C32-C31	-3.97	106.92	110.47
27	b	801	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
28	I	312	KC1	O2D-CGD-CBD	3.96	118.30	111.27
30	M	303	A86	C3-C4-C5	-3.95	115.37	123.47
30	D	206	A86	C10-C9-C8	3.95	135.55	123.22
26	K	303	DD6	C15-C14-C13	-3.95	117.64	125.99
30	D	204	A86	C9-C10-C11	-3.95	114.99	126.61
27	a	839	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
27	M	309	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
32	E	305	BCR	C15-C14-C13	-3.95	121.68	127.31
30	L	302	A86	C4-C5-C6	-3.94	121.68	127.31
27	L	316	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
27	a	808	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
34	b	832	PQN	C11-C12-C13	-3.94	120.23	126.79
32	l	205	BCR	C8-C9-C10	3.94	124.98	118.94
30	m	101	A86	O1-C15-C14	-3.93	105.32	113.21
32	b	840	BCR	C1-C6-C5	-3.93	117.07	122.61
30	K	302	A86	C25-C26-C27	-3.93	121.70	127.31
30	H	203	A86	C26-C25-C24	-3.93	110.96	123.22
26	B	303	DD6	C37-C36-C31	-3.93	119.01	124.35
32	b	837	BCR	C3-C4-C5	-3.92	107.07	114.08
27	a	838	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
27	L	308	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
26	C	303	DD6	C14-C13-C11	-3.92	119.45	125.53
26	F	302	DD6	C3-C2-C1	-3.92	121.72	127.31
30	C	302	A86	C3-C2-C1	3.91	132.90	127.31
30	D	204	A86	C26-C25-C24	-3.91	111.01	123.22
27	F	313	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
26	M	306	DD6	C15-C14-C13	-3.91	117.72	125.99
26	G	305	DD6	O1-C20-C19	-3.91	110.45	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	851	BCR	C20-C21-C22	-3.91	121.73	127.31
26	M	301	DD6	C24-C1-C2	3.91	124.94	118.94
32	j	105	BCR	C15-C14-C13	-3.91	121.73	127.31
30	H	201	A86	C10-C9-C8	3.90	135.40	123.22
30	B	302	A86	C10-C9-C8	3.90	135.39	123.22
27	K	316	CLA	C1-C2-C3	-3.90	119.30	126.04
27	a	804	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
27	a	844	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
29	I	319	LMG	O7-C10-C11	3.89	119.89	111.50
27	A	205	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
27	b	811	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
28	B	313	KC1	O1D-CGD-CBD	-3.89	116.53	124.48
26	B	303	DD6	C4-C5-C6	-3.89	121.76	127.31
26	C	303	DD6	C15-C14-C13	-3.88	117.78	125.99
27	H	209	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
29	l	201	LMG	O7-C10-C11	3.88	119.87	111.50
27	b	807	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
32	j	101	BCR	C16-C17-C18	-3.88	121.77	127.31
27	a	812	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
32	a	835	BCR	C15-C14-C13	-3.88	121.78	127.31
27	I	317	CLA	CMB-C2B-C1B	-3.88	122.51	128.46
27	E	314	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
27	M	312	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
27	K	314	CLA	C3C-C4C-NC	-3.87	106.23	110.57
26	I	304	DD6	C15-C14-C13	-3.87	117.81	125.99
27	a	815	CLA	CAC-C3C-C4C	3.87	129.83	124.81
27	a	829	CLA	CMB-C2B-C1B	-3.86	122.52	128.46
26	L	303	DD6	C24-C1-C2	3.86	124.87	118.94
32	m	102	BCR	C4-C5-C6	-3.86	117.13	122.73
30	B	305	A86	C10-C9-C8	3.86	135.26	123.22
27	I	306	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
27	B	314	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
32	a	847	BCR	C38-C26-C25	-3.85	120.20	124.53
27	G	308	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
26	K	303	DD6	C13-C11-C10	3.85	124.84	118.94
30	F	304	A86	C10-C9-C8	3.85	135.22	123.22
27	K	310	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
27	H	212	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
27	a	821	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
27	B	308	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
26	E	307	DD6	C3-C2-C1	-3.84	121.83	127.31
27	b	823	CLA	CMB-C2B-C3B	3.83	131.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	313	CLA	O2D-CGD-O1D	-3.83	116.34	123.84
30	G	302	A86	C26-C25-C24	-3.83	111.27	123.22
30	D	203	A86	C7-C6-C8	3.83	124.11	118.08
32	a	851	BCR	C16-C17-C18	-3.83	121.85	127.31
32	i	103	BCR	C16-C17-C18	-3.83	121.85	127.31
27	H	208	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
27	a	840	CLA	CMB-C2B-C3B	3.82	131.83	124.68
27	L	309	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
27	M	307	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
27	a	845	CLA	CMB-C2B-C3B	3.82	131.82	124.68
27	b	809	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
27	B	306	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
27	M	317	CLA	C1D-ND-C4D	-3.81	103.63	106.33
27	H	206	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
26	E	307	DD6	C4-C5-C6	-3.80	121.88	127.31
30	K	304	A86	C17-C16-C15	3.80	113.04	109.16
27	a	827	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
27	b	821	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
27	b	803	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
27	b	838	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
32	l	202	BCR	C15-C14-C13	-3.80	121.89	127.31
27	a	841	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
27	E	312	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
27	K	313	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
30	A	213	A86	C34-O4-C38	-3.79	110.83	117.90
26	J	305	DD6	C3-C2-C1	-3.79	121.90	127.31
30	D	206	A86	C35-C34-C33	3.79	116.49	109.88
27	a	849	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
30	I	303	A86	C17-C16-C15	3.78	113.02	109.16
27	I	308	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
32	j	105	BCR	C28-C27-C26	-3.78	107.33	114.08
30	F	304	A86	C4-C5-C6	3.77	132.69	127.31
27	b	816	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
27	L	310	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
27	L	319	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
30	F	304	A86	C7-C6-C8	3.77	124.01	118.08
27	M	313	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
27	I	313	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
30	B	301	A86	C7-C6-C8	3.76	124.01	118.08
31	a	802	LHG	O7-C7-C8	3.76	119.61	111.50
27	A	204	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
27	b	819	CLA	CMB-C2B-C1B	-3.76	122.69	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	309	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
27	D	210	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
27	M	315	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
27	D	213	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
27	a	825	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
32	i	102	BCR	C7-C8-C9	-3.75	120.57	126.23
27	H	207	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
32	a	853	BCR	C24-C23-C22	-3.75	120.58	126.23
27	a	854	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
26	J	305	DD6	C32-C33-C34	-3.74	105.19	113.64
26	L	303	DD6	C21-C20-C19	3.74	118.49	114.28
27	b	820	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
26	E	306	DD6	C25-C24-C1	-3.74	115.91	126.42
27	K	310	CLA	C1-C2-C3	-3.74	119.58	126.04
32	E	304	BCR	C28-C27-C26	-3.74	107.40	114.08
27	H	209	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
27	A	207	CLA	CMB-C2B-C1B	-3.73	122.72	128.46
27	a	844	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
27	l	203	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
32	j	105	BCR	C7-C8-C9	-3.73	120.60	126.23
27	b	846	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
26	C	303	DD6	C32-C31-C36	-3.73	117.37	122.63
30	C	302	A86	C8-C6-C5	-3.73	113.22	118.94
27	a	819	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
27	a	848	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
27	b	815	CLA	CMB-C2B-C3B	3.72	131.64	124.68
29	E	317	LMG	O7-C10-C11	3.72	119.52	111.50
32	j	105	BCR	C11-C10-C9	-3.72	122.01	127.31
30	D	203	A86	C10-C9-C8	3.71	134.81	123.22
32	f	305	BCR	C1-C6-C5	-3.71	117.38	122.61
31	a	833	LHG	O7-C7-C8	3.71	119.50	111.50
30	B	304	A86	C10-C9-C8	3.71	134.80	123.22
27	C	312	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
30	L	304	A86	C8-C6-C5	3.71	124.63	118.94
27	r	201	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
27	a	856	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
26	E	303	DD6	C21-C20-C19	3.71	118.45	114.28
30	B	305	A86	C26-C25-C24	-3.70	111.66	123.22
30	F	301	A86	C25-C24-C1	-3.70	116.01	126.42
26	F	303	DD6	C37-C36-C31	-3.70	119.32	124.35
26	J	302	DD6	C37-C36-C31	-3.70	119.32	124.35
30	I	301	A86	C7-C6-C8	3.70	123.91	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	853	BCR	C11-C10-C9	-3.70	122.03	127.31
30	M	303	A86	C34-O4-C38	-3.70	111.01	117.90
26	I	304	DD6	C25-C24-C1	-3.70	116.03	126.42
27	A	203	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
27	b	843	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
27	L	307	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
26	J	303	DD6	C15-C14-C13	-3.69	118.19	125.99
27	G	307	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
27	L	317	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
27	J	313	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
27	a	805	CLA	O2D-CGD-CBD	3.68	117.82	111.27
27	b	831	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
27	J	311	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
32	r	203	BCR	C16-C17-C18	-3.68	122.06	127.31
27	b	805	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
27	b	845	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
32	f	304	BCR	C20-C21-C22	-3.68	122.06	127.31
27	D	207	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
27	H	205	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
27	D	209	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
30	H	201	A86	C26-C25-C24	-3.68	111.75	123.22
30	B	302	A86	C26-C25-C24	-3.67	111.75	123.22
27	H	213	CLA	CMB-C2B-C3B	3.67	131.55	124.68
27	b	844	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
26	E	307	DD6	C9-C10-C11	-3.67	122.07	127.31
27	a	809	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
27	b	812	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
27	C	316	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
27	K	319	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
27	D	212	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
27	l	204	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
30	r	202	A86	C20-C19-C18	-3.66	105.51	112.75
27	a	830	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
27	H	214	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
27	G	317	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
27	C	314	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
30	B	301	A86	C4-C5-C6	-3.65	122.09	127.31
27	f	302	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
26	C	303	DD6	O1-C20-C19	-3.65	110.64	113.38
26	J	303	DD6	C-C1-C2	-3.65	117.81	122.92
30	C	305	A86	C34-O4-C38	-3.65	111.09	117.90
27	F	307	CLA	CMB-C2B-C1B	-3.65	122.86	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	304	BCR	C16-C17-C18	-3.65	122.10	127.31
30	B	301	A86	C34-O4-C38	-3.65	111.10	117.90
27	b	806	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
30	I	301	A86	C34-O4-C38	-3.64	111.11	117.90
30	K	307	A86	C34-O4-C38	-3.64	111.11	117.90
26	E	306	DD6	C4-C5-C6	-3.64	122.11	127.31
32	a	835	BCR	C24-C23-C22	-3.64	120.73	126.23
30	C	305	A86	C26-C25-C24	-3.64	111.86	123.22
26	M	304	DD6	C15-C14-C13	-3.64	118.30	125.99
27	I	310	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
27	E	315	CLA	CMB-C2B-C3B	3.64	131.49	124.68
27	G	312	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
27	J	308	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
27	D	215	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
32	a	853	BCR	C33-C5-C6	-3.64	120.45	124.53
27	b	808	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
29	L	323	LMG	O2-C2-C3	3.63	118.75	110.35
27	D	217	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
27	A	211	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
30	K	302	A86	C33-C32-C31	3.63	112.73	109.21
27	E	311	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
27	a	820	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
27	M	308	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
27	a	811	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
30	L	304	A86	C9-C10-C11	-3.62	115.96	126.61
30	m	101	A86	C9-C10-C11	-3.62	115.96	126.61
26	J	303	DD6	C24-C1-C2	3.62	124.50	118.94
27	G	314	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
30	I	303	A86	O1-C15-C14	-3.62	105.95	113.21
27	D	208	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
27	I	307	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
28	F	312	KC1	C3D-CAD-CBD	-3.61	102.85	107.61
26	L	303	DD6	C20-C19-C18	-3.61	105.61	112.75
27	A	210	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
27	a	850	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
31	B	315	LHG	O7-C7-C8	3.60	119.27	111.50
27	D	210	CLA	O2D-CGD-O1D	-3.60	116.79	123.84
30	H	203	A86	C41-C32-C31	-3.60	107.25	110.47
28	L	322	KC1	O1D-CGD-CBD	-3.60	117.12	124.48
32	r	203	BCR	C24-C23-C22	-3.59	120.80	126.23
27	J	307	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
27	b	812	CLA	O2D-CGD-O1D	-3.59	116.82	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	102	BCR	C11-C10-C9	-3.59	122.19	127.31
27	F	314	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
30	C	302	A86	C7-C6-C8	3.59	123.73	118.08
32	a	836	BCR	C33-C5-C6	-3.59	120.50	124.53
27	a	815	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
27	G	316	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
32	m	102	BCR	C34-C9-C10	-3.58	117.90	122.92
27	D	208	CLA	C1-C2-C3	-3.58	119.85	126.04
26	I	302	DD6	O1-C20-C19	-3.57	110.70	113.38
26	G	301	DD6	C9-C10-C11	-3.57	122.22	127.31
27	J	310	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
27	b	814	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
32	i	103	BCR	C28-C27-C26	-3.57	107.71	114.08
27	B	312	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
27	a	843	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
27	H	204	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
27	F	310	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
26	G	305	DD6	C37-C36-C31	-3.56	119.51	124.35
27	b	818	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
27	C	315	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
27	E	308	CLA	CMB-C2B-C3B	3.56	131.33	124.68
27	M	310	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
27	D	207	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
27	b	839	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
27	l	206	CLA	CMB-C2B-C3B	3.55	131.33	124.68
27	a	832	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
32	a	853	BCR	C38-C26-C25	-3.55	120.54	124.53
32	b	837	BCR	C28-C27-C26	-3.55	107.74	114.08
27	L	313	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
27	H	206	CLA	CMB-C2B-C3B	3.55	131.32	124.68
27	a	809	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
32	a	851	BCR	C15-C14-C13	-3.55	122.25	127.31
32	a	847	BCR	C7-C8-C9	-3.54	120.88	126.23
30	L	306	A86	C25-C26-C27	-3.54	122.25	127.31
27	b	824	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
32	j	105	BCR	C33-C5-C6	-3.54	120.55	124.53
27	a	807	CLA	CMB-C2B-C3B	3.54	131.30	124.68
27	a	842	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
27	K	312	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
27	M	319	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
26	G	305	DD6	C4-C5-C6	-3.53	122.27	127.31
27	G	311	CLA	CMB-C2B-C1B	-3.53	123.03	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	E	303	DD6	C37-C36-C31	-3.53	119.55	124.35
30	B	304	A86	C26-C25-C24	-3.53	112.20	123.22
32	j	101	BCR	C38-C26-C25	-3.53	120.56	124.53
27	G	315	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
27	I	315	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
30	M	302	A86	C35-C34-C33	3.53	116.03	109.88
26	E	303	DD6	C34-C35-C36	-3.53	104.83	111.85
27	A	206	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
30	L	302	A86	O1-C15-C14	-3.52	106.14	113.21
27	a	824	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
26	C	303	DD6	C-C1-C2	-3.52	117.99	122.92
26	I	302	DD6	C37-C36-C31	-3.52	119.57	124.35
32	j	101	BCR	C33-C5-C6	-3.52	120.58	124.53
32	r	203	BCR	C20-C21-C22	-3.52	122.29	127.31
27	H	210	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
27	a	826	CLA	CMB-C2B-C3B	3.51	131.25	124.68
27	f	303	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
32	a	835	BCR	C3-C4-C5	-3.51	107.80	114.08
26	E	303	DD6	C37-C36-C35	3.51	120.86	114.36
32	l	205	BCR	C3-C4-C5	-3.51	107.81	114.08
30	H	201	A86	C17-C16-C15	3.51	112.74	109.16
32	E	304	BCR	C33-C5-C6	-3.50	120.60	124.53
30	B	301	A86	C20-C19-C18	-3.50	105.83	112.75
27	B	307	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
30	C	305	A86	O1-C15-C14	-3.50	106.19	113.21
27	a	805	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
27	K	314	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
27	C	309	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
28	J	306	KC1	C3D-CAD-CBD	-3.49	103.00	107.61
32	b	833	BCR	C15-C14-C13	-3.49	122.32	127.31
32	a	847	BCR	C24-C23-C22	-3.49	120.96	126.23
27	G	309	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
27	a	839	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
26	F	302	DD6	C14-C13-C11	-3.49	120.11	125.53
27	a	816	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
27	L	318	CLA	CMB-C2B-C3B	3.48	131.20	124.68
30	B	302	A86	C17-C16-C15	3.48	112.72	109.16
27	b	830	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
27	F	306	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
27	b	842	CLA	CMB-C2B-C3B	3.48	131.19	124.68
26	I	302	DD6	C4-C5-C6	-3.48	122.35	127.31
32	b	837	BCR	C7-C8-C9	-3.48	120.98	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	849	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
26	L	301	DD6	C37-C36-C35	3.47	120.79	114.36
34	a	831	PQN	C14-C13-C15	3.47	121.11	115.27
30	D	204	A86	C19-C18-C17	-3.47	104.07	110.77
27	f	301	CLA	CMB-C2B-C3B	3.46	131.16	124.68
27	K	318	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
26	K	303	DD6	C7-C6-C5	-3.46	118.08	122.92
27	b	841	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
30	M	305	A86	C17-C16-C15	3.46	112.69	109.16
32	a	836	BCR	C38-C26-C25	-3.46	120.65	124.53
27	C	307	CLA	CMB-C2B-C3B	3.46	131.14	124.68
30	B	305	A86	C34-O4-C38	-3.45	111.46	117.90
27	b	826	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
32	b	834	BCR	C7-C8-C9	-3.45	121.02	126.23
27	a	817	CLA	CMB-C2B-C3B	3.45	131.13	124.68
32	E	305	BCR	C33-C5-C6	-3.45	120.65	124.53
27	l	204	CLA	O2D-CGD-CBD	3.45	117.40	111.27
26	A	201	DD6	C37-C36-C35	3.45	120.75	114.36
32	E	304	BCR	C11-C10-C9	-3.45	122.39	127.31
27	L	321	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
26	L	301	DD6	C25-C26-C27	-3.45	116.57	126.58
26	A	201	DD6	C14-C13-C11	-3.44	120.19	125.53
27	J	315	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
27	K	319	CLA	CMB-C2B-C3B	3.44	131.12	124.68
27	E	310	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
30	B	301	A86	C25-C24-C1	-3.43	116.77	126.42
27	a	815	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
26	L	303	DD6	C3-C2-C1	-3.43	122.41	127.31
27	B	311	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
30	M	302	A86	C7-C6-C8	3.43	123.48	118.08
27	a	846	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
27	a	806	CLA	CMB-C2B-C3B	3.43	131.10	124.68
27	b	813	CLA	CMB-C2B-C3B	3.43	131.09	124.68
27	K	311	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
30	L	304	A86	C7-C6-C5	-3.43	118.12	122.92
32	j	101	BCR	C28-C27-C26	-3.42	107.96	114.08
32	a	851	BCR	C38-C26-C25	-3.42	120.68	124.53
26	K	303	DD6	C37-C36-C31	-3.42	119.70	124.35
27	F	311	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
30	J	304	A86	C41-C32-C31	-3.42	107.41	110.47
26	E	306	DD6	O1-C20-C19	-3.42	110.82	113.38
27	L	311	CLA	CMB-C2B-C1B	-3.41	123.22	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	i	101	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
27	H	210	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
32	E	305	BCR	C11-C10-C9	-3.41	122.44	127.31
29	A	214	LMG	O7-C10-C11	3.41	118.85	111.50
27	K	316	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
30	I	303	A86	C35-C34-C33	3.41	115.82	109.88
27	K	317	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
27	j	104	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
32	b	833	BCR	C3-C4-C5	-3.40	108.00	114.08
27	H	209	CLA	CMB-C2B-C3B	3.40	131.04	124.68
32	l	205	BCR	C34-C9-C10	-3.40	118.16	122.92
32	i	102	BCR	C15-C14-C13	-3.40	122.46	127.31
27	a	820	CLA	CMB-C2B-C3B	3.40	131.03	124.68
27	G	306	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
28	G	313	KC1	C3D-CAD-CBD	-3.39	103.14	107.61
26	F	302	DD6	C37-C36-C35	3.39	120.64	114.36
32	b	840	BCR	C34-C9-C10	-3.39	118.17	122.92
26	H	202	DD6	C3-C2-C1	-3.39	122.47	127.31
27	b	817	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
30	I	301	A86	C26-C25-C24	-3.39	112.64	123.22
27	K	313	CLA	C1-C2-C3	-3.39	120.19	126.04
32	a	847	BCR	C11-C10-C9	-3.39	122.48	127.31
27	C	311	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
26	L	303	DD6	C37-C36-C31	-3.38	119.75	124.35
27	M	316	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
27	a	823	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
26	H	202	DD6	O1-C20-C19	-3.38	110.85	113.38
32	b	837	BCR	C20-C21-C22	-3.37	122.49	127.31
32	j	101	BCR	C7-C8-C9	-3.37	121.14	126.23
27	b	810	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
27	C	306	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
27	b	822	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
32	f	304	BCR	C28-C27-C26	-3.37	108.07	114.08
27	D	214	CLA	CMB-C2B-C3B	3.37	130.97	124.68
30	C	305	A86	C7-C6-C8	3.36	123.38	118.08
27	a	818	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
32	f	304	BCR	C24-C23-C22	-3.36	121.16	126.23
26	D	205	DD6	C4-C3-C2	3.36	130.35	123.47
27	L	312	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
32	E	305	BCR	C38-C26-C25	-3.36	120.76	124.53
27	b	825	CLA	CMB-C2B-C3B	3.35	130.95	124.68
35	l	207	ET4	C01-C06-C05	-3.35	117.89	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	838	CLA	CMB-C2B-C3B	3.35	130.95	124.68
27	L	319	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
30	H	203	A86	C7-C6-C8	3.35	123.35	118.08
27	G	310	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
26	M	301	DD6	C37-C36-C31	-3.35	119.80	124.35
27	B	310	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
30	J	316	A86	C19-C18-C17	-3.34	104.31	110.77
26	J	302	DD6	C20-C19-C18	-3.34	106.14	112.75
26	E	306	DD6	C20-C19-C18	-3.34	106.14	112.75
27	a	813	CLA	CMB-C2B-C3B	3.34	130.93	124.68
27	b	847	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
27	E	309	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
26	D	205	DD6	C9-C8-C6	-3.34	117.04	126.42
27	F	305	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
26	B	303	DD6	C15-C14-C13	-3.33	118.94	125.99
35	l	207	ET4	C35-C36-C37	-3.33	105.74	110.30
29	C	319	LMG	O8-C28-C29	3.33	122.36	111.91
29	L	323	LMG	C1-C2-C3	-3.33	103.06	110.00
30	G	302	A86	O-C13-C14	-3.33	114.90	121.66
27	F	315	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
27	b	850	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
26	F	303	DD6	C14-C13-C11	-3.32	120.37	125.53
32	b	840	BCR	C24-C23-C22	-3.32	121.21	126.23
30	H	201	A86	O1-C15-C14	-3.32	106.54	113.21
26	G	304	DD6	C15-C14-C13	-3.32	118.97	125.99
27	F	313	CLA	CMB-C2B-C3B	3.32	130.89	124.68
27	J	309	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
27	a	808	CLA	CMB-C2B-C3B	3.32	130.89	124.68
27	D	216	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
27	K	310	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
35	l	207	ET4	C07-C06-C05	-3.32	113.42	121.46
27	M	316	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
27	a	839	CLA	O2D-CGD-CBD	3.32	117.16	111.27
29	L	323	LMG	O6-C1-C2	-3.32	103.33	110.35
30	C	304	A86	O1-C15-C14	-3.32	106.56	113.21
32	f	304	BCR	C33-C5-C6	-3.31	120.81	124.53
32	l	205	BCR	C33-C5-C6	-3.31	120.81	124.53
30	B	301	A86	C9-C10-C11	-3.31	116.88	126.61
27	M	309	CLA	C1-C2-C3	-3.31	120.32	126.04
30	B	302	A86	O1-C15-C14	-3.31	106.57	113.21
27	M	311	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
27	M	312	CLA	CMB-C2B-C3B	3.31	130.87	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	844	CLA	CMB-C2B-C3B	3.31	130.86	124.68
30	E	301	A86	C7-C6-C8	3.30	123.28	118.08
32	m	102	BCR	C2-C1-C6	3.30	115.56	110.48
30	K	306	A86	C34-O4-C38	-3.30	111.74	117.90
27	C	314	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
27	M	307	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
27	J	311	CLA	CMB-C2B-C3B	3.30	130.85	124.68
27	a	830	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
30	b	848	A86	O-C13-C11	-3.29	113.87	121.15
27	A	205	CLA	CMB-C2B-C3B	3.29	130.84	124.68
31	a	834	LHG	O8-C23-C24	3.29	120.02	111.38
27	C	309	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
27	F	317	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
26	J	303	DD6	C9-C10-C11	-3.29	122.62	127.31
27	J	312	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
30	m	101	A86	C8-C6-C5	3.28	123.98	118.94
27	b	821	CLA	O2D-CGD-CBD	3.28	117.10	111.27
27	b	829	CLA	CMB-C2B-C3B	3.28	130.82	124.68
27	M	311	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
27	a	814	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
27	H	205	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
30	I	303	A86	C24-C1-C2	-3.28	113.91	118.94
32	b	840	BCR	C3-C4-C5	-3.28	108.22	114.08
27	I	305	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
27	I	305	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
30	B	302	A86	O-C13-C11	-3.27	113.91	121.15
30	M	302	A86	O1-C15-C14	-3.27	106.65	113.21
30	D	203	A86	C4-C3-C2	-3.27	116.77	123.47
27	I	306	CLA	CMB-C2B-C3B	3.27	130.80	124.68
27	K	309	CLA	CMB-C2B-C3B	3.27	130.79	124.68
27	b	807	CLA	CMB-C2B-C3B	3.27	130.79	124.68
30	H	201	A86	O-C13-C11	-3.27	113.93	121.15
27	G	308	CLA	CMB-C2B-C3B	3.26	130.78	124.68
30	E	301	A86	C26-C25-C24	-3.26	113.03	123.22
32	a	847	BCR	C16-C17-C18	-3.26	122.66	127.31
30	L	302	A86	O4-C34-C33	3.26	115.70	107.59
27	C	310	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
27	H	207	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
27	a	843	CLA	CMB-C2B-C3B	3.25	130.76	124.68
26	A	202	DD6	C32-C31-C36	-3.25	118.05	122.63
27	D	213	CLA	CMB-C2B-C3B	3.25	130.75	124.68
31	E	316	LHG	C5-O7-C7	-3.25	109.80	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	312	CLA	CAA-CBA-CGA	-3.25	103.77	113.25
30	I	301	A86	C-C1-C24	3.25	123.19	118.08
27	L	308	CLA	CMB-C2B-C3B	3.24	130.75	124.68
26	I	304	DD6	C4-C3-C2	-3.24	116.83	123.47
27	a	812	CLA	CMB-C2B-C3B	3.24	130.75	124.68
32	b	833	BCR	C7-C8-C9	-3.24	121.33	126.23
27	E	313	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
30	D	203	A86	C26-C25-C24	3.24	133.34	123.22
27	C	316	CLA	CMB-C2B-C3B	3.24	130.74	124.68
27	K	310	CLA	CMB-C2B-C3B	3.24	130.74	124.68
27	M	313	CLA	CMB-C2B-C3B	3.24	130.74	124.68
27	a	844	CLA	CMB-C2B-C3B	3.24	130.74	124.68
27	J	310	CLA	CMB-C2B-C3B	3.24	130.73	124.68
30	D	206	A86	C26-C25-C24	-3.23	113.13	123.22
27	b	811	CLA	CMB-C2B-C3B	3.23	130.73	124.68
27	a	829	CLA	CMB-C2B-C3B	3.23	130.72	124.68
27	L	316	CLA	CMB-C2B-C3B	3.23	130.72	124.68
27	B	308	CLA	CMB-C2B-C3B	3.23	130.72	124.68
28	M	314	KC1	C2A-C3A-C4A	3.23	108.88	106.49
27	C	318	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
30	E	301	A86	C8-C6-C5	-3.22	114.00	118.94
27	D	211	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
27	b	841	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
26	I	302	DD6	C15-C14-C13	-3.22	119.18	125.99
26	I	304	DD6	C20-C19-C18	-3.22	106.38	112.75
30	L	306	A86	C34-O4-C38	-3.22	111.89	117.90
32	b	833	BCR	C11-C10-C9	-3.22	122.72	127.31
27	F	309	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
26	E	306	DD6	C-C1-C24	-3.22	113.00	118.08
27	K	311	CLA	CMB-C2B-C3B	3.22	130.70	124.68
32	i	103	BCR	C33-C5-C6	-3.22	120.91	124.53
32	b	837	BCR	C11-C10-C9	-3.22	122.72	127.31
27	I	311	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
27	a	822	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
27	A	204	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
31	B	315	LHG	O8-C23-C24	3.21	121.99	111.91
30	C	302	A86	O1-C15-C14	-3.21	106.76	113.21
30	J	316	A86	O1-C15-C14	-3.21	106.76	113.21
32	l	202	BCR	C34-C9-C10	-3.21	118.42	122.92
32	b	834	BCR	C2-C1-C6	3.21	115.43	110.48
30	C	302	A86	C34-O4-C38	-3.21	111.91	117.90
26	H	202	DD6	C9-C10-C11	-3.21	122.73	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	302	DD6	C15-C14-C13	-3.21	119.20	125.99
32	b	834	BCR	C15-C16-C17	-3.21	116.90	123.47
27	A	208	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
26	L	301	DD6	C32-C31-C36	-3.21	118.10	122.63
28	L	322	KC1	O2D-CGD-O1D	-3.21	117.57	123.84
27	M	309	CLA	CMB-C2B-C3B	3.21	130.68	124.68
27	a	821	CLA	CMB-C2B-C3B	3.21	130.68	124.68
30	J	301	A86	C10-C9-C8	3.20	133.21	123.22
28	H	211	KC1	CHB-C1B-C2B	-3.20	118.76	125.48
26	G	303	DD6	C15-C14-C13	-3.20	119.22	125.99
27	a	841	CLA	CMB-C2B-C3B	3.20	130.67	124.68
27	a	828	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
30	K	302	A86	C40-C32-C31	-3.20	107.61	110.47
27	H	208	CLA	CMB-C2B-C3B	3.20	130.66	124.68
32	a	853	BCR	C28-C27-C26	-3.20	108.37	114.08
30	J	304	A86	C26-C25-C24	-3.20	113.24	123.22
32	j	105	BCR	C38-C26-C25	-3.20	120.94	124.53
27	M	308	CLA	CMB-C2B-C3B	3.20	130.66	124.68
27	b	820	CLA	CMB-C2B-C3B	3.20	130.66	124.68
27	J	314	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
30	I	303	A86	C33-C32-C31	3.20	112.32	109.21
27	a	804	CLA	CMB-C2B-C3B	3.20	130.66	124.68
32	E	305	BCR	C3-C4-C5	-3.19	108.37	114.08
32	b	837	BCR	C16-C15-C14	-3.19	116.93	123.47
26	J	302	DD6	C33-C34-C35	-3.19	105.93	110.30
32	b	840	BCR	C8-C9-C10	3.19	123.84	118.94
27	C	312	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
30	L	304	A86	C-C1-C2	-3.19	118.45	122.92
27	F	308	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
27	a	810	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
30	D	204	A86	C24-C1-C2	-3.19	114.05	118.94
31	a	833	LHG	O8-C23-C24	3.19	121.91	111.91
32	E	304	BCR	C3-C4-C5	-3.19	108.39	114.08
27	L	315	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
32	a	835	BCR	C7-C8-C9	-3.18	121.42	126.23
27	b	803	CLA	CMB-C2B-C3B	3.18	130.64	124.68
32	b	834	BCR	C31-C1-C2	3.18	121.64	108.91
30	K	307	A86	C-C1-C2	-3.18	118.47	122.92
27	B	309	CLA	CMB-C2B-C3B	3.18	130.63	124.68
27	I	311	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
27	b	828	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
26	E	306	DD6	C-C1-C2	-3.18	118.47	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	305	DD6	C33-C34-C35	-3.18	105.95	110.30
32	E	305	BCR	C7-C8-C9	-3.18	121.43	126.23
27	a	849	CLA	CMB-C2B-C3B	3.18	130.63	124.68
28	C	308	KC1	C3D-CAD-CBD	-3.18	103.42	107.61
26	G	303	DD6	C4-C5-C6	-3.18	122.77	127.31
30	H	203	A86	C10-C9-C8	3.18	133.13	123.22
27	E	313	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
37	b	835	DGD	C2G-O2G-C1B	-3.18	109.97	117.79
26	G	303	DD6	C37-C36-C31	-3.18	120.03	124.35
27	B	306	CLA	CMB-C2B-C3B	3.17	130.62	124.68
27	G	307	CLA	CMB-C2B-C3B	3.17	130.61	124.68
27	H	212	CLA	CMB-C2B-C3B	3.17	130.61	124.68
27	a	844	CLA	O1D-CGD-CBD	3.17	130.97	124.48
27	A	204	CLA	CMB-C2B-C3B	3.17	130.60	124.68
26	D	205	DD6	C37-C36-C31	-3.17	120.05	124.35
27	a	839	CLA	CMB-C2B-C3B	3.17	130.60	124.68
26	D	205	DD6	C-C1-C2	-3.17	118.49	122.92
30	J	304	A86	C36-C31-C32	3.17	122.84	119.70
26	H	202	DD6	C13-C11-C10	3.16	123.80	118.94
32	b	833	BCR	C24-C23-C22	-3.16	121.46	126.23
27	b	812	CLA	CMB-C2B-C3B	3.16	130.59	124.68
27	K	313	CLA	CMB-C2B-C3B	3.16	130.59	124.68
27	b	819	CLA	CMB-C2B-C3B	3.16	130.59	124.68
27	a	811	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
30	m	101	A86	C4-C3-C2	-3.15	117.02	123.47
28	A	209	KC1	O1D-CGD-CBD	-3.15	118.03	124.48
26	L	301	DD6	C25-C24-C1	-3.15	117.56	126.42
27	a	823	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
26	M	306	DD6	C4-C3-C2	-3.15	117.02	123.47
27	D	209	CLA	CMB-C2B-C3B	3.15	130.57	124.68
27	I	313	CLA	CMB-C2B-C3B	3.15	130.57	124.68
27	a	848	CLA	CMB-C2B-C3B	3.15	130.57	124.68
27	b	816	CLA	CMB-C2B-C3B	3.15	130.57	124.68
27	K	314	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
27	I	317	CLA	CMB-C2B-C3B	3.15	130.56	124.68
27	A	205	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
30	M	303	A86	C35-C34-C33	3.14	115.36	109.88
27	I	308	CLA	CMB-C2B-C3B	3.14	130.55	124.68
27	E	312	CLA	CMB-C2B-C3B	3.14	130.55	124.68
26	M	304	DD6	C19-C18-C17	-3.14	104.71	110.77
27	E	314	CLA	CMB-C2B-C3B	3.14	130.55	124.68
27	a	825	CLA	CMB-C2B-C3B	3.14	130.55	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	305	A86	C10-C9-C8	3.14	133.01	123.22
27	r	201	CLA	CMB-C2B-C3B	3.14	130.55	124.68
27	H	213	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
27	a	854	CLA	CMB-C2B-C3B	3.14	130.54	124.68
28	I	312	KC1	CHC-C4B-C3B	-3.13	119.90	125.26
27	J	308	CLA	CMB-C2B-C3B	3.13	130.53	124.68
27	b	831	CLA	CMB-C2B-C3B	3.13	130.53	124.68
27	b	814	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
28	J	306	KC1	CBD-CHA-C1A	3.13	134.71	128.88
32	f	305	BCR	C33-C5-C4	3.13	119.62	113.62
27	b	838	CLA	O2D-CGD-CBD	3.13	116.82	111.27
27	E	311	CLA	CMB-C2B-C3B	3.13	130.53	124.68
27	L	317	CLA	CMB-C2B-C3B	3.12	130.52	124.68
30	K	305	A86	C34-O4-C38	-3.12	112.08	117.90
27	a	819	CLA	CMB-C2B-C3B	3.12	130.52	124.68
27	J	307	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
27	L	310	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
27	D	215	CLA	CMB-C2B-C3B	3.12	130.52	124.68
27	K	314	CLA	CHD-C1D-C2D	3.12	132.02	125.48
30	H	203	A86	O1-C15-C14	-3.12	106.95	113.21
30	E	301	A86	C10-C9-C8	3.12	132.94	123.22
27	b	849	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
28	L	314	KC1	O1D-CGD-CBD	-3.12	118.11	124.48
27	H	206	CLA	O2D-CGD-CBD	3.12	116.80	111.27
27	a	827	CLA	CMB-C2B-C1B	-3.12	123.68	128.46
30	K	305	A86	C17-C16-C15	3.11	112.34	109.16
30	I	303	A86	C34-O4-C38	-3.11	112.09	117.90
26	G	305	DD6	C9-C10-C11	-3.11	122.87	127.31
27	b	805	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
27	a	806	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
32	f	304	BCR	C38-C26-C25	-3.11	121.04	124.53
30	C	302	A86	C26-C25-C24	-3.11	113.52	123.22
27	A	203	CLA	CMB-C2B-C3B	3.11	130.49	124.68
26	G	301	DD6	C37-C36-C31	-3.11	120.13	124.35
32	a	835	BCR	C38-C26-C25	-3.11	121.04	124.53
27	G	314	CLA	CAA-C2A-C3A	-3.10	108.85	116.10
27	a	830	CLA	CMB-C2B-C3B	3.10	130.49	124.68
27	f	302	CLA	CMB-C2B-C3B	3.10	130.49	124.68
27	D	208	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
27	b	824	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
30	D	204	A86	C-C1-C24	3.10	122.97	118.08
27	H	205	CLA	CMB-C2B-C3B	3.10	130.48	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	303	DD6	C32-C33-C34	-3.10	106.64	113.64
27	I	316	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
32	l	205	BCR	C38-C26-C27	3.10	119.57	113.62
27	b	845	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
35	l	207	ET4	O40-C36-C35	3.10	115.96	109.80
27	F	313	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
27	L	309	CLA	CMB-C2B-C3B	3.10	130.47	124.68
26	E	302	DD6	C37-C36-C31	-3.09	120.14	124.35
27	b	821	CLA	CMB-C2B-C3B	3.09	130.47	124.68
27	K	317	CLA	CMB-C2B-C3B	3.09	130.47	124.68
32	a	853	BCR	C11-C12-C13	-3.09	117.74	126.42
27	b	846	CLA	CMB-C2B-C3B	3.09	130.45	124.68
27	D	208	CLA	CAA-CBA-CGA	-3.09	104.23	113.25
27	I	315	CLA	C1-C2-C3	-3.08	120.71	126.04
30	K	302	A86	C41-C32-C31	-3.08	107.71	110.47
27	M	309	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
27	b	843	CLA	CMB-C2B-C3B	3.08	130.44	124.68
26	F	302	DD6	C37-C36-C31	-3.08	120.16	124.35
29	J	317	LMG	O2-C2-C1	3.08	117.53	110.05
26	I	304	DD6	C37-C36-C31	-3.08	120.16	124.35
30	M	303	A86	C7-C6-C5	-3.08	118.61	122.92
30	L	304	A86	C34-O4-C38	-3.08	112.16	117.90
26	L	303	DD6	C-C1-C2	-3.08	118.61	122.92
30	M	303	A86	C20-C19-C18	-3.08	106.66	112.75
27	b	808	CLA	CMB-C2B-C3B	3.08	130.43	124.68
26	E	306	DD6	C37-C36-C31	-3.08	120.17	124.35
32	m	102	BCR	C16-C15-C14	-3.07	117.18	123.47
30	b	848	A86	C12-C11-C13	3.07	121.18	116.02
31	D	201	LHG	O8-C23-C24	3.07	121.54	111.91
27	I	309	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
30	J	316	A86	C40-C32-C31	-3.07	107.73	110.47
27	I	307	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
30	F	304	A86	C3-C2-C1	3.07	131.69	127.31
27	A	208	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
30	B	301	A86	C28-C27-C26	-3.07	118.63	122.92
28	I	312	KC1	O1D-CGD-CBD	-3.07	118.21	124.48
27	b	819	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
30	C	304	A86	C17-C16-C15	3.07	112.29	109.16
27	F	307	CLA	CMB-C2B-C3B	3.06	130.41	124.68
27	a	828	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
27	M	315	CLA	CMB-C2B-C3B	3.06	130.41	124.68
27	b	806	CLA	CMB-C2B-C3B	3.06	130.41	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	856	CLA	CMB-C2B-C3B	3.06	130.41	124.68
26	G	304	DD6	C4-C5-C6	-3.06	122.94	127.31
27	b	838	CLA	CMB-C2B-C3B	3.06	130.40	124.68
27	K	317	CLA	CHB-C4A-NA	3.06	128.74	124.51
32	b	837	BCR	C33-C5-C6	-3.06	121.09	124.53
30	K	304	A86	O1-C20-C21	-3.06	111.39	115.06
32	f	305	BCR	C3-C4-C5	-3.06	108.62	114.08
27	I	314	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
27	A	207	CLA	CMB-C2B-C3B	3.06	130.39	124.68
27	G	312	CLA	CMB-C2B-C3B	3.06	130.39	124.68
26	G	305	DD6	C15-C14-C13	-3.05	119.53	125.99
30	I	303	A86	C7-C6-C8	3.05	122.89	118.08
26	A	202	DD6	C25-C24-C1	-3.05	117.83	126.42
27	M	316	CLA	CMB-C2B-C3B	3.05	130.39	124.68
27	D	216	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
30	M	302	A86	C25-C26-C27	-3.05	122.95	127.31
30	D	206	A86	C17-C16-C15	3.05	112.27	109.16
26	D	205	DD6	C7-C6-C8	-3.05	113.27	118.08
27	C	317	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
27	H	214	CLA	CMB-C2B-C3B	3.05	130.38	124.68
27	D	212	CLA	CMB-C2B-C3B	3.05	130.38	124.68
27	G	307	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
35	l	207	ET4	C16-C15-C14	3.05	129.71	123.47
30	b	848	A86	C41-C32-C31	-3.04	107.75	110.47
26	M	304	DD6	C24-C1-C2	3.04	123.61	118.94
27	a	854	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
27	b	830	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
32	a	847	BCR	C15-C14-C13	-3.04	122.97	127.31
28	B	313	KC1	CHB-C1B-C2B	-3.04	119.10	125.48
26	M	301	DD6	C-C1-C2	-3.04	118.67	122.92
29	A	214	LMG	O8-C28-C29	3.04	121.44	111.91
30	B	304	A86	C34-O4-C38	-3.04	112.23	117.90
27	b	817	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
27	l	203	CLA	CMB-C2B-C3B	3.04	130.36	124.68
32	a	835	BCR	C38-C26-C27	3.04	119.45	113.62
27	F	314	CLA	CMB-C2B-C3B	3.04	130.36	124.68
27	b	801	CLA	CMB-C2B-C3B	3.04	130.36	124.68
32	m	102	BCR	C8-C9-C10	3.03	123.60	118.94
27	a	841	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
26	I	304	DD6	C32-C31-C36	-3.03	118.35	122.63
26	L	301	DD6	C15-C14-C13	-3.03	119.58	125.99
27	b	805	CLA	CMB-C2B-C3B	3.03	130.35	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	310	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
30	C	302	A86	C19-C18-C17	-3.03	104.92	110.77
30	I	301	A86	O1-C15-C14	-3.03	107.14	113.21
30	E	301	A86	O1-C15-C14	-3.03	107.14	113.21
27	a	855	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
30	I	303	A86	C19-C18-C17	-3.03	104.93	110.77
31	E	318	LHG	O8-C23-C24	3.03	121.40	111.91
27	M	310	CLA	CMB-C2B-C3B	3.03	130.34	124.68
30	C	302	A86	O-C13-C11	-3.03	114.46	121.15
30	F	301	A86	C17-C16-C15	3.02	112.25	109.16
26	E	307	DD6	O1-C20-C19	-3.02	111.11	113.38
27	K	309	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
27	C	307	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
27	C	315	CLA	CMB-C2B-C3B	3.02	130.33	124.68
28	B	313	KC1	C3D-CAD-CBD	-3.02	103.63	107.61
26	D	205	DD6	C26-C25-C24	3.02	132.64	123.22
27	b	845	CLA	CMB-C2B-C3B	3.02	130.32	124.68
27	I	308	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
27	M	307	CLA	CMB-C2B-C3B	3.01	130.32	124.68
27	l	204	CLA	CMB-C2B-C3B	3.01	130.32	124.68
28	L	320	KC1	CHC-C4B-C3B	-3.01	120.10	125.26
27	b	808	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
27	a	811	CLA	CMB-C2B-C3B	3.01	130.32	124.68
27	G	314	CLA	CMB-C2B-C3B	3.01	130.31	124.68
30	F	304	A86	C34-O4-C38	-3.01	112.28	117.90
30	b	848	A86	C7-C6-C5	-3.01	118.70	122.92
32	l	205	BCR	C15-C14-C13	-3.01	123.01	127.31
28	M	314	KC1	CHB-C1B-C2B	-3.01	119.17	125.48
27	a	821	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
27	J	311	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
27	F	316	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
27	D	217	CLA	CMB-C2B-C3B	3.01	130.30	124.68
27	b	839	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
27	b	806	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
27	D	207	CLA	CMB-C2B-C3B	3.00	130.30	124.68
28	J	306	KC1	CHC-C4B-C3B	-3.00	120.12	125.26
27	L	307	CLA	CMB-C2B-C3B	3.00	130.30	124.68
27	a	850	CLA	CMB-C2B-C3B	3.00	130.30	124.68
27	J	313	CLA	CMB-C2B-C3B	3.00	130.29	124.68
29	E	317	LMG	O1-C7-C8	-3.00	103.66	110.90
27	a	845	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
30	K	301	A86	C3-C2-C1	-3.00	123.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	846	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
30	r	202	A86	O4-C38-C39	3.00	116.60	111.09
32	i	103	BCR	C3-C4-C5	-3.00	108.73	114.08
27	I	310	CLA	CMB-C2B-C3B	3.00	130.28	124.68
27	L	316	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
27	H	212	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
32	b	840	BCR	C30-C25-C26	-2.99	118.39	122.61
26	D	205	DD6	C41-C32-C31	-2.99	105.71	110.47
26	D	205	DD6	C33-C34-C35	-2.99	106.21	110.30
27	F	309	CLA	C2D-C1D-ND	-2.99	107.90	110.10
26	I	304	DD6	C19-C18-C17	-2.99	104.99	110.77
30	C	302	A86	C10-C9-C8	2.99	132.56	123.22
30	M	302	A86	C10-C9-C8	2.99	132.55	123.22
27	A	206	CLA	CMB-C2B-C3B	2.99	130.27	124.68
27	F	310	CLA	CMB-C2B-C3B	2.99	130.27	124.68
26	J	305	DD6	C7-C6-C5	-2.99	118.74	122.92
27	A	207	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
27	B	312	CLA	CMB-C2B-C3B	2.99	130.27	124.68
27	b	828	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
27	L	310	CLA	CMB-C2B-C3B	2.99	130.27	124.68
27	a	832	CLA	CMB-C2B-C3B	2.99	130.27	124.68
27	b	842	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
27	M	318	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
27	A	211	CLA	CMB-C2B-C3B	2.99	130.26	124.68
27	C	314	CLA	CMB-C2B-C3B	2.98	130.26	124.68
32	E	304	BCR	C7-C8-C9	-2.98	121.73	126.23
28	K	315	KC1	CHB-C1B-C2B	-2.98	119.22	125.48
26	A	201	DD6	O1-C20-C21	-2.98	111.48	115.06
27	a	832	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
27	M	318	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
30	K	301	A86	C33-C32-C31	2.98	112.11	109.21
30	b	848	A86	C10-C9-C8	-2.98	113.92	123.22
32	l	202	BCR	C3-C4-C5	-2.98	108.76	114.08
26	L	301	DD6	C9-C8-C6	-2.98	118.05	126.42
27	b	823	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
26	G	304	DD6	C3-C4-C5	-2.98	117.38	123.47
27	a	803	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
27	b	809	CLA	CMB-C2B-C3B	2.98	130.25	124.68
30	J	301	A86	O4-C38-O5	-2.98	117.05	122.96
27	H	204	CLA	CMB-C2B-C3B	2.98	130.25	124.68
27	a	822	CLA	CMB-C2B-C3B	2.98	130.25	124.68
26	B	303	DD6	C3-C2-C1	-2.98	123.06	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	303	CLA	CMB-C2B-C3B	2.97	130.24	124.68
26	J	305	DD6	C28-C27-C29	2.97	122.73	116.84
27	b	841	CLA	CMB-C2B-C3B	2.97	130.24	124.68
26	D	205	DD6	C19-C18-C17	-2.97	105.03	110.77
30	D	203	A86	C28-C27-C26	-2.97	118.76	122.92
26	G	304	DD6	C9-C10-C11	-2.97	123.07	127.31
27	K	314	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
27	b	818	CLA	CMB-C2B-C3B	2.97	130.23	124.68
27	a	817	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
26	A	201	DD6	C25-C26-C27	-2.96	117.97	126.58
30	D	204	A86	C34-O4-C38	-2.96	112.38	117.90
30	B	305	A86	C7-C6-C8	2.96	122.74	118.08
27	a	842	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
26	J	302	DD6	C-C1-C2	-2.96	118.78	122.92
30	K	306	A86	C41-C32-C31	-2.96	107.82	110.47
28	M	314	KC1	O2D-CGD-O1D	-2.96	118.05	123.84
27	b	843	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
27	L	311	CLA	CMB-C2B-C3B	2.96	130.21	124.68
27	b	839	CLA	CMB-C2B-C3B	2.96	130.21	124.68
27	B	309	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
27	B	314	CLA	CMB-C2B-C3B	2.96	130.21	124.68
27	D	210	CLA	CMB-C2B-C3B	2.96	130.21	124.68
32	I	202	BCR	C24-C23-C22	-2.95	121.77	126.23
30	E	301	A86	C34-O4-C38	-2.95	112.39	117.90
27	G	317	CLA	CMB-C2B-C3B	2.95	130.20	124.68
27	M	315	CLA	CAA-C2A-C3A	-2.95	109.21	116.10
27	a	809	CLA	CMB-C2B-C3B	2.95	130.20	124.68
28	L	314	KC1	CHB-C1B-C2B	-2.95	119.29	125.48
27	B	311	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
27	a	825	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
27	G	315	CLA	CMB-C2B-C3B	2.95	130.19	124.68
30	I	301	A86	C19-C18-C17	-2.95	105.08	110.77
27	G	316	CLA	CMB-C2B-C3B	2.95	130.19	124.68
27	B	312	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
27	b	801	CLA	O2D-CGD-CBD	2.94	116.50	111.27
27	L	321	CLA	CMB-C2B-C3B	2.94	130.18	124.68
27	C	318	CLA	CMB-C2B-C3B	2.94	130.18	124.68
28	K	308	KC1	O2D-CGD-O1D	-2.94	118.09	123.84
26	E	306	DD6	C32-C31-C36	-2.94	118.48	122.63
27	a	824	CLA	CMB-C2B-C3B	2.94	130.18	124.68
27	L	307	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
30	A	213	A86	C17-C16-C15	2.94	112.16	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	847	BCR	C3-C4-C5	-2.94	108.83	114.08
30	r	202	A86	O-C13-C14	-2.94	115.69	121.66
27	I	307	CLA	CMB-C2B-C3B	2.93	130.17	124.68
28	C	308	KC1	CHC-C4B-C3B	-2.93	120.24	125.26
29	l	201	LMG	O8-C28-C29	2.93	121.11	111.91
27	b	831	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
27	b	846	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
27	b	824	CLA	CMB-C2B-C3B	2.93	130.17	124.68
27	a	808	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
32	m	102	BCR	C28-C27-C26	-2.93	108.84	114.08
27	b	803	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
27	A	210	CLA	CMB-C2B-C3B	2.93	130.16	124.68
27	a	826	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
27	H	214	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
27	a	838	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
27	K	316	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
27	b	827	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	D	202	LMG	O8-C28-C29	2.93	121.10	111.91
32	f	305	BCR	C28-C27-C26	-2.93	108.85	114.08
27	b	810	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
32	j	101	BCR	C3-C4-C5	-2.93	108.85	114.08
27	B	307	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
27	J	312	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
27	M	317	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
32	b	834	BCR	C20-C21-C22	-2.93	123.13	127.31
26	E	306	DD6	C37-C36-C35	2.93	119.78	114.36
27	b	811	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
27	A	203	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
28	C	308	KC1	O1D-CGD-CBD	-2.92	118.50	124.48
30	M	305	A86	O1-C15-C14	-2.92	107.35	113.21
27	b	806	CLA	CHB-C4A-NA	2.92	128.55	124.51
27	G	311	CLA	CMB-C2B-C3B	2.92	130.14	124.68
27	M	310	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
27	b	813	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
30	K	305	A86	C4-C3-C2	-2.92	117.49	123.47
27	E	311	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
27	i	101	CLA	C1-C2-C3	-2.92	120.99	126.04
32	i	103	BCR	C38-C26-C25	-2.92	121.25	124.53
27	b	847	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
27	K	316	CLA	CMB-C2B-C3B	2.92	130.14	124.68
28	K	308	KC1	CHB-C1B-C2B	-2.92	119.36	125.48
30	I	301	A86	C17-C16-C15	2.92	112.14	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	312	CLA	CMB-C2B-C3B	2.91	130.13	124.68
32	l	202	BCR	C16-C17-C18	-2.91	123.15	127.31
27	I	311	CLA	CMB-C2B-C3B	2.91	130.13	124.68
27	H	207	CLA	O2D-CGD-CBD	2.91	116.44	111.27
27	a	818	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
27	J	313	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
27	E	315	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
27	l	206	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
32	f	305	BCR	C16-C17-C18	-2.91	123.16	127.31
27	a	850	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
27	L	319	CLA	CMB-C2B-C3B	2.91	130.12	124.68
27	D	214	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
27	K	318	CLA	CMB-C2B-C3B	2.91	130.12	124.68
32	a	847	BCR	C29-C30-C25	-2.91	106.00	110.48
27	b	829	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
27	l	203	CLA	O2D-CGD-CBD	2.91	116.43	111.27
32	a	835	BCR	C20-C21-C22	-2.91	123.16	127.31
27	a	807	CLA	CHB-C4A-NA	2.91	128.53	124.51
29	C	301	LMG	O8-C28-C29	2.91	121.03	111.91
30	J	304	A86	C34-O4-C38	-2.91	112.48	117.90
32	r	203	BCR	C15-C14-C13	-2.91	123.16	127.31
32	b	840	BCR	C16-C17-C18	-2.91	123.16	127.31
27	j	104	CLA	CAA-C2A-C3A	-2.90	109.32	116.10
27	D	211	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
27	b	801	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
27	a	848	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
27	B	307	CLA	CMB-C2B-C3B	2.90	130.11	124.68
30	C	305	A86	O-C13-C11	-2.90	114.74	121.15
27	H	204	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
29	E	317	LMG	O8-C28-C29	2.90	121.01	111.91
27	K	314	CLA	CMB-C2B-C3B	2.90	130.10	124.68
27	a	816	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
27	b	849	CLA	CMB-C2B-C3B	2.90	130.10	124.68
27	a	814	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
27	M	316	CLA	CAA-CBA-CGA	-2.90	104.79	113.25
27	a	815	CLA	C1-C2-C3	-2.89	121.04	126.04
27	b	816	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
29	j	103	LMG	O8-C28-C29	2.89	120.99	111.91
27	H	210	CLA	CMB-C2B-C3B	2.89	130.09	124.68
30	M	302	A86	C40-C32-C31	-2.89	107.89	110.47
27	I	306	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
29	J	317	LMG	O8-C28-C29	2.89	120.97	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	856	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
27	G	306	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
27	I	309	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
27	E	312	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
32	a	851	BCR	C37-C22-C21	-2.88	118.88	122.92
30	I	303	A86	C40-C32-C31	-2.88	107.89	110.47
30	A	213	A86	C25-C24-C1	-2.88	118.31	126.42
30	J	301	A86	C7-C6-C8	2.88	122.62	118.08
27	F	305	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
30	F	304	A86	C9-C8-C6	2.88	134.51	126.42
27	K	312	CLA	CMB-C2B-C3B	2.88	130.07	124.68
30	J	304	A86	C7-C6-C8	2.88	122.61	118.08
28	A	209	KC1	CHC-C4B-C3B	-2.88	120.33	125.26
27	D	207	CLA	O2D-CGD-CBD	2.88	116.38	111.27
30	D	203	A86	C9-C8-C6	2.88	134.50	126.42
26	D	205	DD6	C13-C11-C10	2.88	123.36	118.94
27	a	816	CLA	CMB-C2B-C3B	2.88	130.06	124.68
27	F	306	CLA	CMB-C2B-C3B	2.88	130.06	124.68
26	H	202	DD6	C20-C19-C18	-2.88	107.06	112.75
27	a	807	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
27	I	315	CLA	CMB-C2B-C3B	2.88	130.06	124.68
27	a	813	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	E	302	DD6	C21-C20-C15	-2.88	117.44	122.26
27	H	208	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
27	a	849	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
27	L	311	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	M	315	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	b	817	CLA	CMB-C2B-C3B	2.87	130.05	124.68
27	a	824	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
28	F	312	KC1	CHC-C4B-C3B	-2.87	120.34	125.26
27	G	312	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	A	211	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	C	306	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	D	213	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	a	805	CLA	CMB-C2B-C3B	2.87	130.05	124.68
26	M	301	DD6	C21-C20-C15	-2.87	117.45	122.26
27	b	807	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	D	202	LMG	O2-C2-C3	-2.87	103.72	110.35
30	L	302	A86	C3-C2-C1	-2.87	123.22	127.31
27	G	309	CLA	CMB-C2B-C3B	2.87	130.04	124.68
27	E	308	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
27	J	314	CLA	O2D-CGD-O1D	-2.87	118.24	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	315	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
27	E	310	CLA	CMB-C2B-C3B	2.86	130.04	124.68
27	G	317	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
27	J	307	CLA	CMB-C2B-C3B	2.86	130.03	124.68
27	b	826	CLA	CMB-C2B-C3B	2.86	130.03	124.68
32	b	840	BCR	C33-C5-C4	2.86	119.11	113.62
27	a	844	CLA	O2A-CGA-O1A	-2.86	116.38	123.59
26	M	301	DD6	C15-C14-C13	-2.86	119.95	125.99
27	I	311	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
27	I	310	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
26	H	202	DD6	C15-C14-C13	-2.85	119.96	125.99
31	E	316	LHG	O8-C23-C24	2.85	120.86	111.91
27	b	826	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	r	202	A86	C12-C11-C10	-2.85	116.52	123.42
27	b	850	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	E	301	A86	C19-C18-C17	-2.85	105.27	110.77
27	D	215	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
27	E	314	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
30	m	101	A86	C34-O4-C38	-2.85	112.59	117.90
27	F	307	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
27	C	311	CLA	CAA-CBA-CGA	-2.84	104.95	113.25
27	a	804	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
27	a	841	CLA	CHB-C4A-NA	2.84	128.44	124.51
27	D	212	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
27	G	306	CLA	CMB-C2B-C3B	2.84	129.99	124.68
26	M	304	DD6	C37-C36-C31	-2.84	120.49	124.35
37	b	835	DGD	O1G-C1A-C2A	2.84	120.82	111.91
27	a	844	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
27	L	312	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	B	303	DD6	C26-C25-C24	-2.84	114.36	123.22
32	E	304	BCR	C24-C23-C22	-2.84	121.95	126.23
26	G	301	DD6	C15-C14-C13	-2.84	119.99	125.99
26	M	306	DD6	C10-C9-C8	-2.84	114.36	123.22
27	j	104	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
27	b	809	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
32	l	205	BCR	C20-C21-C22	-2.84	123.26	127.31
27	f	301	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	A	201	DD6	C10-C9-C8	-2.84	114.37	123.22
30	J	304	A86	C20-C19-C18	-2.83	107.14	112.75
27	F	310	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	a	812	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	L	313	CLA	CMB-C2B-C3B	2.83	129.97	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	819	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	C	317	CLA	CMB-C2B-C3B	2.83	129.97	124.68
32	l	202	BCR	C15-C16-C17	-2.83	117.68	123.47
30	M	302	A86	C19-C18-C17	-2.83	105.31	110.77
27	C	309	CLA	CHB-C4A-NA	2.83	128.43	124.51
30	L	302	A86	C20-C19-C18	-2.83	107.15	112.75
27	a	840	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
31	K	320	LHG	O8-C23-C24	2.83	120.78	111.91
32	E	304	BCR	C16-C17-C18	-2.83	123.28	127.31
32	a	835	BCR	C11-C10-C9	-2.83	123.28	127.31
35	l	207	ET4	C01-C06-C07	2.83	123.78	115.78
27	M	312	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
27	b	820	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	A	201	DD6	C25-C24-C1	-2.83	118.48	126.42
27	G	315	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
27	a	846	CLA	CMB-C2B-C3B	2.82	129.96	124.68
32	a	853	BCR	C38-C26-C27	2.82	119.04	113.62
27	D	210	CLA	O2D-CGD-CBD	2.82	116.28	111.27
27	C	309	CLA	CMB-C2B-C3B	2.82	129.96	124.68
28	H	211	KC1	CBD-CHA-C1A	2.82	134.15	128.88
27	I	311	CLA	CHB-C4A-NA	2.82	128.41	124.51
30	H	201	A86	C12-C11-C10	-2.82	116.59	123.42
27	b	839	CLA	CHB-C4A-NA	2.82	128.41	124.51
26	K	303	DD6	C12-C11-C10	-2.82	118.97	122.92
32	m	102	BCR	C10-C11-C12	-2.82	114.42	123.22
27	F	314	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
27	L	309	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	L	322	KC1	CHB-C1B-C2B	-2.82	119.56	125.48
32	E	305	BCR	C33-C5-C4	2.82	119.03	113.62
32	a	836	BCR	C7-C8-C9	-2.82	121.98	126.23
27	L	313	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
27	a	843	CLA	O2A-CGA-O1A	-2.82	116.48	123.59
27	F	305	CLA	CMB-C2B-C3B	2.82	129.95	124.68
29	A	212	LMG	O8-C28-C29	2.82	120.75	111.91
27	G	310	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	I	311	CLA	CMC-C2C-C1C	2.81	129.32	125.04
27	A	206	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	a	842	CLA	CMB-C2B-C3B	2.81	129.94	124.68
27	G	314	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	E	309	CLA	CMB-C2B-C3B	2.81	129.93	124.68
30	C	305	A86	C19-C18-C17	-2.81	105.35	110.77
27	I	305	CLA	CMB-C2B-C3B	2.81	129.93	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	216	CLA	CMB-C2B-C3B	2.81	129.93	124.68
27	F	315	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
30	K	306	A86	C9-C10-C11	-2.81	118.36	126.61
27	I	314	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
27	b	814	CLA	CMB-C2B-C3B	2.81	129.93	124.68
27	M	317	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
27	L	321	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
27	b	815	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
30	M	303	A86	C4-C3-C2	2.80	129.21	123.47
31	I	318	LHG	O8-C23-C24	2.80	120.69	111.91
27	M	319	CLA	CMB-C2B-C3B	2.80	129.92	124.68
27	J	308	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
26	B	303	DD6	C4-C3-C2	-2.80	117.74	123.47
30	B	301	A86	C3-C4-C5	-2.80	117.74	123.47
27	B	310	CLA	CMB-C2B-C3B	2.80	129.91	124.68
27	b	818	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
27	M	317	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
27	j	104	CLA	CMB-C2B-C3B	2.80	129.91	124.68
30	m	101	A86	C10-C9-C8	2.80	131.94	123.22
27	J	309	CLA	C1-C2-C3	-2.80	121.21	126.04
27	E	309	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
27	a	810	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
28	G	313	KC1	CHC-C4B-C3B	-2.79	120.48	125.26
27	F	306	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
30	B	304	A86	O-C13-C11	-2.79	114.98	121.15
27	f	302	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
28	C	308	KC1	C4B-CHC-C1C	-2.79	120.04	126.06
28	F	312	KC1	CHB-C1B-C2B	-2.79	119.63	125.48
30	J	301	A86	C4-C5-C6	2.79	131.29	127.31
27	a	843	CLA	O2D-CGD-CBD	2.79	116.22	111.27
27	C	318	CLA	CHB-C4A-NA	2.79	128.37	124.51
28	C	313	KC1	CHB-C1B-C2B	-2.79	119.63	125.48
32	b	837	BCR	C24-C23-C22	-2.79	122.03	126.23
27	L	313	CLA	C1-C2-C3	-2.79	121.22	126.04
27	B	308	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
26	D	205	DD6	C25-C24-C1	2.78	134.24	126.42
28	A	209	KC1	C4B-CHC-C1C	-2.78	120.05	126.06
30	B	302	A86	C12-C11-C10	-2.78	116.69	123.42
26	K	303	DD6	C33-C34-C35	-2.78	106.50	110.30
27	L	317	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
27	I	316	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	B	303	DD6	C20-C19-C18	-2.78	107.25	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	l	205	BCR	C38-C26-C25	-2.78	121.41	124.53
27	F	311	CLA	CMB-C2B-C3B	2.78	129.88	124.68
28	K	308	KC1	C3D-CAD-CBD	-2.78	103.95	107.61
28	C	313	KC1	CBD-CHA-C1A	2.78	134.06	128.88
27	a	829	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
30	H	203	A86	C8-C6-C5	-2.77	114.68	118.94
27	J	310	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
28	L	322	KC1	CHC-C4B-C3B	-2.77	120.52	125.26
30	F	301	A86	C28-C27-C26	-2.77	119.04	122.92
27	F	315	CLA	CMB-C2B-C3B	2.77	129.86	124.68
30	B	305	A86	C17-C16-C15	2.77	111.99	109.16
27	I	309	CLA	CHD-C1D-ND	-2.77	121.91	124.45
30	M	305	A86	C34-O4-C38	-2.77	112.74	117.90
30	C	305	A86	C40-C32-C31	-2.77	108.00	110.47
27	C	310	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
28	L	314	KC1	CHC-C4B-C3B	-2.77	120.53	125.26
32	a	847	BCR	C30-C25-C26	-2.77	118.72	122.61
29	M	321	LMG	O1-C1-C2	2.77	112.62	108.30
27	F	311	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
27	E	310	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
30	r	202	A86	C26-C25-C24	2.76	131.84	123.22
27	a	818	CLA	CMB-C2B-C3B	2.76	129.85	124.68
27	b	838	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
27	b	822	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
32	b	840	BCR	C4-C5-C6	-2.76	118.72	122.73
30	F	304	A86	O4-C38-O5	-2.76	117.48	122.96
27	i	101	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
27	i	101	CLA	CMB-C2B-C3B	2.76	129.84	124.68
28	I	312	KC1	C4B-CHC-C1C	-2.76	120.11	126.06
28	M	314	KC1	C4B-CHC-C1C	-2.76	120.11	126.06
31	M	320	LHG	O8-C23-C24	2.76	120.56	111.91
30	M	305	A86	C26-C25-C24	-2.76	114.61	123.22
32	f	305	BCR	C1-C6-C7	2.76	123.58	115.78
31	a	801	LHG	O8-C23-C24	2.76	120.56	111.91
27	a	856	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
32	E	304	BCR	C38-C26-C25	-2.76	121.43	124.53
27	C	315	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
27	b	828	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
30	r	202	A86	C7-C6-C8	2.75	122.42	118.08
28	L	314	KC1	CBD-CHA-C1A	2.75	134.02	128.88
27	G	310	CLA	CMB-C2B-C3B	2.75	129.83	124.68
26	J	302	DD6	C34-C35-C36	-2.75	106.37	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	309	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
26	E	307	DD6	C37-C36-C31	-2.75	120.61	124.35
27	b	810	CLA	CMB-C2B-C3B	2.75	129.83	124.68
27	I	313	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	C	301	LMG	C4-C3-C2	2.75	115.62	110.82
30	J	304	A86	C8-C6-C5	-2.75	114.72	118.94
27	D	215	CLA	CAA-C2A-C3A	-2.75	109.68	116.10
28	C	313	KC1	CHC-C4B-C3B	-2.75	120.56	125.26
28	G	313	KC1	CHB-C1B-C2B	-2.75	119.72	125.48
30	m	101	A86	C3-C4-C5	-2.75	117.85	123.47
30	C	305	A86	C8-C6-C5	-2.75	114.73	118.94
27	K	318	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
27	a	824	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	B	312	CLA	CHB-C4A-NA	2.74	128.31	124.51
32	E	304	BCR	C33-C5-C4	2.74	118.89	113.62
30	K	302	A86	C34-O4-C38	-2.74	112.78	117.90
32	i	102	BCR	C33-C5-C4	2.74	118.88	113.62
30	K	306	A86	C35-C34-C33	2.74	114.66	109.88
30	K	307	A86	C12-C11-C13	2.74	120.62	116.02
27	a	813	CLA	CHB-C4A-NA	2.74	128.30	124.51
27	b	847	CLA	CMB-C2B-C3B	2.74	129.80	124.68
32	a	836	BCR	C28-C27-C26	-2.74	109.19	114.08
32	a	853	BCR	C20-C19-C18	-2.74	118.73	126.42
26	F	303	DD6	C15-C14-C13	-2.74	120.21	125.99
28	J	306	KC1	C4B-CHC-C1C	-2.73	120.16	126.06
27	a	815	CLA	CMB-C2B-C3B	2.73	129.79	124.68
30	I	301	A86	C40-C32-C31	-2.73	108.03	110.47
27	G	316	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	K	301	A86	C40-C32-C31	-2.73	108.03	110.47
27	F	317	CLA	CMB-C2B-C3B	2.73	129.78	124.68
27	L	312	CLA	CMB-C2B-C3B	2.73	129.78	124.68
27	b	822	CLA	CMB-C2B-C3B	2.73	129.78	124.68
28	M	314	KC1	CHC-C4B-C3B	-2.73	120.60	125.26
32	r	203	BCR	C38-C26-C25	-2.72	121.47	124.53
27	L	313	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
30	K	306	A86	C3-C4-C5	-2.72	117.89	123.47
27	A	210	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
26	M	306	DD6	C4-C5-C6	-2.72	123.42	127.31
32	b	834	BCR	C11-C12-C13	-2.72	118.77	126.42
30	J	316	A86	C28-C27-C26	-2.72	119.11	122.92
28	K	315	KC1	O1D-CGD-CBD	-2.72	118.92	124.48
27	J	309	CLA	O2D-CGD-O1D	-2.72	118.52	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	812	CLA	CHB-C4A-NA	2.72	128.28	124.51
30	C	302	A86	C41-C32-C31	-2.72	108.04	110.47
32	b	840	BCR	C15-C14-C13	-2.72	123.43	127.31
30	B	304	A86	O-C13-C14	-2.72	116.13	121.66
26	E	307	DD6	C14-C13-C11	-2.72	121.31	125.53
27	G	308	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
27	E	310	CLA	CHB-C4A-NA	2.72	128.27	124.51
27	E	312	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	G	301	DD6	C21-C20-C15	-2.72	117.71	122.26
27	D	214	CLA	CHB-C4A-NA	2.72	128.27	124.51
27	a	817	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
27	K	313	CLA	CHB-C4A-NA	2.72	128.27	124.51
27	b	801	CLA	C1-C2-C3	-2.72	121.35	126.04
30	B	305	A86	O-C13-C14	-2.71	116.14	121.66
28	H	211	KC1	O1D-CGD-CBD	-2.71	118.93	124.48
27	G	309	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
27	B	311	CLA	CMB-C2B-C3B	2.71	129.75	124.68
30	B	304	A86	C12-C11-C10	-2.71	116.86	123.42
26	I	304	DD6	C4-C5-C6	-2.71	123.44	127.31
27	r	201	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
27	b	819	CLA	CHB-C4A-NA	2.71	128.26	124.51
30	J	316	A86	C10-C9-C8	2.71	131.68	123.22
28	I	312	KC1	O2D-CGD-O1D	-2.71	118.54	123.84
27	C	306	CLA	CMB-C2B-C3B	2.71	129.75	124.68
28	J	306	KC1	CHB-C1B-C2B	-2.71	119.80	125.48
28	A	209	KC1	C3D-CAD-CBD	-2.71	104.04	107.61
27	C	309	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
27	I	314	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
32	b	837	BCR	C38-C26-C27	2.71	118.81	113.62
27	b	812	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
27	a	828	CLA	CHB-C4A-NA	2.71	128.25	124.51
30	C	302	A86	O4-C38-O5	-2.70	117.59	122.96
27	L	315	CLA	CMB-C2B-C3B	2.70	129.73	124.68
32	b	840	BCR	C38-C26-C27	2.70	118.81	113.62
32	b	837	BCR	C20-C19-C18	-2.70	118.83	126.42
27	L	316	CLA	C1-C2-C3	-2.70	121.37	126.04
28	A	209	KC1	C2A-C3A-C4A	2.70	108.49	106.49
27	a	821	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	E	302	DD6	C33-C34-C35	-2.70	106.61	110.30
27	a	809	CLA	C1-C2-C3	-2.70	121.37	126.04
30	I	301	A86	C10-C9-C8	2.70	131.64	123.22
28	H	211	KC1	C3D-CAD-CBD	-2.70	104.05	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	J	301	A86	C8-C6-C5	-2.70	114.80	118.94
26	C	303	DD6	C33-C34-C35	2.70	114.00	110.30
27	F	316	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
26	M	306	DD6	C37-C36-C35	2.70	119.35	114.36
30	K	301	A86	O4-C38-O5	-2.70	117.61	122.96
30	M	303	A86	C19-C18-C17	-2.70	105.57	110.77
28	J	306	KC1	O2D-CGD-O1D	-2.69	118.57	123.84
27	K	314	CLA	CHB-C4A-NA	2.69	128.24	124.51
27	b	823	CLA	CHB-C4A-NA	2.69	128.24	124.51
27	F	308	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
26	J	305	DD6	C-C1-C24	-2.69	113.84	118.08
26	C	303	DD6	C10-C9-C8	-2.69	114.82	123.22
27	K	309	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
29	C	319	LMG	C1-O6-C5	-2.69	108.41	113.69
32	f	305	BCR	C20-C19-C18	-2.69	118.87	126.42
32	l	202	BCR	C8-C9-C10	2.69	123.06	118.94
30	K	301	A86	C41-C32-C31	-2.69	108.07	110.47
27	M	316	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
30	B	305	A86	C19-C18-C17	-2.69	105.59	110.77
27	J	315	CLA	CMB-C2B-C3B	2.69	129.70	124.68
27	a	803	CLA	CMB-C2B-C3B	2.68	129.70	124.68
27	B	306	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
27	K	314	CLA	CHD-C1D-ND	-2.68	121.99	124.45
26	J	303	DD6	C32-C33-C34	-2.68	107.58	113.64
27	b	825	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
27	C	318	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
27	I	314	CLA	CMB-C2B-C3B	2.68	129.70	124.68
30	E	301	A86	C41-C32-C31	-2.68	108.07	110.47
27	D	209	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
27	H	207	CLA	CMB-C2B-C3B	2.68	129.69	124.68
27	a	823	CLA	CHB-C4A-NA	2.68	128.22	124.51
32	r	203	BCR	C33-C5-C6	-2.68	121.52	124.53
27	B	308	CLA	CHB-C4A-NA	2.68	128.22	124.51
28	L	320	KC1	CBD-CHA-C1A	2.68	133.87	128.88
26	A	202	DD6	C15-C14-C13	-2.68	120.33	125.99
32	r	203	BCR	C11-C10-C9	-2.68	123.49	127.31
32	f	305	BCR	C7-C8-C9	-2.67	122.19	126.23
30	K	301	A86	C4-C3-C2	-2.67	118.00	123.47
30	I	301	A86	O4-C38-O5	-2.67	117.65	122.96
26	L	301	DD6	C37-C36-C31	-2.67	120.72	124.35
27	M	311	CLA	CMB-C2B-C3B	2.67	129.68	124.68
27	D	211	CLA	CMB-C2B-C3B	2.67	129.68	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	E	313	CLA	CMB-C2B-C3B	2.67	129.68	124.68
28	L	320	KC1	CHB-C1B-C2B	-2.67	119.88	125.48
27	a	856	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
26	F	303	DD6	C21-C20-C15	-2.67	117.79	122.26
32	a	847	BCR	C38-C26-C27	2.67	118.74	113.62
27	a	814	CLA	CMB-C2B-C3B	2.67	129.67	124.68
30	K	306	A86	C9-C8-C6	-2.67	118.92	126.42
27	L	313	CLA	CHB-C4A-NA	2.67	128.20	124.51
32	i	102	BCR	C3-C4-C5	-2.67	109.31	114.08
30	B	302	A86	C7-C6-C8	2.67	122.28	118.08
27	K	318	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
27	K	313	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
27	b	805	CLA	CHB-C4A-NA	2.67	128.20	124.51
27	b	817	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
26	H	202	DD6	C4-C5-C6	-2.67	123.50	127.31
27	b	827	CLA	CHB-C4A-NA	2.67	128.20	124.51
27	M	318	CLA	CHB-C4A-NA	2.66	128.20	124.51
27	f	303	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
27	C	310	CLA	CMB-C2B-C3B	2.66	129.66	124.68
27	G	306	CLA	CHB-C4A-NA	2.66	128.20	124.51
32	a	853	BCR	C3-C4-C5	-2.66	109.32	114.08
27	b	828	CLA	CMB-C2B-C3B	2.66	129.66	124.68
27	D	209	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	H	201	A86	C7-C6-C8	2.66	122.27	118.08
27	J	312	CLA	CMB-C2B-C3B	2.66	129.66	124.68
29	a	852	LMG	O8-C28-C29	2.66	120.25	111.91
34	b	832	PQN	C14-C13-C15	2.66	119.74	115.27
31	j	102	LHG	O8-C23-C24	2.66	120.25	111.91
27	b	845	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	b	848	A86	C-C1-C24	2.66	122.26	118.08
30	E	301	A86	O-C13-C11	-2.66	115.28	121.15
27	a	823	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
26	A	201	DD6	C37-C36-C31	-2.66	120.74	124.35
27	G	311	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
27	I	309	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
30	L	305	A86	C26-C25-C24	-2.65	114.94	123.22
30	K	304	A86	O1-C15-C14	-2.65	107.89	113.21
28	L	322	KC1	C3D-CAD-CBD	-2.65	104.11	107.61
26	M	301	DD6	C14-C13-C11	-2.65	121.42	125.53
27	F	310	CLA	CHB-C4A-NA	2.65	128.18	124.51
27	B	314	CLA	CMA-C3A-C2A	-2.65	109.92	116.10
30	J	301	A86	C19-C18-C17	-2.65	105.66	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	828	CLA	CMB-C2B-C3B	2.65	129.63	124.68
27	b	815	CLA	CHB-C4A-NA	2.65	128.17	124.51
27	K	312	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
26	J	303	DD6	C7-C6-C5	-2.64	119.22	122.92
27	M	313	CLA	CHB-C4A-NA	2.64	128.17	124.51
27	b	801	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
27	f	302	CLA	CHB-C4A-NA	2.64	128.17	124.51
27	f	303	CLA	CHB-C4A-NA	2.64	128.17	124.51
26	M	301	DD6	O1-C20-C19	-2.64	111.40	113.38
26	E	307	DD6	C15-C14-C13	-2.64	120.41	125.99
27	a	803	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
27	b	813	CLA	CHB-C4A-NA	2.64	128.16	124.51
32	b	837	BCR	C33-C5-C4	2.64	118.69	113.62
27	K	314	CLA	CAA-CBA-CGA	-2.64	105.54	113.25
32	f	305	BCR	C16-C15-C14	-2.64	118.07	123.47
30	b	848	A86	C24-C1-C2	-2.64	114.89	118.94
26	G	305	DD6	C21-C20-C15	-2.64	117.84	122.26
32	a	847	BCR	C23-C24-C25	-2.64	119.80	127.20
26	H	202	DD6	C23-C16-C22	2.64	111.26	107.37
26	L	303	DD6	C34-C35-C36	-2.63	106.61	111.85
26	A	202	DD6	C20-C19-C18	-2.63	107.54	112.75
27	F	309	CLA	CMB-C2B-C3B	2.63	129.60	124.68
27	M	312	CLA	CAA-CBA-CGA	-2.63	105.56	113.25
26	H	202	DD6	C12-C11-C10	-2.63	119.24	122.92
27	L	315	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
30	F	301	A86	C20-C19-C18	-2.63	107.55	112.75
27	C	316	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
27	K	317	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
26	J	305	DD6	C25-C24-C1	-2.63	119.03	126.42
26	B	303	DD6	C-C1-C24	-2.63	113.94	118.08
26	G	304	DD6	C33-C34-C35	-2.63	106.71	110.30
29	J	317	LMG	C8-O7-C10	-2.63	111.32	117.79
32	a	835	BCR	C8-C7-C6	-2.63	119.83	127.20
30	J	316	A86	C17-C16-C15	2.63	111.84	109.16
27	b	850	CLA	CHB-C4A-NA	2.63	128.14	124.51
27	b	814	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
27	b	811	CLA	CHB-C4A-NA	2.62	128.14	124.51
28	A	209	KC1	CBD-CHA-C1A	2.62	133.77	128.88
27	G	314	CLA	CHB-C4A-NA	2.62	128.14	124.51
30	L	306	A86	C40-C32-C31	-2.62	108.13	110.47
27	L	318	CLA	O2D-CGD-O1D	-2.62	118.14	124.09
32	E	304	BCR	C20-C21-C22	-2.62	123.57	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	209	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
27	H	209	CLA	CHB-C4A-NA	2.62	128.13	124.51
32	b	833	BCR	C38-C26-C25	-2.61	121.59	124.53
27	G	312	CLA	CHB-C4A-NA	2.61	128.13	124.51
26	G	303	DD6	C9-C10-C11	-2.61	123.58	127.31
30	G	302	A86	C4-C5-C6	-2.61	123.58	127.31
27	A	203	CLA	CHB-C4A-NA	2.61	128.13	124.51
27	F	308	CLA	CMB-C2B-C3B	2.61	129.57	124.68
26	G	303	DD6	C33-C34-C35	-2.61	106.73	110.30
35	l	207	ET4	C34-C35-C36	-2.61	107.75	113.64
32	j	105	BCR	C38-C26-C27	2.61	118.63	113.62
27	M	308	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
30	r	202	A86	C28-C27-C26	2.61	126.58	122.92
32	E	304	BCR	C15-C16-C17	-2.61	118.13	123.47
27	a	820	CLA	CHB-C4A-NA	2.61	128.12	124.51
27	b	841	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
27	b	844	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
27	a	810	CLA	CMB-C2B-C3B	2.61	129.56	124.68
28	H	211	KC1	CHC-C4B-C3B	-2.61	120.80	125.26
27	C	316	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	B	305	A86	C8-C6-C5	-2.61	114.94	118.94
27	a	845	CLA	CHB-C4A-NA	2.61	128.12	124.51
27	M	311	CLA	O2D-CGD-CBD	2.60	115.90	111.27
30	F	301	A86	C4-C3-C2	-2.60	118.14	123.47
28	C	308	KC1	CHB-C1B-C2B	-2.60	120.02	125.48
27	J	312	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	I	304	DD6	C9-C10-C11	-2.60	123.59	127.31
28	K	308	KC1	O1D-CGD-CBD	-2.60	119.16	124.48
27	G	307	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
27	J	308	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
27	j	104	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	E	301	A86	C3-C2-C1	2.60	131.02	127.31
31	a	837	LHG	O8-C23-C24	2.60	120.07	111.91
30	J	304	A86	C24-C1-C2	-2.60	114.95	118.94
30	G	302	A86	C12-C11-C10	-2.60	117.13	123.42
27	H	213	CLA	C1-C2-C3	-2.60	121.55	126.04
27	E	308	CLA	CHB-C4A-NA	2.60	128.11	124.51
27	G	317	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	F	303	DD6	C9-C8-C6	-2.60	119.11	126.42
27	M	318	CLA	CMB-C2B-C3B	2.60	129.54	124.68
27	G	308	CLA	CHB-C4A-NA	2.60	128.10	124.51
32	i	102	BCR	C33-C5-C6	-2.60	121.61	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I	312	KC1	CHB-C1B-C2B	-2.60	120.04	125.48
26	E	307	DD6	C33-C34-C35	-2.59	106.75	110.30
27	K	309	CLA	CHB-C4A-NA	2.59	128.10	124.51
27	b	812	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
27	b	841	CLA	CHB-C4A-NA	2.59	128.10	124.51
27	E	314	CLA	CHB-C4A-NA	2.59	128.10	124.51
27	a	818	CLA	CHB-C4A-NA	2.59	128.10	124.51
27	J	311	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
27	L	321	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
27	L	318	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
27	a	829	CLA	CHB-C4A-NA	2.59	128.10	124.51
27	I	305	CLA	O2D-CGD-CBD	2.59	115.87	111.27
27	K	318	CLA	CHB-C4A-NA	2.59	128.09	124.51
27	b	810	CLA	CHB-C4A-NA	2.59	128.09	124.51
26	C	303	DD6	C33-C32-C31	-2.59	104.37	109.62
27	H	206	CLA	CAA-CBA-CGA	-2.59	105.69	113.25
27	M	312	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
27	a	855	CLA	CHB-C4A-NA	2.59	128.09	124.51
27	a	840	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
30	F	304	A86	C36-C31-C32	2.59	122.27	119.70
30	L	305	A86	C12-C11-C13	2.59	120.37	116.02
30	C	302	A86	C21-C20-C19	-2.59	111.37	114.28
27	J	309	CLA	CMB-C2B-C3B	2.59	129.52	124.68
32	m	102	BCR	C33-C5-C4	2.59	118.59	113.62
27	K	316	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
32	E	304	BCR	C21-C20-C19	-2.59	115.15	123.22
27	H	207	CLA	C1-C2-C3	-2.59	121.57	126.04
31	b	836	LHG	O8-C23-C24	2.59	120.02	111.91
30	B	302	A86	O4-C38-O5	-2.59	117.83	122.96
27	B	309	CLA	CHB-C4A-NA	2.59	128.09	124.51
31	M	320	LHG	C5-O7-C7	-2.58	111.43	117.79
27	b	843	CLA	CHB-C4A-NA	2.58	128.09	124.51
27	L	319	CLA	O2D-CGD-CBD	2.58	115.86	111.27
27	C	317	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
27	a	842	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
33	J	318	SQD	O7-S-C6	2.58	110.02	106.92
27	a	809	CLA	CBA-CAA-C2A	-2.58	106.25	113.86
26	L	303	DD6	C37-C36-C35	2.58	119.14	114.36
27	a	856	CLA	CHB-C4A-NA	2.58	128.08	124.51
30	H	201	A86	O4-C38-O5	-2.58	117.84	122.96
26	J	303	DD6	C21-C20-C15	-2.58	117.94	122.26
27	A	210	CLA	C1B-CHB-C4A	-2.58	125.01	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	207	ET4	C42-C34-C33	-2.58	106.37	110.47
27	D	208	CLA	CMB-C2B-C3B	2.58	129.50	124.68
26	M	301	DD6	C25-C24-C1	-2.58	119.18	126.42
27	B	307	CLA	CHB-C4A-NA	2.58	128.07	124.51
27	H	214	CLA	CHB-C4A-NA	2.58	128.07	124.51
27	b	849	CLA	CHB-C4A-NA	2.57	128.07	124.51
27	a	823	CLA	CMB-C2B-C3B	2.57	129.49	124.68
27	a	843	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
27	M	315	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	M	304	DD6	C4-C5-C6	-2.57	123.64	127.31
27	A	204	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
27	D	213	CLA	CHB-C4A-NA	2.57	128.07	124.51
27	a	826	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	J	304	A86	C9-C8-C6	2.57	133.64	126.42
28	K	308	KC1	CHC-C4B-C3B	-2.57	120.86	125.26
32	r	203	BCR	C7-C8-C9	-2.57	122.35	126.23
27	a	827	CLA	O1D-CGD-CBD	2.57	129.74	124.48
27	C	311	CLA	CMB-C2B-C3B	2.57	129.48	124.68
27	b	838	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
27	a	810	CLA	CHB-C4A-NA	2.56	128.06	124.51
30	A	213	A86	C12-C11-C13	2.56	120.33	116.02
27	F	313	CLA	CHB-C4A-NA	2.56	128.06	124.51
27	M	311	CLA	CHB-C4A-NA	2.56	128.06	124.51
27	b	812	CLA	CHB-C4A-NA	2.56	128.06	124.51
27	b	850	CLA	CMB-C2B-C3B	2.56	129.47	124.68
27	I	317	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
27	C	312	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
28	B	313	KC1	O2D-CGD-O1D	-2.56	118.83	123.84
26	M	306	DD6	C32-C31-C36	-2.56	119.02	122.63
32	a	851	BCR	C30-C25-C26	-2.56	119.01	122.61
27	C	306	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	L	301	DD6	C4-C3-C2	-2.56	118.23	123.47
27	F	305	CLA	CHB-C4A-NA	2.56	128.05	124.51
30	C	305	A86	O4-C38-O5	-2.56	117.88	122.96
27	l	203	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
27	K	316	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	L	301	DD6	C14-C13-C11	-2.56	121.56	125.53
27	a	841	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
28	L	320	KC1	C4B-CHC-C1C	-2.56	120.54	126.06
30	r	202	A86	C21-C20-C19	-2.56	111.40	114.28
27	A	211	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
32	l	205	BCR	C27-C26-C25	-2.56	119.02	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	319	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
32	I	202	BCR	C21-C20-C19	-2.56	115.24	123.22
27	H	204	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	D	203	A86	C25-C24-C1	2.55	133.59	126.42
27	J	314	CLA	CMB-C2B-C3B	2.55	129.46	124.68
26	L	301	DD6	C12-C11-C10	-2.55	119.35	122.92
27	b	807	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	I	301	A86	C21-C20-C19	-2.55	111.41	114.28
27	F	307	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	F	317	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	a	805	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	b	841	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
28	M	314	KC1	C1A-C2A-C3A	-2.55	105.09	107.11
27	A	208	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
27	a	820	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
30	G	302	A86	O-C13-C11	-2.55	115.51	121.15
30	L	304	A86	C3-C4-C5	-2.55	118.25	123.47
27	L	317	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
27	a	849	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	L	308	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
32	a	851	BCR	C35-C13-C14	-2.55	119.35	122.92
27	D	211	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	a	814	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	L	308	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
27	A	211	CLA	CHB-C4A-NA	2.55	128.03	124.51
27	G	310	CLA	CHB-C4A-NA	2.55	128.03	124.51
27	K	312	CLA	CHB-C4A-NA	2.55	128.03	124.51
30	B	302	A86	C40-C32-C31	-2.55	108.19	110.47
30	C	302	A86	C4-C5-C6	2.54	130.94	127.31
27	I	313	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
26	K	303	DD6	C41-C32-C31	-2.54	106.43	110.47
27	M	312	CLA	CHB-C4A-NA	2.54	128.03	124.51
27	H	212	CLA	CHB-C4A-NA	2.54	128.03	124.51
30	D	204	A86	C17-C16-C15	2.54	111.75	109.16
27	J	314	CLA	CHB-C4A-NA	2.54	128.03	124.51
27	I	309	CLA	CMB-C2B-C3B	2.54	129.43	124.68
32	b	834	BCR	C8-C7-C6	-2.54	120.07	127.20
30	L	305	A86	O4-C38-O5	-2.54	117.92	122.96
30	D	203	A86	O1-C15-C20	-2.54	56.92	59.40
27	B	312	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
27	b	821	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
30	H	203	A86	C24-C1-C2	-2.54	115.05	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	821	CLA	CHB-C4A-NA	2.54	128.02	124.51
26	J	303	DD6	C25-C24-C1	-2.54	119.29	126.42
27	C	310	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
27	F	309	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
27	D	207	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
28	K	308	KC1	CBA-CAA-C2A	-2.54	115.60	125.27
30	H	201	A86	C40-C32-C31	-2.54	108.20	110.47
30	D	203	A86	C19-C18-C17	-2.53	105.88	110.77
30	C	304	A86	C3-C4-C5	-2.53	118.28	123.47
26	D	205	DD6	C14-C13-C11	-2.53	121.60	125.53
27	a	806	CLA	CHB-C4A-NA	2.53	128.01	124.51
32	b	840	BCR	C21-C20-C19	-2.53	115.31	123.22
27	G	315	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	a	854	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	l	206	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	a	803	CLA	C4D-C3D-CAD	-2.53	105.11	108.10
28	L	314	KC1	C3D-CAD-CBD	-2.53	104.27	107.61
27	C	317	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
27	f	301	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	M	317	CLA	CMB-C2B-C3B	2.53	129.41	124.68
27	a	816	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	H	206	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
27	D	213	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
30	M	303	A86	C9-C8-C6	-2.53	119.31	126.42
27	F	317	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
27	K	317	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
27	K	309	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
27	K	311	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
29	l	201	LMG	O2-C2-C3	-2.53	104.51	110.35
27	K	319	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
28	G	313	KC1	C4B-CHC-C1C	-2.52	120.62	126.06
27	A	211	CLA	CBD-CHA-C1A	2.52	131.47	128.50
27	a	832	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	C	313	KC1	O1D-CGD-CBD	-2.52	119.33	124.48
26	I	302	DD6	C37-C36-C35	2.52	119.02	114.36
27	H	206	CLA	CHB-C4A-NA	2.52	128.00	124.51
27	H	208	CLA	CHB-C4A-NA	2.52	128.00	124.51
27	b	803	CLA	CHB-C4A-NA	2.52	128.00	124.51
27	a	839	CLA	CHB-C4A-NA	2.52	127.99	124.51
27	F	316	CLA	CMA-C3A-C2A	-2.52	110.23	116.10
27	C	309	CLA	C1B-CHB-C4A	-2.52	125.14	130.12
27	C	311	CLA	C1B-CHB-C4A	-2.51	125.14	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	833	BCR	C38-C26-C27	2.51	118.45	113.62
26	L	303	DD6	C15-C14-C13	-2.51	120.68	125.99
26	K	303	DD6	C8-C6-C5	2.51	122.80	118.94
32	f	305	BCR	C38-C26-C25	-2.51	121.70	124.53
27	B	310	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
33	J	318	SQD	O48-C23-C24	2.51	119.79	111.91
27	B	311	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	b	808	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	a	846	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	b	844	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	I	317	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
26	D	205	DD6	C4-C5-C6	2.51	130.89	127.31
27	a	827	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
32	l	205	BCR	C33-C5-C4	2.51	118.43	113.62
27	a	808	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	b	816	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	B	314	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
30	K	302	A86	O1-C15-C14	-2.50	108.18	113.21
27	b	820	CLA	CHB-C4A-NA	2.50	127.97	124.51
27	F	311	CLA	CHB-C4A-NA	2.50	127.97	124.51
27	b	824	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	I	303	A86	C8-C6-C5	-2.50	115.10	118.94
27	G	311	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
27	J	308	CLA	CHB-C4A-NA	2.50	127.97	124.51
28	F	312	KC1	C4B-CHC-C1C	-2.50	120.66	126.06
27	a	838	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
26	L	303	DD6	C32-C31-C36	-2.50	119.10	122.63
35	l	207	ET4	C28-C13-C14	-2.50	119.42	122.92
26	G	304	DD6	O1-C20-C19	-2.50	111.50	113.38
27	b	829	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	K	302	A86	C-C1-C2	-2.50	119.42	122.92
27	J	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
27	b	826	CLA	CHB-C4A-NA	2.50	127.97	124.51
27	a	825	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
27	I	307	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
32	f	304	BCR	C38-C26-C27	2.50	118.41	113.62
27	E	313	CLA	O2D-CGD-CBD	2.50	115.70	111.27
27	b	818	CLA	CHB-C4A-NA	2.50	127.96	124.51
27	l	203	CLA	O2A-CGA-O1A	-2.50	117.30	123.59
26	G	304	DD6	C21-C20-C15	-2.49	118.08	122.26
30	D	204	A86	O4-C38-O5	-2.49	118.01	122.96
27	a	829	CLA	O2A-CGA-O1A	-2.49	117.30	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	820	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
27	J	314	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
27	a	830	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
27	E	313	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
27	l	204	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
27	b	809	CLA	CHB-C4A-NA	2.49	127.95	124.51
30	I	301	A86	C8-C6-C5	-2.49	115.12	118.94
27	H	210	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
27	E	311	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
32	i	102	BCR	C30-C25-C26	-2.49	119.11	122.61
27	D	208	CLA	O2D-CGD-CBD	2.49	115.69	111.27
26	I	302	DD6	C10-C9-C8	-2.49	115.45	123.22
27	F	314	CLA	CHB-C4A-NA	2.49	127.95	124.51
27	D	217	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
30	F	304	A86	C26-C25-C24	-2.49	115.46	123.22
32	E	304	BCR	C8-C7-C6	-2.49	120.22	127.20
27	b	831	CLA	CHB-C4A-NA	2.49	127.95	124.51
27	b	829	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
30	F	304	A86	C40-C32-C31	-2.49	108.25	110.47
26	G	303	DD6	C3-C4-C5	-2.48	118.38	123.47
27	H	212	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
27	a	817	CLA	CHB-C4A-NA	2.48	127.95	124.51
30	I	303	A86	O-C13-C11	-2.48	115.66	121.15
30	C	305	A86	C4-C5-C6	2.48	130.85	127.31
28	K	308	KC1	C4B-CHC-C1C	-2.48	120.70	126.06
27	b	804	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
26	M	301	DD6	C33-C34-C35	-2.48	106.91	110.30
27	a	842	CLA	C11-C10-C8	-2.48	107.90	115.92
28	A	209	KC1	O2D-CGD-O1D	-2.48	118.99	123.84
27	I	316	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
27	L	316	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
32	b	837	BCR	C30-C25-C26	-2.48	119.12	122.61
27	a	815	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
28	I	312	KC1	CAA-CBA-CGA	-2.48	114.52	127.26
27	b	838	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	I	308	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
32	E	305	BCR	C38-C26-C27	2.48	118.38	113.62
27	F	308	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	M	303	A86	O1-C15-C20	-2.48	56.98	59.40
27	A	208	CLA	CMB-C2B-C3B	2.48	129.31	124.68
26	E	303	DD6	C4-C3-C2	-2.47	118.41	123.47
27	H	213	CLA	CHD-C1D-ND	-2.47	122.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	838	CLA	CHB-C4A-NA	2.47	127.93	124.51
27	a	850	CLA	CHB-C4A-NA	2.47	127.93	124.51
30	K	304	A86	C19-C18-C17	-2.47	106.00	110.77
27	a	829	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
27	l	204	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
27	A	206	CLA	CHB-C4A-NA	2.47	127.93	124.51
27	L	311	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
30	A	213	A86	O4-C38-O5	-2.47	118.06	122.96
28	I	312	KC1	C3D-CAD-CBD	-2.47	104.35	107.61
34	b	832	PQN	C2M-C2-C3	-2.47	120.37	124.40
27	M	307	CLA	O2D-CGD-CBD	2.47	115.66	111.27
35	l	207	ET4	C35-C34-C33	2.47	114.62	109.62
32	a	835	BCR	C33-C5-C6	-2.47	121.76	124.53
27	a	819	CLA	CHB-C4A-NA	2.47	127.92	124.51
30	L	302	A86	C19-C18-C17	-2.47	106.01	110.77
26	B	303	DD6	C9-C10-C11	-2.47	123.79	127.31
27	E	309	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
27	D	215	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
28	L	314	KC1	C4B-CHC-C1C	-2.47	120.74	126.06
30	D	206	A86	C41-C32-C31	2.47	112.68	110.47
27	F	308	CLA	C1-C2-C3	-2.47	121.78	126.04
27	A	204	CLA	CHB-C4A-NA	2.47	127.92	124.51
26	F	303	DD6	C37-C36-C35	2.47	118.92	114.36
27	b	847	CLA	CHB-C4A-NA	2.46	127.92	124.51
27	b	804	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
27	K	310	CLA	CAA-CBA-CGA	-2.46	106.05	113.25
26	G	303	DD6	O1-C20-C21	-2.46	112.10	115.06
29	C	301	LMG	C6-C5-C4	-2.46	107.23	113.00
30	K	304	A86	C25-C24-C1	-2.46	119.50	126.42
30	D	206	A86	C19-C18-C17	-2.46	106.02	110.77
28	M	314	KC1	O2A-CGA-O1A	-2.46	117.56	122.67
27	F	316	CLA	CMB-C2B-C3B	2.46	129.28	124.68
27	M	307	CLA	CHB-C4A-NA	2.46	127.91	124.51
28	H	211	KC1	C4B-CHC-C1C	-2.46	120.75	126.06
27	L	310	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
27	I	307	CLA	CHB-C4A-NA	2.46	127.91	124.51
27	a	828	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
32	a	835	BCR	C10-C11-C12	-2.46	115.54	123.22
27	H	206	CLA	C16-C15-C13	-2.46	107.97	115.92
27	G	316	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
27	a	827	CLA	CHB-C4A-NA	2.46	127.91	124.51
26	L	301	DD6	C7-C6-C5	-2.46	119.48	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	317	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
27	M	319	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
30	K	306	A86	C25-C26-C27	-2.45	123.81	127.31
27	a	825	CLA	CHB-C4A-NA	2.45	127.91	124.51
27	b	846	CLA	CHB-C4A-NA	2.45	127.91	124.51
27	D	212	CLA	CHB-C4A-NA	2.45	127.91	124.51
27	a	815	CLA	O2D-CGD-CBD	2.45	115.63	111.27
30	L	304	A86	C28-C27-C26	-2.45	119.49	122.92
30	E	301	A86	C12-C11-C10	-2.45	117.49	123.42
27	a	805	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
30	K	305	A86	C9-C8-C6	-2.45	119.53	126.42
27	M	311	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
31	a	802	LHG	O8-C23-C24	2.45	119.60	111.91
30	L	306	A86	C9-C10-C11	-2.45	119.40	126.61
28	L	322	KC1	C4B-CHC-C1C	-2.45	120.77	126.06
27	a	848	CLA	CHB-C4A-NA	2.45	127.90	124.51
27	a	804	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
30	J	316	A86	C25-C24-C1	2.45	133.29	126.42
30	F	301	A86	O4-C38-O5	-2.45	118.10	122.96
27	a	811	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	A	202	DD6	C23-C16-C22	2.45	110.98	107.37
27	M	307	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
27	a	840	CLA	CHD-C1D-ND	-2.45	122.21	124.45
27	a	803	CLA	CBA-CAA-C2A	-2.45	106.64	113.86
27	b	845	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
27	H	207	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
27	J	313	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
32	f	305	BCR	C10-C11-C12	-2.44	115.59	123.22
27	B	311	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
27	E	311	CLA	CHB-C4A-NA	2.44	127.89	124.51
27	b	842	CLA	CHB-C4A-NA	2.44	127.89	124.51
27	H	205	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
32	a	835	BCR	C33-C5-C4	2.44	118.31	113.62
27	D	217	CLA	CMA-C3A-C2A	-2.44	110.40	116.10
26	F	302	DD6	C21-C20-C15	-2.44	118.17	122.26
27	A	208	CLA	CHB-C4A-NA	2.44	127.89	124.51
27	G	307	CLA	CHB-C4A-NA	2.44	127.88	124.51
27	b	815	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
27	I	315	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
27	a	806	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
32	j	101	BCR	C33-C5-C4	2.44	118.30	113.62
32	b	837	BCR	C15-C14-C13	-2.44	123.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	817	CLA	CHB-C4A-NA	2.44	127.88	124.51
26	G	301	DD6	C37-C36-C35	2.44	118.87	114.36
27	A	205	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
27	H	213	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
27	K	310	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
27	b	842	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
29	E	317	LMG	C8-O7-C10	-2.43	111.80	117.79
27	b	849	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
30	E	301	A86	C36-C31-C32	2.43	122.11	119.70
30	K	306	A86	O4-C38-O5	-2.43	118.13	122.96
30	B	305	A86	C9-C8-C6	2.43	133.25	126.42
27	L	312	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
26	A	201	DD6	C32-C31-C36	-2.43	119.20	122.63
27	F	316	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
30	C	304	A86	C24-C1-C2	2.43	122.67	118.94
27	b	830	CLA	C1-C2-C3	-2.43	121.84	126.04
30	C	305	A86	C36-C31-C32	-2.43	117.28	119.70
27	F	305	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
27	b	805	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
27	C	311	CLA	CHB-C4A-NA	2.43	127.87	124.51
27	I	313	CLA	CHB-C4A-NA	2.43	127.87	124.51
27	b	808	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
27	F	307	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
27	C	316	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
29	J	317	LMG	O6-C1-C2	2.43	115.49	110.35
27	a	850	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
30	C	305	A86	C41-C32-C31	-2.43	108.30	110.47
27	H	206	CLA	C1-C2-C3	-2.42	121.85	126.04
27	B	307	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
30	M	302	A86	C34-O4-C38	-2.42	113.38	117.90
32	a	851	BCR	C7-C8-C9	-2.42	122.57	126.23
27	B	314	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
28	C	313	KC1	C4B-CHC-C1C	-2.42	120.83	126.06
27	E	309	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	C	311	CLA	CHD-C1D-ND	-2.42	122.23	124.45
27	C	317	CLA	CHD-C1D-ND	-2.42	122.23	124.45
27	C	315	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	L	321	CLA	CHD-C1D-ND	-2.42	122.23	124.45
27	r	201	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
27	I	306	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	a	824	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
26	H	202	DD6	C33-C32-C31	2.42	114.52	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	815	CLA	CHB-C4A-NA	2.42	127.86	124.51
32	r	203	BCR	C33-C5-C4	2.42	118.26	113.62
27	M	318	CLA	CAA-CBA-CGA	-2.42	106.19	113.25
32	E	305	BCR	C8-C7-C6	-2.42	120.41	127.20
27	b	825	CLA	CHB-C4A-NA	2.42	127.85	124.51
29	A	212	LMG	C1-O6-C5	-2.42	108.94	113.69
27	M	316	CLA	C3A-C2A-C1A	2.42	104.96	101.34
27	b	809	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
27	b	826	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
27	A	206	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	a	832	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
32	f	305	BCR	C37-C22-C21	-2.41	119.54	122.92
27	M	310	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
26	I	302	DD6	C21-C20-C15	-2.41	118.22	122.26
26	L	303	DD6	C4-C5-C6	-2.41	123.87	127.31
27	r	201	CLA	CHB-C4A-NA	2.41	127.85	124.51
27	M	310	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
27	K	312	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	H	204	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	L	307	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
30	E	301	A86	C4-C5-C6	2.41	130.75	127.31
27	D	210	CLA	CHB-C4A-NA	2.41	127.84	124.51
26	M	304	DD6	C23-C16-C22	2.41	110.92	107.37
30	J	301	A86	C36-C31-C32	2.41	122.09	119.70
27	F	311	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
30	D	203	A86	O4-C38-O5	-2.41	118.18	122.96
27	H	208	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
27	b	822	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	J	316	A86	O4-C38-O5	-2.41	118.18	122.96
26	A	202	DD6	C9-C10-C11	-2.41	123.87	127.31
27	A	207	CLA	CAA-CBA-CGA	-2.41	106.22	113.25
32	b	837	BCR	C38-C26-C25	-2.41	121.83	124.53
27	D	215	CLA	CHB-C4A-NA	2.41	127.84	124.51
27	C	307	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
27	L	308	CLA	C1-C2-C3	-2.40	121.89	126.04
32	i	103	BCR	C15-C16-C17	-2.40	118.55	123.47
27	E	308	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
27	M	313	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
30	K	307	A86	C25-C24-C1	-2.40	119.67	126.42
28	F	312	KC1	O1D-CGD-CBD	-2.40	119.57	124.48
30	K	307	A86	O4-C38-O5	-2.40	118.19	122.96
32	a	836	BCR	C38-C26-C27	2.40	118.23	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	825	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
27	b	812	CLA	O2D-CGD-CBD	2.40	115.53	111.27
32	a	847	BCR	C21-C20-C19	-2.40	115.73	123.22
26	M	301	DD6	C7-C6-C5	-2.40	119.56	122.92
30	m	101	A86	C12-C11-C10	-2.40	117.62	123.42
27	A	207	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
27	G	310	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
29	M	321	LMG	O8-C28-C29	2.40	119.43	111.91
27	E	311	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
32	j	105	BCR	C20-C19-C18	-2.40	119.69	126.42
27	a	816	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
27	b	830	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
27	I	317	CLA	CHB-C4A-NA	2.39	127.82	124.51
27	J	310	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
27	D	209	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
26	D	205	DD6	C28-C27-C29	-2.39	112.10	116.84
27	I	305	CLA	CHB-C4A-NA	2.39	127.82	124.51
27	A	203	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
27	I	316	CLA	CMB-C2B-C3B	2.39	129.15	124.68
30	K	301	A86	C12-C11-C13	2.39	120.04	116.02
30	m	101	A86	C41-C32-C31	-2.39	108.33	110.47
27	B	310	CLA	CHB-C4A-NA	2.39	127.81	124.51
27	a	803	CLA	CHB-C4A-NA	2.39	127.81	124.51
27	H	209	CLA	O2D-CGD-CBD	2.39	115.51	111.27
26	I	304	DD6	C37-C36-C35	2.39	118.78	114.36
27	E	313	CLA	CHB-C4A-NA	2.39	127.81	124.51
27	H	205	CLA	O2D-CGD-CBD	2.39	115.51	111.27
30	J	301	A86	C9-C8-C6	2.39	133.12	126.42
27	i	101	CLA	CHB-C4A-NA	2.39	127.81	124.51
27	I	316	CLA	CHB-C4A-NA	2.38	127.81	124.51
27	a	811	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
27	L	317	CLA	CHB-C4A-NA	2.38	127.81	124.51
32	b	840	BCR	C8-C7-C6	-2.38	120.51	127.20
32	a	847	BCR	C20-C21-C22	-2.38	123.91	127.31
27	b	804	CLA	C1-C2-C3	-2.38	121.92	126.04
28	K	315	KC1	C3D-CAD-CBD	-2.38	104.47	107.61
27	a	830	CLA	CHB-C4A-NA	2.38	127.81	124.51
30	M	302	A86	O4-C38-O5	-2.38	118.23	122.96
30	L	304	A86	O4-C38-O5	-2.38	118.23	122.96
28	B	313	KC1	C4B-CHC-C1C	-2.38	120.92	126.06
30	A	213	A86	C40-C32-C31	-2.38	108.34	110.47
26	M	301	DD6	C9-C10-C11	-2.38	123.92	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	833	BCR	C33-C5-C6	-2.38	121.86	124.53
27	A	205	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
30	A	213	A86	C4-C3-C2	-2.38	118.60	123.47
32	b	833	BCR	C16-C15-C14	-2.38	118.61	123.47
32	i	103	BCR	C38-C26-C27	2.38	118.18	113.62
27	K	312	CLA	CAA-CBA-CGA	-2.38	106.31	113.25
27	a	848	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
27	b	813	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
32	l	205	BCR	C35-C13-C14	-2.38	119.60	122.92
32	l	202	BCR	C10-C11-C12	-2.37	115.81	123.22
27	I	310	CLA	CHB-C4A-NA	2.37	127.80	124.51
30	D	206	A86	C12-C11-C10	-2.37	117.68	123.42
30	M	305	A86	C9-C8-C6	-2.37	119.75	126.42
30	J	304	A86	O4-C38-O5	-2.37	118.25	122.96
32	i	102	BCR	C1-C6-C5	-2.37	119.27	122.61
27	H	206	CLA	C2D-C1D-ND	-2.37	108.36	110.10
27	E	315	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
27	J	312	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	L	323	LMG	O8-C28-C29	2.37	119.35	111.91
27	a	840	CLA	CHB-C4A-NA	2.37	127.79	124.51
27	b	831	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
27	b	823	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
30	G	302	A86	C25-C24-C1	2.37	133.07	126.42
27	M	316	CLA	C2A-C1A-CHA	2.37	128.00	123.86
27	A	208	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
32	a	853	BCR	C35-C13-C14	-2.37	119.61	122.92
27	H	207	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	G	305	DD6	C3-C4-C5	-2.37	118.62	123.47
30	G	302	A86	C34-O4-C38	-2.37	113.48	117.90
27	J	307	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
27	J	315	CLA	CHB-C4A-NA	2.37	127.78	124.51
30	M	305	A86	C19-C18-C17	-2.37	106.20	110.77
27	i	101	CLA	C11-C10-C8	-2.37	108.27	115.92
27	F	306	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
27	I	315	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
27	b	821	CLA	O2A-CGA-O1A	-2.36	117.62	123.59
32	a	847	BCR	C16-C15-C14	-2.36	118.63	123.47
27	F	314	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
30	L	306	A86	C9-C8-C6	-2.36	119.78	126.42
27	a	844	CLA	CHB-C4A-NA	2.36	127.78	124.51
32	l	202	BCR	C33-C5-C4	2.36	118.16	113.62
30	r	202	A86	O-C13-C11	-2.36	115.93	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	313	CLA	CHB-C4A-NA	2.36	127.78	124.51
27	i	101	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
26	G	301	DD6	C14-C13-C11	-2.36	121.87	125.53
32	l	202	BCR	C11-C10-C9	-2.36	123.94	127.31
27	M	318	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
32	i	102	BCR	C16-C15-C14	-2.36	118.64	123.47
30	K	306	A86	O1-C15-C14	-2.36	108.47	113.21
35	l	207	ET4	C15-C14-C13	2.36	130.68	127.31
27	F	313	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
27	b	827	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
27	C	309	CLA	C1-C2-C3	-2.36	121.97	126.04
27	G	315	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	E	307	DD6	O1-C20-C21	-2.36	112.23	115.06
27	E	310	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
27	I	305	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
27	G	309	CLA	CHB-C4A-NA	2.36	127.77	124.51
30	F	304	A86	C41-C32-C31	-2.36	108.36	110.47
26	D	205	DD6	C20-C19-C18	-2.36	108.09	112.75
27	a	839	CLA	C1-C2-C3	-2.36	121.97	126.04
32	f	304	BCR	C33-C5-C4	2.36	118.14	113.62
27	H	210	CLA	O2D-CGD-CBD	2.35	115.45	111.27
27	I	309	CLA	CHB-C4A-NA	2.35	127.77	124.51
28	C	308	KC1	C2A-C3A-C4A	2.35	108.23	106.49
26	I	304	DD6	C10-C9-C8	-2.35	115.87	123.22
30	K	302	A86	C35-C34-C33	-2.35	105.77	109.88
32	E	305	BCR	C16-C15-C14	-2.35	118.66	123.47
27	M	312	CLA	CHD-C1D-ND	-2.35	122.29	124.45
30	E	301	A86	C40-C32-C31	-2.35	108.37	110.47
27	a	810	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
26	G	305	DD6	C14-C13-C11	-2.35	121.88	125.53
32	E	305	BCR	C20-C19-C18	-2.35	119.81	126.42
28	B	313	KC1	CBD-CHA-C1A	2.35	133.26	128.88
27	D	217	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
32	b	840	BCR	C30-C25-C24	2.35	122.42	115.78
27	I	308	CLA	C1-C2-C3	-2.35	121.98	126.04
30	G	302	A86	C-C1-C24	-2.35	114.38	118.08
27	b	827	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
27	I	314	CLA	CHB-C4A-NA	2.35	127.76	124.51
27	L	319	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
27	b	830	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	L	320	KC1	O1D-CGD-CBD	-2.35	119.68	124.48
27	F	316	CLA	CHB-C4A-NA	2.35	127.75	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	305	A86	C21-C20-C19	-2.34	111.64	114.28
27	M	317	CLA	O2A-CGA-O1A	-2.34	117.45	123.30
27	C	312	CLA	C1-C2-C3	-2.34	121.99	126.04
27	F	315	CLA	C1-C2-C3	-2.34	121.99	126.04
30	B	301	A86	C7-C6-C5	-2.34	119.64	122.92
30	B	305	A86	C12-C11-C10	-2.34	117.76	123.42
27	J	309	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
27	F	315	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
27	J	315	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	J	301	A86	C12-C11-C10	-2.34	117.76	123.42
32	a	851	BCR	C36-C18-C17	-2.34	119.64	122.92
27	j	104	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
26	E	303	DD6	O2-C18-C17	-2.34	105.15	109.80
28	J	306	KC1	O1D-CGD-CBD	-2.34	119.70	124.48
27	L	312	CLA	CHB-C4A-NA	2.34	127.75	124.51
32	j	101	BCR	C38-C26-C27	2.34	118.11	113.62
32	i	102	BCR	C20-C19-C18	-2.34	119.85	126.42
27	I	306	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
30	D	204	A86	O-C13-C11	-2.34	115.98	121.15
32	b	837	BCR	C27-C26-C25	-2.34	119.34	122.73
27	D	212	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
32	b	837	BCR	C36-C18-C17	-2.34	119.65	122.92
27	C	314	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
27	G	309	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
27	a	822	CLA	CHB-C4A-NA	2.33	127.74	124.51
30	K	304	A86	C12-C11-C13	2.33	119.94	116.02
27	b	806	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	A	213	A86	C35-C34-C33	2.33	113.95	109.88
27	I	315	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
26	I	304	DD6	C23-C16-C22	2.33	110.81	107.37
27	a	845	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	B	302	A86	C19-C18-C17	-2.33	106.27	110.77
27	K	313	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
27	C	306	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
26	L	303	DD6	O2-C18-C19	-2.33	105.17	109.80
27	a	819	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	H	201	A86	O-C13-C14	-2.33	116.93	121.66
30	D	204	A86	C21-C20-C19	-2.33	111.66	114.28
30	K	305	A86	C26-C25-C24	-2.33	115.95	123.22
27	B	306	CLA	CHB-C4A-NA	2.33	127.73	124.51
27	F	306	CLA	CHB-C4A-NA	2.33	127.73	124.51
30	M	303	A86	O4-C38-O5	-2.33	118.34	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	306	A86	O4-C38-O5	-2.33	118.34	122.96
30	r	202	A86	O1-C15-C20	-2.33	57.13	59.40
32	i	102	BCR	C27-C26-C25	-2.33	119.35	122.73
30	H	203	A86	O-C13-C11	-2.33	116.01	121.15
27	f	302	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
27	b	828	CLA	CHB-C4A-NA	2.33	127.73	124.51
30	H	203	A86	C-C1-C24	2.32	121.74	118.08
27	a	804	CLA	CHB-C4A-NA	2.32	127.73	124.51
30	B	305	A86	O1-C15-C14	-2.32	108.55	113.21
27	a	849	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
27	b	847	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
27	b	843	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
30	K	305	A86	C12-C11-C13	2.32	119.92	116.02
30	b	848	A86	C25-C26-C27	-2.32	124.00	127.31
32	a	853	BCR	C33-C5-C4	2.32	118.07	113.62
27	M	319	CLA	CHB-C4A-NA	2.32	127.72	124.51
28	L	314	KC1	O2D-CGD-O1D	-2.32	119.30	123.84
30	F	301	A86	C10-C9-C8	-2.32	115.98	123.22
27	M	308	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
27	b	807	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
29	I	319	LMG	O8-C28-C29	2.32	119.19	111.91
32	a	847	BCR	C33-C5-C4	2.32	118.07	113.62
30	B	302	A86	C-C1-C24	2.32	121.73	118.08
27	J	310	CLA	CHB-C4A-NA	2.32	127.72	124.51
27	a	813	CLA	C1-C2-C3	-2.32	123.00	126.75
32	b	840	BCR	C35-C13-C14	-2.32	119.68	122.92
27	b	804	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
27	a	818	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
30	C	304	A86	C26-C25-C24	-2.32	115.99	123.22
30	M	302	A86	C26-C25-C24	-2.32	115.99	123.22
32	l	202	BCR	C23-C24-C25	-2.32	120.70	127.20
32	m	102	BCR	C20-C19-C18	-2.32	119.91	126.42
26	H	202	DD6	C7-C6-C5	-2.32	119.68	122.92
27	I	311	CLA	C11-C10-C8	-2.32	108.44	115.92
27	D	214	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
30	C	305	A86	C12-C11-C10	-2.31	117.82	123.42
27	E	315	CLA	CHB-C4A-NA	2.31	127.71	124.51
30	L	306	A86	C-C1-C2	-2.31	119.68	122.92
27	a	827	CLA	CMB-C2B-C3B	2.31	129.00	124.68
30	K	305	A86	C9-C10-C11	-2.31	119.81	126.61
30	H	203	A86	C12-C11-C10	-2.31	117.83	123.42
30	L	306	A86	C4-C3-C2	-2.31	118.74	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	310	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
30	I	303	A86	O4-C38-O5	-2.31	118.37	122.96
30	K	302	A86	O4-C38-O5	-2.31	118.37	122.96
27	C	310	CLA	CHB-C4A-NA	2.31	127.71	124.51
32	f	304	BCR	C3-C4-C5	-2.31	109.95	114.08
26	D	205	DD6	C9-C10-C11	-2.31	124.02	127.31
27	H	214	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
27	a	815	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
30	B	302	A86	O1-C15-C20	-2.31	57.14	59.40
30	B	305	A86	O-C13-C11	-2.31	116.05	121.15
30	C	304	A86	C10-C9-C8	-2.31	116.02	123.22
26	F	303	DD6	C4-C3-C2	-2.31	118.75	123.47
26	G	301	DD6	O1-C20-C19	-2.31	111.65	113.38
27	b	846	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
27	M	317	CLA	C2A-C1A-CHA	2.31	127.89	123.86
27	a	855	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
30	H	203	A86	O1-C15-C20	-2.31	57.15	59.40
27	a	839	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
27	M	316	CLA	CHB-C4A-NA	2.31	127.70	124.51
30	H	201	A86	C19-C18-C17	-2.31	106.32	110.77
30	B	302	A86	O-C13-C14	-2.30	116.98	121.66
27	b	830	CLA	CAA-CBA-CGA	-2.30	106.52	113.25
27	G	306	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	I	310	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	a	812	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	a	839	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
30	L	302	A86	O4-C38-O5	-2.30	118.39	122.96
30	K	304	A86	O4-C38-O5	-2.30	118.39	122.96
27	G	311	CLA	C1-C2-C3	-2.30	122.06	126.04
27	D	216	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	b	814	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	E	301	A86	O4-C38-O5	-2.30	118.39	122.96
30	J	301	A86	O1-C15-C14	-2.30	108.60	113.21
27	M	309	CLA	CHB-C4A-NA	2.30	127.69	124.51
26	L	303	DD6	C32-C33-C34	-2.30	108.45	113.64
27	G	308	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	a	803	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
27	b	810	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
28	C	313	KC1	C2A-C3A-C4A	2.30	108.19	106.49
27	A	205	CLA	CHB-C4A-NA	2.30	127.69	124.51
27	E	314	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
27	K	311	CLA	O2A-CGA-O1A	-2.29	117.80	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	208	CLA	C7-C6-C5	-2.29	107.13	113.36
27	D	216	CLA	CHB-C4A-NA	2.29	127.68	124.51
27	C	315	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
28	B	313	KC1	CHC-C4B-C3B	-2.29	121.33	125.26
30	K	307	A86	O1-C15-C14	-2.29	108.61	113.21
30	D	206	A86	O1-C15-C20	-2.29	57.16	59.40
27	M	313	CLA	C1-C2-C3	-2.29	122.08	126.04
26	J	302	DD6	C28-C27-C29	2.29	121.38	116.84
30	H	201	A86	C-C1-C24	2.29	121.69	118.08
27	f	303	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
27	G	312	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
26	G	301	DD6	C33-C34-C35	-2.29	107.17	110.30
30	G	302	A86	C41-C32-C40	2.29	115.55	108.53
27	a	822	CLA	O2D-CGD-CBD	2.29	115.33	111.27
26	K	303	DD6	C4-C3-C2	-2.29	118.79	123.47
26	G	303	DD6	C21-C20-C15	-2.29	118.43	122.26
30	K	306	A86	C26-C25-C24	-2.29	116.08	123.22
27	M	308	CLA	C1-C2-C3	-2.29	122.09	126.04
27	F	315	CLA	CHB-C4A-NA	2.29	127.67	124.51
26	E	303	DD6	C7-C6-C5	-2.29	119.72	122.92
27	G	311	CLA	CHB-C4A-NA	2.29	127.67	124.51
26	K	303	DD6	O1-C20-C21	2.29	117.79	115.06
27	b	830	CLA	CMB-C2B-C3B	2.28	128.95	124.68
32	a	847	BCR	C8-C7-C6	-2.28	120.79	127.20
27	a	822	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
27	I	315	CLA	CHB-C4A-NA	2.28	127.67	124.51
26	A	202	DD6	C19-C18-C17	-2.28	106.36	110.77
27	D	207	CLA	CHB-C4A-NA	2.28	127.67	124.51
27	A	205	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	E	306	DD6	C28-C27-C29	2.28	121.36	116.84
30	C	302	A86	O1-C15-C20	-2.28	57.17	59.40
27	L	311	CLA	CHB-C4A-NA	2.28	127.67	124.51
28	K	315	KC1	CBD-CHA-C1A	2.28	133.13	128.88
30	m	101	A86	O-C13-C11	-2.28	116.11	121.15
26	E	306	DD6	C32-C33-C34	-2.28	108.49	113.64
27	l	204	CLA	C11-C10-C8	-2.28	108.55	115.92
37	b	835	DGD	O2G-C1B-O1B	-2.28	118.19	123.70
32	j	105	BCR	C37-C22-C21	-2.28	119.73	122.92
27	E	312	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
27	J	315	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
27	M	315	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
32	a	853	BCR	C12-C13-C14	2.28	122.44	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	K	315	KC1	O2D-CGD-O1D	-2.28	119.39	123.84
27	M	309	CLA	C2D-C1D-ND	-2.27	108.43	110.10
27	b	822	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
27	a	813	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
27	I	308	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
27	M	309	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
32	b	833	BCR	C20-C19-C18	-2.27	120.03	126.42
32	j	101	BCR	C37-C22-C21	-2.27	119.74	122.92
27	L	318	CLA	CHB-C4A-NA	2.27	127.65	124.51
30	H	201	A86	C8-C6-C5	-2.27	115.45	118.94
27	a	808	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
32	E	305	BCR	C28-C27-C26	-2.27	110.02	114.08
26	I	304	DD6	C32-C33-C34	-2.27	108.52	113.64
27	G	317	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
27	D	210	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
32	f	304	BCR	C11-C12-C13	-2.27	120.04	126.42
27	G	316	CLA	CHB-C4A-NA	2.27	127.65	124.51
27	H	212	CLA	CBA-CAA-C2A	-2.27	107.17	113.86
28	C	308	KC1	O2D-CGD-O1D	-2.27	119.40	123.84
28	C	313	KC1	O2D-CGD-O1D	-2.27	119.40	123.84
30	H	201	A86	O1-C15-C20	-2.27	57.18	59.40
32	r	203	BCR	C2-C1-C6	2.27	113.97	110.48
30	A	213	A86	C19-C18-C17	-2.27	106.39	110.77
27	M	313	CLA	O2D-CGD-CBD	2.27	115.30	111.27
30	K	307	A86	C3-C4-C5	-2.27	118.83	123.47
32	a	836	BCR	C8-C7-C6	-2.27	120.84	127.20
27	F	309	CLA	CHB-C4A-NA	2.26	127.64	124.51
27	D	217	CLA	CHB-C4A-NA	2.26	127.64	124.51
30	J	301	A86	O-C13-C14	-2.26	117.06	121.66
27	G	314	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
27	f	301	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
28	M	314	KC1	O1D-CGD-CBD	-2.26	119.85	124.48
27	L	315	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
30	B	301	A86	C-C1-C2	-2.26	119.75	122.92
27	b	819	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
27	a	846	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
28	L	320	KC1	C3D-CAD-CBD	-2.26	104.63	107.61
32	a	836	BCR	C10-C11-C12	-2.26	116.16	123.22
27	H	206	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
30	K	305	A86	O4-C38-O5	-2.26	118.47	122.96
27	D	217	CLA	CHD-C1D-ND	-2.26	122.38	124.45
27	M	316	CLA	O2D-CGD-CBD	2.26	115.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	308	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
32	b	834	BCR	C38-C26-C27	2.26	117.95	113.62
32	b	834	BCR	C35-C13-C14	-2.26	119.76	122.92
32	j	101	BCR	C8-C7-C6	-2.26	120.87	127.20
32	i	102	BCR	C4-C5-C6	-2.26	119.46	122.73
27	a	810	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
27	C	317	CLA	CHB-C4A-NA	2.25	127.63	124.51
27	L	307	CLA	CHB-C4A-NA	2.25	127.63	124.51
27	a	807	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
30	m	101	A86	C19-C18-C17	-2.25	106.42	110.77
30	D	206	A86	O4-C38-O5	-2.25	118.49	122.96
26	E	306	DD6	O1-C20-C21	-2.25	112.36	115.06
26	G	303	DD6	C10-C9-C8	-2.25	116.19	123.22
28	K	315	KC1	CHC-C4B-C3B	-2.25	121.41	125.26
32	b	837	BCR	C23-C24-C25	-2.25	120.88	127.20
27	b	818	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
26	B	303	DD6	C28-C27-C29	2.25	121.30	116.84
32	i	103	BCR	C33-C5-C4	2.25	117.94	113.62
27	a	827	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
30	D	206	A86	C7-C6-C8	2.25	121.62	118.08
28	L	320	KC1	C2A-C3A-C4A	2.25	108.15	106.49
27	A	210	CLA	CHD-C1D-ND	-2.25	122.39	124.45
27	l	204	CLA	CHB-C4A-NA	2.25	127.62	124.51
26	J	303	DD6	C12-C11-C10	-2.25	119.78	122.92
30	K	305	A86	C-C1-C2	-2.25	119.78	122.92
28	M	314	KC1	C3D-CAD-CBD	-2.25	104.65	107.61
27	M	309	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
27	C	307	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
32	b	834	BCR	C33-C5-C4	2.25	117.93	113.62
27	K	310	CLA	CHB-C4A-NA	2.24	127.62	124.51
30	r	202	A86	O2-C18-C19	2.24	114.26	109.80
32	r	203	BCR	C10-C11-C12	-2.24	116.22	123.22
27	a	842	CLA	CHB-C4A-NA	2.24	127.61	124.51
30	B	304	A86	C7-C6-C8	2.24	121.61	118.08
27	M	313	CLA	CBA-CAA-C2A	-2.24	107.25	113.86
27	H	207	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
32	b	840	BCR	C23-C24-C25	-2.24	120.92	127.20
27	A	207	CLA	CHB-C4A-NA	2.24	127.61	124.51
26	C	303	DD6	C23-C16-C22	2.24	110.67	107.37
27	L	309	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
27	B	309	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
27	F	308	CLA	C1B-CHB-C4A	-2.24	125.69	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	824	CLA	C1-C2-C3	-2.24	122.18	126.04
30	J	316	A86	C-C1-C24	-2.24	114.56	118.08
27	a	821	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
27	l	206	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
32	a	847	BCR	C10-C11-C12	-2.23	116.24	123.22
27	E	313	CLA	CHD-C1D-ND	-2.23	122.40	124.45
31	a	833	LHG	C26-C25-C24	2.23	121.22	113.19
27	G	309	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
27	a	809	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
27	C	307	CLA	CHB-C4A-NA	2.23	127.60	124.51
30	B	302	A86	C8-C6-C5	-2.23	115.52	118.94
32	f	304	BCR	C15-C16-C17	-2.23	118.91	123.47
26	A	201	DD6	C-C1-C2	-2.23	119.80	122.92
27	b	824	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
26	J	302	DD6	C37-C36-C35	2.23	118.48	114.36
30	M	305	A86	C12-C11-C13	2.23	119.76	116.02
32	a	835	BCR	C27-C26-C25	-2.23	119.50	122.73
27	M	308	CLA	CHB-C4A-NA	2.23	127.59	124.51
27	C	312	CLA	CHB-C4A-NA	2.23	127.59	124.51
33	J	318	SQD	C5-C6-S	2.23	119.99	113.20
27	E	313	CLA	CAA-CBA-CGA	-2.23	106.60	112.51
30	M	302	A86	C21-C20-C19	-2.22	111.78	114.28
30	L	304	A86	C4-C3-C2	-2.22	118.92	123.47
32	l	205	BCR	C8-C7-C6	-2.22	120.96	127.20
27	I	308	CLA	CHB-C4A-NA	2.22	127.59	124.51
27	a	856	CLA	O1D-CGD-CBD	2.22	129.03	124.48
27	C	318	CLA	CHD-C1D-ND	-2.22	122.41	124.45
27	a	817	CLA	C1-C2-C3	-2.22	122.20	126.04
28	J	306	KC1	C1A-C2A-C3A	-2.22	105.35	107.11
26	M	304	DD6	C26-C25-C24	-2.22	116.29	123.22
27	F	313	CLA	O2D-CGD-CBD	2.22	115.21	111.27
30	F	304	A86	C12-C11-C10	-2.22	118.05	123.42
35	l	207	ET4	C15-C16-C17	2.22	128.02	123.47
26	J	302	DD6	C9-C8-C6	-2.22	120.18	126.42
32	f	305	BCR	C23-C22-C21	2.22	122.35	118.94
27	K	316	CLA	C6-C5-C3	-2.22	107.64	113.45
27	b	816	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
28	L	320	KC1	O2D-CGD-O1D	-2.22	119.50	123.84
30	C	305	A86	C35-C34-C33	2.22	113.74	109.88
30	M	302	A86	C8-C6-C5	-2.22	115.54	118.94
30	C	305	A86	O1-C15-C20	-2.22	57.23	59.40
30	I	303	A86	C9-C8-C6	2.21	132.64	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	211	CLA	C2A-C1A-CHA	2.21	126.14	122.71
27	L	309	CLA	C1-C2-C3	-2.21	122.21	126.04
27	D	211	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
32	b	840	BCR	C7-C8-C9	-2.21	122.89	126.23
27	b	811	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
27	a	814	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
30	D	204	A86	C41-C32-C31	-2.21	108.49	110.47
26	J	302	DD6	C21-C20-C15	-2.21	118.56	122.26
30	K	306	A86	C17-C16-C15	2.21	111.42	109.16
30	K	306	A86	C12-C11-C13	2.21	119.73	116.02
27	a	820	CLA	O2D-CGD-CBD	2.21	115.19	111.27
26	C	303	DD6	C37-C36-C31	-2.21	121.35	124.35
32	r	203	BCR	C16-C15-C14	-2.21	118.95	123.47
30	C	302	A86	C12-C11-C10	-2.21	118.08	123.42
27	b	805	CLA	CAA-CBA-CGA	-2.21	106.65	112.51
27	I	311	CLA	C1-C2-C3	-2.21	122.22	126.04
26	J	302	DD6	C14-C13-C11	-2.21	122.11	125.53
27	L	311	CLA	CHD-C1D-ND	-2.20	122.43	124.45
27	L	319	CLA	CHB-C4A-NA	2.20	127.56	124.51
27	K	317	CLA	C2A-C1A-CHA	2.20	127.70	123.85
30	K	302	A86	C25-C24-C1	-2.20	120.23	126.42
30	H	203	A86	C19-C18-C17	-2.20	106.52	110.77
30	L	302	A86	O-C13-C14	-2.20	117.18	121.66
27	a	805	CLA	CAA-CBA-CGA	-2.20	106.82	113.25
27	H	213	CLA	CHB-C4A-NA	2.20	127.56	124.51
27	B	314	CLA	CAA-C2A-C3A	-2.20	110.96	116.10
27	L	321	CLA	CAA-CBA-CGA	-2.20	106.66	112.51
28	K	308	KC1	CBD-CHA-C1A	2.20	132.99	128.88
27	a	804	CLA	CHD-C1D-ND	-2.20	122.43	124.45
26	L	303	DD6	C7-C6-C5	-2.20	119.84	122.92
26	D	205	DD6	C33-C32-C31	2.20	114.08	109.62
26	J	303	DD6	C37-C36-C35	2.20	118.43	114.36
27	K	314	CLA	CHD-C4C-C3C	2.20	128.07	124.84
27	K	319	CLA	CHA-C1A-NA	-2.20	121.37	126.40
27	a	846	CLA	CHD-C1D-ND	-2.20	122.44	124.45
30	B	301	A86	C17-C16-C15	2.20	111.40	109.16
27	C	316	CLA	C2D-C1D-ND	-2.20	108.49	110.10
30	C	304	A86	C20-C19-C18	-2.20	108.41	112.75
27	G	307	CLA	CHD-C1D-ND	-2.19	122.44	124.45
27	a	815	CLA	CAC-C3C-C2C	-2.19	123.78	127.53
27	E	314	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
30	L	302	A86	C25-C26-C27	-2.19	124.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	315	LHG	O8-C23-O10	-2.19	118.06	123.59
26	A	202	DD6	C7-C6-C5	-2.19	119.85	122.92
28	G	313	KC1	O1D-CGD-CBD	-2.19	120.00	124.48
27	a	806	CLA	CHD-C1D-ND	-2.19	122.44	124.45
27	a	803	CLA	C2D-C1D-ND	-2.19	108.49	110.10
26	H	202	DD6	C37-C36-C35	2.19	118.41	114.36
31	b	836	LHG	O8-C6-C5	-2.19	102.06	108.43
27	M	311	CLA	CAA-CBA-CGA	-2.19	106.86	113.25
26	E	306	DD6	C8-C6-C5	2.19	122.30	118.94
27	A	210	CLA	CHB-C4A-NA	2.19	127.54	124.51
30	F	301	A86	C-C1-C2	-2.19	119.86	122.92
32	a	836	BCR	C11-C10-C9	-2.19	124.19	127.31
27	L	316	CLA	CHB-C4A-NA	2.19	127.54	124.51
28	K	308	KC1	C2A-C3A-C4A	2.19	108.11	106.49
32	a	835	BCR	C15-C16-C17	-2.19	119.00	123.47
27	i	101	CLA	CHD-C1D-ND	-2.18	122.45	124.45
28	J	306	KC1	C2A-C3A-C4A	2.18	108.11	106.49
27	D	208	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
30	C	304	A86	O1-C15-C20	-2.18	57.27	59.40
27	M	313	CLA	C11-C12-C13	-2.18	108.86	115.92
28	K	315	KC1	C4B-CHC-C1C	-2.18	121.35	126.06
28	C	313	KC1	C3D-CAD-CBD	-2.18	104.73	107.61
27	C	314	CLA	CHB-C4A-NA	2.18	127.53	124.51
26	A	202	DD6	C37-C36-C31	-2.18	121.39	124.35
26	J	305	DD6	C26-C25-C24	-2.18	116.42	123.22
26	A	202	DD6	O4-C34-C33	-2.18	105.47	109.80
27	G	312	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
30	r	202	A86	C-C1-C2	-2.18	119.88	122.92
27	I	313	CLA	CAC-C3C-C4C	2.17	127.63	124.81
27	D	208	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
30	K	307	A86	C10-C9-C8	-2.17	116.43	123.22
30	L	302	A86	C7-C6-C5	-2.17	119.88	122.92
32	a	835	BCR	C29-C30-C25	2.17	113.83	110.48
27	C	311	CLA	C1-C2-C3	-2.17	122.28	126.04
26	G	303	DD6	C25-C24-C1	-2.17	120.31	126.42
27	b	829	CLA	CHD-C1D-ND	-2.17	122.46	124.45
27	b	843	CLA	CHD-C1D-ND	-2.17	122.46	124.45
27	J	307	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
30	L	306	A86	C12-C11-C13	2.17	119.67	116.02
27	a	856	CLA	CHD-C1D-ND	-2.17	122.46	124.45
27	E	308	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	I	302	DD6	C25-C26-C27	-2.17	120.28	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	848	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	G	304	DD6	O1-C20-C21	-2.17	112.46	115.06
29	A	214	LMG	C1-O6-C5	-2.17	109.43	113.69
32	a	847	BCR	C30-C25-C24	2.17	121.91	115.78
26	E	306	DD6	C7-C6-C8	2.17	121.49	118.08
28	L	314	KC1	O2A-CGA-O1A	-2.17	118.17	122.67
27	C	317	CLA	O2D-CGD-CBD	2.17	115.12	111.27
26	G	304	DD6	C14-C13-C11	-2.17	122.17	125.53
27	b	841	CLA	O2D-CGD-CBD	2.17	115.12	111.27
27	K	314	CLA	C4D-C3D-CAD	-2.17	105.54	108.10
27	H	206	CLA	CAA-C2A-C1A	-2.17	104.88	111.97
30	r	202	A86	C-C1-C24	-2.17	114.67	118.08
27	F	310	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
26	K	303	DD6	O2-C18-C19	-2.16	105.50	109.80
30	K	302	A86	C4-C3-C2	-2.16	119.04	123.47
32	E	304	BCR	C38-C26-C27	2.16	117.77	113.62
28	H	211	KC1	O2D-CGD-O1D	-2.16	119.61	123.84
27	H	205	CLA	CHB-C4A-NA	2.16	127.50	124.51
27	b	824	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
32	r	203	BCR	C8-C7-C6	-2.16	121.13	127.20
30	I	301	A86	C35-C34-C33	2.16	113.65	109.88
27	I	311	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
29	A	214	LMG	C7-O1-C1	-2.16	109.51	113.74
27	b	805	CLA	O2D-CGD-CBD	2.16	115.11	111.27
30	H	203	A86	C34-O4-C38	-2.16	113.87	117.90
26	E	307	DD6	C4-C3-C2	-2.16	119.05	123.47
27	C	311	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
27	b	822	CLA	C1-C2-C3	-2.16	123.26	126.75
32	f	304	BCR	C35-C13-C14	-2.16	119.90	122.92
27	K	313	CLA	CHD-C1D-ND	-2.16	122.47	124.45
27	a	854	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
27	D	207	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
27	A	204	CLA	O2D-CGD-CBD	2.16	115.11	111.27
27	C	310	CLA	CHD-C1D-ND	-2.16	122.47	124.45
27	K	310	CLA	CAC-C3C-C4C	2.16	127.61	124.81
27	J	309	CLA	CHB-C4A-NA	2.16	127.49	124.51
30	G	302	A86	C35-C34-C33	2.16	113.64	109.88
30	G	302	A86	O1-C15-C20	-2.16	57.29	59.40
30	r	202	A86	O4-C34-C35	2.16	112.96	107.59
27	a	826	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
27	I	306	CLA	C1-C2-C3	-2.15	122.32	126.04
27	b	809	CLA	O2A-CGA-O1A	-2.15	118.15	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I	302	DD6	C12-C11-C13	2.15	121.47	118.08
27	a	841	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
27	K	311	CLA	CHD-C1D-ND	-2.15	122.48	124.45
27	b	830	CLA	O2D-CGD-CBD	2.15	115.09	111.27
27	b	831	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
28	G	313	KC1	C2A-C3A-C4A	2.15	108.08	106.49
30	K	306	A86	C-C1-C2	-2.15	119.91	122.92
27	L	308	CLA	CHB-C4A-NA	2.15	127.49	124.51
27	l	203	CLA	CHB-C4A-NA	2.15	127.49	124.51
26	E	306	DD6	C15-C14-C13	2.15	130.54	125.99
27	H	209	CLA	CAA-CBA-CGA	-2.15	106.97	113.25
27	J	309	CLA	CHC-C1C-NC	2.15	127.47	124.20
27	a	815	CLA	C2D-C1D-ND	-2.15	108.52	110.10
27	C	307	CLA	O2D-CGD-CBD	2.15	115.09	111.27
27	a	806	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
27	b	839	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
32	b	834	BCR	C21-C20-C19	-2.15	116.51	123.22
27	J	312	CLA	C1-C2-C3	-2.15	122.33	126.04
26	F	302	DD6	O1-C20-C21	-2.15	112.48	115.06
27	a	805	CLA	CHD-C1D-ND	-2.15	122.48	124.45
29	J	317	LMG	C1-C2-C3	2.15	114.47	110.00
30	I	303	A86	C20-C19-C18	-2.15	108.50	112.75
27	K	310	CLA	CHD-C1D-ND	-2.14	122.48	124.45
27	M	313	CLA	CHD-C1D-ND	-2.14	122.48	124.45
27	a	816	CLA	CHD-C1D-ND	-2.14	122.48	124.45
27	b	850	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
30	J	301	A86	C17-C16-C15	2.14	111.35	109.16
27	a	817	CLA	CHD-C1D-ND	-2.14	122.48	124.45
32	l	202	BCR	C38-C26-C27	2.14	117.73	113.62
27	b	811	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
30	K	306	A86	C19-C18-C17	-2.14	106.63	110.77
26	L	301	DD6	C21-C20-C15	-2.14	118.67	122.26
26	L	301	DD6	C-C1-C2	-2.14	119.92	122.92
30	J	316	A86	O4-C34-C35	2.14	112.93	107.59
27	L	308	CLA	O2D-CGD-CBD	2.14	115.07	111.27
27	G	308	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
27	F	316	CLA	CAA-C2A-C3A	-2.14	111.10	116.10
26	G	305	DD6	C37-C36-C35	2.14	118.32	114.36
26	K	303	DD6	C33-C32-C31	2.14	113.96	109.62
27	a	854	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
27	b	817	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
27	a	848	CLA	CHD-C1D-ND	-2.14	122.49	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	304	DD6	C10-C9-C8	-2.14	116.54	123.22
27	C	316	CLA	CAA-C2A-C3A	-2.14	111.10	116.10
27	b	804	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
27	C	316	CLA	C3C-C4C-NC	-2.14	108.17	110.57
27	L	310	CLA	CHD-C1D-ND	-2.14	122.49	124.45
30	B	302	A86	C4-C5-C6	2.14	130.36	127.31
27	I	307	CLA	C1-C2-C3	-2.14	122.35	126.04
27	I	313	CLA	CAA-C2A-C3A	-2.14	111.11	116.10
26	G	305	DD6	C25-C24-C1	-2.14	120.41	126.42
27	H	213	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
27	f	301	CLA	C1-C2-C3	-2.14	122.35	126.04
27	K	318	CLA	CHD-C1D-ND	-2.14	122.49	124.45
30	D	203	A86	C20-C19-C18	-2.14	108.52	112.75
27	b	813	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
27	L	310	CLA	CHB-C4A-NA	2.13	127.46	124.51
28	M	314	KC1	C3C-C4C-NC	-2.13	107.87	109.88
27	b	846	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
30	L	305	A86	C4-C3-C2	-2.13	119.10	123.47
27	K	316	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
27	M	310	CLA	CHB-C4A-NA	2.13	127.46	124.51
27	H	210	CLA	CHB-C4A-NA	2.13	127.46	124.51
27	I	311	CLA	CMD-C2D-C3D	2.13	132.52	127.61
27	B	314	CLA	C2D-C1D-ND	-2.13	108.53	110.10
26	L	301	DD6	O1-C20-C21	-2.13	112.50	115.06
27	F	315	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
32	i	102	BCR	C38-C26-C27	2.13	117.70	113.62
27	K	313	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
27	b	803	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
27	G	309	CLA	CHD-C1D-ND	-2.13	122.50	124.45
30	L	305	A86	C34-O4-C38	-2.12	113.94	117.90
30	I	301	A86	O1-C15-C20	-2.12	57.32	59.40
27	b	843	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
30	A	213	A86	O1-C15-C14	-2.12	108.95	113.21
27	a	839	CLA	CGD-CBD-CAD	-2.12	103.86	110.73
32	a	835	BCR	C21-C20-C19	-2.12	116.59	123.22
26	B	303	DD6	C32-C31-C36	-2.12	119.64	122.63
27	a	827	CLA	C6-C7-C8	-2.12	109.06	115.92
35	l	207	ET4	C26-C01-C06	-2.12	106.86	110.30
27	B	308	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
27	a	838	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
27	D	209	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
30	D	203	A86	C3-C4-C5	-2.12	119.13	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	834	BCR	C16-C17-C18	-2.12	124.28	127.31
30	M	302	A86	O1-C15-C20	-2.12	57.33	59.40
32	a	836	BCR	C20-C19-C18	-2.12	120.46	126.42
30	K	307	A86	C40-C32-C31	-2.12	108.57	110.47
32	f	304	BCR	C23-C24-C25	-2.12	121.25	127.20
27	M	307	CLA	C11-C10-C8	-2.12	109.07	115.92
30	C	304	A86	O4-C38-O5	-2.12	118.75	122.96
27	I	305	CLA	CHD-C1D-ND	-2.12	122.51	124.45
27	L	315	CLA	CHB-C4A-NA	2.12	127.44	124.51
26	C	303	DD6	C25-C24-C1	-2.12	120.46	126.42
27	K	312	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
27	L	310	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
27	M	317	CLA	CAA-CBA-CGA	-2.12	106.89	112.51
27	b	815	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
32	b	840	BCR	C33-C5-C6	-2.12	122.15	124.53
27	a	842	CLA	O2D-CGD-CBD	2.12	115.03	111.27
29	E	317	LMG	O3-C3-C2	-2.12	105.46	110.35
27	C	314	CLA	CAA-C2A-C3A	-2.12	111.16	116.10
27	a	809	CLA	CHB-C4A-NA	2.12	127.44	124.51
27	K	314	CLA	C11-C12-C13	-2.11	109.08	115.92
32	b	840	BCR	C16-C15-C14	-2.11	119.14	123.47
27	E	309	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	b	847	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	J	311	CLA	CHB-C4A-NA	2.11	127.43	124.51
27	a	824	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
29	a	852	LMG	O6-C5-C4	2.11	113.53	109.69
27	M	308	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
26	L	303	DD6	C33-C34-C35	-2.11	107.42	110.30
27	L	319	CLA	CAA-CBA-CGA	-2.11	106.91	112.51
28	L	322	KC1	CBD-CHA-C1A	2.11	132.81	128.88
27	D	210	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
27	M	317	CLA	CHB-C4A-NA	2.11	127.42	124.51
26	G	304	DD6	C37-C36-C31	-2.10	121.49	124.35
27	a	812	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
30	J	316	A86	C36-C31-C32	2.10	121.78	119.70
27	B	308	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
30	K	305	A86	O1-C15-C14	-2.10	108.99	113.21
27	A	204	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
26	B	303	DD6	C33-C34-C35	-2.10	107.43	110.30
30	F	304	A86	O-C13-C11	-2.10	116.50	121.15
30	H	201	A86	C4-C5-C6	2.10	130.31	127.31
32	a	853	BCR	C36-C18-C17	-2.10	119.98	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	828	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
27	b	807	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
30	H	203	A86	C17-C16-C15	2.10	111.31	109.16
26	B	303	DD6	C10-C9-C8	-2.10	116.66	123.22
30	K	301	A86	C17-C16-C15	2.10	111.31	109.16
30	C	304	A86	C19-C18-C17	-2.10	106.72	110.77
27	a	817	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	K	316	CLA	CBA-CAA-C2A	-2.10	107.67	113.86
27	G	316	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
32	b	833	BCR	C36-C18-C17	-2.10	119.98	122.92
27	a	855	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	b	826	CLA	O2A-CGA-O1A	-2.10	118.08	123.30
30	G	302	A86	O3-C36-C37	2.10	113.13	109.39
30	H	203	A86	O4-C38-O5	-2.09	118.80	122.96
30	B	305	A86	O1-C15-C20	-2.09	57.35	59.40
30	m	101	A86	O-C13-C14	-2.09	117.40	121.66
30	J	304	A86	C19-C18-C17	-2.09	106.73	110.77
27	H	205	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
27	a	804	CLA	C1-C2-C3	-2.09	122.42	126.04
27	K	312	CLA	CHD-C1D-ND	-2.09	122.53	124.45
27	b	830	CLA	C11-C10-C8	-2.09	109.15	115.92
27	G	307	CLA	C1-C2-C3	-2.09	122.42	126.04
27	G	317	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
30	D	206	A86	O-C13-C11	-2.09	116.53	121.15
26	I	302	DD6	C-C1-C2	-2.09	119.99	122.92
27	J	307	CLA	C1-C2-C3	-2.09	122.43	126.04
26	G	301	DD6	C3-C4-C5	-2.09	119.19	123.47
26	G	305	DD6	C25-C26-C27	-2.09	120.51	126.58
27	L	309	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
30	B	304	A86	O1-C15-C20	-2.09	57.36	59.40
27	F	315	CLA	CHD-C1D-ND	-2.09	122.53	124.45
32	f	305	BCR	C38-C26-C27	2.09	117.63	113.62
27	E	311	CLA	C11-C12-C13	-2.09	109.17	115.92
27	b	829	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
30	G	302	A86	C28-C27-C29	-2.09	114.09	118.93
32	m	102	BCR	C36-C18-C17	-2.09	120.00	122.92
27	a	809	CLA	O2D-CGD-CBD	2.09	114.98	111.27
27	H	209	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
27	a	822	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
27	D	213	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
26	F	303	DD6	C7-C6-C5	-2.09	120.00	122.92
27	b	804	CLA	CBA-CAA-C2A	-2.09	107.70	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	306	CLA	CHD-C1D-ND	-2.09	122.54	124.45
27	L	312	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
27	b	818	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
26	H	202	DD6	O4-C34-C33	-2.09	105.66	109.80
30	H	201	A86	C9-C8-C6	2.09	132.27	126.42
27	b	842	CLA	CHD-C1D-ND	-2.08	122.54	124.45
28	A	209	KC1	CHB-C1B-C2B	-2.08	121.11	125.48
27	K	311	CLA	O1D-CGD-CBD	2.08	128.75	124.48
26	F	302	DD6	C25-C26-C27	-2.08	120.53	126.58
26	E	306	DD6	C4-C3-C2	2.08	127.74	123.47
27	a	821	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
30	B	302	A86	C9-C8-C6	2.08	132.27	126.42
29	A	212	LMG	O1-C1-C2	2.08	111.55	108.30
31	E	318	LHG	C26-C25-C24	2.08	120.67	113.19
27	b	821	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
27	a	826	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	f	302	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	b	846	CLA	CHD-C1D-ND	-2.08	122.54	124.45
30	F	301	A86	C7-C6-C5	-2.08	120.01	122.92
27	F	311	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	D	208	CLA	CHB-C4A-NA	2.08	127.39	124.51
27	b	815	CLA	CHD-C1D-ND	-2.08	122.55	124.45
27	b	819	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	H	212	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	F	316	CLA	CHD-C1D-ND	-2.08	122.55	124.45
27	L	309	CLA	CHB-C4A-NA	2.08	127.38	124.51
26	J	305	DD6	O1-C20-C19	-2.08	111.82	113.38
30	M	305	A86	C3-C4-C5	-2.08	119.22	123.47
26	F	303	DD6	O1-C20-C21	-2.07	112.57	115.06
27	a	805	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
27	B	312	CLA	CHD-C1D-ND	-2.07	122.55	124.45
30	A	213	A86	C10-C9-C8	-2.07	116.75	123.22
27	K	318	CLA	C2D-C1D-ND	-2.07	108.58	110.10
30	M	302	A86	C12-C11-C10	-2.07	118.41	123.42
27	r	201	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
27	L	311	CLA	CBD-CHA-C1A	2.07	130.94	128.50
30	B	301	A86	O4-C38-O5	-2.07	118.85	122.96
27	M	313	CLA	C16-C15-C13	-2.07	109.23	115.92
32	i	102	BCR	C8-C7-C6	-2.07	121.39	127.20
27	D	214	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
32	r	203	BCR	C21-C20-C19	-2.07	116.77	123.22
30	J	316	A86	O1-C15-C20	-2.07	57.38	59.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	305	A86	C41-C32-C31	-2.07	108.62	110.47
27	H	205	CLA	CHD-C1D-ND	-2.07	122.56	124.45
26	G	303	DD6	C25-C26-C27	-2.07	120.58	126.58
32	E	305	BCR	C36-C18-C17	-2.07	120.03	122.92
28	H	211	KC1	CBA-CAA-C2A	-2.07	117.40	125.27
30	L	302	A86	O1-C15-C20	-2.06	57.38	59.40
29	J	317	LMG	O1-C7-C8	-2.06	105.92	110.90
27	b	804	CLA	CHB-C4A-NA	2.06	127.36	124.51
27	a	809	CLA	CAA-CBA-CGA	-2.06	107.23	113.25
30	m	101	A86	O1-C15-C20	-2.06	57.39	59.40
26	J	302	DD6	C32-C33-C34	-2.06	108.99	113.64
32	E	304	BCR	C36-C18-C19	2.06	121.32	118.08
27	E	310	CLA	C2A-C1A-CHA	2.06	127.46	123.86
27	A	205	CLA	C1-C2-C3	-2.06	122.48	126.04
27	L	321	CLA	CHB-C4A-NA	2.06	127.36	124.51
27	a	844	CLA	C2D-C1D-ND	-2.06	108.59	110.10
27	a	832	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
27	G	316	CLA	CHD-C1D-ND	-2.06	122.56	124.45
30	B	304	A86	O4-C38-O5	-2.06	118.87	122.96
27	I	310	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
27	b	844	CLA	O1D-CGD-CBD	2.06	128.69	124.48
27	F	313	CLA	CAA-C2A-C3A	-2.06	111.30	116.10
30	B	305	A86	C-C1-C24	2.06	121.32	118.08
30	H	203	A86	O-C13-C14	-2.06	117.48	121.66
30	H	203	A86	C21-C20-C19	-2.06	111.97	114.28
26	M	306	DD6	C23-C16-C22	2.05	110.40	107.37
32	a	851	BCR	C23-C22-C21	2.05	122.09	118.94
32	E	304	BCR	C23-C24-C25	-2.05	121.43	127.20
27	C	309	CLA	CAA-CBA-CGA	-2.05	107.25	113.25
26	G	304	DD6	C37-C36-C35	2.05	118.16	114.36
30	K	301	A86	C19-C18-C17	-2.05	106.81	110.77
27	B	311	CLA	CAC-C3C-C4C	2.05	127.47	124.81
27	J	311	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
27	a	816	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
27	b	822	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
27	M	308	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	j	103	LMG	O6-C5-C6	2.05	111.53	106.44
26	E	303	DD6	C10-C9-C8	-2.05	116.82	123.22
28	K	308	KC1	CAC-C3C-C4C	2.05	127.47	124.81
27	E	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
27	J	310	CLA	CHD-C1D-ND	-2.05	122.57	124.45
27	C	307	CLA	CHD-C1D-ND	-2.05	122.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	E	312	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
35	l	207	ET4	C27-C09-C08	2.04	121.30	118.08
27	b	839	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
30	B	305	A86	C4-C5-C6	2.04	130.23	127.31
27	f	301	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
27	a	845	CLA	C2A-C1A-CHA	2.04	127.43	123.86
27	M	319	CLA	CHD-C1D-ND	-2.04	122.58	124.45
27	a	824	CLA	C1-C2-C3	-2.04	123.45	126.75
27	F	306	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
30	m	101	A86	C28-C27-C26	-2.04	120.06	122.92
27	B	307	CLA	CHD-C1D-ND	-2.04	122.58	124.45
27	L	313	CLA	C11-C10-C8	-2.04	109.33	115.92
27	K	311	CLA	CHB-C4A-NA	2.04	127.33	124.51
27	C	309	CLA	O2D-CGD-CBD	2.04	114.89	111.27
30	M	305	A86	O4-C38-O5	-2.04	118.91	122.96
29	D	202	LMG	O7-C10-O9	-2.04	118.78	123.70
29	a	852	LMG	C3-C4-C5	2.04	113.87	110.24
27	F	308	CLA	CHD-C1D-ND	-2.03	122.58	124.45
27	K	319	CLA	C4D-CHA-C1A	2.03	123.72	121.25
27	B	311	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
30	M	303	A86	C26-C25-C24	2.03	129.56	123.22
28	L	314	KC1	C2A-C3A-C4A	2.03	108.00	106.49
28	L	322	KC1	CHD-C4C-NC	2.03	127.29	124.20
27	J	308	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
26	E	307	DD6	C37-C36-C35	2.03	118.12	114.36
27	J	314	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
32	j	105	BCR	C33-C5-C4	2.03	117.52	113.62
30	G	302	A86	O4-C38-O5	-2.03	118.92	122.96
26	H	202	DD6	C19-C18-C17	-2.03	106.85	110.77
27	M	312	CLA	CAA-C2A-C1A	-2.03	105.31	111.97
30	K	305	A86	C19-C18-C17	-2.03	106.85	110.77
27	H	213	CLA	C16-C15-C13	-2.03	109.36	115.92
29	j	103	LMG	C6-C5-C4	-2.03	108.25	113.00
27	b	820	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
30	A	213	A86	C9-C8-C6	-2.03	120.72	126.42
26	C	303	DD6	C21-C20-C15	-2.03	118.86	122.26
32	a	853	BCR	C23-C24-C25	-2.03	121.50	127.20
34	a	831	PQN	C11-C12-C13	-2.03	123.42	126.79
26	E	307	DD6	C34-C35-C36	-2.03	107.81	111.85
32	a	836	BCR	C34-C9-C8	2.03	121.27	118.08
30	L	305	A86	C9-C10-C11	-2.03	120.65	126.61
27	b	808	CLA	O2A-CGA-O1A	-2.03	118.48	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	305	BCR	C8-C7-C6	-2.03	121.51	127.20
27	b	850	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
26	K	303	DD6	C37-C36-C35	2.03	118.11	114.36
27	L	308	CLA	C16-C15-C13	-2.02	109.37	115.92
27	F	305	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
30	B	304	A86	C21-C20-C19	-2.02	112.00	114.28
27	A	207	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
27	b	825	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
30	B	305	A86	O4-C38-O5	-2.02	118.95	122.96
27	a	843	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
32	a	835	BCR	C23-C24-C25	-2.02	121.53	127.20
27	F	314	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
27	F	306	CLA	C1-C2-C3	-2.02	122.55	126.04
27	b	804	CLA	CMB-C2B-C3B	2.02	128.46	124.68
27	K	317	CLA	O1D-CGD-CBD	2.02	128.61	124.48
27	a	803	CLA	C16-C15-C13	-2.02	109.39	115.92
27	a	823	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
27	a	846	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	I	302	DD6	O1-C20-C21	-2.02	112.64	115.06
26	M	306	DD6	O2-C18-C19	-2.02	105.80	109.80
26	F	303	DD6	C-C1-C2	-2.02	120.10	122.92
26	M	301	DD6	C23-C16-C22	2.02	110.34	107.37
28	G	313	KC1	C1A-C2A-C3A	-2.02	105.52	107.11
30	D	206	A86	C9-C8-C6	2.02	132.08	126.42
32	m	102	BCR	C38-C26-C25	-2.01	122.27	124.53
32	a	851	BCR	C8-C7-C6	-2.01	121.55	127.20
27	L	316	CLA	CHD-C1D-ND	-2.01	122.60	124.45
27	a	856	CLA	C2D-C1D-ND	-2.01	108.62	110.10
32	a	835	BCR	C39-C30-C25	-2.01	107.03	110.30
26	E	302	DD6	C15-C14-C13	-2.01	121.74	125.99
26	E	302	DD6	C12-C11-C10	-2.01	120.10	122.92
27	a	842	CLA	C6-C7-C8	-2.01	109.41	115.92
30	K	304	A86	C9-C8-C6	-2.01	120.76	126.42
27	C	314	CLA	O2D-CGD-CBD	2.01	114.84	111.27
31	H	215	LHG	O8-C23-C24	2.01	121.15	112.38
26	A	201	DD6	C4-C3-C2	-2.01	119.35	123.47
31	E	316	LHG	O8-C23-O10	-2.01	118.52	123.59
27	I	313	CLA	CMA-C3A-C2A	-2.01	111.41	116.10
26	G	303	DD6	C14-C13-C11	-2.01	122.41	125.53
27	D	210	CLA	CHD-C1D-ND	-2.01	122.61	124.45
30	D	204	A86	O1-C15-C20	-2.01	57.44	59.40
27	a	828	CLA	O2A-CGA-O1A	-2.01	118.52	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	314	CLA	CBA-CAA-C2A	-2.01	107.94	113.86
27	a	819	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
27	J	310	CLA	CAC-C3C-C4C	2.01	127.41	124.81
30	L	304	A86	C3-C2-C1	-2.01	124.45	127.31
26	A	201	DD6	C13-C11-C10	-2.01	115.86	118.94
27	M	312	CLA	C3C-C4C-NC	-2.01	108.32	110.57
27	B	309	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
27	a	830	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
27	I	314	CLA	CHD-C1D-ND	-2.01	122.61	124.45
27	D	216	CLA	C2D-C1D-ND	-2.00	108.63	110.10
27	a	809	CLA	C3A-C2A-C1A	2.00	104.34	101.34
30	K	301	A86	C26-C25-C24	-2.00	116.97	123.22
30	K	301	A86	O1-C15-C14	-2.00	109.19	113.21
27	L	308	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (228) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	203	CLA	ND
27	A	204	CLA	ND
27	A	205	CLA	ND
27	A	206	CLA	ND
27	A	207	CLA	ND
27	A	208	CLA	ND
27	A	210	CLA	ND
27	A	211	CLA	ND
27	B	306	CLA	ND
27	B	307	CLA	ND
27	B	308	CLA	ND
27	B	309	CLA	ND
27	B	310	CLA	ND
27	B	311	CLA	ND
27	B	312	CLA	ND
27	B	314	CLA	ND
27	C	306	CLA	ND
27	C	307	CLA	ND
27	C	309	CLA	ND
27	C	310	CLA	ND
27	C	311	CLA	ND
27	C	312	CLA	ND
27	C	314	CLA	ND
27	C	315	CLA	ND

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Mol	Chain	Res	Type	Atom
27	C	316	CLA	ND
27	C	317	CLA	ND
27	C	318	CLA	ND
27	E	308	CLA	ND
27	E	309	CLA	ND
27	E	310	CLA	ND
27	E	311	CLA	ND
27	E	312	CLA	ND
27	E	313	CLA	ND
27	E	314	CLA	ND
27	E	315	CLA	ND
27	F	305	CLA	ND
27	F	306	CLA	ND
27	F	307	CLA	ND
27	F	308	CLA	ND
27	F	309	CLA	ND
27	F	310	CLA	ND
27	F	311	CLA	ND
27	F	313	CLA	ND
27	F	314	CLA	ND
27	F	315	CLA	ND
27	F	316	CLA	ND
27	F	317	CLA	ND
27	G	306	CLA	ND
27	G	307	CLA	ND
27	G	308	CLA	ND
27	G	309	CLA	ND
27	G	310	CLA	ND
27	G	311	CLA	ND
27	G	312	CLA	ND
27	G	314	CLA	ND
27	G	315	CLA	ND
27	G	316	CLA	ND
27	G	317	CLA	ND
27	H	204	CLA	ND
27	H	205	CLA	ND
27	H	206	CLA	ND
27	H	207	CLA	ND
27	H	208	CLA	ND
27	H	209	CLA	ND
27	H	210	CLA	ND
27	H	212	CLA	ND

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Mol	Chain	Res	Type	Atom
27	H	213	CLA	ND
27	H	214	CLA	ND
27	I	305	CLA	ND
27	I	306	CLA	ND
27	I	307	CLA	ND
27	I	308	CLA	ND
27	I	309	CLA	ND
27	I	310	CLA	ND
27	I	311	CLA	ND
27	I	313	CLA	ND
27	I	314	CLA	ND
27	I	315	CLA	ND
27	I	316	CLA	ND
27	I	317	CLA	ND
27	J	307	CLA	ND
27	J	308	CLA	ND
27	J	309	CLA	ND
27	J	310	CLA	ND
27	J	311	CLA	ND
27	J	312	CLA	ND
27	J	313	CLA	ND
27	J	314	CLA	ND
27	J	315	CLA	ND
27	K	309	CLA	ND
27	K	310	CLA	ND
27	K	311	CLA	ND
27	K	312	CLA	ND
27	K	313	CLA	ND
27	K	314	CLA	ND
27	K	316	CLA	ND
27	K	317	CLA	ND
27	K	318	CLA	ND
27	K	319	CLA	ND
27	L	307	CLA	ND
27	L	308	CLA	ND
27	L	309	CLA	ND
27	L	310	CLA	ND
27	L	311	CLA	ND
27	L	312	CLA	ND
27	L	313	CLA	ND
27	L	315	CLA	ND
27	L	316	CLA	ND

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Mol	Chain	Res	Type	Atom
27	L	317	CLA	ND
27	L	318	CLA	ND
27	L	319	CLA	ND
27	L	321	CLA	ND
27	M	307	CLA	ND
27	M	308	CLA	ND
27	M	309	CLA	ND
27	M	310	CLA	ND
27	M	311	CLA	ND
27	M	312	CLA	ND
27	M	313	CLA	ND
27	M	315	CLA	ND
27	M	316	CLA	ND
27	M	318	CLA	ND
27	M	319	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
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

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Mol	Chain	Res	Type	Atom
27	a	830	CLA	ND
27	a	832	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	a	845	CLA	ND
27	a	846	CLA	ND
27	a	848	CLA	ND
27	a	849	CLA	ND
27	a	850	CLA	ND
27	a	854	CLA	ND
27	a	855	CLA	ND
27	a	856	CLA	ND
27	f	301	CLA	ND
27	f	302	CLA	ND
27	f	303	CLA	ND
27	i	101	CLA	ND
27	j	104	CLA	ND
27	l	203	CLA	ND
27	l	204	CLA	ND
27	l	206	CLA	ND
27	r	201	CLA	ND
27	D	207	CLA	ND
27	D	208	CLA	ND
27	D	209	CLA	ND
27	D	210	CLA	ND
27	D	211	CLA	ND
27	D	212	CLA	ND
27	D	213	CLA	ND
27	D	214	CLA	ND
27	D	215	CLA	ND
27	D	216	CLA	ND
27	D	217	CLA	ND
27	b	801	CLA	ND
27	b	803	CLA	ND
27	b	804	CLA	ND
27	b	805	CLA	ND
27	b	806	CLA	ND

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Mol	Chain	Res	Type	Atom
27	b	807	CLA	ND
27	b	808	CLA	ND
27	b	809	CLA	ND
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	838	CLA	ND
27	b	839	CLA	ND
27	b	841	CLA	ND
27	b	842	CLA	ND
27	b	843	CLA	ND
27	b	844	CLA	ND
27	b	845	CLA	ND
27	b	846	CLA	ND
27	b	847	CLA	ND
27	b	849	CLA	ND
27	b	850	CLA	ND

All (3471) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	201	DD6	C12-C11-C13-C14
26	A	201	DD6	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	A	202	DD6	C13-C14-C15-C16
26	A	202	DD6	C13-C14-C15-C20
26	E	302	DD6	C10-C11-C13-C14
26	E	302	DD6	C12-C11-C13-C14
26	E	303	DD6	C13-C14-C15-C16
26	E	303	DD6	C13-C14-C15-O1
26	E	306	DD6	C13-C14-C15-C16
26	E	306	DD6	C13-C14-C15-C20
26	E	306	DD6	C13-C14-C15-O1
26	E	306	DD6	C5-C6-C8-C9
26	E	306	DD6	C7-C6-C8-C9
26	G	301	DD6	C10-C11-C13-C14
26	G	301	DD6	C12-C11-C13-C14
26	G	301	DD6	C13-C14-C15-O1
26	H	202	DD6	C27-C29-C30-C31
26	J	302	DD6	C-C1-C24-C25
26	J	302	DD6	C2-C1-C24-C25
26	J	302	DD6	C10-C11-C13-C14
26	J	302	DD6	C12-C11-C13-C14
26	J	302	DD6	C13-C14-C15-O1
26	J	302	DD6	C5-C6-C8-C9
26	J	302	DD6	C7-C6-C8-C9
26	J	303	DD6	C10-C11-C13-C14
26	J	303	DD6	C12-C11-C13-C14
26	J	303	DD6	C5-C6-C8-C9
26	J	303	DD6	C7-C6-C8-C9
26	J	305	DD6	C10-C11-C13-C14
26	J	305	DD6	C12-C11-C13-C14
26	K	303	DD6	C10-C11-C13-C14
26	K	303	DD6	C12-C11-C13-C14
26	K	303	DD6	C13-C14-C15-O1
26	K	303	DD6	C7-C6-C8-C9
26	L	301	DD6	C7-C6-C8-C9
26	M	301	DD6	C13-C14-C15-O1
26	M	306	DD6	C12-C11-C13-C14
27	A	210	CLA	CBD-CGD-O2D-CED
27	B	306	CLA	C1A-C2A-CAA-CBA
27	B	306	CLA	C3A-C2A-CAA-CBA
27	B	309	CLA	C4-C3-C5-C6
27	B	310	CLA	CBA-CGA-O2A-C1
27	B	310	CLA	CBD-CGD-O2D-CED
27	B	310	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	311	CLA	CBD-CGD-O2D-CED
27	B	312	CLA	C3A-C2A-CAA-CBA
27	B	314	CLA	CBD-CGD-O2D-CED
27	C	306	CLA	CHA-CBD-CGD-O1D
27	C	306	CLA	CHA-CBD-CGD-O2D
27	C	310	CLA	CBA-CGA-O2A-C1
27	C	310	CLA	CBD-CGD-O2D-CED
27	C	311	CLA	CBD-CGD-O2D-CED
27	C	312	CLA	C3A-C2A-CAA-CBA
27	C	315	CLA	C1A-C2A-CAA-CBA
27	C	316	CLA	CHA-CBD-CGD-O1D
27	C	317	CLA	C1A-C2A-CAA-CBA
27	C	317	CLA	CHA-CBD-CGD-O1D
27	C	318	CLA	C1A-C2A-CAA-CBA
27	C	318	CLA	C3A-C2A-CAA-CBA
27	E	310	CLA	CBA-CGA-O2A-C1
27	E	310	CLA	O1A-CGA-O2A-C1
27	E	310	CLA	CHA-CBD-CGD-O1D
27	E	310	CLA	CHA-CBD-CGD-O2D
27	E	314	CLA	CHA-CBD-CGD-O1D
27	E	314	CLA	CHA-CBD-CGD-O2D
27	E	314	CLA	CAD-CBD-CGD-O1D
27	F	305	CLA	C3A-C2A-CAA-CBA
27	F	305	CLA	CBD-CGD-O2D-CED
27	F	309	CLA	CBD-CGD-O2D-CED
27	F	310	CLA	C1A-C2A-CAA-CBA
27	F	311	CLA	CBD-CGD-O2D-CED
27	F	315	CLA	C1A-C2A-CAA-CBA
27	F	315	CLA	C3A-C2A-CAA-CBA
27	F	316	CLA	CHA-CBD-CGD-O1D
27	F	316	CLA	CBD-CGD-O2D-CED
27	F	317	CLA	C1A-C2A-CAA-CBA
27	G	309	CLA	C2A-CAA-CBA-CGA
27	G	309	CLA	CHA-CBD-CGD-O1D
27	G	309	CLA	CHA-CBD-CGD-O2D
27	G	311	CLA	C4-C3-C5-C6
27	G	314	CLA	CBD-CGD-O2D-CED
27	G	315	CLA	C3A-C2A-CAA-CBA
27	G	315	CLA	CBD-CGD-O2D-CED
27	H	204	CLA	C1A-C2A-CAA-CBA
27	H	204	CLA	C3A-C2A-CAA-CBA
27	H	204	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	H	210	CLA	C1A-C2A-CAA-CBA
27	H	210	CLA	C3A-C2A-CAA-CBA
27	H	212	CLA	CHA-CBD-CGD-O1D
27	H	212	CLA	CHA-CBD-CGD-O2D
27	H	213	CLA	C2-C3-C5-C6
27	H	213	CLA	C4-C3-C5-C6
27	H	214	CLA	CBD-CGD-O2D-CED
27	H	214	CLA	O1D-CGD-O2D-CED
27	I	308	CLA	C6-C7-C8-C9
27	I	309	CLA	CBA-CGA-O2A-C1
27	I	309	CLA	CHA-CBD-CGD-O1D
27	I	309	CLA	CHA-CBD-CGD-O2D
27	I	310	CLA	C1A-C2A-CAA-CBA
27	I	310	CLA	C3A-C2A-CAA-CBA
27	I	311	CLA	CHA-CBD-CGD-O1D
27	I	311	CLA	CHA-CBD-CGD-O2D
27	I	311	CLA	C2-C3-C5-C6
27	I	311	CLA	C4-C3-C5-C6
27	I	313	CLA	CHA-CBD-CGD-O1D
27	I	313	CLA	CHA-CBD-CGD-O2D
27	I	313	CLA	CAD-CBD-CGD-O1D
27	I	313	CLA	CAD-CBD-CGD-O2D
27	I	314	CLA	CHA-CBD-CGD-O1D
27	I	314	CLA	CHA-CBD-CGD-O2D
27	I	314	CLA	CBD-CGD-O2D-CED
27	I	317	CLA	CBD-CGD-O2D-CED
27	J	309	CLA	C1A-C2A-CAA-CBA
27	J	309	CLA	C3A-C2A-CAA-CBA
27	J	310	CLA	CHA-CBD-CGD-O2D
27	J	310	CLA	CBD-CGD-O2D-CED
27	J	312	CLA	CHA-CBD-CGD-O1D
27	J	312	CLA	CHA-CBD-CGD-O2D
27	J	313	CLA	CBD-CGD-O2D-CED
27	J	314	CLA	CBD-CGD-O2D-CED
27	K	310	CLA	C2-C3-C5-C6
27	K	310	CLA	C4-C3-C5-C6
27	K	311	CLA	CHA-CBD-CGD-O1D
27	K	311	CLA	CHA-CBD-CGD-O2D
27	K	311	CLA	CAD-CBD-CGD-O1D
27	K	311	CLA	CAD-CBD-CGD-O2D
27	K	312	CLA	C2-C3-C5-C6
27	K	312	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	K	316	CLA	C1A-C2A-CAA-CBA
27	K	318	CLA	C1A-C2A-CAA-CBA
27	K	318	CLA	C3A-C2A-CAA-CBA
27	K	319	CLA	CBD-CGD-O2D-CED
27	K	319	CLA	O1D-CGD-O2D-CED
27	L	307	CLA	C1A-C2A-CAA-CBA
27	L	307	CLA	C3A-C2A-CAA-CBA
27	L	310	CLA	CHA-CBD-CGD-O1D
27	L	310	CLA	C11-C10-C8-C9
27	L	311	CLA	CHA-CBD-CGD-O2D
27	L	312	CLA	O2A-C1-C2-C3
27	L	312	CLA	C2-C3-C5-C6
27	L	312	CLA	C4-C3-C5-C6
27	L	313	CLA	C1A-C2A-CAA-CBA
27	L	313	CLA	C3A-C2A-CAA-CBA
27	L	313	CLA	CBD-CGD-O2D-CED
27	L	316	CLA	CBD-CGD-O2D-CED
27	L	317	CLA	CBD-CGD-O2D-CED
27	L	321	CLA	C1A-C2A-CAA-CBA
27	L	321	CLA	C3A-C2A-CAA-CBA
27	M	311	CLA	C1A-C2A-CAA-CBA
27	M	311	CLA	C3A-C2A-CAA-CBA
27	M	311	CLA	CBA-CGA-O2A-C1
27	M	312	CLA	C1A-C2A-CAA-CBA
27	M	312	CLA	C3A-C2A-CAA-CBA
27	M	312	CLA	C2A-CAA-CBA-CGA
27	M	313	CLA	C1A-C2A-CAA-CBA
27	M	313	CLA	C3A-C2A-CAA-CBA
27	M	313	CLA	C11-C10-C8-C9
27	M	316	CLA	C1A-C2A-CAA-CBA
27	M	316	CLA	C2-C3-C5-C6
27	M	316	CLA	C4-C3-C5-C6
27	M	318	CLA	C1A-C2A-CAA-CBA
27	M	318	CLA	C3A-C2A-CAA-CBA
27	M	319	CLA	CAD-CBD-CGD-O1D
27	M	319	CLA	CAD-CBD-CGD-O2D
27	M	319	CLA	CBD-CGD-O2D-CED
27	a	803	CLA	CBD-CGD-O2D-CED
27	a	803	CLA	O1D-CGD-O2D-CED
27	a	804	CLA	CHA-CBD-CGD-O1D
27	a	804	CLA	CHA-CBD-CGD-O2D
27	a	805	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	a	805	CLA	CHA-CBD-CGD-O2D
27	a	806	CLA	C1A-C2A-CAA-CBA
27	a	806	CLA	C3A-C2A-CAA-CBA
27	a	807	CLA	C3A-C2A-CAA-CBA
27	a	811	CLA	C2A-CAA-CBA-CGA
27	a	811	CLA	CHA-CBD-CGD-O1D
27	a	811	CLA	CHA-CBD-CGD-O2D
27	a	815	CLA	C1A-C2A-CAA-CBA
27	a	815	CLA	CHA-CBD-CGD-O1D
27	a	815	CLA	CHA-CBD-CGD-O2D
27	a	816	CLA	C3A-C2A-CAA-CBA
27	a	817	CLA	C1A-C2A-CAA-CBA
27	a	817	CLA	C3A-C2A-CAA-CBA
27	a	818	CLA	C1A-C2A-CAA-CBA
27	a	818	CLA	C3A-C2A-CAA-CBA
27	a	823	CLA	C1A-C2A-CAA-CBA
27	a	823	CLA	C3A-C2A-CAA-CBA
27	a	825	CLA	C1A-C2A-CAA-CBA
27	a	825	CLA	C3A-C2A-CAA-CBA
27	a	825	CLA	CHA-CBD-CGD-O1D
27	a	825	CLA	CHA-CBD-CGD-O2D
27	a	826	CLA	C1A-C2A-CAA-CBA
27	a	826	CLA	CHA-CBD-CGD-O1D
27	a	826	CLA	CHA-CBD-CGD-O2D
27	a	829	CLA	CHA-CBD-CGD-O1D
27	a	830	CLA	CHA-CBD-CGD-O1D
27	a	830	CLA	CHA-CBD-CGD-O2D
27	a	830	CLA	CAD-CBD-CGD-O1D
27	a	839	CLA	C1A-C2A-CAA-CBA
27	a	839	CLA	C3A-C2A-CAA-CBA
27	a	839	CLA	CHA-CBD-CGD-O2D
27	a	840	CLA	C1A-C2A-CAA-CBA
27	a	843	CLA	CHA-CBD-CGD-O1D
27	a	843	CLA	CHA-CBD-CGD-O2D
27	a	843	CLA	CAD-CBD-CGD-O1D
27	a	843	CLA	C11-C12-C13-C14
27	a	846	CLA	C1A-C2A-CAA-CBA
27	a	846	CLA	C3A-C2A-CAA-CBA
27	a	848	CLA	C1A-C2A-CAA-CBA
27	a	848	CLA	C3A-C2A-CAA-CBA
27	a	849	CLA	C2A-CAA-CBA-CGA
27	a	854	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	a	854	CLA	CHA-CBD-CGD-O2D
27	a	854	CLA	CAD-CBD-CGD-O1D
27	a	856	CLA	CBD-CGD-O2D-CED
27	a	856	CLA	C2-C3-C5-C6
27	a	856	CLA	C4-C3-C5-C6
27	f	301	CLA	CBD-CGD-O2D-CED
27	l	204	CLA	C2-C3-C5-C6
27	l	204	CLA	C4-C3-C5-C6
27	l	204	CLA	C11-C10-C8-C9
27	r	201	CLA	C1A-C2A-CAA-CBA
27	r	201	CLA	C3A-C2A-CAA-CBA
27	r	201	CLA	CBD-CGD-O2D-CED
27	D	213	CLA	C2A-CAA-CBA-CGA
27	D	215	CLA	CBD-CGD-O2D-CED
27	D	216	CLA	C1A-C2A-CAA-CBA
27	D	216	CLA	C3A-C2A-CAA-CBA
27	b	801	CLA	C2A-CAA-CBA-CGA
27	b	804	CLA	CHA-CBD-CGD-O1D
27	b	804	CLA	CHA-CBD-CGD-O2D
27	b	804	CLA	CBD-CGD-O2D-CED
27	b	806	CLA	C3A-C2A-CAA-CBA
27	b	807	CLA	CBD-CGD-O2D-CED
27	b	810	CLA	C1A-C2A-CAA-CBA
27	b	813	CLA	O1A-CGA-O2A-C1
27	b	814	CLA	CHA-CBD-CGD-O1D
27	b	814	CLA	CHA-CBD-CGD-O2D
27	b	814	CLA	CAD-CBD-CGD-O1D
27	b	815	CLA	C1A-C2A-CAA-CBA
27	b	815	CLA	C3A-C2A-CAA-CBA
27	b	818	CLA	C1A-C2A-CAA-CBA
27	b	818	CLA	C3A-C2A-CAA-CBA
27	b	818	CLA	CHA-CBD-CGD-O1D
27	b	818	CLA	CHA-CBD-CGD-O2D
27	b	819	CLA	C1A-C2A-CAA-CBA
27	b	819	CLA	C3A-C2A-CAA-CBA
27	b	820	CLA	C1A-C2A-CAA-CBA
27	b	820	CLA	C3A-C2A-CAA-CBA
27	b	820	CLA	CHA-CBD-CGD-O1D
27	b	820	CLA	CHA-CBD-CGD-O2D
27	b	821	CLA	CHA-CBD-CGD-O2D
27	b	821	CLA	C11-C12-C13-C14
27	b	822	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	b	822	CLA	C3A-C2A-CAA-CBA
27	b	823	CLA	C1A-C2A-CAA-CBA
27	b	823	CLA	C3A-C2A-CAA-CBA
27	b	824	CLA	C1A-C2A-CAA-CBA
27	b	825	CLA	C1A-C2A-CAA-CBA
27	b	841	CLA	CHA-CBD-CGD-O2D
27	b	842	CLA	C1A-C2A-CAA-CBA
27	b	842	CLA	C3A-C2A-CAA-CBA
27	b	842	CLA	CBD-CGD-O2D-CED
27	b	844	CLA	C4-C3-C5-C6
27	b	845	CLA	C1A-C2A-CAA-CBA
27	b	846	CLA	C1A-C2A-CAA-CBA
27	b	846	CLA	C3A-C2A-CAA-CBA
27	b	850	CLA	C2-C3-C5-C6
27	b	850	CLA	C4-C3-C5-C6
28	A	209	KC1	C2B-C3B-CAB-CBB
28	A	209	KC1	C4B-C3B-CAB-CBB
28	A	209	KC1	CBD-CGD-O2D-CED
28	B	313	KC1	C2A-CAA-CBA-CGA
28	B	313	KC1	CHA-CBD-CGD-O1D
28	B	313	KC1	CBD-CGD-O2D-CED
28	C	308	KC1	C1A-C2A-CAA-CBA
28	C	308	KC1	C3A-C2A-CAA-CBA
28	C	308	KC1	C2B-C3B-CAB-CBB
28	C	308	KC1	C4B-C3B-CAB-CBB
28	C	308	KC1	C2A-CAA-CBA-CGA
28	C	308	KC1	CHA-CBD-CGD-O1D
28	C	313	KC1	C1A-C2A-CAA-CBA
28	C	313	KC1	C3A-C2A-CAA-CBA
28	C	313	KC1	C2B-C3B-CAB-CBB
28	C	313	KC1	C4B-C3B-CAB-CBB
28	F	312	KC1	C1A-C2A-CAA-CBA
28	F	312	KC1	C2B-C3B-CAB-CBB
28	F	312	KC1	C4B-C3B-CAB-CBB
28	F	312	KC1	C2A-CAA-CBA-CGA
28	G	313	KC1	C1A-C2A-CAA-CBA
28	G	313	KC1	C2B-C3B-CAB-CBB
28	G	313	KC1	C4B-C3B-CAB-CBB
28	I	312	KC1	C2A-CAA-CBA-CGA
28	J	306	KC1	C2A-CAA-CBA-CGA
28	K	308	KC1	C1A-C2A-CAA-CBA
28	K	308	KC1	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	L	314	KC1	C2A-CAA-CBA-CGA
28	L	314	KC1	CHA-CBD-CGD-O1D
28	L	314	KC1	CBD-CGD-O2D-CED
28	L	320	KC1	C1A-C2A-CAA-CBA
28	L	320	KC1	C3A-C2A-CAA-CBA
28	L	320	KC1	C2B-C3B-CAB-CBB
28	L	320	KC1	C4B-C3B-CAB-CBB
28	L	320	KC1	CBD-CGD-O2D-CED
28	L	322	KC1	CHA-CBD-CGD-O1D
29	A	214	LMG	O6-C1-O1-C7
29	C	301	LMG	O6-C1-O1-C7
29	E	317	LMG	O7-C8-C9-O8
29	I	319	LMG	O10-C28-O8-C9
29	I	319	LMG	C29-C28-O8-C9
29	M	321	LMG	C2-C1-O1-C7
29	M	321	LMG	O6-C1-O1-C7
29	a	852	LMG	O7-C8-C9-O8
29	j	103	LMG	O10-C28-O8-C9
29	j	103	LMG	C29-C28-O8-C9
29	l	201	LMG	O6-C1-O1-C7
29	l	201	LMG	O7-C8-C9-O8
29	l	201	LMG	C11-C10-O7-C8
29	D	202	LMG	C2-C1-O1-C7
29	D	202	LMG	O6-C1-O1-C7
30	A	213	A86	C-C1-C24-C25
30	A	213	A86	C2-C1-C24-C25
30	B	301	A86	C26-C27-C29-C30
30	B	301	A86	C28-C27-C29-C30
30	B	302	A86	C39-C38-O4-C34
30	B	302	A86	O5-C38-O4-C34
30	B	305	A86	C1-C2-C3-C4
30	C	304	A86	C35-C34-O4-C38
30	C	305	A86	C1-C2-C3-C4
30	E	301	A86	C1-C2-C3-C4
30	E	301	A86	C35-C34-O4-C38
30	F	301	A86	C-C1-C24-C25
30	F	301	A86	C2-C1-C24-C25
30	F	301	A86	C35-C34-O4-C38
30	F	301	A86	C39-C38-O4-C34
30	F	304	A86	C35-C34-O4-C38
30	G	302	A86	C-C1-C24-C25
30	G	302	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
30	G	302	A86	C35-C34-O4-C38
30	G	302	A86	C39-C38-O4-C34
30	G	302	A86	C3-C4-C5-C6
30	H	201	A86	C39-C38-O4-C34
30	H	201	A86	O5-C38-O4-C34
30	I	301	A86	C28-C27-C29-C30
30	I	303	A86	C1-C2-C3-C4
30	J	301	A86	C1-C2-C3-C4
30	J	316	A86	C26-C27-C29-C30
30	J	316	A86	C39-C38-O4-C34
30	J	316	A86	O5-C38-O4-C34
30	K	301	A86	C-C1-C24-C25
30	K	301	A86	C10-C11-C13-O
30	K	301	A86	C12-C11-C13-O
30	K	301	A86	C33-C34-O4-C38
30	K	302	A86	C-C1-C24-C25
30	K	302	A86	C2-C1-C24-C25
30	K	302	A86	C33-C34-O4-C38
30	K	302	A86	C39-C38-O4-C34
30	K	302	A86	C5-C6-C8-C9
30	K	302	A86	C7-C6-C8-C9
30	K	304	A86	O5-C38-O4-C34
30	K	307	A86	O5-C38-O4-C34
30	L	302	A86	C-C1-C24-C25
30	L	302	A86	C2-C1-C24-C25
30	L	302	A86	C39-C38-O4-C34
30	L	302	A86	O5-C38-O4-C34
30	L	305	A86	C10-C11-C13-O
30	L	305	A86	C12-C11-C13-O
30	L	305	A86	C35-C34-O4-C38
30	L	305	A86	C39-C38-O4-C34
30	L	305	A86	O5-C38-O4-C34
30	L	306	A86	C13-C14-C15-O1
30	L	306	A86	O5-C38-O4-C34
30	M	302	A86	O5-C38-O4-C34
30	M	303	A86	C11-C10-C9-C8
30	M	303	A86	C10-C11-C13-O
30	M	303	A86	C12-C11-C13-O
30	M	303	A86	C24-C25-C26-C27
30	M	305	A86	C-C1-C24-C25
30	m	101	A86	C39-C38-O4-C34
30	D	203	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
30	D	203	A86	C2-C1-C24-C25
30	D	203	A86	O5-C38-O4-C34
30	D	206	A86	C1-C2-C3-C4
30	D	206	A86	C39-C38-O4-C34
30	D	206	A86	O5-C38-O4-C34
30	b	848	A86	C-C1-C24-C25
30	b	848	A86	C2-C1-C24-C25
30	b	848	A86	C11-C10-C9-C8
31	B	315	LHG	O1-C1-C2-C3
31	B	315	LHG	C3-O3-P-O4
31	B	315	LHG	C4-O6-P-O4
31	E	318	LHG	C2-C3-O3-P
31	H	215	LHG	C4-O6-P-O3
31	H	215	LHG	C4-O6-P-O4
31	H	215	LHG	C4-O6-P-O5
31	H	215	LHG	C8-C7-O7-C5
31	I	318	LHG	C3-O3-P-O5
31	I	318	LHG	C4-O6-P-O4
31	K	320	LHG	O7-C5-C6-O8
31	K	320	LHG	C8-C7-O7-C5
31	a	801	LHG	C1-C2-C3-O3
31	a	801	LHG	C8-C7-O7-C5
31	a	802	LHG	C3-O3-P-O4
31	a	802	LHG	C3-O3-P-O5
31	a	834	LHG	C3-O3-P-O4
31	a	834	LHG	C4-O6-P-O3
31	a	834	LHG	C8-C7-O7-C5
31	D	201	LHG	C3-O3-P-O4
31	D	201	LHG	C3-O3-P-O5
31	D	201	LHG	C3-O3-P-O6
32	a	836	BCR	C37-C22-C23-C24
32	a	847	BCR	C23-C24-C25-C26
32	a	847	BCR	C23-C24-C25-C30
32	a	851	BCR	C1-C6-C7-C8
32	a	851	BCR	C5-C6-C7-C8
32	a	853	BCR	C5-C6-C7-C8
32	f	305	BCR	C5-C6-C7-C8
32	f	305	BCR	C17-C18-C19-C20
32	f	305	BCR	C36-C18-C19-C20
32	f	305	BCR	C21-C22-C23-C24
32	f	305	BCR	C37-C22-C23-C24
32	i	103	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
32	i	103	BCR	C37-C22-C23-C24
32	j	105	BCR	C21-C22-C23-C24
32	j	105	BCR	C37-C22-C23-C24
32	l	205	BCR	C1-C6-C7-C8
32	l	205	BCR	C21-C22-C23-C24
32	l	205	BCR	C37-C22-C23-C24
32	m	102	BCR	C7-C8-C9-C10
32	m	102	BCR	C7-C8-C9-C34
32	b	837	BCR	C7-C8-C9-C10
32	b	837	BCR	C7-C8-C9-C34
32	b	837	BCR	C19-C20-C21-C22
32	b	837	BCR	C21-C22-C23-C24
32	b	837	BCR	C37-C22-C23-C24
32	b	840	BCR	C23-C24-C25-C26
32	b	840	BCR	C23-C24-C25-C30
33	J	318	SQD	O49-C7-O47-C45
33	J	318	SQD	O5-C5-C6-S
33	J	318	SQD	C5-C6-S-O7
34	a	831	PQN	C12-C13-C15-C16
34	a	831	PQN	C14-C13-C15-C16
35	l	207	ET4	C05-C06-C07-C08
27	a	815	CLA	C2C-C3C-CAC-CBC
30	B	301	A86	C39-C38-O4-C34
30	C	302	A86	C39-C38-O4-C34
30	C	305	A86	O5-C38-O4-C34
30	E	301	A86	C39-C38-O4-C34
30	F	304	A86	C39-C38-O4-C34
30	I	301	A86	C39-C38-O4-C34
30	K	307	A86	C39-C38-O4-C34
30	L	306	A86	C39-C38-O4-C34
30	M	302	A86	C39-C38-O4-C34
30	D	203	A86	C39-C38-O4-C34
27	B	311	CLA	O1D-CGD-O2D-CED
27	B	314	CLA	O1D-CGD-O2D-CED
27	C	311	CLA	O1D-CGD-O2D-CED
27	C	314	CLA	O1D-CGD-O2D-CED
27	F	309	CLA	O1D-CGD-O2D-CED
27	G	315	CLA	O1D-CGD-O2D-CED
27	I	311	CLA	O1D-CGD-O2D-CED
27	I	317	CLA	O1D-CGD-O2D-CED
27	J	314	CLA	O1D-CGD-O2D-CED
27	L	313	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	L	314	KC1	O1D-CGD-O2D-CED
28	L	320	KC1	O1D-CGD-O2D-CED
27	G	309	CLA	C8-C10-C11-C12
27	G	309	CLA	C13-C15-C16-C17
27	J	312	CLA	C5-C6-C7-C8
27	I	317	CLA	C2C-C3C-CAC-CBC
27	J	310	CLA	C2C-C3C-CAC-CBC
30	A	213	A86	C39-C38-O4-C34
30	B	301	A86	O5-C38-O4-C34
30	C	302	A86	O5-C38-O4-C34
30	C	304	A86	C39-C38-O4-C34
30	C	305	A86	C39-C38-O4-C34
30	F	301	A86	O5-C38-O4-C34
30	F	304	A86	O5-C38-O4-C34
30	J	301	A86	C39-C38-O4-C34
30	K	304	A86	C39-C38-O4-C34
30	K	306	A86	C39-C38-O4-C34
27	G	316	CLA	O1D-CGD-O2D-CED
27	I	314	CLA	O1D-CGD-O2D-CED
27	J	313	CLA	O1D-CGD-O2D-CED
27	M	315	CLA	O1D-CGD-O2D-CED
27	a	804	CLA	O1D-CGD-O2D-CED
27	j	104	CLA	O1D-CGD-O2D-CED
27	b	807	CLA	O1D-CGD-O2D-CED
27	B	307	CLA	CBD-CGD-O2D-CED
27	B	312	CLA	CBD-CGD-O2D-CED
27	C	314	CLA	CBD-CGD-O2D-CED
27	C	315	CLA	CBD-CGD-O2D-CED
27	E	308	CLA	CBD-CGD-O2D-CED
27	E	314	CLA	CBD-CGD-O2D-CED
27	F	307	CLA	CBD-CGD-O2D-CED
27	F	313	CLA	CBD-CGD-O2D-CED
27	F	315	CLA	CBD-CGD-O2D-CED
27	F	317	CLA	CBD-CGD-O2D-CED
27	G	307	CLA	CBD-CGD-O2D-CED
27	G	309	CLA	CBD-CGD-O2D-CED
27	G	316	CLA	CBD-CGD-O2D-CED
27	G	317	CLA	CBD-CGD-O2D-CED
27	I	311	CLA	CBD-CGD-O2D-CED
27	J	309	CLA	CBD-CGD-O2D-CED
27	J	312	CLA	CBD-CGD-O2D-CED
27	L	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	L	315	CLA	CBD-CGD-O2D-CED
27	M	315	CLA	CBD-CGD-O2D-CED
27	a	804	CLA	CBD-CGD-O2D-CED
27	a	823	CLA	CBD-CGD-O2D-CED
27	a	854	CLA	CBD-CGD-O2D-CED
27	j	104	CLA	CBD-CGD-O2D-CED
27	D	211	CLA	CBD-CGD-O2D-CED
27	D	217	CLA	CBD-CGD-O2D-CED
27	b	814	CLA	CBD-CGD-O2D-CED
28	J	306	KC1	CBD-CGD-O2D-CED
27	A	207	CLA	O1A-CGA-O2A-C1
27	E	314	CLA	O1A-CGA-O2A-C1
27	G	309	CLA	O1A-CGA-O2A-C1
31	j	102	LHG	O10-C23-O8-C6
27	B	310	CLA	O1A-CGA-O2A-C1
27	C	310	CLA	O1A-CGA-O2A-C1
27	K	318	CLA	O1A-CGA-O2A-C1
27	J	310	CLA	C4C-C3C-CAC-CBC
27	K	317	CLA	C2C-C3C-CAC-CBC
30	K	306	A86	O5-C38-O4-C34
27	F	313	CLA	O1D-CGD-O2D-CED
27	F	317	CLA	O1D-CGD-O2D-CED
27	G	314	CLA	O1D-CGD-O2D-CED
27	J	310	CLA	O1D-CGD-O2D-CED
27	J	312	CLA	O1D-CGD-O2D-CED
27	M	319	CLA	O1D-CGD-O2D-CED
27	D	217	CLA	O1D-CGD-O2D-CED
27	b	814	CLA	O1D-CGD-O2D-CED
27	K	318	CLA	CBA-CGA-O2A-C1
27	a	815	CLA	C4C-C3C-CAC-CBC
30	H	203	A86	C39-C38-O4-C34
27	A	210	CLA	O1D-CGD-O2D-CED
27	C	310	CLA	O1D-CGD-O2D-CED
27	F	307	CLA	O1D-CGD-O2D-CED
27	F	311	CLA	O1D-CGD-O2D-CED
27	F	316	CLA	O1D-CGD-O2D-CED
27	L	316	CLA	O1D-CGD-O2D-CED
27	a	856	CLA	O1D-CGD-O2D-CED
27	D	215	CLA	O1D-CGD-O2D-CED
27	b	804	CLA	O1D-CGD-O2D-CED
27	A	207	CLA	CBA-CGA-O2A-C1
27	E	314	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	G	309	CLA	CBA-CGA-O2A-C1
31	j	102	LHG	C24-C23-O8-C6
27	C	317	CLA	CBD-CGD-O2D-CED
27	C	318	CLA	CBD-CGD-O2D-CED
27	E	312	CLA	CBD-CGD-O2D-CED
27	F	310	CLA	CBD-CGD-O2D-CED
27	G	306	CLA	CBD-CGD-O2D-CED
27	I	313	CLA	CBD-CGD-O2D-CED
27	I	316	CLA	CBD-CGD-O2D-CED
27	K	311	CLA	CBD-CGD-O2D-CED
27	K	314	CLA	CBD-CGD-O2D-CED
27	K	317	CLA	CBD-CGD-O2D-CED
27	L	321	CLA	CBD-CGD-O2D-CED
27	M	312	CLA	CBD-CGD-O2D-CED
27	a	813	CLA	CBD-CGD-O2D-CED
27	a	830	CLA	CBD-CGD-O2D-CED
27	a	843	CLA	CBD-CGD-O2D-CED
27	a	844	CLA	CBD-CGD-O2D-CED
27	a	846	CLA	CBD-CGD-O2D-CED
27	b	816	CLA	CBD-CGD-O2D-CED
27	b	817	CLA	CBD-CGD-O2D-CED
27	b	818	CLA	CBD-CGD-O2D-CED
27	b	823	CLA	CBD-CGD-O2D-CED
27	b	831	CLA	CBD-CGD-O2D-CED
27	C	317	CLA	C2C-C3C-CAC-CBC
27	K	317	CLA	C4C-C3C-CAC-CBC
27	A	208	CLA	O1A-CGA-O2A-C1
27	E	312	CLA	O1A-CGA-O2A-C1
27	F	315	CLA	O1A-CGA-O2A-C1
27	H	204	CLA	O1A-CGA-O2A-C1
27	I	310	CLA	O1A-CGA-O2A-C1
27	M	313	CLA	O1A-CGA-O2A-C1
27	a	806	CLA	O1A-CGA-O2A-C1
27	a	813	CLA	O1A-CGA-O2A-C1
27	a	815	CLA	O1A-CGA-O2A-C1
27	a	817	CLA	O1A-CGA-O2A-C1
27	a	819	CLA	O1A-CGA-O2A-C1
27	a	840	CLA	O1A-CGA-O2A-C1
27	a	841	CLA	O1A-CGA-O2A-C1
27	b	814	CLA	O1A-CGA-O2A-C1
27	b	827	CLA	O1A-CGA-O2A-C1
27	b	850	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	C	319	LMG	O10-C28-O8-C9
31	a	837	LHG	O10-C23-O8-C6
27	I	309	CLA	O1A-CGA-O2A-C1
27	M	311	CLA	O1A-CGA-O2A-C1
27	f	301	CLA	O1D-CGD-O2D-CED
27	r	201	CLA	O1D-CGD-O2D-CED
28	L	322	KC1	CAA-CBA-CGA-O2A
28	M	314	KC1	CAA-CBA-CGA-O2A
27	A	205	CLA	C4C-C3C-CAC-CBC
30	E	301	A86	O5-C38-O4-C34
30	I	301	A86	O5-C38-O4-C34
27	F	305	CLA	O1D-CGD-O2D-CED
27	b	842	CLA	O1D-CGD-O2D-CED
27	L	311	CLA	CBD-CGD-O2D-CED
27	a	825	CLA	CBD-CGD-O2D-CED
27	b	806	CLA	CBD-CGD-O2D-CED
27	b	838	CLA	CBD-CGD-O2D-CED
27	L	317	CLA	O1D-CGD-O2D-CED
29	L	323	LMG	O9-C10-O7-C8
29	l	201	LMG	O9-C10-O7-C8
31	H	215	LHG	O9-C7-O7-C5
31	K	320	LHG	O9-C7-O7-C5
31	a	801	LHG	O9-C7-O7-C5
31	a	802	LHG	O9-C7-O7-C5
31	a	834	LHG	O9-C7-O7-C5
27	I	317	CLA	CBA-CGA-O2A-C1
27	J	310	CLA	CBA-CGA-O2A-C1
27	K	319	CLA	CBA-CGA-O2A-C1
27	M	319	CLA	CBA-CGA-O2A-C1
30	B	305	A86	C39-C38-O4-C34
27	A	206	CLA	O1A-CGA-O2A-C1
27	G	310	CLA	O1A-CGA-O2A-C1
27	D	211	CLA	O1D-CGD-O2D-CED
27	A	204	CLA	C3-C5-C6-C7
27	A	207	CLA	C3-C5-C6-C7
27	C	309	CLA	C3-C5-C6-C7
27	C	312	CLA	C3-C5-C6-C7
27	E	308	CLA	C3-C5-C6-C7
27	F	306	CLA	C3-C5-C6-C7
27	F	307	CLA	C3-C5-C6-C7
27	F	308	CLA	C3-C5-C6-C7
27	F	311	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	I	311	CLA	C3-C5-C6-C7
27	L	312	CLA	C3-C5-C6-C7
27	L	313	CLA	C3-C5-C6-C7
27	L	316	CLA	C3-C5-C6-C7
27	M	313	CLA	C3-C5-C6-C7
27	M	316	CLA	C3-C5-C6-C7
27	a	809	CLA	C3-C5-C6-C7
27	a	839	CLA	C3-C5-C6-C7
27	a	841	CLA	C3-C5-C6-C7
27	b	807	CLA	C3-C5-C6-C7
27	b	823	CLA	C3-C5-C6-C7
27	b	838	CLA	C3-C5-C6-C7
27	b	847	CLA	C3-C5-C6-C7
27	H	204	CLA	CBA-CGA-O2A-C1
27	J	314	CLA	CBA-CGA-O2A-C1
27	M	313	CLA	CBA-CGA-O2A-C1
27	a	806	CLA	CBA-CGA-O2A-C1
27	a	813	CLA	CBA-CGA-O2A-C1
27	a	815	CLA	CBA-CGA-O2A-C1
27	a	819	CLA	CBA-CGA-O2A-C1
27	a	841	CLA	CBA-CGA-O2A-C1
27	b	813	CLA	CBA-CGA-O2A-C1
27	b	814	CLA	CBA-CGA-O2A-C1
27	b	827	CLA	CBA-CGA-O2A-C1
27	b	850	CLA	CBA-CGA-O2A-C1
29	M	321	LMG	C29-C28-O8-C9
27	A	205	CLA	C2C-C3C-CAC-CBC
27	I	317	CLA	C4C-C3C-CAC-CBC
27	a	805	CLA	C5-C6-C7-C8
29	L	323	LMG	C11-C10-O7-C8
31	a	802	LHG	C8-C7-O7-C5
27	C	315	CLA	O1D-CGD-O2D-CED
27	F	315	CLA	O1D-CGD-O2D-CED
27	C	309	CLA	CBD-CGD-O2D-CED
27	G	312	CLA	CBD-CGD-O2D-CED
27	H	212	CLA	CBD-CGD-O2D-CED
27	H	213	CLA	CBD-CGD-O2D-CED
27	H	204	CLA	C2C-C3C-CAC-CBC
27	I	313	CLA	C2C-C3C-CAC-CBC
30	K	302	A86	O5-C38-O4-C34
27	I	317	CLA	O1A-CGA-O2A-C1
27	K	319	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	M	319	CLA	O1A-CGA-O2A-C1
30	G	302	A86	O5-C38-O4-C34
30	m	101	A86	O5-C38-O4-C34
28	B	313	KC1	CAA-CBA-CGA-O1A
28	B	313	KC1	CAA-CBA-CGA-O2A
27	A	206	CLA	CBA-CGA-O2A-C1
27	G	310	CLA	CBA-CGA-O2A-C1
27	K	311	CLA	C3-C5-C6-C7
30	b	848	A86	C39-C38-O4-C34
27	M	313	CLA	C4-C3-C5-C6
27	a	849	CLA	C4-C3-C5-C6
27	a	850	CLA	C4-C3-C5-C6
27	b	830	CLA	C4-C3-C5-C6
34	b	832	PQN	C14-C13-C15-C16
27	B	309	CLA	C2-C3-C5-C6
27	G	311	CLA	C2-C3-C5-C6
27	a	850	CLA	C2-C3-C5-C6
27	b	844	CLA	C2-C3-C5-C6
27	L	308	CLA	CBD-CGD-O2D-CED
27	a	808	CLA	CBD-CGD-O2D-CED
27	a	838	CLA	CBD-CGD-O2D-CED
27	a	839	CLA	CBD-CGD-O2D-CED
27	b	803	CLA	CBD-CGD-O2D-CED
27	A	208	CLA	C2A-CAA-CBA-CGA
27	B	306	CLA	C2A-CAA-CBA-CGA
27	C	310	CLA	C2A-CAA-CBA-CGA
27	F	311	CLA	C2A-CAA-CBA-CGA
27	F	317	CLA	C2A-CAA-CBA-CGA
27	I	305	CLA	C2A-CAA-CBA-CGA
27	J	309	CLA	C2A-CAA-CBA-CGA
27	J	315	CLA	C2A-CAA-CBA-CGA
27	K	313	CLA	C2A-CAA-CBA-CGA
27	K	318	CLA	C2A-CAA-CBA-CGA
27	a	843	CLA	C2A-CAA-CBA-CGA
27	D	216	CLA	C2A-CAA-CBA-CGA
27	b	809	CLA	C2A-CAA-CBA-CGA
27	b	829	CLA	C2A-CAA-CBA-CGA
27	b	845	CLA	O1A-CGA-O2A-C1
29	a	852	LMG	C31-C32-C33-C34
31	E	318	LHG	C24-C25-C26-C27
31	M	320	LHG	C24-C25-C26-C27
31	a	801	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
31	a	802	LHG	C24-C25-C26-C27
31	a	833	LHG	C24-C25-C26-C27
31	a	837	LHG	C24-C25-C26-C27
31	D	201	LHG	C24-C25-C26-C27
31	b	836	LHG	C24-C25-C26-C27
27	J	310	CLA	O1A-CGA-O2A-C1
27	H	206	CLA	C3-C5-C6-C7
27	H	210	CLA	C3-C5-C6-C7
27	K	309	CLA	C3-C5-C6-C7
27	K	310	CLA	C3-C5-C6-C7
27	a	838	CLA	C3-C5-C6-C7
27	D	213	CLA	C3-C5-C6-C7
27	b	841	CLA	C3-C5-C6-C7
27	A	208	CLA	CBA-CGA-O2A-C1
27	B	308	CLA	CBA-CGA-O2A-C1
27	E	312	CLA	CBA-CGA-O2A-C1
27	F	311	CLA	CBA-CGA-O2A-C1
27	F	315	CLA	CBA-CGA-O2A-C1
27	G	316	CLA	CBA-CGA-O2A-C1
27	I	310	CLA	CBA-CGA-O2A-C1
27	I	311	CLA	CBA-CGA-O2A-C1
27	L	307	CLA	CBA-CGA-O2A-C1
27	a	805	CLA	CBA-CGA-O2A-C1
27	a	817	CLA	CBA-CGA-O2A-C1
27	a	824	CLA	CBA-CGA-O2A-C1
27	a	827	CLA	CBA-CGA-O2A-C1
27	a	840	CLA	CBA-CGA-O2A-C1
27	a	849	CLA	CBA-CGA-O2A-C1
27	a	854	CLA	CBA-CGA-O2A-C1
27	D	207	CLA	CBA-CGA-O2A-C1
27	b	822	CLA	CBA-CGA-O2A-C1
29	C	319	LMG	C29-C28-O8-C9
29	L	323	LMG	C29-C28-O8-C9
31	a	837	LHG	C24-C23-O8-C6
31	D	201	LHG	C15-C16-C17-C18
31	D	201	LHG	C30-C31-C32-C33
27	a	824	CLA	CBD-CGD-O2D-CED
27	b	827	CLA	CBD-CGD-O2D-CED
27	C	317	CLA	C4C-C3C-CAC-CBC
27	B	307	CLA	O1D-CGD-O2D-CED
27	L	315	CLA	O1D-CGD-O2D-CED
27	a	854	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	E	317	LMG	C4-C5-C6-O5
27	F	306	CLA	O1A-CGA-O2A-C1
27	G	316	CLA	O1A-CGA-O2A-C1
27	a	824	CLA	O1A-CGA-O2A-C1
27	a	849	CLA	O1A-CGA-O2A-C1
27	a	850	CLA	O1A-CGA-O2A-C1
29	M	321	LMG	O10-C28-O8-C9
27	b	816	CLA	CBA-CGA-O2A-C1
27	M	307	CLA	C2C-C3C-CAC-CBC
30	A	213	A86	O5-C38-O4-C34
26	C	303	DD6	C1-C2-C3-C4
30	B	302	A86	C1-C2-C3-C4
30	B	304	A86	C1-C2-C3-C4
30	C	302	A86	C1-C2-C3-C4
30	F	301	A86	C1-C2-C3-C4
30	F	301	A86	C3-C4-C5-C6
30	F	304	A86	C1-C2-C3-C4
30	H	201	A86	C1-C2-C3-C4
30	H	203	A86	C1-C2-C3-C4
30	I	301	A86	C1-C2-C3-C4
30	J	304	A86	C1-C2-C3-C4
30	M	302	A86	C1-C2-C3-C4
30	M	303	A86	C3-C4-C5-C6
30	M	305	A86	C24-C25-C26-C27
30	r	202	A86	C1-C2-C3-C4
30	r	202	A86	C24-C25-C26-C27
30	b	848	A86	C24-C25-C26-C27
30	C	304	A86	O5-C38-O4-C34
30	r	202	A86	C39-C38-O4-C34
27	A	207	CLA	CBD-CGD-O2D-CED
27	G	308	CLA	CBD-CGD-O2D-CED
27	I	309	CLA	CBD-CGD-O2D-CED
27	J	308	CLA	CBD-CGD-O2D-CED
27	a	807	CLA	CBD-CGD-O2D-CED
27	a	826	CLA	CBD-CGD-O2D-CED
27	a	850	CLA	CBD-CGD-O2D-CED
27	a	855	CLA	CBD-CGD-O2D-CED
27	D	208	CLA	CBD-CGD-O2D-CED
27	B	312	CLA	O1D-CGD-O2D-CED
27	G	317	CLA	O1D-CGD-O2D-CED
27	a	823	CLA	O1D-CGD-O2D-CED
31	a	837	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	I	307	CLA	C3-C5-C6-C7
27	a	803	CLA	C3-C5-C6-C7
27	b	815	CLA	C3-C5-C6-C7
27	B	311	CLA	CBA-CGA-O2A-C1
27	E	311	CLA	CBA-CGA-O2A-C1
27	F	305	CLA	CBA-CGA-O2A-C1
27	F	306	CLA	CBA-CGA-O2A-C1
27	a	843	CLA	CBA-CGA-O2A-C1
27	b	845	CLA	CBA-CGA-O2A-C1
29	A	212	LMG	C29-C28-O8-C9
31	a	802	LHG	C24-C23-O8-C6
27	I	311	CLA	O1A-CGA-O2A-C1
27	J	314	CLA	O1A-CGA-O2A-C1
27	L	307	CLA	O1A-CGA-O2A-C1
29	A	212	LMG	O6-C5-C6-O5
27	L	309	CLA	O1D-CGD-O2D-CED
31	b	836	LHG	C8-C7-O7-C5
30	r	202	A86	O5-C38-O4-C34
27	K	312	CLA	CBD-CGD-O2D-CED
27	a	814	CLA	CBD-CGD-O2D-CED
27	b	819	CLA	CBD-CGD-O2D-CED
27	b	849	CLA	CBD-CGD-O2D-CED
29	I	319	LMG	C14-C15-C16-C17
31	M	320	LHG	C28-C29-C30-C31
31	a	801	LHG	C28-C29-C30-C31
31	D	201	LHG	C13-C14-C15-C16
31	b	836	LHG	C27-C28-C29-C30
27	E	311	CLA	O1A-CGA-O2A-C1
27	a	805	CLA	O1A-CGA-O2A-C1
29	A	212	LMG	C17-C18-C19-C20
29	C	319	LMG	C13-C14-C15-C16
29	L	323	LMG	C34-C35-C36-C37
29	l	201	LMG	C21-C22-C23-C24
31	K	320	LHG	C10-C11-C12-C13
31	a	802	LHG	C16-C17-C18-C19
31	a	802	LHG	C30-C31-C32-C33
31	a	802	LHG	C34-C35-C36-C37
31	D	201	LHG	C11-C12-C13-C14
27	J	309	CLA	O1D-CGD-O2D-CED
29	C	319	LMG	C11-C12-C13-C14
31	b	836	LHG	C13-C14-C15-C16
27	K	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	a	849	CLA	CBD-CGD-O2D-CED
27	B	311	CLA	C3-C5-C6-C7
27	M	310	CLA	C3-C5-C6-C7
27	a	850	CLA	CBA-CGA-O2A-C1
27	E	308	CLA	O1D-CGD-O2D-CED
29	A	214	LMG	O6-C5-C6-O5
31	b	836	LHG	O9-C7-O7-C5
28	I	312	KC1	CAA-CBA-CGA-O2A
29	J	317	LMG	C13-C14-C15-C16
29	L	323	LMG	C11-C12-C13-C14
31	a	801	LHG	C17-C18-C19-C20
27	B	311	CLA	O1A-CGA-O2A-C1
27	F	305	CLA	O1A-CGA-O2A-C1
27	F	311	CLA	O1A-CGA-O2A-C1
27	a	827	CLA	O1A-CGA-O2A-C1
27	a	843	CLA	O1A-CGA-O2A-C1
27	D	207	CLA	O1A-CGA-O2A-C1
27	b	822	CLA	O1A-CGA-O2A-C1
29	A	212	LMG	O10-C28-O8-C9
29	L	323	LMG	O10-C28-O8-C9
31	a	802	LHG	O10-C23-O8-C6
27	J	313	CLA	CBA-CGA-O2A-C1
30	I	303	A86	C39-C38-O4-C34
27	b	816	CLA	O1A-CGA-O2A-C1
27	A	207	CLA	C15-C16-C17-C18
29	E	317	LMG	O6-C5-C6-O5
27	A	207	CLA	C4-C3-C5-C6
27	B	311	CLA	C4-C3-C5-C6
27	H	206	CLA	C4-C3-C5-C6
27	H	209	CLA	C4-C3-C5-C6
27	J	309	CLA	C4-C3-C5-C6
27	J	311	CLA	C4-C3-C5-C6
27	J	314	CLA	C4-C3-C5-C6
27	K	309	CLA	C4-C3-C5-C6
27	K	314	CLA	C4-C3-C5-C6
27	M	310	CLA	C4-C3-C5-C6
27	a	827	CLA	C4-C3-C5-C6
27	a	843	CLA	C4-C3-C5-C6
27	D	207	CLA	C4-C3-C5-C6
27	A	207	CLA	C2-C3-C5-C6
27	B	311	CLA	C2-C3-C5-C6
27	H	206	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	H	209	CLA	C2-C3-C5-C6
27	J	309	CLA	C2-C3-C5-C6
27	J	311	CLA	C2-C3-C5-C6
27	J	314	CLA	C2-C3-C5-C6
27	K	309	CLA	C2-C3-C5-C6
27	K	314	CLA	C2-C3-C5-C6
27	M	310	CLA	C2-C3-C5-C6
27	M	313	CLA	C2-C3-C5-C6
27	a	827	CLA	C2-C3-C5-C6
27	a	843	CLA	C2-C3-C5-C6
27	D	207	CLA	C2-C3-C5-C6
27	b	830	CLA	C2-C3-C5-C6
27	l	206	CLA	CBD-CGD-O2D-CED
27	A	210	CLA	C2A-CAA-CBA-CGA
27	F	306	CLA	C2A-CAA-CBA-CGA
27	G	310	CLA	C2A-CAA-CBA-CGA
27	K	314	CLA	C2A-CAA-CBA-CGA
27	b	820	CLA	C2A-CAA-CBA-CGA
27	E	314	CLA	O1D-CGD-O2D-CED
27	L	315	CLA	C2C-C3C-CAC-CBC
27	B	308	CLA	O1A-CGA-O2A-C1
27	a	854	CLA	O1A-CGA-O2A-C1
29	I	319	LMG	O6-C1-O1-C7
27	L	321	CLA	O1D-CGD-O2D-CED
27	L	311	CLA	C2C-C3C-CAC-CBC
27	M	317	CLA	C2C-C3C-CAC-CBC
30	J	301	A86	O5-C38-O4-C34
27	b	843	CLA	CBA-CGA-O2A-C1
28	L	322	KC1	C2C-C3C-CAC-CBC
31	M	320	LHG	C30-C31-C32-C33
27	C	312	CLA	CBD-CGD-O2D-CED
27	b	825	CLA	CBD-CGD-O2D-CED
27	C	318	CLA	O1D-CGD-O2D-CED
29	j	103	LMG	O6-C5-C6-O5
37	b	835	DGD	O6E-C5E-C6E-O5E
27	M	316	CLA	C5-C6-C7-C8
29	J	317	LMG	C17-C18-C19-C20
27	E	312	CLA	O1D-CGD-O2D-CED
27	F	310	CLA	O1D-CGD-O2D-CED
27	G	307	CLA	O1D-CGD-O2D-CED
27	G	309	CLA	O1D-CGD-O2D-CED
28	J	306	KC1	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	L	314	KC1	CAA-CBA-CGA-O2A
31	B	315	LHG	C8-C7-O7-C5
27	H	204	CLA	C4C-C3C-CAC-CBC
29	E	317	LMG	C16-C17-C18-C19
31	M	320	LHG	C11-C10-C9-C8
27	G	306	CLA	O1D-CGD-O2D-CED
27	K	314	CLA	O1D-CGD-O2D-CED
27	b	816	CLA	O1D-CGD-O2D-CED
28	H	211	KC1	O1D-CGD-O2D-CED
27	a	819	CLA	CBD-CGD-O2D-CED
31	a	802	LHG	C26-C27-C28-C29
31	B	315	LHG	C1-C2-C3-O3
31	H	215	LHG	C1-C2-C3-O3
31	a	837	LHG	C1-C2-C3-O3
31	D	201	LHG	C1-C2-C3-O3
29	A	212	LMG	C4-C5-C6-O5
29	j	103	LMG	C4-C5-C6-O5
27	b	843	CLA	O1A-CGA-O2A-C1
27	H	212	CLA	C3-C5-C6-C7
27	L	307	CLA	C3-C5-C6-C7
27	b	821	CLA	C3-C5-C6-C7
27	K	317	CLA	O1D-CGD-O2D-CED
27	b	823	CLA	O1D-CGD-O2D-CED
27	E	308	CLA	CBA-CGA-O2A-C1
27	G	308	CLA	CBA-CGA-O2A-C1
27	G	317	CLA	CBA-CGA-O2A-C1
27	J	308	CLA	CBA-CGA-O2A-C1
27	J	309	CLA	CBA-CGA-O2A-C1
27	K	314	CLA	CBA-CGA-O2A-C1
27	K	316	CLA	CBA-CGA-O2A-C1
27	a	808	CLA	CBA-CGA-O2A-C1
27	a	826	CLA	CBA-CGA-O2A-C1
27	b	801	CLA	CBA-CGA-O2A-C1
29	l	201	LMG	C29-C28-O8-C9
31	E	318	LHG	C24-C23-O8-C6
31	a	801	LHG	C24-C23-O8-C6
27	M	317	CLA	CBD-CGD-O2D-CED
29	C	301	LMG	C4-C5-C6-O5
27	M	312	CLA	O1D-CGD-O2D-CED
26	J	302	DD6	C1-C2-C3-C4
26	L	301	DD6	C1-C2-C3-C4
30	M	303	A86	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
30	b	848	A86	C1-C2-C3-C4
27	M	318	CLA	C2C-C3C-CAC-CBC
30	H	203	A86	O5-C38-O4-C34
27	a	815	CLA	C10-C11-C12-C13
29	J	317	LMG	C11-C12-C13-C14
31	E	318	LHG	C34-C35-C36-C37
28	A	209	KC1	CAA-CBA-CGA-O1A
28	L	314	KC1	CAA-CBA-CGA-O1A
27	F	315	CLA	C5-C6-C7-C8
27	I	311	CLA	C5-C6-C7-C8
27	I	311	CLA	C8-C10-C11-C12
27	a	812	CLA	C15-C16-C17-C18
27	a	815	CLA	C13-C15-C16-C17
27	a	827	CLA	C8-C10-C11-C12
27	a	842	CLA	C15-C16-C17-C18
27	a	843	CLA	C5-C6-C7-C8
31	H	215	LHG	O2-C2-C3-O3
31	a	801	LHG	O2-C2-C3-O3
29	l	201	LMG	C2-C1-O1-C7
27	G	317	CLA	O1A-CGA-O2A-C1
27	J	308	CLA	O1A-CGA-O2A-C1
27	J	309	CLA	O1A-CGA-O2A-C1
27	a	826	CLA	O1A-CGA-O2A-C1
27	a	849	CLA	C2-C3-C5-C6
27	A	204	CLA	C6-C7-C8-C9
27	A	205	CLA	C6-C7-C8-C9
27	A	205	CLA	C11-C12-C13-C14
27	B	308	CLA	C11-C12-C13-C14
27	C	311	CLA	C11-C10-C8-C9
27	H	205	CLA	C11-C12-C13-C14
27	H	206	CLA	C6-C7-C8-C9
27	H	212	CLA	C6-C7-C8-C9
27	H	212	CLA	C14-C13-C15-C16
27	I	311	CLA	C11-C12-C13-C14
27	J	307	CLA	C6-C7-C8-C9
27	J	311	CLA	C6-C7-C8-C9
27	J	312	CLA	C11-C12-C13-C14
27	K	309	CLA	C14-C13-C15-C16
27	K	312	CLA	C6-C7-C8-C9
27	K	314	CLA	C6-C7-C8-C9
27	K	314	CLA	C14-C13-C15-C16
27	K	316	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	L	308	CLA	C11-C10-C8-C9
27	L	309	CLA	C11-C10-C8-C9
27	L	309	CLA	C11-C12-C13-C14
27	L	310	CLA	C6-C7-C8-C9
27	L	310	CLA	C14-C13-C15-C16
27	M	307	CLA	C11-C10-C8-C9
27	M	308	CLA	C6-C7-C8-C9
27	M	313	CLA	C6-C7-C8-C9
27	a	815	CLA	C6-C7-C8-C9
27	a	815	CLA	C11-C12-C13-C14
27	a	815	CLA	C14-C13-C15-C16
27	a	856	CLA	C6-C7-C8-C9
27	i	101	CLA	C11-C10-C8-C9
27	D	207	CLA	C11-C10-C8-C9
27	D	208	CLA	C11-C10-C8-C9
27	b	804	CLA	C11-C12-C13-C14
27	b	838	CLA	C11-C10-C8-C9
27	b	844	CLA	C11-C10-C8-C9
27	a	813	CLA	O1D-CGD-O2D-CED
27	a	830	CLA	O1D-CGD-O2D-CED
27	a	843	CLA	O1D-CGD-O2D-CED
28	K	315	KC1	O1D-CGD-O2D-CED
27	a	829	CLA	CBD-CGD-O2D-CED
27	M	316	CLA	C2A-CAA-CBA-CGA
26	A	201	DD6	C-C1-C24-C25
26	C	303	DD6	C12-C11-C13-C14
26	E	303	DD6	C12-C11-C13-C14
26	F	303	DD6	C12-C11-C13-C14
26	F	303	DD6	C7-C6-C8-C9
26	H	202	DD6	C12-C11-C13-C14
26	L	301	DD6	C12-C11-C13-C14
30	B	301	A86	C-C1-C24-C25
30	J	316	A86	C-C1-C24-C25
30	M	303	A86	C-C1-C24-C25
30	b	848	A86	C7-C6-C8-C9
32	a	853	BCR	C11-C12-C13-C35
32	a	853	BCR	C36-C18-C19-C20
32	j	101	BCR	C37-C22-C23-C24
32	j	105	BCR	C36-C18-C19-C20
32	m	102	BCR	C37-C22-C23-C24
32	b	834	BCR	C7-C8-C9-C34
32	b	840	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
26	A	201	DD6	C2-C1-C24-C25
26	A	201	DD6	C10-C11-C13-C14
26	C	303	DD6	C10-C11-C13-C14
26	E	303	DD6	C10-C11-C13-C14
26	H	202	DD6	C10-C11-C13-C14
26	L	301	DD6	C10-C11-C13-C14
26	L	301	DD6	C5-C6-C8-C9
30	B	301	A86	C2-C1-C24-C25
30	J	316	A86	C2-C1-C24-C25
30	M	303	A86	C2-C1-C24-C25
30	b	848	A86	C5-C6-C8-C9
32	a	836	BCR	C21-C22-C23-C24
32	a	853	BCR	C11-C12-C13-C14
32	j	101	BCR	C21-C22-C23-C24
32	m	102	BCR	C21-C22-C23-C24
32	b	840	BCR	C7-C8-C9-C10
28	H	211	KC1	C2C-C3C-CAC-CBC
31	a	802	LHG	C9-C10-C11-C12
29	C	319	LMG	C28-C29-C30-C31
29	D	202	LMG	C28-C29-C30-C31
27	K	316	CLA	O1A-CGA-O2A-C1
27	A	204	CLA	C15-C16-C17-C18
27	C	311	CLA	C10-C11-C12-C13
27	H	205	CLA	C8-C10-C11-C12
27	H	212	CLA	C10-C11-C12-C13
27	I	308	CLA	C13-C15-C16-C17
27	K	314	CLA	C5-C6-C7-C8
27	L	309	CLA	C10-C11-C12-C13
27	b	812	CLA	C10-C11-C12-C13
33	J	318	SQD	C28-C29-C30-C31
29	A	214	LMG	C4-C5-C6-O5
28	I	312	KC1	CAA-CBA-CGA-O1A
28	J	306	KC1	CAA-CBA-CGA-O2A
28	M	314	KC1	CAA-CBA-CGA-O1A
27	I	307	CLA	C2C-C3C-CAC-CBC
27	I	313	CLA	C4C-C3C-CAC-CBC
27	I	313	CLA	O1D-CGD-O2D-CED
27	A	208	CLA	C3-C5-C6-C7
27	H	210	CLA	C8-C10-C11-C12
27	F	310	CLA	CBA-CGA-O2A-C1
27	H	213	CLA	CBA-CGA-O2A-C1
29	D	202	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
27	K	309	CLA	C13-C15-C16-C17
27	M	308	CLA	C8-C10-C11-C12
27	M	313	CLA	C10-C11-C12-C13
27	a	856	CLA	C5-C6-C7-C8
27	b	803	CLA	C13-C15-C16-C17
27	b	804	CLA	C10-C11-C12-C13
29	j	103	LMG	C10-C11-C12-C13
27	L	308	CLA	C2C-C3C-CAC-CBC
31	M	320	LHG	C32-C33-C34-C35
27	A	205	CLA	C15-C16-C17-C18
27	E	311	CLA	C5-C6-C7-C8
27	E	311	CLA	C15-C16-C17-C18
27	F	308	CLA	C8-C10-C11-C12
27	F	315	CLA	C8-C10-C11-C12
27	G	309	CLA	C15-C16-C17-C18
27	M	309	CLA	C10-C11-C12-C13
27	a	808	CLA	C8-C10-C11-C12
27	a	815	CLA	C15-C16-C17-C18
27	a	838	CLA	C8-C10-C11-C12
27	a	840	CLA	C5-C6-C7-C8
27	l	204	CLA	C8-C10-C11-C12
27	D	208	CLA	C8-C10-C11-C12
27	D	213	CLA	C8-C10-C11-C12
27	b	808	CLA	C10-C11-C12-C13
27	b	824	CLA	C5-C6-C7-C8
27	b	825	CLA	C13-C15-C16-C17
27	b	850	CLA	C13-C15-C16-C17
31	D	201	LHG	C26-C27-C28-C29
27	b	818	CLA	O1D-CGD-O2D-CED
31	B	315	LHG	O1-C1-C2-O2
33	J	318	SQD	O5-C1-O6-C44
33	J	318	SQD	O6-C1-O5-C5
29	J	317	LMG	C10-C11-C12-C13
29	a	852	LMG	C10-C11-C12-C13
29	l	201	LMG	C10-C11-C12-C13
31	B	315	LHG	C7-C8-C9-C10
31	b	836	LHG	C7-C8-C9-C10
30	K	305	A86	C39-C38-O4-C34
27	F	306	CLA	CBD-CGD-O2D-CED
27	b	824	CLA	CBD-CGD-O2D-CED
27	I	316	CLA	O1D-CGD-O2D-CED
27	A	204	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	E	308	CLA	C5-C6-C7-C8
27	E	311	CLA	C8-C10-C11-C12
27	H	206	CLA	C8-C10-C11-C12
27	a	815	CLA	C8-C10-C11-C12
27	a	842	CLA	C13-C15-C16-C17
27	a	811	CLA	CBA-CGA-O2A-C1
27	a	855	CLA	CBA-CGA-O2A-C1
27	a	846	CLA	O1D-CGD-O2D-CED
27	b	817	CLA	O1D-CGD-O2D-CED
31	B	315	LHG	O9-C7-O7-C5
28	L	322	KC1	CAA-CBA-CGA-O1A
27	M	307	CLA	C4C-C3C-CAC-CBC
29	A	214	LMG	C12-C13-C14-C15
27	C	307	CLA	C13-C15-C16-C17
27	b	843	CLA	C5-C6-C7-C8
27	b	844	CLA	C10-C11-C12-C13
27	b	846	CLA	C8-C10-C11-C12
29	A	214	LMG	C28-C29-C30-C31
29	C	301	LMG	C28-C29-C30-C31
27	D	216	CLA	CBA-CGA-O2A-C1
27	K	310	CLA	C2C-C3C-CAC-CBC
27	H	212	CLA	C15-C16-C17-C18
27	b	806	CLA	C15-C16-C17-C18
27	L	311	CLA	O1D-CGD-O2D-CED
27	A	204	CLA	C6-C7-C8-C10
27	A	207	CLA	C6-C7-C8-C10
27	B	306	CLA	C11-C12-C13-C15
27	C	309	CLA	C11-C10-C8-C7
27	G	309	CLA	C11-C12-C13-C15
27	J	311	CLA	C12-C13-C15-C16
27	L	312	CLA	C6-C7-C8-C10
27	L	313	CLA	C12-C13-C15-C16
27	M	309	CLA	C11-C10-C8-C7
27	a	803	CLA	C11-C12-C13-C15
27	a	855	CLA	C12-C13-C15-C16
27	a	856	CLA	C6-C7-C8-C10
27	b	801	CLA	C11-C10-C8-C7
27	b	804	CLA	C12-C13-C15-C16
27	E	308	CLA	O1A-CGA-O2A-C1
27	a	808	CLA	O1A-CGA-O2A-C1
27	b	801	CLA	O1A-CGA-O2A-C1
29	l	201	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
31	E	318	LHG	O10-C23-O8-C6
26	A	201	DD6	C3-C4-C5-C6
26	C	303	DD6	C3-C4-C5-C6
26	J	302	DD6	C11-C10-C9-C8
30	G	302	A86	C1-C2-C3-C4
30	J	316	A86	C1-C2-C3-C4
27	M	308	CLA	CBA-CGA-O2A-C1
27	F	305	CLA	C2A-CAA-CBA-CGA
27	F	310	CLA	C2A-CAA-CBA-CGA
27	L	319	CLA	C2A-CAA-CBA-CGA
27	M	310	CLA	C2A-CAA-CBA-CGA
27	M	317	CLA	C2A-CAA-CBA-CGA
27	C	317	CLA	O1D-CGD-O2D-CED
27	K	311	CLA	O1D-CGD-O2D-CED
27	a	825	CLA	O1D-CGD-O2D-CED
27	a	844	CLA	O1D-CGD-O2D-CED
27	b	831	CLA	O1D-CGD-O2D-CED
27	b	838	CLA	O1D-CGD-O2D-CED
27	H	206	CLA	C5-C6-C7-C8
27	H	210	CLA	C5-C6-C7-C8
27	a	803	CLA	C15-C16-C17-C18
27	a	817	CLA	C5-C6-C7-C8
27	a	829	CLA	C13-C15-C16-C17
27	a	838	CLA	C13-C15-C16-C17
27	a	843	CLA	C15-C16-C17-C18
27	a	845	CLA	C5-C6-C7-C8
27	b	818	CLA	C8-C10-C11-C12
27	b	821	CLA	C13-C15-C16-C17
27	b	830	CLA	C13-C15-C16-C17
28	M	314	KC1	C2C-C3C-CAC-CBC
30	B	305	A86	O5-C38-O4-C34
27	G	308	CLA	O1A-CGA-O2A-C1
31	a	801	LHG	O10-C23-O8-C6
27	F	314	CLA	CBD-CGD-O2D-CED
27	K	313	CLA	CBD-CGD-O2D-CED
27	b	844	CLA	CBD-CGD-O2D-CED
27	b	812	CLA	C8-C10-C11-C12
28	L	314	KC1	C2C-C3C-CAC-CBC
31	E	318	LHG	C10-C11-C12-C13
31	K	320	LHG	C24-C25-C26-C27
31	B	315	LHG	O2-C2-C3-O3
31	I	318	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	J	313	CLA	O1A-CGA-O2A-C1
27	F	308	CLA	C13-C15-C16-C17
27	B	306	CLA	C5-C6-C7-C8
27	E	311	CLA	C10-C11-C12-C13
27	E	314	CLA	C5-C6-C7-C8
27	H	205	CLA	C13-C15-C16-C17
27	H	212	CLA	C13-C15-C16-C17
27	K	314	CLA	C13-C15-C16-C17
27	K	316	CLA	C10-C11-C12-C13
27	D	207	CLA	C8-C10-C11-C12
27	D	213	CLA	C10-C11-C12-C13
27	L	313	CLA	CBA-CGA-O2A-C1
27	b	818	CLA	CBA-CGA-O2A-C1
27	K	314	CLA	O1A-CGA-O2A-C1
29	D	202	LMG	O10-C28-O8-C9
27	M	318	CLA	CBA-CGA-O2A-C1
33	J	318	SQD	C23-C24-C25-C26
29	C	301	LMG	C11-C12-C13-C14
27	C	312	CLA	C10-C11-C12-C13
27	G	309	CLA	C5-C6-C7-C8
27	J	309	CLA	C10-C11-C12-C13
27	L	313	CLA	C8-C10-C11-C12
27	M	309	CLA	C8-C10-C11-C12
27	b	804	CLA	C8-C10-C11-C12
27	b	830	CLA	C5-C6-C7-C8
27	M	317	CLA	C4C-C3C-CAC-CBC
27	G	312	CLA	O1D-CGD-O2D-CED
27	b	806	CLA	O1D-CGD-O2D-CED
27	a	828	CLA	CBD-CGD-O2D-CED
27	b	828	CLA	CBD-CGD-O2D-CED
27	F	310	CLA	O1A-CGA-O2A-C1
31	D	201	LHG	C8-C7-O7-C5
27	A	204	CLA	C5-C6-C7-C8
27	A	205	CLA	C5-C6-C7-C8
27	A	205	CLA	C10-C11-C12-C13
27	G	309	CLA	C10-C11-C12-C13
27	J	309	CLA	C8-C10-C11-C12
27	J	311	CLA	C8-C10-C11-C12
27	K	309	CLA	C10-C11-C12-C13
27	M	313	CLA	C13-C15-C16-C17
27	a	845	CLA	C15-C16-C17-C18
27	b	821	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	B	315	LHG	C3-O3-P-O6
31	B	315	LHG	C4-O6-P-O3
31	E	318	LHG	C4-O6-P-O3
31	I	318	LHG	C3-O3-P-O6
31	I	318	LHG	C4-O6-P-O3
31	a	801	LHG	C3-O3-P-O6
31	a	802	LHG	C3-O3-P-O6
31	a	802	LHG	C4-O6-P-O3
31	D	201	LHG	C4-O6-P-O3
27	f	301	CLA	C3-C5-C6-C7
31	a	833	LHG	C11-C12-C13-C14
27	a	838	CLA	CBA-CGA-O2A-C1
27	b	809	CLA	CBA-CGA-O2A-C1
27	b	822	CLA	CBD-CGD-O2D-CED
27	I	311	CLA	C15-C16-C17-C18
27	H	212	CLA	O1D-CGD-O2D-CED
27	a	808	CLA	O1D-CGD-O2D-CED
31	I	318	LHG	C1-C2-C3-O3
31	D	201	LHG	O9-C7-O7-C5
27	G	309	CLA	C4-C3-C5-C6
30	L	304	A86	C39-C38-O4-C34
27	a	855	CLA	O1A-CGA-O2A-C1
27	K	313	CLA	C2C-C3C-CAC-CBC
28	K	308	KC1	C2C-C3C-CAC-CBC
27	a	825	CLA	C2A-CAA-CBA-CGA
27	b	838	CLA	C2A-CAA-CBA-CGA
27	b	839	CLA	C2A-CAA-CBA-CGA
27	M	308	CLA	C3-C5-C6-C7
28	H	211	KC1	CAA-CBA-CGA-O2A
27	J	312	CLA	CBA-CGA-O2A-C1
27	K	309	CLA	CBA-CGA-O2A-C1
27	K	312	CLA	CBA-CGA-O2A-C1
27	f	302	CLA	CBA-CGA-O2A-C1
27	i	101	CLA	CBA-CGA-O2A-C1
27	D	213	CLA	CBA-CGA-O2A-C1
27	b	831	CLA	CBA-CGA-O2A-C1
27	b	812	CLA	CBD-CGD-O2D-CED
27	M	318	CLA	C4C-C3C-CAC-CBC
26	C	303	DD6	C24-C25-C26-C27
26	L	301	DD6	C11-C10-C9-C8
26	L	301	DD6	C3-C4-C5-C6
30	B	301	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	J	316	A86	C24-C25-C26-C27
30	K	302	A86	C11-C10-C9-C8
32	a	853	BCR	C9-C10-C11-C12
31	B	315	LHG	C15-C16-C17-C18
31	E	318	LHG	C25-C26-C27-C28
31	M	320	LHG	C18-C19-C20-C21
31	b	836	LHG	C14-C15-C16-C17
27	L	308	CLA	O1D-CGD-O2D-CED
27	E	315	CLA	CBD-CGD-O2D-CED
27	K	314	CLA	C10-C11-C12-C13
27	K	316	CLA	C13-C15-C16-C17
27	a	805	CLA	C10-C11-C12-C13
29	C	301	LMG	O6-C5-C6-O5
29	A	214	LMG	C16-C17-C18-C19
29	E	317	LMG	C11-C12-C13-C14
29	J	317	LMG	C15-C16-C17-C18
29	j	103	LMG	C30-C31-C32-C33
29	D	202	LMG	C35-C36-C37-C38
31	M	320	LHG	C10-C11-C12-C13
31	M	320	LHG	C17-C18-C19-C20
31	a	801	LHG	C29-C30-C31-C32
31	j	102	LHG	C30-C31-C32-C33
31	D	201	LHG	C18-C19-C20-C21
31	b	836	LHG	C34-C35-C36-C37
37	b	835	DGD	C8A-C9A-CAA-CBA
27	a	811	CLA	O1A-CGA-O2A-C1
27	H	213	CLA	O1D-CGD-O2D-CED
27	a	838	CLA	O1D-CGD-O2D-CED
27	b	803	CLA	O1D-CGD-O2D-CED
28	H	211	KC1	C2A-CAA-CBA-CGA
28	L	322	KC1	C2A-CAA-CBA-CGA
28	M	314	KC1	C2A-CAA-CBA-CGA
27	A	205	CLA	C16-C17-C18-C20
27	a	803	CLA	C16-C17-C18-C19
27	a	827	CLA	C11-C12-C13-C14
27	b	843	CLA	C16-C17-C18-C20
29	A	214	LMG	C20-C21-C22-C23
29	C	319	LMG	C17-C18-C19-C20
29	L	323	LMG	C32-C33-C34-C35
31	E	318	LHG	C17-C18-C19-C20
31	I	318	LHG	C13-C14-C15-C16
31	K	320	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	H	215	LHG	C6-C5-O7-C7
31	a	802	LHG	C4-C5-O7-C7
27	C	309	CLA	O1D-CGD-O2D-CED
27	a	824	CLA	O1D-CGD-O2D-CED
27	a	803	CLA	C8-C10-C11-C12
27	a	829	CLA	C15-C16-C17-C18
29	E	317	LMG	C10-C11-C12-C13
27	A	211	CLA	CBD-CGD-O2D-CED
27	I	307	CLA	CBD-CGD-O2D-CED
29	A	212	LMG	C38-C39-C40-C41
29	I	319	LMG	C11-C12-C13-C14
29	J	317	LMG	C32-C33-C34-C35
31	a	833	LHG	C11-C10-C9-C8
31	b	836	LHG	C30-C31-C32-C33
37	b	835	DGD	C6A-C7A-C8A-C9A
37	b	835	DGD	C6B-C7B-C8B-C9B
27	b	827	CLA	O1D-CGD-O2D-CED
31	a	802	LHG	C5-C4-O6-P
31	D	201	LHG	C2-C3-O3-P
27	H	213	CLA	O1A-CGA-O2A-C1
29	A	212	LMG	C19-C20-C21-C22
29	A	214	LMG	C11-C12-C13-C14
29	A	214	LMG	C18-C19-C20-C21
29	C	319	LMG	C20-C21-C22-C23
31	H	215	LHG	C15-C16-C17-C18
37	b	835	DGD	CEB-CFB-CGB-CHB
27	G	306	CLA	CBA-CGA-O2A-C1
31	D	201	LHG	O2-C2-C3-O3
31	b	836	LHG	O2-C2-C3-O3
29	l	201	LMG	C20-C21-C22-C23
30	b	848	A86	O5-C38-O4-C34
31	E	318	LHG	C14-C15-C16-C17
31	K	320	LHG	C11-C12-C13-C14
31	a	833	LHG	C29-C30-C31-C32
31	b	836	LHG	C23-C24-C25-C26
27	a	839	CLA	O1D-CGD-O2D-CED
29	A	214	LMG	C2-C1-O1-C7
29	M	321	LMG	O7-C8-C9-O8
27	l	203	CLA	CBA-CGA-O2A-C1
29	A	214	LMG	C13-C14-C15-C16
29	C	319	LMG	C29-C30-C31-C32
29	D	202	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	H	215	LHG	C11-C12-C13-C14
31	a	801	LHG	C11-C10-C9-C8
31	b	836	LHG	C26-C27-C28-C29
37	b	835	DGD	CAB-CBB-CCB-CDB
27	K	312	CLA	O1A-CGA-O2A-C1
27	a	838	CLA	O1A-CGA-O2A-C1
27	C	311	CLA	C11-C12-C13-C15
27	F	311	CLA	C11-C12-C13-C14
27	I	306	CLA	C16-C17-C18-C19
27	I	311	CLA	C16-C17-C18-C19
27	a	856	CLA	C16-C17-C18-C19
28	L	322	KC1	O1D-CGD-O2D-CED
27	K	311	CLA	C4-C3-C5-C6
27	b	847	CLA	C4-C3-C5-C6
29	L	323	LMG	C18-C19-C20-C21
31	K	320	LHG	C11-C10-C9-C8
31	a	801	LHG	C11-C12-C13-C14
31	a	802	LHG	C12-C13-C14-C15
31	a	802	LHG	C31-C32-C33-C34
31	a	833	LHG	C26-C27-C28-C29
27	A	205	CLA	C14-C13-C15-C16
27	A	207	CLA	C6-C7-C8-C9
27	A	207	CLA	C11-C10-C8-C9
27	E	308	CLA	C6-C7-C8-C9
27	K	309	CLA	C11-C12-C13-C14
27	M	309	CLA	C6-C7-C8-C9
27	a	809	CLA	C14-C13-C15-C16
27	a	817	CLA	C11-C12-C13-C14
27	a	849	CLA	C11-C10-C8-C9
27	b	807	CLA	C14-C13-C15-C16
27	b	844	CLA	C14-C13-C15-C16
27	a	807	CLA	O1D-CGD-O2D-CED
29	A	212	LMG	C28-C29-C30-C31
28	L	322	KC1	C4C-C3C-CAC-CBC
29	J	317	LMG	C20-C21-C22-C23
29	a	852	LMG	C30-C31-C32-C33
31	B	315	LHG	C26-C27-C28-C29
31	E	318	LHG	C9-C10-C11-C12
31	a	801	LHG	C33-C34-C35-C36
31	a	833	LHG	C14-C15-C16-C17
31	a	833	LHG	C31-C32-C33-C34
31	a	837	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	j	102	LHG	C10-C11-C12-C13
31	D	201	LHG	C11-C10-C9-C8
27	I	311	CLA	C13-C15-C16-C17
27	J	314	CLA	C5-C6-C7-C8
27	b	846	CLA	C13-C15-C16-C17
27	J	313	CLA	C2A-CAA-CBA-CGA
27	a	810	CLA	C2A-CAA-CBA-CGA
27	D	209	CLA	C2A-CAA-CBA-CGA
27	D	210	CLA	C2A-CAA-CBA-CGA
27	b	812	CLA	C2A-CAA-CBA-CGA
27	b	843	CLA	C2A-CAA-CBA-CGA
27	L	313	CLA	O1A-CGA-O2A-C1
27	M	308	CLA	O1A-CGA-O2A-C1
30	G	302	A86	C7-C6-C8-C9
30	J	316	A86	C7-C6-C8-C9
30	M	305	A86	C7-C6-C8-C9
32	a	851	BCR	C37-C22-C23-C24
27	l	203	CLA	C2C-C3C-CAC-CBC
29	L	323	LMG	C15-C16-C17-C18
31	B	315	LHG	C28-C29-C30-C31
31	j	102	LHG	C9-C10-C11-C12
31	b	836	LHG	C29-C30-C31-C32
31	I	318	LHG	O1-C1-C2-C3
31	b	836	LHG	O1-C1-C2-C3
26	F	303	DD6	C10-C11-C13-C14
26	M	306	DD6	C10-C11-C13-C14
30	G	302	A86	C5-C6-C8-C9
30	J	316	A86	C5-C6-C8-C9
32	a	851	BCR	C21-C22-C23-C24
32	b	834	BCR	C7-C8-C9-C10
29	E	317	LMG	C11-C10-O7-C8
29	L	323	LMG	C31-C32-C33-C34
29	M	321	LMG	C30-C31-C32-C33
29	a	852	LMG	C11-C12-C13-C14
31	E	318	LHG	C29-C30-C31-C32
31	H	215	LHG	C13-C14-C15-C16
37	b	835	DGD	C3A-C4A-C5A-C6A
29	A	212	LMG	C10-C11-C12-C13
29	a	852	LMG	C28-C29-C30-C31
29	A	212	LMG	C11-C12-C13-C14
29	A	212	LMG	C18-C19-C20-C21
29	A	212	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
29	C	319	LMG	C31-C32-C33-C34
29	L	323	LMG	C17-C18-C19-C20
29	M	321	LMG	C18-C19-C20-C21
31	B	315	LHG	C10-C11-C12-C13
31	M	320	LHG	C16-C17-C18-C19
31	a	801	LHG	C31-C32-C33-C34
31	a	837	LHG	C31-C32-C33-C34
31	D	201	LHG	C10-C11-C12-C13
31	D	201	LHG	C16-C17-C18-C19
33	J	318	SQD	C24-C25-C26-C27
37	b	835	DGD	C7B-C8B-C9B-CAB
27	A	204	CLA	C16-C17-C18-C19
27	E	312	CLA	C6-C7-C8-C9
27	F	311	CLA	C11-C12-C13-C15
27	G	309	CLA	C16-C17-C18-C19
27	J	311	CLA	C16-C17-C18-C20
27	K	312	CLA	C16-C17-C18-C19
27	M	313	CLA	C16-C17-C18-C20
27	a	827	CLA	C11-C12-C13-C15
27	b	823	CLA	C16-C17-C18-C19
27	b	843	CLA	C16-C17-C18-C19
27	J	314	CLA	C8-C10-C11-C12
27	a	809	CLA	C5-C6-C7-C8
27	D	208	CLA	C5-C6-C7-C8
27	b	807	CLA	C13-C15-C16-C17
27	b	838	CLA	C10-C11-C12-C13
27	b	844	CLA	C5-C6-C7-C8
27	A	207	CLA	O1D-CGD-O2D-CED
27	a	826	CLA	O1D-CGD-O2D-CED
31	I	318	LHG	C12-C13-C14-C15
31	a	802	LHG	C15-C16-C17-C18
31	j	102	LHG	C26-C27-C28-C29
31	D	201	LHG	C28-C29-C30-C31
31	b	836	LHG	C10-C11-C12-C13
27	b	830	CLA	CBD-CGD-O2D-CED
28	A	209	KC1	O1D-CGD-O2D-CED
28	I	312	KC1	C2C-C3C-CAC-CBC
29	C	319	LMG	C16-C17-C18-C19
29	C	319	LMG	C30-C31-C32-C33
29	E	317	LMG	C33-C34-C35-C36
29	j	103	LMG	C14-C15-C16-C17
31	B	315	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	a	801	LHG	C16-C17-C18-C19
31	a	833	LHG	C13-C14-C15-C16
31	a	833	LHG	C15-C16-C17-C18
37	b	835	DGD	C3B-C4B-C5B-C6B
27	H	212	CLA	C5-C6-C7-C8
27	D	213	CLA	O1A-CGA-O2A-C1
29	L	323	LMG	C19-C20-C21-C22
31	E	318	LHG	C12-C13-C14-C15
31	K	320	LHG	C13-C14-C15-C16
27	G	308	CLA	O1D-CGD-O2D-CED
27	I	309	CLA	O1D-CGD-O2D-CED
27	a	850	CLA	O1D-CGD-O2D-CED
27	a	855	CLA	O1D-CGD-O2D-CED
28	I	312	KC1	O1D-CGD-O2D-CED
27	F	317	CLA	C3A-C2A-CAA-CBA
27	G	308	CLA	C3A-C2A-CAA-CBA
27	G	310	CLA	C3A-C2A-CAA-CBA
27	H	213	CLA	C3A-C2A-CAA-CBA
27	I	305	CLA	C3A-C2A-CAA-CBA
27	J	313	CLA	C3A-C2A-CAA-CBA
27	K	310	CLA	C3A-C2A-CAA-CBA
27	K	316	CLA	C3A-C2A-CAA-CBA
27	L	316	CLA	C3A-C2A-CAA-CBA
27	a	808	CLA	C3A-C2A-CAA-CBA
27	a	826	CLA	C3A-C2A-CAA-CBA
27	a	840	CLA	C3A-C2A-CAA-CBA
27	f	303	CLA	C3A-C2A-CAA-CBA
27	D	209	CLA	C3A-C2A-CAA-CBA
27	D	211	CLA	C3A-C2A-CAA-CBA
27	b	809	CLA	C3A-C2A-CAA-CBA
27	b	811	CLA	C3A-C2A-CAA-CBA
27	b	825	CLA	C3A-C2A-CAA-CBA
27	b	826	CLA	C3A-C2A-CAA-CBA
27	b	845	CLA	C3A-C2A-CAA-CBA
37	b	835	DGD	C2G-C1G-O1G-C1A
30	D	204	A86	C1-C2-C3-C4
29	J	317	LMG	C16-C17-C18-C19
31	a	802	LHG	C27-C28-C29-C30
27	J	308	CLA	O1D-CGD-O2D-CED
27	b	809	CLA	O1A-CGA-O2A-C1
27	b	818	CLA	O1A-CGA-O2A-C1
27	A	205	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	E	312	CLA	C6-C7-C8-C10
27	I	306	CLA	C16-C17-C18-C20
27	K	312	CLA	C16-C17-C18-C20
27	a	842	CLA	C16-C17-C18-C19
31	K	320	LHG	C15-C16-C17-C18
31	E	318	LHG	C4-C5-C6-O8
31	b	836	LHG	C4-C5-C6-O8
37	b	835	DGD	O1G-C1G-C2G-C3G
29	C	319	LMG	C12-C13-C14-C15
29	L	323	LMG	C30-C31-C32-C33
29	l	201	LMG	C13-C14-C15-C16
31	b	836	LHG	C31-C32-C33-C34
27	L	310	CLA	O2A-C1-C2-C3
28	J	306	KC1	O1D-CGD-O2D-CED
29	M	321	LMG	C21-C22-C23-C24
27	a	809	CLA	C8-C10-C11-C12
27	a	839	CLA	C5-C6-C7-C8
27	K	311	CLA	CBA-CGA-O2A-C1
27	L	316	CLA	CBA-CGA-O2A-C1
27	M	307	CLA	CBA-CGA-O2A-C1
27	E	309	CLA	C2-C3-C5-C6
27	G	309	CLA	C2-C3-C5-C6
27	K	311	CLA	C2-C3-C5-C6
27	L	316	CLA	C2-C3-C5-C6
27	a	842	CLA	C2-C3-C5-C6
29	C	319	LMG	C11-C10-O7-C8
31	j	102	LHG	C8-C7-O7-C5
27	b	819	CLA	O1D-CGD-O2D-CED
27	L	311	CLA	C4C-C3C-CAC-CBC
29	I	319	LMG	C31-C32-C33-C34
27	b	823	CLA	C2A-CAA-CBA-CGA
31	b	836	LHG	O1-C1-C2-O2
27	a	856	CLA	C15-C16-C17-C18
29	J	317	LMG	C30-C31-C32-C33
31	H	215	LHG	C11-C10-C9-C8
31	a	802	LHG	C25-C26-C27-C28
31	a	834	LHG	C9-C10-C11-C12
37	b	835	DGD	CDB-CEB-CFB-CGB
27	J	312	CLA	O1A-CGA-O2A-C1
27	f	302	CLA	O1A-CGA-O2A-C1
27	i	101	CLA	O1A-CGA-O2A-C1
27	L	315	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
27	H	207	CLA	C5-C6-C7-C8
27	I	308	CLA	C2C-C3C-CAC-CBC
27	J	309	CLA	C2C-C3C-CAC-CBC
27	a	829	CLA	C3-C5-C6-C7
27	D	208	CLA	C3-C5-C6-C7
27	b	838	CLA	CBA-CGA-O2A-C1
27	L	316	CLA	C2C-C3C-CAC-CBC
27	K	309	CLA	O1A-CGA-O2A-C1
27	b	831	CLA	O1A-CGA-O2A-C1
27	b	850	CLA	C15-C16-C17-C18
31	b	836	LHG	C1-C2-C3-O3
27	L	308	CLA	C4C-C3C-CAC-CBC
29	E	317	LMG	C13-C14-C15-C16
31	a	801	LHG	C14-C15-C16-C17
29	E	317	LMG	O9-C10-O7-C8
31	j	102	LHG	O9-C7-O7-C5
27	a	843	CLA	C2-C1-O2A-CGA
30	I	303	A86	O5-C38-O4-C34
31	E	318	LHG	C11-C12-C13-C14
31	a	833	LHG	C28-C29-C30-C31
33	J	318	SQD	C26-C27-C28-C29
31	j	102	LHG	C34-C35-C36-C37
27	a	842	CLA	C16-C17-C18-C20
27	J	309	CLA	C3-C5-C6-C7
32	E	304	BCR	C23-C24-C25-C26
32	E	304	BCR	C23-C24-C25-C30
32	a	836	BCR	C23-C24-C25-C26
32	a	836	BCR	C23-C24-C25-C30
32	a	853	BCR	C1-C6-C7-C8
32	f	305	BCR	C1-C6-C7-C8
32	i	103	BCR	C23-C24-C25-C26
32	i	103	BCR	C23-C24-C25-C30
32	l	202	BCR	C1-C6-C7-C8
32	l	202	BCR	C5-C6-C7-C8
32	l	205	BCR	C5-C6-C7-C8
32	l	205	BCR	C23-C24-C25-C26
32	l	205	BCR	C23-C24-C25-C30
32	r	203	BCR	C1-C6-C7-C8
32	r	203	BCR	C5-C6-C7-C8
32	b	834	BCR	C1-C6-C7-C8
32	b	834	BCR	C5-C6-C7-C8
35	l	207	ET4	C01-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
27	D	217	CLA	C2C-C3C-CAC-CBC
29	A	212	LMG	C12-C13-C14-C15
29	A	214	LMG	C29-C30-C31-C32
31	j	102	LHG	C25-C26-C27-C28
27	A	205	CLA	CBA-CGA-O2A-C1
27	B	306	CLA	CBA-CGA-O2A-C1
27	a	846	CLA	CBA-CGA-O2A-C1
29	a	852	LMG	C29-C28-O8-C9
31	K	320	LHG	C24-C23-O8-C6
27	C	312	CLA	C8-C10-C11-C12
27	H	206	CLA	C13-C15-C16-C17
27	K	312	CLA	C10-C11-C12-C13
27	L	309	CLA	C13-C15-C16-C17
27	a	809	CLA	C10-C11-C12-C13
27	b	841	CLA	C5-C6-C7-C8
29	A	214	LMG	C11-C10-O7-C8
27	l	203	CLA	O1A-CGA-O2A-C1
28	M	314	KC1	CBD-CGD-O2D-CED
27	G	312	CLA	C14-C13-C15-C16
31	E	318	LHG	C7-C8-C9-C10
27	B	308	CLA	C10-C11-C12-C13
27	a	856	CLA	C10-C11-C12-C13
27	E	309	CLA	C4-C3-C5-C6
27	H	207	CLA	C4-C3-C5-C6
27	L	316	CLA	C4-C3-C5-C6
27	a	842	CLA	C4-C3-C5-C6
27	D	208	CLA	C4-C3-C5-C6
27	b	839	CLA	C4-C3-C5-C6
27	K	309	CLA	O1D-CGD-O2D-CED
27	K	312	CLA	O1D-CGD-O2D-CED
27	a	814	CLA	O1D-CGD-O2D-CED
27	b	849	CLA	O1D-CGD-O2D-CED
27	A	207	CLA	C11-C12-C13-C15
27	E	308	CLA	C6-C7-C8-C10
27	E	309	CLA	C12-C13-C15-C16
27	H	207	CLA	C2-C3-C5-C6
27	H	210	CLA	C6-C7-C8-C10
27	I	311	CLA	C12-C13-C15-C16
27	J	311	CLA	C6-C7-C8-C10
27	K	309	CLA	C11-C12-C13-C15
27	K	312	CLA	C6-C7-C8-C10
27	M	308	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
27	M	309	CLA	C6-C7-C8-C10
27	a	804	CLA	C12-C13-C15-C16
27	a	817	CLA	C11-C12-C13-C15
27	a	842	CLA	C11-C10-C8-C7
27	a	849	CLA	C11-C10-C8-C7
27	D	208	CLA	C2-C3-C5-C6
27	D	208	CLA	C11-C12-C13-C15
27	b	804	CLA	C11-C12-C13-C15
27	b	807	CLA	C12-C13-C15-C16
27	b	839	CLA	C2-C3-C5-C6
27	b	843	CLA	C6-C7-C8-C10
27	b	844	CLA	C12-C13-C15-C16
27	b	846	CLA	C12-C13-C15-C16
27	b	847	CLA	C2-C3-C5-C6
34	b	832	PQN	C12-C13-C15-C16
27	G	316	CLA	C3-C5-C6-C7
27	A	205	CLA	O1A-CGA-O2A-C1
27	K	311	CLA	O1A-CGA-O2A-C1
27	L	316	CLA	O1A-CGA-O2A-C1
27	M	307	CLA	O1A-CGA-O2A-C1
27	b	838	CLA	O1A-CGA-O2A-C1
27	a	844	CLA	C2C-C3C-CAC-CBC
29	E	317	LMG	C30-C31-C32-C33
29	j	103	LMG	C31-C32-C33-C34
31	D	201	LHG	C34-C35-C36-C37
27	H	207	CLA	C8-C10-C11-C12
26	E	303	DD6	C24-C25-C26-C27
30	K	305	A86	C1-C2-C3-C4
30	K	306	A86	C1-C2-C3-C4
30	K	306	A86	C3-C4-C5-C6
27	b	820	CLA	CBD-CGD-O2D-CED
27	C	311	CLA	C11-C12-C13-C14
27	I	311	CLA	C16-C17-C18-C20
27	D	208	CLA	O1D-CGD-O2D-CED
28	B	313	KC1	O1D-CGD-O2D-CED
29	C	319	LMG	O9-C10-O7-C8
29	D	202	LMG	O9-C10-O7-C8
31	E	318	LHG	O9-C7-O7-C5
27	K	313	CLA	CBA-CGA-O2A-C1
27	L	310	CLA	CBA-CGA-O2A-C1
27	a	803	CLA	CBA-CGA-O2A-C1
27	a	820	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	L	323	LMG	C12-C13-C14-C15
31	M	320	LHG	C19-C20-C21-C22
31	a	833	LHG	C33-C34-C35-C36
27	H	208	CLA	C2A-CAA-CBA-CGA
27	a	816	CLA	C2A-CAA-CBA-CGA
27	a	818	CLA	C2A-CAA-CBA-CGA
27	a	841	CLA	C2A-CAA-CBA-CGA
27	a	856	CLA	C2A-CAA-CBA-CGA
27	b	842	CLA	C2A-CAA-CBA-CGA
27	C	307	CLA	C15-C16-C17-C18
27	J	312	CLA	C13-C15-C16-C17
27	J	314	CLA	C15-C16-C17-C18
27	M	309	CLA	C15-C16-C17-C18
27	a	842	CLA	C10-C11-C12-C13
27	b	821	CLA	C10-C11-C12-C13
29	C	319	LMG	C32-C33-C34-C35
29	J	317	LMG	C14-C15-C16-C17
29	j	103	LMG	C11-C12-C13-C14
27	K	313	CLA	C4C-C3C-CAC-CBC
27	B	306	CLA	C12-C13-C15-C16
27	M	317	CLA	O1D-CGD-O2D-CED
27	l	203	CLA	C4C-C3C-CAC-CBC
29	l	201	LMG	C29-C30-C31-C32
31	E	318	LHG	C19-C20-C21-C22
28	H	211	KC1	C2B-C3B-CAB-CBB
28	L	314	KC1	C2B-C3B-CAB-CBB
27	F	315	CLA	C2C-C3C-CAC-CBC
27	F	315	CLA	C10-C11-C12-C13
29	I	319	LMG	C13-C14-C15-C16
27	b	847	CLA	CBA-CGA-O2A-C1
27	l	204	CLA	C13-C15-C16-C17
27	a	849	CLA	O1D-CGD-O2D-CED
27	I	315	CLA	C2C-C3C-CAC-CBC
37	b	835	DGD	C8B-C9B-CAB-CBB
29	I	319	LMG	C28-C29-C30-C31
29	C	301	LMG	C11-C10-O7-C8
29	D	202	LMG	C11-C10-O7-C8
31	E	318	LHG	C8-C7-O7-C5
29	a	852	LMG	C4-C5-C6-O5
28	H	211	KC1	C4B-C3B-CAB-CBB
28	L	314	KC1	C4B-C3B-CAB-CBB
27	I	315	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	E	317	LMG	C17-C18-C19-C20
31	B	315	LHG	C24-C25-C26-C27
31	M	320	LHG	C9-C10-C11-C12
29	A	214	LMG	O9-C10-O7-C8
29	C	301	LMG	O9-C10-O7-C8
27	a	843	CLA	C3-C5-C6-C7
27	b	806	CLA	C3-C5-C6-C7
29	C	301	LMG	O7-C8-C9-O8
29	J	317	LMG	O7-C8-C9-O8
31	E	318	LHG	O7-C5-C6-O8
27	A	206	CLA	CBD-CGD-O2D-CED
27	B	306	CLA	O1A-CGA-O2A-C1
29	I	201	LMG	C18-C19-C20-C21
31	a	801	LHG	C10-C11-C12-C13
27	A	207	CLA	C5-C6-C7-C8
27	H	213	CLA	C8-C10-C11-C12
27	a	827	CLA	C5-C6-C7-C8
27	I	206	CLA	O1D-CGD-O2D-CED
27	A	204	CLA	C4-C3-C5-C6
27	b	824	CLA	C4-C3-C5-C6
27	b	841	CLA	C2-C3-C5-C6
31	E	318	LHG	C11-C10-C9-C8
27	A	204	CLA	C11-C10-C8-C9
27	B	306	CLA	C11-C12-C13-C14
27	B	308	CLA	C14-C13-C15-C16
27	E	309	CLA	C14-C13-C15-C16
27	G	309	CLA	C11-C12-C13-C14
27	J	311	CLA	C14-C13-C15-C16
27	M	308	CLA	C11-C10-C8-C9
27	a	803	CLA	C11-C12-C13-C14
27	a	805	CLA	C11-C10-C8-C9
27	a	811	CLA	C14-C13-C15-C16
27	a	842	CLA	C11-C10-C8-C9
27	a	845	CLA	C11-C12-C13-C14
27	a	846	CLA	C11-C12-C13-C14
27	a	855	CLA	C11-C10-C8-C9
27	D	208	CLA	C6-C7-C8-C9
27	D	214	CLA	C6-C7-C8-C9
27	b	803	CLA	C11-C12-C13-C14
27	b	804	CLA	C11-C10-C8-C9
27	b	804	CLA	C14-C13-C15-C16
27	b	806	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	b	823	CLA	C11-C12-C13-C14
27	b	831	CLA	C11-C12-C13-C14
29	A	214	LMG	C14-C15-C16-C17
27	J	307	CLA	C3-C5-C6-C7
27	J	311	CLA	C3-C5-C6-C7
27	H	206	CLA	C2A-CAA-CBA-CGA
27	b	808	CLA	C2A-CAA-CBA-CGA
27	b	817	CLA	C2A-CAA-CBA-CGA
28	H	211	KC1	C4C-C3C-CAC-CBC
27	D	209	CLA	CBA-CGA-O2A-C1
30	K	301	A86	C7-C6-C8-C9
32	l	205	BCR	C7-C8-C9-C34
27	H	205	CLA	C5-C6-C7-C8
27	J	307	CLA	C15-C16-C17-C18
27	b	804	CLA	C5-C6-C7-C8
29	M	321	LMG	C14-C15-C16-C17
30	K	301	A86	C2-C1-C24-C25
32	l	205	BCR	C7-C8-C9-C10
27	a	846	CLA	O1A-CGA-O2A-C1
29	a	852	LMG	O10-C28-O8-C9
31	K	320	LHG	O10-C23-O8-C6
27	A	210	CLA	C1A-C2A-CAA-CBA
27	B	312	CLA	C1A-C2A-CAA-CBA
27	C	310	CLA	C1A-C2A-CAA-CBA
27	C	312	CLA	C1A-C2A-CAA-CBA
27	E	308	CLA	C1A-C2A-CAA-CBA
27	F	305	CLA	C1A-C2A-CAA-CBA
27	G	308	CLA	C1A-C2A-CAA-CBA
27	G	310	CLA	C1A-C2A-CAA-CBA
27	G	312	CLA	C1A-C2A-CAA-CBA
27	G	316	CLA	C1A-C2A-CAA-CBA
27	H	213	CLA	C1A-C2A-CAA-CBA
27	I	305	CLA	C1A-C2A-CAA-CBA
27	I	306	CLA	C1A-C2A-CAA-CBA
27	J	310	CLA	C1A-C2A-CAA-CBA
27	J	313	CLA	C1A-C2A-CAA-CBA
27	K	310	CLA	C1A-C2A-CAA-CBA
27	K	313	CLA	C1A-C2A-CAA-CBA
27	L	316	CLA	C1A-C2A-CAA-CBA
27	M	317	CLA	C1A-C2A-CAA-CBA
27	a	807	CLA	C1A-C2A-CAA-CBA
27	a	808	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	a	816	CLA	C1A-C2A-CAA-CBA
27	f	303	CLA	C1A-C2A-CAA-CBA
27	D	209	CLA	C1A-C2A-CAA-CBA
27	D	211	CLA	C1A-C2A-CAA-CBA
27	b	806	CLA	C1A-C2A-CAA-CBA
27	b	809	CLA	C1A-C2A-CAA-CBA
27	b	811	CLA	C1A-C2A-CAA-CBA
27	b	814	CLA	C1A-C2A-CAA-CBA
27	b	826	CLA	C1A-C2A-CAA-CBA
27	b	828	CLA	C1A-C2A-CAA-CBA
27	b	850	CLA	C1A-C2A-CAA-CBA
27	G	309	CLA	C16-C17-C18-C20
27	J	309	CLA	C16-C17-C18-C19
31	E	318	LHG	C30-C31-C32-C33
31	M	320	LHG	C14-C15-C16-C17
26	J	302	DD6	C3-C4-C5-C6
27	b	825	CLA	O1D-CGD-O2D-CED
27	M	318	CLA	O1A-CGA-O2A-C1
27	H	207	CLA	C15-C16-C17-C18
27	K	314	CLA	C8-C10-C11-C12
27	a	817	CLA	C15-C16-C17-C18
27	a	843	CLA	C8-C10-C11-C12
31	E	318	LHG	C3-O3-P-O6
31	a	834	LHG	C3-O3-P-O6
29	A	214	LMG	C17-C18-C19-C20
29	A	214	LMG	C21-C22-C23-C24
29	M	321	LMG	C10-C11-C12-C13
29	j	103	LMG	C28-C29-C30-C31
27	I	306	CLA	CBD-CGD-O2D-CED
27	E	314	CLA	C3-C5-C6-C7
27	a	808	CLA	C3-C5-C6-C7
27	a	846	CLA	C3-C5-C6-C7
31	K	320	LHG	C5-C4-O6-P
31	a	837	LHG	C2-C3-O3-P
27	C	312	CLA	O1D-CGD-O2D-CED
27	K	309	CLA	C5-C6-C7-C8
27	M	307	CLA	C5-C6-C7-C8
27	H	205	CLA	CBA-CGA-O2A-C1
27	a	819	CLA	O1D-CGD-O2D-CED
31	E	318	LHG	C27-C28-C29-C30
29	A	212	LMG	C31-C32-C33-C34
29	j	103	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	b	823	CLA	C16-C17-C18-C20
27	L	307	CLA	C2C-C3C-CAC-CBC
27	l	204	CLA	C3-C5-C6-C7
27	b	818	CLA	C3-C5-C6-C7
27	B	306	CLA	C8-C10-C11-C12
27	B	312	CLA	C4-C3-C5-C6
27	D	213	CLA	C4-C3-C5-C6
27	b	841	CLA	C4-C3-C5-C6
27	C	315	CLA	C3A-C2A-CAA-CBA
27	C	317	CLA	C3A-C2A-CAA-CBA
29	E	317	LMG	C15-C16-C17-C18
31	a	833	LHG	C34-C35-C36-C37
31	j	102	LHG	C15-C16-C17-C18
37	b	835	DGD	C9B-CAB-CBB-CCB
27	b	820	CLA	C13-C15-C16-C17
28	M	314	KC1	C4C-C3C-CAC-CBC
29	j	103	LMG	C15-C16-C17-C18
31	H	215	LHG	C12-C13-C14-C15
31	K	320	LHG	C23-C24-C25-C26
29	J	317	LMG	C11-C10-O7-C8
27	a	803	CLA	O1A-CGA-O2A-C1
27	E	311	CLA	C2A-CAA-CBA-CGA
27	E	314	CLA	C2A-CAA-CBA-CGA
27	A	207	CLA	C16-C17-C18-C19
27	F	310	CLA	C11-C12-C13-C15
27	a	854	CLA	C6-C7-C8-C9
29	A	212	LMG	C33-C34-C35-C36
29	A	214	LMG	O1-C7-C8-C9
29	A	214	LMG	C7-C8-C9-O8
29	C	301	LMG	C31-C32-C33-C34
29	J	317	LMG	C7-C8-C9-O8
29	a	852	LMG	O1-C7-C8-C9
29	a	852	LMG	C7-C8-C9-O8
29	l	201	LMG	C7-C8-C9-O8
29	D	202	LMG	C7-C8-C9-O8
31	K	320	LHG	C4-C5-C6-O8
31	a	837	LHG	C4-C5-C6-O8
27	C	309	CLA	C5-C6-C7-C8
27	K	313	CLA	O1A-CGA-O2A-C1
27	a	820	CLA	O1A-CGA-O2A-C1
29	L	323	LMG	C8-C7-O1-C1
27	a	829	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	b	824	CLA	O1D-CGD-O2D-CED
29	C	319	LMG	C18-C19-C20-C21
29	C	319	LMG	C21-C22-C23-C24
29	D	202	LMG	C30-C31-C32-C33
31	K	320	LHG	C9-C10-C11-C12
31	M	320	LHG	C33-C34-C35-C36
27	L	310	CLA	C8-C10-C11-C12
27	b	825	CLA	C10-C11-C12-C13
27	M	307	CLA	C14-C13-C15-C16
27	L	307	CLA	C5-C6-C7-C8
27	L	316	CLA	CAA-CBA-CGA-O2A
27	b	803	CLA	CAA-CBA-CGA-O2A
31	a	802	LHG	C23-C24-C25-C26
29	A	214	LMG	C22-C23-C24-C25
31	a	833	LHG	C16-C17-C18-C19
31	a	802	LHG	C35-C36-C37-C38
27	L	310	CLA	O1A-CGA-O2A-C1
27	D	209	CLA	O1A-CGA-O2A-C1
31	j	102	LHG	C12-C13-C14-C15
31	D	201	LHG	C35-C36-C37-C38
31	b	836	LHG	C19-C20-C21-C22
27	J	312	CLA	C10-C11-C12-C13
27	A	208	CLA	C4-C3-C5-C6
27	a	821	CLA	C4-C3-C5-C6
27	a	823	CLA	C4-C3-C5-C6
27	a	844	CLA	C4-C3-C5-C6
27	a	844	CLA	C2-C3-C5-C6
28	C	313	KC1	C2A-CAA-CBA-CGA
27	M	313	CLA	C16-C17-C18-C19
27	a	843	CLA	C16-C17-C18-C19
27	b	830	CLA	C16-C17-C18-C20
27	E	309	CLA	CBA-CGA-O2A-C1
27	I	315	CLA	CBA-CGA-O2A-C1
27	K	310	CLA	CBA-CGA-O2A-C1
31	B	315	LHG	C31-C32-C33-C34
27	H	208	CLA	CBD-CGD-O2D-CED
27	F	306	CLA	O1D-CGD-O2D-CED
29	A	212	LMG	C16-C17-C18-C19
29	I	319	LMG	C32-C33-C34-C35
27	D	216	CLA	O1A-CGA-O2A-C1
29	A	214	LMG	C9-C8-O7-C10
27	A	203	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	M	313	CLA	C2A-CAA-CBA-CGA
27	b	815	CLA	C2A-CAA-CBA-CGA
27	b	825	CLA	C5-C6-C7-C8
29	J	317	LMG	C37-C38-C39-C40
30	K	305	A86	O5-C38-O4-C34
27	b	850	CLA	CBD-CGD-O2D-CED
27	D	207	CLA	C3-C5-C6-C7
27	b	804	CLA	C3-C5-C6-C7
27	b	812	CLA	C3-C5-C6-C7
29	L	323	LMG	C33-C34-C35-C36
27	L	309	CLA	CBA-CGA-O2A-C1
27	b	820	CLA	CBA-CGA-O2A-C1
27	b	847	CLA	O1A-CGA-O2A-C1
28	L	314	KC1	C4C-C3C-CAC-CBC
27	b	844	CLA	O1D-CGD-O2D-CED
29	A	212	LMG	C11-C10-O7-C8
27	b	813	CLA	C5-C6-C7-C8
27	b	845	CLA	C5-C6-C7-C8
29	C	301	LMG	C2-C1-O1-C7
29	j	103	LMG	C17-C18-C19-C20
31	M	320	LHG	C27-C28-C29-C30
29	D	202	LMG	O7-C8-C9-O8
29	J	317	LMG	C12-C13-C14-C15
37	b	835	DGD	C7A-C8A-C9A-CAA
27	b	808	CLA	C5-C6-C7-C8
27	H	205	CLA	O1A-CGA-O2A-C1
27	K	310	CLA	O1A-CGA-O2A-C1
27	J	315	CLA	CBD-CGD-O2D-CED
27	K	313	CLA	O1D-CGD-O2D-CED
28	K	315	KC1	C2C-C3C-CAC-CBC
31	E	318	LHG	C13-C14-C15-C16
27	A	204	CLA	C11-C10-C8-C7
27	A	205	CLA	C6-C7-C8-C10
27	A	205	CLA	C11-C12-C13-C15
27	B	308	CLA	C12-C13-C15-C16
27	F	307	CLA	C11-C10-C8-C7
27	F	310	CLA	C6-C7-C8-C10
27	G	309	CLA	C12-C13-C15-C16
27	H	205	CLA	C12-C13-C15-C16
27	H	206	CLA	C6-C7-C8-C10
27	H	212	CLA	C11-C10-C8-C7
27	H	212	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	I	306	CLA	C11-C12-C13-C15
27	J	312	CLA	C12-C13-C15-C16
27	K	314	CLA	C6-C7-C8-C10
27	K	314	CLA	C11-C10-C8-C7
27	K	314	CLA	C12-C13-C15-C16
27	K	316	CLA	C6-C7-C8-C10
27	L	308	CLA	C11-C10-C8-C7
27	M	307	CLA	C11-C12-C13-C15
27	M	313	CLA	C6-C7-C8-C10
27	a	804	CLA	C6-C7-C8-C10
27	a	807	CLA	C12-C13-C15-C16
27	a	808	CLA	C11-C12-C13-C15
27	a	811	CLA	C12-C13-C15-C16
27	a	815	CLA	C12-C13-C15-C16
27	a	821	CLA	C2-C3-C5-C6
27	a	828	CLA	C11-C12-C13-C15
27	a	839	CLA	C6-C7-C8-C10
27	a	845	CLA	C11-C12-C13-C15
27	a	846	CLA	C11-C12-C13-C15
27	a	855	CLA	C11-C10-C8-C7
27	a	856	CLA	C11-C10-C8-C7
27	f	301	CLA	C11-C10-C8-C7
27	f	302	CLA	C11-C12-C13-C15
27	f	302	CLA	C12-C13-C15-C16
27	l	204	CLA	C6-C7-C8-C10
27	D	207	CLA	C11-C10-C8-C7
27	D	214	CLA	C6-C7-C8-C10
27	b	803	CLA	C11-C12-C13-C15
27	b	804	CLA	C11-C10-C8-C7
27	b	807	CLA	C11-C12-C13-C15
27	b	808	CLA	C11-C12-C13-C15
27	b	821	CLA	C11-C10-C8-C7
27	b	821	CLA	C11-C12-C13-C15
27	b	823	CLA	C11-C12-C13-C15
27	b	831	CLA	C11-C12-C13-C15
27	b	844	CLA	C11-C10-C8-C7
27	A	207	CLA	C11-C12-C13-C14
27	E	309	CLA	C6-C7-C8-C9
27	F	310	CLA	C6-C7-C8-C9
27	G	309	CLA	C14-C13-C15-C16
27	G	312	CLA	C11-C10-C8-C9
27	H	205	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
27	I	306	CLA	C11-C12-C13-C14
27	I	308	CLA	C11-C10-C8-C9
27	I	311	CLA	C14-C13-C15-C16
27	J	312	CLA	C14-C13-C15-C16
27	K	309	CLA	C6-C7-C8-C9
27	K	316	CLA	C6-C7-C8-C9
27	L	313	CLA	C14-C13-C15-C16
27	a	804	CLA	C6-C7-C8-C9
27	a	807	CLA	C14-C13-C15-C16
27	a	808	CLA	C11-C12-C13-C14
27	a	810	CLA	C14-C13-C15-C16
27	a	817	CLA	C6-C7-C8-C9
27	a	828	CLA	C11-C12-C13-C14
27	a	830	CLA	C14-C13-C15-C16
27	a	839	CLA	C6-C7-C8-C9
27	a	842	CLA	C11-C12-C13-C14
27	a	844	CLA	C14-C13-C15-C16
27	a	856	CLA	C11-C10-C8-C9
27	f	301	CLA	C11-C10-C8-C9
27	f	302	CLA	C11-C12-C13-C14
27	f	302	CLA	C14-C13-C15-C16
27	D	210	CLA	C6-C7-C8-C9
27	b	807	CLA	C11-C12-C13-C14
27	b	825	CLA	C11-C12-C13-C14
27	b	843	CLA	C11-C12-C13-C14
27	b	844	CLA	C11-C12-C13-C14
31	E	318	LHG	C16-C17-C18-C19
27	H	206	CLA	CBA-CGA-O2A-C1
27	a	832	CLA	CBA-CGA-O2A-C1
27	K	310	CLA	C5-C6-C7-C8
27	K	312	CLA	C2C-C3C-CAC-CBC
30	L	304	A86	O5-C38-O4-C34
27	a	828	CLA	O1D-CGD-O2D-CED
32	b	834	BCR	C37-C22-C23-C24
27	A	207	CLA	C16-C17-C18-C20
27	a	854	CLA	C6-C7-C8-C10
27	F	314	CLA	O1D-CGD-O2D-CED
30	M	305	A86	C2-C1-C24-C25
27	L	310	CLA	C13-C15-C16-C17
27	L	310	CLA	C15-C16-C17-C18
27	L	316	CLA	C4C-C3C-CAC-CBC
27	b	813	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	G	306	CLA	O1A-CGA-O2A-C1
31	M	320	LHG	C24-C23-O8-C6
27	M	310	CLA	C10-C11-C12-C13
27	I	305	CLA	CBD-CGD-O2D-CED
27	K	310	CLA	CBD-CGD-O2D-CED
27	M	318	CLA	CBD-CGD-O2D-CED
27	F	310	CLA	C11-C12-C13-C14
27	H	207	CLA	C16-C17-C18-C20
27	a	856	CLA	C16-C17-C18-C20
31	K	320	LHG	O6-C4-C5-C6
31	a	802	LHG	O6-C4-C5-C6
27	b	844	CLA	C3-C5-C6-C7
29	A	214	LMG	C10-C11-C12-C13
27	b	812	CLA	O1D-CGD-O2D-CED
27	I	307	CLA	C4C-C3C-CAC-CBC
29	J	317	LMG	C39-C40-C41-C42
29	l	201	LMG	C14-C15-C16-C17
27	I	314	CLA	CBA-CGA-O2A-C1
27	a	812	CLA	CBA-CGA-O2A-C1
27	a	848	CLA	CBA-CGA-O2A-C1
27	b	841	CLA	CBA-CGA-O2A-C1
31	E	316	LHG	C24-C23-O8-C6
27	K	312	CLA	C5-C6-C7-C8
27	b	828	CLA	O1D-CGD-O2D-CED
27	L	307	CLA	C6-C7-C8-C10
37	b	835	DGD	C2B-C3B-C4B-C5B
27	F	315	CLA	C4-C3-C5-C6
27	H	210	CLA	C4-C3-C5-C6
27	I	308	CLA	C4-C3-C5-C6
27	a	811	CLA	C4-C3-C5-C6
27	b	820	CLA	C15-C16-C17-C18
27	f	302	CLA	CBD-CGD-O2D-CED
27	a	850	CLA	C11-C10-C8-C9
27	b	822	CLA	O1D-CGD-O2D-CED
27	H	212	CLA	C16-C17-C18-C20
31	a	801	LHG	C30-C31-C32-C33
27	a	849	CLA	C13-C15-C16-C17
27	L	321	CLA	C2A-CAA-CBA-CGA
33	J	318	SQD	C6-C5-O5-C1
27	a	822	CLA	CBA-CGA-O2A-C1
27	K	316	CLA	CAA-CBA-CGA-O2A
31	a	802	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
27	A	211	CLA	O1D-CGD-O2D-CED
27	F	310	CLA	C3A-C2A-CAA-CBA
27	K	312	CLA	C3A-C2A-CAA-CBA
27	a	815	CLA	C3A-C2A-CAA-CBA
27	a	841	CLA	C3A-C2A-CAA-CBA
27	l	203	CLA	C3A-C2A-CAA-CBA
27	b	810	CLA	C3A-C2A-CAA-CBA
27	b	824	CLA	C3A-C2A-CAA-CBA
27	J	309	CLA	C4C-C3C-CAC-CBC
31	E	318	LHG	C28-C29-C30-C31
26	I	304	DD6	C24-C25-C26-C27
30	D	203	A86	C1-C2-C3-C4
30	C	302	A86	O-C13-C14-C15
30	J	316	A86	O-C13-C14-C15
30	D	203	A86	O-C13-C14-C15
29	A	212	LMG	C14-C15-C16-C17
31	b	836	LHG	C28-C29-C30-C31
27	H	208	CLA	CBA-CGA-O2A-C1
27	E	315	CLA	O1D-CGD-O2D-CED
27	E	309	CLA	O1A-CGA-O2A-C1
31	a	801	LHG	C35-C36-C37-C38
27	J	309	CLA	C16-C17-C18-C20
27	b	830	CLA	C16-C17-C18-C19
27	a	823	CLA	CBA-CGA-O2A-C1
27	b	811	CLA	CBA-CGA-O2A-C1
31	I	318	LHG	C24-C23-O8-C6
27	H	204	CLA	C6-C7-C8-C10
29	M	321	LMG	C16-C17-C18-C19
31	a	801	LHG	C12-C13-C14-C15
31	a	837	LHG	C32-C33-C34-C35
27	a	805	CLA	C15-C16-C17-C18
34	b	832	PQN	C18-C20-C21-C22
29	E	317	LMG	O1-C7-C8-C9
29	M	321	LMG	C7-C8-C9-O8
31	H	215	LHG	C4-C5-C6-O8
31	M	320	LHG	C4-C5-C6-O8
27	A	208	CLA	C5-C6-C7-C8
29	J	317	LMG	C33-C34-C35-C36
31	D	201	LHG	C19-C20-C21-C22
27	L	309	CLA	O1A-CGA-O2A-C1
31	E	318	LHG	C15-C16-C17-C18
31	b	836	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
27	b	821	CLA	O2A-C1-C2-C3
27	b	846	CLA	C10-C11-C12-C13
27	I	315	CLA	C4-C3-C5-C6
27	b	821	CLA	C4-C3-C5-C6
27	H	212	CLA	C16-C17-C18-C19
27	a	843	CLA	C16-C17-C18-C20
27	F	315	CLA	C2-C3-C5-C6
28	I	312	KC1	C4C-C3C-CAC-CBC
27	b	823	CLA	C10-C11-C12-C13
29	j	103	LMG	C13-C14-C15-C16
27	b	830	CLA	C2A-CAA-CBA-CGA
27	J	309	CLA	C13-C15-C16-C17
31	H	215	LHG	O6-C4-C5-O7
27	a	839	CLA	CBA-CGA-O2A-C1
27	b	821	CLA	CBA-CGA-O2A-C1
37	b	835	DGD	C2A-C1A-O1G-C1G
27	I	315	CLA	O1A-CGA-O2A-C1
27	b	820	CLA	O1A-CGA-O2A-C1
28	A	209	KC1	C3A-C2A-CAA-CBA
27	a	803	CLA	C16-C17-C18-C20
27	L	313	CLA	C2C-C3C-CAC-CBC
27	a	804	CLA	C2C-C3C-CAC-CBC
31	a	833	LHG	C12-C13-C14-C15
31	E	318	LHG	C18-C19-C20-C21
29	I	319	LMG	O7-C8-C9-O8
29	a	852	LMG	O1-C7-C8-O7
33	J	318	SQD	O47-C45-C46-O48
27	a	808	CLA	C15-C16-C17-C18
30	I	301	A86	C35-C34-O4-C38
27	I	307	CLA	O1D-CGD-O2D-CED
27	a	845	CLA	C16-C17-C18-C19
27	b	819	CLA	C16-C17-C18-C19
27	L	319	CLA	C2C-C3C-CAC-CBC
31	a	833	LHG	C32-C33-C34-C35
29	E	317	LMG	O6-C1-O1-C7
27	a	807	CLA	C15-C16-C17-C18
27	a	822	CLA	C5-C6-C7-C8
27	a	830	CLA	C5-C6-C7-C8
30	K	301	A86	C10-C11-C13-C14
30	M	303	A86	C10-C11-C13-C14
28	K	315	KC1	CAA-CBA-CGA-O1A
27	a	839	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
27	D	207	CLA	C2-C1-O2A-CGA
27	b	842	CLA	C2-C1-O2A-CGA
27	b	846	CLA	C2-C1-O2A-CGA
27	J	314	CLA	C10-C11-C12-C13
27	A	205	CLA	C11-C10-C8-C9
27	F	311	CLA	C6-C7-C8-C9
27	G	309	CLA	C11-C10-C8-C9
27	H	205	CLA	C6-C7-C8-C9
27	H	213	CLA	C14-C13-C15-C16
27	J	307	CLA	C11-C10-C8-C9
27	J	311	CLA	C11-C12-C13-C14
27	a	846	CLA	C14-C13-C15-C16
27	a	848	CLA	C11-C10-C8-C9
27	a	855	CLA	C6-C7-C8-C9
27	b	808	CLA	C6-C7-C8-C9
27	b	821	CLA	C11-C10-C8-C9
27	b	825	CLA	C6-C7-C8-C9
29	D	202	LMG	C17-C18-C19-C20
31	a	802	LHG	C10-C11-C12-C13
27	B	307	CLA	C15-C16-C17-C18
27	a	855	CLA	C8-C10-C11-C12
27	b	823	CLA	C15-C16-C17-C18
31	M	320	LHG	C2-C3-O3-P
31	a	801	LHG	C5-C4-O6-P
31	a	837	LHG	C5-C4-O6-P
31	j	102	LHG	C14-C15-C16-C17
31	b	836	LHG	C12-C13-C14-C15
27	J	311	CLA	C16-C17-C18-C19
27	G	317	CLA	O2A-C1-C2-C3
32	r	203	BCR	C23-C24-C25-C26
32	r	203	BCR	C23-C24-C25-C30
32	b	840	BCR	C5-C6-C7-C8
27	b	803	CLA	C5-C6-C7-C8
27	I	315	CLA	O1D-CGD-O2D-CED
27	G	306	CLA	CAA-CBA-CGA-O2A
27	a	832	CLA	O1A-CGA-O2A-C1
26	F	303	DD6	C5-C6-C8-C9
26	K	303	DD6	C5-C6-C8-C9
27	G	315	CLA	C1A-C2A-CAA-CBA
30	K	301	A86	C5-C6-C8-C9
30	M	305	A86	C5-C6-C8-C9
32	j	105	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	b	803	CLA	C10-C11-C12-C13
27	b	831	CLA	C8-C10-C11-C12
31	a	833	LHG	C35-C36-C37-C38
29	A	212	LMG	O9-C10-O7-C8
29	J	317	LMG	O9-C10-O7-C8
31	a	834	LHG	C10-C11-C12-C13
27	A	204	CLA	C16-C17-C18-C20
27	H	205	CLA	C16-C17-C18-C19
27	H	207	CLA	C16-C17-C18-C19
27	a	827	CLA	CBD-CGD-O2D-CED
27	B	306	CLA	C14-C13-C15-C16
27	K	310	CLA	C11-C10-C8-C9
27	H	206	CLA	O1A-CGA-O2A-C1
27	b	820	CLA	O1D-CGD-O2D-CED
29	A	212	LMG	C15-C16-C17-C18
29	A	214	LMG	C19-C20-C21-C22
27	M	310	CLA	C8-C10-C11-C12
29	A	212	LMG	C29-C30-C31-C32
27	A	204	CLA	C11-C12-C13-C15
27	A	208	CLA	C2-C3-C5-C6
27	B	306	CLA	C6-C7-C8-C10
27	B	308	CLA	C11-C10-C8-C7
27	B	311	CLA	C6-C7-C8-C10
27	E	308	CLA	C12-C13-C15-C16
27	E	309	CLA	C6-C7-C8-C10
27	F	311	CLA	C6-C7-C8-C10
27	G	309	CLA	C11-C10-C8-C7
27	G	312	CLA	C11-C10-C8-C7
27	H	212	CLA	C6-C7-C8-C10
27	H	213	CLA	C12-C13-C15-C16
27	I	308	CLA	C6-C7-C8-C10
27	I	308	CLA	C11-C10-C8-C7
27	I	315	CLA	C2-C3-C5-C6
27	J	307	CLA	C11-C10-C8-C7
27	J	311	CLA	C11-C12-C13-C15
27	J	312	CLA	C6-C7-C8-C10
27	K	309	CLA	C12-C13-C15-C16
27	K	312	CLA	C11-C10-C8-C7
27	L	310	CLA	C11-C10-C8-C7
27	M	313	CLA	C11-C10-C8-C7
27	a	810	CLA	C12-C13-C15-C16
27	a	817	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
27	a	821	CLA	C11-C12-C13-C15
27	a	822	CLA	C11-C12-C13-C15
27	a	823	CLA	C2-C3-C5-C6
27	a	830	CLA	C12-C13-C15-C16
27	a	838	CLA	C12-C13-C15-C16
27	a	842	CLA	C11-C12-C13-C15
27	a	843	CLA	C11-C12-C13-C15
27	a	844	CLA	C12-C13-C15-C16
27	a	846	CLA	C12-C13-C15-C16
27	a	848	CLA	C11-C10-C8-C7
27	a	855	CLA	C6-C7-C8-C10
27	f	301	CLA	C12-C13-C15-C16
27	i	101	CLA	C11-C10-C8-C7
27	D	208	CLA	C11-C10-C8-C7
27	D	210	CLA	C6-C7-C8-C10
27	b	806	CLA	C11-C10-C8-C7
27	b	813	CLA	C6-C7-C8-C10
27	b	825	CLA	C11-C12-C13-C15
27	b	843	CLA	C11-C12-C13-C15
27	b	844	CLA	C11-C12-C13-C15
31	M	320	LHG	O10-C23-O8-C6
29	I	319	LMG	C29-C30-C31-C32
29	J	317	LMG	C35-C36-C37-C38
31	K	320	LHG	C19-C20-C21-C22
26	K	303	DD6	C11-C10-C9-C8
30	B	301	A86	C11-C10-C9-C8
30	B	304	A86	C3-C4-C5-C6
32	f	305	BCR	C19-C20-C21-C22
27	b	807	CLA	CBA-CGA-O2A-C1
27	A	206	CLA	O1D-CGD-O2D-CED
27	a	811	CLA	C10-C11-C12-C13
27	b	805	CLA	C2A-CAA-CBA-CGA
27	b	818	CLA	C2A-CAA-CBA-CGA
27	b	846	CLA	C2A-CAA-CBA-CGA
27	b	829	CLA	C13-C15-C16-C17
27	a	845	CLA	C3-C5-C6-C7
37	b	835	DGD	C4B-C5B-C6B-C7B
28	G	313	KC1	C2A-CAA-CBA-CGA
27	a	845	CLA	C16-C17-C18-C20
27	b	819	CLA	C16-C17-C18-C20
27	M	313	CLA	C8-C10-C11-C12
27	a	856	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	b	815	CLA	CBA-CGA-O2A-C1
31	D	201	LHG	C24-C23-O8-C6
27	K	310	CLA	C11-C10-C8-C7
27	M	307	CLA	C12-C13-C15-C16
27	a	850	CLA	C11-C10-C8-C7
31	M	320	LHG	C29-C30-C31-C32
27	b	829	CLA	C5-C6-C7-C8
27	F	308	CLA	CBD-CGD-O2D-CED
27	A	203	CLA	CAD-CBD-CGD-O2D
27	B	307	CLA	CAD-CBD-CGD-O2D
27	B	312	CLA	CAD-CBD-CGD-O2D
27	C	311	CLA	CAD-CBD-CGD-O2D
27	E	309	CLA	CAD-CBD-CGD-O2D
27	E	313	CLA	CAD-CBD-CGD-O2D
27	E	315	CLA	CAD-CBD-CGD-O2D
27	F	310	CLA	CAD-CBD-CGD-O2D
27	G	310	CLA	CAD-CBD-CGD-O2D
27	G	311	CLA	CAD-CBD-CGD-O2D
27	G	314	CLA	CAD-CBD-CGD-O2D
27	H	208	CLA	CAD-CBD-CGD-O2D
27	I	315	CLA	CAD-CBD-CGD-O2D
27	K	317	CLA	CAD-CBD-CGD-O2D
27	K	318	CLA	CAD-CBD-CGD-O2D
27	L	307	CLA	CAD-CBD-CGD-O2D
27	L	309	CLA	CAD-CBD-CGD-O2D
27	L	312	CLA	CAD-CBD-CGD-O2D
27	L	321	CLA	CAD-CBD-CGD-O2D
27	M	317	CLA	CAD-CBD-CGD-O2D
27	M	318	CLA	CAD-CBD-CGD-O2D
27	a	806	CLA	CAD-CBD-CGD-O2D
27	a	810	CLA	CAD-CBD-CGD-O2D
27	a	813	CLA	CAD-CBD-CGD-O2D
27	a	816	CLA	CAD-CBD-CGD-O2D
27	a	819	CLA	CAD-CBD-CGD-O2D
27	a	820	CLA	CAD-CBD-CGD-O2D
27	a	830	CLA	CAD-CBD-CGD-O2D
27	a	843	CLA	CAD-CBD-CGD-O2D
27	a	844	CLA	CAD-CBD-CGD-O2D
27	a	845	CLA	CAD-CBD-CGD-O2D
27	a	848	CLA	CAD-CBD-CGD-O2D
27	a	849	CLA	CAD-CBD-CGD-O2D
27	a	854	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	l	203	CLA	CAD-CBD-CGD-O2D
27	D	211	CLA	CAD-CBD-CGD-O2D
27	b	803	CLA	CAD-CBD-CGD-O2D
27	b	828	CLA	CAD-CBD-CGD-O2D
27	b	829	CLA	CAD-CBD-CGD-O2D
27	b	838	CLA	CAD-CBD-CGD-O2D
27	b	847	CLA	CAD-CBD-CGD-O2D
28	H	211	KC1	CAD-CBD-CGD-O2D
28	K	308	KC1	C2B-C3B-CAB-CBB
30	J	316	A86	C28-C27-C29-C30
27	C	311	CLA	C5-C6-C7-C8
27	b	844	CLA	C15-C16-C17-C18
27	H	208	CLA	CAA-CBA-CGA-O2A
27	K	316	CLA	C16-C17-C18-C20
27	M	308	CLA	C11-C12-C13-C14
27	a	809	CLA	C16-C17-C18-C20
27	i	101	CLA	C11-C12-C13-C14
27	J	315	CLA	O1D-CGD-O2D-CED
29	C	301	LMG	C7-C8-C9-O8
29	E	317	LMG	C7-C8-C9-O8
29	L	323	LMG	C7-C8-C9-O8
30	J	316	A86	C12-C11-C13-O
31	I	318	LHG	C2-C3-O3-P
31	a	834	LHG	C4-C5-C6-O8
27	a	812	CLA	O1A-CGA-O2A-C1
27	a	848	CLA	O1A-CGA-O2A-C1
31	a	802	LHG	C11-C12-C13-C14
33	J	318	SQD	C31-C32-C33-C34
31	K	320	LHG	O6-C4-C5-O7
31	M	320	LHG	O6-C4-C5-O7
31	a	802	LHG	O6-C4-C5-O7
31	a	837	LHG	O6-C4-C5-O7
27	a	805	CLA	C13-C15-C16-C17
31	D	201	LHG	C29-C30-C31-C32
28	B	313	KC1	C4B-C3B-CAB-CBB
27	H	205	CLA	C2A-CAA-CBA-CGA
27	a	819	CLA	C2A-CAA-CBA-CGA
27	H	209	CLA	C11-C12-C13-C15
27	b	821	CLA	C16-C17-C18-C20
27	A	208	CLA	CHA-CBD-CGD-O1D
27	A	208	CLA	CHA-CBD-CGD-O2D
27	A	211	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	A	211	CLA	CHA-CBD-CGD-O2D
27	B	309	CLA	CHA-CBD-CGD-O1D
27	B	309	CLA	CHA-CBD-CGD-O2D
27	C	316	CLA	CHA-CBD-CGD-O2D
27	C	317	CLA	CHA-CBD-CGD-O2D
27	F	316	CLA	CHA-CBD-CGD-O2D
27	G	307	CLA	CHA-CBD-CGD-O2D
27	H	207	CLA	CHA-CBD-CGD-O1D
27	H	207	CLA	CHA-CBD-CGD-O2D
27	H	213	CLA	CHA-CBD-CGD-O1D
27	H	213	CLA	CHA-CBD-CGD-O2D
27	J	307	CLA	CHA-CBD-CGD-O1D
27	J	310	CLA	CHA-CBD-CGD-O1D
27	K	312	CLA	CHA-CBD-CGD-O1D
27	K	312	CLA	CHA-CBD-CGD-O2D
27	L	310	CLA	CHA-CBD-CGD-O2D
27	L	311	CLA	CHA-CBD-CGD-O1D
27	L	315	CLA	CHA-CBD-CGD-O1D
27	M	310	CLA	CHA-CBD-CGD-O1D
27	M	310	CLA	CHA-CBD-CGD-O2D
27	M	311	CLA	CHA-CBD-CGD-O1D
27	M	311	CLA	CHA-CBD-CGD-O2D
27	M	313	CLA	CHA-CBD-CGD-O1D
27	M	313	CLA	CHA-CBD-CGD-O2D
27	M	316	CLA	CHA-CBD-CGD-O1D
27	M	316	CLA	CHA-CBD-CGD-O2D
27	a	803	CLA	CHA-CBD-CGD-O1D
27	a	822	CLA	CHA-CBD-CGD-O1D
27	a	822	CLA	CHA-CBD-CGD-O2D
27	a	828	CLA	CHA-CBD-CGD-O1D
27	a	828	CLA	CHA-CBD-CGD-O2D
27	a	829	CLA	CHA-CBD-CGD-O2D
27	a	832	CLA	CHA-CBD-CGD-O1D
27	a	839	CLA	CHA-CBD-CGD-O1D
27	a	846	CLA	CHA-CBD-CGD-O1D
27	r	201	CLA	CHA-CBD-CGD-O1D
27	r	201	CLA	CHA-CBD-CGD-O2D
27	D	210	CLA	CHA-CBD-CGD-O1D
27	D	210	CLA	CHA-CBD-CGD-O2D
27	b	805	CLA	CHA-CBD-CGD-O1D
27	b	821	CLA	CHA-CBD-CGD-O1D
27	b	841	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	B	313	KC1	CHA-CBD-CGD-O2D
28	C	308	KC1	CHA-CBD-CGD-O2D
28	C	313	KC1	CHA-CBD-CGD-O1D
28	K	315	KC1	CHA-CBD-CGD-O1D
28	K	308	KC1	C4C-C3C-CAC-CBC
27	a	815	CLA	C3-C5-C6-C7
27	b	843	CLA	C3-C5-C6-C7
27	I	314	CLA	O1A-CGA-O2A-C1
27	a	822	CLA	O1A-CGA-O2A-C1
27	a	823	CLA	O1A-CGA-O2A-C1
27	b	821	CLA	O1A-CGA-O2A-C1
27	b	841	CLA	O1A-CGA-O2A-C1
29	A	214	LMG	O7-C8-C9-O8
29	E	317	LMG	O1-C7-C8-O7
29	L	323	LMG	O7-C8-C9-O8
31	H	215	LHG	O7-C5-C6-O8
31	a	802	LHG	O7-C5-C6-O8
31	j	102	LHG	C31-C32-C33-C34
27	a	839	CLA	O1A-CGA-O2A-C1
27	b	807	CLA	O1A-CGA-O2A-C1
27	b	811	CLA	O1A-CGA-O2A-C1
27	a	840	CLA	C16-C17-C18-C20
27	b	844	CLA	C16-C17-C18-C19
30	J	304	A86	C13-C14-C15-O1
30	J	316	A86	C10-C11-C13-O
30	K	301	A86	C13-C14-C15-O1
30	K	304	A86	C13-C14-C15-O1
30	L	302	A86	C13-C14-C15-O1
30	M	302	A86	C13-C14-C15-O1
30	M	303	A86	C13-C14-C15-O1
30	D	204	A86	C13-C14-C15-O1
27	b	830	CLA	O1D-CGD-O2D-CED
27	b	850	CLA	O1D-CGD-O2D-CED
27	A	205	CLA	C3-C5-C6-C7
27	a	828	CLA	C3-C5-C6-C7
27	b	850	CLA	C3-C5-C6-C7
27	a	823	CLA	C5-C6-C7-C8
27	i	101	CLA	CBD-CGD-O2D-CED
31	I	318	LHG	O10-C23-O8-C6
37	b	835	DGD	O1A-C1A-O1G-C1G
26	A	202	DD6	C27-C29-C30-C31
26	E	307	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
27	B	308	CLA	C11-C10-C8-C9
27	G	311	CLA	C6-C7-C8-C9
27	H	209	CLA	C11-C10-C8-C9
27	K	312	CLA	C11-C10-C8-C9
27	M	310	CLA	C11-C10-C8-C9
27	a	821	CLA	C11-C12-C13-C14
27	a	840	CLA	C11-C10-C8-C9
27	b	825	CLA	C11-C10-C8-C9
29	a	852	LMG	O6-C5-C6-O5
31	E	316	LHG	O10-C23-O8-C6
31	D	201	LHG	O10-C23-O8-C6
27	b	801	CLA	C5-C6-C7-C8
27	H	208	CLA	O1D-CGD-O2D-CED
27	I	314	CLA	C2A-CAA-CBA-CGA
27	I	315	CLA	C2A-CAA-CBA-CGA
27	a	818	CLA	CBD-CGD-O2D-CED
27	L	312	CLA	C11-C10-C8-C9
27	D	214	CLA	C11-C10-C8-C9
27	L	309	CLA	C2C-C3C-CAC-CBC
31	D	201	LHG	C33-C34-C35-C36
27	F	306	CLA	C1A-C2A-CAA-CBA
27	G	307	CLA	C1A-C2A-CAA-CBA
27	L	318	CLA	C1A-C2A-CAA-CBA
27	a	830	CLA	C1A-C2A-CAA-CBA
27	b	849	CLA	C1A-C2A-CAA-CBA
29	I	319	LMG	C10-C11-C12-C13
27	C	307	CLA	C16-C17-C18-C19
31	b	836	LHG	C11-C10-C9-C8
27	H	204	CLA	C2-C1-O2A-CGA
27	a	815	CLA	C2-C1-O2A-CGA
27	i	101	CLA	C2-C1-O2A-CGA
29	A	214	LMG	C29-C28-O8-C9
29	J	317	LMG	C29-C28-O8-C9
31	H	215	LHG	C14-C15-C16-C17
30	G	302	A86	C24-C25-C26-C27
30	I	301	A86	C3-C4-C5-C6
32	m	102	BCR	C19-C20-C21-C22
27	I	306	CLA	O1D-CGD-O2D-CED
27	K	310	CLA	O1D-CGD-O2D-CED
27	F	308	CLA	O1D-CGD-O2D-CED
31	M	320	LHG	C26-C27-C28-C29
31	M	320	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	K	314	CLA	C3-C5-C6-C7
27	b	846	CLA	C3-C5-C6-C7
27	I	305	CLA	O1D-CGD-O2D-CED
27	A	204	CLA	C2-C3-C5-C6
27	b	824	CLA	C2-C3-C5-C6
31	B	315	LHG	C4-O6-P-O5
31	E	318	LHG	C3-O3-P-O5
31	E	318	LHG	C4-O6-P-O5
31	a	801	LHG	C3-O3-P-O5
31	a	802	LHG	C4-O6-P-O4
31	a	834	LHG	C3-O3-P-O5
31	D	201	LHG	C4-O6-P-O4
31	D	201	LHG	C4-O6-P-O5
31	b	836	LHG	C3-O3-P-O4
27	B	307	CLA	C16-C17-C18-C20
27	b	815	CLA	C16-C17-C18-C20
27	b	821	CLA	C16-C17-C18-C19
27	C	314	CLA	C2C-C3C-CAC-CBC
27	a	819	CLA	O2A-C1-C2-C3
27	l	203	CLA	O2A-C1-C2-C3
31	E	318	LHG	O6-C4-C5-C6
31	M	320	LHG	O6-C4-C5-C6
31	a	833	LHG	O6-C4-C5-C6
27	b	815	CLA	O1A-CGA-O2A-C1
27	f	302	CLA	O1D-CGD-O2D-CED
27	F	315	CLA	C4C-C3C-CAC-CBC
27	B	312	CLA	C8-C10-C11-C12
27	I	308	CLA	C2A-CAA-CBA-CGA
27	L	308	CLA	C2A-CAA-CBA-CGA
27	a	829	CLA	C2A-CAA-CBA-CGA
27	a	850	CLA	C3-C5-C6-C7
27	K	316	CLA	C5-C6-C7-C8
27	a	810	CLA	C15-C16-C17-C18
27	H	205	CLA	C16-C17-C18-C20
27	b	829	CLA	C16-C17-C18-C20
27	B	309	CLA	CAD-CBD-CGD-O1D
27	C	316	CLA	CAD-CBD-CGD-O1D
27	H	213	CLA	CAD-CBD-CGD-O1D
27	K	312	CLA	CAD-CBD-CGD-O1D
27	L	310	CLA	CAD-CBD-CGD-O1D
27	M	310	CLA	CAD-CBD-CGD-O1D
27	a	811	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	a	826	CLA	CAD-CBD-CGD-O1D
27	a	826	CLA	C2-C3-C5-C6
27	r	201	CLA	CAD-CBD-CGD-O1D
30	I	301	A86	C26-C27-C29-C30
27	L	309	CLA	C15-C16-C17-C18
27	a	838	CLA	C5-C6-C7-C8
27	a	843	CLA	C10-C11-C12-C13
31	B	315	LHG	C30-C31-C32-C33
27	L	307	CLA	C4C-C3C-CAC-CBC
27	b	811	CLA	C16-C17-C18-C20
27	b	818	CLA	C11-C12-C13-C15
27	B	308	CLA	C11-C12-C13-C15
27	B	309	CLA	C12-C13-C15-C16
27	B	312	CLA	C12-C13-C15-C16
27	C	309	CLA	C6-C7-C8-C10
27	F	305	CLA	C11-C10-C8-C7
27	G	312	CLA	C6-C7-C8-C10
27	H	209	CLA	C11-C10-C8-C7
27	J	312	CLA	C11-C12-C13-C15
27	L	309	CLA	C11-C10-C8-C7
27	L	309	CLA	C11-C12-C13-C15
27	L	310	CLA	C6-C7-C8-C10
27	L	310	CLA	C12-C13-C15-C16
27	L	316	CLA	C6-C7-C8-C10
27	M	310	CLA	C11-C10-C8-C7
27	a	815	CLA	C11-C12-C13-C15
27	a	816	CLA	C11-C10-C8-C7
27	a	840	CLA	C11-C10-C8-C7
27	a	840	CLA	C12-C13-C15-C16
27	b	815	CLA	C11-C12-C13-C15
27	b	825	CLA	C6-C7-C8-C10
31	E	318	LHG	O6-C4-C5-O7
31	a	833	LHG	O6-C4-C5-O7
29	A	214	LMG	C30-C31-C32-C33
30	I	303	A86	C24-C25-C26-C27
27	D	211	CLA	CBA-CGA-O2A-C1
29	C	301	LMG	C29-C30-C31-C32
29	J	317	LMG	C34-C35-C36-C37
31	D	201	LHG	C9-C10-C11-C12
27	G	311	CLA	C3-C5-C6-C7
27	A	208	CLA	C6-C7-C8-C9
31	a	802	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
33	J	318	SQD	C44-C45-C46-O48
29	A	214	LMG	O1-C7-C8-O7
31	M	320	LHG	O7-C5-C6-O8
31	a	834	LHG	O7-C5-C6-O8
31	b	836	LHG	O7-C5-C6-O8
33	J	318	SQD	O6-C44-C45-O47
37	b	835	DGD	O1G-C1G-C2G-O2G
31	a	802	LHG	C33-C34-C35-C36
27	M	308	CLA	C11-C12-C13-C15
27	a	812	CLA	C8-C10-C11-C12
27	M	318	CLA	O1D-CGD-O2D-CED
27	M	309	CLA	O1A-CGA-O2A-C1
27	M	309	CLA	CBA-CGA-O2A-C1
27	b	829	CLA	CBA-CGA-O2A-C1
31	I	318	LHG	C9-C10-C11-C12
30	L	306	A86	C13-C14-C15-C20
30	b	848	A86	C13-C14-C15-C20
27	K	310	CLA	C4C-C3C-CAC-CBC
29	M	321	LMG	C13-C14-C15-C16
27	A	204	CLA	C11-C12-C13-C14
27	B	306	CLA	C6-C7-C8-C9
27	B	309	CLA	C6-C7-C8-C9
27	B	311	CLA	C6-C7-C8-C9
27	E	308	CLA	C14-C13-C15-C16
27	H	213	CLA	C6-C7-C8-C9
27	J	309	CLA	C11-C10-C8-C9
27	J	312	CLA	C6-C7-C8-C9
27	J	314	CLA	C14-C13-C15-C16
27	L	312	CLA	C6-C7-C8-C9
27	a	822	CLA	C11-C12-C13-C14
27	a	838	CLA	C14-C13-C15-C16
27	a	842	CLA	C14-C13-C15-C16
27	a	855	CLA	C14-C13-C15-C16
27	f	301	CLA	C14-C13-C15-C16
27	l	204	CLA	C6-C7-C8-C9
27	D	208	CLA	C14-C13-C15-C16
27	b	806	CLA	C11-C10-C8-C9
27	b	809	CLA	C11-C12-C13-C14
27	b	813	CLA	C6-C7-C8-C9
29	A	214	LMG	O10-C28-O8-C9
29	J	317	LMG	O10-C28-O8-C9
31	M	320	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	C	311	CLA	C3-C5-C6-C7
27	a	840	CLA	C16-C17-C18-C19
27	b	829	CLA	C16-C17-C18-C19
27	b	847	CLA	C15-C16-C17-C18
27	r	201	CLA	C2C-C3C-CAC-CBC
31	M	320	LHG	O1-C1-C2-O2
27	a	803	CLA	C5-C6-C7-C8
26	E	306	DD6	C6-C8-C9-C10
26	D	205	DD6	C1-C24-C25-C26
30	B	301	A86	C6-C8-C9-C10
30	B	302	A86	C6-C8-C9-C10
30	B	304	A86	C6-C8-C9-C10
30	B	305	A86	C6-C8-C9-C10
30	C	302	A86	C6-C8-C9-C10
30	C	305	A86	C6-C8-C9-C10
30	E	301	A86	C6-C8-C9-C10
30	F	304	A86	C6-C8-C9-C10
30	G	302	A86	C6-C8-C9-C10
30	H	201	A86	C6-C8-C9-C10
30	H	203	A86	C6-C8-C9-C10
30	I	301	A86	C6-C8-C9-C10
30	I	303	A86	C6-C8-C9-C10
30	J	301	A86	C6-C8-C9-C10
30	J	304	A86	C6-C8-C9-C10
30	J	316	A86	C6-C8-C9-C10
30	M	302	A86	C6-C8-C9-C10
30	m	101	A86	C6-C8-C9-C10
30	r	202	A86	C6-C8-C9-C10
30	D	203	A86	C1-C24-C25-C26
30	D	203	A86	C6-C8-C9-C10
30	D	206	A86	C6-C8-C9-C10
30	b	848	A86	C1-C24-C25-C26
27	B	308	CLA	C3-C5-C6-C7
27	a	815	CLA	C5-C6-C7-C8
29	D	202	LMG	C11-C12-C13-C14
27	b	847	CLA	CAA-CBA-CGA-O2A
27	J	307	CLA	C10-C11-C12-C13
37	b	835	DGD	C4E-C5E-C6E-O5E
27	H	209	CLA	C3-C5-C6-C7
27	B	312	CLA	C2-C3-C5-C6
27	a	811	CLA	C2-C3-C5-C6
27	D	213	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	I	308	CLA	C16-C17-C18-C19
31	K	320	LHG	C18-C19-C20-C21
27	J	315	CLA	C1-C2-C3-C4
27	a	819	CLA	C1-C2-C3-C4
27	D	209	CLA	C1-C2-C3-C4
27	b	829	CLA	O1A-CGA-O2A-C1
27	J	315	CLA	C2C-C3C-CAC-CBC
27	K	316	CLA	C3-C5-C6-C7
31	a	801	LHG	C6-C5-O7-C7
31	b	836	LHG	C6-C5-O7-C7
31	a	837	LHG	O6-C4-C5-C6
27	C	307	CLA	C2A-CAA-CBA-CGA
27	H	207	CLA	C2A-CAA-CBA-CGA
27	K	311	CLA	C2A-CAA-CBA-CGA
27	M	308	CLA	C2A-CAA-CBA-CGA
27	a	805	CLA	C2A-CAA-CBA-CGA
27	a	827	CLA	C2A-CAA-CBA-CGA
27	F	307	CLA	O1A-CGA-O2A-C1
27	J	308	CLA	C2-C1-O2A-CGA
27	K	311	CLA	C2-C1-O2A-CGA
27	b	807	CLA	C2-C1-O2A-CGA
27	b	839	CLA	C2-C1-O2A-CGA
27	i	101	CLA	C11-C12-C13-C15
27	a	827	CLA	O1D-CGD-O2D-CED
29	C	319	LMG	C34-C35-C36-C37
31	B	315	LHG	C9-C10-C11-C12
27	I	315	CLA	C5-C6-C7-C8
30	J	301	A86	C12-C11-C13-C14
30	L	302	A86	C12-C11-C13-C14
30	L	305	A86	C12-C11-C13-C14
30	M	303	A86	C12-C11-C13-C14
27	F	307	CLA	CBA-CGA-O2A-C1
27	C	312	CLA	O1A-CGA-O2A-C1
31	E	316	LHG	O6-C4-C5-O7
27	F	306	CLA	C6-C7-C8-C10
27	i	101	CLA	O1D-CGD-O2D-CED
32	j	101	BCR	C23-C24-C25-C26
32	b	840	BCR	C1-C6-C7-C8
31	a	837	LHG	C25-C26-C27-C28
27	a	817	CLA	C10-C11-C12-C13
27	D	208	CLA	C13-C15-C16-C17
27	b	809	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	a	846	CLA	C2A-CAA-CBA-CGA
31	b	836	LHG	C35-C36-C37-C38
29	A	212	LMG	O7-C8-C9-O8
29	C	301	LMG	O1-C7-C8-O7
31	a	837	LHG	O7-C5-C6-O8
27	b	812	CLA	CBA-CGA-O2A-C1
31	E	316	LHG	C3-O3-P-O6
31	a	833	LHG	C3-O3-P-O6
31	a	837	LHG	C4-O6-P-O3
31	j	102	LHG	C4-O6-P-O3
31	b	836	LHG	C3-O3-P-O6
31	a	833	LHG	C27-C28-C29-C30
27	L	313	CLA	C5-C6-C7-C8
29	C	301	LMG	O1-C7-C8-C9
27	a	818	CLA	O1D-CGD-O2D-CED
27	A	205	CLA	C11-C10-C8-C7
27	G	311	CLA	C6-C7-C8-C10
27	I	308	CLA	C2-C3-C5-C6
27	a	815	CLA	C6-C7-C8-C10
27	b	806	CLA	C6-C7-C8-C10
27	b	824	CLA	C11-C10-C8-C7
29	E	317	LMG	C28-C29-C30-C31
27	B	309	CLA	C14-C13-C15-C16
27	B	312	CLA	C14-C13-C15-C16
27	C	309	CLA	C6-C7-C8-C9
27	F	307	CLA	C11-C10-C8-C9
27	G	312	CLA	C6-C7-C8-C9
27	K	314	CLA	C11-C10-C8-C9
27	M	307	CLA	C11-C12-C13-C14
27	M	309	CLA	C11-C10-C8-C9
27	a	816	CLA	C11-C10-C8-C9
27	a	840	CLA	C14-C13-C15-C16
27	b	801	CLA	C11-C10-C8-C9
27	b	808	CLA	C11-C12-C13-C14
27	b	815	CLA	C11-C12-C13-C14
27	b	846	CLA	C14-C13-C15-C16
26	A	201	DD6	C24-C25-C26-C27
32	j	105	BCR	C19-C20-C21-C22
27	B	307	CLA	C16-C17-C18-C19
27	D	217	CLA	C4C-C3C-CAC-CBC
37	b	835	DGD	CBB-CCB-CDB-CEB
27	L	316	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	b	847	CLA	C5-C6-C7-C8
27	b	812	CLA	O1A-CGA-O2A-C1
27	b	815	CLA	C16-C17-C18-C19
31	b	836	LHG	C5-C4-O6-P
27	J	312	CLA	C8-C10-C11-C12
27	b	819	CLA	C13-C15-C16-C17
27	A	207	CLA	C2C-C3C-CAC-CBC
27	G	312	CLA	C12-C13-C15-C16
27	A	205	CLA	C4-C3-C5-C6
31	I	318	LHG	O1-C1-C2-O2
27	H	210	CLA	C2-C3-C5-C6
31	a	801	LHG	C25-C26-C27-C28
27	b	811	CLA	C16-C17-C18-C19
27	C	312	CLA	CBA-CGA-O2A-C1
27	a	828	CLA	C10-C11-C12-C13
37	b	835	DGD	C1B-C2B-C3B-C4B
28	H	211	KC1	CAA-CBA-CGA-O1A
27	B	307	CLA	C2A-CAA-CBA-CGA
27	B	312	CLA	C2A-CAA-CBA-CGA
27	f	303	CLA	C2A-CAA-CBA-CGA
30	B	302	A86	C3-C4-C5-C6
30	H	201	A86	C3-C4-C5-C6
30	L	306	A86	C24-C25-C26-C27
32	a	853	BCR	C19-C20-C21-C22
29	J	317	LMG	C19-C20-C21-C22
31	H	215	LHG	O6-C4-C5-C6
31	a	833	LHG	C25-C26-C27-C28
31	D	201	LHG	C32-C33-C34-C35
27	a	809	CLA	C13-C15-C16-C17
29	M	321	LMG	C17-C18-C19-C20
27	J	315	CLA	O1A-CGA-O2A-C1
29	L	323	LMG	C14-C15-C16-C17
28	K	308	KC1	C4B-C3B-CAB-CBB
27	H	212	CLA	C4-C3-C5-C6
27	a	846	CLA	C4-C3-C5-C6
27	b	814	CLA	C4-C3-C5-C6
27	b	814	CLA	C2-C3-C5-C6
27	b	818	CLA	C2-C3-C5-C6
27	H	208	CLA	O1A-CGA-O2A-C1
27	K	312	CLA	C13-C15-C16-C17
27	l	204	CLA	C15-C16-C17-C18
27	C	311	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
27	E	308	CLA	C2-C1-O2A-CGA
27	L	307	CLA	C2-C1-O2A-CGA
27	b	830	CLA	C2-C1-O2A-CGA
30	G	302	A86	C33-C34-O4-C38
27	B	309	CLA	C15-C16-C17-C18
27	E	309	CLA	C10-C11-C12-C13
27	a	812	CLA	C2A-CAA-CBA-CGA
27	a	815	CLA	C2A-CAA-CBA-CGA
27	J	315	CLA	CBA-CGA-O2A-C1
27	b	803	CLA	CAA-CBA-CGA-O1A
27	I	308	CLA	C4C-C3C-CAC-CBC
31	a	833	LHG	C9-C10-C11-C12
27	A	205	CLA	C3A-C2A-CAA-CBA
27	I	309	CLA	C3A-C2A-CAA-CBA
29	a	852	LMG	O9-C10-O7-C8
29	L	323	LMG	O8-C28-C29-C30
31	M	320	LHG	O8-C23-C24-C25
27	H	209	CLA	C2C-C3C-CAC-CBC
27	M	308	CLA	C4-C3-C5-C6
27	a	832	CLA	C4-C3-C5-C6
27	b	818	CLA	C4-C3-C5-C6
27	M	308	CLA	C2-C3-C5-C6
27	a	832	CLA	C2-C3-C5-C6
26	G	305	DD6	C27-C29-C30-C31
27	C	307	CLA	C6-C7-C8-C9
27	C	312	CLA	C6-C7-C8-C9
27	I	311	CLA	C11-C10-C8-C9
27	J	314	CLA	C11-C12-C13-C14
27	L	316	CLA	C6-C7-C8-C9
27	M	309	CLA	C11-C12-C13-C14
27	M	313	CLA	C11-C12-C13-C14
27	b	801	CLA	C6-C7-C8-C9
27	b	803	CLA	C6-C7-C8-C9
27	b	807	CLA	C11-C10-C8-C9
27	A	204	CLA	C10-C11-C12-C13
27	E	309	CLA	C15-C16-C17-C18
26	E	306	DD6	C9-C10-C11-C12
26	E	306	DD6	C4-C5-C6-C7
26	D	205	DD6	C4-C5-C6-C7
30	L	304	A86	C-C1-C2-C3
30	L	304	A86	C4-C5-C6-C7
30	m	101	A86	C-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	m	101	A86	C4-C5-C6-C7
30	D	204	A86	C4-C5-C6-C7
30	b	848	A86	C-C1-C2-C3
32	f	304	BCR	C35-C13-C14-C15
32	l	202	BCR	C11-C10-C9-C34
32	m	102	BCR	C11-C10-C9-C34
29	L	323	LMG	C20-C21-C22-C23
31	a	837	LHG	C23-C24-C25-C26
32	f	305	BCR	C7-C8-C9-C34
32	b	834	BCR	C21-C22-C23-C24
31	K	320	LHG	C6-C5-O7-C7
27	a	817	CLA	C4-C3-C5-C6
27	E	310	CLA	C1A-C2A-CAA-CBA
27	F	311	CLA	C1A-C2A-CAA-CBA
27	I	309	CLA	C1A-C2A-CAA-CBA
27	K	312	CLA	C1A-C2A-CAA-CBA
27	K	319	CLA	C1A-C2A-CAA-CBA
27	a	810	CLA	C1A-C2A-CAA-CBA
27	a	820	CLA	C1A-C2A-CAA-CBA
27	a	838	CLA	C1A-C2A-CAA-CBA
27	a	841	CLA	C1A-C2A-CAA-CBA
27	l	203	CLA	C1A-C2A-CAA-CBA
31	a	801	LHG	C15-C16-C17-C18
27	b	803	CLA	C16-C17-C18-C19
27	C	311	CLA	C11-C10-C8-C7
27	E	311	CLA	C12-C13-C15-C16
27	I	306	CLA	C6-C7-C8-C10
27	I	311	CLA	C11-C12-C13-C15
27	J	309	CLA	C11-C10-C8-C7
27	M	307	CLA	C11-C10-C8-C7
27	M	308	CLA	C6-C7-C8-C10
27	a	817	CLA	C2-C3-C5-C6
27	a	827	CLA	C6-C7-C8-C10
27	a	828	CLA	C11-C10-C8-C7
27	l	204	CLA	C11-C10-C8-C7
27	b	818	CLA	C11-C10-C8-C7
27	b	827	CLA	C11-C10-C8-C7
27	b	838	CLA	C11-C10-C8-C7
27	a	811	CLA	C3-C5-C6-C7
27	r	201	CLA	C4C-C3C-CAC-CBC
29	J	317	LMG	C36-C37-C38-C39
27	b	845	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	b	841	CLA	O1D-CGD-O2D-CED
27	G	312	CLA	C2A-CAA-CBA-CGA
27	b	822	CLA	C2A-CAA-CBA-CGA
27	J	313	CLA	C2C-C3C-CAC-CBC
27	b	829	CLA	C15-C16-C17-C18
29	E	317	LMG	C18-C19-C20-C21
28	F	312	KC1	C3A-C2A-CAA-CBA
28	G	313	KC1	C3A-C2A-CAA-CBA
27	b	830	CLA	C8-C10-C11-C12
27	L	317	CLA	CAA-CBA-CGA-O1A
27	L	317	CLA	CAA-CBA-CGA-O2A
27	b	806	CLA	C4-C3-C5-C6
37	b	835	DGD	C2A-C3A-C4A-C5A
27	E	311	CLA	C13-C15-C16-C17
27	b	838	CLA	C8-C10-C11-C12
29	D	202	LMG	C20-C21-C22-C23
27	b	813	CLA	C3-C5-C6-C7
27	b	845	CLA	CBD-CGD-O2D-CED
37	b	835	DGD	O1B-C1B-O2G-C2G
31	M	320	LHG	C11-C12-C13-C14
31	j	102	LHG	C16-C17-C18-C19
26	E	306	DD6	C9-C10-C11-C13
26	E	306	DD6	C4-C5-C6-C8
26	D	205	DD6	C4-C5-C6-C8
30	F	301	A86	C13-C14-C15-C16
30	I	301	A86	C13-C14-C15-C16
30	L	304	A86	C24-C1-C2-C3
30	L	304	A86	C4-C5-C6-C8
30	m	101	A86	C24-C1-C2-C3
30	m	101	A86	C4-C5-C6-C8
30	D	204	A86	C4-C5-C6-C8
30	b	848	A86	C24-C1-C2-C3
32	f	304	BCR	C12-C13-C14-C15
32	l	202	BCR	C11-C10-C9-C8
32	m	102	BCR	C11-C10-C9-C8
29	j	103	LMG	O7-C8-C9-O8
27	a	856	CLA	C2C-C3C-CAC-CBC
27	a	816	CLA	CAA-CBA-CGA-O2A
27	C	311	CLA	C4C-C3C-CAC-CBC
37	b	835	DGD	C9A-CAA-CBA-CCA
26	E	303	DD6	C1-C2-C3-C4
26	M	301	DD6	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	K	307	A86	C24-C25-C26-C27
27	a	842	CLA	C8-C10-C11-C12
27	l	204	CLA	C16-C17-C18-C19
31	a	833	LHG	C17-C18-C19-C20
30	B	301	A86	C10-C11-C13-C14
30	G	302	A86	C10-C11-C13-C14
30	L	305	A86	C10-C11-C13-C14
27	b	825	CLA	C2C-C3C-CAC-CBC
27	a	810	CLA	C8-C10-C11-C12
27	b	850	CLA	C10-C11-C12-C13
27	F	306	CLA	C2-C1-O2A-CGA
27	I	307	CLA	C2-C1-O2A-CGA
27	a	805	CLA	C2-C1-O2A-CGA
27	a	844	CLA	C2-C1-O2A-CGA
27	b	825	CLA	C2-C1-O2A-CGA
27	H	212	CLA	C2-C3-C5-C6
27	a	807	CLA	C2-C3-C5-C6
27	I	315	CLA	C4C-C3C-CAC-CBC
27	H	206	CLA	C10-C11-C12-C13
27	b	843	CLA	C10-C11-C12-C13
29	C	319	LMG	C15-C16-C17-C18
27	J	314	CLA	CAA-CBA-CGA-O2A
27	I	308	CLA	C16-C17-C18-C20
27	K	309	CLA	C16-C17-C18-C19
27	C	309	CLA	C11-C10-C8-C9
27	b	811	CLA	C6-C7-C8-C9
31	B	315	LHG	C23-C24-C25-C26
31	a	834	LHG	O2-C2-C3-O3
27	B	309	CLA	C2A-CAA-CBA-CGA
27	K	316	CLA	C2A-CAA-CBA-CGA
27	b	807	CLA	C2A-CAA-CBA-CGA
27	b	827	CLA	C2A-CAA-CBA-CGA
27	K	316	CLA	C16-C17-C18-C19
27	D	209	CLA	O2A-C1-C2-C3
27	C	309	CLA	C4C-C3C-CAC-CBC
32	j	101	BCR	C23-C24-C25-C30
32	l	202	BCR	C23-C24-C25-C30
27	a	803	CLA	CAA-CBA-CGA-O2A
31	M	320	LHG	O1-C1-C2-C3
29	l	201	LMG	C12-C13-C14-C15
26	F	302	DD6	C1-C2-C3-C4
26	I	304	DD6	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	I	304	DD6	C3-C4-C5-C6
26	L	301	DD6	C24-C25-C26-C27
30	J	316	A86	C3-C4-C5-C6
30	M	305	A86	C11-C10-C9-C8
27	a	839	CLA	C4-C3-C5-C6
27	b	801	CLA	C4-C3-C5-C6
27	b	804	CLA	C4-C3-C5-C6
27	b	838	CLA	C4-C3-C5-C6
32	a	853	BCR	C17-C18-C19-C20
27	L	309	CLA	C8-C10-C11-C12
29	a	852	LMG	C32-C33-C34-C35
31	B	315	LHG	C13-C14-C15-C16
27	H	214	CLA	CAA-CBA-CGA-O2A
27	K	312	CLA	C4C-C3C-CAC-CBC
27	H	209	CLA	C10-C11-C12-C13
29	j	103	LMG	C8-C7-O1-C1
37	b	835	DGD	C2B-C1B-O2G-C2G
27	J	315	CLA	C4C-C3C-CAC-CBC
28	K	308	KC1	CAA-CBA-CGA-O2A
29	A	212	LMG	C36-C37-C38-C39
27	J	314	CLA	C16-C17-C18-C20
27	a	828	CLA	C2A-CAA-CBA-CGA
27	b	825	CLA	C2A-CAA-CBA-CGA
27	E	313	CLA	O1D-CGD-O2D-CED
27	b	841	CLA	CBD-CGD-O2D-CED
27	B	306	CLA	C4-C3-C5-C6
27	B	308	CLA	C4-C3-C5-C6
27	b	849	CLA	C5-C6-C7-C8
27	a	805	CLA	C11-C12-C13-C15
27	b	809	CLA	C11-C12-C13-C15
27	b	811	CLA	C6-C7-C8-C10
27	b	821	CLA	C2-C3-C5-C6
29	E	317	LMG	C31-C32-C33-C34
35	l	207	ET4	C19-C20-C21-C22
27	a	807	CLA	CAA-CBA-CGA-O2A
27	L	308	CLA	C16-C17-C18-C20
27	L	319	CLA	C4C-C3C-CAC-CBC
27	i	101	CLA	C10-C11-C12-C13
27	b	823	CLA	CBA-CGA-O2A-C1
27	B	311	CLA	C13-C15-C16-C17
27	a	845	CLA	C13-C15-C16-C17
27	a	825	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	D	214	CLA	O1D-CGD-O2D-CED
27	b	845	CLA	O1D-CGD-O2D-CED
29	a	852	LMG	C11-C10-O7-C8
31	I	318	LHG	C25-C26-C27-C28
27	C	306	CLA	CAA-CBA-CGA-O2A
27	G	311	CLA	CBA-CGA-O2A-C1
27	M	310	CLA	CBA-CGA-O2A-C1
27	D	214	CLA	CBA-CGA-O2A-C1
31	K	320	LHG	C4-O6-P-O4
27	F	317	CLA	CAA-CBA-CGA-O2A
27	b	825	CLA	CAA-CBA-CGA-O2A
27	a	820	CLA	C2C-C3C-CAC-CBC
27	a	844	CLA	C4C-C3C-CAC-CBC
30	I	301	A86	C33-C34-O4-C38
27	M	310	CLA	C2C-C3C-CAC-CBC
27	b	823	CLA	O1A-CGA-O2A-C1
31	a	833	LHG	C30-C31-C32-C33
27	F	305	CLA	C11-C10-C8-C9
27	I	306	CLA	C6-C7-C8-C9
27	a	828	CLA	C11-C10-C8-C9
27	i	101	CLA	C6-C7-C8-C9
27	l	204	CLA	C11-C12-C13-C14
31	j	102	LHG	C18-C19-C20-C21
27	A	204	CLA	C3A-C2A-CAA-CBA
27	E	312	CLA	C3A-C2A-CAA-CBA
27	E	315	CLA	C3A-C2A-CAA-CBA
27	b	844	CLA	C3A-C2A-CAA-CBA
27	b	850	CLA	C3A-C2A-CAA-CBA
27	a	829	CLA	C5-C6-C7-C8
27	a	838	CLA	C15-C16-C17-C18
27	G	311	CLA	O1A-CGA-O2A-C1
27	D	214	CLA	O1A-CGA-O2A-C1
31	H	215	LHG	C17-C18-C19-C20
27	a	814	CLA	CAA-CBA-CGA-O2A
27	C	307	CLA	CAD-CBD-CGD-O2D
27	C	318	CLA	CAD-CBD-CGD-O2D
27	F	308	CLA	CAD-CBD-CGD-O2D
27	F	317	CLA	CAD-CBD-CGD-O2D
27	I	317	CLA	CAD-CBD-CGD-O2D
27	J	311	CLA	CAD-CBD-CGD-O2D
27	J	315	CLA	CAD-CBD-CGD-O2D
27	K	310	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	K	313	CLA	CAD-CBD-CGD-O2D
27	L	313	CLA	CAD-CBD-CGD-O2D
27	L	317	CLA	CAD-CBD-CGD-O2D
27	L	319	CLA	CAD-CBD-CGD-O2D
27	M	309	CLA	CAD-CBD-CGD-O2D
27	a	808	CLA	CAD-CBD-CGD-O2D
27	a	812	CLA	CAD-CBD-CGD-O2D
27	a	827	CLA	CAD-CBD-CGD-O2D
27	a	855	CLA	CAD-CBD-CGD-O2D
27	f	302	CLA	CAD-CBD-CGD-O2D
27	l	206	CLA	CAD-CBD-CGD-O2D
27	D	212	CLA	CAD-CBD-CGD-O2D
27	D	217	CLA	CAD-CBD-CGD-O2D
27	b	806	CLA	CAD-CBD-CGD-O2D
27	b	807	CLA	CAD-CBD-CGD-O2D
27	b	811	CLA	CAD-CBD-CGD-O2D
27	b	814	CLA	CAD-CBD-CGD-O2D
27	b	822	CLA	CAD-CBD-CGD-O2D
27	b	826	CLA	CAD-CBD-CGD-O2D
27	b	830	CLA	CAD-CBD-CGD-O2D
27	b	844	CLA	CAD-CBD-CGD-O2D
27	b	846	CLA	CAD-CBD-CGD-O2D
28	A	209	KC1	CAD-CBD-CGD-O2D
28	C	313	KC1	CAD-CBD-CGD-O2D
28	K	308	KC1	CAD-CBD-CGD-O2D
28	M	314	KC1	CAD-CBD-CGD-O2D
30	b	848	A86	C28-C27-C29-C30
31	K	320	LHG	C4-C5-O7-C7
27	I	311	CLA	C10-C11-C12-C13
27	M	318	CLA	C2A-CAA-CBA-CGA
27	J	313	CLA	C4C-C3C-CAC-CBC
27	D	214	CLA	CBD-CGD-O2D-CED
27	b	811	CLA	C15-C16-C17-C18
27	F	305	CLA	C2-C1-O2A-CGA
27	L	309	CLA	C2-C1-O2A-CGA
31	K	320	LHG	C16-C17-C18-C19
33	J	318	SQD	C25-C26-C27-C28
29	D	202	LMG	C10-C11-C12-C13
27	a	815	CLA	CAA-CBA-CGA-O2A
27	b	807	CLA	C10-C11-C12-C13
27	C	309	CLA	C4-C3-C5-C6
27	a	807	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	b	847	CLA	C16-C17-C18-C20
27	H	214	CLA	CAA-CBA-CGA-O1A
27	I	307	CLA	C2-C3-C5-C6
27	b	806	CLA	C2-C3-C5-C6
27	b	838	CLA	C2-C3-C5-C6
27	b	843	CLA	C2-C3-C5-C6
27	B	306	CLA	CAA-CBA-CGA-O2A
27	F	311	CLA	CAA-CBA-CGA-O2A
27	M	312	CLA	CAA-CBA-CGA-O2A
27	D	209	CLA	CAA-CBA-CGA-O2A
26	E	302	DD6	C13-C14-C15-O1
26	F	303	DD6	C13-C14-C15-O1
26	G	305	DD6	C13-C14-C15-O1
26	I	302	DD6	C13-C14-C15-O1
30	B	301	A86	C12-C11-C13-O
30	G	302	A86	C12-C11-C13-O
30	J	301	A86	C12-C11-C13-O
30	L	302	A86	C12-C11-C13-O
30	b	848	A86	C12-C11-C13-O
27	a	810	CLA	CAA-CBA-CGA-O2A
27	D	211	CLA	CAA-CBA-CGA-O2A
27	b	818	CLA	CAA-CBA-CGA-O2A
27	b	845	CLA	CAA-CBA-CGA-O2A
31	E	316	LHG	C16-C17-C18-C19
27	M	309	CLA	O2A-C1-C2-C3
27	a	838	CLA	O2A-C1-C2-C3
27	M	310	CLA	O1A-CGA-O2A-C1
31	a	801	LHG	C9-C10-C11-C12
27	E	308	CLA	C2A-CAA-CBA-CGA
27	b	814	CLA	C2A-CAA-CBA-CGA
27	K	314	CLA	C15-C16-C17-C18
27	H	209	CLA	C11-C12-C13-C14
27	E	313	CLA	CBD-CGD-O2D-CED
31	a	837	LHG	C27-C28-C29-C30
27	B	311	CLA	CHA-CBD-CGD-O2D
27	F	305	CLA	CHA-CBD-CGD-O1D
27	F	305	CLA	CHA-CBD-CGD-O2D
27	F	315	CLA	CHA-CBD-CGD-O1D
27	G	306	CLA	CHA-CBD-CGD-O1D
27	G	306	CLA	CHA-CBD-CGD-O2D
27	G	307	CLA	CHA-CBD-CGD-O1D
27	G	308	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	H	206	CLA	CHA-CBD-CGD-O1D
27	H	206	CLA	CHA-CBD-CGD-O2D
27	I	310	CLA	CHA-CBD-CGD-O2D
27	I	316	CLA	CHA-CBD-CGD-O1D
27	I	316	CLA	CHA-CBD-CGD-O2D
27	J	307	CLA	CHA-CBD-CGD-O2D
27	J	313	CLA	CHA-CBD-CGD-O2D
27	K	316	CLA	CHA-CBD-CGD-O1D
27	K	316	CLA	CHA-CBD-CGD-O2D
27	L	308	CLA	CHA-CBD-CGD-O1D
27	L	308	CLA	CHA-CBD-CGD-O2D
27	L	315	CLA	CHA-CBD-CGD-O2D
27	a	803	CLA	CHA-CBD-CGD-O2D
27	a	807	CLA	CHA-CBD-CGD-O1D
27	a	813	CLA	CHA-CBD-CGD-O1D
27	a	818	CLA	CHA-CBD-CGD-O2D
27	a	823	CLA	CHA-CBD-CGD-O1D
27	a	832	CLA	CHA-CBD-CGD-O2D
27	a	841	CLA	CHA-CBD-CGD-O1D
27	a	841	CLA	CHA-CBD-CGD-O2D
27	a	845	CLA	CHA-CBD-CGD-O2D
27	a	846	CLA	CHA-CBD-CGD-O2D
27	f	301	CLA	CHA-CBD-CGD-O1D
27	f	301	CLA	CHA-CBD-CGD-O2D
27	l	204	CLA	CHA-CBD-CGD-O1D
27	l	204	CLA	CHA-CBD-CGD-O2D
27	b	805	CLA	CHA-CBD-CGD-O2D
27	b	808	CLA	CHA-CBD-CGD-O1D
27	b	808	CLA	CHA-CBD-CGD-O2D
27	b	813	CLA	CHA-CBD-CGD-O2D
27	b	816	CLA	CHA-CBD-CGD-O1D
27	b	823	CLA	CHA-CBD-CGD-O1D
27	b	823	CLA	CHA-CBD-CGD-O2D
27	b	824	CLA	CHA-CBD-CGD-O1D
27	b	824	CLA	CHA-CBD-CGD-O2D
27	b	839	CLA	CHA-CBD-CGD-O1D
27	b	842	CLA	CHA-CBD-CGD-O1D
27	b	842	CLA	CHA-CBD-CGD-O2D
27	b	849	CLA	CHA-CBD-CGD-O1D
27	b	849	CLA	CHA-CBD-CGD-O2D
28	J	306	KC1	CHA-CBD-CGD-O2D
28	L	314	KC1	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	L	322	KC1	CHA-CBD-CGD-O2D
30	J	304	A86	C3-C4-C5-C6
30	L	306	A86	C1-C2-C3-C4
27	C	306	CLA	CAA-CBA-CGA-O1A
27	a	825	CLA	CAA-CBA-CGA-O1A
27	G	317	CLA	CAA-CBA-CGA-O2A
27	a	819	CLA	CAA-CBA-CGA-O2A
31	B	315	LHG	O7-C7-C8-C9
27	b	801	CLA	C2-C3-C5-C6
27	A	207	CLA	C8-C10-C11-C12
31	E	316	LHG	O6-C4-C5-C6
31	a	801	LHG	C32-C33-C34-C35
27	b	808	CLA	C16-C17-C18-C19
31	a	833	LHG	O8-C23-C24-C25
33	J	318	SQD	C33-C34-C35-C36
27	l	204	CLA	O1A-CGA-O2A-C1
27	a	840	CLA	C13-C15-C16-C17
27	a	814	CLA	CAA-CBA-CGA-O1A
27	D	211	CLA	O1A-CGA-O2A-C1
27	F	307	CLA	CAA-CBA-CGA-O2A
27	b	850	CLA	CAA-CBA-CGA-O2A
31	a	837	LHG	C29-C30-C31-C32
27	J	307	CLA	C2A-CAA-CBA-CGA
27	F	306	CLA	C6-C7-C8-C9
30	B	301	A86	C10-C11-C13-O
30	J	301	A86	C10-C11-C13-O
30	L	302	A86	C10-C11-C13-O
30	D	206	A86	C13-C14-C15-O1
30	b	848	A86	C13-C14-C15-O1
27	l	204	CLA	CBA-CGA-O2A-C1
31	a	802	LHG	C17-C18-C19-C20
27	G	309	CLA	CAA-CBA-CGA-O2A
27	a	813	CLA	CAA-CBA-CGA-O2A
29	A	212	LMG	C21-C22-C23-C24
27	G	316	CLA	C4-C3-C5-C6
27	A	205	CLA	C2-C3-C5-C6
27	a	809	CLA	C16-C17-C18-C19
27	B	306	CLA	C10-C11-C12-C13
27	I	310	CLA	CAA-CBA-CGA-O2A
27	L	309	CLA	CAA-CBA-CGA-O2A
29	J	317	LMG	O7-C10-C11-C12
27	G	309	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	J	308	CLA	C6-C7-C8-C9
27	K	314	CLA	C11-C12-C13-C14
27	a	804	CLA	C14-C13-C15-C16
27	a	817	CLA	C11-C10-C8-C9
27	a	827	CLA	C6-C7-C8-C9
27	a	848	CLA	C14-C13-C15-C16
27	b	820	CLA	C11-C10-C8-C9
27	b	824	CLA	C11-C10-C8-C9
27	b	827	CLA	C11-C10-C8-C9
27	b	843	CLA	C6-C7-C8-C9
30	D	206	A86	C3-C4-C5-C6
27	b	830	CLA	C2C-C3C-CAC-CBC
27	b	847	CLA	C13-C15-C16-C17
29	D	202	LMG	C21-C22-C23-C24
27	K	319	CLA	CAA-CBA-CGA-O2A
27	L	307	CLA	CAA-CBA-CGA-O2A
33	J	318	SQD	O48-C23-C24-C25
27	K	316	CLA	CAA-CBA-CGA-O1A
27	E	312	CLA	C2A-CAA-CBA-CGA
27	L	316	CLA	C2A-CAA-CBA-CGA
27	r	201	CLA	C2A-CAA-CBA-CGA
27	D	209	CLA	CAA-CBA-CGA-O1A
29	M	321	LMG	C12-C13-C14-C15
27	b	849	CLA	CBA-CGA-O2A-C1
27	F	317	CLA	CAA-CBA-CGA-O1A
27	b	825	CLA	CAA-CBA-CGA-O1A
31	D	201	LHG	C17-C18-C19-C20
27	a	849	CLA	CAA-CBA-CGA-O2A
27	G	317	CLA	CAA-CBA-CGA-O1A
27	D	211	CLA	CAA-CBA-CGA-O1A
30	K	306	A86	C5-C6-C8-C9
27	a	807	CLA	CBA-CGA-O2A-C1
31	b	836	LHG	C24-C23-O8-C6
29	L	323	LMG	C35-C36-C37-C38
27	A	204	CLA	C1A-C2A-CAA-CBA
27	A	205	CLA	C1A-C2A-CAA-CBA
27	E	309	CLA	C1A-C2A-CAA-CBA
27	E	312	CLA	C1A-C2A-CAA-CBA
27	E	315	CLA	C1A-C2A-CAA-CBA
27	a	812	CLA	C1A-C2A-CAA-CBA
27	a	845	CLA	C1A-C2A-CAA-CBA
27	a	855	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	f	301	CLA	C1A-C2A-CAA-CBA
27	F	311	CLA	CAA-CBA-CGA-O1A
27	a	810	CLA	CAA-CBA-CGA-O1A
27	b	818	CLA	CAA-CBA-CGA-O1A
31	b	836	LHG	O10-C23-O8-C6
27	L	307	CLA	CAA-CBA-CGA-O1A
27	a	819	CLA	CAA-CBA-CGA-O1A
31	M	320	LHG	C15-C16-C17-C18
29	I	319	LMG	C7-C8-C9-O8
27	b	809	CLA	CAA-CBA-CGA-O2A
27	F	308	CLA	C2A-CAA-CBA-CGA
27	G	307	CLA	C2A-CAA-CBA-CGA
27	I	306	CLA	C2A-CAA-CBA-CGA
27	L	307	CLA	C2A-CAA-CBA-CGA
27	b	847	CLA	C16-C17-C18-C19
31	a	833	LHG	O10-C23-C24-C25
27	H	206	CLA	O1D-CGD-O2D-CED
31	j	102	LHG	C29-C30-C31-C32
27	I	310	CLA	CAA-CBA-CGA-O1A
27	b	849	CLA	O1A-CGA-O2A-C1
27	M	313	CLA	C5-C6-C7-C8
28	K	315	KC1	C4C-C3C-CAC-CBC
31	E	318	LHG	C3-O3-P-O4
31	E	318	LHG	C4-O6-P-O4
31	a	837	LHG	C4-O6-P-O5
31	j	102	LHG	C3-O3-P-O5
27	F	307	CLA	CAA-CBA-CGA-O1A
27	G	306	CLA	CAA-CBA-CGA-O1A
27	L	309	CLA	CAA-CBA-CGA-O1A
27	M	312	CLA	CAA-CBA-CGA-O1A
27	a	810	CLA	C5-C6-C7-C8
27	a	818	CLA	CAA-CBA-CGA-O2A
27	C	309	CLA	C10-C11-C12-C13
31	B	315	LHG	O9-C7-C8-C9
33	J	318	SQD	O10-C23-C24-C25
27	r	201	CLA	CAA-CBA-CGA-O2A
27	C	309	CLA	C2C-C3C-CAC-CBC
27	E	315	CLA	C2A-CAA-CBA-CGA
27	B	306	CLA	CAA-CBA-CGA-O1A
27	f	302	CLA	C5-C6-C7-C8
29	L	323	LMG	C29-C30-C31-C32
28	A	209	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	a	815	CLA	CAA-CBA-CGA-O1A
27	b	845	CLA	CAA-CBA-CGA-O1A
27	H	204	CLA	O1D-CGD-O2D-CED
27	b	808	CLA	C16-C17-C18-C20
27	b	846	CLA	C16-C17-C18-C20
27	J	314	CLA	C4C-C3C-CAC-CBC
27	C	314	CLA	CAD-CBD-CGD-O1D
27	F	315	CLA	C3-C5-C6-C7
27	I	308	CLA	CAD-CBD-CGD-O1D
27	J	312	CLA	CAD-CBD-CGD-O1D
27	L	316	CLA	CAD-CBD-CGD-O1D
27	a	807	CLA	CAD-CBD-CGD-O1D
27	a	846	CLA	CAD-CBD-CGD-O1D
27	b	812	CLA	CAD-CBD-CGD-O1D
27	b	823	CLA	CAD-CBD-CGD-O1D
27	b	827	CLA	CAD-CBD-CGD-O1D
27	b	842	CLA	CAD-CBD-CGD-O1D
30	D	203	A86	C26-C27-C29-C30
27	a	813	CLA	CAA-CBA-CGA-O1A
27	E	311	CLA	C11-C10-C8-C9
27	a	805	CLA	C14-C13-C15-C16
27	a	822	CLA	C14-C13-C15-C16
27	a	830	CLA	C6-C7-C8-C9
27	b	812	CLA	C11-C10-C8-C9
27	b	819	CLA	C6-C7-C8-C9
27	r	201	CLA	CAA-CBA-CGA-O1A
27	K	312	CLA	C15-C16-C17-C18
27	a	804	CLA	C15-C16-C17-C18
27	H	208	CLA	CAA-CBA-CGA-O1A
27	E	310	CLA	CAA-CBA-CGA-O2A
27	G	312	CLA	CAA-CBA-CGA-O2A
27	J	315	CLA	CAA-CBA-CGA-O2A
27	M	318	CLA	CAA-CBA-CGA-O2A
27	a	824	CLA	CAA-CBA-CGA-O2A
27	D	214	CLA	CAA-CBA-CGA-O2A
27	b	807	CLA	CAA-CBA-CGA-O2A
27	L	313	CLA	C4C-C3C-CAC-CBC
29	J	317	LMG	C40-C41-C42-C43
27	b	809	CLA	C13-C15-C16-C17
27	a	841	CLA	C10-C11-C12-C13
27	A	203	CLA	O1D-CGD-O2D-CED
27	E	308	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	a	829	CLA	CAA-CBA-CGA-O2A
27	D	207	CLA	CAA-CBA-CGA-O2A
29	E	317	LMG	O7-C10-C11-C12
27	K	319	CLA	CAA-CBA-CGA-O1A
27	I	307	CLA	C4-C3-C5-C6
27	b	843	CLA	C4-C3-C5-C6
27	I	306	CLA	C15-C16-C17-C18
27	K	309	CLA	C15-C16-C17-C18
27	B	309	CLA	C6-C7-C8-C10
27	E	311	CLA	C11-C10-C8-C7
27	G	309	CLA	C6-C7-C8-C10
27	J	307	CLA	C6-C7-C8-C10
27	J	308	CLA	C6-C7-C8-C10
27	K	310	CLA	C6-C7-C8-C10
27	M	319	CLA	C3A-C2A-CAA-CBA
27	a	807	CLA	C6-C7-C8-C10
27	a	817	CLA	C11-C10-C8-C7
27	a	822	CLA	C12-C13-C15-C16
27	a	846	CLA	C2-C3-C5-C6
27	b	819	CLA	C6-C7-C8-C10
27	b	820	CLA	C11-C10-C8-C7
27	b	830	CLA	C11-C10-C8-C7
27	G	308	CLA	CAA-CBA-CGA-O1A
27	b	807	CLA	CAA-CBA-CGA-O1A
27	b	850	CLA	CAA-CBA-CGA-O1A
27	l	206	CLA	CAA-CBA-CGA-O2A
27	B	309	CLA	CAA-CBA-CGA-O2A
27	C	307	CLA	CAA-CBA-CGA-O2A
27	F	308	CLA	CAA-CBA-CGA-O2A
27	F	314	CLA	CAA-CBA-CGA-O2A
27	G	308	CLA	CAA-CBA-CGA-O2A
27	J	309	CLA	CAA-CBA-CGA-O2A
27	M	309	CLA	CAA-CBA-CGA-O2A
27	a	809	CLA	CAA-CBA-CGA-O2A
27	b	810	CLA	CAA-CBA-CGA-O2A
27	b	823	CLA	CAA-CBA-CGA-O2A
31	a	834	LHG	O8-C23-C24-C25
27	b	815	CLA	C13-C15-C16-C17
32	f	305	BCR	C7-C8-C9-C10
32	l	202	BCR	C21-C22-C23-C24
27	F	308	CLA	CAA-CBA-CGA-O1A
30	D	203	A86	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
27	a	808	CLA	C16-C17-C18-C20
30	F	301	A86	O-C13-C14-C15
27	F	315	CLA	CAA-CBA-CGA-O2A
27	a	828	CLA	CAA-CBA-CGA-O2A
27	b	813	CLA	CAA-CBA-CGA-O2A
31	j	102	LHG	C17-C18-C19-C20
27	a	806	CLA	O1D-CGD-O2D-CED
27	b	820	CLA	C10-C11-C12-C13
27	a	807	CLA	O1A-CGA-O2A-C1
27	G	309	CLA	CAA-CBA-CGA-O1A
27	D	214	CLA	CAA-CBA-CGA-O1A
27	D	210	CLA	O1A-CGA-O2A-C1
27	E	315	CLA	CAA-CBA-CGA-O2A
27	M	311	CLA	CAA-CBA-CGA-O2A
27	b	804	CLA	CAA-CBA-CGA-O2A
27	G	312	CLA	CAA-CBA-CGA-O1A
27	a	849	CLA	CAA-CBA-CGA-O1A
27	b	826	CLA	C2A-CAA-CBA-CGA
28	A	209	KC1	C2C-C3C-CAC-CBC
27	J	309	CLA	CAA-CBA-CGA-O1A
27	J	315	CLA	CAA-CBA-CGA-O1A
27	a	845	CLA	CAA-CBA-CGA-O2A
27	b	828	CLA	CAA-CBA-CGA-O2A
27	b	838	CLA	CAA-CBA-CGA-O2A
27	J	311	CLA	C10-C11-C12-C13

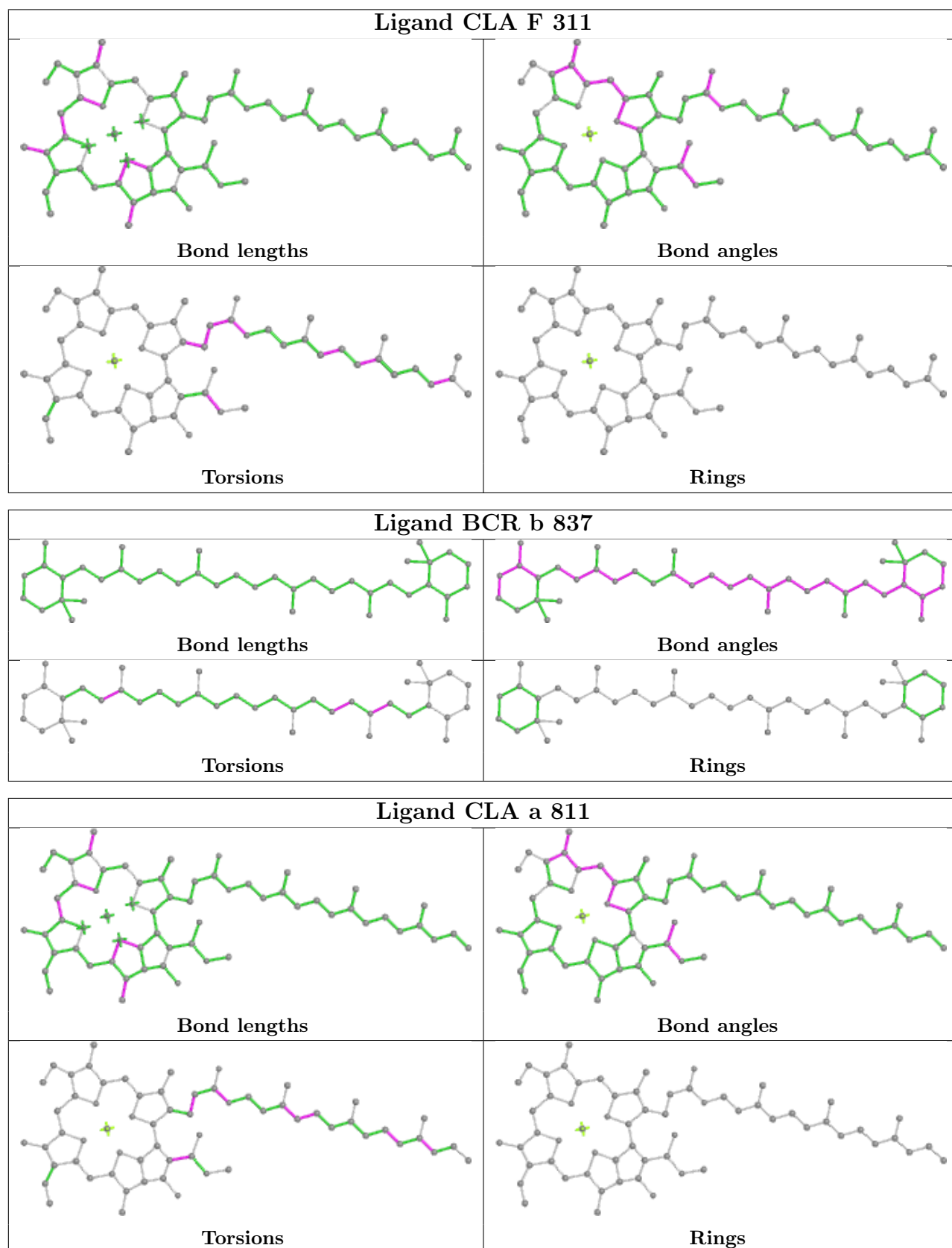
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	K	307	A86	C31-C32-C33-C34-C35-C36

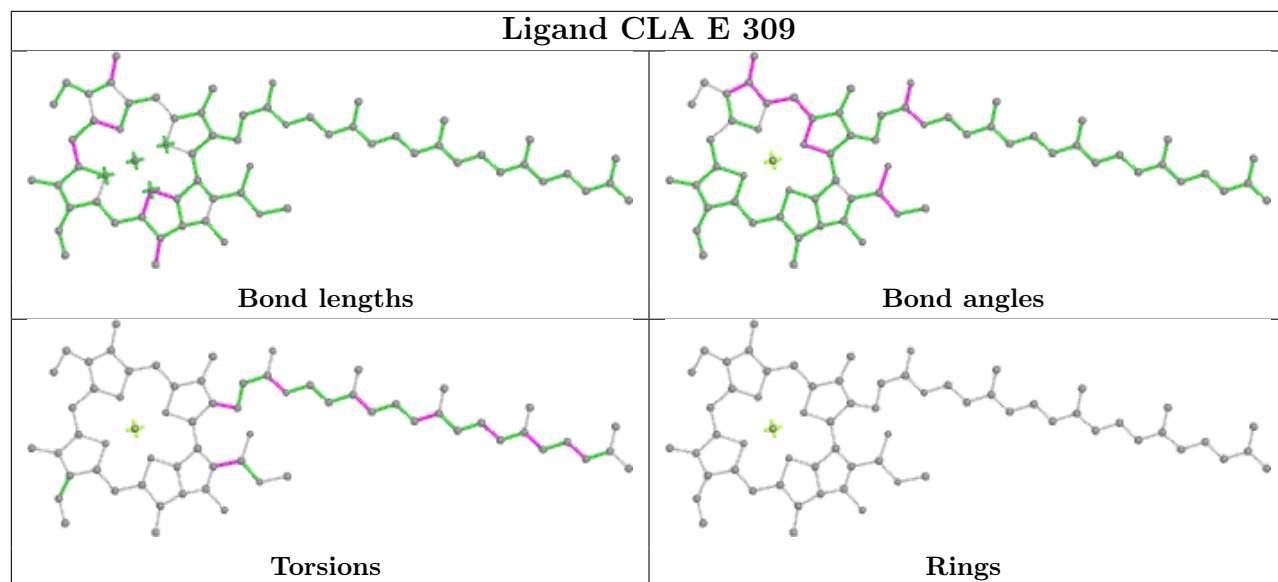
No monomer is involved in short contacts.

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.

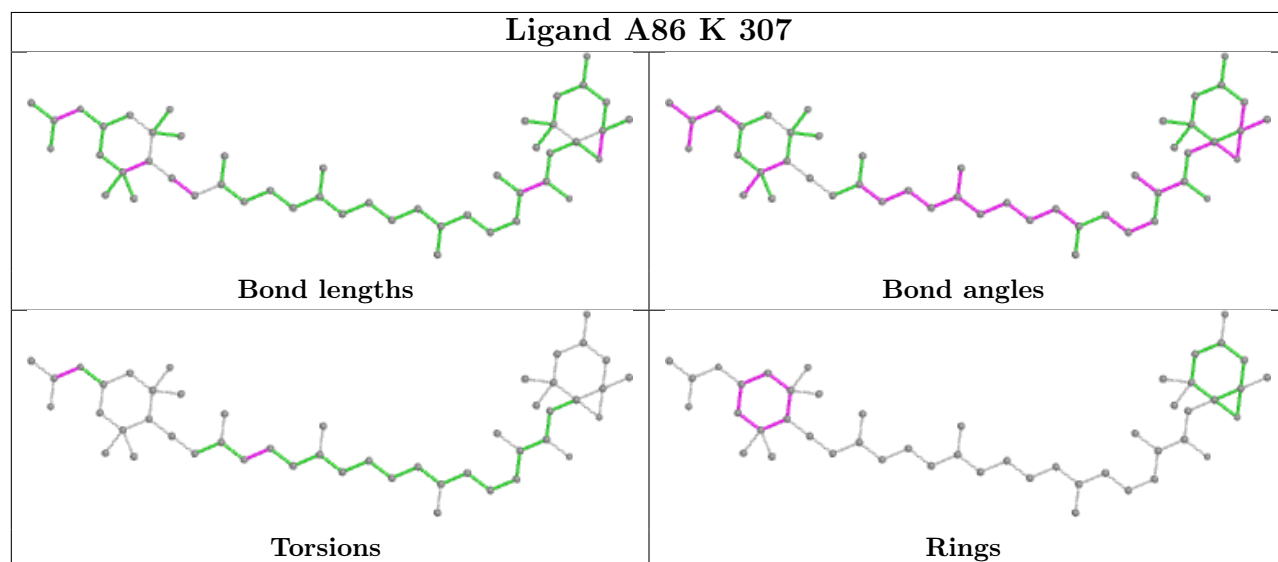
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



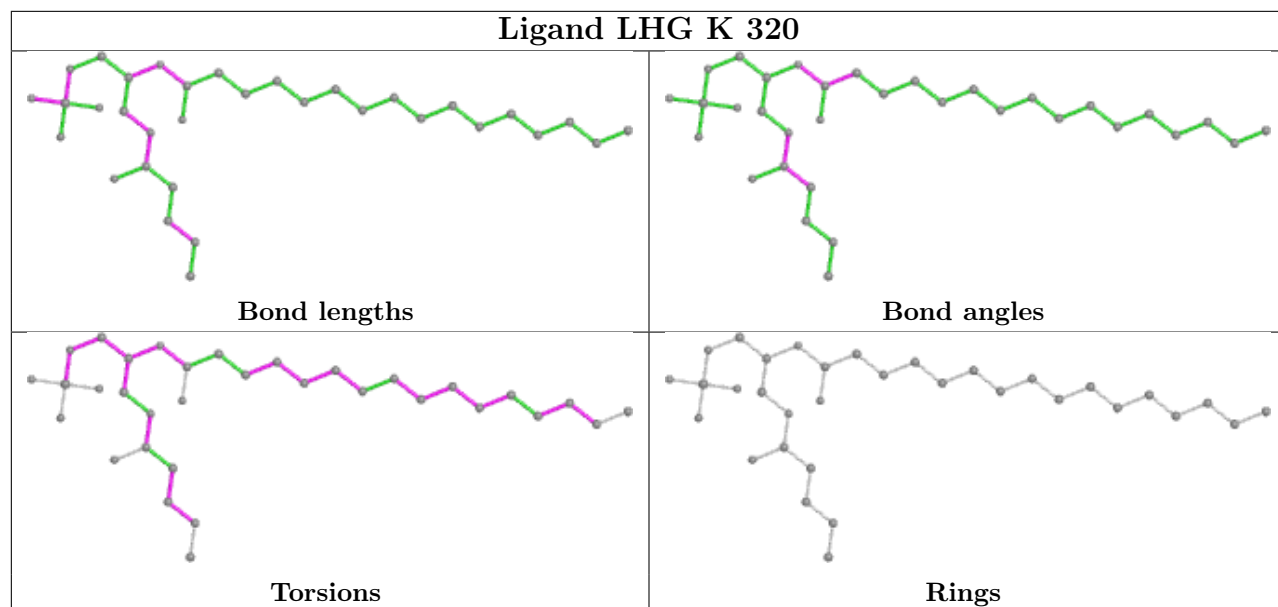
## Ligand CLA E 309



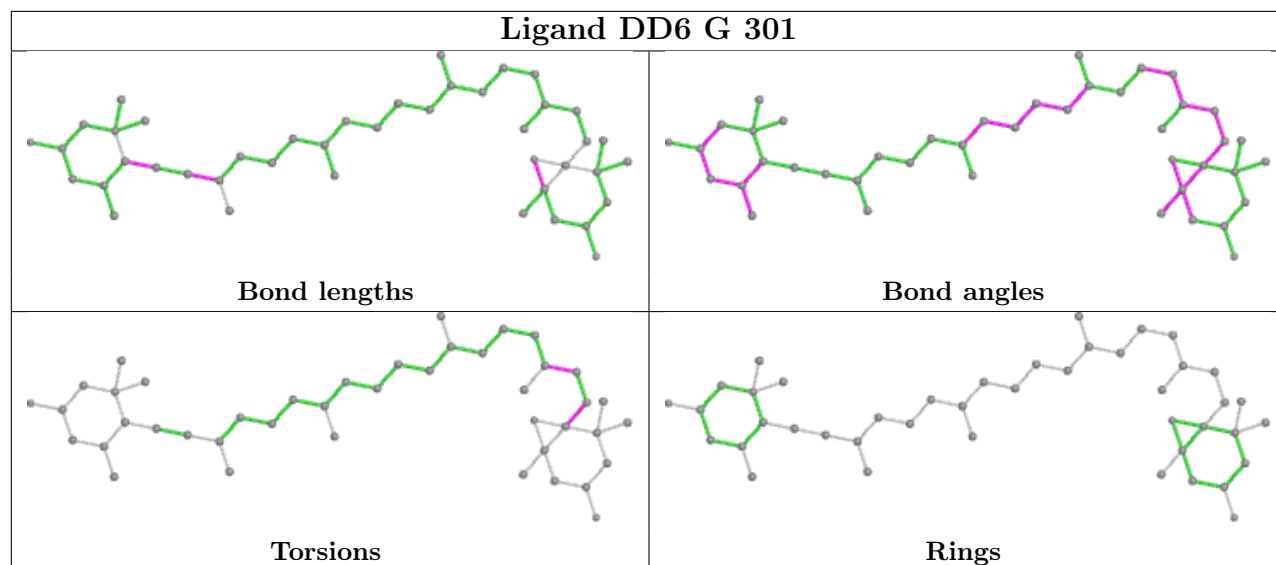
## Ligand A86 K 307



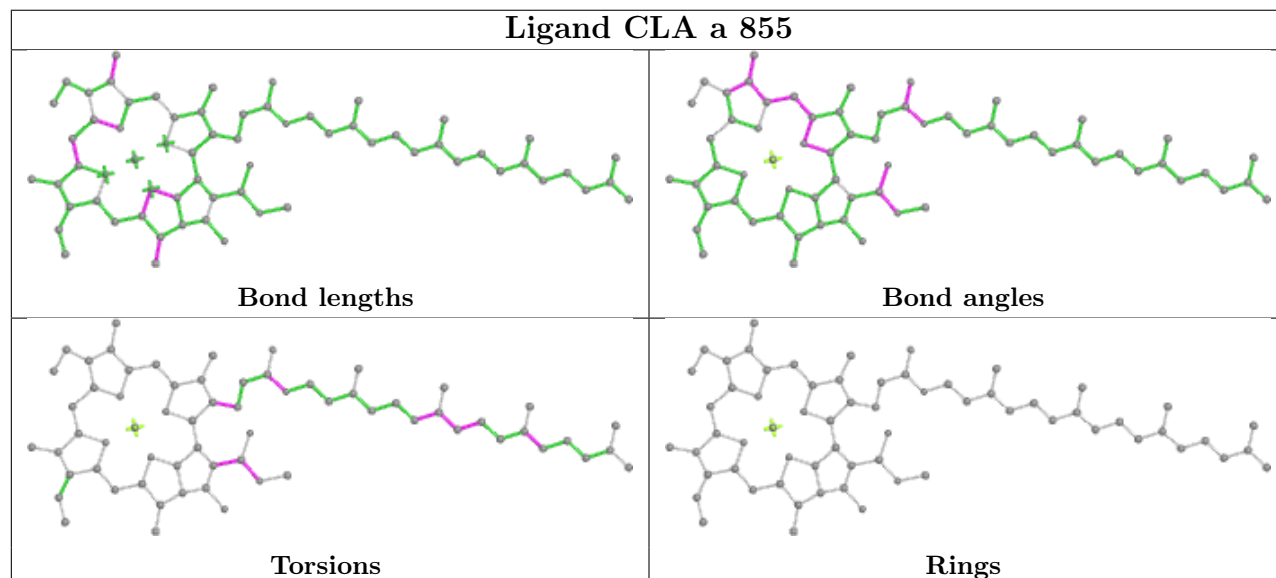
## Ligand LHG K 320



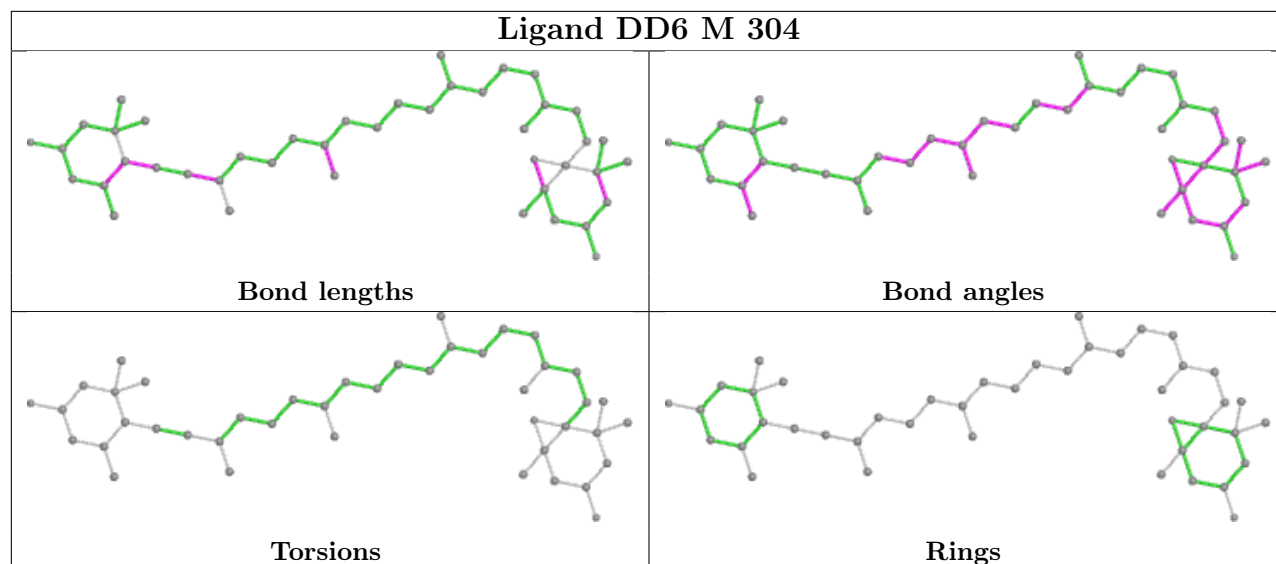
## Ligand DD6 G 301

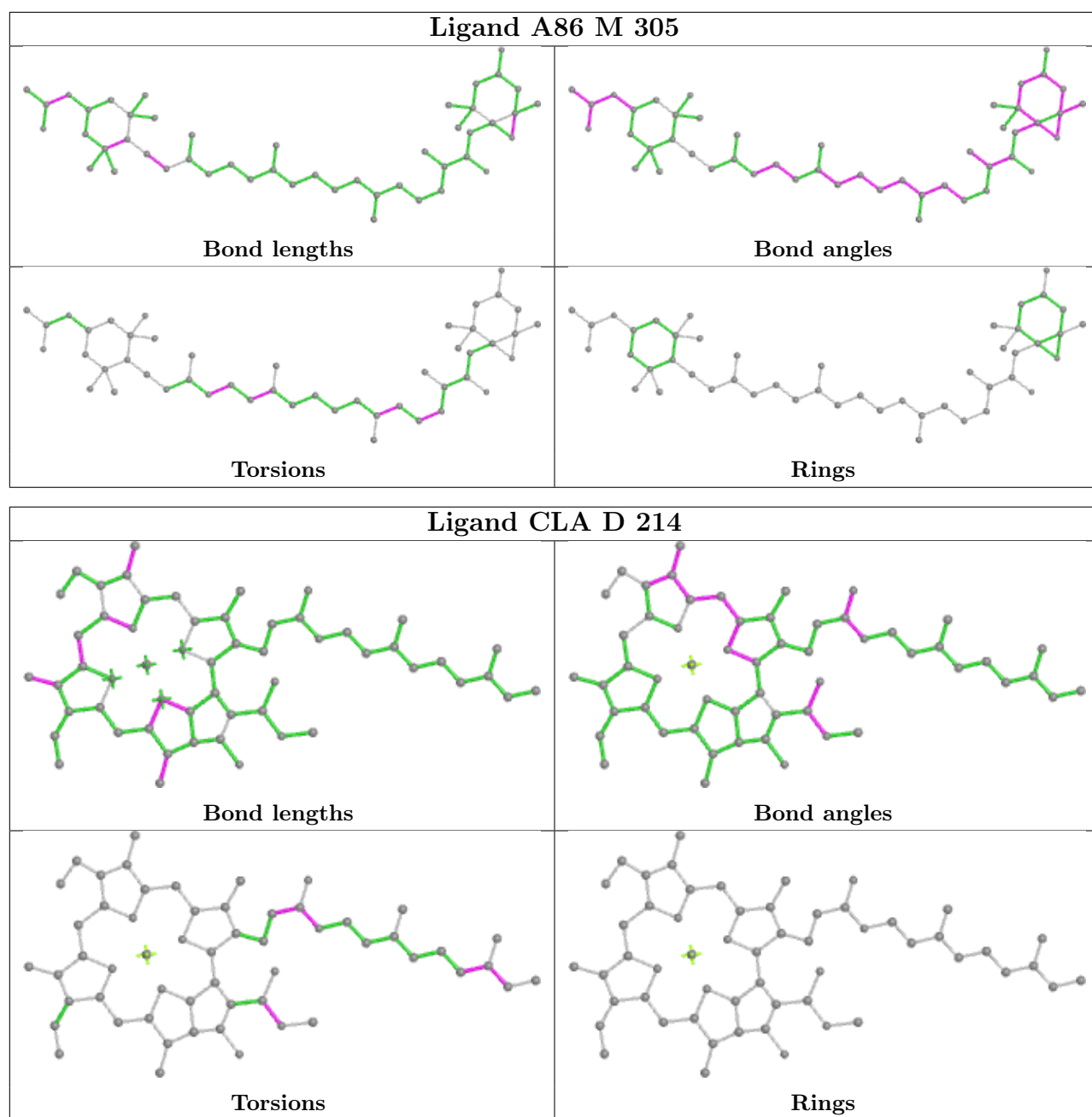


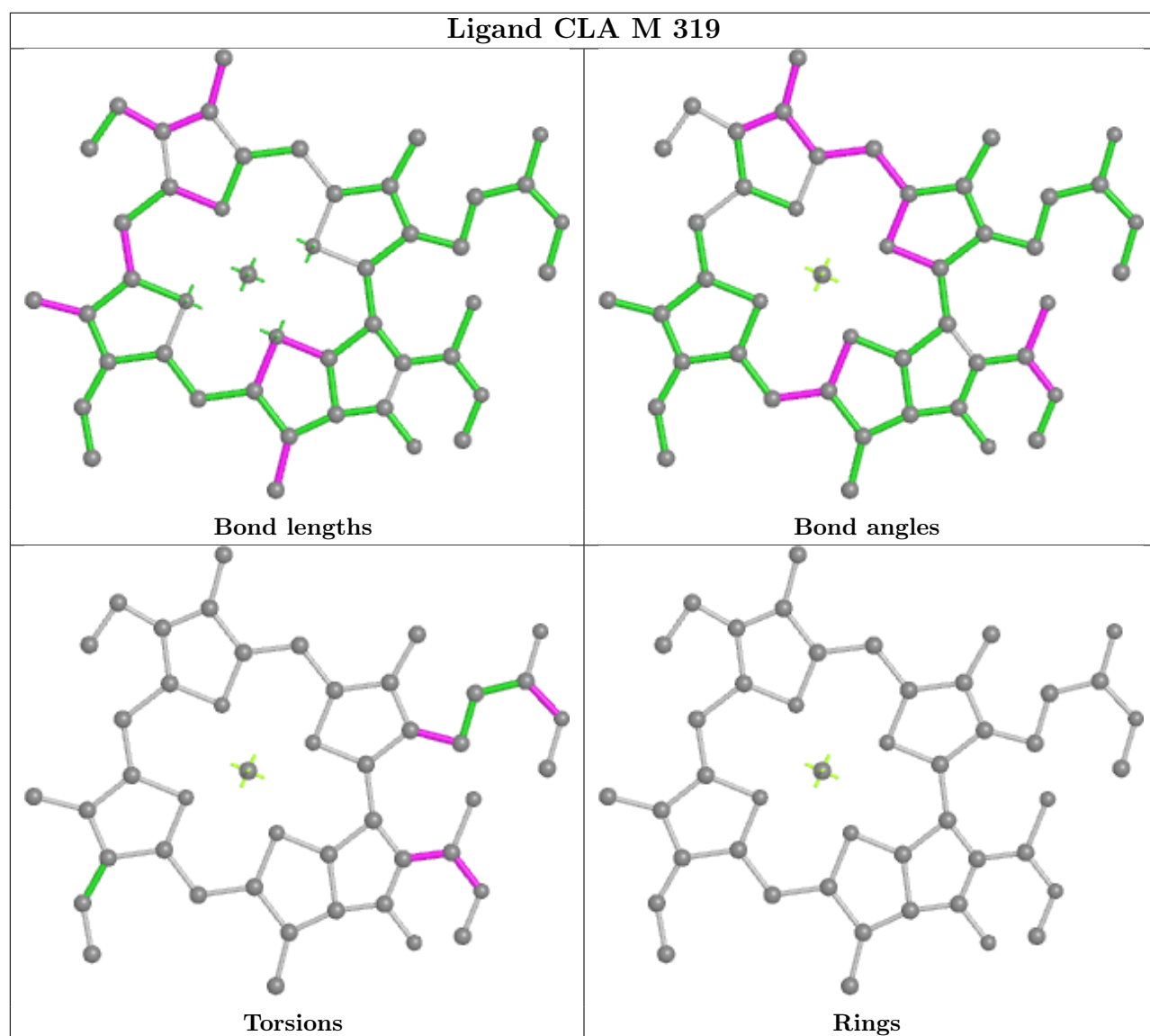
## Ligand CLA a 855



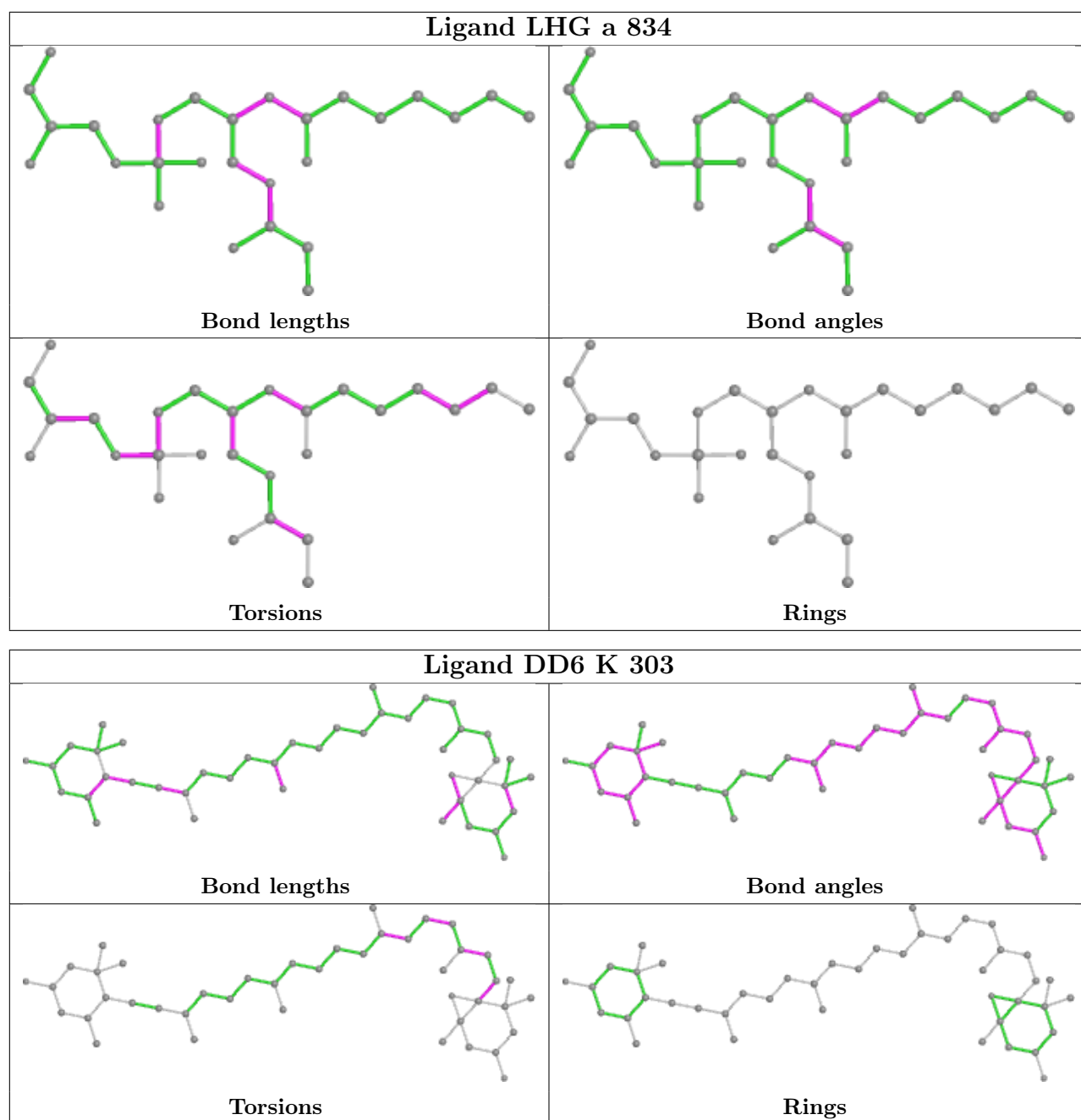
## Ligand DD6 M 304



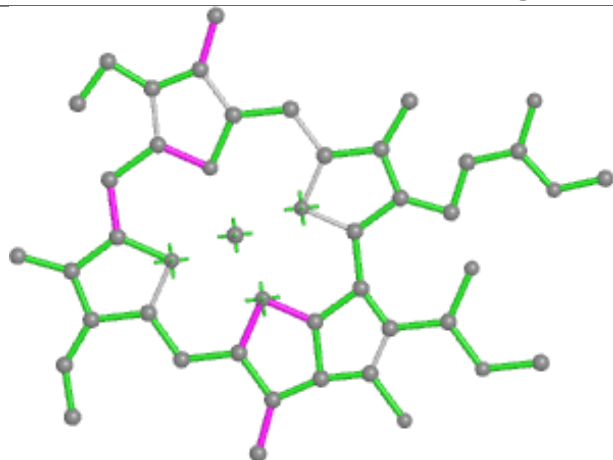




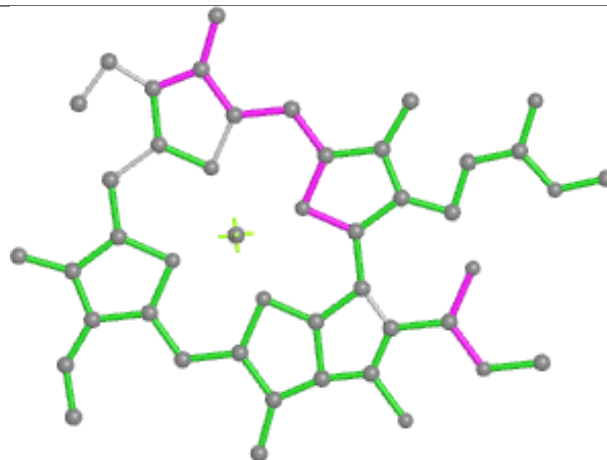




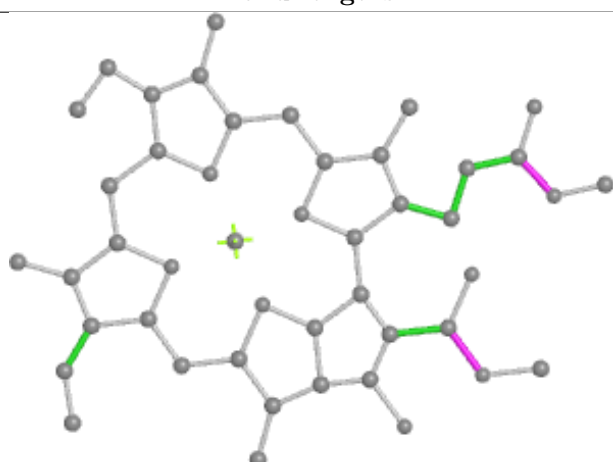
## Ligand CLA B 310



Bond lengths



Bond angles

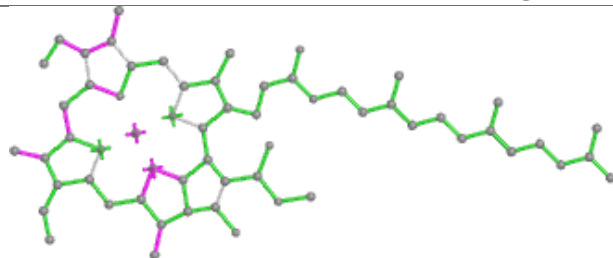


Torsions

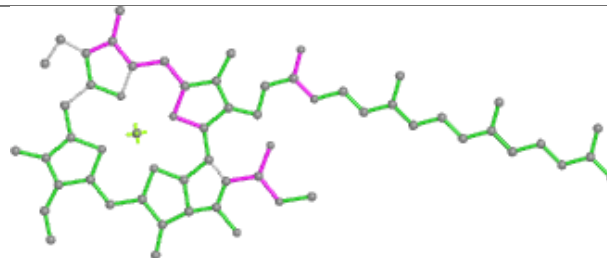


Rings

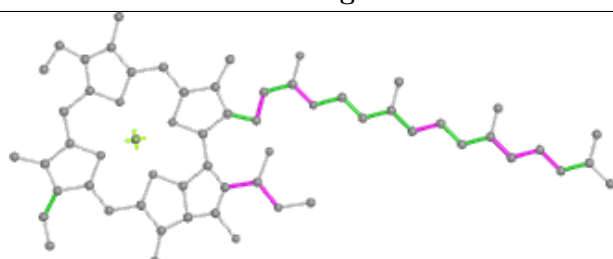
## Ligand CLA b 812



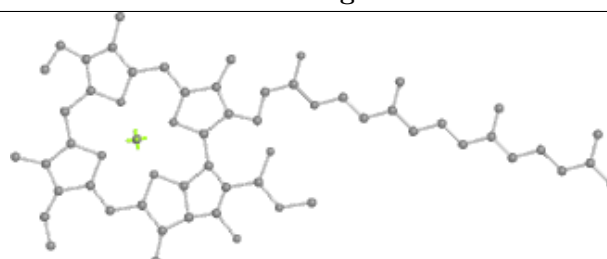
Bond lengths



Bond angles

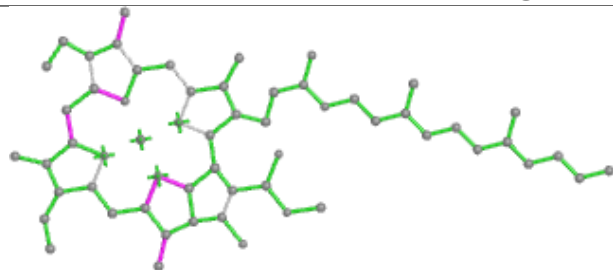


Torsions

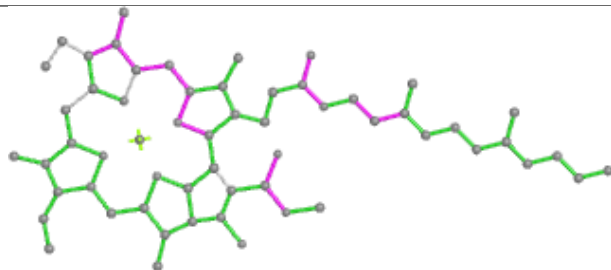


Rings

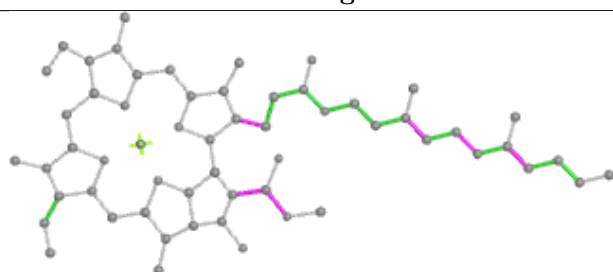
## Ligand CLA b 824



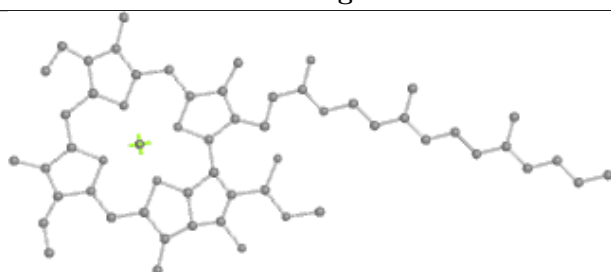
Bond lengths



Bond angles

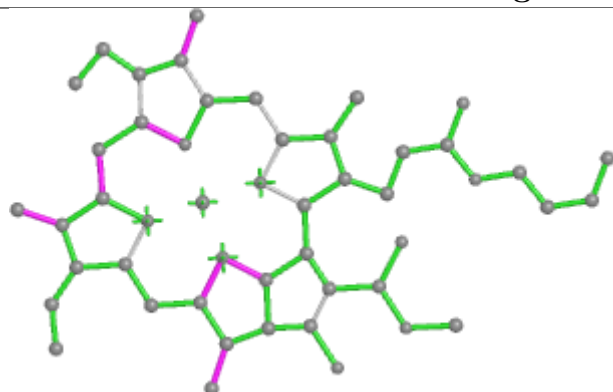


Torsions

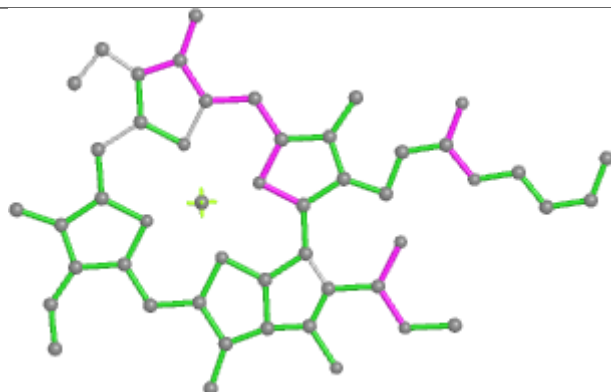


Rings

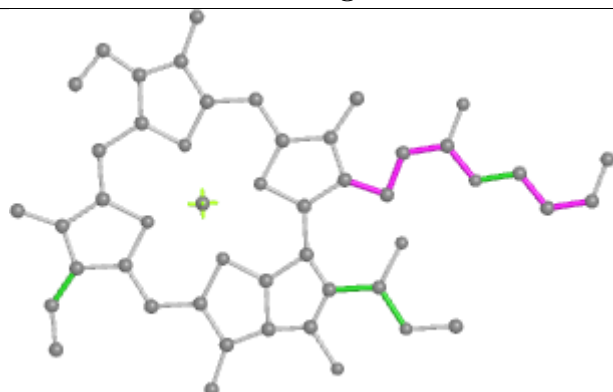
## Ligand CLA D 209



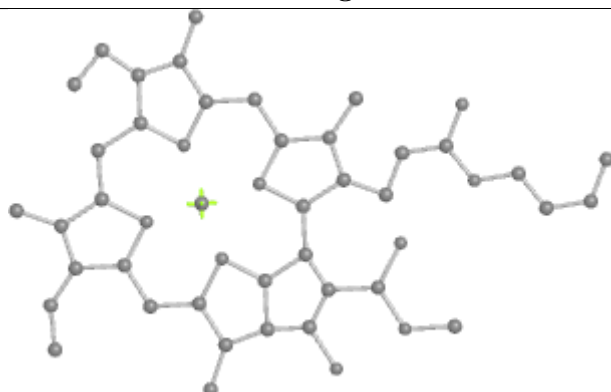
Bond lengths



Bond angles

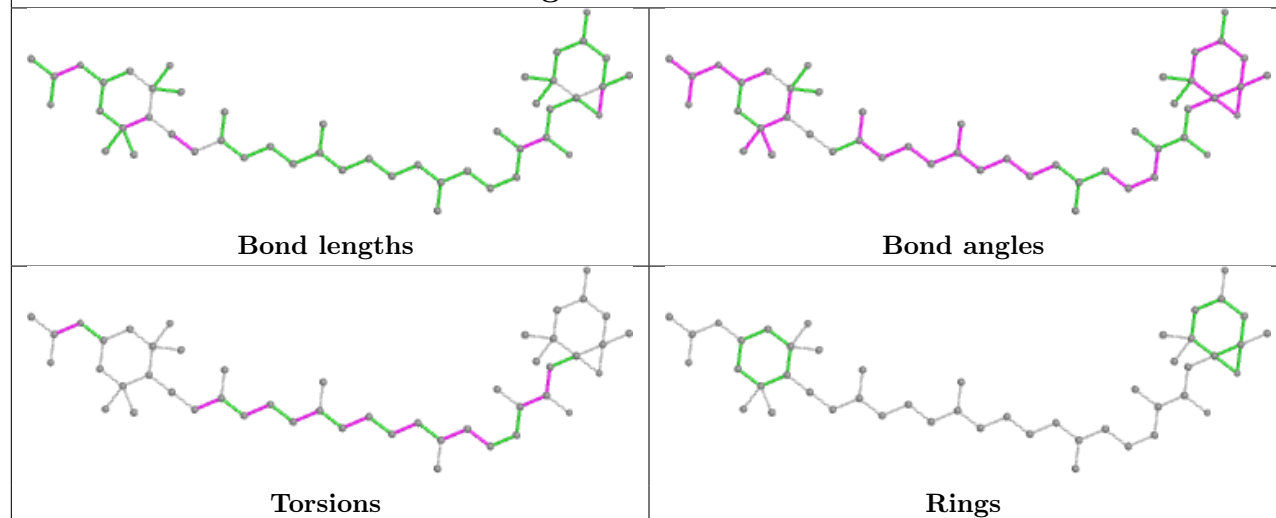


Torsions

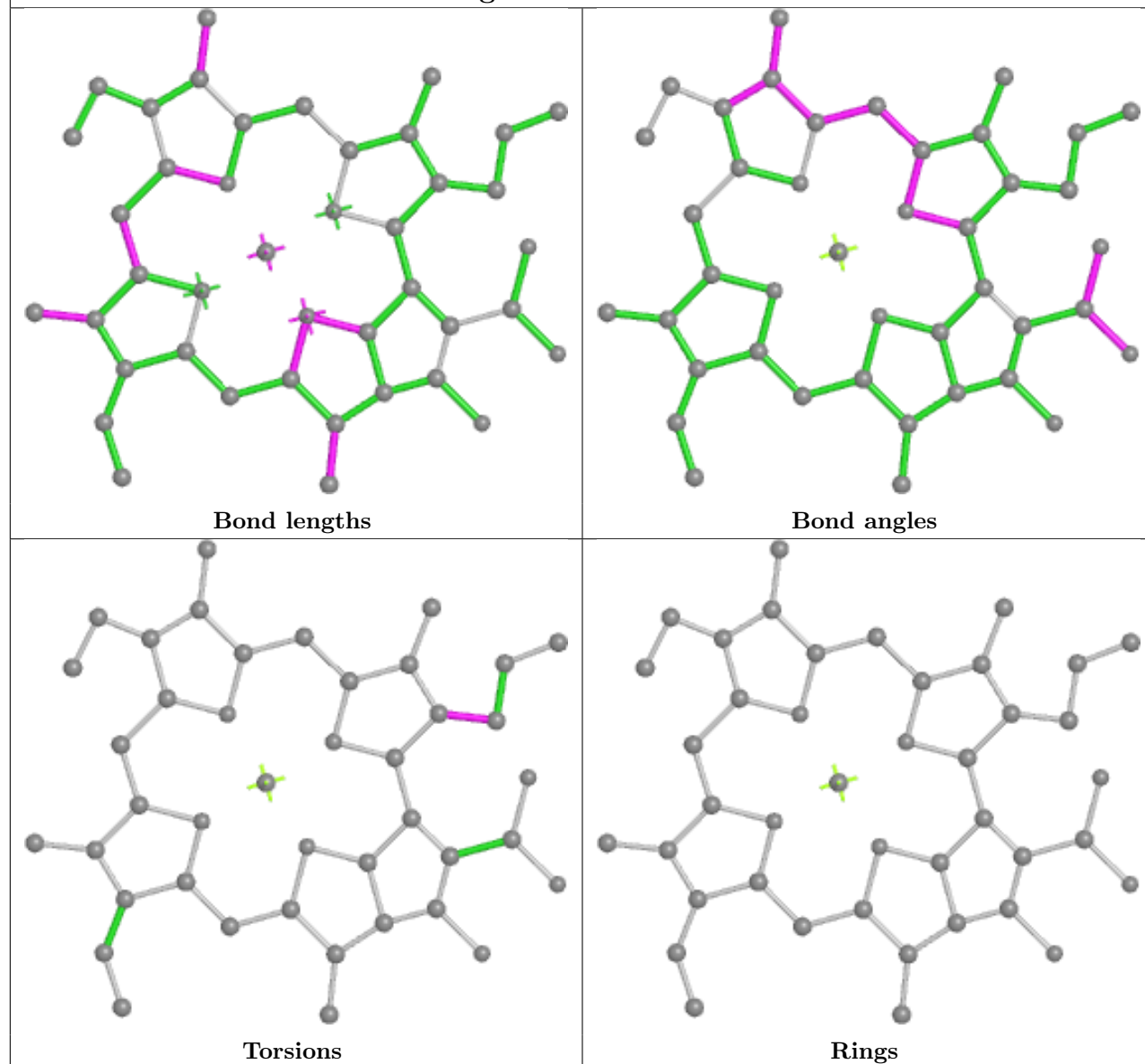


Rings

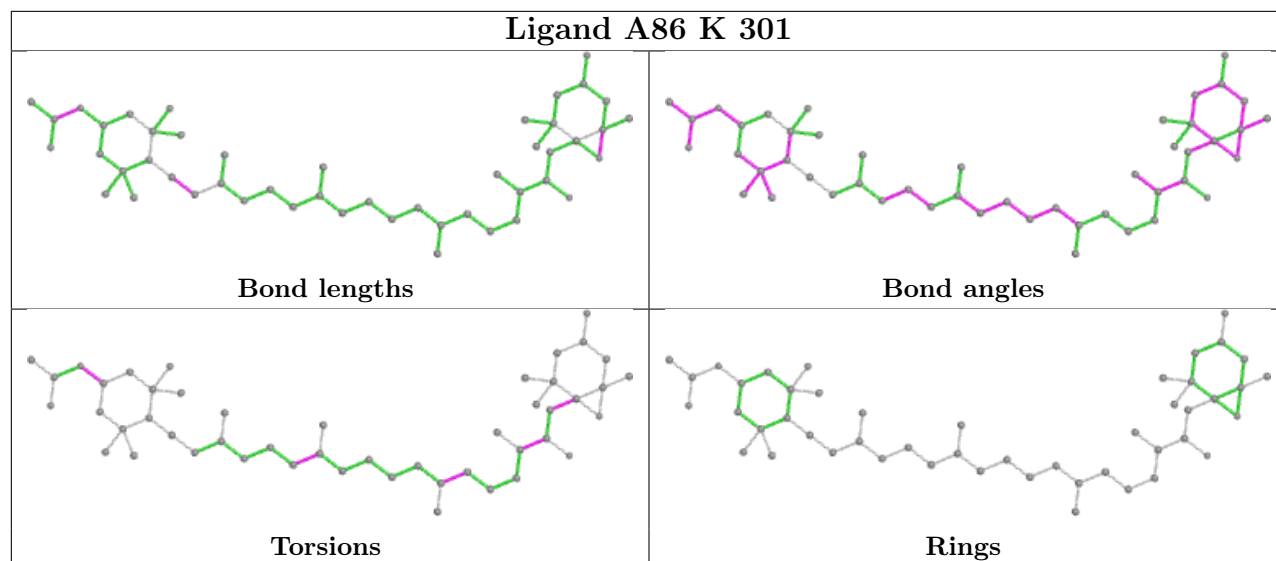
## Ligand A86 J 316



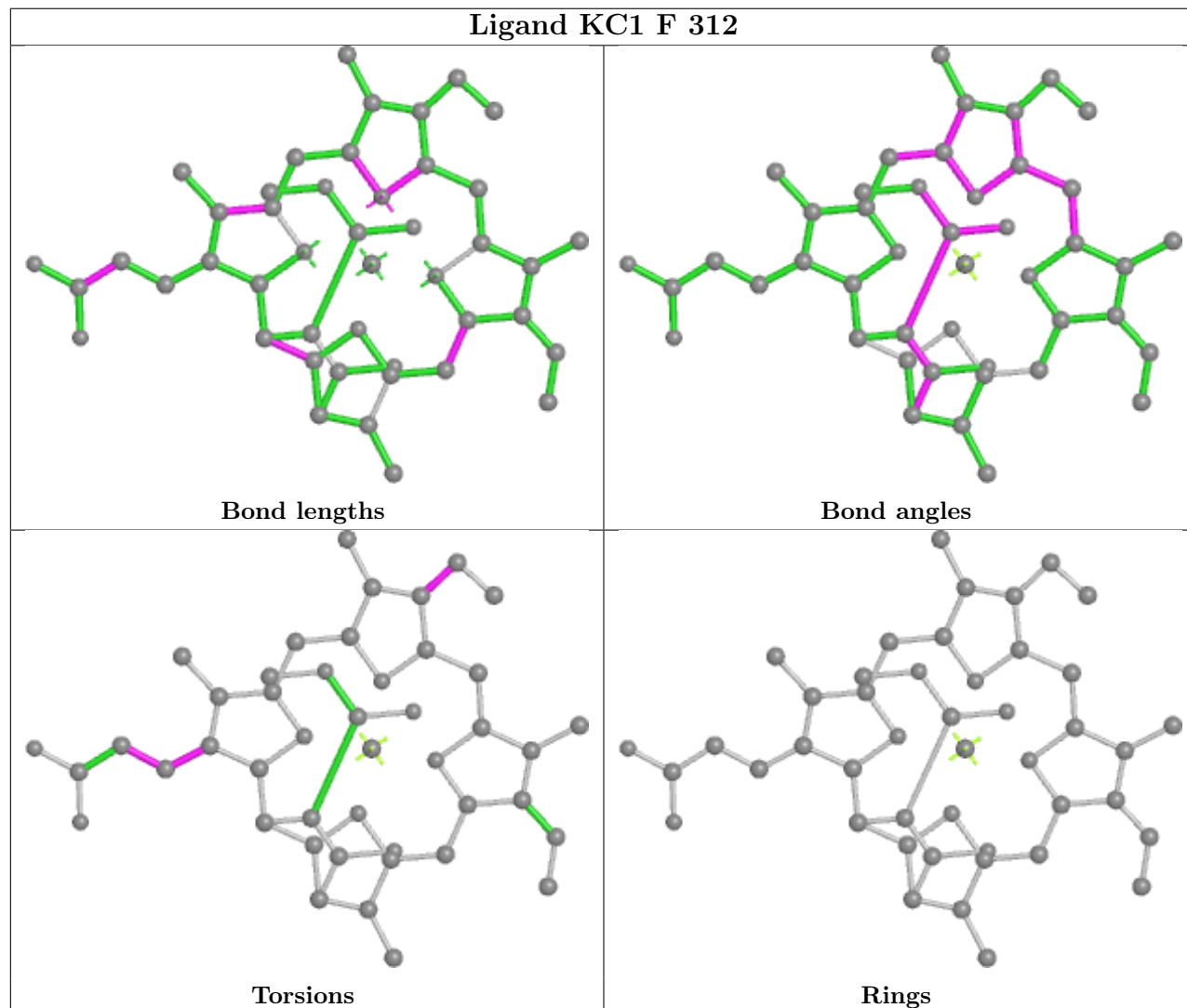
## Ligand CLA L 318



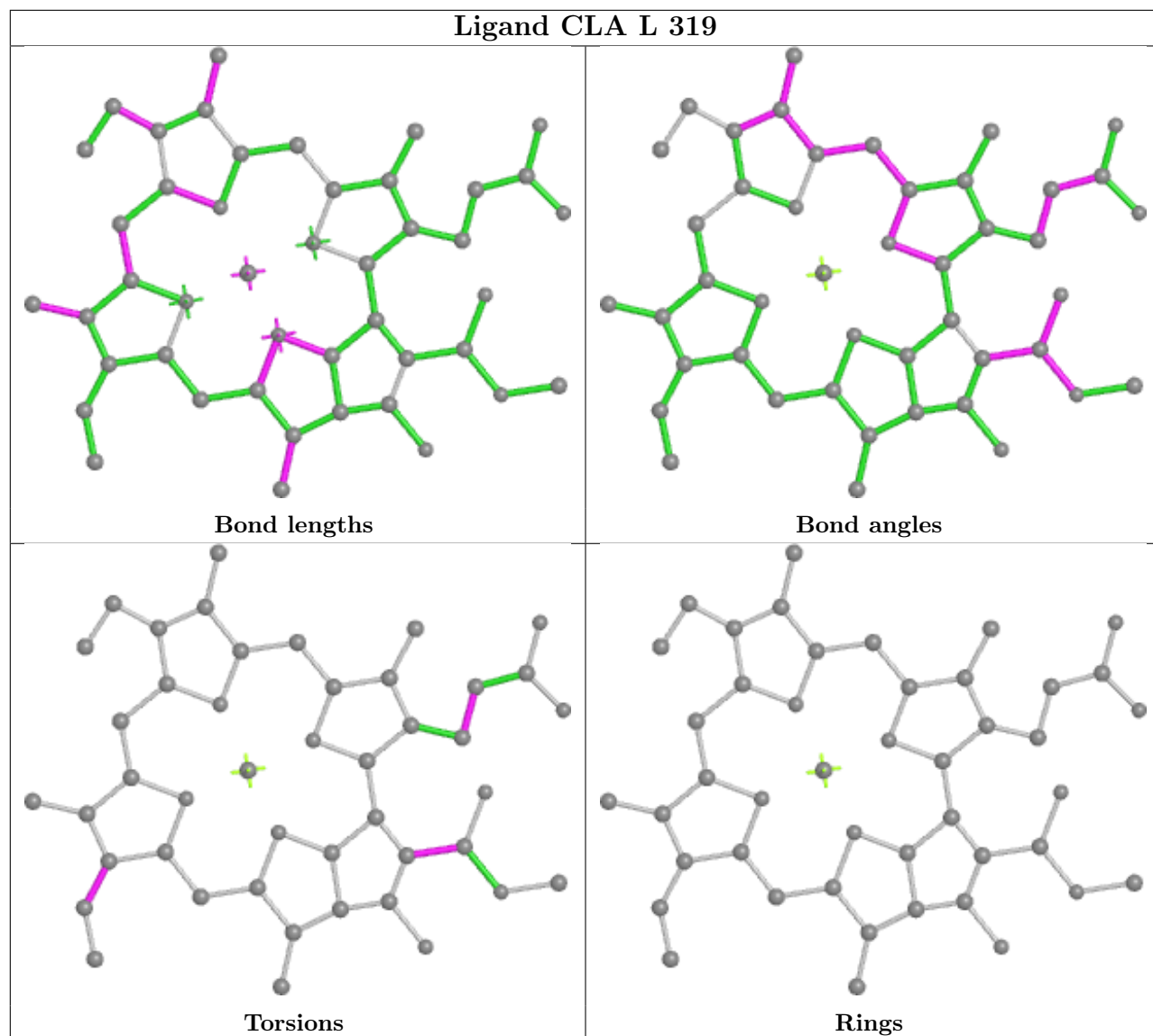
## Ligand A86 K 301

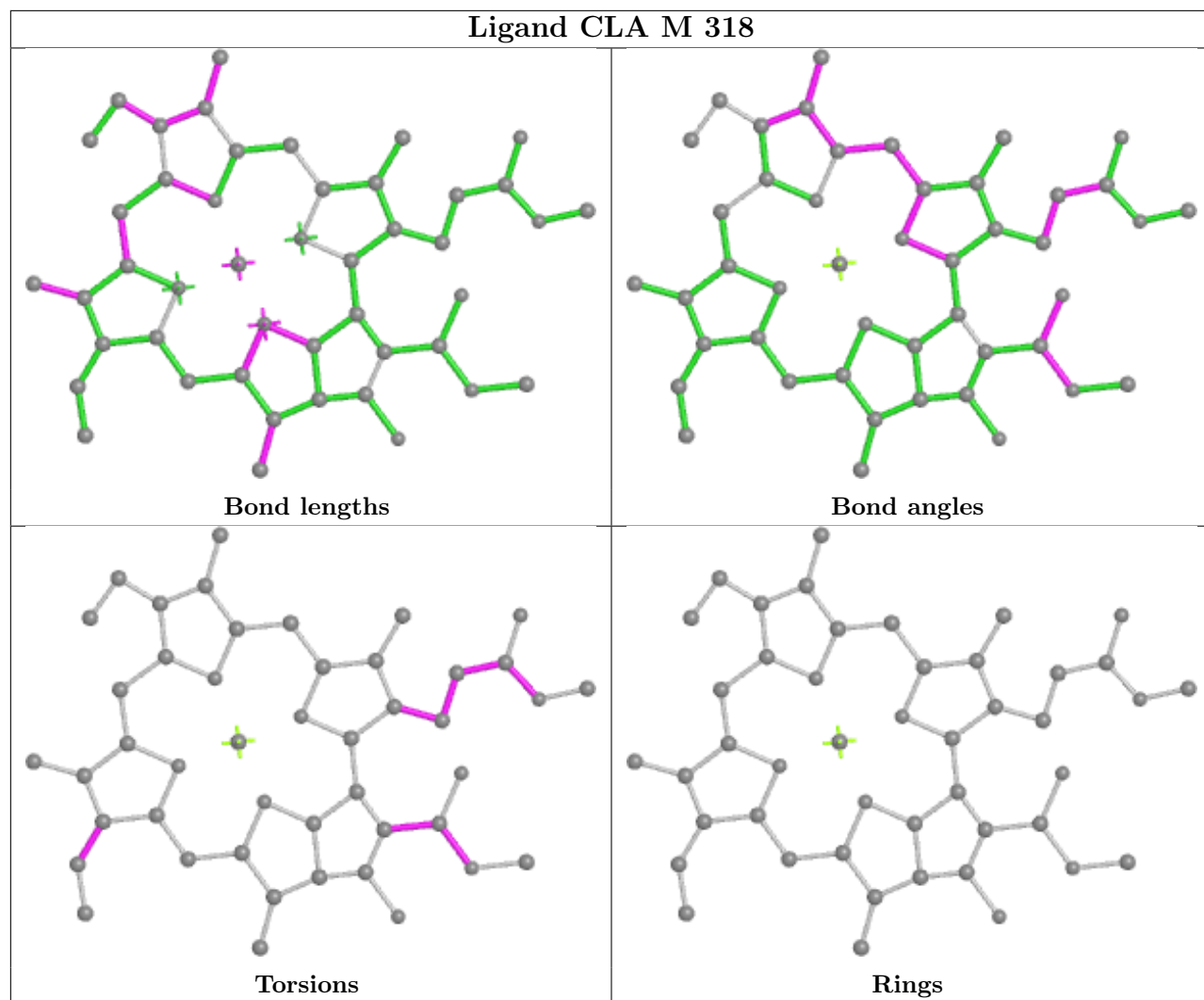


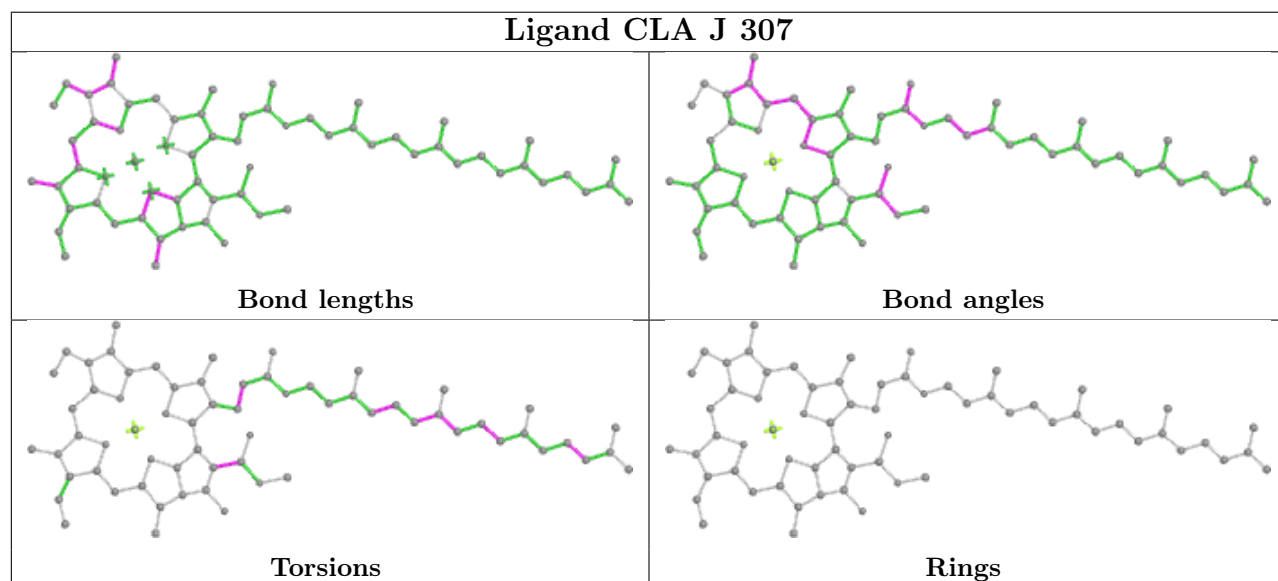
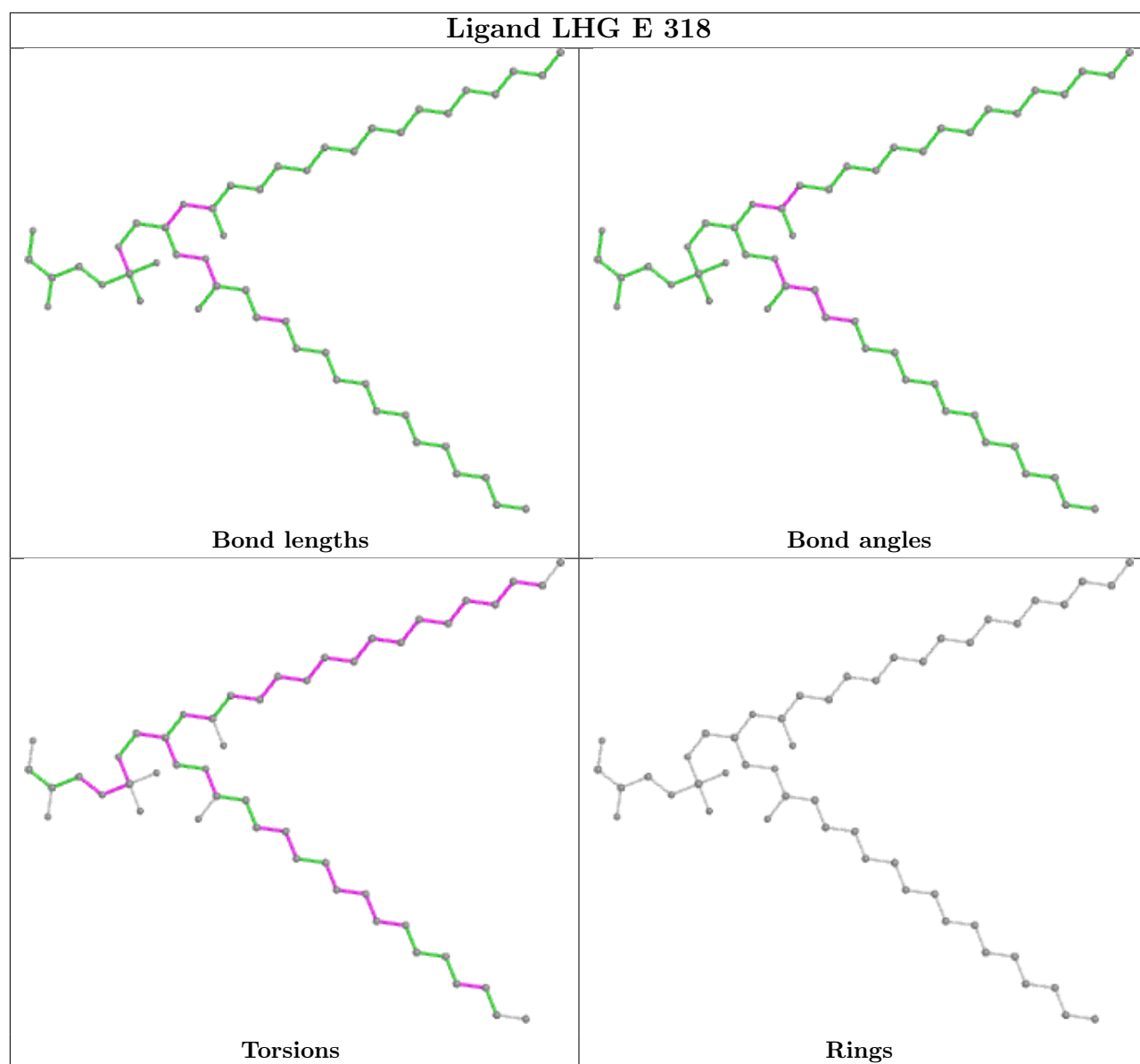
## Ligand KC1 F 312



## Ligand CLA L 319

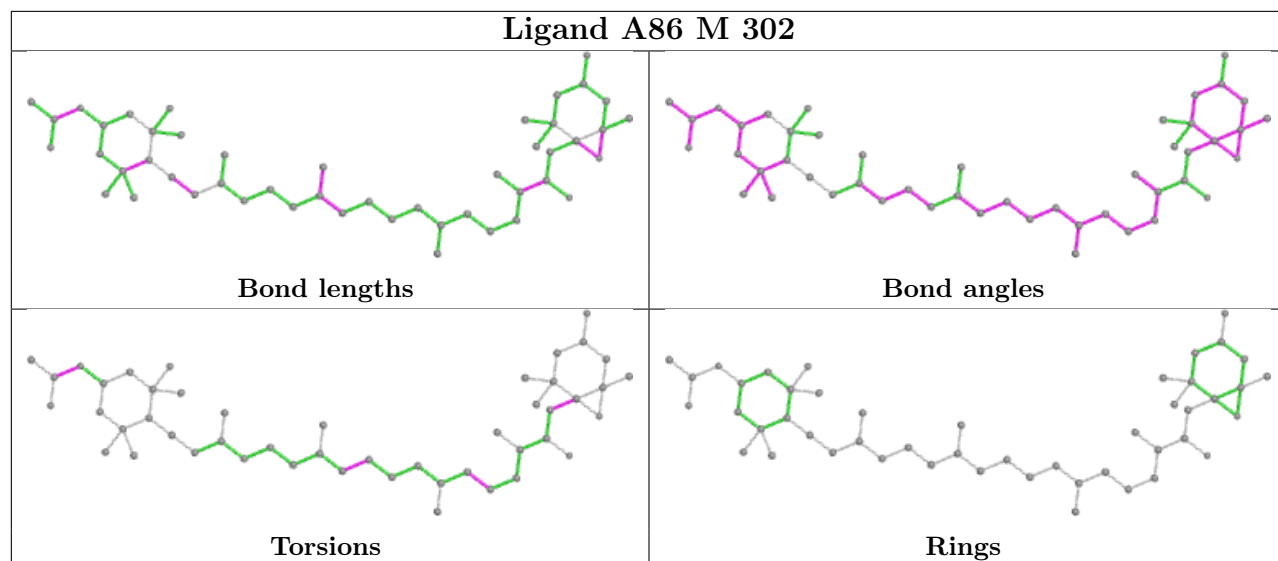




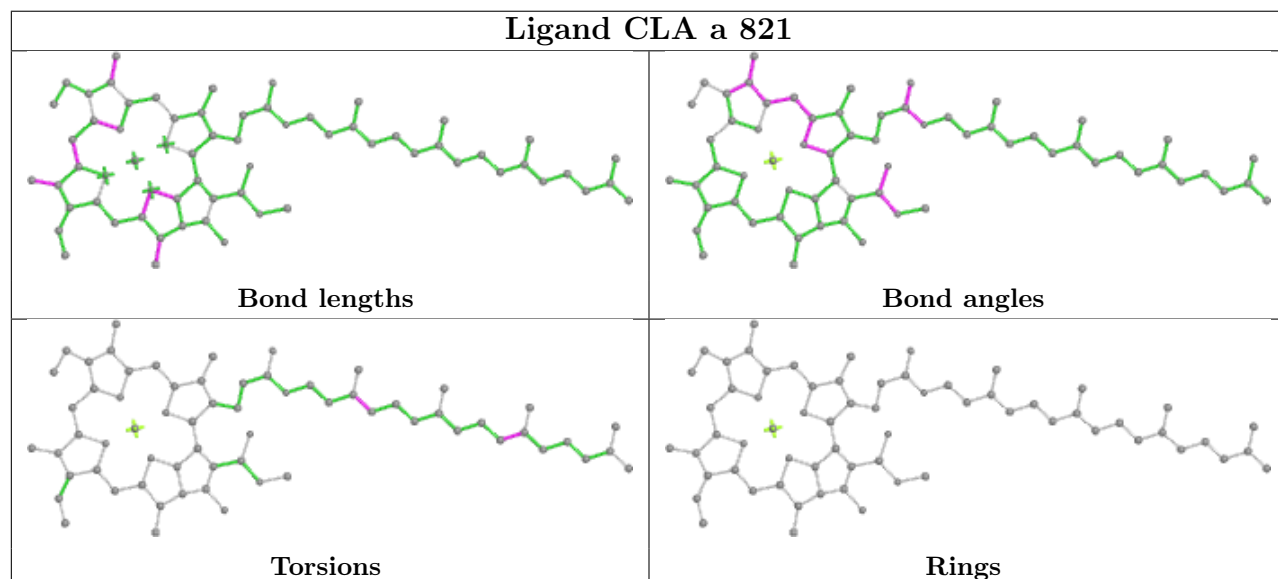




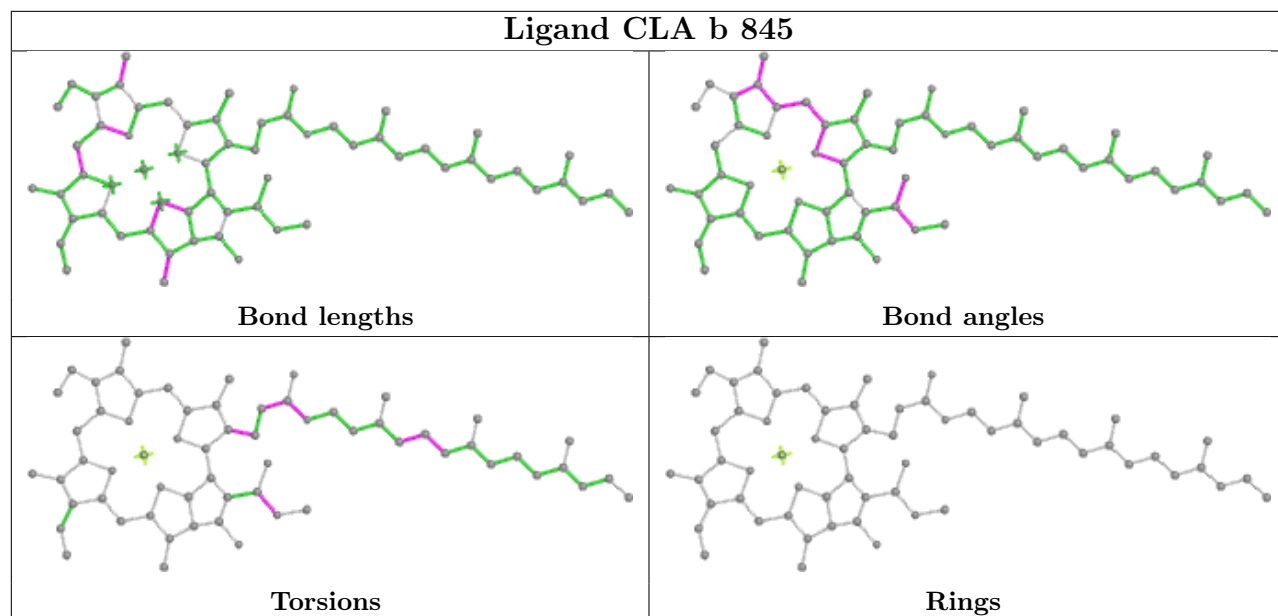
## Ligand A86 M 302



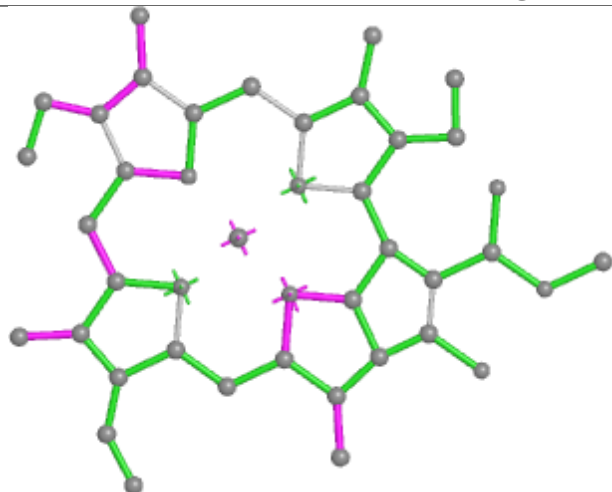
## Ligand CLA a 821



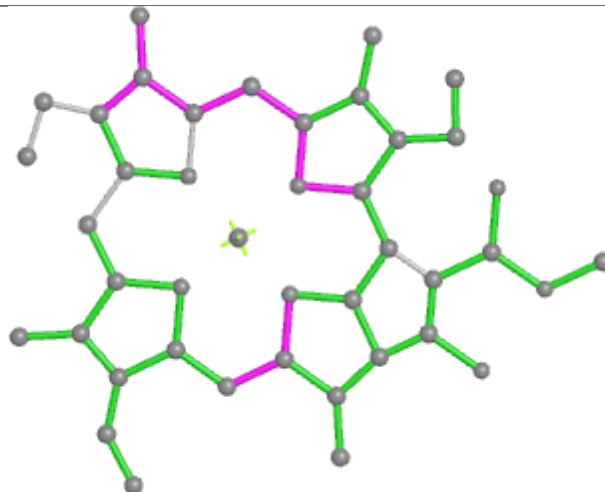
## Ligand CLA b 845



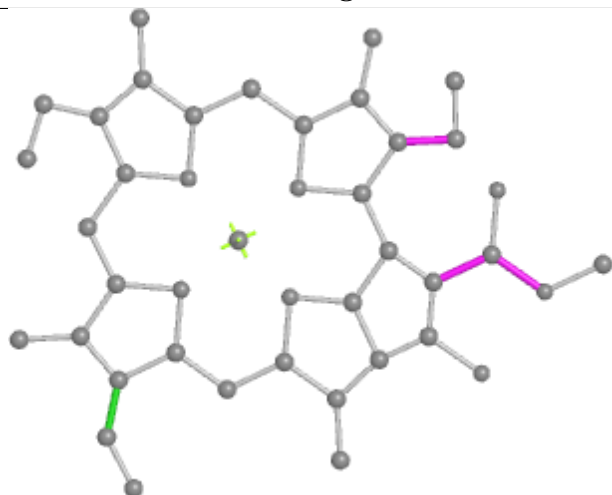
## Ligand CLA C 318



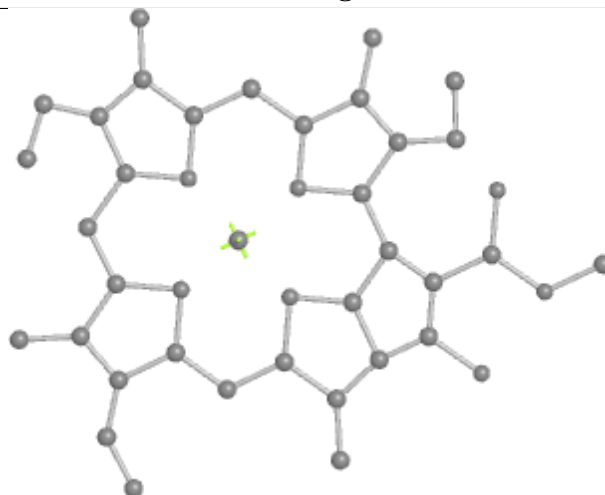
Bond lengths



Bond angles

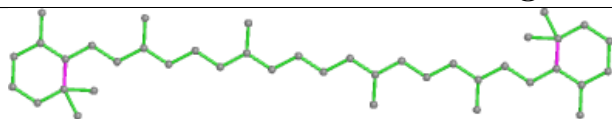


Torsions

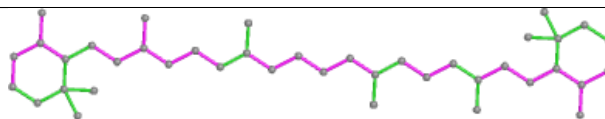


Rings

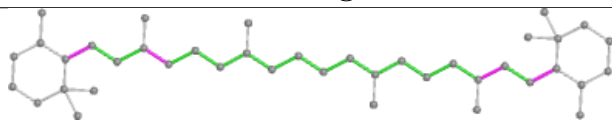
## Ligand BCR 1 202



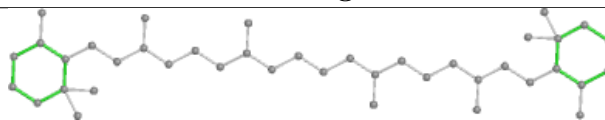
Bond lengths



Bond angles

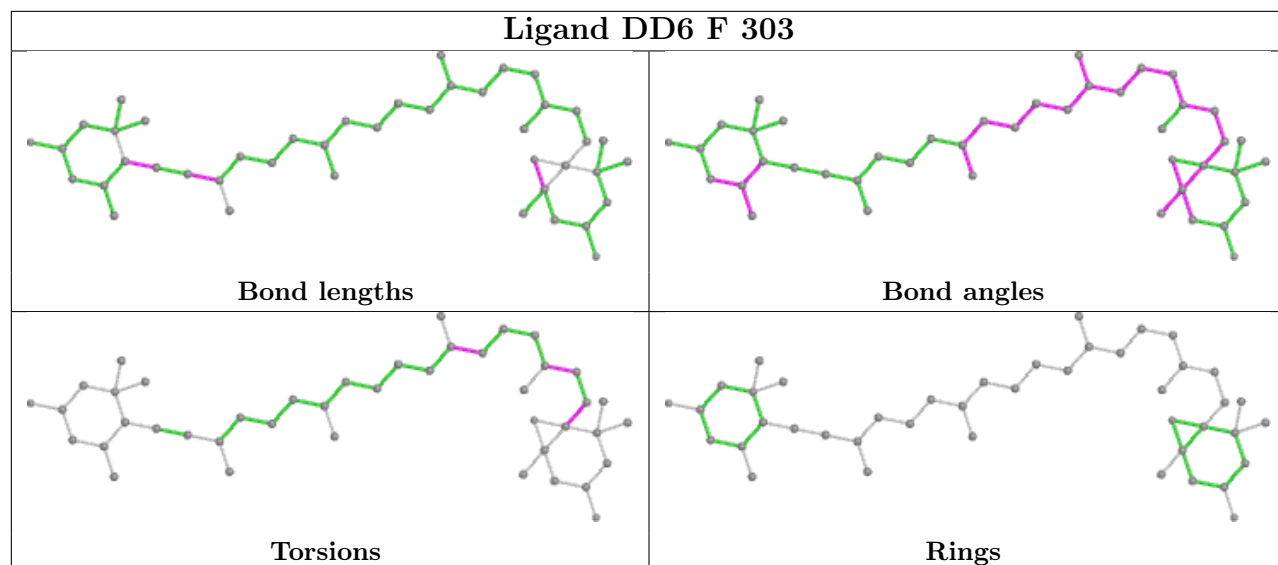


Torsions

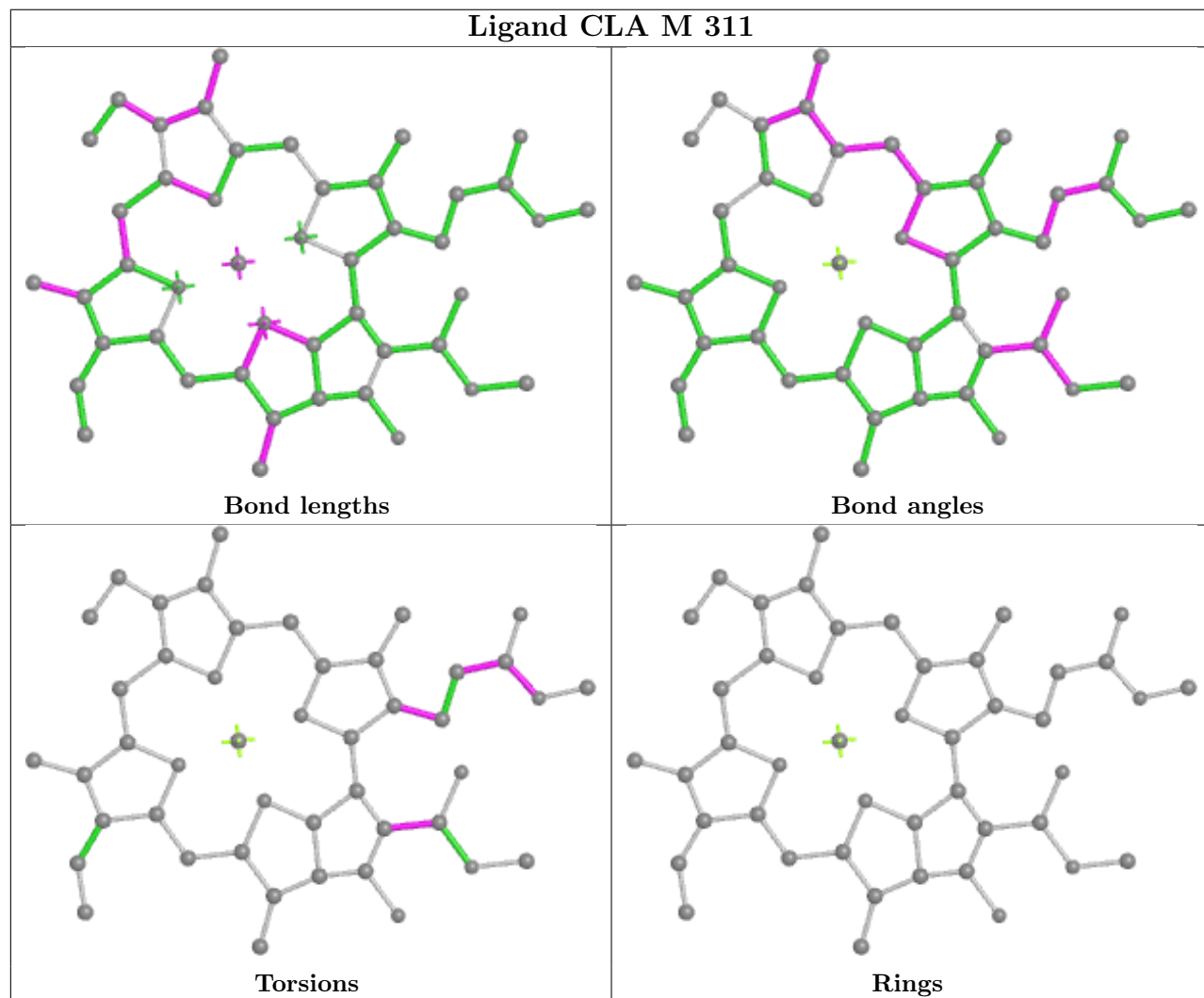


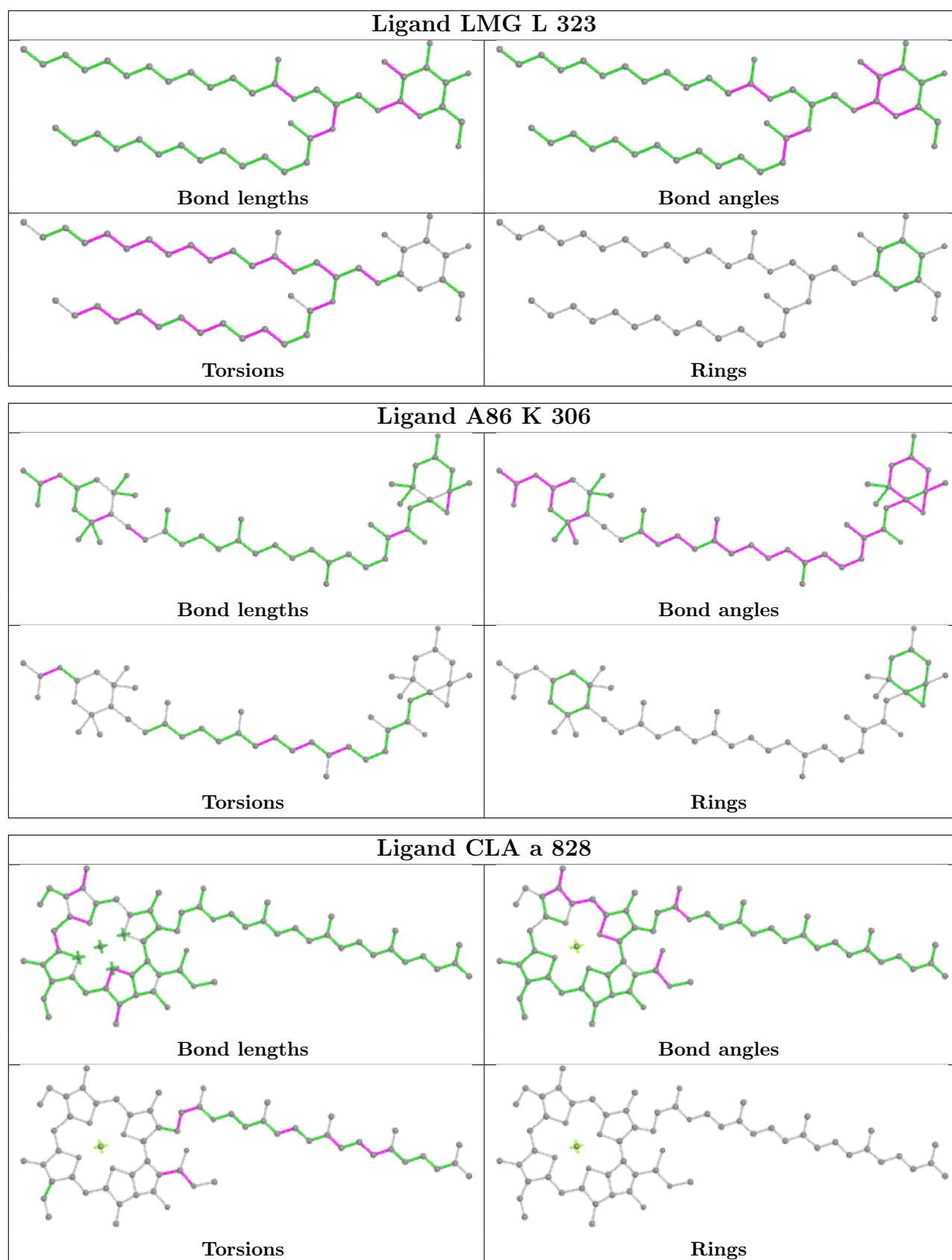
Rings

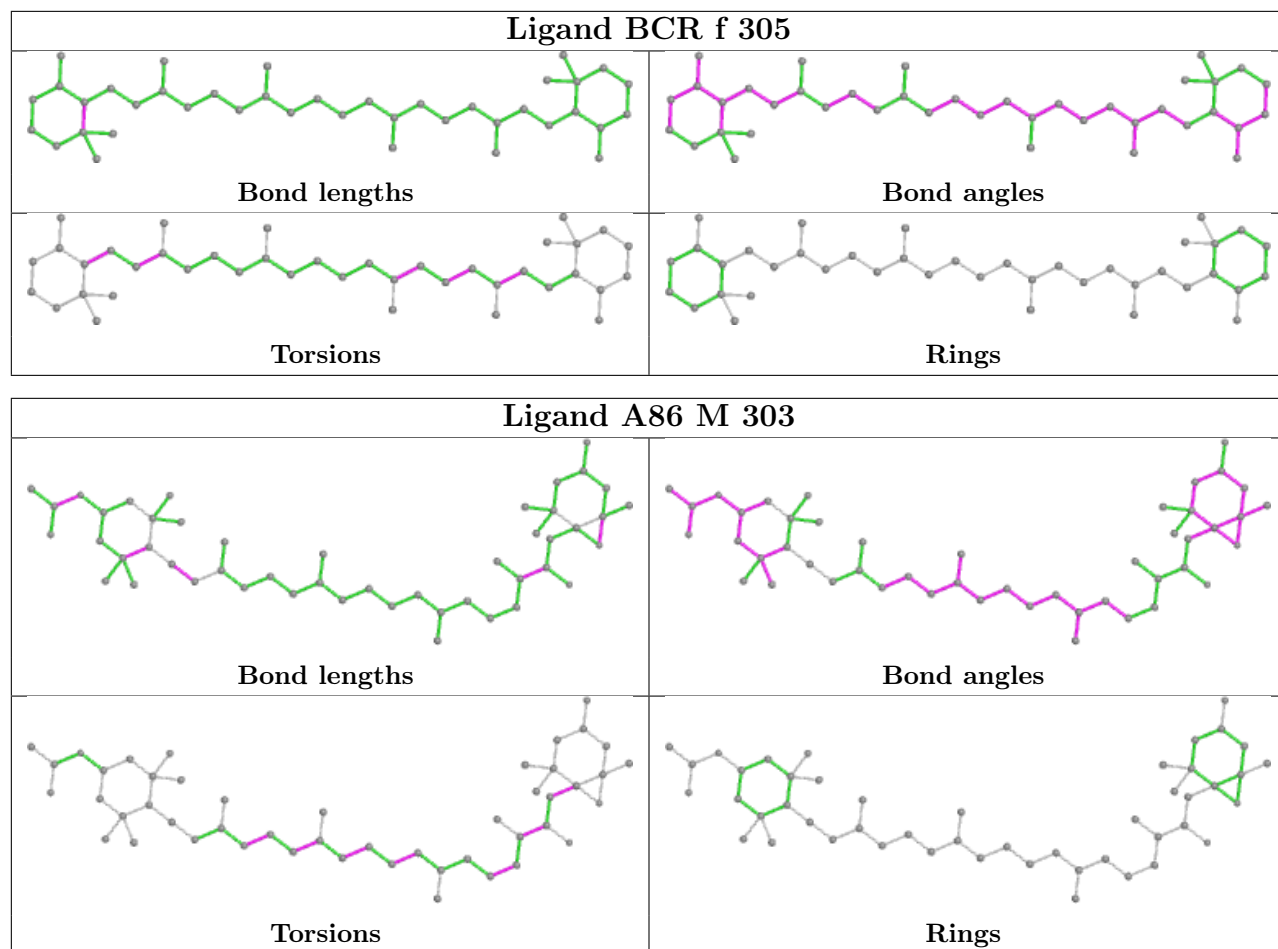
## Ligand DD6 F 303



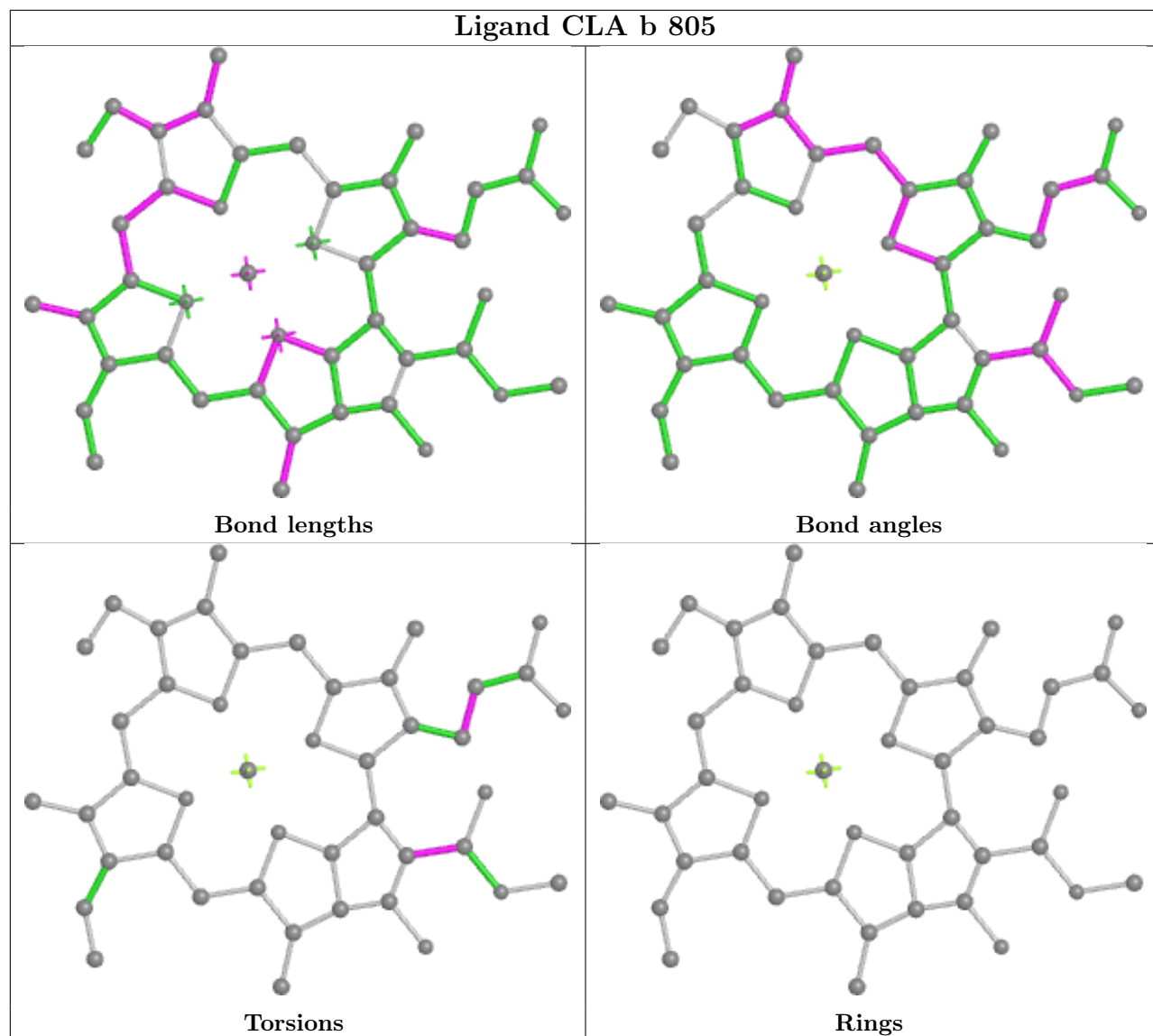
## Ligand CLA M 311



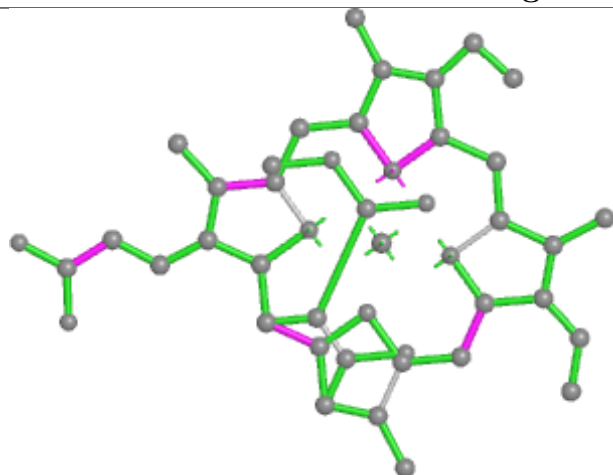




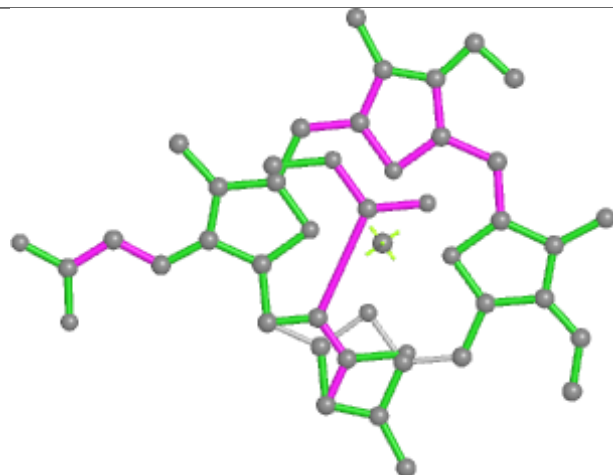
## Ligand CLA b 805



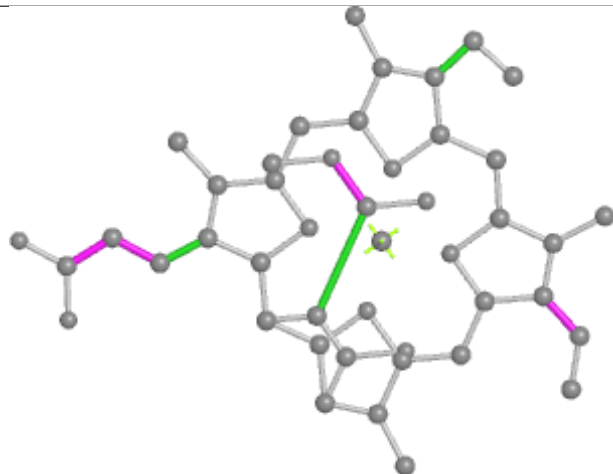
## Ligand KC1 I 312



Bond lengths



Bond angles

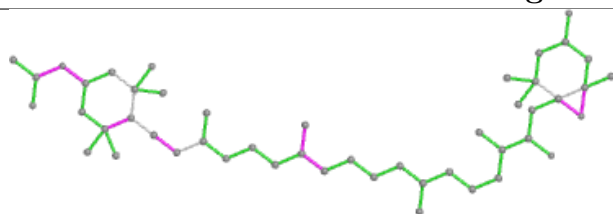


Torsions

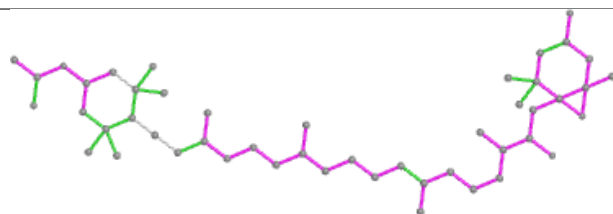


Rings

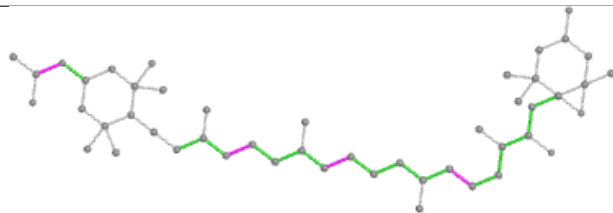
## Ligand A86 r 202



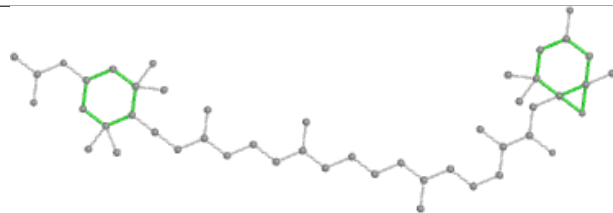
Bond lengths



Bond angles

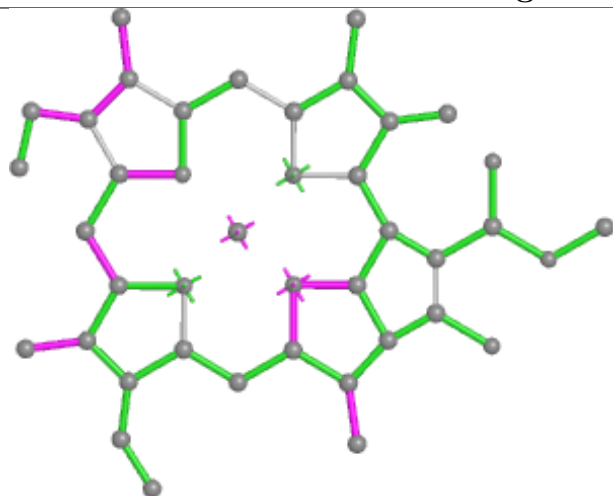


Torsions

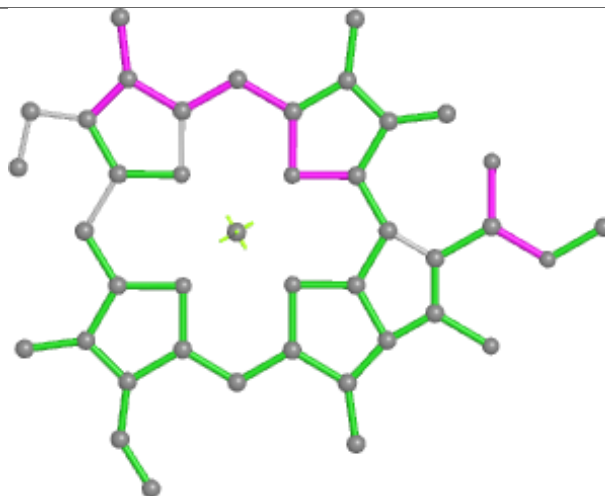


Rings

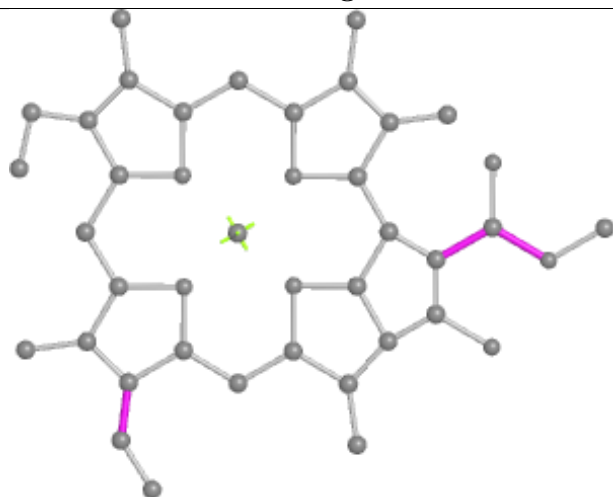
## Ligand CLA L 315



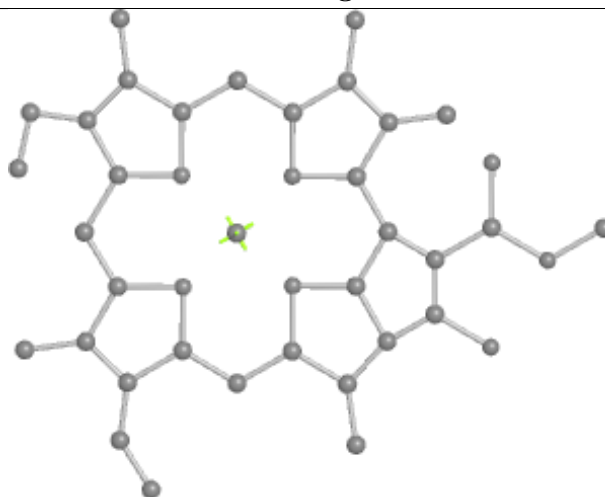
Bond lengths



Bond angles



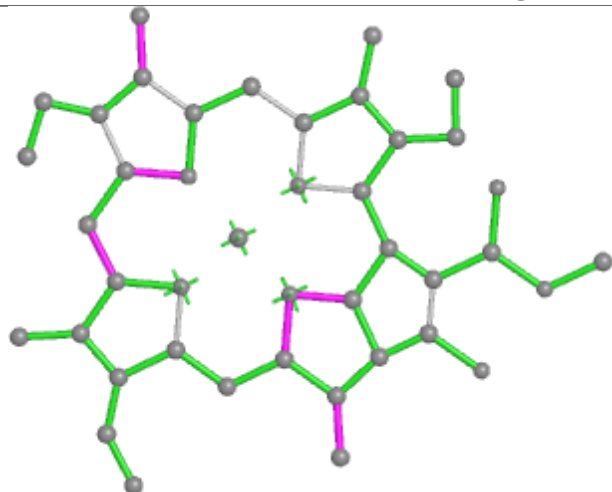
Torsions



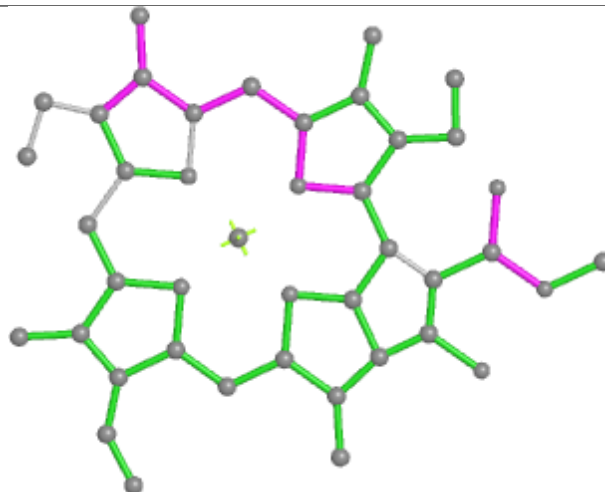
Rings



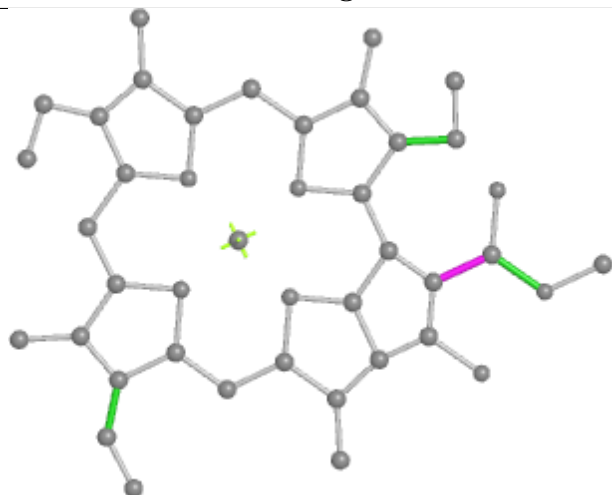
## Ligand CLA D 212



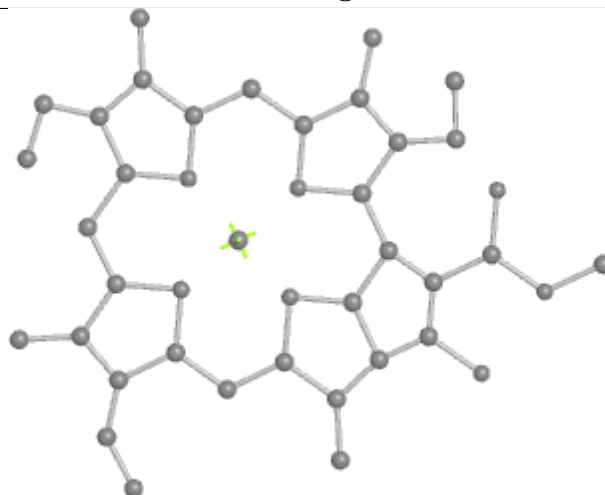
Bond lengths



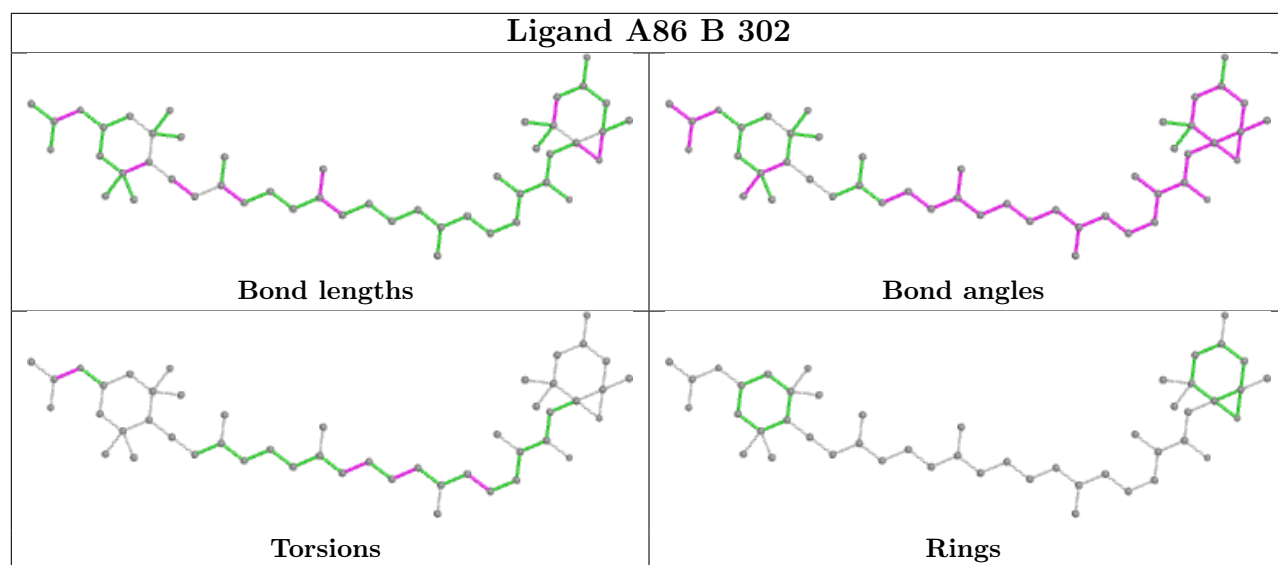
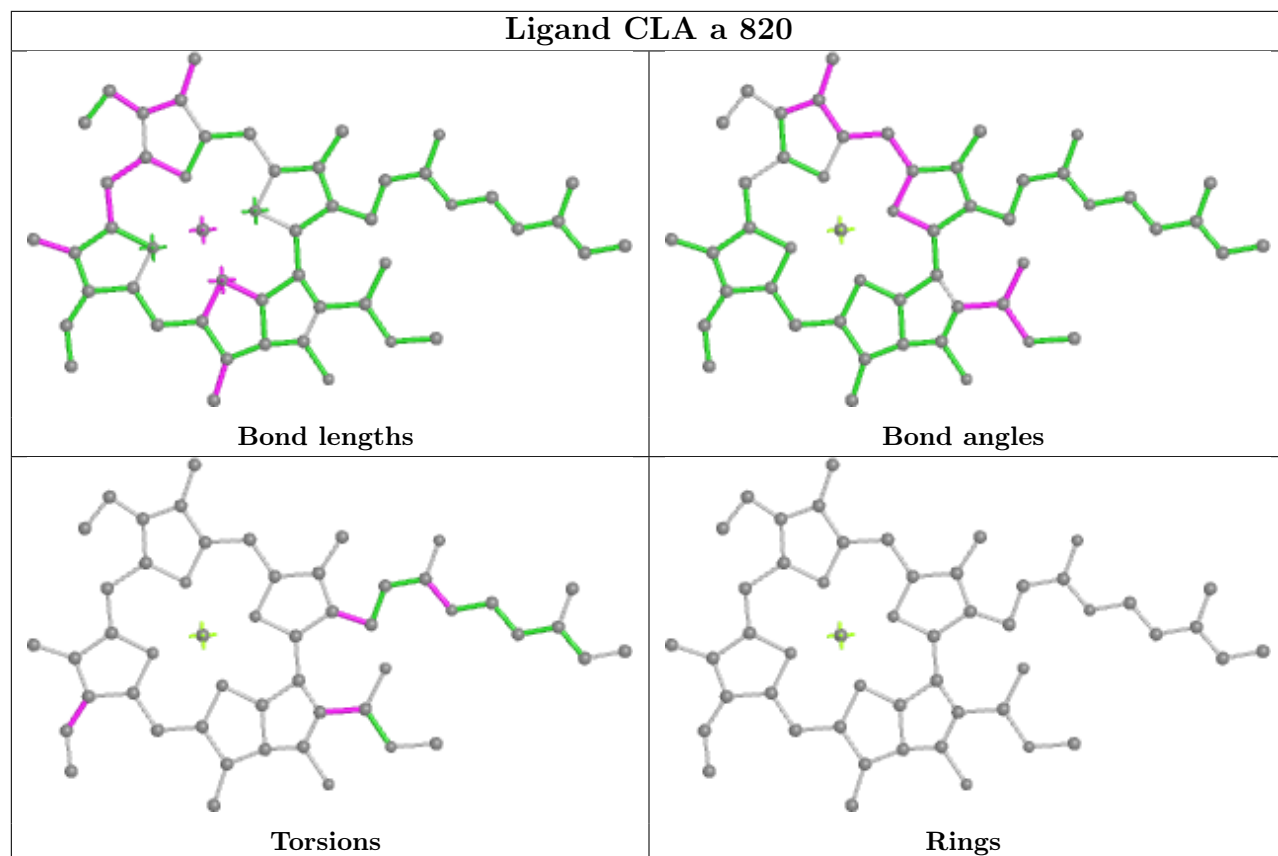
Bond angles



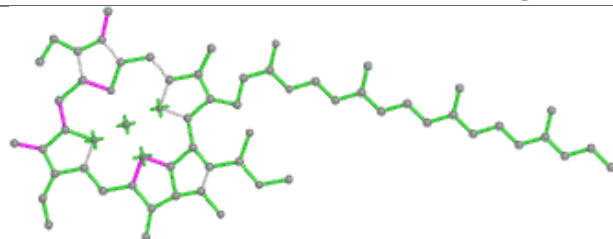
Torsions



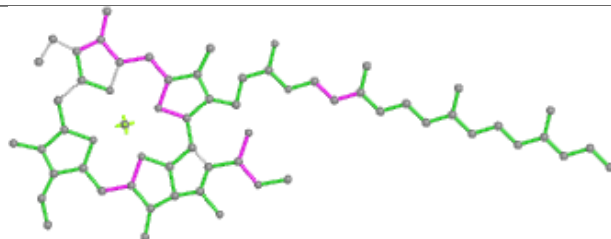
Rings



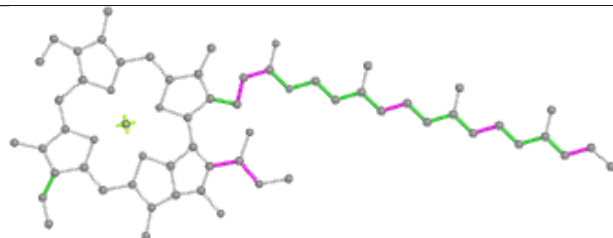
## Ligand CLA F 308



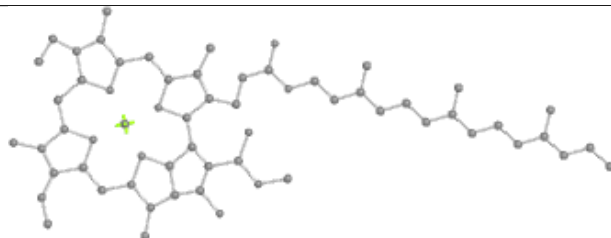
Bond lengths



Bond angles

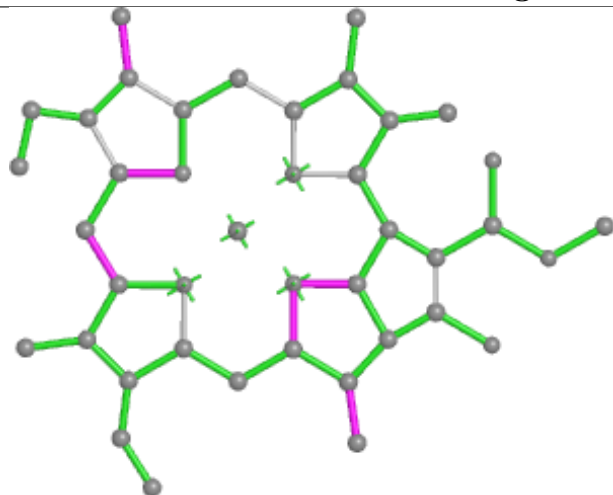


Torsions

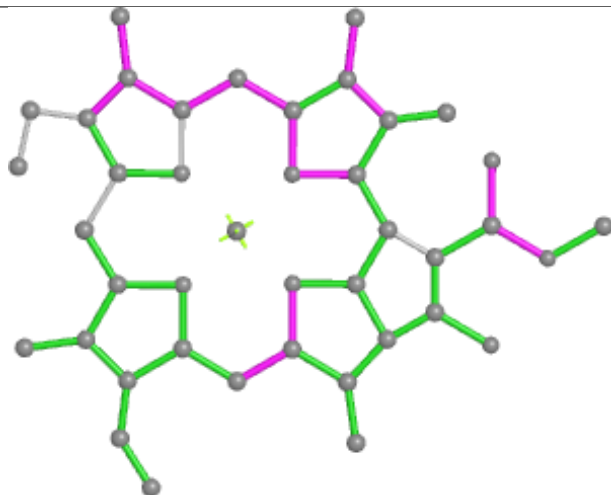


Rings

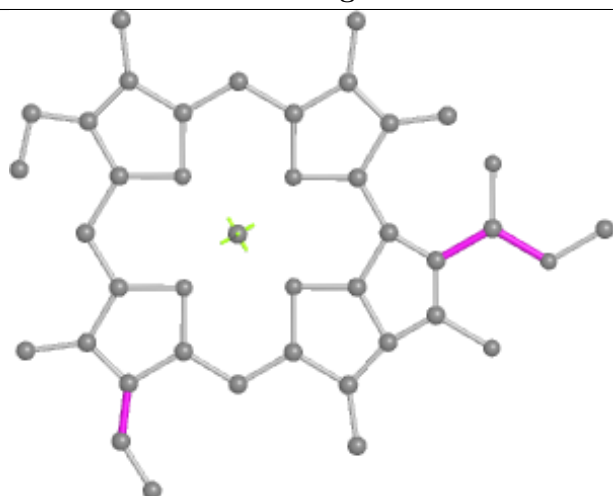
## Ligand CLA D 217



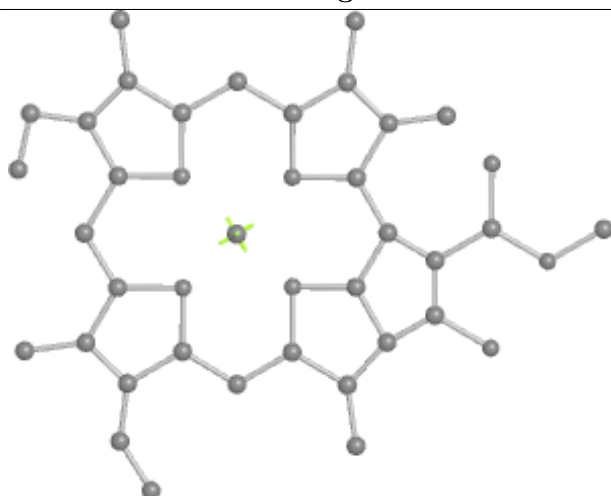
Bond lengths



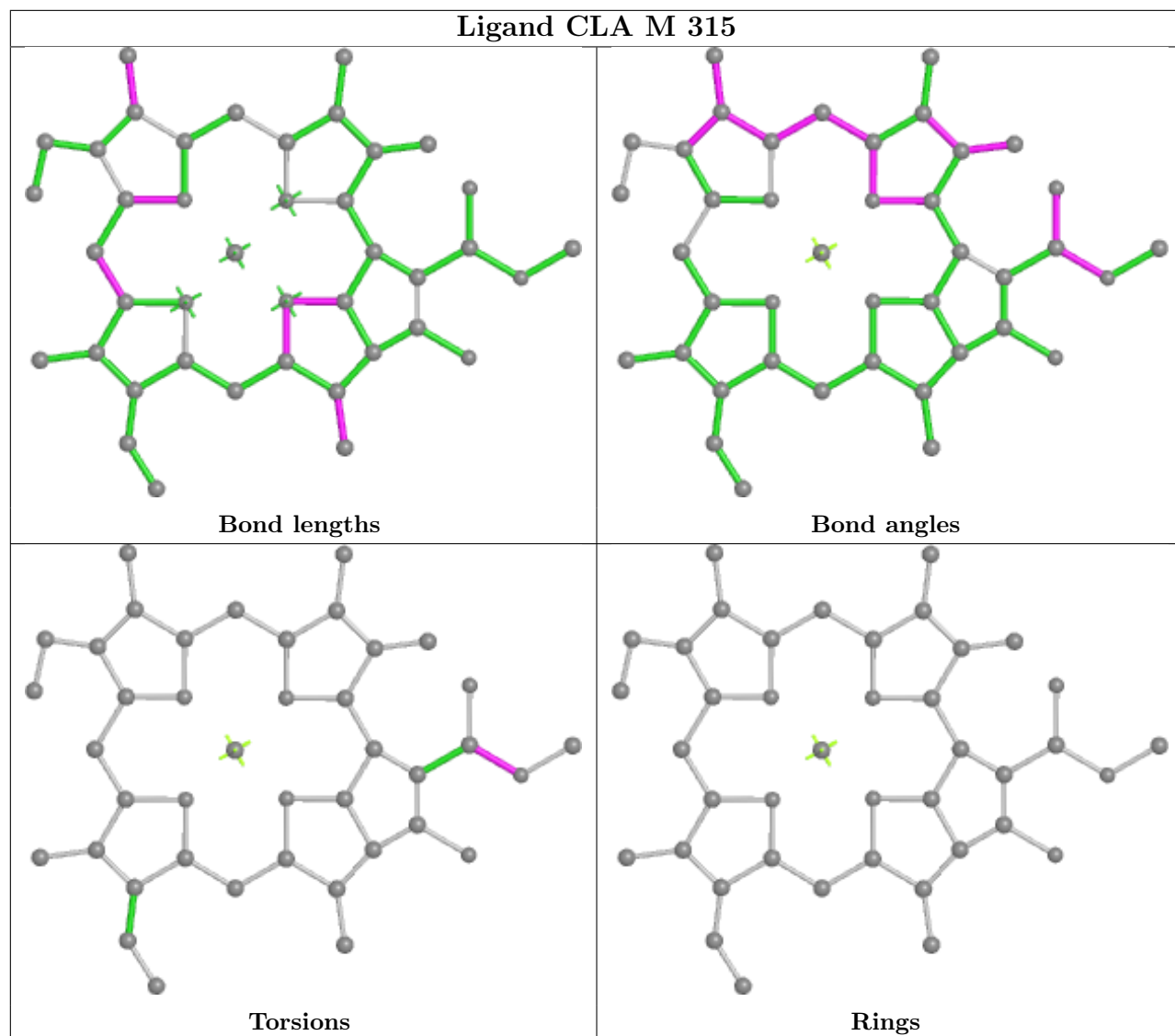
Bond angles

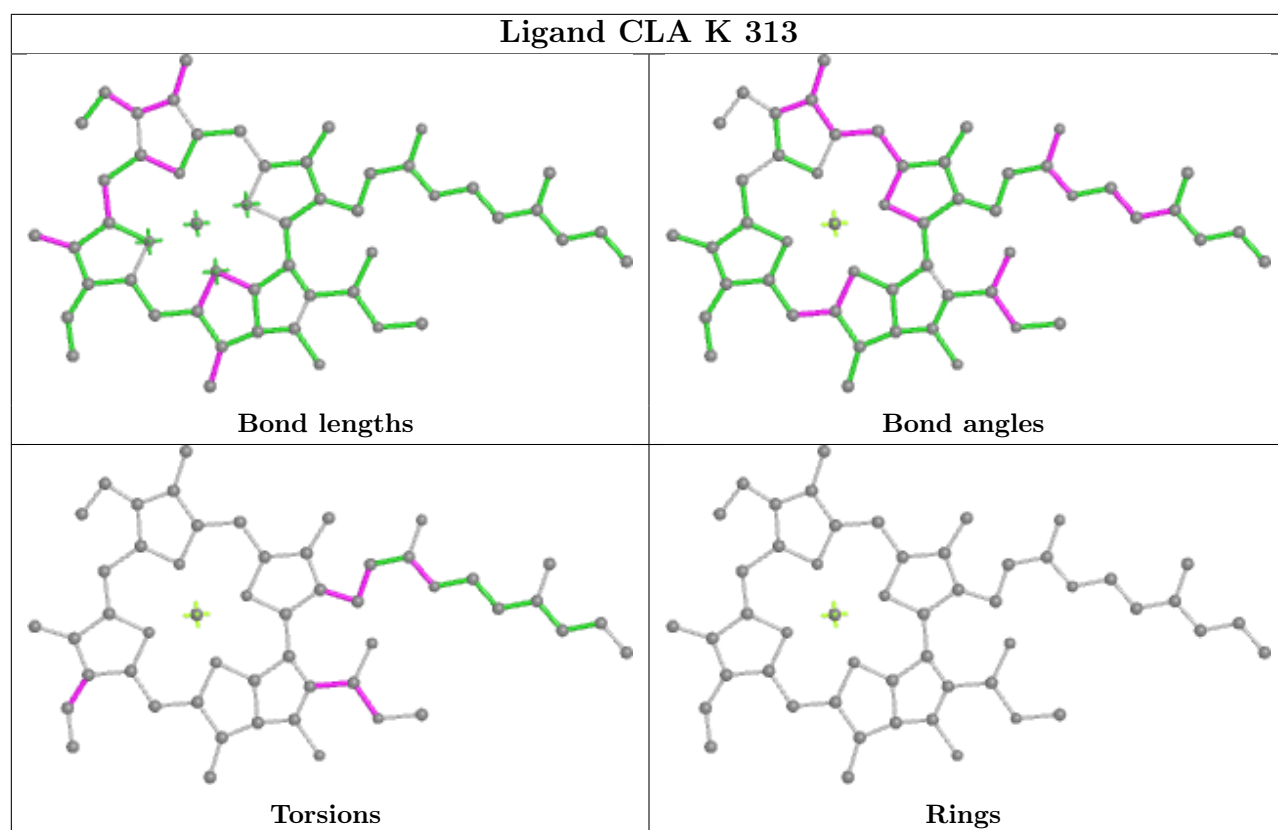


Torsions

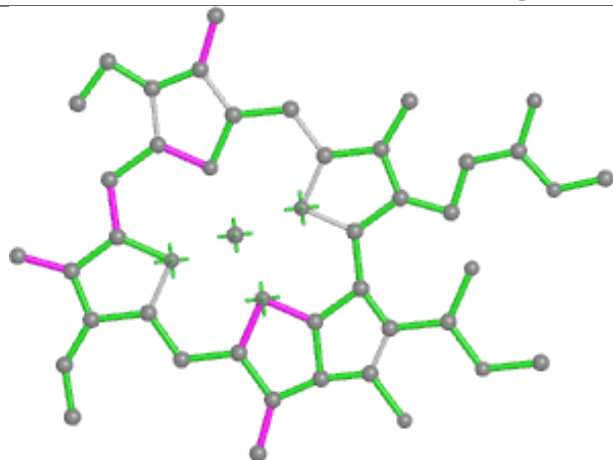


Rings

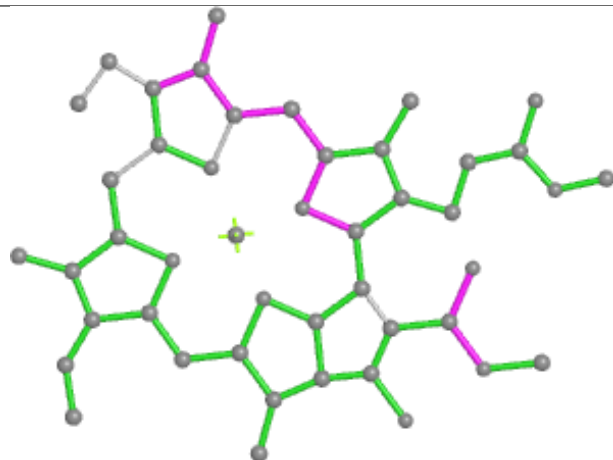




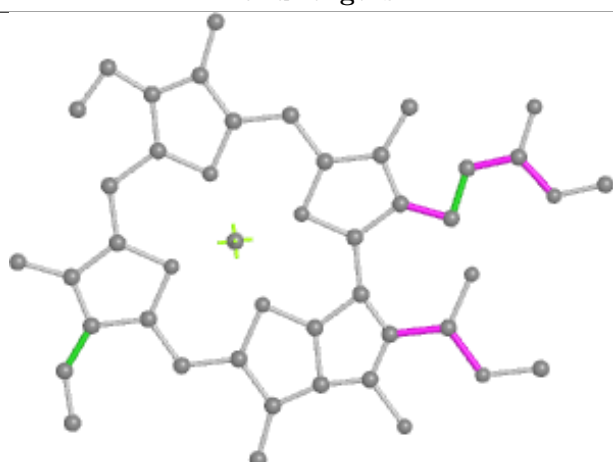
## Ligand CLA D 211



Bond lengths



Bond angles

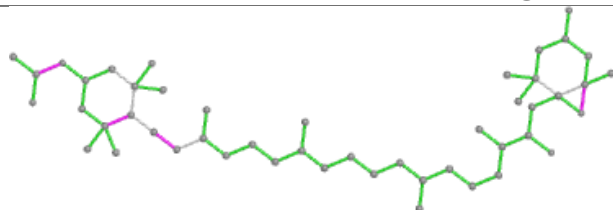


Torsions

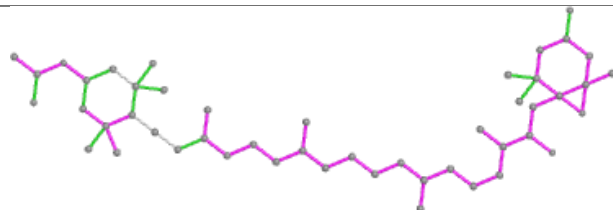


Rings

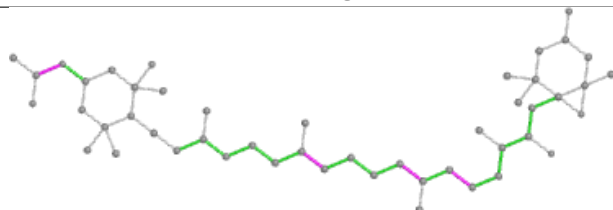
## Ligand A86 m 101



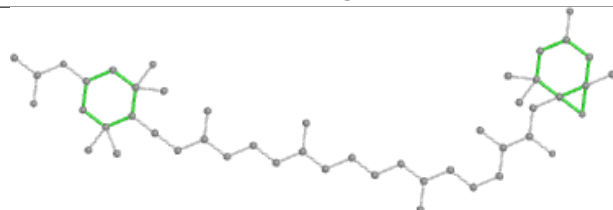
Bond lengths



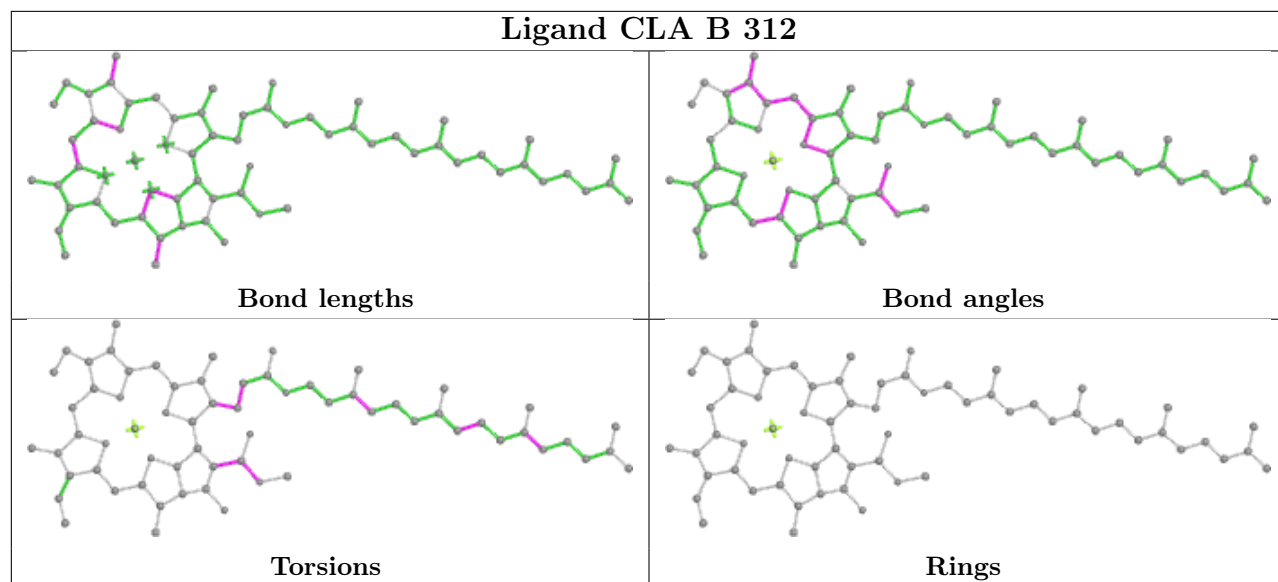
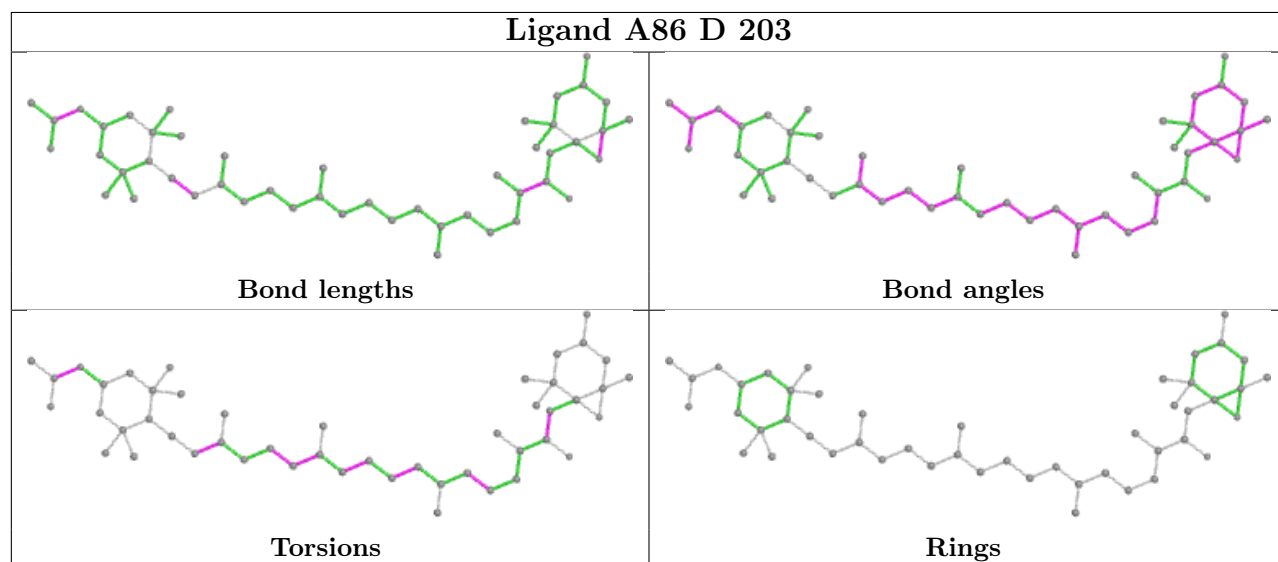
Bond angles



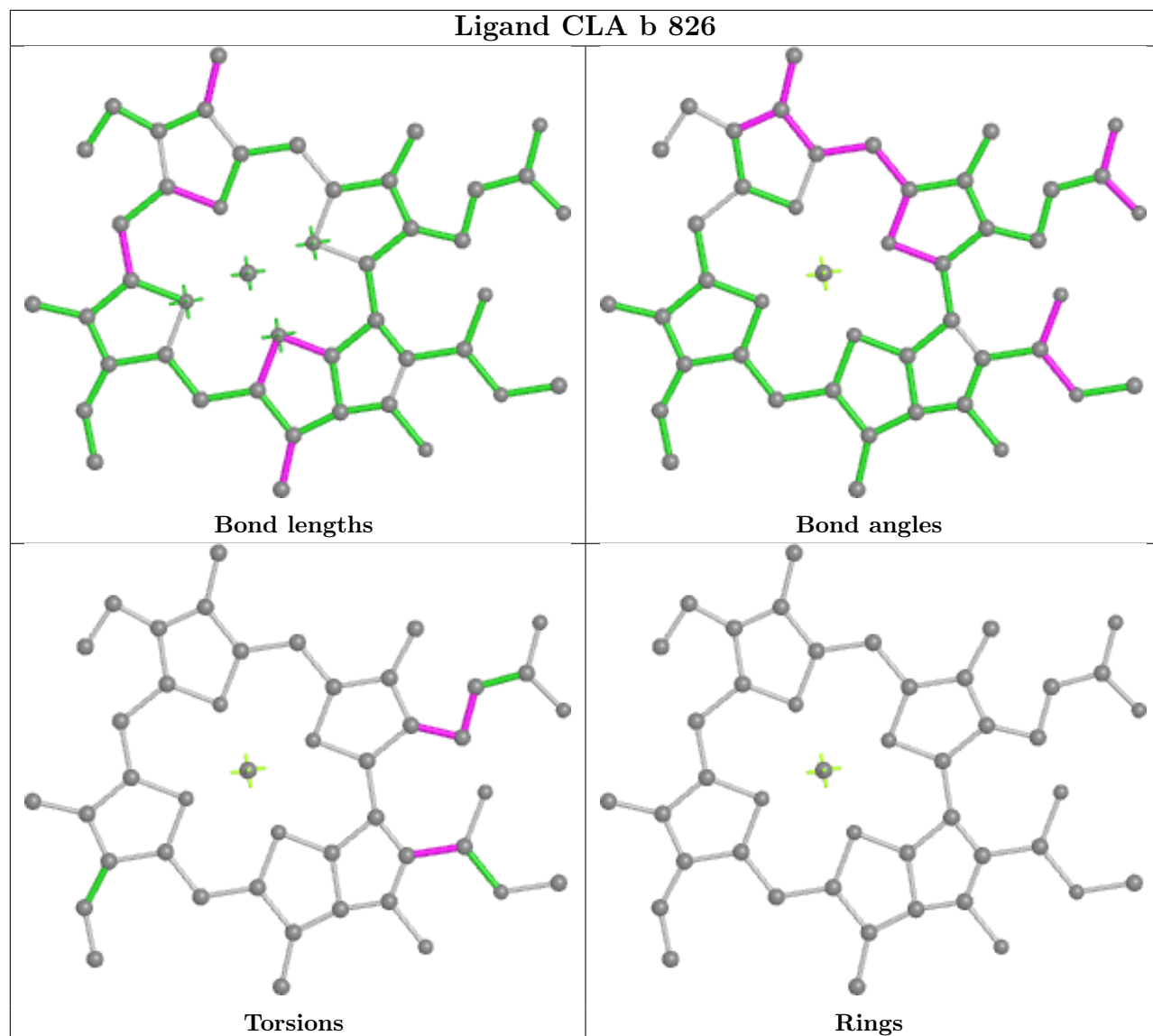
Torsions



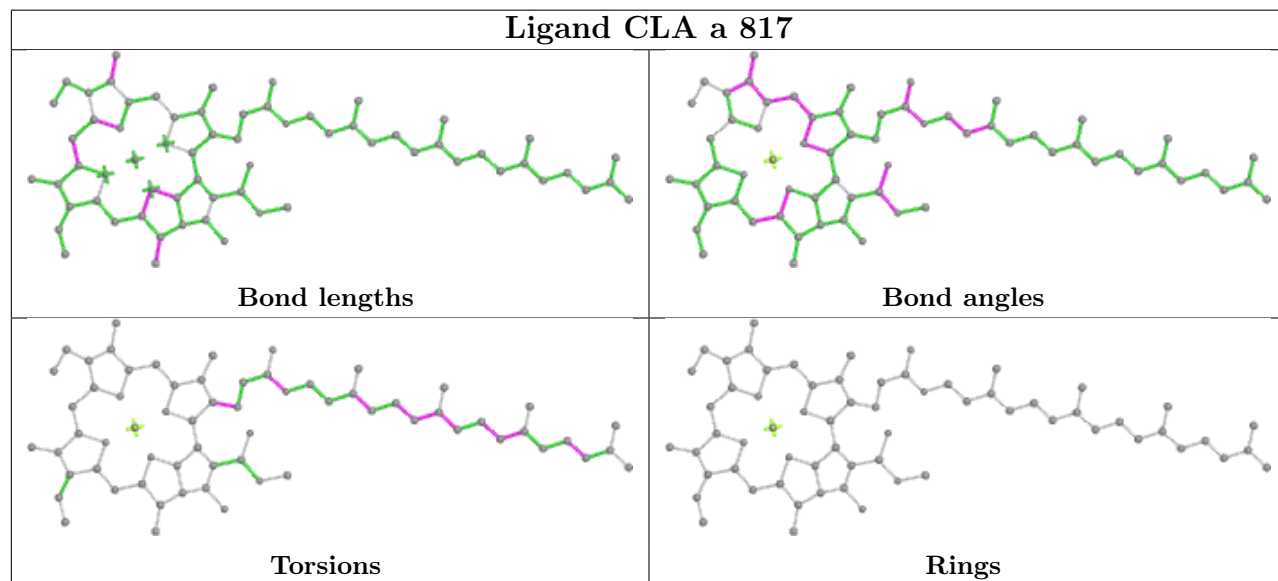
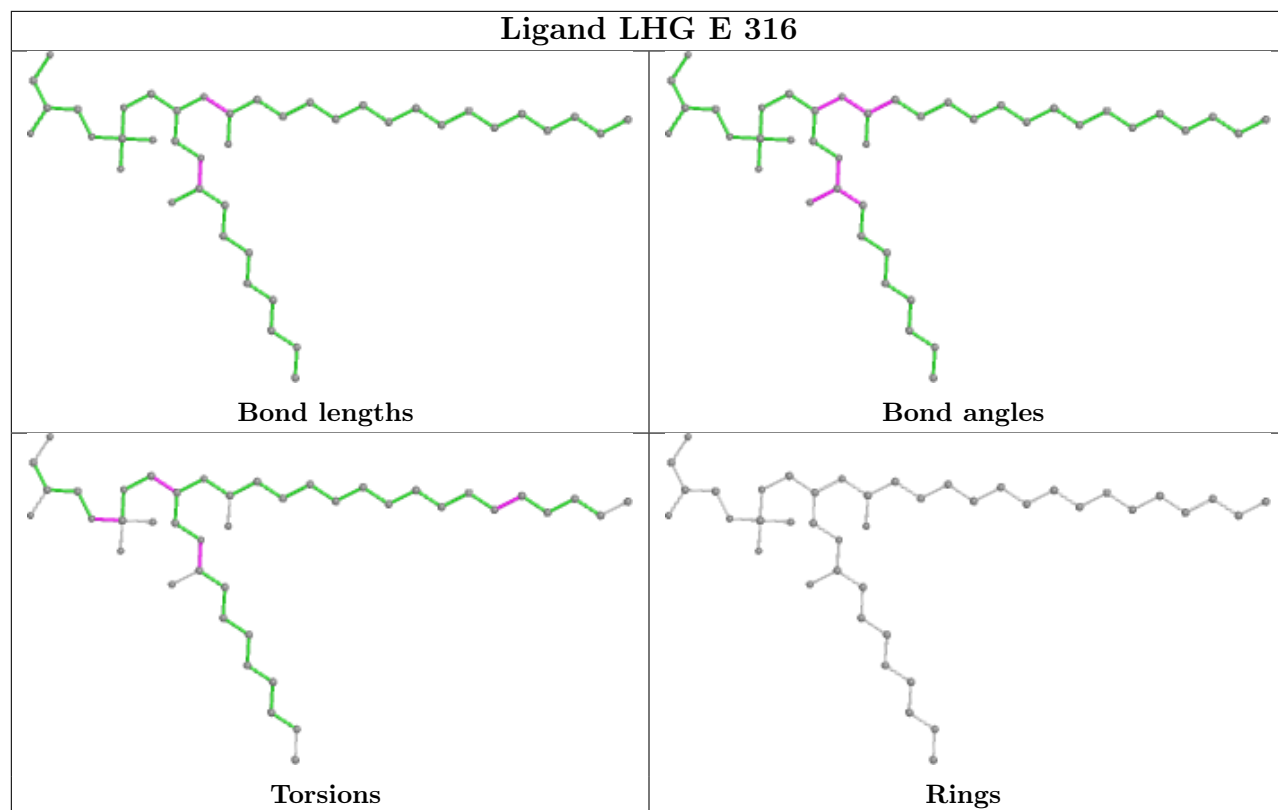
Rings

**Ligand CLA B 312****Ligand A86 D 203**

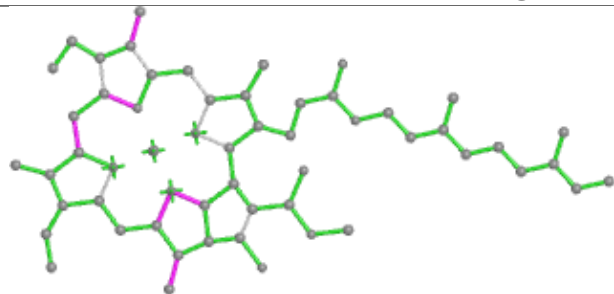
## Ligand CLA b 826



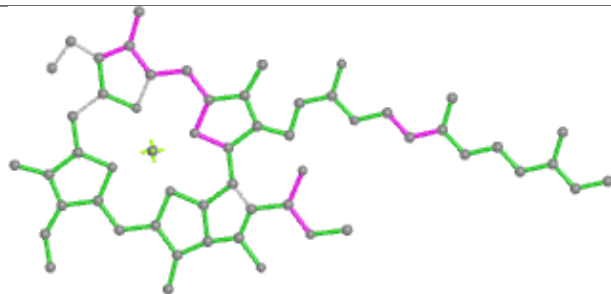




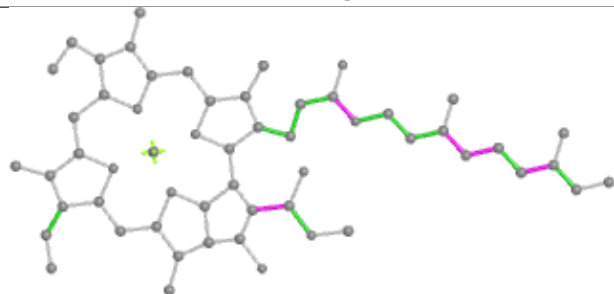
## Ligand CLA G 311



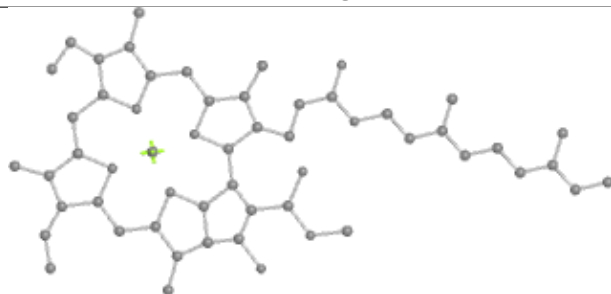
Bond lengths



Bond angles

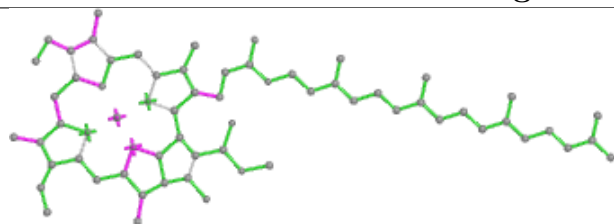


Torsions

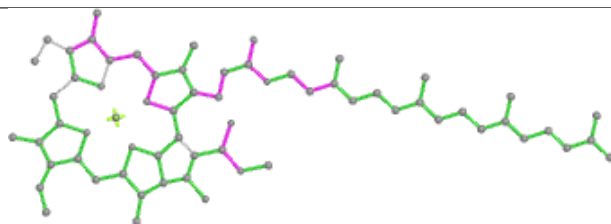


Rings

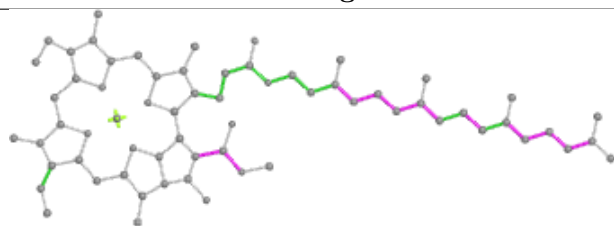
## Ligand CLA H 212



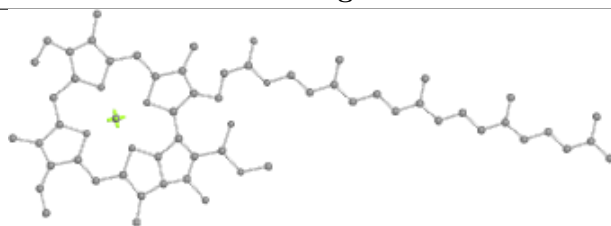
Bond lengths



Bond angles

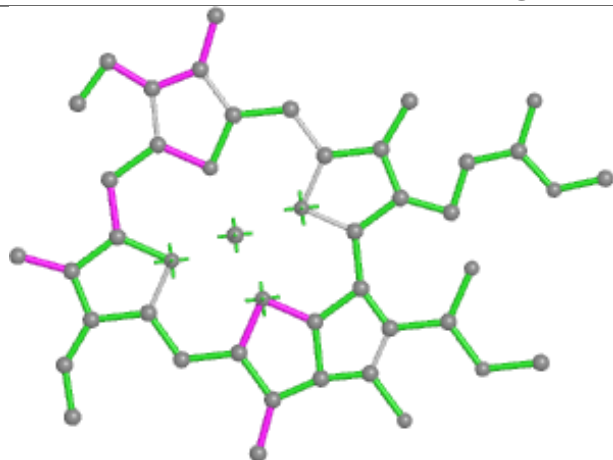


Torsions

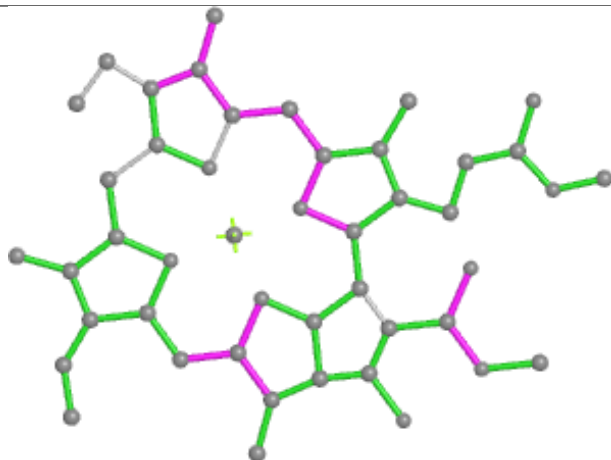


Rings

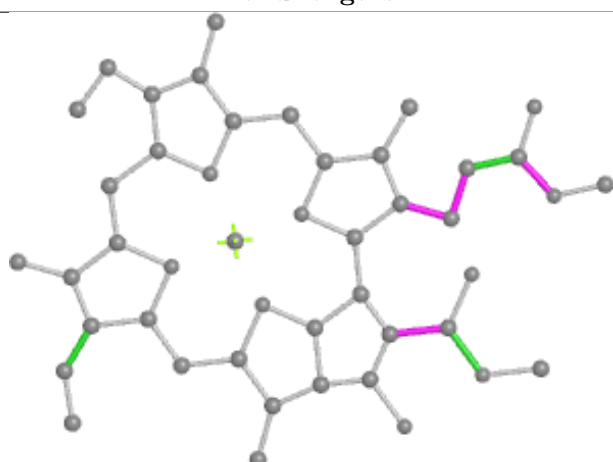
## Ligand CLA K 318



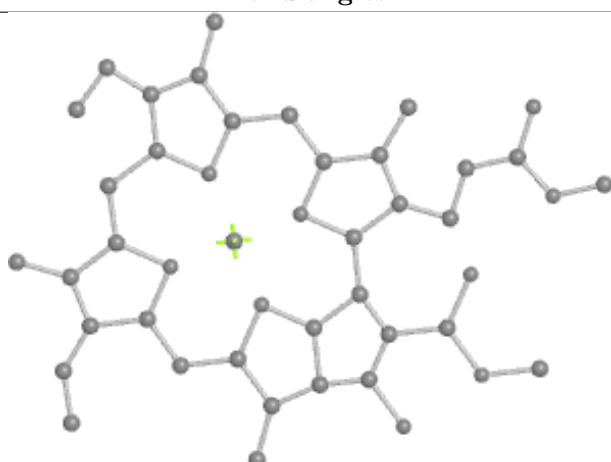
Bond lengths



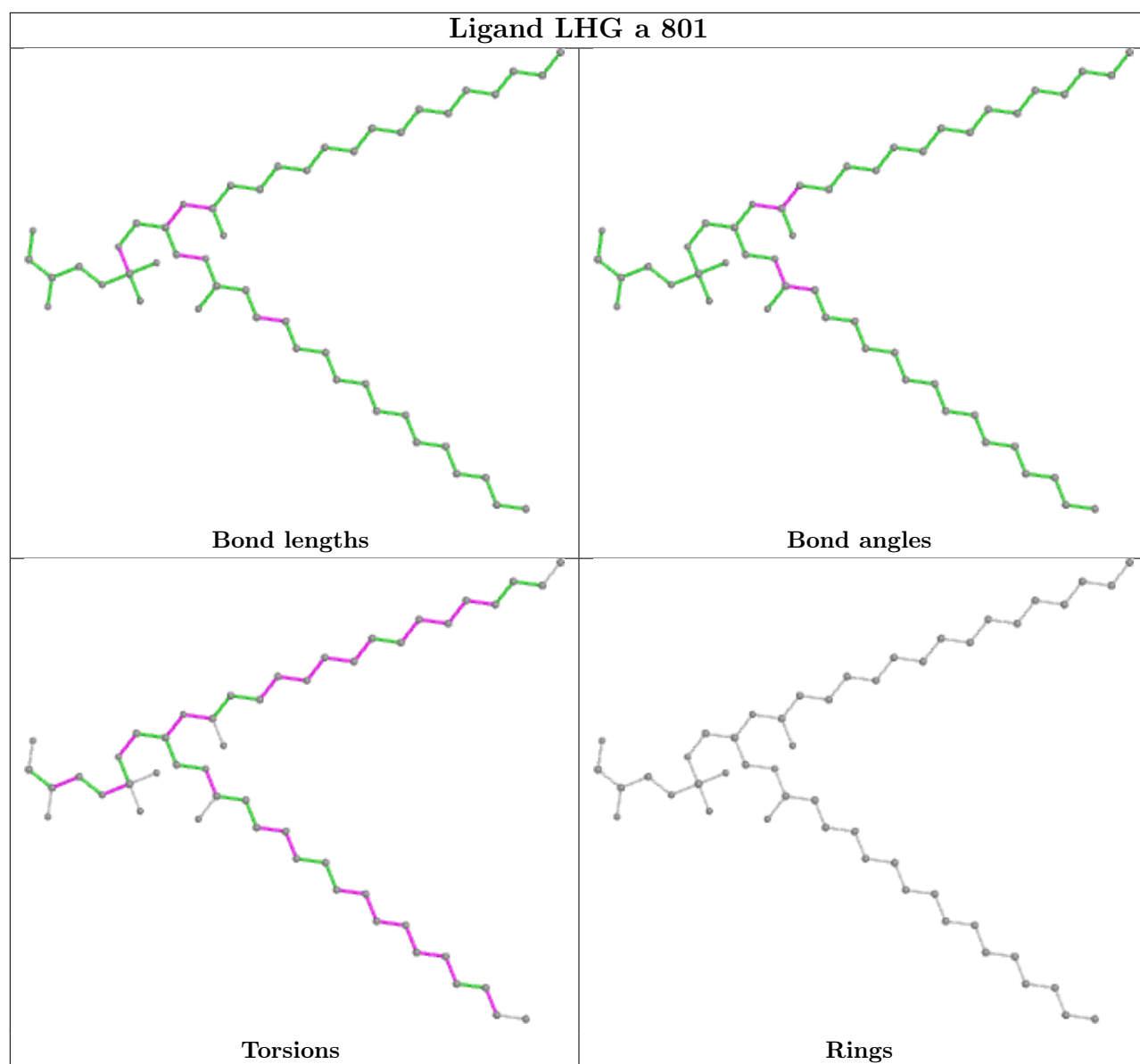
Bond angles

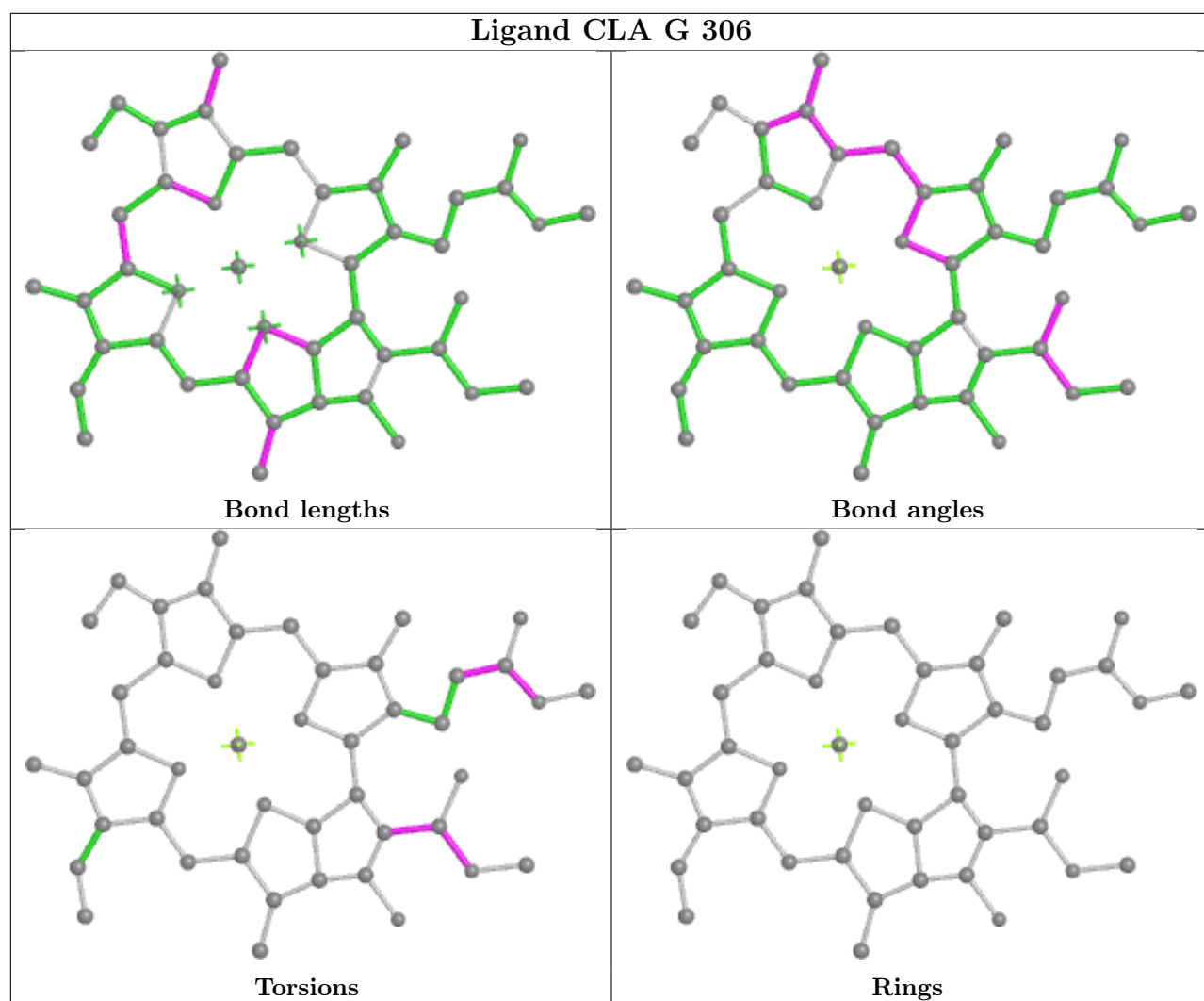


Torsions

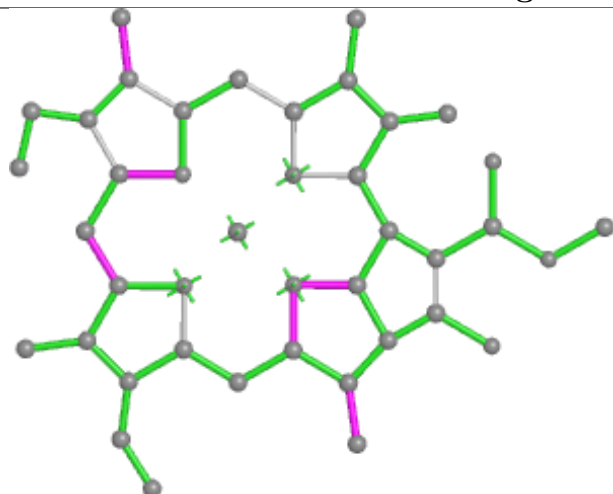


Rings

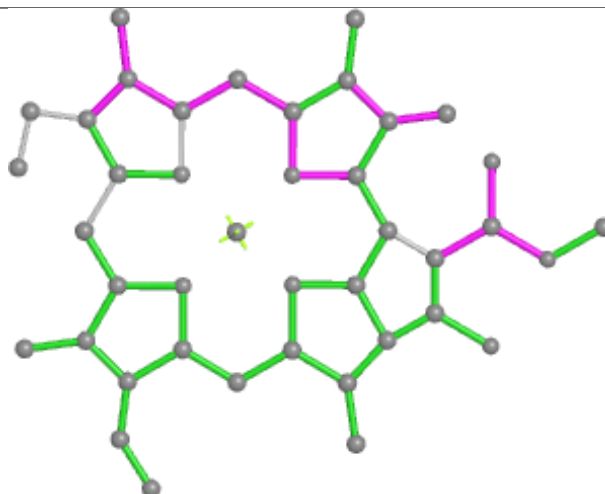




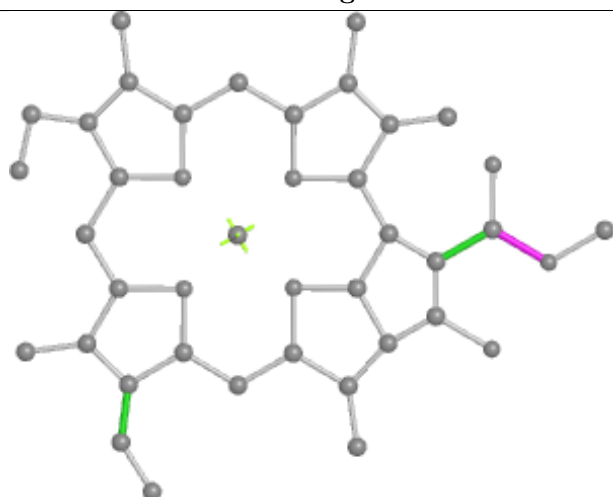
## Ligand CLA F 313



Bond lengths



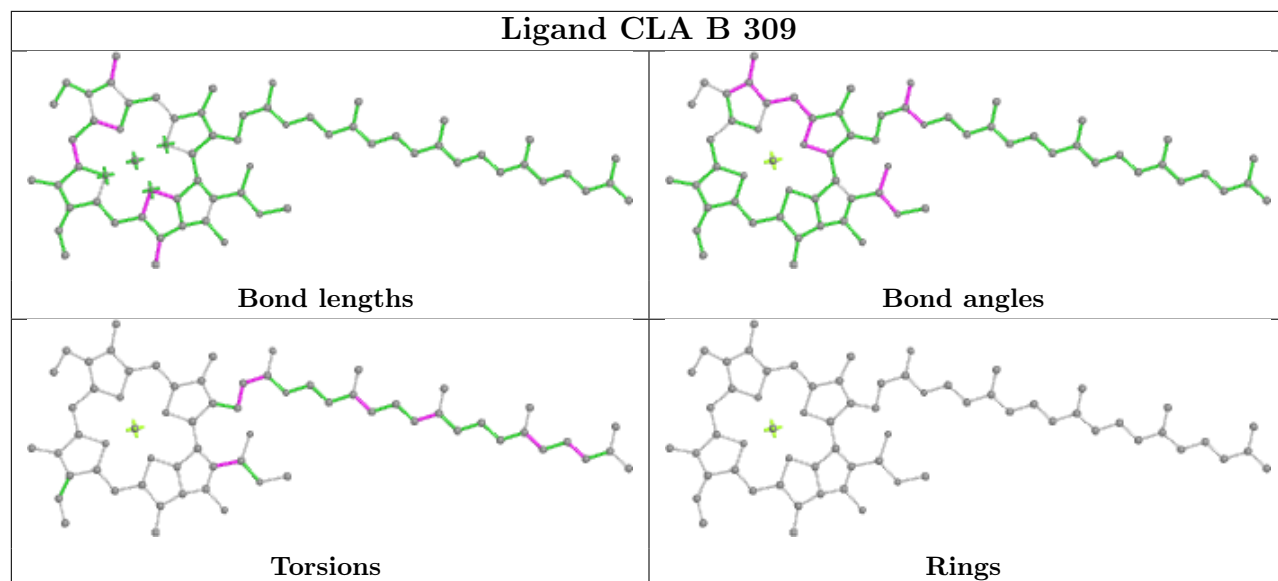
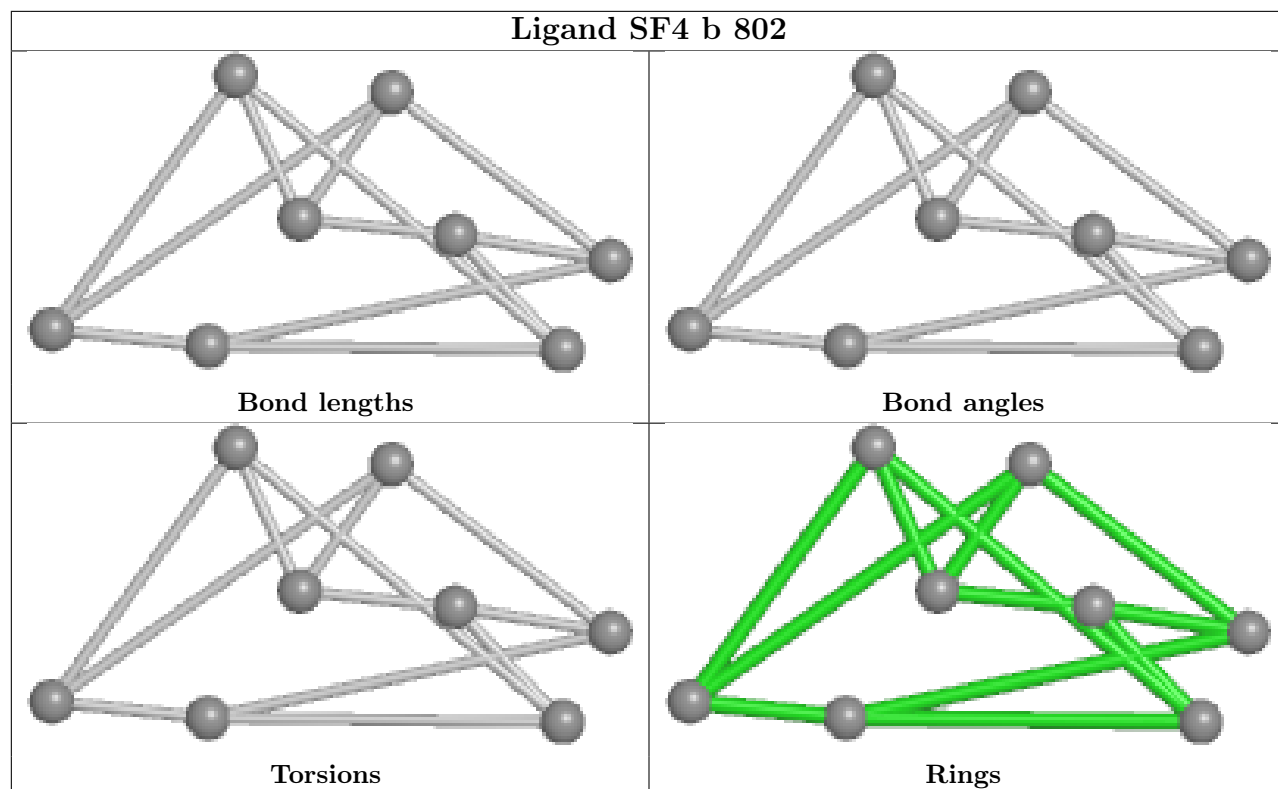
Bond angles



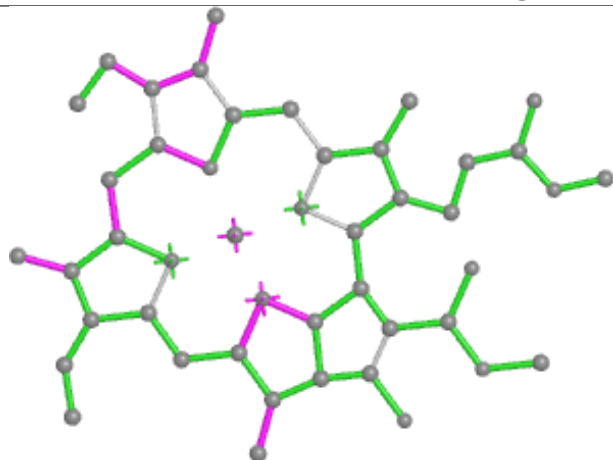
Torsions



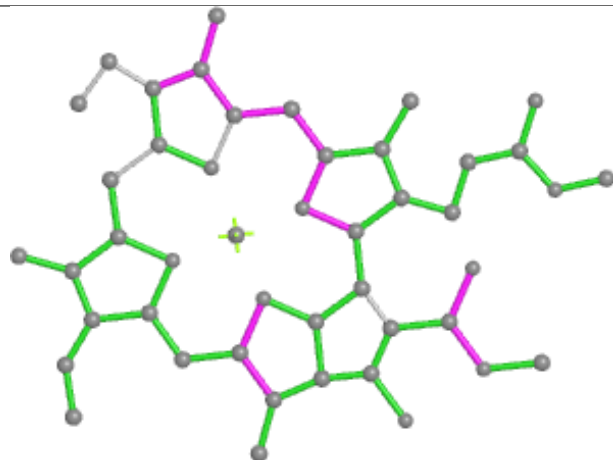
Rings



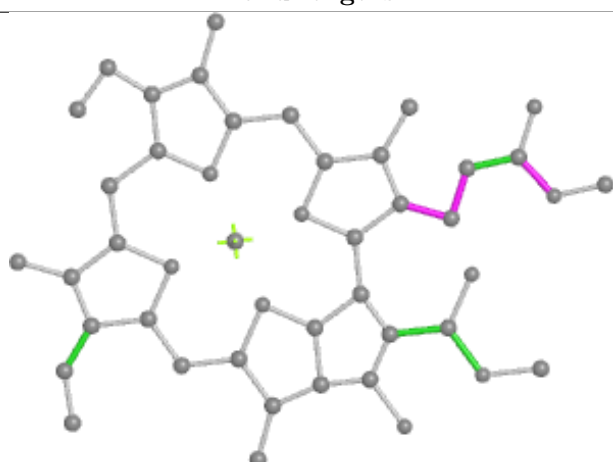
## Ligand CLA D 216



Bond lengths



Bond angles

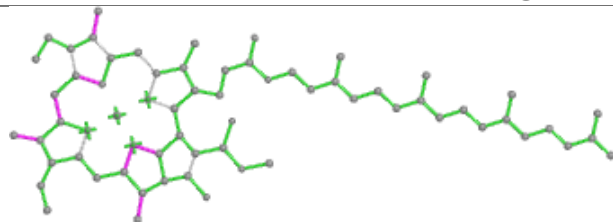


Torsions

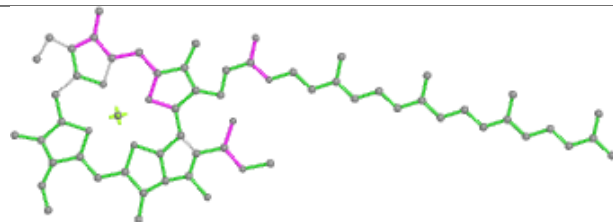


Rings

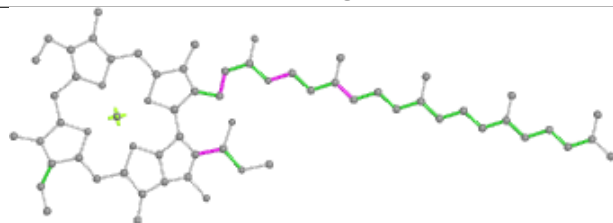
## Ligand CLA b 839



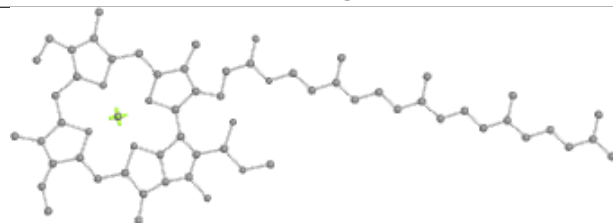
Bond lengths



Bond angles



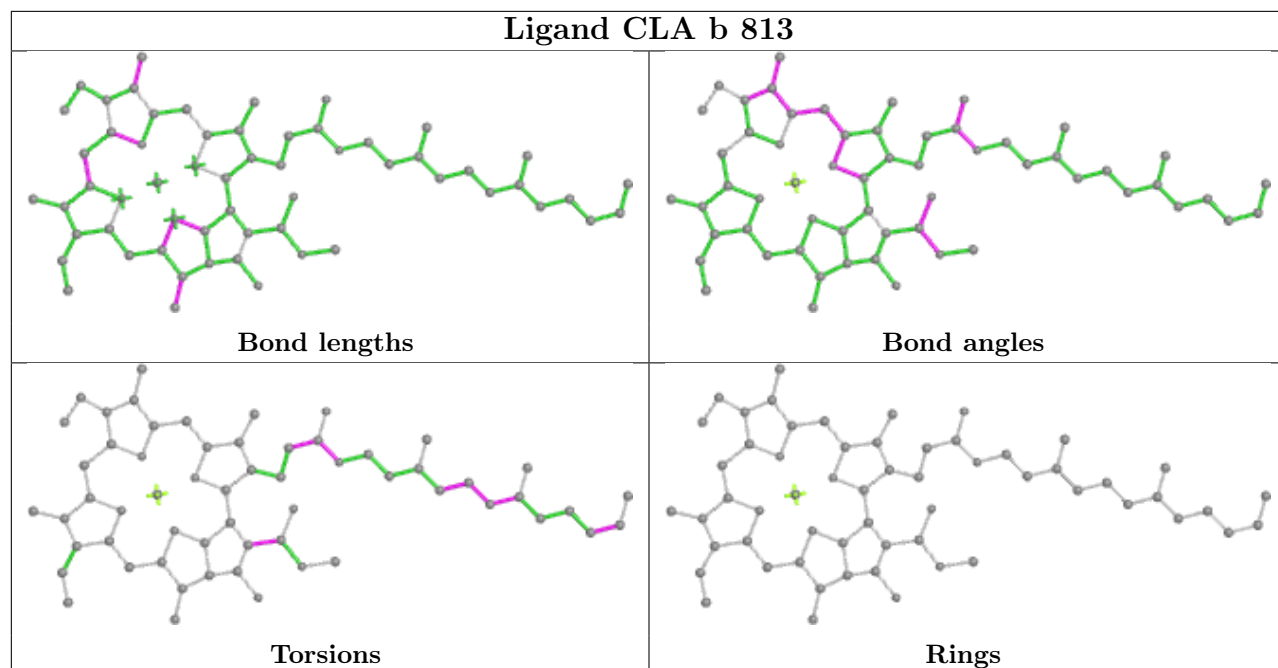
Torsions



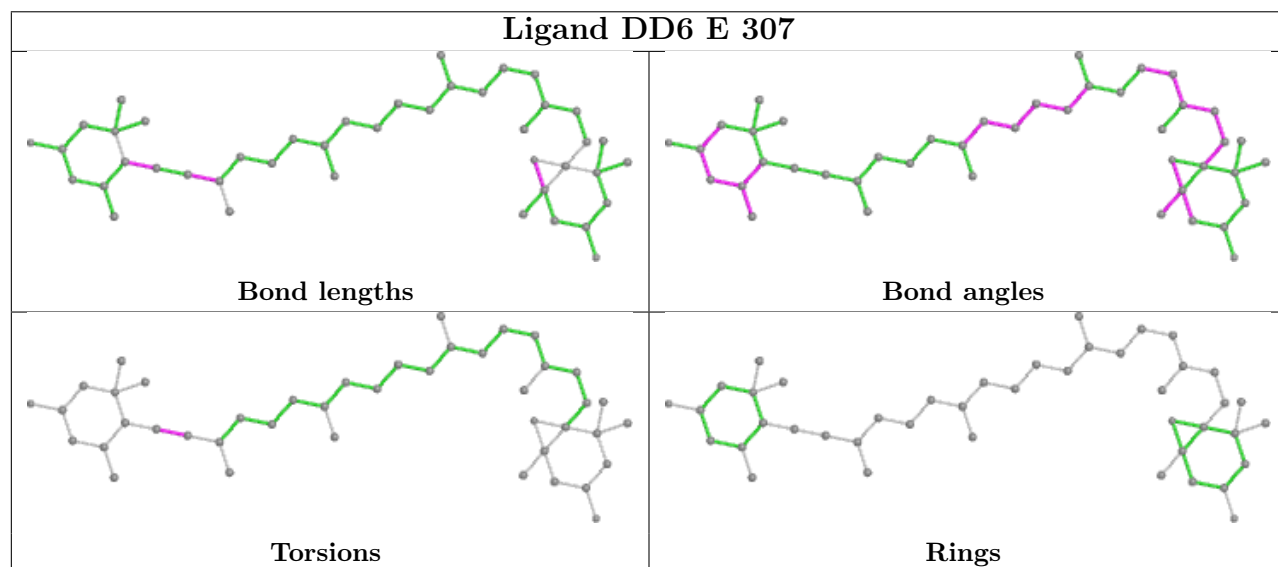
Rings



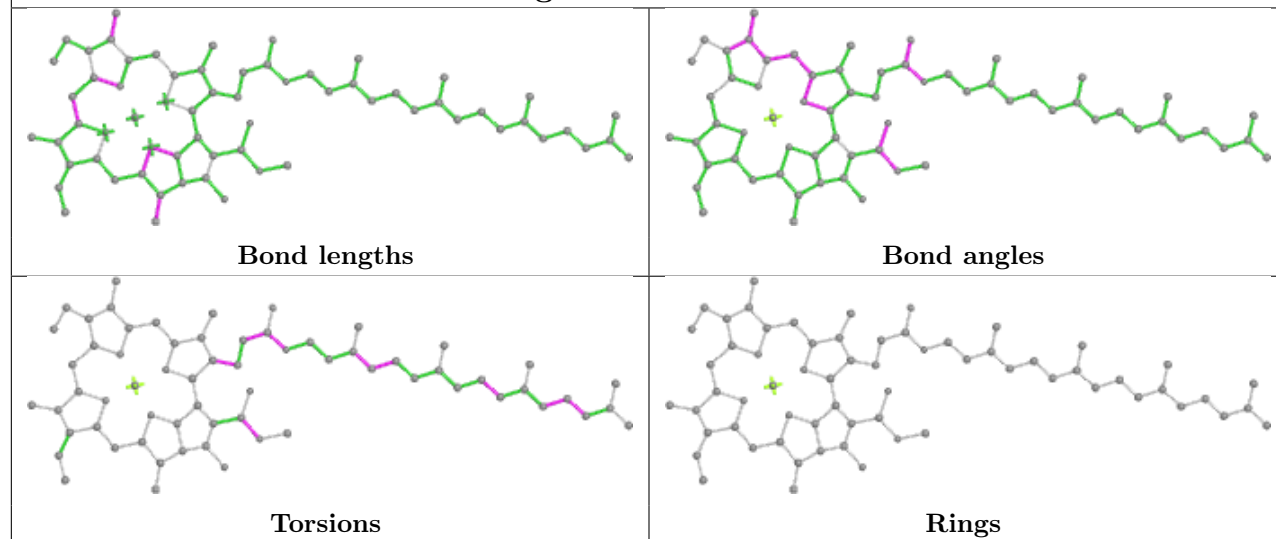
## Ligand CLA b 813



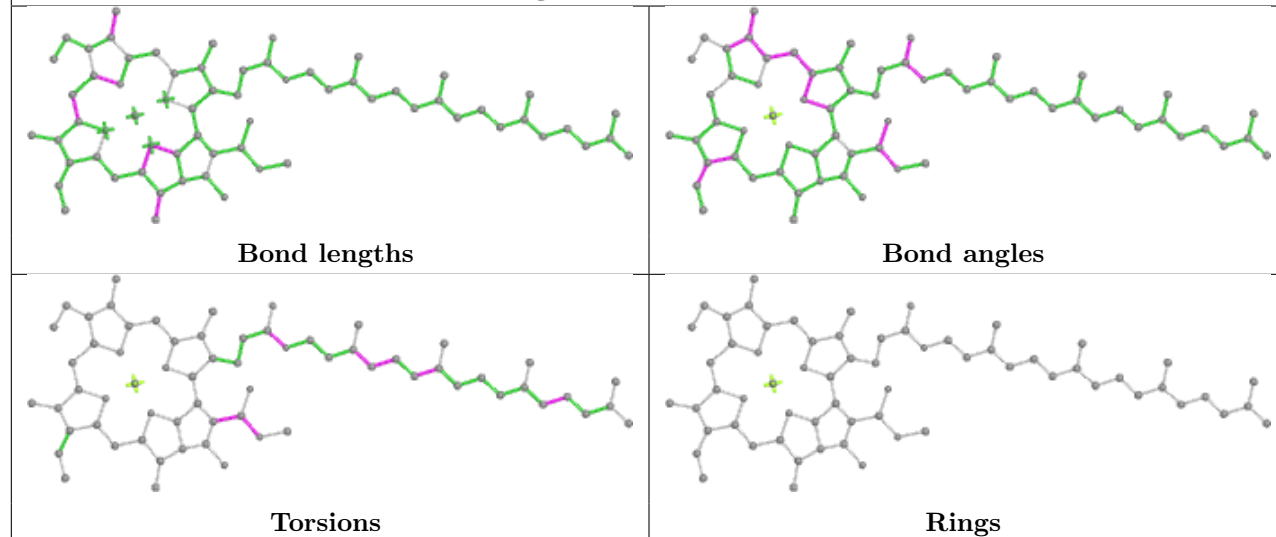
## Ligand DD6 E 307



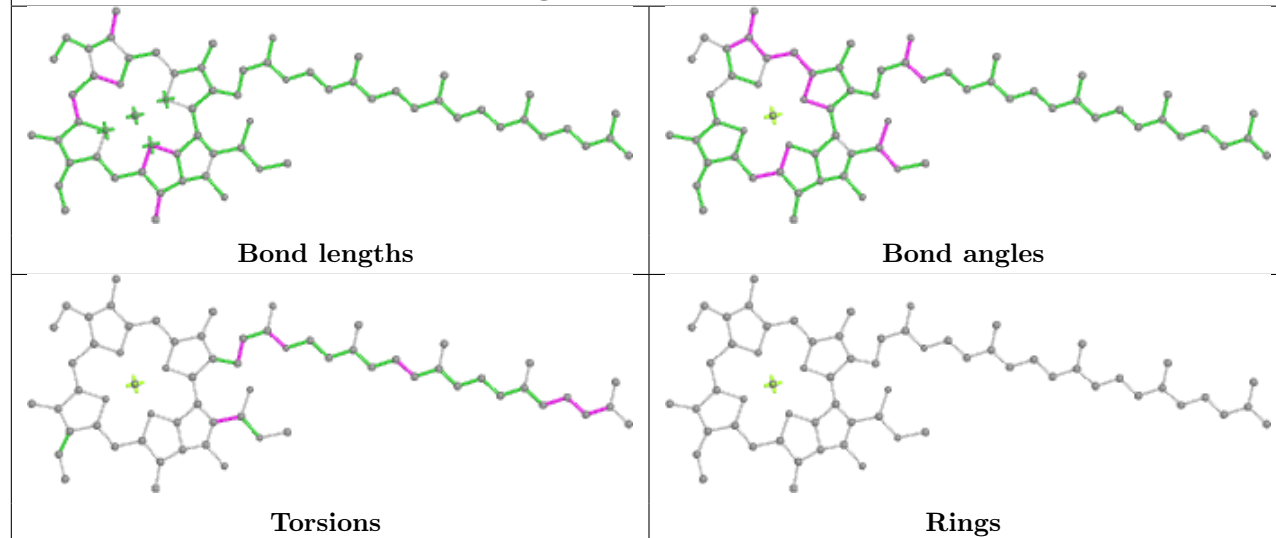
## Ligand CLA b 850



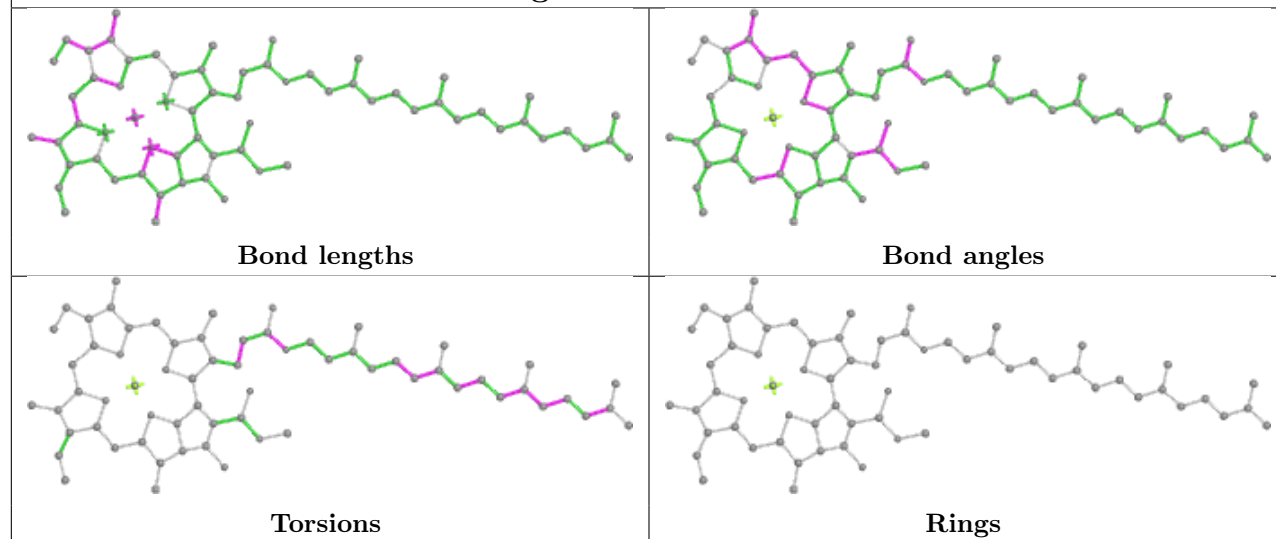
## Ligand CLA B 311



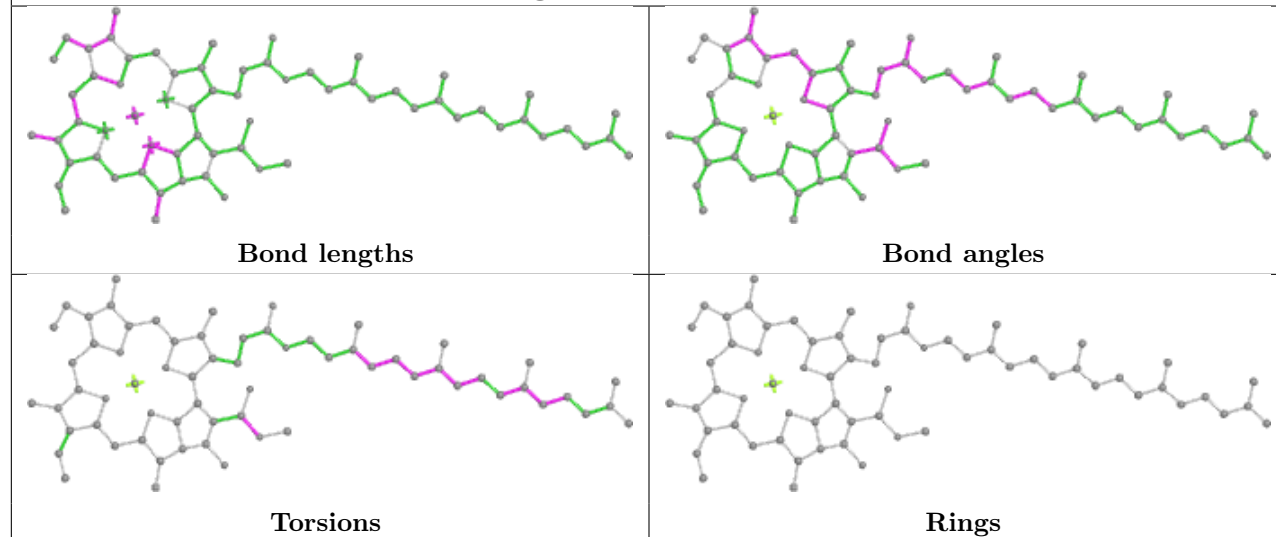
## Ligand CLA b 829



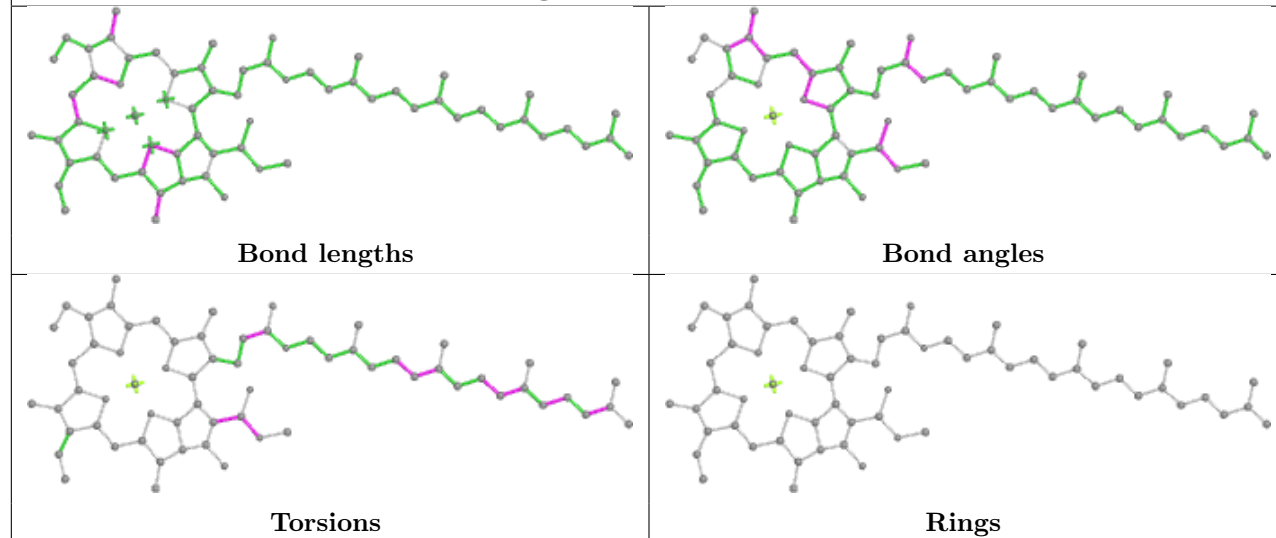
## Ligand CLA H 205



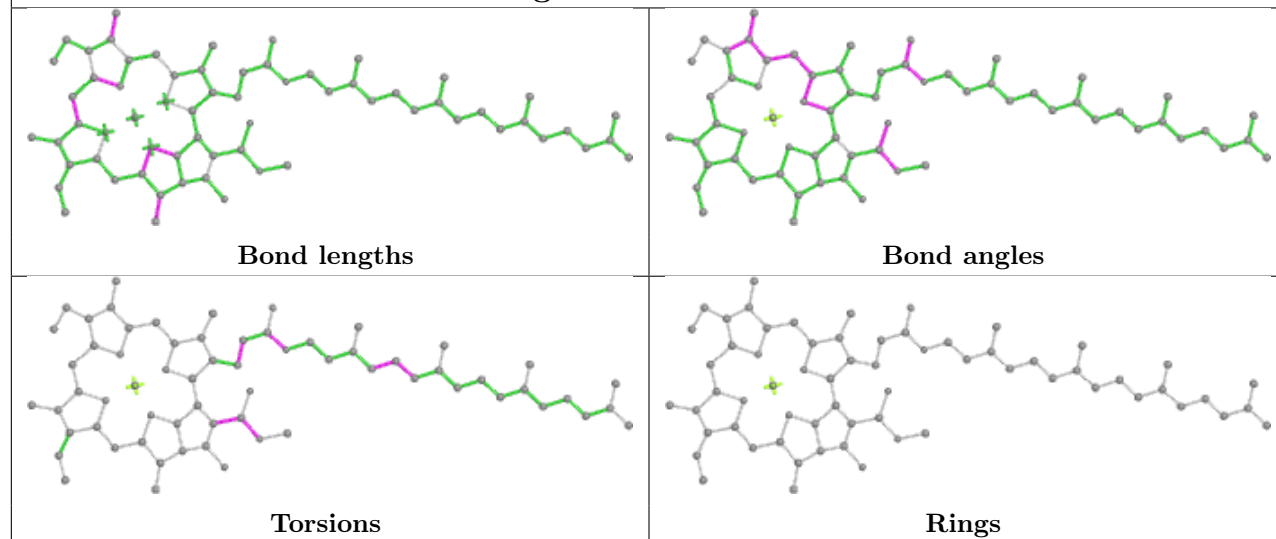
## Ligand CLA D 208



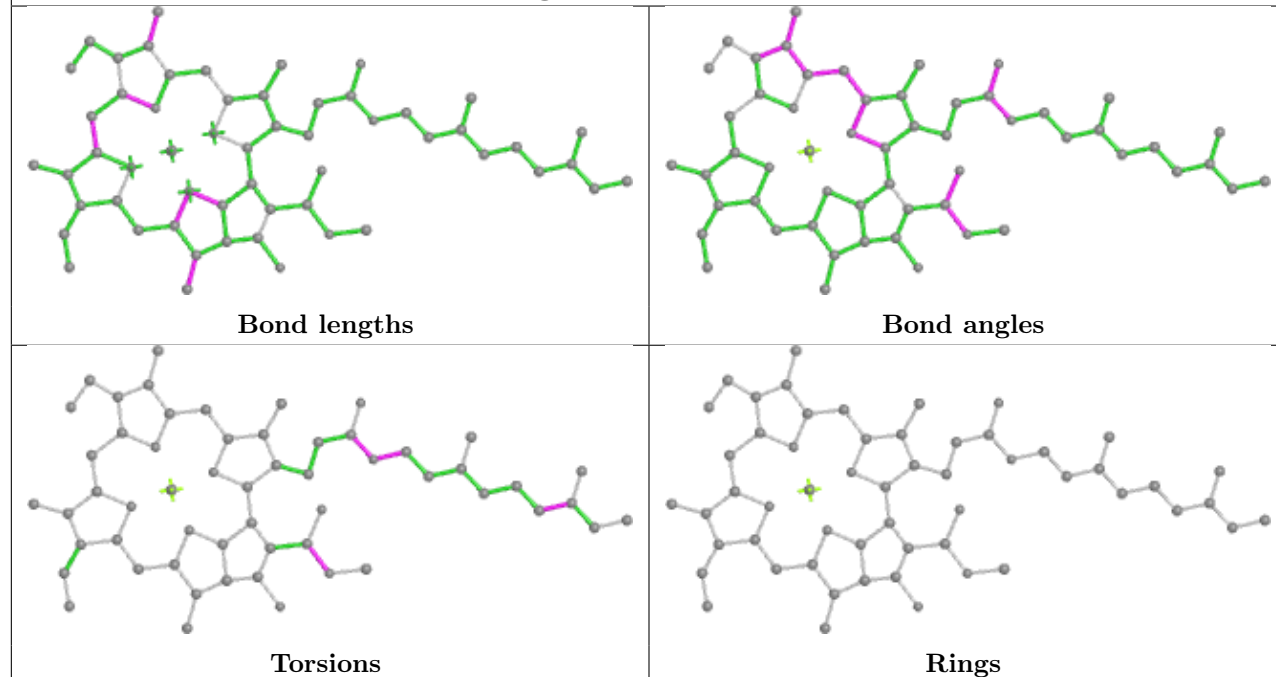
## Ligand CLA b 803



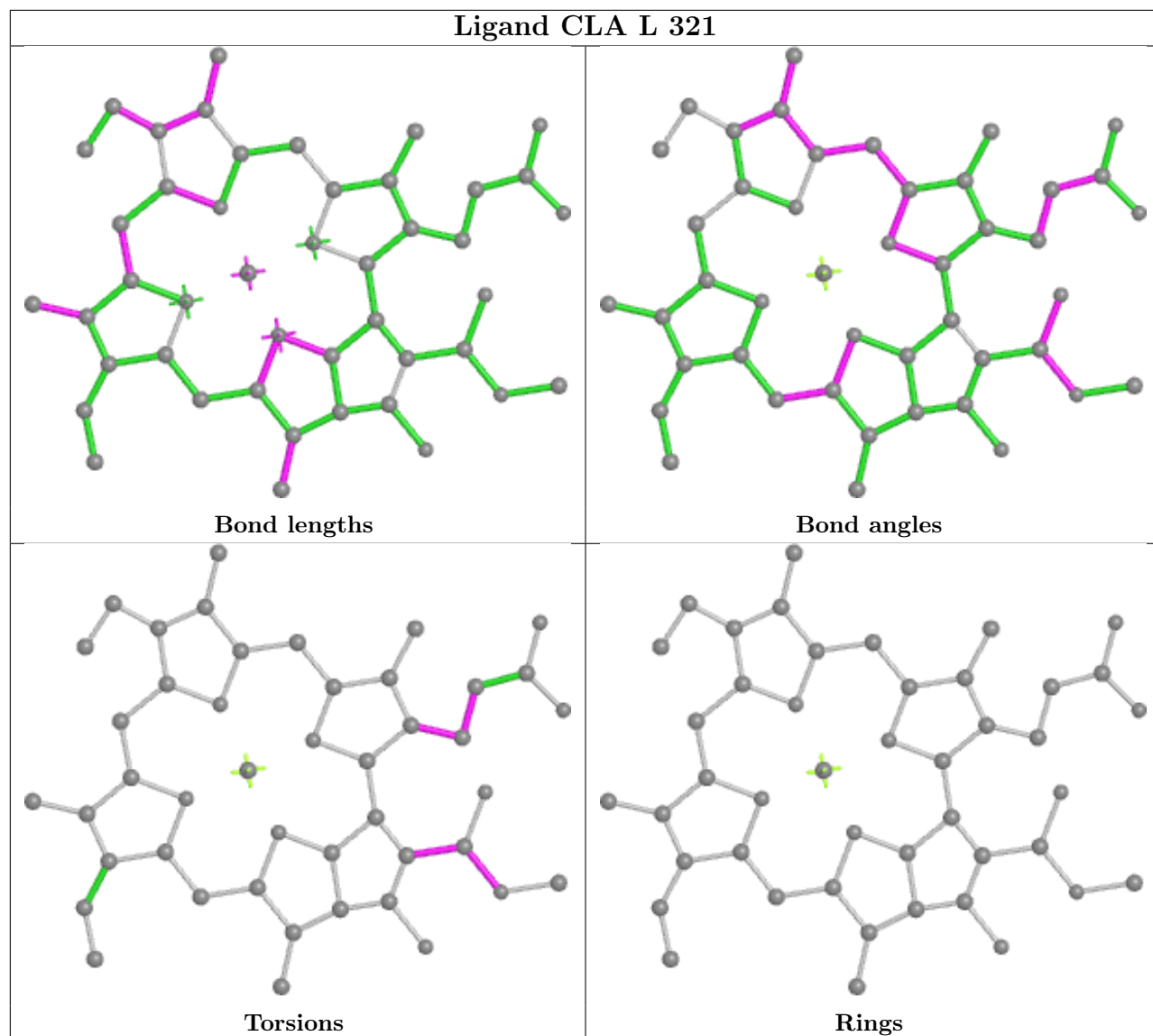
## Ligand CLA E 314



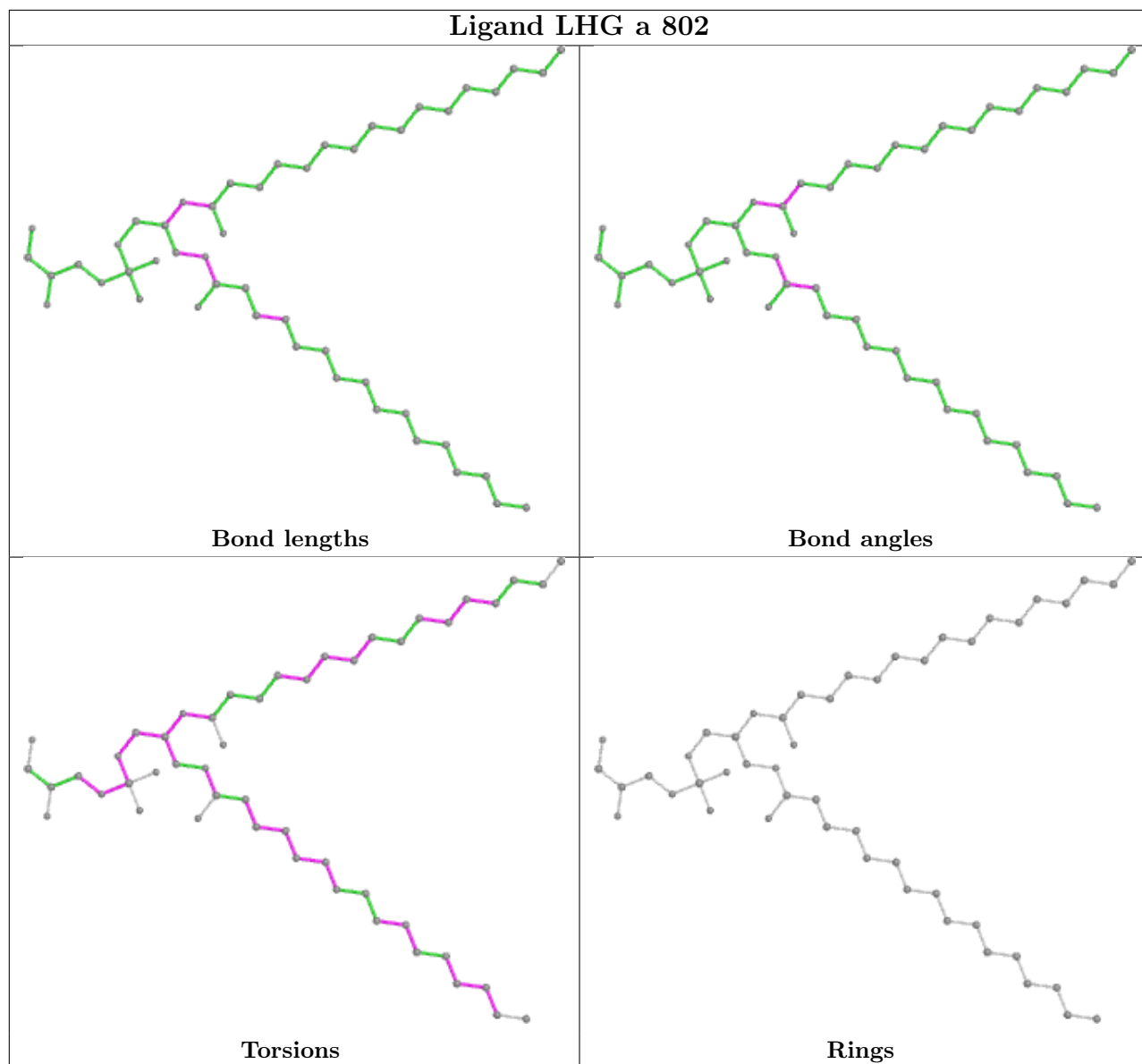
## Ligand CLA J 308



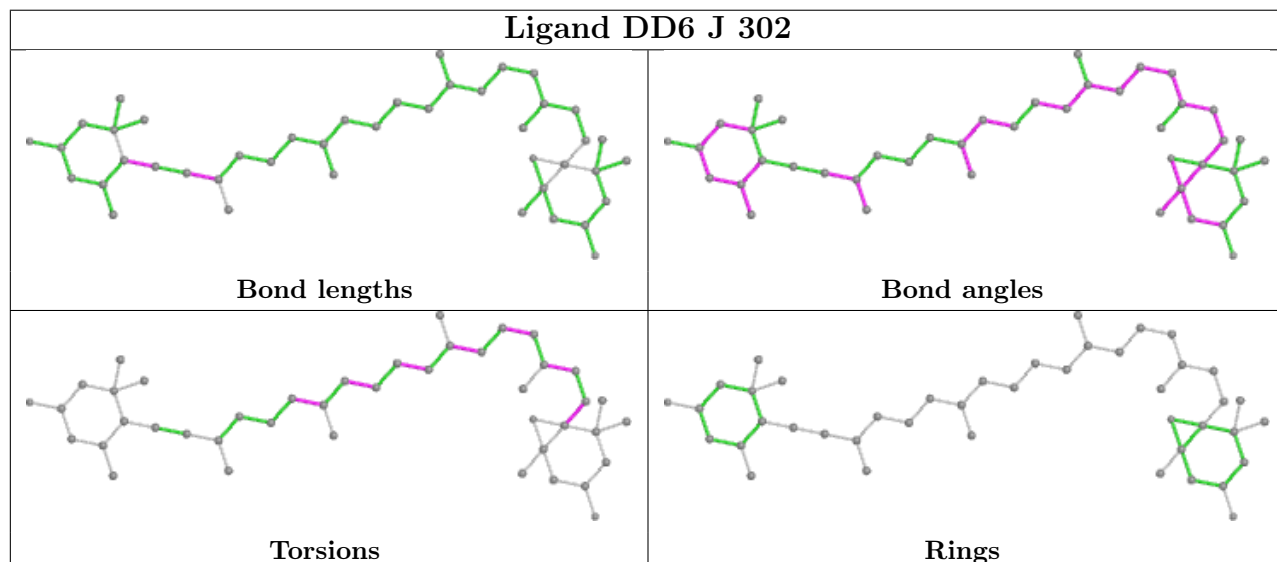
## Ligand CLA L 321

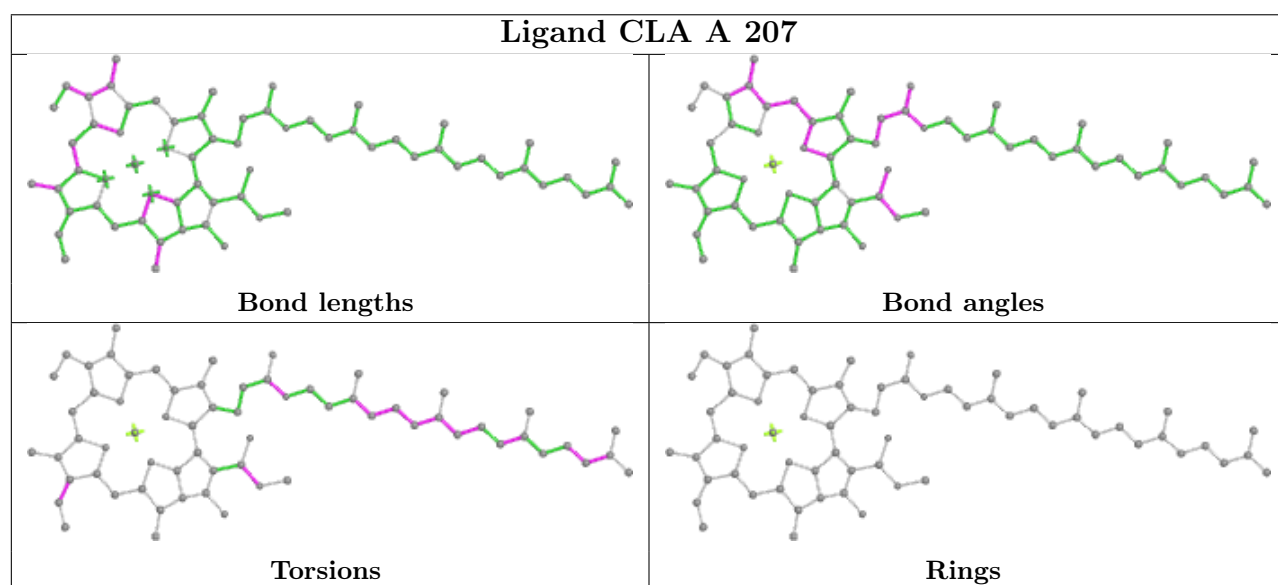
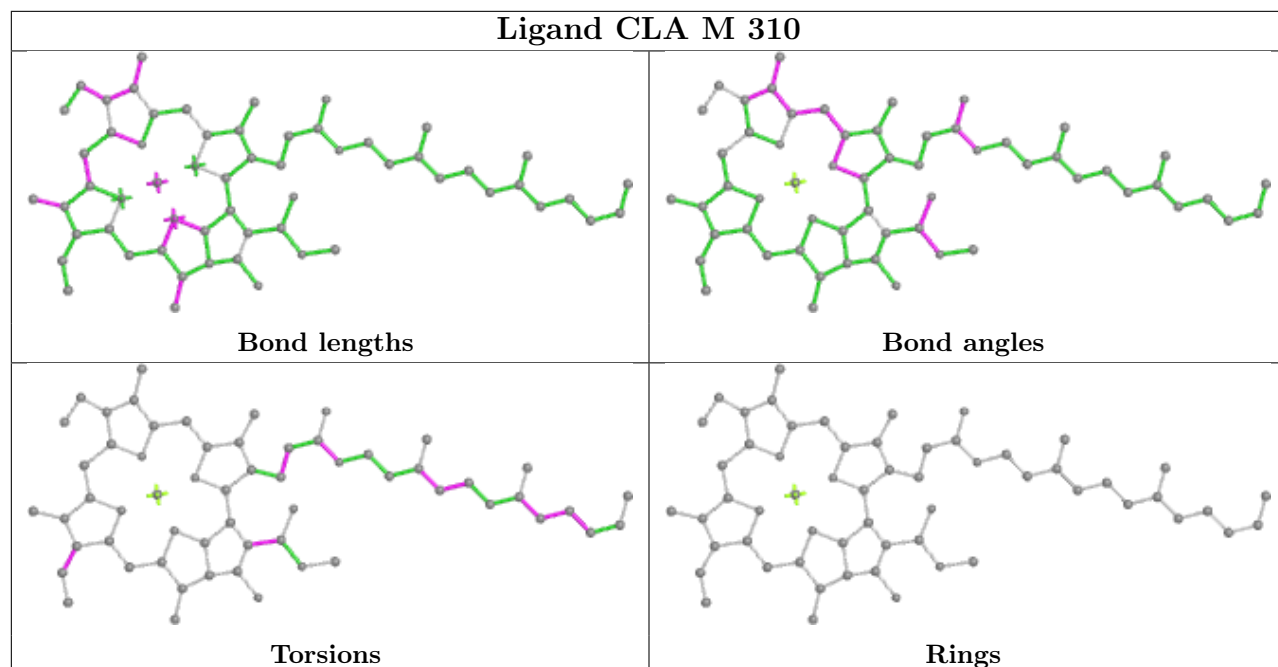
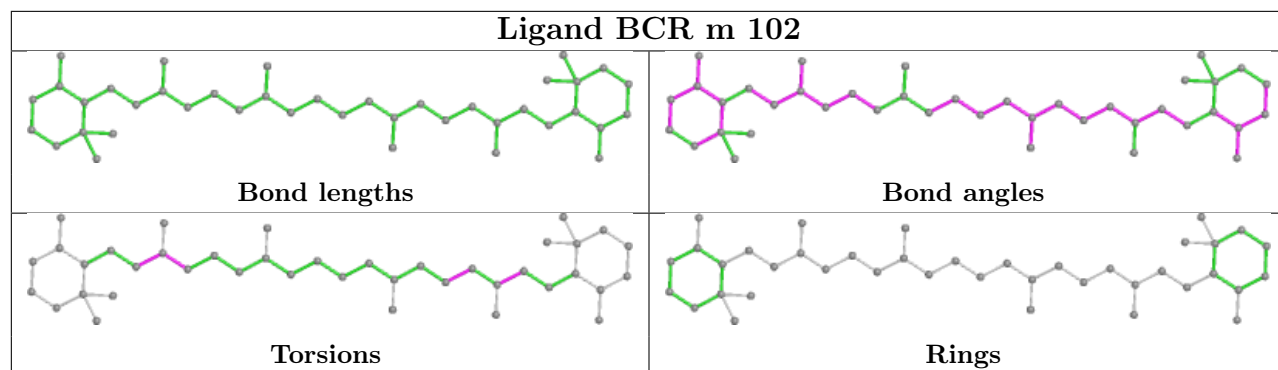


## Ligand LHG a 802

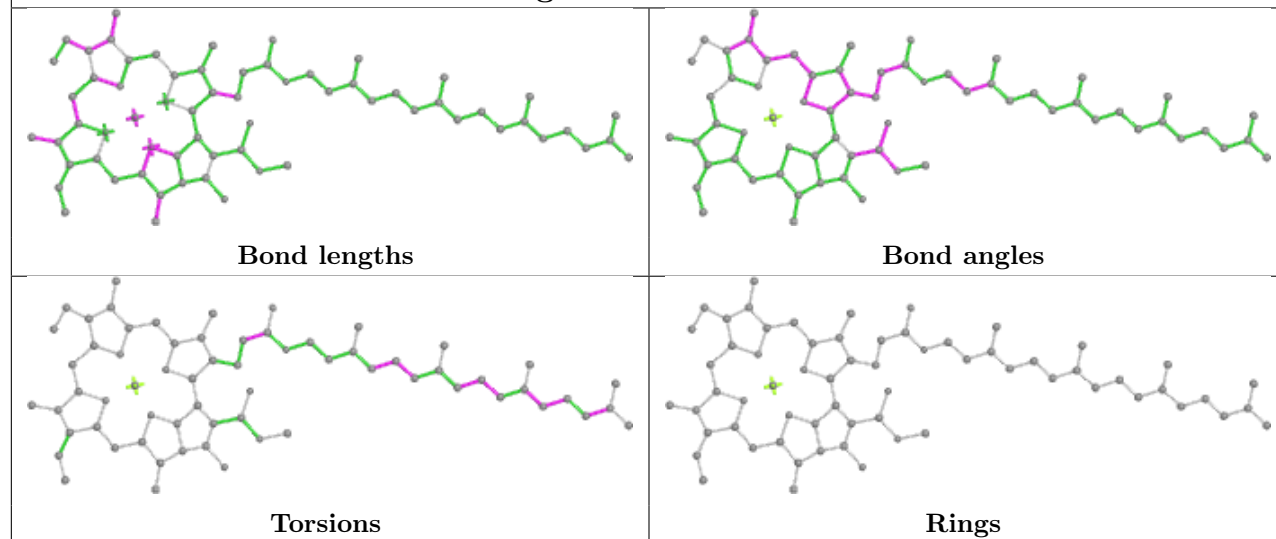


## Ligand DD6 J 302

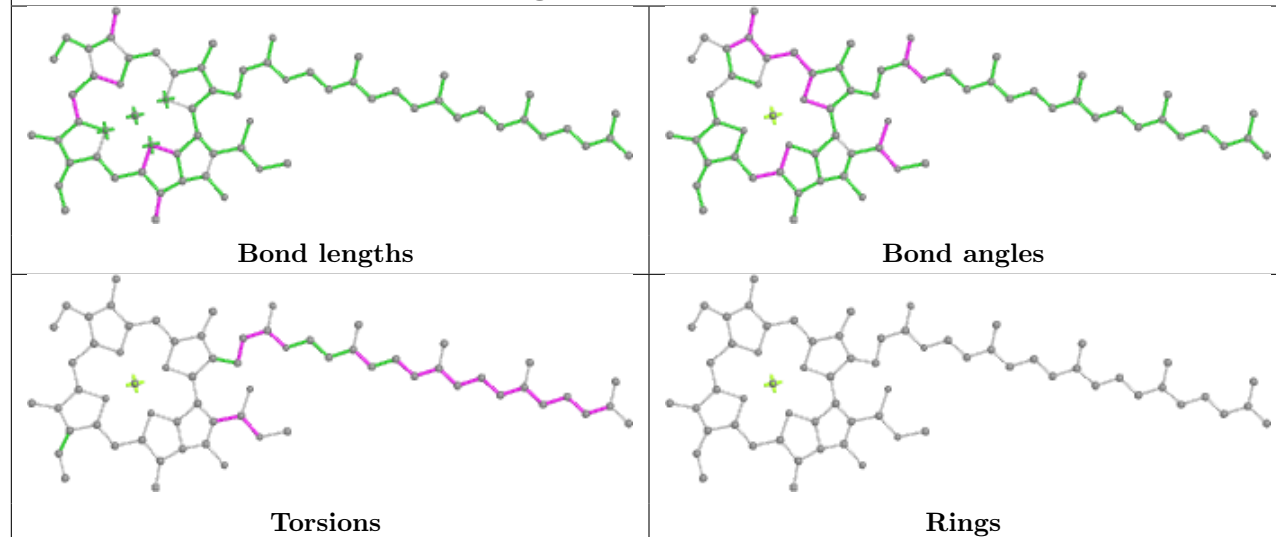




## Ligand CLA a 809

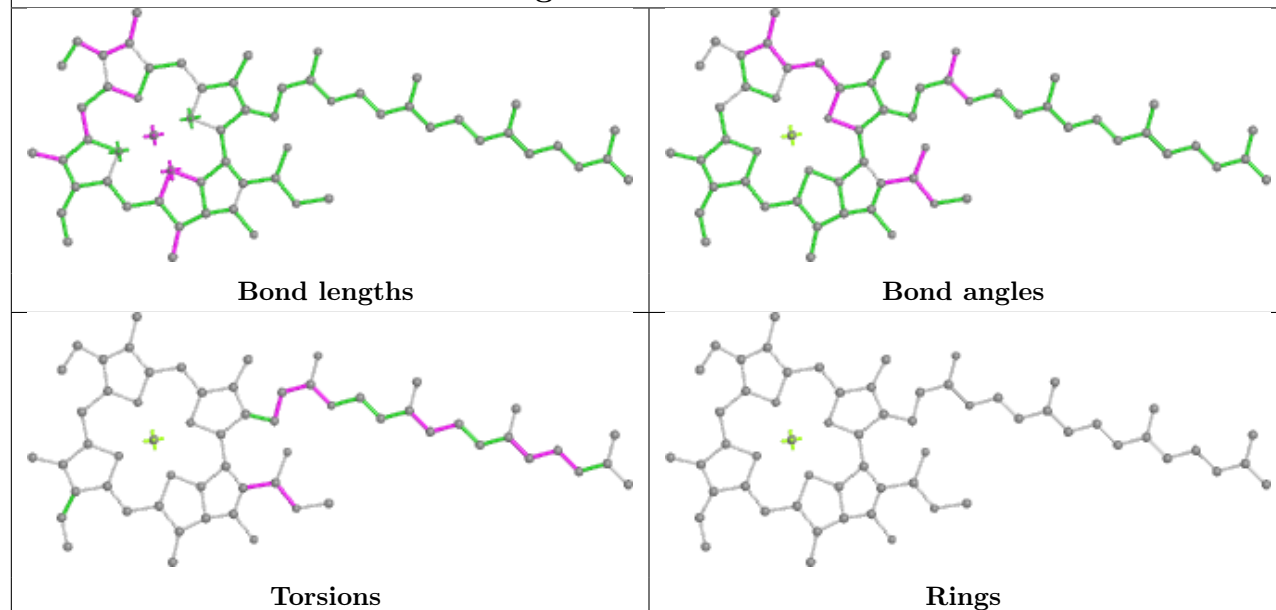


## Ligand CLA G 309

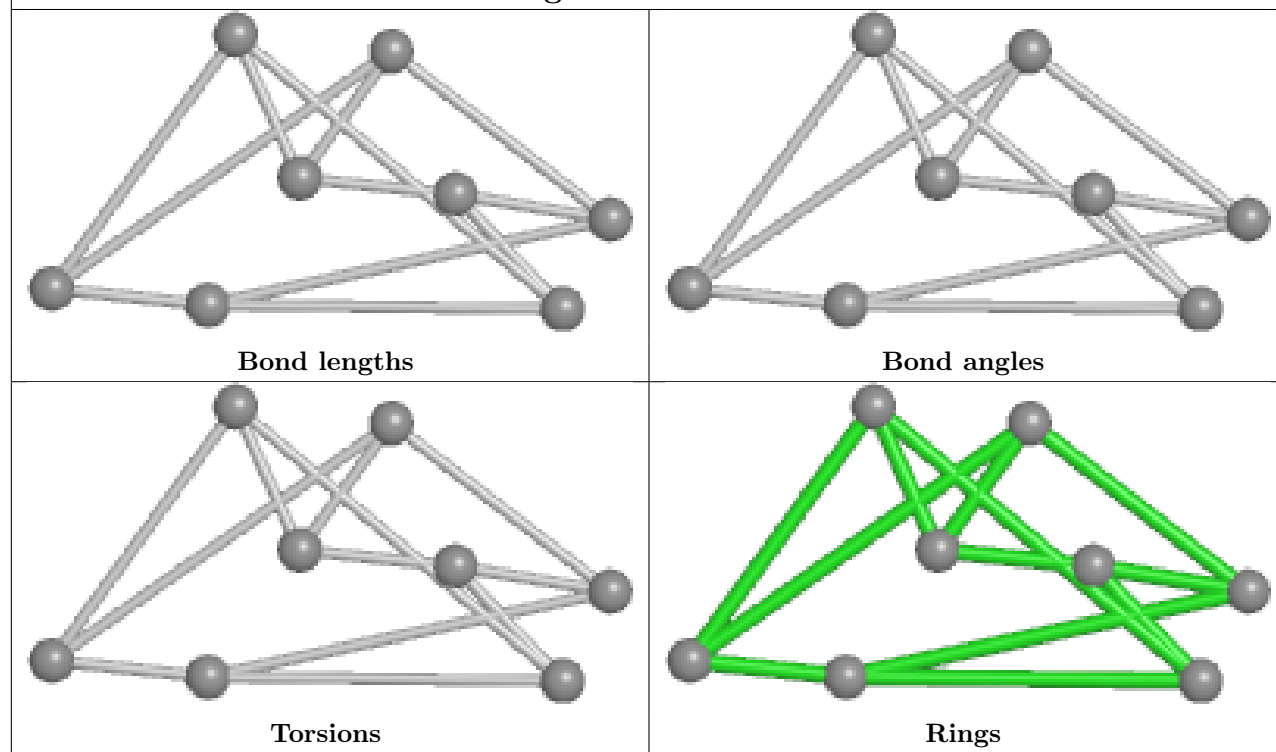




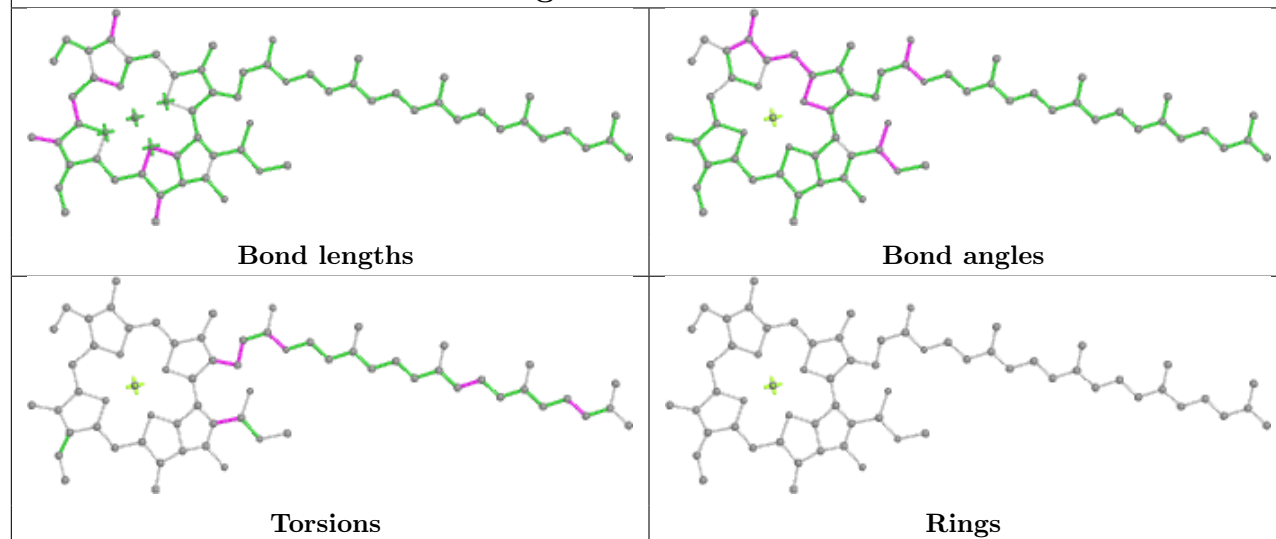
## Ligand CLA b 838



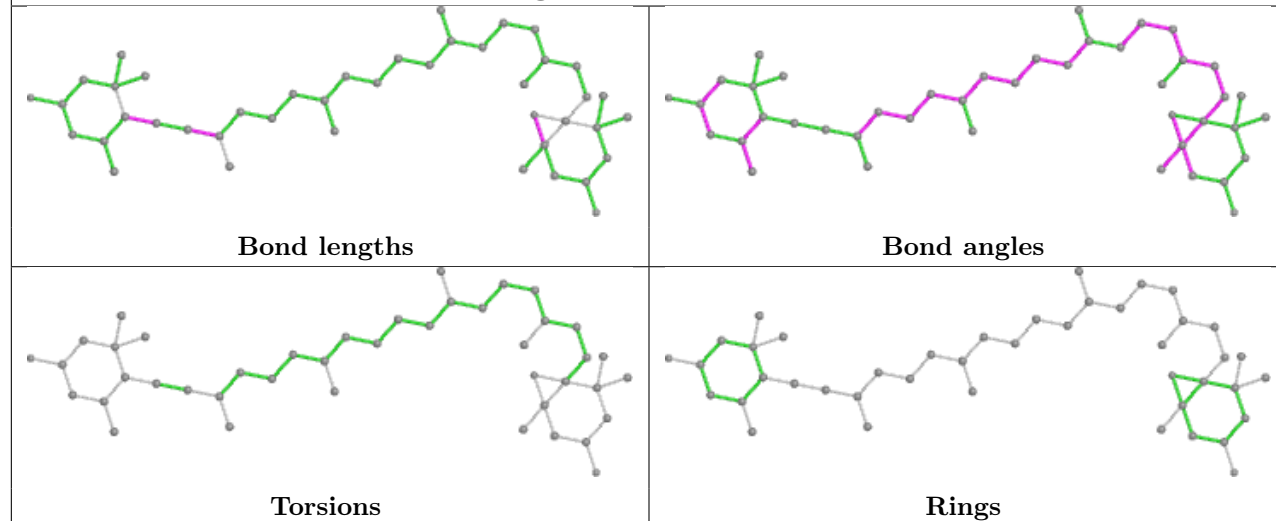
## Ligand SF4 c 102



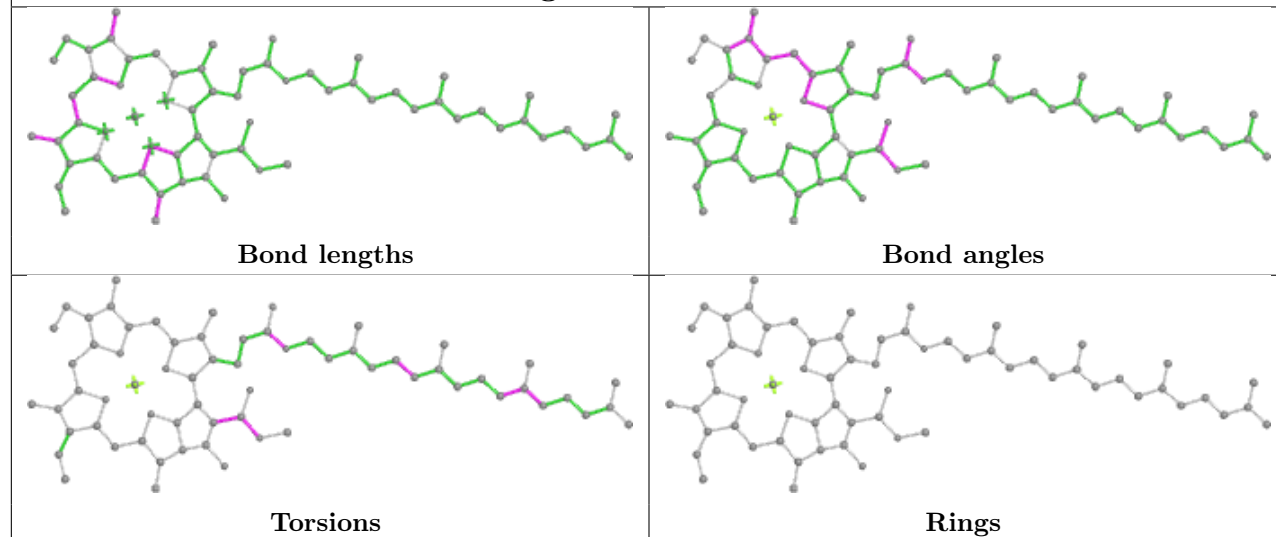
## Ligand CLA a 812

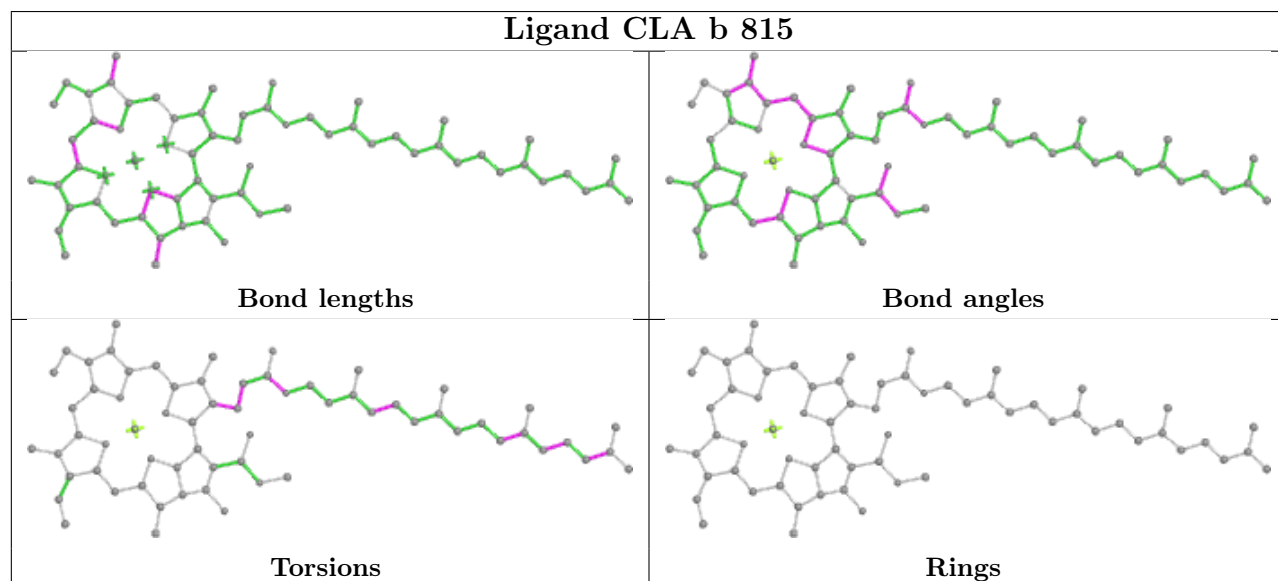
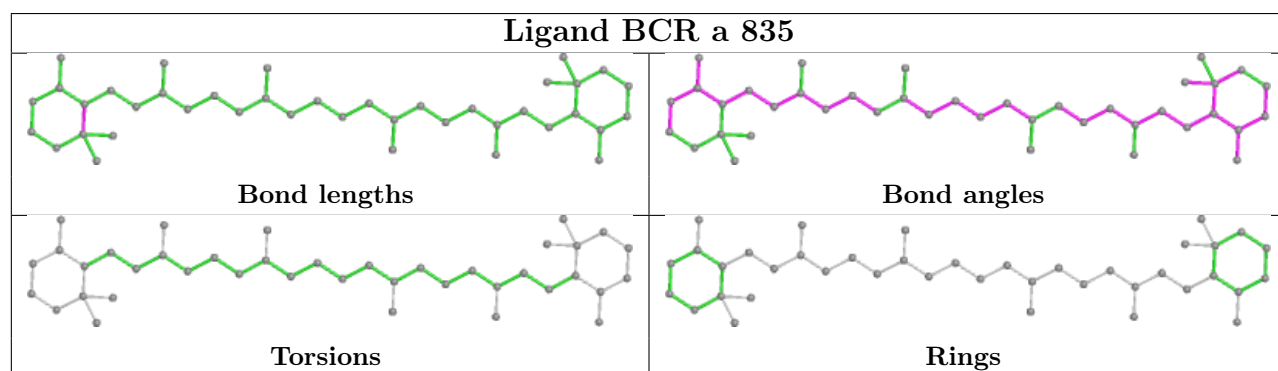
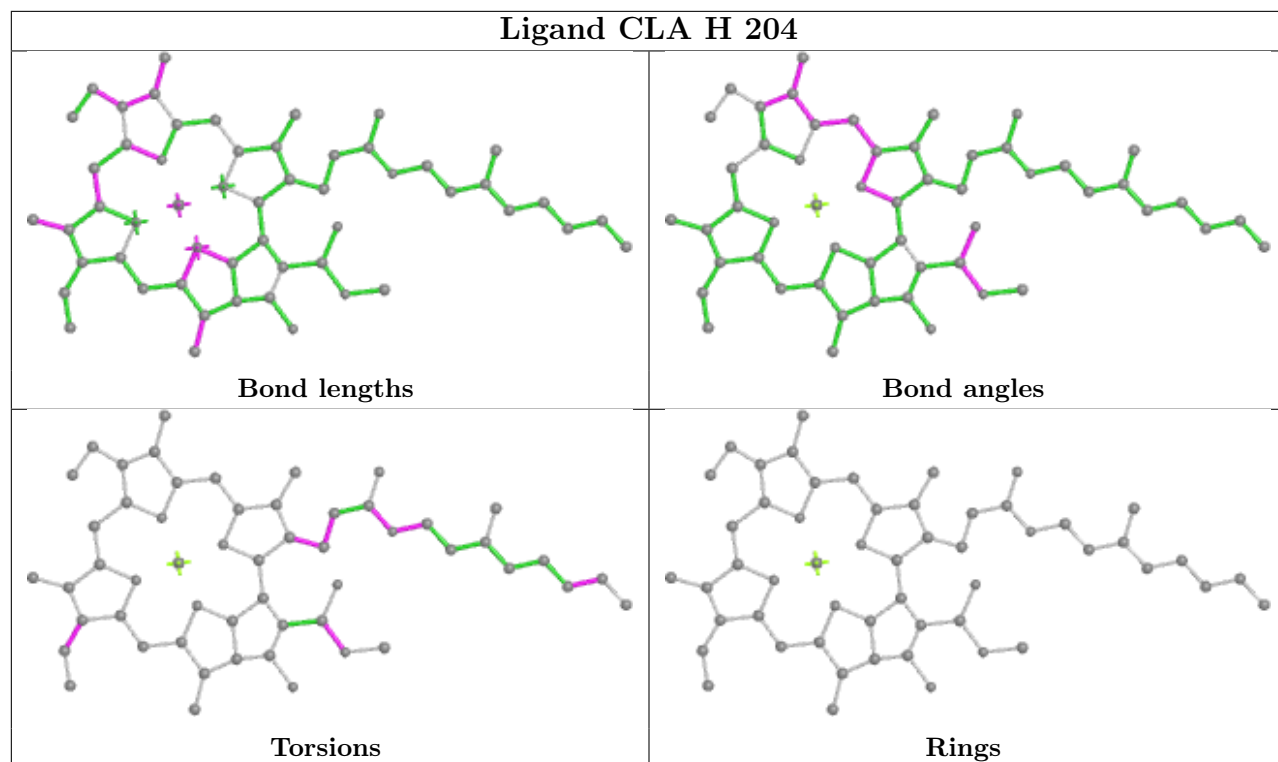


## Ligand DD6 G 303

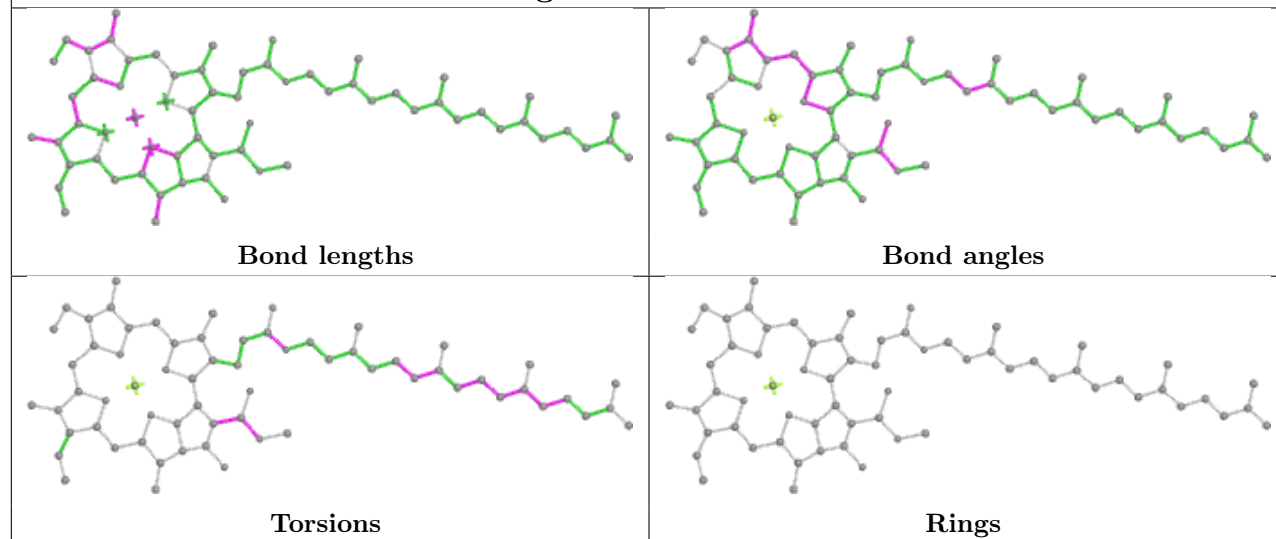


## Ligand CLA f 302

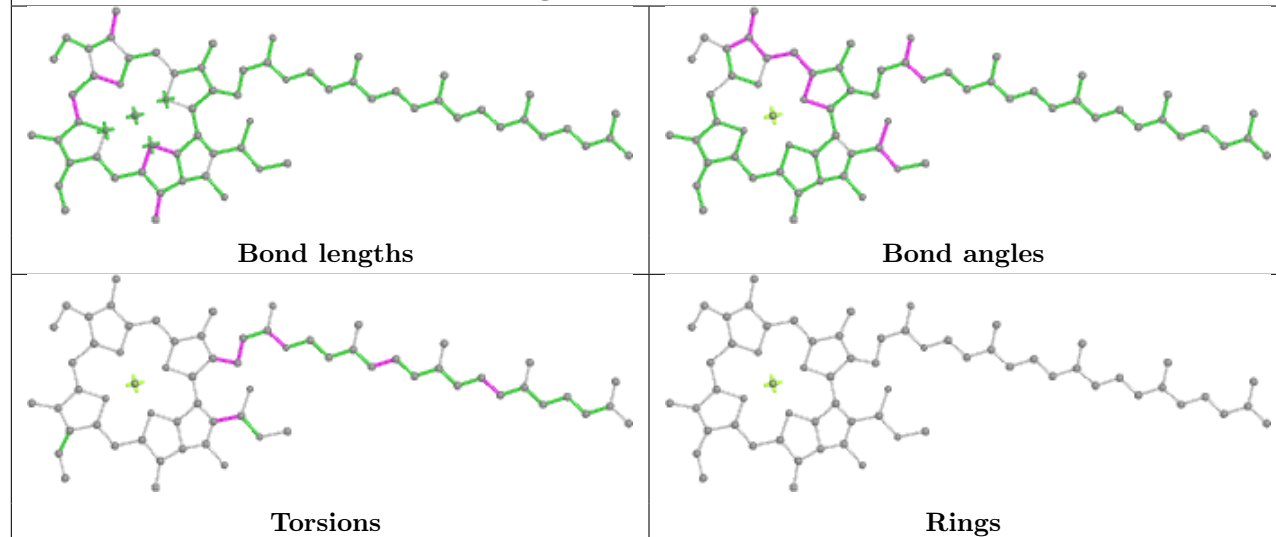




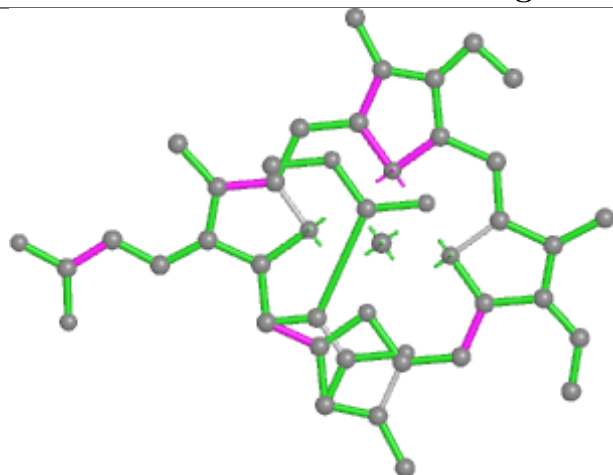
## Ligand CLA J 312



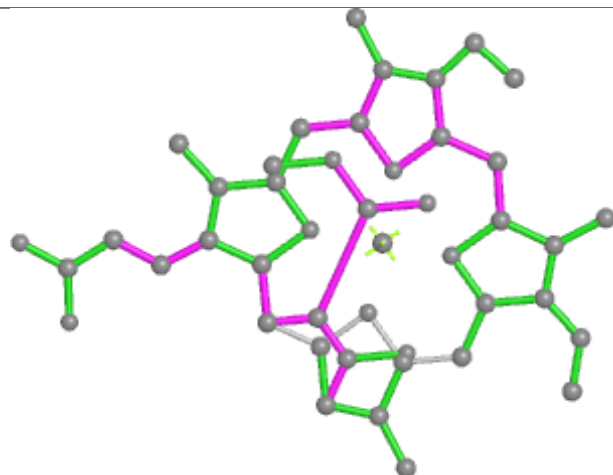
## Ligand CLA a 841



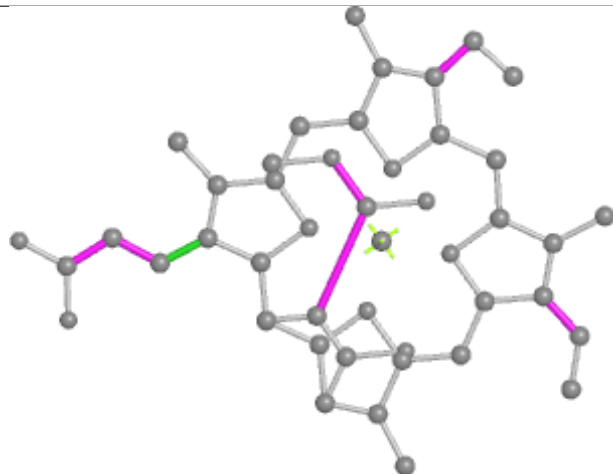
## Ligand KC1 H 211



Bond lengths



Bond angles

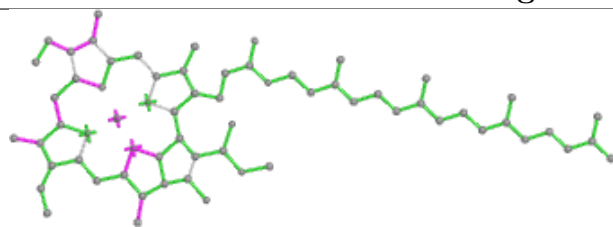


Torsions

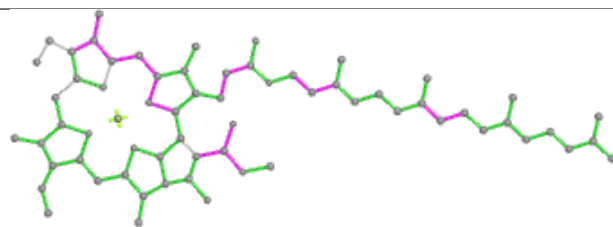


Rings

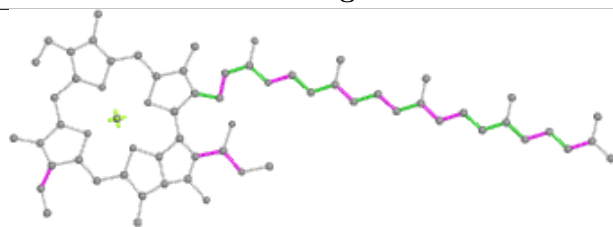
## Ligand CLA b 830



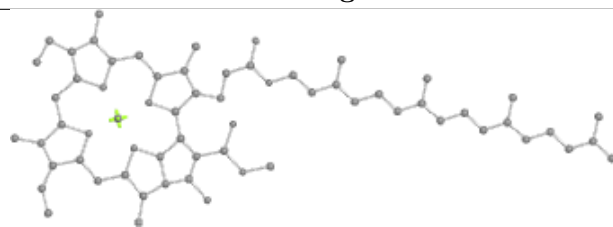
Bond lengths



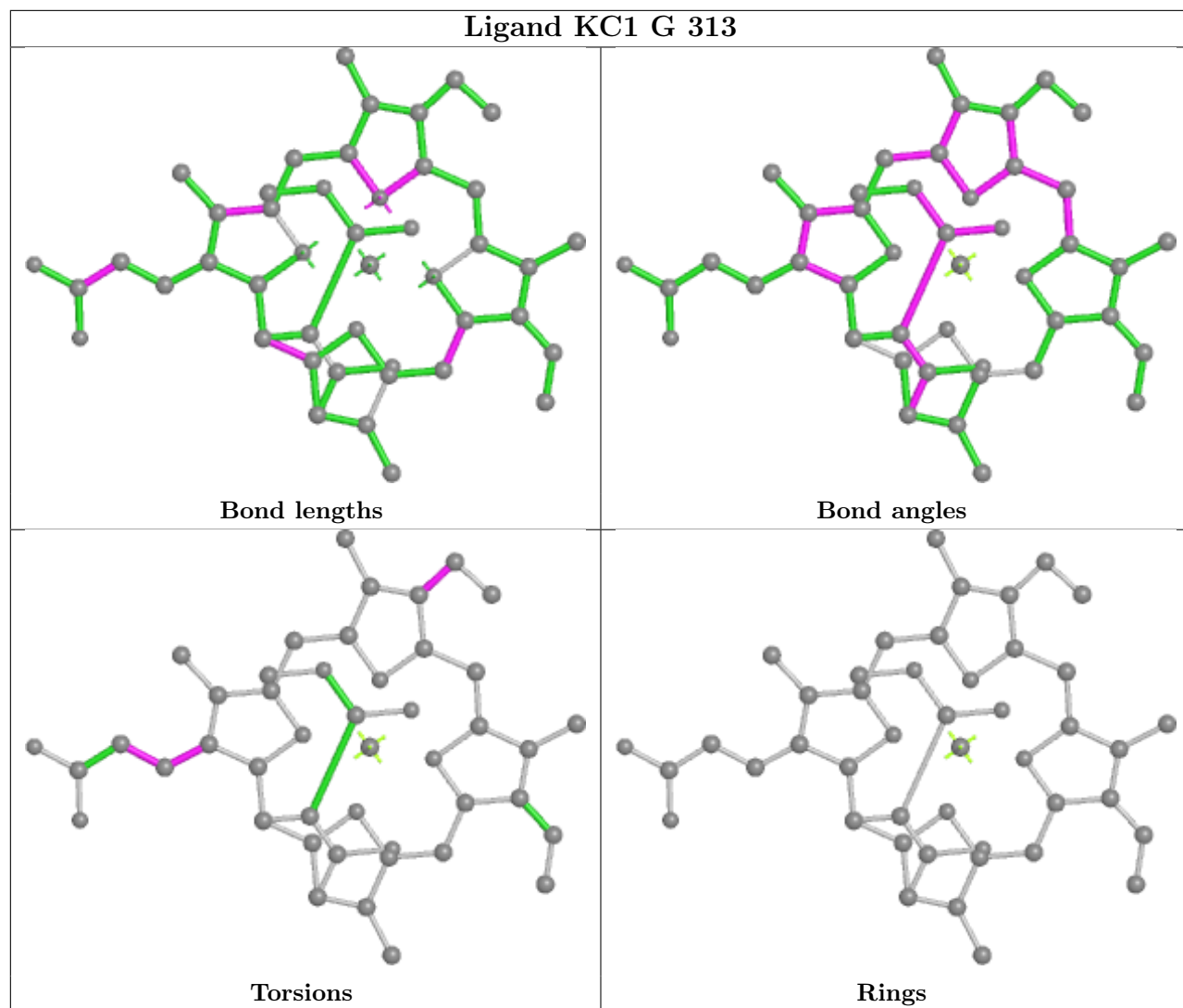
Bond angles



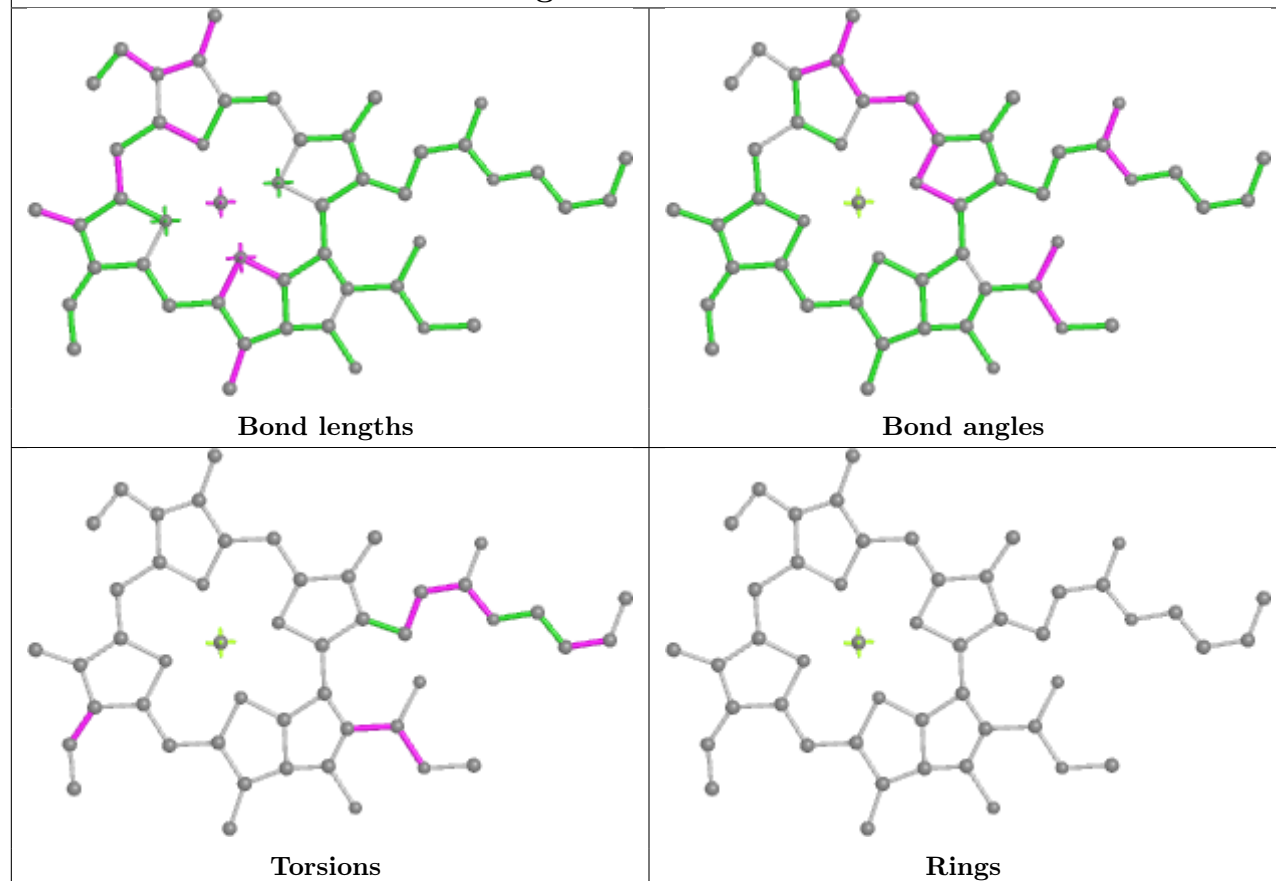
Torsions



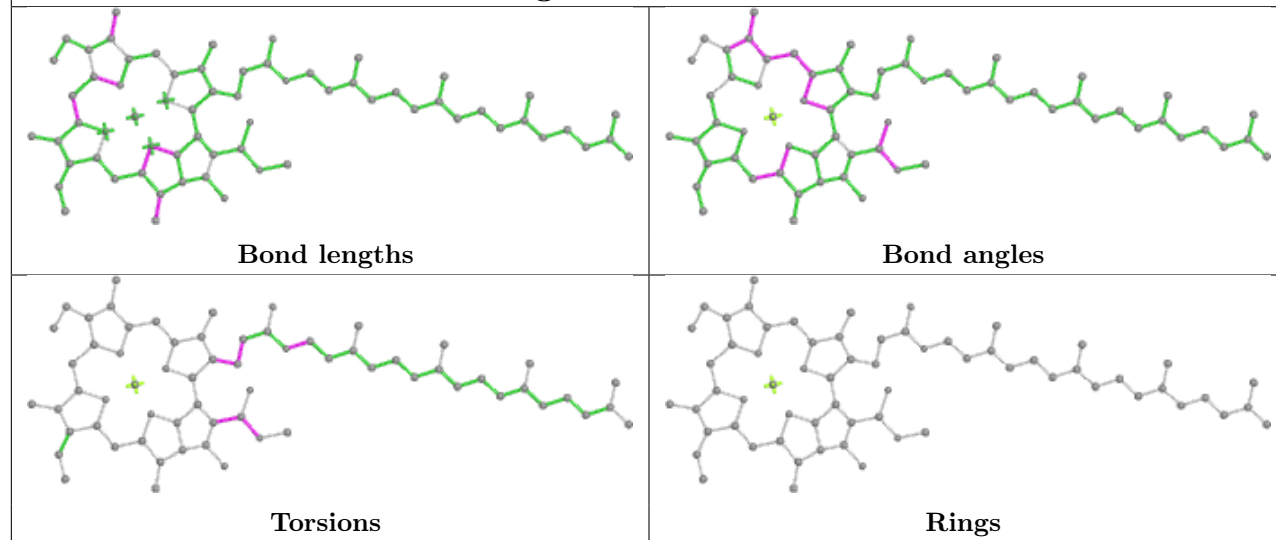
Rings

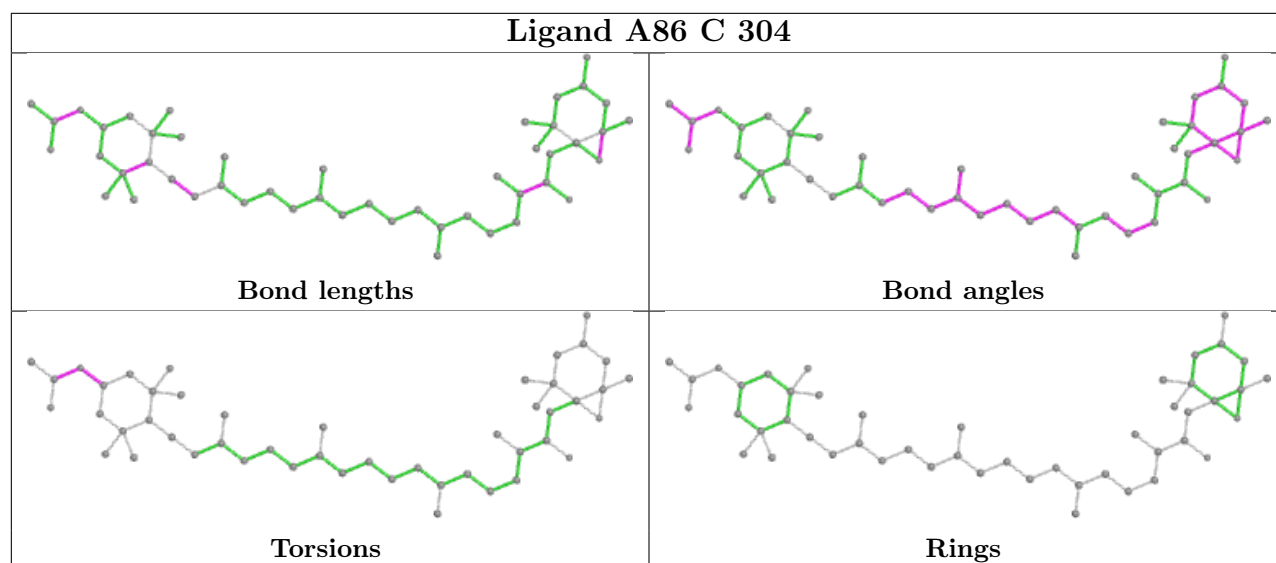
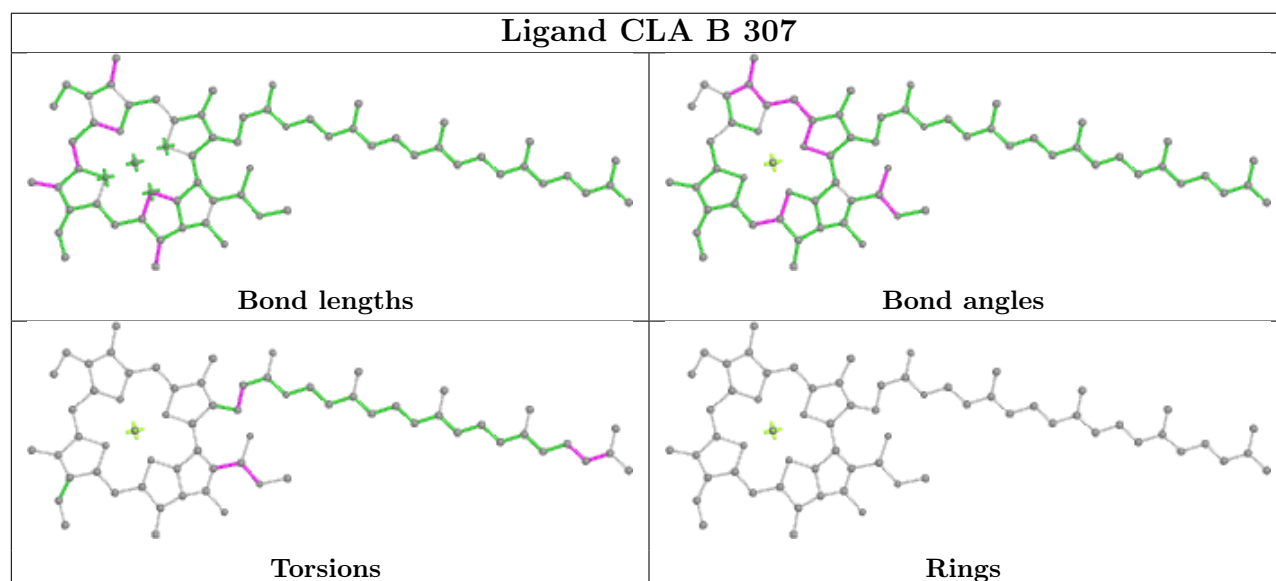
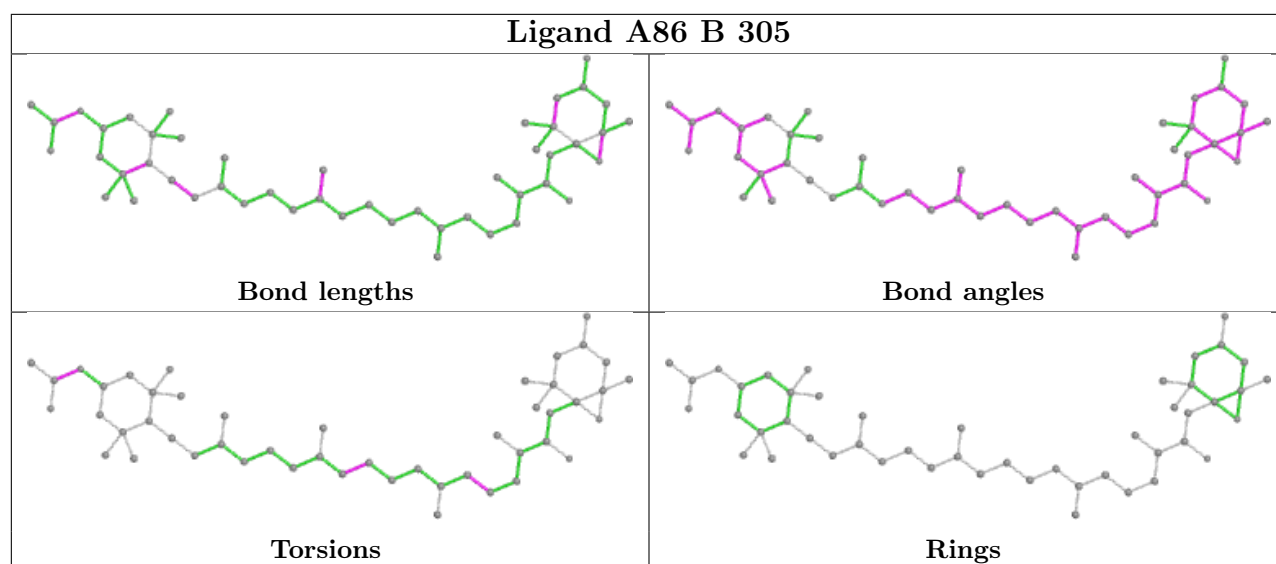


## Ligand CLA J 315



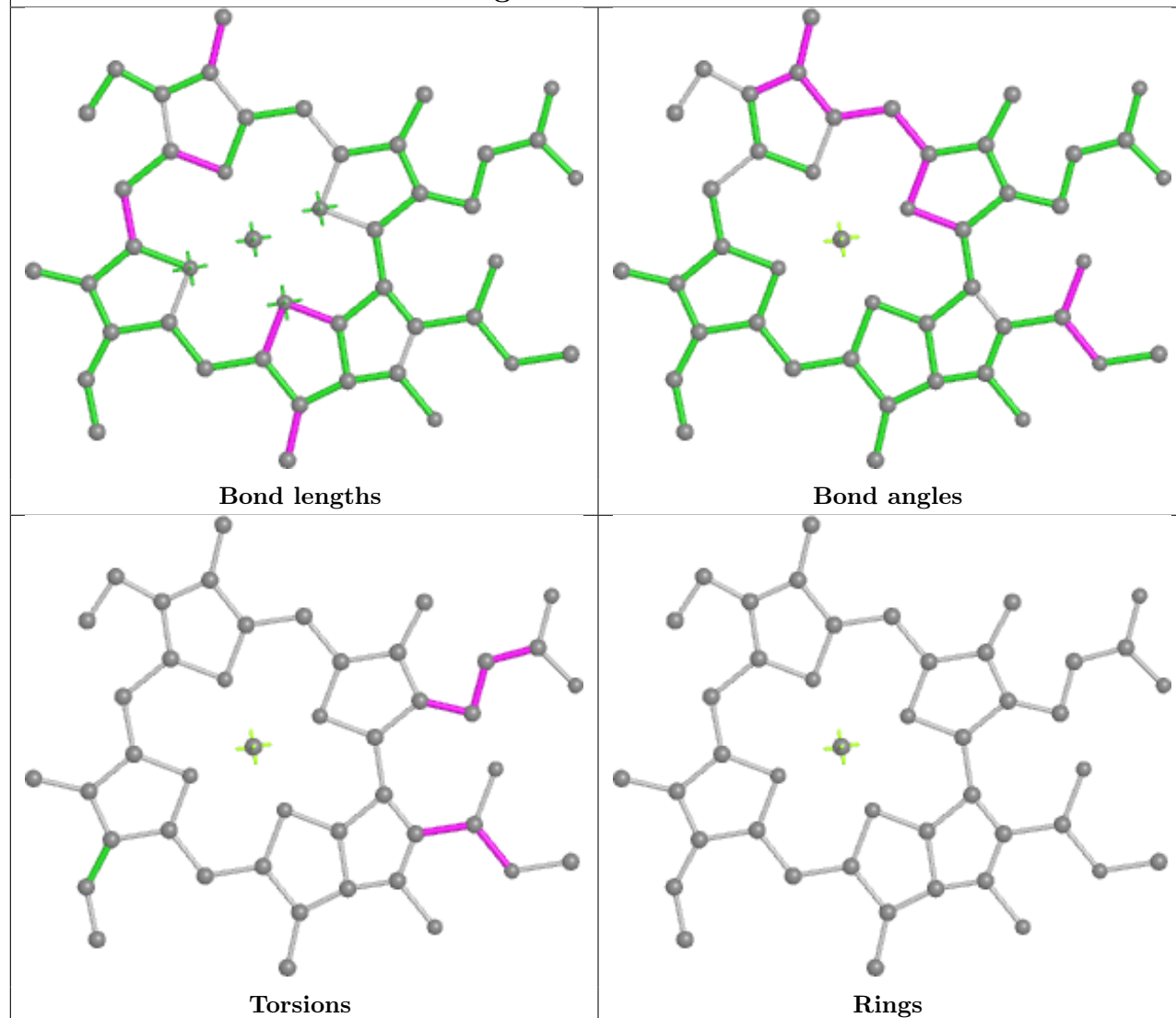
## Ligand CLA b 842



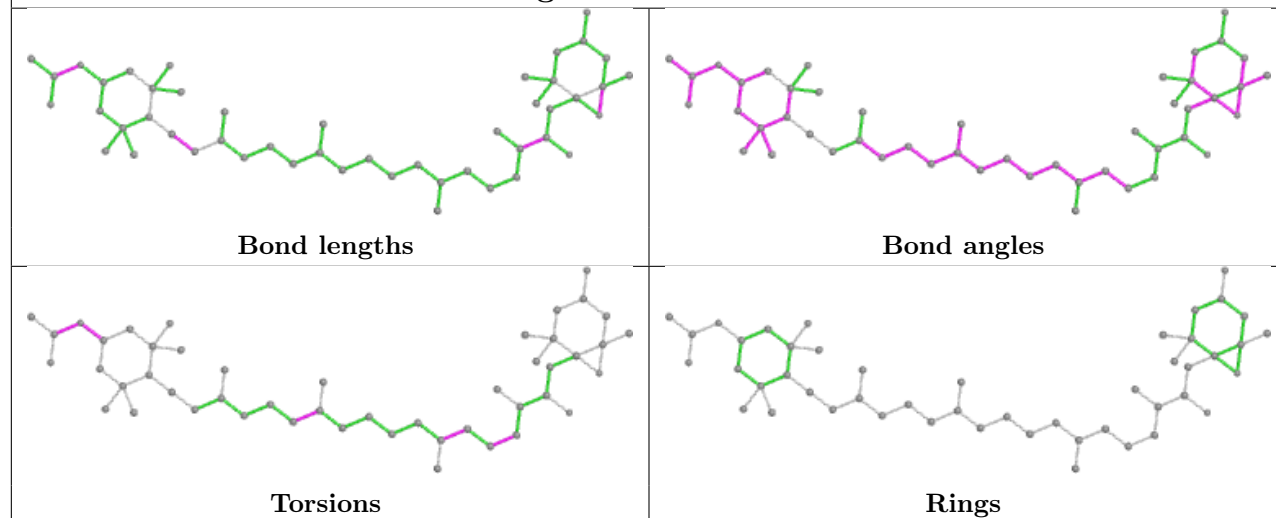




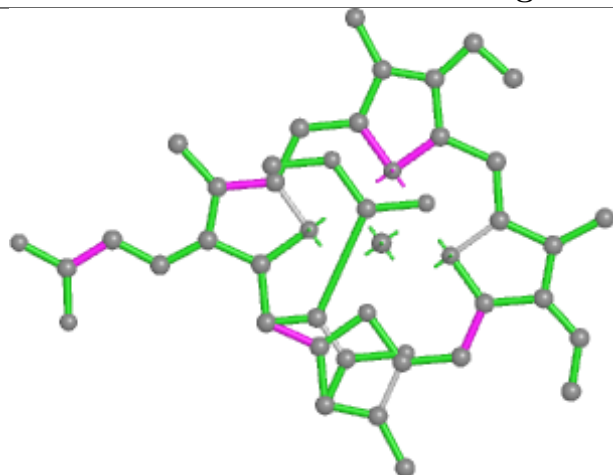
## Ligand CLA a 818



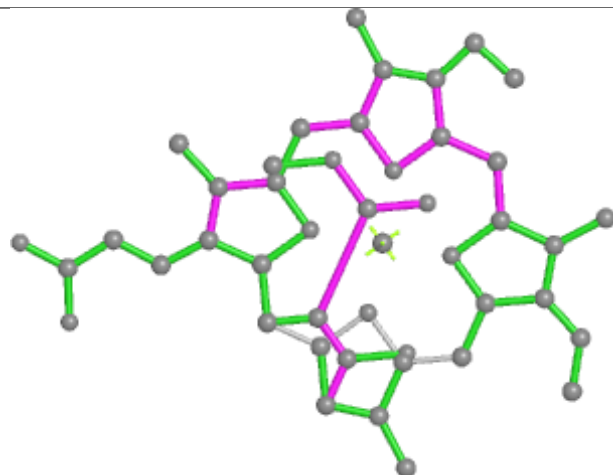
## Ligand A86 K 302



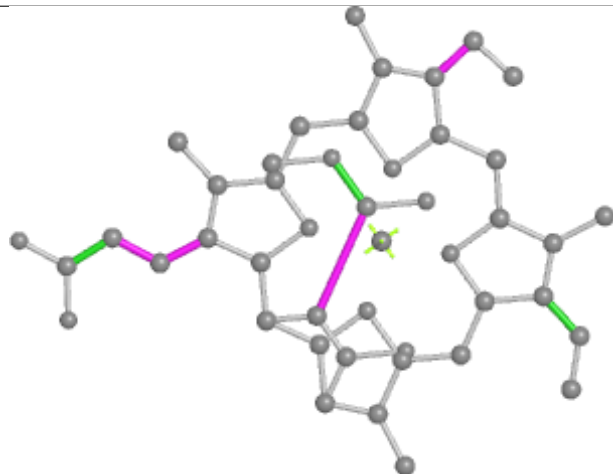
## Ligand KC1 C 308



Bond lengths



Bond angles

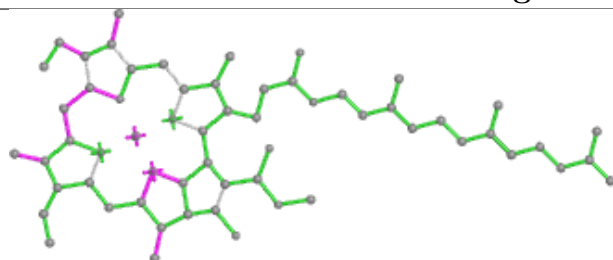


Torsions

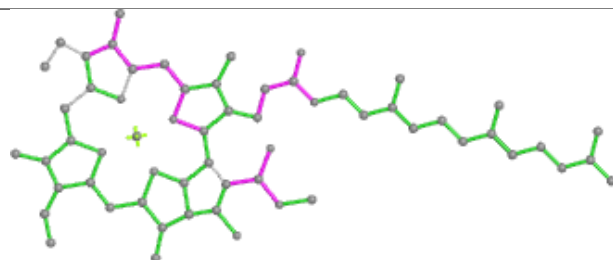


Rings

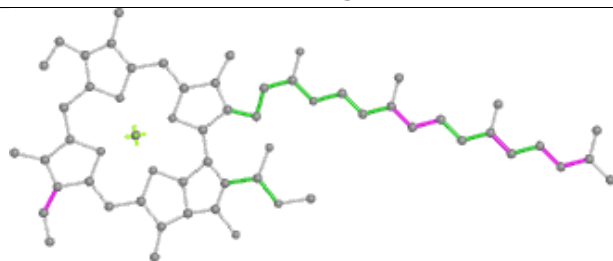
## Ligand CLA H 209



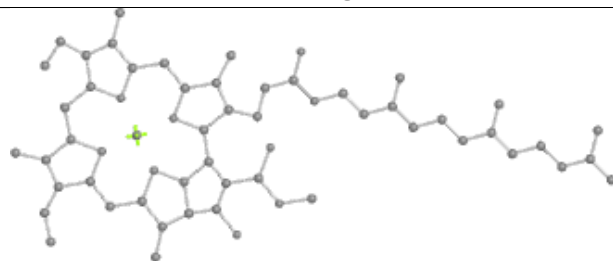
Bond lengths



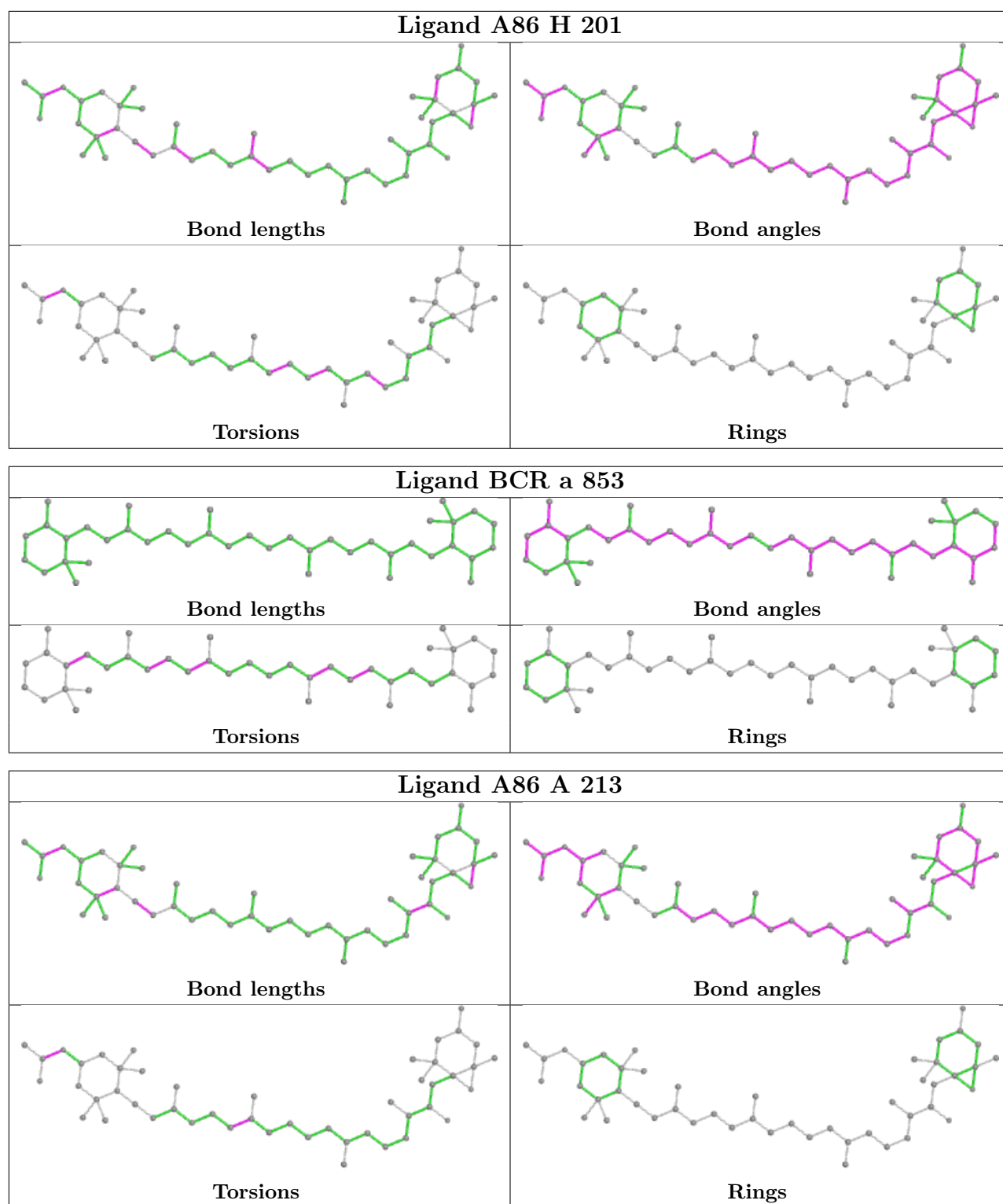
Bond angles



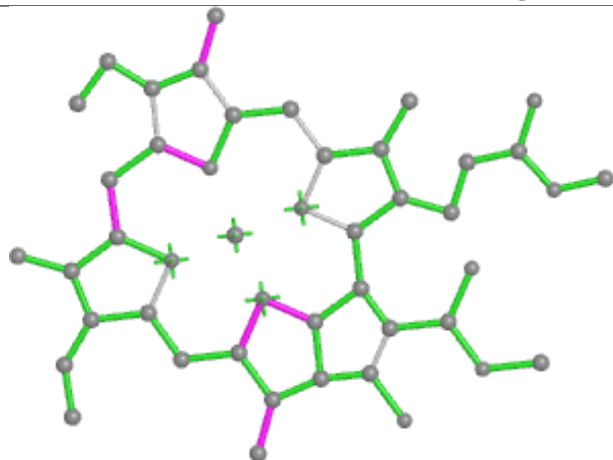
Torsions



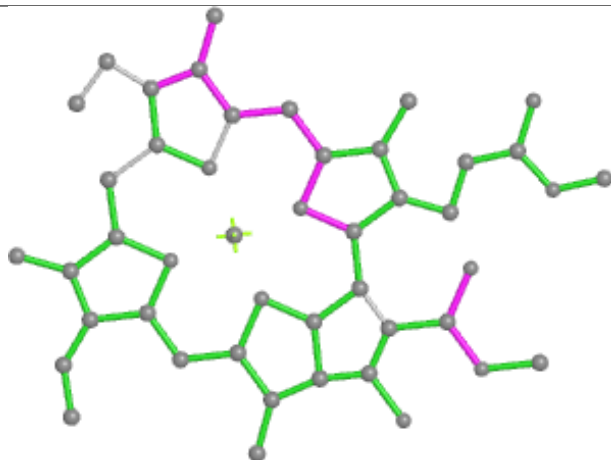
Rings



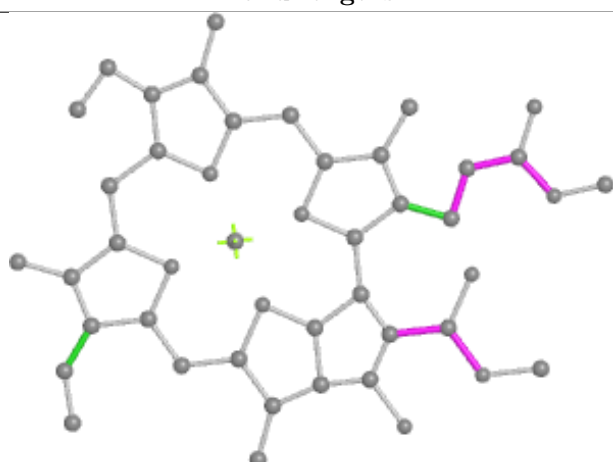
## Ligand CLA H 208



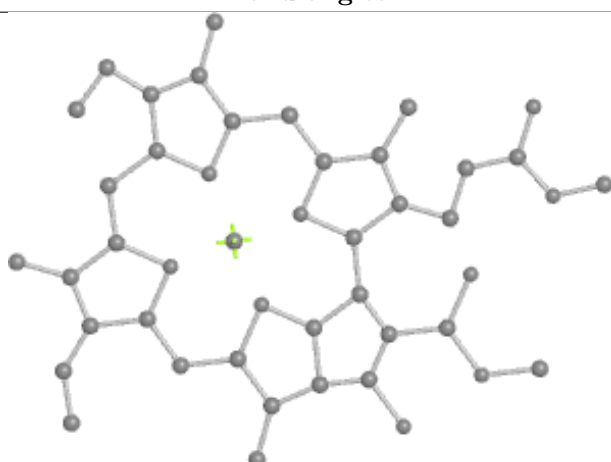
Bond lengths



Bond angles

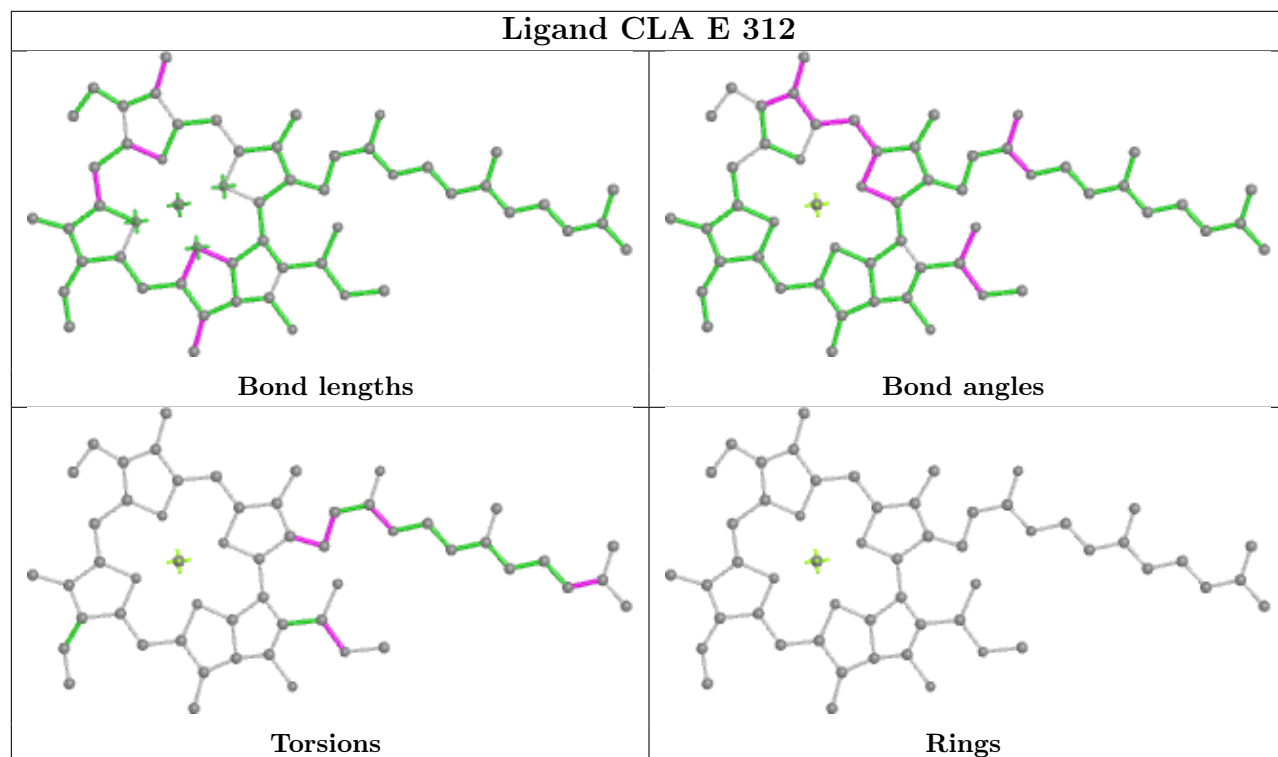


Torsions

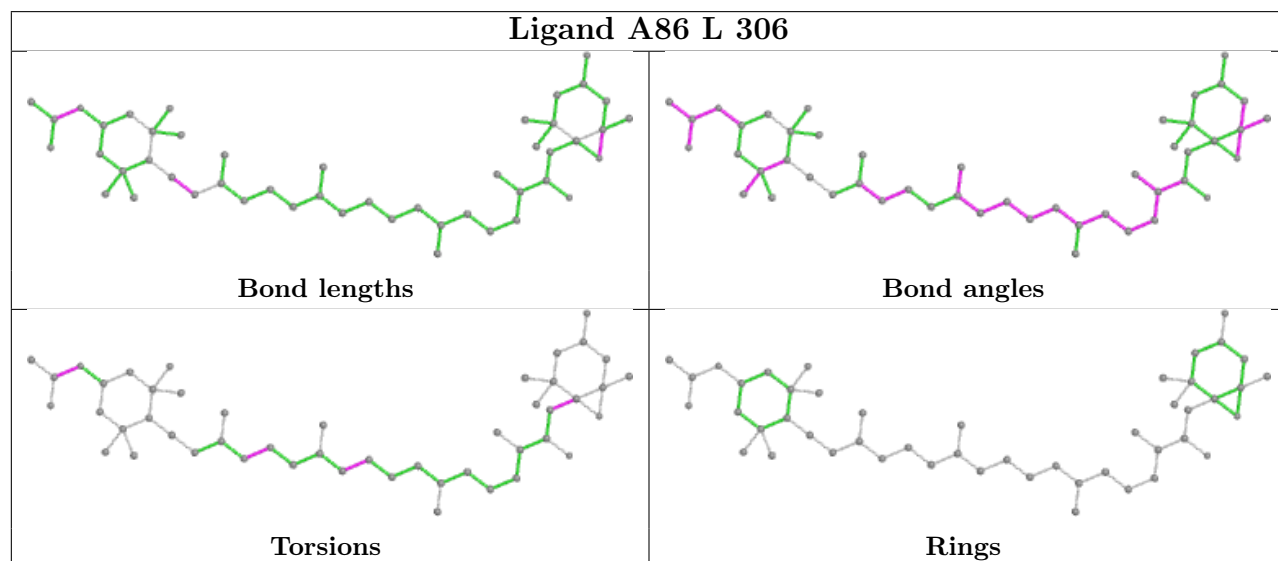


Rings

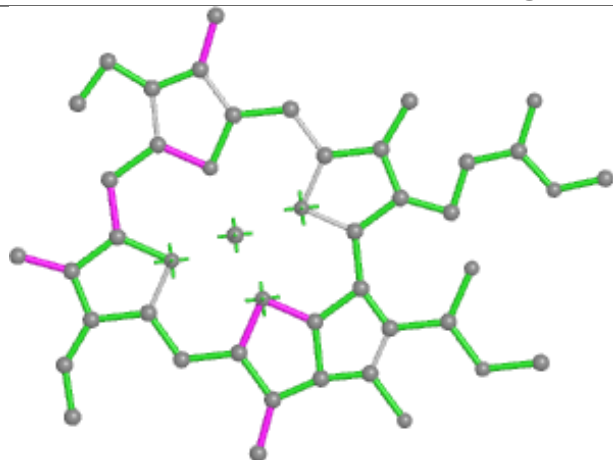
## Ligand CLA E 312



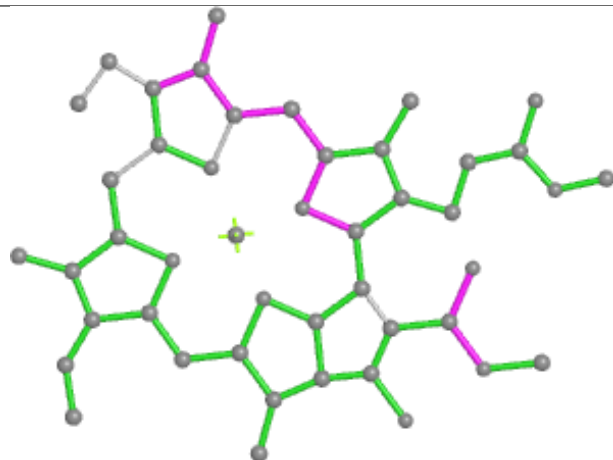
## Ligand A86 L 306



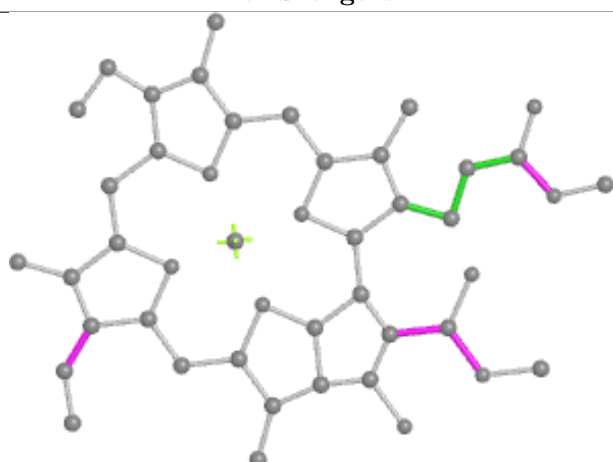
## Ligand CLA I 317



Bond lengths



Bond angles

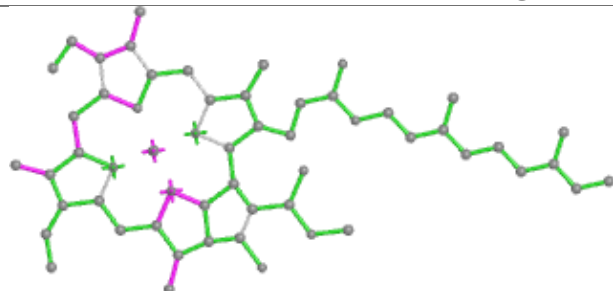


Torsions

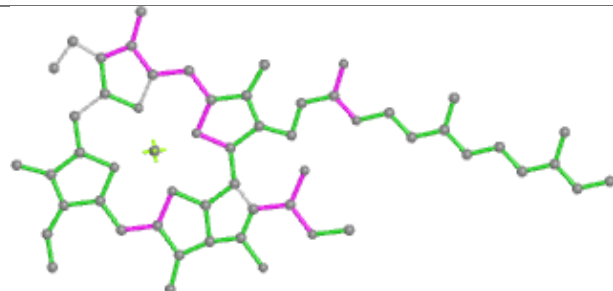


Rings

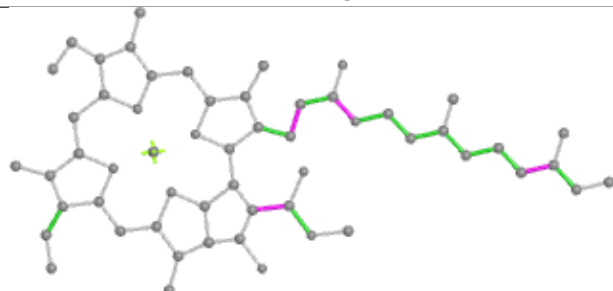
## Ligand CLA D 210



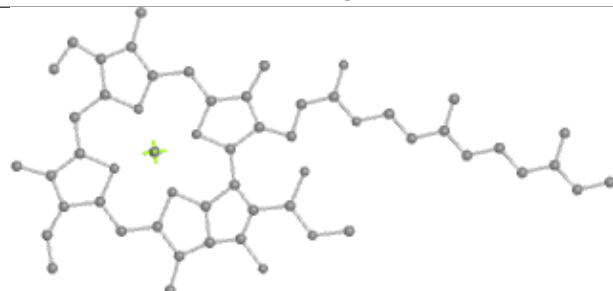
Bond lengths



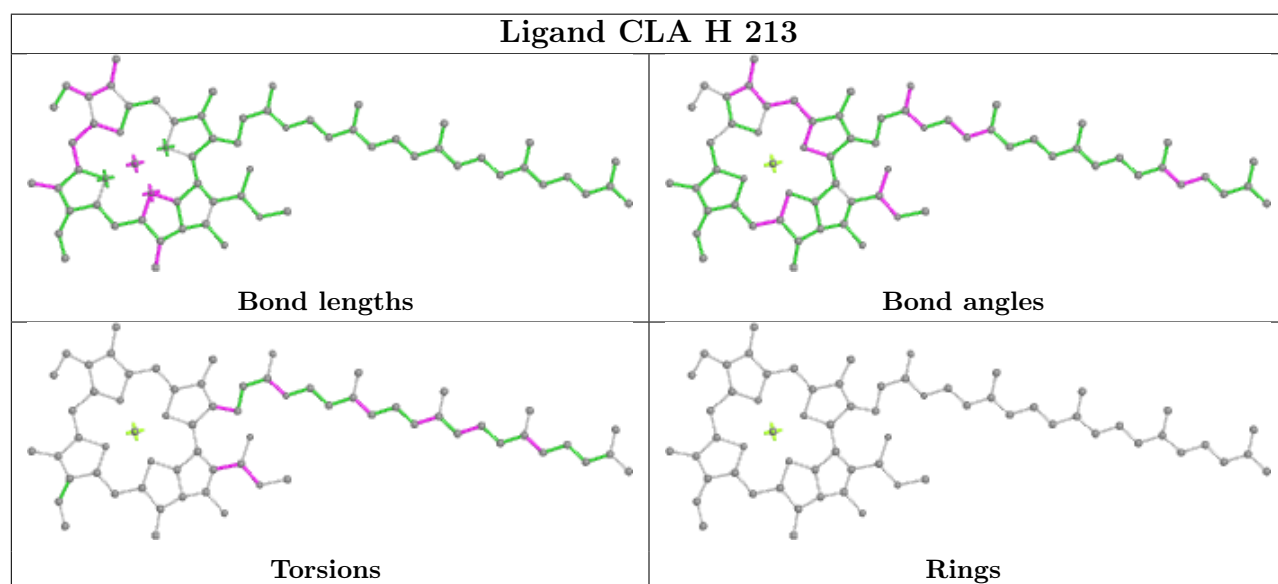
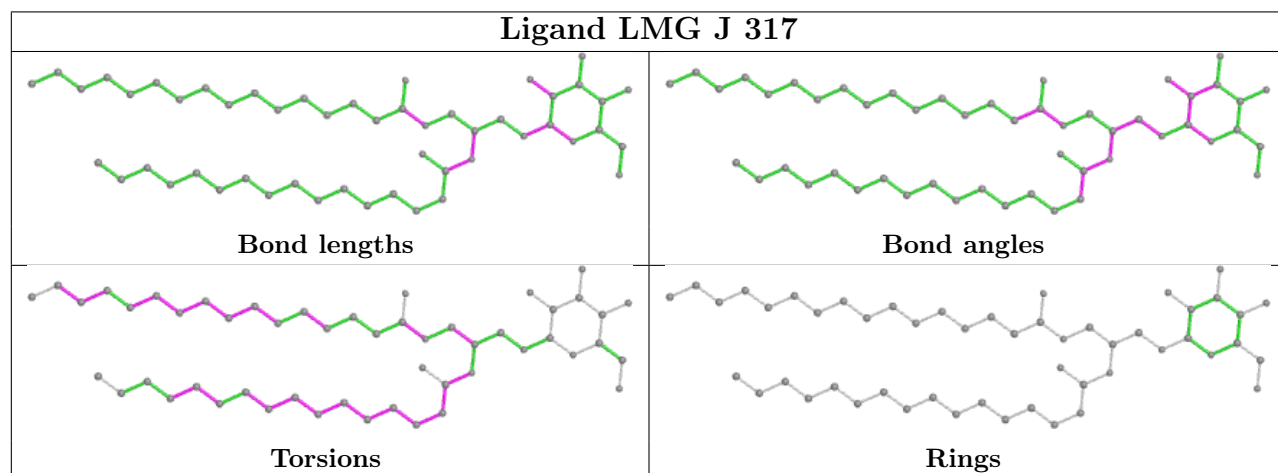
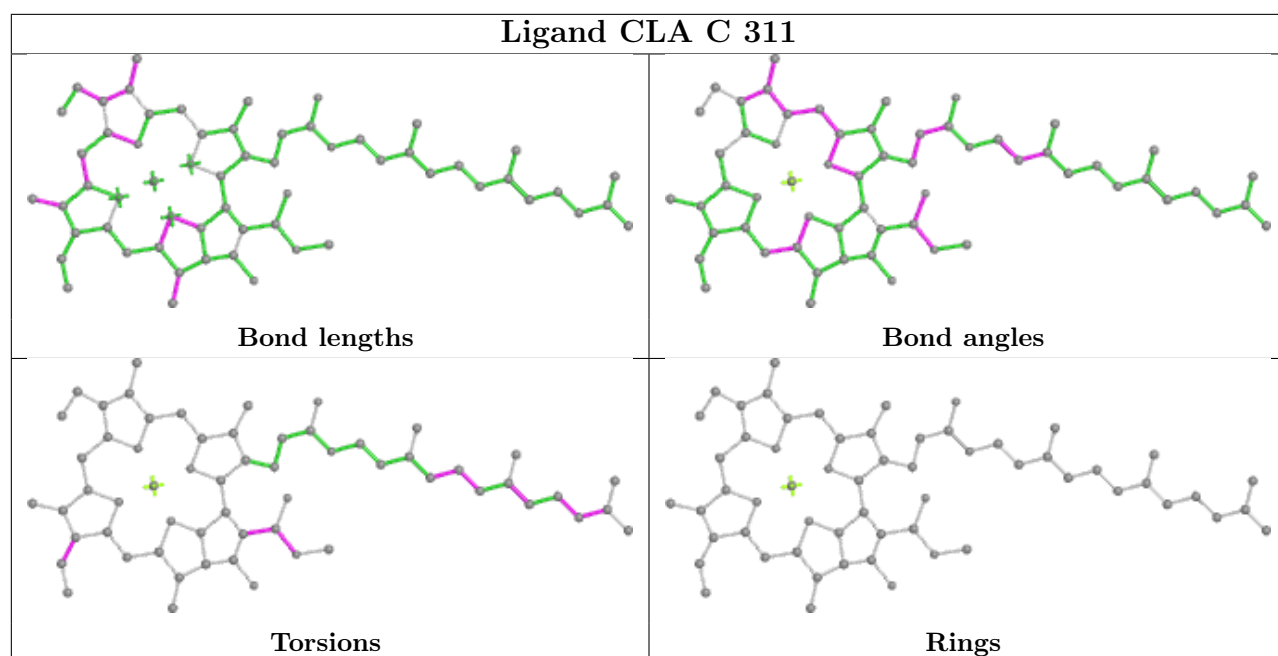
Bond angles



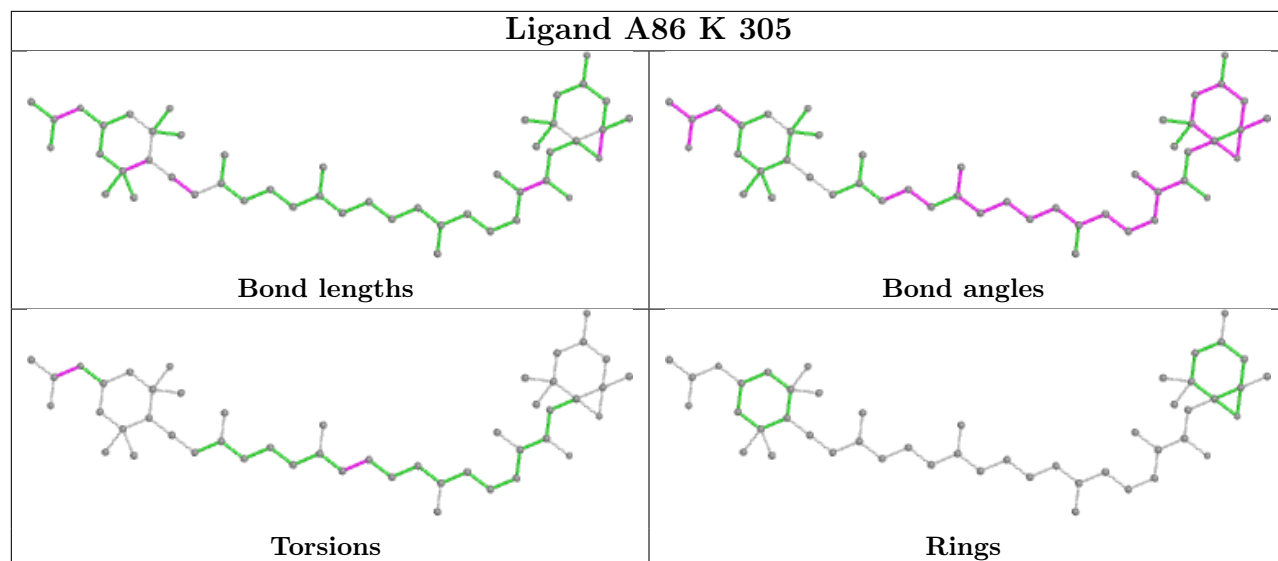
Torsions



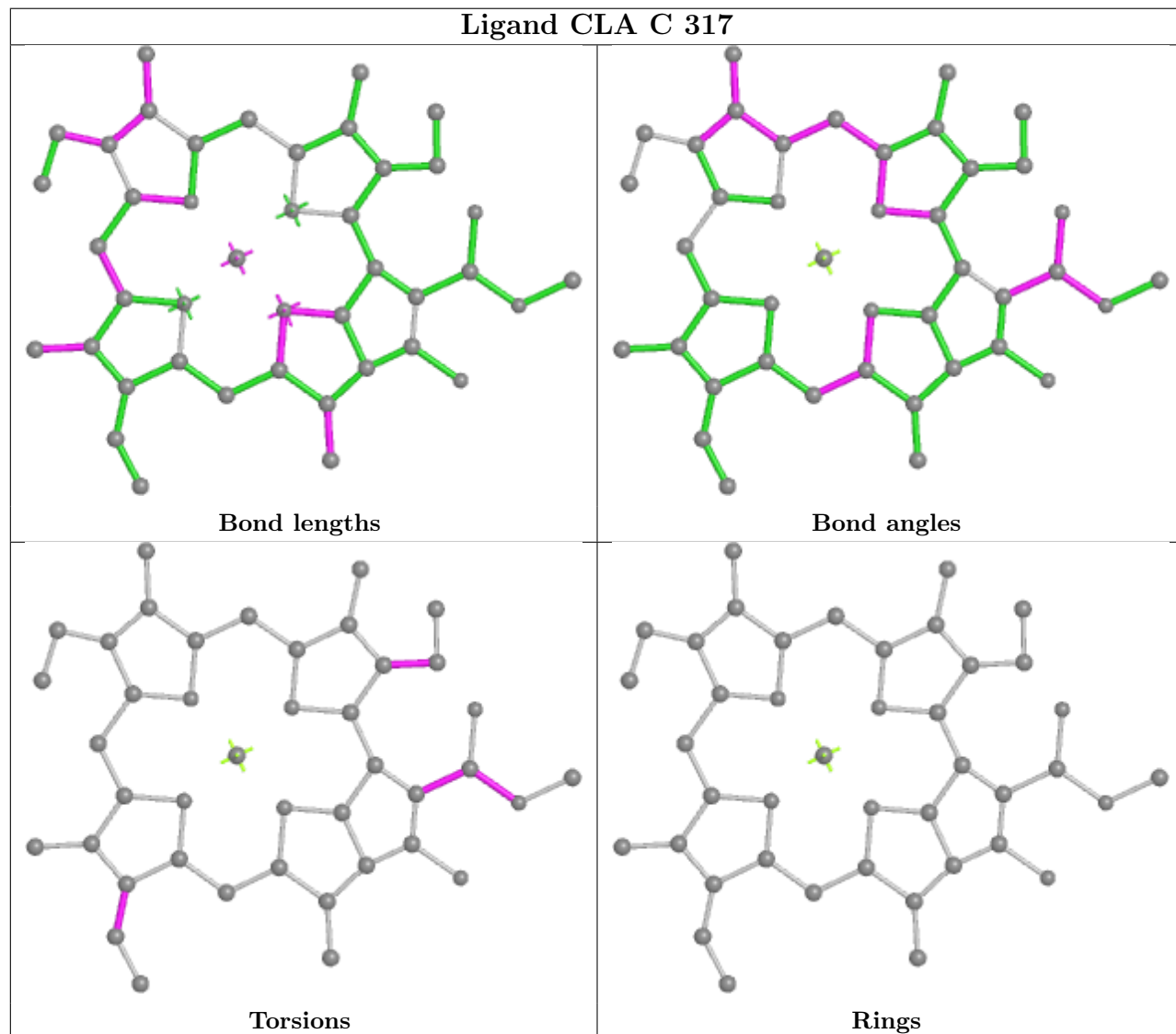
Rings



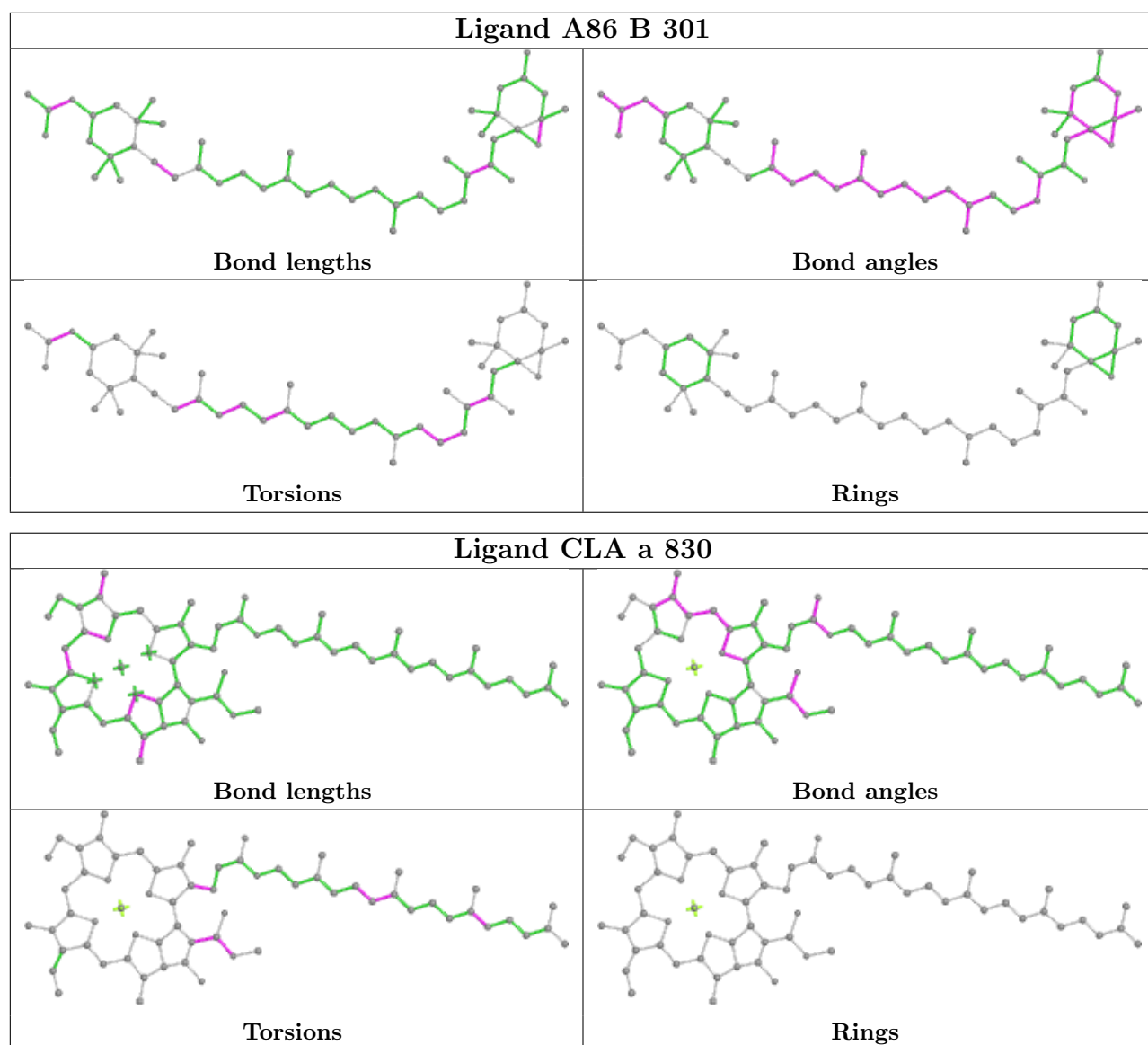
## Ligand A86 K 305



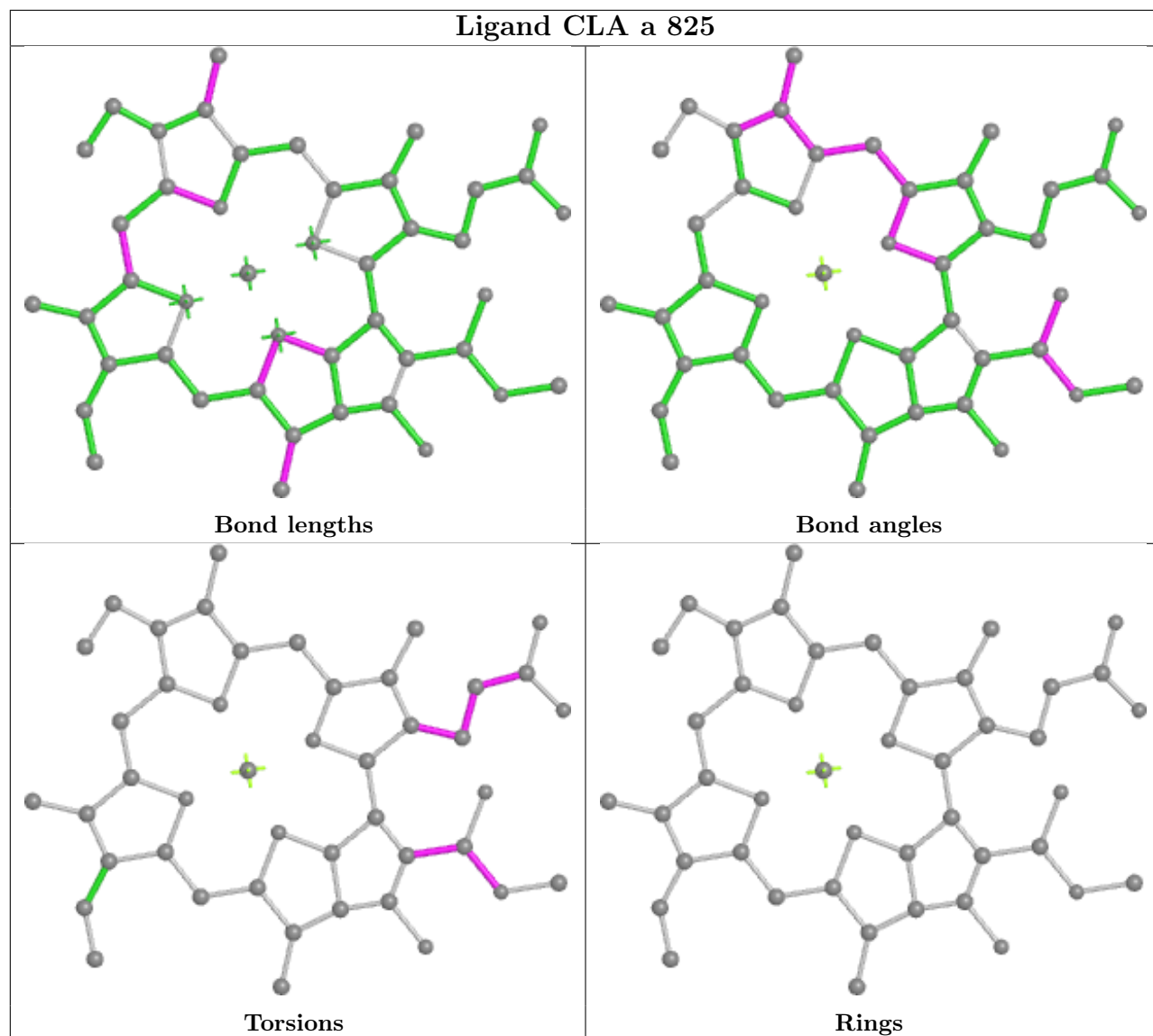
## Ligand CLA C 317

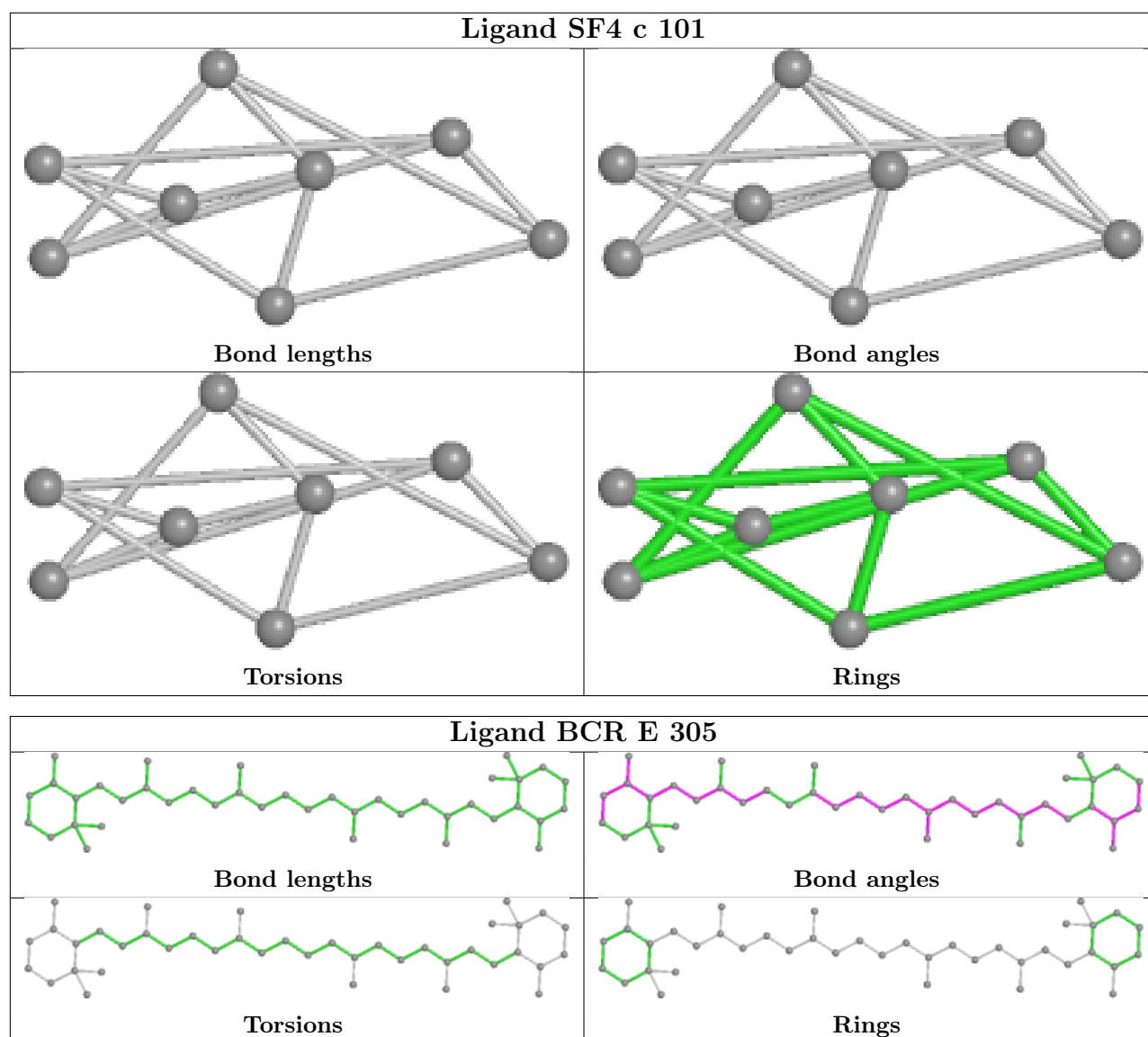




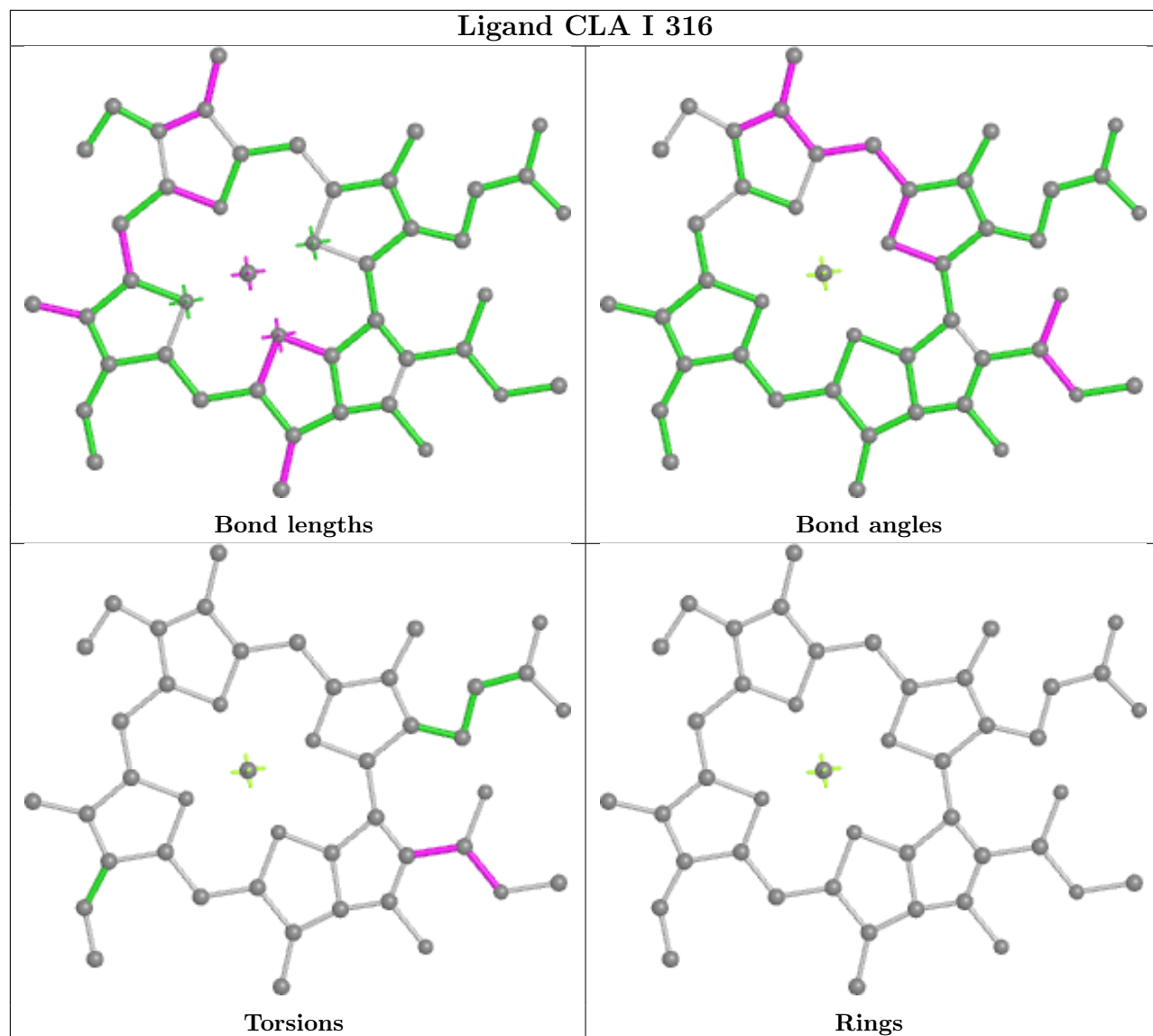


## Ligand CLA a 825

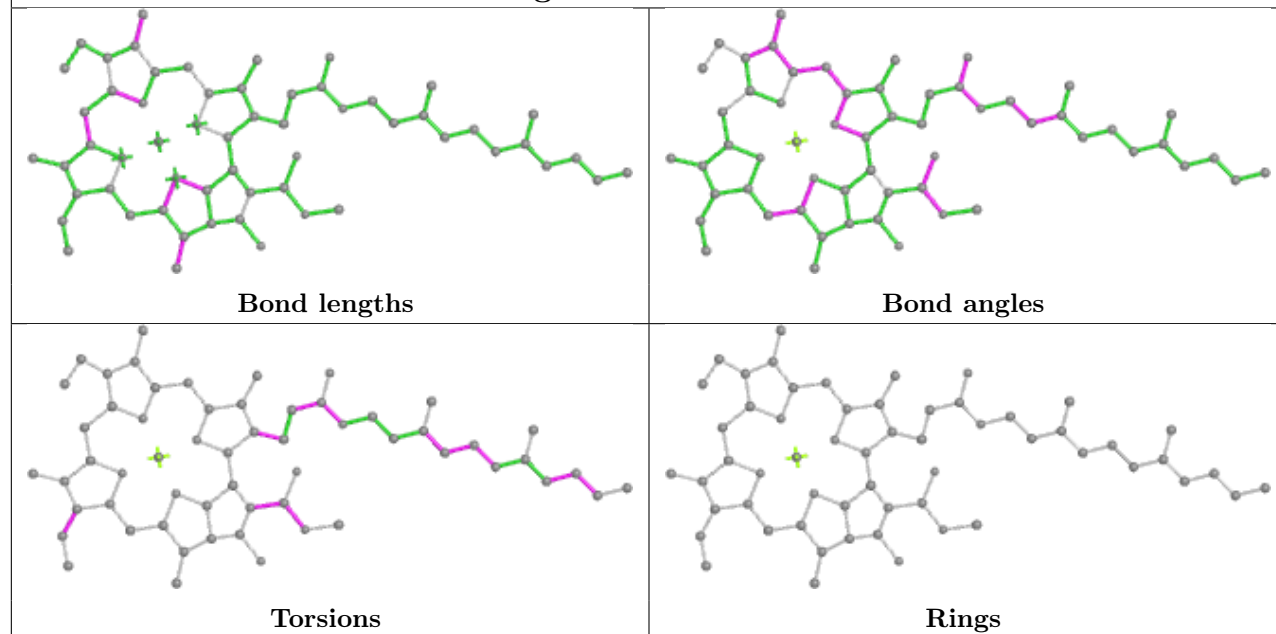




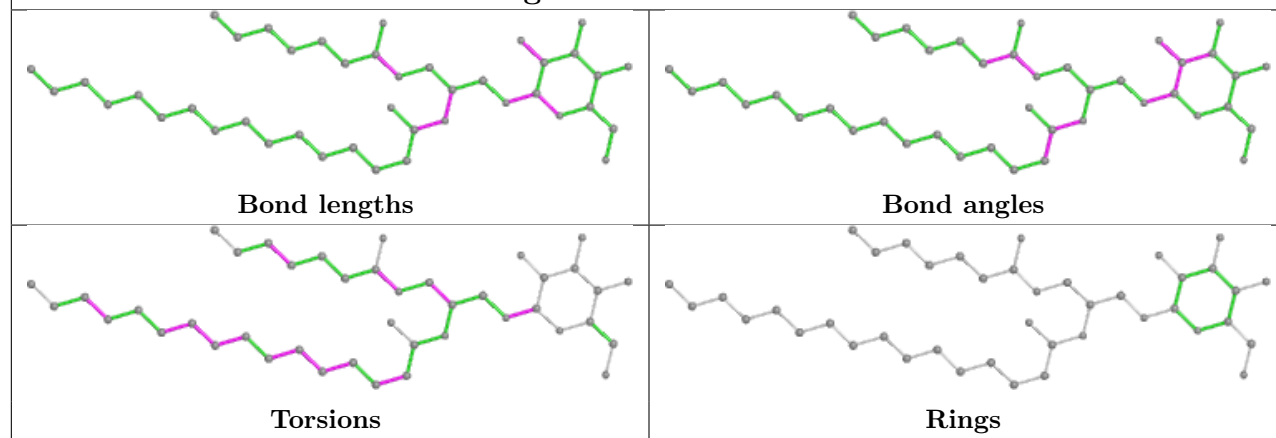
## Ligand CLA I 316



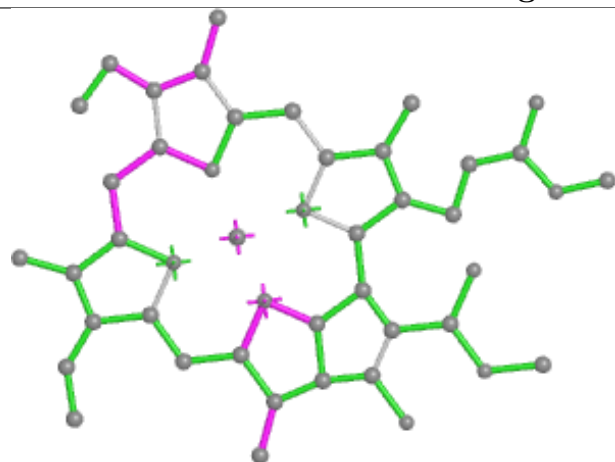
## Ligand CLA F 315



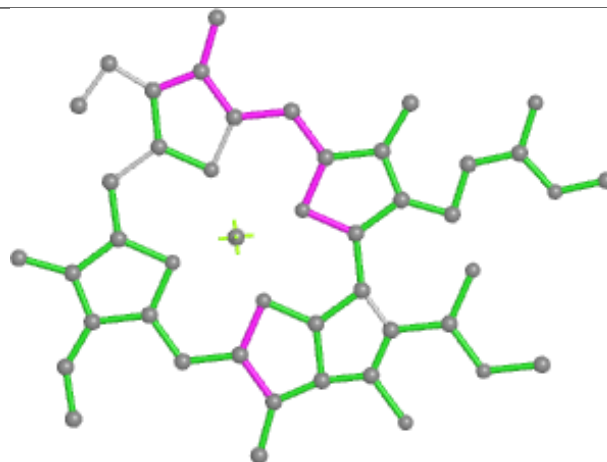
## Ligand LMG M 321



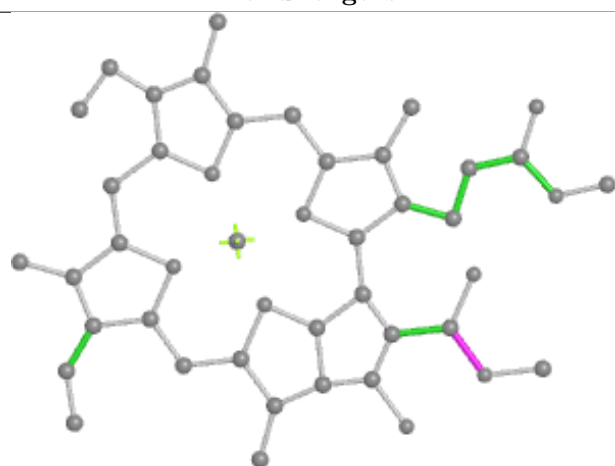
## Ligand CLA F 309



Bond lengths



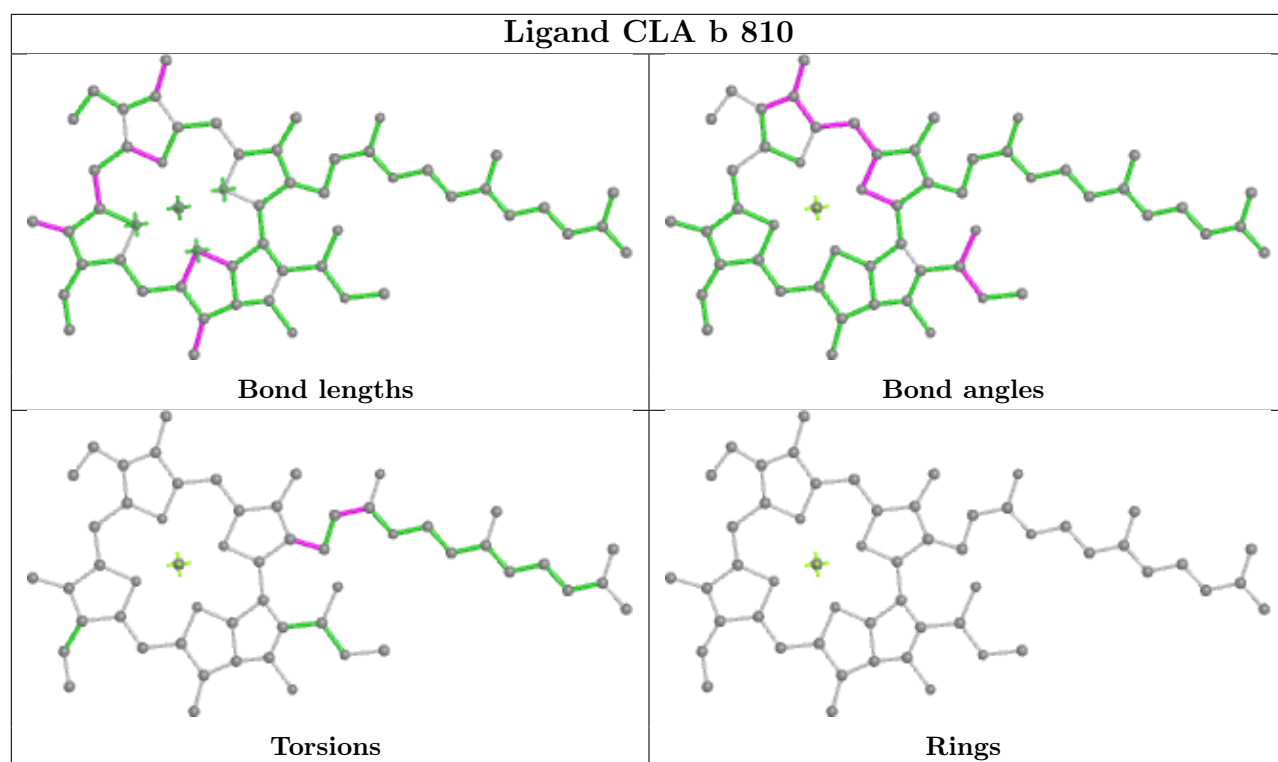
Bond angles



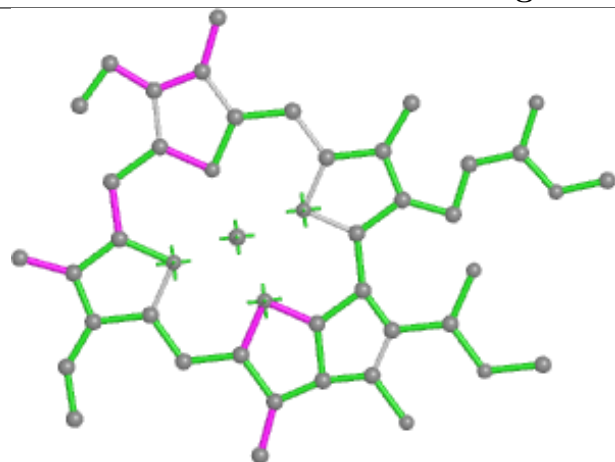
Torsions



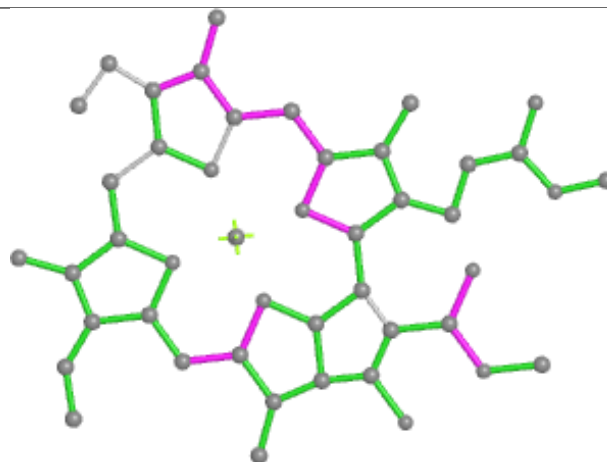
Rings



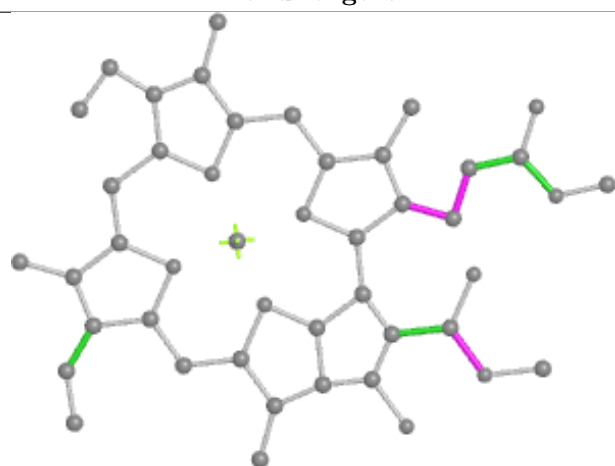
## Ligand CLA A 210



Bond lengths



Bond angles



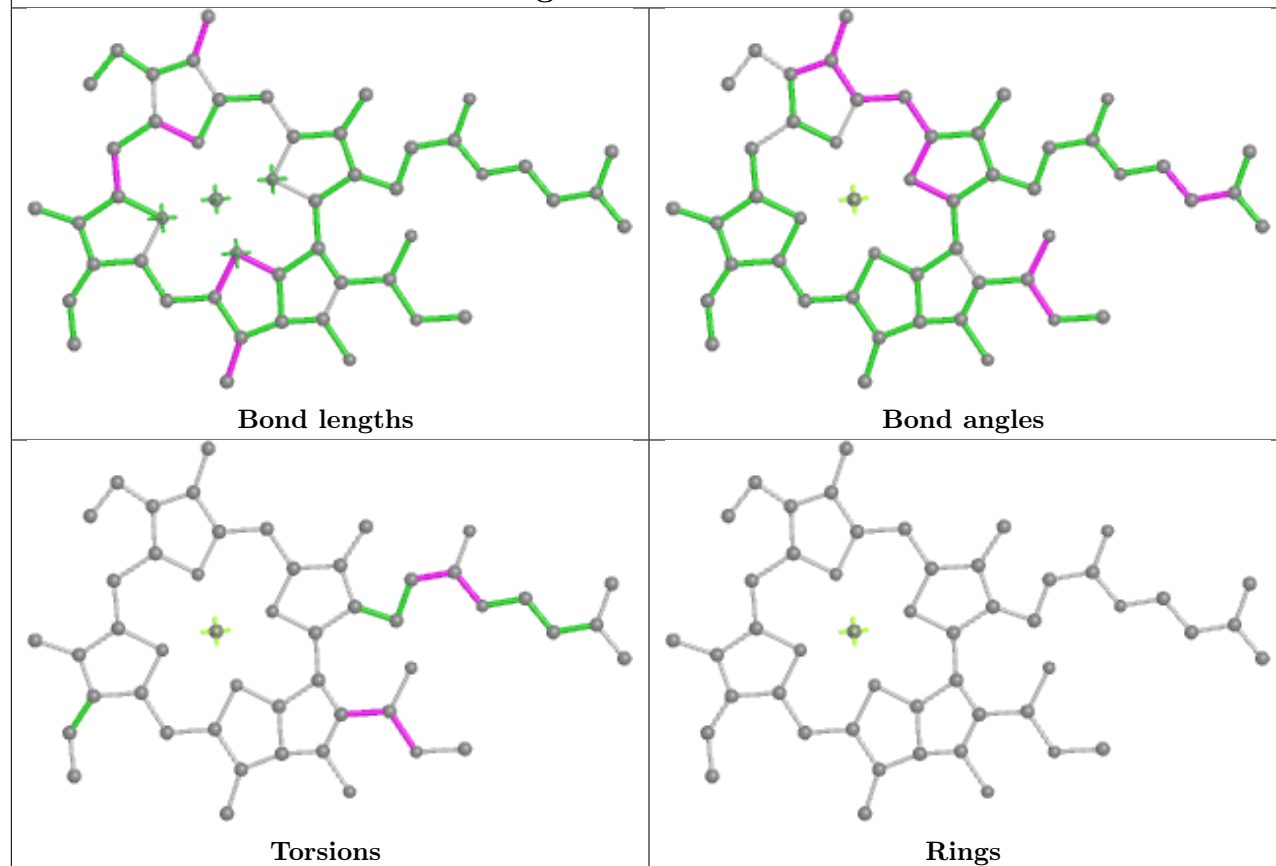
Torsions



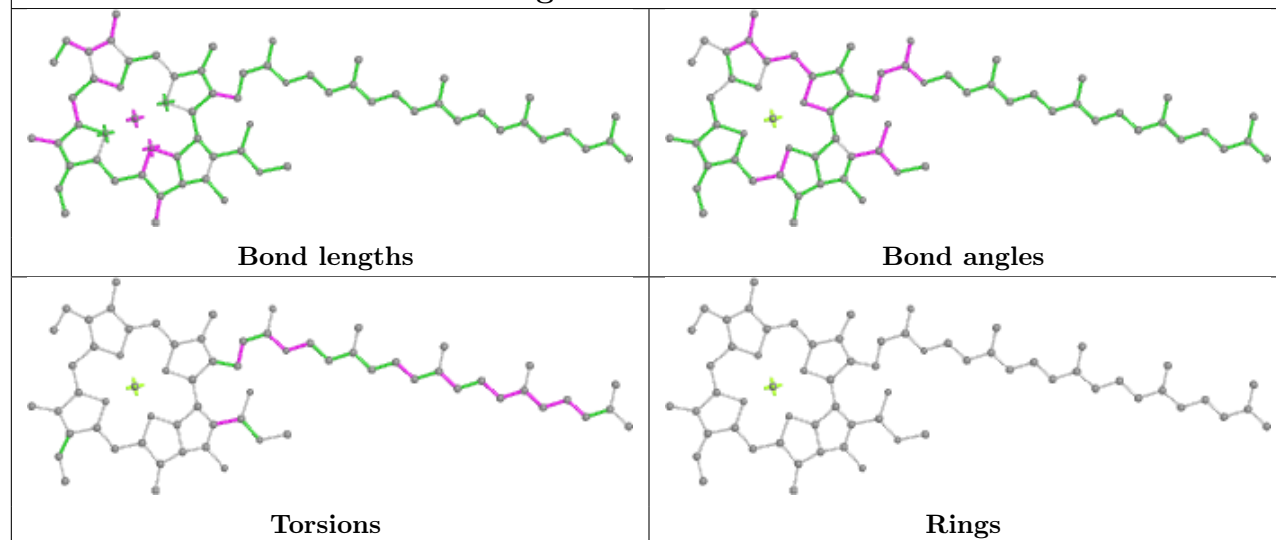
Rings



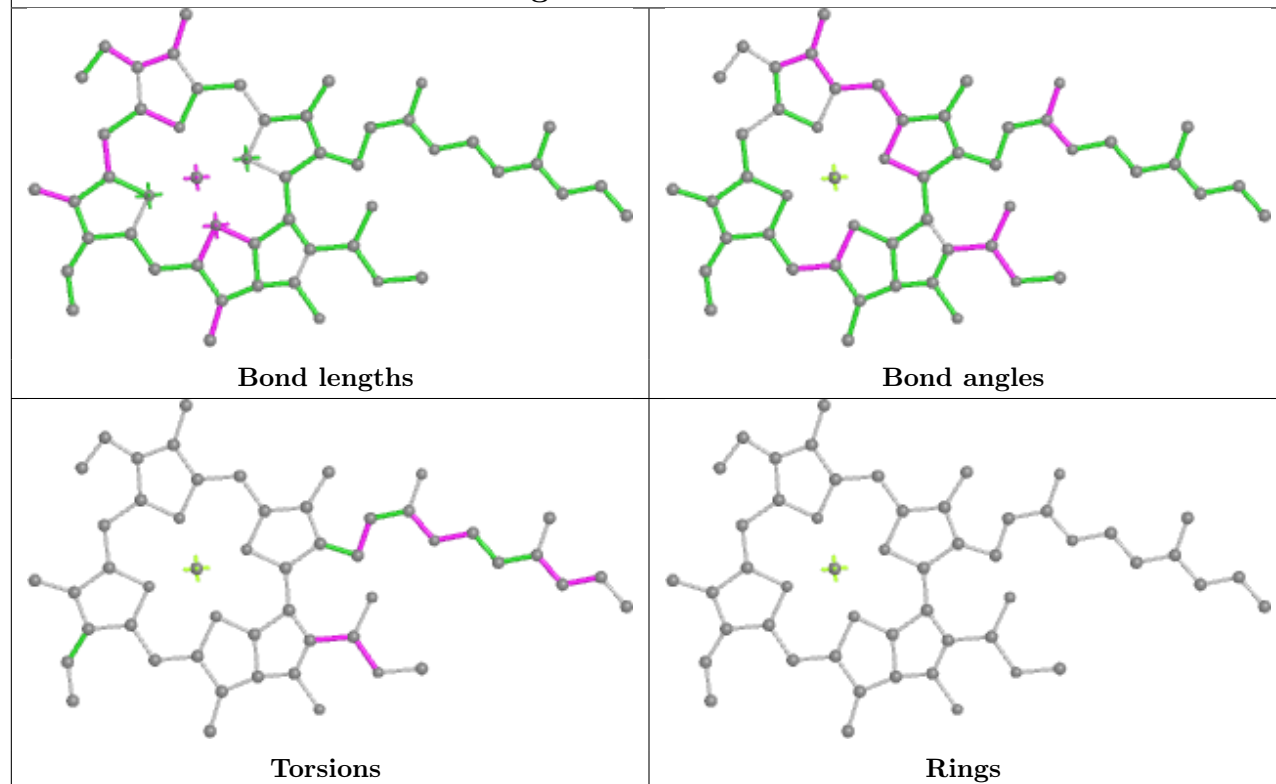
## Ligand CLA a 813



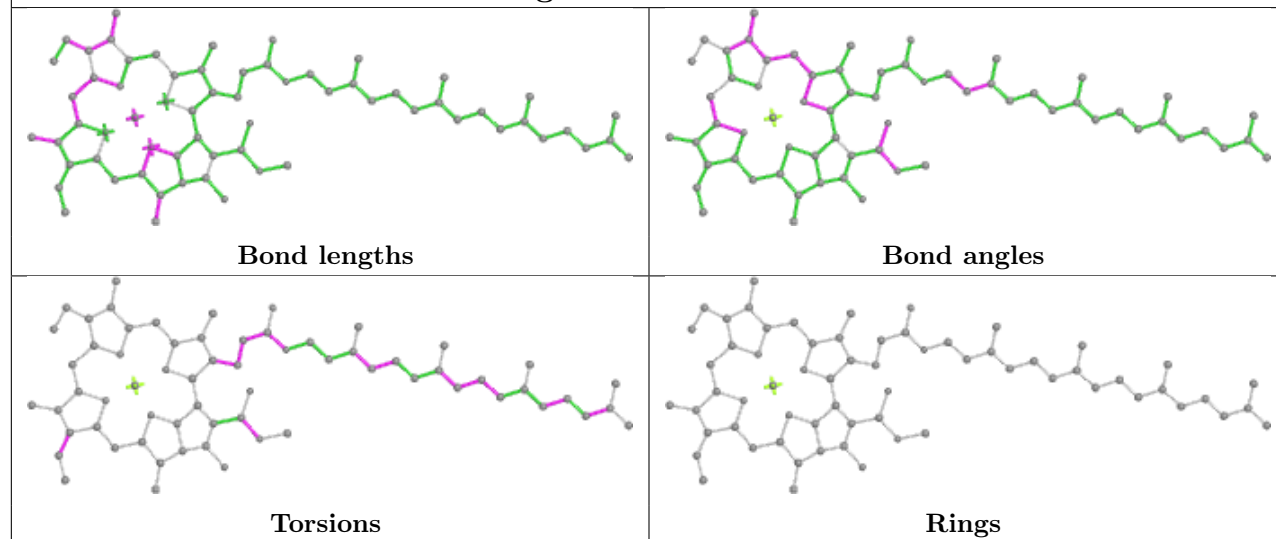
## Ligand CLA a 805



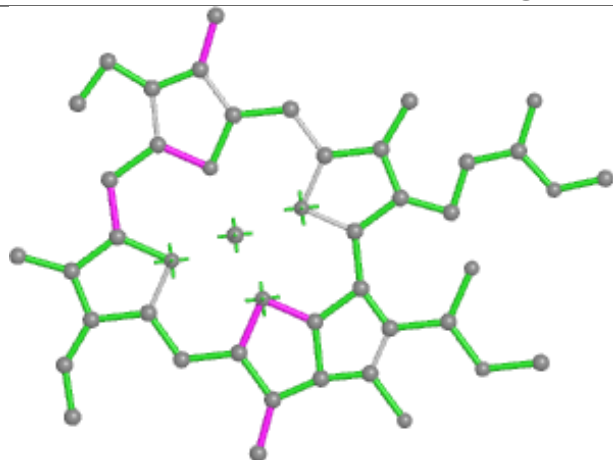
## Ligand CLA K 311



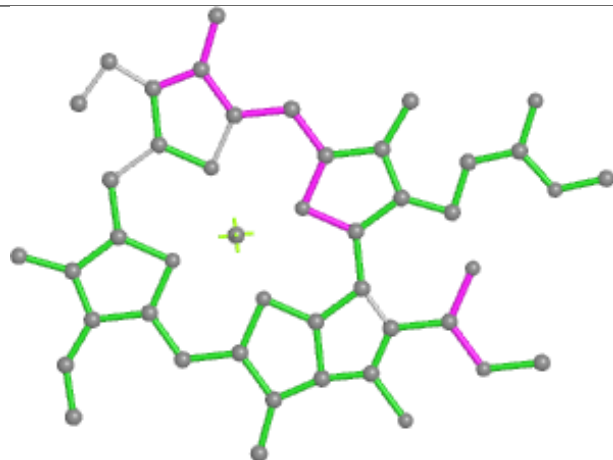
## Ligand CLA J 309



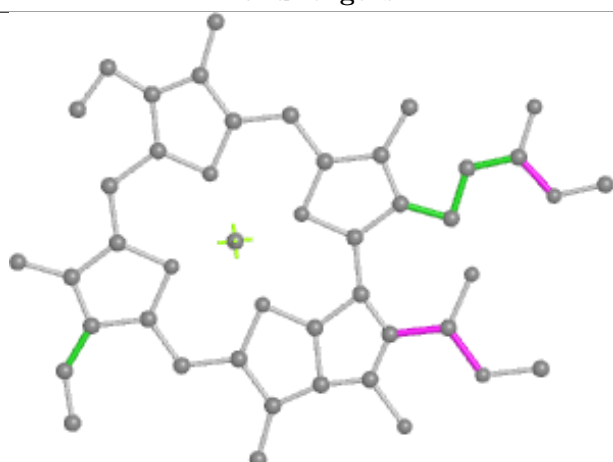
## Ligand CLA b 816



Bond lengths



Bond angles

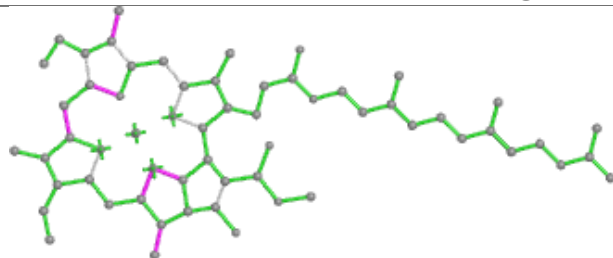


Torsions

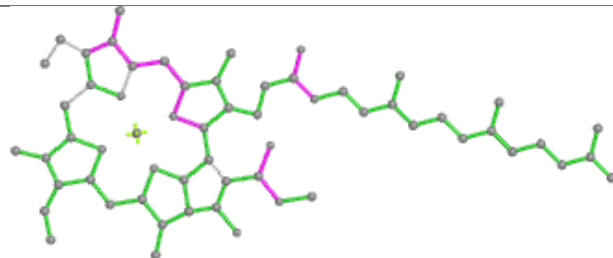


Rings

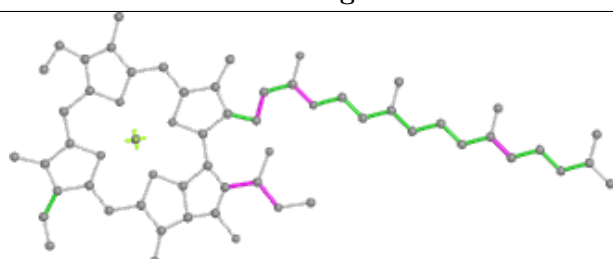
## Ligand CLA b 827



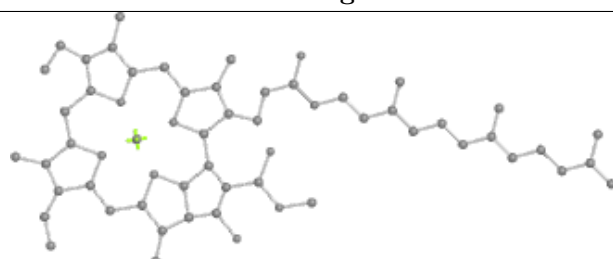
Bond lengths



Bond angles

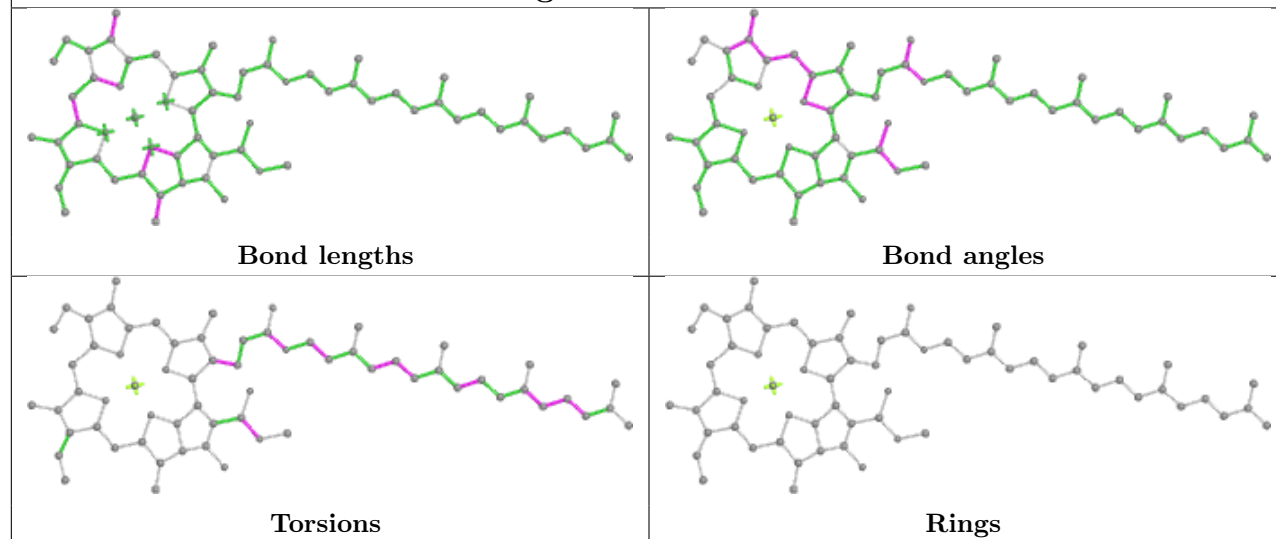


Torsions

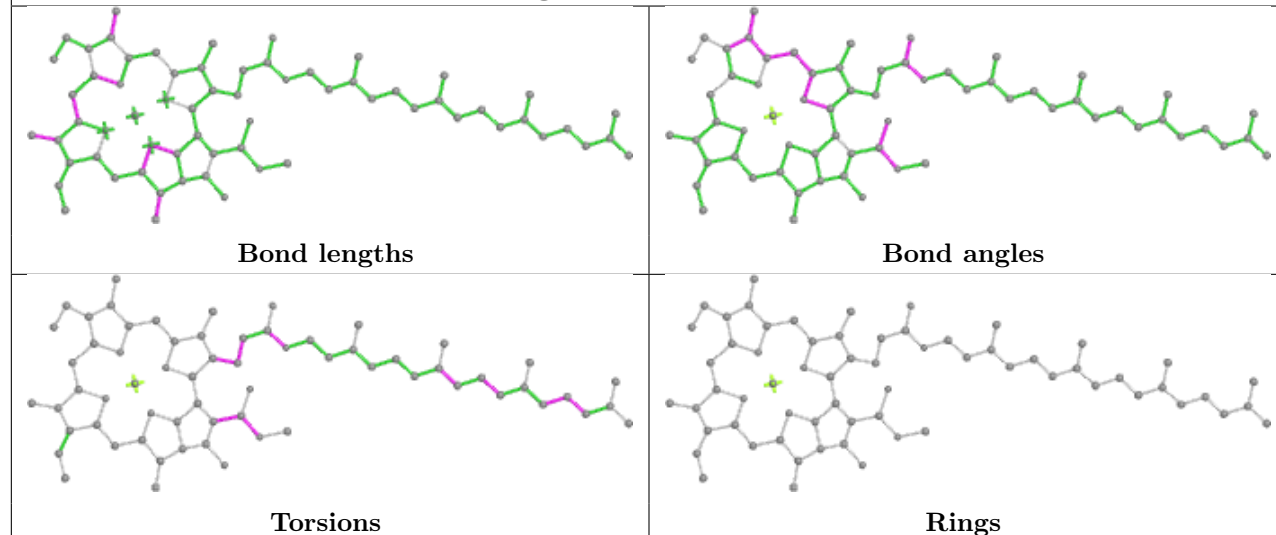


Rings

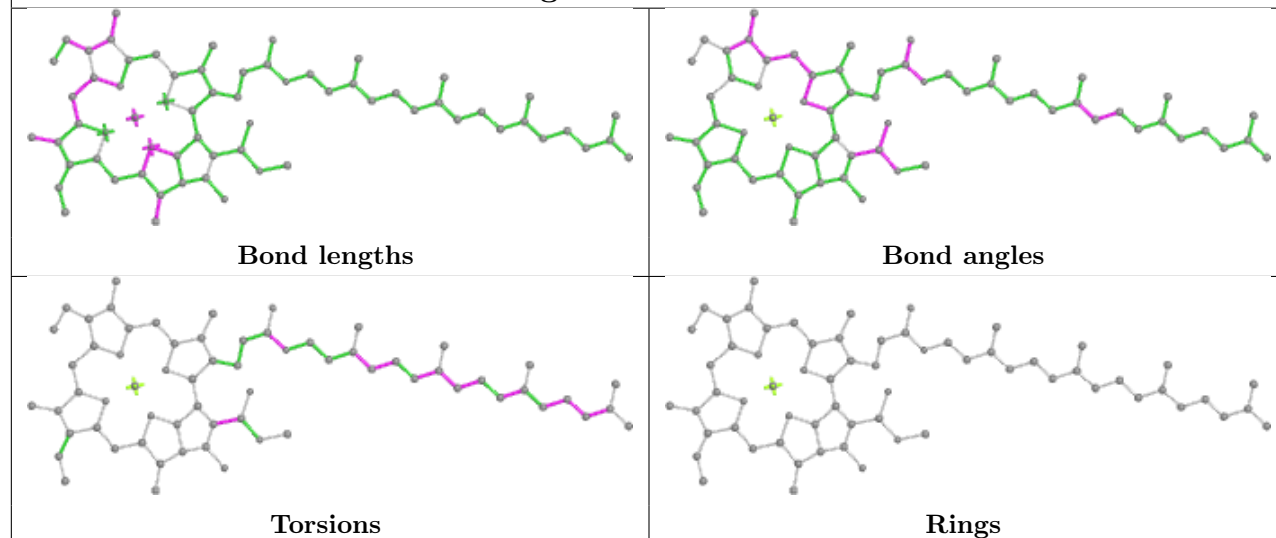
## Ligand CLA a 838



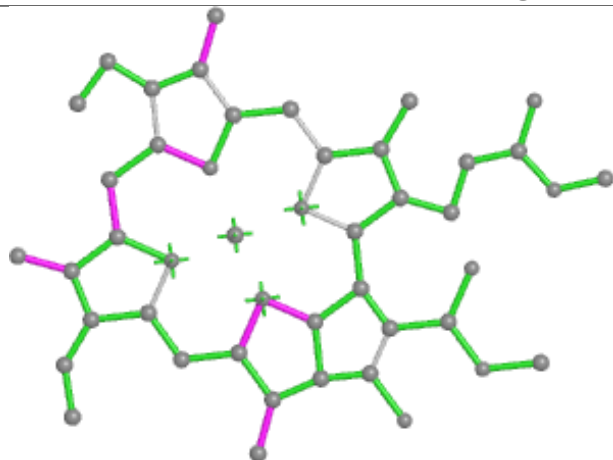
## Ligand CLA b 820



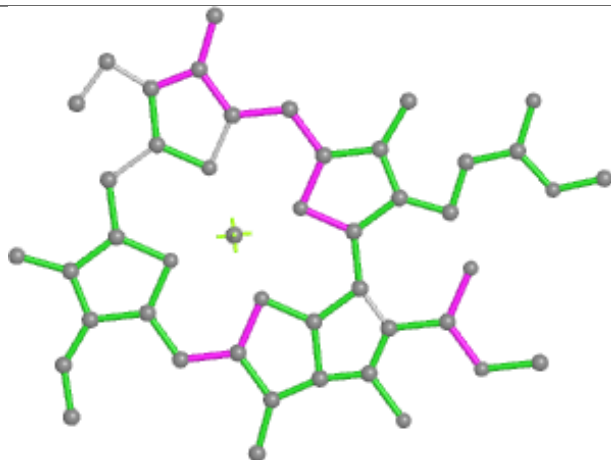
## Ligand CLA l 204



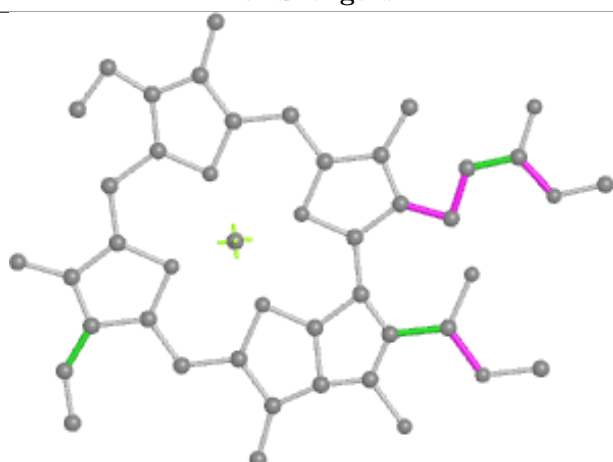
## Ligand CLA C 310



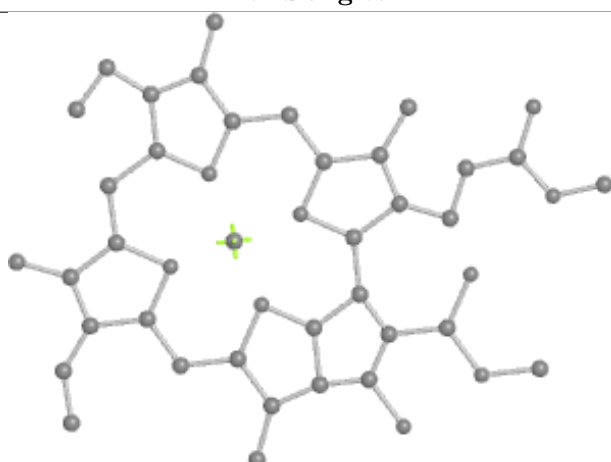
Bond lengths



Bond angles

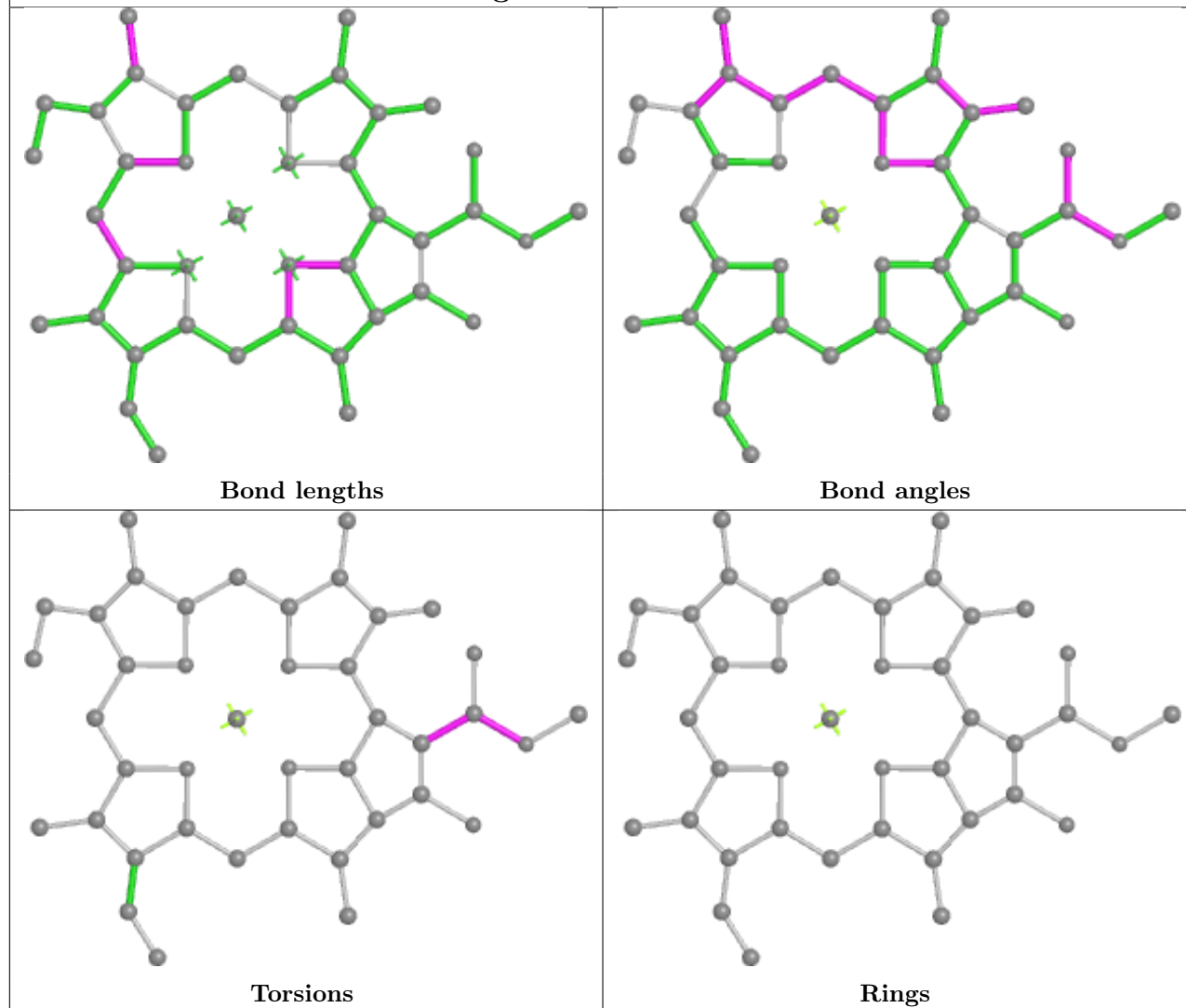


Torsions

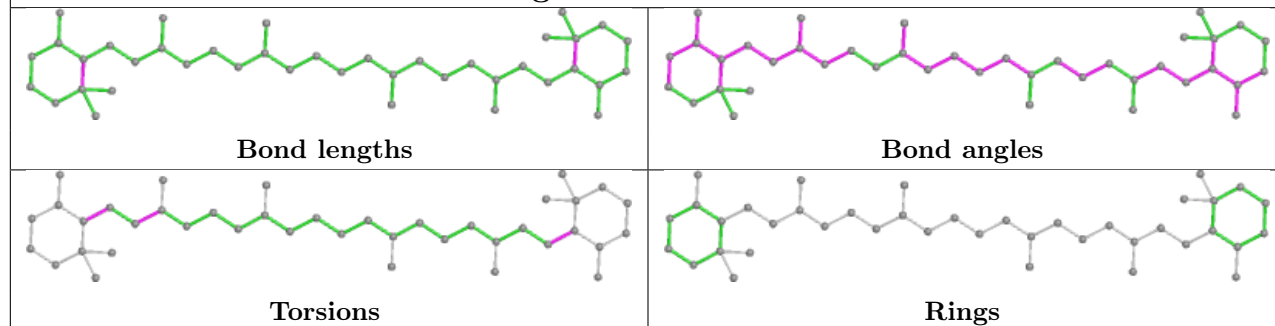


Rings

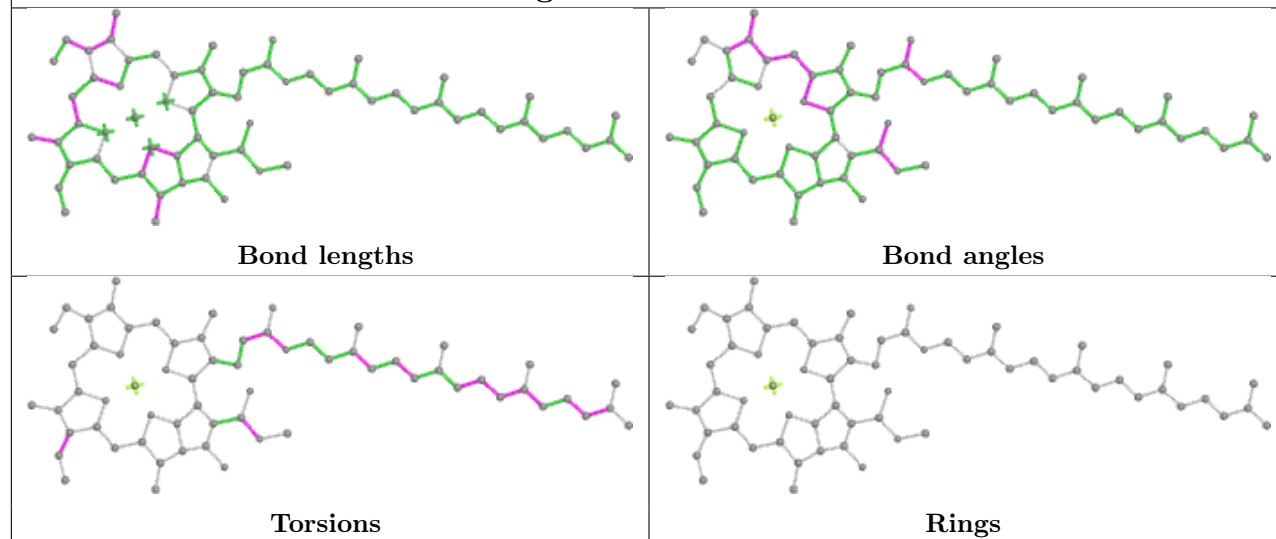
## Ligand CLA G 314



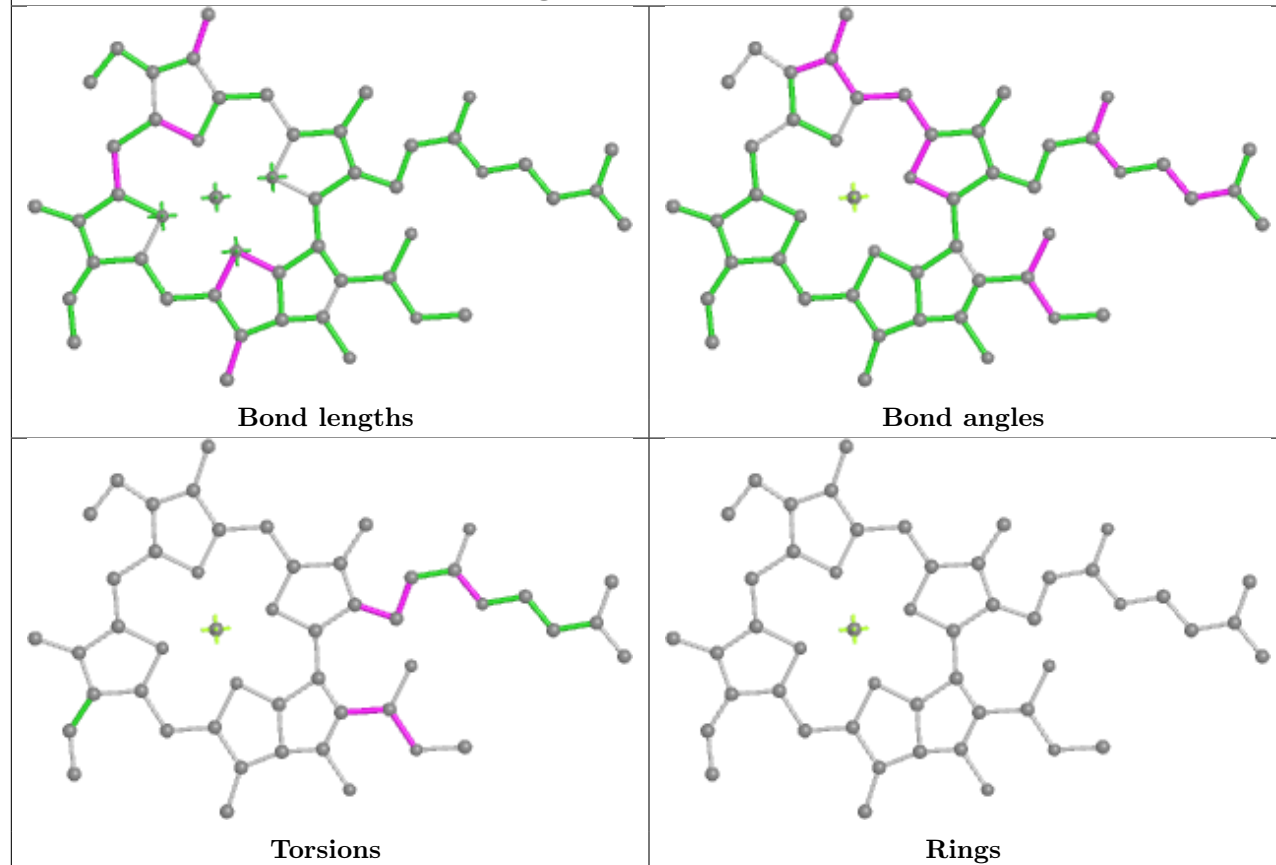
## Ligand BCR b 840



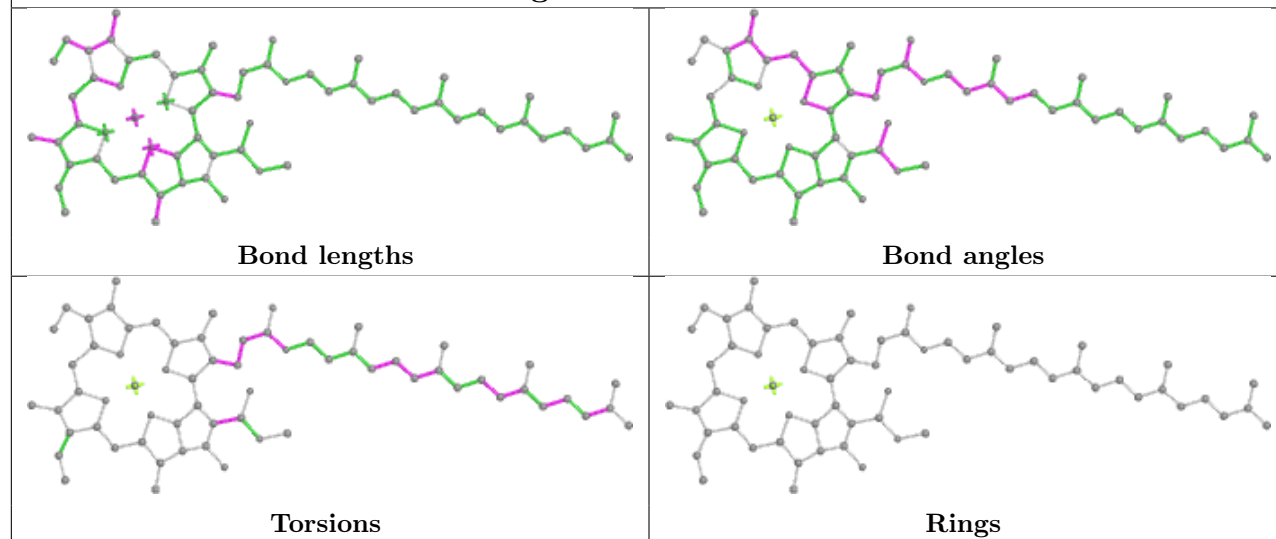
## Ligand CLA J 314



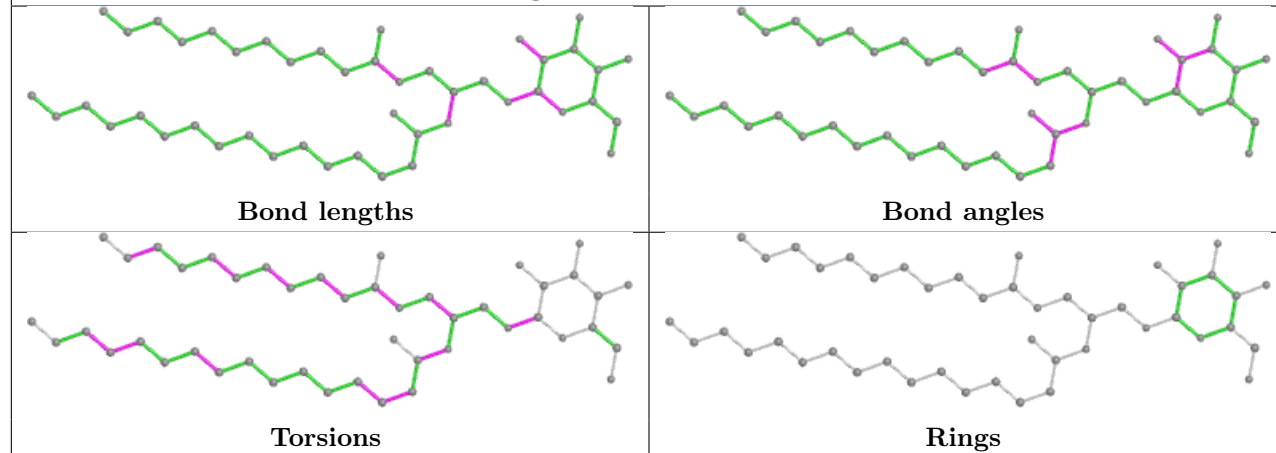
## Ligand CLA b 822



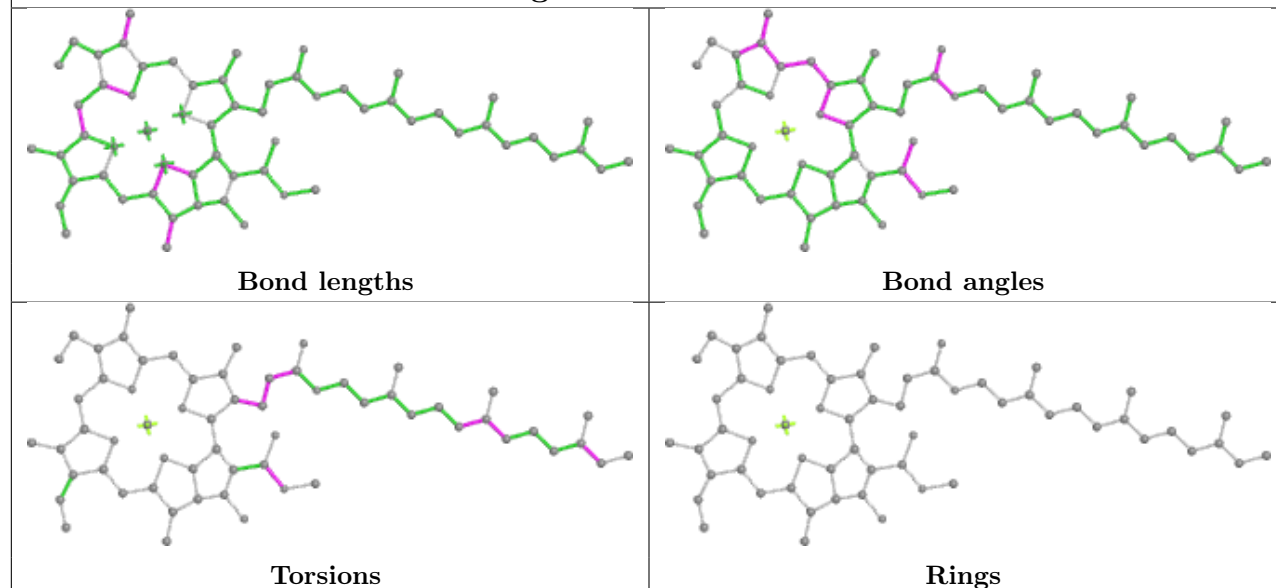
## Ligand CLA K 316



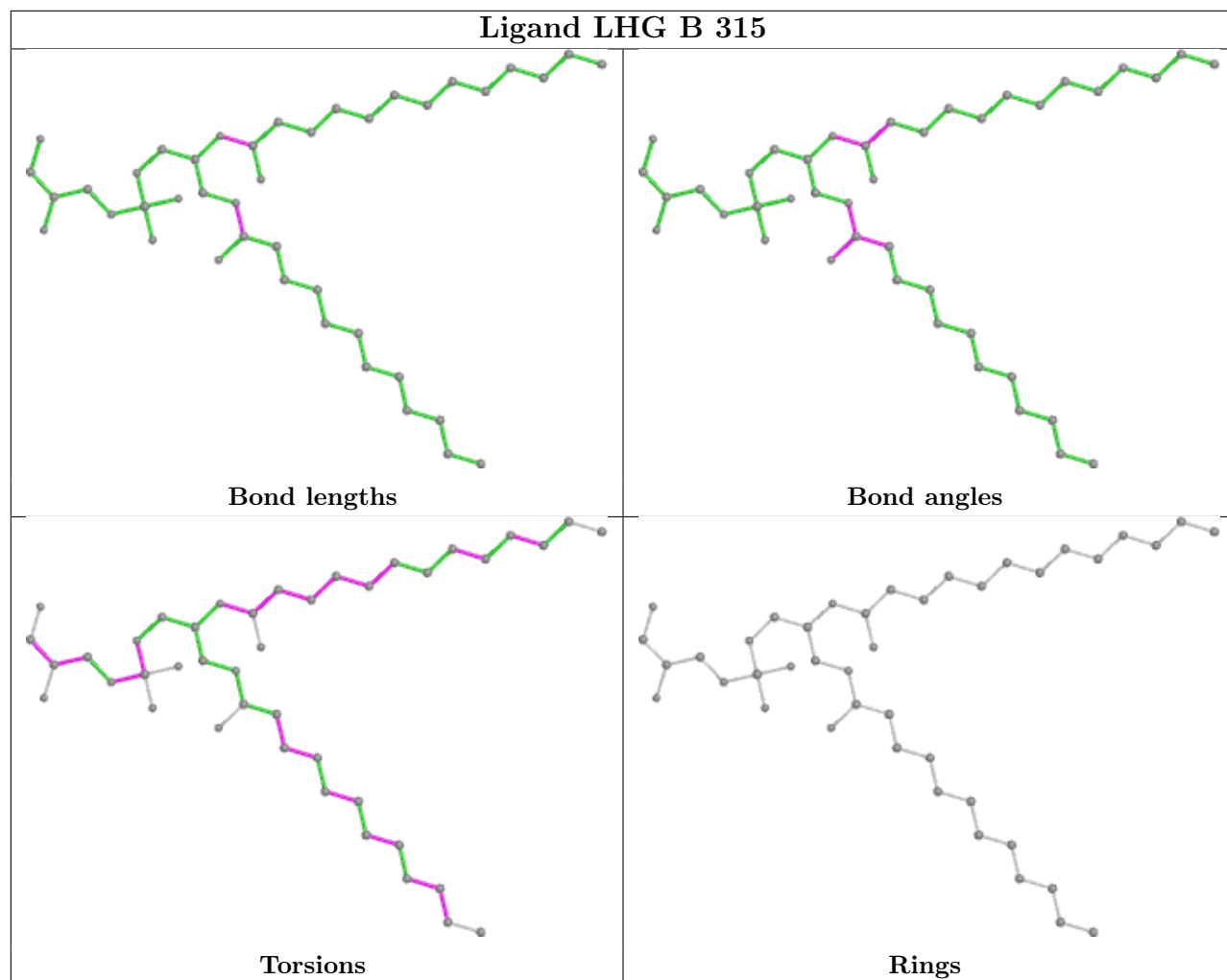
## Ligand LMG D 202



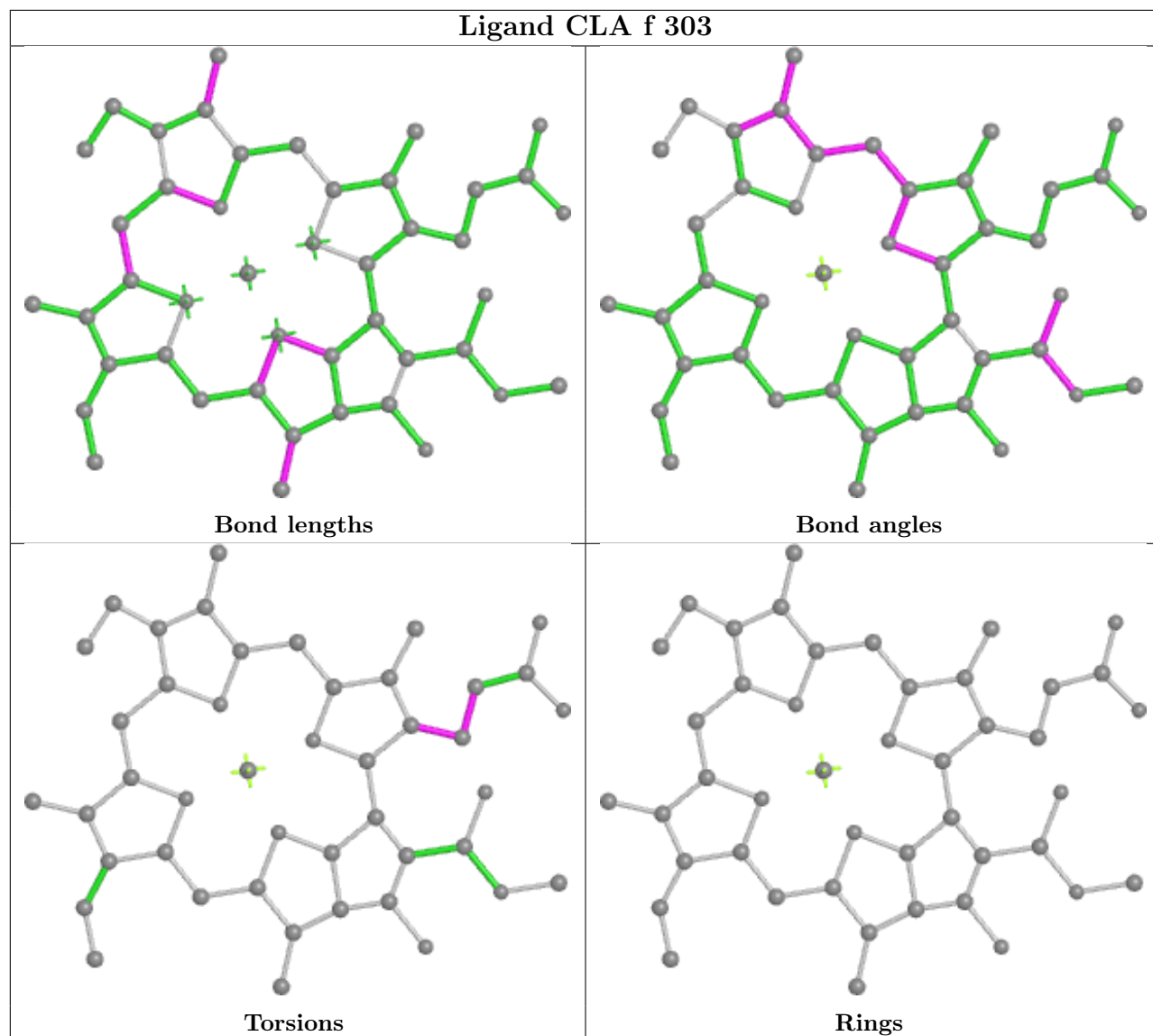
## Ligand CLA G 312



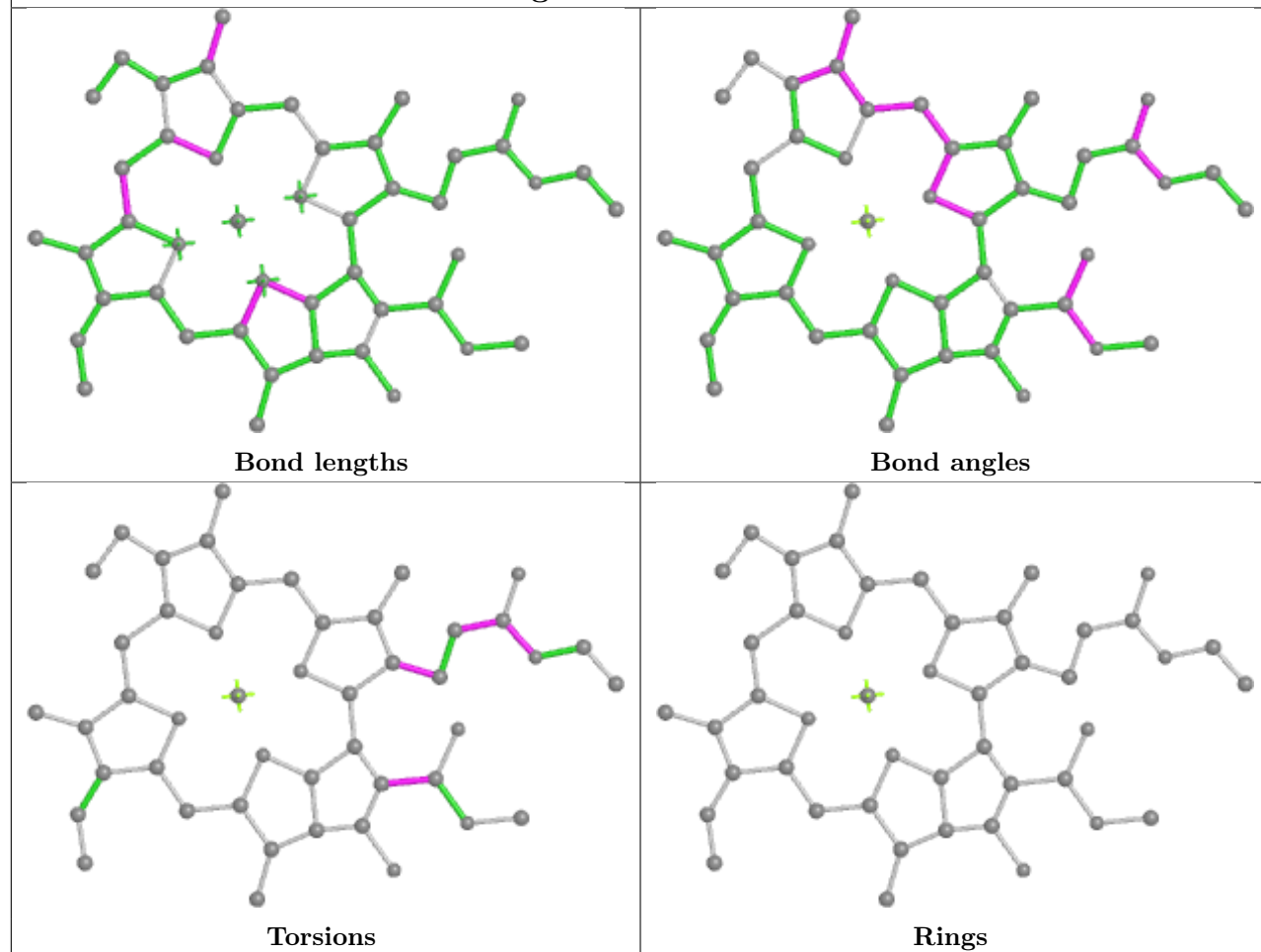




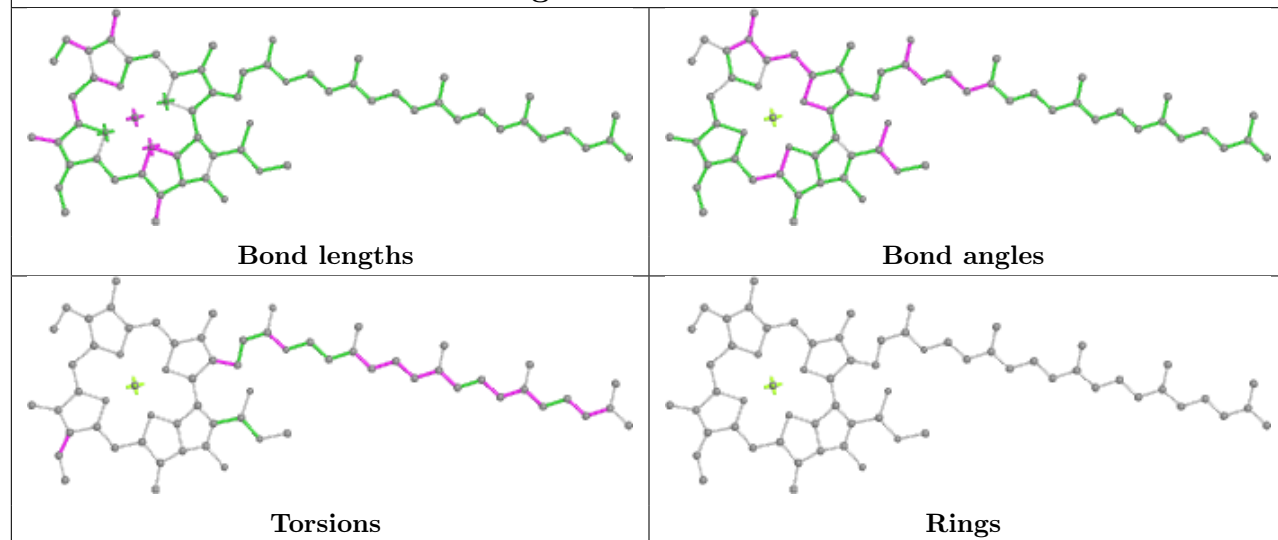
## Ligand CLA f 303

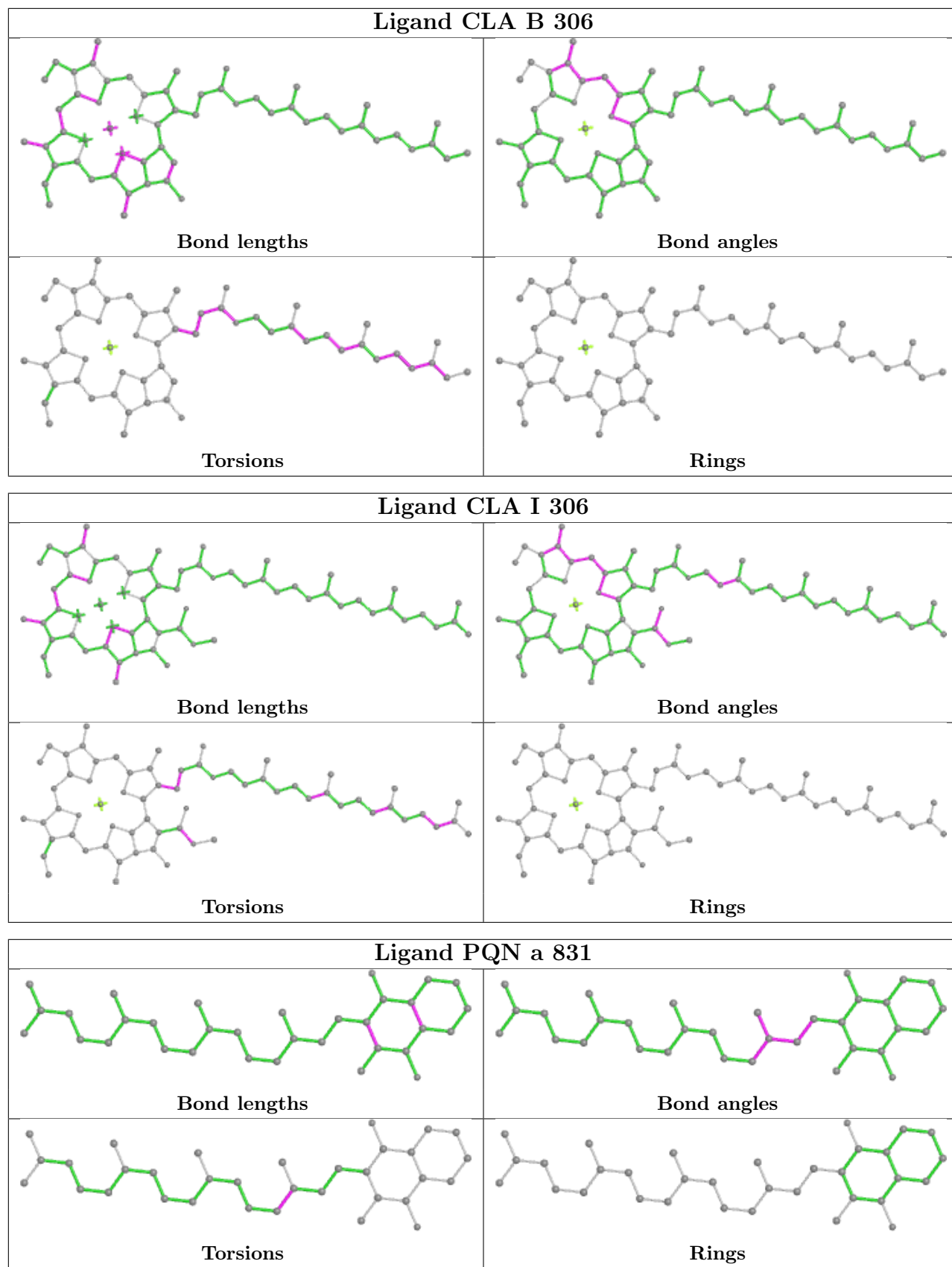


## Ligand CLA I 310

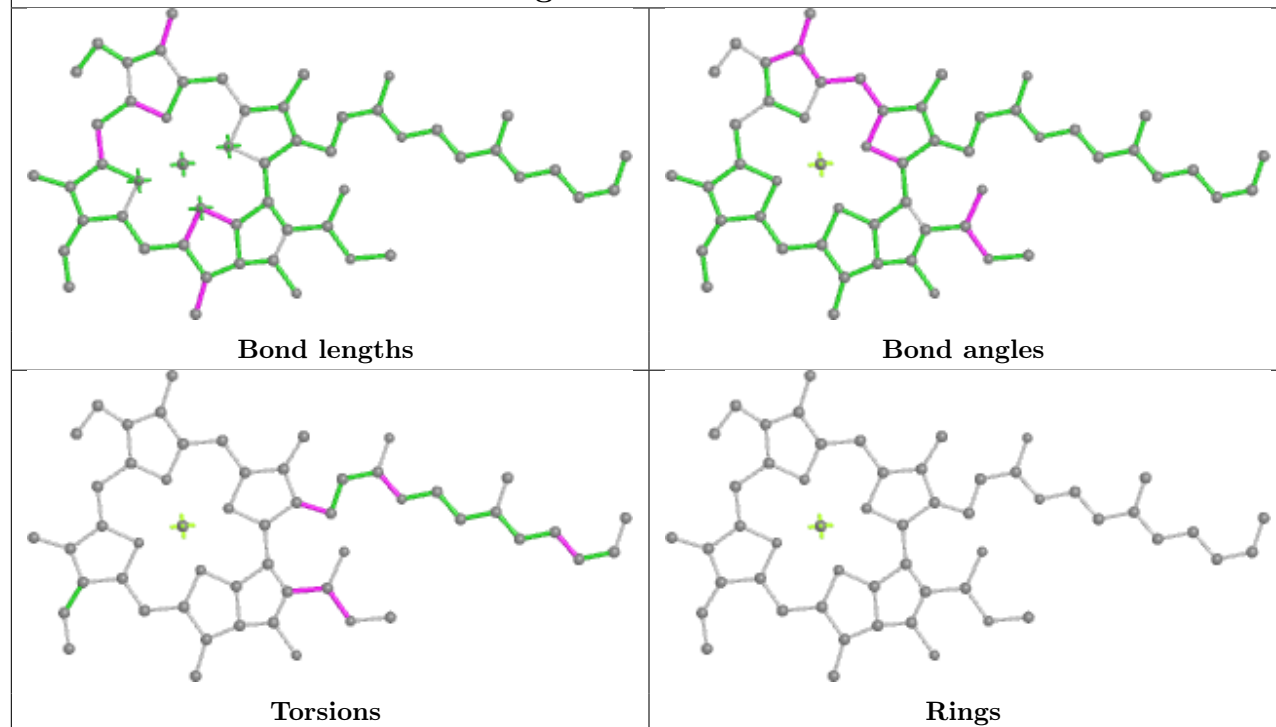


## Ligand CLA A 205

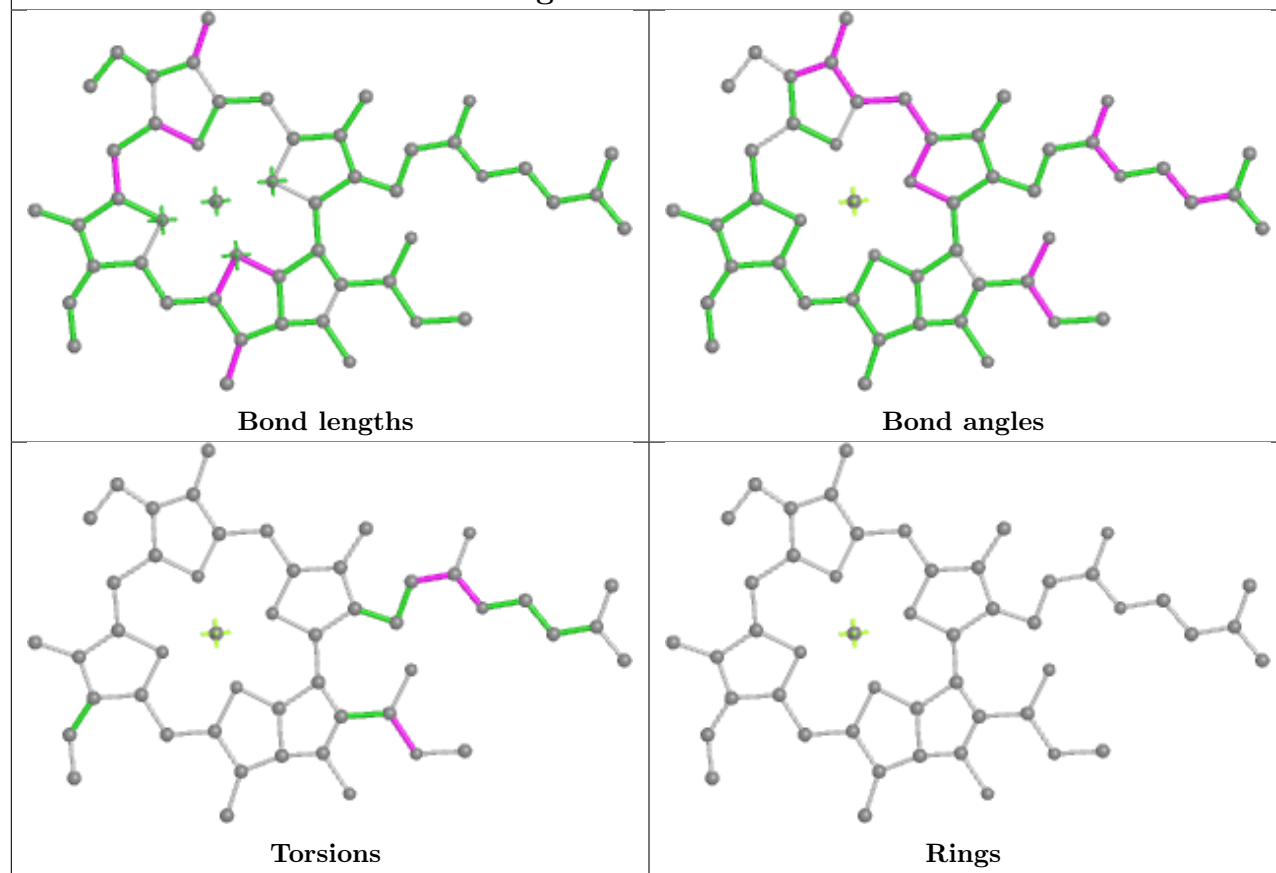




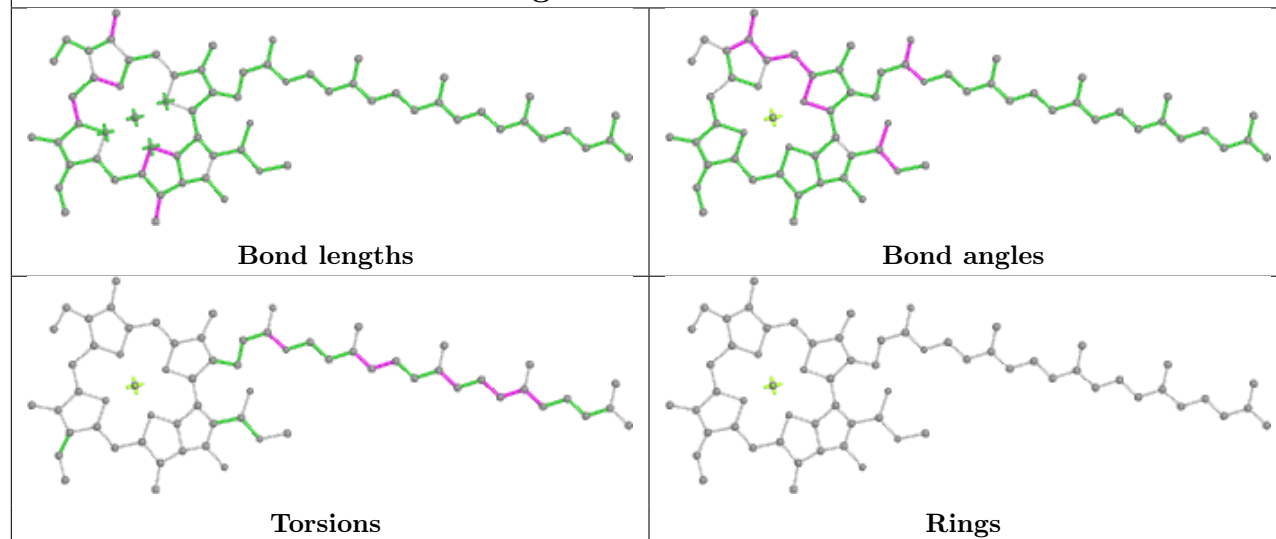
## Ligand CLA b 849



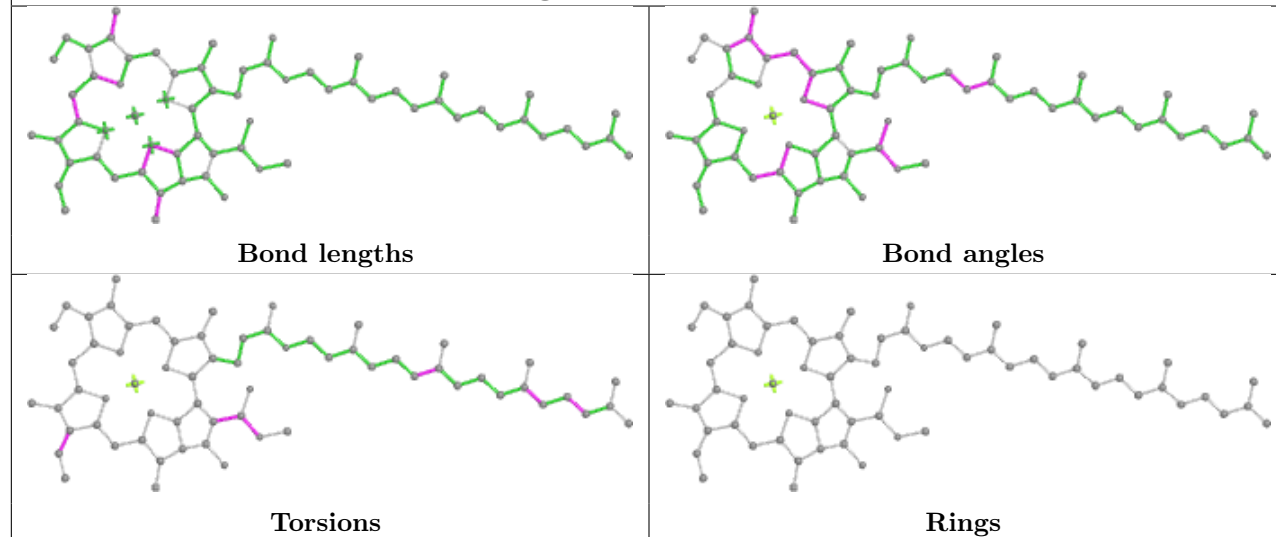
## Ligand CLA a 824



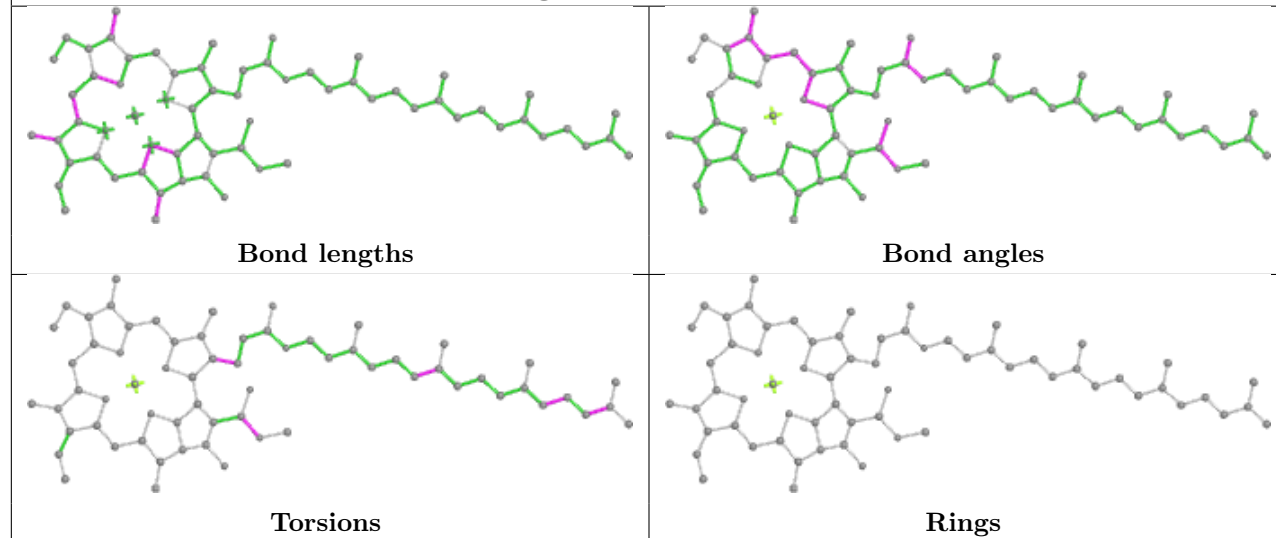
## Ligand CLA B 308



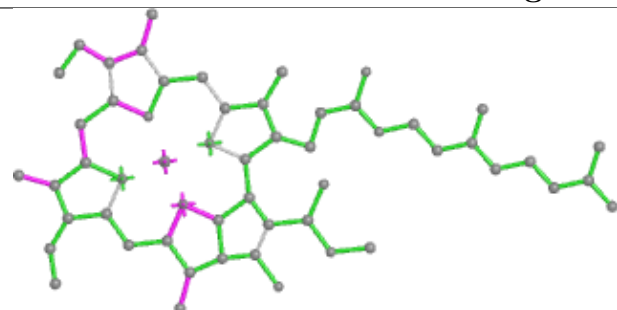
## Ligand CLA a 804



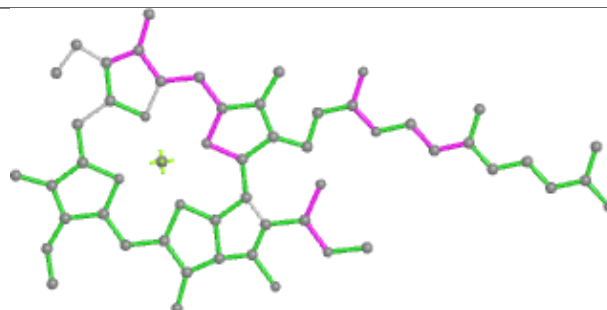
## Ligand CLA b 819



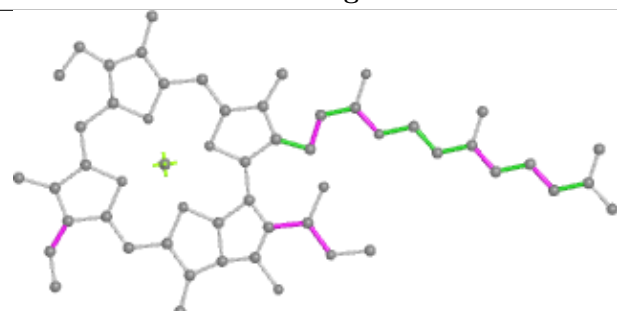
## Ligand CLA I 315



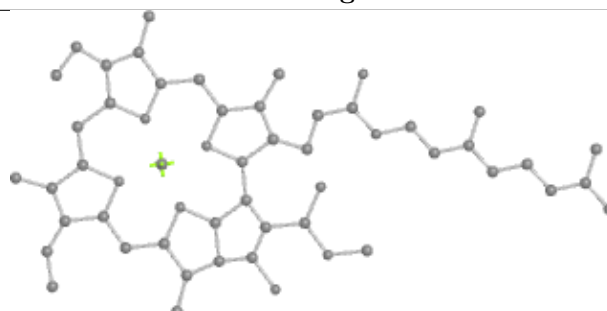
Bond lengths



Bond angles

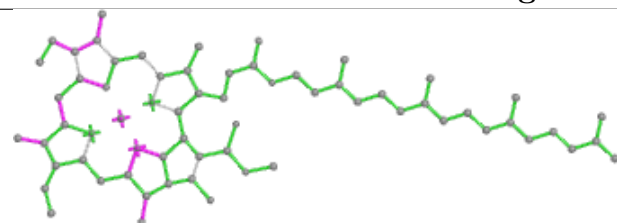


Torsions

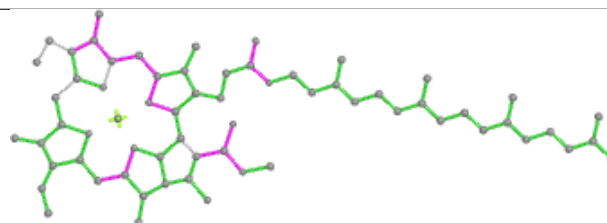


Rings

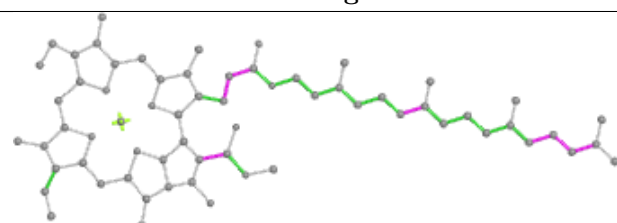
## Ligand CLA C 307



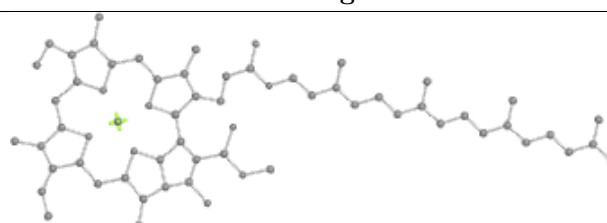
Bond lengths



Bond angles

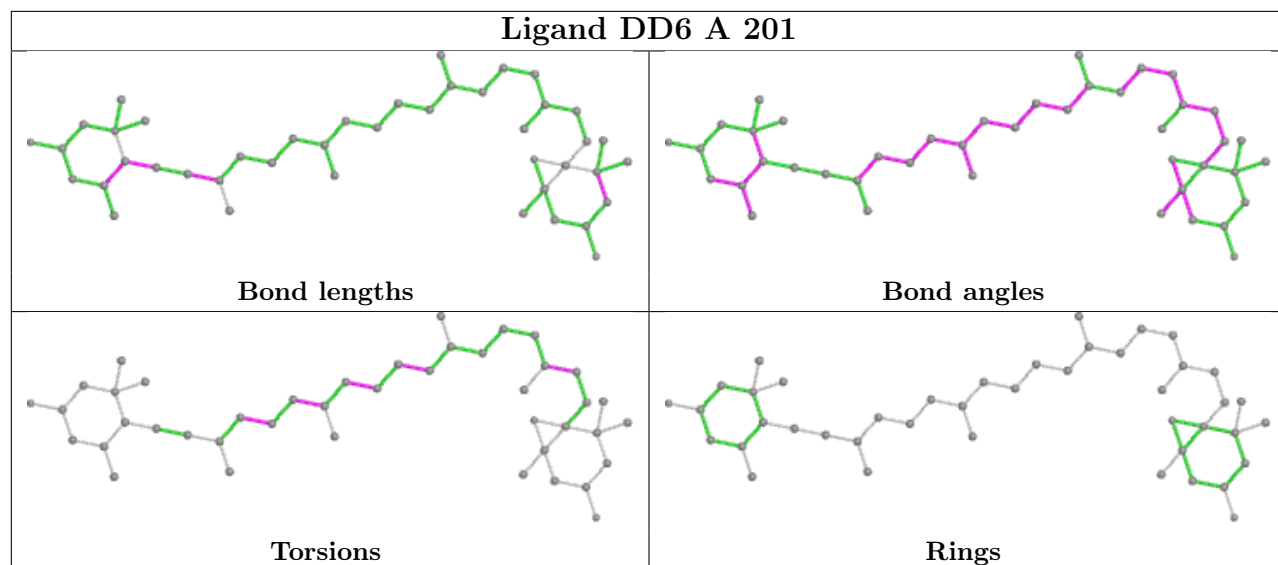


Torsions

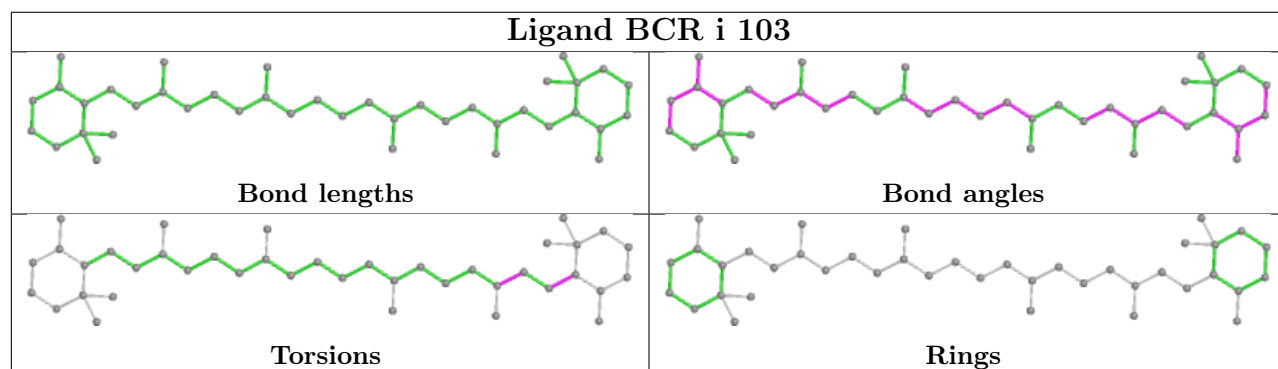


Rings

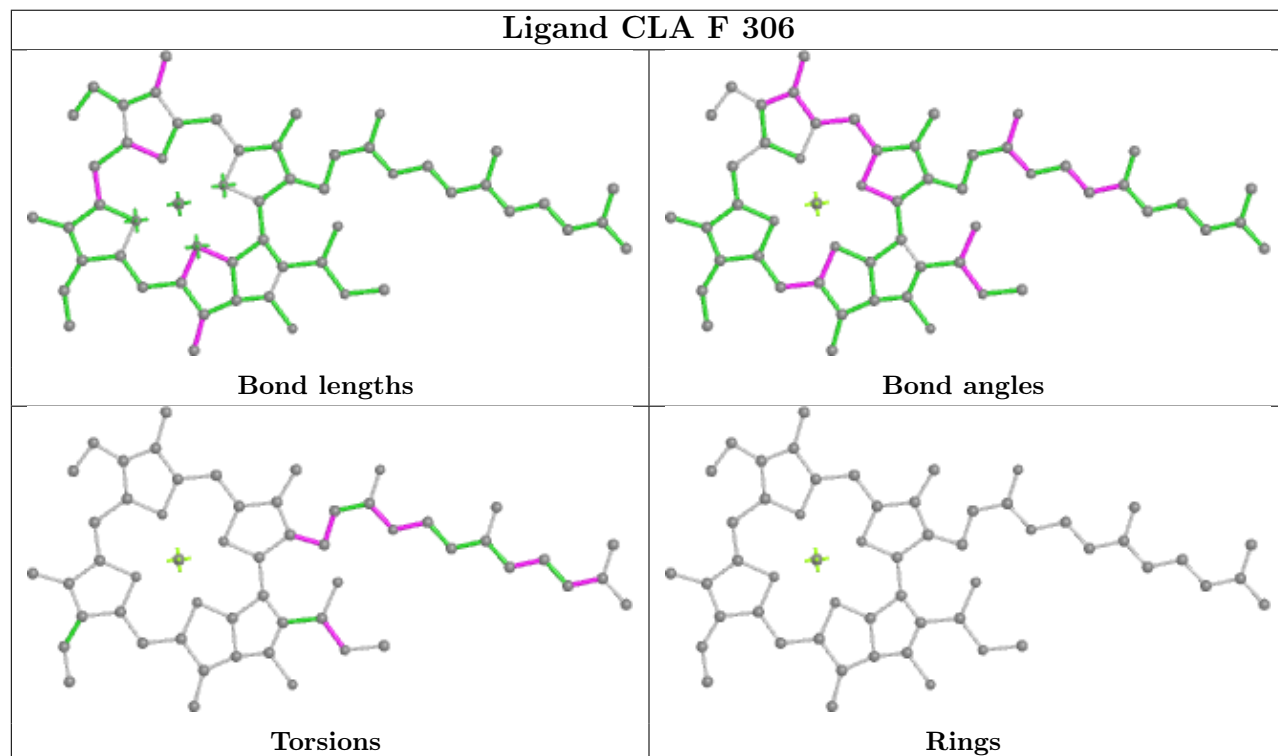
## Ligand DD6 A 201



## Ligand BCR i 103

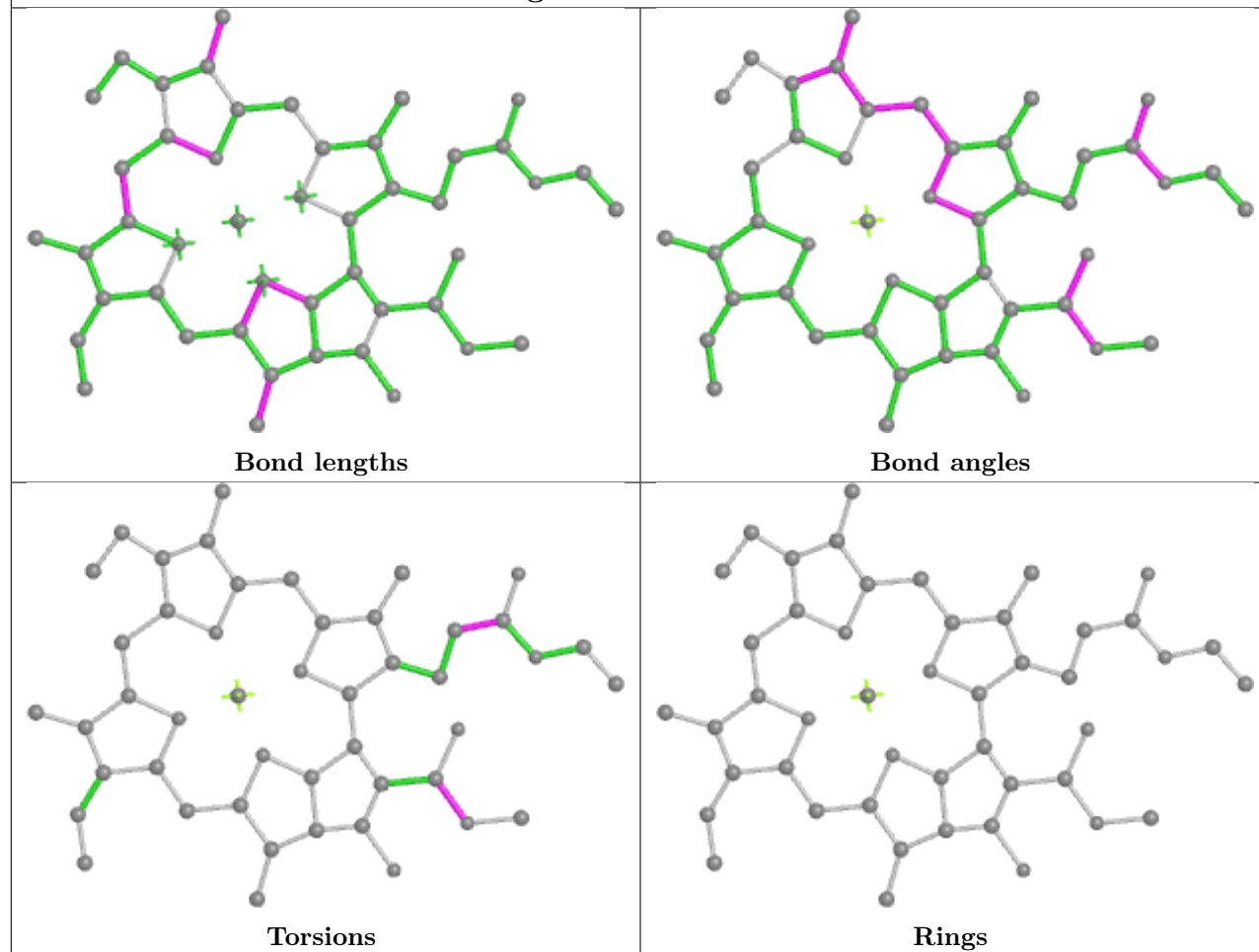


## Ligand CLA F 306

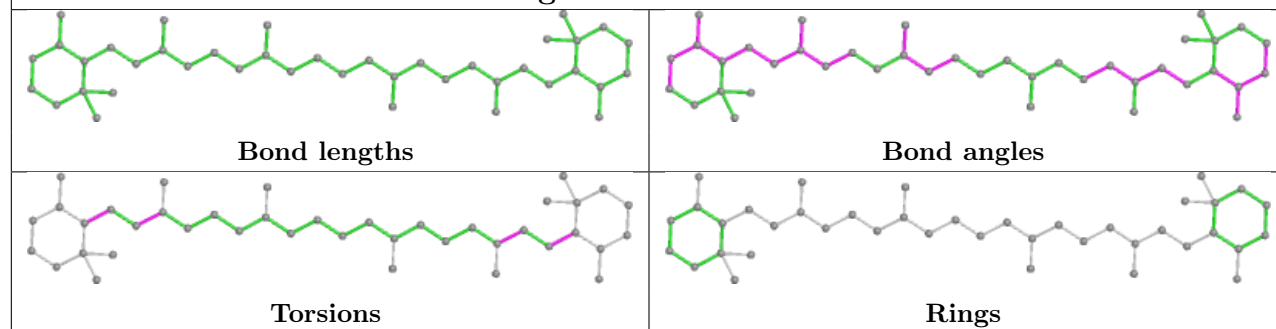




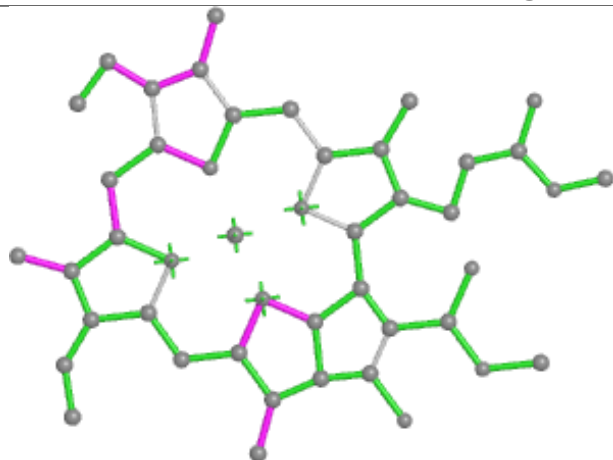
## Ligand CLA F 314



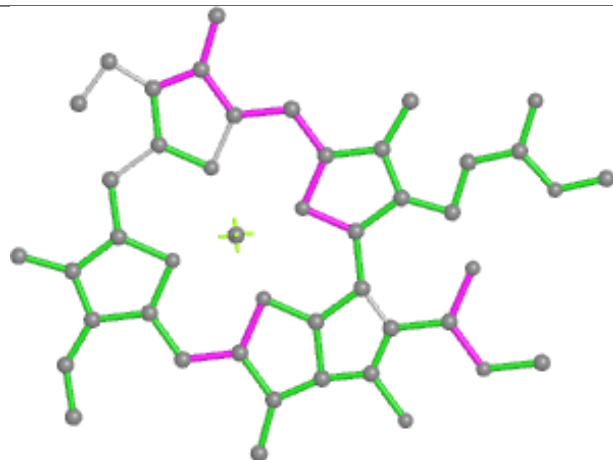
## Ligand BCR 1 205



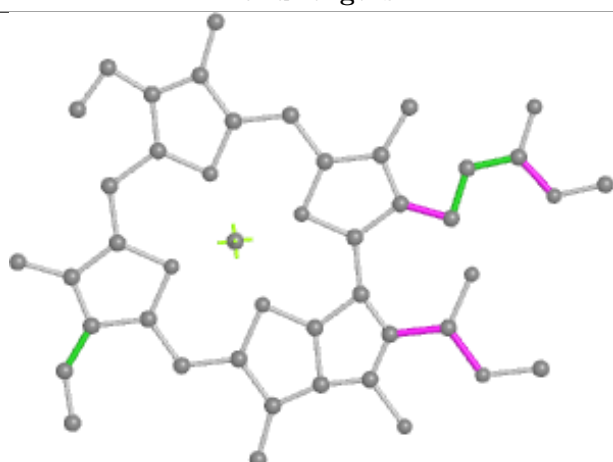
## Ligand CLA I 309



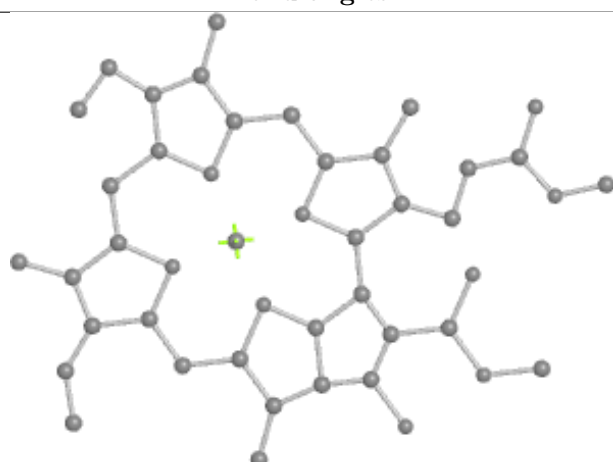
Bond lengths



Bond angles

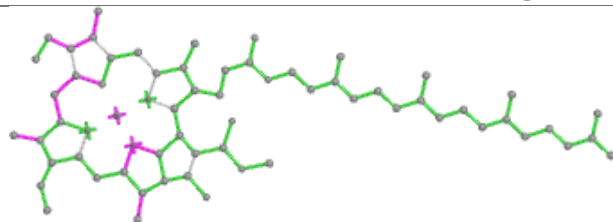


Torsions

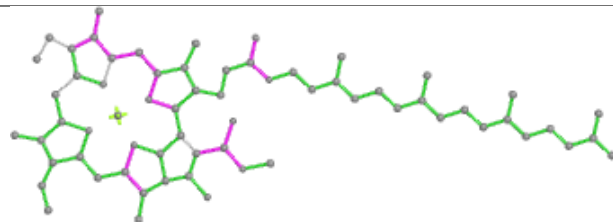


Rings

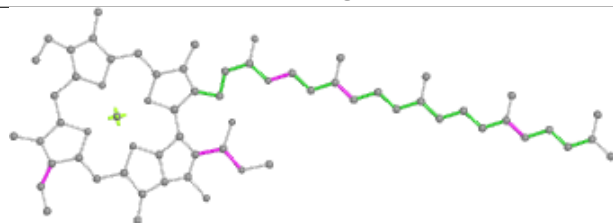
## Ligand CLA a 844



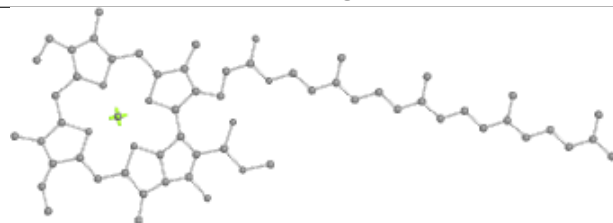
Bond lengths



Bond angles

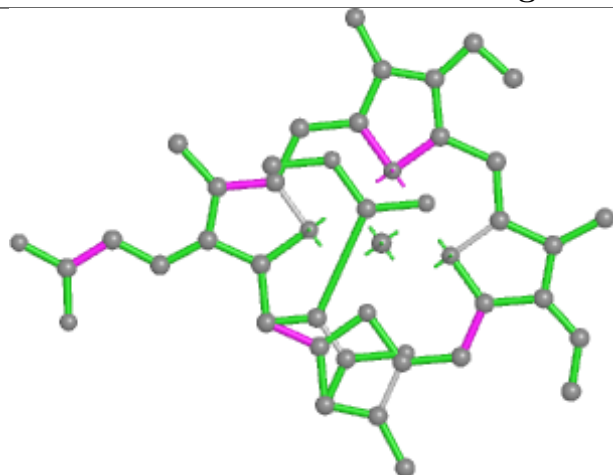


Torsions

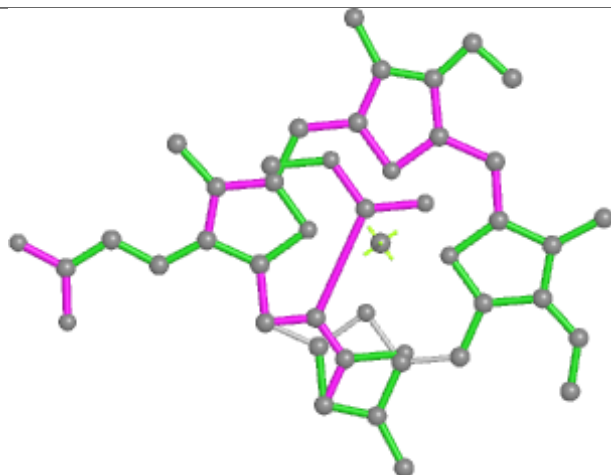


Rings

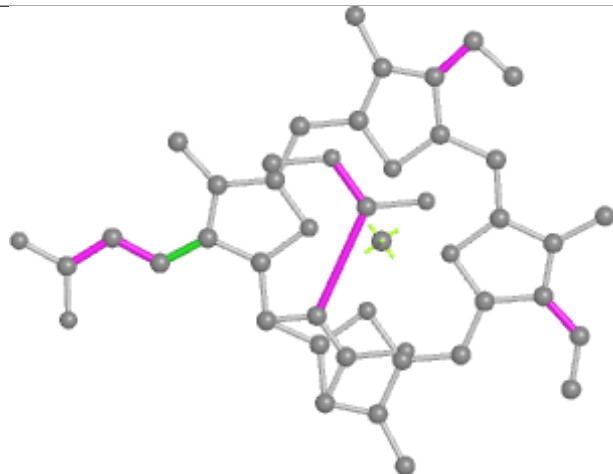
## Ligand KC1 L 314



Bond lengths



Bond angles

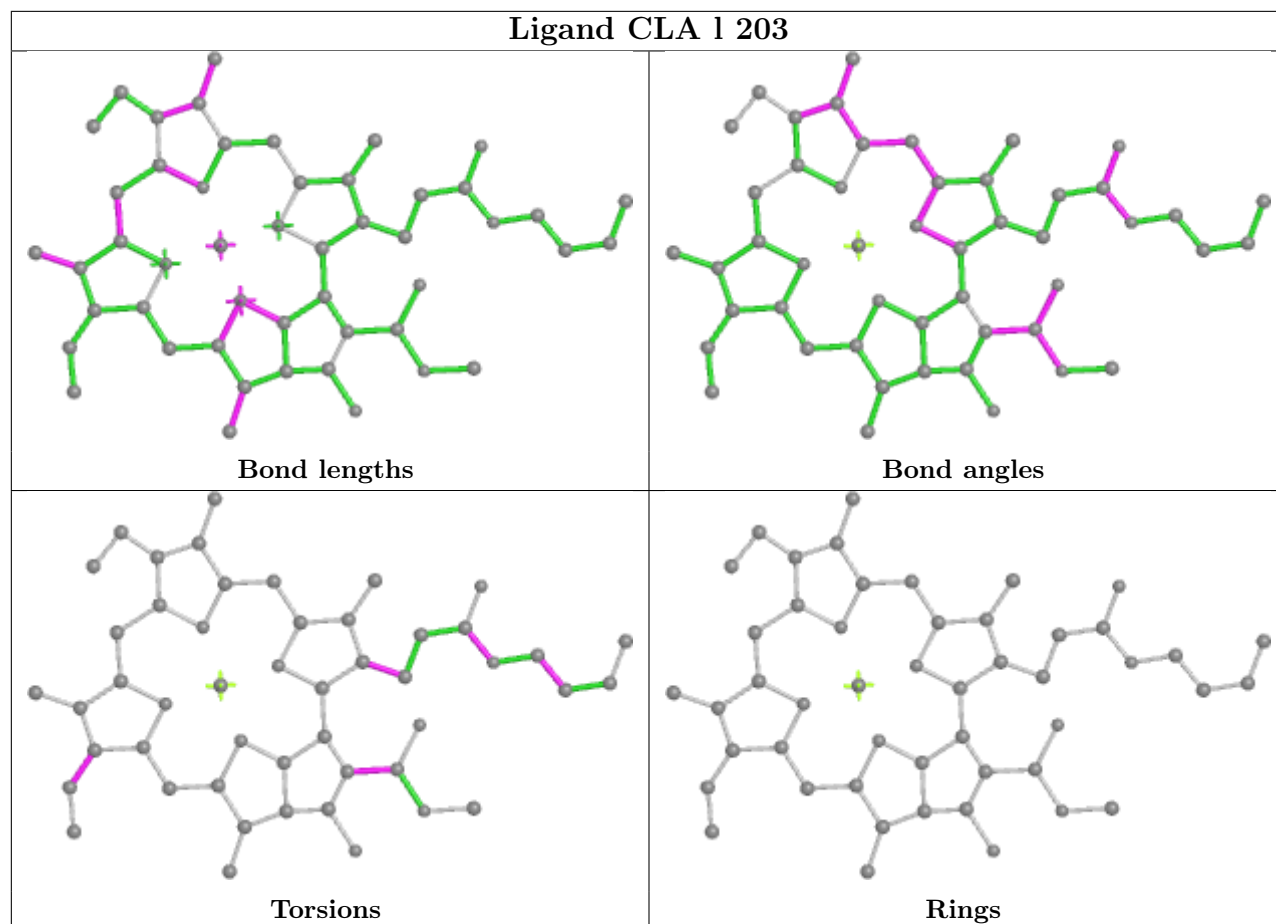


Torsions

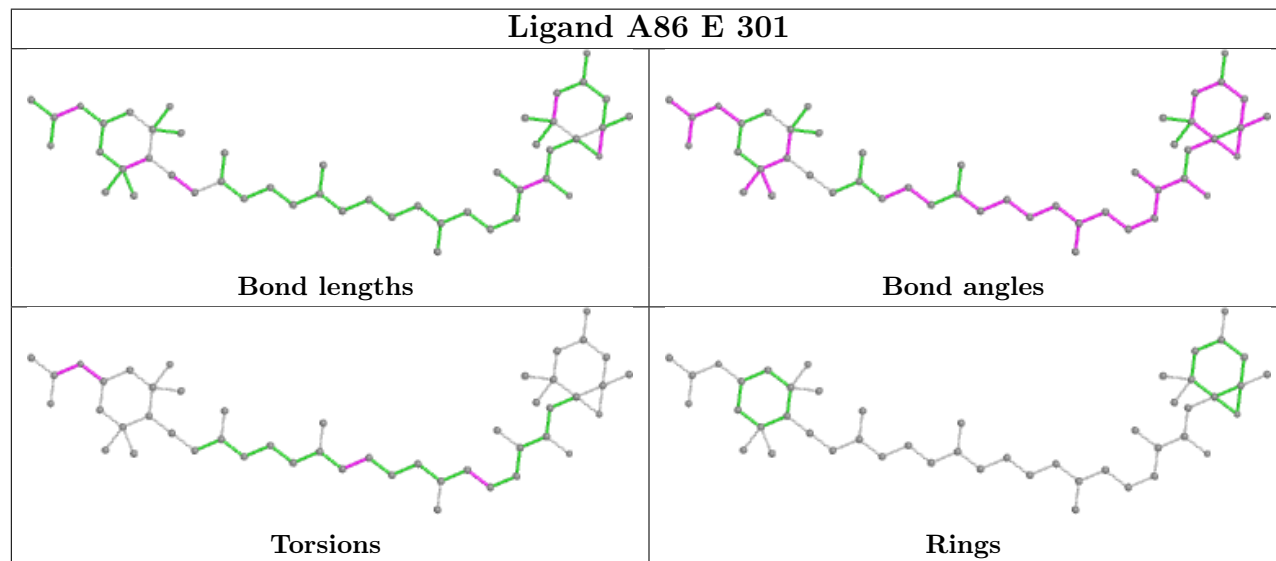


Rings

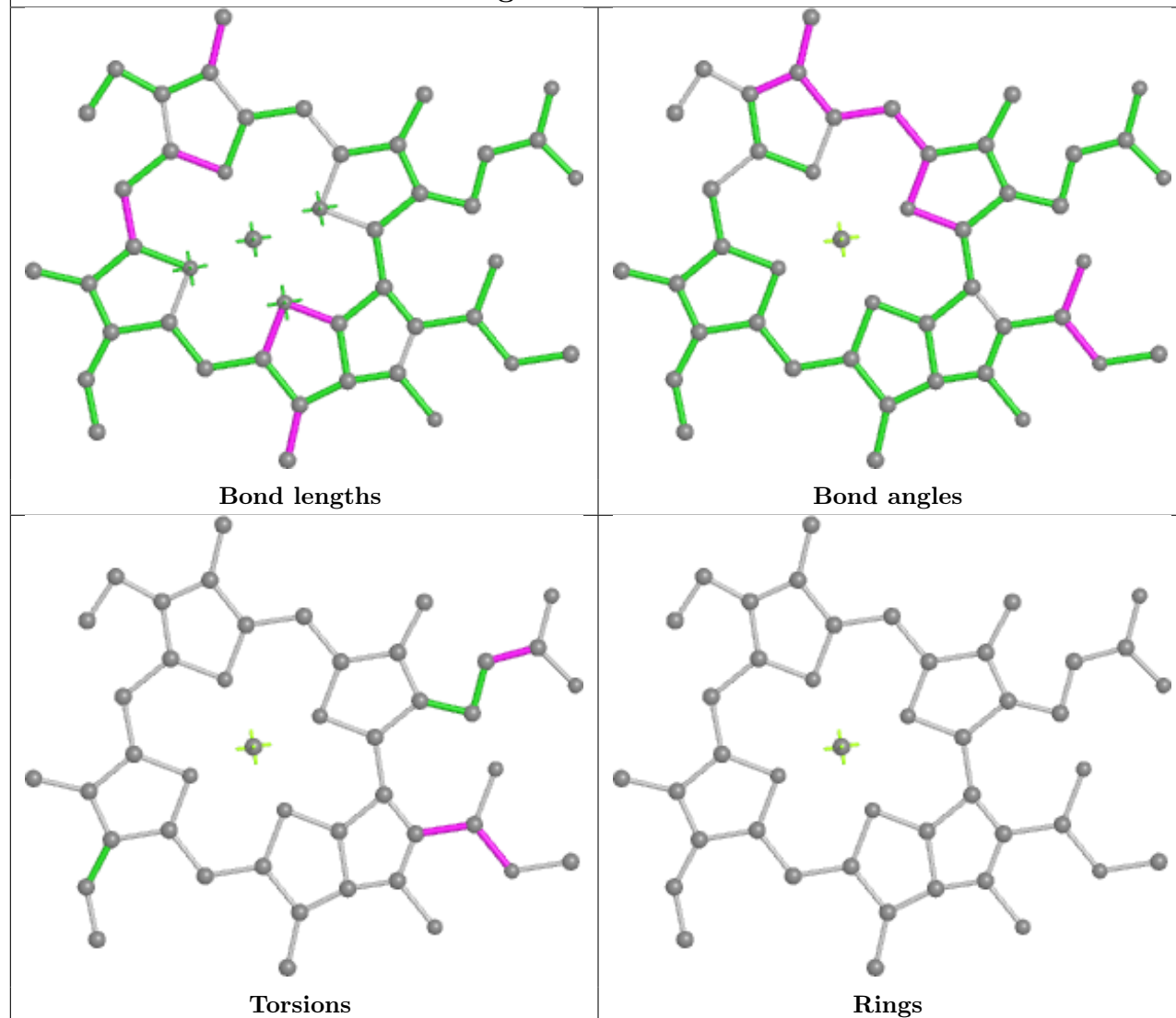
## Ligand CLA 1 203



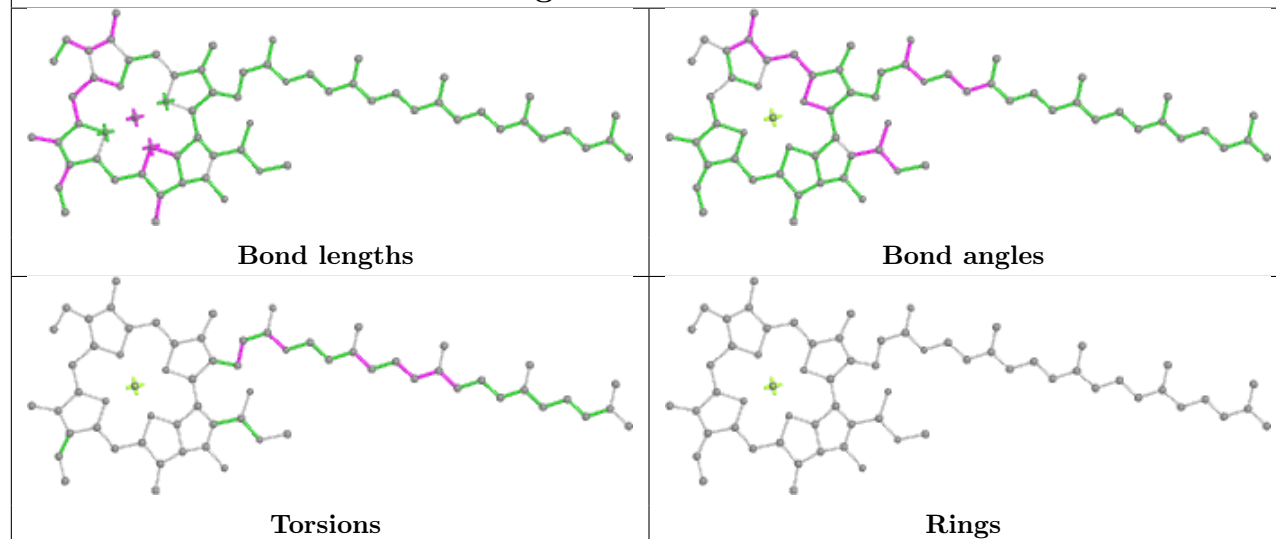
## Ligand A86 E 301



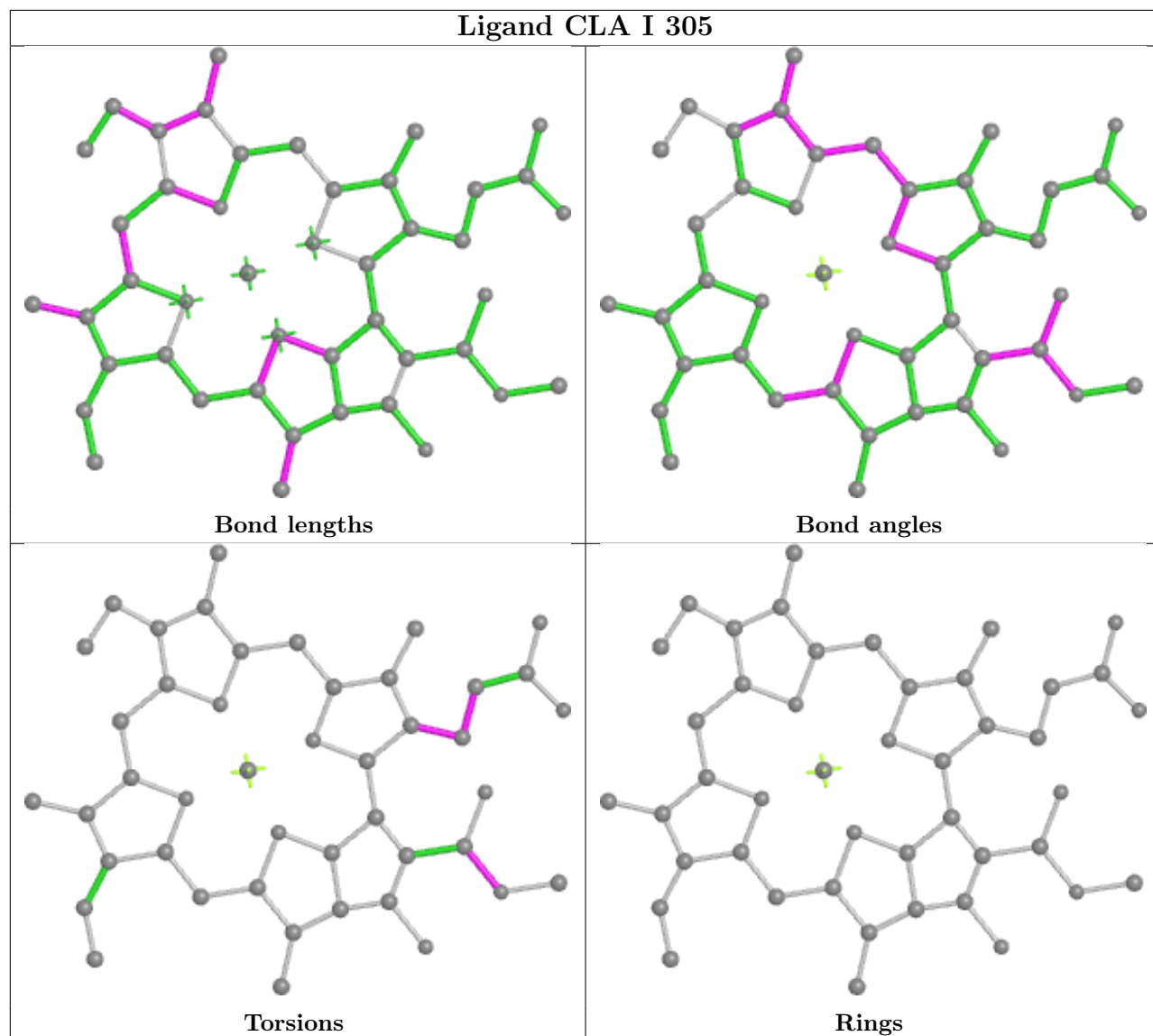
## Ligand CLA l 206



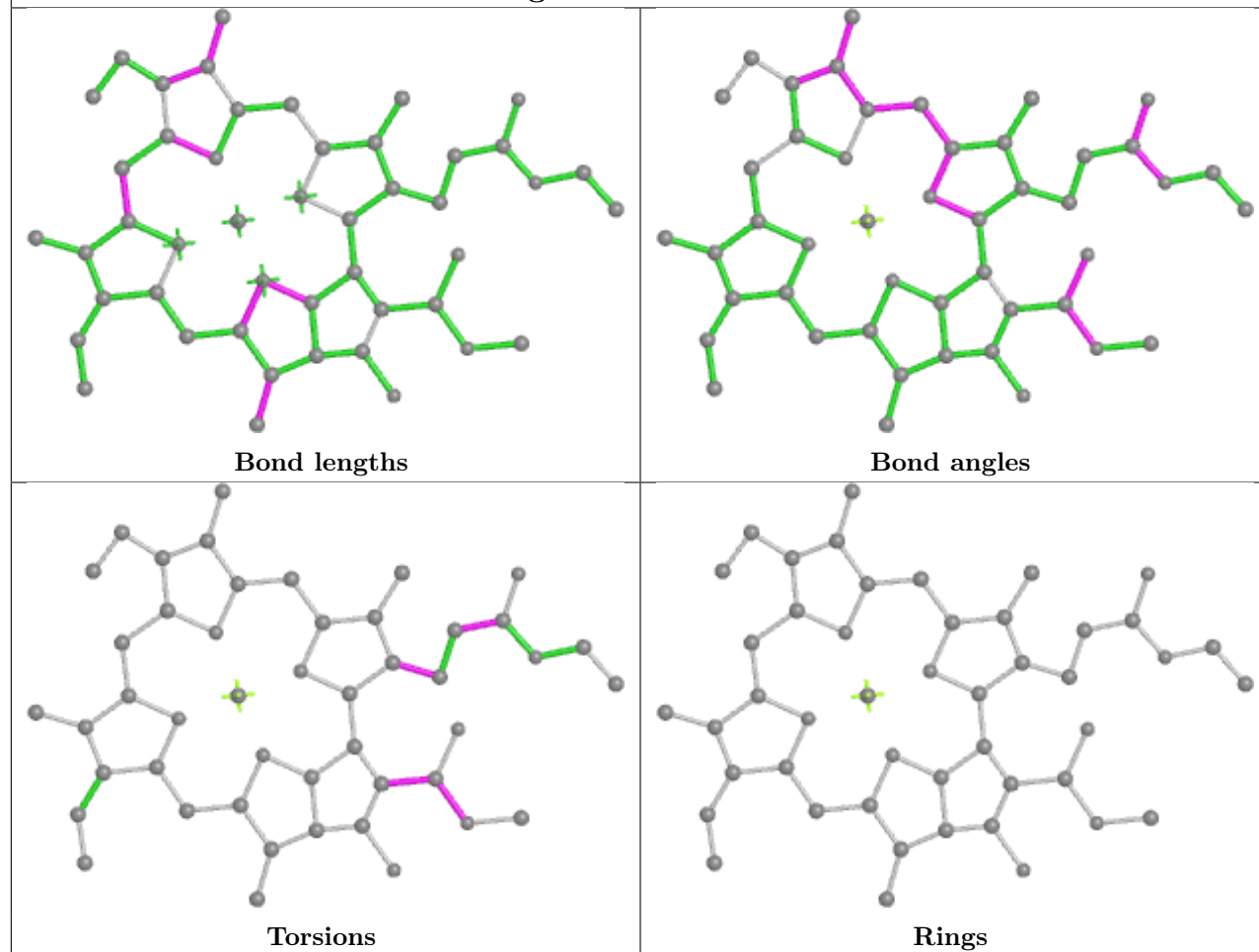
## Ligand CLA b 801



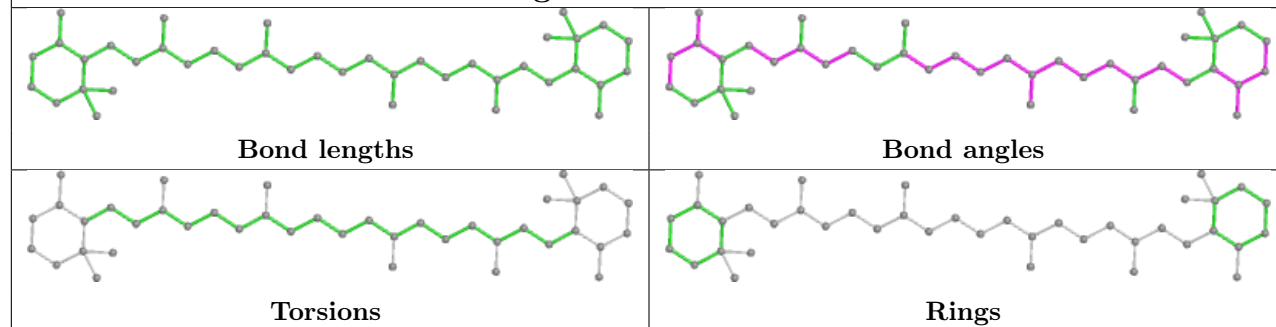
## Ligand CLA I 305



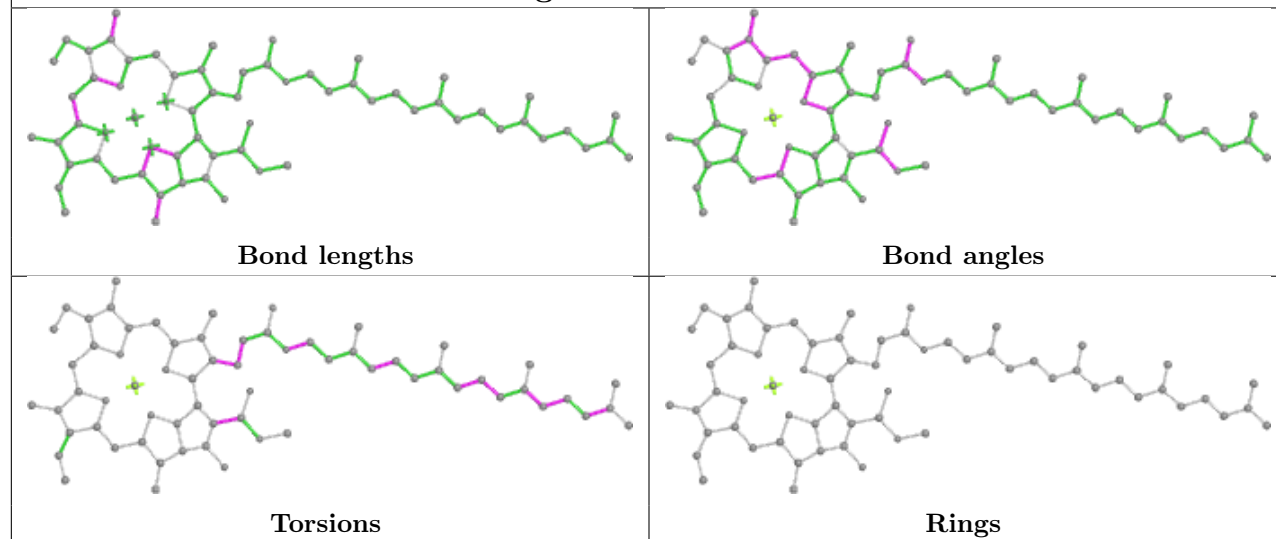
## Ligand CLA b 828



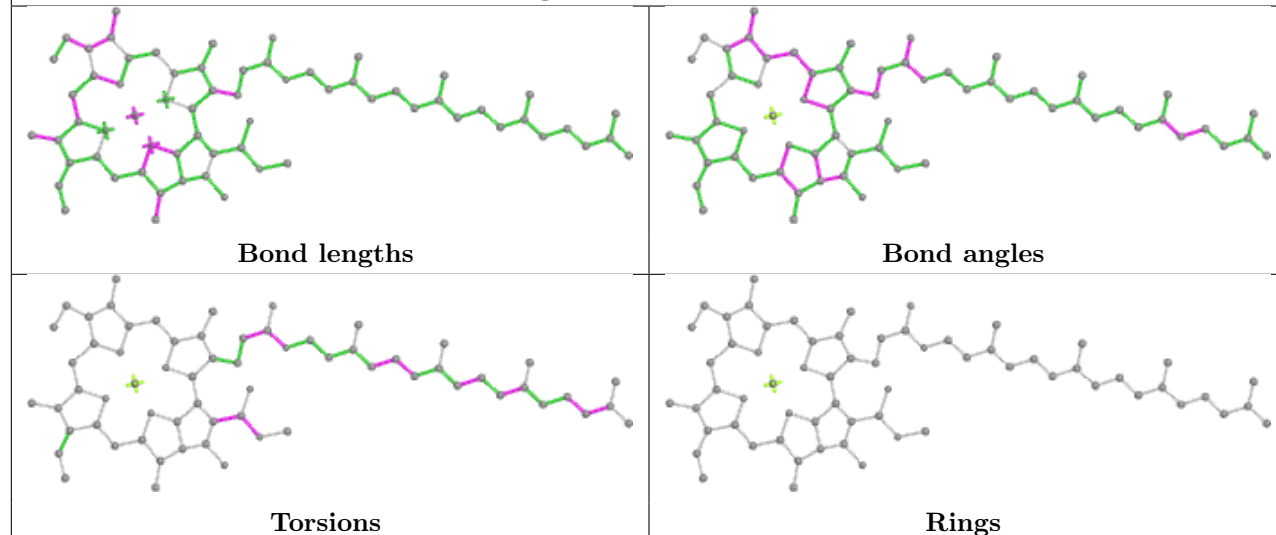
## Ligand BCR b 833



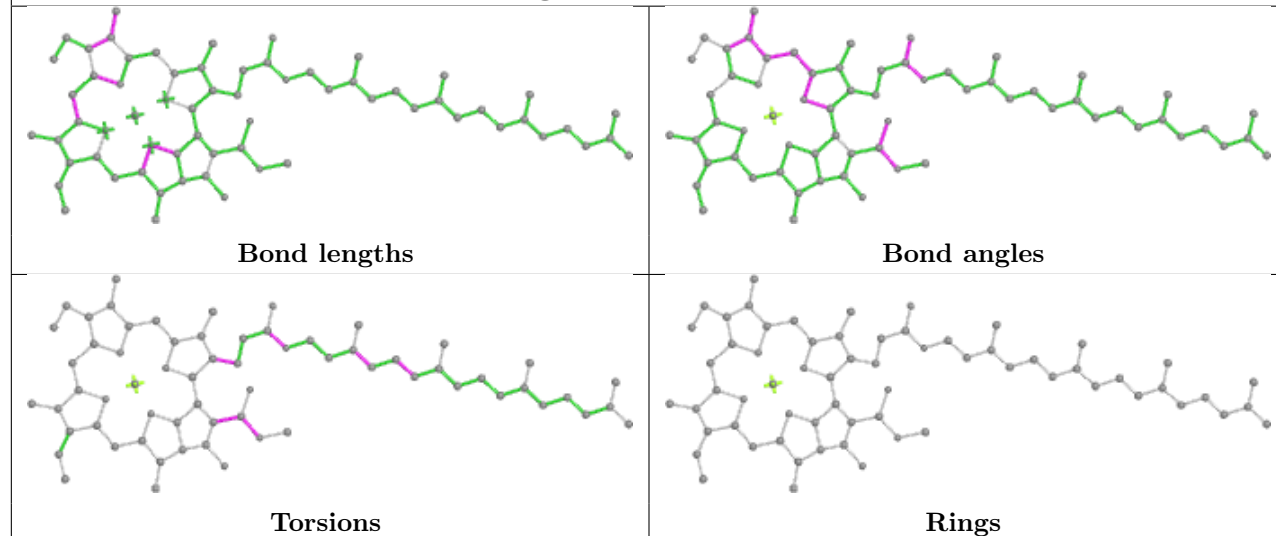
## Ligand CLA b 846



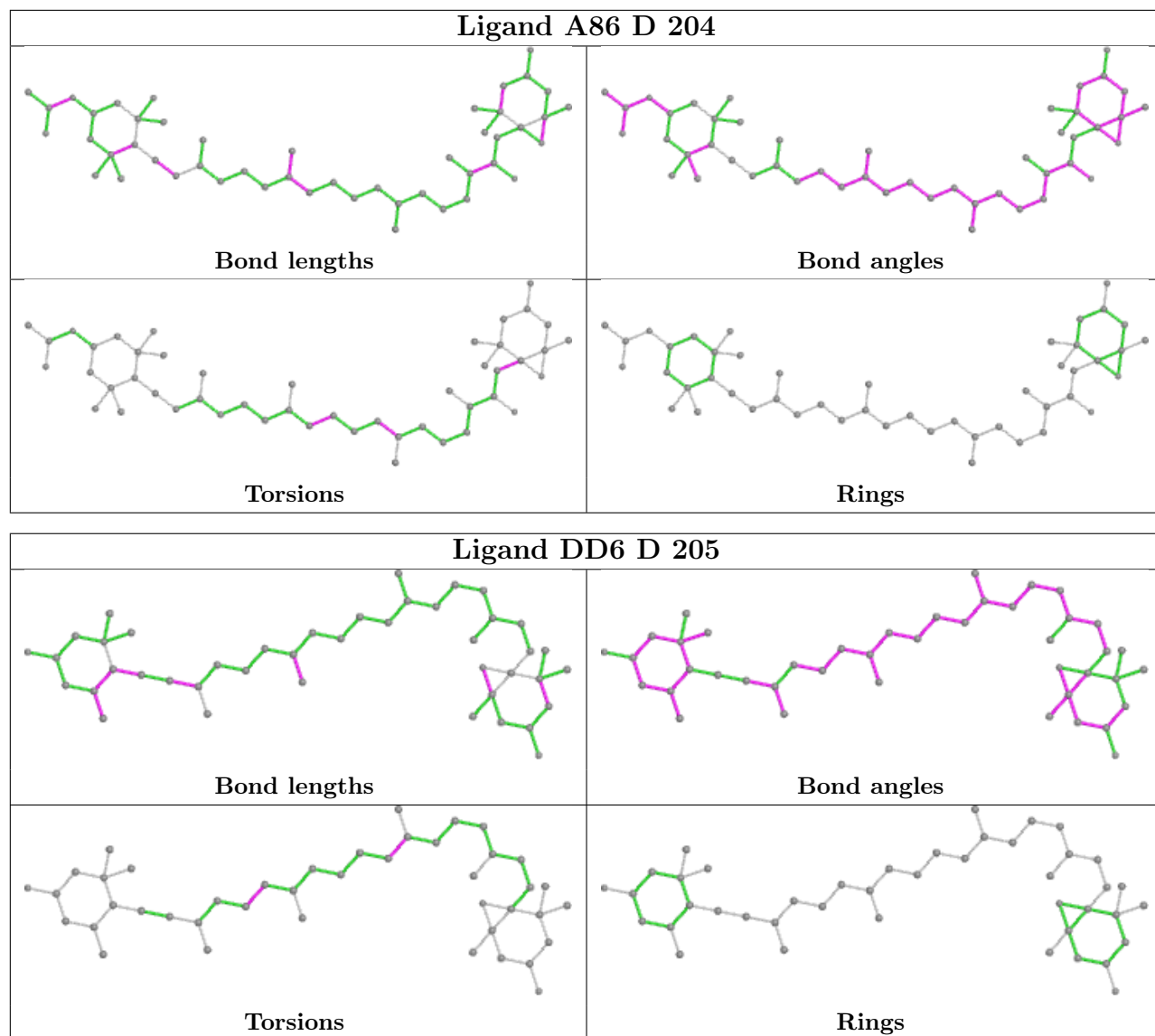
## Ligand CLA a 803



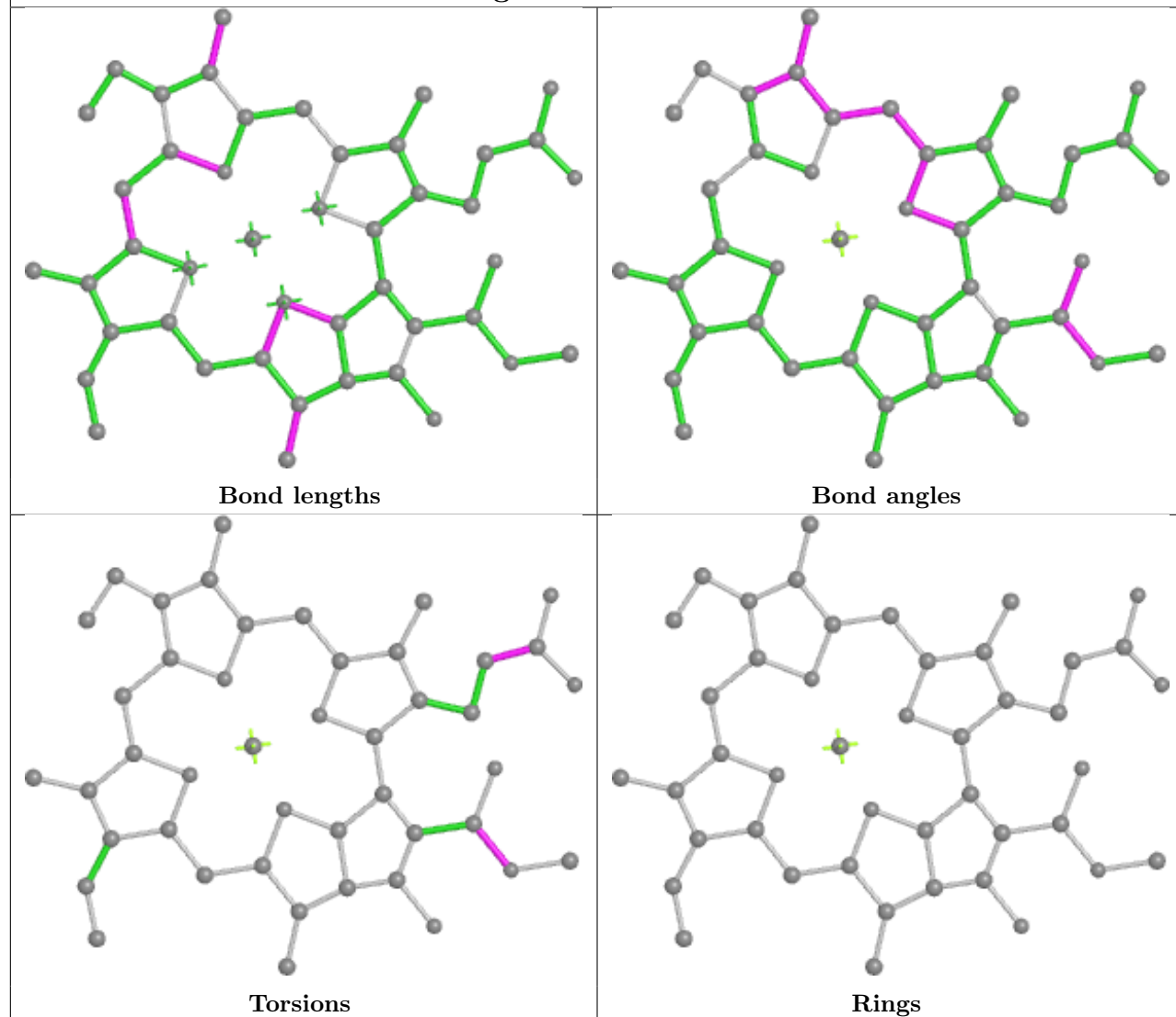
## Ligand CLA a 823



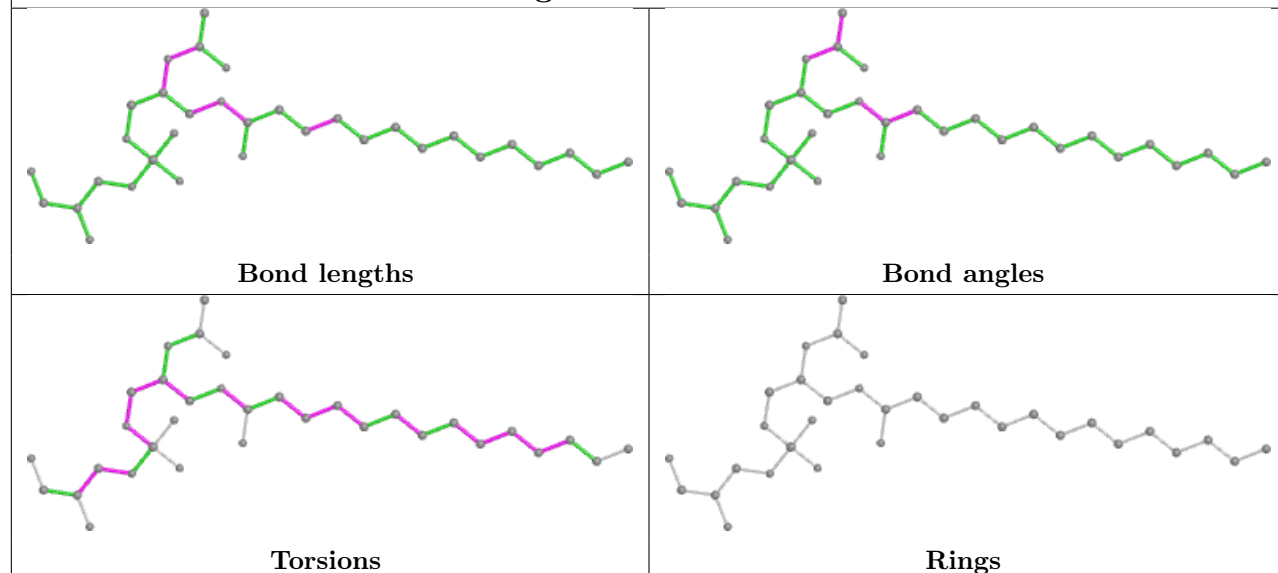


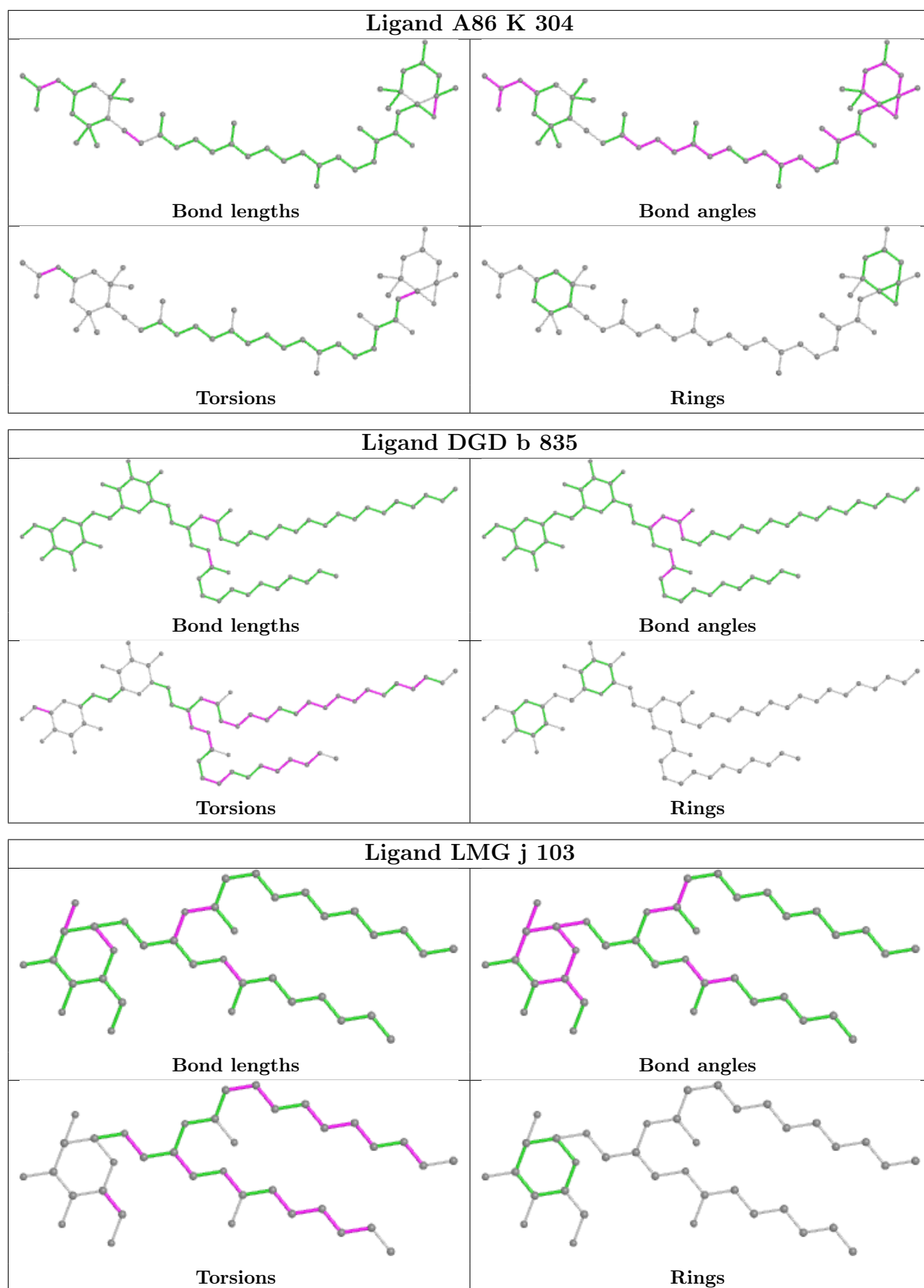


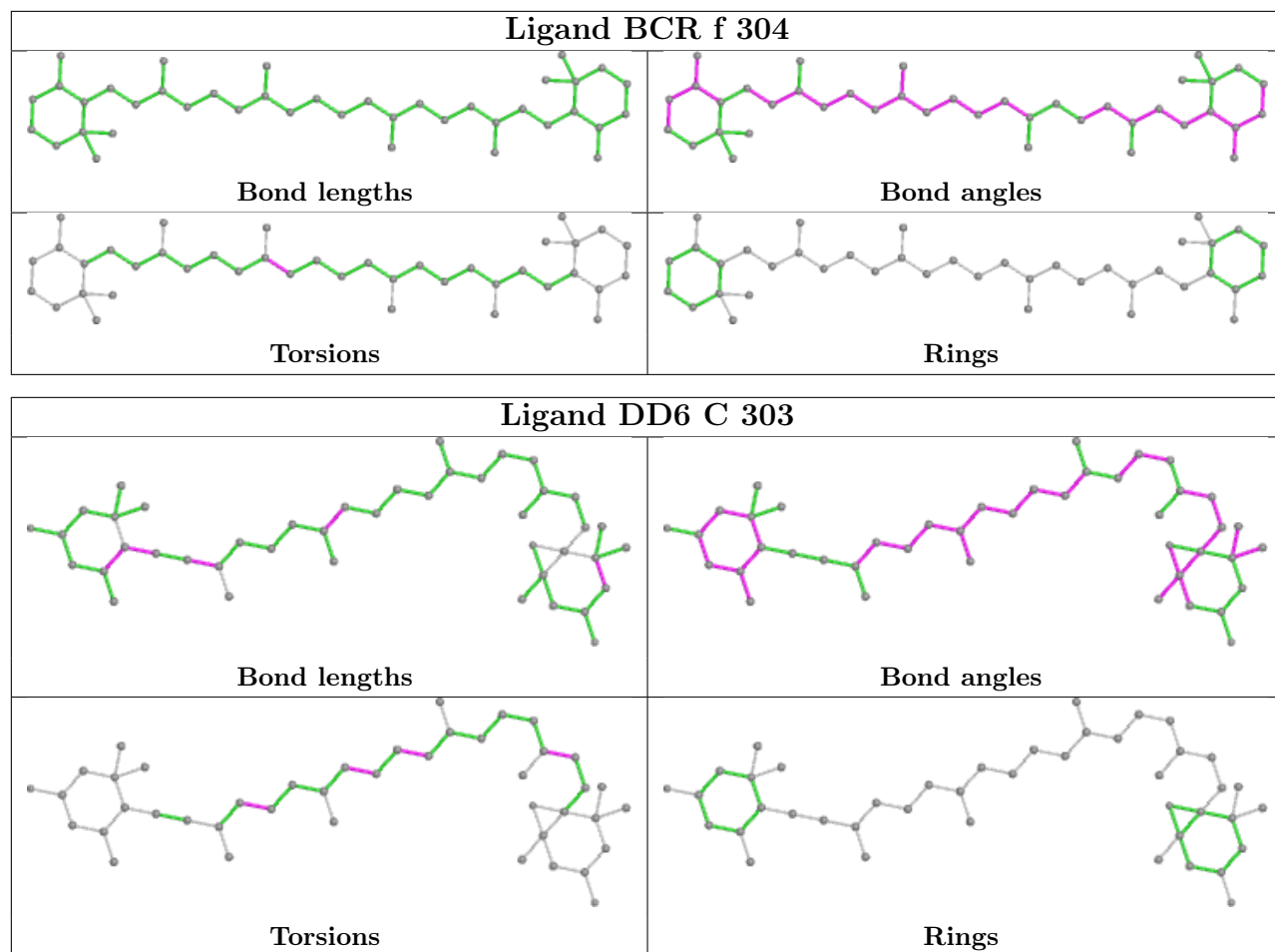
## Ligand CLA a 814



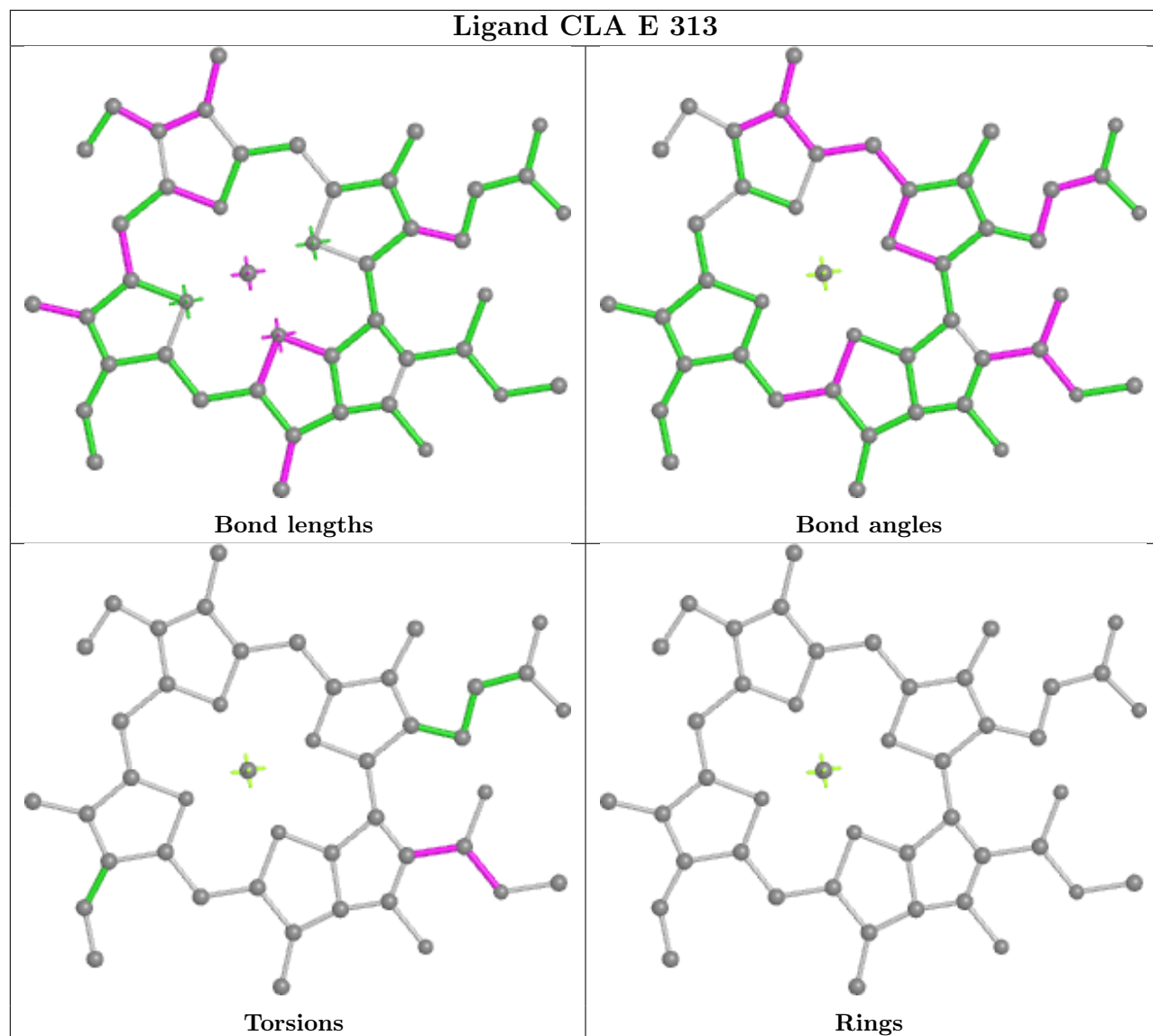
## Ligand LHG a 837



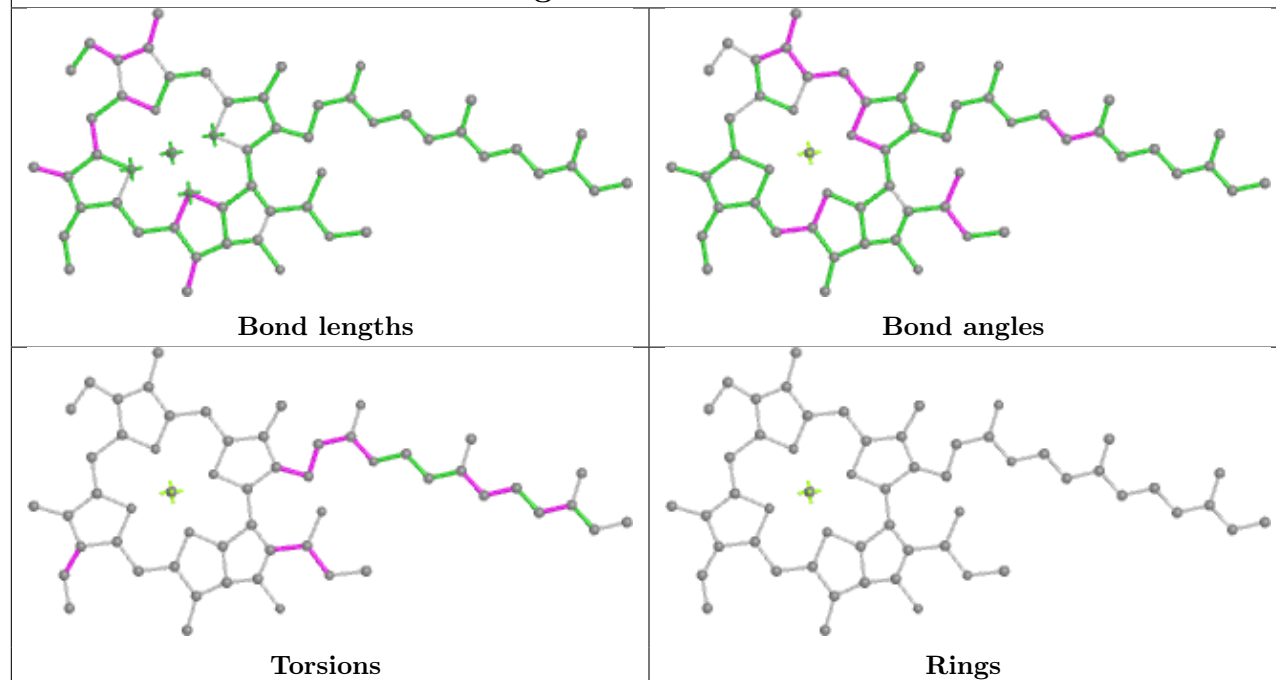




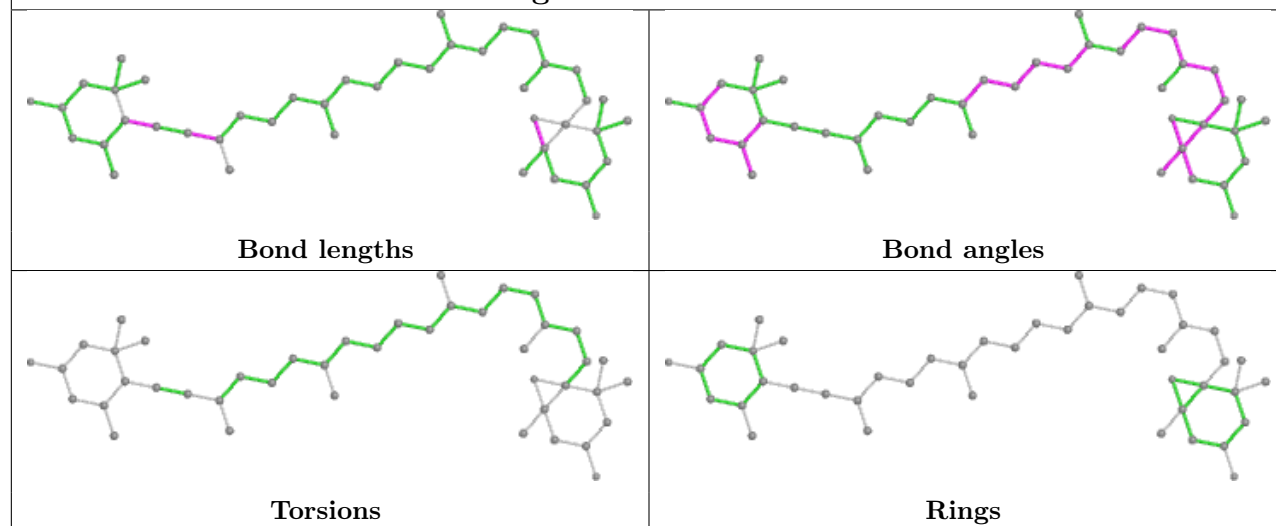
## Ligand CLA E 313

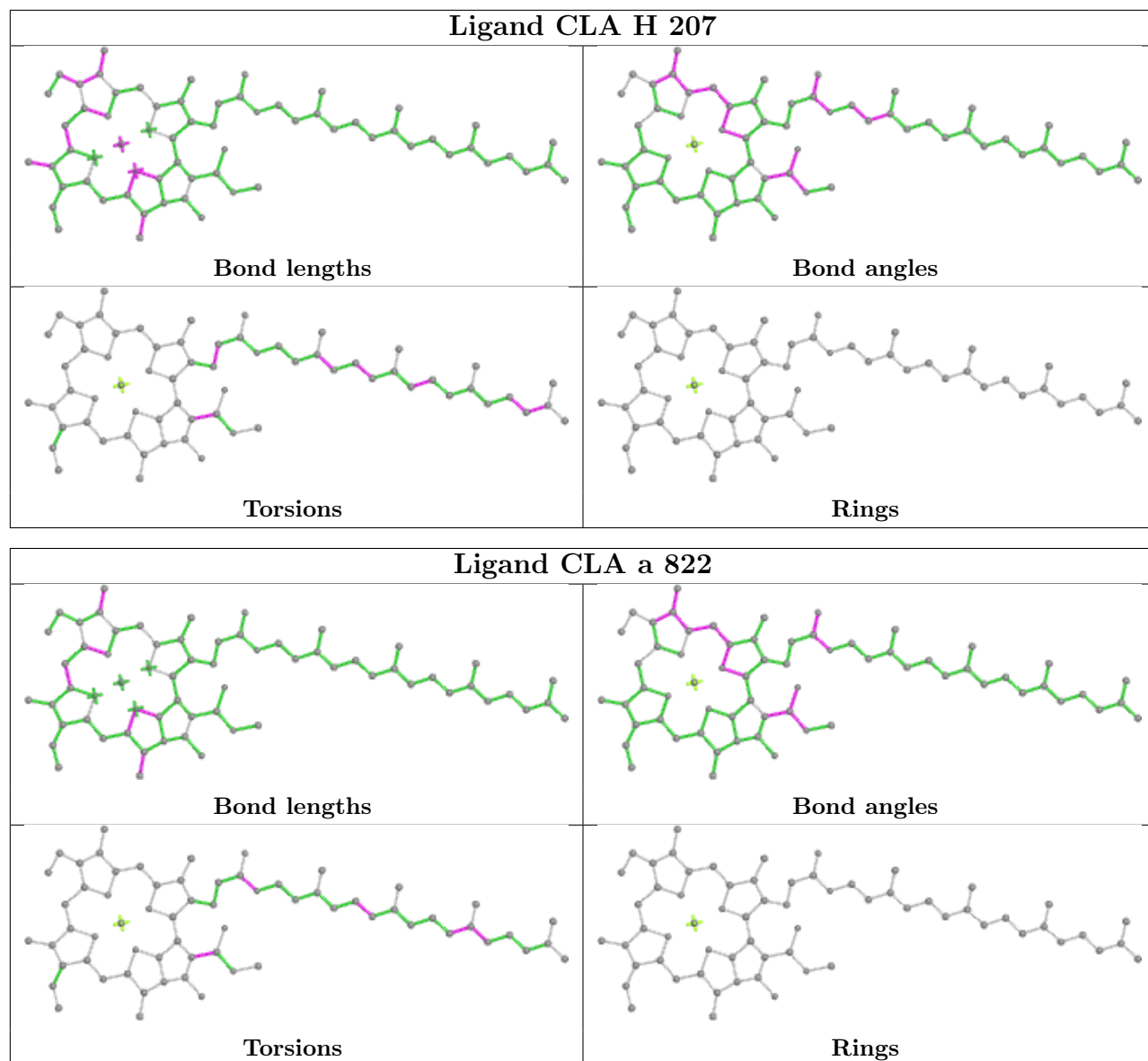


## Ligand CLA L 316

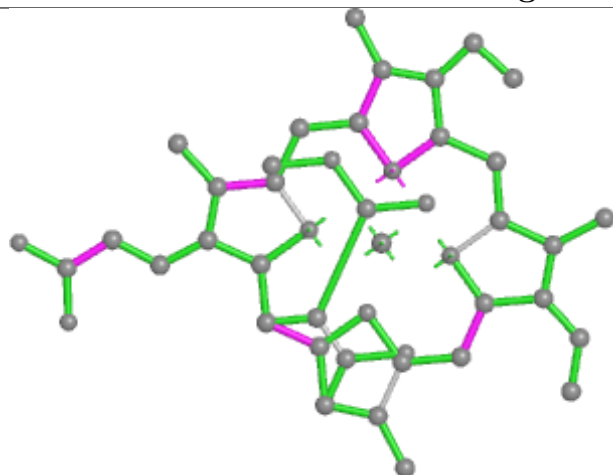


## Ligand DD6 G 304

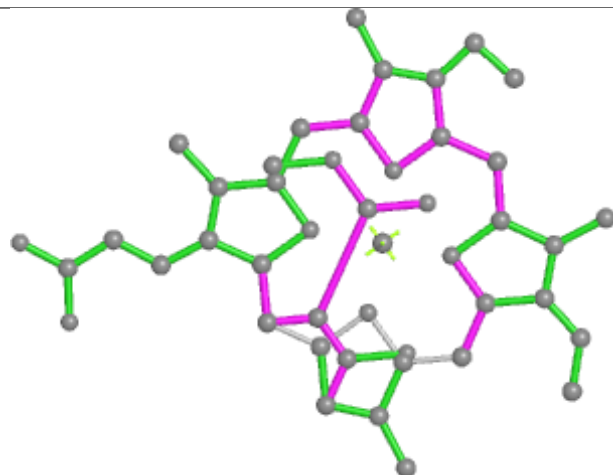




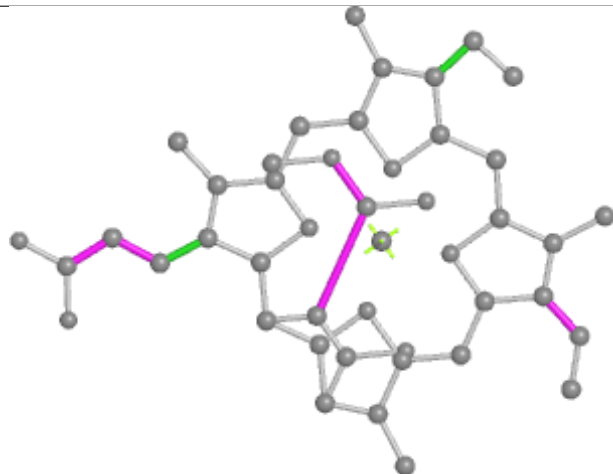
## Ligand KC1 L 322



Bond lengths



Bond angles



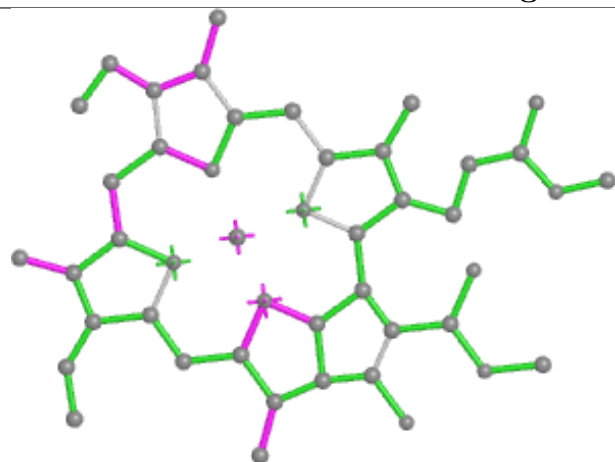
Torsions



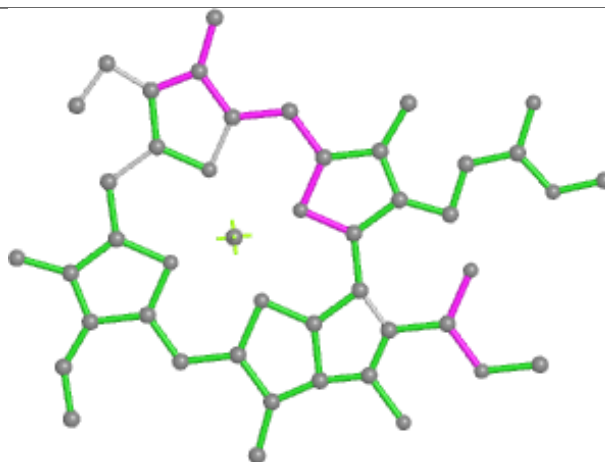
Rings



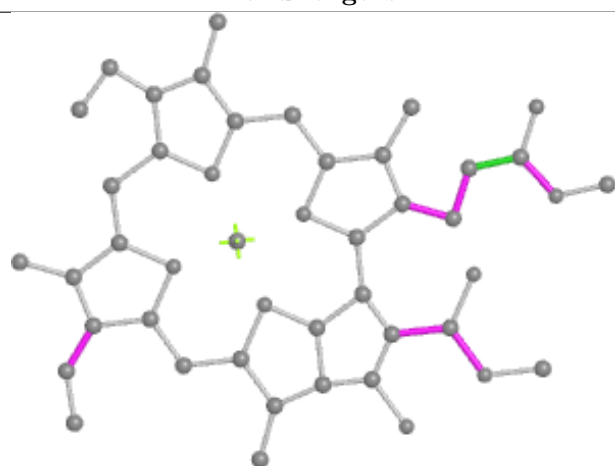
## Ligand CLA J 313



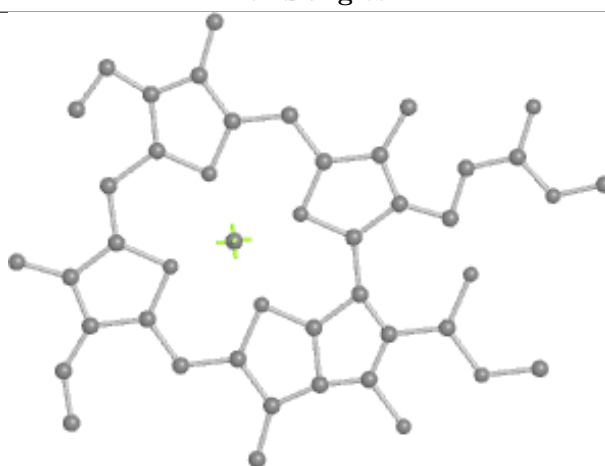
Bond lengths



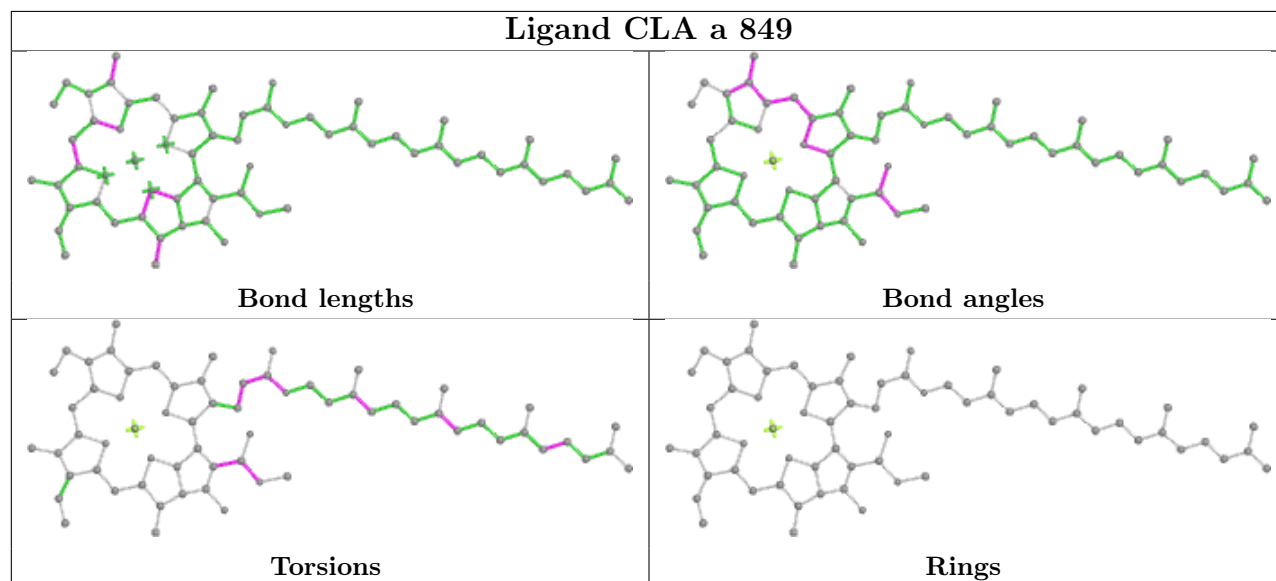
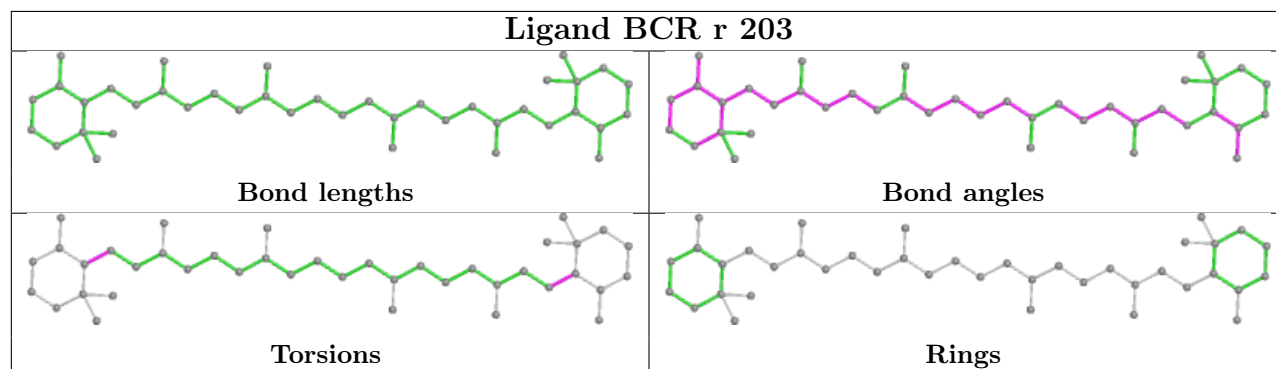
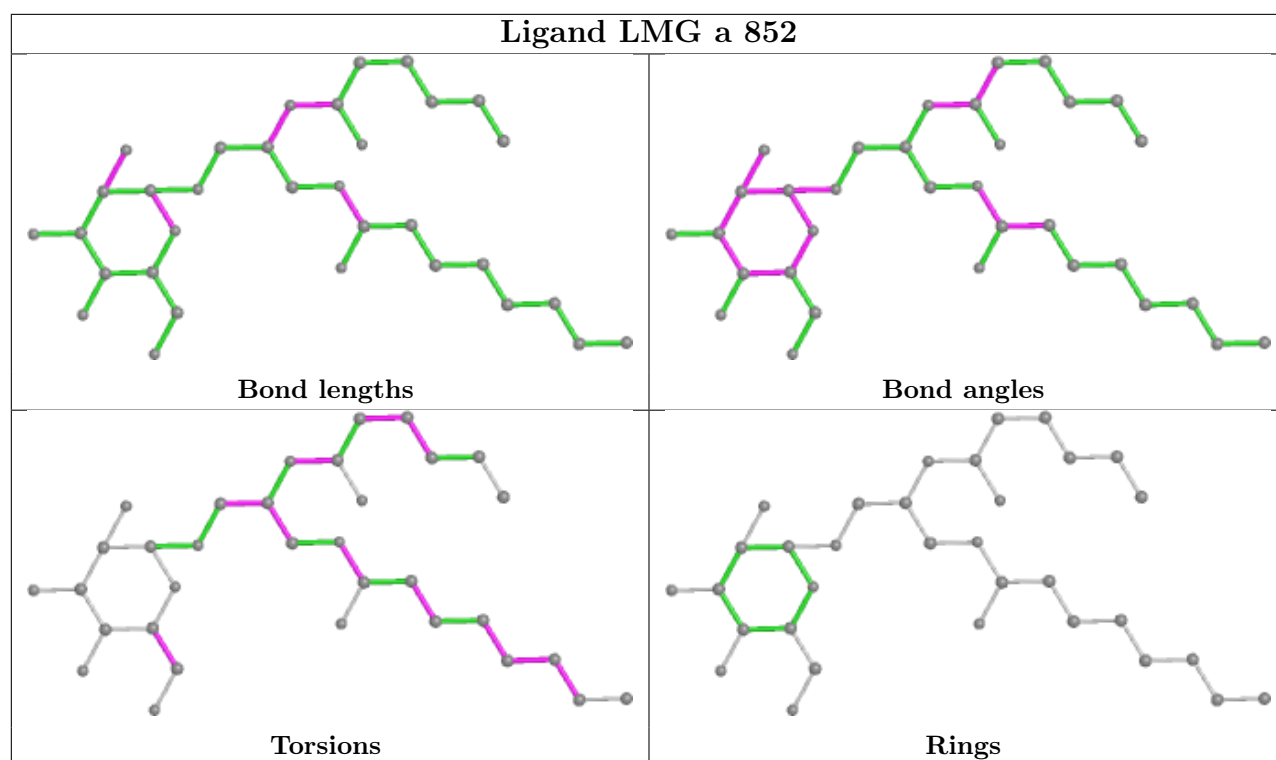
Bond angles



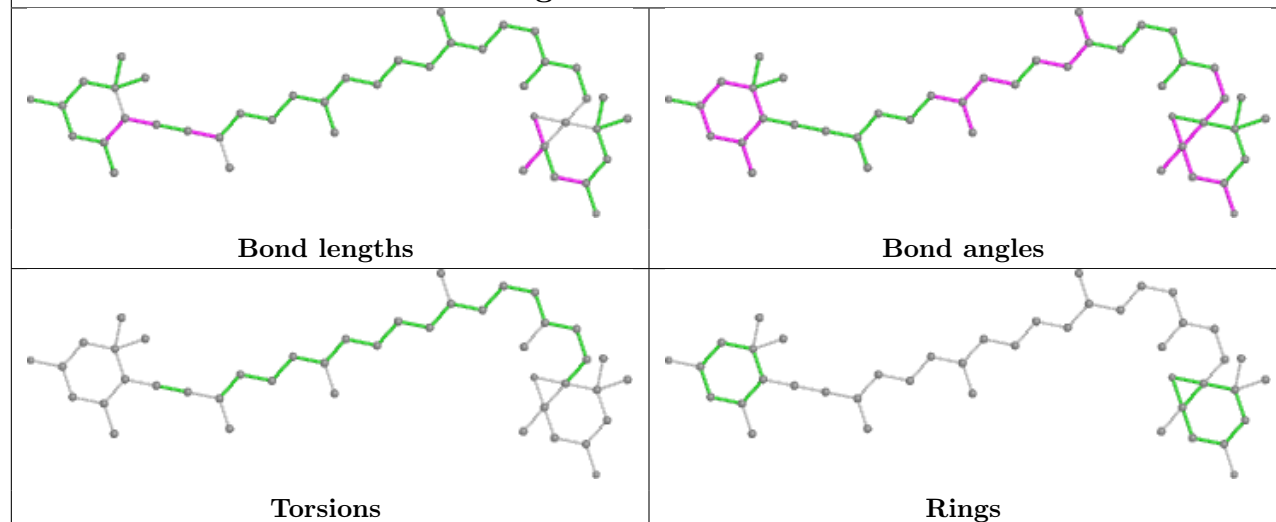
Torsions



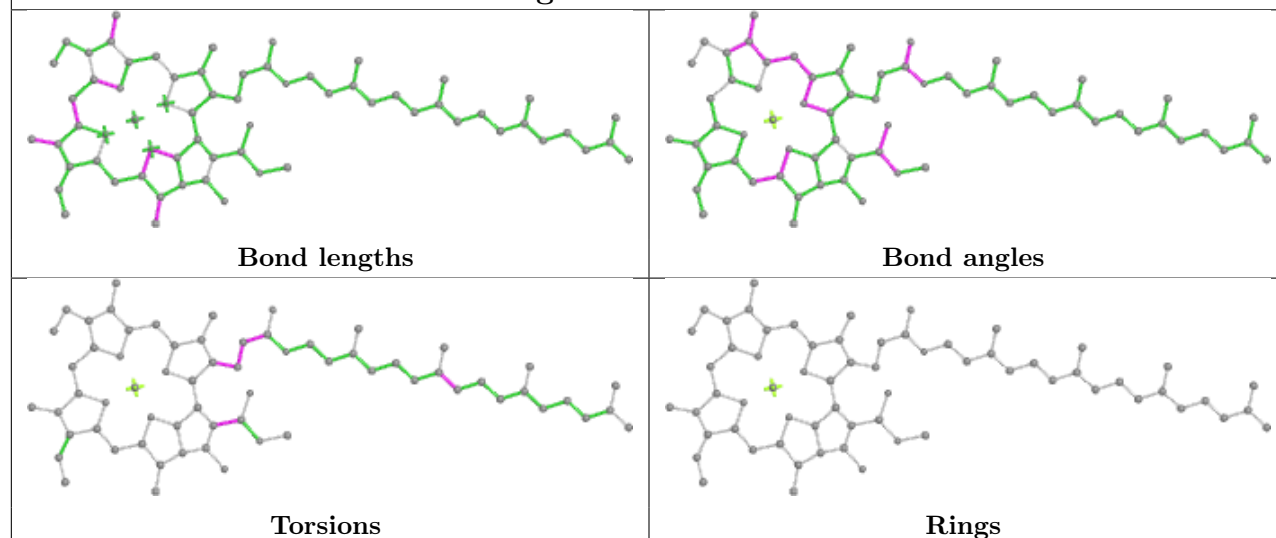
Rings



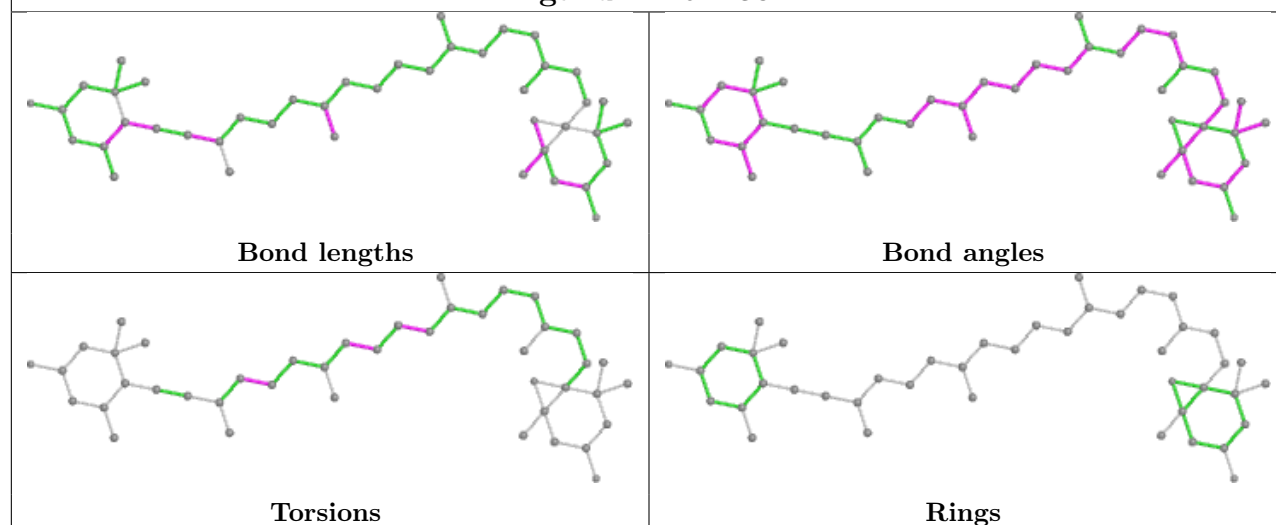
## Ligand DD6 L 303



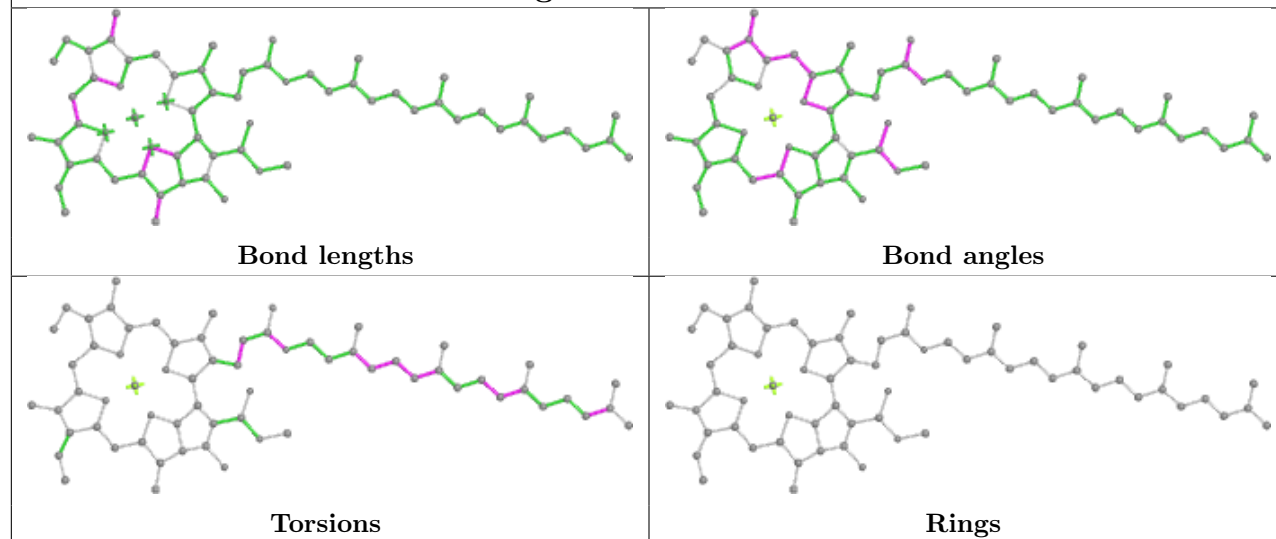
## Ligand CLA a 816



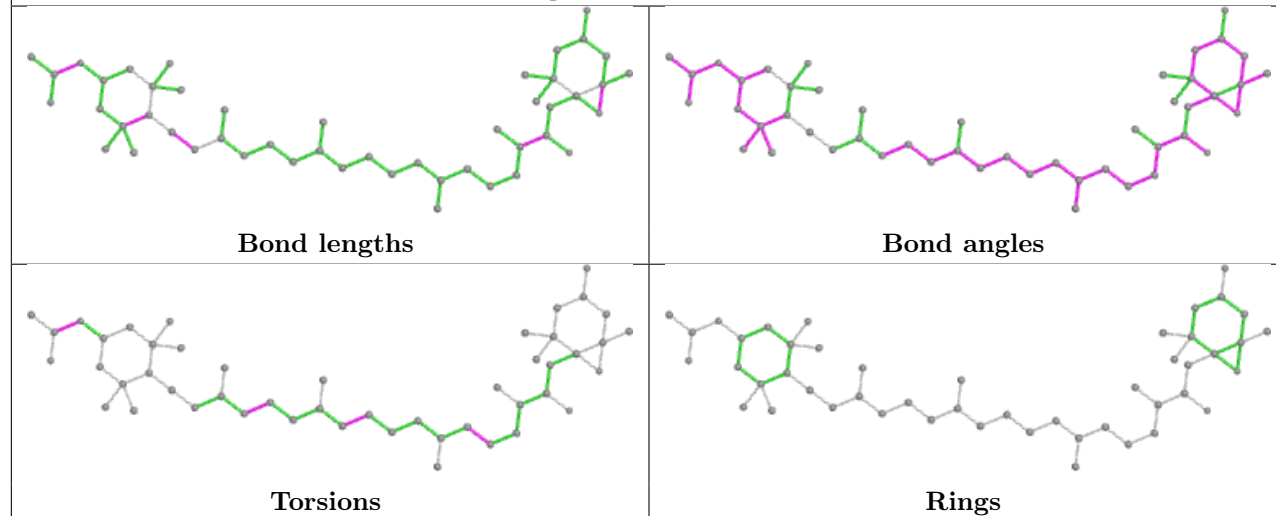
## Ligand DD6 I 304



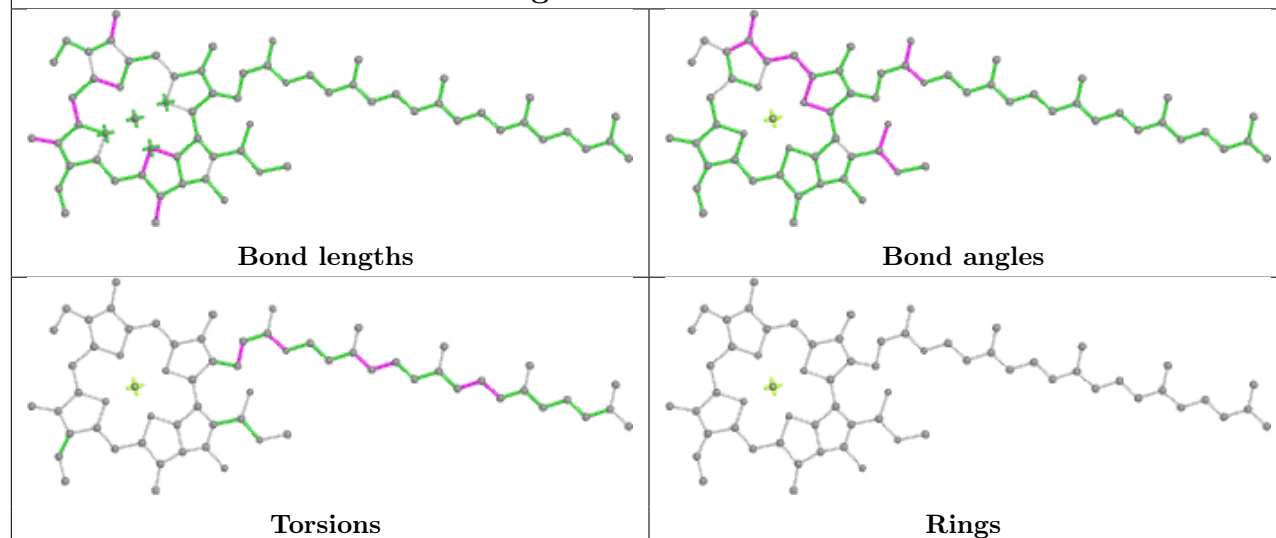
## Ligand CLA b 843

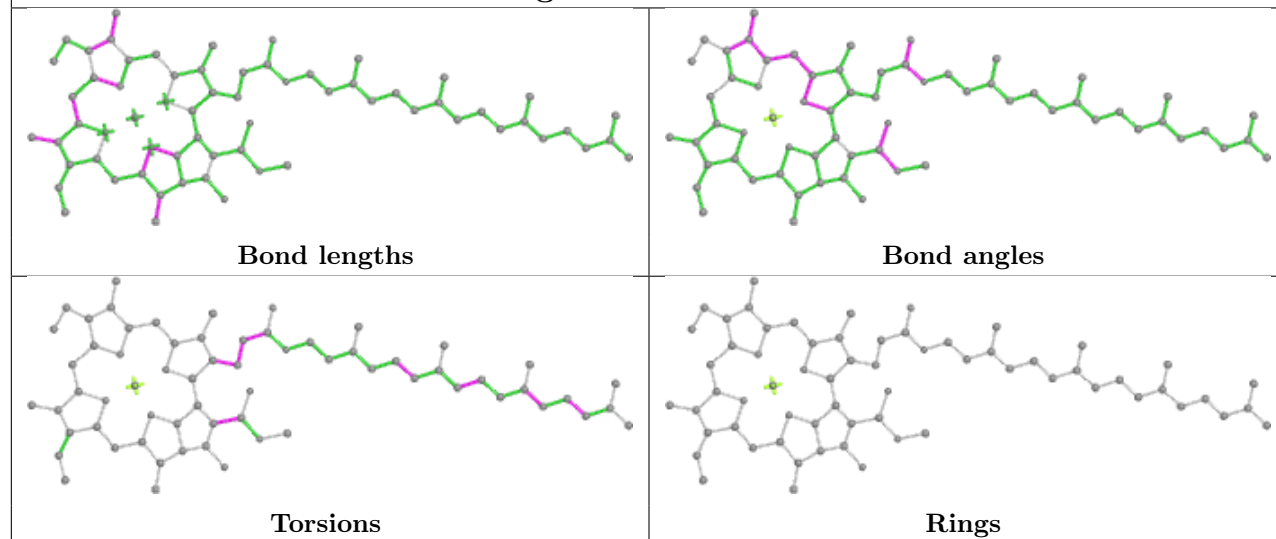
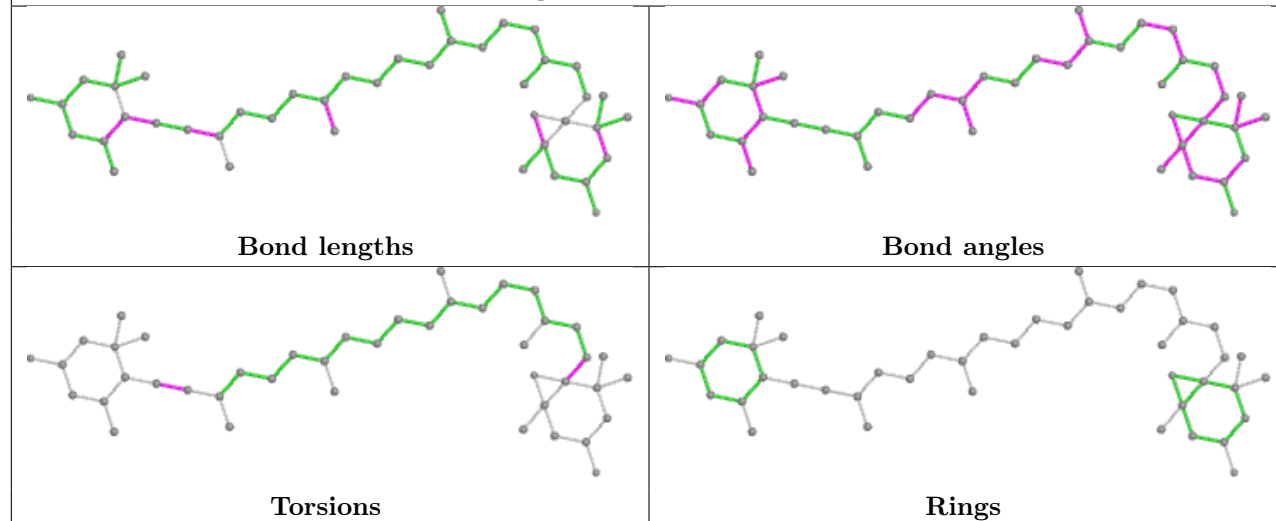


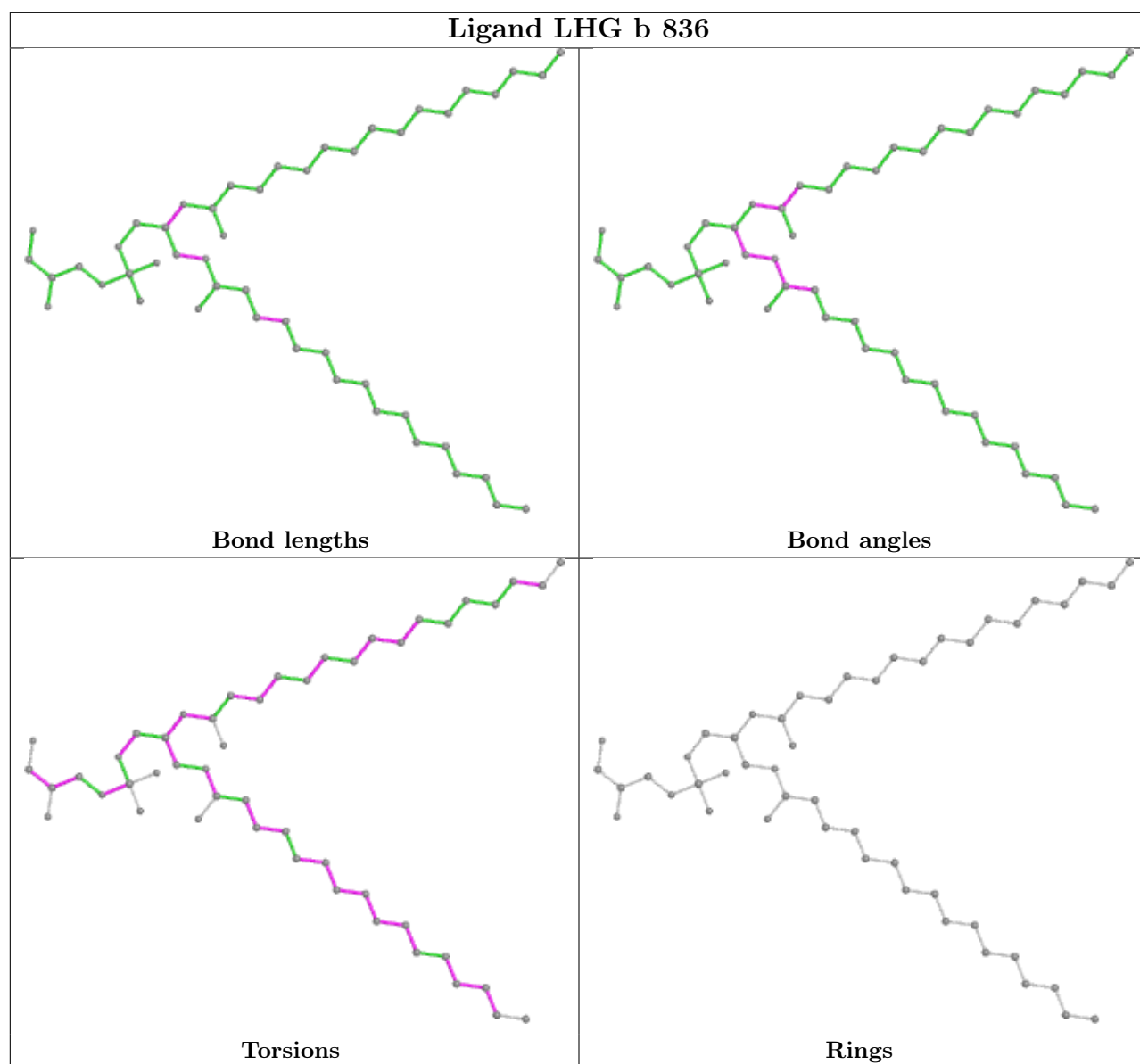
## Ligand A86 I 303



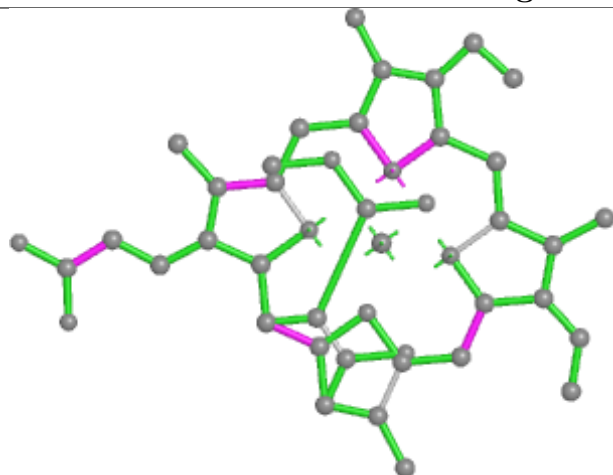
## Ligand CLA D 213



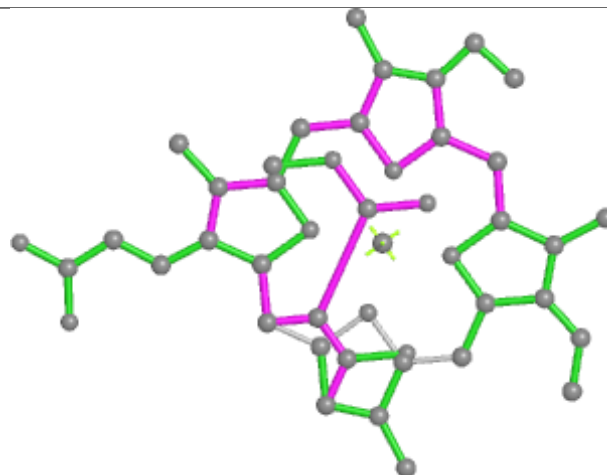
**Ligand CLA a 810****Ligand DD6 A 202**



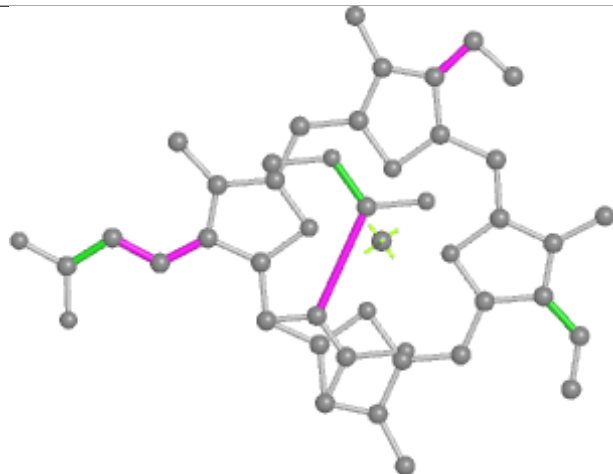
## Ligand KC1 C 313



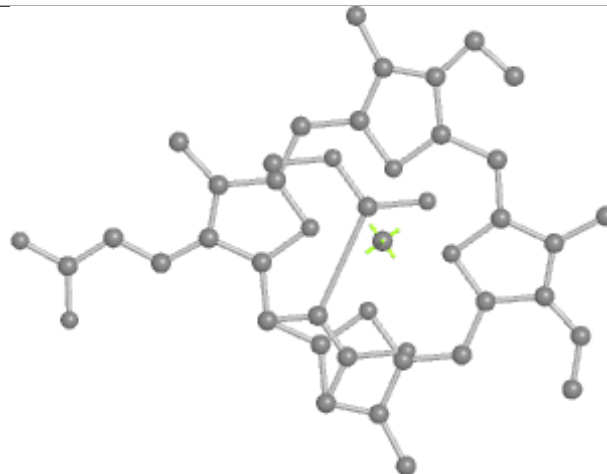
Bond lengths



Bond angles

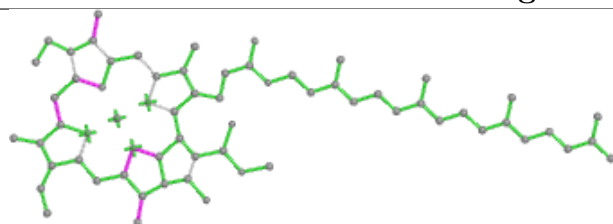


Torsions

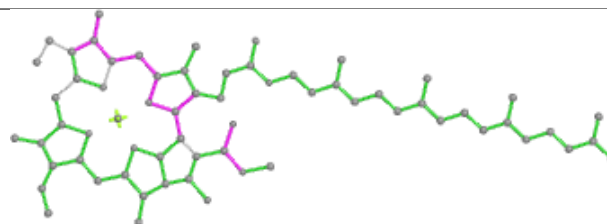


Rings

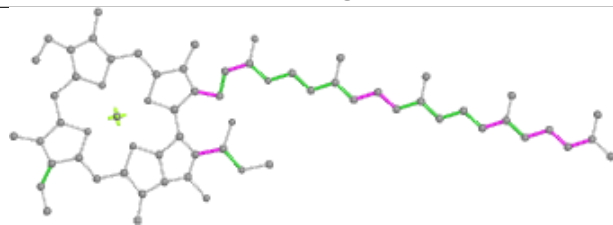
## Ligand CLA a 845



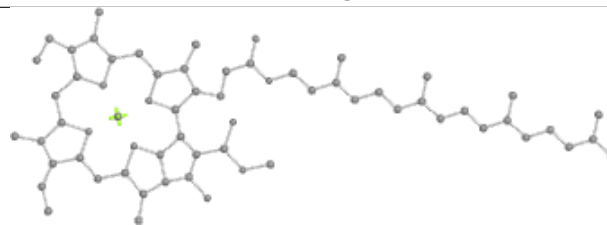
Bond lengths



Bond angles

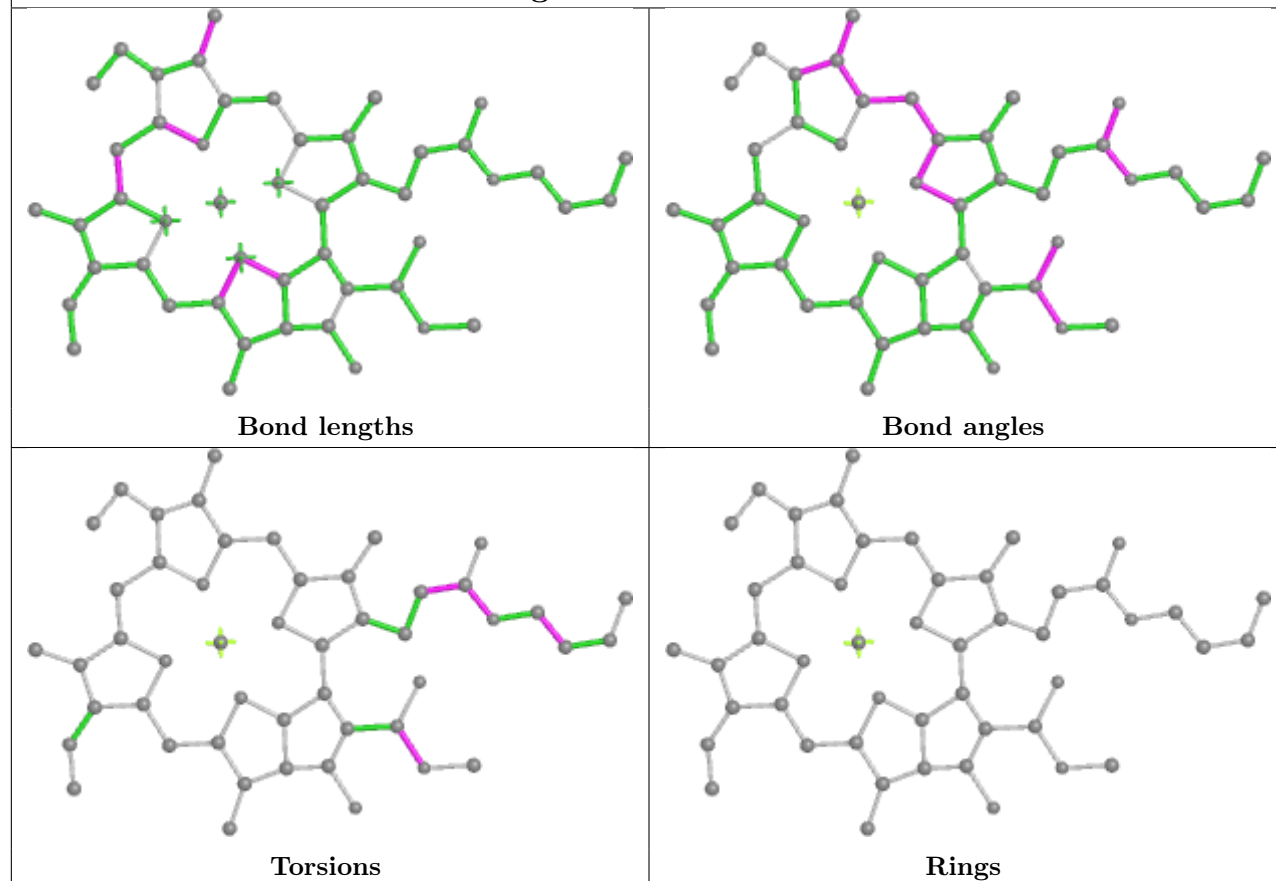


Torsions

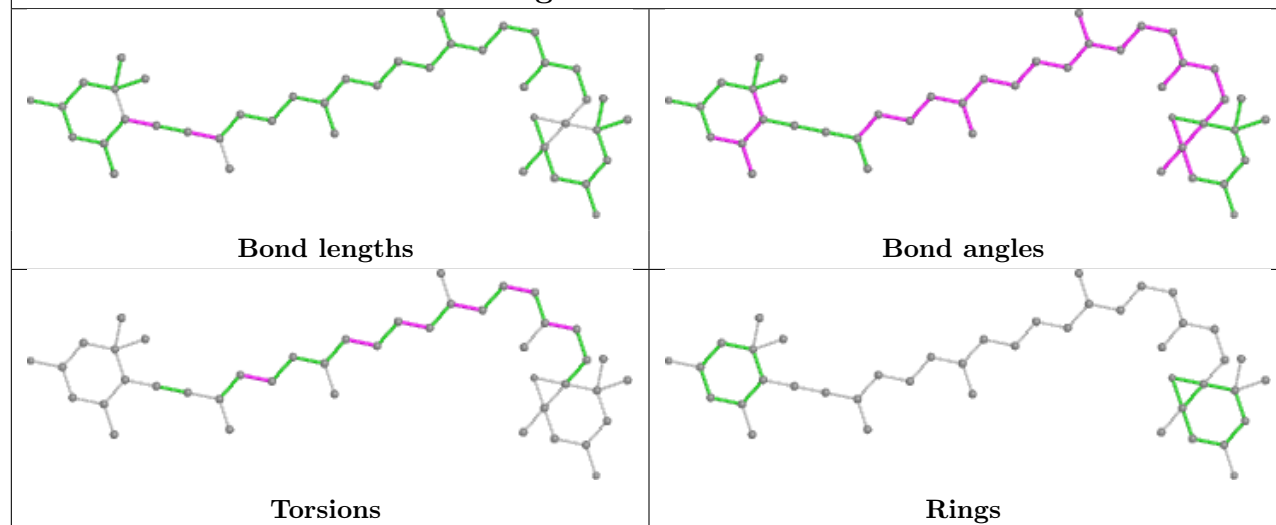


Rings

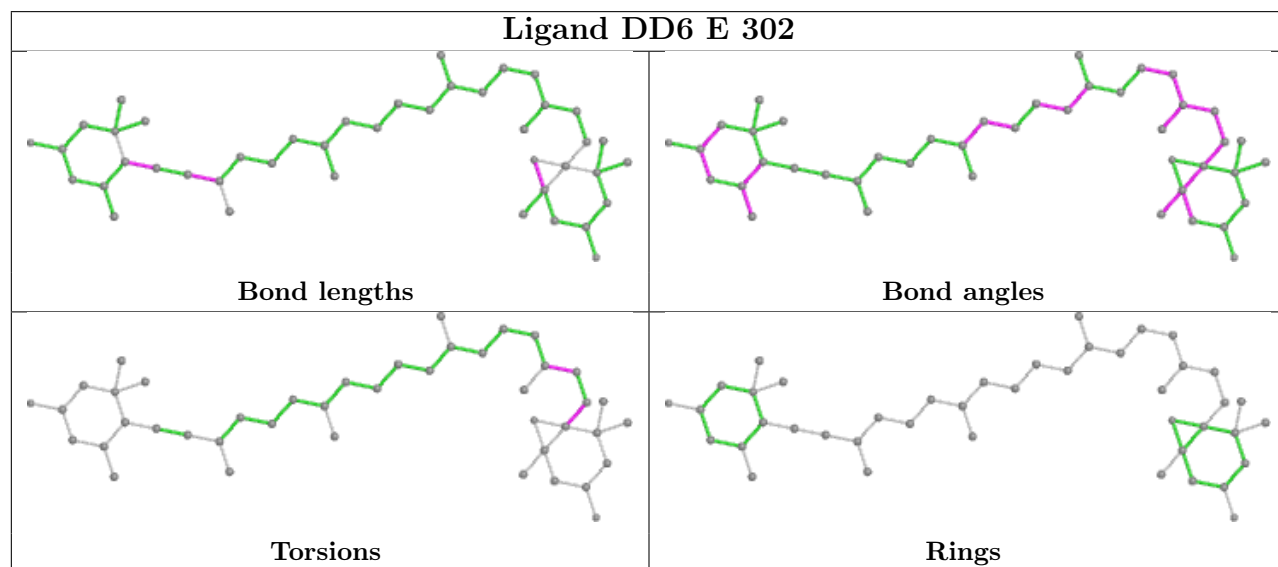
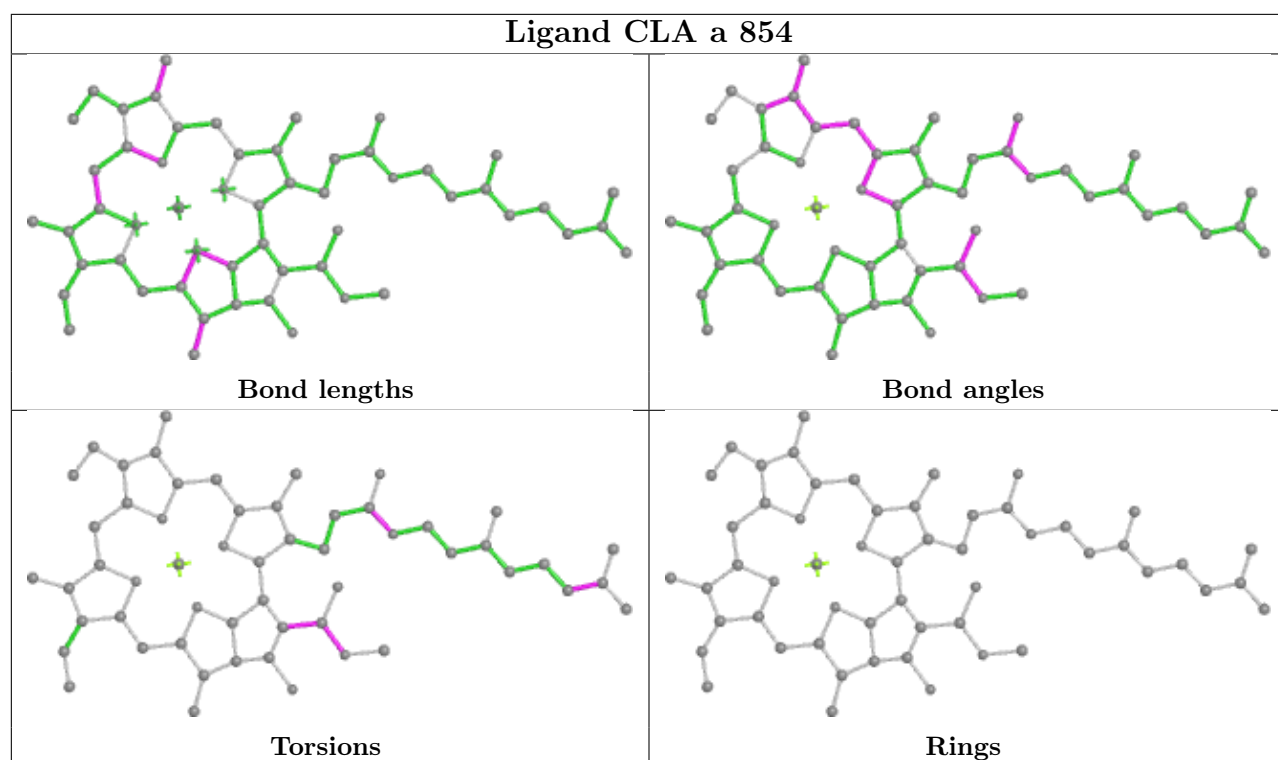
## Ligand CLA G 317



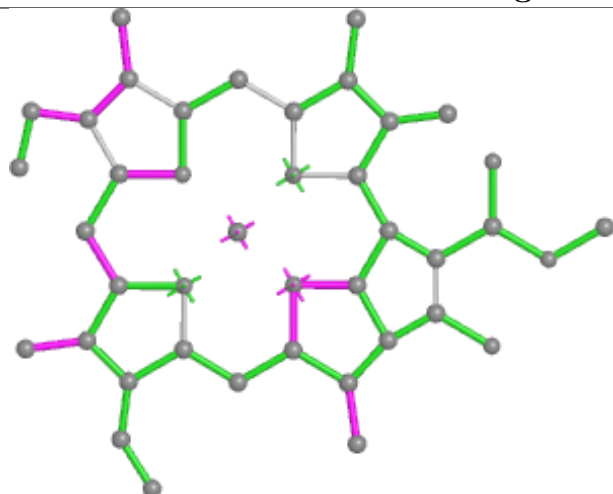
## Ligand DD6 L 301



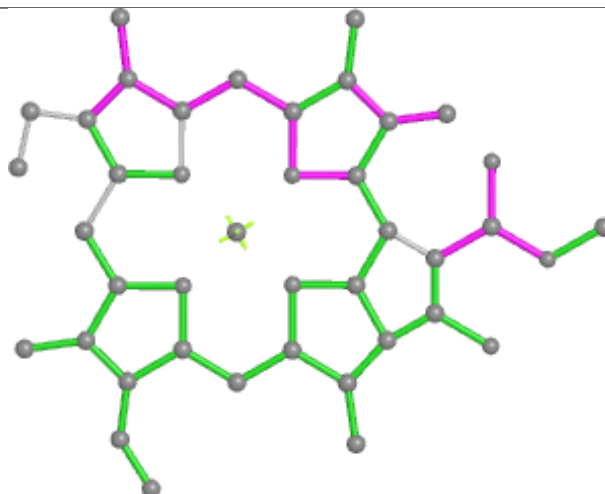




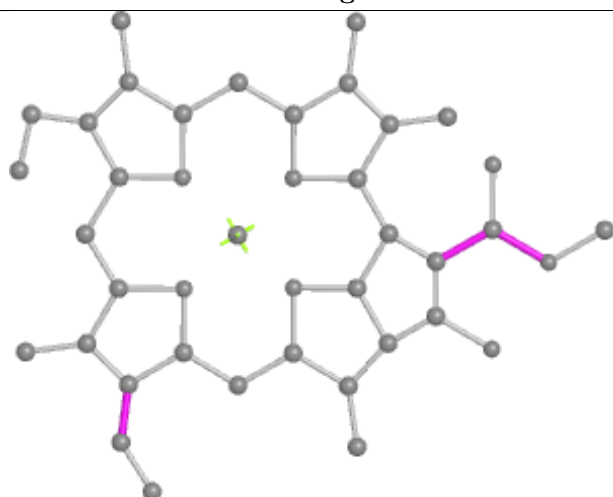
## Ligand CLA C 314



Bond lengths



Bond angles

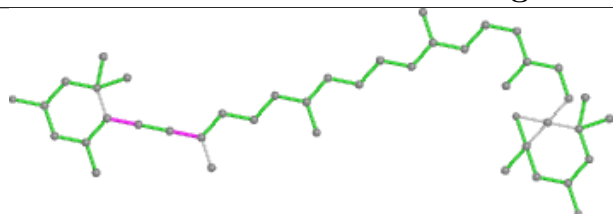


Torsions

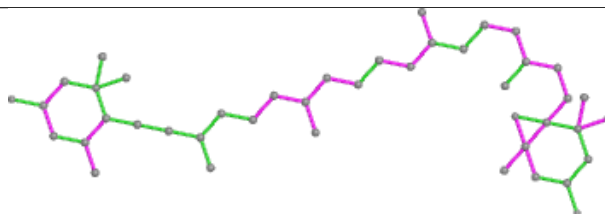


Rings

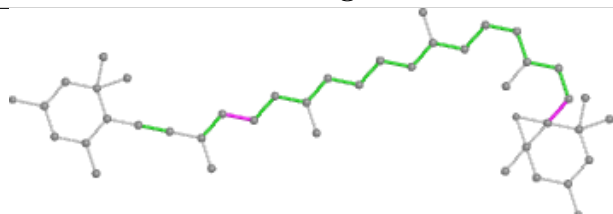
## Ligand DD6 M 301



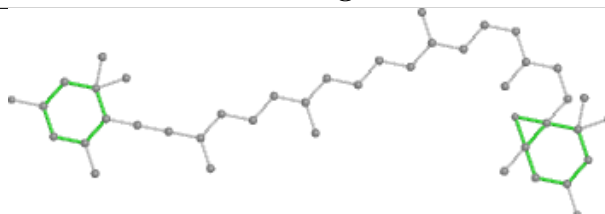
Bond lengths



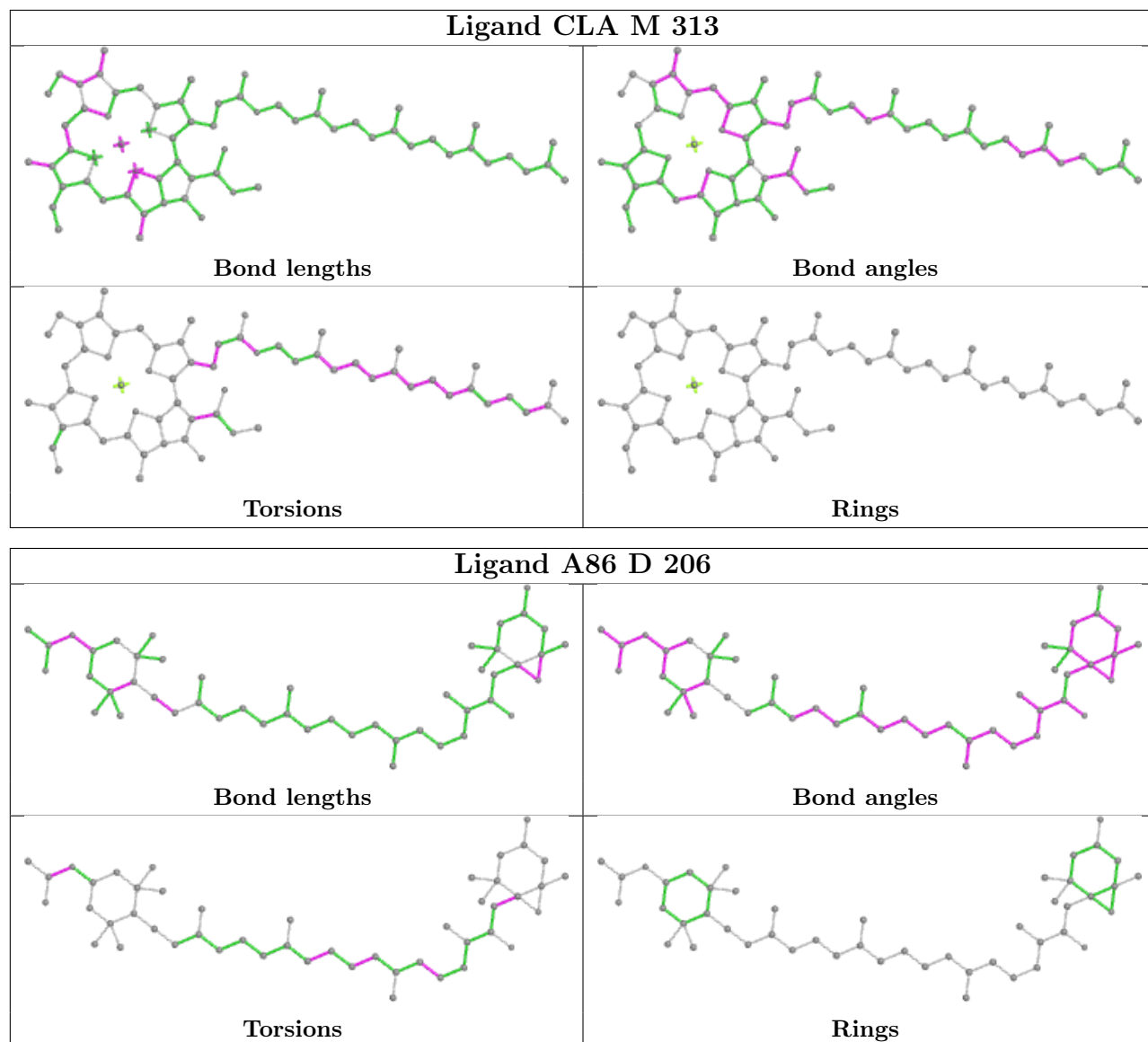
Bond angles

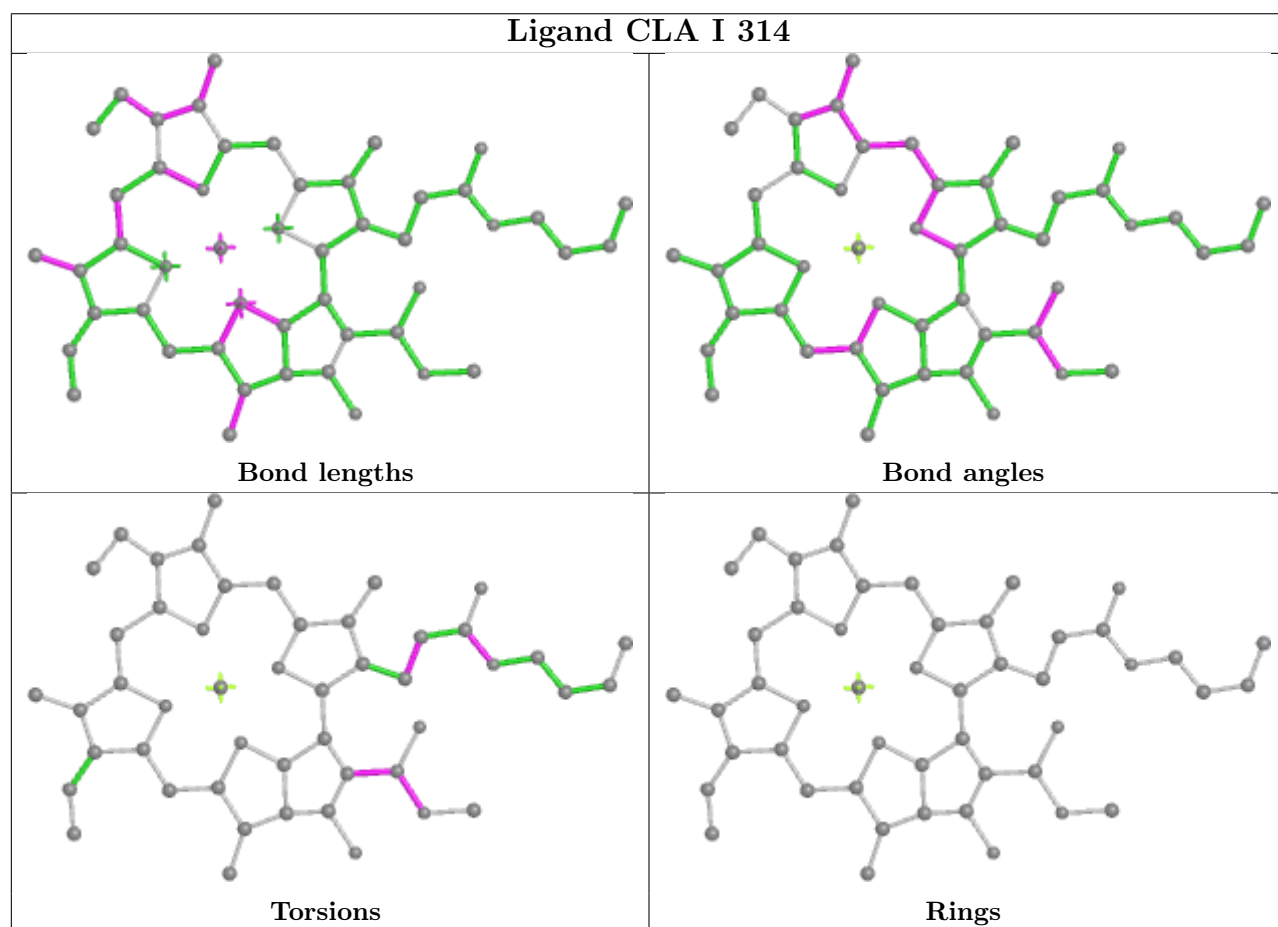
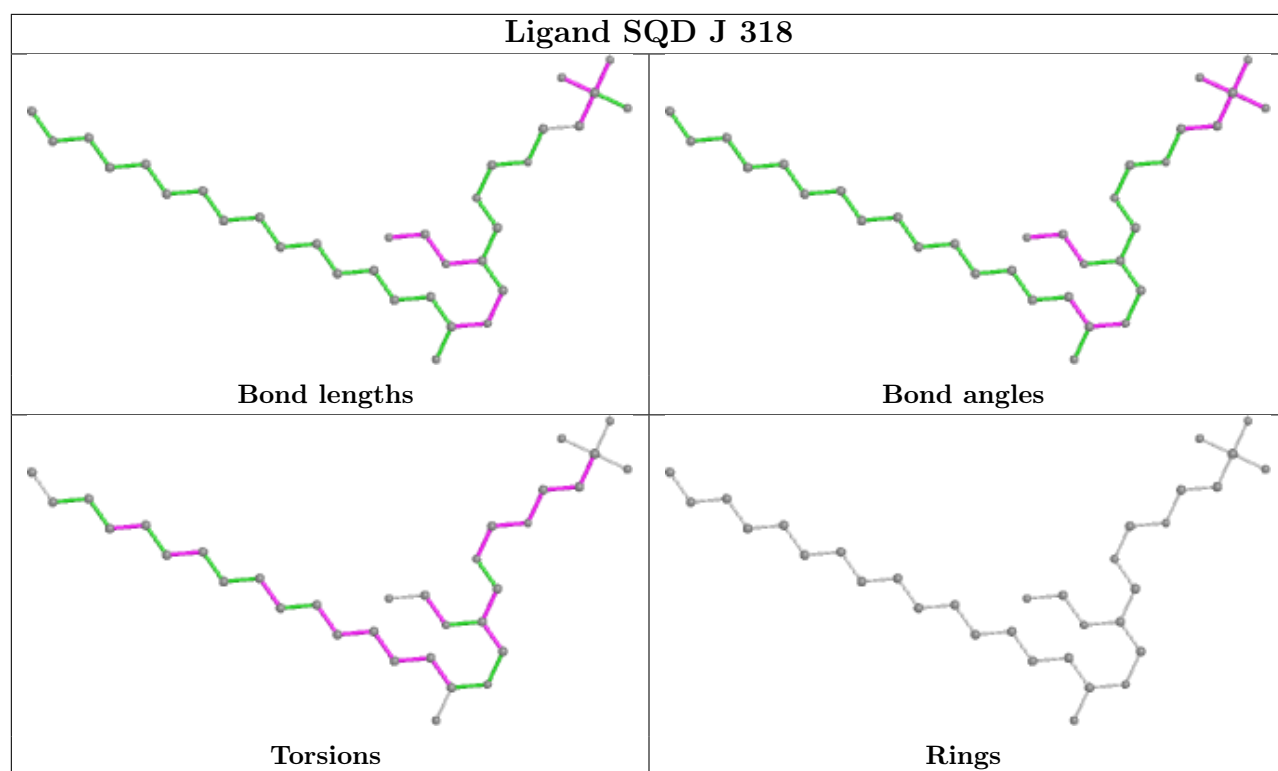


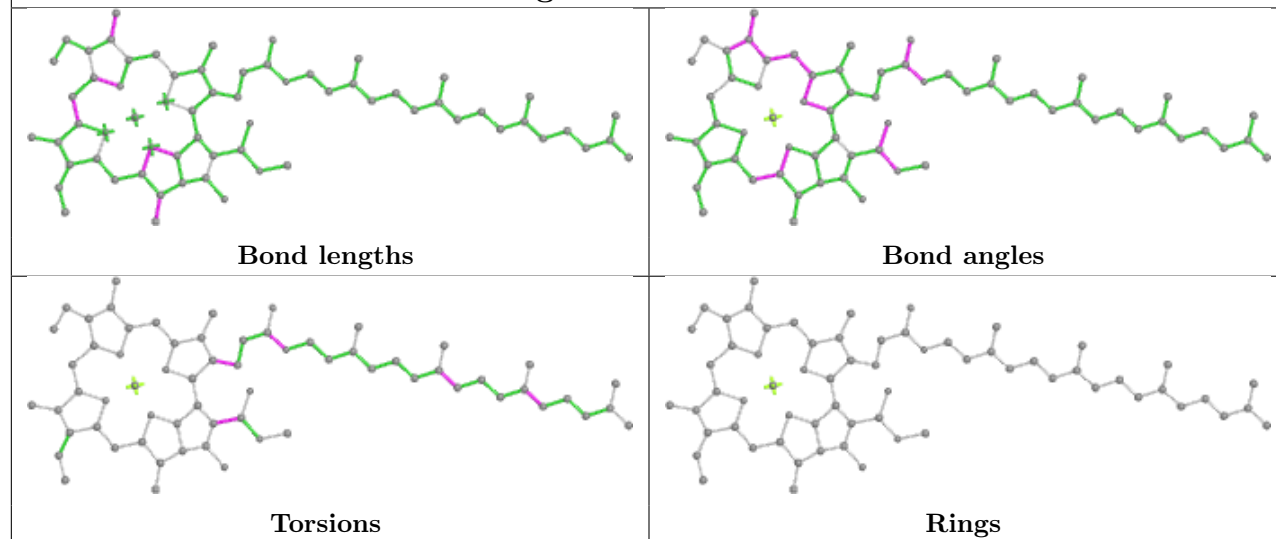
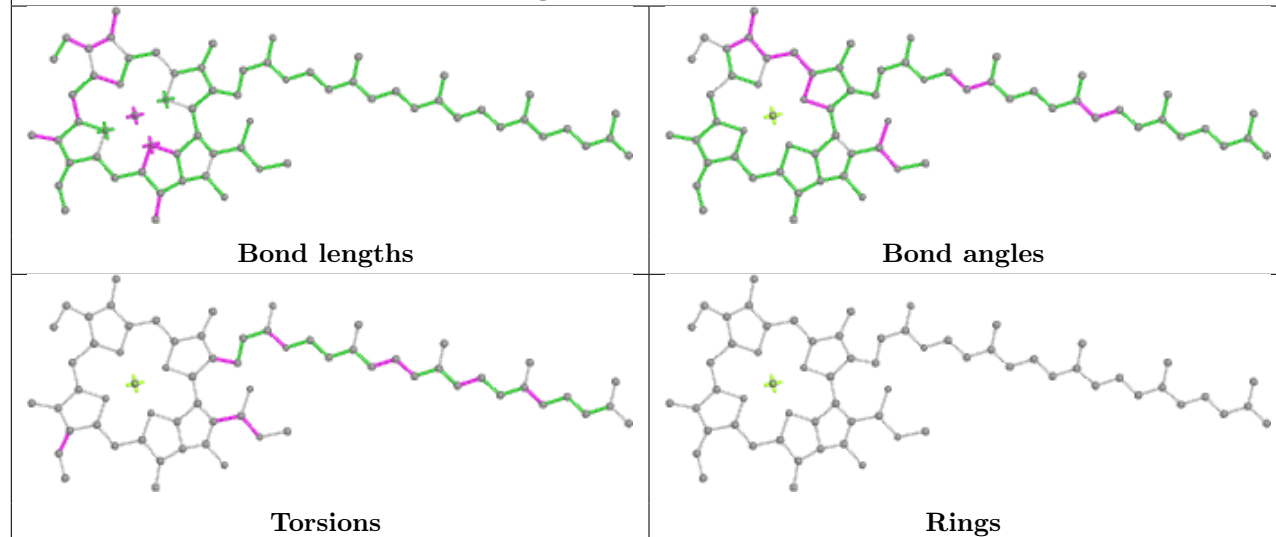
Torsions

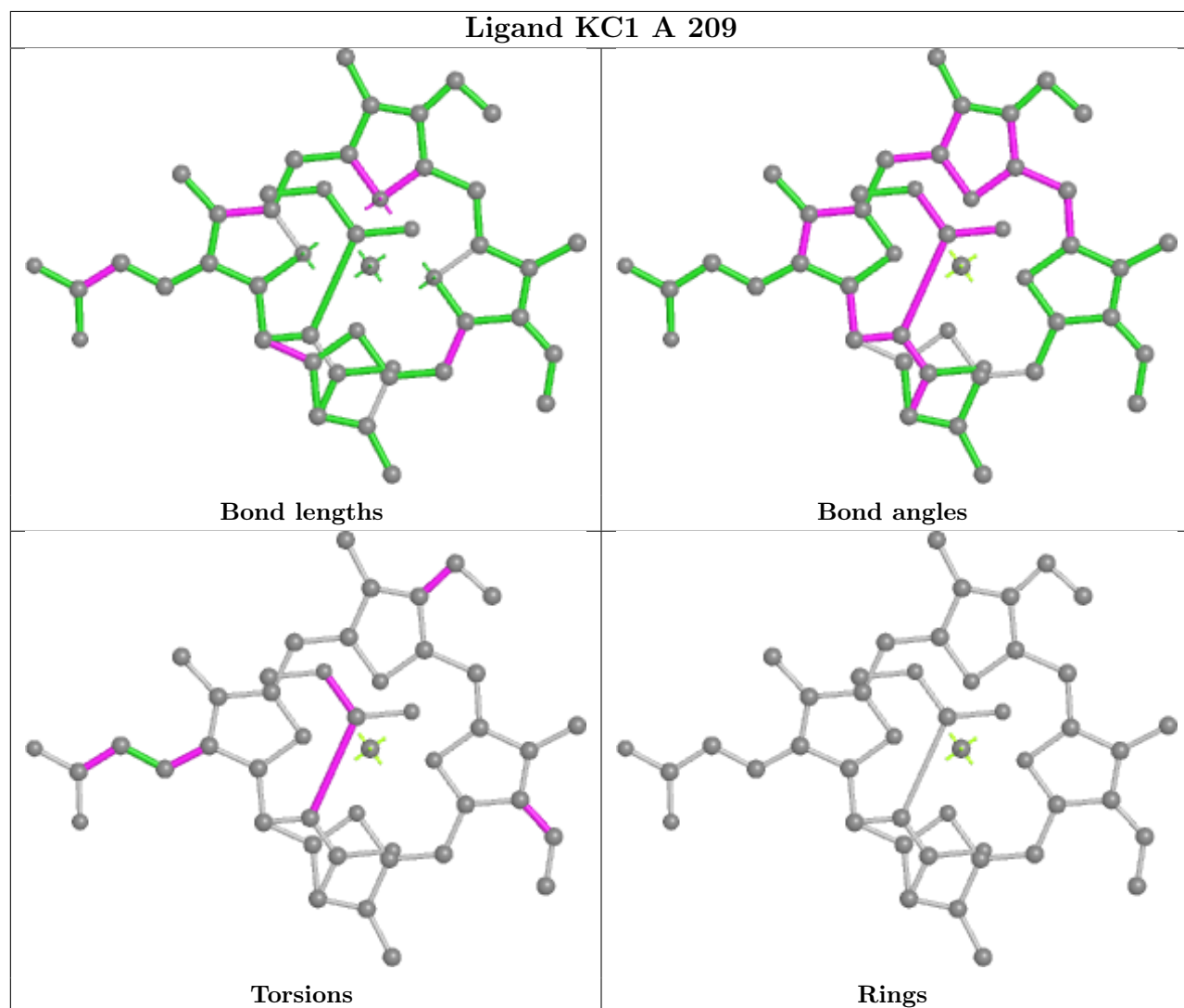
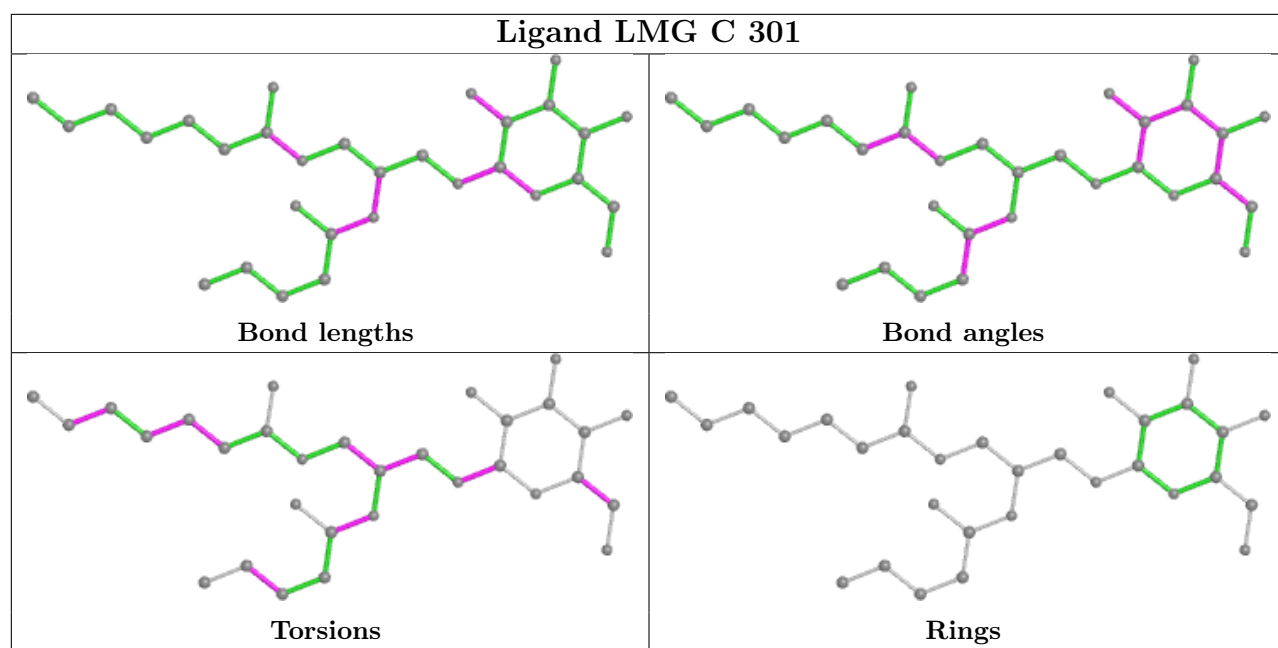


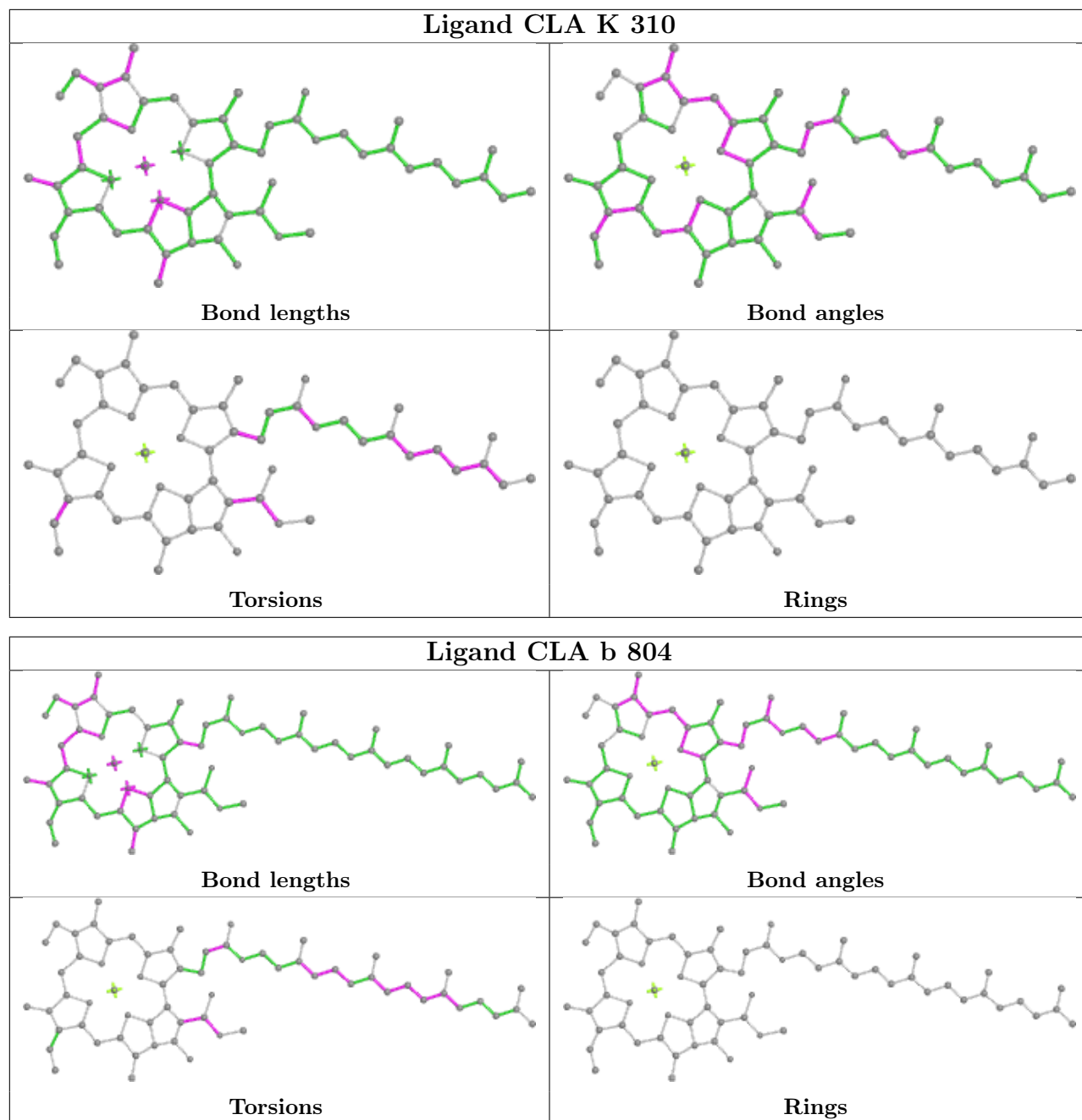
Rings



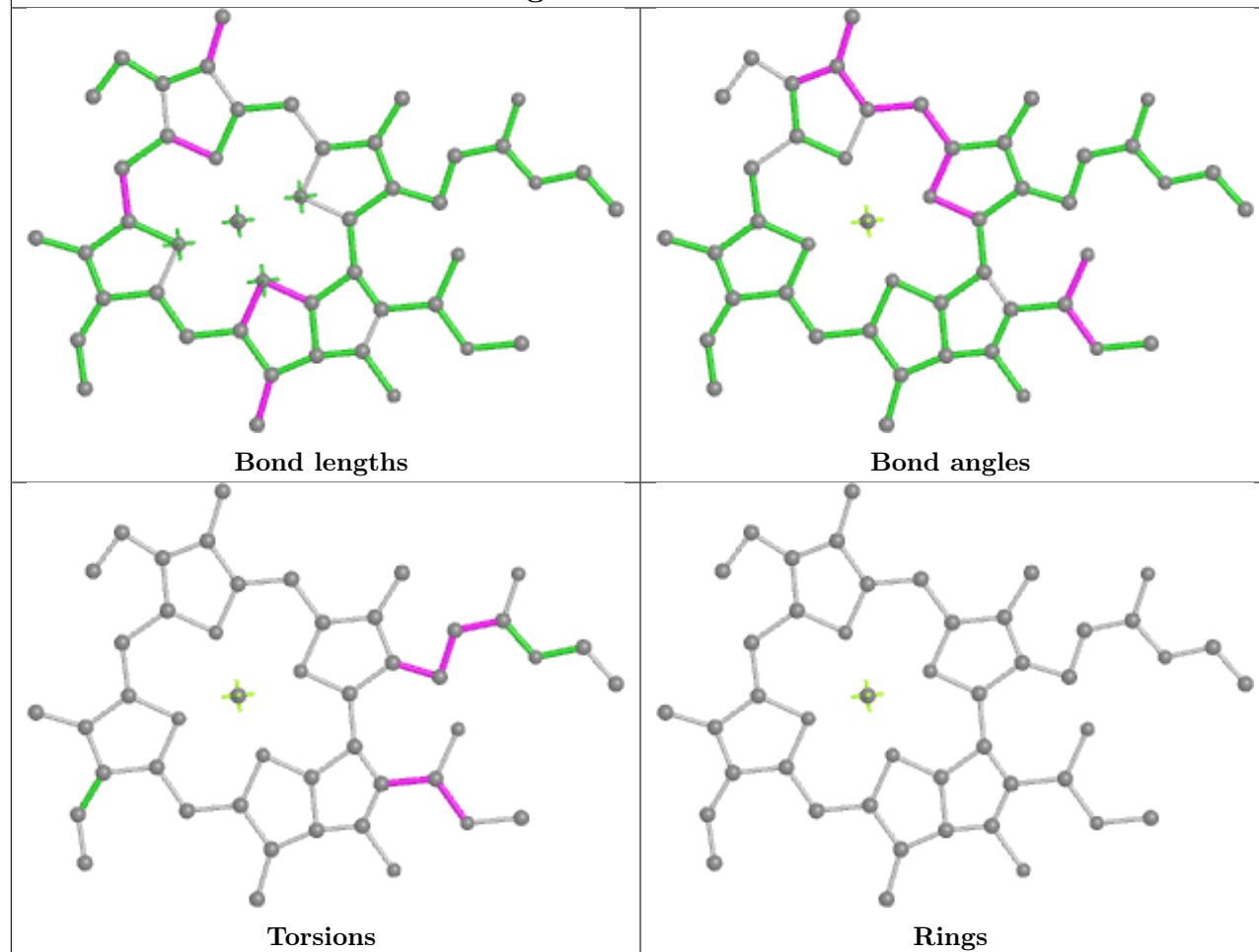


**Ligand CLA a 848****Ligand CLA L 313**

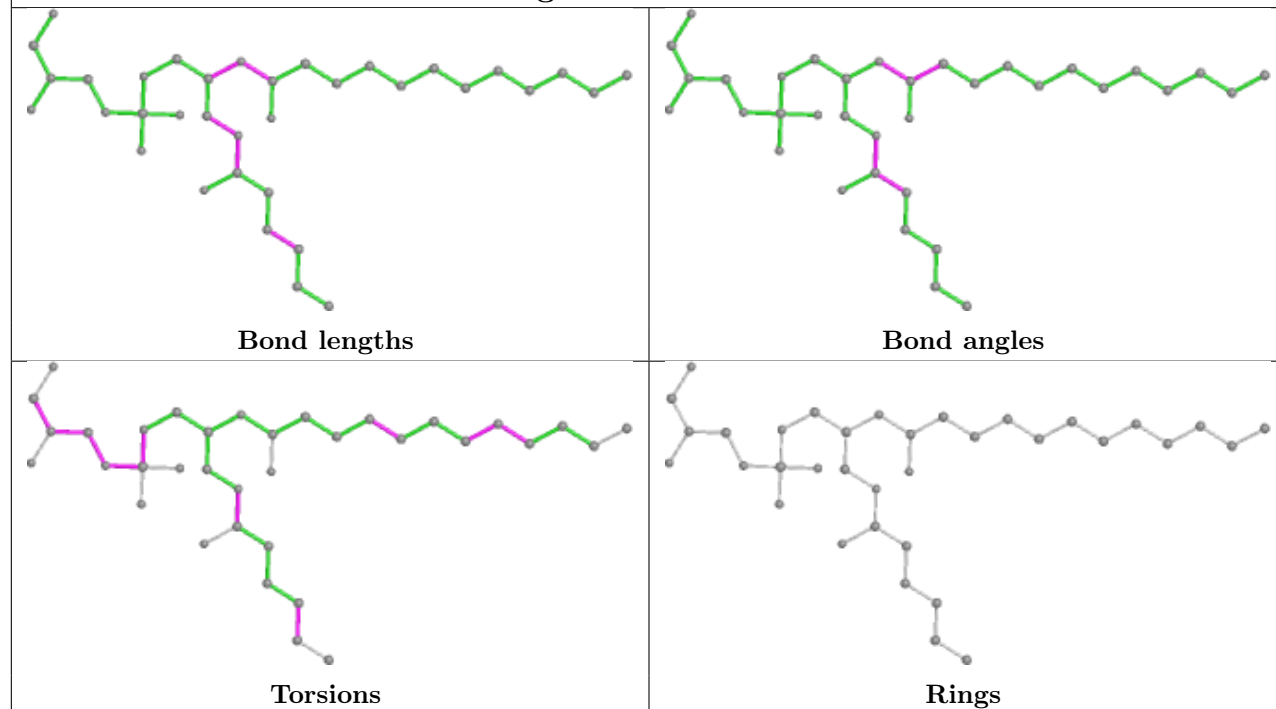




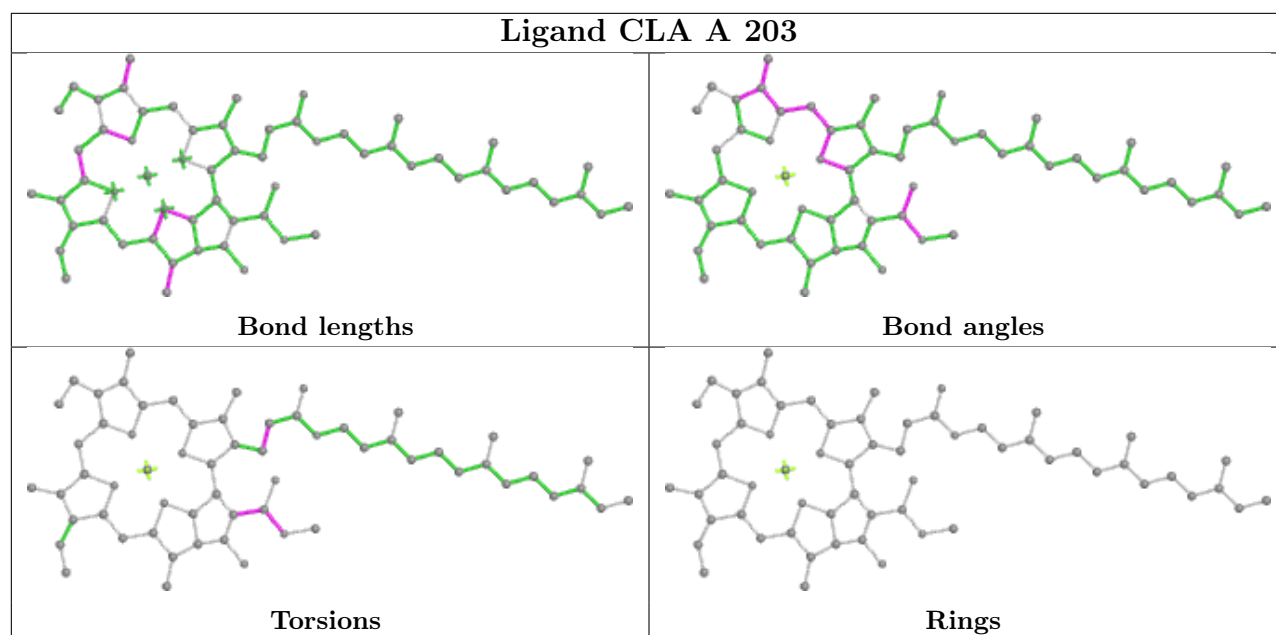
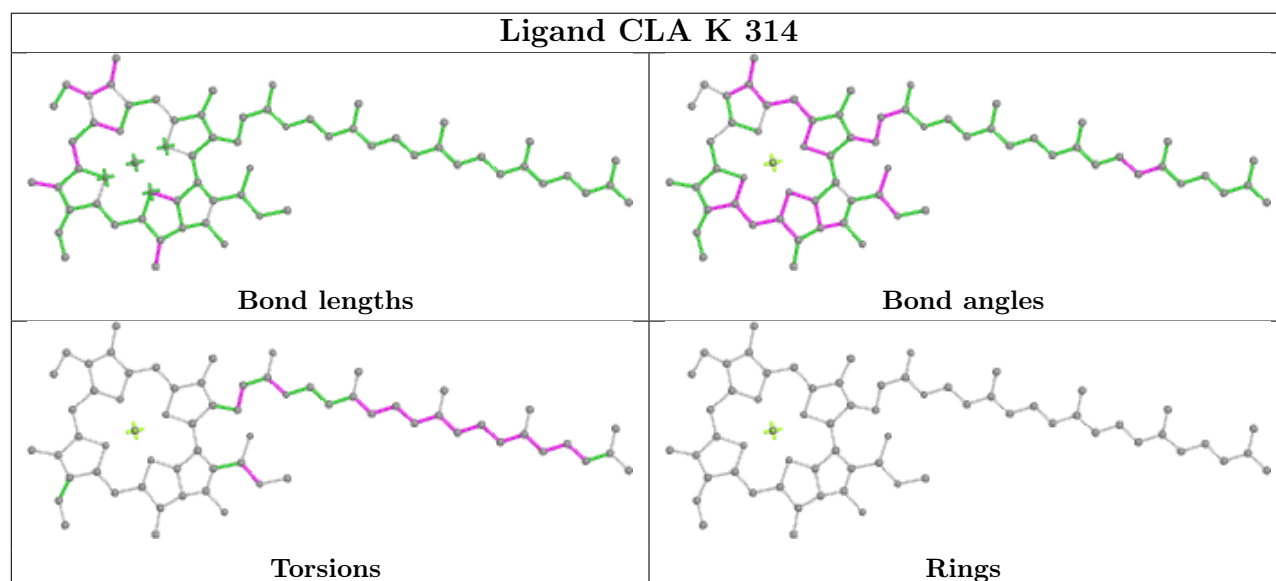
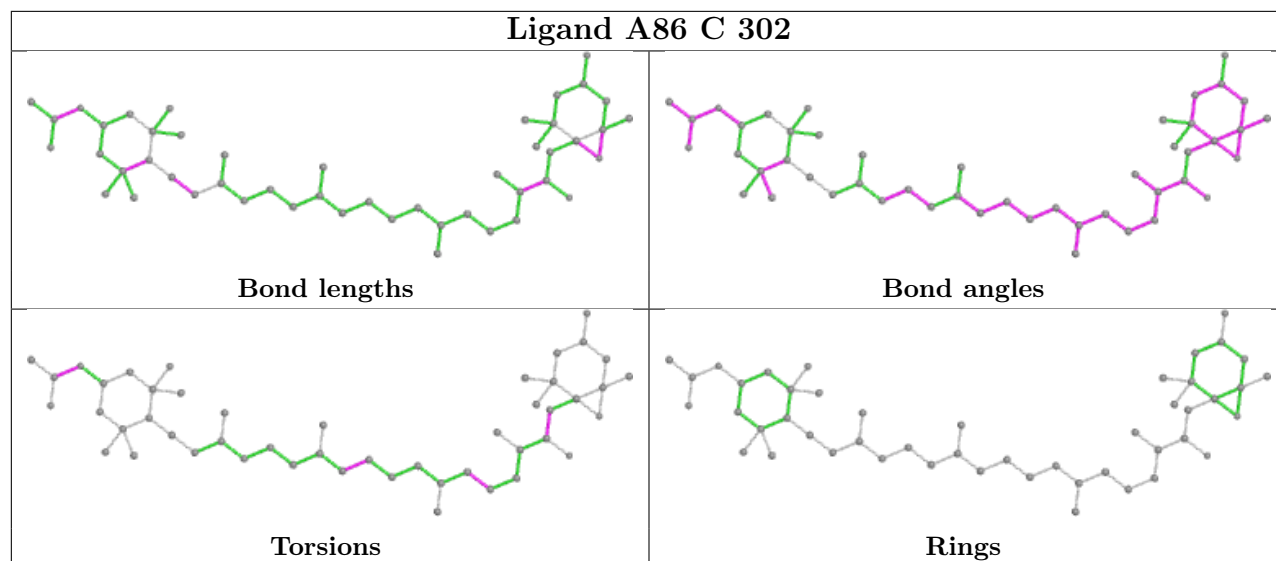
## Ligand CLA F 317

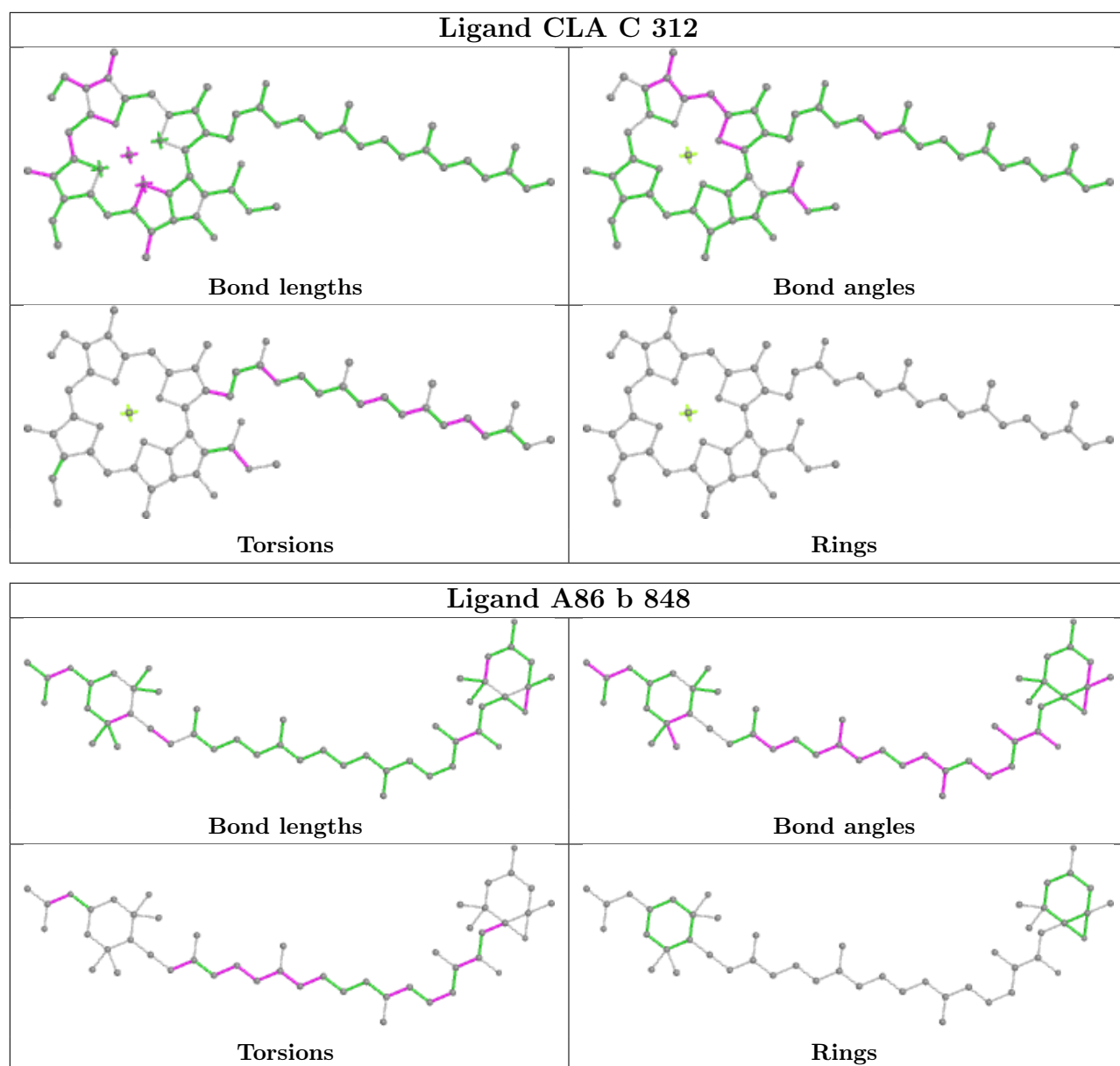


## Ligand LHG I 318

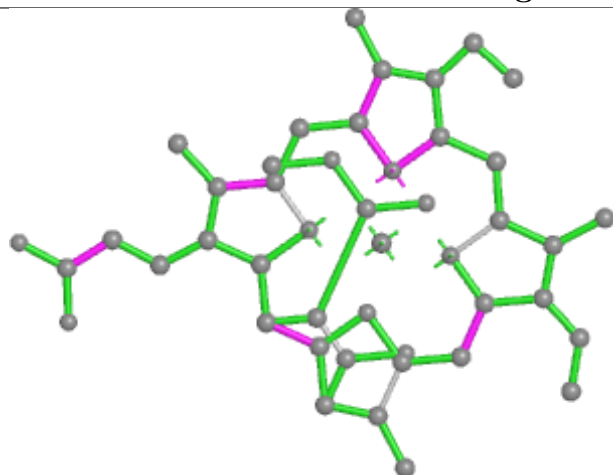




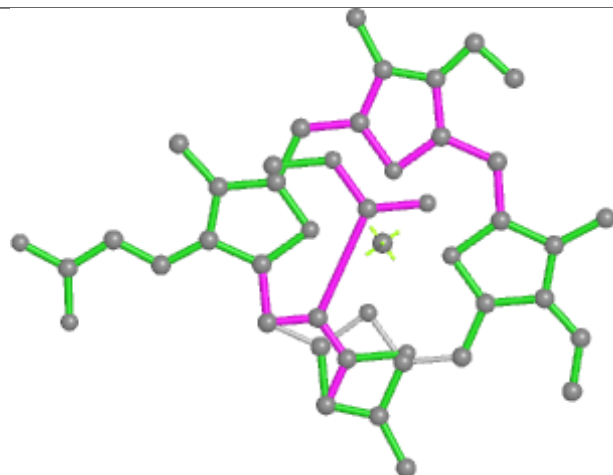




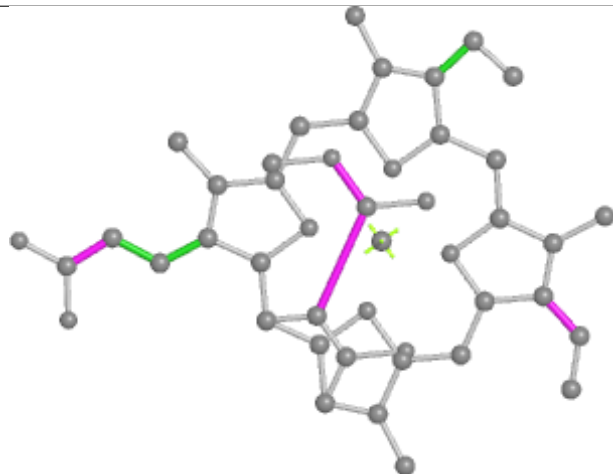
## Ligand KC1 K 315



Bond lengths



Bond angles

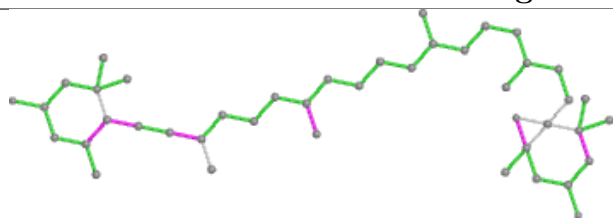


Torsions

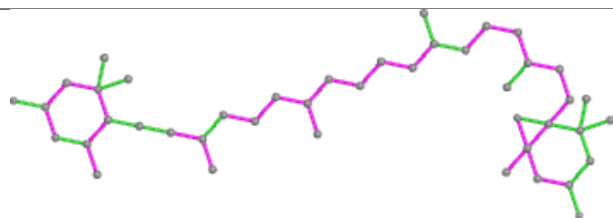


Rings

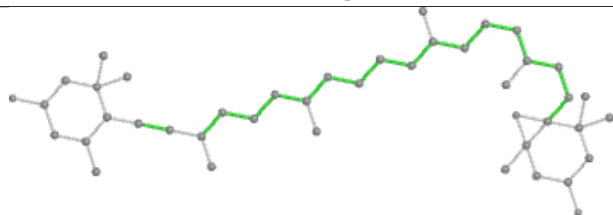
## Ligand DD6 B 303



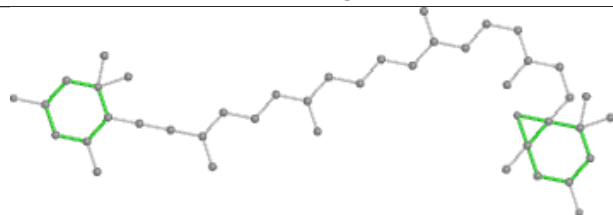
Bond lengths



Bond angles

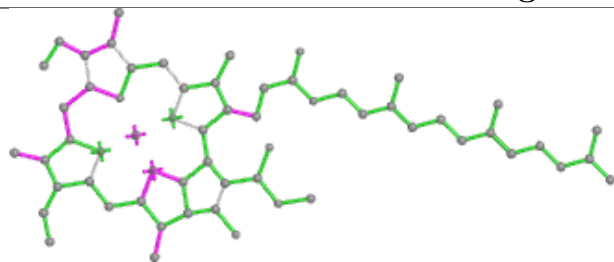


Torsions

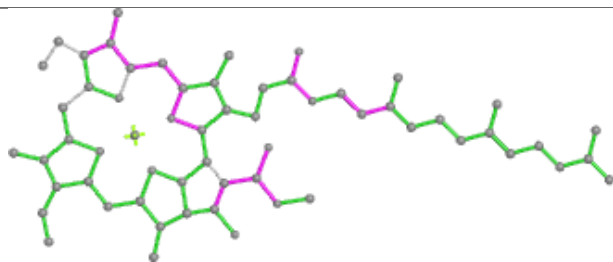


Rings

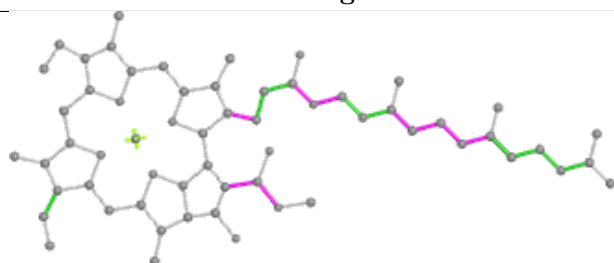
## Ligand CLA a 839



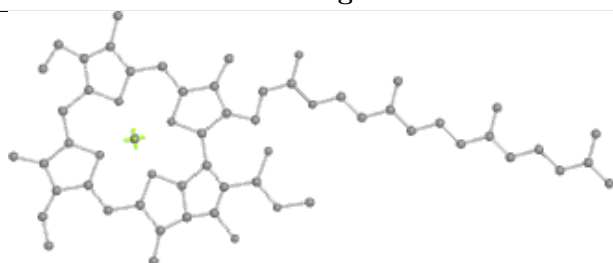
Bond lengths



Bond angles

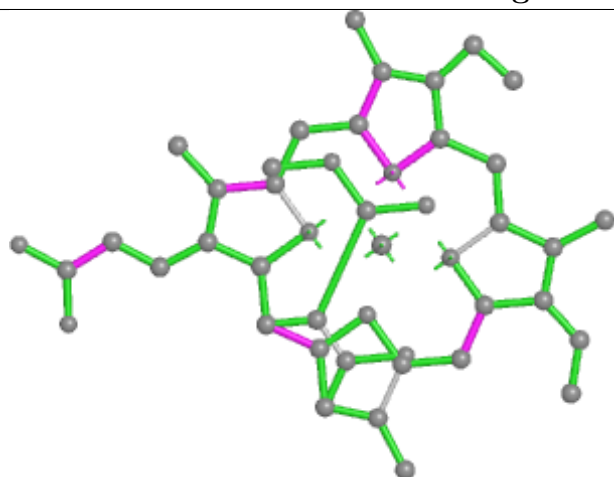


Torsions

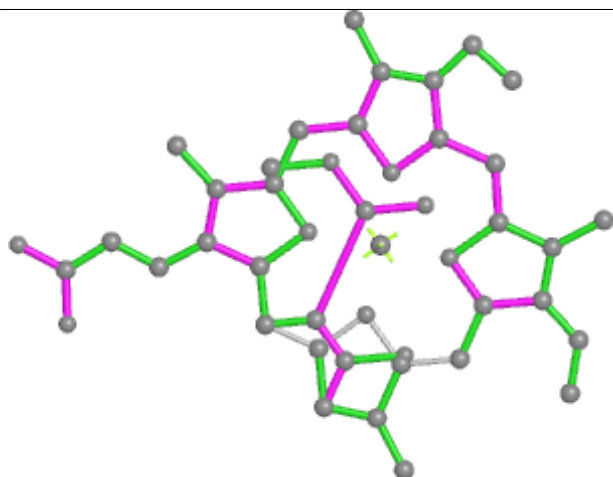


Rings

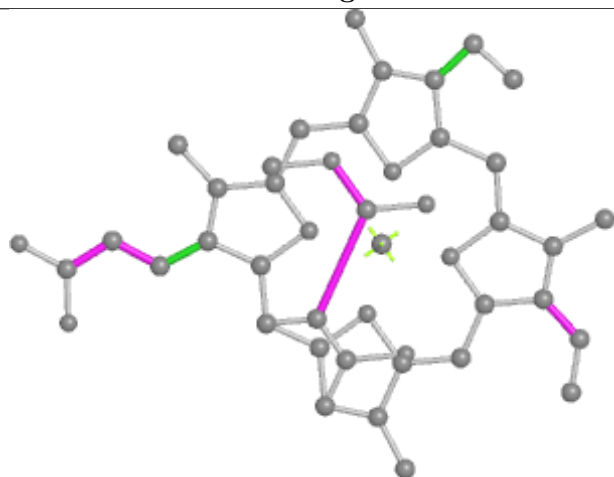
## Ligand KC1 M 314



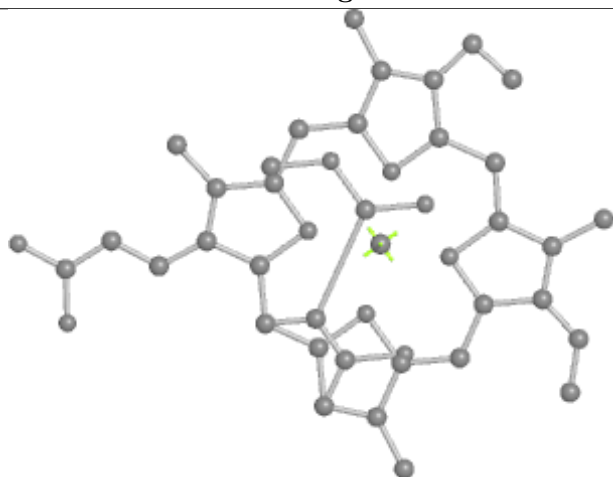
Bond lengths



Bond angles

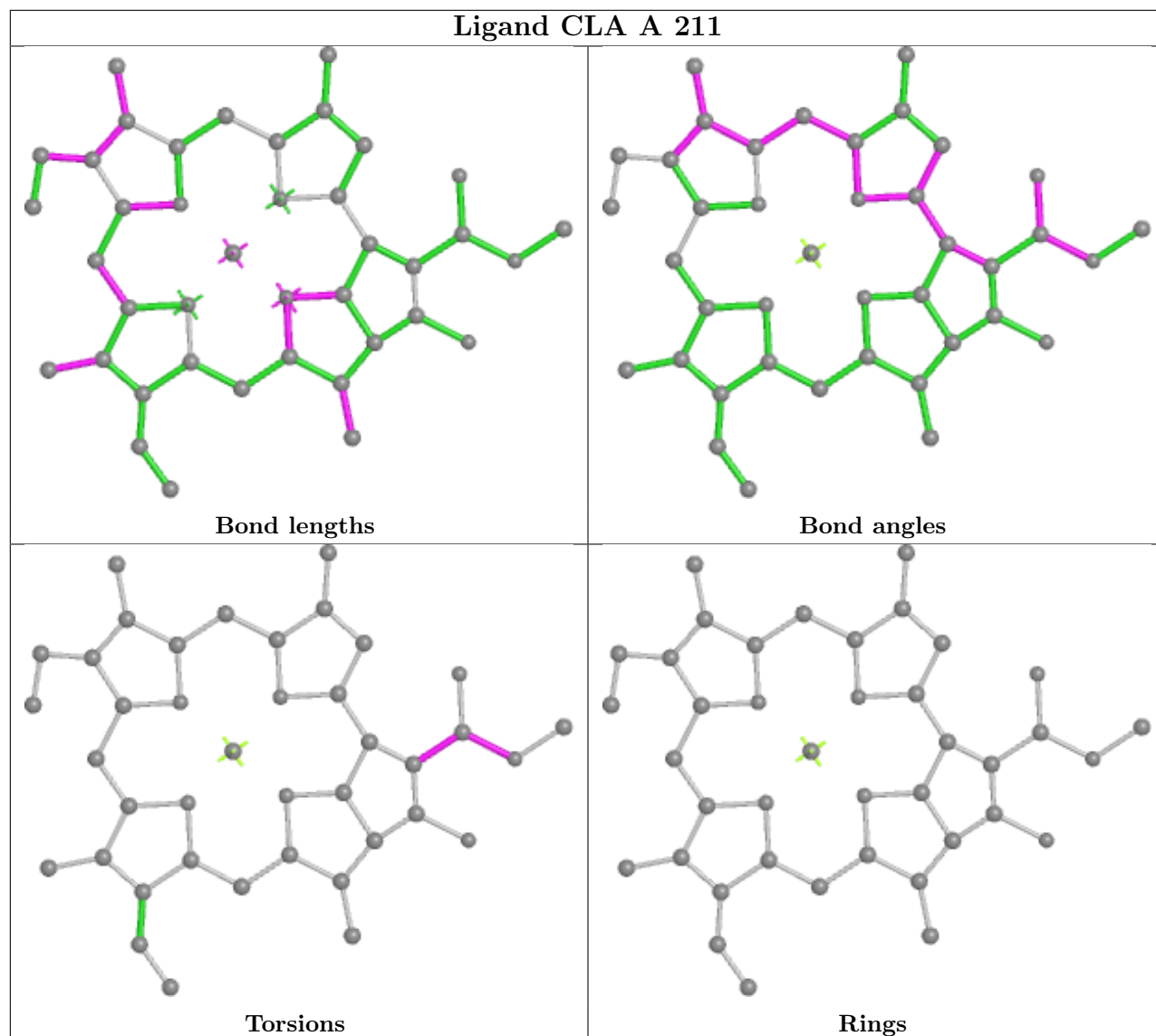


Torsions

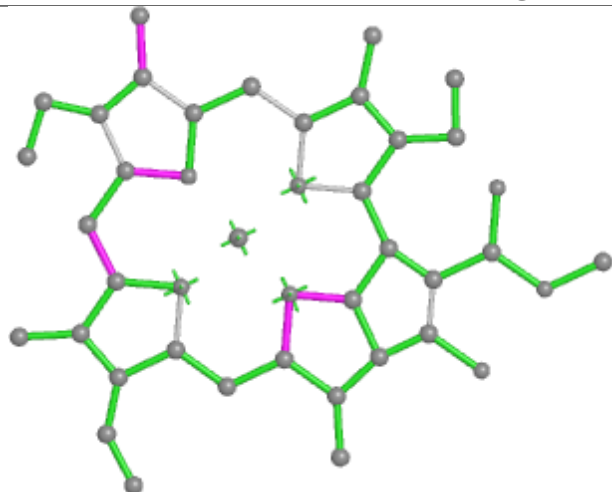


Rings

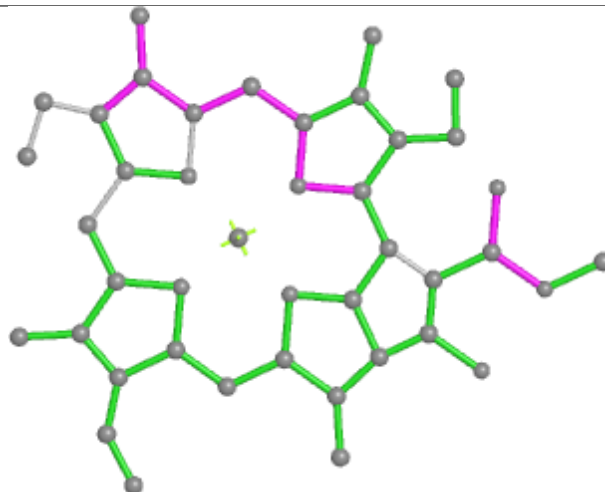
## Ligand CLA A 211



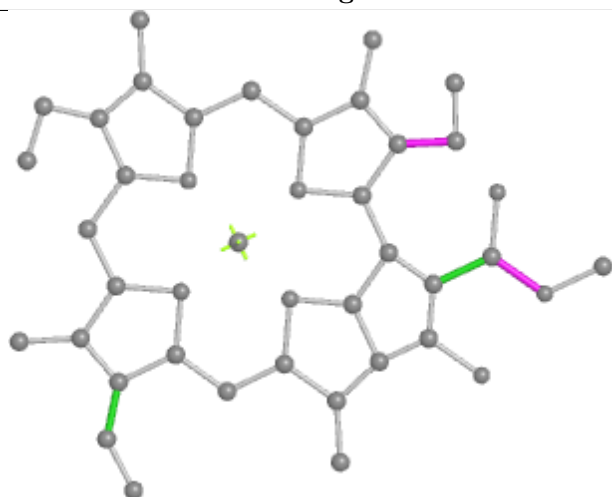
## Ligand CLA C 315



Bond lengths



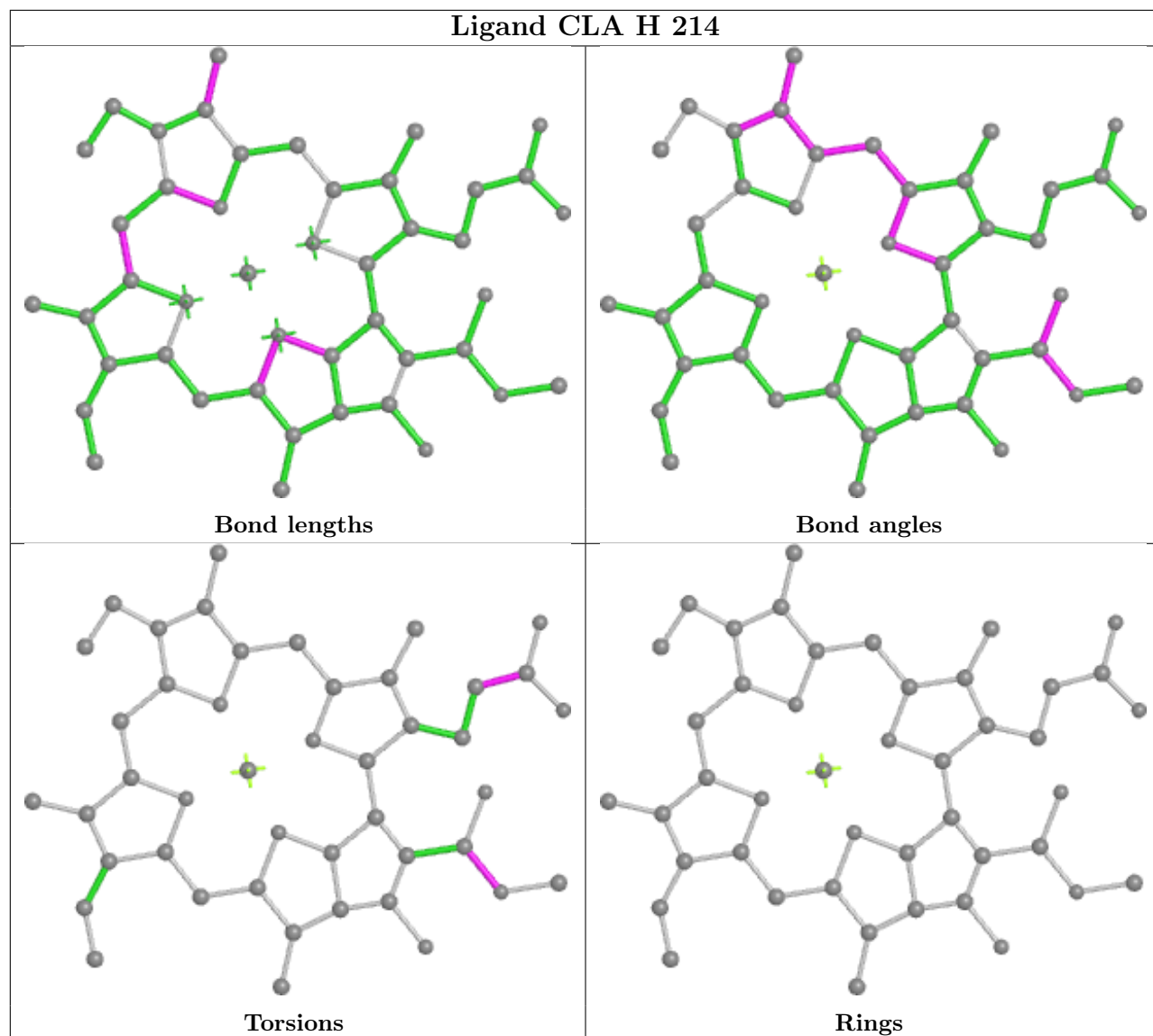
Bond angles

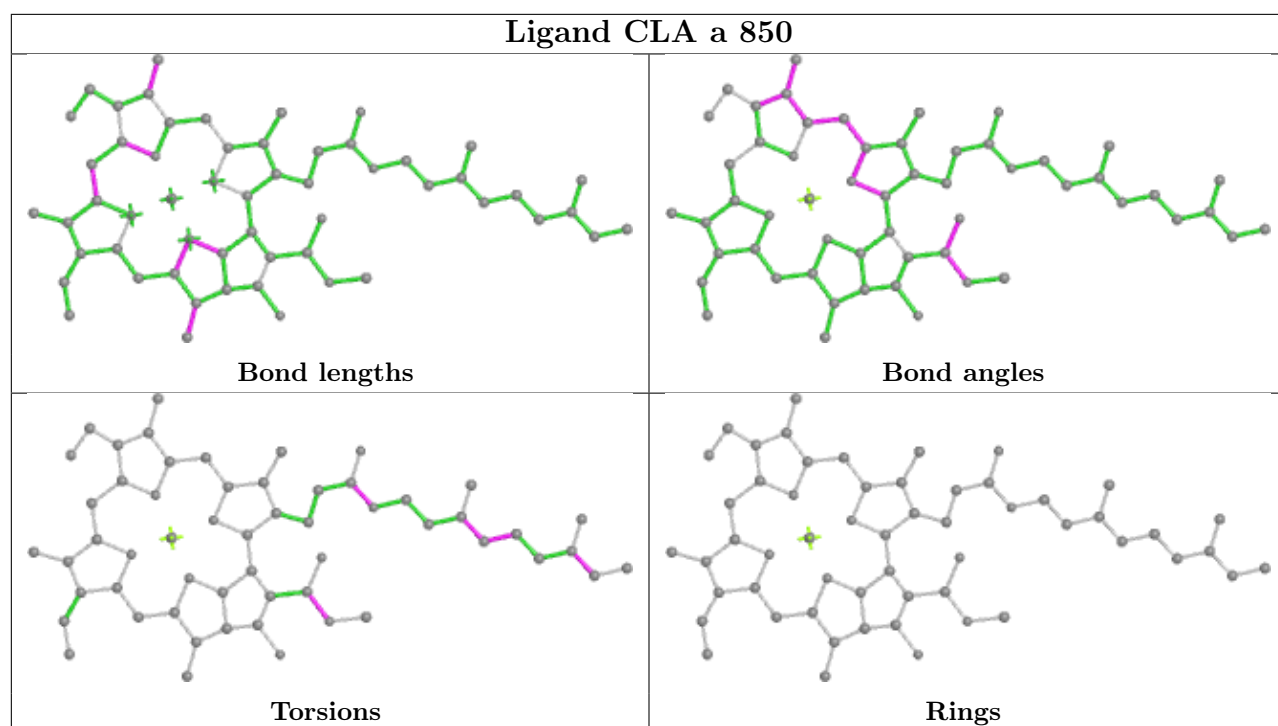


Torsions



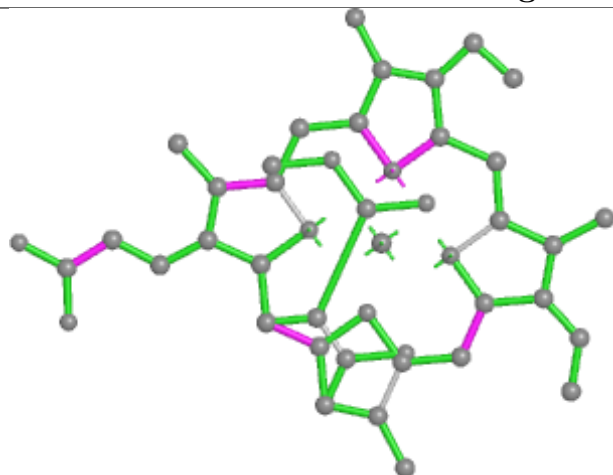
Rings



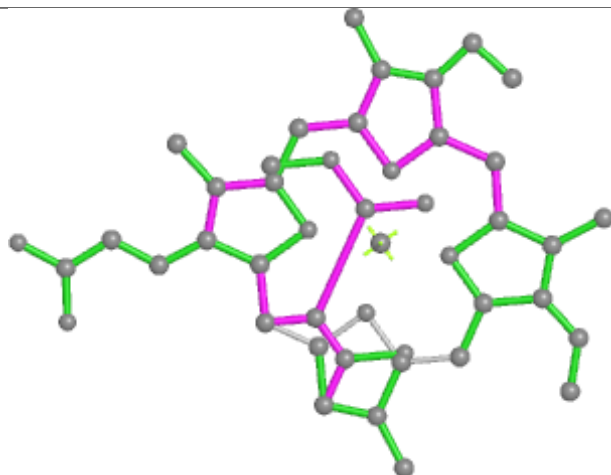




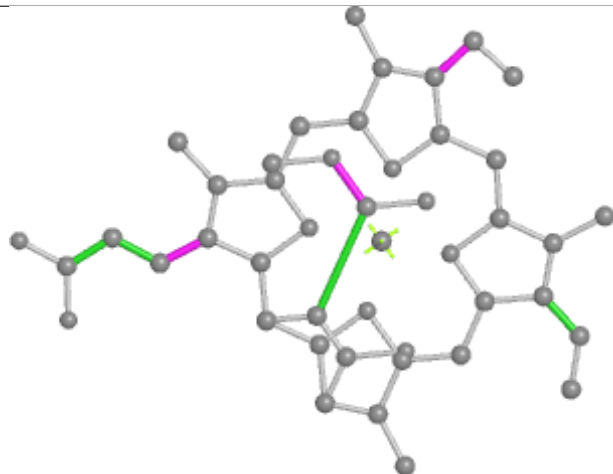
## Ligand KC1 L 320



Bond lengths



Bond angles

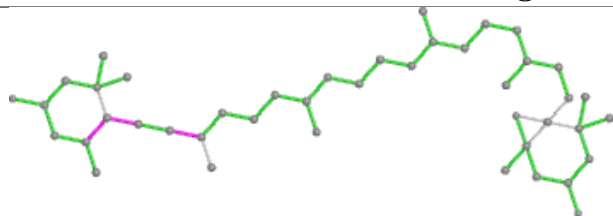


Torsions

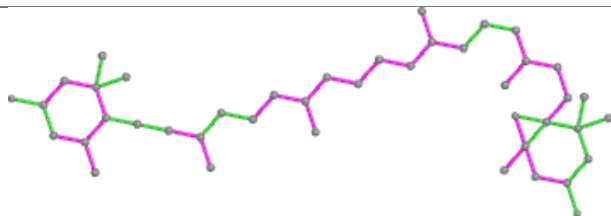


Rings

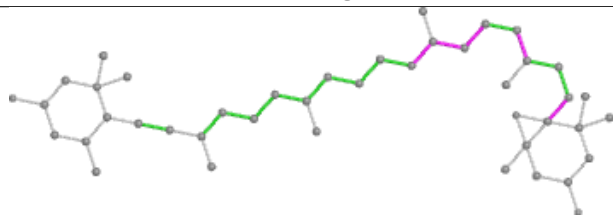
## Ligand DD6 E 306



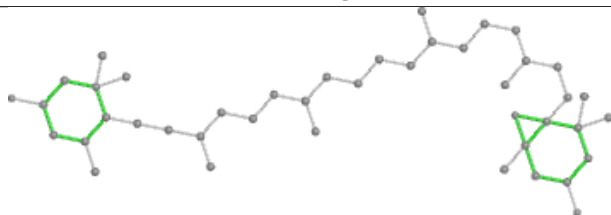
Bond lengths



Bond angles

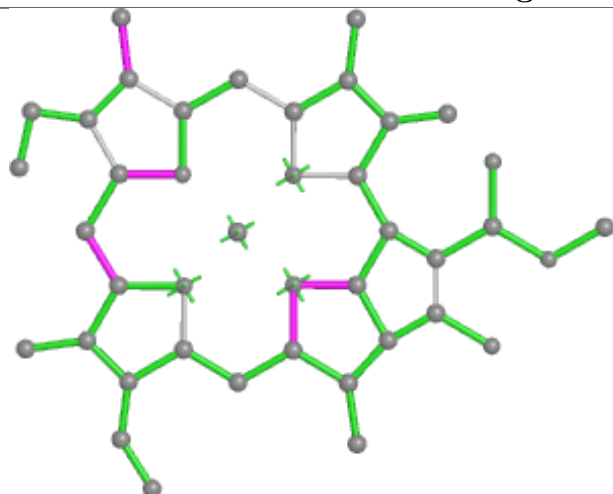


Torsions

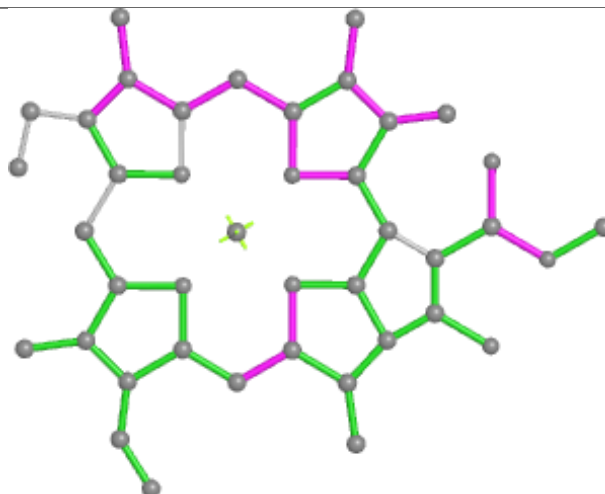


Rings

## Ligand CLA F 316



Bond lengths



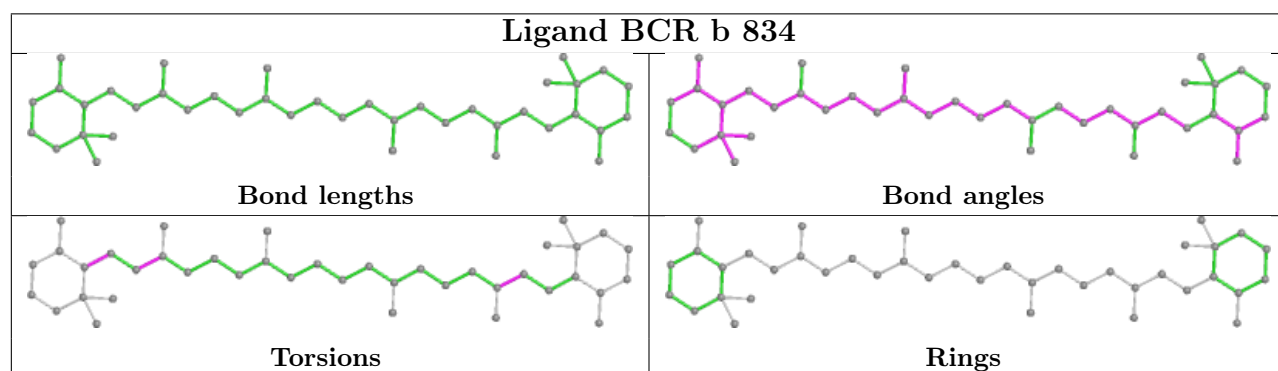
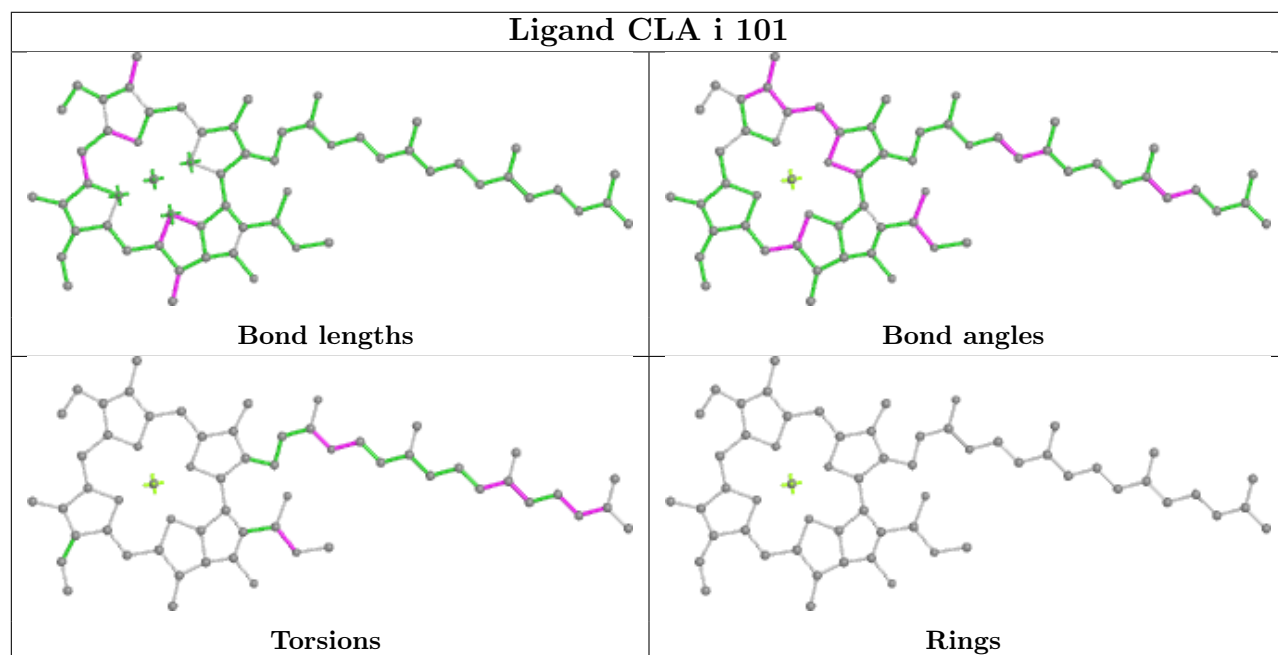
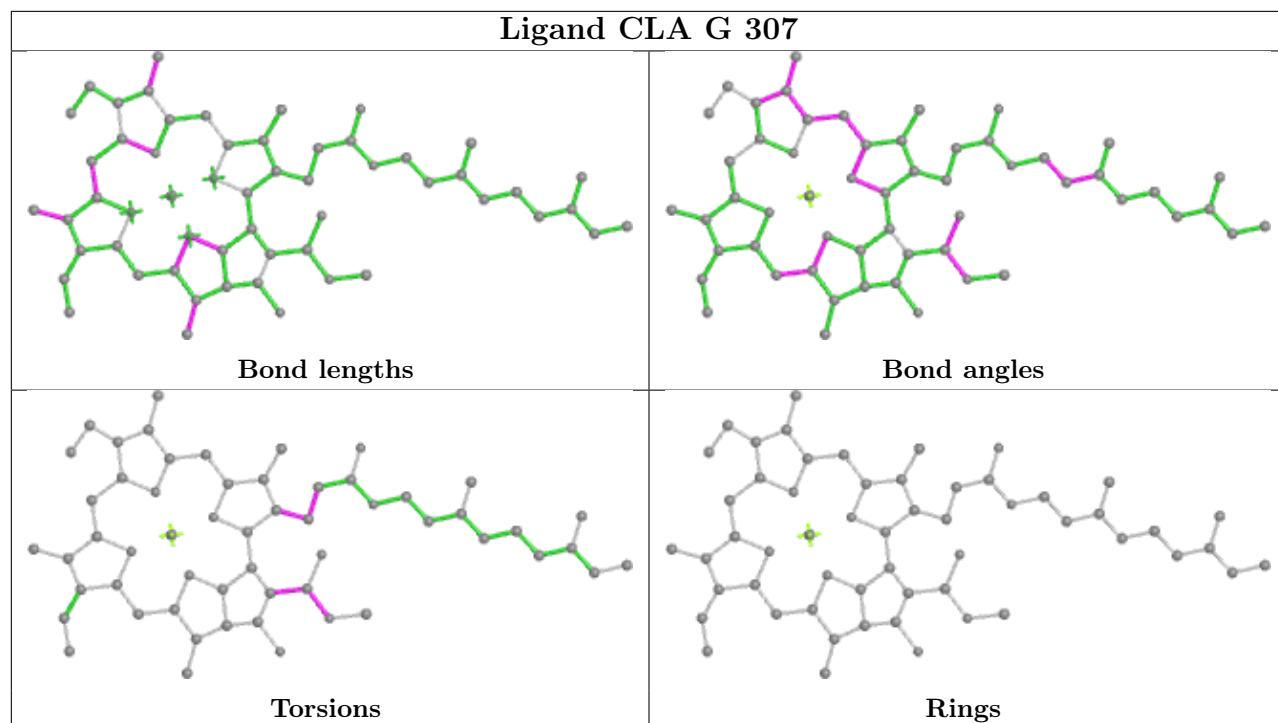
Bond angles



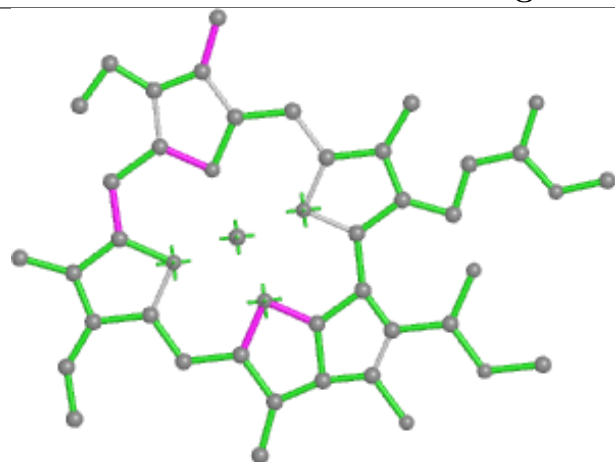
Torsions



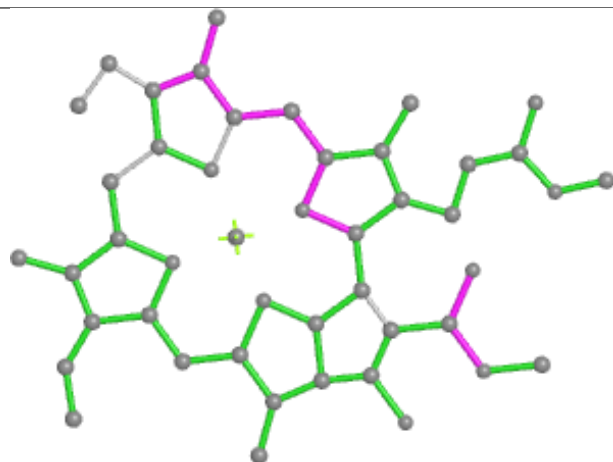
Rings



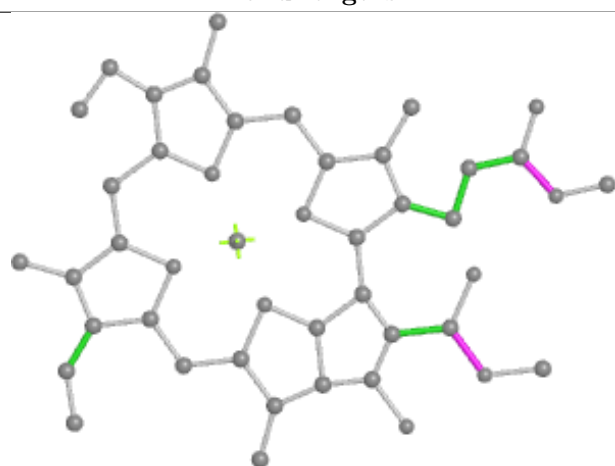
## Ligand CLA A 206



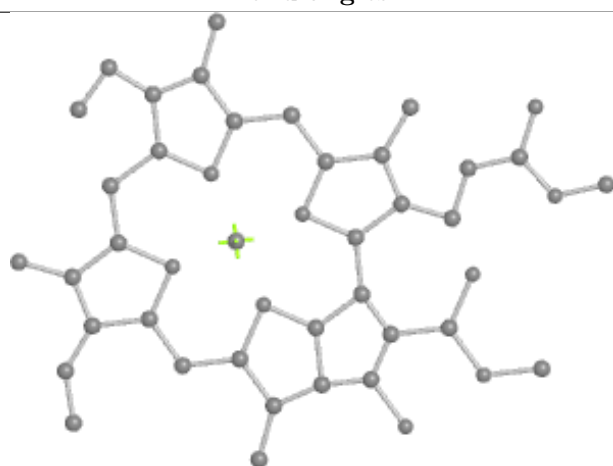
Bond lengths



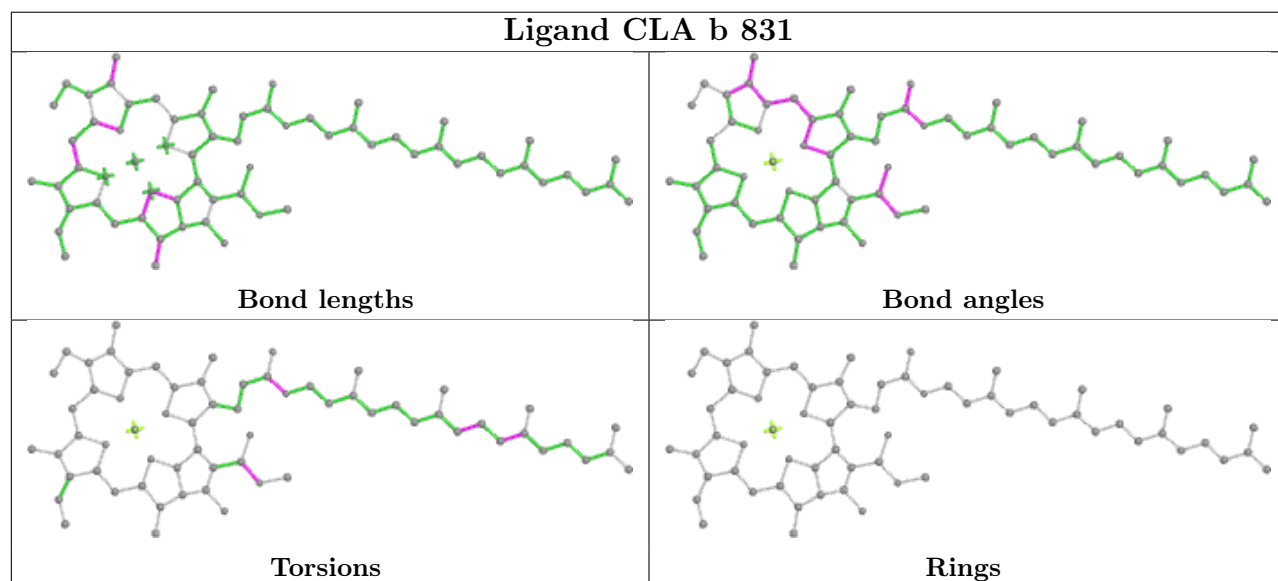
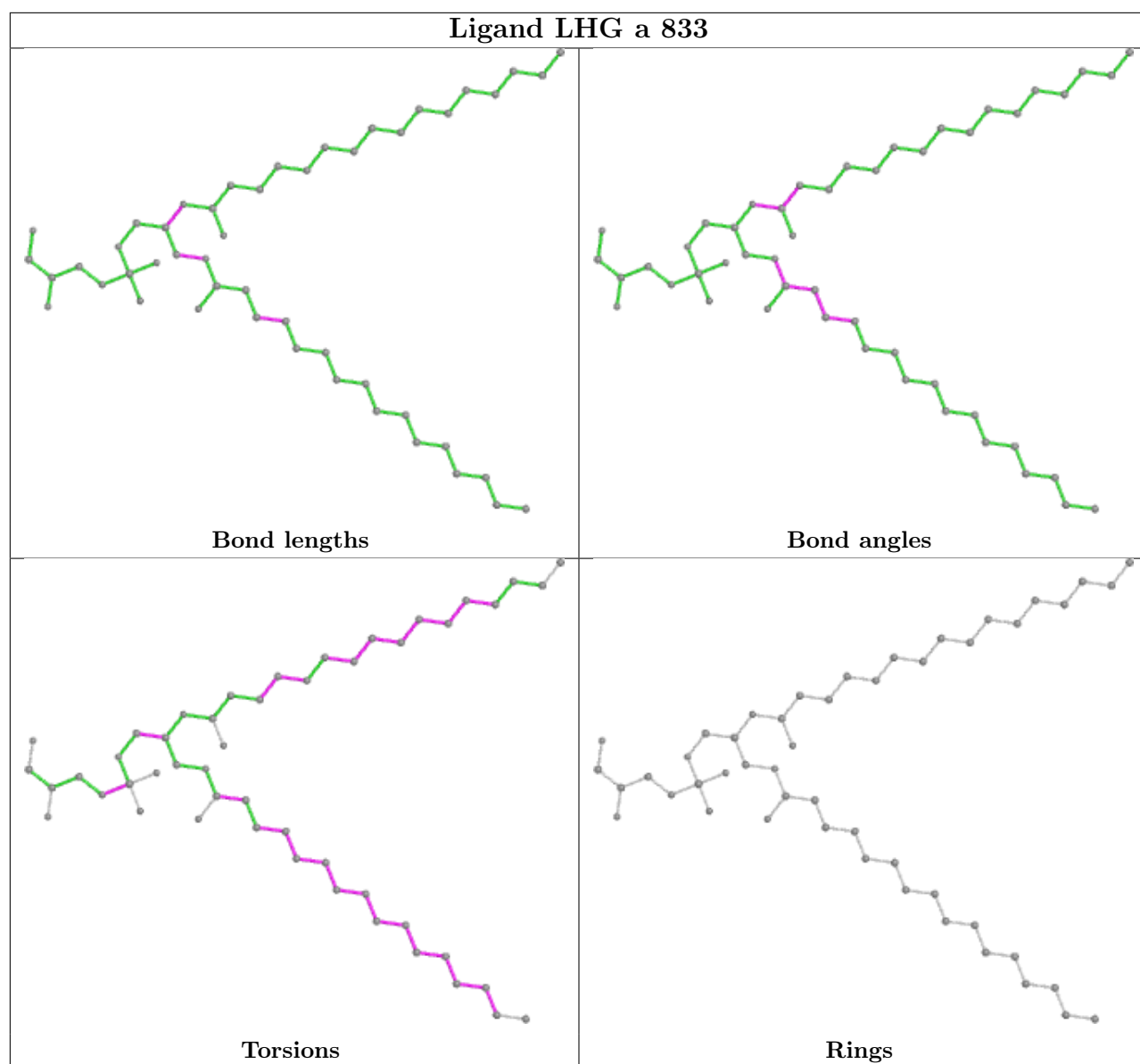
Bond angles

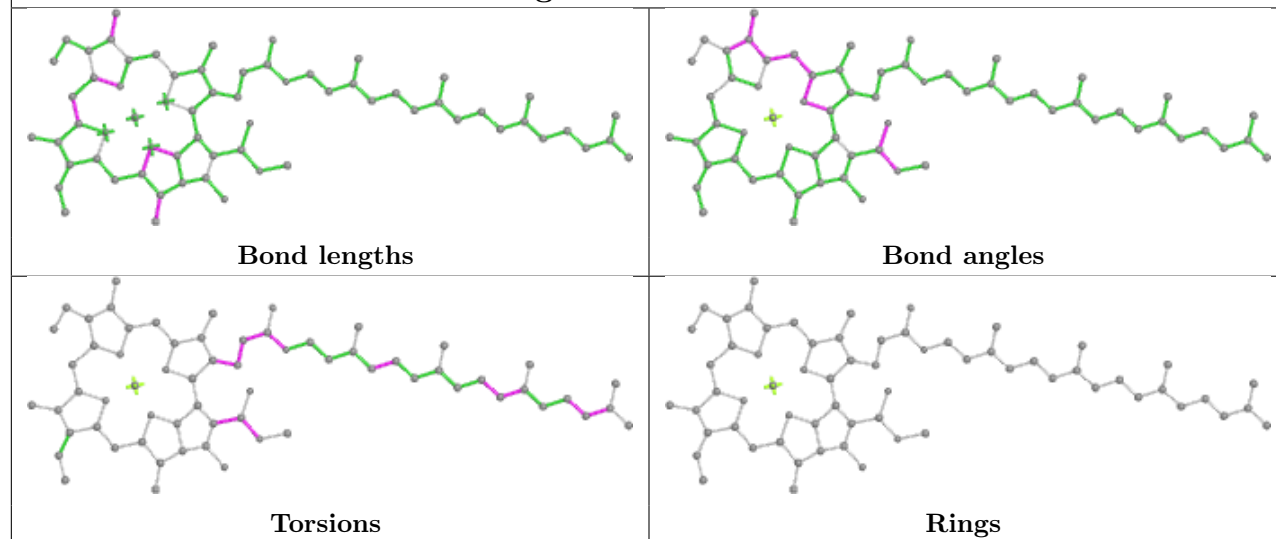
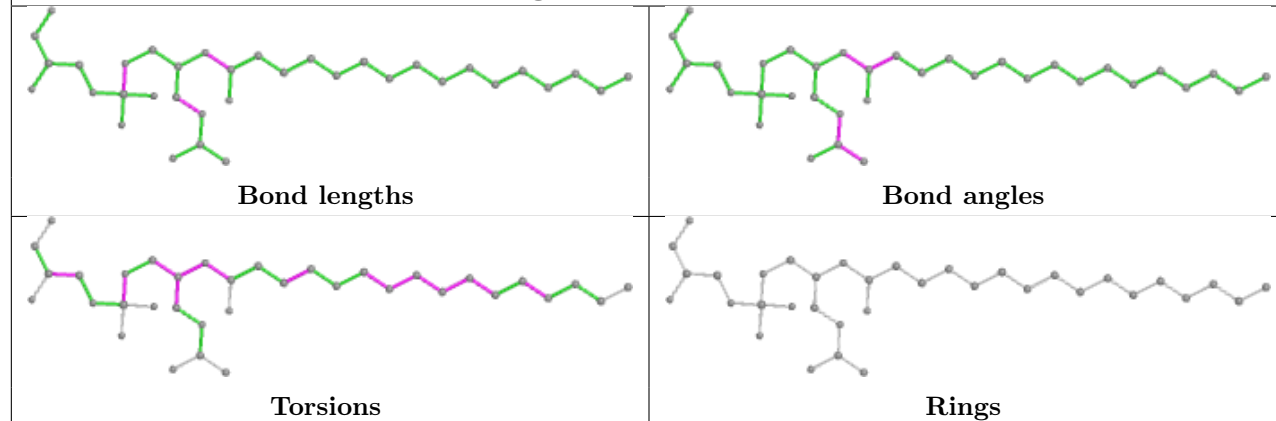


Torsions

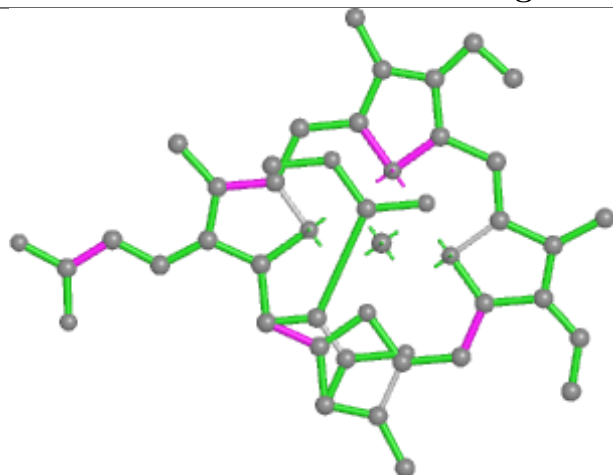


Rings

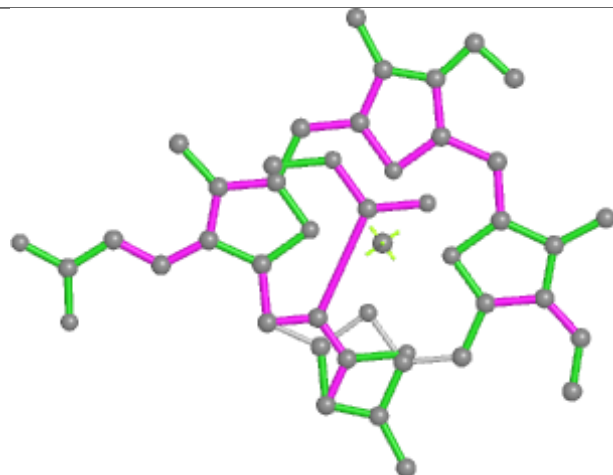


**Ligand CLA b 823****Ligand LHG H 215**

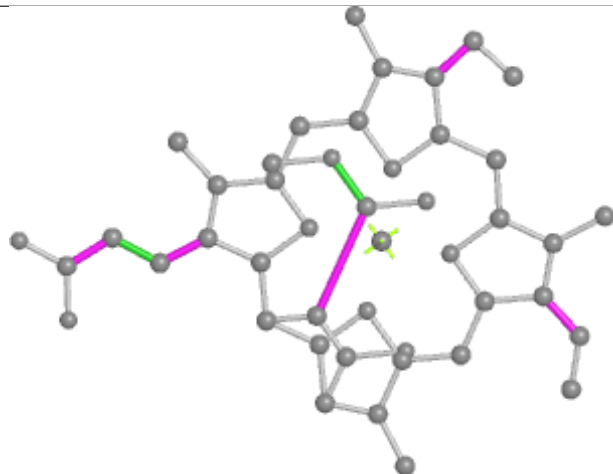
## Ligand KC1 K 308



Bond lengths



Bond angles

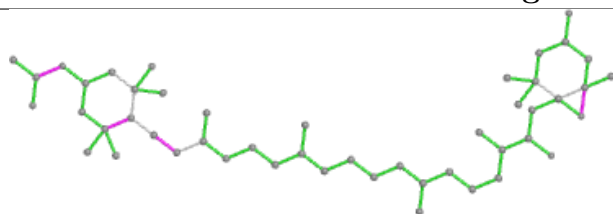


Torsions

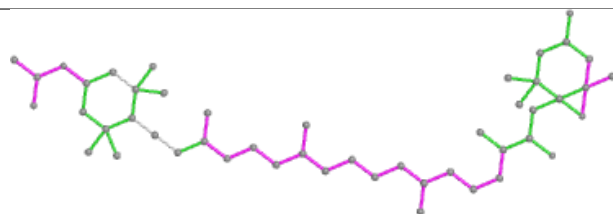


Rings

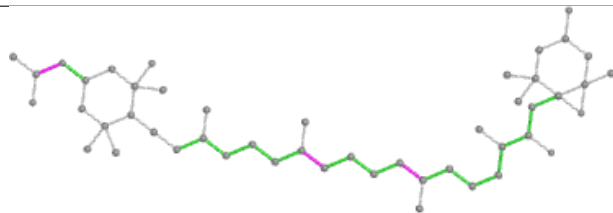
## Ligand A86 L 304



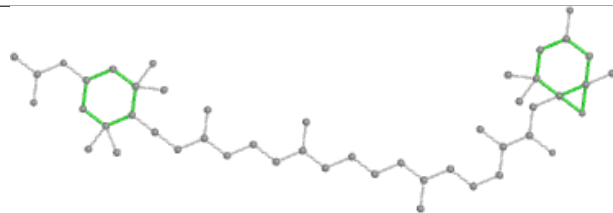
Bond lengths



Bond angles

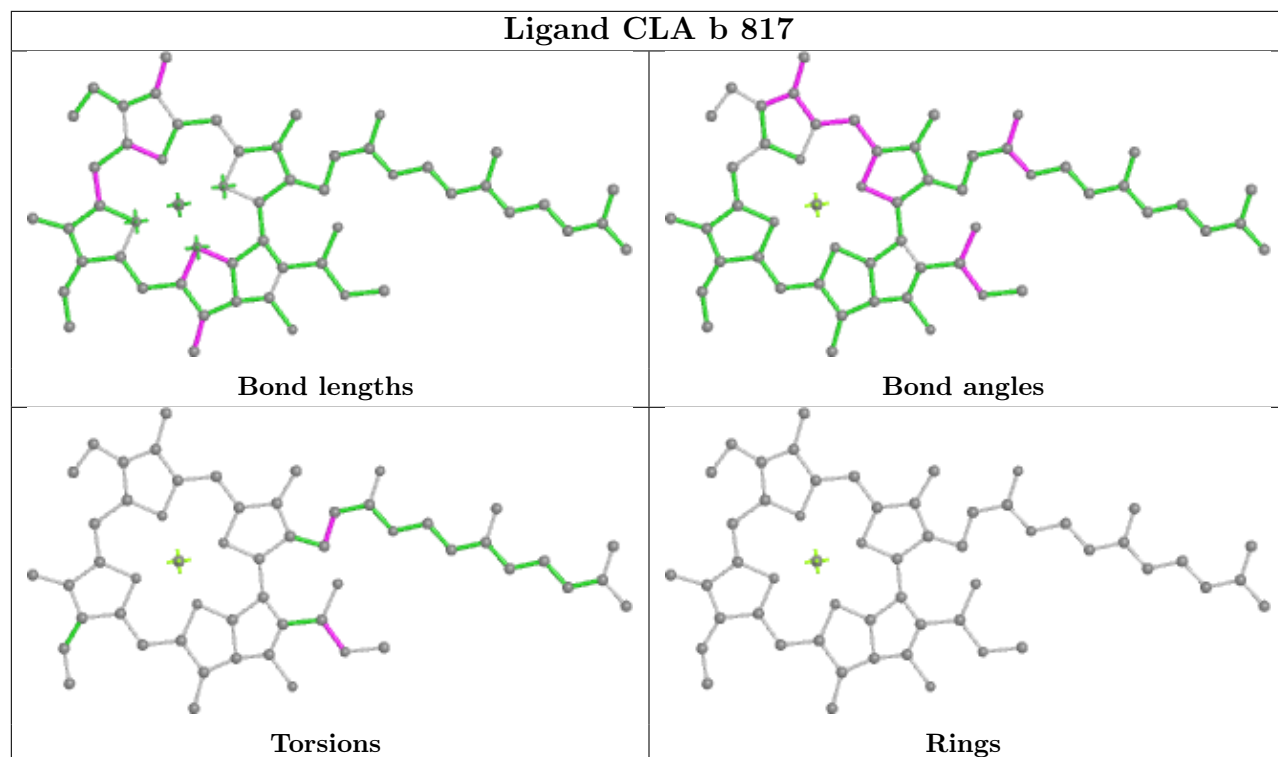


Torsions

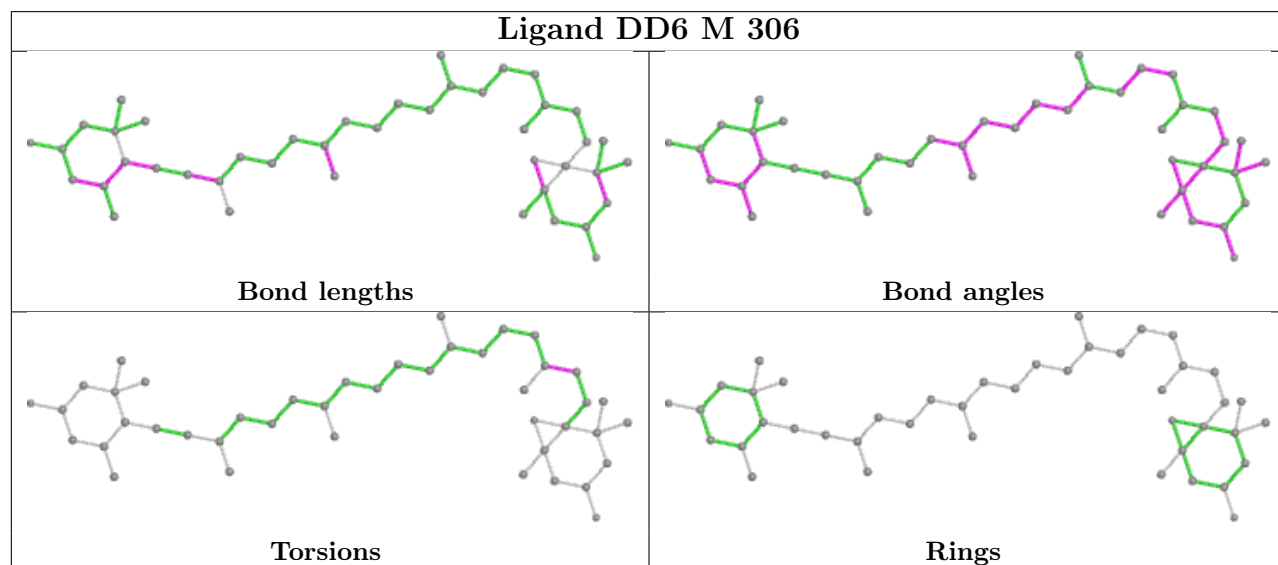


Rings

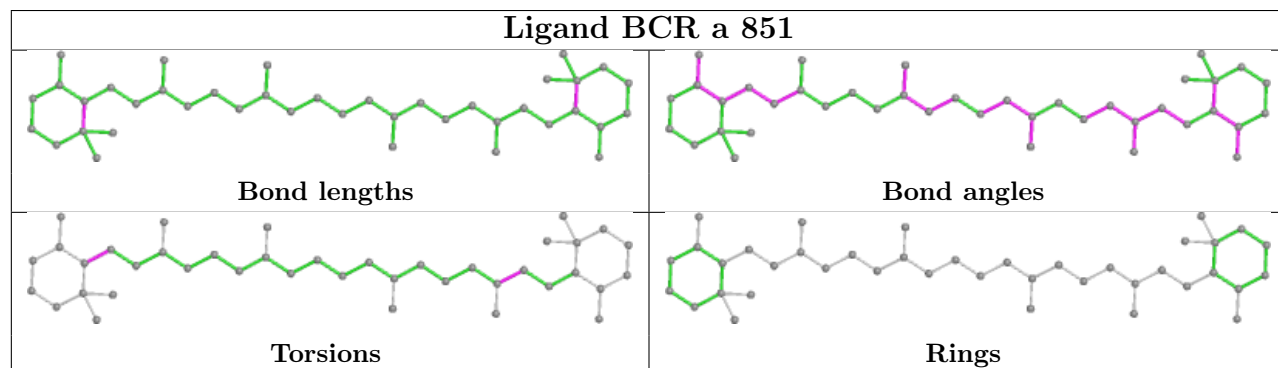
## Ligand CLA b 817



## Ligand DD6 M 306

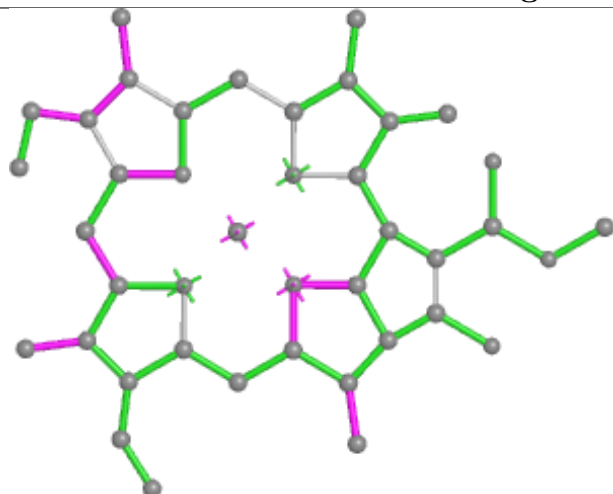


## Ligand BCR a 851

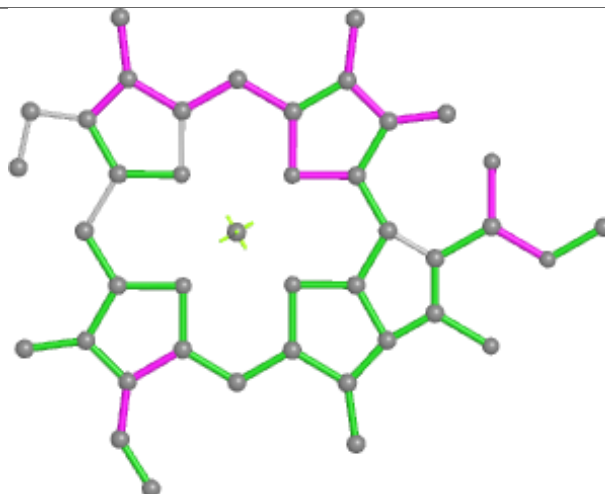




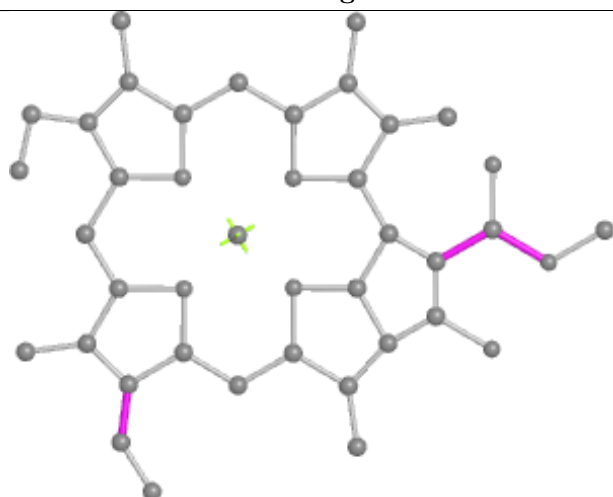
## Ligand CLA I 313



Bond lengths



Bond angles

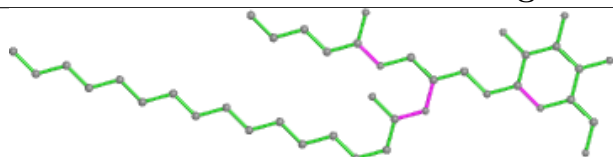


Torsions

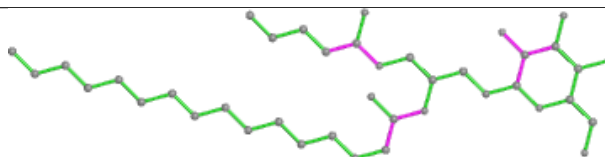


Rings

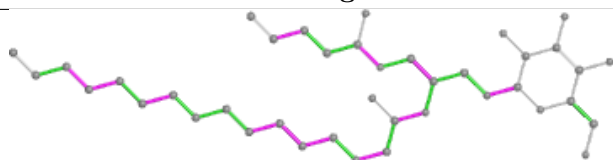
## Ligand LMG I 201



Bond lengths



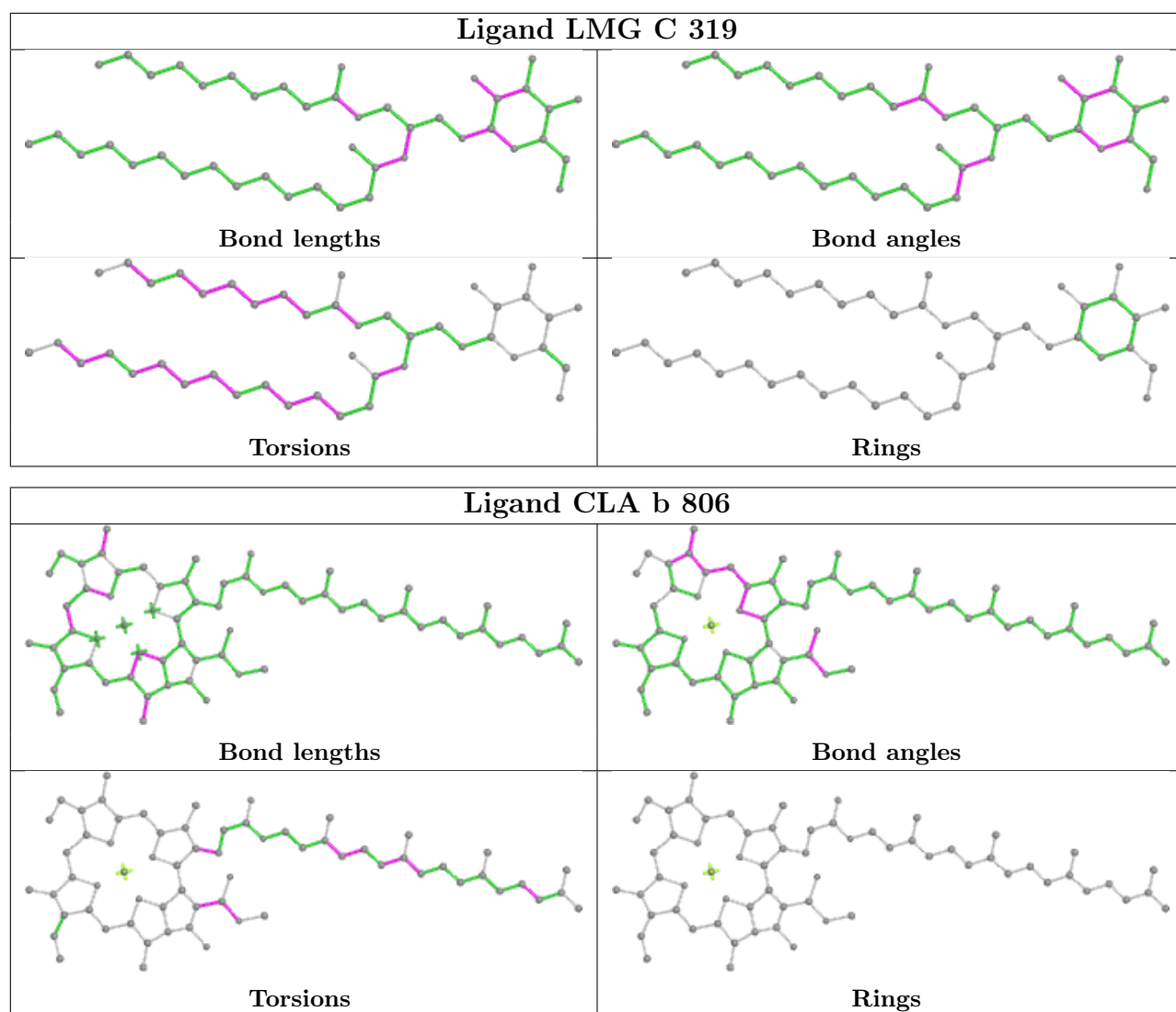
Bond angles



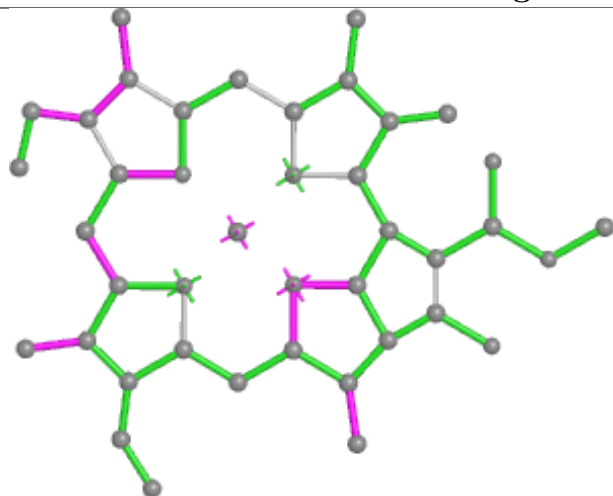
Torsions



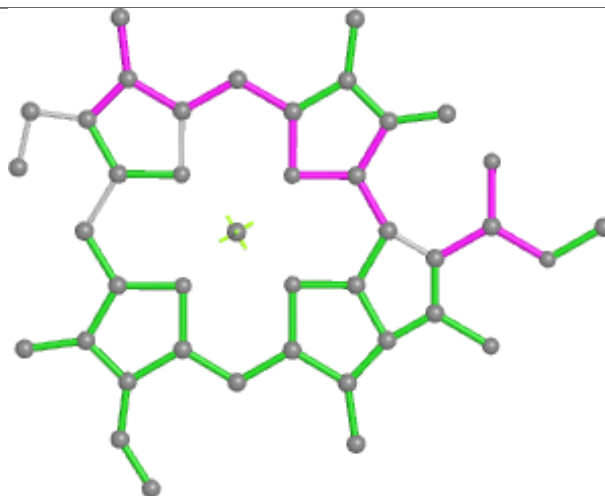
Rings



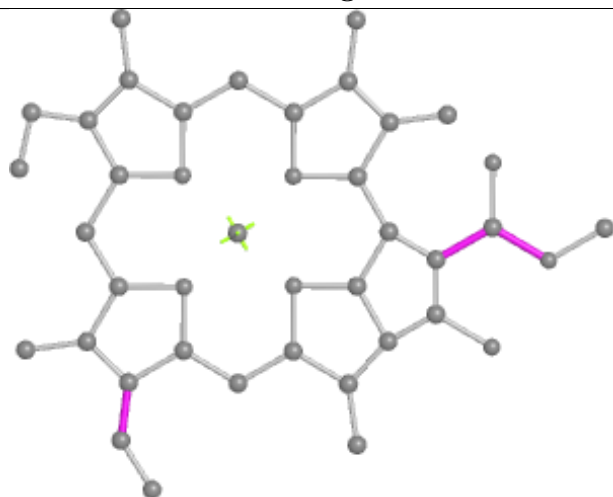
## Ligand CLA K 317



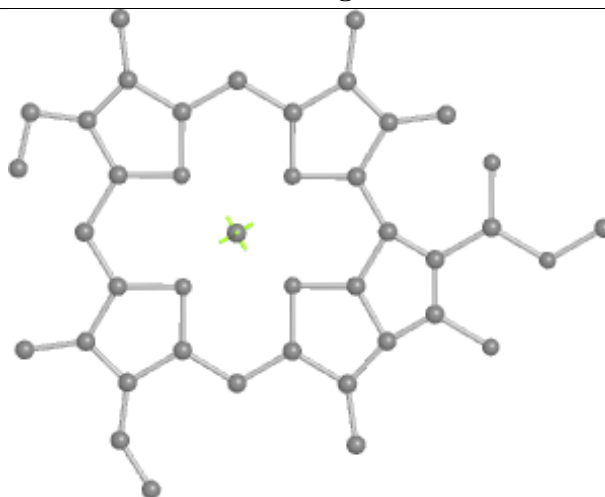
Bond lengths



Bond angles

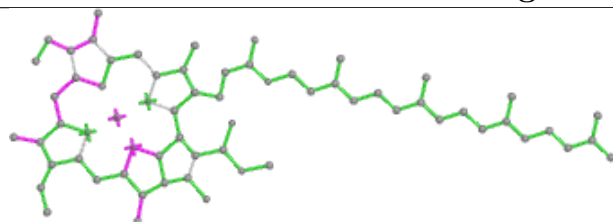


Torsions

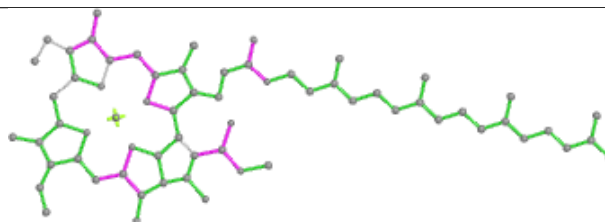


Rings

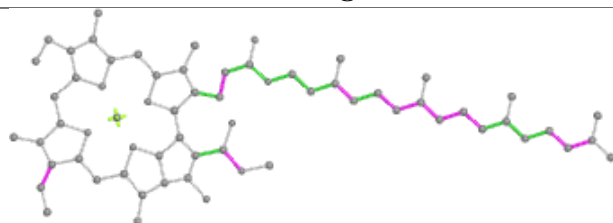
## Ligand CLA a 856



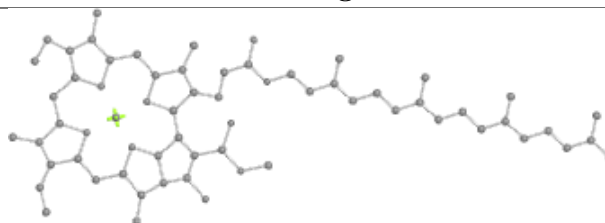
Bond lengths



Bond angles

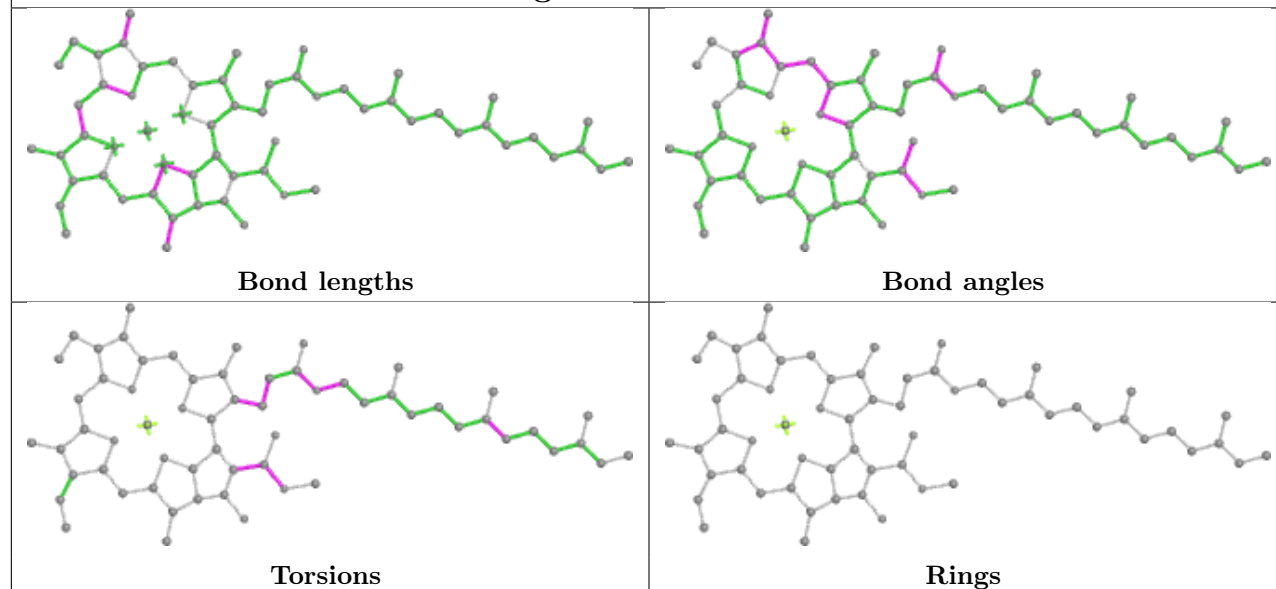


Torsions

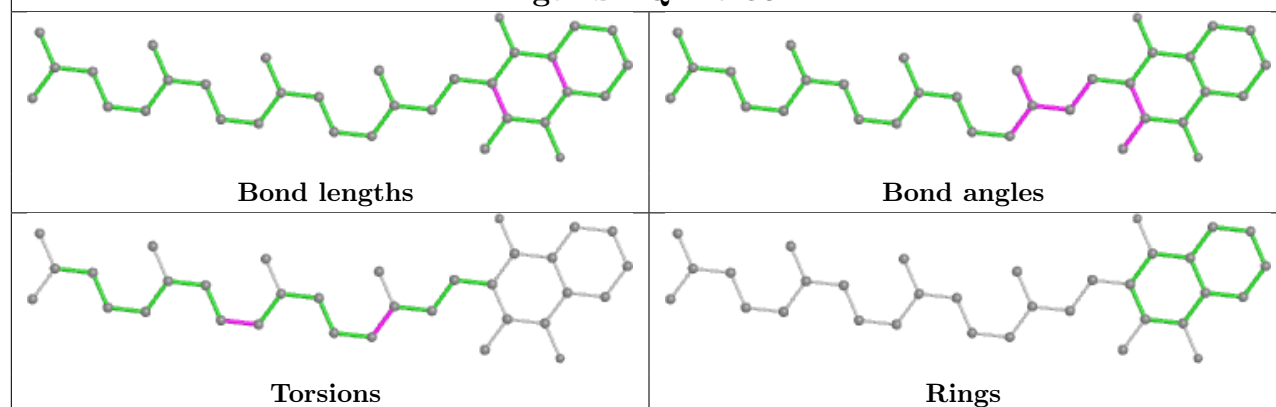


Rings

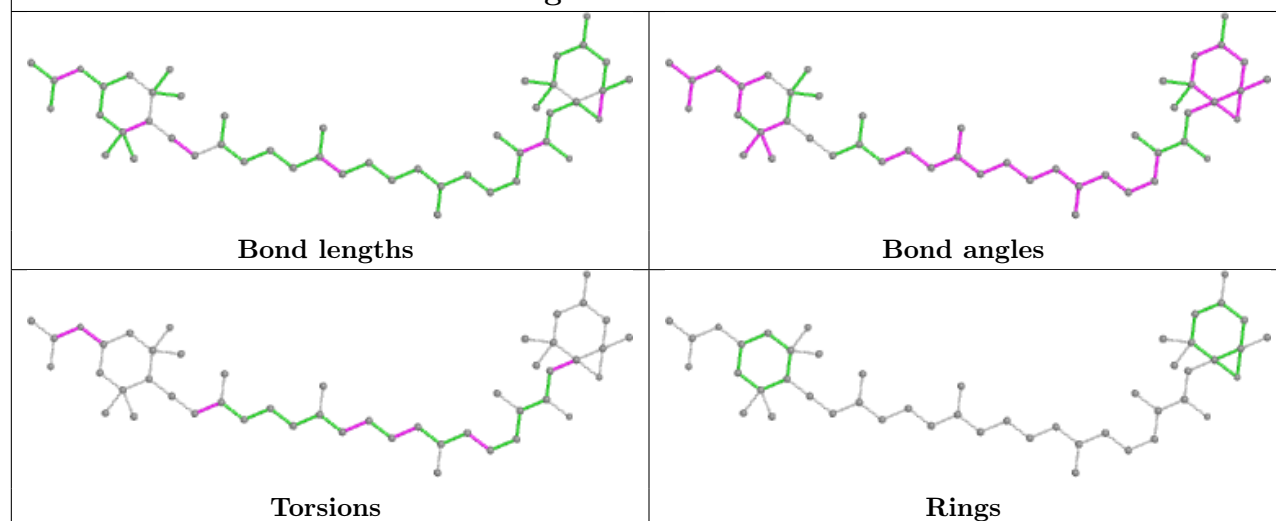
## Ligand CLA F 305



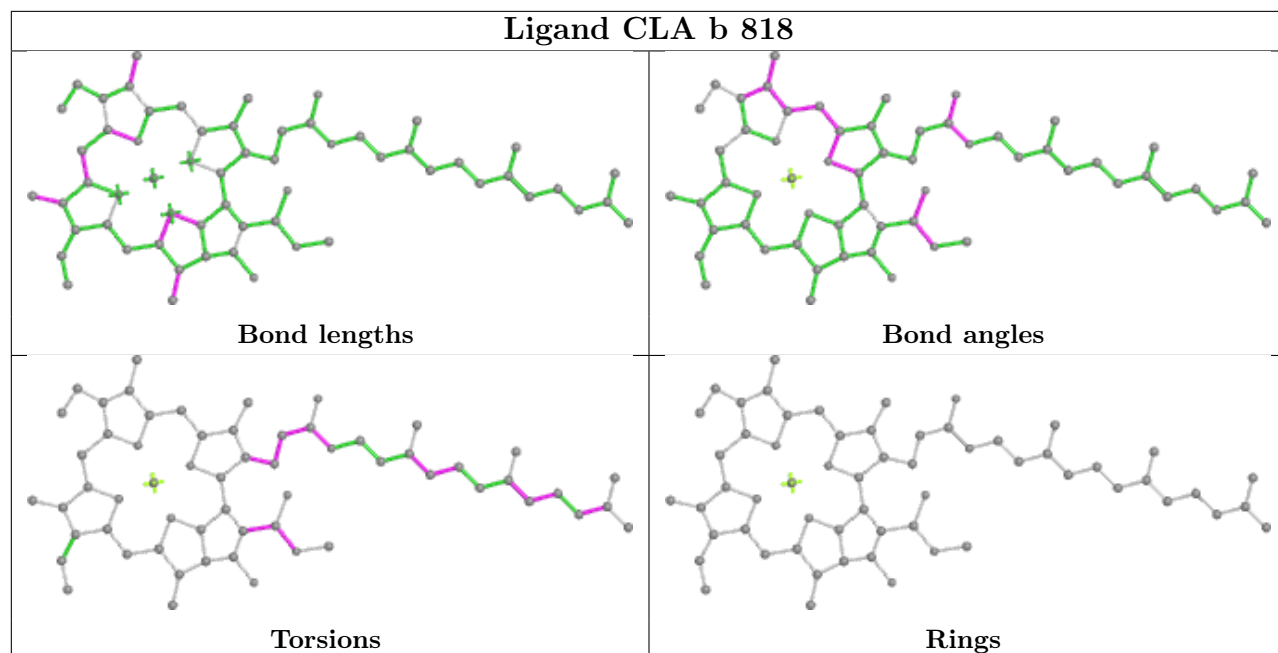
## Ligand PQN b 832



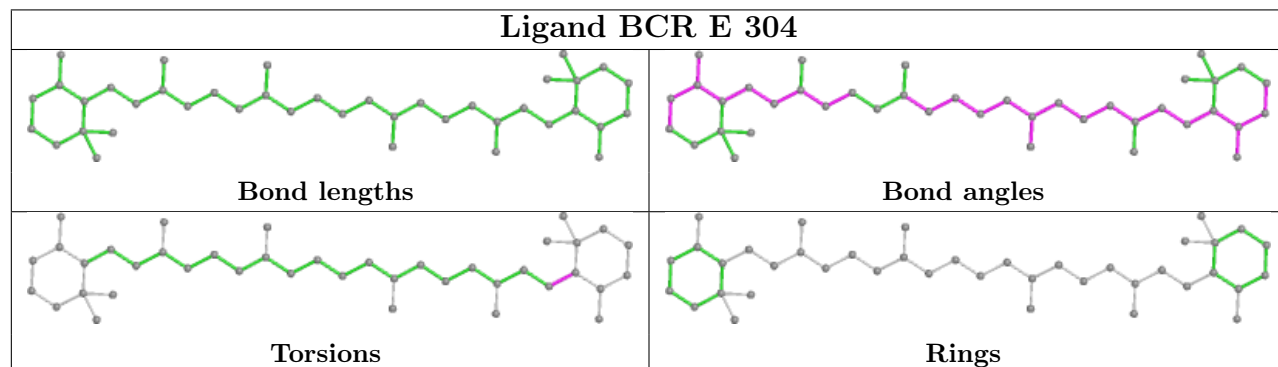
## Ligand A86 I 301



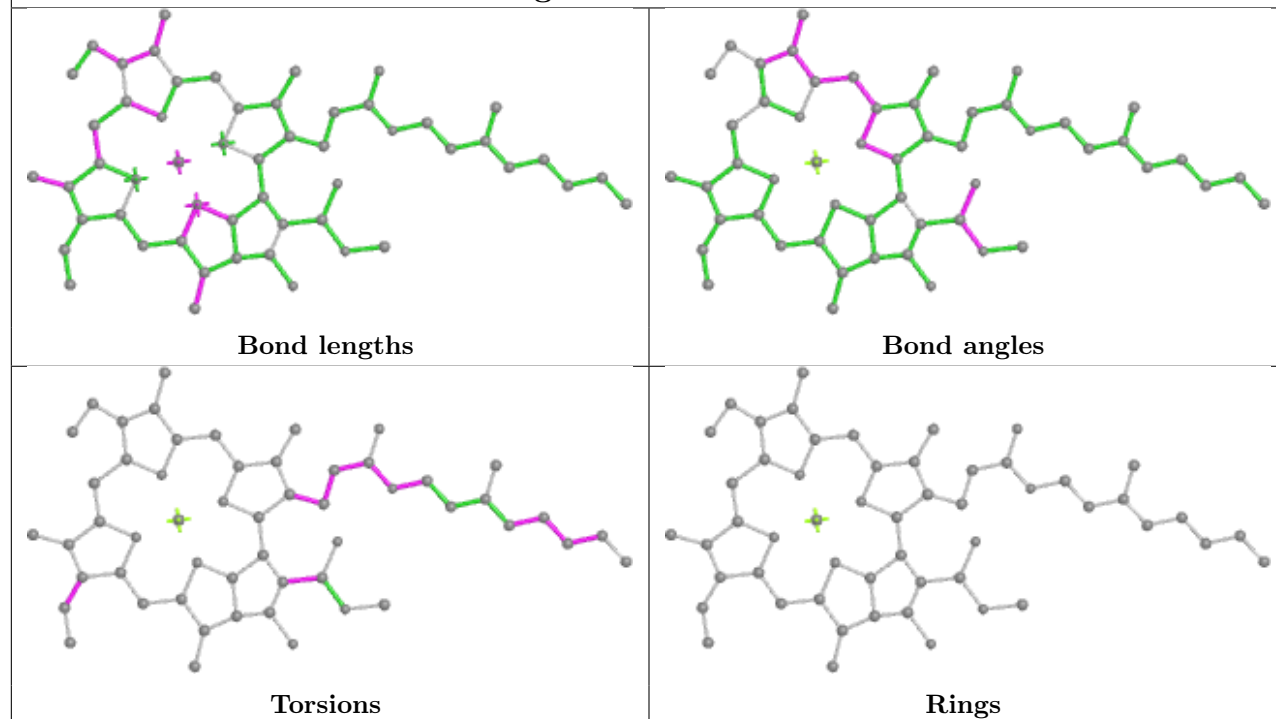
## Ligand CLA b 818



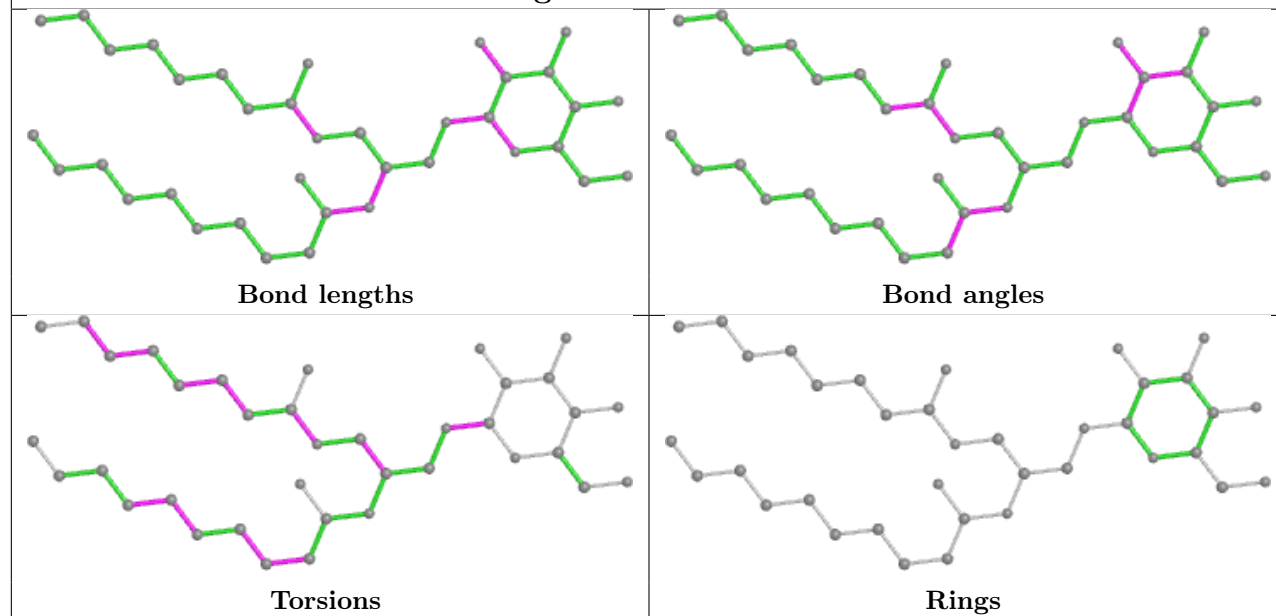
## Ligand BCR E 304



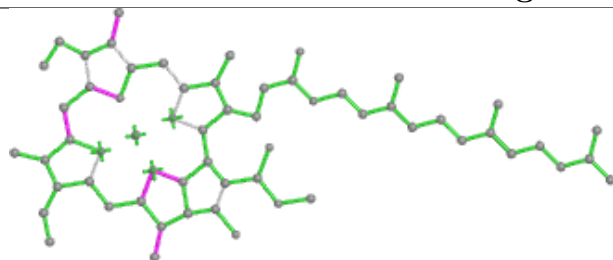
## Ligand CLA L 307



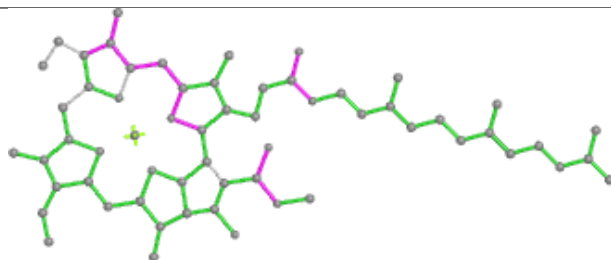
## Ligand LMG I 319



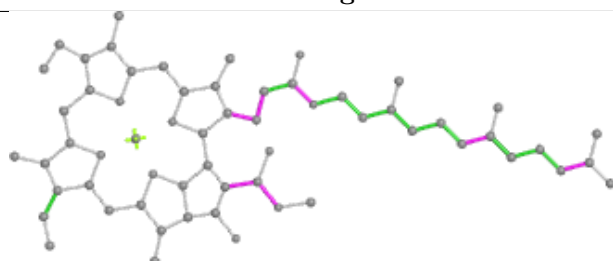
## Ligand CLA F 310



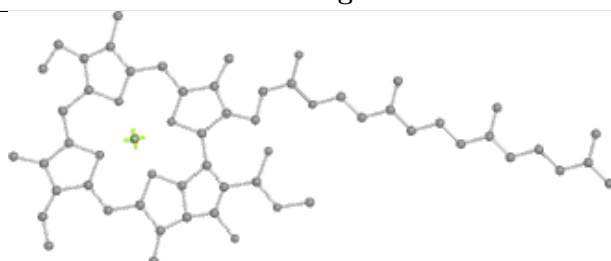
Bond lengths



Bond angles

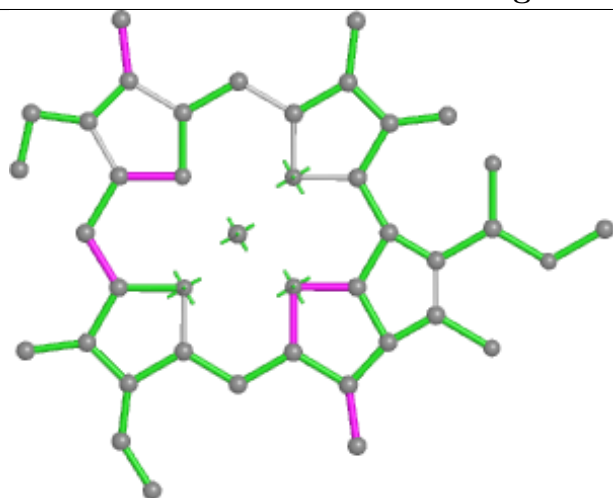


Torsions

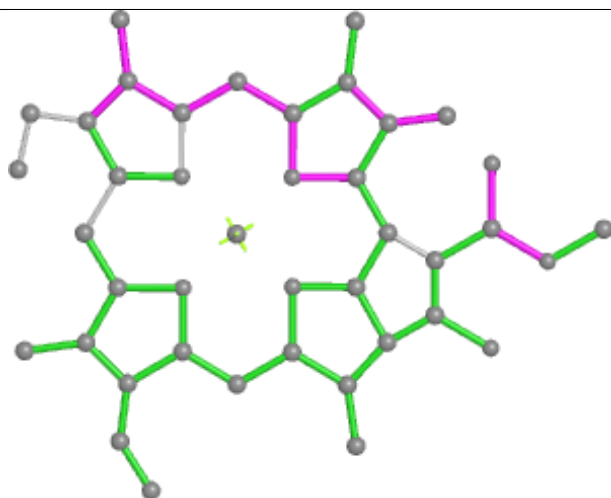


Rings

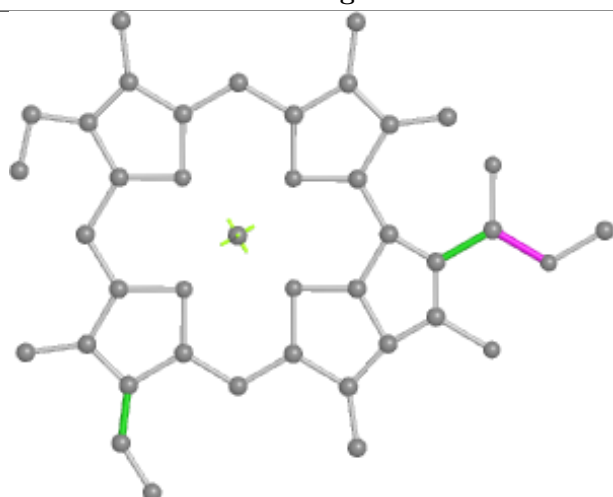
## Ligand CLA D 215



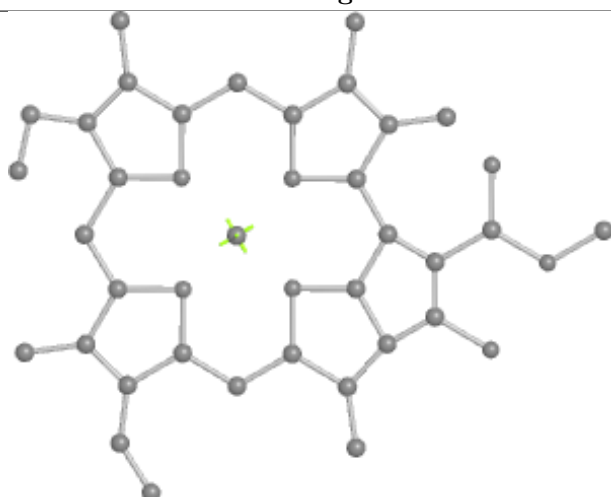
Bond lengths



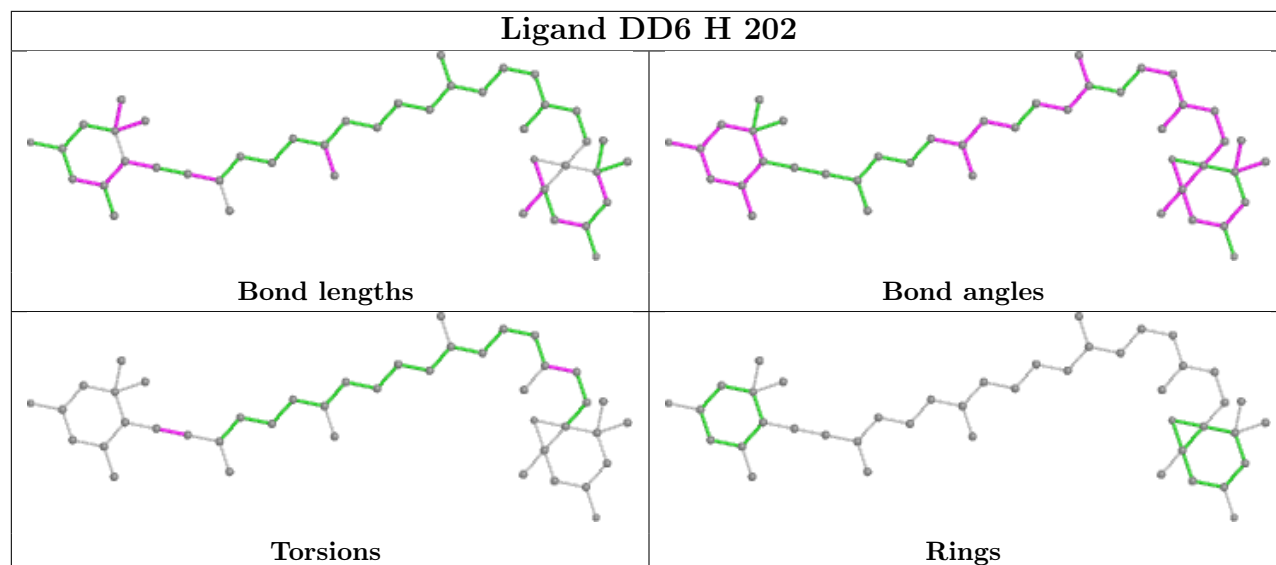
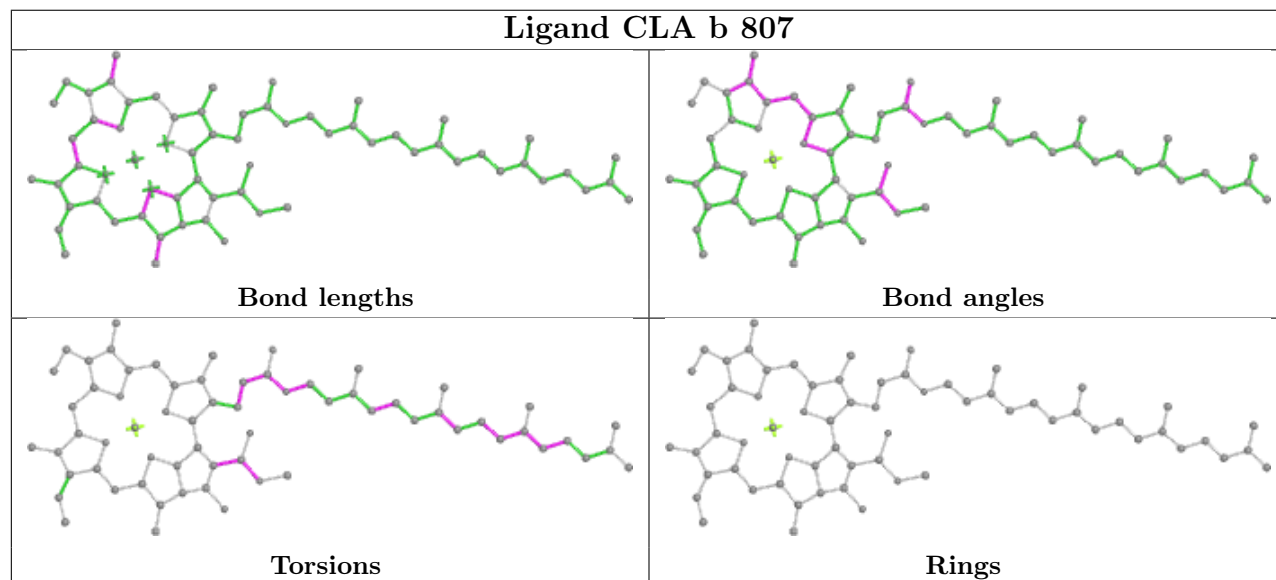
Bond angles



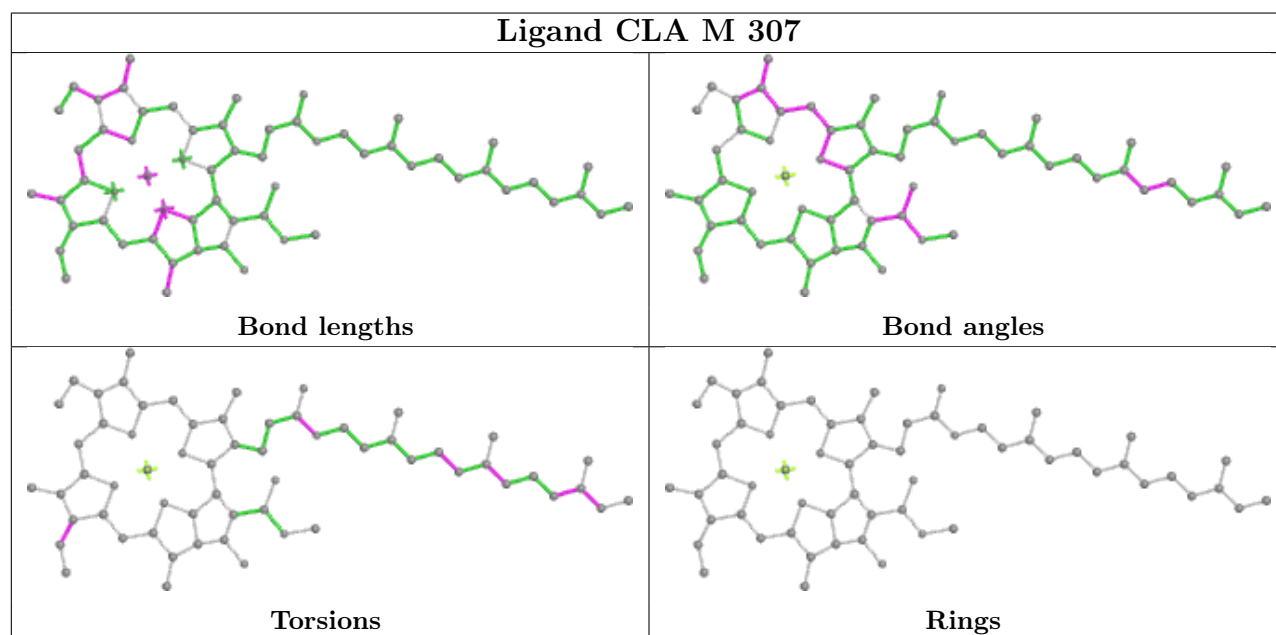
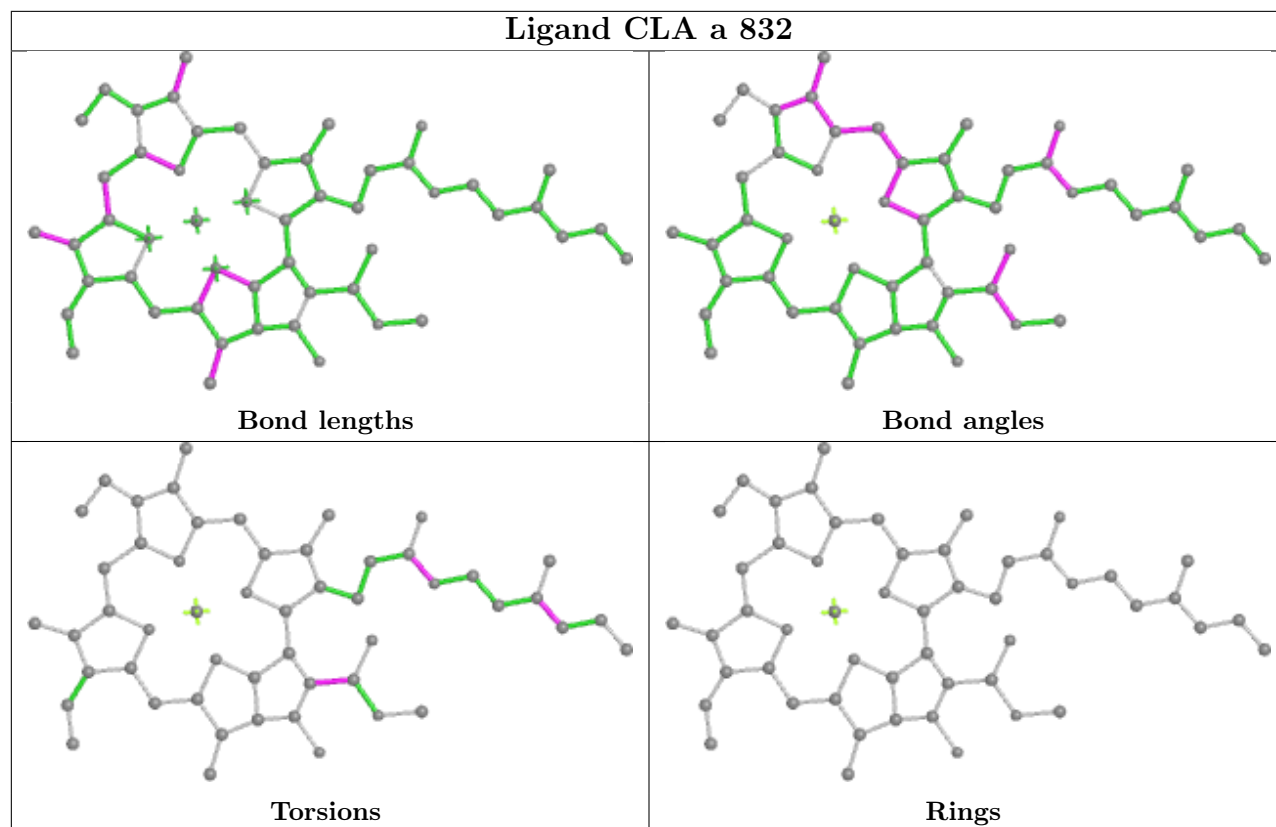
Torsions

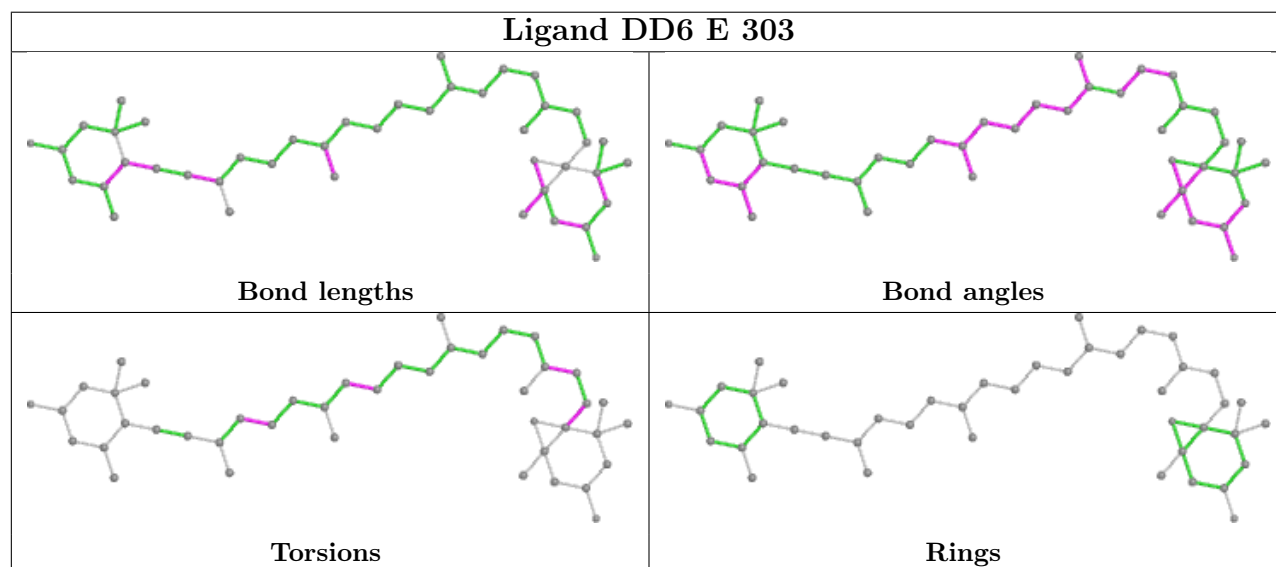
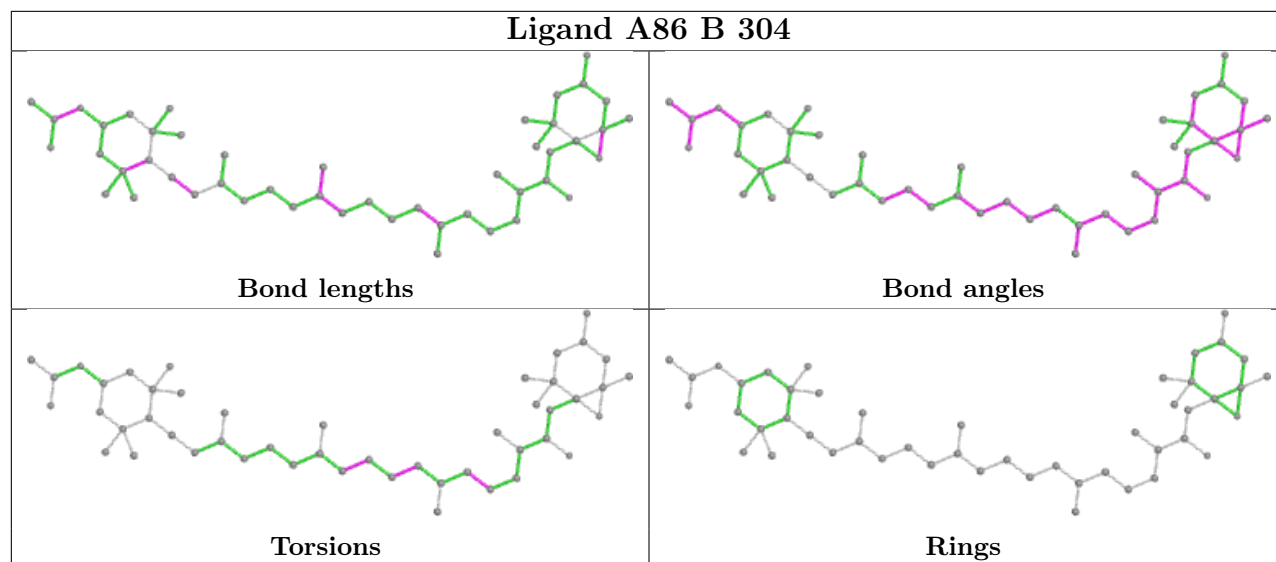
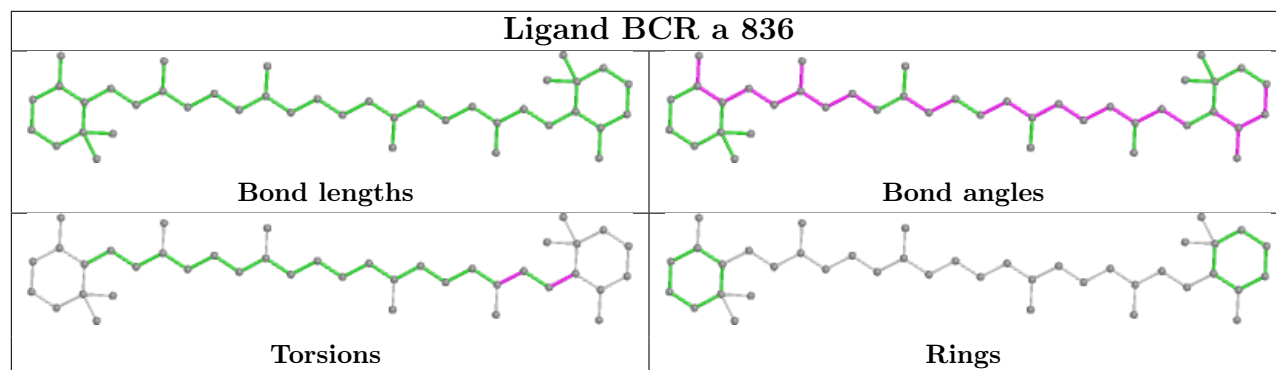


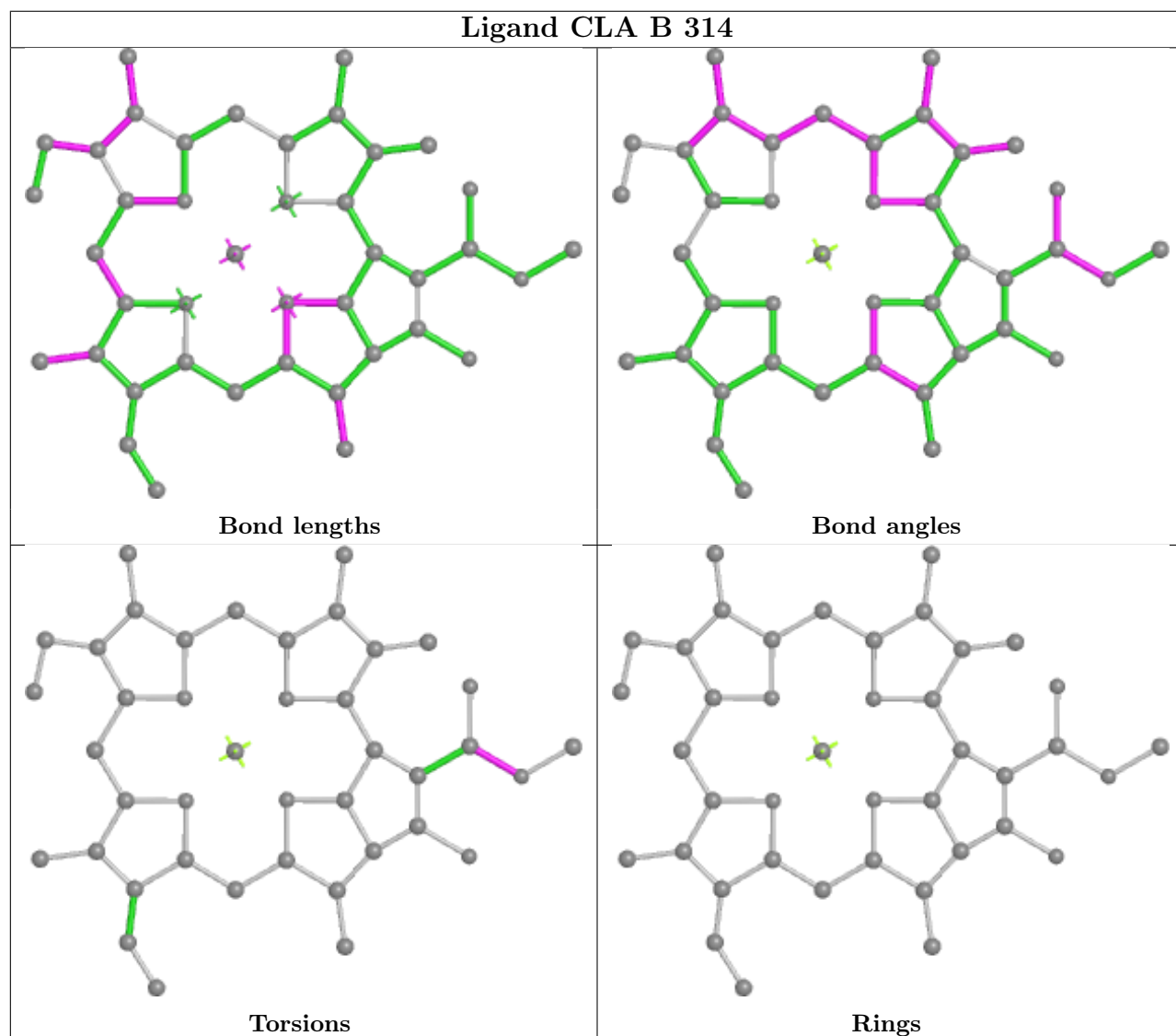
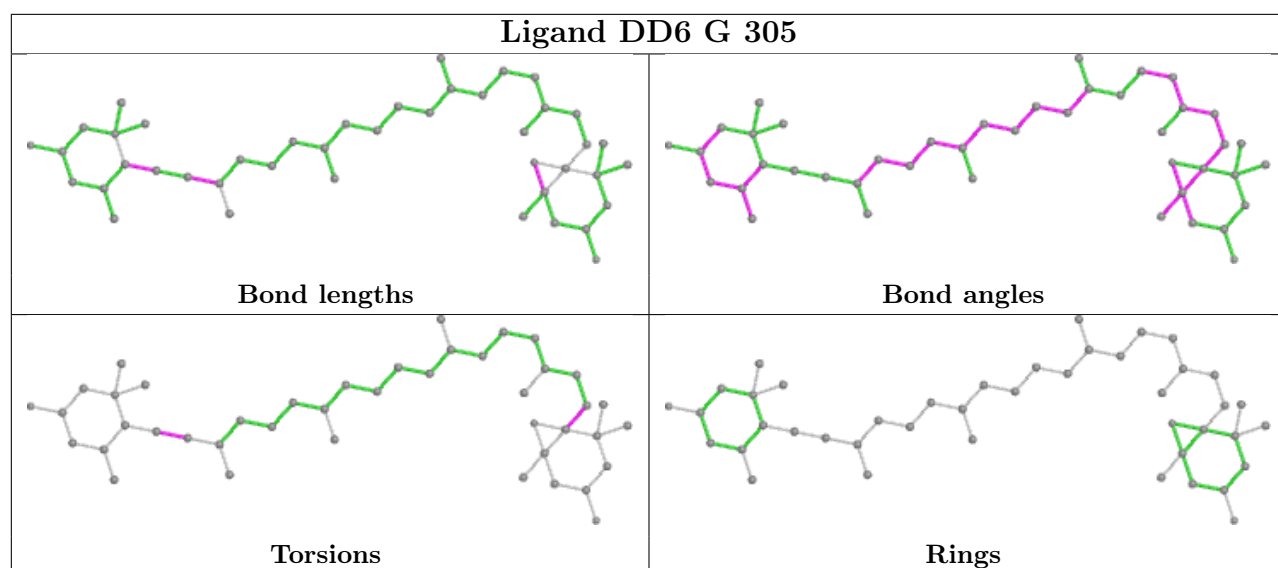
Rings

**Ligand DD6 H 202****Ligand CLA b 807**

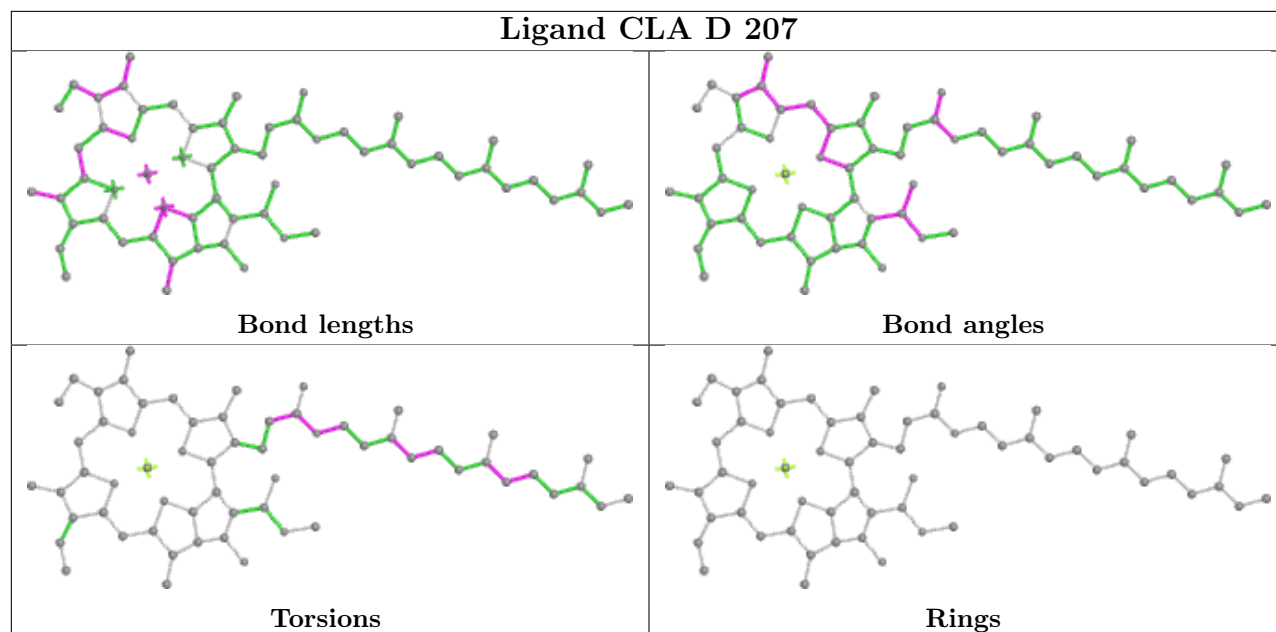




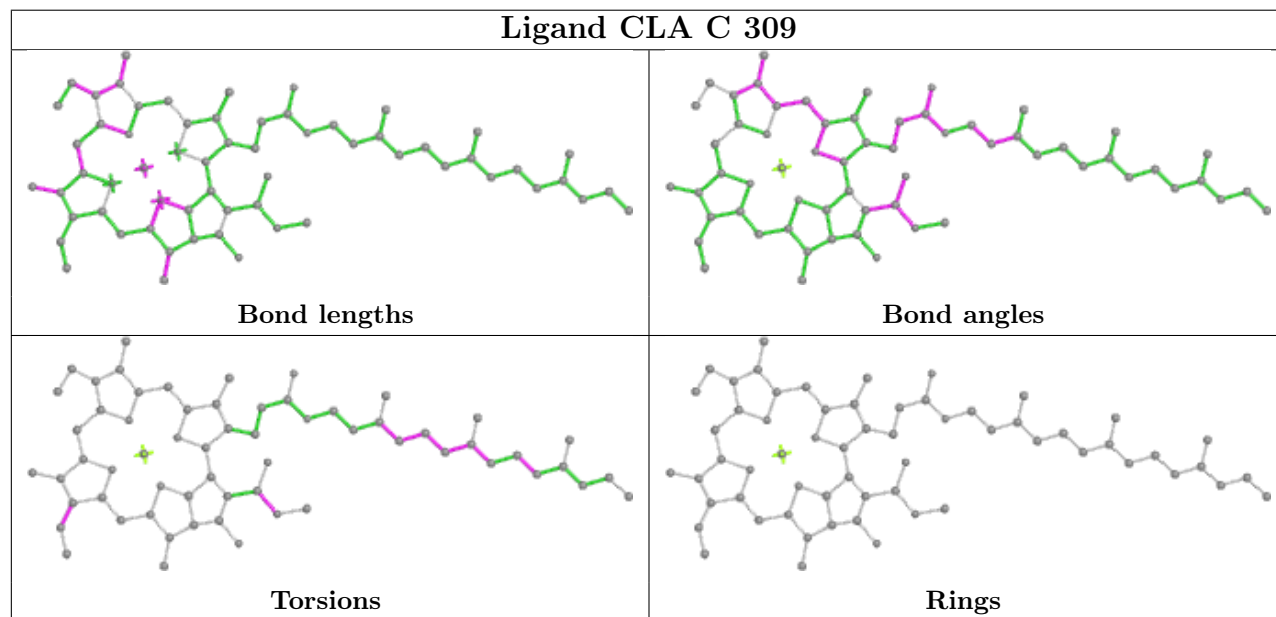


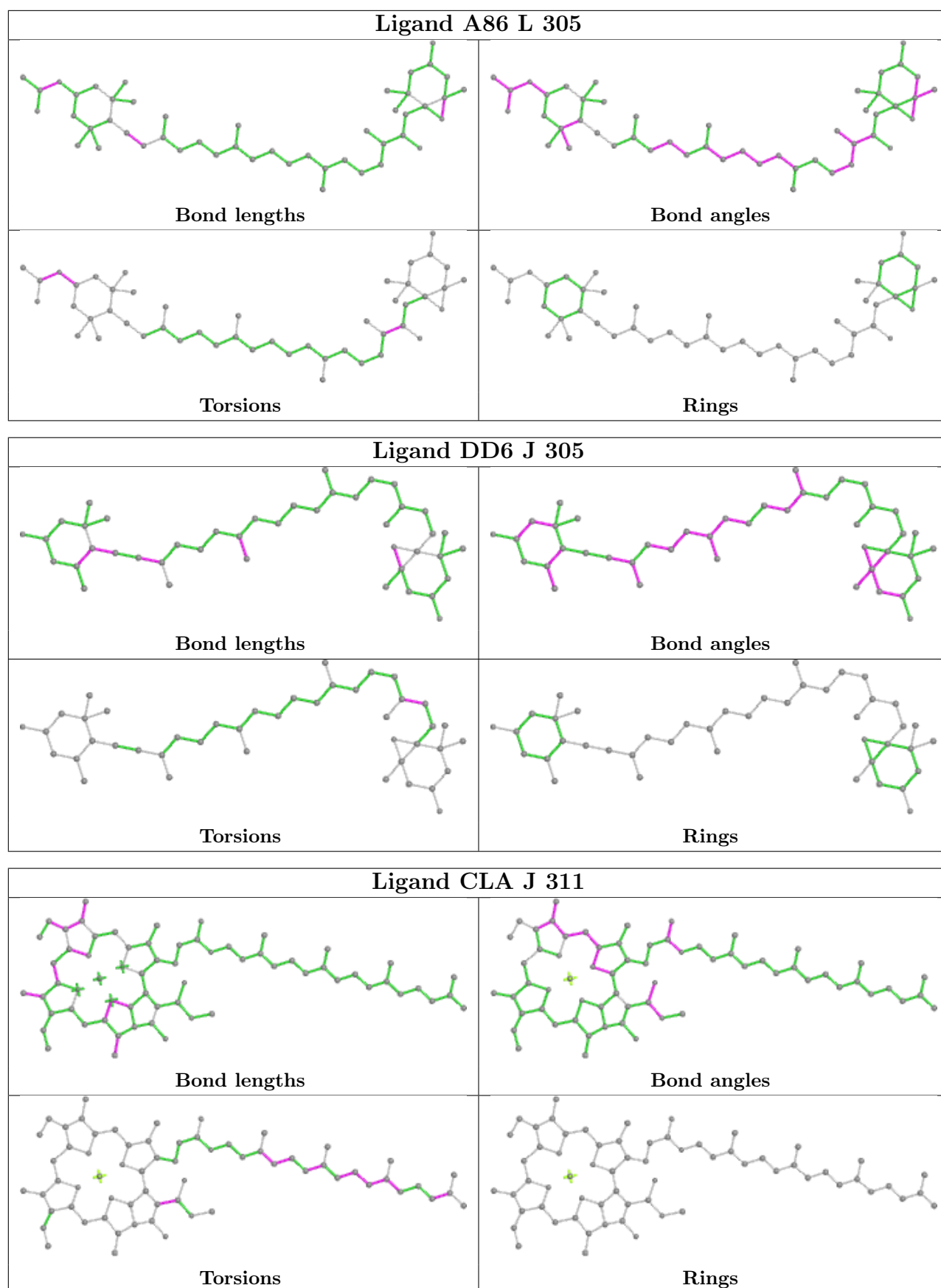


## Ligand CLA D 207

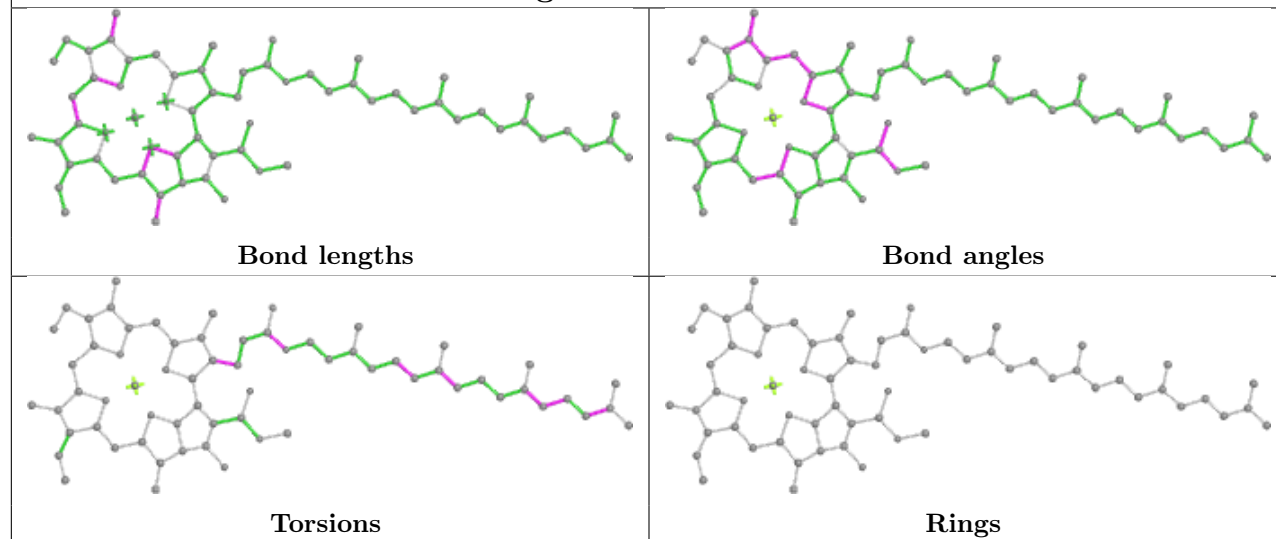


## Ligand CLA C 309

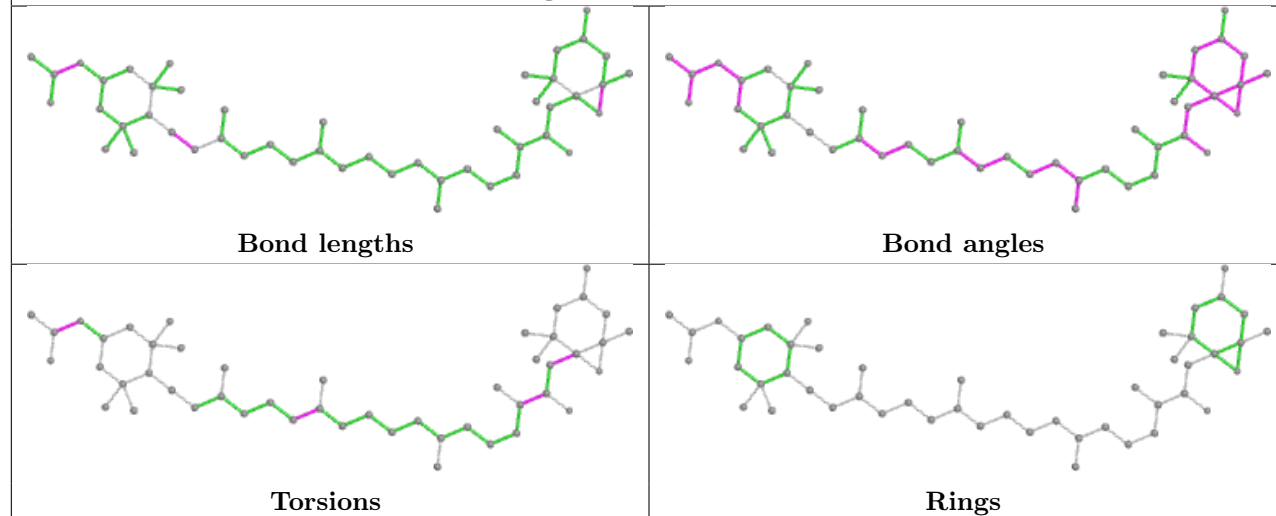




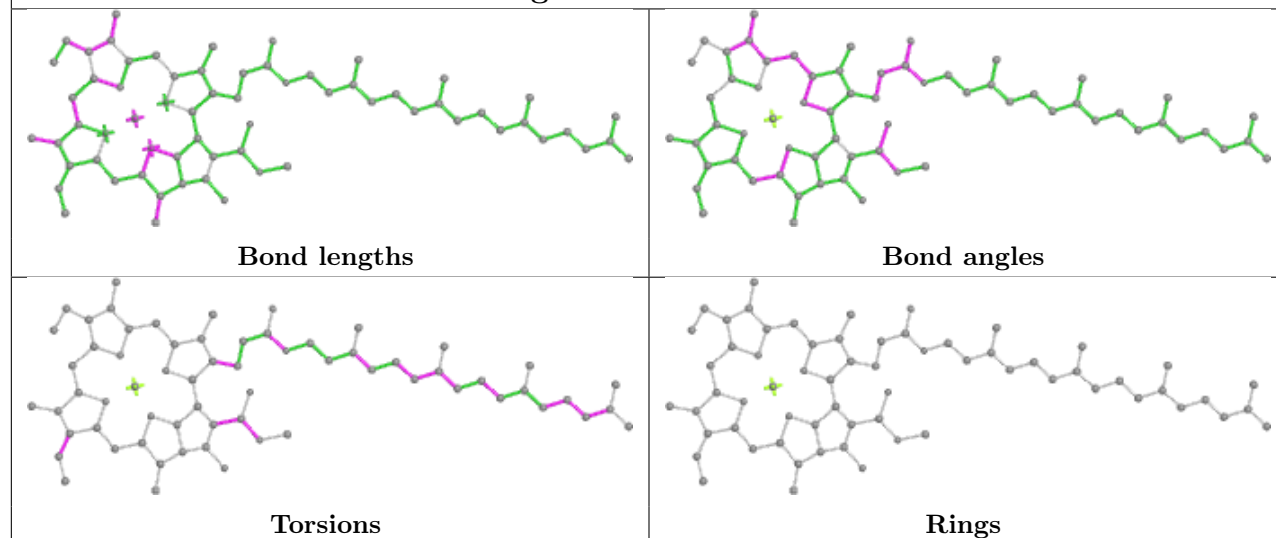
## Ligand CLA a 840



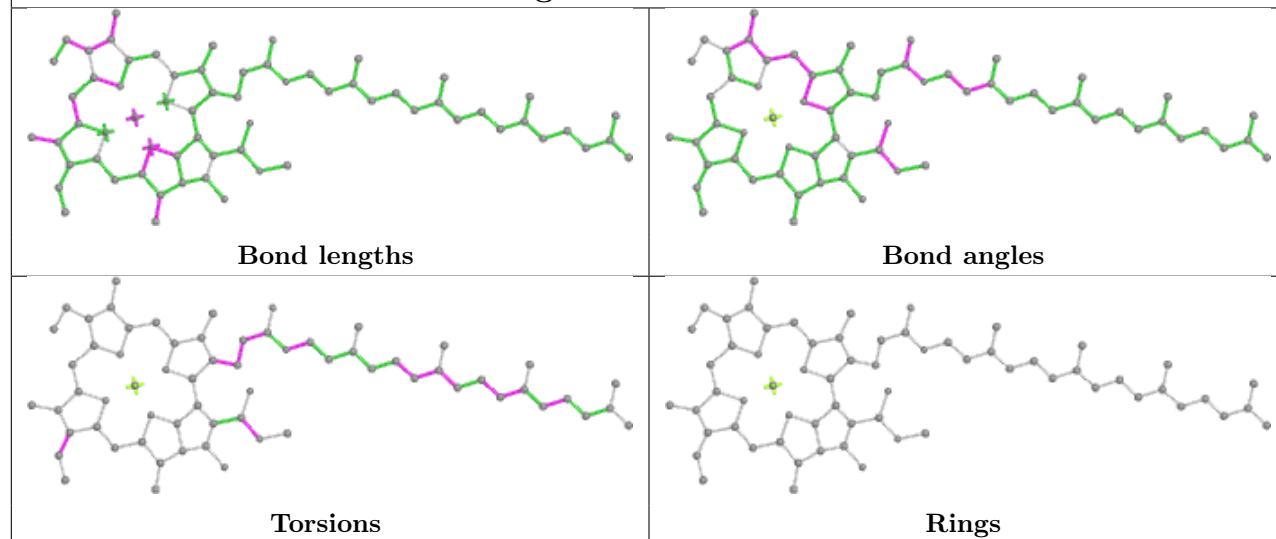
## Ligand A86 L 302



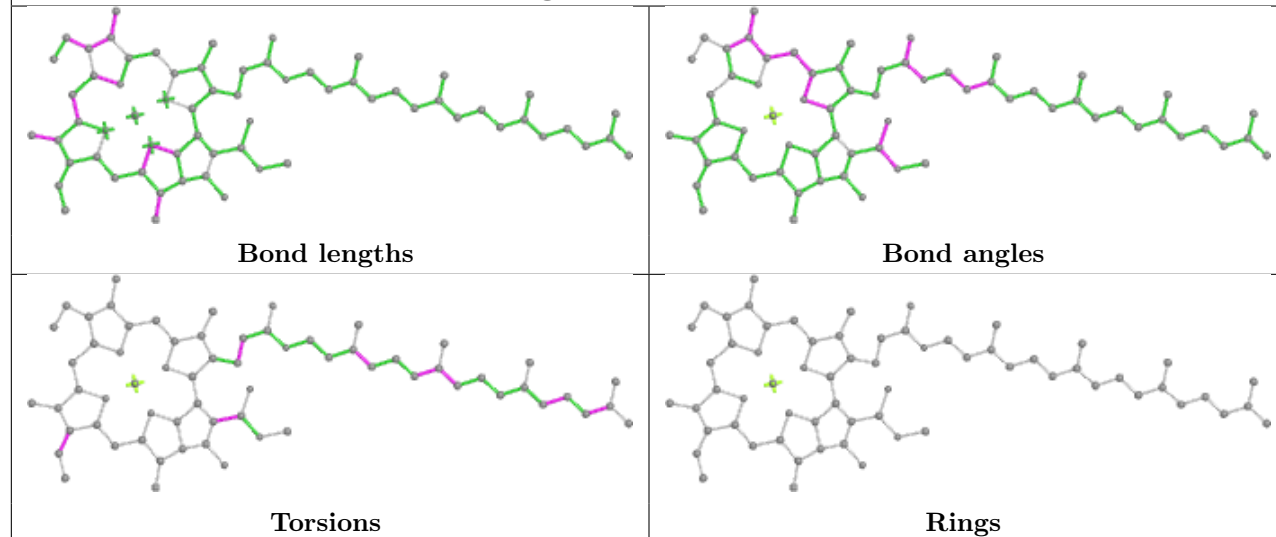
## Ligand CLA K 312



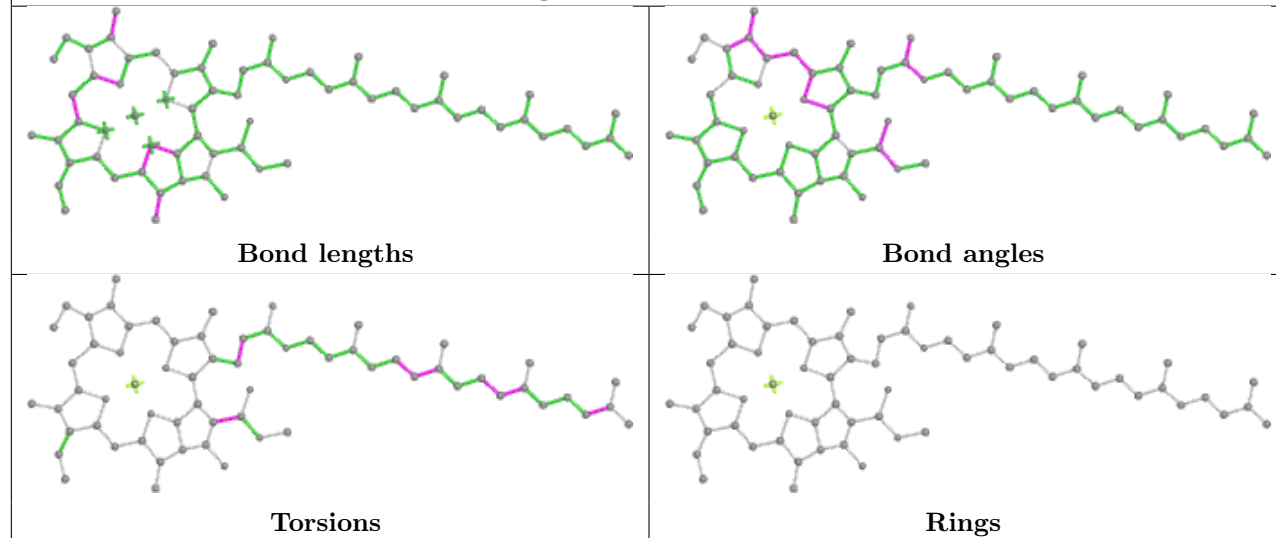
## Ligand CLA b 825

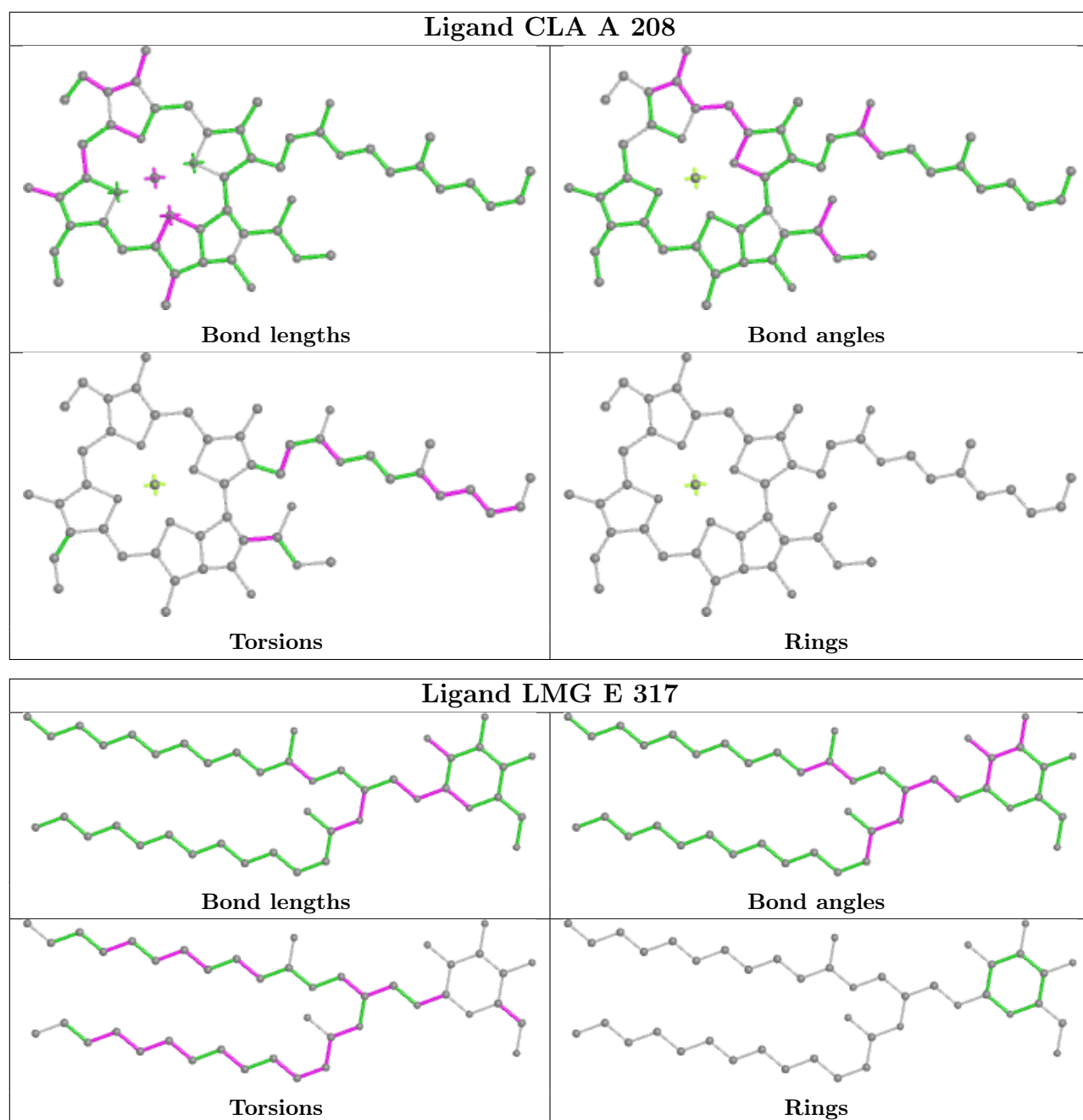


## Ligand CLA I 308



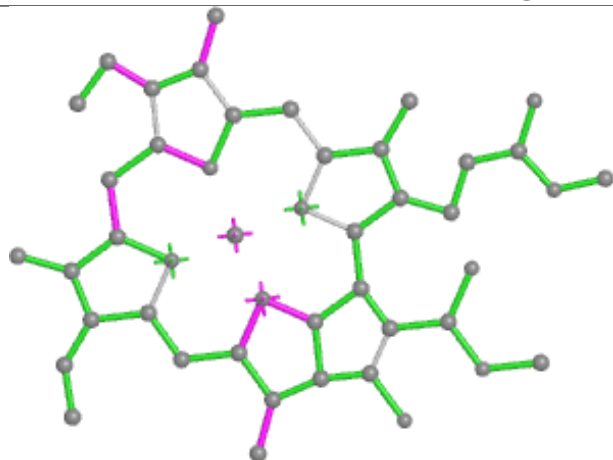
## Ligand CLA b 808



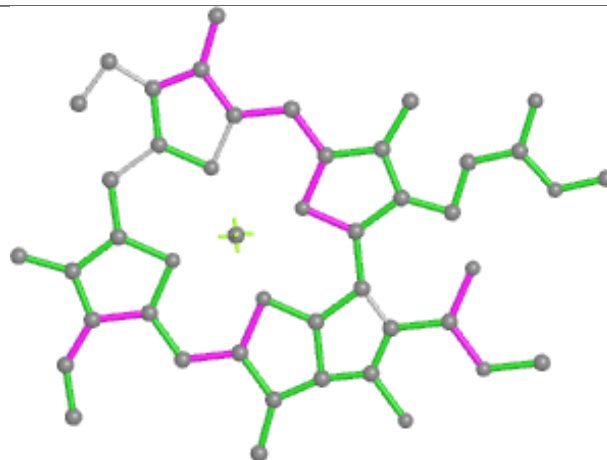




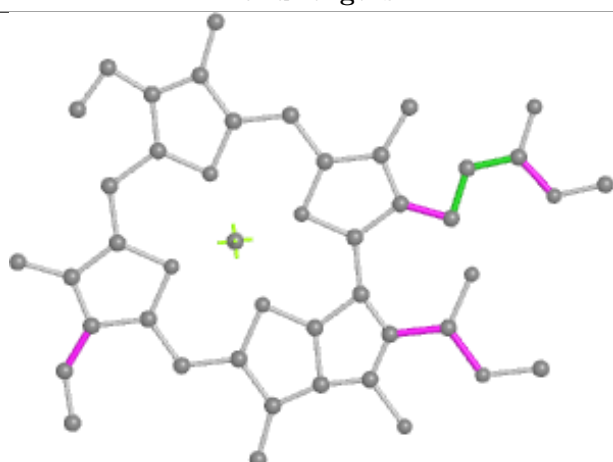
## Ligand CLA J 310



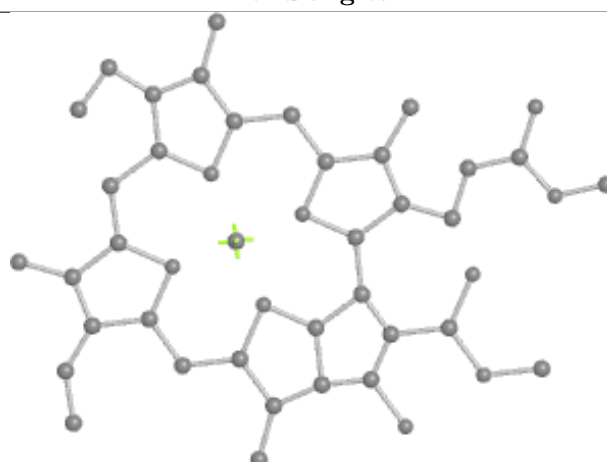
Bond lengths



Bond angles

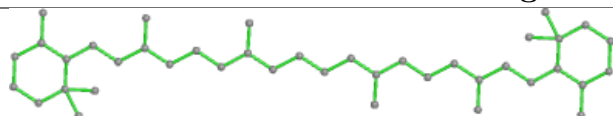


Torsions

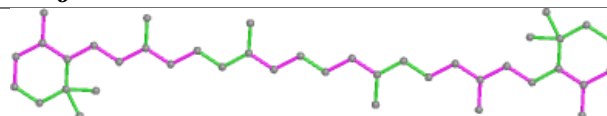


Rings

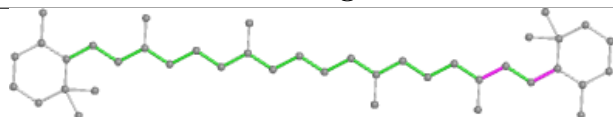
## Ligand BCR j 101



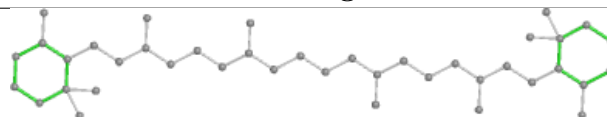
Bond lengths



Bond angles

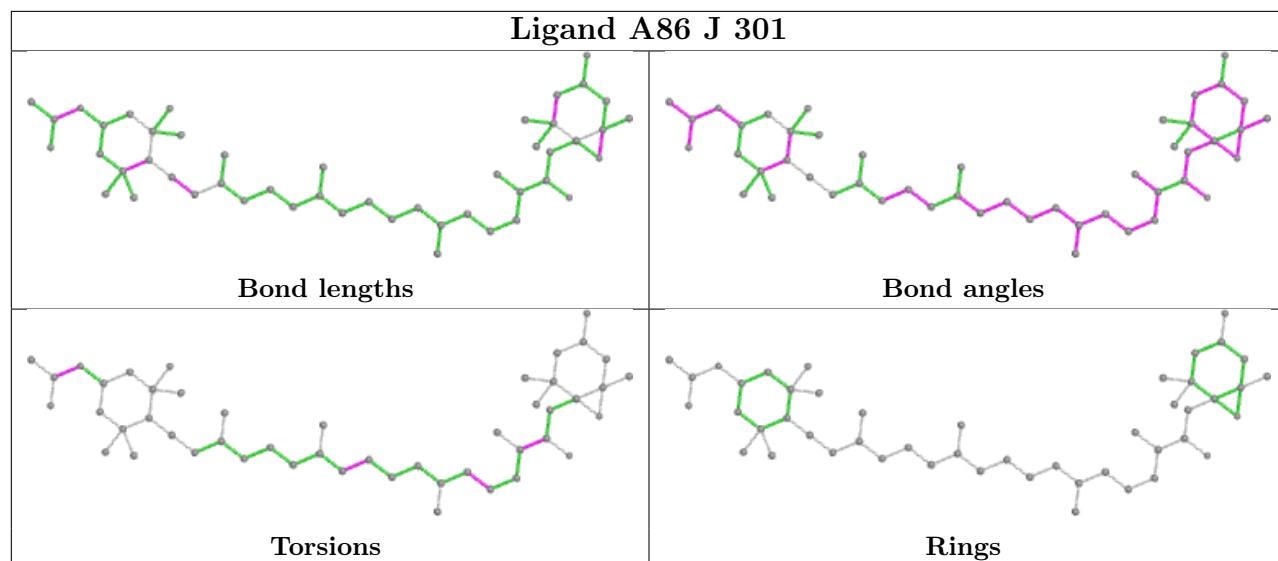


Torsions

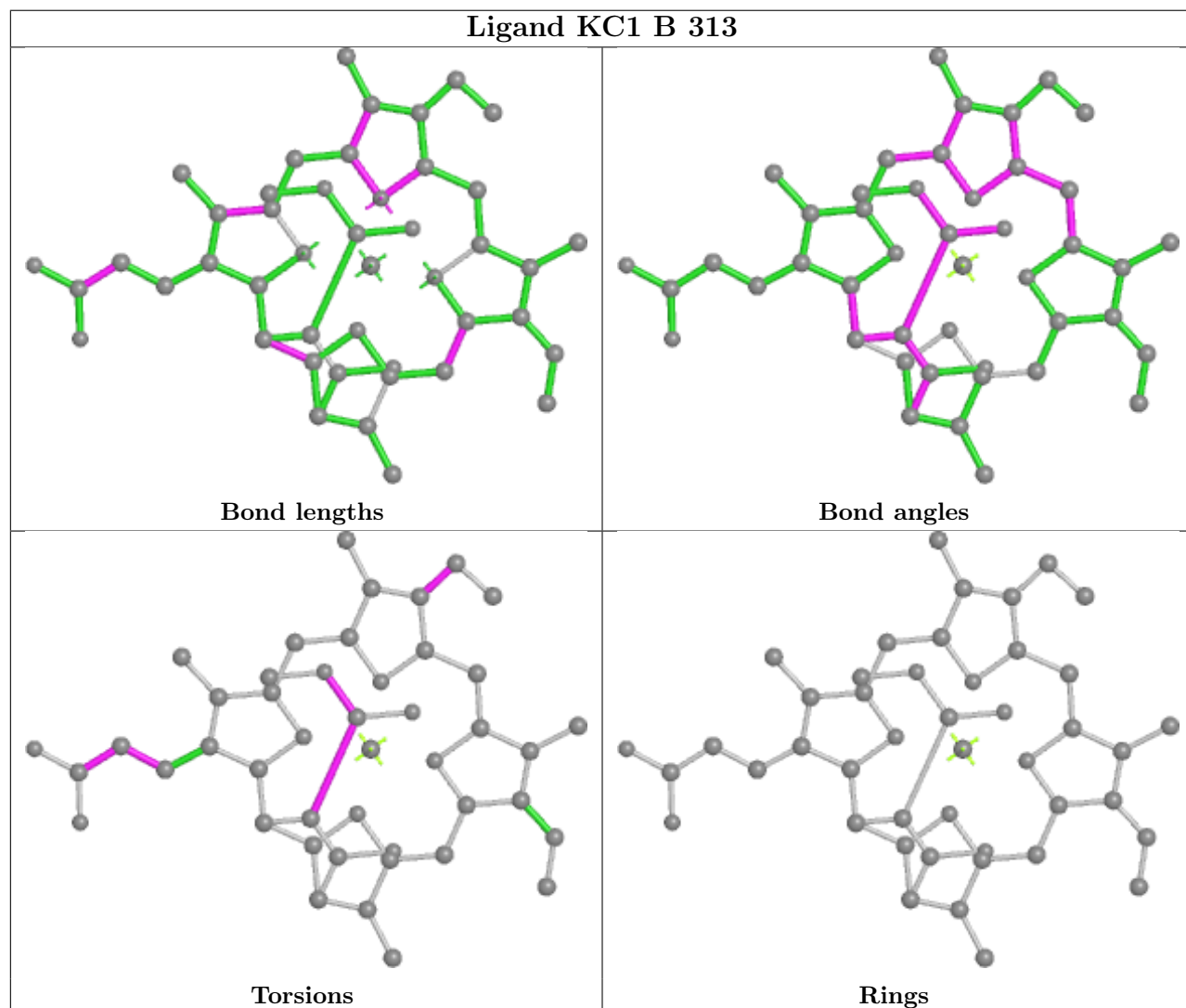


Rings

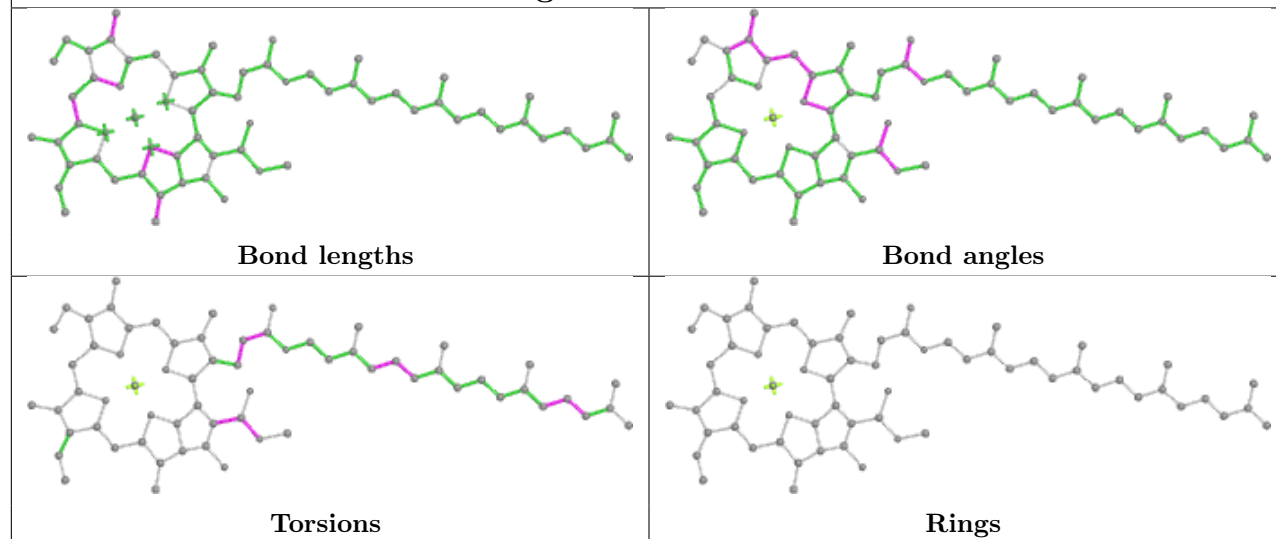
## Ligand A86 J 301



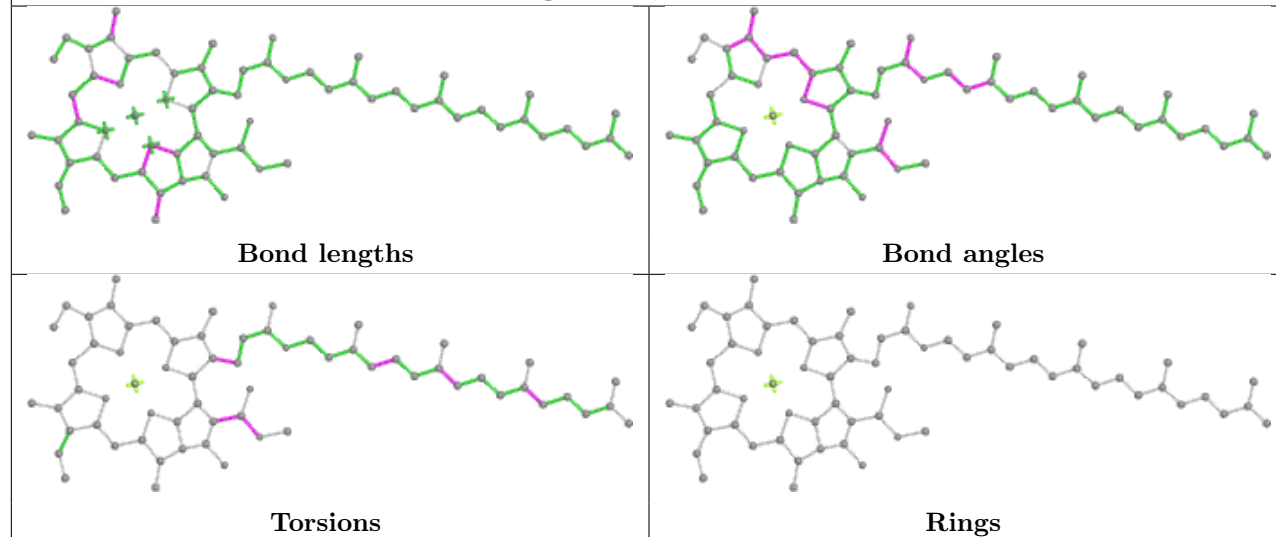
## Ligand KC1 B 313

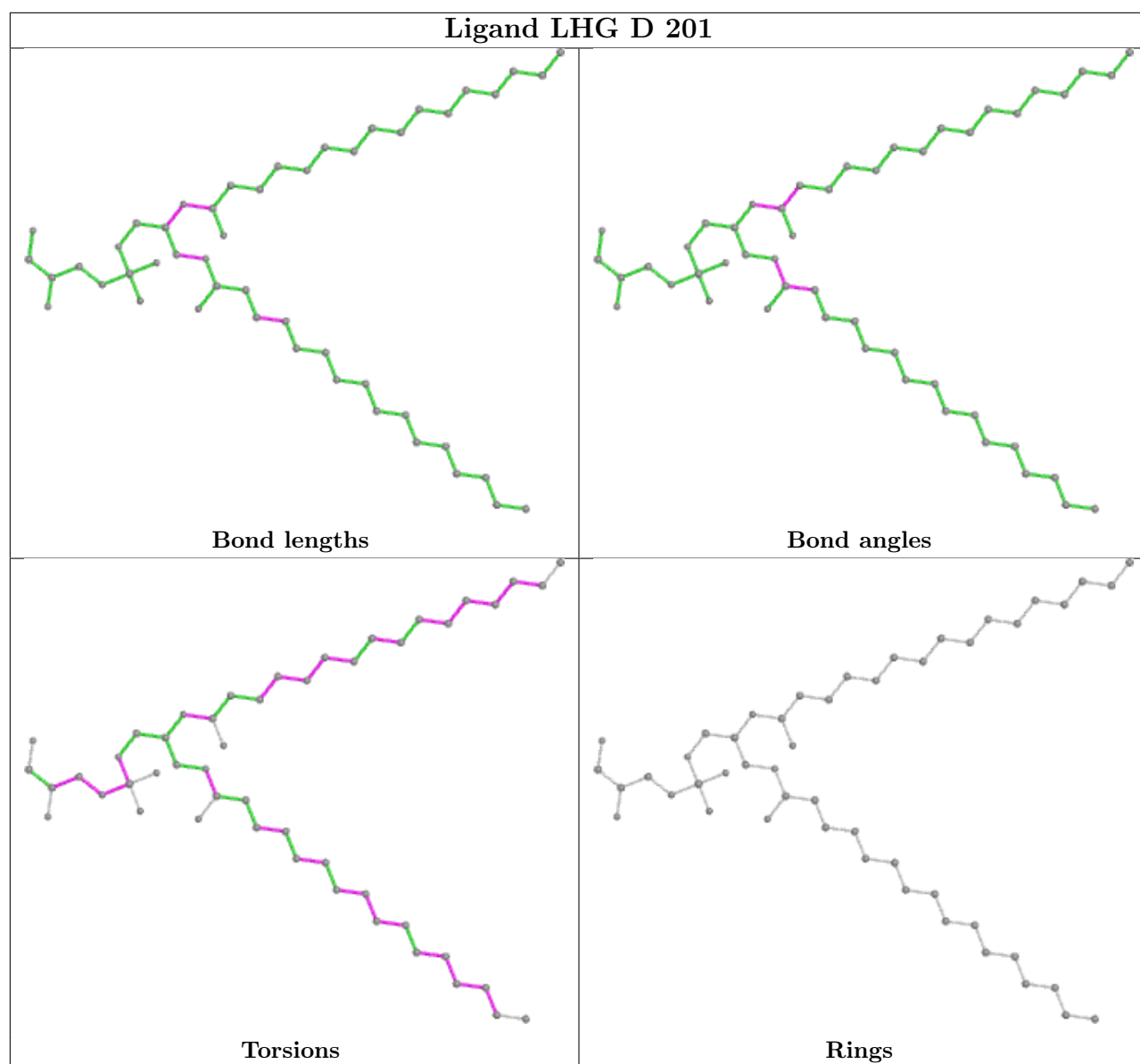


## Ligand CLA a 829

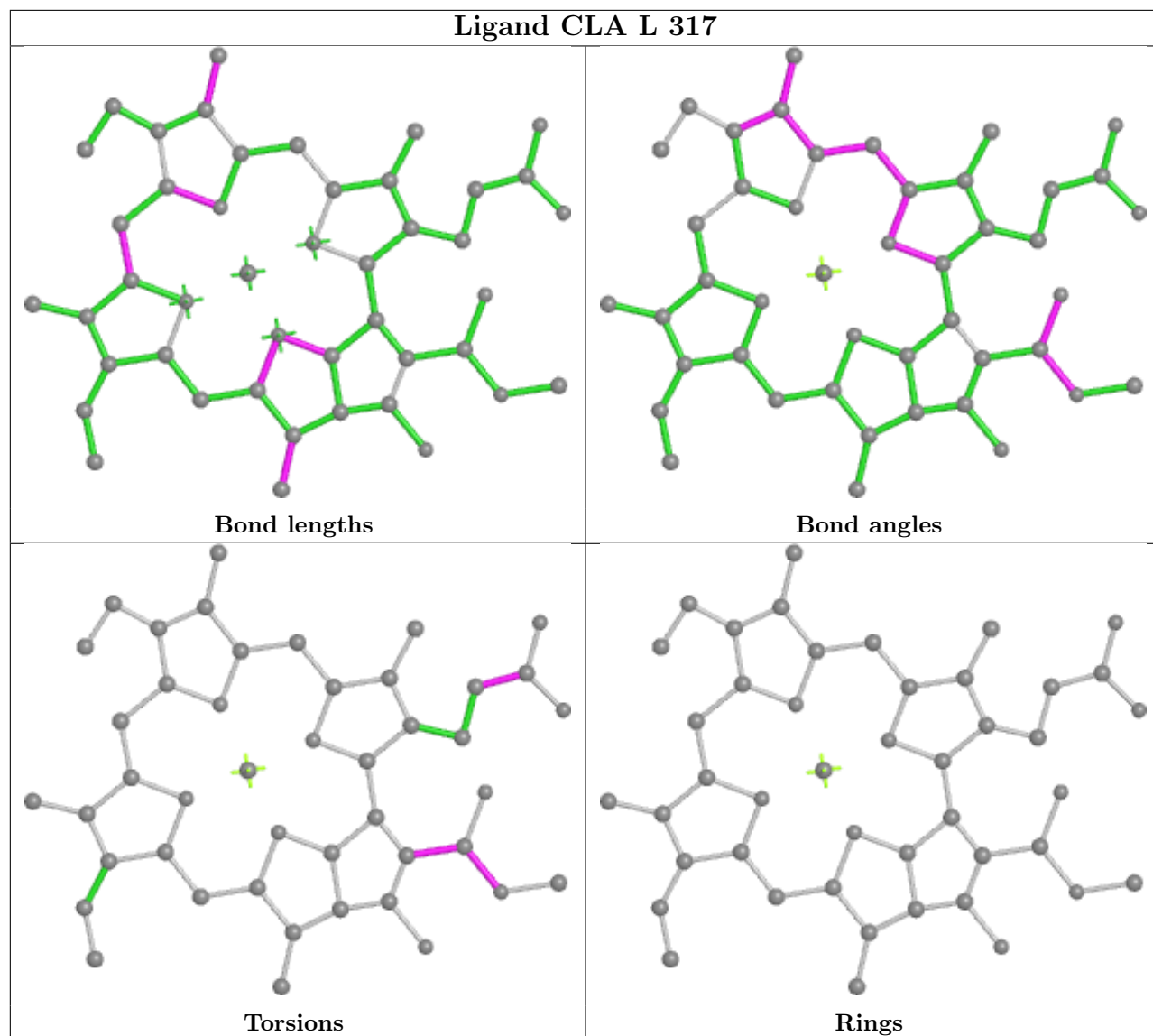


## Ligand CLA f 301

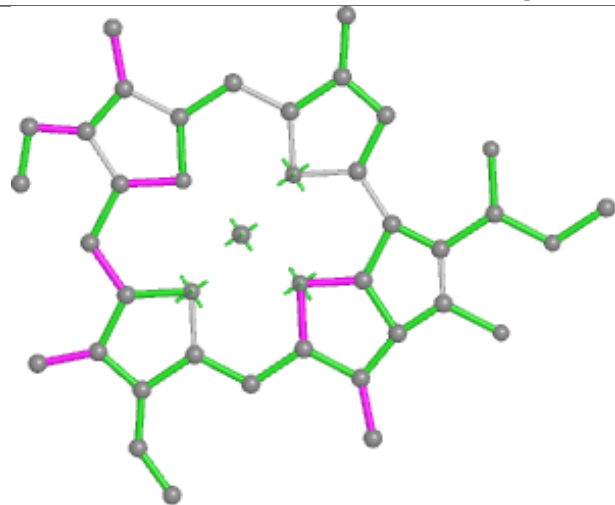




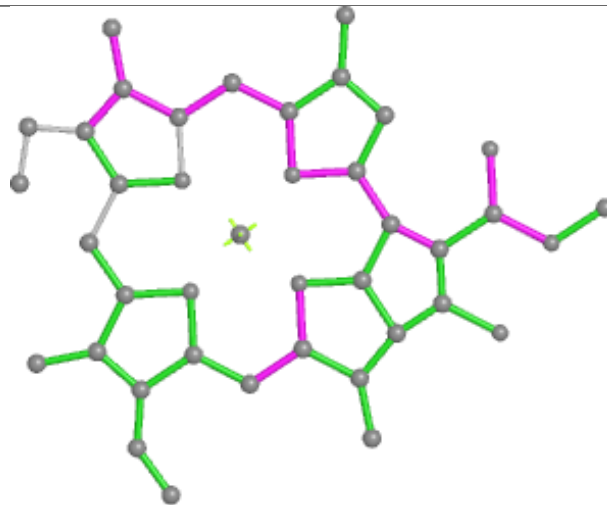
## Ligand CLA L 317



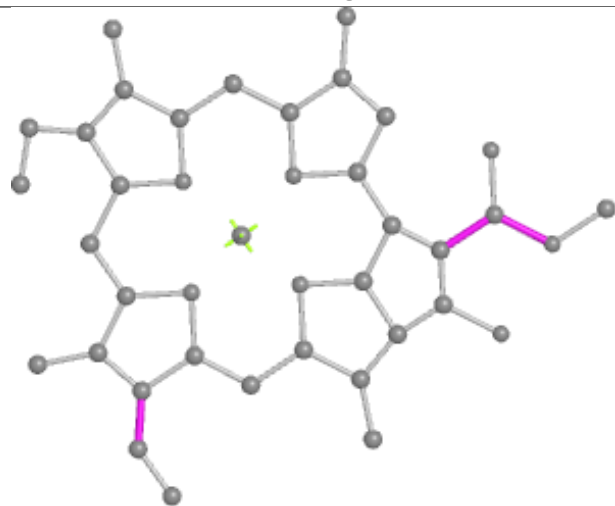
## Ligand CLA L 311



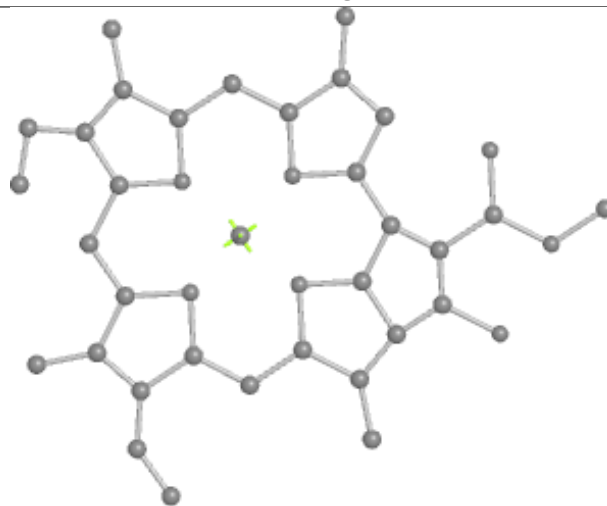
Bond lengths



Bond angles

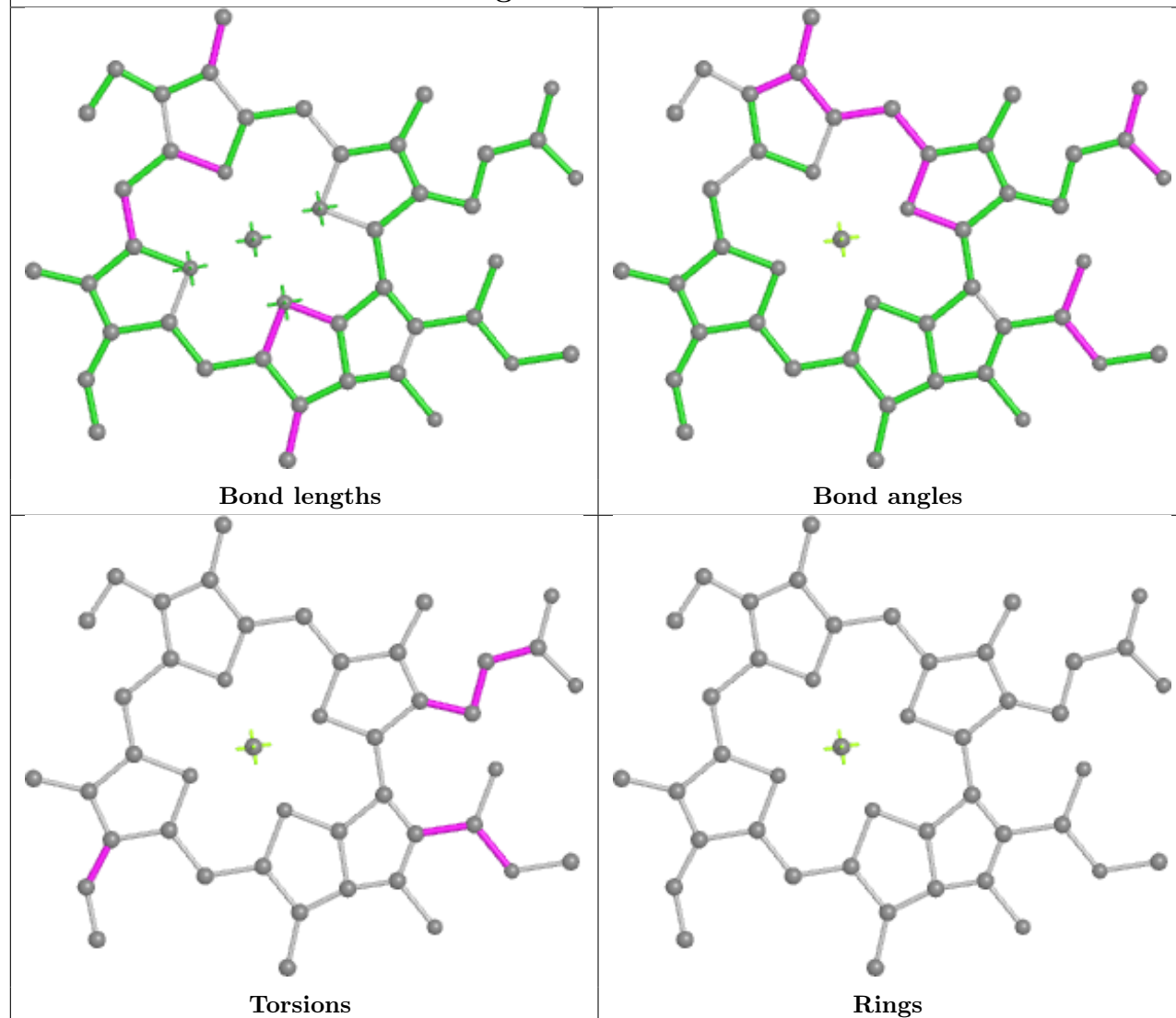


Torsions

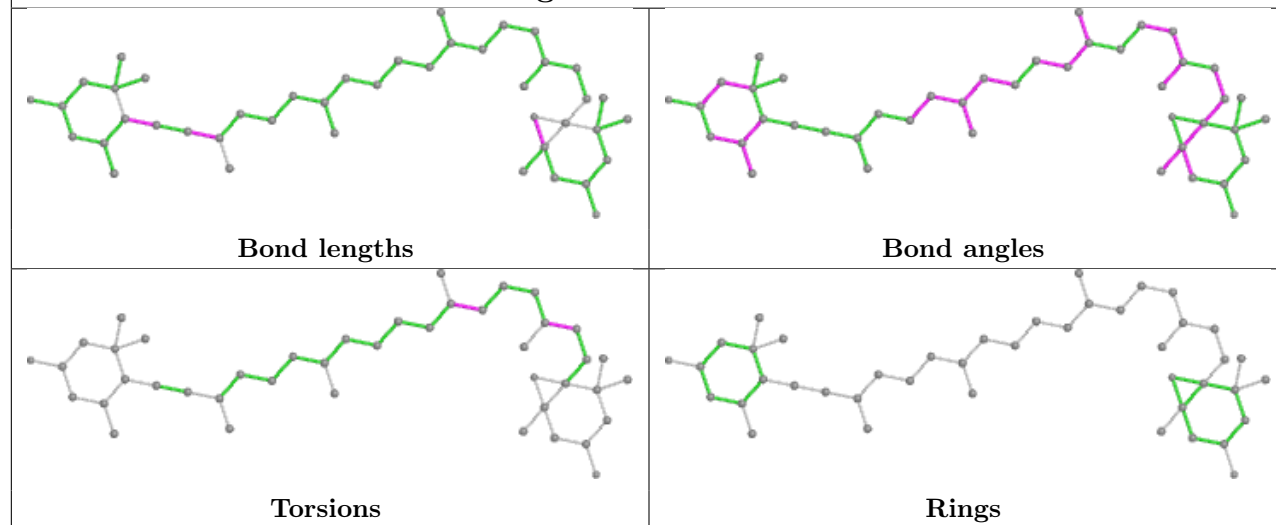


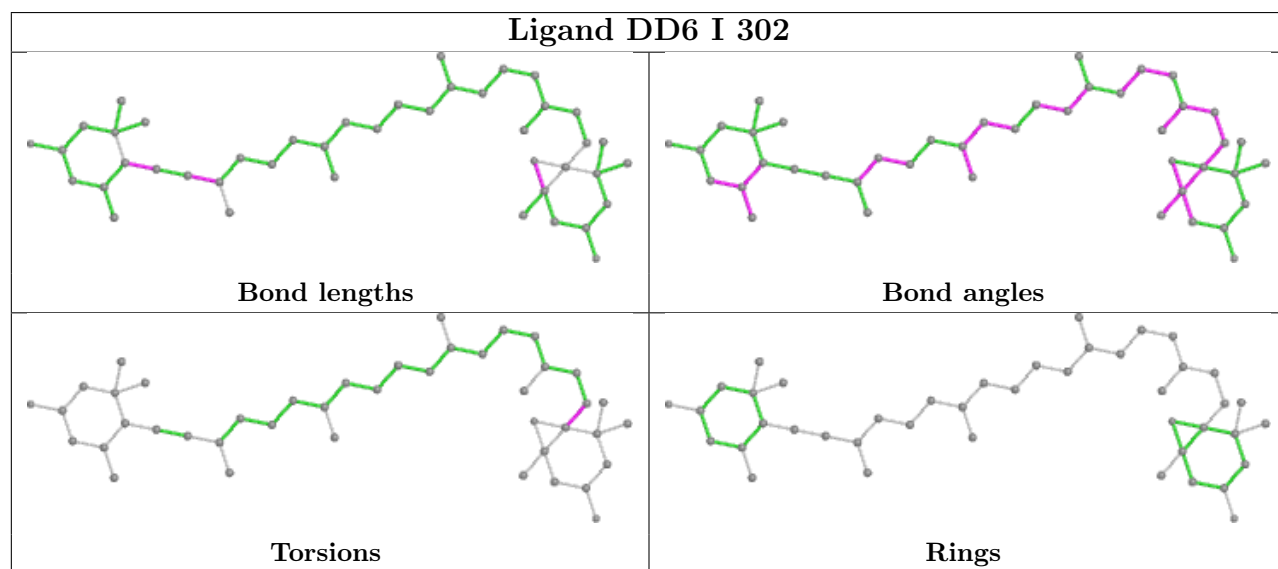
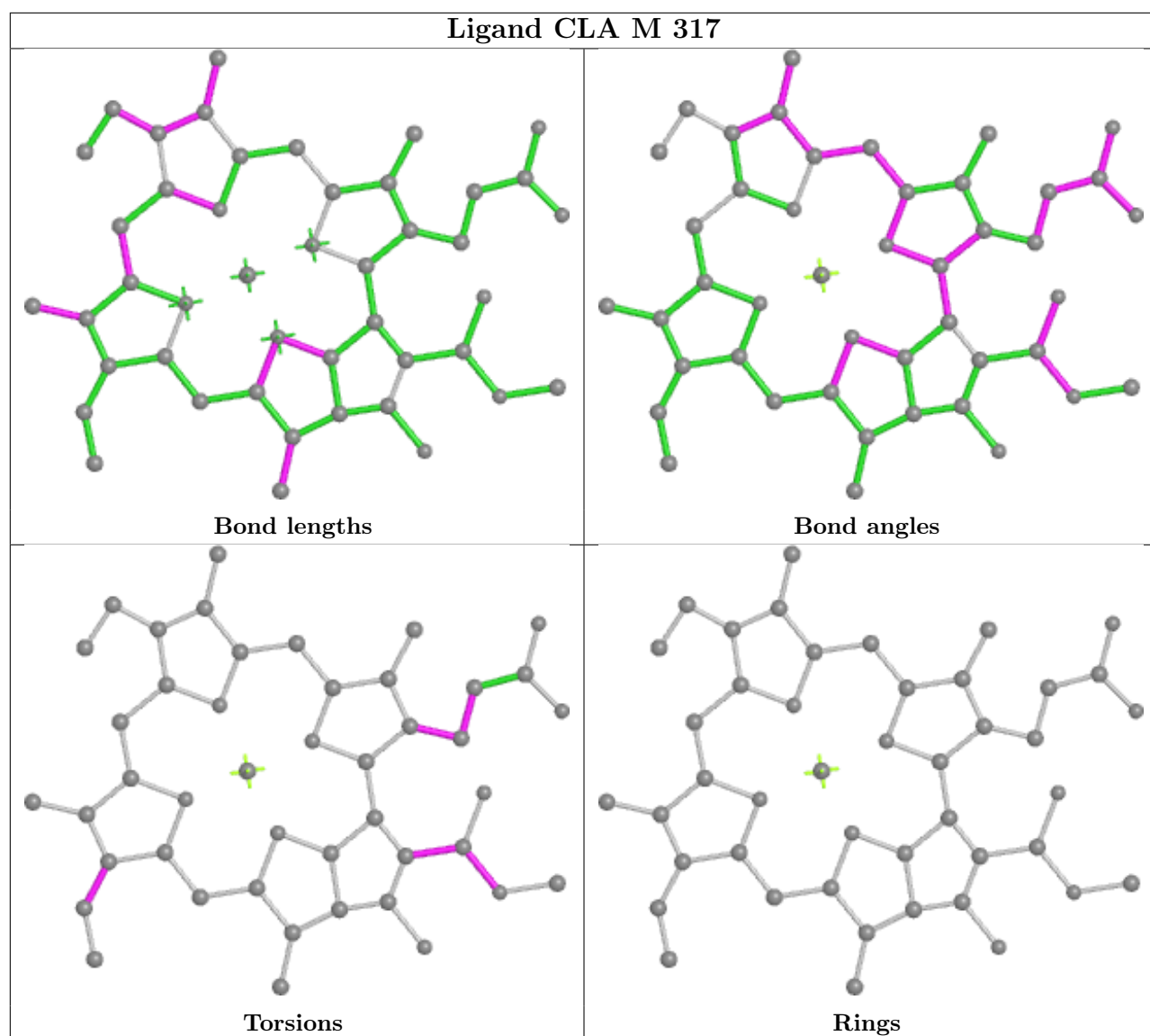
Rings

## Ligand CLA r 201

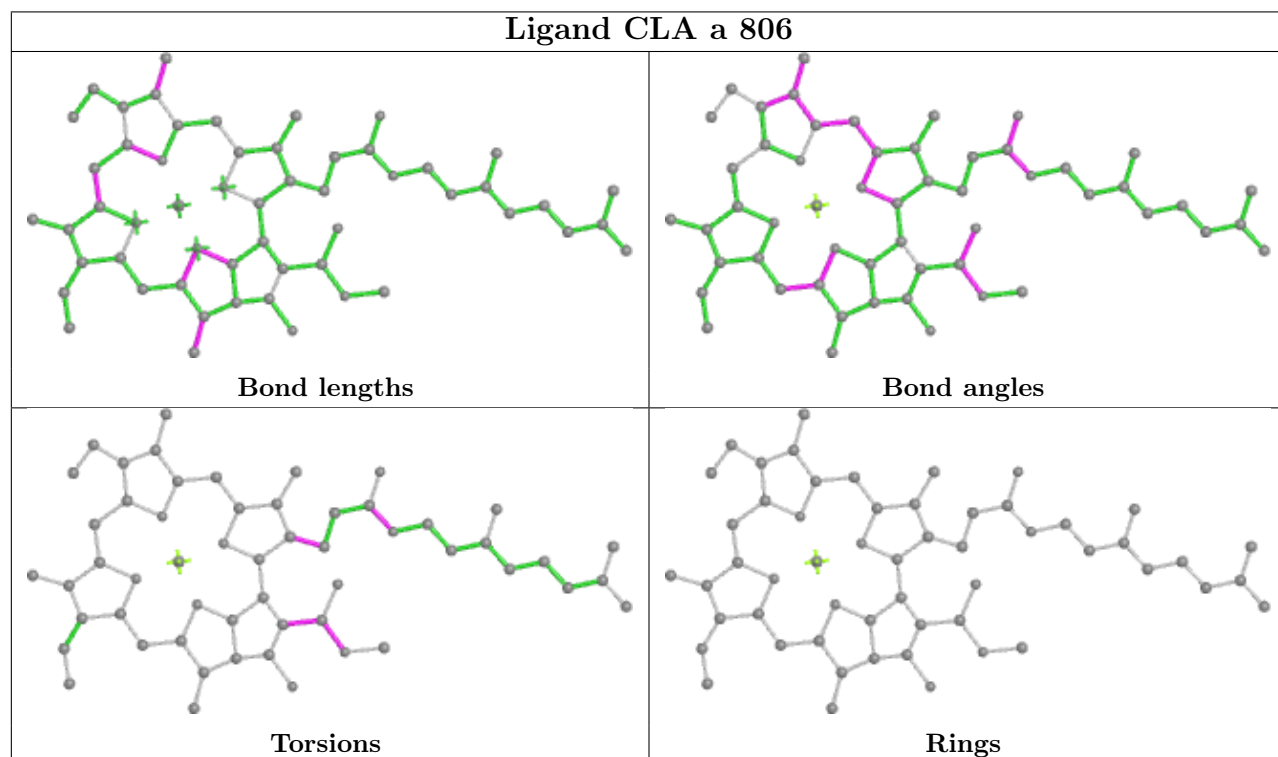
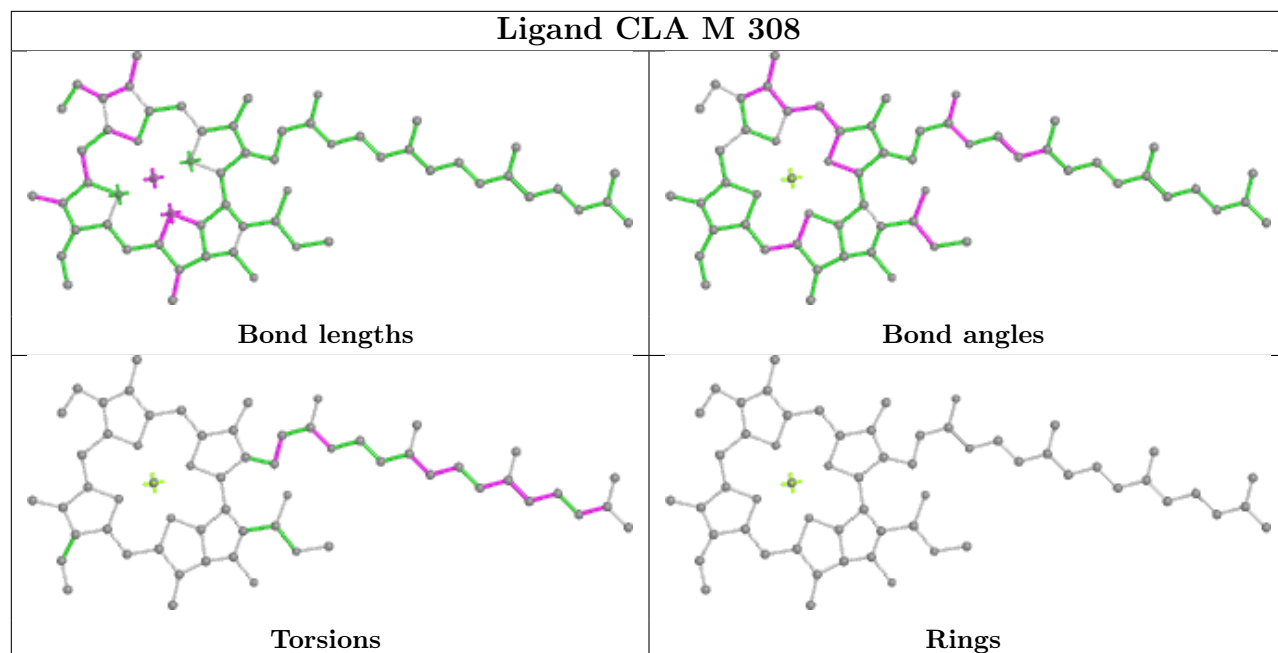


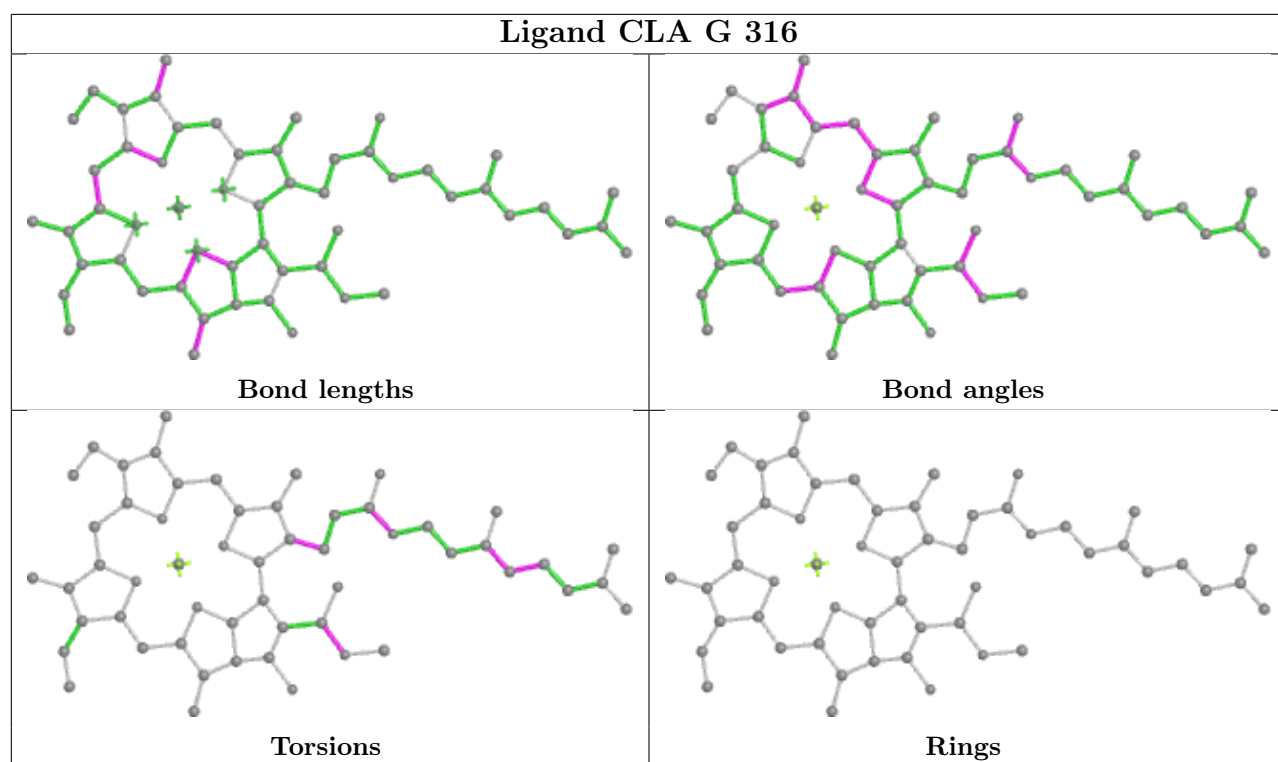
## Ligand DD6 J 303



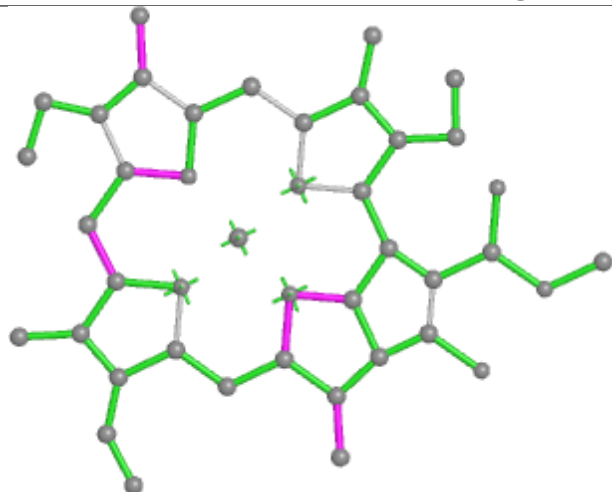




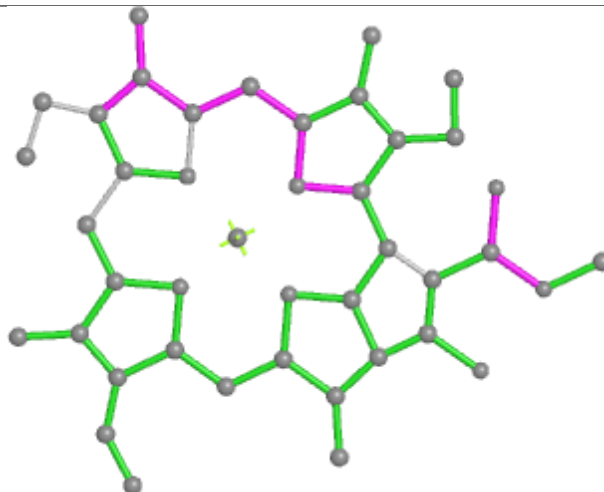




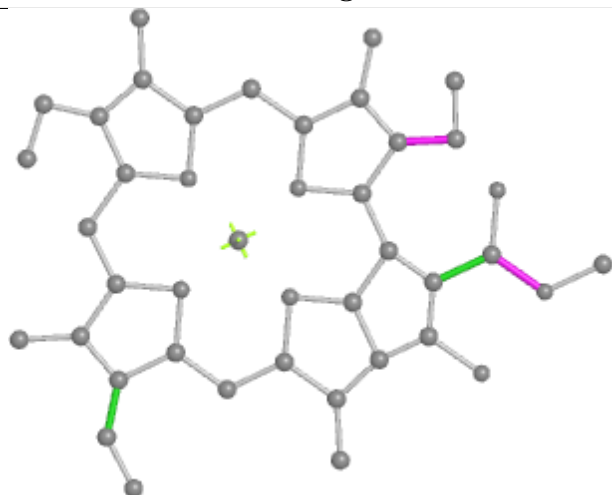
## Ligand CLA G 315



Bond lengths



Bond angles

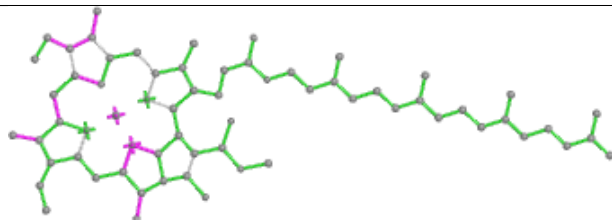


Torsions

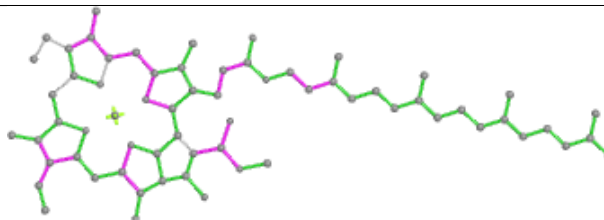


Rings

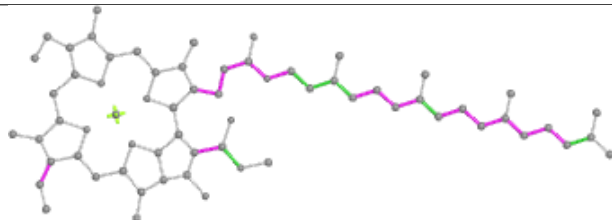
## Ligand CLA a 815



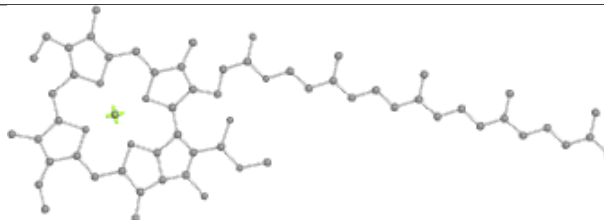
Bond lengths



Bond angles

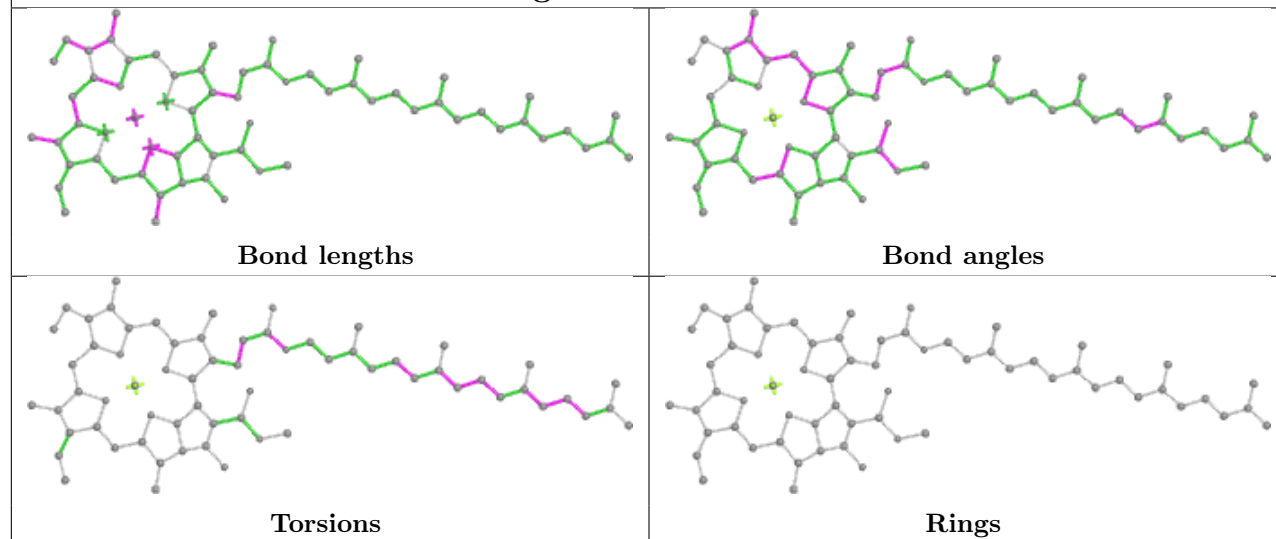


Torsions

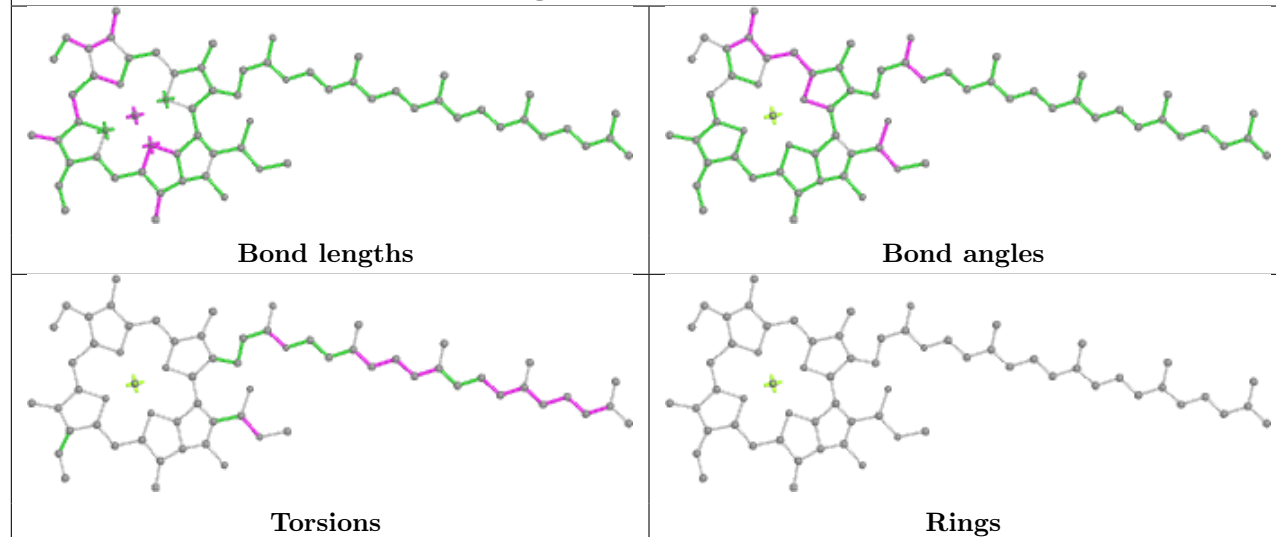


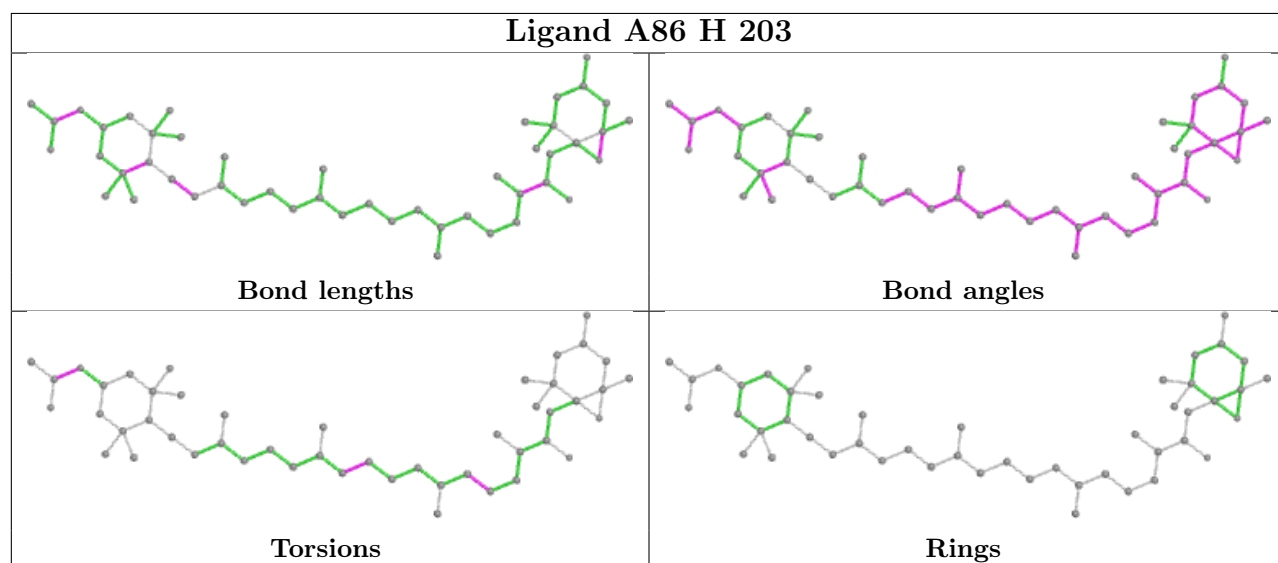
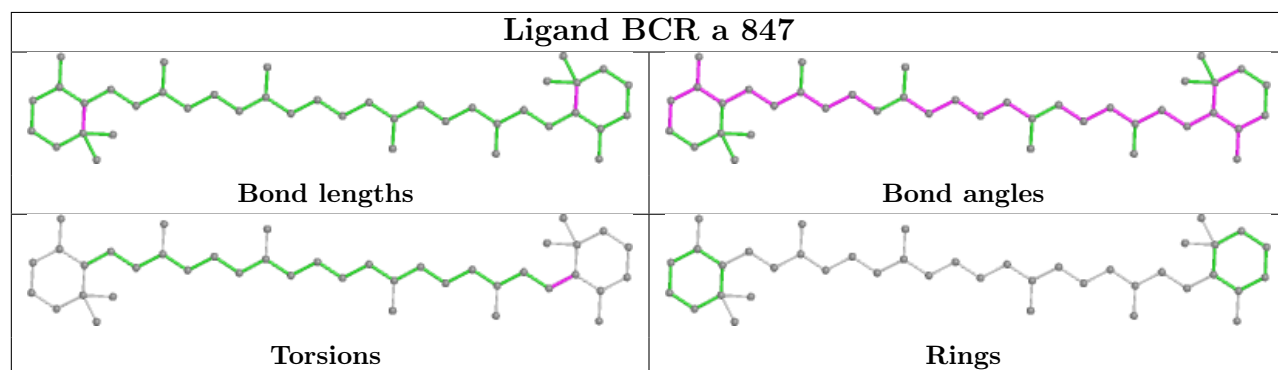
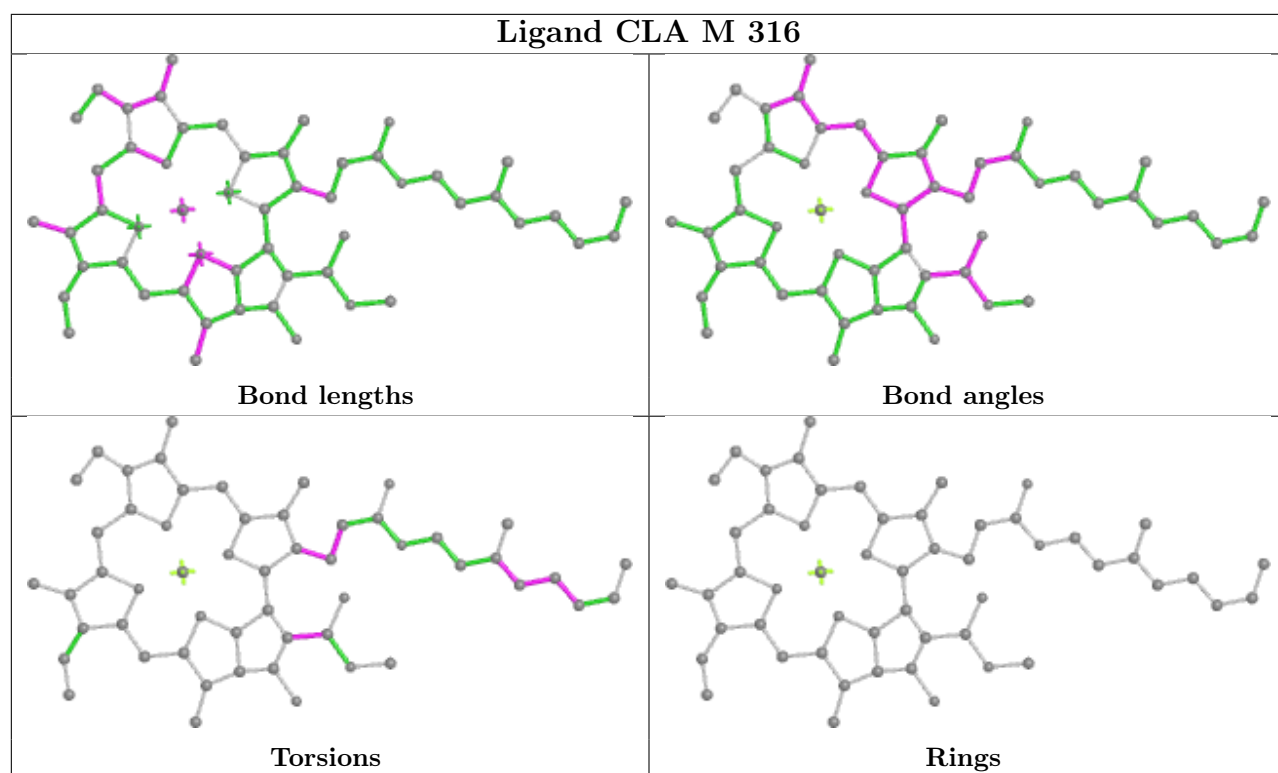
Rings

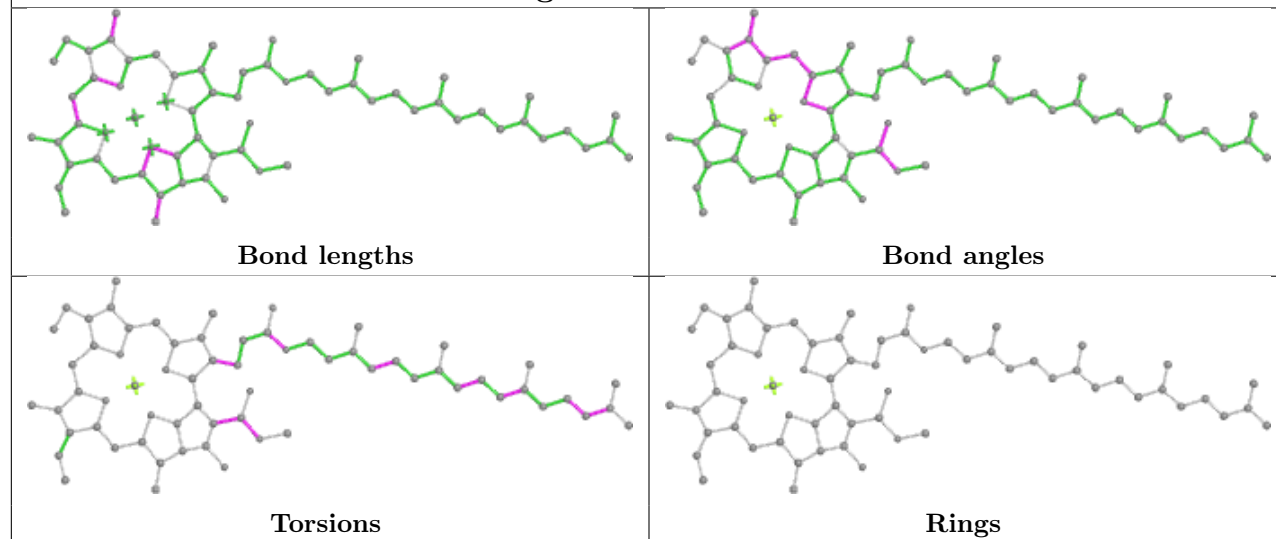
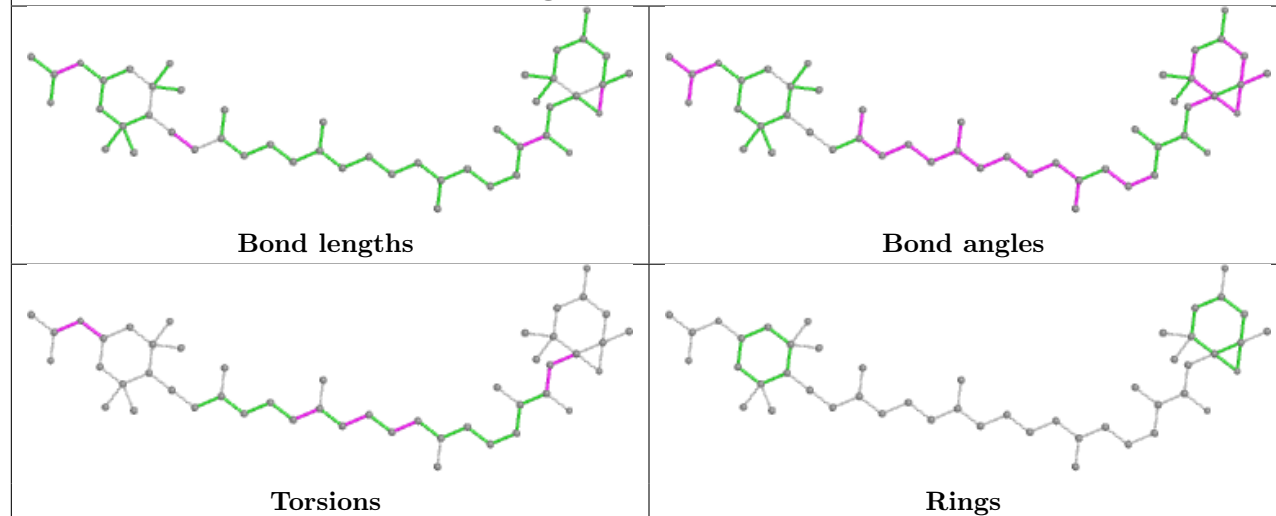
## Ligand CLA E 311

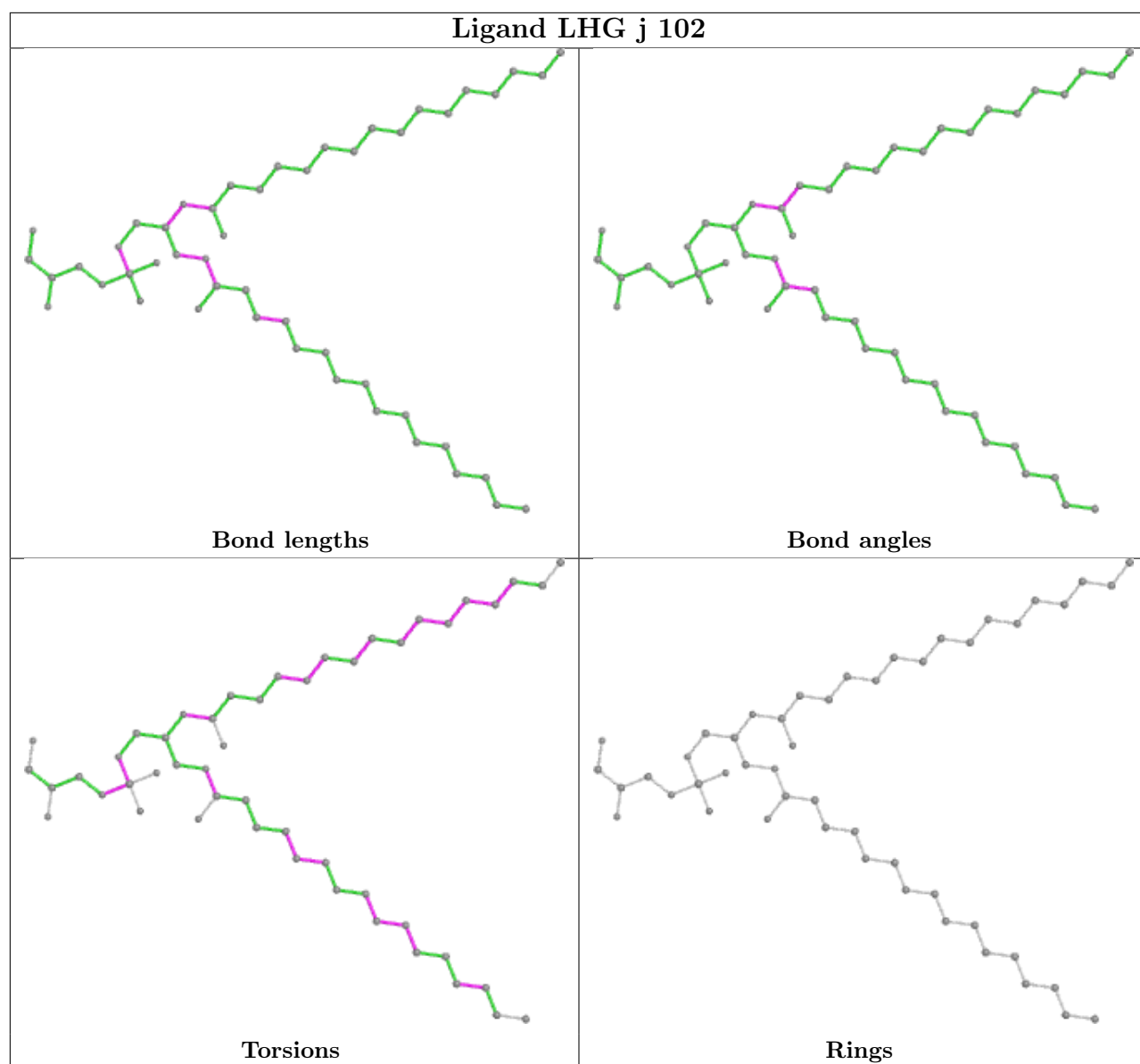


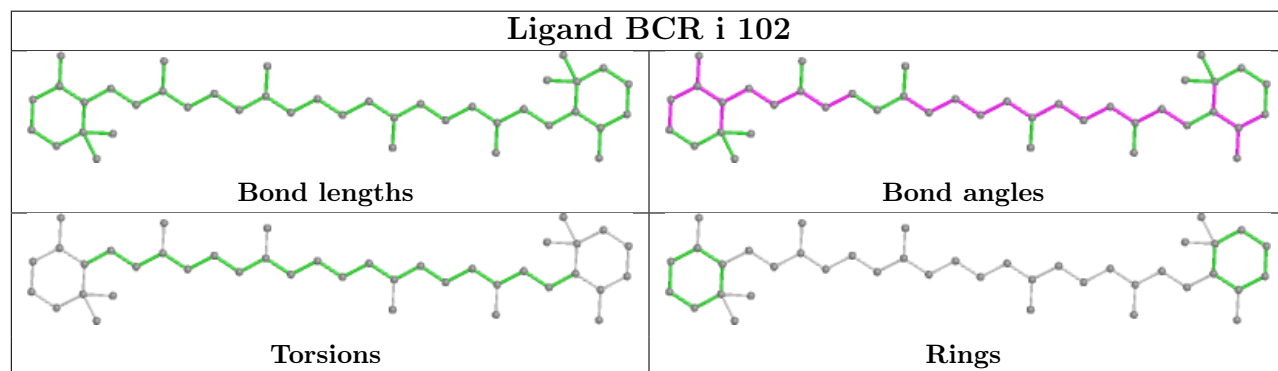
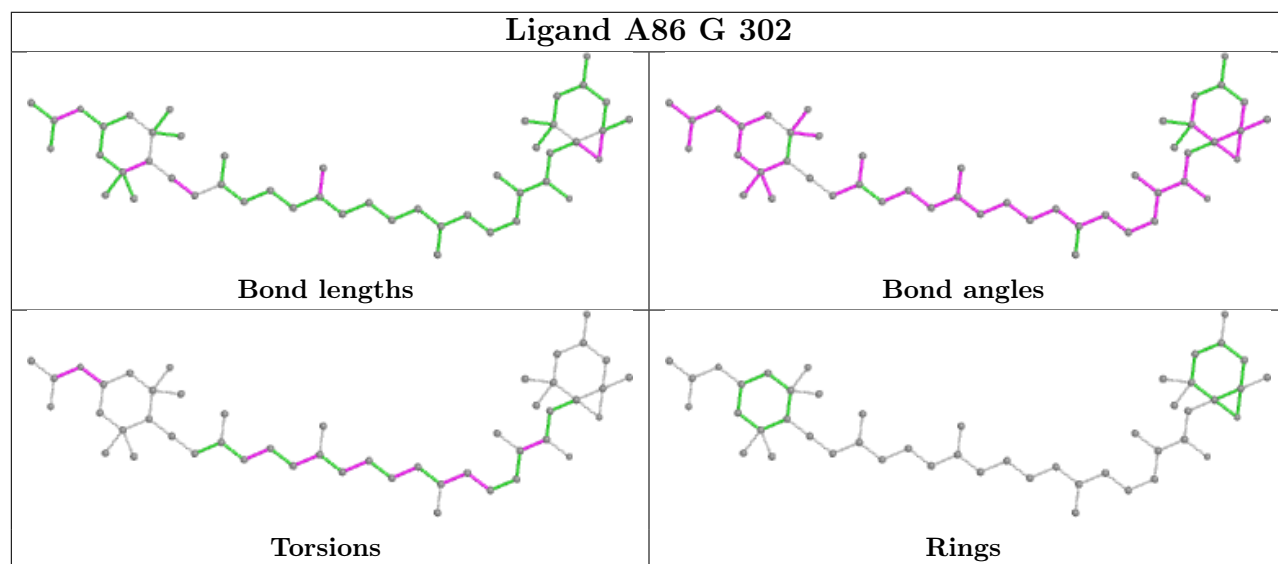
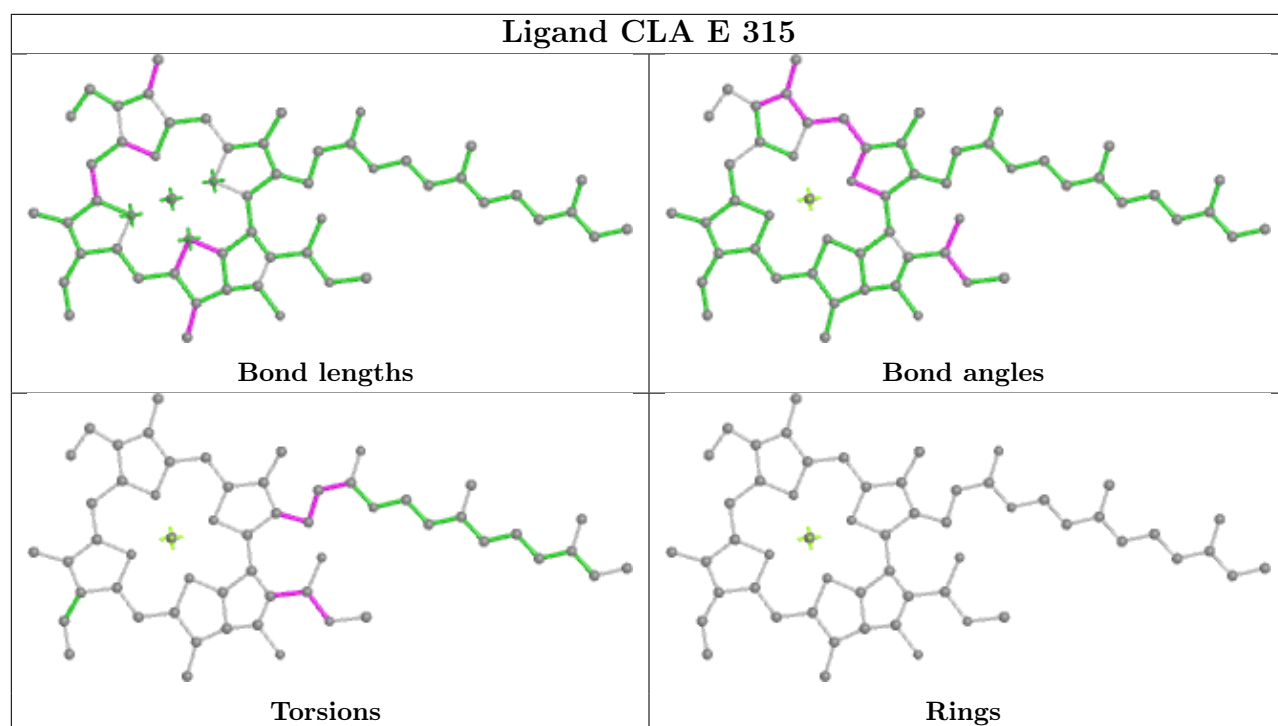
## Ligand CLA K 309





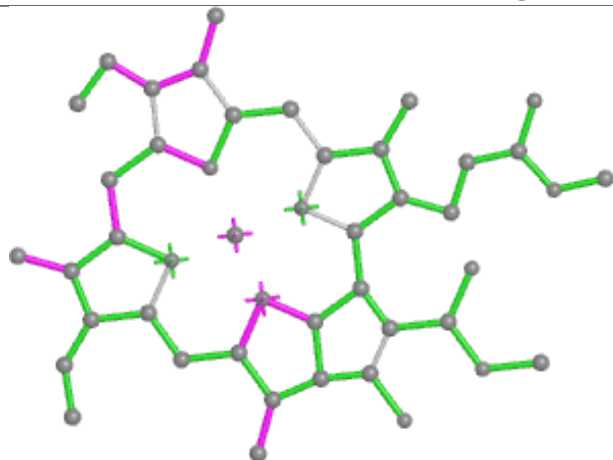
**Ligand CLA a 808****Ligand A86 F 301**



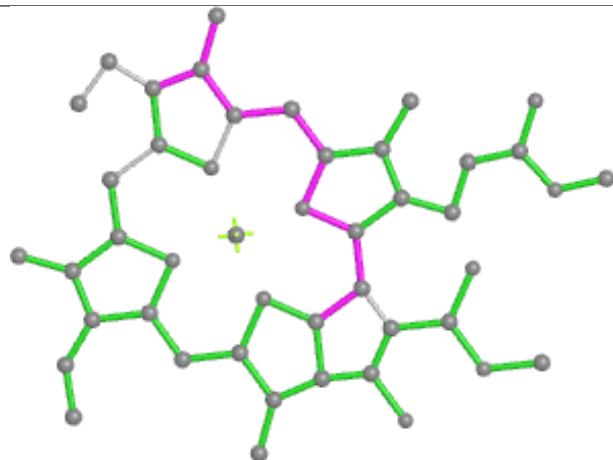




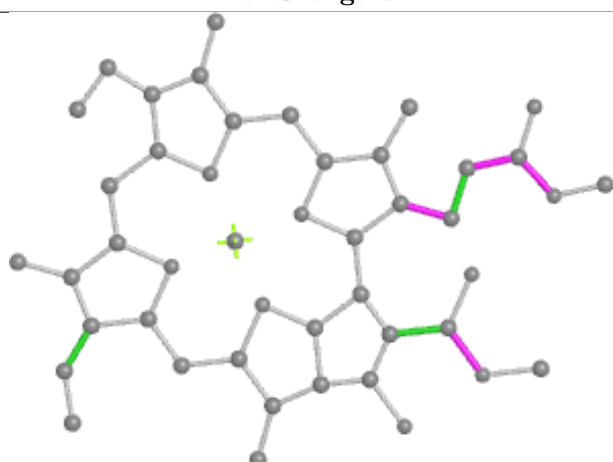
## Ligand CLA K 319



Bond lengths



Bond angles

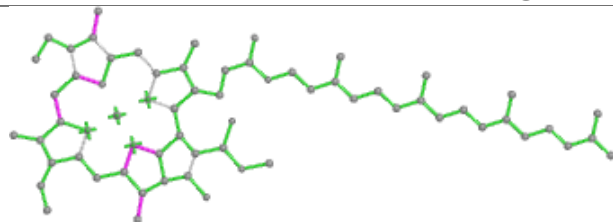


Torsions

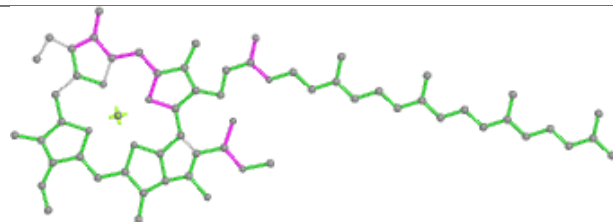


Rings

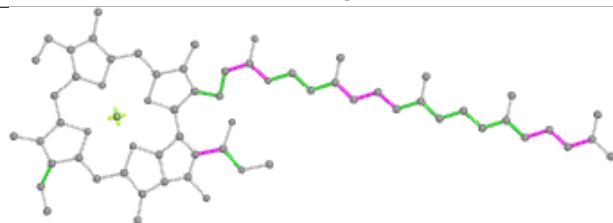
## Ligand CLA b 847



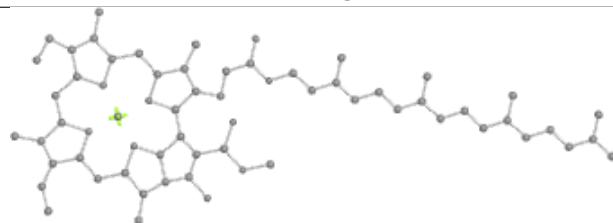
Bond lengths



Bond angles

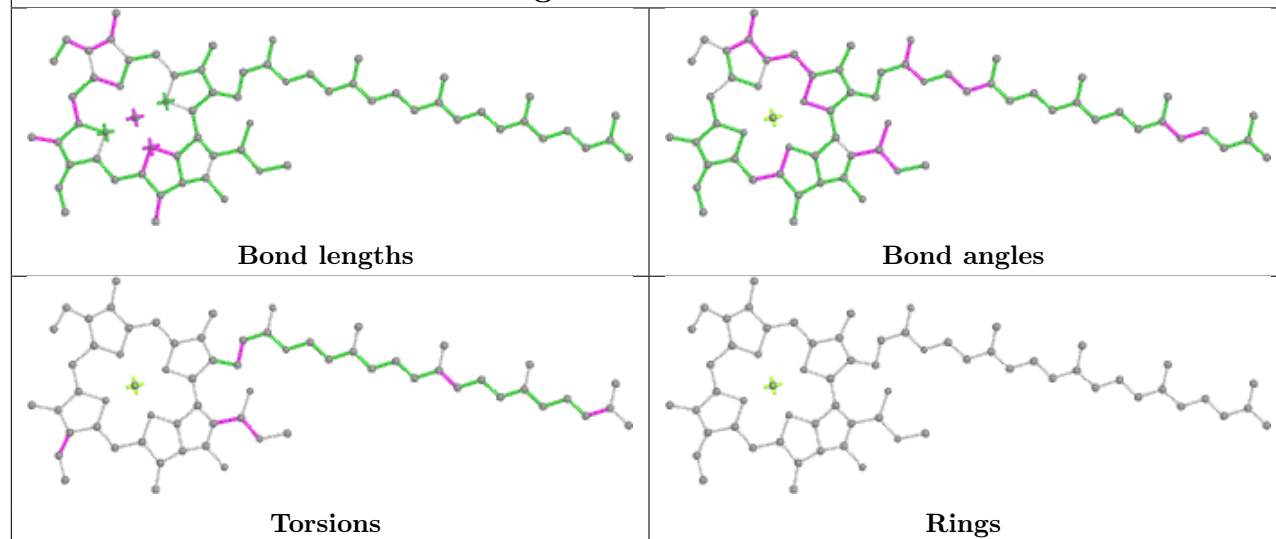


Torsions

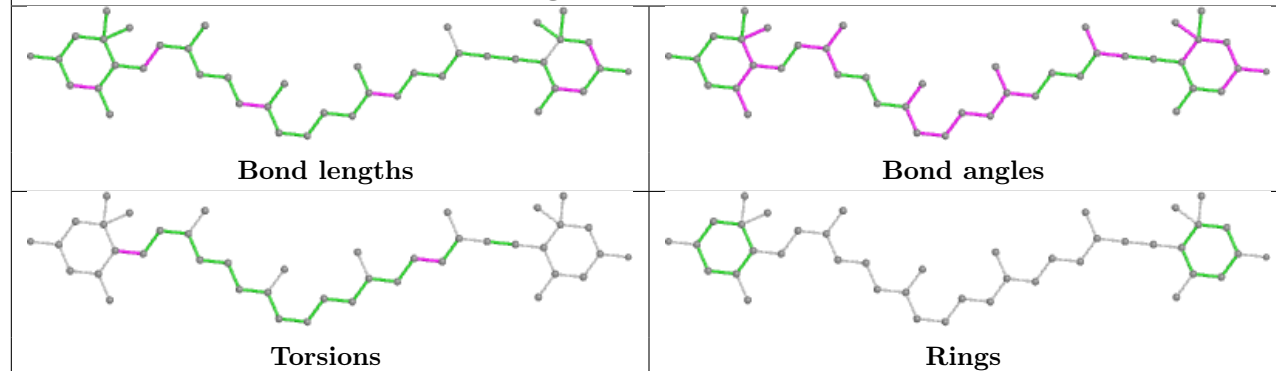


Rings

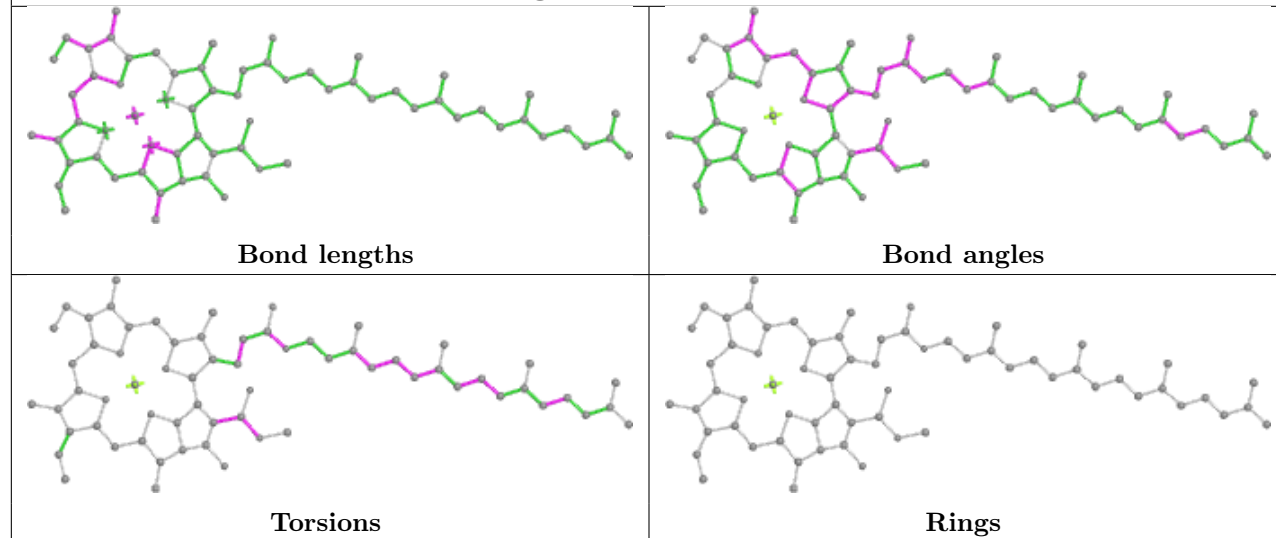
## Ligand CLA L 308



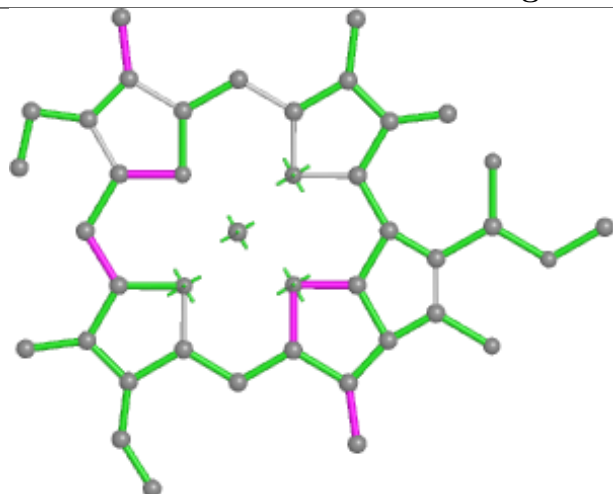
## Ligand ET4 l 207



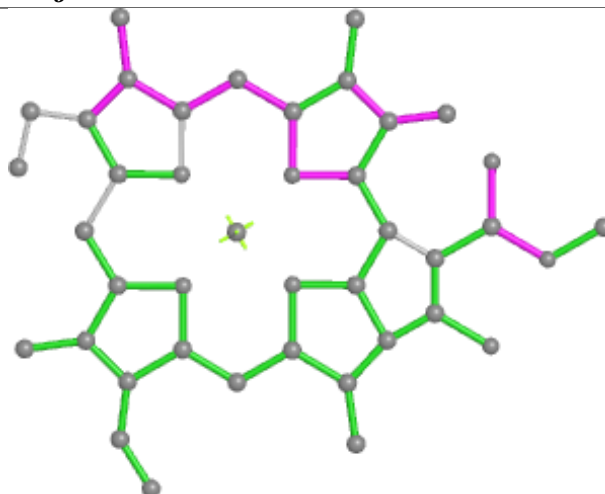
## Ligand CLA H 206



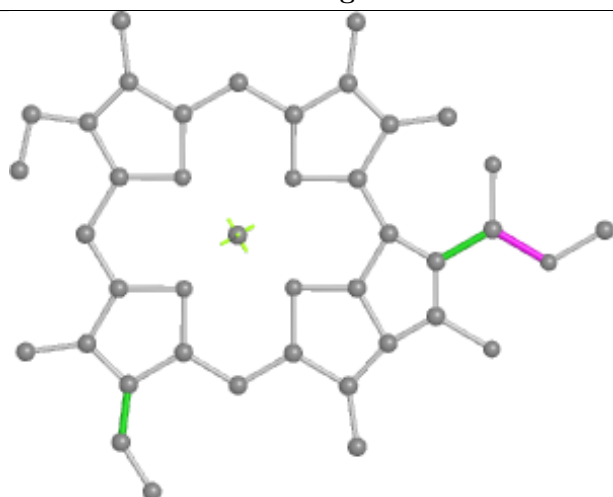
## Ligand CLA j 104



Bond lengths



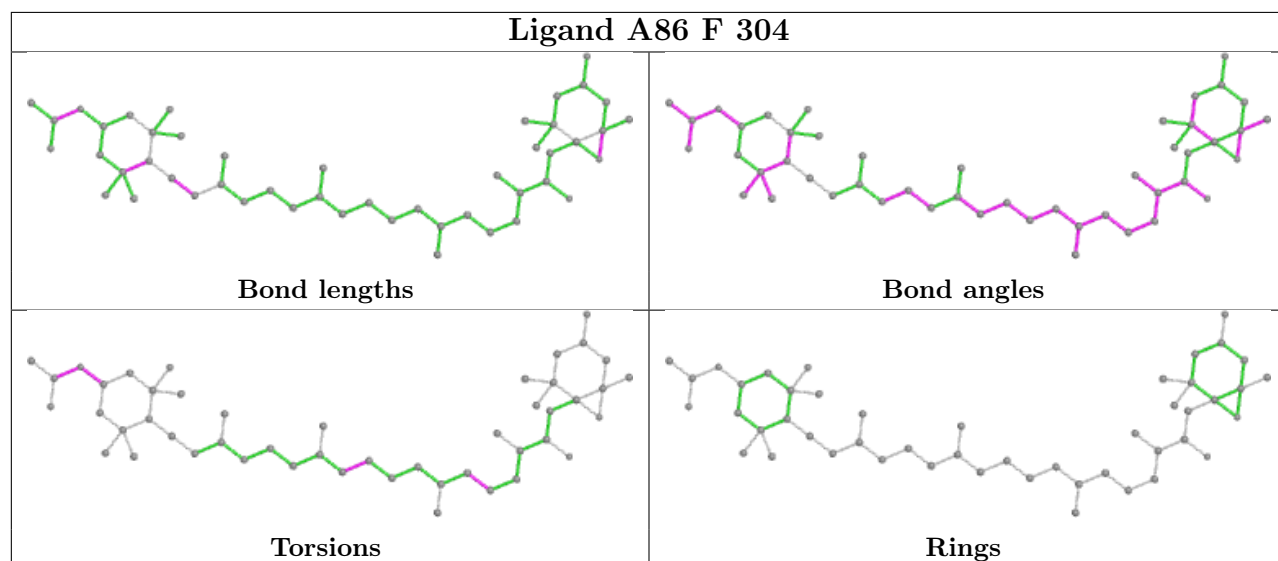
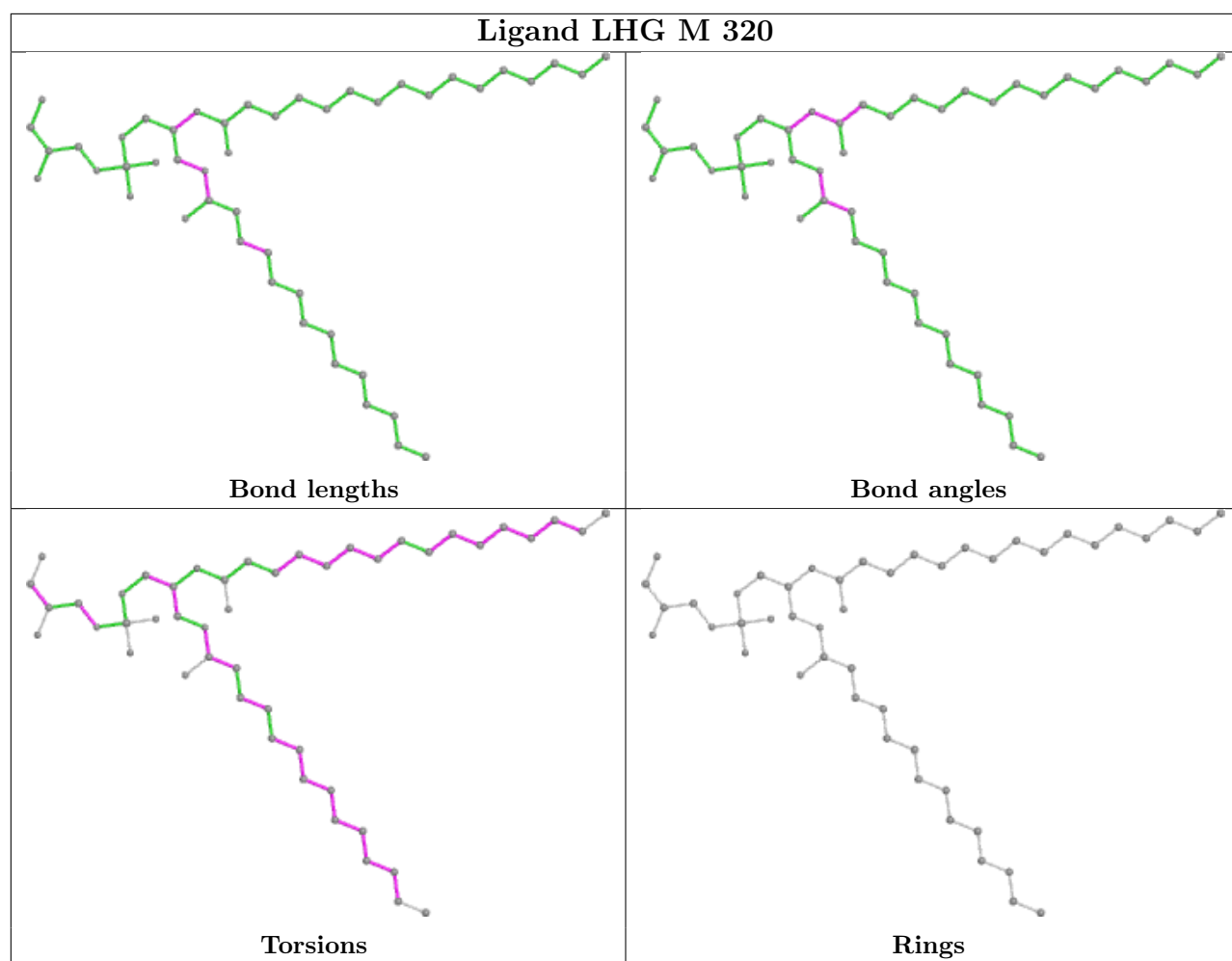
Bond angles

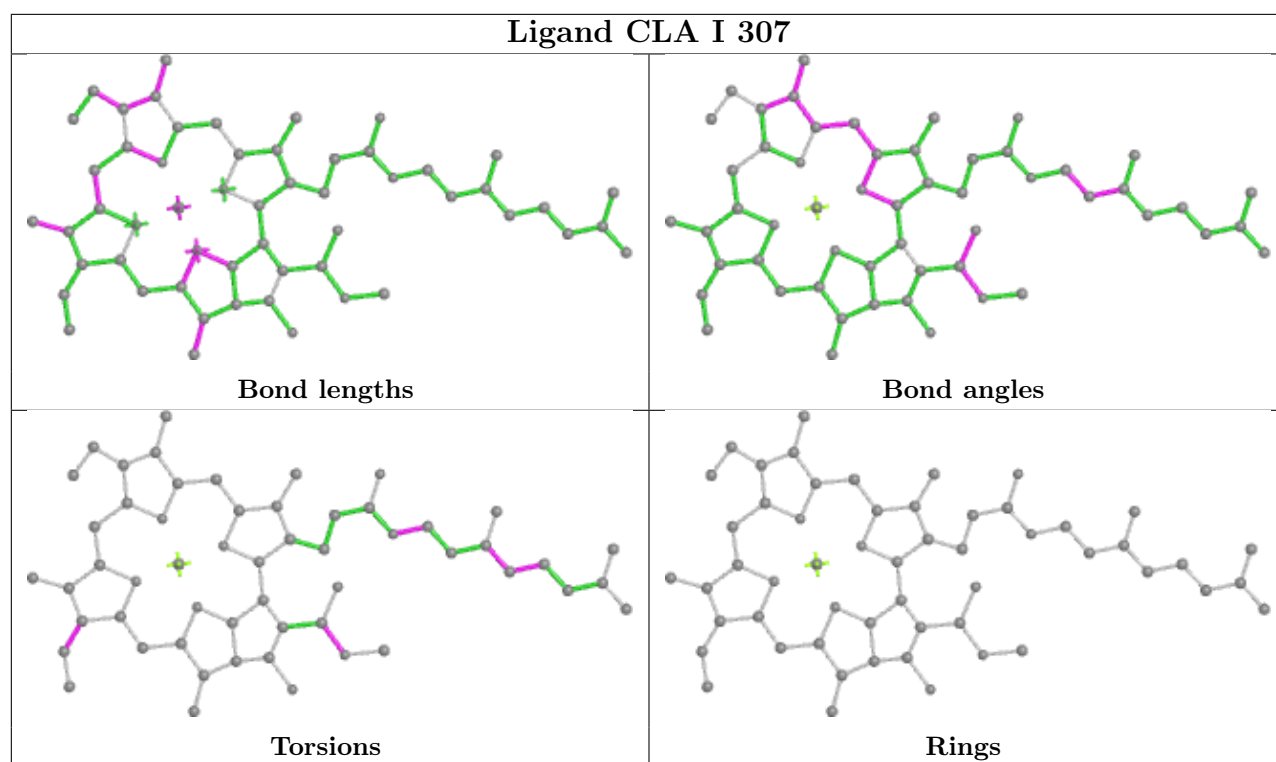


Torsions

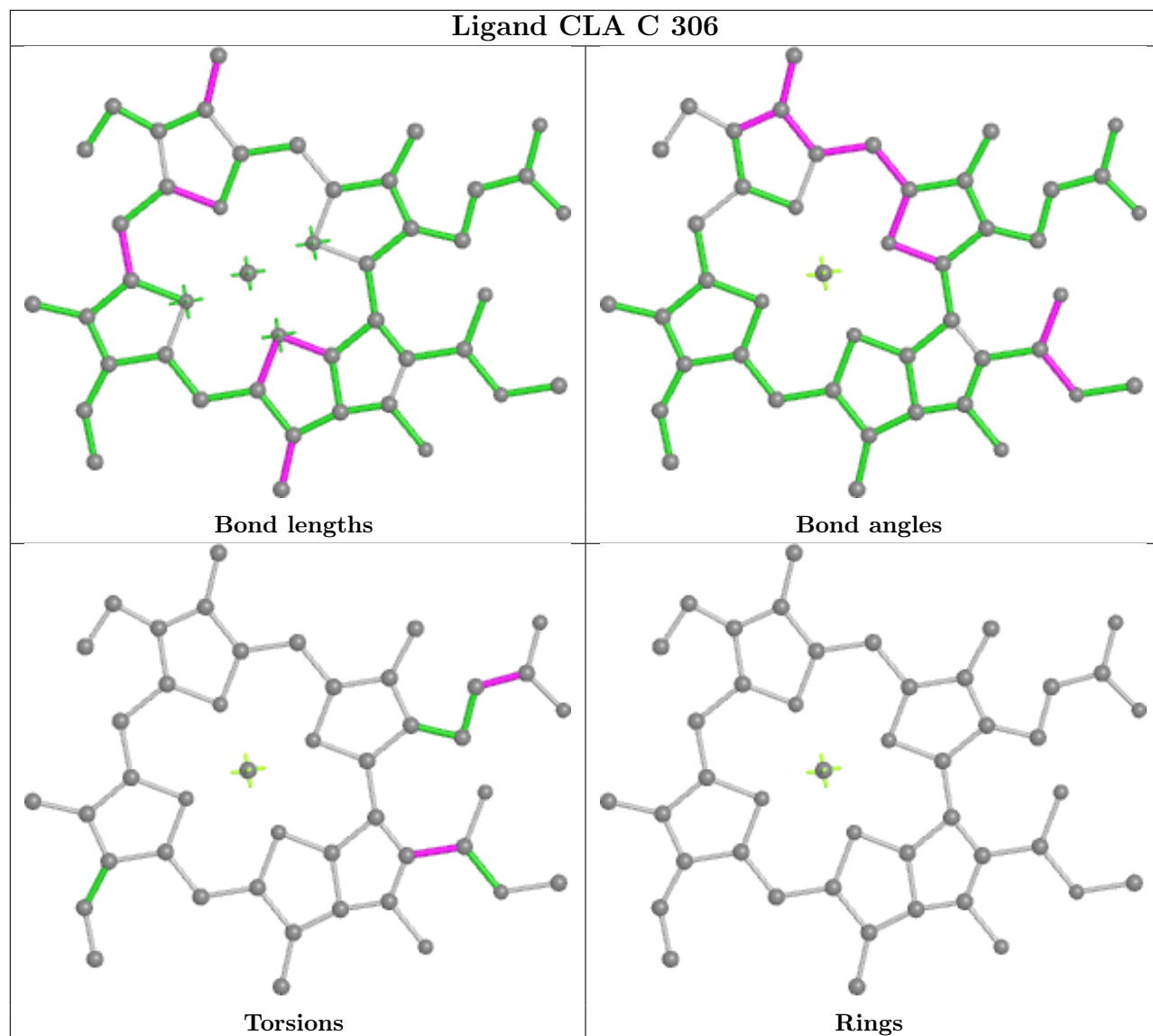


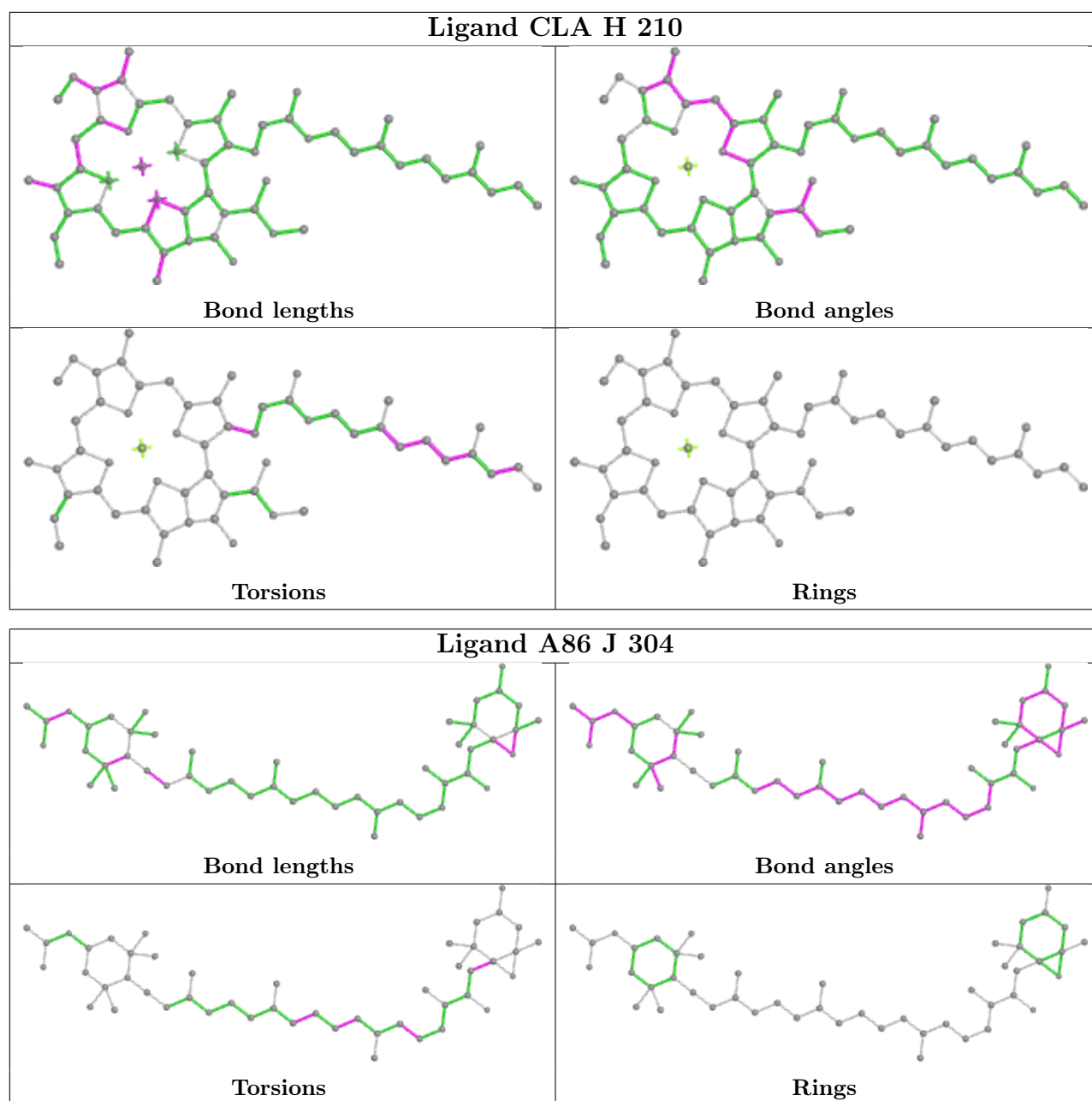
Rings



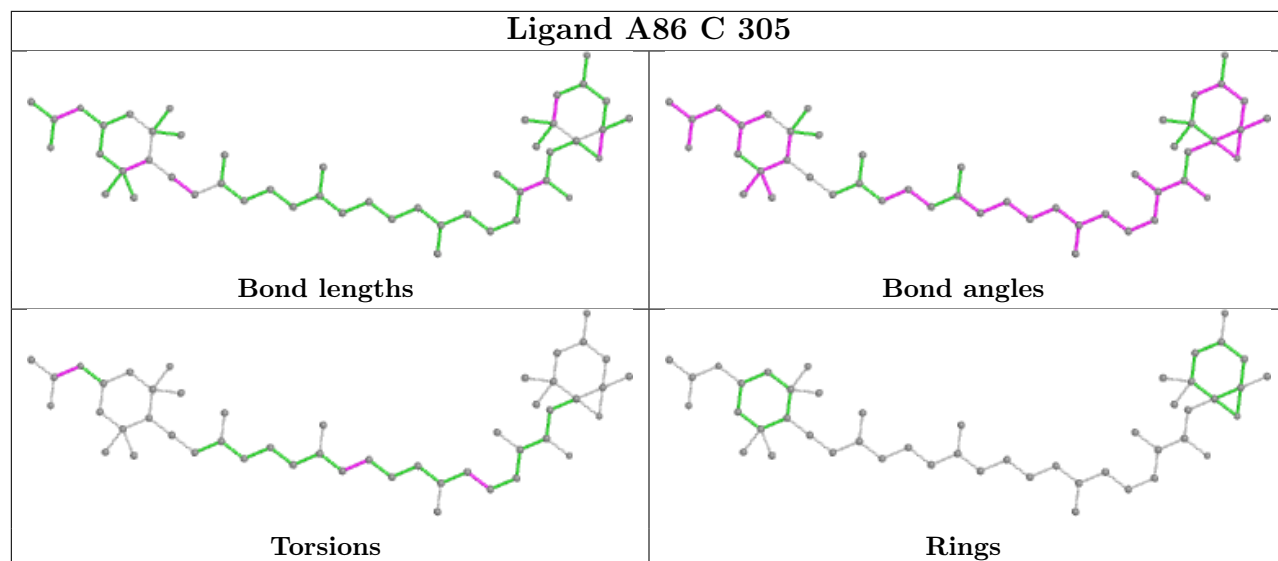


## Ligand CLA C 306

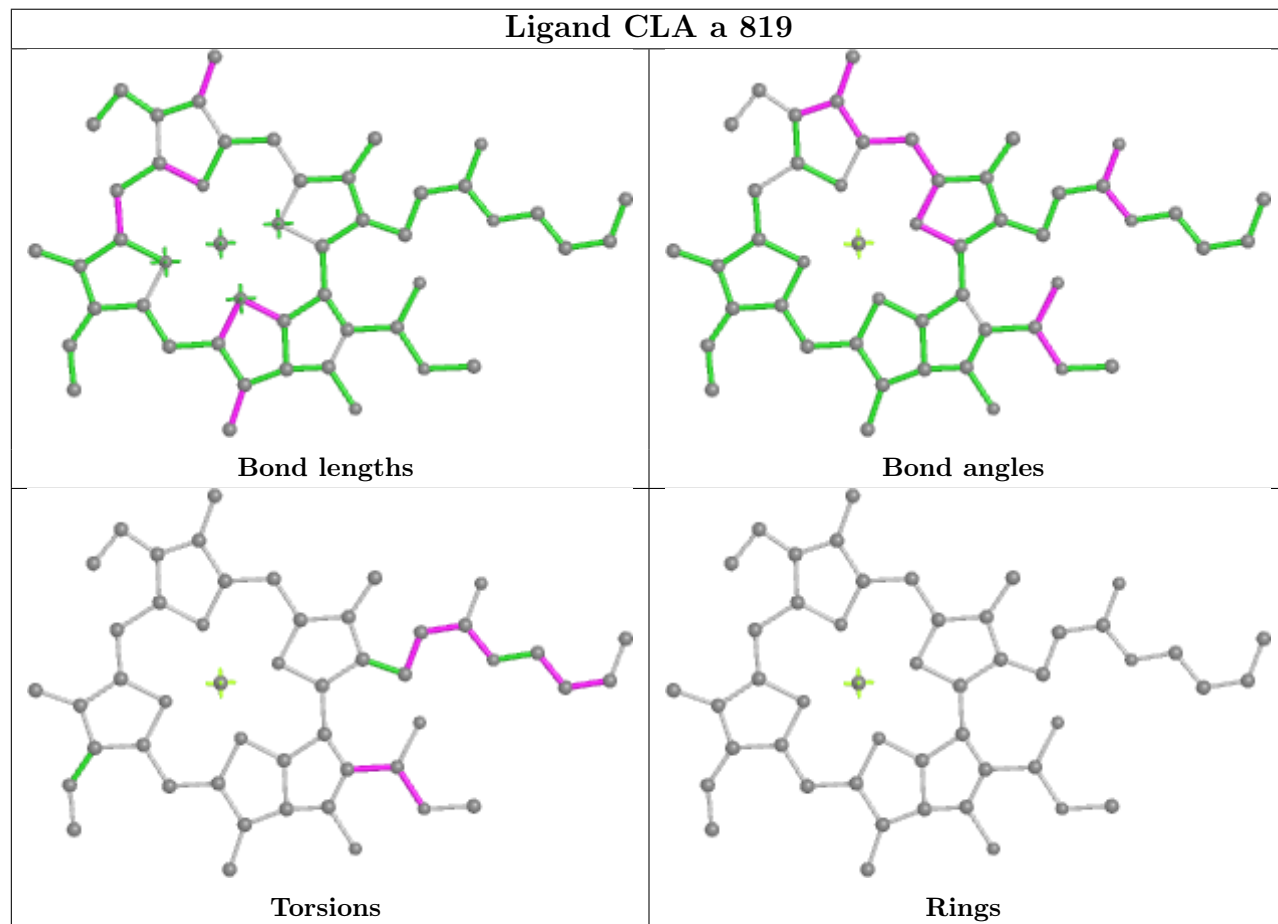




## Ligand A86 C 305

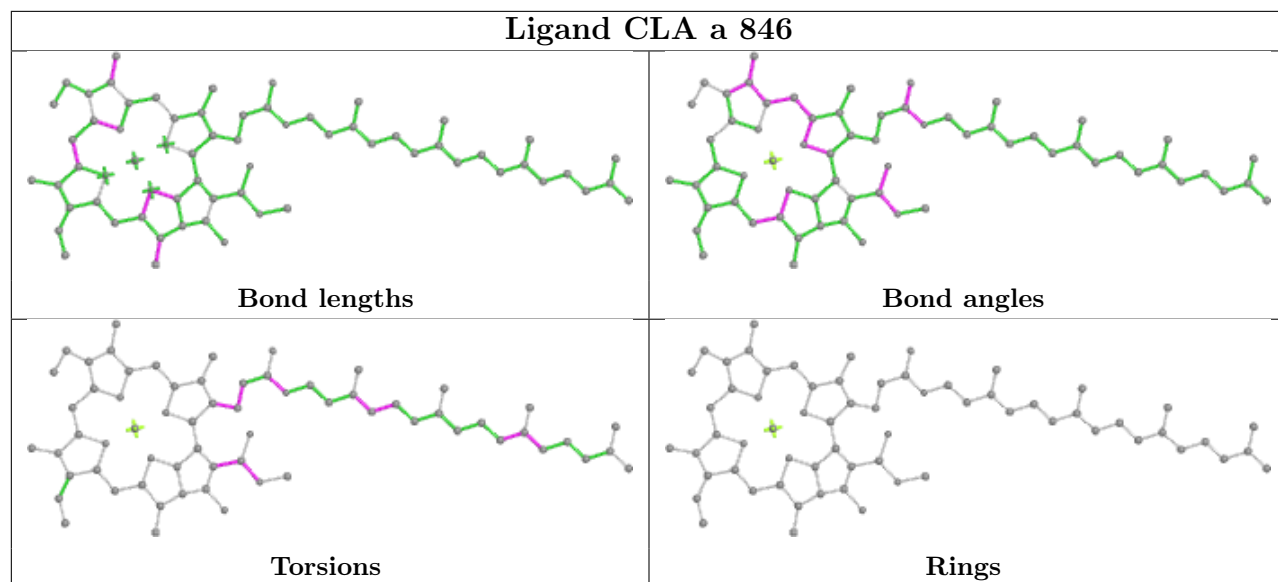


## Ligand CLA a 819

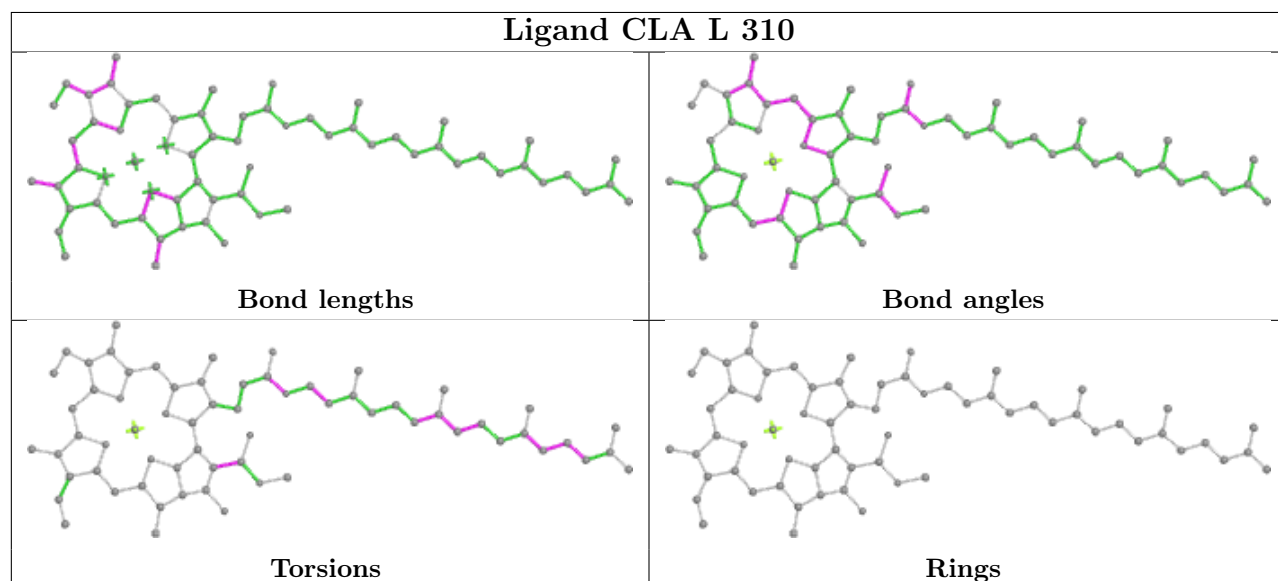




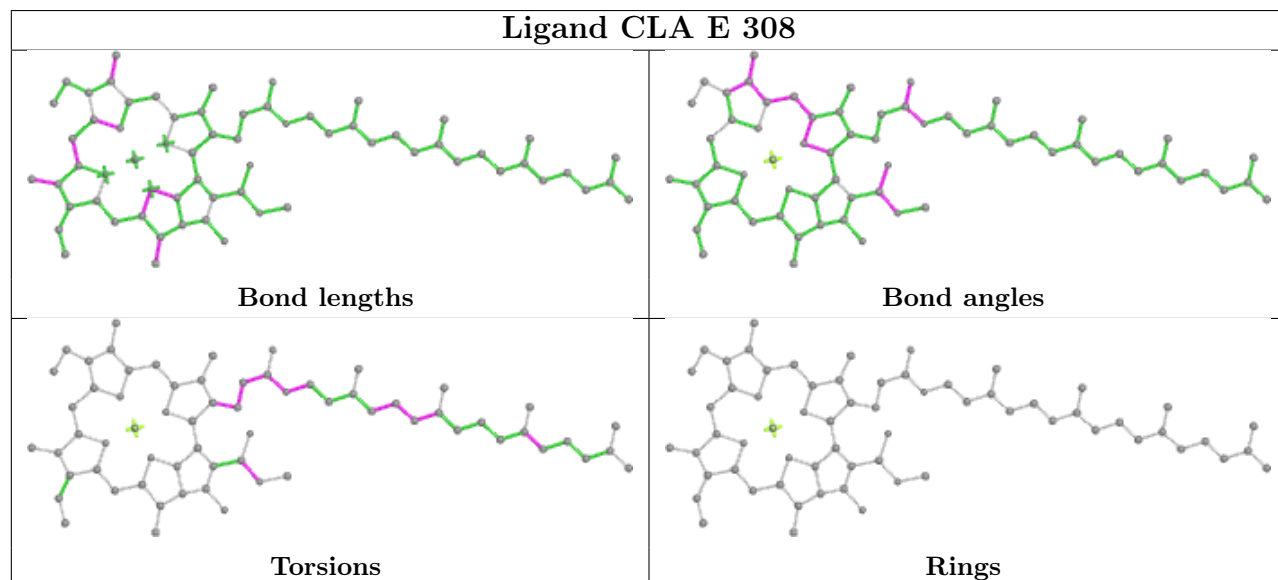
## Ligand CLA a 846



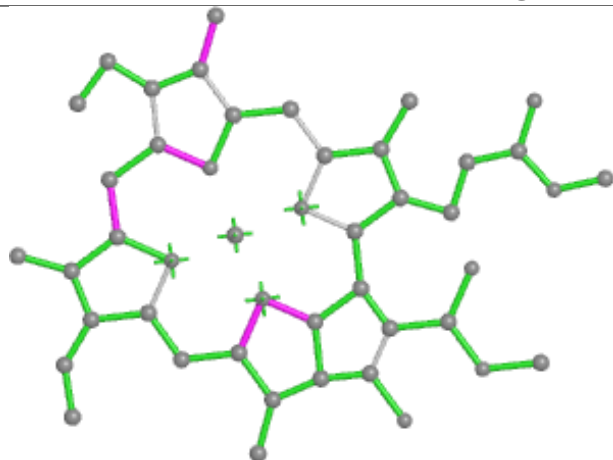
## Ligand CLA L 310



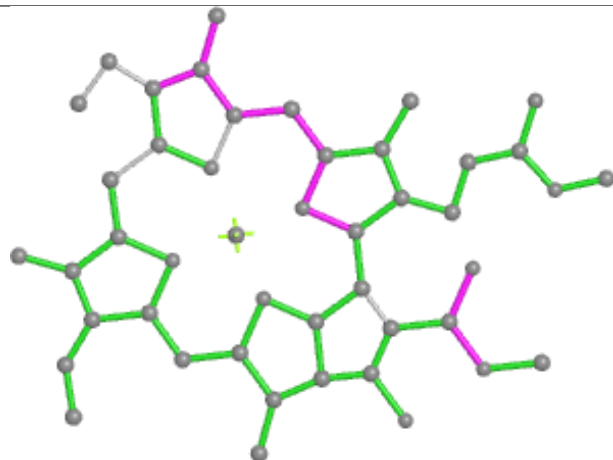
## Ligand CLA E 308



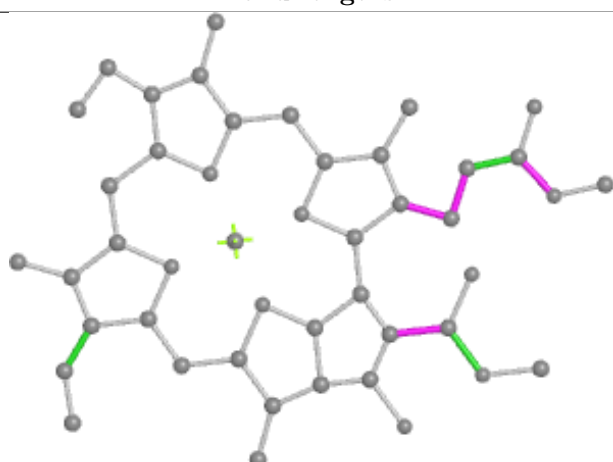
## Ligand CLA G 310



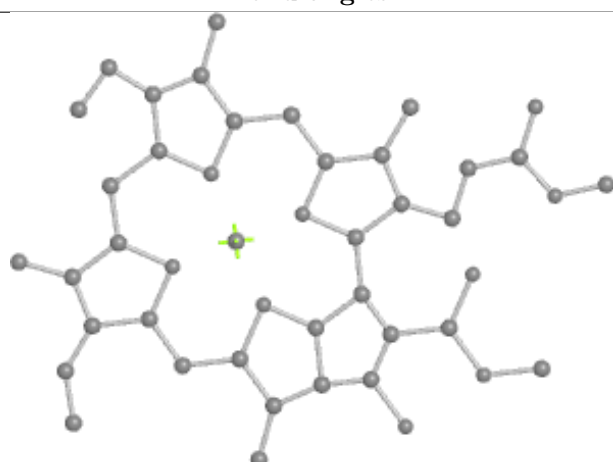
Bond lengths



Bond angles

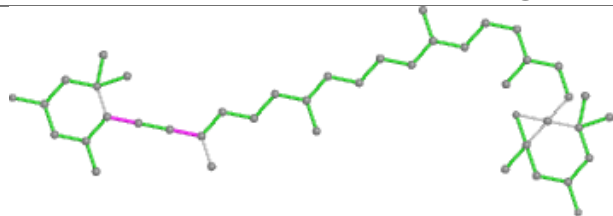


Torsions

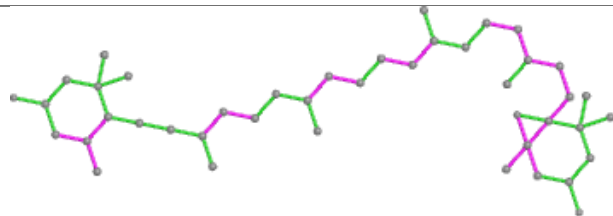


Rings

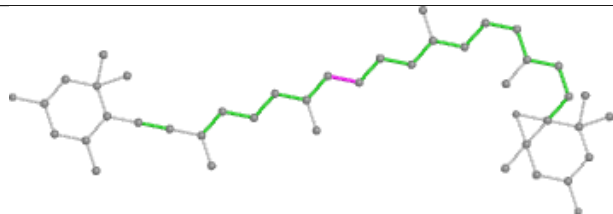
## Ligand DD6 F 302



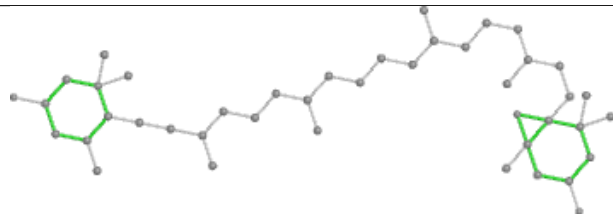
Bond lengths



Bond angles

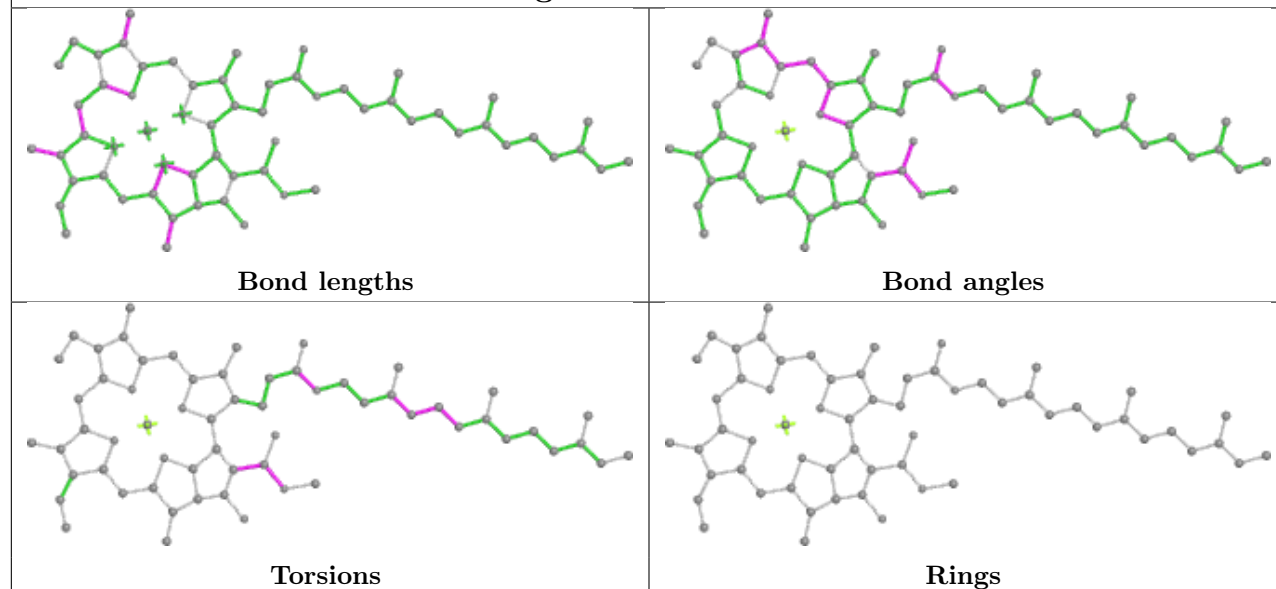


Torsions

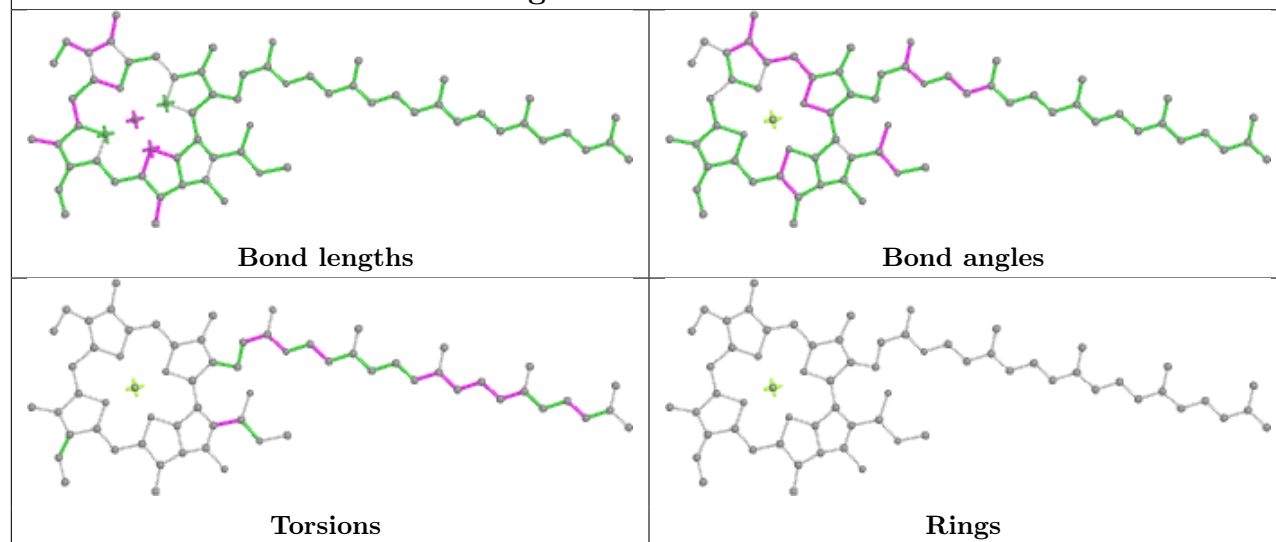


Rings

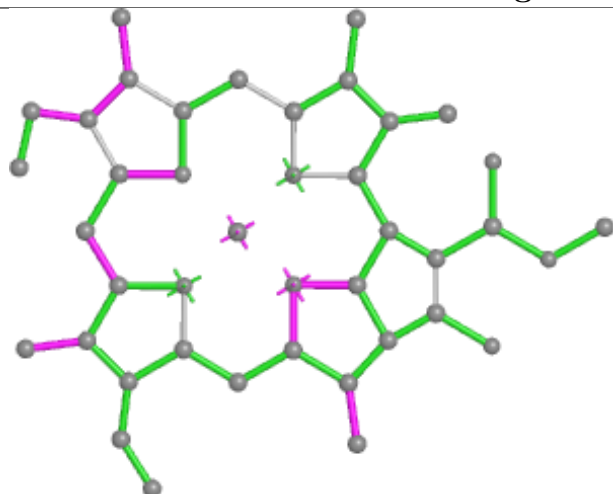
## Ligand CLA b 841



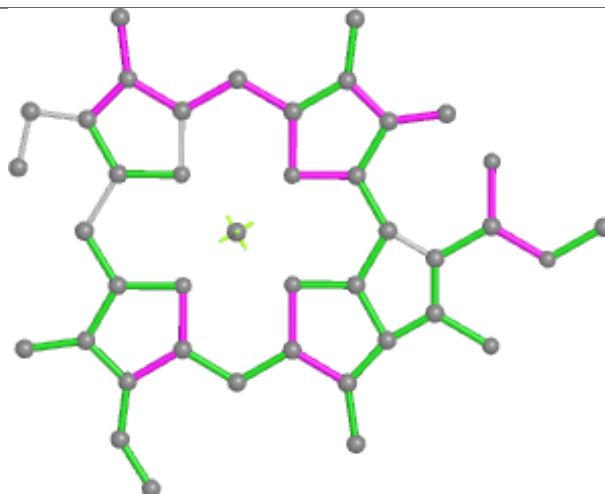
## Ligand CLA M 309



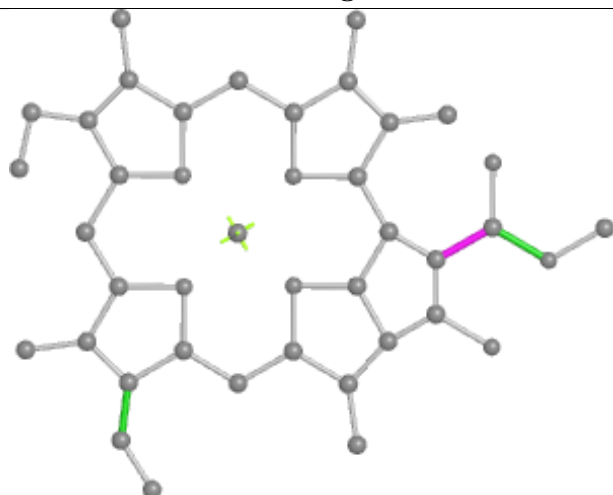
## Ligand CLA C 316



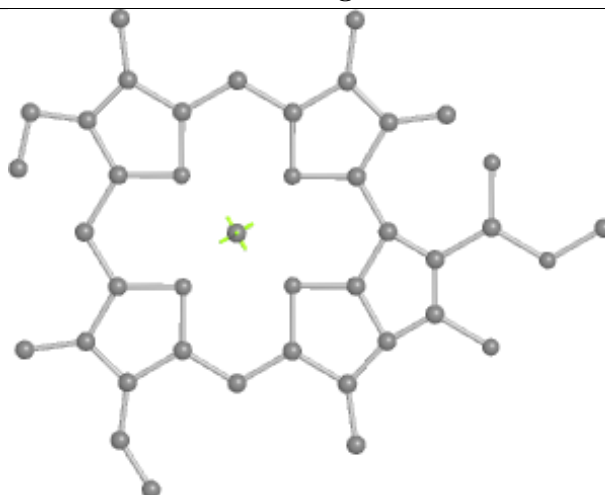
Bond lengths



Bond angles

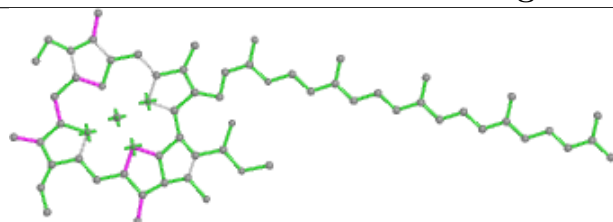


Torsions

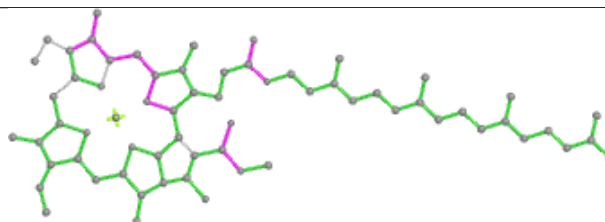


Rings

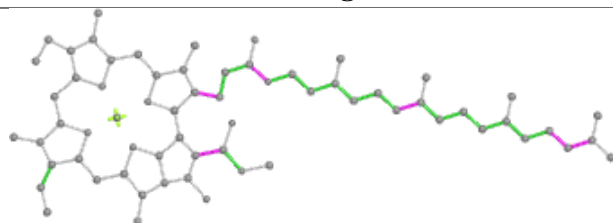
## Ligand CLA b 811



Bond lengths



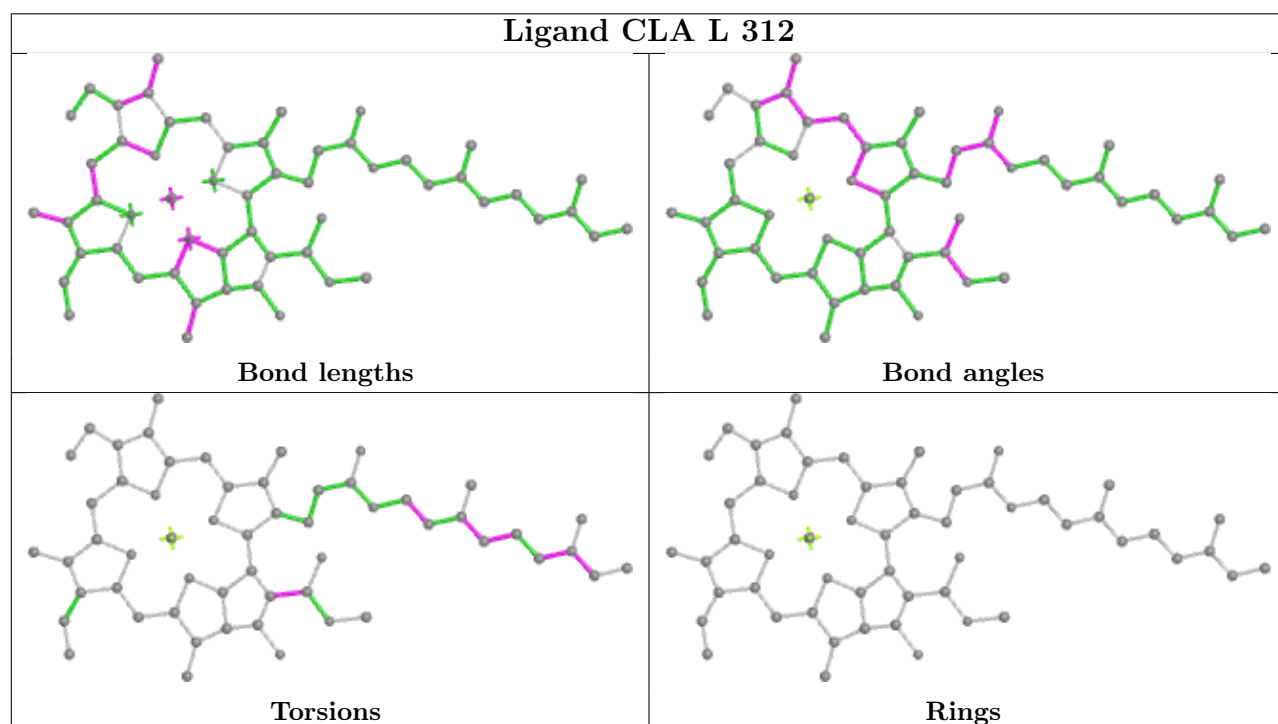
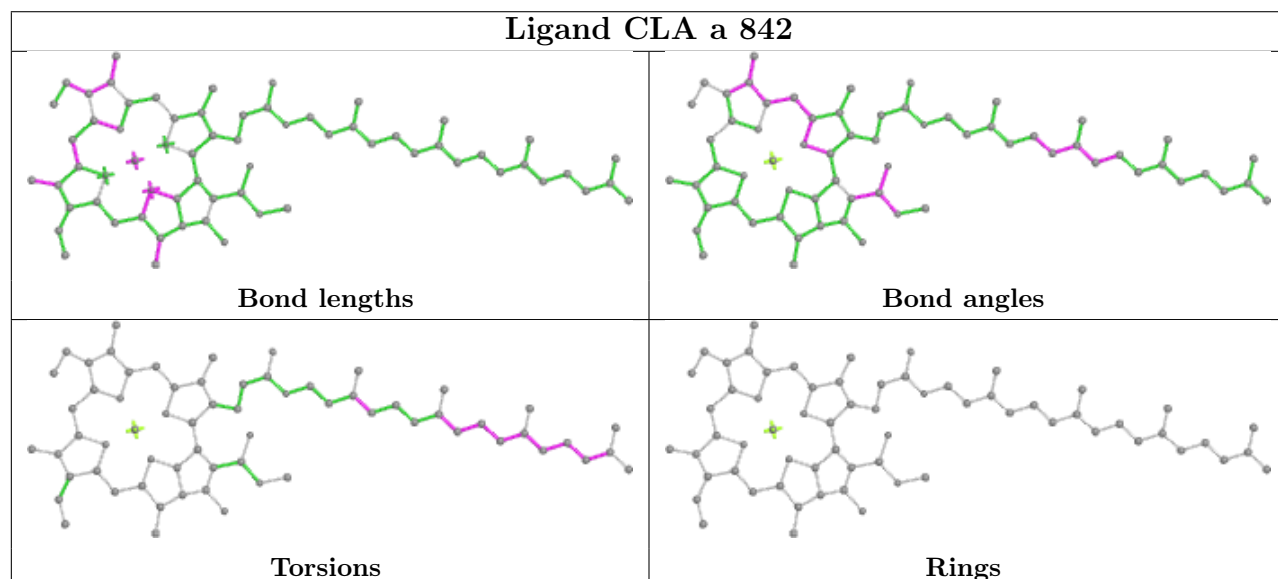
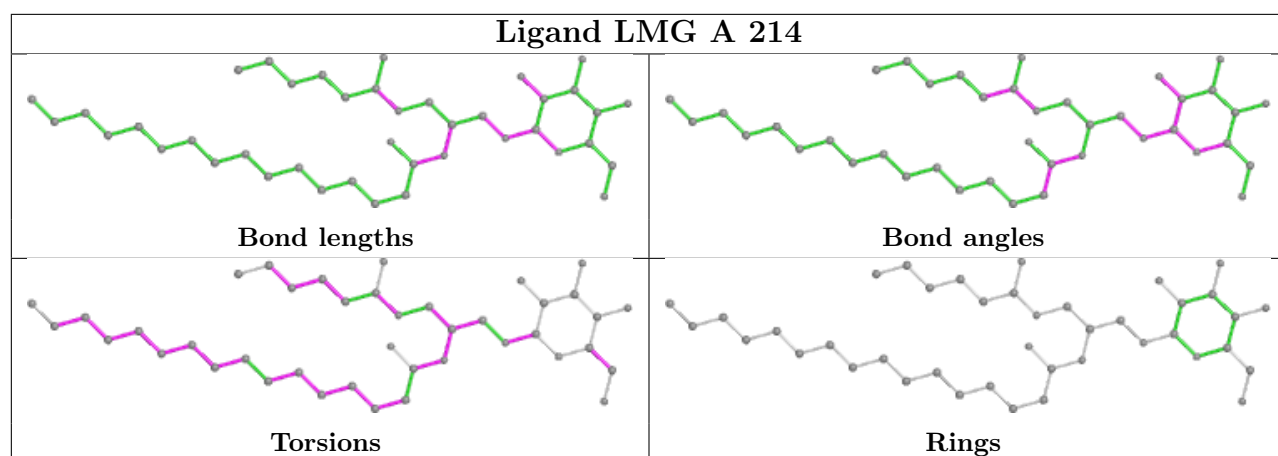
Bond angles



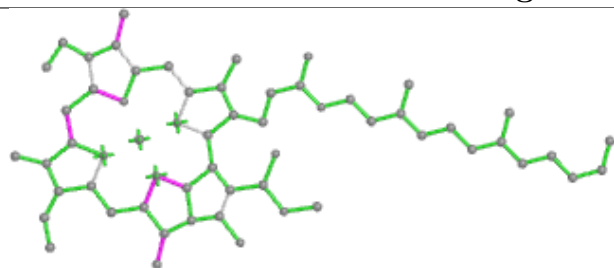
Torsions



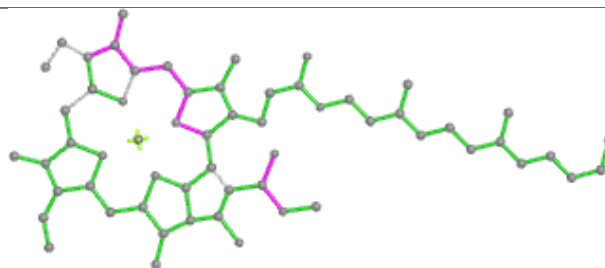
Rings



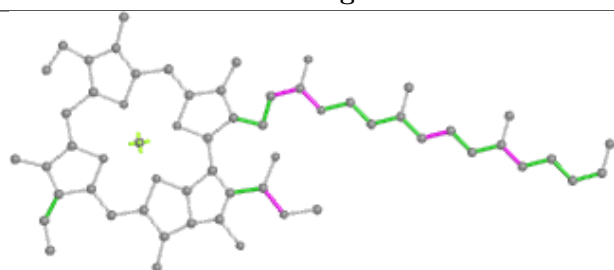
## Ligand CLA F 307



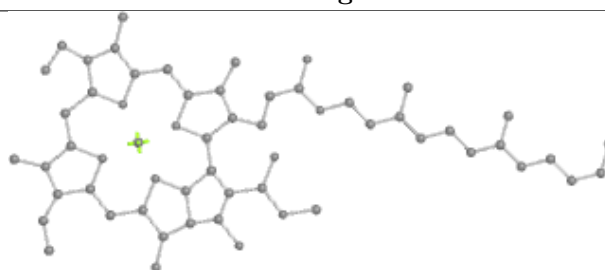
Bond lengths



Bond angles

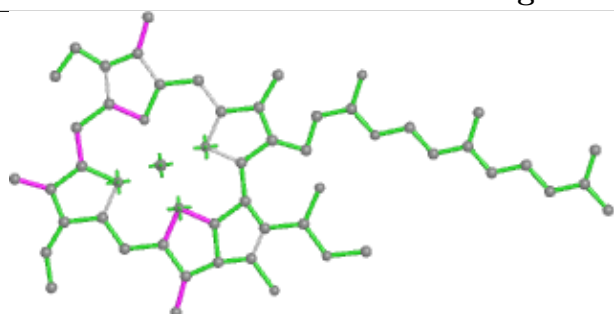


Torsions

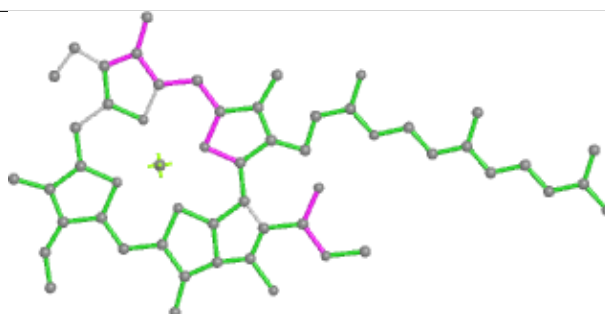


Rings

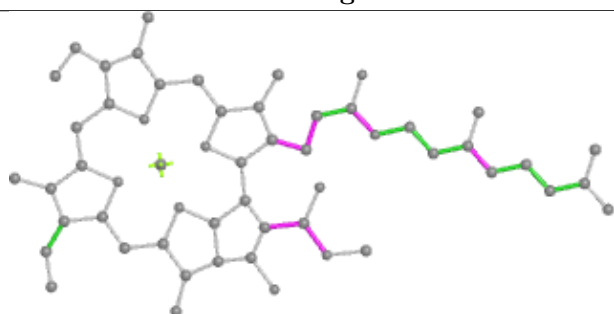
## Ligand CLA b 814



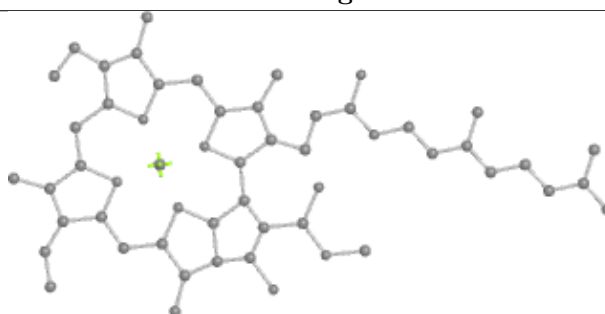
Bond lengths



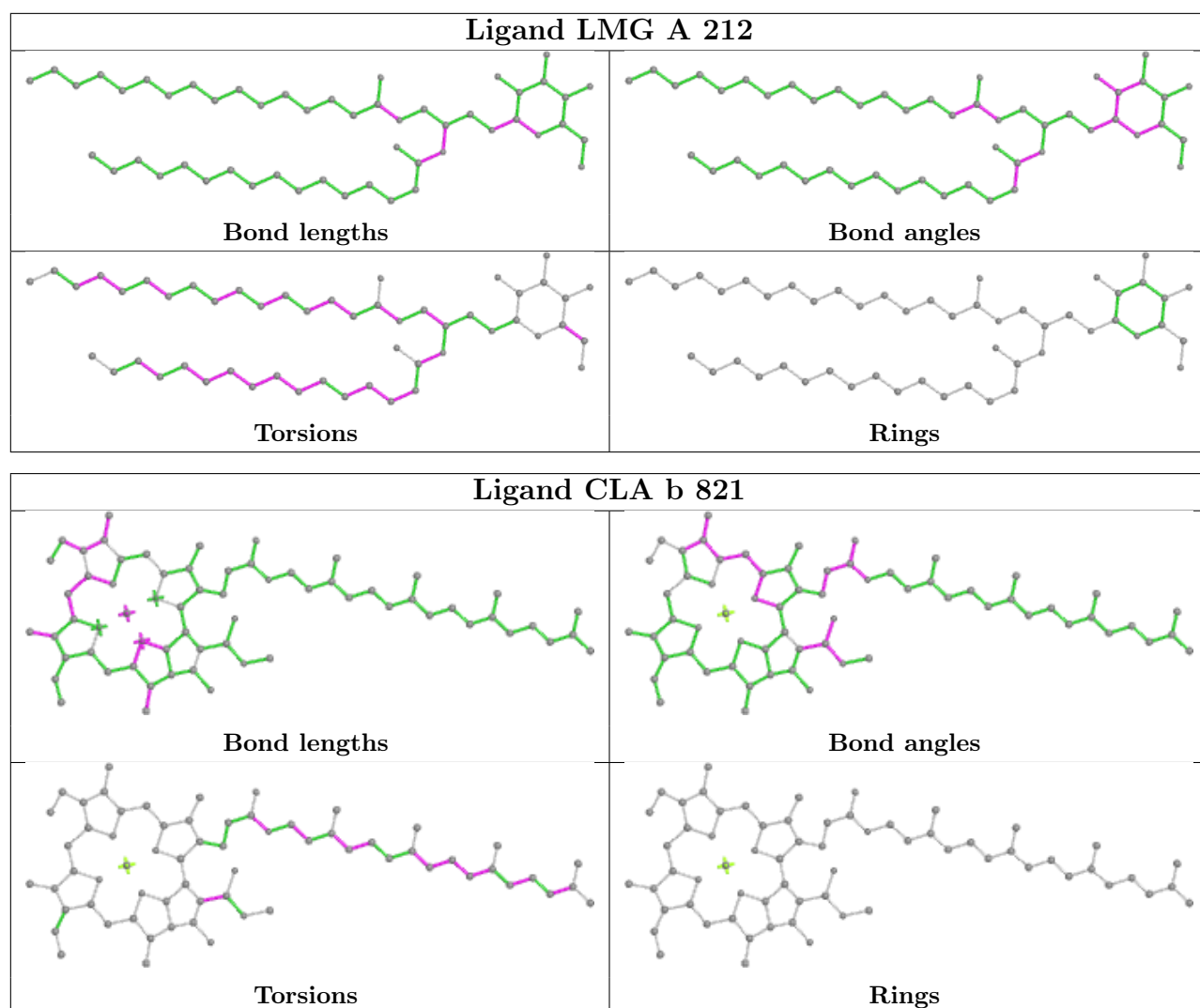
Bond angles

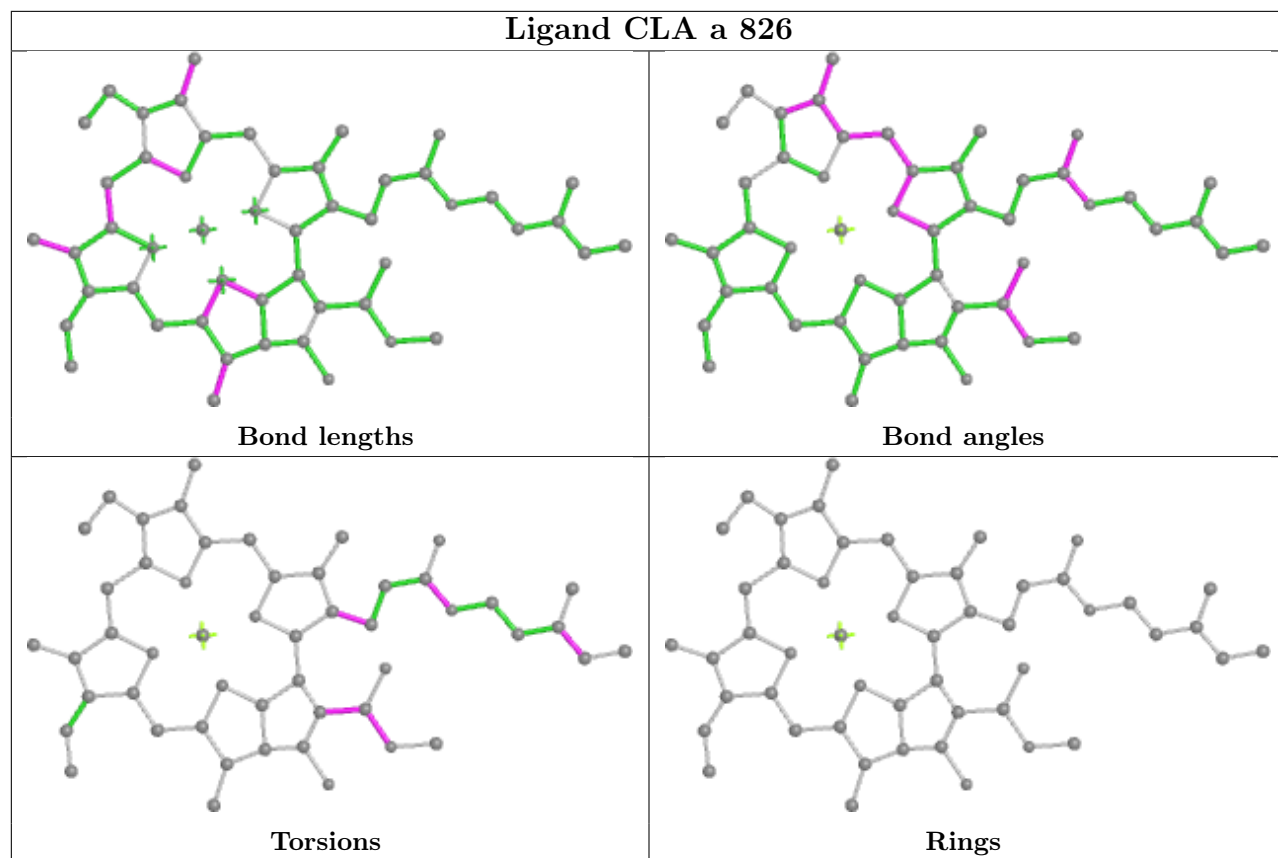


Torsions

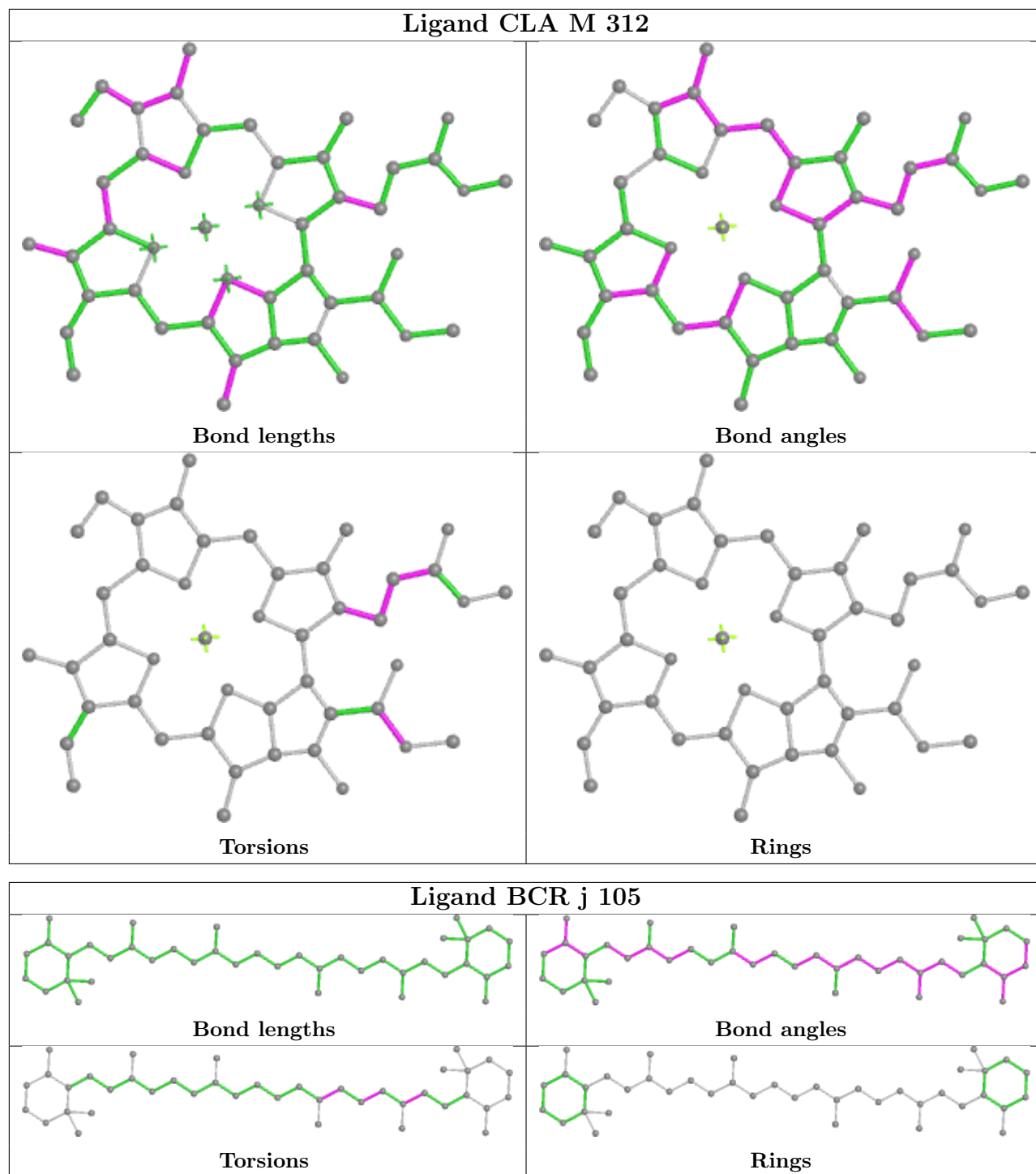


Rings

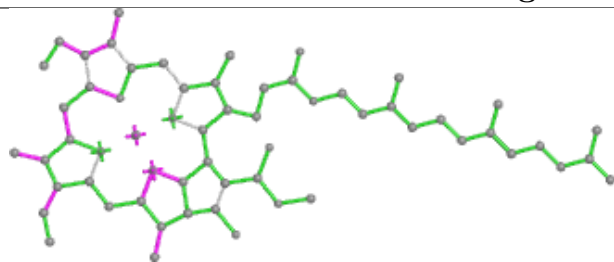




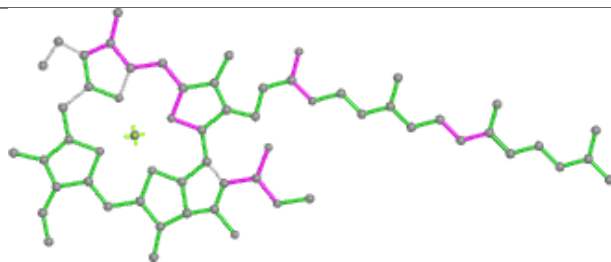




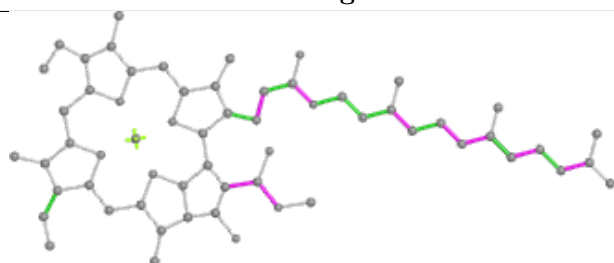
## Ligand CLA a 827



Bond lengths



Bond angles

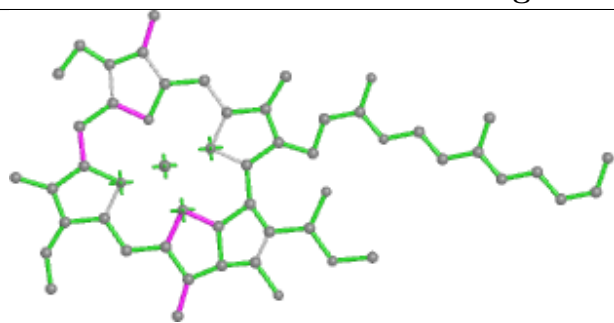


Torsions

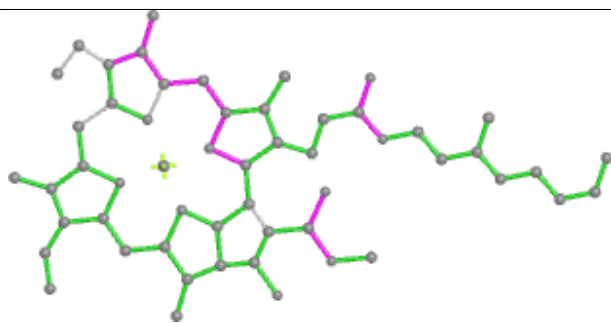


Rings

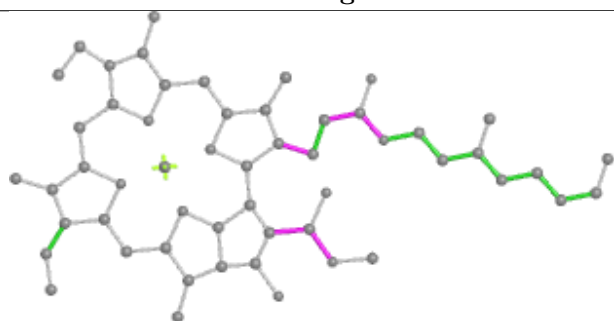
## Ligand CLA G 308



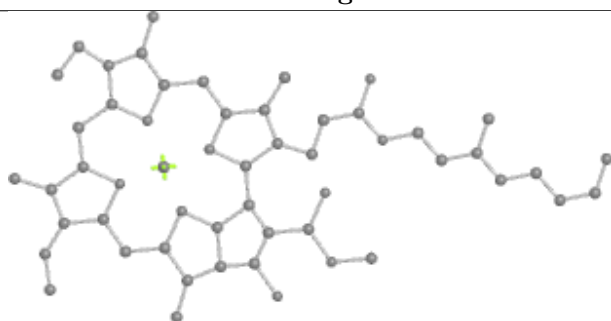
Bond lengths



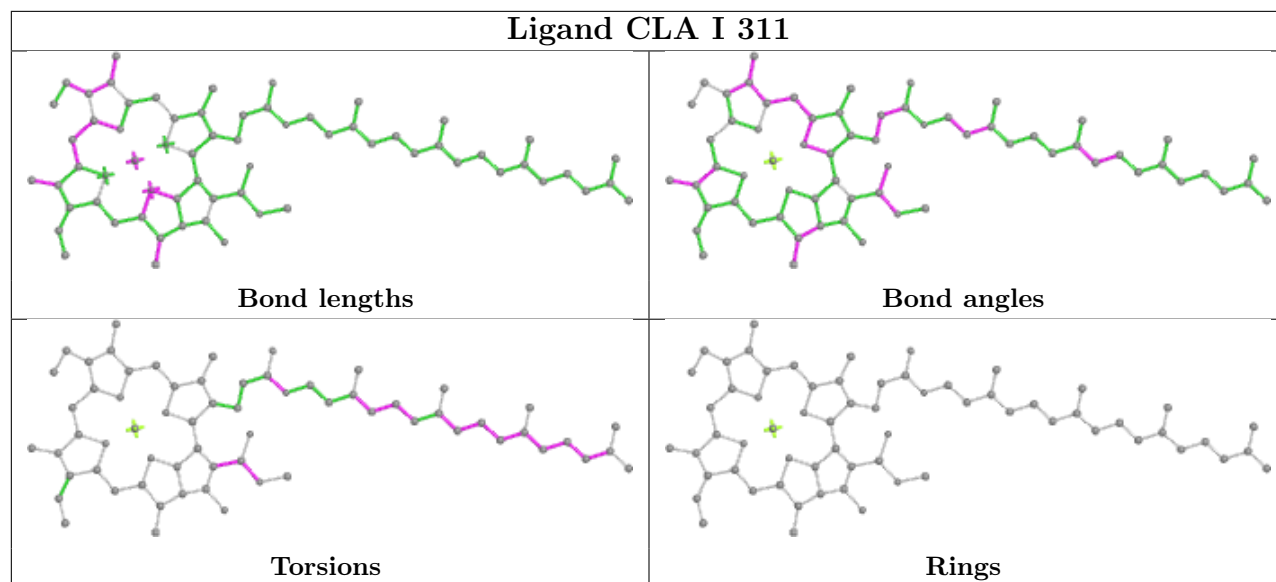
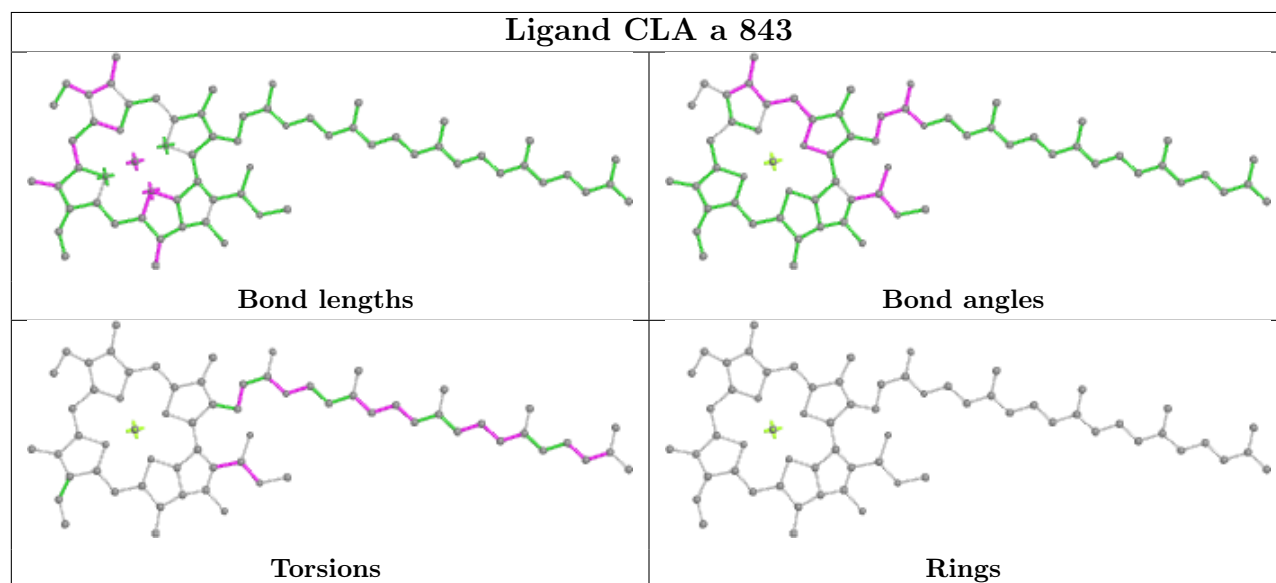
Bond angles



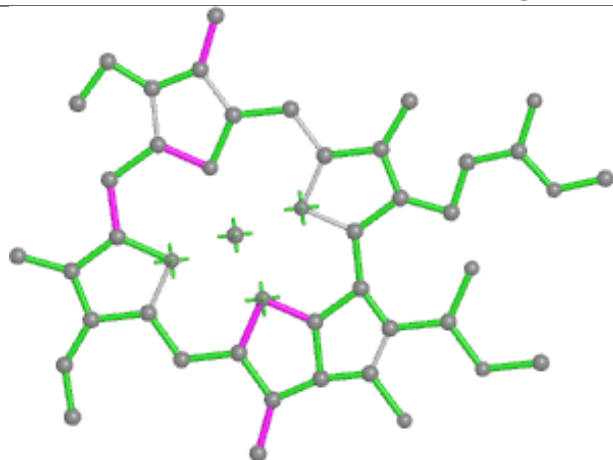
Torsions



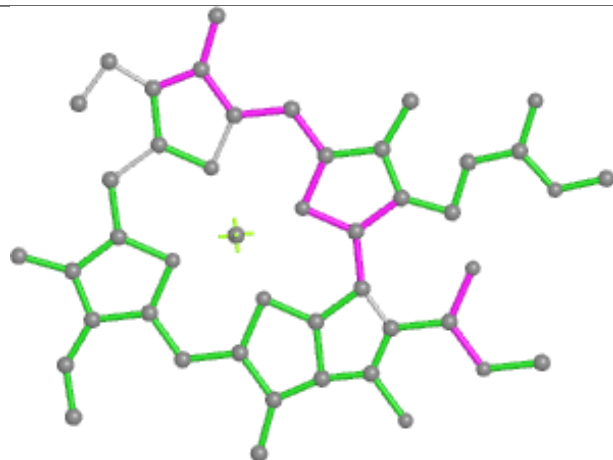
Rings

**Ligand CLA I 311****Ligand CLA a 843**

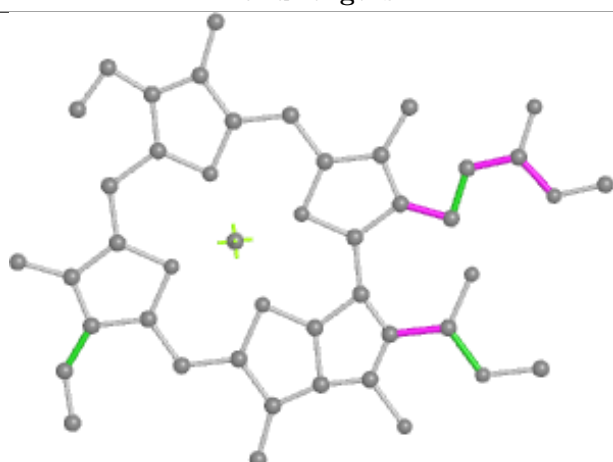
## Ligand CLA E 310



Bond lengths



Bond angles

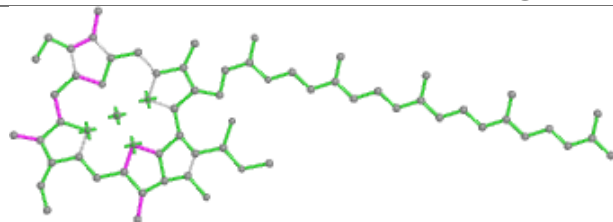


Torsions

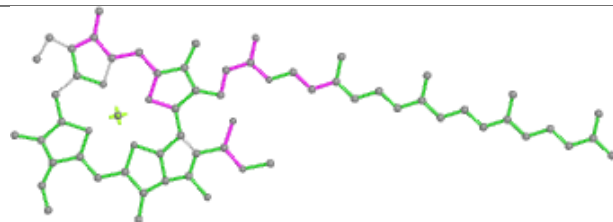


Rings

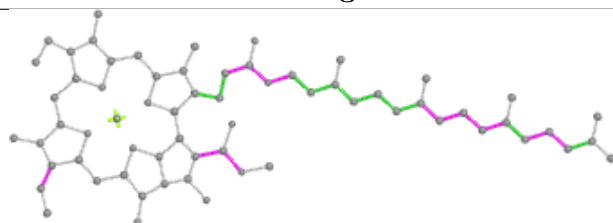
## Ligand CLA L 309



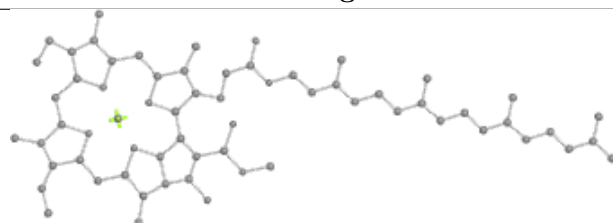
Bond lengths



Bond angles

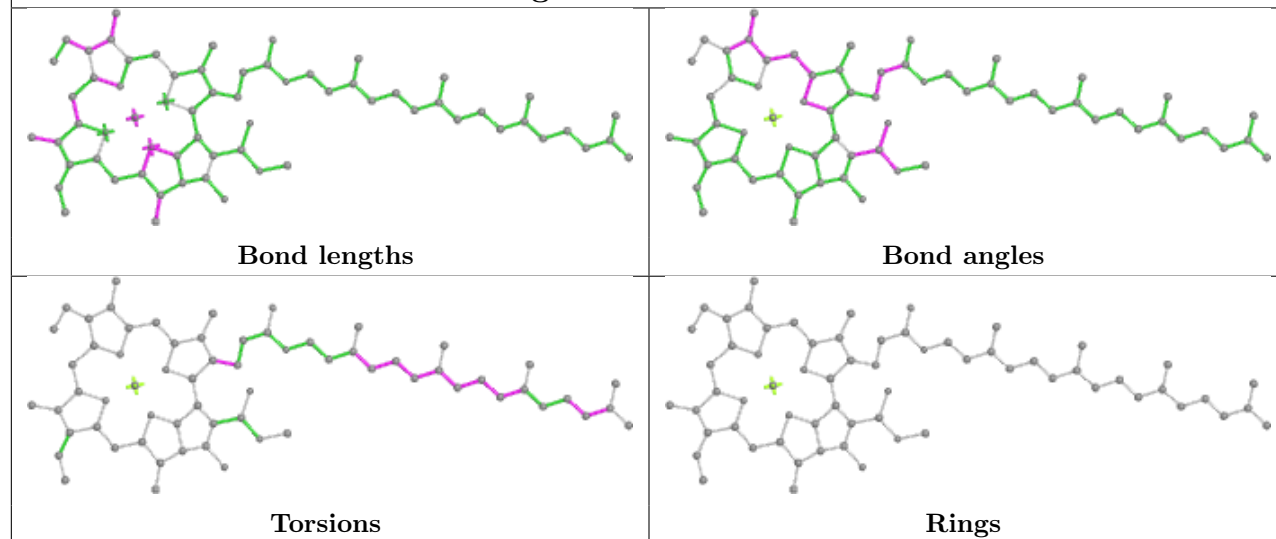


Torsions

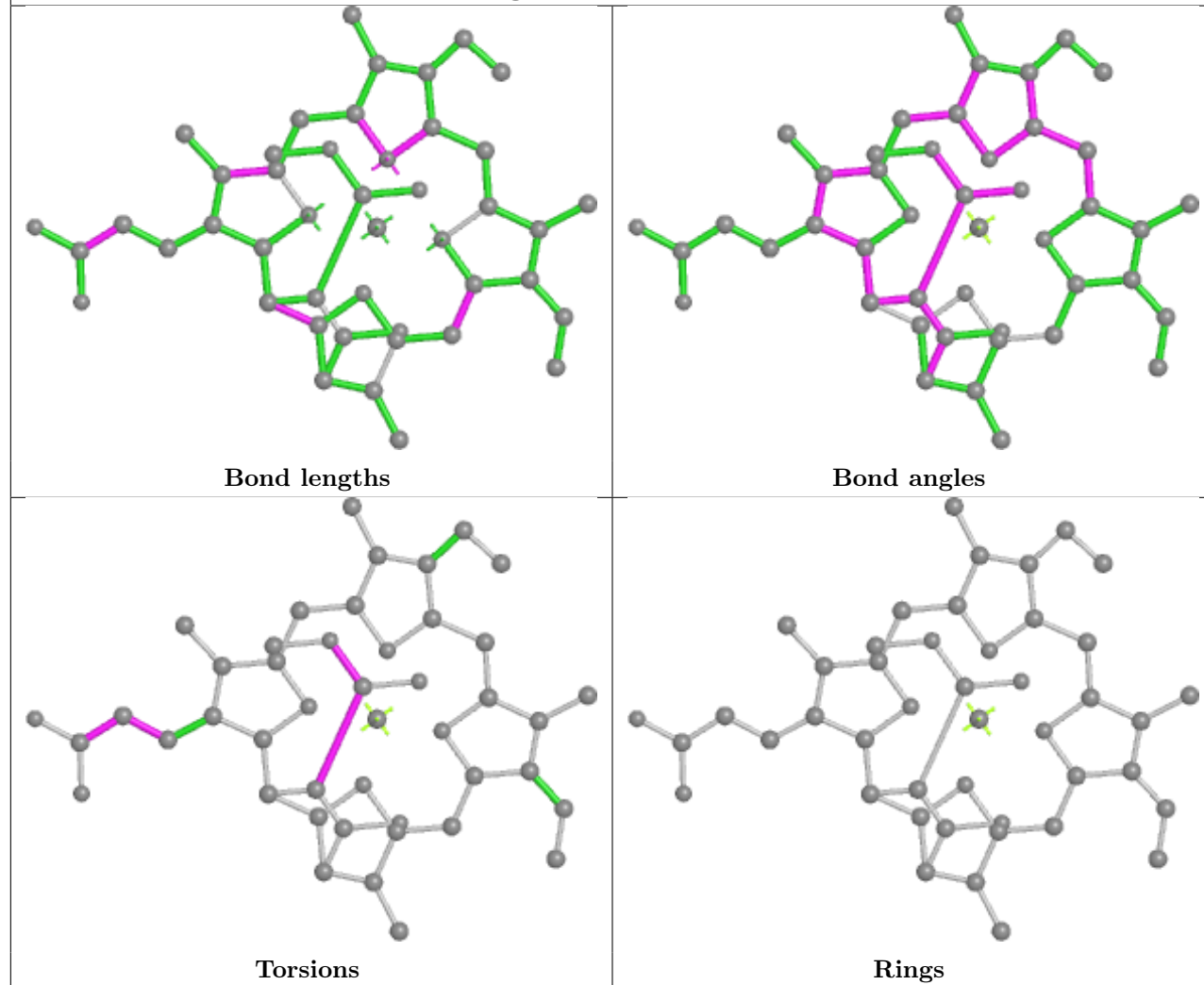


Rings

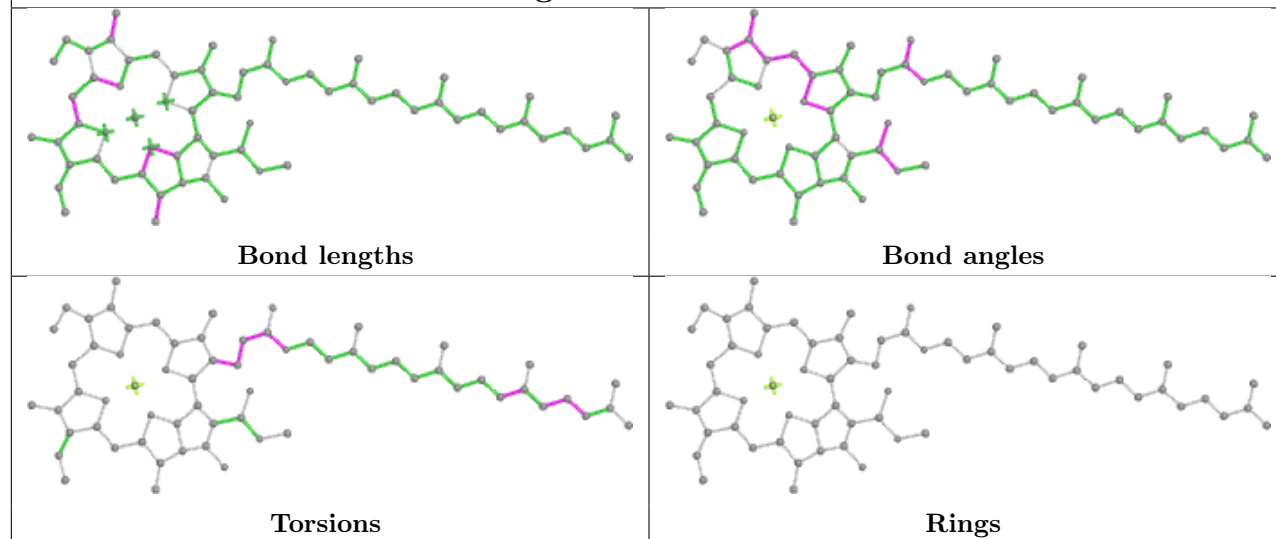
## Ligand CLA A 204



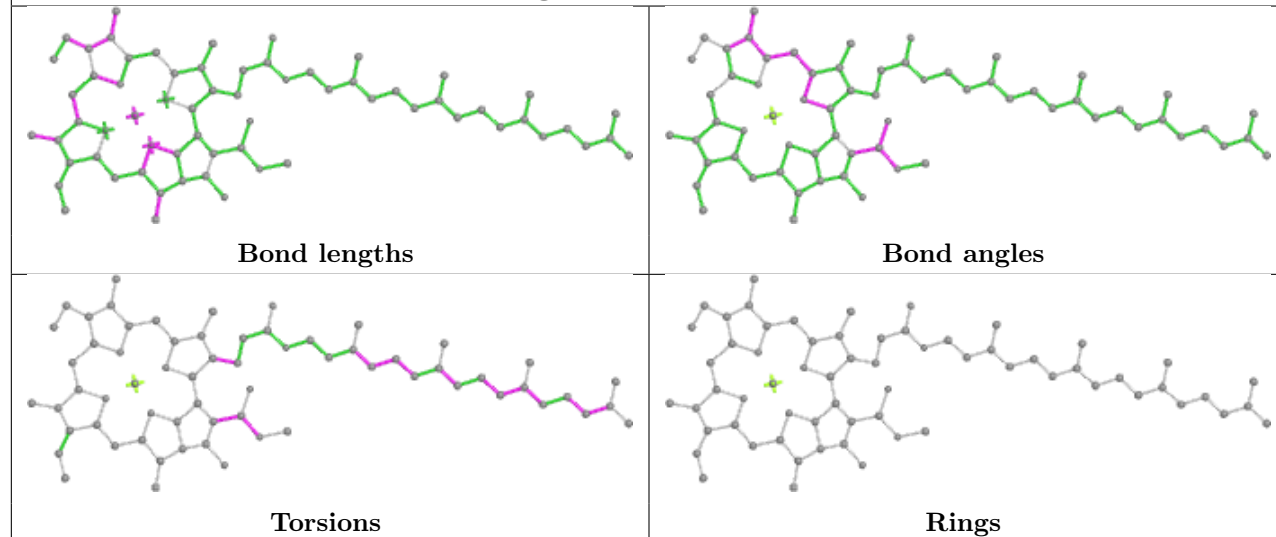
## Ligand KC1 J 306



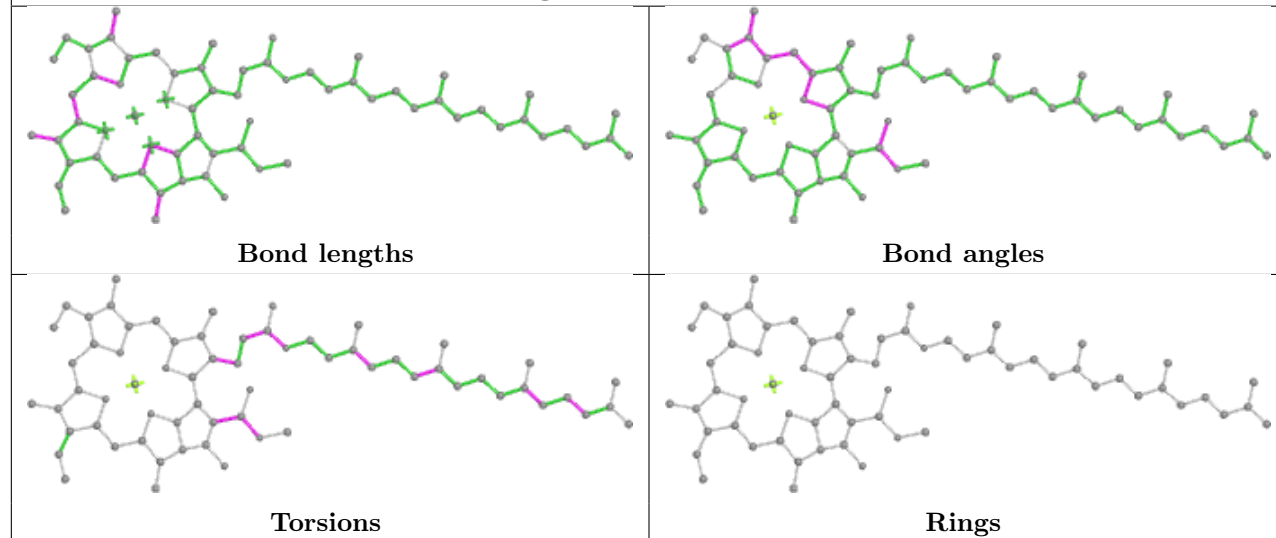
## Ligand CLA b 809



## Ligand CLA b 844



## Ligand CLA a 807



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

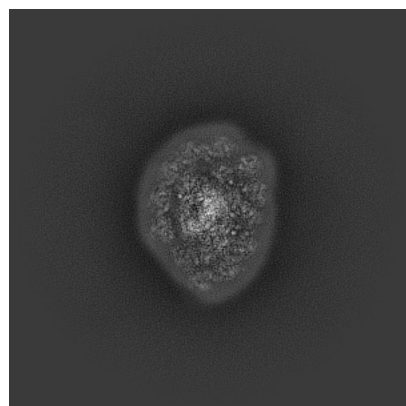
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60032. These allow visual inspection of the internal detail of the map and identification of artifacts.

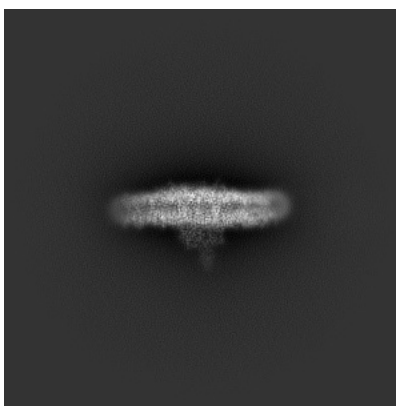
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

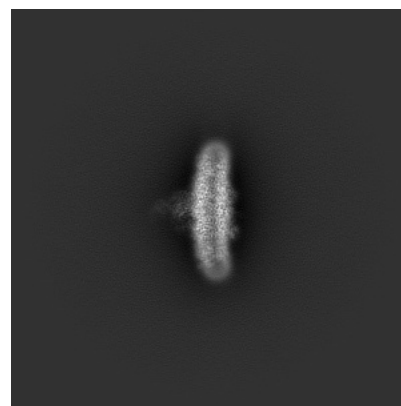
#### 6.1.1 Primary map



X

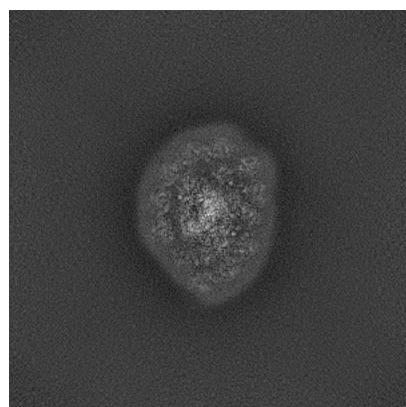


Y

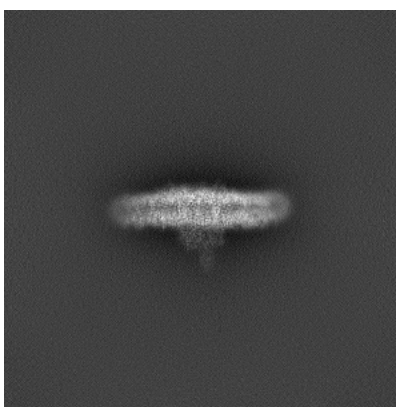


Z

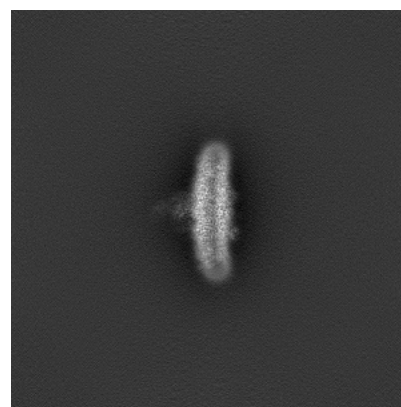
#### 6.1.2 Raw map



X



Y



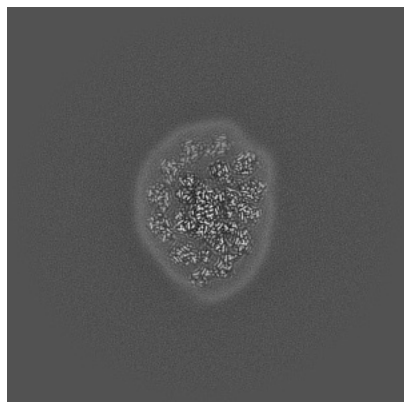
Z

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

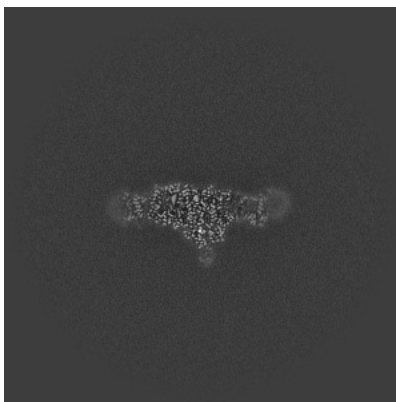


## 6.2 Central slices [i](#)

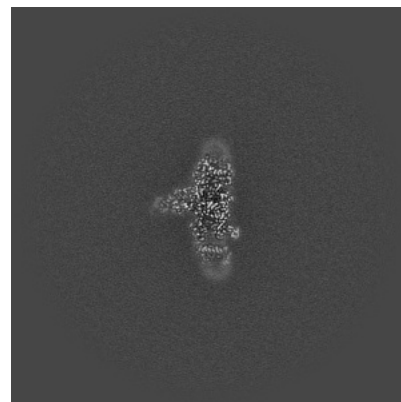
### 6.2.1 Primary map



X Index: 256

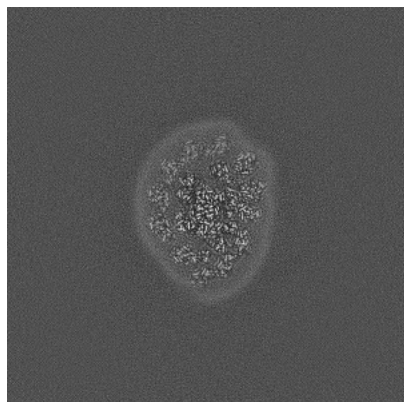


Y Index: 256

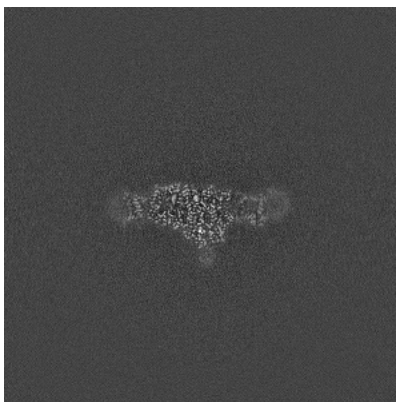


Z Index: 256

### 6.2.2 Raw map



X Index: 256



Y Index: 256

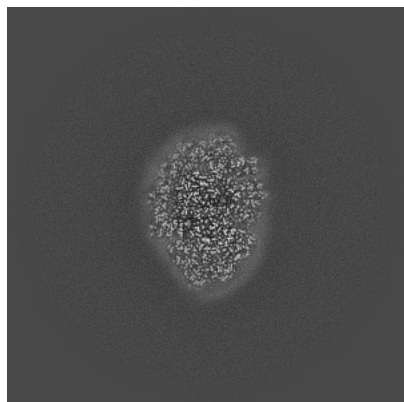


Z Index: 256

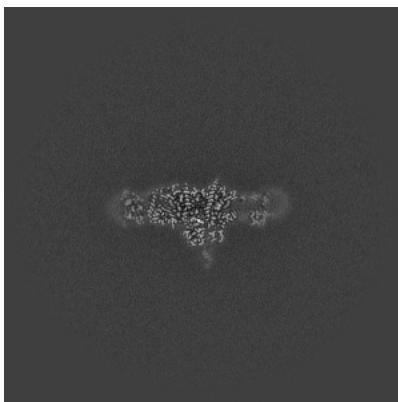
The images above show central slices of the map in three orthogonal directions.

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

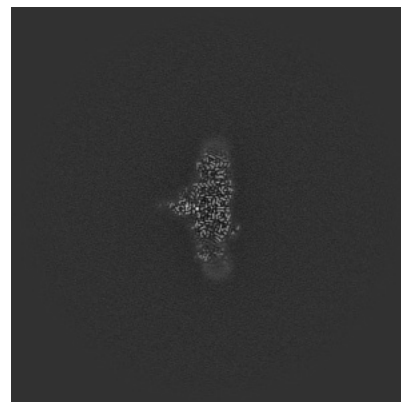
### 6.3.1 Primary map



X Index: 245

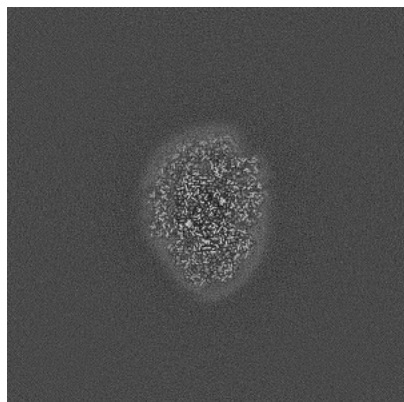


Y Index: 252

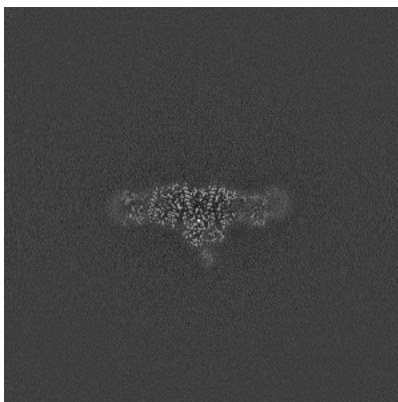


Z Index: 249

### 6.3.2 Raw map



X Index: 246



Y Index: 253

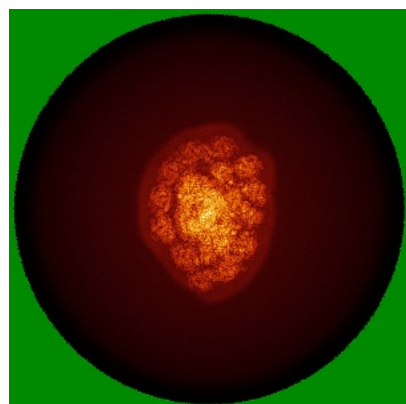


Z Index: 249

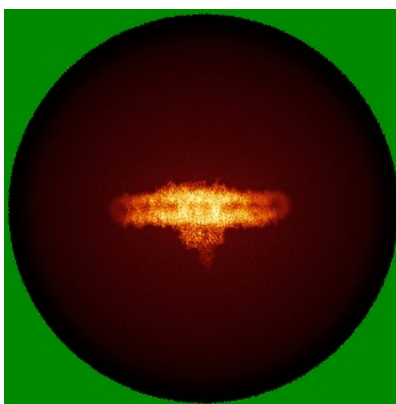
The images above show the largest variance slices of the map in three orthogonal directions.

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

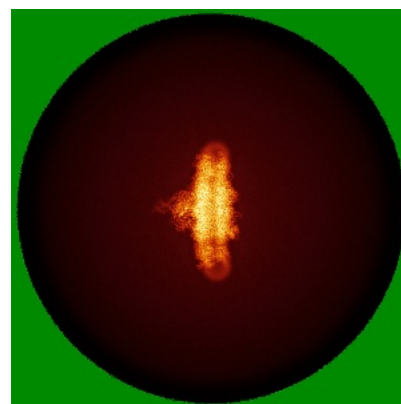
### 6.4.1 Primary map



X

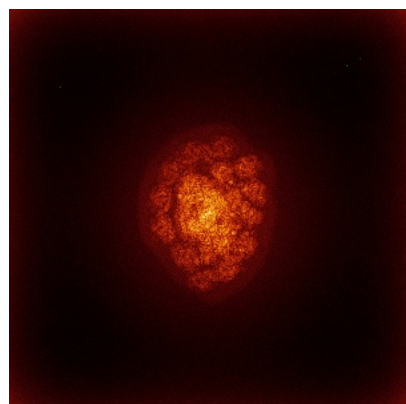


Y

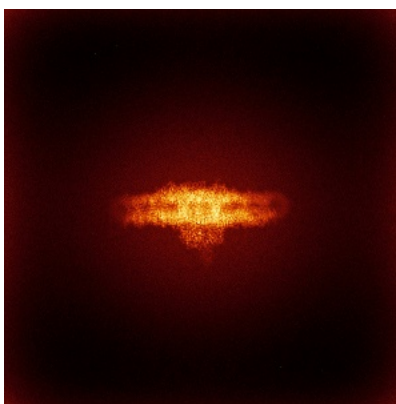


Z

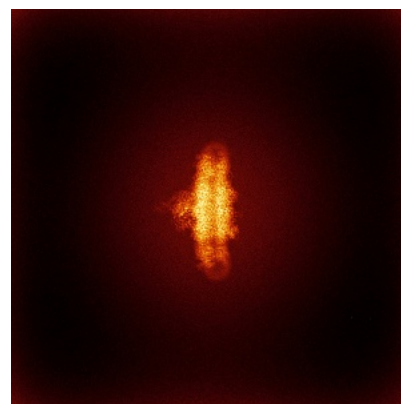
### 6.4.2 Raw map



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



X



Y



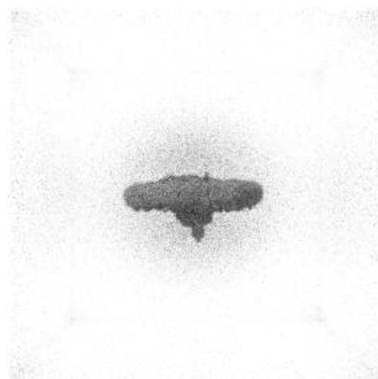
Z

The images above show the 3D surface view of the map at the recommended contour level 0.088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

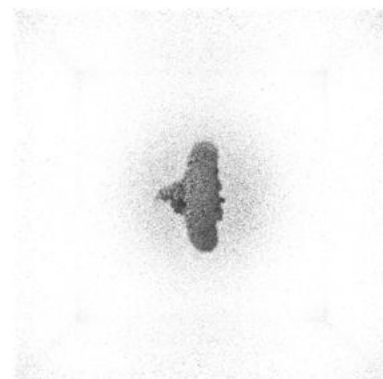
### 6.5.2 Raw map



X



Y



Z

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.

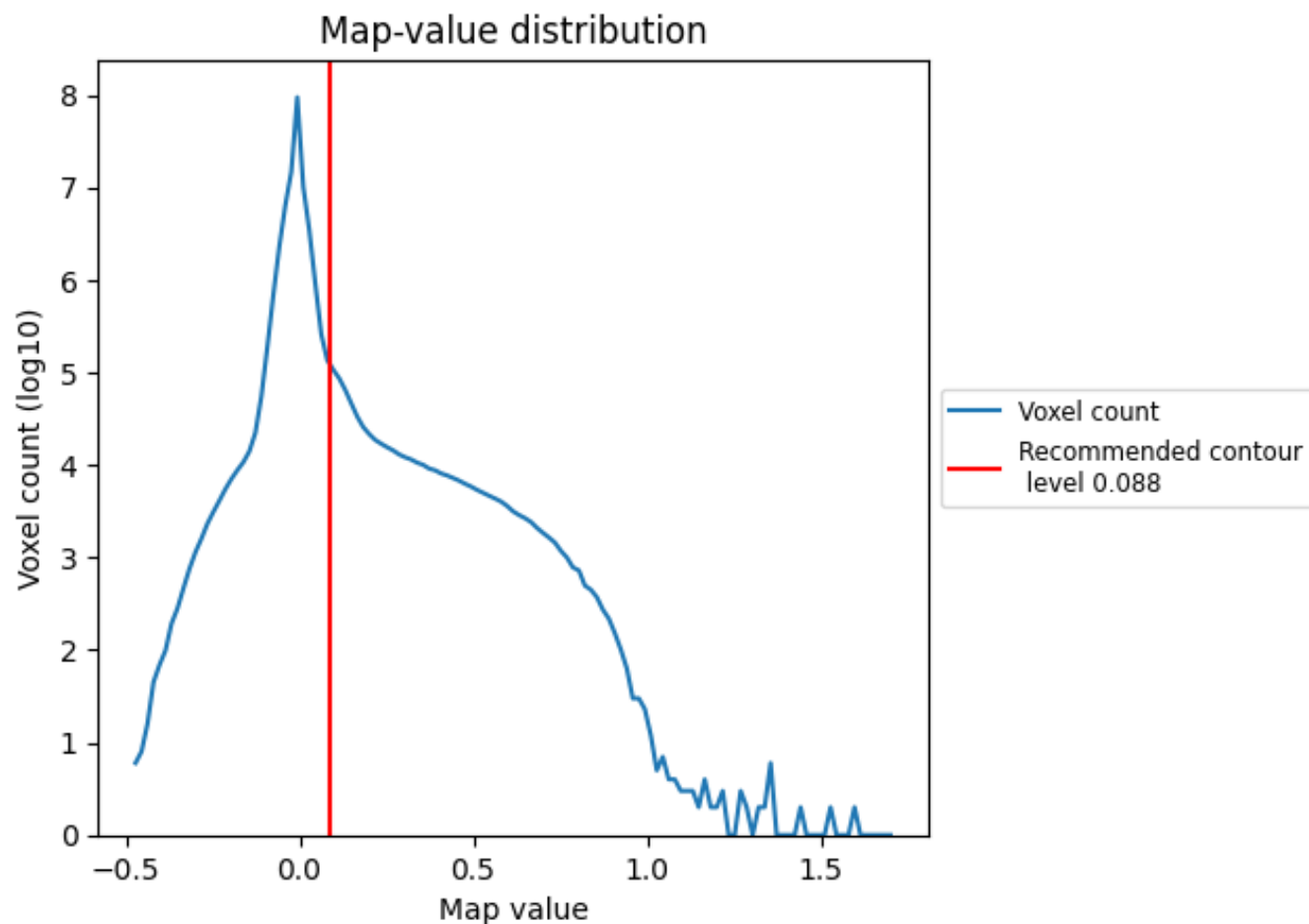
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

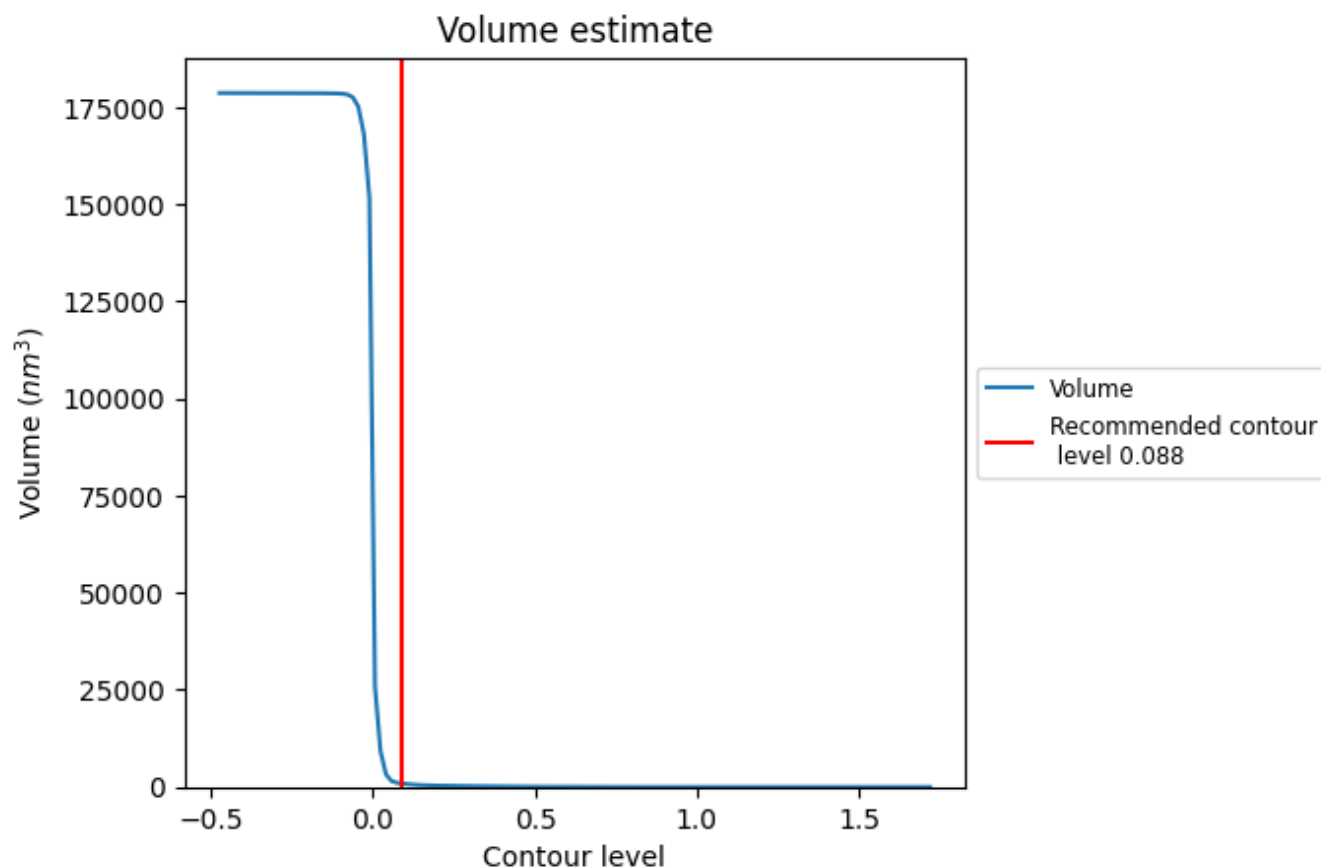
This section contains the results of statistical analysis of the map.

### 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.

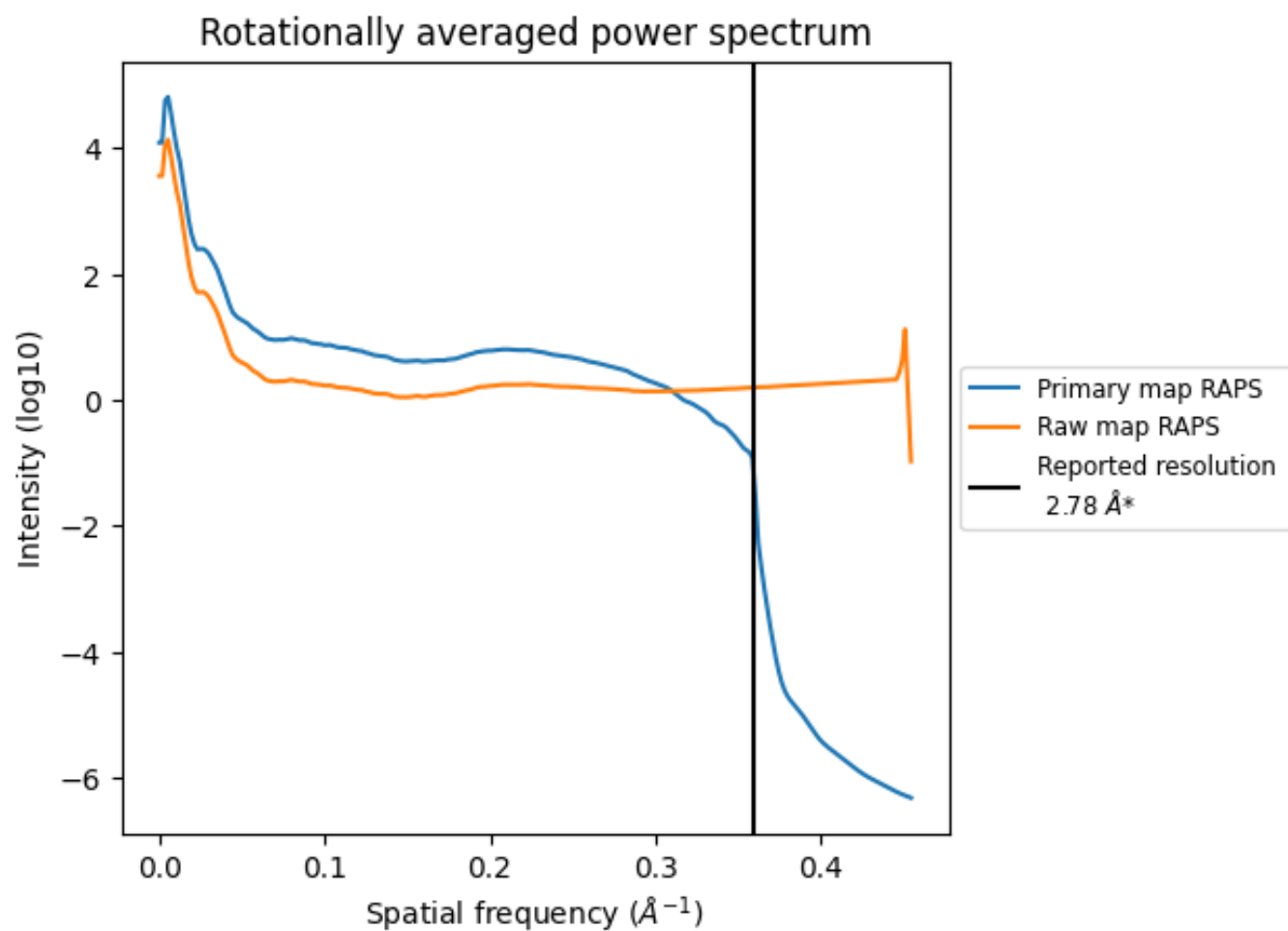
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 920 nm<sup>3</sup>; this corresponds to an approximate mass of 831 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 ⓘ



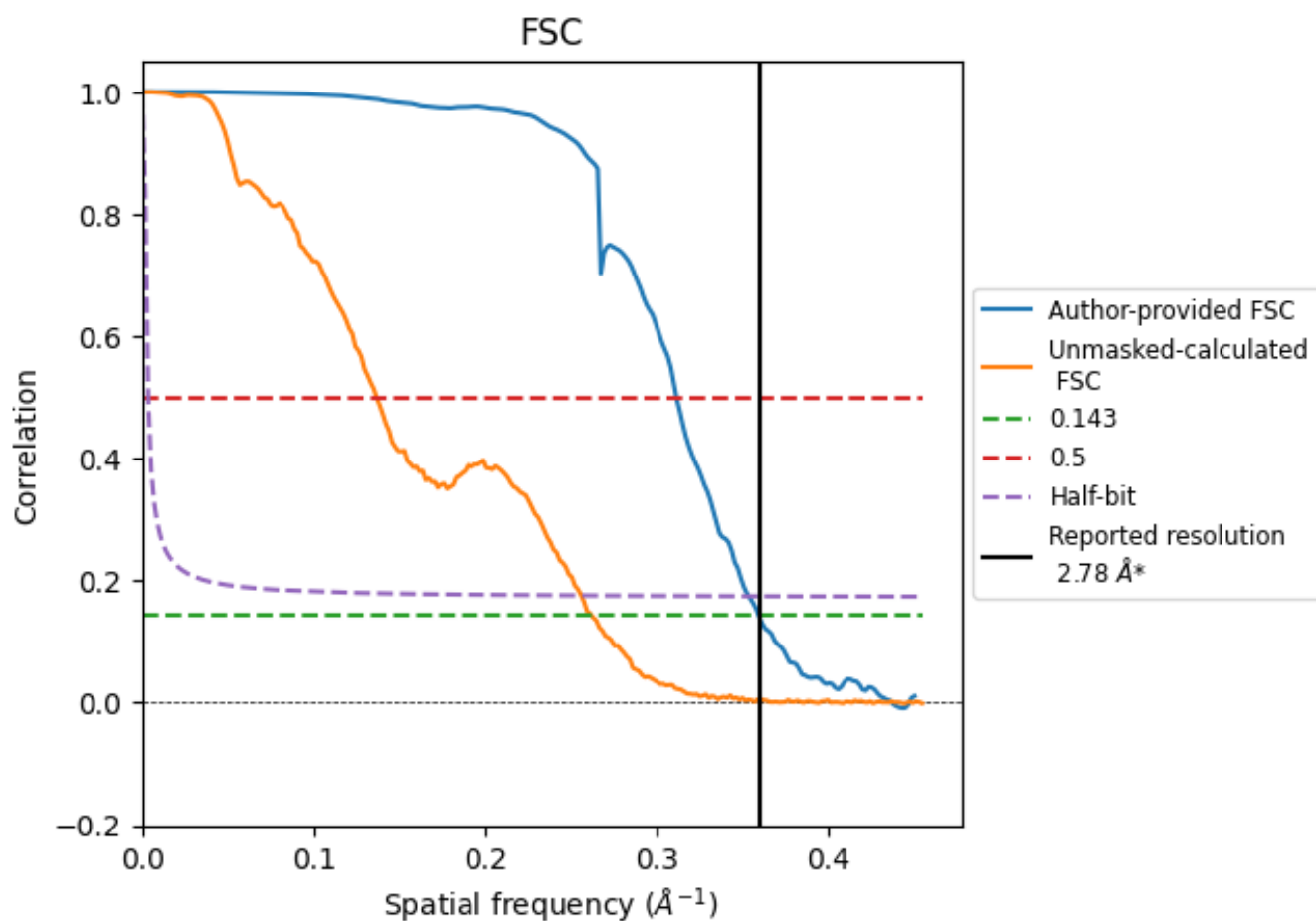
\*Reported resolution corresponds to spatial frequency of 0.360 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.360  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

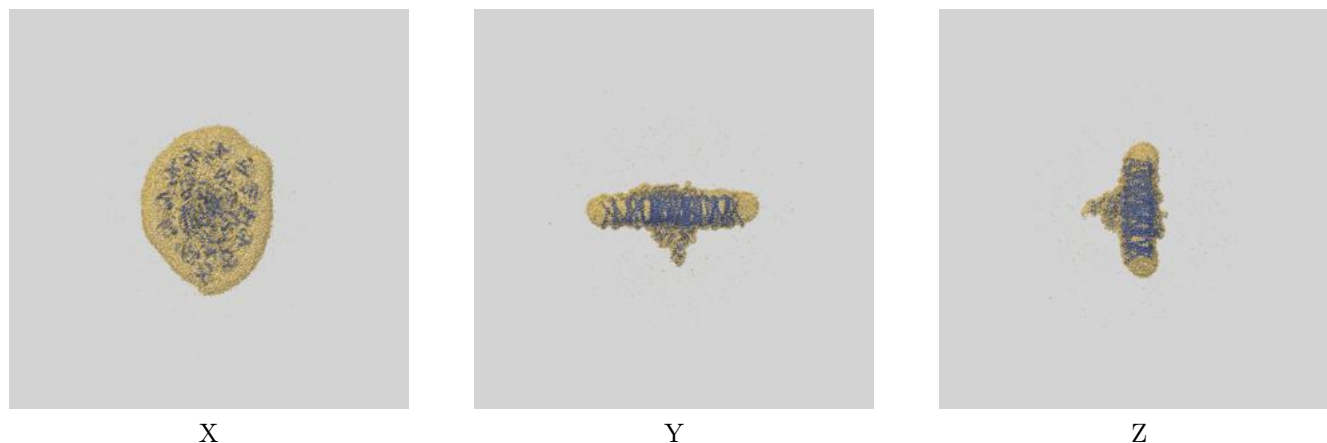
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.21	2.83
Unmasked-calculated*	3.82	7.32	3.91

\*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 3.82 differs from the reported value 2.78 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-60032 and PDB model 8ZEH. Per-residue inclusion information can be found in section 3 on page 38.

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



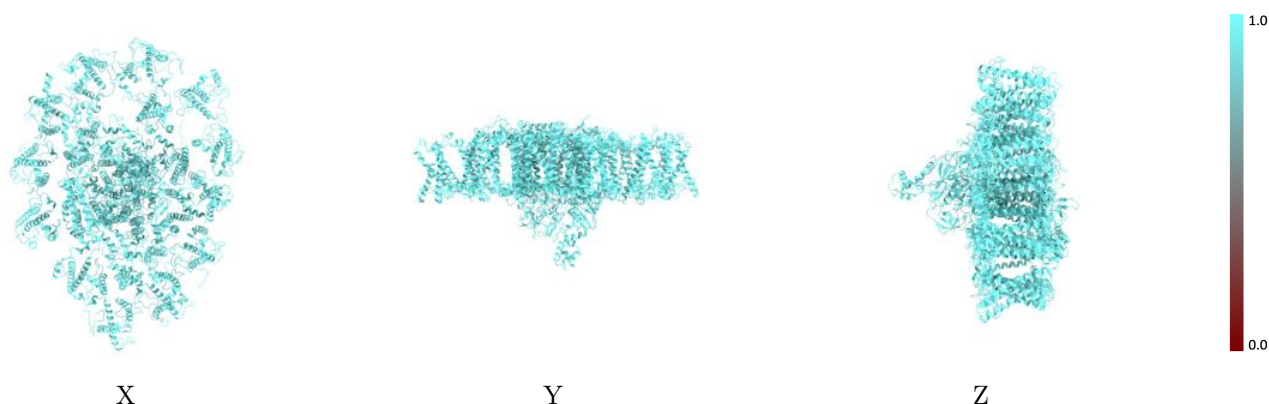
The images above show the 3D surface view of the map at the recommended contour level 0.088 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



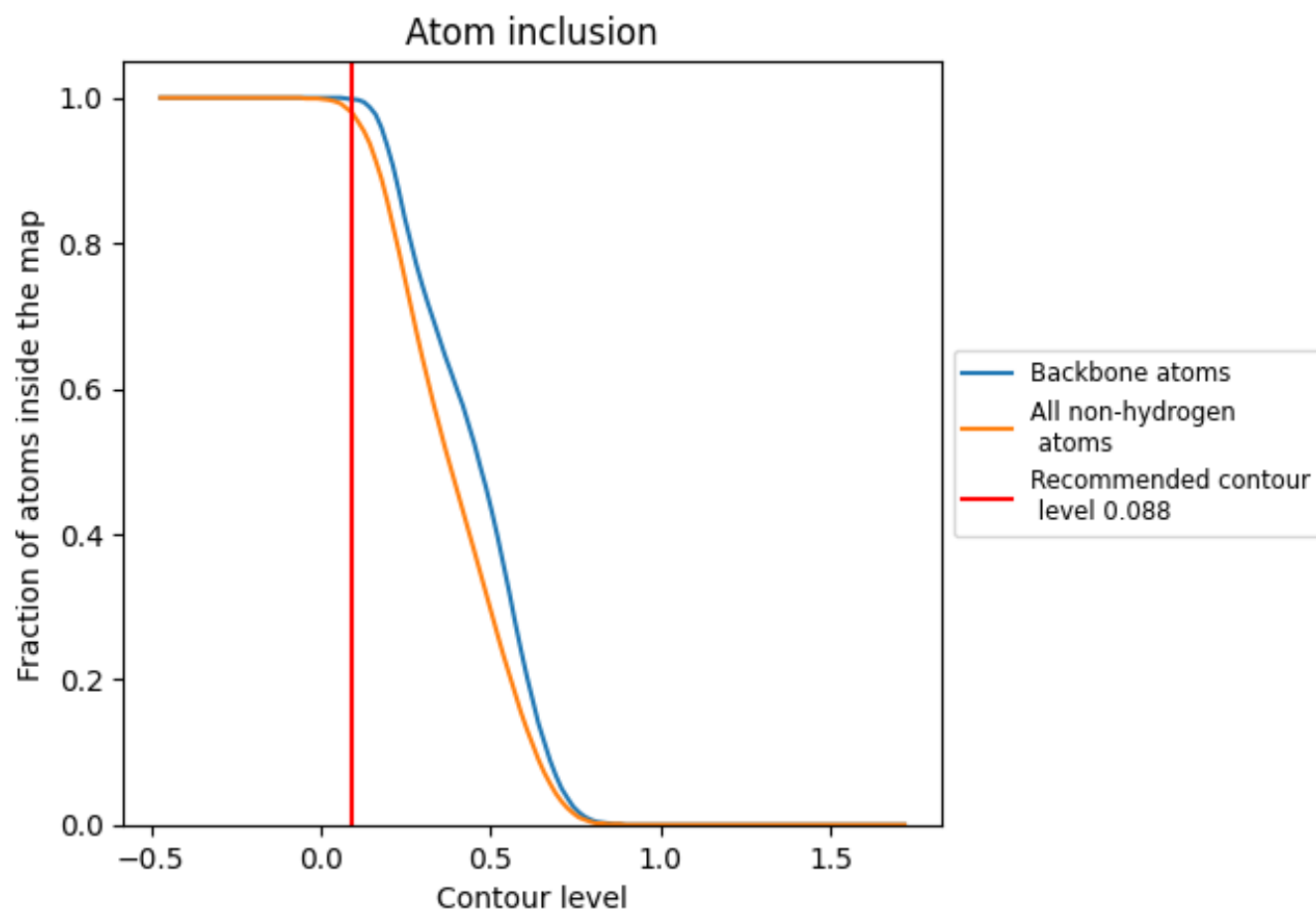
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.088).





















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.5660
A	 0.9750	 0.5410
B	 0.9790	 0.5580
C	 0.9820	 0.5480
D	 0.9770	 0.5730
E	 0.9840	 0.5710
F	 0.9540	 0.4550
G	 0.9760	 0.5470
H	 0.9870	 0.5760
I	 0.9800	 0.5430
J	 0.9780	 0.5160
K	 0.9810	 0.5730
L	 0.9710	 0.5180
M	 0.9850	 0.5780
a	 0.9890	 0.5990
b	 0.9860	 0.5970
c	 0.9900	 0.5880
d	 0.9940	 0.5920
e	 0.9710	 0.5630
f	 0.9800	 0.5790
g	 0.9490	 0.5090
i	 0.9900	 0.5990
j	 0.9680	 0.5650
l	 0.9940	 0.5920
m	 0.9770	 0.5700
r	 0.9820	 0.5740

