



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 05:38 PM JST

PDB ID : 6LY5 / pdb\_00006ly5  
EMDB ID : EMD-30012  
Title : Organization and energy transfer in a huge diatom PSI-FCPI supercomplex  
Authors : Xiong, P.; Caizhe, X.  
Deposited on : 2020-02-13  
Resolution : 2.38 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

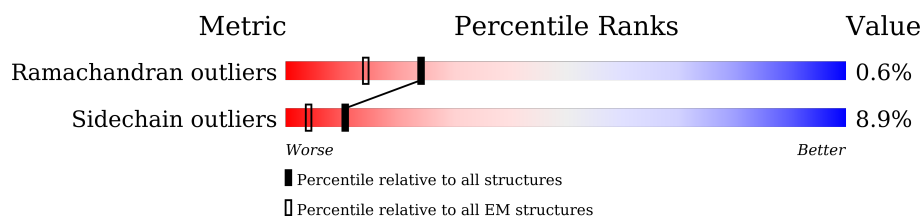
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.38 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





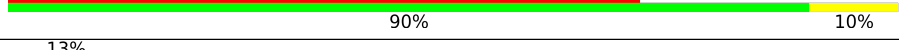

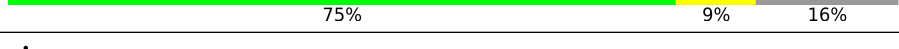
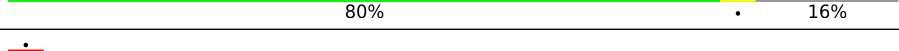
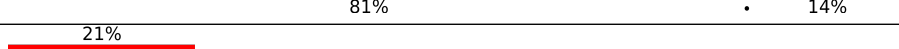
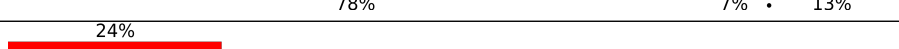
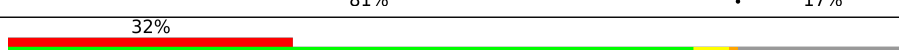

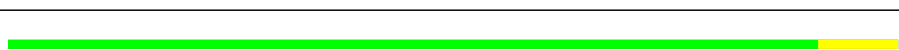




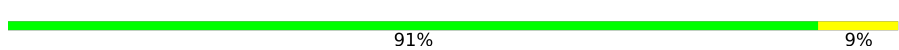


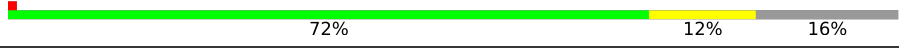
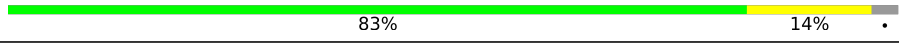
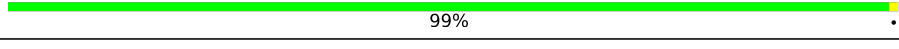


The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey 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	168	
2	B	223	
3	C	198	
4	D	207	
5	E	222	
6	F	215	
7	G	245	
8	H	203	
9	I	195	

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Mol	Chain	Length	Quality of chain
10	J	200	
11	K	207	
12	L	229	
13	M	306	
14	N	219	
15	O	205	
15	P	205	
15	Q	205	
16	R	246	
17	S	254	
18	T	207	
19	W	198	
19	X	198	
20	a	743	
21	b	733	
22	c	80	
23	d	132	
24	e	63	
25	f	162	
26	i	40	
27	j	42	
28	l	172	
29	m	29	
30	g	134	
31	h	139	

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Mol	Chain	Length	Quality of chain
32	U	160	
33	V	179	

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
36	CLA	A	305	X	-	-	-
36	CLA	A	306	X	-	-	-
36	CLA	A	307	X	-	-	-
36	CLA	A	308	X	-	-	-
36	CLA	A	309	X	-	-	-
36	CLA	A	310	X	-	-	-
36	CLA	A	311	X	-	-	-
36	CLA	A	313	X	-	-	-
36	CLA	A	314	X	-	-	-
36	CLA	B	305	X	-	-	-
36	CLA	B	306	X	-	-	-
36	CLA	B	307	X	-	-	-
36	CLA	B	308	X	-	-	-
36	CLA	B	309	X	-	-	-
36	CLA	B	311	X	-	-	-
36	CLA	C	205	X	-	-	-
36	CLA	C	206	X	-	-	-
36	CLA	C	207	X	-	-	-
36	CLA	C	208	X	-	-	-
36	CLA	C	209	X	-	-	-
36	CLA	C	210	X	-	-	-
36	CLA	C	211	X	-	-	-
36	CLA	C	212	X	-	-	-
36	CLA	C	214	X	-	-	-
36	CLA	D	306	X	-	-	-
36	CLA	D	307	X	-	-	-
36	CLA	D	308	X	-	-	-
36	CLA	D	309	X	-	-	-
36	CLA	D	310	X	-	-	-
36	CLA	D	312	X	-	-	-
36	CLA	D	313	X	-	-	-
36	CLA	D	315	X	-	-	-
36	CLA	D	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	D	317	X	-	-	-
36	CLA	E	308	X	-	-	-
36	CLA	E	311	X	-	-	-
36	CLA	E	312	X	-	-	-
36	CLA	E	313	X	-	-	-
36	CLA	E	314	X	-	-	-
36	CLA	E	315	X	-	-	-
36	CLA	E	316	X	-	-	-
36	CLA	E	317	X	-	-	-
36	CLA	F	309	X	-	-	-
36	CLA	F	310	X	-	-	-
36	CLA	F	311	X	-	-	-
36	CLA	F	312	X	-	-	-
36	CLA	F	313	X	-	-	-
36	CLA	F	314	X	-	-	-
36	CLA	F	316	X	-	-	-
36	CLA	F	317	X	-	-	-
36	CLA	G	309	X	-	-	-
36	CLA	G	310	X	-	-	-
36	CLA	G	311	X	-	-	-
36	CLA	G	312	X	-	-	-
36	CLA	G	313	X	-	-	-
36	CLA	G	314	X	-	-	-
36	CLA	G	315	X	-	-	-
36	CLA	G	316	X	-	-	-
36	CLA	G	319	X	-	-	-
36	CLA	H	305	X	-	-	-
36	CLA	H	306	X	-	-	-
36	CLA	H	307	X	-	-	-
36	CLA	H	308	X	-	-	-
36	CLA	H	309	X	-	-	-
36	CLA	H	310	X	-	-	-
36	CLA	H	311	X	-	-	-
36	CLA	H	312	X	-	-	-
36	CLA	H	314	X	-	-	-
36	CLA	H	315	X	-	-	-
36	CLA	H	316	X	-	-	-
36	CLA	H	317	X	-	-	-
36	CLA	H	318	X	-	-	-
36	CLA	I	305	X	-	-	-
36	CLA	I	306	X	-	-	-
36	CLA	I	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	I	308	X	-	-	-
36	CLA	I	309	X	-	-	-
36	CLA	I	310	X	-	-	-
36	CLA	I	311	X	-	-	-
36	CLA	I	312	X	-	-	-
36	CLA	I	313	X	-	-	-
36	CLA	I	314	X	-	-	-
36	CLA	J	307	X	-	-	-
36	CLA	J	309	X	-	-	-
36	CLA	J	310	X	-	-	-
36	CLA	J	311	X	-	-	-
36	CLA	J	312	X	-	-	-
36	CLA	J	313	X	-	-	-
36	CLA	J	315	X	-	-	-
36	CLA	J	316	X	-	-	-
36	CLA	J	317	X	-	-	-
36	CLA	K	307	X	-	-	-
36	CLA	K	308	X	-	-	-
36	CLA	K	309	X	-	-	-
36	CLA	K	310	X	-	-	-
36	CLA	K	311	X	-	-	-
36	CLA	K	312	X	-	-	-
36	CLA	K	313	X	-	-	-
36	CLA	K	315	X	-	-	-
36	CLA	K	316	X	-	-	-
36	CLA	L	308	X	-	-	-
36	CLA	L	309	X	-	-	-
36	CLA	L	310	X	-	-	-
36	CLA	L	311	X	-	-	-
36	CLA	L	313	X	-	-	-
36	CLA	L	314	X	-	-	-
36	CLA	L	316	X	-	-	-
36	CLA	L	320	X	-	-	-
36	CLA	M	306	X	-	-	-
36	CLA	M	307	X	-	-	-
36	CLA	M	308	X	-	-	-
36	CLA	M	309	X	-	-	-
36	CLA	M	310	X	-	-	-
36	CLA	M	311	X	-	-	-
36	CLA	M	312	X	-	-	-
36	CLA	M	314	X	-	-	-
36	CLA	M	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	N	307	X	-	-	-
36	CLA	N	308	X	-	-	-
36	CLA	N	309	X	-	-	-
36	CLA	N	310	X	-	-	-
36	CLA	N	311	X	-	-	-
36	CLA	N	312	X	-	-	-
36	CLA	N	313	X	-	-	-
36	CLA	N	316	X	-	-	-
36	CLA	N	317	X	-	-	-
36	CLA	N	318	X	-	-	-
36	CLA	N	319	X	-	-	-
36	CLA	O	306	X	-	-	-
36	CLA	O	307	X	-	-	-
36	CLA	O	308	X	-	-	-
36	CLA	O	309	X	-	-	-
36	CLA	O	310	X	-	-	-
36	CLA	O	311	X	-	-	-
36	CLA	O	314	X	-	-	-
36	CLA	O	316	X	-	-	-
36	CLA	P	301	X	-	-	-
36	CLA	P	308	X	-	-	-
36	CLA	P	309	X	-	-	-
36	CLA	P	310	X	-	-	-
36	CLA	P	311	X	-	-	-
36	CLA	P	312	X	-	-	-
36	CLA	P	313	X	-	-	-
36	CLA	P	316	X	-	-	-
36	CLA	P	318	X	-	-	-
36	CLA	P	319	X	-	-	-
36	CLA	Q	305	X	-	-	-
36	CLA	Q	306	X	-	-	-
36	CLA	Q	307	X	-	-	-
36	CLA	Q	308	X	-	-	-
36	CLA	Q	309	X	-	-	-
36	CLA	Q	312	X	-	-	-
36	CLA	Q	314	X	-	-	-
36	CLA	R	310	X	-	-	-
36	CLA	R	311	X	-	-	-
36	CLA	R	312	X	-	-	-
36	CLA	R	313	X	-	-	-
36	CLA	R	314	X	-	-	-
36	CLA	R	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	R	316	X	-	-	-
36	CLA	R	318	X	-	-	-
36	CLA	R	319	X	-	-	-
36	CLA	R	320	X	-	-	-
36	CLA	R	322	X	-	-	-
36	CLA	S	309	X	-	-	-
36	CLA	S	310	X	-	-	-
36	CLA	S	311	X	-	-	-
36	CLA	S	313	X	-	-	-
36	CLA	S	315	X	-	-	-
36	CLA	S	317	X	-	-	-
36	CLA	S	318	X	-	-	-
36	CLA	S	319	X	-	-	-
36	CLA	T	308	X	-	-	-
36	CLA	T	309	X	-	-	-
36	CLA	T	311	X	-	-	-
36	CLA	T	312	X	-	-	-
36	CLA	T	313	X	-	-	-
36	CLA	T	314	X	-	-	-
36	CLA	T	316	X	-	-	-
36	CLA	U	305	X	-	-	-
36	CLA	U	306	X	-	-	-
36	CLA	U	307	X	-	-	-
36	CLA	U	308	X	-	-	-
36	CLA	U	310	X	-	-	-
36	CLA	U	311	X	-	-	-
36	CLA	U	313	X	-	-	-
36	CLA	V	305	X	-	-	-
36	CLA	V	306	X	-	-	-
36	CLA	V	307	X	-	-	-
36	CLA	V	308	X	-	-	-
36	CLA	V	309	X	-	-	-
36	CLA	V	310	X	-	-	-
36	CLA	V	311	X	-	-	-
36	CLA	V	313	X	-	-	-
36	CLA	V	314	X	-	-	-
36	CLA	W	201	X	-	-	-
36	CLA	W	206	X	-	-	-
36	CLA	W	207	X	-	-	-
36	CLA	W	208	X	-	-	-
36	CLA	W	209	X	-	-	-
36	CLA	W	210	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	W	211	X	-	-	-
36	CLA	W	215	X	-	-	-
36	CLA	W	216	X	-	-	-
36	CLA	W	218	X	-	-	-
36	CLA	X	306	X	-	-	-
36	CLA	X	308	X	-	-	-
36	CLA	X	310	X	-	-	-
36	CLA	X	312	X	-	-	-
36	CLA	a	801	X	-	-	-
36	CLA	a	802	X	-	-	-
36	CLA	a	803	X	-	-	-
36	CLA	a	804	X	-	-	-
36	CLA	a	805	X	-	-	-
36	CLA	a	806	X	-	-	-
36	CLA	a	807	X	-	-	-
36	CLA	a	808	X	-	-	-
36	CLA	a	809	X	-	-	-
36	CLA	a	810	X	-	-	-
36	CLA	a	811	X	-	-	-
36	CLA	a	812	X	-	-	-
36	CLA	a	813	X	-	-	-
36	CLA	a	814	X	-	-	-
36	CLA	a	815	X	-	-	-
36	CLA	a	816	X	-	-	-
36	CLA	a	817	X	-	-	-
36	CLA	a	818	X	-	-	-
36	CLA	a	819	X	-	-	-
36	CLA	a	820	X	-	-	-
36	CLA	a	821	X	-	-	-
36	CLA	a	822	X	-	-	-
36	CLA	a	823	X	-	-	-
36	CLA	a	824	X	-	-	-
36	CLA	a	825	X	-	-	-
36	CLA	a	826	X	-	-	-
36	CLA	a	827	X	-	-	-
36	CLA	a	828	X	-	-	-
36	CLA	a	829	X	-	-	-
36	CLA	a	831	X	-	-	-
36	CLA	a	832	X	-	-	-
36	CLA	a	833	X	-	-	-
36	CLA	a	834	X	-	-	-
36	CLA	a	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	a	836	X	-	-	-
36	CLA	a	837	X	-	-	-
36	CLA	a	838	X	-	-	-
36	CLA	a	839	X	-	-	-
36	CLA	a	841	X	-	-	-
36	CLA	a	848	X	-	-	-
36	CLA	b	801	X	-	-	-
36	CLA	b	802	X	-	-	-
36	CLA	b	805	X	-	-	-
36	CLA	b	806	X	-	-	-
36	CLA	b	807	X	-	-	-
36	CLA	b	808	X	-	-	-
36	CLA	b	809	X	-	-	-
36	CLA	b	810	X	-	-	-
36	CLA	b	811	X	-	-	-
36	CLA	b	812	X	-	-	-
36	CLA	b	813	X	-	-	-
36	CLA	b	814	X	-	-	-
36	CLA	b	815	X	-	-	-
36	CLA	b	816	X	-	-	-
36	CLA	b	817	X	-	-	-
36	CLA	b	819	X	-	-	-
36	CLA	b	820	X	-	-	-
36	CLA	b	821	X	-	-	-
36	CLA	b	822	X	-	-	-
36	CLA	b	823	X	-	-	-
36	CLA	b	824	X	-	-	-
36	CLA	b	825	X	-	-	-
36	CLA	b	826	X	-	-	-
36	CLA	b	827	X	-	-	-
36	CLA	b	828	X	-	-	-
36	CLA	b	829	X	-	-	-
36	CLA	b	830	X	-	-	-
36	CLA	b	831	X	-	-	-
36	CLA	b	832	X	-	-	-
36	CLA	b	833	X	-	-	-
36	CLA	b	834	X	-	-	-
36	CLA	b	835	X	-	-	-
36	CLA	b	836	X	-	-	-
36	CLA	b	837	X	-	-	-
36	CLA	b	838	X	-	-	-
36	CLA	b	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	b	840	X	-	-	-
36	CLA	b	841	X	-	-	-
36	CLA	f	802	X	-	-	-
36	CLA	f	803	X	-	-	-
36	CLA	f	804	X	-	-	-
36	CLA	f	805	X	-	-	-
36	CLA	h	203	X	-	-	-
36	CLA	i	102	X	-	-	-
36	CLA	j	101	X	-	-	-
36	CLA	j	102	X	-	-	-
36	CLA	j	106	X	-	-	-
36	CLA	l	201	X	-	-	-
36	CLA	l	202	X	-	-	-
36	CLA	l	205	X	-	-	-
36	CLA	l	206	X	-	-	-

## 2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 81344 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 FCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	168	Total	C	N	O	S	0	0
			1287	825	213	237	12		

- Molecule 2 is a protein called FCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1013	662	166	176	9		

- Molecule 3 is a protein called FCPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	163	Total	C	N	O	S	0	0
			1247	796	210	232	9		

- Molecule 4 is a protein called FCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	172	Total	C	N	O	S	0	0
			1337	870	214	245	8		

- Molecule 5 is a protein called FCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	188	Total	C	N	O	S	0	0
			1411	891	240	265	15		

- Molecule 6 is a protein called FCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	180	Total	C	N	O	S	0	0
			1375	880	230	253	12		

- Molecule 7 is a protein called FCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	214	Total	C	N	O	S	0	0
			1668	1079	276	305	8		

- Molecule 8 is a protein called FCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	170	Total	C	N	O	S	0	0
			1291	832	213	236	10		

- Molecule 9 is a protein called FCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	161	Total	C	N	O	S	0	0
			1250	807	208	228	7		

- Molecule 10 is a protein called FCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1301	843	217	236	5		

- Molecule 11 is a protein called FCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	169	Total	C	N	O	S	0	0
			1304	850	214	232	8		

- Molecule 12 is a protein called FCPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	196	Total	C	N	O	S	0	0
			1523	989	250	276	8		

- Molecule 13 is a protein called FCPI-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	187	Total	C	N	O	S	0	0
			1423	914	248	255	6		

- Molecule 14 is a protein called FCPI-21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	219	Total	C	N	O	S	0	0
			1716	1119	282	309	6		

- Molecule 15 is a protein called FCPI.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	173	Total	C	N	O	S	0	0
			1302	837	216	241	8		
15	P	173	Total	C	N	O	S	0	0
			1296	834	213	241	8		
15	Q	173	Total	C	N	O	S	0	0
			1302	837	216	241	8		

- Molecule 16 is a protein called FCPI-24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	211	Total	C	N	O	S	0	0
			1628	1061	266	294	7		

- Molecule 17 is a protein called FCPI-23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	220	Total	C	N	O	S	0	0
			1722	1122	283	311	6		

- Molecule 18 is a protein called FCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	172	Total	C	N	O	S	0	0
			1326	848	226	247	5		

- Molecule 19 is a protein called FCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	160	Total	C	N	O	S	0	0
			1239	799	203	233	4		
19	X	161	Total	C	N	O	S	1	0
			1253	808	207	234	4		

- Molecule 20 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	742	Total	C	N	O	S	0	0
			5858	3826	991	1013	28		

- Molecule 21 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	732	Total	C	N	O	S	1	0
			5820	3828	980	994	18		

- Molecule 22 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	80	Total	C	N	O	S	0	0
			597	368	104	114	11		

- Molecule 23 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	132	Total	C	N	O	S	1	0
			1056	681	186	186	3		

- Molecule 24 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	63	Total	C	N	O	0	0
			507	321	90	96		

- Molecule 25 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	162	Total	C	N	O	S	0	0
			1223	789	211	220	3		

- Molecule 26 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	i	33	Total	C	N	O	S	0	0
			256	176	40	38	2		

- Molecule 27 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	41	Total	C	N	O	S	0	0
			324	219	50	54	1		

- Molecule 28 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	l	144	Total	C	N	O	S	0	0
			1094	726	178	187	3		

- Molecule 29 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	m	28	Total	C	N	O	S	0	0
			198	130	32	34	2		

- Molecule 30 is a protein called PsaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	134	Total	C	N	O	S	0	0
			670	402	134	134			

- Molecule 31 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	89	Total	C	N	O	S	0	0
			676	440	110	120	6		

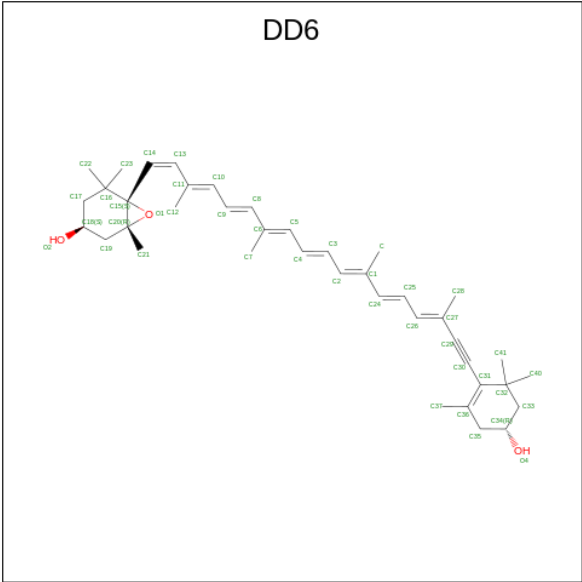
- Molecule 32 is a protein called FCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	156	Total	C	N	O	S	0	0
			1194	766	199	221	8		

- Molecule 33 is a protein called FCPI-19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	179	Total	C	N	O	S	0	0
			1361	871	234	252	4		

- Molecule 34 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>).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	B	1	Total	C	O	0
			43	40	3	
34	B	1	Total	C	O	0
			43	40	3	
34	C	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	

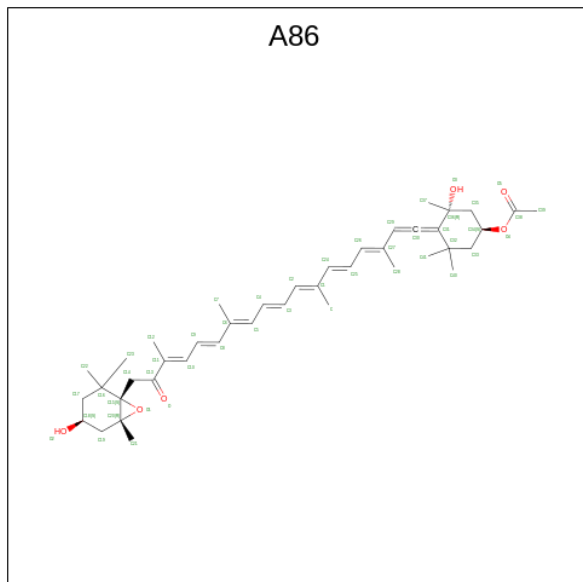
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Mol	Chain	Residues	Atoms			AltConf
34	F	1	Total 43	C 40	O 3	0
34	G	1	Total 43	C 40	O 3	0
34	H	1	Total 43	C 40	O 3	0
34	H	1	Total 43	C 40	O 3	0
34	I	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	K	1	Total 43	C 40	O 3	0
34	K	1	Total 43	C 40	O 3	0
34	L	1	Total 43	C 40	O 3	0
34	M	1	Total 43	C 40	O 3	0
34	O	1	Total 43	C 40	O 3	0
34	P	1	Total 43	C 40	O 3	0
34	Q	1	Total 43	C 40	O 3	0
34	R	1	Total 43	C 40	O 3	0
34	R	1	Total 43	C 40	O 3	0
34	S	1	Total 43	C 40	O 3	0
34	S	1	Total 43	C 40	O 3	0
34	W	1	Total 43	C 40	O 3	0
34	W	1	Total 43	C 40	O 3	0
34	a	1	Total 43	C 40	O 3	0
34	j	1	Total 43	C 40	O 3	0



- Molecule 35 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:  $C_{42}H_{58}O_6$ ).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			48	42	6	
35	A	1	Total	C	O	0
			48	42	6	
35	B	1	Total	C	O	0
			48	42	6	
35	B	1	Total	C	O	0
			48	42	6	
35	C	1	Total	C	O	0
			48	42	6	
35	C	1	Total	C	O	0
			48	42	6	
35	C	1	Total	C	O	0
			48	42	6	
35	D	1	Total	C	O	0
			48	42	6	
35	E	1	Total	C	O	0
			48	42	6	
35	E	1	Total	C	O	0
			48	42	6	
35	E	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	H	1	Total	C	O	0
			48	42	6	
35	H	1	Total	C	O	0
			48	42	6	
35	I	1	Total	C	O	0
			48	42	6	
35	I	1	Total	C	O	0
			48	42	6	
35	I	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	K	1	Total	C	O	0
			48	42	6	
35	K	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	K	1	Total	C	O	0
			48	42	6	
35	K	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	L	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	M	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	N	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	

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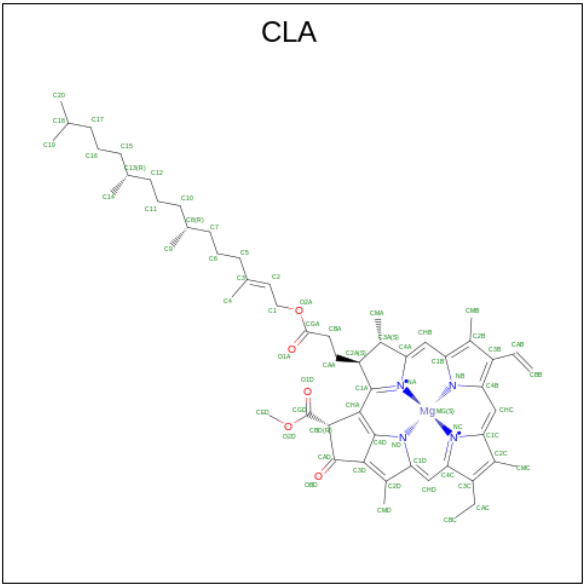
Mol	Chain	Residues	Atoms			AltConf
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	T	1	Total	C	O	0
			48	42	6	
35	W	1	Total	C	O	0
			48	42	6	
35	W	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	X	1	Total	C	O	0
			48	42	6	
35	h	1	Total	C	O	0
			48	42	6	
35	h	1	Total	C	O	0
			48	42	6	
35	U	1	Total	C	O	0
			48	42	6	
35	U	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	U	1	Total	C	O	0
			48	42	6	
35	U	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	

- Molecule 36 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	C	1	Total 43	C 35	Mg 1	N 4	O 3	0
36	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	D	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	D	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	D	1	Total 58	C 48	Mg 1	N 4	O 5	0
36	E	1	Total 49	C 39	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	F	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	F	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	F	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	F	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
36	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
36	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	H	1	Total 48	C 38	Mg 1	N 4	O 5	0
36	H	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	H	1	Total 64	C 54	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	I	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	I	1	Total 54	C 44	Mg 1	N 4	O 5	0
36	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	I	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	I	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	I	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	I	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	J	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	J	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	J	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	K	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	K	1	Total 59	C 49	Mg 1	N 4	O 5	0
36	K	1	Total 62	C 52	Mg 1	N 4	O 5	0
36	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	L	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	L	1	Total 54	C 44	Mg 1	N 4	O 5	0
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	M	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	M	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	M	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	M	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	M	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	M	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	N	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	N	1	Total 51	C 41	Mg 1	N 4	O 5	0
36	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	N	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	N	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
36	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
36	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	N	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	O	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	O	1	Total 58	C 48	Mg 1	N 4	O 5	0
36	O	1	Total 40	C 32	Mg 1	N 4	O 3	0
36	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	P	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	P	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	P	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	P	1	Total 51	C 41	Mg 1	N 4	O 5	0
36	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	Q	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	R	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 45	C 37	Mg 1	N 4	O 3	0
36	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	S	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	T	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	T	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	T	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	W	1	Total 48	C 38	Mg 1	N 4	O 5	0
36	W	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	W	1	Total 57	C 47	Mg 1	N 4	O 5	0
36	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	W	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	W	1	Total 48	C 38	Mg 1	N 4	O 5	0
36	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	W	1	Total 43	C 35	Mg 1	N 4	O 3	0
36	X	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
36	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	X	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	X	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	X	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	X	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
36	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
36	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
36	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
36	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	b	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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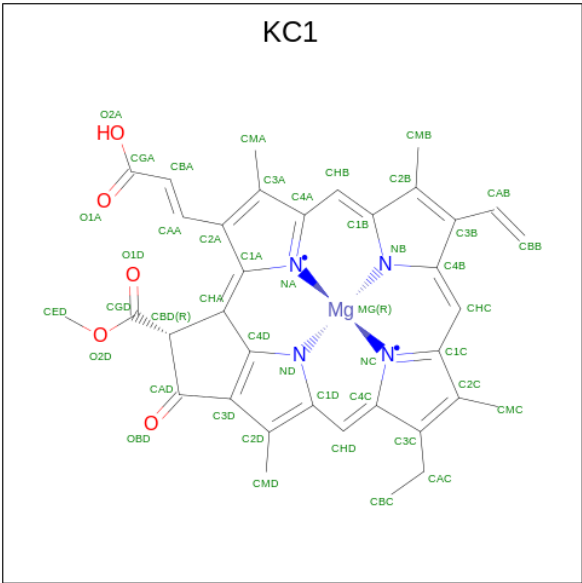
Mol	Chain	Residues	Atoms					AltConf
36	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	j	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	l	1	Total 49	C 39	Mg 1	N 4	O 5	0
36	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	l	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	U	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	V	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	V	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 37 is Chlorophyll c1 (CCD ID: KC1) (formula: C<sub>35</sub>H<sub>30</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
37	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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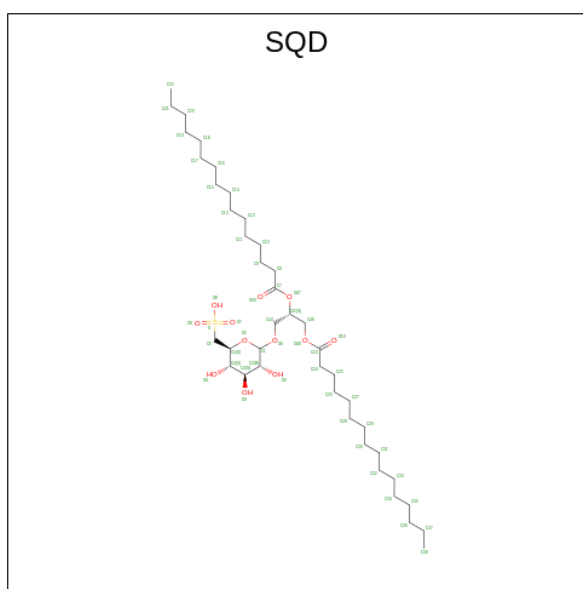
Mol	Chain	Residues	Atoms					AltConf
37	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	R	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
37	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

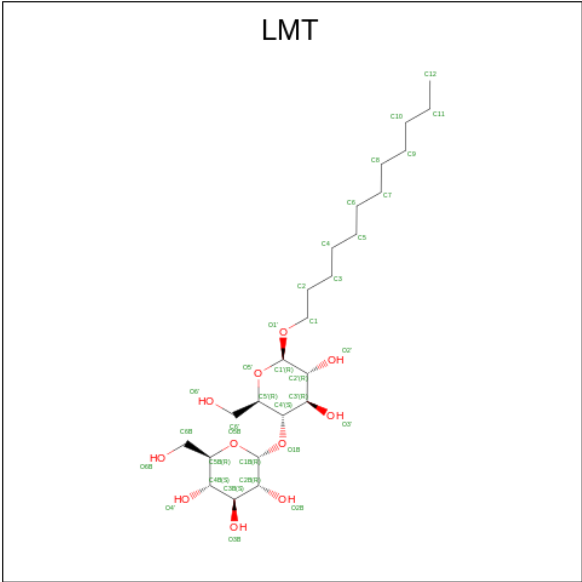
- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	O	S	0
			28	15	12	1	
38	b	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 39 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).





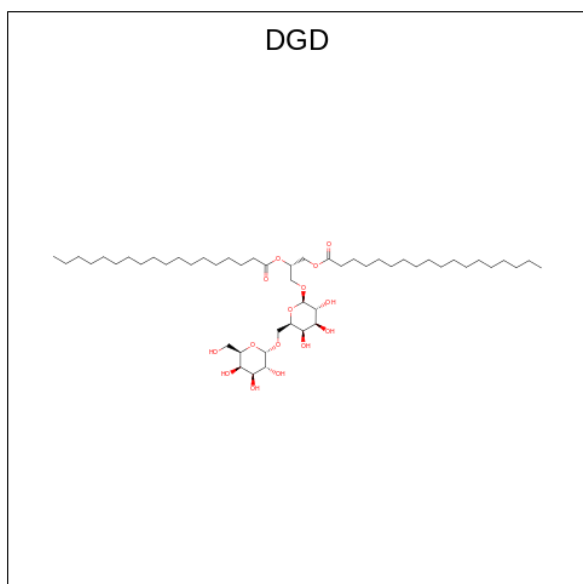
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			35	24	11	
39	B	1	Total	C	O	0
			35	24	11	
39	E	1	Total	C	O	0
			35	24	11	
39	E	1	Total	C	O	0
			23	17	6	
39	E	1	Total	C	O	0
			35	24	11	
39	F	1	Total	C	O	0
			35	24	11	
39	F	1	Total	C	O	0
			33	22	11	
39	G	1	Total	C	O	0
			35	24	11	
39	G	1	Total	C	O	0
			35	24	11	
39	I	1	Total	C	O	0
			35	24	11	
39	I	1	Total	C	O	0
			35	24	11	
39	K	1	Total	C	O	0
			31	20	11	
39	K	1	Total	C	O	0
			35	24	11	
39	L	1	Total	C	O	0
			35	24	11	

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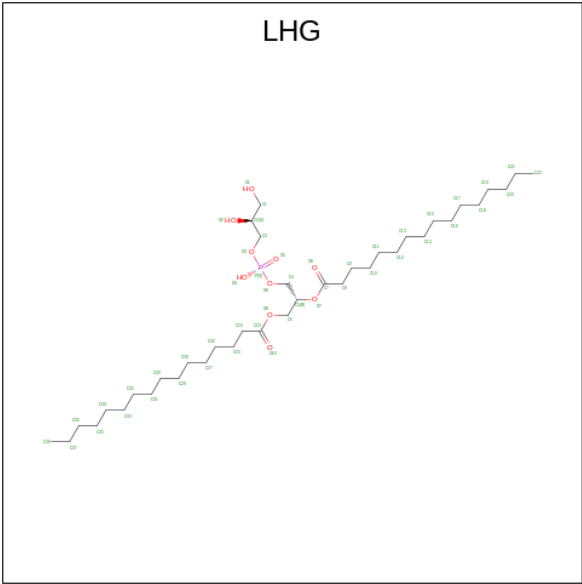
Mol	Chain	Residues	Atoms			AltConf
39	L	1	Total	C	O	0
			31	20	11	
39	P	1	Total	C	O	0
			23	17	6	
39	P	1	Total	C	O	0
			23	17	6	
39	a	1	Total	C	O	0
			35	24	11	
39	a	1	Total	C	O	0
			32	21	11	
39	a	1	Total	C	O	0
			35	24	11	
39	b	1	Total	C	O	0
			35	24	11	
39	b	1	Total	C	O	0
			24	19	5	
39	f	1	Total	C	O	0
			24	18	6	
39	h	1	Total	C	O	0
			35	24	11	
39	U	1	Total	C	O	0
			35	24	11	
39	U	1	Total	C	O	0
			35	24	11	

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
40	C	1	Total	C	O	0
			57	42	15	
40	L	1	Total	C	O	0
			47	32	15	
40	b	1	Total	C	O	0
			60	45	15	

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



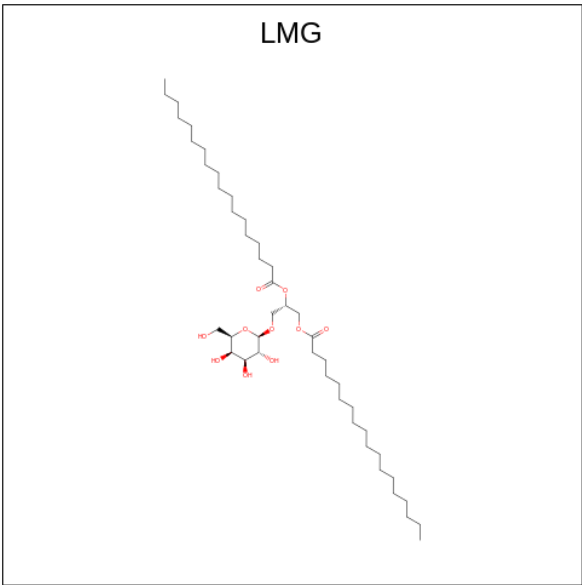
Mol	Chain	Residues	Atoms				AltConf
41	D	1	Total	C	O	P	0
			46	35	10	1	
41	D	1	Total	C	O	P	0
			49	38	10	1	
41	E	1	Total	C	O	P	0
			49	38	10	1	
41	F	1	Total	C	O	P	0
			33	24	8	1	
41	F	1	Total	C	O	P	0
			41	30	10	1	
41	G	1	Total	C	O	P	0
			49	38	10	1	
41	G	1	Total	C	O	P	0
			40	29	10	1	
41	G	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
41	I	1	Total	C	O	P	0
			49	38	10	1	
41	O	1	Total	C	O	P	0
			42	31	10	1	
41	O	1	Total	C	O	P	0
			49	38	10	1	
41	Q	1	Total	C	O	P	0
			49	38	10	1	
41	R	1	Total	C	O	P	0
			49	38	10	1	
41	a	1	Total	C	O	P	0
			48	37	10	1	
41	a	1	Total	C	O	P	0
			27	16	10	1	
41	a	1	Total	C	O	P	0
			47	36	10	1	
41	b	1	Total	C	O	P	0
			49	38	10	1	
41	f	1	Total	C	O	P	0
			49	38	10	1	
41	f	1	Total	C	O	P	0
			42	31	10	1	
41	i	1	Total	C	O	P	0
			46	35	10	1	
41	j	1	Total	C	O	P	0
			49	38	10	1	
41	l	1	Total	C	O	P	0
			48	37	10	1	

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



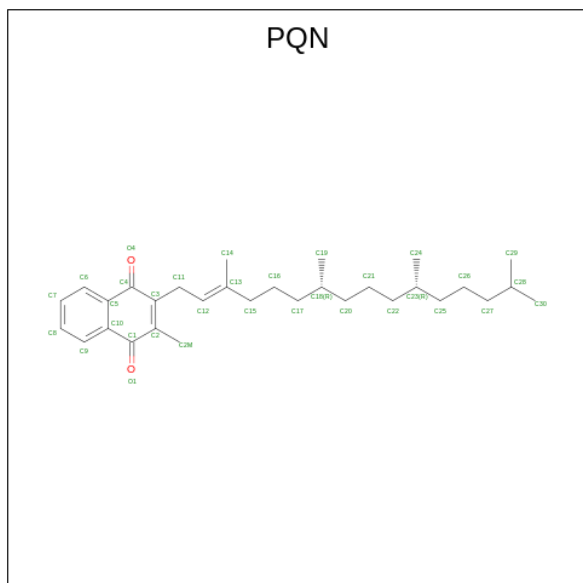
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			46	36	10	
42	D	1	Total	C	O	0
			37	27	10	
42	E	1	Total	C	O	0
			46	36	10	
42	E	1	Total	C	O	0
			40	30	10	
42	G	1	Total	C	O	0
			55	45	10	
42	G	1	Total	C	O	0
			55	45	10	
42	I	1	Total	C	O	0
			55	45	10	
42	J	1	Total	C	O	0
			55	45	10	
42	J	1	Total	C	O	0
			44	34	10	
42	L	1	Total	C	O	0
			33	23	10	
42	a	1	Total	C	O	0
			54	44	10	
42	j	1	Total	C	O	0
			52	42	10	
42	m	1	Total	C	O	0
			37	27	10	
42	h	1	Total	C	O	0
			45	35	10	

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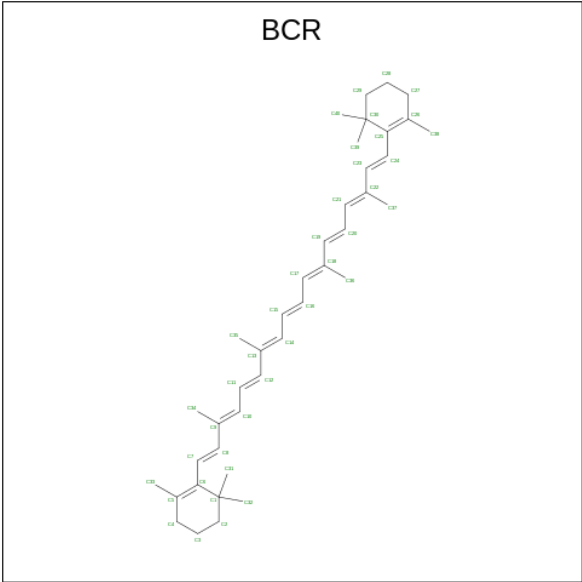
Mol	Chain	Residues	Atoms			AltConf
42	V	1	Total	C	O	0
			46	36	10	
42	V	1	Total	C	O	0
			46	36	10	

- Molecule 43 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 44 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



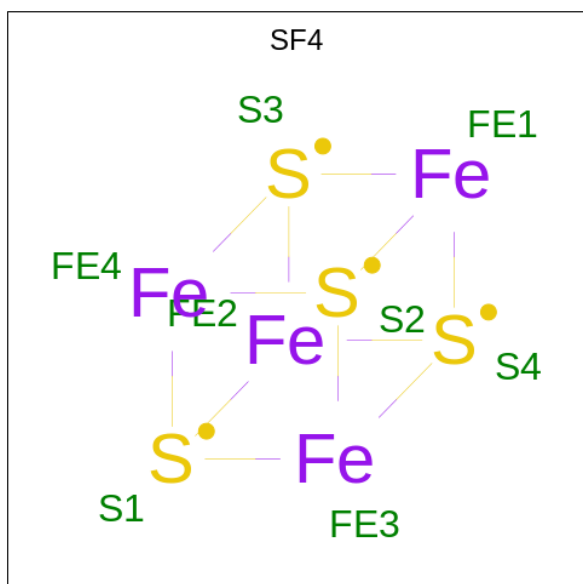
Mol	Chain	Residues	Atoms	AltConf
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	f	1	Total C 40 40	0
44	f	1	Total C 40 40	0
44	i	1	Total C 40 40	0
44	i	1	Total C 40 40	0
44	j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
44	l	1	Total C 40 40	0
44	l	1	Total C 40 40	0
44	m	1	Total C 40 40	0
44	h	1	Total C 40 40	0

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 46 is water.

Mol	Chain	Residues	Atoms	AltConf
46	a	64	Total O 64 64	0
46	b	72	Total O 72 72	0


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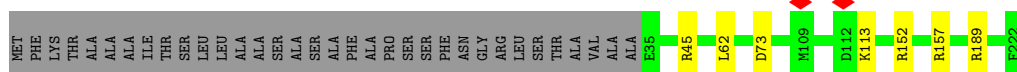


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Mol	Chain	Residues	Atoms		AltConf
46	c	7	Total 7	O 7	0
46	d	4	Total 4	O 4	0
46	f	2	Total 2	O 2	0
46	j	1	Total 1	O 1	0
46	l	3	Total 3	O 3	0

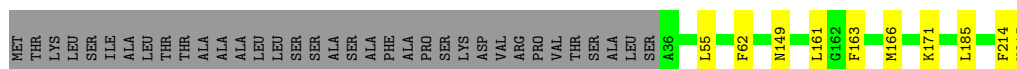


Chain E:  82% 15%




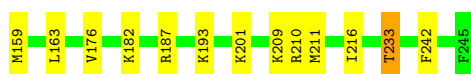
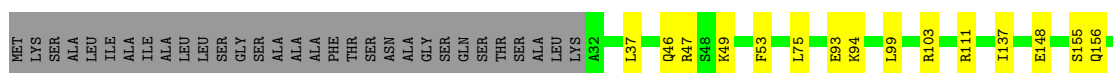
• Molecule 6: FCPI-8

Chain F:  79% 5% 16%




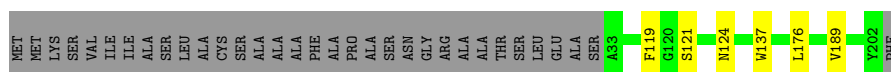
• Molecule 7: FCPI-4

Chain G:  76% 11% 13%



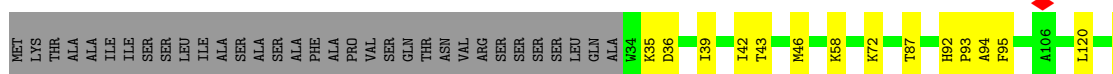
• Molecule 8: FCPI-10

Chain H:  81% 16%




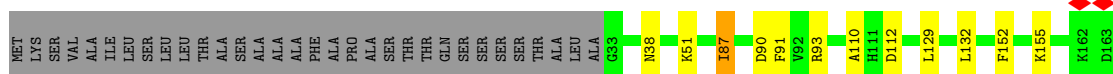
• Molecule 9: FCPI-3

Chain I:  70% 13% 17%

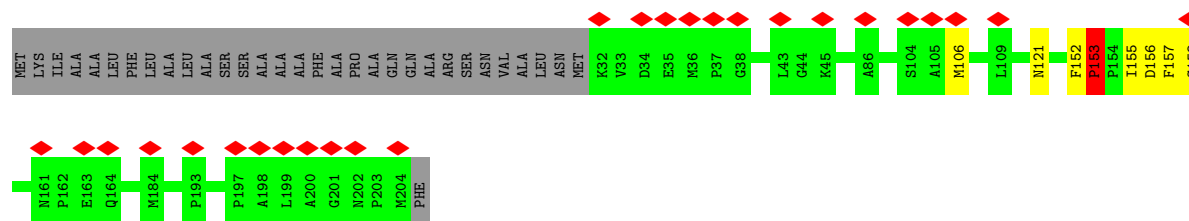
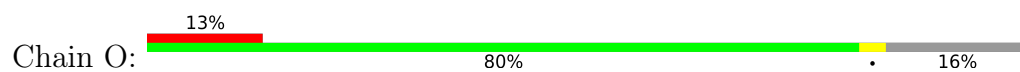


• Molecule 10: FCPI-9

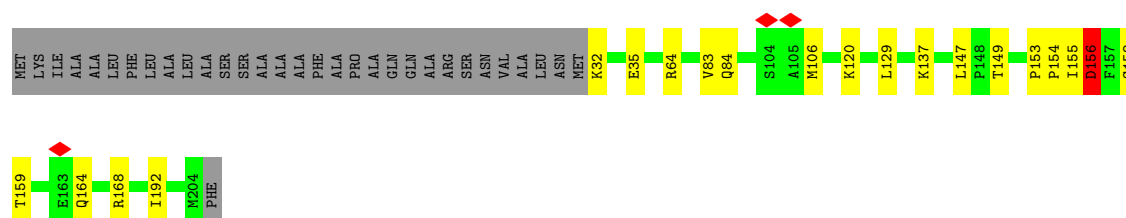
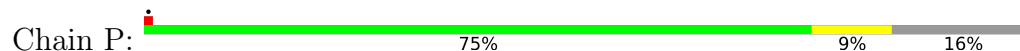
Chain J:  77% 6% 16%



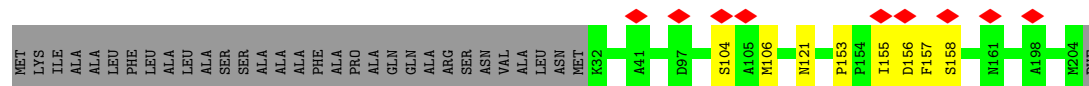
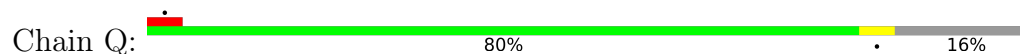




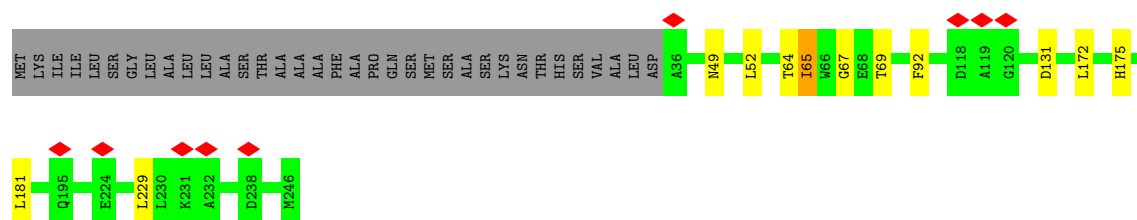
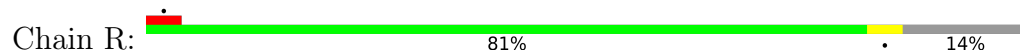
• Molecule 15: FCPI



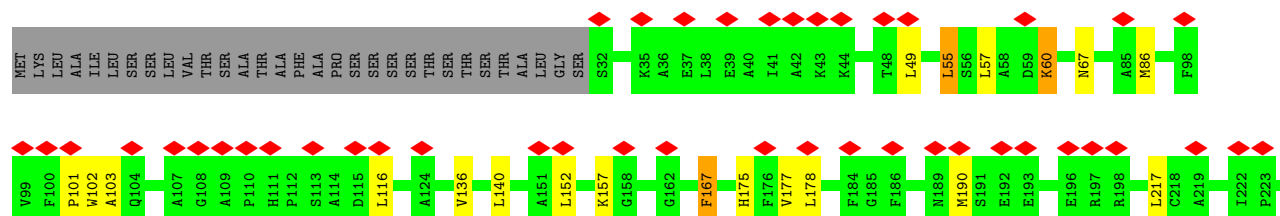
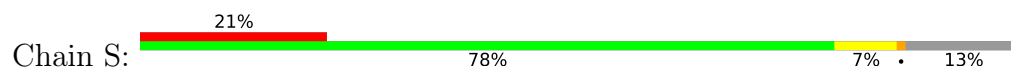
• Molecule 15: FCPI

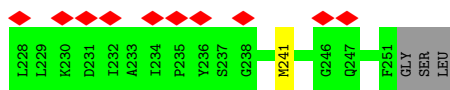


• Molecule 16: FCPI-24

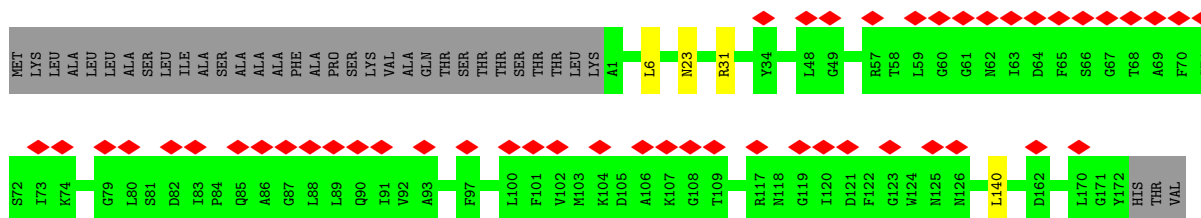
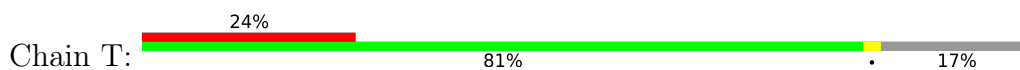


• Molecule 17: FCPI-23

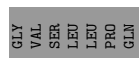
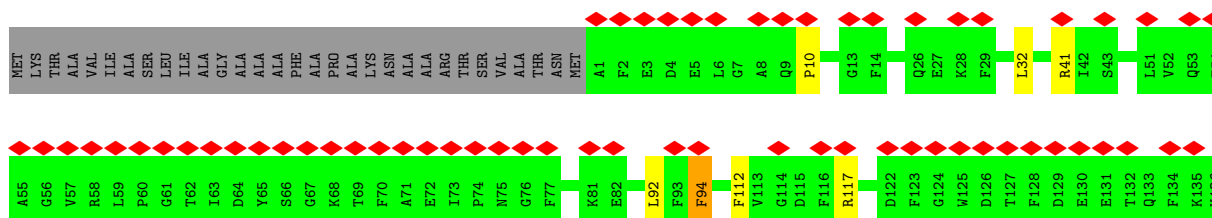
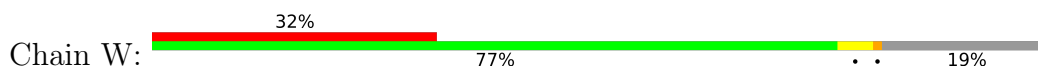




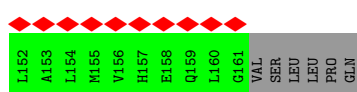
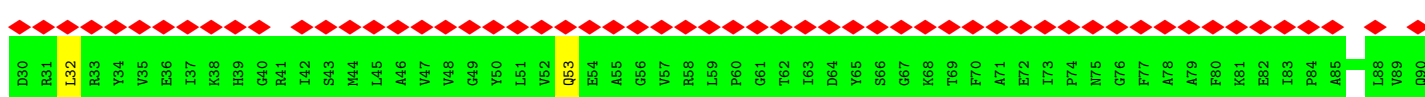
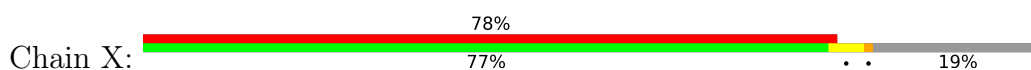
• Molecule 18: FCPI-12



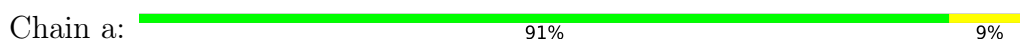
• Molecule 19: FCPI-17



• Molecule 19: FCPI-17



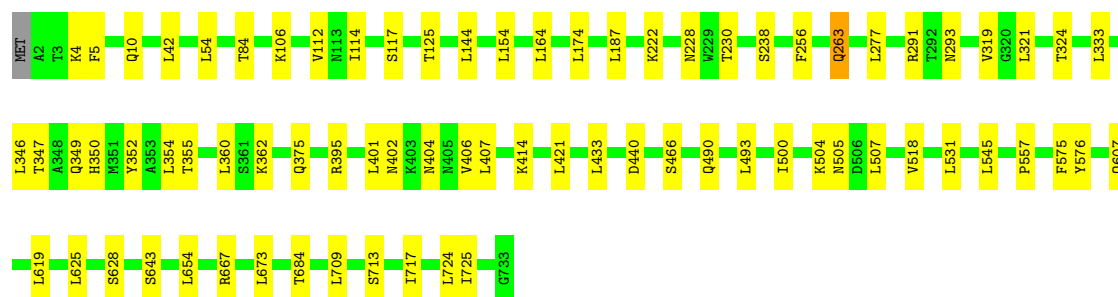
• Molecule 20: PsaA





• Molecule 21: PsaB

Chain b: 89% 10%



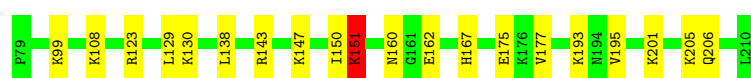
• Molecule 22: PsaC

Chain c: 90% 10%



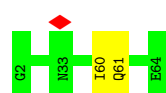
• Molecule 23: PsaD

Chain d: 85% 14%



• Molecule 24: PsaE

Chain e: 97%



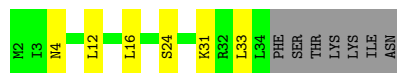
• Molecule 25: PsaF

Chain f: 91% 9%




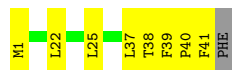
- Molecule 26: PsaI

Chain i:  68% 15% 18%



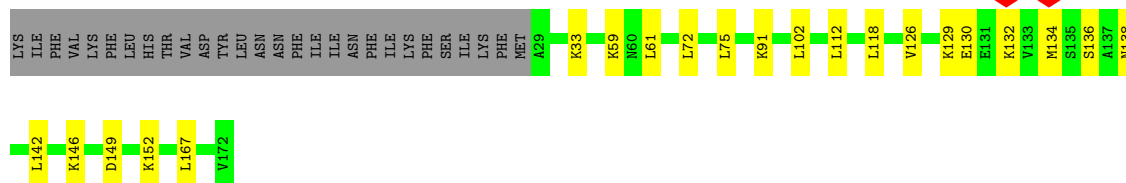
- Molecule 27: PsaJ

Chain j:  79% 19% .




- Molecule 28: PsaL

Chain l:  72% 12% 16%



- Molecule 29: PsaM

Chain m:  83% 14% .



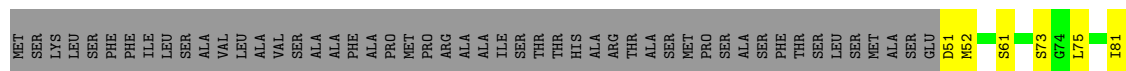
- Molecule 30: PsaS

Chain g:  99% .



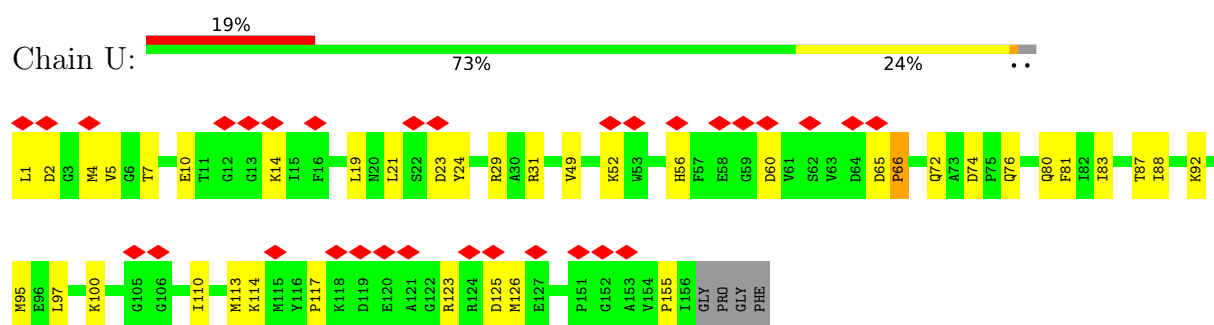
- Molecule 31: PsaR

Chain h:  53% 11% 36%

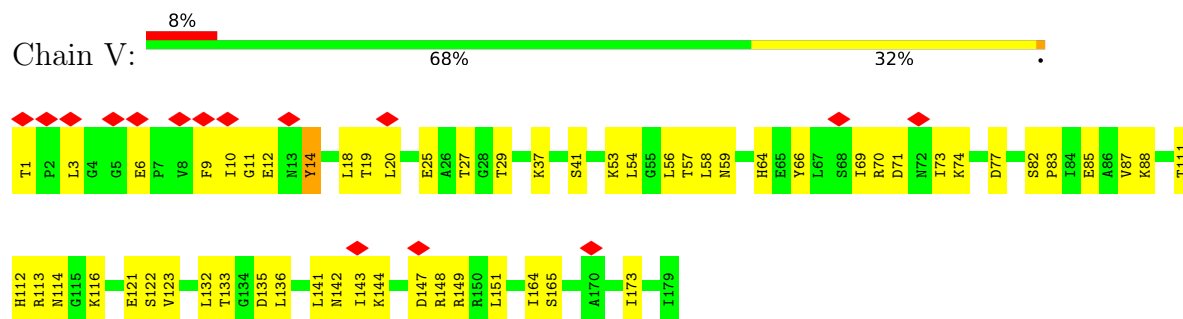


- Molecule 32: FCPI-2





• Molecule 33: FCPI-19



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	164480	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	567.32, 567.32, 567.32	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, SF4, PQN, LMT, BCR, A86, KC1, CLA, DGD, LMG, LHG, DD6

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	0.47	0/1319	0.67	1/1786 (0.1%)
2	B	0.51	2/1039 (0.2%)	0.98	7/1412 (0.5%)
3	C	0.37	0/1275	0.63	1/1726 (0.1%)
4	D	0.54	3/1373 (0.2%)	0.70	1/1860 (0.1%)
5	E	0.49	0/1439	0.70	2/1944 (0.1%)
6	F	0.47	0/1411	0.68	2/1908 (0.1%)
7	G	0.43	1/1714 (0.1%)	0.59	0/2321
8	H	0.55	1/1326 (0.1%)	0.79	3/1798 (0.2%)
9	I	0.40	0/1285	0.67	5/1746 (0.3%)
10	J	0.46	0/1339	0.73	3/1811 (0.2%)
11	K	0.51	0/1346	0.72	1/1826 (0.1%)
12	L	0.53	1/1571 (0.1%)	0.73	3/2141 (0.1%)
13	M	0.46	1/1464 (0.1%)	0.72	1/1982 (0.1%)
14	N	0.53	0/1770	0.90	6/2405 (0.2%)
15	O	0.55	3/1335 (0.2%)	0.81	4/1817 (0.2%)
15	P	0.40	1/1329 (0.1%)	0.93	4/1810 (0.2%)
15	Q	0.56	3/1335 (0.2%)	0.80	2/1817 (0.1%)
16	R	0.40	0/1680	0.71	5/2282 (0.2%)
17	S	0.44	0/1776	0.84	8/2413 (0.3%)
18	T	0.40	0/1353	0.64	2/1823 (0.1%)
19	W	0.55	1/1265 (0.1%)	0.88	8/1707 (0.5%)
19	X	0.59	3/1282 (0.2%)	0.98	11/1729 (0.6%)
20	a	0.44	3/6053 (0.0%)	0.59	5/8238 (0.1%)
21	b	0.39	0/6031	0.57	8/8231 (0.1%)
22	c	0.46	0/607	0.61	0/822
23	d	1.90	2/1086 (0.2%)	1.23	8/1461 (0.5%)
24	e	0.57	0/517	0.56	0/701
25	f	0.47	1/1248 (0.1%)	0.58	2/1687 (0.1%)
26	i	0.49	0/262	0.75	0/356
27	j	0.46	0/333	0.79	2/455 (0.4%)
28	l	0.47	1/1121 (0.1%)	0.69	6/1520 (0.4%)
29	m	0.44	0/198	0.58	1/269 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	h	0.33	0/698	0.54	0/951
32	U	0.42	0/1225	0.83	4/1657 (0.2%)
33	V	0.26	0/1393	0.48	0/1894
All	All	0.53	27/51798 (0.1%)	0.72	116/70306 (0.2%)

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
10	J	0	1
12	L	0	2
14	N	0	7
15	O	0	1
15	P	0	1
15	Q	0	1
17	S	0	2
19	W	0	3
23	d	0	5
30	g	0	1
33	V	0	1
All	All	0	25

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	151[A]	LYS	CA-C	43.55	2.66	1.52
23	d	151[B]	LYS	CA-C	43.55	2.66	1.52
19	X	94	PHE	CE2-CZ	9.29	1.55	1.37
2	B	186	MET	C-N	8.97	1.54	1.34
4	D	73	GLU	CB-CG	-7.17	1.38	1.52
15	O	157	PHE	CB-CG	-6.58	1.40	1.51
15	Q	157	PHE	CB-CG	-6.55	1.40	1.51
15	Q	157	PHE	CD1-CE1	-6.37	1.26	1.39
15	O	157	PHE	CD1-CE1	-6.35	1.26	1.39
19	X	94	PHE	CD2-CE2	6.29	1.51	1.39
15	P	156	ASP	C-N	6.16	1.48	1.34
19	W	41	ARG	CG-CD	-6.10	1.36	1.51
28	l	126	VAL	CB-CG2	-5.96	1.40	1.52
12	L	44	GLU	CD-OE2	-5.94	1.19	1.25
20	a	623	VAL	CB-CG2	-5.71	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	158	SER	CB-OG	5.61	1.49	1.42
15	Q	158	SER	CB-OG	5.58	1.49	1.42
2	B	183	GLU	C-N	-5.54	1.21	1.34
19	X	94	PHE	CD1-CE1	-5.53	1.28	1.39
8	H	189	VAL	CB-CG1	-5.51	1.41	1.52
4	D	193	VAL	CB-CG1	-5.37	1.41	1.52
13	M	91	GLU	CB-CG	-5.32	1.42	1.52
25	f	187	GLU	CG-CD	-5.23	1.44	1.51
7	G	53	PHE	C-N	-5.14	1.22	1.34
4	D	193	VAL	CB-CG2	-5.03	1.42	1.52
20	a	580	CYS	CB-SG	-5.03	1.73	1.81
20	a	127	VAL	CB-CG1	-5.02	1.42	1.52

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	151[A]	LYS	CB-CA-C	-22.80	64.81	110.40
23	d	151[B]	LYS	CB-CA-C	-22.80	64.81	110.40
15	P	156	ASP	O-C-N	-20.21	90.36	122.70
32	U	65	ASP	C-N-CD	-19.93	76.74	120.60
23	d	151[A]	LYS	CA-C-N	-15.35	83.44	117.20
23	d	151[B]	LYS	CA-C-N	-15.35	83.44	117.20
2	B	183	GLU	O-C-N	13.97	145.06	122.70
32	U	65	ASP	C-N-CA	13.79	179.93	122.00
15	P	156	ASP	CA-C-N	13.59	147.09	117.20
15	P	156	ASP	C-N-CA	12.25	152.33	121.70
19	X	94	PHE	CB-CG-CD2	11.52	128.87	120.80
19	X	94	PHE	CD1-CE1-CZ	10.66	132.89	120.10
2	B	183	GLU	CA-C-N	-10.28	94.58	117.20
19	W	141	LEU	CB-CG-CD2	-8.75	96.12	111.00
19	X	53	GLN	CA-CB-CG	-8.65	94.36	113.40
2	B	151	LEU	CA-CB-CG	8.57	135.00	115.30
19	X	94	PHE	CB-CG-CD1	-8.53	114.83	120.80
27	j	25	LEU	CA-CB-CG	8.44	134.72	115.30
8	H	137	TRP	CA-CB-CG	8.32	129.50	113.70
23	d	151[A]	LYS	N-CA-C	8.26	133.30	111.00
23	d	151[B]	LYS	N-CA-C	8.26	133.30	111.00
23	d	151[A]	LYS	CA-C-O	8.21	137.33	120.10
23	d	151[B]	LYS	CA-C-O	8.21	137.33	120.10
2	B	183	GLU	C-N-CA	-8.12	101.39	121.70
9	I	93	PRO	N-CA-C	7.99	132.87	112.10
5	E	62	LEU	CA-CB-CG	7.95	133.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	186	MET	O-C-N	-7.81	110.20	122.70
19	X	53	GLN	CB-CG-CD	7.75	131.75	111.60
15	O	157	PHE	CB-CG-CD1	-7.69	115.42	120.80
20	a	127	VAL	CG1-CB-CG2	-7.67	98.63	110.90
8	H	176	LEU	CA-CB-CG	7.66	132.91	115.30
15	Q	157	PHE	CB-CG-CD1	-7.63	115.46	120.80
18	T	6	LEU	CA-CB-CG	7.56	132.69	115.30
8	H	176	LEU	CB-CG-CD1	-7.37	98.48	111.00
17	S	217	LEU	CA-CB-CG	7.26	132.00	115.30
17	S	116	LEU	CA-CB-CG	7.20	131.86	115.30
20	a	589	CYS	CA-CB-SG	6.98	126.56	114.00
16	R	52	LEU	CA-CB-CG	6.87	131.10	115.30
11	K	161	LEU	CA-CB-CG	6.84	131.04	115.30
14	N	229	LEU	CA-CB-CG	6.78	130.90	115.30
2	B	137	LEU	CA-CB-CG	6.78	130.90	115.30
10	J	186	ILE	CG1-CB-CG2	-6.67	96.72	111.40
2	B	197	ILE	CA-CB-CG1	-6.66	98.35	111.00
12	L	117	LEU	CA-CB-CG	6.61	130.50	115.30
15	O	153	PRO	CA-N-CD	-6.59	102.28	111.50
28	l	61	LEU	CB-CG-CD1	-6.54	99.88	111.00
19	W	32	LEU	CA-CB-CG	6.40	130.01	115.30
12	L	198	LEU	CA-CB-CG	6.37	129.94	115.30
19	X	94	PHE	CE1-CZ-CE2	-6.24	108.77	120.00
3	C	197	LEU	CA-CB-CG	6.20	129.56	115.30
16	R	181	LEU	CA-CB-CG	6.20	129.56	115.30
19	X	53	GLN	CG-CD-OE1	6.17	133.94	121.60
27	j	22	LEU	CB-CG-CD2	-6.15	100.55	111.00
15	Q	158	SER	CB-CA-C	6.14	121.77	110.10
15	O	158	SER	CB-CA-C	6.13	121.75	110.10
25	f	185	ARG	NE-CZ-NH2	-6.06	117.27	120.30
16	R	172	LEU	CA-CB-CG	6.01	129.13	115.30
28	l	118	LEU	CA-CB-CG	6.00	129.11	115.30
21	b	277	LEU	CA-CB-CG	6.00	129.11	115.30
9	I	94	ALA	N-CA-C	6.00	127.20	111.00
20	a	57	LEU	CA-CB-CG	6.00	129.10	115.30
10	J	112	ASP	CB-CG-OD1	5.96	123.67	118.30
21	b	321	LEU	CB-CG-CD1	-5.95	100.89	111.00
17	S	190	MET	CB-CG-SD	5.95	130.24	112.40
32	U	66	PRO	CA-N-CD	-5.93	103.19	111.50
6	F	55	LEU	CA-CB-CG	5.92	128.92	115.30
13	M	127	LEU	CA-CB-CG	5.92	128.92	115.30
21	b	164	LEU	CA-CB-CG	5.91	128.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	73	ASP	CB-CG-OD1	5.87	123.58	118.30
14	N	186	PHE	CB-CG-CD2	5.85	124.90	120.80
17	S	49	LEU	CA-CB-CG	5.84	128.74	115.30
17	S	152	LEU	CA-CB-CG	5.83	128.71	115.30
14	N	49	LEU	CA-CB-CG	5.82	128.70	115.30
19	W	117	ARG	CB-CG-CD	5.72	126.47	111.60
19	W	117	ARG	CD-NE-CZ	5.71	131.59	123.60
17	S	140	LEU	CA-CB-CG	5.67	128.35	115.30
19	X	121	ILE	CG1-CB-CG2	-5.66	98.94	111.40
20	a	580	CYS	CA-CB-SG	-5.61	103.90	114.00
21	b	654	LEU	CA-CB-CG	5.60	128.19	115.30
25	f	221	LEU	CA-CB-CG	-5.59	102.43	115.30
17	S	167	PHE	CB-CG-CD1	5.58	124.70	120.80
12	L	87	LEU	CA-CB-CG	5.52	128.00	115.30
21	b	667	ARG	N-CA-C	5.52	125.89	111.00
20	a	91	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	88	LEU	CA-CB-CG	5.49	127.94	115.30
19	W	94	PHE	CB-CG-CD1	5.49	124.64	120.80
9	I	128	LEU	CA-CB-CG	5.41	127.74	115.30
19	X	53	GLN	CG-CD-NE2	-5.40	103.73	116.70
28	l	75	LEU	CA-CB-CG	5.40	127.72	115.30
14	N	228	LEU	CA-CB-CG	5.36	127.62	115.30
28	l	167	LEU	CA-CB-CG	5.33	127.56	115.30
4	D	37	GLN	CA-CB-CG	5.31	125.08	113.40
9	I	154	ASP	N-CA-C	-5.31	96.67	111.00
28	l	142	LEU	CA-CB-CG	5.30	127.49	115.30
18	T	140	LEU	CB-CG-CD1	-5.28	102.03	111.00
9	I	182	ASP	CB-CG-OD1	5.24	123.02	118.30
10	J	90	ASP	CB-CG-OD2	5.23	123.00	118.30
21	b	263[A]	GLN	CA-C-O	5.22	131.07	120.10
21	b	263[B]	GLN	CA-C-O	5.22	131.07	120.10
16	R	229	LEU	CB-CG-CD1	5.21	119.86	111.00
32	U	60	ASP	CB-CG-OD2	5.18	122.96	118.30
28	l	112	LEU	CA-CB-CG	5.17	127.19	115.30
15	O	153	PRO	N-CA-CB	-5.15	96.93	102.60
17	S	167	PHE	CB-CA-C	-5.13	100.13	110.40
19	W	41	ARG	CB-CG-CD	-5.12	98.29	111.60
19	X	117	ARG	CG-CD-NE	5.10	122.50	111.80
19	X	32	LEU	CB-CG-CD1	-5.09	102.35	111.00
19	W	92	LEU	CA-CB-CG	5.08	126.99	115.30
14	N	116	LEU	CA-CB-CG	5.07	126.97	115.30
29	m	11	LEU	CA-CB-CG	5.04	126.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	W	94	PHE	CB-CG-CD2	-5.04	117.27	120.80
16	R	131	ASP	CB-CG-OD1	5.03	122.83	118.30
14	N	61	ASP	CB-CG-OD1	5.03	122.83	118.30
21	b	144	LEU	CA-CB-CG	5.02	126.86	115.30
6	F	62	PHE	N-CA-C	-5.02	97.45	111.00
15	P	159	THR	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	91	PHE	Mainchain
12	L	228	HIS	Peptide
12	L	47	ASN	Peptide
14	N	112	PRO	Peptide
14	N	172	ASP	Peptide
14	N	224	GLY	Peptide
14	N	225	SER	Peptide
14	N	231	ASP	Peptide
14	N	233	ALA	Peptide
14	N	246	GLY	Peptide
15	O	156	ASP	Peptide
15	P	156	ASP	Mainchain
15	Q	156	ASP	Peptide
17	S	102	TRP	Mainchain
17	S	136	VAL	Mainchain
33	V	11	GLY	Mainchain
19	W	10	PRO	Peptide
19	W	112	PHE	Peptide
19	W	94	PHE	Peptide
23	d	151[A]	LYS	Mainchain,Peptide
23	d	151[B]	LYS	Mainchain,Peptide
23	d	167	HIS	Peptide
30	g	50	UNK	Peptide

## 5.2 Too-close contacts ⓘ

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



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/168 (99%)	150 (90%)	14 (8%)	2 (1%)	11	14
2	B	128/223 (57%)	121 (94%)	7 (6%)	0	100	100
3	C	161/198 (81%)	150 (93%)	9 (6%)	2 (1%)	11	14
4	D	170/207 (82%)	160 (94%)	9 (5%)	1 (1%)	22	30
5	E	186/222 (84%)	178 (96%)	8 (4%)	0	100	100
6	F	178/215 (83%)	165 (93%)	13 (7%)	0	100	100
7	G	212/245 (86%)	197 (93%)	14 (7%)	1 (0%)	25	35
8	H	168/203 (83%)	151 (90%)	17 (10%)	0	100	100
9	I	159/195 (82%)	146 (92%)	13 (8%)	0	100	100
10	J	165/200 (82%)	145 (88%)	17 (10%)	3 (2%)	7	8
11	K	167/207 (81%)	152 (91%)	15 (9%)	0	100	100
12	L	194/229 (85%)	176 (91%)	18 (9%)	0	100	100
13	M	185/306 (60%)	169 (91%)	15 (8%)	1 (0%)	25	35
14	N	217/219 (99%)	174 (80%)	40 (18%)	3 (1%)	9	12
15	O	171/205 (83%)	147 (86%)	21 (12%)	3 (2%)	7	8
15	P	171/205 (83%)	153 (90%)	16 (9%)	2 (1%)	11	14
15	Q	171/205 (83%)	150 (88%)	19 (11%)	2 (1%)	11	14
16	R	209/246 (85%)	182 (87%)	25 (12%)	2 (1%)	13	18
17	S	218/254 (86%)	184 (84%)	29 (13%)	5 (2%)	5	5
18	T	170/207 (82%)	164 (96%)	6 (4%)	0	100	100
19	W	158/198 (80%)	133 (84%)	25 (16%)	0	100	100
19	X	160/198 (81%)	146 (91%)	13 (8%)	1 (1%)	22	30
20	a	740/743 (100%)	713 (96%)	26 (4%)	1 (0%)	48	63
21	b	731/733 (100%)	699 (96%)	31 (4%)	1 (0%)	48	63
22	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	d	131/132 (99%)	125 (95%)	6 (5%)	0	100	100
24	e	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
25	f	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
26	i	31/40 (78%)	31 (100%)	0	0	100	100
27	j	39/42 (93%)	37 (95%)	1 (3%)	1 (3%)	4	4
28	l	142/172 (83%)	131 (92%)	11 (8%)	0	100	100
29	m	26/29 (90%)	26 (100%)	0	0	100	100
31	h	87/139 (63%)	87 (100%)	0	0	100	100
32	U	154/160 (96%)	123 (80%)	26 (17%)	5 (3%)	3	2
33	V	177/179 (99%)	152 (86%)	20 (11%)	5 (3%)	4	3
All	All	6441/7429 (87%)	5903 (92%)	497 (8%)	41 (1%)	24	30

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	87	ILE
15	O	153	PRO
15	O	155	ILE
15	Q	153	PRO
17	S	103	ALA
32	U	66	PRO
33	V	14	TYR
33	V	70	ARG
3	C	42	PHE
10	J	110	ALA
14	N	186	PHE
17	S	167	PHE
19	X	130	GLU
32	U	7	THR
33	V	82	SER
33	V	112	HIS
7	G	233	THR
13	M	234	THR
15	O	106	MET
17	S	60	LYS
1	A	198	THR
4	D	55	ALA
10	J	152	PHE

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Mol	Chain	Res	Type
15	Q	155	ILE
21	b	557	PRO
32	U	117	PRO
33	V	83	PRO
1	A	48	ASN
14	N	227	PRO
16	R	65	ILE
17	S	55	LEU
32	U	113	MET
32	U	155	PRO
15	P	153	PRO
15	P	154	PRO
17	S	101	PRO
27	j	40	PRO
20	a	158	ILE
3	C	161	PRO
14	N	183	PRO
16	R	67	GLY

### 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	137/137 (100%)	131 (96%)	6 (4%)	24	38
2	B	105/180 (58%)	99 (94%)	6 (6%)	17	27
3	C	131/153 (86%)	121 (92%)	10 (8%)	11	16
4	D	140/163 (86%)	126 (90%)	14 (10%)	6	8
5	E	142/164 (87%)	137 (96%)	5 (4%)	31	48
6	F	142/169 (84%)	134 (94%)	8 (6%)	17	27
7	G	172/193 (89%)	145 (84%)	27 (16%)	2	2
8	H	131/154 (85%)	128 (98%)	3 (2%)	45	64
9	I	124/152 (82%)	104 (84%)	20 (16%)	2	2
10	J	130/154 (84%)	123 (95%)	7 (5%)	18	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	133/160 (83%)	130 (98%)	3 (2%)	45	64
12	L	159/180 (88%)	158 (99%)	1 (1%)	84	92
13	M	142/247 (58%)	137 (96%)	5 (4%)	31	48
14	N	176/176 (100%)	169 (96%)	7 (4%)	27	42
15	O	138/159 (87%)	135 (98%)	3 (2%)	47	65
15	P	137/159 (86%)	120 (88%)	17 (12%)	4	4
15	Q	138/159 (87%)	135 (98%)	3 (2%)	47	65
16	R	167/193 (86%)	161 (96%)	6 (4%)	30	46
17	S	177/204 (87%)	167 (94%)	10 (6%)	17	27
18	T	136/163 (83%)	134 (98%)	2 (2%)	60	76
19	W	125/151 (83%)	125 (100%)	0	100	100
19	X	127/151 (84%)	124 (98%)	3 (2%)	44	62
20	a	606/606 (100%)	548 (90%)	58 (10%)	7	9
21	b	593/593 (100%)	523 (88%)	70 (12%)	4	5
22	c	67/69 (97%)	59 (88%)	8 (12%)	4	5
23	d	111/111 (100%)	91 (82%)	20 (18%)	1	1
24	e	55/55 (100%)	53 (96%)	2 (4%)	30	46
25	f	119/125 (95%)	108 (91%)	11 (9%)	7	10
26	i	29/36 (81%)	23 (79%)	6 (21%)	1	1
27	j	34/35 (97%)	29 (85%)	5 (15%)	2	3
28	l	114/143 (80%)	100 (88%)	14 (12%)	4	4
29	m	20/23 (87%)	17 (85%)	3 (15%)	2	2
31	h	70/109 (64%)	55 (79%)	15 (21%)	1	1
32	U	119/121 (98%)	87 (73%)	32 (27%)	0	0
33	V	137/137 (100%)	84 (61%)	53 (39%)	0	0
All	All	5183/5884 (88%)	4720 (91%)	463 (9%)	10	11

All (463) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASP
1	A	109	LEU
1	A	119	MET

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Mol	Chain	Res	Type
1	A	169	GLU
1	A	172	GLU
1	A	196	TRP
2	B	93	LEU
2	B	96	ASP
2	B	105	GLU
2	B	191	LEU
2	B	194	LEU
2	B	207	GLN
3	C	35	GLU
3	C	36	MET
3	C	40	LEU
3	C	45	ARG
3	C	64	LEU
3	C	114	ILE
3	C	158	ASN
3	C	165	MET
3	C	168	LYS
3	C	172	ILE
4	D	61	ARG
4	D	97	ARG
4	D	117	LEU
4	D	125	GLN
4	D	145	LEU
4	D	151	ARG
4	D	152	GLU
4	D	155	ASN
4	D	165	LYS
4	D	177	LEU
4	D	180	ILE
4	D	184	ARG
4	D	204	PHE
4	D	206	TYR
5	E	45	ARG
5	E	113	LYS
5	E	152	ARG
5	E	157	ARG
5	E	189	ARG
6	F	149	ASN
6	F	161	LEU
6	F	163	PHE
6	F	166	MET

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Mol	Chain	Res	Type
6	F	171	LYS
6	F	185	LEU
6	F	214	PHE
6	F	215	ASN
7	G	37	LEU
7	G	46	GLN
7	G	47	ARG
7	G	49	LYS
7	G	75	LEU
7	G	93	GLU
7	G	94	LYS
7	G	99	LEU
7	G	103	ARG
7	G	111	ARG
7	G	137	ILE
7	G	148	GLU
7	G	155	SER
7	G	156	GLN
7	G	159	MET
7	G	163	LEU
7	G	176	VAL
7	G	182	LYS
7	G	187	ARG
7	G	193	LYS
7	G	201	LYS
7	G	209	LYS
7	G	210	ARG
7	G	211	MET
7	G	216	ILE
7	G	233	THR
7	G	242	PHE
8	H	119	PHE
8	H	121	SER
8	H	124	ASN
9	I	35	LYS
9	I	36	ASP
9	I	39	ILE
9	I	42	ILE
9	I	43	THR
9	I	46	MET
9	I	58	LYS
9	I	72	LYS

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Mol	Chain	Res	Type
9	I	87	THR
9	I	92	HIS
9	I	95	PHE
9	I	120	LEU
9	I	133	LYS
9	I	135	ARG
9	I	144	LEU
9	I	150	VAL
9	I	170	LEU
9	I	176	MET
9	I	185	PHE
9	I	194	ARG
10	J	38	ASN
10	J	51	LYS
10	J	87	ILE
10	J	93	ARG
10	J	129	LEU
10	J	132	LEU
10	J	155	LYS
11	K	53	ARG
11	K	151	ARG
11	K	166	THR
12	L	36	ASN
13	M	74	GLU
13	M	75	ILE
13	M	77	ARG
13	M	172	ARG
13	M	173	ARG
14	N	63	TRP
14	N	67	ASN
14	N	86	MET
14	N	169	LEU
14	N	171	ARG
14	N	178	LEU
14	N	241	MET
15	O	121	ASN
15	O	152	PHE
15	O	153	PRO
15	P	32	LYS
15	P	35	GLU
15	P	64	ARG
15	P	83	VAL

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Mol	Chain	Res	Type
15	P	84	GLN
15	P	106	MET
15	P	120	LYS
15	P	129	LEU
15	P	137	LYS
15	P	147	LEU
15	P	149	THR
15	P	155	ILE
15	P	156	ASP
15	P	158	SER
15	P	164	GLN
15	P	168	ARG
15	P	192	ILE
15	Q	104	SER
15	Q	106	MET
15	Q	121	ASN
16	R	49	ASN
16	R	64	THR
16	R	65	ILE
16	R	69	THR
16	R	92	PHE
16	R	175	HIS
17	S	55	LEU
17	S	57	LEU
17	S	60	LYS
17	S	67	ASN
17	S	86	MET
17	S	157	LYS
17	S	175	HIS
17	S	177	VAL
17	S	178	LEU
17	S	241	MET
18	T	23	ASN
18	T	31	ARG
19	X	117	ARG
19	X	127	THR
19	X	129	ASP
20	a	17	ASN
20	a	29	THR
20	a	32	GLU
20	a	49	LYS
20	a	85	GLN

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Mol	Chain	Res	Type
20	a	110	LEU
20	a	115	LYS
20	a	139	ASN
20	a	147	SER
20	a	154	ARG
20	a	179	LEU
20	a	188	LYS
20	a	193	LEU
20	a	216	LEU
20	a	217	SER
20	a	252	ARG
20	a	254	LEU
20	a	280	PHE
20	a	283	PHE
20	a	284	LYS
20	a	288	ASN
20	a	304	LEU
20	a	309	LEU
20	a	326	SER
20	a	327	MET
20	a	335	LYS
20	a	344	LYS
20	a	348	GLU
20	a	353	SER
20	a	358	LEU
20	a	364	MET
20	a	365	ILE
20	a	377	TYR
20	a	393	LEU
20	a	407	VAL
20	a	427	ASN
20	a	430	ASN
20	a	432	LEU
20	a	453	LEU
20	a	466	THR
20	a	468	ARG
20	a	480	LYS
20	a	503	THR
20	a	518	ASP
20	a	521	GLU
20	a	532	LYS
20	a	553	LEU

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Mol	Chain	Res	Type
20	a	556	LEU
20	a	567	LEU
20	a	588	THR
20	a	626	THR
20	a	649	ASN
20	a	652	LEU
20	a	702	LEU
20	a	728	GLN
20	a	739	LEU
20	a	755	SER
20	a	757	THR
21	b	4	LYS
21	b	5	PHE
21	b	10	GLN
21	b	42	LEU
21	b	54	LEU
21	b	84	THR
21	b	106	LYS
21	b	112	VAL
21	b	114	ILE
21	b	117	SER
21	b	125	THR
21	b	154	LEU
21	b	174	LEU
21	b	187	LEU
21	b	222	LYS
21	b	228	ASN
21	b	230	THR
21	b	238	SER
21	b	256	PHE
21	b	263[A]	GLN
21	b	263[B]	GLN
21	b	291	ARG
21	b	293	ASN
21	b	319	VAL
21	b	324	THR
21	b	333	LEU
21	b	346	LEU
21	b	347	THR
21	b	349	GLN
21	b	350	HIS
21	b	352	TYR

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Mol	Chain	Res	Type
21	b	354	LEU
21	b	355	THR
21	b	360	LEU
21	b	362	LYS
21	b	375	GLN
21	b	395	ARG
21	b	401	LEU
21	b	402	ASN
21	b	404	ASN
21	b	406	VAL
21	b	407	LEU
21	b	414	LYS
21	b	421	LEU
21	b	433	LEU
21	b	440	ASP
21	b	466	SER
21	b	490	GLN
21	b	493	LEU
21	b	500	ILE
21	b	504	LYS
21	b	505	ASN
21	b	507	LEU
21	b	518	VAL
21	b	531	LEU
21	b	545	LEU
21	b	575	PHE
21	b	576	TYR
21	b	607	GLN
21	b	619	LEU
21	b	625	LEU
21	b	628	SER
21	b	643	SER
21	b	673	LEU
21	b	684	THR
21	b	709	LEU
21	b	713	SER
21	b	717	ILE
21	b	724	LEU
21	b	725	ILE
22	c	4	SER
22	c	26	LEU
22	c	35	LYS

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Mol	Chain	Res	Type
22	c	37	LYS
22	c	66	ARG
22	c	69	LEU
22	c	72	GLU
22	c	77	MET
23	d	99	LYS
23	d	108	LYS
23	d	123	ARG
23	d	129	LEU
23	d	130	LYS
23	d	138	LEU
23	d	143	ARG
23	d	147	LYS
23	d	150	ILE
23	d	151[A]	LYS
23	d	151[B]	LYS
23	d	160	ASN
23	d	162	GLU
23	d	175	GLU
23	d	177	VAL
23	d	193	LYS
23	d	195	VAL
23	d	201	LYS
23	d	205	LYS
23	d	206	GLN
24	e	60	ILE
24	e	61	GLN
25	f	78	ILE
25	f	99	LYS
25	f	134	LYS
25	f	154	ARG
25	f	178	ARG
25	f	179	SER
25	f	201	LEU
25	f	203	SER
25	f	204	ARG
25	f	207	PHE
25	f	218	ARG
26	i	4	ASN
26	i	12	LEU
26	i	16	LEU
26	i	24	SER

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Mol	Chain	Res	Type
26	i	31	LYS
26	i	33	LEU
27	j	1	MET
27	j	37	LEU
27	j	38	THR
27	j	39	PHE
27	j	41	PHE
28	l	33	LYS
28	l	59	LYS
28	l	72	LEU
28	l	91	LYS
28	l	102	LEU
28	l	129	LYS
28	l	130	GLU
28	l	132	LYS
28	l	134	MET
28	l	136	SER
28	l	138	ASN
28	l	146	LYS
28	l	149	ASP
28	l	152	LYS
29	m	2	ILE
29	m	24	LEU
29	m	27	GLN
31	h	51	ASP
31	h	52	MET
31	h	61	SER
31	h	73	SER
31	h	75	LEU
31	h	81	ILE
31	h	90	SER
31	h	94	SER
31	h	99	GLN
31	h	105	GLU
31	h	113	TYR
31	h	127	THR
31	h	128	HIS
31	h	131	SER
31	h	136	LYS
32	U	1	LEU
32	U	2	ASP
32	U	4	MET

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Mol	Chain	Res	Type
32	U	5	VAL
32	U	10	GLU
32	U	14	LYS
32	U	19	LEU
32	U	21	LEU
32	U	23	ASP
32	U	24	TYR
32	U	29	ARG
32	U	31	ARG
32	U	49	VAL
32	U	52	LYS
32	U	56	HIS
32	U	72	GLN
32	U	74	ASP
32	U	76	GLN
32	U	80	GLN
32	U	81	PHE
32	U	83	ILE
32	U	87	THR
32	U	88	ILE
32	U	92	LYS
32	U	95	MET
32	U	97	LEU
32	U	100	LYS
32	U	110	ILE
32	U	114	LYS
32	U	123	ARG
32	U	125	ASP
32	U	126	MET
33	V	1	THR
33	V	3	LEU
33	V	6	GLU
33	V	9	PHE
33	V	10	ILE
33	V	12	GLU
33	V	14	TYR
33	V	18	LEU
33	V	19	THR
33	V	20	LEU
33	V	25	GLU
33	V	27	THR
33	V	29	THR

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Mol	Chain	Res	Type
33	V	37	LYS
33	V	41	SER
33	V	53	LYS
33	V	54	LEU
33	V	56	LEU
33	V	57	THR
33	V	58	LEU
33	V	59	ASN
33	V	64	HIS
33	V	66	TYR
33	V	69	ILE
33	V	71	ASP
33	V	73	ILE
33	V	74	LYS
33	V	77	ASP
33	V	85	GLU
33	V	87	VAL
33	V	88	LYS
33	V	111	THR
33	V	113	ARG
33	V	114	ASN
33	V	116	LYS
33	V	121	GLU
33	V	122	SER
33	V	123	VAL
33	V	132	LEU
33	V	133	THR
33	V	135	ASP
33	V	136	LEU
33	V	141	LEU
33	V	142	ASN
33	V	143	ILE
33	V	144	LYS
33	V	147	ASP
33	V	148	ARG
33	V	149	ARG
33	V	151	LEU
33	V	164	ILE
33	V	165	SER
33	V	173	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	137	ASN
1	A	193	HIS
1	A	195	ASN
3	C	68	GLN
3	C	95	GLN
3	C	99	HIS
3	C	107	ASN
3	C	140	HIS
3	C	158	ASN
3	C	174	HIS
4	D	155	ASN
5	E	126	HIS
5	E	187	ASN
5	E	212	ASN
6	F	94	HIS
6	F	103	HIS
6	F	149	ASN
7	G	46	GLN
7	G	142	ASN
7	G	156	GLN
7	G	232	GLN
7	G	240	HIS
8	H	46	ASN
9	I	64	ASN
9	I	92	HIS
9	I	181	GLN
9	I	191	GLN
10	J	38	ASN
12	L	75	HIS
12	L	94	HIS
12	L	108	HIS
12	L	163	GLN
13	M	170	HIS
14	N	81	HIS
14	N	111	HIS
14	N	187	ASN
14	N	204	ASN
15	O	70	HIS
15	O	84	GLN
15	O	121	ASN
15	O	140	HIS
15	P	121	ASN

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Mol	Chain	Res	Type
15	P	140	HIS
15	P	164	GLN
15	Q	70	HIS
15	Q	140	HIS
15	Q	191	ASN
16	R	49	ASN
16	R	154	HIS
16	R	175	HIS
17	S	154	HIS
17	S	173	ASN
17	S	175	HIS
17	S	204	ASN
17	S	239	GLN
18	T	9	GLN
18	T	23	ASN
18	T	39	HIS
19	W	26	GLN
19	X	157	HIS
20	a	17	ASN
20	a	141	GLN
20	a	273	GLN
20	a	288	ASN
20	a	343	HIS
20	a	392	GLN
20	a	426	ASN
20	a	427	ASN
20	a	429	ASN
20	a	430	ASN
20	a	447	ASN
20	a	456	HIS
20	a	485	GLN
20	a	596	HIS
20	a	649	ASN
20	a	662	GLN
20	a	700	GLN
20	a	720	GLN
21	b	14	GLN
21	b	71	GLN
21	b	89	HIS
21	b	131	ASN
21	b	132	GLN
21	b	195	HIS

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Mol	Chain	Res	Type
21	b	217	HIS
21	b	276	GLN
21	b	288	HIS
21	b	298	HIS
21	b	349	GLN
21	b	350	HIS
21	b	375	GLN
21	b	404	ASN
21	b	405	ASN
21	b	490	GLN
21	b	505	ASN
21	b	597	HIS
21	b	607	GLN
21	b	641	ASN
21	b	671	GLN
21	b	681	HIS
23	d	206	GLN
26	i	4	ASN
28	l	81	HIS
28	l	143	GLN
29	m	5	ASN
31	h	93	GLN
32	U	56	HIS
32	U	72	GLN
32	U	80	GLN
32	U	148	HIS
33	V	64	HIS
33	V	89	HIS
33	V	112	HIS
33	V	114	ASN
33	V	128	GLN
33	V	142	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

589 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$
35	A86	M	304	-	44,50,50	1.23	3 (6%)	51,76,76	2.06	14 (27%)
39	LMT	G	322	-	36,36,36	0.39	0	47,47,47	0.69	0
39	LMT	L	303	-	36,36,36	1.33	6 (16%)	47,47,47	0.96	1 (2%)
36	CLA	W	215	-	48,56,73	1.88	8 (16%)	55,92,113	1.50	8 (14%)
37	KC1	Q	313	-	48,53,53	3.07	20 (41%)	55,89,89	6.90	36 (65%)
35	A86	J	302	-	44,50,50	1.26	4 (9%)	51,76,76	2.08	12 (23%)
36	CLA	F	310	-	56,64,73	1.50	7 (12%)	65,102,113	1.64	12 (18%)
36	CLA	a	829	-	65,73,73	1.45	9 (13%)	76,113,113	1.74	12 (15%)
36	CLA	T	308	18	61,69,73	1.50	5 (8%)	71,108,113	1.53	9 (12%)
36	CLA	b	816	-	60,68,73	1.92	12 (20%)	70,107,113	2.01	18 (25%)
36	CLA	E	310	-	65,73,73	1.47	6 (9%)	76,113,113	1.59	9 (11%)
39	LMT	b	851	-	24,24,36	0.42	0	29,29,47	0.81	0
35	A86	S	305	-	44,50,50	1.27	3 (6%)	51,76,76	2.95	20 (39%)
36	CLA	F	311	-	52,60,73	1.62	9 (17%)	60,97,113	1.62	8 (13%)
36	CLA	M	306	13,37	55,63,73	1.52	10 (18%)	64,101,113	1.57	11 (17%)
36	CLA	A	305	1	49,57,73	1.65	8 (16%)	55,93,113	1.54	7 (12%)
36	CLA	a	801	-	65,73,73	1.44	10 (15%)	76,113,113	1.61	14 (18%)
35	A86	N	303	-	44,50,50	1.31	5 (11%)	51,76,76	3.31	22 (43%)
34	DD6	D	303	-	39,45,45	2.97	8 (20%)	52,67,67	2.65	18 (34%)
36	CLA	D	309	-	55,63,73	2.08	13 (23%)	64,101,113	2.97	25 (39%)
36	CLA	J	307	10	61,69,73	1.46	7 (11%)	71,108,113	1.58	11 (15%)
34	DD6	W	204	36	39,45,45	2.04	3 (7%)	52,67,67	2.01	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	J	315	-	41,49,73	1.77	7 (17%)	47,84,113	1.81	8 (17%)
37	KC1	U	312	35,32	48,53,53	3.16	21 (43%)	55,89,89	4.86	31 (56%)
36	CLA	D	306	4	45,53,73	1.81	9 (20%)	52,89,113	1.80	10 (19%)
36	CLA	K	312	-	65,73,73	1.42	7 (10%)	76,113,113	1.45	7 (9%)
36	CLA	H	315	8	65,73,73	1.48	9 (13%)	76,113,113	1.60	14 (18%)
36	CLA	J	317	10	47,55,73	1.70	9 (19%)	54,91,113	1.50	6 (11%)
36	CLA	l	206	46	50,58,73	1.59	7 (14%)	58,95,113	1.63	8 (13%)
36	CLA	a	827	-	62,70,73	1.46	8 (12%)	72,109,113	1.70	10 (13%)
42	LMG	E	318	-	46,46,55	0.98	2 (4%)	54,54,63	1.06	2 (3%)
34	DD6	E	306	-	39,45,45	2.03	3 (7%)	52,67,67	2.04	10 (19%)
36	CLA	A	308	-	65,73,73	1.41	7 (10%)	76,113,113	1.59	9 (11%)
36	CLA	I	307	-	54,62,73	1.51	8 (14%)	62,99,113	1.66	8 (12%)
36	CLA	a	804	-	65,73,73	1.44	10 (15%)	76,113,113	1.42	11 (14%)
36	CLA	C	206	-	61,69,73	1.48	7 (11%)	71,108,113	1.48	7 (9%)
36	CLA	P	314	-	60,68,73	1.66	9 (15%)	70,107,113	1.70	14 (20%)
36	CLA	b	833	-	58,66,73	1.50	8 (13%)	67,104,113	1.63	11 (16%)
36	CLA	a	812	-	65,73,73	1.41	7 (10%)	76,113,113	1.54	8 (10%)
36	CLA	O	306	-	61,69,73	1.49	9 (14%)	71,108,113	1.46	6 (8%)
36	CLA	a	820	-	65,73,73	1.39	8 (12%)	76,113,113	1.54	10 (13%)
34	DD6	P	305	-	39,45,45	2.02	3 (7%)	52,67,67	2.06	16 (30%)
36	CLA	C	208	-	65,73,73	1.45	9 (13%)	76,113,113	1.43	9 (11%)
36	CLA	V	311	33	65,73,73	1.40	8 (12%)	76,113,113	1.76	13 (17%)
41	LHG	i	104	-	45,45,48	0.98	2 (4%)	48,51,54	1.03	2 (4%)
34	DD6	S	306	-	39,45,45	1.96	3 (7%)	52,67,67	2.00	13 (25%)
36	CLA	b	835	-	45,53,73	1.74	9 (20%)	52,89,113	1.74	10 (19%)
35	A86	I	302	-	44,50,50	1.30	4 (9%)	51,76,76	2.66	17 (33%)
41	LHG	I	316	-	48,48,48	0.95	2 (4%)	51,54,54	1.00	2 (3%)
39	LMT	I	317	-	36,36,36	0.41	0	47,47,47	0.75	1 (2%)
34	DD6	K	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	13 (25%)
35	A86	O	302	-	44,50,50	1.44	6 (13%)	51,76,76	3.47	23 (45%)
36	CLA	L	314	12	65,73,73	1.41	8 (12%)	76,113,113	1.58	10 (13%)
36	CLA	X	315	-	41,49,73	1.83	5 (12%)	47,84,113	1.78	8 (17%)
36	CLA	G	314	7	41,49,73	1.79	9 (21%)	47,84,113	1.82	9 (19%)
35	A86	E	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.19	13 (25%)
42	LMG	D	320	41	46,46,55	0.98	2 (4%)	54,54,63	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	I	305	-	61,69,73	2.03	11 (18%)	71,108,113	1.76	12 (16%)
36	CLA	b	832	-	49,57,73	1.52	8 (16%)	55,93,113	1.75	8 (14%)
36	CLA	N	311	14	46,54,73	1.72	7 (15%)	53,90,113	1.86	10 (18%)
36	CLA	L	312	12	46,54,73	1.77	8 (17%)	53,90,113	1.91	10 (18%)
36	CLA	O	308	15	65,73,73	1.45	8 (12%)	76,113,113	1.53	9 (11%)
36	CLA	b	807	-	45,53,73	1.66	7 (15%)	52,89,113	1.76	8 (15%)
36	CLA	b	823	-	55,63,73	1.49	7 (12%)	64,101,113	1.61	7 (10%)
35	A86	A	316	-	44,50,50	1.23	4 (9%)	51,76,76	2.16	16 (31%)
37	KC1	T	310	-	48,53,53	4.86	28 (58%)	55,89,89	7.31	33 (60%)
35	A86	T	304	-	44,50,50	1.11	3 (6%)	51,76,76	1.69	11 (21%)
36	CLA	a	806	-	65,73,73	1.72	9 (13%)	76,113,113	1.90	17 (22%)
37	KC1	K	314	11	48,53,53	2.91	19 (39%)	55,89,89	5.96	36 (65%)
36	CLA	L	308	-	61,69,73	1.83	12 (19%)	71,108,113	2.35	17 (23%)
42	LMG	E	319	-	40,40,55	1.04	2 (5%)	48,48,63	1.11	3 (6%)
39	LMT	L	318	-	32,32,36	0.45	0	43,43,47	0.79	1 (2%)
37	KC1	W	217	-	48,53,53	3.14	19 (39%)	55,89,89	4.85	35 (63%)
39	LMT	f	807	-	24,24,36	0.43	0	29,29,47	0.58	0
36	CLA	l	201	-	65,73,73	1.40	8 (12%)	76,113,113	1.55	10 (13%)
44	BCR	a	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	3 (5%)
36	CLA	b	837	-	65,73,73	1.40	8 (12%)	76,113,113	1.59	11 (14%)
36	CLA	b	812	21	65,73,73	1.41	9 (13%)	76,113,113	1.61	13 (17%)
36	CLA	P	312	15	46,54,73	1.72	7 (15%)	53,90,113	1.71	10 (18%)
44	BCR	f	806	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	7 (12%)
36	CLA	l	205	-	65,73,73	1.53	10 (15%)	76,113,113	2.19	18 (23%)
39	LMT	a	854	-	36,36,36	0.40	0	47,47,47	0.75	0
35	A86	O	305	-	44,50,50	1.42	4 (9%)	51,76,76	1.95	16 (31%)
36	CLA	C	210	3	46,54,73	1.79	6 (13%)	53,90,113	1.68	9 (16%)
36	CLA	E	315	-	65,73,73	1.96	15 (23%)	76,113,113	2.57	24 (31%)
42	LMG	D	321	-	37,37,55	1.08	2 (5%)	45,45,63	1.02	2 (4%)
45	SF4	b	803	21,20	0,12,12	-	-	-	-	-
37	KC1	G	317	-	48,53,53	2.92	22 (45%)	55,89,89	5.07	35 (63%)
36	CLA	b	802	-	65,73,73	1.45	8 (12%)	76,113,113	1.42	9 (11%)
36	CLA	R	321	16	65,73,73	1.47	7 (10%)	76,113,113	1.58	9 (11%)
36	CLA	E	308	5	49,57,73	1.63	10 (20%)	55,93,113	1.62	9 (16%)
36	CLA	a	836	-	65,73,73	1.34	8 (12%)	76,113,113	1.71	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
41	LHG	F	319	-	40,40,48	1.03	2 (5%)	43,46,54	1.10	3 (6%)
44	BCR	f	801	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	5 (8%)
36	CLA	D	308	-	65,73,73	1.43	8 (12%)	76,113,113	1.65	12 (15%)
36	CLA	S	319	17	65,73,73	1.49	8 (12%)	76,113,113	1.57	11 (14%)
38	SQD	b	804	-	45,46,54	1.27	4 (8%)	54,57,65	1.21	4 (7%)
35	A86	P	304	-	44,50,50	1.33	5 (11%)	51,76,76	2.74	17 (33%)
36	CLA	H	317	8	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
39	LMT	U	315	-	36,36,36	0.40	0	47,47,47	0.74	1 (2%)
36	CLA	J	316	-	46,54,73	1.72	10 (21%)	53,90,113	1.84	10 (18%)
36	CLA	b	841	41	65,73,73	1.42	12 (18%)	76,113,113	1.99	17 (22%)
36	CLA	A	313	-	41,49,73	1.84	9 (21%)	47,84,113	1.83	7 (14%)
44	BCR	b	847	-	41,41,41	1.18	3 (7%)	56,56,56	1.26	7 (12%)
35	A86	T	302	18	44,50,50	1.24	3 (6%)	51,76,76	2.85	21 (41%)
35	A86	Q	303	-	44,50,50	1.33	5 (11%)	51,76,76	2.05	15 (29%)
36	CLA	U	305	-	61,69,73	1.52	6 (9%)	71,108,113	1.43	7 (9%)
35	A86	L	304	-	44,50,50	1.39	4 (9%)	51,76,76	2.99	15 (29%)
44	BCR	i	103	-	41,41,41	1.19	3 (7%)	56,56,56	1.32	7 (12%)
35	A86	X	303	36	44,50,50	1.47	5 (11%)	51,76,76	3.76	24 (47%)
36	CLA	W	210	-	46,54,73	1.69	6 (13%)	53,90,113	2.10	14 (26%)
36	CLA	H	318	-	50,58,73	1.63	10 (20%)	58,95,113	1.63	10 (17%)
36	CLA	a	825	-	65,73,73	1.53	7 (10%)	76,113,113	1.77	11 (14%)
36	CLA	C	207	-	65,73,73	2.00	14 (21%)	76,113,113	2.81	23 (30%)
36	CLA	T	311	18	65,73,73	1.52	9 (13%)	76,113,113	2.03	16 (21%)
42	LMG	J	318	-	55,55,55	0.89	2 (3%)	63,63,63	1.02	3 (4%)
45	SF4	c	102	-	0,12,12	-	-	-	-	-
36	CLA	U	306	32	65,73,73	2.14	16 (24%)	76,113,113	2.65	23 (30%)
36	CLA	U	311	32	65,73,73	1.46	8 (12%)	76,113,113	1.65	12 (15%)
44	BCR	j	107	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	7 (12%)
36	CLA	L	309	12	65,73,73	1.43	8 (12%)	76,113,113	1.45	8 (10%)
36	CLA	b	829	-	65,73,73	1.44	9 (13%)	76,113,113	1.37	7 (9%)
34	DD6	R	307	-	39,45,45	2.00	2 (5%)	52,67,67	2.11	15 (28%)
35	A86	R	306	-	44,50,50	1.34	4 (9%)	51,76,76	2.91	16 (31%)
36	CLA	D	312	-	65,73,73	1.46	9 (13%)	76,113,113	1.40	9 (11%)
42	LMG	L	321	40	33,33,55	1.13	2 (6%)	41,41,63	1.15	3 (7%)
36	CLA	Q	307	15	50,58,73	1.63	8 (16%)	56,94,113	1.59	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DD6	B	304	-	39,45,45	2.01	3 (7%)	52,67,67	2.14	16 (30%)
36	CLA	P	301	15	65,73,73	1.44	8 (12%)	76,113,113	1.56	10 (13%)
36	CLA	a	819	-	45,53,73	1.74	10 (22%)	52,89,113	2.32	10 (19%)
36	CLA	P	319	-	60,68,73	2.34	11 (18%)	70,107,113	2.21	15 (21%)
36	CLA	R	313	-	65,73,73	1.41	8 (12%)	76,113,113	1.37	7 (9%)
36	CLA	Q	309	15	46,54,73	1.73	7 (15%)	53,90,113	1.73	10 (18%)
41	LHG	l	208	-	47,47,48	0.95	2 (4%)	50,53,54	1.02	3 (6%)
36	CLA	N	309	14	51,59,73	1.67	9 (17%)	59,96,113	1.81	8 (13%)
35	A86	V	301	35	44,50,50	1.23	4 (9%)	51,76,76	2.22	16 (31%)
34	DD6	G	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	10 (19%)
36	CLA	b	810	-	65,73,73	1.36	9 (13%)	76,113,113	1.42	8 (10%)
41	LHG	G	321	36	46,46,48	0.96	2 (4%)	49,52,54	1.06	2 (4%)
34	DD6	E	304	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	10 (19%)
35	A86	B	303	-	44,50,50	1.30	3 (6%)	51,76,76	4.01	27 (52%)
36	CLA	b	827	-	65,73,73	1.57	8 (12%)	76,113,113	1.44	10 (13%)
36	CLA	P	313	-	65,73,73	1.42	7 (10%)	76,113,113	1.44	6 (7%)
36	CLA	a	848	36	65,73,73	1.72	11 (16%)	76,113,113	1.97	19 (25%)
35	A86	F	306	-	44,50,50	1.26	4 (9%)	51,76,76	2.04	13 (25%)
35	A86	P	303	-	44,50,50	1.44	6 (13%)	51,76,76	3.47	23 (45%)
36	CLA	G	319	7	50,58,73	2.05	14 (28%)	58,95,113	3.97	26 (44%)
36	CLA	a	841	41	52,60,73	1.65	8 (15%)	60,97,113	1.64	9 (15%)
36	CLA	W	218	19	43,51,73	1.75	8 (18%)	49,86,113	1.90	9 (18%)
36	CLA	Q	306	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	6 (7%)
36	CLA	L	313	-	65,73,73	1.39	7 (10%)	76,113,113	1.59	7 (9%)
36	CLA	a	830	-	50,58,73	2.05	12 (24%)	58,95,113	3.35	18 (31%)
36	CLA	f	804	46	65,73,73	2.02	17 (26%)	76,113,113	2.93	29 (38%)
42	LMG	V	315	-	46,46,55	0.98	2 (4%)	54,54,63	4.29	4 (7%)
35	A86	K	306	11	44,50,50	1.22	3 (6%)	51,76,76	3.50	21 (41%)
35	A86	L	307	-	44,50,50	1.24	4 (9%)	51,76,76	1.93	11 (21%)
44	BCR	b	845	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	8 (14%)
36	CLA	b	831	-	50,58,73	1.66	10 (20%)	58,95,113	1.65	8 (13%)
36	CLA	F	316	6	41,49,73	1.78	9 (21%)	47,84,113	1.66	9 (19%)
37	KC1	F	308	6	48,53,53	2.95	21 (43%)	55,89,89	6.07	33 (60%)
36	CLA	b	805	36	65,73,73	1.42	10 (15%)	76,113,113	1.40	14 (18%)
35	A86	E	305	5	44,50,50	1.23	4 (9%)	51,76,76	2.04	14 (27%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	G	313	7	65,73,73	1.49	6 (9%)	76,113,113	1.96	14 (18%)
35	A86	O	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.07	14 (27%)
36	CLA	K	316	-	65,73,73	1.45	9 (13%)	76,113,113	1.32	5 (6%)
36	CLA	b	820	21	60,68,73	1.50	9 (15%)	70,107,113	1.47	8 (11%)
36	CLA	R	316	-	46,54,73	1.73	9 (19%)	53,90,113	2.13	16 (30%)
34	DD6	H	302	-	39,45,45	1.98	3 (7%)	52,67,67	1.92	15 (28%)
36	CLA	a	833	-	50,58,73	1.65	11 (22%)	58,95,113	1.69	7 (12%)
36	CLA	P	316	-	41,49,73	1.84	8 (19%)	47,84,113	1.81	7 (14%)
36	CLA	X	313	19	42,50,73	2.62	8 (19%)	48,85,113	4.07	18 (37%)
37	KC1	M	318	-	48,53,53	5.42	28 (58%)	55,89,89	6.65	32 (58%)
37	KC1	O	313	15	48,53,53	3.07	21 (43%)	55,89,89	6.91	36 (65%)
37	KC1	X	311	-	48,53,53	3.14	19 (39%)	55,89,89	4.85	34 (61%)
39	LMT	E	321	-	23,23,36	0.45	0	28,28,47	0.59	0
36	CLA	f	803	-	65,73,73	1.81	14 (21%)	76,113,113	2.45	24 (31%)
36	CLA	J	313	-	65,73,73	1.44	9 (13%)	76,113,113	1.44	8 (10%)
36	CLA	b	819	-	59,67,73	1.63	9 (15%)	68,105,113	2.04	15 (22%)
36	CLA	H	307	8	60,68,73	1.48	8 (13%)	70,107,113	1.99	18 (25%)
36	CLA	J	309	-	65,73,73	1.45	6 (9%)	76,113,113	1.34	7 (9%)
35	A86	R	303	-	44,50,50	1.36	5 (11%)	51,76,76	3.63	21 (41%)
36	CLA	a	813	-	45,53,73	1.62	10 (22%)	52,89,113	1.89	9 (17%)
36	CLA	a	821	-	49,57,73	1.57	8 (16%)	55,93,113	1.70	6 (10%)
37	KC1	B	310	2	48,53,53	3.13	20 (41%)	55,89,89	5.04	34 (61%)
36	CLA	K	307	-	61,69,73	1.91	13 (21%)	71,108,113	2.94	22 (30%)
37	KC1	E	309	-	48,53,53	2.94	20 (41%)	55,89,89	5.56	37 (67%)
42	LMG	G	324	-	55,55,55	0.90	2 (3%)	63,63,63	1.00	3 (4%)
36	CLA	P	318	-	51,59,73	1.66	7 (13%)	59,96,113	1.56	7 (11%)
35	A86	U	302	-	44,50,50	1.33	4 (9%)	51,76,76	3.12	22 (43%)
35	A86	J	301	-	44,50,50	1.26	4 (9%)	51,76,76	2.23	18 (35%)
35	A86	E	307	36	44,50,50	1.24	4 (9%)	51,76,76	2.07	12 (23%)
35	A86	N	304	-	44,50,50	2.90	7 (15%)	51,76,76	7.45	18 (35%)
36	CLA	a	807	20	65,73,73	1.37	7 (10%)	76,113,113	1.63	12 (15%)
36	CLA	Q	314	-	65,73,73	1.45	6 (9%)	76,113,113	4.16	13 (17%)
36	CLA	W	206	19	61,69,73	1.51	5 (8%)	71,108,113	1.63	7 (9%)
35	A86	O	319	35,36	44,50,50	1.28	5 (11%)	51,76,76	2.93	18 (35%)
39	LMT	U	314	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	LMT	h	205	-	36,36,36	0.41	0	47,47,47	0.70	1 (2%)
37	KC1	D	314	4	48,53,53	2.90	19 (39%)	55,89,89	5.52	34 (61%)
35	A86	I	301	-	44,50,50	1.23	3 (6%)	51,76,76	2.39	18 (35%)
36	CLA	a	815	46	45,53,73	1.73	8 (17%)	52,89,113	1.63	6 (11%)
36	CLA	G	310	-	65,73,73	1.41	9 (13%)	76,113,113	1.36	6 (7%)
36	CLA	V	313	-	65,73,73	1.46	8 (12%)	76,113,113	1.34	8 (10%)
36	CLA	V	309	33	43,51,73	1.76	8 (18%)	49,86,113	2.05	12 (24%)
35	A86	V	304	-	44,50,50	1.48	6 (13%)	51,76,76	3.49	18 (35%)
34	DD6	a	849	-	39,45,45	2.01	3 (7%)	52,67,67	1.84	13 (25%)
36	CLA	P	302	-	42,50,73	1.72	7 (16%)	48,85,113	1.92	9 (18%)
36	CLA	S	310	17	65,73,73	1.45	7 (10%)	76,113,113	1.70	12 (15%)
41	LHG	O	318	15	48,48,48	0.88	3 (6%)	51,54,54	1.22	4 (7%)
36	CLA	a	828	-	65,73,73	1.36	7 (10%)	76,113,113	1.57	8 (10%)
36	CLA	U	308	35,32	56,64,73	1.59	8 (14%)	65,102,113	1.75	10 (15%)
36	CLA	b	817	-	59,67,73	1.91	11 (18%)	68,105,113	2.25	18 (26%)
36	CLA	V	307	-	51,59,73	1.67	6 (11%)	59,96,113	1.49	6 (10%)
42	LMG	I	315	-	55,55,55	0.89	2 (3%)	63,63,63	1.00	3 (4%)
36	CLA	E	313	-	65,73,73	1.95	13 (20%)	76,113,113	2.19	20 (26%)
36	CLA	a	811	-	54,62,73	1.60	8 (14%)	62,99,113	1.51	7 (11%)
42	LMG	G	325	-	55,55,55	0.89	2 (3%)	63,63,63	1.01	3 (4%)
36	CLA	S	315	17	43,51,73	1.91	9 (20%)	49,86,113	2.11	10 (20%)
35	A86	G	302	-	44,50,50	1.18	3 (6%)	51,76,76	1.92	13 (25%)
36	CLA	a	810	36	62,70,73	1.44	8 (12%)	72,109,113	1.51	8 (11%)
36	CLA	B	309	2	52,60,73	2.05	10 (19%)	60,97,113	2.20	19 (31%)
39	LMT	F	321	-	34,34,36	0.65	0	45,45,47	1.61	6 (13%)
36	CLA	b	821	46	65,73,73	1.43	10 (15%)	76,113,113	1.49	9 (11%)
35	A86	U	301	-	44,50,50	1.37	3 (6%)	51,76,76	3.80	25 (49%)
35	A86	N	320	-	44,50,50	1.38	6 (13%)	51,76,76	3.30	24 (47%)
35	A86	C	203	-	44,50,50	1.24	4 (9%)	51,76,76	2.07	16 (31%)
36	CLA	B	307	-	46,54,73	1.74	8 (17%)	53,90,113	1.65	9 (16%)
36	CLA	F	314	6,35	65,73,73	1.42	7 (10%)	76,113,113	1.56	10 (13%)
36	CLA	S	321	-	52,60,73	1.66	8 (15%)	60,97,113	1.76	10 (16%)
36	CLA	f	805	25	52,60,73	1.55	7 (13%)	60,97,113	1.65	9 (15%)
36	CLA	N	313	14	41,49,73	1.89	8 (19%)	47,84,113	1.90	12 (25%)
37	KC1	L	317	-	48,53,53	2.96	20 (41%)	55,89,89	5.42	36 (65%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
42	LMG	V	316	-	46,46,55	0.98	2 (4%)	54,54,63	1.04	3 (5%)
39	LMT	a	853	-	33,33,36	0.42	0	44,44,47	0.74	1 (2%)
42	LMG	J	319	-	44,44,55	0.99	2 (4%)	52,52,63	1.11	3 (5%)
34	DD6	A	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.86	9 (17%)
35	A86	F	301	-	44,50,50	1.24	4 (9%)	51,76,76	2.32	16 (31%)
36	CLA	Q	312	-	41,49,73	1.85	8 (19%)	47,84,113	1.81	7 (14%)
40	DGD	b	849	-	61,61,67	1.05	7 (11%)	75,75,81	1.49	11 (14%)
36	CLA	D	310	-	65,73,73	1.35	8 (12%)	76,113,113	1.57	8 (10%)
35	A86	N	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.68	15 (29%)
35	A86	K	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.26	13 (25%)
35	A86	C	204	-	44,50,50	1.84	14 (31%)	51,76,76	2.68	16 (31%)
36	CLA	R	314	16	46,54,73	1.74	8 (17%)	53,90,113	1.91	11 (20%)
36	CLA	a	816	-	65,73,73	1.69	9 (13%)	76,113,113	2.11	16 (21%)
35	A86	V	303	35	44,50,50	1.28	4 (9%)	51,76,76	3.25	22 (43%)
36	CLA	R	320	16	45,53,73	1.80	8 (17%)	52,89,113	1.86	14 (26%)
36	CLA	a	831	-	65,73,73	1.42	10 (15%)	76,113,113	1.38	9 (11%)
36	CLA	N	316	14	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
36	CLA	b	825	-	65,73,73	1.40	9 (13%)	76,113,113	1.54	10 (13%)
35	A86	P	306	-	44,50,50	1.22	3 (6%)	51,76,76	1.89	13 (25%)
37	KC1	P	317	15	48,53,53	2.81	20 (41%)	55,89,89	5.84	35 (63%)
36	CLA	N	308	14	65,73,73	1.67	7 (10%)	76,113,113	1.84	20 (26%)
41	LHG	D	319	42	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
36	CLA	b	811	-	65,73,73	1.43	8 (12%)	76,113,113	1.63	10 (13%)
36	CLA	a	838	-	65,73,73	1.41	10 (15%)	76,113,113	1.44	9 (11%)
36	CLA	b	814	-	55,63,73	1.52	9 (16%)	64,101,113	1.50	7 (10%)
35	A86	U	304	37,32	44,50,50	1.21	3 (6%)	51,76,76	2.34	19 (37%)
36	CLA	b	828	-	65,73,73	1.45	8 (12%)	76,113,113	1.58	14 (18%)
36	CLA	C	214	-	41,49,73	1.77	9 (21%)	47,84,113	1.72	9 (19%)
34	DD6	O	304	-	39,45,45	1.90	3 (7%)	52,67,67	2.00	14 (26%)
36	CLA	H	316	-	65,73,73	1.45	9 (13%)	76,113,113	1.45	7 (9%)
36	CLA	a	809	-	56,64,73	1.49	9 (16%)	65,102,113	1.51	9 (13%)
41	LHG	G	320	-	39,39,48	1.04	2 (5%)	42,45,54	1.11	3 (7%)
36	CLA	A	311	-	65,73,73	1.42	9 (13%)	76,113,113	1.43	7 (9%)
36	CLA	a	839	46	65,73,73	1.38	8 (12%)	76,113,113	1.49	9 (11%)
39	LMT	K	318	-	36,36,36	0.41	0	47,47,47	0.72	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	E	312	-	65,73,73	1.42	7 (10%)	76,113,113	1.57	9 (11%)
36	CLA	A	310	-	65,73,73	1.40	8 (12%)	76,113,113	1.49	7 (9%)
36	CLA	S	317	-	41,49,73	1.84	6 (14%)	47,84,113	1.70	8 (17%)
35	A86	G	306	-	44,50,50	1.21	4 (9%)	51,76,76	2.34	18 (35%)
36	CLA	X	308	19	47,55,73	3.10	10 (21%)	54,91,113	2.43	19 (35%)
44	BCR	h	201	-	41,41,41	1.26	5 (12%)	56,56,56	1.42	10 (17%)
34	DD6	D	301	-	39,45,45	2.01	3 (7%)	52,67,67	1.99	13 (25%)
36	CLA	M	312	13,36	47,55,73	1.71	9 (19%)	54,91,113	1.71	9 (16%)
44	BCR	i	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	7 (12%)
35	A86	h	202	-	44,50,50	1.24	4 (9%)	51,76,76	1.74	10 (19%)
36	CLA	L	320	12	65,73,73	1.43	7 (10%)	76,113,113	1.44	6 (7%)
36	CLA	N	310	14	41,49,73	1.96	10 (24%)	47,84,113	2.42	15 (31%)
36	CLA	O	316	-	65,73,73	1.83	11 (16%)	76,113,113	2.59	25 (32%)
36	CLA	O	312	-	39,48,73	2.10	10 (25%)	45,82,113	1.56	8 (17%)
36	CLA	M	315	13	47,55,73	1.81	10 (21%)	54,91,113	1.68	8 (14%)
36	CLA	N	312	-	47,55,73	1.62	6 (12%)	54,91,113	1.65	6 (11%)
36	CLA	N	315	-	41,49,73	1.82	6 (14%)	47,84,113	1.98	10 (21%)
34	DD6	j	103	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	12 (23%)
35	A86	K	303	-	44,50,50	1.31	4 (9%)	51,76,76	2.80	17 (33%)
35	A86	Q	301	-	44,50,50	1.33	5 (11%)	51,76,76	2.73	17 (33%)
35	A86	S	301	-	44,50,50	1.46	4 (9%)	51,76,76	3.73	26 (50%)
44	BCR	a	847	-	41,41,41	1.23	4 (9%)	56,56,56	1.25	5 (8%)
35	A86	T	306	-	44,50,50	1.23	4 (9%)	51,76,76	2.88	18 (35%)
36	CLA	b	818	-	55,63,73	1.53	7 (12%)	64,101,113	1.79	11 (17%)
36	CLA	J	308	-	61,69,73	1.47	6 (9%)	71,108,113	1.76	11 (15%)
41	LHG	R	323	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
35	A86	G	305	-	44,50,50	1.23	3 (6%)	51,76,76	2.23	15 (29%)
36	CLA	K	315	-	41,49,73	1.76	7 (17%)	47,84,113	1.86	7 (14%)
36	CLA	T	313	18	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
36	CLA	A	314	-	65,73,73	1.56	9 (13%)	76,113,113	1.92	12 (15%)
36	CLA	R	311	16	65,73,73	1.44	6 (9%)	76,113,113	1.48	8 (10%)
35	A86	X	305	-	44,50,50	1.29	4 (9%)	51,76,76	3.04	18 (35%)
41	LHG	b	850	36	48,48,48	0.92	2 (4%)	51,54,54	1.04	3 (5%)
39	LMT	b	848	-	36,36,36	0.38	0	47,47,47	0.67	1 (2%)
36	CLA	U	309	32	46,54,73	1.84	7 (15%)	53,90,113	1.84	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	A86	J	305	-	44,50,50	1.24	3 (6%)	51,76,76	2.08	15 (29%)
36	CLA	a	835	-	51,59,73	1.65	10 (19%)	59,96,113	1.49	9 (15%)
35	A86	Q	304	-	44,50,50	1.39	6 (13%)	51,76,76	3.30	24 (47%)
41	LHG	j	104	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
36	CLA	a	824	-	65,73,73	1.45	8 (12%)	76,113,113	1.94	18 (23%)
36	CLA	L	311	-	65,73,73	1.42	8 (12%)	76,113,113	1.48	9 (11%)
34	DD6	D	304	-	39,45,45	1.97	3 (7%)	52,67,67	1.91	12 (23%)
36	CLA	b	808	-	65,73,73	1.42	8 (12%)	76,113,113	1.49	10 (13%)
44	BCR	l	207	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	8 (14%)
35	A86	A	302	-	44,50,50	1.61	6 (13%)	51,76,76	4.76	25 (49%)
36	CLA	V	314	-	65,73,73	1.98	14 (21%)	76,113,113	2.97	22 (28%)
36	CLA	b	809	-	65,73,73	1.40	8 (12%)	76,113,113	1.39	7 (9%)
36	CLA	b	813	-	54,62,73	1.58	9 (16%)	67,100,113	1.47	11 (16%)
36	CLA	H	310	8	46,54,73	2.01	10 (21%)	53,90,113	2.83	19 (35%)
36	CLA	O	309	-	65,73,73	1.46	8 (12%)	76,113,113	1.53	10 (13%)
36	CLA	J	312	10	65,73,73	1.43	7 (10%)	76,113,113	1.57	8 (10%)
36	CLA	M	311	13,35	65,73,73	1.47	7 (10%)	76,113,113	1.41	6 (7%)
36	CLA	R	322	16	52,60,73	1.66	7 (13%)	60,97,113	1.77	11 (18%)
36	CLA	H	312	8	65,73,73	1.41	10 (15%)	76,113,113	1.57	13 (17%)
34	DD6	B	302	-	39,45,45	2.01	3 (7%)	52,67,67	2.07	16 (30%)
34	DD6	I	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	15 (28%)
35	A86	B	301	-	44,50,50	1.23	4 (9%)	51,76,76	1.98	13 (25%)
36	CLA	a	837	-	65,73,73	1.38	7 (10%)	76,113,113	1.53	8 (10%)
35	A86	X	304	19	44,50,50	1.34	4 (9%)	51,76,76	3.26	20 (39%)
39	LMT	G	323	-	36,36,36	0.39	0	47,47,47	0.82	0
41	LHG	G	301	-	48,48,48	0.77	2 (4%)	51,54,54	1.28	6 (11%)
41	LHG	D	318	36	45,45,48	0.30	0	48,51,54	0.39	0
41	LHG	E	322	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
36	CLA	A	309	1	46,54,73	1.73	9 (19%)	53,90,113	1.61	6 (11%)
36	CLA	K	311	-	46,54,73	1.75	7 (15%)	53,90,113	1.63	10 (18%)
36	CLA	W	207	34	65,73,73	1.47	6 (9%)	76,113,113	1.52	9 (11%)
36	CLA	l	204	28	49,57,73	2.30	14 (28%)	55,93,113	2.26	17 (30%)
36	CLA	T	316	-	41,49,73	1.82	7 (17%)	47,84,113	1.71	7 (14%)
36	CLA	A	307	-	60,68,73	1.46	7 (11%)	70,107,113	1.50	10 (14%)
36	CLA	a	832	-	65,73,73	1.40	9 (13%)	76,113,113	1.59	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	B	311	2	55,63,73	1.63	6 (10%)	64,101,113	1.79	13 (20%)
39	LMT	F	320	-	36,36,36	0.38	0	47,47,47	0.67	1 (2%)
36	CLA	F	317	6	56,64,73	1.95	13 (23%)	65,102,113	2.70	23 (35%)
36	CLA	X	306	-	61,69,73	1.54	5 (8%)	71,108,113	1.46	8 (11%)
36	CLA	D	313	-	65,73,73	1.36	7 (10%)	76,113,113	1.66	11 (14%)
35	A86	X	301	-	44,50,50	1.55	5 (11%)	51,76,76	3.61	28 (54%)
36	CLA	C	205	-	43,51,73	1.69	7 (16%)	49,86,113	1.74	9 (18%)
36	CLA	C	211	-	65,73,73	1.44	10 (15%)	76,113,113	1.46	8 (10%)
42	LMG	m	102	-	37,37,55	1.08	2 (5%)	45,45,63	1.08	3 (6%)
36	CLA	S	314	17	65,73,73	1.57	9 (13%)	76,113,113	1.56	13 (17%)
39	LMT	B	312	-	36,36,36	0.42	0	47,47,47	0.66	1 (2%)
42	LMG	j	105	-	52,52,55	0.91	2 (3%)	60,60,63	1.00	3 (5%)
44	BCR	b	843	-	41,41,41	1.18	3 (7%)	56,56,56	1.18	5 (8%)
35	A86	H	301	-	44,50,50	1.29	3 (6%)	51,76,76	4.88	20 (39%)
36	CLA	O	310	15	46,54,73	1.72	8 (17%)	53,90,113	1.73	10 (18%)
36	CLA	Q	310	15	65,73,73	2.92	15 (23%)	76,113,113	2.92	21 (27%)
36	CLA	a	817	-	65,73,73	1.38	8 (12%)	76,113,113	1.84	13 (17%)
36	CLA	O	307	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	6 (7%)
37	KC1	M	317	-	48,53,53	2.95	21 (43%)	55,89,89	5.39	34 (61%)
36	CLA	R	319	16	45,53,73	1.75	9 (20%)	52,89,113	2.00	14 (26%)
37	KC1	H	313	-	48,53,53	2.88	21 (43%)	55,89,89	5.03	32 (58%)
36	CLA	b	826	21,46	64,72,73	1.48	10 (15%)	74,111,113	2.11	17 (22%)
36	CLA	T	312	18	46,54,73	1.74	6 (13%)	53,90,113	1.79	11 (20%)
36	CLA	J	311	-	46,54,73	1.74	10 (21%)	53,90,113	1.59	9 (16%)
36	CLA	N	318	-	47,55,73	1.74	6 (12%)	54,91,113	1.84	10 (18%)
44	BCR	a	844	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	5 (8%)
39	LMT	P	321	-	23,23,36	0.43	0	28,28,47	0.61	0
36	CLA	W	216	35,19	45,53,73	2.27	10 (22%)	52,89,113	2.80	14 (26%)
36	CLA	H	309	8	65,73,73	1.44	8 (12%)	76,113,113	1.44	7 (9%)
36	CLA	H	311	-	65,73,73	1.36	7 (10%)	76,113,113	1.59	9 (11%)
36	CLA	B	306	-	46,54,73	1.71	8 (17%)	53,90,113	1.76	8 (15%)
36	CLA	I	309	9	46,54,73	1.74	7 (15%)	53,90,113	2.08	10 (18%)
36	CLA	V	310	33	65,73,73	1.44	7 (10%)	76,113,113	1.43	7 (9%)
36	CLA	E	317	-	46,54,73	1.76	7 (15%)	53,90,113	1.54	7 (13%)
36	CLA	K	309	-	59,67,73	1.53	9 (15%)	68,105,113	1.41	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	BCR	m	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.34	7 (12%)
36	CLA	V	306	33	65,73,73	1.50	6 (9%)	76,113,113	1.62	11 (14%)
34	DD6	L	305	-	39,45,45	2.04	3 (7%)	52,67,67	2.00	15 (28%)
35	A86	P	307	-	44,50,50	1.22	3 (6%)	51,76,76	2.05	13 (25%)
36	CLA	a	814	-	50,58,73	1.62	9 (18%)	58,95,113	1.87	10 (17%)
35	A86	S	308	37	44,50,50	1.23	4 (9%)	51,76,76	2.12	16 (31%)
35	A86	X	302	35	44,50,50	1.22	4 (9%)	51,76,76	2.97	18 (35%)
36	CLA	a	802	-	65,73,73	1.45	7 (10%)	76,113,113	1.83	12 (15%)
37	KC1	C	213	-	48,53,53	2.99	19 (39%)	55,89,89	4.91	31 (56%)
36	CLA	b	801	46	65,73,73	1.46	8 (12%)	76,113,113	1.57	11 (14%)
36	CLA	l	202	28	65,73,73	1.44	9 (13%)	76,113,113	1.40	10 (13%)
36	CLA	I	306	9	65,73,73	1.65	13 (20%)	76,113,113	2.44	22 (28%)
34	DD6	E	301	-	39,45,45	1.98	3 (7%)	52,67,67	1.93	10 (19%)
35	A86	M	302	-	44,50,50	1.29	4 (9%)	51,76,76	2.78	16 (31%)
41	LHG	a	842	-	47,47,48	0.76	1 (2%)	50,53,54	1.27	4 (8%)
34	DD6	A	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	12 (23%)
35	A86	O	303	-	44,50,50	1.34	5 (11%)	51,76,76	2.73	17 (33%)
36	CLA	a	808	20	65,73,73	1.44	10 (15%)	76,113,113	1.50	10 (13%)
34	DD6	C	201	-	39,45,45	2.03	3 (7%)	52,67,67	1.92	13 (25%)
34	DD6	D	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.63	9 (17%)
35	A86	D	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.08	11 (21%)
35	A86	J	303	-	44,50,50	1.41	4 (9%)	51,76,76	2.80	20 (39%)
36	CLA	D	311	-	46,54,73	1.71	9 (19%)	53,90,113	1.63	7 (13%)
36	CLA	i	102	26	65,73,73	1.44	7 (10%)	76,113,113	1.59	8 (10%)
36	CLA	W	214	19	41,49,73	2.04	7 (17%)	47,84,113	2.00	14 (29%)
36	CLA	Q	305	-	61,69,73	1.50	8 (13%)	71,108,113	1.46	6 (8%)
43	PQN	a	840	-	34,34,34	1.58	2 (5%)	42,45,45	1.15	4 (9%)
35	A86	F	304	36	44,50,50	1.25	4 (9%)	51,76,76	2.03	13 (25%)
36	CLA	Q	308	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	10 (13%)
36	CLA	S	320	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
38	SQD	A	315	-	27,28,54	1.50	4 (14%)	36,39,65	1.29	5 (13%)
40	DGD	L	302	42	48,48,67	0.98	2 (4%)	62,62,81	1.05	4 (6%)
36	CLA	b	839	-	65,73,73	1.42	8 (12%)	76,113,113	1.52	9 (11%)
34	DD6	F	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	14 (26%)
34	DD6	R	308	-	39,45,45	2.02	3 (7%)	52,67,67	2.12	13 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	F	309	-	65,73,73	1.42	6 (9%)	76,113,113	1.57	11 (14%)
37	KC1	A	312	1	48,53,53	2.88	19 (39%)	55,89,89	6.87	40 (72%)
36	CLA	b	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.82	13 (17%)
35	A86	R	302	16	44,50,50	1.38	5 (11%)	51,76,76	2.80	15 (29%)
36	CLA	R	318	35	41,49,73	1.83	7 (17%)	47,84,113	1.76	9 (19%)
35	A86	L	319	-	44,50,50	1.43	6 (13%)	51,76,76	3.47	24 (47%)
36	CLA	a	822	-	51,59,73	1.89	8 (15%)	59,96,113	2.05	14 (23%)
35	A86	I	304	-	44,50,50	1.47	4 (9%)	51,76,76	3.38	21 (41%)
41	LHG	f	808	25	48,48,48	0.95	2 (4%)	51,54,54	1.02	3 (5%)
36	CLA	V	305	35	61,69,73	1.66	7 (11%)	71,108,113	1.57	9 (12%)
35	A86	L	306	37	44,50,50	1.24	3 (6%)	51,76,76	2.98	19 (37%)
36	CLA	T	314	-	65,73,73	1.44	7 (10%)	76,113,113	1.68	12 (15%)
37	KC1	G	318	-	48,53,53	2.98	21 (43%)	55,89,89	4.77	36 (65%)
36	CLA	M	314	-	41,49,73	1.81	7 (17%)	47,84,113	1.71	7 (14%)
36	CLA	I	313	-	41,49,73	1.79	7 (17%)	47,84,113	1.73	7 (14%)
36	CLA	F	313	-	52,60,73	1.60	9 (17%)	60,97,113	1.55	8 (13%)
36	CLA	b	836	-	58,66,73	2.01	13 (22%)	67,104,113	3.05	24 (35%)
36	CLA	M	316	36	42,50,73	1.78	8 (19%)	48,85,113	1.61	6 (12%)
35	A86	N	306	-	44,50,50	1.22	3 (6%)	51,76,76	2.83	16 (31%)
36	CLA	a	805	20	65,73,73	1.40	10 (15%)	76,113,113	1.43	9 (11%)
36	CLA	O	311	-	58,66,73	1.51	7 (12%)	67,104,113	1.51	6 (8%)
36	CLA	P	311	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	10 (13%)
36	CLA	D	316	-	52,60,73	1.61	10 (19%)	60,97,113	1.82	13 (21%)
35	A86	Q	316	15,36	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
36	CLA	E	311	-	65,73,73	1.40	7 (10%)	76,113,113	1.47	6 (7%)
36	CLA	P	308	-	61,69,73	1.50	9 (14%)	71,108,113	1.46	6 (8%)
36	CLA	H	306	-	61,69,73	1.48	9 (14%)	71,108,113	1.42	6 (8%)
39	LMT	a	851	-	36,36,36	0.43	0	47,47,47	0.74	1 (2%)
36	CLA	D	307	41	61,69,73	1.45	8 (13%)	71,108,113	1.73	16 (22%)
36	CLA	D	315	-	41,49,73	1.70	7 (17%)	47,84,113	2.05	9 (19%)
39	LMT	E	320	-	36,36,36	0.37	0	47,47,47	0.67	0
36	CLA	M	307	-	65,73,73	1.46	9 (13%)	76,113,113	1.56	9 (11%)
36	CLA	H	305	8	48,56,73	1.71	7 (14%)	55,92,113	1.59	8 (14%)
36	CLA	R	312	-	65,73,73	1.49	9 (13%)	76,113,113	1.59	11 (14%)
40	DGD	C	215	-	58,58,67	0.90	2 (3%)	72,72,81	0.96	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	b	815	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	7 (9%)
36	CLA	W	211	19	65,73,73	1.45	7 (10%)	76,113,113	1.60	11 (14%)
36	CLA	M	309	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
36	CLA	W	208	-	45,53,73	1.75	7 (15%)	52,89,113	1.60	6 (11%)
36	CLA	I	308	9	65,73,73	2.07	15 (23%)	76,113,113	2.55	21 (27%)
37	KC1	R	317	-	48,53,53	2.91	20 (41%)	55,89,89	6.06	36 (65%)
36	CLA	G	311	-	65,73,73	1.40	9 (13%)	76,113,113	1.40	8 (10%)
36	CLA	E	316	-	65,73,73	1.45	6 (9%)	76,113,113	1.63	11 (14%)
36	CLA	K	308	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	8 (10%)
37	KC1	O	315	15	48,53,53	3.07	20 (41%)	55,89,89	6.90	36 (65%)
36	CLA	O	314	-	41,49,73	1.83	8 (19%)	47,84,113	1.80	7 (14%)
39	LMT	I	318	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
36	CLA	b	824	-	53,61,73	2.22	14 (26%)	61,98,113	2.40	22 (36%)
42	LMG	a	852	-	54,54,55	0.90	2 (3%)	62,62,63	1.03	3 (4%)
36	CLA	H	308	8	63,72,73	1.45	8 (12%)	73,112,113	1.44	10 (13%)
36	CLA	R	315	-	65,73,73	1.44	7 (10%)	76,113,113	1.47	7 (9%)
36	CLA	L	316	-	41,49,73	1.81	6 (14%)	47,84,113	1.75	8 (17%)
37	KC1	J	314	-	48,53,53	2.92	19 (39%)	55,89,89	6.21	35 (63%)
36	CLA	b	822	-	46,54,73	1.66	8 (17%)	53,90,113	1.62	9 (16%)
36	CLA	G	316	-	49,57,73	1.66	9 (18%)	55,93,113	1.61	7 (12%)
36	CLA	j	106	27	42,50,73	1.75	9 (21%)	48,85,113	1.74	8 (16%)
37	KC1	F	315	-	48,53,53	2.84	18 (37%)	55,89,89	6.66	33 (60%)
35	A86	R	305	-	44,50,50	1.22	4 (9%)	51,76,76	1.81	11 (21%)
36	CLA	G	315	-	56,64,73	1.92	12 (21%)	65,102,113	2.50	19 (29%)
35	A86	T	303	-	44,50,50	1.22	4 (9%)	51,76,76	3.14	21 (41%)
36	CLA	L	310	-	54,62,73	1.61	7 (12%)	62,99,113	1.41	6 (9%)
41	LHG	O	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.08	3 (6%)
36	CLA	j	101	27	65,73,73	1.40	8 (12%)	76,113,113	1.37	7 (9%)
41	LHG	Q	315	36	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
36	CLA	S	313	-	46,54,73	1.74	6 (13%)	53,90,113	1.99	12 (22%)
36	CLA	P	310	15,41	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
36	CLA	S	318	-	42,50,73	1.83	6 (14%)	48,85,113	1.77	9 (18%)
34	DD6	W	205	-	39,45,45	1.99	3 (7%)	52,67,67	2.03	15 (28%)
34	DD6	J	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.87	12 (23%)
35	A86	F	307	-	44,50,50	1.31	3 (6%)	51,76,76	3.94	22 (43%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	BCR	l	203	-	41,41,41	1.23	4 (9%)	56,56,56	1.21	5 (8%)
36	CLA	N	307	-	61,69,73	1.53	6 (9%)	71,108,113	1.45	6 (8%)
35	A86	R	304	16,36	44,50,50	1.30	3 (6%)	51,76,76	2.95	17 (33%)
44	BCR	b	846	-	41,41,41	1.15	4 (9%)	56,56,56	1.44	10 (17%)
36	CLA	b	840	-	65,73,73	1.40	9 (13%)	76,113,113	1.56	13 (17%)
36	CLA	A	306	-	61,69,73	1.93	13 (21%)	71,108,113	2.41	25 (35%)
35	A86	X	314	19	44,50,50	1.26	4 (9%)	51,76,76	2.07	13 (25%)
37	KC1	S	316	-	48,53,53	3.10	20 (41%)	55,89,89	6.04	36 (65%)
35	A86	F	302	-	44,50,50	1.24	4 (9%)	51,76,76	1.92	11 (21%)
36	CLA	I	312	9	52,60,73	1.67	8 (15%)	60,97,113	1.50	7 (11%)
35	A86	M	305	-	44,50,50	1.34	4 (9%)	51,76,76	2.88	15 (29%)
37	KC1	G	308	-	48,53,53	2.94	21 (43%)	55,89,89	5.62	35 (63%)
44	BCR	a	845	-	41,41,41	1.18	2 (4%)	56,56,56	1.19	5 (8%)
37	KC1	P	315	35	48,53,53	3.07	21 (43%)	55,89,89	6.91	36 (65%)
39	LMT	P	320	-	23,23,36	0.43	0	28,28,47	0.62	0
35	A86	V	302	-	44,50,50	1.32	4 (9%)	51,76,76	2.92	21 (41%)
42	LMG	h	206	-	45,45,55	0.99	2 (4%)	53,53,63	1.03	3 (5%)
36	CLA	U	313	-	41,49,73	1.87	7 (17%)	47,84,113	1.92	11 (23%)
36	CLA	S	312	17	65,73,73	1.46	7 (10%)	76,113,113	1.50	9 (11%)
36	CLA	K	310	-	62,70,73	1.98	16 (25%)	72,109,113	2.51	26 (36%)
36	CLA	j	102	-	65,73,73	1.77	10 (15%)	76,113,113	2.26	18 (23%)
36	CLA	R	310	-	61,69,73	1.51	8 (13%)	71,108,113	1.51	6 (8%)
36	CLA	G	312	7	58,66,73	1.48	10 (17%)	67,104,113	1.57	8 (11%)
36	CLA	N	319	14	42,50,73	3.74	14 (33%)	48,85,113	6.10	30 (62%)
37	KC1	L	315	12,35	48,53,53	3.06	19 (39%)	55,89,89	6.27	36 (65%)
44	BCR	b	844	-	41,41,41	1.11	3 (7%)	56,56,56	1.31	5 (8%)
36	CLA	V	308	-	65,73,73	1.43	7 (10%)	76,113,113	1.50	9 (11%)
36	CLA	D	317	-	58,66,73	1.52	8 (13%)	67,104,113	1.50	8 (11%)
39	LMT	E	323	-	36,36,36	0.35	0	47,47,47	0.82	1 (2%)
36	CLA	X	312	-	41,49,73	1.81	7 (17%)	47,84,113	1.95	8 (17%)
35	A86	J	306	-	44,50,50	1.25	3 (6%)	51,76,76	1.96	11 (21%)
35	A86	S	302	-	44,50,50	1.20	3 (6%)	51,76,76	2.68	15 (29%)
36	CLA	b	806	-	65,73,73	1.42	9 (13%)	76,113,113	1.76	12 (15%)
36	CLA	a	823	-	55,63,73	1.95	11 (20%)	64,101,113	2.18	18 (28%)
36	CLA	h	203	-	65,73,73	1.40	8 (12%)	76,113,113	1.59	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	W	201	19	48,56,73	1.72	7 (14%)	55,92,113	1.57	7 (12%)
36	CLA	M	310	13,35	46,54,73	2.28	10 (21%)	53,90,113	1.84	13 (24%)
35	A86	H	304	-	44,50,50	1.24	4 (9%)	51,76,76	2.31	17 (33%)
36	CLA	T	309	18	65,73,73	1.45	7 (10%)	76,113,113	1.51	9 (11%)
34	DD6	Q	302	-	39,45,45	2.04	3 (7%)	52,67,67	2.04	16 (30%)
35	A86	M	301	-	44,50,50	1.36	4 (9%)	51,76,76	3.39	22 (43%)
35	A86	N	305	-	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
37	KC1	N	314	14	48,53,53	3.16	22 (45%)	55,89,89	4.92	33 (60%)
37	KC1	W	213	-	48,53,53	3.12	20 (41%)	55,89,89	5.79	34 (61%)
34	DD6	S	307	-	39,45,45	2.03	3 (7%)	52,67,67	2.07	15 (28%)
36	CLA	f	802	-	65,73,73	1.51	8 (12%)	76,113,113	1.43	10 (13%)
35	A86	W	203	36	44,50,50	1.37	4 (9%)	51,76,76	2.83	20 (39%)
34	DD6	E	303	-	39,45,45	2.00	3 (7%)	52,67,67	2.00	10 (19%)
34	DD6	H	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.97	12 (23%)
36	CLA	F	312	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	8 (10%)
45	SF4	c	101	22	0,12,12	-	-	-	-	-
34	DD6	K	305	-	39,45,45	2.00	3 (7%)	52,67,67	2.00	14 (26%)
36	CLA	a	818	-	65,73,73	1.40	10 (15%)	76,113,113	1.71	10 (13%)
34	DD6	M	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.96	11 (21%)
35	A86	G	304	-	44,50,50	1.43	5 (11%)	51,76,76	3.69	25 (49%)
36	CLA	a	803	36	55,63,73	1.53	8 (14%)	64,101,113	1.72	12 (18%)
36	CLA	C	212	35	65,73,73	1.38	8 (12%)	76,113,113	1.68	12 (15%)
35	A86	K	302	-	44,50,50	1.38	4 (9%)	51,76,76	3.29	20 (39%)
36	CLA	C	209	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	9 (11%)
36	CLA	B	305	2	65,73,73	1.44	7 (10%)	76,113,113	1.50	9 (11%)
36	CLA	a	834	20	45,53,73	1.75	7 (15%)	52,89,113	1.70	8 (15%)
36	CLA	B	308	-	65,73,73	1.41	7 (10%)	76,113,113	1.64	12 (15%)
36	CLA	I	314	-	41,49,73	1.84	7 (17%)	47,84,113	1.68	6 (12%)
39	LMT	K	317	-	32,32,36	0.43	0	43,43,47	0.70	0
36	CLA	M	308	-	52,60,73	1.65	10 (19%)	60,97,113	1.71	9 (15%)
36	CLA	N	317	14	54,62,73	1.64	6 (11%)	62,99,113	1.66	9 (14%)
35	A86	T	307	-	44,50,50	1.24	3 (6%)	51,76,76	3.14	21 (41%)
35	A86	R	301	-	44,50,50	1.47	4 (9%)	51,76,76	3.48	24 (47%)
36	CLA	E	314	-	65,73,73	1.36	8 (12%)	76,113,113	1.66	13 (17%)
36	CLA	J	310	-	65,73,73	1.39	7 (10%)	76,113,113	1.50	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	U	310	-	65,73,73	1.48	7 (10%)	76,113,113	1.62	13 (17%)
36	CLA	a	826	-	65,73,73	1.40	7 (10%)	76,113,113	1.65	9 (11%)
35	A86	F	305	-	44,50,50	1.35	6 (13%)	51,76,76	2.84	20 (39%)
36	CLA	H	314	-	41,49,73	1.74	8 (19%)	47,84,113	1.95	7 (14%)
35	A86	L	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.01	14 (27%)
35	A86	T	305	18	44,50,50	1.48	5 (11%)	51,76,76	3.68	22 (43%)
37	KC1	T	315	-	48,53,53	3.05	19 (39%)	55,89,89	5.84	34 (61%)
35	A86	U	303	36	44,50,50	1.23	4 (9%)	51,76,76	2.00	14 (27%)
37	KC1	V	312	33	48,53,53	3.13	21 (43%)	55,89,89	5.51	34 (61%)
36	CLA	K	313	-	65,73,73	1.44	9 (13%)	76,113,113	1.62	10 (13%)
36	CLA	I	310	35	65,73,73	1.39	7 (10%)	76,113,113	1.55	7 (9%)
36	CLA	X	310	19	41,49,73	1.88	7 (17%)	47,84,113	2.18	11 (23%)
36	CLA	U	307	-	50,58,73	1.68	8 (16%)	58,95,113	1.51	6 (10%)
37	KC1	M	313	13,36	48,53,53	2.95	20 (41%)	55,89,89	6.15	36 (65%)
36	CLA	P	309	41	65,73,73	1.44	8 (12%)	76,113,113	1.48	6 (7%)
35	A86	N	301	-	44,50,50	1.46	4 (9%)	51,76,76	3.73	26 (50%)
35	A86	S	304	-	44,50,50	1.24	4 (9%)	51,76,76	2.13	16 (31%)
36	CLA	I	311	9	65,73,73	1.36	7 (10%)	76,113,113	1.64	9 (11%)
36	CLA	W	212	19	65,73,73	1.48	6 (9%)	76,113,113	1.75	10 (13%)
36	CLA	W	209	19	57,65,73	1.59	7 (12%)	66,103,113	1.55	10 (15%)
34	DD6	A	301	-	39,45,45	2.04	3 (7%)	52,67,67	2.08	15 (28%)
35	A86	C	202	3,36	44,50,50	1.40	5 (11%)	51,76,76	3.09	17 (33%)
41	LHG	a	850	-	46,46,48	0.96	2 (4%)	49,52,54	1.04	3 (6%)
37	KC1	Q	311	15	48,53,53	3.07	20 (41%)	55,89,89	6.90	36 (65%)
43	PQN	b	842	-	34,34,34	1.56	2 (5%)	42,45,45	1.19	4 (9%)
36	CLA	S	309	-	61,69,73	1.53	8 (13%)	71,108,113	1.41	8 (11%)
36	CLA	S	311	35	46,54,73	1.81	9 (19%)	53,90,113	1.64	10 (18%)
35	A86	R	309	-	44,50,50	1.23	4 (9%)	51,76,76	2.84	16 (31%)
35	A86	S	303	17	44,50,50	1.32	5 (11%)	51,76,76	3.30	22 (43%)
36	CLA	G	309	7	65,73,73	1.38	8 (12%)	76,113,113	1.95	14 (18%)
41	LHG	a	843	36	26,26,48	1.24	2 (7%)	29,32,54	1.31	2 (6%)
41	LHG	F	318	-	32,32,48	0.88	1 (3%)	36,37,54	1.72	6 (16%)
36	CLA	X	309	19	44,53,73	1.82	6 (13%)	50,89,113	1.83	12 (24%)
35	A86	T	301	36	44,50,50	1.25	4 (9%)	51,76,76	2.07	16 (31%)
36	CLA	G	307	-	41,50,73	2.21	12 (29%)	46,85,113	3.26	17 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	b	834	-	65,73,73	1.47	8 (12%)	76,113,113	1.41	8 (10%)
39	LMT	B	313	-	36,36,36	0.43	0	47,47,47	0.73	1 (2%)
35	A86	h	204	-	44,50,50	1.23	4 (9%)	51,76,76	2.14	11 (21%)
36	CLA	X	307	35,19	50,58,73	1.76	7 (14%)	58,95,113	1.94	13 (22%)
41	LHG	f	809	-	41,41,48	1.01	2 (4%)	44,47,54	1.09	3 (6%)
36	CLA	b	838	-	47,55,73	1.59	7 (14%)	54,91,113	1.66	8 (14%)
35	A86	W	202	19,36	44,50,50	1.50	6 (13%)	51,76,76	3.63	29 (56%)

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
35	A86	M	304	-	-	14/34/90/90	0/3/3/3
39	LMT	G	322	-	-	17/21/61/61	0/2/2/2
39	LMT	L	303	-	-	10/21/61/61	0/2/2/2
36	CLA	W	215	-	1/1/11/20	4/17/95/115	-
37	KC1	Q	313	-	-	2/15/71/71	-
35	A86	J	302	-	-	5/34/90/90	1/3/3/3
36	CLA	F	310	-	1/1/13/20	10/27/105/115	-
36	CLA	a	829	-	1/1/15/20	13/37/115/115	-
36	CLA	T	308	18	1/1/14/20	8/33/111/115	-
36	CLA	b	816	-	2/2/14/20	17/31/109/115	-
36	CLA	E	310	-	-	7/37/115/115	-
39	LMT	b	851	-	-	7/15/35/61	0/1/1/2
36	CLA	F	311	-	1/1/12/20	8/22/100/115	-
35	A86	S	305	-	-	9/34/90/90	0/3/3/3
36	CLA	M	306	13,37	1/1/13/20	8/25/103/115	-
36	CLA	A	305	1	1/1/11/20	4/18/96/115	-
36	CLA	a	801	-	1/1/15/20	10/37/115/115	-
35	A86	N	303	-	-	4/34/90/90	0/3/3/3
34	DD6	D	303	-	-	9/26/80/80	0/3/3/3
36	CLA	D	309	-	2/2/13/20	6/25/103/115	-
36	CLA	J	307	10	1/1/14/20	9/33/111/115	-
36	CLA	J	315	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DD6	W	204	36	-	7/26/80/80	0/3/3/3
37	KC1	U	312	35,32	-	4/15/71/71	-
36	CLA	D	306	4	1/1/11/20	4/13/91/115	-
36	CLA	K	312	-	1/1/15/20	6/37/115/115	-
36	CLA	H	315	8	1/1/15/20	14/37/115/115	-
36	CLA	J	317	10	1/1/11/20	3/16/94/115	-
36	CLA	l	206	46	1/1/12/20	6/19/97/115	-
36	CLA	a	827	-	1/1/14/20	14/34/112/115	-
42	LMG	E	318	-	-	24/41/61/70	0/1/1/1
34	DD6	E	306	-	-	4/26/80/80	0/3/3/3
36	CLA	A	308	-	1/1/15/20	13/37/115/115	-
36	CLA	I	307	-	1/1/12/20	4/24/102/115	-
36	CLA	a	804	-	1/1/15/20	16/37/115/115	-
36	CLA	C	206	-	1/1/14/20	15/33/111/115	-
36	CLA	P	314	-	-	21/31/109/115	-
36	CLA	b	833	-	1/1/13/20	9/29/107/115	-
36	CLA	a	812	-	1/1/15/20	14/37/115/115	-
36	CLA	O	306	-	1/1/14/20	9/33/111/115	-
36	CLA	a	820	-	1/1/15/20	11/37/115/115	-
34	DD6	P	305	-	-	2/26/80/80	0/3/3/3
36	CLA	C	208	-	1/1/15/20	17/37/115/115	-
36	CLA	V	311	33	1/1/15/20	13/37/115/115	-
41	LHG	i	104	-	-	29/50/50/53	-
34	DD6	S	306	-	-	5/26/80/80	0/3/3/3
36	CLA	b	835	-	1/1/11/20	3/13/91/115	-
35	A86	I	302	-	-	7/34/90/90	0/3/3/3
41	LHG	I	316	-	-	30/53/53/53	-
39	LMT	I	317	-	-	13/21/61/61	0/2/2/2
34	DD6	K	304	-	-	2/26/80/80	0/3/3/3
35	A86	O	302	-	-	9/34/90/90	0/3/3/3
36	CLA	L	314	12	1/1/15/20	19/37/115/115	-
36	CLA	X	315	-	-	3/8/86/115	-
36	CLA	G	314	7	1/1/10/20	2/8/86/115	-
35	A86	E	302	-	-	4/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	LMG	D	320	41	-	24/41/61/70	0/1/1/1
36	CLA	I	305	-	2/2/14/20	10/33/111/115	-
36	CLA	b	832	-	1/1/11/20	4/18/96/115	-
36	CLA	N	311	14	1/1/11/20	4/15/93/115	-
36	CLA	O	308	15	1/1/15/20	13/37/115/115	-
36	CLA	L	312	12	-	6/15/93/115	-
36	CLA	b	807	-	1/1/11/20	3/13/91/115	-
36	CLA	b	823	-	1/1/13/20	4/25/103/115	-
35	A86	A	316	-	-	9/34/90/90	0/3/3/3
37	KC1	T	310	-	-	11/15/71/71	-
36	CLA	a	806	-	2/2/15/20	10/37/115/115	-
35	A86	T	304	-	-	0/34/90/90	0/3/3/3
37	KC1	K	314	11	-	5/15/71/71	-
36	CLA	L	308	-	2/2/14/20	20/33/111/115	-
42	LMG	E	319	-	-	23/35/55/70	0/1/1/1
39	LMT	L	318	-	-	13/17/57/61	0/2/2/2
37	KC1	W	217	-	-	4/15/71/71	-
39	LMT	f	807	-	-	7/15/35/61	0/1/1/2
36	CLA	l	201	-	1/1/15/20	16/37/115/115	-
44	BCR	a	846	-	-	7/29/63/63	0/2/2/2
36	CLA	b	837	-	1/1/15/20	8/37/115/115	-
36	CLA	b	812	21	1/1/15/20	6/37/115/115	-
36	CLA	P	312	15	1/1/11/20	7/15/93/115	-
44	BCR	f	806	-	-	9/29/63/63	0/2/2/2
36	CLA	l	205	-	2/2/15/20	14/37/115/115	-
39	LMT	a	854	-	-	16/21/61/61	0/2/2/2
35	A86	O	305	-	-	14/34/90/90	0/3/3/3
36	CLA	C	210	3	1/1/11/20	4/15/93/115	-
36	CLA	E	315	-	2/2/15/20	16/37/115/115	-
42	LMG	D	321	-	-	21/32/52/70	0/1/1/1
45	SF4	b	803	21,20	-	-	0/6/5/5
37	KC1	G	317	-	-	6/15/71/71	-
36	CLA	b	802	-	1/1/15/20	10/37/115/115	-
36	CLA	R	321	16	-	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	E	308	5	1/1/11/20	8/18/96/115	-
36	CLA	a	836	-	1/1/15/20	11/37/115/115	-
41	LHG	F	319	-	-	33/45/45/53	-
44	BCR	f	801	-	-	9/29/63/63	0/2/2/2
36	CLA	D	308	-	1/1/15/20	16/37/115/115	-
36	CLA	S	319	17	1/1/15/20	6/37/115/115	-
38	SQD	b	804	-	-	23/41/61/69	0/1/1/1
35	A86	P	304	-	-	6/34/90/90	0/3/3/3
36	CLA	H	317	8	1/1/15/20	8/37/115/115	-
39	LMT	U	315	-	-	17/21/61/61	0/2/2/2
36	CLA	J	316	-	1/1/11/20	6/15/93/115	-
36	CLA	b	841	41	1/1/15/20	9/37/115/115	-
36	CLA	A	313	-	1/1/10/20	2/8/86/115	-
44	BCR	b	847	-	-	8/29/63/63	0/2/2/2
35	A86	T	302	18	-	7/34/90/90	0/3/3/3
35	A86	Q	303	-	-	8/34/90/90	0/3/3/3
36	CLA	U	305	-	1/1/14/20	11/33/111/115	-
35	A86	L	304	-	-	6/34/90/90	0/3/3/3
44	BCR	i	103	-	-	11/29/63/63	0/2/2/2
35	A86	X	303	36	-	9/34/90/90	0/3/3/3
36	CLA	W	210	-	1/1/11/20	7/15/93/115	-
36	CLA	H	318	-	1/1/12/20	8/19/97/115	-
36	CLA	a	825	-	2/2/15/20	15/37/115/115	-
36	CLA	C	207	-	1/1/15/20	16/37/115/115	-
36	CLA	T	311	18	1/1/15/20	11/37/115/115	-
42	LMG	J	318	-	-	28/50/70/70	0/1/1/1
45	SF4	c	102	-	-	-	0/6/5/5
36	CLA	U	306	32	1/1/15/20	20/37/115/115	-
36	CLA	U	311	32	1/1/15/20	21/37/115/115	-
44	BCR	j	107	-	-	5/29/63/63	0/2/2/2
36	CLA	L	309	12	1/1/15/20	12/37/115/115	-
36	CLA	b	829	-	1/1/15/20	9/37/115/115	-
36	CLA	D	312	-	1/1/15/20	11/37/115/115	-
34	DD6	R	307	-	-	11/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	R	306	-	-	8/34/90/90	0/3/3/3
42	LMG	L	321	40	-	15/28/48/70	0/1/1/1
36	CLA	Q	307	15	1/1/11/20	4/19/97/115	-
36	CLA	P	301	15	1/1/15/20	16/37/115/115	-
36	CLA	a	819	-	1/1/11/20	3/13/91/115	-
34	DD6	B	304	-	-	2/26/80/80	0/3/3/3
36	CLA	P	319	-	1/1/14/20	14/31/109/115	-
36	CLA	R	313	-	1/1/15/20	13/37/115/115	-
36	CLA	Q	309	15	1/1/11/20	7/15/93/115	-
41	LHG	l	208	-	-	34/52/52/53	-
36	CLA	N	309	14	1/1/12/20	7/21/99/115	-
35	A86	V	301	35	-	10/34/90/90	1/3/3/3
34	DD6	G	303	-	-	4/26/80/80	0/3/3/3
36	CLA	b	810	-	1/1/15/20	8/37/115/115	-
41	LHG	G	321	36	-	27/51/51/53	-
36	CLA	b	827	-	1/1/15/20	10/37/115/115	-
34	DD6	E	304	-	-	4/26/80/80	0/3/3/3
35	A86	B	303	-	-	13/34/90/90	0/3/3/3
36	CLA	P	313	-	1/1/15/20	12/37/115/115	-
36	CLA	a	848	36	2/2/15/20	12/37/115/115	-
35	A86	F	306	-	-	0/34/90/90	1/3/3/3
36	CLA	G	319	7	1/1/12/20	8/19/97/115	-
36	CLA	a	841	41	1/1/12/20	7/22/100/115	-
35	A86	P	303	-	-	9/34/90/90	0/3/3/3
36	CLA	W	218	19	1/1/10/20	9/11/89/115	-
36	CLA	Q	306	-	1/1/15/20	14/37/115/115	-
36	CLA	L	313	-	1/1/15/20	8/37/115/115	-
36	CLA	f	804	46	2/2/15/20	10/37/115/115	-
36	CLA	a	830	-	-	10/19/97/115	-
42	LMG	V	315	-	-	24/41/61/70	0/1/1/1
35	A86	K	306	11	-	8/34/90/90	0/3/3/3
35	A86	L	307	-	-	8/34/90/90	1/3/3/3
44	BCR	b	845	-	-	7/29/63/63	0/2/2/2
36	CLA	b	831	-	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	F	316	6	1/1/10/20	1/8/86/115	-
37	KC1	F	308	6	-	7/15/71/71	-
36	CLA	b	805	36	1/1/15/20	16/37/115/115	-
36	CLA	G	313	7	1/1/15/20	16/37/115/115	-
35	A86	E	305	5	-	5/34/90/90	0/3/3/3
35	A86	O	301	-	-	4/34/90/90	0/3/3/3
36	CLA	K	316	-	1/1/15/20	10/37/115/115	-
36	CLA	b	820	21	1/1/14/20	15/31/109/115	-
36	CLA	R	316	-	1/1/11/20	8/15/93/115	-
34	DD6	H	302	-	-	2/26/80/80	0/3/3/3
36	CLA	a	833	-	1/1/12/20	2/19/97/115	-
36	CLA	P	316	-	1/1/10/20	3/8/86/115	-
36	CLA	X	313	19	-	5/10/88/115	-
37	KC1	M	318	-	-	10/15/71/71	-
37	KC1	O	313	15	-	2/15/71/71	-
37	KC1	X	311	-	-	3/15/71/71	-
39	LMT	E	321	-	-	9/15/35/61	0/1/1/2
36	CLA	f	803	-	2/2/15/20	13/37/115/115	-
36	CLA	J	313	-	1/1/15/20	13/37/115/115	-
36	CLA	b	819	-	1/1/13/20	5/30/108/115	-
36	CLA	H	307	8	1/1/14/20	5/31/109/115	-
36	CLA	J	309	-	1/1/15/20	8/37/115/115	-
36	CLA	a	813	-	1/1/11/20	2/13/91/115	-
36	CLA	a	821	-	1/1/11/20	4/18/96/115	-
35	A86	R	303	-	-	7/34/90/90	0/3/3/3
37	KC1	B	310	2	-	3/15/71/71	-
36	CLA	K	307	-	2/2/14/20	21/33/111/115	-
37	KC1	E	309	-	-	5/15/71/71	-
42	LMG	G	324	-	-	31/50/70/70	0/1/1/1
36	CLA	P	318	-	1/1/12/20	7/21/99/115	-
35	A86	U	302	-	-	9/34/90/90	0/3/3/3
35	A86	J	301	-	-	11/34/90/90	0/3/3/3
35	A86	E	307	36	-	3/34/90/90	0/3/3/3
35	A86	N	304	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	a	807	20	1/1/15/20	13/37/115/115	-
36	CLA	Q	314	-	1/1/15/20	22/37/115/115	-
36	CLA	W	206	19	1/1/14/20	10/33/111/115	-
35	A86	O	319	35,36	-	8/34/90/90	0/3/3/3
39	LMT	U	314	-	-	14/21/61/61	0/2/2/2
39	LMT	h	205	-	-	10/21/61/61	0/2/2/2
37	KC1	D	314	4	-	5/15/71/71	-
35	A86	I	301	-	-	10/34/90/90	0/3/3/3
36	CLA	a	815	46	1/1/11/20	5/13/91/115	-
36	CLA	G	310	-	1/1/15/20	5/37/115/115	-
36	CLA	V	313	-	1/1/15/20	13/37/115/115	-
36	CLA	V	309	33	1/1/10/20	2/11/89/115	-
35	A86	V	304	-	-	9/34/90/90	0/3/3/3
34	DD6	a	849	-	-	6/26/80/80	0/3/3/3
36	CLA	S	310	17	1/1/15/20	14/37/115/115	-
36	CLA	P	302	-	-	5/10/88/115	-
41	LHG	O	318	15	-	30/53/53/53	-
36	CLA	a	828	-	1/1/15/20	20/37/115/115	-
36	CLA	U	308	35,32	1/1/13/20	10/27/105/115	-
36	CLA	b	817	-	2/2/13/20	9/30/108/115	-
36	CLA	V	307	-	1/1/12/20	5/21/99/115	-
42	LMG	I	315	-	-	32/50/70/70	0/1/1/1
36	CLA	E	313	-	2/2/15/20	8/37/115/115	-
36	CLA	a	811	-	1/1/12/20	6/24/102/115	-
42	LMG	G	325	-	-	27/50/70/70	0/1/1/1
36	CLA	S	315	17	1/1/10/20	3/11/89/115	-
35	A86	G	302	-	-	7/34/90/90	0/3/3/3
36	CLA	a	810	36	1/1/14/20	15/34/112/115	-
36	CLA	B	309	2	1/1/12/20	6/22/100/115	-
39	LMT	F	321	-	-	11/19/59/61	0/2/2/2
36	CLA	b	821	46	1/1/15/20	11/37/115/115	-
35	A86	U	301	-	-	8/34/90/90	0/3/3/3
35	A86	N	320	-	-	10/34/90/90	0/3/3/3
36	CLA	B	307	-	1/1/11/20	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	C	203	-	-	8/34/90/90	1/3/3/3
36	CLA	F	314	6,35	1/1/15/20	14/37/115/115	-
36	CLA	S	321	-	-	10/22/100/115	-
36	CLA	f	805	25	1/1/12/20	9/22/100/115	-
36	CLA	N	313	14	1/1/10/20	2/8/86/115	-
37	KC1	L	317	-	-	3/15/71/71	-
42	LMG	V	316	-	-	24/41/61/70	0/1/1/1
39	LMT	a	853	-	-	10/18/58/61	0/2/2/2
42	LMG	J	319	-	-	23/39/59/70	0/1/1/1
34	DD6	A	303	-	-	5/26/80/80	0/3/3/3
35	A86	F	301	-	-	4/34/90/90	0/3/3/3
36	CLA	Q	312	-	1/1/10/20	3/8/86/115	-
40	DGD	b	849	-	-	21/49/89/95	0/2/2/2
36	CLA	D	310	-	1/1/15/20	9/37/115/115	-
35	A86	N	302	-	-	6/34/90/90	0/3/3/3
35	A86	K	301	-	-	6/34/90/90	1/3/3/3
35	A86	C	204	-	-	12/34/90/90	0/3/3/3
36	CLA	R	314	16	1/1/11/20	9/15/93/115	-
36	CLA	a	816	-	1/1/15/20	20/37/115/115	-
35	A86	V	303	35	-	8/34/90/90	0/3/3/3
36	CLA	R	320	16	1/1/11/20	3/13/91/115	-
36	CLA	a	831	-	1/1/15/20	14/37/115/115	-
36	CLA	N	316	14	1/1/15/20	11/37/115/115	-
36	CLA	b	825	-	1/1/15/20	13/37/115/115	-
35	A86	P	306	-	-	3/34/90/90	0/3/3/3
37	KC1	P	317	15	-	4/15/71/71	-
36	CLA	N	308	14	1/1/15/20	15/37/115/115	-
41	LHG	D	319	42	-	30/53/53/53	-
36	CLA	b	811	-	1/1/15/20	10/37/115/115	-
36	CLA	a	838	-	1/1/15/20	6/37/115/115	-
36	CLA	b	814	-	1/1/13/20	3/25/103/115	-
35	A86	U	304	37,32	-	11/34/90/90	0/3/3/3
36	CLA	b	828	-	1/1/15/20	14/37/115/115	-
36	CLA	C	214	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DD6	O	304	-	-	5/26/80/80	0/3/3/3
36	CLA	H	316	-	1/1/15/20	16/37/115/115	-
36	CLA	a	809	-	1/1/13/20	9/27/105/115	-
41	LHG	G	320	-	-	18/44/44/53	-
36	CLA	A	311	-	1/1/15/20	18/37/115/115	-
36	CLA	a	839	46	1/1/15/20	15/37/115/115	-
39	LMT	K	318	-	-	12/21/61/61	0/2/2/2
36	CLA	E	312	-	1/1/15/20	15/37/115/115	-
36	CLA	A	310	-	1/1/15/20	11/37/115/115	-
36	CLA	S	317	-	1/1/10/20	3/8/86/115	-
36	CLA	X	308	19	1/1/11/20	10/16/94/115	-
35	A86	G	306	-	-	6/34/90/90	1/3/3/3
44	BCR	h	201	-	-	9/29/63/63	0/2/2/2
34	DD6	D	301	-	-	11/26/80/80	0/3/3/3
36	CLA	M	312	13,36	1/1/11/20	10/16/94/115	-
44	BCR	i	101	-	-	2/29/63/63	0/2/2/2
35	A86	h	202	-	-	3/34/90/90	1/3/3/3
36	CLA	L	320	12	1/1/15/20	11/37/115/115	-
36	CLA	N	310	14	1/1/10/20	1/8/86/115	-
36	CLA	O	316	-	1/1/15/20	26/37/115/115	-
36	CLA	O	312	-	-	4/8/82/115	-
36	CLA	M	315	13	-	6/16/94/115	-
36	CLA	N	312	-	1/1/11/20	7/16/94/115	-
36	CLA	N	315	-	-	0/8/86/115	-
34	DD6	j	103	-	-	9/26/80/80	0/3/3/3
35	A86	K	303	-	-	5/34/90/90	0/3/3/3
35	A86	Q	301	-	-	6/34/90/90	0/3/3/3
35	A86	S	301	-	-	8/34/90/90	0/3/3/3
44	BCR	a	847	-	-	6/29/63/63	0/2/2/2
35	A86	T	306	-	-	6/34/90/90	0/3/3/3
36	CLA	b	818	-	-	4/25/103/115	-
36	CLA	J	308	-	-	12/33/111/115	-
41	LHG	R	323	-	-	29/53/53/53	-
35	A86	G	305	-	-	4/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	K	315	-	1/1/10/20	3/8/86/115	-
36	CLA	T	313	18	1/1/15/20	8/37/115/115	-
36	CLA	A	314	-	1/1/15/20	20/37/115/115	-
36	CLA	R	311	16	1/1/15/20	13/37/115/115	-
35	A86	X	305	-	-	8/34/90/90	0/3/3/3
41	LHG	b	850	36	-	27/53/53/53	-
39	LMT	b	848	-	-	12/21/61/61	0/2/2/2
36	CLA	U	309	32	-	4/15/93/115	-
36	CLA	a	835	-	1/1/12/20	1/21/99/115	-
35	A86	J	305	-	-	6/34/90/90	0/3/3/3
35	A86	Q	304	-	-	10/34/90/90	0/3/3/3
41	LHG	j	104	-	-	32/53/53/53	-
36	CLA	a	824	-	1/1/15/20	11/37/115/115	-
36	CLA	L	311	-	1/1/15/20	14/37/115/115	-
34	DD6	D	304	-	-	8/26/80/80	0/3/3/3
36	CLA	b	808	-	1/1/15/20	12/37/115/115	-
44	BCR	l	207	-	-	7/29/63/63	0/2/2/2
35	A86	A	302	-	-	9/34/90/90	0/3/3/3
36	CLA	V	314	-	1/1/15/20	17/37/115/115	-
36	CLA	b	809	-	1/1/15/20	16/37/115/115	-
36	CLA	b	813	-	1/1/13/20	3/25/101/115	-
36	CLA	H	310	8	1/1/11/20	5/15/93/115	-
36	CLA	O	309	-	1/1/15/20	17/37/115/115	-
36	CLA	J	312	10	1/1/15/20	10/37/115/115	-
36	CLA	M	311	13,35	1/1/15/20	10/37/115/115	-
36	CLA	R	322	16	1/1/12/20	11/22/100/115	-
36	CLA	H	312	8	1/1/15/20	17/37/115/115	-
34	DD6	B	302	-	-	4/26/80/80	0/3/3/3
34	DD6	I	303	-	-	4/26/80/80	0/3/3/3
35	A86	B	301	-	-	10/34/90/90	0/3/3/3
36	CLA	a	837	-	1/1/15/20	10/37/115/115	-
35	A86	X	304	19	-	7/34/90/90	0/3/3/3
39	LMT	G	323	-	-	16/21/61/61	0/2/2/2
41	LHG	G	301	-	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	D	318	36	-	30/50/50/53	-
41	LHG	E	322	-	-	28/53/53/53	-
36	CLA	A	309	1	1/1/11/20	7/15/93/115	-
36	CLA	K	311	-	1/1/11/20	6/15/93/115	-
36	CLA	W	207	34	1/1/15/20	15/37/115/115	-
36	CLA	l	204	28	-	8/18/96/115	-
36	CLA	T	316	-	1/1/10/20	0/8/86/115	-
36	CLA	A	307	-	1/1/14/20	10/31/109/115	-
36	CLA	a	832	-	1/1/15/20	14/37/115/115	-
36	CLA	B	311	2	1/1/13/20	13/25/103/115	-
39	LMT	F	320	-	-	12/21/61/61	0/2/2/2
36	CLA	F	317	6	2/2/13/20	10/27/105/115	-
36	CLA	X	306	-	1/1/14/20	9/33/111/115	-
36	CLA	D	313	-	1/1/15/20	8/37/115/115	-
35	A86	X	301	-	-	8/34/90/90	0/3/3/3
36	CLA	C	205	-	1/1/10/20	2/11/89/115	-
36	CLA	C	211	-	1/1/15/20	11/37/115/115	-
42	LMG	m	102	-	-	14/32/52/70	0/1/1/1
36	CLA	S	314	17	-	9/37/115/115	-
39	LMT	B	312	-	-	14/21/61/61	0/2/2/2
42	LMG	j	105	-	-	31/47/67/70	0/1/1/1
44	BCR	b	843	-	-	9/29/63/63	0/2/2/2
36	CLA	O	310	15	1/1/11/20	7/15/93/115	-
35	A86	H	301	-	-	5/34/90/90	0/3/3/3
36	CLA	Q	310	15	-	20/37/115/115	-
36	CLA	a	817	-	1/1/15/20	15/37/115/115	-
36	CLA	O	307	-	1/1/15/20	14/37/115/115	-
37	KC1	M	317	-	-	3/15/71/71	-
36	CLA	R	319	16	1/1/11/20	5/13/91/115	-
37	KC1	H	313	-	-	6/15/71/71	-
36	CLA	b	826	21,46	1/1/14/20	10/36/114/115	-
36	CLA	T	312	18	1/1/11/20	5/15/93/115	-
36	CLA	J	311	-	1/1/11/20	3/15/93/115	-
36	CLA	N	318	-	1/1/11/20	5/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	BCR	a	844	-	-	6/29/63/63	0/2/2/2
39	LMT	P	321	-	-	10/14/34/61	0/1/1/2
36	CLA	W	216	35,19	1/1/11/20	3/13/91/115	-
36	CLA	H	309	8	1/1/15/20	15/37/115/115	-
36	CLA	H	311	-	1/1/15/20	9/37/115/115	-
36	CLA	B	306	-	1/1/11/20	4/15/93/115	-
36	CLA	I	309	9	1/1/11/20	6/15/93/115	-
36	CLA	V	310	33	1/1/15/20	8/37/115/115	-
36	CLA	E	317	-	1/1/11/20	5/15/93/115	-
36	CLA	K	309	-	1/1/13/20	12/30/108/115	-
44	BCR	m	101	-	-	9/29/63/63	0/2/2/2
36	CLA	V	306	33	1/1/15/20	19/37/115/115	-
34	DD6	L	305	-	-	7/26/80/80	0/3/3/3
36	CLA	a	814	-	1/1/12/20	2/19/97/115	-
35	A86	P	307	-	-	2/34/90/90	0/3/3/3
35	A86	S	308	37	-	12/34/90/90	0/3/3/3
35	A86	X	302	35	-	6/34/90/90	0/3/3/3
36	CLA	a	802	-	2/2/15/20	11/37/115/115	-
37	KC1	C	213	-	-	6/15/71/71	-
36	CLA	b	801	46	1/1/15/20	8/37/115/115	-
36	CLA	l	202	28	1/1/15/20	11/37/115/115	-
36	CLA	I	306	9	2/2/15/20	15/37/115/115	-
34	DD6	E	301	-	-	4/26/80/80	0/3/3/3
35	A86	M	302	-	-	7/34/90/90	0/3/3/3
41	LHG	a	842	-	-	24/52/52/53	-
34	DD6	A	304	-	-	4/26/80/80	0/3/3/3
35	A86	O	303	-	-	6/34/90/90	0/3/3/3
36	CLA	a	808	20	1/1/15/20	9/37/115/115	-
34	DD6	C	201	-	-	7/26/80/80	0/3/3/3
34	DD6	D	305	-	-	3/26/80/80	0/3/3/3
35	A86	D	302	-	-	7/34/90/90	0/3/3/3
36	CLA	i	102	26	1/1/15/20	20/37/115/115	-
35	A86	J	303	-	-	7/34/90/90	0/3/3/3
36	CLA	D	311	-	-	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	W	214	19	-	3/8/86/115	-
36	CLA	Q	305	-	1/1/14/20	9/33/111/115	-
43	PQN	a	840	-	-	7/23/43/43	0/2/2/2
35	A86	F	304	36	-	4/34/90/90	0/3/3/3
36	CLA	Q	308	-	1/1/15/20	18/37/115/115	-
36	CLA	S	320	-	-	16/37/115/115	-
38	SQD	A	315	-	-	11/22/42/69	0/1/1/1
40	DGD	L	302	42	-	21/36/76/95	0/2/2/2
36	CLA	b	839	-	1/1/15/20	4/37/115/115	-
34	DD6	F	303	-	-	8/26/80/80	0/3/3/3
34	DD6	R	308	-	-	10/26/80/80	0/3/3/3
36	CLA	F	309	-	1/1/15/20	13/37/115/115	-
37	KC1	A	312	1	-	2/15/71/71	-
36	CLA	b	830	-	1/1/15/20	5/37/115/115	-
36	CLA	R	318	35	1/1/10/20	2/8/86/115	-
35	A86	R	302	16	-	6/34/90/90	0/3/3/3
35	A86	L	319	-	-	9/34/90/90	0/3/3/3
36	CLA	a	822	-	1/1/12/20	4/21/99/115	-
35	A86	I	304	-	-	9/34/90/90	0/3/3/3
41	LHG	f	808	25	-	29/53/53/53	-
36	CLA	V	305	35	1/1/14/20	11/33/111/115	-
35	A86	L	306	37	-	10/34/90/90	0/3/3/3
36	CLA	T	314	-	1/1/15/20	15/37/115/115	-
37	KC1	G	318	-	-	5/15/71/71	-
36	CLA	M	314	-	1/1/10/20	2/8/86/115	-
36	CLA	I	313	-	1/1/10/20	3/8/86/115	-
36	CLA	F	313	-	1/1/12/20	6/22/100/115	-
36	CLA	b	836	-	1/1/13/20	8/29/107/115	-
36	CLA	M	316	36	1/1/10/20	4/10/88/115	-
35	A86	N	306	-	-	8/34/90/90	0/3/3/3
36	CLA	a	805	20	1/1/15/20	16/37/115/115	-
36	CLA	O	311	-	1/1/13/20	9/29/107/115	-
36	CLA	P	311	-	1/1/15/20	17/37/115/115	-
36	CLA	D	316	-	1/1/12/20	9/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	Q	316	15,36	-	2/34/90/90	0/3/3/3
36	CLA	E	311	-	1/1/15/20	16/37/115/115	-
36	CLA	P	308	-	1/1/14/20	9/33/111/115	-
36	CLA	H	306	-	1/1/14/20	6/33/111/115	-
39	LMT	a	851	-	-	15/21/61/61	0/2/2/2
36	CLA	D	307	41	1/1/14/20	17/33/111/115	-
36	CLA	D	315	-	1/1/10/20	2/8/86/115	-
39	LMT	E	320	-	-	13/21/61/61	0/2/2/2
36	CLA	M	307	-	1/1/15/20	12/37/115/115	-
36	CLA	H	305	8	1/1/11/20	8/17/95/115	-
36	CLA	R	312	-	1/1/15/20	12/37/115/115	-
40	DGD	C	215	-	-	31/46/86/95	0/2/2/2
36	CLA	b	815	-	1/1/15/20	19/37/115/115	-
36	CLA	W	211	19	1/1/15/20	8/37/115/115	-
36	CLA	M	309	-	1/1/15/20	13/37/115/115	-
36	CLA	W	208	-	1/1/11/20	5/13/91/115	-
36	CLA	I	308	9	1/1/15/20	19/37/115/115	-
37	KC1	R	317	-	-	3/15/71/71	-
36	CLA	G	311	-	1/1/15/20	17/37/115/115	-
36	CLA	E	316	-	1/1/15/20	17/37/115/115	-
36	CLA	K	308	-	1/1/15/20	11/37/115/115	-
37	KC1	O	315	15	-	2/15/71/71	-
36	CLA	O	314	-	1/1/10/20	3/8/86/115	-
39	LMT	I	318	-	-	17/21/61/61	0/2/2/2
36	CLA	b	824	-	1/1/12/20	12/23/101/115	-
42	LMG	a	852	-	-	26/49/69/70	0/1/1/1
36	CLA	H	308	8	1/1/15/20	15/35/113/115	-
36	CLA	R	315	-	1/1/15/20	11/37/115/115	-
36	CLA	L	316	-	1/1/10/20	1/8/86/115	-
37	KC1	J	314	-	-	4/15/71/71	-
36	CLA	b	822	-	1/1/11/20	5/15/93/115	-
36	CLA	G	316	-	1/1/11/20	8/18/96/115	-
36	CLA	j	106	27	1/1/10/20	6/10/88/115	-
37	KC1	F	315	-	-	3/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	R	305	-	-	5/34/90/90	0/3/3/3
36	CLA	G	315	-	2/2/13/20	11/27/105/115	-
35	A86	T	303	-	-	6/34/90/90	0/3/3/3
36	CLA	L	310	-	1/1/12/20	2/24/102/115	-
41	LHG	O	317	-	-	33/46/46/53	-
36	CLA	j	101	27	1/1/15/20	17/37/115/115	-
41	LHG	Q	315	36	-	33/53/53/53	-
36	CLA	S	313	-	1/1/11/20	6/15/93/115	-
36	CLA	P	310	15,41	1/1/15/20	11/37/115/115	-
36	CLA	S	318	-	1/1/10/20	7/10/88/115	-
34	DD6	J	304	-	-	5/26/80/80	0/3/3/3
34	DD6	W	205	-	-	8/26/80/80	0/3/3/3
35	A86	F	307	-	-	6/34/90/90	0/3/3/3
44	BCR	l	203	-	-	10/29/63/63	0/2/2/2
36	CLA	N	307	-	1/1/14/20	7/33/111/115	-
35	A86	R	304	16,36	-	8/34/90/90	0/3/3/3
44	BCR	b	846	-	-	8/29/63/63	0/2/2/2
36	CLA	b	840	-	1/1/15/20	12/37/115/115	-
36	CLA	A	306	-	2/2/14/20	19/33/111/115	-
35	A86	X	314	19	-	3/34/90/90	1/3/3/3
37	KC1	S	316	-	-	6/15/71/71	-
35	A86	F	302	-	-	8/34/90/90	0/3/3/3
36	CLA	I	312	9	1/1/12/20	4/22/100/115	-
35	A86	M	305	-	-	8/34/90/90	0/3/3/3
37	KC1	G	308	-	-	5/15/71/71	-
44	BCR	a	845	-	-	9/29/63/63	0/2/2/2
37	KC1	P	315	35	-	2/15/71/71	-
39	LMT	P	320	-	-	8/14/34/61	0/1/1/2
35	A86	V	302	-	-	5/34/90/90	0/3/3/3
42	LMG	h	206	-	-	24/40/60/70	0/1/1/1
36	CLA	U	313	-	1/1/10/20	2/8/86/115	-
36	CLA	S	312	17	-	17/37/115/115	-
36	CLA	K	310	-	2/2/14/20	14/34/112/115	-
36	CLA	j	102	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	R	310	-	1/1/14/20	16/33/111/115	-
36	CLA	G	312	7	1/1/13/20	4/29/107/115	-
36	CLA	N	319	14	1/1/10/20	3/10/88/115	-
37	KC1	L	315	12,35	-	6/15/71/71	-
44	BCR	b	844	-	-	6/29/63/63	0/2/2/2
36	CLA	V	308	-	1/1/15/20	18/37/115/115	-
36	CLA	D	317	-	1/1/13/20	10/29/107/115	-
39	LMT	E	323	-	-	11/21/61/61	0/2/2/2
36	CLA	X	312	-	1/1/10/20	3/8/86/115	-
35	A86	J	306	-	-	10/34/90/90	0/3/3/3
35	A86	S	302	-	-	6/34/90/90	0/3/3/3
36	CLA	b	806	-	1/1/15/20	14/37/115/115	-
36	CLA	a	823	-	2/2/13/20	10/25/103/115	-
36	CLA	h	203	-	1/1/15/20	20/37/115/115	-
36	CLA	W	201	19	1/1/11/20	2/17/95/115	-
36	CLA	M	310	13,35	1/1/11/20	5/15/93/115	-
36	CLA	T	309	18	1/1/15/20	18/37/115/115	-
35	A86	H	304	-	-	8/34/90/90	0/3/3/3
34	DD6	Q	302	-	-	8/26/80/80	0/3/3/3
35	A86	M	301	-	-	8/34/90/90	0/3/3/3
35	A86	N	305	-	-	2/34/90/90	0/3/3/3
37	KC1	N	314	14	-	7/15/71/71	-
37	KC1	W	213	-	-	5/15/71/71	-
34	DD6	S	307	-	-	6/26/80/80	0/3/3/3
36	CLA	f	802	-	1/1/15/20	16/37/115/115	-
35	A86	W	203	36	-	6/34/90/90	0/3/3/3
34	DD6	E	303	-	-	7/26/80/80	0/3/3/3
34	DD6	H	303	-	-	6/26/80/80	0/3/3/3
36	CLA	F	312	-	1/1/15/20	20/37/115/115	-
45	SF4	c	101	22	-	-	0/6/5/5
36	CLA	a	818	-	1/1/15/20	14/37/115/115	-
34	DD6	K	305	-	-	0/26/80/80	0/3/3/3
34	DD6	M	303	-	-	3/26/80/80	0/3/3/3
35	A86	G	304	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	a	803	36	1/1/13/20	5/25/103/115	-
36	CLA	C	212	35	1/1/15/20	23/37/115/115	-
35	A86	K	302	-	-	8/34/90/90	0/3/3/3
36	CLA	C	209	-	1/1/15/20	10/37/115/115	-
36	CLA	B	305	2	1/1/15/20	24/37/115/115	-
36	CLA	a	834	20	1/1/11/20	5/13/91/115	-
36	CLA	B	308	-	1/1/15/20	14/37/115/115	-
36	CLA	I	314	-	1/1/10/20	0/8/86/115	-
39	LMT	K	317	-	-	14/17/57/61	0/2/2/2
36	CLA	M	308	-	1/1/12/20	5/22/100/115	-
36	CLA	N	317	14	1/1/12/20	8/24/102/115	-
35	A86	T	307	-	-	9/34/90/90	0/3/3/3
35	A86	R	301	-	-	9/34/90/90	0/3/3/3
36	CLA	E	314	-	1/1/15/20	8/37/115/115	-
36	CLA	J	310	-	1/1/15/20	11/37/115/115	-
36	CLA	U	310	-	1/1/15/20	17/37/115/115	-
36	CLA	a	826	-	1/1/15/20	12/37/115/115	-
36	CLA	H	314	-	1/1/10/20	3/8/86/115	-
35	A86	F	305	-	-	8/34/90/90	0/3/3/3
35	A86	L	301	-	-	5/34/90/90	1/3/3/3
35	A86	T	305	18	-	7/34/90/90	0/3/3/3
37	KC1	T	315	-	-	7/15/71/71	-
35	A86	U	303	36	-	17/34/90/90	0/3/3/3
37	KC1	V	312	33	-	7/15/71/71	-
36	CLA	K	313	-	1/1/15/20	13/37/115/115	-
36	CLA	U	307	-	1/1/12/20	1/19/97/115	-
36	CLA	I	310	35	1/1/15/20	10/37/115/115	-
36	CLA	X	310	19	1/1/10/20	2/8/86/115	-
37	KC1	M	313	13,36	-	5/15/71/71	-
36	CLA	P	309	41	1/1/15/20	14/37/115/115	-
35	A86	N	301	-	-	8/34/90/90	0/3/3/3
35	A86	S	304	-	-	9/34/90/90	0/3/3/3
36	CLA	I	311	9	1/1/15/20	17/37/115/115	-
36	CLA	W	212	19	-	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	W	209	19	1/1/13/20	13/28/106/115	-
34	DD6	A	301	-	-	7/26/80/80	0/3/3/3
35	A86	C	202	3,36	-	8/34/90/90	0/3/3/3
41	LHG	a	850	-	-	36/51/51/53	-
37	KC1	Q	311	15	-	2/15/71/71	-
43	PQN	b	842	-	-	11/23/43/43	0/2/2/2
36	CLA	S	309	-	1/1/14/20	8/33/111/115	-
36	CLA	S	311	35	1/1/11/20	2/15/93/115	-
35	A86	R	309	-	-	8/34/90/90	0/3/3/3
35	A86	S	303	17	-	4/34/90/90	0/3/3/3
36	CLA	G	309	7	1/1/15/20	13/37/115/115	-
41	LHG	a	843	36	-	10/31/31/53	-
41	LHG	F	318	-	-	15/34/34/53	-
36	CLA	X	309	19	-	6/13/91/115	-
35	A86	T	301	36	-	4/34/90/90	1/3/3/3
36	CLA	G	307	-	-	2/9/87/115	-
36	CLA	b	834	-	1/1/15/20	10/37/115/115	-
39	LMT	B	313	-	-	16/21/61/61	0/2/2/2
35	A86	h	204	-	-	1/34/90/90	0/3/3/3
36	CLA	X	307	35,19	-	6/19/97/115	-
41	LHG	f	809	-	-	28/46/46/53	-
36	CLA	b	838	-	1/1/11/20	3/16/94/115	-
35	A86	W	202	19,36	-	8/34/90/90	0/3/3/3

All (4148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	M	318	KC1	C4C-NC	17.10	1.63	1.37
36	Q	310	CLA	CAA-C2A	15.78	1.83	1.54
37	M	318	KC1	C1A-NA	15.77	1.68	1.38
37	T	310	KC1	C1A-NA	14.39	1.66	1.38
36	X	308	CLA	C4B-NB	13.90	1.47	1.35
37	T	310	KC1	C4C-NC	13.45	1.57	1.37
36	X	313	CLA	C4B-NB	13.27	1.47	1.35
35	N	304	A86	C19-C18	-13.20	1.33	1.52
36	N	319	CLA	C1D-C2D	12.32	1.69	1.45
36	X	308	CLA	C1B-NB	-12.24	1.24	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	P	319	CLA	C4B-NB	12.01	1.45	1.35
34	D	303	DD6	C2-C1	11.88	1.51	1.35
36	N	319	CLA	C1D-ND	11.78	1.52	1.37
37	M	318	KC1	C4D-ND	10.90	1.44	1.35
35	N	304	A86	C19-C20	9.83	1.66	1.52
37	M	318	KC1	C3C-C2C	9.71	1.57	1.36
37	M	318	KC1	C4D-CHA	9.59	1.57	1.45
37	T	310	KC1	C4D-CHA	9.57	1.57	1.45
36	N	319	CLA	C4B-NB	9.37	1.43	1.35
37	M	318	KC1	C2A-C3A	9.35	1.56	1.37
37	T	310	KC1	C2A-C3A	9.21	1.55	1.37
37	M	318	KC1	C4C-C3C	8.87	1.60	1.45
36	N	308	CLA	C4B-NB	8.77	1.43	1.35
34	A	301	DD6	C29-C27	-8.76	1.25	1.42
34	L	305	DD6	C29-C27	-8.72	1.25	1.42
34	Q	302	DD6	C29-C27	-8.71	1.25	1.42
34	M	303	DD6	C29-C27	-8.69	1.25	1.42
34	E	306	DD6	C29-C27	-8.68	1.25	1.42
34	W	204	DD6	C29-C27	-8.65	1.25	1.42
34	C	201	DD6	C29-C27	-8.65	1.25	1.42
34	S	307	DD6	C29-C27	-8.64	1.25	1.42
34	a	849	DD6	C29-C27	-8.63	1.25	1.42
34	D	301	DD6	C29-C27	-8.61	1.26	1.42
34	K	304	DD6	C29-C27	-8.60	1.26	1.42
34	P	305	DD6	C29-C27	-8.60	1.26	1.42
34	D	305	DD6	C29-C27	-8.60	1.26	1.42
34	E	303	DD6	C29-C27	-8.59	1.26	1.42
34	J	304	DD6	C29-C27	-8.59	1.26	1.42
34	I	303	DD6	C29-C27	-8.58	1.26	1.42
34	R	308	DD6	C29-C27	-8.58	1.26	1.42
34	A	304	DD6	C29-C27	-8.55	1.26	1.42
34	A	303	DD6	C29-C27	-8.54	1.26	1.42
34	R	307	DD6	C29-C27	-8.52	1.26	1.42
34	H	303	DD6	C29-C27	-8.51	1.26	1.42
34	B	302	DD6	C29-C27	-8.51	1.26	1.42
34	B	304	DD6	C29-C27	-8.51	1.26	1.42
34	F	303	DD6	C29-C27	-8.50	1.26	1.42
34	K	305	DD6	C29-C27	-8.50	1.26	1.42
34	W	205	DD6	C29-C27	-8.50	1.26	1.42
34	G	303	DD6	C29-C27	-8.49	1.26	1.42
34	E	304	DD6	C29-C27	-8.48	1.26	1.42
34	j	103	DD6	C29-C27	-8.48	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	301	DD6	C29-C27	-8.47	1.26	1.42
34	H	302	DD6	C29-C27	-8.47	1.26	1.42
34	D	303	DD6	C29-C27	-8.41	1.26	1.42
34	S	306	DD6	C29-C27	-8.41	1.26	1.42
34	D	304	DD6	C29-C27	-8.38	1.26	1.42
37	T	310	KC1	C3C-C2C	8.29	1.54	1.36
36	W	214	CLA	C4B-NB	8.16	1.42	1.35
36	Q	310	CLA	C4B-NB	8.14	1.42	1.35
34	O	304	DD6	C29-C27	-8.13	1.26	1.42
36	P	319	CLA	C1B-NB	-8.07	1.28	1.35
36	O	312	CLA	C4B-NB	8.02	1.42	1.35
36	W	216	CLA	C4B-NB	8.02	1.42	1.35
36	P	314	CLA	C4B-NB	7.98	1.42	1.35
34	L	305	DD6	C30-C31	-7.97	1.25	1.42
36	Q	310	CLA	O1A-CGA	7.94	1.46	1.22
36	B	311	CLA	C4B-NB	7.94	1.42	1.35
34	S	307	DD6	C30-C31	-7.93	1.25	1.42
34	A	301	DD6	C30-C31	-7.92	1.25	1.42
34	Q	302	DD6	C30-C31	-7.92	1.25	1.42
34	W	204	DD6	C30-C31	-7.92	1.25	1.42
34	M	303	DD6	C30-C31	-7.89	1.25	1.42
37	V	312	KC1	C4C-NC	7.89	1.49	1.37
34	C	201	DD6	C30-C31	-7.87	1.25	1.42
34	R	308	DD6	C30-C31	-7.86	1.25	1.42
34	E	306	DD6	C30-C31	-7.85	1.26	1.42
34	J	304	DD6	C30-C31	-7.84	1.26	1.42
34	K	304	DD6	C30-C31	-7.84	1.26	1.42
36	X	307	CLA	C4B-NB	7.83	1.42	1.35
34	P	305	DD6	C30-C31	-7.82	1.26	1.42
36	M	315	CLA	C4B-NB	7.81	1.42	1.35
34	E	303	DD6	C30-C31	-7.81	1.26	1.42
34	D	301	DD6	C30-C31	-7.81	1.26	1.42
34	R	307	DD6	C30-C31	-7.80	1.26	1.42
37	Q	313	KC1	C4C-NC	7.80	1.49	1.37
37	T	315	KC1	C4D-ND	7.80	1.42	1.35
34	K	305	DD6	C30-C31	-7.79	1.26	1.42
34	I	303	DD6	C30-C31	-7.79	1.26	1.42
37	B	310	KC1	C4C-NC	7.79	1.49	1.37
34	B	302	DD6	C30-C31	-7.78	1.26	1.42
34	A	304	DD6	C30-C31	-7.78	1.26	1.42
34	a	849	DD6	C30-C31	-7.77	1.26	1.42
37	U	312	KC1	C4C-NC	7.76	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	302	DD6	C30-C31	-7.75	1.26	1.42
34	B	304	DD6	C30-C31	-7.75	1.26	1.42
37	Q	311	KC1	C4C-NC	7.75	1.49	1.37
37	O	315	KC1	C4C-NC	7.74	1.49	1.37
34	W	205	DD6	C30-C31	-7.74	1.26	1.42
36	S	318	CLA	C4B-NB	7.73	1.42	1.35
34	A	303	DD6	C30-C31	-7.73	1.26	1.42
34	j	103	DD6	C30-C31	-7.73	1.26	1.42
36	U	309	CLA	C4B-NB	7.72	1.42	1.35
34	G	303	DD6	C30-C31	-7.71	1.26	1.42
34	E	304	DD6	C30-C31	-7.70	1.26	1.42
36	M	310	CLA	C1D-ND	7.69	1.47	1.37
36	b	819	CLA	C4B-NB	7.69	1.42	1.35
34	D	304	DD6	C30-C31	-7.68	1.26	1.42
34	S	306	DD6	C30-C31	-7.67	1.26	1.42
34	E	301	DD6	C30-C31	-7.67	1.26	1.42
37	P	315	KC1	C4C-NC	7.67	1.49	1.37
34	H	303	DD6	C30-C31	-7.66	1.26	1.42
34	F	303	DD6	C30-C31	-7.66	1.26	1.42
34	D	303	DD6	C30-C31	-7.66	1.26	1.42
37	O	313	KC1	C4C-NC	7.64	1.49	1.37
36	T	311	CLA	C4B-NB	7.64	1.42	1.35
36	N	318	CLA	C4B-NB	7.63	1.42	1.35
37	N	314	KC1	C4D-ND	7.63	1.42	1.35
36	b	827	CLA	C4B-NB	7.63	1.42	1.35
43	a	840	PQN	C3-C2	7.61	1.49	1.35
36	S	315	CLA	C4B-NB	7.56	1.42	1.35
36	U	307	CLA	C4B-NB	7.55	1.41	1.35
34	D	305	DD6	C30-C31	-7.55	1.26	1.42
36	X	315	CLA	C4B-NB	7.54	1.41	1.35
36	U	313	CLA	C4B-NB	7.53	1.41	1.35
37	V	312	KC1	C4D-ND	7.52	1.41	1.35
43	b	842	PQN	C3-C2	7.52	1.48	1.35
36	W	201	CLA	C4B-NB	7.52	1.41	1.35
36	W	206	CLA	C4B-NB	7.51	1.41	1.35
36	X	310	CLA	C4B-NB	7.51	1.41	1.35
36	a	830	CLA	C4B-NB	7.51	1.41	1.35
36	I	309	CLA	C4B-NB	7.50	1.41	1.35
36	R	318	CLA	C4B-NB	7.50	1.41	1.35
36	A	314	CLA	C4B-NB	7.49	1.41	1.35
36	A	313	CLA	C4B-NB	7.49	1.41	1.35
36	S	314	CLA	C4B-NB	7.48	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	816	CLA	C1D-ND	7.47	1.47	1.37
37	X	311	KC1	C4C-NC	7.47	1.49	1.37
37	W	217	KC1	C4C-NC	7.47	1.49	1.37
36	S	317	CLA	C4B-NB	7.46	1.41	1.35
36	L	312	CLA	C4B-NB	7.46	1.41	1.35
37	N	314	KC1	C4C-NC	7.45	1.48	1.37
36	S	311	CLA	C4B-NB	7.45	1.41	1.35
37	M	318	KC1	C3B-C2B	7.44	1.52	1.37
36	C	210	CLA	C4B-NB	7.44	1.41	1.35
36	X	306	CLA	C4B-NB	7.43	1.41	1.35
36	T	312	CLA	C4B-NB	7.43	1.41	1.35
36	H	310	CLA	C4B-NB	7.43	1.41	1.35
36	f	802	CLA	C4B-NB	7.43	1.41	1.35
36	H	305	CLA	C4B-NB	7.42	1.41	1.35
36	U	310	CLA	C4B-NB	7.41	1.41	1.35
37	M	317	KC1	C4C-NC	7.41	1.48	1.37
36	P	316	CLA	C4B-NB	7.41	1.41	1.35
36	I	312	CLA	C4B-NB	7.40	1.41	1.35
37	S	316	KC1	C4C-NC	7.39	1.48	1.37
36	Q	312	CLA	C4B-NB	7.39	1.41	1.35
37	L	317	KC1	C4C-NC	7.39	1.48	1.37
36	S	321	CLA	C4B-NB	7.37	1.41	1.35
36	N	313	CLA	C4B-NB	7.37	1.41	1.35
36	X	312	CLA	C4B-NB	7.36	1.41	1.35
37	R	317	KC1	C4C-NC	7.36	1.48	1.37
37	J	314	KC1	C4C-NC	7.36	1.48	1.37
36	l	204	CLA	C4B-NB	7.35	1.41	1.35
36	X	309	CLA	C4B-NB	7.35	1.41	1.35
36	V	305	CLA	C4B-NB	7.35	1.41	1.35
36	N	307	CLA	C4B-NB	7.34	1.41	1.35
36	O	314	CLA	C4B-NB	7.34	1.41	1.35
36	P	318	CLA	C4B-NB	7.34	1.41	1.35
36	K	311	CLA	C4B-NB	7.33	1.41	1.35
37	T	310	KC1	C4C-C3C	7.33	1.57	1.45
36	N	310	CLA	C4B-NB	7.32	1.41	1.35
37	M	313	KC1	C4C-NC	7.32	1.48	1.37
36	S	309	CLA	C4B-NB	7.32	1.41	1.35
36	W	216	CLA	C1B-NB	7.32	1.41	1.35
37	T	310	KC1	C3B-C2B	7.31	1.52	1.37
36	S	320	CLA	C4B-NB	7.31	1.41	1.35
36	V	307	CLA	C4B-NB	7.31	1.41	1.35
36	W	209	CLA	C4B-NB	7.30	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	315	CLA	C4B-NB	7.27	1.41	1.35
36	K	308	CLA	C4B-NB	7.26	1.41	1.35
37	W	213	KC1	C4C-NC	7.26	1.48	1.37
36	N	317	CLA	C4B-NB	7.25	1.41	1.35
36	S	313	CLA	C4B-NB	7.25	1.41	1.35
36	T	314	CLA	C4B-NB	7.25	1.41	1.35
37	T	315	KC1	C4C-NC	7.24	1.48	1.37
37	F	308	KC1	C4C-NC	7.23	1.48	1.37
36	V	306	CLA	C4B-NB	7.23	1.41	1.35
36	M	309	CLA	C4B-NB	7.22	1.41	1.35
37	L	315	KC1	C4C-NC	7.22	1.48	1.37
36	b	834	CLA	C4B-NB	7.21	1.41	1.35
36	U	306	CLA	C4B-NB	7.21	1.41	1.35
37	K	314	KC1	C4C-NC	7.21	1.48	1.37
36	M	314	CLA	C4B-NB	7.20	1.41	1.35
34	O	304	DD6	C30-C31	-7.20	1.27	1.42
36	L	310	CLA	C4B-NB	7.19	1.41	1.35
36	R	310	CLA	C4B-NB	7.18	1.41	1.35
36	M	316	CLA	C4B-NB	7.17	1.41	1.35
36	S	319	CLA	C4B-NB	7.17	1.41	1.35
37	D	314	KC1	C4C-NC	7.17	1.48	1.37
37	A	312	KC1	C4C-NC	7.16	1.48	1.37
36	I	305	CLA	C11-C12	-7.16	1.21	1.52
36	W	212	CLA	C4B-NB	7.16	1.41	1.35
36	T	313	CLA	C4B-NB	7.16	1.41	1.35
36	T	316	CLA	C4B-NB	7.15	1.41	1.35
36	B	309	CLA	C4B-NB	7.15	1.41	1.35
36	R	320	CLA	C4B-NB	7.15	1.41	1.35
36	U	305	CLA	C4B-NB	7.14	1.41	1.35
37	X	311	KC1	C4D-ND	7.14	1.41	1.35
37	G	308	KC1	C4C-NC	7.14	1.48	1.37
36	Q	309	CLA	C4B-NB	7.14	1.41	1.35
37	W	217	KC1	C4D-ND	7.14	1.41	1.35
37	S	316	KC1	C4D-ND	7.14	1.41	1.35
36	H	315	CLA	C4B-NB	7.13	1.41	1.35
37	C	213	KC1	C4C-NC	7.13	1.48	1.37
36	H	317	CLA	C4B-NB	7.13	1.41	1.35
37	H	313	KC1	C4C-NC	7.12	1.48	1.37
36	a	815	CLA	C4B-NB	7.12	1.41	1.35
36	a	811	CLA	C4B-NB	7.11	1.41	1.35
36	I	314	CLA	C4B-NB	7.11	1.41	1.35
36	C	209	CLA	C4B-NB	7.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	P	312	CLA	C4B-NB	7.11	1.41	1.35
36	E	316	CLA	C4B-NB	7.09	1.41	1.35
36	T	309	CLA	C4B-NB	7.09	1.41	1.35
36	N	316	CLA	C4B-NB	7.09	1.41	1.35
36	W	211	CLA	C4B-NB	7.08	1.41	1.35
37	G	317	KC1	C4C-NC	7.08	1.48	1.37
36	V	309	CLA	C4B-NB	7.08	1.41	1.35
36	W	207	CLA	C4B-NB	7.07	1.41	1.35
37	F	315	KC1	C4C-NC	7.07	1.48	1.37
36	J	309	CLA	C4B-NB	7.06	1.41	1.35
36	M	311	CLA	C4B-NB	7.06	1.41	1.35
36	B	307	CLA	C4B-NB	7.06	1.41	1.35
36	E	317	CLA	C4B-NB	7.06	1.41	1.35
37	G	318	KC1	C4C-NC	7.06	1.48	1.37
36	R	312	CLA	C4B-NB	7.06	1.41	1.35
36	O	310	CLA	C4B-NB	7.05	1.41	1.35
36	Q	314	CLA	C4B-NB	7.05	1.41	1.35
36	R	314	CLA	C4B-NB	7.03	1.41	1.35
36	R	321	CLA	C4B-NB	7.03	1.41	1.35
37	C	213	KC1	C4D-ND	7.03	1.41	1.35
36	J	312	CLA	C4B-NB	7.03	1.41	1.35
36	V	310	CLA	C4B-NB	7.03	1.41	1.35
36	I	313	CLA	C4B-NB	7.02	1.41	1.35
36	U	311	CLA	C4B-NB	7.01	1.41	1.35
36	R	311	CLA	C4B-NB	7.01	1.41	1.35
36	C	207	CLA	C1D-ND	6.99	1.46	1.37
36	M	308	CLA	C4B-NB	6.99	1.41	1.35
36	R	319	CLA	C4B-NB	6.99	1.41	1.35
37	E	309	KC1	C4C-NC	6.99	1.48	1.37
36	B	305	CLA	C4B-NB	6.99	1.41	1.35
36	S	310	CLA	C4B-NB	6.99	1.41	1.35
36	G	314	CLA	C4B-NB	6.98	1.41	1.35
37	W	213	KC1	C4D-ND	6.98	1.41	1.35
36	L	316	CLA	C4B-NB	6.98	1.41	1.35
36	P	311	CLA	C4B-NB	6.98	1.41	1.35
37	P	317	KC1	C4C-NC	6.96	1.48	1.37
36	A	309	CLA	C4B-NB	6.96	1.41	1.35
36	a	848	CLA	C4B-NB	6.96	1.41	1.35
36	U	308	CLA	C4B-NB	6.95	1.41	1.35
36	D	311	CLA	C4B-NB	6.95	1.41	1.35
37	K	314	KC1	C4D-ND	6.95	1.41	1.35
36	D	306	CLA	C4B-NB	6.95	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	W	218	CLA	C4B-NB	6.94	1.41	1.35
36	P	308	CLA	C4B-NB	6.94	1.41	1.35
36	S	312	CLA	C4B-NB	6.94	1.41	1.35
36	W	215	CLA	C4B-NB	6.94	1.41	1.35
36	O	309	CLA	C4B-NB	6.94	1.41	1.35
36	W	208	CLA	C4B-NB	6.93	1.41	1.35
36	R	322	CLA	C4B-NB	6.92	1.41	1.35
36	B	306	CLA	C4B-NB	6.91	1.41	1.35
36	H	316	CLA	C4B-NB	6.91	1.41	1.35
36	P	309	CLA	C4B-NB	6.90	1.41	1.35
36	Q	305	CLA	C4B-NB	6.90	1.41	1.35
36	O	306	CLA	C4B-NB	6.89	1.41	1.35
36	J	317	CLA	C4B-NB	6.88	1.41	1.35
36	Q	308	CLA	C4B-NB	6.88	1.41	1.35
36	b	830	CLA	C4B-NB	6.87	1.41	1.35
36	K	309	CLA	C4B-NB	6.87	1.41	1.35
36	Q	306	CLA	C4B-NB	6.87	1.41	1.35
36	a	834	CLA	C4B-NB	6.87	1.41	1.35
37	G	318	KC1	C4D-ND	6.86	1.41	1.35
36	N	309	CLA	C4B-NB	6.85	1.41	1.35
36	N	311	CLA	C4B-NB	6.84	1.41	1.35
36	R	316	CLA	C4B-NB	6.83	1.41	1.35
36	a	806	CLA	C1B-NB	6.83	1.41	1.35
36	P	301	CLA	C4B-NB	6.81	1.41	1.35
36	K	312	CLA	C4B-NB	6.81	1.41	1.35
36	O	307	CLA	C4B-NB	6.80	1.41	1.35
36	R	315	CLA	C4B-NB	6.80	1.41	1.35
36	F	312	CLA	C4B-NB	6.80	1.41	1.35
36	i	102	CLA	C4B-NB	6.80	1.41	1.35
36	F	316	CLA	C4B-NB	6.79	1.41	1.35
36	j	106	CLA	C4B-NB	6.79	1.41	1.35
37	D	314	KC1	C4D-ND	6.79	1.41	1.35
36	a	841	CLA	C4B-NB	6.79	1.41	1.35
36	L	320	CLA	C4B-NB	6.79	1.41	1.35
36	N	312	CLA	C4B-NB	6.78	1.41	1.35
36	b	802	CLA	C4B-NB	6.78	1.41	1.35
36	a	824	CLA	C4B-NB	6.77	1.41	1.35
36	G	316	CLA	C4B-NB	6.77	1.41	1.35
36	P	310	CLA	C4B-NB	6.77	1.41	1.35
37	B	310	KC1	C4D-ND	6.77	1.41	1.35
36	O	308	CLA	C4B-NB	6.77	1.41	1.35
36	K	315	CLA	C4B-NB	6.76	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	311	CLA	C4B-NB	6.76	1.41	1.35
37	L	315	KC1	C4D-ND	6.75	1.41	1.35
36	T	308	CLA	C4B-NB	6.75	1.41	1.35
36	M	307	CLA	C4B-NB	6.75	1.41	1.35
36	H	314	CLA	C4B-NB	6.75	1.41	1.35
36	Q	307	CLA	C4B-NB	6.74	1.41	1.35
36	C	214	CLA	C4B-NB	6.74	1.41	1.35
36	L	314	CLA	C4B-NB	6.73	1.41	1.35
36	M	312	CLA	C4B-NB	6.73	1.41	1.35
36	J	315	CLA	C4B-NB	6.73	1.41	1.35
36	P	313	CLA	C4B-NB	6.73	1.41	1.35
36	L	309	CLA	C4B-NB	6.72	1.41	1.35
36	V	308	CLA	C4B-NB	6.72	1.41	1.35
36	F	311	CLA	C4B-NB	6.71	1.41	1.35
36	O	311	CLA	C4B-NB	6.71	1.41	1.35
36	H	306	CLA	C4B-NB	6.71	1.41	1.35
36	a	822	CLA	C4B-NB	6.70	1.41	1.35
37	M	318	KC1	C1D-ND	6.70	1.41	1.35
36	U	306	CLA	C1D-ND	6.67	1.46	1.37
36	M	310	CLA	MG-ND	-6.65	1.92	2.05
36	V	311	CLA	C4B-NB	6.65	1.41	1.35
36	H	309	CLA	C4B-NB	6.65	1.41	1.35
36	I	308	CLA	C4B-NB	6.64	1.41	1.35
36	D	317	CLA	C4B-NB	6.64	1.41	1.35
36	a	819	CLA	C4B-NB	6.64	1.41	1.35
36	A	308	CLA	C4B-NB	6.63	1.41	1.35
36	K	316	CLA	C4B-NB	6.63	1.41	1.35
36	a	833	CLA	C4B-NB	6.60	1.41	1.35
36	b	817	CLA	C4B-NB	6.60	1.41	1.35
36	E	310	CLA	C4B-NB	6.60	1.41	1.35
36	J	316	CLA	C4B-NB	6.60	1.41	1.35
36	J	308	CLA	C4B-NB	6.60	1.41	1.35
36	C	208	CLA	C4B-NB	6.58	1.41	1.35
37	T	310	KC1	CHB-C4A	-6.58	1.24	1.39
36	b	835	CLA	C4B-NB	6.56	1.41	1.35
36	J	307	CLA	C4B-NB	6.56	1.41	1.35
36	D	312	CLA	C4B-NB	6.56	1.41	1.35
36	F	314	CLA	C4B-NB	6.56	1.41	1.35
36	C	206	CLA	C4B-NB	6.56	1.41	1.35
36	W	210	CLA	C4B-NB	6.55	1.41	1.35
36	b	821	CLA	C4B-NB	6.55	1.41	1.35
37	E	309	KC1	C4D-ND	6.54	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	L	311	CLA	C4B-NB	6.53	1.41	1.35
36	b	808	CLA	C4B-NB	6.53	1.41	1.35
36	V	313	CLA	C4B-NB	6.51	1.41	1.35
36	L	313	CLA	C4B-NB	6.51	1.41	1.35
36	A	305	CLA	C4B-NB	6.50	1.41	1.35
36	R	313	CLA	C4B-NB	6.50	1.41	1.35
36	l	206	CLA	C4B-NB	6.50	1.41	1.35
36	C	211	CLA	C4B-NB	6.50	1.41	1.35
36	I	310	CLA	C4B-NB	6.50	1.41	1.35
36	I	305	CLA	C4B-NB	6.49	1.41	1.35
36	D	316	CLA	C4B-NB	6.48	1.41	1.35
36	b	807	CLA	C4B-NB	6.48	1.41	1.35
35	U	301	A86	O4-C38	6.48	1.49	1.35
37	M	313	KC1	C4D-ND	6.47	1.41	1.35
36	H	318	CLA	C4B-NB	6.47	1.41	1.35
37	H	313	KC1	C4D-ND	6.46	1.41	1.35
36	N	319	CLA	CHD-C4C	6.46	1.54	1.39
36	E	308	CLA	C4B-NB	6.45	1.41	1.35
36	b	820	CLA	C4B-NB	6.45	1.41	1.35
36	J	310	CLA	C4B-NB	6.45	1.41	1.35
37	T	310	KC1	OBD-CAD	6.44	1.31	1.22
36	A	311	CLA	C4B-NB	6.43	1.40	1.35
36	H	312	CLA	C4B-NB	6.43	1.40	1.35
36	A	310	CLA	C4B-NB	6.43	1.40	1.35
36	F	310	CLA	C4B-NB	6.43	1.40	1.35
36	H	308	CLA	C4B-NB	6.42	1.40	1.35
36	a	835	CLA	C4B-NB	6.41	1.40	1.35
37	G	308	KC1	C4D-ND	6.40	1.40	1.35
36	b	831	CLA	C4B-NB	6.40	1.40	1.35
36	E	312	CLA	C4B-NB	6.40	1.40	1.35
36	b	839	CLA	C4B-NB	6.39	1.40	1.35
36	V	314	CLA	C1D-ND	6.39	1.45	1.37
36	j	102	CLA	C4B-NB	6.38	1.40	1.35
36	F	309	CLA	C4B-NB	6.38	1.40	1.35
36	h	203	CLA	C4B-NB	6.38	1.40	1.35
36	A	307	CLA	C4B-NB	6.37	1.40	1.35
36	l	202	CLA	C4B-NB	6.36	1.40	1.35
37	M	318	KC1	OBD-CAD	6.36	1.31	1.22
36	J	313	CLA	C4B-NB	6.35	1.40	1.35
36	a	808	CLA	C4B-NB	6.35	1.40	1.35
36	b	833	CLA	C4B-NB	6.35	1.40	1.35
36	a	803	CLA	C4B-NB	6.34	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	810	CLA	C4B-NB	6.34	1.40	1.35
36	H	311	CLA	C4B-NB	6.34	1.40	1.35
36	F	313	CLA	C4B-NB	6.34	1.40	1.35
36	a	838	CLA	C4B-NB	6.33	1.40	1.35
36	D	315	CLA	C4B-NB	6.33	1.40	1.35
36	a	829	CLA	C4B-NB	6.33	1.40	1.35
36	I	308	CLA	C1D-ND	6.33	1.45	1.37
36	G	310	CLA	C4B-NB	6.32	1.40	1.35
36	l	201	CLA	C4B-NB	6.32	1.40	1.35
36	a	812	CLA	C4B-NB	6.31	1.40	1.35
36	j	101	CLA	C4B-NB	6.30	1.40	1.35
36	D	307	CLA	C4B-NB	6.28	1.40	1.35
36	I	307	CLA	C4B-NB	6.28	1.40	1.35
36	b	813	CLA	C4B-NB	6.28	1.40	1.35
36	b	824	CLA	C4B-NB	6.28	1.40	1.35
36	I	305	CLA	C15-C13	-6.28	1.06	1.51
36	V	314	CLA	MG-NA	6.28	2.21	2.06
37	F	308	KC1	C4D-ND	6.27	1.40	1.35
36	b	829	CLA	C4B-NB	6.27	1.40	1.35
36	b	811	CLA	C4B-NB	6.26	1.40	1.35
36	f	805	CLA	C4B-NB	6.26	1.40	1.35
36	b	837	CLA	C4B-NB	6.24	1.40	1.35
37	P	315	KC1	C1A-NA	6.24	1.50	1.38
36	G	307	CLA	C1D-ND	6.22	1.45	1.37
36	E	313	CLA	C4B-NB	6.21	1.40	1.35
36	a	839	CLA	C4B-NB	6.21	1.40	1.35
37	O	315	KC1	C1A-NA	6.20	1.50	1.38
37	Q	311	KC1	C1A-NA	6.19	1.50	1.38
37	A	312	KC1	C1A-NA	6.19	1.50	1.38
36	b	809	CLA	C4B-NB	6.19	1.40	1.35
36	b	825	CLA	C4B-NB	6.19	1.40	1.35
37	Q	313	KC1	C1A-NA	6.19	1.50	1.38
36	a	820	CLA	C4B-NB	6.19	1.40	1.35
36	G	312	CLA	C4B-NB	6.19	1.40	1.35
36	a	823	CLA	C4B-NB	6.19	1.40	1.35
36	b	815	CLA	C4B-NB	6.19	1.40	1.35
37	O	313	KC1	C1A-NA	6.18	1.50	1.38
36	C	205	CLA	C4B-NB	6.18	1.40	1.35
36	b	801	CLA	C4B-NB	6.17	1.40	1.35
36	b	818	CLA	C4B-NB	6.17	1.40	1.35
36	b	812	CLA	C4B-NB	6.17	1.40	1.35
36	b	814	CLA	C4B-NB	6.17	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	K	307	CLA	C1D-ND	6.16	1.45	1.37
36	a	825	CLA	C4B-NB	6.15	1.40	1.35
36	E	311	CLA	C4B-NB	6.14	1.40	1.35
36	a	816	CLA	C1D-ND	6.13	1.45	1.37
36	b	840	CLA	C4B-NB	6.13	1.40	1.35
36	P	302	CLA	C4B-NB	6.13	1.40	1.35
37	J	314	KC1	C4D-ND	6.12	1.40	1.35
36	a	837	CLA	C4B-NB	6.11	1.40	1.35
37	P	317	KC1	C4D-ND	6.10	1.40	1.35
37	U	312	KC1	C4D-ND	6.10	1.40	1.35
37	M	317	KC1	C4D-ND	6.10	1.40	1.35
36	G	311	CLA	C4B-NB	6.09	1.40	1.35
36	b	836	CLA	C1D-ND	6.08	1.45	1.37
36	a	805	CLA	C4B-NB	6.08	1.40	1.35
36	a	828	CLA	C4B-NB	6.08	1.40	1.35
36	C	212	CLA	C4B-NB	6.08	1.40	1.35
36	a	826	CLA	C4B-NB	6.08	1.40	1.35
36	b	823	CLA	C4B-NB	6.08	1.40	1.35
36	b	822	CLA	C4B-NB	6.07	1.40	1.35
36	a	807	CLA	C4B-NB	6.07	1.40	1.35
36	L	308	CLA	CHC-C1C	6.07	1.50	1.35
37	T	310	KC1	C4D-ND	6.07	1.40	1.35
37	N	314	KC1	C3C-C2C	6.04	1.49	1.36
36	I	311	CLA	C4B-NB	6.04	1.40	1.35
36	a	821	CLA	C4B-NB	6.04	1.40	1.35
36	D	313	CLA	C4B-NB	6.03	1.40	1.35
36	G	309	CLA	C4B-NB	6.03	1.40	1.35
36	a	814	CLA	C4B-NB	6.02	1.40	1.35
36	D	308	CLA	C4B-NB	6.02	1.40	1.35
36	H	310	CLA	O2D-CGD	6.01	1.47	1.33
37	W	217	KC1	CHD-C4C	6.00	1.50	1.35
37	B	310	KC1	CHD-C4C	5.99	1.50	1.35
36	a	809	CLA	C4B-NB	5.99	1.40	1.35
37	X	311	KC1	CHD-C4C	5.98	1.50	1.35
37	W	217	KC1	C1A-NA	5.97	1.49	1.38
36	b	805	CLA	C4B-NB	5.96	1.40	1.35
36	b	826	CLA	C4B-NB	5.95	1.40	1.35
37	T	310	KC1	C1D-ND	5.94	1.40	1.35
37	V	312	KC1	CHD-C4C	5.94	1.50	1.35
36	a	827	CLA	C4B-NB	5.93	1.40	1.35
37	U	312	KC1	C1A-NA	5.93	1.49	1.38
37	X	311	KC1	C1A-NA	5.93	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	L	317	KC1	C4D-ND	5.92	1.40	1.35
37	L	315	KC1	C2A-C3A	5.92	1.49	1.37
37	U	312	KC1	C2A-C3A	5.91	1.49	1.37
36	D	309	CLA	C1D-ND	5.91	1.45	1.37
36	b	838	CLA	C4B-NB	5.90	1.40	1.35
37	W	217	KC1	C2A-C3A	5.89	1.49	1.37
36	Q	310	CLA	CBA-CGA	5.89	1.67	1.50
36	D	310	CLA	C4B-NB	5.89	1.40	1.35
37	X	311	KC1	C2A-C3A	5.87	1.49	1.37
36	a	836	CLA	C4B-NB	5.85	1.40	1.35
37	O	315	KC1	C2A-C3A	5.84	1.49	1.37
37	S	316	KC1	CHD-C4C	5.84	1.49	1.35
37	F	308	KC1	C3C-C2C	5.84	1.49	1.36
37	P	315	KC1	C2A-C3A	5.83	1.49	1.37
37	E	309	KC1	C3C-C2C	5.83	1.49	1.36
36	E	314	CLA	C4B-NB	5.83	1.40	1.35
36	a	817	CLA	C4B-NB	5.83	1.40	1.35
37	O	313	KC1	C2A-C3A	5.83	1.49	1.37
37	Q	311	KC1	C2A-C3A	5.82	1.49	1.37
37	Q	313	KC1	C2A-C3A	5.82	1.49	1.37
36	N	319	CLA	CHD-C1D	5.81	1.49	1.38
37	S	316	KC1	C2A-C3A	5.81	1.49	1.37
37	N	314	KC1	CHD-C4C	5.80	1.49	1.35
36	j	102	CLA	C1D-ND	5.80	1.44	1.37
36	K	313	CLA	C4B-NB	5.79	1.40	1.35
37	U	312	KC1	CHD-C4C	5.79	1.49	1.35
37	G	318	KC1	CHD-C4C	5.79	1.49	1.35
37	G	308	KC1	CHD-C4C	5.78	1.49	1.35
36	b	810	CLA	C4B-NB	5.78	1.40	1.35
37	S	316	KC1	C3C-C2C	5.78	1.49	1.36
37	B	310	KC1	C1A-NA	5.78	1.49	1.38
37	L	317	KC1	C1A-NA	5.78	1.49	1.38
37	G	318	KC1	C3C-C2C	5.78	1.49	1.36
37	F	308	KC1	CHD-C4C	5.77	1.49	1.35
36	a	831	CLA	C4B-NB	5.77	1.40	1.35
37	W	213	KC1	C2A-C3A	5.77	1.49	1.37
37	W	213	KC1	CHD-C4C	5.75	1.49	1.35
37	J	314	KC1	C1A-NA	5.74	1.49	1.38
37	L	317	KC1	CHD-C4C	5.72	1.49	1.35
37	C	213	KC1	CHD-C4C	5.72	1.49	1.35
37	F	315	KC1	C1A-NA	5.72	1.49	1.38
37	L	315	KC1	C1A-NA	5.71	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	832	CLA	C4B-NB	5.71	1.40	1.35
37	V	312	KC1	C3C-C2C	5.70	1.48	1.36
37	M	317	KC1	CHD-C4C	5.70	1.49	1.35
35	X	303	A86	O4-C38	5.69	1.48	1.35
36	B	308	CLA	C4B-NB	5.68	1.40	1.35
36	W	214	CLA	C1D-ND	5.67	1.44	1.37
37	R	317	KC1	C1A-NA	5.67	1.49	1.38
37	S	316	KC1	C1A-NA	5.66	1.49	1.38
37	E	309	KC1	CHD-C4C	5.66	1.49	1.35
36	O	316	CLA	C1D-ND	5.66	1.44	1.37
37	A	312	KC1	CHD-C4C	5.66	1.49	1.35
37	A	312	KC1	C2A-C3A	5.65	1.48	1.37
37	U	312	KC1	C3B-C2B	5.65	1.48	1.37
37	V	312	KC1	C2A-C3A	5.65	1.48	1.37
37	T	315	KC1	CHD-C4C	5.65	1.49	1.35
36	G	313	CLA	C4B-NB	5.65	1.40	1.35
36	a	818	CLA	C4B-NB	5.64	1.40	1.35
36	a	801	CLA	C4B-NB	5.64	1.40	1.35
37	G	308	KC1	C3C-C2C	5.63	1.48	1.36
37	J	314	KC1	CHD-C4C	5.63	1.49	1.35
37	F	308	KC1	C1A-NA	5.63	1.49	1.38
35	T	305	A86	O4-C38	5.62	1.47	1.35
37	H	313	KC1	CHD-C4C	5.62	1.49	1.35
37	B	310	KC1	C2A-C3A	5.62	1.48	1.37
37	W	217	KC1	C3C-C2C	5.62	1.48	1.36
37	X	311	KC1	C3C-C2C	5.61	1.48	1.36
37	F	315	KC1	C2A-C3A	5.60	1.48	1.37
37	D	314	KC1	CHD-C4C	5.60	1.49	1.35
35	X	301	A86	O4-C38	5.59	1.47	1.35
37	B	310	KC1	C3C-C2C	5.58	1.48	1.36
36	b	828	CLA	C4B-NB	5.58	1.40	1.35
37	O	315	KC1	CHD-C4C	5.58	1.49	1.35
36	a	804	CLA	C4B-NB	5.58	1.40	1.35
35	A	302	A86	O4-C38	5.58	1.47	1.35
37	Q	311	KC1	CHD-C4C	5.58	1.49	1.35
37	G	317	KC1	CHD-C4C	5.57	1.49	1.35
36	b	806	CLA	C4B-NB	5.57	1.40	1.35
37	R	317	KC1	CHD-C4C	5.56	1.49	1.35
37	P	315	KC1	CHD-C4C	5.56	1.49	1.35
37	M	317	KC1	C3C-C2C	5.55	1.48	1.36
37	U	312	KC1	CHB-C1B	5.55	1.49	1.38
37	Q	313	KC1	CHD-C4C	5.55	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	213	KC1	C1A-NA	5.55	1.48	1.38
37	G	318	KC1	C2A-C3A	5.55	1.48	1.37
36	M	310	CLA	C4B-NB	5.54	1.40	1.35
37	R	317	KC1	C3C-C2C	5.54	1.48	1.36
35	N	301	A86	O4-C38	5.53	1.47	1.35
37	O	313	KC1	CHD-C4C	5.52	1.49	1.35
35	R	304	A86	O4-C38	5.52	1.47	1.35
37	W	213	KC1	C3C-C2C	5.52	1.48	1.36
35	S	301	A86	O4-C38	5.52	1.47	1.35
37	K	314	KC1	CHD-C4C	5.52	1.49	1.35
37	P	317	KC1	CHD-C4C	5.51	1.49	1.35
37	N	314	KC1	C2A-C3A	5.51	1.48	1.37
37	G	317	KC1	C1A-NA	5.50	1.48	1.38
37	D	314	KC1	C3C-C2C	5.49	1.48	1.36
35	M	301	A86	O4-C38	5.48	1.47	1.35
37	M	313	KC1	CHD-C4C	5.48	1.49	1.35
35	S	303	A86	O4-C38	5.47	1.47	1.35
35	X	304	A86	O4-C38	5.47	1.47	1.35
35	R	301	A86	O4-C38	5.47	1.47	1.35
35	K	302	A86	O4-C38	5.46	1.47	1.35
35	N	303	A86	O4-C38	5.46	1.47	1.35
36	K	310	CLA	C1D-ND	5.46	1.44	1.37
37	T	315	KC1	C2A-C3A	5.46	1.48	1.37
35	W	202	A86	O4-C38	5.44	1.47	1.35
37	A	312	KC1	C3D-C2D	5.44	1.49	1.39
37	E	309	KC1	C1A-NA	5.44	1.48	1.38
36	H	307	CLA	C4B-NB	5.43	1.40	1.35
37	M	317	KC1	C2A-C3A	5.43	1.48	1.37
37	R	317	KC1	C4D-ND	5.43	1.40	1.35
36	a	830	CLA	C3B-C2B	5.42	1.47	1.40
36	M	306	CLA	C4B-NB	5.42	1.40	1.35
36	a	832	CLA	C4B-NB	5.41	1.40	1.35
37	G	317	KC1	C4D-ND	5.40	1.40	1.35
37	F	315	KC1	CHD-C4C	5.40	1.48	1.35
37	M	313	KC1	C3C-C2C	5.40	1.48	1.36
37	C	213	KC1	C3C-C2C	5.40	1.48	1.36
37	H	313	KC1	C3C-C2C	5.39	1.48	1.36
37	J	314	KC1	C3C-C2C	5.38	1.48	1.36
37	C	213	KC1	C2A-C3A	5.38	1.48	1.37
35	I	302	A86	O4-C38	5.37	1.47	1.35
36	a	813	CLA	C4B-NB	5.36	1.40	1.35
37	N	314	KC1	C3B-C2B	5.35	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	318	KC1	O2D-CGD	5.34	1.46	1.33
37	L	315	KC1	CHD-C4C	5.34	1.48	1.35
37	T	315	KC1	C3C-C2C	5.34	1.48	1.36
37	B	310	KC1	O2D-CGD	5.33	1.46	1.33
37	P	317	KC1	C2A-C3A	5.33	1.48	1.37
35	R	303	A86	O4-C38	5.32	1.47	1.35
37	G	317	KC1	O2D-CGD	5.31	1.46	1.33
37	L	317	KC1	C3C-C2C	5.30	1.48	1.36
36	P	319	CLA	MG-ND	-5.29	1.95	2.05
36	F	317	CLA	C1D-ND	5.28	1.44	1.37
37	N	314	KC1	C1A-NA	5.27	1.48	1.38
37	G	317	KC1	C3C-C2C	5.27	1.47	1.36
35	I	304	A86	O4-C38	5.26	1.47	1.35
36	U	306	CLA	C3C-C2C	5.26	1.47	1.36
37	J	314	KC1	C2A-C3A	5.25	1.47	1.37
37	O	313	KC1	C3C-C2C	5.25	1.47	1.36
34	D	303	DD6	C-C1	5.25	1.61	1.50
37	W	213	KC1	C3B-C2B	5.25	1.47	1.37
37	P	315	KC1	C3C-C2C	5.25	1.47	1.36
37	H	313	KC1	C1A-NA	5.25	1.48	1.38
37	G	308	KC1	C1A-NA	5.23	1.48	1.38
36	W	215	CLA	OBD-CAD	5.22	1.31	1.22
37	Q	311	KC1	C3C-C2C	5.22	1.47	1.36
37	Q	313	KC1	C3C-C2C	5.22	1.47	1.36
37	L	317	KC1	C2A-C3A	5.22	1.47	1.37
37	N	314	KC1	O2D-CGD	5.21	1.45	1.33
37	O	315	KC1	C3C-C2C	5.21	1.47	1.36
37	M	313	KC1	C2A-C3A	5.21	1.47	1.37
37	C	213	KC1	C3B-C2B	5.20	1.47	1.37
37	Q	313	KC1	C3B-C2B	5.20	1.47	1.37
37	Q	311	KC1	C3B-C2B	5.19	1.47	1.37
37	G	318	KC1	C1A-NA	5.19	1.48	1.38
37	O	313	KC1	C3B-C2B	5.19	1.47	1.37
36	f	804	CLA	C1D-ND	5.19	1.44	1.37
37	T	315	KC1	O2D-CGD	5.19	1.45	1.33
37	W	217	KC1	O2D-CGD	5.18	1.45	1.33
37	S	316	KC1	C3B-C2B	5.18	1.47	1.37
37	M	318	KC1	C1A-CHA	5.18	1.54	1.40
35	C	202	A86	O4-C38	5.18	1.46	1.35
37	S	316	KC1	O2D-CGD	5.17	1.45	1.33
36	B	309	CLA	O2D-CGD	5.17	1.45	1.33
37	P	315	KC1	C3B-C2B	5.17	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	310	KC1	C3B-C2B	5.16	1.47	1.37
37	X	311	KC1	O2D-CGD	5.16	1.45	1.33
36	K	310	CLA	O2D-CGD	5.15	1.45	1.33
37	O	315	KC1	C3B-C2B	5.15	1.47	1.37
37	G	317	KC1	C2A-C3A	5.15	1.47	1.37
36	b	824	CLA	C3B-C2B	5.14	1.47	1.40
35	N	304	A86	O1-C15	-5.14	1.36	1.45
35	J	303	A86	O4-C38	5.14	1.46	1.35
37	M	318	KC1	O2D-CGD	5.13	1.45	1.33
37	L	315	KC1	C3B-C2B	5.13	1.47	1.37
37	U	312	KC1	O2D-CGD	5.13	1.45	1.33
37	L	317	KC1	O2D-CGD	5.13	1.45	1.33
37	M	313	KC1	C1A-NA	5.13	1.48	1.38
36	a	806	CLA	C3B-C2B	5.12	1.47	1.40
37	G	308	KC1	C2A-C3A	5.12	1.47	1.37
36	a	802	CLA	O2D-CGD	5.12	1.45	1.33
36	O	316	CLA	O2D-CGD	5.12	1.45	1.33
37	M	313	KC1	C3B-C2B	5.12	1.47	1.37
36	V	314	CLA	O2D-CGD	5.11	1.45	1.33
36	I	308	CLA	O2D-CGD	5.11	1.45	1.33
35	R	306	A86	O4-C38	5.11	1.46	1.35
35	F	307	A86	O4-C38	5.11	1.46	1.35
35	K	303	A86	O4-C38	5.11	1.46	1.35
35	V	303	A86	O4-C38	5.11	1.46	1.35
36	L	308	CLA	O2D-CGD	5.11	1.45	1.33
37	U	312	KC1	C3C-C2C	5.11	1.47	1.36
35	T	303	A86	O4-C38	5.10	1.46	1.35
37	K	314	KC1	O2D-CGD	5.10	1.45	1.33
37	V	312	KC1	O2D-CGD	5.10	1.45	1.33
37	X	311	KC1	C3D-C2D	5.10	1.48	1.39
36	U	306	CLA	O2D-CGD	5.10	1.45	1.33
37	L	315	KC1	C3C-C2C	5.10	1.47	1.36
36	I	308	CLA	C3B-C2B	5.10	1.47	1.40
37	T	315	KC1	C3B-C2B	5.10	1.47	1.37
36	D	309	CLA	O2D-CGD	5.10	1.45	1.33
37	V	312	KC1	C1A-NA	5.10	1.48	1.38
36	K	310	CLA	C3C-C2C	5.09	1.47	1.36
36	D	309	CLA	CHC-C1C	5.09	1.48	1.35
37	W	217	KC1	C3D-C2D	5.09	1.48	1.39
37	W	213	KC1	O2D-CGD	5.09	1.45	1.33
37	L	315	KC1	O2D-CGD	5.09	1.45	1.33
37	M	317	KC1	C1A-NA	5.08	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	319	CLA	O2D-CGD	5.08	1.45	1.33
36	F	317	CLA	O2D-CGD	5.08	1.45	1.33
36	b	824	CLA	CHC-C1C	5.08	1.48	1.35
36	K	307	CLA	O2D-CGD	5.08	1.45	1.33
37	D	314	KC1	C2A-C3A	5.08	1.47	1.37
36	a	823	CLA	O2D-CGD	5.07	1.45	1.33
37	F	308	KC1	C2A-C3A	5.07	1.47	1.37
36	G	315	CLA	O2D-CGD	5.07	1.45	1.33
37	T	310	KC1	O2D-CGD	5.07	1.45	1.33
35	P	303	A86	O4-C38	5.07	1.46	1.35
37	W	217	KC1	C3B-C2B	5.06	1.47	1.37
37	T	315	KC1	C1A-NA	5.06	1.47	1.38
37	K	314	KC1	C3C-C2C	5.06	1.47	1.36
37	X	311	KC1	C3B-C2B	5.06	1.47	1.37
37	W	213	KC1	C3D-C2D	5.06	1.48	1.39
37	M	313	KC1	O2D-CGD	5.06	1.45	1.33
36	a	830	CLA	O2D-CGD	5.06	1.45	1.33
36	A	306	CLA	O2D-CGD	5.06	1.45	1.33
35	L	319	A86	O4-C38	5.05	1.46	1.35
37	M	317	KC1	C3B-C2B	5.05	1.47	1.37
35	O	302	A86	O4-C38	5.05	1.46	1.35
36	b	836	CLA	O2D-CGD	5.05	1.45	1.33
36	I	306	CLA	O2D-CGD	5.05	1.45	1.33
37	L	317	KC1	C3B-C2B	5.05	1.47	1.37
37	Q	313	KC1	O2D-CGD	5.05	1.45	1.33
36	f	803	CLA	O2D-CGD	5.05	1.45	1.33
36	b	824	CLA	O2D-CGD	5.04	1.45	1.33
37	O	313	KC1	C4D-ND	5.04	1.39	1.35
37	E	309	KC1	C2A-C3A	5.04	1.47	1.37
37	R	317	KC1	C2A-C3A	5.04	1.47	1.37
35	W	203	A86	O4-C38	5.04	1.46	1.35
37	R	317	KC1	O2D-CGD	5.03	1.45	1.33
37	V	312	KC1	C3B-C2B	5.03	1.47	1.37
35	X	305	A86	O4-C38	5.03	1.46	1.35
37	P	315	KC1	C4D-ND	5.03	1.39	1.35
36	E	313	CLA	O2D-CGD	5.03	1.45	1.33
37	Q	311	KC1	O2D-CGD	5.03	1.45	1.33
37	P	315	KC1	C3D-C2D	5.02	1.48	1.39
36	f	804	CLA	CHC-C1C	5.02	1.47	1.35
36	G	319	CLA	C1D-ND	5.02	1.44	1.37
36	a	825	CLA	O2D-CGD	5.02	1.45	1.33
37	P	317	KC1	C3C-C2C	5.02	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	O	315	KC1	O2D-CGD	5.02	1.45	1.33
36	j	102	CLA	O2D-CGD	5.01	1.45	1.33
36	G	313	CLA	C4D-ND	-5.01	1.30	1.37
36	G	315	CLA	C3D-C4D	-5.00	1.32	1.44
36	E	313	CLA	C3D-C4D	-5.00	1.32	1.44
36	a	816	CLA	O2D-CGD	5.00	1.45	1.33
35	M	302	A86	O4-C38	5.00	1.46	1.35
36	E	313	CLA	C3B-C2B	5.00	1.47	1.40
36	E	315	CLA	C3C-C2C	5.00	1.47	1.36
37	C	213	KC1	C1A-NA	5.00	1.47	1.38
37	P	315	KC1	O2D-CGD	5.00	1.45	1.33
36	a	848	CLA	O2D-CGD	4.99	1.45	1.33
36	C	207	CLA	O2D-CGD	4.99	1.45	1.33
37	O	313	KC1	O2D-CGD	4.99	1.45	1.33
37	Q	313	KC1	C3D-C2D	4.98	1.48	1.39
37	Q	311	KC1	C3D-C2D	4.98	1.48	1.39
37	O	313	KC1	C3D-C2D	4.98	1.48	1.39
37	K	314	KC1	C2A-C3A	4.98	1.47	1.37
36	E	315	CLA	O2D-CGD	4.98	1.45	1.33
37	J	314	KC1	O2D-CGD	4.98	1.45	1.33
36	D	309	CLA	C3C-C2C	4.98	1.47	1.36
36	f	804	CLA	O2D-CGD	4.98	1.45	1.33
36	b	836	CLA	CHC-C1C	4.97	1.47	1.35
37	F	315	KC1	C4D-ND	4.97	1.39	1.35
37	D	314	KC1	O2D-CGD	4.97	1.45	1.33
36	l	204	CLA	O2D-CGD	4.97	1.45	1.33
36	l	204	CLA	C3B-C2B	4.97	1.47	1.40
35	O	305	A86	C32-C31	-4.96	1.46	1.54
36	O	316	CLA	CHC-C1C	4.96	1.47	1.35
37	W	213	KC1	CHB-C1B	4.96	1.48	1.38
36	a	806	CLA	O2D-CGD	4.96	1.45	1.33
36	a	822	CLA	O2D-CGD	4.95	1.45	1.33
35	T	302	A86	O4-C38	4.95	1.46	1.35
37	O	315	KC1	C3D-C2D	4.94	1.48	1.39
37	Q	313	KC1	C4D-ND	4.94	1.39	1.35
37	Q	311	KC1	C4D-ND	4.94	1.39	1.35
37	N	314	KC1	C3D-C2D	4.94	1.48	1.39
37	H	313	KC1	O2D-CGD	4.93	1.45	1.33
36	C	207	CLA	CHC-C1C	4.93	1.47	1.35
37	B	310	KC1	C3D-C2D	4.93	1.48	1.39
37	S	316	KC1	C3D-C2D	4.93	1.48	1.39
36	a	823	CLA	C3B-C2B	4.93	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	824	CLA	C3C-C2C	4.93	1.47	1.36
35	M	305	A86	O4-C38	4.93	1.46	1.35
36	j	102	CLA	C3C-C2C	4.93	1.47	1.36
36	l	205	CLA	O2D-CGD	4.93	1.45	1.33
36	b	817	CLA	O2D-CGD	4.92	1.45	1.33
35	V	302	A86	O4-C38	4.92	1.46	1.35
37	P	317	KC1	C1A-NA	4.92	1.47	1.38
35	Q	303	A86	O4-C38	4.92	1.46	1.35
37	O	315	KC1	C4D-ND	4.92	1.39	1.35
37	H	313	KC1	C3B-C2B	4.92	1.47	1.37
37	G	308	KC1	C3B-C2B	4.91	1.47	1.37
36	b	836	CLA	C3C-C2C	4.91	1.47	1.36
37	J	314	KC1	C3B-C2B	4.91	1.47	1.37
37	L	315	KC1	CHB-C1B	4.90	1.47	1.38
36	B	309	CLA	C3C-C2C	4.90	1.47	1.36
37	M	317	KC1	O2D-CGD	4.90	1.45	1.33
36	B	308	CLA	C1D-ND	4.90	1.43	1.37
37	K	314	KC1	C3B-C2B	4.89	1.47	1.37
36	N	319	CLA	C4C-C3C	4.89	1.53	1.45
36	C	207	CLA	C3C-C2C	4.89	1.47	1.36
35	K	306	A86	O4-C38	4.89	1.46	1.35
37	O	315	KC1	CHB-C1B	4.88	1.47	1.38
36	f	804	CLA	C3C-C2C	4.88	1.47	1.36
37	Q	311	KC1	CHB-C1B	4.88	1.47	1.38
35	D	302	A86	O4-C38	4.88	1.46	1.35
37	F	315	KC1	C3B-C2B	4.88	1.47	1.37
36	A	306	CLA	CHC-C1C	4.87	1.47	1.35
37	K	314	KC1	C1A-NA	4.87	1.47	1.38
36	G	319	CLA	CHC-C1C	4.87	1.47	1.35
37	Q	313	KC1	CHB-C1B	4.87	1.47	1.38
36	W	216	CLA	C1D-ND	4.86	1.43	1.37
37	C	213	KC1	O2D-CGD	4.86	1.45	1.33
36	I	306	CLA	C3C-C2C	4.86	1.47	1.36
36	E	315	CLA	CHC-C1C	4.86	1.47	1.35
37	O	313	KC1	CHB-C1B	4.86	1.47	1.38
35	F	306	A86	O4-C38	4.86	1.46	1.35
36	A	306	CLA	C3C-C2C	4.85	1.47	1.36
37	A	312	KC1	C3B-C2B	4.84	1.47	1.37
37	P	315	KC1	CHB-C1B	4.84	1.47	1.38
37	U	312	KC1	C3D-C2D	4.84	1.48	1.39
35	G	304	A86	O4-C38	4.84	1.46	1.35
37	G	317	KC1	C3B-C2B	4.84	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	315	CLA	C1D-ND	4.83	1.43	1.37
35	R	302	A86	O4-C38	4.83	1.46	1.35
35	H	301	A86	O4-C38	4.83	1.46	1.35
35	V	304	A86	O4-C38	4.83	1.46	1.35
36	O	316	CLA	C3C-C2C	4.82	1.47	1.36
37	D	314	KC1	C1A-NA	4.82	1.47	1.38
35	J	306	A86	O4-C38	4.82	1.46	1.35
37	P	317	KC1	O2D-CGD	4.81	1.44	1.33
37	B	310	KC1	OBD-CAD	4.81	1.29	1.22
35	O	303	A86	O4-C38	4.81	1.46	1.35
35	X	302	A86	O4-C38	4.81	1.46	1.35
37	N	314	KC1	CHC-C4B	4.81	1.47	1.38
37	L	315	KC1	CHC-C4B	4.80	1.47	1.38
37	G	308	KC1	O2D-CGD	4.80	1.44	1.33
35	Q	301	A86	O4-C38	4.80	1.46	1.35
37	H	313	KC1	C2A-C3A	4.79	1.47	1.37
37	R	317	KC1	C3B-C2B	4.79	1.47	1.37
35	U	304	A86	O4-C38	4.79	1.46	1.35
35	N	304	A86	O4-C38	4.79	1.46	1.35
36	a	822	CLA	C3B-C2B	4.79	1.47	1.40
36	b	816	CLA	O2D-CGD	4.79	1.44	1.33
37	E	309	KC1	C3B-C2B	4.78	1.47	1.37
37	T	310	KC1	C4B-NB	-4.78	1.31	1.37
43	a	840	PQN	C10-C5	4.78	1.48	1.40
36	f	803	CLA	CHC-C1C	4.78	1.47	1.35
37	T	310	KC1	C3D-C2D	4.78	1.48	1.39
36	a	816	CLA	C3D-C4D	-4.78	1.33	1.44
36	a	802	CLA	C1B-NB	4.78	1.39	1.35
35	S	308	A86	O4-C38	4.77	1.46	1.35
35	F	301	A86	O4-C38	4.77	1.46	1.35
35	O	305	A86	O4-C38	4.77	1.46	1.35
37	W	213	KC1	OBD-CAD	4.77	1.29	1.22
35	I	301	A86	O4-C38	4.77	1.46	1.35
43	b	842	PQN	C10-C5	4.77	1.48	1.40
37	S	316	KC1	CHC-C4B	4.76	1.47	1.38
35	P	304	A86	O4-C38	4.76	1.46	1.35
36	G	319	CLA	C3C-C2C	4.76	1.46	1.36
37	A	312	KC1	C3C-C2C	4.76	1.46	1.36
35	G	302	A86	O4-C38	4.76	1.46	1.35
36	f	803	CLA	C3C-C2C	4.76	1.46	1.36
35	J	302	A86	O4-C38	4.76	1.46	1.35
36	a	823	CLA	C3C-C2C	4.76	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	203	A86	O4-C38	4.75	1.45	1.35
35	T	301	A86	O4-C38	4.75	1.45	1.35
35	F	302	A86	O4-C38	4.75	1.45	1.35
35	G	306	A86	O4-C38	4.74	1.45	1.35
35	C	204	A86	O4-C38	4.74	1.45	1.35
35	T	306	A86	O4-C38	4.74	1.45	1.35
37	M	313	KC1	CHC-C4B	4.74	1.47	1.38
37	R	317	KC1	C3D-C2D	4.74	1.47	1.39
35	H	304	A86	O4-C38	4.74	1.45	1.35
37	F	315	KC1	C3C-C2C	4.73	1.46	1.36
35	M	304	A86	O4-C38	4.73	1.45	1.35
35	S	302	A86	O4-C38	4.73	1.45	1.35
36	b	817	CLA	C3C-C2C	4.72	1.46	1.36
35	L	304	A86	O4-C38	4.72	1.45	1.35
35	P	306	A86	O4-C38	4.72	1.45	1.35
35	N	306	A86	O4-C38	4.72	1.45	1.35
37	D	314	KC1	C3B-C2B	4.72	1.46	1.37
35	N	302	A86	O4-C38	4.72	1.45	1.35
35	X	314	A86	O4-C38	4.71	1.45	1.35
36	C	207	CLA	C3B-C2B	4.71	1.46	1.40
35	J	305	A86	O4-C38	4.71	1.45	1.35
37	M	318	KC1	CHC-C4B	4.71	1.47	1.38
37	E	309	KC1	O2D-CGD	4.71	1.44	1.33
36	K	307	CLA	CHC-C1C	4.71	1.47	1.35
35	S	304	A86	O4-C38	4.71	1.45	1.35
37	A	312	KC1	O2D-CGD	4.70	1.44	1.33
35	R	305	A86	O4-C38	4.70	1.45	1.35
35	E	307	A86	O4-C38	4.70	1.45	1.35
37	W	213	KC1	CHC-C4B	4.69	1.47	1.38
36	V	305	CLA	C1D-ND	4.69	1.43	1.37
35	A	316	A86	O4-C38	4.69	1.45	1.35
37	B	310	KC1	CHB-C1B	4.69	1.47	1.38
37	M	318	KC1	CHB-C1B	4.68	1.47	1.38
35	G	305	A86	O4-C38	4.68	1.45	1.35
37	V	312	KC1	CHC-C4B	4.68	1.47	1.38
35	B	303	A86	O4-C38	4.68	1.45	1.35
35	L	301	A86	O4-C38	4.68	1.45	1.35
37	N	314	KC1	CHB-C1B	4.67	1.47	1.38
35	h	202	A86	O4-C38	4.67	1.45	1.35
35	O	301	A86	O4-C38	4.67	1.45	1.35
35	K	301	A86	O4-C38	4.67	1.45	1.35
35	P	307	A86	O4-C38	4.67	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	L	307	A86	O4-C38	4.66	1.45	1.35
35	V	301	A86	O4-C38	4.66	1.45	1.35
35	U	303	A86	O4-C38	4.66	1.45	1.35
37	F	315	KC1	O2D-CGD	4.65	1.44	1.33
37	L	315	KC1	OBD-CAD	4.65	1.28	1.22
37	C	213	KC1	CHC-C4B	4.65	1.47	1.38
36	A	306	CLA	C3D-C4D	-4.65	1.33	1.44
37	G	318	KC1	C3B-C2B	4.65	1.46	1.37
37	L	315	KC1	C3D-C2D	4.64	1.47	1.39
37	O	313	KC1	CHC-C4B	4.64	1.47	1.38
37	R	317	KC1	CHC-C4B	4.64	1.47	1.38
35	E	305	A86	O4-C38	4.64	1.45	1.35
35	U	302	A86	O4-C38	4.64	1.45	1.35
35	J	301	A86	O4-C38	4.64	1.45	1.35
37	V	312	KC1	CHB-C1B	4.64	1.47	1.38
35	F	304	A86	O4-C38	4.64	1.45	1.35
37	C	213	KC1	CHB-C1B	4.63	1.47	1.38
38	b	804	SQD	O8-S	4.63	1.64	1.47
37	Q	313	KC1	CHC-C4B	4.63	1.47	1.38
36	U	306	CLA	C3B-C2B	4.63	1.46	1.40
37	Q	311	KC1	CHC-C4B	4.62	1.47	1.38
37	F	308	KC1	O2D-CGD	4.62	1.44	1.33
36	I	305	CLA	C14-C13	4.62	1.67	1.52
36	l	205	CLA	CHC-C1C	4.62	1.46	1.35
35	O	319	A86	O4-C38	4.61	1.45	1.35
36	A	306	CLA	C1D-ND	4.61	1.43	1.37
35	B	301	A86	O4-C38	4.61	1.45	1.35
37	M	313	KC1	C3D-C2D	4.61	1.47	1.39
36	b	841	CLA	C4B-NB	4.61	1.39	1.35
37	P	315	KC1	OBD-CAD	4.60	1.28	1.22
38	A	315	SQD	O8-S	4.60	1.63	1.47
37	N	314	KC1	OBD-CAD	4.59	1.28	1.22
37	O	313	KC1	OBD-CAD	4.59	1.28	1.22
37	G	318	KC1	C3D-C2D	4.59	1.47	1.39
37	O	315	KC1	CHC-C4B	4.58	1.47	1.38
37	M	317	KC1	CHC-C4B	4.58	1.47	1.38
37	F	308	KC1	C3B-C2B	4.58	1.46	1.37
37	Q	313	KC1	OBD-CAD	4.58	1.28	1.22
35	N	305	A86	O4-C38	4.57	1.45	1.35
37	P	315	KC1	CHC-C4B	4.57	1.47	1.38
35	Q	316	A86	O4-C38	4.57	1.45	1.35
37	T	315	KC1	CHC-C4B	4.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	U	312	KC1	CHC-C4B	4.56	1.47	1.38
37	J	314	KC1	C3D-C2D	4.56	1.47	1.39
37	Q	311	KC1	OBD-CAD	4.56	1.28	1.22
37	O	315	KC1	OBD-CAD	4.56	1.28	1.22
35	E	302	A86	O4-C38	4.55	1.45	1.35
37	R	317	KC1	OBD-CAD	4.55	1.28	1.22
37	K	314	KC1	CHB-C1B	4.54	1.47	1.38
35	h	204	A86	O4-C38	4.54	1.45	1.35
37	H	313	KC1	C3D-C2D	4.54	1.47	1.39
37	X	311	KC1	OBD-CAD	4.53	1.28	1.22
36	X	313	CLA	C1D-ND	4.53	1.43	1.37
35	S	305	A86	O4-C38	4.52	1.45	1.35
36	G	307	CLA	O2D-CGD	4.52	1.45	1.30
37	X	311	KC1	CHB-C1B	4.52	1.47	1.38
37	W	217	KC1	OBD-CAD	4.51	1.28	1.22
37	H	313	KC1	CHC-C4B	4.51	1.47	1.38
37	T	315	KC1	OBD-CAD	4.51	1.28	1.22
36	G	307	CLA	C3D-C4D	-4.51	1.34	1.44
37	V	312	KC1	C3D-C2D	4.51	1.47	1.39
37	S	316	KC1	OBD-CAD	4.51	1.28	1.22
36	a	848	CLA	C3D-C4D	-4.51	1.34	1.44
37	M	317	KC1	CHB-C1B	4.51	1.47	1.38
37	G	308	KC1	C3D-C2D	4.51	1.47	1.39
36	f	803	CLA	C3B-C2B	4.50	1.46	1.40
35	L	306	A86	O4-C38	4.50	1.45	1.35
37	F	315	KC1	C3D-C2D	4.50	1.47	1.39
36	b	841	CLA	C4D-ND	-4.50	1.31	1.37
36	M	310	CLA	C1B-NB	-4.49	1.31	1.35
37	F	308	KC1	C3D-C2D	4.49	1.47	1.39
36	I	308	CLA	C3D-C4D	-4.49	1.34	1.44
37	E	309	KC1	C3D-C2D	4.48	1.47	1.39
37	W	217	KC1	CHB-C1B	4.48	1.47	1.38
35	R	309	A86	O4-C38	4.47	1.45	1.35
37	D	314	KC1	C3D-C2D	4.46	1.47	1.39
37	C	213	KC1	C3D-C2D	4.46	1.47	1.39
37	P	317	KC1	C3B-C2B	4.46	1.46	1.37
36	H	307	CLA	C1D-ND	4.45	1.43	1.37
37	E	309	KC1	CHC-C4B	4.45	1.47	1.38
37	B	310	KC1	CHC-C4B	4.44	1.47	1.38
37	L	317	KC1	CHC-C4B	4.43	1.47	1.38
35	G	304	A86	O1-C20	-4.43	1.39	1.46
36	E	310	CLA	C4D-ND	-4.43	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	309	CLA	C3B-C2B	4.42	1.46	1.40
37	G	317	KC1	OBD-CAD	4.41	1.28	1.22
37	M	318	KC1	C2A-C1A	4.41	1.58	1.44
37	U	312	KC1	CHB-C4A	4.41	1.49	1.39
36	E	313	CLA	CHC-C1C	4.40	1.46	1.35
37	F	315	KC1	OBD-CAD	4.40	1.28	1.22
37	D	314	KC1	CHB-C1B	4.40	1.46	1.38
37	K	314	KC1	C3D-C2D	4.40	1.47	1.39
37	P	317	KC1	C3D-C2D	4.40	1.47	1.39
37	M	318	KC1	C3B-C4B	4.40	1.54	1.46
37	L	317	KC1	C3D-C2D	4.39	1.47	1.39
37	X	311	KC1	CHC-C4B	4.39	1.46	1.38
37	W	217	KC1	CHC-C4B	4.38	1.46	1.38
37	G	308	KC1	CHB-C1B	4.38	1.46	1.38
37	T	315	KC1	C3D-C2D	4.37	1.47	1.39
36	F	317	CLA	CHC-C1C	4.37	1.46	1.35
36	b	817	CLA	C3D-C4D	-4.36	1.34	1.44
36	l	204	CLA	C3D-C4D	-4.36	1.34	1.44
36	V	314	CLA	CHC-C1C	4.36	1.46	1.35
37	T	310	KC1	C2A-C1A	4.36	1.58	1.44
35	Q	304	A86	O4-C38	4.36	1.45	1.35
36	G	319	CLA	O2A-CGA	4.35	1.46	1.33
37	F	315	KC1	CHC-C4B	4.35	1.46	1.38
35	N	305	A86	O1-C20	-4.35	1.40	1.46
37	G	308	KC1	CHC-C4B	4.34	1.46	1.38
36	b	828	CLA	C4D-ND	-4.34	1.31	1.37
42	V	316	LMG	O8-C28	4.34	1.46	1.33
36	V	314	CLA	C3C-C2C	4.34	1.45	1.36
36	G	319	CLA	C3B-C2B	4.34	1.46	1.40
36	E	313	CLA	C3C-C2C	4.33	1.45	1.36
35	A	302	A86	C30-C29	-4.33	1.24	1.32
41	I	316	LHG	O8-C23	4.33	1.46	1.33
37	D	314	KC1	CHC-C4B	4.32	1.46	1.38
35	Q	316	A86	O1-C20	-4.32	1.40	1.46
35	R	301	A86	C30-C29	-4.32	1.24	1.32
36	I	308	CLA	O2A-CGA	4.32	1.46	1.33
36	G	315	CLA	CHC-C1C	4.32	1.46	1.35
42	G	324	LMG	O8-C28	4.32	1.46	1.33
35	N	320	A86	O4-C38	4.31	1.44	1.35
37	G	317	KC1	C3D-C2D	4.31	1.47	1.39
42	V	315	LMG	O8-C28	4.30	1.45	1.33
40	L	302	DGD	O1G-C1A	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	h	206	LMG	O8-C28	4.30	1.45	1.33
36	K	307	CLA	O2A-CGA	4.30	1.45	1.33
41	F	319	LHG	O8-C23	4.29	1.45	1.33
36	E	315	CLA	C3D-C4D	-4.29	1.34	1.44
37	E	309	KC1	CHB-C1B	4.29	1.46	1.38
36	K	307	CLA	C3C-C2C	4.29	1.45	1.36
37	K	314	KC1	CHC-C4B	4.29	1.46	1.38
41	G	320	LHG	O8-C23	4.29	1.45	1.33
41	f	808	LHG	O8-C23	4.29	1.45	1.33
37	F	315	KC1	CHB-C1B	4.29	1.46	1.38
37	L	317	KC1	CHB-C1B	4.29	1.46	1.38
36	U	306	CLA	O2A-CGA	4.28	1.45	1.33
41	f	809	LHG	O8-C23	4.28	1.45	1.33
36	L	308	CLA	O2A-CGA	4.28	1.45	1.33
41	i	104	LHG	O8-C23	4.28	1.45	1.33
37	G	317	KC1	CHC-C4B	4.28	1.46	1.38
42	E	318	LMG	O8-C28	4.28	1.45	1.33
36	G	315	CLA	O2A-CGA	4.27	1.45	1.33
37	G	317	KC1	CHB-C1B	4.27	1.46	1.38
36	D	309	CLA	C3B-C2B	4.27	1.46	1.40
42	m	102	LMG	O8-C28	4.27	1.45	1.33
37	P	317	KC1	CHB-C1B	4.27	1.46	1.38
36	A	306	CLA	O2A-CGA	4.27	1.45	1.33
37	M	313	KC1	CHB-C1B	4.26	1.46	1.38
36	b	816	CLA	C3D-C4D	-4.26	1.34	1.44
41	l	208	LHG	O8-C23	4.26	1.45	1.33
37	L	317	KC1	OBD-CAD	4.26	1.28	1.22
41	G	321	LHG	O8-C23	4.26	1.45	1.33
41	a	850	LHG	O8-C23	4.26	1.45	1.33
36	E	315	CLA	C3B-C2B	4.26	1.46	1.40
37	T	310	KC1	CHB-C1B	4.26	1.46	1.38
35	F	305	A86	O4-C38	4.26	1.44	1.35
42	G	325	LMG	O8-C28	4.26	1.45	1.33
36	a	822	CLA	O2A-CGA	4.26	1.45	1.33
36	b	817	CLA	O2A-CGA	4.26	1.45	1.33
36	b	801	CLA	C4D-ND	-4.25	1.31	1.37
36	l	205	CLA	O2A-CGA	4.25	1.45	1.33
36	b	816	CLA	O2A-CGA	4.25	1.45	1.33
36	I	308	CLA	C3C-C2C	4.25	1.45	1.36
36	f	803	CLA	O2A-CGA	4.25	1.45	1.33
36	F	317	CLA	O2A-CGA	4.25	1.45	1.33
41	Q	315	LHG	O8-C23	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	D	321	LMG	O8-C28	4.24	1.45	1.33
41	R	323	LHG	O8-C23	4.24	1.45	1.33
35	T	304	A86	O4-C38	4.24	1.44	1.35
36	V	314	CLA	O2A-CGA	4.24	1.45	1.33
36	a	802	CLA	O2A-CGA	4.24	1.45	1.33
36	f	804	CLA	O2A-CGA	4.24	1.45	1.33
36	a	823	CLA	O2A-CGA	4.24	1.45	1.33
36	j	102	CLA	O2A-CGA	4.23	1.45	1.33
37	P	317	KC1	CHC-C4B	4.23	1.46	1.38
42	D	320	LMG	O8-C28	4.23	1.45	1.33
37	G	318	KC1	CHB-C1B	4.23	1.46	1.38
41	E	322	LHG	O8-C23	4.23	1.45	1.33
36	l	204	CLA	O2A-CGA	4.23	1.45	1.33
38	b	804	SQD	O48-C23	4.23	1.45	1.33
40	C	215	DGD	O1G-C1A	4.23	1.45	1.33
42	a	852	LMG	O8-C28	4.22	1.45	1.33
42	J	319	LMG	O8-C28	4.22	1.45	1.33
37	A	312	KC1	OBD-CAD	4.22	1.28	1.22
36	F	317	CLA	C3C-C2C	4.22	1.45	1.36
36	D	308	CLA	C4D-ND	-4.22	1.31	1.37
36	b	836	CLA	O2A-CGA	4.22	1.45	1.33
42	E	319	LMG	O8-C28	4.22	1.45	1.33
36	E	313	CLA	O2A-CGA	4.22	1.45	1.33
37	T	315	KC1	CHB-C1B	4.22	1.46	1.38
36	l	204	CLA	CHC-C1C	4.21	1.45	1.35
41	j	104	LHG	O8-C23	4.21	1.45	1.33
36	B	309	CLA	O2A-CGA	4.21	1.45	1.33
41	i	104	LHG	O7-C7	4.21	1.46	1.34
36	D	309	CLA	O2A-CGA	4.21	1.45	1.33
42	L	321	LMG	O8-C28	4.21	1.45	1.33
36	a	806	CLA	O2A-CGA	4.20	1.45	1.33
37	A	312	KC1	CHC-C4B	4.20	1.46	1.38
36	a	816	CLA	C1B-NB	4.20	1.39	1.35
36	O	316	CLA	O2A-CGA	4.20	1.45	1.33
41	D	319	LHG	O8-C23	4.20	1.45	1.33
37	J	314	KC1	CHC-C4B	4.19	1.46	1.38
36	W	212	CLA	C4D-ND	-4.19	1.31	1.37
41	b	850	LHG	O8-C23	4.19	1.45	1.33
36	f	804	CLA	C3B-C2B	4.19	1.46	1.40
36	E	315	CLA	O2A-CGA	4.19	1.45	1.33
36	G	307	CLA	CHC-C1C	4.19	1.45	1.35
41	a	843	LHG	O8-C23	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	816	CLA	O2A-CGA	4.18	1.45	1.33
36	a	825	CLA	O2A-CGA	4.18	1.45	1.33
36	b	824	CLA	C3D-C4D	-4.18	1.34	1.44
37	T	310	KC1	CAB-C3B	4.18	1.58	1.47
41	O	317	LHG	O8-C23	4.17	1.45	1.33
36	A	306	CLA	C3B-C2B	4.17	1.46	1.40
36	a	848	CLA	O2A-CGA	4.17	1.45	1.33
42	j	105	LMG	O8-C28	4.17	1.45	1.33
36	I	306	CLA	O2A-CGA	4.17	1.45	1.33
36	b	824	CLA	O2A-CGA	4.17	1.45	1.33
36	K	310	CLA	C3D-C4D	-4.17	1.34	1.44
37	G	318	KC1	CHC-C4B	4.17	1.46	1.38
36	a	830	CLA	O2A-CGA	4.16	1.45	1.33
37	M	313	KC1	OBD-CAD	4.16	1.28	1.22
36	U	309	CLA	C1D-ND	4.16	1.42	1.37
37	U	312	KC1	OBD-CAD	4.16	1.28	1.22
36	C	207	CLA	O2A-CGA	4.16	1.45	1.33
42	I	315	LMG	O8-C28	4.16	1.45	1.33
41	f	808	LHG	O7-C7	4.15	1.46	1.34
36	S	314	CLA	C1D-ND	4.15	1.42	1.37
37	J	314	KC1	CHB-C1B	4.15	1.46	1.38
37	F	308	KC1	CHB-C1B	4.15	1.46	1.38
41	G	321	LHG	O7-C7	4.15	1.46	1.34
42	G	324	LMG	O7-C10	4.14	1.46	1.34
36	K	313	CLA	C4D-ND	-4.14	1.32	1.37
37	F	308	KC1	OBD-CAD	4.14	1.28	1.22
41	G	320	LHG	O7-C7	4.14	1.46	1.34
36	X	307	CLA	C1D-ND	4.14	1.42	1.37
35	S	301	A86	O1-C20	-4.13	1.40	1.46
35	N	301	A86	O1-C20	-4.13	1.40	1.46
37	E	309	KC1	OBD-CAD	4.13	1.28	1.22
42	J	318	LMG	O8-C28	4.12	1.45	1.33
41	I	316	LHG	O7-C7	4.12	1.45	1.34
36	X	310	CLA	C1D-ND	4.12	1.42	1.37
36	C	210	CLA	C1D-ND	4.11	1.42	1.37
42	a	852	LMG	O7-C10	4.11	1.45	1.34
36	N	315	CLA	C1D-ND	4.11	1.42	1.37
36	K	310	CLA	O2A-CGA	4.11	1.45	1.33
37	G	308	KC1	OBD-CAD	4.11	1.28	1.22
42	D	321	LMG	O7-C10	4.11	1.45	1.34
41	F	319	LHG	O7-C7	4.10	1.45	1.34
42	D	320	LMG	O7-C10	4.10	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	V	315	LMG	O7-C10	4.10	1.45	1.34
40	C	215	DGD	O2G-C1B	4.10	1.45	1.34
36	f	804	CLA	MG-NA	4.10	2.16	2.06
42	V	316	LMG	O7-C10	4.09	1.45	1.34
41	a	850	LHG	O7-C7	4.09	1.45	1.34
36	X	308	CLA	C3B-C2B	-4.09	1.34	1.40
42	J	318	LMG	O7-C10	4.09	1.45	1.34
38	b	804	SQD	O47-C7	4.08	1.45	1.34
42	E	319	LMG	O7-C10	4.08	1.45	1.34
37	V	312	KC1	OBD-CAD	4.08	1.28	1.22
42	I	315	LMG	O7-C10	4.08	1.45	1.34
42	m	102	LMG	O7-C10	4.07	1.45	1.34
41	f	809	LHG	O7-C7	4.07	1.45	1.34
41	j	104	LHG	O7-C7	4.07	1.45	1.34
41	E	322	LHG	O7-C7	4.07	1.45	1.34
41	Q	315	LHG	O7-C7	4.07	1.45	1.34
38	A	315	SQD	O47-C7	4.07	1.45	1.34
41	R	323	LHG	O7-C7	4.06	1.45	1.34
36	f	804	CLA	C3D-C4D	-4.06	1.35	1.44
42	J	319	LMG	O7-C10	4.05	1.45	1.34
42	G	325	LMG	O7-C10	4.05	1.45	1.34
36	a	848	CLA	C4D-ND	-4.05	1.32	1.37
41	l	208	LHG	O7-C7	4.05	1.45	1.34
37	F	308	KC1	CHC-C4B	4.04	1.46	1.38
36	L	308	CLA	C3B-C2B	4.04	1.46	1.40
36	L	308	CLA	C4B-CHC	4.04	1.52	1.41
42	L	321	LMG	O7-C10	4.04	1.45	1.34
41	O	317	LHG	O7-C7	4.04	1.45	1.34
42	E	318	LMG	O7-C10	4.04	1.45	1.34
36	E	317	CLA	C1D-ND	4.03	1.42	1.37
37	C	213	KC1	OBD-CAD	4.03	1.27	1.22
36	G	307	CLA	C3C-C2C	4.03	1.45	1.36
41	D	319	LHG	O7-C7	4.02	1.45	1.34
37	M	317	KC1	OBD-CAD	4.02	1.27	1.22
35	A	302	A86	O1-C20	-4.01	1.40	1.46
36	S	315	CLA	C1D-ND	4.01	1.42	1.37
36	K	310	CLA	C3B-C2B	4.01	1.45	1.40
42	h	206	LMG	O7-C10	4.00	1.45	1.34
36	a	827	CLA	C4D-ND	-4.00	1.32	1.37
41	a	843	LHG	O7-C7	4.00	1.45	1.34
36	C	207	CLA	C3D-C2D	4.00	1.50	1.39
35	T	307	A86	O4-C38	3.99	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	U	302	A86	O1-C20	-3.99	1.40	1.46
35	M	301	A86	O1-C20	-3.99	1.40	1.46
36	A	314	CLA	OBD-CAD	3.98	1.29	1.22
40	L	302	DGD	O2G-C1B	3.97	1.45	1.34
36	W	209	CLA	C1D-ND	3.97	1.42	1.37
35	Q	303	A86	C30-C29	-3.96	1.25	1.32
36	N	309	CLA	C1D-ND	3.95	1.42	1.37
37	H	313	KC1	OBD-CAD	3.95	1.27	1.22
35	L	304	A86	O1-C20	-3.95	1.40	1.46
35	O	305	A86	C30-C29	-3.95	1.25	1.32
36	a	829	CLA	CMB-C2B	-3.95	1.43	1.51
36	U	305	CLA	C1D-ND	3.95	1.42	1.37
36	G	315	CLA	C1D-ND	3.93	1.42	1.37
42	j	105	LMG	O7-C10	3.93	1.45	1.34
36	X	306	CLA	C1D-ND	3.93	1.42	1.37
35	I	304	A86	O1-C20	-3.92	1.40	1.46
36	S	311	CLA	C1D-ND	3.92	1.42	1.37
36	L	316	CLA	C1D-ND	3.92	1.42	1.37
37	O	313	KC1	CHB-C4A	3.91	1.48	1.39
37	N	314	KC1	C4D-CHA	3.91	1.49	1.45
37	P	315	KC1	CHB-C4A	3.90	1.48	1.39
36	b	806	CLA	C4D-ND	-3.90	1.32	1.37
36	f	803	CLA	C1D-ND	3.90	1.42	1.37
35	O	302	A86	O1-C20	-3.89	1.40	1.46
35	C	202	A86	O1-C20	-3.89	1.40	1.46
35	X	301	A86	C30-C29	-3.89	1.25	1.32
36	f	803	CLA	C3D-C4D	-3.89	1.35	1.44
37	Q	313	KC1	CHB-C4A	3.89	1.48	1.39
35	X	304	A86	O1-C20	-3.89	1.40	1.46
37	O	315	KC1	CHB-C4A	3.89	1.48	1.39
41	b	850	LHG	O7-C7	3.89	1.45	1.34
37	L	315	KC1	CHB-C4A	3.89	1.48	1.39
37	Q	311	KC1	CHB-C4A	3.89	1.48	1.39
36	G	315	CLA	C3B-C2B	3.88	1.45	1.40
36	G	315	CLA	C3C-C2C	3.87	1.44	1.36
36	b	818	CLA	C4D-ND	-3.87	1.32	1.37
37	A	312	KC1	CHB-C1B	3.87	1.45	1.38
36	S	320	CLA	C1D-ND	3.86	1.42	1.37
37	T	315	KC1	C4D-CHA	3.86	1.49	1.45
37	X	311	KC1	C4D-CHA	3.86	1.49	1.45
35	R	301	A86	O1-C20	-3.86	1.40	1.46
36	J	313	CLA	C4D-ND	-3.86	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	K	314	KC1	OBD-CAD	3.86	1.27	1.22
37	M	317	KC1	C3D-C2D	3.85	1.46	1.39
35	W	203	A86	C30-C29	-3.85	1.25	1.32
35	R	304	A86	O1-C20	-3.84	1.40	1.46
37	M	318	KC1	CHB-C4A	-3.84	1.30	1.39
36	b	826	CLA	O2D-CGD	3.84	1.42	1.33
35	S	304	A86	C30-C29	-3.84	1.25	1.32
36	a	801	CLA	C4D-ND	-3.84	1.32	1.37
36	L	312	CLA	C1D-ND	3.84	1.42	1.37
36	O	316	CLA	C3B-C2B	3.84	1.45	1.40
35	L	319	A86	O1-C20	-3.83	1.40	1.46
35	L	304	A86	C30-C29	-3.83	1.25	1.32
37	W	217	KC1	C4D-CHA	3.83	1.49	1.45
36	a	813	CLA	C4D-ND	-3.83	1.32	1.37
35	H	301	A86	O1-C20	-3.83	1.40	1.46
36	a	802	CLA	C4D-ND	-3.82	1.32	1.37
36	a	831	CLA	C4D-ND	-3.82	1.32	1.37
36	R	322	CLA	C4D-ND	-3.82	1.32	1.37
36	W	210	CLA	C1D-ND	3.81	1.42	1.37
36	Q	310	CLA	C2-C3	3.81	1.42	1.33
36	a	817	CLA	C4D-ND	-3.81	1.32	1.37
37	R	317	KC1	CHB-C1B	3.81	1.45	1.38
35	B	303	A86	O1-C20	-3.81	1.40	1.46
36	A	314	CLA	C1D-ND	3.80	1.42	1.37
36	a	841	CLA	C4D-ND	-3.80	1.32	1.37
35	K	302	A86	O1-C20	-3.80	1.40	1.46
36	B	307	CLA	C1D-ND	3.80	1.42	1.37
36	W	215	CLA	C4D-ND	-3.80	1.32	1.37
36	a	824	CLA	C4D-ND	-3.80	1.32	1.37
35	P	303	A86	O1-C20	-3.80	1.40	1.46
35	T	307	A86	O1-C20	-3.79	1.40	1.46
36	S	317	CLA	C1D-ND	3.79	1.42	1.37
34	D	303	DD6	C24-C1	3.79	1.54	1.45
36	a	810	CLA	C4D-ND	-3.79	1.32	1.37
35	R	309	A86	O1-C20	-3.79	1.40	1.46
35	X	303	A86	O1-C20	-3.79	1.40	1.46
36	R	319	CLA	C1D-ND	3.78	1.42	1.37
37	A	312	KC1	C4D-ND	3.78	1.38	1.35
36	V	306	CLA	C4D-ND	-3.78	1.32	1.37
35	J	306	A86	C30-C29	-3.78	1.25	1.32
36	L	308	CLA	C1D-ND	3.78	1.42	1.37
35	V	304	A86	C19-C20	3.78	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	O	301	A86	C30-C29	-3.77	1.25	1.32
35	X	305	A86	O1-C20	-3.77	1.40	1.46
36	A	307	CLA	C4D-ND	-3.77	1.32	1.37
36	U	313	CLA	C1D-ND	3.77	1.42	1.37
37	J	314	KC1	OBD-CAD	3.77	1.27	1.22
36	R	314	CLA	C1D-ND	3.77	1.42	1.37
36	O	312	CLA	C2A-C1A	3.76	1.56	1.51
36	M	310	CLA	C4D-ND	-3.76	1.32	1.37
36	X	313	CLA	C3B-C2B	3.76	1.45	1.40
35	F	304	A86	C30-C29	-3.76	1.25	1.32
35	K	303	A86	O1-C20	-3.76	1.40	1.46
36	K	311	CLA	C1D-ND	3.76	1.42	1.37
37	W	213	KC1	CHB-C4A	3.75	1.47	1.39
37	P	317	KC1	OBD-CAD	3.75	1.27	1.22
36	N	313	CLA	C1D-ND	3.75	1.42	1.37
36	M	307	CLA	C4D-ND	-3.74	1.32	1.37
35	C	204	A86	C30-C29	-3.74	1.25	1.32
35	J	301	A86	C30-C29	-3.74	1.25	1.32
36	J	308	CLA	C1D-ND	3.74	1.42	1.37
37	T	310	KC1	CHC-C4B	3.74	1.45	1.38
36	J	311	CLA	C1D-ND	3.74	1.42	1.37
35	V	304	A86	C17-C18	-3.73	1.47	1.52
35	Q	304	A86	O1-C20	-3.73	1.40	1.46
36	N	318	CLA	C1D-ND	3.73	1.42	1.37
36	Q	310	CLA	CAA-CBA	3.73	1.64	1.52
37	T	310	KC1	C4A-C3A	3.73	1.51	1.44
36	K	310	CLA	CHD-C4C	3.73	1.47	1.39
36	U	306	CLA	OBD-CAD	3.73	1.28	1.22
36	S	313	CLA	C1D-ND	3.73	1.42	1.37
36	N	307	CLA	C1D-ND	3.73	1.42	1.37
35	M	305	A86	O1-C20	-3.73	1.40	1.46
35	N	320	A86	O1-C20	-3.72	1.40	1.46
36	R	320	CLA	C1D-ND	3.72	1.42	1.37
36	G	315	CLA	CHD-C4C	3.72	1.47	1.39
36	a	826	CLA	C4D-ND	-3.72	1.32	1.37
36	Q	310	CLA	C4D-ND	-3.72	1.32	1.37
35	H	304	A86	C30-C29	-3.72	1.25	1.32
36	V	307	CLA	C1D-ND	3.71	1.42	1.37
36	E	315	CLA	CHD-C4C	3.71	1.47	1.39
35	X	302	A86	O1-C20	-3.71	1.40	1.46
36	a	804	CLA	C4D-ND	-3.71	1.32	1.37
35	B	301	A86	C30-C29	-3.70	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	T	316	CLA	C1D-ND	3.70	1.42	1.37
36	N	311	CLA	C1D-ND	3.70	1.42	1.37
36	a	808	CLA	C4D-ND	-3.70	1.32	1.37
36	N	308	CLA	C4D-ND	-3.70	1.32	1.37
36	N	317	CLA	C1D-ND	3.70	1.42	1.37
36	J	315	CLA	C1D-ND	3.69	1.42	1.37
36	F	317	CLA	C1B-NB	-3.69	1.31	1.35
36	S	321	CLA	C1D-ND	3.69	1.42	1.37
36	a	829	CLA	C4D-ND	-3.69	1.32	1.37
36	T	313	CLA	C1D-ND	3.69	1.42	1.37
36	T	311	CLA	C4D-ND	-3.69	1.32	1.37
36	P	312	CLA	C1D-ND	3.69	1.42	1.37
36	b	816	CLA	CHD-C1D	3.69	1.45	1.38
36	I	306	CLA	C1B-NB	-3.69	1.31	1.35
35	J	305	A86	C30-C29	-3.69	1.25	1.32
36	Q	309	CLA	C1D-ND	3.69	1.42	1.37
36	b	824	CLA	C4D-ND	-3.68	1.32	1.37
36	b	831	CLA	C4D-ND	-3.68	1.32	1.37
36	I	308	CLA	OBD-CAD	3.68	1.28	1.22
35	L	301	A86	C30-C29	-3.68	1.25	1.32
36	X	312	CLA	C1D-ND	3.68	1.42	1.37
37	S	316	KC1	CHB-C1B	3.68	1.45	1.38
36	P	318	CLA	C4D-ND	-3.67	1.32	1.37
36	N	313	CLA	CHC-C1C	3.67	1.44	1.35
36	f	804	CLA	CHD-C4C	3.67	1.47	1.39
36	M	314	CLA	C1D-ND	3.67	1.42	1.37
36	a	825	CLA	C4D-ND	-3.67	1.32	1.37
36	N	316	CLA	C1D-ND	3.67	1.42	1.37
36	F	309	CLA	C4D-ND	-3.67	1.32	1.37
36	W	206	CLA	C1D-ND	3.67	1.42	1.37
36	Q	314	CLA	CHC-C1C	3.66	1.44	1.35
36	b	838	CLA	C4D-ND	-3.66	1.32	1.37
36	B	309	CLA	OBD-CAD	3.66	1.28	1.22
35	A	316	A86	C30-C29	-3.66	1.25	1.32
35	Q	301	A86	C30-C29	-3.66	1.25	1.32
36	X	315	CLA	C1D-ND	3.66	1.42	1.37
36	V	308	CLA	C1D-ND	3.66	1.42	1.37
36	L	308	CLA	OBD-CAD	3.66	1.28	1.22
36	b	815	CLA	C4D-ND	-3.66	1.32	1.37
36	l	204	CLA	C1C-NC	-3.66	1.32	1.37
35	J	302	A86	C30-C29	-3.65	1.25	1.32
37	B	310	KC1	CHB-C4A	3.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	312	CLA	C4D-ND	-3.65	1.32	1.37
36	f	802	CLA	C4D-ND	-3.65	1.32	1.37
35	P	307	A86	C30-C29	-3.65	1.25	1.32
35	V	301	A86	C30-C29	-3.65	1.25	1.32
36	S	318	CLA	C1D-ND	3.65	1.42	1.37
37	H	313	KC1	CHB-C1B	3.65	1.45	1.38
36	C	206	CLA	C1D-ND	3.65	1.42	1.37
36	T	308	CLA	C1D-ND	3.65	1.42	1.37
36	b	808	CLA	C4D-ND	-3.65	1.32	1.37
35	E	305	A86	C30-C29	-3.64	1.25	1.32
35	Q	316	A86	C30-C29	-3.64	1.25	1.32
36	B	311	CLA	C1D-ND	3.64	1.42	1.37
35	K	301	A86	C30-C29	-3.64	1.25	1.32
35	X	314	A86	C30-C29	-3.64	1.25	1.32
35	X	301	A86	C32-C31	3.64	1.60	1.54
36	R	318	CLA	C1D-ND	3.64	1.42	1.37
36	P	314	CLA	C4D-ND	-3.64	1.32	1.37
37	V	312	KC1	C4D-CHA	3.63	1.49	1.45
36	K	315	CLA	C1D-ND	3.63	1.42	1.37
37	V	312	KC1	CHB-C4A	3.63	1.47	1.39
36	E	311	CLA	C4D-ND	-3.63	1.32	1.37
36	K	310	CLA	C4D-ND	-3.63	1.32	1.37
36	H	312	CLA	C4D-ND	-3.63	1.32	1.37
35	N	305	A86	C30-C29	-3.63	1.25	1.32
35	E	307	A86	C30-C29	-3.63	1.25	1.32
36	b	839	CLA	C4D-ND	-3.63	1.32	1.37
37	F	308	KC1	C1B-NB	-3.63	1.33	1.37
36	F	309	CLA	C1D-ND	3.62	1.42	1.37
36	S	319	CLA	C1D-ND	3.62	1.42	1.37
36	G	307	CLA	OBD-CAD	3.62	1.28	1.22
36	O	316	CLA	OBD-CAD	3.62	1.28	1.22
36	Q	312	CLA	C1D-ND	3.62	1.42	1.37
36	W	207	CLA	C1D-ND	3.62	1.42	1.37
36	O	310	CLA	C1D-ND	3.62	1.42	1.37
36	O	312	CLA	C4D-ND	-3.62	1.32	1.37
35	F	302	A86	C30-C29	-3.62	1.25	1.32
36	F	312	CLA	C1D-ND	3.62	1.42	1.37
35	L	307	A86	C30-C29	-3.61	1.25	1.32
35	O	303	A86	C30-C29	-3.61	1.25	1.32
37	G	318	KC1	OBD-CAD	3.61	1.27	1.22
36	E	315	CLA	C4D-ND	-3.61	1.32	1.37
36	I	311	CLA	C4D-ND	-3.61	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	313	CLA	C4D-ND	-3.61	1.32	1.37
35	W	202	A86	C30-C29	-3.61	1.25	1.32
37	D	314	KC1	OBD-CAD	3.61	1.27	1.22
35	C	204	A86	C24-C1	3.61	1.53	1.45
36	a	822	CLA	C4D-ND	-3.61	1.32	1.37
35	S	305	A86	O1-C20	-3.61	1.41	1.46
35	P	304	A86	C30-C29	-3.61	1.26	1.32
35	P	306	A86	C30-C29	-3.61	1.26	1.32
36	G	315	CLA	OBD-CAD	3.61	1.28	1.22
35	U	303	A86	C30-C29	-3.60	1.26	1.32
36	a	839	CLA	C4D-ND	-3.60	1.32	1.37
36	A	305	CLA	C1D-ND	3.60	1.42	1.37
36	I	306	CLA	OBD-CAD	3.60	1.28	1.22
36	E	314	CLA	C4D-ND	-3.60	1.32	1.37
36	L	311	CLA	C4D-ND	-3.60	1.32	1.37
35	h	204	A86	C30-C29	-3.60	1.26	1.32
36	b	837	CLA	C4D-ND	-3.60	1.32	1.37
36	K	307	CLA	OBD-CAD	3.60	1.28	1.22
36	E	312	CLA	C4D-ND	-3.60	1.32	1.37
35	E	302	A86	C30-C29	-3.60	1.26	1.32
36	C	211	CLA	C4D-ND	-3.60	1.32	1.37
36	b	817	CLA	OBD-CAD	3.59	1.28	1.22
35	S	308	A86	C30-C29	-3.59	1.26	1.32
35	F	306	A86	C30-C29	-3.59	1.26	1.32
36	F	317	CLA	OBD-CAD	3.59	1.28	1.22
36	a	822	CLA	OBD-CAD	3.59	1.28	1.22
35	R	306	A86	O1-C20	-3.59	1.41	1.46
36	V	313	CLA	C4D-ND	-3.59	1.32	1.37
36	V	314	CLA	OBD-CAD	3.59	1.28	1.22
36	L	308	CLA	C3D-C4D	-3.59	1.36	1.44
36	P	316	CLA	C1D-ND	3.58	1.42	1.37
36	V	313	CLA	C1D-ND	3.58	1.42	1.37
37	W	217	KC1	CHB-C4A	3.58	1.47	1.39
37	X	311	KC1	CHB-C4A	3.58	1.47	1.39
36	W	201	CLA	C1D-ND	3.58	1.42	1.37
37	N	314	KC1	CHB-C4A	3.58	1.47	1.39
36	D	309	CLA	CHD-C4C	3.58	1.47	1.39
36	b	827	CLA	C4D-ND	-3.58	1.32	1.37
36	W	211	CLA	C1D-ND	3.58	1.42	1.37
36	h	203	CLA	C4D-ND	-3.58	1.32	1.37
36	b	820	CLA	C4D-ND	-3.58	1.32	1.37
36	W	208	CLA	C1D-ND	3.58	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	W	202	A86	O1-C20	-3.58	1.41	1.46
36	E	315	CLA	OBD-CAD	3.58	1.28	1.22
36	K	310	CLA	OBD-CAD	3.57	1.28	1.22
36	O	314	CLA	C1D-ND	3.57	1.42	1.37
37	S	316	KC1	CHC-C1C	3.57	1.47	1.39
36	b	830	CLA	CMB-C2B	-3.57	1.44	1.51
36	G	313	CLA	C1D-ND	3.57	1.42	1.37
36	C	208	CLA	C4D-ND	-3.57	1.32	1.37
36	H	308	CLA	C4D-ND	-3.57	1.32	1.37
36	W	216	CLA	C4D-ND	-3.56	1.32	1.37
36	a	825	CLA	OBD-CAD	3.56	1.28	1.22
36	l	205	CLA	OBD-CAD	3.56	1.28	1.22
36	b	836	CLA	C1B-NB	-3.56	1.32	1.35
36	b	816	CLA	OBD-CAD	3.56	1.28	1.22
35	M	304	A86	C30-C29	-3.55	1.26	1.32
36	a	803	CLA	C4D-ND	-3.55	1.32	1.37
37	M	318	KC1	C3D-C2D	3.55	1.45	1.39
36	a	801	CLA	CMD-C2D	-3.55	1.43	1.50
35	h	202	A86	C30-C29	-3.55	1.26	1.32
35	I	301	A86	C30-C29	-3.55	1.26	1.32
36	b	806	CLA	C1D-ND	3.55	1.42	1.37
36	P	310	CLA	C1D-ND	3.55	1.42	1.37
37	C	213	KC1	CHB-C4A	3.55	1.47	1.39
35	T	305	A86	O1-C20	-3.55	1.41	1.46
36	a	814	CLA	C4D-ND	-3.55	1.32	1.37
35	X	303	A86	C30-C29	-3.55	1.26	1.32
36	A	306	CLA	OBD-CAD	3.55	1.28	1.22
35	D	302	A86	C30-C29	-3.54	1.26	1.32
36	A	306	CLA	CHD-C4C	3.54	1.47	1.39
36	O	308	CLA	C1D-ND	3.54	1.42	1.37
36	b	813	CLA	CAB-C3B	-3.54	1.44	1.51
36	a	823	CLA	OBD-CAD	3.54	1.28	1.22
36	B	305	CLA	C4D-ND	-3.54	1.32	1.37
35	T	301	A86	C30-C29	-3.54	1.26	1.32
36	O	307	CLA	C4D-ND	-3.54	1.32	1.37
36	a	820	CLA	C4D-ND	-3.54	1.32	1.37
36	W	215	CLA	C1D-ND	3.53	1.42	1.37
35	R	305	A86	C30-C29	-3.53	1.26	1.32
36	f	804	CLA	OBD-CAD	3.53	1.28	1.22
36	T	312	CLA	C1D-ND	3.53	1.42	1.37
36	C	207	CLA	C3D-C4D	-3.53	1.36	1.44
35	G	305	A86	C30-C29	-3.53	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	806	CLA	OBD-CAD	3.53	1.28	1.22
36	G	310	CLA	C4D-ND	-3.53	1.32	1.37
36	b	824	CLA	CHD-C4C	3.53	1.47	1.39
36	P	309	CLA	C4D-ND	-3.53	1.32	1.37
36	b	832	CLA	C4D-ND	-3.53	1.32	1.37
36	Q	308	CLA	C1D-ND	3.53	1.42	1.37
36	V	306	CLA	CHC-C1C	3.53	1.44	1.35
35	C	204	A86	C26-C27	3.53	1.40	1.35
36	D	309	CLA	OBD-CAD	3.53	1.28	1.22
36	M	311	CLA	C4D-ND	-3.53	1.32	1.37
36	P	319	CLA	C3B-C2B	-3.53	1.35	1.40
36	Q	305	CLA	C1D-ND	3.53	1.42	1.37
36	a	819	CLA	C4D-ND	-3.52	1.32	1.37
36	Q	307	CLA	C1D-ND	3.52	1.42	1.37
36	R	312	CLA	C1D-ND	3.52	1.42	1.37
36	E	313	CLA	OBD-CAD	3.52	1.28	1.22
36	A	308	CLA	C4D-ND	-3.52	1.32	1.37
36	b	836	CLA	OBD-CAD	3.52	1.28	1.22
36	b	802	CLA	C4D-ND	-3.52	1.32	1.37
36	l	201	CLA	C4D-ND	-3.52	1.32	1.37
36	a	806	CLA	C4D-ND	-3.52	1.32	1.37
36	H	309	CLA	C4D-ND	-3.51	1.32	1.37
36	b	830	CLA	C4D-ND	-3.51	1.32	1.37
36	V	309	CLA	C1D-ND	3.51	1.42	1.37
36	I	312	CLA	C4D-ND	-3.51	1.32	1.37
36	b	810	CLA	C4D-ND	-3.51	1.32	1.37
36	C	207	CLA	OBD-CAD	3.51	1.28	1.22
36	P	308	CLA	C1D-ND	3.51	1.42	1.37
36	f	803	CLA	OBD-CAD	3.51	1.28	1.22
36	a	838	CLA	C4D-ND	-3.51	1.32	1.37
36	U	307	CLA	C1D-ND	3.51	1.42	1.37
36	j	101	CLA	C4D-ND	-3.51	1.32	1.37
36	X	309	CLA	C4D-ND	-3.51	1.32	1.37
37	A	312	KC1	CHB-C4A	3.51	1.47	1.39
36	a	816	CLA	OBD-CAD	3.50	1.28	1.22
35	F	301	A86	C30-C29	-3.50	1.26	1.32
36	b	817	CLA	C4D-ND	-3.50	1.32	1.37
35	F	305	A86	O1-C20	-3.50	1.41	1.46
36	R	315	CLA	C1D-ND	3.50	1.42	1.37
35	C	203	A86	C30-C29	-3.50	1.26	1.32
36	O	309	CLA	C1D-ND	3.50	1.42	1.37
37	M	318	KC1	CAB-C3B	3.50	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	319	CLA	C1B-NB	3.50	1.38	1.35
36	a	805	CLA	C4D-ND	-3.50	1.32	1.37
36	a	818	CLA	C4D-ND	-3.50	1.32	1.37
35	J	303	A86	O1-C20	-3.50	1.41	1.46
36	H	316	CLA	C4D-ND	-3.50	1.32	1.37
36	G	319	CLA	OBD-CAD	3.50	1.28	1.22
36	a	830	CLA	OBD-CAD	3.50	1.28	1.22
37	D	314	KC1	CHB-C4A	3.49	1.47	1.39
36	l	204	CLA	OBD-CAD	3.49	1.28	1.22
36	C	207	CLA	CHD-C4C	3.49	1.47	1.39
36	a	821	CLA	C4D-ND	-3.49	1.32	1.37
36	L	309	CLA	C4D-ND	-3.49	1.32	1.37
36	L	310	CLA	C1D-ND	3.48	1.42	1.37
36	A	309	CLA	C1D-ND	3.48	1.42	1.37
37	N	314	KC1	CHC-C1C	3.48	1.47	1.39
36	Q	306	CLA	C4D-ND	-3.48	1.32	1.37
36	a	823	CLA	C4D-ND	-3.48	1.32	1.37
36	I	305	CLA	C4D-ND	-3.48	1.32	1.37
36	l	202	CLA	C4D-ND	-3.48	1.32	1.37
36	F	310	CLA	C4D-ND	-3.47	1.32	1.37
36	a	832	CLA	C4D-ND	-3.47	1.32	1.37
36	A	311	CLA	C4D-ND	-3.47	1.32	1.37
36	a	809	CLA	C4D-ND	-3.47	1.32	1.37
44	a	847	BCR	C30-C25	-3.47	1.49	1.53
36	f	804	CLA	MG-ND	-3.47	1.98	2.05
37	V	312	KC1	CHC-C1C	3.47	1.47	1.39
36	N	310	CLA	C1B-NB	-3.47	1.32	1.35
36	P	311	CLA	C1D-ND	3.47	1.42	1.37
36	T	309	CLA	C1D-ND	3.47	1.42	1.37
37	G	318	KC1	C4D-CHA	3.47	1.49	1.45
36	L	313	CLA	C1D-ND	3.46	1.42	1.37
36	M	309	CLA	C1D-ND	3.46	1.42	1.37
36	O	306	CLA	C1D-ND	3.46	1.42	1.37
37	A	312	KC1	C1B-NB	-3.46	1.33	1.37
37	K	314	KC1	CHB-C4A	3.46	1.47	1.39
35	K	302	A86	C30-C29	-3.46	1.26	1.32
36	N	310	CLA	CHC-C1C	3.46	1.43	1.35
36	S	314	CLA	C4D-ND	-3.46	1.32	1.37
36	F	313	CLA	C4D-ND	-3.46	1.32	1.37
36	C	205	CLA	C1D-ND	3.45	1.42	1.37
36	M	306	CLA	C4D-ND	-3.45	1.33	1.37
36	S	312	CLA	C4D-ND	-3.45	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	316	CLA	C1D-ND	3.45	1.42	1.37
36	a	823	CLA	C1D-ND	3.45	1.42	1.37
36	a	837	CLA	C4D-ND	-3.45	1.33	1.37
36	S	310	CLA	C1D-ND	3.45	1.42	1.37
36	b	827	CLA	C1D-ND	3.44	1.42	1.37
36	a	833	CLA	C4D-ND	-3.44	1.33	1.37
36	M	312	CLA	C4D-ND	-3.44	1.33	1.37
35	R	302	A86	C30-C29	-3.44	1.26	1.32
36	i	102	CLA	C1D-ND	3.44	1.42	1.37
36	a	811	CLA	C4D-ND	-3.44	1.33	1.37
36	b	824	CLA	OBD-CAD	3.44	1.28	1.22
36	J	312	CLA	C4D-ND	-3.44	1.33	1.37
36	V	311	CLA	C4D-ND	-3.44	1.33	1.37
37	B	310	KC1	C4D-CHA	3.44	1.49	1.45
36	l	205	CLA	C1C-NC	-3.44	1.32	1.37
36	K	309	CLA	C1D-ND	3.43	1.42	1.37
36	D	309	CLA	C3D-C4D	-3.43	1.36	1.44
36	I	307	CLA	C4D-ND	-3.43	1.33	1.37
36	P	302	CLA	C1D-ND	3.43	1.42	1.37
36	a	812	CLA	C4D-ND	-3.43	1.33	1.37
36	l	205	CLA	C4D-ND	-3.43	1.33	1.37
36	V	310	CLA	C1D-ND	3.43	1.42	1.37
36	b	836	CLA	C3D-C4D	-3.43	1.36	1.44
36	a	834	CLA	C1D-ND	3.43	1.42	1.37
36	b	840	CLA	C4D-ND	-3.43	1.33	1.37
36	X	308	CLA	CHC-C1C	3.43	1.43	1.35
36	R	321	CLA	C1D-ND	3.43	1.42	1.37
36	H	306	CLA	C4D-ND	-3.42	1.33	1.37
35	X	301	A86	O1-C20	-3.42	1.41	1.46
36	C	212	CLA	C4D-ND	-3.42	1.33	1.37
36	D	307	CLA	C1D-ND	3.42	1.42	1.37
36	N	308	CLA	MG-ND	-3.42	1.99	2.05
36	H	315	CLA	C4D-ND	-3.42	1.33	1.37
36	R	316	CLA	C1D-ND	3.42	1.42	1.37
36	j	102	CLA	OBD-CAD	3.42	1.28	1.22
36	X	313	CLA	C4B-CHC	-3.42	1.31	1.41
36	U	308	CLA	C1D-ND	3.41	1.42	1.37
35	M	305	A86	C30-C29	-3.41	1.26	1.32
36	A	310	CLA	C4D-ND	-3.41	1.33	1.37
36	a	836	CLA	C4D-ND	-3.41	1.33	1.37
36	b	807	CLA	C4D-ND	-3.41	1.33	1.37
35	L	306	A86	O1-C20	-3.41	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	L	317	KC1	CHB-C4A	3.41	1.47	1.39
37	G	317	KC1	C4D-CHA	3.41	1.49	1.45
36	D	312	CLA	C1D-ND	3.41	1.42	1.37
36	G	316	CLA	C1D-ND	3.41	1.42	1.37
36	j	106	CLA	C4D-ND	-3.41	1.33	1.37
37	G	308	KC1	CHB-C4A	3.41	1.47	1.39
37	L	315	KC1	C4D-CHA	3.41	1.49	1.45
35	N	304	A86	C30-C29	-3.41	1.26	1.32
36	F	317	CLA	C4D-ND	-3.41	1.33	1.37
37	M	317	KC1	CHC-C1C	3.40	1.47	1.39
36	L	311	CLA	C1D-ND	3.40	1.42	1.37
36	f	805	CLA	C4D-ND	-3.40	1.33	1.37
36	H	317	CLA	C1D-ND	3.40	1.42	1.37
36	W	218	CLA	C1D-ND	3.40	1.42	1.37
37	C	213	KC1	C4D-CHA	3.40	1.49	1.45
36	P	301	CLA	C4D-ND	-3.40	1.33	1.37
36	a	835	CLA	C4D-ND	-3.40	1.33	1.37
36	L	314	CLA	C1D-ND	3.40	1.42	1.37
36	M	315	CLA	C1D-ND	3.40	1.42	1.37
35	W	203	A86	O1-C20	-3.40	1.41	1.46
36	b	811	CLA	C4D-ND	-3.40	1.33	1.37
36	F	311	CLA	C4D-ND	-3.40	1.33	1.37
36	b	816	CLA	C4D-ND	-3.40	1.33	1.37
36	V	305	CLA	C4D-ND	-3.40	1.33	1.37
35	F	307	A86	C30-C29	-3.40	1.26	1.32
36	R	311	CLA	C4D-ND	-3.39	1.33	1.37
36	b	829	CLA	C4D-ND	-3.39	1.33	1.37
36	D	317	CLA	C4D-ND	-3.39	1.33	1.37
36	A	308	CLA	C1D-ND	3.39	1.42	1.37
36	a	807	CLA	C4D-ND	-3.39	1.33	1.37
36	Q	314	CLA	C4D-ND	-3.39	1.33	1.37
36	b	821	CLA	C4D-ND	-3.39	1.33	1.37
36	l	204	CLA	C1D-ND	3.39	1.42	1.37
36	U	306	CLA	CHD-C4C	3.39	1.47	1.39
36	a	802	CLA	OBD-CAD	3.38	1.28	1.22
36	b	809	CLA	C4D-ND	-3.38	1.33	1.37
36	V	306	CLA	C1D-ND	3.38	1.41	1.37
36	b	813	CLA	C4D-ND	-3.38	1.33	1.37
36	b	835	CLA	C4D-ND	-3.38	1.33	1.37
36	G	319	CLA	CHD-C4C	3.38	1.46	1.39
35	K	306	A86	O1-C20	-3.38	1.41	1.46
44	b	843	BCR	C1-C6	-3.38	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	M	308	CLA	C4D-ND	-3.38	1.33	1.37
37	S	316	KC1	C4D-CHA	3.38	1.49	1.45
36	L	320	CLA	C1D-ND	3.37	1.41	1.37
44	l	203	BCR	C30-C25	-3.37	1.49	1.53
36	a	828	CLA	C4D-ND	-3.37	1.33	1.37
36	a	814	CLA	C1D-ND	3.37	1.41	1.37
36	E	316	CLA	C4D-ND	-3.37	1.33	1.37
36	J	316	CLA	C1D-ND	3.37	1.41	1.37
36	X	308	CLA	C1D-ND	3.37	1.41	1.37
36	H	318	CLA	C4D-ND	-3.37	1.33	1.37
36	C	206	CLA	C4D-ND	-3.36	1.33	1.37
36	S	310	CLA	C4D-ND	-3.36	1.33	1.37
36	S	309	CLA	C1D-ND	3.36	1.41	1.37
37	M	313	KC1	CHC-C1C	3.36	1.46	1.39
36	a	833	CLA	CMB-C2B	-3.36	1.44	1.51
37	M	318	KC1	C4A-C3A	3.36	1.51	1.44
36	D	310	CLA	C4D-ND	-3.36	1.33	1.37
36	J	309	CLA	C4D-ND	-3.36	1.33	1.37
36	X	307	CLA	C4D-ND	-3.35	1.33	1.37
36	b	833	CLA	C4D-ND	-3.35	1.33	1.37
36	N	319	CLA	C4D-ND	-3.35	1.33	1.37
36	A	306	CLA	C3D-C2D	3.35	1.48	1.39
36	F	311	CLA	C1D-ND	3.35	1.41	1.37
44	i	103	BCR	C1-C6	-3.35	1.49	1.53
36	D	315	CLA	C4D-ND	-3.35	1.33	1.37
36	O	311	CLA	C1D-ND	3.35	1.41	1.37
37	W	213	KC1	C4D-CHA	3.35	1.49	1.45
35	C	204	A86	C28-C27	-3.35	1.44	1.50
36	I	309	CLA	C1D-ND	3.35	1.41	1.37
35	I	302	A86	O1-C20	-3.34	1.41	1.46
36	J	317	CLA	C1D-ND	3.34	1.41	1.37
36	F	314	CLA	C4D-ND	-3.34	1.33	1.37
36	G	307	CLA	CHD-C4C	3.34	1.46	1.39
36	E	313	CLA	C3D-C2D	3.34	1.48	1.39
36	F	317	CLA	C3D-C4D	-3.34	1.36	1.44
37	T	315	KC1	CHC-C1C	3.33	1.46	1.39
36	N	317	CLA	C4D-ND	-3.33	1.33	1.37
36	M	311	CLA	C1D-ND	3.33	1.41	1.37
36	b	822	CLA	C1D-ND	3.33	1.41	1.37
36	P	313	CLA	C1D-ND	3.33	1.41	1.37
36	b	829	CLA	CHC-C1C	3.33	1.43	1.35
36	K	308	CLA	C4D-ND	-3.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	f	803	CLA	CHD-C4C	3.33	1.46	1.39
36	J	311	CLA	C4D-ND	-3.33	1.33	1.37
37	M	317	KC1	CHB-C4A	3.32	1.46	1.39
36	H	306	CLA	C1D-ND	3.32	1.41	1.37
35	T	302	A86	O1-C20	-3.32	1.41	1.46
37	H	313	KC1	CHC-C1C	3.32	1.46	1.39
36	C	205	CLA	C4D-ND	-3.32	1.33	1.37
36	i	102	CLA	C4D-ND	-3.32	1.33	1.37
36	l	202	CLA	C1D-ND	3.32	1.41	1.37
36	R	321	CLA	CMB-C2B	-3.32	1.44	1.51
36	B	306	CLA	C1D-ND	3.32	1.41	1.37
36	a	830	CLA	C3D-C4D	-3.32	1.36	1.44
36	E	308	CLA	C4D-ND	-3.32	1.33	1.37
36	L	309	CLA	C1D-ND	3.32	1.41	1.37
36	M	316	CLA	C1D-ND	3.32	1.41	1.37
35	R	302	A86	O1-C20	-3.32	1.41	1.46
36	H	314	CLA	C1D-ND	3.32	1.41	1.37
35	G	306	A86	C30-C29	-3.31	1.26	1.32
36	E	310	CLA	C1D-ND	3.31	1.41	1.37
37	G	318	KC1	CHB-C4A	3.31	1.46	1.39
35	R	303	A86	O1-C20	-3.31	1.41	1.46
36	O	309	CLA	C4D-ND	-3.31	1.33	1.37
36	P	302	CLA	C4D-ND	-3.31	1.33	1.37
36	a	834	CLA	C4D-ND	-3.31	1.33	1.37
36	B	306	CLA	C4D-ND	-3.31	1.33	1.37
35	V	302	A86	C30-C29	-3.31	1.26	1.32
36	H	305	CLA	C1D-ND	3.31	1.41	1.37
36	J	310	CLA	C1D-ND	3.31	1.41	1.37
36	V	314	CLA	CHD-C4C	3.31	1.46	1.39
37	J	314	KC1	CHB-C4A	3.31	1.46	1.39
36	K	316	CLA	C4D-ND	-3.31	1.33	1.37
36	b	835	CLA	C1D-ND	3.31	1.41	1.37
36	b	823	CLA	C4D-ND	-3.30	1.33	1.37
35	U	304	A86	C30-C29	-3.30	1.26	1.32
36	O	308	CLA	C4D-ND	-3.30	1.33	1.37
36	G	315	CLA	C3D-C2D	3.30	1.48	1.39
36	b	814	CLA	C4D-ND	-3.30	1.33	1.37
36	W	216	CLA	C3B-C2B	-3.30	1.35	1.40
36	b	834	CLA	C4D-ND	-3.29	1.33	1.37
35	V	302	A86	O1-C20	-3.29	1.41	1.46
36	V	314	CLA	C3B-C2B	3.29	1.44	1.40
36	T	309	CLA	C4D-ND	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	313	CLA	C1D-ND	3.29	1.41	1.37
36	G	316	CLA	C4D-ND	-3.29	1.33	1.37
36	B	305	CLA	CHC-C1C	3.29	1.43	1.35
36	S	311	CLA	CHC-C1C	3.29	1.43	1.35
37	X	311	KC1	CHC-C1C	3.29	1.46	1.39
36	a	815	CLA	C4D-ND	-3.29	1.33	1.37
36	X	309	CLA	C1D-ND	3.28	1.41	1.37
35	M	302	A86	O1-C20	-3.28	1.41	1.46
35	M	302	A86	C30-C29	-3.28	1.26	1.32
36	K	313	CLA	C1D-ND	3.28	1.41	1.37
36	a	801	CLA	C1D-ND	3.28	1.41	1.37
36	D	307	CLA	C4D-ND	-3.28	1.33	1.37
36	b	827	CLA	CHC-C1C	3.28	1.43	1.35
36	l	206	CLA	C1D-ND	3.28	1.41	1.37
36	T	314	CLA	C4D-ND	-3.28	1.33	1.37
37	H	313	KC1	C1B-NB	-3.28	1.33	1.37
36	P	311	CLA	C4D-ND	-3.28	1.33	1.37
37	F	315	KC1	CHB-C4A	3.28	1.46	1.39
36	I	310	CLA	C4D-ND	-3.27	1.33	1.37
36	b	816	CLA	CHD-C4C	3.27	1.46	1.39
36	R	318	CLA	CHC-C1C	3.27	1.43	1.35
36	b	814	CLA	C1D-ND	3.27	1.41	1.37
36	W	207	CLA	C4D-ND	-3.27	1.33	1.37
35	V	303	A86	O1-C20	-3.27	1.41	1.46
36	j	106	CLA	C1D-ND	3.27	1.41	1.37
36	b	818	CLA	C1D-ND	3.27	1.41	1.37
44	h	201	BCR	C1-C6	-3.27	1.49	1.53
36	b	836	CLA	CHD-C4C	3.27	1.46	1.39
36	G	311	CLA	C4D-ND	-3.27	1.33	1.37
36	T	308	CLA	C4D-ND	-3.26	1.33	1.37
36	G	312	CLA	C4D-ND	-3.26	1.33	1.37
36	W	212	CLA	CHC-C1C	3.26	1.43	1.35
36	W	207	CLA	CHC-C1C	3.26	1.43	1.35
36	l	206	CLA	C4D-ND	-3.26	1.33	1.37
37	W	217	KC1	CHC-C1C	3.26	1.46	1.39
35	O	302	A86	C30-C29	-3.26	1.26	1.32
36	b	812	CLA	CMB-C2B	-3.26	1.44	1.51
37	C	213	KC1	CHC-C1C	3.26	1.46	1.39
35	N	306	A86	O1-C20	-3.25	1.41	1.46
36	K	316	CLA	C1D-ND	3.25	1.41	1.37
36	U	311	CLA	CHC-C1C	3.25	1.43	1.35
37	E	309	KC1	CHB-C4A	3.25	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	R	317	KC1	CHC-C1C	3.25	1.46	1.39
36	B	309	CLA	CHC-C1C	3.25	1.43	1.35
36	U	313	CLA	CHC-C1C	3.25	1.43	1.35
36	Q	308	CLA	C4D-ND	-3.25	1.33	1.37
36	R	312	CLA	C4D-ND	-3.25	1.33	1.37
37	P	317	KC1	CHB-C4A	3.24	1.46	1.39
36	b	805	CLA	CMD-C2D	-3.24	1.43	1.50
36	L	310	CLA	C4D-ND	-3.24	1.33	1.37
36	J	317	CLA	C4D-ND	-3.24	1.33	1.37
36	M	312	CLA	C1D-ND	3.24	1.41	1.37
36	A	313	CLA	C4D-ND	-3.24	1.33	1.37
36	H	307	CLA	CHC-C1C	3.24	1.43	1.35
37	Q	313	KC1	CHC-C1C	3.24	1.46	1.39
36	b	831	CLA	CMB-C2B	-3.24	1.44	1.51
36	G	307	CLA	C3D-C2D	3.24	1.48	1.39
37	O	315	KC1	CHC-C1C	3.24	1.46	1.39
36	b	812	CLA	C4D-ND	-3.24	1.33	1.37
36	C	208	CLA	C1D-ND	3.24	1.41	1.37
36	H	308	CLA	C1D-ND	3.24	1.41	1.37
36	a	826	CLA	C1D-ND	3.23	1.41	1.37
36	j	101	CLA	C1D-ND	3.23	1.41	1.37
36	V	308	CLA	C4D-ND	-3.23	1.33	1.37
37	Q	311	KC1	CHC-C1C	3.23	1.46	1.39
36	f	802	CLA	CHC-C1C	3.23	1.43	1.35
36	O	311	CLA	C4D-ND	-3.23	1.33	1.37
36	R	313	CLA	C4D-ND	-3.23	1.33	1.37
36	S	315	CLA	CHC-C1C	3.23	1.43	1.35
36	D	306	CLA	C4D-ND	-3.23	1.33	1.37
37	D	314	KC1	C4D-CHA	3.23	1.49	1.45
37	P	315	KC1	CHC-C1C	3.22	1.46	1.39
35	P	303	A86	C30-C29	-3.22	1.26	1.32
36	L	314	CLA	C4D-ND	-3.22	1.33	1.37
35	L	319	A86	C30-C29	-3.22	1.26	1.32
35	N	306	A86	C30-C29	-3.22	1.26	1.32
36	a	802	CLA	CHC-C1C	3.22	1.43	1.35
36	a	832	CLA	C1D-ND	3.22	1.41	1.37
36	Q	307	CLA	C4D-ND	-3.22	1.33	1.37
36	U	306	CLA	C4D-ND	-3.22	1.33	1.37
36	b	817	CLA	C3D-C2D	3.22	1.47	1.39
36	b	828	CLA	C1D-ND	3.22	1.41	1.37
36	N	308	CLA	C1C-C2C	3.22	1.50	1.44
36	P	318	CLA	C1D-ND	3.22	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	U	306	CLA	CHC-C1C	3.22	1.43	1.35
37	S	316	KC1	CHB-C4A	3.21	1.46	1.39
36	P	310	CLA	C4D-ND	-3.21	1.33	1.37
36	R	313	CLA	C1D-ND	3.21	1.41	1.37
36	E	313	CLA	C1D-ND	3.21	1.41	1.37
36	K	315	CLA	C4D-ND	-3.21	1.33	1.37
36	C	212	CLA	CHC-C1C	3.21	1.43	1.35
36	H	314	CLA	C4D-ND	-3.21	1.33	1.37
36	I	314	CLA	C4D-ND	-3.21	1.33	1.37
36	b	825	CLA	C4D-ND	-3.21	1.33	1.37
36	E	312	CLA	C1D-ND	3.21	1.41	1.37
36	E	310	CLA	CHC-C1C	3.21	1.43	1.35
36	b	811	CLA	CMC-C2C	-3.21	1.44	1.50
36	V	310	CLA	C4D-ND	-3.21	1.33	1.37
36	b	809	CLA	C1D-ND	3.20	1.41	1.37
36	K	307	CLA	C1C-NC	-3.20	1.33	1.37
36	I	308	CLA	C3D-C2D	3.20	1.47	1.39
36	J	308	CLA	CHC-C1C	3.20	1.43	1.35
36	a	830	CLA	C1D-ND	3.20	1.41	1.37
36	C	214	CLA	C4D-ND	-3.20	1.33	1.37
36	J	316	CLA	C4D-ND	-3.20	1.33	1.37
37	O	313	KC1	CHC-C1C	3.20	1.46	1.39
36	T	314	CLA	C1D-ND	3.20	1.41	1.37
36	b	822	CLA	C4D-ND	-3.20	1.33	1.37
36	Q	314	CLA	C1D-ND	3.20	1.41	1.37
36	D	316	CLA	C4D-ND	-3.20	1.33	1.37
36	P	313	CLA	C4D-ND	-3.20	1.33	1.37
36	a	824	CLA	CHC-C1C	3.20	1.43	1.35
36	D	316	CLA	C1D-ND	3.20	1.41	1.37
35	I	304	A86	C30-C29	-3.19	1.26	1.32
36	l	204	CLA	C3D-C2D	3.19	1.47	1.39
36	X	309	CLA	CHC-C1C	3.19	1.43	1.35
36	U	311	CLA	C4D-ND	-3.19	1.33	1.37
36	C	211	CLA	C1D-ND	3.19	1.41	1.37
36	D	311	CLA	C1D-ND	3.19	1.41	1.37
36	D	315	CLA	C1D-ND	3.19	1.41	1.37
36	G	314	CLA	C1D-ND	3.19	1.41	1.37
36	L	311	CLA	CHC-C1C	3.19	1.43	1.35
36	F	309	CLA	CHC-C1C	3.19	1.43	1.35
36	b	806	CLA	CHC-C1C	3.19	1.43	1.35
36	J	315	CLA	C4D-ND	-3.19	1.33	1.37
36	A	313	CLA	C1D-ND	3.19	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	312	CLA	CHC-C1C	3.19	1.43	1.35
36	X	308	CLA	C4D-ND	-3.19	1.33	1.37
36	N	309	CLA	CMB-C2B	-3.19	1.45	1.51
37	T	315	KC1	CHB-C4A	3.19	1.46	1.39
36	a	803	CLA	CHC-C1C	3.19	1.43	1.35
36	b	818	CLA	CHC-C1C	3.19	1.43	1.35
36	G	313	CLA	CHC-C1C	3.18	1.43	1.35
36	J	307	CLA	C4D-ND	-3.18	1.33	1.37
37	M	318	KC1	C1B-NB	-3.18	1.33	1.37
37	F	308	KC1	CHB-C4A	3.18	1.46	1.39
36	H	307	CLA	C4D-ND	-3.18	1.33	1.37
36	W	209	CLA	CHC-C1C	3.18	1.43	1.35
36	N	319	CLA	C3C-C2C	3.18	1.43	1.36
36	N	319	CLA	MG-ND	3.18	2.12	2.05
37	G	317	KC1	CHB-C4A	3.18	1.46	1.39
36	f	805	CLA	C1D-ND	3.18	1.41	1.37
37	M	313	KC1	CHB-C4A	3.18	1.46	1.39
36	Q	306	CLA	CHC-C1C	3.18	1.43	1.35
35	V	304	A86	C30-C29	-3.18	1.26	1.32
35	O	303	A86	O1-C20	-3.18	1.41	1.46
36	K	309	CLA	C4D-ND	-3.18	1.33	1.37
37	J	314	KC1	CHC-C1C	3.17	1.46	1.39
36	I	312	CLA	C1D-ND	3.17	1.41	1.37
36	V	305	CLA	C1B-NB	3.17	1.38	1.35
36	P	309	CLA	CHC-C1C	3.17	1.43	1.35
36	b	825	CLA	C1D-ND	3.17	1.41	1.37
35	O	319	A86	O1-C20	-3.17	1.41	1.46
36	A	305	CLA	C4D-ND	-3.17	1.33	1.37
36	O	307	CLA	CHC-C1C	3.17	1.43	1.35
36	I	314	CLA	C1D-ND	3.17	1.41	1.37
36	J	310	CLA	C4D-ND	-3.17	1.33	1.37
36	X	315	CLA	CHC-C1C	3.17	1.43	1.35
36	D	306	CLA	C1D-ND	3.17	1.41	1.37
37	M	313	KC1	C4D-CHA	3.17	1.49	1.45
35	P	304	A86	O1-C20	-3.17	1.41	1.46
36	F	314	CLA	C1D-ND	3.17	1.41	1.37
36	L	320	CLA	C4D-ND	-3.17	1.33	1.37
36	b	805	CLA	C4D-ND	-3.16	1.33	1.37
36	a	848	CLA	OBD-CAD	3.16	1.27	1.22
36	H	316	CLA	C1D-ND	3.16	1.41	1.37
37	F	315	KC1	C1B-NB	-3.16	1.33	1.37
37	K	314	KC1	C4D-CHA	3.16	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	313	CLA	CHC-C1C	3.16	1.43	1.35
36	G	307	CLA	C1B-NB	-3.16	1.32	1.35
36	H	317	CLA	CHC-C1C	3.16	1.43	1.35
36	W	215	CLA	CHC-C1C	3.16	1.43	1.35
36	R	322	CLA	C1D-ND	3.16	1.41	1.37
36	I	306	CLA	C1D-ND	3.16	1.41	1.37
35	N	302	A86	O1-C20	-3.16	1.41	1.46
36	b	841	CLA	C1D-ND	3.16	1.41	1.37
36	a	837	CLA	C1D-ND	3.15	1.41	1.37
36	b	837	CLA	CHC-C1C	3.15	1.43	1.35
36	f	804	CLA	C3D-C2D	3.15	1.47	1.39
35	B	303	A86	C30-C29	-3.15	1.26	1.32
36	S	319	CLA	C4D-ND	-3.15	1.33	1.37
36	P	308	CLA	C4D-ND	-3.15	1.33	1.37
36	Q	305	CLA	C4D-ND	-3.15	1.33	1.37
35	N	304	A86	C13-C11	-3.15	1.43	1.49
36	a	831	CLA	C1D-ND	3.15	1.41	1.37
36	Q	310	CLA	C1D-ND	3.15	1.41	1.37
36	J	313	CLA	C1D-ND	3.14	1.41	1.37
36	P	314	CLA	C1D-ND	3.14	1.41	1.37
36	b	801	CLA	CHC-C1C	3.14	1.43	1.35
36	M	306	CLA	C3B-CAB	-3.14	1.41	1.47
36	X	312	CLA	CHC-C1C	3.14	1.43	1.35
36	R	311	CLA	C1D-ND	3.14	1.41	1.37
35	S	302	A86	O1-C20	-3.14	1.41	1.46
36	l	202	CLA	CHC-C1C	3.14	1.43	1.35
36	M	308	CLA	C1D-ND	3.13	1.41	1.37
36	b	815	CLA	C1D-ND	3.13	1.41	1.37
36	S	313	CLA	C4D-ND	-3.13	1.33	1.37
36	D	313	CLA	C1D-ND	3.13	1.41	1.37
36	F	316	CLA	CHC-C1C	3.13	1.43	1.35
36	N	316	CLA	C4D-ND	-3.13	1.33	1.37
36	S	320	CLA	CHC-C1C	3.13	1.43	1.35
36	W	218	CLA	CHC-C1C	3.13	1.43	1.35
36	K	308	CLA	CHC-C1C	3.13	1.43	1.35
35	L	306	A86	C13-C11	-3.13	1.43	1.49
36	I	310	CLA	C1D-ND	3.13	1.41	1.37
36	A	308	CLA	CHC-C1C	3.13	1.43	1.35
36	M	307	CLA	C1D-ND	3.13	1.41	1.37
36	l	201	CLA	C1D-ND	3.12	1.41	1.37
36	R	311	CLA	CHC-C1C	3.12	1.43	1.35
36	G	313	CLA	CMB-C2B	-3.12	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	322	CLA	CHC-C1C	3.12	1.43	1.35
36	a	825	CLA	CHC-C1C	3.12	1.43	1.35
36	H	309	CLA	C1D-ND	3.12	1.41	1.37
36	R	312	CLA	CHC-C1C	3.12	1.43	1.35
36	b	819	CLA	CMB-C2B	-3.12	1.45	1.51
36	O	316	CLA	CHD-C4C	3.12	1.46	1.39
36	S	320	CLA	C4D-ND	-3.12	1.33	1.37
36	J	317	CLA	CHC-C1C	3.12	1.43	1.35
36	R	315	CLA	C4D-ND	-3.12	1.33	1.37
37	W	213	KC1	CHC-C1C	3.12	1.46	1.39
36	a	815	CLA	C1D-ND	3.12	1.41	1.37
35	Q	301	A86	O1-C20	-3.12	1.41	1.46
36	J	312	CLA	CHC-C1C	3.12	1.43	1.35
36	l	204	CLA	CHD-C4C	3.11	1.46	1.39
37	L	317	KC1	CHC-C1C	3.11	1.46	1.39
36	N	319	CLA	CHC-C1C	3.11	1.42	1.35
36	H	305	CLA	C4D-ND	-3.11	1.33	1.37
36	K	308	CLA	C1D-ND	3.11	1.41	1.37
36	I	312	CLA	CHC-C1C	3.11	1.42	1.35
36	T	309	CLA	CHC-C1C	3.11	1.42	1.35
36	M	307	CLA	CHC-C1C	3.11	1.42	1.35
36	S	321	CLA	CHC-C1C	3.11	1.42	1.35
36	b	833	CLA	CMB-C2B	-3.11	1.45	1.51
36	N	313	CLA	C4D-ND	-3.11	1.33	1.37
36	X	315	CLA	C4D-ND	-3.11	1.33	1.37
36	K	312	CLA	C4D-ND	-3.11	1.33	1.37
36	O	312	CLA	C1D-ND	3.11	1.41	1.37
36	S	315	CLA	C4D-ND	-3.11	1.33	1.37
36	E	317	CLA	CHC-C1C	3.10	1.42	1.35
35	F	305	A86	C30-C29	-3.10	1.26	1.32
44	h	201	BCR	C30-C25	-3.10	1.49	1.53
36	N	310	CLA	C1D-C2D	3.10	1.51	1.45
36	a	848	CLA	CHC-C1C	3.10	1.42	1.35
36	D	313	CLA	CHC-C1C	3.10	1.42	1.35
36	O	306	CLA	C4D-ND	-3.10	1.33	1.37
36	a	828	CLA	C1D-ND	3.10	1.41	1.37
37	E	309	KC1	C1B-NB	-3.10	1.34	1.37
36	b	834	CLA	CHC-C1C	3.10	1.42	1.35
36	K	312	CLA	CHC-C1C	3.10	1.42	1.35
36	W	208	CLA	CHC-C1C	3.10	1.42	1.35
35	T	303	A86	O1-C20	-3.10	1.41	1.46
36	E	311	CLA	C1D-ND	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	817	CLA	CHC-C1C	3.10	1.42	1.35
36	N	316	CLA	CHC-C1C	3.09	1.42	1.35
36	A	309	CLA	C4D-ND	-3.09	1.33	1.37
37	F	308	KC1	C4D-CHA	3.09	1.48	1.45
44	f	806	BCR	C1-C6	-3.09	1.49	1.53
37	U	312	KC1	C4D-CHA	3.09	1.48	1.45
36	T	313	CLA	CHC-C1C	3.09	1.42	1.35
36	K	309	CLA	CHC-C1C	3.09	1.42	1.35
36	D	308	CLA	CHC-C1C	3.09	1.42	1.35
36	R	316	CLA	C4D-ND	-3.09	1.33	1.37
36	a	818	CLA	CMB-C2B	-3.09	1.45	1.51
36	H	311	CLA	C4D-ND	-3.09	1.33	1.37
36	a	804	CLA	C3B-C2B	-3.09	1.36	1.40
36	B	305	CLA	C1D-ND	3.08	1.41	1.37
36	a	816	CLA	C3D-C2D	3.08	1.47	1.39
36	b	823	CLA	C1D-ND	3.08	1.41	1.37
37	E	309	KC1	CHC-C1C	3.08	1.46	1.39
36	M	309	CLA	CHC-C1C	3.08	1.42	1.35
36	M	315	CLA	C4D-ND	-3.08	1.33	1.37
36	a	835	CLA	C3B-C2B	-3.08	1.36	1.40
36	a	820	CLA	C1D-ND	3.08	1.41	1.37
36	L	310	CLA	CHC-C1C	3.08	1.42	1.35
36	L	316	CLA	C4D-ND	-3.08	1.33	1.37
36	F	313	CLA	C1D-ND	3.08	1.41	1.37
36	a	807	CLA	C1D-ND	3.07	1.41	1.37
36	H	317	CLA	C4D-ND	-3.07	1.33	1.37
36	K	310	CLA	C3D-C2D	3.07	1.47	1.39
37	B	310	KC1	CHC-C1C	3.07	1.46	1.39
36	F	316	CLA	C4D-ND	-3.07	1.33	1.37
36	I	313	CLA	C4D-ND	-3.07	1.33	1.37
36	S	309	CLA	C4D-ND	-3.07	1.33	1.37
36	A	307	CLA	CHC-C1C	3.07	1.42	1.35
36	S	310	CLA	CHC-C1C	3.07	1.42	1.35
36	a	812	CLA	CHC-C1C	3.07	1.42	1.35
36	b	802	CLA	CHC-C1C	3.07	1.42	1.35
36	J	312	CLA	C1D-ND	3.07	1.41	1.37
36	a	811	CLA	CHC-C1C	3.07	1.42	1.35
36	b	835	CLA	CHC-C1C	3.07	1.42	1.35
36	E	314	CLA	C1D-ND	3.07	1.41	1.37
36	S	309	CLA	CHC-C1C	3.07	1.42	1.35
36	N	312	CLA	C1D-ND	3.06	1.41	1.37
36	b	807	CLA	C1D-ND	3.06	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	822	CLA	CHC-C1C	3.06	1.42	1.35
36	L	313	CLA	C4D-ND	-3.06	1.33	1.37
36	R	313	CLA	CHC-C1C	3.06	1.42	1.35
36	H	310	CLA	C1D-ND	3.06	1.41	1.37
37	O	313	KC1	C1B-NB	-3.06	1.34	1.37
36	R	314	CLA	C4D-ND	-3.06	1.33	1.37
37	L	317	KC1	C4D-CHA	3.06	1.48	1.45
36	b	830	CLA	CMD-C2D	-3.06	1.44	1.50
36	H	316	CLA	CHC-C1C	3.06	1.42	1.35
36	I	305	CLA	C1D-ND	3.06	1.41	1.37
36	D	317	CLA	CHC-C1C	3.06	1.42	1.35
36	K	313	CLA	CHC-C1C	3.06	1.42	1.35
36	S	312	CLA	C1D-ND	3.06	1.41	1.37
36	N	310	CLA	C1D-ND	3.06	1.41	1.37
37	O	315	KC1	C1B-NB	-3.06	1.34	1.37
36	X	306	CLA	CHC-C1C	3.06	1.42	1.35
36	i	102	CLA	CHC-C1C	3.06	1.42	1.35
36	E	316	CLA	C1D-ND	3.06	1.41	1.37
36	B	309	CLA	C1D-ND	3.06	1.41	1.37
36	C	211	CLA	CHC-C1C	3.06	1.42	1.35
36	T	316	CLA	C4D-ND	-3.06	1.33	1.37
35	S	301	A86	C32-C31	-3.05	1.49	1.54
36	M	308	CLA	CHC-C1C	3.05	1.42	1.35
36	f	805	CLA	CHC-C1C	3.05	1.42	1.35
36	b	816	CLA	C3D-C2D	3.05	1.47	1.39
36	F	313	CLA	CHC-C1C	3.05	1.42	1.35
36	J	307	CLA	C1D-ND	3.05	1.41	1.37
36	G	310	CLA	C1D-ND	3.05	1.41	1.37
36	U	307	CLA	CHC-C1C	3.05	1.42	1.35
36	G	314	CLA	C4D-ND	-3.05	1.33	1.37
36	R	310	CLA	C4D-ND	-3.05	1.33	1.37
36	G	309	CLA	CHC-C1C	3.05	1.42	1.35
36	l	201	CLA	CHC-C1C	3.05	1.42	1.35
36	V	307	CLA	C4D-ND	-3.04	1.33	1.37
36	I	311	CLA	CHC-C1C	3.04	1.42	1.35
36	M	314	CLA	CHC-C1C	3.04	1.42	1.35
36	W	208	CLA	C4D-ND	-3.04	1.33	1.37
36	O	309	CLA	CHC-C1C	3.04	1.42	1.35
36	E	315	CLA	C3D-C2D	3.04	1.47	1.39
36	T	314	CLA	CHC-C1C	3.04	1.42	1.35
37	Q	311	KC1	C1B-NB	-3.04	1.34	1.37
36	b	817	CLA	C1D-ND	3.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Q	313	KC1	C1B-NB	-3.04	1.34	1.37
36	M	314	CLA	C4D-ND	-3.04	1.33	1.37
36	U	305	CLA	C4D-ND	-3.04	1.33	1.37
36	D	311	CLA	C4D-ND	-3.04	1.33	1.37
35	F	307	A86	O1-C20	-3.03	1.41	1.46
35	T	302	A86	C30-C29	-3.03	1.26	1.32
36	I	306	CLA	CHD-C4C	3.03	1.46	1.39
36	U	305	CLA	CHC-C1C	3.03	1.42	1.35
36	X	306	CLA	C4D-ND	-3.03	1.33	1.37
36	a	808	CLA	C1D-ND	3.03	1.41	1.37
36	b	808	CLA	C1D-ND	3.03	1.41	1.37
36	L	309	CLA	CHC-C1C	3.03	1.42	1.35
36	a	835	CLA	CHC-C1C	3.03	1.42	1.35
35	N	301	A86	C32-C31	-3.03	1.49	1.54
36	S	311	CLA	C4D-ND	-3.03	1.33	1.37
36	b	810	CLA	C1D-ND	3.03	1.41	1.37
36	a	811	CLA	C1D-ND	3.03	1.41	1.37
36	F	312	CLA	C4D-ND	-3.03	1.33	1.37
37	L	315	KC1	CHC-C1C	3.03	1.46	1.39
36	D	312	CLA	CHC-C1C	3.03	1.42	1.35
36	S	317	CLA	CHC-C1C	3.03	1.42	1.35
35	U	302	A86	C30-C29	-3.03	1.26	1.32
36	G	310	CLA	CHC-C1C	3.03	1.42	1.35
36	H	308	CLA	CHC-C1C	3.03	1.42	1.35
36	N	307	CLA	CHC-C1C	3.03	1.42	1.35
36	D	308	CLA	C1D-ND	3.03	1.41	1.37
36	b	813	CLA	CHC-C1C	3.03	1.42	1.35
36	I	311	CLA	C1D-ND	3.03	1.41	1.37
36	B	309	CLA	C4D-ND	-3.03	1.33	1.37
36	N	311	CLA	C4D-ND	-3.03	1.33	1.37
36	l	204	CLA	C4D-ND	-3.03	1.33	1.37
37	P	315	KC1	C1B-NB	-3.03	1.34	1.37
36	b	831	CLA	CHC-C1C	3.02	1.42	1.35
37	G	317	KC1	CHC-C1C	3.02	1.46	1.39
36	R	315	CLA	CHC-C1C	3.02	1.42	1.35
36	P	319	CLA	CHC-C1C	3.02	1.42	1.35
36	P	301	CLA	CHC-C1C	3.02	1.42	1.35
36	a	822	CLA	CHC-C1C	3.02	1.42	1.35
36	W	206	CLA	CHC-C1C	3.02	1.42	1.35
36	a	827	CLA	CHC-C1C	3.02	1.42	1.35
36	J	309	CLA	CHC-C1C	3.02	1.42	1.35
36	b	801	CLA	C1D-ND	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	311	CLA	CHC-C1C	3.02	1.42	1.35
36	T	312	CLA	CHC-C1C	3.02	1.42	1.35
36	Q	309	CLA	C4D-ND	-3.02	1.33	1.37
35	N	320	A86	C32-C31	-3.02	1.49	1.54
36	P	311	CLA	CHC-C1C	3.02	1.42	1.35
36	O	314	CLA	C4D-ND	-3.02	1.33	1.37
36	S	314	CLA	CHC-C1C	3.02	1.42	1.35
36	M	316	CLA	C4D-ND	-3.01	1.33	1.37
36	a	805	CLA	C1D-ND	3.01	1.41	1.37
36	h	203	CLA	C1D-ND	3.01	1.41	1.37
36	J	313	CLA	CHC-C1C	3.01	1.42	1.35
36	a	816	CLA	CHC-C1C	3.01	1.42	1.35
36	W	201	CLA	C4D-ND	-3.01	1.33	1.37
37	M	317	KC1	C1B-NB	-3.01	1.34	1.37
36	l	206	CLA	CHC-C1C	3.01	1.42	1.35
36	X	313	CLA	O2D-CGD	3.01	1.40	1.33
36	N	317	CLA	CHC-C1C	3.01	1.42	1.35
35	U	301	A86	C30-C29	-3.01	1.26	1.32
35	M	301	A86	C30-C29	-3.01	1.26	1.32
37	G	308	KC1	CHC-C1C	3.01	1.46	1.39
35	R	303	A86	C30-C29	-3.01	1.26	1.32
36	X	310	CLA	CHC-C1C	3.01	1.42	1.35
36	a	807	CLA	CHC-C1C	3.01	1.42	1.35
36	F	317	CLA	CHD-C4C	3.01	1.46	1.39
36	U	310	CLA	C4D-ND	-3.01	1.33	1.37
36	E	312	CLA	CHC-C1C	3.01	1.42	1.35
35	T	306	A86	O1-C20	-3.01	1.41	1.46
36	G	316	CLA	CHC-C1C	3.00	1.42	1.35
36	A	311	CLA	CHC-C1C	3.00	1.42	1.35
36	F	314	CLA	CHC-C1C	3.00	1.42	1.35
36	U	309	CLA	C4D-ND	-3.00	1.33	1.37
36	b	811	CLA	C1D-ND	3.00	1.41	1.37
36	V	305	CLA	CHC-C1C	3.00	1.42	1.35
36	V	307	CLA	CHC-C1C	3.00	1.42	1.35
36	b	816	CLA	CHC-C1C	3.00	1.42	1.35
37	K	314	KC1	CHC-C1C	3.00	1.46	1.39
36	N	319	CLA	C4D-CHA	3.00	1.49	1.38
37	S	316	KC1	C1B-NB	-3.00	1.34	1.37
35	I	302	A86	C30-C29	-3.00	1.27	1.32
36	a	809	CLA	C1D-ND	3.00	1.41	1.37
37	G	317	KC1	C1B-NB	-3.00	1.34	1.37
36	V	308	CLA	CHC-C1C	2.99	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	317	CLA	CMB-C2B	-2.99	1.45	1.51
36	Q	306	CLA	C1D-ND	2.99	1.41	1.37
35	T	307	A86	C30-C29	-2.99	1.27	1.32
37	P	317	KC1	CHC-C1C	2.99	1.46	1.39
36	a	810	CLA	CHC-C1C	2.99	1.42	1.35
36	R	320	CLA	CHC-C1C	2.99	1.42	1.35
36	b	820	CLA	C1D-ND	2.99	1.41	1.37
36	a	836	CLA	C1D-ND	2.99	1.41	1.37
36	V	313	CLA	CHC-C1C	2.99	1.42	1.35
36	b	807	CLA	CHC-C1C	2.99	1.42	1.35
36	l	205	CLA	C1D-ND	2.99	1.41	1.37
35	S	303	A86	O1-C20	-2.99	1.41	1.46
35	Q	304	A86	C32-C31	-2.99	1.49	1.54
35	R	309	A86	C30-C29	-2.99	1.27	1.32
36	I	306	CLA	CHC-C1C	2.99	1.42	1.35
36	D	317	CLA	C1D-ND	2.99	1.41	1.37
36	a	822	CLA	C1D-ND	2.99	1.41	1.37
36	N	318	CLA	CHC-C1C	2.99	1.42	1.35
36	S	313	CLA	CHC-C1C	2.99	1.42	1.35
36	R	310	CLA	CMB-C2B	-2.99	1.45	1.51
36	K	315	CLA	CHC-C1C	2.99	1.42	1.35
36	X	312	CLA	C4D-ND	-2.99	1.33	1.37
36	G	309	CLA	C1D-ND	2.99	1.41	1.37
36	J	310	CLA	CHC-C1C	2.99	1.42	1.35
36	D	310	CLA	C1D-ND	2.99	1.41	1.37
37	D	314	KC1	CHC-C1C	2.98	1.46	1.39
36	N	312	CLA	CHC-C1C	2.98	1.42	1.35
36	R	310	CLA	C1D-ND	2.98	1.41	1.37
36	R	318	CLA	C4D-ND	-2.98	1.33	1.37
37	T	310	KC1	C3B-C4B	2.98	1.51	1.46
37	U	312	KC1	CHC-C1C	2.98	1.46	1.39
36	b	806	CLA	CMC-C2C	-2.98	1.44	1.50
36	P	309	CLA	C1D-ND	2.98	1.41	1.37
36	a	835	CLA	CMD-C2D	-2.98	1.44	1.50
36	b	839	CLA	C1D-ND	2.98	1.41	1.37
36	G	311	CLA	CMD-C2D	-2.98	1.44	1.50
36	Q	308	CLA	CHC-C1C	2.98	1.42	1.35
36	H	306	CLA	CHC-C1C	2.98	1.42	1.35
36	O	310	CLA	C4D-ND	-2.98	1.33	1.37
37	R	317	KC1	CHB-C4A	2.98	1.46	1.39
35	K	303	A86	C30-C29	-2.98	1.27	1.32
36	G	312	CLA	C1D-ND	2.98	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	210	CLA	CHC-C1C	2.97	1.42	1.35
36	C	209	CLA	CMD-C2D	-2.97	1.44	1.50
36	C	214	CLA	CHC-C1C	2.97	1.42	1.35
36	Q	312	CLA	C4D-ND	-2.97	1.33	1.37
36	b	809	CLA	CHC-C1C	2.97	1.42	1.35
36	a	818	CLA	C1D-ND	2.97	1.41	1.37
37	J	314	KC1	C4D-CHA	2.97	1.48	1.45
36	a	804	CLA	CMB-C2B	-2.97	1.45	1.51
36	H	315	CLA	C1D-ND	2.97	1.41	1.37
36	R	316	CLA	CHC-C1C	2.97	1.42	1.35
36	O	307	CLA	C1D-ND	2.97	1.41	1.37
36	J	309	CLA	C1D-ND	2.97	1.41	1.37
36	b	821	CLA	C1D-ND	2.97	1.41	1.37
44	a	846	BCR	C1-C6	-2.97	1.49	1.53
44	a	845	BCR	C30-C25	-2.97	1.49	1.53
36	b	819	CLA	CHC-C1C	2.96	1.42	1.35
36	a	830	CLA	C3D-C2D	2.96	1.47	1.39
37	E	309	KC1	C4D-CHA	2.96	1.48	1.45
36	R	321	CLA	C4D-ND	-2.96	1.33	1.37
36	P	319	CLA	C3D-C4D	2.96	1.50	1.44
36	I	305	CLA	CHC-C1C	2.96	1.42	1.35
36	P	301	CLA	C1D-ND	2.96	1.41	1.37
36	C	209	CLA	CMB-C2B	-2.96	1.45	1.51
36	F	312	CLA	CHC-C1C	2.96	1.42	1.35
36	P	312	CLA	C4D-ND	-2.96	1.33	1.37
36	b	839	CLA	CHC-C1C	2.96	1.42	1.35
36	a	841	CLA	C1D-ND	2.96	1.41	1.37
36	E	308	CLA	C1D-ND	2.96	1.41	1.37
36	b	824	CLA	C1D-ND	2.96	1.41	1.37
36	I	310	CLA	CHC-C1C	2.96	1.42	1.35
36	T	316	CLA	CHC-C1C	2.96	1.42	1.35
37	G	318	KC1	C1B-NB	-2.96	1.34	1.37
36	E	313	CLA	CHD-C4C	2.96	1.46	1.39
36	a	834	CLA	CHC-C1C	2.96	1.42	1.35
36	I	307	CLA	C1D-ND	2.96	1.41	1.37
36	b	838	CLA	C1D-ND	2.96	1.41	1.37
36	P	318	CLA	CHC-C1C	2.95	1.42	1.35
36	C	214	CLA	C1D-ND	2.95	1.41	1.37
36	D	310	CLA	CHC-C1C	2.95	1.42	1.35
36	V	309	CLA	CHC-C1C	2.95	1.42	1.35
36	a	812	CLA	C1D-ND	2.95	1.41	1.37
36	a	815	CLA	CHC-C1C	2.95	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	T	310	KC1	C1D-CHD	2.95	1.49	1.41
36	T	311	CLA	C1D-ND	2.95	1.41	1.37
36	a	803	CLA	C1D-ND	2.95	1.41	1.37
36	K	307	CLA	C3D-C4D	-2.95	1.37	1.44
36	B	306	CLA	CHC-C1C	2.95	1.42	1.35
36	P	316	CLA	C4D-ND	-2.95	1.33	1.37
36	S	315	CLA	CMC-C2C	-2.94	1.44	1.50
36	b	836	CLA	C3B-C2B	2.94	1.44	1.40
36	a	802	CLA	C1D-ND	2.94	1.41	1.37
36	M	309	CLA	C4D-ND	-2.94	1.33	1.37
36	a	809	CLA	CHC-C1C	2.94	1.42	1.35
36	J	308	CLA	C4D-ND	-2.94	1.33	1.37
36	S	318	CLA	C4D-ND	-2.94	1.33	1.37
36	A	313	CLA	CHC-C1C	2.94	1.42	1.35
36	b	821	CLA	CHC-C1C	2.94	1.42	1.35
36	a	826	CLA	CHC-C1C	2.94	1.42	1.35
35	N	303	A86	O1-C20	-2.94	1.42	1.46
36	W	201	CLA	CHC-C1C	2.94	1.42	1.35
36	T	311	CLA	C3C-C2C	2.94	1.43	1.36
36	b	823	CLA	CHC-C1C	2.94	1.42	1.35
36	F	310	CLA	C1D-ND	2.94	1.41	1.37
36	I	314	CLA	CMB-C2B	-2.94	1.45	1.51
36	A	310	CLA	CHC-C1C	2.94	1.42	1.35
36	I	308	CLA	CHD-C1D	2.94	1.44	1.38
37	T	310	KC1	CHC-C1C	-2.94	1.32	1.39
36	a	828	CLA	CHC-C1C	2.93	1.42	1.35
36	h	203	CLA	CHC-C1C	2.93	1.42	1.35
36	b	830	CLA	C1D-ND	2.93	1.41	1.37
36	b	826	CLA	CMD-C2D	-2.93	1.44	1.50
36	L	316	CLA	CHC-C1C	2.93	1.42	1.35
36	U	309	CLA	CHC-C1C	2.93	1.42	1.35
37	V	312	KC1	C4C-C3C	2.93	1.50	1.45
36	T	313	CLA	C4D-ND	-2.93	1.33	1.37
36	j	101	CLA	CHC-C1C	2.93	1.42	1.35
36	H	315	CLA	CHC-C1C	2.93	1.42	1.35
36	a	838	CLA	CHC-C1C	2.93	1.42	1.35
36	A	305	CLA	CHC-C1C	2.93	1.42	1.35
36	S	321	CLA	C4D-ND	-2.93	1.33	1.37
36	M	316	CLA	CHC-C1C	2.93	1.42	1.35
37	X	311	KC1	C1A-CHA	2.93	1.48	1.40
36	L	320	CLA	CHC-C1C	2.93	1.42	1.35
36	b	835	CLA	C3B-C2B	-2.92	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	820	CLA	CHC-C1C	2.92	1.42	1.35
37	W	217	KC1	C1A-CHA	2.92	1.48	1.40
36	G	313	CLA	CMD-C2D	-2.92	1.44	1.50
36	I	306	CLA	C3B-C2B	2.92	1.44	1.40
36	b	815	CLA	CMC-C2C	-2.92	1.44	1.50
37	G	308	KC1	C1B-NB	-2.92	1.34	1.37
36	X	313	CLA	C1B-NB	-2.92	1.32	1.35
36	K	311	CLA	C4D-ND	-2.92	1.33	1.37
36	V	311	CLA	CHC-C1C	2.92	1.42	1.35
44	l	203	BCR	C1-C6	-2.92	1.49	1.53
44	b	846	BCR	C30-C25	-2.92	1.49	1.53
36	M	306	CLA	MG-ND	-2.92	2.00	2.05
36	S	319	CLA	CHC-C1C	2.92	1.42	1.35
36	b	826	CLA	C1D-ND	2.92	1.41	1.37
36	A	309	CLA	CHC-C1C	2.92	1.42	1.35
36	B	308	CLA	CHC-C1C	2.92	1.42	1.35
36	J	311	CLA	CHC-C1C	2.92	1.42	1.35
36	a	821	CLA	CHC-C1C	2.92	1.42	1.35
38	A	315	SQD	C6-S	-2.92	1.66	1.77
36	R	319	CLA	CHC-C1C	2.92	1.42	1.35
36	b	808	CLA	CHC-C1C	2.91	1.42	1.35
36	C	208	CLA	CHC-C1C	2.91	1.42	1.35
36	K	307	CLA	CHD-C4C	2.91	1.45	1.39
36	A	311	CLA	CMB-C2B	-2.91	1.45	1.51
36	E	316	CLA	CHC-C1C	2.91	1.42	1.35
36	G	314	CLA	CHC-C1C	2.91	1.42	1.35
36	b	802	CLA	C3B-C2B	-2.91	1.36	1.40
36	W	216	CLA	C1B-CHB	2.91	1.49	1.41
35	Q	316	A86	O1-C15	-2.91	1.40	1.45
36	Q	309	CLA	CHC-C1C	2.91	1.42	1.35
36	C	205	CLA	CHC-C1C	2.90	1.42	1.35
36	P	313	CLA	CHC-C1C	2.90	1.42	1.35
36	b	838	CLA	CHC-C1C	2.90	1.42	1.35
37	F	315	KC1	CHC-C1C	2.90	1.45	1.39
36	b	831	CLA	CMD-C2D	-2.90	1.44	1.50
36	N	315	CLA	CHC-C1C	2.90	1.42	1.35
36	j	106	CLA	CHC-C1C	2.90	1.42	1.35
36	L	312	CLA	CHC-C1C	2.90	1.42	1.35
36	K	310	CLA	CHC-C1C	2.90	1.42	1.35
36	O	311	CLA	CHC-C1C	2.90	1.42	1.35
36	R	321	CLA	CHC-C1C	2.90	1.42	1.35
36	E	308	CLA	CMB-C2B	-2.90	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	K	312	CLA	C1D-ND	2.90	1.41	1.37
36	K	307	CLA	C3B-C2B	2.90	1.44	1.40
35	N	305	A86	O1-C15	-2.90	1.40	1.45
36	F	313	CLA	CMB-C2B	-2.90	1.45	1.51
36	K	311	CLA	CHC-C1C	2.90	1.42	1.35
36	b	813	CLA	CMD-C2D	-2.90	1.44	1.50
36	J	315	CLA	CHC-C1C	2.89	1.42	1.35
36	O	310	CLA	CHC-C1C	2.89	1.42	1.35
36	Q	307	CLA	CHC-C1C	2.89	1.42	1.35
36	b	814	CLA	CHC-C1C	2.89	1.42	1.35
36	b	819	CLA	C4D-ND	-2.89	1.33	1.37
36	M	312	CLA	CHC-C1C	2.89	1.42	1.35
36	b	815	CLA	CHC-C1C	2.89	1.42	1.35
36	O	308	CLA	CHC-C1C	2.89	1.42	1.35
36	O	306	CLA	CHC-C1C	2.89	1.42	1.35
36	a	831	CLA	CHC-C1C	2.89	1.42	1.35
36	F	311	CLA	CHC-C1C	2.89	1.42	1.35
38	b	804	SQD	C6-S	-2.89	1.66	1.77
36	I	308	CLA	CHD-C4C	2.89	1.45	1.39
36	F	310	CLA	CHC-C1C	2.89	1.42	1.35
37	G	318	KC1	CHC-C1C	2.89	1.45	1.39
36	Q	305	CLA	CHC-C1C	2.89	1.42	1.35
36	S	315	CLA	C3B-C2B	-2.89	1.36	1.40
36	b	841	CLA	CMB-C2B	-2.89	1.45	1.51
36	R	320	CLA	C4D-ND	-2.88	1.33	1.37
36	b	829	CLA	C3B-C2B	-2.88	1.36	1.40
36	H	314	CLA	CHC-C1C	2.88	1.42	1.35
36	b	833	CLA	CHC-C1C	2.88	1.42	1.35
35	G	302	A86	C30-C29	-2.88	1.27	1.32
36	X	308	CLA	CMD-C2D	-2.88	1.44	1.50
36	C	209	CLA	CHC-C1C	2.88	1.42	1.35
36	P	310	CLA	CHC-C1C	2.88	1.42	1.35
36	a	836	CLA	CHC-C1C	2.88	1.42	1.35
36	P	312	CLA	CHC-C1C	2.88	1.42	1.35
36	b	828	CLA	CHC-C1C	2.88	1.42	1.35
36	N	311	CLA	CHC-C1C	2.88	1.42	1.35
36	U	310	CLA	CMD-C2D	-2.88	1.44	1.50
37	J	314	KC1	C1B-NB	-2.88	1.34	1.37
36	B	307	CLA	CHC-C1C	2.87	1.42	1.35
36	N	308	CLA	CHC-C1C	2.87	1.42	1.35
37	U	312	KC1	C4A-C3A	2.87	1.50	1.44
36	P	308	CLA	CHC-C1C	2.87	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	832	CLA	CHC-C1C	2.87	1.42	1.35
36	b	811	CLA	CHC-C1C	2.87	1.42	1.35
36	j	102	CLA	CHC-C1C	2.87	1.42	1.35
36	R	310	CLA	CHC-C1C	2.87	1.42	1.35
37	G	308	KC1	C4D-CHA	2.87	1.48	1.45
36	C	209	CLA	C1D-ND	2.86	1.41	1.37
36	b	823	CLA	CMB-C2B	-2.86	1.45	1.51
36	b	834	CLA	C1D-ND	2.86	1.41	1.37
36	A	314	CLA	CHC-C1C	2.86	1.42	1.35
36	W	211	CLA	CHC-C1C	2.86	1.42	1.35
36	L	313	CLA	CHC-C1C	2.86	1.42	1.35
37	F	308	KC1	CHC-C1C	2.86	1.45	1.39
36	K	316	CLA	CMB-C2B	-2.86	1.45	1.51
36	H	310	CLA	CHC-C1C	2.86	1.42	1.35
35	J	303	A86	C30-C29	-2.86	1.27	1.32
36	W	206	CLA	C4D-ND	-2.86	1.33	1.37
36	N	308	CLA	CMB-C2B	-2.86	1.45	1.51
36	U	308	CLA	CHC-C1C	2.86	1.42	1.35
36	b	841	CLA	C4B-CHC	-2.86	1.33	1.41
36	I	305	CLA	C16-C15	2.86	1.68	1.51
35	S	302	A86	C30-C29	-2.86	1.27	1.32
36	l	205	CLA	C1D-C2D	2.86	1.51	1.45
36	a	827	CLA	CMC-C2C	-2.86	1.44	1.50
36	a	804	CLA	C3B-CAB	-2.85	1.42	1.47
35	N	302	A86	C30-C29	-2.85	1.27	1.32
36	B	311	CLA	CHC-C1C	2.85	1.42	1.35
36	A	310	CLA	CMD-C2D	-2.85	1.44	1.50
37	A	312	KC1	CHC-C1C	2.85	1.45	1.39
36	b	829	CLA	C1D-ND	2.85	1.41	1.37
36	D	315	CLA	CHC-C1C	2.85	1.42	1.35
36	J	307	CLA	CHC-C1C	2.85	1.42	1.35
44	a	847	BCR	C1-C6	-2.85	1.49	1.53
36	M	307	CLA	CMB-C2B	-2.85	1.45	1.51
36	f	802	CLA	C3B-C2B	-2.85	1.36	1.40
39	L	303	LMT	O3'-C3'	-2.85	1.36	1.43
36	a	805	CLA	CHC-C1C	2.85	1.42	1.35
36	b	802	CLA	CMB-C2B	-2.85	1.45	1.51
39	L	303	LMT	O2'-C2'	-2.84	1.36	1.43
36	b	821	CLA	CMB-C2B	-2.84	1.45	1.51
36	a	834	CLA	CMB-C2B	-2.84	1.45	1.51
36	b	827	CLA	C3B-C2B	-2.84	1.36	1.40
36	A	309	CLA	CMB-C2B	-2.84	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	317	CLA	C4D-ND	-2.84	1.33	1.37
36	Q	310	CLA	O2A-CGA	2.84	1.41	1.33
36	T	308	CLA	CHC-C1C	2.84	1.42	1.35
36	b	801	CLA	CMC-C2C	-2.84	1.44	1.50
36	E	308	CLA	CHC-C1C	2.84	1.42	1.35
36	A	307	CLA	C1D-ND	2.84	1.41	1.37
36	Q	310	CLA	CHC-C1C	2.84	1.42	1.35
36	U	310	CLA	CHC-C1C	2.84	1.42	1.35
35	S	305	A86	C30-C29	-2.84	1.27	1.32
36	a	841	CLA	CMB-C2B	-2.84	1.45	1.51
36	b	801	CLA	CMB-C2B	-2.84	1.45	1.51
36	V	310	CLA	CHC-C1C	2.83	1.42	1.35
35	X	305	A86	C30-C29	-2.83	1.27	1.32
36	M	315	CLA	C3B-C2B	-2.83	1.36	1.40
36	W	210	CLA	C4D-ND	-2.83	1.33	1.37
35	T	303	A86	C30-C29	-2.83	1.27	1.32
36	a	814	CLA	CMB-C2B	-2.83	1.45	1.51
36	a	839	CLA	CMB-C2B	-2.83	1.45	1.51
36	U	311	CLA	C1D-ND	2.83	1.41	1.37
36	R	314	CLA	CHC-C1C	2.83	1.42	1.35
36	l	202	CLA	CMB-C2B	-2.83	1.45	1.51
36	a	832	CLA	CHC-C1C	2.83	1.42	1.35
36	H	318	CLA	CHC-C1C	2.83	1.42	1.35
36	H	318	CLA	CMD-C2D	-2.83	1.44	1.50
36	C	212	CLA	C1D-ND	2.83	1.41	1.37
36	G	311	CLA	CHC-C1C	2.83	1.42	1.35
36	P	314	CLA	CHC-C1C	2.83	1.42	1.35
36	C	209	CLA	C4D-ND	-2.83	1.33	1.37
36	L	314	CLA	CHC-C1C	2.83	1.42	1.35
36	N	309	CLA	C4D-ND	-2.83	1.33	1.37
36	O	312	CLA	CHC-C1C	2.83	1.42	1.35
36	Q	312	CLA	CHC-C1C	2.83	1.42	1.35
36	X	307	CLA	CMB-C2B	-2.82	1.45	1.51
36	a	820	CLA	CHC-C1C	2.82	1.42	1.35
36	D	306	CLA	CHC-C1C	2.82	1.42	1.35
36	E	314	CLA	CHC-C1C	2.82	1.42	1.35
36	a	838	CLA	CMB-C2B	-2.82	1.45	1.51
36	U	311	CLA	CMD-C2D	-2.82	1.44	1.50
37	T	310	KC1	CHD-C4C	-2.82	1.27	1.35
36	W	214	CLA	CHC-C1C	2.82	1.42	1.35
36	H	312	CLA	C1D-ND	2.82	1.41	1.37
36	N	307	CLA	C4D-ND	-2.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	W	209	CLA	C4D-ND	-2.82	1.33	1.37
36	H	309	CLA	CHC-C1C	2.82	1.42	1.35
36	b	829	CLA	CMB-C2B	-2.81	1.45	1.51
36	N	309	CLA	C3B-C2B	-2.81	1.36	1.40
36	a	841	CLA	C3B-C2B	-2.81	1.36	1.40
36	H	305	CLA	CHC-C1C	2.81	1.42	1.35
36	L	308	CLA	C3B-CAB	-2.81	1.42	1.47
36	a	806	CLA	CHC-C1C	2.81	1.42	1.35
36	D	308	CLA	CMB-C2B	-2.81	1.45	1.51
37	L	317	KC1	C1B-NB	-2.81	1.34	1.37
36	b	840	CLA	CMB-C2B	-2.81	1.45	1.51
35	C	204	A86	C25-C26	2.81	1.52	1.43
36	B	309	CLA	C1B-NB	-2.81	1.32	1.35
37	H	313	KC1	CHB-C4A	2.81	1.45	1.39
36	J	316	CLA	C3B-C2B	-2.81	1.36	1.40
36	b	828	CLA	CMC-C2C	-2.81	1.44	1.50
37	H	313	KC1	C4D-CHA	2.81	1.48	1.45
36	P	316	CLA	CHC-C1C	2.81	1.42	1.35
36	I	309	CLA	CHC-C1C	2.81	1.42	1.35
36	T	311	CLA	CHC-C1C	2.81	1.42	1.35
36	D	311	CLA	CHC-C1C	2.80	1.42	1.35
36	I	306	CLA	C1D-C2D	2.80	1.50	1.45
36	a	812	CLA	CMC-C2C	-2.80	1.44	1.50
36	a	833	CLA	C3B-C2B	-2.80	1.36	1.40
36	C	210	CLA	C4D-ND	-2.80	1.33	1.37
36	I	308	CLA	CHC-C1C	2.80	1.42	1.35
36	a	827	CLA	C1D-ND	2.80	1.41	1.37
37	R	317	KC1	C1B-NB	-2.80	1.34	1.37
36	I	308	CLA	C1D-C2D	2.79	1.50	1.45
36	M	306	CLA	C1D-ND	2.79	1.41	1.37
44	b	845	BCR	C30-C25	-2.79	1.49	1.53
36	a	832	CLA	C3B-C2B	-2.79	1.36	1.40
36	O	314	CLA	CHC-C1C	2.79	1.42	1.35
36	j	102	CLA	C1D-C2D	2.79	1.50	1.45
36	a	810	CLA	C1D-ND	2.79	1.41	1.37
36	J	309	CLA	CMB-C2B	-2.79	1.45	1.51
36	P	302	CLA	CHC-C1C	2.79	1.42	1.35
36	S	317	CLA	C4D-ND	-2.79	1.33	1.37
36	a	801	CLA	CHC-C1C	2.79	1.42	1.35
36	a	813	CLA	CHC-C1C	2.78	1.42	1.35
36	I	307	CLA	CHC-C1C	2.78	1.42	1.35
36	G	307	CLA	C1D-C2D	2.78	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	312	CLA	CHC-C1C	2.78	1.42	1.35
37	M	318	KC1	CHC-C1C	-2.78	1.32	1.39
36	B	307	CLA	C4D-ND	-2.78	1.33	1.37
36	T	312	CLA	C4D-ND	-2.78	1.33	1.37
36	a	806	CLA	CHD-C4C	2.78	1.45	1.39
36	C	206	CLA	CHC-C1C	2.78	1.42	1.35
36	U	308	CLA	OBD-CAD	2.78	1.27	1.22
36	a	833	CLA	C1D-ND	2.78	1.41	1.37
36	a	823	CLA	CHC-C1C	2.78	1.42	1.35
36	G	314	CLA	CMB-C2B	-2.78	1.45	1.51
36	b	820	CLA	CMB-C2B	-2.77	1.45	1.51
36	I	314	CLA	C3B-C2B	-2.77	1.36	1.40
36	a	837	CLA	CHC-C1C	2.77	1.42	1.35
35	T	305	A86	C17-C18	-2.77	1.48	1.52
36	b	805	CLA	MG-ND	-2.77	2.00	2.05
37	M	317	KC1	C4D-CHA	2.77	1.48	1.45
36	M	310	CLA	C3B-C2B	-2.77	1.36	1.40
36	b	812	CLA	CMD-C2D	-2.77	1.44	1.50
36	b	826	CLA	C4D-ND	-2.77	1.33	1.37
36	D	307	CLA	CHC-C1C	2.77	1.42	1.35
36	a	806	CLA	C1D-ND	2.77	1.41	1.37
36	G	309	CLA	C4D-ND	-2.77	1.33	1.37
35	J	303	A86	C13-C11	-2.77	1.44	1.49
36	f	802	CLA	C1D-ND	2.77	1.41	1.37
36	M	306	CLA	CMB-C2B	-2.76	1.45	1.51
36	a	835	CLA	CMB-C2B	-2.76	1.45	1.51
36	N	315	CLA	C4D-ND	-2.76	1.33	1.37
44	b	847	BCR	C30-C25	-2.76	1.50	1.53
36	D	307	CLA	CMB-C2B	-2.76	1.45	1.51
36	a	801	CLA	CMB-C2B	-2.76	1.45	1.51
36	J	307	CLA	CMB-C2B	-2.76	1.45	1.51
36	W	218	CLA	CMD-C2D	-2.76	1.44	1.50
36	U	313	CLA	C4D-ND	-2.76	1.33	1.37
36	a	839	CLA	CHC-C1C	2.76	1.42	1.35
37	M	318	KC1	C1C-C2C	2.76	1.49	1.44
36	E	311	CLA	CMB-C2B	-2.76	1.45	1.51
36	D	316	CLA	CHC-C1C	2.76	1.42	1.35
36	I	314	CLA	CHC-C1C	2.76	1.42	1.35
35	R	306	A86	C30-C29	-2.76	1.27	1.32
36	a	808	CLA	CHC-C1C	2.76	1.42	1.35
44	m	101	BCR	C30-C25	-2.75	1.50	1.53
36	a	818	CLA	CHC-C1C	2.75	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	311	CLA	CHC-C1C	2.75	1.42	1.35
36	b	805	CLA	CHC-C1C	2.75	1.42	1.35
36	a	835	CLA	C1D-ND	2.75	1.41	1.37
36	O	312	CLA	CMD-C2D	-2.75	1.45	1.50
36	b	839	CLA	CMB-C2B	-2.75	1.45	1.51
36	b	827	CLA	CMB-C2B	-2.75	1.45	1.51
36	D	306	CLA	CMB-C2B	-2.75	1.45	1.51
36	b	837	CLA	C1D-ND	2.75	1.41	1.37
37	T	310	KC1	CMD-C2D	2.75	1.57	1.51
36	G	312	CLA	CMB-C2B	-2.75	1.45	1.51
35	C	204	A86	C3-C2	2.74	1.51	1.43
36	G	307	CLA	CHD-C1D	2.74	1.43	1.38
44	b	847	BCR	C1-C6	-2.74	1.50	1.53
36	b	825	CLA	CHC-C1C	2.74	1.42	1.35
36	M	311	CLA	CMB-C2B	-2.74	1.45	1.51
36	Q	310	CLA	CMD-C2D	-2.74	1.45	1.50
36	D	311	CLA	CMB-C2B	-2.74	1.45	1.51
36	a	808	CLA	CMB-C2B	-2.74	1.45	1.51
36	M	311	CLA	CHC-C1C	2.74	1.42	1.35
36	b	832	CLA	C1D-ND	2.74	1.41	1.37
36	H	312	CLA	CHC-C1C	2.74	1.42	1.35
36	O	312	CLA	CMB-C2B	-2.74	1.45	1.51
36	S	318	CLA	CHC-C1C	2.74	1.42	1.35
37	P	315	KC1	C4D-CHA	2.74	1.48	1.45
36	B	311	CLA	C3B-C2B	-2.73	1.36	1.40
36	V	305	CLA	C1D-C2D	2.73	1.50	1.45
36	a	829	CLA	CMD-C2D	-2.73	1.45	1.50
36	a	821	CLA	CMD-C2D	-2.73	1.45	1.50
36	a	820	CLA	CMB-C2B	-2.73	1.46	1.51
37	O	313	KC1	C4D-CHA	2.73	1.48	1.45
36	I	309	CLA	C4D-ND	-2.73	1.33	1.37
36	W	218	CLA	C4D-ND	-2.73	1.33	1.37
36	K	309	CLA	CMB-C2B	-2.73	1.46	1.51
36	M	308	CLA	CMB-C2B	-2.73	1.46	1.51
36	P	314	CLA	CMB-C2B	-2.73	1.46	1.51
44	m	101	BCR	C1-C6	-2.73	1.50	1.53
36	a	811	CLA	CMB-C2B	-2.72	1.46	1.51
36	l	201	CLA	CMB-C2B	-2.72	1.46	1.51
36	K	316	CLA	CHC-C1C	2.72	1.41	1.35
36	T	316	CLA	CMB-C2B	-2.72	1.46	1.51
36	a	832	CLA	C3B-CAB	-2.72	1.42	1.47
36	a	824	CLA	CMD-C2D	-2.72	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	N	318	CLA	C4D-ND	-2.72	1.33	1.37
36	J	316	CLA	CHC-C1C	2.72	1.41	1.35
37	R	317	KC1	C4D-CHA	2.72	1.48	1.45
36	K	310	CLA	CHD-C1D	2.72	1.43	1.38
36	a	811	CLA	C3B-C2B	-2.72	1.36	1.40
36	I	312	CLA	CMB-C2B	-2.72	1.46	1.51
36	Q	310	CLA	CMB-C2B	-2.71	1.46	1.51
36	b	815	CLA	CMB-C2B	-2.71	1.46	1.51
36	a	809	CLA	CMB-C2B	-2.71	1.46	1.51
36	C	208	CLA	CMB-C2B	-2.71	1.46	1.51
36	a	817	CLA	CHC-C1C	2.71	1.41	1.35
36	A	311	CLA	C1D-ND	2.71	1.41	1.37
35	V	303	A86	C13-C11	-2.71	1.44	1.49
36	H	318	CLA	CMB-C2B	-2.71	1.46	1.51
36	b	826	CLA	CMB-C2B	-2.71	1.46	1.51
37	C	213	KC1	C1B-NB	-2.71	1.34	1.37
35	H	301	A86	C13-C11	-2.71	1.44	1.49
36	a	841	CLA	CHC-C1C	2.71	1.41	1.35
36	R	319	CLA	C4D-ND	-2.71	1.34	1.37
36	b	826	CLA	CHC-C1C	2.70	1.41	1.35
36	A	305	CLA	CMB-C2B	-2.70	1.46	1.51
36	K	312	CLA	CMB-C2B	-2.70	1.46	1.51
37	Q	313	KC1	C4D-CHA	2.70	1.48	1.45
36	P	314	CLA	CMD-C2D	-2.70	1.45	1.50
36	U	310	CLA	C1D-ND	2.70	1.41	1.37
36	a	816	CLA	C4B-NB	2.70	1.37	1.35
36	l	204	CLA	C1D-C2D	2.70	1.50	1.45
37	U	312	KC1	C1B-NB	-2.70	1.34	1.37
36	H	316	CLA	CMB-C2B	-2.70	1.46	1.51
37	M	318	KC1	CMD-C2D	2.69	1.57	1.51
36	a	832	CLA	CMB-C2B	-2.69	1.46	1.51
36	N	312	CLA	C4D-ND	-2.69	1.34	1.37
36	b	808	CLA	CMB-C2B	-2.69	1.46	1.51
36	O	309	CLA	CMB-C2B	-2.69	1.46	1.51
36	b	812	CLA	CHC-C1C	2.69	1.41	1.35
36	V	311	CLA	CMD-C2D	-2.69	1.45	1.50
36	U	308	CLA	C4D-ND	-2.69	1.34	1.37
36	W	210	CLA	CHC-C1C	2.69	1.41	1.35
36	j	106	CLA	CMB-C2B	-2.69	1.46	1.51
37	Q	311	KC1	C4D-CHA	2.69	1.48	1.45
36	M	310	CLA	CHC-C1C	2.69	1.41	1.35
36	b	811	CLA	CMB-C2B	-2.69	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	835	CLA	CMB-C2B	-2.69	1.46	1.51
36	a	814	CLA	CHC-C1C	2.69	1.41	1.35
36	M	306	CLA	CMD-C2D	-2.69	1.45	1.50
36	L	312	CLA	C4D-ND	-2.69	1.34	1.37
36	a	821	CLA	C1D-ND	2.69	1.41	1.37
36	J	316	CLA	CMB-C2B	-2.68	1.46	1.51
36	E	316	CLA	CMB-C2B	-2.68	1.46	1.51
36	b	810	CLA	CHC-C1C	2.68	1.41	1.35
37	G	317	KC1	O1D-CGD	2.68	1.28	1.21
36	S	309	CLA	CMD-C2D	-2.68	1.45	1.50
36	C	211	CLA	CMB-C2B	-2.68	1.46	1.51
36	H	315	CLA	CMB-C2B	-2.68	1.46	1.51
36	a	810	CLA	CMB-C2B	-2.68	1.46	1.51
37	M	313	KC1	C1B-NB	-2.68	1.34	1.37
36	W	214	CLA	C4D-ND	-2.68	1.34	1.37
36	Q	307	CLA	CMB-C2B	-2.68	1.46	1.51
36	a	819	CLA	CMB-C2B	-2.68	1.46	1.51
36	l	206	CLA	CMB-C2B	-2.68	1.46	1.51
36	K	307	CLA	C1D-C2D	2.68	1.50	1.45
36	l	205	CLA	C3B-C2B	2.68	1.44	1.40
36	j	102	CLA	C3D-C2D	2.68	1.46	1.39
36	E	310	CLA	CMD-C2D	-2.68	1.45	1.50
36	I	305	CLA	CMB-C2B	-2.67	1.46	1.51
36	Q	308	CLA	CMB-C2B	-2.67	1.46	1.51
36	a	839	CLA	C1D-ND	2.67	1.41	1.37
36	b	827	CLA	CMC-C2C	-2.67	1.45	1.50
35	R	302	A86	C13-C11	-2.67	1.44	1.49
36	b	829	CLA	CMD-C2D	-2.67	1.45	1.50
36	F	311	CLA	CMB-C2B	-2.67	1.46	1.51
36	b	828	CLA	CMB-C2B	-2.67	1.46	1.51
36	P	319	CLA	CMB-C2B	-2.67	1.46	1.51
36	H	305	CLA	CMB-C2B	-2.67	1.46	1.51
36	G	311	CLA	C1D-ND	2.67	1.41	1.37
36	b	817	CLA	C1D-C2D	2.67	1.50	1.45
36	a	833	CLA	CHC-C1C	2.67	1.41	1.35
36	J	311	CLA	CMB-C2B	-2.66	1.46	1.51
36	D	316	CLA	CMB-C2B	-2.66	1.46	1.51
36	a	819	CLA	CMD-C2D	-2.66	1.45	1.50
36	b	838	CLA	CMB-C2B	-2.66	1.46	1.51
36	D	317	CLA	CMB-C2B	-2.66	1.46	1.51
36	H	312	CLA	CMB-C2B	-2.66	1.46	1.51
36	E	312	CLA	CMB-C2B	-2.66	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	l	205	CLA	C3D-C2D	2.66	1.46	1.39
36	P	301	CLA	CMB-C2B	-2.66	1.46	1.51
44	b	846	BCR	C1-C6	-2.66	1.50	1.53
36	a	819	CLA	C1D-ND	2.66	1.41	1.37
36	b	814	CLA	CMB-C2B	-2.66	1.46	1.51
36	V	306	CLA	CMC-C2C	-2.66	1.45	1.50
37	T	315	KC1	C1A-CHA	2.66	1.47	1.40
36	C	214	CLA	CMB-C2B	-2.66	1.46	1.51
36	O	308	CLA	CMB-C2B	-2.65	1.46	1.51
36	P	310	CLA	CMB-C2B	-2.65	1.46	1.51
37	B	310	KC1	C4C-C3C	2.65	1.49	1.45
36	b	834	CLA	CMB-C2B	-2.65	1.46	1.51
36	i	102	CLA	CMB-C2B	-2.65	1.46	1.51
35	V	304	A86	O1-C20	-2.65	1.42	1.46
36	H	310	CLA	CMB-C2B	-2.65	1.46	1.51
39	L	303	LMT	O2B-C2B	-2.65	1.36	1.43
36	X	307	CLA	CHC-C1C	2.65	1.41	1.35
37	O	315	KC1	C4D-CHA	2.65	1.48	1.45
36	a	810	CLA	C3B-C2B	-2.65	1.36	1.40
36	R	311	CLA	CMB-C2B	-2.64	1.46	1.51
37	K	314	KC1	C1B-NB	-2.64	1.34	1.37
36	a	815	CLA	CMB-C2B	-2.64	1.46	1.51
36	b	810	CLA	CMB-C2B	-2.64	1.46	1.51
36	I	306	CLA	C3D-C2D	2.64	1.46	1.39
36	E	315	CLA	C1D-C2D	2.64	1.50	1.45
37	P	317	KC1	C4D-CHA	2.64	1.48	1.45
36	M	310	CLA	CMB-C2B	-2.64	1.46	1.51
36	B	311	CLA	CMB-C2B	-2.64	1.46	1.51
36	P	311	CLA	CMB-C2B	-2.64	1.46	1.51
36	V	307	CLA	CMB-C2B	-2.64	1.46	1.51
36	G	312	CLA	CMD-C2D	-2.64	1.45	1.50
36	H	318	CLA	C1D-ND	2.64	1.41	1.37
36	b	825	CLA	CMD-C2D	-2.64	1.45	1.50
36	S	311	CLA	CMB-C2B	-2.64	1.46	1.51
36	H	309	CLA	CMD-C2D	-2.64	1.45	1.50
36	a	804	CLA	CHC-C1C	2.64	1.41	1.35
36	b	805	CLA	CMB-C2B	-2.64	1.46	1.51
36	f	802	CLA	CMB-C2B	-2.64	1.46	1.51
36	b	833	CLA	C1D-ND	2.63	1.41	1.37
36	a	805	CLA	CMB-C2B	-2.63	1.46	1.51
35	N	304	A86	C21-C20	2.63	1.56	1.51
36	A	310	CLA	C1D-ND	2.63	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	206	CLA	CMB-C2B	-2.63	1.46	1.51
37	G	317	KC1	C1A-CHA	2.63	1.47	1.40
36	J	313	CLA	CMB-C2B	-2.63	1.46	1.51
36	b	819	CLA	C3B-C2B	-2.63	1.36	1.40
36	F	310	CLA	CMB-C2B	-2.63	1.46	1.51
36	a	817	CLA	CMB-C2B	-2.63	1.46	1.51
36	J	312	CLA	CMB-C2B	-2.63	1.46	1.51
37	W	217	KC1	C1B-NB	-2.63	1.34	1.37
37	X	311	KC1	C1B-NB	-2.63	1.34	1.37
36	B	306	CLA	CMB-C2B	-2.63	1.46	1.51
35	Q	316	A86	C13-C11	-2.63	1.44	1.49
36	G	316	CLA	CMB-C2B	-2.63	1.46	1.51
36	a	848	CLA	C1D-ND	2.62	1.41	1.37
37	F	308	KC1	C4C-C3C	2.62	1.49	1.45
36	b	840	CLA	C1D-ND	2.62	1.41	1.37
36	G	309	CLA	O2D-CGD	2.62	1.39	1.33
36	H	309	CLA	CMB-C2B	-2.62	1.46	1.51
36	R	314	CLA	CMB-C2B	-2.62	1.46	1.51
35	X	304	A86	C30-C29	-2.62	1.27	1.32
36	H	306	CLA	CMB-C2B	-2.62	1.46	1.51
36	b	831	CLA	C3B-C2B	-2.62	1.36	1.40
36	A	307	CLA	CMB-C2B	-2.62	1.46	1.51
36	a	829	CLA	MG-ND	-2.62	2.00	2.05
36	V	314	CLA	C3D-C4D	-2.62	1.38	1.44
36	b	822	CLA	CMB-C2B	-2.62	1.46	1.51
37	O	315	KC1	C1A-CHA	2.62	1.47	1.40
35	N	305	A86	C13-C11	-2.62	1.44	1.49
36	a	841	CLA	CMC-C2C	-2.62	1.45	1.50
36	a	826	CLA	CMC-C2C	-2.62	1.45	1.50
36	H	310	CLA	CBD-CGD	2.61	1.60	1.52
36	K	307	CLA	C1B-NB	-2.61	1.32	1.35
36	K	311	CLA	CMB-C2B	-2.61	1.46	1.51
36	L	310	CLA	CMB-C2B	-2.61	1.46	1.51
36	P	313	CLA	CMB-C2B	-2.61	1.46	1.51
36	V	313	CLA	CMB-C2B	-2.61	1.46	1.51
35	Q	303	A86	C32-C31	-2.61	1.50	1.54
36	a	812	CLA	CMB-C2B	-2.61	1.46	1.51
37	Q	313	KC1	C1A-CHA	2.61	1.47	1.40
36	C	212	CLA	CMD-C2D	-2.61	1.45	1.50
36	a	829	CLA	CHC-C1C	2.61	1.41	1.35
41	O	318	LHG	C13-C12	2.61	1.66	1.51
35	U	301	A86	O1-C20	-2.61	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	M	315	CLA	CMB-C2B	-2.60	1.46	1.51
36	b	840	CLA	C3B-C2B	-2.60	1.36	1.40
36	b	825	CLA	CMB-C2B	-2.60	1.46	1.51
36	O	316	CLA	C3D-C2D	2.60	1.46	1.39
36	D	312	CLA	CMB-C2B	-2.60	1.46	1.51
36	W	201	CLA	CMB-C2B	-2.60	1.46	1.51
36	a	821	CLA	CMB-C2B	-2.60	1.46	1.51
36	b	809	CLA	CMB-C2B	-2.60	1.46	1.51
36	F	317	CLA	C3D-C2D	2.60	1.46	1.39
37	Q	311	KC1	C1A-CHA	2.60	1.47	1.40
35	C	204	A86	C2-C1	2.60	1.39	1.35
36	B	308	CLA	C4D-ND	-2.60	1.34	1.37
35	U	302	A86	C13-C11	-2.60	1.44	1.49
36	R	320	CLA	CMB-C2B	-2.60	1.46	1.51
37	M	318	KC1	C3D-CAD	2.59	1.53	1.47
36	J	315	CLA	CMB-C2B	-2.59	1.46	1.51
36	A	313	CLA	CMB-C2B	-2.59	1.46	1.51
37	W	213	KC1	C4A-C3A	2.59	1.49	1.44
36	L	320	CLA	CMB-C2B	-2.59	1.46	1.51
36	a	826	CLA	CMB-C2B	-2.59	1.46	1.51
35	L	304	A86	C13-C11	-2.59	1.44	1.49
36	H	308	CLA	CMB-C2B	-2.59	1.46	1.51
36	R	316	CLA	CMB-C2B	-2.59	1.46	1.51
37	P	315	KC1	C1A-CHA	2.59	1.47	1.40
36	b	832	CLA	CMB-C2B	-2.59	1.46	1.51
36	b	837	CLA	CMB-C2B	-2.58	1.46	1.51
36	V	314	CLA	C1B-NB	-2.58	1.32	1.35
36	a	817	CLA	C1D-ND	2.58	1.41	1.37
36	a	804	CLA	CMD-C2D	-2.58	1.45	1.50
36	G	319	CLA	C1D-C2D	2.58	1.50	1.45
36	H	307	CLA	C1D-C2D	2.58	1.50	1.45
36	V	310	CLA	CMB-C2B	-2.58	1.46	1.51
36	h	203	CLA	CMB-C2B	-2.58	1.46	1.51
36	K	310	CLA	C1D-C2D	2.58	1.50	1.45
37	P	317	KC1	C1B-NB	-2.58	1.34	1.37
36	R	320	CLA	CMD-C2D	-2.57	1.45	1.50
36	a	828	CLA	CMD-C2D	-2.57	1.45	1.50
36	b	841	CLA	CMC-C2C	-2.57	1.45	1.50
36	P	302	CLA	CMB-C2B	-2.57	1.46	1.51
37	L	317	KC1	C1A-CHA	2.57	1.47	1.40
36	b	811	CLA	C3B-C2B	-2.57	1.36	1.40
36	S	311	CLA	C3B-C2B	-2.57	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	307	CLA	CMB-C2B	-2.57	1.46	1.51
36	j	101	CLA	CMB-C2B	-2.57	1.46	1.51
37	D	314	KC1	C1B-NB	-2.57	1.34	1.37
37	O	313	KC1	C1A-CHA	2.57	1.47	1.40
37	W	213	KC1	C1A-CHA	2.57	1.47	1.40
36	O	311	CLA	CMB-C2B	-2.57	1.46	1.51
36	E	317	CLA	CMB-C2B	-2.57	1.46	1.51
36	P	312	CLA	CMB-C2B	-2.57	1.46	1.51
36	H	311	CLA	C1D-ND	2.57	1.40	1.37
36	b	802	CLA	C1D-ND	2.57	1.40	1.37
44	a	846	BCR	C30-C25	-2.57	1.50	1.53
36	M	312	CLA	CMB-C2B	-2.57	1.46	1.51
36	W	210	CLA	CMB-C2B	-2.57	1.46	1.51
35	S	304	A86	C32-C31	-2.57	1.50	1.54
36	a	825	CLA	C1D-ND	2.57	1.40	1.37
36	P	309	CLA	CMB-C2B	-2.57	1.46	1.51
36	V	314	CLA	C3D-C2D	2.56	1.46	1.39
36	E	308	CLA	C3B-C2B	-2.56	1.36	1.40
36	N	310	CLA	C4D-ND	-2.56	1.34	1.37
36	b	819	CLA	CMD-C2D	-2.56	1.45	1.50
36	W	215	CLA	CMB-C2B	-2.56	1.46	1.51
37	F	308	KC1	C1D-CHD	2.56	1.48	1.41
36	C	205	CLA	CMB-C2B	-2.56	1.46	1.51
36	a	831	CLA	CMB-C2B	-2.56	1.46	1.51
36	V	309	CLA	CMB-C2B	-2.56	1.46	1.51
44	b	844	BCR	C1-C6	-2.56	1.50	1.53
36	Q	309	CLA	CMB-C2B	-2.55	1.46	1.51
36	F	313	CLA	C3B-C2B	-2.55	1.36	1.40
36	a	823	CLA	CHD-C1D	2.55	1.43	1.38
36	H	314	CLA	CMB-C2B	-2.55	1.46	1.51
36	U	307	CLA	CMB-C2B	-2.55	1.46	1.51
37	W	213	KC1	C1D-CHD	2.55	1.48	1.41
36	H	317	CLA	CMB-C2B	-2.55	1.46	1.51
36	Q	306	CLA	CMB-C2B	-2.55	1.46	1.51
36	K	313	CLA	CMB-C2B	-2.55	1.46	1.51
36	b	813	CLA	CMB-C2B	-2.55	1.46	1.51
36	a	837	CLA	CMB-C2B	-2.55	1.46	1.51
36	b	819	CLA	C1D-ND	2.55	1.40	1.37
37	T	310	KC1	C1B-NB	-2.55	1.34	1.37
36	F	314	CLA	CMB-C2B	-2.54	1.46	1.51
36	a	808	CLA	C3B-C2B	-2.54	1.36	1.40
36	a	817	CLA	CMC-C2C	-2.54	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	O	303	A86	C32-C31	-2.54	1.50	1.54
36	O	310	CLA	CMB-C2B	-2.54	1.46	1.51
36	C	214	CLA	CMD-C2D	-2.54	1.45	1.50
36	J	312	CLA	CMC-C2C	-2.54	1.45	1.50
37	L	315	KC1	C1A-CHA	2.54	1.47	1.40
44	b	844	BCR	C30-C25	-2.54	1.50	1.53
36	V	309	CLA	C4D-ND	-2.54	1.34	1.37
36	f	805	CLA	CMB-C2B	-2.54	1.46	1.51
35	I	304	A86	C13-C11	-2.54	1.44	1.49
36	F	317	CLA	C3B-C2B	2.54	1.43	1.40
36	S	312	CLA	CMD-C2D	-2.54	1.45	1.50
36	a	836	CLA	CMB-C2B	-2.54	1.46	1.51
36	N	318	CLA	CMB-C2B	-2.54	1.46	1.51
36	a	807	CLA	CMB-C2B	-2.53	1.46	1.51
36	D	313	CLA	CMB-C2B	-2.53	1.46	1.51
36	Q	312	CLA	CMB-C2B	-2.53	1.46	1.51
36	T	308	CLA	CMB-C2B	-2.53	1.46	1.51
35	C	204	A86	C4-C5	2.53	1.51	1.43
36	b	839	CLA	C3B-C2B	-2.53	1.36	1.40
36	E	314	CLA	CMB-C2B	-2.53	1.46	1.51
36	R	313	CLA	CMB-C2B	-2.53	1.46	1.51
36	U	308	CLA	CMB-C2B	-2.53	1.46	1.51
37	V	312	KC1	C1A-CHA	2.53	1.47	1.40
36	M	309	CLA	CMB-C2B	-2.53	1.46	1.51
36	V	308	CLA	CMB-C2B	-2.53	1.46	1.51
36	O	314	CLA	CMB-C2B	-2.53	1.46	1.51
36	b	834	CLA	C3B-C2B	-2.53	1.36	1.40
36	J	317	CLA	CMB-C2B	-2.53	1.46	1.51
36	H	315	CLA	CMD-C2D	-2.53	1.45	1.50
34	D	303	DD6	C4-C5	2.53	1.51	1.43
37	G	318	KC1	C1D-CHD	2.53	1.48	1.41
36	U	306	CLA	C1D-C2D	2.53	1.50	1.45
36	J	310	CLA	CMB-C2B	-2.53	1.46	1.51
36	R	319	CLA	CMB-C2B	-2.52	1.46	1.51
36	a	827	CLA	CMB-C2B	-2.52	1.46	1.51
44	f	801	BCR	C30-C25	-2.52	1.50	1.53
36	K	313	CLA	OBD-CAD	-2.52	1.18	1.22
38	A	315	SQD	O48-C23	2.52	1.45	1.33
36	F	309	CLA	CMB-C2B	-2.52	1.46	1.51
36	S	315	CLA	CMB-C2B	-2.52	1.46	1.51
36	a	824	CLA	CMB-C2B	-2.52	1.46	1.51
36	a	830	CLA	CHC-C1C	2.52	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	314	CLA	CMB-C2B	-2.52	1.46	1.51
35	S	303	A86	C30-C29	-2.52	1.27	1.32
36	W	212	CLA	CMB-C2B	-2.52	1.46	1.51
36	S	319	CLA	CMB-C2B	-2.52	1.46	1.51
41	G	301	LHG	O7-C5	-2.52	1.40	1.46
36	M	315	CLA	CHC-C1C	2.52	1.41	1.35
36	b	833	CLA	C3B-C2B	-2.52	1.36	1.40
44	b	843	BCR	C30-C25	-2.52	1.50	1.53
35	Q	303	A86	C13-C11	-2.51	1.44	1.49
35	X	302	A86	C30-C29	-2.51	1.27	1.32
37	B	310	KC1	C1D-CHD	2.51	1.48	1.41
36	M	310	CLA	CMD-C2D	-2.51	1.45	1.50
36	G	309	CLA	CMB-C2B	-2.51	1.46	1.51
36	S	310	CLA	CMB-C2B	-2.51	1.46	1.51
36	R	322	CLA	O1D-CGD	2.51	1.27	1.21
36	K	316	CLA	C3B-C2B	-2.51	1.36	1.40
36	W	212	CLA	MG-ND	-2.51	2.00	2.05
36	L	312	CLA	CMB-C2B	-2.51	1.46	1.51
39	L	303	LMT	O4'-C4B	-2.51	1.37	1.43
36	P	316	CLA	CMB-C2B	-2.51	1.46	1.51
36	b	813	CLA	C1D-ND	2.51	1.40	1.37
36	C	210	CLA	CMB-C2B	-2.51	1.46	1.51
36	O	307	CLA	CMB-C2B	-2.51	1.46	1.51
36	G	307	CLA	C3B-C2B	2.51	1.43	1.40
36	a	817	CLA	MG-ND	-2.51	2.00	2.05
36	i	102	CLA	CMC-C2C	-2.51	1.45	1.50
36	K	307	CLA	C3D-C2D	2.51	1.46	1.39
36	b	841	CLA	CHC-C1C	2.51	1.41	1.35
35	P	304	A86	C32-C31	-2.50	1.50	1.54
36	D	315	CLA	CMB-C2B	-2.50	1.46	1.51
36	I	313	CLA	CMB-C2B	-2.50	1.46	1.51
36	b	830	CLA	CHC-C1C	2.50	1.41	1.35
36	G	310	CLA	CMB-C2B	-2.50	1.46	1.51
36	a	815	CLA	C3B-C2B	-2.50	1.36	1.40
36	a	804	CLA	MG-ND	-2.50	2.00	2.05
36	a	819	CLA	CHC-C1C	2.50	1.41	1.35
35	N	303	A86	C30-C29	-2.50	1.27	1.32
36	Q	305	CLA	CMB-C2B	-2.50	1.46	1.51
36	b	822	CLA	C3B-C2B	-2.50	1.36	1.40
36	M	316	CLA	CMB-C2B	-2.50	1.46	1.51
36	X	309	CLA	CMB-C2B	-2.49	1.46	1.51
36	J	308	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	803	CLA	CMB-C2B	-2.49	1.46	1.51
36	a	814	CLA	C3B-C2B	-2.49	1.36	1.40
36	a	818	CLA	CMC-C2C	-2.49	1.45	1.50
36	b	807	CLA	CMB-C2B	-2.49	1.46	1.51
36	F	316	CLA	CMB-C2B	-2.49	1.46	1.51
36	b	840	CLA	CMD-C2D	-2.49	1.45	1.50
34	G	303	DD6	O1-C20	-2.49	1.42	1.46
44	j	107	BCR	C1-C6	-2.49	1.50	1.53
36	S	309	CLA	CMB-C2B	-2.49	1.46	1.51
36	M	306	CLA	CHC-C1C	2.49	1.41	1.35
36	U	306	CLA	C1B-NB	-2.49	1.33	1.35
36	f	804	CLA	CHD-C1D	2.49	1.43	1.38
36	H	311	CLA	CMB-C2B	-2.48	1.46	1.51
35	W	202	A86	C33-C34	2.48	1.56	1.51
36	V	311	CLA	CMB-C2B	-2.48	1.46	1.51
36	M	306	CLA	C3B-C2B	-2.48	1.36	1.40
36	A	310	CLA	CMB-C2B	-2.48	1.46	1.51
37	P	317	KC1	C4B-NB	-2.48	1.34	1.37
36	W	208	CLA	CMB-C2B	-2.48	1.46	1.51
37	E	309	KC1	C1A-CHA	2.48	1.47	1.40
35	C	204	A86	C5-C6	2.48	1.39	1.35
37	T	315	KC1	C1B-NB	-2.48	1.34	1.37
36	W	209	CLA	CMB-C2B	-2.48	1.46	1.51
36	I	312	CLA	C3B-C2B	-2.48	1.36	1.40
36	C	207	CLA	C1D-C2D	2.48	1.50	1.45
36	b	818	CLA	CMC-C2C	-2.48	1.45	1.50
35	Q	301	A86	C32-C31	-2.48	1.50	1.54
36	L	309	CLA	CMB-C2B	-2.48	1.46	1.51
36	U	306	CLA	C1C-NC	2.48	1.41	1.37
36	S	320	CLA	CMB-C2B	-2.48	1.46	1.51
36	D	316	CLA	CMD-C2D	-2.48	1.45	1.50
36	a	801	CLA	C3B-C2B	-2.47	1.36	1.40
36	P	318	CLA	CMB-C2B	-2.47	1.46	1.51
36	W	214	CLA	CMB-C2B	-2.47	1.46	1.51
36	X	310	CLA	CMB-C2B	-2.47	1.46	1.51
36	P	308	CLA	CMB-C2B	-2.47	1.46	1.51
36	D	309	CLA	C1D-C2D	2.47	1.50	1.45
36	V	314	CLA	C1D-C2D	2.47	1.50	1.45
40	b	849	DGD	C3G-C2G	2.47	1.58	1.50
36	a	834	CLA	C3B-C2B	-2.47	1.36	1.40
36	E	308	CLA	CMD-C2D	-2.47	1.45	1.50
37	X	311	KC1	C1D-CHD	2.47	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	K	315	CLA	CMB-C2B	-2.47	1.46	1.51
36	a	824	CLA	MG-ND	-2.47	2.00	2.05
36	A	314	CLA	C4D-ND	-2.47	1.34	1.37
36	H	311	CLA	CMD-C2D	-2.47	1.45	1.50
36	X	312	CLA	CMC-C2C	-2.47	1.45	1.50
36	D	316	CLA	C3B-C2B	-2.47	1.36	1.40
36	N	319	CLA	C3B-C2B	-2.47	1.36	1.40
36	b	823	CLA	CMD-C2D	-2.47	1.45	1.50
35	X	303	A86	C13-C11	-2.47	1.45	1.49
36	b	820	CLA	CMD-C2D	-2.47	1.45	1.50
36	I	310	CLA	CMB-C2B	-2.47	1.46	1.51
36	J	313	CLA	C3B-C2B	-2.46	1.36	1.40
36	W	211	CLA	C4D-ND	-2.46	1.34	1.37
35	N	320	A86	C37-C36	-2.46	1.48	1.52
37	B	310	KC1	C1A-CHA	2.46	1.47	1.40
37	N	314	KC1	C4C-C3C	2.46	1.49	1.45
36	B	307	CLA	CMB-C2B	-2.46	1.46	1.51
35	C	202	A86	C32-C31	-2.46	1.50	1.54
36	R	315	CLA	CMB-C2B	-2.46	1.46	1.51
36	G	314	CLA	C3B-C2B	-2.46	1.37	1.40
35	T	305	A86	C13-C11	-2.46	1.45	1.49
36	a	814	CLA	CMC-C2C	-2.46	1.45	1.50
36	b	808	CLA	CMC-C2C	-2.46	1.45	1.50
36	F	311	CLA	CMC-C2C	-2.46	1.45	1.50
36	a	813	CLA	CMB-C2B	-2.46	1.46	1.51
36	a	813	CLA	CMC-C2C	-2.46	1.45	1.50
35	W	203	A86	C13-C11	-2.46	1.45	1.49
36	D	309	CLA	C3D-C2D	2.46	1.45	1.39
36	B	308	CLA	CMB-C2B	-2.46	1.46	1.51
36	b	821	CLA	C3B-C2B	-2.46	1.37	1.40
44	b	845	BCR	C1-C6	-2.46	1.50	1.53
35	T	306	A86	C30-C29	-2.45	1.27	1.32
36	R	322	CLA	CMB-C2B	-2.45	1.46	1.51
36	b	836	CLA	C3D-C2D	2.45	1.45	1.39
36	W	211	CLA	CMB-C2B	-2.45	1.46	1.51
36	C	209	CLA	CMC-C2C	-2.45	1.45	1.50
36	F	312	CLA	CMB-C2B	-2.45	1.46	1.51
36	O	306	CLA	CMB-C2B	-2.45	1.46	1.51
36	T	311	CLA	CMB-C2B	-2.45	1.46	1.51
35	W	202	A86	C32-C31	2.45	1.58	1.54
36	J	308	CLA	CMC-C2C	-2.45	1.45	1.50
36	I	306	CLA	C4D-CHA	2.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	U	312	KC1	C1A-CHA	2.45	1.47	1.40
37	W	217	KC1	C1D-CHD	2.44	1.47	1.41
35	Q	304	A86	C37-C36	-2.44	1.48	1.52
36	A	308	CLA	CMC-C2C	-2.44	1.45	1.50
36	H	310	CLA	C4D-CHA	2.44	1.47	1.38
36	a	803	CLA	CMD-C2D	-2.44	1.45	1.50
36	b	814	CLA	C3B-C2B	-2.44	1.37	1.40
37	N	314	KC1	C1A-CHA	2.44	1.47	1.40
36	A	308	CLA	CMB-C2B	-2.44	1.46	1.51
36	l	204	CLA	C1B-CHB	2.44	1.47	1.41
36	F	311	CLA	C3B-C2B	-2.44	1.37	1.40
36	b	811	CLA	CMD-C2D	-2.44	1.45	1.50
36	P	319	CLA	CMD-C2D	-2.44	1.45	1.50
35	J	301	A86	O1-C20	-2.44	1.42	1.46
36	C	209	CLA	C3B-C2B	-2.44	1.37	1.40
36	M	314	CLA	CMB-C2B	-2.44	1.46	1.51
36	R	310	CLA	CMD-C2D	-2.44	1.45	1.50
36	b	806	CLA	CMB-C2B	-2.44	1.46	1.51
36	L	316	CLA	CMB-C2B	-2.44	1.46	1.51
36	C	212	CLA	CMB-C2B	-2.44	1.46	1.51
36	N	312	CLA	CMB-C2B	-2.44	1.46	1.51
37	G	318	KC1	C4B-NB	-2.44	1.34	1.37
36	I	309	CLA	CMB-C2B	-2.44	1.46	1.51
36	N	315	CLA	CMB-C2B	-2.44	1.46	1.51
36	a	819	CLA	C3B-C2B	-2.44	1.37	1.40
36	O	316	CLA	C1D-C2D	2.44	1.50	1.45
36	b	837	CLA	CMD-C2D	-2.44	1.45	1.50
36	C	208	CLA	CMD-C2D	-2.44	1.45	1.50
36	b	828	CLA	MG-ND	-2.43	2.01	2.05
41	F	318	LHG	P-O6	2.43	1.68	1.60
36	L	313	CLA	CMB-C2B	-2.43	1.46	1.51
36	a	804	CLA	C1D-ND	2.43	1.40	1.37
36	H	310	CLA	O2D-CED	2.43	1.51	1.45
36	M	308	CLA	C3B-C2B	-2.43	1.37	1.40
37	G	318	KC1	C1A-CHA	2.43	1.47	1.40
36	P	301	CLA	CMC-C2C	-2.43	1.45	1.50
36	S	317	CLA	CMB-C2B	-2.43	1.46	1.51
36	D	310	CLA	CMB-C2B	-2.43	1.46	1.51
36	a	813	CLA	CMD-C2D	-2.43	1.45	1.50
37	S	316	KC1	C1A-CHA	2.43	1.47	1.40
37	A	312	KC1	C4D-CHA	2.42	1.48	1.45
36	S	315	CLA	C3B-CAB	-2.42	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	312	CLA	CMB-C2B	-2.42	1.46	1.51
36	O	316	CLA	C4D-CHA	2.42	1.47	1.38
36	K	312	CLA	CMD-C2D	-2.42	1.45	1.50
36	R	312	CLA	CMB-C2B	-2.42	1.46	1.51
36	f	803	CLA	C4D-ND	-2.42	1.34	1.37
37	X	311	KC1	C4C-C3C	2.42	1.49	1.45
41	G	301	LHG	O8-C6	-2.42	1.39	1.45
37	E	309	KC1	C4B-NB	-2.42	1.34	1.37
36	U	313	CLA	CMB-C2B	-2.42	1.46	1.51
36	V	311	CLA	C1D-ND	2.42	1.40	1.37
36	G	311	CLA	CMB-C2B	-2.42	1.46	1.51
36	U	309	CLA	CMB-C2B	-2.42	1.46	1.51
37	N	314	KC1	C1D-CHD	2.42	1.47	1.41
36	l	202	CLA	CMD-C2D	-2.42	1.45	1.50
37	U	312	KC1	C4C-C3C	2.42	1.49	1.45
36	A	314	CLA	CMB-C2B	-2.41	1.46	1.51
36	S	318	CLA	CMB-C2B	-2.41	1.46	1.51
37	W	217	KC1	C4C-C3C	2.41	1.49	1.45
36	D	312	CLA	C3B-C2B	-2.41	1.37	1.40
44	f	801	BCR	C1-C6	-2.41	1.50	1.53
36	S	321	CLA	CMB-C2B	-2.41	1.46	1.51
37	R	317	KC1	C1A-CHA	2.41	1.47	1.40
36	U	310	CLA	MG-ND	-2.41	2.01	2.05
39	L	303	LMT	O3B-C3B	-2.41	1.37	1.43
37	F	308	KC1	C1A-CHA	2.41	1.47	1.40
36	b	810	CLA	C3B-C2B	-2.41	1.37	1.40
36	T	309	CLA	CMB-C2B	-2.41	1.46	1.51
36	f	803	CLA	C3D-C2D	2.41	1.45	1.39
36	b	818	CLA	CMB-C2B	-2.41	1.46	1.51
36	U	305	CLA	CMB-C2B	-2.41	1.46	1.51
36	f	804	CLA	C1D-C2D	2.40	1.50	1.45
36	B	305	CLA	CMB-C2B	-2.40	1.46	1.51
35	C	202	A86	C30-C29	-2.40	1.28	1.32
36	G	319	CLA	C3D-C2D	2.40	1.45	1.39
36	a	828	CLA	CMB-C2B	-2.40	1.46	1.51
35	F	301	A86	O1-C20	-2.40	1.42	1.46
36	T	314	CLA	CMB-C2B	-2.40	1.46	1.51
35	Q	304	A86	C30-C29	-2.40	1.28	1.32
37	S	316	KC1	C1D-CHD	2.40	1.47	1.41
36	I	305	CLA	CMD-C2D	-2.40	1.45	1.50
36	R	312	CLA	C3B-CAB	-2.40	1.43	1.47
36	b	816	CLA	C1D-C2D	2.40	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	841	CLA	C3C-C2C	2.40	1.41	1.36
37	D	314	KC1	C1D-CHD	2.40	1.47	1.41
36	S	313	CLA	CMB-C2B	-2.39	1.46	1.51
36	l	202	CLA	C3B-C2B	-2.39	1.37	1.40
36	a	829	CLA	C3B-C2B	-2.39	1.37	1.40
35	N	320	A86	C33-C34	2.39	1.56	1.51
36	b	824	CLA	C1B-CHB	2.39	1.47	1.41
36	R	318	CLA	CMC-C2C	-2.39	1.45	1.50
36	I	311	CLA	CMB-C2B	-2.39	1.46	1.51
36	K	308	CLA	CMB-C2B	-2.39	1.46	1.51
36	E	315	CLA	CHD-C1D	2.39	1.43	1.38
35	X	301	A86	C13-C11	-2.39	1.45	1.49
36	R	318	CLA	CMB-C2B	-2.38	1.46	1.51
36	a	838	CLA	CMD-C2D	-2.38	1.45	1.50
36	f	804	CLA	C1B-CHB	2.38	1.47	1.41
36	N	316	CLA	CMB-C2B	-2.38	1.46	1.51
34	F	303	DD6	O1-C20	-2.38	1.42	1.46
36	R	313	CLA	CMD-C2D	-2.38	1.45	1.50
36	a	838	CLA	C3B-C2B	-2.38	1.37	1.40
36	b	831	CLA	C1D-ND	2.38	1.40	1.37
37	G	317	KC1	C4B-NB	-2.38	1.34	1.37
36	T	312	CLA	CMB-C2B	-2.38	1.46	1.51
35	F	306	A86	O1-C20	-2.38	1.42	1.46
36	A	311	CLA	CMD-C2D	-2.38	1.45	1.50
36	b	812	CLA	C1D-ND	2.38	1.40	1.37
34	a	849	DD6	O1-C20	-2.38	1.42	1.46
35	C	204	A86	C8-C6	2.38	1.51	1.45
36	W	216	CLA	CHC-C1C	2.38	1.41	1.35
34	B	304	DD6	O1-C20	-2.38	1.42	1.46
36	Q	314	CLA	CMB-C2B	-2.38	1.46	1.51
36	a	813	CLA	MG-ND	-2.38	2.01	2.05
36	F	317	CLA	MG-ND	-2.37	2.01	2.05
36	G	316	CLA	CMD-C2D	-2.37	1.45	1.50
36	N	311	CLA	CMB-C2B	-2.37	1.46	1.51
36	b	840	CLA	CHC-C1C	2.37	1.41	1.35
36	N	312	CLA	CMD-C2D	-2.37	1.45	1.50
36	E	314	CLA	CAC-C3C	-2.37	1.45	1.51
37	T	310	KC1	C3D-CAD	2.37	1.52	1.47
36	a	848	CLA	C3D-C2D	2.37	1.45	1.39
36	S	311	CLA	CMD-C2D	-2.37	1.45	1.50
36	X	306	CLA	CMB-C2B	-2.37	1.46	1.51
36	b	806	CLA	CMD-C2D	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	U	310	CLA	CMB-C2B	-2.37	1.46	1.51
36	U	311	CLA	CMB-C2B	-2.37	1.46	1.51
36	a	835	CLA	C3B-CAB	-2.37	1.43	1.47
35	C	203	A86	C32-C31	-2.37	1.50	1.54
34	D	305	DD6	O1-C20	-2.36	1.42	1.46
39	L	303	LMT	O1'-C1'	-2.36	1.36	1.40
35	N	320	A86	C30-C29	-2.36	1.28	1.32
36	J	317	CLA	CMD-C2D	-2.36	1.45	1.50
37	R	317	KC1	C4B-NB	-2.36	1.34	1.37
37	B	310	KC1	C1B-NB	-2.36	1.34	1.37
36	B	305	CLA	CMC-C2C	-2.36	1.45	1.50
36	b	805	CLA	CMC-C2C	-2.36	1.45	1.50
36	E	310	CLA	CMB-C2B	-2.36	1.46	1.51
36	S	314	CLA	O2D-CGD	2.36	1.39	1.33
36	A	314	CLA	C3D-C4D	2.36	1.49	1.44
36	R	312	CLA	CMD-C2D	-2.36	1.45	1.50
34	D	301	DD6	O1-C20	-2.36	1.42	1.46
35	V	303	A86	C30-C29	-2.36	1.28	1.32
37	C	213	KC1	C1A-CHA	2.36	1.46	1.40
35	R	302	A86	C32-C31	-2.36	1.50	1.54
36	a	818	CLA	C3B-C2B	-2.36	1.37	1.40
35	J	305	A86	O1-C20	-2.36	1.42	1.46
36	U	307	CLA	C4D-ND	-2.36	1.34	1.37
41	O	318	LHG	C12-C11	2.36	1.64	1.51
36	A	307	CLA	CMC-C2C	-2.36	1.45	1.50
36	b	815	CLA	CMD-C2D	-2.36	1.45	1.50
36	F	313	CLA	C3B-CAB	-2.36	1.43	1.47
36	A	309	CLA	C3B-C2B	-2.36	1.37	1.40
36	b	834	CLA	CMD-C2D	-2.35	1.45	1.50
37	V	312	KC1	C1D-CHD	2.35	1.47	1.41
36	J	309	CLA	CMD-C2D	-2.35	1.45	1.50
37	G	308	KC1	C1D-CHD	2.35	1.47	1.41
36	a	809	CLA	C3B-C2B	-2.35	1.37	1.40
35	F	305	A86	C13-C11	-2.35	1.45	1.49
36	K	310	CLA	C1C-C2C	2.35	1.49	1.44
36	L	308	CLA	C4D-ND	-2.35	1.34	1.37
35	I	301	A86	O1-C20	-2.35	1.42	1.46
36	K	313	CLA	MG-ND	-2.35	2.01	2.05
37	V	312	KC1	C1B-NB	-2.35	1.34	1.37
36	P	314	CLA	MG-ND	-2.35	2.01	2.05
34	K	304	DD6	O1-C20	-2.35	1.42	1.46
36	H	315	CLA	C3B-C2B	-2.35	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	U	311	CLA	CMC-C2C	-2.35	1.45	1.50
36	A	309	CLA	CMC-C2C	-2.35	1.45	1.50
36	L	309	CLA	CMC-C2C	-2.35	1.45	1.50
36	J	307	CLA	CMD-C2D	-2.35	1.45	1.50
36	R	316	CLA	CMD-C2D	-2.35	1.45	1.50
36	D	306	CLA	C3B-C2B	-2.35	1.37	1.40
36	Q	310	CLA	MG-ND	-2.34	2.01	2.05
37	A	312	KC1	C1D-CHD	2.34	1.47	1.41
37	C	213	KC1	C1D-CHD	2.34	1.47	1.41
36	T	313	CLA	CMB-C2B	-2.34	1.46	1.51
36	O	312	CLA	MG-ND	-2.34	2.01	2.05
36	b	838	CLA	CMD-C2D	-2.34	1.45	1.50
36	X	310	CLA	C3B-CAB	-2.34	1.43	1.47
35	Q	304	A86	C33-C34	2.34	1.55	1.51
44	a	845	BCR	C1-C6	-2.34	1.50	1.53
36	H	312	CLA	CMC-C2C	-2.34	1.45	1.50
36	W	211	CLA	O2D-CGD	2.34	1.38	1.33
44	l	207	BCR	C1-C6	-2.34	1.50	1.53
36	D	308	CLA	CMD-C2D	-2.33	1.45	1.50
37	U	312	KC1	C1D-CHD	2.33	1.47	1.41
36	V	311	CLA	CMC-C2C	-2.33	1.45	1.50
36	E	314	CLA	CMC-C2C	-2.33	1.45	1.50
34	D	303	DD6	O1-C20	-2.33	1.42	1.46
35	O	301	A86	O1-C20	-2.33	1.42	1.46
36	U	306	CLA	C3D-C2D	2.33	1.45	1.39
35	T	301	A86	C32-C31	-2.33	1.50	1.54
36	b	824	CLA	C1C-C2C	2.33	1.49	1.44
36	a	804	CLA	CMC-C2C	-2.33	1.45	1.50
36	a	808	CLA	CMD-C2D	-2.33	1.45	1.50
37	T	315	KC1	C1D-CHD	2.33	1.47	1.41
35	O	319	A86	C30-C29	-2.33	1.28	1.32
36	a	841	CLA	CMD-C2D	-2.32	1.45	1.50
36	b	827	CLA	CMD-C2D	-2.32	1.45	1.50
36	b	833	CLA	CMC-C2C	-2.32	1.45	1.50
36	L	314	CLA	CMD-C2D	-2.32	1.45	1.50
36	H	314	CLA	CMD-C2D	-2.32	1.45	1.50
44	j	107	BCR	C30-C25	-2.32	1.50	1.53
37	L	315	KC1	C1B-NB	-2.32	1.34	1.37
36	B	308	CLA	CMD-C2D	-2.32	1.45	1.50
37	D	314	KC1	C4B-NB	-2.32	1.34	1.37
36	W	218	CLA	CMC-C2C	-2.32	1.45	1.50
36	J	313	CLA	C3B-CAB	-2.32	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	W	213	KC1	C4C-C3C	2.32	1.49	1.45
36	W	218	CLA	CMB-C2B	-2.32	1.46	1.51
36	a	824	CLA	C1D-ND	2.32	1.40	1.37
37	G	318	KC1	O2A-CGA	-2.32	1.24	1.30
37	J	314	KC1	C1A-CHA	2.32	1.46	1.40
35	G	304	A86	C13-C11	-2.31	1.45	1.49
36	b	818	CLA	CMD-C2D	-2.31	1.45	1.50
41	O	318	LHG	P-O6	2.31	1.68	1.59
36	b	801	CLA	MG-ND	-2.31	2.01	2.05
36	M	311	CLA	CMD-C2D	-2.31	1.45	1.50
36	D	317	CLA	C3B-C2B	-2.31	1.37	1.40
36	b	835	CLA	CMD-C2D	-2.31	1.45	1.50
36	a	818	CLA	CMD-C2D	-2.31	1.45	1.50
41	a	842	LHG	O8-C6	-2.31	1.39	1.45
36	a	807	CLA	CMD-C2D	-2.31	1.45	1.50
36	a	838	CLA	MG-ND	-2.31	2.01	2.05
35	F	301	A86	C32-C31	-2.31	1.50	1.54
35	O	302	A86	C33-C34	2.31	1.55	1.51
36	D	312	CLA	CMD-C2D	-2.30	1.45	1.50
35	F	305	A86	O3-C36	-2.30	1.39	1.43
35	L	301	A86	C32-C31	-2.30	1.50	1.54
44	i	101	BCR	C1-C6	-2.30	1.50	1.53
36	K	308	CLA	CMC-C2C	-2.30	1.45	1.50
35	G	304	A86	C30-C29	-2.30	1.28	1.32
35	L	319	A86	C33-C34	2.30	1.55	1.51
36	a	812	CLA	CMD-C2D	-2.30	1.45	1.50
37	G	317	KC1	C1D-CHD	2.30	1.47	1.41
37	G	308	KC1	C1A-CHA	2.30	1.46	1.40
36	A	305	CLA	CMD-C2D	-2.30	1.45	1.50
36	b	836	CLA	C1C-C2C	2.30	1.49	1.44
36	L	311	CLA	CMB-C2B	-2.30	1.46	1.51
36	G	316	CLA	CMC-C2C	-2.30	1.45	1.50
36	b	826	CLA	MG-ND	-2.30	2.01	2.05
36	B	311	CLA	CMD-C2D	-2.29	1.45	1.50
36	N	309	CLA	CHC-C1C	2.29	1.40	1.35
36	V	311	CLA	MG-ND	-2.29	2.01	2.05
36	D	312	CLA	C3B-CAB	-2.29	1.43	1.47
36	a	814	CLA	CMD-C2D	-2.29	1.45	1.50
36	R	320	CLA	C3B-C2B	-2.29	1.37	1.40
36	J	307	CLA	MG-ND	-2.29	2.01	2.05
44	a	844	BCR	C1-C6	-2.29	1.50	1.53
36	P	316	CLA	C3B-C2B	-2.29	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	W	207	CLA	CMB-C2B	-2.29	1.46	1.51
36	E	314	CLA	CMD-C2D	-2.29	1.45	1.50
35	E	307	A86	O1-C20	-2.29	1.42	1.46
36	I	206	CLA	CMD-C2D	-2.29	1.45	1.50
34	H	303	DD6	O1-C20	-2.29	1.42	1.46
37	M	317	KC1	C1A-CHA	2.29	1.46	1.40
36	P	302	CLA	CMC-C2C	-2.29	1.46	1.50
36	a	839	CLA	CMD-C2D	-2.28	1.46	1.50
35	F	304	A86	O1-C20	-2.28	1.42	1.46
37	A	312	KC1	C1A-CHA	2.28	1.46	1.40
36	U	306	CLA	C4C-C3C	2.28	1.49	1.45
36	V	305	CLA	C3B-C2B	-2.28	1.37	1.40
36	C	211	CLA	CMD-C2D	-2.28	1.46	1.50
36	G	311	CLA	MG-ND	-2.28	2.01	2.05
36	U	311	CLA	MG-ND	-2.28	2.01	2.05
34	A	303	DD6	O1-C20	-2.28	1.43	1.46
36	R	316	CLA	C1D-C2D	2.28	1.49	1.45
35	V	301	A86	C32-C31	-2.28	1.50	1.54
36	b	802	CLA	CMD-C2D	-2.28	1.46	1.50
36	a	839	CLA	CMC-C2C	-2.28	1.46	1.50
36	f	802	CLA	CMD-C2D	-2.28	1.46	1.50
36	G	316	CLA	C3B-C2B	-2.28	1.37	1.40
34	S	307	DD6	O1-C20	-2.28	1.43	1.46
36	C	214	CLA	C3B-C2B	-2.28	1.37	1.40
36	b	821	CLA	CMD-C2D	-2.28	1.46	1.50
35	X	302	A86	C13-C11	-2.28	1.45	1.49
35	X	314	A86	C32-C31	-2.27	1.50	1.54
36	A	305	CLA	C3B-C2B	-2.27	1.37	1.40
37	F	308	KC1	C4B-NB	-2.27	1.35	1.37
36	M	316	CLA	CMD-C2D	-2.27	1.46	1.50
36	P	302	CLA	CMD-C2D	-2.27	1.46	1.50
36	b	808	CLA	C3B-C2B	-2.27	1.37	1.40
36	a	821	CLA	MG-ND	-2.27	2.01	2.05
36	A	306	CLA	C4C-C3C	2.27	1.48	1.45
35	E	302	A86	O1-C20	-2.27	1.43	1.46
36	I	312	CLA	CMC-C2C	-2.27	1.46	1.50
36	a	832	CLA	CMD-C2D	-2.27	1.46	1.50
37	J	314	KC1	C1D-CHD	2.27	1.47	1.41
36	E	316	CLA	CMD-C2D	-2.27	1.46	1.50
36	W	206	CLA	CMB-C2B	-2.27	1.46	1.51
37	G	318	KC1	C4C-C3C	2.27	1.48	1.45
36	X	308	CLA	CMB-C2B	-2.27	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	820	CLA	CMD-C2D	-2.27	1.46	1.50
35	A	316	A86	O1-C20	-2.27	1.43	1.46
44	b	845	BCR	C38-C26	-2.27	1.47	1.50
35	E	305	A86	O1-C20	-2.26	1.43	1.46
37	E	309	KC1	C1D-CHD	2.26	1.47	1.41
36	K	309	CLA	CMD-C2D	-2.26	1.46	1.50
37	M	318	KC1	C1D-CHD	2.26	1.47	1.41
36	C	208	CLA	C3B-C2B	-2.26	1.37	1.40
37	R	317	KC1	C1D-CHD	2.26	1.47	1.41
35	T	306	A86	C13-C11	-2.26	1.45	1.49
37	P	317	KC1	C1A-CHA	2.26	1.46	1.40
36	A	311	CLA	CMC-C2C	-2.26	1.46	1.50
35	P	303	A86	C33-C34	2.26	1.55	1.51
36	f	805	CLA	CMD-C2D	-2.26	1.46	1.50
35	R	303	A86	C35-C34	2.26	1.55	1.51
36	b	822	CLA	CMD-C2D	-2.26	1.46	1.50
35	h	202	A86	C32-C31	-2.26	1.50	1.54
36	a	811	CLA	CMD-C2D	-2.26	1.46	1.50
35	G	306	A86	O1-C20	-2.26	1.43	1.46
37	M	313	KC1	C1D-CHD	2.26	1.47	1.41
36	G	310	CLA	CMD-C2D	-2.26	1.46	1.50
36	a	837	CLA	CMD-C2D	-2.26	1.46	1.50
37	H	313	KC1	C1D-CHD	2.25	1.47	1.41
36	H	310	CLA	CMD-C2D	-2.25	1.46	1.50
36	C	205	CLA	CMD-C2D	-2.25	1.46	1.50
36	a	809	CLA	CMD-C2D	-2.25	1.46	1.50
34	j	103	DD6	O1-C20	-2.25	1.43	1.46
36	f	803	CLA	C4C-C3C	2.25	1.48	1.45
36	b	802	CLA	CMC-C2C	-2.25	1.46	1.50
37	T	310	KC1	C1C-C2C	2.25	1.48	1.44
35	L	301	A86	O1-C20	-2.25	1.43	1.46
36	R	316	CLA	CMC-C2C	-2.25	1.46	1.50
36	b	822	CLA	C3B-CAB	-2.25	1.43	1.47
36	M	312	CLA	CMD-C2D	-2.25	1.46	1.50
35	C	204	A86	C32-C31	-2.25	1.50	1.54
35	U	304	A86	O1-C20	-2.25	1.43	1.46
36	a	808	CLA	C3B-CAB	-2.25	1.43	1.47
36	b	819	CLA	CMC-C2C	-2.25	1.46	1.50
36	N	308	CLA	C3B-CAB	-2.25	1.43	1.47
37	M	313	KC1	C4C-C3C	2.25	1.48	1.45
36	D	311	CLA	CMD-C2D	-2.25	1.46	1.50
36	E	311	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	U	307	CLA	CMD-C2D	-2.25	1.46	1.50
35	T	305	A86	C30-C29	-2.25	1.28	1.32
36	b	807	CLA	CMD-C2D	-2.25	1.46	1.50
36	B	306	CLA	CMD-C2D	-2.25	1.46	1.50
36	I	307	CLA	CMD-C2D	-2.25	1.46	1.50
36	R	322	CLA	CMD-C2D	-2.25	1.46	1.50
36	a	827	CLA	CMD-C2D	-2.25	1.46	1.50
36	i	102	CLA	CMD-C2D	-2.25	1.46	1.50
36	F	316	CLA	C3B-CAB	-2.24	1.43	1.47
35	R	301	A86	C13-C11	-2.24	1.45	1.49
36	a	823	CLA	CHD-C4C	2.24	1.44	1.39
36	b	820	CLA	C3B-C2B	-2.24	1.37	1.40
36	N	307	CLA	CMB-C2B	-2.24	1.47	1.51
36	R	314	CLA	CMC-C2C	-2.24	1.46	1.50
36	H	305	CLA	CMD-C2D	-2.24	1.46	1.50
36	I	310	CLA	CMD-C2D	-2.24	1.46	1.50
36	L	312	CLA	C3B-C2B	-2.24	1.37	1.40
36	O	314	CLA	C3B-C2B	-2.24	1.37	1.40
36	a	832	CLA	CMC-C2C	-2.24	1.46	1.50
34	P	305	DD6	O1-C20	-2.24	1.43	1.46
35	O	319	A86	C3-C2	2.24	1.50	1.43
36	L	314	CLA	CMB-C2B	-2.24	1.47	1.51
36	D	306	CLA	O2A-CGA	2.24	1.38	1.30
36	D	309	CLA	C1C-C2C	2.24	1.48	1.44
37	L	315	KC1	C4A-C3A	2.24	1.48	1.44
36	h	203	CLA	CMD-C2D	-2.24	1.46	1.50
36	H	318	CLA	C3B-C2B	-2.24	1.37	1.40
36	b	836	CLA	C1D-C2D	2.24	1.49	1.45
36	b	832	CLA	CMD-C2D	-2.24	1.46	1.50
36	b	816	CLA	C1B-CHB	2.24	1.47	1.41
36	C	208	CLA	CMC-C2C	-2.24	1.46	1.50
36	G	319	CLA	C4C-C3C	2.24	1.48	1.45
36	R	311	CLA	CMD-C2D	-2.23	1.46	1.50
36	V	309	CLA	CMD-C2D	-2.23	1.46	1.50
37	W	213	KC1	C1B-NB	-2.23	1.35	1.37
36	a	824	CLA	C3C-C2C	2.23	1.41	1.36
34	E	301	DD6	O1-C20	-2.23	1.43	1.46
36	Q	312	CLA	C3B-C2B	-2.23	1.37	1.40
36	a	848	CLA	MG-ND	-2.23	2.01	2.05
35	G	305	A86	O1-C20	-2.23	1.43	1.46
36	K	316	CLA	CMD-C2D	-2.23	1.46	1.50
36	b	828	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	P	307	A86	O1-C20	-2.23	1.43	1.46
36	b	841	CLA	CMD-C2D	-2.23	1.46	1.50
34	E	304	DD6	O1-C20	-2.23	1.43	1.46
37	S	316	KC1	C3B-C4B	2.23	1.50	1.46
35	D	302	A86	C32-C31	-2.23	1.50	1.54
36	J	310	CLA	CMD-C2D	-2.23	1.46	1.50
36	H	315	CLA	MG-ND	-2.23	2.01	2.05
35	S	301	A86	C13-C11	-2.23	1.45	1.49
34	A	301	DD6	O1-C20	-2.23	1.43	1.46
34	I	303	DD6	O1-C20	-2.23	1.43	1.46
35	L	307	A86	C32-C31	-2.23	1.50	1.54
36	L	313	CLA	CMD-C2D	-2.23	1.46	1.50
36	W	212	CLA	C1A-CHA	-2.23	1.33	1.43
36	a	833	CLA	CMC-C2C	-2.23	1.46	1.50
36	F	313	CLA	CMD-C2D	-2.23	1.46	1.50
36	I	311	CLA	CMC-C2C	-2.23	1.46	1.50
36	b	841	CLA	C1C-NC	-2.23	1.34	1.37
36	G	319	CLA	C3D-C4D	-2.23	1.39	1.44
36	T	311	CLA	C4B-CHC	-2.23	1.34	1.41
36	U	306	CLA	C1C-C2C	2.23	1.48	1.44
36	F	314	CLA	CMD-C2D	-2.23	1.46	1.50
36	K	313	CLA	CMD-C2D	-2.23	1.46	1.50
36	a	834	CLA	CMD-C2D	-2.23	1.46	1.50
36	A	311	CLA	C3B-C2B	-2.23	1.37	1.40
36	P	318	CLA	CMD-C2D	-2.22	1.46	1.50
36	a	808	CLA	CMC-C2C	-2.22	1.46	1.50
36	a	838	CLA	C1D-ND	2.22	1.40	1.37
36	P	301	CLA	CMD-C2D	-2.22	1.46	1.50
36	a	815	CLA	CMC-C2C	-2.22	1.46	1.50
36	b	825	CLA	MG-ND	-2.22	2.01	2.05
36	a	831	CLA	CMC-C2C	-2.22	1.46	1.50
36	I	311	CLA	CMD-C2D	-2.22	1.46	1.50
36	X	315	CLA	CMB-C2B	-2.22	1.47	1.51
36	B	308	CLA	CAC-C3C	-2.22	1.45	1.51
35	M	302	A86	C13-C11	-2.22	1.45	1.49
34	H	302	DD6	O1-C20	-2.22	1.43	1.46
37	P	315	KC1	C1D-CHD	2.22	1.47	1.41
36	A	306	CLA	C1C-C2C	2.22	1.48	1.44
36	Q	308	CLA	CMD-C2D	-2.22	1.46	1.50
36	a	810	CLA	CMD-C2D	-2.22	1.46	1.50
35	V	302	A86	C17-C18	-2.22	1.49	1.52
36	G	312	CLA	C3B-C2B	-2.22	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	M	312	CLA	C3B-C2B	-2.22	1.37	1.40
36	a	807	CLA	CMC-C2C	-2.22	1.46	1.50
36	H	314	CLA	CMC-C2C	-2.22	1.46	1.50
36	b	814	CLA	CMC-C2C	-2.22	1.46	1.50
37	U	312	KC1	C1B-C2B	2.22	1.49	1.45
37	O	315	KC1	C1D-CHD	2.22	1.47	1.41
36	b	814	CLA	CMD-C2D	-2.22	1.46	1.50
37	O	313	KC1	C1D-CHD	2.22	1.47	1.41
35	M	301	A86	C33-C34	2.22	1.55	1.51
35	R	306	A86	O3-C36	-2.22	1.39	1.43
35	N	303	A86	C13-C11	-2.21	1.45	1.49
36	H	308	CLA	CMD-C2D	-2.21	1.46	1.50
37	L	317	KC1	C1D-CHD	2.21	1.47	1.41
36	b	812	CLA	C3B-C2B	-2.21	1.37	1.40
35	N	301	A86	C13-C11	-2.21	1.45	1.49
36	b	812	CLA	MG-ND	-2.21	2.01	2.05
34	R	308	DD6	O1-C20	-2.21	1.43	1.46
35	G	304	A86	C17-C18	-2.21	1.49	1.52
36	N	319	CLA	CMB-C2B	-2.21	1.47	1.51
37	Q	313	KC1	C1D-CHD	2.21	1.47	1.41
36	H	318	CLA	MG-ND	-2.21	2.01	2.05
36	a	808	CLA	MG-ND	-2.21	2.01	2.05
36	b	830	CLA	MG-ND	-2.21	2.01	2.05
36	F	310	CLA	CMD-C2D	-2.21	1.46	1.50
36	H	316	CLA	CMD-C2D	-2.21	1.46	1.50
36	I	201	CLA	CMD-C2D	-2.21	1.46	1.50
36	C	212	CLA	CMC-C2C	-2.21	1.46	1.50
36	M	308	CLA	CMD-C2D	-2.21	1.46	1.50
36	a	817	CLA	CMD-C2D	-2.21	1.46	1.50
36	b	810	CLA	CMD-C2D	-2.21	1.46	1.50
36	j	106	CLA	C3B-C2B	-2.21	1.37	1.40
36	a	831	CLA	CMD-C2D	-2.21	1.46	1.50
36	W	214	CLA	C3B-C2B	-2.21	1.37	1.40
36	E	313	CLA	C1B-CHB	2.21	1.47	1.41
36	C	209	CLA	MG-ND	-2.21	2.01	2.05
36	O	306	CLA	CMD-C2D	-2.21	1.46	1.50
36	R	313	CLA	MG-ND	-2.21	2.01	2.05
36	b	833	CLA	CMD-C2D	-2.21	1.46	1.50
36	K	315	CLA	CMD-C2D	-2.21	1.46	1.50
36	b	839	CLA	CMD-C2D	-2.21	1.46	1.50
36	a	814	CLA	C4B-CHC	-2.21	1.34	1.41
35	J	301	A86	C32-C31	-2.21	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	311	CLA	CMD-C2D	-2.21	1.46	1.50
36	A	307	CLA	CMD-C2D	-2.21	1.46	1.50
36	P	314	CLA	CMC-C2C	-2.21	1.46	1.50
36	b	812	CLA	CMC-C2C	-2.21	1.46	1.50
36	Q	310	CLA	CMC-C2C	-2.20	1.46	1.50
37	Q	311	KC1	C1D-CHD	2.20	1.47	1.41
36	W	216	CLA	C3D-C4D	2.20	1.49	1.44
35	S	303	A86	C13-C11	-2.20	1.45	1.49
35	K	301	A86	O1-C20	-2.20	1.43	1.46
36	I	308	CLA	C1B-CHB	2.20	1.47	1.41
36	E	315	CLA	C1C-C2C	2.20	1.48	1.44
36	b	809	CLA	CMD-C2D	-2.20	1.46	1.50
35	K	303	A86	C13-C11	-2.20	1.45	1.49
36	a	839	CLA	C3B-C2B	-2.20	1.37	1.40
36	D	313	CLA	CMD-C2D	-2.20	1.46	1.50
36	J	311	CLA	CMD-C2D	-2.20	1.46	1.50
36	K	313	CLA	CMC-C2C	-2.20	1.46	1.50
36	b	813	CLA	MG-ND	-2.20	2.01	2.05
37	G	308	KC1	C4B-NB	-2.20	1.35	1.37
35	F	306	A86	C32-C31	-2.20	1.50	1.54
35	Q	316	A86	C2-C1	-2.20	1.32	1.35
36	L	311	CLA	CMC-C2C	-2.20	1.46	1.50
35	U	303	A86	C32-C31	-2.20	1.50	1.54
36	L	308	CLA	MG-ND	2.20	2.10	2.05
35	Q	316	A86	C17-C18	-2.20	1.49	1.52
37	M	317	KC1	C4B-NB	-2.20	1.35	1.37
36	A	314	CLA	CMD-C2D	-2.20	1.46	1.50
36	O	312	CLA	CMC-C2C	-2.20	1.46	1.50
35	X	314	A86	O1-C20	-2.20	1.43	1.46
36	E	312	CLA	CMC-C2C	-2.20	1.46	1.50
36	S	312	CLA	MG-ND	-2.20	2.01	2.05
36	I	312	CLA	CMD-C2D	-2.20	1.46	1.50
37	S	316	KC1	C4C-C3C	2.20	1.48	1.45
36	O	309	CLA	CMD-C2D	-2.20	1.46	1.50
36	U	309	CLA	CMD-C2D	-2.20	1.46	1.50
44	l	207	BCR	C30-C25	-2.20	1.50	1.53
36	a	801	CLA	C3B-CAB	-2.20	1.43	1.47
36	N	310	CLA	CMD-C2D	-2.20	1.46	1.50
37	Q	313	KC1	C4A-C3A	2.20	1.48	1.44
34	D	303	DD6	C3-C2	2.20	1.50	1.43
36	G	314	CLA	CMD-C2D	-2.20	1.46	1.50
36	T	309	CLA	CMC-C2C	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	305	A86	C32-C31	-2.20	1.50	1.54
36	I	306	CLA	C3D-C4D	-2.20	1.39	1.44
44	i	103	BCR	C38-C26	-2.19	1.47	1.50
36	A	313	CLA	CMD-C2D	-2.19	1.46	1.50
36	H	307	CLA	CAC-C3C	-2.19	1.45	1.51
35	W	202	A86	C13-C11	-2.19	1.45	1.49
35	G	302	A86	O1-C20	-2.19	1.43	1.46
36	F	310	CLA	CMC-C2C	-2.19	1.46	1.50
34	B	302	DD6	O1-C20	-2.19	1.43	1.46
35	F	302	A86	O1-C20	-2.19	1.43	1.46
36	b	832	CLA	CMC-C2C	-2.19	1.46	1.50
36	N	307	CLA	CMD-C2D	-2.19	1.46	1.50
36	Q	305	CLA	CMD-C2D	-2.19	1.46	1.50
36	a	819	CLA	C3C-C2C	2.19	1.41	1.36
36	H	310	CLA	C3B-C2B	-2.19	1.37	1.40
36	X	308	CLA	MG-ND	-2.19	2.01	2.05
34	D	304	DD6	O1-C20	-2.19	1.43	1.46
36	W	207	CLA	CMC-C2C	-2.19	1.46	1.50
36	a	826	CLA	CMD-C2D	-2.19	1.46	1.50
44	f	806	BCR	C33-C5	-2.19	1.47	1.50
36	a	833	CLA	CMD-C2D	-2.19	1.46	1.50
37	O	315	KC1	CAA-C2A	2.19	1.53	1.46
36	a	819	CLA	C4B-CHC	-2.19	1.34	1.41
36	M	315	CLA	CMC-C2C	-2.19	1.46	1.50
37	L	317	KC1	C4C-C3C	2.19	1.48	1.45
37	O	313	KC1	C4A-C3A	2.19	1.48	1.44
36	N	313	CLA	CMC-C2C	-2.19	1.46	1.50
36	P	311	CLA	CMD-C2D	-2.19	1.46	1.50
36	b	834	CLA	CMC-C2C	-2.19	1.46	1.50
36	G	316	CLA	C3B-CAB	-2.19	1.43	1.47
36	b	841	CLA	C3B-C2B	-2.19	1.37	1.40
36	D	310	CLA	CMD-C2D	-2.19	1.46	1.50
36	V	307	CLA	CMD-C2D	-2.19	1.46	1.50
35	C	203	A86	O1-C20	-2.19	1.43	1.46
35	O	301	A86	C32-C31	-2.19	1.50	1.54
36	C	207	CLA	C4C-C3C	2.18	1.48	1.45
36	P	308	CLA	CMD-C2D	-2.18	1.46	1.50
35	G	306	A86	C32-C31	-2.18	1.50	1.54
36	a	848	CLA	CHD-C1D	2.18	1.42	1.38
36	a	827	CLA	C3B-CAB	-2.18	1.43	1.47
36	N	309	CLA	C4B-CHC	-2.18	1.34	1.41
37	E	309	KC1	O2A-CGA	-2.18	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	806	BCR	C30-C25	-2.18	1.50	1.53
35	h	204	A86	O1-C20	-2.18	1.43	1.46
36	P	319	CLA	CMC-C2C	-2.18	1.46	1.50
36	K	315	CLA	CMC-C2C	-2.18	1.46	1.50
35	C	202	A86	C13-C11	-2.18	1.45	1.49
34	Q	302	DD6	O1-C20	-2.18	1.43	1.46
37	T	315	KC1	C4C-C3C	2.18	1.48	1.45
36	W	211	CLA	CMD-C2D	-2.18	1.46	1.50
36	B	307	CLA	C3B-C2B	-2.18	1.37	1.40
36	T	309	CLA	CMD-C2D	-2.18	1.46	1.50
36	A	310	CLA	CMC-C2C	-2.18	1.46	1.50
36	b	807	CLA	CMC-C2C	-2.18	1.46	1.50
36	E	317	CLA	C3B-C2B	-2.18	1.37	1.40
36	f	804	CLA	C1C-C2C	2.18	1.48	1.44
34	W	204	DD6	O1-C20	-2.18	1.43	1.46
35	B	301	A86	O1-C20	-2.18	1.43	1.46
36	G	312	CLA	CMC-C2C	-2.18	1.46	1.50
36	a	803	CLA	CMC-C2C	-2.18	1.46	1.50
35	O	303	A86	C13-C11	-2.18	1.45	1.49
36	F	311	CLA	C3B-CAB	-2.18	1.43	1.47
36	j	106	CLA	CMD-C2D	-2.18	1.46	1.50
35	R	303	A86	C13-C11	-2.18	1.45	1.49
37	F	308	KC1	O2A-CGA	-2.18	1.24	1.30
36	L	311	CLA	CMD-C2D	-2.18	1.46	1.50
36	R	314	CLA	CMD-C2D	-2.18	1.46	1.50
36	O	307	CLA	CMC-C2C	-2.18	1.46	1.50
37	T	310	KC1	C1A-CHA	2.17	1.46	1.40
35	N	305	A86	C2-C1	-2.17	1.32	1.35
35	P	304	A86	C13-C11	-2.17	1.45	1.49
36	D	313	CLA	CMC-C2C	-2.17	1.46	1.50
36	O	307	CLA	CMD-C2D	-2.17	1.46	1.50
36	a	805	CLA	CMD-C2D	-2.17	1.46	1.50
37	Q	311	KC1	CAA-C2A	2.17	1.53	1.46
36	P	313	CLA	CMD-C2D	-2.17	1.46	1.50
36	b	801	CLA	CMD-C2D	-2.17	1.46	1.50
36	b	825	CLA	CMC-C2C	-2.17	1.46	1.50
37	M	317	KC1	O2A-CGA	-2.17	1.24	1.30
37	Q	313	KC1	CAA-C2A	2.17	1.53	1.46
36	M	315	CLA	CAC-C3C	-2.17	1.45	1.51
34	K	305	DD6	O1-C20	-2.17	1.43	1.46
36	P	309	CLA	CMD-C2D	-2.17	1.46	1.50
35	N	305	A86	C17-C16	-2.17	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	211	CLA	CMC-C2C	-2.17	1.46	1.50
36	D	307	CLA	CMD-C2D	-2.17	1.46	1.50
36	b	837	CLA	CMC-C2C	-2.17	1.46	1.50
36	H	307	CLA	C3B-C2B	-2.17	1.37	1.40
35	Q	301	A86	C13-C11	-2.17	1.45	1.49
36	a	835	CLA	CMC-C2C	-2.17	1.46	1.50
37	N	314	KC1	C1B-NB	-2.17	1.35	1.37
36	M	315	CLA	CMD-C2D	-2.17	1.46	1.50
36	U	309	CLA	C3B-C2B	-2.17	1.37	1.40
35	N	305	A86	C17-C18	-2.17	1.49	1.52
37	K	314	KC1	C1A-CHA	2.17	1.46	1.40
36	M	316	CLA	C3B-C2B	-2.17	1.37	1.40
35	O	302	A86	C26-C27	-2.17	1.32	1.35
36	H	316	CLA	CMC-C2C	-2.17	1.46	1.50
36	a	810	CLA	C3B-CAB	-2.17	1.43	1.47
36	B	307	CLA	CMD-C2D	-2.17	1.46	1.50
36	L	314	CLA	CMC-C2C	-2.17	1.46	1.50
36	R	315	CLA	CMD-C2D	-2.17	1.46	1.50
35	P	306	A86	O1-C20	-2.17	1.43	1.46
36	K	312	CLA	CMC-C2C	-2.17	1.46	1.50
36	P	309	CLA	CMC-C2C	-2.17	1.46	1.50
36	Q	308	CLA	MG-ND	-2.17	2.01	2.05
36	D	317	CLA	CMD-C2D	-2.17	1.46	1.50
36	P	311	CLA	MG-ND	-2.17	2.01	2.05
35	E	307	A86	C32-C31	-2.16	1.50	1.54
34	C	201	DD6	O1-C20	-2.16	1.43	1.46
36	X	313	CLA	C3D-C4D	2.16	1.49	1.44
36	C	206	CLA	CMD-C2D	-2.16	1.46	1.50
36	M	312	CLA	MG-ND	-2.16	2.01	2.05
36	N	309	CLA	CMD-C2D	-2.16	1.46	1.50
37	M	318	KC1	C4B-NB	-2.16	1.35	1.37
36	R	321	CLA	CMD-C2D	-2.16	1.46	1.50
37	P	315	KC1	CAA-C2A	2.16	1.53	1.46
36	a	831	CLA	C3B-C2B	-2.16	1.37	1.40
36	M	312	CLA	C3B-CAB	-2.16	1.43	1.47
35	F	302	A86	C32-C31	-2.16	1.50	1.54
36	K	309	CLA	C3B-C2B	-2.16	1.37	1.40
36	R	312	CLA	C3B-C2B	-2.16	1.37	1.40
44	a	844	BCR	C30-C25	-2.16	1.50	1.53
37	A	312	KC1	C4B-NB	-2.16	1.35	1.37
36	Q	306	CLA	CMC-C2C	-2.16	1.46	1.50
36	a	821	CLA	CMC-C2C	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	S	311	CLA	C3B-CAB	-2.16	1.43	1.47
35	T	304	A86	C30-C29	-2.16	1.28	1.32
37	O	315	KC1	C4A-C3A	2.16	1.48	1.44
34	M	303	DD6	O1-C20	-2.16	1.43	1.46
36	E	315	CLA	C4C-C3C	2.16	1.48	1.45
37	C	213	KC1	C4C-C3C	2.16	1.48	1.45
36	Q	306	CLA	CMD-C2D	-2.16	1.46	1.50
36	R	310	CLA	MG-ND	-2.16	2.01	2.05
34	E	306	DD6	O1-C20	-2.15	1.43	1.46
35	Q	316	A86	C17-C16	-2.15	1.51	1.54
36	H	311	CLA	CMC-C2C	-2.15	1.46	1.50
36	P	312	CLA	CMD-C2D	-2.15	1.46	1.50
44	h	201	BCR	C33-C5	-2.15	1.47	1.50
36	O	310	CLA	CMC-C2C	-2.15	1.46	1.50
37	Q	311	KC1	C4A-C3A	2.15	1.48	1.44
36	N	313	CLA	CMB-C2B	-2.15	1.47	1.51
36	A	310	CLA	MG-ND	-2.15	2.01	2.05
36	D	308	CLA	MG-ND	-2.15	2.01	2.05
36	a	829	CLA	CMC-C2C	-2.15	1.46	1.50
34	O	304	DD6	O1-C20	-2.15	1.43	1.46
35	S	308	A86	O1-C20	-2.15	1.43	1.46
36	D	310	CLA	C3B-CAB	-2.15	1.43	1.47
36	X	307	CLA	CAC-C3C	-2.15	1.45	1.51
36	G	310	CLA	CMC-C2C	-2.15	1.46	1.50
36	J	313	CLA	CMC-C2C	-2.15	1.46	1.50
36	j	101	CLA	CMD-C2D	-2.15	1.46	1.50
36	U	305	CLA	CMD-C2D	-2.15	1.46	1.50
36	a	818	CLA	C3B-CAB	-2.15	1.43	1.47
36	a	833	CLA	C3B-CAB	-2.15	1.43	1.47
35	U	303	A86	O1-C20	-2.15	1.43	1.46
36	L	314	CLA	MG-ND	-2.15	2.01	2.05
36	J	312	CLA	CMD-C2D	-2.15	1.46	1.50
37	O	313	KC1	CAA-C2A	2.15	1.53	1.46
35	P	303	A86	C26-C27	-2.15	1.32	1.35
36	J	316	CLA	C3B-CAB	-2.15	1.43	1.47
36	H	312	CLA	CMD-C2D	-2.15	1.46	1.50
36	M	315	CLA	C4B-CHC	-2.15	1.35	1.41
35	J	306	A86	O1-C20	-2.15	1.43	1.46
36	b	839	CLA	CMC-C2C	-2.15	1.46	1.50
35	J	302	A86	C32-C31	-2.15	1.50	1.54
44	h	201	BCR	C39-C30	-2.15	1.49	1.53
36	D	311	CLA	C3B-C2B	-2.15	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	207	CLA	C1B-CHB	2.15	1.47	1.41
36	J	316	CLA	CMC-C2C	-2.15	1.46	1.50
36	H	307	CLA	CMB-C2B	-2.15	1.47	1.51
36	R	316	CLA	MG-ND	-2.15	2.01	2.05
36	a	831	CLA	MG-ND	-2.15	2.01	2.05
36	I	309	CLA	CAC-C3C	-2.15	1.45	1.51
36	A	314	CLA	C3B-C2B	-2.15	1.37	1.40
40	b	849	DGD	O3D-C3D	-2.15	1.37	1.43
36	S	314	CLA	C3B-C2B	-2.14	1.37	1.40
36	O	311	CLA	CMD-C2D	-2.14	1.46	1.50
37	M	313	KC1	C1A-CHA	2.14	1.46	1.40
36	a	805	CLA	CMC-C2C	-2.14	1.46	1.50
36	K	316	CLA	C3B-CAB	-2.14	1.43	1.47
37	P	315	KC1	C4A-C3A	2.14	1.48	1.44
36	X	309	CLA	C3D-C4D	2.14	1.49	1.44
36	J	316	CLA	CMD-C2D	-2.14	1.46	1.50
36	l	201	CLA	C3B-C2B	-2.14	1.37	1.40
36	W	201	CLA	CMD-C2D	-2.14	1.46	1.50
36	F	312	CLA	CMC-C2C	-2.14	1.46	1.50
36	E	311	CLA	CMC-C2C	-2.14	1.46	1.50
35	S	308	A86	C32-C31	-2.14	1.51	1.54
36	a	830	CLA	C1D-C2D	2.14	1.49	1.45
36	b	813	CLA	CMC-C2C	-2.14	1.46	1.50
36	P	301	CLA	C3B-C2B	-2.14	1.37	1.40
36	H	306	CLA	C3B-CAB	-2.14	1.43	1.47
36	a	836	CLA	CMC-C2C	-2.14	1.46	1.50
35	K	301	A86	C32-C31	-2.14	1.51	1.54
36	I	305	CLA	CMC-C2C	-2.14	1.46	1.50
35	F	304	A86	C32-C31	-2.14	1.51	1.54
36	I	313	CLA	CMD-C2D	-2.14	1.46	1.50
36	L	310	CLA	CMD-C2D	-2.14	1.46	1.50
36	N	311	CLA	CMD-C2D	-2.14	1.46	1.50
36	X	312	CLA	CMD-C2D	-2.14	1.46	1.50
36	K	311	CLA	CMD-C2D	-2.14	1.46	1.50
37	N	314	KC1	C4A-C3A	2.14	1.48	1.44
36	N	313	CLA	C3B-CAB	-2.14	1.43	1.47
36	O	309	CLA	MG-ND	-2.14	2.01	2.05
36	V	313	CLA	MG-ND	-2.14	2.01	2.05
35	H	304	A86	C32-C31	-2.14	1.51	1.54
36	J	310	CLA	CMC-C2C	-2.14	1.46	1.50
36	J	311	CLA	C3B-CAB	-2.14	1.43	1.47
36	J	317	CLA	C3B-C2B	-2.14	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	813	CLA	CMA-C3A	-2.13	1.48	1.53
37	M	317	KC1	C1D-CHD	2.13	1.46	1.41
36	C	207	CLA	C1C-C2C	2.13	1.48	1.44
36	N	317	CLA	CMC-C2C	-2.13	1.46	1.50
36	b	808	CLA	CMD-C2D	-2.13	1.46	1.50
44	b	846	BCR	C33-C5	-2.13	1.47	1.50
36	C	208	CLA	C3B-CAB	-2.13	1.43	1.47
36	L	320	CLA	CMD-C2D	-2.13	1.46	1.50
36	H	309	CLA	CMC-C2C	-2.13	1.46	1.50
36	Q	309	CLA	CMD-C2D	-2.13	1.46	1.50
35	V	301	A86	O1-C20	-2.13	1.43	1.46
36	I	309	CLA	CMD-C2D	-2.13	1.46	1.50
36	D	308	CLA	CMC-C2C	-2.13	1.46	1.50
36	Q	312	CLA	CMD-C2D	-2.13	1.46	1.50
34	L	305	DD6	O1-C20	-2.13	1.43	1.46
36	R	319	CLA	CMC-C2C	-2.13	1.46	1.50
36	a	836	CLA	CMD-C2D	-2.13	1.46	1.50
37	G	308	KC1	C4C-C3C	2.13	1.48	1.45
36	E	317	CLA	C3B-CAB	-2.13	1.43	1.47
36	D	317	CLA	CMC-C2C	-2.13	1.46	1.50
36	M	309	CLA	CMC-C2C	-2.13	1.46	1.50
37	K	314	KC1	C4A-C3A	2.13	1.48	1.44
36	D	316	CLA	CMC-C2C	-2.13	1.46	1.50
35	h	202	A86	O1-C20	-2.13	1.43	1.46
36	X	312	CLA	CMB-C2B	-2.13	1.47	1.51
36	Q	309	CLA	CMC-C2C	-2.13	1.46	1.50
36	X	310	CLA	C4D-ND	-2.13	1.34	1.37
35	I	302	A86	C13-C11	-2.12	1.45	1.49
36	T	316	CLA	CMD-C2D	-2.12	1.46	1.50
36	U	308	CLA	CMD-C2D	-2.12	1.46	1.50
36	a	803	CLA	MG-ND	-2.12	2.01	2.05
35	T	301	A86	O1-C20	-2.12	1.43	1.46
36	I	307	CLA	CMC-C2C	-2.12	1.46	1.50
36	C	206	CLA	C3B-C2B	-2.12	1.37	1.40
36	H	316	CLA	C3B-C2B	-2.12	1.37	1.40
36	M	311	CLA	MG-ND	-2.12	2.01	2.05
36	V	310	CLA	CMD-C2D	-2.12	1.46	1.50
36	D	316	CLA	C3B-CAB	-2.12	1.43	1.47
37	M	318	KC1	CHD-C4C	2.12	1.40	1.35
34	A	304	DD6	O1-C20	-2.12	1.43	1.46
36	N	318	CLA	CMD-C2D	-2.12	1.46	1.50
36	S	321	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	830	CLA	CMC-C2C	-2.12	1.46	1.50
36	V	309	CLA	C3B-C2B	-2.12	1.37	1.40
36	F	309	CLA	CMC-C2C	-2.12	1.46	1.50
36	a	805	CLA	C3B-CAB	-2.12	1.43	1.47
35	A	302	A86	C35-C34	2.12	1.55	1.51
36	a	809	CLA	CMC-C2C	-2.12	1.46	1.50
35	Q	303	A86	O1-C20	-2.12	1.43	1.46
36	b	819	CLA	C3B-CAB	-2.12	1.43	1.47
36	H	312	CLA	C3B-C2B	-2.12	1.37	1.40
35	D	302	A86	O1-C20	-2.12	1.43	1.46
36	D	312	CLA	CMC-C2C	-2.12	1.46	1.50
36	a	801	CLA	CMC-C2C	-2.12	1.46	1.50
36	b	829	CLA	C3B-CAB	-2.12	1.43	1.47
36	K	316	CLA	CMC-C2C	-2.12	1.46	1.50
36	T	314	CLA	CMC-C2C	-2.12	1.46	1.50
35	L	319	A86	C26-C27	-2.12	1.33	1.35
36	D	310	CLA	CMC-C2C	-2.12	1.46	1.50
36	A	306	CLA	MG-ND	-2.12	2.01	2.05
36	S	311	CLA	MG-ND	-2.12	2.01	2.05
36	E	312	CLA	CMD-C2D	-2.12	1.46	1.50
36	A	311	CLA	C3B-CAB	-2.12	1.43	1.47
36	J	315	CLA	CMC-C2C	-2.12	1.46	1.50
36	S	315	CLA	C1B-NB	2.12	1.37	1.35
36	b	820	CLA	CMC-C2C	-2.12	1.46	1.50
36	G	310	CLA	MG-ND	-2.11	2.01	2.05
37	G	317	KC1	C4C-C3C	2.11	1.48	1.45
36	J	313	CLA	MG-ND	-2.11	2.01	2.05
36	b	829	CLA	CMC-C2C	-2.11	1.46	1.50
36	W	210	CLA	MG-ND	-2.11	2.01	2.05
37	L	315	KC1	C1D-CHD	2.11	1.46	1.41
37	P	317	KC1	O2A-CGA	-2.11	1.24	1.30
36	G	309	CLA	CMD-C2D	-2.11	1.46	1.50
36	V	308	CLA	CMD-C2D	-2.11	1.46	1.50
36	A	305	CLA	CMC-C2C	-2.11	1.46	1.50
44	b	847	BCR	C38-C26	-2.11	1.47	1.50
36	V	306	CLA	CMB-C2B	-2.11	1.47	1.51
36	M	307	CLA	CMC-C2C	-2.11	1.46	1.50
36	b	806	CLA	C3B-CAB	-2.11	1.43	1.47
36	O	306	CLA	CMC-C2C	-2.11	1.46	1.50
36	S	319	CLA	CMD-C2D	-2.11	1.46	1.50
36	I	314	CLA	CMD-C2D	-2.11	1.46	1.50
36	a	835	CLA	MG-ND	-2.11	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	820	CLA	MG-ND	-2.11	2.01	2.05
36	P	316	CLA	CMD-C2D	-2.11	1.46	1.50
36	a	815	CLA	CMD-C2D	-2.11	1.46	1.50
40	b	849	DGD	O4D-C4D	-2.11	1.38	1.43
36	D	311	CLA	CMC-C2C	-2.11	1.46	1.50
36	L	308	CLA	MG-NA	2.11	2.11	2.06
35	X	303	A86	C26-C27	-2.11	1.33	1.35
36	H	317	CLA	CMD-C2D	-2.11	1.46	1.50
35	T	303	A86	C13-C11	-2.11	1.45	1.49
37	G	317	KC1	O2A-CGA	-2.11	1.24	1.30
36	G	310	CLA	C3B-CAB	-2.10	1.43	1.47
36	M	307	CLA	CMD-C2D	-2.10	1.46	1.50
36	P	319	CLA	MG-NA	2.10	2.11	2.06
36	A	313	CLA	CMC-C2C	-2.10	1.46	1.50
36	b	823	CLA	CMC-C2C	-2.10	1.46	1.50
36	b	826	CLA	CMC-C2C	-2.10	1.46	1.50
36	C	211	CLA	C3B-C2B	-2.10	1.37	1.40
36	D	306	CLA	MG-ND	-2.10	2.01	2.05
36	b	806	CLA	MG-ND	-2.10	2.01	2.05
35	L	307	A86	O1-C20	-2.10	1.43	1.46
36	V	313	CLA	C3B-CAB	-2.10	1.43	1.47
36	Q	305	CLA	CMC-C2C	-2.10	1.46	1.50
36	b	835	CLA	C3B-CAB	-2.10	1.43	1.47
36	O	308	CLA	CMD-C2D	-2.10	1.46	1.50
36	O	310	CLA	CMD-C2D	-2.10	1.46	1.50
35	H	304	A86	O1-C20	-2.10	1.43	1.46
36	A	309	CLA	C3B-CAB	-2.10	1.43	1.47
36	b	809	CLA	C3B-C2B	-2.10	1.37	1.40
36	Q	306	CLA	MG-ND	-2.10	2.01	2.05
36	H	312	CLA	MG-ND	-2.10	2.01	2.05
36	A	309	CLA	CMD-C2D	-2.10	1.46	1.50
36	I	313	CLA	CMC-C2C	-2.10	1.46	1.50
35	X	304	A86	C13-C11	-2.10	1.45	1.49
37	F	315	KC1	C1A-CHA	2.10	1.46	1.40
44	a	847	BCR	C33-C5	-2.10	1.47	1.50
36	D	306	CLA	CMD-C2D	-2.10	1.46	1.50
36	a	811	CLA	CMC-C2C	-2.10	1.46	1.50
40	b	849	DGD	C1E-C2E	2.10	1.58	1.52
36	G	311	CLA	C3B-C2B	-2.10	1.37	1.40
36	a	809	CLA	C3B-CAB	-2.10	1.43	1.47
36	b	831	CLA	MG-ND	-2.10	2.01	2.05
36	b	830	CLA	C4B-CHC	-2.10	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	831	CLA	C3B-CAB	-2.10	1.43	1.47
37	V	312	KC1	C4B-NB	-2.10	1.35	1.37
36	b	805	CLA	C4B-CHC	-2.10	1.35	1.41
36	F	316	CLA	CMD-C2D	-2.10	1.46	1.50
36	R	319	CLA	CMD-C2D	-2.10	1.46	1.50
36	b	810	CLA	CMC-C2C	-2.10	1.46	1.50
37	L	317	KC1	O2A-CGA	-2.10	1.24	1.30
36	b	810	CLA	C3B-CAB	-2.09	1.43	1.47
36	P	310	CLA	CMD-C2D	-2.09	1.46	1.50
36	f	803	CLA	C1C-C2C	2.09	1.48	1.44
36	L	311	CLA	MG-ND	-2.09	2.01	2.05
36	D	307	CLA	C3B-C2B	-2.09	1.37	1.40
36	Q	307	CLA	CMD-C2D	-2.09	1.46	1.50
36	O	311	CLA	CMC-C2C	-2.09	1.46	1.50
36	D	315	CLA	CMC-C2C	-2.09	1.46	1.50
36	U	307	CLA	C3B-C2B	-2.09	1.37	1.40
36	T	313	CLA	CMD-C2D	-2.09	1.46	1.50
36	T	314	CLA	CMD-C2D	-2.09	1.46	1.50
37	H	313	KC1	C3B-C4B	2.09	1.49	1.46
35	A	316	A86	C32-C31	-2.09	1.51	1.54
36	M	307	CLA	C3B-C2B	-2.09	1.37	1.40
36	S	321	CLA	C3B-C2B	-2.09	1.37	1.40
36	b	821	CLA	C3B-CAB	-2.09	1.43	1.47
35	K	302	A86	C33-C34	2.09	1.55	1.51
36	B	307	CLA	C3B-CAB	-2.09	1.43	1.47
37	G	308	KC1	O2A-CGA	-2.09	1.24	1.30
35	R	305	A86	O1-C20	-2.09	1.43	1.46
36	G	312	CLA	MG-ND	-2.09	2.01	2.05
36	M	308	CLA	C3B-CAB	-2.09	1.43	1.47
36	N	316	CLA	CMD-C2D	-2.09	1.46	1.50
36	b	809	CLA	CMC-C2C	-2.09	1.46	1.50
36	j	106	CLA	CMC-C2C	-2.09	1.46	1.50
36	N	311	CLA	C3B-CAB	-2.09	1.43	1.47
36	P	313	CLA	CMC-C2C	-2.09	1.46	1.50
36	T	316	CLA	CMC-C2C	-2.09	1.46	1.50
35	A	302	A86	C26-C27	-2.09	1.33	1.35
36	F	312	CLA	CMD-C2D	-2.09	1.46	1.50
36	J	317	CLA	CMC-C2C	-2.09	1.46	1.50
36	M	314	CLA	CMC-C2C	-2.09	1.46	1.50
36	j	101	CLA	CMC-C2C	-2.09	1.46	1.50
36	K	310	CLA	MG-ND	-2.09	2.01	2.05
36	M	314	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	830	CLA	C4B-CHC	-2.09	1.35	1.41
36	B	305	CLA	CMD-C2D	-2.09	1.46	1.50
35	X	305	A86	C13-C11	-2.09	1.45	1.49
36	L	312	CLA	CMD-C2D	-2.09	1.46	1.50
36	H	318	CLA	CMC-C2C	-2.08	1.46	1.50
36	B	306	CLA	C3B-C2B	-2.08	1.37	1.40
36	J	315	CLA	CMD-C2D	-2.08	1.46	1.50
35	J	302	A86	O1-C20	-2.08	1.43	1.46
34	J	304	DD6	O1-C20	-2.08	1.43	1.46
36	b	815	CLA	MG-ND	-2.08	2.01	2.05
36	S	310	CLA	CMD-C2D	-2.08	1.46	1.50
36	W	208	CLA	CMD-C2D	-2.08	1.46	1.50
36	W	216	CLA	CMD-C2D	-2.08	1.46	1.50
36	E	308	CLA	MG-ND	-2.08	2.01	2.05
36	H	308	CLA	MG-ND	-2.08	2.01	2.05
36	H	312	CLA	C4B-CHC	-2.08	1.35	1.41
36	E	313	CLA	MG-ND	-2.08	2.01	2.05
36	D	315	CLA	CMD-C2D	-2.08	1.46	1.50
37	D	314	KC1	C1A-CHA	2.08	1.46	1.40
36	J	311	CLA	C3B-C2B	-2.08	1.37	1.40
36	b	830	CLA	C3B-C2B	-2.08	1.37	1.40
36	L	312	CLA	CMC-C2C	-2.08	1.46	1.50
36	L	309	CLA	CMD-C2D	-2.08	1.46	1.50
36	K	309	CLA	C3B-CAB	-2.08	1.43	1.47
36	C	214	CLA	CMC-C2C	-2.08	1.46	1.50
36	f	805	CLA	CMC-C2C	-2.08	1.46	1.50
37	K	314	KC1	C1D-CHD	2.08	1.46	1.41
36	N	310	CLA	C3C-C2C	2.08	1.41	1.36
36	J	311	CLA	MG-ND	-2.08	2.01	2.05
37	F	315	KC1	O2A-CGA	-2.08	1.24	1.30
36	a	818	CLA	C4B-CHC	-2.08	1.35	1.41
36	a	805	CLA	C3B-C2B	-2.08	1.37	1.40
36	X	313	CLA	CMD-C2D	-2.08	1.46	1.50
37	P	317	KC1	C1D-CHD	2.08	1.46	1.41
36	S	314	CLA	CMD-C2D	-2.07	1.46	1.50
35	V	304	A86	C17-C16	-2.07	1.51	1.54
36	P	308	CLA	CMC-C2C	-2.07	1.46	1.50
36	G	309	CLA	O2A-CGA	2.07	1.39	1.33
36	R	314	CLA	C3B-C2B	-2.07	1.37	1.40
36	j	101	CLA	C3B-C2B	-2.07	1.37	1.40
36	G	314	CLA	C3B-CAB	-2.07	1.43	1.47
37	R	317	KC1	C4C-C3C	2.07	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	831	CLA	CMC-C2C	-2.07	1.46	1.50
36	P	309	CLA	MG-ND	-2.07	2.01	2.05
36	b	838	CLA	CMC-C2C	-2.07	1.46	1.50
37	P	315	KC1	C4C-C3C	2.07	1.48	1.45
34	E	303	DD6	O1-C20	-2.07	1.43	1.46
34	W	205	DD6	O1-C20	-2.07	1.43	1.46
36	J	317	CLA	C3B-CAB	-2.07	1.43	1.47
36	H	317	CLA	CMC-C2C	-2.07	1.46	1.50
36	f	802	CLA	CMC-C2C	-2.07	1.46	1.50
36	W	215	CLA	C3B-CAB	-2.07	1.43	1.47
36	P	312	CLA	CMC-C2C	-2.07	1.46	1.50
35	R	304	A86	C30-C29	-2.07	1.28	1.32
36	C	212	CLA	MG-ND	-2.07	2.01	2.05
44	b	843	BCR	C33-C5	-2.07	1.47	1.50
36	L	309	CLA	C3B-CAB	-2.07	1.43	1.47
37	N	314	KC1	C1C-C2C	2.07	1.48	1.44
36	A	308	CLA	CMD-C2D	-2.07	1.46	1.50
36	W	216	CLA	CMC-C2C	-2.07	1.46	1.50
36	b	824	CLA	C4C-C3C	2.07	1.48	1.45
36	H	308	CLA	CMC-C2C	-2.07	1.46	1.50
36	b	805	CLA	C3B-CAB	-2.07	1.43	1.47
36	W	201	CLA	C3B-C2B	-2.07	1.37	1.40
36	l	202	CLA	CMC-C2C	-2.07	1.46	1.50
36	b	840	CLA	MG-ND	-2.07	2.01	2.05
36	H	309	CLA	C3B-CAB	-2.07	1.43	1.47
36	b	831	CLA	C3B-CAB	-2.07	1.43	1.47
36	J	316	CLA	C4B-CHC	-2.07	1.35	1.41
36	H	306	CLA	C3B-C2B	-2.07	1.37	1.40
36	L	313	CLA	CMC-C2C	-2.07	1.46	1.50
36	b	805	CLA	C3B-C2B	-2.06	1.37	1.40
36	H	306	CLA	CMD-C2D	-2.06	1.46	1.50
36	L	320	CLA	CMC-C2C	-2.06	1.46	1.50
36	M	306	CLA	CMC-C2C	-2.06	1.46	1.50
36	W	209	CLA	CMD-C2D	-2.06	1.46	1.50
35	h	204	A86	C32-C31	-2.06	1.51	1.54
44	m	101	BCR	C38-C26	-2.06	1.47	1.50
44	h	201	BCR	C38-C26	-2.06	1.47	1.50
35	C	204	A86	O1-C20	-2.06	1.43	1.46
36	O	314	CLA	CMD-C2D	-2.06	1.46	1.50
36	b	826	CLA	C3B-C2B	-2.06	1.37	1.40
36	R	319	CLA	C3B-C2B	-2.06	1.37	1.40
36	l	206	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	O	313	KC1	C4C-C3C	2.06	1.48	1.45
36	U	313	CLA	C3B-CAB	-2.06	1.43	1.47
36	f	804	CLA	C4C-C3C	2.06	1.48	1.45
36	O	310	CLA	C3B-C2B	-2.06	1.37	1.40
36	H	314	CLA	MG-ND	-2.06	2.01	2.05
36	h	203	CLA	CMC-C2C	-2.06	1.46	1.50
35	R	305	A86	C32-C31	-2.06	1.51	1.54
36	P	308	CLA	C3B-CAB	-2.06	1.43	1.47
36	a	813	CLA	C3B-CAB	-2.06	1.43	1.47
35	O	319	A86	C13-C11	-2.06	1.45	1.49
36	S	314	CLA	O1D-CGD	2.06	1.26	1.21
36	Q	305	CLA	C3B-CAB	-2.06	1.43	1.47
40	b	849	DGD	O2D-C2D	-2.06	1.38	1.43
36	f	803	CLA	C4B-CHC	2.05	1.46	1.41
36	S	313	CLA	CMD-C2D	-2.05	1.46	1.50
36	S	309	CLA	MG-ND	-2.05	2.01	2.05
36	D	316	CLA	C4B-CHC	-2.05	1.35	1.41
36	S	319	CLA	CMC-C2C	-2.05	1.46	1.50
36	S	321	CLA	CMC-C2C	-2.05	1.46	1.50
36	W	215	CLA	MG-ND	-2.05	2.01	2.05
36	G	314	CLA	CMC-C2C	-2.05	1.46	1.50
36	F	316	CLA	C3B-C2B	-2.05	1.37	1.40
36	S	309	CLA	CMC-C2C	-2.05	1.46	1.50
37	H	313	KC1	O2A-CGA	-2.05	1.25	1.30
36	P	319	CLA	C4D-ND	2.05	1.40	1.37
36	H	317	CLA	C3B-C2B	-2.05	1.37	1.40
36	h	203	CLA	C3B-C2B	-2.05	1.37	1.40
36	b	821	CLA	MG-ND	-2.05	2.01	2.05
36	A	313	CLA	C3B-CAB	-2.05	1.43	1.47
44	m	101	BCR	C33-C5	-2.05	1.47	1.50
36	D	311	CLA	C3B-CAB	-2.05	1.43	1.47
37	V	312	KC1	C4A-C3A	2.05	1.48	1.44
36	l	202	CLA	C3B-CAB	-2.05	1.43	1.47
36	K	311	CLA	CMC-C2C	-2.05	1.46	1.50
36	N	310	CLA	C1B-CHB	-2.05	1.35	1.41
36	R	319	CLA	C3C-C2C	2.05	1.41	1.36
36	R	315	CLA	C3B-C2B	-2.05	1.37	1.40
36	V	314	CLA	C4D-CHA	2.05	1.45	1.38
36	O	307	CLA	MG-ND	-2.05	2.01	2.05
36	P	318	CLA	CMC-C2C	-2.05	1.46	1.50
36	a	838	CLA	CMC-C2C	-2.05	1.46	1.50
36	N	309	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	835	CLA	CMC-C2C	-2.05	1.46	1.50
44	l	203	BCR	C38-C26	-2.05	1.47	1.50
35	T	304	A86	C13-C11	-2.04	1.45	1.49
35	C	204	A86	C9-C10	2.04	1.49	1.43
36	Q	312	CLA	CMC-C2C	-2.04	1.46	1.50
36	A	313	CLA	C3B-C2B	-2.04	1.37	1.40
36	G	319	CLA	C1A-CHA	2.04	1.51	1.43
35	O	302	A86	C13-C11	-2.04	1.45	1.49
36	G	312	CLA	C3B-CAB	-2.04	1.43	1.47
36	O	306	CLA	C3B-CAB	-2.04	1.43	1.47
35	B	301	A86	C32-C31	-2.04	1.51	1.54
36	M	308	CLA	CMC-C2C	-2.04	1.46	1.50
35	K	306	A86	C13-C11	-2.04	1.45	1.49
37	J	314	KC1	O2A-CGA	-2.04	1.25	1.30
36	a	801	CLA	C4B-CHC	-2.04	1.35	1.41
36	J	311	CLA	CMC-C2C	-2.04	1.46	1.50
36	a	833	CLA	C4B-CHC	-2.04	1.35	1.41
36	a	828	CLA	CMC-C2C	-2.04	1.46	1.50
36	b	821	CLA	CMC-C2C	-2.04	1.46	1.50
36	b	840	CLA	CMC-C2C	-2.04	1.46	1.50
44	i	101	BCR	C30-C25	-2.04	1.51	1.53
36	a	820	CLA	MG-ND	-2.04	2.01	2.05
36	T	311	CLA	CMD-C2D	-2.04	1.46	1.50
36	b	825	CLA	C4B-CHC	-2.04	1.35	1.41
40	b	849	DGD	C2A-C1A	-2.04	1.44	1.50
35	M	304	A86	O1-C20	-2.03	1.43	1.46
36	I	308	CLA	MG-ND	-2.03	2.01	2.05
36	X	308	CLA	CMC-C2C	-2.03	1.46	1.50
44	b	846	BCR	C38-C26	-2.03	1.47	1.50
36	P	310	CLA	CMC-C2C	-2.03	1.46	1.50
36	S	310	CLA	CMC-C2C	-2.03	1.46	1.50
44	b	844	BCR	C38-C26	-2.03	1.47	1.50
36	V	310	CLA	CMC-C2C	-2.03	1.46	1.50
36	I	310	CLA	MG-ND	-2.03	2.01	2.05
36	a	805	CLA	MG-ND	-2.03	2.01	2.05
36	H	305	CLA	C3B-C2B	-2.03	1.37	1.40
36	a	829	CLA	C4B-CHC	-2.03	1.35	1.41
36	N	313	CLA	CMD-C2D	-2.03	1.46	1.50
36	Q	307	CLA	CMC-C2C	-2.03	1.46	1.50
37	N	314	KC1	C3B-C4B	2.03	1.49	1.46
44	a	847	BCR	C38-C26	-2.03	1.47	1.50
36	F	313	CLA	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	O	308	CLA	CMC-C2C	-2.03	1.46	1.50
37	M	317	KC1	C4C-C3C	2.03	1.48	1.45
44	l	203	BCR	C33-C5	-2.03	1.47	1.50
36	W	208	CLA	O2A-CGA	2.03	1.37	1.30
36	R	321	CLA	MG-ND	-2.03	2.01	2.05
36	D	307	CLA	C3B-CAB	-2.03	1.43	1.47
36	H	316	CLA	C3B-CAB	-2.03	1.43	1.47
36	X	307	CLA	CMD-C2D	-2.03	1.46	1.50
36	O	312	CLA	C3A-C4A	2.03	1.54	1.51
35	O	305	A86	O1-C20	-2.03	1.43	1.46
35	E	302	A86	C32-C31	-2.03	1.51	1.54
36	M	308	CLA	MG-ND	-2.03	2.01	2.05
36	M	309	CLA	CMD-C2D	-2.03	1.46	1.50
36	N	316	CLA	CMC-C2C	-2.03	1.46	1.50
36	O	314	CLA	CMC-C2C	-2.03	1.46	1.50
36	V	313	CLA	CMD-C2D	-2.03	1.46	1.50
36	C	210	CLA	CMD-C2D	-2.03	1.46	1.50
36	W	214	CLA	CMD-C2D	-2.03	1.46	1.50
36	a	837	CLA	CMC-C2C	-2.02	1.46	1.50
36	M	310	CLA	C4B-CHC	-2.02	1.35	1.41
36	F	316	CLA	CMC-C2C	-2.02	1.46	1.50
36	S	320	CLA	CMC-C2C	-2.02	1.46	1.50
36	W	209	CLA	CMC-C2C	-2.02	1.46	1.50
36	G	311	CLA	C3B-CAB	-2.02	1.43	1.47
44	i	103	BCR	C30-C25	-2.02	1.51	1.53
36	R	310	CLA	C3B-C2B	-2.02	1.37	1.40
36	F	314	CLA	MG-ND	-2.02	2.01	2.05
37	B	310	KC1	C4A-C3A	2.02	1.48	1.44
35	R	309	A86	C13-C11	-2.02	1.45	1.49
36	a	838	CLA	C3B-CAB	-2.02	1.43	1.47
36	G	315	CLA	MG-ND	-2.02	2.01	2.05
36	S	319	CLA	MG-ND	-2.02	2.01	2.05
36	b	832	CLA	MG-ND	-2.02	2.01	2.05
36	Q	310	CLA	MG-NA	2.02	2.11	2.06
36	V	308	CLA	CMC-C2C	-2.02	1.46	1.50
36	K	310	CLA	C4C-C3C	2.02	1.48	1.45
36	W	218	CLA	MG-ND	-2.02	2.01	2.05
36	a	820	CLA	CMC-C2C	-2.02	1.46	1.50
34	S	306	DD6	O1-C20	-2.02	1.43	1.46
36	G	319	CLA	C1C-C2C	2.02	1.48	1.44
36	B	306	CLA	C3B-CAB	-2.02	1.43	1.47
37	M	313	KC1	O2A-CGA	-2.02	1.25	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	308	CLA	CMC-C2C	-2.02	1.46	1.50
36	j	102	CLA	MG-ND	-2.02	2.01	2.05
36	S	318	CLA	CMD-C2D	-2.02	1.46	1.50
36	C	214	CLA	C3B-CAB	-2.02	1.43	1.47
36	a	836	CLA	O2D-CED	-2.02	1.40	1.45
37	F	315	KC1	C1D-CHD	2.02	1.46	1.41
35	L	319	A86	C13-C11	-2.02	1.45	1.49
36	C	211	CLA	C3B-CAB	-2.02	1.43	1.47
36	H	318	CLA	CAA-C2A	-2.02	1.50	1.54
36	b	837	CLA	C3B-C2B	-2.02	1.37	1.40
35	S	303	A86	C5-C6	-2.02	1.33	1.35
36	T	311	CLA	C4C-C3C	-2.02	1.41	1.45
36	S	317	CLA	CMD-C2D	-2.02	1.46	1.50
36	V	309	CLA	C3B-CAB	-2.02	1.43	1.47
36	H	315	CLA	CMC-C2C	-2.02	1.46	1.50
36	L	316	CLA	CMD-C2D	-2.01	1.46	1.50
35	P	303	A86	C13-C11	-2.01	1.45	1.49
36	U	308	CLA	C3B-C2B	-2.01	1.37	1.40
37	H	313	KC1	C1A-CHA	2.01	1.45	1.40
36	l	201	CLA	CMC-C2C	-2.01	1.46	1.50
36	N	310	CLA	MG-ND	-2.01	2.01	2.05
36	Q	307	CLA	MG-ND	-2.01	2.01	2.05
36	a	813	CLA	C1D-ND	2.01	1.40	1.37
37	H	313	KC1	C4B-NB	-2.01	1.35	1.37
36	O	309	CLA	CMC-C2C	-2.01	1.46	1.50
36	P	316	CLA	CMC-C2C	-2.01	1.46	1.50
36	U	313	CLA	CMC-C2C	-2.01	1.46	1.50
36	b	841	CLA	MG-ND	-2.01	2.01	2.05
35	S	304	A86	O1-C20	-2.01	1.43	1.46
36	M	316	CLA	CMC-C2C	-2.01	1.46	1.50
36	C	205	CLA	MG-ND	-2.01	2.01	2.05
36	b	814	CLA	C3B-CAB	-2.01	1.43	1.47
36	K	309	CLA	CMC-C2C	-2.01	1.46	1.50
36	N	315	CLA	CMD-C2D	-2.01	1.46	1.50
36	j	106	CLA	C3B-CAB	-2.01	1.43	1.47
36	a	833	CLA	MG-ND	-2.01	2.01	2.05
44	a	846	BCR	C38-C26	-2.01	1.47	1.50
35	M	305	A86	C13-C11	-2.01	1.45	1.49
36	a	830	CLA	C4D-CHA	2.01	1.45	1.38
35	A	302	A86	C2-C1	-2.01	1.33	1.35
36	Q	314	CLA	CMD-C2D	-2.01	1.46	1.50
36	P	314	CLA	MG-NA	2.01	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	819	CLA	CAC-C3C	-2.01	1.46	1.51
36	U	307	CLA	CMC-C2C	-2.01	1.46	1.50
35	N	303	A86	C5-C6	-2.01	1.33	1.35
40	b	849	DGD	O4E-C4E	-2.01	1.38	1.43
36	L	310	CLA	C3B-C2B	-2.01	1.37	1.40
36	I	307	CLA	MG-ND	-2.01	2.01	2.05
36	O	306	CLA	C3B-C2B	-2.01	1.37	1.40
36	O	308	CLA	C3B-C2B	-2.01	1.37	1.40
36	R	318	CLA	CMD-C2D	-2.01	1.46	1.50
36	D	309	CLA	C4C-C3C	2.01	1.48	1.45
36	R	320	CLA	CMC-C2C	-2.00	1.46	1.50
36	X	310	CLA	C3B-C2B	-2.00	1.37	1.40
36	C	211	CLA	MG-ND	-2.00	2.01	2.05
36	R	312	CLA	CMC-C2C	-2.00	1.46	1.50
35	E	305	A86	C32-C31	-2.00	1.51	1.54
36	E	308	CLA	C3B-CAB	-2.00	1.43	1.47
36	H	306	CLA	CMC-C2C	-2.00	1.46	1.50
36	R	313	CLA	CMC-C2C	-2.00	1.46	1.50
36	M	307	CLA	MG-ND	-2.00	2.01	2.05
36	G	315	CLA	C4B-NB	-2.00	1.33	1.35
36	P	308	CLA	C3B-C2B	-2.00	1.37	1.40
36	T	312	CLA	CMD-C2D	-2.00	1.46	1.50

All (7259) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	N	304	A86	O1-C20-C21	-47.08	58.64	115.06
36	Q	314	CLA	C4-C3-C5	-24.40	74.22	115.27
42	V	315	LMG	O7-C10-C11	22.29	159.53	111.50
35	A	302	A86	C33-C32-C31	-21.39	88.43	109.21
36	N	319	CLA	CHD-C1D-ND	-21.33	104.86	124.45
37	T	310	KC1	CHD-C4C-NC	20.41	155.17	124.20
37	A	312	KC1	CMD-C2D-C1D	-20.11	97.55	128.46
35	H	301	A86	O4-C38-O5	19.83	162.35	122.96
37	P	315	KC1	C1A-NA-C4A	-19.18	98.08	106.71
37	O	315	KC1	C1A-NA-C4A	-19.17	98.09	106.71
37	Q	313	KC1	C1A-NA-C4A	-19.15	98.10	106.71
37	Q	311	KC1	C1A-NA-C4A	-19.15	98.10	106.71
37	O	313	KC1	C1A-NA-C4A	-19.13	98.11	106.71
37	W	213	KC1	CMD-C2D-C1D	-18.94	99.35	128.46
37	M	318	KC1	C3C-C4C-NC	-18.74	92.23	109.88
37	A	312	KC1	C1A-NA-C4A	-18.73	98.29	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	V	315	LMG	O7-C10-O9	-18.46	79.09	123.70
37	F	315	KC1	CMD-C2D-C1D	-18.29	100.35	128.46
36	N	319	CLA	CMD-C2D-C1D	18.11	156.62	124.71
36	X	313	CLA	C4A-NA-C1A	18.00	114.80	106.71
37	P	317	KC1	CMD-C2D-C1D	-17.76	101.17	128.46
37	O	313	KC1	C1A-C2A-C3A	-17.55	93.18	107.11
37	O	315	KC1	C1A-C2A-C3A	-17.53	93.20	107.11
37	Q	311	KC1	C1A-C2A-C3A	-17.51	93.21	107.11
37	P	315	KC1	C1A-C2A-C3A	-17.49	93.23	107.11
37	Q	313	KC1	C1A-C2A-C3A	-17.48	93.23	107.11
37	L	315	KC1	CMD-C2D-C1D	-17.45	101.64	128.46
36	N	319	CLA	C1D-ND-C4D	-17.43	93.96	106.33
37	M	313	KC1	CMD-C2D-C1D	-17.40	101.72	128.46
37	M	318	KC1	C1A-C2A-C3A	17.37	120.91	107.11
37	S	316	KC1	CMD-C2D-C1D	-17.37	101.76	128.46
37	J	314	KC1	CMD-C2D-C1D	-17.32	101.85	128.46
37	A	312	KC1	CMD-C2D-C3D	17.32	157.08	124.68
37	O	313	KC1	CMD-C2D-C1D	-17.31	101.85	128.46
37	P	315	KC1	CMD-C2D-C1D	-17.31	101.86	128.46
37	O	315	KC1	CMD-C2D-C1D	-17.29	101.88	128.46
37	Q	311	KC1	CMD-C2D-C1D	-17.29	101.89	128.46
37	Q	313	KC1	CMD-C2D-C1D	-17.26	101.94	128.46
37	W	213	KC1	CMD-C2D-C3D	17.06	156.59	124.68
36	Q	314	CLA	C4-C3-C2	-16.76	80.68	123.68
36	Q	314	CLA	C5-C3-C2	16.68	154.87	121.12
35	H	301	A86	O4-C38-C39	-16.60	80.54	111.09
37	L	315	KC1	CMD-C2D-C3D	16.60	155.73	124.68
37	T	310	KC1	C3C-C4C-NC	-16.50	94.34	109.88
37	P	317	KC1	CMD-C2D-C3D	16.50	155.54	124.68
37	F	315	KC1	CMD-C2D-C3D	16.46	155.47	124.68
37	Q	311	KC1	CMD-C2D-C3D	16.26	155.11	124.68
37	O	315	KC1	CMD-C2D-C3D	16.26	155.10	124.68
37	O	313	KC1	CMD-C2D-C3D	16.26	155.10	124.68
37	Q	313	KC1	CMD-C2D-C3D	16.25	155.08	124.68
37	P	315	KC1	CMD-C2D-C3D	16.25	155.08	124.68
37	T	310	KC1	C1A-C2A-C3A	16.19	119.97	107.11
37	F	308	KC1	CMD-C2D-C1D	-16.17	103.61	128.46
37	M	313	KC1	CMD-C2D-C3D	16.08	154.77	124.68
37	K	314	KC1	CMD-C2D-C1D	-16.06	103.78	128.46
37	J	314	KC1	CMD-C2D-C3D	15.98	154.57	124.68
37	M	317	KC1	OBD-CAD-CBD	15.92	148.63	125.89
37	A	312	KC1	C1A-C2A-C3A	-15.75	94.61	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	319	CLA	C4A-NA-C1A	15.74	113.78	106.71
36	a	830	CLA	C4A-NA-C1A	15.73	113.78	106.71
37	T	315	KC1	OBD-CAD-CBD	15.67	148.28	125.89
37	S	316	KC1	CMD-C2D-C3D	15.64	153.93	124.68
37	L	315	KC1	OBD-CAD-CBD	15.61	148.20	125.89
37	K	314	KC1	CMD-C2D-C3D	15.32	153.34	124.68
37	G	308	KC1	OBD-CAD-CBD	15.30	147.75	125.89
37	F	315	KC1	C1A-NA-C4A	-15.18	99.88	106.71
36	W	216	CLA	C4A-NA-C1A	15.02	113.46	106.71
37	R	317	KC1	OBD-CAD-CBD	14.99	147.32	125.89
37	E	309	KC1	OBD-CAD-CBD	14.99	147.32	125.89
37	M	318	KC1	OBD-CAD-C3D	-14.92	103.21	127.98
37	L	317	KC1	OBD-CAD-CBD	14.92	147.21	125.89
37	K	314	KC1	OBD-CAD-CBD	14.90	147.19	125.89
37	F	315	KC1	C1A-C2A-C3A	-14.86	95.32	107.11
37	F	308	KC1	OBD-CAD-CBD	14.74	146.95	125.89
37	R	317	KC1	CMD-C2D-C1D	-14.71	105.85	128.46
37	T	310	KC1	OBD-CAD-C3D	-14.71	103.56	127.98
37	P	315	KC1	OBD-CAD-CBD	14.67	146.85	125.89
37	Q	311	KC1	OBD-CAD-CBD	14.66	146.84	125.89
37	Q	313	KC1	OBD-CAD-CBD	14.63	146.80	125.89
37	O	313	KC1	OBD-CAD-CBD	14.63	146.80	125.89
37	O	315	KC1	OBD-CAD-CBD	14.63	146.80	125.89
37	T	315	KC1	CMD-C2D-C1D	-14.63	105.98	128.46
37	F	308	KC1	CMD-C2D-C3D	14.60	151.99	124.68
37	V	312	KC1	OBD-CAD-CBD	14.50	146.62	125.89
37	D	314	KC1	OBD-CAD-CBD	14.46	146.55	125.89
37	T	310	KC1	CHC-C4B-NB	14.12	137.43	124.45
37	D	314	KC1	CMD-C2D-C1D	-14.11	106.77	128.46
37	C	213	KC1	OBD-CAD-CBD	14.09	146.02	125.89
37	M	313	KC1	OBD-CAD-CBD	14.09	146.02	125.89
37	T	315	KC1	CMD-C2D-C3D	14.06	150.99	124.68
37	F	315	KC1	OBD-CAD-CBD	14.05	145.97	125.89
35	F	307	A86	C41-C32-C31	14.01	123.01	110.47
37	S	316	KC1	OBD-CAD-CBD	13.98	145.87	125.89
35	A	302	A86	C40-C32-C31	13.98	122.98	110.47
36	X	313	CLA	CMB-C2B-C1B	-13.96	107.01	128.46
35	T	305	A86	O1-C15-C14	-13.96	85.20	113.21
37	W	213	KC1	OBD-CAD-CBD	13.94	145.81	125.89
35	L	304	A86	O1-C15-C14	-13.90	85.31	113.21
35	X	303	A86	O1-C15-C14	-13.86	85.39	113.21
35	J	303	A86	O1-C15-C14	-13.76	85.60	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	314	KC1	OBD-CAD-CBD	13.76	145.55	125.89
35	I	304	A86	O1-C15-C14	-13.74	85.64	113.21
37	R	317	KC1	CMD-C2D-C3D	13.73	150.37	124.68
37	B	310	KC1	OBD-CAD-CBD	13.71	145.49	125.89
35	U	302	A86	O1-C15-C14	-13.71	85.70	113.21
37	G	317	KC1	OBD-CAD-CBD	13.69	145.45	125.89
35	V	304	A86	O1-C20-C19	13.60	123.59	113.38
35	T	307	A86	O1-C15-C14	-13.56	86.00	113.21
35	F	307	A86	C33-C32-C31	-13.37	96.21	109.21
35	R	304	A86	O1-C15-C14	-13.30	86.52	113.21
35	A	302	A86	O1-C15-C14	-13.24	86.63	113.21
37	U	312	KC1	OBD-CAD-CBD	13.21	144.77	125.89
37	D	314	KC1	CMD-C2D-C3D	13.20	149.38	124.68
35	R	301	A86	O1-C15-C14	-13.19	86.75	113.21
36	f	804	CLA	C4A-NA-C1A	13.18	112.63	106.71
37	T	310	KC1	CHB-C4A-C3A	-13.15	104.43	124.98
35	X	305	A86	O1-C15-C14	-13.13	86.87	113.21
35	L	306	A86	O1-C15-C14	-13.11	86.89	113.21
37	T	310	KC1	CHD-C4C-C3C	-13.11	100.73	125.33
37	X	311	KC1	OBD-CAD-CBD	13.09	144.60	125.89
37	W	217	KC1	OBD-CAD-CBD	13.08	144.58	125.89
35	R	309	A86	O1-C15-C14	-13.04	87.04	113.21
35	C	202	A86	O1-C15-C14	-13.02	87.08	113.21
35	B	303	A86	O1-C15-C14	-12.99	87.15	113.21
35	R	306	A86	O1-C15-C14	-12.96	87.21	113.21
35	O	302	A86	O1-C15-C14	-12.91	87.31	113.21
35	L	319	A86	O1-C15-C14	-12.90	87.32	113.21
35	P	303	A86	O1-C15-C14	-12.88	87.36	113.21
37	P	317	KC1	OBD-CAD-CBD	12.83	144.23	125.89
35	N	304	A86	O1-C20-C19	-12.83	103.74	113.38
37	V	312	KC1	CMD-C2D-C1D	-12.82	108.76	128.46
35	M	305	A86	O1-C15-C14	-12.80	87.52	113.21
35	N	306	A86	O1-C15-C14	-12.72	87.69	113.21
37	J	314	KC1	OBD-CAD-CBD	12.71	144.05	125.89
35	Q	304	A86	O1-C15-C14	-12.65	87.81	113.21
35	N	320	A86	O1-C15-C14	-12.65	87.82	113.21
35	K	306	A86	O1-C15-C14	-12.63	87.87	113.21
35	X	304	A86	O1-C15-C14	-12.62	87.87	113.21
37	H	313	KC1	OBD-CAD-CBD	12.54	143.81	125.89
35	M	301	A86	O1-C15-C14	-12.54	88.04	113.21
37	P	317	KC1	CHC-C4B-NB	12.52	135.96	124.45
37	L	315	KC1	OBD-CAD-C3D	-12.50	107.23	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	O	319	A86	O1-C15-C14	-12.49	88.15	113.21
37	D	314	KC1	OBD-CAD-C3D	-12.48	107.25	127.98
37	G	308	KC1	OBD-CAD-C3D	-12.48	107.25	127.98
35	K	302	A86	O1-C15-C14	-12.48	88.17	113.21
35	B	303	A86	C40-C32-C31	-12.44	99.34	110.47
35	X	301	A86	O1-C15-C14	-12.40	88.33	113.21
37	V	312	KC1	CMD-C2D-C3D	12.38	147.84	124.68
37	K	314	KC1	OBD-CAD-C3D	-12.35	107.47	127.98
37	F	308	KC1	OBD-CAD-C3D	-12.33	107.50	127.98
37	M	317	KC1	OBD-CAD-C3D	-12.31	107.54	127.98
37	E	309	KC1	OBD-CAD-C3D	-12.29	107.57	127.98
35	P	304	A86	O1-C15-C14	-12.21	88.71	113.21
35	Q	301	A86	O1-C15-C14	-12.20	88.72	113.21
35	O	303	A86	O1-C15-C14	-12.19	88.75	113.21
37	M	318	KC1	C1A-NA-C4A	12.18	112.18	106.71
37	S	316	KC1	CAB-C3B-C4B	12.16	154.28	124.90
37	U	312	KC1	C1A-C2A-C3A	-12.16	97.46	107.11
35	I	302	A86	O1-C15-C14	-12.15	88.82	113.21
37	T	315	KC1	OBD-CAD-C3D	-12.11	107.88	127.98
37	R	317	KC1	OBD-CAD-C3D	-12.10	107.89	127.98
37	F	308	KC1	C1A-NA-C4A	-12.09	101.27	106.71
35	F	305	A86	O1-C15-C14	-12.06	89.01	113.21
35	T	306	A86	O1-C15-C14	-12.04	89.04	113.21
35	K	303	A86	O1-C15-C14	-12.02	89.09	113.21
35	N	303	A86	O1-C15-C14	-11.98	89.17	113.21
35	S	303	A86	O1-C15-C14	-11.97	89.18	113.21
37	E	309	KC1	CMD-C2D-C1D	-11.96	110.08	128.46
37	M	313	KC1	OBD-CAD-C3D	-11.96	108.13	127.98
35	V	302	A86	O1-C15-C14	-11.94	89.25	113.21
35	S	302	A86	O1-C15-C14	-11.93	89.26	113.21
35	N	302	A86	O1-C15-C14	-11.93	89.27	113.21
37	H	313	KC1	C1A-NA-C4A	-11.88	101.37	106.71
37	F	315	KC1	OBD-CAD-C3D	-11.87	108.28	127.98
37	P	315	KC1	OBD-CAD-C3D	-11.84	108.32	127.98
37	G	308	KC1	CMD-C2D-C1D	-11.84	110.26	128.46
37	L	317	KC1	OBD-CAD-C3D	-11.84	108.33	127.98
35	T	303	A86	O1-C15-C14	-11.84	89.46	113.21
37	Q	311	KC1	OBD-CAD-C3D	-11.82	108.35	127.98
37	Q	313	KC1	OBD-CAD-C3D	-11.82	108.35	127.98
37	O	315	KC1	OBD-CAD-C3D	-11.81	108.36	127.98
37	O	313	KC1	OBD-CAD-C3D	-11.81	108.37	127.98
37	T	310	KC1	OBD-CAD-CBD	11.81	142.77	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	L	315	KC1	C1A-C2A-C3A	-11.78	97.76	107.11
35	X	303	A86	O1-C20-C21	-11.74	100.98	115.06
35	T	302	A86	O1-C15-C14	-11.73	89.68	113.21
35	T	305	A86	O1-C20-C19	11.72	122.18	113.38
37	G	317	KC1	OBD-CAD-C3D	-11.72	108.53	127.98
35	N	304	A86	C21-C20-C19	11.71	127.45	114.28
37	S	316	KC1	OBD-CAD-C3D	-11.68	108.58	127.98
37	C	213	KC1	OBD-CAD-C3D	-11.68	108.60	127.98
37	M	313	KC1	CAB-C3B-C4B	11.66	153.06	124.90
37	M	318	KC1	OBD-CAD-CBD	11.60	142.47	125.89
35	H	301	A86	O1-C15-C14	-11.60	89.93	113.21
37	V	312	KC1	OBD-CAD-C3D	-11.58	108.75	127.98
35	R	302	A86	O1-C15-C14	-11.58	89.97	113.21
37	B	310	KC1	OBD-CAD-C3D	-11.58	108.76	127.98
37	U	312	KC1	OBD-CAD-C3D	-11.57	108.78	127.98
36	Q	310	CLA	CAA-CBA-CGA	11.56	147.04	113.25
37	F	308	KC1	C1A-C2A-C3A	-11.56	97.94	107.11
37	D	314	KC1	CHC-C4B-NB	11.55	135.06	124.45
35	M	302	A86	O1-C15-C14	-11.54	90.05	113.21
37	T	310	KC1	C2A-C3A-C4A	-11.47	97.98	106.49
35	W	202	A86	O1-C15-C14	-11.45	90.24	113.21
35	R	303	A86	O1-C15-C14	-11.43	90.27	113.21
37	N	314	KC1	OBD-CAD-C3D	-11.39	109.07	127.98
37	R	317	KC1	CAB-C3B-C4B	11.38	152.38	124.90
37	E	309	KC1	CMD-C2D-C3D	11.37	145.95	124.68
35	H	301	A86	O5-C38-C39	-11.34	83.52	124.81
37	J	314	KC1	C1A-C2A-C3A	-11.33	98.12	107.11
37	G	308	KC1	CMD-C2D-C3D	11.32	145.86	124.68
37	H	313	KC1	OBD-CAD-C3D	-11.30	109.22	127.98
37	W	213	KC1	OBD-CAD-C3D	-11.30	109.23	127.98
37	J	314	KC1	OBD-CAD-C3D	-11.26	109.29	127.98
35	X	302	A86	O1-C15-C14	-11.21	90.71	113.21
37	T	310	KC1	CHB-C1B-NB	11.19	134.74	124.45
35	B	303	A86	C35-C34-C33	-11.18	90.37	109.88
35	W	203	A86	O1-C15-C14	-11.15	90.84	113.21
37	L	317	KC1	C1A-C2A-C3A	-11.14	98.27	107.11
37	W	217	KC1	OBD-CAD-C3D	-11.14	109.49	127.98
37	A	312	KC1	CHC-C4B-NB	11.14	134.69	124.45
37	X	311	KC1	OBD-CAD-C3D	-11.14	109.49	127.98
37	N	314	KC1	CAB-C3B-C4B	11.13	151.77	124.90
37	P	317	KC1	OBD-CAD-C3D	-11.11	109.53	127.98
37	M	317	KC1	CMD-C2D-C1D	-11.11	111.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	314	CLA	C4A-NA-C1A	11.10	111.70	106.71
42	V	315	LMG	O9-C10-C11	-11.10	80.44	123.73
34	D	303	DD6	C-C1-C24	-11.08	100.62	118.08
36	A	314	CLA	C4A-NA-C1A	11.01	111.65	106.71
35	C	204	A86	C-C1-C2	-10.99	107.53	122.92
37	F	308	KC1	CHB-C1B-NB	10.96	134.53	124.45
35	F	307	A86	O1-C15-C14	-10.93	91.27	113.21
37	L	315	KC1	CHC-C4B-NB	10.92	134.49	124.45
35	N	304	A86	C17-C16-C15	10.92	120.30	109.16
37	V	312	KC1	CAC-C3C-C4C	10.90	138.95	124.81
37	B	310	KC1	C1A-C2A-C3A	-10.88	98.48	107.11
37	B	310	KC1	CHC-C4B-NB	10.86	134.44	124.45
36	a	830	CLA	C4D-CHA-C1A	-10.86	108.04	121.25
37	G	317	KC1	CHC-C4B-NB	10.85	134.42	124.45
37	A	312	KC1	CHD-C4C-C3C	-10.84	104.98	125.33
37	H	313	KC1	CHB-C1B-NB	10.82	134.40	124.45
37	X	311	KC1	CHC-C4B-NB	10.81	134.39	124.45
37	K	314	KC1	CHC-C4B-NB	10.81	134.39	124.45
37	L	317	KC1	CHC-C4B-NB	10.81	134.39	124.45
37	W	217	KC1	CHC-C4B-NB	10.80	134.38	124.45
36	N	319	CLA	C3D-C2D-C1D	-10.77	91.14	105.83
35	V	303	A86	O1-C15-C14	-10.75	91.65	113.21
37	K	314	KC1	CHD-C4C-C3C	-10.74	105.16	125.33
37	L	315	KC1	CHD-C4C-C3C	-10.69	105.26	125.33
37	A	312	KC1	CAB-C3B-C4B	10.68	150.68	124.90
37	G	308	KC1	CHC-C4B-NB	10.67	134.26	124.45
37	C	213	KC1	CAB-C3B-C4B	10.64	150.60	124.90
37	O	313	KC1	CHC-C4B-NB	10.63	134.22	124.45
35	G	304	A86	O1-C20-C21	-10.63	102.32	115.06
37	O	315	KC1	CHC-C4B-NB	10.61	134.21	124.45
37	P	315	KC1	CHC-C4B-NB	10.61	134.20	124.45
37	M	318	KC1	C2A-C1A-NA	-10.60	92.40	109.40
37	G	308	KC1	CAB-C3B-C4B	10.60	150.49	124.90
37	Q	313	KC1	CHC-C4B-NB	10.58	134.18	124.45
36	G	319	CLA	C1D-ND-C4D	-10.58	98.82	106.33
37	Q	311	KC1	CHC-C4B-NB	10.57	134.17	124.45
37	G	318	KC1	CHC-C4B-NB	10.56	134.16	124.45
37	J	314	KC1	C1A-NA-C4A	-10.54	101.97	106.71
37	E	309	KC1	CHC-C4B-NB	10.53	134.13	124.45
37	M	317	KC1	CHC-C4B-NB	10.52	134.12	124.45
37	R	317	KC1	CHC-C4B-NB	10.52	134.12	124.45
37	J	314	KC1	CAB-C3B-C4B	10.51	150.29	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	F	315	KC1	CHC-C4B-NB	10.49	134.10	124.45
37	T	315	KC1	CHC-C4B-NB	10.45	134.06	124.45
37	V	312	KC1	CAB-C3B-C4B	10.44	150.12	124.90
37	J	314	KC1	CHC-C4B-NB	10.43	134.04	124.45
37	Q	313	KC1	CAB-C3B-C4B	10.40	150.00	124.90
37	Q	311	KC1	CAB-C3B-C4B	10.39	150.00	124.90
37	O	313	KC1	CAB-C3B-C4B	10.39	149.98	124.90
37	M	317	KC1	CAB-C3B-C4B	10.37	149.95	124.90
37	O	315	KC1	CAB-C3B-C4B	10.37	149.95	124.90
37	T	315	KC1	CAB-C3B-C4B	10.37	149.93	124.90
37	F	315	KC1	CAB-C3B-C4B	10.36	149.91	124.90
37	P	315	KC1	CAB-C3B-C4B	10.36	149.91	124.90
37	G	318	KC1	CAB-C3B-C4B	10.36	149.91	124.90
37	R	317	KC1	C1A-NA-C4A	-10.35	102.05	106.71
37	F	308	KC1	CHC-C4B-NB	10.35	133.97	124.45
37	L	317	KC1	CAB-C3B-C4B	10.33	149.84	124.90
36	b	836	CLA	C1D-ND-C4D	-10.29	99.03	106.33
37	P	315	KC1	CHD-C4C-C3C	-10.27	106.05	125.33
37	O	313	KC1	CHD-C4C-C3C	-10.27	106.05	125.33
37	G	318	KC1	OBD-CAD-C3D	-10.25	110.96	127.98
37	Q	311	KC1	CHD-C4C-C3C	-10.25	106.10	125.33
37	M	318	KC1	CHC-C4B-NB	10.25	133.87	124.45
37	O	315	KC1	CHD-C4C-C3C	-10.24	106.11	125.33
37	Q	313	KC1	CHD-C4C-C3C	-10.23	106.12	125.33
37	G	318	KC1	OBD-CAD-CBD	10.23	140.51	125.89
37	E	309	KC1	CAB-C3B-C4B	10.22	149.59	124.90
37	M	317	KC1	CMD-C2D-C3D	10.20	143.75	124.68
37	J	314	KC1	CHD-C4C-C3C	-10.15	106.28	125.33
35	R	303	A86	C33-C32-C31	-10.13	99.36	109.21
37	K	314	KC1	CAB-C3B-C4B	10.11	149.31	124.90
37	C	213	KC1	CHC-C4B-NB	10.07	133.71	124.45
35	Q	316	A86	C17-C16-C15	10.07	119.43	109.16
35	N	305	A86	C17-C16-C15	10.06	119.43	109.16
37	F	315	KC1	CHD-C4C-C3C	-10.06	106.45	125.33
35	G	304	A86	O1-C15-C14	-10.04	93.06	113.21
37	P	317	KC1	CHD-C4C-C3C	-10.02	106.53	125.33
37	W	213	KC1	CHC-C4B-NB	10.01	133.66	124.45
37	R	317	KC1	CHB-C1B-NB	10.01	133.65	124.45
37	L	315	KC1	CHD-C4C-NC	9.97	139.34	124.20
37	M	313	KC1	CHB-C1B-NB	9.97	133.62	124.45
37	M	318	KC1	C2A-C3A-C4A	-9.96	99.09	106.49
37	U	312	KC1	CHD-C4C-C3C	-9.96	106.64	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	308	KC1	C1A-C2A-C3A	-9.96	99.21	107.11
37	S	316	KC1	C1A-C2A-C3A	-9.94	99.23	107.11
35	N	301	A86	O1-C15-C14	-9.86	93.43	113.21
35	S	301	A86	O1-C15-C14	-9.85	93.44	113.21
37	L	317	KC1	CHD-C4C-C3C	-9.85	106.84	125.33
37	M	313	KC1	CHC-C4B-NB	9.84	133.50	124.45
37	W	217	KC1	CAB-C3B-C4B	9.82	148.62	124.90
37	B	310	KC1	CAB-C3B-C4B	9.82	148.62	124.90
37	X	311	KC1	CAB-C3B-C4B	9.82	148.61	124.90
37	T	315	KC1	CBD-CHA-C1A	9.81	147.16	128.88
37	M	318	KC1	C4B-C3B-C2B	-9.76	98.73	106.75
36	b	826	CLA	C4A-NA-C1A	9.76	111.09	106.71
37	J	314	KC1	CHD-C4C-NC	9.75	139.00	124.20
37	R	317	KC1	CHD-C4C-C3C	-9.75	107.03	125.33
36	K	307	CLA	C4A-NA-C1A	9.74	111.08	106.71
37	F	315	KC1	CHD-C4C-NC	9.70	138.92	124.20
37	H	313	KC1	C1A-C2A-C3A	-9.69	99.42	107.11
37	M	313	KC1	CHD-C4C-C3C	-9.62	107.28	125.33
36	N	319	CLA	C3C-C4C-NC	-9.61	99.79	110.57
37	W	213	KC1	CHD-C4C-C3C	-9.61	107.29	125.33
37	G	317	KC1	CHD-C4C-NC	9.60	138.77	124.20
37	R	317	KC1	C1A-C2A-C3A	-9.57	99.52	107.11
37	V	312	KC1	CHC-C4B-NB	9.56	133.24	124.45
37	W	213	KC1	CAB-C3B-C4B	9.55	147.96	124.90
37	G	317	KC1	CHD-C4C-C3C	-9.54	107.42	125.33
37	T	315	KC1	CHD-C4C-C3C	-9.54	107.43	125.33
36	I	309	CLA	C4A-NA-C1A	9.48	110.97	106.71
36	N	309	CLA	C4A-NA-C1A	9.48	110.97	106.71
37	C	213	KC1	CHD-C4C-C3C	-9.48	107.54	125.33
37	T	315	KC1	CHD-C4C-NC	9.46	138.56	124.20
36	G	319	CLA	CHD-C1D-ND	-9.43	115.79	124.45
37	M	318	KC1	C4C-C3C-C2C	9.42	120.62	106.90
36	T	311	CLA	C4A-NA-C1A	9.41	110.94	106.71
36	a	833	CLA	C4A-NA-C1A	9.37	110.92	106.71
36	G	307	CLA	CHD-C1D-ND	-9.36	115.85	124.45
35	K	306	A86	C33-C32-C31	-9.34	100.13	109.21
37	T	310	KC1	CHB-C4A-NA	9.24	138.76	124.20
37	H	313	KC1	CHD-C4C-C3C	-9.23	108.01	125.33
37	G	317	KC1	CAB-C3B-C4B	9.22	147.17	124.90
37	P	317	KC1	CHD-C4C-NC	9.21	138.18	124.20
36	C	207	CLA	CMD-C2D-C1D	9.21	140.95	124.71
35	S	305	A86	O1-C15-C14	-9.19	94.76	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	U	301	A86	C3-C2-C1	-9.19	114.19	127.31
36	b	841	CLA	C4A-NA-C1A	9.18	110.83	106.71
37	S	316	KC1	CHC-C4B-NB	9.17	132.88	124.45
37	G	308	KC1	CHD-C4C-C3C	-9.16	108.13	125.33
37	V	312	KC1	CHD-C4C-C3C	-9.14	108.17	125.33
37	D	314	KC1	CAB-C3B-C4B	9.13	146.95	124.90
36	a	817	CLA	CMB-C2B-C1B	-9.11	114.46	128.46
37	S	316	KC1	CHD-C4C-C3C	-9.11	108.24	125.33
36	U	308	CLA	C4A-NA-C1A	9.10	110.80	106.71
36	I	306	CLA	C4A-NA-C1A	9.06	110.78	106.71
37	U	312	KC1	CHC-C4B-NB	9.06	132.78	124.45
36	I	308	CLA	CHD-C1D-ND	-9.05	116.14	124.45
36	S	321	CLA	C4A-NA-C1A	9.05	110.77	106.71
35	U	301	A86	C3-C4-C5	-9.04	104.95	123.47
37	M	318	KC1	CHB-C4A-C3A	-9.02	110.89	124.98
37	T	315	KC1	CHB-C1B-NB	8.98	132.71	124.45
37	N	314	KC1	CBD-CHA-C1A	8.97	145.59	128.88
36	G	313	CLA	C4A-NA-C1A	8.95	110.73	106.71
37	P	317	KC1	CHB-C1B-NB	8.94	132.67	124.45
37	C	213	KC1	CHB-C1B-NB	8.93	132.66	124.45
36	Q	310	CLA	C1-O2A-CGA	8.91	139.81	116.44
37	M	313	KC1	C1A-C2A-C3A	-8.89	100.06	107.11
37	B	310	KC1	CHD-C4C-C3C	-8.89	108.65	125.33
36	a	819	CLA	C4A-NA-C1A	8.88	110.70	106.71
37	K	314	KC1	C1A-C2A-C3A	-8.88	100.07	107.11
36	P	319	CLA	C4A-NA-C1A	8.86	110.69	106.71
37	N	314	KC1	CHB-C1B-NB	8.85	132.59	124.45
37	X	311	KC1	C1A-C2A-C3A	-8.83	100.11	107.11
37	W	217	KC1	C1A-C2A-C3A	-8.83	100.11	107.11
36	H	310	CLA	O2D-CGD-CBD	8.83	126.95	111.27
37	F	308	KC1	CHD-C4C-C3C	-8.82	108.77	125.33
36	S	315	CLA	C4A-NA-C1A	8.82	110.67	106.71
36	U	306	CLA	CMD-C2D-C1D	8.81	140.25	124.71
37	J	314	KC1	CHB-C1B-NB	8.81	132.55	124.45
35	V	304	A86	O1-C15-C14	-8.81	95.53	113.21
37	E	309	KC1	C1A-C2A-C3A	-8.80	100.13	107.11
36	f	804	CLA	CHD-C1D-ND	-8.76	116.40	124.45
36	K	307	CLA	C1D-ND-C4D	-8.74	100.12	106.33
35	I	304	A86	O4-C38-C39	8.73	127.15	111.09
36	V	314	CLA	CHD-C1D-ND	-8.72	116.44	124.45
35	S	305	A86	C17-C16-C15	8.71	118.05	109.16
37	X	311	KC1	CHD-C4C-C3C	-8.71	108.98	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	301	A86	O1-C20-C19	-8.70	106.84	113.38
37	W	217	KC1	CHD-C4C-C3C	-8.70	108.99	125.33
35	O	302	A86	O4-C38-C39	8.70	127.09	111.09
35	L	319	A86	O4-C38-C39	8.70	127.09	111.09
35	P	303	A86	O4-C38-C39	8.70	127.09	111.09
35	W	202	A86	O4-C38-C39	8.67	127.04	111.09
35	X	303	A86	O4-C38-C39	8.67	127.04	111.09
37	K	314	KC1	CHB-C1B-NB	8.66	132.41	124.45
35	T	307	A86	O1-C20-C21	-8.66	104.68	115.06
37	A	312	KC1	CHD-C4C-NC	8.65	137.33	124.20
36	D	309	CLA	C1D-ND-C4D	-8.65	100.19	106.33
35	U	301	A86	O1-C15-C14	-8.64	95.86	113.21
36	R	316	CLA	C4A-NA-C1A	8.62	110.58	106.71
36	T	314	CLA	C4A-NA-C1A	8.61	110.58	106.71
36	D	309	CLA	CMD-C2D-C1D	8.60	139.87	124.71
37	V	312	KC1	CBD-CHA-C1A	8.60	144.90	128.88
35	S	301	A86	O4-C38-C39	8.59	126.90	111.09
36	G	319	CLA	CMD-C2D-C1D	8.59	139.85	124.71
36	H	310	CLA	CED-O2D-CGD	8.58	135.33	115.94
36	K	307	CLA	CMD-C2D-C1D	8.57	139.82	124.71
35	N	301	A86	O4-C38-C39	8.56	126.84	111.09
35	X	301	A86	O4-C38-C39	8.56	126.84	111.09
37	T	310	KC1	CHC-C4B-C3B	-8.56	110.62	125.26
35	N	301	A86	C17-C16-C15	8.52	117.85	109.16
36	S	313	CLA	C4A-NA-C1A	8.52	110.53	106.71
36	X	307	CLA	C4A-NA-C1A	8.52	110.53	106.71
37	N	314	KC1	CHC-C4B-NB	8.51	132.28	124.45
35	R	301	A86	O4-C38-C39	8.51	126.75	111.09
37	M	318	KC1	CAC-C3C-C2C	-8.51	112.97	127.53
35	S	301	A86	C17-C16-C15	8.51	117.84	109.16
35	R	303	A86	O4-C38-C39	8.49	126.72	111.09
36	b	836	CLA	CMD-C2D-C1D	8.49	139.68	124.71
36	V	314	CLA	CMD-C2D-C1D	8.48	139.65	124.71
36	K	310	CLA	CHD-C1D-ND	-8.47	116.67	124.45
36	a	813	CLA	C4A-NA-C1A	8.46	110.51	106.71
36	V	309	CLA	C4A-NA-C1A	8.45	110.51	106.71
37	E	309	KC1	CHD-C4C-C3C	-8.44	109.49	125.33
37	H	313	KC1	CHC-C4B-NB	8.43	132.20	124.45
36	E	315	CLA	CHD-C1D-ND	-8.43	116.71	124.45
37	M	317	KC1	CHB-C1B-NB	8.40	132.17	124.45
36	b	811	CLA	C4A-NA-C1A	8.38	110.47	106.71
37	M	317	KC1	CHD-C4C-C3C	-8.38	109.61	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	F	308	KC1	C2C-C1C-NC	8.37	119.71	110.57
36	N	319	CLA	CHD-C1D-C2D	8.36	143.01	125.48
37	N	314	KC1	CHD-C4C-C3C	-8.35	109.65	125.33
36	f	803	CLA	CMD-C2D-C1D	8.35	139.43	124.71
36	F	311	CLA	C4A-NA-C1A	8.34	110.45	106.71
36	O	316	CLA	CMD-C2D-C1D	8.34	139.41	124.71
36	O	316	CLA	C1D-ND-C4D	-8.33	100.42	106.33
36	F	317	CLA	CMD-C2D-C1D	8.33	139.39	124.71
36	a	814	CLA	C4A-NA-C1A	8.30	110.44	106.71
35	K	301	A86	O1-C20-C19	-8.30	107.15	113.38
36	b	817	CLA	C4A-NA-C1A	8.29	110.43	106.71
37	M	318	KC1	CHB-C1B-NB	8.29	132.07	124.45
36	a	836	CLA	C4A-NA-C1A	8.28	110.43	106.71
36	G	309	CLA	C4A-NA-C1A	8.28	110.43	106.71
37	L	317	KC1	CHD-C4C-NC	8.28	136.76	124.20
36	E	315	CLA	CMD-C2D-C1D	8.28	139.30	124.71
37	T	310	KC1	C2A-C1A-NA	-8.27	96.15	109.40
36	a	826	CLA	C4A-NA-C1A	8.25	110.42	106.71
36	K	310	CLA	CMD-C2D-C1D	8.24	139.24	124.71
36	l	205	CLA	C4A-NA-C1A	8.24	110.41	106.71
36	W	206	CLA	C4A-NA-C1A	8.23	110.40	106.71
37	G	308	KC1	CHB-C1B-NB	8.22	132.01	124.45
35	T	303	A86	O4-C38-C39	8.20	126.18	111.09
36	N	318	CLA	C4A-NA-C1A	8.19	110.39	106.71
37	L	317	KC1	CHB-C1B-NB	8.18	131.97	124.45
37	G	318	KC1	C2C-C1C-NC	8.16	119.49	110.57
36	H	312	CLA	C4A-NA-C1A	8.16	110.38	106.71
36	I	306	CLA	CMD-C2D-C1D	8.15	139.08	124.71
35	V	303	A86	C17-C16-C15	8.15	117.48	109.16
36	B	306	CLA	C4A-NA-C1A	8.14	110.37	106.71
36	B	311	CLA	C4A-NA-C1A	8.14	110.37	106.71
35	E	302	A86	O1-C20-C19	-8.13	107.27	113.38
37	L	317	KC1	C1A-NA-C4A	-8.12	103.05	106.71
37	K	314	KC1	CBD-CHA-C1A	8.11	144.00	128.88
37	N	314	KC1	CMD-C2D-C3D	8.10	139.83	124.68
36	b	835	CLA	C4A-NA-C1A	8.10	110.35	106.71
37	D	314	KC1	C1A-C2A-C3A	-8.09	100.69	107.11
37	S	316	KC1	CAB-C3B-C2B	-8.09	101.97	128.60
36	L	312	CLA	C4A-NA-C1A	8.09	110.34	106.71
37	G	318	KC1	CHD-C4C-C3C	-8.08	110.15	125.33
36	b	826	CLA	CED-O2D-CGD	8.08	134.22	115.94
36	l	205	CLA	CMD-C2D-C1D	8.08	138.94	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	311	CLA	C4A-NA-C1A	8.07	110.34	106.71
35	H	301	A86	O1-C20-C21	-8.07	105.39	115.06
37	V	312	KC1	CHB-C1B-NB	8.07	131.87	124.45
36	N	311	CLA	C4A-NA-C1A	8.06	110.33	106.71
37	C	213	KC1	CBD-CHA-C1A	8.06	143.90	128.88
36	H	309	CLA	C4A-NA-C1A	8.05	110.33	106.71
37	E	309	KC1	CHB-C1B-NB	8.04	131.84	124.45
37	D	314	KC1	CHD-C4C-C3C	-8.04	110.24	125.33
35	h	204	A86	O1-C20-C19	-8.04	107.34	113.38
36	j	102	CLA	CMD-C2D-C1D	8.03	138.86	124.71
36	D	315	CLA	C4A-NA-C1A	8.02	110.31	106.71
36	R	314	CLA	C4A-NA-C1A	8.02	110.31	106.71
36	Q	312	CLA	C4A-NA-C1A	8.01	110.31	106.71
35	C	202	A86	O4-C38-C39	8.01	125.82	111.09
37	M	318	KC1	C1C-C2C-C3C	-8.00	98.54	106.96
36	P	316	CLA	C4A-NA-C1A	8.00	110.30	106.71
35	G	305	A86	O1-C20-C19	-8.00	107.37	113.38
36	G	307	CLA	CMD-C2D-C1D	7.99	138.80	124.71
36	J	312	CLA	C4A-NA-C1A	7.99	110.30	106.71
36	A	313	CLA	C4A-NA-C1A	7.98	110.29	106.71
37	G	318	KC1	C1A-C2A-C3A	-7.98	100.78	107.11
36	U	306	CLA	CHD-C1D-ND	-7.97	117.13	124.45
37	S	316	KC1	CHB-C1B-NB	7.97	131.77	124.45
36	L	313	CLA	C4A-NA-C1A	7.96	110.29	106.71
37	G	318	KC1	CHB-C1B-NB	7.96	131.77	124.45
35	T	305	A86	O4-C38-C39	7.95	125.71	111.09
35	G	304	A86	C17-C16-C15	7.94	117.27	109.16
36	O	314	CLA	C4A-NA-C1A	7.93	110.27	106.71
36	J	308	CLA	C4A-NA-C1A	7.93	110.27	106.71
35	N	303	A86	O4-C38-C39	7.92	125.66	111.09
37	E	309	KC1	C2C-C1C-NC	7.92	119.22	110.57
37	R	317	KC1	CAB-C3B-C2B	-7.92	102.52	128.60
35	V	303	A86	O4-C38-C39	7.92	125.65	111.09
36	I	308	CLA	CMD-C2D-C1D	7.91	138.65	124.71
35	S	303	A86	O4-C38-C39	7.91	125.64	111.09
37	D	314	KC1	CBD-CHA-C1A	7.90	143.61	128.88
36	T	312	CLA	C4A-NA-C1A	7.90	110.26	106.71
37	Q	311	KC1	C2A-C3A-C4A	7.90	112.34	106.49
37	O	315	KC1	C2A-C3A-C4A	7.89	112.34	106.49
37	U	312	KC1	C1A-NA-C4A	-7.89	103.16	106.71
36	Q	310	CLA	O2A-C1-C2	7.88	129.35	108.64
37	A	312	KC1	CHB-C1B-NB	7.88	131.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	I	301	A86	O1-C20-C19	-7.87	107.47	113.38
36	U	306	CLA	C4A-NA-C1A	7.87	110.24	106.71
36	b	816	CLA	CMD-C2D-C1D	7.87	138.58	124.71
36	I	311	CLA	C4A-NA-C1A	7.86	110.24	106.71
36	R	319	CLA	C4A-NA-C1A	7.86	110.24	106.71
37	O	313	KC1	C2A-C3A-C4A	7.85	112.31	106.49
37	P	315	KC1	C2A-C3A-C4A	7.85	112.31	106.49
36	b	807	CLA	C4A-NA-C1A	7.85	110.24	106.71
35	F	307	A86	C17-C16-C15	7.85	117.17	109.16
36	C	207	CLA	CHD-C1D-ND	-7.84	117.25	124.45
36	X	312	CLA	C4A-NA-C1A	7.84	110.23	106.71
36	G	307	CLA	C1C-C2C-C3C	-7.83	98.73	106.96
37	A	312	KC1	CHB-C4A-C3A	-7.82	112.76	124.98
36	b	806	CLA	C4A-NA-C1A	7.82	110.22	106.71
37	Q	313	KC1	C2A-C3A-C4A	7.82	112.29	106.49
37	B	310	KC1	C1A-NA-C4A	-7.81	103.20	106.71
36	f	804	CLA	CMD-C2D-C1D	7.81	138.47	124.71
36	L	308	CLA	CHB-C4A-NA	7.80	135.29	124.51
37	M	318	KC1	CHD-C4C-C3C	-7.79	110.70	125.33
36	a	828	CLA	C4A-NA-C1A	7.78	110.20	106.71
37	S	316	KC1	CHB-C4A-C3A	-7.76	112.86	124.98
37	D	314	KC1	CHB-C1B-NB	7.75	131.58	124.45
36	i	102	CLA	C4A-NA-C1A	7.75	110.19	106.71
36	D	313	CLA	C4A-NA-C1A	7.75	110.19	106.71
36	b	819	CLA	C4A-NA-C1A	7.74	110.19	106.71
36	b	839	CLA	C4A-NA-C1A	7.74	110.18	106.71
36	b	817	CLA	CMD-C2D-C1D	7.74	138.35	124.71
36	S	318	CLA	C4A-NA-C1A	7.73	110.18	106.71
37	W	213	KC1	CHB-C1B-NB	7.73	131.55	124.45
37	A	312	KC1	CBD-CHA-C1A	-7.72	114.49	128.88
36	l	204	CLA	CMD-C2D-C1D	7.72	138.32	124.71
37	G	317	KC1	CMD-C2D-C3D	7.71	139.11	124.68
37	G	308	KC1	CHD-C4C-NC	7.70	135.89	124.20
36	f	805	CLA	C4A-NA-C1A	7.70	110.17	106.71
37	N	314	KC1	CMD-C2D-C1D	-7.68	116.66	128.46
36	a	824	CLA	C4A-NA-C1A	7.68	110.16	106.71
36	A	306	CLA	CMD-C2D-C1D	7.68	138.25	124.71
35	K	306	A86	C40-C32-C31	7.68	117.34	110.47
37	R	317	KC1	CHB-C4A-C3A	-7.67	112.99	124.98
35	M	301	A86	C17-C16-C15	7.66	116.98	109.16
36	K	312	CLA	C4A-NA-C1A	7.66	110.15	106.71
35	K	302	A86	O4-C38-C39	7.65	125.16	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	M	313	KC1	CAB-C3B-C2B	-7.65	103.41	128.60
37	T	310	KC1	CAC-C3C-C2C	-7.64	114.46	127.53
36	T	309	CLA	C4A-NA-C1A	7.64	110.14	106.71
36	E	314	CLA	C4A-NA-C1A	7.64	110.14	106.71
37	O	315	KC1	C2C-C1C-NC	7.63	118.91	110.57
35	K	302	A86	C35-C34-C33	-7.63	96.57	109.88
37	Q	313	KC1	C2C-C1C-NC	7.63	118.90	110.57
35	X	305	A86	O1-C20-C21	-7.62	105.92	115.06
36	a	802	CLA	C4A-NA-C1A	7.62	110.13	106.71
36	b	832	CLA	C4A-NA-C1A	7.62	110.13	106.71
37	Q	311	KC1	C2C-C1C-NC	7.62	118.89	110.57
37	T	310	KC1	C2A-C1A-CHA	7.61	152.64	127.44
36	a	830	CLA	CMD-C2D-C1D	7.61	138.13	124.71
36	h	203	CLA	C4A-NA-C1A	7.61	110.13	106.71
37	P	315	KC1	C2C-C1C-NC	7.61	118.88	110.57
36	a	818	CLA	C4A-NA-C1A	7.61	110.13	106.71
36	a	808	CLA	C4A-NA-C1A	7.59	110.12	106.71
36	C	209	CLA	C4A-NA-C1A	7.59	110.12	106.71
37	O	315	KC1	C2A-C1A-NA	7.58	121.56	109.40
36	Q	309	CLA	C4A-NA-C1A	7.57	110.11	106.71
37	K	314	KC1	CHD-C4C-NC	7.57	135.69	124.20
37	O	313	KC1	C2A-C1A-NA	7.57	121.54	109.40
37	Q	313	KC1	C2A-C1A-NA	7.57	121.54	109.40
37	P	317	KC1	CAB-C3B-C4B	7.56	143.16	124.90
37	Q	311	KC1	C2A-C1A-NA	7.56	121.53	109.40
37	L	315	KC1	CHB-C1B-NB	7.56	131.40	124.45
37	P	315	KC1	C2A-C1A-NA	7.55	121.51	109.40
37	A	312	KC1	OBD-CAD-C3D	-7.55	115.44	127.98
37	M	318	KC1	CHC-C4B-C3B	-7.54	112.36	125.26
36	a	823	CLA	C4A-NA-C1A	7.54	110.09	106.71
37	O	313	KC1	C2C-C1C-NC	7.54	118.80	110.57
35	V	304	A86	C17-C16-C15	7.54	116.85	109.16
37	B	310	KC1	CHB-C1B-NB	7.53	131.38	124.45
36	H	316	CLA	C4A-NA-C1A	7.53	110.09	106.71
36	b	825	CLA	C4A-NA-C1A	7.52	110.09	106.71
36	b	824	CLA	CMD-C2D-C1D	7.52	137.96	124.71
36	D	310	CLA	C4A-NA-C1A	7.51	110.08	106.71
36	a	807	CLA	C4A-NA-C1A	7.51	110.08	106.71
37	O	313	KC1	CHD-C4C-NC	7.51	135.60	124.20
36	G	319	CLA	C2D-C1D-ND	7.51	115.64	110.10
36	a	817	CLA	CMB-C2B-C3B	7.51	138.73	124.68
36	O	310	CLA	C4A-NA-C1A	7.50	110.08	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	M	301	A86	O4-C38-C39	7.50	124.89	111.09
36	S	310	CLA	C4A-NA-C1A	7.50	110.08	106.71
35	G	304	A86	C21-C20-C19	-7.50	105.85	114.28
35	S	301	A86	C21-C20-C19	-7.49	105.85	114.28
37	P	315	KC1	CHD-C4C-NC	7.49	135.57	124.20
35	N	301	A86	C21-C20-C19	-7.49	105.86	114.28
37	Q	311	KC1	CHD-C4C-NC	7.47	135.54	124.20
37	O	315	KC1	CHD-C4C-NC	7.47	135.53	124.20
37	Q	313	KC1	CHD-C4C-NC	7.47	135.53	124.20
37	M	317	KC1	C1A-C2A-C3A	-7.47	101.19	107.11
36	A	308	CLA	C4A-NA-C1A	7.46	110.06	106.71
36	E	316	CLA	C4A-NA-C1A	7.46	110.06	106.71
36	a	841	CLA	C4A-NA-C1A	7.46	110.06	106.71
37	H	313	KC1	CHB-C4A-C3A	-7.45	113.34	124.98
36	C	206	CLA	C4A-NA-C1A	7.44	110.05	106.71
36	H	307	CLA	C4A-NA-C1A	7.43	110.05	106.71
36	G	312	CLA	C4A-NA-C1A	7.43	110.05	106.71
35	K	302	A86	C17-C16-C15	7.42	116.73	109.16
37	F	308	KC1	CHD-C4C-NC	7.42	135.46	124.20
36	a	816	CLA	CMD-C2D-C1D	7.41	137.78	124.71
36	V	306	CLA	C4A-NA-C1A	7.41	110.04	106.71
36	B	305	CLA	C4A-NA-C1A	7.41	110.04	106.71
36	J	315	CLA	C4A-NA-C1A	7.41	110.04	106.71
36	a	815	CLA	C4A-NA-C1A	7.41	110.04	106.71
36	P	301	CLA	C4A-NA-C1A	7.40	110.03	106.71
35	X	304	A86	O1-C20-C21	-7.39	106.20	115.06
36	L	314	CLA	C4A-NA-C1A	7.39	110.03	106.71
36	V	314	CLA	C1C-C2C-C3C	-7.39	99.19	106.96
36	G	315	CLA	C1C-C2C-C3C	-7.38	99.19	106.96
35	B	303	A86	C17-C16-C15	7.38	116.69	109.16
36	N	312	CLA	C4A-NA-C1A	7.37	110.02	106.71
36	P	312	CLA	C4A-NA-C1A	7.37	110.02	106.71
36	W	218	CLA	C4A-NA-C1A	7.37	110.02	106.71
36	V	314	CLA	C1D-ND-C4D	-7.36	101.10	106.33
36	a	827	CLA	C4A-NA-C1A	7.36	110.02	106.71
36	N	319	CLA	C4D-C3D-CAD	-7.36	99.42	108.10
36	R	315	CLA	C4A-NA-C1A	7.36	110.02	106.71
37	W	217	KC1	CHB-C1B-NB	7.36	131.22	124.45
36	G	316	CLA	C4A-NA-C1A	7.36	110.01	106.71
36	L	320	CLA	C4A-NA-C1A	7.36	110.01	106.71
37	G	317	KC1	CHB-C1B-NB	7.35	131.21	124.45
36	H	310	CLA	C4D-CHA-C1A	-7.34	112.31	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	212	CLA	C4A-NA-C1A	7.34	110.01	106.71
37	M	313	KC1	CHD-C4C-NC	7.34	135.34	124.20
36	Q	308	CLA	C4A-NA-C1A	7.34	110.00	106.71
36	C	210	CLA	C4A-NA-C1A	7.33	110.00	106.71
36	U	310	CLA	C4A-NA-C1A	7.33	110.00	106.71
36	C	207	CLA	C3D-C2D-C1D	-7.33	95.83	105.83
36	b	836	CLA	CHD-C1D-ND	-7.33	117.72	124.45
37	L	315	KC1	CAB-C3B-C4B	7.33	142.59	124.90
36	a	834	CLA	C4A-NA-C1A	7.32	110.00	106.71
36	a	821	CLA	C4A-NA-C1A	7.31	109.99	106.71
36	G	314	CLA	C4A-NA-C1A	7.31	109.99	106.71
35	M	301	A86	C35-C34-C33	-7.30	97.13	109.88
36	C	207	CLA	C1D-ND-C4D	-7.30	101.15	106.33
36	P	311	CLA	C4A-NA-C1A	7.30	109.99	106.71
35	Q	304	A86	C33-C32-C31	-7.30	102.12	109.21
36	T	311	CLA	CAC-C3C-C4C	-7.29	115.35	124.81
36	O	311	CLA	C4A-NA-C1A	7.29	109.98	106.71
37	X	311	KC1	CHB-C1B-NB	7.29	131.15	124.45
36	G	315	CLA	C2C-C1C-NC	7.28	116.79	109.97
36	U	306	CLA	C2D-C1D-ND	7.28	115.47	110.10
36	L	308	CLA	CMD-C2D-C1D	7.28	137.54	124.71
35	X	304	A86	O4-C38-C39	7.27	124.47	111.09
36	X	310	CLA	O1D-CGD-CBD	7.27	139.36	124.48
35	N	320	A86	C33-C32-C31	-7.27	102.15	109.21
36	J	310	CLA	C4A-NA-C1A	7.26	109.97	106.71
36	O	309	CLA	C4A-NA-C1A	7.25	109.97	106.71
36	X	308	CLA	C4A-NA-C1A	7.25	109.97	106.71
36	G	315	CLA	CMD-C2D-C1D	7.24	137.48	124.71
35	V	304	A86	C20-C19-C18	7.24	127.08	112.75
37	F	315	KC1	CHB-C1B-NB	7.24	131.11	124.45
36	b	808	CLA	C4A-NA-C1A	7.23	109.96	106.71
37	A	312	KC1	C2C-C1C-NC	7.23	118.46	110.57
36	a	812	CLA	C4A-NA-C1A	7.23	109.95	106.71
37	L	315	KC1	C2C-C1C-NC	7.22	118.45	110.57
36	a	810	CLA	C4A-NA-C1A	7.21	109.95	106.71
36	J	313	CLA	C4A-NA-C1A	7.21	109.95	106.71
35	G	304	A86	O4-C38-C39	7.19	124.32	111.09
36	P	313	CLA	C4A-NA-C1A	7.19	109.94	106.71
36	F	314	CLA	C4A-NA-C1A	7.19	109.94	106.71
36	a	848	CLA	CMD-C2D-C1D	7.19	137.38	124.71
36	Q	306	CLA	C4A-NA-C1A	7.18	109.94	106.71
35	R	302	A86	C17-C16-C15	7.18	116.49	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	J	314	KC1	C2C-C1C-NC	7.17	118.41	110.57
36	M	307	CLA	C4A-NA-C1A	7.17	109.93	106.71
36	X	306	CLA	C4A-NA-C1A	7.17	109.93	106.71
36	U	309	CLA	C4A-NA-C1A	7.17	109.93	106.71
37	W	217	KC1	CHB-C4A-C3A	-7.17	113.78	124.98
37	X	311	KC1	CHB-C4A-C3A	-7.16	113.79	124.98
36	H	314	CLA	C4A-NA-C1A	7.16	109.93	106.71
37	S	316	KC1	CHD-C4C-NC	7.16	135.07	124.20
36	a	837	CLA	C4A-NA-C1A	7.16	109.92	106.71
35	N	301	A86	O1-C20-C21	-7.16	106.48	115.06
36	P	308	CLA	C4A-NA-C1A	7.16	109.92	106.71
37	N	314	KC1	CAB-C3B-C2B	-7.15	105.04	128.60
36	b	815	CLA	C4A-NA-C1A	7.15	109.92	106.71
35	T	303	A86	C17-C16-C15	7.15	116.46	109.16
35	S	301	A86	O1-C20-C21	-7.15	106.49	115.06
36	a	832	CLA	C4A-NA-C1A	7.14	109.92	106.71
37	F	315	KC1	CAC-C3C-C4C	7.14	134.08	124.81
35	V	302	A86	O1-C20-C19	7.14	118.75	113.38
36	V	310	CLA	C4A-NA-C1A	7.14	109.92	106.71
36	P	309	CLA	C4A-NA-C1A	7.14	109.91	106.71
36	O	306	CLA	C4A-NA-C1A	7.13	109.91	106.71
36	a	819	CLA	CAC-C3C-C4C	-7.13	115.56	124.81
37	W	213	KC1	C1A-C2A-C3A	-7.12	101.46	107.11
35	U	301	A86	O1-C20-C19	-7.12	108.03	113.38
36	T	308	CLA	C4A-NA-C1A	7.12	109.91	106.71
36	V	308	CLA	C4A-NA-C1A	7.12	109.91	106.71
37	G	308	KC1	C2C-C1C-NC	7.12	118.34	110.57
36	U	311	CLA	C4A-NA-C1A	7.12	109.91	106.71
36	a	829	CLA	CMB-C2B-C1B	-7.11	117.54	128.46
36	M	315	CLA	C4A-NA-C1A	7.11	109.90	106.71
36	D	309	CLA	CHD-C1D-ND	-7.11	117.92	124.45
36	O	307	CLA	C4A-NA-C1A	7.10	109.90	106.71
36	b	820	CLA	C4A-NA-C1A	7.10	109.90	106.71
35	R	301	A86	O1-C20-C21	-7.10	106.55	115.06
36	C	211	CLA	C4A-NA-C1A	7.09	109.89	106.71
35	J	301	A86	O1-C20-C19	-7.09	108.06	113.38
36	a	829	CLA	C4A-NA-C1A	7.08	109.89	106.71
36	a	816	CLA	C4A-NA-C1A	7.08	109.89	106.71
36	I	307	CLA	C4A-NA-C1A	7.08	109.89	106.71
36	b	810	CLA	C4A-NA-C1A	7.08	109.89	106.71
36	W	207	CLA	C4A-NA-C1A	7.07	109.89	106.71
37	W	213	KC1	C2C-C1C-NC	7.07	118.29	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	S	316	KC1	C1A-NA-C4A	-7.07	103.53	106.71
36	Q	305	CLA	C4A-NA-C1A	7.07	109.88	106.71
35	S	301	A86	C25-C26-C27	-7.06	117.23	127.31
37	U	312	KC1	C2C-C1C-NC	7.06	118.28	110.57
36	W	201	CLA	C4A-NA-C1A	7.06	109.88	106.71
36	V	305	CLA	C4A-NA-C1A	7.06	109.88	106.71
35	N	301	A86	C25-C26-C27	-7.06	117.24	127.31
36	I	308	CLA	C4A-NA-C1A	7.06	109.88	106.71
36	l	206	CLA	C4A-NA-C1A	7.05	109.88	106.71
35	U	301	A86	C4-C3-C2	7.04	137.90	123.47
37	U	312	KC1	CMD-C2D-C3D	7.04	137.85	124.68
37	D	314	KC1	CHC-C4B-C3B	-7.03	113.23	125.26
36	H	315	CLA	C4A-NA-C1A	7.03	109.86	106.71
36	I	308	CLA	C1D-ND-C4D	-7.03	101.34	106.33
36	E	313	CLA	CMD-C2D-C1D	7.02	137.09	124.71
36	A	311	CLA	C4A-NA-C1A	7.02	109.86	106.71
36	a	839	CLA	C4A-NA-C1A	7.02	109.86	106.71
36	E	310	CLA	C4A-NA-C1A	7.02	109.86	106.71
36	X	309	CLA	C4A-NA-C1A	7.02	109.86	106.71
37	X	311	KC1	C2C-C1C-NC	7.01	118.22	110.57
35	W	202	A86	C17-C16-C15	7.01	116.31	109.16
37	B	310	KC1	C2C-C1C-NC	7.00	118.22	110.57
37	W	217	KC1	C2C-C1C-NC	7.00	118.21	110.57
36	U	305	CLA	C4A-NA-C1A	7.00	109.85	106.71
36	M	311	CLA	C4A-NA-C1A	6.99	109.85	106.71
37	F	315	KC1	CHB-C4A-C3A	-6.99	114.06	124.98
36	N	307	CLA	C4A-NA-C1A	6.98	109.84	106.71
37	M	318	KC1	CHB-C4A-NA	6.98	135.20	124.20
36	R	320	CLA	C4A-NA-C1A	6.97	109.84	106.71
36	F	317	CLA	C1C-C2C-C3C	-6.96	99.64	106.96
37	M	318	KC1	CMD-C2D-C3D	6.96	137.70	124.68
36	b	823	CLA	C4A-NA-C1A	6.95	109.83	106.71
37	P	317	KC1	CHC-C4B-C3B	-6.95	113.37	125.26
35	R	304	A86	O4-C38-C39	6.95	123.87	111.09
36	I	305	CLA	C4A-NA-C1A	6.94	109.83	106.71
36	F	310	CLA	C4A-NA-C1A	6.94	109.83	106.71
37	G	317	KC1	C2C-C1C-NC	6.94	118.15	110.57
37	A	312	KC1	CHC-C4B-C3B	-6.94	113.39	125.26
36	b	836	CLA	C4A-NA-C1A	6.94	109.82	106.71
36	j	106	CLA	C4A-NA-C1A	6.93	109.82	106.71
37	R	317	KC1	C2C-C1C-NC	6.92	118.13	110.57
36	K	307	CLA	CHD-C1D-ND	-6.91	118.11	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S	304	A86	C33-C32-C31	6.90	115.92	109.21
37	L	317	KC1	CHB-C4A-C3A	-6.89	114.21	124.98
36	N	315	CLA	C4A-NA-C1A	6.89	109.81	106.71
37	G	317	KC1	CHB-C4A-C3A	-6.89	114.22	124.98
37	G	318	KC1	C1A-NA-C4A	-6.89	103.61	106.71
37	D	314	KC1	C2C-C1C-NC	6.88	118.09	110.57
37	T	310	KC1	C4C-C3C-C2C	6.88	116.92	106.90
36	F	312	CLA	C4A-NA-C1A	6.88	109.80	106.71
37	A	312	KC1	CAB-C3B-C2B	-6.88	105.93	128.60
36	O	316	CLA	CHD-C1D-ND	-6.88	118.13	124.45
35	V	304	A86	O1-C20-C21	6.88	123.30	115.06
37	X	311	KC1	CHC-C4B-C3B	-6.88	113.50	125.26
37	T	310	KC1	CHC-C1C-C2C	6.88	135.72	124.98
36	f	802	CLA	C4A-NA-C1A	6.88	109.80	106.71
37	C	213	KC1	CAB-C3B-C2B	-6.87	105.97	128.60
37	W	217	KC1	CHC-C4B-C3B	-6.87	113.51	125.26
37	A	312	KC1	C2A-C1A-NA	6.87	120.41	109.40
37	L	317	KC1	C2C-C1C-NC	6.87	118.07	110.57
36	P	318	CLA	C4A-NA-C1A	6.86	109.79	106.71
35	N	301	A86	C35-C34-C33	-6.85	97.92	109.88
37	M	313	KC1	C1A-NA-C4A	-6.85	103.62	106.71
37	K	314	KC1	CHC-C4B-C3B	-6.85	113.54	125.26
35	L	304	A86	O1-C20-C21	-6.85	106.85	115.06
35	S	301	A86	C35-C34-C33	-6.85	97.93	109.88
37	G	317	KC1	CMD-C2D-C1D	-6.85	117.94	128.46
37	H	313	KC1	CHD-C4C-NC	6.85	134.59	124.20
36	X	313	CLA	C3B-C4B-NB	6.84	118.06	109.21
36	A	310	CLA	C4A-NA-C1A	6.84	109.78	106.71
36	K	316	CLA	C4A-NA-C1A	6.84	109.78	106.71
37	G	308	KC1	CAB-C3B-C2B	-6.84	106.07	128.60
36	M	308	CLA	C4A-NA-C1A	6.84	109.78	106.71
36	a	806	CLA	C4A-NA-C1A	6.84	109.78	106.71
35	R	303	A86	C40-C32-C31	6.83	116.58	110.47
37	V	312	KC1	CAB-C3B-C2B	-6.83	106.12	128.60
37	M	317	KC1	CAB-C3B-C2B	-6.82	106.12	128.60
36	M	309	CLA	C4A-NA-C1A	6.82	109.77	106.71
36	b	830	CLA	C4A-NA-C1A	6.82	109.77	106.71
36	b	814	CLA	C4A-NA-C1A	6.82	109.77	106.71
37	O	313	KC1	CHB-C1B-NB	6.82	130.72	124.45
36	K	308	CLA	C4A-NA-C1A	6.82	109.77	106.71
36	E	308	CLA	C4A-NA-C1A	6.81	109.77	106.71
36	E	313	CLA	C1C-C2C-C3C	-6.81	99.80	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	L	315	KC1	C1A-NA-C4A	-6.81	103.64	106.71
37	Q	311	KC1	CHB-C1B-NB	6.80	130.71	124.45
36	U	307	CLA	C4A-NA-C1A	6.80	109.76	106.71
36	G	307	CLA	C2C-C1C-NC	6.80	116.34	109.97
36	H	317	CLA	C4A-NA-C1A	6.79	109.76	106.71
36	I	204	CLA	C4A-NA-C1A	6.79	109.76	106.71
36	M	316	CLA	C4A-NA-C1A	6.79	109.76	106.71
37	O	315	KC1	CHB-C1B-NB	6.79	130.69	124.45
36	N	319	CLA	CMD-C2D-C3D	-6.78	112.01	127.61
37	T	310	KC1	C4B-C3B-C2B	-6.78	101.18	106.75
35	W	202	A86	C35-C34-C33	-6.78	98.05	109.88
36	D	307	CLA	C4A-NA-C1A	6.77	109.75	106.71
35	M	302	A86	C17-C16-C15	6.77	116.07	109.16
37	J	314	KC1	CHC-C4B-C3B	-6.77	113.67	125.26
37	Q	313	KC1	CHB-C1B-NB	6.77	130.68	124.45
36	a	816	CLA	C1D-ND-C4D	-6.77	101.53	106.33
36	M	314	CLA	C4A-NA-C1A	6.76	109.75	106.71
35	R	303	A86	C17-C16-C15	6.76	116.06	109.16
36	a	809	CLA	C4A-NA-C1A	6.76	109.74	106.71
36	W	208	CLA	C4A-NA-C1A	6.75	109.74	106.71
37	P	315	KC1	CHB-C1B-NB	6.75	130.66	124.45
36	P	319	CLA	C2D-C1D-ND	6.75	115.08	110.10
37	G	318	KC1	CAB-C3B-C2B	-6.74	106.38	128.60
37	T	315	KC1	CAB-C3B-C2B	-6.74	106.40	128.60
36	C	208	CLA	C4A-NA-C1A	6.74	109.74	106.71
36	b	821	CLA	C4A-NA-C1A	6.74	109.74	106.71
37	G	318	KC1	CHD-C4C-NC	6.74	134.43	124.20
35	L	319	A86	C35-C34-C33	-6.74	98.12	109.88
37	U	312	KC1	CMD-C2D-C1D	-6.74	118.11	128.46
36	D	317	CLA	C4A-NA-C1A	6.74	109.73	106.71
36	I	314	CLA	C4A-NA-C1A	6.74	109.73	106.71
35	O	302	A86	C35-C34-C33	-6.73	98.13	109.88
36	f	803	CLA	C2C-C1C-NC	6.73	116.27	109.97
35	R	306	A86	C25-C26-C27	-6.72	117.72	127.31
35	B	303	A86	C25-C26-C27	-6.72	117.72	127.31
36	W	214	CLA	C4A-NA-C1A	6.72	109.73	106.71
36	P	302	CLA	C4A-NA-C1A	6.72	109.72	106.71
36	j	102	CLA	C4A-NA-C1A	6.71	109.72	106.71
36	b	830	CLA	CMB-C2B-C1B	-6.71	118.15	128.46
37	J	314	KC1	CHB-C4A-C3A	-6.70	114.50	124.98
35	P	303	A86	C35-C34-C33	-6.70	98.18	109.88
35	N	303	A86	C35-C34-C33	-6.70	98.18	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	K	314	KC1	C2C-C1C-NC	6.70	117.89	110.57
36	D	312	CLA	C4A-NA-C1A	6.70	109.72	106.71
35	S	303	A86	C35-C34-C33	-6.70	98.19	109.88
36	B	307	CLA	C4A-NA-C1A	6.70	109.72	106.71
36	C	214	CLA	C4A-NA-C1A	6.69	109.72	106.71
36	U	313	CLA	C4A-NA-C1A	6.69	109.71	106.71
37	J	314	KC1	CAB-C3B-C2B	-6.69	106.57	128.60
37	R	317	KC1	CHD-C4C-NC	6.68	134.34	124.20
37	L	317	KC1	CAB-C3B-C2B	-6.68	106.59	128.60
36	N	316	CLA	C4A-NA-C1A	6.68	109.71	106.71
36	D	308	CLA	C4A-NA-C1A	6.68	109.71	106.71
37	E	309	KC1	CAB-C3B-C2B	-6.67	106.62	128.60
34	D	303	DD6	C-C1-C2	-6.67	113.58	122.92
36	a	811	CLA	C4A-NA-C1A	6.66	109.70	106.71
37	F	315	KC1	CAB-C3B-C2B	-6.66	106.66	128.60
37	Q	313	KC1	CAB-C3B-C2B	-6.66	106.66	128.60
37	M	313	KC1	CAC-C3C-C4C	6.66	133.45	124.81
37	Q	311	KC1	CAB-C3B-C2B	-6.66	106.67	128.60
37	O	313	KC1	CAB-C3B-C2B	-6.66	106.67	128.60
37	U	312	KC1	CAC-C3C-C4C	6.65	133.43	124.81
37	G	308	KC1	CHC-C4B-C3B	-6.64	113.89	125.26
37	P	315	KC1	CAB-C3B-C2B	-6.64	106.72	128.60
37	O	315	KC1	CAB-C3B-C2B	-6.64	106.72	128.60
35	G	306	A86	O1-C20-C19	-6.64	108.39	113.38
36	b	829	CLA	C4A-NA-C1A	6.64	109.69	106.71
36	F	309	CLA	C4A-NA-C1A	6.63	109.69	106.71
36	P	310	CLA	C4A-NA-C1A	6.63	109.69	106.71
37	O	313	KC1	CHB-C4A-C3A	-6.62	114.64	124.98
37	Q	313	KC1	CHB-C4A-C3A	-6.62	114.64	124.98
37	L	315	KC1	CHC-C4B-C3B	-6.62	113.94	125.26
36	Q	307	CLA	C4A-NA-C1A	6.62	109.68	106.71
35	A	316	A86	O1-C20-C19	-6.62	108.41	113.38
37	P	317	KC1	C2C-C1C-NC	6.62	117.79	110.57
36	K	315	CLA	C4A-NA-C1A	6.62	109.68	106.71
37	O	315	KC1	CHB-C4A-C3A	-6.61	114.65	124.98
37	F	308	KC1	CHB-C4A-C3A	-6.61	114.65	124.98
36	R	312	CLA	C4A-NA-C1A	6.61	109.68	106.71
37	Q	311	KC1	CHB-C4A-C3A	-6.60	114.66	124.98
36	W	211	CLA	C4A-NA-C1A	6.60	109.67	106.71
36	E	311	CLA	C4A-NA-C1A	6.60	109.67	106.71
36	O	308	CLA	C4A-NA-C1A	6.60	109.67	106.71
37	M	317	KC1	CBD-CHA-C1A	6.60	141.18	128.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	P	315	KC1	CHB-C4A-C3A	-6.59	114.68	124.98
34	S	307	DD6	C21-C20-C19	6.59	121.70	114.28
36	Q	310	CLA	O2A-CGA-CBA	-6.59	91.22	111.91
36	H	306	CLA	C4A-NA-C1A	6.59	109.67	106.71
36	A	306	CLA	C2C-C1C-NC	6.59	116.15	109.97
37	P	317	KC1	C1A-C2A-C3A	-6.59	101.88	107.11
37	F	315	KC1	C2C-C1C-NC	6.58	117.76	110.57
36	a	805	CLA	C4A-NA-C1A	6.58	109.66	106.71
36	R	310	CLA	C4A-NA-C1A	6.58	109.66	106.71
37	G	318	KC1	CHC-C4B-C3B	-6.57	114.02	125.26
37	L	315	KC1	CHC-C1C-NC	-6.57	113.85	124.20
36	R	318	CLA	C4A-NA-C1A	6.57	109.66	106.71
37	F	308	KC1	CHC-C4B-C3B	-6.57	114.03	125.26
36	D	316	CLA	C4A-NA-C1A	6.56	109.66	106.71
36	K	311	CLA	C4A-NA-C1A	6.56	109.66	106.71
37	L	317	KC1	CHC-C4B-C3B	-6.56	114.04	125.26
36	G	307	CLA	C4A-NA-C1A	6.55	109.65	106.71
37	F	315	KC1	CHC-C4B-C3B	-6.55	114.06	125.26
36	D	309	CLA	C4A-NA-C1A	6.55	109.65	106.71
36	H	311	CLA	C4A-NA-C1A	6.55	109.65	106.71
36	F	317	CLA	C2C-C1C-NC	6.55	116.11	109.97
36	a	848	CLA	C4A-NA-C1A	6.54	109.65	106.71
37	B	310	KC1	CHC-C4B-C3B	-6.53	114.08	125.26
35	K	306	A86	C17-C16-C15	6.53	115.83	109.16
36	W	212	CLA	CHD-C1D-ND	-6.53	118.46	124.45
37	G	317	KC1	CHC-C4B-C3B	-6.52	114.10	125.26
36	J	309	CLA	C4A-NA-C1A	6.52	109.64	106.71
35	S	303	A86	C17-C16-C15	6.51	115.81	109.16
36	S	317	CLA	C4A-NA-C1A	6.51	109.63	106.71
37	N	314	KC1	C2C-C1C-NC	6.51	117.68	110.57
37	T	310	KC1	C1B-CHB-C4A	-6.50	112.03	126.06
35	N	303	A86	C17-C16-C15	6.50	115.80	109.16
35	X	304	A86	C17-C16-C15	6.50	115.80	109.16
37	A	312	KC1	C2A-C3A-C4A	6.50	111.31	106.49
36	G	319	CLA	C2C-C1C-NC	6.50	116.06	109.97
35	F	305	A86	C17-C16-C15	6.49	115.78	109.16
34	D	303	DD6	C21-C20-C19	6.48	121.58	114.28
35	X	303	A86	C3-C2-C1	-6.48	118.06	127.31
36	b	819	CLA	CMB-C2B-C1B	-6.48	118.50	128.46
35	F	304	A86	O1-C20-C19	-6.48	108.51	113.38
36	E	313	CLA	C2C-C1C-NC	6.47	116.03	109.97
35	R	301	A86	C35-C34-C33	-6.47	98.59	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	U	312	KC1	CHB-C1B-NB	6.46	130.40	124.45
35	N	302	A86	C17-C16-C15	6.46	115.75	109.16
36	a	803	CLA	C4A-NA-C1A	6.46	109.61	106.71
36	b	809	CLA	C4A-NA-C1A	6.45	109.61	106.71
34	S	307	DD6	C3-C2-C1	-6.45	118.11	127.31
37	K	314	KC1	CAB-C3B-C2B	-6.45	107.36	128.60
35	S	302	A86	C17-C16-C15	6.45	115.74	109.16
36	S	320	CLA	C4A-NA-C1A	6.44	109.60	106.71
35	N	320	A86	C17-C16-C15	6.44	115.73	109.16
35	X	304	A86	C35-C34-C33	-6.44	98.64	109.88
35	E	307	A86	O1-C20-C19	-6.43	108.55	113.38
36	A	307	CLA	C4A-NA-C1A	6.43	109.60	106.71
37	O	313	KC1	CHC-C4B-C3B	-6.43	114.25	125.26
36	J	317	CLA	C4A-NA-C1A	6.43	109.60	106.71
36	I	312	CLA	C4A-NA-C1A	6.43	109.59	106.71
35	P	303	A86	O1-C20-C21	-6.42	107.36	115.06
37	B	310	KC1	CAB-C3B-C2B	-6.42	107.44	128.60
37	Q	313	KC1	CHC-C4B-C3B	-6.42	114.28	125.26
36	a	820	CLA	C4A-NA-C1A	6.41	109.59	106.71
35	R	302	A86	C25-C26-C27	-6.41	118.16	127.31
37	T	315	KC1	CHC-C4B-C3B	-6.41	114.29	125.26
36	b	833	CLA	C4A-NA-C1A	6.41	109.59	106.71
37	Q	311	KC1	CHC-C4B-C3B	-6.41	114.30	125.26
35	L	319	A86	O1-C20-C21	-6.41	107.38	115.06
36	N	308	CLA	CMC-C2C-C1C	6.40	134.79	125.04
36	C	207	CLA	C2C-C1C-NC	6.40	115.97	109.97
36	A	309	CLA	C4A-NA-C1A	6.40	109.58	106.71
37	P	315	KC1	CHC-C4B-C3B	-6.39	114.32	125.26
35	O	302	A86	O1-C20-C21	-6.39	107.40	115.06
37	O	315	KC1	CHC-C4B-C3B	-6.39	114.33	125.26
36	L	308	CLA	CHC-C1C-NC	-6.38	114.52	124.20
35	N	320	A86	C25-C26-C27	-6.38	118.20	127.31
36	N	317	CLA	C4A-NA-C1A	6.38	109.58	106.71
35	T	305	A86	O2-C18-C17	-6.38	97.12	109.80
34	E	301	DD6	C21-C20-C19	6.38	121.46	114.28
35	Q	304	A86	C17-C16-C15	6.38	115.67	109.16
36	b	841	CLA	CMC-C2C-C1C	-6.38	115.33	125.04
36	b	837	CLA	C4A-NA-C1A	6.37	109.57	106.71
36	a	825	CLA	C4A-NA-C1A	6.37	109.57	106.71
35	T	302	A86	C17-C16-C15	6.36	115.66	109.16
34	K	305	DD6	C21-C20-C19	6.36	121.44	114.28
36	b	822	CLA	C4A-NA-C1A	6.36	109.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	Q	304	A86	C25-C26-C27	-6.35	118.24	127.31
36	L	308	CLA	C4D-C3D-CAD	6.35	115.58	108.10
37	G	317	KC1	C1A-C2A-C3A	-6.35	102.07	107.11
37	H	313	KC1	CHB-C1B-C2B	-6.35	112.16	125.48
36	R	322	CLA	C4A-NA-C1A	6.35	109.56	106.71
34	E	306	DD6	C21-C20-C19	6.35	121.42	114.28
36	b	840	CLA	C4A-NA-C1A	6.35	109.56	106.71
34	O	304	DD6	C21-C20-C19	6.35	121.42	114.28
36	j	102	CLA	C1D-ND-C4D	-6.35	101.83	106.33
36	I	313	CLA	C4A-NA-C1A	6.34	109.56	106.71
36	l	201	CLA	C4A-NA-C1A	6.34	109.56	106.71
37	G	308	KC1	C1A-NA-C4A	-6.34	103.86	106.71
37	U	312	KC1	CHC-C4B-C3B	-6.34	114.42	125.26
35	M	304	A86	C4-C5-C6	-6.33	118.27	127.31
37	C	213	KC1	CMD-C2D-C3D	6.33	136.52	124.68
36	j	101	CLA	C4A-NA-C1A	6.33	109.55	106.71
36	B	309	CLA	CMD-C2D-C1D	6.33	135.86	124.71
37	E	309	KC1	CHC-C4B-C3B	-6.33	114.44	125.26
36	W	210	CLA	CMB-C2B-C1B	-6.33	118.74	128.46
36	S	319	CLA	C4A-NA-C1A	6.32	109.55	106.71
37	M	318	KC1	CHC-C1C-NC	-6.32	114.25	124.20
37	T	315	KC1	C2C-C1C-NC	6.32	117.47	110.57
34	H	303	DD6	C21-C20-C19	6.32	121.39	114.28
37	C	213	KC1	C2C-C1C-NC	6.32	117.47	110.57
37	F	315	KC1	C2A-C3A-C4A	6.31	111.17	106.49
37	M	317	KC1	CAC-C3C-C4C	6.31	132.99	124.81
36	b	834	CLA	C4A-NA-C1A	6.30	109.54	106.71
36	S	314	CLA	C4A-NA-C1A	6.30	109.54	106.71
35	D	302	A86	O1-C20-C19	-6.29	108.65	113.38
36	L	309	CLA	C4A-NA-C1A	6.29	109.53	106.71
36	I	310	CLA	C4A-NA-C1A	6.29	109.53	106.71
36	a	822	CLA	CMD-C2D-C1D	6.29	135.79	124.71
34	R	308	DD6	C9-C10-C11	-6.28	118.34	127.31
34	S	306	DD6	C21-C20-C19	6.28	121.35	114.28
37	W	217	KC1	CAB-C3B-C2B	-6.28	107.92	128.60
35	G	304	A86	O1-C20-C19	6.28	118.10	113.38
35	E	305	A86	O1-C20-C19	-6.27	108.67	113.38
36	W	209	CLA	C4A-NA-C1A	6.27	109.52	106.71
35	U	304	A86	C4-C5-C6	-6.27	118.37	127.31
37	X	311	KC1	CAB-C3B-C2B	-6.26	107.97	128.60
34	A	301	DD6	C3-C2-C1	-6.26	118.37	127.31
36	L	316	CLA	C4A-NA-C1A	6.26	109.52	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	R	311	CLA	C4A-NA-C1A	6.26	109.52	106.71
36	J	316	CLA	C4A-NA-C1A	6.26	109.52	106.71
36	P	319	CLA	CHD-C1D-ND	-6.26	118.70	124.45
35	O	303	A86	C17-C16-C15	6.26	115.55	109.16
35	T	306	A86	C23-C16-C22	-6.25	98.15	107.37
37	S	316	KC1	C2C-C1C-NC	6.25	117.40	110.57
36	E	315	CLA	C2C-C1C-NC	6.25	115.83	109.97
36	b	838	CLA	C4A-NA-C1A	6.25	109.52	106.71
34	D	304	DD6	C21-C20-C19	6.25	121.31	114.28
35	J	305	A86	O1-C20-C19	-6.25	108.69	113.38
36	X	310	CLA	C4A-NA-C1A	6.25	109.51	106.71
36	W	210	CLA	C4A-NA-C1A	6.24	109.51	106.71
37	R	317	KC1	CHC-C1C-NC	-6.24	114.37	124.20
35	U	302	A86	O1-C20-C21	-6.24	107.58	115.06
35	X	302	A86	C17-C16-C15	6.24	115.53	109.16
37	W	213	KC1	CHC-C4B-C3B	-6.24	114.59	125.26
36	N	319	CLA	CAA-C2A-C3A	-6.23	98.69	114.26
36	J	307	CLA	C4A-NA-C1A	6.23	109.51	106.71
36	H	310	CLA	C4A-NA-C1A	6.22	109.50	106.71
36	T	316	CLA	C4A-NA-C1A	6.22	109.50	106.71
35	P	304	A86	C17-C16-C15	6.22	115.51	109.16
35	Q	301	A86	C17-C16-C15	6.22	115.50	109.16
37	B	310	KC1	CHB-C4A-C3A	-6.21	115.27	124.98
36	b	802	CLA	C4A-NA-C1A	6.21	109.50	106.71
35	X	301	A86	C35-C34-C33	-6.20	99.06	109.88
34	C	201	DD6	C21-C20-C19	6.20	121.25	114.28
34	L	305	DD6	C3-C2-C1	-6.19	118.47	127.31
36	a	825	CLA	CMD-C2D-C1D	6.19	135.62	124.71
34	G	303	DD6	C21-C20-C19	6.19	121.24	114.28
36	E	312	CLA	C4A-NA-C1A	6.18	109.49	106.71
36	S	309	CLA	C4A-NA-C1A	6.18	109.49	106.71
34	B	302	DD6	C3-C2-C1	-6.17	118.50	127.31
36	V	314	CLA	C2C-C1C-NC	6.17	115.75	109.97
36	X	315	CLA	C4A-NA-C1A	6.17	109.48	106.71
35	S	305	A86	C21-C20-C19	-6.17	107.34	114.28
36	M	310	CLA	C4A-NA-C1A	6.16	109.48	106.71
37	G	318	KC1	O2D-CGD-CBD	6.16	122.22	111.27
36	H	305	CLA	C4A-NA-C1A	6.16	109.48	106.71
35	L	319	A86	C17-C16-C15	6.16	115.45	109.16
35	P	303	A86	C17-C16-C15	6.15	115.44	109.16
37	F	315	KC1	C2A-C1A-NA	6.15	119.26	109.40
35	O	302	A86	C17-C16-C15	6.14	115.43	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	O	305	A86	C3-C2-C1	-6.14	118.54	127.31
36	K	313	CLA	C4A-NA-C1A	6.14	109.47	106.71
34	E	303	DD6	C21-C20-C19	6.14	121.19	114.28
35	H	304	A86	O1-C20-C19	-6.14	108.77	113.38
35	W	202	A86	C23-C16-C17	-6.13	98.32	108.98
36	C	205	CLA	C4A-NA-C1A	6.13	109.46	106.71
36	b	836	CLA	C2C-C1C-NC	6.12	115.71	109.97
35	M	305	A86	C17-C16-C15	6.12	115.41	109.16
35	U	301	A86	C8-C6-C5	6.12	128.33	118.94
36	M	306	CLA	C4A-NA-C1A	6.12	109.46	106.71
35	K	306	A86	O3-C36-C37	-6.12	98.50	109.39
36	U	306	CLA	C3D-C2D-C1D	-6.11	97.49	105.83
34	M	303	DD6	C21-C20-C19	6.11	121.16	114.28
36	R	321	CLA	CMB-C2B-C1B	-6.11	119.07	128.46
35	X	302	A86	O1-C20-C21	-6.11	107.73	115.06
36	P	319	CLA	C1D-ND-C4D	-6.11	101.99	106.33
37	M	313	KC1	C2C-C1C-NC	6.10	117.23	110.57
36	D	311	CLA	C4A-NA-C1A	6.10	109.45	106.71
37	H	313	KC1	C2C-C1C-NC	6.10	117.23	110.57
36	a	806	CLA	CMD-C2D-C1D	6.09	135.45	124.71
37	L	315	KC1	CBD-CHA-C1A	6.09	140.24	128.88
35	F	306	A86	O1-C20-C19	-6.09	108.81	113.38
37	E	309	KC1	CHB-C4A-C3A	-6.09	115.47	124.98
37	M	317	KC1	C2C-C1C-NC	6.08	117.22	110.57
35	T	305	A86	C35-C34-C33	-6.08	99.26	109.88
37	W	213	KC1	CAB-C3B-C2B	-6.08	108.56	128.60
37	U	312	KC1	C4B-C3B-C2B	-6.08	101.76	106.75
36	V	307	CLA	C4A-NA-C1A	6.08	109.44	106.71
35	A	302	A86	O1-C20-C21	-6.08	107.77	115.06
34	I	303	DD6	C21-C20-C19	6.08	121.12	114.28
34	E	304	DD6	C21-C20-C19	6.08	121.11	114.28
34	J	304	DD6	C21-C20-C19	6.07	121.11	114.28
36	a	823	CLA	CMD-C2D-C1D	6.07	135.40	124.71
37	U	312	KC1	C2A-C3A-C4A	6.06	110.98	106.49
36	b	801	CLA	C4A-NA-C1A	6.04	109.42	106.71
36	f	804	CLA	C2C-C1C-NC	6.04	115.63	109.97
37	M	313	KC1	CHC-C4B-C3B	-6.04	114.94	125.26
36	D	309	CLA	C2C-C1C-NC	6.03	115.62	109.97
37	S	316	KC1	CHB-C4A-NA	6.03	133.70	124.20
36	a	822	CLA	C4A-NA-C1A	6.02	109.41	106.71
37	C	213	KC1	C1A-C2A-C3A	-6.02	102.33	107.11
34	R	307	DD6	C21-C20-C19	6.02	121.05	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	213	KC1	CHC-C4B-C3B	-6.02	114.96	125.26
36	b	828	CLA	C4A-NA-C1A	6.02	109.41	106.71
37	P	317	KC1	CHC-C1C-NC	-6.02	114.73	124.20
36	L	310	CLA	C4A-NA-C1A	6.01	109.41	106.71
36	K	309	CLA	C4A-NA-C1A	6.01	109.41	106.71
37	A	312	KC1	C4B-CHC-C1C	-6.01	113.09	126.06
35	H	301	A86	C17-C16-C15	6.01	115.29	109.16
37	T	315	KC1	CHB-C4A-C3A	-6.01	115.59	124.98
36	F	317	CLA	CHD-C1D-ND	-6.00	118.94	124.45
37	M	317	KC1	CHC-C4B-C3B	-6.00	114.99	125.26
35	R	301	A86	C25-C26-C27	-6.00	118.75	127.31
35	N	306	A86	C17-C16-C15	5.99	115.27	109.16
36	M	312	CLA	C4A-NA-C1A	5.99	109.40	106.71
37	N	314	KC1	CHC-C1C-NC	-5.99	114.78	124.20
36	b	824	CLA	C2C-C1C-NC	5.98	115.57	109.97
34	W	204	DD6	C21-C20-C19	5.98	121.00	114.28
36	G	307	CLA	C1D-ND-C4D	-5.97	102.09	106.33
35	J	302	A86	O1-C20-C19	-5.97	108.90	113.38
36	N	315	CLA	CMB-C2B-C1B	-5.96	119.30	128.46
36	D	306	CLA	C4A-NA-C1A	5.96	109.39	106.71
37	G	317	KC1	CAB-C3B-C2B	-5.96	108.98	128.60
36	T	313	CLA	C4A-NA-C1A	5.95	109.38	106.71
35	V	301	A86	O1-C20-C19	-5.95	108.91	113.38
34	D	303	DD6	C24-C1-C2	-5.95	109.82	118.94
36	a	835	CLA	C4A-NA-C1A	5.95	109.38	106.71
37	O	315	KC1	CHC-C1C-NC	-5.94	114.85	124.20
36	H	318	CLA	C4A-NA-C1A	5.94	109.38	106.71
34	A	304	DD6	C21-C20-C19	5.94	120.96	114.28
37	P	315	KC1	CHC-C1C-NC	-5.94	114.85	124.20
36	X	308	CLA	CAA-C2A-C1A	-5.94	92.53	111.97
35	O	301	A86	O1-C20-C19	-5.93	108.92	113.38
37	M	317	KC1	CHC-C1C-NC	-5.93	114.86	124.20
35	C	202	A86	O1-C20-C21	-5.93	107.95	115.06
36	E	313	CLA	C4A-NA-C1A	5.93	109.37	106.71
36	S	311	CLA	C4A-NA-C1A	5.93	109.37	106.71
35	V	302	A86	C35-C34-C33	-5.92	99.54	109.88
35	X	301	A86	C40-C32-C31	-5.92	105.17	110.47
37	Q	311	KC1	CHC-C1C-NC	-5.92	114.88	124.20
37	Q	313	KC1	CHC-C1C-NC	-5.92	114.88	124.20
37	V	312	KC1	CHC-C4B-C3B	-5.92	115.14	125.26
36	a	801	CLA	C4A-NA-C1A	5.91	109.36	106.71
36	J	311	CLA	C4A-NA-C1A	5.91	109.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	R	306	A86	C17-C16-C15	5.91	115.19	109.16
36	A	305	CLA	C4A-NA-C1A	5.91	109.36	106.71
37	D	314	KC1	CAB-C3B-C2B	-5.90	109.15	128.60
37	E	309	KC1	CHC-C1C-NC	-5.90	114.91	124.20
36	R	321	CLA	C4A-NA-C1A	5.90	109.36	106.71
36	Q	310	CLA	CAA-C2A-C3A	5.89	128.92	112.78
37	O	313	KC1	CHC-C1C-NC	-5.89	114.93	124.20
36	b	836	CLA	C2D-C1D-ND	5.88	114.43	110.10
36	b	812	CLA	C4A-NA-C1A	5.87	109.35	106.71
36	a	824	CLA	CAC-C3C-C2C	5.87	137.57	127.53
37	G	318	KC1	CHB-C4A-C3A	-5.87	115.81	124.98
37	M	313	KC1	CHB-C4A-C3A	-5.87	115.81	124.98
37	L	315	KC1	C3C-C4C-NC	5.86	115.40	109.88
36	F	313	CLA	C4A-NA-C1A	5.86	109.34	106.71
36	a	802	CLA	CMD-C2D-C1D	5.86	135.05	124.71
35	R	303	A86	O3-C36-C37	-5.86	98.96	109.39
34	A	303	DD6	C21-C20-C19	5.86	120.87	114.28
34	W	205	DD6	C21-C20-C19	5.86	120.87	114.28
36	b	818	CLA	C4A-NA-C1A	5.86	109.34	106.71
37	M	313	KC1	CHC-C1C-NC	-5.86	114.98	124.20
36	C	207	CLA	C2D-C1D-ND	5.86	114.42	110.10
37	T	310	KC1	CMD-C2D-C3D	5.85	135.63	124.68
36	l	205	CLA	O2D-CGD-CBD	5.85	121.67	111.27
35	K	303	A86	C17-C16-C15	5.85	115.13	109.16
36	N	319	CLA	CHD-C4C-C3C	5.85	133.44	124.84
36	l	204	CLA	O2D-CGD-CBD	5.84	121.65	111.27
36	W	216	CLA	C1B-CHB-C4A	-5.84	118.55	130.12
37	T	310	KC1	CHC-C1C-NC	-5.84	115.01	124.20
35	F	307	A86	O4-C38-C39	5.83	121.82	111.09
36	F	317	CLA	C3D-C2D-C1D	-5.83	97.87	105.83
35	V	301	A86	C4-C5-C6	-5.83	118.99	127.31
34	R	307	DD6	C3-C2-C1	-5.83	118.99	127.31
37	F	308	KC1	CAA-C2A-C1A	5.83	151.53	124.75
35	W	203	A86	C17-C16-C15	5.83	115.11	109.16
37	W	213	KC1	CHC-C1C-NC	-5.82	115.04	124.20
37	D	314	KC1	C4B-CHC-C1C	-5.81	113.53	126.06
36	X	313	CLA	CMB-C2B-C3B	5.81	135.54	124.68
35	K	301	A86	C4-C5-C6	-5.80	119.03	127.31
35	R	303	A86	C34-O4-C38	5.80	128.70	117.90
37	L	315	KC1	CAC-C3C-C4C	5.80	132.33	124.81
36	X	308	CLA	C1B-CHB-C4A	-5.79	118.65	130.12
37	V	312	KC1	C2C-C1C-NC	5.79	116.89	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	X	302	A86	C4-C5-C6	-5.79	119.05	127.31
37	S	316	KC1	CHC-C4B-C3B	-5.79	115.36	125.26
35	O	319	A86	C17-C16-C15	5.78	115.06	109.16
36	b	831	CLA	C4A-NA-C1A	5.78	109.31	106.71
34	H	302	DD6	C21-C20-C19	5.78	120.78	114.28
37	H	313	KC1	C4B-CHC-C1C	-5.77	113.60	126.06
37	L	315	KC1	C2A-C3A-C4A	5.77	110.77	106.49
35	U	301	A86	C25-C24-C1	-5.77	110.20	126.42
36	b	806	CLA	CMB-C2B-C1B	-5.77	119.60	128.46
36	V	314	CLA	C2D-C1D-ND	5.76	114.35	110.10
35	O	319	A86	C25-C26-C27	-5.76	119.09	127.31
36	C	207	CLA	C4A-NA-C1A	5.75	109.29	106.71
36	O	316	CLA	C1C-C2C-C3C	-5.75	100.91	106.96
36	b	817	CLA	O2D-CGD-CBD	5.74	121.47	111.27
36	Q	310	CLA	C1-C2-C3	5.74	135.97	126.04
37	N	314	KC1	C4B-CHC-C1C	-5.74	113.68	126.06
36	f	803	CLA	C3D-C2D-C1D	-5.73	98.01	105.83
35	T	303	A86	C25-C26-C27	-5.73	119.14	127.31
35	R	309	A86	C17-C16-C15	5.73	115.00	109.16
36	f	803	CLA	CHD-C1D-ND	-5.73	119.19	124.45
36	N	313	CLA	CMB-C2B-C1B	-5.72	119.67	128.46
37	C	213	KC1	CHC-C1C-NC	-5.71	115.21	124.20
36	J	316	CLA	CAC-C3C-C4C	5.71	132.22	124.81
37	T	310	KC1	C3A-C4A-NA	5.71	116.81	110.57
34	D	301	DD6	C3-C2-C1	-5.71	119.16	127.31
36	a	830	CLA	CHB-C4A-NA	5.71	132.41	124.51
36	G	319	CLA	C3D-C2D-C1D	-5.70	98.05	105.83
34	E	306	DD6	C14-C13-C11	-5.70	116.69	125.53
37	T	315	KC1	CAC-C3C-C4C	5.70	132.20	124.81
36	S	319	CLA	CBA-CAA-C2A	-5.69	97.06	113.86
37	R	317	KC1	CHC-C4B-C3B	-5.69	115.53	125.26
36	N	310	CLA	CMB-C2B-C3B	5.69	135.32	124.68
36	V	314	CLA	C3D-C2D-C1D	-5.69	98.07	105.83
35	J	302	A86	C4-C5-C6	-5.68	119.20	127.31
41	F	318	LHG	O4-P-O5	5.68	132.92	110.68
37	G	317	KC1	CHC-C1C-NC	-5.68	115.26	124.20
35	G	306	A86	C25-C26-C27	-5.68	119.21	127.31
37	W	217	KC1	CHB-C4A-NA	5.67	133.14	124.20
37	X	311	KC1	CHB-C4A-NA	5.67	133.14	124.20
37	G	308	KC1	CHC-C1C-NC	-5.67	115.27	124.20
35	A	302	A86	C36-C31-C32	5.67	125.32	119.70
37	C	213	KC1	CHD-C4C-NC	5.66	132.80	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	317	KC1	CAC-C3C-C4C	5.66	132.16	124.81
35	U	304	A86	O1-C20-C19	-5.66	109.13	113.38
36	I	310	CLA	CMB-C2B-C1B	-5.66	119.76	128.46
37	R	317	KC1	CHB-C1B-C2B	-5.66	113.61	125.48
36	b	836	CLA	C3D-C2D-C1D	-5.66	98.11	105.83
36	a	822	CLA	O2D-CGD-CBD	5.65	121.32	111.27
37	L	317	KC1	C2A-C3A-C4A	5.65	110.68	106.49
37	L	317	KC1	CHB-C4A-NA	5.65	133.10	124.20
36	N	319	CLA	CHA-C4D-ND	5.64	144.31	132.50
36	Q	310	CLA	C5-C3-C2	5.64	132.53	121.12
35	I	302	A86	C17-C16-C15	5.64	114.91	109.16
35	H	304	A86	C17-C16-C15	5.63	114.91	109.16
37	J	314	KC1	CHC-C1C-NC	-5.63	115.33	124.20
34	R	308	DD6	C4-C5-C6	-5.63	119.27	127.31
37	G	308	KC1	CHB-C4A-C3A	-5.63	116.18	124.98
37	P	317	KC1	CBD-CHA-C1A	5.63	139.37	128.88
37	M	313	KC1	CBD-CHA-C1A	5.63	139.37	128.88
35	h	204	A86	C3-C2-C1	-5.62	119.28	127.31
37	T	315	KC1	CHC-C1C-NC	-5.62	115.35	124.20
36	A	306	CLA	CHD-C1D-ND	-5.62	119.29	124.45
36	b	827	CLA	C4A-NA-C1A	5.62	109.23	106.71
36	a	824	CLA	CAC-C3C-C4C	-5.61	117.53	124.81
36	W	215	CLA	C4A-NA-C1A	5.61	109.23	106.71
36	a	801	CLA	O2D-CGD-CBD	5.61	121.24	111.27
37	Q	313	KC1	C4B-CHC-C1C	-5.61	113.97	126.06
34	E	303	DD6	C14-C13-C11	-5.60	116.83	125.53
37	L	317	KC1	CMD-C2D-C3D	5.60	135.16	124.68
37	F	308	KC1	C4B-CHC-C1C	-5.60	113.99	126.06
37	O	313	KC1	C4B-CHC-C1C	-5.60	113.99	126.06
35	C	204	A86	C8-C6-C5	5.59	127.53	118.94
36	a	816	CLA	O2D-CGD-CBD	5.59	121.21	111.27
37	L	317	KC1	CAA-C2A-C1A	5.59	150.45	124.75
36	B	309	CLA	C4A-NA-C1A	5.59	109.22	106.71
37	F	315	KC1	C4B-CHC-C1C	-5.59	114.00	126.06
36	G	310	CLA	C4A-NA-C1A	5.59	109.22	106.71
37	Q	311	KC1	C4B-CHC-C1C	-5.59	114.01	126.06
35	I	304	A86	O1-C20-C21	-5.59	108.36	115.06
36	F	316	CLA	C4A-NA-C1A	5.59	109.22	106.71
35	U	301	A86	C4-C5-C6	5.58	135.28	127.31
37	P	315	KC1	C4B-CHC-C1C	-5.58	114.03	126.06
36	b	813	CLA	C4A-NA-C1A	5.58	109.21	106.71
37	O	315	KC1	C4B-CHC-C1C	-5.58	114.03	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	317	CLA	C4A-NA-C1A	5.57	109.21	106.71
35	K	306	A86	O4-C38-C39	5.57	121.34	111.09
37	M	318	KC1	C2A-C1A-CHA	5.57	145.87	127.44
36	G	311	CLA	C4A-NA-C1A	5.57	109.21	106.71
37	H	313	KC1	CHC-C1C-NC	-5.57	115.44	124.20
37	F	308	KC1	C4B-C3B-C2B	-5.56	102.18	106.75
37	M	317	KC1	C1A-NA-C4A	-5.56	104.20	106.71
34	L	305	DD6	C21-C20-C19	5.56	120.54	114.28
36	Q	310	CLA	CAA-C2A-C1A	5.56	130.18	111.97
36	A	308	CLA	CMB-C2B-C1B	-5.56	119.92	128.46
35	U	301	A86	C7-C6-C5	-5.55	115.14	122.92
37	L	317	KC1	CHC-C1C-NC	-5.55	115.47	124.20
37	J	314	KC1	CAA-C2A-C1A	5.54	150.22	124.75
37	G	318	KC1	CHC-C1C-NC	-5.53	115.49	124.20
35	X	301	A86	C17-C16-C15	5.53	114.80	109.16
35	V	303	A86	O1-C20-C19	-5.52	109.23	113.38
35	M	305	A86	O1-C20-C21	-5.51	108.45	115.06
36	N	317	CLA	CMB-C2B-C1B	-5.51	120.00	128.46
36	j	102	CLA	O2D-CGD-CBD	5.51	121.05	111.27
36	l	202	CLA	C4A-NA-C1A	5.51	109.18	106.71
37	H	313	KC1	CHC-C4B-C3B	-5.50	115.85	125.26
37	E	309	KC1	CBD-CHA-C1A	5.50	139.13	128.88
37	F	308	KC1	O2D-CGD-CBD	5.49	121.03	111.27
36	L	311	CLA	CMB-C2B-C1B	-5.49	120.02	128.46
35	U	302	A86	C17-C16-C15	5.49	114.77	109.16
35	X	303	A86	C4-C5-C6	-5.49	119.47	127.31
36	a	804	CLA	C4A-NA-C1A	5.49	109.17	106.71
35	L	301	A86	O1-C20-C19	-5.49	109.26	113.38
37	B	310	KC1	CAC-C3C-C4C	5.48	131.92	124.81
36	N	310	CLA	C4A-NA-C1A	5.48	109.17	106.71
37	N	314	KC1	CHC-C4B-C3B	-5.48	115.89	125.26
35	X	305	A86	C17-C16-C15	5.47	114.75	109.16
37	B	310	KC1	CHC-C1C-NC	-5.47	115.58	124.20
35	A	316	A86	C4-C5-C6	-5.47	119.50	127.31
34	K	305	DD6	C3-C2-C1	-5.47	119.51	127.31
37	X	311	KC1	C1A-NA-C4A	-5.47	104.25	106.71
35	L	306	A86	C17-C16-C15	5.46	114.74	109.16
35	J	301	A86	O1-C20-C21	-5.46	108.51	115.06
36	C	207	CLA	O2D-CGD-CBD	5.45	120.96	111.27
37	X	311	KC1	C4B-CHC-C1C	-5.45	114.30	126.06
37	W	217	KC1	C4B-CHC-C1C	-5.45	114.31	126.06
36	a	818	CLA	CMB-C2B-C1B	-5.45	120.09	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	W	213	KC1	C4B-CHC-C1C	-5.43	114.34	126.06
35	X	304	A86	C25-C26-C27	-5.43	119.56	127.31
37	A	312	KC1	O2D-CGD-CBD	5.43	120.92	111.27
37	V	312	KC1	C1A-C2A-C3A	-5.43	102.81	107.11
35	V	304	A86	C35-C34-C33	-5.43	100.41	109.88
35	I	304	A86	C34-O4-C38	5.42	128.00	117.90
37	W	217	KC1	C1A-NA-C4A	-5.42	104.27	106.71
35	C	202	A86	C17-C16-C15	5.42	114.69	109.16
37	C	213	KC1	CMD-C2D-C1D	-5.42	120.14	128.46
37	J	314	KC1	C4B-CHC-C1C	-5.42	114.37	126.06
36	W	210	CLA	CMB-C2B-C3B	5.42	134.81	124.68
37	R	317	KC1	CHB-C4A-NA	5.42	132.74	124.20
35	N	305	A86	O4-C38-C39	5.41	121.04	111.09
37	E	309	KC1	C1A-NA-C4A	-5.41	104.27	106.71
36	N	313	CLA	CMB-C2B-C3B	5.40	134.79	124.68
35	S	308	A86	C4-C5-C6	-5.40	119.61	127.31
37	M	313	KC1	C3C-C4C-NC	5.39	114.95	109.88
35	Q	316	A86	O4-C38-C39	5.39	121.01	111.09
37	W	213	KC1	CHD-C4C-NC	5.39	132.38	124.20
37	V	312	KC1	CHB-C4A-C3A	-5.39	116.56	124.98
35	G	304	A86	C35-C34-C33	-5.39	100.47	109.88
35	H	304	A86	C25-C26-C27	-5.39	119.62	127.31
36	G	313	CLA	CMB-C2B-C1B	-5.39	120.18	128.46
36	I	306	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
37	B	310	KC1	C4B-CHC-C1C	-5.39	114.44	126.06
37	G	317	KC1	C4B-CHC-C1C	-5.39	114.44	126.06
37	A	312	KC1	OBD-CAD-CBD	5.39	133.59	125.89
37	W	213	KC1	CBD-CHA-C1A	5.38	138.92	128.88
36	U	306	CLA	O2D-CGD-CBD	5.38	120.83	111.27
34	S	306	DD6	C3-C2-C1	-5.38	119.63	127.31
36	a	838	CLA	C4A-NA-C1A	5.38	109.12	106.71
36	F	317	CLA	C4A-NA-C1A	5.38	109.12	106.71
37	M	313	KC1	C4B-CHC-C1C	-5.38	114.46	126.06
35	V	302	A86	C23-C16-C22	-5.37	99.44	107.37
35	V	303	A86	C4-C5-C6	-5.37	119.65	127.31
37	E	309	KC1	CAC-C3C-C2C	5.37	136.71	127.53
36	K	310	CLA	C4A-NA-C1A	5.37	109.12	106.71
34	F	303	DD6	C9-C10-C11	-5.37	119.65	127.31
36	R	313	CLA	C4A-NA-C1A	5.37	109.12	106.71
36	D	316	CLA	CAC-C3C-C4C	5.36	131.76	124.81
36	L	311	CLA	C4A-NA-C1A	5.36	109.11	106.71
36	X	313	CLA	CED-O2D-CGD	5.36	128.05	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	W	203	A86	C35-C34-C33	-5.36	100.53	109.88
37	K	314	KC1	CHC-C1C-NC	-5.35	115.77	124.20
36	a	827	CLA	CMB-C2B-C1B	-5.35	120.24	128.46
35	X	314	A86	O1-C20-C19	-5.35	109.36	113.38
37	P	317	KC1	C4B-CHC-C1C	-5.35	114.52	126.06
36	b	818	CLA	CMB-C2B-C1B	-5.35	120.25	128.46
36	a	806	CLA	O2D-CGD-CBD	5.34	120.77	111.27
35	T	303	A86	C34-O4-C38	5.34	127.85	117.90
36	D	315	CLA	CMB-C2B-C1B	-5.34	120.26	128.46
35	U	301	A86	C9-C8-C6	-5.33	111.43	126.42
35	X	301	A86	C4-C5-C6	-5.33	119.70	127.31
35	C	203	A86	O1-C20-C19	-5.33	109.38	113.38
35	X	301	A86	O1-C20-C21	-5.33	108.67	115.06
37	H	313	KC1	C1B-CHB-C4A	-5.33	114.56	126.06
35	T	302	A86	C35-C34-C33	-5.33	100.58	109.88
37	D	314	KC1	CHC-C1C-NC	-5.33	115.82	124.20
36	X	313	CLA	C4D-CHA-C1A	-5.32	114.77	121.25
36	K	307	CLA	C2D-C1D-ND	5.32	114.03	110.10
37	M	313	KC1	O2D-CGD-CBD	5.32	120.72	111.27
37	T	310	KC1	CHB-C1B-C2B	-5.32	114.33	125.48
37	M	313	KC1	CHB-C1B-C2B	-5.31	114.33	125.48
35	M	302	A86	C3-C2-C1	-5.31	119.73	127.31
37	P	317	KC1	CHB-C4A-C3A	-5.31	116.68	124.98
36	b	836	CLA	C3B-C4B-NB	5.31	116.07	109.21
35	U	304	A86	C3-C2-C1	-5.31	119.74	127.31
36	D	309	CLA	C3D-C2D-C1D	-5.30	98.59	105.83
37	F	308	KC1	CHB-C1B-C2B	-5.30	114.36	125.48
37	B	310	KC1	CAA-C2A-C1A	5.30	149.10	124.75
36	L	308	CLA	O2D-CGD-CBD	5.29	120.68	111.27
36	O	316	CLA	O2D-CGD-CBD	5.29	120.67	111.27
37	G	308	KC1	CAA-C2A-C1A	5.29	149.07	124.75
36	E	315	CLA	O2D-CGD-CBD	5.29	120.66	111.27
35	N	306	A86	C25-C26-C27	-5.29	119.77	127.31
35	U	302	A86	C4-C5-C6	-5.29	119.77	127.31
36	b	812	CLA	CMB-C2B-C1B	-5.28	120.34	128.46
37	T	310	KC1	O2D-CGD-CBD	5.28	120.65	111.27
36	N	310	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
36	E	310	CLA	CMB-C2B-C1B	-5.27	120.36	128.46
37	G	317	KC1	CHB-C4A-NA	5.27	132.51	124.20
37	S	316	KC1	C4B-CHC-C1C	-5.27	114.69	126.06
35	W	203	A86	C4-C5-C6	-5.27	119.79	127.31
36	I	306	CLA	O2D-CGD-CBD	5.27	120.63	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	M	301	A86	O1-C20-C19	-5.27	109.43	113.38
35	N	320	A86	C3-C2-C1	-5.26	119.80	127.31
37	A	312	KC1	CAC-C3C-C4C	5.26	131.64	124.81
37	F	308	KC1	CHC-C1C-NC	-5.26	115.92	124.20
37	F	315	KC1	CHC-C1C-NC	-5.26	115.92	124.20
37	S	316	KC1	CHB-C1B-C2B	-5.26	114.44	125.48
34	B	304	DD6	C4-C5-C6	-5.26	119.80	127.31
37	M	317	KC1	C3C-C4C-NC	5.26	114.83	109.88
35	L	306	A86	C4-C5-C6	-5.25	119.81	127.31
36	a	830	CLA	O2D-CGD-CBD	5.25	120.61	111.27
35	N	303	A86	C3-C4-C5	-5.25	112.71	123.47
35	S	303	A86	C3-C4-C5	-5.25	112.72	123.47
35	C	202	A86	C34-O4-C38	5.25	127.68	117.90
36	I	311	CLA	CMB-C2B-C1B	-5.24	120.40	128.46
35	R	302	A86	C35-C34-C33	-5.24	100.73	109.88
36	S	312	CLA	CMB-C2B-C1B	-5.24	120.41	128.46
37	P	315	KC1	C3C-C4C-NC	5.24	114.81	109.88
36	b	836	CLA	O2D-CGD-CBD	5.24	120.58	111.27
37	K	314	KC1	C4B-CHC-C1C	-5.24	114.75	126.06
36	K	307	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
34	B	304	DD6	C9-C10-C11	-5.24	119.83	127.31
37	A	312	KC1	CHC-C1C-NC	-5.24	115.95	124.20
36	T	311	CLA	CAC-C3C-C2C	5.24	136.49	127.53
36	j	102	CLA	C2D-C1D-ND	5.24	113.96	110.10
36	K	310	CLA	O2D-CGD-CBD	5.23	120.57	111.27
35	R	309	A86	C4-C5-C6	-5.23	119.84	127.31
37	F	315	KC1	O2D-CGD-CBD	5.23	120.57	111.27
35	W	202	A86	C25-C26-C27	-5.23	119.84	127.31
35	U	303	A86	C3-C2-C1	-5.23	119.84	127.31
35	Q	304	A86	O1-C20-C21	-5.23	108.79	115.06
36	O	316	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
37	C	213	KC1	C4B-CHC-C1C	-5.22	114.79	126.06
37	U	312	KC1	CHC-C1C-NC	-5.22	115.98	124.20
37	L	315	KC1	O2D-CGD-CBD	5.22	120.55	111.27
37	S	316	KC1	CHC-C1C-NC	-5.22	115.98	124.20
35	P	307	A86	O1-C20-C19	-5.22	109.46	113.38
36	a	824	CLA	CMB-C2B-C1B	-5.22	120.44	128.46
35	N	320	A86	O1-C20-C21	-5.22	108.81	115.06
37	X	311	KC1	CHC-C1C-NC	-5.22	115.99	124.20
36	L	313	CLA	CMB-C2B-C1B	-5.21	120.45	128.46
37	R	317	KC1	C1B-CHB-C4A	-5.21	114.81	126.06
36	V	311	CLA	CMB-C2B-C1B	-5.21	120.45	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	T	315	KC1	C1B-CHB-C4A	-5.21	114.81	126.06
37	O	313	KC1	C3C-C4C-NC	5.21	114.78	109.88
37	N	314	KC1	C1A-C2A-C3A	-5.21	102.98	107.11
36	a	825	CLA	O2D-CGD-CBD	5.21	120.52	111.27
35	Q	304	A86	C3-C2-C1	-5.21	119.88	127.31
37	Q	313	KC1	C3C-C4C-NC	5.21	114.78	109.88
35	J	306	A86	O1-C20-C19	-5.21	109.47	113.38
36	a	823	CLA	O2D-CGD-CBD	5.21	120.52	111.27
35	P	307	A86	C3-C2-C1	-5.20	119.88	127.31
37	W	217	KC1	CHC-C1C-NC	-5.20	116.01	124.20
37	Q	311	KC1	C3C-C4C-NC	5.20	114.78	109.88
36	X	310	CLA	O2D-CGD-O1D	-5.20	113.67	123.84
35	V	303	A86	C34-O4-C38	5.20	127.58	117.90
35	A	302	A86	C17-C16-C15	5.19	114.46	109.16
35	T	306	A86	O4-C38-C39	5.19	120.64	111.09
35	W	203	A86	C25-C26-C27	-5.19	119.91	127.31
36	S	312	CLA	C4A-NA-C1A	5.18	109.04	106.71
35	S	305	A86	C25-C26-C27	-5.18	119.91	127.31
36	b	816	CLA	O2D-CGD-CBD	5.18	120.48	111.27
37	U	312	KC1	CAB-C3B-C4B	5.18	137.41	124.90
36	D	309	CLA	C2D-C1D-ND	5.18	113.92	110.10
37	O	315	KC1	C3C-C4C-NC	5.17	114.75	109.88
35	G	305	A86	O1-C20-C21	-5.17	108.86	115.06
36	R	312	CLA	O2D-CGD-CBD	5.17	120.46	111.27
37	T	310	KC1	C1A-NA-C4A	5.17	109.03	106.71
35	X	304	A86	C23-C16-C17	-5.17	100.00	108.98
36	C	207	CLA	C3B-C4B-NB	5.17	115.89	109.21
37	L	317	KC1	C4B-CHC-C1C	-5.17	114.90	126.06
35	C	204	A86	C-C1-C24	5.17	126.22	118.08
35	C	203	A86	C3-C2-C1	-5.16	119.94	127.31
36	O	316	CLA	C2D-C1D-ND	5.16	113.91	110.10
36	a	820	CLA	CMB-C2B-C1B	-5.16	120.54	128.46
36	O	316	CLA	C2C-C1C-NC	5.15	114.80	109.97
35	U	302	A86	C25-C26-C27	-5.15	119.96	127.31
35	X	301	A86	C23-C16-C17	-5.15	100.03	108.98
35	R	301	A86	C17-C16-C15	5.15	114.42	109.16
35	K	303	A86	C35-C34-C33	-5.15	100.89	109.88
36	I	307	CLA	CMB-C2B-C1B	-5.15	120.56	128.46
34	Q	302	DD6	C3-C2-C1	-5.14	119.97	127.31
36	H	314	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
37	V	312	KC1	CHC-C1C-NC	-5.14	116.11	124.20
36	G	307	CLA	C3B-C4B-NB	5.14	115.85	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	301	DD6	C21-C20-C19	5.13	120.05	114.28
37	E	309	KC1	CAA-C2A-C1A	5.13	148.32	124.75
35	B	301	A86	O1-C20-C19	-5.12	109.53	113.38
36	b	805	CLA	C4A-NA-C1A	5.12	109.01	106.71
35	B	303	A86	O4-C38-C39	5.12	120.51	111.09
36	K	307	CLA	O2D-CGD-CBD	5.12	120.36	111.27
36	K	313	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
35	R	304	A86	C17-C16-C15	5.11	114.38	109.16
36	V	313	CLA	C4A-NA-C1A	5.11	109.00	106.71
35	X	305	A86	C35-C34-C33	-5.11	100.96	109.88
34	B	302	DD6	C9-C10-C11	-5.11	120.02	127.31
36	S	310	CLA	C1-C2-C3	5.11	134.87	126.04
36	b	831	CLA	CMB-C2B-C1B	-5.11	120.62	128.46
35	L	301	A86	C4-C5-C6	-5.11	120.02	127.31
35	Q	303	A86	C3-C2-C1	-5.11	120.02	127.31
35	U	301	A86	C24-C1-C2	5.10	126.77	118.94
37	K	314	KC1	C1B-CHB-C4A	-5.10	115.06	126.06
36	Q	310	CLA	C4A-NA-C1A	5.10	109.00	106.71
37	M	318	KC1	C3D-CAD-CBD	5.10	114.31	107.61
37	R	317	KC1	C4B-CHC-C1C	-5.09	115.07	126.06
36	R	310	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
37	B	310	KC1	C2A-C3A-C4A	5.09	110.26	106.49
36	b	801	CLA	CMB-C2B-C1B	-5.09	120.65	128.46
36	b	836	CLA	C3C-C4C-NC	5.08	116.27	110.57
35	V	304	A86	C14-C15-C16	-5.08	99.29	118.75
36	l	205	CLA	C3B-C4B-NB	5.08	115.78	109.21
36	a	819	CLA	CAC-C3C-C2C	5.08	136.22	127.53
34	Q	302	DD6	C9-C10-C11	-5.08	120.06	127.31
36	K	315	CLA	CMB-C2B-C1B	-5.07	120.66	128.46
37	T	315	KC1	CHB-C4A-NA	5.07	132.20	124.20
34	W	204	DD6	C3-C2-C1	-5.07	120.07	127.31
36	P	314	CLA	C4A-NA-C1A	5.07	108.99	106.71
36	I	306	CLA	C3B-C4B-NB	5.07	115.77	109.21
37	X	311	KC1	CAA-C2A-C1A	5.07	148.06	124.75
35	B	303	A86	C4-C5-C6	-5.07	120.07	127.31
37	T	315	KC1	C4B-CHC-C1C	-5.07	115.12	126.06
37	W	217	KC1	CAA-C2A-C1A	5.07	148.05	124.75
36	J	307	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
36	U	306	CLA	C1D-ND-C4D	-5.07	102.74	106.33
36	X	307	CLA	CMB-C2B-C1B	-5.06	120.68	128.46
37	P	317	KC1	CAB-C3B-C2B	-5.06	111.92	128.60
36	G	315	CLA	C4A-NA-C1A	5.06	108.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	P	305	DD6	C9-C10-C11	-5.06	120.09	127.31
35	U	303	A86	C25-C26-C27	-5.06	120.09	127.31
35	G	304	A86	C20-C19-C18	5.06	122.75	112.75
37	M	317	KC1	CHB-C4A-C3A	-5.05	117.08	124.98
35	X	301	A86	C3-C2-C1	-5.05	120.10	127.31
35	R	304	A86	C21-C20-C19	5.05	119.96	114.28
36	X	310	CLA	CAA-C2A-C3A	-5.05	104.32	116.10
35	I	301	A86	C4-C5-C6	-5.04	120.11	127.31
35	X	314	A86	C4-C5-C6	-5.04	120.11	127.31
34	W	205	DD6	C3-C2-C1	-5.04	120.12	127.31
36	H	310	CLA	O2D-CGD-O1D	-5.04	113.99	123.84
37	M	313	KC1	C1B-CHB-C4A	-5.03	115.21	126.06
36	D	313	CLA	CMB-C2B-C1B	-5.02	120.75	128.46
37	M	318	KC1	O2D-CGD-CBD	5.02	120.18	111.27
36	O	312	CLA	C4A-NA-C1A	5.01	108.96	106.71
36	E	315	CLA	C3B-C4B-NB	5.01	115.69	109.21
37	U	312	KC1	C4B-CHC-C1C	-5.01	115.26	126.06
35	X	302	A86	O4-C38-C39	5.01	120.30	111.09
35	I	301	A86	C25-C26-C27	-5.00	120.17	127.31
37	T	315	KC1	CHB-C1B-C2B	-5.00	114.99	125.48
36	N	310	CLA	C2D-C1D-ND	-5.00	106.42	110.10
36	G	319	CLA	C3C-C4C-NC	5.00	116.18	110.57
36	a	812	CLA	CMB-C2B-C1B	-4.99	120.79	128.46
35	X	302	A86	C23-C16-C22	-4.99	100.01	107.37
36	i	102	CLA	CMB-C2B-C1B	-4.99	120.80	128.46
35	h	202	A86	C4-C5-C6	-4.99	120.19	127.31
37	D	314	KC1	C1B-CHB-C4A	-4.99	115.30	126.06
37	S	316	KC1	C2B-C1B-NB	4.98	113.77	110.10
37	E	309	KC1	CHB-C4A-NA	4.97	132.04	124.20
35	B	301	A86	C4-C5-C6	-4.97	120.22	127.31
34	A	301	DD6	C9-C10-C11	-4.97	120.22	127.31
37	G	318	KC1	C4B-CHC-C1C	-4.97	115.34	126.06
36	Q	314	CLA	C4A-NA-C1A	4.97	108.94	106.71
34	P	305	DD6	C4-C5-C6	-4.96	120.23	127.31
35	W	203	A86	C3-C2-C1	-4.96	120.23	127.31
36	a	828	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
37	R	317	KC1	CAA-C2A-C1A	4.96	147.55	124.75
34	R	308	DD6	C21-C20-C19	4.96	119.86	114.28
36	V	314	CLA	O2D-CGD-CBD	4.96	120.08	111.27
37	B	310	KC1	CHB-C4A-NA	4.96	132.01	124.20
36	E	311	CLA	CMB-C2B-C1B	-4.96	120.85	128.46
35	F	305	A86	C23-C16-C17	-4.96	100.37	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	f	803	CLA	C3C-C4C-NC	4.95	116.13	110.57
35	S	308	A86	O1-C20-C19	-4.95	109.66	113.38
37	G	308	KC1	C4B-CHC-C1C	-4.95	115.38	126.06
35	T	301	A86	O1-C20-C19	-4.95	109.66	113.38
37	R	317	KC1	O2D-CGD-CBD	4.95	120.06	111.27
35	H	304	A86	C4-C5-C6	-4.95	120.25	127.31
36	K	307	CLA	C3B-C4B-NB	4.95	115.61	109.21
35	M	301	A86	O4-C34-C33	4.95	119.91	107.59
34	Q	302	DD6	C4-C5-C6	-4.94	120.25	127.31
35	R	305	A86	C3-C2-C1	-4.94	120.26	127.31
36	D	309	CLA	O2D-CGD-CBD	4.94	120.05	111.27
37	P	315	KC1	O2D-CGD-CBD	4.94	120.04	111.27
36	Q	310	CLA	O1A-CGA-CBA	4.94	142.99	123.73
35	K	303	A86	O1-C20-C21	-4.94	109.14	115.06
36	J	312	CLA	CMB-C2B-C1B	-4.93	120.88	128.46
37	X	311	KC1	CHD-C4C-NC	4.93	131.69	124.20
37	L	315	KC1	C4B-CHC-C1C	-4.93	115.42	126.06
37	E	309	KC1	O2D-CGD-CBD	4.93	120.03	111.27
36	A	306	CLA	C3C-C4C-NC	4.93	116.10	110.57
36	I	310	CLA	CMB-C2B-C3B	4.93	133.90	124.68
34	B	304	DD6	C21-C20-C19	4.93	119.82	114.28
35	J	303	A86	C25-C26-C27	-4.93	120.28	127.31
36	a	848	CLA	O2D-CGD-CBD	4.92	120.02	111.27
36	X	312	CLA	CMB-C2B-C1B	-4.92	120.90	128.46
36	b	806	CLA	CMB-C2B-C3B	4.92	133.89	124.68
35	F	305	A86	C4-C5-C6	-4.91	120.30	127.31
35	X	303	A86	C34-O4-C38	4.91	127.05	117.90
36	f	803	CLA	O2D-CGD-CBD	4.91	119.99	111.27
36	B	308	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
37	E	309	KC1	C4B-CHC-C1C	-4.91	115.47	126.06
37	O	313	KC1	O2D-CGD-CBD	4.91	119.99	111.27
36	A	306	CLA	C3B-C4B-NB	4.91	115.55	109.21
37	P	317	KC1	CAC-C3C-C4C	4.90	131.17	124.81
37	G	308	KC1	CBD-CHA-C1A	4.90	138.02	128.88
34	I	303	DD6	C3-C2-C1	-4.90	120.32	127.31
36	W	212	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
37	W	217	KC1	CHD-C4C-NC	4.90	131.63	124.20
35	R	302	A86	C3-C2-C1	-4.89	120.33	127.31
37	J	314	KC1	CHB-C4A-NA	4.89	131.91	124.20
36	I	308	CLA	O2D-CGD-CBD	4.89	119.96	111.27
35	U	301	A86	O1-C20-C21	-4.89	109.19	115.06
37	Q	313	KC1	O2D-CGD-CBD	4.89	119.95	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	P	317	KC1	O2D-CGD-CBD	4.88	119.95	111.27
36	K	307	CLA	C4C-C3C-C2C	-4.88	99.78	106.90
37	Q	311	KC1	O2D-CGD-CBD	4.88	119.94	111.27
36	a	803	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
37	J	314	KC1	CHB-C1B-C2B	-4.88	115.24	125.48
36	F	317	CLA	C3B-C4B-NB	4.88	115.52	109.21
35	M	302	A86	O4-C38-C39	4.88	120.07	111.09
36	Q	314	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
35	L	306	A86	C24-C1-C2	4.88	126.43	118.94
35	G	305	A86	C4-C5-C6	-4.88	120.35	127.31
37	J	314	KC1	C3C-C4C-NC	4.87	114.47	109.88
35	M	305	A86	O4-C38-C39	4.87	120.05	111.09
37	P	317	KC1	C1B-CHB-C4A	-4.87	115.55	126.06
36	a	821	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
37	A	312	KC1	CHB-C4A-NA	4.87	131.87	124.20
35	N	303	A86	C-C1-C24	4.86	125.74	118.08
35	I	302	A86	C35-C34-C33	-4.86	101.39	109.88
35	J	303	A86	C35-C34-C33	-4.86	101.39	109.88
37	O	315	KC1	O2D-CGD-CBD	4.86	119.91	111.27
39	F	321	LMT	C3B-C4B-C5B	-4.86	101.57	110.24
37	V	312	KC1	C1B-CHB-C4A	-4.86	115.58	126.06
36	G	315	CLA	O2D-CGD-CBD	4.86	119.90	111.27
36	H	311	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
35	L	304	A86	C4-C5-C6	-4.85	120.38	127.31
36	F	309	CLA	CMB-C2B-C1B	-4.85	121.00	128.46
37	J	314	KC1	C2A-C3A-C4A	4.85	110.08	106.49
35	M	301	A86	C3-C2-C1	-4.85	120.39	127.31
36	f	804	CLA	O2D-CGD-CBD	4.85	119.89	111.27
36	N	308	CLA	CMB-C2B-C1B	-4.85	121.01	128.46
36	K	310	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
36	N	308	CLA	C4A-NA-C1A	4.85	108.89	106.71
35	S	303	A86	C-C1-C24	4.85	125.71	118.08
36	N	315	CLA	CMB-C2B-C3B	4.84	133.74	124.68
36	U	311	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
37	W	213	KC1	O2D-CGD-CBD	4.84	119.87	111.27
37	J	314	KC1	O2D-CGD-CBD	4.83	119.86	111.27
37	H	313	KC1	CMD-C2D-C3D	4.83	133.72	124.68
35	O	319	A86	O4-C38-C39	4.83	119.98	111.09
37	L	317	KC1	CAC-C3C-C4C	4.83	131.08	124.81
35	K	302	A86	O4-C34-C33	4.83	119.62	107.59
36	E	315	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
36	L	311	CLA	CMB-C2B-C3B	4.83	133.71	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	T	301	A86	C4-C5-C6	-4.83	120.42	127.31
35	N	306	A86	O4-C38-C39	4.83	119.97	111.09
35	N	301	A86	C3-C2-C1	-4.82	120.42	127.31
37	M	317	KC1	C4B-CHC-C1C	-4.82	115.66	126.06
36	H	308	CLA	C4A-NA-C1A	4.82	108.87	106.71
35	E	302	A86	C4-C5-C6	-4.82	120.43	127.31
35	S	301	A86	C3-C2-C1	-4.82	120.43	127.31
35	D	302	A86	C3-C2-C1	-4.82	120.43	127.31
36	b	824	CLA	O2D-CGD-CBD	4.81	119.82	111.27
37	N	314	KC1	C1B-CHB-C4A	-4.81	115.67	126.06
35	H	304	A86	O4-C38-C39	4.81	119.95	111.09
37	H	313	KC1	CHB-C4A-NA	4.81	131.79	124.20
34	A	301	DD6	C21-C20-C19	4.81	119.69	114.28
36	B	309	CLA	O2D-CGD-CBD	4.80	119.81	111.27
35	G	304	A86	O-C13-C11	-4.80	110.53	121.15
35	W	202	A86	C4-C5-C6	-4.80	120.45	127.31
36	X	313	CLA	O2D-CGD-O1D	-4.80	114.45	123.84
37	F	308	KC1	C2A-C3A-C4A	4.80	110.05	106.49
35	R	306	A86	C35-C34-C33	-4.80	101.50	109.88
36	b	818	CLA	CMB-C2B-C3B	4.80	133.66	124.68
34	P	305	DD6	C21-C20-C19	4.80	119.68	114.28
35	P	306	A86	C4-C5-C6	-4.80	120.47	127.31
35	G	306	A86	O4-C38-C39	4.79	119.91	111.09
36	E	314	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
34	M	303	DD6	C3-C2-C1	-4.79	120.48	127.31
37	E	309	KC1	CHD-C4C-NC	4.79	131.47	124.20
34	A	304	DD6	C3-C2-C1	-4.79	120.48	127.31
35	T	303	A86	C35-C34-C33	-4.78	101.53	109.88
35	B	303	A86	O1-C20-C21	-4.78	109.33	115.06
36	b	819	CLA	CMB-C2B-C3B	4.78	133.61	124.68
36	b	826	CLA	C4D-CHA-C1A	-4.77	115.44	121.25
35	G	305	A86	O4-C38-C39	4.77	119.87	111.09
37	L	315	KC1	CHB-C4A-C3A	-4.77	117.52	124.98
37	V	312	KC1	C3C-C4C-NC	4.77	114.37	109.88
37	N	314	KC1	CHB-C4A-C3A	-4.77	117.53	124.98
36	P	302	CLA	CMB-C2B-C1B	-4.76	121.14	128.46
37	H	313	KC1	O2D-CGD-CBD	4.76	119.73	111.27
35	J	301	A86	C4-C5-C6	-4.76	120.51	127.31
37	C	213	KC1	CHB-C4A-C3A	-4.76	117.54	124.98
36	I	308	CLA	C4C-C3C-C2C	-4.76	99.96	106.90
36	N	310	CLA	CHD-C1D-ND	-4.75	120.08	124.45
34	R	307	DD6	C9-C10-C11	-4.75	120.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	824	CLA	C3C-C4C-NC	4.75	115.90	110.57
35	K	306	A86	C41-C32-C31	4.75	114.72	110.47
36	F	317	CLA	O2D-CGD-CBD	4.75	119.70	111.27
35	J	305	A86	O1-C20-C21	-4.75	109.37	115.06
36	a	827	CLA	CMB-C2B-C3B	4.74	133.55	124.68
37	B	310	KC1	O2D-CGD-CBD	4.74	119.70	111.27
35	P	304	A86	C3-C2-C1	-4.74	120.54	127.31
36	W	218	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
35	X	303	A86	C25-C26-C27	-4.74	120.55	127.31
37	U	312	KC1	O2D-CGD-CBD	4.73	119.68	111.27
36	b	837	CLA	CMB-C2B-C1B	-4.73	121.19	128.46
35	N	306	A86	C4-C5-C6	-4.73	120.56	127.31
36	G	319	CLA	O2D-CGD-CBD	4.73	119.67	111.27
36	b	830	CLA	CMB-C2B-C3B	4.73	133.52	124.68
35	I	304	A86	C17-C16-C15	4.72	113.98	109.16
37	M	313	KC1	CAA-C2A-C1A	4.72	146.44	124.75
35	U	303	A86	C4-C5-C6	-4.72	120.57	127.31
34	S	307	DD6	C15-C14-C13	-4.72	116.02	125.99
37	A	312	KC1	CHB-C1B-C2B	-4.72	115.58	125.48
37	M	317	KC1	O2D-CGD-CBD	4.72	119.65	111.27
37	F	308	KC1	C1B-CHB-C4A	-4.71	115.89	126.06
35	C	204	A86	C24-C1-C2	4.71	126.17	118.94
36	a	836	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
36	N	310	CLA	CMD-C2D-C1D	4.71	133.02	124.71
34	K	304	DD6	C4-C5-C6	-4.71	120.59	127.31
36	a	831	CLA	C4A-NA-C1A	4.71	108.82	106.71
37	K	314	KC1	C2A-C3A-C4A	4.71	109.98	106.49
35	Q	301	A86	C3-C2-C1	-4.71	120.59	127.31
35	O	303	A86	C3-C2-C1	-4.71	120.59	127.31
36	G	310	CLA	CMB-C2B-C1B	-4.70	121.23	128.46
35	G	304	A86	O1-C15-C20	-4.70	54.80	59.40
37	L	317	KC1	CMD-C2D-C1D	-4.70	121.24	128.46
36	V	305	CLA	C1B-CHB-C4A	-4.70	120.81	130.12
37	H	313	KC1	CAA-C2A-C1A	4.70	146.35	124.75
35	S	301	A86	C20-C19-C18	4.70	122.05	112.75
35	W	202	A86	C34-O4-C38	4.70	126.66	117.90
35	N	301	A86	C20-C19-C18	4.70	122.04	112.75
34	j	103	DD6	C14-C13-C11	-4.70	118.24	125.53
35	M	304	A86	O1-C20-C21	-4.70	109.43	115.06
35	X	302	A86	C3-C2-C1	-4.70	120.61	127.31
35	H	304	A86	C3-C2-C1	-4.69	120.61	127.31
35	S	308	A86	O1-C20-C21	-4.69	109.44	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	308	CLA	CMB-C2B-C3B	4.69	133.45	124.68
36	G	315	CLA	CHD-C1D-ND	-4.69	120.14	124.45
35	L	319	A86	O4-C34-C35	4.69	119.26	107.59
35	K	301	A86	O1-C20-C21	-4.69	109.44	115.06
37	N	314	KC1	CHB-C1B-C2B	-4.68	115.66	125.48
35	E	302	A86	O1-C20-C21	-4.68	109.44	115.06
35	E	305	A86	O4-C38-C39	4.68	119.70	111.09
36	K	307	CLA	C3C-C4C-NC	4.68	115.82	110.57
37	F	315	KC1	CHB-C4A-NA	4.68	131.57	124.20
35	F	306	A86	C3-C2-C1	-4.68	120.63	127.31
36	M	310	CLA	C1D-ND-C4D	-4.67	103.01	106.33
37	F	315	KC1	C3C-C4C-NC	4.67	114.28	109.88
35	H	301	A86	C4-C5-C6	-4.67	120.64	127.31
35	X	302	A86	C25-C26-C27	-4.67	120.64	127.31
36	A	306	CLA	O2D-CGD-CBD	4.67	119.57	111.27
37	G	308	KC1	C2A-C3A-C4A	4.67	109.95	106.49
35	O	302	A86	O4-C34-C35	4.67	119.21	107.59
36	C	207	CLA	C3C-C4C-NC	4.67	115.80	110.57
35	L	304	A86	O4-C38-C39	4.66	119.67	111.09
35	P	303	A86	O4-C34-C35	4.66	119.21	107.59
35	I	304	A86	C3-C2-C1	-4.66	120.66	127.31
35	L	307	A86	C3-C2-C1	-4.66	120.66	127.31
36	b	838	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
36	Q	310	CLA	C6-C5-C3	4.66	125.68	113.45
36	f	804	CLA	C3C-C4C-NC	4.66	115.80	110.57
36	X	308	CLA	CAC-C3C-C4C	4.66	130.86	124.81
35	L	307	A86	O1-C20-C21	-4.66	109.47	115.06
35	O	301	A86	O1-C20-C21	-4.66	109.47	115.06
35	W	202	A86	C3-C2-C1	-4.66	120.66	127.31
34	H	303	DD6	C9-C10-C11	-4.66	120.67	127.31
36	K	308	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
35	X	305	A86	O4-C38-C39	4.65	119.64	111.09
36	D	309	CLA	C3B-C4B-NB	4.65	115.22	109.21
35	T	307	A86	C17-C16-C15	4.64	113.90	109.16
36	G	309	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
36	L	314	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
36	a	814	CLA	CMC-C2C-C1C	-4.64	117.97	125.04
36	I	311	CLA	CMB-C2B-C3B	4.64	133.36	124.68
36	V	306	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
35	J	302	A86	O1-C20-C21	-4.64	109.50	115.06
37	V	312	KC1	CHB-C4A-NA	4.64	131.51	124.20
36	P	309	CLA	CMB-C2B-C1B	-4.64	121.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	837	CLA	CMB-C2B-C1B	-4.64	121.34	128.46
36	l	201	CLA	CMB-C2B-C1B	-4.64	121.34	128.46
36	b	832	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
37	G	308	KC1	CHB-C4A-NA	4.63	131.50	124.20
35	W	202	A86	O1-C20-C21	-4.63	109.50	115.06
35	B	303	A86	C23-C16-C17	-4.63	100.94	108.98
36	A	310	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
35	G	302	A86	C3-C2-C1	-4.63	120.70	127.31
35	K	303	A86	C4-C5-C6	-4.63	120.70	127.31
37	K	314	KC1	CHB-C1B-C2B	-4.63	115.77	125.48
35	U	301	A86	C25-C26-C27	4.63	133.91	127.31
35	C	203	A86	O4-C38-C39	4.62	119.60	111.09
36	B	305	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
36	D	309	CLA	C3C-C4C-NC	4.62	115.75	110.57
35	U	301	A86	C-C1-C2	-4.62	116.45	122.92
35	M	305	A86	C35-C34-C33	-4.62	101.81	109.88
36	a	829	CLA	CMB-C2B-C3B	4.62	133.32	124.68
34	P	305	DD6	C3-C2-C1	-4.62	120.72	127.31
35	Q	303	A86	O4-C38-C39	4.62	119.59	111.09
36	Q	306	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
36	O	307	CLA	CMB-C2B-C1B	-4.62	121.37	128.46
35	J	306	A86	O1-C20-C21	-4.62	109.53	115.06
34	H	303	DD6	C3-C2-C1	-4.61	120.72	127.31
36	W	206	CLA	CMB-C2B-C1B	-4.61	121.37	128.46
36	S	315	CLA	CBA-CAA-C2A	4.61	123.75	114.02
37	T	310	KC1	C3D-CAD-CBD	4.61	113.67	107.61
35	S	305	A86	C4-C5-C6	-4.61	120.73	127.31
35	I	304	A86	C7-C6-C5	-4.61	116.47	122.92
35	F	302	A86	C4-C5-C6	-4.61	120.73	127.31
36	a	807	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
37	K	314	KC1	CAA-C2A-C1A	4.61	145.92	124.75
36	K	313	CLA	CMB-C2B-C3B	4.61	133.30	124.68
35	O	305	A86	O4-C38-C39	4.60	119.56	111.09
36	N	319	CLA	C1B-CHB-C4A	-4.60	121.00	130.12
35	F	301	A86	C4-C5-C6	-4.60	120.74	127.31
37	V	312	KC1	O2D-CGD-CBD	4.60	119.45	111.27
35	P	304	A86	C4-C5-C6	-4.60	120.74	127.31
36	R	322	CLA	O1D-CGD-CBD	4.60	133.90	124.48
35	F	307	A86	O4-C34-C33	4.60	119.04	107.59
36	X	315	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
34	H	303	DD6	C4-C5-C6	-4.60	120.75	127.31
35	R	309	A86	O4-C38-C39	4.60	119.55	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	315	CLA	CMB-C2B-C3B	4.60	133.28	124.68
35	J	306	A86	C3-C2-C1	-4.60	120.75	127.31
37	S	316	KC1	O2D-CGD-CBD	4.59	119.43	111.27
35	U	301	A86	O4-C38-C39	4.59	119.54	111.09
36	I	308	CLA	C3C-C4C-NC	4.59	115.72	110.57
36	L	309	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
36	B	309	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
35	Q	301	A86	C4-C5-C6	-4.59	120.76	127.31
35	P	306	A86	O4-C38-C39	4.59	119.53	111.09
34	A	304	DD6	C9-C10-C11	-4.59	120.76	127.31
35	M	304	A86	C25-C26-C27	-4.59	120.76	127.31
36	B	308	CLA	C4A-NA-C1A	4.59	108.77	106.71
35	T	306	A86	C3-C2-C1	-4.59	120.77	127.31
35	O	303	A86	C4-C5-C6	-4.58	120.77	127.31
36	D	310	CLA	CMB-C2B-C1B	-4.58	121.42	128.46
35	K	306	A86	C23-C16-C17	-4.58	101.02	108.98
35	M	301	A86	O1-C20-C21	-4.58	109.56	115.06
37	S	316	KC1	C1B-CHB-C4A	-4.58	116.17	126.06
36	b	823	CLA	CMB-C2B-C1B	-4.58	121.42	128.46
35	M	302	A86	C35-C34-C33	-4.58	101.88	109.88
35	N	304	A86	C3-C2-C1	-4.57	120.78	127.31
36	F	317	CLA	C4D-CHA-C1A	-4.57	115.69	121.25
36	b	807	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
35	J	306	A86	O4-C38-C39	4.57	119.50	111.09
35	W	202	A86	C12-C11-C13	4.57	123.70	116.02
35	U	302	A86	O4-C38-C39	4.57	119.50	111.09
35	L	306	A86	C3-C2-C1	-4.57	120.79	127.31
37	J	314	KC1	C1B-CHB-C4A	-4.57	116.21	126.06
37	P	317	KC1	CHB-C1B-C2B	-4.57	115.91	125.48
36	W	211	CLA	O2D-CGD-CBD	4.57	119.38	111.27
35	B	303	A86	C3-C2-C1	-4.56	120.80	127.31
35	T	301	A86	C3-C2-C1	-4.56	120.80	127.31
35	T	301	A86	C25-C26-C27	-4.56	120.80	127.31
37	W	213	KC1	CHB-C4A-C3A	-4.56	117.85	124.98
35	N	301	A86	C4-C5-C6	-4.56	120.80	127.31
37	R	317	KC1	C3C-C4C-NC	4.56	114.17	109.88
36	B	309	CLA	CHD-C1D-ND	-4.56	120.26	124.45
35	S	303	A86	C24-C1-C2	-4.56	111.94	118.94
35	F	302	A86	O4-C38-C39	4.56	119.48	111.09
36	L	308	CLA	C4A-NA-C1A	4.56	108.76	106.71
35	M	304	A86	O4-C38-C39	4.56	119.48	111.09
36	E	310	CLA	CMB-C2B-C3B	4.56	133.21	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	W	203	A86	C23-C16-C17	-4.56	101.06	108.98
35	F	306	A86	O1-C20-C21	-4.56	109.60	115.06
35	N	303	A86	C24-C1-C2	-4.56	111.95	118.94
35	P	304	A86	O4-C38-C39	4.56	119.47	111.09
36	R	311	CLA	CMB-C2B-C1B	-4.55	121.46	128.46
36	l	205	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
36	a	826	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
35	X	314	A86	C25-C26-C27	-4.55	120.82	127.31
36	E	312	CLA	CAA-C2A-C3A	-4.55	100.33	112.78
37	C	213	KC1	CHB-C1B-C2B	-4.54	115.95	125.48
36	D	308	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
36	F	310	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
35	R	303	A86	C3-C2-C1	-4.54	120.83	127.31
35	S	301	A86	C4-C5-C6	-4.54	120.83	127.31
35	O	319	A86	C4-C3-C2	-4.54	114.18	123.47
37	T	315	KC1	O2D-CGD-CBD	4.54	119.33	111.27
36	G	309	CLA	O2D-CGD-CBD	4.54	119.33	111.27
35	N	304	A86	O1-C15-C14	-4.54	104.11	113.21
35	W	202	A86	O4-C38-O5	-4.54	113.95	122.96
37	M	318	KC1	CHC-C1C-C2C	4.54	132.06	124.98
34	B	304	DD6	O1-C20-C19	-4.53	109.98	113.38
35	R	305	A86	O4-C38-C39	4.53	119.42	111.09
35	A	302	A86	O4-C34-C33	4.53	118.87	107.59
35	B	301	A86	O4-C38-C39	4.53	119.42	111.09
35	G	302	A86	O4-C38-C39	4.53	119.42	111.09
35	O	303	A86	O4-C38-C39	4.53	119.42	111.09
35	R	304	A86	C3-C4-C5	-4.53	114.20	123.47
35	L	319	A86	C3-C2-C1	-4.52	120.85	127.31
34	H	302	DD6	C3-C2-C1	-4.52	120.85	127.31
37	H	313	KC1	C2B-C1B-NB	4.52	113.44	110.10
35	R	306	A86	C4-C5-C6	-4.52	120.86	127.31
36	M	307	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
35	O	302	A86	C3-C2-C1	-4.52	120.86	127.31
35	I	301	A86	O4-C38-C39	4.52	119.40	111.09
34	K	304	DD6	C21-C20-C19	4.52	119.36	114.28
35	S	304	A86	C3-C2-C1	-4.52	120.86	127.31
37	M	317	KC1	C1B-CHB-C4A	-4.52	116.31	126.06
35	M	301	A86	C23-C16-C17	-4.52	101.13	108.98
35	Q	301	A86	O4-C38-C39	4.52	119.40	111.09
35	T	304	A86	O4-C38-C39	4.51	119.39	111.09
35	h	202	A86	O4-C38-C39	4.51	119.39	111.09
35	I	304	A86	C4-C5-C6	-4.51	120.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	302	A86	O1-C20-C19	-4.51	109.99	113.38
34	C	201	DD6	C3-C2-C1	-4.51	120.87	127.31
35	X	305	A86	C25-C26-C27	-4.51	120.87	127.31
36	f	803	CLA	C1D-ND-C4D	-4.51	103.13	106.33
35	L	307	A86	O4-C38-C39	4.51	119.38	111.09
35	P	303	A86	C3-C2-C1	-4.51	120.88	127.31
36	a	813	CLA	CMB-C2B-C1B	-4.51	121.54	128.46
36	G	319	CLA	C3B-C4B-NB	4.50	115.03	109.21
34	E	306	DD6	C4-C5-C6	-4.50	120.89	127.31
36	L	312	CLA	O1D-CGD-CBD	4.49	133.68	124.48
36	L	313	CLA	CMB-C2B-C3B	4.49	133.09	124.68
35	K	306	A86	C36-C31-C32	-4.49	115.24	119.70
35	U	303	A86	O4-C38-C39	4.49	119.36	111.09
35	T	301	A86	O4-C38-C39	4.49	119.35	111.09
35	Q	304	A86	O4-C38-C39	4.49	119.35	111.09
35	N	320	A86	O4-C38-C39	4.49	119.35	111.09
36	E	315	CLA	C3C-C4C-NC	4.49	115.60	110.57
35	N	304	A86	C19-C18-C17	-4.49	102.11	110.77
37	G	317	KC1	C1B-CHB-C4A	-4.48	116.38	126.06
35	F	304	A86	O4-C38-C39	4.48	119.34	111.09
35	N	303	A86	C40-C32-C31	4.48	114.48	110.47
37	C	213	KC1	C1B-CHB-C4A	-4.48	116.40	126.06
37	F	308	KC1	C2A-C1A-NA	4.48	116.58	109.40
37	D	314	KC1	CHB-C4A-C3A	-4.48	117.98	124.98
37	L	317	KC1	CHB-C1B-C2B	-4.47	116.09	125.48
35	S	305	A86	O4-C38-C39	4.47	119.32	111.09
37	V	312	KC1	C4B-CHC-C1C	-4.47	116.41	126.06
36	H	308	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
37	G	318	KC1	CHB-C1B-C2B	-4.47	116.10	125.48
35	M	302	A86	C4-C5-C6	-4.47	120.93	127.31
35	F	301	A86	O4-C38-C39	4.47	119.31	111.09
35	P	304	A86	C35-C34-C33	-4.47	102.08	109.88
35	S	303	A86	C40-C32-C31	4.47	114.47	110.47
35	P	307	A86	O1-C20-C21	-4.46	109.71	115.06
37	L	315	KC1	CAB-C3B-C2B	-4.46	113.90	128.60
35	S	304	A86	O4-C38-C39	4.46	119.30	111.09
35	T	306	A86	C4-C5-C6	-4.46	120.94	127.31
35	X	305	A86	C4-C5-C6	-4.46	120.95	127.31
35	L	301	A86	O4-C38-C39	4.46	119.29	111.09
37	L	317	KC1	C1B-CHB-C4A	-4.46	116.44	126.06
35	J	302	A86	O4-C38-C39	4.46	119.29	111.09
35	T	307	A86	C3-C2-C1	-4.45	120.95	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	301	A86	O1-C20-C21	-4.45	109.72	115.06
35	I	304	A86	O4-C38-O5	-4.45	114.12	122.96
34	F	303	DD6	C21-C20-C19	4.45	119.28	114.28
35	V	301	A86	O4-C38-C39	4.45	119.27	111.09
36	S	312	CLA	CMB-C2B-C3B	4.44	132.99	124.68
34	F	303	DD6	C4-C5-C6	-4.44	120.97	127.31
35	L	304	A86	C35-C34-C33	-4.44	102.12	109.88
35	J	305	A86	O4-C38-C39	4.44	119.26	111.09
36	I	307	CLA	CMB-C2B-C3B	4.44	132.99	124.68
35	Q	301	A86	C35-C34-C33	-4.44	102.12	109.88
35	O	303	A86	C35-C34-C33	-4.44	102.12	109.88
37	E	309	KC1	C1B-CHB-C4A	-4.44	116.48	126.06
37	G	318	KC1	CBD-CHA-C1A	4.44	137.16	128.88
37	F	308	KC1	CHB-C4A-NA	4.44	131.20	124.20
36	W	212	CLA	C4A-NA-C1A	4.44	108.70	106.71
35	E	307	A86	C4-C5-C6	-4.44	120.98	127.31
35	E	302	A86	C3-C2-C1	-4.43	120.98	127.31
34	W	205	DD6	C4-C5-C6	-4.43	120.98	127.31
37	V	312	KC1	C4C-C3C-C2C	-4.43	100.44	106.90
37	E	309	KC1	CHB-C1B-C2B	-4.43	116.19	125.48
35	D	302	A86	O4-C38-C39	4.43	119.24	111.09
35	J	305	A86	C4-C5-C6	-4.43	120.99	127.31
36	L	312	CLA	O2D-CGD-O1D	-4.43	115.18	123.84
36	I	305	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
35	X	314	A86	O4-C38-C39	4.43	119.23	111.09
36	J	310	CLA	CMB-C2B-C1B	-4.42	121.66	128.46
35	V	301	A86	C25-C26-C27	-4.42	121.00	127.31
36	G	309	CLA	O2D-CGD-O1D	-4.42	115.20	123.84
37	N	314	KC1	CHB-C4A-NA	4.42	131.17	124.20
37	U	312	KC1	C2A-C1A-NA	4.42	116.49	109.40
37	G	308	KC1	CHB-C1B-C2B	-4.42	116.21	125.48
35	U	304	A86	O1-C20-C21	-4.42	109.76	115.06
36	I	314	CLA	CMA-C3A-C2A	-4.42	105.80	116.10
37	L	317	KC1	O2D-CGD-CBD	4.41	119.11	111.27
35	A	316	A86	O4-C38-C39	4.41	119.21	111.09
34	Q	302	DD6	C21-C20-C19	4.41	119.25	114.28
35	G	302	A86	O1-C20-C21	-4.41	109.77	115.06
35	T	302	A86	C3-C2-C1	-4.41	121.01	127.31
35	C	204	A86	O4-C38-C39	4.41	119.21	111.09
35	L	304	A86	C17-C16-C15	4.41	113.66	109.16
36	l	205	CLA	C2D-C1D-ND	4.41	113.35	110.10
34	C	201	DD6	C4-C5-C6	-4.41	121.02	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	308	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
37	D	314	KC1	CHB-C4A-NA	4.40	131.14	124.20
37	J	314	KC1	C4B-C3B-C2B	-4.40	103.14	106.75
40	b	849	DGD	O5D-C6D-C5D	-4.40	100.91	109.05
35	J	301	A86	O4-C38-C39	4.40	119.18	111.09
36	I	309	CLA	CBA-CAA-C2A	-4.40	100.89	113.86
35	S	308	A86	O4-C38-C39	4.40	119.18	111.09
37	M	317	KC1	CHB-C1B-C2B	-4.39	116.26	125.48
35	I	301	A86	C17-C16-C15	4.39	113.64	109.16
37	H	313	KC1	C3C-C4C-NC	4.39	114.01	109.88
36	a	818	CLA	CMB-C2B-C3B	4.39	132.89	124.68
35	O	301	A86	O4-C38-C39	4.39	119.16	111.09
37	A	312	KC1	C3A-C4A-NA	4.39	115.36	110.57
35	K	301	A86	O4-C38-C39	4.39	119.16	111.09
35	R	309	A86	O1-C20-C21	-4.39	109.80	115.06
37	D	314	KC1	CAC-C3C-C4C	4.39	130.50	124.81
35	N	301	A86	O1-C15-C20	-4.38	55.11	59.40
34	E	306	DD6	C3-C2-C1	-4.38	121.05	127.31
35	D	302	A86	C17-C16-C15	4.38	113.63	109.16
35	X	314	A86	O1-C20-C21	-4.38	109.81	115.06
35	X	305	A86	C3-C2-C1	-4.38	121.06	127.31
37	H	313	KC1	C4B-C3B-C2B	-4.38	103.16	106.75
35	S	301	A86	O1-C15-C20	-4.38	55.12	59.40
36	O	309	CLA	CMB-C2B-C1B	-4.38	121.74	128.46
36	a	839	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
36	E	312	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
35	S	302	A86	O4-C38-C39	4.37	119.14	111.09
37	D	314	KC1	C3C-C4C-NC	4.37	113.99	109.88
36	j	102	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
37	G	308	KC1	C1B-CHB-C4A	-4.37	116.63	126.06
36	I	306	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
37	P	317	KC1	CHB-C4A-NA	4.37	131.09	124.20
35	T	304	A86	C17-C16-C15	4.37	113.62	109.16
37	M	313	KC1	CHB-C4A-NA	4.37	131.09	124.20
37	V	312	KC1	CHB-C1B-C2B	-4.37	116.32	125.48
36	P	311	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
36	U	309	CLA	CBA-CAA-C2A	-4.36	100.98	113.86
35	S	305	A86	C20-C19-C18	4.36	121.38	112.75
35	P	307	A86	O4-C38-C39	4.36	119.11	111.09
36	U	313	CLA	CAA-C2A-C3A	-4.36	105.93	116.10
37	K	314	KC1	O2D-CGD-CBD	4.36	119.02	111.27
35	R	301	A86	O4-C34-C35	4.36	118.44	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	304	DD6	C3-C2-C1	-4.36	121.09	127.31
36	G	319	CLA	CHB-C4A-NA	4.35	130.53	124.51
36	B	308	CLA	CMB-C2B-C3B	4.35	132.82	124.68
35	G	304	A86	C28-C27-C26	-4.35	116.83	122.92
35	O	319	A86	C36-C31-C32	-4.35	115.38	119.70
36	b	824	CLA	C4D-C3D-CAD	4.35	113.22	108.10
36	K	315	CLA	CMB-C2B-C3B	4.35	132.81	124.68
37	N	314	KC1	C4B-C3B-C2B	-4.35	103.18	106.75
37	G	318	KC1	C3C-C4C-NC	4.35	113.97	109.88
35	N	302	A86	O4-C38-C39	4.35	119.09	111.09
35	N	301	A86	O4-C34-C33	4.35	118.42	107.59
34	a	849	DD6	C21-C20-C19	4.35	119.17	114.28
36	a	823	CLA	CHD-C4C-C3C	-4.34	118.46	124.84
36	R	313	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
35	E	307	A86	O1-C20-C21	-4.34	109.85	115.06
35	S	301	A86	O4-C34-C33	4.34	118.40	107.59
35	R	303	A86	C25-C26-C27	-4.34	121.12	127.31
35	X	303	A86	O4-C38-O5	-4.34	114.34	122.96
36	R	321	CLA	CMB-C2B-C3B	4.34	132.79	124.68
36	a	802	CLA	CMD-C2D-C3D	-4.34	117.64	127.61
35	I	301	A86	C3-C2-C1	-4.34	121.12	127.31
36	X	308	CLA	CBC-CAC-C3C	4.34	124.38	112.43
36	Q	308	CLA	CMB-C2B-C1B	-4.33	121.80	128.46
35	M	301	A86	C25-C26-C27	-4.33	121.13	127.31
36	b	819	CLA	CAA-C2A-C3A	-4.33	100.92	112.78
35	T	307	A86	C40-C32-C31	4.33	114.35	110.47
35	M	305	A86	C25-C26-C27	-4.33	121.14	127.31
35	S	308	A86	C17-C16-C15	4.33	113.58	109.16
35	N	304	A86	O4-C38-C39	4.33	119.05	111.09
36	E	313	CLA	O2D-CGD-CBD	4.32	118.95	111.27
37	C	213	KC1	O2D-CGD-CBD	4.32	118.95	111.27
35	O	302	A86	C4-C5-C6	-4.32	121.15	127.31
36	R	318	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
36	f	804	CLA	C3B-C4B-NB	4.31	114.79	109.21
36	C	212	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
36	i	102	CLA	CMB-C2B-C3B	4.31	132.75	124.68
41	F	318	LHG	O3-P-O6	-4.31	95.26	106.73
37	X	311	KC1	CBD-CHA-C1A	4.31	136.92	128.88
36	A	306	CLA	C4A-NA-C1A	4.31	108.64	106.71
35	E	302	A86	O4-C38-C39	4.31	119.02	111.09
36	H	315	CLA	CBC-CAC-C3C	4.31	124.31	112.43
35	R	303	A86	C4-C5-C6	-4.31	121.16	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	T	305	A86	C3-C2-C1	-4.31	121.16	127.31
35	O	301	A86	C3-C2-C1	-4.31	121.16	127.31
36	D	313	CLA	CMB-C2B-C3B	4.31	132.74	124.68
35	G	306	A86	O1-C20-C21	-4.31	109.90	115.06
35	X	303	A86	C21-C20-C19	-4.31	109.44	114.28
35	C	203	A86	O1-C20-C21	-4.30	109.90	115.06
37	W	217	KC1	CBD-CHA-C1A	4.30	136.90	128.88
36	b	816	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
35	K	302	A86	C3-C2-C1	-4.30	121.18	127.31
35	S	308	A86	C3-C2-C1	-4.30	121.18	127.31
37	T	315	KC1	C3C-C4C-NC	4.30	113.92	109.88
36	W	209	CLA	CMB-C2B-C1B	-4.29	121.86	128.46
35	P	303	A86	O4-C38-O5	-4.29	114.43	122.96
35	P	303	A86	C4-C5-C6	-4.29	121.18	127.31
36	G	307	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
35	R	306	A86	O1-C20-C21	-4.29	109.92	115.06
35	T	302	A86	C23-C16-C22	-4.29	101.04	107.37
35	B	301	A86	O1-C20-C21	-4.29	109.92	115.06
36	T	314	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
35	h	204	A86	C25-C26-C27	-4.29	121.19	127.31
35	O	301	A86	C4-C5-C6	-4.29	121.19	127.31
41	G	321	LHG	O7-C7-C8	4.29	120.74	111.50
35	T	301	A86	O1-C20-C21	-4.28	109.92	115.06
36	f	803	CLA	C1C-C2C-C3C	-4.28	102.45	106.96
35	R	309	A86	C35-C34-C33	-4.28	102.41	109.88
35	L	319	A86	C4-C5-C6	-4.28	121.20	127.31
35	C	204	A86	C3-C2-C1	-4.28	121.20	127.31
35	P	307	A86	C4-C5-C6	-4.28	121.20	127.31
35	M	302	A86	C25-C26-C27	-4.28	121.20	127.31
37	M	318	KC1	CHB-C1B-C2B	-4.28	116.51	125.48
36	a	824	CLA	CMB-C2B-C3B	4.28	132.68	124.68
35	E	307	A86	O4-C38-C39	4.28	118.96	111.09
35	X	301	A86	O4-C38-O5	-4.28	114.47	122.96
35	H	301	A86	C23-C16-C17	-4.28	101.56	108.98
37	W	217	KC1	O2D-CGD-CBD	4.27	118.86	111.27
35	F	306	A86	O4-C38-C39	4.27	118.94	111.09
35	O	302	A86	O4-C38-O5	-4.27	114.49	122.96
36	H	311	CLA	CMB-C2B-C3B	4.27	132.66	124.68
37	G	318	KC1	C1B-CHB-C4A	-4.27	116.86	126.06
37	W	217	KC1	C1B-CHB-C4A	-4.26	116.86	126.06
36	a	828	CLA	CMB-C2B-C3B	4.26	132.66	124.68
35	U	304	A86	O4-C38-C39	4.26	118.93	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	J	314	KC1	C2A-C1A-NA	4.26	116.24	109.40
34	B	302	DD6	C21-C20-C19	4.26	119.07	114.28
36	Q	314	CLA	CMB-C2B-C3B	4.26	132.65	124.68
35	h	204	A86	O1-C20-C21	-4.26	109.95	115.06
37	X	311	KC1	O2D-CGD-CBD	4.26	118.83	111.27
35	Q	303	A86	C4-C5-C6	-4.26	121.23	127.31
36	P	302	CLA	CMB-C2B-C3B	4.26	132.64	124.68
36	P	314	CLA	CAA-C2A-C3A	-4.26	101.12	112.78
35	G	304	A86	O4-C38-O5	-4.26	114.51	122.96
35	L	319	A86	O4-C38-O5	-4.26	114.51	122.96
37	R	317	KC1	C3B-C2B-C1B	-4.26	103.01	107.08
36	D	307	CLA	O2D-CGD-O1D	-4.26	115.52	123.84
37	X	311	KC1	C1B-CHB-C4A	-4.25	116.88	126.06
34	O	304	DD6	C9-C10-C11	-4.25	121.24	127.31
35	L	304	A86	C25-C26-C27	-4.25	121.24	127.31
35	N	302	A86	C35-C34-C33	-4.25	102.46	109.88
35	F	304	A86	C4-C5-C6	-4.25	121.25	127.31
36	V	311	CLA	CMB-C2B-C3B	4.25	132.63	124.68
35	T	305	A86	C20-C19-C18	4.25	121.15	112.75
35	S	304	A86	O1-C20-C21	-4.25	109.97	115.06
34	A	303	DD6	C3-C2-C1	-4.25	121.25	127.31
35	T	303	A86	C4-C5-C6	-4.24	121.25	127.31
36	a	803	CLA	CMB-C2B-C3B	4.24	132.62	124.68
35	F	302	A86	C3-C2-C1	-4.24	121.26	127.31
36	B	309	CLA	CMD-C2D-C3D	-4.24	117.86	127.61
36	f	804	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
37	W	217	KC1	CAC-C3C-C4C	4.24	130.31	124.81
37	X	311	KC1	CAC-C3C-C4C	4.24	130.31	124.81
35	K	306	A86	C25-C26-C27	-4.24	121.27	127.31
35	S	302	A86	C35-C34-C33	-4.24	102.48	109.88
36	b	841	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
36	C	207	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
34	E	301	DD6	C9-C10-C11	-4.23	121.27	127.31
35	R	301	A86	C4-C5-C6	-4.23	121.27	127.31
34	D	305	DD6	O1-C20-C19	-4.23	110.20	113.38
37	G	308	KC1	O2D-CGD-CBD	4.23	118.79	111.27
37	K	314	KC1	CAC-C3C-C4C	4.23	130.30	124.81
35	R	301	A86	C3-C2-C1	-4.22	121.28	127.31
34	E	303	DD6	C4-C5-C6	-4.22	121.28	127.31
35	Q	301	A86	C25-C26-C27	-4.22	121.28	127.31
36	D	310	CLA	CMB-C2B-C3B	4.22	132.58	124.68
35	F	304	A86	O1-C20-C21	-4.22	110.00	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	310	CLA	C2D-C1D-ND	-4.22	107.00	110.10
36	I	305	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
35	T	306	A86	C35-C34-C33	-4.22	102.52	109.88
36	N	318	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
36	U	306	CLA	C3C-C4C-NC	4.21	115.30	110.57
36	K	310	CLA	C2C-C1C-NC	4.21	113.92	109.97
34	S	306	DD6	C9-C10-C11	-4.21	121.30	127.31
35	O	303	A86	C25-C26-C27	-4.21	121.30	127.31
35	F	301	A86	C3-C2-C1	-4.21	121.31	127.31
35	E	307	A86	C3-C2-C1	-4.21	121.31	127.31
36	C	212	CLA	CAC-C3C-C4C	4.21	130.27	124.81
35	P	304	A86	C25-C26-C27	-4.20	121.31	127.31
34	R	307	DD6	C4-C5-C6	-4.20	121.31	127.31
40	L	302	DGD	O2G-C1B-C2B	4.20	120.55	111.50
36	I	308	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
35	S	301	A86	O4-C38-O5	-4.20	114.62	122.96
37	D	314	KC1	CAA-C2A-C1A	4.20	144.04	124.75
34	S	306	DD6	C37-C36-C31	-4.20	118.64	124.35
35	O	319	A86	C35-C34-C33	-4.20	102.55	109.88
35	N	303	A86	C28-C27-C26	-4.20	117.05	122.92
37	G	317	KC1	C1A-NA-C4A	-4.20	104.82	106.71
36	J	308	CLA	O2D-CGD-CBD	4.19	118.72	111.27
35	O	302	A86	C23-C16-C17	-4.19	101.69	108.98
36	A	314	CLA	CHB-C4A-NA	4.19	130.31	124.51
36	S	309	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
41	G	301	LHG	O4-P-O5	4.19	132.96	112.24
36	N	319	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
36	a	816	CLA	CHD-C1D-ND	-4.19	120.61	124.45
34	M	303	DD6	C4-C5-C6	-4.19	121.33	127.31
36	V	309	CLA	C2A-C1A-CHA	4.19	131.18	123.86
36	V	309	CLA	CBA-CAA-C2A	-4.19	105.18	114.02
35	O	319	A86	C3-C2-C1	4.19	133.28	127.31
35	C	202	A86	C33-C32-C31	4.18	113.28	109.21
37	W	217	KC1	CHB-C1B-C2B	-4.18	116.70	125.48
36	f	803	CLA	C2D-C1D-ND	4.18	113.19	110.10
34	J	304	DD6	C3-C2-C1	-4.18	121.34	127.31
35	R	301	A86	O4-C38-O5	-4.18	114.65	122.96
35	N	301	A86	O4-C38-O5	-4.18	114.66	122.96
36	b	841	CLA	CMC-C2C-C3C	4.18	137.47	126.12
35	L	319	A86	C23-C16-C17	-4.18	101.72	108.98
35	P	303	A86	C23-C16-C17	-4.18	101.72	108.98
36	b	818	CLA	O2D-CGD-O1D	-4.18	115.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	F	321	LMT	O5B-C1B-C2B	-4.18	101.50	110.35
37	D	314	KC1	CHB-C1B-C2B	-4.18	116.72	125.48
36	H	314	CLA	CMB-C2B-C3B	4.18	132.49	124.68
35	X	314	A86	C3-C2-C1	-4.18	121.35	127.31
36	E	315	CLA	C1C-C2C-C3C	-4.18	102.57	106.96
36	P	314	CLA	CAA-C2A-C1A	-4.18	98.29	111.97
36	F	314	CLA	C7-C6-C5	-4.18	102.02	113.36
37	X	311	KC1	CHB-C1B-C2B	-4.18	116.72	125.48
37	H	313	KC1	CAC-C3C-C4C	4.17	130.23	124.81
35	T	306	A86	C17-C16-C15	4.17	113.42	109.16
35	L	306	A86	C23-C16-C17	-4.17	101.73	108.98
37	K	314	KC1	C4B-C3B-C2B	-4.17	103.33	106.75
34	E	301	DD6	C3-C2-C1	-4.17	121.36	127.31
35	A	302	A86	C26-C25-C24	-4.17	110.21	123.22
37	O	315	KC1	C4B-C3B-C2B	-4.17	103.33	106.75
37	Q	311	KC1	C4B-C3B-C2B	-4.17	103.33	106.75
35	S	303	A86	C28-C27-C26	-4.17	117.09	122.92
37	W	213	KC1	C1B-CHB-C4A	-4.17	117.07	126.06
36	X	312	CLA	CMB-C2B-C3B	4.16	132.47	124.68
37	H	313	KC1	CMD-C2D-C1D	-4.16	122.06	128.46
42	J	318	LMG	O7-C10-C11	4.16	120.47	111.50
36	N	317	CLA	CMB-C2B-C3B	4.16	132.47	124.68
42	V	316	LMG	O7-C10-C11	4.16	120.47	111.50
37	Q	313	KC1	C4B-C3B-C2B	-4.16	103.33	106.75
41	O	318	LHG	O4-P-O5	4.16	132.80	112.24
35	S	303	A86	C23-C16-C17	-4.16	101.76	108.98
42	E	319	LMG	O7-C10-C11	4.16	120.46	111.50
35	W	202	A86	O4-C34-C33	4.16	117.94	107.59
34	J	304	DD6	C37-C36-C31	-4.15	118.70	124.35
36	I	309	CLA	C2A-C1A-CHA	4.15	131.12	123.86
36	Q	310	CLA	C2A-C3A-C4A	4.15	108.58	101.87
37	D	314	KC1	C2A-C3A-C4A	4.15	109.57	106.49
35	V	303	A86	O4-C38-O5	-4.15	114.71	122.96
36	U	311	CLA	CMB-C2B-C3B	4.15	132.45	124.68
36	K	312	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
36	G	315	CLA	C3B-C4B-NB	4.15	114.58	109.21
36	D	309	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
35	T	302	A86	O1-C20-C21	-4.15	110.08	115.06
37	O	313	KC1	C4B-C3B-C2B	-4.15	103.34	106.75
36	H	307	CLA	C3C-C4C-NC	-4.15	105.92	110.57
35	T	306	A86	C25-C26-C27	-4.15	121.39	127.31
35	N	303	A86	C23-C16-C17	-4.15	101.78	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	W	205	DD6	C9-C10-C11	-4.15	121.39	127.31
36	a	831	CLA	CMB-C2B-C1B	-4.14	122.09	128.46
36	H	307	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
35	V	303	A86	C23-C16-C17	-4.14	101.79	108.98
36	a	812	CLA	CMB-C2B-C3B	4.14	132.42	124.68
36	R	322	CLA	CED-O2D-CGD	4.14	125.30	115.94
35	L	301	A86	O1-C20-C21	-4.14	110.10	115.06
36	P	314	CLA	C2A-C3A-C4A	4.14	108.55	101.87
35	S	304	A86	C41-C32-C31	-4.14	106.77	110.47
35	N	301	A86	C34-O4-C38	4.14	125.60	117.90
36	P	302	CLA	O2D-CGD-O1D	-4.13	115.75	123.84
42	J	319	LMG	O7-C10-C11	4.13	120.41	111.50
35	F	305	A86	O4-C38-C39	4.13	118.70	111.09
35	V	303	A86	C28-C27-C26	-4.13	117.13	122.92
34	K	304	DD6	C3-C2-C1	-4.13	121.41	127.31
36	a	820	CLA	CMB-C2B-C3B	4.13	132.41	124.68
36	b	837	CLA	CMB-C2B-C3B	4.13	132.41	124.68
36	J	307	CLA	CMB-C2B-C3B	4.13	132.41	124.68
35	h	204	A86	O4-C38-C39	4.13	118.69	111.09
36	W	218	CLA	CMB-C2B-C3B	4.13	132.41	124.68
34	E	301	DD6	C14-C13-C11	-4.13	119.12	125.53
35	X	301	A86	O4-C34-C35	4.13	117.87	107.59
35	N	303	A86	C25-C26-C27	-4.13	121.42	127.31
36	S	310	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
36	J	312	CLA	CMB-C2B-C3B	4.12	132.39	124.68
37	P	315	KC1	C4B-C3B-C2B	-4.12	103.37	106.75
41	F	319	LHG	O7-C7-C8	4.12	120.38	111.50
35	S	303	A86	C25-C26-C27	-4.12	121.43	127.31
37	G	317	KC1	C3C-C4C-NC	4.12	113.75	109.88
37	B	310	KC1	C1B-CHB-C4A	-4.12	117.17	126.06
36	b	836	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
36	G	309	CLA	CMB-C2B-C3B	4.12	132.38	124.68
36	b	801	CLA	CMB-C2B-C3B	4.12	132.38	124.68
41	a	843	LHG	O7-C7-C8	4.12	120.37	111.50
36	S	313	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
35	D	302	A86	C4-C5-C6	-4.12	121.44	127.31
35	S	301	A86	C34-O4-C38	4.12	125.57	117.90
42	G	325	LMG	O7-C10-C11	4.11	120.37	111.50
37	E	309	KC1	C3C-C4C-NC	4.11	113.75	109.88
40	C	215	DGD	O2G-C1B-C2B	4.11	120.36	111.50
41	j	104	LHG	O7-C7-C8	4.11	120.36	111.50
42	a	852	LMG	O7-C10-C11	4.11	120.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	K	307	CLA	CAC-C3C-C4C	4.11	130.14	124.81
35	K	306	A86	C4-C5-C6	-4.11	121.45	127.31
34	j	103	DD6	C37-C36-C31	-4.11	118.77	124.35
41	G	320	LHG	O7-C7-C8	4.10	120.35	111.50
36	E	315	CLA	C4A-NA-C1A	4.10	108.55	106.71
34	B	302	DD6	C4-C5-C6	-4.10	121.45	127.31
35	H	301	A86	C35-C34-C33	-4.10	102.72	109.88
35	R	302	A86	C23-C16-C17	-4.10	101.86	108.98
35	K	302	A86	C4-C5-C6	-4.10	121.46	127.31
36	G	319	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
41	a	842	LHG	O4-P-O5	4.10	132.50	112.24
34	A	304	DD6	C4-C5-C6	-4.10	121.46	127.31
37	M	313	KC1	C4C-C3C-C2C	-4.10	100.93	106.90
36	a	806	CLA	CMD-C2D-C3D	-4.10	118.19	127.61
37	A	312	KC1	C4B-C3B-C2B	-4.10	103.39	106.75
35	J	306	A86	C4-C5-C6	-4.10	121.47	127.31
35	K	302	A86	O1-C20-C19	-4.09	110.31	113.38
41	f	808	LHG	O7-C7-C8	4.09	120.33	111.50
37	B	310	KC1	CHB-C1B-C2B	-4.09	116.89	125.48
36	A	307	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
35	X	302	A86	C35-C34-C33	-4.09	102.73	109.88
36	a	836	CLA	CMB-C2B-C3B	4.09	132.33	124.68
35	N	305	A86	C34-O4-C38	-4.09	110.27	117.90
37	F	315	KC1	CHB-C1B-C2B	-4.09	116.90	125.48
35	Q	304	A86	C36-C31-C32	-4.09	115.64	119.70
36	a	822	CLA	CMD-C2D-C3D	-4.09	118.21	127.61
37	N	314	KC1	CAA-C2A-C1A	4.09	143.54	124.75
36	b	817	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
35	N	320	A86	C36-C31-C32	-4.09	115.64	119.70
36	f	804	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
36	b	828	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
36	N	308	CLA	CHC-C1C-NC	-4.08	118.01	124.20
36	A	306	CLA	C1C-C2C-C3C	-4.08	102.66	106.96
35	V	301	A86	O1-C20-C21	-4.08	110.17	115.06
37	M	317	KC1	CHD-C4C-NC	4.08	130.39	124.20
36	F	309	CLA	CMB-C2B-C3B	4.08	132.31	124.68
35	Q	316	A86	C34-O4-C38	-4.08	110.30	117.90
36	l	201	CLA	CMB-C2B-C3B	4.08	132.31	124.68
36	b	815	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
36	N	319	CLA	CMB-C2B-C3B	4.07	132.30	124.68
34	j	103	DD6	C9-C10-C11	-4.07	121.50	127.31
42	D	320	LMG	O7-C10-C11	4.07	120.28	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	314	CLA	CMB-C2B-C3B	4.07	132.30	124.68
35	L	307	A86	C4-C5-C6	-4.07	121.50	127.31
34	D	304	DD6	C9-C10-C11	-4.07	121.50	127.31
36	a	821	CLA	CMB-C2B-C3B	4.07	132.29	124.68
35	R	304	A86	O1-C20-C21	-4.07	110.18	115.06
34	W	204	DD6	C4-C5-C6	-4.06	121.51	127.31
34	A	303	DD6	C9-C10-C11	-4.06	121.51	127.31
35	S	305	A86	O1-C15-C20	-4.06	55.43	59.40
35	X	303	A86	C35-C34-C33	-4.06	102.79	109.88
35	B	303	A86	O1-C20-C19	-4.06	110.33	113.38
37	V	312	KC1	CAC-C3C-C2C	-4.06	120.59	127.53
37	D	314	KC1	O2D-CGD-CBD	4.06	118.48	111.27
35	S	301	A86	O4-C34-C35	4.06	117.70	107.59
35	D	302	A86	O1-C20-C21	-4.06	110.19	115.06
35	F	305	A86	C3-C2-C1	-4.06	121.52	127.31
37	X	311	KC1	C4B-C3B-C2B	-4.05	103.42	106.75
37	N	314	KC1	O2D-CGD-CBD	4.05	118.47	111.27
35	K	302	A86	C23-C16-C17	-4.05	101.94	108.98
35	U	304	A86	C17-C16-C15	4.05	113.30	109.16
42	h	206	LMG	O7-C10-C11	4.05	120.24	111.50
41	f	809	LHG	O7-C7-C8	4.05	120.23	111.50
35	V	301	A86	C3-C2-C1	-4.05	121.53	127.31
36	T	313	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
35	J	305	A86	C3-C2-C1	-4.05	121.53	127.31
34	E	304	DD6	C37-C36-C31	-4.05	118.85	124.35
35	E	305	A86	O1-C20-C21	-4.05	110.21	115.06
35	N	301	A86	O4-C34-C35	4.05	117.67	107.59
36	b	838	CLA	CMB-C2B-C3B	4.05	132.25	124.68
35	Q	303	A86	O1-C20-C21	-4.05	110.21	115.06
42	I	315	LMG	O7-C10-C11	4.05	120.22	111.50
37	F	315	KC1	C4B-C3B-C2B	-4.04	103.43	106.75
41	i	104	LHG	O7-C7-C8	4.04	120.22	111.50
36	J	309	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
34	E	303	DD6	C37-C36-C31	-4.04	118.86	124.35
38	A	315	SQD	O47-C7-C8	4.04	120.21	111.50
37	E	309	KC1	C2A-C3A-C4A	4.04	109.48	106.49
36	a	807	CLA	CMB-C2B-C3B	4.04	132.24	124.68
35	X	301	A86	C41-C32-C31	4.04	114.09	110.47
37	C	213	KC1	C4B-C3B-C2B	-4.04	103.44	106.75
37	L	315	KC1	C1B-CHB-C4A	-4.04	117.35	126.06
38	b	804	SQD	O47-C7-C8	4.03	120.20	111.50
41	l	208	LHG	O7-C7-C8	4.03	120.20	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	P	305	DD6	C14-C13-C11	-4.03	119.27	125.53
35	I	304	A86	C12-C11-C13	-4.03	109.25	116.02
37	G	308	KC1	C4B-C3B-C2B	-4.03	103.44	106.75
36	j	101	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
41	R	323	LHG	O7-C7-C8	4.03	120.19	111.50
36	b	820	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
35	P	307	A86	C25-C26-C27	-4.03	121.56	127.31
36	I	305	CLA	C11-C12-C13	4.03	128.95	115.92
35	S	305	A86	C35-C34-C33	-4.03	102.84	109.88
37	L	315	KC1	CAA-C2A-C1A	4.03	143.26	124.75
37	O	315	KC1	CHB-C4A-NA	4.03	130.55	124.20
35	T	305	A86	O4-C38-O5	-4.03	114.96	122.96
34	G	303	DD6	C37-C36-C31	-4.03	118.88	124.35
36	H	307	CLA	CHD-C1D-ND	-4.03	120.75	124.45
35	F	302	A86	O1-C20-C21	-4.02	110.23	115.06
35	P	306	A86	O1-C20-C21	-4.02	110.23	115.06
35	U	303	A86	O1-C20-C21	-4.02	110.23	115.06
35	F	304	A86	C3-C2-C1	-4.02	121.57	127.31
36	V	307	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
35	W	202	A86	O4-C34-C35	4.02	117.61	107.59
36	a	813	CLA	CMB-C2B-C3B	4.02	132.20	124.68
37	Q	311	KC1	CHB-C4A-NA	4.02	130.54	124.20
37	M	317	KC1	C4C-C3C-C2C	-4.02	101.04	106.90
36	j	102	CLA	CHD-C1D-ND	-4.02	120.76	124.45
35	R	303	A86	O4-C38-O5	-4.02	114.98	122.96
36	l	206	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
36	h	203	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
36	W	216	CLA	CMB-C2B-C3B	-4.02	117.16	124.68
37	C	213	KC1	CHB-C4A-NA	4.02	130.53	124.20
37	Q	313	KC1	CHB-C4A-NA	4.02	130.53	124.20
37	G	308	KC1	C3C-C4C-NC	4.02	113.66	109.88
36	L	320	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
37	W	217	KC1	C4B-C3B-C2B	-4.02	103.45	106.75
35	V	302	A86	C3-C2-C1	-4.02	121.58	127.31
36	E	311	CLA	CMB-C2B-C3B	4.02	132.19	124.68
35	R	301	A86	C34-O4-C38	4.02	125.38	117.90
37	O	313	KC1	CHB-C4A-NA	4.02	130.53	124.20
36	O	311	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
41	Q	315	LHG	O7-C7-C8	4.02	120.16	111.50
36	T	316	CLA	CMB-C2B-C1B	-4.01	122.29	128.46
36	l	204	CLA	C3D-C2D-C1D	-4.01	100.35	105.83
36	C	205	CLA	CMB-C2B-C1B	-4.01	122.29	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	824	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
36	D	307	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
34	D	304	DD6	C37-C36-C31	-4.01	118.90	124.35
35	R	303	A86	C23-C16-C17	-4.01	102.02	108.98
36	G	309	CLA	C1-C2-C3	4.01	132.97	126.04
34	R	308	DD6	C3-C2-C1	-4.01	121.59	127.31
34	E	301	DD6	C4-C5-C6	-4.00	121.59	127.31
34	O	304	DD6	C37-C36-C31	-4.00	118.91	124.35
44	f	801	BCR	C2-C1-C6	4.00	116.64	110.48
36	G	319	CLA	C4D-C3D-CAD	-4.00	103.38	108.10
41	O	317	LHG	O7-C7-C8	4.00	120.12	111.50
35	C	202	A86	O4-C38-O5	-4.00	115.02	122.96
41	a	850	LHG	O7-C7-C8	4.00	120.11	111.50
37	H	313	KC1	C2A-C1A-NA	3.99	115.81	109.40
35	U	302	A86	C21-C20-C19	3.99	118.77	114.28
35	P	303	A86	C34-O4-C38	3.99	125.34	117.90
36	P	313	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
37	S	316	KC1	CBD-CHA-C1A	3.99	136.32	128.88
36	D	315	CLA	CAA-C2A-C3A	-3.99	106.78	116.10
35	M	305	A86	C4-C5-C6	-3.99	121.61	127.31
37	G	317	KC1	CHB-C1B-C2B	-3.99	117.11	125.48
36	U	310	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
36	a	825	CLA	CMD-C2D-C3D	-3.99	118.44	127.61
36	G	310	CLA	CMB-C2B-C3B	3.99	132.14	124.68
37	W	213	KC1	CHB-C1B-C2B	-3.99	117.11	125.48
35	T	306	A86	O1-C20-C21	-3.99	110.28	115.06
42	G	324	LMG	O7-C10-C11	3.99	120.09	111.50
37	W	213	KC1	C4B-C3B-C2B	-3.99	103.48	106.75
35	U	301	A86	C17-C16-C15	3.99	113.23	109.16
37	P	315	KC1	CHB-C4A-NA	3.98	130.48	124.20
37	F	315	KC1	C1B-CHB-C4A	-3.98	117.47	126.06
36	b	832	CLA	CMB-C2B-C3B	3.98	132.13	124.68
42	m	102	LMG	O7-C10-C11	3.98	120.08	111.50
37	G	318	KC1	CAC-C3C-C2C	3.98	134.34	127.53
35	L	319	A86	C34-O4-C38	3.98	125.31	117.90
35	O	302	A86	C34-O4-C38	3.98	125.31	117.90
35	K	306	A86	C28-C27-C26	-3.98	117.35	122.92
37	A	312	KC1	CAA-C2A-C1A	3.98	143.03	124.75
36	L	314	CLA	CMB-C2B-C3B	3.98	132.12	124.68
34	E	304	DD6	C3-C2-C1	-3.98	121.63	127.31
37	F	308	KC1	C3C-C4C-NC	3.98	113.62	109.88
35	M	305	A86	C3-C2-C1	-3.98	121.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	304	DD6	C14-C13-C11	-3.97	119.36	125.53
37	M	313	KC1	C4B-C3B-C2B	-3.97	103.49	106.75
36	X	313	CLA	C2C-C1C-NC	3.97	113.69	109.97
36	a	801	CLA	C1D-ND-C4D	-3.97	103.51	106.33
36	I	308	CLA	CAC-C3C-C4C	3.97	129.97	124.81
36	W	216	CLA	CHB-C4A-NA	3.97	130.00	124.51
35	N	302	A86	C4-C5-C6	-3.97	121.65	127.31
36	D	311	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
35	V	301	A86	C17-C16-C15	3.97	113.21	109.16
36	B	305	CLA	CMB-C2B-C3B	3.97	132.10	124.68
36	C	211	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
36	a	848	CLA	CHD-C4C-NC	3.97	130.45	124.20
34	G	303	DD6	C3-C2-C1	-3.96	121.65	127.31
36	M	311	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
37	L	315	KC1	C2A-C1A-NA	3.96	115.76	109.40
37	S	316	KC1	C2A-C3A-C4A	3.96	109.42	106.49
36	D	308	CLA	CAC-C3C-C4C	3.96	129.95	124.81
35	N	320	A86	C23-C16-C17	-3.96	102.11	108.98
36	b	840	CLA	CAC-C3C-C4C	3.96	129.95	124.81
35	S	302	A86	C4-C5-C6	-3.96	121.67	127.31
42	L	321	LMG	O7-C10-C11	3.96	120.03	111.50
35	H	304	A86	O1-C20-C21	-3.96	110.32	115.06
41	I	316	LHG	O7-C7-C8	3.95	120.02	111.50
37	W	213	KC1	CAC-C3C-C4C	3.95	129.94	124.81
35	h	202	A86	O1-C20-C21	-3.95	110.32	115.06
37	S	316	KC1	C3B-C2B-C1B	-3.95	103.30	107.08
36	a	837	CLA	CMB-C2B-C3B	3.95	132.07	124.68
34	M	303	DD6	C37-C36-C31	-3.95	118.98	124.35
36	E	315	CLA	CHB-C4A-NA	3.95	129.98	124.51
36	R	312	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
37	L	315	KC1	C4B-C3B-C2B	-3.95	103.51	106.75
35	I	302	A86	C25-C26-C27	-3.95	121.67	127.31
36	a	830	CLA	CHA-C4D-ND	3.95	140.76	132.50
34	O	304	DD6	C15-C14-C13	-3.95	117.64	125.99
36	X	315	CLA	CMB-C2B-C3B	3.95	132.06	124.68
35	S	303	A86	O4-C38-O5	-3.95	115.12	122.96
36	R	316	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
36	X	315	CLA	CAA-C2A-C3A	-3.95	106.89	116.10
36	M	309	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
35	N	303	A86	O4-C38-O5	-3.94	115.13	122.96
35	T	307	A86	C25-C26-C27	-3.94	121.68	127.31
36	a	817	CLA	C4A-NA-C1A	3.94	108.48	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	305	DD6	C21-C20-C19	3.94	118.71	114.28
37	L	315	KC1	CHB-C4A-NA	3.94	130.41	124.20
36	W	210	CLA	C2A-C1A-CHA	3.94	130.75	123.86
37	F	315	KC1	CAA-C2A-C1A	3.94	142.85	124.75
35	A	302	A86	C3-C4-C5	-3.94	115.41	123.47
36	W	212	CLA	CMB-C2B-C3B	3.94	132.05	124.68
36	a	823	CLA	CMD-C2D-C3D	-3.94	118.56	127.61
37	H	313	KC1	C3A-C4A-NA	3.94	114.87	110.57
35	T	304	A86	O1-C20-C19	-3.94	110.42	113.38
36	l	201	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
42	E	318	LMG	O7-C10-C11	3.93	119.98	111.50
36	b	826	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
36	B	311	CLA	O1D-CGD-CBD	3.93	132.53	124.48
36	b	809	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
36	J	315	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
35	A	316	A86	O1-C20-C21	-3.93	110.35	115.06
36	b	817	CLA	C4C-C3C-C2C	-3.93	101.17	106.90
41	D	319	LHG	O7-C7-C8	3.93	119.97	111.50
36	V	306	CLA	CMB-C2B-C3B	3.93	132.03	124.68
37	T	315	KC1	C4D-C3D-CAD	3.93	114.16	107.81
36	N	309	CLA	O2A-CGA-O1A	-3.92	113.69	123.59
37	T	310	KC1	C1C-C2C-C3C	-3.92	102.83	106.96
35	R	309	A86	C3-C2-C1	-3.92	121.71	127.31
36	f	803	CLA	C4A-NA-C1A	3.92	108.47	106.71
36	A	310	CLA	CMB-C2B-C3B	3.92	132.02	124.68
36	R	319	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
34	O	304	DD6	C4-C5-C6	-3.92	121.71	127.31
34	A	301	DD6	C37-C36-C31	-3.92	119.02	124.35
37	L	315	KC1	CHB-C1B-C2B	-3.92	117.25	125.48
34	B	304	DD6	C14-C13-C11	-3.92	119.44	125.53
36	a	824	CLA	CBC-CAC-C3C	3.92	123.24	112.43
35	X	301	A86	C28-C27-C26	-3.92	117.43	122.92
35	S	305	A86	C3-C2-C1	-3.92	121.72	127.31
44	a	844	BCR	C2-C1-C6	3.92	116.52	110.48
35	V	304	A86	O1-C15-C20	-3.92	55.57	59.40
35	Q	304	A86	C23-C16-C17	-3.92	102.17	108.98
36	G	315	CLA	CMC-C2C-C1C	3.92	131.01	125.04
35	O	319	A86	O1-C20-C21	-3.92	110.36	115.06
41	b	850	LHG	O7-C7-C8	3.92	119.94	111.50
37	A	312	KC1	C2A-C1A-CHA	3.91	140.40	127.44
36	b	807	CLA	CMB-C2B-C3B	3.91	132.00	124.68
36	a	802	CLA	O2D-CGD-CBD	3.91	118.22	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	J	308	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
37	P	315	KC1	C3A-C4A-NA	3.91	114.84	110.57
35	T	307	A86	C35-C34-C33	-3.91	103.05	109.88
35	O	305	A86	O1-C20-C21	-3.91	110.37	115.06
36	W	206	CLA	CMB-C2B-C3B	3.91	131.99	124.68
35	V	303	A86	C40-C32-C31	3.91	113.97	110.47
37	L	317	KC1	C3C-C4C-NC	3.90	113.55	109.88
36	a	826	CLA	CMB-C2B-C3B	3.90	131.98	124.68
36	J	316	CLA	CAC-C3C-C2C	-3.90	120.85	127.53
34	D	301	DD6	O1-C20-C19	-3.90	110.45	113.38
36	B	308	CLA	C2D-C1D-ND	-3.90	107.23	110.10
36	P	309	CLA	CMB-C2B-C3B	3.90	131.98	124.68
37	G	318	KC1	CHB-C4A-NA	3.90	130.35	124.20
35	V	303	A86	C9-C10-C11	-3.90	115.14	126.61
36	K	308	CLA	CMB-C2B-C3B	3.90	131.98	124.68
37	O	313	KC1	C3A-C4A-NA	3.90	114.83	110.57
39	F	321	LMT	O5B-C5B-C4B	3.90	116.78	109.69
36	Q	306	CLA	CMB-C2B-C3B	3.90	131.97	124.68
36	a	829	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
34	A	303	DD6	C4-C5-C6	-3.90	121.75	127.31
36	a	848	CLA	CHD-C4C-C3C	-3.90	119.11	124.84
34	A	303	DD6	C37-C36-C31	-3.90	119.05	124.35
36	O	308	CLA	C4-C3-C5	3.90	121.83	115.27
35	R	301	A86	C23-C16-C17	-3.90	102.21	108.98
36	C	212	CLA	CMB-C2B-C3B	3.89	131.97	124.68
37	Q	313	KC1	C3A-C4A-NA	3.89	114.82	110.57
37	L	317	KC1	CBD-CHA-C1A	3.89	136.14	128.88
37	U	312	KC1	CAA-C2A-C1A	3.89	142.64	124.75
36	a	832	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
35	T	307	A86	C4-C5-C6	-3.89	121.76	127.31
35	V	302	A86	O4-C38-C39	3.89	118.24	111.09
36	b	816	CLA	C3B-C4B-NB	3.88	114.23	109.21
36	G	313	CLA	CMB-C2B-C3B	3.88	131.94	124.68
36	A	314	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
36	B	311	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
36	J	310	CLA	CMB-C2B-C3B	3.88	131.93	124.68
35	F	307	A86	C25-C26-C27	-3.88	121.78	127.31
37	G	317	KC1	CAA-C2A-C1A	3.88	142.56	124.75
35	F	307	A86	C3-C2-C1	-3.87	121.78	127.31
36	L	309	CLA	CMB-C2B-C3B	3.87	131.93	124.68
34	H	303	DD6	C37-C36-C31	-3.87	119.08	124.35
34	E	303	DD6	C3-C2-C1	-3.87	121.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	O	307	CLA	CMB-C2B-C3B	3.87	131.92	124.68
37	L	317	KC1	C4B-C3B-C2B	-3.87	103.57	106.75
37	O	315	KC1	C3A-C4A-NA	3.87	114.80	110.57
37	Q	311	KC1	C3A-C4A-NA	3.87	114.80	110.57
35	I	304	A86	C25-C26-C27	-3.87	121.79	127.31
36	b	833	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
36	E	313	CLA	CHB-C4A-NA	3.87	129.86	124.51
35	J	301	A86	C3-C2-C1	-3.87	121.79	127.31
34	B	304	DD6	C3-C2-C1	-3.87	121.79	127.31
35	X	304	A86	C4-C5-C6	-3.87	121.79	127.31
36	X	308	CLA	O2A-CGA-O1A	-3.87	113.83	123.59
36	D	308	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
35	G	305	A86	C3-C2-C1	-3.87	121.79	127.31
36	b	825	CLA	CMB-C2B-C1B	-3.86	122.52	128.46
35	U	302	A86	C35-C34-C33	-3.86	103.14	109.88
37	M	318	KC1	CMC-C2C-C1C	3.86	130.92	125.04
36	K	310	CLA	CHB-C4A-NA	3.86	129.85	124.51
36	K	310	CLA	C3B-C4B-NB	3.86	114.20	109.21
35	L	306	A86	C9-C8-C6	-3.86	115.58	126.42
36	V	305	CLA	CHD-C1D-ND	-3.85	120.91	124.45
35	T	303	A86	O4-C38-O5	-3.85	115.31	122.96
34	K	305	DD6	C4-C5-C6	-3.85	121.82	127.31
34	A	301	DD6	C14-C13-C11	-3.85	119.56	125.53
35	A	316	A86	C17-C16-C15	3.85	113.09	109.16
37	P	315	KC1	O2D-CGD-O1D	-3.84	116.32	123.84
34	j	103	DD6	C4-C5-C6	-3.84	121.82	127.31
35	E	307	A86	C25-C26-C27	-3.84	121.82	127.31
36	H	307	CLA	CMB-C2B-C3B	3.84	131.87	124.68
36	E	316	CLA	CBC-CAC-C3C	3.84	123.02	112.43
36	X	312	CLA	CAA-C2A-C3A	-3.84	107.14	116.10
36	G	313	CLA	C1B-CHB-C4A	-3.84	122.51	130.12
36	F	312	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
36	D	316	CLA	CAC-C3C-C2C	-3.84	120.96	127.53
36	G	307	CLA	CMC-C2C-C1C	3.84	130.88	125.04
35	X	303	A86	O1-C15-C20	-3.84	55.65	59.40
42	j	105	LMG	O7-C10-C11	3.83	119.76	111.50
36	K	313	CLA	O2D-CGD-O1D	-3.83	116.34	123.84
35	G	304	A86	C41-C32-C31	3.83	113.90	110.47
35	S	308	A86	C25-C26-C27	-3.83	121.84	127.31
36	J	308	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
36	K	310	CLA	C3C-C4C-NC	3.83	114.87	110.57
35	X	301	A86	O4-C34-C33	3.83	117.13	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	L	306	A86	O4-C38-C39	3.83	118.13	111.09
37	Q	313	KC1	O2D-CGD-O1D	-3.82	116.36	123.84
36	V	314	CLA	C3B-C4B-NB	3.82	114.15	109.21
35	F	305	A86	C35-C34-C33	-3.82	103.20	109.88
35	E	305	A86	C3-C2-C1	-3.82	121.85	127.31
36	l	202	CLA	O2D-CGD-O1D	-3.82	116.36	123.84
35	C	204	A86	O1-C20-C21	-3.82	110.48	115.06
34	W	205	DD6	C37-C36-C31	-3.82	119.16	124.35
35	A	302	A86	C8-C6-C5	-3.82	113.08	118.94
36	a	830	CLA	C2A-C3A-C4A	3.82	108.04	101.87
36	b	821	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
36	G	309	CLA	CED-O2D-CGD	3.82	124.58	115.94
35	N	306	A86	C35-C34-C33	-3.82	103.21	109.88
44	m	101	BCR	C2-C1-C6	3.82	116.36	110.48
34	a	849	DD6	C37-C36-C31	-3.82	119.16	124.35
36	f	804	CLA	CHB-C4A-NA	3.82	129.79	124.51
35	T	305	A86	C23-C16-C22	-3.81	101.74	107.37
36	I	306	CLA	C2D-C1D-ND	3.81	112.92	110.10
35	I	304	A86	C23-C16-C17	-3.81	102.36	108.98
35	X	304	A86	O1-C15-C20	-3.81	55.67	59.40
36	b	830	CLA	C2D-C1D-ND	-3.81	107.30	110.10
36	M	308	CLA	CBC-CAC-C3C	3.81	122.94	112.43
35	N	302	A86	C25-C26-C27	-3.81	121.87	127.31
35	X	301	A86	C12-C11-C13	3.81	122.42	116.02
42	D	321	LMG	O7-C10-C11	3.81	119.71	111.50
37	K	314	KC1	CHB-C4A-C3A	-3.81	119.03	124.98
34	a	849	DD6	C4-C5-C6	-3.81	121.88	127.31
35	J	303	A86	C4-C5-C6	-3.81	121.88	127.31
44	b	847	BCR	C2-C1-C6	3.81	116.34	110.48
37	Q	311	KC1	O2D-CGD-O1D	-3.80	116.40	123.84
36	F	314	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
37	O	313	KC1	O2D-CGD-O1D	-3.80	116.40	123.84
36	V	309	CLA	CAA-C2A-C1A	3.80	124.44	111.97
36	b	812	CLA	CMB-C2B-C3B	3.80	131.79	124.68
36	A	313	CLA	CAA-C2A-C3A	-3.80	107.23	116.10
37	T	310	KC1	CMA-C3A-C4A	3.80	130.82	125.04
35	S	302	A86	C25-C26-C27	-3.80	121.89	127.31
37	M	317	KC1	C4D-C3D-CAD	3.80	113.95	107.81
36	E	316	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
34	a	849	DD6	C3-C2-C1	-3.80	121.89	127.31
35	P	303	A86	O4-C34-C33	3.79	117.04	107.59
36	I	313	CLA	CMB-C2B-C1B	-3.79	122.63	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	E	301	DD6	C37-C36-C31	-3.79	119.19	124.35
37	K	314	KC1	CHB-C4A-NA	3.79	130.18	124.20
36	a	822	CLA	C4-C3-C5	3.79	120.32	115.98
36	b	821	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
36	P	319	CLA	C2A-C1A-CHA	3.79	130.49	123.86
35	R	304	A86	C3-C2-C1	-3.79	121.90	127.31
34	I	303	DD6	C4-C5-C6	-3.79	121.90	127.31
35	L	319	A86	O4-C34-C33	3.79	117.03	107.59
35	U	301	A86	C26-C25-C24	3.78	135.03	123.22
36	N	319	CLA	C3D-C4D-CHA	-3.78	104.06	112.72
37	O	315	KC1	O2D-CGD-O1D	-3.78	116.44	123.84
36	a	819	CLA	CMC-C2C-C3C	3.78	136.38	126.12
35	Q	303	A86	C12-C11-C13	3.78	122.37	116.02
37	K	314	KC1	C2A-C1A-CHA	-3.78	114.94	127.44
35	I	301	A86	O1-C20-C21	-3.78	110.53	115.06
36	T	316	CLA	CAA-C2A-C3A	-3.78	107.29	116.10
36	S	313	CLA	C2A-C1A-CHA	3.78	130.46	123.86
36	P	314	CLA	CBA-CAA-C2A	3.78	125.01	113.86
35	O	302	A86	O4-C34-C33	3.77	116.99	107.59
36	R	318	CLA	CAA-C2A-C3A	-3.77	107.30	116.10
35	Q	304	A86	C41-C32-C31	3.77	113.85	110.47
36	J	308	CLA	CHD-C1D-ND	-3.77	120.99	124.45
36	a	848	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
35	M	305	A86	C23-C16-C17	-3.77	102.43	108.98
41	E	322	LHG	O7-C7-C8	3.77	119.62	111.50
34	K	305	DD6	C37-C36-C31	-3.77	119.23	124.35
36	a	836	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
35	M	304	A86	C3-C2-C1	-3.76	121.94	127.31
35	X	304	A86	C3-C2-C1	-3.76	121.94	127.31
36	I	308	CLA	CHB-C4A-NA	3.76	129.71	124.51
37	T	315	KC1	C4B-C3B-C2B	-3.76	103.67	106.75
44	h	201	BCR	C40-C30-C25	3.76	116.39	110.30
36	L	308	CLA	CMB-C2B-C3B	3.76	131.71	124.68
36	N	319	CLA	C4D-CHA-C1A	3.76	125.82	121.25
35	T	302	A86	O4-C38-C39	3.75	118.00	111.09
36	U	311	CLA	C1-C2-C3	-3.75	119.56	126.04
34	F	303	DD6	C3-C2-C1	-3.75	121.96	127.31
35	G	306	A86	C9-C8-C6	-3.75	115.88	126.42
37	A	312	KC1	C1B-CHB-C4A	-3.75	117.97	126.06
34	E	303	DD6	C9-C10-C11	-3.75	121.96	127.31
36	G	315	CLA	CHB-C4A-NA	3.75	129.69	124.51
36	a	801	CLA	CGD-CBD-CAD	3.75	122.87	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	307	CLA	C1B-CHB-C4A	-3.74	122.70	130.12
37	B	310	KC1	C3C-C4C-NC	3.74	113.40	109.88
36	A	309	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
36	G	315	CLA	CMD-C2D-C3D	-3.74	119.02	127.61
36	P	301	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
37	O	313	KC1	CAC-C3C-C4C	3.74	129.66	124.81
36	R	314	CLA	CAC-C3C-C4C	3.73	129.65	124.81
36	W	211	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
36	a	830	CLA	C4D-C3D-CAD	3.73	112.49	108.10
35	S	304	A86	C4-C5-C6	-3.73	121.99	127.31
35	C	204	A86	C7-C6-C8	-3.73	112.20	118.08
35	F	301	A86	O1-C15-C14	-3.73	105.73	113.21
35	X	305	A86	O1-C15-C20	-3.73	55.76	59.40
36	W	214	CLA	C3C-C4C-NC	-3.73	106.39	110.57
37	P	317	KC1	C3C-C4C-NC	3.72	113.38	109.88
35	I	302	A86	O4-C38-C39	3.72	117.94	111.09
36	W	218	CLA	CBC-CAC-C3C	3.72	122.70	112.43
37	P	315	KC1	CAC-C3C-C4C	3.72	129.64	124.81
36	N	310	CLA	CHD-C1D-C2D	3.72	133.29	125.48
36	b	827	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
37	Q	313	KC1	CAC-C3C-C4C	3.72	129.64	124.81
43	b	842	PQN	C11-C12-C13	-3.72	120.60	126.79
34	D	303	DD6	C15-C14-C13	-3.72	118.13	125.99
36	L	316	CLA	CAA-C2A-C3A	-3.72	107.42	116.10
35	K	302	A86	O4-C38-O5	-3.72	115.58	122.96
37	Q	311	KC1	CAC-C3C-C4C	3.72	129.63	124.81
36	X	309	CLA	C2A-C1A-CHA	3.71	130.35	123.86
37	S	316	KC1	CAA-C2A-C1A	3.71	141.81	124.75
37	G	317	KC1	CBD-CHA-C1A	3.71	135.80	128.88
35	S	303	A86	C3-C2-C1	-3.71	122.02	127.31
35	R	301	A86	O4-C34-C33	3.71	116.83	107.59
37	O	315	KC1	CAC-C3C-C4C	3.71	129.62	124.81
36	H	314	CLA	CAA-C2A-C3A	-3.71	107.45	116.10
37	B	310	KC1	C2A-C1A-NA	3.71	115.35	109.40
34	K	305	DD6	C9-C10-C11	-3.71	122.02	127.31
35	R	305	A86	C4-C5-C6	-3.71	122.02	127.31
35	K	303	A86	C23-C16-C17	-3.71	102.54	108.98
37	G	318	KC1	C4B-C3B-C2B	-3.71	103.71	106.75
35	N	320	A86	C41-C32-C31	3.71	113.79	110.47
36	a	819	CLA	CMC-C2C-C1C	-3.71	119.39	125.04
37	B	310	KC1	CMD-C2D-C3D	3.71	131.61	124.68
34	Q	302	DD6	C14-C13-C11	-3.70	119.78	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	N	310	CLA	CAA-C2A-C3A	-3.70	107.46	116.10
36	f	804	CLA	C1D-ND-C4D	-3.70	103.70	106.33
36	X	308	CLA	CBA-CAA-C2A	3.70	124.79	113.86
36	W	207	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
35	N	303	A86	C3-C2-C1	-3.70	122.03	127.31
36	K	307	CLA	CHD-C4C-C3C	-3.70	119.40	124.84
36	H	305	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
34	H	302	DD6	C37-C36-C31	-3.70	119.32	124.35
37	U	312	KC1	C3C-C4C-NC	3.70	113.36	109.88
36	T	314	CLA	CMB-C2B-C3B	3.70	131.60	124.68
36	P	316	CLA	CMA-C3A-C2A	-3.70	107.47	116.10
36	T	309	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
36	V	305	CLA	CMD-C2D-C1D	3.70	131.23	124.71
34	j	103	DD6	C3-C2-C1	-3.70	122.04	127.31
36	H	308	CLA	CMB-C2B-C3B	3.69	131.59	124.68
36	b	823	CLA	CMB-C2B-C3B	3.69	131.59	124.68
35	X	305	A86	C23-C16-C17	-3.69	102.56	108.98
37	A	312	KC1	CBC-CAC-C3C	-3.69	102.25	112.43
34	G	303	DD6	C4-C5-C6	-3.69	122.04	127.31
36	Q	312	CLA	CMA-C3A-C2A	-3.69	107.48	116.10
35	V	304	A86	C25-C26-C27	-3.69	122.05	127.31
36	D	308	CLA	CMB-C2B-C3B	3.69	131.58	124.68
36	U	313	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
36	O	314	CLA	CMA-C3A-C2A	-3.69	107.49	116.10
36	H	306	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
37	L	317	KC1	C2A-C1A-NA	3.69	115.31	109.40
35	X	304	A86	O4-C38-O5	-3.69	115.64	122.96
36	b	841	CLA	CAC-C3C-C2C	3.68	133.83	127.53
36	a	805	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
36	V	308	CLA	CMB-C2B-C3B	3.68	131.57	124.68
34	D	301	DD6	C37-C36-C31	-3.68	119.34	124.35
36	M	312	CLA	CAA-C2A-C3A	-3.68	102.69	112.78
36	f	804	CLA	C4D-CHA-C1A	-3.68	116.77	121.25
34	A	304	DD6	C37-C36-C31	-3.68	119.35	124.35
34	j	103	DD6	C21-C20-C19	3.68	118.42	114.28
35	T	303	A86	C3-C2-C1	-3.68	122.06	127.31
34	B	304	DD6	C32-C31-C36	-3.68	117.44	122.63
36	D	313	CLA	O2A-CGA-O1A	-3.68	114.31	123.59
36	A	306	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
36	H	311	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
35	U	302	A86	C41-C32-C31	3.68	113.76	110.47
36	Q	312	CLA	CAA-C2A-C3A	-3.68	107.52	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	F	308	KC1	O2D-CGD-O1D	-3.68	116.65	123.84
34	Q	302	DD6	C37-C36-C31	-3.68	119.36	124.35
36	P	316	CLA	CAA-C2A-C3A	-3.67	107.53	116.10
36	R	313	CLA	CMB-C2B-C3B	3.67	131.55	124.68
35	Q	303	A86	C33-C32-C31	3.67	112.78	109.21
35	F	301	A86	C17-C16-C15	3.67	112.91	109.16
36	W	209	CLA	CMB-C2B-C3B	3.67	131.54	124.68
34	D	301	DD6	C9-C10-C11	-3.67	122.08	127.31
36	O	314	CLA	CAA-C2A-C3A	-3.66	107.55	116.10
35	E	302	A86	C25-C26-C27	-3.66	122.08	127.31
36	T	314	CLA	CHB-C4A-NA	3.66	129.58	124.51
35	M	301	A86	O4-C38-O5	-3.66	115.68	122.96
36	G	313	CLA	CAA-C2A-C3A	-3.66	102.75	112.78
36	I	306	CLA	C2C-C1C-NC	3.66	113.40	109.97
36	R	310	CLA	CMB-C2B-C3B	3.66	131.53	124.68
36	V	314	CLA	CHB-C4A-NA	3.66	129.57	124.51
35	N	306	A86	C3-C2-C1	-3.66	122.09	127.31
36	L	316	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
36	T	311	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
36	E	312	CLA	CMB-C2B-C3B	3.66	131.52	124.68
37	S	316	KC1	C4B-C3B-C2B	-3.66	103.75	106.75
36	I	308	CLA	C3D-C4D-ND	3.65	116.15	110.24
37	C	213	KC1	CAC-C3C-C4C	3.65	129.55	124.81
34	D	303	DD6	C3-C4-C5	3.65	130.95	123.47
35	G	306	A86	C7-C6-C5	-3.65	117.81	122.92
35	L	319	A86	C28-C27-C26	-3.65	117.81	122.92
37	M	318	KC1	C1B-CHB-C4A	-3.65	118.19	126.06
36	I	204	CLA	C2C-C1C-NC	3.65	113.39	109.97
36	S	313	CLA	CMB-C2B-C3B	3.65	131.50	124.68
37	O	313	KC1	CHB-C1B-C2B	-3.65	117.83	125.48
37	U	312	KC1	CHB-C4A-C3A	-3.64	119.28	124.98
35	X	301	A86	C25-C26-C27	-3.64	122.11	127.31
35	T	303	A86	C28-C27-C26	-3.64	117.82	122.92
37	Q	311	KC1	CHB-C1B-C2B	-3.64	117.84	125.48
36	N	313	CLA	CAA-C2A-C3A	-3.64	107.60	116.10
36	F	310	CLA	CMB-C2B-C3B	3.64	131.49	124.68
35	G	306	A86	C8-C6-C5	3.64	124.53	118.94
37	W	213	KC1	CHB-C4A-NA	3.64	129.94	124.20
37	V	312	KC1	C4B-C3B-C2B	-3.64	103.76	106.75
36	V	306	CLA	CMC-C2C-C1C	3.64	130.58	125.04
35	C	204	A86	C4-C3-C2	3.64	130.93	123.47
37	O	315	KC1	CHB-C1B-C2B	-3.64	117.85	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	Q	313	KC1	CHB-C1B-C2B	-3.64	117.85	125.48
36	b	816	CLA	CHD-C1D-ND	-3.64	121.11	124.45
35	T	305	A86	O2-C18-C19	-3.64	102.57	109.80
36	a	831	CLA	CMB-C2B-C3B	3.64	131.48	124.68
36	S	311	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
37	P	315	KC1	CHB-C1B-C2B	-3.63	117.86	125.48
37	G	318	KC1	O2D-CGD-O1D	-3.63	116.73	123.84
37	W	213	KC1	CAA-C2A-C1A	3.63	141.45	124.75
36	b	817	CLA	CAC-C3C-C4C	3.63	129.52	124.81
36	V	310	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
35	F	306	A86	C4-C5-C6	-3.63	122.13	127.31
36	F	313	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
36	M	307	CLA	C1-C2-C3	3.63	132.32	126.04
35	X	301	A86	C23-C16-C22	-3.63	102.02	107.37
36	M	314	CLA	CAA-C2A-C3A	-3.63	107.63	116.10
36	j	106	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
35	M	304	A86	O1-C20-C19	-3.63	110.66	113.38
36	V	313	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
36	a	834	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
36	N	312	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
35	T	305	A86	O1-C15-C20	-3.63	55.86	59.40
35	F	305	A86	C41-C32-C31	3.62	113.72	110.47
34	C	201	DD6	C9-C10-C11	-3.62	122.14	127.31
36	R	319	CLA	CMC-C2C-C1C	-3.62	119.53	125.04
36	O	308	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
35	F	307	A86	C41-C32-C33	3.62	125.30	109.05
36	O	309	CLA	CMB-C2B-C3B	3.62	131.45	124.68
35	B	303	A86	O1-C15-C20	-3.62	55.86	59.40
36	G	309	CLA	C1-O2A-CGA	3.62	125.93	116.44
37	F	315	KC1	C4C-C3C-C2C	-3.61	101.63	106.90
36	B	309	CLA	C6-C5-C3	-3.61	108.71	114.62
36	b	841	CLA	CMB-C2B-C3B	3.61	131.44	124.68
37	E	309	KC1	C4B-C3B-C2B	-3.61	103.78	106.75
36	Q	307	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
35	O	302	A86	C28-C27-C26	-3.61	117.86	122.92
35	Q	316	A86	O1-C15-C14	-3.61	105.96	113.21
36	a	830	CLA	C1-C2-C3	-3.61	120.91	126.75
36	E	315	CLA	C3D-C4D-ND	3.61	116.08	110.24
35	N	305	A86	O1-C15-C14	-3.61	105.96	113.21
36	P	318	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
35	C	204	A86	C25-C26-C27	3.61	132.46	127.31
37	W	217	KC1	C2A-C3A-C4A	3.61	109.16	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	J	304	DD6	C4-C5-C6	-3.61	122.16	127.31
44	b	846	BCR	C11-C10-C9	-3.61	122.16	127.31
36	a	809	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
35	C	202	A86	C3-C2-C1	-3.61	122.17	127.31
35	R	304	A86	C25-C26-C27	-3.61	122.17	127.31
37	S	316	KC1	C3C-C4C-NC	3.60	113.27	109.88
35	O	302	A86	O1-C15-C20	-3.60	55.88	59.40
37	R	317	KC1	C2A-C1A-NA	3.60	115.18	109.40
34	S	306	DD6	C15-C14-C13	-3.60	118.38	125.99
35	K	301	A86	C34-O4-C38	-3.60	111.19	117.90
35	P	303	A86	C28-C27-C26	-3.60	117.88	122.92
36	K	307	CLA	CHB-C4A-NA	3.60	129.49	124.51
36	P	311	CLA	CMB-C2B-C3B	3.60	131.41	124.68
35	M	305	A86	O1-C15-C20	-3.60	55.88	59.40
36	R	311	CLA	CMB-C2B-C3B	3.60	131.41	124.68
36	Q	308	CLA	CMB-C2B-C3B	3.60	131.41	124.68
36	L	308	CLA	CMD-C2D-C3D	-3.60	119.34	127.61
36	N	307	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
35	W	202	A86	C41-C32-C31	-3.59	107.25	110.47
36	I	306	CLA	C1D-ND-C4D	-3.59	103.78	106.33
37	X	311	KC1	C2A-C3A-C4A	3.59	109.15	106.49
36	H	318	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
34	M	303	DD6	C15-C14-C13	-3.59	118.40	125.99
36	R	322	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
36	I	305	CLA	CMB-C2B-C3B	3.59	131.39	124.68
36	b	831	CLA	CMB-C2B-C3B	3.58	131.38	124.68
35	T	302	A86	C41-C32-C31	-3.58	107.27	110.47
36	a	823	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
36	E	308	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
36	E	315	CLA	C1-C2-C3	-3.58	119.86	126.04
36	K	315	CLA	CAA-C2A-C3A	-3.58	107.75	116.10
35	R	301	A86	O1-C15-C20	-3.58	55.90	59.40
36	H	310	CLA	CMD-C2D-C1D	-3.57	118.41	124.71
36	R	312	CLA	CMB-C2B-C3B	3.57	131.37	124.68
35	A	316	A86	C3-C2-C1	-3.57	122.21	127.31
36	S	314	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
35	X	301	A86	C34-O4-C38	3.57	124.55	117.90
37	L	315	KC1	C4C-C3C-C2C	-3.57	101.69	106.90
36	F	316	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
36	P	310	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
36	b	808	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
37	R	317	KC1	C2B-C1B-NB	3.57	112.73	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	Q	304	A86	O1-C15-C20	-3.57	55.91	59.40
36	j	102	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
36	R	315	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
35	L	319	A86	O1-C15-C20	-3.57	55.91	59.40
36	X	307	CLA	CMB-C2B-C3B	3.57	131.35	124.68
36	b	812	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
36	X	307	CLA	CBC-CAC-C3C	-3.56	102.61	112.43
35	P	303	A86	O1-C15-C20	-3.56	55.92	59.40
44	b	846	BCR	C2-C1-C6	3.56	115.97	110.48
36	a	802	CLA	C1-C2-C3	-3.56	119.88	126.04
36	U	306	CLA	C2C-C1C-NC	3.56	113.31	109.97
34	D	305	DD6	C3-C2-C1	-3.56	122.23	127.31
36	j	102	CLA	CAC-C3C-C4C	3.56	129.43	124.81
36	X	309	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
34	W	204	DD6	C9-C10-C11	-3.56	122.23	127.31
35	F	306	A86	C25-C26-C27	-3.56	122.23	127.31
35	N	320	A86	O1-C15-C20	-3.56	55.92	59.40
35	R	306	A86	C23-C16-C17	-3.56	102.80	108.98
35	T	302	A86	C4-C5-C6	-3.56	122.23	127.31
37	N	314	KC1	C3C-C4C-NC	3.56	113.22	109.88
36	W	212	CLA	CMA-C3A-C2A	-3.56	99.48	113.83
35	I	301	A86	O1-C15-C14	-3.56	106.08	113.21
34	H	302	DD6	C4-C5-C6	-3.55	122.24	127.31
36	b	839	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
36	A	307	CLA	CMB-C2B-C3B	3.55	131.32	124.68
36	H	318	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
36	a	828	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
37	B	310	KC1	CHD-C4C-NC	3.55	129.59	124.20
37	A	312	KC1	C2B-C1B-NB	3.55	112.72	110.10
35	K	303	A86	C4-C3-C2	-3.54	116.21	123.47
34	D	304	DD6	C4-C5-C6	-3.54	122.25	127.31
36	A	305	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
44	b	844	BCR	C28-C27-C26	-3.54	107.75	114.08
35	E	305	A86	C4-C5-C6	-3.54	122.26	127.31
36	Q	312	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
36	G	309	CLA	CHB-C4A-NA	3.54	129.41	124.51
35	K	306	A86	C34-O4-C38	-3.54	111.30	117.90
35	F	302	A86	C25-C26-C27	-3.54	122.26	127.31
36	S	310	CLA	CMB-C2B-C3B	3.54	131.30	124.68
36	N	319	CLA	O1D-CGD-CBD	3.54	131.72	124.48
35	T	307	A86	C41-C32-C31	-3.54	107.31	110.47
36	K	311	CLA	CMB-C2B-C1B	-3.54	123.03	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	317	KC1	C4B-C3B-C2B	-3.54	103.85	106.75
36	N	313	CLA	C4A-NA-C1A	3.53	108.30	106.71
36	P	316	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
36	G	314	CLA	CAA-C2A-C3A	-3.53	107.86	116.10
36	S	311	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
35	X	302	A86	C9-C8-C6	-3.53	116.50	126.42
36	b	828	CLA	CMB-C2B-C3B	3.53	131.28	124.68
35	N	304	A86	C24-C1-C2	3.53	124.36	118.94
36	F	317	CLA	CMC-C2C-C1C	3.53	130.41	125.04
35	G	304	A86	C33-C32-C31	-3.53	105.78	109.21
37	V	312	KC1	CHD-C4C-NC	3.53	129.55	124.20
34	D	301	DD6	C14-C13-C11	-3.53	120.06	125.53
36	X	309	CLA	CAA-C2A-C1A	3.53	123.53	111.97
35	C	203	A86	C4-C5-C6	-3.53	122.28	127.31
36	O	314	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
35	B	301	A86	C34-O4-C38	-3.52	111.33	117.90
35	W	202	A86	O1-C15-C20	-3.52	55.95	59.40
39	F	321	LMT	C1B-C2B-C3B	3.52	117.33	110.00
36	I	306	CLA	CHB-C4A-NA	3.52	129.38	124.51
36	E	315	CLA	C1D-ND-C4D	-3.52	103.83	106.33
36	b	818	CLA	C1B-CHB-C4A	-3.52	123.14	130.12
35	I	302	A86	C4-C5-C6	-3.52	122.29	127.31
36	N	316	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
36	T	312	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
36	G	313	CLA	CBA-CAA-C2A	3.52	124.24	113.86
35	A	302	A86	C3-C2-C1	-3.51	122.30	127.31
35	B	303	A86	O-C13-C14	-3.51	114.52	121.66
36	b	819	CLA	CAA-C2A-C1A	-3.51	100.47	111.97
36	N	312	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
35	A	316	A86	C25-C26-C27	-3.51	122.30	127.31
35	W	203	A86	C9-C8-C6	-3.51	116.57	126.42
37	B	310	KC1	CBD-CHA-C1A	3.51	135.42	128.88
34	K	305	DD6	C15-C14-C13	-3.51	118.58	125.99
36	N	318	CLA	CMB-C2B-C3B	3.51	131.24	124.68
35	G	306	A86	C-C1-C2	-3.51	118.01	122.92
35	G	302	A86	O1-C20-C19	-3.51	110.75	113.38
34	a	849	DD6	C14-C13-C11	-3.50	120.09	125.53
36	h	203	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
35	M	301	A86	O1-C15-C20	-3.50	55.98	59.40
37	A	312	KC1	O2D-CGD-O1D	-3.50	116.99	123.84
36	a	822	CLA	C1-C2-C3	-3.50	119.99	126.04
36	E	308	CLA	CMB-C2B-C1B	-3.50	123.08	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	W	215	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
35	A	302	A86	C23-C16-C17	-3.50	102.91	108.98
36	R	312	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
36	R	316	CLA	CBC-CAC-C3C	3.49	122.06	112.43
36	M	314	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
36	R	320	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
36	I	313	CLA	CAA-C2A-C3A	-3.49	107.95	116.10
37	M	318	KC1	CMA-C3A-C4A	3.49	130.36	125.04
35	J	301	A86	C17-C16-C15	3.49	112.72	109.16
36	a	836	CLA	O1D-CGD-CBD	3.49	131.63	124.48
36	S	320	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
36	R	315	CLA	CHB-C4A-NA	3.49	129.34	124.51
35	K	302	A86	O1-C20-C21	-3.49	110.88	115.06
34	W	204	DD6	C14-C13-C11	-3.48	120.12	125.53
36	O	316	CLA	C1-C2-C3	-3.48	120.02	126.04
35	N	304	A86	C-C1-C2	-3.48	118.04	122.92
35	T	307	A86	O1-C15-C20	-3.48	56.00	59.40
35	T	307	A86	O4-C34-C35	-3.48	98.92	107.59
36	S	321	CLA	CHB-C4A-NA	3.48	129.32	124.51
36	M	310	CLA	C2A-C1A-CHA	3.48	129.94	123.86
37	R	317	KC1	CAC-C3C-C4C	3.48	129.32	124.81
37	D	314	KC1	C4B-C3B-C2B	-3.48	103.90	106.75
35	X	303	A86	C23-C16-C22	-3.48	102.24	107.37
35	J	302	A86	C3-C2-C1	-3.48	122.35	127.31
35	J	302	A86	C25-C26-C27	-3.48	122.35	127.31
35	R	305	A86	O1-C20-C21	-3.48	110.89	115.06
37	F	315	KC1	C3A-C4A-NA	3.48	114.37	110.57
36	N	308	CLA	CMB-C2B-C3B	3.47	131.18	124.68
36	S	317	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
36	S	313	CLA	CHB-C4A-NA	3.47	129.31	124.51
36	C	205	CLA	CMB-C2B-C3B	3.47	131.17	124.68
37	N	314	KC1	C2A-C1A-CHA	-3.47	115.97	127.44
35	W	202	A86	C33-C32-C31	-3.47	105.84	109.21
34	O	304	DD6	C3-C2-C1	-3.47	122.36	127.31
36	f	805	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
36	J	315	CLA	CAA-C2A-C3A	-3.47	108.01	116.10
37	D	314	KC1	C4C-C3C-C2C	-3.46	101.85	106.90
35	R	302	A86	C4-C5-C6	-3.46	122.37	127.31
35	P	306	A86	C34-O4-C38	-3.46	111.44	117.90
36	X	313	CLA	O1D-CGD-CBD	3.46	131.57	124.48
36	O	310	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
36	C	207	CLA	CHB-C4A-NA	3.46	129.30	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	V	304	A86	C4-C5-C6	-3.46	122.37	127.31
35	L	306	A86	C36-C31-C32	-3.46	116.26	119.70
35	C	202	A86	O1-C15-C20	-3.46	56.02	59.40
36	B	306	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
37	O	313	KC1	CAA-C2A-C1A	3.46	140.65	124.75
34	L	305	DD6	C4-C5-C6	-3.46	122.37	127.31
41	a	843	LHG	O8-C23-C24	3.46	120.45	111.38
36	a	838	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
36	R	322	CLA	O2D-CGD-CBD	-3.46	105.12	111.27
36	X	308	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
36	W	210	CLA	CAA-C2A-C1A	3.45	123.30	111.97
36	I	305	CLA	C12-C11-C10	3.45	129.11	113.24
34	H	302	DD6	C15-C14-C13	-3.45	118.69	125.99
37	P	317	KC1	C3B-C2B-C1B	-3.45	103.78	107.08
37	P	315	KC1	CAA-C2A-C1A	3.45	140.60	124.75
36	b	822	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
36	D	306	CLA	CAA-CBA-CGA	3.45	121.66	112.51
35	X	302	A86	O1-C15-C20	-3.45	56.03	59.40
35	A	302	A86	O1-C15-C20	-3.45	56.03	59.40
35	I	304	A86	C35-C34-C33	-3.45	103.86	109.88
36	M	307	CLA	CMB-C2B-C3B	3.45	131.13	124.68
36	L	312	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
37	O	315	KC1	CAA-C2A-C1A	3.45	140.59	124.75
36	O	312	CLA	CHA-C1A-NA	-3.45	118.66	126.41
37	Q	311	KC1	CAA-C2A-C1A	3.45	140.59	124.75
34	R	308	DD6	C14-C13-C11	-3.45	120.18	125.53
36	H	311	CLA	O2D-CGD-CBD	3.45	117.39	111.27
35	J	301	A86	C34-O4-C38	-3.45	111.48	117.90
36	f	803	CLA	C1-C2-C3	-3.44	120.08	126.04
36	U	313	CLA	CMB-C2B-C3B	3.44	131.12	124.68
36	b	819	CLA	C3A-C2A-C1A	3.44	106.50	101.34
37	Q	313	KC1	CAA-C2A-C1A	3.44	140.58	124.75
35	A	302	A86	C40-C32-C33	3.44	124.51	109.05
44	h	201	BCR	C39-C30-C25	-3.44	104.72	110.30
35	M	301	A86	C4-C5-C6	-3.44	122.40	127.31
36	U	305	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
37	H	313	KC1	CBD-CHA-C1A	3.44	135.30	128.88
35	R	305	A86	C25-C26-C27	-3.44	122.40	127.31
35	H	301	A86	C4-C3-C2	-3.44	116.43	123.47
36	a	839	CLA	CMB-C2B-C3B	3.44	131.11	124.68
37	M	317	KC1	C4B-C3B-C2B	-3.44	103.93	106.75
35	Q	304	A86	C25-C24-C1	-3.44	116.77	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	I	308	CLA	CHD-C4C-C3C	-3.43	119.79	124.84
36	R	318	CLA	CMB-C2B-C3B	3.43	131.10	124.68
35	N	320	A86	C25-C24-C1	-3.43	116.77	126.42
35	T	305	A86	C25-C26-C27	-3.43	122.41	127.31
36	f	803	CLA	C3B-C4B-NB	3.43	113.65	109.21
37	W	213	KC1	C3C-C4C-NC	3.43	113.11	109.88
34	A	301	DD6	C4-C5-C6	-3.43	122.41	127.31
36	G	315	CLA	C1-C2-C3	-3.43	120.11	126.04
36	L	310	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
34	W	205	DD6	O1-C20-C19	3.43	115.96	113.38
36	Q	309	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
36	N	311	CLA	C2A-C1A-CHA	3.43	129.86	123.86
36	E	316	CLA	CAC-C3C-C2C	3.43	133.39	127.53
36	b	814	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
35	R	309	A86	O1-C15-C20	-3.43	56.05	59.40
37	B	310	KC1	C4B-C3B-C2B	-3.43	103.94	106.75
36	W	211	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
36	b	824	CLA	C1-C2-C3	-3.42	120.12	126.04
36	U	306	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
36	a	803	CLA	O2A-CGA-O1A	-3.42	114.96	123.59
36	P	312	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
36	C	214	CLA	CAA-C2A-C3A	-3.42	108.12	116.10
36	T	313	CLA	CMB-C2B-C3B	3.42	131.08	124.68
35	E	305	A86	C17-C16-C15	3.42	112.65	109.16
35	P	306	A86	O1-C20-C19	-3.42	110.81	113.38
36	W	208	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
37	P	317	KC1	CAA-C2A-C1A	3.42	140.46	124.75
36	f	803	CLA	CAC-C3C-C4C	3.42	129.24	124.81
36	G	319	CLA	C1-C2-C3	-3.42	121.22	126.75
36	b	815	CLA	CMB-C2B-C3B	3.42	131.07	124.68
35	B	301	A86	C3-C2-C1	-3.42	122.44	127.31
37	V	312	KC1	C4D-C3D-CAD	3.42	113.33	107.81
35	K	302	A86	O1-C15-C20	-3.41	56.06	59.40
36	H	315	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
36	j	101	CLA	CMB-C2B-C3B	3.41	131.07	124.68
36	a	802	CLA	C4D-C3D-CAD	-3.41	104.07	108.10
35	L	304	A86	C23-C16-C17	-3.41	103.05	108.98
36	K	310	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
35	U	301	A86	C9-C10-C11	-3.41	116.58	126.61
36	b	811	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
36	l	206	CLA	CMB-C2B-C3B	3.41	131.06	124.68
36	b	828	CLA	O2D-CGD-O1D	-3.41	117.17	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	K	304	DD6	C9-C10-C11	-3.41	122.44	127.31
36	W	214	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
36	V	309	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
36	W	212	CLA	CAA-C2A-C3A	-3.41	103.44	112.78
36	b	830	CLA	O2D-CGD-CBD	3.41	117.32	111.27
36	R	316	CLA	CAA-C2A-C3A	-3.41	103.45	112.78
37	E	309	KC1	CAC-C3C-C4C	-3.41	120.39	124.81
36	D	307	CLA	CMB-C2B-C3B	3.41	131.05	124.68
35	U	302	A86	C4-C3-C2	-3.40	116.50	123.47
36	X	310	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
35	L	306	A86	C-C1-C2	-3.40	118.16	122.92
37	M	317	KC1	CHB-C4A-NA	3.40	129.57	124.20
36	P	308	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
35	N	306	A86	C23-C16-C17	-3.40	103.07	108.98
36	R	311	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
36	b	808	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
36	S	310	CLA	O2A-C1-C2	3.40	117.57	108.64
36	R	314	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
34	a	849	DD6	C9-C10-C11	-3.40	122.46	127.31
36	Q	305	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
35	L	304	A86	C3-C2-C1	-3.39	122.47	127.31
37	R	317	KC1	C3A-C4A-NA	3.39	114.27	110.57
35	R	309	A86	C23-C16-C17	-3.39	103.09	108.98
36	O	306	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
37	K	314	KC1	C3C-C4C-NC	3.39	113.07	109.88
35	X	302	A86	C9-C10-C11	-3.39	116.65	126.61
36	S	315	CLA	CHB-C4A-NA	3.39	129.20	124.51
36	G	307	CLA	C3D-C4D-ND	3.39	115.72	110.24
36	H	309	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
34	P	305	DD6	C37-C36-C35	3.39	120.63	114.36
35	G	302	A86	C4-C5-C6	-3.39	122.48	127.31
36	D	308	CLA	CBC-CAC-C3C	3.38	121.76	112.43
36	a	809	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
36	b	819	CLA	CHB-C4A-NA	3.38	129.19	124.51
35	L	306	A86	C26-C25-C24	-3.38	112.66	123.22
36	A	314	CLA	CGD-CBD-CAD	3.38	121.69	110.73
36	b	840	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
36	P	314	CLA	CHA-C1A-NA	-3.38	118.66	126.40
35	U	303	A86	C34-O4-C38	-3.38	111.60	117.90
36	D	306	CLA	CAC-C3C-C4C	3.38	129.19	124.81
36	l	202	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
36	B	311	CLA	CHB-C4A-NA	3.38	129.18	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	I	314	CLA	CAA-C2A-C3A	-3.38	108.22	116.10
36	Q	310	CLA	CHA-C1A-NA	-3.38	118.66	126.40
36	G	313	CLA	CAA-CBA-CGA	3.38	123.12	113.25
34	E	304	DD6	C4-C5-C6	-3.38	122.49	127.31
36	K	313	CLA	O2D-CGD-CBD	3.37	117.26	111.27
36	H	310	CLA	CHB-C4A-NA	3.37	129.18	124.51
35	I	304	A86	O1-C15-C20	-3.37	56.10	59.40
35	J	303	A86	O1-C20-C21	-3.37	111.01	115.06
36	a	808	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
35	G	306	A86	C25-C24-C1	-3.37	116.94	126.42
35	V	302	A86	C4-C5-C6	-3.37	122.50	127.31
35	X	301	A86	O1-C15-C20	-3.37	56.11	59.40
36	G	314	CLA	O2D-CGD-O1D	-3.37	117.26	123.84
35	R	304	A86	C35-C34-C33	-3.37	104.00	109.88
39	F	321	LMT	C1B-O5B-C5B	3.36	120.29	113.69
36	h	203	CLA	CMB-C2B-C3B	3.36	130.97	124.68
36	b	823	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
36	U	308	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
36	M	308	CLA	CAC-C3C-C2C	3.36	133.28	127.53
36	M	308	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
34	O	304	DD6	C34-C35-C36	-3.36	105.16	111.85
36	S	309	CLA	CMB-C2B-C3B	3.36	130.96	124.68
34	P	305	DD6	C32-C31-C36	-3.36	117.89	122.63
36	H	307	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
36	G	307	CLA	CHB-C4A-NA	3.36	129.16	124.51
34	E	306	DD6	C37-C36-C35	3.36	120.57	114.36
34	E	306	DD6	C32-C31-C36	-3.36	117.89	122.63
36	b	826	CLA	CHB-C4A-NA	3.35	129.15	124.51
37	R	317	KC1	C2A-C3A-C4A	3.35	108.97	106.49
36	P	319	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
36	a	821	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
36	L	308	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
36	b	830	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
35	P	303	A86	C41-C32-C31	-3.35	107.47	110.47
36	J	311	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
36	a	811	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
36	a	837	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
35	T	305	A86	C23-C16-C17	-3.35	103.17	108.98
36	H	307	CLA	C4D-CHA-C1A	3.35	125.32	121.25
36	b	834	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
36	S	319	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
36	C	211	CLA	CMB-C2B-C3B	3.34	130.93	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	839	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
36	T	308	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
36	E	313	CLA	CMC-C2C-C1C	3.34	130.13	125.04
35	X	303	A86	C3-C4-C5	-3.34	116.63	123.47
35	R	302	A86	C3-C4-C5	-3.34	116.63	123.47
36	W	201	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
35	J	303	A86	C4-C3-C2	-3.34	116.63	123.47
37	E	309	KC1	C1C-C2C-C3C	-3.34	103.44	106.96
36	W	216	CLA	CMB-C2B-C1B	3.34	133.60	128.46
34	C	201	DD6	C37-C36-C31	-3.34	119.81	124.35
37	X	311	KC1	CMD-C2D-C3D	3.34	130.92	124.68
37	C	213	KC1	CAA-C2A-C1A	3.34	140.08	124.75
34	B	304	DD6	C37-C36-C35	3.34	120.54	114.36
35	L	306	A86	C9-C10-C11	-3.34	116.80	126.61
36	b	813	CLA	CAB-C3B-C4B	-3.34	123.34	128.46
37	G	317	KC1	O2D-CGD-O1D	-3.34	117.32	123.84
36	F	313	CLA	O2D-CGD-O1D	-3.34	117.32	123.84
36	K	310	CLA	C3D-C4D-ND	3.34	115.63	110.24
35	K	303	A86	O4-C38-C39	3.33	117.22	111.09
36	b	829	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
35	O	302	A86	C41-C32-C31	-3.33	107.49	110.47
37	W	217	KC1	C3C-C4C-NC	3.33	113.02	109.88
35	R	306	A86	O4-C38-C39	3.33	117.22	111.09
37	W	217	KC1	CMD-C2D-C3D	3.33	130.91	124.68
36	L	320	CLA	CMB-C2B-C3B	3.33	130.91	124.68
36	U	309	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
36	B	308	CLA	CHD-C1D-ND	-3.33	121.39	124.45
36	a	823	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
36	G	312	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
35	R	306	A86	O1-C15-C20	-3.33	56.14	59.40
36	K	312	CLA	CMB-C2B-C3B	3.33	130.91	124.68
35	S	305	A86	C28-C27-C26	-3.33	118.26	122.92
36	U	313	CLA	C2A-C1A-CHA	3.33	129.66	123.85
35	I	304	A86	C7-C6-C8	3.33	123.32	118.08
35	C	202	A86	C23-C16-C17	-3.33	103.20	108.98
36	a	816	CLA	CMD-C2D-C3D	-3.32	119.97	127.61
36	H	311	CLA	CHB-C4A-NA	3.32	129.11	124.51
36	D	311	CLA	CMB-C2B-C3B	3.32	130.90	124.68
36	a	817	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
34	R	308	DD6	C37-C36-C31	-3.32	119.83	124.35
37	H	313	KC1	C4C-C3C-C2C	-3.32	102.06	106.90
35	L	319	A86	C41-C32-C31	-3.32	107.50	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	312	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
36	a	816	CLA	C1-C2-C3	-3.32	120.30	126.04
37	G	317	KC1	O1D-CGD-CBD	3.32	131.28	124.48
35	R	303	A86	O1-C20-C21	-3.32	111.08	115.06
36	K	309	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
36	U	310	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
36	U	313	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
36	P	319	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
36	V	310	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
36	b	831	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
36	P	319	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
36	b	805	CLA	C7-C6-C5	-3.31	104.36	113.36
36	O	311	CLA	CMB-C2B-C3B	3.31	130.88	124.68
36	P	313	CLA	CMB-C2B-C3B	3.31	130.88	124.68
36	R	316	CLA	CMB-C2B-C3B	3.31	130.87	124.68
36	N	316	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
35	G	302	A86	C34-O4-C38	-3.31	111.73	117.90
36	J	315	CLA	CMB-C2B-C3B	3.31	130.87	124.68
36	U	310	CLA	C2D-C1D-ND	-3.31	107.67	110.10
35	L	307	A86	O1-C20-C19	-3.31	110.90	113.38
36	f	804	CLA	C1-C2-C3	-3.31	120.32	126.04
36	W	214	CLA	CAC-C3C-C2C	-3.31	121.87	127.53
34	R	307	DD6	C21-C20-C15	-3.31	116.72	122.26
36	U	309	CLA	CAA-C2A-C1A	3.31	122.81	111.97
37	X	311	KC1	C3C-C4C-NC	3.31	112.99	109.88
34	S	307	DD6	C37-C36-C31	-3.30	119.86	124.35
36	A	311	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
36	a	834	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
35	X	303	A86	O1-C20-C19	3.30	115.86	113.38
36	X	313	CLA	CHC-C1C-C2C	-3.30	117.59	126.72
35	F	307	A86	O4-C34-C35	-3.30	99.37	107.59
35	L	306	A86	C21-C20-C19	3.30	117.99	114.28
36	N	311	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
37	P	315	KC1	CMA-C3A-C4A	-3.30	120.01	125.04
36	D	309	CLA	C1-C2-C3	-3.30	120.34	126.04
36	E	317	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
36	U	308	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
36	F	312	CLA	CMB-C2B-C3B	3.30	130.85	124.68
35	G	304	A86	C4-C3-C2	-3.30	116.72	123.47
35	X	303	A86	C25-C24-C1	-3.30	117.16	126.42
36	b	821	CLA	O2D-CGD-CBD	3.30	117.12	111.27
35	M	302	A86	C23-C16-C17	-3.30	103.26	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	312	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
37	O	313	KC1	CMA-C3A-C4A	-3.30	120.02	125.04
36	M	311	CLA	CMB-C2B-C3B	3.29	130.84	124.68
36	E	313	CLA	C1-C2-C3	-3.29	120.35	126.04
36	H	307	CLA	CHB-C4A-NA	3.29	129.07	124.51
36	N	318	CLA	CHB-C4A-NA	3.29	129.07	124.51
35	L	304	A86	O1-C15-C20	-3.29	56.18	59.40
36	C	210	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
35	K	301	A86	C9-C10-C11	-3.29	116.94	126.61
36	I	311	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
36	M	309	CLA	CMB-C2B-C3B	3.29	130.83	124.68
36	I	306	CLA	C1-C2-C3	-3.29	120.36	126.04
35	E	307	A86	C17-C16-C15	3.29	112.52	109.16
35	S	304	A86	C40-C32-C31	-3.29	107.53	110.47
36	U	313	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
36	F	314	CLA	CMB-C2B-C3B	3.29	130.83	124.68
37	L	315	KC1	C4D-C3D-CAD	3.29	113.12	107.81
36	G	319	CLA	CAC-C3C-C4C	3.29	129.07	124.81
35	I	302	A86	C3-C2-C1	-3.29	122.62	127.31
34	I	303	DD6	C37-C36-C35	3.29	120.44	114.36
37	G	308	KC1	C2A-C1A-NA	3.29	114.67	109.40
37	Q	311	KC1	CMA-C3A-C4A	-3.28	120.04	125.04
36	N	311	CLA	CHB-C4A-NA	3.28	129.05	124.51
35	N	306	A86	C28-C27-C26	-3.28	118.32	122.92
36	a	808	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
36	a	830	CLA	C3D-C2D-C1D	-3.28	101.35	105.83
36	a	838	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
36	T	308	CLA	CAC-C3C-C4C	3.28	129.07	124.81
36	V	309	CLA	CHB-C4A-NA	3.28	129.05	124.51
36	S	312	CLA	CMA-C3A-C2A	-3.28	100.60	113.83
35	H	301	A86	O1-C15-C20	-3.28	56.19	59.40
36	V	314	CLA	CMC-C2C-C1C	3.28	130.03	125.04
39	F	321	LMT	C4B-C3B-C2B	3.28	116.55	110.82
35	R	303	A86	O1-C20-C19	-3.28	110.92	113.38
37	S	316	KC1	CMA-C3A-C4A	-3.28	120.05	125.04
35	Q	303	A86	O1-C20-C19	-3.27	110.92	113.38
37	F	308	KC1	C3A-C4A-NA	3.27	114.15	110.57
36	C	214	CLA	CMA-C3A-C2A	-3.27	108.46	116.10
36	X	313	CLA	C1D-ND-C4D	-3.27	104.01	106.33
36	b	813	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
37	O	315	KC1	CMA-C3A-C4A	-3.27	120.05	125.04
36	D	306	CLA	C2A-C1A-CHA	3.27	129.58	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	L	307	A86	C34-O4-C38	-3.27	111.80	117.90
36	U	311	CLA	CHB-C4A-NA	3.27	129.04	124.51
37	Q	313	KC1	CMA-C3A-C4A	-3.27	120.06	125.04
36	a	815	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
35	G	304	A86	C7-C6-C8	3.27	123.23	118.08
34	G	303	DD6	C15-C14-C13	-3.27	119.08	125.99
35	O	301	A86	C25-C26-C27	-3.27	122.64	127.31
36	E	316	CLA	CAC-C3C-C4C	-3.27	120.57	124.81
36	X	306	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
35	H	301	A86	C25-C26-C27	-3.27	122.65	127.31
35	L	301	A86	C3-C2-C1	-3.27	122.65	127.31
35	O	319	A86	C23-C16-C17	-3.27	103.31	108.98
37	J	314	KC1	C4C-C3C-C2C	-3.27	102.14	106.90
35	K	303	A86	C25-C26-C27	-3.26	122.65	127.31
35	J	303	A86	C17-C16-C15	3.26	112.49	109.16
36	S	317	CLA	CAA-C2A-C3A	-3.26	108.48	116.10
36	C	207	CLA	C1-C2-C3	-3.26	120.40	126.04
36	N	308	CLA	CMA-C3A-C4A	3.26	120.54	111.77
35	F	304	A86	C17-C16-C15	3.26	112.49	109.16
37	J	314	KC1	CAC-C3C-C4C	3.26	129.04	124.81
36	A	314	CLA	C2A-C1A-CHA	3.26	129.56	123.86
37	T	310	KC1	C4B-CHC-C1C	-3.26	119.03	126.06
36	a	832	CLA	O2D-CGD-CBD	3.26	117.06	111.27
36	D	306	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
36	I	313	CLA	CMB-C2B-C3B	3.26	130.77	124.68
36	b	833	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
35	N	301	A86	O-C13-C11	-3.26	113.95	121.15
35	L	307	A86	C25-C26-C27	-3.26	122.66	127.31
37	F	308	KC1	C1C-C2C-C3C	-3.25	103.53	106.96
36	b	825	CLA	CMB-C2B-C3B	3.25	130.76	124.68
36	S	318	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
36	b	824	CLA	C4A-NA-C1A	3.25	108.17	106.71
36	R	314	CLA	C2A-C1A-CHA	3.25	129.54	123.86
35	S	301	A86	O-C13-C11	-3.25	113.97	121.15
36	M	312	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
36	W	207	CLA	CMB-C2B-C3B	3.25	130.76	124.68
34	E	306	DD6	C9-C10-C11	-3.25	122.67	127.31
36	A	314	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
35	U	304	A86	C25-C26-C27	-3.25	122.68	127.31
36	b	820	CLA	CMB-C2B-C3B	3.25	130.75	124.68
36	S	314	CLA	C1B-CHB-C4A	-3.25	123.69	130.12
34	D	303	DD6	C37-C36-C31	-3.25	119.94	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	208	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
36	L	308	CLA	C1-C2-C3	-3.24	120.44	126.04
36	I	312	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
35	E	305	A86	C34-O4-C38	-3.24	111.86	117.90
36	O	310	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
36	D	316	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
36	G	319	CLA	CHD-C4C-C3C	-3.24	120.08	124.84
36	b	805	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
36	F	310	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
36	H	316	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
36	R	316	CLA	CHB-C4A-NA	3.24	128.99	124.51
34	a	849	DD6	O1-C20-C19	-3.24	110.95	113.38
36	a	801	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
36	P	312	CLA	O2D-CGD-O1D	-3.23	117.51	123.84
37	F	308	KC1	CAC-C3C-C2C	3.23	133.06	127.53
36	F	309	CLA	CHD-C1D-ND	-3.23	121.48	124.45
35	G	306	A86	C9-C10-C11	-3.23	117.10	126.61
36	b	809	CLA	CMB-C2B-C3B	3.23	130.73	124.68
36	J	308	CLA	CMB-C2B-C3B	3.23	130.72	124.68
36	U	309	CLA	C2A-C1A-CHA	3.23	129.51	123.86
35	V	302	A86	C41-C32-C31	-3.23	107.58	110.47
36	Q	310	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
35	T	305	A86	C10-C9-C8	-3.23	113.15	123.22
36	B	307	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
36	R	319	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
36	K	307	CLA	C3D-C4D-ND	3.23	115.46	110.24
37	H	313	KC1	C3B-C2B-C1B	-3.23	104.00	107.08
36	J	317	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
34	W	204	DD6	C37-C36-C35	3.23	120.33	114.36
36	T	316	CLA	CMB-C2B-C3B	3.23	130.71	124.68
36	Q	309	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
36	b	826	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
36	J	313	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
36	P	314	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
36	a	803	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
36	b	835	CLA	CHB-C4A-NA	3.22	128.97	124.51
35	T	306	A86	O1-C20-C19	3.22	115.80	113.38
36	H	307	CLA	O2D-CGD-CBD	3.22	116.99	111.27
36	I	309	CLA	CAA-C2A-C1A	3.22	122.52	111.97
35	X	303	A86	C7-C6-C8	3.22	123.15	118.08
37	A	312	KC1	C3B-C2B-C1B	-3.22	104.00	107.08
36	W	209	CLA	O2D-CGD-O1D	-3.22	117.55	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	809	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
35	V	303	A86	C4-C3-C2	-3.22	116.89	123.47
36	N	308	CLA	CMC-C2C-C3C	-3.21	117.39	126.12
36	E	313	CLA	CMD-C2D-C3D	-3.21	120.22	127.61
36	R	319	CLA	CHB-C4A-NA	3.21	128.96	124.51
36	B	311	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
36	b	826	CLA	CHA-C4D-ND	3.21	139.22	132.50
36	M	310	CLA	CAA-C2A-C1A	3.21	122.50	111.97
36	U	310	CLA	CMB-C2B-C3B	3.21	130.68	124.68
35	J	301	A86	O1-C15-C14	-3.21	106.77	113.21
36	S	314	CLA	CMB-C2B-C3B	3.21	130.68	124.68
36	H	318	CLA	C1-O2A-CGA	3.21	124.86	116.44
35	W	203	A86	O1-C15-C20	-3.21	56.27	59.40
36	D	313	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
36	F	316	CLA	CMB-C2B-C3B	3.20	130.67	124.68
35	G	306	A86	C24-C1-C2	3.20	123.86	118.94
36	i	102	CLA	CHB-C4A-NA	3.20	128.94	124.51
35	N	306	A86	O1-C15-C20	-3.20	56.27	59.40
36	b	817	CLA	C1-C2-C3	-3.20	120.51	126.04
36	H	308	CLA	O2D-CGD-O1D	-3.20	116.82	124.09
36	S	315	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
35	B	303	A86	C34-O4-C38	-3.20	111.93	117.90
35	X	305	A86	C9-C8-C6	-3.20	117.43	126.42
36	I	305	CLA	C14-C13-C12	-3.20	99.71	111.29
36	N	311	CLA	CAA-C2A-C1A	3.20	122.45	111.97
34	R	307	DD6	C14-C13-C11	-3.20	120.57	125.53
35	V	303	A86	O1-C20-C21	-3.20	111.22	115.06
35	K	303	A86	O1-C15-C20	-3.20	56.27	59.40
36	b	830	CLA	CAC-C3C-C4C	3.20	128.96	124.81
35	S	305	A86	C19-C18-C17	-3.20	104.60	110.77
36	l	202	CLA	CAA-C2A-C3A	-3.20	104.03	112.78
35	V	303	A86	C9-C8-C6	-3.19	117.44	126.42
37	M	313	KC1	C2A-C3A-C4A	3.19	108.86	106.49
35	T	303	A86	C23-C16-C17	-3.19	103.43	108.98
34	I	303	DD6	C14-C13-C11	-3.19	120.58	125.53
36	M	306	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
36	M	306	CLA	CMB-C2B-C3B	3.19	130.65	124.68
36	V	314	CLA	C4D-C3D-CAD	-3.19	104.33	108.10
36	R	314	CLA	CHB-C4A-NA	3.19	128.93	124.51
36	a	814	CLA	CHB-C4A-NA	3.19	128.92	124.51
35	A	302	A86	C34-O4-C38	3.19	123.84	117.90
36	C	212	CLA	CHB-C4A-NA	3.19	128.92	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	R	316	CLA	CAC-C3C-C2C	3.19	132.98	127.53
36	j	106	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
36	C	206	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
35	V	302	A86	C12-C11-C13	3.18	121.37	116.02
36	N	315	CLA	CAA-C2A-C3A	-3.18	108.67	116.10
36	D	309	CLA	C3D-C4D-ND	3.18	115.39	110.24
36	M	306	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
36	G	319	CLA	C3D-C4D-ND	3.18	115.38	110.24
36	b	813	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
36	R	321	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
36	S	321	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
36	T	312	CLA	C2A-C1A-CHA	3.18	129.42	123.86
36	A	306	CLA	CMD-C2D-C3D	-3.18	120.30	127.61
36	K	310	CLA	C1D-ND-C4D	-3.18	104.08	106.33
36	O	312	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
36	E	316	CLA	CMB-C2B-C3B	3.18	130.62	124.68
35	A	302	A86	C4-C3-C2	-3.18	116.97	123.47
34	K	304	DD6	C37-C36-C31	-3.18	120.03	124.35
37	B	310	KC1	C3B-C2B-C1B	-3.17	104.04	107.08
35	I	304	A86	C36-C31-C32	-3.17	116.55	119.70
35	X	314	A86	C34-O4-C38	-3.17	111.98	117.90
36	D	317	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
36	U	306	CLA	C1-C2-C3	-3.17	120.56	126.04
35	W	203	A86	C9-C10-C11	-3.17	117.28	126.61
36	C	209	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
37	G	318	KC1	C1C-C2C-C3C	-3.17	103.62	106.96
35	O	301	A86	C34-O4-C38	-3.17	111.99	117.90
35	J	305	A86	C17-C16-C15	3.17	112.40	109.16
36	G	313	CLA	C3A-C2A-C1A	3.17	106.09	101.34
37	K	314	KC1	C4D-C3D-CAD	3.17	112.93	107.81
36	b	824	CLA	CMD-C2D-C3D	-3.17	120.33	127.61
34	S	307	DD6	C37-C36-C35	3.17	120.22	114.36
35	A	316	A86	C34-O4-C38	-3.17	111.99	117.90
36	G	312	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
36	X	309	CLA	CMB-C2B-C3B	3.17	130.60	124.68
36	a	825	CLA	C1-C2-C3	-3.17	120.57	126.04
36	a	824	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
36	F	317	CLA	C4D-C3D-CAD	3.17	111.83	108.10
35	R	303	A86	O4-C34-C35	3.17	115.47	107.59
35	T	301	A86	C34-O4-C38	-3.16	112.00	117.90
36	G	313	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
36	a	841	CLA	O2D-CGD-O1D	-3.16	117.65	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	E	304	DD6	C9-C10-C11	-3.16	122.79	127.31
35	I	301	A86	C34-O4-C38	-3.16	112.00	117.90
36	a	827	CLA	C1B-CHB-C4A	-3.16	123.85	130.12
36	S	314	CLA	CED-O2D-CGD	3.16	123.09	115.94
36	D	310	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
36	E	313	CLA	CHD-C1D-ND	-3.16	121.55	124.45
35	F	307	A86	C23-C16-C17	-3.16	103.49	108.98
36	A	313	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
36	M	315	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
37	G	317	KC1	C4C-C3C-C2C	-3.16	102.30	106.90
35	P	306	A86	C3-C2-C1	-3.16	122.80	127.31
35	L	306	A86	C41-C32-C31	3.16	113.30	110.47
36	U	308	CLA	CHB-C4A-NA	3.16	128.88	124.51
36	R	320	CLA	C2D-C1D-ND	-3.16	107.78	110.10
36	S	318	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
35	V	301	A86	C34-O4-C38	-3.16	112.02	117.90
37	T	315	KC1	C4C-C3C-C2C	-3.15	102.30	106.90
37	C	213	KC1	C3C-C4C-NC	3.15	112.84	109.88
36	B	311	CLA	C4D-CHA-C1A	-3.15	117.41	121.25
34	K	304	DD6	C15-C14-C13	-3.15	119.33	125.99
35	T	302	A86	O1-C15-C20	-3.15	56.32	59.40
36	W	216	CLA	CMA-C3A-C4A	3.15	120.24	111.77
35	A	302	A86	C9-C10-C11	-3.15	117.35	126.61
36	b	836	CLA	CHD-C4C-C3C	-3.15	120.21	124.84
35	U	301	A86	C34-O4-C38	3.15	123.76	117.90
36	M	315	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
36	O	316	CLA	C3B-C4B-NB	3.15	113.28	109.21
36	A	307	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
34	A	303	DD6	C21-C20-C15	-3.15	116.99	122.26
36	H	307	CLA	C1-O2A-CGA	3.15	124.70	116.44
34	J	304	DD6	C15-C14-C13	-3.15	119.34	125.99
36	V	314	CLA	C1-C2-C3	-3.14	120.60	126.04
36	b	832	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
36	a	848	CLA	C3D-C2D-C1D	-3.14	101.54	105.83
36	S	318	CLA	CAA-C2A-C3A	-3.14	106.41	114.26
36	i	102	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
35	R	305	A86	C34-O4-C38	-3.14	112.05	117.90
36	b	816	CLA	C1-C2-C3	-3.14	120.61	126.04
36	V	309	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
35	T	305	A86	C4-C5-C6	-3.14	122.83	127.31
37	W	213	KC1	C1A-NA-C4A	-3.14	105.30	106.71
43	a	840	PQN	C11-C12-C13	-3.14	121.57	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	305	A86	O1-C15-C20	-3.14	56.33	59.40
36	N	310	CLA	C3C-C4C-NC	-3.14	107.06	110.57
36	E	315	CLA	CHD-C4C-C3C	-3.13	120.23	124.84
36	b	820	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
36	a	814	CLA	CMC-C2C-C3C	3.13	134.63	126.12
36	b	825	CLA	CHB-C4A-NA	3.13	128.84	124.51
35	C	202	A86	C35-C34-C33	-3.13	104.41	109.88
36	W	215	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
36	G	316	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
36	X	308	CLA	C2A-C1A-CHA	3.13	129.33	123.86
36	G	315	CLA	CMB-C2B-C3B	3.13	130.53	124.68
36	b	827	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
36	K	309	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
35	K	302	A86	C25-C26-C27	-3.13	122.85	127.31
36	f	802	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
36	V	313	CLA	CMB-C2B-C3B	3.12	130.52	124.68
44	b	845	BCR	C31-C1-C6	3.12	115.36	110.30
35	T	307	A86	C33-C32-C31	-3.12	106.18	109.21
35	K	301	A86	C25-C26-C27	-3.12	122.86	127.31
36	H	306	CLA	CMB-C2B-C3B	3.12	130.52	124.68
36	S	319	CLA	CHB-C4A-NA	3.12	128.83	124.51
36	b	811	CLA	CHB-C4A-NA	3.12	128.83	124.51
34	L	305	DD6	C37-C36-C35	3.12	120.14	114.36
36	R	320	CLA	CHB-C4A-NA	3.12	128.82	124.51
36	K	310	CLA	CMB-C2B-C3B	3.12	130.51	124.68
35	O	301	A86	C9-C8-C6	-3.12	117.66	126.42
36	h	203	CLA	CBA-CAA-C2A	3.12	123.06	113.86
36	R	315	CLA	CMB-C2B-C3B	3.12	130.51	124.68
35	V	304	A86	C23-C16-C17	-3.11	103.57	108.98
37	G	318	KC1	C3B-C2B-C1B	-3.11	104.10	107.08
36	N	312	CLA	CMB-C2B-C3B	3.11	130.50	124.68
36	b	818	CLA	CAA-CBA-CGA	3.11	122.35	113.25
36	G	314	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
36	L	312	CLA	CHB-C4A-NA	3.11	128.81	124.51
36	b	840	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
36	P	301	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
36	J	309	CLA	CMB-C2B-C3B	3.11	130.50	124.68
37	S	316	KC1	C2A-C1A-NA	3.11	114.39	109.40
36	D	307	CLA	O2D-CGD-CBD	3.11	116.79	111.27
36	a	816	CLA	C3D-C2D-C1D	-3.11	101.59	105.83
36	K	311	CLA	CHB-C4A-NA	3.11	128.81	124.51
36	P	301	CLA	CMB-C2B-C3B	3.11	130.49	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	H	302	DD6	C33-C34-C35	-3.10	106.05	110.30
36	b	836	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
36	X	309	CLA	CHB-C4A-NA	3.10	128.80	124.51
36	E	310	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
34	B	302	DD6	C14-C13-C11	-3.10	120.72	125.53
44	a	845	BCR	C2-C1-C6	3.10	115.26	110.48
36	A	306	CLA	CHD-C4C-C3C	-3.10	120.28	124.84
36	b	839	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
36	P	301	CLA	CHB-C4A-NA	3.10	128.80	124.51
35	U	302	A86	O1-C15-C20	-3.10	56.37	59.40
34	R	307	DD6	C37-C36-C35	3.10	120.10	114.36
34	B	302	DD6	C37-C36-C31	-3.10	120.14	124.35
36	b	837	CLA	O1D-CGD-CBD	3.10	130.83	124.48
36	W	216	CLA	CAA-C2A-C1A	-3.10	101.82	111.97
36	W	201	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
36	W	212	CLA	C4D-C3D-CAD	-3.10	104.44	108.10
36	T	312	CLA	CHB-C4A-NA	3.10	128.79	124.51
36	K	307	CLA	C4D-C3D-CAD	-3.10	104.45	108.10
36	b	819	CLA	CHD-C1D-ND	-3.09	121.61	124.45
36	a	830	CLA	CMD-C2D-C3D	-3.09	120.50	127.61
36	C	205	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
36	F	313	CLA	O2D-CGD-CBD	3.09	116.76	111.27
36	S	310	CLA	C1-O2A-CGA	3.09	124.56	116.44
36	X	308	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
36	b	841	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
36	b	841	CLA	CAC-C3C-C4C	-3.09	120.80	124.81
35	V	303	A86	C25-C26-C27	-3.09	122.90	127.31
37	E	309	KC1	C3B-C2B-C1B	-3.09	104.12	107.08
36	b	810	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
36	V	311	CLA	CMD-C2D-C1D	-3.09	119.27	124.71
37	M	313	KC1	C2A-C1A-NA	3.09	114.36	109.40
34	M	303	DD6	C9-C10-C11	-3.09	122.90	127.31
36	D	306	CLA	CHB-C4A-NA	3.09	128.78	124.51
35	M	304	A86	C34-O4-C38	-3.09	112.14	117.90
36	b	825	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
36	H	317	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
35	Q	303	A86	C41-C32-C31	-3.09	107.71	110.47
36	I	309	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
36	b	802	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
35	L	301	A86	C17-C16-C15	3.08	112.31	109.16
36	T	314	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
36	W	211	CLA	CHB-C4A-NA	3.08	128.77	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	E	323	LMT	C1B-O1B-C4'	-3.08	110.34	117.96
36	C	214	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
35	E	305	A86	C25-C26-C27	-3.08	122.91	127.31
36	N	313	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
36	T	311	CLA	CHD-C1D-ND	-3.08	121.62	124.45
37	A	312	KC1	C1C-C2C-C3C	-3.08	103.72	106.96
36	a	805	CLA	CMB-C2B-C3B	3.08	130.44	124.68
36	L	316	CLA	CMB-C2B-C3B	3.08	130.44	124.68
36	b	822	CLA	CMB-C2B-C3B	3.08	130.44	124.68
36	f	803	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
37	R	317	KC1	C4C-C3C-C2C	-3.08	102.41	106.90
36	T	309	CLA	CMB-C2B-C3B	3.08	130.44	124.68
34	B	302	DD6	C37-C36-C35	3.08	120.05	114.36
35	R	303	A86	C41-C32-C31	3.07	113.22	110.47
36	b	805	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
36	T	309	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
35	R	304	A86	O1-C15-C20	-3.07	56.40	59.40
36	a	814	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
37	G	317	KC1	C3B-C2B-C1B	-3.07	104.14	107.08
35	B	301	A86	C17-C16-C15	3.07	112.30	109.16
36	H	312	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
36	b	824	CLA	C3D-C2D-C1D	-3.07	101.64	105.83
35	R	309	A86	C25-C26-C27	-3.07	122.93	127.31
36	H	310	CLA	CHA-C4D-ND	3.07	138.92	132.50
36	N	316	CLA	CMB-C2B-C3B	3.07	130.42	124.68
34	I	303	DD6	C32-C31-C36	-3.07	118.30	122.63
35	C	202	A86	C4-C5-C6	-3.07	122.93	127.31
36	J	309	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
35	V	303	A86	C3-C2-C1	-3.07	122.93	127.31
36	f	805	CLA	CMB-C2B-C3B	3.07	130.42	124.68
36	H	315	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
36	b	829	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
35	T	304	A86	C25-C26-C27	-3.07	122.93	127.31
36	B	307	CLA	C2A-C1A-CHA	3.07	129.22	123.86
36	V	311	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
37	T	315	KC1	C3B-C2B-C1B	-3.06	104.15	107.08
36	b	816	CLA	C3D-C4D-ND	3.06	115.19	110.24
36	I	309	CLA	CHB-C4A-NA	3.06	128.75	124.51
36	A	311	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
36	H	316	CLA	CED-O2D-CGD	3.06	122.86	115.94
36	F	316	CLA	CAA-C2A-C3A	-3.06	108.95	116.10
36	H	314	CLA	O2D-CGD-O1D	-3.06	117.85	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	802	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
36	A	306	CLA	CHB-C4A-NA	3.06	128.74	124.51
34	L	305	DD6	C25-C24-C1	-3.06	117.82	126.42
36	R	319	CLA	CBC-CAC-C3C	3.06	120.86	112.43
35	T	305	A86	O-C13-C11	-3.06	114.39	121.15
34	D	305	DD6	C15-C14-C13	-3.06	119.53	125.99
37	M	318	KC1	C3A-C4A-NA	3.06	113.91	110.57
35	R	306	A86	C3-C2-C1	-3.06	122.95	127.31
35	V	302	A86	O1-C15-C20	-3.06	56.41	59.40
36	a	820	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
35	M	302	A86	C3-C4-C5	-3.05	117.22	123.47
36	N	311	CLA	CMB-C2B-C3B	3.05	130.39	124.68
35	L	304	A86	C4-C3-C2	-3.05	117.22	123.47
36	R	314	CLA	CBA-CAA-C2A	-3.05	104.85	113.86
36	T	311	CLA	CMB-C2B-C3B	3.05	130.39	124.68
36	C	208	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
36	K	307	CLA	C2C-C1C-NC	3.05	112.83	109.97
44	i	103	BCR	C15-C16-C17	-3.05	117.22	123.47
36	H	307	CLA	CMD-C2D-C1D	3.05	130.09	124.71
35	V	304	A86	O4-C38-C39	3.05	116.70	111.09
36	B	309	CLA	C4-C3-C5	3.05	120.40	115.27
36	a	823	CLA	CAC-C3C-C4C	3.05	128.76	124.81
37	V	312	KC1	C3B-C2B-C1B	-3.05	104.17	107.08
44	j	107	BCR	C2-C1-C6	3.04	115.17	110.48
36	D	312	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
35	h	202	A86	C3-C2-C1	-3.04	122.97	127.31
34	R	307	DD6	C37-C36-C31	-3.04	120.22	124.35
36	V	313	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
36	O	316	CLA	CMB-C2B-C3B	3.04	130.36	124.68
36	a	801	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
37	P	315	KC1	C4C-C3C-C2C	-3.04	102.47	106.90
36	M	316	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
36	b	824	CLA	C4-C3-C5	3.04	120.38	115.27
36	S	315	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
36	j	106	CLA	CMB-C2B-C3B	3.04	130.36	124.68
36	D	306	CLA	CAA-C2A-C1A	3.04	121.92	111.97
36	a	807	CLA	CHB-C4A-NA	3.04	128.71	124.51
36	M	306	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
36	a	818	CLA	CHB-C4A-NA	3.03	128.71	124.51
37	O	313	KC1	C4C-C3C-C2C	-3.03	102.48	106.90
37	Q	313	KC1	C4C-C3C-C2C	-3.03	102.48	106.90
36	a	809	CLA	CMB-C2B-C3B	3.03	130.35	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	M	308	CLA	CAC-C3C-C4C	-3.03	120.88	124.81
34	W	204	DD6	C21-C20-C15	-3.03	117.19	122.26
36	W	210	CLA	CHB-C4A-NA	3.03	128.70	124.51
36	a	826	CLA	CHB-C4A-NA	3.03	128.70	124.51
36	N	310	CLA	CMD-C2D-C3D	-3.03	120.65	127.61
36	a	811	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
36	a	819	CLA	CHB-C4A-NA	3.03	128.70	124.51
36	b	826	CLA	OBD-CAD-C3D	-3.03	121.24	128.52
36	l	205	CLA	CHB-C4A-NA	3.03	128.70	124.51
35	K	301	A86	C3-C2-C1	-3.03	122.99	127.31
35	J	305	A86	C34-O4-C38	-3.03	112.26	117.90
36	N	319	CLA	CAC-C3C-C2C	-3.02	122.36	127.53
36	U	307	CLA	CMB-C2B-C1B	-3.02	123.81	128.46
36	W	207	CLA	C1-C2-C3	3.02	131.27	126.04
36	J	315	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
36	H	305	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
36	A	314	CLA	C3A-C2A-C1A	3.02	105.87	101.34
36	N	307	CLA	CMB-C2B-C3B	3.02	130.33	124.68
36	b	810	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
36	b	837	CLA	CHB-C4A-NA	3.02	128.69	124.51
34	L	305	DD6	O1-C20-C19	3.02	115.65	113.38
37	D	314	KC1	C3B-C2B-C1B	-3.02	104.19	107.08
36	b	808	CLA	CHB-C4A-NA	3.02	128.69	124.51
36	J	312	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
36	A	306	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
35	R	303	A86	O1-C15-C20	-3.02	56.45	59.40
36	j	102	CLA	C4-C3-C5	3.02	120.35	115.27
34	R	307	DD6	C15-C14-C13	-3.02	119.61	125.99
36	A	305	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
36	L	316	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
36	C	210	CLA	CHB-C4A-NA	3.02	128.68	124.51
36	N	319	CLA	CHB-C4A-NA	3.02	128.68	124.51
36	Q	309	CLA	CHB-C4A-NA	3.02	128.68	124.51
36	G	311	CLA	C2D-C1D-ND	-3.02	107.88	110.10
36	b	836	CLA	C1-C2-C3	-3.01	120.83	126.04
37	Q	311	KC1	C4C-C3C-C2C	-3.01	102.51	106.90
35	W	203	A86	O4-C38-C39	3.01	116.63	111.09
35	N	302	A86	O1-C15-C20	-3.01	56.46	59.40
36	E	314	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
36	b	811	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
36	b	813	CLA	CMA-C3A-C2A	-3.01	101.69	113.83
36	a	806	CLA	C1-C2-C3	-3.01	120.84	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	841	CLA	CHC-C1C-NC	3.01	128.77	124.20
36	G	313	CLA	CMA-C3A-C4A	3.01	119.86	111.77
37	U	312	KC1	CHB-C1B-C2B	-3.01	119.17	125.48
35	C	204	A86	C17-C16-C15	3.01	112.23	109.16
36	b	814	CLA	CHB-C4A-NA	3.01	128.67	124.51
36	a	810	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
36	F	317	CLA	C1-C2-C3	-3.00	120.85	126.04
35	V	303	A86	C33-C32-C31	3.00	112.13	109.21
36	b	833	CLA	O2D-CGD-CBD	3.00	116.61	111.27
34	W	204	DD6	C32-C31-C36	-3.00	118.39	122.63
36	G	316	CLA	CHB-C4A-NA	3.00	128.66	124.51
36	O	316	CLA	CHB-C4A-NA	3.00	128.66	124.51
36	R	314	CLA	CAA-C2A-C1A	3.00	121.81	111.97
35	F	307	A86	C3-C4-C5	-3.00	117.33	123.47
35	F	307	A86	O4-C38-O5	-3.00	117.00	122.96
35	G	306	A86	C17-C16-C15	3.00	112.22	109.16
35	S	302	A86	O1-C15-C20	-3.00	56.47	59.40
34	M	303	DD6	C21-C20-C15	-3.00	117.23	122.26
35	B	303	A86	O-C13-C11	-3.00	114.52	121.15
36	I	312	CLA	CHB-C4A-NA	3.00	128.66	124.51
36	J	311	CLA	CHB-C4A-NA	3.00	128.66	124.51
36	b	812	CLA	C2D-C1D-ND	-3.00	107.89	110.10
37	O	315	KC1	C4C-C3C-C2C	-3.00	102.53	106.90
34	R	308	DD6	C15-C14-C13	-3.00	119.65	125.99
44	m	101	BCR	C3-C4-C5	-3.00	108.72	114.08
36	b	821	CLA	CMB-C2B-C3B	3.00	130.28	124.68
36	J	308	CLA	CHB-C4A-NA	3.00	128.66	124.51
35	Q	304	A86	C-C1-C2	-3.00	118.73	122.92
36	D	309	CLA	C4-C3-C5	3.00	120.31	115.27
36	B	308	CLA	C3C-C4C-NC	-3.00	107.21	110.57
34	O	304	DD6	C21-C20-C15	-3.00	117.24	122.26
35	V	303	A86	O1-C15-C20	-2.99	56.47	59.40
36	b	819	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
36	a	832	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
36	a	804	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
37	G	318	KC1	C3A-C4A-NA	2.99	113.84	110.57
36	f	805	CLA	CHB-C4A-NA	2.99	128.65	124.51
44	b	843	BCR	C29-C30-C25	2.99	115.09	110.48
36	b	824	CLA	CHB-C4A-NA	2.99	128.65	124.51
34	B	302	DD6	C21-C20-C15	-2.99	117.25	122.26
35	O	319	A86	C25-C24-C1	-2.99	118.02	126.42
34	E	304	DD6	C14-C13-C11	-2.99	120.89	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	835	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
36	a	823	CLA	CHD-C4C-NC	2.99	128.91	124.20
34	S	307	DD6	C3-C4-C5	-2.99	117.35	123.47
36	G	319	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
37	L	317	KC1	C4D-C3D-CAD	2.99	112.64	107.81
34	W	205	DD6	C14-C13-C11	-2.99	120.89	125.53
36	a	832	CLA	CMB-C2B-C3B	2.99	130.27	124.68
35	S	305	A86	C14-C15-C16	-2.99	107.31	118.75
37	M	317	KC1	C3B-C2B-C1B	-2.99	104.22	107.08
34	W	205	DD6	C15-C14-C13	-2.99	119.68	125.99
36	W	207	CLA	O2A-CGA-O1A	-2.99	116.05	123.59
36	Q	310	CLA	C4-C3-C2	-2.99	116.02	123.68
36	M	308	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
34	S	307	DD6	C4-C5-C6	-2.99	123.05	127.31
36	W	209	CLA	CHB-C4A-NA	2.99	128.64	124.51
36	a	830	CLA	CHD-C1D-ND	2.98	127.20	124.45
34	E	303	DD6	C21-C20-C15	-2.98	117.26	122.26
36	l	206	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
35	F	304	A86	C34-O4-C38	-2.98	112.34	117.90
36	V	309	CLA	CMB-C2B-C3B	2.98	130.26	124.68
36	f	804	CLA	O2A-CGA-CBA	2.98	121.27	111.91
36	A	306	CLA	CAC-C3C-C4C	2.98	128.68	124.81
35	C	204	A86	C34-O4-C38	-2.98	112.34	117.90
36	C	212	CLA	CBC-CAC-C3C	2.98	120.65	112.43
37	T	315	KC1	C2B-C1B-NB	2.98	112.30	110.10
40	b	849	DGD	O3E-C3E-C2E	-2.98	103.46	110.35
36	S	319	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
36	R	322	CLA	CMB-C2B-C3B	2.98	130.25	124.68
36	F	313	CLA	CMB-C2B-C3B	2.98	130.25	124.68
36	V	307	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
36	P	311	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
37	C	213	KC1	C4D-C3D-CAD	2.98	112.62	107.81
36	b	838	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
36	N	315	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
36	V	307	CLA	CMB-C2B-C3B	2.97	130.24	124.68
36	S	315	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
35	W	202	A86	C10-C9-C8	-2.97	113.94	123.22
36	V	310	CLA	CMB-C2B-C3B	2.97	130.24	124.68
36	O	309	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
36	W	214	CLA	C1D-ND-C4D	-2.97	104.22	106.33
35	T	306	A86	O1-C15-C20	-2.97	56.50	59.40
36	R	316	CLA	C2A-C1A-CHA	2.97	129.05	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	N	320	A86	C-C1-C2	-2.97	118.76	122.92
36	f	802	CLA	C6-C7-C8	-2.97	106.32	115.92
36	B	309	CLA	C2C-C1C-NC	2.97	112.75	109.97
36	B	307	CLA	CHB-C4A-NA	2.97	128.62	124.51
37	D	314	KC1	C2A-C1A-CHA	-2.97	117.62	127.44
35	N	320	A86	C4-C5-C6	-2.97	123.07	127.31
36	C	209	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
36	S	313	CLA	CAA-C2A-C1A	2.97	121.70	111.97
36	N	319	CLA	CED-O2D-CGD	2.97	122.65	115.94
36	a	826	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
35	Q	304	A86	O3-C36-C37	-2.96	104.12	109.39
36	C	212	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
36	O	316	CLA	CHD-C4C-C3C	-2.96	120.48	124.84
36	W	215	CLA	CMB-C2B-C3B	2.96	130.22	124.68
35	J	303	A86	O4-C38-C39	2.96	116.54	111.09
36	a	815	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
37	G	308	KC1	C4C-C3C-C2C	-2.96	102.58	106.90
36	O	310	CLA	CHB-C4A-NA	2.96	128.61	124.51
35	M	302	A86	C9-C10-C11	-2.96	117.90	126.61
37	G	318	KC1	C4C-C3C-C2C	-2.96	102.58	106.90
36	X	306	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
36	b	824	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
36	T	308	CLA	CHB-C4A-NA	2.96	128.61	124.51
35	S	303	A86	C4-C5-C6	-2.96	123.08	127.31
36	a	841	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
36	W	208	CLA	CMB-C2B-C3B	2.96	130.22	124.68
36	l	205	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
36	O	306	CLA	CMB-C2B-C3B	2.96	130.21	124.68
36	S	320	CLA	CMB-C2B-C3B	2.96	130.21	124.68
36	X	310	CLA	CMB-C2B-C3B	2.96	130.21	124.68
36	J	310	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
36	a	836	CLA	O2A-CGA-O1A	-2.96	116.13	123.59
35	T	303	A86	C33-C32-C31	-2.96	106.34	109.21
35	V	304	A86	C40-C32-C31	2.96	113.12	110.47
35	N	303	A86	C4-C5-C6	-2.96	123.09	127.31
34	W	204	DD6	C37-C36-C31	-2.96	120.33	124.35
35	L	304	A86	O-C13-C11	-2.96	114.62	121.15
36	H	317	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
36	Q	305	CLA	CMB-C2B-C3B	2.96	130.21	124.68
36	a	833	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
36	Q	307	CLA	CMB-C2B-C3B	2.95	130.21	124.68
36	F	314	CLA	CHB-C4A-NA	2.95	128.59	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	U	306	CLA	C4D-C3D-CAD	-2.95	104.62	108.10
36	P	308	CLA	CMB-C2B-C3B	2.95	130.20	124.68
39	I	317	LMT	C1B-O1B-C4'	-2.95	110.66	117.96
36	U	310	CLA	O1D-CGD-CBD	2.95	130.52	124.48
36	b	839	CLA	CMB-C2B-C3B	2.95	130.20	124.68
35	K	306	A86	O1-C15-C20	-2.95	56.52	59.40
36	b	824	CLA	CHD-C4C-C3C	-2.95	120.50	124.84
36	I	313	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
36	b	815	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
36	U	305	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
36	T	312	CLA	CMB-C2B-C3B	2.95	130.20	124.68
35	Q	304	A86	C4-C5-C6	-2.95	123.10	127.31
36	Q	308	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
35	G	302	A86	C3-C4-C5	-2.95	117.43	123.47
35	L	301	A86	C34-O4-C38	-2.95	112.40	117.90
34	L	305	DD6	C15-C14-C13	-2.95	119.76	125.99
44	b	845	BCR	C40-C30-C25	2.95	115.08	110.30
35	N	320	A86	O3-C36-C37	-2.95	104.15	109.39
36	E	316	CLA	CHB-C4A-NA	2.95	128.59	124.51
36	a	803	CLA	CHB-C4A-NA	2.95	128.59	124.51
36	b	821	CLA	CHB-C4A-NA	2.94	128.58	124.51
35	C	203	A86	C28-C27-C26	-2.94	118.80	122.92
35	J	303	A86	O1-C15-C20	-2.94	56.52	59.40
35	W	202	A86	C4-C3-C2	-2.94	117.45	123.47
36	A	309	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
37	G	318	KC1	CED-O2D-CGD	2.94	122.59	115.94
37	W	217	KC1	C3B-C2B-C1B	-2.94	104.27	107.08
36	f	802	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
36	R	319	CLA	O2D-CGD-CBD	2.94	116.49	111.27
36	F	316	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
36	a	816	CLA	C4-C3-C5	2.94	120.22	115.27
37	J	314	KC1	CBD-CHA-C1A	2.94	134.36	128.88
36	M	314	CLA	CMB-C2B-C3B	2.94	130.18	124.68
36	O	308	CLA	CMB-C2B-C3B	2.94	130.18	124.68
36	B	311	CLA	C2D-C1D-ND	-2.94	107.94	110.10
36	b	808	CLA	CMB-C2B-C3B	2.94	130.17	124.68
35	S	304	A86	C34-O4-C38	-2.94	112.42	117.90
34	R	308	DD6	C37-C36-C35	2.94	119.80	114.36
35	U	302	A86	C9-C8-C6	-2.94	118.17	126.42
36	T	309	CLA	CHB-C4A-NA	2.94	128.57	124.51
35	F	305	A86	O-C13-C11	-2.94	114.66	121.15
36	D	311	CLA	CHB-C4A-NA	2.93	128.57	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	315	CLA	C4-C3-C5	2.93	120.21	115.27
36	a	823	CLA	C1-C2-C3	-2.93	120.97	126.04
36	D	317	CLA	CHB-C4A-NA	2.93	128.57	124.51
35	A	302	A86	C-C1-C24	2.93	122.70	118.08
36	H	316	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
36	J	316	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
35	O	319	A86	O1-C15-C20	-2.93	56.53	59.40
35	U	302	A86	C23-C16-C17	-2.93	103.89	108.98
34	A	303	DD6	C14-C13-C11	-2.93	120.98	125.53
36	I	310	CLA	CHB-C4A-NA	2.93	128.56	124.51
37	T	310	KC1	CAC-C3C-C4C	2.93	128.61	124.81
35	A	302	A86	C7-C6-C8	2.93	122.69	118.08
36	b	816	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
36	B	306	CLA	CHB-C4A-NA	2.93	128.56	124.51
36	B	306	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
35	T	302	A86	C25-C26-C27	-2.93	123.14	127.31
36	P	312	CLA	CHB-C4A-NA	2.93	128.56	124.51
36	W	214	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
36	D	309	CLA	CHD-C4C-C3C	-2.92	120.54	124.84
36	B	306	CLA	CMB-C2B-C3B	2.92	130.15	124.68
35	B	303	A86	O4-C38-O5	-2.92	117.16	122.96
35	P	307	A86	C34-O4-C38	-2.92	112.45	117.90
35	T	304	A86	C3-C4-C5	-2.92	117.49	123.47
36	U	313	CLA	CHB-C4A-NA	2.92	128.55	124.51
36	b	814	CLA	CMB-C2B-C3B	2.92	130.14	124.68
36	b	811	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
37	B	310	KC1	C4C-C3C-C2C	-2.92	102.64	106.90
37	U	312	KC1	CHB-C4A-NA	2.92	128.81	124.20
36	H	316	CLA	CHB-C4A-NA	2.92	128.55	124.51
36	L	312	CLA	C2A-C1A-CHA	2.92	128.96	123.86
35	I	302	A86	O1-C15-C20	-2.92	56.55	59.40
37	N	314	KC1	C4D-C3D-CAD	2.92	112.52	107.81
36	b	841	CLA	CHB-C4A-NA	2.92	128.55	124.51
37	X	311	KC1	C3B-C2B-C1B	-2.92	104.29	107.08
36	E	313	CLA	C4-C3-C5	2.92	120.18	115.27
36	M	311	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
34	Q	302	DD6	C37-C36-C35	2.92	119.76	114.36
35	M	301	A86	C41-C32-C31	-2.91	107.86	110.47
36	N	307	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
36	a	848	CLA	CMD-C2D-C3D	-2.91	120.91	127.61
37	M	318	KC1	C4B-CHC-C1C	-2.91	119.77	126.06
35	V	302	A86	C17-C16-C15	2.91	112.14	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	807	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
36	J	313	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
36	b	835	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
35	C	203	A86	C25-C26-C27	-2.91	123.15	127.31
36	S	317	CLA	CMB-C2B-C3B	2.91	130.13	124.68
35	F	307	A86	C23-C16-C22	-2.91	103.08	107.37
36	Q	310	CLA	C3A-C2A-C1A	-2.91	96.98	101.34
37	L	317	KC1	C3B-C2B-C1B	-2.91	104.30	107.08
34	A	304	DD6	C14-C13-C11	-2.91	121.01	125.53
36	L	314	CLA	CHB-C4A-NA	2.91	128.53	124.51
39	B	312	LMT	C1B-O1B-C4'	-2.91	110.77	117.96
35	Q	303	A86	C34-O4-C38	-2.91	112.47	117.90
36	B	305	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
36	P	310	CLA	CMB-C2B-C3B	2.91	130.12	124.68
36	L	308	CLA	C4-C3-C5	2.91	120.16	115.27
34	G	303	DD6	C14-C13-C11	-2.91	121.02	125.53
34	W	205	DD6	C21-C20-C15	-2.91	117.39	122.26
36	S	320	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
35	J	305	A86	C25-C26-C27	-2.91	123.16	127.31
36	G	311	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
36	E	317	CLA	CMB-C2B-C3B	2.91	130.11	124.68
36	I	312	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
36	D	312	CLA	CMB-C2B-C3B	2.90	130.11	124.68
36	J	311	CLA	CMB-C2B-C3B	2.90	130.11	124.68
35	N	301	A86	C33-C32-C31	-2.90	106.39	109.21
35	T	302	A86	C40-C32-C31	2.90	113.07	110.47
36	T	309	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
37	U	312	KC1	C4C-C3C-C2C	-2.90	102.67	106.90
36	a	819	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
36	D	310	CLA	CHB-C4A-NA	2.90	128.53	124.51
36	Q	308	CLA	CHB-C4A-NA	2.90	128.53	124.51
37	M	313	KC1	O2D-CGD-O1D	-2.90	118.17	123.84
36	b	825	CLA	O2D-CGD-CBD	2.90	116.42	111.27
35	U	304	A86	C28-C27-C26	-2.90	118.86	122.92
35	N	320	A86	O4-C34-C33	2.90	114.81	107.59
35	G	304	A86	C26-C25-C24	-2.90	114.17	123.22
36	j	102	CLA	C1-C2-C3	-2.90	121.03	126.04
36	T	311	CLA	CHB-C4A-NA	2.90	128.52	124.51
34	F	303	DD6	C37-C36-C31	-2.90	120.41	124.35
35	T	305	A86	O1-C20-C21	-2.90	111.59	115.06
36	a	835	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
36	R	312	CLA	C1B-CHB-C4A	-2.90	124.38	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	802	CLA	C4-C3-C5	2.90	120.14	115.27
35	R	306	A86	C4-C3-C2	-2.89	117.55	123.47
36	b	802	CLA	CHB-C4A-NA	2.89	128.51	124.51
36	P	302	CLA	CAA-C2A-C3A	-2.89	107.03	114.26
35	Q	303	A86	C40-C32-C31	-2.89	107.88	110.47
36	V	305	CLA	CMA-C3A-C2A	-2.89	102.16	113.83
35	U	304	A86	C7-C6-C5	-2.89	118.87	122.92
36	j	106	CLA	CHB-C4A-NA	2.89	128.51	124.51
36	b	817	CLA	CHB-C4A-NA	2.89	128.51	124.51
36	C	207	CLA	C4-C3-C5	2.89	120.13	115.27
36	M	314	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
36	X	312	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
35	L	306	A86	O1-C15-C20	-2.89	56.58	59.40
36	a	833	CLA	CHB-C4A-NA	2.89	128.50	124.51
36	R	316	CLA	CAC-C3C-C4C	-2.89	121.07	124.81
36	G	311	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
36	a	827	CLA	CHB-C4A-NA	2.88	128.50	124.51
36	f	804	CLA	CAC-C3C-C4C	2.88	128.55	124.81
36	b	817	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
36	a	832	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
36	F	311	CLA	CHB-C4A-NA	2.88	128.50	124.51
34	I	303	DD6	C9-C10-C11	-2.88	123.20	127.31
35	X	304	A86	C28-C27-C26	-2.88	118.89	122.92
44	b	845	BCR	C27-C26-C25	2.88	126.91	122.73
36	N	319	CLA	CAA-C2A-C1A	-2.88	105.77	112.14
34	H	303	DD6	C14-C13-C11	-2.88	121.06	125.53
36	b	807	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
36	U	305	CLA	CMB-C2B-C3B	2.88	130.06	124.68
36	P	314	CLA	C3A-C2A-C1A	-2.88	97.03	101.34
37	K	314	KC1	CBC-CAC-C3C	-2.88	104.50	112.43
36	P	311	CLA	CHB-C4A-NA	2.88	128.49	124.51
36	G	315	CLA	C4-C3-C5	2.88	120.11	115.27
35	T	307	A86	C3-C4-C5	-2.88	117.58	123.47
35	O	305	A86	C12-C11-C13	2.88	120.85	116.02
34	A	301	DD6	C3-C4-C5	-2.87	117.58	123.47
35	O	305	A86	C-C1-C2	-2.87	118.90	122.92
36	a	848	CLA	O2A-CGA-CBA	2.87	120.92	111.91
36	S	321	CLA	CGD-CBD-CAD	-2.87	101.43	110.73
35	Q	304	A86	O4-C34-C33	2.87	114.75	107.59
36	a	824	CLA	C2A-C1A-CHA	2.87	128.88	123.86
37	F	308	KC1	CBD-CHA-C1A	2.87	134.24	128.88
36	D	309	CLA	C4C-C3C-C2C	-2.87	102.71	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	T	306	A86	C28-C27-C26	-2.87	118.90	122.92
36	U	306	CLA	CHB-C4A-NA	2.87	128.48	124.51
36	C	207	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
36	b	816	CLA	O2A-CGA-CBA	2.87	120.92	111.91
44	i	101	BCR	C31-C1-C6	2.87	114.95	110.30
36	A	308	CLA	CHB-C4A-NA	2.87	128.48	124.51
36	E	315	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
36	b	833	CLA	CAA-C2A-C1A	-2.87	102.57	111.97
35	S	302	A86	C23-C16-C17	-2.87	104.00	108.98
37	M	317	KC1	C3D-CAD-CBD	-2.87	103.83	107.61
36	U	311	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
36	b	831	CLA	O2D-CGD-CBD	2.87	116.36	111.27
39	K	318	LMT	C1B-O1B-C4'	-2.87	110.87	117.96
35	K	302	A86	O4-C34-C35	2.87	114.73	107.59
36	f	802	CLA	CHD-C1D-ND	-2.87	121.82	124.45
44	a	847	BCR	C24-C23-C22	-2.87	121.90	126.23
36	V	308	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
35	N	302	A86	C23-C16-C17	-2.86	104.00	108.98
36	C	214	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
36	A	306	CLA	C1-C2-C3	-2.86	121.09	126.04
36	O	309	CLA	CHB-C4A-NA	2.86	128.47	124.51
37	W	213	KC1	C1C-C2C-C3C	-2.86	103.95	106.96
36	a	818	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
36	Q	314	CLA	O2D-CGD-CBD	2.86	116.36	111.27
35	R	302	A86	O4-C38-C39	2.86	116.36	111.09
36	a	808	CLA	CMB-C2B-C3B	2.86	130.03	124.68
35	K	306	A86	O4-C38-O5	-2.86	117.28	122.96
36	W	211	CLA	CMB-C2B-C3B	2.86	130.03	124.68
36	E	315	CLA	O2A-CGA-CBA	2.86	120.89	111.91
35	L	301	A86	C25-C26-C27	-2.86	123.23	127.31
35	M	302	A86	O1-C15-C20	-2.86	56.60	59.40
35	S	301	A86	C33-C32-C31	-2.86	106.43	109.21
37	T	315	KC1	C3D-CAD-CBD	-2.86	103.84	107.61
37	F	315	KC1	C3B-C2B-C1B	-2.86	104.34	107.08
35	H	301	A86	C28-C27-C26	-2.86	118.92	122.92
36	W	206	CLA	CHB-C4A-NA	2.86	128.47	124.51
36	H	318	CLA	O1D-CGD-CBD	2.86	130.33	124.48
35	N	306	A86	O1-C20-C21	-2.86	111.63	115.06
35	B	303	A86	C8-C6-C5	2.86	123.33	118.94
36	L	314	CLA	O2A-CGA-O1A	-2.86	116.38	123.59
36	H	312	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
36	H	318	CLA	CMB-C2B-C3B	2.86	130.02	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	303	A86	C25-C24-C1	-2.86	118.39	126.42
36	C	211	CLA	CHB-C4A-NA	2.86	128.46	124.51
36	f	804	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
37	J	314	KC1	C2B-C1B-NB	2.86	112.21	110.10
35	U	304	A86	O1-C15-C14	-2.86	107.48	113.21
36	T	312	CLA	CBA-CAA-C2A	-2.86	105.43	113.86
35	N	306	A86	C40-C32-C31	2.85	113.03	110.47
36	R	319	CLA	CAC-C3C-C2C	2.85	132.41	127.53
36	M	315	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
36	I	306	CLA	CMD-C2D-C3D	-2.85	121.05	127.61
36	A	305	CLA	CMB-C2B-C3B	2.85	130.02	124.68
35	G	305	A86	C25-C26-C27	-2.85	123.24	127.31
36	D	316	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
36	O	316	CLA	C4D-C3D-CAD	-2.85	104.73	108.10
36	D	308	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
36	b	824	CLA	O2A-CGA-CBA	2.85	120.86	111.91
35	F	301	A86	C34-O4-C38	-2.85	112.58	117.90
36	b	806	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
35	R	301	A86	C25-C24-C1	-2.85	118.40	126.42
35	X	303	A86	C20-C19-C18	2.85	118.39	112.75
35	T	303	A86	C40-C32-C31	2.85	113.02	110.47
36	M	316	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	P	302	CLA	O2D-CGD-CBD	2.85	116.33	111.27
37	F	308	KC1	C4C-C3C-C2C	-2.85	102.74	106.90
36	X	308	CLA	C3B-C4B-NB	-2.85	105.53	109.21
36	S	311	CLA	CMB-C2B-C3B	2.85	130.01	124.68
36	N	319	CLA	CHA-C1A-NA	-2.85	119.87	126.40
36	S	317	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	a	832	CLA	CHD-C1D-ND	-2.85	121.84	124.45
36	U	308	CLA	CMB-C2B-C3B	2.85	130.01	124.68
35	T	304	A86	O1-C20-C21	-2.85	111.64	115.06
36	G	315	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
36	X	313	CLA	CHC-C1C-NC	2.85	128.52	124.20
37	M	313	KC1	C3B-C2B-C1B	-2.85	104.36	107.08
36	R	320	CLA	CMB-C2B-C3B	2.85	130.00	124.68
35	N	320	A86	C40-C32-C31	2.84	113.02	110.47
37	U	312	KC1	CBD-CHA-C1A	2.84	134.19	128.88
36	R	314	CLA	CMB-C2B-C3B	2.84	130.00	124.68
44	b	845	BCR	C38-C26-C27	-2.84	108.15	113.62
36	N	319	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
41	D	319	LHG	O8-C23-C24	2.84	120.83	111.91
36	b	826	CLA	O2D-CGD-CBD	2.84	116.32	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	307	CLA	CMB-C2B-C3B	2.84	130.00	124.68
36	b	825	CLA	C2A-C1A-CHA	2.84	128.83	123.86
34	J	304	DD6	C9-C10-C11	-2.84	123.25	127.31
36	K	307	CLA	C1-C2-C3	-2.84	121.13	126.04
36	C	206	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
36	a	827	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
36	N	319	CLA	CMC-C2C-C3C	2.84	133.83	126.12
37	G	318	KC1	C2A-C1A-NA	2.84	113.96	109.40
36	O	316	CLA	CMC-C2C-C1C	2.84	129.36	125.04
36	E	316	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
36	N	307	CLA	CHB-C4A-NA	2.84	128.44	124.51
34	L	305	DD6	C37-C36-C31	-2.84	120.49	124.35
36	N	309	CLA	CHB-C4A-NA	2.84	128.44	124.51
36	T	313	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
36	a	825	CLA	C4-C3-C5	2.84	120.04	115.27
36	I	306	CLA	O2A-CGA-CBA	2.84	120.81	111.91
44	j	107	BCR	C29-C30-C25	2.83	114.84	110.48
36	J	310	CLA	CHB-C4A-NA	2.83	128.43	124.51
36	C	207	CLA	CAC-C3C-C4C	2.83	128.49	124.81
36	G	307	CLA	CMD-C2D-C3D	-2.83	121.09	127.61
36	H	309	CLA	CMB-C2B-C3B	2.83	129.98	124.68
36	C	211	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
36	b	811	CLA	O2D-CGD-CBD	2.83	116.30	111.27
36	h	203	CLA	CHB-C4A-NA	2.83	128.43	124.51
34	F	303	DD6	O1-C20-C19	-2.83	111.25	113.38
35	M	304	A86	C9-C10-C11	-2.83	118.28	126.61
35	K	303	A86	C28-C27-C26	-2.83	118.95	122.92
36	b	833	CLA	CMD-C2D-C1D	-2.83	119.72	124.71
36	T	314	CLA	CMA-C3A-C4A	-2.83	104.16	111.77
35	C	202	A86	C28-C27-C26	-2.83	118.96	122.92
36	Q	314	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
34	S	306	DD6	C4-C5-C6	-2.83	123.27	127.31
37	G	308	KC1	C4D-C3D-CAD	2.83	112.38	107.81
36	C	212	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
36	b	832	CLA	CHB-C4A-NA	2.83	128.43	124.51
36	N	318	CLA	C2A-C1A-CHA	2.83	128.81	123.86
36	G	314	CLA	CHB-C4A-NA	2.83	128.42	124.51
35	U	303	A86	O1-C20-C19	-2.83	111.26	113.38
35	N	304	A86	C34-O4-C38	-2.83	112.63	117.90
36	X	307	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
44	l	207	BCR	C2-C1-C6	2.83	114.83	110.48
36	N	319	CLA	C1D-CHD-C4C	2.83	132.15	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	N	317	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
36	b	801	CLA	CAC-C3C-C4C	2.83	128.48	124.81
35	N	301	A86	C19-C18-C17	-2.83	105.32	110.77
37	G	308	KC1	C3B-C2B-C1B	-2.82	104.38	107.08
36	D	315	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
36	l	202	CLA	CMB-C2B-C3B	2.82	129.96	124.68
36	N	315	CLA	C2A-C1A-CHA	2.82	128.78	123.85
35	K	301	A86	C9-C8-C6	-2.82	118.48	126.42
36	W	218	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
34	F	303	DD6	C32-C31-C36	-2.82	118.65	122.63
36	I	306	CLA	CHD-C4C-C3C	-2.82	120.69	124.84
36	W	210	CLA	C2D-C1D-ND	-2.82	108.03	110.10
36	K	311	CLA	CMB-C2B-C3B	2.82	129.96	124.68
36	a	832	CLA	CHB-C4A-NA	2.82	128.41	124.51
36	W	212	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
36	a	822	CLA	O2A-CGA-CBA	2.82	120.76	111.91
36	S	310	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
37	L	317	KC1	C4C-C3C-C2C	-2.82	102.79	106.90
35	L	307	A86	C12-C11-C13	2.82	120.76	116.02
35	F	306	A86	C12-C11-C13	2.82	120.75	116.02
35	R	304	A86	O4-C38-O5	-2.82	117.36	122.96
36	K	310	CLA	C1-C2-C3	-2.82	121.17	126.04
36	A	314	CLA	CMB-C2B-C3B	2.82	129.95	124.68
36	a	805	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
36	a	814	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
36	I	309	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
36	C	210	CLA	C2A-C1A-CHA	2.82	128.78	123.86
37	L	315	KC1	CMC-C2C-C1C	2.81	129.32	125.04
44	l	203	BCR	C27-C26-C25	2.81	126.82	122.73
36	E	315	CLA	CMB-C2B-C3B	2.81	129.94	124.68
36	T	308	CLA	CMB-C2B-C3B	2.81	129.94	124.68
35	E	302	A86	C9-C10-C11	-2.81	118.34	126.61
36	C	207	CLA	CHD-C4C-C3C	-2.81	120.71	124.84
36	P	319	CLA	CMB-C2B-C3B	2.81	129.94	124.68
36	b	837	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
36	a	834	CLA	CMB-C2B-C3B	2.81	129.94	124.68
35	S	301	A86	C19-C18-C17	-2.81	105.34	110.77
36	I	307	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
36	R	316	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
36	b	801	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
36	f	804	CLA	CHD-C4C-C3C	-2.81	120.71	124.84
34	D	305	DD6	C33-C34-C35	-2.81	106.46	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	310	KC1	CMD-C2D-C1D	-2.81	124.14	128.46
36	D	311	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
37	E	309	KC1	C4D-C3D-CAD	2.81	112.35	107.81
35	h	204	A86	C3-C4-C5	-2.81	117.72	123.47
36	I	308	CLA	CMD-C2D-C3D	-2.81	121.15	127.61
36	X	315	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
36	D	307	CLA	CHB-C4A-NA	2.81	128.40	124.51
36	G	312	CLA	CHB-C4A-NA	2.81	128.40	124.51
36	a	838	CLA	CMB-C2B-C3B	2.81	129.93	124.68
36	a	813	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
35	V	303	A86	C35-C34-C33	-2.81	104.98	109.88
36	A	309	CLA	CMB-C2B-C3B	2.81	129.93	124.68
36	l	201	CLA	O2D-CGD-CBD	2.81	116.25	111.27
44	b	846	BCR	C3-C4-C5	-2.81	109.07	114.08
36	j	102	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
35	N	302	A86	O1-C20-C21	-2.81	111.69	115.06
35	N	302	A86	C28-C27-C26	-2.81	118.99	122.92
35	Q	304	A86	C40-C32-C31	2.80	112.98	110.47
36	J	313	CLA	CMB-C2B-C3B	2.80	129.93	124.68
36	W	216	CLA	C1D-ND-C4D	-2.80	104.34	106.33
36	D	306	CLA	CHA-C1A-NA	-2.80	119.98	126.40
34	C	201	DD6	C15-C14-C13	-2.80	120.07	125.99
36	P	309	CLA	CHB-C4A-NA	2.80	128.39	124.51
34	I	303	DD6	C25-C26-C27	-2.80	118.44	126.58
36	C	206	CLA	CHB-C4A-NA	2.80	128.38	124.51
36	b	811	CLA	CMB-C2B-C3B	2.80	129.92	124.68
36	R	319	CLA	CMC-C2C-C3C	2.80	133.72	126.12
35	J	306	A86	C25-C26-C27	-2.80	123.31	127.31
36	b	839	CLA	CHB-C4A-NA	2.80	128.38	124.51
36	a	823	CLA	C4-C3-C5	2.80	119.98	115.27
36	a	829	CLA	CMD-C2D-C1D	-2.80	119.78	124.71
36	M	312	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
36	J	312	CLA	CHB-C4A-NA	2.80	128.38	124.51
36	J	312	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
35	h	202	A86	O1-C20-C19	-2.80	111.28	113.38
34	K	304	DD6	C37-C36-C35	2.80	119.54	114.36
40	L	302	DGD	C2G-O2G-C1B	-2.80	110.90	117.79
36	b	816	CLA	CHD-C4C-NC	2.80	128.61	124.20
36	V	314	CLA	C4-C3-C5	2.80	119.98	115.27
36	P	301	CLA	C5-C3-C2	-2.80	115.46	121.12
36	R	310	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
36	b	833	CLA	CAA-CBA-CGA	-2.80	105.08	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	f	803	CLA	C4-C3-C5	2.80	119.97	115.27
35	N	305	A86	C-C1-C2	-2.79	119.01	122.92
35	K	301	A86	C4-C3-C2	-2.79	117.75	123.47
35	O	305	A86	C3-C4-C5	-2.79	117.75	123.47
36	L	312	CLA	CMB-C2B-C3B	2.79	129.91	124.68
37	E	309	KC1	O2D-CGD-O1D	-2.79	118.38	123.84
44	b	844	BCR	C29-C30-C25	2.79	114.78	110.48
36	O	312	CLA	C2A-C3A-C4A	2.79	108.57	103.59
36	R	312	CLA	C6-C7-C8	-2.79	106.89	115.92
36	X	308	CLA	C3A-C2A-C1A	2.79	105.52	101.34
36	a	819	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
36	b	812	CLA	CAC-C3C-C4C	2.79	128.43	124.81
42	E	318	LMG	O8-C28-C29	2.79	120.67	111.91
35	S	302	A86	C28-C27-C26	-2.79	119.01	122.92
37	A	312	KC1	C3C-C4C-NC	2.79	112.50	109.88
36	G	307	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
42	D	320	LMG	O8-C28-C29	2.79	120.67	111.91
36	V	308	CLA	CHB-C4A-NA	2.79	128.37	124.51
36	T	312	CLA	CAA-C2A-C1A	2.79	121.12	111.97
44	a	847	BCR	C27-C26-C25	2.79	126.78	122.73
36	P	308	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
36	I	308	CLA	C1-C2-C3	-2.79	121.22	126.04
36	A	310	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
34	B	302	DD6	C32-C31-C36	-2.79	118.70	122.63
36	h	203	CLA	O1D-CGD-CBD	2.79	130.19	124.48
36	E	315	CLA	CMD-C2D-C3D	-2.79	121.20	127.61
44	b	844	BCR	C30-C25-C26	-2.79	118.69	122.61
36	D	315	CLA	CHB-C4A-NA	2.79	128.37	124.51
36	N	308	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
36	a	812	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
35	X	302	A86	C25-C24-C1	-2.79	118.59	126.42
36	R	320	CLA	CMD-C2D-C1D	2.79	129.62	124.71
36	P	319	CLA	CHA-C1A-NA	-2.79	120.02	126.40
36	E	314	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
35	Q	316	A86	C-C1-C2	-2.79	119.02	122.92
44	i	101	BCR	C29-C30-C25	2.79	114.77	110.48
35	S	302	A86	O1-C20-C21	-2.79	111.72	115.06
35	F	307	A86	C40-C32-C33	-2.78	96.54	109.05
36	f	804	CLA	CMD-C2D-C3D	-2.78	121.21	127.61
41	I	316	LHG	O8-C23-C24	2.78	120.65	111.91
36	H	306	CLA	CHB-C4A-NA	2.78	128.36	124.51
36	Q	306	CLA	CHB-C4A-NA	2.78	128.36	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	309	CLA	O2A-CGA-CBA	2.78	120.64	111.91
43	a	840	PQN	C14-C13-C15	2.78	119.95	115.27
35	R	303	A86	C3-C4-C5	-2.78	117.77	123.47
36	O	307	CLA	CHB-C4A-NA	2.78	128.36	124.51
36	Q	305	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
36	R	316	CLA	CMC-C2C-C1C	-2.78	120.80	125.04
36	I	307	CLA	CHB-C4A-NA	2.78	128.36	124.51
36	A	306	CLA	CMB-C2B-C3B	2.78	129.88	124.68
36	T	311	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
36	S	319	CLA	CMB-C2B-C3B	2.78	129.88	124.68
35	G	302	A86	C12-C11-C13	2.78	120.69	116.02
36	B	309	CLA	C1-C2-C3	-2.78	121.24	126.04
36	R	313	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
36	N	309	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
37	G	318	KC1	CAA-CBA-CGA	-2.78	112.99	127.26
36	N	308	CLA	C1-C2-C3	2.78	130.84	126.04
36	N	318	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
36	E	313	CLA	C3D-C2D-C1D	-2.78	102.04	105.83
36	W	214	CLA	CAA-C2A-C3A	-2.77	109.62	116.10
36	K	310	CLA	CMD-C2D-C3D	-2.77	121.23	127.61
36	M	310	CLA	CHA-C1A-NA	-2.77	120.05	126.40
36	l	201	CLA	CHD-C1D-ND	-2.77	121.91	124.45
36	N	315	CLA	CHB-C4A-NA	2.77	128.35	124.51
44	b	846	BCR	C8-C9-C10	2.77	123.20	118.94
40	b	849	DGD	C6D-O5D-C1E	2.77	119.16	113.74
36	V	311	CLA	C1-C2-C3	-2.77	121.25	126.04
34	j	103	DD6	C9-C8-C6	-2.77	118.63	126.42
36	b	819	CLA	C2D-C1D-ND	-2.77	108.06	110.10
36	J	311	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
36	M	307	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
36	b	816	CLA	CMD-C2D-C3D	-2.77	121.24	127.61
36	a	810	CLA	CAA-CBA-CGA	2.77	121.35	113.25
36	O	310	CLA	CMB-C2B-C3B	2.77	129.86	124.68
36	f	804	CLA	C3D-C4D-ND	2.77	114.72	110.24
35	G	305	A86	C9-C10-C11	-2.77	118.46	126.61
35	T	305	A86	C28-C27-C26	-2.77	119.04	122.92
35	X	304	A86	O-C13-C11	-2.77	115.03	121.15
35	R	306	A86	C25-C24-C1	-2.77	118.64	126.42
40	L	302	DGD	O1G-C1A-C2A	2.77	120.60	111.91
36	b	837	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
36	A	313	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
35	T	304	A86	O1-C15-C14	-2.77	107.65	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	309	CLA	O2A-C1-C2	-2.77	101.36	108.64
35	V	304	A86	C3-C2-C1	-2.77	123.36	127.31
35	C	203	A86	C17-C16-C15	2.77	111.99	109.16
36	K	310	CLA	C4-C3-C5	2.77	119.93	115.27
36	b	819	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
35	S	305	A86	O-C13-C11	-2.77	115.04	121.15
37	E	309	KC1	CBC-CAC-C3C	2.77	120.06	112.43
37	L	317	KC1	CED-O2D-CGD	2.77	122.19	115.94
36	D	313	CLA	CHB-C4A-NA	2.77	128.34	124.51
35	O	319	A86	O4-C38-O5	-2.76	117.47	122.96
36	B	309	CLA	CMC-C2C-C1C	2.76	129.25	125.04
37	M	318	KC1	C2C-C1C-NC	2.76	113.59	110.57
44	b	845	BCR	C30-C25-C26	-2.76	118.72	122.61
35	S	302	A86	C23-C16-C22	-2.76	103.29	107.37
36	b	816	CLA	C1D-ND-C4D	-2.76	104.37	106.33
36	F	317	CLA	C4-C3-C5	2.76	119.92	115.27
36	a	822	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
36	T	314	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
36	j	102	CLA	CMD-C2D-C3D	-2.76	121.26	127.61
35	D	302	A86	O1-C15-C14	-2.76	107.67	113.21
34	H	302	DD6	C21-C20-C15	-2.76	117.63	122.26
36	a	806	CLA	CHD-C1D-ND	-2.76	121.92	124.45
35	F	307	A86	O1-C15-C20	-2.76	56.70	59.40
37	S	316	KC1	C4C-C3C-C2C	-2.76	102.87	106.90
36	E	317	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
36	a	806	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
36	U	309	CLA	CMB-C2B-C3B	2.76	129.84	124.68
36	A	306	CLA	O2A-CGA-CBA	2.76	120.57	111.91
36	b	815	CLA	CBC-CAC-C3C	2.76	120.04	112.43
35	O	301	A86	C3-C4-C5	-2.76	117.82	123.47
35	O	305	A86	O1-C20-C19	-2.76	111.31	113.38
36	W	207	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
37	H	313	KC1	C2A-C3A-C4A	2.76	108.53	106.49
36	U	305	CLA	CHB-C4A-NA	2.76	128.33	124.51
35	S	301	A86	C25-C24-C1	-2.76	118.67	126.42
41	F	318	LHG	O8-C23-C24	2.76	120.56	111.91
41	b	850	LHG	O8-C23-C24	2.76	120.56	111.91
36	A	306	CLA	C4-C3-C5	2.76	119.91	115.27
35	J	303	A86	C3-C2-C1	-2.76	123.38	127.31
36	R	315	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
42	D	321	LMG	O8-C28-C29	2.76	120.56	111.91
37	J	314	KC1	C3A-C4A-NA	2.76	113.58	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	818	CLA	O2D-CGD-CBD	2.76	116.17	111.27
37	U	312	KC1	C1B-CHB-C4A	-2.76	120.11	126.06
34	P	305	DD6	C37-C36-C31	-2.76	120.61	124.35
36	P	308	CLA	CHB-C4A-NA	2.76	128.32	124.51
36	O	306	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
36	M	309	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
37	D	314	KC1	CAA-CBA-CGA	-2.75	113.11	127.26
36	S	314	CLA	CAA-C2A-C3A	-2.75	105.24	112.78
36	a	816	CLA	CHB-C4A-NA	2.75	128.32	124.51
36	N	315	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
35	G	304	A86	C19-C18-C17	-2.75	105.46	110.77
36	b	810	CLA	CHB-C4A-NA	2.75	128.32	124.51
35	O	305	A86	C4-C5-C6	-2.75	123.38	127.31
36	I	308	CLA	C4-C3-C5	2.75	119.90	115.27
36	b	816	CLA	C4D-CHA-C1A	-2.75	117.90	121.25
36	U	306	CLA	O2A-CGA-CBA	2.75	120.54	111.91
37	A	312	KC1	CMA-C3A-C4A	-2.75	120.85	125.04
36	W	207	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
35	R	303	A86	C9-C10-C11	-2.75	118.52	126.61
36	Q	309	CLA	CMB-C2B-C3B	2.75	129.82	124.68
35	N	302	A86	C23-C16-C22	-2.75	103.31	107.37
36	b	837	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
35	T	303	A86	O1-C15-C20	-2.75	56.71	59.40
37	F	308	KC1	CMC-C2C-C3C	2.75	133.58	126.12
36	M	312	CLA	CMB-C2B-C3B	2.75	129.82	124.68
35	S	301	A86	C14-C15-C16	-2.75	108.23	118.75
36	P	318	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
36	a	823	CLA	O2A-CGA-CBA	2.75	120.53	111.91
44	i	103	BCR	C29-C30-C25	2.75	114.71	110.48
36	J	317	CLA	CMB-C2B-C3B	2.75	129.82	124.68
36	L	313	CLA	CHB-C4A-NA	2.75	128.31	124.51
36	P	312	CLA	CMB-C2B-C3B	2.75	129.81	124.68
36	a	825	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
37	G	318	KC1	C2B-C1B-NB	2.75	112.13	110.10
37	N	314	KC1	C4C-C3C-C2C	-2.74	102.90	106.90
36	a	841	CLA	CAC-C3C-C4C	2.74	128.37	124.81
35	U	304	A86	C9-C8-C6	-2.74	118.71	126.42
37	X	311	KC1	C2B-C1B-NB	2.74	112.13	110.10
36	B	309	CLA	CHA-C4D-ND	2.74	138.24	132.50
35	O	305	A86	C41-C32-C31	-2.74	108.02	110.47
42	I	315	LMG	O8-C28-C29	2.74	120.52	111.91
36	K	315	CLA	O2D-CGD-O1D	-2.74	118.47	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	I	303	DD6	C37-C36-C31	-2.74	120.62	124.35
37	E	309	KC1	C4C-C3C-C2C	-2.74	102.90	106.90
41	R	323	LHG	O8-C23-C24	2.74	120.51	111.91
36	a	806	CLA	O2A-CGA-CBA	2.74	120.51	111.91
36	U	307	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
42	j	105	LMG	O8-C28-C29	2.74	120.51	111.91
36	D	316	CLA	CMB-C2B-C3B	2.74	129.81	124.68
36	b	836	CLA	CHB-C4A-NA	2.74	128.30	124.51
35	T	305	A86	C3-C4-C5	-2.74	117.86	123.47
36	l	204	CLA	CMD-C2D-C3D	-2.74	121.31	127.61
36	I	306	CLA	CMC-C2C-C1C	2.74	129.21	125.04
36	b	801	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
36	D	312	CLA	CHB-C4A-NA	2.74	128.30	124.51
36	D	316	CLA	C2D-C1D-ND	-2.74	108.08	110.10
36	Q	305	CLA	CHB-C4A-NA	2.74	128.30	124.51
36	O	306	CLA	CHB-C4A-NA	2.74	128.30	124.51
36	L	314	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
34	C	201	DD6	C37-C36-C35	2.74	119.43	114.36
35	N	301	A86	C14-C15-C16	-2.74	108.27	118.75
36	A	306	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
35	U	304	A86	C41-C32-C31	-2.74	108.02	110.47
35	B	301	A86	C4-C3-C2	-2.74	117.87	123.47
36	X	306	CLA	CMB-C2B-C3B	2.74	129.80	124.68
41	b	850	LHG	C5-O7-C7	-2.74	111.05	117.79
43	a	840	PQN	C2M-C2-C3	-2.74	119.94	124.40
35	M	301	A86	C34-O4-C38	2.74	123.00	117.90
42	G	324	LMG	O8-C28-C29	2.74	120.50	111.91
35	S	304	A86	C12-C11-C13	2.74	120.62	116.02
36	V	311	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
35	N	301	A86	C25-C24-C1	-2.74	118.73	126.42
35	R	303	A86	C9-C8-C6	-2.74	118.73	126.42
36	b	824	CLA	CAC-C3C-C4C	2.74	128.36	124.81
34	D	303	DD6	C10-C9-C8	-2.73	114.68	123.22
36	b	834	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
35	K	306	A86	C3-C2-C1	-2.73	123.41	127.31
36	I	305	CLA	O2D-CGD-CBD	2.73	116.12	111.27
36	D	309	CLA	CAC-C3C-C4C	2.73	128.36	124.81
36	M	310	CLA	CAC-C3C-C4C	2.73	128.36	124.81
36	M	316	CLA	CHB-C4A-NA	2.73	128.29	124.51
36	O	308	CLA	CHB-C4A-NA	2.73	128.29	124.51
36	b	836	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
35	U	304	A86	C-C1-C2	-2.73	119.09	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	K	305	DD6	C14-C13-C11	-2.73	121.29	125.53
36	N	319	CLA	CMC-C2C-C1C	-2.73	120.88	125.04
36	G	310	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
37	P	317	KC1	C4C-C3C-C2C	-2.73	102.92	106.90
36	B	305	CLA	CHB-C4A-NA	2.73	128.29	124.51
36	L	309	CLA	O2A-CGA-O1A	-2.73	116.70	123.59
35	F	301	A86	C25-C26-C27	-2.73	123.41	127.31
43	b	842	PQN	C2M-C2-C3	-2.73	119.94	124.40
37	F	315	KC1	CMA-C3A-C4A	-2.73	120.88	125.04
36	b	814	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
36	B	308	CLA	CHB-C4A-NA	2.73	128.29	124.51
36	K	307	CLA	C4-C3-C5	2.73	119.86	115.27
36	H	309	CLA	CHB-C4A-NA	2.73	128.29	124.51
34	B	302	DD6	C15-C14-C13	-2.73	120.22	125.99
37	J	314	KC1	C3B-C2B-C1B	-2.73	104.47	107.08
36	G	319	CLA	CHA-C4D-ND	-2.73	126.79	132.50
36	S	321	CLA	O2D-CGD-CBD	2.73	116.12	111.27
36	a	810	CLA	CHB-C4A-NA	2.73	128.29	124.51
35	F	302	A86	C34-O4-C38	-2.73	112.81	117.90
35	W	203	A86	O1-C20-C21	-2.73	111.79	115.06
41	G	320	LHG	O8-C23-C24	2.73	120.47	111.91
36	U	306	CLA	C4-C3-C5	2.73	119.86	115.27
35	T	307	A86	C23-C16-C17	-2.73	104.24	108.98
36	E	311	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
37	G	317	KC1	CED-O2D-CGD	2.73	122.11	115.94
35	T	302	A86	C36-C31-C32	-2.73	116.99	119.70
36	Q	314	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
37	G	318	KC1	CBC-CAC-C3C	2.73	119.94	112.43
36	C	211	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
37	V	312	KC1	CAA-C2A-C1A	2.72	137.27	124.75
35	O	303	A86	C25-C24-C1	-2.72	118.76	126.42
35	R	302	A86	O1-C15-C20	-2.72	56.74	59.40
35	U	302	A86	C23-C16-C22	-2.72	103.35	107.37
36	M	308	CLA	CMB-C2B-C3B	2.72	129.77	124.68
36	P	318	CLA	CMB-C2B-C3B	2.72	129.77	124.68
41	Q	315	LHG	O8-C23-C24	2.72	120.45	111.91
36	S	314	CLA	CHB-C4A-NA	2.72	128.28	124.51
36	S	312	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
42	a	852	LMG	O8-C28-C29	2.72	120.45	111.91
36	M	307	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
35	h	204	A86	C4-C5-C6	-2.72	123.43	127.31
34	H	302	DD6	O1-C20-C19	2.72	115.43	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	F	319	LHG	O8-C23-C24	2.72	120.44	111.91
36	K	316	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
36	L	308	CLA	CHC-C1C-C2C	2.72	134.25	126.72
36	W	201	CLA	CHB-C4A-NA	2.72	128.27	124.51
42	L	321	LMG	O8-C28-C29	2.72	120.44	111.91
35	O	303	A86	O1-C15-C20	-2.72	56.74	59.40
36	G	307	CLA	CHD-C1D-C2D	2.72	131.18	125.48
36	a	824	CLA	O2D-CGD-CBD	2.72	116.10	111.27
36	a	811	CLA	CHB-C4A-NA	2.72	128.27	124.51
37	T	315	KC1	CAA-C2A-C1A	2.72	137.24	124.75
36	b	806	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
36	V	314	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
36	b	836	CLA	C4-C3-C5	2.72	119.84	115.27
35	P	304	A86	C25-C24-C1	-2.72	118.78	126.42
36	l	204	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
36	S	321	CLA	CMB-C2B-C3B	2.72	129.76	124.68
36	a	823	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
36	W	207	CLA	CHB-C4A-NA	2.72	128.27	124.51
36	R	320	CLA	C2A-C1A-CHA	2.72	128.61	123.86
36	S	313	CLA	C3A-C2A-C1A	2.72	105.41	101.34
36	X	308	CLA	CMB-C2B-C3B	2.71	129.76	124.68
41	a	850	LHG	O8-C23-C24	2.71	120.43	111.91
36	W	208	CLA	CHB-C4A-NA	2.71	128.26	124.51
36	V	311	CLA	CMD-C2D-C3D	2.71	133.86	127.61
36	b	829	CLA	CMB-C2B-C3B	2.71	129.75	124.68
36	A	308	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
36	K	312	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
36	F	312	CLA	CHB-C4A-NA	2.71	128.26	124.51
34	C	201	DD6	C21-C20-C15	-2.71	117.72	122.26
36	W	216	CLA	C2A-C3A-C4A	2.71	106.25	101.87
35	G	304	A86	C9-C8-C6	2.71	134.03	126.42
34	C	201	DD6	C14-C13-C11	-2.71	121.32	125.53
36	F	311	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
36	W	214	CLA	CMB-C2B-C3B	2.71	129.75	124.68
35	G	304	A86	C36-C31-C32	-2.71	117.01	119.70
36	b	802	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
36	N	317	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
36	G	312	CLA	CMB-C2B-C3B	2.71	129.75	124.68
36	U	306	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
42	V	315	LMG	O8-C28-C29	2.71	120.40	111.91
36	D	313	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
36	B	308	CLA	O2D-CGD-O1D	-2.71	118.55	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	h	201	BCR	C29-C30-C25	2.71	114.65	110.48
36	J	308	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
36	J	316	CLA	CBC-CAC-C3C	2.71	119.89	112.43
38	b	804	SQD	O9-S-C6	2.71	110.15	106.94
35	M	302	A86	C9-C8-C6	-2.70	118.82	126.42
44	b	847	BCR	C27-C26-C25	2.70	126.66	122.73
35	A	316	A86	C4-C3-C2	-2.70	117.94	123.47
35	O	305	A86	C35-C34-C33	-2.70	105.16	109.88
36	b	817	CLA	CMD-C2D-C3D	-2.70	121.39	127.61
36	C	210	CLA	CMB-C2B-C3B	2.70	129.74	124.68
35	Q	301	A86	C25-C24-C1	-2.70	118.82	126.42
36	R	322	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
36	H	314	CLA	CAC-C3C-C4C	2.70	128.32	124.81
37	F	315	KC1	O2D-CGD-O1D	-2.70	118.56	123.84
35	P	306	A86	C25-C26-C27	-2.70	123.45	127.31
36	b	826	CLA	C2D-C1D-ND	-2.70	108.11	110.10
36	N	316	CLA	CHB-C4A-NA	2.70	128.25	124.51
36	a	823	CLA	CHB-C4A-NA	2.70	128.25	124.51
36	D	306	CLA	CMB-C2B-C3B	2.70	129.73	124.68
36	h	203	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
36	P	313	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
35	N	304	A86	C26-C25-C24	-2.70	114.80	123.22
35	M	301	A86	O4-C34-C35	2.70	114.31	107.59
35	J	306	A86	C12-C11-C13	2.70	120.55	116.02
36	a	831	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
36	a	813	CLA	CHB-C4A-NA	2.70	128.24	124.51
37	Q	311	KC1	C1B-CHB-C4A	-2.70	120.24	126.06
36	S	313	CLA	CAC-C3C-C4C	2.70	128.31	124.81
44	a	844	BCR	C24-C23-C22	-2.70	122.16	126.23
34	E	306	DD6	C21-C20-C15	-2.70	117.74	122.26
37	O	313	KC1	C1B-CHB-C4A	-2.70	120.24	126.06
36	K	309	CLA	CMB-C2B-C3B	2.69	129.72	124.68
36	b	805	CLA	CMB-C2B-C3B	2.69	129.72	124.68
37	O	315	KC1	C1B-CHB-C4A	-2.69	120.25	126.06
37	S	316	KC1	CAC-C3C-C4C	2.69	128.31	124.81
36	S	311	CLA	CHB-C4A-NA	2.69	128.24	124.51
36	X	312	CLA	CHB-C4A-NA	2.69	128.24	124.51
36	O	316	CLA	O2A-CGA-CBA	2.69	120.36	111.91
37	D	314	KC1	C4D-C3D-CAD	2.69	112.16	107.81
36	I	205	CLA	CMD-C2D-C3D	-2.69	121.42	127.61
35	J	302	A86	C9-C10-C11	-2.69	118.69	126.61
42	G	325	LMG	O8-C28-C29	2.69	120.36	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	834	CLA	CHB-C4A-NA	2.69	128.24	124.51
36	b	831	CLA	C2D-C1D-ND	-2.69	108.12	110.10
36	C	207	CLA	CMB-C2B-C3B	2.69	129.72	124.68
35	U	302	A86	C9-C10-C11	-2.69	118.69	126.61
35	E	307	A86	C34-O4-C38	-2.69	112.88	117.90
36	P	310	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	f	802	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	F	314	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
36	b	833	CLA	CMD-C2D-C3D	2.69	133.80	127.61
36	l	205	CLA	C4-C3-C5	2.69	119.80	115.27
37	Q	313	KC1	C1B-CHB-C4A	-2.69	120.25	126.06
36	H	312	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	G	316	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
36	P	309	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
36	G	319	CLA	CMB-C2B-C3B	2.69	129.71	124.68
36	M	310	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
36	J	308	CLA	C6-C5-C3	2.69	120.50	113.45
36	O	307	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
35	R	304	A86	C23-C16-C17	-2.69	104.31	108.98
36	a	810	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
37	W	217	KC1	C1C-C2C-C3C	-2.69	104.13	106.96
36	E	312	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	I	311	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	b	811	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
36	R	322	CLA	CMA-C3A-C2A	-2.69	102.99	113.83
35	I	302	A86	O1-C20-C21	-2.69	111.84	115.06
36	D	316	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	G	309	CLA	CBA-CAA-C2A	2.69	121.79	113.86
41	G	301	LHG	O8-C23-C24	2.69	120.34	111.91
34	R	307	DD6	O1-C20-C19	2.69	115.40	113.38
36	S	313	CLA	CBA-CAA-C2A	-2.69	105.94	113.86
36	M	310	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
36	V	311	CLA	CHB-C4A-NA	2.69	128.22	124.51
36	E	312	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
36	H	315	CLA	CAA-C2A-C1A	2.68	120.77	111.97
37	W	217	KC1	C2B-C1B-NB	2.68	112.08	110.10
36	K	310	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
36	b	835	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
34	L	305	DD6	C3-C4-C5	-2.68	117.98	123.47
36	E	317	CLA	CHB-C4A-NA	2.68	128.22	124.51
36	a	814	CLA	CHC-C1C-NC	2.68	128.27	124.20
36	S	311	CLA	C1B-CHB-C4A	-2.68	124.80	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	307	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
36	E	315	CLA	CAC-C3C-C4C	2.68	128.29	124.81
36	E	310	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
36	D	307	CLA	CAA-CBA-CGA	-2.68	105.42	113.25
36	j	102	CLA	O2A-CGA-CBA	2.68	120.32	111.91
41	j	104	LHG	O8-C23-C24	2.68	120.32	111.91
36	a	836	CLA	CHB-C4A-NA	2.68	128.22	124.51
36	a	802	CLA	O2A-CGA-CBA	2.68	120.32	111.91
36	W	211	CLA	CED-O2D-CGD	2.68	122.00	115.94
34	K	304	DD6	C32-C31-C36	-2.68	118.85	122.63
40	C	215	DGD	O1G-C1A-C2A	2.68	120.32	111.91
36	D	309	CLA	CMB-C2B-C3B	2.68	129.69	124.68
36	D	308	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
35	P	304	A86	O1-C15-C20	-2.68	56.78	59.40
36	Q	307	CLA	CHB-C4A-NA	2.68	128.22	124.51
36	b	827	CLA	CMB-C2B-C3B	2.68	129.69	124.68
37	X	311	KC1	C1C-C2C-C3C	-2.68	104.14	106.96
35	N	301	A86	C3-C4-C5	-2.68	117.99	123.47
36	K	308	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
36	W	216	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
36	C	206	CLA	CMB-C2B-C3B	2.68	129.69	124.68
36	U	307	CLA	CHB-C4A-NA	2.68	128.21	124.51
36	V	306	CLA	CHB-C4A-NA	2.68	128.21	124.51
35	X	302	A86	C23-C16-C17	-2.68	104.33	108.98
36	F	317	CLA	O2A-CGA-CBA	2.68	120.31	111.91
36	L	312	CLA	CAA-C2A-C1A	2.68	120.75	111.97
35	E	305	A86	C12-C11-C13	2.68	120.52	116.02
41	G	321	LHG	O8-C23-C24	2.68	120.30	111.91
36	O	311	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
36	J	313	CLA	CHB-C4A-NA	2.67	128.21	124.51
41	E	322	LHG	O8-C23-C24	2.67	120.30	111.91
37	G	318	KC1	CBA-CAA-C2A	2.67	135.47	125.27
36	a	825	CLA	O2A-CGA-CBA	2.67	120.30	111.91
35	Q	301	A86	O1-C15-C20	-2.67	56.79	59.40
36	H	310	CLA	O1D-CGD-CBD	-2.67	119.02	124.48
36	a	815	CLA	CHB-C4A-NA	2.67	128.21	124.51
35	P	306	A86	C40-C32-C31	-2.67	108.08	110.47
35	N	320	A86	C3-C4-C5	-2.67	118.00	123.47
36	N	318	CLA	C3A-C2A-C1A	2.67	105.34	101.34
36	O	316	CLA	C3C-C4C-NC	2.67	113.57	110.57
36	F	311	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
36	E	315	CLA	O2D-CGD-O1D	-2.67	118.62	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	849	DD6	C25-C26-C27	-2.67	118.83	126.58
35	S	301	A86	C3-C4-C5	-2.67	118.00	123.47
35	X	302	A86	O4-C38-O5	-2.67	117.66	122.96
36	G	307	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
36	b	834	CLA	CHB-C4A-NA	2.67	128.20	124.51
36	I	306	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
37	P	315	KC1	C1B-CHB-C4A	-2.67	120.30	126.06
36	R	315	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
36	A	311	CLA	CMB-C2B-C3B	2.67	129.67	124.68
36	a	816	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
36	A	313	CLA	CHB-C4A-NA	2.67	128.20	124.51
34	I	303	DD6	C21-C20-C15	-2.67	117.79	122.26
36	B	306	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
36	K	307	CLA	CMD-C2D-C3D	-2.66	121.48	127.61
37	M	313	KC1	C4D-C3D-CAD	2.66	112.11	107.81
36	F	312	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
36	W	206	CLA	CHD-C1D-ND	-2.66	122.01	124.45
35	O	303	A86	C23-C16-C17	-2.66	104.36	108.98
36	b	826	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
34	K	305	DD6	C21-C20-C15	-2.66	117.80	122.26
36	L	320	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
36	f	805	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
36	P	310	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
36	I	309	CLA	CMB-C2B-C3B	2.66	129.66	124.68
36	H	315	CLA	C2A-C1A-CHA	2.66	128.51	123.86
36	Q	307	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
35	V	303	A86	O4-C34-C35	2.66	114.22	107.59
36	K	307	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
35	P	304	A86	C23-C16-C17	-2.66	104.36	108.98
35	Q	304	A86	C3-C4-C5	-2.66	118.03	123.47
35	S	303	A86	O1-C15-C20	-2.66	56.80	59.40
36	S	312	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
36	b	834	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
36	P	319	CLA	C3B-C4B-NB	-2.66	105.77	109.21
40	b	849	DGD	CDB-CCB-CBB	-2.66	100.93	114.42
35	V	304	A86	C19-C18-C17	-2.66	105.64	110.77
35	I	302	A86	C23-C16-C22	-2.66	103.45	107.37
35	Q	301	A86	C23-C16-C17	-2.66	104.36	108.98
36	R	320	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
36	J	313	CLA	CHD-C1D-ND	-2.66	122.01	124.45
36	E	308	CLA	CMB-C2B-C3B	2.66	129.65	124.68
37	W	213	KC1	C3B-C2B-C1B	-2.66	104.54	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	W	202	A86	C25-C24-C1	-2.66	118.95	126.42
36	O	308	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
36	S	320	CLA	CHB-C4A-NA	2.65	128.18	124.51
36	K	311	CLA	CAA-C2A-C1A	2.65	120.67	111.97
36	b	841	CLA	O2D-CGD-CBD	2.65	115.98	111.27
36	N	308	CLA	C1-O2A-CGA	2.65	123.41	116.44
37	G	318	KC1	CMC-C2C-C3C	2.65	133.32	126.12
36	a	806	CLA	C4-C3-C5	2.65	119.73	115.27
36	C	207	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
35	R	304	A86	C25-C24-C1	-2.65	118.96	126.42
36	a	812	CLA	CHB-C4A-NA	2.65	128.18	124.51
36	j	101	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
36	G	319	CLA	O2A-CGA-CBA	2.65	120.23	111.91
36	W	210	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
36	I	306	CLA	C4-C3-C5	2.65	119.73	115.27
36	F	309	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
37	K	314	KC1	C3B-C2B-C1B	-2.65	104.54	107.08
42	m	102	LMG	O8-C28-C29	2.65	120.23	111.91
36	Q	306	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
42	h	206	LMG	O8-C28-C29	2.65	120.22	111.91
36	b	806	CLA	C3C-C4C-NC	-2.65	107.60	110.57
36	H	315	CLA	CHB-C4A-NA	2.65	128.18	124.51
36	P	319	CLA	CHB-C4A-NA	2.65	128.18	124.51
34	S	306	DD6	C21-C20-C15	-2.65	117.82	122.26
36	a	830	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
36	b	823	CLA	CHB-C4A-NA	2.65	128.17	124.51
34	F	303	DD6	C21-C20-C15	-2.65	117.82	122.26
36	W	210	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
35	S	303	A86	C9-C8-C6	-2.65	118.98	126.42
36	a	835	CLA	CHB-C4A-NA	2.65	128.17	124.51
36	B	305	CLA	CHD-C1D-ND	-2.65	122.02	124.45
36	X	309	CLA	CHA-C1A-NA	-2.65	120.34	126.40
35	J	302	A86	C34-O4-C38	-2.64	112.97	117.90
36	D	317	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
36	a	839	CLA	CHB-C4A-NA	2.64	128.17	124.51
36	D	309	CLA	CMD-C2D-C3D	-2.64	121.53	127.61
36	X	306	CLA	CHB-C4A-NA	2.64	128.17	124.51
34	A	301	DD6	C37-C36-C35	2.64	119.25	114.36
36	a	806	CLA	CMB-C2B-C3B	2.64	129.62	124.68
34	Q	302	DD6	C21-C20-C15	-2.64	117.83	122.26
36	a	804	CLA	C2D-C1D-ND	-2.64	108.16	110.10
36	a	808	CLA	CHB-C4A-NA	2.64	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	801	CLA	C2A-C1A-CHA	2.64	128.48	123.86
44	l	203	BCR	C15-C16-C17	-2.64	118.06	123.47
35	A	302	A86	O-C13-C11	-2.64	115.31	121.15
36	a	848	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
41	F	318	LHG	C11-C10-C9	-2.64	101.02	114.42
36	V	314	CLA	O2A-CGA-CBA	2.64	120.19	111.91
36	K	310	CLA	CAC-C3C-C4C	2.64	128.24	124.81
36	K	311	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
34	C	201	DD6	C25-C26-C27	-2.64	118.92	126.58
36	V	314	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
35	N	303	A86	O1-C15-C20	-2.64	56.82	59.40
36	C	205	CLA	CHB-C4A-NA	2.64	128.16	124.51
36	L	311	CLA	CHB-C4A-NA	2.64	128.16	124.51
36	b	817	CLA	C4-C3-C5	2.64	119.71	115.27
35	N	303	A86	C9-C8-C6	-2.64	119.01	126.42
36	b	817	CLA	O2A-CGA-CBA	2.64	120.18	111.91
35	N	305	A86	C28-C27-C26	-2.64	119.23	122.92
41	a	842	LHG	O8-C23-C24	2.64	120.18	111.91
36	N	313	CLA	C2A-C1A-CHA	2.63	128.45	123.85
36	I	314	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
42	J	318	LMG	O8-C28-C29	2.63	120.17	111.91
36	F	309	CLA	C1-C2-C3	2.63	130.60	126.04
36	B	309	CLA	O2A-CGA-CBA	2.63	120.17	111.91
36	l	204	CLA	O2A-CGA-CBA	2.63	120.17	111.91
36	H	311	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
36	a	802	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
37	M	313	KC1	C2B-C1B-NB	2.63	112.05	110.10
35	S	308	A86	C34-O4-C38	-2.63	112.99	117.90
35	X	301	A86	O3-C36-C37	-2.63	104.71	109.39
41	F	318	LHG	C20-C19-C18	-2.63	101.06	114.42
36	E	313	CLA	CHD-C4C-C3C	-2.63	120.97	124.84
44	b	846	BCR	C27-C26-C25	2.63	126.55	122.73
36	J	317	CLA	CHB-C4A-NA	2.63	128.15	124.51
35	K	302	A86	C9-C10-C11	-2.63	118.87	126.61
42	E	319	LMG	O8-C28-C29	2.63	120.17	111.91
36	J	313	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
35	X	304	A86	C40-C32-C31	-2.63	108.12	110.47
34	B	302	DD6	C25-C26-C27	-2.63	118.94	126.58
41	f	808	LHG	O8-C23-C24	2.63	120.16	111.91
37	C	213	KC1	C2A-C1A-CHA	-2.63	118.74	127.44
44	b	846	BCR	C15-C14-C13	-2.63	123.56	127.31
41	f	809	LHG	O8-C23-C24	2.63	120.16	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	303	DD6	C37-C36-C35	2.63	119.23	114.36
35	F	307	A86	C41-C32-C40	-2.63	100.46	108.53
36	b	810	CLA	CMB-C2B-C3B	2.63	129.60	124.68
36	M	309	CLA	CHB-C4A-NA	2.63	128.15	124.51
36	a	807	CLA	O2A-C1-C2	2.63	115.55	108.64
36	C	208	CLA	CMB-C2B-C3B	2.63	129.60	124.68
36	N	309	CLA	CMC-C2C-C1C	-2.63	121.04	125.04
36	a	804	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
41	D	319	LHG	C5-O7-C7	-2.63	111.32	117.79
36	W	206	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
35	R	304	A86	C9-C10-C11	-2.63	118.88	126.61
35	F	304	A86	C12-C11-C13	2.63	120.44	116.02
34	B	302	DD6	C25-C24-C1	-2.63	119.03	126.42
36	U	309	CLA	CHB-C4A-NA	2.63	128.15	124.51
36	K	307	CLA	O2A-CGA-CBA	2.63	120.15	111.91
41	i	104	LHG	O8-C23-C24	2.63	120.15	111.91
36	T	309	CLA	CAA-C2A-C3A	-2.63	105.59	112.78
37	E	309	KC1	CMC-C2C-C3C	2.63	133.25	126.12
36	C	205	CLA	C2D-C1D-ND	-2.63	108.17	110.10
36	N	315	CLA	CAA-C2A-C1A	2.63	118.29	111.81
36	l	204	CLA	CAC-C3C-C4C	2.63	128.22	124.81
36	L	320	CLA	CHB-C4A-NA	2.62	128.14	124.51
36	M	306	CLA	CHB-C4A-NA	2.62	128.14	124.51
37	E	309	KC1	C2A-C1A-NA	2.62	113.61	109.40
37	T	315	KC1	C1A-C2A-C3A	-2.62	105.03	107.11
36	L	308	CLA	O2A-CGA-CBA	2.62	120.14	111.91
36	S	310	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
36	R	310	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
36	I	308	CLA	CMB-C2B-C3B	2.62	129.59	124.68
35	W	202	A86	O2-C18-C19	2.62	115.02	109.80
36	b	807	CLA	CHB-C4A-NA	2.62	128.14	124.51
35	Q	316	A86	C28-C27-C26	-2.62	119.25	122.92
36	b	837	CLA	CHD-C1D-ND	-2.62	122.05	124.45
36	T	316	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
36	R	319	CLA	CMB-C2B-C3B	2.62	129.58	124.68
36	F	317	CLA	C2D-C1D-ND	2.62	112.03	110.10
36	b	819	CLA	C3C-C4C-NC	-2.62	107.63	110.57
37	S	316	KC1	C3A-C4A-NA	2.62	113.43	110.57
35	J	301	A86	C25-C26-C27	-2.62	123.57	127.31
36	a	801	CLA	CHA-C1A-NA	-2.62	120.40	126.40
36	A	310	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
36	E	313	CLA	O2A-CGA-CBA	2.62	120.12	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	T	311	CLA	CHD-C4C-C3C	-2.62	120.99	124.84
36	E	314	CLA	CHB-C4A-NA	2.62	128.13	124.51
36	M	315	CLA	CBC-CAC-C3C	-2.62	105.22	112.43
35	F	302	A86	C12-C11-C13	2.62	120.42	116.02
36	B	308	CLA	CHD-C1D-C2D	2.62	130.97	125.48
35	B	301	A86	C12-C11-C13	2.62	120.42	116.02
35	V	301	A86	C9-C10-C11	-2.62	118.92	126.61
41	O	317	LHG	O8-C23-C24	2.61	120.11	111.91
34	L	305	DD6	C14-C13-C11	-2.61	121.47	125.53
36	O	311	CLA	CHB-C4A-NA	2.61	128.13	124.51
36	G	316	CLA	CMB-C2B-C3B	2.61	129.57	124.68
35	I	302	A86	C23-C16-C17	-2.61	104.44	108.98
43	b	842	PQN	C14-C13-C15	2.61	119.67	115.27
35	U	304	A86	C12-C11-C13	2.61	120.41	116.02
35	K	306	A86	C4-C3-C2	-2.61	118.12	123.47
36	G	315	CLA	O2A-CGA-CBA	2.61	120.11	111.91
36	H	305	CLA	CMB-C2B-C3B	2.61	129.57	124.68
36	I	306	CLA	C2A-C3A-C4A	2.61	106.09	101.87
35	R	301	A86	O-C13-C11	-2.61	115.38	121.15
35	M	304	A86	C7-C6-C5	-2.61	119.27	122.92
36	a	816	CLA	O2A-CGA-CBA	2.61	120.10	111.91
36	b	826	CLA	CMB-C2B-C3B	2.61	129.56	124.68
36	M	310	CLA	C3B-C4B-NB	-2.61	105.83	109.21
36	E	312	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
34	R	308	DD6	C21-C20-C15	-2.61	117.89	122.26
36	T	311	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
36	L	316	CLA	CHB-C4A-NA	2.61	128.12	124.51
37	L	315	KC1	O2D-CGD-O1D	-2.61	118.74	123.84
36	H	307	CLA	C2A-C1A-CHA	2.61	128.42	123.86
36	S	318	CLA	CMB-C2B-C3B	2.61	129.56	124.68
36	K	315	CLA	CHB-C4A-NA	2.61	128.12	124.51
36	W	216	CLA	CAA-CBA-CGA	2.61	119.43	112.51
36	O	316	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
36	H	315	CLA	CMB-C2B-C3B	2.61	129.56	124.68
36	a	819	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
36	a	830	CLA	O2A-CGA-CBA	2.61	120.09	111.91
36	D	308	CLA	O2D-CGD-CBD	2.61	115.90	111.27
41	l	208	LHG	O8-C23-C24	2.61	120.08	111.91
40	b	849	DGD	C1E-O6E-C5E	2.61	118.80	113.69
36	a	820	CLA	C2D-C1D-ND	-2.61	108.18	110.10
36	I	310	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
36	V	306	CLA	O2D-CGD-O1D	-2.60	118.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	214	CLA	CMB-C2B-C3B	2.60	129.55	124.68
36	L	310	CLA	CMB-C2B-C3B	2.60	129.55	124.68
35	T	306	A86	O4-C38-O5	-2.60	117.79	122.96
35	X	302	A86	C4-C3-C2	-2.60	118.14	123.47
35	E	305	A86	O1-C15-C14	-2.60	107.99	113.21
35	K	302	A86	C34-O4-C38	2.60	122.75	117.90
36	D	317	CLA	CMB-C2B-C3B	2.60	129.55	124.68
35	K	303	A86	C36-C31-C32	-2.60	117.11	119.70
42	J	318	LMG	C8-O7-C10	-2.60	111.39	117.79
44	f	801	BCR	C27-C26-C25	2.60	126.51	122.73
35	L	319	A86	C28-C27-C29	2.60	124.95	118.93
36	P	313	CLA	CHB-C4A-NA	2.60	128.11	124.51
44	m	101	BCR	C11-C10-C9	-2.60	123.60	127.31
36	D	317	CLA	CMA-C3A-C2A	-2.60	103.34	113.83
36	M	310	CLA	CHB-C4A-NA	2.60	128.10	124.51
36	b	822	CLA	CHB-C4A-NA	2.60	128.10	124.51
36	W	201	CLA	CMB-C2B-C3B	2.60	129.54	124.68
35	C	203	A86	C12-C11-C13	2.60	120.39	116.02
36	R	318	CLA	CHB-C4A-NA	2.60	128.10	124.51
35	H	301	A86	C21-C20-C19	-2.60	111.36	114.28
35	B	303	A86	C41-C32-C31	2.60	112.80	110.47
36	J	307	CLA	CAA-C2A-C3A	-2.60	105.67	112.78
44	b	843	BCR	C7-C8-C9	-2.60	122.31	126.23
36	C	205	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
36	D	310	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
36	S	310	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
35	A	302	A86	C24-C1-C2	-2.60	114.96	118.94
36	l	206	CLA	CHB-C4A-NA	2.60	128.10	124.51
34	S	307	DD6	C25-C24-C1	-2.59	119.13	126.42
35	J	303	A86	C26-C25-C24	-2.59	115.12	123.22
36	R	316	CLA	C2D-C1D-ND	-2.59	108.19	110.10
36	a	801	CLA	CMB-C2B-C3B	2.59	129.53	124.68
36	b	828	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
34	D	301	DD6	C25-C26-C27	-2.59	119.06	126.58
36	T	314	CLA	CAA-C2A-C1A	-2.59	103.48	111.97
34	S	307	DD6	C9-C10-C11	-2.59	123.61	127.31
36	P	312	CLA	C2A-C1A-CHA	2.59	128.39	123.86
34	J	304	DD6	C21-C20-C15	-2.59	117.92	122.26
34	R	308	DD6	C32-C31-C36	-2.59	118.98	122.63
35	O	319	A86	C28-C27-C26	-2.59	119.30	122.92
36	f	803	CLA	O2A-CGA-CBA	2.59	120.03	111.91
35	X	303	A86	C10-C9-C8	-2.59	115.14	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	R	313	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
35	O	305	A86	C25-C26-C27	-2.59	123.61	127.31
35	P	303	A86	C28-C27-C29	2.59	124.92	118.93
35	W	202	A86	C3-C4-C5	-2.59	118.17	123.47
36	K	312	CLA	CHB-C4A-NA	2.59	128.09	124.51
35	H	304	A86	O4-C38-O5	-2.59	117.82	122.96
36	M	312	CLA	CHB-C4A-NA	2.59	128.09	124.51
36	W	208	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
35	J	303	A86	C23-C16-C17	-2.59	104.49	108.98
42	E	319	LMG	C8-O7-C10	-2.59	111.42	117.79
36	a	810	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
35	Q	303	A86	C35-C34-C33	-2.59	105.36	109.88
36	a	821	CLA	CHB-C4A-NA	2.59	128.09	124.51
37	K	314	KC1	C4C-C3C-C2C	-2.59	103.13	106.90
36	F	317	CLA	CHD-C4C-C3C	-2.59	121.04	124.84
34	R	307	DD6	C32-C31-C36	-2.59	118.98	122.63
36	M	314	CLA	CHB-C4A-NA	2.59	128.09	124.51
36	a	841	CLA	CHB-C4A-NA	2.58	128.09	124.51
38	A	315	SQD	C45-O47-C7	-2.58	111.43	117.79
35	B	301	A86	C26-C25-C24	-2.58	115.15	123.22
36	f	805	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
44	i	103	BCR	C37-C22-C21	-2.58	119.30	122.92
37	F	308	KC1	C4D-C3D-CAD	2.58	111.98	107.81
35	V	301	A86	C9-C8-C6	-2.58	119.16	126.42
36	b	841	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
35	O	302	A86	C28-C27-C29	2.58	124.91	118.93
36	O	310	CLA	C2A-C1A-CHA	2.58	128.37	123.86
36	D	312	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
36	K	310	CLA	O2A-CGA-CBA	2.58	120.00	111.91
36	Q	309	CLA	C2A-C1A-CHA	2.58	128.37	123.86
36	R	322	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
35	N	306	A86	O4-C38-O5	-2.58	117.84	122.96
35	F	305	A86	C28-C27-C26	-2.58	119.31	122.92
34	a	849	DD6	C15-C14-C13	-2.58	120.54	125.99
36	G	309	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
36	l	205	CLA	C2C-C1C-NC	2.58	112.39	109.97
36	B	308	CLA	CMA-C3A-C2A	-2.58	103.42	113.83
36	S	315	CLA	C3A-C2A-C1A	2.58	105.20	101.34
36	A	309	CLA	CHB-C4A-NA	2.58	128.08	124.51
35	J	301	A86	C26-C25-C24	-2.58	115.17	123.22
34	A	301	DD6	O1-C20-C19	-2.58	111.45	113.38
34	F	303	DD6	C15-C14-C13	-2.58	120.54	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	W	204	DD6	C15-C14-C13	-2.58	120.54	125.99
36	G	309	CLA	C6-C5-C3	2.58	120.21	113.45
34	D	301	DD6	C37-C36-C35	2.58	119.13	114.36
36	H	310	CLA	CHD-C4C-C3C	2.58	128.63	124.84
34	B	302	DD6	C-C1-C2	-2.58	119.31	122.92
34	B	304	DD6	O1-C20-C21	-2.58	111.97	115.06
36	F	313	CLA	CHB-C4A-NA	2.58	128.07	124.51
35	U	301	A86	C36-C31-C32	2.57	122.25	119.70
37	O	313	KC1	C3B-C2B-C1B	-2.57	104.62	107.08
36	j	102	CLA	CHB-C4A-NA	2.57	128.07	124.51
36	U	310	CLA	CMC-C2C-C1C	-2.57	121.12	125.04
37	V	312	KC1	C2A-C1A-CHA	-2.57	118.93	127.44
35	Q	304	A86	C24-C1-C2	2.57	122.89	118.94
36	H	318	CLA	CAA-CBA-CGA	-2.57	105.74	113.25
36	H	318	CLA	CHB-C4A-NA	2.57	128.07	124.51
35	J	301	A86	C12-C11-C13	2.57	120.34	116.02
36	V	310	CLA	CHB-C4A-NA	2.57	128.07	124.51
36	b	817	CLA	CHD-C4C-C3C	-2.57	121.06	124.84
36	I	313	CLA	CHB-C4A-NA	2.57	128.06	124.51
36	b	830	CLA	CAC-C3C-C2C	-2.57	123.14	127.53
36	W	211	CLA	C2D-C1D-ND	-2.57	108.21	110.10
36	R	312	CLA	CHB-C4A-NA	2.57	128.06	124.51
36	S	315	CLA	C1D-ND-C4D	-2.57	104.51	106.33
36	K	312	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
34	P	305	DD6	C21-C20-C15	-2.57	117.96	122.26
36	S	321	CLA	C2A-C1A-CHA	2.57	128.35	123.86
35	U	302	A86	O4-C38-O5	-2.57	117.86	122.96
35	G	305	A86	C41-C32-C31	-2.57	108.17	110.47
35	h	202	A86	C34-O4-C38	-2.57	113.11	117.90
36	K	316	CLA	CHB-C4A-NA	2.57	128.06	124.51
34	K	305	DD6	C37-C36-C35	2.57	119.11	114.36
35	S	303	A86	C9-C10-C11	-2.57	119.07	126.61
36	J	316	CLA	CHB-C4A-NA	2.57	128.06	124.51
36	a	807	CLA	C11-C10-C8	-2.57	107.63	115.92
34	W	205	DD6	C32-C33-C34	-2.56	107.85	113.64
37	C	213	KC1	O2D-CGD-O1D	-2.56	118.82	123.84
36	D	307	CLA	C2A-C1A-CHA	2.56	128.34	123.86
36	I	308	CLA	CHD-C1D-C2D	2.56	130.86	125.48
36	F	310	CLA	O2D-CGD-CBD	2.56	115.82	111.27
35	N	304	A86	C40-C32-C31	-2.56	108.18	110.47
36	b	801	CLA	C4D-C3D-CAD	-2.56	105.08	108.10
42	V	316	LMG	O8-C28-C29	2.56	119.95	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	309	CLA	CMC-C2C-C1C	2.56	128.94	125.04
37	C	213	KC1	C4C-C3C-C2C	-2.56	103.16	106.90
37	T	310	KC1	O2D-CGD-O1D	-2.56	118.83	123.84
36	U	306	CLA	CAC-C3C-C4C	2.56	128.13	124.81
36	a	829	CLA	CMD-C2D-C3D	2.56	133.51	127.61
42	J	319	LMG	O8-C28-C29	2.56	119.94	111.91
36	F	310	CLA	CHB-C4A-NA	2.56	128.05	124.51
34	S	307	DD6	C21-C20-C15	-2.56	117.97	122.26
36	I	308	CLA	C4D-CHA-C1A	-2.56	118.14	121.25
35	N	303	A86	C9-C10-C11	-2.56	119.08	126.61
35	K	302	A86	C9-C8-C6	-2.56	119.23	126.42
36	b	836	CLA	CMC-C2C-C1C	2.56	128.94	125.04
36	b	805	CLA	CMA-C3A-C2A	-2.56	103.51	113.83
36	N	308	CLA	CMA-C3A-C2A	-2.56	103.51	113.83
36	C	208	CLA	O2D-CGD-CBD	2.56	115.81	111.27
36	J	307	CLA	CHB-C4A-NA	2.56	128.05	124.51
36	A	314	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
36	L	311	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
36	M	307	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
36	b	840	CLA	CHB-C4A-NA	2.56	128.05	124.51
35	H	304	A86	O1-C15-C14	-2.56	108.08	113.21
36	b	811	CLA	CBA-CAA-C2A	2.56	121.41	113.86
34	O	304	DD6	C25-C26-C27	-2.55	119.16	126.58
35	X	305	A86	C9-C10-C11	-2.55	119.10	126.61
34	Q	302	DD6	C15-C14-C13	-2.55	120.59	125.99
34	D	303	DD6	C32-C31-C36	-2.55	119.03	122.63
36	B	308	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
37	T	315	KC1	C2A-C1A-CHA	-2.55	119.00	127.44
36	f	803	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
35	X	314	A86	C12-C11-C13	2.55	120.31	116.02
36	L	310	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
35	N	305	A86	C23-C16-C17	-2.55	104.55	108.98
44	m	101	BCR	C15-C14-C13	-2.55	123.67	127.31
35	J	305	A86	C12-C11-C13	2.55	120.31	116.02
36	O	316	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
44	l	207	BCR	C3-C4-C5	-2.55	109.52	114.08
36	I	311	CLA	O2D-CGD-CBD	2.55	115.80	111.27
36	b	834	CLA	CHD-C1D-ND	-2.55	122.11	124.45
35	S	304	A86	O1-C20-C19	-2.55	111.47	113.38
35	X	305	A86	C25-C24-C1	-2.55	119.25	126.42
35	G	302	A86	O1-C15-C14	-2.55	108.09	113.21
35	V	302	A86	C22-C16-C17	2.55	113.41	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	306	A86	C34-O4-C38	-2.55	113.15	117.90
35	N	302	A86	C4-C3-C2	-2.55	118.25	123.47
35	S	302	A86	C4-C3-C2	-2.55	118.25	123.47
36	a	822	CLA	CHB-C4A-NA	2.55	128.03	124.51
37	M	317	KC1	C2A-C1A-NA	2.55	113.49	109.40
35	I	304	A86	C4-C3-C2	-2.55	118.26	123.47
35	T	307	A86	C9-C10-C11	-2.55	119.12	126.61
36	f	803	CLA	CHD-C4C-C3C	-2.55	121.10	124.84
37	M	317	KC1	C3A-C4A-NA	2.55	113.35	110.57
37	P	315	KC1	C3B-C2B-C1B	-2.55	104.64	107.08
36	a	820	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
36	W	214	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
36	T	308	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
37	F	315	KC1	C2B-C1B-NB	2.55	111.98	110.10
38	b	804	SQD	O48-C23-C24	2.55	119.89	111.91
36	G	315	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
36	N	308	CLA	C3C-C4C-NC	2.54	113.42	110.57
36	b	836	CLA	C3D-C4D-ND	2.54	114.35	110.24
35	E	305	A86	O4-C38-O5	-2.54	117.91	122.96
35	U	301	A86	C40-C32-C31	-2.54	108.19	110.47
36	b	811	CLA	C1-C2-C3	-2.54	121.64	126.04
36	f	803	CLA	CMC-C2C-C1C	2.54	128.91	125.04
36	a	802	CLA	CED-O2D-CGD	2.54	121.69	115.94
36	Q	312	CLA	CHB-C4A-NA	2.54	128.03	124.51
36	f	804	CLA	C4-C3-C5	2.54	119.55	115.27
37	A	312	KC1	C3D-CAD-CBD	2.54	110.95	107.61
36	F	309	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
36	T	312	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
35	C	203	A86	C3-C4-C5	-2.54	118.27	123.47
36	a	806	CLA	CHB-C4A-NA	2.54	128.03	124.51
36	b	828	CLA	CHB-C4A-NA	2.54	128.03	124.51
39	b	848	LMT	C1B-O1B-C4'	-2.54	111.68	117.96
37	Q	313	KC1	C3B-C2B-C1B	-2.54	104.65	107.08
36	G	311	CLA	CMB-C2B-C3B	2.54	129.43	124.68
36	P	316	CLA	CHB-C4A-NA	2.54	128.02	124.51
34	W	205	DD6	C37-C36-C35	2.54	119.06	114.36
35	P	306	A86	C4-C3-C2	-2.54	118.27	123.47
37	B	310	KC1	O2D-CGD-O1D	-2.54	118.87	123.84
35	N	320	A86	C24-C1-C2	2.54	122.84	118.94
36	h	203	CLA	CHD-C1D-ND	-2.54	122.12	124.45
36	X	310	CLA	O2D-CGD-CBD	-2.54	106.76	111.27
36	a	848	CLA	OBD-CAD-C3D	-2.54	122.41	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	b	846	BCR	C15-C16-C17	-2.54	118.27	123.47
37	P	317	KC1	C1A-NA-C4A	-2.54	105.56	106.71
36	C	207	CLA	O2A-CGA-CBA	2.54	119.87	111.91
36	H	317	CLA	CHB-C4A-NA	2.54	128.02	124.51
35	N	304	A86	C41-C32-C31	-2.54	108.20	110.47
36	S	314	CLA	C2A-C1A-CHA	2.54	128.29	123.86
36	a	818	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
36	a	839	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
37	Q	311	KC1	C3B-C2B-C1B	-2.54	104.65	107.08
36	X	313	CLA	CMC-C2C-C3C	2.54	133.00	126.12
36	T	311	CLA	CMC-C2C-C3C	2.53	133.00	126.12
36	F	313	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
36	A	313	CLA	CMB-C2B-C3B	2.53	129.42	124.68
34	D	304	DD6	C21-C20-C15	-2.53	118.01	122.26
44	a	844	BCR	C27-C26-C25	2.53	126.41	122.73
42	a	852	LMG	C8-O7-C10	-2.53	111.55	117.79
35	J	301	A86	C4-C3-C2	-2.53	118.28	123.47
35	J	302	A86	C9-C8-C6	-2.53	119.30	126.42
36	b	824	CLA	CMC-C2C-C1C	2.53	128.90	125.04
36	W	212	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
35	Q	316	A86	C23-C16-C17	-2.53	104.58	108.98
35	Q	316	A86	O4-C34-C33	2.53	113.90	107.59
37	W	213	KC1	C4D-C3D-CAD	2.53	111.90	107.81
35	F	305	A86	C4-C3-C2	-2.53	118.29	123.47
36	V	308	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
36	N	308	CLA	CHD-C4C-C3C	-2.53	121.12	124.84
36	W	210	CLA	CBA-CAA-C2A	-2.53	106.39	113.86
35	P	306	A86	C12-C11-C13	2.53	120.27	116.02
35	F	304	A86	C25-C26-C27	-2.53	123.70	127.31
36	E	312	CLA	CHD-C1D-ND	-2.53	122.13	124.45
34	A	301	DD6	C15-C14-C13	-2.53	120.64	125.99
34	I	303	DD6	C15-C14-C13	-2.53	120.64	125.99
36	H	310	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
36	L	320	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
36	X	313	CLA	C2A-C1A-CHA	2.53	128.28	123.86
34	L	305	DD6	C25-C26-C27	-2.53	119.24	126.58
35	N	305	A86	O4-C34-C33	2.53	113.89	107.59
36	S	317	CLA	CHB-C4A-NA	2.53	128.01	124.51
36	a	809	CLA	CHB-C4A-NA	2.53	128.01	124.51
37	E	309	KC1	C2B-C1B-NB	2.53	111.97	110.10
36	P	313	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
35	W	203	A86	O1-C20-C19	-2.53	111.48	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	L	301	A86	C4-C3-C2	-2.52	118.30	123.47
36	S	313	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
36	l	205	CLA	CHD-C1D-ND	-2.52	122.13	124.45
36	H	308	CLA	O1A-CGA-CBA	2.52	133.58	123.73
36	R	318	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
36	D	313	CLA	CHD-C1D-ND	-2.52	122.14	124.45
36	E	313	CLA	C3C-C4C-NC	2.52	113.40	110.57
35	G	304	A86	C14-C15-C16	-2.52	109.09	118.75
36	H	306	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
37	N	314	KC1	C1C-C2C-C3C	-2.52	104.30	106.96
36	V	305	CLA	CMA-C3A-C4A	2.52	118.55	111.77
34	K	304	DD6	C14-C13-C11	-2.52	121.62	125.53
35	G	305	A86	O4-C38-O5	-2.52	117.95	122.96
36	l	205	CLA	O2A-CGA-CBA	2.52	119.82	111.91
36	G	315	CLA	C3D-C2D-C1D	-2.52	102.39	105.83
36	H	307	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
36	j	106	CLA	CAA-C2A-C3A	-2.52	107.96	114.26
36	j	106	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
36	R	311	CLA	O2D-CGD-CBD	2.52	115.75	111.27
36	F	311	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
36	B	311	CLA	C3A-C2A-C1A	2.52	105.11	101.34
35	T	307	A86	O4-C34-C33	2.52	113.87	107.59
34	j	103	DD6	O1-C20-C21	-2.52	112.04	115.06
36	L	311	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
36	K	313	CLA	CHB-C4A-NA	2.52	128.00	124.51
36	T	311	CLA	CMC-C2C-C1C	-2.52	121.20	125.04
36	b	823	CLA	O2D-CGD-CBD	2.52	115.74	111.27
36	O	314	CLA	CHB-C4A-NA	2.52	128.00	124.51
36	b	838	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
35	S	305	A86	C25-C24-C1	-2.52	119.34	126.42
36	G	314	CLA	CAC-C3C-C4C	2.52	128.08	124.81
35	T	303	A86	C25-C24-C1	-2.52	119.34	126.42
36	V	306	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
37	W	217	KC1	O2D-CGD-O1D	-2.52	118.92	123.84
35	D	302	A86	C25-C26-C27	-2.52	123.72	127.31
36	S	321	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
34	F	303	DD6	C14-C13-C11	-2.52	121.63	125.53
35	V	304	A86	C4-C3-C2	-2.52	118.32	123.47
36	a	804	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
37	L	315	KC1	C3B-C2B-C1B	-2.51	104.67	107.08
36	N	318	CLA	CGD-CBD-CAD	-2.51	102.59	110.73
34	W	204	DD6	O1-C20-C19	2.51	115.27	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	314	CLA	CHD-C1D-ND	-2.51	122.14	124.45
37	O	315	KC1	C1C-C2C-C3C	-2.51	104.31	106.96
35	P	303	A86	C9-C10-C11	-2.51	119.22	126.61
34	D	301	DD6	C21-C20-C15	-2.51	118.05	122.26
36	H	305	CLA	CHB-C4A-NA	2.51	127.99	124.51
35	R	302	A86	C9-C10-C11	-2.51	119.22	126.61
34	j	103	DD6	C4-C3-C2	-2.51	118.33	123.47
35	M	301	A86	C3-C4-C5	-2.51	118.33	123.47
36	b	836	CLA	CAC-C3C-C4C	2.51	128.07	124.81
36	K	313	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
36	S	309	CLA	C2D-C1D-ND	-2.51	108.25	110.10
35	B	303	A86	C10-C9-C8	-2.51	115.38	123.22
35	L	319	A86	C9-C10-C11	-2.51	119.23	126.61
35	S	301	A86	O1-C20-C19	2.51	115.27	113.38
44	m	101	BCR	C27-C26-C25	2.51	126.37	122.73
35	F	305	A86	C40-C32-C31	2.51	112.72	110.47
35	S	305	A86	C4-C3-C2	-2.51	118.34	123.47
37	X	311	KC1	O2D-CGD-O1D	-2.51	118.94	123.84
36	R	321	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
35	O	302	A86	C3-C4-C5	-2.51	118.34	123.47
36	F	317	CLA	CHA-C4D-ND	2.51	137.74	132.50
35	L	319	A86	C3-C4-C5	-2.51	118.34	123.47
35	V	303	A86	C25-C24-C1	-2.51	119.38	126.42
36	b	822	CLA	CAA-C2A-C3A	-2.51	105.92	112.78
36	V	309	CLA	C3A-C2A-C1A	2.50	105.09	101.34
36	G	313	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
35	P	303	A86	C3-C4-C5	-2.50	118.34	123.47
35	N	301	A86	O1-C20-C19	2.50	115.26	113.38
37	G	308	KC1	CED-O2D-CGD	2.50	121.60	115.94
36	G	313	CLA	C6-C7-C8	-2.50	107.83	115.92
36	b	813	CLA	CAB-C3B-C2B	2.50	129.59	124.69
36	S	313	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
34	H	302	DD6	C37-C36-C35	2.50	118.99	114.36
36	V	311	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
35	R	302	A86	C9-C8-C6	-2.50	119.39	126.42
36	H	306	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
37	Q	311	KC1	C1C-C2C-C3C	-2.50	104.33	106.96
36	H	316	CLA	CMB-C2B-C3B	2.50	129.36	124.68
37	X	311	KC1	C2A-C1A-NA	2.50	113.41	109.40
44	b	846	BCR	C35-C13-C14	-2.50	119.42	122.92
36	N	318	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
36	O	311	CLA	C1B-CHB-C4A	-2.50	125.17	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Q	310	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
35	O	319	A86	C-C1-C24	-2.50	114.14	118.08
36	a	830	CLA	C5-C3-C4	2.50	120.12	114.60
37	O	315	KC1	C3B-C2B-C1B	-2.50	104.69	107.08
35	R	301	A86	C23-C16-C22	-2.50	103.69	107.37
36	N	311	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
36	O	312	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
36	b	813	CLA	C2D-C1D-ND	-2.50	108.26	110.10
36	W	216	CLA	O2A-CGA-O1A	-2.50	117.08	123.30
36	G	312	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
35	T	302	A86	C3-C4-C5	-2.50	118.36	123.47
35	O	302	A86	C9-C10-C11	-2.50	119.27	126.61
37	P	315	KC1	C1C-C2C-C3C	-2.50	104.33	106.96
34	L	305	DD6	C9-C10-C11	-2.50	123.75	127.31
34	F	303	DD6	C37-C36-C35	2.50	118.98	114.36
34	O	304	DD6	C12-C11-C10	-2.50	119.43	122.92
35	X	301	A86	C25-C24-C1	-2.50	119.41	126.42
35	X	301	A86	C9-C8-C6	-2.50	119.41	126.42
36	J	315	CLA	CHB-C4A-NA	2.49	127.96	124.51
35	h	202	A86	C4-C3-C2	-2.49	118.36	123.47
44	f	801	BCR	C30-C25-C26	-2.49	119.10	122.61
36	E	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
36	S	315	CLA	CBC-CAC-C3C	2.49	119.31	112.43
36	E	313	CLA	CMB-C2B-C3B	2.49	129.34	124.68
36	b	816	CLA	C4-C3-C5	2.49	119.47	115.27
36	a	838	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
36	a	825	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
34	S	306	DD6	C3-C4-C5	-2.49	118.37	123.47
35	T	302	A86	O4-C34-C33	2.49	113.80	107.59
36	A	306	CLA	CMC-C2C-C1C	2.49	128.84	125.04
36	b	839	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
39	L	318	LMT	C1B-O1B-C4'	-2.49	111.80	117.96
36	P	314	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
35	T	307	A86	C9-C8-C6	-2.49	119.42	126.42
35	S	305	A86	O4-C38-O5	-2.49	118.01	122.96
36	M	316	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
35	U	302	A86	C25-C24-C1	-2.49	119.42	126.42
36	C	210	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
34	E	306	DD6	C37-C36-C31	-2.49	120.97	124.35
36	M	310	CLA	C3D-C4D-ND	2.49	114.27	110.24
35	N	305	A86	O4-C38-O5	-2.49	118.02	122.96
44	a	847	BCR	C11-C10-C9	-2.49	123.76	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	835	CLA	C2D-C1D-ND	-2.49	108.27	110.10
36	D	316	CLA	C3C-C4C-NC	-2.49	107.78	110.57
36	M	315	CLA	CHB-C4A-NA	2.49	127.95	124.51
36	S	318	CLA	CHB-C4A-NA	2.49	127.95	124.51
35	V	302	A86	O1-C20-C21	-2.49	112.08	115.06
36	b	830	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
36	b	805	CLA	O2D-CGD-CBD	2.49	115.69	111.27
36	A	308	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
37	C	213	KC1	C3B-C2B-C1B	-2.49	104.70	107.08
36	b	816	CLA	C1D-CHD-C4C	-2.49	120.69	126.06
35	H	301	A86	C9-C10-C11	-2.49	119.30	126.61
44	i	103	BCR	C28-C27-C26	-2.49	109.64	114.08
37	X	311	KC1	C4C-C3C-C2C	-2.49	103.28	106.90
36	E	308	CLA	O2D-CGD-CBD	2.49	115.68	111.27
36	Q	308	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
36	M	308	CLA	CHB-C4A-NA	2.48	127.95	124.51
37	L	317	KC1	C2B-C1B-NB	2.48	111.94	110.10
37	W	217	KC1	C4C-C3C-C2C	-2.48	103.28	106.90
35	N	303	A86	C26-C25-C24	-2.48	115.46	123.22
36	A	305	CLA	CHB-C4A-NA	2.48	127.95	124.51
35	R	309	A86	C9-C8-C6	-2.48	119.44	126.42
36	a	804	CLA	CHB-C4A-NA	2.48	127.95	124.51
44	l	207	BCR	C11-C10-C9	-2.48	123.77	127.31
35	F	301	A86	C19-C18-C17	-2.48	105.98	110.77
35	F	307	A86	C40-C32-C31	2.48	112.69	110.47
35	R	304	A86	C14-C15-C16	2.48	128.26	118.75
36	M	312	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
36	S	314	CLA	C17-C16-C15	-2.48	101.83	113.24
36	U	309	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
34	W	205	DD6	C25-C26-C27	-2.48	119.37	126.58
37	S	316	KC1	C4D-C3D-CAD	2.48	111.82	107.81
35	Q	316	A86	C14-C15-C16	2.48	128.26	118.75
36	b	824	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
36	H	317	CLA	CMB-C2B-C3B	2.48	129.32	124.68
35	N	305	A86	C14-C15-C16	2.48	128.25	118.75
36	S	321	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
44	f	806	BCR	C35-C13-C14	-2.48	119.45	122.92
37	O	313	KC1	C1C-C2C-C3C	-2.48	104.35	106.96
36	a	837	CLA	CHB-C4A-NA	2.48	127.94	124.51
35	T	301	A86	C33-C32-C31	-2.48	106.80	109.21
36	A	305	CLA	C2D-C1D-ND	-2.48	108.28	110.10
36	D	317	CLA	CHD-C1D-ND	-2.48	122.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	R	322	CLA	CHD-C1D-ND	-2.48	122.18	124.45
35	T	307	A86	C21-C20-C19	-2.48	111.49	114.28
37	W	217	KC1	C2A-C1A-NA	2.48	113.38	109.40
34	F	303	DD6	C12-C11-C10	-2.48	119.45	122.92
35	K	303	A86	C9-C8-C6	-2.48	119.46	126.42
34	O	304	DD6	C7-C6-C5	-2.48	119.45	122.92
36	b	806	CLA	CHB-C4A-NA	2.48	127.94	124.51
35	N	303	A86	C7-C6-C8	2.48	121.98	118.08
35	Q	303	A86	C3-C4-C5	-2.47	118.41	123.47
36	b	818	CLA	CHD-C1D-ND	-2.47	122.18	124.45
36	b	836	CLA	O2A-CGA-CBA	2.47	119.67	111.91
35	Q	316	A86	O4-C38-O5	-2.47	118.05	122.96
35	F	305	A86	C36-C31-C32	-2.47	117.24	119.70
35	V	302	A86	C25-C26-C27	-2.47	123.78	127.31
36	H	314	CLA	CHB-C4A-NA	2.47	127.93	124.51
37	G	317	KC1	C3A-C4A-NA	2.47	113.27	110.57
36	T	313	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
35	G	304	A86	C8-C6-C5	-2.47	115.15	118.94
35	S	303	A86	C26-C25-C24	-2.47	115.51	123.22
37	G	308	KC1	C1C-C2C-C3C	-2.47	104.36	106.96
36	a	811	CLA	CMB-C2B-C3B	2.47	129.30	124.68
36	f	804	CLA	CHA-C4D-ND	2.47	137.67	132.50
35	C	203	A86	C34-O4-C38	-2.47	113.29	117.90
35	U	304	A86	C25-C24-C1	-2.47	119.48	126.42
36	C	208	CLA	CHB-C4A-NA	2.47	127.93	124.51
36	W	214	CLA	CAC-C3C-C4C	2.47	128.01	124.81
36	a	813	CLA	O2D-CGD-CBD	2.47	115.66	111.27
35	O	301	A86	C9-C10-C11	-2.47	119.35	126.61
35	J	302	A86	C4-C3-C2	-2.47	118.42	123.47
36	N	313	CLA	CHB-C4A-NA	2.47	127.92	124.51
36	F	317	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
36	a	808	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
36	H	312	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
35	U	302	A86	O1-C20-C19	-2.47	111.53	113.38
36	b	802	CLA	CMB-C2B-C3B	2.47	129.29	124.68
36	S	314	CLA	C4D-CHA-C1A	2.47	124.25	121.25
35	T	302	A86	O4-C34-C35	-2.47	101.45	107.59
37	Q	313	KC1	C1C-C2C-C3C	-2.47	104.36	106.96
36	F	317	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
36	W	211	CLA	CHD-C1D-ND	-2.46	122.19	124.45
36	P	318	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
34	O	304	DD6	C33-C34-C35	-2.46	106.93	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	a	846	BCR	C27-C26-C25	2.46	126.31	122.73
36	T	311	CLA	C2C-C1C-NC	-2.46	107.67	109.97
36	E	314	CLA	C1-O2A-CGA	2.46	122.91	116.44
34	O	304	DD6	C37-C36-C35	2.46	118.92	114.36
36	P	302	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
36	N	317	CLA	C2A-C1A-CHA	2.46	128.16	123.86
35	R	309	A86	C4-C3-C2	-2.46	118.43	123.47
35	C	202	A86	C36-C31-C32	-2.46	117.25	119.70
36	E	317	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
36	U	308	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
36	b	813	CLA	O2D-CGD-CBD	2.46	115.64	111.27
36	P	311	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
34	S	307	DD6	C-C1-C2	-2.46	119.48	122.92
34	L	305	DD6	C10-C9-C8	-2.46	115.54	123.22
36	i	102	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
37	N	314	KC1	CAA-CBA-CGA	-2.46	114.62	127.26
35	B	301	A86	O4-C38-O5	-2.46	118.08	122.96
36	b	840	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
35	N	305	A86	C3-C2-C1	-2.46	123.80	127.31
36	O	308	CLA	C4-C3-C2	-2.46	117.37	123.68
36	R	321	CLA	CHB-C4A-NA	2.46	127.91	124.51
35	h	204	A86	C-C1-C2	-2.46	119.48	122.92
36	Q	314	CLA	CED-O2D-CGD	2.46	121.49	115.94
36	H	315	CLA	O2D-CGD-CBD	2.46	115.63	111.27
35	R	305	A86	C40-C32-C31	-2.46	108.27	110.47
36	D	317	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
36	W	206	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
36	b	840	CLA	CBC-CAC-C3C	2.46	119.20	112.43
36	C	206	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
36	F	312	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
36	b	824	CLA	CMB-C2B-C3B	2.45	129.27	124.68
44	f	806	BCR	C38-C26-C27	-2.45	108.90	113.62
36	X	310	CLA	CHB-C4A-NA	2.45	127.90	124.51
36	U	310	CLA	CHB-C4A-NA	2.45	127.90	124.51
35	H	304	A86	C9-C10-C11	-2.45	119.40	126.61
35	Q	316	A86	C3-C2-C1	-2.45	123.81	127.31
35	C	203	A86	O4-C38-O5	-2.45	118.09	122.96
35	S	308	A86	C12-C11-C13	2.45	120.14	116.02
44	j	107	BCR	C11-C10-C9	-2.45	123.81	127.31
36	G	314	CLA	CMB-C2B-C3B	2.45	129.26	124.68
36	L	308	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
36	a	806	CLA	CHD-C4C-C3C	-2.45	121.24	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	L	304	A86	O4-C38-O5	-2.45	118.09	122.96
36	R	311	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
37	N	314	KC1	C3B-C2B-C1B	-2.45	104.74	107.08
35	U	301	A86	O4-C38-O5	-2.45	118.09	122.96
35	P	303	A86	C9-C8-C6	-2.45	119.53	126.42
36	M	306	CLA	CMD-C2D-C3D	2.45	133.25	127.61
36	b	829	CLA	CHB-C4A-NA	2.45	127.90	124.51
34	B	302	DD6	C3-C4-C5	-2.45	118.46	123.47
36	b	826	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
34	R	308	DD6	C12-C11-C10	-2.45	119.49	122.92
35	S	303	A86	C7-C6-C8	2.45	121.94	118.08
35	L	319	A86	C9-C8-C6	-2.45	119.54	126.42
36	l	205	CLA	C1-C2-C3	-2.45	121.81	126.04
36	a	825	CLA	CHD-C1D-ND	-2.45	122.20	124.45
36	b	826	CLA	CAA-C2A-C1A	-2.45	103.96	111.97
35	F	306	A86	C17-C16-C15	2.45	111.66	109.16
36	a	801	CLA	OBD-CAD-C3D	2.45	134.41	128.52
36	l	201	CLA	CHB-C4A-NA	2.45	127.89	124.51
36	a	803	CLA	C1-O2A-CGA	2.45	122.86	116.44
37	W	213	KC1	C4C-C3C-C2C	-2.45	103.33	106.90
36	W	209	CLA	O2D-CGD-CBD	2.45	115.61	111.27
36	X	308	CLA	C1D-ND-C4D	-2.45	104.60	106.33
36	b	830	CLA	CHB-C4A-NA	2.44	127.89	124.51
36	l	206	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
36	O	308	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
36	Q	307	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
35	G	305	A86	C9-C8-C6	-2.44	119.55	126.42
36	I	310	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
36	O	309	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
35	X	304	A86	C25-C24-C1	-2.44	119.55	126.42
36	a	814	CLA	CMB-C2B-C3B	2.44	129.25	124.68
44	f	806	BCR	C16-C15-C14	-2.44	118.47	123.47
36	S	318	CLA	O2D-CGD-CBD	2.44	115.61	111.27
36	R	311	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
36	X	315	CLA	CHB-C4A-NA	2.44	127.89	124.51
36	a	805	CLA	CHB-C4A-NA	2.44	127.89	124.51
36	a	828	CLA	CHB-C4A-NA	2.44	127.89	124.51
34	E	304	DD6	C15-C14-C13	-2.44	120.83	125.99
36	N	317	CLA	CHB-C4A-NA	2.44	127.89	124.51
35	J	302	A86	C7-C6-C5	-2.44	119.51	122.92
35	U	301	A86	C41-C32-C31	-2.44	108.29	110.47
35	M	305	A86	O4-C38-O5	-2.44	118.12	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	826	CLA	C3A-C2A-C1A	2.44	104.99	101.34
36	f	804	CLA	CMC-C2C-C1C	2.44	128.75	125.04
36	L	313	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
36	P	318	CLA	CHB-C4A-NA	2.44	127.88	124.51
36	X	309	CLA	CHD-C1D-ND	-2.44	122.21	124.45
36	M	316	CLA	CMB-C2B-C3B	2.44	129.24	124.68
38	A	315	SQD	O8-S-C6	2.44	109.62	105.74
35	H	304	A86	C7-C6-C5	-2.44	119.51	122.92
35	X	301	A86	C4-C3-C2	-2.44	118.48	123.47
36	b	806	CLA	O1D-CGD-CBD	2.44	129.47	124.48
36	B	306	CLA	CHD-C1D-ND	-2.44	122.22	124.45
36	D	306	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
35	F	304	A86	O4-C38-O5	-2.43	118.12	122.96
36	b	821	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
36	M	312	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
36	b	805	CLA	C1-C2-C3	-2.43	121.83	126.04
36	J	317	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
36	b	828	CLA	CGD-CBD-CAD	2.43	118.61	110.73
35	O	302	A86	C9-C8-C6	-2.43	119.58	126.42
35	U	304	A86	C34-O4-C38	-2.43	113.36	117.90
36	I	306	CLA	C4D-CHA-C1A	2.43	124.21	121.25
41	G	320	LHG	C5-O7-C7	-2.43	111.80	117.79
36	a	827	CLA	O1D-CGD-CBD	2.43	129.46	124.48
34	H	302	DD6	C9-C10-C11	-2.43	123.84	127.31
36	a	809	CLA	CHD-C1D-ND	-2.43	122.22	124.45
35	R	303	A86	C25-C24-C1	-2.43	119.59	126.42
36	P	310	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
36	W	218	CLA	C2D-C1D-ND	-2.43	108.31	110.10
36	R	320	CLA	CHD-C1D-ND	-2.43	122.22	124.45
36	H	315	CLA	CAC-C3C-C2C	2.43	131.68	127.53
35	P	306	A86	O4-C38-O5	-2.43	118.14	122.96
35	N	301	A86	C4-C3-C2	-2.43	118.50	123.47
36	b	835	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
35	C	204	A86	O1-C15-C14	2.43	118.08	113.21
36	C	212	CLA	CAC-C3C-C2C	-2.43	123.38	127.53
36	b	802	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
36	a	824	CLA	CMC-C2C-C1C	-2.43	121.34	125.04
35	I	301	A86	C40-C32-C31	-2.43	108.30	110.47
35	I	304	A86	O1-C20-C19	-2.43	111.56	113.38
36	a	813	CLA	CHD-C1D-ND	-2.43	122.22	124.45
36	a	802	CLA	CHB-C4A-NA	2.43	127.87	124.51
35	G	304	A86	C34-O4-C38	2.43	122.42	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	S	313	CLA	CHD-C1D-ND	-2.43	122.22	124.45
36	J	307	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
36	U	307	CLA	CMB-C2B-C3B	2.43	129.22	124.68
35	R	309	A86	O4-C38-O5	-2.43	118.14	122.96
35	P	304	A86	C9-C10-C11	-2.43	119.48	126.61
36	U	309	CLA	C3A-C2A-C1A	2.42	104.97	101.34
35	G	302	A86	C26-C25-C24	-2.42	115.65	123.22
34	H	303	DD6	C37-C36-C35	2.42	118.85	114.36
36	b	838	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
34	A	301	DD6	O1-C20-C21	-2.42	112.15	115.06
36	b	812	CLA	CHB-C4A-NA	2.42	127.86	124.51
35	D	302	A86	C12-C11-C13	2.42	120.09	116.02
36	J	316	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
37	R	317	KC1	CBB-CAB-C3B	-2.42	115.56	127.62
39	L	303	LMT	C3'-C4'-C5'	-2.42	105.37	110.93
36	b	813	CLA	CMB-C2B-C3B	2.42	129.43	124.69
36	b	825	CLA	C2D-C1D-ND	-2.42	108.32	110.10
35	X	304	A86	C20-C19-C18	2.42	117.54	112.75
39	U	314	LMT	C1B-O1B-C4'	-2.42	111.97	117.96
36	X	313	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
36	V	311	CLA	CBA-CAA-C2A	2.42	121.01	113.86
37	H	313	KC1	CAA-CBA-CGA	-2.42	114.81	127.26
36	a	824	CLA	CHD-C4C-C3C	-2.42	121.28	124.84
35	J	306	A86	O4-C38-O5	-2.42	118.15	122.96
36	M	306	CLA	CMD-C2D-C1D	-2.42	120.45	124.71
36	A	307	CLA	CHB-C4A-NA	2.42	127.86	124.51
36	T	313	CLA	CHB-C4A-NA	2.42	127.86	124.51
36	L	309	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
36	X	308	CLA	CAA-CBA-CGA	2.42	120.33	113.25
36	N	309	CLA	CMC-C2C-C3C	2.42	132.69	126.12
36	V	311	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
37	P	317	KC1	O2D-CGD-O1D	-2.42	119.11	123.84
36	H	310	CLA	CAC-C3C-C4C	2.42	127.95	124.81
36	A	314	CLA	O1D-CGD-CBD	2.42	129.44	124.48
36	D	307	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
35	N	320	A86	C9-C10-C11	-2.42	119.50	126.61
35	L	306	A86	C35-C34-C33	-2.42	105.66	109.88
35	M	301	A86	C9-C8-C6	-2.42	119.62	126.42
37	R	317	KC1	O2D-CGD-O1D	-2.42	119.11	123.84
35	O	303	A86	C9-C10-C11	-2.42	119.50	126.61
35	P	307	A86	C12-C11-C13	2.42	120.08	116.02
36	O	307	CLA	C1B-CHB-C4A	-2.42	125.33	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S	301	A86	C4-C3-C2	-2.42	118.52	123.47
41	G	301	LHG	C11-C10-C9	-2.42	102.15	114.42
36	T	316	CLA	CHB-C4A-NA	2.42	127.86	124.51
36	W	214	CLA	CHB-C4A-NA	2.42	127.86	124.51
34	D	303	DD6	C3-C2-C1	-2.42	123.86	127.31
36	E	315	CLA	CMC-C2C-C1C	2.42	128.72	125.04
37	D	314	KC1	CHD-C4C-NC	2.42	127.87	124.20
35	Q	301	A86	C9-C8-C6	-2.42	119.63	126.42
42	G	325	LMG	C8-O7-C10	-2.42	111.84	117.79
35	P	304	A86	C9-C8-C6	-2.42	119.63	126.42
36	N	313	CLA	CHA-C1A-NA	-2.42	120.87	126.40
36	B	309	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
35	V	301	A86	C33-C32-C31	-2.41	106.86	109.21
36	b	830	CLA	C3C-C4C-NC	-2.41	107.86	110.57
36	C	212	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
35	V	303	A86	C14-C15-C16	-2.41	109.51	118.75
36	P	319	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
36	a	848	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
36	F	313	CLA	CHD-C1D-ND	-2.41	122.24	124.45
36	a	820	CLA	CHB-C4A-NA	2.41	127.85	124.51
36	W	216	CLA	C2C-C1C-NC	2.41	112.23	109.97
35	U	303	A86	O4-C38-O5	-2.41	118.17	122.96
35	E	302	A86	C34-O4-C38	-2.41	113.40	117.90
35	G	306	A86	C34-O4-C38	-2.41	113.40	117.90
44	b	847	BCR	C30-C25-C26	-2.41	119.22	122.61
36	A	308	CLA	O1D-CGD-CBD	2.41	129.42	124.48
34	H	303	DD6	C15-C14-C13	-2.41	120.89	125.99
36	G	316	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
36	I	307	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
36	N	311	CLA	C3A-C2A-C1A	2.41	104.95	101.34
36	H	312	CLA	CBA-CAA-C2A	2.41	120.98	113.86
34	D	305	DD6	C25-C24-C1	-2.41	119.65	126.42
36	a	848	CLA	C4-C3-C5	2.41	119.32	115.27
36	b	806	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
35	U	301	A86	C12-C11-C13	2.41	120.07	116.02
35	O	303	A86	C9-C8-C6	-2.41	119.65	126.42
41	O	318	LHG	C20-C19-C18	-2.41	102.20	114.42
44	b	844	BCR	C2-C1-C6	2.41	114.19	110.48
44	b	844	BCR	C24-C23-C22	-2.41	122.60	126.23
34	R	307	DD6	C25-C26-C27	-2.41	119.59	126.58
36	B	307	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
36	K	313	CLA	C4D-C3D-CAD	-2.41	105.26	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	319	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
35	T	306	A86	C3-C4-C5	-2.41	118.54	123.47
36	a	829	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
36	U	311	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
41	Q	315	LHG	C5-O7-C7	-2.41	111.87	117.79
35	I	304	A86	C40-C32-C31	2.41	112.62	110.47
34	S	306	DD6	C33-C34-C35	-2.41	107.01	110.30
35	M	302	A86	O4-C38-O5	-2.41	118.18	122.96
36	M	315	CLA	CMB-C2B-C3B	2.40	129.18	124.68
36	S	310	CLA	CAA-C2A-C3A	-2.40	106.19	112.78
36	W	215	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
35	J	301	A86	O4-C38-O5	-2.40	118.19	122.96
36	W	208	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
36	N	308	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
36	R	321	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
36	N	319	CLA	C2A-C1A-CHA	2.40	128.06	123.86
36	N	319	CLA	CHC-C1C-NC	2.40	127.85	124.20
36	A	311	CLA	CHB-C4A-NA	2.40	127.83	124.51
36	l	206	CLA	C1-C2-C3	-2.40	122.86	126.75
36	P	309	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
36	P	301	CLA	O2D-CGD-CBD	2.40	115.54	111.27
36	K	310	CLA	CHC-C1C-C2C	-2.40	120.08	126.72
35	O	305	A86	O4-C38-O5	-2.40	118.19	122.96
36	b	817	CLA	C3D-C4D-ND	2.40	114.12	110.24
35	I	301	A86	C41-C32-C31	-2.40	108.32	110.47
35	F	306	A86	O1-C15-C14	-2.40	108.39	113.21
35	Q	304	A86	C28-C27-C26	-2.40	119.56	122.92
37	K	314	KC1	C2A-C1A-NA	2.40	113.25	109.40
36	M	307	CLA	CHB-C4A-NA	2.40	127.83	124.51
36	S	320	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
36	L	308	CLA	CHD-C1D-ND	-2.40	122.25	124.45
36	b	802	CLA	C1-C2-C3	-2.40	121.89	126.04
36	b	818	CLA	C4D-CHA-C1A	2.40	124.17	121.25
35	Q	304	A86	C9-C10-C11	-2.40	119.56	126.61
36	a	803	CLA	O2A-CGA-CBA	2.40	119.43	111.91
36	M	310	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
35	S	301	A86	C9-C10-C11	-2.40	119.56	126.61
35	Q	301	A86	C9-C10-C11	-2.40	119.56	126.61
34	B	304	DD6	C37-C36-C31	-2.40	121.09	124.35
36	L	310	CLA	CHB-C4A-NA	2.40	127.83	124.51
34	L	305	DD6	C-C1-C2	-2.40	119.57	122.92
36	L	313	CLA	O2D-CGD-O1D	-2.40	119.15	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	W	213	KC1	O2D-CGD-O1D	-2.40	119.15	123.84
36	S	315	CLA	CMC-C2C-C1C	-2.40	121.39	125.04
36	b	808	CLA	O2A-C1-C2	-2.40	102.34	108.64
36	N	316	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
36	a	824	CLA	CHA-C1A-NA	-2.40	120.91	126.40
36	D	309	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
35	G	306	A86	O4-C38-O5	-2.39	118.20	122.96
36	b	840	CLA	CAA-CBA-CGA	-2.39	106.26	113.25
36	b	827	CLA	CHD-C1D-ND	-2.39	122.25	124.45
37	M	318	KC1	O2D-CGD-O1D	-2.39	119.16	123.84
35	L	307	A86	O4-C38-O5	-2.39	118.21	122.96
35	T	302	A86	C9-C10-C11	-2.39	119.57	126.61
36	a	838	CLA	CHB-C4A-NA	2.39	127.82	124.51
36	E	310	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
36	B	309	CLA	C3A-C2A-C1A	2.39	104.92	101.34
36	C	212	CLA	C3A-C2A-C1A	2.39	104.92	101.34
39	I	318	LMT	C1B-O1B-C4'	-2.39	112.04	117.96
35	N	320	A86	C28-C27-C26	-2.39	119.57	122.92
36	G	319	CLA	CHC-C1C-C2C	-2.39	120.11	126.72
34	D	304	DD6	C37-C36-C35	2.39	118.78	114.36
36	b	823	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
36	W	210	CLA	CHA-C1A-NA	-2.39	120.93	126.40
36	a	808	CLA	C2A-C1A-CHA	2.39	128.04	123.86
35	N	301	A86	C9-C10-C11	-2.39	119.58	126.61
35	A	316	A86	C12-C11-C13	2.39	120.03	116.02
36	N	312	CLA	CHB-C4A-NA	2.39	127.81	124.51
35	F	302	A86	O4-C38-O5	-2.39	118.22	122.96
36	A	314	CLA	C1D-ND-C4D	-2.39	104.64	106.33
36	f	804	CLA	CMB-C2B-C3B	2.39	129.14	124.68
39	F	320	LMT	C1B-O1B-C4'	-2.39	112.06	117.96
36	X	307	CLA	C1-C2-C3	-2.39	122.89	126.75
36	N	310	CLA	CHA-C1A-NA	-2.39	120.93	126.40
37	M	317	KC1	CAA-C2A-C1A	2.39	135.72	124.75
36	Q	306	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
44	f	806	BCR	C27-C26-C25	2.39	126.20	122.73
36	a	835	CLA	CMB-C2B-C3B	2.39	129.14	124.68
37	L	317	KC1	C3D-CAD-CBD	-2.39	104.46	107.61
36	G	315	CLA	C2D-C1D-ND	-2.39	108.35	110.10
35	T	305	A86	C34-O4-C38	2.39	122.34	117.90
35	R	306	A86	C28-C27-C26	-2.39	119.58	122.92
35	M	301	A86	C9-C10-C11	-2.38	119.60	126.61
36	b	816	CLA	C2A-C1A-CHA	-2.38	119.69	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	L	312	CLA	CBA-CAA-C2A	-2.38	106.82	113.86
36	U	310	CLA	C1D-ND-C4D	2.38	108.03	106.33
36	J	307	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
35	I	301	A86	C28-C27-C26	-2.38	119.58	122.92
36	J	308	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
34	J	304	DD6	C14-C13-C11	-2.38	121.83	125.53
35	Q	303	A86	O4-C38-O5	-2.38	118.23	122.96
36	K	310	CLA	CHD-C1D-C2D	2.38	130.48	125.48
35	I	302	A86	C9-C8-C6	-2.38	119.72	126.42
36	E	313	CLA	CHC-C1C-C2C	-2.38	120.13	126.72
34	a	849	DD6	O1-C20-C21	-2.38	112.20	115.06
35	S	302	A86	O4-C38-O5	-2.38	118.23	122.96
34	M	303	DD6	C37-C36-C35	2.38	118.77	114.36
36	H	316	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
43	b	842	PQN	C2M-C2-C1	2.38	120.21	116.27
36	I	305	CLA	CHB-C4A-NA	2.38	127.80	124.51
41	f	809	LHG	C5-O7-C7	-2.38	111.93	117.79
35	V	301	A86	O4-C38-O5	-2.38	118.24	122.96
35	R	301	A86	C28-C27-C26	-2.38	119.59	122.92
36	A	307	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
36	b	827	CLA	CHB-C4A-NA	2.38	127.80	124.51
36	V	313	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
35	V	301	A86	C7-C6-C5	-2.38	119.59	122.92
36	b	837	CLA	CBA-CAA-C2A	2.38	120.88	113.86
36	D	311	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
36	a	832	CLA	C3C-C4C-NC	-2.38	107.91	110.57
36	A	310	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
36	N	311	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
35	O	301	A86	C12-C11-C13	2.38	120.02	116.02
36	D	307	CLA	C3A-C2A-C1A	2.38	104.90	101.34
36	b	806	CLA	C2A-C1A-CHA	2.38	128.01	123.86
36	F	314	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
35	R	306	A86	C9-C8-C6	-2.38	119.74	126.42
41	O	318	LHG	O8-C23-C24	2.38	119.36	111.91
35	R	305	A86	C3-C4-C5	-2.37	118.61	123.47
35	L	301	A86	C12-C11-C13	2.37	120.01	116.02
35	R	302	A86	C25-C24-C1	-2.37	119.75	126.42
36	a	806	CLA	CAC-C3C-C4C	2.37	127.89	124.81
36	b	829	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
36	D	309	CLA	CHB-C4A-NA	2.37	127.79	124.51
36	B	305	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
36	N	310	CLA	CHC-C1C-NC	2.37	127.80	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	S	314	CLA	CHA-C1A-NA	-2.37	120.96	126.40
35	A	302	A86	C4-C5-C6	-2.37	123.92	127.31
37	M	317	KC1	O2D-CGD-O1D	-2.37	119.20	123.84
39	h	205	LMT	C1B-O1B-C4'	-2.37	112.10	117.96
34	Q	302	DD6	C25-C24-C1	-2.37	119.76	126.42
36	D	316	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
36	P	308	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
36	I	308	CLA	O2A-CGA-CBA	2.37	119.34	111.91
36	O	306	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
36	a	817	CLA	CHB-C4A-NA	2.37	127.79	124.51
35	M	302	A86	C25-C24-C1	-2.37	119.76	126.42
35	R	305	A86	O1-C20-C19	-2.37	111.60	113.38
36	N	313	CLA	CMA-C3A-C2A	-2.37	110.57	116.10
36	Q	305	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
34	D	305	DD6	C9-C10-C11	-2.37	123.93	127.31
36	N	307	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
35	T	307	A86	C28-C27-C26	-2.37	119.61	122.92
36	H	307	CLA	CHC-C1C-NC	2.37	127.79	124.20
35	A	302	A86	C12-C11-C13	-2.37	112.05	116.02
36	a	803	CLA	C2D-C1D-ND	-2.37	108.36	110.10
36	F	309	CLA	C4-C3-C2	-2.37	117.61	123.68
36	L	316	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
36	F	317	CLA	CHB-C4A-NA	2.37	127.78	124.51
36	b	818	CLA	CHB-C4A-NA	2.37	127.78	124.51
36	a	830	CLA	CMB-C2B-C3B	2.37	129.10	124.68
34	A	304	DD6	C37-C36-C35	2.37	118.74	114.36
34	D	301	DD6	C4-C5-C6	-2.37	123.93	127.31
44	i	101	BCR	C30-C25-C26	-2.37	119.28	122.61
36	b	810	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
36	V	314	CLA	CMD-C2D-C3D	-2.36	122.17	127.61
35	J	303	A86	C3-C4-C5	-2.36	118.63	123.47
35	H	301	A86	C3-C2-C1	-2.36	123.94	127.31
37	C	213	KC1	C1C-C2C-C3C	-2.36	104.47	106.96
36	D	308	CLA	CAA-CBA-CGA	-2.36	106.35	113.25
39	a	853	LMT	C1B-O1B-C4'	-2.36	112.11	117.96
36	X	313	CLA	CHA-C4D-ND	2.36	137.44	132.50
35	O	301	A86	C17-C16-C15	2.36	111.57	109.16
36	R	319	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
35	F	307	A86	C9-C10-C11	-2.36	119.66	126.61
35	K	301	A86	O4-C38-O5	-2.36	118.27	122.96
34	R	307	DD6	C-C1-C2	-2.36	119.61	122.92
36	I	308	CLA	O2D-CGD-O1D	-2.36	119.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	J	310	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
36	b	814	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
37	U	312	KC1	CAB-C3B-C2B	-2.36	120.82	128.60
36	a	809	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
34	E	304	DD6	C32-C33-C34	-2.36	108.31	113.64
35	X	304	A86	C36-C31-C32	-2.36	117.35	119.70
35	N	302	A86	O4-C38-O5	-2.36	118.27	122.96
34	D	303	DD6	C7-C6-C8	2.36	121.80	118.08
36	I	305	CLA	C15-C13-C12	2.36	133.40	113.58
34	D	301	DD6	C15-C14-C13	-2.36	121.00	125.99
44	b	845	BCR	C24-C23-C22	-2.36	122.67	126.23
35	E	305	A86	C41-C32-C31	-2.36	108.36	110.47
36	N	308	CLA	CHC-C1C-C2C	2.36	133.25	126.72
35	N	305	A86	C20-C19-C18	2.36	117.41	112.75
35	L	301	A86	O4-C38-O5	-2.36	118.28	122.96
36	K	307	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
36	U	309	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
34	K	304	DD6	C21-C20-C15	-2.36	118.31	122.26
36	H	312	CLA	C4-C3-C5	2.36	119.24	115.27
36	C	209	CLA	CMD-C2D-C1D	-2.36	120.56	124.71
36	W	209	CLA	C2A-C1A-CHA	2.36	127.98	123.86
36	F	316	CLA	CHB-C4A-NA	2.36	127.77	124.51
37	R	317	KC1	C1C-C2C-C3C	-2.36	104.48	106.96
35	Q	303	A86	C10-C9-C8	-2.36	115.86	123.22
36	R	313	CLA	CHB-C4A-NA	2.36	127.77	124.51
35	R	305	A86	O4-C38-O5	-2.36	118.28	122.96
36	f	803	CLA	CMB-C2B-C3B	2.36	129.09	124.68
44	m	101	BCR	C7-C8-C9	-2.36	122.68	126.23
36	U	305	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
36	a	808	CLA	O1D-CGD-CBD	2.36	129.30	124.48
36	H	312	CLA	CHD-C1D-ND	-2.35	122.29	124.45
35	h	204	A86	C9-C10-C11	-2.35	119.69	126.61
36	E	313	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
36	L	309	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
36	Q	310	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
36	M	311	CLA	O1D-CGD-CBD	2.35	129.30	124.48
36	a	811	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
36	a	806	CLA	C3C-C4C-NC	2.35	113.21	110.57
44	a	845	BCR	C27-C26-C25	2.35	126.15	122.73
36	S	309	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
36	A	307	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
36	S	318	CLA	C1B-CHB-C4A	-2.35	125.46	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	831	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
35	F	305	A86	C10-C9-C8	-2.35	115.88	123.22
34	P	305	DD6	C15-C14-C13	-2.35	121.02	125.99
36	C	214	CLA	CHB-C4A-NA	2.35	127.76	124.51
36	H	310	CLA	C1D-ND-C4D	2.35	108.00	106.33
36	S	309	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
44	i	101	BCR	C2-C1-C6	2.35	114.10	110.48
37	V	312	KC1	O2D-CGD-O1D	-2.35	119.24	123.84
35	P	307	A86	C41-C32-C31	-2.35	108.37	110.47
35	Q	304	A86	O4-C38-O5	-2.35	118.30	122.96
36	b	836	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
36	V	307	CLA	CHB-C4A-NA	2.35	127.76	124.51
36	a	804	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
35	G	306	A86	C3-C4-C5	-2.35	118.66	123.47
44	b	843	BCR	C27-C26-C25	2.35	126.14	122.73
36	G	307	CLA	O2D-CGD-O1D	-2.35	118.76	124.09
41	O	318	LHG	C13-C12-C11	-2.35	102.51	114.42
36	G	307	CLA	CHD-C4C-C3C	-2.35	121.39	124.84
36	l	202	CLA	CHB-C4A-NA	2.35	127.76	124.51
37	G	318	KC1	CAA-C2A-C1A	2.35	135.53	124.75
36	V	314	CLA	C3D-C4D-ND	2.35	114.03	110.24
37	P	317	KC1	CBB-CAB-C3B	-2.35	115.95	127.62
36	E	314	CLA	C3C-C4C-NC	-2.35	107.94	110.57
36	b	828	CLA	C1-C2-C3	-2.35	121.99	126.04
36	f	804	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
35	Q	316	A86	C20-C19-C18	2.35	117.39	112.75
36	a	841	CLA	C2A-C1A-CHA	2.34	127.96	123.86
36	b	835	CLA	CGD-CBD-CAD	-2.34	103.14	110.73
35	S	308	A86	C9-C8-C6	-2.34	119.83	126.42
36	G	319	CLA	C5-C3-C4	2.34	119.78	114.60
36	C	212	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
35	W	202	A86	O1-C20-C19	-2.34	111.62	113.38
37	W	213	KC1	C2A-C3A-C4A	2.34	108.22	106.49
35	X	314	A86	O4-C38-O5	-2.34	118.31	122.96
34	A	304	DD6	C25-C26-C27	-2.34	119.78	126.58
36	P	302	CLA	CHB-C4A-NA	2.34	127.75	124.51
36	R	316	CLA	CHA-C1A-NA	-2.34	121.04	126.40
35	N	305	A86	C41-C32-C31	-2.34	108.38	110.47
36	b	828	CLA	CHA-C4D-ND	2.34	137.40	132.50
36	a	832	CLA	CBA-CAA-C2A	2.34	120.77	113.86
36	A	305	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
36	a	817	CLA	C1B-CHB-C4A	-2.34	125.48	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	S	311	CLA	O1D-CGD-CBD	2.34	129.27	124.48
36	a	838	CLA	CMD-C2D-C1D	-2.34	120.59	124.71
36	a	816	CLA	C3A-C2A-C1A	2.34	104.84	101.34
36	P	314	CLA	CMA-C3A-C4A	-2.34	105.49	111.77
36	Q	314	CLA	CHD-C1D-ND	-2.34	122.31	124.45
34	B	304	DD6	C7-C6-C5	-2.34	119.65	122.92
36	F	309	CLA	CHB-C4A-NA	2.34	127.74	124.51
36	L	309	CLA	CHB-C4A-NA	2.34	127.74	124.51
34	B	302	DD6	C12-C11-C10	-2.34	119.65	122.92
36	a	830	CLA	C3A-C2A-C1A	2.34	104.84	101.34
35	Q	316	A86	C41-C32-C31	-2.34	108.38	110.47
36	H	315	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
36	a	824	CLA	CHB-C4A-NA	2.33	127.74	124.51
36	U	306	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
35	W	202	A86	C36-C31-C32	2.33	122.01	119.70
35	Q	303	A86	C26-C25-C24	-2.33	115.93	123.22
35	T	304	A86	C4-C5-C6	-2.33	123.98	127.31
36	T	308	CLA	CAC-C3C-C2C	-2.33	123.54	127.53
36	N	316	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
35	X	305	A86	C20-C19-C18	2.33	117.36	112.75
35	h	202	A86	C26-C25-C24	-2.33	115.94	123.22
35	N	304	A86	C9-C10-C11	-2.33	119.75	126.61
36	N	313	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
35	L	306	A86	C25-C24-C1	2.33	132.97	126.42
35	N	320	A86	O4-C38-O5	-2.33	118.33	122.96
35	G	305	A86	C34-O4-C38	-2.33	113.55	117.90
35	T	306	A86	C9-C10-C11	-2.33	119.76	126.61
44	f	801	BCR	C38-C26-C27	-2.33	109.14	113.62
36	a	805	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
37	H	313	KC1	O2D-CGD-O1D	-2.33	119.28	123.84
36	a	833	CLA	CMB-C2B-C1B	-2.33	124.88	128.46
35	I	301	A86	O4-C38-O5	-2.33	118.33	122.96
37	K	314	KC1	C1C-C2C-C3C	-2.33	104.51	106.96
36	D	307	CLA	C2D-C1D-ND	-2.33	108.39	110.10
35	M	304	A86	C25-C24-C1	-2.33	119.88	126.42
36	S	312	CLA	CED-O2D-CGD	2.33	121.20	115.94
37	R	317	KC1	C4D-C3D-CAD	2.33	111.57	107.81
36	X	312	CLA	C2A-C1A-CHA	2.33	127.92	123.85
35	T	303	A86	C36-C31-C32	-2.33	117.39	119.70
36	b	833	CLA	CMB-C2B-C3B	2.33	129.03	124.68
36	N	319	CLA	C4C-C3C-C2C	2.33	110.29	106.90
34	K	305	DD6	C-C1-C2	-2.33	119.66	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	U	308	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
35	X	305	A86	C12-C11-C13	2.32	119.93	116.02
36	K	309	CLA	CHB-C4A-NA	2.32	127.73	124.51
35	R	304	A86	C36-C31-C32	-2.32	117.39	119.70
36	b	817	CLA	C2A-C3A-C4A	2.32	105.62	101.87
35	O	305	A86	C33-C32-C31	2.32	111.47	109.21
36	A	311	CLA	C1-C2-C3	-2.32	122.02	126.04
44	i	103	BCR	C30-C25-C26	-2.32	119.34	122.61
36	A	306	CLA	C1D-ND-C4D	-2.32	104.68	106.33
36	F	309	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
36	a	827	CLA	C6-C5-C3	-2.32	107.36	113.45
36	a	823	CLA	CMB-C2B-C3B	2.32	129.03	124.68
34	W	204	DD6	C25-C26-C27	-2.32	119.83	126.58
35	J	303	A86	C-C1-C24	2.32	121.74	118.08
36	R	311	CLA	CHB-C4A-NA	2.32	127.72	124.51
36	W	218	CLA	CHB-C4A-NA	2.32	127.72	124.51
36	I	311	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
36	U	307	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
36	A	310	CLA	CHB-C4A-NA	2.32	127.72	124.51
35	T	301	A86	C12-C11-C13	2.32	119.92	116.02
34	R	307	DD6	C25-C24-C1	-2.32	119.89	126.42
36	D	312	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
36	E	310	CLA	CHB-C4A-NA	2.32	127.72	124.51
36	E	311	CLA	CHB-C4A-NA	2.32	127.72	124.51
44	i	101	BCR	C1-C6-C5	-2.32	119.34	122.61
36	a	803	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
35	G	304	A86	C10-C9-C8	-2.32	115.98	123.22
35	R	305	A86	C12-C11-C13	2.32	119.92	116.02
37	M	313	KC1	C3A-C4A-NA	2.32	113.10	110.57
36	a	817	CLA	C2D-C1D-ND	-2.32	108.39	110.10
35	E	307	A86	C12-C11-C13	2.32	119.92	116.02
36	A	314	CLA	CHD-C1D-ND	-2.32	122.32	124.45
35	J	303	A86	C21-C20-C19	2.32	116.89	114.28
36	H	309	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
37	U	312	KC1	O2D-CGD-O1D	-2.32	119.31	123.84
35	H	304	A86	C34-O4-C38	-2.32	113.58	117.90
44	i	101	BCR	C28-C27-C26	-2.32	109.94	114.08
35	M	304	A86	O4-C38-O5	-2.31	118.36	122.96
34	J	304	DD6	C37-C36-C35	2.31	118.64	114.36
35	I	304	A86	O-C13-C11	-2.31	116.03	121.15
36	P	319	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
37	L	315	KC1	C3D-CAD-CBD	-2.31	104.56	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	303	DD6	C37-C36-C35	2.31	118.64	114.36
36	M	309	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
36	R	320	CLA	CAC-C3C-C4C	2.31	127.81	124.81
44	I	207	BCR	C15-C14-C13	-2.31	124.01	127.31
35	T	302	A86	C23-C16-C17	-2.31	104.97	108.98
36	Q	314	CLA	CHB-C4A-NA	2.31	127.71	124.51
36	b	815	CLA	CHB-C4A-NA	2.31	127.71	124.51
35	J	305	A86	O4-C38-O5	-2.31	118.37	122.96
36	b	825	CLA	CHA-C1A-NA	-2.31	121.11	126.40
36	b	835	CLA	O2A-CGA-O1A	-2.31	117.54	123.30
36	V	309	CLA	O2D-CGD-CBD	2.31	115.37	111.27
36	W	214	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
35	A	316	A86	C41-C32-C31	-2.31	108.41	110.47
36	J	307	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
36	a	803	CLA	CAA-CBA-CGA	-2.31	106.50	113.25
34	K	305	DD6	C3-C4-C5	-2.31	118.74	123.47
36	E	315	CLA	CHD-C1D-C2D	2.31	130.32	125.48
36	a	822	CLA	CMB-C2B-C3B	2.31	129.00	124.68
37	V	312	KC1	C2B-C1B-NB	2.31	111.81	110.10
36	F	311	CLA	C3A-C2A-C1A	2.31	104.80	101.34
36	J	317	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
36	R	319	CLA	CAC-C3C-C4C	-2.31	121.82	124.81
35	X	303	A86	O-C13-C11	-2.31	116.05	121.15
35	J	305	A86	C41-C32-C31	-2.31	108.41	110.47
36	W	218	CLA	CMC-C2C-C1C	-2.31	121.53	125.04
36	a	805	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
35	C	204	A86	C28-C27-C26	-2.31	119.69	122.92
36	b	839	CLA	CHD-C1D-ND	-2.31	122.33	124.45
44	b	846	BCR	C1-C6-C5	-2.31	119.37	122.61
36	a	801	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
34	R	307	DD6	C3-C4-C5	-2.31	118.75	123.47
35	S	305	A86	C9-C10-C11	-2.31	119.83	126.61
36	F	310	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
36	G	310	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
36	I	306	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
36	b	831	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
35	V	302	A86	C36-C31-C32	-2.30	117.41	119.70
37	G	308	KC1	CAC-C3C-C4C	2.30	127.80	124.81
35	O	301	A86	O4-C38-O5	-2.30	118.38	122.96
34	D	303	DD6	C9-C10-C11	-2.30	124.02	127.31
35	G	302	A86	O4-C38-O5	-2.30	118.39	122.96
36	P	314	CLA	C1-C2-C3	2.30	130.03	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	307	CLA	C4-C3-C5	2.30	119.15	115.27
34	Q	302	DD6	C25-C26-C27	-2.30	119.89	126.58
36	S	309	CLA	CHB-C4A-NA	2.30	127.70	124.51
36	E	313	CLA	C4D-CHA-C1A	-2.30	118.45	121.25
36	M	307	CLA	C1-O2A-CGA	2.30	122.48	116.44
44	b	847	BCR	C38-C26-C27	-2.30	109.19	113.62
35	h	202	A86	C12-C11-C13	2.30	119.89	116.02
35	W	203	A86	C36-C31-C32	-2.30	117.41	119.70
37	Q	311	KC1	CGD-CBD-CAD	-2.30	103.28	110.73
37	K	314	KC1	C2B-C1B-NB	2.30	111.80	110.10
44	h	201	BCR	C33-C5-C6	-2.30	121.94	124.53
36	a	822	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
36	f	803	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
36	a	832	CLA	C3A-C2A-C1A	2.30	104.78	101.34
37	O	315	KC1	CGD-CBD-CAD	-2.30	103.29	110.73
36	J	311	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
36	T	313	CLA	C2D-C1D-ND	-2.30	108.41	110.10
36	G	319	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
35	S	304	A86	O4-C38-O5	-2.30	118.40	122.96
35	R	309	A86	C9-C10-C11	-2.30	119.86	126.61
36	G	319	CLA	CMC-C2C-C1C	2.30	128.53	125.04
35	Q	301	A86	C33-C32-C31	2.30	111.44	109.21
35	R	302	A86	O4-C34-C35	-2.30	101.88	107.59
37	L	317	KC1	C1C-C2C-C3C	-2.30	104.54	106.96
36	F	317	CLA	C3C-C4C-NC	2.30	113.14	110.57
35	K	301	A86	C7-C6-C5	-2.30	119.71	122.92
36	X	308	CLA	C2A-C3A-C4A	-2.29	98.16	101.87
36	a	825	CLA	CHB-C4A-NA	2.29	127.68	124.51
35	R	301	A86	C20-C19-C18	2.29	117.29	112.75
41	O	317	LHG	C5-O7-C7	-2.29	112.14	117.79
35	M	305	A86	C40-C32-C31	-2.29	108.42	110.47
36	R	316	CLA	CMC-C2C-C3C	2.29	132.34	126.12
36	A	307	CLA	CHD-C1D-ND	-2.29	122.35	124.45
36	a	817	CLA	C2A-C1A-CHA	2.29	127.87	123.86
36	P	301	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
34	S	306	DD6	C37-C36-C35	2.29	118.60	114.36
35	C	204	A86	O4-C38-O5	-2.29	118.41	122.96
36	R	314	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
35	X	314	A86	C9-C8-C6	-2.29	119.98	126.42
37	P	317	KC1	C1C-C2C-C3C	-2.29	104.55	106.96
36	a	818	CLA	CHC-C1C-NC	2.29	127.68	124.20
37	Q	313	KC1	CGD-CBD-CAD	-2.29	103.31	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	303	DD6	O1-C20-C21	-2.29	112.31	115.06
35	F	302	A86	C40-C32-C31	-2.29	108.42	110.47
37	W	217	KC1	C3A-C4A-NA	2.29	113.07	110.57
36	S	314	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
39	B	313	LMT	C1B-O1B-C4'	-2.29	112.30	117.96
41	G	301	LHG	C27-C26-C25	-2.29	102.80	114.42
35	O	303	A86	O4-C38-O5	-2.29	118.41	122.96
35	T	302	A86	C34-O4-C38	2.29	122.16	117.90
41	F	319	LHG	C5-O7-C7	-2.29	112.16	117.79
37	V	312	KC1	CAA-CBA-CGA	-2.29	115.50	127.26
36	b	828	CLA	C4D-C3D-CAD	-2.29	105.40	108.10
36	O	316	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
35	K	303	A86	C-C1-C24	2.29	121.68	118.08
41	a	842	LHG	C11-C10-C9	-2.29	102.81	114.42
36	H	311	CLA	C2D-C1D-ND	-2.29	108.42	110.10
36	G	314	CLA	O1D-CGD-CBD	2.29	129.16	124.48
36	b	819	CLA	CHD-C1D-C2D	2.29	130.28	125.48
36	b	806	CLA	CAC-C3C-C4C	2.29	127.78	124.81
37	O	313	KC1	CGD-CBD-CAD	-2.29	103.33	110.73
37	X	311	KC1	C3A-C4A-NA	2.29	113.07	110.57
37	P	315	KC1	CGD-CBD-CAD	-2.29	103.33	110.73
36	U	310	CLA	CMC-C2C-C3C	2.29	132.32	126.12
34	I	303	DD6	O1-C20-C19	2.29	115.10	113.38
35	X	301	A86	O-C13-C11	-2.29	116.10	121.15
36	H	312	CLA	CMB-C2B-C3B	2.29	128.95	124.68
35	M	302	A86	C23-C16-C22	-2.29	104.00	107.37
36	W	216	CLA	O1A-CGA-CBA	2.29	130.42	123.08
36	D	313	CLA	C3A-C2A-C1A	2.28	104.76	101.34
36	b	825	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
36	b	806	CLA	CHC-C1C-NC	2.28	127.67	124.20
36	W	209	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
42	I	315	LMG	C8-O7-C10	-2.28	112.17	117.79
44	a	844	BCR	C40-C30-C25	2.28	114.00	110.30
35	O	302	A86	C25-C24-C1	-2.28	120.00	126.42
36	l	205	CLA	C3A-C2A-C1A	2.28	104.76	101.34
41	G	301	LHG	C20-C19-C18	-2.28	102.83	114.42
36	D	309	CLA	C4D-C3D-CAD	-2.28	105.41	108.10
35	S	304	A86	C35-C34-C33	-2.28	105.89	109.88
36	a	808	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
36	X	308	CLA	CHB-C4A-NA	2.28	127.67	124.51
35	N	304	A86	C14-C15-C16	2.28	127.50	118.75
35	Q	301	A86	O4-C38-O5	-2.28	118.43	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	l	205	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
36	L	314	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
35	U	301	A86	O1-C15-C20	-2.28	57.17	59.40
35	P	303	A86	C25-C24-C1	-2.28	120.01	126.42
44	m	101	BCR	C15-C16-C17	-2.28	118.80	123.47
36	B	309	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
34	a	849	DD6	C37-C36-C35	2.28	118.58	114.36
35	V	302	A86	O2-C18-C17	-2.28	105.27	109.80
35	T	305	A86	C12-C11-C13	2.28	119.85	116.02
35	W	203	A86	C41-C32-C31	2.28	112.51	110.47
36	C	209	CLA	CHB-C4A-NA	2.28	127.67	124.51
36	C	207	CLA	CMC-C2C-C1C	2.28	128.51	125.04
36	a	806	CLA	C4D-C3D-CAD	-2.28	105.41	108.10
36	N	308	CLA	C3B-C4B-NB	-2.28	106.26	109.21
34	A	304	DD6	C-C1-C2	-2.28	119.73	122.92
36	a	832	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
35	L	319	A86	C25-C24-C1	-2.28	120.01	126.42
36	S	319	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
36	l	204	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
36	D	308	CLA	CHB-C4A-NA	2.28	127.66	124.51
36	K	310	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
39	U	315	LMT	C1B-O1B-C4'	-2.28	112.33	117.96
36	N	311	CLA	CBA-CAA-C2A	-2.28	107.14	113.86
42	G	324	LMG	C8-O7-C10	-2.28	112.18	117.79
35	T	306	A86	C25-C24-C1	-2.28	120.02	126.42
34	J	304	DD6	C33-C34-C35	-2.28	107.19	110.30
36	l	204	CLA	CHB-C4A-NA	2.28	127.66	124.51
35	O	301	A86	C41-C32-C31	-2.28	108.43	110.47
36	H	308	CLA	C2D-C1D-ND	-2.28	108.43	110.10
36	U	313	CLA	O1D-CGD-CBD	2.28	129.14	124.48
35	S	303	A86	C36-C31-C32	-2.28	117.44	119.70
36	J	311	CLA	CHA-C1A-NA	-2.28	121.19	126.40
35	R	302	A86	C4-C3-C2	-2.28	118.81	123.47
35	G	306	A86	C28-C27-C26	-2.28	119.73	122.92
36	J	316	CLA	C3C-C4C-NC	-2.28	108.02	110.57
36	H	305	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
36	R	318	CLA	CHD-C1D-ND	-2.28	122.36	124.45
36	j	101	CLA	CHB-C4A-NA	2.28	127.66	124.51
34	K	304	DD6	O1-C20-C19	-2.27	111.67	113.38
36	a	836	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
36	T	309	CLA	O2D-CGD-CBD	2.27	115.31	111.27
35	R	309	A86	C28-C27-C26	-2.27	119.74	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	814	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
36	h	203	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
35	O	303	A86	C33-C32-C31	2.27	111.42	109.21
36	a	804	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
35	I	301	A86	C7-C6-C5	-2.27	119.74	122.92
35	A	316	A86	O4-C38-O5	-2.27	118.44	122.96
36	b	833	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
44	a	846	BCR	C7-C8-C9	-2.27	122.80	126.23
36	b	834	CLA	CMB-C2B-C3B	2.27	128.93	124.68
36	V	314	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
37	G	308	KC1	C2B-C1B-NB	2.27	111.78	110.10
36	B	311	CLA	CMB-C2B-C3B	2.27	128.93	124.68
34	K	304	DD6	O1-C20-C21	-2.27	112.33	115.06
36	i	102	CLA	CAA-CBA-CGA	-2.27	106.62	113.25
36	N	312	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
35	P	304	A86	C33-C32-C31	2.27	111.42	109.21
36	U	313	CLA	CAA-C2A-C1A	2.27	117.42	111.81
36	E	308	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
37	N	314	KC1	CED-O2D-CGD	2.27	121.07	115.94
36	a	810	CLA	CMB-C2B-C3B	2.27	128.93	124.68
36	K	311	CLA	C2A-C1A-CHA	2.27	127.83	123.86
36	b	840	CLA	CMB-C2B-C3B	2.27	128.92	124.68
36	Q	310	CLA	C4-C3-C5	-2.27	111.45	115.27
36	a	831	CLA	CHD-C1D-ND	-2.27	122.37	124.45
36	T	308	CLA	C3C-C4C-NC	-2.27	108.03	110.57
36	R	316	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
35	H	301	A86	C-C1-C24	2.27	121.65	118.08
36	f	804	CLA	CHD-C1D-C2D	2.27	130.24	125.48
36	K	316	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
35	L	307	A86	C3-C4-C5	-2.27	118.83	123.47
36	W	210	CLA	C1D-ND-C4D	2.27	107.94	106.33
36	H	309	CLA	C1-C2-C3	-2.27	122.12	126.04
37	P	315	KC1	CBA-CAA-C2A	2.27	133.91	125.27
36	E	314	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
36	b	817	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
36	b	809	CLA	CHB-C4A-NA	2.27	127.64	124.51
36	b	808	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
35	I	302	A86	C7-C6-C8	2.27	121.65	118.08
35	K	303	A86	C3-C2-C1	-2.26	124.08	127.31
36	I	312	CLA	CMB-C2B-C3B	2.26	128.91	124.68
36	U	313	CLA	CHA-C1A-NA	-2.26	121.21	126.40
35	P	304	A86	O4-C38-O5	-2.26	118.46	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S	301	A86	C40-C32-C33	2.26	119.21	109.05
36	J	312	CLA	O1D-CGD-CBD	2.26	129.12	124.48
36	X	313	CLA	C3A-C2A-C1A	2.26	104.73	101.34
34	H	303	DD6	C7-C6-C5	-2.26	119.75	122.92
36	L	314	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
36	a	817	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
36	j	101	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
35	B	303	A86	C-C1-C2	-2.26	119.76	122.92
36	a	822	CLA	CHD-C1D-ND	-2.26	122.38	124.45
37	O	313	KC1	CBA-CAA-C2A	2.26	133.89	125.27
36	H	305	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
35	F	301	A86	C9-C10-C11	-2.26	119.97	126.61
34	E	303	DD6	C9-C8-C6	-2.26	120.07	126.42
36	K	309	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
36	b	832	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
36	a	801	CLA	CHA-C4D-ND	2.26	137.22	132.50
36	a	812	CLA	CHD-C1D-ND	-2.26	122.38	124.45
35	A	316	A86	O1-C15-C14	-2.26	108.68	113.21
36	W	211	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
35	C	202	A86	C9-C10-C11	-2.26	119.97	126.61
41	R	323	LHG	C5-O7-C7	-2.26	112.23	117.79
35	T	305	A86	C25-C24-C1	-2.26	120.07	126.42
35	X	314	A86	C4-C3-C2	-2.26	118.85	123.47
34	C	201	DD6	C-C1-C2	-2.26	119.76	122.92
37	V	312	KC1	C3D-CAD-CBD	-2.26	104.63	107.61
35	R	301	A86	C9-C8-C6	-2.26	120.08	126.42
35	E	302	A86	O4-C38-O5	-2.26	118.48	122.96
35	K	306	A86	C21-C20-C19	2.26	116.82	114.28
37	Q	313	KC1	CBA-CAA-C2A	2.26	133.88	125.27
35	N	301	A86	C40-C32-C33	2.26	119.18	109.05
36	a	838	CLA	CMD-C2D-C3D	2.26	132.80	127.61
35	B	303	A86	C28-C27-C26	-2.26	119.76	122.92
35	D	302	A86	O4-C38-O5	-2.26	118.48	122.96
35	S	308	A86	C41-C32-C31	-2.25	108.45	110.47
36	F	311	CLA	CMB-C2B-C3B	2.25	128.90	124.68
35	I	302	A86	C36-C31-C32	-2.25	117.46	119.70
35	X	302	A86	C36-C31-C32	-2.25	117.46	119.70
36	U	308	CLA	C3A-C2A-C1A	2.25	104.72	101.34
37	P	317	KC1	CMB-C2B-C1B	2.25	128.69	124.71
44	a	845	BCR	C24-C23-C22	-2.25	122.83	126.23
34	R	308	DD6	C7-C6-C5	-2.25	119.77	122.92
35	K	306	A86	C-C1-C2	-2.25	119.77	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	X	314	A86	C33-C32-C31	-2.25	107.02	109.21
35	M	304	A86	C40-C32-C31	-2.25	108.46	110.47
36	E	308	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
36	O	308	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
36	T	316	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
36	a	839	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
36	f	805	CLA	C6-C5-C3	-2.25	110.94	114.62
36	H	312	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
36	a	815	CLA	CMB-C2B-C3B	2.25	128.89	124.68
36	l	202	CLA	O1D-CGD-CBD	2.25	129.09	124.48
36	H	310	CLA	CMD-C2D-C3D	2.25	132.79	127.61
36	G	311	CLA	C4-C3-C5	2.25	119.06	115.27
36	V	314	CLA	CHD-C4C-C3C	-2.25	121.53	124.84
35	C	203	A86	C36-C31-C32	-2.25	117.46	119.70
35	X	304	A86	C21-C20-C19	-2.25	111.75	114.28
37	B	310	KC1	C4D-C3D-CAD	2.25	111.44	107.81
36	L	312	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
35	X	301	A86	C20-C19-C18	2.25	117.20	112.75
36	X	309	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
36	L	316	CLA	O2D-CGD-CBD	2.25	115.26	111.27
34	A	301	DD6	C-C1-C2	-2.25	119.78	122.92
35	N	303	A86	C36-C31-C32	-2.25	117.47	119.70
36	A	309	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
36	b	831	CLA	CHB-C4A-NA	2.25	127.62	124.51
36	b	807	CLA	O2A-CGA-O1A	-2.25	117.70	123.30
36	H	318	CLA	CAA-C2A-C3A	-2.25	106.63	112.78
36	A	311	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
37	P	317	KC1	C4B-C3B-C2B	-2.25	104.91	106.75
36	X	315	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
34	D	301	DD6	C-C1-C2	-2.25	119.78	122.92
36	a	807	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
35	J	302	A86	O4-C38-O5	-2.24	118.50	122.96
36	A	306	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
37	Q	311	KC1	CBA-CAA-C2A	2.24	133.83	125.27
36	V	308	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
34	S	306	DD6	C25-C26-C27	-2.24	120.07	126.58
36	I	313	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
35	X	303	A86	C4-C3-C2	-2.24	118.88	123.47
36	H	317	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
36	b	820	CLA	C2D-C1D-ND	-2.24	108.45	110.10
36	a	836	CLA	CHD-C1D-ND	-2.24	122.39	124.45
43	a	840	PQN	C2M-C2-C1	2.24	119.99	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	O	315	KC1	CBA-CAA-C2A	2.24	133.82	125.27
36	H	308	CLA	CHB-C4A-NA	2.24	127.61	124.51
36	G	316	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
38	b	804	SQD	O8-S-C6	2.24	109.31	105.74
35	M	301	A86	C33-C32-C31	-2.24	107.03	109.21
36	W	215	CLA	CHA-C1A-NA	-2.24	121.27	126.40
36	C	208	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
36	b	815	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
36	b	840	CLA	CAC-C3C-C2C	-2.24	123.70	127.53
36	G	312	CLA	C2D-C1D-ND	-2.24	108.45	110.10
36	X	308	CLA	O2A-CGA-CBA	2.24	118.94	111.91
44	h	201	BCR	C16-C15-C14	-2.24	118.89	123.47
36	b	812	CLA	C3C-C4C-NC	-2.24	108.06	110.57
35	V	301	A86	C12-C11-C13	2.24	119.78	116.02
36	R	322	CLA	CHB-C4A-NA	2.24	127.61	124.51
36	C	209	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
36	C	210	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
35	W	202	A86	C28-C27-C29	2.24	124.12	118.93
41	F	318	LHG	C18-C17-C16	-2.24	103.06	114.42
36	b	820	CLA	CHB-C4A-NA	2.24	127.61	124.51
36	V	313	CLA	CHB-C4A-NA	2.24	127.61	124.51
34	D	303	DD6	C21-C20-C15	-2.24	118.51	122.26
37	N	314	KC1	C2B-C1B-NB	2.24	111.75	110.10
36	P	314	CLA	C4D-CHA-C1A	2.24	123.97	121.25
34	W	205	DD6	C12-C11-C10	-2.24	119.79	122.92
42	L	321	LMG	C8-O7-C10	-2.24	112.28	117.79
36	a	832	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
35	R	304	A86	O-C13-C11	-2.24	116.21	121.15
36	N	317	CLA	CHA-C1A-NA	-2.24	121.28	126.40
36	S	310	CLA	C3A-C2A-C1A	2.24	104.69	101.34
37	S	316	KC1	C1C-C2C-C3C	-2.24	104.61	106.96
36	j	102	CLA	C3A-C2A-C1A	2.24	104.69	101.34
35	X	301	A86	O-C13-C14	-2.24	117.12	121.66
36	F	314	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
34	B	304	DD6	C15-C14-C13	-2.24	121.27	125.99
36	I	314	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
35	U	303	A86	C-C1-C2	-2.23	119.79	122.92
36	R	312	CLA	CED-O2D-CGD	-2.23	110.88	115.94
36	a	828	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
35	P	306	A86	C41-C32-C31	-2.23	108.47	110.47
36	f	804	CLA	C3D-C4D-CHA	-2.23	107.61	112.72
36	F	317	CLA	CMD-C2D-C3D	-2.23	122.48	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	210	CLA	CAA-C2A-C1A	2.23	119.29	111.97
35	F	305	A86	C26-C25-C24	-2.23	116.25	123.22
37	K	314	KC1	CMA-C3A-C2A	-2.23	122.83	128.30
36	R	310	CLA	CHB-C4A-NA	2.23	127.60	124.51
35	N	302	A86	C3-C2-C1	-2.23	124.12	127.31
34	B	304	DD6	C21-C20-C15	-2.23	118.52	122.26
34	D	305	DD6	C25-C26-C27	-2.23	120.10	126.58
44	b	845	BCR	C1-C6-C5	-2.23	119.47	122.61
36	Q	307	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
34	B	304	DD6	C9-C8-C6	-2.23	120.15	126.42
35	E	302	A86	C9-C8-C6	-2.23	120.15	126.42
36	a	806	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
36	I	311	CLA	CHD-C1D-ND	-2.23	122.41	124.45
36	a	834	CLA	CHD-C1D-ND	-2.23	122.41	124.45
36	P	310	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
36	D	308	CLA	O2A-CGA-CBA	2.23	118.90	111.91
35	F	301	A86	C7-C6-C5	-2.23	119.80	122.92
34	E	301	DD6	C37-C36-C35	2.23	118.48	114.36
34	S	306	DD6	C25-C24-C1	-2.23	120.15	126.42
36	b	810	CLA	CHD-C1D-ND	-2.23	122.41	124.45
35	J	306	A86	C3-C4-C5	-2.23	118.91	123.47
37	M	313	KC1	C2A-C1A-CHA	-2.23	120.07	127.44
36	C	209	CLA	CMB-C2B-C3B	2.23	128.85	124.68
36	N	308	CLA	C6-C5-C3	2.23	119.30	113.45
36	U	310	CLA	CBC-CAC-C3C	2.23	118.57	112.43
34	M	303	DD6	C25-C26-C27	-2.23	120.11	126.58
36	W	201	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
36	a	804	CLA	CAA-CBA-CGA	-2.23	106.74	113.25
35	P	307	A86	O4-C38-O5	-2.23	118.54	122.96
36	O	314	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
44	l	203	BCR	C2-C1-C6	2.23	113.91	110.48
36	R	313	CLA	C2D-C1D-ND	-2.23	108.46	110.10
36	B	311	CLA	CHA-C4D-ND	2.23	137.16	132.50
36	B	311	CLA	CBC-CAC-C3C	2.23	118.57	112.43
36	J	316	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
36	Q	310	CLA	C4D-CHA-C1A	2.23	123.96	121.25
36	b	810	CLA	O2D-CGD-CBD	2.22	115.22	111.27
36	a	826	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
36	a	837	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
35	K	302	A86	C28-C27-C26	-2.22	119.81	122.92
36	b	841	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
37	N	314	KC1	CAC-C3C-C2C	2.22	131.33	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	821	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
36	G	313	CLA	C16-C15-C13	-2.22	108.73	115.92
42	h	206	LMG	C8-O7-C10	-2.22	112.32	117.79
36	J	315	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
36	R	314	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
34	K	305	DD6	C25-C26-C27	-2.22	120.13	126.58
41	j	104	LHG	C5-O7-C7	-2.22	112.32	117.79
36	f	802	CLA	CMB-C2B-C3B	2.22	128.83	124.68
35	F	301	A86	O4-C38-O5	-2.22	118.55	122.96
36	a	831	CLA	C4D-C3D-CAD	-2.22	105.48	108.10
36	D	309	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
36	H	307	CLA	CHD-C4C-C3C	2.22	128.10	124.84
36	C	214	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
35	K	303	A86	C40-C32-C31	2.22	112.46	110.47
37	P	317	KC1	C4D-C3D-CAD	2.22	111.39	107.81
35	J	303	A86	C9-C10-C11	-2.22	120.08	126.61
36	C	205	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
36	f	802	CLA	C2A-C1A-CHA	2.22	127.74	123.86
36	P	314	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
35	U	303	A86	C28-C27-C26	-2.22	119.82	122.92
36	F	309	CLA	C5-C3-C2	2.22	125.61	121.12
36	X	307	CLA	CHB-C4A-NA	2.22	127.58	124.51
35	S	301	A86	C9-C8-C6	-2.22	120.19	126.42
35	T	307	A86	C20-C19-C18	2.22	117.14	112.75
36	Q	312	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
44	l	207	BCR	C28-C27-C26	-2.22	110.12	114.08
35	I	302	A86	C3-C4-C5	-2.22	118.94	123.47
35	N	306	A86	C25-C24-C1	-2.22	120.19	126.42
35	N	301	A86	C9-C8-C6	-2.21	120.19	126.42
36	O	312	CLA	C4D-CHA-C1A	2.21	123.94	121.25
36	X	307	CLA	C2A-C1A-CHA	2.21	127.73	123.86
35	M	305	A86	C3-C4-C5	-2.21	118.94	123.47
36	T	314	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
35	X	301	A86	C3-C4-C5	-2.21	118.94	123.47
35	A	302	A86	C28-C27-C26	-2.21	119.82	122.92
37	T	310	KC1	CBD-CHA-C1A	-2.21	124.76	128.88
36	X	312	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
36	b	816	CLA	CHB-C4A-NA	2.21	127.57	124.51
35	S	302	A86	C3-C2-C1	-2.21	124.15	127.31
44	h	201	BCR	C27-C26-C25	2.21	125.94	122.73
36	E	316	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
35	U	303	A86	C9-C8-C6	-2.21	120.20	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	S	311	CLA	CHA-C4D-ND	2.21	137.12	132.50
36	E	311	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
35	G	305	A86	C33-C32-C31	2.21	111.36	109.21
36	a	807	CLA	CHD-C1D-ND	-2.21	122.42	124.45
36	P	319	CLA	O2D-CGD-CBD	2.21	115.20	111.27
36	b	822	CLA	O1D-CGD-CBD	2.21	129.01	124.48
42	V	316	LMG	C8-O7-C10	-2.21	112.35	117.79
36	a	841	CLA	CAA-CBA-CGA	-2.21	106.79	113.25
36	P	316	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
35	T	302	A86	C9-C8-C6	-2.21	120.21	126.42
35	h	202	A86	O4-C38-O5	-2.21	118.57	122.96
34	I	303	DD6	C-C1-C2	-2.21	119.83	122.92
36	X	306	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
35	J	306	A86	C17-C16-C15	2.21	111.42	109.16
35	S	305	A86	O1-C20-C21	-2.21	112.41	115.06
36	W	211	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
35	S	308	A86	C9-C10-C11	-2.21	120.12	126.61
36	I	309	CLA	CBC-CAC-C3C	2.21	118.52	112.43
35	F	305	A86	C33-C32-C31	2.21	111.36	109.21
36	E	314	CLA	O2A-C1-C2	2.21	114.44	108.64
36	R	316	CLA	CHD-C1D-ND	-2.21	122.43	124.45
36	L	310	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
34	F	303	DD6	C7-C6-C5	-2.21	119.83	122.92
36	b	834	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
36	b	805	CLA	CHA-C1A-NA	-2.21	121.35	126.40
36	H	309	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
36	a	824	CLA	CAA-CBA-CGA	-2.21	106.81	113.25
37	B	310	KC1	C2B-C1B-NB	2.21	111.73	110.10
35	L	319	A86	C33-C32-C31	-2.20	107.07	109.21
36	X	307	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
36	b	835	CLA	CMB-C2B-C3B	2.20	128.80	124.68
36	b	808	CLA	CHD-C1D-ND	-2.20	122.43	124.45
35	U	302	A86	C28-C27-C26	-2.20	119.83	122.92
36	V	308	CLA	C1-C2-C3	-2.20	122.23	126.04
36	E	313	CLA	CED-O2D-CGD	2.20	120.92	115.94
36	b	807	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
36	b	816	CLA	C3C-C4C-NC	-2.20	108.10	110.57
35	C	202	A86	C26-C25-C24	-2.20	116.34	123.22
40	C	215	DGD	C2G-O2G-C1B	-2.20	112.37	117.79
36	a	810	CLA	C1-O2A-CGA	2.20	122.22	116.44
36	I	305	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
34	S	306	DD6	C-C1-C2	-2.20	119.84	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	f	804	CLA	C2A-C3A-C4A	2.20	105.42	101.87
36	S	319	CLA	CHA-C1A-NA	-2.20	121.36	126.40
36	S	314	CLA	CHD-C1D-ND	-2.20	122.43	124.45
36	b	824	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
35	V	304	A86	C28-C27-C26	-2.20	119.84	122.92
34	B	302	DD6	O1-C20-C21	-2.20	112.42	115.06
36	l	201	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
36	a	837	CLA	C2A-C1A-CHA	2.20	127.70	123.86
35	C	203	A86	O1-C15-C14	-2.20	108.80	113.21
36	I	314	CLA	CHB-C4A-NA	2.20	127.55	124.51
44	i	103	BCR	C15-C14-C13	-2.20	124.17	127.31
36	f	803	CLA	C3D-C4D-ND	2.20	113.79	110.24
35	T	307	A86	C23-C16-C22	-2.20	104.13	107.37
36	K	315	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
36	l	202	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
36	K	310	CLA	CMC-C2C-C1C	2.20	128.38	125.04
36	b	824	CLA	CHD-C1D-ND	-2.20	122.44	124.45
36	A	307	CLA	O2D-CGD-CBD	2.20	115.17	111.27
36	D	313	CLA	CBA-CAA-C2A	2.20	120.35	113.86
44	l	207	BCR	C24-C23-C22	-2.20	122.92	126.23
34	Q	302	DD6	C9-C8-C6	-2.20	120.25	126.42
35	T	306	A86	C4-C3-C2	-2.20	118.97	123.47
35	W	203	A86	C3-C4-C5	-2.20	118.97	123.47
36	H	315	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
36	a	816	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
36	b	801	CLA	C2D-C1D-ND	-2.20	108.49	110.10
36	a	839	CLA	O2D-CGD-CBD	2.20	115.17	111.27
36	I	306	CLA	C3C-C4C-NC	2.20	113.03	110.57
35	T	301	A86	O4-C38-O5	-2.20	118.60	122.96
36	b	841	CLA	C2A-C1A-CHA	2.19	127.70	123.86
36	G	312	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
35	M	305	A86	C9-C8-C6	-2.19	120.25	126.42
35	R	301	A86	C40-C32-C33	2.19	118.90	109.05
36	H	317	CLA	CAC-C3C-C4C	2.19	127.66	124.81
36	M	312	CLA	C2D-C1D-ND	-2.19	108.49	110.10
35	F	304	A86	C3-C4-C5	-2.19	118.98	123.47
36	b	827	CLA	CHA-C4D-ND	2.19	137.09	132.50
37	S	316	KC1	O2D-CGD-O1D	-2.19	119.55	123.84
35	T	304	A86	O4-C38-O5	-2.19	118.60	122.96
36	B	309	CLA	CHB-C4A-NA	2.19	127.55	124.51
36	b	830	CLA	C6-C7-C8	-2.19	108.83	115.92
36	b	832	CLA	O2A-CGA-O1A	-2.19	118.06	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	K	303	A86	C9-C10-C11	-2.19	120.16	126.61
36	N	309	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
36	U	306	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
36	a	829	CLA	O2D-CGD-CBD	2.19	115.16	111.27
37	K	314	KC1	CAA-CBA-CGA	-2.19	116.00	127.26
36	C	206	CLA	CHD-C1D-ND	-2.19	122.44	124.45
36	a	807	CLA	C1-C2-C3	-2.19	122.25	126.04
36	a	824	CLA	C16-C15-C13	-2.19	108.84	115.92
36	J	313	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
34	A	301	DD6	C21-C20-C15	-2.19	118.59	122.26
36	P	301	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
36	a	833	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
36	S	318	CLA	C2A-C1A-CHA	2.19	127.69	123.86
36	a	824	CLA	CMC-C2C-C3C	2.19	132.06	126.12
36	I	306	CLA	C3D-C4D-ND	2.19	113.78	110.24
37	J	314	KC1	O2D-CGD-O1D	-2.19	119.56	123.84
34	a	849	DD6	C9-C8-C6	-2.19	120.27	126.42
36	N	315	CLA	CHA-C1A-NA	-2.19	121.38	126.40
34	I	303	DD6	C33-C34-C35	2.19	113.30	110.30
36	a	841	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
36	S	317	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
36	N	319	CLA	C3A-C2A-C1A	2.19	104.62	101.34
36	a	818	CLA	CHD-C1D-ND	-2.19	122.44	124.45
36	S	312	CLA	CHB-C4A-NA	2.19	127.54	124.51
36	b	829	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
35	U	303	A86	C9-C10-C11	-2.19	120.18	126.61
34	P	305	DD6	C9-C8-C6	-2.19	120.27	126.42
35	H	301	A86	C26-C25-C24	-2.19	116.39	123.22
35	U	302	A86	C14-C15-C16	2.19	127.13	118.75
36	X	313	CLA	C2A-C3A-C4A	2.19	105.40	101.87
37	P	317	KC1	CAA-CBA-CGA	-2.19	116.02	127.26
44	j	107	BCR	C24-C23-C22	-2.19	122.93	126.23
35	P	303	A86	C33-C32-C31	-2.19	107.09	109.21
36	M	310	CLA	CMB-C2B-C3B	2.19	128.77	124.68
35	W	203	A86	C21-C20-C19	-2.19	111.82	114.28
36	a	837	CLA	O2D-CGD-CBD	2.19	115.15	111.27
36	H	307	CLA	C4D-C3D-CAD	-2.19	105.52	108.10
36	C	209	CLA	O2D-CGD-CBD	2.19	115.15	111.27
36	b	809	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
36	b	812	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
36	T	308	CLA	C2D-C1D-ND	-2.18	108.50	110.10
37	F	308	KC1	CAB-C3B-C2B	2.18	135.80	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	P	305	DD6	O1-C20-C21	-2.18	112.44	115.06
36	b	827	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
36	H	315	CLA	CAA-CBA-CGA	-2.18	106.87	113.25
36	R	320	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
35	H	304	A86	C9-C8-C6	-2.18	120.28	126.42
36	W	212	CLA	CHD-C1D-C2D	2.18	130.06	125.48
37	T	315	KC1	C1A-NA-C4A	2.18	107.69	106.71
36	f	803	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
36	S	309	CLA	O2D-CGD-CBD	2.18	115.14	111.27
36	l	202	CLA	CHD-C1D-ND	-2.18	122.45	124.45
41	a	842	LHG	C27-C26-C25	-2.18	103.35	114.42
36	a	807	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
36	U	306	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
36	F	316	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
34	Q	302	DD6	C-C1-C2	-2.18	119.87	122.92
36	F	310	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
36	B	305	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
35	h	204	A86	C34-O4-C38	-2.18	113.83	117.90
36	B	307	CLA	CHA-C1A-NA	-2.18	121.41	126.40
36	I	312	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
36	F	316	CLA	CMA-C3A-C2A	-2.18	111.02	116.10
35	P	307	A86	C-C1-C2	-2.18	119.87	122.92
36	V	309	CLA	CHA-C1A-NA	-2.18	121.41	126.40
36	M	308	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
35	P	307	A86	C3-C4-C5	-2.18	119.01	123.47
35	T	306	A86	C7-C6-C8	2.18	121.51	118.08
37	T	310	KC1	C3B-C2B-C1B	-2.18	105.00	107.08
41	a	850	LHG	C5-O7-C7	-2.18	112.43	117.79
35	P	304	A86	C3-C4-C5	-2.18	119.01	123.47
36	J	311	CLA	C2A-C1A-CHA	2.18	127.67	123.86
36	U	306	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
37	J	314	KC1	C1C-C2C-C3C	-2.18	104.67	106.96
36	D	307	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
44	f	806	BCR	C40-C30-C25	2.18	113.83	110.30
36	X	307	CLA	CED-O2D-CGD	2.18	120.86	115.94
36	B	305	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
36	L	313	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
34	S	307	DD6	C32-C31-C36	-2.18	119.56	122.63
36	b	838	CLA	CHB-C4A-NA	2.18	127.52	124.51
36	F	310	CLA	CAC-C3C-C4C	2.17	127.63	124.81
36	T	311	CLA	C11-C12-C13	-2.17	108.89	115.92
36	U	306	CLA	C2A-C3A-C4A	2.17	105.38	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	L	317	KC1	O1D-CGD-CBD	-2.17	120.03	124.48
36	D	316	CLA	CHD-C1D-ND	-2.17	122.46	124.45
35	W	203	A86	C25-C24-C1	-2.17	120.31	126.42
35	F	305	A86	O-C13-C14	-2.17	117.24	121.66
35	I	301	A86	C9-C10-C11	-2.17	120.22	126.61
36	l	204	CLA	C3D-C4D-ND	2.17	113.75	110.24
34	H	303	DD6	C25-C26-C27	-2.17	120.27	126.58
36	a	820	CLA	CHD-C1D-ND	-2.17	122.46	124.45
36	M	315	CLA	C3C-C4C-NC	-2.17	108.13	110.57
35	R	301	A86	C4-C3-C2	-2.17	119.02	123.47
34	Q	302	DD6	O1-C20-C21	-2.17	112.45	115.06
36	I	309	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
34	E	301	DD6	C21-C20-C15	-2.17	118.62	122.26
37	Q	311	KC1	C3D-CAD-CBD	-2.17	104.75	107.61
35	S	305	A86	C9-C8-C6	-2.17	120.31	126.42
36	a	834	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
36	b	801	CLA	CAA-CBA-CGA	-2.17	106.91	113.25
36	I	307	CLA	C2A-C1A-CHA	2.17	127.66	123.86
36	a	822	CLA	C4D-C3D-CAD	-2.17	105.54	108.10
36	S	310	CLA	CHB-C4A-NA	2.17	127.51	124.51
36	b	808	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
36	H	310	CLA	C3D-C2D-C1D	2.17	108.79	105.83
35	N	306	A86	C4-C3-C2	-2.17	119.03	123.47
34	D	304	DD6	C25-C26-C27	-2.17	120.28	126.58
36	l	204	CLA	CMB-C2B-C3B	2.17	128.74	124.68
36	M	314	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
36	a	816	CLA	C3D-C4D-ND	2.17	113.75	110.24
35	O	303	A86	C3-C4-C5	-2.17	119.03	123.47
36	B	307	CLA	CAA-C2A-C1A	2.17	119.08	111.97
36	U	309	CLA	CHA-C1A-NA	-2.17	121.43	126.40
36	K	310	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
36	b	821	CLA	C2D-C1D-ND	-2.17	108.51	110.10
35	M	305	A86	C20-C19-C18	2.17	117.04	112.75
37	P	317	KC1	CBC-CAC-C3C	-2.17	106.45	112.43
36	O	316	CLA	C4-C3-C5	2.17	118.92	115.27
35	U	302	A86	C3-C2-C1	-2.17	124.22	127.31
35	H	304	A86	C40-C32-C31	-2.17	108.53	110.47
36	R	318	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
36	T	313	CLA	CAC-C3C-C4C	2.17	127.62	124.81
35	F	307	A86	C21-C20-C19	-2.17	111.84	114.28
36	D	313	CLA	C1-C2-C3	-2.17	122.30	126.04
44	b	847	BCR	C2-C3-C4	2.17	116.22	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	312	CLA	CAA-C2A-C1A	2.17	119.07	111.97
36	D	316	CLA	CHD-C4C-C3C	2.17	128.02	124.84
36	G	310	CLA	CHB-C4A-NA	2.17	127.51	124.51
44	j	107	BCR	C1-C6-C5	-2.17	119.56	122.61
37	D	314	KC1	C2B-C1B-NB	2.17	111.70	110.10
36	K	309	CLA	C4-C3-C5	2.17	118.91	115.27
36	b	802	CLA	CHD-C1D-ND	-2.17	122.46	124.45
35	G	302	A86	C17-C16-C15	2.17	111.37	109.16
36	a	848	CLA	C4D-C3D-CAD	2.17	110.65	108.10
35	N	304	A86	O-C13-C11	-2.17	116.36	121.15
36	J	307	CLA	C4-C3-C5	2.17	118.91	115.27
36	J	307	CLA	C2A-C1A-CHA	2.16	127.64	123.86
36	D	311	CLA	C2D-C1D-ND	-2.16	108.51	110.10
34	C	201	DD6	C32-C31-C36	-2.16	119.58	122.63
36	j	102	CLA	C2A-C1A-CHA	2.16	127.64	123.86
34	I	303	DD6	C25-C24-C1	-2.16	120.34	126.42
36	N	310	CLA	C1B-CHB-C4A	2.16	134.40	130.12
36	L	311	CLA	O2D-CGD-CBD	2.16	115.11	111.27
36	b	826	CLA	C2A-C1A-CHA	2.16	127.64	123.86
36	E	316	CLA	CMC-C2C-C3C	2.16	131.99	126.12
35	O	302	A86	C33-C32-C31	-2.16	107.11	109.21
37	A	312	KC1	C4D-C3D-CAD	-2.16	104.31	107.81
36	J	312	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
36	a	811	CLA	CHD-C1D-ND	-2.16	122.47	124.45
37	P	315	KC1	C3D-CAD-CBD	-2.16	104.76	107.61
42	m	102	LMG	C8-O7-C10	-2.16	112.47	117.79
40	b	849	DGD	O3D-C3D-C4D	-2.16	105.35	110.35
35	S	308	A86	O4-C38-O5	-2.16	118.67	122.96
35	B	303	A86	C20-C19-C18	2.16	117.02	112.75
36	O	312	CLA	CBD-CHA-C1A	2.16	131.04	128.50
37	O	313	KC1	C3D-CAD-CBD	-2.16	104.76	107.61
36	b	837	CLA	C2D-C1D-ND	-2.16	108.51	110.10
35	Q	316	A86	C25-C26-C27	-2.16	124.23	127.31
35	F	306	A86	C10-C9-C8	-2.16	116.48	123.22
35	U	303	A86	C12-C11-C13	2.16	119.65	116.02
36	S	311	CLA	C2D-C1D-ND	-2.16	108.51	110.10
35	K	306	A86	C9-C10-C11	-2.16	120.27	126.61
36	b	819	CLA	C2A-C1A-CHA	2.16	127.63	123.86
37	T	315	KC1	CAA-CBA-CGA	-2.16	116.18	127.26
35	C	204	A86	C9-C8-C6	-2.16	120.36	126.42
35	N	305	A86	O1-C15-C20	-2.16	57.29	59.40
35	Q	301	A86	C3-C4-C5	-2.16	119.06	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	T	314	CLA	CHD-C1D-ND	-2.16	122.47	124.45
37	B	310	KC1	C1C-C2C-C3C	-2.16	104.69	106.96
35	T	304	A86	C10-C9-C8	-2.16	116.49	123.22
36	R	320	CLA	CHD-C1D-C2D	2.16	130.00	125.48
35	S	304	A86	C26-C25-C24	-2.15	116.49	123.22
36	A	313	CLA	O1D-CGD-CBD	2.15	128.89	124.48
36	V	306	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
35	A	316	A86	C9-C8-C6	-2.15	120.36	126.42
35	F	307	A86	C7-C6-C8	2.15	121.47	118.08
35	X	301	A86	C40-C32-C33	2.15	118.72	109.05
36	V	305	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
34	Q	302	DD6	C32-C31-C36	-2.15	119.59	122.63
42	J	319	LMG	C8-O7-C10	-2.15	112.49	117.79
36	a	848	CLA	C4-C3-C2	-2.15	118.16	123.68
44	b	847	BCR	C15-C16-C17	-2.15	119.06	123.47
36	K	310	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
36	G	313	CLA	C2D-C1D-ND	-2.15	108.52	110.10
35	F	305	A86	O4-C38-O5	-2.15	118.69	122.96
36	l	204	CLA	C1C-C2C-C3C	-2.15	104.69	106.96
37	O	315	KC1	C3D-CAD-CBD	-2.15	104.77	107.61
35	Q	316	A86	O1-C15-C20	-2.15	57.30	59.40
36	b	838	CLA	C2D-C1D-ND	-2.15	108.52	110.10
35	I	301	A86	C9-C8-C6	-2.15	120.37	126.42
36	M	309	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
36	X	310	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
35	P	304	A86	C12-C11-C13	2.15	119.64	116.02
35	N	306	A86	C9-C8-C6	-2.15	120.38	126.42
37	Q	313	KC1	C3D-CAD-CBD	-2.15	104.77	107.61
36	D	316	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
35	Q	316	A86	O1-C20-C21	-2.15	112.48	115.06
36	K	316	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
34	M	303	DD6	C-C1-C2	-2.15	119.91	122.92
34	P	305	DD6	C12-C11-C10	-2.15	119.91	122.92
36	N	313	CLA	C4D-CHA-C1A	2.15	123.86	121.25
36	W	210	CLA	C3A-C2A-C1A	2.15	104.56	101.34
36	V	311	CLA	C2A-C1A-CHA	2.15	127.61	123.86
35	N	305	A86	O1-C20-C21	-2.15	112.48	115.06
36	B	308	CLA	CHD-C4C-NC	2.15	127.59	124.20
35	I	301	A86	C12-C11-C13	2.15	119.63	116.02
34	E	303	DD6	C37-C36-C35	2.15	118.33	114.36
35	C	203	A86	C41-C32-C31	-2.15	108.55	110.47
36	H	308	CLA	CHA-C1A-NA	-2.15	121.48	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	f	805	CLA	C1B-CHB-C4A	-2.15	125.87	130.12
36	K	308	CLA	CHB-C4A-NA	2.15	127.48	124.51
36	P	302	CLA	CBA-CAA-C2A	-2.14	108.69	113.47
36	X	310	CLA	C2A-C1A-CHA	2.14	127.59	123.85
36	a	829	CLA	CHB-C4A-NA	2.14	127.48	124.51
36	R	314	CLA	C3A-C2A-C1A	2.14	104.55	101.34
36	a	813	CLA	O2A-CGA-O1A	-2.14	117.96	123.30
44	l	207	BCR	C29-C30-C25	2.14	113.78	110.48
36	a	803	CLA	O2D-CGD-CBD	2.14	115.07	111.27
36	R	319	CLA	C3A-C2A-C1A	2.14	104.55	101.34
36	X	315	CLA	CHA-C1A-NA	-2.14	121.49	126.40
35	I	302	A86	C9-C10-C11	-2.14	120.31	126.61
35	O	303	A86	C12-C11-C13	2.14	119.62	116.02
36	a	826	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
35	U	304	A86	C40-C32-C31	-2.14	108.56	110.47
36	F	311	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
36	a	836	CLA	C3A-C2A-C1A	2.14	104.55	101.34
44	f	806	BCR	C30-C25-C26	-2.14	119.60	122.61
35	P	306	A86	C26-C25-C24	-2.14	116.54	123.22
44	a	845	BCR	C1-C6-C5	-2.14	119.60	122.61
36	A	307	CLA	C1-C2-C3	-2.14	122.34	126.04
35	Q	301	A86	C12-C11-C13	2.14	119.62	116.02
34	K	305	DD6	C25-C24-C1	-2.14	120.41	126.42
36	A	308	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
36	U	306	CLA	CMC-C2C-C1C	2.14	128.29	125.04
34	W	205	DD6	C25-C24-C1	-2.14	120.41	126.42
36	V	310	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
36	W	218	CLA	O1D-CGD-CBD	2.14	128.86	124.48
35	S	304	A86	C3-C4-C5	-2.14	119.10	123.47
35	J	301	A86	C19-C18-C17	-2.14	106.65	110.77
36	V	306	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
35	J	303	A86	O3-C36-C37	-2.14	105.59	109.39
36	a	819	CLA	CMB-C2B-C3B	2.14	128.68	124.68
36	I	312	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
35	J	305	A86	C19-C18-C17	-2.14	106.65	110.77
36	a	823	CLA	C4D-C3D-CAD	-2.14	105.58	108.10
36	U	311	CLA	CMD-C2D-C1D	-2.14	120.95	124.71
36	U	311	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
36	N	318	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
36	T	314	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
36	G	311	CLA	CHB-C4A-NA	2.14	127.47	124.51
35	G	305	A86	C40-C32-C31	-2.14	108.56	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	313	CLA	CHA-C1A-NA	-2.14	121.51	126.40
36	C	209	CLA	C3A-C2A-C1A	2.14	104.54	101.34
36	O	316	CLA	C2A-C3A-C4A	2.13	105.32	101.87
36	R	321	CLA	C2D-C1D-ND	-2.13	108.53	110.10
36	i	102	CLA	C2A-C1A-CHA	2.13	127.59	123.86
37	R	317	KC1	C3D-CAD-CBD	-2.13	104.80	107.61
36	L	308	CLA	CMB-C2B-C1B	2.13	131.74	128.46
35	E	302	A86	C7-C6-C5	-2.13	119.93	122.92
36	b	805	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
35	L	301	A86	C9-C10-C11	-2.13	120.33	126.61
36	F	310	CLA	C1-C2-C3	-2.13	122.35	126.04
34	A	301	DD6	C12-C11-C10	-2.13	119.94	122.92
35	E	307	A86	O4-C38-O5	-2.13	118.73	122.96
35	T	302	A86	C33-C32-C31	-2.13	107.14	109.21
34	H	302	DD6	C10-C9-C8	-2.13	116.56	123.22
44	a	846	BCR	C38-C26-C27	-2.13	109.52	113.62
35	G	306	A86	C19-C18-C17	-2.13	106.66	110.77
36	H	315	CLA	CHA-C1A-NA	-2.13	121.52	126.40
36	b	820	CLA	O2A-C1-C2	-2.13	103.03	108.64
36	G	314	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
35	X	305	A86	C4-C3-C2	-2.13	119.11	123.47
40	b	849	DGD	C3D-C4D-C5D	-2.13	106.44	110.24
36	P	312	CLA	CAA-C2A-C1A	2.13	118.95	111.97
36	b	805	CLA	C2D-C1D-ND	-2.13	108.53	110.10
36	K	308	CLA	C1-C2-C3	-2.13	122.36	126.04
36	S	319	CLA	C2A-C1A-CHA	2.13	127.58	123.86
36	V	305	CLA	CHD-C1D-C2D	2.13	129.94	125.48
36	N	308	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
37	G	317	KC1	C2B-C1B-NB	2.13	111.67	110.10
36	R	312	CLA	C2A-C1A-CHA	2.13	127.58	123.86
34	R	308	DD6	O1-C20-C21	-2.13	112.51	115.06
36	b	820	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
35	I	302	A86	C4-C3-C2	-2.13	119.12	123.47
36	S	320	CLA	C2A-C1A-CHA	2.13	127.58	123.86
35	N	303	A86	C33-C32-C31	-2.13	107.14	109.21
42	j	105	LMG	C8-O7-C10	-2.13	112.56	117.79
37	D	314	KC1	O2D-CGD-O1D	-2.13	119.68	123.84
36	T	313	CLA	CHD-C1D-ND	-2.13	122.50	124.45
44	b	843	BCR	C30-C25-C26	-2.13	119.62	122.61
36	a	835	CLA	CBA-CAA-C2A	-2.13	107.59	113.86
36	Q	309	CLA	CAA-C2A-C1A	2.13	118.94	111.97
36	E	310	CLA	CMD-C2D-C3D	2.12	132.50	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	O	302	A86	C40-C32-C33	2.12	118.59	109.05
35	N	305	A86	C25-C26-C27	-2.12	124.28	127.31
36	N	308	CLA	C1D-ND-C4D	-2.12	104.83	106.33
37	W	213	KC1	C2A-C1A-NA	2.12	112.81	109.40
36	R	315	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
36	V	310	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
35	P	303	A86	C40-C32-C33	2.12	118.58	109.05
37	M	318	KC1	CAB-C3B-C4B	2.12	130.02	124.90
36	b	824	CLA	CED-O2D-CGD	2.12	120.74	115.94
35	Q	304	A86	C9-C8-C6	-2.12	120.46	126.42
36	H	312	CLA	O1D-CGD-CBD	2.12	128.82	124.48
35	T	303	A86	C9-C10-C11	-2.12	120.37	126.61
37	U	312	KC1	CAC-C3C-C2C	-2.12	123.90	127.53
36	b	833	CLA	C4-C3-C5	2.12	118.84	115.27
36	I	305	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
35	J	305	A86	C9-C8-C6	-2.12	120.46	126.42
35	X	303	A86	C23-C16-C17	-2.12	105.30	108.98
36	J	309	CLA	CHB-C4A-NA	2.12	127.44	124.51
36	a	831	CLA	CHA-C1A-NA	-2.12	121.55	126.40
36	O	310	CLA	CAA-C2A-C1A	2.12	118.92	111.97
36	U	311	CLA	CMC-C2C-C1C	2.12	128.26	125.04
36	P	311	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
36	b	830	CLA	CHA-C4D-ND	2.12	136.93	132.50
35	L	319	A86	C40-C32-C33	2.12	118.56	109.05
36	C	210	CLA	CHA-C1A-NA	-2.12	121.55	126.40
36	D	315	CLA	C2A-C1A-CHA	2.12	127.55	123.85
36	Q	314	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
36	J	310	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
35	V	302	A86	C23-C16-C17	-2.12	105.30	108.98
36	b	812	CLA	C6-C7-C8	-2.12	109.08	115.92
35	I	304	A86	C25-C24-C1	-2.12	120.47	126.42
44	a	847	BCR	C2-C1-C6	2.12	113.74	110.48
35	T	301	A86	C9-C10-C11	-2.12	120.39	126.61
35	W	202	A86	C20-C19-C18	2.12	116.94	112.75
34	B	304	DD6	C12-C11-C10	-2.12	119.96	122.92
34	D	303	DD6	C8-C6-C5	-2.11	115.70	118.94
36	D	307	CLA	CGD-CBD-CAD	2.11	117.58	110.73
36	A	306	CLA	C3D-C4D-ND	2.11	113.66	110.24
36	D	312	CLA	CHD-C1D-ND	-2.11	122.51	124.45
36	E	317	CLA	CHD-C1D-ND	-2.11	122.51	124.45
35	W	202	A86	C19-C18-C17	-2.11	106.69	110.77
35	E	307	A86	C19-C18-C17	-2.11	106.69	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	314	KC1	CMB-C2B-C1B	2.11	128.44	124.71
36	a	804	CLA	C1-C2-C3	2.11	129.70	126.04
35	R	301	A86	C41-C32-C31	2.11	112.36	110.47
41	G	301	LHG	C18-C17-C16	-2.11	103.70	114.42
37	G	308	KC1	O2D-CGD-O1D	-2.11	119.71	123.84
36	l	204	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
36	a	828	CLA	O2D-CGD-CBD	2.11	115.02	111.27
34	J	304	DD6	C25-C26-C27	-2.11	120.45	126.58
36	E	316	CLA	CMC-C2C-C1C	-2.11	121.83	125.04
36	b	839	CLA	C3A-C2A-C1A	2.11	104.50	101.34
36	a	816	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
38	A	315	SQD	O9-S-C6	2.11	109.45	106.94
37	G	317	KC1	C4D-C3D-CAD	2.11	111.22	107.81
36	M	311	CLA	CHB-C4A-NA	2.11	127.43	124.51
36	a	831	CLA	CHB-C4A-NA	2.11	127.43	124.51
35	E	305	A86	C19-C18-C17	-2.11	106.70	110.77
36	H	305	CLA	C2D-C1D-ND	-2.11	108.55	110.10
36	C	207	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
36	Q	308	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
36	H	310	CLA	CGD-CBD-CAD	2.11	117.57	110.73
36	T	312	CLA	C3A-C2A-C1A	2.11	104.50	101.34
34	A	304	DD6	C25-C24-C1	-2.11	120.49	126.42
35	G	305	A86	C36-C31-C32	2.11	121.79	119.70
36	U	308	CLA	C1-C2-C3	-2.11	122.40	126.04
36	K	309	CLA	O1D-CGD-CBD	2.11	128.80	124.48
36	J	315	CLA	CMA-C3A-C2A	-2.11	111.18	116.10
36	b	839	CLA	O2D-CGD-CBD	2.11	115.01	111.27
36	J	309	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
37	T	315	KC1	O2D-CGD-O1D	-2.11	119.72	123.84
44	f	801	BCR	C40-C30-C25	2.11	113.72	110.30
36	b	813	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
35	J	301	A86	C41-C32-C31	-2.11	108.59	110.47
36	Q	308	CLA	C2D-C1D-ND	-2.11	108.55	110.10
35	T	303	A86	O4-C34-C35	-2.11	102.35	107.59
34	D	304	DD6	C25-C24-C1	-2.11	120.50	126.42
35	L	304	A86	C9-C10-C11	-2.11	120.42	126.61
36	L	309	CLA	O1D-CGD-CBD	2.11	128.79	124.48
36	a	805	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
36	P	310	CLA	C11-C12-C13	-2.10	109.12	115.92
36	D	310	CLA	C3A-C2A-C1A	2.10	104.49	101.34
44	h	201	BCR	C11-C10-C9	-2.10	124.31	127.31
36	a	809	CLA	O2A-CGA-O1A	-2.10	118.28	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	306	CLA	C2C-C1C-NC	-2.10	108.00	109.97
36	b	805	CLA	CHA-C4D-ND	2.10	136.90	132.50
37	G	317	KC1	CAA-CBA-CGA	-2.10	116.45	127.26
36	j	101	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
36	F	312	CLA	C3A-C2A-C1A	2.10	104.49	101.34
36	b	840	CLA	O2D-CGD-CBD	2.10	115.01	111.27
35	B	303	A86	C41-C32-C40	2.10	114.98	108.53
35	T	301	A86	C25-C24-C1	-2.10	120.51	126.42
35	U	303	A86	C7-C6-C5	-2.10	119.98	122.92
36	a	817	CLA	C6-C7-C8	-2.10	109.13	115.92
36	I	311	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
36	P	314	CLA	C6-C7-C8	-2.10	109.13	115.92
36	V	307	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
36	F	314	CLA	C2A-C1A-CHA	2.10	127.53	123.86
34	P	305	DD6	C25-C26-C27	-2.10	120.48	126.58
35	U	304	A86	C8-C6-C5	2.10	122.16	118.94
36	b	840	CLA	C11-C12-C13	-2.10	109.13	115.92
35	T	303	A86	C9-C8-C6	-2.10	120.52	126.42
36	K	310	CLA	CHD-C4C-C3C	-2.10	121.75	124.84
35	S	308	A86	C7-C6-C5	-2.10	119.98	122.92
34	A	303	DD6	C25-C26-C27	-2.10	120.49	126.58
36	D	310	CLA	O2D-CGD-CBD	2.10	115.00	111.27
36	a	820	CLA	O2D-CGD-CBD	2.10	115.00	111.27
35	T	301	A86	C7-C6-C5	-2.10	119.98	122.92
36	G	309	CLA	C4D-CHA-C1A	-2.10	118.70	121.25
35	K	302	A86	C7-C6-C5	-2.10	119.98	122.92
36	a	823	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
36	C	211	CLA	CHD-C1D-ND	-2.10	122.53	124.45
35	L	304	A86	C10-C9-C8	-2.10	116.68	123.22
35	H	301	A86	C23-C16-C22	-2.10	104.28	107.37
35	F	301	A86	C12-C11-C13	2.09	119.54	116.02
36	b	805	CLA	C2A-C1A-CHA	2.09	127.52	123.86
36	f	802	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
35	Q	316	A86	O1-C20-C19	2.09	114.95	113.38
36	K	311	CLA	CHA-C1A-NA	-2.09	121.60	126.40
36	b	822	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
35	B	303	A86	C23-C16-C22	2.09	110.46	107.37
35	O	319	A86	C40-C32-C31	2.09	112.34	110.47
36	b	822	CLA	C2D-C1D-ND	-2.09	108.56	110.10
34	H	303	DD6	C12-C11-C10	-2.09	119.99	122.92
35	X	305	A86	C28-C27-C26	-2.09	119.99	122.92
36	O	309	CLA	O2A-CGA-O1A	-2.09	118.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	U	302	A86	C36-C31-C32	-2.09	117.62	119.70
36	E	314	CLA	CHD-C4C-NC	2.09	127.50	124.20
35	S	303	A86	C33-C32-C31	-2.09	107.18	109.21
35	J	305	A86	C4-C3-C2	-2.09	119.19	123.47
41	I	208	LHG	C5-O7-C7	-2.09	112.64	117.79
36	O	310	CLA	O2D-CGD-CBD	2.09	114.98	111.27
35	N	304	A86	O4-C38-O5	-2.09	118.81	122.96
36	X	309	CLA	C1D-ND-C4D	-2.09	104.85	106.33
36	L	314	CLA	C2A-C1A-CHA	2.09	127.51	123.86
34	D	301	DD6	C25-C24-C1	-2.09	120.54	126.42
36	O	312	CLA	C2A-C1A-CHA	2.09	125.95	122.71
36	f	804	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
34	S	307	DD6	C7-C6-C8	2.09	121.37	118.08
36	b	827	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
34	D	304	DD6	C-C1-C2	-2.09	120.00	122.92
35	H	304	A86	C19-C18-C17	-2.09	106.74	110.77
36	K	308	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
36	Q	309	CLA	O2D-CGD-CBD	2.09	114.98	111.27
37	M	317	KC1	CAA-CBA-CGA	-2.09	116.53	127.26
35	S	304	A86	C-C1-C2	-2.09	120.00	122.92
36	b	828	CLA	C16-C15-C13	-2.09	109.17	115.92
36	K	308	CLA	CAC-C3C-C4C	2.09	127.52	124.81
35	J	301	A86	O1-C15-C20	-2.09	57.36	59.40
36	I	201	CLA	C4-C3-C5	2.09	118.78	115.27
36	a	835	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
36	T	312	CLA	CAC-C3C-C4C	2.09	127.52	124.81
36	a	826	CLA	C3A-C2A-C1A	2.09	104.47	101.34
35	X	305	A86	O4-C38-O5	-2.09	118.82	122.96
34	E	301	DD6	C12-C11-C10	-2.09	120.00	122.92
36	a	826	CLA	C6-C5-C3	2.09	118.93	113.45
34	j	103	DD6	C32-C33-C34	-2.09	108.93	113.64
36	b	835	CLA	CHD-C1D-ND	-2.09	122.54	124.45
36	J	311	CLA	CHA-C4D-ND	2.09	136.86	132.50
36	E	310	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
34	J	304	DD6	C3-C4-C5	-2.08	119.20	123.47
36	F	317	CLA	C1D-ND-C4D	-2.08	104.85	106.33
44	h	201	BCR	C24-C23-C22	-2.08	123.08	126.23
34	D	303	DD6	C25-C24-C1	-2.08	120.56	126.42
36	a	824	CLA	CBA-CAA-C2A	2.08	120.02	113.86
34	H	302	DD6	C20-C19-C18	-2.08	108.63	112.75
37	X	311	KC1	C4D-C3D-CAD	2.08	111.17	107.81
35	L	307	A86	C33-C32-C31	-2.08	107.19	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	817	CLA	C3A-C2A-C1A	2.08	104.46	101.34
35	Q	304	A86	C20-C19-C18	2.08	116.87	112.75
36	I	308	CLA	C2D-C1D-ND	2.08	111.64	110.10
36	R	320	CLA	CHA-C4D-ND	2.08	136.86	132.50
36	P	311	CLA	CBC-CAC-C3C	2.08	118.17	112.43
44	j	107	BCR	C30-C25-C26	-2.08	119.68	122.61
36	a	827	CLA	CHD-C1D-ND	-2.08	122.54	124.45
36	b	814	CLA	CHD-C1D-ND	-2.08	122.54	124.45
34	a	849	DD6	C4-C3-C2	-2.08	119.21	123.47
36	P	312	CLA	O2D-CGD-CBD	2.08	114.97	111.27
36	N	310	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
36	O	309	CLA	C2D-C1D-ND	-2.08	108.57	110.10
35	T	303	A86	O4-C34-C33	2.08	112.78	107.59
36	Q	309	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
36	a	823	CLA	C3A-C2A-C1A	2.08	104.46	101.34
35	K	306	A86	C9-C8-C6	-2.08	120.57	126.42
36	a	839	CLA	CHD-C1D-ND	-2.08	122.54	124.45
36	R	312	CLA	C3A-C2A-C1A	2.08	104.45	101.34
36	S	319	CLA	CAA-C2A-C1A	2.08	118.79	111.97
36	O	309	CLA	CBC-CAC-C3C	2.08	118.16	112.43
35	M	304	A86	C28-C27-C26	-2.08	120.01	122.92
35	O	305	A86	C24-C1-C2	2.08	122.13	118.94
36	E	312	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
36	U	310	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
36	b	832	CLA	O2D-CGD-CBD	2.08	114.96	111.27
35	L	301	A86	C9-C8-C6	-2.08	120.58	126.42
40	b	849	DGD	C7A-C6A-C5A	-2.08	103.88	114.42
36	W	209	CLA	CHA-C1A-NA	-2.08	121.64	126.40
36	a	848	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
36	a	806	CLA	C2A-C3A-C4A	2.08	105.22	101.87
36	b	841	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
36	H	308	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
36	a	801	CLA	O2A-C1-C2	-2.08	103.18	108.64
36	j	102	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
35	V	302	A86	C20-C19-C18	2.08	116.86	112.75
36	b	819	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
34	P	305	DD6	C7-C6-C5	-2.08	120.02	122.92
34	A	304	DD6	C12-C11-C10	-2.08	120.02	122.92
35	K	301	A86	C41-C32-C31	-2.07	108.61	110.47
36	Q	308	CLA	CBC-CAC-C3C	2.07	118.15	112.43
35	S	308	A86	C4-C3-C2	-2.07	119.22	123.47
35	W	203	A86	C14-C15-C16	-2.07	110.81	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	303	DD6	C25-C26-C27	-2.07	120.56	126.58
35	R	301	A86	C9-C10-C11	-2.07	120.51	126.61
35	J	306	A86	C26-C25-C24	-2.07	116.75	123.22
36	O	316	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
40	b	849	DGD	CBB-CAB-C9B	-2.07	103.90	114.42
36	b	828	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
44	h	201	BCR	C7-C8-C9	-2.07	123.10	126.23
34	D	303	DD6	C14-C13-C11	-2.07	122.31	125.53
37	J	314	KC1	C4D-C3D-CAD	2.07	111.16	107.81
35	N	320	A86	C9-C8-C6	-2.07	120.60	126.42
36	b	841	CLA	C16-C15-C13	-2.07	109.22	115.92
44	l	203	BCR	C24-C23-C22	-2.07	123.11	126.23
34	S	307	DD6	C10-C9-C8	-2.07	116.75	123.22
36	K	311	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
36	J	316	CLA	C2D-C1D-ND	-2.07	108.58	110.10
37	W	217	KC1	C4D-C3D-CAD	2.07	111.15	107.81
34	G	303	DD6	C12-C11-C13	2.07	121.34	118.08
36	a	822	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
36	E	308	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
36	b	817	CLA	C1C-C2C-C3C	2.07	109.13	106.96
36	b	835	CLA	C2A-C1A-CHA	2.07	127.48	123.86
36	X	306	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
34	G	303	DD6	C37-C36-C35	2.07	118.19	114.36
36	O	316	CLA	CAC-C3C-C4C	2.07	127.50	124.81
36	T	312	CLA	CHA-C1A-NA	-2.07	121.66	126.40
35	E	305	A86	C26-C25-C24	-2.07	116.76	123.22
36	Q	310	CLA	CBA-CAA-C2A	2.07	119.97	113.86
36	J	308	CLA	CMD-C2D-C1D	2.07	128.36	124.71
34	P	305	DD6	O1-C20-C19	-2.07	111.83	113.38
36	B	309	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
36	C	207	CLA	C3D-C4D-ND	2.07	113.58	110.24
36	P	311	CLA	C2D-C1D-ND	-2.07	108.58	110.10
34	C	201	DD6	C25-C24-C1	-2.07	120.61	126.42
36	a	809	CLA	O2D-CGD-CBD	2.07	114.94	111.27
35	F	305	A86	C3-C4-C5	-2.07	119.24	123.47
35	V	301	A86	C19-C18-C17	-2.07	106.78	110.77
36	b	805	CLA	C6-C5-C3	2.07	118.88	113.45
35	F	306	A86	C3-C4-C5	-2.07	119.24	123.47
36	C	208	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
35	N	320	A86	C20-C19-C18	2.07	116.84	112.75
36	X	307	CLA	C3C-C4C-NC	-2.07	108.25	110.57
34	W	204	DD6	C-C1-C2	-2.07	120.03	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	R	309	A86	C20-C19-C18	2.07	116.84	112.75
35	M	301	A86	C25-C24-C1	-2.07	120.61	126.42
40	L	302	DGD	O2G-C1B-O1B	-2.07	118.71	123.70
35	T	303	A86	C4-C3-C2	-2.07	119.24	123.47
36	O	316	CLA	CHA-C4D-ND	-2.07	128.18	132.50
36	K	312	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
36	a	848	CLA	CMB-C2B-C1B	-2.07	125.29	128.46
35	B	301	A86	C25-C26-C27	-2.06	124.36	127.31
35	N	302	A86	C26-C25-C24	-2.06	116.77	123.22
35	N	305	A86	O1-C20-C19	2.06	114.93	113.38
36	l	204	CLA	C4C-C3C-C2C	-2.06	103.89	106.90
36	D	312	CLA	O1D-CGD-CBD	2.06	128.71	124.48
34	G	303	DD6	C32-C33-C34	-2.06	108.98	113.64
36	R	321	CLA	O2D-CGD-CBD	2.06	114.94	111.27
36	H	308	CLA	C1-C2-C3	-2.06	122.47	126.04
44	h	201	BCR	C40-C30-C39	-2.06	102.19	108.53
34	D	305	DD6	C21-C20-C15	-2.06	118.80	122.26
44	b	843	BCR	C16-C15-C14	-2.06	119.25	123.47
36	W	215	CLA	C2A-C1A-CHA	2.06	127.47	123.86
36	R	319	CLA	C2A-C1A-CHA	2.06	127.47	123.86
36	a	829	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
35	I	301	A86	C19-C18-C17	-2.06	106.79	110.77
36	H	310	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
36	X	309	CLA	CBA-CAA-C2A	-2.06	107.78	113.86
34	L	305	DD6	C7-C6-C8	2.06	121.33	118.08
34	G	303	DD6	C10-C9-C8	-2.06	116.78	123.22
36	C	208	CLA	C4-C3-C5	2.06	118.74	115.27
36	J	307	CLA	CHA-C1A-NA	-2.06	121.68	126.40
34	K	304	DD6	C7-C6-C5	-2.06	120.04	122.92
34	S	307	DD6	C12-C11-C13	2.06	121.32	118.08
36	C	205	CLA	O2D-CGD-CBD	2.06	114.93	111.27
36	F	310	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
35	A	316	A86	C7-C6-C5	-2.06	120.04	122.92
35	H	304	A86	C-C1-C2	-2.06	120.04	122.92
36	b	809	CLA	O1D-CGD-CBD	2.06	128.70	124.48
36	l	202	CLA	O2A-C1-C2	-2.06	103.22	108.64
36	A	306	CLA	C2A-C3A-C4A	2.06	105.19	101.87
35	W	202	A86	C23-C16-C22	-2.06	104.33	107.37
36	b	836	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
44	b	846	BCR	C29-C30-C25	2.06	113.65	110.48
36	P	318	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
35	N	303	A86	C34-O4-C38	2.06	121.73	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	O	310	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
36	A	308	CLA	C3A-C2A-C1A	2.06	104.42	101.34
35	D	302	A86	C19-C18-C17	-2.06	106.80	110.77
34	j	103	DD6	C37-C36-C35	2.06	118.16	114.36
37	N	314	KC1	O2D-CGD-O1D	-2.06	119.82	123.84
36	L	308	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
36	a	813	CLA	C2A-C3A-C4A	2.06	105.19	101.87
36	a	841	CLA	C1B-CHB-C4A	-2.06	126.05	130.12
36	a	820	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
35	L	306	A86	C3-C4-C5	-2.05	119.27	123.47
36	a	821	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
36	a	838	CLA	O2D-CGD-CBD	2.05	114.92	111.27
35	S	302	A86	C26-C25-C24	-2.05	116.81	123.22
36	a	815	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
36	l	205	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
34	E	304	DD6	C-C1-C2	-2.05	120.05	122.92
34	K	305	DD6	C32-C33-C34	-2.05	109.01	113.64
35	M	302	A86	C40-C32-C31	-2.05	108.64	110.47
36	N	317	CLA	CHD-C1D-ND	-2.05	122.57	124.45
36	N	313	CLA	CHD-C1D-ND	-2.05	122.57	124.45
35	h	204	A86	O4-C38-O5	-2.05	118.89	122.96
36	X	308	CLA	CAC-C3C-C2C	-2.05	124.02	127.53
37	G	317	KC1	C1C-C2C-C3C	-2.05	104.80	106.96
35	X	302	A86	C14-C15-C16	-2.05	110.90	118.75
35	F	304	A86	C26-C25-C24	-2.05	116.82	123.22
40	b	849	DGD	O5E-C6E-C5E	-2.05	104.26	111.29
36	a	801	CLA	C2D-C1D-ND	-2.05	108.59	110.10
36	N	309	CLA	C3A-C2A-C1A	2.05	104.41	101.34
36	P	312	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
36	V	305	CLA	CHB-C4A-NA	2.05	127.35	124.51
35	F	301	A86	O1-C15-C20	-2.05	57.40	59.40
35	W	202	A86	O-C13-C11	-2.05	116.62	121.15
36	N	308	CLA	C4C-C3C-C2C	-2.05	103.91	106.90
36	R	320	CLA	CHA-C1A-NA	-2.05	121.70	126.40
34	W	205	DD6	C-C1-C2	-2.05	120.05	122.92
34	B	304	DD6	C4-C3-C2	-2.05	119.28	123.47
36	L	314	CLA	O2A-CGA-CBA	2.05	118.34	111.91
36	a	817	CLA	CHA-C1A-NA	-2.05	121.71	126.40
36	W	210	CLA	CAC-C3C-C4C	2.05	127.47	124.81
36	S	311	CLA	C2A-C1A-CHA	2.05	127.44	123.86
36	b	840	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
34	D	304	DD6	C15-C14-C13	-2.05	121.66	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	808	CLA	O1D-CGD-CBD	2.05	128.68	124.48
36	b	826	CLA	C1D-ND-C4D	2.05	107.79	106.33
36	W	201	CLA	O2D-CGD-CBD	2.05	114.91	111.27
36	H	307	CLA	CHD-C1D-C2D	2.05	129.78	125.48
35	V	302	A86	C9-C8-C6	-2.05	120.66	126.42
35	G	305	A86	C7-C6-C5	-2.05	120.06	122.92
36	a	834	CLA	C2A-C1A-CHA	2.05	127.44	123.86
44	a	847	BCR	C31-C1-C6	2.05	113.62	110.30
36	K	313	CLA	CHA-C4D-ND	2.05	136.78	132.50
36	b	841	CLA	C4D-CHA-C1A	2.05	123.74	121.25
35	L	319	A86	C4-C3-C2	-2.05	119.28	123.47
36	a	824	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
36	X	309	CLA	O2D-CGD-O1D	-2.05	119.44	124.09
36	l	201	CLA	C3C-C4C-NC	-2.05	108.28	110.57
36	a	830	CLA	C1D-ND-C4D	2.05	107.79	106.33
35	J	301	A86	C9-C10-C11	-2.05	120.59	126.61
36	M	306	CLA	C3B-C4B-NB	-2.05	106.57	109.21
41	f	808	LHG	C5-O7-C7	-2.04	112.76	117.79
35	G	302	A86	C25-C26-C27	-2.04	124.39	127.31
44	b	845	BCR	C15-C16-C17	-2.04	119.29	123.47
36	U	311	CLA	CMD-C2D-C3D	2.04	132.32	127.61
36	U	311	CLA	C2A-C1A-CHA	2.04	127.43	123.86
44	j	107	BCR	C28-C27-C26	-2.04	110.43	114.08
35	G	306	A86	C3-C2-C1	-2.04	124.39	127.31
36	B	306	CLA	CAC-C3C-C4C	2.04	127.46	124.81
35	K	302	A86	C3-C4-C5	-2.04	119.29	123.47
36	B	311	CLA	C1B-CHB-C4A	-2.04	126.07	130.12
35	X	303	A86	C28-C27-C26	-2.04	120.06	122.92
36	C	214	CLA	C2D-C1D-ND	-2.04	108.60	110.10
36	S	319	CLA	C2D-C1D-ND	-2.04	108.60	110.10
36	W	215	CLA	CHB-C4A-NA	2.04	127.33	124.51
36	V	306	CLA	C2A-C1A-CHA	2.04	127.43	123.86
34	H	303	DD6	C-C1-C2	-2.04	120.06	122.92
36	b	822	CLA	CED-O2D-CGD	2.04	120.55	115.94
35	J	303	A86	C9-C8-C6	-2.04	120.68	126.42
36	b	813	CLA	CHB-C4A-NA	2.04	127.33	124.51
35	B	303	A86	C19-C18-C17	-2.04	106.83	110.77
36	O	309	CLA	C1-C2-C3	-2.04	122.51	126.04
35	F	301	A86	C33-C32-C31	-2.04	107.23	109.21
35	J	305	A86	C40-C32-C31	-2.04	108.65	110.47
35	O	302	A86	C4-C3-C2	-2.04	119.30	123.47
36	f	804	CLA	CHC-C1C-C2C	-2.04	121.08	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	828	CLA	O1D-CGD-CBD	2.04	128.66	124.48
35	L	301	A86	C19-C18-C17	-2.04	106.83	110.77
35	F	302	A86	C4-C3-C2	-2.04	119.30	123.47
36	W	214	CLA	C2D-C1D-ND	-2.04	108.60	110.10
36	b	807	CLA	C2A-C1A-CHA	2.04	127.42	123.86
40	b	849	DGD	CAB-C9B-C8B	-2.04	104.07	114.42
35	P	307	A86	C40-C32-C31	-2.04	108.65	110.47
36	j	106	CLA	CHD-C1D-ND	-2.04	122.58	124.45
44	i	103	BCR	C27-C26-C25	2.04	125.69	122.73
36	l	206	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
44	a	845	BCR	C38-C26-C27	-2.04	109.70	113.62
39	a	851	LMT	C1B-O1B-C4'	-2.04	112.92	117.96
36	a	828	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
35	A	316	A86	C26-C25-C24	-2.04	116.86	123.22
34	Q	302	DD6	C12-C11-C10	-2.04	120.07	122.92
34	E	303	DD6	C4-C3-C2	-2.04	119.30	123.47
36	P	311	CLA	C1-C2-C3	-2.04	122.52	126.04
36	S	321	CLA	C3A-C2A-C1A	2.04	104.39	101.34
36	D	307	CLA	CMC-C2C-C1C	-2.04	121.94	125.04
36	V	309	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
36	F	310	CLA	CHD-C1D-ND	-2.04	122.58	124.45
35	S	303	A86	C34-O4-C38	2.04	121.69	117.90
35	E	307	A86	C40-C32-C31	-2.04	108.65	110.47
35	P	303	A86	C4-C3-C2	-2.04	119.30	123.47
35	P	304	A86	O1-C20-C21	-2.04	112.62	115.06
36	a	829	CLA	C2D-C1D-ND	-2.04	108.60	110.10
35	V	301	A86	C25-C24-C1	-2.04	120.70	126.42
36	a	802	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
36	f	802	CLA	C3B-C4B-NB	-2.04	106.58	109.21
36	I	307	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
36	a	812	CLA	C1B-CHB-C4A	-2.04	126.09	130.12
36	W	209	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
36	a	808	CLA	CHA-C1A-NA	-2.03	121.74	126.40
35	J	303	A86	C33-C32-C31	-2.03	107.23	109.21
36	W	207	CLA	C1-O2A-CGA	2.03	121.78	116.44
36	T	309	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
34	M	303	DD6	C14-C13-C11	-2.03	122.38	125.53
36	P	312	CLA	CBA-CAA-C2A	-2.03	107.86	113.86
36	C	211	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
36	V	313	CLA	O2D-CGD-CBD	2.03	114.88	111.27
36	b	817	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
38	A	315	SQD	O7-S-C6	2.03	109.35	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	H	304	A86	C28-C27-C26	-2.03	120.08	122.92
44	I	207	BCR	C31-C1-C6	2.03	113.59	110.30
36	H	312	CLA	C2A-C1A-CHA	2.03	127.41	123.86
36	a	807	CLA	C2A-C1A-CHA	2.03	127.41	123.86
35	C	202	A86	O-C13-C11	-2.03	116.66	121.15
36	b	836	CLA	C2A-C3A-C4A	2.03	105.15	101.87
34	E	301	DD6	C15-C14-C13	-2.03	121.70	125.99
36	U	308	CLA	CGD-CBD-CAD	2.03	117.31	110.73
36	G	311	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
36	B	311	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
35	X	304	A86	C4-C3-C2	-2.03	119.32	123.47
36	O	310	CLA	CBA-CAA-C2A	-2.03	107.88	113.86
36	L	311	CLA	CHD-C1D-ND	-2.03	122.59	124.45
35	G	304	A86	C4-C5-C6	-2.03	124.42	127.31
36	I	204	CLA	C2A-C3A-C4A	2.03	105.14	101.87
36	A	306	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
35	T	301	A86	C9-C8-C6	-2.03	120.72	126.42
36	I	310	CLA	CHD-C1D-ND	-2.03	122.59	124.45
35	O	305	A86	C4-C3-C2	-2.03	119.32	123.47
36	M	306	CLA	C1D-ND-C4D	2.03	107.77	106.33
36	U	310	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
36	O	314	CLA	C2A-C3A-C4A	2.03	104.37	101.78
36	a	835	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
36	a	833	CLA	CMD-C2D-C3D	2.02	132.27	127.61
35	X	304	A86	C41-C32-C31	2.02	112.28	110.47
36	E	315	CLA	C4D-CHA-C1A	-2.02	118.78	121.25
35	M	301	A86	C19-C18-C17	-2.02	106.86	110.77
35	J	303	A86	O-C13-C11	-2.02	116.68	121.15
36	b	812	CLA	C11-C10-C8	-2.02	109.38	115.92
37	M	313	KC1	CAA-CBA-CGA	-2.02	116.86	127.26
36	X	310	CLA	CHA-C4D-ND	2.02	136.73	132.50
36	B	309	CLA	C4D-CHA-C1A	-2.02	118.79	121.25
35	F	306	A86	C33-C32-C31	-2.02	107.25	109.21
35	M	304	A86	C41-C32-C31	-2.02	108.66	110.47
34	E	306	DD6	C25-C26-C27	-2.02	120.71	126.58
34	j	103	DD6	C21-C20-C15	-2.02	118.87	122.26
36	T	311	CLA	C1-C2-C3	-2.02	122.55	126.04
36	a	829	CLA	O1D-CGD-CBD	2.02	128.62	124.48
35	R	306	A86	C9-C10-C11	-2.02	120.66	126.61
36	a	805	CLA	C2A-C1A-CHA	2.02	127.39	123.86
36	J	309	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
36	T	311	CLA	O2A-CGA-O1A	-2.02	118.49	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Q	309	CLA	CBA-CAA-C2A	-2.02	107.90	113.86
35	X	303	A86	O2-C18-C19	-2.02	105.79	109.80
36	K	313	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
37	W	217	KC1	CMD-C2D-C1D	-2.02	125.36	128.46
36	a	818	CLA	CMC-C2C-C1C	-2.02	121.96	125.04
36	M	306	CLA	C2D-C1D-ND	-2.02	108.62	110.10
36	b	801	CLA	CHA-C1A-NA	-2.02	121.77	126.40
36	b	818	CLA	CHA-C1A-NA	-2.02	121.77	126.40
35	O	319	A86	C20-C19-C18	2.02	116.74	112.75
37	R	317	KC1	C4B-C3B-C2B	-2.02	105.09	106.75
42	D	320	LMG	C8-O7-C10	-2.02	112.82	117.79
36	b	812	CLA	CAC-C3C-C2C	-2.02	124.08	127.53
37	A	312	KC1	CAC-C3C-C2C	-2.02	124.08	127.53
44	i	101	BCR	C38-C26-C27	-2.02	109.74	113.62
35	O	305	A86	C26-C25-C24	-2.02	116.92	123.22
36	D	315	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
36	S	320	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
36	S	317	CLA	CHD-C1D-ND	-2.02	122.60	124.45
36	H	311	CLA	CHD-C1D-ND	-2.02	122.60	124.45
35	L	319	A86	C20-C19-C18	2.02	116.74	112.75
34	H	302	DD6	C-C1-C2	-2.02	120.10	122.92
36	D	315	CLA	CBC-CAC-C3C	2.02	117.99	112.43
36	a	814	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
36	H	310	CLA	C3C-C4C-NC	-2.02	108.31	110.57
35	L	306	A86	O3-C36-C37	-2.02	105.81	109.39
36	H	318	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
37	L	315	KC1	C1C-C2C-C3C	-2.01	104.84	106.96
36	a	848	CLA	CHB-C4A-NA	2.01	127.30	124.51
35	J	301	A86	C9-C8-C6	-2.01	120.76	126.42
35	E	302	A86	C-C1-C2	-2.01	120.10	122.92
36	b	812	CLA	O2D-CGD-CBD	2.01	114.85	111.27
36	P	316	CLA	C2A-C3A-C4A	2.01	104.35	101.78
36	f	803	CLA	CHB-C4A-NA	2.01	127.30	124.51
36	W	214	CLA	CHA-C1A-NA	-2.01	121.79	126.40
35	W	203	A86	C4-C3-C2	-2.01	119.35	123.47
36	T	314	CLA	C2A-C1A-CHA	2.01	127.38	123.86
35	X	314	A86	C28-C27-C26	-2.01	120.10	122.92
36	b	801	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
44	l	203	BCR	C31-C1-C6	2.01	113.56	110.30
34	O	304	DD6	C-C1-C2	-2.01	120.11	122.92
36	S	312	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
34	A	301	DD6	C25-C24-C1	-2.01	120.77	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	316	CLA	C2D-C1D-ND	-2.01	108.62	110.10
37	U	312	KC1	C1C-C2C-C3C	-2.01	104.84	106.96
35	Q	301	A86	O1-C20-C21	-2.01	112.65	115.06
44	a	844	BCR	C30-C25-C26	-2.01	119.78	122.61
35	V	302	A86	C4-C3-C2	-2.01	119.36	123.47
36	X	306	CLA	CHA-C4D-ND	2.01	136.70	132.50
34	E	304	DD6	C37-C36-C35	2.01	118.08	114.36
35	S	304	A86	C14-C15-C16	2.01	126.45	118.75
35	O	303	A86	O1-C20-C21	-2.01	112.65	115.06
35	B	303	A86	C7-C6-C5	-2.01	120.11	122.92
35	X	303	A86	C7-C6-C5	-2.01	120.11	122.92
36	D	307	CLA	CMC-C2C-C3C	2.01	131.57	126.12
36	L	311	CLA	CHA-C1A-NA	-2.01	121.80	126.40
34	A	304	DD6	C15-C14-C13	-2.01	121.75	125.99
35	R	306	A86	C12-C11-C13	2.01	119.40	116.02
36	a	833	CLA	C2A-C1A-CHA	2.01	127.37	123.86
35	T	301	A86	C28-C27-C26	-2.01	120.11	122.92
37	W	213	KC1	C3D-CAD-CBD	-2.01	104.96	107.61
44	f	806	BCR	C33-C5-C6	-2.01	122.27	124.53
36	l	205	CLA	C2A-C1A-CHA	2.01	127.37	123.86
35	U	304	A86	C4-C3-C2	-2.01	119.36	123.47
36	F	314	CLA	CHA-C1A-NA	-2.01	121.80	126.40
37	L	315	KC1	C2A-C1A-CHA	-2.01	120.80	127.44
35	V	304	A86	C33-C32-C31	-2.01	107.26	109.21
35	F	307	A86	C28-C27-C26	-2.01	120.11	122.92
37	A	312	KC1	CMC-C2C-C1C	2.01	128.10	125.04
36	U	305	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
36	P	301	CLA	C1-C2-C3	2.01	129.51	126.04
36	G	315	CLA	C3D-C4D-ND	2.01	113.48	110.24
36	Q	312	CLA	C2A-C3A-C4A	2.01	104.34	101.78
36	a	848	CLA	CAC-C3C-C4C	2.01	127.41	124.81
36	X	307	CLA	CBA-CAA-C2A	2.01	119.78	113.86
35	O	319	A86	C3-C4-C5	2.01	127.58	123.47
36	a	817	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
35	A	302	A86	O4-C38-C39	2.01	114.78	111.09
35	F	304	A86	C41-C32-C31	-2.01	108.68	110.47
36	X	307	CLA	CHD-C1D-ND	-2.01	122.61	124.45
36	N	310	CLA	CHA-C4D-ND	2.01	136.69	132.50
36	b	828	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
36	a	818	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
36	b	827	CLA	CHA-C1A-NA	-2.00	121.81	126.40
34	H	302	DD6	C25-C26-C27	-2.00	120.76	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	H	302	DD6	C3-C4-C5	-2.00	119.37	123.47
36	R	318	CLA	CMA-C3A-C2A	-2.00	111.42	116.10
35	E	302	A86	C4-C3-C2	-2.00	119.37	123.47
36	f	805	CLA	O1D-CGD-CBD	2.00	128.58	124.48
36	E	314	CLA	CMC-C2C-C1C	2.00	128.09	125.04
35	T	304	A86	C28-C27-C26	-2.00	120.12	122.92
35	B	301	A86	C40-C32-C31	-2.00	108.68	110.47
44	b	847	BCR	C10-C11-C12	-2.00	116.97	123.22
36	a	804	CLA	C1D-ND-C4D	2.00	107.76	106.33
35	T	301	A86	C-C1-C2	-2.00	120.12	122.92
36	Q	308	CLA	C1-C2-C3	-2.00	122.58	126.04
36	a	827	CLA	C3A-C2A-C1A	2.00	104.34	101.34
35	H	301	A86	C34-O4-C38	-2.00	114.17	117.90
35	C	203	A86	C10-C9-C8	-2.00	116.97	123.22
36	V	308	CLA	CHD-C1D-ND	-2.00	122.61	124.45
36	a	812	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
35	S	308	A86	C19-C18-C17	-2.00	106.91	110.77
36	K	311	CLA	CMA-C3A-C4A	-2.00	106.40	111.77
35	V	302	A86	C9-C10-C11	-2.00	120.73	126.61

All (321) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	A	305	CLA	ND
36	A	306	CLA	C8
36	A	306	CLA	ND
36	A	307	CLA	ND
36	A	308	CLA	ND
36	A	309	CLA	ND
36	A	310	CLA	ND
36	A	311	CLA	ND
36	A	313	CLA	ND
36	A	314	CLA	ND
36	B	305	CLA	ND
36	B	306	CLA	ND
36	B	307	CLA	ND
36	B	308	CLA	ND
36	B	309	CLA	ND
36	B	311	CLA	ND
36	C	205	CLA	ND
36	C	206	CLA	ND
36	C	207	CLA	C8

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Mol	Chain	Res	Type	Atom
36	C	208	CLA	ND
36	C	209	CLA	ND
36	C	210	CLA	ND
36	C	211	CLA	ND
36	C	212	CLA	ND
36	C	214	CLA	ND
36	D	306	CLA	ND
36	D	307	CLA	ND
36	D	308	CLA	ND
36	D	309	CLA	C8
36	D	309	CLA	ND
36	D	310	CLA	ND
36	D	312	CLA	ND
36	D	313	CLA	ND
36	D	315	CLA	ND
36	D	316	CLA	ND
36	D	317	CLA	ND
36	E	308	CLA	ND
36	E	311	CLA	ND
36	E	312	CLA	ND
36	E	313	CLA	C8
36	E	313	CLA	ND
36	E	314	CLA	ND
36	E	315	CLA	C8
36	E	315	CLA	ND
36	E	316	CLA	ND
36	E	317	CLA	ND
36	F	309	CLA	ND
36	F	310	CLA	ND
36	F	311	CLA	ND
36	F	312	CLA	ND
36	F	313	CLA	ND
36	F	314	CLA	ND
36	F	316	CLA	ND
36	F	317	CLA	C8
36	F	317	CLA	ND
36	G	309	CLA	ND
36	G	310	CLA	ND
36	G	311	CLA	ND
36	G	312	CLA	ND
36	G	313	CLA	ND
36	G	314	CLA	ND

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Mol	Chain	Res	Type	Atom
36	G	315	CLA	C8
36	G	315	CLA	ND
36	G	316	CLA	ND
36	G	319	CLA	ND
36	H	305	CLA	ND
36	H	306	CLA	ND
36	H	307	CLA	ND
36	H	308	CLA	ND
36	H	309	CLA	ND
36	H	310	CLA	ND
36	H	311	CLA	ND
36	H	312	CLA	ND
36	H	314	CLA	ND
36	H	315	CLA	ND
36	H	316	CLA	ND
36	H	317	CLA	ND
36	H	318	CLA	ND
36	I	305	CLA	C13
36	I	305	CLA	ND
36	I	306	CLA	C8
36	I	306	CLA	ND
36	I	307	CLA	ND
36	I	308	CLA	C8
36	I	309	CLA	ND
36	I	310	CLA	ND
36	I	311	CLA	ND
36	I	312	CLA	ND
36	I	313	CLA	ND
36	I	314	CLA	ND
36	J	307	CLA	ND
36	J	309	CLA	ND
36	J	310	CLA	ND
36	J	311	CLA	ND
36	J	312	CLA	ND
36	J	313	CLA	ND
36	J	315	CLA	ND
36	J	316	CLA	ND
36	J	317	CLA	ND
36	K	307	CLA	C8
36	K	307	CLA	ND
36	K	308	CLA	ND
36	K	309	CLA	ND

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Mol	Chain	Res	Type	Atom
36	K	310	CLA	C8
36	K	310	CLA	ND
36	K	311	CLA	ND
36	K	312	CLA	ND
36	K	313	CLA	ND
36	K	315	CLA	ND
36	K	316	CLA	ND
36	L	308	CLA	C8
36	L	308	CLA	ND
36	L	309	CLA	ND
36	L	310	CLA	ND
36	L	311	CLA	ND
36	L	313	CLA	ND
36	L	314	CLA	ND
36	L	316	CLA	ND
36	L	320	CLA	ND
36	M	306	CLA	ND
36	M	307	CLA	ND
36	M	308	CLA	ND
36	M	309	CLA	ND
36	M	310	CLA	ND
36	M	311	CLA	ND
36	M	312	CLA	ND
36	M	314	CLA	ND
36	M	316	CLA	ND
36	N	307	CLA	ND
36	N	308	CLA	ND
36	N	309	CLA	ND
36	N	310	CLA	ND
36	N	311	CLA	ND
36	N	312	CLA	ND
36	N	313	CLA	ND
36	N	316	CLA	ND
36	N	317	CLA	ND
36	N	318	CLA	ND
36	N	319	CLA	ND
36	O	306	CLA	ND
36	O	307	CLA	ND
36	O	308	CLA	ND
36	O	309	CLA	ND
36	O	310	CLA	ND
36	O	311	CLA	ND

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Mol	Chain	Res	Type	Atom
36	O	314	CLA	ND
36	O	316	CLA	C8
36	P	301	CLA	ND
36	P	308	CLA	ND
36	P	309	CLA	ND
36	P	310	CLA	ND
36	P	311	CLA	ND
36	P	312	CLA	ND
36	P	313	CLA	ND
36	P	316	CLA	ND
36	P	318	CLA	ND
36	P	319	CLA	ND
36	Q	305	CLA	ND
36	Q	306	CLA	ND
36	Q	307	CLA	ND
36	Q	308	CLA	ND
36	Q	309	CLA	ND
36	Q	312	CLA	ND
36	Q	314	CLA	ND
36	R	310	CLA	ND
36	R	311	CLA	ND
36	R	312	CLA	ND
36	R	313	CLA	ND
36	R	314	CLA	ND
36	R	315	CLA	ND
36	R	316	CLA	ND
36	R	318	CLA	ND
36	R	319	CLA	ND
36	R	320	CLA	ND
36	R	322	CLA	ND
36	S	309	CLA	ND
36	S	310	CLA	ND
36	S	311	CLA	ND
36	S	313	CLA	ND
36	S	315	CLA	ND
36	S	317	CLA	ND
36	S	318	CLA	ND
36	S	319	CLA	ND
36	T	308	CLA	ND
36	T	309	CLA	ND
36	T	311	CLA	ND
36	T	312	CLA	ND

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Mol	Chain	Res	Type	Atom
36	T	313	CLA	ND
36	T	314	CLA	ND
36	T	316	CLA	ND
36	W	201	CLA	ND
36	W	206	CLA	ND
36	W	207	CLA	ND
36	W	208	CLA	ND
36	W	209	CLA	ND
36	W	210	CLA	ND
36	W	211	CLA	ND
36	W	215	CLA	ND
36	W	216	CLA	ND
36	W	218	CLA	ND
36	X	306	CLA	ND
36	X	308	CLA	ND
36	X	310	CLA	ND
36	X	312	CLA	ND
36	a	801	CLA	ND
36	a	802	CLA	ND
36	a	802	CLA	C8
36	a	803	CLA	ND
36	a	804	CLA	ND
36	a	805	CLA	ND
36	a	806	CLA	C8
36	a	806	CLA	ND
36	a	807	CLA	ND
36	a	808	CLA	ND
36	a	809	CLA	ND
36	a	810	CLA	ND
36	a	811	CLA	ND
36	a	812	CLA	ND
36	a	813	CLA	ND
36	a	814	CLA	ND
36	a	815	CLA	ND
36	a	816	CLA	C8
36	a	817	CLA	ND
36	a	818	CLA	ND
36	a	819	CLA	ND
36	a	820	CLA	ND
36	a	821	CLA	ND
36	a	822	CLA	ND
36	a	823	CLA	C8

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Mol	Chain	Res	Type	Atom
36	a	823	CLA	ND
36	a	824	CLA	ND
36	a	825	CLA	C8
36	a	825	CLA	ND
36	a	826	CLA	ND
36	a	827	CLA	ND
36	a	828	CLA	ND
36	a	829	CLA	ND
36	a	831	CLA	ND
36	a	832	CLA	ND
36	a	833	CLA	ND
36	a	834	CLA	ND
36	a	835	CLA	ND
36	a	836	CLA	ND
36	a	837	CLA	ND
36	a	838	CLA	ND
36	a	839	CLA	ND
36	a	841	CLA	ND
36	a	848	CLA	C8
36	a	848	CLA	ND
36	b	801	CLA	ND
36	b	802	CLA	ND
36	b	805	CLA	ND
36	b	806	CLA	ND
36	b	807	CLA	ND
36	b	808	CLA	ND
36	b	809	CLA	ND
36	b	810	CLA	ND
36	b	811	CLA	ND
36	b	812	CLA	ND
36	b	813	CLA	ND
36	b	814	CLA	ND
36	b	815	CLA	ND
36	b	816	CLA	C8
36	b	816	CLA	ND
36	b	817	CLA	C8
36	b	817	CLA	ND
36	b	819	CLA	ND
36	b	820	CLA	ND
36	b	821	CLA	ND
36	b	822	CLA	ND
36	b	823	CLA	ND

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Mol	Chain	Res	Type	Atom
36	b	824	CLA	ND
36	b	825	CLA	ND
36	b	826	CLA	ND
36	b	827	CLA	ND
36	b	828	CLA	ND
36	b	829	CLA	ND
36	b	830	CLA	ND
36	b	831	CLA	ND
36	b	832	CLA	ND
36	b	833	CLA	ND
36	b	834	CLA	ND
36	b	835	CLA	ND
36	b	836	CLA	C8
36	b	837	CLA	ND
36	b	838	CLA	ND
36	b	839	CLA	ND
36	b	840	CLA	ND
36	b	841	CLA	ND
36	f	802	CLA	ND
36	f	803	CLA	C8
36	f	803	CLA	ND
36	f	804	CLA	C8
36	f	804	CLA	ND
36	f	805	CLA	ND
36	i	102	CLA	ND
36	j	101	CLA	ND
36	j	102	CLA	C8
36	j	106	CLA	ND
36	l	201	CLA	ND
36	l	202	CLA	ND
36	l	205	CLA	C8
36	l	205	CLA	ND
36	l	206	CLA	ND
36	h	203	CLA	ND
36	U	305	CLA	ND
36	U	306	CLA	C8
36	U	307	CLA	ND
36	U	308	CLA	ND
36	U	310	CLA	ND
36	U	311	CLA	ND
36	U	313	CLA	ND
36	V	305	CLA	ND

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Mol	Chain	Res	Type	Atom
36	V	306	CLA	ND
36	V	307	CLA	ND
36	V	308	CLA	ND
36	V	309	CLA	ND
36	V	310	CLA	ND
36	V	311	CLA	ND
36	V	313	CLA	ND
36	V	314	CLA	C8

All (5822) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	301	DD6	C10-C11-C13-C14
34	A	301	DD6	C12-C11-C13-C14
34	A	301	DD6	C13-C14-C15-C20
34	A	301	DD6	C13-C14-C15-O1
34	A	303	DD6	C10-C11-C13-C14
34	A	303	DD6	C12-C11-C13-C14
34	A	303	DD6	C13-C14-C15-C16
34	A	303	DD6	C13-C14-C15-C20
34	A	303	DD6	C13-C14-C15-O1
34	A	304	DD6	C10-C11-C13-C14
34	A	304	DD6	C12-C11-C13-C14
34	A	304	DD6	C13-C14-C15-C20
34	A	304	DD6	C13-C14-C15-O1
34	B	302	DD6	C10-C11-C13-C14
34	B	302	DD6	C12-C11-C13-C14
34	B	302	DD6	C13-C14-C15-O1
34	C	201	DD6	C13-C14-C15-C16
34	C	201	DD6	C13-C14-C15-C20
34	C	201	DD6	C13-C14-C15-O1
34	C	201	DD6	C5-C6-C8-C9
34	C	201	DD6	C7-C6-C8-C9
34	D	301	DD6	C10-C11-C13-C14
34	D	301	DD6	C12-C11-C13-C14
34	D	301	DD6	C13-C14-C15-C16
34	D	301	DD6	C13-C14-C15-C20
34	D	301	DD6	C3-C4-C5-C6
34	D	301	DD6	C5-C6-C8-C9
34	D	301	DD6	C7-C6-C8-C9
34	D	303	DD6	C-C1-C2-C3
34	D	303	DD6	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
34	D	303	DD6	C2-C1-C24-C25
34	D	303	DD6	C13-C14-C15-O1
34	D	304	DD6	C13-C14-C15-C20
34	D	304	DD6	C5-C6-C8-C9
34	D	304	DD6	C7-C6-C8-C9
34	E	301	DD6	C13-C14-C15-C16
34	E	303	DD6	C10-C11-C13-C14
34	E	303	DD6	C13-C14-C15-C16
34	E	303	DD6	C13-C14-C15-C20
34	E	303	DD6	C5-C6-C8-C9
34	E	303	DD6	C7-C6-C8-C9
34	E	304	DD6	C13-C14-C15-C16
34	E	304	DD6	C13-C14-C15-C20
34	F	303	DD6	C10-C11-C13-C14
34	F	303	DD6	C12-C11-C13-C14
34	F	303	DD6	C13-C14-C15-C16
34	F	303	DD6	C13-C14-C15-C20
34	F	303	DD6	C13-C14-C15-O1
34	G	303	DD6	C13-C14-C15-C16
34	G	303	DD6	C13-C14-C15-C20
34	H	302	DD6	C13-C14-C15-O1
34	H	303	DD6	C10-C11-C13-C14
34	H	303	DD6	C12-C11-C13-C14
34	H	303	DD6	C13-C14-C15-C20
34	H	303	DD6	C13-C14-C15-O1
34	H	303	DD6	C5-C6-C8-C9
34	H	303	DD6	C7-C6-C8-C9
34	I	303	DD6	C10-C11-C13-C14
34	I	303	DD6	C12-C11-C13-C14
34	I	303	DD6	C13-C14-C15-C16
34	I	303	DD6	C13-C14-C15-C20
34	J	304	DD6	C10-C11-C13-C14
34	J	304	DD6	C12-C11-C13-C14
34	J	304	DD6	C13-C14-C15-O1
34	L	305	DD6	C10-C11-C13-C14
34	L	305	DD6	C12-C11-C13-C14
34	L	305	DD6	C13-C14-C15-C16
34	L	305	DD6	C13-C14-C15-C20
34	M	303	DD6	C10-C11-C13-C14
34	M	303	DD6	C12-C11-C13-C14
34	O	304	DD6	C10-C11-C13-C14
34	O	304	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
34	O	304	DD6	C13-C14-C15-O1
34	O	304	DD6	C5-C6-C8-C9
34	O	304	DD6	C7-C6-C8-C9
34	Q	302	DD6	C-C1-C24-C25
34	Q	302	DD6	C2-C1-C24-C25
34	Q	302	DD6	C13-C14-C15-C16
34	Q	302	DD6	C13-C14-C15-C20
34	R	307	DD6	C-C1-C24-C25
34	R	307	DD6	C2-C1-C24-C25
34	R	307	DD6	C10-C11-C13-C14
34	R	307	DD6	C12-C11-C13-C14
34	R	307	DD6	C13-C14-C15-C16
34	R	307	DD6	C13-C14-C15-C20
34	R	307	DD6	C5-C6-C8-C9
34	R	307	DD6	C7-C6-C8-C9
34	R	308	DD6	C-C1-C24-C25
34	R	308	DD6	C2-C1-C24-C25
34	R	308	DD6	C11-C10-C9-C8
34	R	308	DD6	C13-C14-C15-O1
34	S	306	DD6	C13-C14-C15-O1
34	S	306	DD6	C5-C6-C8-C9
34	S	306	DD6	C7-C6-C8-C9
34	S	307	DD6	C-C1-C24-C25
34	W	204	DD6	C-C1-C24-C25
34	W	204	DD6	C2-C1-C24-C25
34	W	204	DD6	C10-C11-C13-C14
34	W	204	DD6	C12-C11-C13-C14
34	W	204	DD6	C13-C14-C15-C16
34	W	205	DD6	C13-C14-C15-C20
34	W	205	DD6	C5-C6-C8-C9
34	W	205	DD6	C7-C6-C8-C9
34	a	849	DD6	C13-C14-C15-C16
34	a	849	DD6	C13-C14-C15-C20
34	a	849	DD6	C7-C6-C8-C9
34	j	103	DD6	C10-C11-C13-C14
34	j	103	DD6	C12-C11-C13-C14
34	j	103	DD6	C13-C14-C15-C16
34	j	103	DD6	C13-C14-C15-C20
35	A	316	A86	C13-C14-C15-C16
35	A	316	A86	C13-C14-C15-O1
35	A	316	A86	C26-C27-C29-C30
35	A	316	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
35	A	316	A86	C39-C38-O4-C34
35	B	303	A86	C11-C10-C9-C8
35	B	303	A86	C12-C11-C13-C14
35	B	303	A86	O-C13-C14-C15
35	B	303	A86	C11-C13-C14-C15
35	B	303	A86	C39-C38-O4-C34
35	C	203	A86	C-C1-C24-C25
35	C	203	A86	C2-C1-C24-C25
35	C	203	A86	C33-C34-O4-C38
35	C	203	A86	C39-C38-O4-C34
35	C	203	A86	O5-C38-O4-C34
35	C	204	A86	C28-C27-C29-C30
35	C	204	A86	C33-C34-O4-C38
35	D	302	A86	C35-C34-O4-C38
35	D	302	A86	C5-C6-C8-C9
35	D	302	A86	C7-C6-C8-C9
35	E	302	A86	C13-C14-C15-O1
35	E	305	A86	C39-C38-O4-C34
35	E	305	A86	O5-C38-O4-C34
35	E	305	A86	C5-C6-C8-C9
35	E	305	A86	C7-C6-C8-C9
35	E	307	A86	C13-C14-C15-O1
35	F	301	A86	C-C1-C24-C25
35	F	301	A86	C2-C1-C24-C25
35	F	302	A86	C35-C34-O4-C38
35	F	302	A86	C39-C38-O4-C34
35	F	304	A86	C13-C14-C15-O1
35	F	307	A86	C39-C38-O4-C34
35	G	302	A86	C-C1-C24-C25
35	G	302	A86	C2-C1-C24-C25
35	G	302	A86	C35-C34-O4-C38
35	G	304	A86	C12-C11-C13-C14
35	G	304	A86	C13-C14-C15-C20
35	G	305	A86	C39-C38-O4-C34
35	G	305	A86	O5-C38-O4-C34
35	H	304	A86	C-C1-C24-C25
35	H	304	A86	C2-C1-C24-C25
35	H	304	A86	C24-C25-C26-C27
35	H	304	A86	C26-C27-C29-C30
35	H	304	A86	C33-C34-O4-C38
35	H	304	A86	C39-C38-O4-C34
35	H	304	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
35	I	301	A86	C-C1-C24-C25
35	I	301	A86	C2-C1-C24-C25
35	I	301	A86	C24-C25-C26-C27
35	I	301	A86	C5-C6-C8-C9
35	I	301	A86	C7-C6-C8-C9
35	J	301	A86	C-C1-C24-C25
35	J	301	A86	C13-C14-C15-C20
35	J	301	A86	C13-C14-C15-O1
35	J	302	A86	C13-C14-C15-O1
35	J	305	A86	C35-C34-O4-C38
35	J	305	A86	C5-C6-C8-C9
35	J	305	A86	C7-C6-C8-C9
35	J	306	A86	C-C1-C24-C25
35	J	306	A86	C2-C1-C24-C25
35	J	306	A86	C12-C11-C13-C14
35	J	306	A86	C13-C14-C15-O1
35	J	306	A86	C33-C34-O4-C38
35	K	301	A86	C-C1-C24-C25
35	K	301	A86	C2-C1-C24-C25
35	K	301	A86	C13-C14-C15-O1
35	K	301	A86	O5-C38-O4-C34
35	K	302	A86	C12-C11-C13-C14
35	K	306	A86	C12-C11-C13-O
35	K	306	A86	C12-C11-C13-C14
35	K	306	A86	C39-C38-O4-C34
35	L	301	A86	C-C1-C24-C25
35	L	301	A86	C2-C1-C24-C25
35	L	304	A86	C39-C38-O4-C34
35	L	306	A86	C-C1-C24-C25
35	L	306	A86	C2-C1-C24-C25
35	L	306	A86	C10-C11-C13-O
35	L	306	A86	C12-C11-C13-O
35	L	306	A86	C39-C38-O4-C34
35	L	307	A86	C-C1-C24-C25
35	L	307	A86	C2-C1-C24-C25
35	L	307	A86	C11-C10-C9-C8
35	L	307	A86	C5-C6-C8-C9
35	L	307	A86	C7-C6-C8-C9
35	L	319	A86	C12-C11-C13-C14
35	M	301	A86	C12-C11-C13-C14
35	M	302	A86	C12-C11-C13-O
35	M	302	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
35	M	304	A86	C-C1-C24-C25
35	M	304	A86	C2-C1-C24-C25
35	M	304	A86	C5-C6-C8-C9
35	M	304	A86	C7-C6-C8-C9
35	M	305	A86	C12-C11-C13-C14
35	M	305	A86	C39-C38-O4-C34
35	N	301	A86	C12-C11-C13-C14
35	N	301	A86	C13-C14-C15-C20
35	N	304	A86	C-C1-C24-C25
35	N	304	A86	C2-C1-C24-C25
35	N	304	A86	C33-C34-O4-C38
35	N	304	A86	C5-C6-C8-C9
35	N	304	A86	C7-C6-C8-C9
35	N	306	A86	C10-C11-C13-O
35	N	306	A86	C12-C11-C13-O
35	N	306	A86	C12-C11-C13-C14
35	N	306	A86	C39-C38-O4-C34
35	N	320	A86	C12-C11-C13-C14
35	N	320	A86	C39-C38-O4-C34
35	O	301	A86	C5-C6-C8-C9
35	O	301	A86	C7-C6-C8-C9
35	O	302	A86	C12-C11-C13-C14
35	O	303	A86	C39-C38-O4-C34
35	O	305	A86	C39-C38-O4-C34
35	O	305	A86	O5-C38-O4-C34
35	O	305	A86	C5-C6-C8-C9
35	O	305	A86	C7-C6-C8-C9
35	O	319	A86	C11-C10-C9-C8
35	O	319	A86	C12-C11-C13-O
35	P	303	A86	C12-C11-C13-C14
35	P	304	A86	C39-C38-O4-C34
35	P	306	A86	C39-C38-O4-C34
35	P	306	A86	O5-C38-O4-C34
35	Q	301	A86	C39-C38-O4-C34
35	Q	303	A86	C-C1-C24-C25
35	Q	303	A86	C2-C1-C24-C25
35	Q	303	A86	C39-C38-O4-C34
35	Q	303	A86	O5-C38-O4-C34
35	Q	304	A86	C12-C11-C13-O
35	Q	304	A86	C12-C11-C13-C14
35	Q	304	A86	C39-C38-O4-C34
35	R	305	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
35	R	305	A86	C2-C1-C24-C25
35	R	306	A86	C12-C11-C13-C14
35	R	309	A86	C12-C11-C13-C14
35	R	309	A86	C39-C38-O4-C34
35	S	301	A86	C12-C11-C13-C14
35	S	301	A86	C13-C14-C15-C20
35	S	304	A86	C-C1-C24-C25
35	S	304	A86	C2-C1-C24-C25
35	S	304	A86	C13-C14-C15-C16
35	S	304	A86	C33-C34-O4-C38
35	S	304	A86	C39-C38-O4-C34
35	S	305	A86	C12-C11-C13-O
35	S	305	A86	C12-C11-C13-C14
35	S	305	A86	C13-C14-C15-C20
35	S	305	A86	C39-C38-O4-C34
35	S	308	A86	C-C1-C24-C25
35	S	308	A86	C28-C27-C29-C30
35	S	308	A86	C35-C34-O4-C38
35	T	306	A86	C39-C38-O4-C34
35	T	307	A86	C39-C38-O4-C34
35	W	202	A86	C12-C11-C13-C14
35	X	301	A86	C12-C11-C13-C14
35	X	302	A86	C39-C38-O4-C34
35	X	305	A86	C39-C38-O4-C34
35	X	314	A86	O5-C38-O4-C34
35	h	202	A86	C13-C14-C15-O1
35	h	202	A86	C39-C38-O4-C34
35	U	302	A86	C39-C38-O4-C34
35	U	303	A86	C-C1-C24-C25
35	U	303	A86	C2-C1-C24-C25
35	U	303	A86	C11-C10-C9-C8
35	U	303	A86	C13-C14-C15-C16
35	U	303	A86	C33-C34-O4-C38
35	U	303	A86	C5-C6-C8-C9
35	U	303	A86	C7-C6-C8-C9
35	U	304	A86	C-C1-C24-C25
35	U	304	A86	C2-C1-C24-C25
35	U	304	A86	C12-C11-C13-C14
35	U	304	A86	C13-C14-C15-C16
35	U	304	A86	C13-C14-C15-O1
35	U	304	A86	C1-C2-C3-C4
35	V	301	A86	C-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
35	V	301	A86	C2-C1-C24-C25
35	V	301	A86	C13-C14-C15-C16
35	V	301	A86	C13-C14-C15-C20
35	V	301	A86	C13-C14-C15-O1
35	V	301	A86	C33-C34-O4-C38
35	V	301	A86	C39-C38-O4-C34
35	V	304	A86	C13-C14-C15-C20
35	V	304	A86	C39-C38-O4-C34
36	A	306	CLA	C1A-C2A-CAA-CBA
36	A	307	CLA	CHA-CBD-CGD-O1D
36	A	307	CLA	CHA-CBD-CGD-O2D
36	A	309	CLA	CBA-CGA-O2A-C1
36	A	309	CLA	CBD-CGD-O2D-CED
36	A	311	CLA	C1A-C2A-CAA-CBA
36	A	311	CLA	C3A-C2A-CAA-CBA
36	A	314	CLA	C1A-C2A-CAA-CBA
36	A	314	CLA	C3A-C2A-CAA-CBA
36	B	305	CLA	CHA-CBD-CGD-O1D
36	B	305	CLA	CHA-CBD-CGD-O2D
36	B	308	CLA	CBD-CGD-O2D-CED
36	B	308	CLA	C2-C3-C5-C6
36	B	308	CLA	C4-C3-C5-C6
36	C	206	CLA	C2-C3-C5-C6
36	C	206	CLA	C4-C3-C5-C6
36	C	206	CLA	C11-C10-C8-C7
36	C	207	CLA	C11-C12-C13-C14
36	C	208	CLA	C2-C3-C5-C6
36	C	208	CLA	C4-C3-C5-C6
36	C	209	CLA	CHA-CBD-CGD-O1D
36	C	209	CLA	CHA-CBD-CGD-O2D
36	C	210	CLA	C1A-C2A-CAA-CBA
36	C	210	CLA	CBA-CGA-O2A-C1
36	C	212	CLA	CHA-CBD-CGD-O1D
36	D	307	CLA	C1A-C2A-CAA-CBA
36	D	307	CLA	C2-C3-C5-C6
36	D	307	CLA	C4-C3-C5-C6
36	D	308	CLA	C11-C10-C8-C7
36	D	309	CLA	CBD-CGD-O2D-CED
36	D	311	CLA	CBD-CGD-O2D-CED
36	D	312	CLA	CBD-CGD-O2D-CED
36	D	316	CLA	CBD-CGD-O2D-CED
36	D	316	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	E	308	CLA	CHA-CBD-CGD-O1D
36	E	312	CLA	C1A-C2A-CAA-CBA
36	E	316	CLA	C1A-C2A-CAA-CBA
36	E	316	CLA	C3A-C2A-CAA-CBA
36	E	316	CLA	CHA-CBD-CGD-O1D
36	E	316	CLA	CHA-CBD-CGD-O2D
36	E	317	CLA	C3A-C2A-CAA-CBA
36	F	309	CLA	C2-C3-C5-C6
36	F	309	CLA	C4-C3-C5-C6
36	F	311	CLA	CHA-CBD-CGD-O1D
36	F	311	CLA	CHA-CBD-CGD-O2D
36	F	314	CLA	C1A-C2A-CAA-CBA
36	F	314	CLA	C3A-C2A-CAA-CBA
36	F	314	CLA	C6-C7-C8-C10
36	F	317	CLA	C1A-C2A-CAA-CBA
36	G	311	CLA	C2-C3-C5-C6
36	G	311	CLA	C4-C3-C5-C6
36	G	313	CLA	CHA-CBD-CGD-O1D
36	G	313	CLA	CHA-CBD-CGD-O2D
36	G	315	CLA	CBA-CGA-O2A-C1
36	G	315	CLA	O1A-CGA-O2A-C1
36	G	315	CLA	CBD-CGD-O2D-CED
36	G	315	CLA	C2-C3-C5-C6
36	G	315	CLA	C4-C3-C5-C6
36	G	316	CLA	CBD-CGD-O2D-CED
36	H	307	CLA	CBA-CGA-O2A-C1
36	H	307	CLA	O1A-CGA-O2A-C1
36	H	308	CLA	CAD-CBD-CGD-O1D
36	H	308	CLA	CAD-CBD-CGD-O2D
36	H	310	CLA	CBA-CGA-O2A-C1
36	H	310	CLA	O1A-CGA-O2A-C1
36	H	312	CLA	C1A-C2A-CAA-CBA
36	H	316	CLA	C6-C7-C8-C9
36	H	317	CLA	CBD-CGD-O2D-CED
36	H	318	CLA	CBD-CGD-O2D-CED
36	I	305	CLA	C6-C7-C8-C9
36	I	308	CLA	CAD-CBD-CGD-O1D
36	I	308	CLA	CAD-CBD-CGD-O2D
36	I	313	CLA	CBD-CGD-O2D-CED
36	J	307	CLA	C2-C3-C5-C6
36	J	307	CLA	C4-C3-C5-C6
36	J	311	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	J	311	CLA	O1A-CGA-O2A-C1
36	J	312	CLA	CBD-CGD-O2D-CED
36	J	316	CLA	CBD-CGD-O2D-CED
36	K	307	CLA	C1A-C2A-CAA-CBA
36	K	307	CLA	C3A-C2A-CAA-CBA
36	K	307	CLA	CBD-CGD-O2D-CED
36	K	311	CLA	C2A-CAA-CBA-CGA
36	K	311	CLA	CBA-CGA-O2A-C1
36	K	313	CLA	CHA-CBD-CGD-O1D
36	K	313	CLA	CHA-CBD-CGD-O2D
36	L	308	CLA	C1A-C2A-CAA-CBA
36	L	308	CLA	C3A-C2A-CAA-CBA
36	L	308	CLA	C2-C3-C5-C6
36	L	308	CLA	C4-C3-C5-C6
36	L	312	CLA	C3A-C2A-CAA-CBA
36	L	312	CLA	CBD-CGD-O2D-CED
36	L	312	CLA	O1D-CGD-O2D-CED
36	L	314	CLA	C1A-C2A-CAA-CBA
36	M	306	CLA	CHA-CBD-CGD-O1D
36	M	306	CLA	CHA-CBD-CGD-O2D
36	M	307	CLA	CBA-CGA-O2A-C1
36	M	307	CLA	O1A-CGA-O2A-C1
36	M	307	CLA	O2A-C1-C2-C3
36	M	309	CLA	CBD-CGD-O2D-CED
36	M	310	CLA	C3A-C2A-CAA-CBA
36	M	310	CLA	CBA-CGA-O2A-C1
36	M	310	CLA	O1A-CGA-O2A-C1
36	M	316	CLA	C1A-C2A-CAA-CBA
36	M	316	CLA	C3A-C2A-CAA-CBA
36	M	316	CLA	CBD-CGD-O2D-CED
36	N	308	CLA	CBD-CGD-O2D-CED
36	N	309	CLA	C2-C3-C5-C6
36	N	311	CLA	C3A-C2A-CAA-CBA
36	N	317	CLA	CBD-CGD-O2D-CED
36	N	319	CLA	CAD-CBD-CGD-O1D
36	N	319	CLA	CBD-CGD-O2D-CED
36	O	306	CLA	CHA-CBD-CGD-O1D
36	O	306	CLA	CHA-CBD-CGD-O2D
36	O	309	CLA	CHA-CBD-CGD-O1D
36	O	309	CLA	CHA-CBD-CGD-O2D
36	O	310	CLA	C1A-C2A-CAA-CBA
36	O	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	O	310	CLA	O1A-CGA-O2A-C1
36	O	310	CLA	CBD-CGD-O2D-CED
36	O	316	CLA	C1A-C2A-CAA-CBA
36	O	316	CLA	C3A-C2A-CAA-CBA
36	O	316	CLA	O2A-C1-C2-C3
36	P	302	CLA	C1A-C2A-CAA-CBA
36	P	302	CLA	C3A-C2A-CAA-CBA
36	P	308	CLA	CHA-CBD-CGD-O1D
36	P	308	CLA	CHA-CBD-CGD-O2D
36	P	311	CLA	CHA-CBD-CGD-O1D
36	P	311	CLA	CHA-CBD-CGD-O2D
36	P	312	CLA	C1A-C2A-CAA-CBA
36	P	312	CLA	CBA-CGA-O2A-C1
36	P	312	CLA	O1A-CGA-O2A-C1
36	P	312	CLA	CBD-CGD-O2D-CED
36	P	314	CLA	C1A-C2A-CAA-CBA
36	P	314	CLA	C3A-C2A-CAA-CBA
36	P	314	CLA	O2A-C1-C2-C3
36	P	318	CLA	C1A-C2A-CAA-CBA
36	Q	305	CLA	CHA-CBD-CGD-O1D
36	Q	305	CLA	CHA-CBD-CGD-O2D
36	Q	308	CLA	CHA-CBD-CGD-O1D
36	Q	308	CLA	CHA-CBD-CGD-O2D
36	Q	309	CLA	C1A-C2A-CAA-CBA
36	Q	309	CLA	CBA-CGA-O2A-C1
36	Q	309	CLA	O1A-CGA-O2A-C1
36	Q	309	CLA	CBD-CGD-O2D-CED
36	Q	314	CLA	CBD-CGD-O2D-CED
36	R	310	CLA	CHA-CBD-CGD-O1D
36	R	310	CLA	CHA-CBD-CGD-O2D
36	R	310	CLA	C2-C3-C5-C6
36	R	310	CLA	C4-C3-C5-C6
36	R	311	CLA	CBD-CGD-O2D-CED
36	R	311	CLA	C4-C3-C5-C6
36	R	314	CLA	C3A-C2A-CAA-CBA
36	R	314	CLA	CBA-CGA-O2A-C1
36	R	316	CLA	C1A-C2A-CAA-CBA
36	R	318	CLA	CBD-CGD-O2D-CED
36	R	322	CLA	C1A-C2A-CAA-CBA
36	R	322	CLA	CHA-CBD-CGD-O2D
36	R	322	CLA	CBD-CGD-O2D-CED
36	S	309	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
36	S	309	CLA	CHA-CBD-CGD-O2D
36	S	310	CLA	CBD-CGD-O2D-CED
36	S	310	CLA	O2A-C1-C2-C3
36	S	311	CLA	CBD-CGD-O2D-CED
36	S	312	CLA	CHA-CBD-CGD-O1D
36	S	312	CLA	CHA-CBD-CGD-O2D
36	S	312	CLA	CAD-CBD-CGD-O1D
36	S	312	CLA	CBD-CGD-O2D-CED
36	S	313	CLA	C3A-C2A-CAA-CBA
36	S	313	CLA	CBA-CGA-O2A-C1
36	S	314	CLA	C1A-C2A-CAA-CBA
36	S	314	CLA	CBD-CGD-O2D-CED
36	S	314	CLA	O1D-CGD-O2D-CED
36	S	314	CLA	C2-C3-C5-C6
36	S	314	CLA	C4-C3-C5-C6
36	S	318	CLA	C1A-C2A-CAA-CBA
36	S	318	CLA	C3A-C2A-CAA-CBA
36	S	318	CLA	CHA-CBD-CGD-O1D
36	S	318	CLA	CHA-CBD-CGD-O2D
36	S	320	CLA	C1A-C2A-CAA-CBA
36	S	321	CLA	C1A-C2A-CAA-CBA
36	S	321	CLA	CHA-CBD-CGD-O1D
36	S	321	CLA	CHA-CBD-CGD-O2D
36	T	308	CLA	CBD-CGD-O2D-CED
36	T	312	CLA	C1A-C2A-CAA-CBA
36	T	314	CLA	C1A-C2A-CAA-CBA
36	T	314	CLA	CHA-CBD-CGD-O1D
36	W	206	CLA	CHA-CBD-CGD-O1D
36	W	206	CLA	CHA-CBD-CGD-O2D
36	W	209	CLA	CHA-CBD-CGD-O1D
36	W	209	CLA	CHA-CBD-CGD-O2D
36	W	210	CLA	C3A-C2A-CAA-CBA
36	W	212	CLA	C1A-C2A-CAA-CBA
36	X	306	CLA	CHA-CBD-CGD-O1D
36	X	306	CLA	CHA-CBD-CGD-O2D
36	X	307	CLA	CBD-CGD-O2D-CED
36	X	308	CLA	C1A-C2A-CAA-CBA
36	X	309	CLA	C1A-C2A-CAA-CBA
36	X	310	CLA	CBD-CGD-O2D-CED
36	X	312	CLA	CBD-CGD-O2D-CED
36	X	313	CLA	C1A-C2A-CAA-CBA
36	X	313	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	X	313	CLA	CBD-CGD-O2D-CED
36	a	803	CLA	C1A-C2A-CAA-CBA
36	a	803	CLA	CBA-CGA-O2A-C1
36	a	804	CLA	CHA-CBD-CGD-O1D
36	a	804	CLA	CHA-CBD-CGD-O2D
36	a	804	CLA	CAD-CBD-CGD-O1D
36	a	805	CLA	C1A-C2A-CAA-CBA
36	a	805	CLA	C3A-C2A-CAA-CBA
36	a	807	CLA	C3A-C2A-CAA-CBA
36	a	809	CLA	CHA-CBD-CGD-O1D
36	a	809	CLA	CHA-CBD-CGD-O2D
36	a	812	CLA	C11-C10-C8-C9
36	a	816	CLA	C1A-C2A-CAA-CBA
36	a	816	CLA	C3A-C2A-CAA-CBA
36	a	816	CLA	CHA-CBD-CGD-O1D
36	a	816	CLA	CHA-CBD-CGD-O2D
36	a	817	CLA	C3A-C2A-CAA-CBA
36	a	818	CLA	C1A-C2A-CAA-CBA
36	a	818	CLA	C3A-C2A-CAA-CBA
36	a	821	CLA	C1A-C2A-CAA-CBA
36	a	821	CLA	C3A-C2A-CAA-CBA
36	a	821	CLA	C2A-CAA-CBA-CGA
36	a	822	CLA	C2-C3-C5-C6
36	a	823	CLA	C4-C3-C5-C6
36	a	825	CLA	C3A-C2A-CAA-CBA
36	a	825	CLA	C11-C10-C8-C9
36	a	827	CLA	C11-C12-C13-C14
36	a	830	CLA	C1A-C2A-CAA-CBA
36	a	830	CLA	C3A-C2A-CAA-CBA
36	a	832	CLA	CHA-CBD-CGD-O1D
36	a	832	CLA	CHA-CBD-CGD-O2D
36	a	834	CLA	C2A-CAA-CBA-CGA
36	a	836	CLA	CBD-CGD-O2D-CED
36	a	836	CLA	C2-C3-C5-C6
36	a	836	CLA	C4-C3-C5-C6
36	a	841	CLA	C3A-C2A-CAA-CBA
36	a	848	CLA	CBD-CGD-O2D-CED
36	a	848	CLA	C2-C3-C5-C6
36	a	848	CLA	C4-C3-C5-C6
36	b	805	CLA	CHA-CBD-CGD-O1D
36	b	805	CLA	CHA-CBD-CGD-O2D
36	b	808	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	b	808	CLA	C3A-C2A-CAA-CBA
36	b	809	CLA	C6-C7-C8-C9
36	b	816	CLA	C1A-C2A-CAA-CBA
36	b	816	CLA	C3A-C2A-CAA-CBA
36	b	817	CLA	C4-C3-C5-C6
36	b	818	CLA	C2-C3-C5-C6
36	b	818	CLA	C4-C3-C5-C6
36	b	820	CLA	C3A-C2A-CAA-CBA
36	b	821	CLA	CHA-CBD-CGD-O1D
36	b	821	CLA	CHA-CBD-CGD-O2D
36	b	824	CLA	C1A-C2A-CAA-CBA
36	b	824	CLA	CHA-CBD-CGD-O1D
36	b	824	CLA	CHA-CBD-CGD-O2D
36	b	824	CLA	C2-C3-C5-C6
36	b	824	CLA	C4-C3-C5-C6
36	b	826	CLA	CBD-CGD-O2D-CED
36	b	826	CLA	C11-C10-C8-C9
36	b	827	CLA	C1A-C2A-CAA-CBA
36	b	828	CLA	C1A-C2A-CAA-CBA
36	b	828	CLA	C3A-C2A-CAA-CBA
36	b	829	CLA	C1A-C2A-CAA-CBA
36	b	829	CLA	C3A-C2A-CAA-CBA
36	b	831	CLA	C1A-C2A-CAA-CBA
36	b	831	CLA	C3A-C2A-CAA-CBA
36	b	832	CLA	C2A-CAA-CBA-CGA
36	b	836	CLA	C2-C3-C5-C6
36	b	836	CLA	C4-C3-C5-C6
36	f	803	CLA	C11-C10-C8-C9
36	f	804	CLA	CBD-CGD-O2D-CED
36	f	804	CLA	C2-C3-C5-C6
36	f	804	CLA	C4-C3-C5-C6
36	i	102	CLA	C1A-C2A-CAA-CBA
36	i	102	CLA	C3A-C2A-CAA-CBA
36	i	102	CLA	CHA-CBD-CGD-O1D
36	i	102	CLA	CHA-CBD-CGD-O2D
36	i	102	CLA	CAD-CBD-CGD-O1D
36	i	102	CLA	CBD-CGD-O2D-CED
36	j	101	CLA	C4-C3-C5-C6
36	j	106	CLA	CHA-CBD-CGD-O1D
36	j	106	CLA	CHA-CBD-CGD-O2D
36	j	106	CLA	CAD-CBD-CGD-O1D
36	l	202	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	l	204	CLA	C3A-C2A-CAA-CBA
36	h	203	CLA	C1A-C2A-CAA-CBA
36	h	203	CLA	CHA-CBD-CGD-O1D
36	h	203	CLA	CHA-CBD-CGD-O2D
36	h	203	CLA	C2-C3-C5-C6
36	h	203	CLA	C4-C3-C5-C6
36	U	305	CLA	CHA-CBD-CGD-O1D
36	U	305	CLA	CHA-CBD-CGD-O2D
36	U	309	CLA	C1A-C2A-CAA-CBA
36	U	309	CLA	CBA-CGA-O2A-C1
36	U	310	CLA	CBD-CGD-O2D-CED
36	U	311	CLA	C3A-C2A-CAA-CBA
36	V	306	CLA	CBD-CGD-O2D-CED
36	V	309	CLA	C3A-C2A-CAA-CBA
36	V	311	CLA	C1A-C2A-CAA-CBA
36	V	313	CLA	C1A-C2A-CAA-CBA
36	V	313	CLA	CBD-CGD-O2D-CED
36	V	314	CLA	C1A-C2A-CAA-CBA
36	V	314	CLA	CBD-CGD-O2D-CED
37	C	213	KC1	C1A-C2A-CAA-CBA
37	C	213	KC1	C3A-C2A-CAA-CBA
37	D	314	KC1	C1A-C2A-CAA-CBA
37	D	314	KC1	C3A-C2A-CAA-CBA
37	F	308	KC1	C2B-C3B-CAB-CBB
37	F	308	KC1	C4B-C3B-CAB-CBB
37	F	315	KC1	CBD-CGD-O2D-CED
37	G	317	KC1	C1A-C2A-CAA-CBA
37	G	317	KC1	C3A-C2A-CAA-CBA
37	G	317	KC1	CBD-CGD-O2D-CED
37	H	313	KC1	C1A-C2A-CAA-CBA
37	H	313	KC1	C3A-C2A-CAA-CBA
37	K	314	KC1	C1A-C2A-CAA-CBA
37	K	314	KC1	C3A-C2A-CAA-CBA
37	K	314	KC1	CAA-CBA-CGA-O1A
37	K	314	KC1	CAA-CBA-CGA-O2A
37	L	315	KC1	C1A-C2A-CAA-CBA
37	L	315	KC1	C3A-C2A-CAA-CBA
37	M	313	KC1	CBD-CGD-O2D-CED
37	M	317	KC1	C1A-C2A-CAA-CBA
37	M	318	KC1	C1A-C2A-CAA-CBA
37	M	318	KC1	C3A-C2A-CAA-CBA
37	M	318	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
37	M	318	KC1	CBD-CGD-O2D-CED
37	N	314	KC1	C1A-C2A-CAA-CBA
37	N	314	KC1	C3A-C2A-CAA-CBA
37	P	317	KC1	C1A-C2A-CAA-CBA
37	P	317	KC1	C3A-C2A-CAA-CBA
37	R	317	KC1	CAA-CBA-CGA-O1A
37	R	317	KC1	CAA-CBA-CGA-O2A
37	S	316	KC1	C3A-C2A-CAA-CBA
37	S	316	KC1	C4B-C3B-CAB-CBB
37	T	315	KC1	C1A-C2A-CAA-CBA
37	T	315	KC1	C3A-C2A-CAA-CBA
37	T	315	KC1	CAA-CBA-CGA-O1A
37	T	315	KC1	CAA-CBA-CGA-O2A
37	W	213	KC1	C1A-C2A-CAA-CBA
37	W	213	KC1	C3A-C2A-CAA-CBA
37	W	217	KC1	C2B-C3B-CAB-CBB
37	W	217	KC1	C4B-C3B-CAB-CBB
37	W	217	KC1	CAD-CBD-CGD-O2D
37	X	311	KC1	C1A-C2A-CAA-CBA
37	X	311	KC1	C3A-C2A-CAA-CBA
37	U	312	KC1	C1A-C2A-CAA-CBA
37	U	312	KC1	C3A-C2A-CAA-CBA
37	V	312	KC1	C1A-C2A-CAA-CBA
37	V	312	KC1	C3A-C2A-CAA-CBA
38	b	804	SQD	C2-C1-O6-C44
38	b	804	SQD	O5-C1-O6-C44
38	b	804	SQD	O5-C5-C6-S
39	B	312	LMT	O5'-C1'-O1'-C1
39	E	321	LMT	C2'-C1'-O1'-C1
39	E	321	LMT	O5'-C1'-O1'-C1
39	E	323	LMT	O5'-C1'-O1'-C1
39	E	323	LMT	C2-C1-O1'-C1'
39	F	320	LMT	O5'-C1'-O1'-C1
39	F	321	LMT	C2-C1-O1'-C1'
39	G	322	LMT	C2'-C1'-O1'-C1
39	G	322	LMT	O5'-C1'-O1'-C1
39	G	322	LMT	C2-C1-O1'-C1'
39	G	323	LMT	C2-C1-O1'-C1'
39	I	317	LMT	O5'-C1'-O1'-C1
39	I	318	LMT	C2'-C1'-O1'-C1
39	I	318	LMT	O5'-C1'-O1'-C1
39	K	318	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
39	L	318	LMT	C2'-C1'-O1'-C1
39	P	320	LMT	O5'-C1'-O1'-C1
39	P	320	LMT	C2-C1-O1'-C1'
39	P	321	LMT	C2'-C1'-O1'-C1
39	P	321	LMT	O5'-C1'-O1'-C1
39	a	853	LMT	C2'-C1'-O1'-C1
39	a	853	LMT	O5'-C1'-O1'-C1
39	a	854	LMT	C2'-C1'-O1'-C1
39	a	854	LMT	O5'-C1'-O1'-C1
39	b	848	LMT	C2'-C1'-O1'-C1
39	b	848	LMT	O5'-C1'-O1'-C1
39	b	848	LMT	C2-C1-O1'-C1'
39	f	807	LMT	O5'-C1'-O1'-C1
39	h	205	LMT	C2-C1-O1'-C1'
39	U	315	LMT	C2-C1-O1'-C1'
40	C	215	DGD	C2B-C1B-O2G-C2G
40	C	215	DGD	C2G-C3G-O3G-C1D
40	C	215	DGD	C2D-C1D-O3G-C3G
40	C	215	DGD	O6D-C1D-O3G-C3G
40	L	302	DGD	O1A-C1A-O1G-C1G
40	L	302	DGD	C2D-C1D-O3G-C3G
40	L	302	DGD	O6D-C1D-O3G-C3G
40	b	849	DGD	O2G-C2G-C3G-O3G
41	D	318	LHG	C3-O3-P-O5
41	D	318	LHG	O9-C7-O7-C5
41	D	318	LHG	C8-C7-O7-C5
41	D	319	LHG	O1-C1-C2-C3
41	D	319	LHG	C3-O3-P-O5
41	D	319	LHG	C8-C7-O7-C5
41	E	322	LHG	C4-O6-P-O3
41	E	322	LHG	C4-O6-P-O4
41	E	322	LHG	C4-O6-P-O5
41	F	319	LHG	C3-O3-P-O4
41	F	319	LHG	C4-O6-P-O5
41	F	319	LHG	C8-C7-O7-C5
41	G	301	LHG	C1-C2-C3-O3
41	G	301	LHG	C4-O6-P-O5
41	G	321	LHG	C3-O3-P-O4
41	G	321	LHG	C4-O6-P-O5
41	I	316	LHG	C1-C2-C3-O3
41	I	316	LHG	C4-O6-P-O4
41	O	317	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
41	O	317	LHG	C3-O3-P-O5
41	O	317	LHG	C4-O6-P-O5
41	O	318	LHG	O1-C1-C2-O2
41	O	318	LHG	O1-C1-C2-C3
41	O	318	LHG	C3-O3-P-O4
41	Q	315	LHG	C1-C2-C3-O3
41	Q	315	LHG	C3-O3-P-O5
41	Q	315	LHG	C4-O6-P-O5
41	Q	315	LHG	C5-C4-O6-P
41	Q	315	LHG	C8-C7-O7-C5
41	R	323	LHG	O1-C1-C2-O2
41	R	323	LHG	O1-C1-C2-C3
41	R	323	LHG	C4-O6-P-O5
41	R	323	LHG	O9-C7-O7-C5
41	a	842	LHG	O1-C1-C2-C3
41	a	842	LHG	C3-O3-P-O5
41	a	842	LHG	C4-O6-P-O4
41	a	843	LHG	C3-O3-P-O5
41	a	850	LHG	C3-O3-P-O5
41	a	850	LHG	O9-C7-O7-C5
41	a	850	LHG	C8-C7-O7-C5
41	b	850	LHG	C4-O6-P-O3
41	b	850	LHG	C4-O6-P-O4
41	b	850	LHG	C4-O6-P-O5
41	b	850	LHG	O9-C7-O7-C5
41	b	850	LHG	C8-C7-O7-C5
41	f	808	LHG	C1-C2-C3-O3
41	f	808	LHG	C2-C3-O3-P
41	f	809	LHG	C2-C3-O3-P
41	f	809	LHG	C4-O6-P-O3
41	f	809	LHG	C4-O6-P-O4
41	f	809	LHG	C4-O6-P-O5
41	i	104	LHG	C2-C3-O3-P
41	i	104	LHG	C4-O6-P-O3
41	i	104	LHG	C4-O6-P-O4
41	i	104	LHG	C4-O6-P-O5
41	i	104	LHG	O10-C23-O8-C6
41	i	104	LHG	C24-C23-O8-C6
41	j	104	LHG	C3-O3-P-O5
41	l	208	LHG	C4-O6-P-O4
41	l	208	LHG	C8-C7-O7-C5
42	D	320	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
42	D	320	LMG	O6-C1-O1-C7
42	D	320	LMG	C11-C10-O7-C8
42	D	321	LMG	O6-C1-O1-C7
42	E	318	LMG	O6-C1-O1-C7
42	E	319	LMG	C2-C1-O1-C7
42	E	319	LMG	O6-C1-O1-C7
42	E	319	LMG	C11-C10-O7-C8
42	G	324	LMG	O10-C28-O8-C9
42	G	324	LMG	C29-C28-O8-C9
42	I	315	LMG	C11-C10-O7-C8
42	J	318	LMG	O9-C10-O7-C8
42	J	319	LMG	O9-C10-O7-C8
42	a	852	LMG	C11-C10-O7-C8
42	j	105	LMG	O6-C1-O1-C7
42	j	105	LMG	O10-C28-O8-C9
42	j	105	LMG	C29-C28-O8-C9
42	m	102	LMG	C11-C10-O7-C8
42	h	206	LMG	C2-C1-O1-C7
42	h	206	LMG	O6-C1-O1-C7
42	h	206	LMG	O10-C28-O8-C9
42	h	206	LMG	C29-C28-O8-C9
42	V	315	LMG	O9-C10-O7-C8
42	V	316	LMG	C2-C1-O1-C7
42	V	316	LMG	O6-C1-O1-C7
43	a	840	PQN	C21-C22-C23-C24
44	a	844	BCR	C7-C8-C9-C34
44	a	845	BCR	C7-C8-C9-C10
44	a	845	BCR	C7-C8-C9-C34
44	a	845	BCR	C21-C22-C23-C24
44	a	846	BCR	C7-C8-C9-C10
44	a	846	BCR	C7-C8-C9-C34
44	a	847	BCR	C21-C22-C23-C24
44	b	843	BCR	C1-C6-C7-C8
44	b	843	BCR	C7-C8-C9-C10
44	b	843	BCR	C7-C8-C9-C34
44	b	843	BCR	C37-C22-C23-C24
44	b	844	BCR	C11-C10-C9-C8
44	b	844	BCR	C21-C22-C23-C24
44	b	844	BCR	C37-C22-C23-C24
44	f	801	BCR	C7-C8-C9-C34
44	f	801	BCR	C21-C22-C23-C24
44	f	801	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
44	f	806	BCR	C7-C8-C9-C34
44	f	806	BCR	C35-C13-C14-C15
44	f	806	BCR	C37-C22-C23-C24
44	i	103	BCR	C1-C6-C7-C8
44	i	103	BCR	C7-C8-C9-C34
44	i	103	BCR	C21-C22-C23-C24
44	i	103	BCR	C23-C24-C25-C26
44	i	103	BCR	C23-C24-C25-C30
44	j	107	BCR	C7-C8-C9-C10
44	j	107	BCR	C7-C8-C9-C34
44	l	203	BCR	C1-C6-C7-C8
44	l	203	BCR	C11-C10-C9-C8
44	l	203	BCR	C21-C22-C23-C24
44	l	203	BCR	C37-C22-C23-C24
44	l	203	BCR	C23-C24-C25-C30
44	l	207	BCR	C7-C8-C9-C10
44	m	101	BCR	C7-C8-C9-C10
44	m	101	BCR	C7-C8-C9-C34
44	m	101	BCR	C20-C21-C22-C37
44	m	101	BCR	C23-C24-C25-C30
44	h	201	BCR	C7-C8-C9-C10
44	h	201	BCR	C22-C23-C24-C25
44	h	201	BCR	C23-C24-C25-C30
35	A	302	A86	C39-C38-O4-C34
35	D	302	A86	C39-C38-O4-C34
35	F	301	A86	C39-C38-O4-C34
35	F	302	A86	O5-C38-O4-C34
35	F	304	A86	O5-C38-O4-C34
35	F	305	A86	C39-C38-O4-C34
35	G	302	A86	C39-C38-O4-C34
35	G	306	A86	C39-C38-O4-C34
35	G	306	A86	O5-C38-O4-C34
35	I	301	A86	C39-C38-O4-C34
35	I	302	A86	C39-C38-O4-C34
35	J	301	A86	C39-C38-O4-C34
35	J	302	A86	C39-C38-O4-C34
35	J	303	A86	C39-C38-O4-C34
35	J	306	A86	C39-C38-O4-C34
35	K	301	A86	C39-C38-O4-C34
35	K	303	A86	C39-C38-O4-C34
35	L	301	A86	C39-C38-O4-C34
35	M	304	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
35	N	302	A86	C39-C38-O4-C34
35	N	305	A86	C39-C38-O4-C34
35	O	319	A86	C39-C38-O4-C34
35	Q	316	A86	C39-C38-O4-C34
35	R	302	A86	C39-C38-O4-C34
35	R	306	A86	C39-C38-O4-C34
35	S	302	A86	C39-C38-O4-C34
35	T	302	A86	C39-C38-O4-C34
35	W	203	A86	C39-C38-O4-C34
35	X	314	A86	C39-C38-O4-C34
35	U	303	A86	C39-C38-O4-C34
35	V	302	A86	C39-C38-O4-C34
36	K	310	CLA	C2C-C3C-CAC-CBC
36	L	308	CLA	C4C-C3C-CAC-CBC
36	a	819	CLA	C4C-C3C-CAC-CBC
36	a	824	CLA	C4C-C3C-CAC-CBC
37	G	318	KC1	C4C-C3C-CAC-CBC
39	F	321	LMT	C3'-C4'-O1B-C1B
36	G	314	CLA	O1D-CGD-O2D-CED
36	G	316	CLA	O1D-CGD-O2D-CED
36	H	316	CLA	O1D-CGD-O2D-CED
36	K	307	CLA	O1D-CGD-O2D-CED
36	N	312	CLA	O1D-CGD-O2D-CED
36	Q	314	CLA	O1D-CGD-O2D-CED
36	W	212	CLA	O1D-CGD-O2D-CED
36	X	310	CLA	O1D-CGD-O2D-CED
36	a	848	CLA	O1D-CGD-O2D-CED
36	h	203	CLA	O1D-CGD-O2D-CED
36	V	306	CLA	O1D-CGD-O2D-CED
37	F	315	KC1	O1D-CGD-O2D-CED
39	K	317	LMT	C2B-C1B-O1B-C4'
36	O	316	CLA	C15-C16-C17-C18
36	j	102	CLA	C8-C10-C11-C12
35	A	316	A86	O5-C38-O4-C34
35	B	301	A86	C39-C38-O4-C34
35	C	204	A86	C39-C38-O4-C34
35	D	302	A86	O5-C38-O4-C34
35	F	304	A86	C39-C38-O4-C34
35	G	302	A86	O5-C38-O4-C34
35	J	305	A86	C39-C38-O4-C34
35	M	304	A86	O5-C38-O4-C34
35	N	304	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
35	N	305	A86	O5-C38-O4-C34
35	Q	316	A86	O5-C38-O4-C34
35	R	304	A86	C39-C38-O4-C34
35	S	304	A86	O5-C38-O4-C34
35	U	303	A86	O5-C38-O4-C34
35	V	301	A86	O5-C38-O4-C34
36	L	308	CLA	C2C-C3C-CAC-CBC
36	X	308	CLA	C2C-C3C-CAC-CBC
36	B	308	CLA	O1D-CGD-O2D-CED
36	B	309	CLA	O1D-CGD-O2D-CED
36	D	309	CLA	O1D-CGD-O2D-CED
36	N	317	CLA	O1D-CGD-O2D-CED
36	O	310	CLA	O1D-CGD-O2D-CED
36	P	312	CLA	O1D-CGD-O2D-CED
36	P	319	CLA	O1D-CGD-O2D-CED
36	Q	309	CLA	O1D-CGD-O2D-CED
36	R	322	CLA	O1D-CGD-O2D-CED
36	W	209	CLA	O1D-CGD-O2D-CED
36	X	315	CLA	O1D-CGD-O2D-CED
36	b	826	CLA	O1D-CGD-O2D-CED
36	i	102	CLA	O1D-CGD-O2D-CED
36	V	308	CLA	O1D-CGD-O2D-CED
36	V	314	CLA	O1D-CGD-O2D-CED
37	M	318	KC1	O1D-CGD-O2D-CED
36	A	307	CLA	CBD-CGD-O2D-CED
36	A	311	CLA	CBD-CGD-O2D-CED
36	A	313	CLA	CBD-CGD-O2D-CED
36	B	306	CLA	CBD-CGD-O2D-CED
36	B	309	CLA	CBD-CGD-O2D-CED
36	B	311	CLA	CBD-CGD-O2D-CED
36	D	313	CLA	CBD-CGD-O2D-CED
36	F	312	CLA	CBD-CGD-O2D-CED
36	G	309	CLA	CBD-CGD-O2D-CED
36	G	313	CLA	CBD-CGD-O2D-CED
36	G	314	CLA	CBD-CGD-O2D-CED
36	H	305	CLA	CBD-CGD-O2D-CED
36	H	312	CLA	CBD-CGD-O2D-CED
36	H	316	CLA	CBD-CGD-O2D-CED
36	J	315	CLA	CBD-CGD-O2D-CED
36	K	309	CLA	CBD-CGD-O2D-CED
36	K	310	CLA	CBD-CGD-O2D-CED
36	K	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	L	311	CLA	CBD-CGD-O2D-CED
36	L	314	CLA	CBD-CGD-O2D-CED
36	M	308	CLA	CBD-CGD-O2D-CED
36	M	312	CLA	CBD-CGD-O2D-CED
36	M	314	CLA	CBD-CGD-O2D-CED
36	M	315	CLA	CBD-CGD-O2D-CED
36	N	312	CLA	CBD-CGD-O2D-CED
36	N	318	CLA	CBD-CGD-O2D-CED
36	O	309	CLA	CBD-CGD-O2D-CED
36	P	311	CLA	CBD-CGD-O2D-CED
36	P	318	CLA	CBD-CGD-O2D-CED
36	P	319	CLA	CBD-CGD-O2D-CED
36	Q	308	CLA	CBD-CGD-O2D-CED
36	R	313	CLA	CBD-CGD-O2D-CED
36	S	315	CLA	CBD-CGD-O2D-CED
36	S	318	CLA	CBD-CGD-O2D-CED
36	S	321	CLA	CBD-CGD-O2D-CED
36	T	309	CLA	CBD-CGD-O2D-CED
36	T	311	CLA	CBD-CGD-O2D-CED
36	T	313	CLA	CBD-CGD-O2D-CED
36	W	209	CLA	CBD-CGD-O2D-CED
36	W	212	CLA	CBD-CGD-O2D-CED
36	W	214	CLA	CBD-CGD-O2D-CED
36	X	308	CLA	CBD-CGD-O2D-CED
36	X	315	CLA	CBD-CGD-O2D-CED
36	a	817	CLA	CBD-CGD-O2D-CED
36	a	827	CLA	CBD-CGD-O2D-CED
36	b	835	CLA	CBD-CGD-O2D-CED
36	b	840	CLA	CBD-CGD-O2D-CED
36	j	106	CLA	CBD-CGD-O2D-CED
36	h	203	CLA	CBD-CGD-O2D-CED
36	U	308	CLA	CBD-CGD-O2D-CED
36	U	311	CLA	CBD-CGD-O2D-CED
36	U	313	CLA	CBD-CGD-O2D-CED
36	V	307	CLA	CBD-CGD-O2D-CED
36	V	308	CLA	CBD-CGD-O2D-CED
36	V	311	CLA	CBD-CGD-O2D-CED
36	A	306	CLA	O1A-CGA-O2A-C1
36	D	307	CLA	O1A-CGA-O2A-C1
36	D	308	CLA	O1A-CGA-O2A-C1
36	H	311	CLA	O1A-CGA-O2A-C1
36	I	310	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	a	803	CLA	O1A-CGA-O2A-C1
41	G	301	LHG	O10-C23-O8-C6
42	E	319	LMG	O10-C28-O8-C9
42	J	318	LMG	O10-C28-O8-C9
36	A	309	CLA	O1A-CGA-O2A-C1
36	C	210	CLA	O1A-CGA-O2A-C1
36	R	314	CLA	O1A-CGA-O2A-C1
36	S	313	CLA	O1A-CGA-O2A-C1
36	W	210	CLA	O1A-CGA-O2A-C1
36	U	309	CLA	O1A-CGA-O2A-C1
35	J	306	A86	O5-C38-O4-C34
35	P	307	A86	C39-C38-O4-C34
36	K	310	CLA	C4C-C3C-CAC-CBC
36	R	316	CLA	C4C-C3C-CAC-CBC
36	R	319	CLA	C4C-C3C-CAC-CBC
36	a	819	CLA	C2C-C3C-CAC-CBC
36	a	824	CLA	C2C-C3C-CAC-CBC
37	F	308	KC1	C4C-C3C-CAC-CBC
37	G	318	KC1	C2C-C3C-CAC-CBC
39	G	322	LMT	C5'-C4'-O1B-C1B
36	B	311	CLA	O1D-CGD-O2D-CED
36	H	312	CLA	O1D-CGD-O2D-CED
36	I	313	CLA	O1D-CGD-O2D-CED
36	K	310	CLA	O1D-CGD-O2D-CED
36	W	214	CLA	O1D-CGD-O2D-CED
36	X	313	CLA	O1D-CGD-O2D-CED
36	U	308	CLA	O1D-CGD-O2D-CED
36	U	313	CLA	O1D-CGD-O2D-CED
37	G	317	KC1	O1D-CGD-O2D-CED
36	W	210	CLA	CBA-CGA-O2A-C1
36	E	316	CLA	C4C-C3C-CAC-CBC
37	F	308	KC1	C2C-C3C-CAC-CBC
37	T	310	KC1	C4C-C3C-CAC-CBC
35	O	305	A86	C35-C34-O4-C38
39	L	318	LMT	C2B-C1B-O1B-C4'
36	D	311	CLA	O1D-CGD-O2D-CED
36	G	315	CLA	O1D-CGD-O2D-CED
36	H	318	CLA	O1D-CGD-O2D-CED
36	J	312	CLA	O1D-CGD-O2D-CED
36	J	316	CLA	O1D-CGD-O2D-CED
36	L	311	CLA	O1D-CGD-O2D-CED
36	M	316	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	N	308	CLA	O1D-CGD-O2D-CED
36	R	311	CLA	O1D-CGD-O2D-CED
36	R	318	CLA	O1D-CGD-O2D-CED
36	S	310	CLA	O1D-CGD-O2D-CED
36	S	312	CLA	O1D-CGD-O2D-CED
36	T	308	CLA	O1D-CGD-O2D-CED
36	X	308	CLA	O1D-CGD-O2D-CED
36	U	310	CLA	O1D-CGD-O2D-CED
37	M	313	KC1	O1D-CGD-O2D-CED
36	A	306	CLA	CBA-CGA-O2A-C1
36	D	307	CLA	CBA-CGA-O2A-C1
36	D	308	CLA	CBA-CGA-O2A-C1
40	L	302	DGD	C2A-C1A-O1G-C1G
42	E	319	LMG	C29-C28-O8-C9
42	J	318	LMG	C29-C28-O8-C9
36	A	305	CLA	CBD-CGD-O2D-CED
36	A	306	CLA	CBD-CGD-O2D-CED
36	A	308	CLA	CBD-CGD-O2D-CED
36	A	314	CLA	CBD-CGD-O2D-CED
36	B	305	CLA	CBD-CGD-O2D-CED
36	C	212	CLA	CBD-CGD-O2D-CED
36	C	214	CLA	CBD-CGD-O2D-CED
36	E	315	CLA	CBD-CGD-O2D-CED
36	G	319	CLA	CBD-CGD-O2D-CED
36	H	314	CLA	CBD-CGD-O2D-CED
36	J	310	CLA	CBD-CGD-O2D-CED
36	K	315	CLA	CBD-CGD-O2D-CED
36	N	307	CLA	CBD-CGD-O2D-CED
36	N	309	CLA	CBD-CGD-O2D-CED
36	O	316	CLA	CBD-CGD-O2D-CED
36	R	310	CLA	CBD-CGD-O2D-CED
36	R	312	CLA	CBD-CGD-O2D-CED
36	S	317	CLA	CBD-CGD-O2D-CED
36	S	320	CLA	CBD-CGD-O2D-CED
36	W	210	CLA	CBD-CGD-O2D-CED
36	W	216	CLA	CBD-CGD-O2D-CED
36	a	802	CLA	CBD-CGD-O2D-CED
36	a	808	CLA	CBD-CGD-O2D-CED
36	a	809	CLA	CBD-CGD-O2D-CED
36	a	828	CLA	CBD-CGD-O2D-CED
36	a	832	CLA	CBD-CGD-O2D-CED
36	a	837	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	a	838	CLA	CBD-CGD-O2D-CED
36	b	805	CLA	CBD-CGD-O2D-CED
36	b	806	CLA	CBD-CGD-O2D-CED
36	b	818	CLA	CBD-CGD-O2D-CED
36	b	824	CLA	CBD-CGD-O2D-CED
36	b	828	CLA	CBD-CGD-O2D-CED
36	l	206	CLA	CBD-CGD-O2D-CED
36	U	305	CLA	CBD-CGD-O2D-CED
37	H	313	KC1	CBD-CGD-O2D-CED
35	J	301	A86	O5-C38-O4-C34
35	J	302	A86	O5-C38-O4-C34
35	M	305	A86	O5-C38-O4-C34
35	N	306	A86	O5-C38-O4-C34
36	M	308	CLA	C4C-C3C-CAC-CBC
37	E	309	KC1	C2C-C3C-CAC-CBC
36	A	310	CLA	O1A-CGA-O2A-C1
36	B	308	CLA	O1A-CGA-O2A-C1
36	D	312	CLA	O1A-CGA-O2A-C1
36	F	314	CLA	O1A-CGA-O2A-C1
36	G	311	CLA	O1A-CGA-O2A-C1
36	G	312	CLA	O1A-CGA-O2A-C1
36	G	319	CLA	O1A-CGA-O2A-C1
36	J	307	CLA	O1A-CGA-O2A-C1
36	L	309	CLA	O1A-CGA-O2A-C1
36	L	313	CLA	O1A-CGA-O2A-C1
36	N	312	CLA	O1A-CGA-O2A-C1
36	O	308	CLA	O1A-CGA-O2A-C1
36	P	310	CLA	O1A-CGA-O2A-C1
36	Q	307	CLA	O1A-CGA-O2A-C1
36	R	311	CLA	O1A-CGA-O2A-C1
36	T	309	CLA	O1A-CGA-O2A-C1
36	T	313	CLA	O1A-CGA-O2A-C1
36	W	207	CLA	O1A-CGA-O2A-C1
36	a	804	CLA	O1A-CGA-O2A-C1
36	a	816	CLA	O1A-CGA-O2A-C1
36	a	818	CLA	O1A-CGA-O2A-C1
36	a	839	CLA	O1A-CGA-O2A-C1
36	b	834	CLA	O1A-CGA-O2A-C1
36	f	804	CLA	O1A-CGA-O2A-C1
36	V	306	CLA	O1A-CGA-O2A-C1
41	a	850	LHG	O10-C23-O8-C6
41	f	809	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
42	D	321	LMG	O10-C28-O8-C9
42	a	852	LMG	O10-C28-O8-C9
42	m	102	LMG	O10-C28-O8-C9
36	D	312	CLA	O1D-CGD-O2D-CED
36	N	319	CLA	O1D-CGD-O2D-CED
36	S	311	CLA	O1D-CGD-O2D-CED
36	X	307	CLA	O1D-CGD-O2D-CED
36	X	312	CLA	O1D-CGD-O2D-CED
36	f	804	CLA	O1D-CGD-O2D-CED
36	O	308	CLA	C5-C6-C7-C8
36	b	817	CLA	C8-C10-C11-C12
37	S	316	KC1	CAA-CBA-CGA-O1A
35	A	302	A86	O5-C38-O4-C34
35	B	303	A86	O5-C38-O4-C34
35	I	302	A86	O5-C38-O4-C34
35	J	303	A86	O5-C38-O4-C34
35	K	303	A86	O5-C38-O4-C34
35	L	301	A86	O5-C38-O4-C34
35	L	304	A86	O5-C38-O4-C34
35	M	302	A86	O5-C38-O4-C34
35	N	302	A86	O5-C38-O4-C34
35	N	320	A86	O5-C38-O4-C34
35	O	319	A86	O5-C38-O4-C34
35	Q	304	A86	O5-C38-O4-C34
35	R	302	A86	O5-C38-O4-C34
35	R	306	A86	O5-C38-O4-C34
35	S	302	A86	O5-C38-O4-C34
35	T	302	A86	O5-C38-O4-C34
35	T	306	A86	O5-C38-O4-C34
35	W	203	A86	O5-C38-O4-C34
35	X	302	A86	O5-C38-O4-C34
35	X	305	A86	O5-C38-O4-C34
35	U	302	A86	O5-C38-O4-C34
35	V	302	A86	O5-C38-O4-C34
36	E	316	CLA	C2C-C3C-CAC-CBC
37	E	309	KC1	C4C-C3C-CAC-CBC
39	a	851	LMT	C3'-C4'-O1B-C1B
36	A	309	CLA	O1D-CGD-O2D-CED
36	H	317	CLA	O1D-CGD-O2D-CED
36	M	309	CLA	O1D-CGD-O2D-CED
36	a	836	CLA	O1D-CGD-O2D-CED
35	C	202	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
35	G	304	A86	C39-C38-O4-C34
35	K	306	A86	O5-C38-O4-C34
35	L	306	A86	O5-C38-O4-C34
35	R	305	A86	C39-C38-O4-C34
35	S	305	A86	O5-C38-O4-C34
35	V	304	A86	O5-C38-O4-C34
36	D	308	CLA	CBD-CGD-O2D-CED
36	I	306	CLA	C8-C10-C11-C12
36	A	307	CLA	O1D-CGD-O2D-CED
36	G	309	CLA	O1D-CGD-O2D-CED
36	K	309	CLA	O1D-CGD-O2D-CED
36	V	313	CLA	O1D-CGD-O2D-CED
38	b	804	SQD	O49-C7-O47-C45
40	C	215	DGD	O1B-C1B-O2G-C2G
40	L	302	DGD	O1B-C1B-O2G-C2G
41	D	319	LHG	O9-C7-O7-C5
41	F	319	LHG	O9-C7-O7-C5
41	Q	315	LHG	O9-C7-O7-C5
41	l	208	LHG	O9-C7-O7-C5
42	D	320	LMG	O9-C10-O7-C8
42	E	319	LMG	O9-C10-O7-C8
42	I	315	LMG	O9-C10-O7-C8
42	a	852	LMG	O9-C10-O7-C8
42	m	102	LMG	O9-C10-O7-C8
36	B	306	CLA	CBA-CGA-O2A-C1
35	F	307	A86	O5-C38-O4-C34
35	O	303	A86	O5-C38-O4-C34
35	P	304	A86	O5-C38-O4-C34
35	Q	301	A86	O5-C38-O4-C34
35	R	309	A86	O5-C38-O4-C34
35	T	307	A86	O5-C38-O4-C34
35	h	202	A86	O5-C38-O4-C34
36	R	319	CLA	C2C-C3C-CAC-CBC
36	T	311	CLA	C2C-C3C-CAC-CBC
37	T	310	KC1	C2C-C3C-CAC-CBC
36	X	309	CLA	O1A-CGA-O2A-C1
35	R	309	A86	C35-C34-O4-C38
39	B	312	LMT	O5B-C1B-O1B-C4'
36	A	306	CLA	C3-C5-C6-C7
36	A	314	CLA	C3-C5-C6-C7
36	B	305	CLA	C3-C5-C6-C7
36	C	208	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
36	C	211	CLA	C3-C5-C6-C7
36	C	212	CLA	C3-C5-C6-C7
36	D	307	CLA	C3-C5-C6-C7
36	D	313	CLA	C3-C5-C6-C7
36	E	315	CLA	C3-C5-C6-C7
36	E	316	CLA	C3-C5-C6-C7
36	G	313	CLA	C3-C5-C6-C7
36	H	308	CLA	C3-C5-C6-C7
36	I	306	CLA	C3-C5-C6-C7
36	I	308	CLA	C3-C5-C6-C7
36	J	313	CLA	C3-C5-C6-C7
36	K	307	CLA	C3-C5-C6-C7
36	K	308	CLA	C3-C5-C6-C7
36	K	313	CLA	C3-C5-C6-C7
36	M	307	CLA	C3-C5-C6-C7
36	O	306	CLA	C3-C5-C6-C7
36	P	301	CLA	C3-C5-C6-C7
36	P	308	CLA	C3-C5-C6-C7
36	P	314	CLA	C3-C5-C6-C7
36	Q	305	CLA	C3-C5-C6-C7
36	Q	310	CLA	C3-C5-C6-C7
36	S	310	CLA	C3-C5-C6-C7
36	W	207	CLA	C3-C5-C6-C7
36	W	211	CLA	C3-C5-C6-C7
36	a	829	CLA	C3-C5-C6-C7
36	b	811	CLA	C3-C5-C6-C7
36	b	816	CLA	C3-C5-C6-C7
36	b	819	CLA	C3-C5-C6-C7
36	j	101	CLA	C3-C5-C6-C7
36	U	310	CLA	C3-C5-C6-C7
36	H	311	CLA	CBA-CGA-O2A-C1
36	I	307	CLA	CBA-CGA-O2A-C1
36	I	310	CLA	CBA-CGA-O2A-C1
36	J	307	CLA	CBA-CGA-O2A-C1
36	L	313	CLA	CBA-CGA-O2A-C1
36	M	311	CLA	CBA-CGA-O2A-C1
36	N	312	CLA	CBA-CGA-O2A-C1
36	O	308	CLA	CBA-CGA-O2A-C1
36	P	310	CLA	CBA-CGA-O2A-C1
36	Q	307	CLA	CBA-CGA-O2A-C1
36	R	311	CLA	CBA-CGA-O2A-C1
36	S	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	T	309	CLA	CBA-CGA-O2A-C1
36	W	207	CLA	CBA-CGA-O2A-C1
36	f	804	CLA	CBA-CGA-O2A-C1
36	V	306	CLA	CBA-CGA-O2A-C1
41	F	319	LHG	C24-C23-O8-C6
41	G	301	LHG	C24-C23-O8-C6
41	a	850	LHG	C24-C23-O8-C6
41	f	808	LHG	C24-C23-O8-C6
41	f	809	LHG	C24-C23-O8-C6
42	D	321	LMG	C29-C28-O8-C9
42	a	852	LMG	C29-C28-O8-C9
42	m	102	LMG	C29-C28-O8-C9
36	W	218	CLA	C2C-C3C-CAC-CBC
38	A	315	SQD	C24-C23-O48-C46
38	b	804	SQD	C8-C7-O47-C45
40	L	302	DGD	C2B-C1B-O2G-C2G
41	R	323	LHG	C8-C7-O7-C5
42	J	318	LMG	C11-C10-O7-C8
42	J	319	LMG	C11-C10-O7-C8
36	B	306	CLA	O1D-CGD-O2D-CED
36	D	307	CLA	CBD-CGD-O2D-CED
36	a	820	CLA	CBD-CGD-O2D-CED
36	a	830	CLA	CBD-CGD-O2D-CED
35	F	305	A86	O5-C38-O4-C34
36	R	316	CLA	C2C-C3C-CAC-CBC
36	K	312	CLA	O1A-CGA-O2A-C1
36	B	306	CLA	O1A-CGA-O2A-C1
39	I	318	LMT	O5B-C1B-O1B-C4'
39	a	851	LMT	O5B-C1B-O1B-C4'
37	V	312	KC1	C2C-C3C-CAC-CBC
39	G	323	LMT	C3'-C4'-O1B-C1B
37	C	213	KC1	CAA-CBA-CGA-O1A
37	C	213	KC1	CAA-CBA-CGA-O2A
37	S	316	KC1	CAA-CBA-CGA-O2A
37	T	310	KC1	CAA-CBA-CGA-O1A
37	T	310	KC1	CAA-CBA-CGA-O2A
37	V	312	KC1	CAA-CBA-CGA-O1A
36	I	309	CLA	CBA-CGA-O2A-C1
36	X	309	CLA	CBA-CGA-O2A-C1
36	F	313	CLA	C3-C5-C6-C7
36	H	315	CLA	C4C-C3C-CAC-CBC
39	K	317	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
36	B	311	CLA	C4-C3-C5-C6
36	D	308	CLA	C4-C3-C5-C6
36	E	314	CLA	C4-C3-C5-C6
36	F	314	CLA	C4-C3-C5-C6
36	H	316	CLA	C4-C3-C5-C6
36	L	309	CLA	C4-C3-C5-C6
36	O	307	CLA	C4-C3-C5-C6
36	P	309	CLA	C4-C3-C5-C6
36	Q	306	CLA	C4-C3-C5-C6
36	W	206	CLA	C4-C3-C5-C6
36	U	310	CLA	C4-C3-C5-C6
39	I	317	LMT	C4'-C5'-C6'-O6'
36	B	311	CLA	C2-C3-C5-C6
36	F	314	CLA	C2-C3-C5-C6
36	H	316	CLA	C2-C3-C5-C6
36	R	311	CLA	C2-C3-C5-C6
36	W	206	CLA	C2-C3-C5-C6
36	a	823	CLA	C2-C3-C5-C6
36	U	310	CLA	C2-C3-C5-C6
36	O	312	CLA	CBD-CGD-O2D-CED
36	O	314	CLA	CBD-CGD-O2D-CED
36	P	314	CLA	CBD-CGD-O2D-CED
36	P	316	CLA	CBD-CGD-O2D-CED
36	Q	310	CLA	CBD-CGD-O2D-CED
36	Q	312	CLA	CBD-CGD-O2D-CED
36	W	206	CLA	CBD-CGD-O2D-CED
36	X	306	CLA	CBD-CGD-O2D-CED
36	a	815	CLA	CBD-CGD-O2D-CED
36	a	829	CLA	CBD-CGD-O2D-CED
36	b	808	CLA	CBD-CGD-O2D-CED
36	b	816	CLA	CBD-CGD-O2D-CED
36	l	202	CLA	CBD-CGD-O2D-CED
36	G	313	CLA	C2A-CAA-CBA-CGA
36	G	319	CLA	C2A-CAA-CBA-CGA
36	H	316	CLA	C2A-CAA-CBA-CGA
36	a	807	CLA	C2A-CAA-CBA-CGA
36	a	819	CLA	C2A-CAA-CBA-CGA
36	a	823	CLA	C2A-CAA-CBA-CGA
36	a	828	CLA	C2A-CAA-CBA-CGA
36	b	816	CLA	C2A-CAA-CBA-CGA
36	b	839	CLA	C2A-CAA-CBA-CGA
36	f	802	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
35	F	301	A86	O5-C38-O4-C34
35	I	301	A86	O5-C38-O4-C34
36	A	311	CLA	C3-C5-C6-C7
36	C	207	CLA	C3-C5-C6-C7
36	F	314	CLA	C3-C5-C6-C7
36	L	313	CLA	C3-C5-C6-C7
36	M	306	CLA	C3-C5-C6-C7
36	P	319	CLA	C3-C5-C6-C7
36	R	310	CLA	C3-C5-C6-C7
36	R	311	CLA	C3-C5-C6-C7
36	R	312	CLA	C3-C5-C6-C7
36	S	312	CLA	C3-C5-C6-C7
36	a	806	CLA	C3-C5-C6-C7
36	a	812	CLA	C3-C5-C6-C7
36	b	812	CLA	C3-C5-C6-C7
36	b	824	CLA	C3-C5-C6-C7
36	j	102	CLA	C3-C5-C6-C7
36	A	310	CLA	CBA-CGA-O2A-C1
36	B	308	CLA	CBA-CGA-O2A-C1
36	D	312	CLA	CBA-CGA-O2A-C1
36	D	317	CLA	CBA-CGA-O2A-C1
36	E	313	CLA	CBA-CGA-O2A-C1
36	F	312	CLA	CBA-CGA-O2A-C1
36	F	314	CLA	CBA-CGA-O2A-C1
36	G	311	CLA	CBA-CGA-O2A-C1
36	G	312	CLA	CBA-CGA-O2A-C1
36	G	316	CLA	CBA-CGA-O2A-C1
36	G	319	CLA	CBA-CGA-O2A-C1
36	L	309	CLA	CBA-CGA-O2A-C1
36	M	312	CLA	CBA-CGA-O2A-C1
36	N	308	CLA	CBA-CGA-O2A-C1
36	P	314	CLA	CBA-CGA-O2A-C1
36	S	320	CLA	CBA-CGA-O2A-C1
36	T	313	CLA	CBA-CGA-O2A-C1
36	a	804	CLA	CBA-CGA-O2A-C1
36	a	816	CLA	CBA-CGA-O2A-C1
36	a	818	CLA	CBA-CGA-O2A-C1
36	a	839	CLA	CBA-CGA-O2A-C1
36	b	833	CLA	CBA-CGA-O2A-C1
36	b	834	CLA	CBA-CGA-O2A-C1
36	U	306	CLA	CBA-CGA-O2A-C1
40	C	215	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
41	Q	315	LHG	C24-C23-O8-C6
42	G	325	LMG	C29-C28-O8-C9
39	F	320	LMT	O5'-C5'-C6'-O6'
39	G	322	LMT	O5B-C5B-C6B-O6B
35	R	304	A86	O5-C38-O4-C34
36	H	305	CLA	O1D-CGD-O2D-CED
36	a	817	CLA	O1D-CGD-O2D-CED
40	C	215	DGD	C4D-C5D-C6D-O5D
36	b	837	CLA	CBD-CGD-O2D-CED
36	M	308	CLA	C2C-C3C-CAC-CBC
36	X	308	CLA	C4C-C3C-CAC-CBC
36	G	313	CLA	O1D-CGD-O2D-CED
36	L	314	CLA	O1D-CGD-O2D-CED
36	M	312	CLA	O1D-CGD-O2D-CED
36	M	314	CLA	O1D-CGD-O2D-CED
36	P	318	CLA	O1D-CGD-O2D-CED
36	S	315	CLA	O1D-CGD-O2D-CED
36	j	106	CLA	O1D-CGD-O2D-CED
36	U	311	CLA	O1D-CGD-O2D-CED
42	j	105	LMG	C4-C5-C6-O5
36	B	305	CLA	O1A-CGA-O2A-C1
36	C	211	CLA	O1A-CGA-O2A-C1
36	D	317	CLA	O1A-CGA-O2A-C1
36	E	313	CLA	O1A-CGA-O2A-C1
36	F	312	CLA	O1A-CGA-O2A-C1
36	I	307	CLA	O1A-CGA-O2A-C1
36	J	312	CLA	O1A-CGA-O2A-C1
36	M	311	CLA	O1A-CGA-O2A-C1
36	N	308	CLA	O1A-CGA-O2A-C1
36	O	316	CLA	O1A-CGA-O2A-C1
36	P	314	CLA	O1A-CGA-O2A-C1
36	Q	310	CLA	O1A-CGA-O2A-C1
36	S	310	CLA	O1A-CGA-O2A-C1
36	S	320	CLA	O1A-CGA-O2A-C1
36	W	211	CLA	O1A-CGA-O2A-C1
36	b	820	CLA	O1A-CGA-O2A-C1
36	b	833	CLA	O1A-CGA-O2A-C1
36	U	306	CLA	O1A-CGA-O2A-C1
36	V	310	CLA	O1A-CGA-O2A-C1
41	F	319	LHG	O10-C23-O8-C6
41	G	321	LHG	O10-C23-O8-C6
41	f	808	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
41	D	318	LHG	C31-C32-C33-C34
36	K	311	CLA	O1A-CGA-O2A-C1
36	A	313	CLA	O1D-CGD-O2D-CED
36	V	311	CLA	O1D-CGD-O2D-CED
34	Q	302	DD6	C3-C4-C5-C6
34	R	307	DD6	C1-C2-C3-C4
34	j	103	DD6	C11-C10-C9-C8
35	S	308	A86	C3-C4-C5-C6
35	U	301	A86	C24-C25-C26-C27
35	U	303	A86	C3-C4-C5-C6
35	V	301	A86	C3-C4-C5-C6
39	U	315	LMT	O5B-C1B-O1B-C4'
39	B	312	LMT	C2B-C1B-O1B-C4'
39	K	317	LMT	C4B-C5B-C6B-O6B
35	L	307	A86	C39-C38-O4-C34
35	T	303	A86	C39-C38-O4-C34
35	X	301	A86	C39-C38-O4-C34
36	H	315	CLA	C2C-C3C-CAC-CBC
36	J	316	CLA	C2C-C3C-CAC-CBC
37	V	312	KC1	CAA-CBA-CGA-O2A
36	C	205	CLA	CBD-CGD-O2D-CED
36	J	309	CLA	CBD-CGD-O2D-CED
36	K	311	CLA	CBD-CGD-O2D-CED
36	M	307	CLA	CBD-CGD-O2D-CED
36	N	316	CLA	CBD-CGD-O2D-CED
36	P	302	CLA	CBD-CGD-O2D-CED
36	R	316	CLA	CBD-CGD-O2D-CED
36	R	321	CLA	CBD-CGD-O2D-CED
36	S	319	CLA	CBD-CGD-O2D-CED
36	T	312	CLA	CBD-CGD-O2D-CED
36	b	815	CLA	CBD-CGD-O2D-CED
37	T	315	KC1	CBD-CGD-O2D-CED
37	U	312	KC1	CBD-CGD-O2D-CED
36	J	315	CLA	O1D-CGD-O2D-CED
41	G	301	LHG	O2-C2-C3-O3
41	I	316	LHG	O2-C2-C3-O3
41	O	318	LHG	O2-C2-C3-O3
41	Q	315	LHG	O2-C2-C3-O3
41	a	843	LHG	O2-C2-C3-O3
41	j	104	LHG	O2-C2-C3-O3
41	l	208	LHG	O2-C2-C3-O3
36	E	314	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
36	F	310	CLA	C3-C5-C6-C7
36	L	310	CLA	C3-C5-C6-C7
36	L	320	CLA	C3-C5-C6-C7
36	O	311	CLA	C3-C5-C6-C7
36	P	313	CLA	C3-C5-C6-C7
36	W	206	CLA	C3-C5-C6-C7
36	a	839	CLA	C3-C5-C6-C7
36	b	805	CLA	C3-C5-C6-C7
36	l	205	CLA	C3-C5-C6-C7
36	U	311	CLA	C3-C5-C6-C7
36	V	306	CLA	C3-C5-C6-C7
36	B	305	CLA	CBA-CGA-O2A-C1
36	C	211	CLA	CBA-CGA-O2A-C1
36	J	312	CLA	CBA-CGA-O2A-C1
36	K	312	CLA	CBA-CGA-O2A-C1
36	K	313	CLA	CBA-CGA-O2A-C1
36	Q	310	CLA	CBA-CGA-O2A-C1
36	X	306	CLA	CBA-CGA-O2A-C1
36	V	310	CLA	CBA-CGA-O2A-C1
41	G	321	LHG	C24-C23-O8-C6
42	D	320	LMG	C29-C28-O8-C9
42	V	315	LMG	C29-C28-O8-C9
35	H	301	A86	O5-C38-O4-C34
35	I	304	A86	C39-C38-O4-C34
35	K	302	A86	C39-C38-O4-C34
35	L	307	A86	O5-C38-O4-C34
35	L	319	A86	C39-C38-O4-C34
35	M	301	A86	C39-C38-O4-C34
35	N	301	A86	C39-C38-O4-C34
35	N	303	A86	C39-C38-O4-C34
35	O	302	A86	C39-C38-O4-C34
35	P	303	A86	C39-C38-O4-C34
35	R	301	A86	C39-C38-O4-C34
35	R	303	A86	C39-C38-O4-C34
35	R	303	A86	O5-C38-O4-C34
35	S	301	A86	C39-C38-O4-C34
35	S	303	A86	C39-C38-O4-C34
35	T	303	A86	O5-C38-O4-C34
35	T	305	A86	C39-C38-O4-C34
35	W	202	A86	C39-C38-O4-C34
35	X	303	A86	C39-C38-O4-C34
35	X	304	A86	C39-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
35	U	301	A86	C39-C38-O4-C34
35	V	303	A86	C39-C38-O4-C34
36	G	316	CLA	O1A-CGA-O2A-C1
38	b	804	SQD	O10-C23-O48-C46
42	D	320	LMG	O10-C28-O8-C9
42	G	325	LMG	O10-C28-O8-C9
39	I	318	LMT	O5'-C5'-C6'-O6'
39	a	851	LMT	O5'-C5'-C6'-O6'
39	U	315	LMT	O5'-C5'-C6'-O6'
42	G	325	LMG	O6-C5-C6-O5
42	J	319	LMG	O6-C5-C6-O5
42	L	321	LMG	O6-C5-C6-O5
36	M	315	CLA	O1D-CGD-O2D-CED
36	O	309	CLA	O1D-CGD-O2D-CED
36	P	311	CLA	O1D-CGD-O2D-CED
36	Q	308	CLA	O1D-CGD-O2D-CED
36	S	318	CLA	O1D-CGD-O2D-CED
36	K	313	CLA	C5-C6-C7-C8
41	f	809	LHG	C8-C7-O7-C5
35	C	202	A86	O5-C38-O4-C34
35	G	304	A86	O5-C38-O4-C34
35	I	304	A86	O5-C38-O4-C34
35	K	302	A86	O5-C38-O4-C34
35	L	319	A86	O5-C38-O4-C34
35	M	301	A86	O5-C38-O4-C34
35	N	301	A86	O5-C38-O4-C34
35	N	303	A86	O5-C38-O4-C34
35	O	302	A86	O5-C38-O4-C34
35	P	303	A86	O5-C38-O4-C34
35	R	301	A86	O5-C38-O4-C34
35	S	301	A86	O5-C38-O4-C34
35	S	303	A86	O5-C38-O4-C34
35	T	305	A86	O5-C38-O4-C34
35	W	202	A86	O5-C38-O4-C34
35	X	301	A86	O5-C38-O4-C34
35	X	303	A86	O5-C38-O4-C34
35	X	304	A86	O5-C38-O4-C34
35	U	301	A86	O5-C38-O4-C34
35	V	303	A86	O5-C38-O4-C34
36	N	318	CLA	O1D-CGD-O2D-CED
36	D	311	CLA	CBA-CGA-O2A-C1
36	N	311	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	J	308	CLA	CBD-CGD-O2D-CED
36	L	308	CLA	CBD-CGD-O2D-CED
36	R	315	CLA	CBD-CGD-O2D-CED
39	B	313	LMT	O5'-C5'-C6'-O6'
39	F	321	LMT	O5B-C5B-C6B-O6B
39	K	318	LMT	O5'-C5'-C6'-O6'
39	L	318	LMT	O5'-C5'-C6'-O6'
39	a	851	LMT	O5B-C5B-C6B-O6B
42	J	318	LMG	O6-C5-C6-O5
42	V	316	LMG	O6-C5-C6-O5
36	b	836	CLA	C2C-C3C-CAC-CBC
41	D	319	LHG	C14-C15-C16-C17
41	D	319	LHG	C34-C35-C36-C37
41	a	842	LHG	C28-C29-C30-C31
41	a	850	LHG	C11-C10-C9-C8
41	b	850	LHG	C11-C10-C9-C8
42	D	320	LMG	C23-C24-C25-C26
42	G	325	LMG	C14-C15-C16-C17
42	I	315	LMG	C13-C14-C15-C16
41	b	850	LHG	C5-C6-O8-C23
35	X	305	A86	C35-C34-O4-C38
36	T	309	CLA	O1D-CGD-O2D-CED
39	B	313	LMT	O5B-C1B-O1B-C4'
39	I	317	LMT	C2-C3-C4-C5
40	C	215	DGD	C4B-C5B-C6B-C7B
41	E	322	LHG	C18-C19-C20-C21
41	G	321	LHG	C11-C10-C9-C8
41	Q	315	LHG	C28-C29-C30-C31
41	a	850	LHG	C10-C11-C12-C13
41	a	850	LHG	C28-C29-C30-C31
41	f	808	LHG	C24-C25-C26-C27
41	i	104	LHG	C12-C13-C14-C15
41	j	104	LHG	C11-C10-C9-C8
41	j	104	LHG	C17-C18-C19-C20
42	E	318	LMG	C20-C21-C22-C23
42	I	315	LMG	C36-C37-C38-C39
39	B	312	LMT	O5'-C5'-C6'-O6'
39	I	317	LMT	O5'-C5'-C6'-O6'
40	b	849	DGD	O6E-C5E-C6E-O5E
42	D	320	LMG	O6-C5-C6-O5
42	V	315	LMG	O6-C5-C6-O5
39	F	320	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
42	E	319	LMG	C4-C5-C6-O5
42	J	318	LMG	C4-C5-C6-O5
36	I	309	CLA	O1A-CGA-O2A-C1
36	R	313	CLA	O1D-CGD-O2D-CED
36	S	321	CLA	O1D-CGD-O2D-CED
36	T	313	CLA	O1D-CGD-O2D-CED
39	a	854	LMT	C3'-C4'-O1B-C1B
41	Q	315	LHG	C11-C10-C9-C8
41	a	850	LHG	C30-C31-C32-C33
42	J	318	LMG	C23-C24-C25-C26
36	N	316	CLA	C13-C15-C16-C17
36	a	824	CLA	C8-C10-C11-C12
36	E	310	CLA	C3-C5-C6-C7
36	O	308	CLA	C3-C5-C6-C7
36	T	309	CLA	C3-C5-C6-C7
36	a	803	CLA	C3-C5-C6-C7
36	b	820	CLA	C3-C5-C6-C7
36	b	825	CLA	C3-C5-C6-C7
36	O	316	CLA	CBA-CGA-O2A-C1
36	W	211	CLA	CBA-CGA-O2A-C1
36	b	817	CLA	CBA-CGA-O2A-C1
36	b	820	CLA	CBA-CGA-O2A-C1
38	b	804	SQD	C24-C23-O48-C46
36	F	312	CLA	O1D-CGD-O2D-CED
41	f	809	LHG	O9-C7-O7-C5
37	H	313	KC1	CAA-CBA-CGA-O2A
40	C	215	DGD	C2B-C3B-C4B-C5B
41	E	322	LHG	C2-C3-O3-P
41	Q	315	LHG	C2-C3-O3-P
41	j	104	LHG	C2-C3-O3-P
36	E	314	CLA	O1A-CGA-O2A-C1
36	M	312	CLA	O1A-CGA-O2A-C1
36	X	306	CLA	O1A-CGA-O2A-C1
40	C	215	DGD	O1A-C1A-O1G-C1G
41	Q	315	LHG	O10-C23-O8-C6
36	S	321	CLA	C3-C5-C6-C7
35	J	305	A86	O5-C38-O4-C34
35	N	304	A86	O5-C38-O4-C34
35	S	308	A86	C39-C38-O4-C34
42	E	318	LMG	C15-C16-C17-C18
42	j	105	LMG	C19-C20-C21-C22
39	B	313	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
39	F	321	LMT	O5'-C5'-C6'-O6'
42	E	319	LMG	O6-C5-C6-O5
36	A	306	CLA	C4-C3-C5-C6
36	C	212	CLA	C4-C3-C5-C6
36	E	313	CLA	C4-C3-C5-C6
36	E	315	CLA	C4-C3-C5-C6
36	K	307	CLA	C4-C3-C5-C6
36	K	309	CLA	C4-C3-C5-C6
36	L	314	CLA	C4-C3-C5-C6
36	M	306	CLA	C4-C3-C5-C6
36	O	316	CLA	C4-C3-C5-C6
36	a	811	CLA	C4-C3-C5-C6
36	b	833	CLA	C4-C3-C5-C6
36	l	201	CLA	C4-C3-C5-C6
39	G	322	LMT	C4B-C5B-C6B-O6B
36	A	306	CLA	C2-C3-C5-C6
36	C	212	CLA	C2-C3-C5-C6
36	E	313	CLA	C2-C3-C5-C6
36	E	314	CLA	C2-C3-C5-C6
36	E	315	CLA	C2-C3-C5-C6
36	K	307	CLA	C2-C3-C5-C6
36	K	309	CLA	C2-C3-C5-C6
36	L	314	CLA	C2-C3-C5-C6
36	M	306	CLA	C2-C3-C5-C6
36	O	316	CLA	C2-C3-C5-C6
36	a	811	CLA	C2-C3-C5-C6
36	b	817	CLA	C2-C3-C5-C6
36	b	833	CLA	C2-C3-C5-C6
36	j	101	CLA	C2-C3-C5-C6
36	l	201	CLA	C2-C3-C5-C6
36	a	834	CLA	CBD-CGD-O2D-CED
35	L	304	A86	C35-C34-O4-C38
36	S	321	CLA	C2A-CAA-CBA-CGA
36	a	802	CLA	O1D-CGD-O2D-CED
36	a	827	CLA	O1D-CGD-O2D-CED
36	b	828	CLA	O1D-CGD-O2D-CED
36	b	840	CLA	O1D-CGD-O2D-CED
36	V	307	CLA	O1D-CGD-O2D-CED
41	E	322	LHG	C14-C15-C16-C17
41	b	850	LHG	C10-C11-C12-C13
39	K	317	LMT	O5B-C5B-C6B-O6B
40	L	302	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
42	a	852	LMG	O6-C5-C6-O5
42	j	105	LMG	O6-C5-C6-O5
36	K	313	CLA	O1A-CGA-O2A-C1
36	b	817	CLA	O1A-CGA-O2A-C1
42	V	315	LMG	O10-C28-O8-C9
39	G	323	LMT	C4B-C5B-C6B-O6B
39	U	315	LMT	C4'-C5'-C6'-O6'
39	L	318	LMT	O5'-C1'-O1'-C1
39	a	851	LMT	O5'-C1'-O1'-C1
40	L	302	DGD	O6E-C1E-O5D-C6D
42	G	324	LMG	O6-C1-O1-C7
36	D	313	CLA	O1D-CGD-O2D-CED
35	C	204	A86	O5-C38-O4-C34
41	R	323	LHG	C30-C31-C32-C33
42	a	852	LMG	C15-C16-C17-C18
39	U	315	LMT	C2B-C1B-O1B-C4'
36	E	314	CLA	CBA-CGA-O2A-C1
36	N	318	CLA	CBA-CGA-O2A-C1
36	A	311	CLA	O1D-CGD-O2D-CED
36	R	316	CLA	CBA-CGA-O2A-C1
36	W	218	CLA	C4C-C3C-CAC-CBC
36	A	308	CLA	O1D-CGD-O2D-CED
36	K	313	CLA	O1D-CGD-O2D-CED
36	M	308	CLA	O1D-CGD-O2D-CED
36	S	317	CLA	O1D-CGD-O2D-CED
36	T	311	CLA	O1D-CGD-O2D-CED
36	W	216	CLA	O1D-CGD-O2D-CED
36	b	806	CLA	O1D-CGD-O2D-CED
36	b	835	CLA	O1D-CGD-O2D-CED
37	H	313	KC1	O1D-CGD-O2D-CED
37	B	310	KC1	CAA-CBA-CGA-O1A
37	G	317	KC1	CAA-CBA-CGA-O1A
37	G	318	KC1	CAA-CBA-CGA-O2A
37	H	313	KC1	CAA-CBA-CGA-O1A
37	W	213	KC1	CAA-CBA-CGA-O2A
41	F	318	LHG	C8-C7-O7-C5
35	B	303	A86	C35-C34-O4-C38
35	N	302	A86	C35-C34-O4-C38
35	S	302	A86	C35-C34-O4-C38
35	T	303	A86	C35-C34-O4-C38
35	W	202	A86	C33-C34-O4-C38
35	V	303	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
39	a	853	LMT	C4B-C5B-C6B-O6B
39	U	315	LMT	C4B-C5B-C6B-O6B
35	B	301	A86	O5-C38-O4-C34
41	Q	315	LHG	C25-C26-C27-C28
42	D	321	LMG	C13-C14-C15-C16
36	C	212	CLA	O1D-CGD-O2D-CED
36	J	310	CLA	O1D-CGD-O2D-CED
36	a	828	CLA	O1D-CGD-O2D-CED
36	H	308	CLA	O1A-CGA-O2A-C1
35	P	307	A86	O5-C38-O4-C34
36	J	312	CLA	C3-C5-C6-C7
36	a	816	CLA	C3-C5-C6-C7
36	a	808	CLA	O1D-CGD-O2D-CED
36	a	832	CLA	O1D-CGD-O2D-CED
36	a	837	CLA	O1D-CGD-O2D-CED
36	A	314	CLA	CBA-CGA-O2A-C1
36	D	316	CLA	CBA-CGA-O2A-C1
36	E	308	CLA	CBA-CGA-O2A-C1
36	H	308	CLA	CBA-CGA-O2A-C1
36	I	305	CLA	CBA-CGA-O2A-C1
36	K	308	CLA	CBA-CGA-O2A-C1
36	M	306	CLA	CBA-CGA-O2A-C1
36	O	306	CLA	CBA-CGA-O2A-C1
36	P	308	CLA	CBA-CGA-O2A-C1
36	Q	305	CLA	CBA-CGA-O2A-C1
36	R	312	CLA	CBA-CGA-O2A-C1
36	a	822	CLA	CBA-CGA-O2A-C1
36	a	836	CLA	CBA-CGA-O2A-C1
36	b	824	CLA	CBA-CGA-O2A-C1
36	b	831	CLA	CBA-CGA-O2A-C1
36	b	840	CLA	CBA-CGA-O2A-C1
36	l	202	CLA	CBA-CGA-O2A-C1
36	l	204	CLA	CBA-CGA-O2A-C1
36	U	305	CLA	CBA-CGA-O2A-C1
41	I	316	LHG	C24-C23-O8-C6
36	W	218	CLA	CBD-CGD-O2D-CED
36	a	811	CLA	CBD-CGD-O2D-CED
42	a	852	LMG	C4-C5-C6-O5
41	j	104	LHG	C11-C12-C13-C14
36	D	311	CLA	O1A-CGA-O2A-C1
36	b	824	CLA	O1D-CGD-O2D-CED
34	D	303	DD6	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
34	D	303	DD6	C3-C4-C5-C6
34	L	305	DD6	C24-C25-C26-C27
34	W	204	DD6	C24-C25-C26-C27
35	N	304	A86	C11-C10-C9-C8
35	U	303	A86	C1-C2-C3-C4
35	F	305	A86	C35-C34-O4-C38
36	G	309	CLA	C13-C15-C16-C17
36	S	320	CLA	C13-C15-C16-C17
36	a	820	CLA	C5-C6-C7-C8
36	a	822	CLA	O1A-CGA-O2A-C1
39	F	321	LMT	C4'-C5'-C6'-O6'
40	L	302	DGD	C4E-C5E-C6E-O5E
42	G	325	LMG	C4-C5-C6-O5
35	O	301	A86	C39-C38-O4-C34
37	N	314	KC1	C2C-C3C-CAC-CBC
37	E	309	KC1	CAA-CBA-CGA-O1A
37	E	309	KC1	CAA-CBA-CGA-O2A
37	F	308	KC1	CAA-CBA-CGA-O2A
37	G	308	KC1	CAA-CBA-CGA-O1A
37	G	318	KC1	CAA-CBA-CGA-O1A
37	J	314	KC1	CAA-CBA-CGA-O1A
37	M	313	KC1	CAA-CBA-CGA-O1A
36	a	809	CLA	O1D-CGD-O2D-CED
42	V	315	LMG	C32-C33-C34-C35
39	B	313	LMT	C4B-C5B-C6B-O6B
42	J	319	LMG	C4-C5-C6-O5
36	A	307	CLA	C10-C11-C12-C13
36	D	308	CLA	C5-C6-C7-C8
36	F	309	CLA	C13-C15-C16-C17
36	H	316	CLA	C5-C6-C7-C8
36	P	301	CLA	C5-C6-C7-C8
36	P	311	CLA	C8-C10-C11-C12
36	Q	308	CLA	C8-C10-C11-C12
36	a	810	CLA	C8-C10-C11-C12
36	a	812	CLA	C10-C11-C12-C13
36	b	809	CLA	C10-C11-C12-C13
36	b	837	CLA	C13-C15-C16-C17
36	U	306	CLA	C13-C15-C16-C17
36	V	313	CLA	C8-C10-C11-C12
36	B	307	CLA	CBA-CGA-O2A-C1
41	F	319	LHG	O2-C2-C3-O3
41	O	317	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
41	a	850	LHG	O2-C2-C3-O3
41	f	808	LHG	O2-C2-C3-O3
36	l	201	CLA	C3-C5-C6-C7
38	b	804	SQD	C23-C24-C25-C26
41	F	318	LHG	C23-C24-C25-C26
42	a	852	LMG	C28-C29-C30-C31
36	F	311	CLA	C3-C5-C6-C7
36	O	316	CLA	O1D-CGD-O2D-CED
39	E	323	LMT	C2'-C1'-O1'-C1
39	F	320	LMT	C2'-C1'-O1'-C1
39	K	318	LMT	C2'-C1'-O1'-C1
39	P	320	LMT	C2'-C1'-O1'-C1
39	a	851	LMT	C2'-C1'-O1'-C1
39	f	807	LMT	C2'-C1'-O1'-C1
40	L	302	DGD	C2E-C1E-O5D-C6D
42	D	321	LMG	C2-C1-O1-C7
42	E	318	LMG	C2-C1-O1-C7
38	A	315	SQD	O10-C23-O48-C46
36	A	314	CLA	O1A-CGA-O2A-C1
36	K	308	CLA	O1A-CGA-O2A-C1
36	R	312	CLA	O1A-CGA-O2A-C1
36	b	824	CLA	O1A-CGA-O2A-C1
39	G	323	LMT	O5B-C5B-C6B-O6B
39	F	321	LMT	C4B-C5B-C6B-O6B
36	D	308	CLA	C2-C3-C5-C6
36	L	309	CLA	C2-C3-C5-C6
36	O	307	CLA	C2-C3-C5-C6
36	P	309	CLA	C2-C3-C5-C6
36	Q	306	CLA	C2-C3-C5-C6
36	B	305	CLA	C14-C13-C15-C16
36	C	206	CLA	C6-C7-C8-C9
36	C	207	CLA	C11-C10-C8-C9
36	C	208	CLA	C6-C7-C8-C9
36	C	212	CLA	C14-C13-C15-C16
36	D	307	CLA	C11-C10-C8-C9
36	D	308	CLA	C6-C7-C8-C9
36	E	311	CLA	C11-C10-C8-C9
36	E	315	CLA	C11-C12-C13-C14
36	E	315	CLA	C14-C13-C15-C16
36	E	316	CLA	C6-C7-C8-C9
36	F	317	CLA	C6-C7-C8-C9
36	G	309	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	G	309	CLA	C14-C13-C15-C16
36	G	313	CLA	C11-C12-C13-C14
36	H	315	CLA	C6-C7-C8-C9
36	I	306	CLA	C11-C12-C13-C14
36	I	308	CLA	C11-C10-C8-C9
36	I	308	CLA	C11-C12-C13-C14
36	J	309	CLA	C11-C12-C13-C14
36	J	313	CLA	C14-C13-C15-C16
36	K	310	CLA	C6-C7-C8-C9
36	K	313	CLA	C11-C12-C13-C14
36	L	309	CLA	C6-C7-C8-C9
36	M	311	CLA	C11-C12-C13-C14
36	N	308	CLA	C14-C13-C15-C16
36	O	309	CLA	C6-C7-C8-C9
36	O	316	CLA	C11-C10-C8-C9
36	P	301	CLA	C6-C7-C8-C9
36	P	301	CLA	C11-C12-C13-C14
36	P	311	CLA	C6-C7-C8-C9
36	Q	308	CLA	C6-C7-C8-C9
36	Q	310	CLA	C11-C10-C8-C9
36	R	312	CLA	C11-C12-C13-C14
36	S	310	CLA	C6-C7-C8-C9
36	T	309	CLA	C6-C7-C8-C9
36	T	314	CLA	C6-C7-C8-C9
36	W	207	CLA	C6-C7-C8-C9
36	a	806	CLA	C11-C10-C8-C9
36	a	825	CLA	C11-C12-C13-C14
36	a	831	CLA	C11-C10-C8-C9
36	a	839	CLA	C11-C10-C8-C9
36	a	839	CLA	C14-C13-C15-C16
36	b	816	CLA	C11-C10-C8-C9
36	b	817	CLA	C6-C7-C8-C9
36	b	821	CLA	C6-C7-C8-C9
36	i	102	CLA	C6-C7-C8-C9
36	l	205	CLA	C11-C10-C8-C9
36	h	203	CLA	C6-C7-C8-C9
36	U	305	CLA	C6-C7-C8-C9
36	V	306	CLA	C6-C7-C8-C9
36	V	314	CLA	C11-C12-C13-C14
43	b	842	PQN	C24-C23-C25-C26
36	A	305	CLA	O1D-CGD-O2D-CED
36	A	314	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	B	305	CLA	O1D-CGD-O2D-CED
36	H	314	CLA	O1D-CGD-O2D-CED
36	l	206	CLA	O1D-CGD-O2D-CED
35	H	301	A86	C35-C34-O4-C38
35	S	305	A86	C35-C34-O4-C38
36	a	823	CLA	C2C-C3C-CAC-CBC
41	a	850	LHG	C17-C18-C19-C20
36	J	313	CLA	C5-C6-C7-C8
36	L	309	CLA	C5-C6-C7-C8
36	O	309	CLA	C8-C10-C11-C12
36	U	311	CLA	C5-C6-C7-C8
36	V	308	CLA	C10-C11-C12-C13
36	C	208	CLA	C2A-CAA-CBA-CGA
36	D	317	CLA	C2A-CAA-CBA-CGA
36	F	317	CLA	C2A-CAA-CBA-CGA
36	J	311	CLA	C2A-CAA-CBA-CGA
36	R	312	CLA	C2A-CAA-CBA-CGA
36	R	322	CLA	C2A-CAA-CBA-CGA
36	l	206	CLA	C2A-CAA-CBA-CGA
34	B	304	DD6	C12-C11-C13-C14
34	C	201	DD6	C12-C11-C13-C14
34	D	301	DD6	C-C1-C24-C25
34	D	303	DD6	C12-C11-C13-C14
34	E	303	DD6	C12-C11-C13-C14
34	E	304	DD6	C12-C11-C13-C14
34	E	306	DD6	C12-C11-C13-C14
34	G	303	DD6	C12-C11-C13-C14
34	K	304	DD6	C7-C6-C8-C9
34	L	305	DD6	C-C1-C24-C25
34	P	305	DD6	C-C1-C24-C25
34	R	308	DD6	C12-C11-C13-C14
34	R	308	DD6	C7-C6-C8-C9
34	W	205	DD6	C12-C11-C13-C14
34	a	849	DD6	C12-C11-C13-C14
34	j	103	DD6	C7-C6-C8-C9
35	F	302	A86	C7-C6-C8-C9
35	O	305	A86	C-C1-C24-C25
44	a	845	BCR	C37-C22-C23-C24
44	a	846	BCR	C37-C22-C23-C24
44	a	847	BCR	C37-C22-C23-C24
44	b	845	BCR	C7-C8-C9-C34
44	b	846	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
44	b	847	BCR	C7-C8-C9-C34
44	h	201	BCR	C7-C8-C9-C34
34	B	304	DD6	C10-C11-C13-C14
34	C	201	DD6	C10-C11-C13-C14
34	D	303	DD6	C10-C11-C13-C14
34	E	306	DD6	C10-C11-C13-C14
34	G	303	DD6	C10-C11-C13-C14
34	L	305	DD6	C2-C1-C24-C25
34	R	308	DD6	C5-C6-C8-C9
34	W	205	DD6	C10-C11-C13-C14
34	j	103	DD6	C5-C6-C8-C9
35	J	301	A86	C2-C1-C24-C25
35	O	305	A86	C2-C1-C24-C25
35	S	308	A86	C2-C1-C24-C25
44	b	846	BCR	C7-C8-C9-C10
41	O	317	LHG	C8-C7-O7-C5
41	D	319	LHG	C12-C13-C14-C15
42	D	321	LMG	C4-C5-C6-O5
40	L	302	DGD	C1B-C2B-C3B-C4B
41	G	320	LHG	C23-C24-C25-C26
41	G	321	LHG	C7-C8-C9-C10
42	I	315	LMG	C10-C11-C12-C13
42	L	321	LMG	C10-C11-C12-C13
42	j	105	LMG	C10-C11-C12-C13
36	D	316	CLA	O1A-CGA-O2A-C1
36	I	305	CLA	O1A-CGA-O2A-C1
36	b	831	CLA	O1A-CGA-O2A-C1
36	U	305	CLA	O1A-CGA-O2A-C1
36	F	309	CLA	C15-C16-C17-C18
36	H	309	CLA	C13-C15-C16-C17
36	I	311	CLA	C15-C16-C17-C18
36	K	308	CLA	C15-C16-C17-C18
36	L	308	CLA	C5-C6-C7-C8
36	O	307	CLA	C8-C10-C11-C12
36	P	309	CLA	C8-C10-C11-C12
36	Q	306	CLA	C8-C10-C11-C12
36	Q	314	CLA	C10-C11-C12-C13
36	R	312	CLA	C8-C10-C11-C12
36	R	321	CLA	C13-C15-C16-C17
36	S	314	CLA	C10-C11-C12-C13
36	a	829	CLA	C10-C11-C12-C13
36	b	802	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	b	820	CLA	C5-C6-C7-C8
36	b	837	CLA	C5-C6-C7-C8
42	D	321	LMG	C31-C32-C33-C34
42	j	105	LMG	C15-C16-C17-C18
37	B	310	KC1	CAA-CBA-CGA-O2A
37	D	314	KC1	CAA-CBA-CGA-O2A
37	G	308	KC1	CAA-CBA-CGA-O2A
37	G	317	KC1	CAA-CBA-CGA-O2A
37	J	314	KC1	CAA-CBA-CGA-O2A
37	M	313	KC1	CAA-CBA-CGA-O2A
37	N	314	KC1	CAA-CBA-CGA-O2A
37	W	213	KC1	CAA-CBA-CGA-O1A
36	A	306	CLA	C2C-C3C-CAC-CBC
36	R	310	CLA	O1D-CGD-O2D-CED
36	R	315	CLA	C3-C5-C6-C7
36	R	310	CLA	CBA-CGA-O2A-C1
36	h	203	CLA	CBA-CGA-O2A-C1
41	b	850	LHG	C24-C23-O8-C6
36	A	314	CLA	C15-C16-C17-C18
36	B	305	CLA	C15-C16-C17-C18
36	C	207	CLA	C13-C15-C16-C17
36	C	211	CLA	C10-C11-C12-C13
36	C	212	CLA	C13-C15-C16-C17
36	D	307	CLA	C8-C10-C11-C12
36	E	311	CLA	C5-C6-C7-C8
36	F	314	CLA	C15-C16-C17-C18
36	H	308	CLA	C10-C11-C12-C13
36	H	308	CLA	C15-C16-C17-C18
36	H	316	CLA	C15-C16-C17-C18
36	J	308	CLA	C8-C10-C11-C12
36	K	310	CLA	C5-C6-C7-C8
36	L	320	CLA	C10-C11-C12-C13
36	M	309	CLA	C15-C16-C17-C18
36	M	311	CLA	C10-C11-C12-C13
36	O	307	CLA	C10-C11-C12-C13
36	P	309	CLA	C10-C11-C12-C13
36	P	310	CLA	C5-C6-C7-C8
36	P	313	CLA	C10-C11-C12-C13
36	Q	306	CLA	C10-C11-C12-C13
36	Q	314	CLA	C13-C15-C16-C17
36	R	311	CLA	C13-C15-C16-C17
36	R	311	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	R	321	CLA	C15-C16-C17-C18
36	S	310	CLA	C13-C15-C16-C17
36	T	309	CLA	C15-C16-C17-C18
36	T	314	CLA	C5-C6-C7-C8
36	W	207	CLA	C5-C6-C7-C8
36	a	802	CLA	C13-C15-C16-C17
36	a	807	CLA	C5-C6-C7-C8
36	b	808	CLA	C15-C16-C17-C18
36	b	815	CLA	C8-C10-C11-C12
36	b	825	CLA	C5-C6-C7-C8
36	b	826	CLA	C10-C11-C12-C13
36	V	308	CLA	C15-C16-C17-C18
36	V	313	CLA	C5-C6-C7-C8
43	b	842	PQN	C15-C16-C17-C18
39	b	848	LMT	O5B-C5B-C6B-O6B
35	T	302	A86	C35-C34-O4-C38
41	E	322	LHG	C23-C24-C25-C26
41	a	850	LHG	C23-C24-C25-C26
42	h	206	LMG	C10-C11-C12-C13
36	H	310	CLA	CBD-CGD-O2D-CED
36	C	212	CLA	C2C-C3C-CAC-CBC
37	V	312	KC1	C4C-C3C-CAC-CBC
36	a	838	CLA	O1D-CGD-O2D-CED
39	L	303	LMT	O5'-C5'-C6'-O6'
36	A	308	CLA	C10-C11-C12-C13
36	B	305	CLA	C13-C15-C16-C17
36	E	311	CLA	C13-C15-C16-C17
36	E	315	CLA	C5-C6-C7-C8
36	G	313	CLA	C10-C11-C12-C13
36	H	308	CLA	C5-C6-C7-C8
36	H	315	CLA	C10-C11-C12-C13
36	I	310	CLA	C13-C15-C16-C17
36	J	313	CLA	C13-C15-C16-C17
36	M	307	CLA	C15-C16-C17-C18
36	O	316	CLA	C5-C6-C7-C8
36	O	316	CLA	C10-C11-C12-C13
36	R	315	CLA	C13-C15-C16-C17
36	S	319	CLA	C8-C10-C11-C12
36	W	212	CLA	C15-C16-C17-C18
36	a	802	CLA	C15-C16-C17-C18
36	a	820	CLA	C13-C15-C16-C17
36	a	825	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	a	825	CLA	C8-C10-C11-C12
36	a	827	CLA	C10-C11-C12-C13
36	a	831	CLA	C5-C6-C7-C8
36	a	839	CLA	C15-C16-C17-C18
36	l	201	CLA	C10-C11-C12-C13
36	h	203	CLA	C15-C16-C17-C18
36	U	310	CLA	C13-C15-C16-C17
36	U	311	CLA	C8-C10-C11-C12
36	V	308	CLA	C8-C10-C11-C12
36	V	314	CLA	C15-C16-C17-C18
39	B	313	LMT	C4'-C5'-C6'-O6'
39	K	318	LMT	C4'-C5'-C6'-O6'
36	N	311	CLA	O1A-CGA-O2A-C1
35	R	305	A86	O5-C38-O4-C34
36	C	214	CLA	O1D-CGD-O2D-CED
36	G	319	CLA	O1D-CGD-O2D-CED
36	K	315	CLA	O1D-CGD-O2D-CED
36	O	306	CLA	O1A-CGA-O2A-C1
38	b	804	SQD	C7-C8-C9-C10
40	C	215	DGD	C1A-C2A-C3A-C4A
41	D	318	LHG	C23-C24-C25-C26
41	F	319	LHG	C23-C24-C25-C26
41	G	321	LHG	C23-C24-C25-C26
41	a	842	LHG	C7-C8-C9-C10
41	f	808	LHG	C23-C24-C25-C26
41	f	809	LHG	C7-C8-C9-C10
42	D	321	LMG	C10-C11-C12-C13
42	I	315	LMG	C28-C29-C30-C31
42	J	319	LMG	C28-C29-C30-C31
42	a	852	LMG	C10-C11-C12-C13
42	V	315	LMG	C28-C29-C30-C31
40	C	215	DGD	C6B-C7B-C8B-C9B
36	a	816	CLA	CBD-CGD-O2D-CED
36	E	315	CLA	O1D-CGD-O2D-CED
36	S	320	CLA	O1D-CGD-O2D-CED
36	B	305	CLA	C10-C11-C12-C13
36	B	308	CLA	C13-C15-C16-C17
36	C	208	CLA	C5-C6-C7-C8
36	D	310	CLA	C15-C16-C17-C18
36	L	311	CLA	C10-C11-C12-C13
36	L	313	CLA	C10-C11-C12-C13
36	O	307	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	P	309	CLA	C5-C6-C7-C8
36	Q	306	CLA	C5-C6-C7-C8
36	R	313	CLA	C10-C11-C12-C13
36	b	808	CLA	C10-C11-C12-C13
36	b	809	CLA	C5-C6-C7-C8
36	b	815	CLA	C10-C11-C12-C13
36	b	841	CLA	C15-C16-C17-C18
36	l	201	CLA	C8-C10-C11-C12
36	K	310	CLA	C3-C5-C6-C7
36	f	804	CLA	C3-C5-C6-C7
36	V	311	CLA	C3-C5-C6-C7
36	S	309	CLA	CBA-CGA-O2A-C1
36	V	314	CLA	CBA-CGA-O2A-C1
41	O	317	LHG	C24-C23-O8-C6
39	I	318	LMT	O1'-C1-C2-C3
39	P	321	LMT	O1'-C1-C2-C3
42	a	852	LMG	C22-C23-C24-C25
35	E	302	A86	C33-C34-O4-C38
35	F	307	A86	C33-C34-O4-C38
35	I	302	A86	C35-C34-O4-C38
35	N	301	A86	C33-C34-O4-C38
35	N	320	A86	C35-C34-O4-C38
35	O	319	A86	C35-C34-O4-C38
35	Q	304	A86	C35-C34-O4-C38
35	R	306	A86	C35-C34-O4-C38
35	S	301	A86	C33-C34-O4-C38
36	A	306	CLA	O1D-CGD-O2D-CED
36	D	308	CLA	O1D-CGD-O2D-CED
36	R	312	CLA	O1D-CGD-O2D-CED
36	W	210	CLA	O1D-CGD-O2D-CED
36	b	805	CLA	O1D-CGD-O2D-CED
36	b	818	CLA	O1D-CGD-O2D-CED
37	D	314	KC1	CAA-CBA-CGA-O1A
37	F	308	KC1	CAA-CBA-CGA-O1A
37	N	314	KC1	CAA-CBA-CGA-O1A
36	a	804	CLA	C2-C1-O2A-CGA
36	C	208	CLA	C8-C10-C11-C12
36	H	311	CLA	C10-C11-C12-C13
36	I	311	CLA	C10-C11-C12-C13
36	K	307	CLA	C10-C11-C12-C13
36	K	316	CLA	C13-C15-C16-C17
36	a	809	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	a	817	CLA	C8-C10-C11-C12
36	b	811	CLA	C13-C15-C16-C17
36	b	830	CLA	C10-C11-C12-C13
40	C	215	DGD	C1B-C2B-C3B-C4B
41	G	301	LHG	C23-C24-C25-C26
41	a	850	LHG	C7-C8-C9-C10
42	L	321	LMG	C28-C29-C30-C31
36	C	211	CLA	CBD-CGD-O2D-CED
36	W	209	CLA	C8-C10-C11-C12
36	a	827	CLA	C13-C15-C16-C17
39	G	323	LMT	O1'-C1-C2-C3
36	I	312	CLA	C3-C5-C6-C7
36	W	215	CLA	O2A-C1-C2-C3
36	H	309	CLA	C15-C16-C17-C18
36	H	316	CLA	C13-C15-C16-C17
36	I	308	CLA	C13-C15-C16-C17
36	h	203	CLA	C8-C10-C11-C12
42	L	321	LMG	C4-C5-C6-O5
36	A	308	CLA	C12-C13-C15-C16
36	C	207	CLA	C12-C13-C15-C16
36	G	309	CLA	C12-C13-C15-C16
36	H	309	CLA	C11-C12-C13-C15
36	H	315	CLA	C12-C13-C15-C16
36	I	310	CLA	C12-C13-C15-C16
36	J	308	CLA	C6-C7-C8-C10
36	K	307	CLA	C11-C10-C8-C7
36	K	309	CLA	C11-C10-C8-C7
36	K	313	CLA	C11-C12-C13-C15
36	N	316	CLA	C11-C12-C13-C15
36	P	301	CLA	C11-C10-C8-C7
36	T	314	CLA	C6-C7-C8-C10
36	a	801	CLA	C12-C13-C15-C16
36	b	809	CLA	C11-C10-C8-C7
36	b	811	CLA	C11-C10-C8-C7
36	b	820	CLA	C11-C10-C8-C7
36	b	825	CLA	C12-C13-C15-C16
36	f	802	CLA	C6-C7-C8-C10
36	l	201	CLA	C11-C12-C13-C15
36	l	205	CLA	C12-C13-C15-C16
36	T	313	CLA	C3-C5-C6-C7
36	M	306	CLA	O1A-CGA-O2A-C1
36	P	308	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	Q	305	CLA	O1A-CGA-O2A-C1
36	b	840	CLA	O1A-CGA-O2A-C1
36	l	202	CLA	O1A-CGA-O2A-C1
36	l	204	CLA	O1A-CGA-O2A-C1
34	F	303	DD6	C11-C10-C9-C8
34	R	307	DD6	C11-C10-C9-C8
35	M	304	A86	C11-C10-C9-C8
35	M	304	A86	C1-C2-C3-C4
35	M	304	A86	C24-C25-C26-C27
35	M	304	A86	C3-C4-C5-C6
35	U	303	A86	C24-C25-C26-C27
36	E	308	CLA	CBD-CGD-O2D-CED
35	N	306	A86	C35-C34-O4-C38
36	B	308	CLA	C2A-CAA-CBA-CGA
36	O	308	CLA	C2A-CAA-CBA-CGA
36	P	310	CLA	C2A-CAA-CBA-CGA
36	Q	307	CLA	C2A-CAA-CBA-CGA
36	b	834	CLA	C2A-CAA-CBA-CGA
36	N	307	CLA	O1D-CGD-O2D-CED
36	N	309	CLA	O1D-CGD-O2D-CED
36	X	306	CLA	O1D-CGD-O2D-CED
36	U	305	CLA	O1D-CGD-O2D-CED
36	A	314	CLA	C13-C15-C16-C17
36	F	310	CLA	C5-C6-C7-C8
36	G	309	CLA	C10-C11-C12-C13
36	H	312	CLA	C8-C10-C11-C12
36	S	314	CLA	C13-C15-C16-C17
36	T	311	CLA	C8-C10-C11-C12
36	b	806	CLA	C13-C15-C16-C17
36	b	839	CLA	C5-C6-C7-C8
36	j	101	CLA	C5-C6-C7-C8
36	U	310	CLA	C15-C16-C17-C18
36	V	308	CLA	C13-C15-C16-C17
36	V	314	CLA	C13-C15-C16-C17
42	D	320	LMG	C15-C16-C17-C18
37	L	317	KC1	CAA-CBA-CGA-O2A
39	U	315	LMT	O5B-C5B-C6B-O6B
36	E	308	CLA	O1A-CGA-O2A-C1
36	N	318	CLA	O1A-CGA-O2A-C1
41	I	316	LHG	O10-C23-O8-C6
36	b	812	CLA	CBD-CGD-O2D-CED
36	V	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	I	317	LMT	C4B-C5B-C6B-O6B
36	D	316	CLA	C2C-C3C-CAC-CBC
44	b	846	BCR	C10-C11-C12-C13
44	m	101	BCR	C18-C19-C20-C21
39	G	323	LMT	O5'-C5'-C6'-O6'
41	R	323	LHG	O2-C2-C3-O3
41	i	104	LHG	O2-C2-C3-O3
39	L	303	LMT	C4'-C5'-C6'-O6'
36	K	309	CLA	C3-C5-C6-C7
36	O	316	CLA	C3-C5-C6-C7
36	a	820	CLA	C3-C5-C6-C7
36	U	306	CLA	C3-C5-C6-C7
36	A	306	CLA	C8-C10-C11-C12
36	B	308	CLA	C8-C10-C11-C12
36	E	311	CLA	C8-C10-C11-C12
36	F	312	CLA	C8-C10-C11-C12
36	F	312	CLA	C10-C11-C12-C13
36	I	308	CLA	C8-C10-C11-C12
36	L	320	CLA	C5-C6-C7-C8
36	O	309	CLA	C15-C16-C17-C18
36	O	311	CLA	C5-C6-C7-C8
36	P	311	CLA	C15-C16-C17-C18
36	P	313	CLA	C5-C6-C7-C8
36	Q	308	CLA	C15-C16-C17-C18
36	R	310	CLA	C5-C6-C7-C8
36	R	312	CLA	C13-C15-C16-C17
36	W	212	CLA	C5-C6-C7-C8
36	a	831	CLA	C8-C10-C11-C12
36	b	815	CLA	C15-C16-C17-C18
36	b	826	CLA	C13-C15-C16-C17
36	f	804	CLA	C13-C15-C16-C17
36	j	102	CLA	C13-C15-C16-C17
36	l	201	CLA	C5-C6-C7-C8
36	U	306	CLA	C8-C10-C11-C12
36	V	311	CLA	C15-C16-C17-C18
43	a	840	PQN	C20-C21-C22-C23
41	D	319	LHG	C24-C23-O8-C6
36	R	310	CLA	O1A-CGA-O2A-C1
36	a	836	CLA	O1A-CGA-O2A-C1
39	G	323	LMT	C4'-C5'-C6'-O6'
39	G	322	LMT	O1'-C1-C2-C3
36	A	308	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	K	316	CLA	C8-C10-C11-C12
36	N	316	CLA	C10-C11-C12-C13
36	O	308	CLA	C13-C15-C16-C17
36	S	310	CLA	C5-C6-C7-C8
36	T	309	CLA	C5-C6-C7-C8
36	a	810	CLA	C10-C11-C12-C13
36	a	812	CLA	C8-C10-C11-C12
36	a	817	CLA	C10-C11-C12-C13
36	a	839	CLA	C13-C15-C16-C17
36	b	805	CLA	C8-C10-C11-C12
36	b	820	CLA	C10-C11-C12-C13
36	l	201	CLA	C13-C15-C16-C17
36	U	311	CLA	C10-C11-C12-C13
39	L	303	LMT	O1'-C1-C2-C3
39	I	318	LMT	C4B-C5B-C6B-O6B
39	I	318	LMT	C4'-C5'-C6'-O6'
36	h	203	CLA	O1A-CGA-O2A-C1
41	b	850	LHG	O10-C23-O8-C6
41	G	320	LHG	C15-C16-C17-C18
36	D	307	CLA	C5-C6-C7-C8
36	E	316	CLA	C5-C6-C7-C8
36	K	307	CLA	C8-C10-C11-C12
36	O	316	CLA	C13-C15-C16-C17
36	P	310	CLA	C13-C15-C16-C17
36	W	207	CLA	C15-C16-C17-C18
36	a	836	CLA	C13-C15-C16-C17
36	b	820	CLA	C8-C10-C11-C12
36	b	827	CLA	C10-C11-C12-C13
36	V	305	CLA	C10-C11-C12-C13
36	V	306	CLA	C5-C6-C7-C8
36	V	311	CLA	C5-C6-C7-C8
36	V	311	CLA	C13-C15-C16-C17
36	V	314	CLA	C5-C6-C7-C8
35	M	302	A86	C35-C34-O4-C38
35	O	303	A86	C35-C34-O4-C38
35	P	304	A86	C35-C34-O4-C38
35	Q	301	A86	C35-C34-O4-C38
35	R	301	A86	C33-C34-O4-C38
41	D	318	LHG	C3-O3-P-O6
41	F	319	LHG	C4-O6-P-O3
41	G	301	LHG	C4-O6-P-O3
41	G	321	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
41	G	321	LHG	C4-O6-P-O3
41	I	316	LHG	C4-O6-P-O3
41	O	317	LHG	C3-O3-P-O6
41	O	318	LHG	C3-O3-P-O6
41	a	850	LHG	C3-O3-P-O6
41	j	104	LHG	C4-O6-P-O3
41	l	208	LHG	C4-O6-P-O3
41	I	316	LHG	C7-C8-C9-C10
42	E	319	LMG	C28-C29-C30-C31
36	H	306	CLA	C3-C5-C6-C7
36	H	316	CLA	CBA-CGA-O2A-C1
36	V	305	CLA	CBA-CGA-O2A-C1
36	A	306	CLA	C10-C11-C12-C13
36	b	819	CLA	C5-C6-C7-C8
36	f	802	CLA	C15-C16-C17-C18
36	l	205	CLA	C8-C10-C11-C12
43	a	840	PQN	C25-C26-C27-C28
42	V	315	LMG	C4-C5-C6-O5
36	Q	312	CLA	O1D-CGD-O2D-CED
36	D	308	CLA	C2C-C3C-CAC-CBC
41	D	319	LHG	C23-C24-C25-C26
36	O	314	CLA	O1D-CGD-O2D-CED
36	P	316	CLA	O1D-CGD-O2D-CED
36	a	815	CLA	O1D-CGD-O2D-CED
36	a	820	CLA	O1D-CGD-O2D-CED
36	b	808	CLA	O1D-CGD-O2D-CED
41	F	319	LHG	C1-C2-C3-O3
41	R	323	LHG	C1-C2-C3-O3
41	i	104	LHG	C1-C2-C3-O3
41	F	318	LHG	O9-C7-O7-C5
41	O	317	LHG	O9-C7-O7-C5
36	F	313	CLA	C4-C3-C5-C6
36	S	312	CLA	C4-C3-C5-C6
36	a	828	CLA	C4-C3-C5-C6
40	b	849	DGD	C4E-C5E-C6E-O5E
35	T	301	A86	C39-C38-O4-C34
36	D	312	CLA	C13-C15-C16-C17
36	E	312	CLA	C10-C11-C12-C13
36	L	308	CLA	C8-C10-C11-C12
36	P	314	CLA	C10-C11-C12-C13
36	R	310	CLA	C8-C10-C11-C12
36	j	102	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	b	836	CLA	C4C-C3C-CAC-CBC
36	A	309	CLA	C2A-CAA-CBA-CGA
36	E	316	CLA	C2A-CAA-CBA-CGA
36	L	312	CLA	C2A-CAA-CBA-CGA
36	P	301	CLA	C2A-CAA-CBA-CGA
36	P	319	CLA	C2A-CAA-CBA-CGA
36	b	825	CLA	C2A-CAA-CBA-CGA
36	a	826	CLA	C16-C17-C18-C20
36	l	201	CLA	C16-C17-C18-C20
39	I	318	LMT	O5B-C5B-C6B-O6B
36	D	312	CLA	C3-C5-C6-C7
37	M	318	KC1	CAA-CBA-CGA-O2A
36	W	212	CLA	CBA-CGA-O2A-C1
41	E	322	LHG	C24-C23-O8-C6
36	a	807	CLA	C8-C10-C11-C12
39	h	205	LMT	O5B-C5B-C6B-O6B
36	a	825	CLA	C10-C11-C12-C13
36	l	205	CLA	C15-C16-C17-C18
36	a	829	CLA	O1D-CGD-O2D-CED
35	H	301	A86	C39-C38-O4-C34
38	b	804	SQD	C11-C10-C9-C8
34	E	306	DD6	C24-C25-C26-C27
34	Q	302	DD6	C1-C2-C3-C4
39	a	851	LMT	C4'-C5'-C6'-O6'
35	J	303	A86	C35-C34-O4-C38
35	T	306	A86	C35-C34-O4-C38
35	X	302	A86	C35-C34-O4-C38
41	R	323	LHG	C23-C24-C25-C26
39	F	321	LMT	C5-C6-C7-C8
39	a	851	LMT	C2-C3-C4-C5
41	O	318	LHG	C13-C14-C15-C16
41	l	208	LHG	C30-C31-C32-C33
42	G	325	LMG	C19-C20-C21-C22
42	j	105	LMG	C40-C41-C42-C43
36	a	830	CLA	O1D-CGD-O2D-CED
36	O	311	CLA	CBD-CGD-O2D-CED
36	P	313	CLA	CBD-CGD-O2D-CED
36	H	308	CLA	C8-C10-C11-C12
36	a	832	CLA	C5-C6-C7-C8
36	b	837	CLA	C15-C16-C17-C18
39	P	321	LMT	O5'-C5'-C6'-O6'
44	a	845	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
44	b	844	BCR	C11-C10-C9-C34
44	l	203	BCR	C11-C10-C9-C34
44	l	203	BCR	C20-C21-C22-C37
38	b	804	SQD	C28-C29-C30-C31
39	a	851	LMT	C11-C10-C9-C8
40	C	215	DGD	C3A-C4A-C5A-C6A
41	E	322	LHG	C9-C10-C11-C12
41	F	319	LHG	C16-C17-C18-C19
41	F	319	LHG	C17-C18-C19-C20
41	G	321	LHG	C30-C31-C32-C33
41	R	323	LHG	C27-C28-C29-C30
41	a	842	LHG	C24-C25-C26-C27
41	a	850	LHG	C15-C16-C17-C18
41	a	850	LHG	C32-C33-C34-C35
41	f	808	LHG	C25-C26-C27-C28
41	f	809	LHG	C9-C10-C11-C12
41	i	104	LHG	C15-C16-C17-C18
41	l	208	LHG	C11-C10-C9-C8
42	D	321	LMG	C30-C31-C32-C33
42	L	321	LMG	C13-C14-C15-C16
42	V	315	LMG	C15-C16-C17-C18
42	V	316	LMG	C17-C18-C19-C20
36	A	307	CLA	C11-C12-C13-C15
36	B	311	CLA	C6-C7-C8-C9
36	O	308	CLA	C16-C17-C18-C19
36	b	810	CLA	C16-C17-C18-C20
36	j	101	CLA	C16-C17-C18-C20
36	C	207	CLA	CBA-CGA-O2A-C1
36	K	309	CLA	CBA-CGA-O2A-C1
39	B	312	LMT	C11-C10-C9-C8
39	E	320	LMT	C6-C7-C8-C9
39	G	322	LMT	C2-C3-C4-C5
39	h	205	LMT	C4-C5-C6-C7
40	b	849	DGD	C3A-C4A-C5A-C6A
40	b	849	DGD	C4A-C5A-C6A-C7A
41	D	318	LHG	C12-C13-C14-C15
41	G	301	LHG	C17-C18-C19-C20
41	G	321	LHG	C29-C30-C31-C32
41	Q	315	LHG	C34-C35-C36-C37
42	E	318	LMG	C14-C15-C16-C17
42	E	319	LMG	C12-C13-C14-C15
42	G	324	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
42	G	325	LMG	C33-C34-C35-C36
42	I	315	LMG	C11-C12-C13-C14
42	J	318	LMG	C21-C22-C23-C24
42	J	318	LMG	C22-C23-C24-C25
42	j	105	LMG	C16-C17-C18-C19
42	h	206	LMG	C23-C24-C25-C26
36	b	837	CLA	O1D-CGD-O2D-CED
37	M	317	KC1	CAA-CBA-CGA-O1A
36	L	320	CLA	CBD-CGD-O2D-CED
41	D	319	LHG	C10-C11-C12-C13
41	G	301	LHG	C29-C30-C31-C32
41	G	321	LHG	C28-C29-C30-C31
41	Q	315	LHG	C32-C33-C34-C35
41	i	104	LHG	C28-C29-C30-C31
42	G	324	LMG	C12-C13-C14-C15
42	j	105	LMG	C17-C18-C19-C20
42	h	206	LMG	C11-C12-C13-C14
42	V	316	LMG	C15-C16-C17-C18
36	O	312	CLA	O1D-CGD-O2D-CED
36	P	314	CLA	O1D-CGD-O2D-CED
36	Q	310	CLA	O1D-CGD-O2D-CED
36	b	816	CLA	O1D-CGD-O2D-CED
35	L	306	A86	C33-C34-O4-C38
39	E	323	LMT	C5-C6-C7-C8
39	K	318	LMT	C7-C8-C9-C10
39	U	314	LMT	C3-C4-C5-C6
41	G	301	LHG	C27-C28-C29-C30
41	G	321	LHG	C15-C16-C17-C18
41	O	317	LHG	C26-C27-C28-C29
41	Q	315	LHG	C13-C14-C15-C16
41	j	104	LHG	C12-C13-C14-C15
42	E	318	LMG	C33-C34-C35-C36
42	I	315	LMG	C40-C41-C42-C43
39	a	851	LMT	C4B-C5B-C6B-O6B
36	a	814	CLA	C2C-C3C-CAC-CBC
39	E	321	LMT	C5-C6-C7-C8
39	U	314	LMT	C4-C5-C6-C7
39	U	315	LMT	O1'-C1-C2-C3
41	F	318	LHG	C12-C13-C14-C15
41	f	809	LHG	C33-C34-C35-C36
41	l	208	LHG	C10-C11-C12-C13
41	l	208	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
42	E	318	LMG	C11-C12-C13-C14
42	G	325	LMG	C40-C41-C42-C43
36	H	316	CLA	C3-C5-C6-C7
36	a	827	CLA	C3-C5-C6-C7
36	R	316	CLA	O1D-CGD-O2D-CED
36	l	202	CLA	O1D-CGD-O2D-CED
38	A	315	SQD	C2-C1-O6-C44
39	B	313	LMT	C2'-C1'-O1'-C1
39	E	320	LMT	C2'-C1'-O1'-C1
39	U	314	LMT	C2'-C1'-O1'-C1
44	f	806	BCR	C11-C10-C9-C8
44	f	806	BCR	C12-C13-C14-C15
44	l	203	BCR	C20-C21-C22-C23
44	h	201	BCR	C20-C21-C22-C23
36	L	320	CLA	CBA-CGA-O2A-C1
36	O	311	CLA	CBA-CGA-O2A-C1
36	P	313	CLA	CBA-CGA-O2A-C1
39	E	323	LMT	C11-C10-C9-C8
41	D	318	LHG	C25-C26-C27-C28
41	D	319	LHG	C31-C32-C33-C34
41	E	322	LHG	C16-C17-C18-C19
41	I	316	LHG	C16-C17-C18-C19
41	O	317	LHG	C16-C17-C18-C19
41	R	323	LHG	C34-C35-C36-C37
41	b	850	LHG	C15-C16-C17-C18
41	b	850	LHG	C28-C29-C30-C31
36	S	309	CLA	O1A-CGA-O2A-C1
36	V	314	CLA	O1A-CGA-O2A-C1
36	A	311	CLA	C16-C17-C18-C20
36	B	305	CLA	C16-C17-C18-C20
36	G	313	CLA	C16-C17-C18-C20
36	a	828	CLA	C16-C17-C18-C19
36	b	821	CLA	C16-C17-C18-C20
36	U	306	CLA	C16-C17-C18-C20
36	U	310	CLA	C16-C17-C18-C20
36	V	311	CLA	C16-C17-C18-C20
36	M	307	CLA	O1D-CGD-O2D-CED
36	P	302	CLA	O1D-CGD-O2D-CED
36	S	319	CLA	O1D-CGD-O2D-CED
36	W	206	CLA	O1D-CGD-O2D-CED
39	a	853	LMT	O5B-C5B-C6B-O6B
42	D	321	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
36	I	312	CLA	C4-C3-C5-C6
36	J	310	CLA	C4-C3-C5-C6
39	a	854	LMT	C5'-C4'-O1B-C1B
39	a	854	LMT	C6-C7-C8-C9
40	b	849	DGD	C6A-C7A-C8A-C9A
41	G	320	LHG	C25-C26-C27-C28
41	f	808	LHG	C12-C13-C14-C15
42	G	324	LMG	C36-C37-C38-C39
42	G	325	LMG	C11-C12-C13-C14
42	j	105	LMG	C35-C36-C37-C38
36	a	828	CLA	C2-C3-C5-C6
36	b	834	CLA	C2-C3-C5-C6
36	G	311	CLA	C11-C12-C13-C14
36	I	308	CLA	C14-C13-C15-C16
36	J	310	CLA	C11-C12-C13-C14
36	M	307	CLA	C6-C7-C8-C9
36	M	309	CLA	C11-C12-C13-C14
36	R	310	CLA	C6-C7-C8-C9
36	S	312	CLA	C11-C10-C8-C9
36	a	805	CLA	C11-C10-C8-C9
36	a	836	CLA	C6-C7-C8-C9
36	b	811	CLA	C11-C10-C8-C9
36	V	311	CLA	C6-C7-C8-C9
36	J	309	CLA	O1D-CGD-O2D-CED
36	b	815	CLA	O1D-CGD-O2D-CED
35	B	301	A86	C33-C34-O4-C38
35	I	304	A86	C33-C34-O4-C38
35	X	301	A86	C33-C34-O4-C38
35	X	303	A86	C33-C34-O4-C38
42	J	319	LMG	C10-C11-C12-C13
39	E	321	LMT	C3-C4-C5-C6
39	F	321	LMT	C4-C5-C6-C7
39	G	323	LMT	C3-C4-C5-C6
39	G	323	LMT	C4-C5-C6-C7
39	U	315	LMT	C7-C8-C9-C10
40	b	849	DGD	C4B-C5B-C6B-C7B
41	E	322	LHG	C11-C10-C9-C8
41	F	318	LHG	C10-C11-C12-C13
41	I	316	LHG	C27-C28-C29-C30
41	O	317	LHG	C25-C26-C27-C28
41	a	850	LHG	C13-C14-C15-C16
41	b	850	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
42	G	324	LMG	C38-C39-C40-C41
42	G	325	LMG	C16-C17-C18-C19
42	G	325	LMG	C38-C39-C40-C41
42	I	315	LMG	C30-C31-C32-C33
42	V	315	LMG	C16-C17-C18-C19
36	H	311	CLA	C13-C15-C16-C17
36	I	305	CLA	C5-C6-C7-C8
36	R	311	CLA	C8-C10-C11-C12
36	a	805	CLA	C8-C10-C11-C12
36	b	815	CLA	C13-C15-C16-C17
37	L	317	KC1	CAA-CBA-CGA-O1A
37	M	318	KC1	CAA-CBA-CGA-O1A
40	C	215	DGD	O6E-C5E-C6E-O5E
36	D	311	CLA	C2A-CAA-CBA-CGA
36	a	808	CLA	C2A-CAA-CBA-CGA
36	a	848	CLA	C2A-CAA-CBA-CGA
36	V	305	CLA	O1A-CGA-O2A-C1
41	O	317	LHG	O10-C23-O8-C6
34	D	304	DD6	C12-C11-C13-C14
35	D	302	A86	C-C1-C24-C25
44	i	103	BCR	C37-C22-C23-C24
39	B	313	LMT	C6-C7-C8-C9
39	P	321	LMT	C3-C4-C5-C6
41	F	319	LHG	C9-C10-C11-C12
41	a	842	LHG	C29-C30-C31-C32
41	b	850	LHG	C29-C30-C31-C32
41	l	208	LHG	C33-C34-C35-C36
42	G	324	LMG	C18-C19-C20-C21
42	J	318	LMG	C39-C40-C41-C42
41	D	318	LHG	O1-C1-C2-C3
41	F	319	LHG	O1-C1-C2-C3
41	G	320	LHG	O1-C1-C2-C3
41	a	850	LHG	O1-C1-C2-C3
41	b	850	LHG	O1-C1-C2-C3
41	f	808	LHG	O1-C1-C2-C3
41	l	208	LHG	O1-C1-C2-C3
34	D	304	DD6	C10-C11-C13-C14
34	R	308	DD6	C10-C11-C13-C14
34	S	307	DD6	C2-C1-C24-C25
34	a	849	DD6	C5-C6-C8-C9
35	B	303	A86	C5-C6-C8-C9
35	D	302	A86	C2-C1-C24-C25

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Mol	Chain	Res	Type	Atoms
36	E	313	CLA	C3-C5-C6-C7
36	F	309	CLA	C3-C5-C6-C7
36	K	312	CLA	C3-C5-C6-C7
36	a	836	CLA	C3-C5-C6-C7
36	f	803	CLA	C3-C5-C6-C7
36	S	310	CLA	C15-C16-C17-C18
36	b	808	CLA	C13-C15-C16-C17
36	V	313	CLA	C10-C11-C12-C13
39	F	320	LMT	C7-C8-C9-C10
39	P	321	LMT	C2-C3-C4-C5
39	a	851	LMT	C5-C6-C7-C8
41	D	319	LHG	C11-C12-C13-C14
41	G	301	LHG	C12-C13-C14-C15
41	f	809	LHG	C10-C11-C12-C13
41	i	104	LHG	C25-C26-C27-C28
36	b	809	CLA	CBD-CGD-O2D-CED
42	D	320	LMG	C4-C5-C6-O5
36	N	316	CLA	O1D-CGD-O2D-CED
39	B	313	LMT	C4-C5-C6-C7
39	G	323	LMT	C5-C6-C7-C8
39	G	323	LMT	C11-C10-C9-C8
39	L	318	LMT	C4-C5-C6-C7
39	P	321	LMT	C4-C5-C6-C7
39	a	853	LMT	C4-C5-C6-C7
39	a	854	LMT	C7-C8-C9-C10
39	U	314	LMT	C7-C8-C9-C10
39	U	315	LMT	C11-C10-C9-C8
40	b	849	DGD	C2A-C3A-C4A-C5A
40	b	849	DGD	CEB-CFB-CGB-CHB
41	D	319	LHG	C11-C10-C9-C8
41	F	318	LHG	C16-C17-C18-C19
41	F	319	LHG	C18-C19-C20-C21
41	G	301	LHG	C32-C33-C34-C35
41	O	318	LHG	C24-C25-C26-C27
41	Q	315	LHG	C14-C15-C16-C17
41	R	323	LHG	C17-C18-C19-C20
41	a	843	LHG	C11-C10-C9-C8
41	l	208	LHG	C31-C32-C33-C34
42	J	319	LMG	C15-C16-C17-C18
42	a	852	LMG	C14-C15-C16-C17
42	a	852	LMG	C35-C36-C37-C38
42	j	105	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
42	j	105	LMG	C31-C32-C33-C34
42	h	206	LMG	C12-C13-C14-C15
42	h	206	LMG	C21-C22-C23-C24
39	L	303	LMT	O5B-C5B-C6B-O6B
36	A	307	CLA	C11-C12-C13-C14
36	B	311	CLA	C6-C7-C8-C10
36	H	316	CLA	C16-C17-C18-C19
36	H	316	CLA	C16-C17-C18-C20
36	O	308	CLA	C16-C17-C18-C20
36	P	319	CLA	C11-C12-C13-C14
36	P	319	CLA	C11-C12-C13-C15
36	Q	314	CLA	C16-C17-C18-C20
36	R	315	CLA	C16-C17-C18-C20
36	a	807	CLA	C16-C17-C18-C20
36	b	820	CLA	C11-C12-C13-C14
36	b	825	CLA	C16-C17-C18-C20
36	U	310	CLA	C16-C17-C18-C19
36	U	311	CLA	C16-C17-C18-C20
38	A	315	SQD	O5-C1-O6-C44
39	B	313	LMT	O5'-C1'-O1'-C1
39	E	320	LMT	O5'-C1'-O1'-C1
36	C	212	CLA	C5-C6-C7-C8
36	D	310	CLA	C8-C10-C11-C12
36	D	313	CLA	C8-C10-C11-C12
36	H	309	CLA	C10-C11-C12-C13
36	I	311	CLA	C13-C15-C16-C17
36	M	309	CLA	C10-C11-C12-C13
36	a	832	CLA	C13-C15-C16-C17
36	h	203	CLA	C10-C11-C12-C13
36	U	306	CLA	C5-C6-C7-C8
35	K	303	A86	C35-C34-O4-C38
35	M	305	A86	C35-C34-O4-C38
39	F	321	LMT	C3-C4-C5-C6
39	b	848	LMT	C5-C6-C7-C8
39	U	314	LMT	C5-C6-C7-C8
41	I	316	LHG	C12-C13-C14-C15
41	I	316	LHG	C14-C15-C16-C17
41	I	316	LHG	C24-C25-C26-C27
41	f	809	LHG	C24-C25-C26-C27
41	j	104	LHG	C34-C35-C36-C37
42	G	325	LMG	C18-C19-C20-C21
42	m	102	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
36	Q	306	CLA	CBD-CGD-O2D-CED
39	I	318	LMT	C1-C2-C3-C4
37	U	312	KC1	O1D-CGD-O2D-CED
39	P	320	LMT	C6-C7-C8-C9
39	a	851	LMT	C4-C5-C6-C7
39	U	314	LMT	C2-C3-C4-C5
41	G	321	LHG	C10-C11-C12-C13
41	G	321	LHG	C33-C34-C35-C36
42	D	320	LMG	C20-C21-C22-C23
42	G	324	LMG	C17-C18-C19-C20
42	V	315	LMG	C20-C21-C22-C23
42	V	316	LMG	C32-C33-C34-C35
41	i	104	LHG	C7-C8-C9-C10
41	l	208	LHG	C23-C24-C25-C26
42	j	105	LMG	C28-C29-C30-C31
36	M	307	CLA	C13-C15-C16-C17
36	b	809	CLA	C15-C16-C17-C18
36	b	812	CLA	C8-C10-C11-C12
36	b	821	CLA	C15-C16-C17-C18
36	l	205	CLA	C13-C15-C16-C17
39	a	851	LMT	C7-C8-C9-C10
39	b	848	LMT	C4-C5-C6-C7
41	a	850	LHG	C16-C17-C18-C19
41	i	104	LHG	C13-C14-C15-C16
42	E	318	LMG	C17-C18-C19-C20
42	E	319	LMG	C13-C14-C15-C16
42	J	318	LMG	C29-C30-C31-C32
36	A	311	CLA	CBA-CGA-O2A-C1
36	T	314	CLA	CBA-CGA-O2A-C1
36	a	805	CLA	CBA-CGA-O2A-C1
36	f	805	CLA	CBA-CGA-O2A-C1
36	l	201	CLA	CBA-CGA-O2A-C1
36	U	310	CLA	CBA-CGA-O2A-C1
39	I	317	LMT	C5-C6-C7-C8
39	P	321	LMT	C5-C6-C7-C8
41	D	318	LHG	C27-C28-C29-C30
41	O	317	LHG	C18-C19-C20-C21
41	i	104	LHG	C14-C15-C16-C17
41	j	104	LHG	C24-C25-C26-C27
42	I	315	LMG	C41-C42-C43-C44
36	C	205	CLA	O1D-CGD-O2D-CED
36	D	307	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	K	311	CLA	O1D-CGD-O2D-CED
36	R	315	CLA	O1D-CGD-O2D-CED
36	R	321	CLA	O1D-CGD-O2D-CED
36	B	307	CLA	C3A-C2A-CAA-CBA
36	C	210	CLA	C3A-C2A-CAA-CBA
36	E	312	CLA	C3A-C2A-CAA-CBA
36	F	310	CLA	C3A-C2A-CAA-CBA
36	F	312	CLA	C3A-C2A-CAA-CBA
36	F	317	CLA	C3A-C2A-CAA-CBA
36	G	307	CLA	C3A-C2A-CAA-CBA
36	H	312	CLA	C3A-C2A-CAA-CBA
36	I	309	CLA	C3A-C2A-CAA-CBA
36	M	312	CLA	C3A-C2A-CAA-CBA
36	O	310	CLA	C3A-C2A-CAA-CBA
36	P	312	CLA	C3A-C2A-CAA-CBA
36	Q	309	CLA	C3A-C2A-CAA-CBA
36	Q	310	CLA	C3A-C2A-CAA-CBA
36	S	314	CLA	C3A-C2A-CAA-CBA
36	S	320	CLA	C3A-C2A-CAA-CBA
36	T	312	CLA	C3A-C2A-CAA-CBA
36	X	309	CLA	C3A-C2A-CAA-CBA
36	a	831	CLA	C3A-C2A-CAA-CBA
36	b	801	CLA	C3A-C2A-CAA-CBA
36	b	815	CLA	C3A-C2A-CAA-CBA
36	b	827	CLA	C3A-C2A-CAA-CBA
36	f	805	CLA	C3A-C2A-CAA-CBA
36	h	203	CLA	C3A-C2A-CAA-CBA
36	U	309	CLA	C3A-C2A-CAA-CBA
36	V	311	CLA	C3A-C2A-CAA-CBA
36	I	306	CLA	C5-C6-C7-C8
36	J	310	CLA	C8-C10-C11-C12
36	W	211	CLA	C10-C11-C12-C13
39	B	313	LMT	C2-C1-O1'-C1'
39	K	318	LMT	C2-C1-O1'-C1'
39	b	851	LMT	C2-C1-O1'-C1'
36	N	317	CLA	C5-C6-C7-C8
37	N	314	KC1	C4C-C3C-CAC-CBC
38	b	804	SQD	C13-C14-C15-C16
41	D	319	LHG	C25-C26-C27-C28
41	E	322	LHG	C31-C32-C33-C34
41	O	318	LHG	C16-C17-C18-C19
41	f	808	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
42	h	206	LMG	C17-C18-C19-C20
35	L	319	A86	C33-C34-O4-C38
35	O	302	A86	C33-C34-O4-C38
35	P	303	A86	C33-C34-O4-C38
35	U	302	A86	C35-C34-O4-C38
36	J	316	CLA	CBA-CGA-O2A-C1
36	T	312	CLA	O1D-CGD-O2D-CED
36	H	316	CLA	O1A-CGA-O2A-C1
41	D	319	LHG	O10-C23-O8-C6
36	G	313	CLA	C16-C17-C18-C19
36	H	312	CLA	C16-C17-C18-C20
36	Q	314	CLA	C16-C17-C18-C19
36	R	315	CLA	C16-C17-C18-C19
36	a	807	CLA	C16-C17-C18-C19
36	b	825	CLA	C16-C17-C18-C19
42	D	320	LMG	C21-C22-C23-C24
42	G	325	LMG	C21-C22-C23-C24
42	J	318	LMG	C33-C34-C35-C36
42	J	318	LMG	C40-C41-C42-C43
42	J	319	LMG	C30-C31-C32-C33
42	j	105	LMG	C14-C15-C16-C17
42	m	102	LMG	C12-C13-C14-C15
42	V	316	LMG	C18-C19-C20-C21
41	R	323	LHG	C4-C5-C6-O8
42	I	315	LMG	O6-C5-C6-O5
36	O	307	CLA	CBD-CGD-O2D-CED
36	P	309	CLA	CBD-CGD-O2D-CED
36	b	801	CLA	CBD-CGD-O2D-CED
36	b	833	CLA	CBD-CGD-O2D-CED
36	U	306	CLA	CBD-CGD-O2D-CED
39	K	318	LMT	C6-C7-C8-C9
39	b	848	LMT	O1'-C1-C2-C3
40	C	215	DGD	C8B-C9B-CAB-CBB
41	D	319	LHG	C30-C31-C32-C33
42	E	318	LMG	C19-C20-C21-C22
42	I	315	LMG	C15-C16-C17-C18
36	Q	314	CLA	O2A-C1-C2-C3
36	F	312	CLA	C3-C5-C6-C7
36	b	809	CLA	C3-C5-C6-C7
39	G	322	LMT	C1-C2-C3-C4
39	E	323	LMT	C2-C3-C4-C5
39	L	303	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
42	V	315	LMG	C29-C30-C31-C32
36	b	805	CLA	C13-C15-C16-C17
36	a	818	CLA	C4-C3-C5-C6
36	a	832	CLA	C4-C3-C5-C6
36	D	313	CLA	CBA-CGA-O2A-C1
36	T	308	CLA	CBA-CGA-O2A-C1
36	a	810	CLA	CBA-CGA-O2A-C1
36	l	206	CLA	CBA-CGA-O2A-C1
36	H	309	CLA	C2-C3-C5-C6
36	I	312	CLA	C2-C3-C5-C6
36	J	310	CLA	C2-C3-C5-C6
36	a	818	CLA	C2-C3-C5-C6
36	U	308	CLA	C2-C3-C5-C6
42	D	321	LMG	C11-C10-O7-C8
42	L	321	LMG	C11-C10-O7-C8
39	K	317	LMT	C2-C3-C4-C5
35	B	301	A86	C35-C34-O4-C38
35	K	306	A86	C35-C34-O4-C38
41	D	318	LHG	O1-C1-C2-O2
41	D	319	LHG	O1-C1-C2-O2
41	G	320	LHG	O1-C1-C2-O2
41	a	842	LHG	O1-C1-C2-O2
41	l	208	LHG	O1-C1-C2-O2
36	R	313	CLA	C15-C16-C17-C18
39	K	318	LMT	C5-C6-C7-C8
41	D	318	LHG	C9-C10-C11-C12
41	O	318	LHG	C32-C33-C34-C35
41	Q	315	LHG	C27-C28-C29-C30
41	R	323	LHG	C16-C17-C18-C19
41	j	104	LHG	C27-C28-C29-C30
41	l	208	LHG	C28-C29-C30-C31
42	I	315	LMG	C14-C15-C16-C17
36	W	212	CLA	O1A-CGA-O2A-C1
39	E	323	LMT	O5'-C5'-C6'-O6'
36	A	311	CLA	C16-C17-C18-C19
36	b	840	CLA	C16-C17-C18-C20
40	L	302	DGD	C2B-C3B-C4B-C5B
41	D	318	LHG	C17-C18-C19-C20
41	I	316	LHG	C18-C19-C20-C21
36	B	307	CLA	O1A-CGA-O2A-C1
36	R	316	CLA	O1A-CGA-O2A-C1
39	G	323	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
36	I	311	CLA	C5-C6-C7-C8
36	T	313	CLA	C15-C16-C17-C18
36	b	834	CLA	C15-C16-C17-C18
42	V	316	LMG	C14-C15-C16-C17
36	H	317	CLA	C3-C5-C6-C7
36	b	833	CLA	C3-C5-C6-C7
41	Q	315	LHG	C24-C25-C26-C27
41	a	843	LHG	C9-C10-C11-C12
42	G	324	LMG	C15-C16-C17-C18
36	C	207	CLA	O1A-CGA-O2A-C1
36	K	309	CLA	O1A-CGA-O2A-C1
41	E	322	LHG	O10-C23-O8-C6
36	T	314	CLA	C10-C11-C12-C13
41	G	320	LHG	C1-C2-C3-O3
40	b	849	DGD	C3B-C4B-C5B-C6B
41	D	318	LHG	C29-C30-C31-C32
41	I	316	LHG	C11-C12-C13-C14
41	O	318	LHG	C33-C34-C35-C36
41	b	850	LHG	C17-C18-C19-C20
41	f	808	LHG	C34-C35-C36-C37
41	j	104	LHG	C32-C33-C34-C35
42	E	319	LMG	C32-C33-C34-C35
42	J	318	LMG	C38-C39-C40-C41
42	J	319	LMG	C11-C12-C13-C14
41	a	842	LHG	O9-C7-O7-C5
42	D	321	LMG	O9-C10-O7-C8
42	L	321	LMG	O9-C10-O7-C8
39	L	318	LMT	C1-C2-C3-C4
39	U	315	LMT	C1-C2-C3-C4
36	K	307	CLA	C2-C1-O2A-CGA
36	b	824	CLA	C2-C1-O2A-CGA
36	i	102	CLA	C2-C1-O2A-CGA
35	S	308	A86	O5-C38-O4-C34
36	R	314	CLA	C2C-C3C-CAC-CBC
41	E	322	LHG	C25-C26-C27-C28
41	G	321	LHG	C27-C28-C29-C30
39	L	318	LMT	O5B-C5B-C6B-O6B
36	A	308	CLA	C5-C6-C7-C8
36	b	816	CLA	C10-C11-C12-C13
36	i	102	CLA	C5-C6-C7-C8
41	G	321	LHG	C2-C3-O3-P
36	A	311	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	L	320	CLA	O1A-CGA-O2A-C1
36	O	311	CLA	O1A-CGA-O2A-C1
36	P	313	CLA	O1A-CGA-O2A-C1
36	U	310	CLA	O1A-CGA-O2A-C1
39	B	312	LMT	C1-C2-C3-C4
39	L	318	LMT	C4'-C5'-C6'-O6'
39	B	313	LMT	C5-C6-C7-C8
39	I	317	LMT	C9-C10-C11-C12
40	C	215	DGD	C9B-CAB-CBB-CCB
41	j	104	LHG	C31-C32-C33-C34
42	J	319	LMG	C17-C18-C19-C20
36	I	306	CLA	C16-C17-C18-C19
36	a	826	CLA	C16-C17-C18-C19
36	b	810	CLA	C16-C17-C18-C19
41	O	318	LHG	C23-C24-C25-C26
42	D	321	LMG	C28-C29-C30-C31
42	E	318	LMG	C28-C29-C30-C31
36	P	310	CLA	C3-C5-C6-C7
36	a	805	CLA	C3-C5-C6-C7
44	a	846	BCR	C1-C6-C7-C8
44	a	846	BCR	C5-C6-C7-C8
44	a	847	BCR	C1-C6-C7-C8
44	a	847	BCR	C5-C6-C7-C8
44	a	847	BCR	C23-C24-C25-C26
44	a	847	BCR	C23-C24-C25-C30
44	b	843	BCR	C5-C6-C7-C8
44	b	844	BCR	C5-C6-C7-C8
44	b	846	BCR	C1-C6-C7-C8
44	b	846	BCR	C5-C6-C7-C8
44	b	846	BCR	C23-C24-C25-C26
44	b	846	BCR	C23-C24-C25-C30
44	b	847	BCR	C5-C6-C7-C8
44	f	806	BCR	C1-C6-C7-C8
44	f	806	BCR	C5-C6-C7-C8
44	i	103	BCR	C5-C6-C7-C8
44	l	203	BCR	C5-C6-C7-C8
44	l	203	BCR	C23-C24-C25-C26
44	m	101	BCR	C23-C24-C25-C26
44	h	201	BCR	C1-C6-C7-C8
44	h	201	BCR	C5-C6-C7-C8
44	h	201	BCR	C23-C24-C25-C26
36	a	810	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
36	I	307	CLA	C5-C6-C7-C8
39	G	323	LMT	C2-C3-C4-C5
40	C	215	DGD	C5A-C6A-C7A-C8A
41	D	318	LHG	C11-C12-C13-C14
41	D	319	LHG	C27-C28-C29-C30
41	R	323	LHG	C31-C32-C33-C34
42	G	325	LMG	C37-C38-C39-C40
42	V	315	LMG	C22-C23-C24-C25
36	H	310	CLA	O1D-CGD-O2D-CED
36	H	318	CLA	CBA-CGA-O2A-C1
36	J	309	CLA	CBA-CGA-O2A-C1
36	L	308	CLA	CBA-CGA-O2A-C1
36	N	307	CLA	CBA-CGA-O2A-C1
42	V	316	LMG	C29-C28-O8-C9
35	N	320	A86	C33-C34-O4-C38
35	Q	304	A86	C33-C34-O4-C38
36	A	310	CLA	C15-C16-C17-C18
36	B	308	CLA	C5-C6-C7-C8
36	B	308	CLA	C10-C11-C12-C13
36	C	208	CLA	C13-C15-C16-C17
36	I	310	CLA	C10-C11-C12-C13
36	K	308	CLA	C8-C10-C11-C12
36	L	308	CLA	C10-C11-C12-C13
36	W	209	CLA	C5-C6-C7-C8
36	a	816	CLA	C8-C10-C11-C12
36	b	805	CLA	C15-C16-C17-C18
36	b	829	CLA	C5-C6-C7-C8
36	b	830	CLA	C8-C10-C11-C12
36	i	102	CLA	C13-C15-C16-C17
39	G	322	LMT	O5B-C1B-O1B-C4'
41	f	808	LHG	C8-C7-O7-C5
41	I	316	LHG	C11-C10-C9-C8
41	O	317	LHG	C13-C14-C15-C16
41	f	809	LHG	C29-C30-C31-C32
42	h	206	LMG	C24-C25-C26-C27
36	f	805	CLA	O1A-CGA-O2A-C1
36	G	315	CLA	C11-C10-C8-C9
42	E	319	LMG	C31-C32-C33-C34
36	E	311	CLA	C10-C11-C12-C13
36	G	309	CLA	C5-C6-C7-C8
36	O	307	CLA	C13-C15-C16-C17
36	O	316	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	P	309	CLA	C13-C15-C16-C17
36	Q	306	CLA	C13-C15-C16-C17
37	M	317	KC1	CAA-CBA-CGA-O2A
41	a	842	LHG	C11-C10-C9-C8
41	f	808	LHG	C33-C34-C35-C36
42	G	325	LMG	C17-C18-C19-C20
36	D	317	CLA	C4-C3-C5-C6
36	H	309	CLA	C4-C3-C5-C6
36	a	837	CLA	C4-C3-C5-C6
36	b	805	CLA	C4-C3-C5-C6
36	b	834	CLA	C4-C3-C5-C6
36	U	306	CLA	C4-C3-C5-C6
36	U	308	CLA	C4-C3-C5-C6
36	V	313	CLA	C4-C3-C5-C6
36	A	310	CLA	C12-C13-C15-C16
36	A	311	CLA	C12-C13-C15-C16
36	C	206	CLA	C6-C7-C8-C10
36	C	207	CLA	C11-C10-C8-C7
36	D	307	CLA	C11-C10-C8-C7
36	D	308	CLA	C6-C7-C8-C10
36	D	312	CLA	C11-C10-C8-C7
36	D	312	CLA	C12-C13-C15-C16
36	F	317	CLA	C6-C7-C8-C10
36	G	309	CLA	C6-C7-C8-C10
36	G	311	CLA	C11-C12-C13-C15
36	I	305	CLA	C11-C12-C13-C15
36	I	308	CLA	C12-C13-C15-C16
36	I	311	CLA	C6-C7-C8-C10
36	J	307	CLA	C6-C7-C8-C10
36	J	308	CLA	C11-C10-C8-C7
36	J	310	CLA	C11-C12-C13-C15
36	J	313	CLA	C12-C13-C15-C16
36	L	311	CLA	C12-C13-C15-C16
36	M	309	CLA	C11-C12-C13-C15
36	O	309	CLA	C12-C13-C15-C16
36	P	301	CLA	C11-C12-C13-C15
36	P	311	CLA	C12-C13-C15-C16
36	P	314	CLA	C2-C3-C5-C6
36	Q	308	CLA	C12-C13-C15-C16
36	S	309	CLA	C11-C12-C13-C15
36	S	312	CLA	C11-C10-C8-C7
36	W	207	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
36	X	306	CLA	C11-C12-C13-C15
36	a	801	CLA	C11-C12-C13-C15
36	a	804	CLA	C2-C3-C5-C6
36	a	805	CLA	C11-C10-C8-C7
36	a	806	CLA	C11-C10-C8-C7
36	a	810	CLA	C11-C10-C8-C7
36	a	829	CLA	C11-C10-C8-C7
36	a	836	CLA	C6-C7-C8-C10
36	a	837	CLA	C2-C3-C5-C6
36	a	838	CLA	C12-C13-C15-C16
36	b	805	CLA	C2-C3-C5-C6
36	b	816	CLA	C11-C10-C8-C7
36	l	202	CLA	C11-C12-C13-C15
36	U	306	CLA	C2-C3-C5-C6
36	V	313	CLA	C2-C3-C5-C6
39	G	323	LMT	O5B-C1B-O1B-C4'
36	J	309	CLA	O1A-CGA-O2A-C1
36	T	308	CLA	O1A-CGA-O2A-C1
36	T	314	CLA	O1A-CGA-O2A-C1
36	l	201	CLA	O1A-CGA-O2A-C1
39	K	317	LMT	C4-C5-C6-C7
39	U	314	LMT	O1'-C1-C2-C3
41	O	317	LHG	C19-C20-C21-C22
41	f	809	LHG	C30-C31-C32-C33
41	j	104	LHG	C35-C36-C37-C38
42	E	319	LMG	C29-C30-C31-C32
36	G	313	CLA	C13-C15-C16-C17
36	K	308	CLA	C13-C15-C16-C17
36	L	314	CLA	C5-C6-C7-C8
36	M	309	CLA	C8-C10-C11-C12
36	b	841	CLA	C13-C15-C16-C17
36	j	102	CLA	C15-C16-C17-C18
36	V	313	CLA	C15-C16-C17-C18
34	R	308	DD6	C3-C4-C5-C6
34	S	307	DD6	C24-C25-C26-C27
35	I	301	A86	C11-C10-C9-C8
35	O	305	A86	C3-C4-C5-C6
36	E	317	CLA	CBD-CGD-O2D-CED
36	B	305	CLA	C16-C17-C18-C19
36	V	311	CLA	C16-C17-C18-C19
40	C	215	DGD	O6D-C5D-C6D-O5D
35	R	302	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
35	W	203	A86	C35-C34-O4-C38
37	T	315	KC1	O1D-CGD-O2D-CED
41	f	808	LHG	O9-C7-O7-C5
42	E	318	LMG	O9-C10-O7-C8
36	C	206	CLA	CBA-CGA-O2A-C1
36	F	309	CLA	CBA-CGA-O2A-C1
36	P	319	CLA	CBA-CGA-O2A-C1
36	a	809	CLA	CBA-CGA-O2A-C1
36	a	823	CLA	CBA-CGA-O2A-C1
36	a	848	CLA	CBA-CGA-O2A-C1
36	j	101	CLA	CBA-CGA-O2A-C1
42	E	318	LMG	C29-C28-O8-C9
39	U	315	LMT	C6-C7-C8-C9
42	G	325	LMG	C13-C14-C15-C16
42	G	325	LMG	C42-C43-C44-C45
36	C	209	CLA	C2A-CAA-CBA-CGA
36	D	308	CLA	C2A-CAA-CBA-CGA
36	M	307	CLA	C2A-CAA-CBA-CGA
36	M	315	CLA	C2A-CAA-CBA-CGA
36	T	309	CLA	C2A-CAA-CBA-CGA
36	b	801	CLA	C2A-CAA-CBA-CGA
36	b	806	CLA	C2A-CAA-CBA-CGA
36	b	829	CLA	C2A-CAA-CBA-CGA
36	V	306	CLA	C2A-CAA-CBA-CGA
36	V	313	CLA	C2A-CAA-CBA-CGA
36	M	311	CLA	C5-C6-C7-C8
36	a	828	CLA	C13-C15-C16-C17
36	b	816	CLA	C5-C6-C7-C8
36	b	829	CLA	C8-C10-C11-C12
42	E	318	LMG	C31-C32-C33-C34
42	E	319	LMG	C33-C34-C35-C36
36	a	811	CLA	O1D-CGD-O2D-CED
36	f	805	CLA	CBD-CGD-O2D-CED
42	I	315	LMG	C31-C32-C33-C34
42	j	105	LMG	C18-C19-C20-C21
36	I	305	CLA	C12-C13-C15-C16
36	K	307	CLA	C12-C13-C15-C16
42	V	316	LMG	C28-C29-C30-C31
36	L	308	CLA	O1D-CGD-O2D-CED
36	C	212	CLA	C8-C10-C11-C12
36	E	310	CLA	C13-C15-C16-C17
36	H	306	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	a	804	CLA	C13-C15-C16-C17
36	a	805	CLA	C5-C6-C7-C8
39	B	313	LMT	C5'-C4'-O1B-C1B
40	L	302	DGD	C2A-C3A-C4A-C5A
40	L	302	DGD	C4B-C5B-C6B-C7B
40	b	849	DGD	C5A-C6A-C7A-C8A
41	f	808	LHG	C14-C15-C16-C17
42	E	319	LMG	C11-C12-C13-C14
37	L	315	KC1	C2B-C3B-CAB-CBB
37	P	317	KC1	C2B-C3B-CAB-CBB
37	S	316	KC1	C2B-C3B-CAB-CBB
37	T	310	KC1	C2B-C3B-CAB-CBB
36	a	837	CLA	C3-C5-C6-C7
37	A	312	KC1	CAA-CBA-CGA-O2A
36	b	840	CLA	C2C-C3C-CAC-CBC
39	K	317	LMT	O1'-C1-C2-C3
42	D	320	LMG	C32-C33-C34-C35
36	a	805	CLA	O1A-CGA-O2A-C1
36	E	315	CLA	CBA-CGA-O2A-C1
36	H	312	CLA	CBA-CGA-O2A-C1
39	h	205	LMT	O5'-C1'-O1'-C1
39	U	314	LMT	O5'-C1'-O1'-C1
42	L	321	LMG	O6-C1-O1-C7
36	a	839	CLA	C5-C6-C7-C8
36	V	306	CLA	C15-C16-C17-C18
39	G	322	LMT	C6-C7-C8-C9
40	C	215	DGD	CAB-CBB-CCB-CDB
41	E	322	LHG	C29-C30-C31-C32
41	O	318	LHG	C15-C16-C17-C18
42	G	324	LMG	C29-C30-C31-C32
42	I	315	LMG	C23-C24-C25-C26
42	j	105	LMG	C30-C31-C32-C33
42	j	105	LMG	C41-C42-C43-C44
42	m	102	LMG	C30-C31-C32-C33
41	I	316	LHG	C8-C7-O7-C5
41	a	843	LHG	C8-C7-O7-C5
41	i	104	LHG	C8-C7-O7-C5
42	E	318	LMG	C11-C10-O7-C8
42	G	325	LMG	C11-C10-O7-C8
42	V	315	LMG	C11-C10-O7-C8
41	D	318	LHG	O6-C4-C5-O7
39	a	851	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
40	b	849	DGD	CAB-CBB-CCB-CDB
41	j	104	LHG	C18-C19-C20-C21
37	F	315	KC1	C4B-C3B-CAB-CBB
37	L	315	KC1	C4B-C3B-CAB-CBB
37	M	318	KC1	C4B-C3B-CAB-CBB
37	P	317	KC1	C4B-C3B-CAB-CBB
37	R	317	KC1	C4B-C3B-CAB-CBB
39	b	851	LMT	C1-C2-C3-C4
36	a	831	CLA	C13-C15-C16-C17
36	F	310	CLA	CBD-CGD-O2D-CED
36	j	101	CLA	CBD-CGD-O2D-CED
36	l	206	CLA	O1A-CGA-O2A-C1
36	J	316	CLA	C4C-C3C-CAC-CBC
39	a	854	LMT	O1'-C1-C2-C3
40	b	849	DGD	C2B-C3B-C4B-C5B
41	D	318	LHG	C11-C10-C9-C8
41	Q	315	LHG	C17-C18-C19-C20
41	j	104	LHG	C33-C34-C35-C36
41	i	104	LHG	O9-C7-O7-C5
35	C	202	A86	C33-C34-O4-C38
41	f	808	LHG	C30-C31-C32-C33
42	L	321	LMG	C2-C1-O1-C7
40	C	215	DGD	C2A-C3A-C4A-C5A
41	O	317	LHG	C11-C10-C9-C8
42	L	321	LMG	C11-C12-C13-C14
36	H	318	CLA	O1A-CGA-O2A-C1
36	L	308	CLA	O1A-CGA-O2A-C1
36	N	307	CLA	O1A-CGA-O2A-C1
36	b	821	CLA	C16-C17-C18-C19
39	K	317	LMT	C3-C4-C5-C6
41	b	850	LHG	C11-C12-C13-C14
41	j	104	LHG	C10-C11-C12-C13
36	K	309	CLA	C8-C10-C11-C12
36	Q	310	CLA	C4-C3-C5-C6
36	T	309	CLA	C4-C3-C5-C6
36	a	804	CLA	C4-C3-C5-C6
36	a	829	CLA	C4-C3-C5-C6
36	V	306	CLA	C4-C3-C5-C6
41	E	322	LHG	C7-C8-C9-C10
36	F	313	CLA	C2-C3-C5-C6
36	S	312	CLA	C2-C3-C5-C6
36	a	832	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
34	D	305	DD6	C27-C29-C30-C31
36	U	310	CLA	C4C-C3C-CAC-CBC
39	E	323	LMT	C6-C7-C8-C9
42	G	324	LMG	C19-C20-C21-C22
42	L	321	LMG	C12-C13-C14-C15
42	V	316	LMG	C11-C12-C13-C14
39	E	323	LMT	C1-C2-C3-C4
36	A	308	CLA	C14-C13-C15-C16
36	A	310	CLA	C14-C13-C15-C16
36	A	311	CLA	C14-C13-C15-C16
36	B	305	CLA	C11-C10-C8-C9
36	D	312	CLA	C11-C10-C8-C9
36	D	312	CLA	C14-C13-C15-C16
36	F	309	CLA	C6-C7-C8-C9
36	H	308	CLA	C6-C7-C8-C9
36	H	309	CLA	C11-C12-C13-C14
36	I	305	CLA	C11-C12-C13-C14
36	I	310	CLA	C14-C13-C15-C16
36	J	308	CLA	C6-C7-C8-C9
36	J	308	CLA	C11-C10-C8-C9
36	K	307	CLA	C11-C10-C8-C9
36	N	307	CLA	C11-C12-C13-C14
36	O	309	CLA	C14-C13-C15-C16
36	P	311	CLA	C14-C13-C15-C16
36	Q	308	CLA	C14-C13-C15-C16
36	S	309	CLA	C11-C12-C13-C14
36	T	308	CLA	C11-C12-C13-C14
36	X	306	CLA	C11-C12-C13-C14
36	a	801	CLA	C11-C12-C13-C14
36	a	810	CLA	C11-C10-C8-C9
36	a	810	CLA	C11-C12-C13-C14
36	a	824	CLA	C11-C10-C8-C9
36	a	829	CLA	C11-C10-C8-C9
36	a	838	CLA	C14-C13-C15-C16
36	b	815	CLA	C11-C10-C8-C9
36	b	825	CLA	C14-C13-C15-C16
36	b	827	CLA	C6-C7-C8-C9
36	b	827	CLA	C11-C12-C13-C14
36	f	802	CLA	C6-C7-C8-C9
36	h	203	CLA	C11-C12-C13-C14
36	D	313	CLA	O1A-CGA-O2A-C1
35	O	301	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
39	B	313	LMT	C3'-C4'-O1B-C1B
42	D	321	LMG	C15-C16-C17-C18
36	G	315	CLA	C3-C5-C6-C7
36	b	814	CLA	C3-C5-C6-C7
36	i	102	CLA	C3-C5-C6-C7
36	E	312	CLA	C2A-CAA-CBA-CGA
36	P	314	CLA	C2A-CAA-CBA-CGA
36	a	839	CLA	C2A-CAA-CBA-CGA
36	b	820	CLA	C2A-CAA-CBA-CGA
36	b	828	CLA	C2A-CAA-CBA-CGA
36	V	305	CLA	C2A-CAA-CBA-CGA
36	A	306	CLA	C4C-C3C-CAC-CBC
38	b	804	SQD	C14-C15-C16-C17
40	b	849	DGD	C8A-C9A-CAA-CBA
41	f	808	LHG	C27-C28-C29-C30
42	D	320	LMG	C29-C30-C31-C32
35	B	303	A86	C7-C6-C8-C9
36	J	308	CLA	O1D-CGD-O2D-CED
36	W	218	CLA	O1D-CGD-O2D-CED
36	J	313	CLA	C15-C16-C17-C18
36	W	212	CLA	C8-C10-C11-C12
36	G	319	CLA	C2C-C3C-CAC-CBC
36	a	823	CLA	C4C-C3C-CAC-CBC
41	D	318	LHG	C13-C14-C15-C16
41	F	319	LHG	C24-C25-C26-C27
42	a	852	LMG	C39-C40-C41-C42
36	a	810	CLA	O1A-CGA-O2A-C1
36	j	101	CLA	O1A-CGA-O2A-C1
42	V	316	LMG	O10-C28-O8-C9
36	B	305	CLA	C1A-C2A-CAA-CBA
36	B	307	CLA	C1A-C2A-CAA-CBA
36	C	212	CLA	C1A-C2A-CAA-CBA
36	D	316	CLA	C1A-C2A-CAA-CBA
36	D	317	CLA	C1A-C2A-CAA-CBA
36	E	317	CLA	C1A-C2A-CAA-CBA
36	F	310	CLA	C1A-C2A-CAA-CBA
36	F	312	CLA	C1A-C2A-CAA-CBA
36	F	313	CLA	C1A-C2A-CAA-CBA
36	G	307	CLA	C1A-C2A-CAA-CBA
36	G	313	CLA	C1A-C2A-CAA-CBA
36	H	311	CLA	C1A-C2A-CAA-CBA
36	I	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	L	312	CLA	C1A-C2A-CAA-CBA
36	M	310	CLA	C1A-C2A-CAA-CBA
36	M	311	CLA	C1A-C2A-CAA-CBA
36	N	308	CLA	C1A-C2A-CAA-CBA
36	N	311	CLA	C1A-C2A-CAA-CBA
36	N	312	CLA	C1A-C2A-CAA-CBA
36	P	319	CLA	C1A-C2A-CAA-CBA
36	Q	310	CLA	C1A-C2A-CAA-CBA
36	Q	314	CLA	C1A-C2A-CAA-CBA
36	R	311	CLA	C1A-C2A-CAA-CBA
36	R	314	CLA	C1A-C2A-CAA-CBA
36	S	309	CLA	C1A-C2A-CAA-CBA
36	S	310	CLA	C1A-C2A-CAA-CBA
36	S	313	CLA	C1A-C2A-CAA-CBA
36	T	309	CLA	C1A-C2A-CAA-CBA
36	W	210	CLA	C1A-C2A-CAA-CBA
36	W	218	CLA	C1A-C2A-CAA-CBA
36	X	307	CLA	C1A-C2A-CAA-CBA
36	a	807	CLA	C1A-C2A-CAA-CBA
36	a	809	CLA	C1A-C2A-CAA-CBA
36	a	810	CLA	C1A-C2A-CAA-CBA
36	a	817	CLA	C1A-C2A-CAA-CBA
36	a	823	CLA	C1A-C2A-CAA-CBA
36	a	825	CLA	C1A-C2A-CAA-CBA
36	a	831	CLA	C1A-C2A-CAA-CBA
36	a	832	CLA	C1A-C2A-CAA-CBA
36	a	841	CLA	C1A-C2A-CAA-CBA
36	b	801	CLA	C1A-C2A-CAA-CBA
36	b	815	CLA	C1A-C2A-CAA-CBA
36	b	820	CLA	C1A-C2A-CAA-CBA
36	b	822	CLA	C1A-C2A-CAA-CBA
36	b	823	CLA	C1A-C2A-CAA-CBA
36	b	832	CLA	C1A-C2A-CAA-CBA
36	b	838	CLA	C1A-C2A-CAA-CBA
36	f	805	CLA	C1A-C2A-CAA-CBA
36	l	204	CLA	C1A-C2A-CAA-CBA
36	l	206	CLA	C1A-C2A-CAA-CBA
36	U	311	CLA	C1A-C2A-CAA-CBA
36	V	305	CLA	C1A-C2A-CAA-CBA
36	V	309	CLA	C1A-C2A-CAA-CBA
36	F	312	CLA	C16-C17-C18-C19
36	F	312	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
36	H	315	CLA	C16-C17-C18-C20
36	a	828	CLA	C16-C17-C18-C20
36	b	840	CLA	C16-C17-C18-C19
36	j	101	CLA	C16-C17-C18-C19
36	l	201	CLA	C16-C17-C18-C19
36	U	306	CLA	C16-C17-C18-C19
36	U	311	CLA	C16-C17-C18-C19
42	G	325	LMG	O9-C10-O7-C8
41	F	318	LHG	C11-C10-C9-C8
41	a	850	LHG	C12-C13-C14-C15
41	i	104	LHG	C32-C33-C34-C35
41	l	208	LHG	C9-C10-C11-C12
42	a	852	LMG	C18-C19-C20-C21
42	a	852	LMG	C32-C33-C34-C35
35	J	301	A86	C24-C25-C26-C27
35	R	305	A86	C11-C10-C9-C8
36	K	310	CLA	C10-C11-C12-C13
36	R	313	CLA	C5-C6-C7-C8
35	E	302	A86	C35-C34-O4-C38
41	R	323	LHG	C4-O6-P-O3
41	f	809	LHG	C3-O3-P-O6
41	I	316	LHG	C26-C27-C28-C29
42	E	318	LMG	C32-C33-C34-C35
41	D	319	LHG	C7-C8-C9-C10
42	m	102	LMG	C10-C11-C12-C13
41	D	319	LHG	C2-C3-O3-P
41	O	318	LHG	C25-C26-C27-C28
41	a	842	LHG	C12-C13-C14-C15
42	V	316	LMG	C22-C23-C24-C25
36	F	312	CLA	C13-C15-C16-C17
36	K	312	CLA	C10-C11-C12-C13
36	L	320	CLA	C8-C10-C11-C12
36	O	311	CLA	C8-C10-C11-C12
36	P	313	CLA	C8-C10-C11-C12
36	P	314	CLA	C8-C10-C11-C12
36	W	206	CLA	C10-C11-C12-C13
36	V	306	CLA	C13-C15-C16-C17
36	E	312	CLA	CBA-CGA-O2A-C1
36	J	317	CLA	CBA-CGA-O2A-C1
36	f	802	CLA	CBA-CGA-O2A-C1
41	a	842	LHG	C24-C23-O8-C6
41	O	317	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
39	K	318	LMT	C2-C3-C4-C5
42	G	324	LMG	C37-C38-C39-C40
41	b	850	LHG	C32-C33-C34-C35
42	I	315	LMG	C22-C23-C24-C25
42	h	206	LMG	C22-C23-C24-C25
35	U	303	A86	C35-C34-O4-C38
36	D	306	CLA	C2C-C3C-CAC-CBC
41	F	318	LHG	C11-C12-C13-C14
37	A	312	KC1	CAA-CBA-CGA-O1A
41	a	842	LHG	C16-C17-C18-C19
41	f	808	LHG	C28-C29-C30-C31
42	D	321	LMG	C29-C30-C31-C32
42	E	318	LMG	C10-C11-C12-C13
42	E	319	LMG	C10-C11-C12-C13
36	N	312	CLA	C2-C1-O2A-CGA
41	a	850	LHG	C25-C26-C27-C28
41	j	104	LHG	C1-C2-C3-O3
41	l	208	LHG	C1-C2-C3-O3
41	I	316	LHG	O9-C7-O7-C5
36	P	314	CLA	C4-C3-C5-C6
36	Q	314	CLA	C4-C3-C5-C6
39	G	322	LMT	C7-C8-C9-C10
41	I	316	LHG	C32-C33-C34-C35
41	Q	315	LHG	C15-C16-C17-C18
42	h	206	LMG	C30-C31-C32-C33
43	b	842	PQN	C20-C21-C22-C23
36	a	834	CLA	O1D-CGD-O2D-CED
41	R	323	LHG	C11-C10-C9-C8
42	I	315	LMG	C34-C35-C36-C37
42	J	318	LMG	C11-C12-C13-C14
35	W	202	A86	C35-C34-O4-C38
36	F	309	CLA	O1A-CGA-O2A-C1
42	E	318	LMG	O10-C28-O8-C9
41	E	322	LHG	O2-C2-C3-O3
41	a	850	LHG	C29-C30-C31-C32
42	J	319	LMG	C22-C23-C24-C25
36	Q	310	CLA	C16-C17-C18-C20
36	l	202	CLA	C16-C17-C18-C19
36	G	311	CLA	C3-C5-C6-C7
36	R	321	CLA	C3-C5-C6-C7
40	b	849	DGD	C1G-C2G-C3G-O3G
41	D	319	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
41	F	319	LHG	C4-C5-C6-O8
41	G	301	LHG	C4-C5-C6-O8
41	G	320	LHG	C4-C5-C6-O8
41	O	318	LHG	C4-C5-C6-O8
41	I	208	LHG	C25-C26-C27-C28
42	D	320	LMG	C7-C8-C9-O8
42	G	325	LMG	C34-C35-C36-C37
42	J	319	LMG	C18-C19-C20-C21
42	L	321	LMG	C7-C8-C9-O8
42	V	315	LMG	C7-C8-C9-O8
39	a	854	LMT	C9-C10-C11-C12
41	R	323	LHG	C14-C15-C16-C17
36	a	823	CLA	O1A-CGA-O2A-C1
36	a	848	CLA	O1A-CGA-O2A-C1
39	I	317	LMT	O5B-C1B-O1B-C4'
42	D	321	LMG	C8-C7-O1-C1
42	G	324	LMG	C8-C7-O1-C1
42	I	315	LMG	C8-C7-O1-C1
39	L	303	LMT	C4-C5-C6-C7
39	P	320	LMT	O1'-C1-C2-C3
40	L	302	DGD	C4A-C5A-C6A-C7A
41	j	104	LHG	C19-C20-C21-C22
42	E	318	LMG	C21-C22-C23-C24
42	m	102	LMG	C32-C33-C34-C35
42	V	316	LMG	C24-C25-C26-C27
36	B	305	CLA	C5-C6-C7-C8
39	E	320	LMT	C4B-C5B-C6B-O6B
39	E	323	LMT	C9-C10-C11-C12
41	l	208	LHG	C14-C15-C16-C17
41	F	319	LHG	C7-C8-C9-C10
36	P	319	CLA	O1A-CGA-O2A-C1
40	C	215	DGD	C4A-C5A-C6A-C7A
41	D	319	LHG	C19-C20-C21-C22
41	I	316	LHG	C34-C35-C36-C37
42	D	321	LMG	C16-C17-C18-C19
42	a	852	LMG	C31-C32-C33-C34
42	a	852	LMG	C37-C38-C39-C40
42	I	315	LMG	O6-C1-O1-C7
36	a	828	CLA	C8-C10-C11-C12
36	a	829	CLA	C8-C10-C11-C12
36	U	306	CLA	C15-C16-C17-C18
41	f	809	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
41	i	104	LHG	C35-C36-C37-C38
42	j	105	LMG	C36-C37-C38-C39
42	V	315	LMG	C18-C19-C20-C21
36	b	816	CLA	CBA-CGA-O2A-C1
40	L	302	DGD	C7B-C8B-C9B-CAB
41	R	323	LHG	C15-C16-C17-C18
41	l	208	LHG	C18-C19-C20-C21
35	R	303	A86	C33-C34-O4-C38
35	V	304	A86	C35-C34-O4-C38
36	A	314	CLA	C10-C11-C12-C13
36	H	311	CLA	C15-C16-C17-C18
36	C	206	CLA	O1A-CGA-O2A-C1
39	a	854	LMT	C5-C6-C7-C8
41	D	319	LHG	C33-C34-C35-C36
42	j	105	LMG	C20-C21-C22-C23
42	G	325	LMG	C29-C30-C31-C32
36	K	313	CLA	C10-C11-C12-C13
39	E	323	LMT	O5B-C5B-C6B-O6B
39	a	854	LMT	O5'-C5'-C6'-O6'
39	f	807	LMT	O5'-C5'-C6'-O6'
44	b	843	BCR	C20-C21-C22-C37
44	i	103	BCR	C11-C10-C9-C34
36	D	310	CLA	C4-C3-C5-C6
36	l	202	CLA	C4-C3-C5-C6
36	V	308	CLA	C4-C3-C5-C6
36	b	817	CLA	C10-C11-C12-C13
41	a	850	LHG	C24-C25-C26-C27
39	B	312	LMT	C4'-C5'-C6'-O6'
42	V	316	LMG	C4-C5-C6-O5
36	V	310	CLA	O1D-CGD-O2D-CED
36	R	315	CLA	CBA-CGA-O2A-C1
36	a	826	CLA	CBA-CGA-O2A-C1
41	O	318	LHG	C24-C23-O8-C6
39	G	323	LMT	C9-C10-C11-C12
42	a	852	LMG	C20-C21-C22-C23
36	a	824	CLA	CBD-CGD-O2D-CED
36	E	315	CLA	C15-C16-C17-C18
36	N	308	CLA	C15-C16-C17-C18
40	C	215	DGD	C6A-C7A-C8A-C9A
38	b	804	SQD	C46-C45-O47-C7
41	D	318	LHG	C6-C5-O7-C7
41	O	317	LHG	C6-C5-O7-C7

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Mol	Chain	Res	Type	Atoms
42	D	321	LMG	C9-C8-O7-C10
42	h	206	LMG	O6-C5-C6-O5
36	A	314	CLA	C2A-CAA-CBA-CGA
36	S	309	CLA	C2A-CAA-CBA-CGA
36	E	315	CLA	C8-C10-C11-C12
36	R	311	CLA	C5-C6-C7-C8
36	S	320	CLA	C8-C10-C11-C12
36	b	815	CLA	C5-C6-C7-C8
36	D	309	CLA	C2-C1-O2A-CGA
36	F	317	CLA	C2-C1-O2A-CGA
39	L	303	LMT	C2-C3-C4-C5
41	l	208	LHG	C19-C20-C21-C22
42	J	319	LMG	C13-C14-C15-C16
42	a	852	LMG	C33-C34-C35-C36
36	a	831	CLA	C3-C5-C6-C7
39	P	320	LMT	C11-C10-C9-C8
36	a	816	CLA	O1D-CGD-O2D-CED
36	P	301	CLA	C8-C10-C11-C12
39	E	320	LMT	O5B-C1B-O1B-C4'
36	O	311	CLA	C10-C11-C12-C13
39	h	205	LMT	C9-C10-C11-C12
41	Q	315	LHG	C35-C36-C37-C38
41	a	850	LHG	C33-C34-C35-C36
41	f	808	LHG	C35-C36-C37-C38
36	C	212	CLA	CBA-CGA-O2A-C1
36	E	311	CLA	CBA-CGA-O2A-C1
36	X	307	CLA	CBA-CGA-O2A-C1
36	H	315	CLA	C16-C17-C18-C19
36	Q	310	CLA	C16-C17-C18-C19
36	W	208	CLA	CBD-CGD-O2D-CED
39	F	320	LMT	C3-C4-C5-C6
39	K	318	LMT	C11-C10-C9-C8
41	I	316	LHG	C15-C16-C17-C18
41	f	808	LHG	C29-C30-C31-C32
42	m	102	LMG	C11-C12-C13-C14
41	D	319	LHG	C24-C25-C26-C27
36	C	211	CLA	O1D-CGD-O2D-CED
36	E	315	CLA	O1A-CGA-O2A-C1
36	H	312	CLA	O1A-CGA-O2A-C1
36	J	317	CLA	O1A-CGA-O2A-C1
36	a	809	CLA	O1A-CGA-O2A-C1
36	f	802	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
41	a	843	LHG	C7-C8-C9-C10
36	S	312	CLA	C10-C11-C12-C13
43	b	842	PQN	C23-C25-C26-C27
42	j	105	LMG	C2-C1-O1-C7
44	f	801	BCR	C11-C10-C9-C8
39	L	318	LMT	C5-C6-C7-C8
41	G	301	LHG	C35-C36-C37-C38
39	E	320	LMT	C1-C2-C3-C4
42	G	325	LMG	O1-C7-C8-O7
35	F	307	A86	C35-C34-O4-C38
41	a	843	LHG	O9-C7-O7-C5
36	a	807	CLA	C15-C16-C17-C18
36	E	312	CLA	O1A-CGA-O2A-C1
39	B	313	LMT	C9-C10-C11-C12
39	F	321	LMT	C7-C8-C9-C10
41	f	809	LHG	C25-C26-C27-C28
37	G	308	KC1	C2C-C3C-CAC-CBC
42	J	318	LMG	C24-C25-C26-C27
36	A	306	CLA	C6-C7-C8-C10
36	A	311	CLA	C6-C7-C8-C10
36	A	311	CLA	C11-C10-C8-C7
36	A	311	CLA	C11-C12-C13-C15
36	B	305	CLA	C11-C10-C8-C7
36	C	208	CLA	C6-C7-C8-C10
36	C	208	CLA	C12-C13-C15-C16
36	C	212	CLA	C6-C7-C8-C10
36	C	212	CLA	C12-C13-C15-C16
36	D	310	CLA	C2-C3-C5-C6
36	E	313	CLA	C6-C7-C8-C10
36	E	315	CLA	C12-C13-C15-C16
36	E	316	CLA	C6-C7-C8-C10
36	F	312	CLA	C12-C13-C15-C16
36	G	309	CLA	C11-C10-C8-C7
36	G	313	CLA	C11-C12-C13-C15
36	H	312	CLA	C11-C12-C13-C15
36	I	306	CLA	C11-C12-C13-C15
36	I	308	CLA	C11-C10-C8-C7
36	I	308	CLA	C11-C12-C13-C15
36	J	312	CLA	C12-C13-C15-C16
36	L	313	CLA	C12-C13-C15-C16
36	L	314	CLA	C11-C12-C13-C15
36	M	311	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
36	N	307	CLA	C11-C12-C13-C15
36	N	308	CLA	C11-C12-C13-C15
36	O	307	CLA	C12-C13-C15-C16
36	O	308	CLA	C6-C7-C8-C10
36	O	316	CLA	C12-C13-C15-C16
36	P	301	CLA	C6-C7-C8-C10
36	P	309	CLA	C12-C13-C15-C16
36	Q	306	CLA	C12-C13-C15-C16
36	Q	310	CLA	C2-C3-C5-C6
36	R	313	CLA	C12-C13-C15-C16
36	S	310	CLA	C6-C7-C8-C10
36	T	308	CLA	C11-C12-C13-C15
36	a	810	CLA	C11-C12-C13-C15
36	a	812	CLA	C6-C7-C8-C10
36	a	812	CLA	C11-C10-C8-C7
36	a	816	CLA	C11-C12-C13-C15
36	a	824	CLA	C11-C10-C8-C7
36	a	828	CLA	C11-C12-C13-C15
36	a	828	CLA	C12-C13-C15-C16
36	a	829	CLA	C2-C3-C5-C6
36	a	839	CLA	C11-C10-C8-C7
36	a	839	CLA	C11-C12-C13-C15
36	a	839	CLA	C12-C13-C15-C16
36	b	802	CLA	C11-C10-C8-C7
36	b	805	CLA	C6-C7-C8-C10
36	b	809	CLA	C12-C13-C15-C16
36	b	821	CLA	C11-C10-C8-C7
36	b	827	CLA	C6-C7-C8-C10
36	b	827	CLA	C11-C12-C13-C15
36	f	803	CLA	C11-C10-C8-C7
36	i	102	CLA	C6-C7-C8-C10
36	j	102	CLA	C12-C13-C15-C16
36	l	202	CLA	C2-C3-C5-C6
36	h	203	CLA	C6-C7-C8-C10
36	h	203	CLA	C11-C12-C13-C15
36	V	305	CLA	C11-C10-C8-C7
36	V	308	CLA	C2-C3-C5-C6
36	V	314	CLA	C11-C12-C13-C15
43	a	840	PQN	C17-C18-C20-C21
43	b	842	PQN	C22-C23-C25-C26
36	A	310	CLA	C3-C5-C6-C7
39	b	851	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
36	A	306	CLA	C6-C7-C8-C9
36	A	311	CLA	C11-C12-C13-C14
36	C	206	CLA	C11-C10-C8-C9
36	C	206	CLA	C11-C12-C13-C14
36	C	207	CLA	C14-C13-C15-C16
36	C	211	CLA	C14-C13-C15-C16
36	C	212	CLA	C6-C7-C8-C9
36	D	308	CLA	C11-C10-C8-C9
36	E	313	CLA	C6-C7-C8-C9
36	F	312	CLA	C6-C7-C8-C9
36	F	312	CLA	C14-C13-C15-C16
36	G	309	CLA	C11-C10-C8-C9
36	H	311	CLA	C14-C13-C15-C16
36	H	312	CLA	C11-C12-C13-C14
36	H	312	CLA	C14-C13-C15-C16
36	H	315	CLA	C14-C13-C15-C16
36	I	306	CLA	C6-C7-C8-C9
36	I	308	CLA	C6-C7-C8-C9
36	J	308	CLA	C11-C12-C13-C14
36	J	312	CLA	C14-C13-C15-C16
36	J	313	CLA	C6-C7-C8-C9
36	J	313	CLA	C11-C10-C8-C9
36	L	308	CLA	C11-C10-C8-C9
36	L	311	CLA	C14-C13-C15-C16
36	L	313	CLA	C14-C13-C15-C16
36	L	314	CLA	C11-C12-C13-C14
36	O	307	CLA	C14-C13-C15-C16
36	O	316	CLA	C14-C13-C15-C16
36	P	309	CLA	C14-C13-C15-C16
36	Q	306	CLA	C14-C13-C15-C16
36	R	310	CLA	C11-C12-C13-C14
36	T	314	CLA	C11-C12-C13-C14
36	W	206	CLA	C11-C12-C13-C14
36	W	212	CLA	C11-C12-C13-C14
36	a	801	CLA	C14-C13-C15-C16
36	a	802	CLA	C6-C7-C8-C9
36	a	802	CLA	C14-C13-C15-C16
36	a	817	CLA	C11-C10-C8-C9
36	a	828	CLA	C11-C12-C13-C14
36	a	828	CLA	C14-C13-C15-C16
36	a	829	CLA	C6-C7-C8-C9
36	a	831	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	a	839	CLA	C11-C12-C13-C14
36	b	802	CLA	C11-C10-C8-C9
36	b	805	CLA	C6-C7-C8-C9
36	b	805	CLA	C11-C10-C8-C9
36	b	806	CLA	C11-C10-C8-C9
36	b	809	CLA	C11-C10-C8-C9
36	j	101	CLA	C11-C12-C13-C14
36	j	102	CLA	C14-C13-C15-C16
36	l	205	CLA	C14-C13-C15-C16
36	U	311	CLA	C11-C10-C8-C9
36	V	306	CLA	C11-C12-C13-C14
43	b	842	PQN	C21-C22-C23-C24
35	T	301	A86	O5-C38-O4-C34
36	a	816	CLA	C2C-C3C-CAC-CBC
39	b	851	LMT	C6-C7-C8-C9
41	O	317	LHG	C9-C10-C11-C12
41	f	808	LHG	C31-C32-C33-C34
42	I	315	LMG	C21-C22-C23-C24
36	b	836	CLA	CBA-CGA-O2A-C1
36	G	315	CLA	C5-C6-C7-C8
36	l	201	CLA	C15-C16-C17-C18
39	K	317	LMT	C5-C6-C7-C8
41	a	850	LHG	C26-C27-C28-C29
36	b	816	CLA	O1A-CGA-O2A-C1
44	b	847	BCR	C11-C12-C13-C35
44	l	207	BCR	C7-C8-C9-C34
36	l	205	CLA	C16-C17-C18-C20
39	b	848	LMT	C9-C10-C11-C12
34	a	849	DD6	C10-C11-C13-C14
36	b	819	CLA	C11-C12-C13-C14
40	C	215	DGD	C7B-C8B-C9B-CAB
41	E	322	LHG	C35-C36-C37-C38
41	a	843	LHG	C10-C11-C12-C13
42	J	318	LMG	C42-C43-C44-C45
36	C	206	CLA	C3-C5-C6-C7
36	K	316	CLA	C3-C5-C6-C7
36	b	810	CLA	C3-C5-C6-C7
36	h	203	CLA	C3-C5-C6-C7
36	E	308	CLA	O1D-CGD-O2D-CED
36	b	812	CLA	O1D-CGD-O2D-CED
41	E	322	LHG	C1-C2-C3-O3
36	I	308	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	I	310	CLA	C15-C16-C17-C18
36	L	314	CLA	C13-C15-C16-C17
42	a	852	LMG	C40-C41-C42-C43
36	a	826	CLA	O1A-CGA-O2A-C1
36	C	209	CLA	CBA-CGA-O2A-C1
36	F	317	CLA	CBA-CGA-O2A-C1
36	b	829	CLA	CBA-CGA-O2A-C1
36	j	102	CLA	CBA-CGA-O2A-C1
39	P	321	LMT	C7-C8-C9-C10
40	C	215	DGD	CFB-CGB-CHB-CIB
41	j	104	LHG	C9-C10-C11-C12
41	j	104	LHG	C23-C24-C25-C26
36	D	313	CLA	C15-C16-C17-C18
36	B	309	CLA	C3-C5-C6-C7
36	a	825	CLA	CBD-CGD-O2D-CED
39	G	323	LMT	C5'-C4'-O1B-C1B
41	F	319	LHG	C14-C15-C16-C17
36	A	308	CLA	C16-C17-C18-C19
36	A	310	CLA	C10-C11-C12-C13
41	G	301	LHG	O6-C4-C5-C6
41	Q	315	LHG	O6-C4-C5-C6
41	i	104	LHG	O6-C4-C5-C6
36	a	801	CLA	C3-C5-C6-C7
36	b	821	CLA	C3-C5-C6-C7
35	V	302	A86	C35-C34-O4-C38
39	a	854	LMT	C3-C4-C5-C6
39	U	315	LMT	C4-C5-C6-C7
41	j	104	LHG	C13-C14-C15-C16
42	I	315	LMG	C19-C20-C21-C22
36	a	807	CLA	CBA-CGA-O2A-C1
36	U	311	CLA	CBA-CGA-O2A-C1
36	b	840	CLA	C8-C10-C11-C12
41	b	850	LHG	C33-C34-C35-C36
41	O	318	LHG	C7-C8-C9-C10
39	E	321	LMT	C4-C5-C6-C7
42	G	324	LMG	C33-C34-C35-C36
36	L	320	CLA	O1D-CGD-O2D-CED
36	P	313	CLA	O1D-CGD-O2D-CED
36	I	306	CLA	C10-C11-C12-C13
39	G	322	LMT	C2B-C1B-O1B-C4'
35	K	302	A86	C35-C34-O4-C38
35	T	305	A86	C35-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
42	V	316	LMG	C31-C32-C33-C34
36	O	311	CLA	O1D-CGD-O2D-CED
36	N	308	CLA	C3-C5-C6-C7
36	b	823	CLA	C3-C5-C6-C7
36	A	308	CLA	C16-C17-C18-C20
36	b	813	CLA	C6-C7-C8-C9
36	b	823	CLA	C6-C7-C8-C9
39	E	320	LMT	C7-C8-C9-C10
42	J	319	LMG	C19-C20-C21-C22
41	O	317	LHG	C2-C3-O3-P
41	R	323	LHG	C2-C3-O3-P
36	W	201	CLA	CBD-CGD-O2D-CED
36	b	833	CLA	O1D-CGD-O2D-CED
36	P	319	CLA	C3A-C2A-CAA-CBA
36	R	316	CLA	C3A-C2A-CAA-CBA
36	a	803	CLA	C3A-C2A-CAA-CBA
36	b	814	CLA	C3A-C2A-CAA-CBA
36	b	832	CLA	C3A-C2A-CAA-CBA
36	V	313	CLA	C3A-C2A-CAA-CBA
36	V	314	CLA	C3A-C2A-CAA-CBA
36	U	310	CLA	C2C-C3C-CAC-CBC
41	G	301	LHG	C19-C20-C21-C22
41	E	322	LHG	C5-C6-O8-C23
34	S	307	DD6	C11-C10-C9-C8
35	E	302	A86	O-C13-C14-C15
35	P	306	A86	O-C13-C14-C15
35	S	304	A86	O-C13-C14-C15
35	T	301	A86	O-C13-C14-C15
35	U	303	A86	O-C13-C14-C15
39	B	312	LMT	C2-C1-O1'-C1'
39	K	317	LMT	C2-C1-O1'-C1'
39	a	853	LMT	C2-C1-O1'-C1'
41	D	318	LHG	C32-C33-C34-C35
41	a	850	LHG	C18-C19-C20-C21
42	a	852	LMG	C36-C37-C38-C39
35	N	303	A86	C35-C34-O4-C38
35	S	303	A86	C35-C34-O4-C38
43	a	840	PQN	C23-C25-C26-C27
39	E	321	LMT	C2-C3-C4-C5
41	E	322	LHG	C26-C27-C28-C29
41	j	104	LHG	C28-C29-C30-C31
36	T	311	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
36	b	823	CLA	C6-C7-C8-C10
36	b	826	CLA	CBA-CGA-O2A-C1
36	b	841	CLA	CBA-CGA-O2A-C1
41	D	318	LHG	C24-C23-O8-C6
41	j	104	LHG	C24-C23-O8-C6
42	I	315	LMG	C12-C13-C14-C15
42	V	315	LMG	C33-C34-C35-C36
36	A	311	CLA	C10-C11-C12-C13
36	a	837	CLA	C10-C11-C12-C13
36	b	828	CLA	C8-C10-C11-C12
36	b	840	CLA	C15-C16-C17-C18
39	I	317	LMT	O5B-C5B-C6B-O6B
42	G	324	LMG	C7-C8-C9-O8
42	J	318	LMG	O1-C7-C8-C9
42	j	105	LMG	O1-C7-C8-C9
41	F	319	LHG	C19-C20-C21-C22
36	b	809	CLA	O1D-CGD-O2D-CED
36	a	830	CLA	C2C-C3C-CAC-CBC
39	I	318	LMT	C3-C4-C5-C6
41	E	322	LHG	C19-C20-C21-C22
36	I	308	CLA	O2A-C1-C2-C3
36	W	207	CLA	O2A-C1-C2-C3
36	a	804	CLA	O2A-C1-C2-C3
35	G	304	A86	C35-C34-O4-C38
35	M	301	A86	C35-C34-O4-C38
41	O	317	LHG	C17-C18-C19-C20
36	O	307	CLA	O1D-CGD-O2D-CED
36	P	309	CLA	O1D-CGD-O2D-CED
41	f	809	LHG	C27-C28-C29-C30
42	j	105	LMG	C39-C40-C41-C42
36	R	315	CLA	O1A-CGA-O2A-C1
36	F	309	CLA	C5-C6-C7-C8
36	f	804	CLA	C15-C16-C17-C18
36	H	308	CLA	C4-C3-C5-C6
36	Q	306	CLA	O1D-CGD-O2D-CED
41	Q	315	LHG	C12-C13-C14-C15
41	a	842	LHG	C34-C35-C36-C37
39	U	314	LMT	C1-C2-C3-C4
36	f	805	CLA	O1D-CGD-O2D-CED
41	F	319	LHG	C3-O3-P-O6
41	O	317	LHG	C4-O6-P-O3
41	f	808	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
36	X	307	CLA	O1A-CGA-O2A-C1
39	a	853	LMT	C3-C4-C5-C6
39	U	314	LMT	C9-C10-C11-C12
41	O	318	LHG	C28-C29-C30-C31
41	f	808	LHG	C11-C10-C9-C8
42	G	325	LMG	C41-C42-C43-C44
36	O	310	CLA	C2A-CAA-CBA-CGA
36	P	312	CLA	C2A-CAA-CBA-CGA
36	Q	309	CLA	C2A-CAA-CBA-CGA
36	a	817	CLA	C2A-CAA-CBA-CGA
41	f	808	LHG	O1-C1-C2-O2
36	R	315	CLA	C15-C16-C17-C18
36	a	831	CLA	C15-C16-C17-C18
36	b	825	CLA	C13-C15-C16-C17
41	F	319	LHG	O6-C4-C5-O7
41	a	850	LHG	O6-C4-C5-O7
41	i	104	LHG	O6-C4-C5-O7
41	G	321	LHG	C17-C18-C19-C20
36	C	212	CLA	O1A-CGA-O2A-C1
36	A	314	CLA	C16-C17-C18-C20
36	H	312	CLA	C16-C17-C18-C19
36	I	306	CLA	C16-C17-C18-C20
36	l	205	CLA	C16-C17-C18-C19
36	C	207	CLA	C5-C6-C7-C8
36	L	309	CLA	C15-C16-C17-C18
39	b	851	LMT	C7-C8-C9-C10
41	D	319	LHG	C32-C33-C34-C35
42	G	324	LMG	C24-C25-C26-C27
42	J	318	LMG	C20-C21-C22-C23
36	N	310	CLA	C4C-C3C-CAC-CBC
39	a	854	LMT	C4-C5-C6-C7
36	C	209	CLA	C10-C11-C12-C13
36	I	306	CLA	C13-C15-C16-C17
36	L	309	CLA	C13-C15-C16-C17
36	E	311	CLA	O1A-CGA-O2A-C1
36	b	836	CLA	O1A-CGA-O2A-C1
41	I	316	LHG	C19-C20-C21-C22
38	b	804	SQD	O47-C45-C46-O48
41	F	319	LHG	O7-C5-C6-O8
41	f	809	LHG	O7-C5-C6-O8
42	E	319	LMG	O1-C7-C8-O7
42	G	324	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
42	I	315	LMG	O7-C8-C9-O8
42	J	318	LMG	O1-C7-C8-O7
42	h	206	LMG	O7-C8-C9-O8
39	a	853	LMT	C1-C2-C3-C4
36	f	803	CLA	C5-C6-C7-C8
36	E	317	CLA	O1D-CGD-O2D-CED
39	L	303	LMT	C9-C10-C11-C12
41	G	321	LHG	C13-C14-C15-C16
35	S	301	A86	C35-C34-O4-C38
36	b	813	CLA	C6-C7-C8-C10
36	G	311	CLA	C4C-C3C-CAC-CBC
41	R	323	LHG	C19-C20-C21-C22
41	i	104	LHG	C34-C35-C36-C37
36	J	312	CLA	C15-C16-C17-C18
36	a	801	CLA	C8-C10-C11-C12
35	A	302	A86	C10-C11-C13-C14
35	B	301	A86	C10-C11-C13-C14
35	B	303	A86	C10-C11-C13-C14
35	C	204	A86	C10-C11-C13-C14
35	G	304	A86	C10-C11-C13-C14
35	I	302	A86	C10-C11-C13-C14
35	I	304	A86	C10-C11-C13-C14
35	K	302	A86	C10-C11-C13-C14
35	K	306	A86	C10-C11-C13-C14
35	L	304	A86	C10-C11-C13-C14
35	L	306	A86	C10-C11-C13-C14
35	L	319	A86	C10-C11-C13-C14
35	M	301	A86	C10-C11-C13-C14
35	M	302	A86	C10-C11-C13-C14
35	M	305	A86	C10-C11-C13-C14
35	N	306	A86	C10-C11-C13-C14
35	N	320	A86	C10-C11-C13-C14
35	O	302	A86	C10-C11-C13-C14
35	O	319	A86	C10-C11-C13-C14
35	P	303	A86	C10-C11-C13-C14
35	Q	303	A86	C10-C11-C13-C14
35	Q	304	A86	C10-C11-C13-C14
35	R	301	A86	C10-C11-C13-C14
35	R	303	A86	C10-C11-C13-C14
35	R	304	A86	C10-C11-C13-C14
35	R	306	A86	C10-C11-C13-C14
35	R	309	A86	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
35	S	305	A86	C10-C11-C13-C14
35	T	302	A86	C10-C11-C13-C14
35	T	305	A86	C10-C11-C13-C14
35	T	307	A86	C10-C11-C13-C14
35	X	301	A86	C10-C11-C13-C14
35	X	304	A86	C10-C11-C13-C14
35	U	302	A86	C10-C11-C13-C14
35	V	303	A86	C10-C11-C13-C14
41	O	318	LHG	C1-C2-C3-O3
41	a	843	LHG	C1-C2-C3-O3
41	l	208	LHG	C32-C33-C34-C35
36	B	311	CLA	C3-C5-C6-C7
36	G	319	CLA	C2-C1-O2A-CGA
36	H	306	CLA	C2-C1-O2A-CGA
36	Q	314	CLA	C2-C1-O2A-CGA
36	T	314	CLA	C2-C1-O2A-CGA
36	a	808	CLA	C2-C1-O2A-CGA
36	a	830	CLA	C2-C1-O2A-CGA
36	b	802	CLA	C2-C1-O2A-CGA
36	b	806	CLA	C2-C1-O2A-CGA
36	b	827	CLA	C2-C1-O2A-CGA
39	U	315	LMT	C3-C4-C5-C6
36	H	312	CLA	C15-C16-C17-C18
42	D	320	LMG	C10-C11-C12-C13
36	A	306	CLA	C11-C10-C8-C9
36	F	314	CLA	C6-C7-C8-C9
36	G	310	CLA	C11-C12-C13-C14
36	H	316	CLA	C14-C13-C15-C16
36	M	311	CLA	C14-C13-C15-C16
36	O	307	CLA	C11-C10-C8-C9
36	O	316	CLA	C11-C12-C13-C14
36	P	309	CLA	C11-C10-C8-C9
36	P	314	CLA	C11-C10-C8-C9
36	Q	306	CLA	C11-C10-C8-C9
36	W	211	CLA	C14-C13-C15-C16
36	a	805	CLA	C11-C12-C13-C14
36	a	818	CLA	C11-C12-C13-C14
36	a	826	CLA	C11-C12-C13-C14
36	a	828	CLA	C6-C7-C8-C9
36	a	831	CLA	C6-C7-C8-C9
36	a	837	CLA	C11-C10-C8-C9
36	b	809	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
36	b	816	CLA	C6-C7-C8-C9
36	f	802	CLA	C14-C13-C15-C16
36	i	102	CLA	C14-C13-C15-C16
36	U	305	CLA	C11-C12-C13-C14
36	U	306	CLA	C6-C7-C8-C9
36	U	311	CLA	C6-C7-C8-C9
36	R	314	CLA	CBD-CGD-O2D-CED
35	N	301	A86	C35-C34-O4-C38
35	R	303	A86	C35-C34-O4-C38
39	b	848	LMT	C2-C3-C4-C5
39	U	315	LMT	C9-C10-C11-C12
41	i	104	LHG	C11-C10-C9-C8
42	E	319	LMG	C14-C15-C16-C17
42	J	319	LMG	C20-C21-C22-C23
36	H	312	CLA	C5-C6-C7-C8
36	W	207	CLA	C13-C15-C16-C17
36	a	822	CLA	C4-C3-C5-C6
41	O	317	LHG	C5-C4-O6-P
39	b	848	LMT	C4B-C5B-C6B-O6B
41	i	104	LHG	C26-C27-C28-C29
42	J	318	LMG	C15-C16-C17-C18
36	R	315	CLA	C2A-CAA-CBA-CGA
36	W	207	CLA	C2A-CAA-CBA-CGA
36	a	812	CLA	C2A-CAA-CBA-CGA
36	l	202	CLA	C16-C17-C18-C20
36	b	841	CLA	CBD-CGD-O2D-CED
44	a	844	BCR	C1-C6-C7-C8
44	a	844	BCR	C5-C6-C7-C8
44	a	844	BCR	C23-C24-C25-C26
44	a	844	BCR	C23-C24-C25-C30
44	a	845	BCR	C23-C24-C25-C26
44	a	846	BCR	C23-C24-C25-C26
44	b	843	BCR	C23-C24-C25-C26
44	b	843	BCR	C23-C24-C25-C30
44	b	844	BCR	C1-C6-C7-C8
44	b	845	BCR	C5-C6-C7-C8
44	b	847	BCR	C1-C6-C7-C8
44	b	847	BCR	C23-C24-C25-C26
44	f	806	BCR	C23-C24-C25-C26
44	i	101	BCR	C5-C6-C7-C8
44	l	207	BCR	C5-C6-C7-C8
44	l	207	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
44	m	101	BCR	C5-C6-C7-C8
36	T	313	CLA	C13-C15-C16-C17
36	b	821	CLA	C13-C15-C16-C17
41	G	321	LHG	C31-C32-C33-C34
42	D	320	LMG	C33-C34-C35-C36
36	U	306	CLA	O1D-CGD-O2D-CED
34	W	205	DD6	C-C1-C24-C25
44	b	845	BCR	C37-C22-C23-C24
36	f	803	CLA	C2C-C3C-CAC-CBC
34	E	304	DD6	C10-C11-C13-C14
35	C	204	A86	C2-C1-C24-C25
35	R	301	A86	C35-C34-O4-C38
36	M	309	CLA	C5-C6-C7-C8
36	R	310	CLA	C10-C11-C12-C13
36	a	828	CLA	C15-C16-C17-C18
39	a	853	LMT	C6-C7-C8-C9
42	j	105	LMG	C21-C22-C23-C24
40	b	849	DGD	O1B-C1B-O2G-C2G
41	G	301	LHG	O9-C7-O7-C5
36	G	311	CLA	C8-C10-C11-C12
41	b	850	LHG	C13-C14-C15-C16
36	H	309	CLA	C16-C17-C18-C20
36	a	808	CLA	C16-C17-C18-C20
36	b	820	CLA	C11-C12-C13-C15
36	F	310	CLA	C11-C10-C8-C9
36	K	307	CLA	C14-C13-C15-C16
36	U	310	CLA	C8-C10-C11-C12
36	C	209	CLA	O1A-CGA-O2A-C1
36	j	102	CLA	O1A-CGA-O2A-C1
36	j	101	CLA	O1D-CGD-O2D-CED
42	a	852	LMG	C12-C13-C14-C15
36	I	311	CLA	CBD-CGD-O2D-CED
36	G	310	CLA	C8-C10-C11-C12
36	G	311	CLA	C13-C15-C16-C17
41	O	318	LHG	O6-C4-C5-C6
41	b	850	LHG	O6-C4-C5-C6
41	G	320	LHG	O2-C2-C3-O3
41	b	850	LHG	O2-C2-C3-O3
36	J	316	CLA	O1A-CGA-O2A-C1
36	b	801	CLA	O1D-CGD-O2D-CED
39	U	315	LMT	C5-C6-C7-C8
41	i	104	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
36	A	314	CLA	C11-C12-C13-C15
36	B	305	CLA	C11-C12-C13-C15
36	B	305	CLA	C12-C13-C15-C16
36	C	206	CLA	C11-C12-C13-C15
36	C	207	CLA	C11-C12-C13-C15
36	C	211	CLA	C12-C13-C15-C16
36	F	312	CLA	C6-C7-C8-C10
36	G	310	CLA	C11-C12-C13-C15
36	H	307	CLA	C11-C10-C8-C7
36	H	311	CLA	C12-C13-C15-C16
36	H	315	CLA	C6-C7-C8-C10
36	H	316	CLA	C6-C7-C8-C10
36	I	305	CLA	C6-C7-C8-C10
36	I	306	CLA	C6-C7-C8-C10
36	I	308	CLA	C6-C7-C8-C10
36	I	311	CLA	C11-C10-C8-C7
36	J	308	CLA	C11-C12-C13-C15
36	J	313	CLA	C11-C10-C8-C7
36	K	310	CLA	C11-C12-C13-C15
36	K	312	CLA	C12-C13-C15-C16
36	L	308	CLA	C11-C10-C8-C7
36	N	316	CLA	C6-C7-C8-C10
36	O	316	CLA	C11-C10-C8-C7
36	O	316	CLA	C11-C12-C13-C15
36	P	310	CLA	C12-C13-C15-C16
36	Q	306	CLA	C11-C10-C8-C7
36	Q	314	CLA	C12-C13-C15-C16
36	R	310	CLA	C11-C12-C13-C15
36	S	310	CLA	C11-C12-C13-C15
36	T	314	CLA	C11-C12-C13-C15
36	T	314	CLA	C12-C13-C15-C16
36	W	206	CLA	C11-C12-C13-C15
36	W	211	CLA	C12-C13-C15-C16
36	W	212	CLA	C11-C12-C13-C15
36	a	802	CLA	C6-C7-C8-C10
36	a	805	CLA	C11-C12-C13-C15
36	a	817	CLA	C11-C10-C8-C7
36	a	818	CLA	C11-C12-C13-C15
36	a	825	CLA	C11-C10-C8-C7
36	a	825	CLA	C11-C12-C13-C15
36	a	826	CLA	C11-C12-C13-C15
36	a	828	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
36	a	831	CLA	C6-C7-C8-C10
36	a	831	CLA	C11-C10-C8-C7
36	a	831	CLA	C11-C12-C13-C15
36	a	848	CLA	C11-C10-C8-C7
36	b	805	CLA	C11-C10-C8-C7
36	b	806	CLA	C11-C10-C8-C7
36	b	826	CLA	C6-C7-C8-C10
36	b	826	CLA	C11-C10-C8-C7
36	b	828	CLA	C12-C13-C15-C16
36	b	837	CLA	C12-C13-C15-C16
36	f	802	CLA	C12-C13-C15-C16
36	f	805	CLA	C2-C3-C5-C6
36	i	102	CLA	C12-C13-C15-C16
36	j	101	CLA	C6-C7-C8-C10
36	j	101	CLA	C11-C12-C13-C15
36	l	205	CLA	C11-C10-C8-C7
36	U	305	CLA	C11-C12-C13-C15
36	U	306	CLA	C6-C7-C8-C10
36	U	311	CLA	C11-C10-C8-C7
36	V	306	CLA	C6-C7-C8-C10
36	V	306	CLA	C11-C12-C13-C15
36	V	308	CLA	C6-C7-C8-C10
36	V	311	CLA	C12-C13-C15-C16
43	a	840	PQN	C21-C22-C23-C25
43	b	842	PQN	C21-C22-C23-C25
39	I	317	LMT	C1-C2-C3-C4
41	f	809	LHG	C26-C27-C28-C29
42	G	324	LMG	C42-C43-C44-C45
42	V	315	LMG	C17-C18-C19-C20
36	L	314	CLA	C15-C16-C17-C18
36	f	802	CLA	C13-C15-C16-C17
34	A	301	DD6	C24-C25-C26-C27
34	M	303	DD6	C24-C25-C26-C27
34	R	308	DD6	C1-C2-C3-C4
35	S	304	A86	C11-C10-C9-C8
35	S	308	A86	C11-C10-C9-C8
36	T	311	CLA	C16-C17-C18-C20
41	F	319	LHG	C12-C13-C14-C15
41	F	319	LHG	C10-C11-C12-C13
42	G	324	LMG	C41-C42-C43-C44
36	S	312	CLA	C8-C10-C11-C12
42	V	316	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
42	a	852	LMG	C38-C39-C40-C41
44	a	844	BCR	C20-C21-C22-C37
44	b	846	BCR	C11-C10-C9-C34
36	G	312	CLA	C3-C5-C6-C7
36	J	308	CLA	C3-C5-C6-C7
36	b	802	CLA	C15-C16-C17-C18
36	b	834	CLA	C10-C11-C12-C13
36	W	209	CLA	CBA-CGA-O2A-C1
36	V	307	CLA	CBA-CGA-O2A-C1
42	G	324	LMG	C11-C12-C13-C14
39	L	318	LMT	O5B-C1B-O1B-C4'
36	E	313	CLA	C15-C16-C17-C18
36	b	840	CLA	C10-C11-C12-C13
36	a	807	CLA	O1A-CGA-O2A-C1
36	W	207	CLA	CBD-CGD-O2D-CED
35	H	304	A86	C28-C27-C29-C30
35	I	301	A86	C28-C27-C29-C30
35	J	301	A86	C28-C27-C29-C30
35	U	303	A86	C28-C27-C29-C30
36	A	310	CLA	CAD-CBD-CGD-O2D
36	D	315	CLA	CAD-CBD-CGD-O2D
36	D	316	CLA	CAD-CBD-CGD-O2D
36	E	311	CLA	CAD-CBD-CGD-O2D
36	F	316	CLA	CAD-CBD-CGD-O2D
36	G	316	CLA	CAD-CBD-CGD-O2D
36	I	313	CLA	CAD-CBD-CGD-O2D
36	J	317	CLA	CAD-CBD-CGD-O2D
36	K	307	CLA	CAD-CBD-CGD-O2D
36	K	309	CLA	CAD-CBD-CGD-O2D
36	K	316	CLA	CAD-CBD-CGD-O2D
36	L	308	CLA	CAD-CBD-CGD-O2D
36	L	316	CLA	CAD-CBD-CGD-O2D
36	M	310	CLA	CAD-CBD-CGD-O2D
36	M	311	CLA	CAD-CBD-CGD-O2D
36	N	309	CLA	CAD-CBD-CGD-O2D
36	N	312	CLA	CAD-CBD-CGD-O2D
36	P	319	CLA	CAD-CBD-CGD-O2D
36	R	314	CLA	CAD-CBD-CGD-O2D
36	S	312	CLA	CAD-CBD-CGD-O2D
36	S	319	CLA	CAD-CBD-CGD-O2D
36	T	312	CLA	CAD-CBD-CGD-O2D
36	W	210	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
36	W	214	CLA	CAD-CBD-CGD-O2D
36	X	312	CLA	CAD-CBD-CGD-O2D
36	X	315	CLA	CAD-CBD-CGD-O2D
36	a	805	CLA	CAD-CBD-CGD-O2D
36	a	806	CLA	CAD-CBD-CGD-O2D
36	a	830	CLA	CAD-CBD-CGD-O2D
36	a	831	CLA	CAD-CBD-CGD-O2D
36	b	808	CLA	CAD-CBD-CGD-O2D
36	b	827	CLA	CAD-CBD-CGD-O2D
36	b	833	CLA	CAD-CBD-CGD-O2D
36	i	102	CLA	CAD-CBD-CGD-O2D
36	j	106	CLA	CAD-CBD-CGD-O2D
36	l	201	CLA	CAD-CBD-CGD-O2D
36	V	307	CLA	CAD-CBD-CGD-O2D
36	V	313	CLA	CAD-CBD-CGD-O2D
37	C	213	KC1	CAD-CBD-CGD-O2D
37	M	318	KC1	CAD-CBD-CGD-O2D
37	O	313	KC1	CAD-CBD-CGD-O2D
37	O	315	KC1	CAD-CBD-CGD-O2D
37	P	315	KC1	CAD-CBD-CGD-O2D
37	Q	311	KC1	CAD-CBD-CGD-O2D
37	Q	313	KC1	CAD-CBD-CGD-O2D
37	X	311	KC1	CAD-CBD-CGD-O2D
40	C	215	DGD	C1G-C2G-O2G-C1B
41	Q	315	LHG	C4-C5-O7-C7
41	a	842	LHG	C6-C5-O7-C7
41	l	208	LHG	C6-C5-O7-C7
42	a	852	LMG	C9-C8-O7-C10
39	B	312	LMT	C6-C7-C8-C9
42	j	105	LMG	C12-C13-C14-C15
42	j	105	LMG	C32-C33-C34-C35
35	J	302	A86	C35-C34-O4-C38
36	I	311	CLA	C8-C10-C11-C12
36	a	802	CLA	C10-C11-C12-C13
36	a	804	CLA	C15-C16-C17-C18
44	b	847	BCR	C6-C7-C8-C9
36	b	829	CLA	O1A-CGA-O2A-C1
36	C	207	CLA	CBD-CGD-O2D-CED
36	T	311	CLA	CBA-CGA-O2A-C1
36	H	315	CLA	C4-C3-C5-C6
36	R	322	CLA	C4-C3-C5-C6
36	f	805	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	a	808	CLA	C16-C17-C18-C19
36	M	312	CLA	C4C-C3C-CAC-CBC
39	L	303	LMT	O5'-C1'-O1'-C1
39	U	315	LMT	O5'-C1'-O1'-C1
35	A	316	A86	C12-C11-C13-O
35	B	301	A86	C12-C11-C13-O
35	B	303	A86	C12-C11-C13-O
35	C	202	A86	C12-C11-C13-O
35	F	305	A86	C12-C11-C13-O
35	F	307	A86	C12-C11-C13-O
35	G	304	A86	C12-C11-C13-O
35	H	301	A86	C12-C11-C13-O
35	I	302	A86	C12-C11-C13-O
35	I	304	A86	C12-C11-C13-O
35	J	303	A86	C12-C11-C13-O
35	J	306	A86	C12-C11-C13-O
35	K	302	A86	C12-C11-C13-O
35	K	303	A86	C12-C11-C13-O
35	L	319	A86	C12-C11-C13-O
35	M	301	A86	C12-C11-C13-O
35	M	304	A86	C12-C11-C13-O
35	M	305	A86	C12-C11-C13-O
35	N	301	A86	C12-C11-C13-O
35	N	302	A86	C12-C11-C13-O
35	N	320	A86	C12-C11-C13-O
35	O	302	A86	C12-C11-C13-O
35	O	303	A86	C12-C11-C13-O
35	O	305	A86	C12-C11-C13-O
35	P	303	A86	C12-C11-C13-O
35	P	304	A86	C12-C11-C13-O
35	Q	301	A86	C12-C11-C13-O
35	Q	303	A86	C12-C11-C13-O
35	R	301	A86	C12-C11-C13-O
35	R	302	A86	C12-C11-C13-O
35	R	303	A86	C12-C11-C13-O
35	R	304	A86	C12-C11-C13-O
35	R	306	A86	C12-C11-C13-O
35	R	309	A86	C12-C11-C13-O
35	S	301	A86	C12-C11-C13-O
35	S	302	A86	C12-C11-C13-O
35	T	302	A86	C12-C11-C13-O
35	T	303	A86	C12-C11-C13-O

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Mol	Chain	Res	Type	Atoms
35	T	306	A86	C12-C11-C13-O
35	T	307	A86	C12-C11-C13-O
35	W	202	A86	C12-C11-C13-O
35	W	203	A86	C12-C11-C13-O
35	X	301	A86	C12-C11-C13-O
35	X	302	A86	C12-C11-C13-O
35	X	303	A86	C12-C11-C13-O
35	X	305	A86	C12-C11-C13-O
35	U	302	A86	C12-C11-C13-O
35	U	304	A86	C12-C11-C13-O
35	V	303	A86	C12-C11-C13-O
35	V	304	A86	C12-C11-C13-O
38	A	315	SQD	C44-C45-C46-O48
41	D	318	LHG	C5-C4-O6-P
41	E	322	LHG	C5-C4-O6-P
41	G	321	LHG	C5-C4-O6-P
41	O	317	LHG	C4-C5-C6-O8
42	D	321	LMG	C7-C8-C9-O8
42	G	325	LMG	O1-C7-C8-C9
42	I	315	LMG	C7-C8-C9-O8
42	h	206	LMG	C7-C8-C9-O8
36	b	841	CLA	O1A-CGA-O2A-C1
36	V	307	CLA	O1A-CGA-O2A-C1
41	F	318	LHG	O6-C4-C5-O7
41	G	301	LHG	O6-C4-C5-O7
41	Q	315	LHG	O6-C4-C5-O7
36	J	307	CLA	C3-C5-C6-C7
36	L	308	CLA	C3-C5-C6-C7
35	L	306	A86	C35-C34-O4-C38
35	X	301	A86	C35-C34-O4-C38
41	F	318	LHG	C9-C10-C11-C12
41	a	842	LHG	C27-C28-C29-C30
41	j	104	LHG	C29-C30-C31-C32
37	B	310	KC1	C4B-C3B-CAB-CBB
37	C	213	KC1	C4B-C3B-CAB-CBB
37	E	309	KC1	C4B-C3B-CAB-CBB
37	G	308	KC1	C4B-C3B-CAB-CBB
37	J	314	KC1	C4B-C3B-CAB-CBB
37	K	314	KC1	C4B-C3B-CAB-CBB
37	L	317	KC1	C4B-C3B-CAB-CBB
37	N	314	KC1	C4B-C3B-CAB-CBB
37	O	313	KC1	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
37	O	315	KC1	C4B-C3B-CAB-CBB
37	P	315	KC1	C4B-C3B-CAB-CBB
37	Q	311	KC1	C4B-C3B-CAB-CBB
37	Q	313	KC1	C4B-C3B-CAB-CBB
37	T	315	KC1	C4B-C3B-CAB-CBB
37	W	213	KC1	C4B-C3B-CAB-CBB
39	F	320	LMT	O5B-C5B-C6B-O6B
36	F	314	CLA	C2A-CAA-CBA-CGA
36	X	306	CLA	C2A-CAA-CBA-CGA
36	O	308	CLA	C10-C11-C12-C13
36	b	819	CLA	C10-C11-C12-C13
41	i	104	LHG	C27-C28-C29-C30
36	J	313	CLA	CBD-CGD-O2D-CED
36	a	820	CLA	C16-C17-C18-C19
36	a	814	CLA	C4C-C3C-CAC-CBC
41	O	318	LHG	O9-C7-O7-C5
36	A	308	CLA	CHA-CBD-CGD-O1D
36	A	308	CLA	CHA-CBD-CGD-O2D
36	B	311	CLA	CHA-CBD-CGD-O1D
36	B	311	CLA	CHA-CBD-CGD-O2D
36	C	208	CLA	CHA-CBD-CGD-O1D
36	C	208	CLA	CHA-CBD-CGD-O2D
36	C	212	CLA	CHA-CBD-CGD-O2D
36	E	308	CLA	CHA-CBD-CGD-O2D
36	E	312	CLA	CHA-CBD-CGD-O1D
36	E	312	CLA	CHA-CBD-CGD-O2D
36	G	311	CLA	CHA-CBD-CGD-O1D
36	G	311	CLA	CHA-CBD-CGD-O2D
36	H	315	CLA	CHA-CBD-CGD-O1D
36	Q	314	CLA	CHA-CBD-CGD-O1D
36	Q	314	CLA	CHA-CBD-CGD-O2D
36	R	313	CLA	CHA-CBD-CGD-O1D
36	R	313	CLA	CHA-CBD-CGD-O2D
36	S	320	CLA	CHA-CBD-CGD-O1D
36	S	320	CLA	CHA-CBD-CGD-O2D
36	T	314	CLA	CHA-CBD-CGD-O2D
36	X	308	CLA	CHA-CBD-CGD-O1D
36	X	308	CLA	CHA-CBD-CGD-O2D
36	a	801	CLA	CHA-CBD-CGD-O1D
36	a	801	CLA	CHA-CBD-CGD-O2D
36	a	834	CLA	CHA-CBD-CGD-O1D
36	b	802	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
36	b	811	CLA	CHA-CBD-CGD-O1D
36	b	811	CLA	CHA-CBD-CGD-O2D
36	b	815	CLA	CHA-CBD-CGD-O1D
36	b	817	CLA	CHA-CBD-CGD-O1D
36	b	817	CLA	CHA-CBD-CGD-O2D
36	b	825	CLA	CHA-CBD-CGD-O1D
36	b	825	CLA	CHA-CBD-CGD-O2D
36	b	841	CLA	CHA-CBD-CGD-O1D
36	V	305	CLA	CHA-CBD-CGD-O1D
36	V	305	CLA	CHA-CBD-CGD-O2D
41	a	850	LHG	C19-C20-C21-C22
41	D	318	LHG	O10-C23-O8-C6
41	j	104	LHG	O10-C23-O8-C6
42	V	315	LMG	C31-C32-C33-C34
39	f	807	LMT	C1-C2-C3-C4
39	b	851	LMT	C2-C3-C4-C5
42	G	325	LMG	C22-C23-C24-C25
42	J	318	LMG	C32-C33-C34-C35
40	C	215	DGD	O1G-C1G-C2G-O2G
41	G	301	LHG	O7-C5-C6-O8
41	G	321	LHG	O7-C5-C6-O8
41	O	317	LHG	O7-C5-C6-O8
41	O	318	LHG	O7-C5-C6-O8
41	R	323	LHG	O7-C5-C6-O8
42	G	324	LMG	O7-C8-C9-O8
42	L	321	LMG	O7-C8-C9-O8
42	j	105	LMG	O1-C7-C8-O7
42	V	315	LMG	O1-C7-C8-O7
42	V	315	LMG	O7-C8-C9-O8
41	f	808	LHG	C16-C17-C18-C19
42	V	316	LMG	C12-C13-C14-C15
36	H	309	CLA	C8-C10-C11-C12
36	F	317	CLA	O1A-CGA-O2A-C1
36	b	826	CLA	O1A-CGA-O2A-C1
39	L	318	LMT	O1'-C1-C2-C3
39	U	314	LMT	C6-C7-C8-C9
42	j	105	LMG	C42-C43-C44-C45
39	E	321	LMT	C3'-C4'-O1B-C1B
36	H	309	CLA	C16-C17-C18-C19
35	A	316	A86	C10-C11-C13-O
35	B	301	A86	C10-C11-C13-O
35	B	303	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
35	C	202	A86	C10-C11-C13-O
35	C	204	A86	C13-C14-C15-O1
35	F	302	A86	C13-C14-C15-O1
35	F	305	A86	C10-C11-C13-O
35	F	307	A86	C10-C11-C13-O
35	G	304	A86	C10-C11-C13-O
35	H	301	A86	C10-C11-C13-O
35	I	302	A86	C10-C11-C13-O
35	I	304	A86	C10-C11-C13-O
35	J	303	A86	C10-C11-C13-O
35	K	302	A86	C10-C11-C13-O
35	K	303	A86	C10-C11-C13-O
35	K	306	A86	C10-C11-C13-O
35	L	301	A86	C13-C14-C15-O1
35	L	304	A86	C10-C11-C13-O
35	L	319	A86	C10-C11-C13-O
35	M	301	A86	C10-C11-C13-O
35	M	302	A86	C10-C11-C13-O
35	M	304	A86	C10-C11-C13-O
35	M	305	A86	C10-C11-C13-O
35	N	301	A86	C10-C11-C13-O
35	N	302	A86	C10-C11-C13-O
35	N	303	A86	C10-C11-C13-O
35	N	320	A86	C10-C11-C13-O
35	O	302	A86	C10-C11-C13-O
35	O	303	A86	C10-C11-C13-O
35	O	305	A86	C10-C11-C13-O
35	O	319	A86	C10-C11-C13-O
35	P	303	A86	C10-C11-C13-O
35	P	304	A86	C10-C11-C13-O
35	Q	301	A86	C10-C11-C13-O
35	Q	303	A86	C10-C11-C13-O
35	Q	304	A86	C10-C11-C13-O
35	R	301	A86	C10-C11-C13-O
35	R	302	A86	C10-C11-C13-O
35	R	303	A86	C10-C11-C13-O
35	R	304	A86	C10-C11-C13-O
35	R	306	A86	C10-C11-C13-O
35	R	309	A86	C10-C11-C13-O
35	S	301	A86	C10-C11-C13-O
35	S	302	A86	C10-C11-C13-O
35	S	303	A86	C10-C11-C13-O

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Mol	Chain	Res	Type	Atoms
35	S	305	A86	C10-C11-C13-O
35	S	305	A86	C13-C14-C15-O1
35	T	302	A86	C10-C11-C13-O
35	T	303	A86	C10-C11-C13-O
35	T	305	A86	C10-C11-C13-O
35	T	306	A86	C10-C11-C13-O
35	T	307	A86	C10-C11-C13-O
35	W	202	A86	C10-C11-C13-O
35	W	203	A86	C10-C11-C13-O
35	X	301	A86	C10-C11-C13-O
35	X	302	A86	C10-C11-C13-O
35	X	303	A86	C10-C11-C13-O
35	X	304	A86	C10-C11-C13-O
35	X	305	A86	C10-C11-C13-O
35	U	302	A86	C10-C11-C13-O
35	U	304	A86	C10-C11-C13-O
35	V	302	A86	C10-C11-C13-O
35	V	303	A86	C10-C11-C13-O
35	V	304	A86	C10-C11-C13-O
41	Q	315	LHG	O1-C1-C2-O2
41	b	850	LHG	O1-C1-C2-O2
36	F	310	CLA	O1D-CGD-O2D-CED
39	h	205	LMT	C6-C7-C8-C9
41	F	319	LHG	C25-C26-C27-C28
41	O	317	LHG	C12-C13-C14-C15
41	R	323	LHG	C13-C14-C15-C16
42	J	319	LMG	C23-C24-C25-C26
36	O	309	CLA	C3-C5-C6-C7
36	P	311	CLA	C3-C5-C6-C7
36	Q	308	CLA	C3-C5-C6-C7
36	a	820	CLA	C4-C3-C5-C6
39	E	321	LMT	C7-C8-C9-C10
36	U	311	CLA	O1A-CGA-O2A-C1
36	T	309	CLA	C2-C3-C5-C6
34	D	304	DD6	C27-C29-C30-C31
42	D	320	LMG	C24-C25-C26-C27
42	V	316	LMG	O9-C10-O7-C8
36	U	311	CLA	C15-C16-C17-C18
36	A	314	CLA	C11-C12-C13-C14
36	F	310	CLA	C6-C7-C8-C9
36	H	306	CLA	C11-C12-C13-C14
36	H	307	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
36	K	312	CLA	C14-C13-C15-C16
36	L	314	CLA	C14-C13-C15-C16
36	N	308	CLA	C11-C12-C13-C14
36	N	316	CLA	C6-C7-C8-C9
36	O	306	CLA	C11-C10-C8-C9
36	P	308	CLA	C11-C10-C8-C9
36	Q	305	CLA	C11-C10-C8-C9
36	Q	314	CLA	C14-C13-C15-C16
36	b	809	CLA	C11-C12-C13-C14
36	b	826	CLA	C6-C7-C8-C9
36	j	101	CLA	C6-C7-C8-C9
36	U	311	CLA	C11-C12-C13-C14
36	V	308	CLA	C14-C13-C15-C16
41	I	316	LHG	C9-C10-C11-C12
36	W	209	CLA	O1A-CGA-O2A-C1
36	a	839	CLA	C16-C17-C18-C19
36	a	839	CLA	C16-C17-C18-C20
36	b	806	CLA	C3-C5-C6-C7
36	V	310	CLA	C3-C5-C6-C7
36	W	208	CLA	O1D-CGD-O2D-CED
40	C	215	DGD	CBB-CCB-CDB-CEB
36	B	309	CLA	C2A-CAA-CBA-CGA
36	J	313	CLA	C2A-CAA-CBA-CGA
36	F	317	CLA	C11-C10-C8-C9
36	b	828	CLA	CAA-CBA-CGA-O2A
39	a	851	LMT	C5'-C4'-O1B-C1B
42	h	206	LMG	C14-C15-C16-C17
34	F	303	DD6	C7-C6-C8-C9
34	Q	302	DD6	C12-C11-C13-C14
34	S	307	DD6	C7-C6-C8-C9
44	b	847	BCR	C37-C22-C23-C24
36	a	802	CLA	C8-C10-C11-C12
42	m	102	LMG	C16-C17-C18-C19
34	D	301	DD6	C2-C1-C24-C25
34	P	305	DD6	C2-C1-C24-C25
34	Q	302	DD6	C10-C11-C13-C14
35	F	302	A86	C5-C6-C8-C9
39	B	312	LMT	C9-C10-C11-C12
36	A	307	CLA	C1A-C2A-CAA-CBA
36	C	206	CLA	C1A-C2A-CAA-CBA
36	E	314	CLA	C1A-C2A-CAA-CBA
36	T	313	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	a	827	CLA	C1A-C2A-CAA-CBA
36	b	813	CLA	C1A-C2A-CAA-CBA
36	b	835	CLA	C1A-C2A-CAA-CBA
42	G	324	LMG	C28-C29-C30-C31
36	T	309	CLA	C16-C17-C18-C19
42	h	206	LMG	O9-C10-O7-C8
36	Q	314	CLA	C5-C6-C7-C8
41	D	318	LHG	C26-C27-C28-C29
36	B	308	CLA	C2-C1-O2A-CGA
36	G	316	CLA	C2-C1-O2A-CGA
36	b	816	CLA	C2-C1-O2A-CGA
38	b	804	SQD	C10-C11-C12-C13
42	G	324	LMG	C40-C41-C42-C43
35	G	302	A86	C11-C10-C9-C8
36	a	824	CLA	O1D-CGD-O2D-CED
42	E	318	LMG	C36-C37-C38-C39
42	I	315	LMG	C33-C34-C35-C36
36	b	840	CLA	C3-C5-C6-C7
41	I	316	LHG	C2-C3-O3-P
36	D	317	CLA	C2-C3-C5-C6
36	a	820	CLA	C2-C3-C5-C6
39	I	318	LMT	C5-C6-C7-C8
42	D	320	LMG	C14-C15-C16-C17
41	D	318	LHG	C3-O3-P-O4
41	D	319	LHG	C3-O3-P-O4
41	F	319	LHG	C3-O3-P-O5
41	F	319	LHG	C4-O6-P-O4
41	G	321	LHG	C4-O6-P-O4
41	O	317	LHG	C3-O3-P-O4
41	a	850	LHG	C3-O3-P-O4
41	f	809	LHG	C3-O3-P-O4
41	f	809	LHG	C3-O3-P-O5
41	j	104	LHG	C4-O6-P-O5
36	C	207	CLA	C16-C17-C18-C19
36	O	316	CLA	C16-C17-C18-C19
36	a	816	CLA	C16-C17-C18-C19
36	a	820	CLA	C16-C17-C18-C20
40	b	849	DGD	C1B-C2B-C3B-C4B
42	V	315	LMG	C10-C11-C12-C13
39	B	313	LMT	C3-C4-C5-C6
41	D	318	LHG	O6-C4-C5-C6
41	l	208	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
35	T	307	A86	C35-C34-O4-C38
40	C	215	DGD	CEB-CFB-CGB-CHB
39	L	303	LMT	C5-C6-C7-C8
36	K	307	CLA	C2A-CAA-CBA-CGA
36	S	314	CLA	C2A-CAA-CBA-CGA
36	I	307	CLA	C3-C5-C6-C7
43	b	842	PQN	C13-C15-C16-C17
41	a	842	LHG	C9-C10-C11-C12
42	G	324	LMG	C14-C15-C16-C17
36	K	316	CLA	C16-C17-C18-C20
35	C	204	A86	C26-C27-C29-C30
35	I	301	A86	C26-C27-C29-C30
35	S	308	A86	C26-C27-C29-C30
36	A	308	CLA	CAD-CBD-CGD-O1D
36	B	309	CLA	CAD-CBD-CGD-O1D
36	C	209	CLA	CAD-CBD-CGD-O1D
36	E	312	CLA	CAD-CBD-CGD-O1D
36	F	311	CLA	CAD-CBD-CGD-O1D
36	G	311	CLA	CAD-CBD-CGD-O1D
36	O	309	CLA	CAD-CBD-CGD-O1D
36	O	316	CLA	CAD-CBD-CGD-O1D
36	P	311	CLA	CAD-CBD-CGD-O1D
36	Q	308	CLA	CAD-CBD-CGD-O1D
36	R	313	CLA	CAD-CBD-CGD-O1D
36	X	308	CLA	CAD-CBD-CGD-O1D
36	V	314	CLA	CAD-CBD-CGD-O1D
37	W	217	KC1	CAD-CBD-CGD-O1D
38	A	315	SQD	C5-C6-S-O9
36	E	316	CLA	C13-C15-C16-C17
40	C	215	DGD	CCB-CDB-CEB-CFB
41	G	301	LHG	C33-C34-C35-C36
42	V	316	LMG	C13-C14-C15-C16
36	T	311	CLA	O1A-CGA-O2A-C1
36	G	312	CLA	C10-C11-C12-C13
36	f	802	CLA	C3-C5-C6-C7
36	C	212	CLA	C10-C11-C12-C13
39	b	848	LMT	C6-C7-C8-C9
41	D	319	LHG	C29-C30-C31-C32
41	O	317	LHG	C24-C25-C26-C27
41	l	208	LHG	C7-C8-C9-C10
36	I	311	CLA	CBA-CGA-O2A-C1
36	S	321	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
41	a	850	LHG	C1-C2-C3-O3
42	G	324	LMG	C39-C40-C41-C42
42	j	105	LMG	C13-C14-C15-C16
36	A	314	CLA	C12-C13-C15-C16
36	C	208	CLA	C11-C10-C8-C7
36	E	311	CLA	C12-C13-C15-C16
36	E	315	CLA	C11-C12-C13-C15
36	E	316	CLA	C12-C13-C15-C16
36	F	309	CLA	C11-C12-C13-C15
36	J	309	CLA	C11-C12-C13-C15
36	K	310	CLA	C6-C7-C8-C10
36	L	308	CLA	C11-C12-C13-C15
36	L	309	CLA	C6-C7-C8-C10
36	N	308	CLA	C12-C13-C15-C16
36	O	307	CLA	C11-C10-C8-C7
36	P	309	CLA	C11-C10-C8-C7
36	P	314	CLA	C6-C7-C8-C10
36	Q	310	CLA	C11-C10-C8-C7
36	Q	314	CLA	C11-C12-C13-C15
36	R	321	CLA	C3A-C2A-CAA-CBA
36	T	309	CLA	C6-C7-C8-C10
36	W	209	CLA	C6-C7-C8-C10
36	a	804	CLA	C6-C7-C8-C10
36	a	817	CLA	C6-C7-C8-C10
36	a	825	CLA	C6-C7-C8-C10
36	a	827	CLA	C11-C12-C13-C15
36	a	832	CLA	C6-C7-C8-C10
36	b	808	CLA	C11-C12-C13-C15
36	b	809	CLA	C6-C7-C8-C10
36	b	810	CLA	C11-C10-C8-C7
36	b	815	CLA	C6-C7-C8-C10
36	b	820	CLA	C6-C7-C8-C10
36	f	803	CLA	C6-C7-C8-C10
36	U	306	CLA	C11-C10-C8-C7
36	U	308	CLA	C6-C7-C8-C10
36	U	311	CLA	C11-C12-C13-C15
36	V	305	CLA	C6-C7-C8-C10
36	V	308	CLA	C12-C13-C15-C16
41	O	317	LHG	C7-C8-C9-C10
41	O	318	LHG	O6-C4-C5-O7
41	b	850	LHG	O6-C4-C5-O7
41	l	208	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
36	E	315	CLA	C13-C15-C16-C17
38	b	804	SQD	C11-C12-C13-C14
34	D	303	DD6	C11-C10-C9-C8
35	J	301	A86	C11-C10-C9-C8
35	V	301	A86	C1-C2-C3-C4
39	I	318	LMT	C2-C1-O1'-C1'
41	I	316	LHG	C35-C36-C37-C38
41	O	318	LHG	C10-C11-C12-C13
41	j	104	LHG	C26-C27-C28-C29
35	P	303	A86	C35-C34-O4-C38
36	P	301	CLA	C10-C11-C12-C13
36	b	806	CLA	C8-C10-C11-C12
36	U	306	CLA	C10-C11-C12-C13
39	B	312	LMT	C4B-C5B-C6B-O6B
38	A	315	SQD	C8-C7-O47-C45
42	h	206	LMG	C11-C10-O7-C8
36	b	801	CLA	C15-C16-C17-C18
36	N	317	CLA	C6-C7-C8-C9
39	G	322	LMT	C3-C4-C5-C6
42	V	316	LMG	C33-C34-C35-C36
36	X	309	CLA	CAD-CBD-CGD-O1D
38	b	804	SQD	C44-C45-C46-O48
39	F	320	LMT	C6-C7-C8-C9
41	l	208	LHG	C4-C5-C6-O8
42	E	318	LMG	O6-C5-C6-O5
42	V	315	LMG	O1-C7-C8-C9
35	L	319	A86	C35-C34-O4-C38
41	D	319	LHG	O7-C5-C6-O8
41	l	208	LHG	O7-C5-C6-O8
42	D	320	LMG	O1-C7-C8-O7
42	D	321	LMG	O7-C8-C9-O8
42	I	315	LMG	O1-C7-C8-O7
41	R	323	LHG	C32-C33-C34-C35
37	G	308	KC1	C4C-C3C-CAC-CBC
41	E	322	LHG	C28-C29-C30-C31
41	f	809	LHG	C34-C35-C36-C37
42	D	321	LMG	C12-C13-C14-C15
38	b	804	SQD	C45-C44-O6-C1
40	L	302	DGD	C2G-C3G-O3G-C1D
42	J	319	LMG	C8-C7-O1-C1
36	T	311	CLA	C13-C15-C16-C17
36	a	808	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	D	317	CLA	O1D-CGD-O2D-CED
42	E	318	LMG	C29-C30-C31-C32
36	b	806	CLA	C15-C16-C17-C18
36	S	319	CLA	C4-C3-C5-C6
36	a	827	CLA	C4-C3-C5-C6
36	b	802	CLA	C4-C3-C5-C6
36	b	828	CLA	C4-C3-C5-C6
36	f	803	CLA	C4-C3-C5-C6
36	C	208	CLA	CBA-CGA-O2A-C1
36	H	309	CLA	CBA-CGA-O2A-C1
42	m	102	LMG	C13-C14-C15-C16
36	V	306	CLA	C2-C3-C5-C6
35	A	302	A86	C13-C14-C15-C20
35	A	316	A86	C13-C14-C15-C20
35	C	202	A86	C13-C14-C15-C20
35	F	305	A86	C13-C14-C15-C20
35	I	304	A86	C13-C14-C15-C20
35	K	302	A86	C13-C14-C15-C20
35	L	304	A86	C13-C14-C15-C20
35	L	319	A86	C13-C14-C15-C20
35	M	301	A86	C13-C14-C15-C20
35	M	305	A86	C13-C14-C15-C20
35	N	306	A86	C13-C14-C15-C20
35	N	320	A86	C13-C14-C15-C20
35	O	302	A86	C13-C14-C15-C20
35	P	303	A86	C13-C14-C15-C20
35	Q	304	A86	C13-C14-C15-C20
35	R	301	A86	C13-C14-C15-C20
35	R	304	A86	C13-C14-C15-C20
35	R	306	A86	C13-C14-C15-C20
35	R	309	A86	C13-C14-C15-C20
35	T	305	A86	C13-C14-C15-C20
35	T	307	A86	C13-C14-C15-C20
35	W	202	A86	C13-C14-C15-C20
35	X	303	A86	C13-C14-C15-C20
35	X	304	A86	C13-C14-C15-C20
35	X	305	A86	C13-C14-C15-C20
35	U	302	A86	C13-C14-C15-C20
35	U	303	A86	C13-C14-C15-C20
36	A	311	CLA	C6-C7-C8-C9
36	C	208	CLA	C14-C13-C15-C16
36	E	316	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	K	307	CLA	C11-C12-C13-C14
36	K	309	CLA	C11-C10-C8-C9
36	K	310	CLA	C11-C12-C13-C14
36	L	314	CLA	C6-C7-C8-C9
36	N	316	CLA	C11-C12-C13-C14
36	P	310	CLA	C14-C13-C15-C16
36	R	313	CLA	C14-C13-C15-C16
36	S	310	CLA	C11-C12-C13-C14
36	S	320	CLA	C11-C10-C8-C9
36	T	314	CLA	C14-C13-C15-C16
36	a	808	CLA	C14-C13-C15-C16
36	a	817	CLA	C6-C7-C8-C9
36	a	848	CLA	C11-C10-C8-C9
36	b	821	CLA	C11-C10-C8-C9
36	b	828	CLA	C14-C13-C15-C16
36	b	837	CLA	C14-C13-C15-C16
36	f	803	CLA	C14-C13-C15-C16
36	V	308	CLA	C6-C7-C8-C9
36	V	311	CLA	C14-C13-C15-C16
43	a	840	PQN	C19-C18-C20-C21
44	i	103	BCR	C22-C23-C24-C25
44	l	207	BCR	C6-C7-C8-C9
42	J	318	LMG	C37-C38-C39-C40
35	O	302	A86	C35-C34-O4-C38
42	J	319	LMG	O6-C1-O1-C7
36	a	837	CLA	C13-C15-C16-C17
41	R	323	LHG	C33-C34-C35-C36
42	I	315	LMG	C37-C38-C39-C40
39	B	312	LMT	C5-C6-C7-C8
34	D	305	DD6	C7-C6-C8-C9
35	F	302	A86	C-C1-C24-C25
36	T	309	CLA	C13-C15-C16-C17
38	b	804	SQD	C26-C27-C28-C29
42	D	320	LMG	C30-C31-C32-C33
42	J	318	LMG	C14-C15-C16-C17
36	W	201	CLA	O1D-CGD-O2D-CED
34	K	304	DD6	C5-C6-C8-C9
36	C	212	CLA	C15-C16-C17-C18
41	G	301	LHG	C24-C25-C26-C27
36	a	825	CLA	O1D-CGD-O2D-CED
36	a	817	CLA	C13-C15-C16-C17
35	K	306	A86	C33-C34-O4-C38

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Mol	Chain	Res	Type	Atoms
38	b	804	SQD	C27-C28-C29-C30
36	a	810	CLA	C4-C3-C5-C6
36	a	817	CLA	CAA-CBA-CGA-O2A
41	b	850	LHG	C31-C32-C33-C34
36	I	311	CLA	O1A-CGA-O2A-C1
36	H	312	CLA	C13-C15-C16-C17
41	O	318	LHG	C11-C12-C13-C14
39	E	321	LMT	O5'-C5'-C6'-O6'
42	G	324	LMG	O6-C5-C6-O5
41	l	208	LHG	C24-C25-C26-C27
42	h	206	LMG	C29-C30-C31-C32
36	a	806	CLA	CBD-CGD-O2D-CED
36	H	317	CLA	C8-C10-C11-C12
36	Q	314	CLA	C15-C16-C17-C18
36	A	305	CLA	C1-C2-C3-C4
36	E	308	CLA	C1-C2-C3-C4
36	a	821	CLA	C1-C2-C3-C4
36	b	832	CLA	C1-C2-C3-C4
36	G	311	CLA	C2C-C3C-CAC-CBC
42	m	102	LMG	C28-C29-C30-C31
42	D	320	LMG	C9-C8-O7-C10
42	I	315	LMG	C9-C8-O7-C10
41	F	318	LHG	O6-C4-C5-C6
41	a	850	LHG	O6-C4-C5-C6
41	a	842	LHG	C1-C2-C3-O3
36	B	311	CLA	C2A-CAA-CBA-CGA
36	G	311	CLA	C2A-CAA-CBA-CGA
36	I	308	CLA	C2A-CAA-CBA-CGA
36	K	308	CLA	C2A-CAA-CBA-CGA
36	K	313	CLA	C2A-CAA-CBA-CGA
36	T	311	CLA	C2A-CAA-CBA-CGA
36	a	811	CLA	C2A-CAA-CBA-CGA
36	a	816	CLA	C2A-CAA-CBA-CGA
36	b	807	CLA	C2A-CAA-CBA-CGA
38	A	315	SQD	O49-C7-O47-C45
36	K	307	CLA	CBA-CGA-O2A-C1
36	a	830	CLA	CBA-CGA-O2A-C1
36	C	207	CLA	O1D-CGD-O2D-CED
36	E	312	CLA	C5-C6-C7-C8
36	J	312	CLA	C10-C11-C12-C13
36	A	310	CLA	C2-C1-O2A-CGA
36	D	316	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
36	F	313	CLA	C2-C1-O2A-CGA
36	P	314	CLA	C2-C1-O2A-CGA
36	W	215	CLA	C2-C1-O2A-CGA
36	b	833	CLA	C2-C1-O2A-CGA
36	l	204	CLA	C2-C1-O2A-CGA
36	U	305	CLA	C2-C1-O2A-CGA
36	V	306	CLA	C2-C1-O2A-CGA
36	D	307	CLA	C4C-C3C-CAC-CBC
36	M	312	CLA	C2C-C3C-CAC-CBC
39	P	321	LMT	C4'-C5'-C6'-O6'
35	I	304	A86	C35-C34-O4-C38
42	L	321	LMG	O7-C10-C11-C12
39	P	320	LMT	C4'-C5'-C6'-O6'
36	C	206	CLA	C8-C10-C11-C12
36	K	307	CLA	O1A-CGA-O2A-C1
39	a	854	LMT	C2-C3-C4-C5
39	K	317	LMT	C3'-C4'-O1B-C1B
35	A	302	A86	C12-C11-C13-C14
35	B	301	A86	C12-C11-C13-C14
35	C	202	A86	C12-C11-C13-C14
35	C	204	A86	C12-C11-C13-C14
35	F	305	A86	C12-C11-C13-C14
35	I	302	A86	C12-C11-C13-C14
35	I	304	A86	C12-C11-C13-C14
35	J	303	A86	C12-C11-C13-C14
35	L	306	A86	C12-C11-C13-C14
35	M	302	A86	C12-C11-C13-C14
35	O	305	A86	C12-C11-C13-C14
35	O	319	A86	C12-C11-C13-C14
35	Q	303	A86	C12-C11-C13-C14
35	R	301	A86	C12-C11-C13-C14
35	R	304	A86	C12-C11-C13-C14
35	T	302	A86	C12-C11-C13-C14
35	T	307	A86	C12-C11-C13-C14
35	X	303	A86	C12-C11-C13-C14
35	X	305	A86	C12-C11-C13-C14
35	U	301	A86	C12-C11-C13-C14
35	U	302	A86	C12-C11-C13-C14
35	V	303	A86	C12-C11-C13-C14
35	V	304	A86	C12-C11-C13-C14
41	F	318	LHG	C4-O6-P-O5
35	S	308	A86	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
36	a	830	CLA	O1A-CGA-O2A-C1
41	O	317	LHG	O6-C4-C5-O7
39	I	317	LMT	C4-C5-C6-C7
36	W	211	CLA	C13-C15-C16-C17
36	a	836	CLA	C15-C16-C17-C18
42	h	206	LMG	C20-C21-C22-C23
44	a	845	BCR	C5-C6-C7-C8
44	a	845	BCR	C23-C24-C25-C30
44	a	846	BCR	C23-C24-C25-C30
44	b	847	BCR	C23-C24-C25-C30
44	f	801	BCR	C5-C6-C7-C8
44	f	806	BCR	C23-C24-C25-C30
44	j	107	BCR	C23-C24-C25-C26
44	j	107	BCR	C23-C24-C25-C30
44	l	207	BCR	C23-C24-C25-C30
44	m	101	BCR	C1-C6-C7-C8
36	H	315	CLA	C2-C3-C5-C6
36	T	311	CLA	C4C-C3C-CAC-CBC
36	V	314	CLA	C2C-C3C-CAC-CBC
39	a	853	LMT	C5-C6-C7-C8
41	j	104	LHG	C15-C16-C17-C18
38	b	804	SQD	O48-C23-C24-C25
41	D	318	LHG	O2-C2-C3-O3
36	C	207	CLA	C16-C17-C18-C20
39	K	317	LMT	O5'-C1'-O1'-C1
42	E	318	LMG	C30-C31-C32-C33
42	G	325	LMG	C24-C25-C26-C27
42	J	319	LMG	C2-C1-O1-C7
44	i	103	BCR	C20-C21-C22-C23
41	G	320	LHG	O7-C5-C6-O8
42	D	320	LMG	O7-C8-C9-O8
36	a	825	CLA	C15-C16-C17-C18
40	b	849	DGD	C9B-CAB-CBB-CCB
36	D	317	CLA	CBD-CGD-O2D-CED
41	D	318	LHG	C4-O6-P-O3
41	D	319	LHG	C3-O3-P-O6
41	G	320	LHG	C3-O3-P-O6
41	G	320	LHG	C4-O6-P-O3
41	Q	315	LHG	C3-O3-P-O6
41	R	323	LHG	C3-O3-P-O6
41	a	842	LHG	C3-O3-P-O6
41	a	843	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
39	h	205	LMT	C5-C6-C7-C8
41	G	301	LHG	C28-C29-C30-C31
36	a	818	CLA	C16-C17-C18-C19
36	I	311	CLA	O1D-CGD-O2D-CED
41	l	208	LHG	C34-C35-C36-C37
42	G	324	LMG	C35-C36-C37-C38
36	M	307	CLA	C5-C6-C7-C8
39	I	317	LMT	C3-C4-C5-C6
36	A	306	CLA	C11-C10-C8-C7
36	C	209	CLA	C11-C12-C13-C15
36	E	311	CLA	C11-C10-C8-C7
36	E	316	CLA	C11-C12-C13-C15
36	H	306	CLA	C11-C12-C13-C15
36	H	308	CLA	C11-C12-C13-C15
36	J	313	CLA	C6-C7-C8-C10
36	L	314	CLA	C12-C13-C15-C16
36	L	320	CLA	C12-C13-C15-C16
36	O	306	CLA	C11-C10-C8-C7
36	P	308	CLA	C11-C10-C8-C7
36	P	313	CLA	C12-C13-C15-C16
36	Q	305	CLA	C11-C10-C8-C7
36	R	312	CLA	C6-C7-C8-C10
36	a	820	CLA	C11-C10-C8-C7
36	a	829	CLA	C6-C7-C8-C10
36	a	832	CLA	C11-C12-C13-C15
36	b	809	CLA	C11-C12-C13-C15
36	b	815	CLA	C11-C10-C8-C7
36	b	816	CLA	C6-C7-C8-C10
36	l	201	CLA	C6-C7-C8-C10
39	I	317	LMT	C2B-C1B-O1B-C4'
39	I	318	LMT	C11-C10-C9-C8
41	f	809	LHG	C28-C29-C30-C31
36	A	311	CLA	C11-C10-C8-C9
36	B	305	CLA	C11-C12-C13-C14
36	E	316	CLA	C14-C13-C15-C16
36	F	309	CLA	C11-C12-C13-C14
36	I	311	CLA	C6-C7-C8-C9
36	O	308	CLA	C6-C7-C8-C9
36	a	816	CLA	C11-C12-C13-C14
36	a	832	CLA	C6-C7-C8-C9
36	b	820	CLA	C11-C10-C8-C9
36	l	201	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
36	U	311	CLA	C13-C15-C16-C17
34	W	204	DD6	C1-C2-C3-C4
34	j	103	DD6	C24-C25-C26-C27
35	K	301	A86	C24-C25-C26-C27
35	X	314	A86	C24-C25-C26-C27
36	D	310	CLA	C16-C17-C18-C19
36	G	310	CLA	C16-C17-C18-C19
36	L	314	CLA	C16-C17-C18-C20
36	V	314	CLA	C4C-C3C-CAC-CBC
39	I	318	LMT	C7-C8-C9-C10
36	a	848	CLA	C5-C6-C7-C8
36	V	310	CLA	C10-C11-C12-C13
36	C	208	CLA	O1A-CGA-O2A-C1
36	N	307	CLA	C2A-CAA-CBA-CGA
39	I	318	LMT	C3'-C4'-O1B-C1B
39	I	318	LMT	C6-C7-C8-C9
39	P	320	LMT	C1-C2-C3-C4
36	S	321	CLA	O1A-CGA-O2A-C1
44	m	101	BCR	C37-C22-C23-C24
36	a	818	CLA	C16-C17-C18-C20
36	b	828	CLA	CBA-CGA-O2A-C1
42	h	206	LMG	C15-C16-C17-C18
34	S	307	DD6	C5-C6-C8-C9
41	a	842	LHG	C10-C11-C12-C13
36	D	308	CLA	C4C-C3C-CAC-CBC
36	A	306	CLA	C12-C13-C15-C16
36	F	310	CLA	C11-C10-C8-C7
36	F	317	CLA	C11-C10-C8-C7
36	G	315	CLA	C11-C10-C8-C7
36	l	204	CLA	O2A-C1-C2-C3
36	G	310	CLA	C16-C17-C18-C20
36	M	309	CLA	C16-C17-C18-C20
36	V	308	CLA	CBA-CGA-O2A-C1
41	G	320	LHG	C24-C23-O8-C6
36	D	307	CLA	C2C-C3C-CAC-CBC
42	h	206	LMG	C31-C32-C33-C34
36	W	207	CLA	O1D-CGD-O2D-CED
35	R	304	A86	C33-C34-O4-C38
35	S	308	A86	C33-C34-O4-C38
40	b	849	DGD	C6B-C7B-C8B-C9B
40	L	302	DGD	C3A-C4A-C5A-C6A
36	K	316	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	F	309	CLA	C2A-CAA-CBA-CGA
36	Q	306	CLA	C2A-CAA-CBA-CGA
36	U	308	CLA	C2A-CAA-CBA-CGA
36	U	311	CLA	C2A-CAA-CBA-CGA
36	a	816	CLA	C16-C17-C18-C20
34	B	302	DD6	C11-C10-C9-C8
41	R	323	LHG	O6-C4-C5-C6
36	H	309	CLA	O1A-CGA-O2A-C1
41	E	322	LHG	C27-C28-C29-C30
36	N	308	CLA	C13-C15-C16-C17
36	b	816	CLA	C8-C10-C11-C12
41	G	320	LHG	O10-C23-O8-C6
36	L	310	CLA	C6-C7-C8-C9
36	V	306	CLA	C16-C17-C18-C19
37	T	310	KC1	C4B-C3B-CAB-CBB
42	J	318	LMG	C18-C19-C20-C21
36	C	209	CLA	C4-C3-C5-C6
36	a	841	CLA	C4-C3-C5-C6
36	R	321	CLA	C10-C11-C12-C13
36	C	209	CLA	C2-C3-C5-C6
36	a	841	CLA	C2-C3-C5-C6
41	O	317	LHG	C11-C12-C13-C14
36	B	308	CLA	C15-C16-C17-C18
41	l	208	LHG	C13-C14-C15-C16
36	H	312	CLA	CAA-CBA-CGA-O2A
36	E	308	CLA	C2-C1-O2A-CGA
36	E	311	CLA	C2-C1-O2A-CGA
36	M	307	CLA	C2-C1-O2A-CGA
36	P	319	CLA	C2-C1-O2A-CGA
36	a	806	CLA	C2-C1-O2A-CGA
36	a	838	CLA	C2-C1-O2A-CGA
36	B	311	CLA	C5-C6-C7-C8
36	E	311	CLA	C16-C17-C18-C20
36	O	316	CLA	C16-C17-C18-C20
36	D	316	CLA	C4C-C3C-CAC-CBC
39	K	317	LMT	C2'-C1'-O1'-C1
36	K	310	CLA	C13-C15-C16-C17
36	A	307	CLA	C8-C10-C11-C12
36	i	102	CLA	O1A-CGA-O2A-C1
36	E	310	CLA	C2A-CAA-CBA-CGA
36	F	313	CLA	C2A-CAA-CBA-CGA
36	L	309	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
36	L	311	CLA	C2A-CAA-CBA-CGA
36	O	307	CLA	C2A-CAA-CBA-CGA
36	P	309	CLA	C2A-CAA-CBA-CGA
36	R	313	CLA	C2A-CAA-CBA-CGA
36	W	209	CLA	C2A-CAA-CBA-CGA
36	a	802	CLA	C2A-CAA-CBA-CGA
36	b	810	CLA	C2A-CAA-CBA-CGA
42	J	319	LMG	O7-C8-C9-O8
39	B	313	LMT	C1-C2-C3-C4
41	F	319	LHG	C26-C27-C28-C29
41	l	208	LHG	C12-C13-C14-C15
41	G	301	LHG	C2-C3-O3-P
39	h	205	LMT	C2-C3-C4-C5
42	G	324	LMG	C34-C35-C36-C37
42	I	315	LMG	C29-C30-C31-C32
36	A	306	CLA	C3A-C2A-CAA-CBA
36	P	301	CLA	C3A-C2A-CAA-CBA
36	T	314	CLA	C3A-C2A-CAA-CBA
36	W	212	CLA	C3A-C2A-CAA-CBA
36	a	827	CLA	C3A-C2A-CAA-CBA
36	l	202	CLA	C3A-C2A-CAA-CBA
36	A	314	CLA	C16-C17-C18-C19
36	P	310	CLA	C16-C17-C18-C20
36	a	848	CLA	C16-C17-C18-C19
36	P	301	CLA	CAA-CBA-CGA-O2A
40	b	849	DGD	C7B-C8B-C9B-CAB
34	S	306	DD6	C11-C10-C9-C8
35	C	204	A86	O-C13-C14-C15
39	F	320	LMT	C5-C6-C7-C8
39	f	807	LMT	C6-C7-C8-C9
35	X	304	A86	C35-C34-O4-C38
41	b	850	LHG	C16-C17-C18-C19
36	S	319	CLA	C2-C3-C5-C6
36	a	827	CLA	C2-C3-C5-C6
34	A	301	DD6	C27-C29-C30-C31
34	J	304	DD6	C27-C29-C30-C31
36	V	314	CLA	CAA-CBA-CGA-O2A
36	F	312	CLA	C11-C12-C13-C14
36	F	314	CLA	C11-C10-C8-C9
36	K	310	CLA	C14-C13-C15-C16
36	N	308	CLA	C6-C7-C8-C9
36	b	811	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
36	b	825	CLA	C6-C7-C8-C9
36	U	306	CLA	C11-C10-C8-C9
36	V	314	CLA	C11-C10-C8-C9
36	G	311	CLA	C10-C11-C12-C13
36	K	316	CLA	CBA-CGA-O2A-C1
42	I	315	LMG	C39-C40-C41-C42
42	m	102	LMG	C15-C16-C17-C18
39	F	320	LMT	C1-C2-C3-C4
36	S	313	CLA	C2C-C3C-CAC-CBC
39	E	320	LMT	C11-C10-C9-C8
41	F	318	LHG	C24-C25-C26-C27
35	C	203	A86	C25-C26-C27-C28
35	G	306	A86	C-C1-C2-C3
35	G	306	A86	C4-C5-C6-C7
35	U	301	A86	C4-C5-C6-C7
35	U	304	A86	C25-C26-C27-C28
40	L	302	DGD	C1G-C2G-C3G-O3G
41	D	319	LHG	C4-C5-C6-O8
41	G	321	LHG	C4-C5-C6-O8
42	D	320	LMG	O1-C7-C8-C9
44	b	845	BCR	C20-C21-C22-C37
42	E	319	LMG	C15-C16-C17-C18
36	W	218	CLA	C2A-CAA-CBA-CGA
36	V	308	CLA	O1A-CGA-O2A-C1
36	E	310	CLA	C16-C17-C18-C20
35	T	307	A86	C33-C34-O4-C38
41	i	104	LHG	C10-C11-C12-C13
39	E	320	LMT	C4-C5-C6-C7
36	Q	314	CLA	C3-C5-C6-C7
34	W	205	DD6	C2-C1-C24-C25
39	G	322	LMT	C3'-C4'-O1B-C1B
41	a	842	LHG	C26-C27-C28-C29
35	J	302	A86	C33-C34-O4-C38
36	V	314	CLA	C8-C10-C11-C12
36	b	811	CLA	C4-C3-C5-C6
36	b	815	CLA	C4-C3-C5-C6
36	I	310	CLA	C1A-C2A-CAA-CBA
36	M	312	CLA	C1A-C2A-CAA-CBA
36	W	211	CLA	C1A-C2A-CAA-CBA
36	a	812	CLA	C1A-C2A-CAA-CBA
36	a	833	CLA	C1A-C2A-CAA-CBA
36	a	835	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	b	814	CLA	C1A-C2A-CAA-CBA
36	b	830	CLA	C1A-C2A-CAA-CBA
36	j	102	CLA	C1A-C2A-CAA-CBA
39	E	320	LMT	C9-C10-C11-C12
36	C	211	CLA	C6-C7-C8-C10
36	C	212	CLA	C11-C10-C8-C7
36	F	310	CLA	C6-C7-C8-C10
36	Q	310	CLA	C12-C13-C15-C16
36	a	807	CLA	C12-C13-C15-C16
36	a	810	CLA	C6-C7-C8-C10
36	b	802	CLA	C2-C3-C5-C6
36	b	821	CLA	C6-C7-C8-C10
36	f	803	CLA	C12-C13-C15-C16
36	h	203	CLA	C11-C10-C8-C7
36	U	310	CLA	C12-C13-C15-C16
36	U	311	CLA	C6-C7-C8-C10
36	U	310	CLA	C10-C11-C12-C13
36	D	306	CLA	CAA-CBA-CGA-O1A
34	D	304	DD6	C11-C10-C9-C8
35	E	307	A86	C11-C10-C9-C8
39	U	314	LMT	C5'-C4'-O1B-C1B
41	Q	315	LHG	C4-O6-P-O3
41	a	842	LHG	C4-O6-P-O3
39	b	848	LMT	C11-C10-C9-C8
36	A	310	CLA	C16-C17-C18-C20
39	E	320	LMT	O5B-C5B-C6B-O6B
42	a	852	LMG	C11-C12-C13-C14
36	Q	314	CLA	C2A-CAA-CBA-CGA
36	S	313	CLA	C2A-CAA-CBA-CGA
36	b	831	CLA	C2A-CAA-CBA-CGA
36	V	308	CLA	C2A-CAA-CBA-CGA
41	F	319	LHG	O1-C1-C2-O2
36	C	206	CLA	C10-C11-C12-C13
36	L	311	CLA	C8-C10-C11-C12
36	L	313	CLA	C15-C16-C17-C18
36	b	811	CLA	C10-C11-C12-C13
36	j	101	CLA	C10-C11-C12-C13
36	V	308	CLA	C5-C6-C7-C8
41	l	208	LHG	C29-C30-C31-C32
42	j	105	LMG	C38-C39-C40-C41
36	G	319	CLA	C4C-C3C-CAC-CBC
41	j	104	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	M	313	KC1	C3A-C2A-CAA-CBA
36	a	816	CLA	C4C-C3C-CAC-CBC
36	b	815	CLA	C4C-C3C-CAC-CBC
41	Q	315	LHG	C31-C32-C33-C34
37	T	310	KC1	CBD-CGD-O2D-CED
36	A	306	CLA	C14-C13-C15-C16
41	G	321	LHG	C5-C6-O8-C23
37	T	310	KC1	O1D-CGD-O2D-CED
41	O	317	LHG	C14-C15-C16-C17
35	X	303	A86	C35-C34-O4-C38
35	V	303	A86	C35-C34-O4-C38
36	I	306	CLA	C4-C3-C5-C6
36	I	310	CLA	C4-C3-C5-C6
36	N	316	CLA	C4-C3-C5-C6
36	b	828	CLA	C2-C3-C5-C6
42	E	318	LMG	C16-C17-C18-C19
36	O	309	CLA	C10-C11-C12-C13
36	P	311	CLA	C10-C11-C12-C13
36	Q	308	CLA	C10-C11-C12-C13
36	a	827	CLA	C5-C6-C7-C8
36	l	205	CLA	C5-C6-C7-C8
36	a	806	CLA	O1D-CGD-O2D-CED
39	U	314	LMT	C3'-C4'-O1B-C1B
35	C	203	A86	C25-C26-C27-C29
35	G	306	A86	C24-C1-C2-C3
35	G	306	A86	C4-C5-C6-C8
35	J	301	A86	C13-C14-C15-C16
35	L	307	A86	C13-C14-C15-C16
35	O	305	A86	C13-C14-C15-C16
35	U	301	A86	C4-C5-C6-C8
35	U	304	A86	C25-C26-C27-C29
36	a	826	CLA	C13-C15-C16-C17
42	G	325	LMG	C30-C31-C32-C33
41	j	104	LHG	O7-C5-C6-O8
42	V	316	LMG	O7-C8-C9-O8
36	H	309	CLA	C2A-CAA-CBA-CGA
39	K	318	LMT	C9-C10-C11-C12
39	h	205	LMT	C5'-C4'-O1B-C1B
41	a	842	LHG	C11-C12-C13-C14
34	D	301	DD6	C24-C25-C26-C27
34	R	307	DD6	C3-C4-C5-C6
35	B	301	A86	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
36	J	313	CLA	O1D-CGD-O2D-CED
36	D	306	CLA	CAA-CBA-CGA-O2A
36	F	314	CLA	C16-C17-C18-C20
36	C	206	CLA	C5-C6-C7-C8
36	K	313	CLA	C15-C16-C17-C18
41	I	316	LHG	C17-C18-C19-C20
35	C	202	A86	C10-C11-C13-C14
35	F	305	A86	C10-C11-C13-C14
35	J	303	A86	C10-C11-C13-C14
35	J	306	A86	C10-C11-C13-C14
35	N	302	A86	C10-C11-C13-C14
35	O	303	A86	C10-C11-C13-C14
35	O	305	A86	C10-C11-C13-C14
35	P	304	A86	C10-C11-C13-C14
35	Q	301	A86	C10-C11-C13-C14
35	R	302	A86	C10-C11-C13-C14
35	S	302	A86	C10-C11-C13-C14
35	T	303	A86	C10-C11-C13-C14
35	T	306	A86	C10-C11-C13-C14
35	W	203	A86	C10-C11-C13-C14
35	X	302	A86	C10-C11-C13-C14
35	X	303	A86	C10-C11-C13-C14
35	X	305	A86	C10-C11-C13-C14
35	U	304	A86	C10-C11-C13-C14
35	V	304	A86	C10-C11-C13-C14
39	F	320	LMT	C3'-C4'-O1B-C1B
36	R	314	CLA	O1D-CGD-O2D-CED
36	H	317	CLA	C4-C3-C5-C6
36	I	305	CLA	C4-C3-C5-C6
36	N	317	CLA	C4-C3-C5-C6
36	b	806	CLA	C4-C3-C5-C6
39	G	322	LMT	C11-C10-C9-C8
36	D	317	CLA	C2-C1-O2A-CGA
36	E	312	CLA	C2-C1-O2A-CGA
36	F	309	CLA	C2-C1-O2A-CGA
36	H	308	CLA	C2-C1-O2A-CGA
36	H	312	CLA	C2-C1-O2A-CGA
36	a	825	CLA	C2-C1-O2A-CGA
36	b	829	CLA	C2-C1-O2A-CGA
36	f	803	CLA	C2-C3-C5-C6
42	J	319	LMG	C12-C13-C14-C15
36	f	804	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	P	308	CLA	O1D-CGD-O2D-CED
39	I	318	LMT	C5'-C4'-O1B-C1B
36	A	314	CLA	C14-C13-C15-C16
36	M	311	CLA	C11-C10-C8-C9
36	O	308	CLA	C11-C10-C8-C9
36	P	313	CLA	C14-C13-C15-C16
36	a	806	CLA	C10-C11-C12-C13
41	O	318	LHG	C35-C36-C37-C38
36	a	808	CLA	C3-C5-C6-C7
42	V	316	LMG	C29-C30-C31-C32
41	F	318	LHG	C15-C16-C17-C18
36	H	315	CLA	C8-C10-C11-C12
36	D	309	CLA	C2A-CAA-CBA-CGA
36	J	310	CLA	C2A-CAA-CBA-CGA
36	K	309	CLA	C2A-CAA-CBA-CGA
36	N	317	CLA	O1A-CGA-O2A-C1
41	a	842	LHG	O10-C23-O8-C6
44	a	845	BCR	C1-C6-C7-C8
44	b	845	BCR	C1-C6-C7-C8
44	b	845	BCR	C23-C24-C25-C30
44	f	801	BCR	C1-C6-C7-C8
44	f	801	BCR	C23-C24-C25-C26
44	f	801	BCR	C23-C24-C25-C30
44	i	101	BCR	C1-C6-C7-C8
44	l	207	BCR	C1-C6-C7-C8
39	G	322	LMT	C4-C5-C6-C7
36	Q	305	CLA	O1D-CGD-O2D-CED
36	B	309	CLA	CAA-CBA-CGA-O2A
36	H	318	CLA	CAA-CBA-CGA-O2A
40	C	215	DGD	O1G-C1G-C2G-C3G
42	I	315	LMG	O1-C7-C8-C9
36	l	205	CLA	C10-C11-C12-C13
41	G	320	LHG	C19-C20-C21-C22
34	A	301	DD6	C11-C10-C9-C8
34	S	306	DD6	C24-C25-C26-C27
35	E	305	A86	C24-C25-C26-C27
35	J	305	A86	C24-C25-C26-C27
36	E	312	CLA	C4-C3-C5-C6
36	O	309	CLA	C4-C3-C5-C6
36	P	311	CLA	C4-C3-C5-C6
36	Q	308	CLA	C4-C3-C5-C6
36	a	805	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
44	b	843	BCR	C21-C22-C23-C24
36	i	102	CLA	C16-C17-C18-C20
36	L	311	CLA	C5-C6-C7-C8
36	P	301	CLA	C13-C15-C16-C17
36	a	826	CLA	C5-C6-C7-C8
36	R	322	CLA	C2-C3-C5-C6
39	a	854	LMT	O5B-C1B-O1B-C4'
36	a	838	CLA	C8-C10-C11-C12
36	O	306	CLA	O1D-CGD-O2D-CED
39	h	205	LMT	C3'-C4'-O1B-C1B
42	L	321	LMG	C29-C30-C31-C32
36	A	308	CLA	C3-C5-C6-C7
36	E	312	CLA	C8-C10-C11-C12
36	M	306	CLA	C5-C6-C7-C8
41	f	809	LHG	O6-C4-C5-O7
41	D	318	LHG	C24-C25-C26-C27
36	b	807	CLA	CAA-CBA-CGA-O2A
37	M	318	KC1	C2C-C3C-CAC-CBC
39	b	851	LMT	C9-C10-C11-C12
36	j	102	CLA	C16-C17-C18-C19
42	I	315	LMG	C4-C5-C6-O5
36	f	803	CLA	C15-C16-C17-C18
41	F	319	LHG	O6-C4-C5-C6
36	K	316	CLA	C4-C3-C5-C6
36	W	209	CLA	C4-C3-C5-C6
36	F	312	CLA	C11-C10-C8-C7
36	H	308	CLA	C2-C3-C5-C6
36	H	317	CLA	C6-C7-C8-C10
36	N	317	CLA	C2-C3-C5-C6
36	Q	314	CLA	C2-C3-C5-C6
36	S	312	CLA	C6-C7-C8-C10
36	S	320	CLA	C11-C10-C8-C7
36	f	802	CLA	C2-C3-C5-C6
36	U	305	CLA	C6-C7-C8-C10
36	b	807	CLA	CAA-CBA-CGA-O1A
36	F	311	CLA	CBA-CGA-O2A-C1
41	G	321	LHG	C11-C12-C13-C14
34	J	304	DD6	C1-C2-C3-C4
41	a	850	LHG	O7-C7-C8-C9
36	a	823	CLA	CBD-CGD-O2D-CED
36	E	315	CLA	C16-C17-C18-C19
36	M	309	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
36	a	801	CLA	C16-C17-C18-C20
36	W	208	CLA	CAA-CBA-CGA-O2A
41	F	319	LHG	C2-C3-O3-P
41	a	850	LHG	O7-C5-C6-O8
36	I	306	CLA	CBA-CGA-O2A-C1
36	a	817	CLA	CBA-CGA-O2A-C1
43	b	842	PQN	C18-C20-C21-C22
36	a	830	CLA	C4C-C3C-CAC-CBC
42	J	318	LMG	C17-C18-C19-C20
36	E	311	CLA	C16-C17-C18-C19
39	U	314	LMT	C4B-C5B-C6B-O6B
36	R	320	CLA	CAA-CBA-CGA-O2A
36	i	102	CLA	CBA-CGA-O2A-C1
41	E	322	LHG	O7-C7-C8-C9
42	V	315	LMG	O7-C10-C11-C12
38	b	804	SQD	C45-C46-O48-C23
36	B	305	CLA	C4-C3-C5-C6
36	P	301	CLA	C4-C3-C5-C6
36	b	801	CLA	C4-C3-C5-C6
41	O	318	LHG	C11-C10-C9-C8
41	I	316	LHG	C3-O3-P-O6
36	b	806	CLA	C2-C3-C5-C6
36	b	811	CLA	C2-C3-C5-C6
36	b	815	CLA	C2-C3-C5-C6
36	I	309	CLA	CAA-CBA-CGA-O2A
36	D	307	CLA	C12-C13-C15-C16
36	C	208	CLA	C11-C10-C8-C9
36	E	311	CLA	C14-C13-C15-C16
36	E	314	CLA	C6-C7-C8-C9
36	G	309	CLA	C6-C7-C8-C9
36	H	311	CLA	C6-C7-C8-C9
36	J	307	CLA	C6-C7-C8-C9
36	J	310	CLA	C11-C10-C8-C9
36	K	308	CLA	C14-C13-C15-C16
36	L	308	CLA	C11-C12-C13-C14
36	Q	310	CLA	C14-C13-C15-C16
36	Q	314	CLA	C11-C12-C13-C14
36	S	312	CLA	C6-C7-C8-C9
36	S	320	CLA	C6-C7-C8-C9
36	W	209	CLA	C6-C7-C8-C9
36	a	804	CLA	C6-C7-C8-C9
36	a	812	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
36	a	820	CLA	C11-C10-C8-C9
36	a	825	CLA	C6-C7-C8-C9
36	a	837	CLA	C14-C13-C15-C16
36	b	808	CLA	C6-C7-C8-C9
36	b	808	CLA	C11-C12-C13-C14
36	b	810	CLA	C11-C10-C8-C9
36	b	815	CLA	C6-C7-C8-C9
36	U	308	CLA	C6-C7-C8-C9
36	U	310	CLA	C14-C13-C15-C16
43	b	842	PQN	C19-C18-C20-C21
42	J	319	LMG	C24-C25-C26-C27
41	i	104	LHG	C16-C17-C18-C19
36	D	307	CLA	C3A-C2A-CAA-CBA
36	G	315	CLA	C3A-C2A-CAA-CBA
36	L	314	CLA	C3A-C2A-CAA-CBA
36	O	309	CLA	C3A-C2A-CAA-CBA
36	P	311	CLA	C3A-C2A-CAA-CBA
36	P	318	CLA	C3A-C2A-CAA-CBA
36	Q	308	CLA	C3A-C2A-CAA-CBA
36	S	321	CLA	C3A-C2A-CAA-CBA
36	a	812	CLA	C3A-C2A-CAA-CBA
36	b	824	CLA	C3A-C2A-CAA-CBA
36	I	306	CLA	O1A-CGA-O2A-C1
36	L	311	CLA	CAA-CBA-CGA-O2A
36	Q	310	CLA	CAA-CBA-CGA-O2A
36	f	802	CLA	CAA-CBA-CGA-O2A
36	P	308	CLA	CBD-CGD-O2D-CED
36	R	319	CLA	CAA-CBA-CGA-O2A
35	B	303	A86	C28-C27-C29-C30
35	M	304	A86	C28-C27-C29-C30
35	N	320	A86	C28-C27-C29-C30
35	Q	304	A86	C28-C27-C29-C30
36	A	305	CLA	CAD-CBD-CGD-O2D
36	A	309	CLA	CAD-CBD-CGD-O2D
36	D	306	CLA	CAD-CBD-CGD-O2D
36	D	308	CLA	CAD-CBD-CGD-O2D
36	D	309	CLA	CAD-CBD-CGD-O2D
36	D	317	CLA	CAD-CBD-CGD-O2D
36	H	305	CLA	CAD-CBD-CGD-O2D
36	J	310	CLA	CAD-CBD-CGD-O2D
36	K	310	CLA	CAD-CBD-CGD-O2D
36	K	315	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
36	L	311	CLA	CAD-CBD-CGD-O2D
36	L	312	CLA	CAD-CBD-CGD-O2D
36	M	308	CLA	CAD-CBD-CGD-O2D
36	M	315	CLA	CAD-CBD-CGD-O2D
36	O	308	CLA	CAD-CBD-CGD-O2D
36	P	302	CLA	CAD-CBD-CGD-O2D
36	P	310	CLA	CAD-CBD-CGD-O2D
36	Q	307	CLA	CAD-CBD-CGD-O2D
36	R	319	CLA	CAD-CBD-CGD-O2D
36	R	320	CLA	CAD-CBD-CGD-O2D
36	S	317	CLA	CAD-CBD-CGD-O2D
36	W	208	CLA	CAD-CBD-CGD-O2D
36	W	216	CLA	CAD-CBD-CGD-O2D
36	X	307	CLA	CAD-CBD-CGD-O2D
36	a	804	CLA	CAD-CBD-CGD-O2D
36	a	810	CLA	CAD-CBD-CGD-O2D
36	a	813	CLA	CAD-CBD-CGD-O2D
36	a	826	CLA	CAD-CBD-CGD-O2D
36	a	848	CLA	CAD-CBD-CGD-O2D
36	b	822	CLA	CAD-CBD-CGD-O2D
36	b	831	CLA	CAD-CBD-CGD-O2D
36	b	837	CLA	CAD-CBD-CGD-O2D
36	j	101	CLA	CAD-CBD-CGD-O2D
36	U	306	CLA	CAD-CBD-CGD-O2D
36	U	307	CLA	CAD-CBD-CGD-O2D
37	F	308	KC1	CAD-CBD-CGD-O2D
37	V	312	KC1	CAD-CBD-CGD-O2D
36	b	830	CLA	C16-C17-C18-C20
39	K	318	LMT	C4-C5-C6-C7
36	C	207	CLA	C8-C10-C11-C12
36	a	816	CLA	C15-C16-C17-C18
35	J	301	A86	C3-C4-C5-C6
36	b	840	CLA	C2A-CAA-CBA-CGA
41	G	321	LHG	C32-C33-C34-C35
36	T	309	CLA	CAA-CBA-CGA-O2A
36	a	804	CLA	CAA-CBA-CGA-O2A
42	a	852	LMG	C16-C17-C18-C19
36	a	823	CLA	O1D-CGD-O2D-CED
36	L	311	CLA	C4-C3-C5-C6
39	K	317	LMT	C4'-C5'-C6'-O6'
39	F	321	LMT	O5'-C1'-O1'-C1
36	D	312	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	L	313	CLA	C13-C15-C16-C17
36	I	306	CLA	C2-C3-C5-C6
36	K	316	CLA	C2-C3-C5-C6
36	N	316	CLA	C2-C3-C5-C6
36	W	209	CLA	C2-C3-C5-C6
36	K	307	CLA	CAA-CBA-CGA-O2A
36	O	306	CLA	CBD-CGD-O2D-CED
34	F	303	DD6	C5-C6-C8-C9
35	F	302	A86	C2-C1-C24-C25
44	f	801	BCR	C7-C8-C9-C10
36	D	307	CLA	C14-C13-C15-C16
34	D	301	DD6	C13-C14-C15-O1
34	D	304	DD6	C13-C14-C15-O1
34	E	301	DD6	C13-C14-C15-O1
34	E	303	DD6	C13-C14-C15-O1
34	E	306	DD6	C13-C14-C15-O1
34	W	205	DD6	C13-C14-C15-O1
35	A	302	A86	C12-C11-C13-O
35	T	305	A86	C12-C11-C13-O
35	X	304	A86	C12-C11-C13-O
35	U	301	A86	C12-C11-C13-O
35	V	302	A86	C12-C11-C13-O
41	f	809	LHG	C4-C5-C6-O8
42	E	319	LMG	O1-C7-C8-C9
42	G	324	LMG	O1-C7-C8-C9
36	W	208	CLA	CAA-CBA-CGA-O1A
36	Q	305	CLA	CBD-CGD-O2D-CED
36	b	828	CLA	O1A-CGA-O2A-C1
36	M	312	CLA	CAA-CBA-CGA-O2A
36	b	808	CLA	CAA-CBA-CGA-O2A
36	U	308	CLA	CAA-CBA-CGA-O2A
40	L	302	DGD	C1A-C2A-C3A-C4A
36	F	312	CLA	O2A-C1-C2-C3
36	R	311	CLA	O2A-C1-C2-C3
36	T	309	CLA	O2A-C1-C2-C3
36	a	809	CLA	O2A-C1-C2-C3
36	a	827	CLA	O2A-C1-C2-C3
36	b	819	CLA	O2A-C1-C2-C3
36	b	834	CLA	O2A-C1-C2-C3
36	f	802	CLA	O2A-C1-C2-C3
36	i	102	CLA	O2A-C1-C2-C3
36	V	306	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
36	A	307	CLA	C2A-CAA-CBA-CGA
36	B	307	CLA	C2A-CAA-CBA-CGA
36	H	307	CLA	C2A-CAA-CBA-CGA
36	E	311	CLA	CAA-CBA-CGA-O2A
36	L	309	CLA	C3-C5-C6-C7
36	R	319	CLA	CAA-CBA-CGA-O1A
36	F	314	CLA	C16-C17-C18-C19
36	a	802	CLA	C16-C17-C18-C20
34	E	301	DD6	C24-C25-C26-C27
36	D	310	CLA	CHA-CBD-CGD-O1D
36	E	310	CLA	CHA-CBD-CGD-O1D
36	E	310	CLA	CHA-CBD-CGD-O2D
36	E	317	CLA	CHA-CBD-CGD-O2D
36	H	309	CLA	CHA-CBD-CGD-O1D
36	H	309	CLA	CHA-CBD-CGD-O2D
36	H	315	CLA	CHA-CBD-CGD-O2D
36	H	318	CLA	CHA-CBD-CGD-O1D
36	H	318	CLA	CHA-CBD-CGD-O2D
36	I	308	CLA	CHA-CBD-CGD-O1D
36	I	308	CLA	CHA-CBD-CGD-O2D
36	I	311	CLA	CHA-CBD-CGD-O1D
36	I	311	CLA	CHA-CBD-CGD-O2D
36	K	308	CLA	CHA-CBD-CGD-O1D
36	K	308	CLA	CHA-CBD-CGD-O2D
36	N	313	CLA	CHA-CBD-CGD-O1D
36	N	313	CLA	CHA-CBD-CGD-O2D
36	O	312	CLA	CHA-CBD-CGD-O1D
36	O	312	CLA	CHA-CBD-CGD-O2D
36	P	314	CLA	CHA-CBD-CGD-O1D
36	P	314	CLA	CHA-CBD-CGD-O2D
36	Q	310	CLA	CHA-CBD-CGD-O1D
36	Q	310	CLA	CHA-CBD-CGD-O2D
36	R	322	CLA	CHA-CBD-CGD-O1D
36	T	308	CLA	CHA-CBD-CGD-O1D
36	T	308	CLA	CHA-CBD-CGD-O2D
36	W	212	CLA	CHA-CBD-CGD-O1D
36	W	212	CLA	CHA-CBD-CGD-O2D
36	W	218	CLA	CHA-CBD-CGD-O1D
36	W	218	CLA	CHA-CBD-CGD-O2D
36	a	813	CLA	CHA-CBD-CGD-O1D
36	a	815	CLA	CHA-CBD-CGD-O1D
36	a	815	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
36	a	818	CLA	CHA-CBD-CGD-O1D
36	a	818	CLA	CHA-CBD-CGD-O2D
36	a	824	CLA	CHA-CBD-CGD-O1D
36	a	824	CLA	CHA-CBD-CGD-O2D
36	a	827	CLA	CHA-CBD-CGD-O2D
36	a	828	CLA	CHA-CBD-CGD-O2D
36	a	829	CLA	CHA-CBD-CGD-O1D
36	a	829	CLA	CHA-CBD-CGD-O2D
36	a	834	CLA	CHA-CBD-CGD-O2D
36	b	802	CLA	CHA-CBD-CGD-O2D
36	b	815	CLA	CHA-CBD-CGD-O2D
36	b	822	CLA	CHA-CBD-CGD-O1D
36	b	830	CLA	CHA-CBD-CGD-O2D
36	b	836	CLA	CHA-CBD-CGD-O2D
36	j	102	CLA	CHA-CBD-CGD-O2D
36	l	204	CLA	CHA-CBD-CGD-O1D
36	l	205	CLA	CHA-CBD-CGD-O1D
36	l	205	CLA	CHA-CBD-CGD-O2D
36	V	308	CLA	CHA-CBD-CGD-O1D
36	V	310	CLA	CHA-CBD-CGD-O1D
36	V	310	CLA	CHA-CBD-CGD-O2D
37	G	318	KC1	CHA-CBD-CGD-O2D
37	T	310	KC1	CHA-CBD-CGD-O1D
37	T	310	KC1	CHA-CBD-CGD-O2D
36	b	806	CLA	CAA-CBA-CGA-O2A
36	R	313	CLA	CBA-CGA-O2A-C1
36	R	312	CLA	C15-C16-C17-C18
36	b	838	CLA	C2-C1-O2A-CGA
44	b	845	BCR	C20-C21-C22-C23
39	f	807	LMT	C2-C3-C4-C5
41	O	318	LHG	C12-C13-C14-C15
42	E	318	LMG	C35-C36-C37-C38
39	a	854	LMT	C2B-C1B-O1B-C4'
36	a	812	CLA	C15-C16-C17-C18
36	M	309	CLA	CAA-CBA-CGA-O2A
36	a	841	CLA	CAA-CBA-CGA-O2A
36	b	812	CLA	CAA-CBA-CGA-O2A
40	L	302	DGD	O1G-C1G-C2G-O2G
41	D	318	LHG	O7-C5-C6-O8
42	J	318	LMG	O7-C8-C9-O8
35	A	302	A86	C33-C34-O4-C38
36	J	310	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	S	318	CLA	C4C-C3C-CAC-CBC
42	J	318	LMG	C41-C42-C43-C44
37	L	315	KC1	CAA-CBA-CGA-O2A
36	R	313	CLA	O1A-CGA-O2A-C1
36	b	809	CLA	CAA-CBA-CGA-O2A
41	I	316	LHG	O7-C7-C8-C9
36	D	310	CLA	C2A-CAA-CBA-CGA
36	F	311	CLA	C2A-CAA-CBA-CGA
36	Q	310	CLA	C2A-CAA-CBA-CGA
35	A	302	A86	C10-C11-C13-O
35	B	301	A86	C13-C14-C15-O1
35	C	204	A86	C10-C11-C13-O
35	G	305	A86	C13-C14-C15-O1
35	J	306	A86	C10-C11-C13-O
35	S	308	A86	C13-C14-C15-O1
35	h	204	A86	C13-C14-C15-O1
35	U	301	A86	C10-C11-C13-O
35	V	304	A86	C13-C14-C15-O1
41	E	322	LHG	O1-C1-C2-O2
36	D	313	CLA	C13-C15-C16-C17
36	O	309	CLA	C4C-C3C-CAC-CBC
36	P	311	CLA	C4C-C3C-CAC-CBC
36	N	317	CLA	CBA-CGA-O2A-C1
36	Q	308	CLA	C4C-C3C-CAC-CBC
36	S	315	CLA	C4C-C3C-CAC-CBC
36	P	318	CLA	CAA-CBA-CGA-O2A
36	G	309	CLA	C4-C3-C5-C6
41	f	808	LHG	C19-C20-C21-C22
36	A	314	CLA	C11-C10-C8-C7
36	E	316	CLA	C11-C10-C8-C7
36	H	306	CLA	C6-C7-C8-C10
36	J	307	CLA	C11-C12-C13-C15
36	J	309	CLA	C2-C3-C5-C6
36	L	311	CLA	C2-C3-C5-C6
36	L	314	CLA	C6-C7-C8-C10
36	O	316	CLA	C6-C7-C8-C10
36	P	319	CLA	C6-C7-C8-C10
36	a	805	CLA	C12-C13-C15-C16
36	a	810	CLA	C2-C3-C5-C6
36	b	801	CLA	C2-C3-C5-C6
36	b	839	CLA	C11-C10-C8-C7
36	F	312	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	L	314	CLA	CAA-CBA-CGA-O2A
36	N	309	CLA	CAA-CBA-CGA-O2A
36	a	824	CLA	CAA-CBA-CGA-O2A
36	b	841	CLA	CAA-CBA-CGA-O2A
41	R	323	LHG	O7-C7-C8-C9
36	R	320	CLA	CAA-CBA-CGA-O1A
36	E	312	CLA	C4C-C3C-CAC-CBC
36	C	211	CLA	C6-C7-C8-C9
36	C	212	CLA	C11-C10-C8-C9
36	I	311	CLA	C11-C10-C8-C9
36	O	316	CLA	C6-C7-C8-C9
36	P	301	CLA	C11-C10-C8-C9
36	P	314	CLA	C6-C7-C8-C9
36	S	320	CLA	C11-C12-C13-C14
36	W	207	CLA	C11-C10-C8-C9
36	a	810	CLA	C6-C7-C8-C9
36	a	816	CLA	C14-C13-C15-C16
36	a	832	CLA	C11-C12-C13-C14
36	b	820	CLA	C6-C7-C8-C9
36	b	839	CLA	C11-C10-C8-C9
36	f	803	CLA	C6-C7-C8-C9
36	V	305	CLA	C6-C7-C8-C9
36	I	309	CLA	CAA-CBA-CGA-O1A
34	j	103	DD6	C3-C4-C5-C6
44	h	201	BCR	C19-C20-C21-C22
39	F	320	LMT	C5'-C4'-O1B-C1B
36	E	310	CLA	CBA-CGA-O2A-C1
36	G	316	CLA	CAA-CBA-CGA-O2A
36	X	308	CLA	CAA-CBA-CGA-O2A
38	A	315	SQD	C4-C5-C6-S
38	A	315	SQD	C5-C6-S-O8
36	a	812	CLA	O1A-CGA-O2A-C1
36	b	825	CLA	O1A-CGA-O2A-C1
36	K	316	CLA	C5-C6-C7-C8
36	J	308	CLA	C2A-CAA-CBA-CGA
36	f	805	CLA	C2A-CAA-CBA-CGA
36	N	318	CLA	C2-C1-O2A-CGA
36	C	212	CLA	C4C-C3C-CAC-CBC
41	O	318	LHG	C27-C28-C29-C30
42	G	324	LMG	C22-C23-C24-C25
35	C	204	A86	C-C1-C24-C25
36	f	802	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
36	D	310	CLA	C16-C17-C18-C20
36	P	313	CLA	C16-C17-C18-C20
36	I	311	CLA	C4-C3-C5-C6
36	a	806	CLA	C4-C3-C5-C6
41	G	301	LHG	C18-C19-C20-C21
41	Q	315	LHG	O1-C1-C2-C3
41	j	104	LHG	O1-C1-C2-C3
36	a	801	CLA	CAA-CBA-CGA-O2A
44	i	103	BCR	C7-C8-C9-C10
36	O	307	CLA	CBA-CGA-O2A-C1
36	P	309	CLA	CBA-CGA-O2A-C1
36	Q	306	CLA	CBA-CGA-O2A-C1
36	a	812	CLA	CBA-CGA-O2A-C1
36	F	311	CLA	O1D-CGD-O2D-CED
36	a	817	CLA	O1A-CGA-O2A-C1
41	O	318	LHG	C31-C32-C33-C34
36	A	309	CLA	C1A-C2A-CAA-CBA
36	D	309	CLA	C1A-C2A-CAA-CBA
36	G	311	CLA	C1A-C2A-CAA-CBA
36	H	305	CLA	C1A-C2A-CAA-CBA
36	I	305	CLA	C1A-C2A-CAA-CBA
36	K	311	CLA	C1A-C2A-CAA-CBA
36	N	309	CLA	C1A-C2A-CAA-CBA
36	O	309	CLA	C1A-C2A-CAA-CBA
36	P	301	CLA	C1A-C2A-CAA-CBA
36	P	311	CLA	C1A-C2A-CAA-CBA
36	Q	308	CLA	C1A-C2A-CAA-CBA
36	R	321	CLA	C1A-C2A-CAA-CBA
36	f	802	CLA	C1A-C2A-CAA-CBA
36	f	803	CLA	C1A-C2A-CAA-CBA
36	U	308	CLA	C1A-C2A-CAA-CBA
39	a	854	LMT	C11-C10-C9-C8
41	G	320	LHG	C18-C19-C20-C21
36	G	316	CLA	CAA-CBA-CGA-O1A
41	E	322	LHG	O9-C7-C8-C9
41	R	323	LHG	O9-C7-C8-C9
36	b	822	CLA	O1D-CGD-O2D-CED
36	D	308	CLA	C2-C1-O2A-CGA
36	a	833	CLA	C2-C1-O2A-CGA
36	b	805	CLA	C2-C1-O2A-CGA
36	E	314	CLA	C8-C10-C11-C12
36	I	308	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	E	311	CLA	CAA-CBA-CGA-O1A
36	Q	310	CLA	CAA-CBA-CGA-O1A
36	U	308	CLA	CAA-CBA-CGA-O1A
42	V	315	LMG	O9-C10-C11-C12
39	B	312	LMT	C4-C5-C6-C7
42	J	319	LMG	C7-C8-C9-O8
37	J	314	KC1	C4C-C3C-CAC-CBC
39	E	320	LMT	C5-C6-C7-C8
36	M	309	CLA	C2A-CAA-CBA-CGA
36	S	312	CLA	C2A-CAA-CBA-CGA
36	X	308	CLA	C2A-CAA-CBA-CGA
36	l	204	CLA	C2A-CAA-CBA-CGA
41	i	104	LHG	C29-C30-C31-C32
36	b	841	CLA	C16-C17-C18-C19
41	a	850	LHG	O9-C7-C8-C9
36	V	305	CLA	C8-C10-C11-C12
36	F	311	CLA	O1A-CGA-O2A-C1
40	b	849	DGD	C7A-C8A-C9A-CAA
36	O	309	CLA	CAA-CBA-CGA-O2A
36	P	311	CLA	CAA-CBA-CGA-O2A
36	Q	308	CLA	CAA-CBA-CGA-O2A
36	W	207	CLA	CAA-CBA-CGA-O2A
36	b	805	CLA	C5-C6-C7-C8
36	b	810	CLA	C15-C16-C17-C18
36	M	312	CLA	CAA-CBA-CGA-O1A
36	a	804	CLA	CAA-CBA-CGA-O1A
36	a	824	CLA	CAA-CBA-CGA-O1A
41	I	316	LHG	O9-C7-C8-C9
35	U	302	A86	C33-C34-O4-C38
36	C	211	CLA	C15-C16-C17-C18
36	a	818	CLA	C8-C10-C11-C12
41	G	320	LHG	C3-O3-P-O5
41	G	320	LHG	C4-O6-P-O5
41	I	316	LHG	C3-O3-P-O5
41	Q	315	LHG	C4-O6-P-O4
41	f	808	LHG	C4-O6-P-O5
41	l	208	LHG	C4-O6-P-O5
36	L	314	CLA	C16-C17-C18-C19
36	a	841	CLA	CAA-CBA-CGA-O1A
36	b	809	CLA	CAA-CBA-CGA-O1A
39	L	318	LMT	C4B-C5B-C6B-O6B
44	j	107	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	A	310	CLA	C13-C15-C16-C17
36	L	311	CLA	CAA-CBA-CGA-O1A
36	M	309	CLA	CAA-CBA-CGA-O1A
36	b	806	CLA	CAA-CBA-CGA-O1A
36	b	812	CLA	CAA-CBA-CGA-O1A
36	S	312	CLA	CAA-CBA-CGA-O2A
41	G	320	LHG	O9-C7-O7-C5
41	Q	315	LHG	C19-C20-C21-C22
36	K	307	CLA	CAA-CBA-CGA-O1A
36	T	309	CLA	CAA-CBA-CGA-O1A
36	b	828	CLA	CAA-CBA-CGA-O1A
36	a	828	CLA	C3-C5-C6-C7
36	R	315	CLA	C5-C6-C7-C8
36	H	310	CLA	CAA-CBA-CGA-O2A
36	I	312	CLA	CAA-CBA-CGA-O2A
36	Q	314	CLA	CAA-CBA-CGA-O2A
42	V	316	LMG	O8-C28-C29-C30
36	b	829	CLA	C4-C3-C5-C6
43	b	842	PQN	C14-C13-C15-C16
39	E	320	LMT	C2B-C1B-O1B-C4'
36	E	312	CLA	C2-C3-C5-C6
36	a	805	CLA	C2-C3-C5-C6
36	D	315	CLA	C4C-C3C-CAC-CBC
35	M	304	A86	C26-C27-C29-C30
35	U	303	A86	C26-C27-C29-C30
36	D	310	CLA	CAD-CBD-CGD-O1D
36	H	314	CLA	CAD-CBD-CGD-O1D
36	H	318	CLA	CAD-CBD-CGD-O1D
36	I	311	CLA	CAD-CBD-CGD-O1D
36	O	314	CLA	CAD-CBD-CGD-O1D
36	P	316	CLA	CAD-CBD-CGD-O1D
36	P	318	CLA	C2-C3-C5-C6
36	Q	312	CLA	CAD-CBD-CGD-O1D
36	W	212	CLA	CAD-CBD-CGD-O1D
36	W	218	CLA	CAD-CBD-CGD-O1D
36	X	313	CLA	CAD-CBD-CGD-O1D
36	a	812	CLA	CAD-CBD-CGD-O1D
36	a	815	CLA	CAD-CBD-CGD-O1D
36	a	818	CLA	CAD-CBD-CGD-O1D
36	a	828	CLA	CAD-CBD-CGD-O1D
36	a	832	CLA	CAD-CBD-CGD-O1D
36	b	802	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
36	b	815	CLA	CAD-CBD-CGD-O1D
36	b	822	CLA	CAD-CBD-CGD-O1D
36	b	831	CLA	CAD-CBD-CGD-O1D
36	b	841	CLA	CAD-CBD-CGD-O1D
36	V	308	CLA	CAD-CBD-CGD-O1D
37	T	310	KC1	CAD-CBD-CGD-O1D
38	A	315	SQD	O5-C5-C6-S
42	E	319	LMG	O8-C28-C29-C30
36	A	314	CLA	C11-C10-C8-C9
36	G	313	CLA	C6-C7-C8-C9
36	H	317	CLA	C6-C7-C8-C9
36	J	312	CLA	C11-C10-C8-C9
36	L	320	CLA	C11-C12-C13-C14
36	P	310	CLA	C11-C10-C8-C9
36	P	319	CLA	C6-C7-C8-C9
36	R	312	CLA	C6-C7-C8-C9
36	a	807	CLA	C14-C13-C15-C16
36	j	101	CLA	C11-C10-C8-C9
36	h	203	CLA	C11-C10-C8-C9
41	a	850	LHG	O1-C1-C2-O2
41	f	809	LHG	O1-C1-C2-O2
37	L	315	KC1	CAA-CBA-CGA-O1A
36	W	212	CLA	C10-C11-C12-C13
36	L	314	CLA	C3-C5-C6-C7
36	P	314	CLA	CAA-CBA-CGA-O2A
36	A	314	CLA	C8-C10-C11-C12
36	B	305	CLA	C2A-CAA-CBA-CGA
35	A	302	A86	C35-C34-O4-C38
36	a	828	CLA	CBA-CGA-O2A-C1
36	B	311	CLA	CAA-CBA-CGA-O2A
36	R	321	CLA	CAA-CBA-CGA-O2A
36	a	826	CLA	CAA-CBA-CGA-O2A
41	F	319	LHG	O8-C23-C24-C25
36	L	320	CLA	C4-C3-C5-C6
36	O	311	CLA	C4-C3-C5-C6
36	P	313	CLA	C4-C3-C5-C6
36	f	802	CLA	C4-C3-C5-C6
36	V	313	CLA	C13-C15-C16-C17
36	H	305	CLA	O1A-CGA-O2A-C1
36	B	308	CLA	C6-C7-C8-C10
36	G	313	CLA	C6-C7-C8-C10
36	H	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
36	H	308	CLA	CHA-CBD-CGD-O1D
36	H	317	CLA	C11-C10-C8-C7
36	I	310	CLA	C2-C3-C5-C6
36	K	308	CLA	C11-C12-C13-C15
36	L	311	CLA	C11-C12-C13-C15
36	N	308	CLA	C6-C7-C8-C10
36	N	316	CLA	C11-C10-C8-C7
36	R	322	CLA	C3A-C2A-CAA-CBA
36	S	320	CLA	C11-C12-C13-C15
36	X	309	CLA	CAD-CBD-CGD-O2D
36	a	807	CLA	C6-C7-C8-C10
36	a	816	CLA	C12-C13-C15-C16
36	a	826	CLA	C12-C13-C15-C16
36	a	837	CLA	C12-C13-C15-C16
36	b	827	CLA	C11-C10-C8-C7
36	j	102	CLA	C3A-C2A-CAA-CBA
36	U	306	CLA	C11-C12-C13-C15
36	B	311	CLA	CAA-CBA-CGA-O1A
36	P	314	CLA	CAA-CBA-CGA-O1A
36	P	318	CLA	CAA-CBA-CGA-O1A
35	E	307	A86	C39-C38-O4-C34
41	O	318	LHG	C18-C19-C20-C21
41	a	850	LHG	C9-C10-C11-C12
36	B	305	CLA	CAA-CBA-CGA-O2A
36	H	305	CLA	CAA-CBA-CGA-O2A
36	J	307	CLA	CAA-CBA-CGA-O2A
36	L	308	CLA	CAA-CBA-CGA-O2A
36	M	315	CLA	CAA-CBA-CGA-O2A
36	W	215	CLA	CAA-CBA-CGA-O2A
36	a	811	CLA	CAA-CBA-CGA-O2A
36	b	816	CLA	CAA-CBA-CGA-O2A
36	b	834	CLA	CAA-CBA-CGA-O2A
36	b	838	CLA	CAA-CBA-CGA-O2A
41	O	317	LHG	C23-C24-C25-C26
34	D	305	DD6	C5-C6-C8-C9
34	E	301	DD6	C10-C11-C13-C14
34	H	302	DD6	C10-C11-C13-C14
35	S	304	A86	C5-C6-C8-C9
36	N	309	CLA	CAA-CBA-CGA-O1A
35	G	302	A86	C24-C25-C26-C27
35	G	305	A86	C11-C10-C9-C8
35	T	301	A86	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
35	C	203	A86	O-C13-C14-C15
35	O	305	A86	O-C13-C14-C15
39	L	318	LMT	C2-C1-O1'-C1'
39	f	807	LMT	C2-C1-O1'-C1'
36	L	309	CLA	CAA-CBA-CGA-O2A
41	f	808	LHG	O8-C23-C24-C25
36	R	314	CLA	C4C-C3C-CAC-CBC
36	a	841	CLA	O1D-CGD-O2D-CED
36	a	806	CLA	C15-C16-C17-C18
36	b	834	CLA	C5-C6-C7-C8
36	M	315	CLA	CAA-CBA-CGA-O1A
36	R	322	CLA	CAA-CBA-CGA-O1A
36	b	825	CLA	CBA-CGA-O2A-C1
37	D	314	KC1	CBD-CGD-O2D-CED
36	S	320	CLA	C5-C6-C7-C8
37	S	316	KC1	C4C-C3C-CAC-CBC
36	R	322	CLA	CAA-CBA-CGA-O2A
36	b	810	CLA	CAA-CBA-CGA-O2A
39	B	312	LMT	O1'-C1-C2-C3
36	b	836	CLA	C8-C10-C11-C12
36	H	305	CLA	CAA-CBA-CGA-O1A
36	W	215	CLA	CAA-CBA-CGA-O1A
41	F	318	LHG	O10-C23-C24-C25
36	R	310	CLA	C2A-CAA-CBA-CGA
35	F	304	A86	C33-C34-O4-C38
41	b	850	LHG	C30-C31-C32-C33
36	a	805	CLA	C15-C16-C17-C18
36	a	826	CLA	C10-C11-C12-C13
36	B	305	CLA	CAA-CBA-CGA-O1A
36	Q	308	CLA	CAA-CBA-CGA-O1A
36	W	207	CLA	CAA-CBA-CGA-O1A
42	E	319	LMG	O10-C28-C29-C30
36	J	309	CLA	C4-C3-C5-C6
36	G	313	CLA	CAA-CBA-CGA-O2A
36	J	308	CLA	CAA-CBA-CGA-O2A
36	N	308	CLA	CAA-CBA-CGA-O2A
36	V	306	CLA	CAA-CBA-CGA-O2A
42	h	206	LMG	O7-C10-C11-C12

All (11) ring outliers are listed below:

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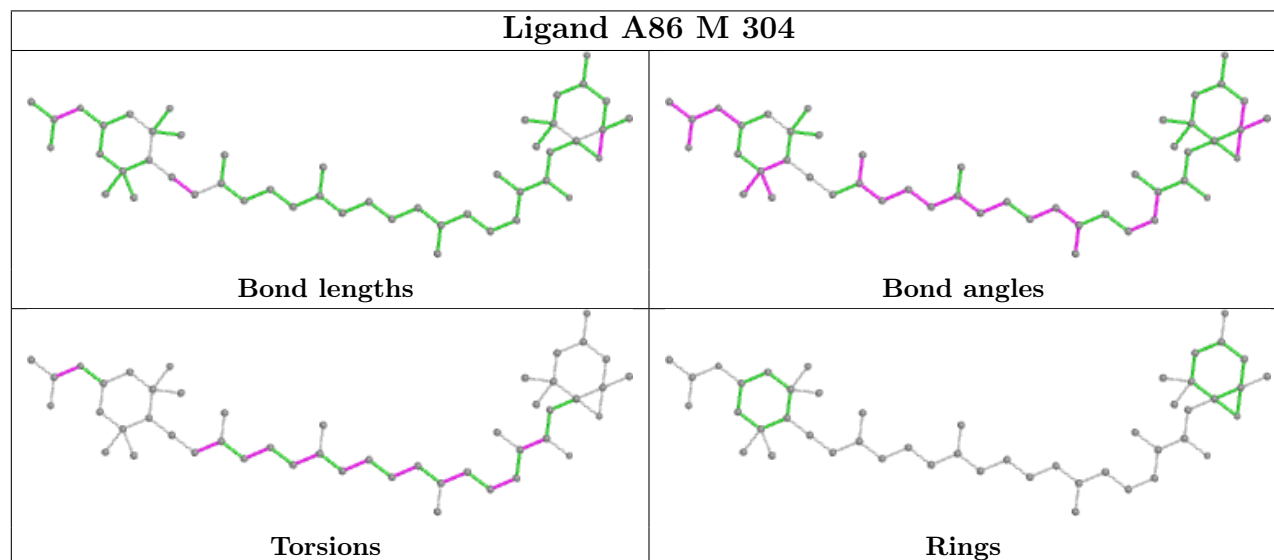
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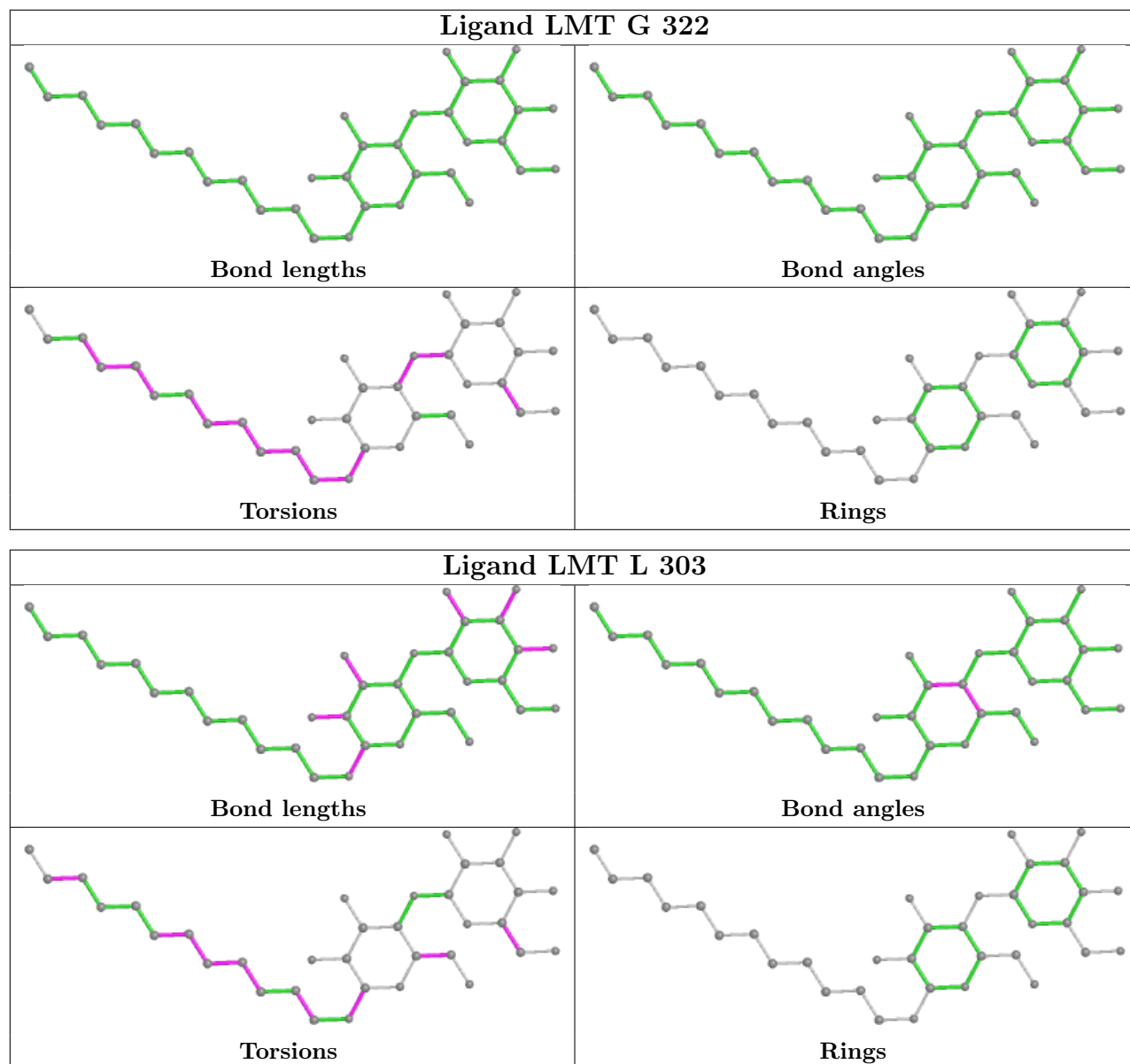
Mol	Chain	Res	Type	Atoms
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Mol	Chain	Res	Type	Atoms
35	V	301	A86	C31-C32-C33-C34-C35-C36
35	J	302	A86	C31-C32-C33-C34-C35-C36
35	K	301	A86	C31-C32-C33-C34-C35-C36
35	G	306	A86	C31-C32-C33-C34-C35-C36
35	T	301	A86	C31-C32-C33-C34-C35-C36
35	X	314	A86	C31-C32-C33-C34-C35-C36
35	C	203	A86	C31-C32-C33-C34-C35-C36
35	h	202	A86	C31-C32-C33-C34-C35-C36
35	L	301	A86	C31-C32-C33-C34-C35-C36
35	L	307	A86	C31-C32-C33-C34-C35-C36
35	F	306	A86	C31-C32-C33-C34-C35-C36

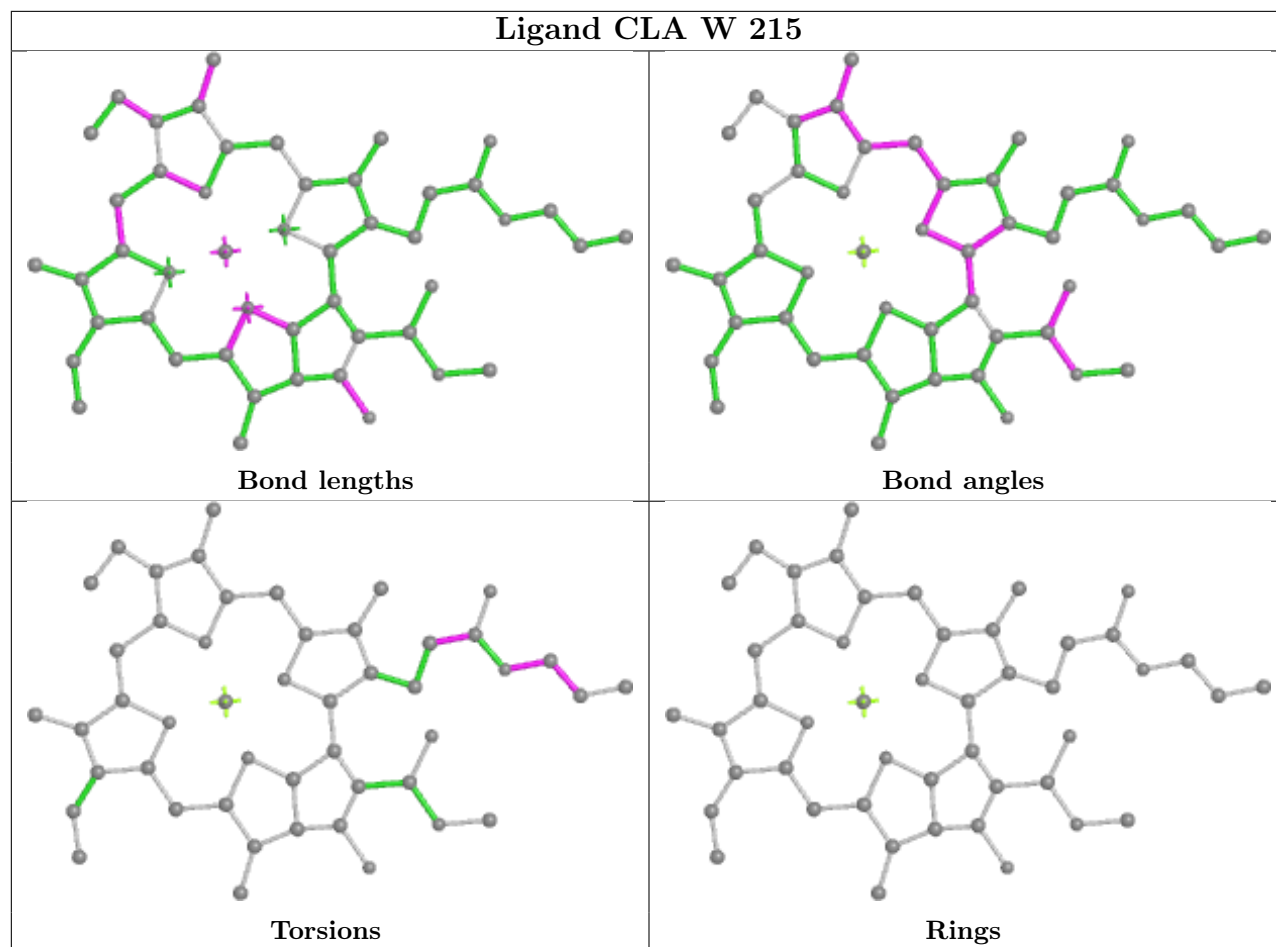
No monomer is involved in short contacts.

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.

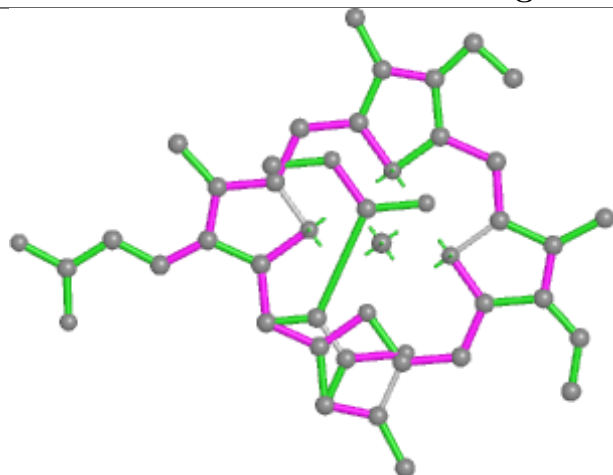




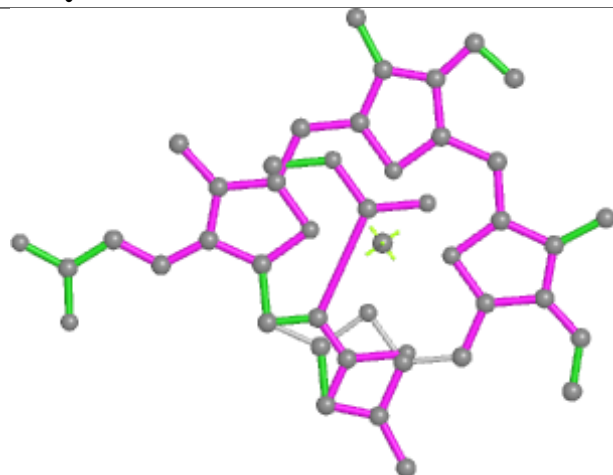




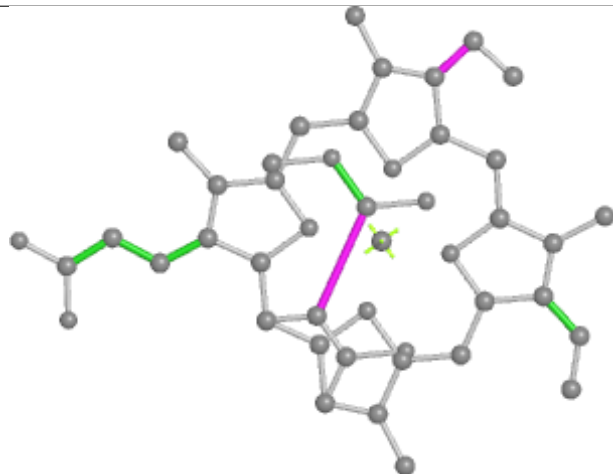
## Ligand KC1 Q 313



Bond lengths



Bond angles

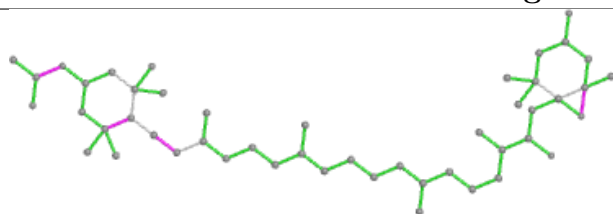


Torsions

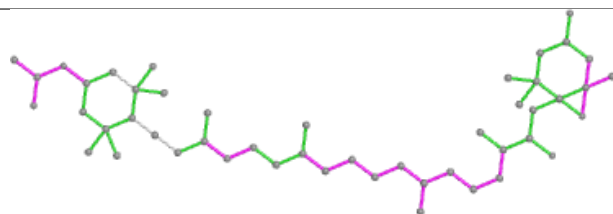


Rings

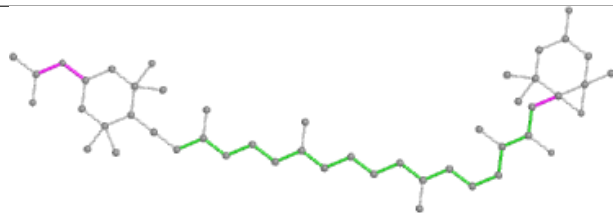
## Ligand A86 J 302



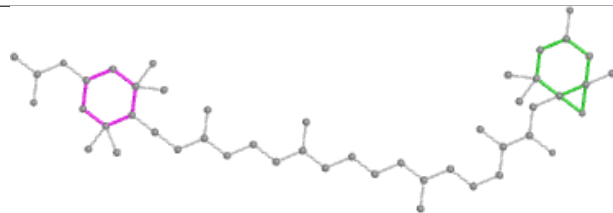
Bond lengths



Bond angles

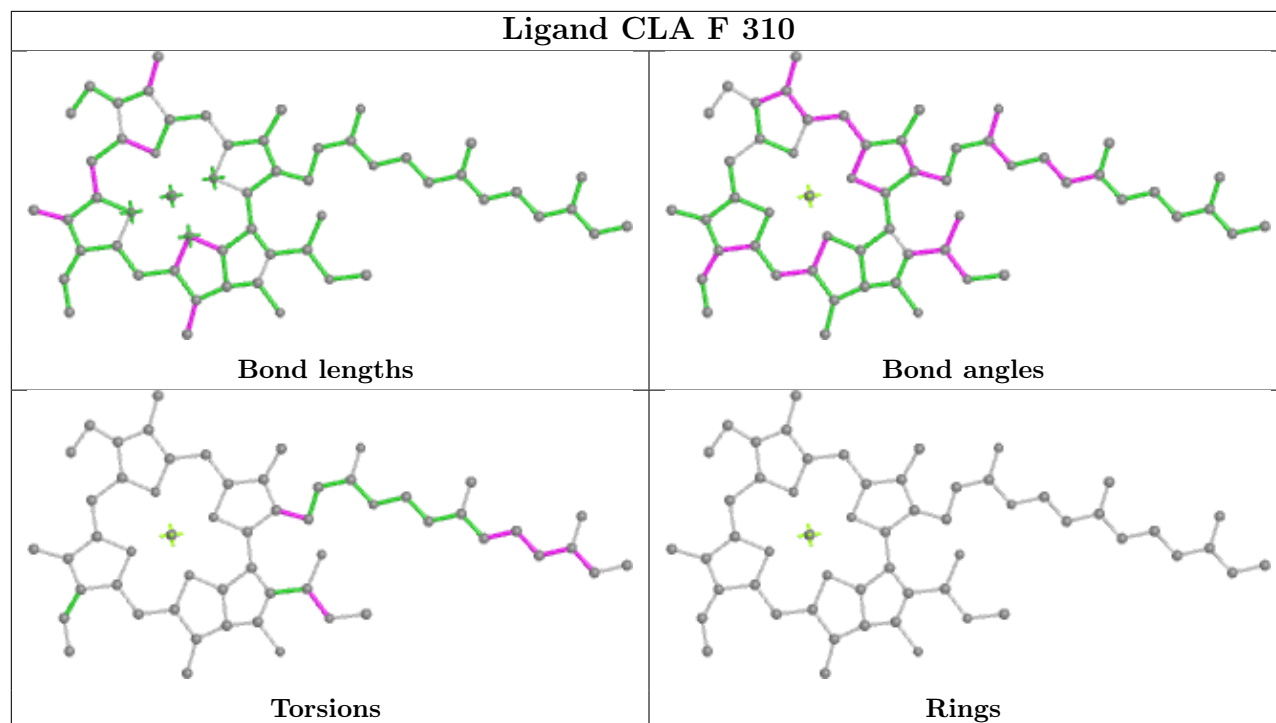


Torsions

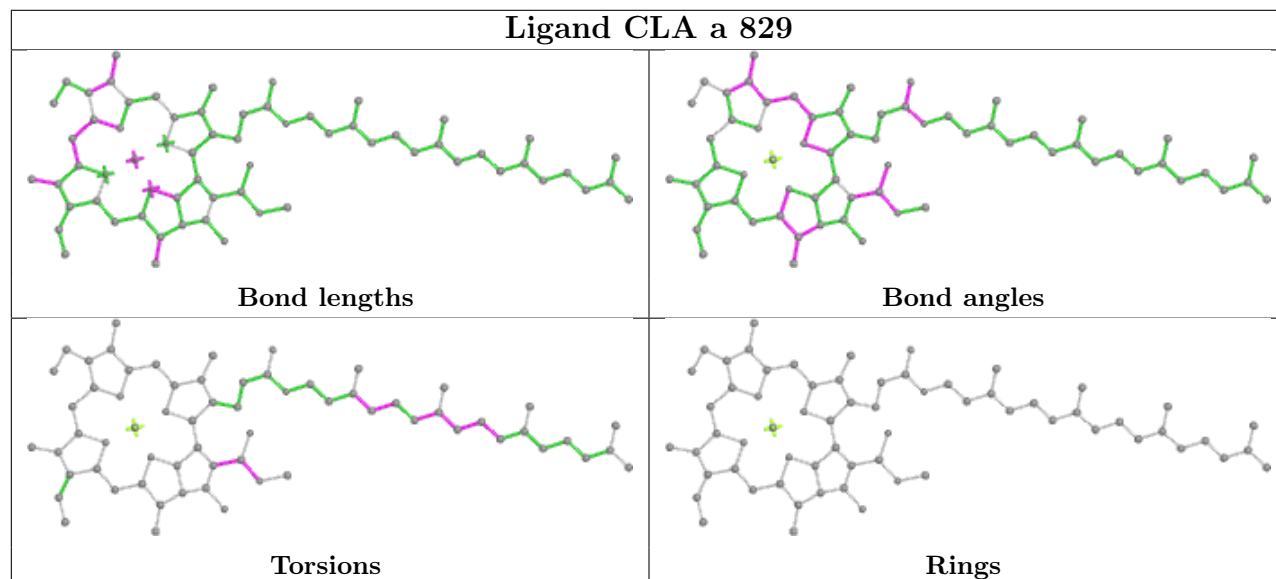


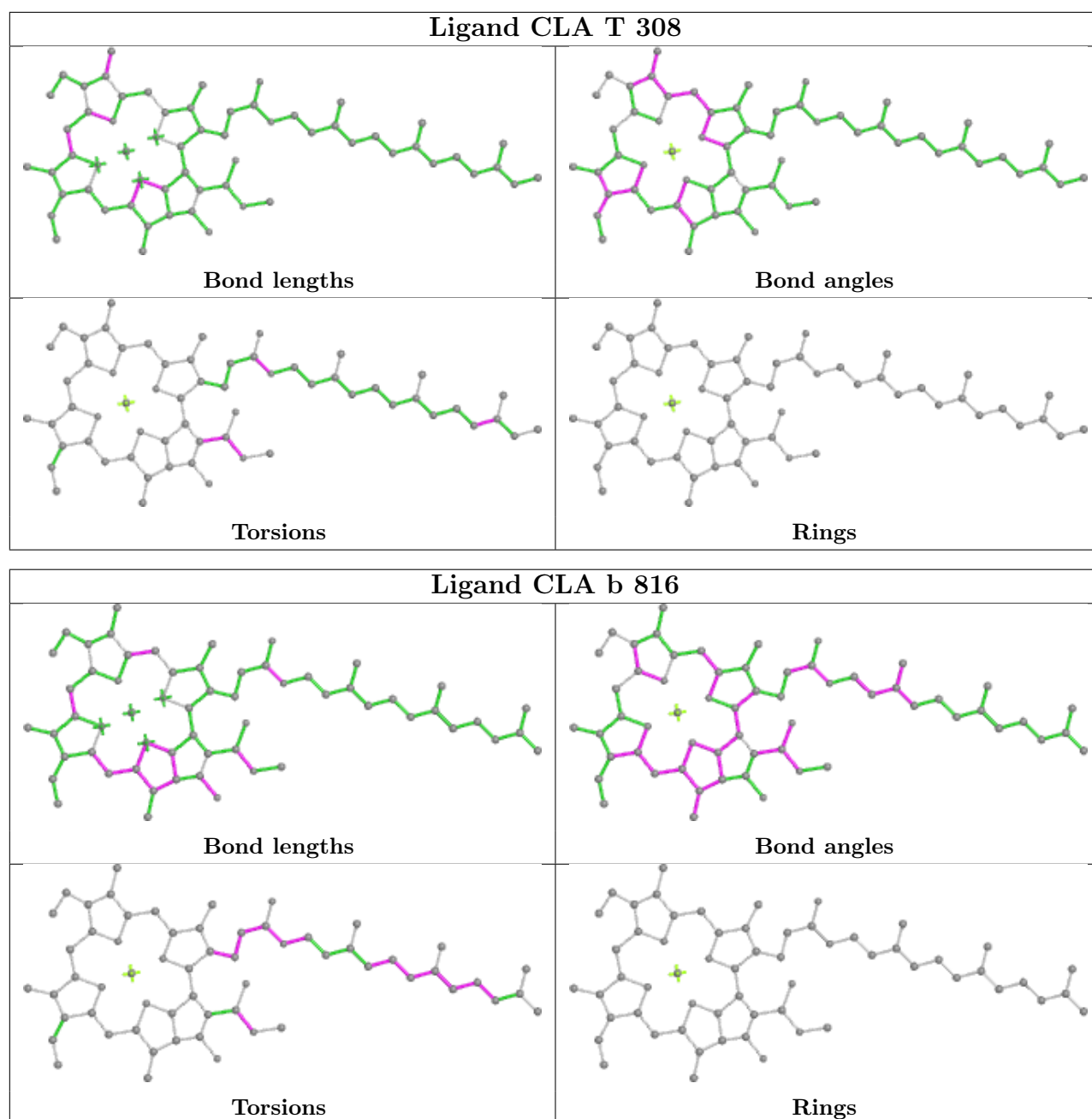
Rings

## Ligand CLA F 310

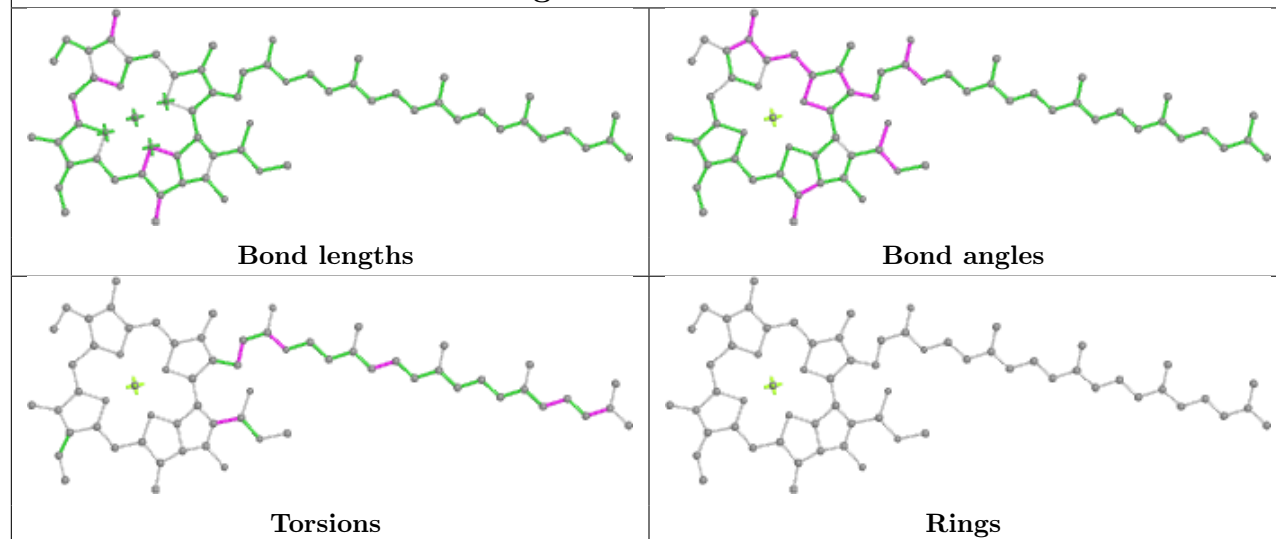


## Ligand CLA a 829

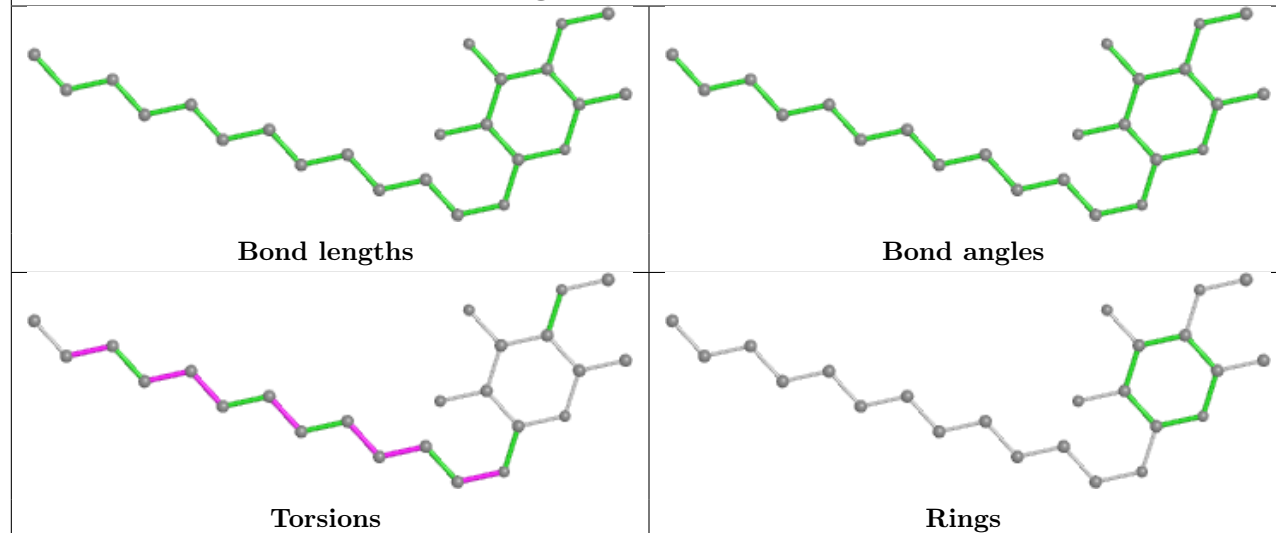




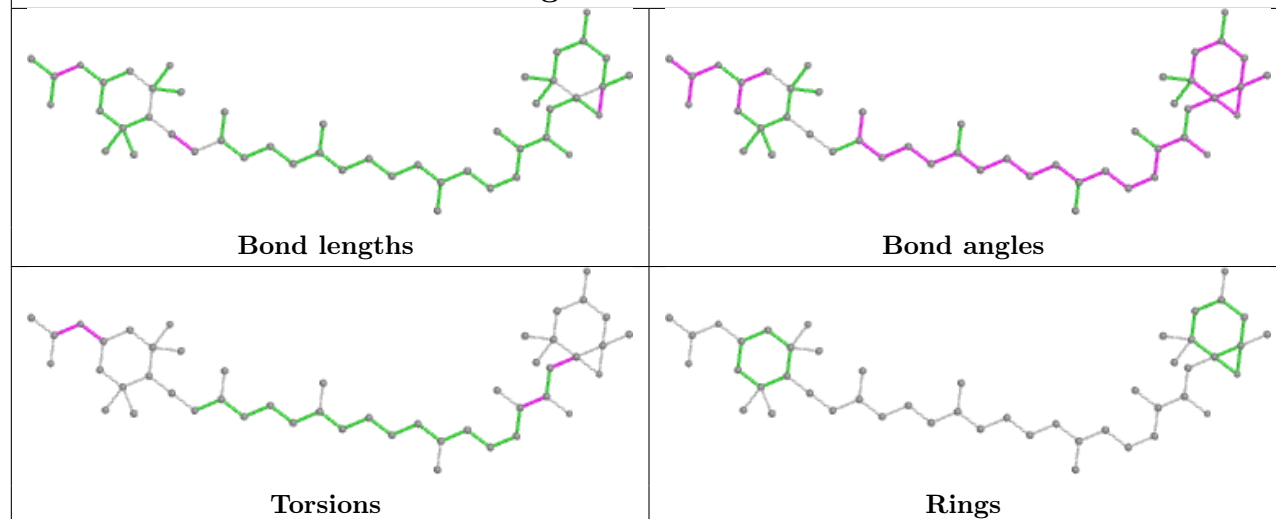
## Ligand CLA E 310



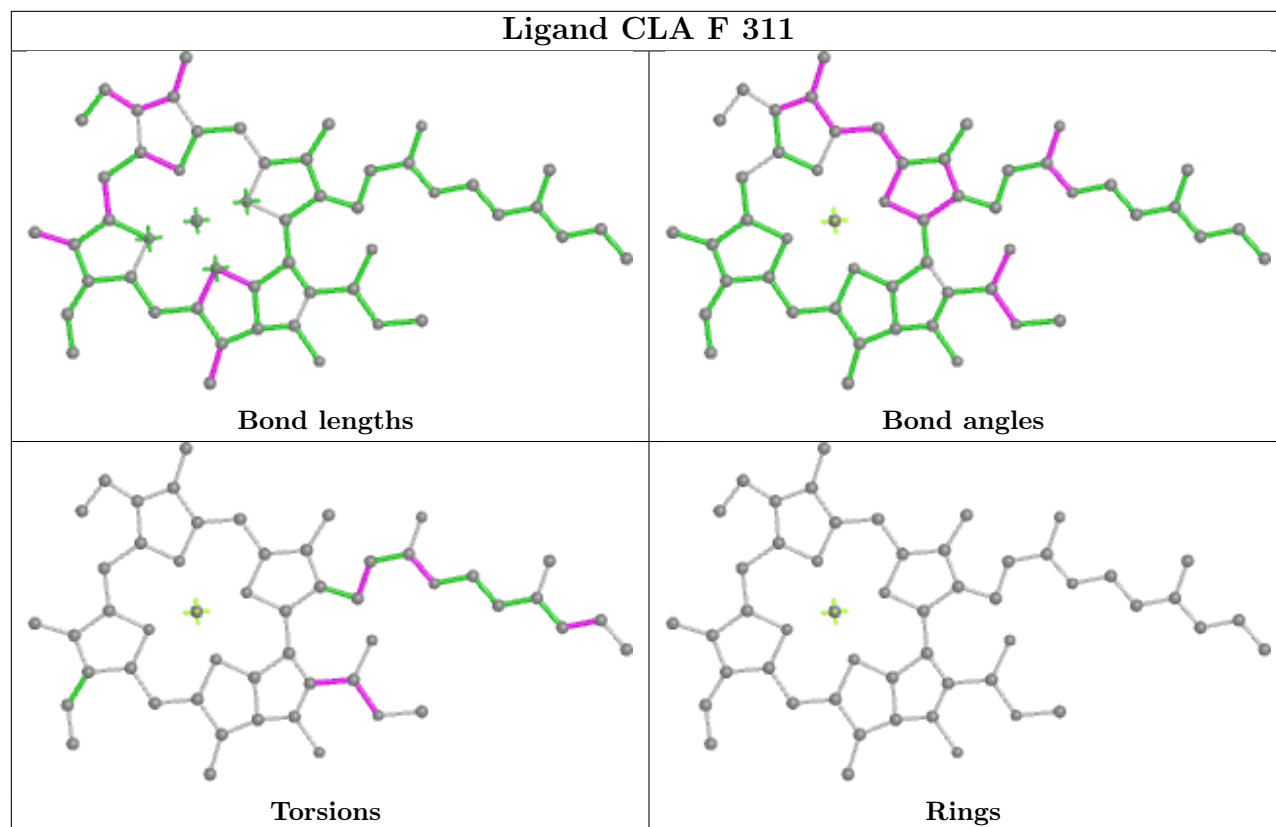
## Ligand LMT b 851



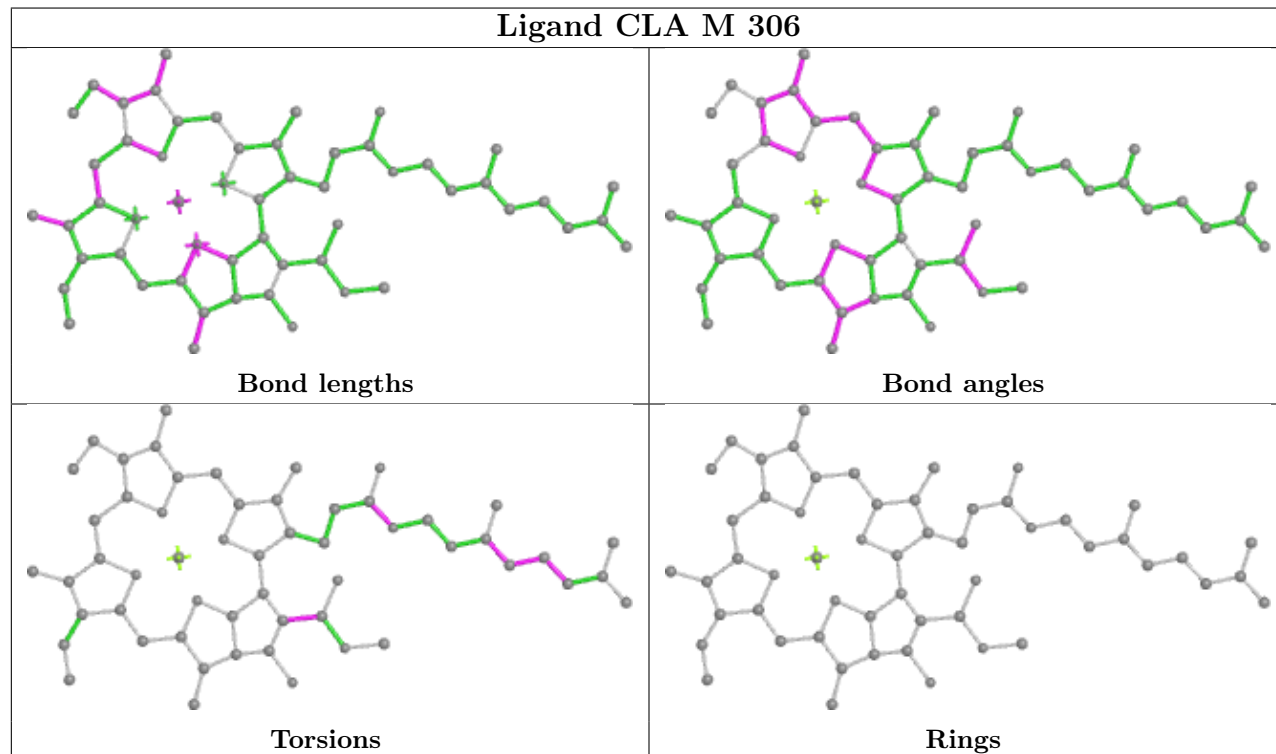
## Ligand A86 S 305



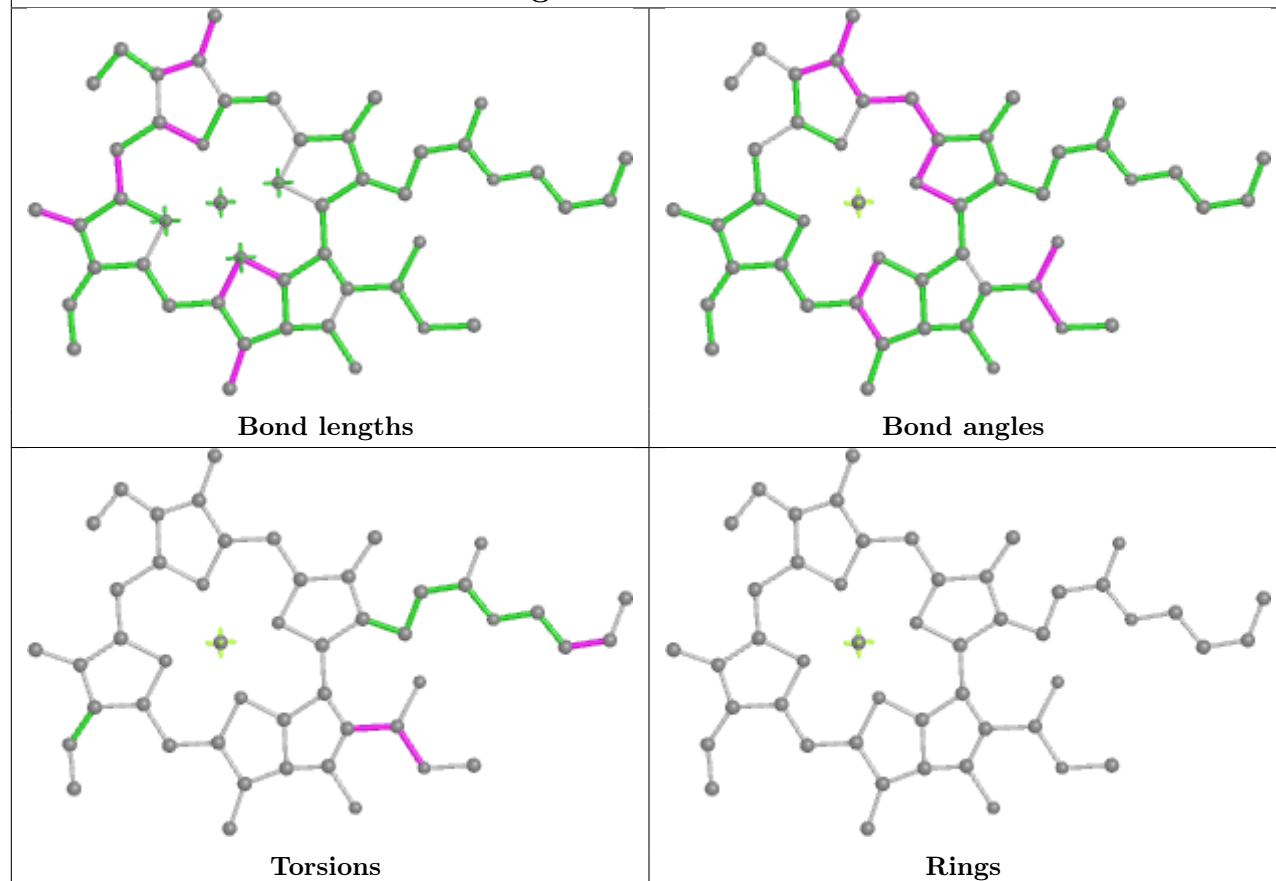
## Ligand CLA F 311



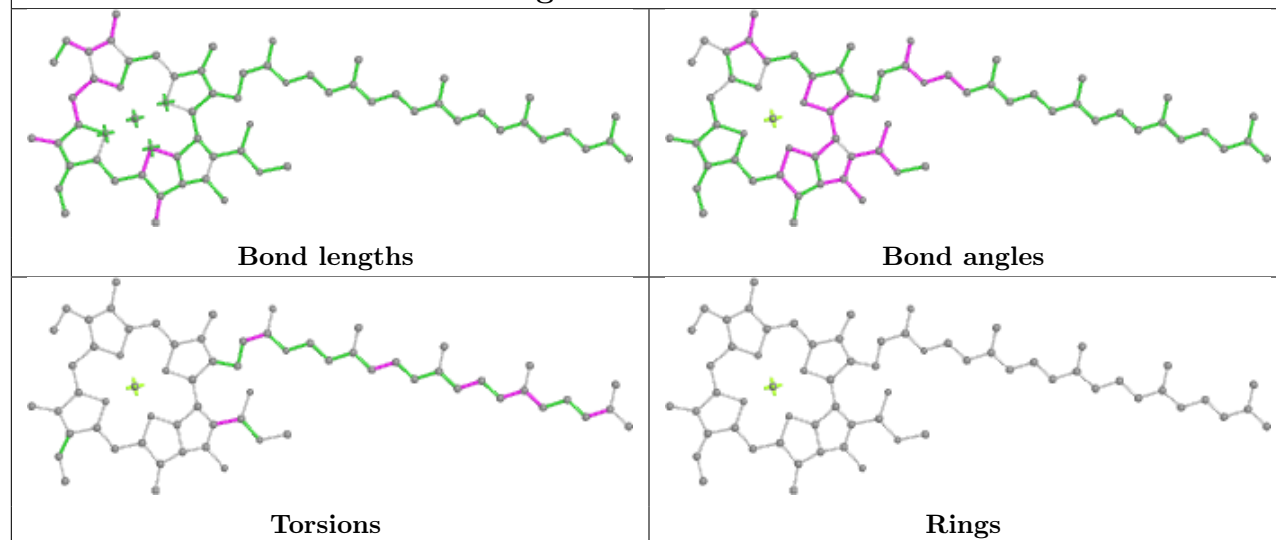
## Ligand CLA M 306

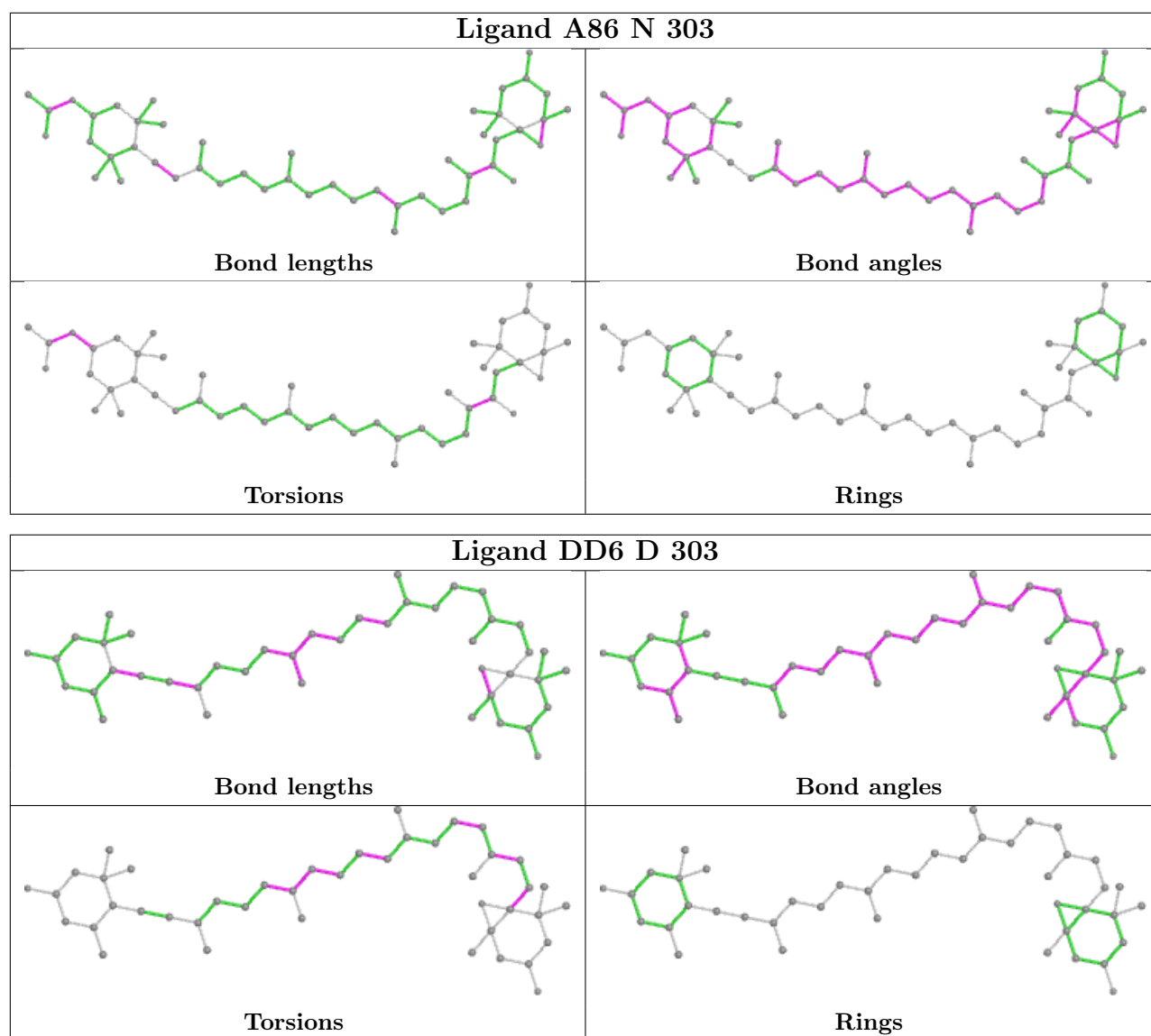


## Ligand CLA A 305



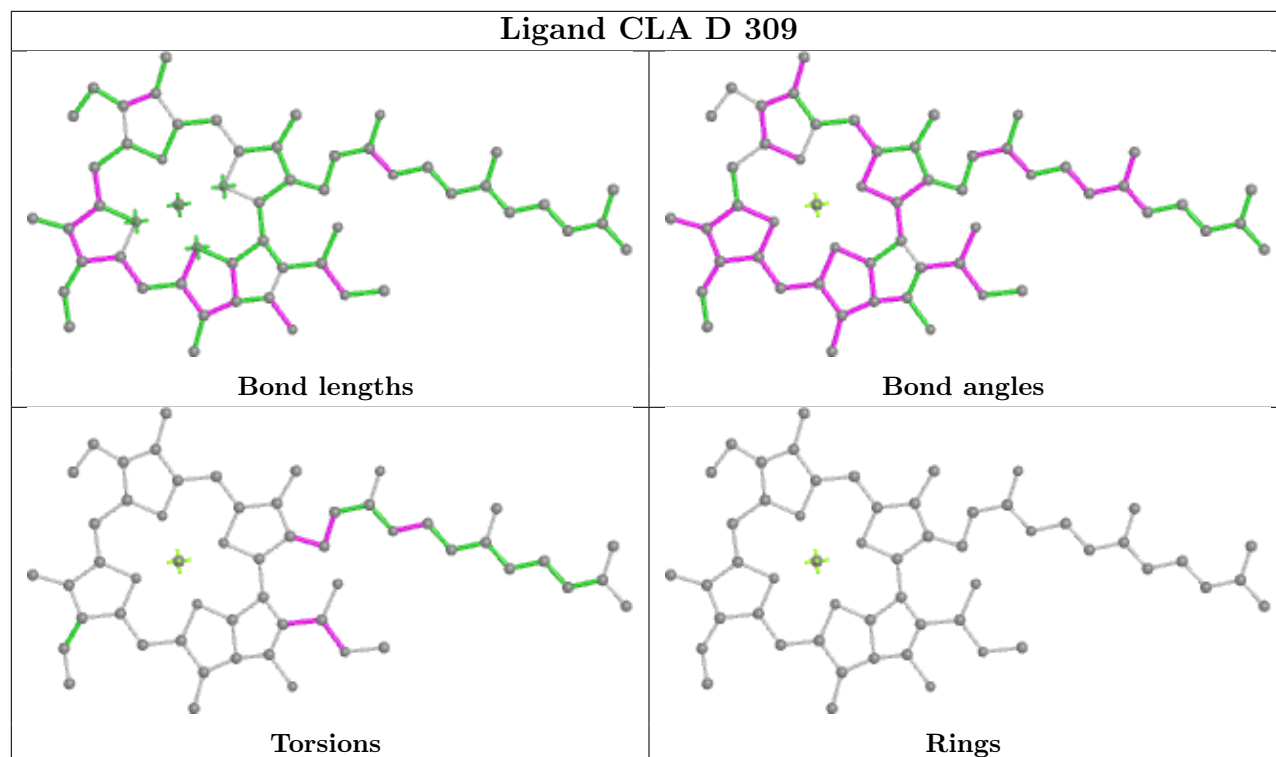
## Ligand CLA a 801



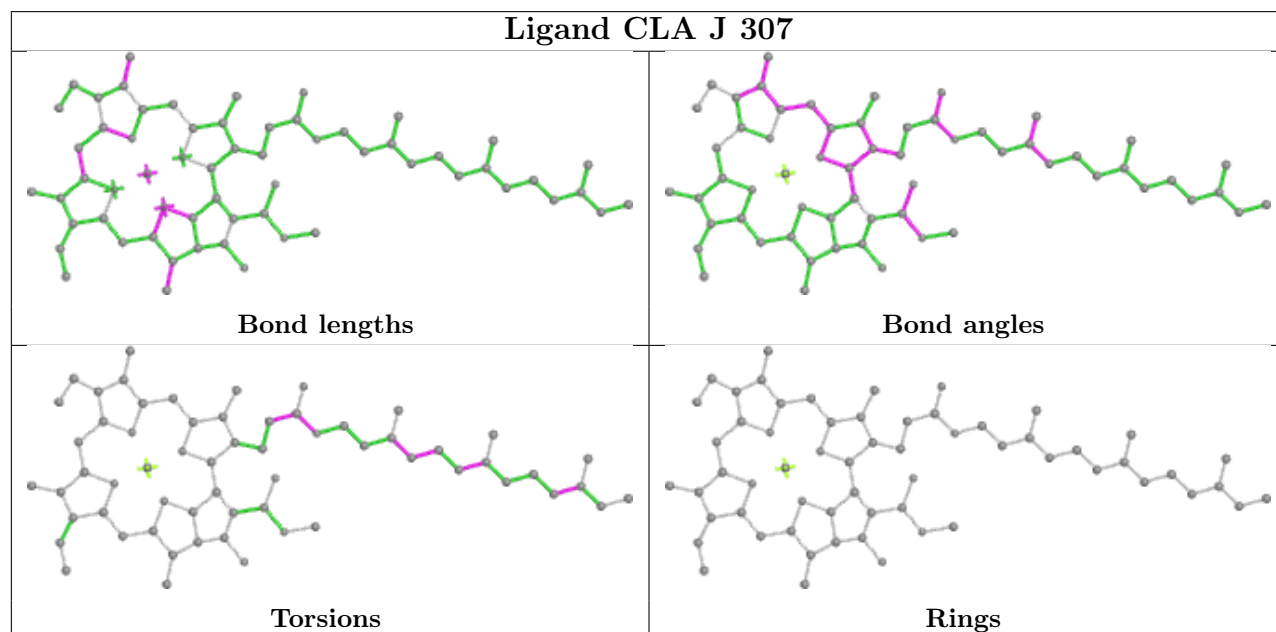


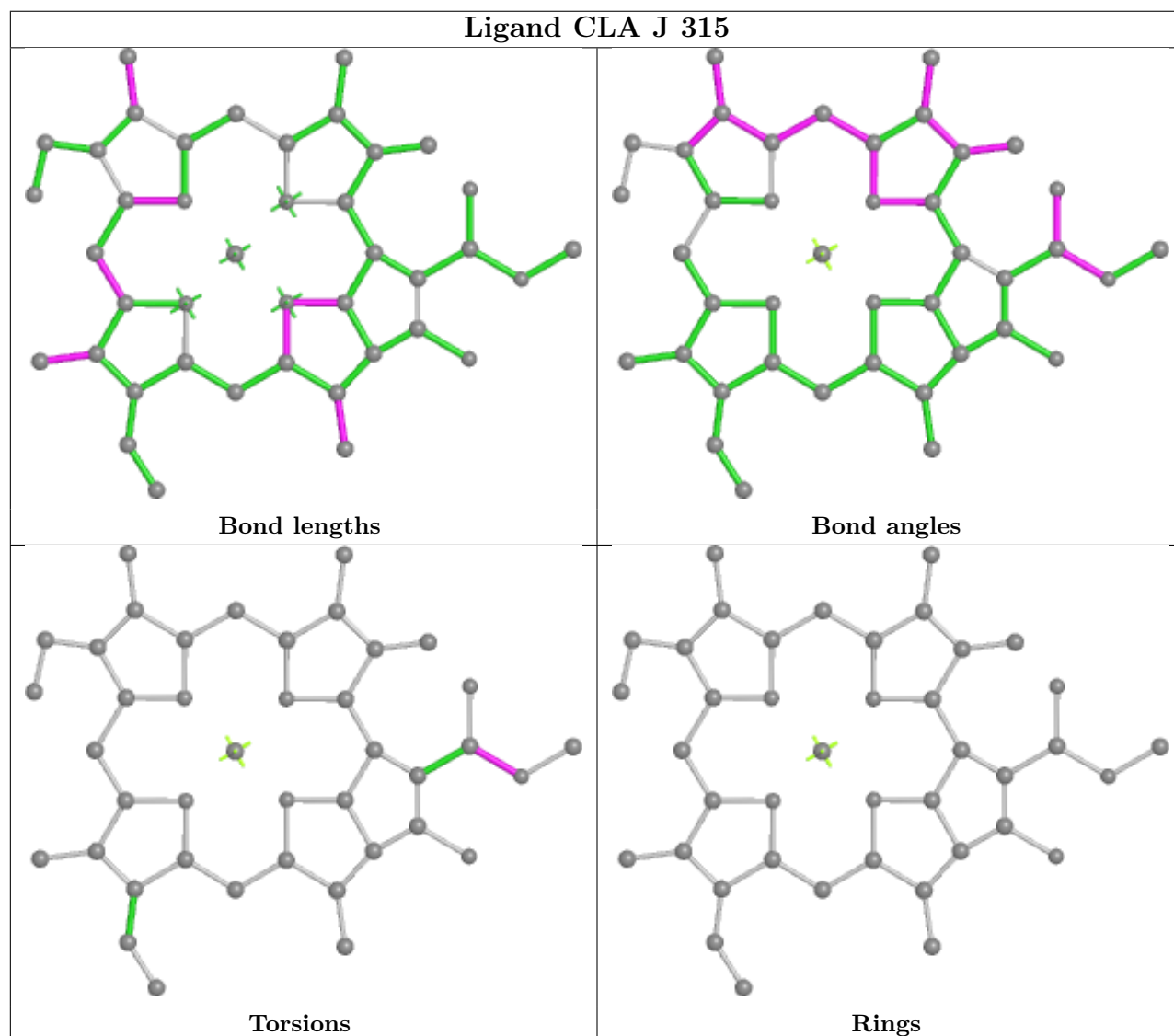
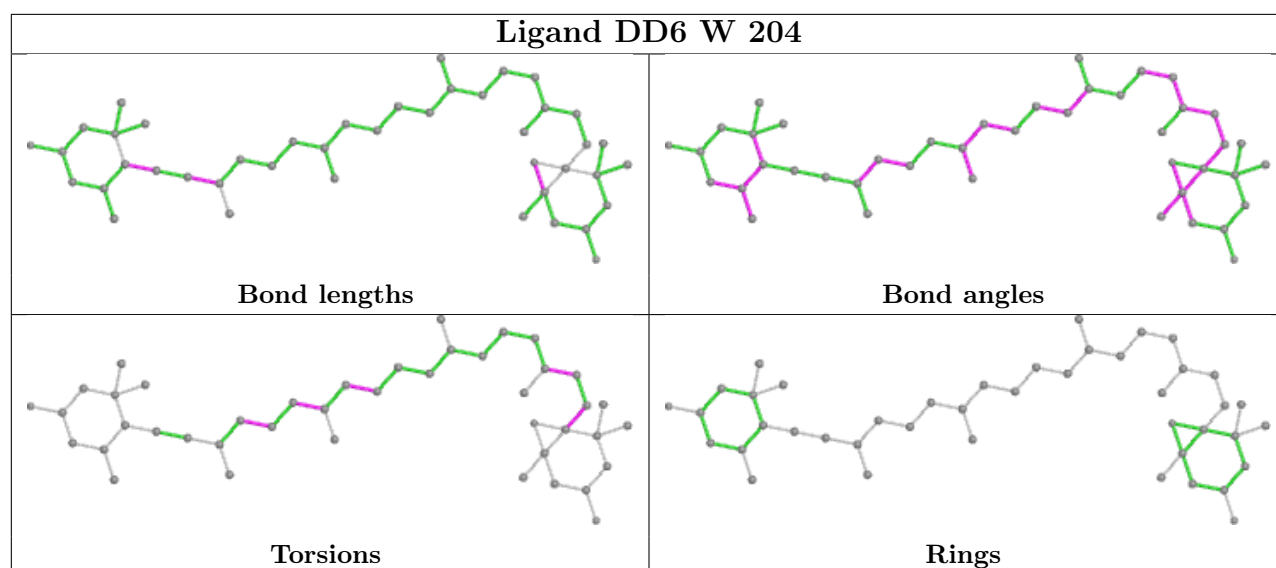


## Ligand CLA D 309

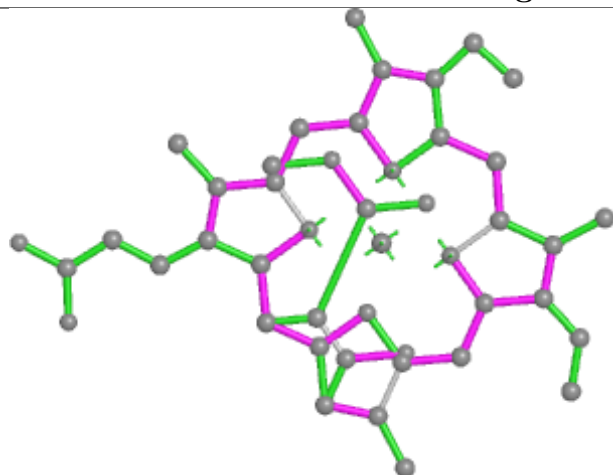


## Ligand CLA J 307

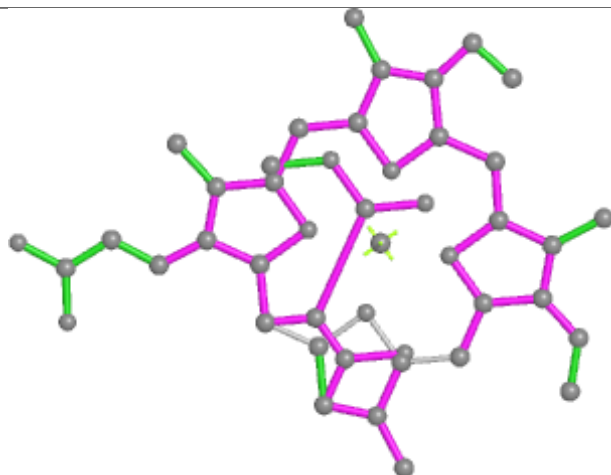




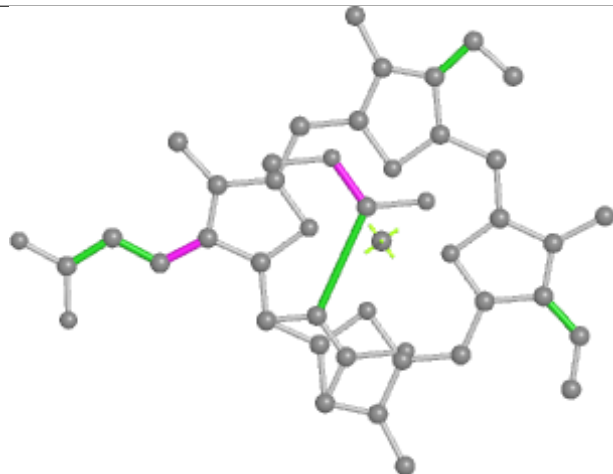
## Ligand KC1 U 312



Bond lengths



Bond angles

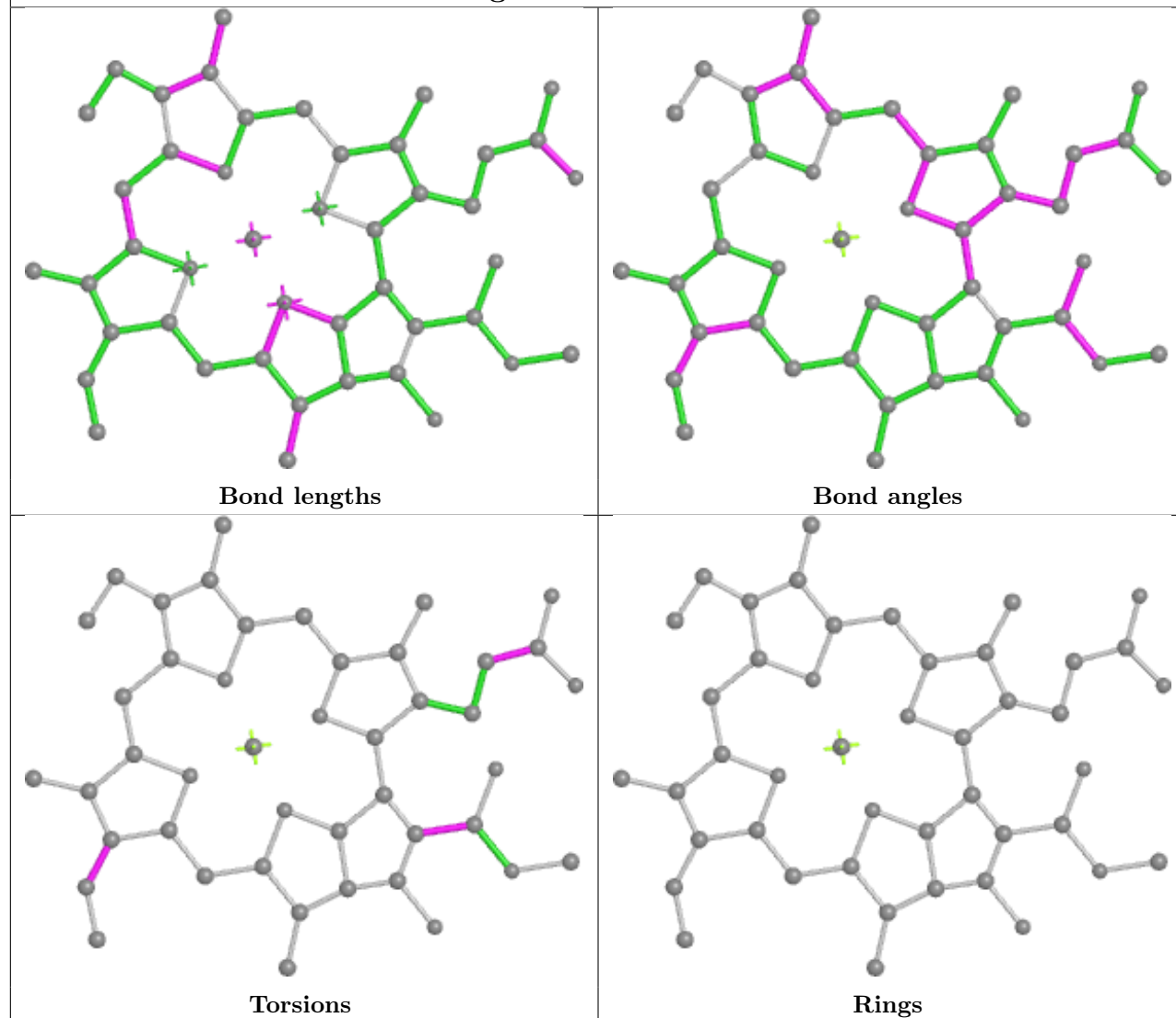


Torsions

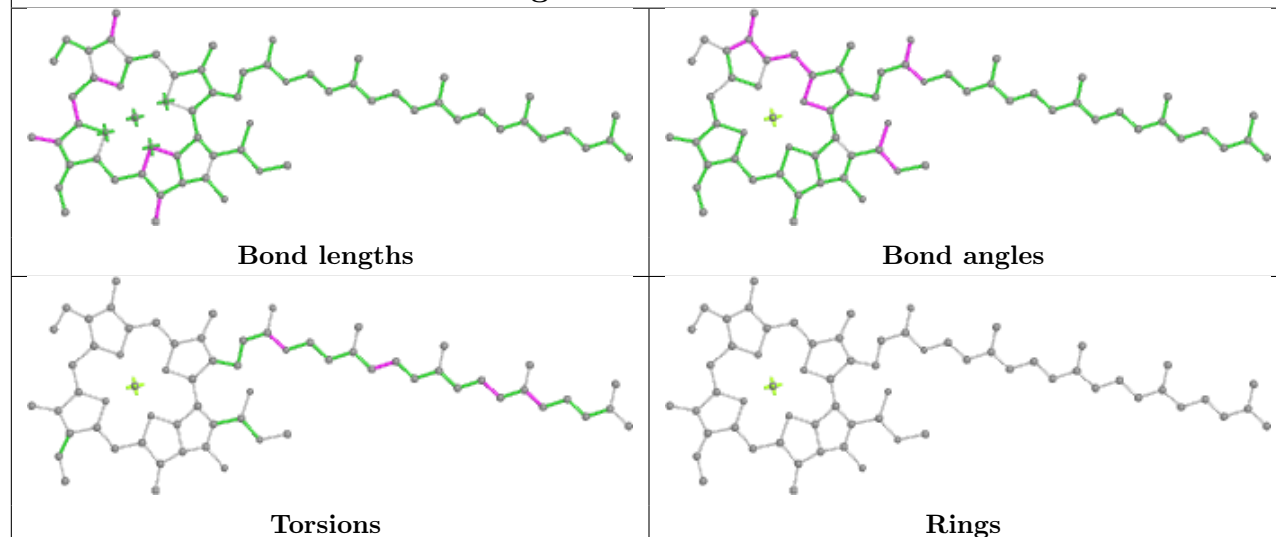


Rings

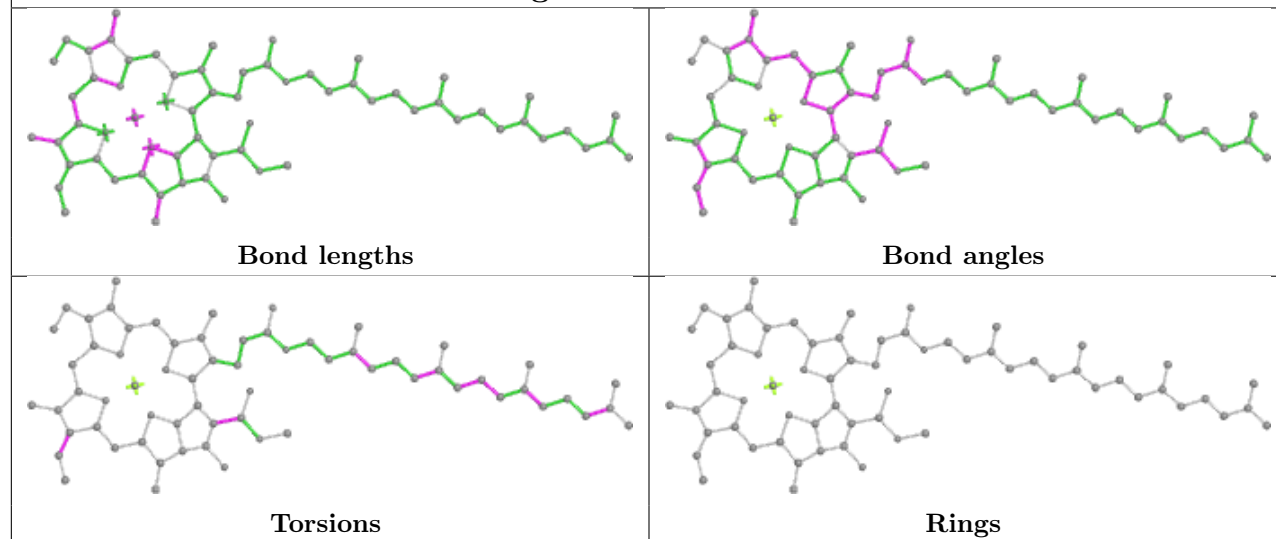
## Ligand CLA D 306



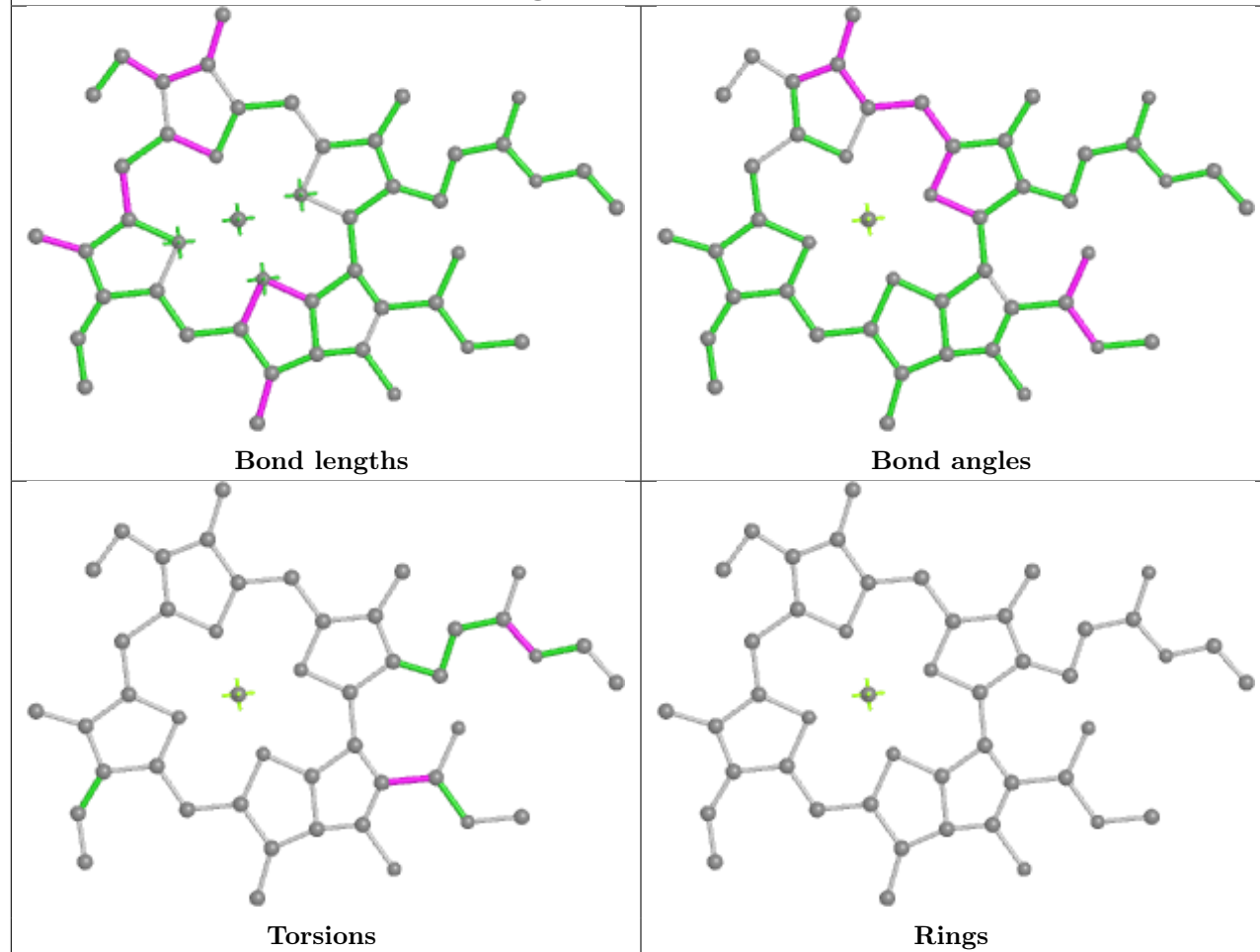
## Ligand CLA K 312



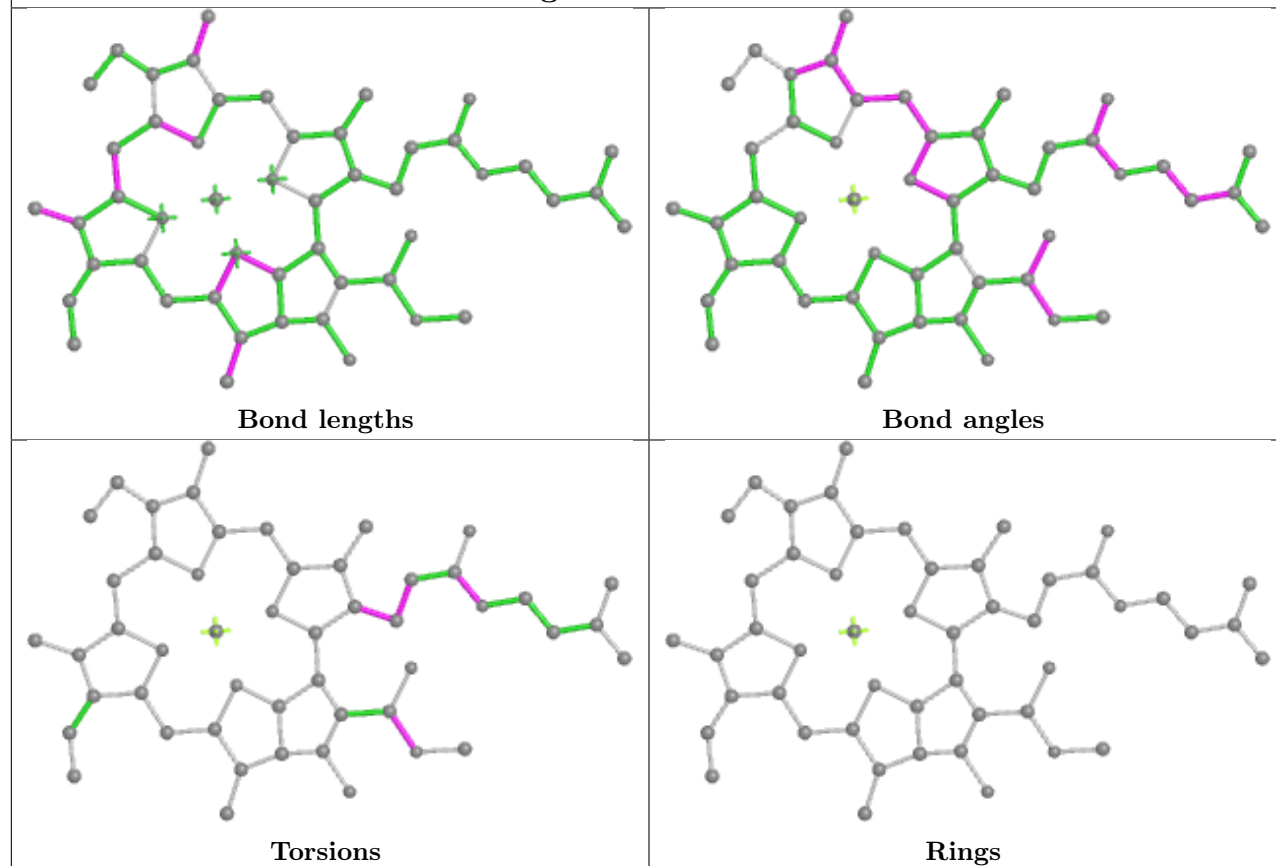
## Ligand CLA H 315



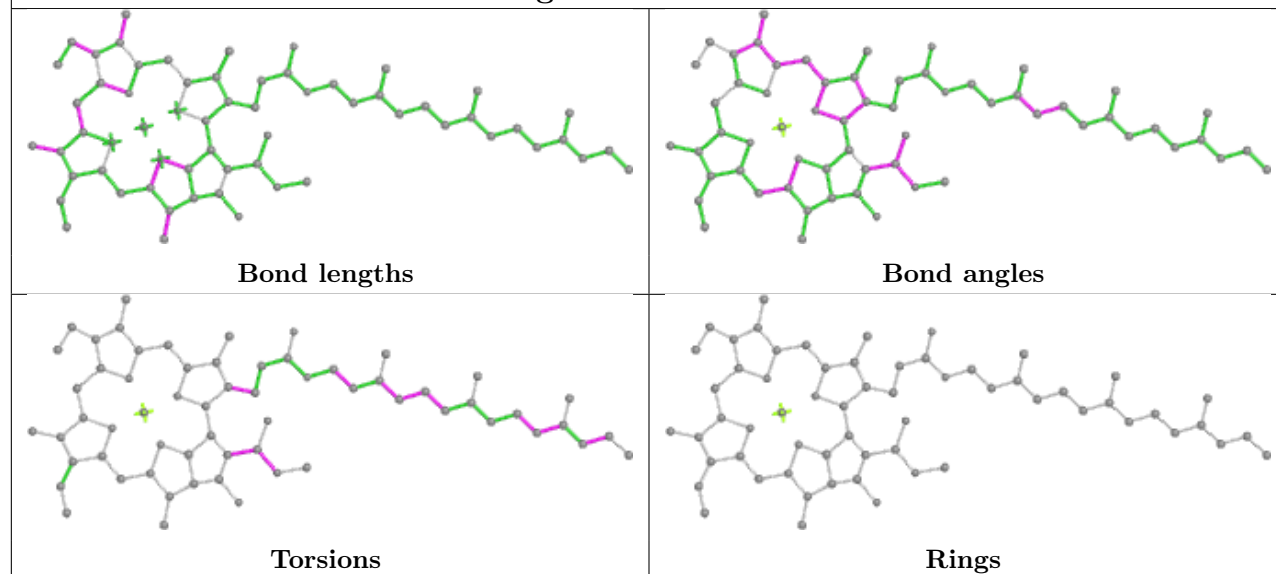
## Ligand CLA J 317

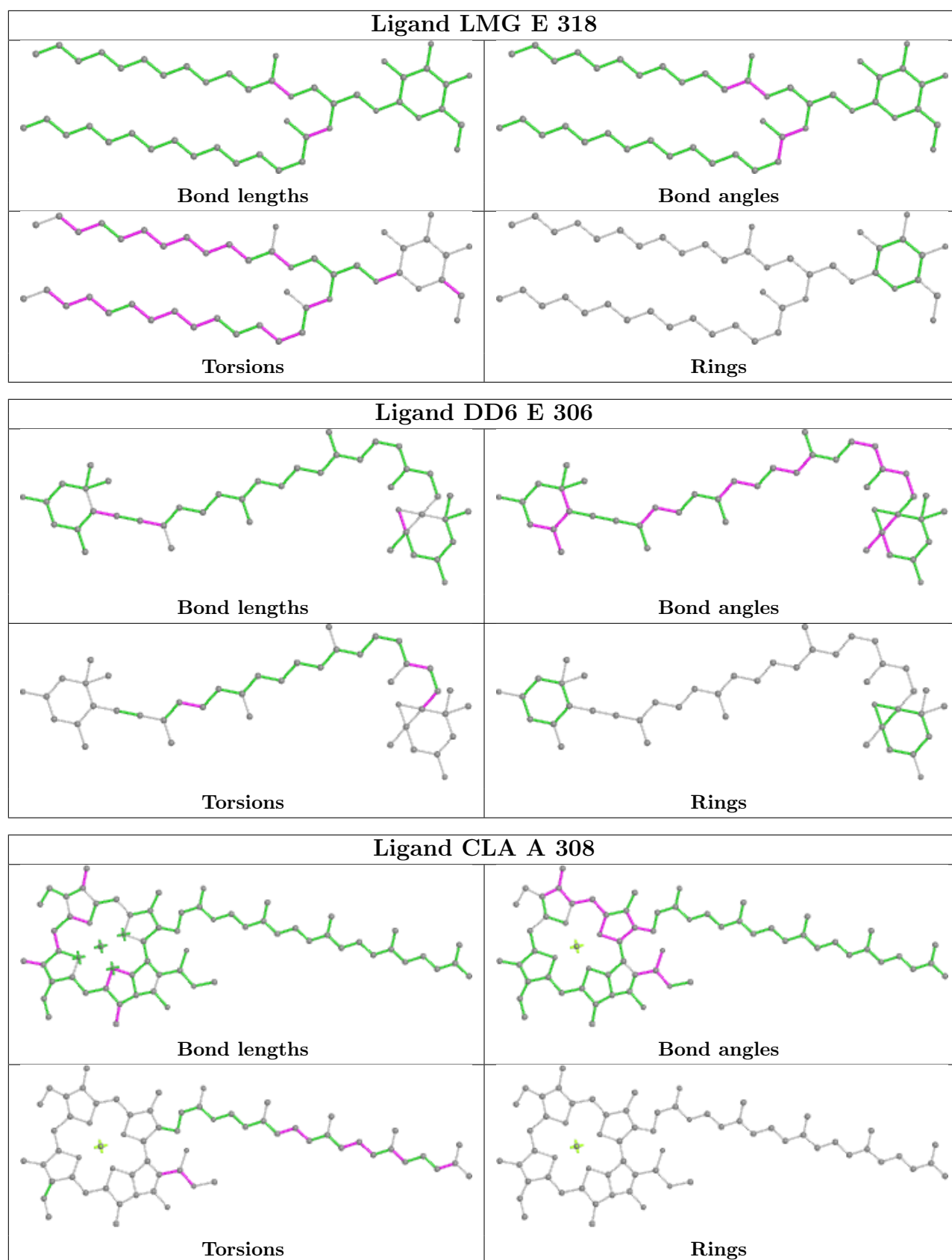


## Ligand CLA l 206

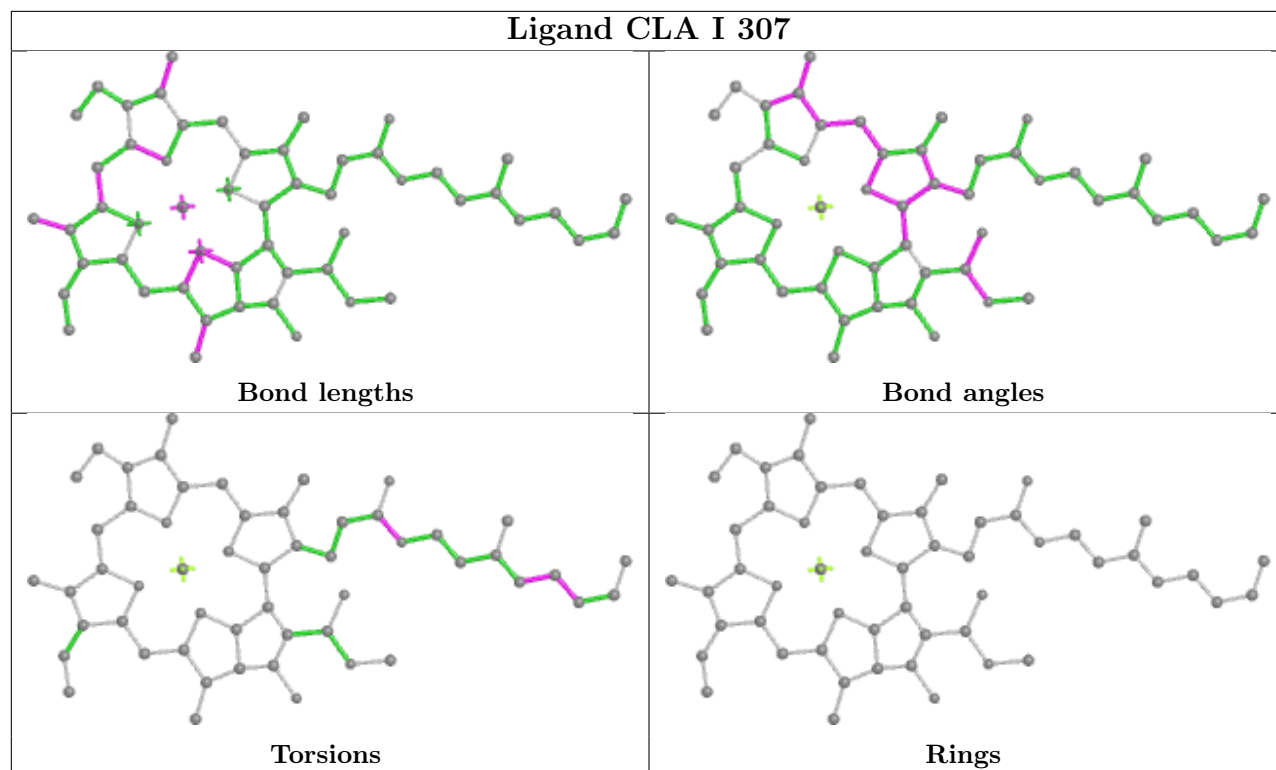


## Ligand CLA a 827

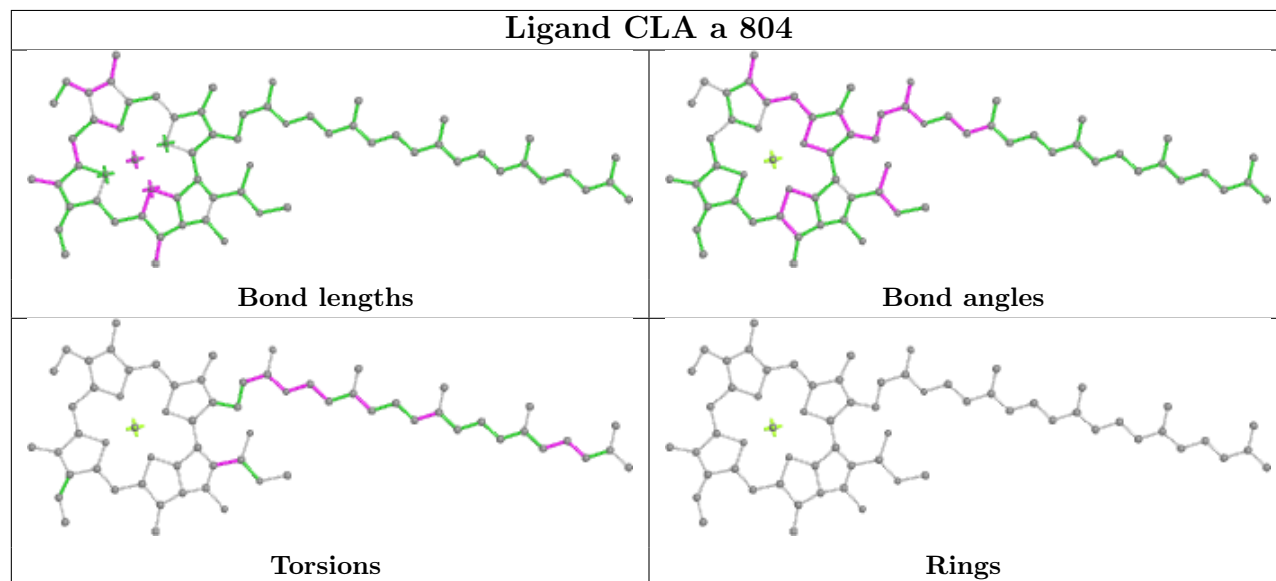




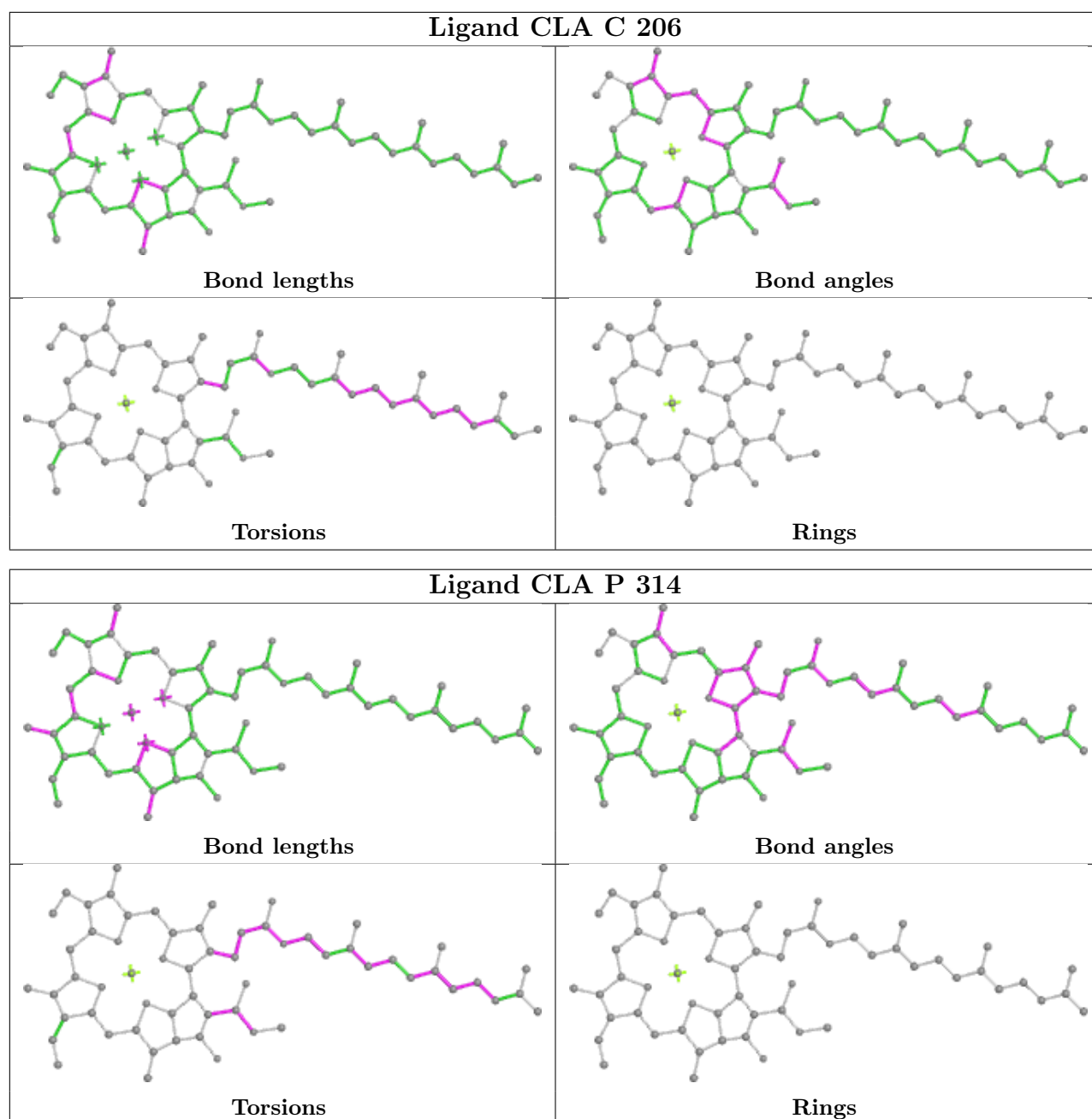
## Ligand CLA I 307

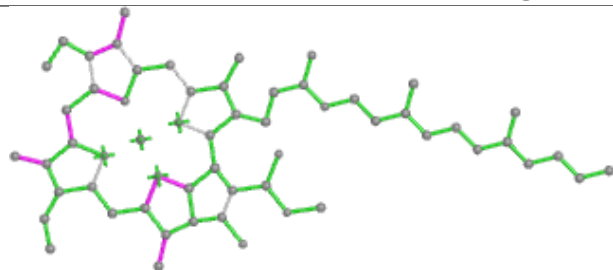
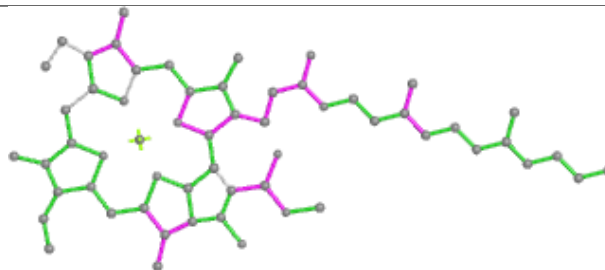
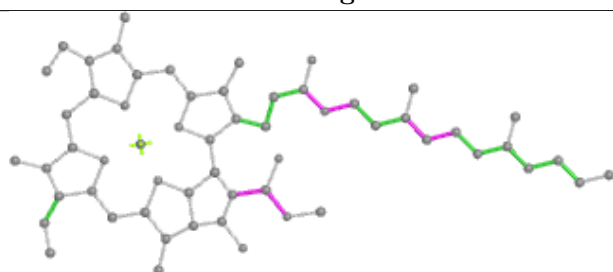
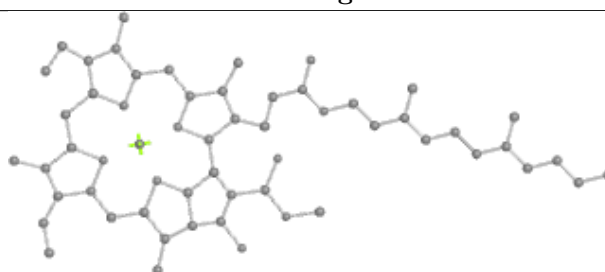
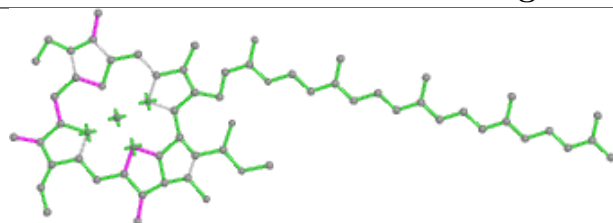
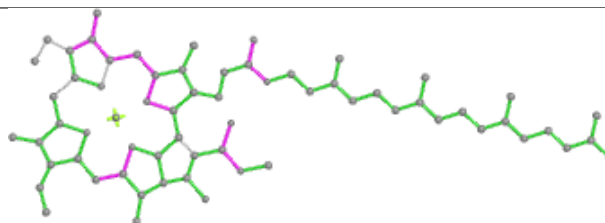
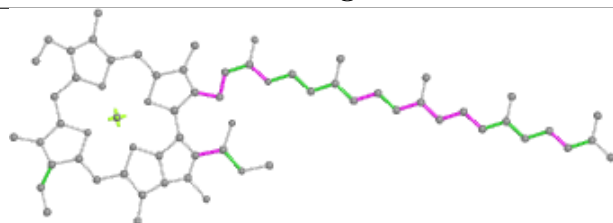
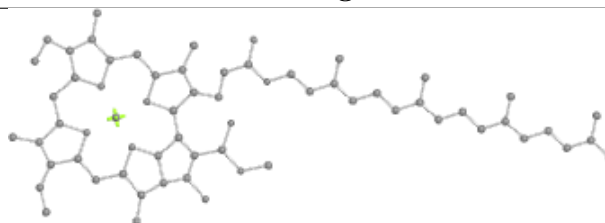


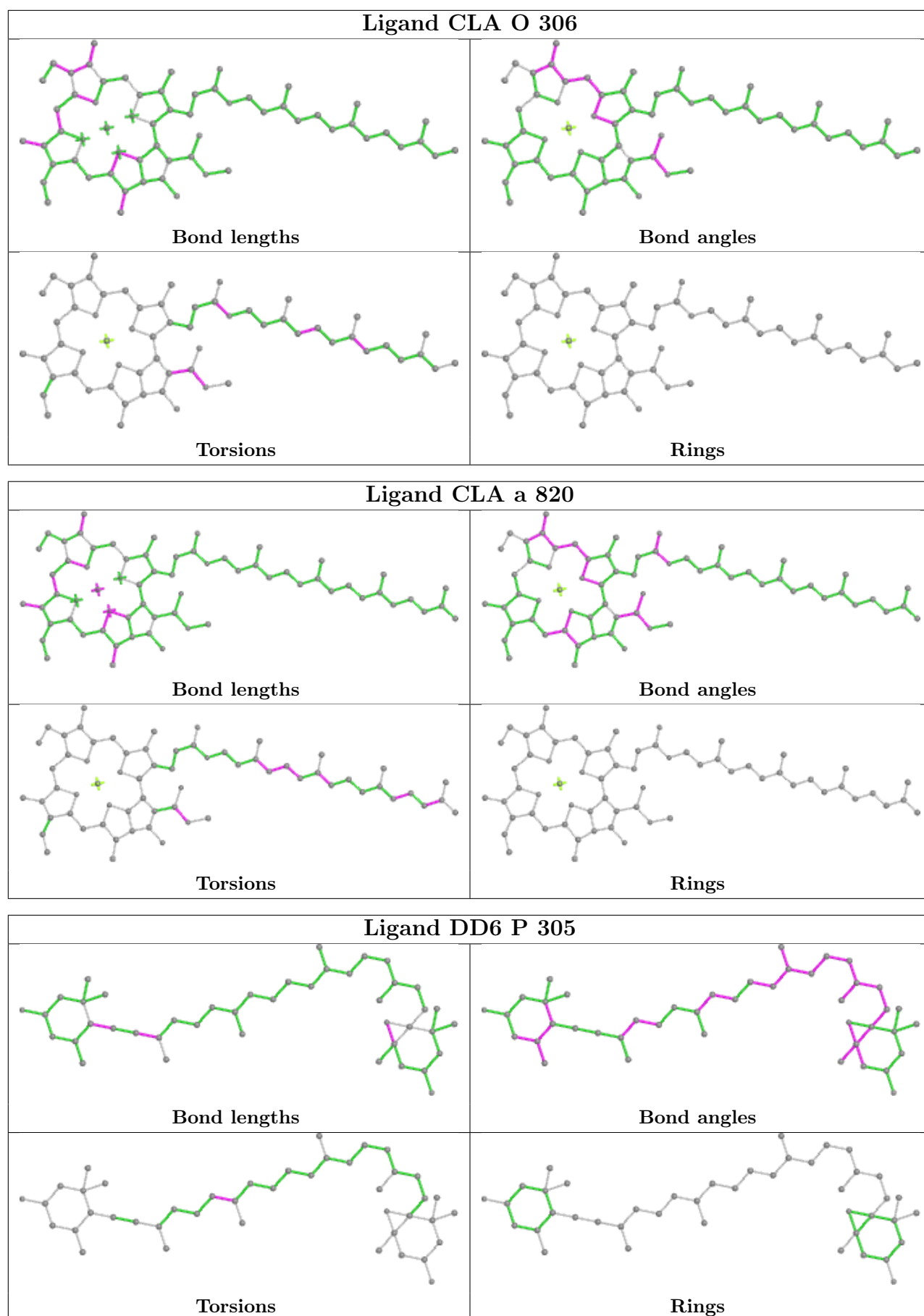
## Ligand CLA a 804

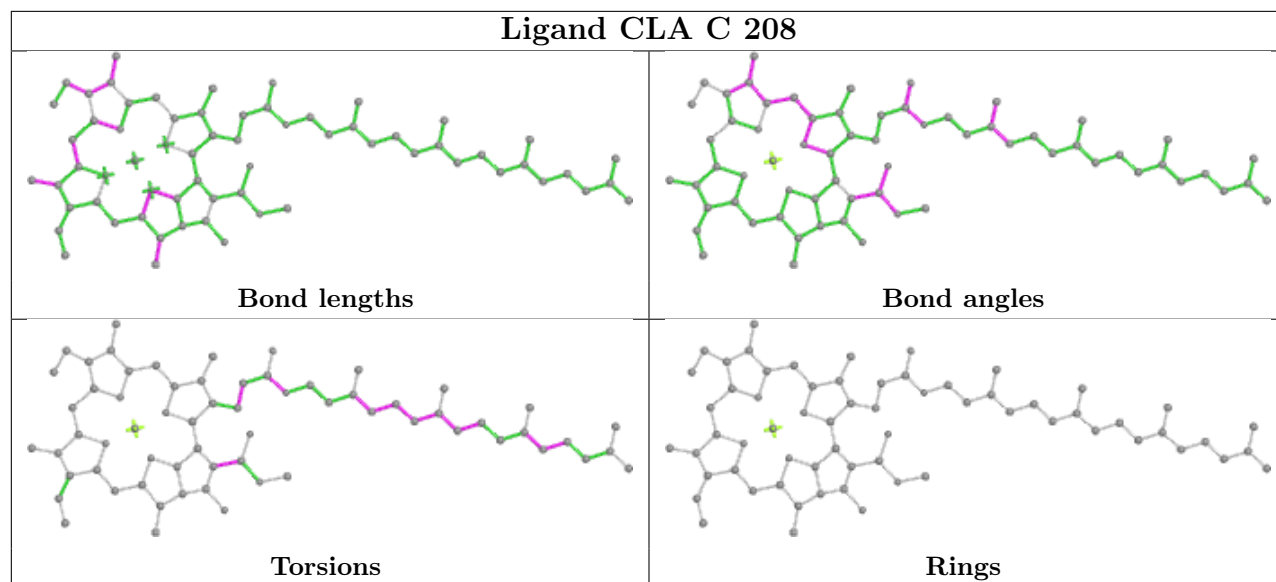
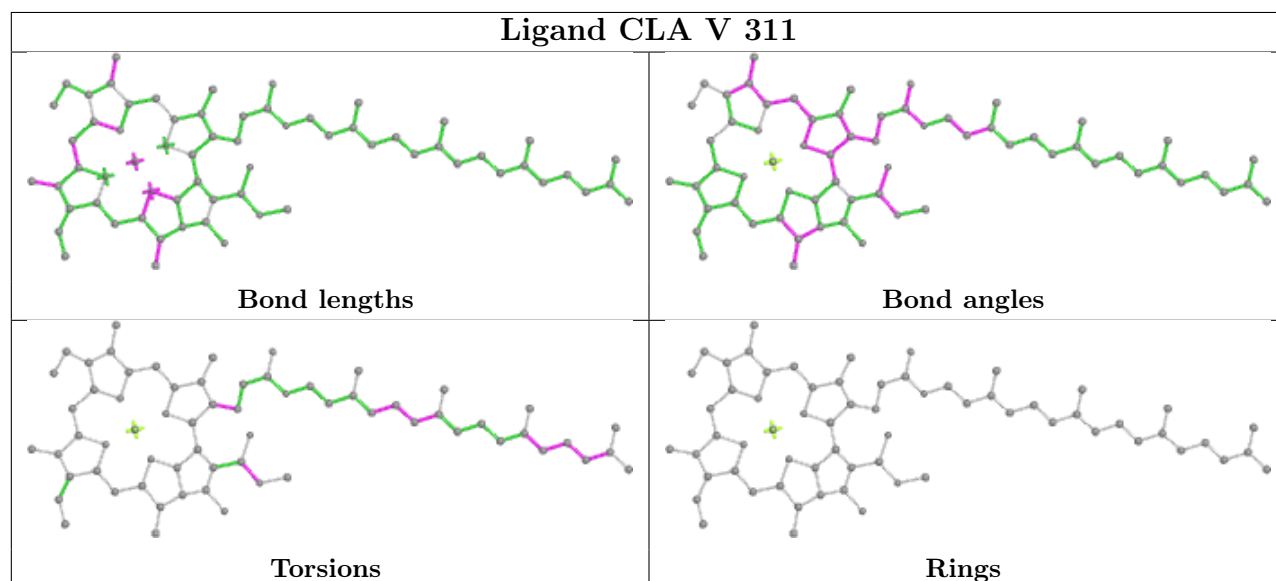




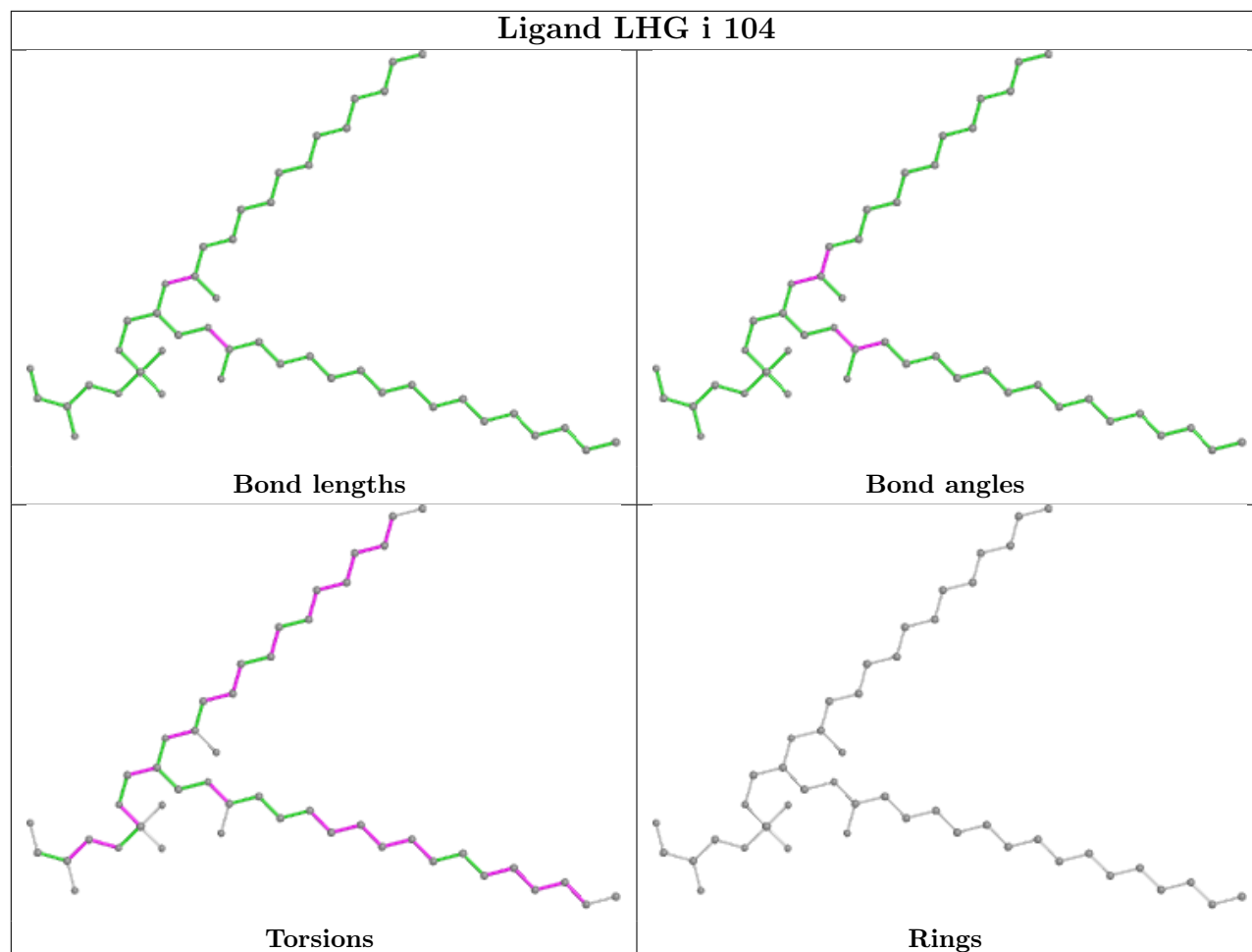


**Ligand CLA b 833****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA a 812****Bond lengths****Bond angles****Torsions****Rings**

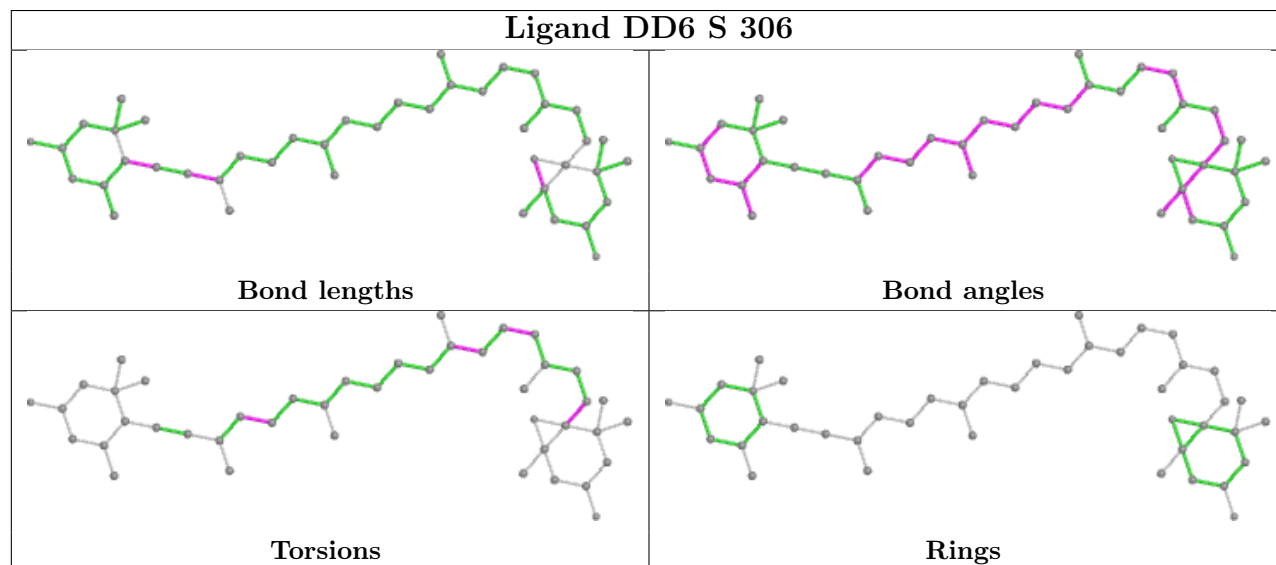


**Ligand CLA C 208****Ligand CLA V 311**

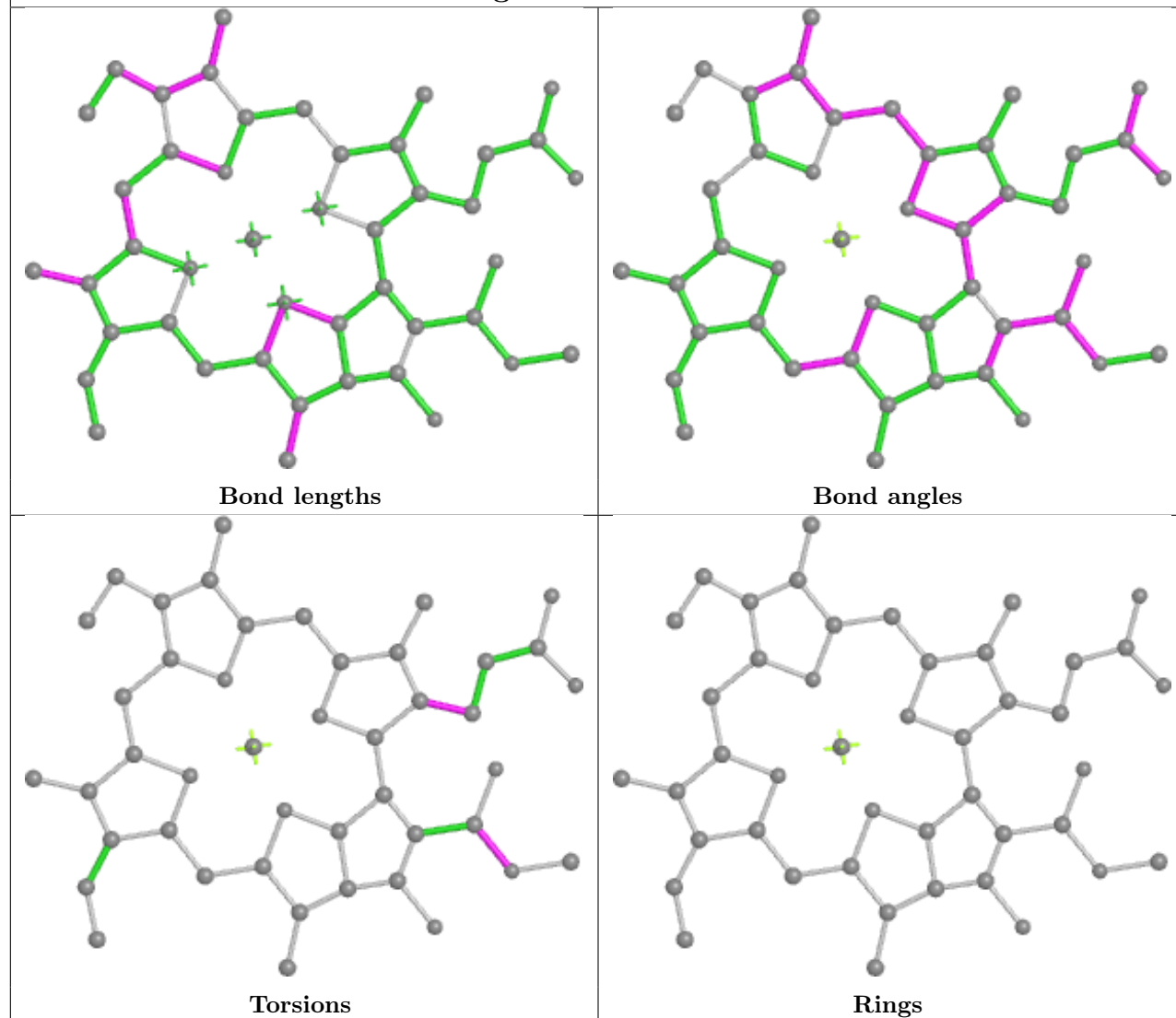
## Ligand LHG i 104



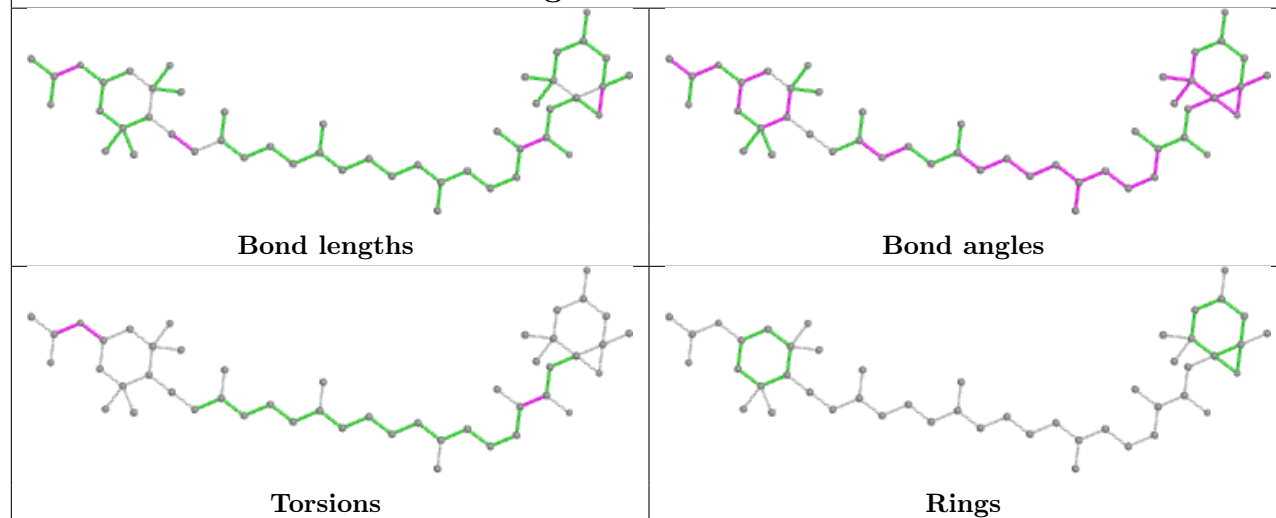
## Ligand DD6 S 306

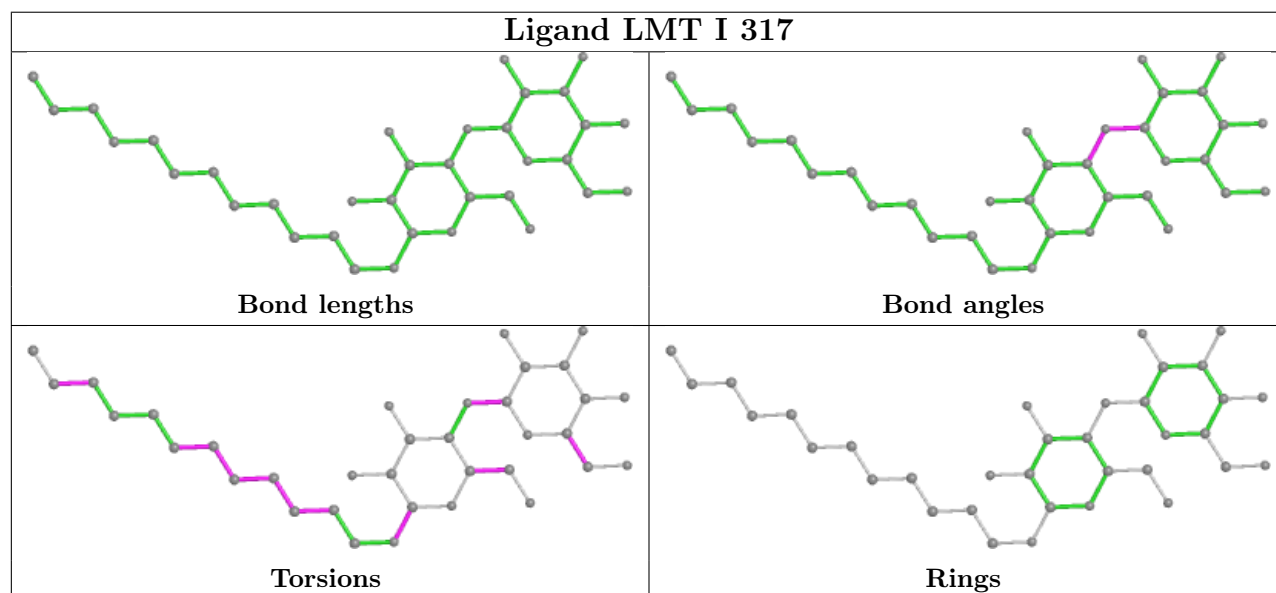
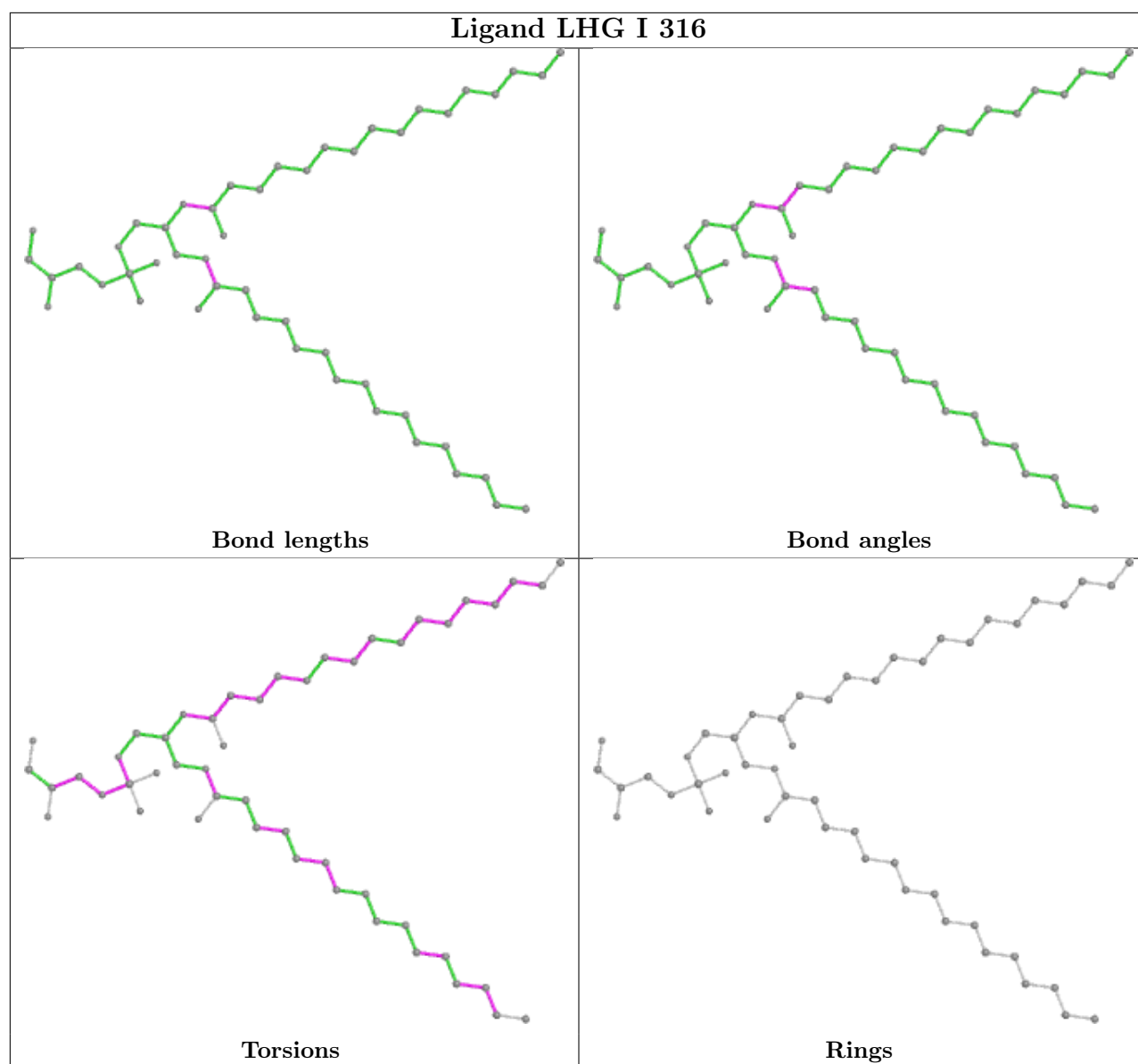


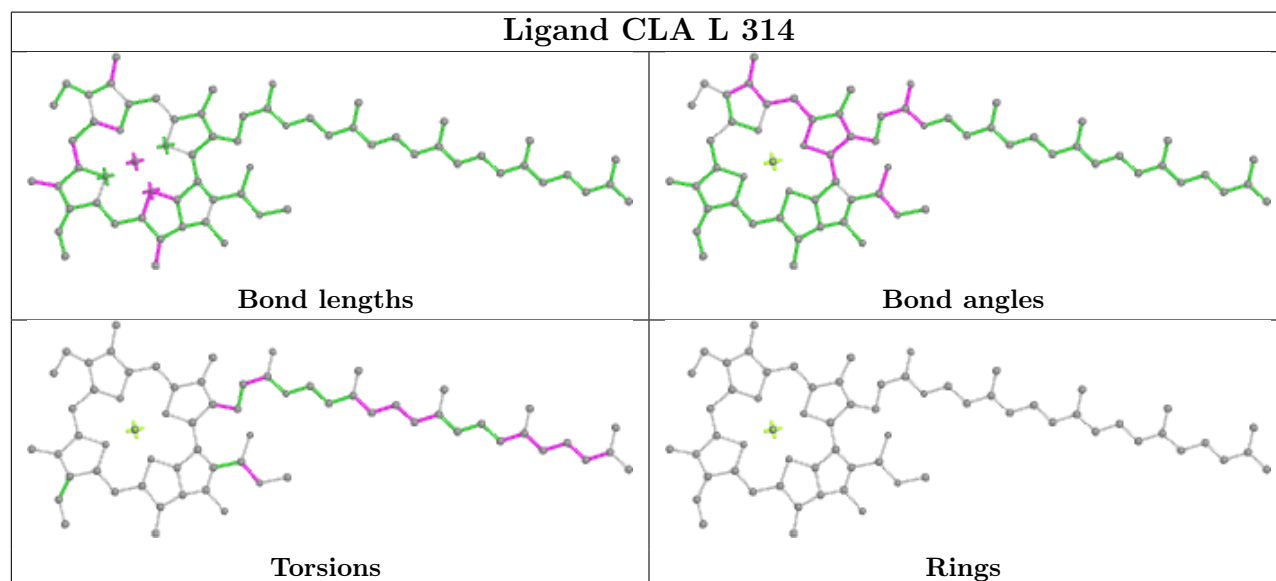
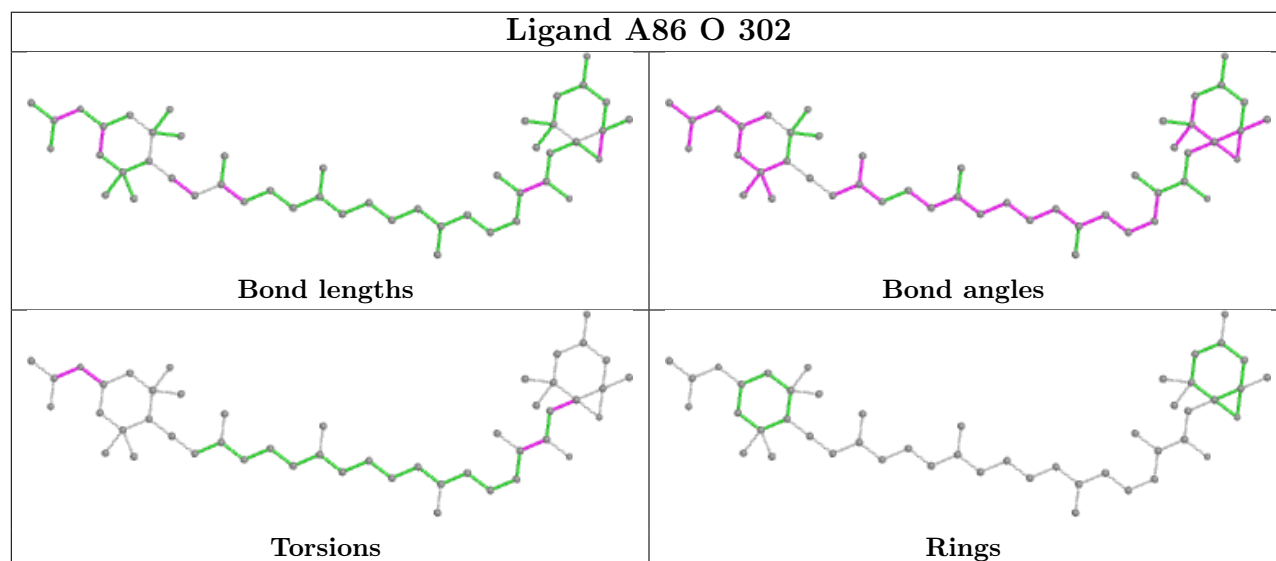
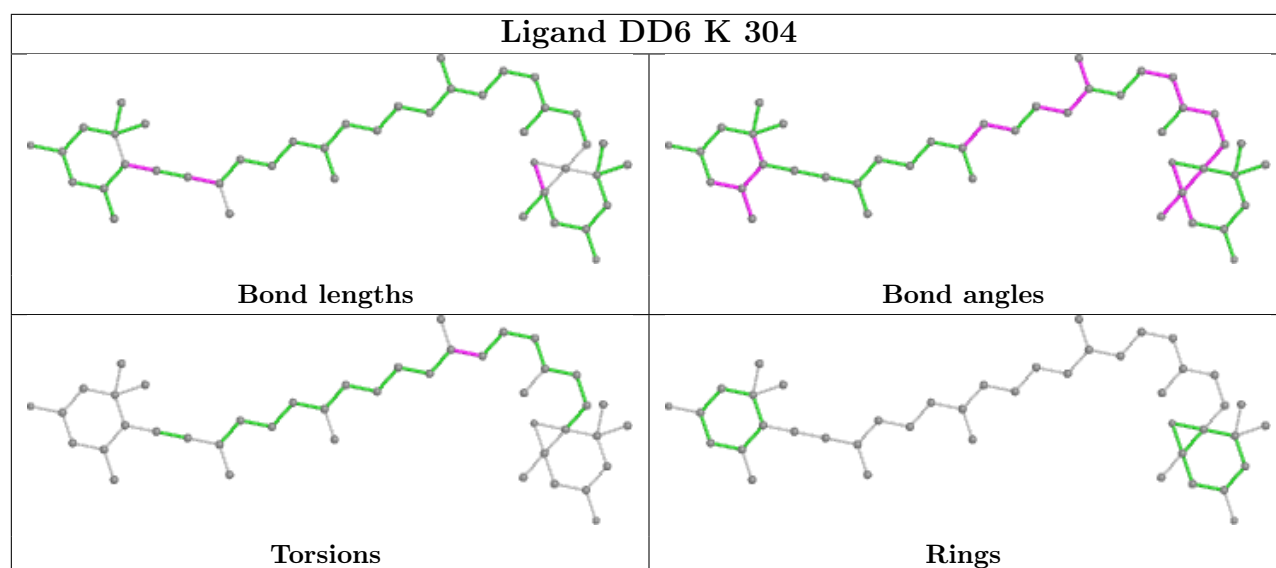
## Ligand CLA b 835



## Ligand A86 I 302

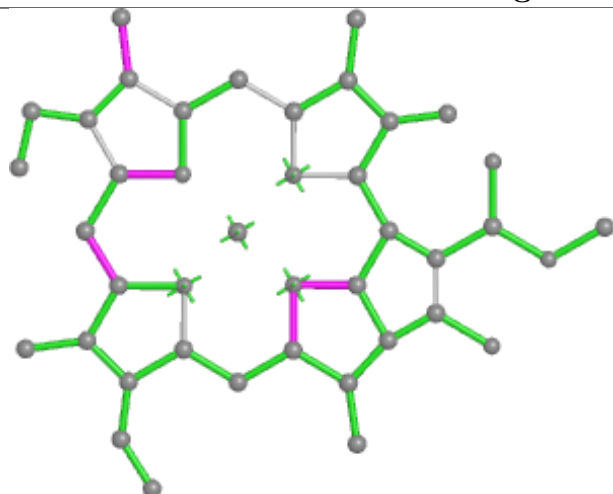




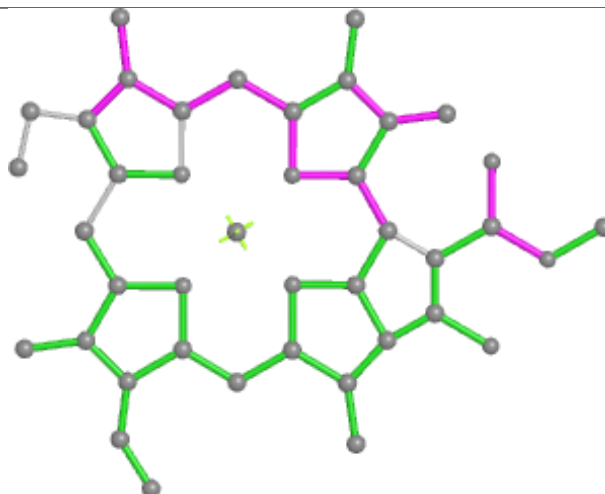




## Ligand CLA X 315



Bond lengths



Bond angles

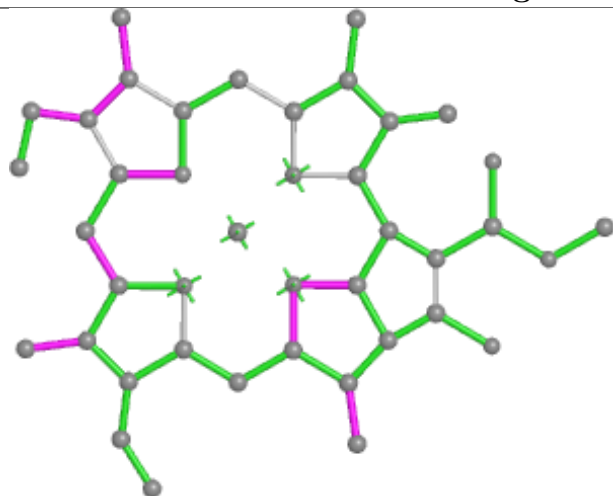


Torsions

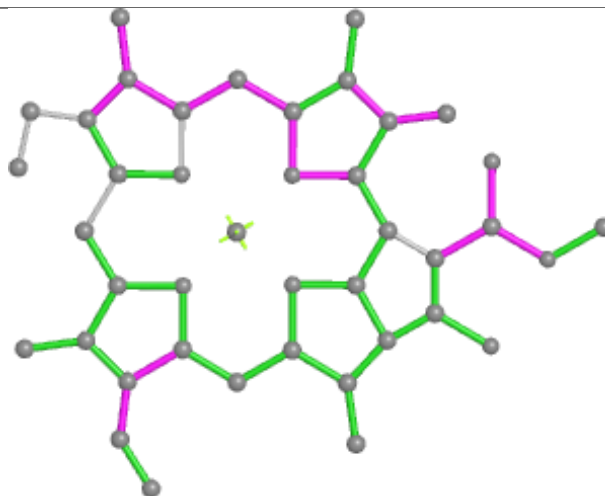


Rings

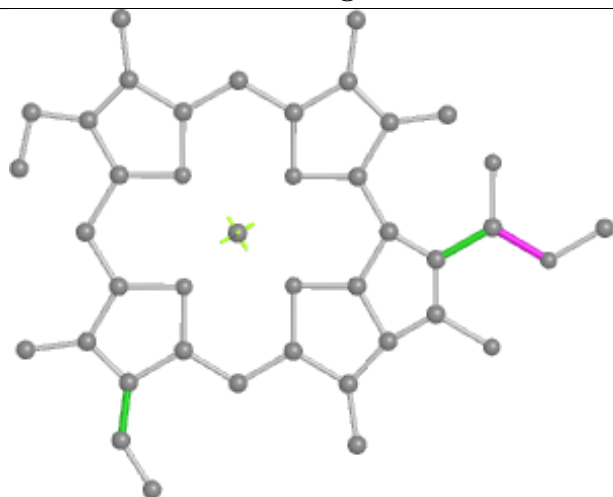
## Ligand CLA G 314



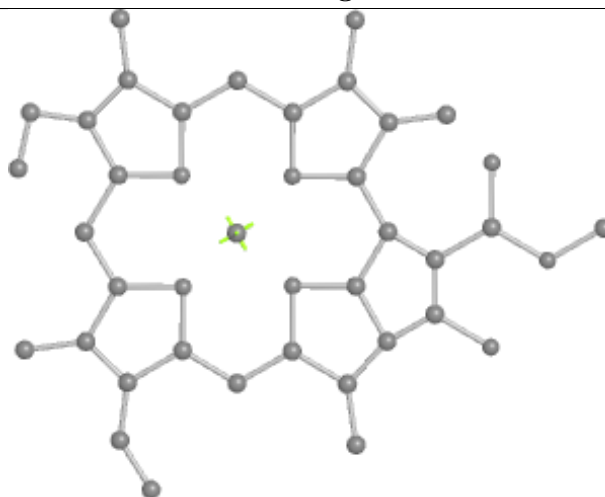
Bond lengths



Bond angles

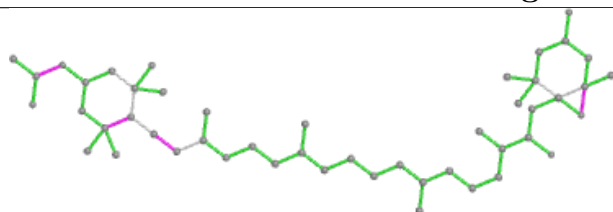


Torsions

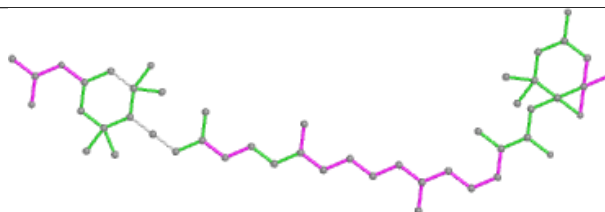


Rings

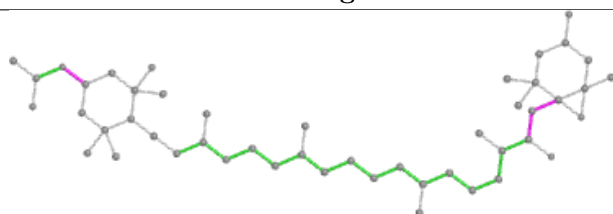
## Ligand A86 E 302



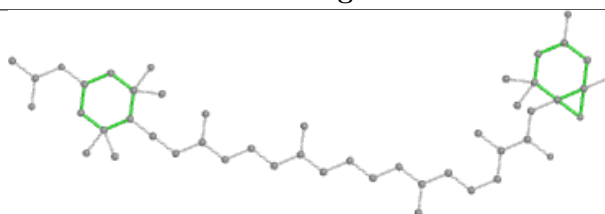
Bond lengths



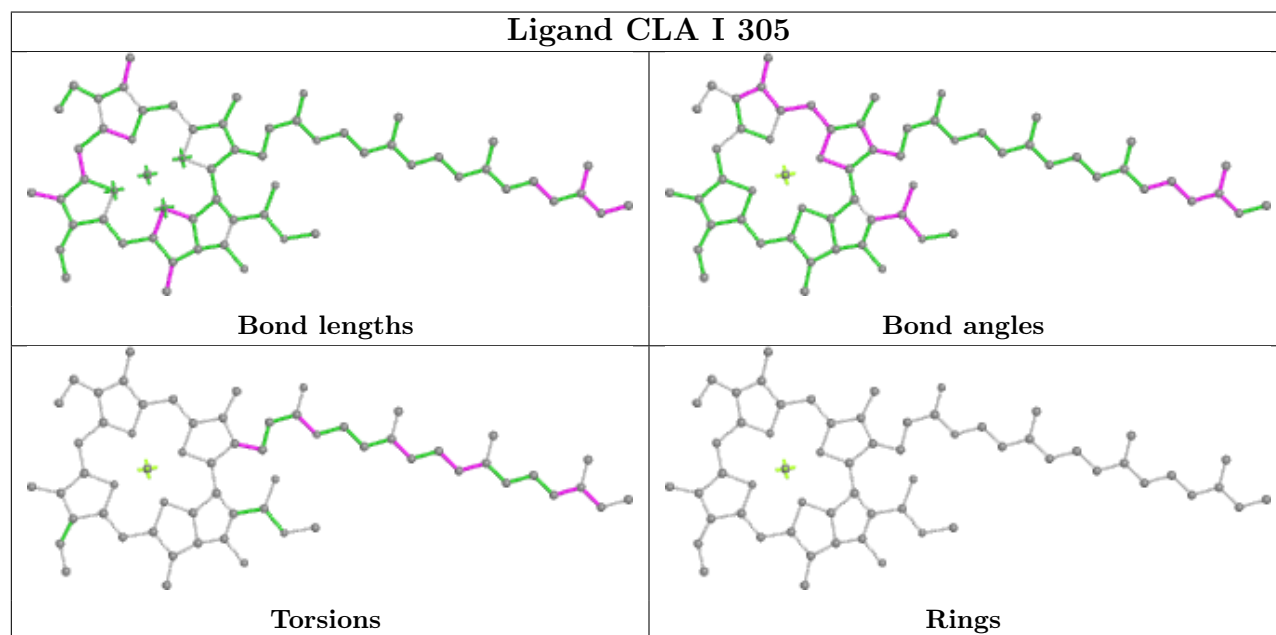
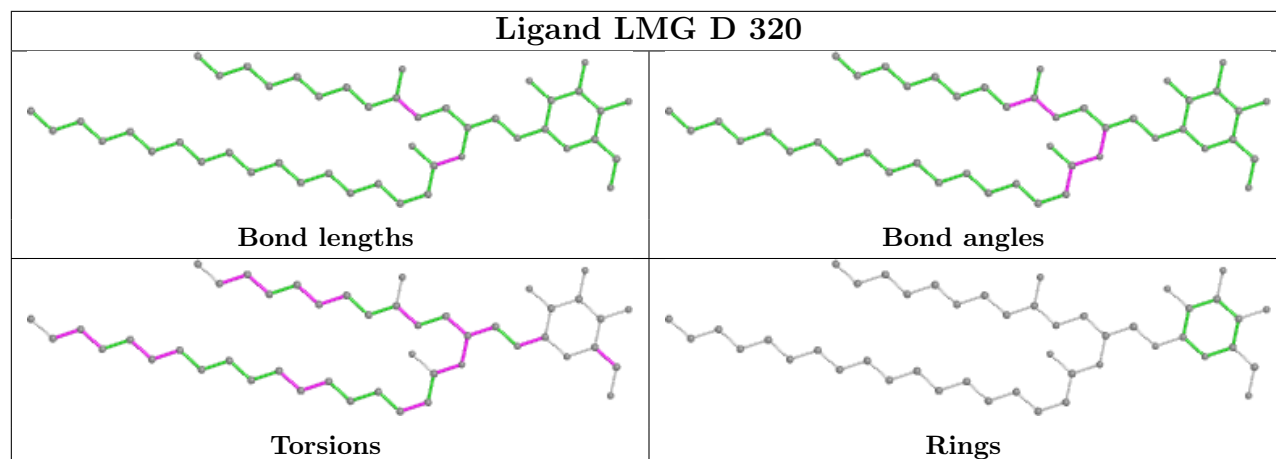
Bond angles

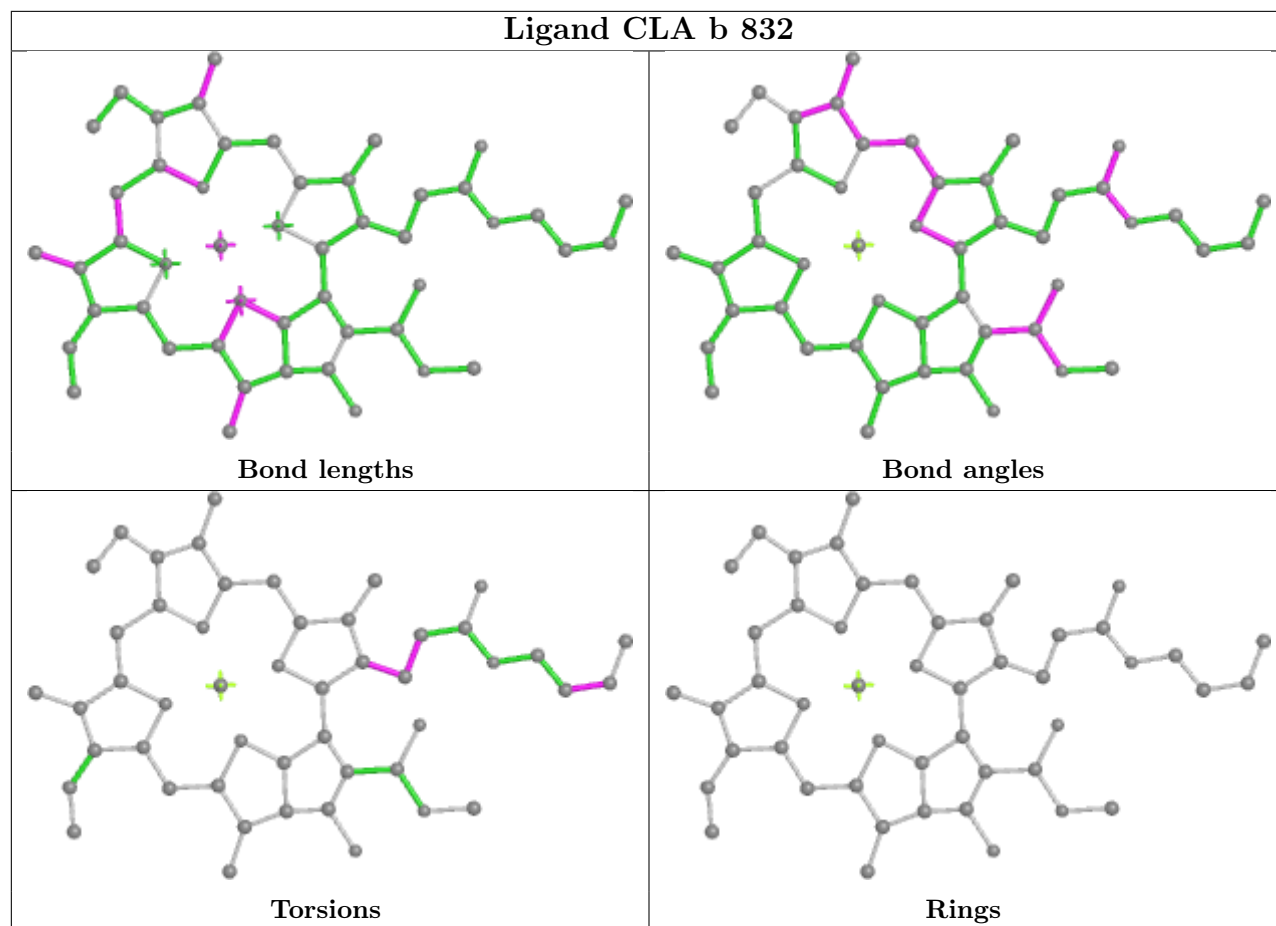


Torsions

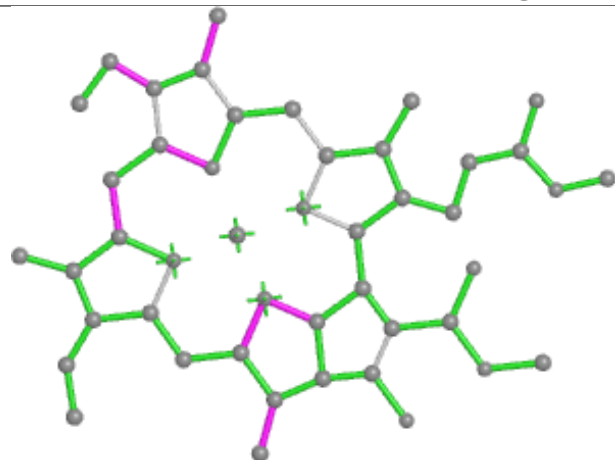


Rings

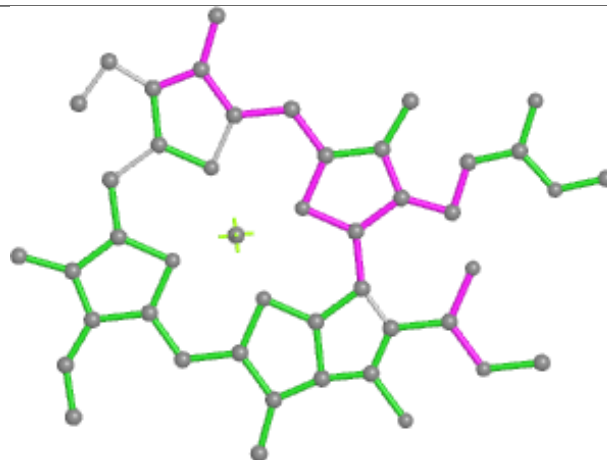




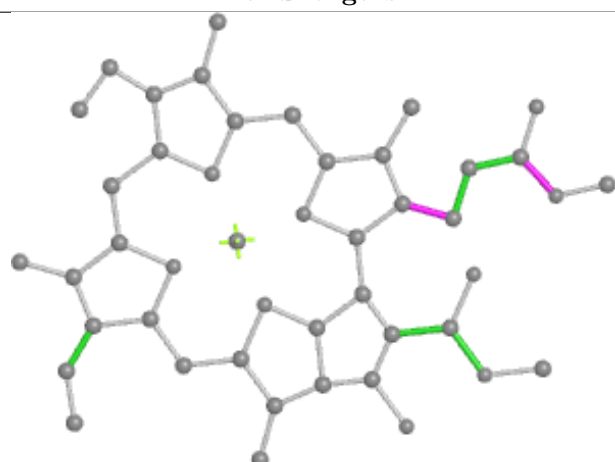
## Ligand CLA N 311



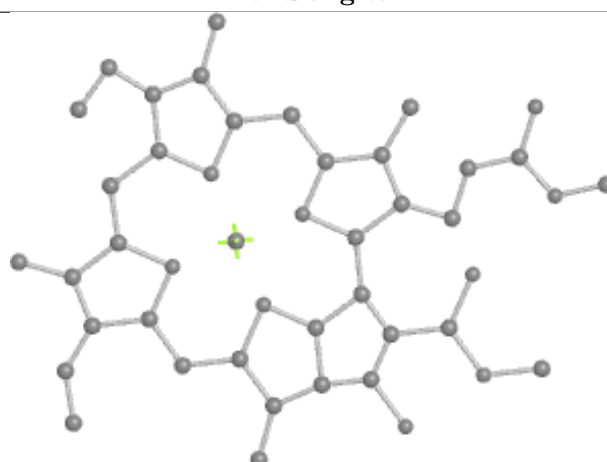
Bond lengths



Bond angles

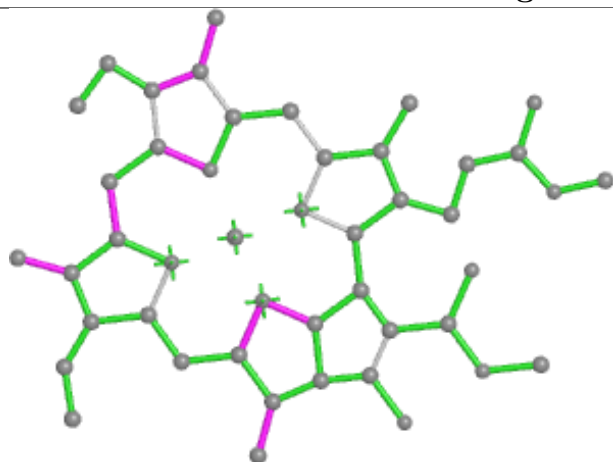


Torsions

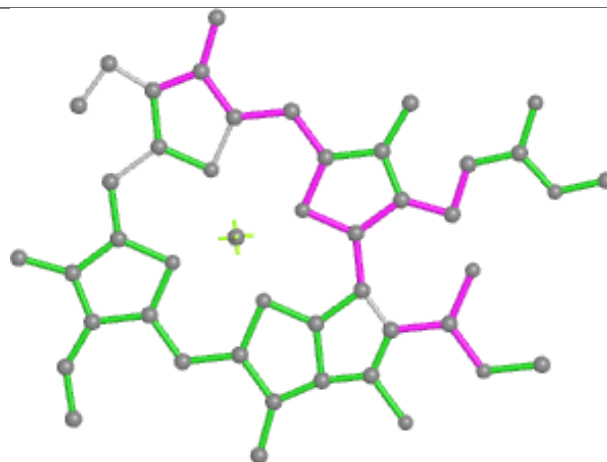


Rings

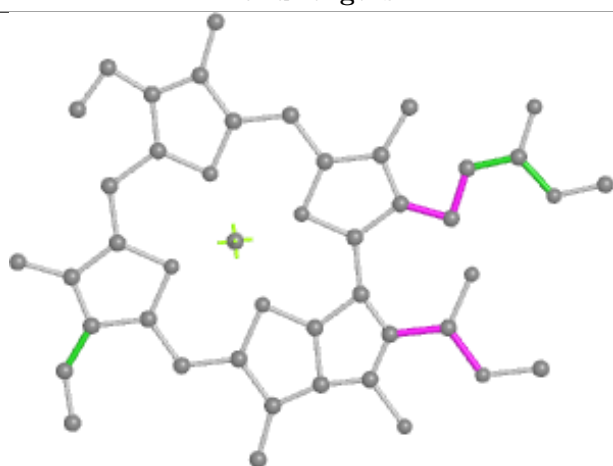
## Ligand CLA L 312



Bond lengths



Bond angles

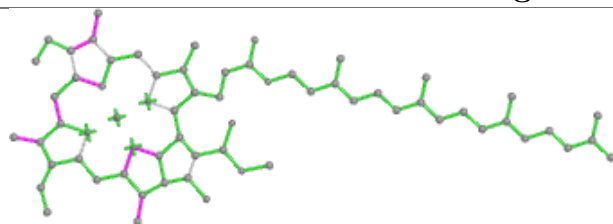


Torsions

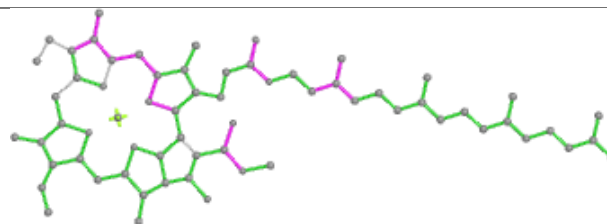


Rings

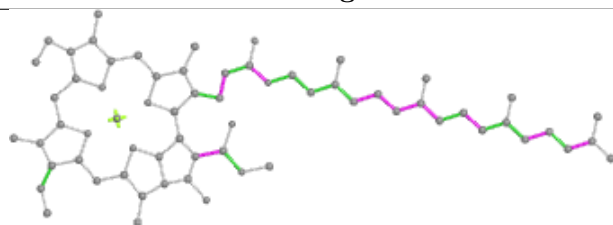
## Ligand CLA O 308



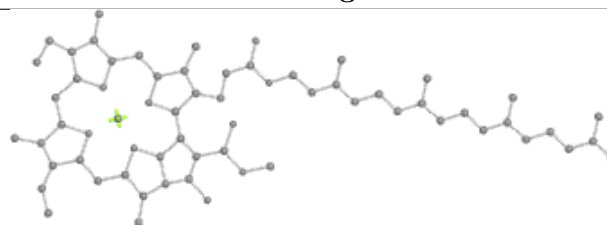
Bond lengths



Bond angles

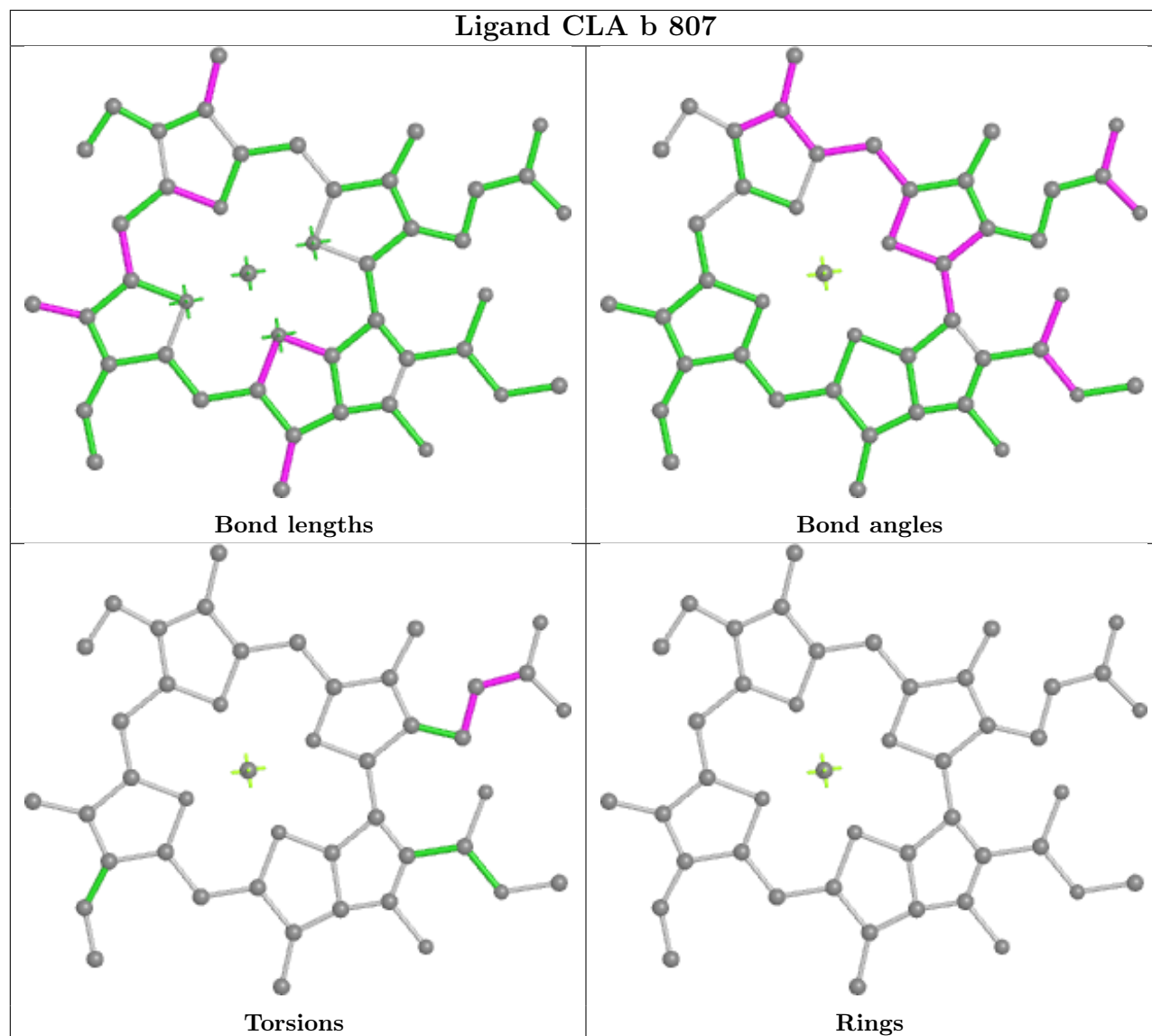


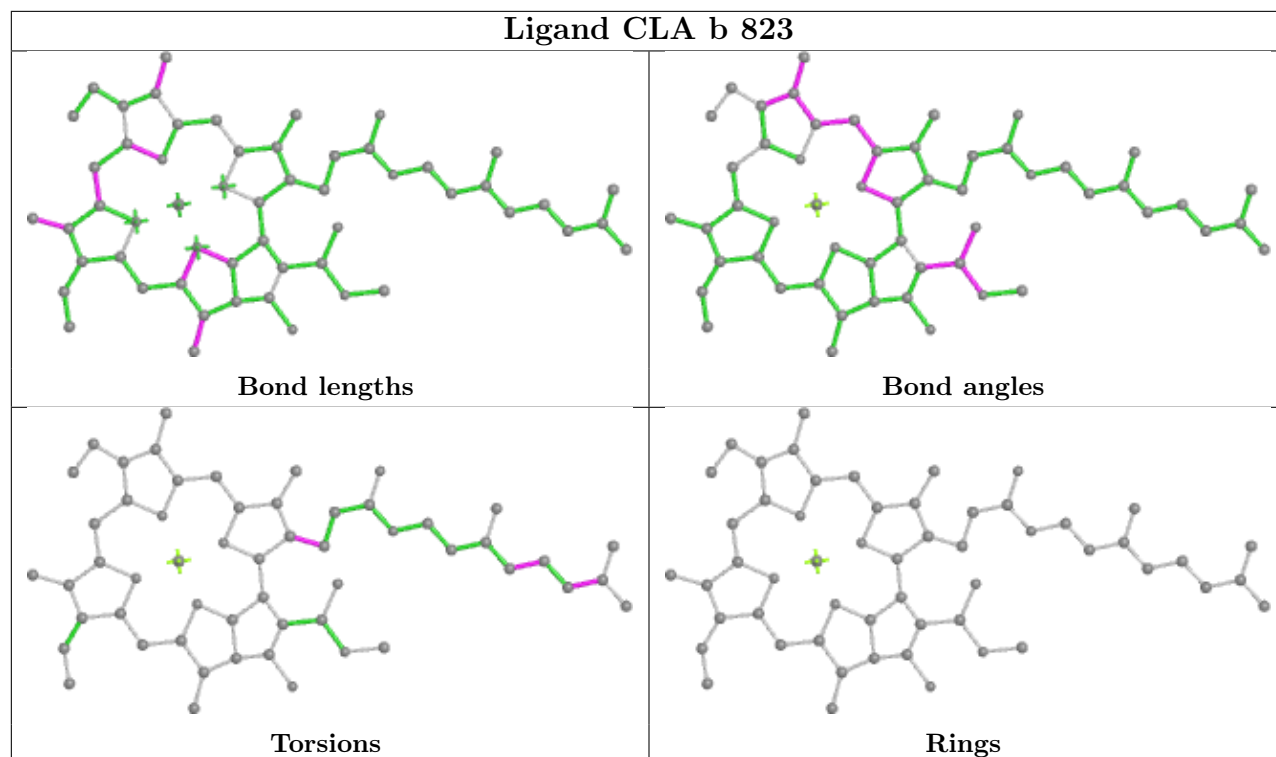
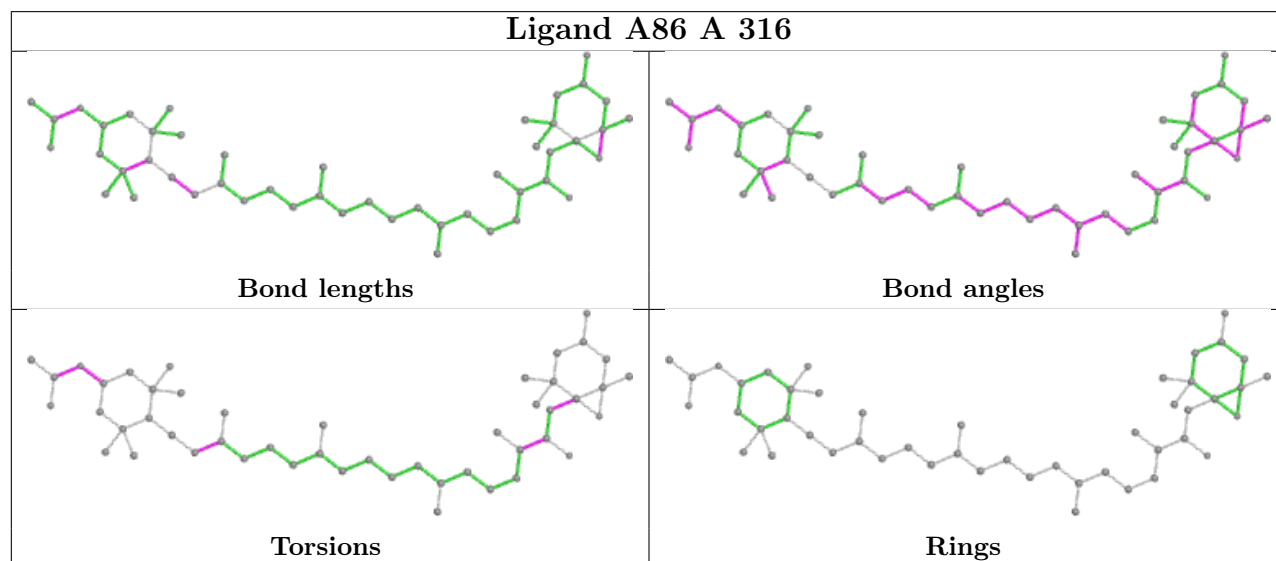
Torsions



Rings

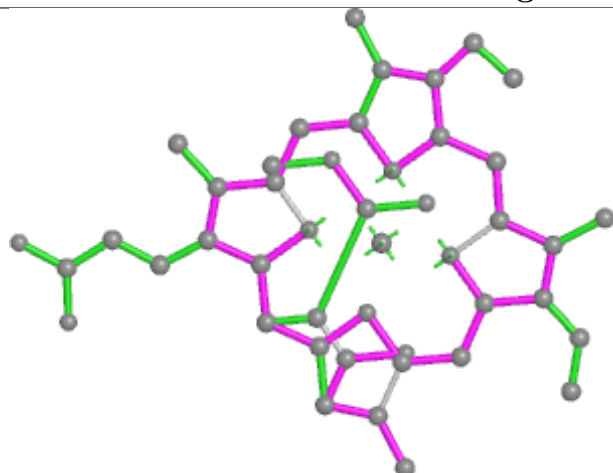
## Ligand CLA b 807



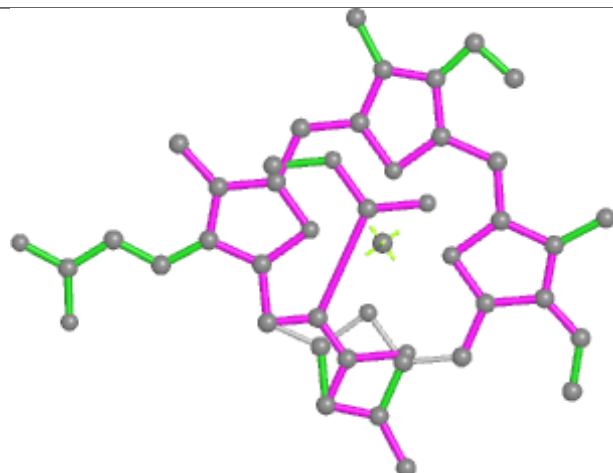
**Ligand CLA b 823****Ligand A86 A 316**



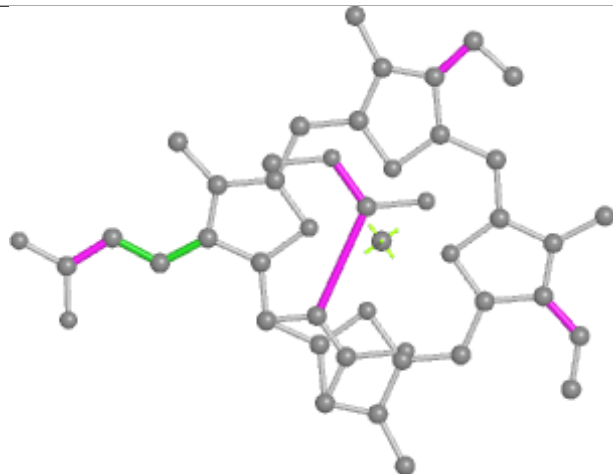
## Ligand KC1 T 310



Bond lengths



Bond angles

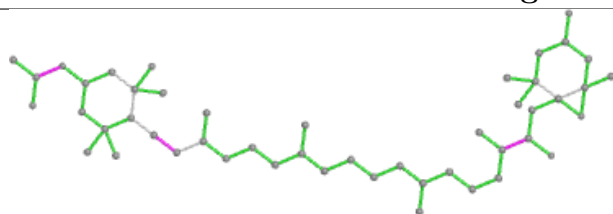


Torsions

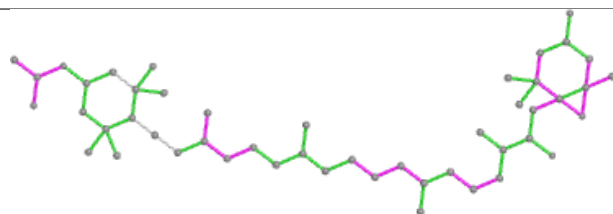


Rings

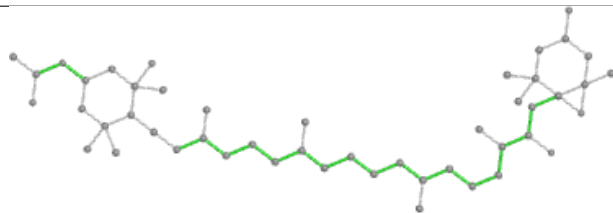
## Ligand A86 T 304



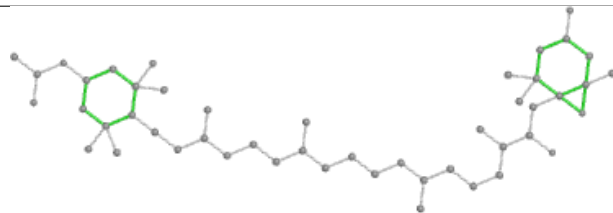
Bond lengths



Bond angles

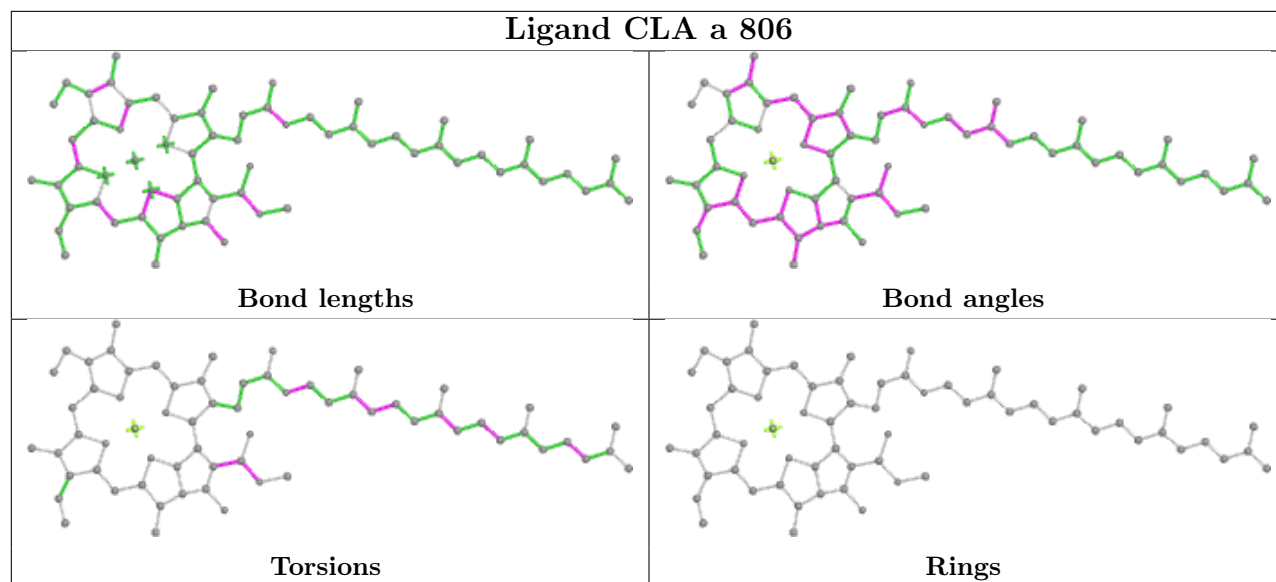


Torsions

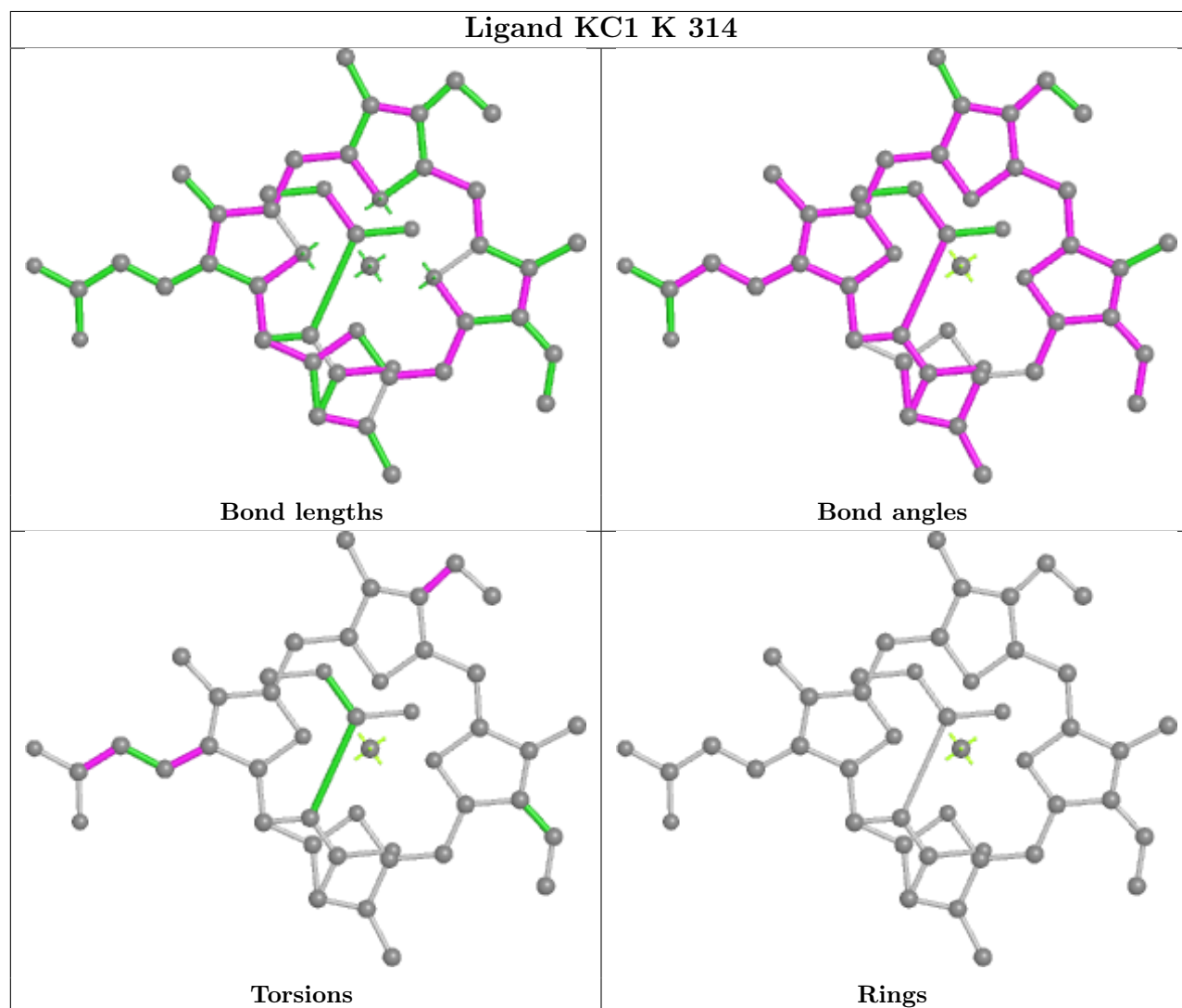


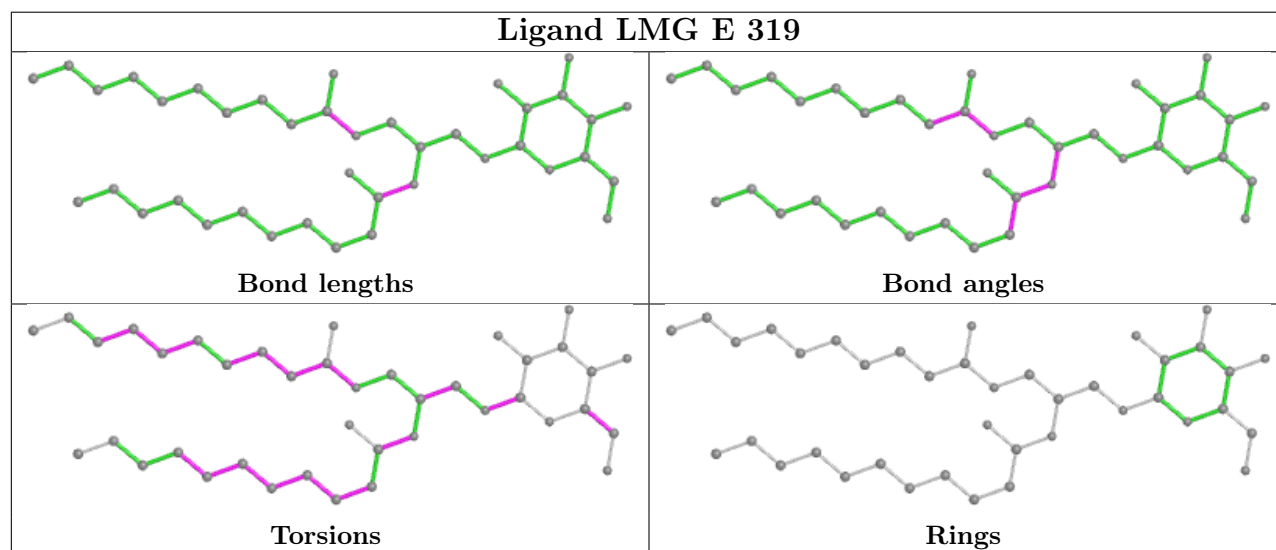
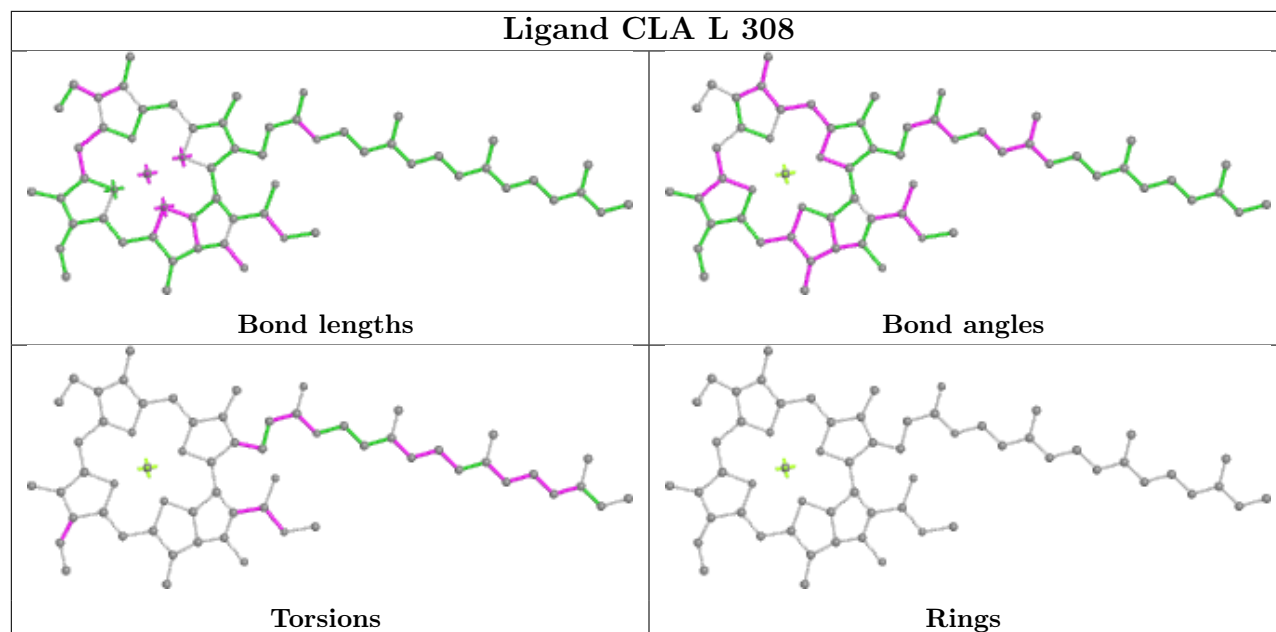
Rings

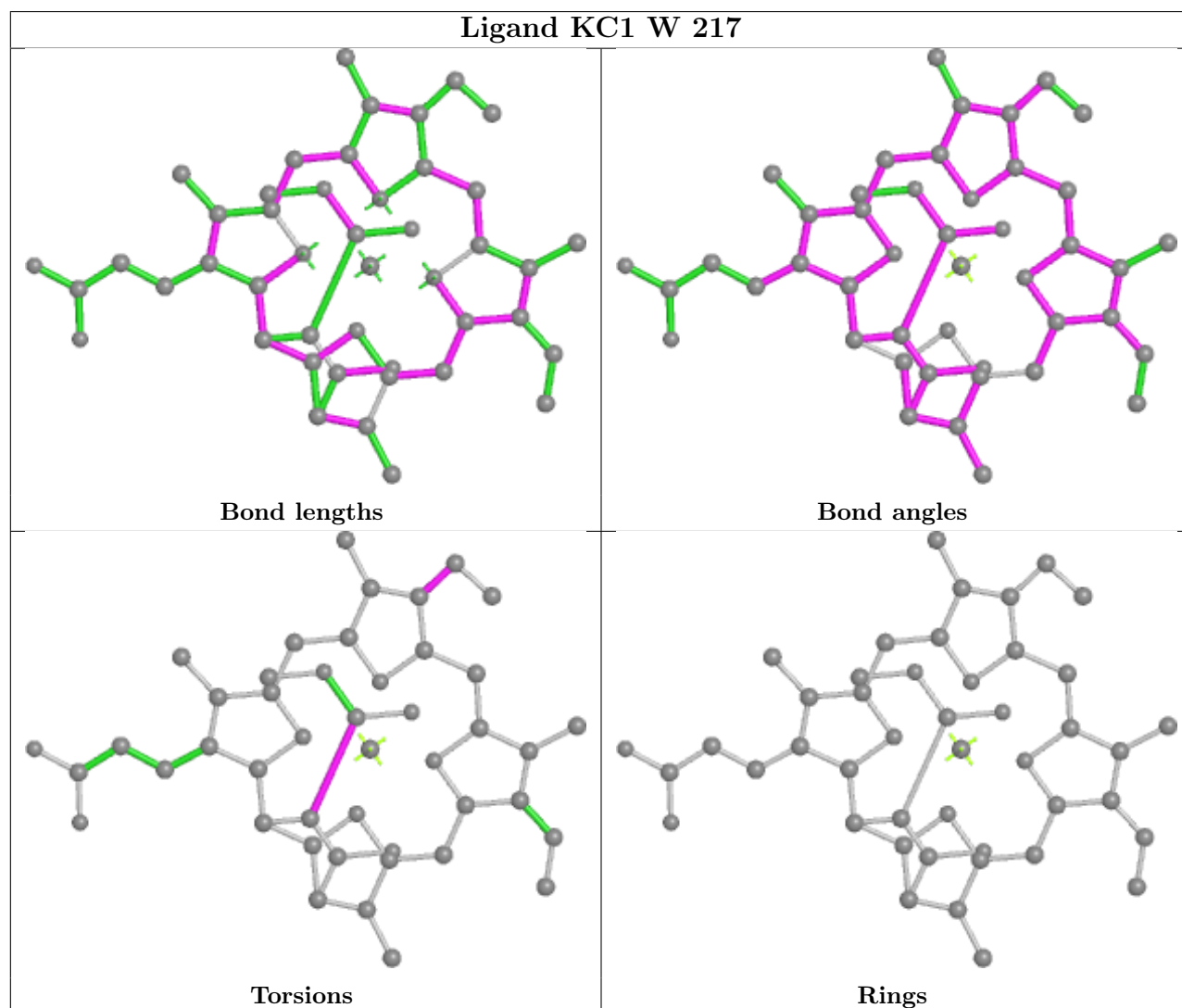
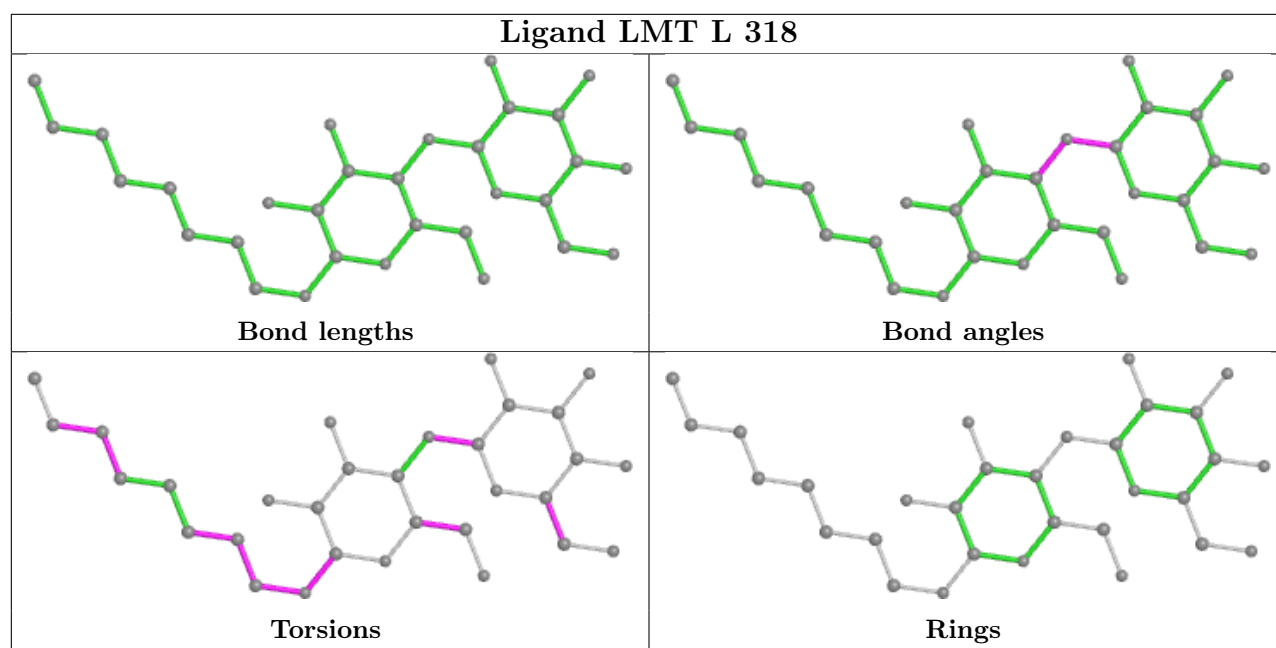
## Ligand CLA a 806

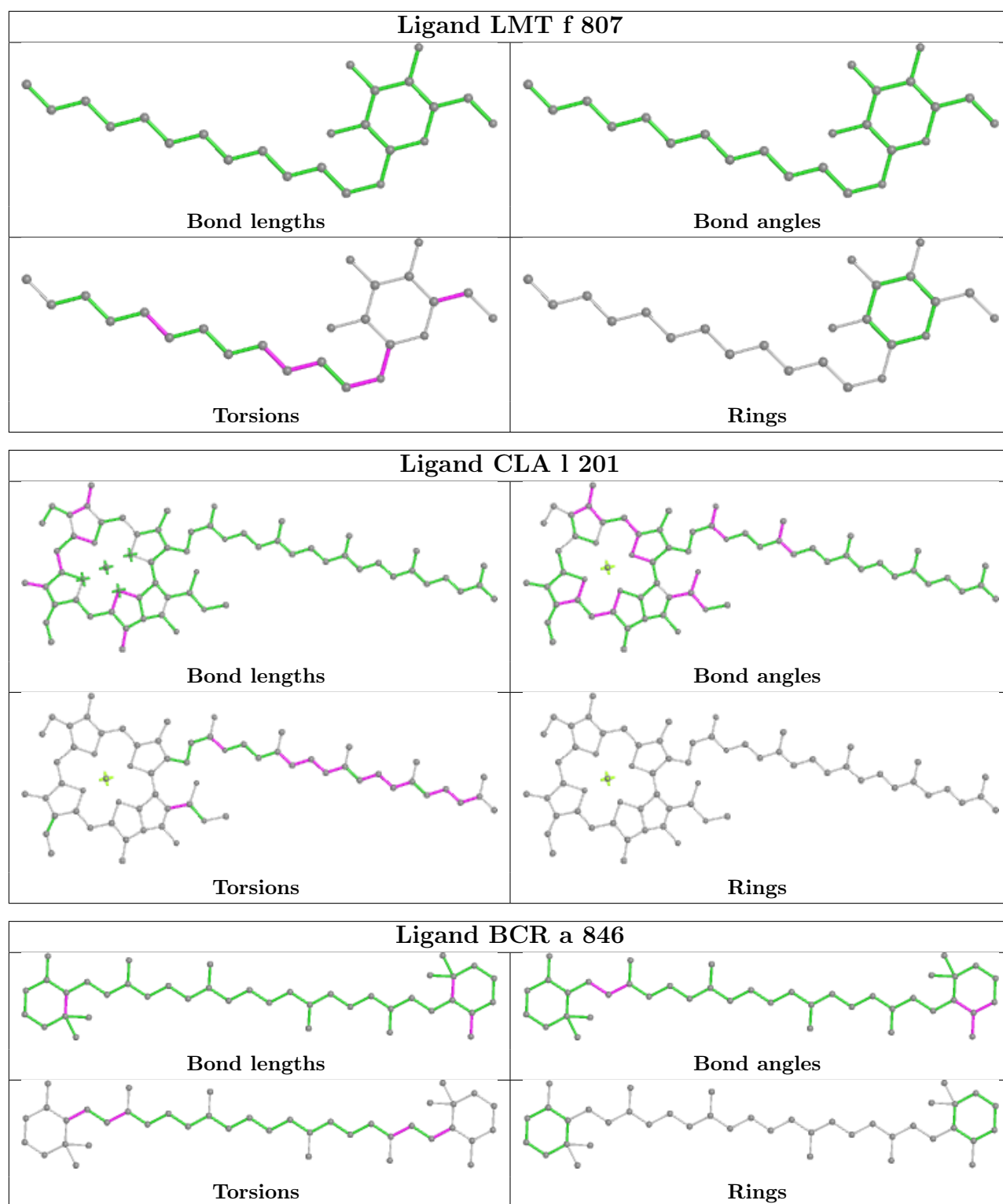


## Ligand KC1 K 314

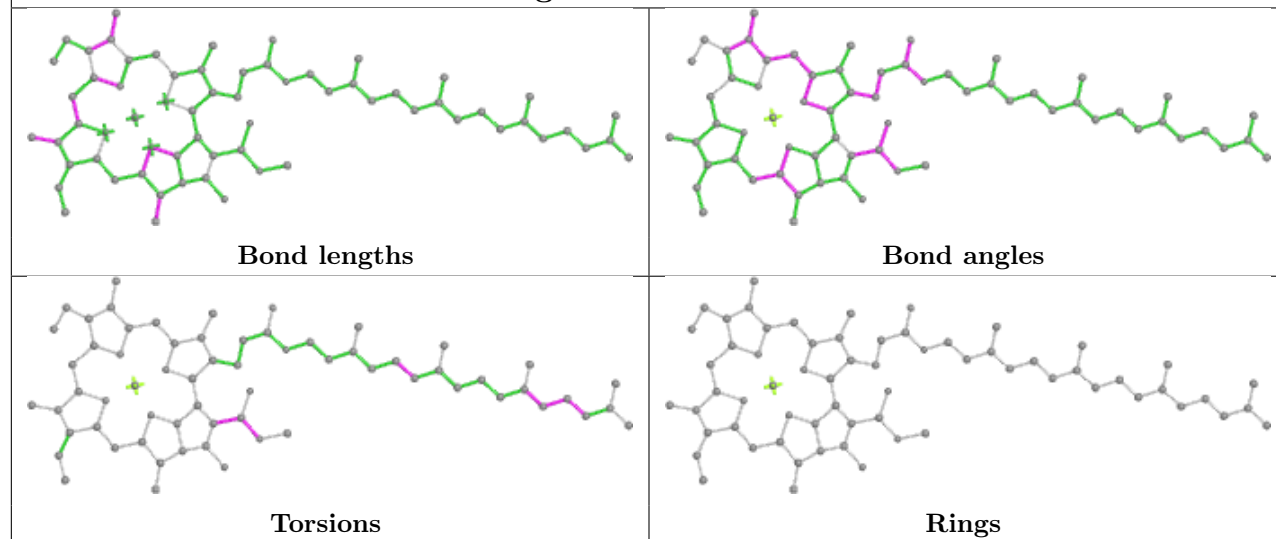




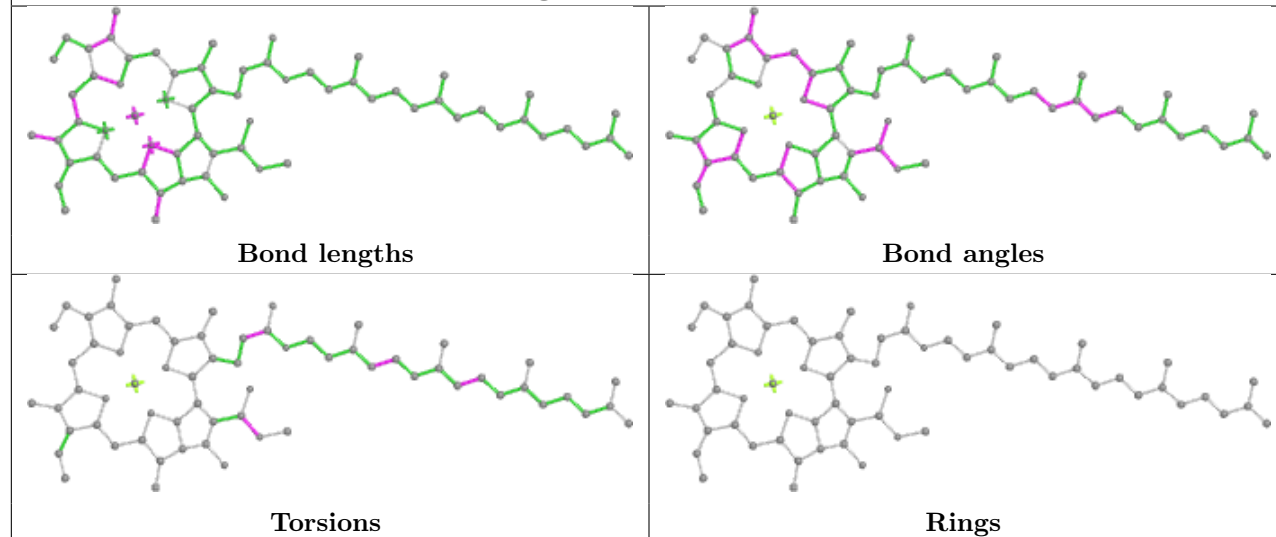




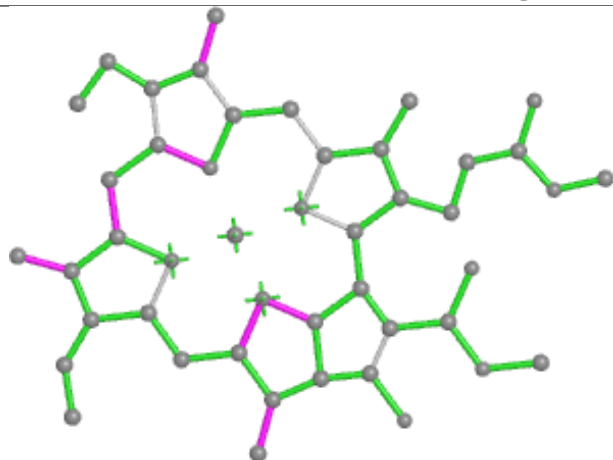
## Ligand CLA b 837



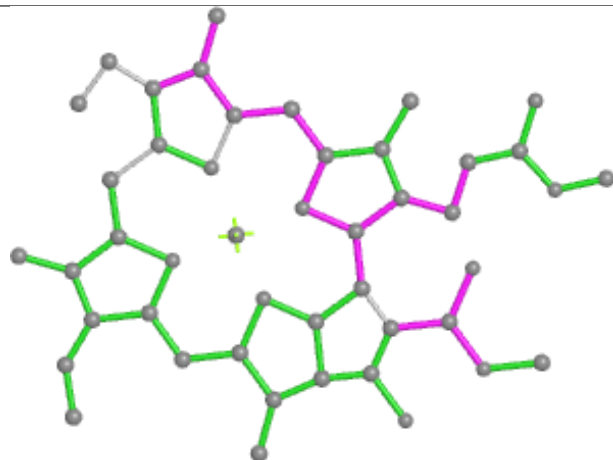
## Ligand CLA b 812



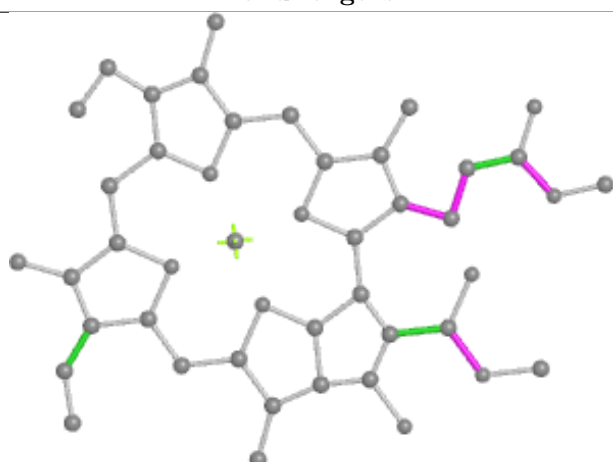
## Ligand CLA P 312



Bond lengths



Bond angles

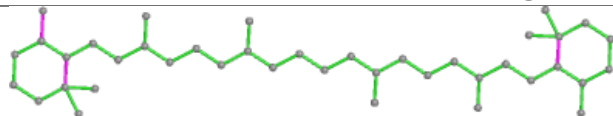


Torsions

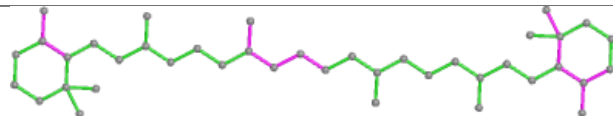


Rings

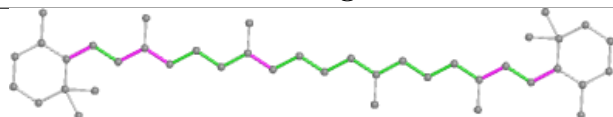
## Ligand BCR f 806



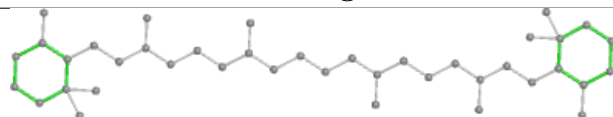
Bond lengths



Bond angles

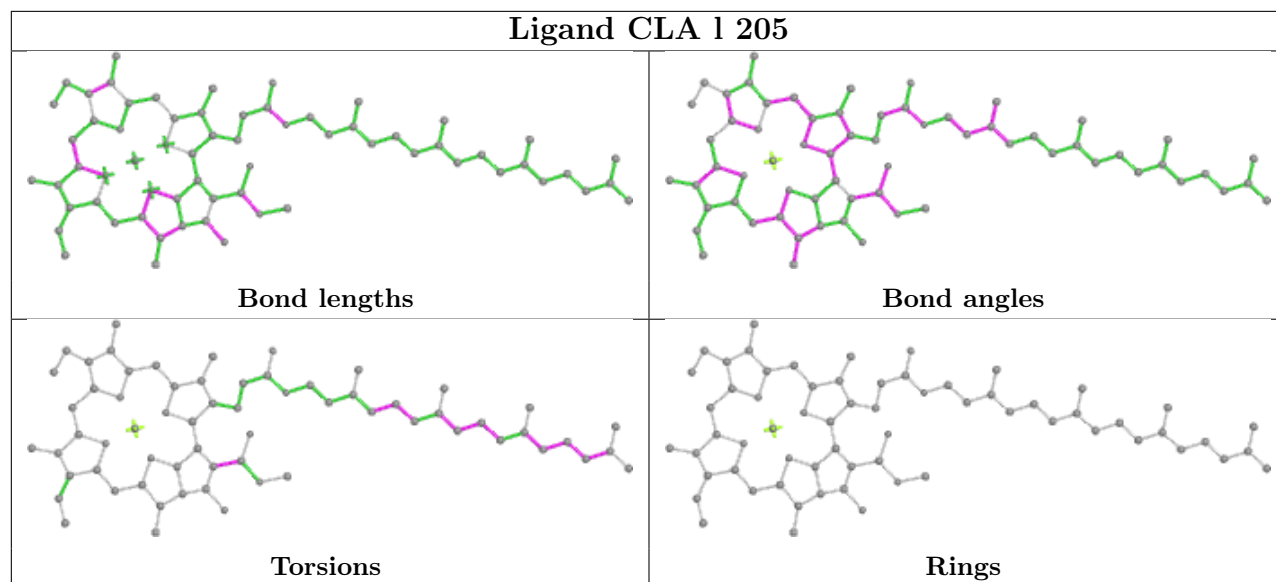


Torsions

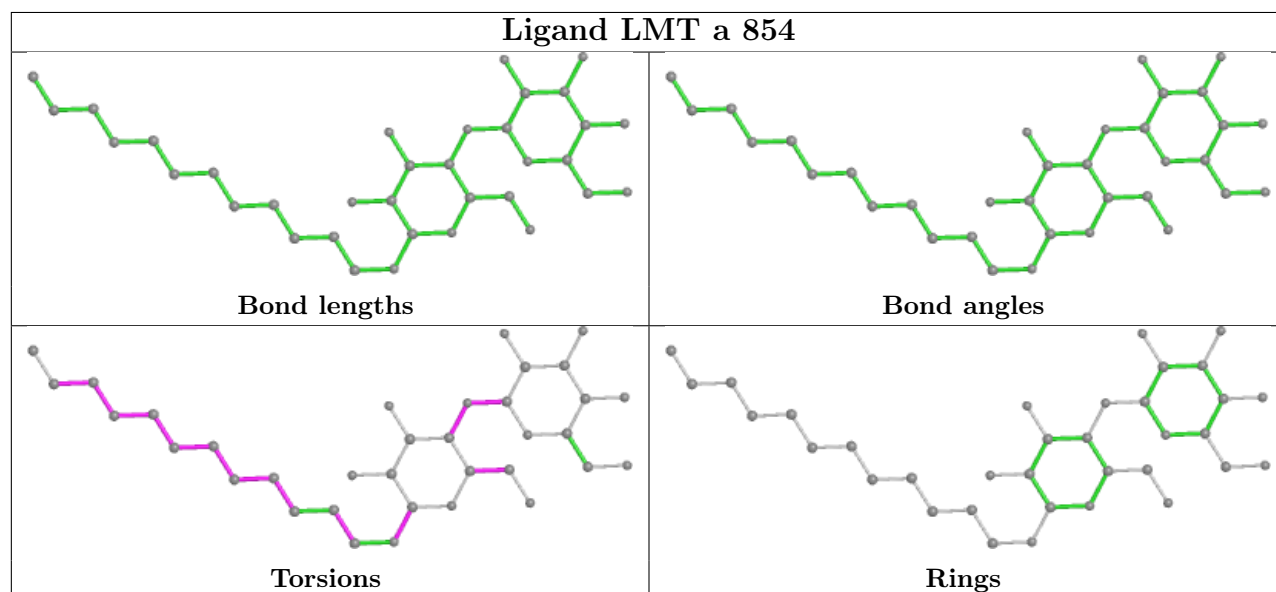


Rings

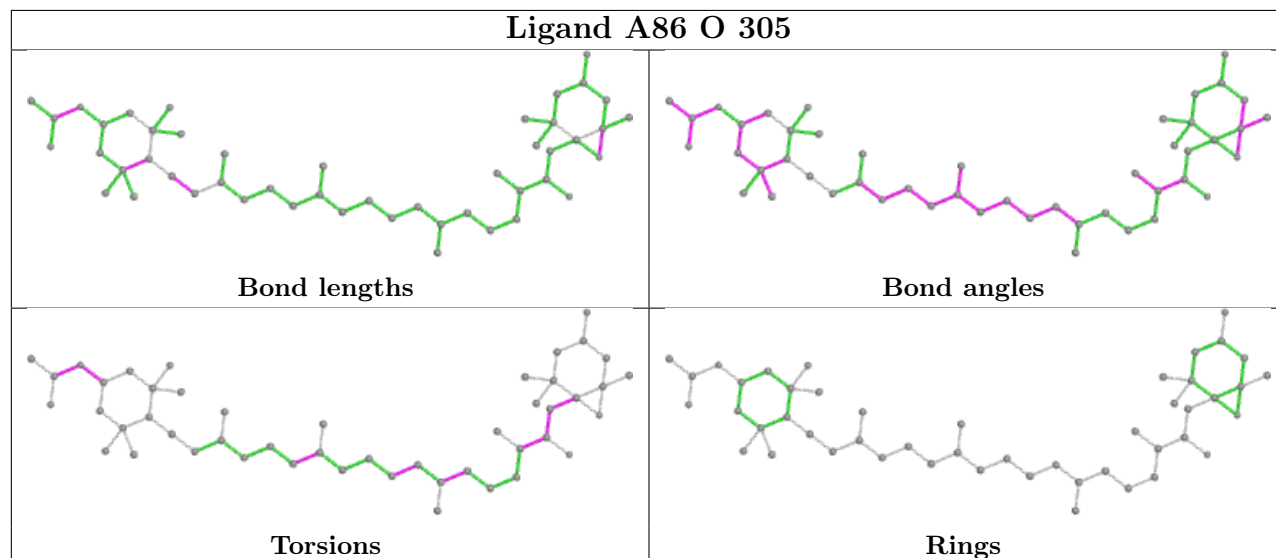
## Ligand CLA 1 205



## Ligand LMT a 854

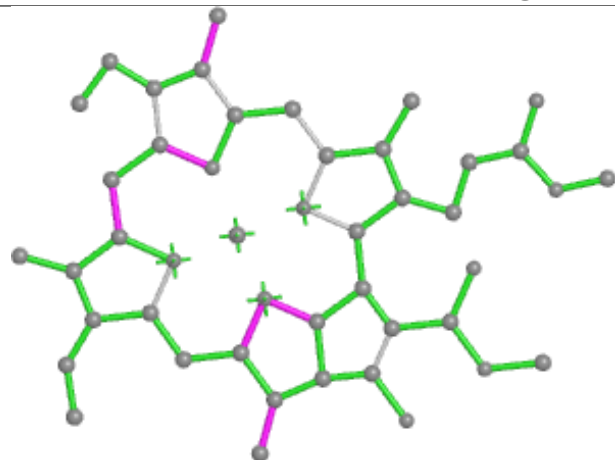


## Ligand A86 O 305

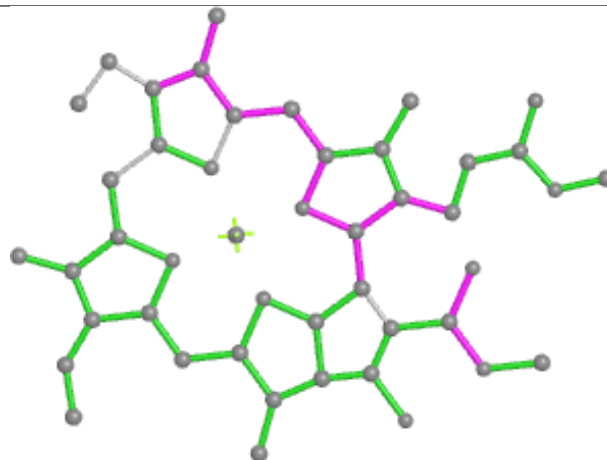




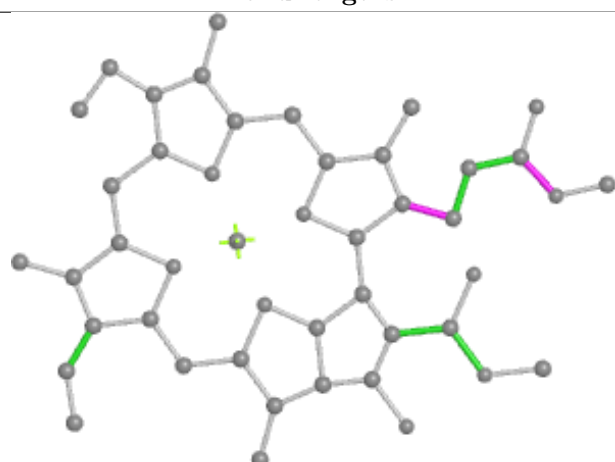
## Ligand CLA C 210



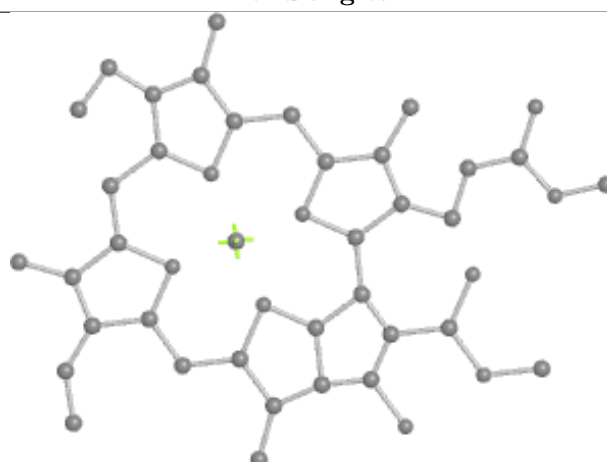
Bond lengths



Bond angles

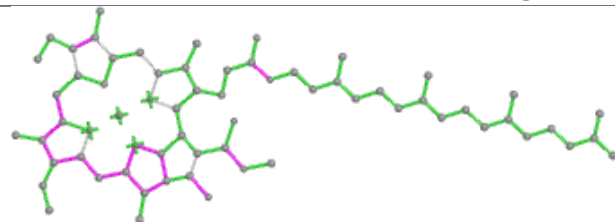


Torsions

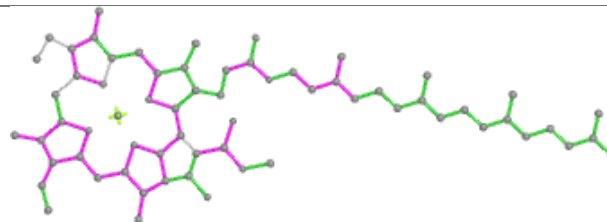


Rings

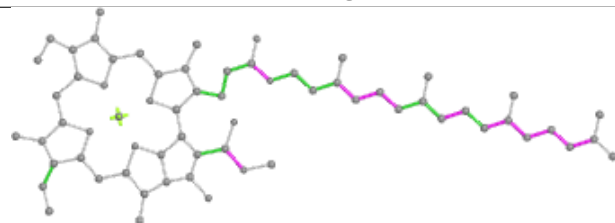
## Ligand CLA E 315



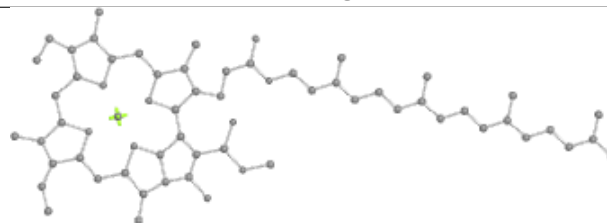
Bond lengths



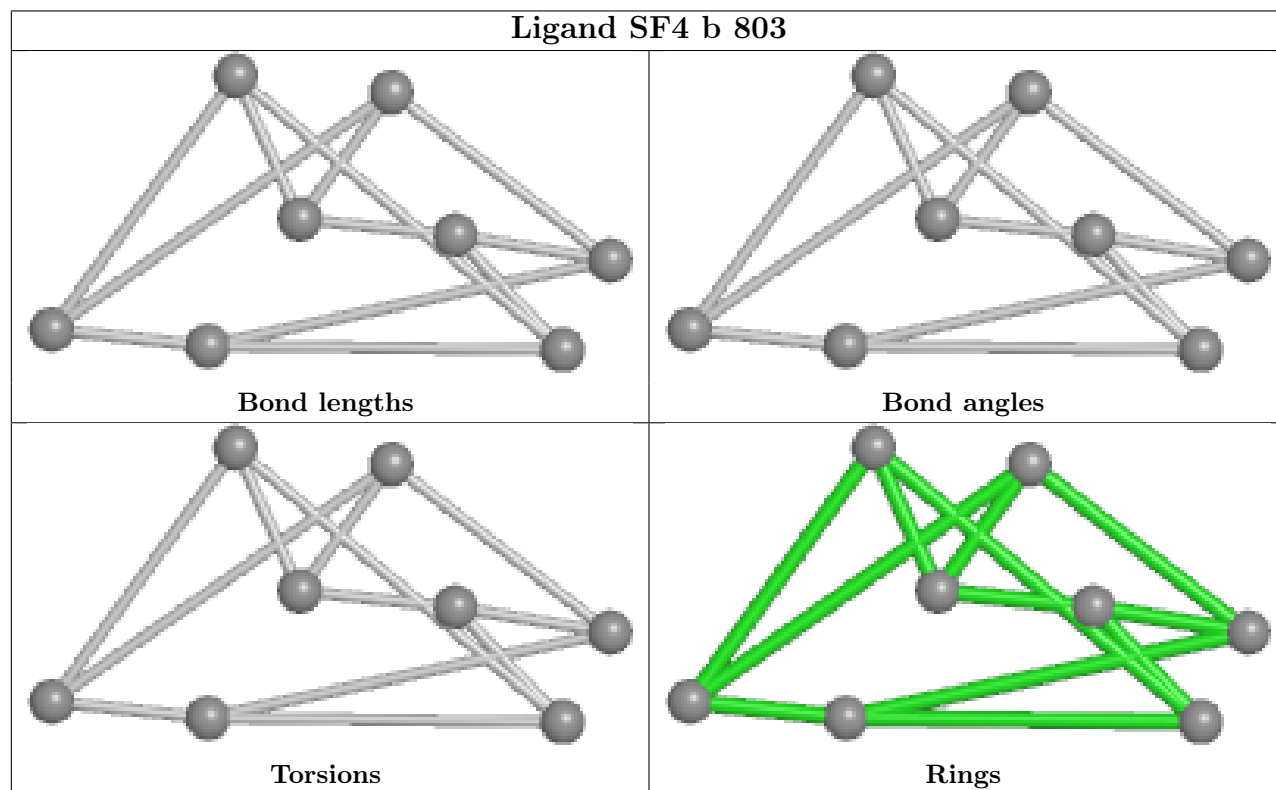
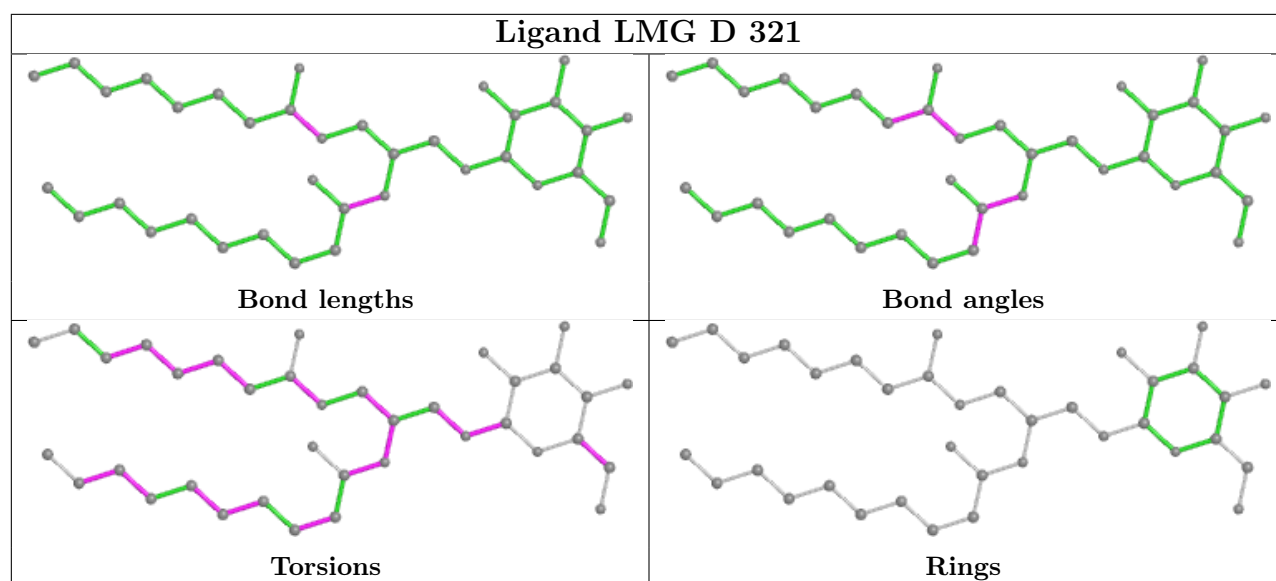
Bond angles



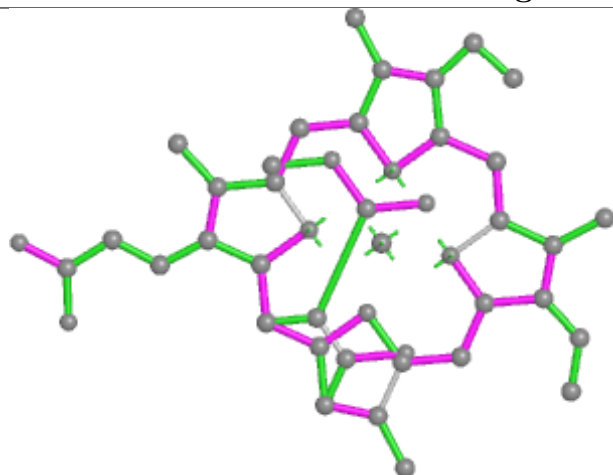
Torsions



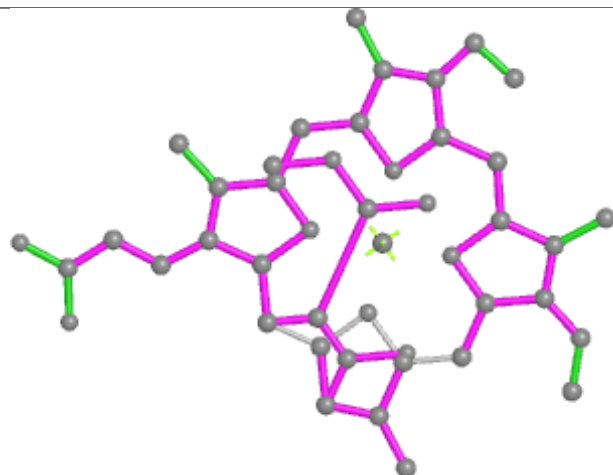
Rings



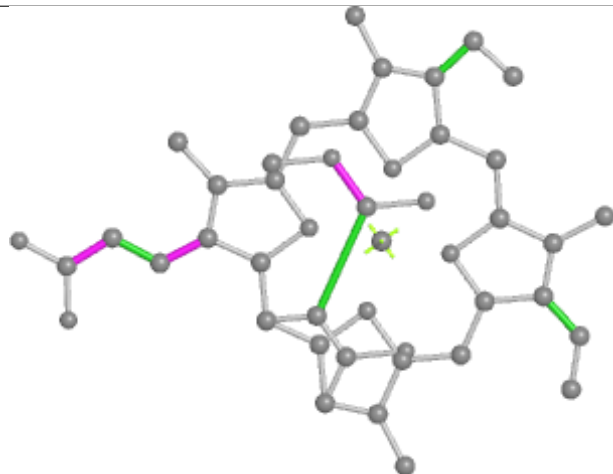
## Ligand KC1 G 317



Bond lengths



Bond angles

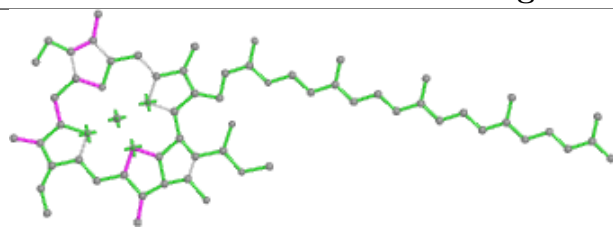


Torsions

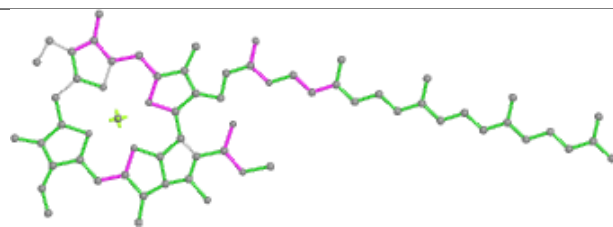


Rings

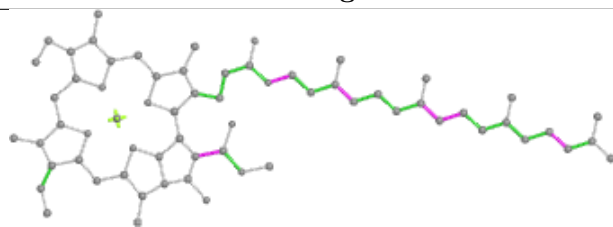
## Ligand CLA b 802



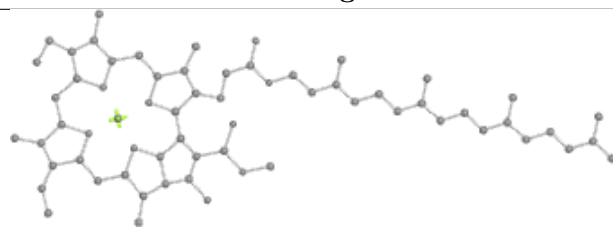
Bond lengths



Bond angles

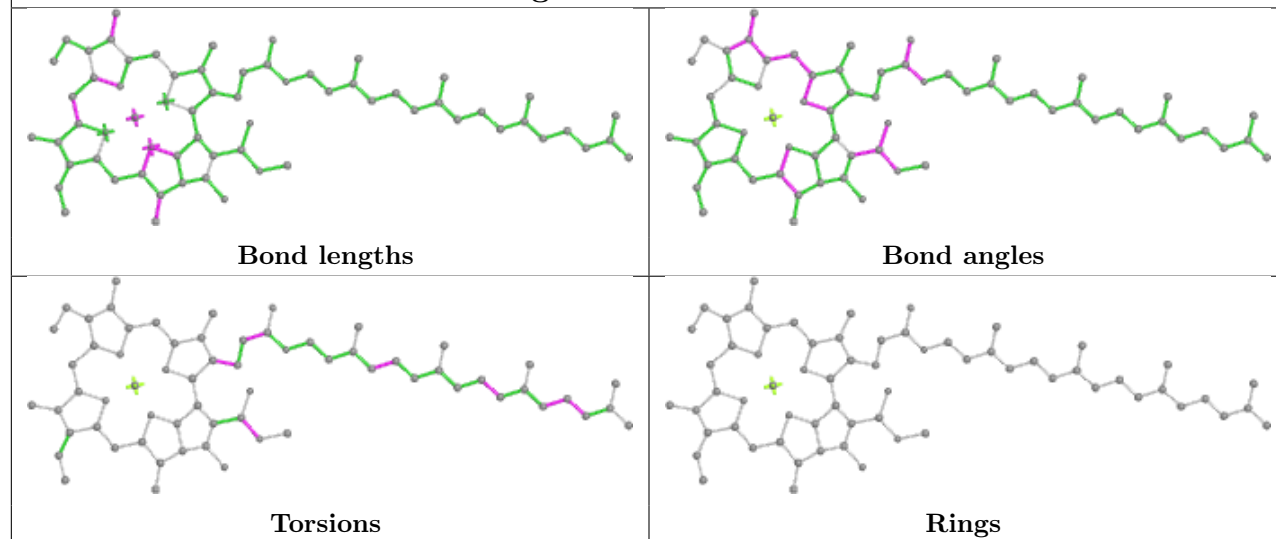


Torsions

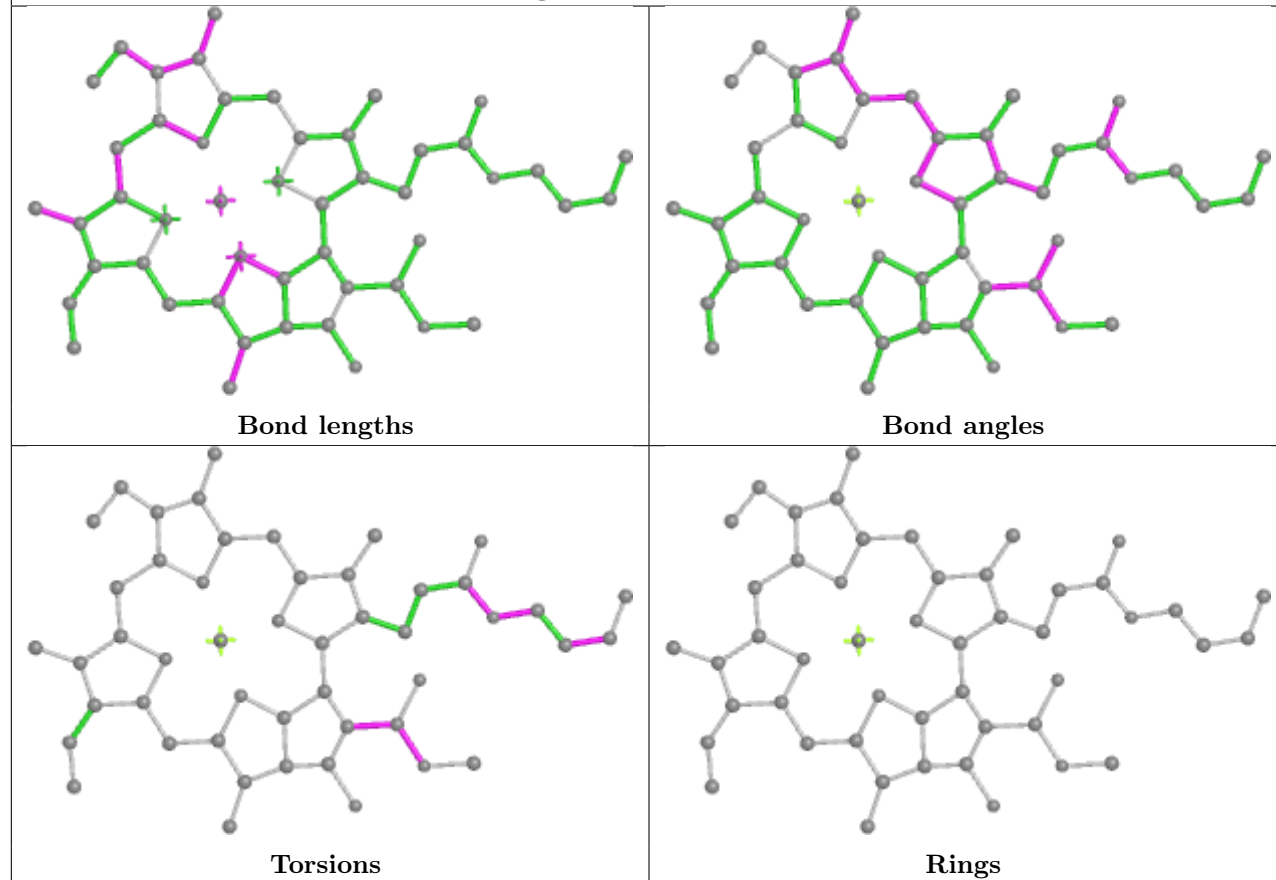


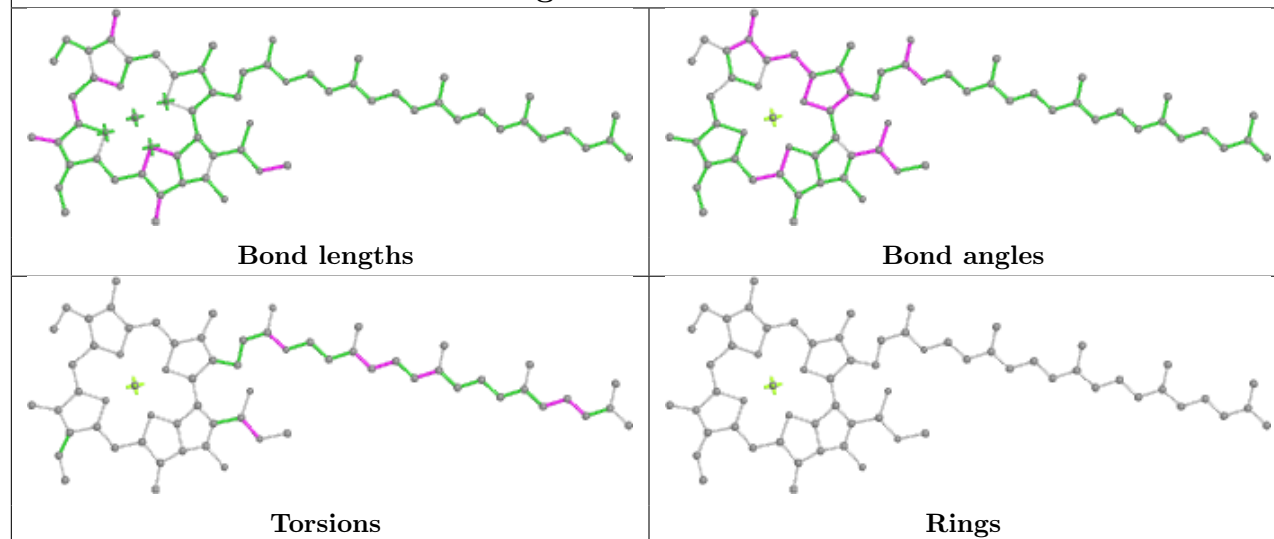
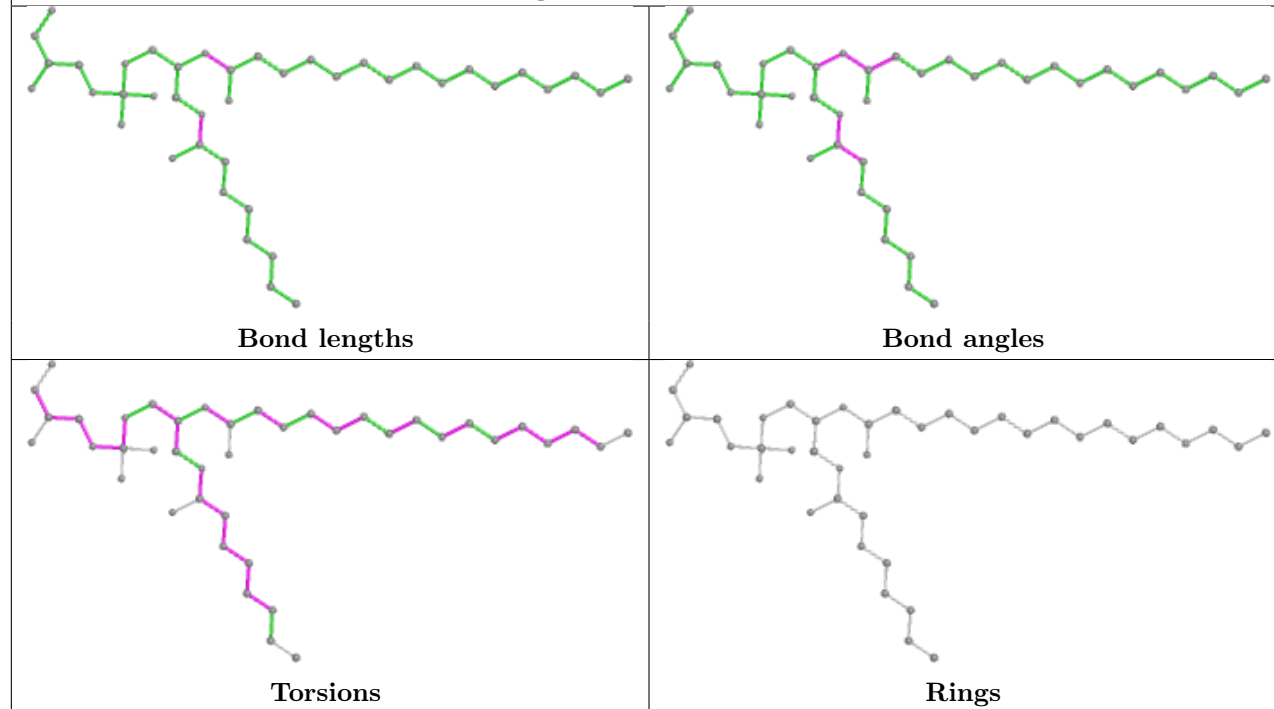
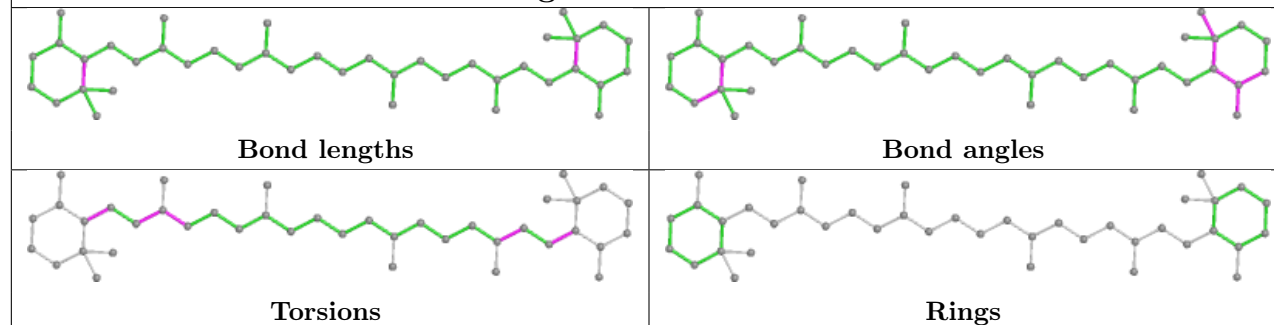
Rings

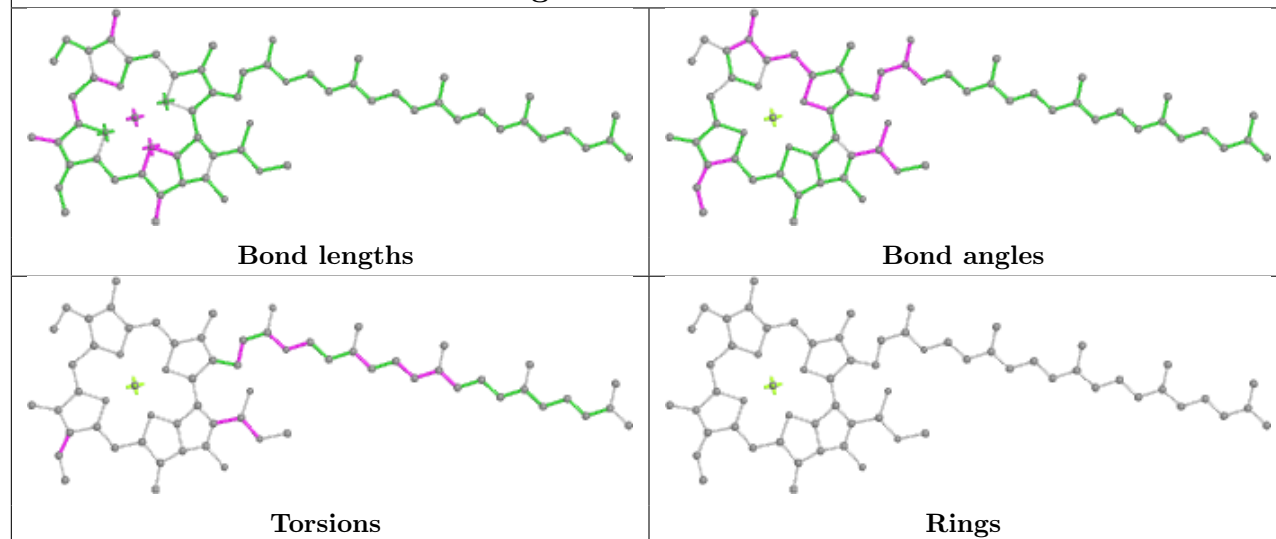
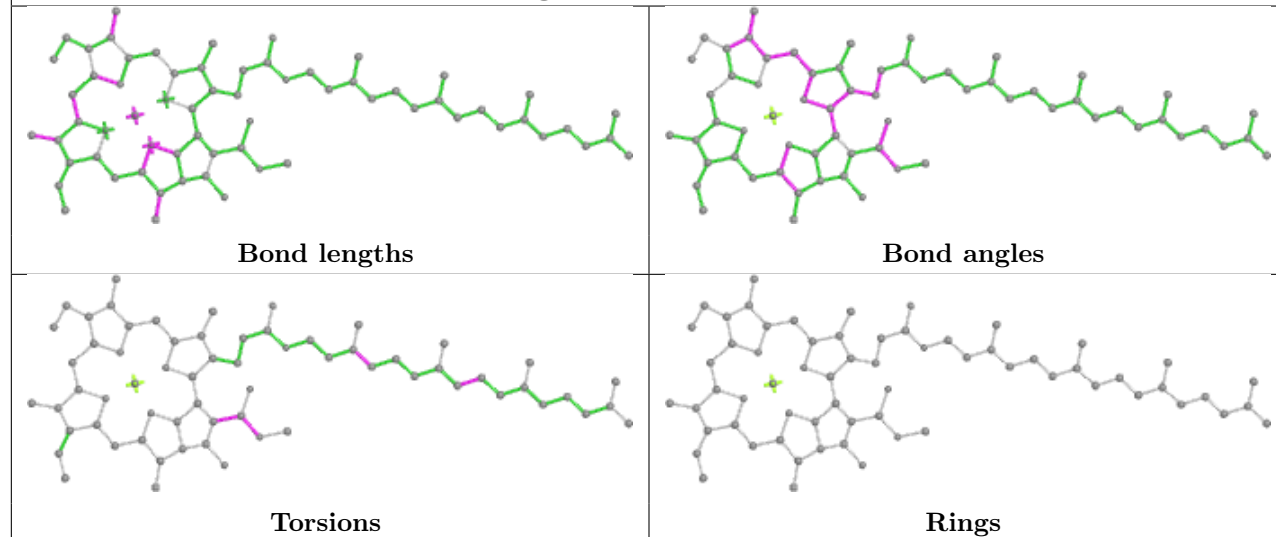
## Ligand CLA R 321



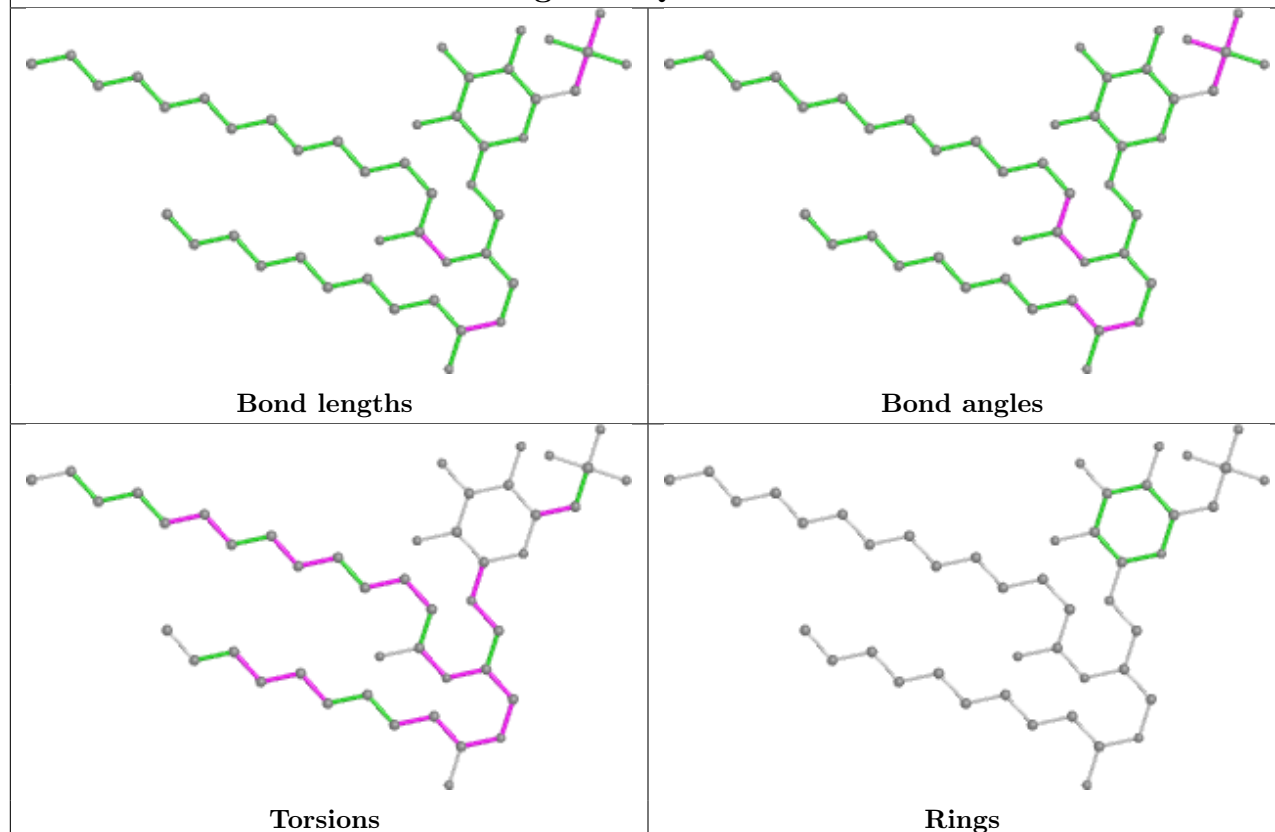
## Ligand CLA E 308



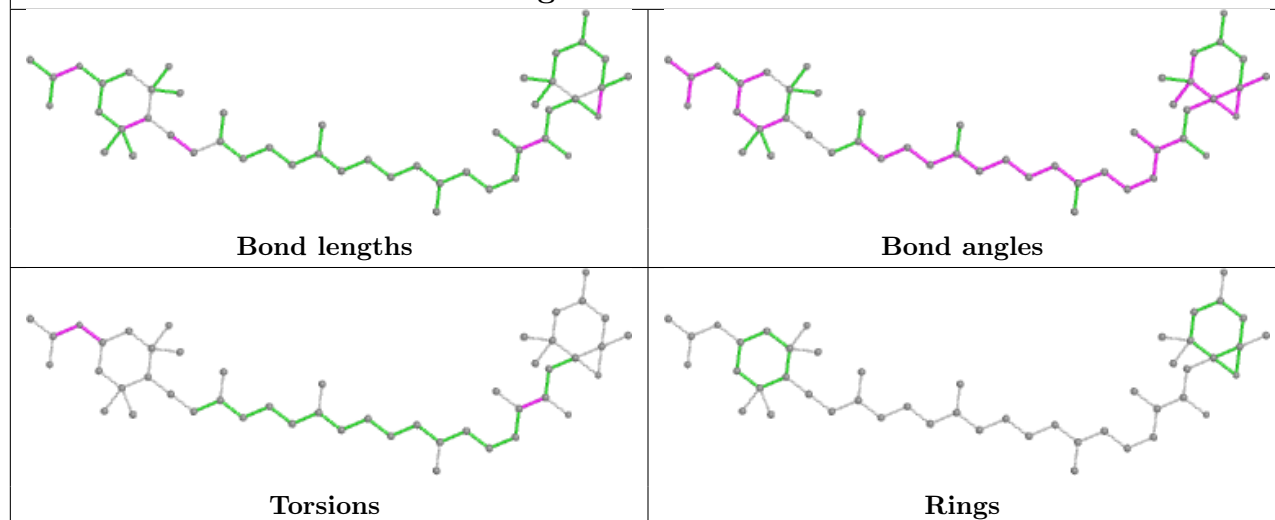
**Ligand CLA a 836****Ligand LHG F 319****Ligand BCR f 801**

**Ligand CLA D 308****Ligand CLA S 319**

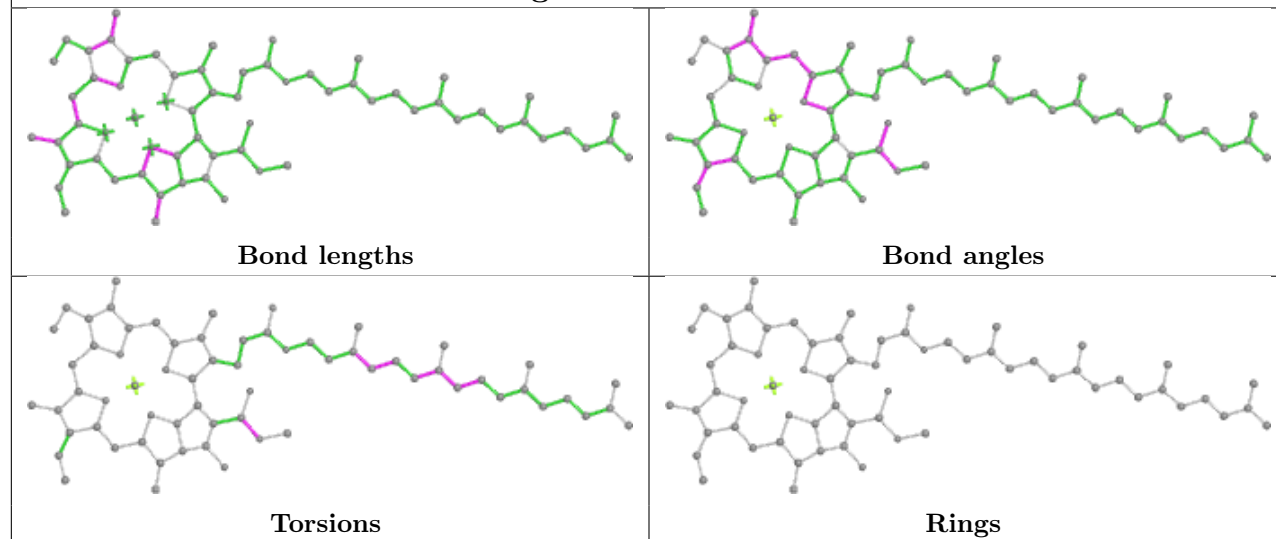
## Ligand SQD b 804



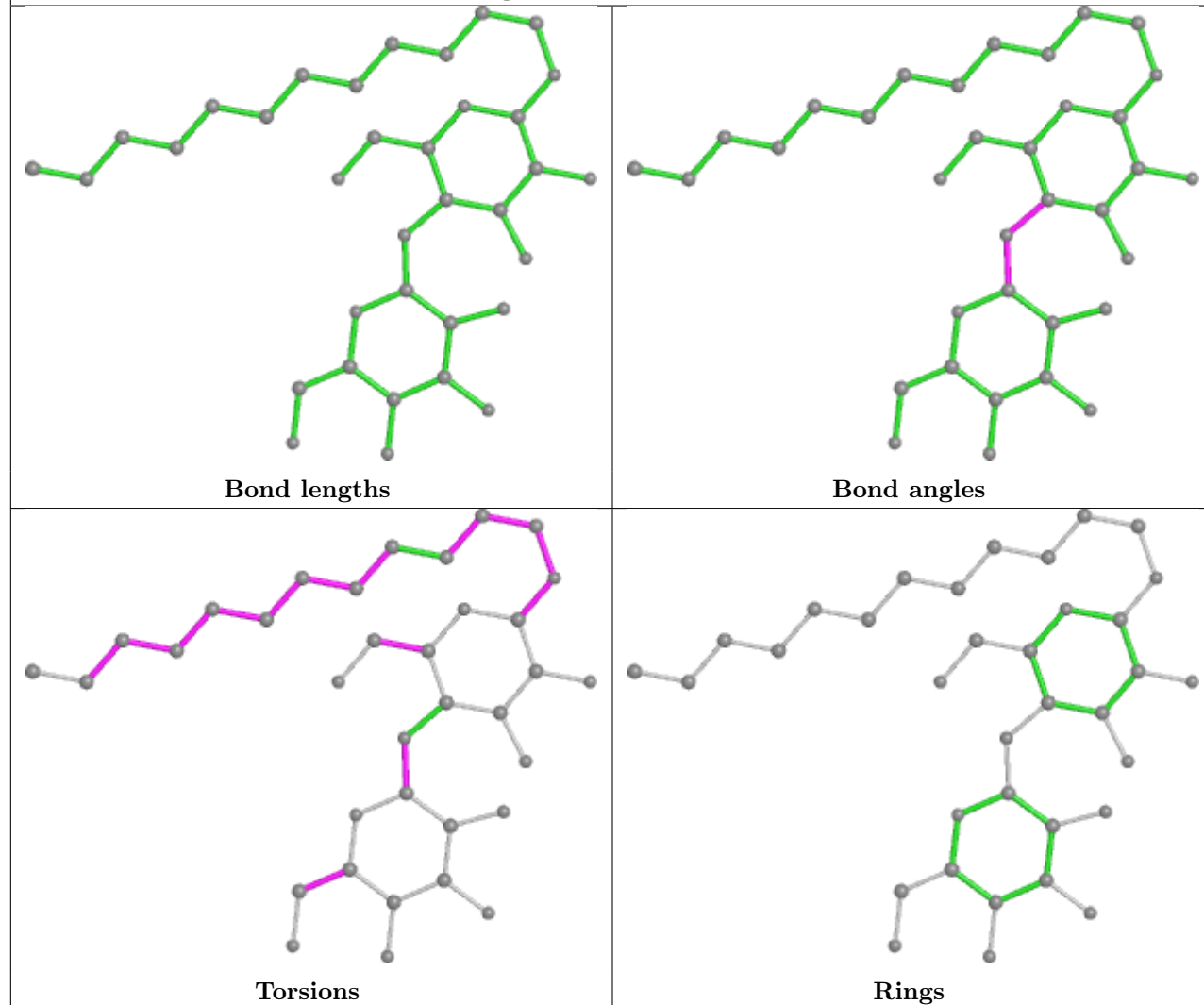
## Ligand A86 P 304



## Ligand CLA H 317

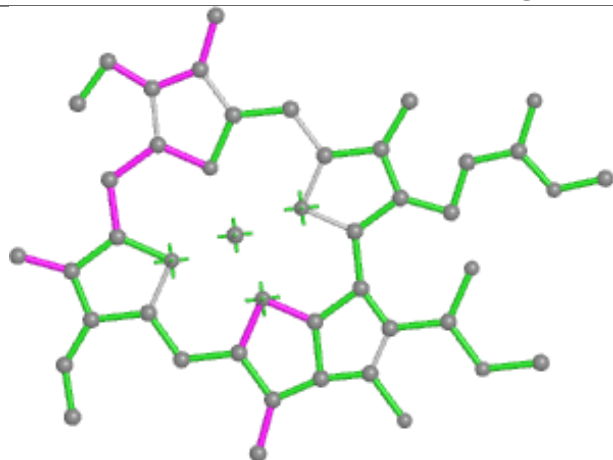


## Ligand LMT U 315

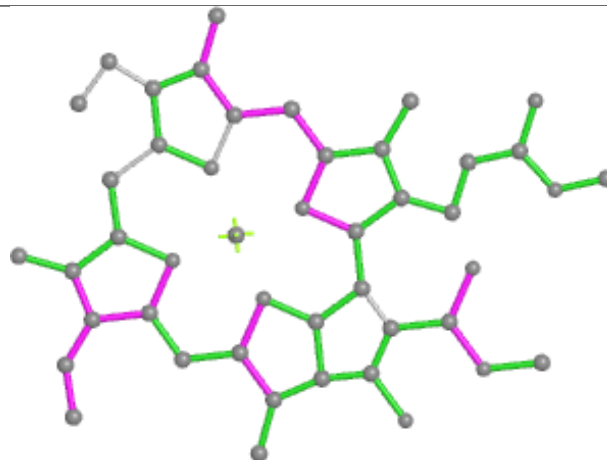




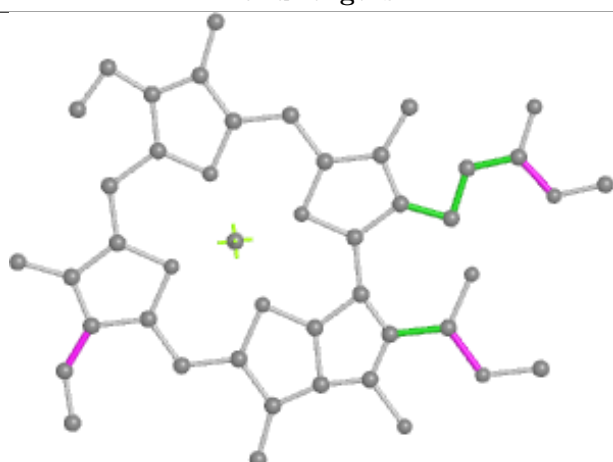
## Ligand CLA J 316



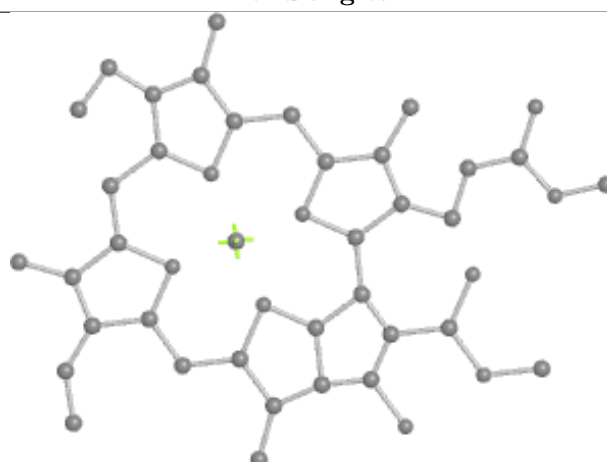
Bond lengths



Bond angles

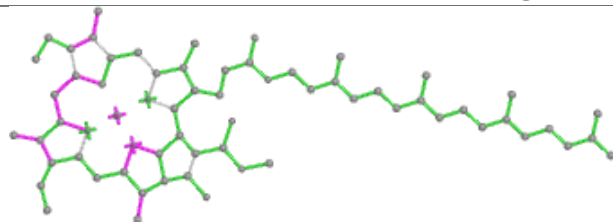


Torsions

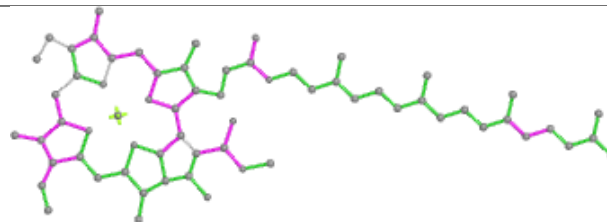


Rings

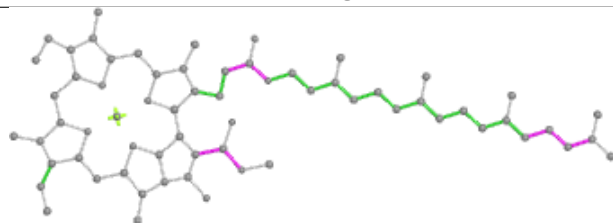
## Ligand CLA b 841



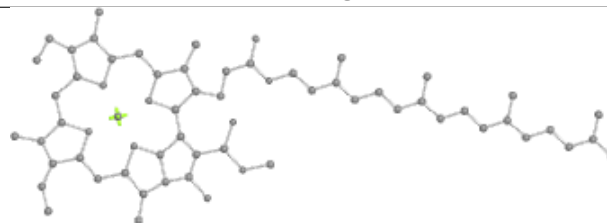
Bond lengths



Bond angles

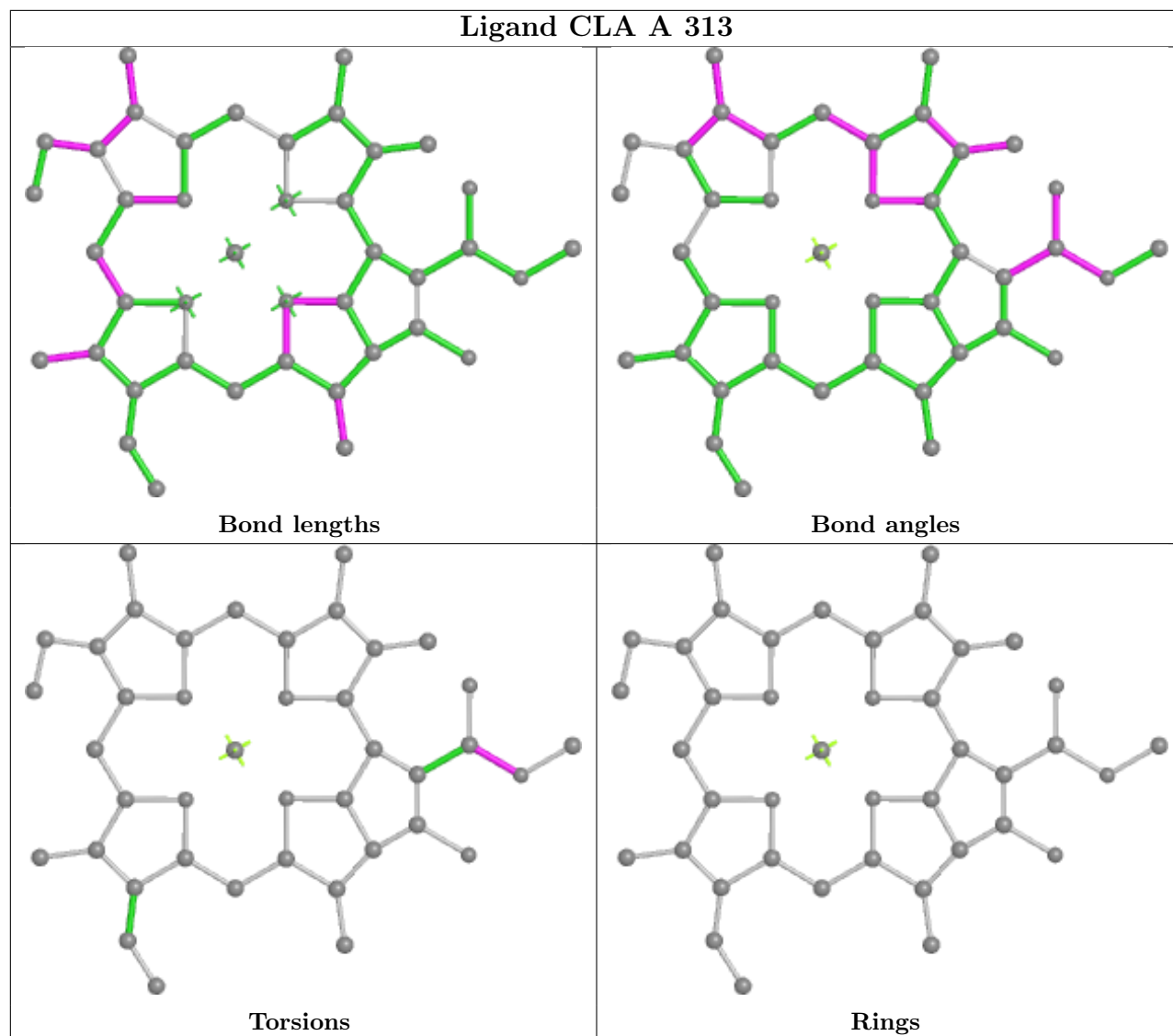


Torsions

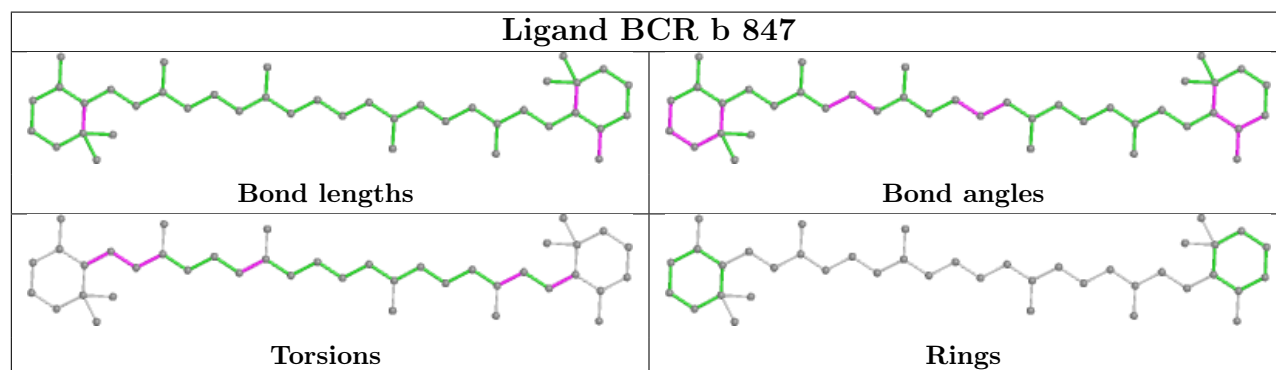


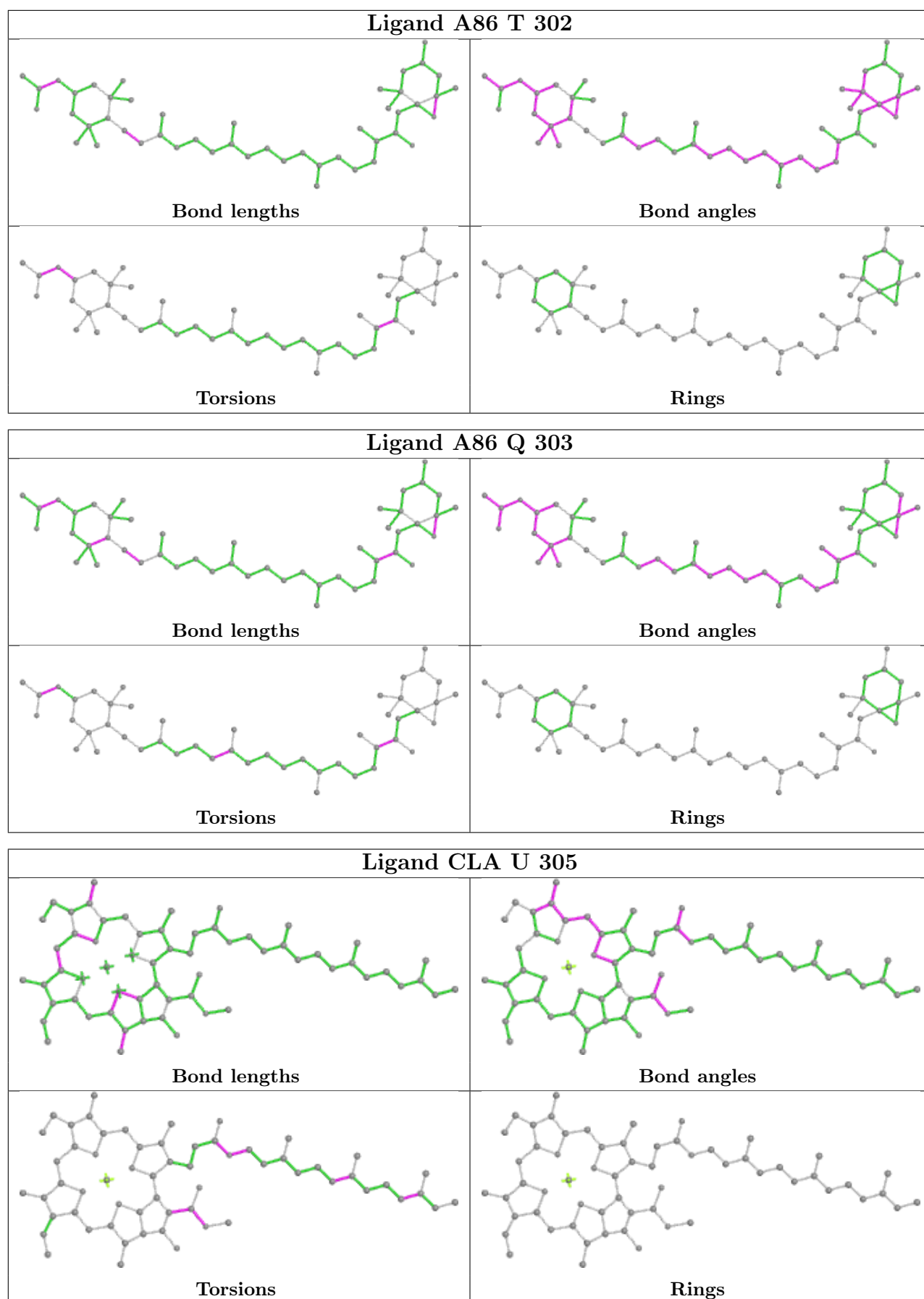
Rings

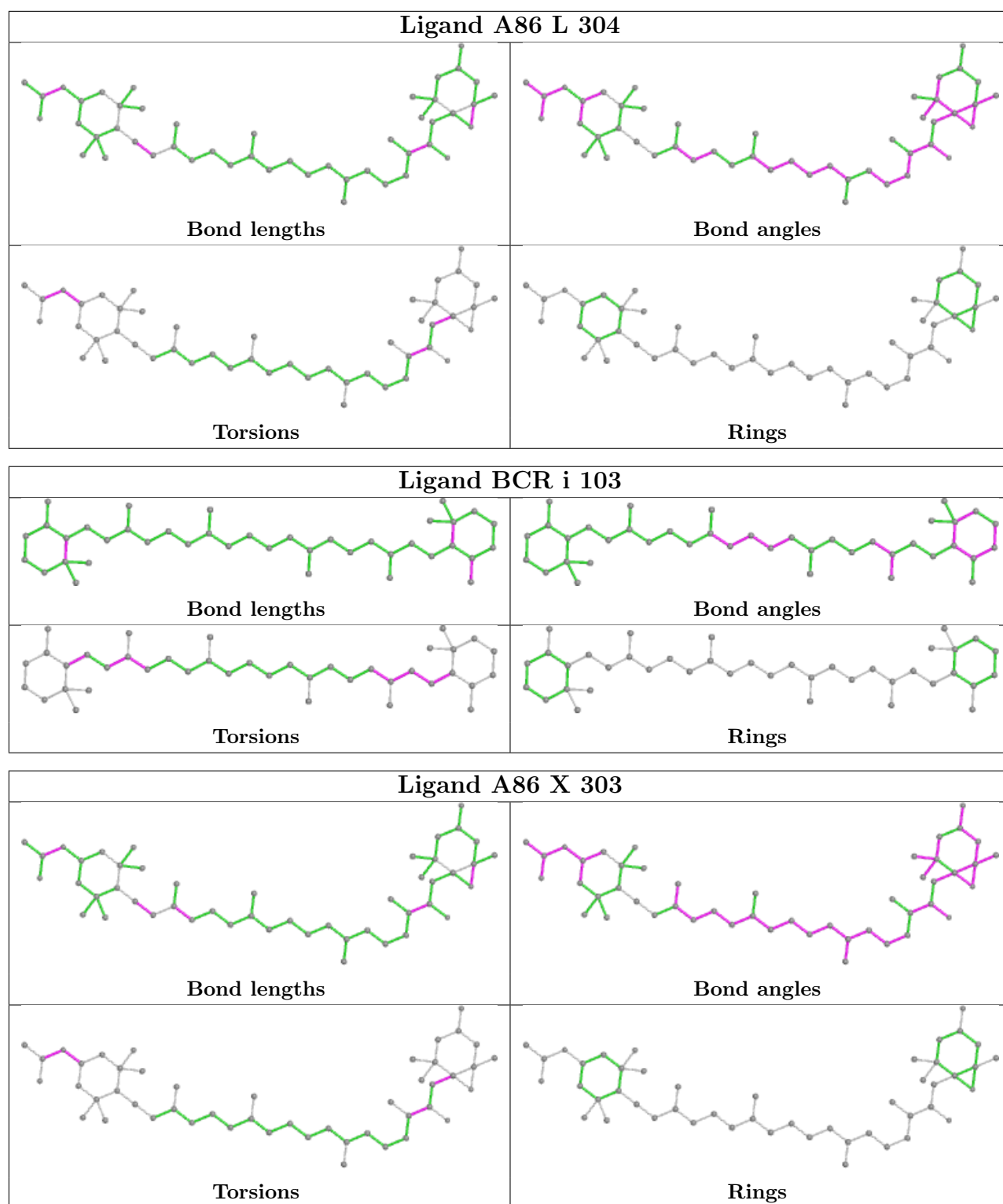
## Ligand CLA A 313

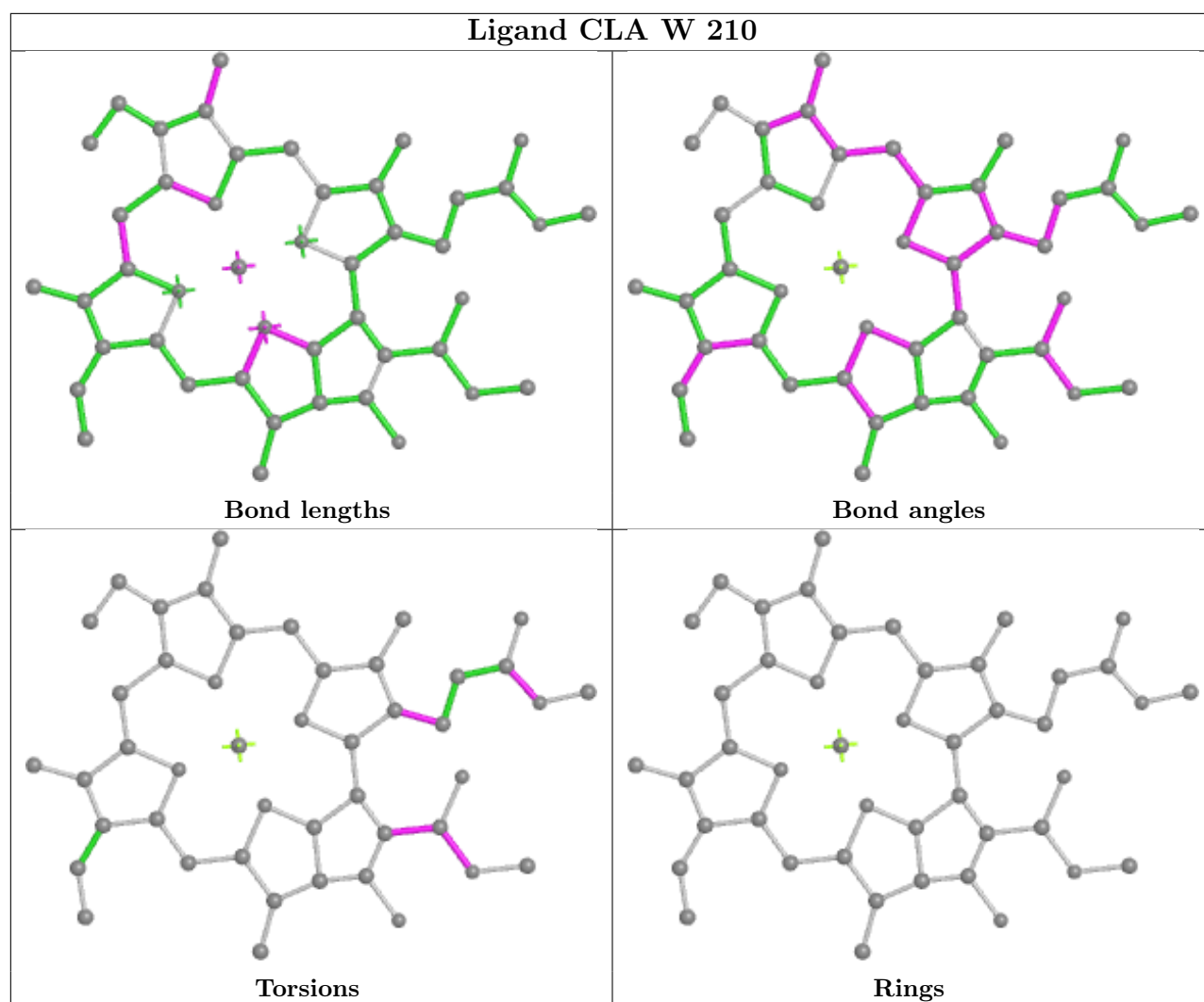


## Ligand BCR b 847

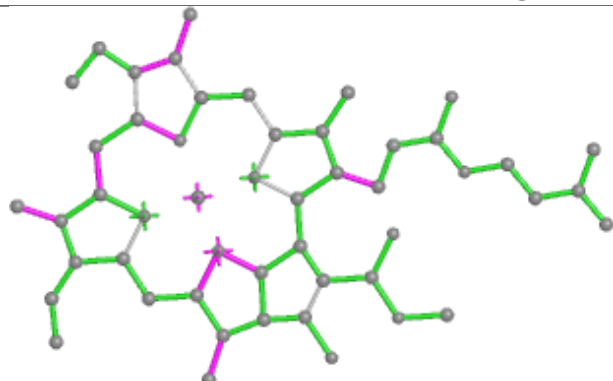




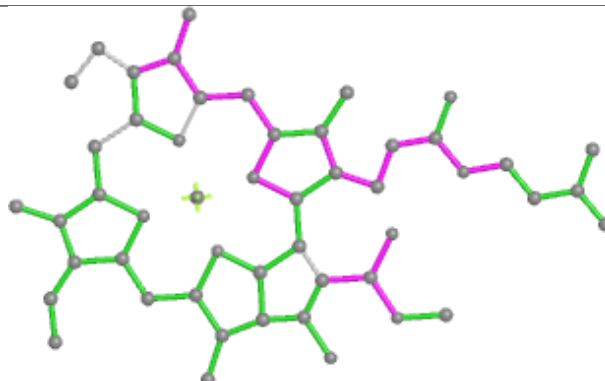




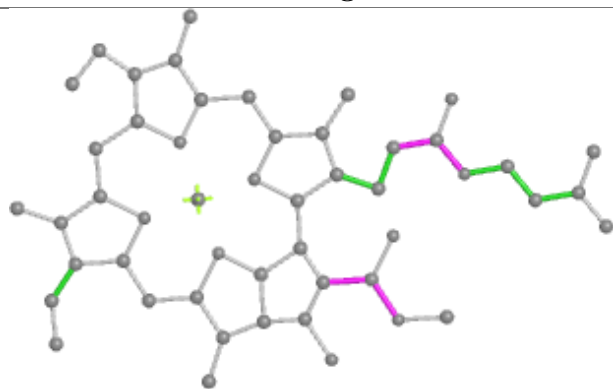
## Ligand CLA H 318



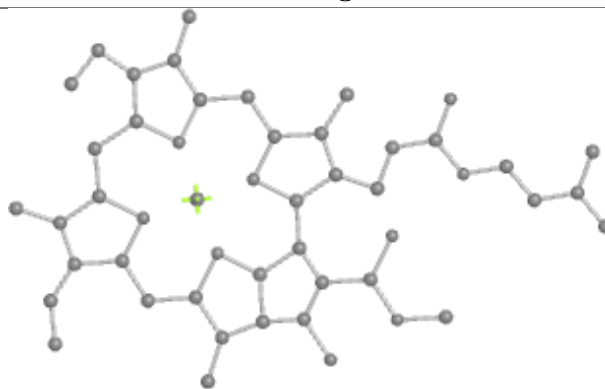
Bond lengths



Bond angles

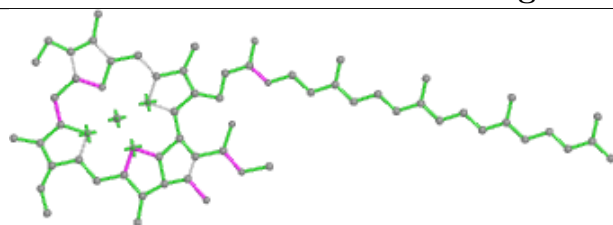


Torsions

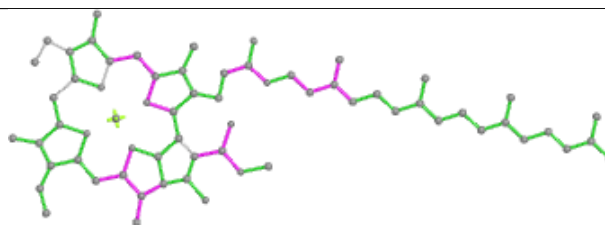


Rings

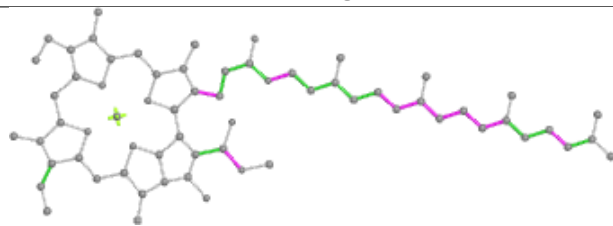
## Ligand CLA a 825



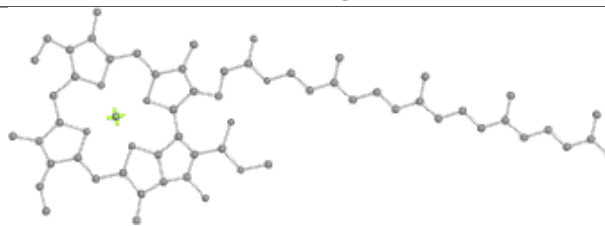
Bond lengths



Bond angles

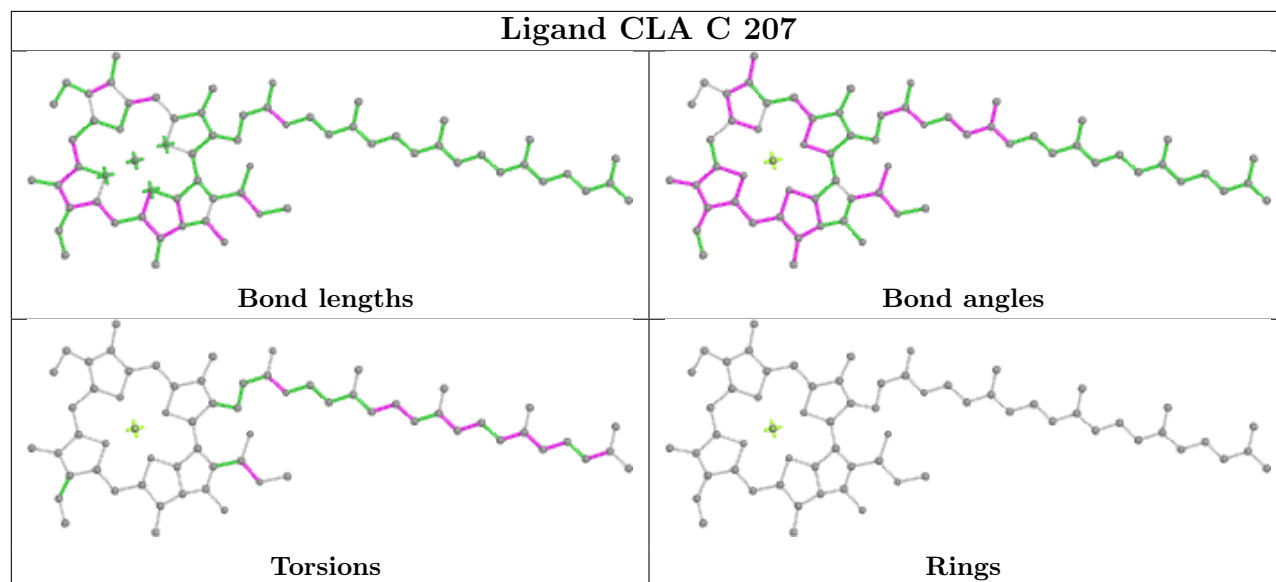


Torsions

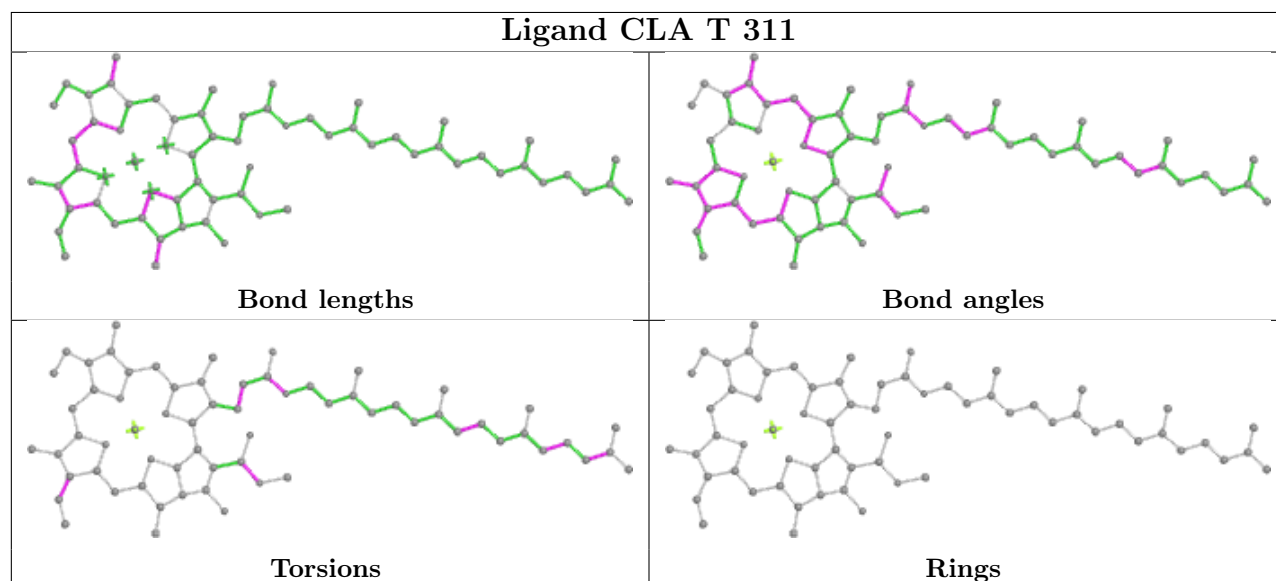


Rings

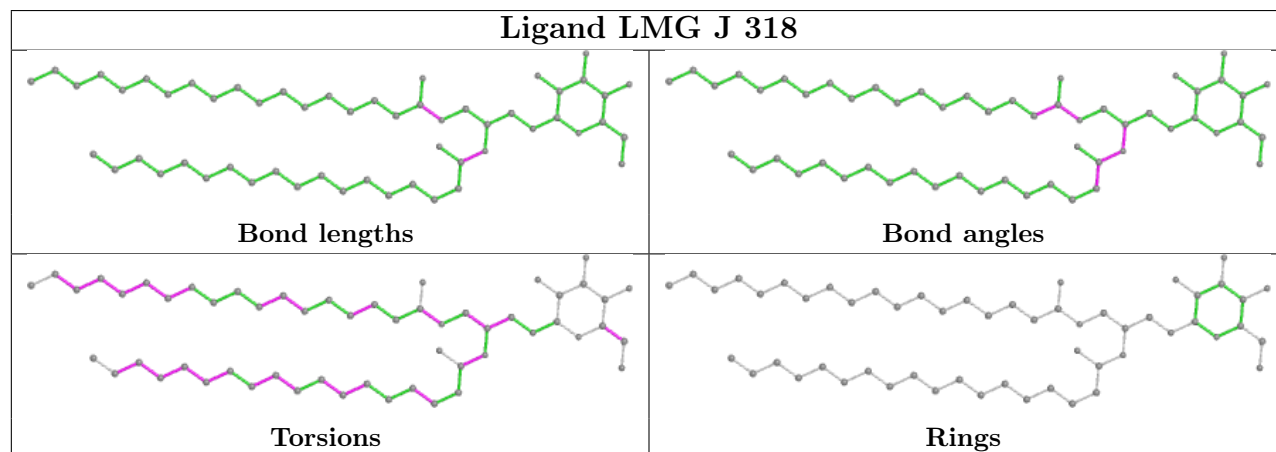
## Ligand CLA C 207

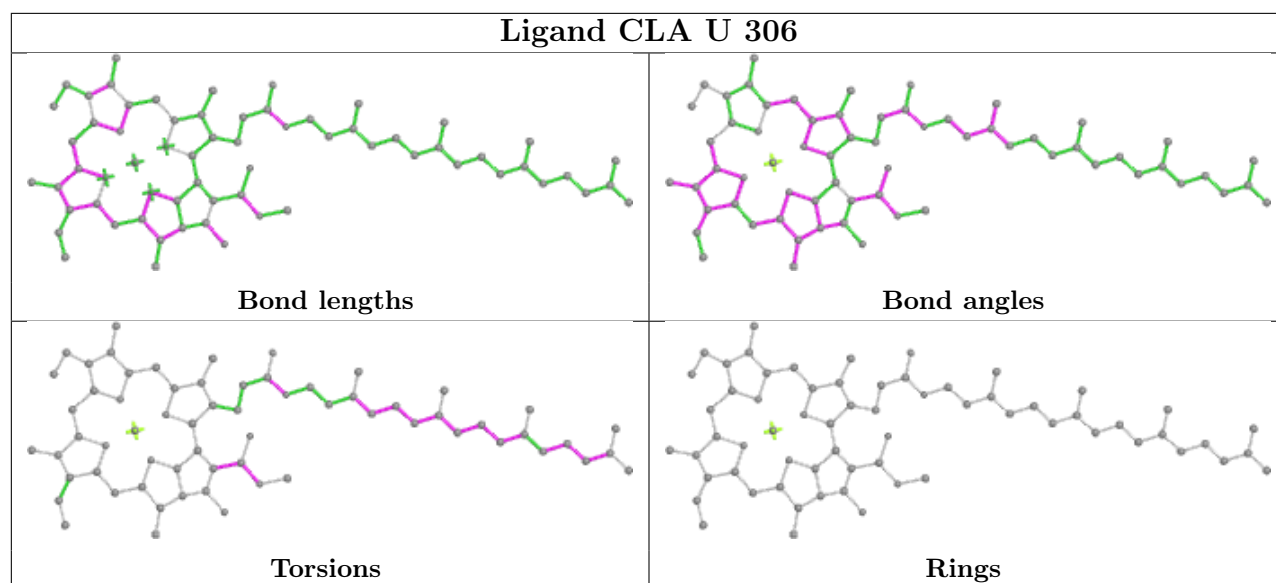
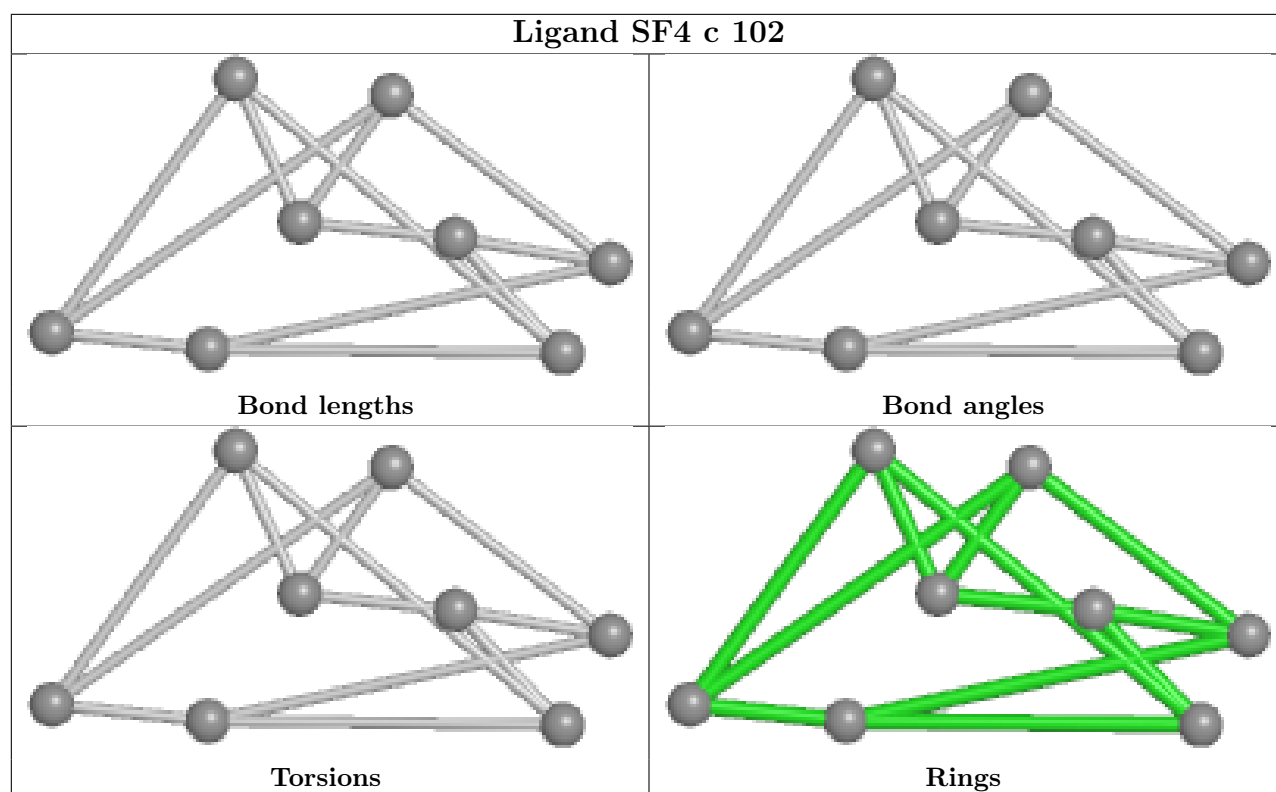


## Ligand CLA T 311



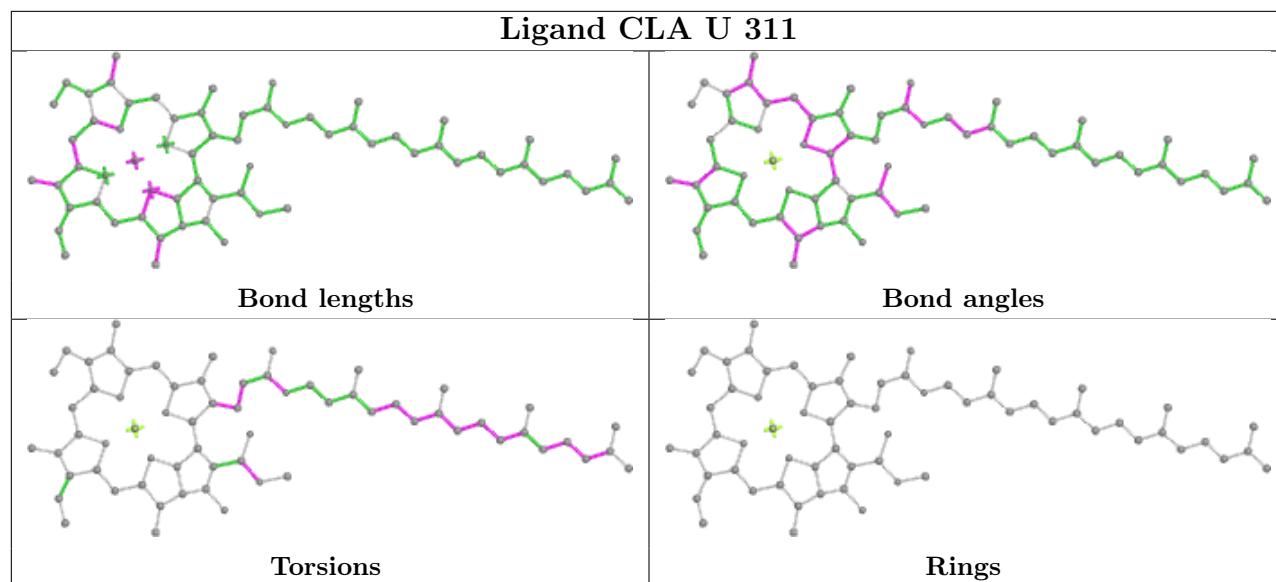
## Ligand LMG J 318



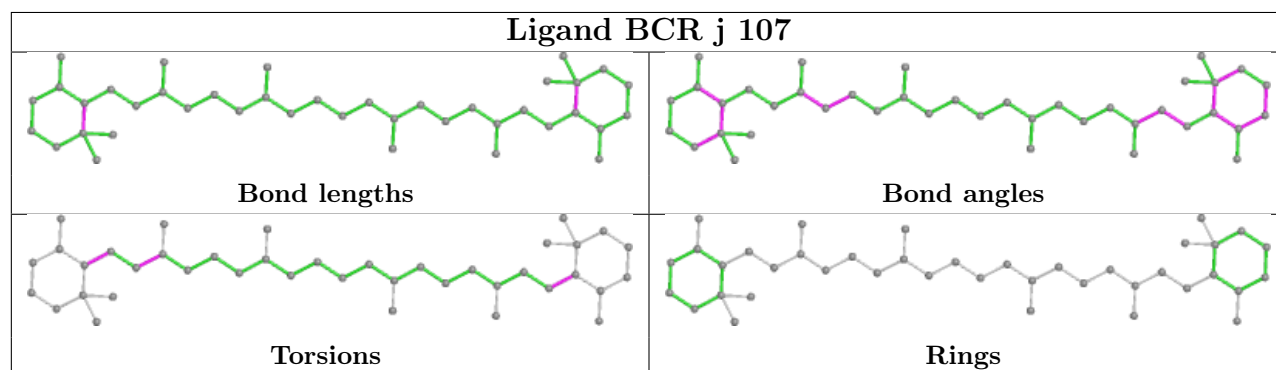




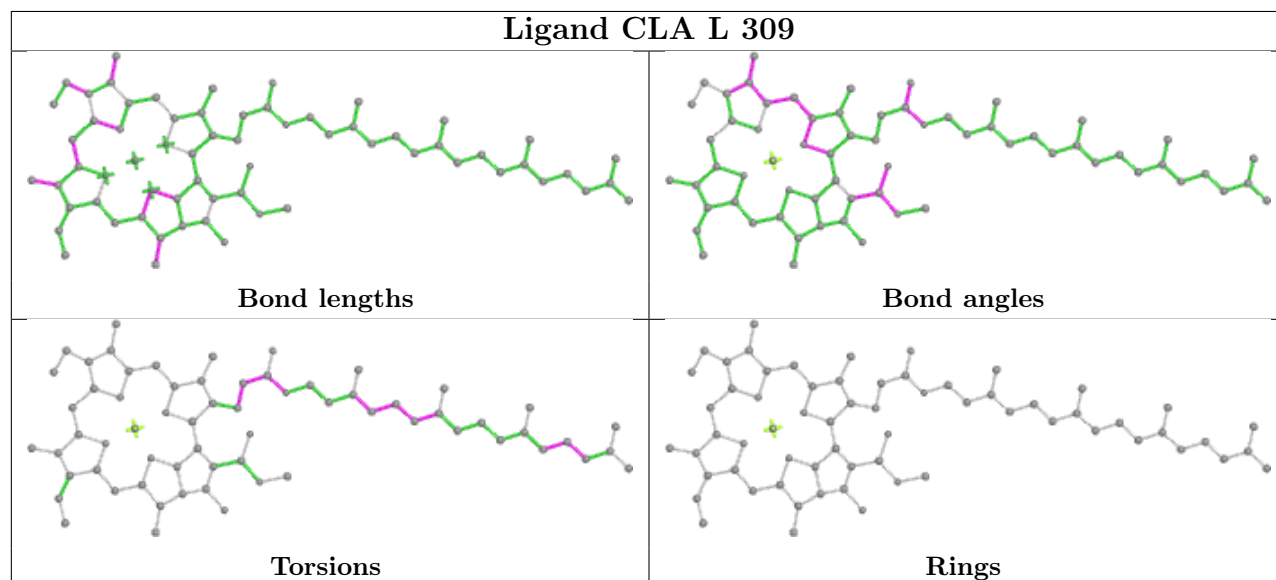
## Ligand CLA U 311

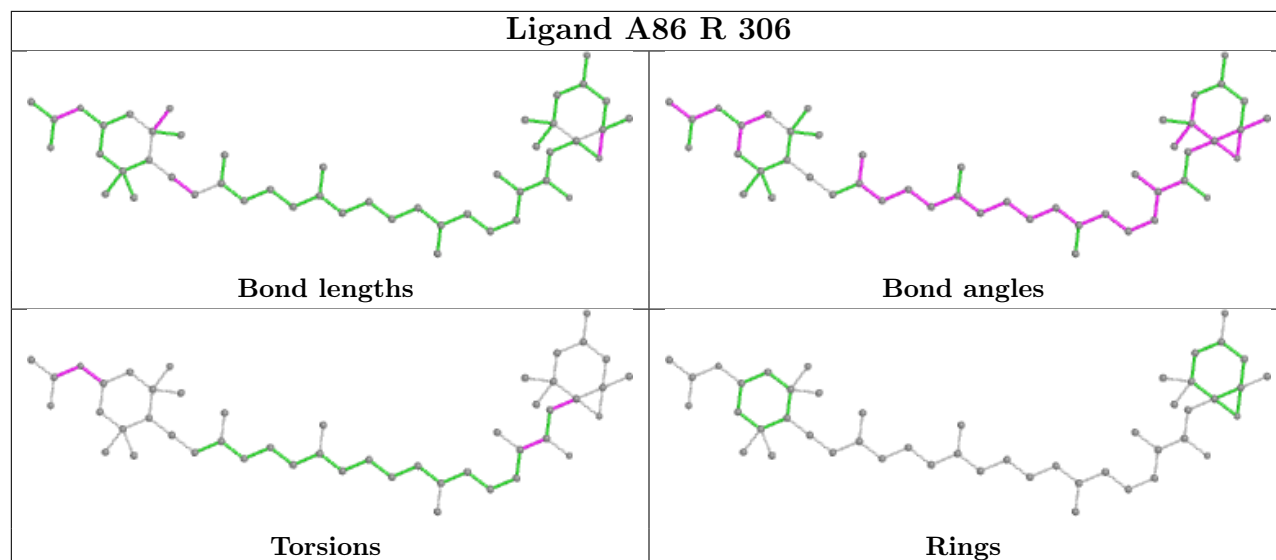
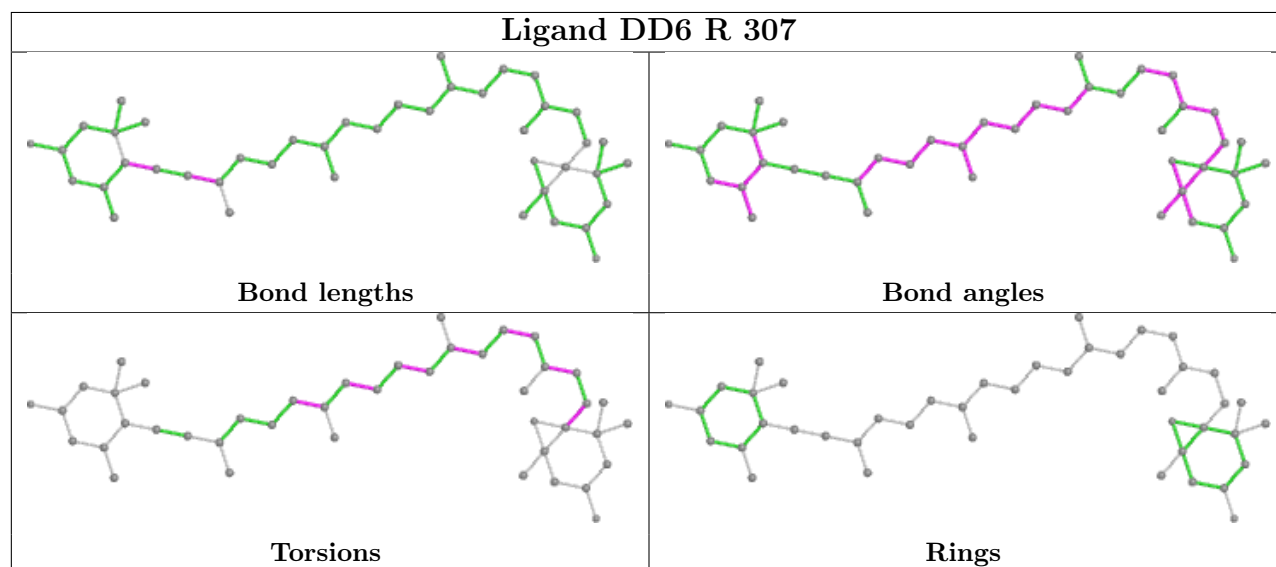
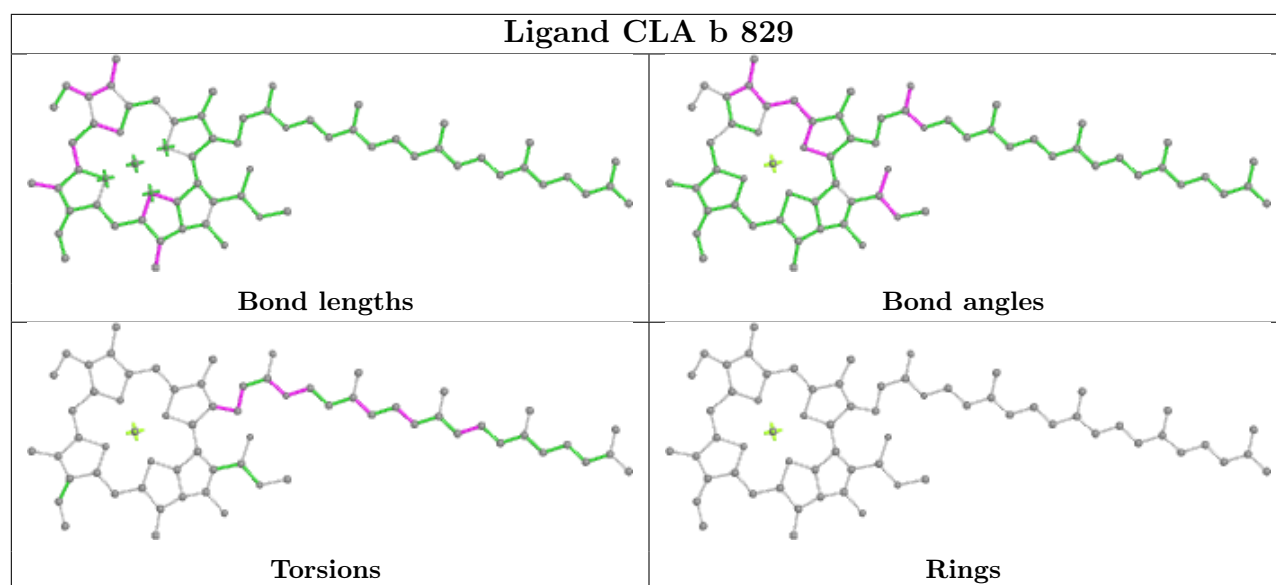


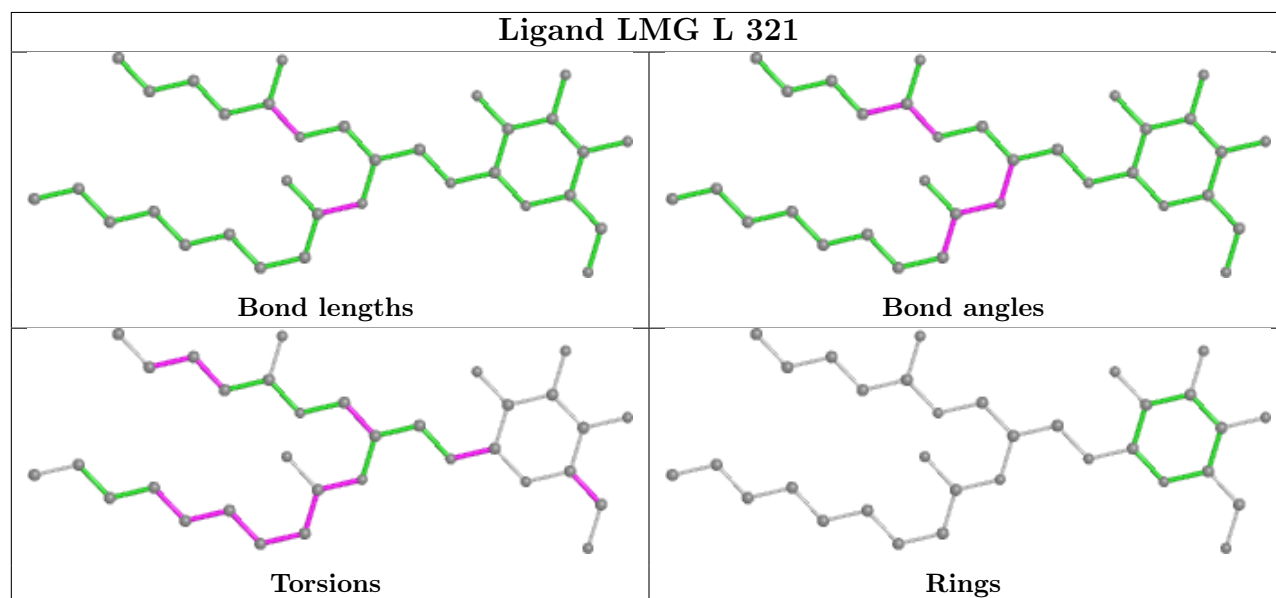
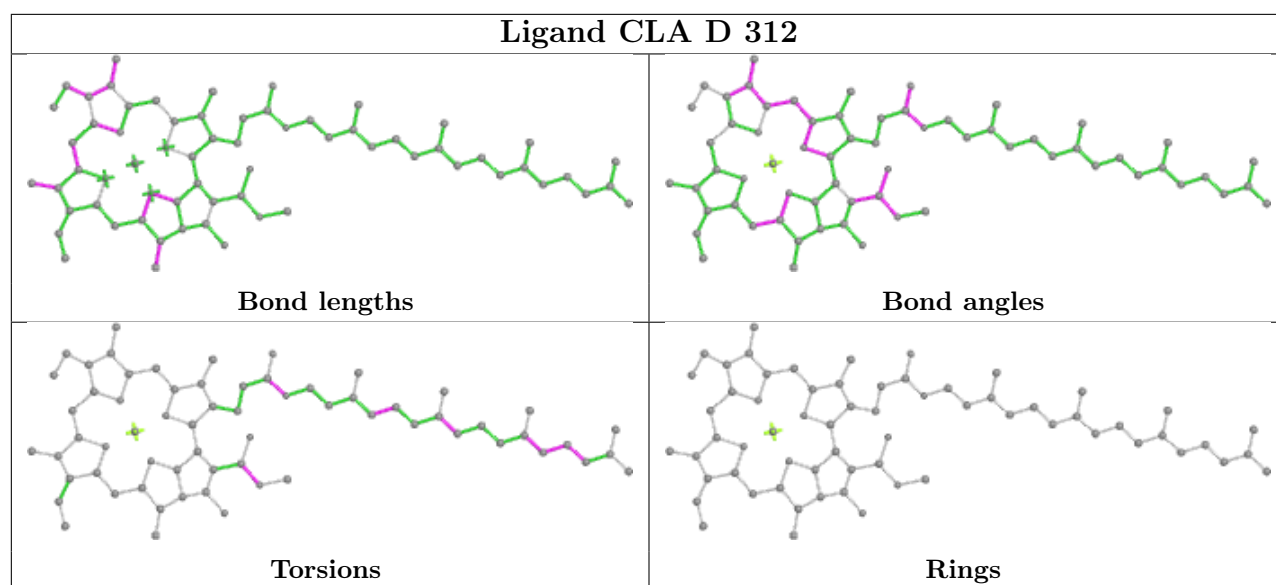
## Ligand BCR j 107

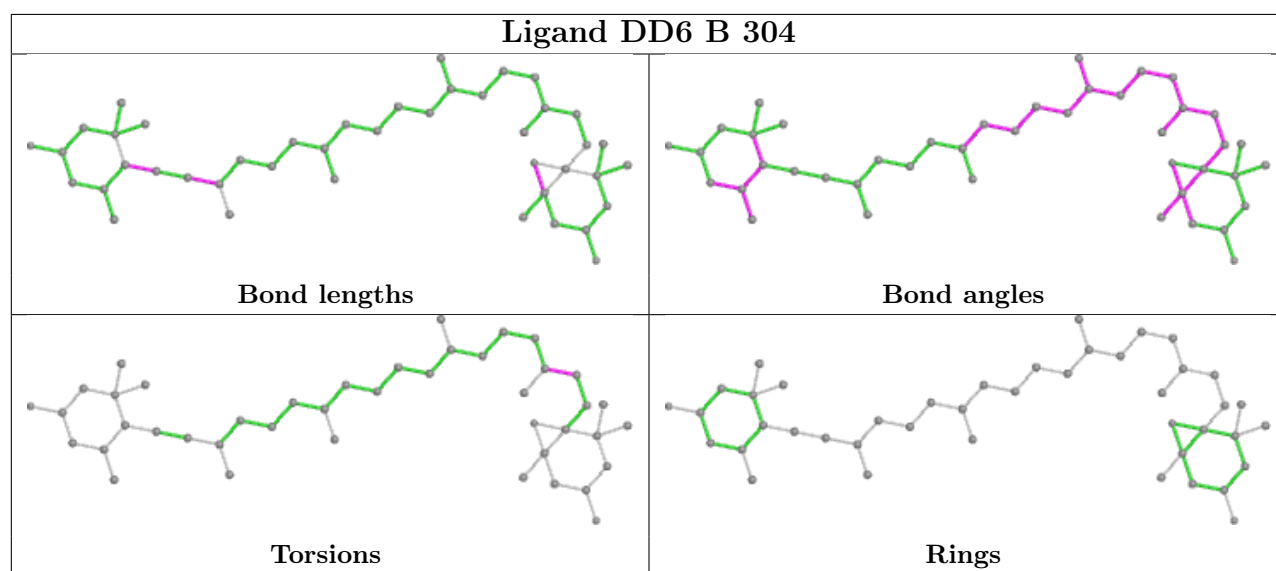
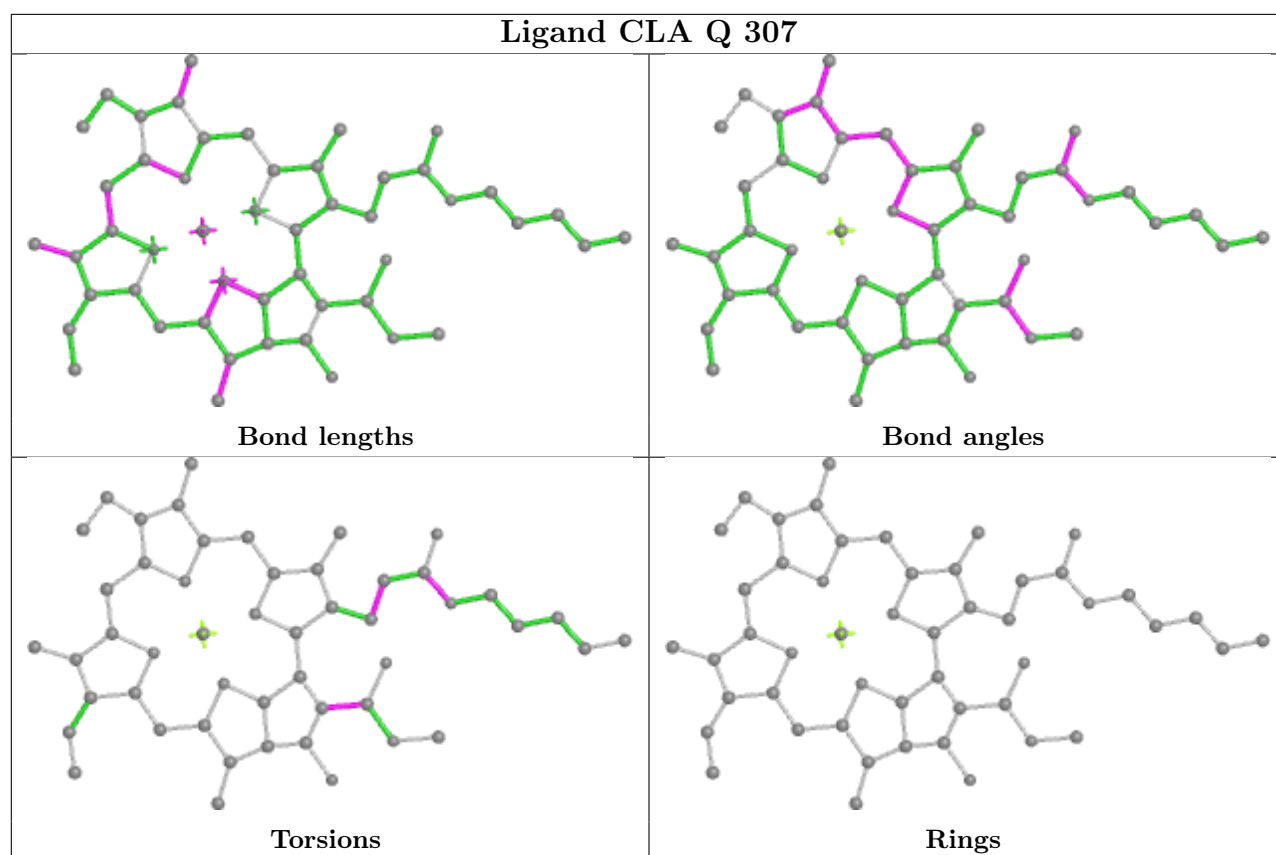


## Ligand CLA L 309

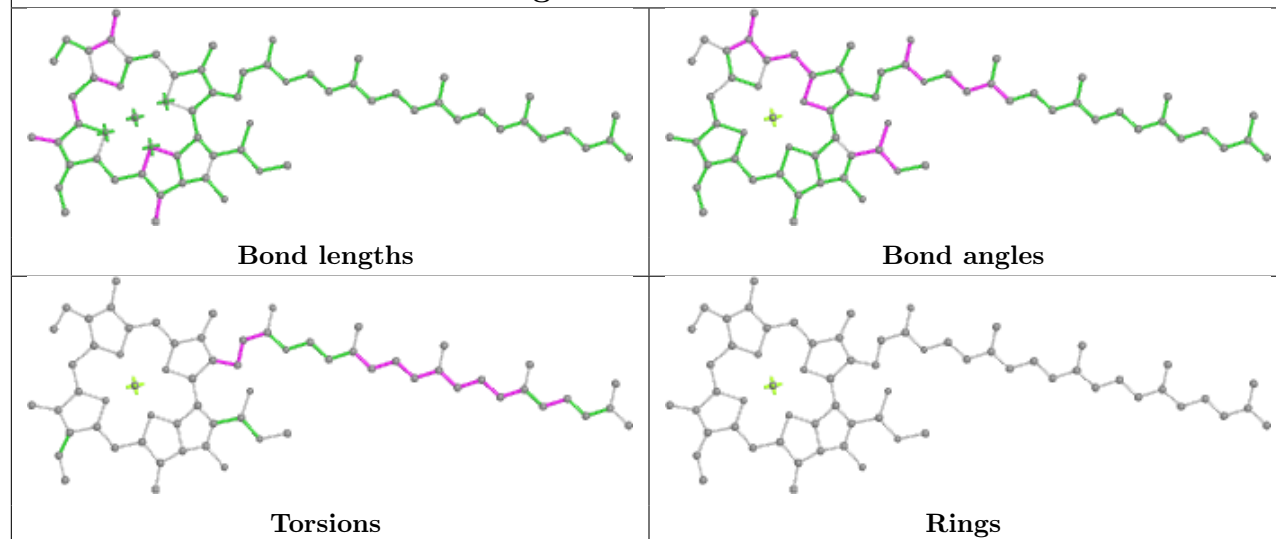




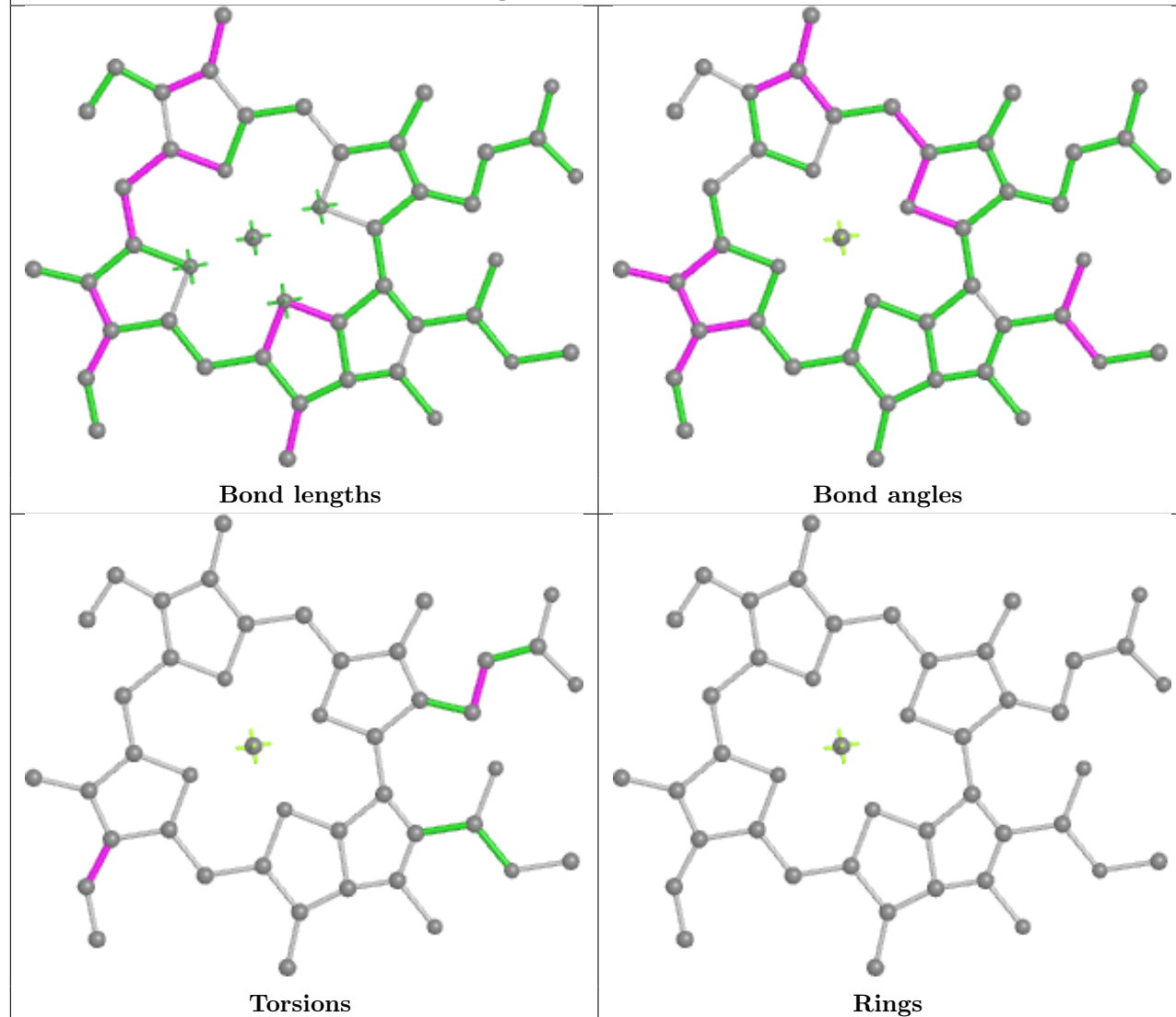




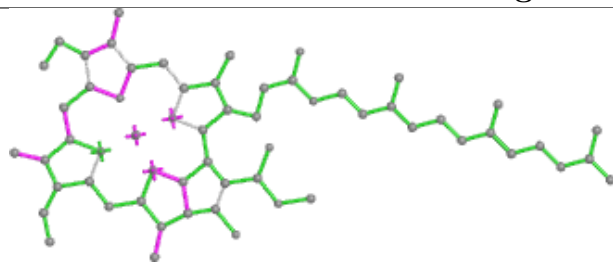
## Ligand CLA P 301



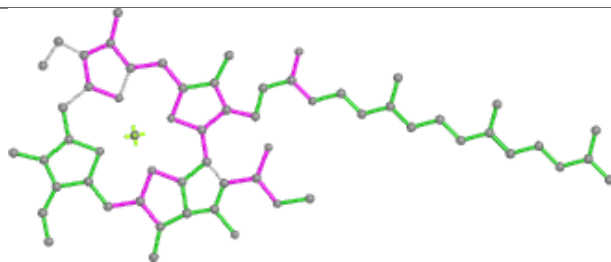
## Ligand CLA a 819



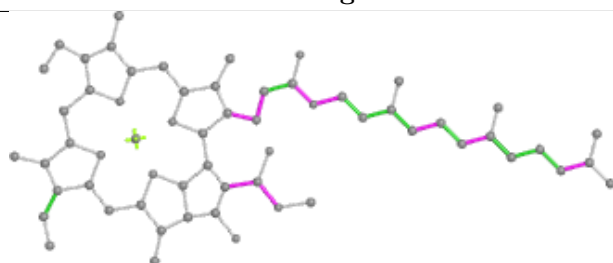
## Ligand CLA P 319



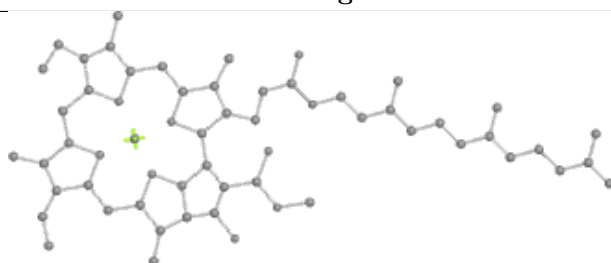
Bond lengths



Bond angles

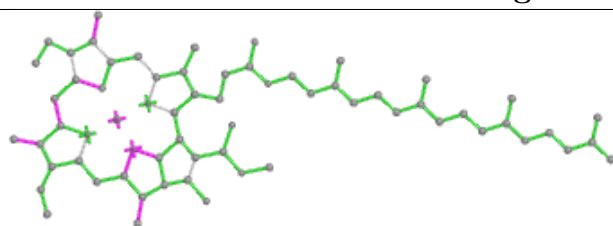


Torsions

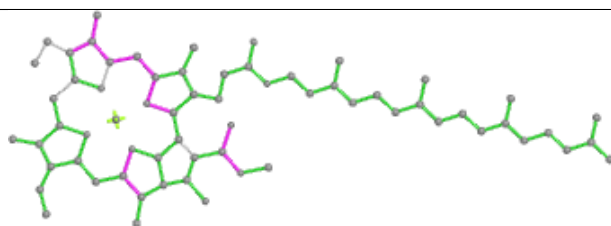


Rings

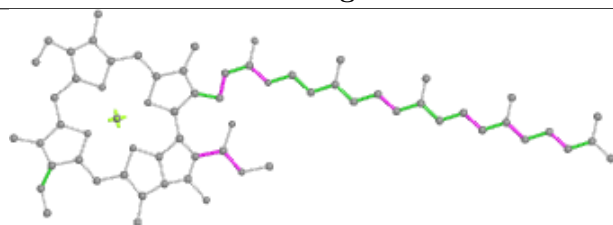
## Ligand CLA R 313



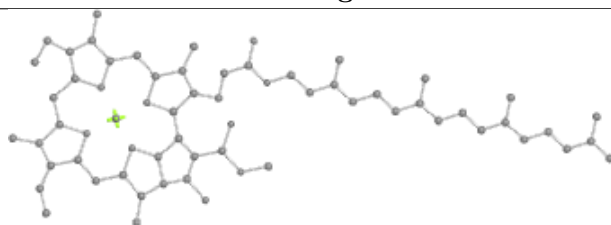
Bond lengths



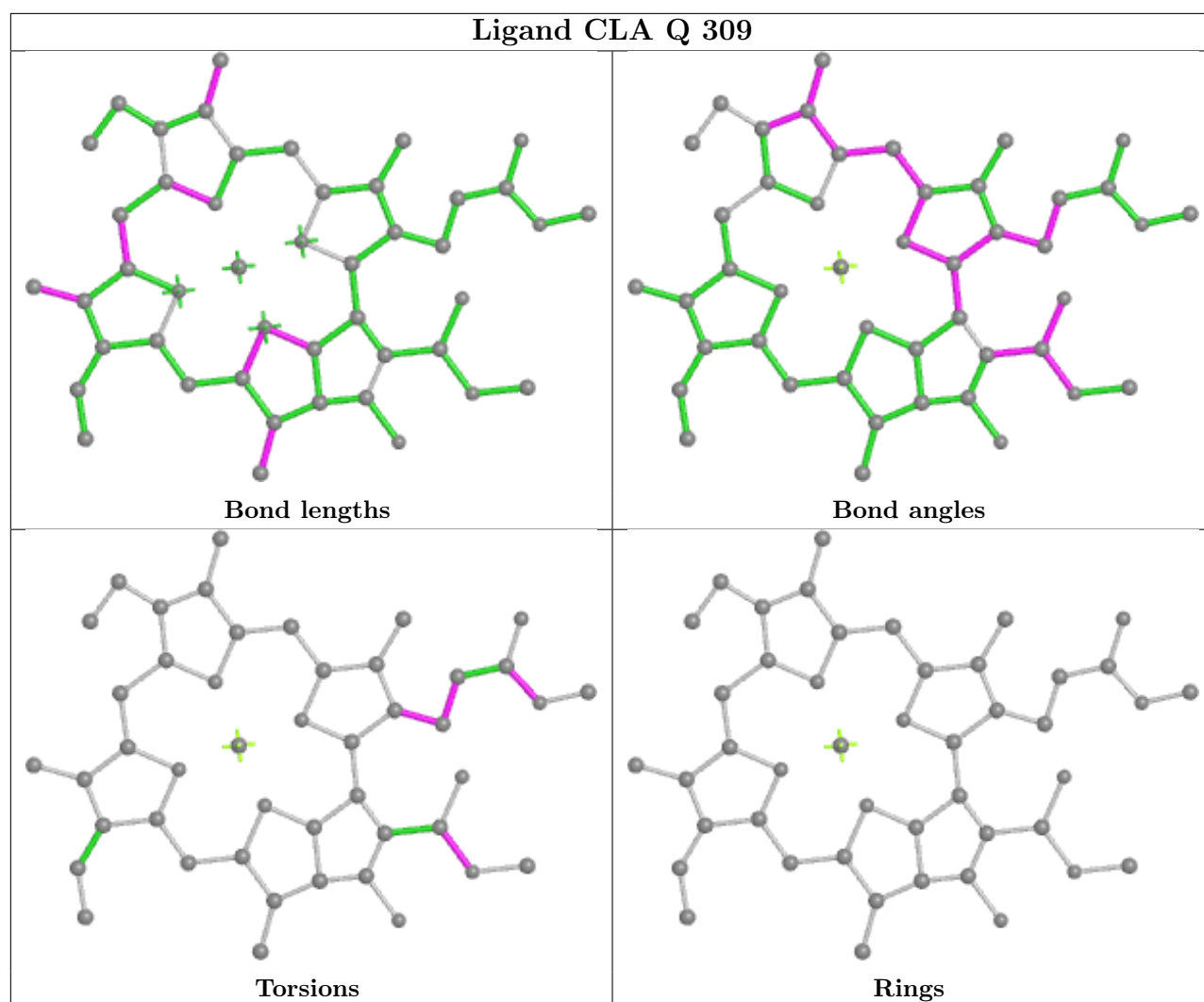
Bond angles

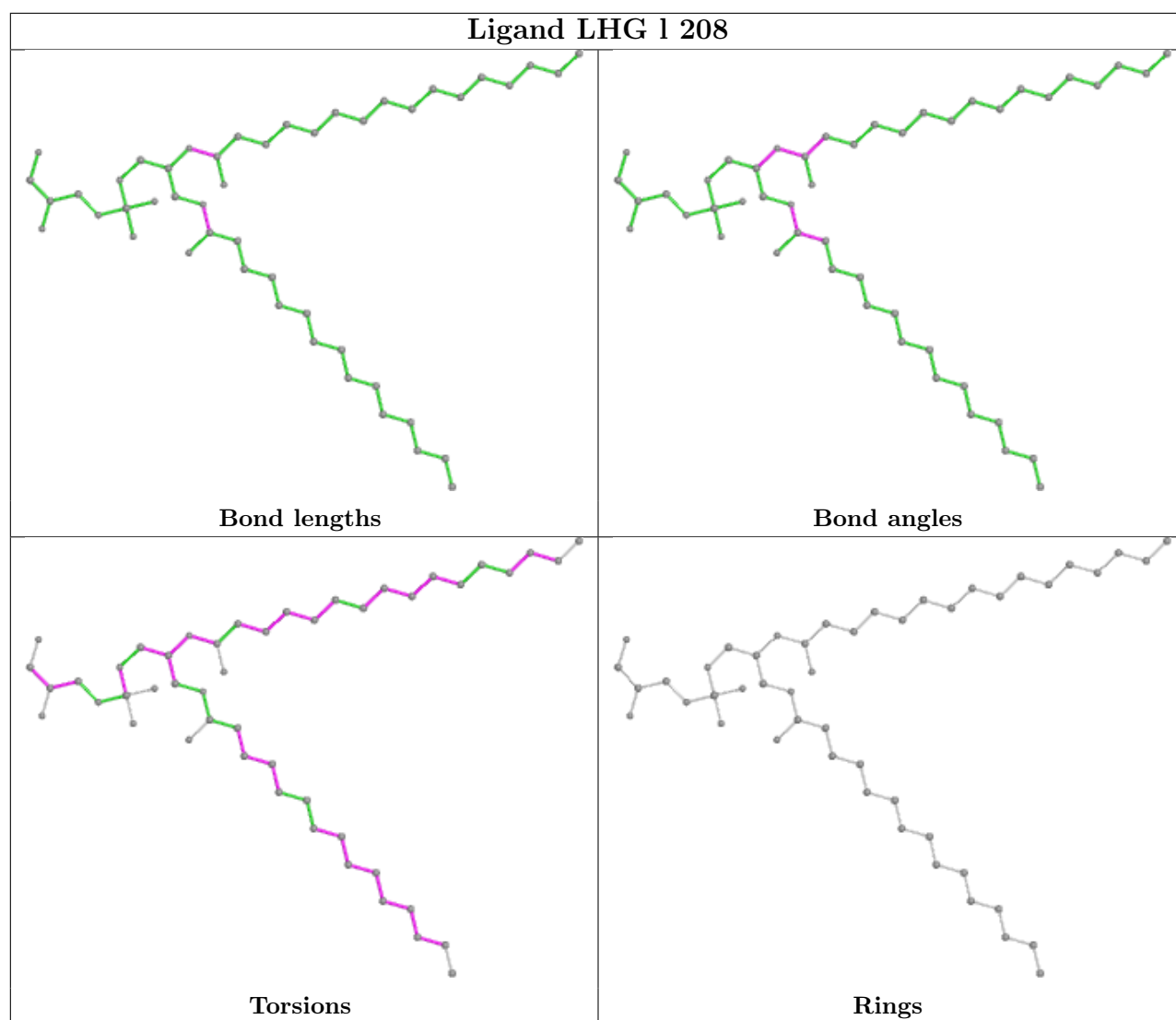


Torsions

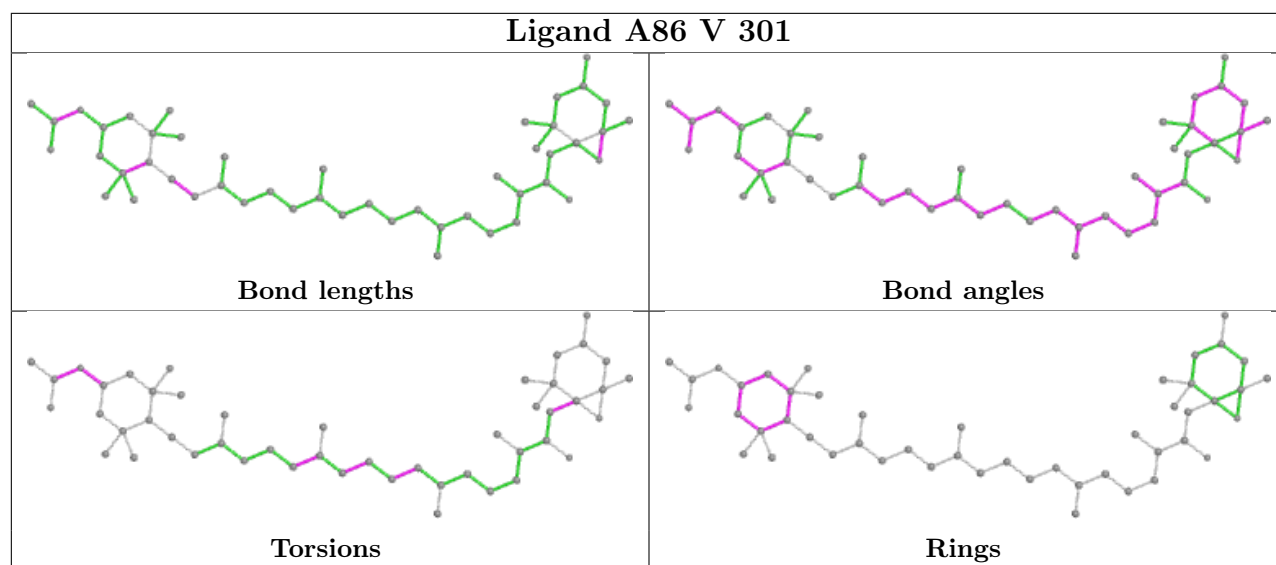
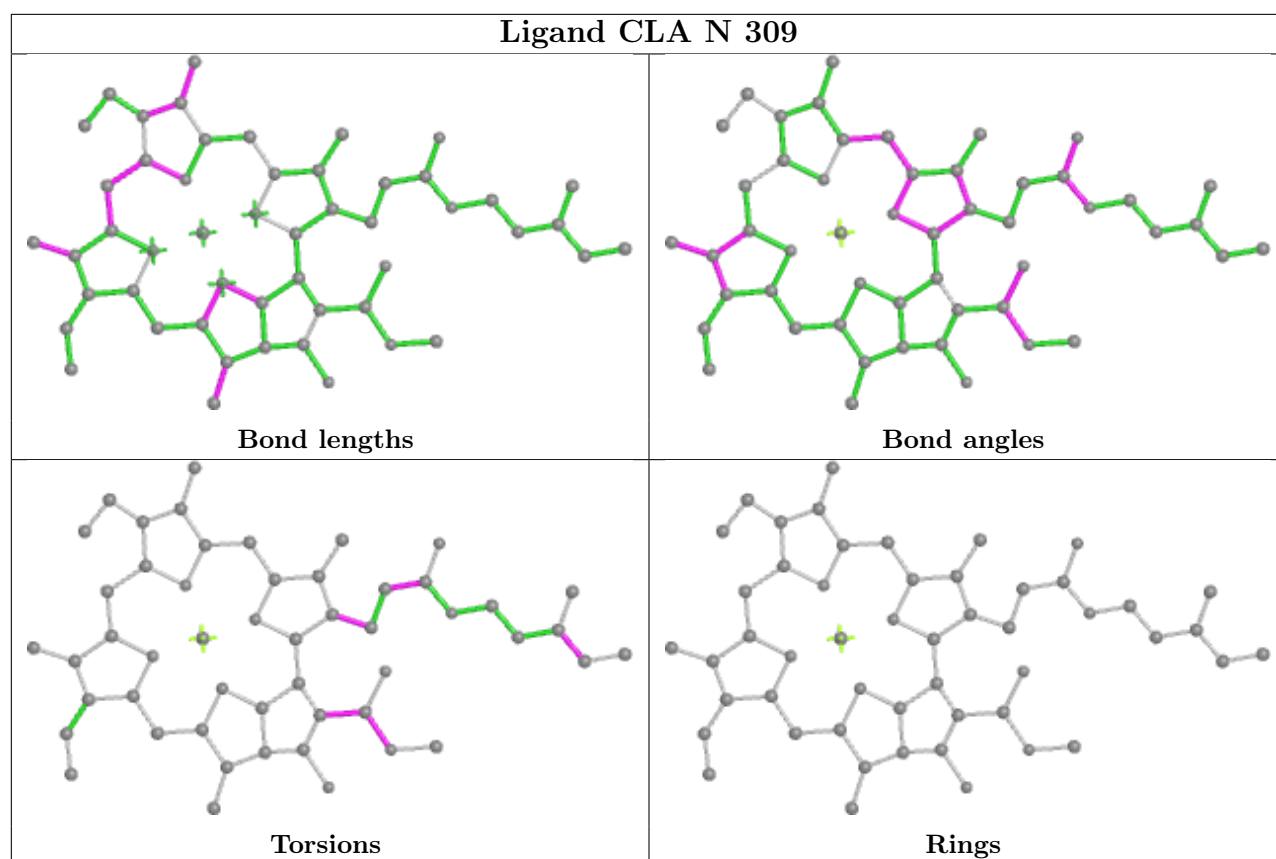


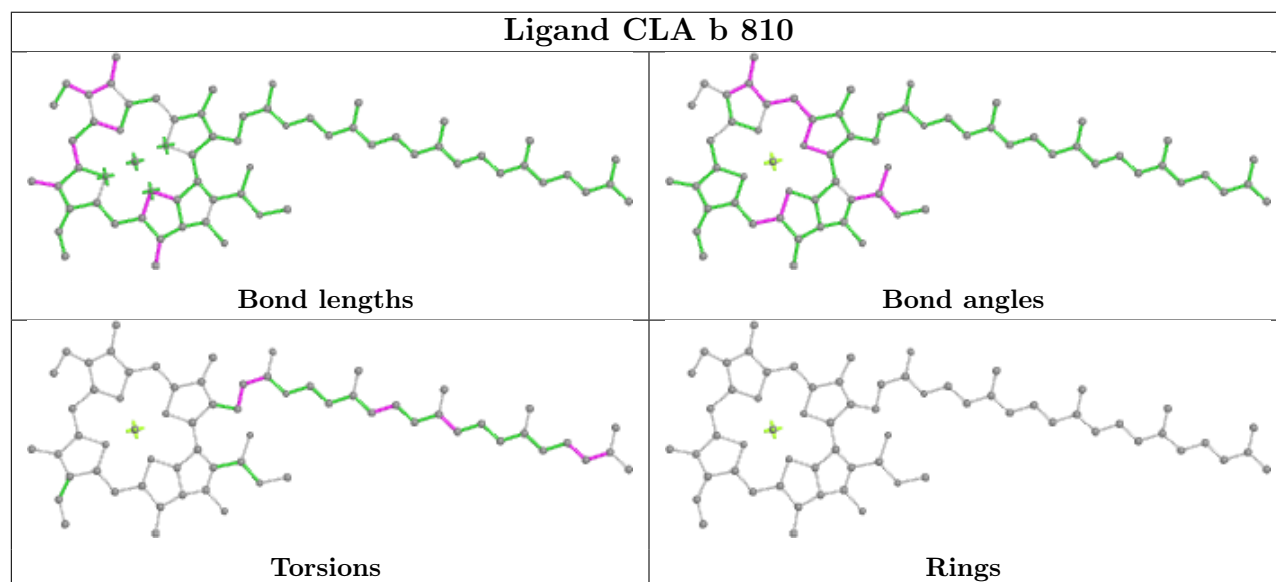
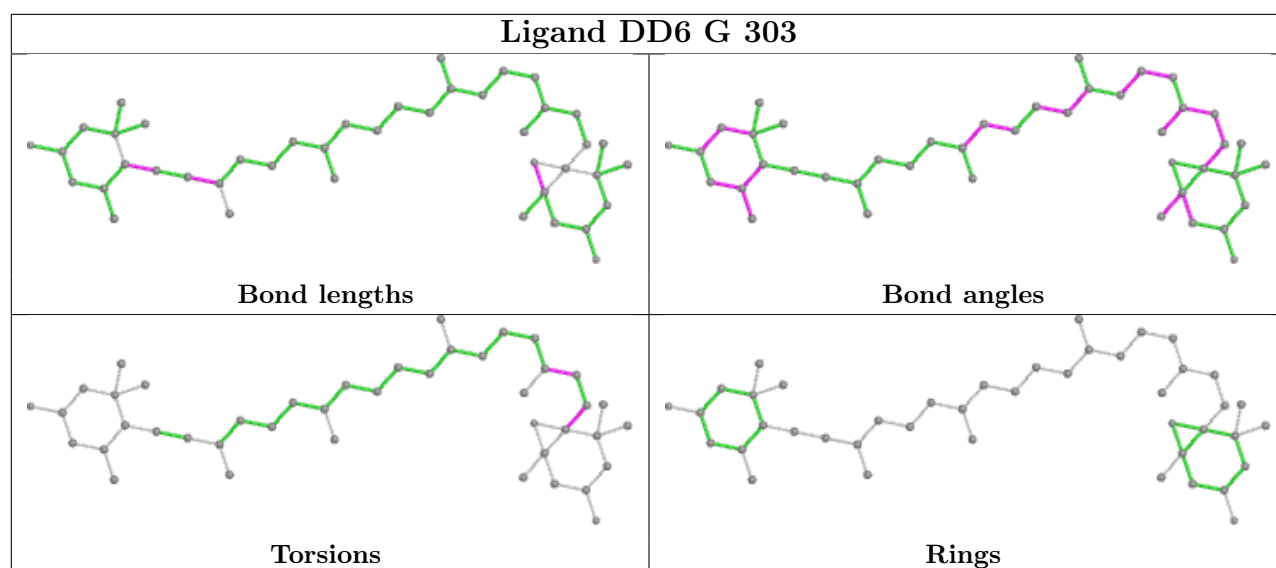
Rings

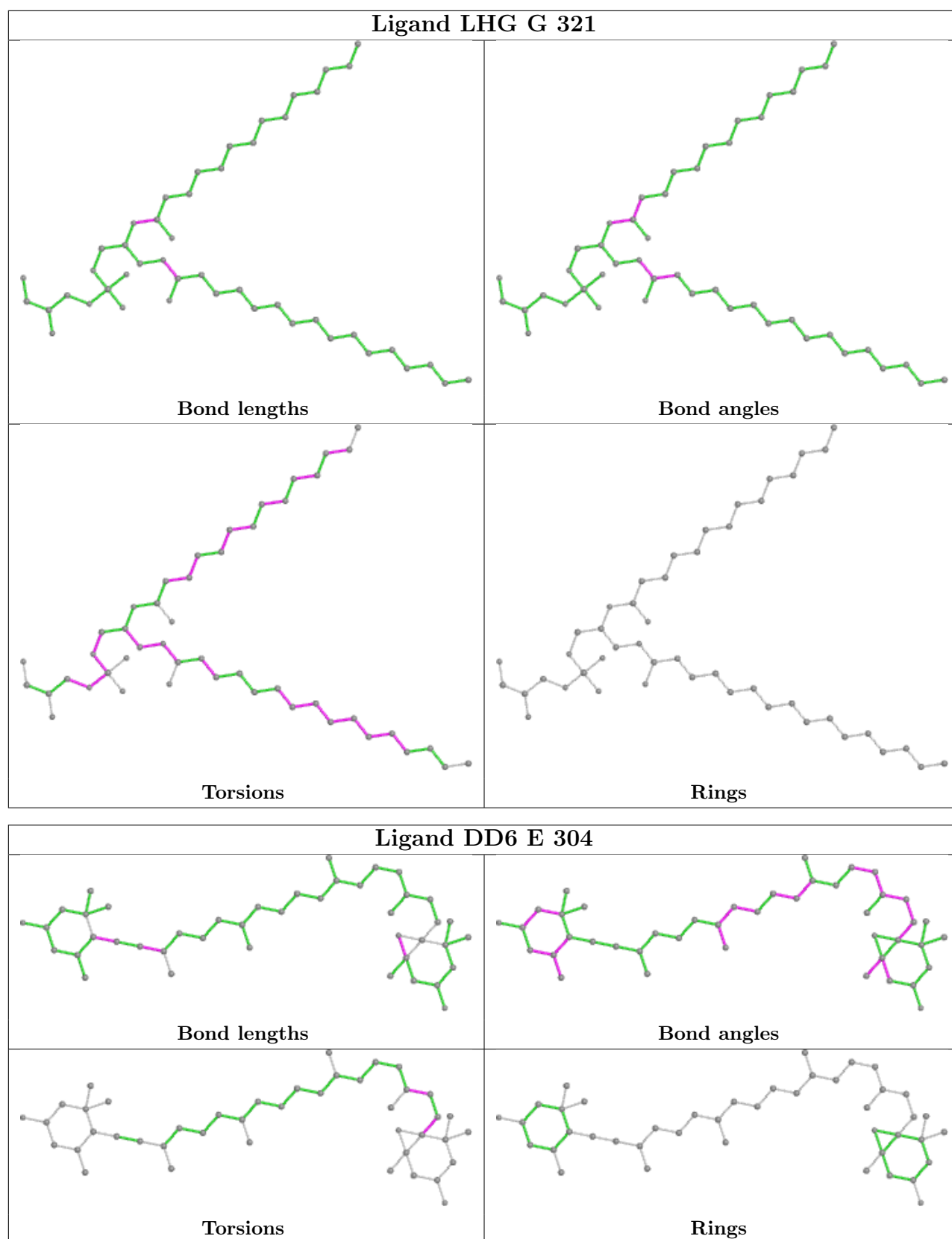


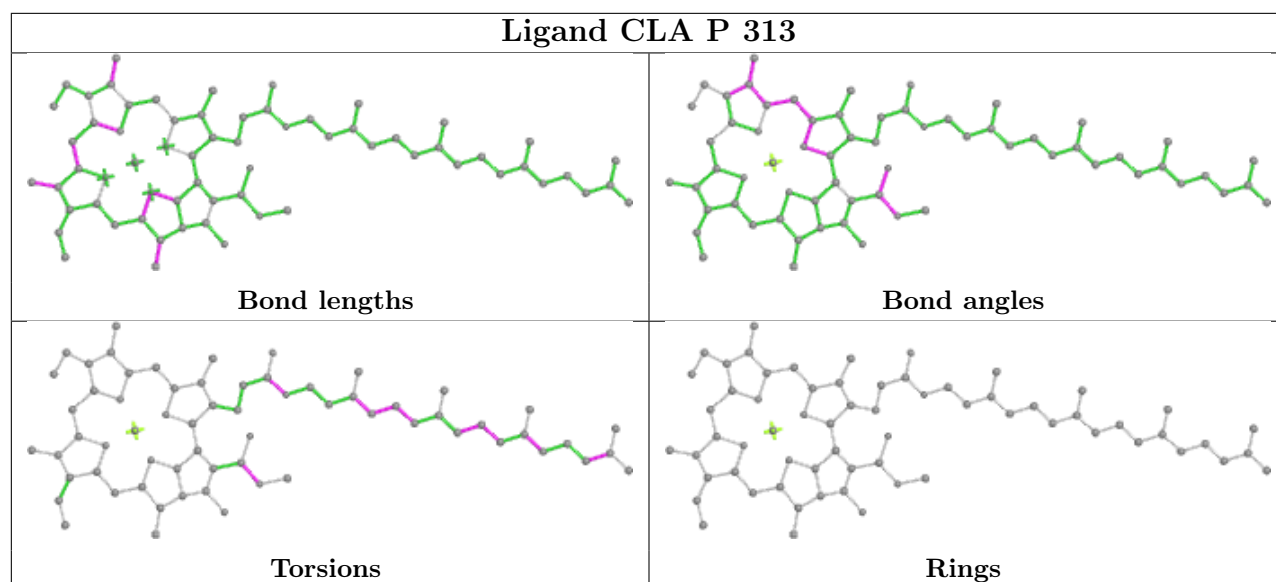
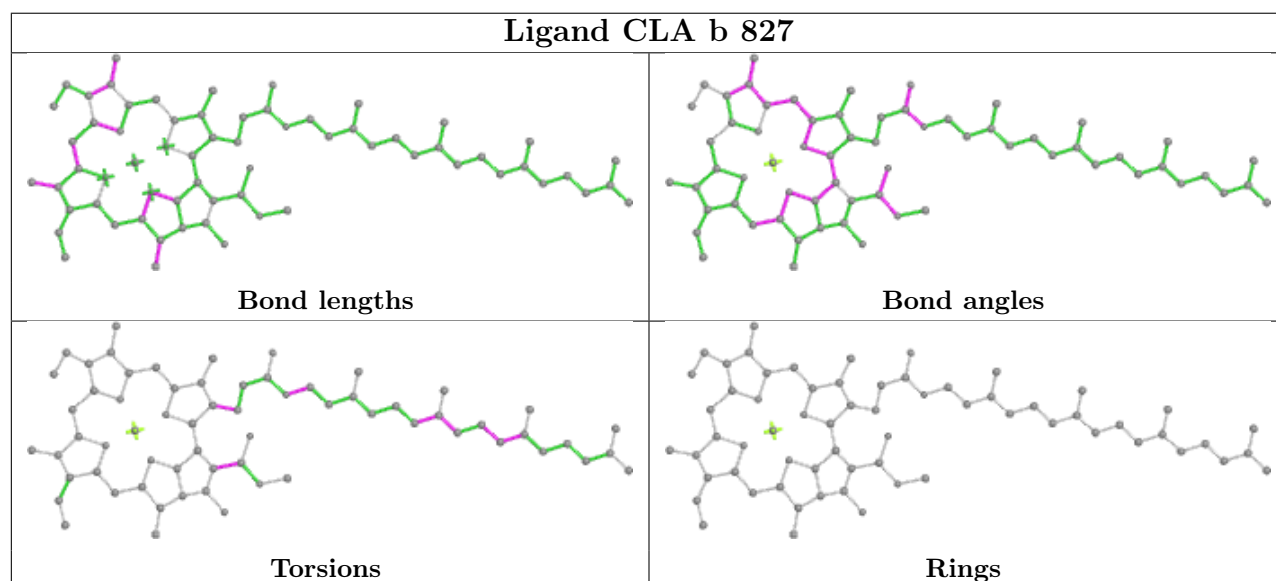
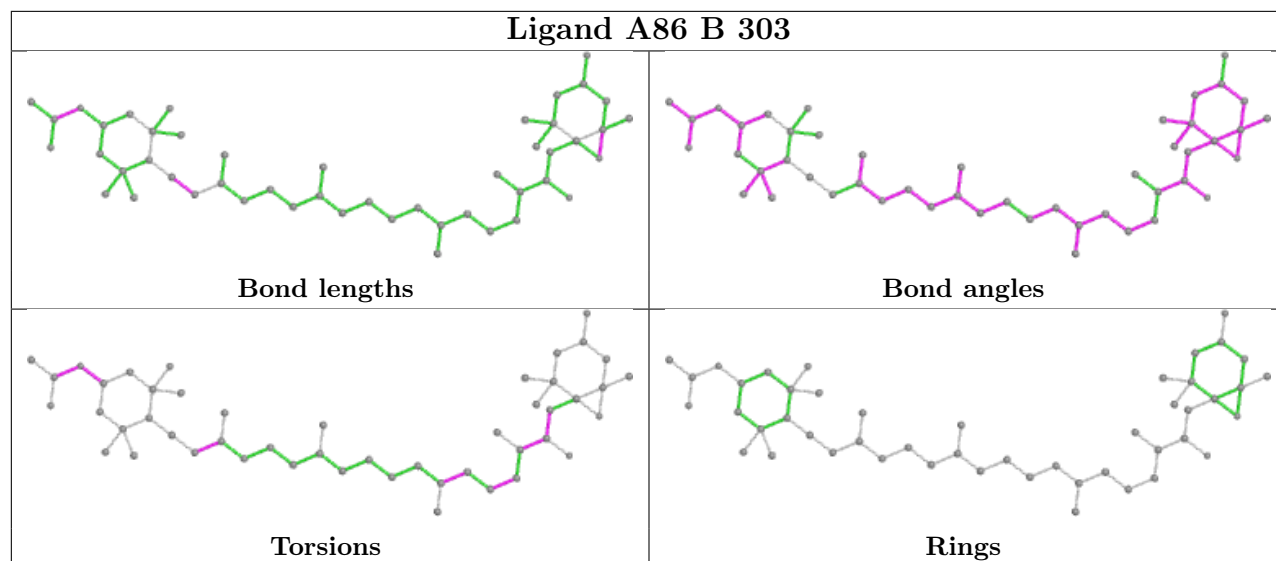




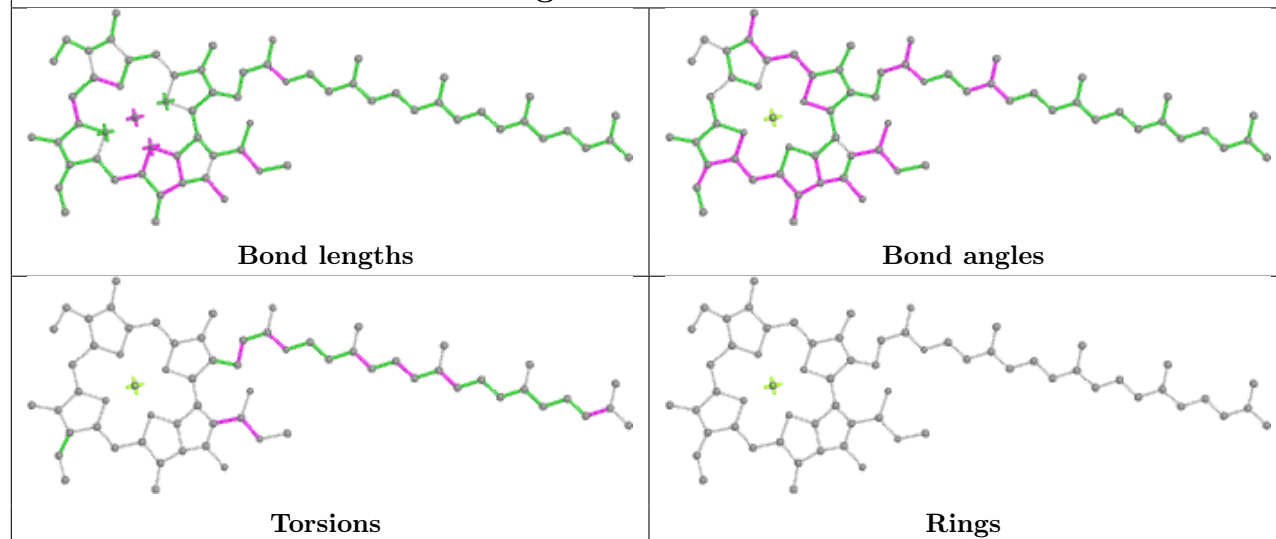




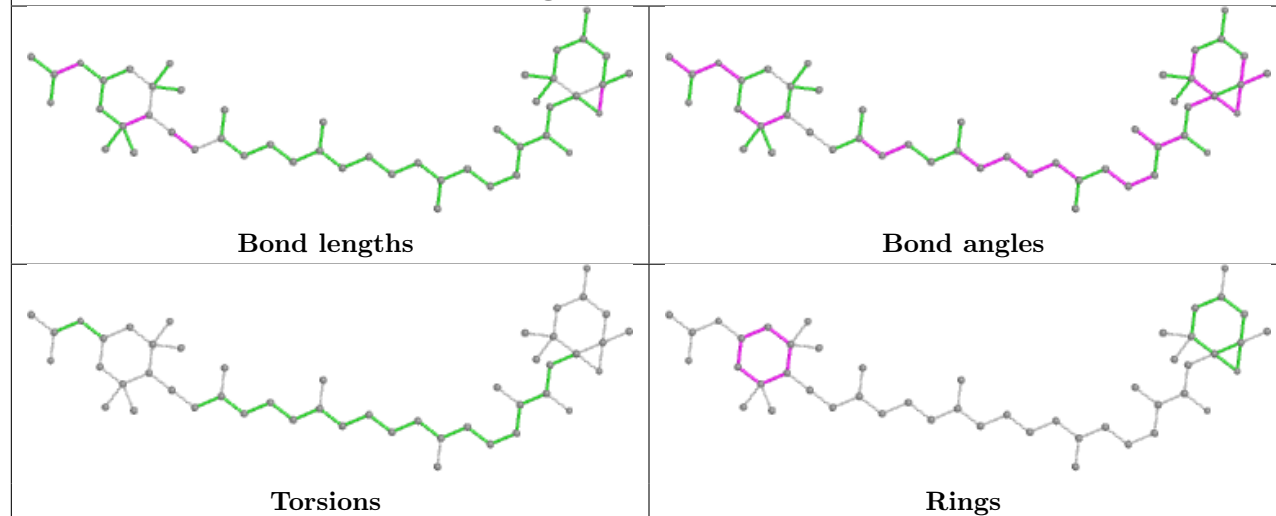




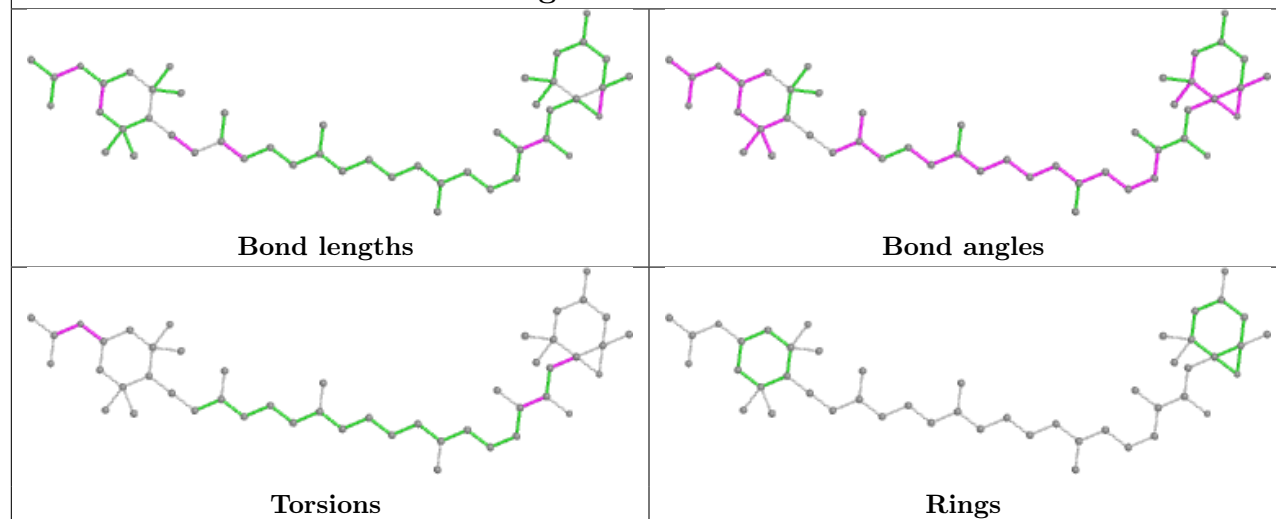
## Ligand CLA a 848



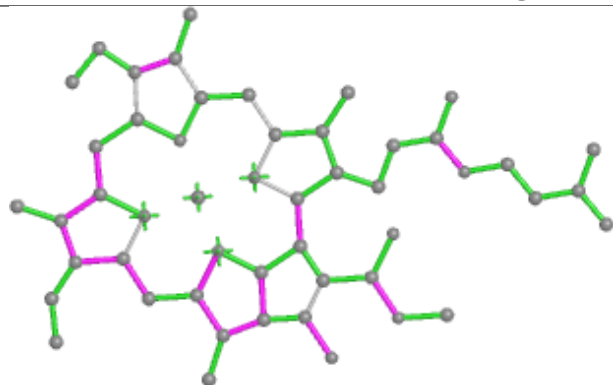
## Ligand A86 F 306



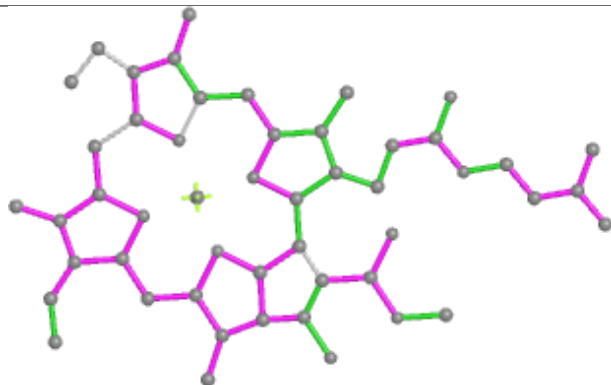
## Ligand A86 P 303



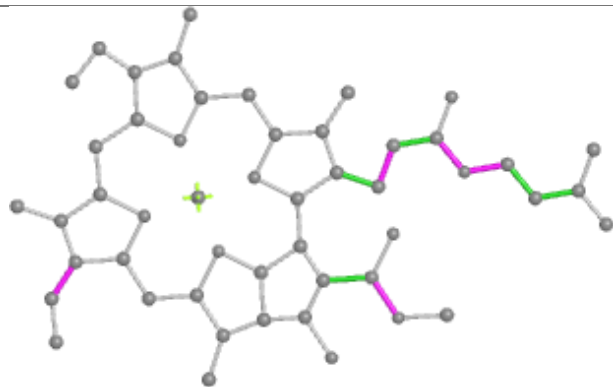
## Ligand CLA G 319



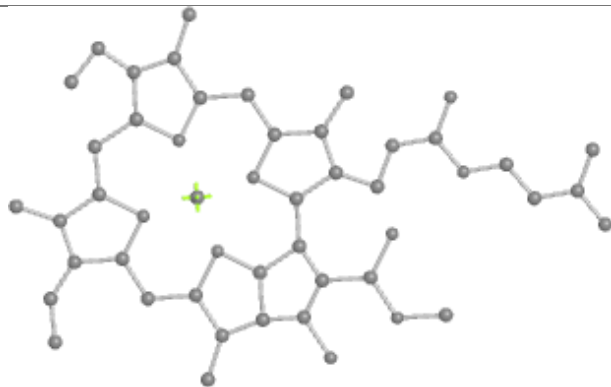
Bond lengths



Bond angles

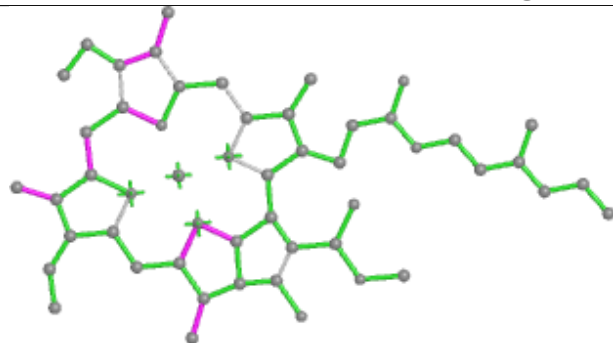


Torsions

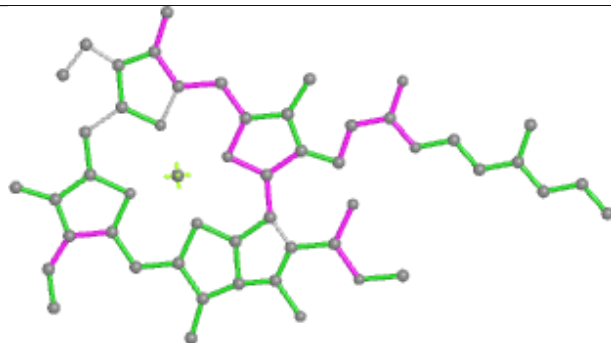


Rings

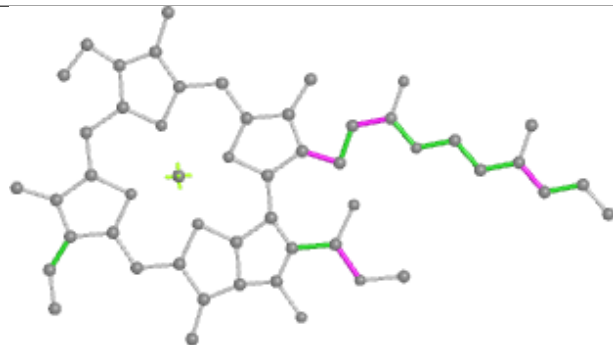
## Ligand CLA a 841



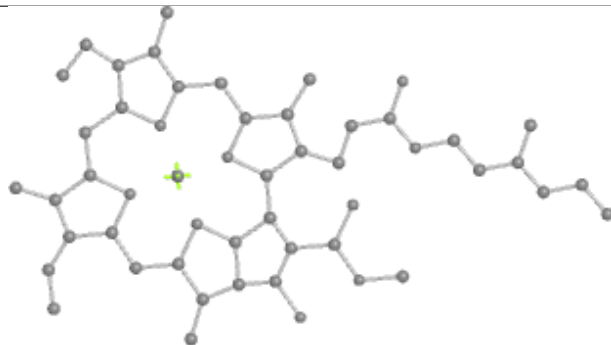
Bond lengths



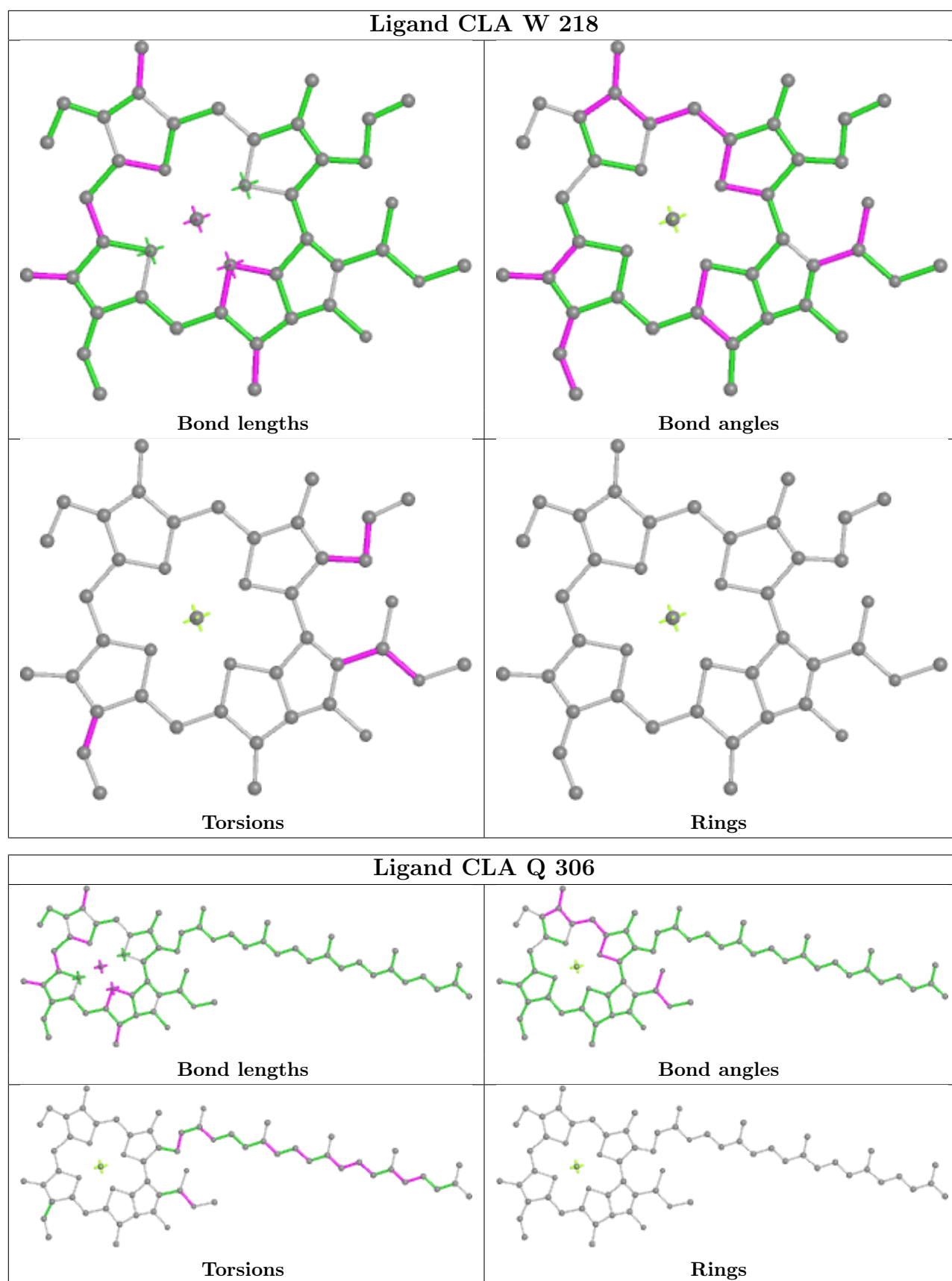
Bond angles



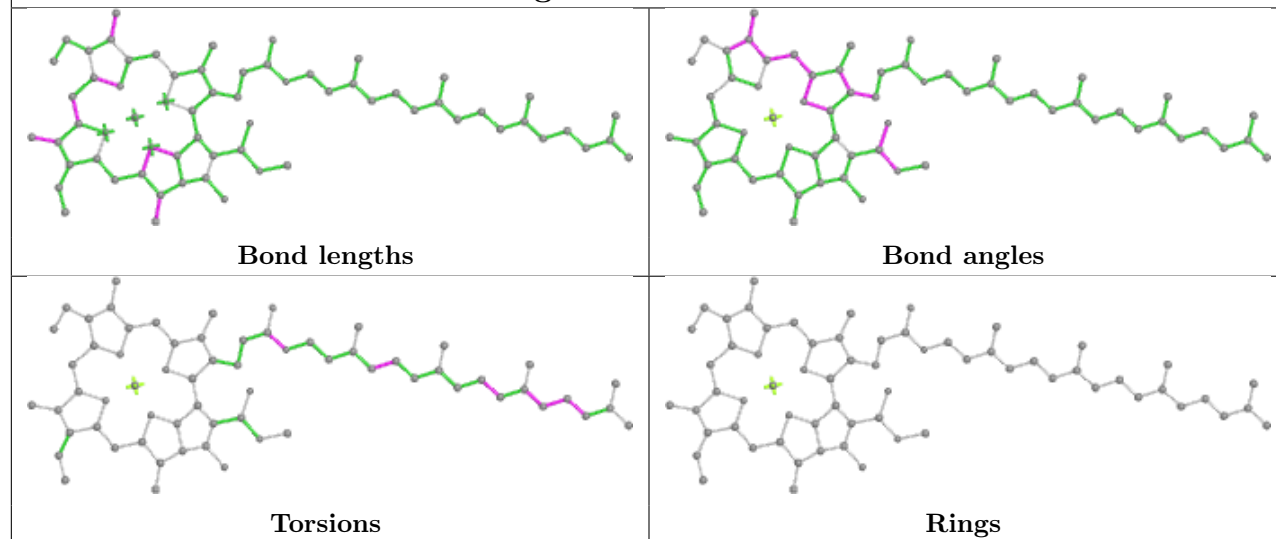
Torsions



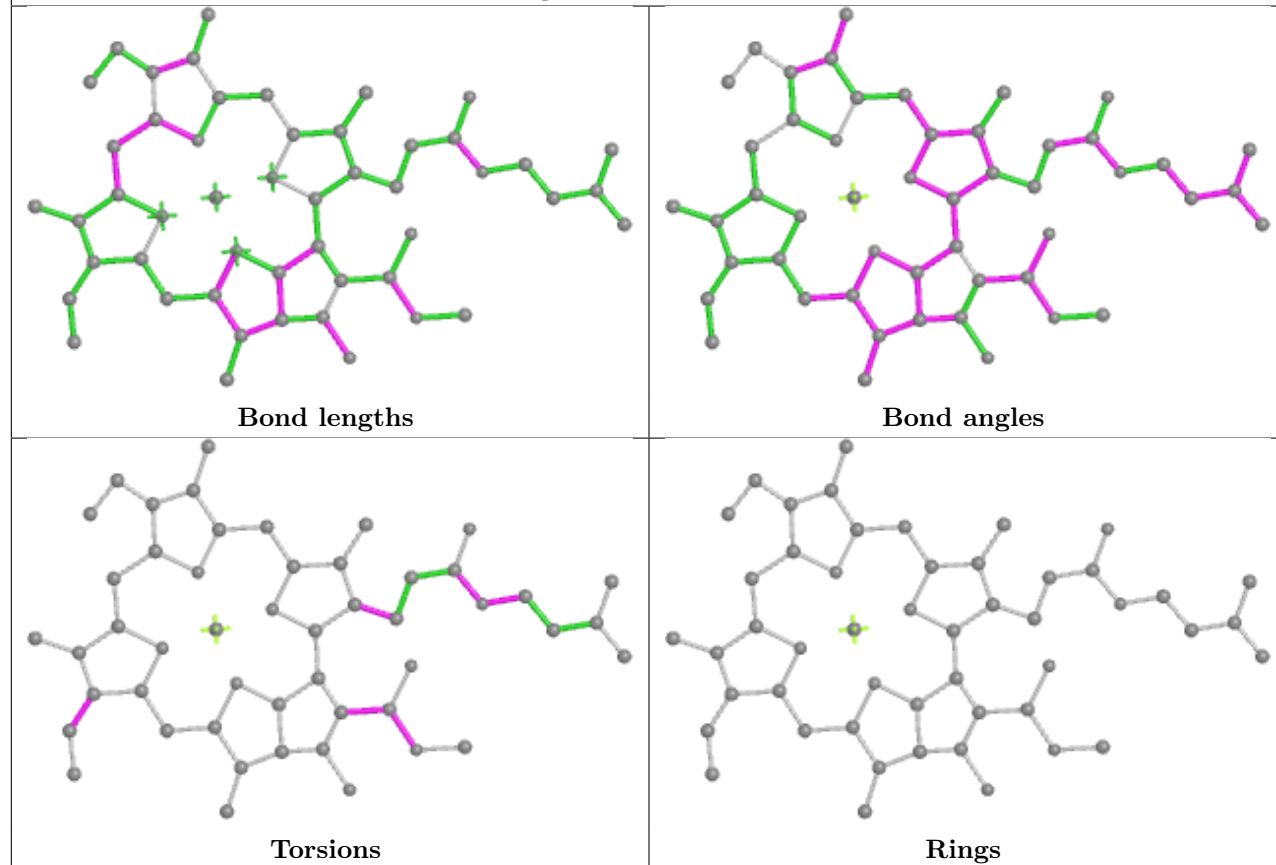
Rings



## Ligand CLA L 313

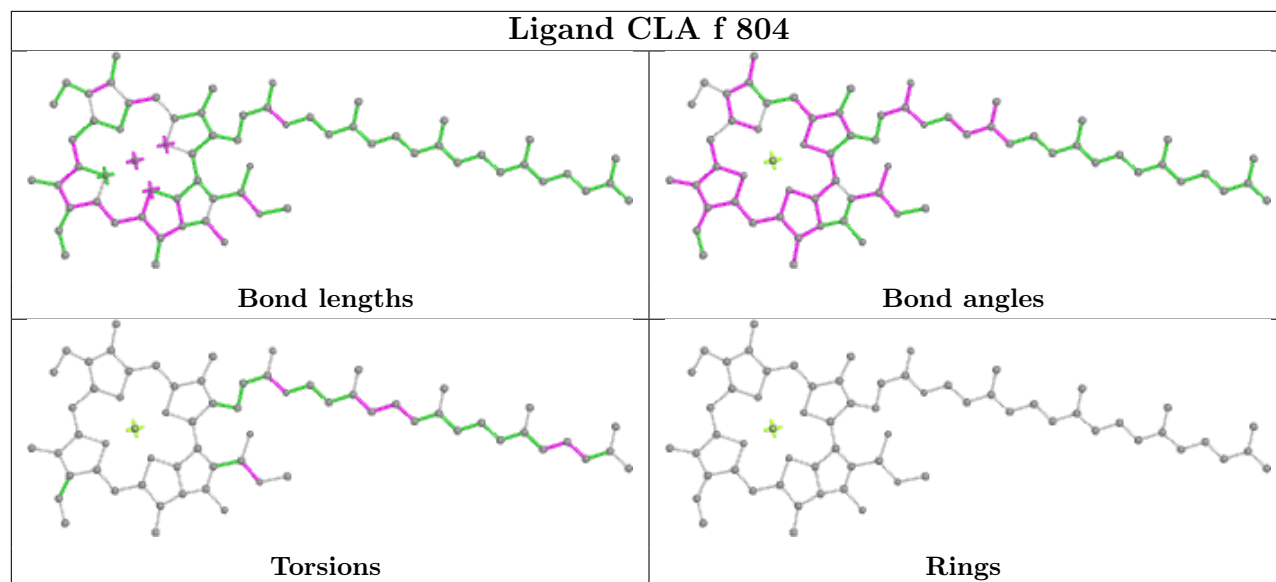


## Ligand CLA a 830

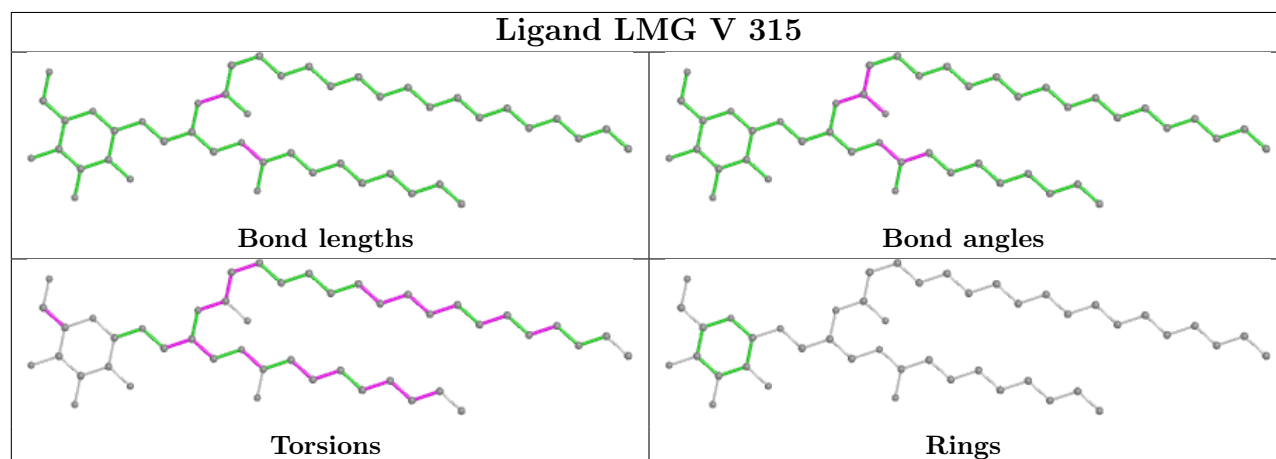




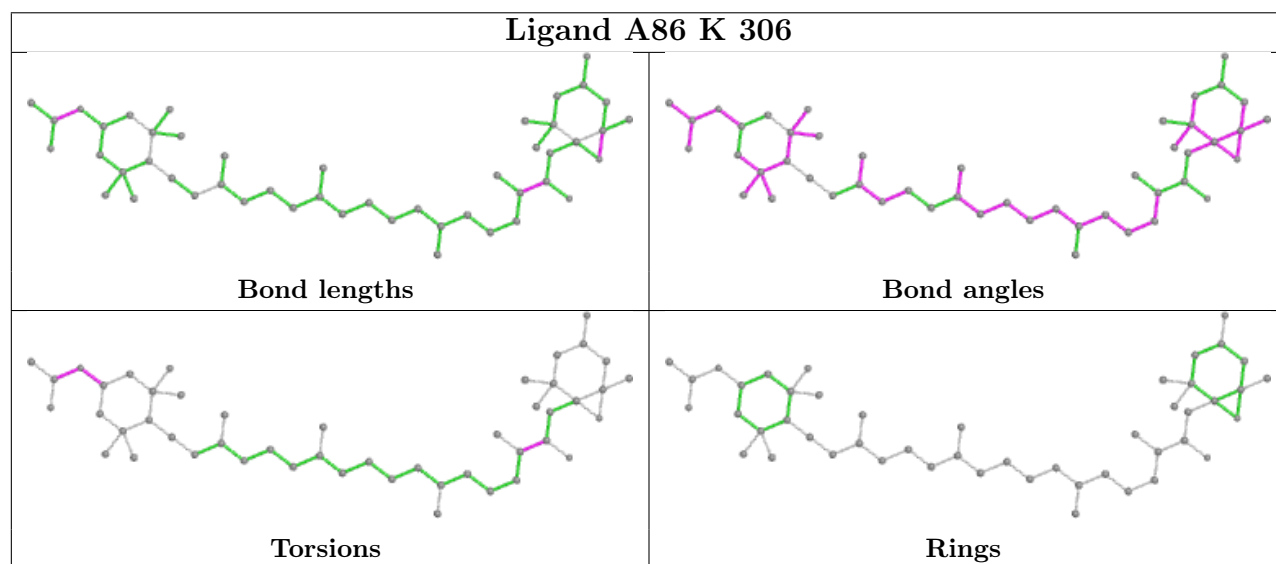
## Ligand CLA f 804

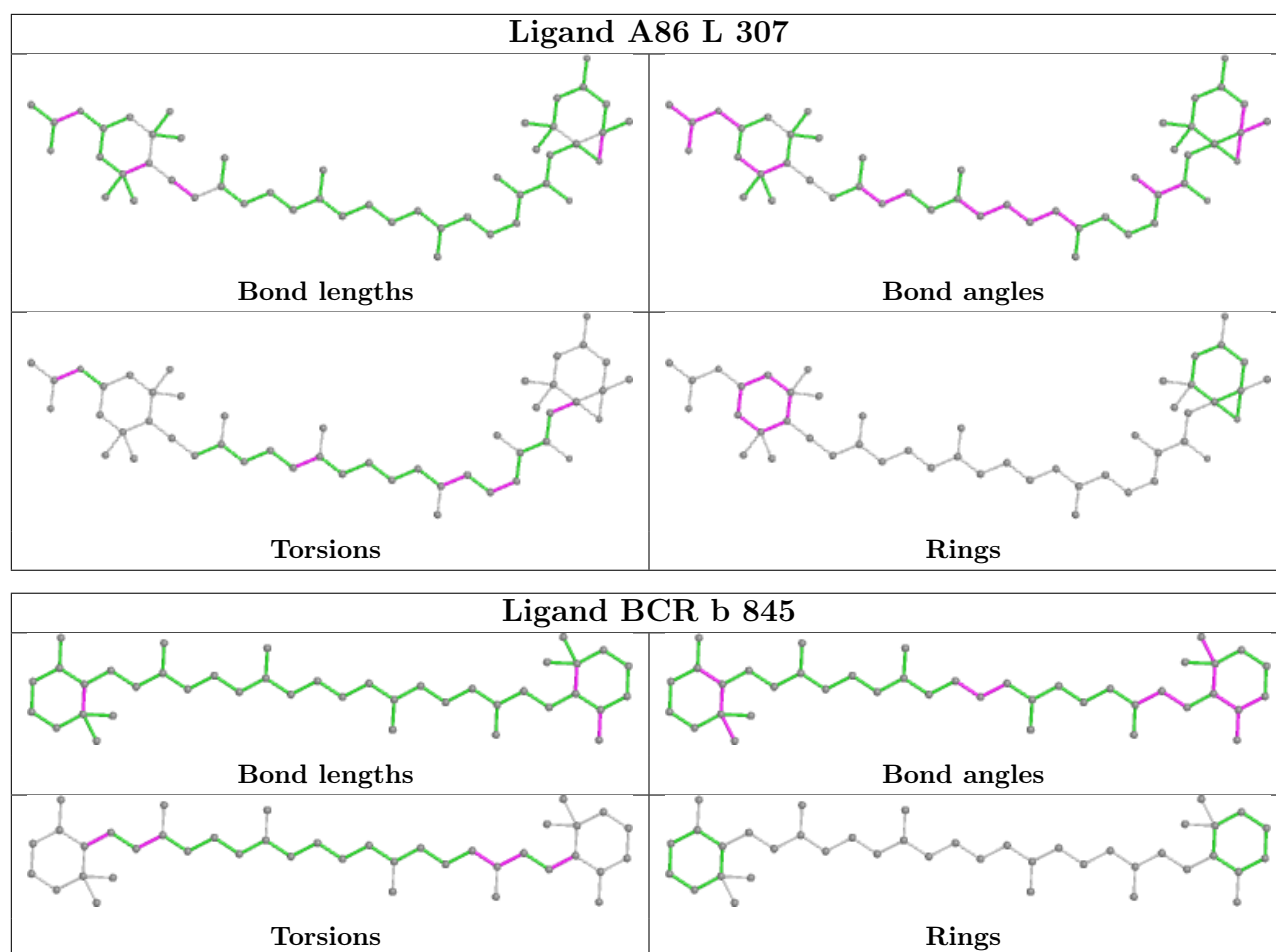


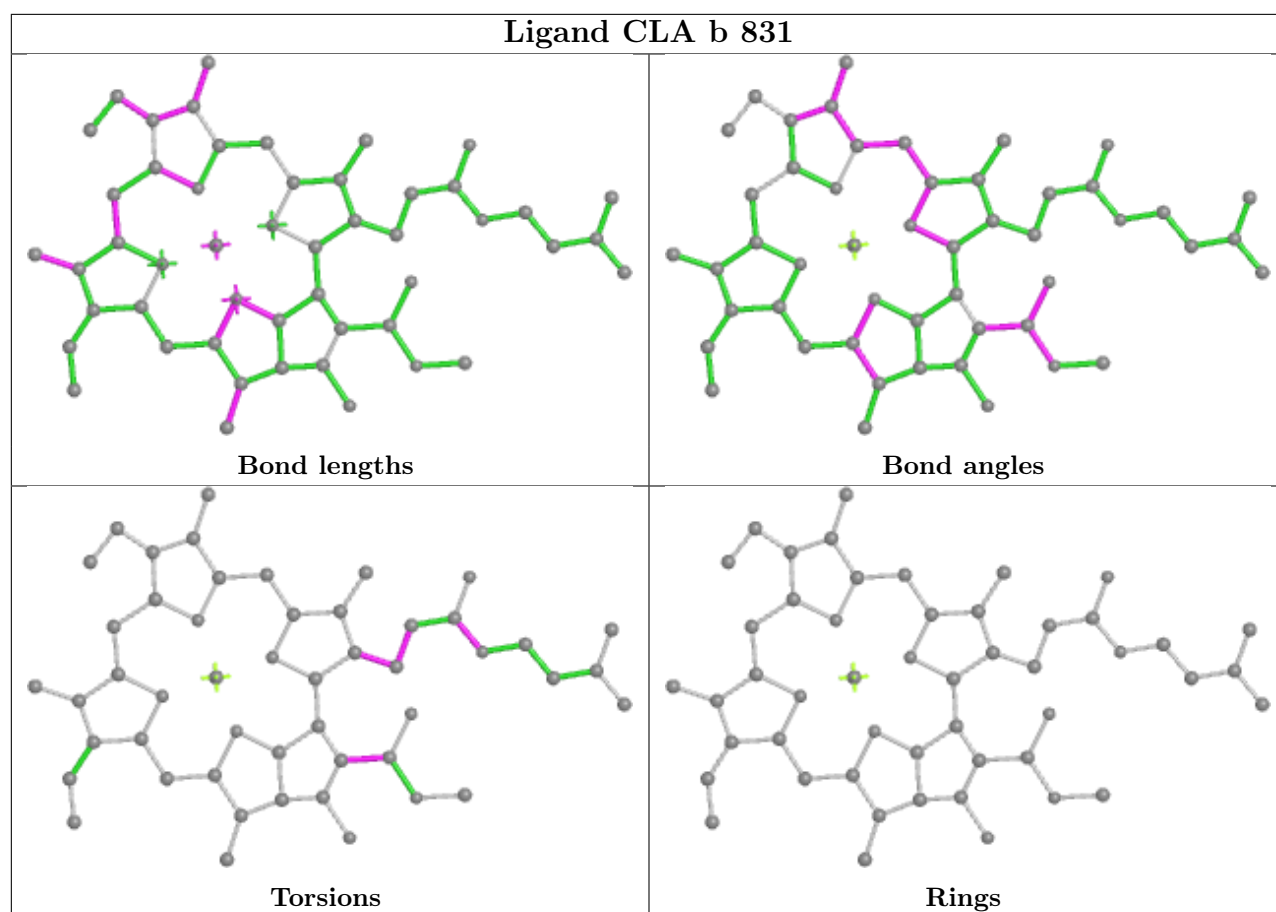
## Ligand LMG V 315



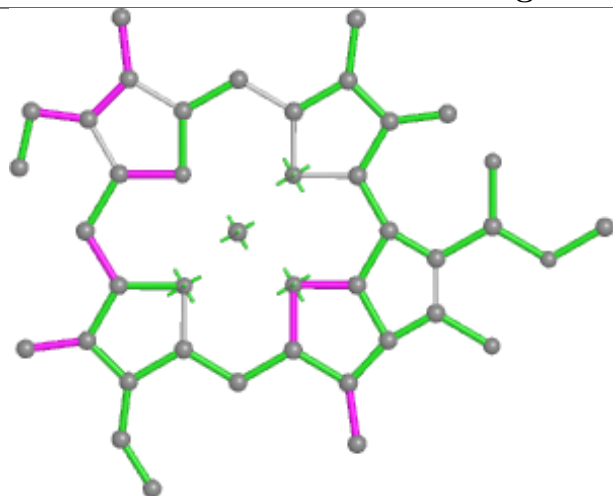
## Ligand A86 K 306



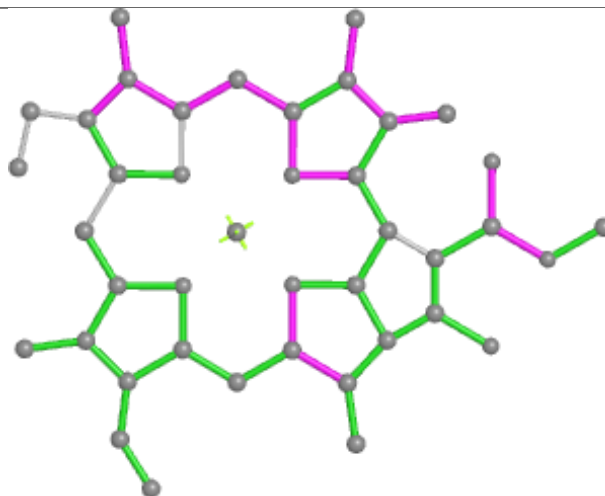




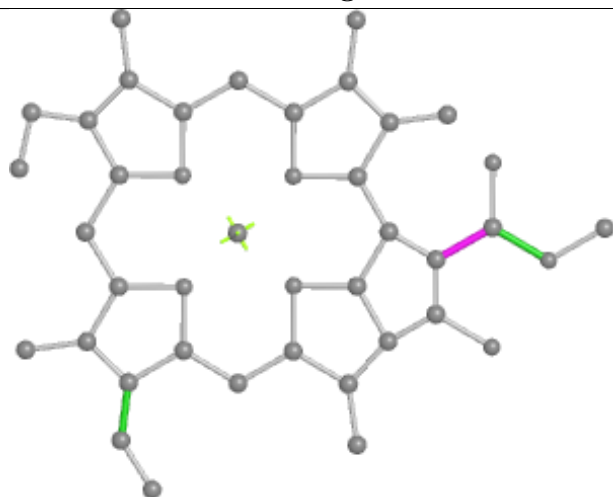
## Ligand CLA F 316



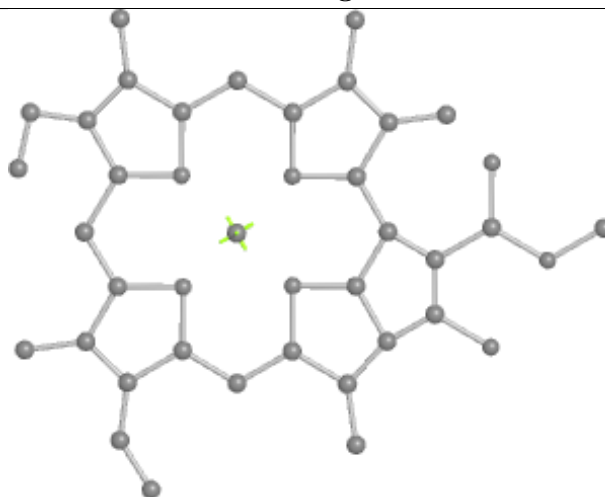
Bond lengths



Bond angles

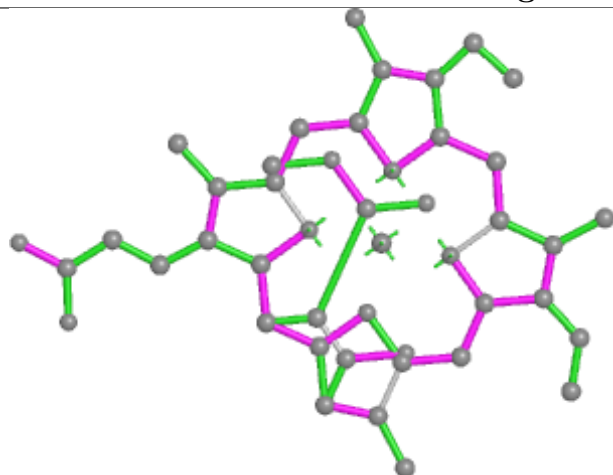


Torsions

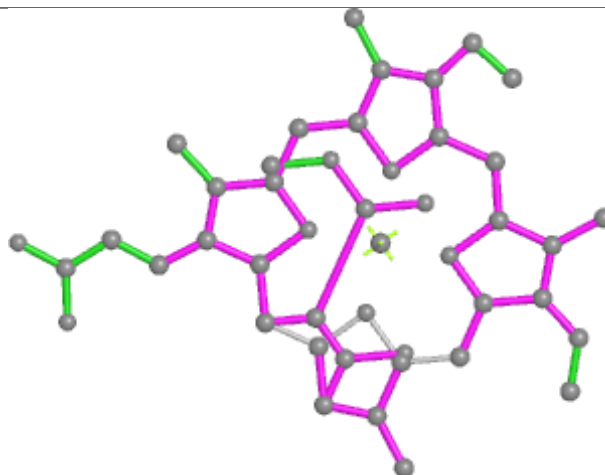


Rings

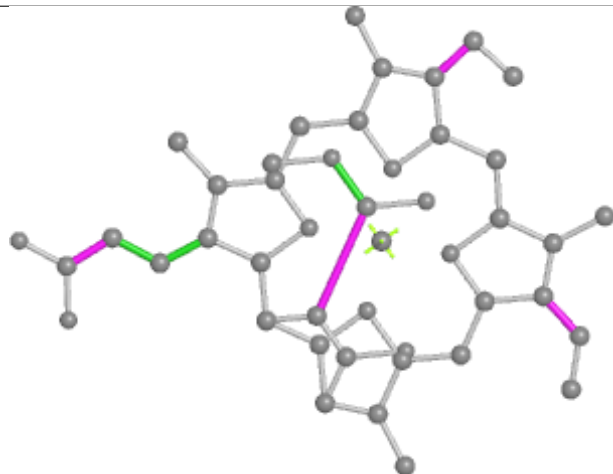
## Ligand KC1 F 308



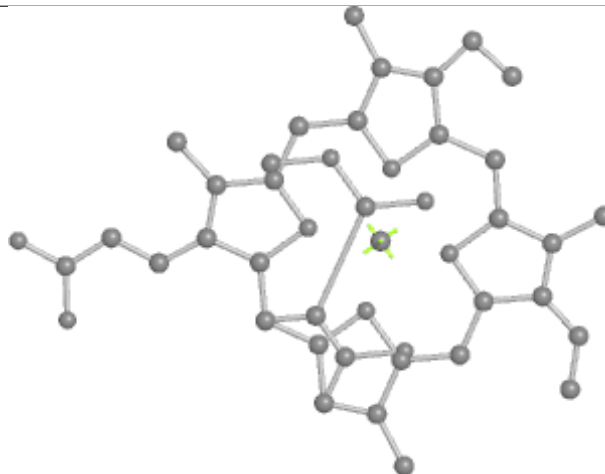
Bond lengths



Bond angles

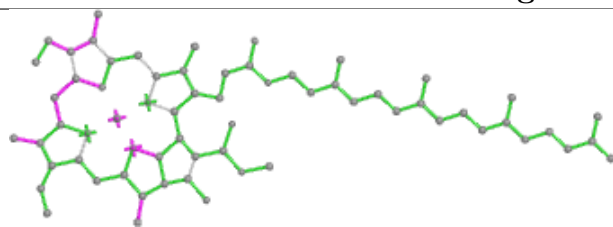


Torsions

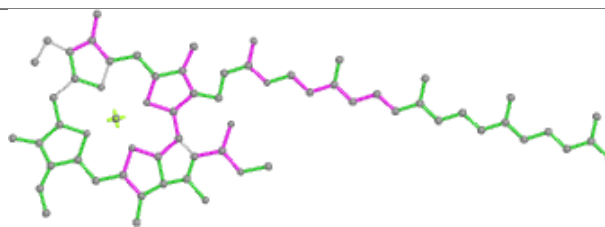


Rings

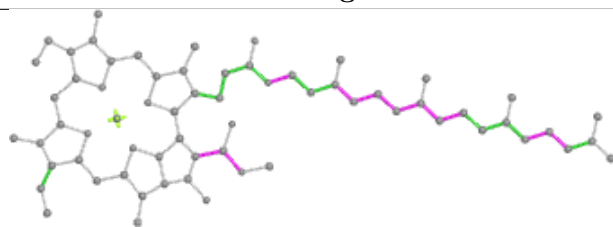
## Ligand CLA b 805



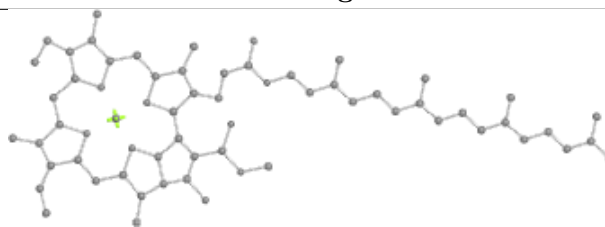
Bond lengths



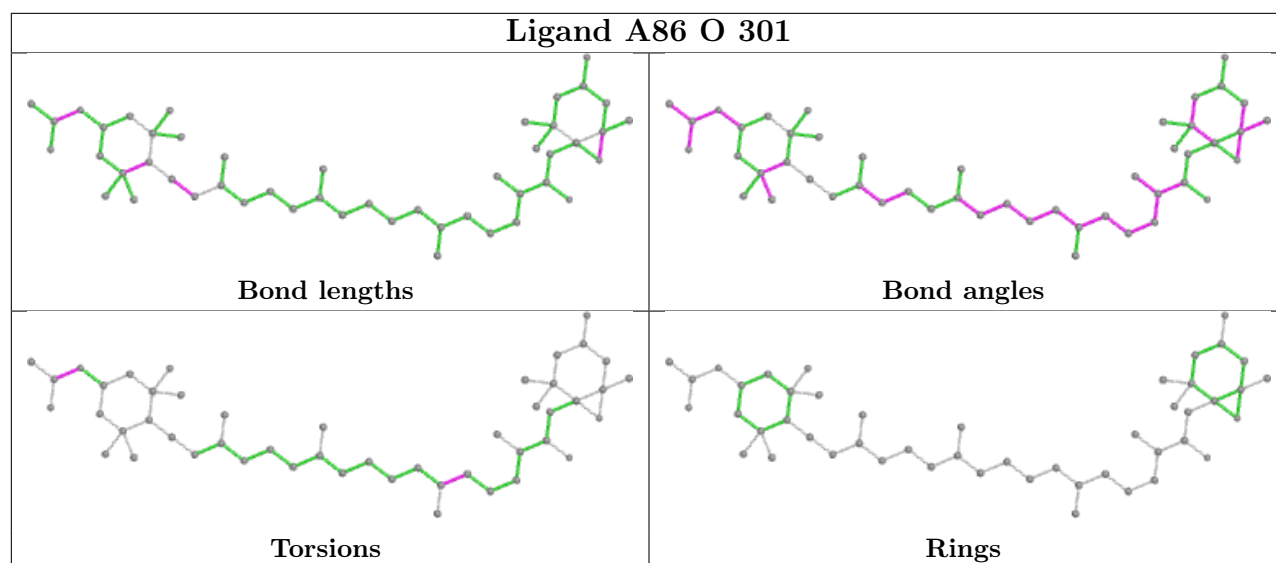
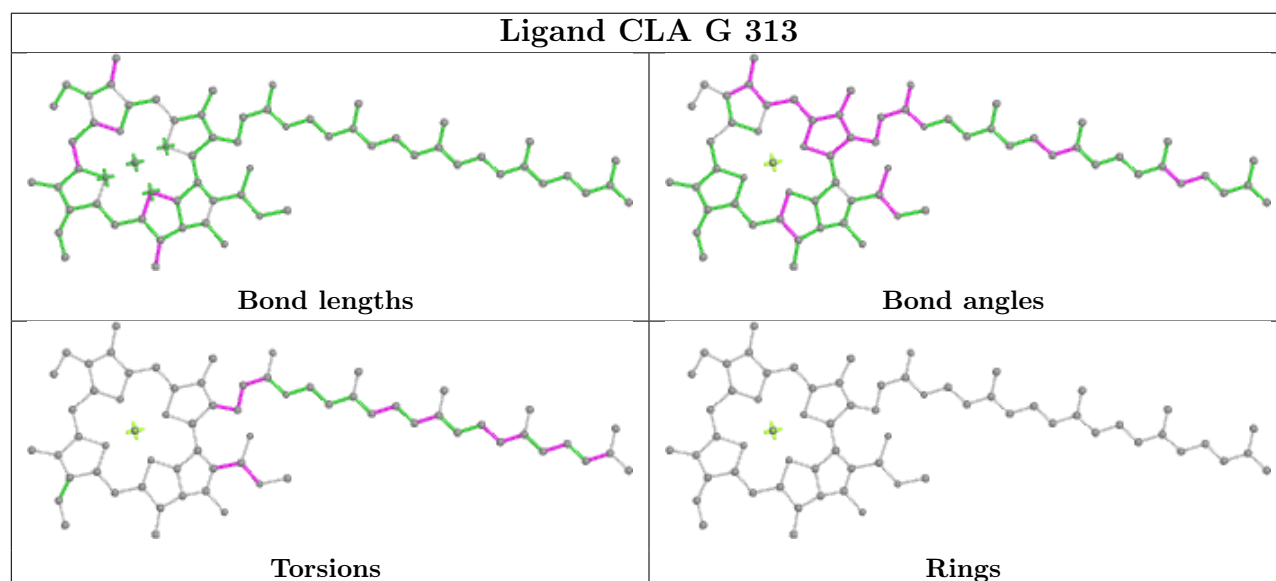
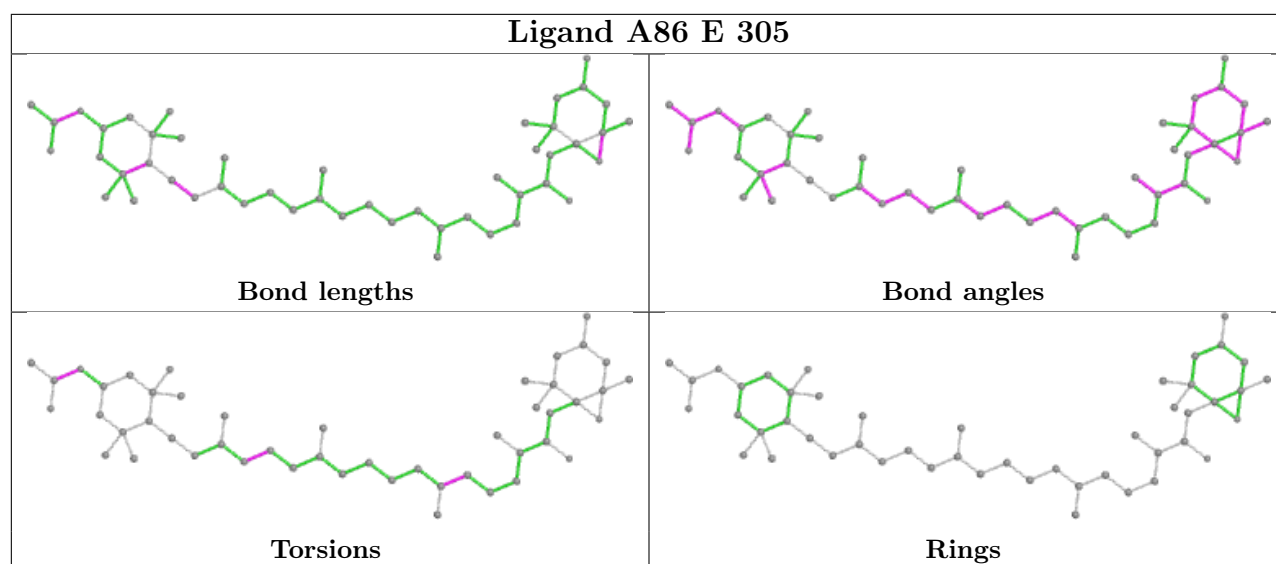
Bond angles



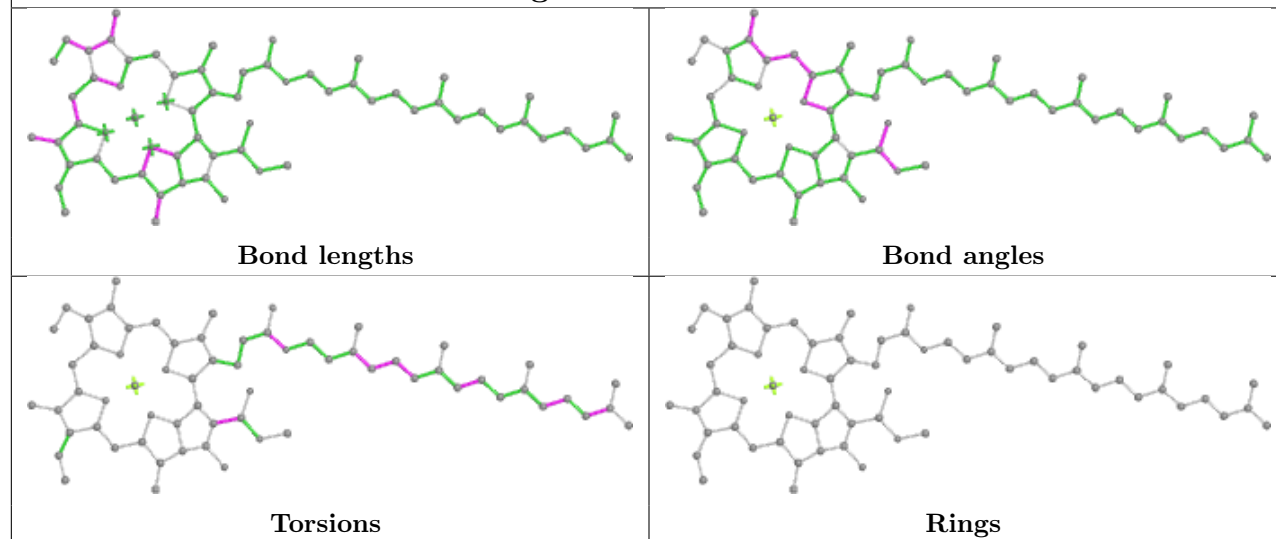
Torsions



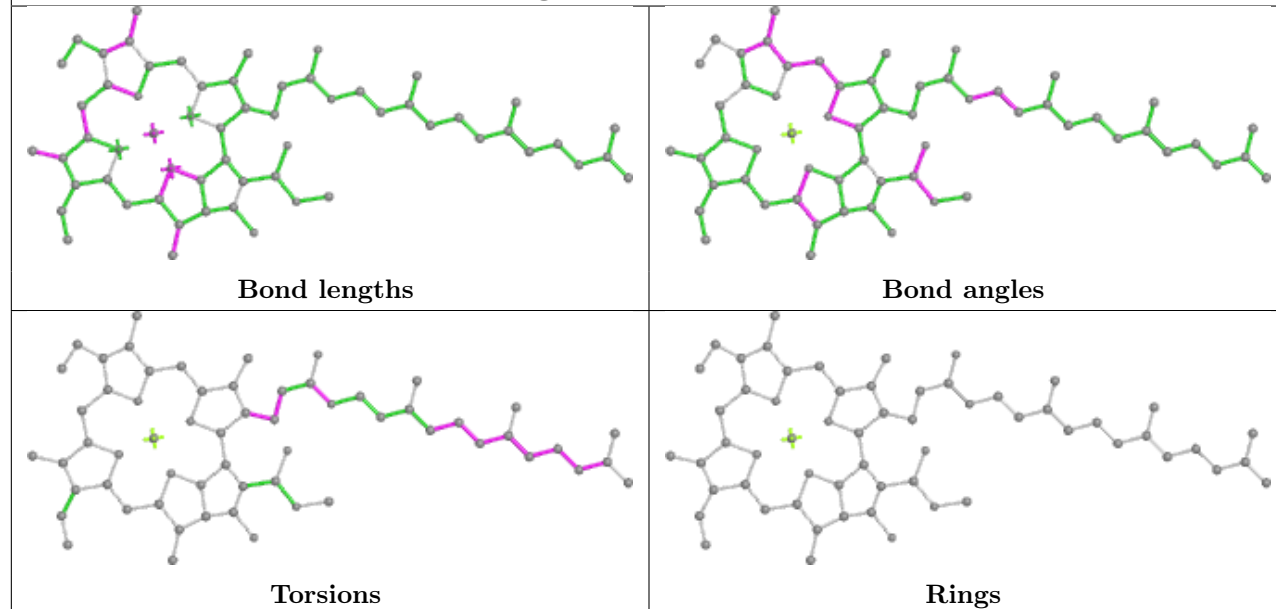
Rings



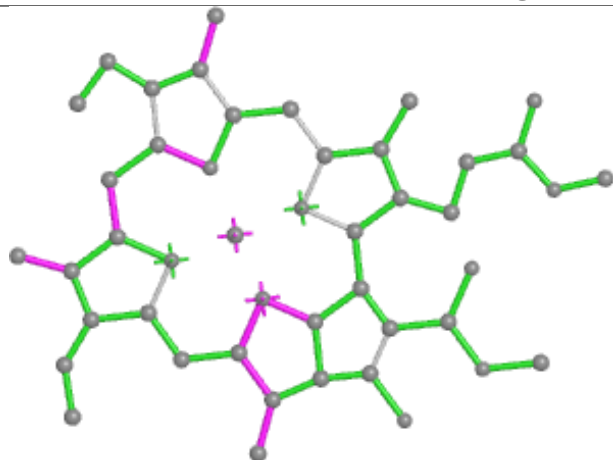
## Ligand CLA K 316



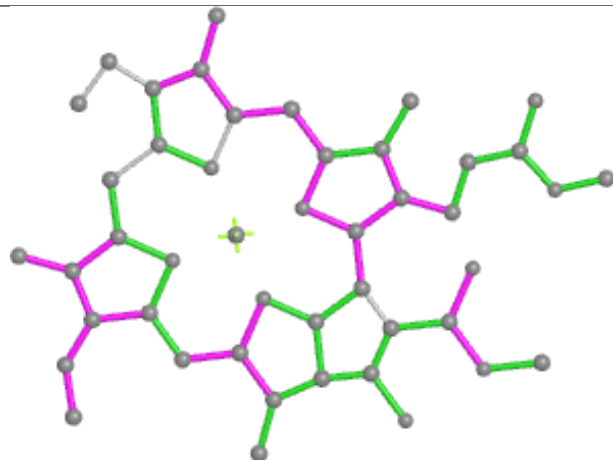
## Ligand CLA b 820



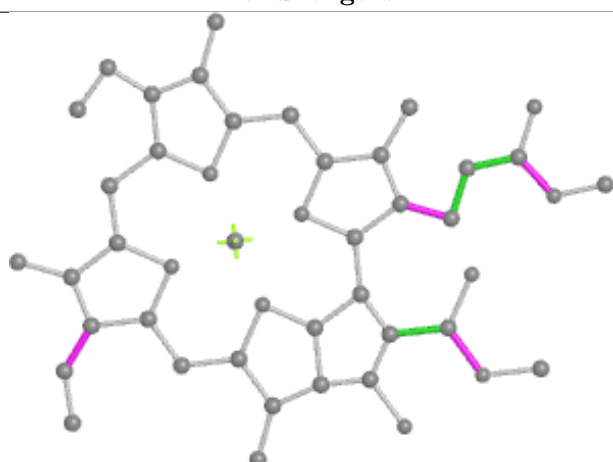
## Ligand CLA R 316



Bond lengths



Bond angles

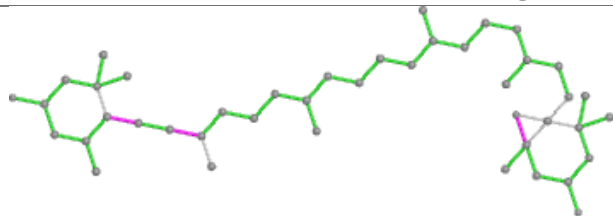


Torsions

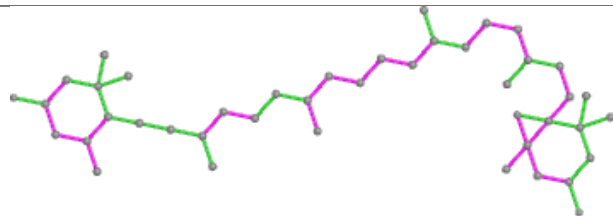


Rings

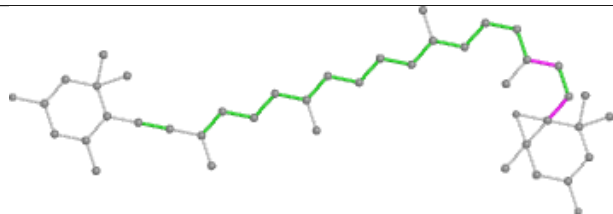
## Ligand DD6 H 302



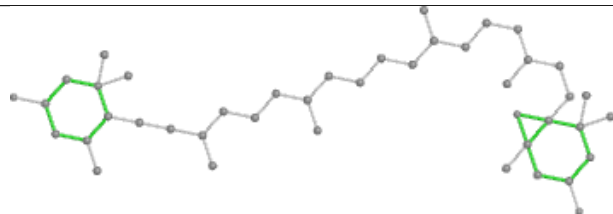
Bond lengths



Bond angles

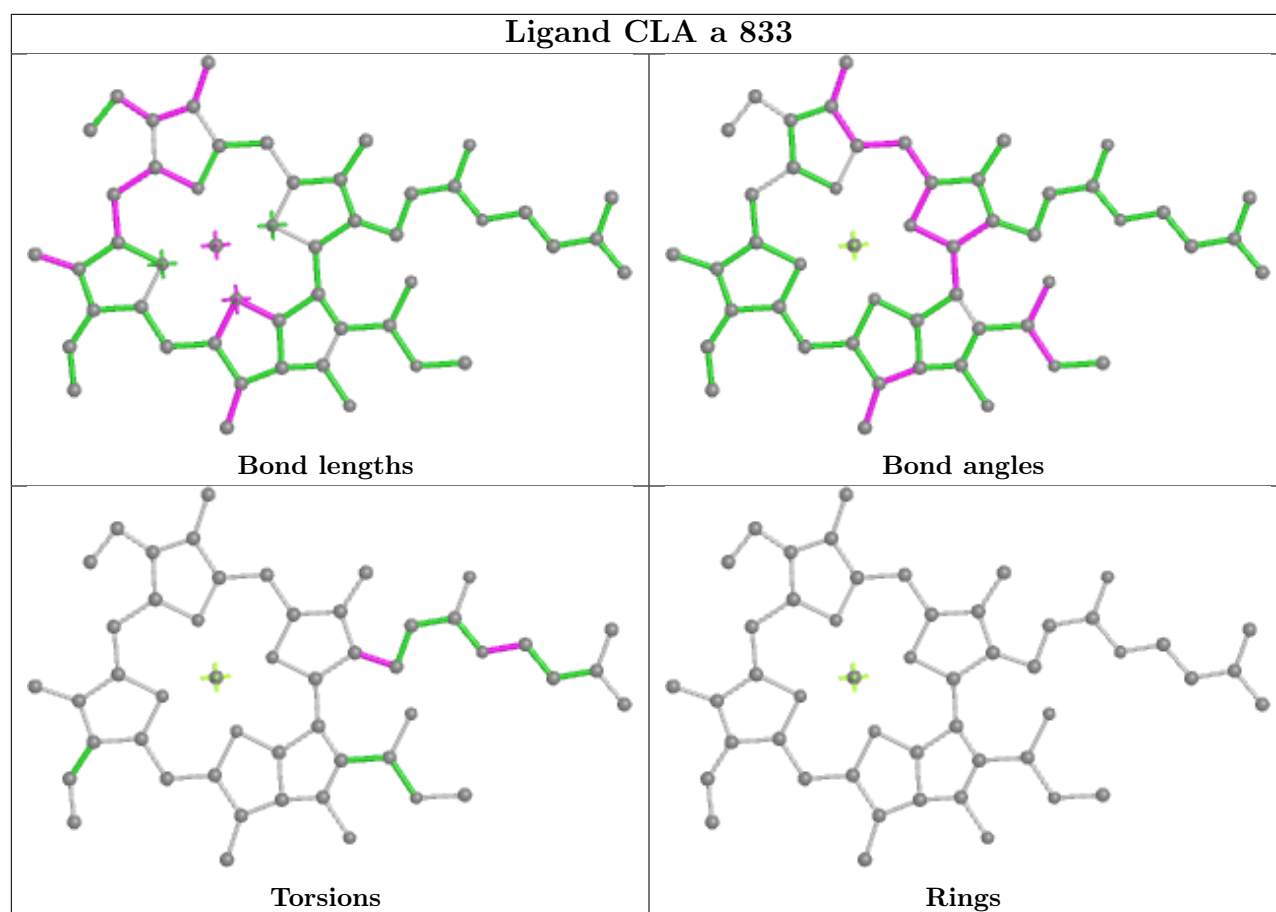


Torsions

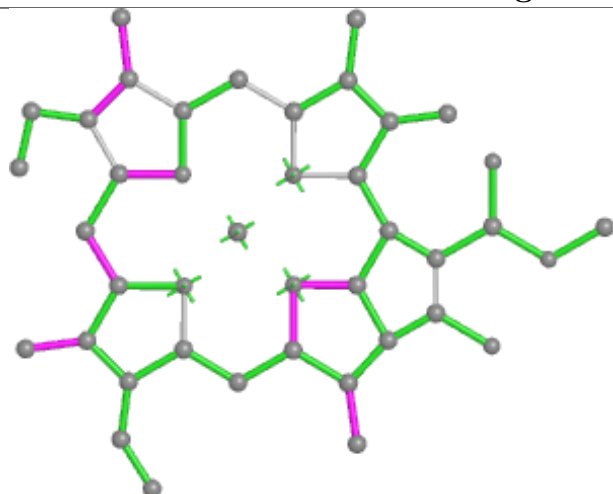


Rings

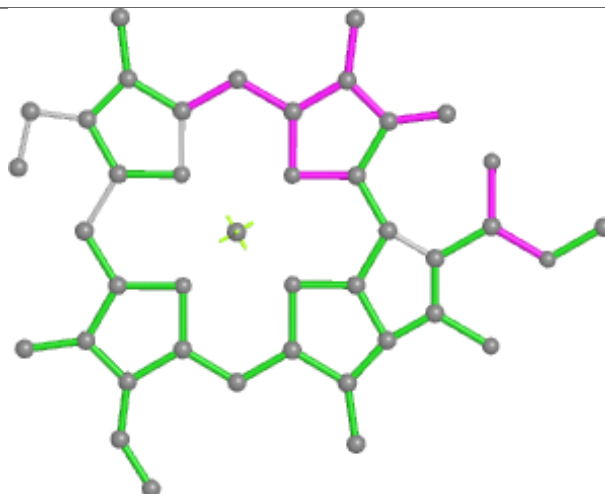




## Ligand CLA P 316



Bond lengths



Bond angles

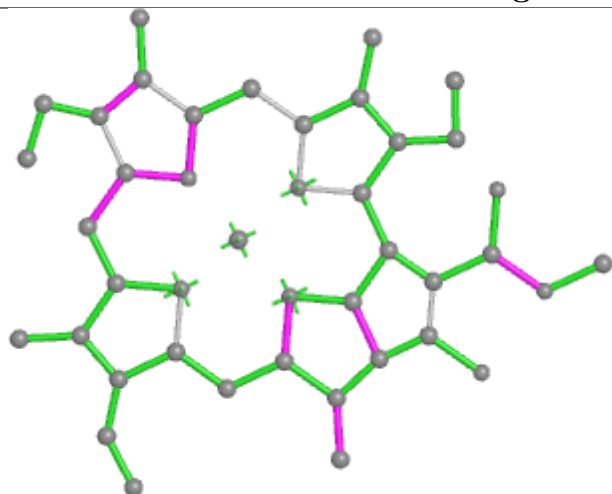


Torsions

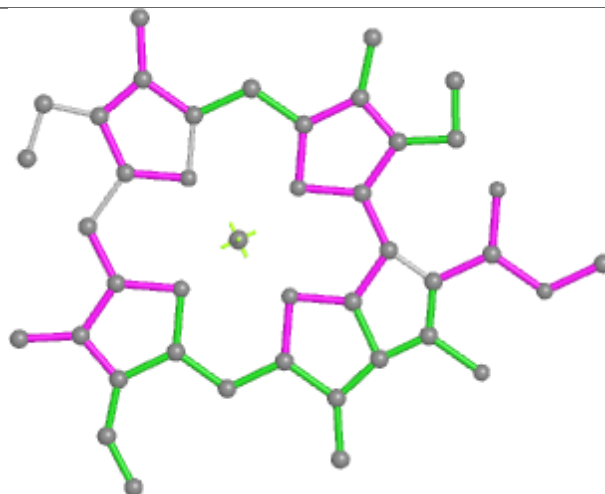


Rings

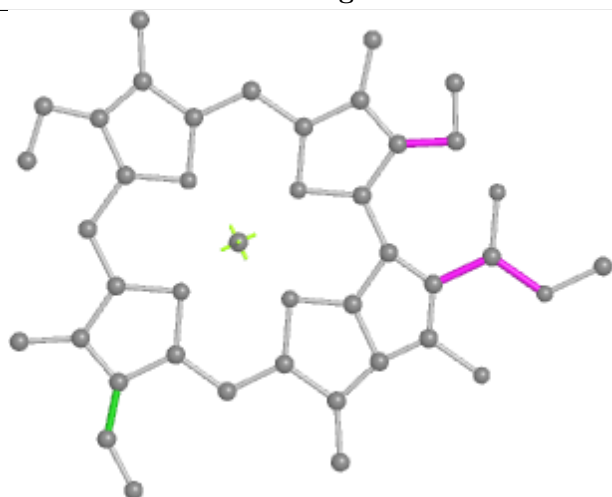
## Ligand CLA X 313



Bond lengths



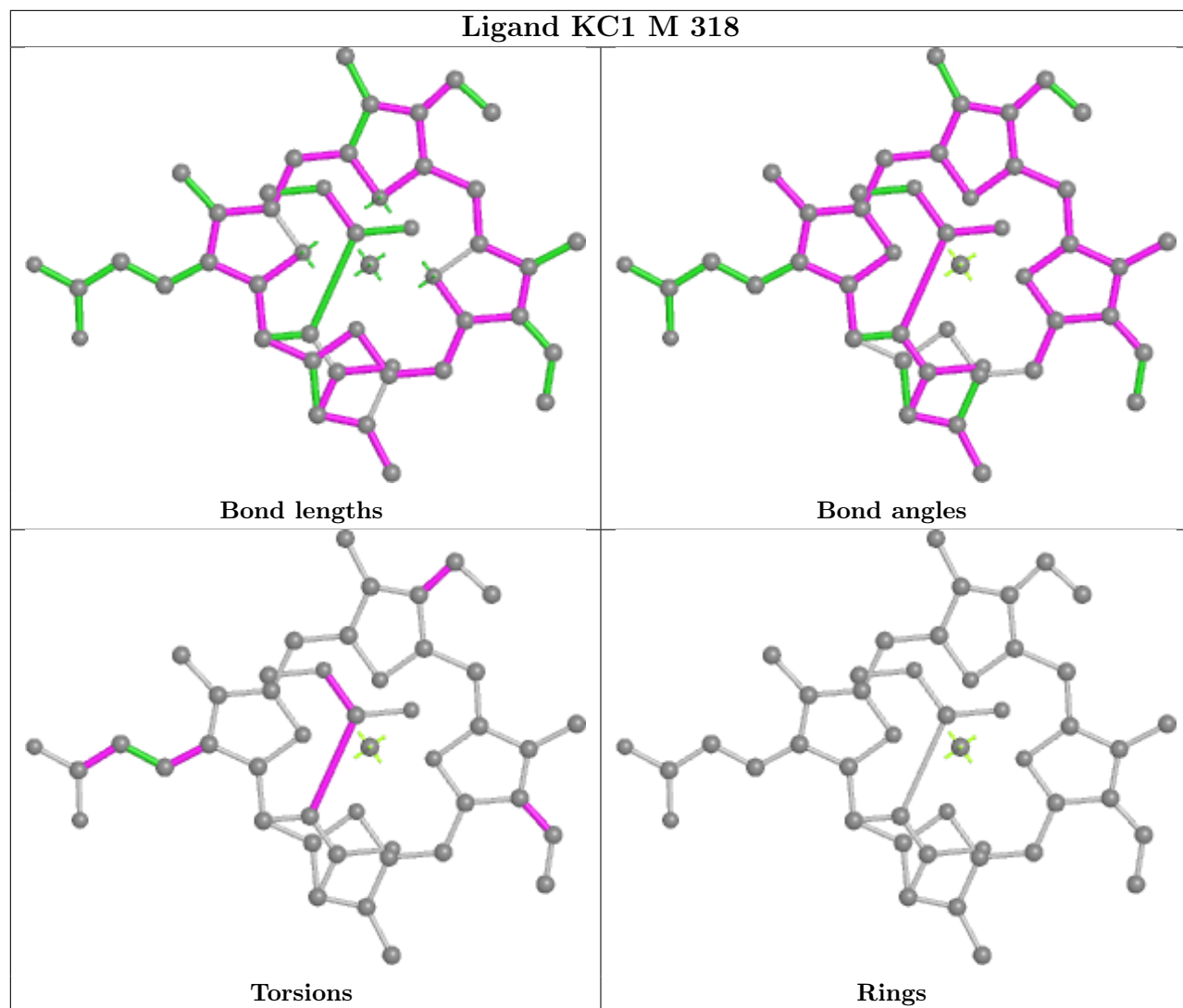
Bond angles



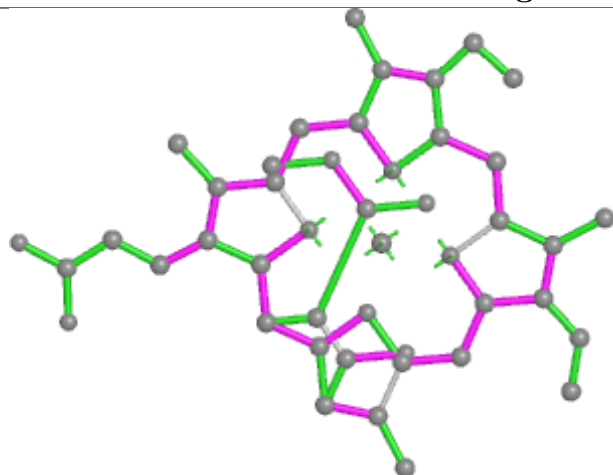
Torsions



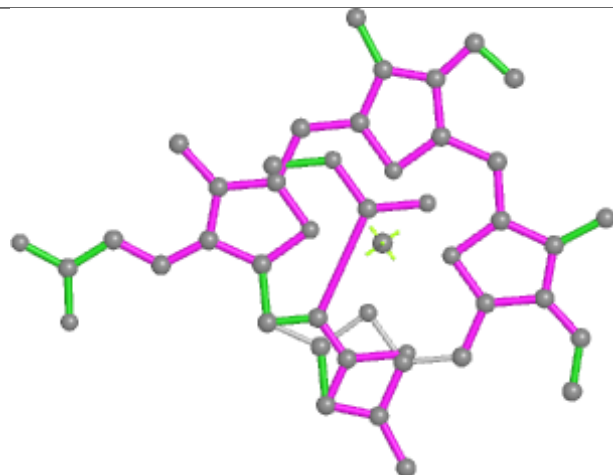
Rings



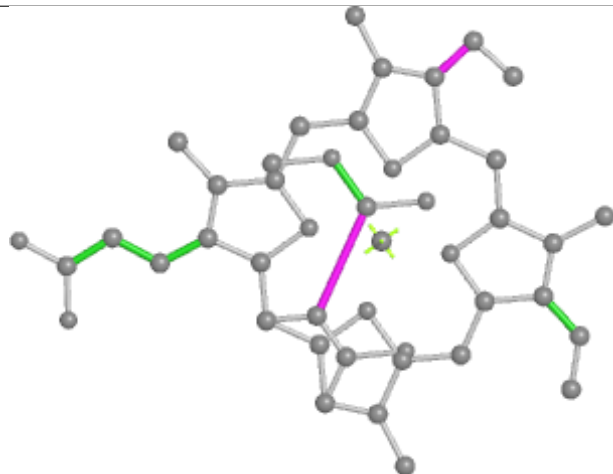
## Ligand KC1 O 313



Bond lengths



Bond angles

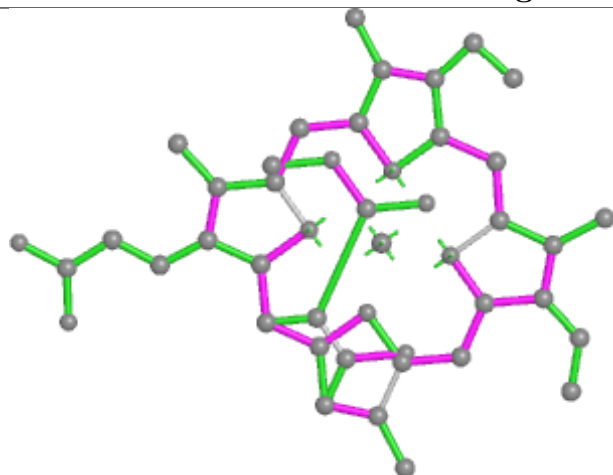


Torsions

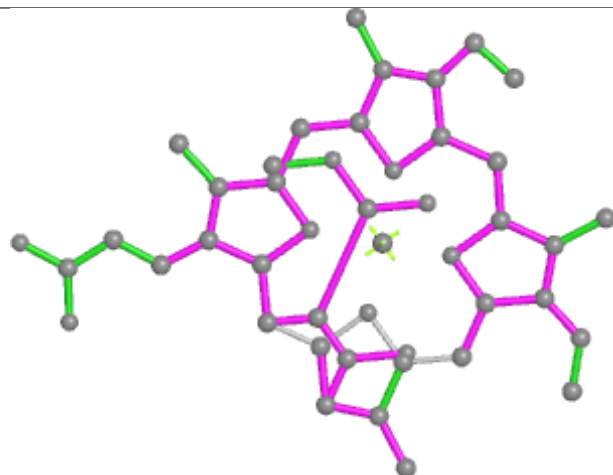


Rings

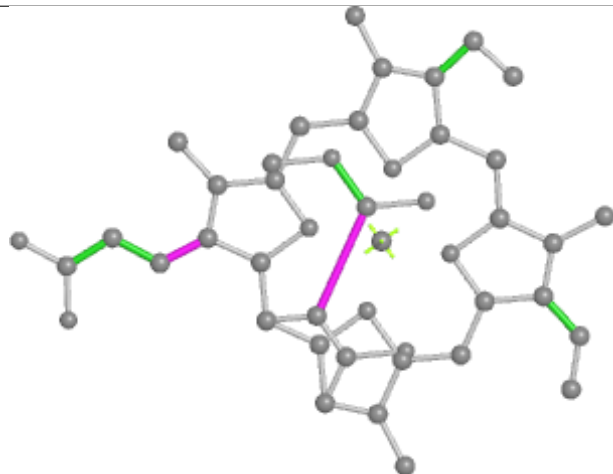
## Ligand KC1 X 311



Bond lengths



Bond angles

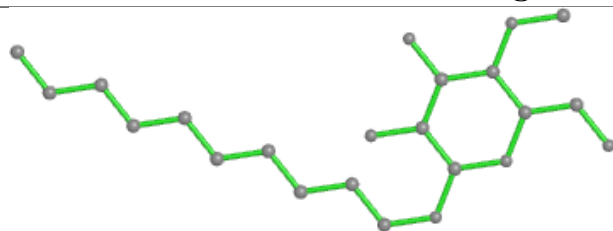


Torsions

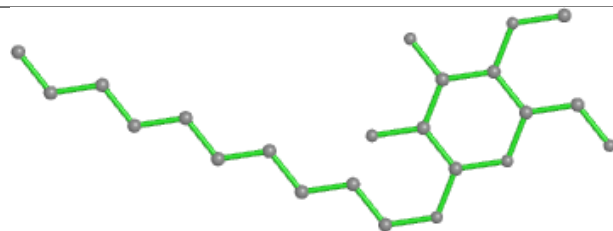


Rings

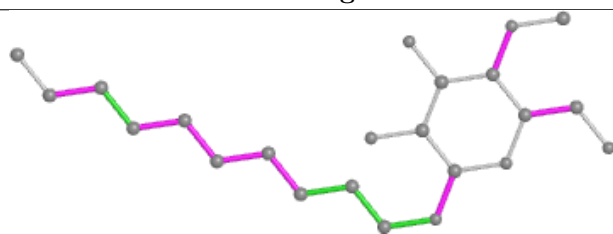
## Ligand LMT E 321



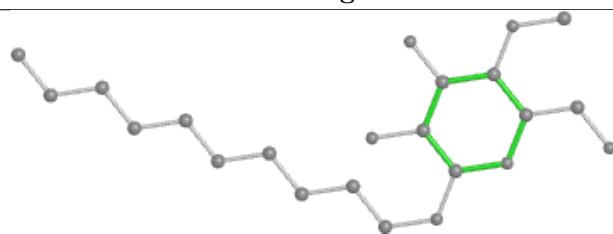
Bond lengths



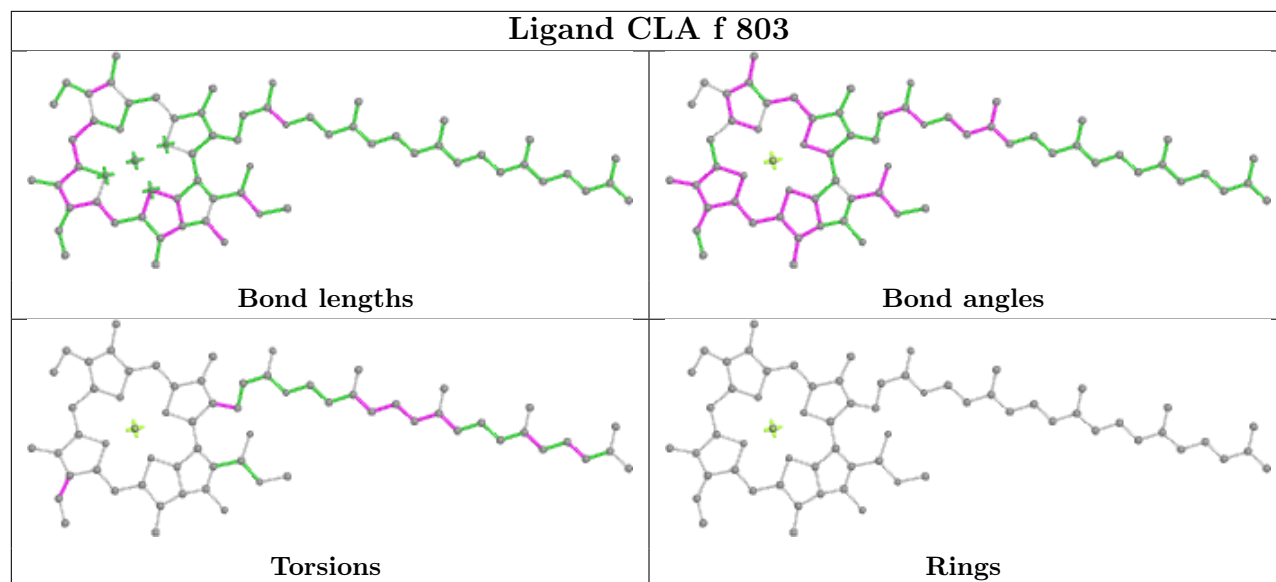
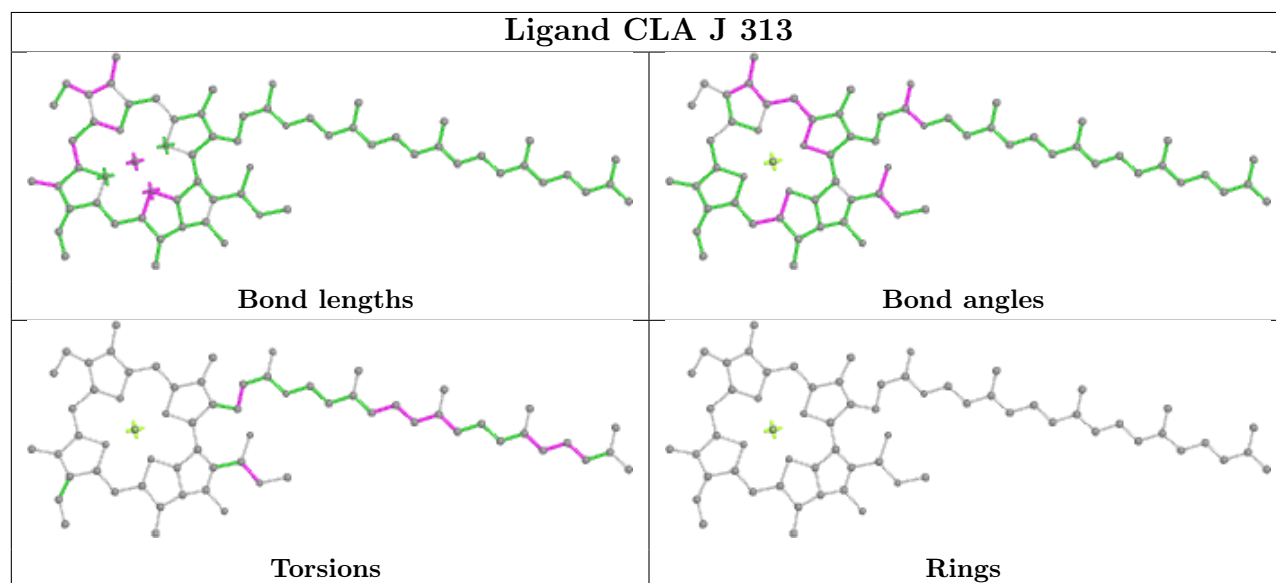
Bond angles



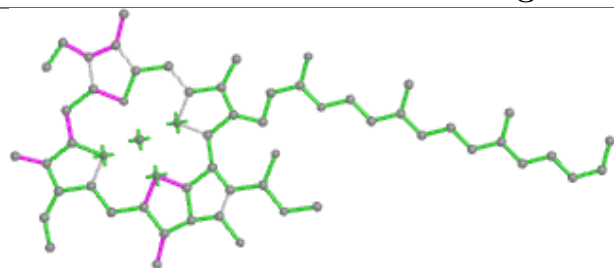
Torsions



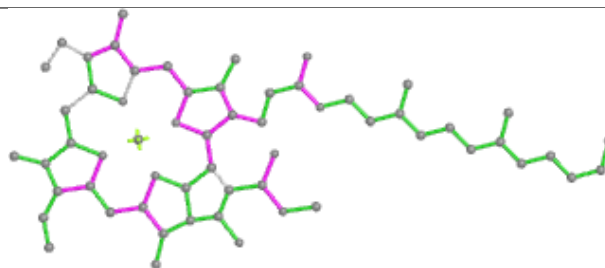
Rings

**Ligand CLA f 803****Ligand CLA J 313**

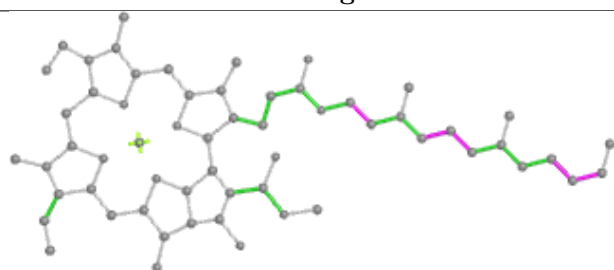
## Ligand CLA b 819



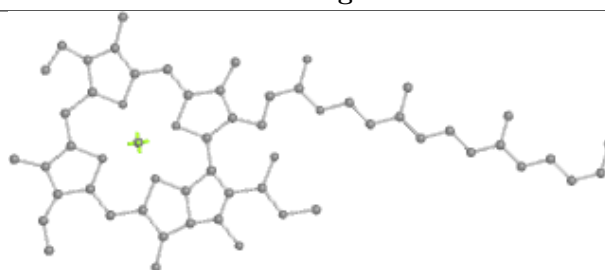
Bond lengths



Bond angles

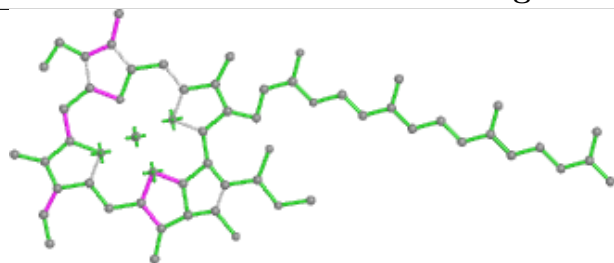


Torsions

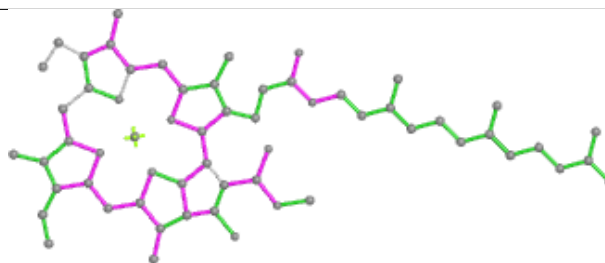


Rings

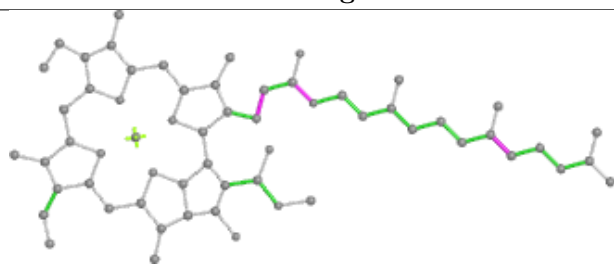
## Ligand CLA H 307



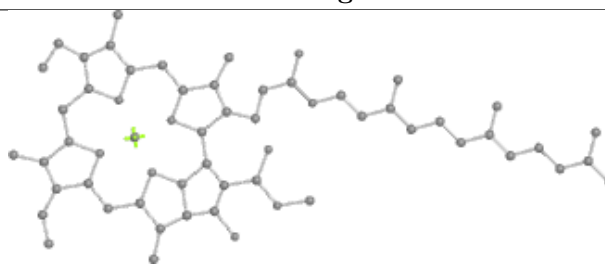
Bond lengths



Bond angles

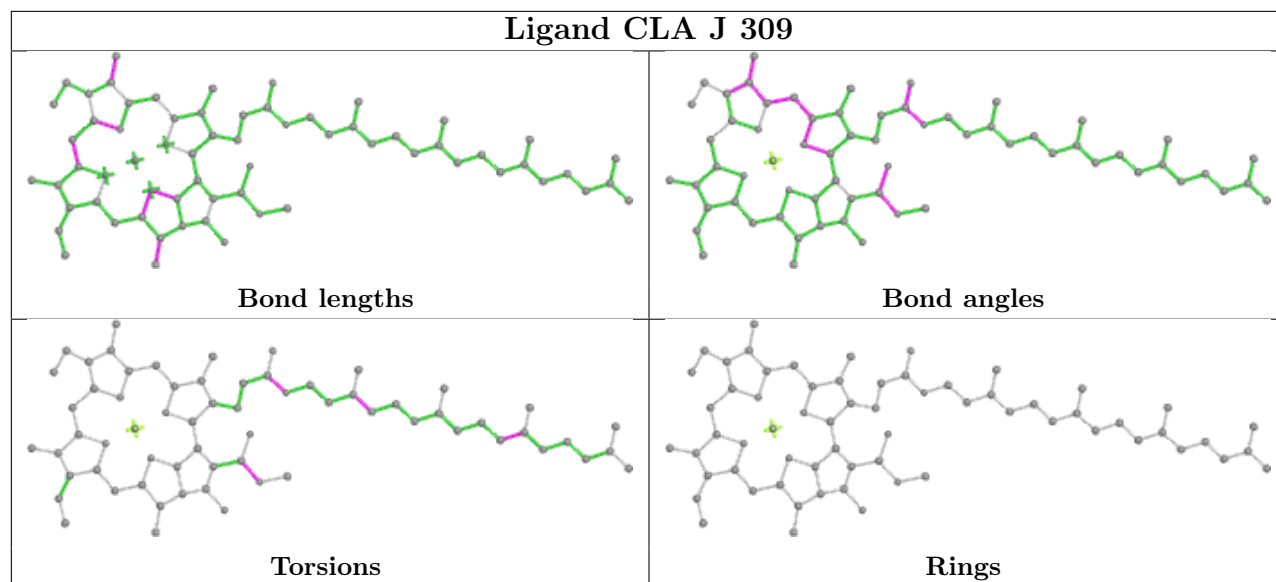
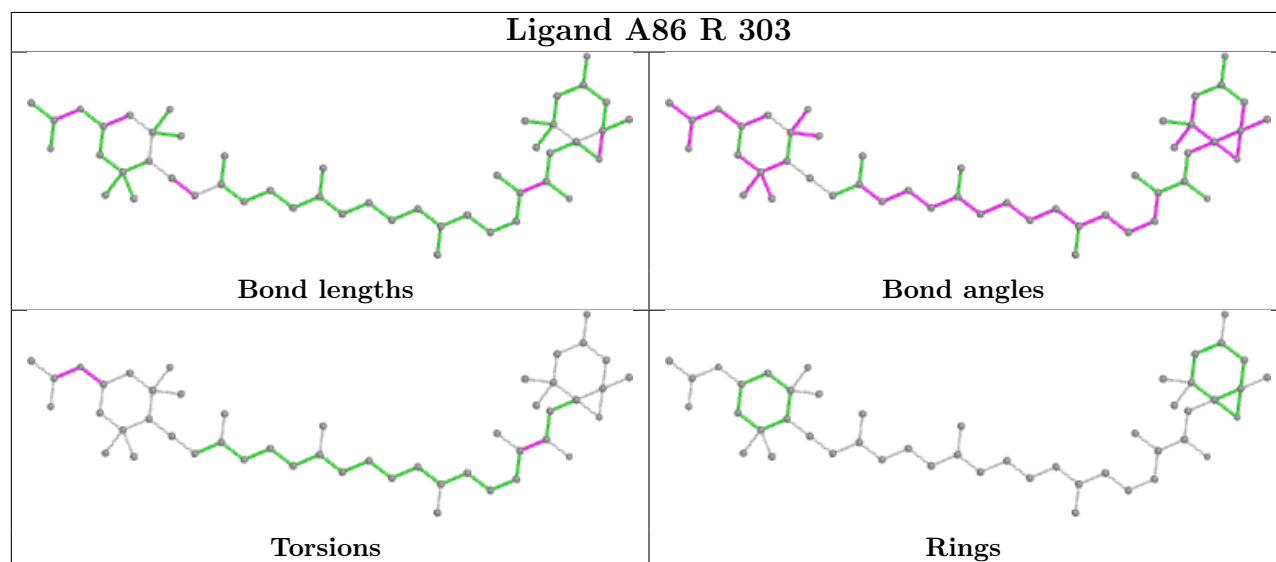


Torsions

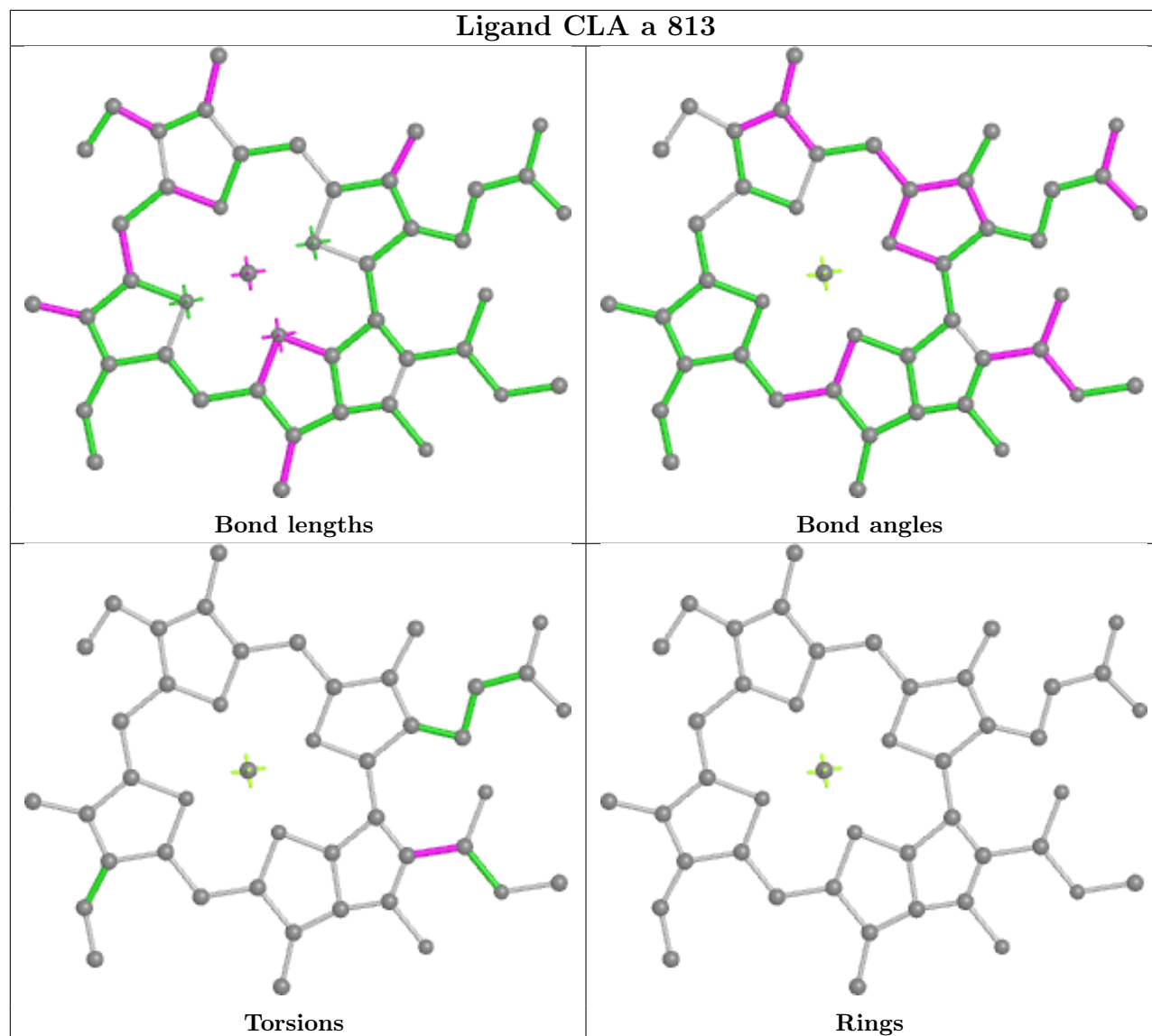


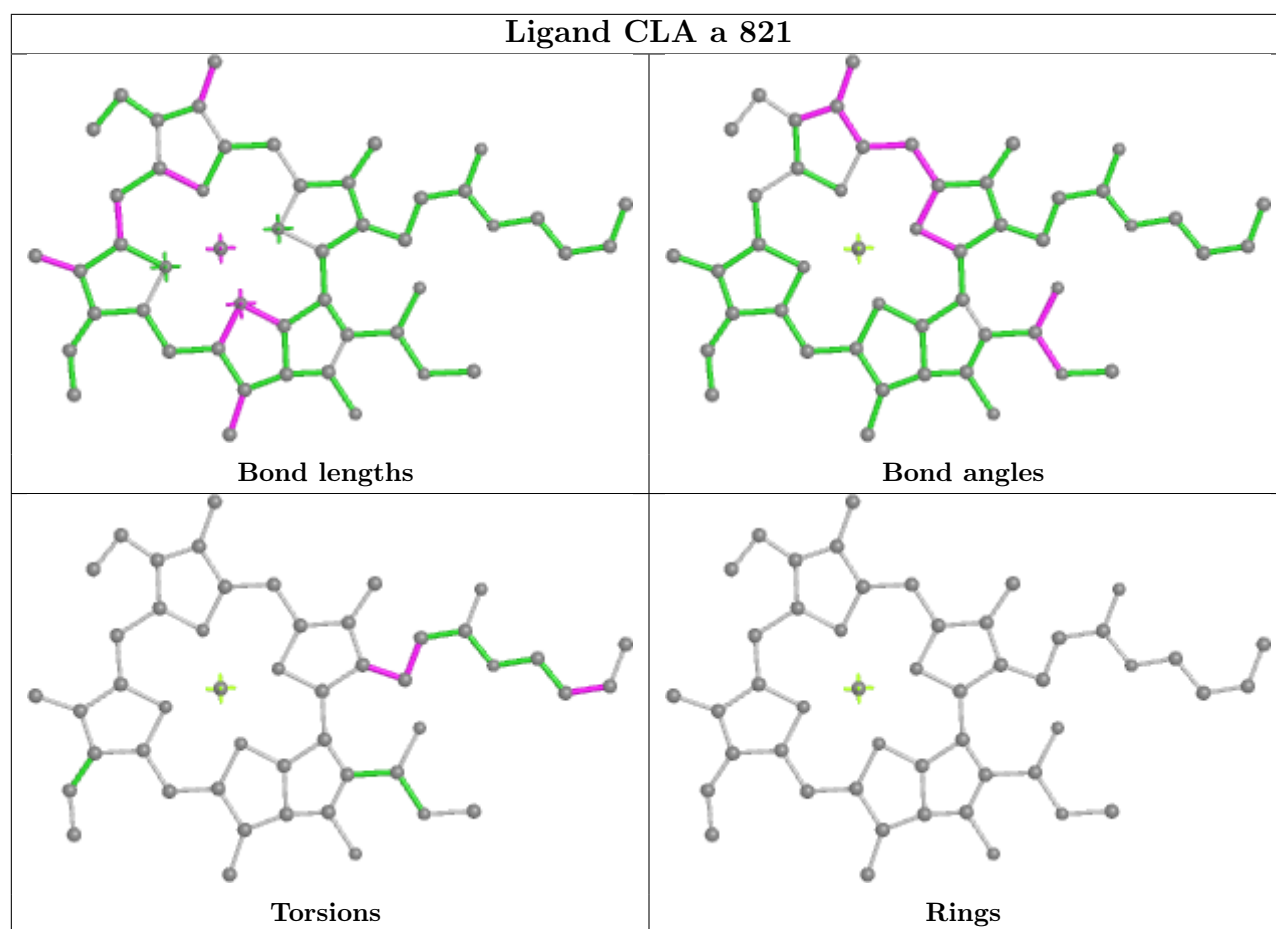
Rings



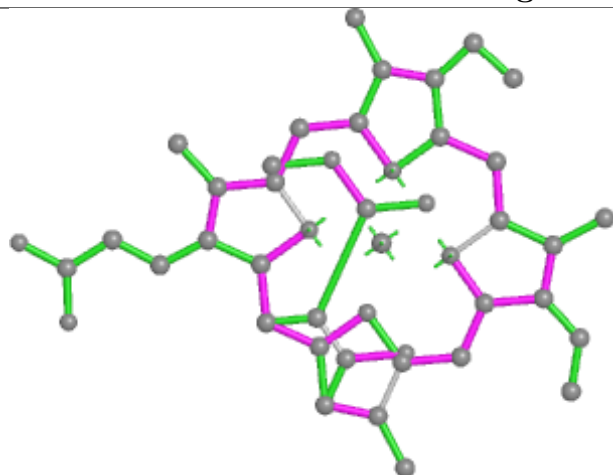
**Ligand CLA J 309****Ligand A86 R 303**

## Ligand CLA a 813

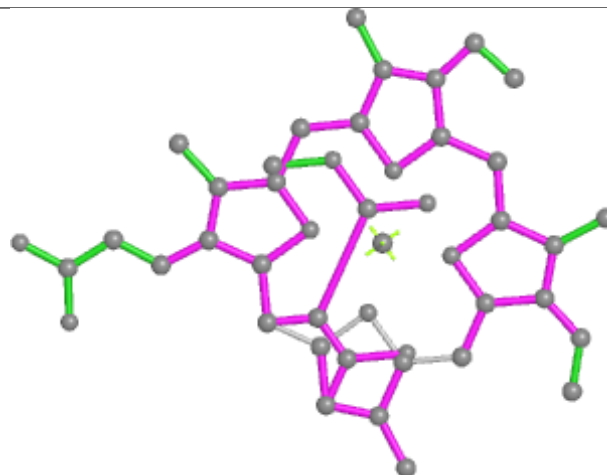




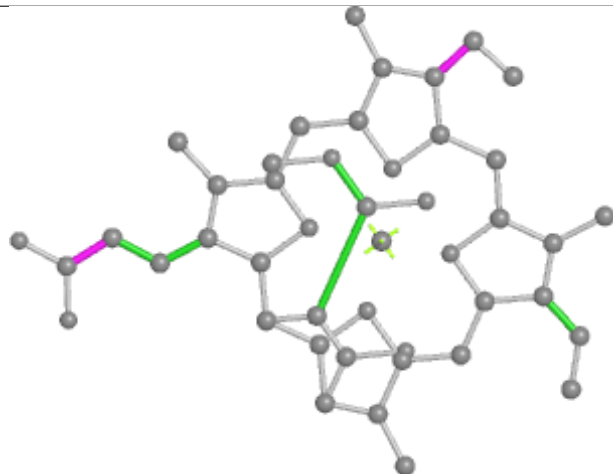
## Ligand KC1 B 310



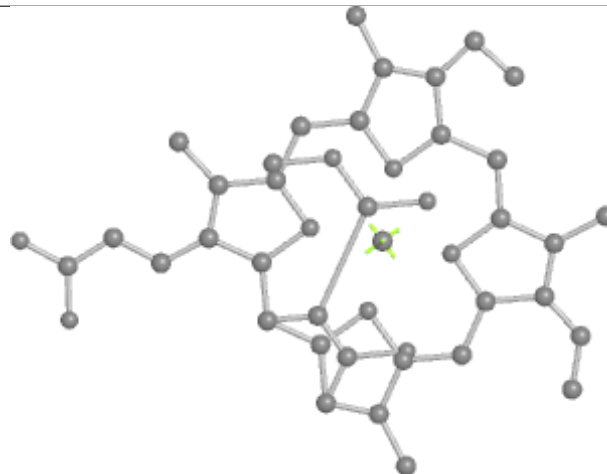
Bond lengths



Bond angles

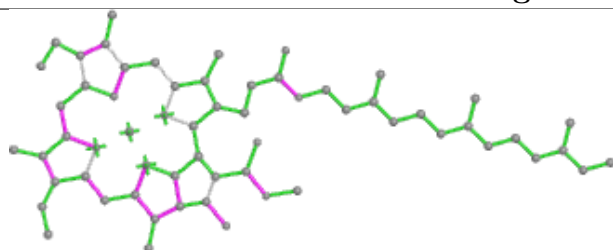


Torsions

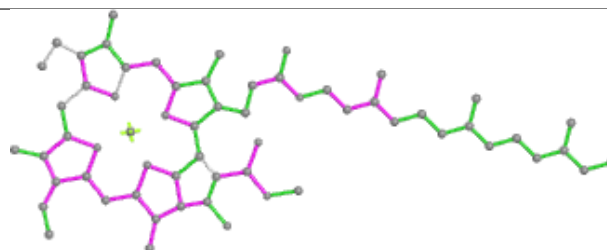


Rings

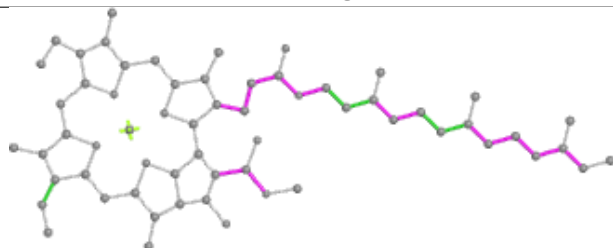
## Ligand CLA K 307



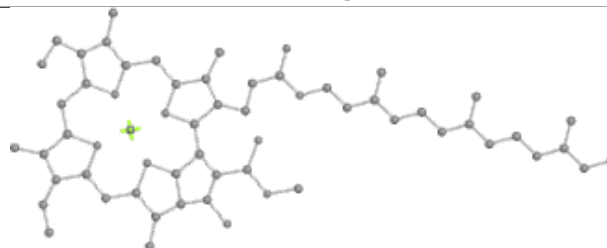
Bond lengths



Bond angles

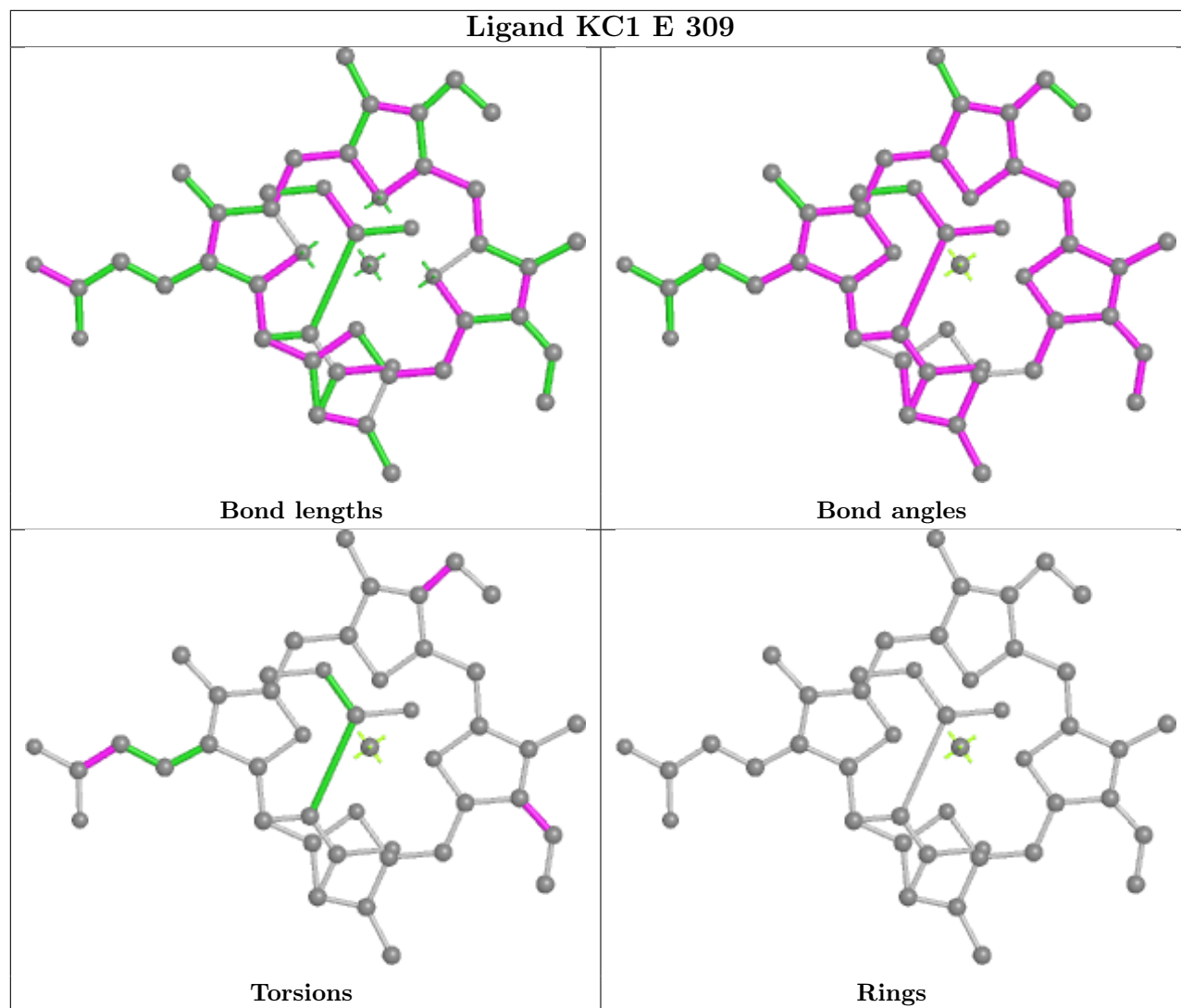


Torsions

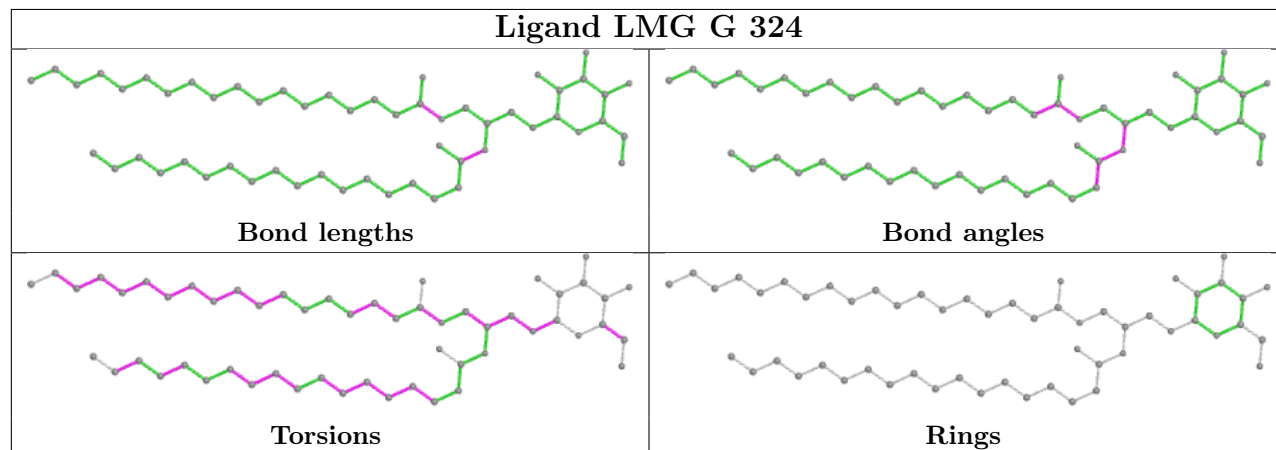


Rings

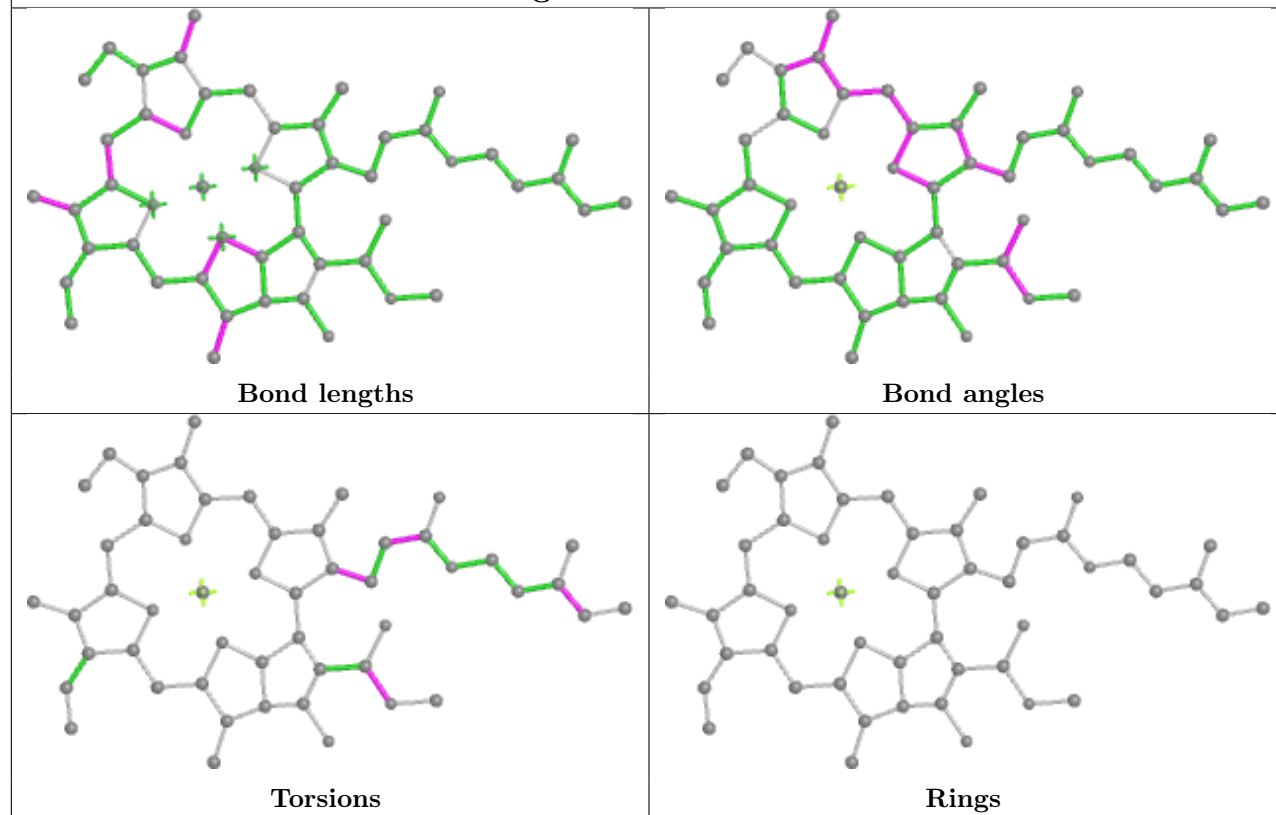
## Ligand KC1 E 309



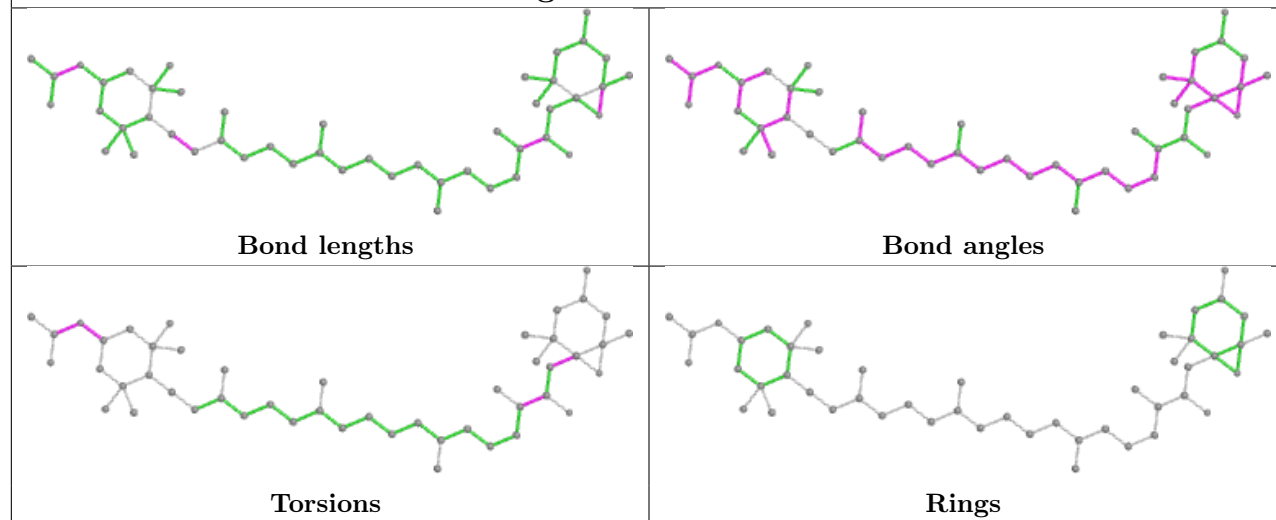
## Ligand LMG G 324

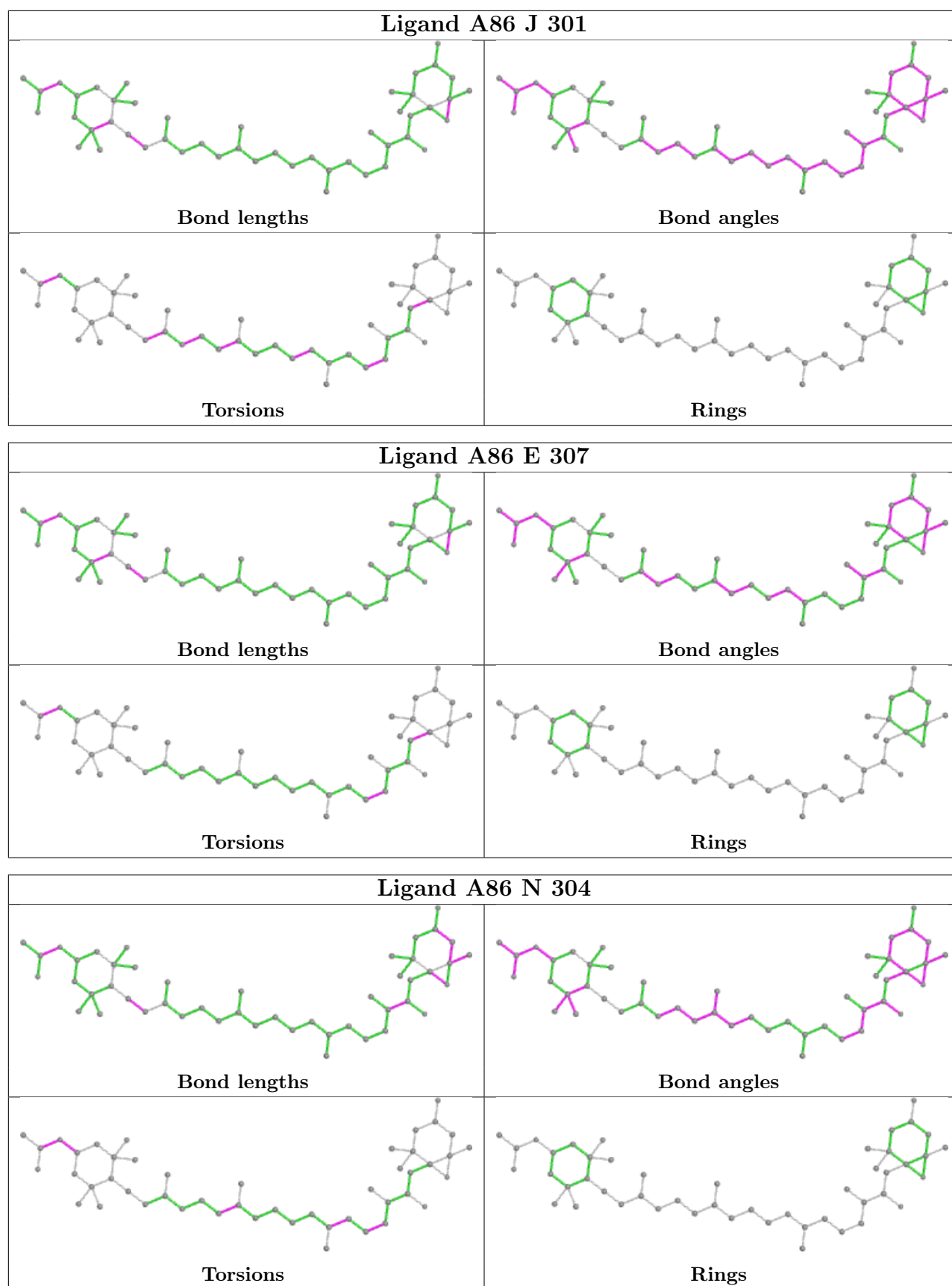


## Ligand CLA P 318

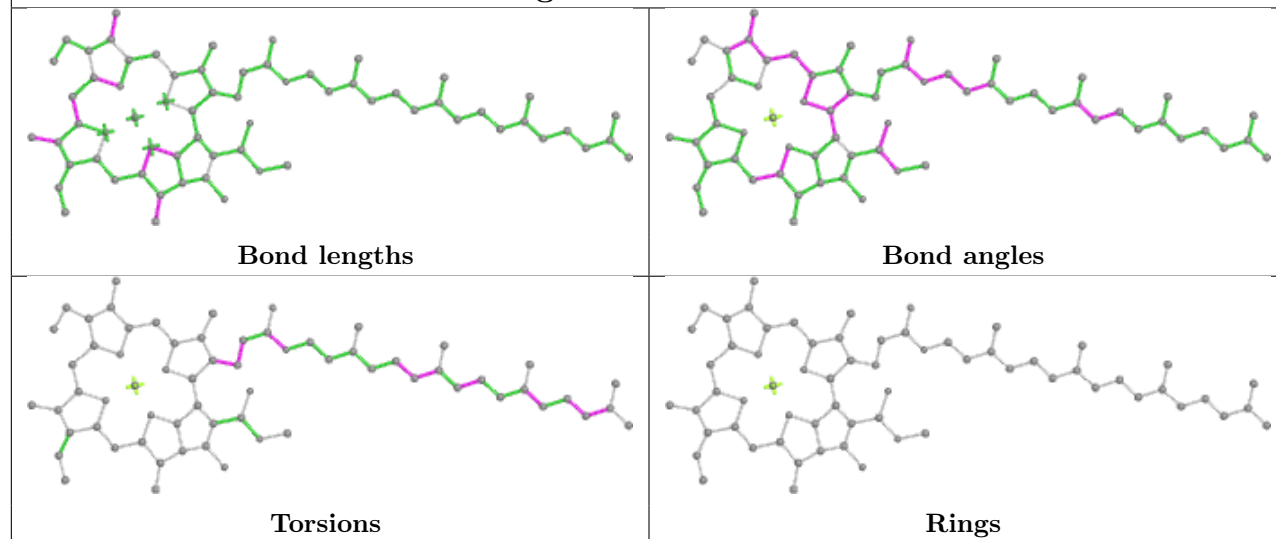


## Ligand A86 U 302

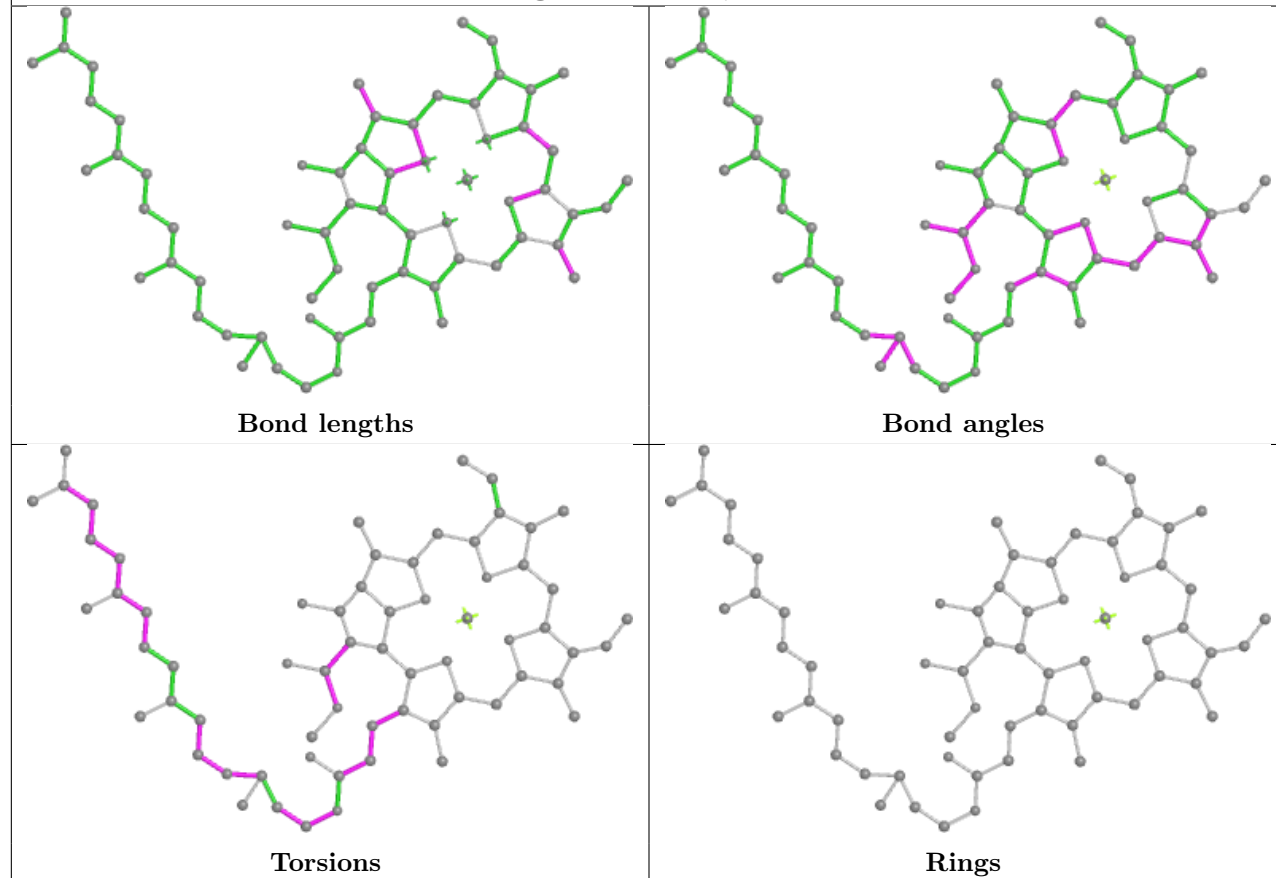




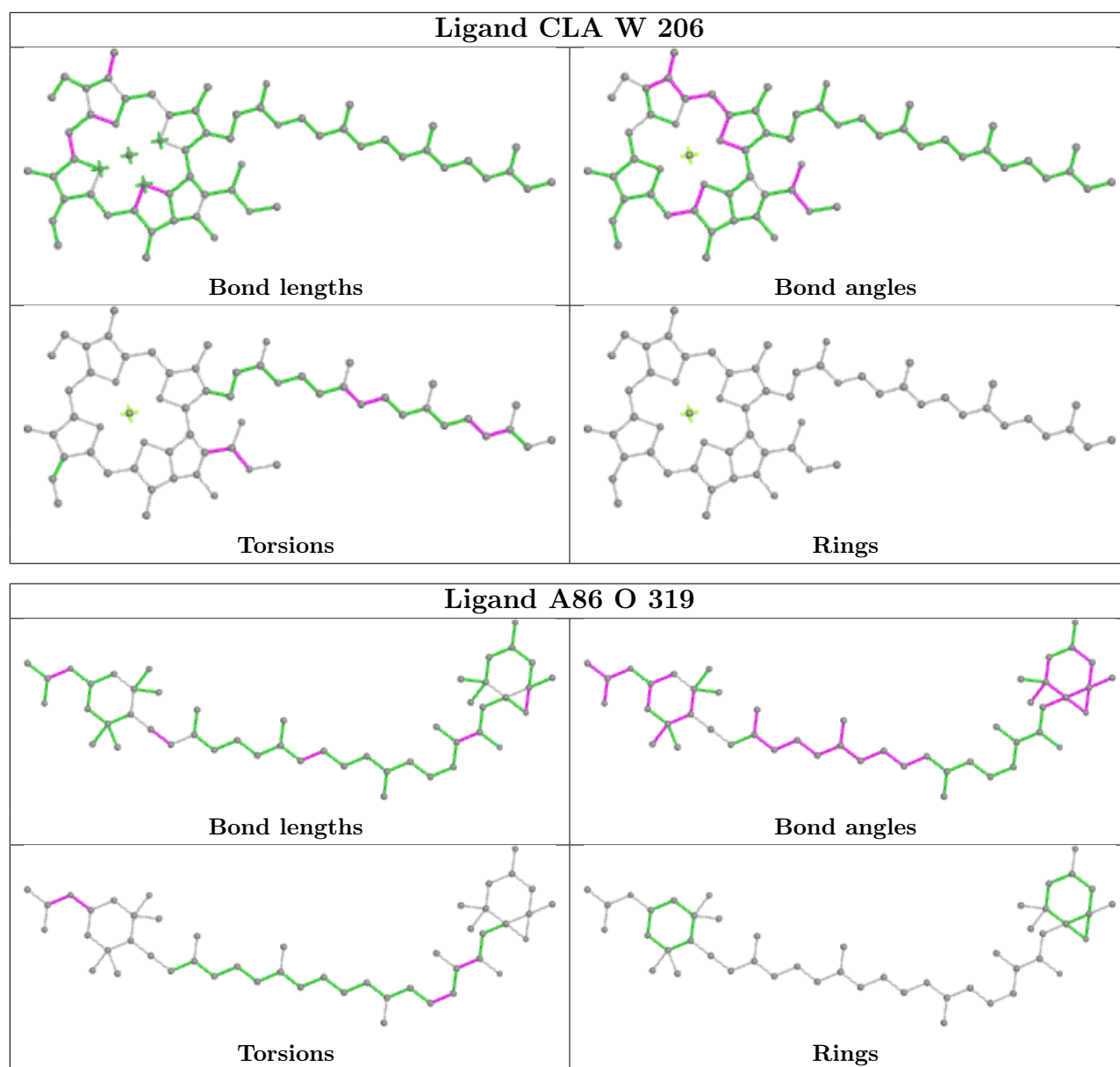
## Ligand CLA a 807

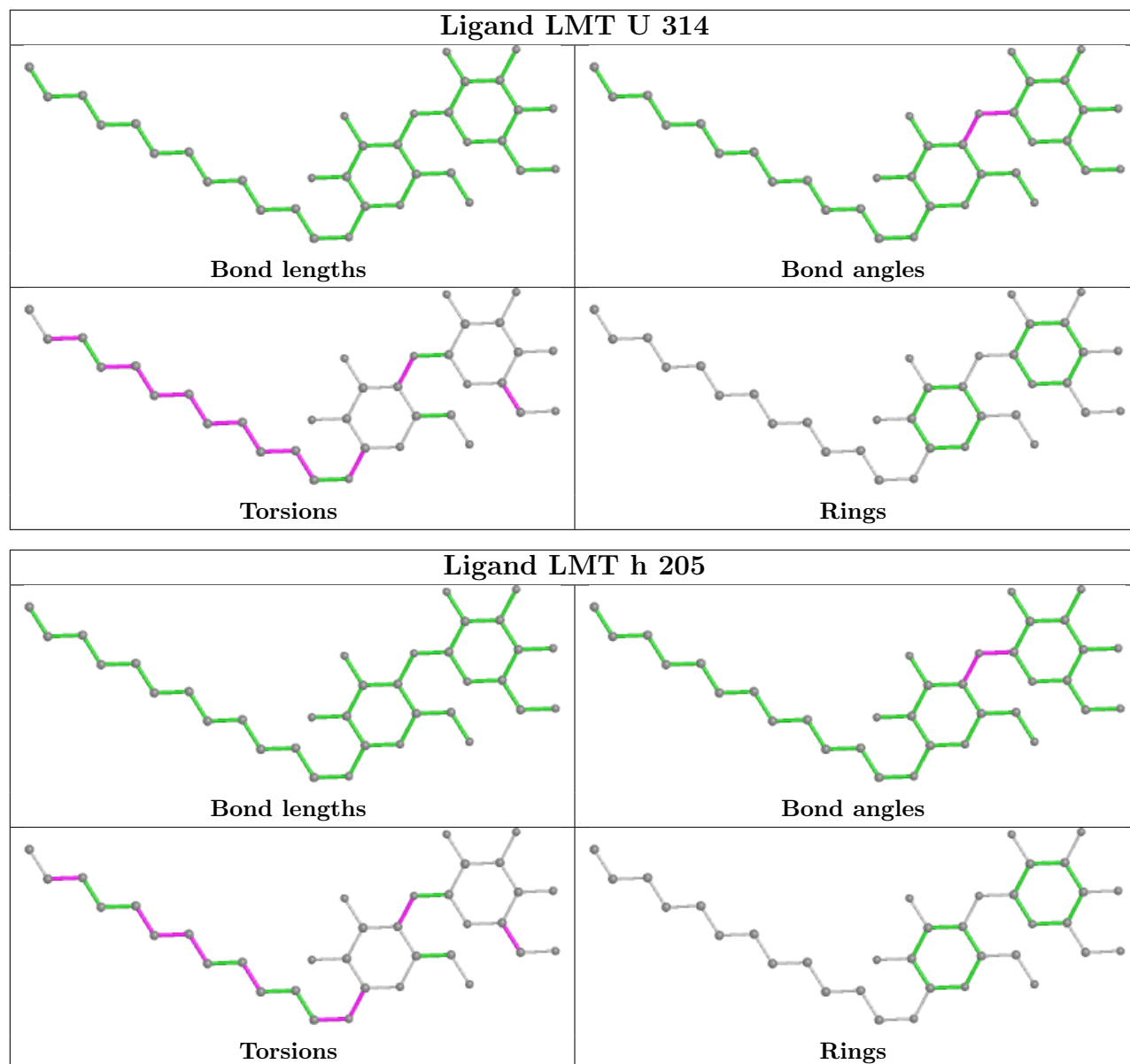


## Ligand CLA Q 314

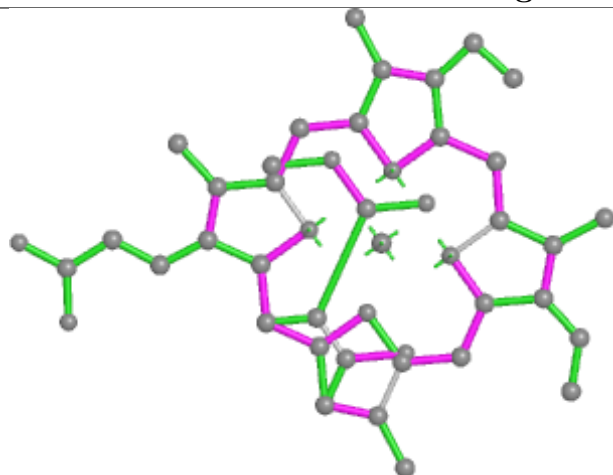




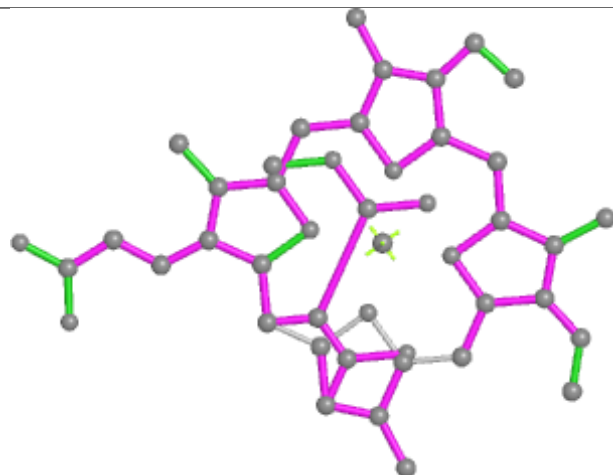




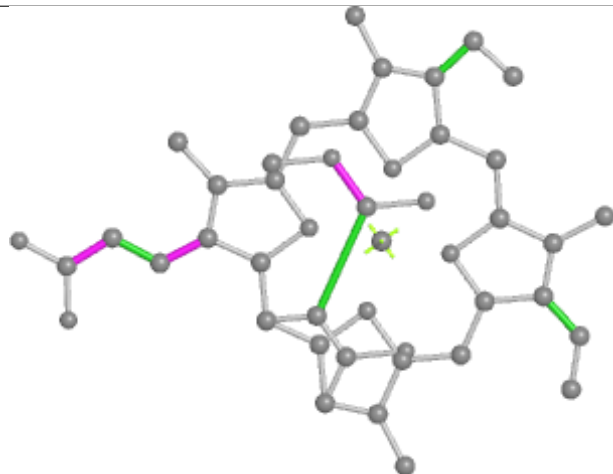
## Ligand KC1 D 314



Bond lengths



Bond angles

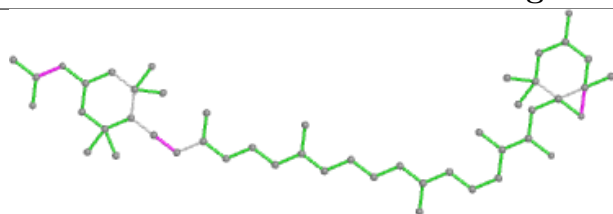


Torsions

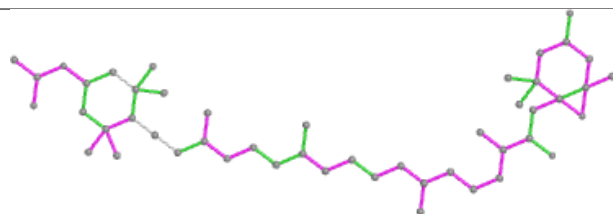


Rings

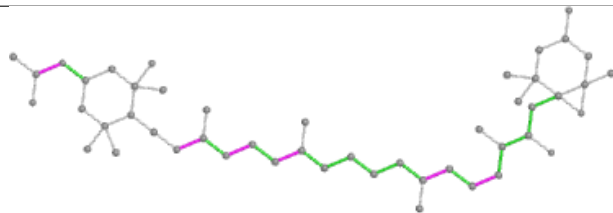
## Ligand A86 I 301



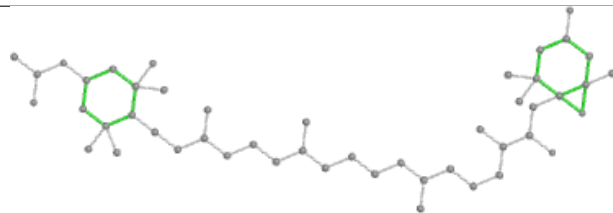
Bond lengths



Bond angles

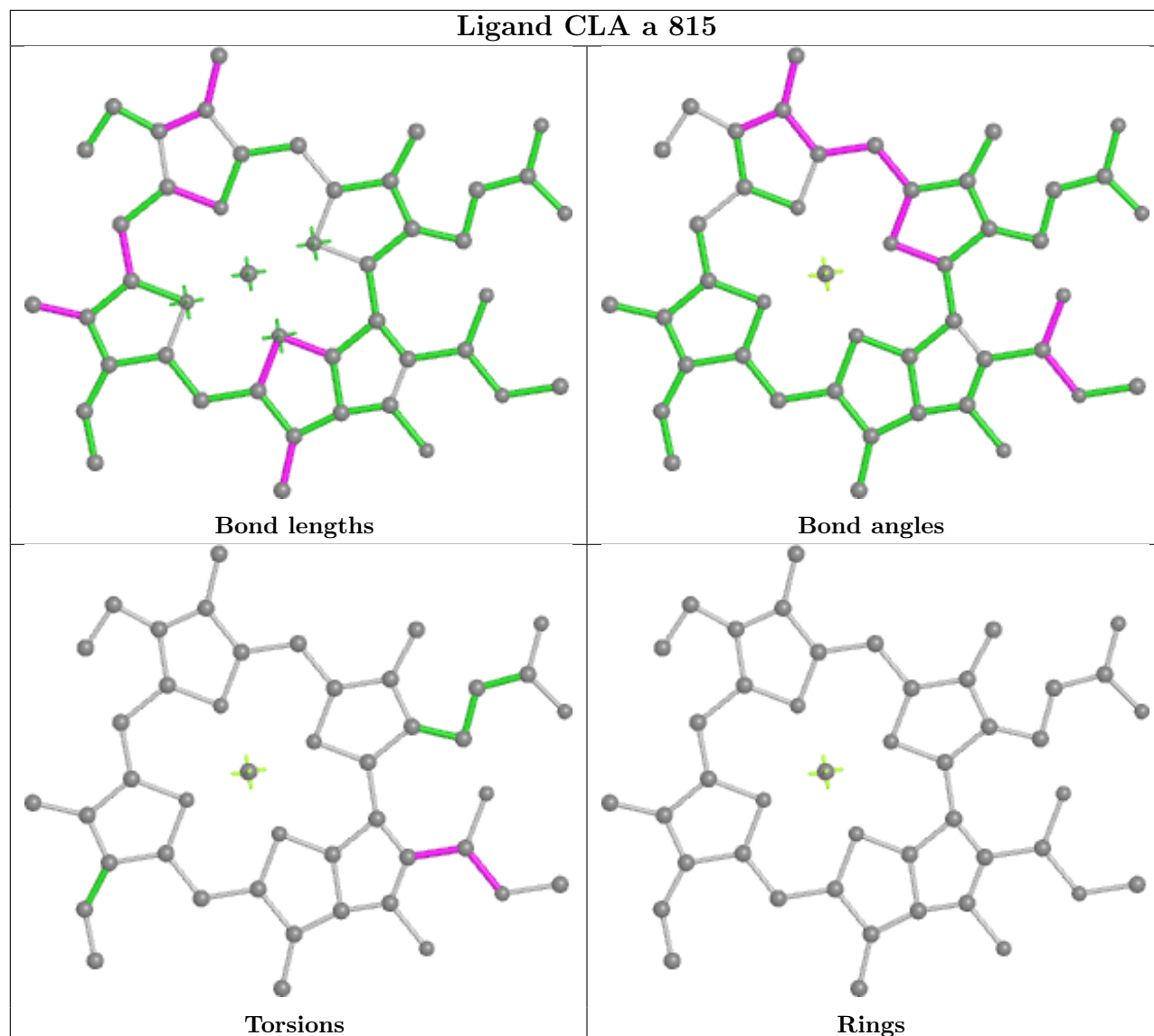


Torsions

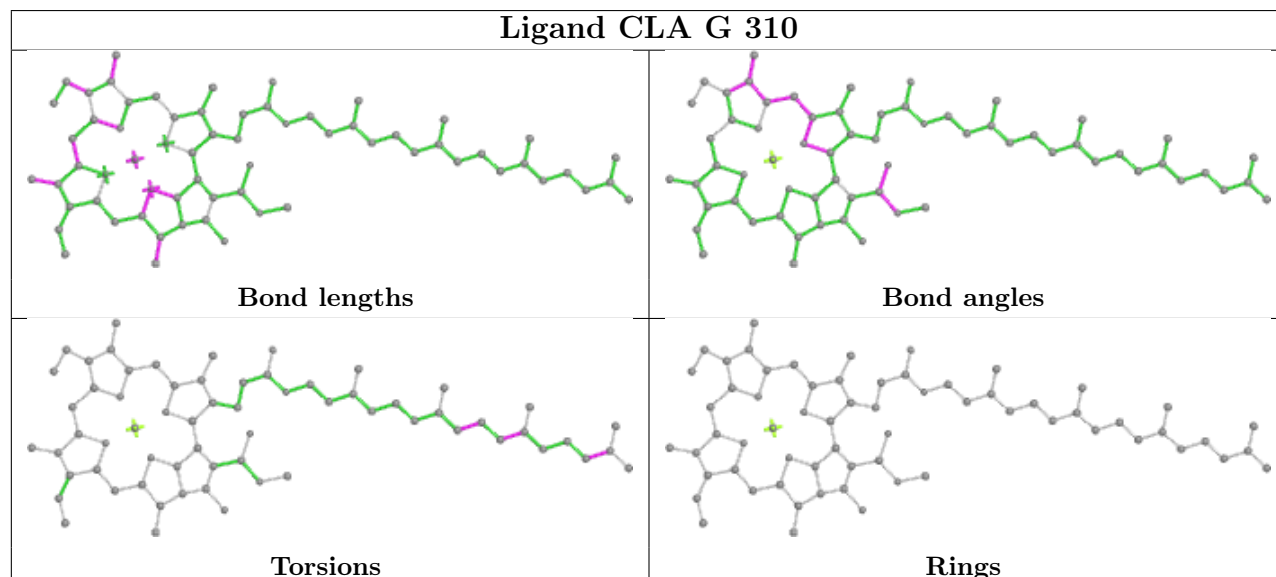


Rings

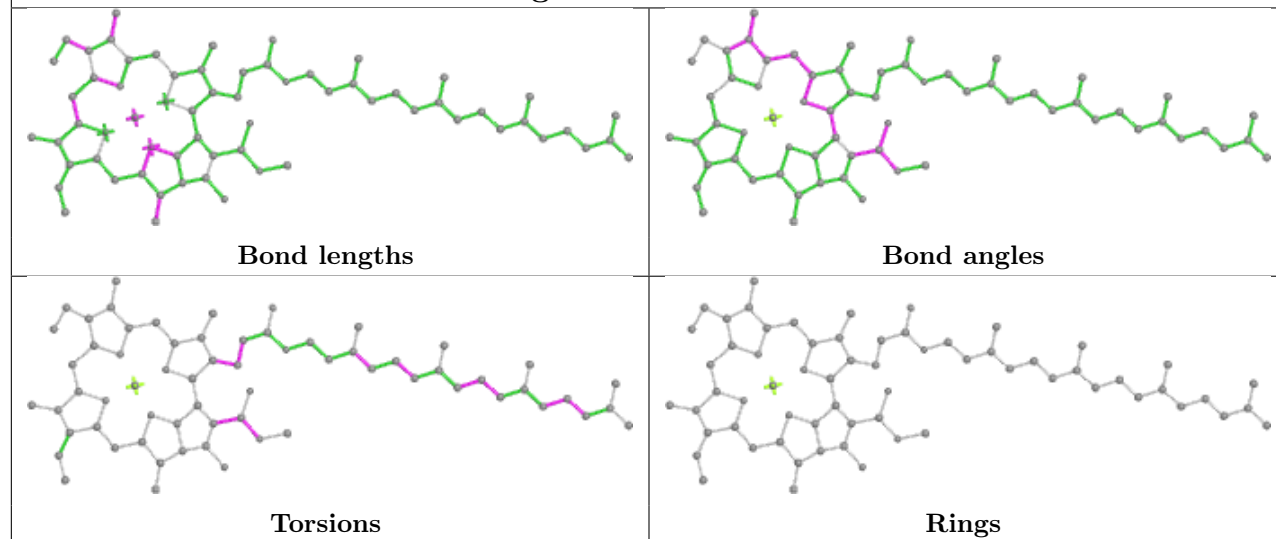
## Ligand CLA a 815



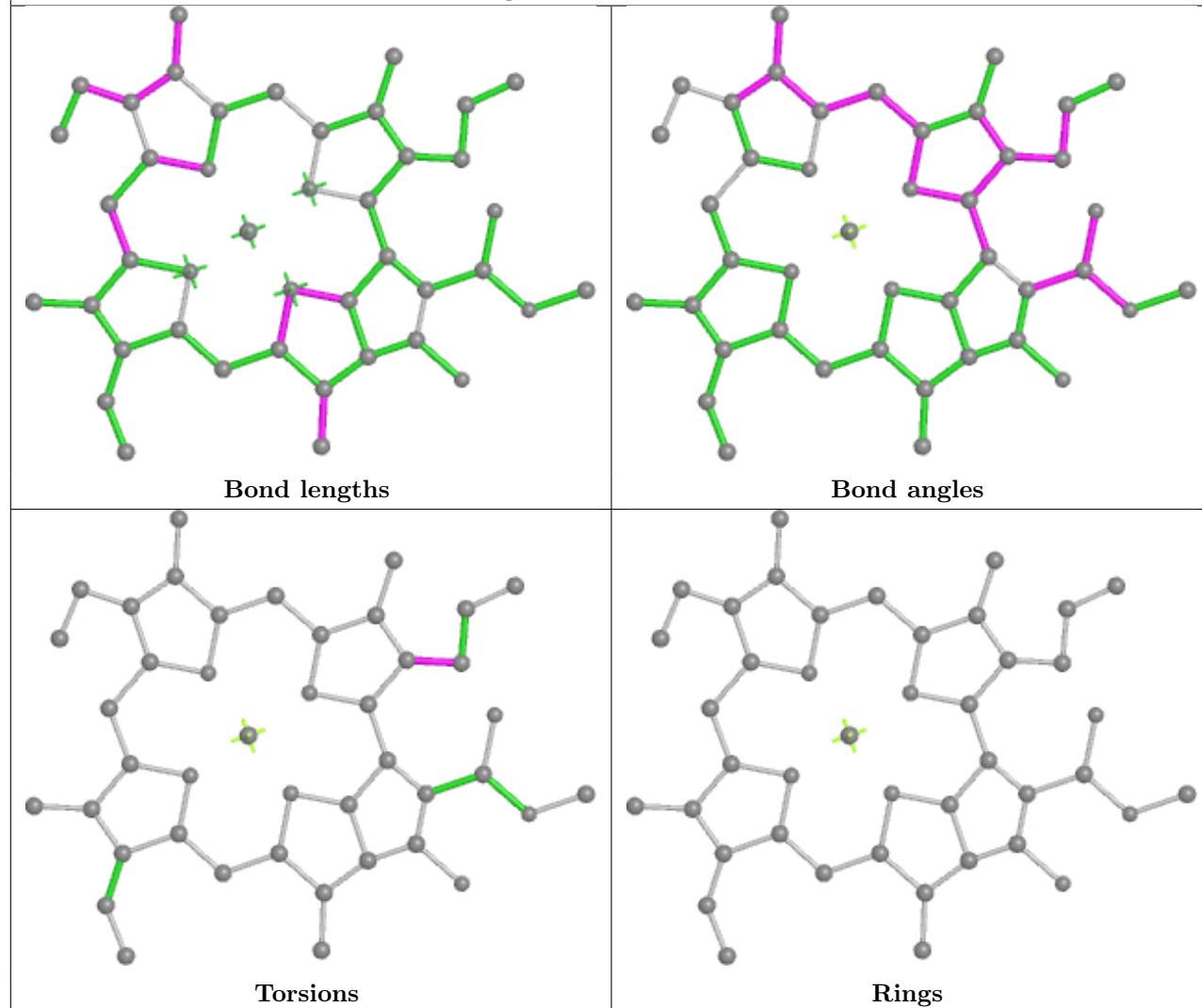
## Ligand CLA G 310

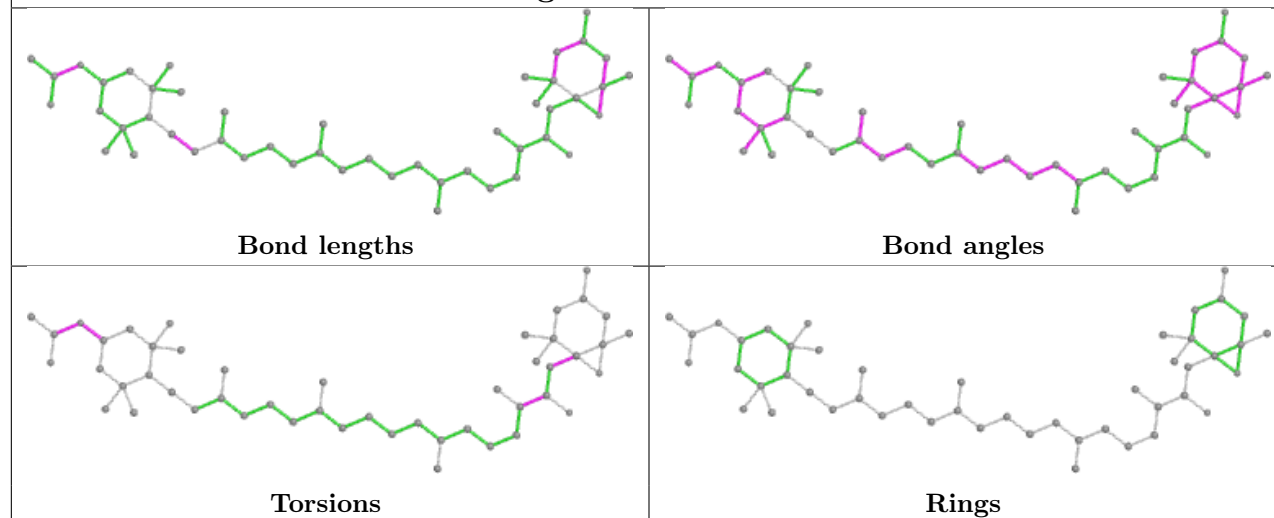
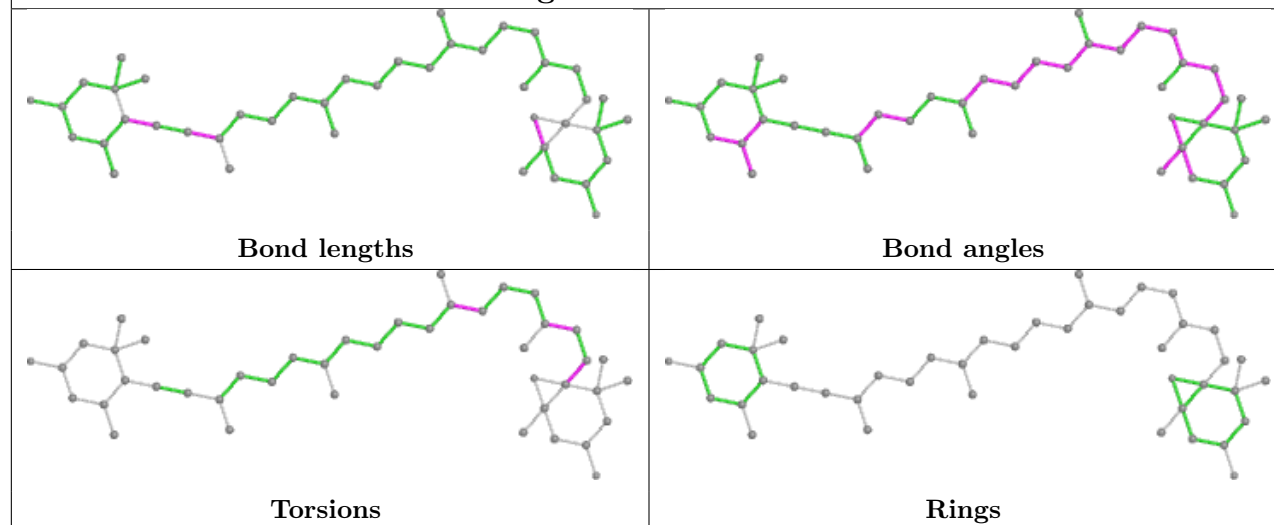


## Ligand CLA V 313

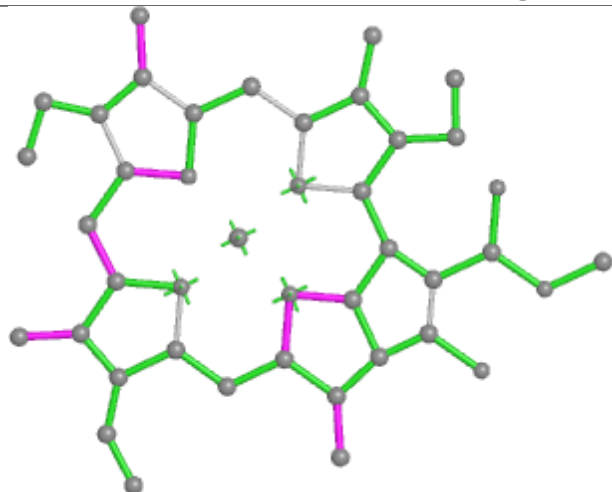


## Ligand CLA V 309

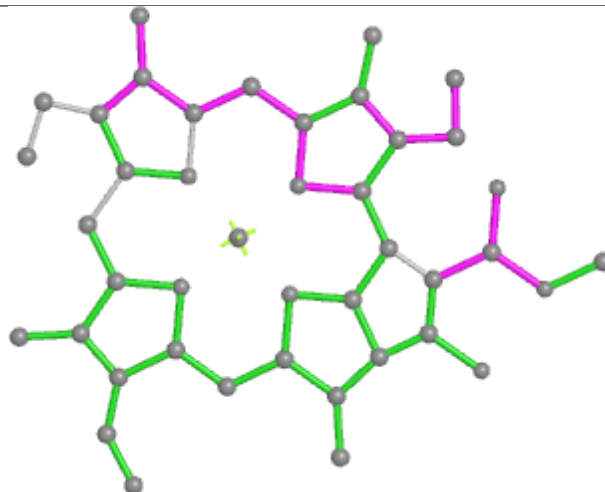


**Ligand A86 V 304****Ligand DD6 a 849**

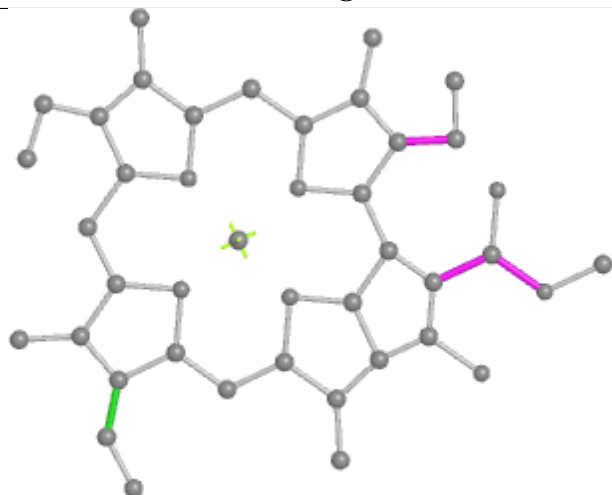
## Ligand CLA P 302



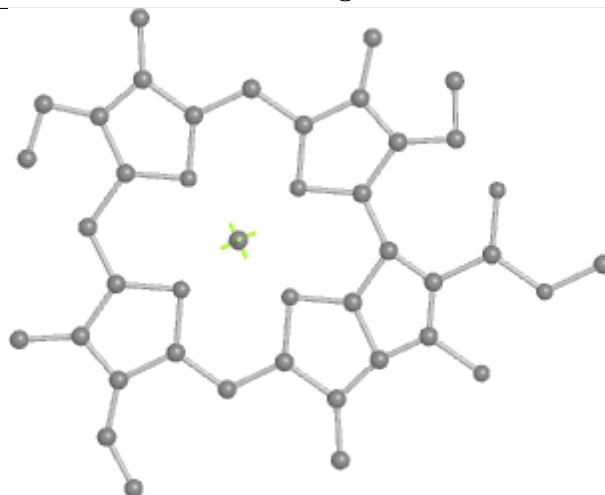
Bond lengths



Bond angles

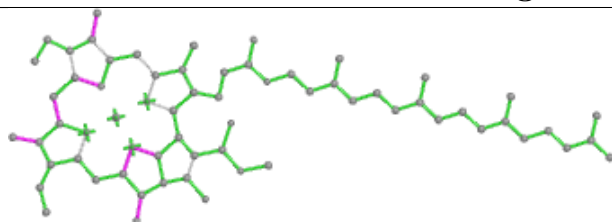


Torsions

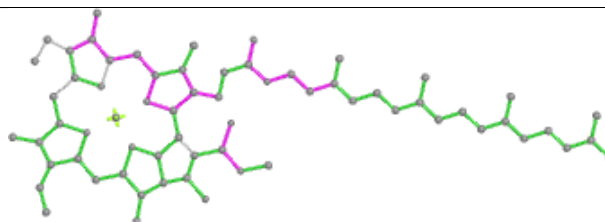


Rings

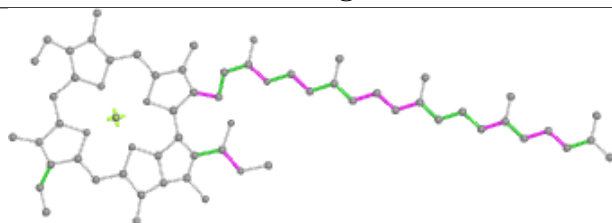
## Ligand CLA S 310



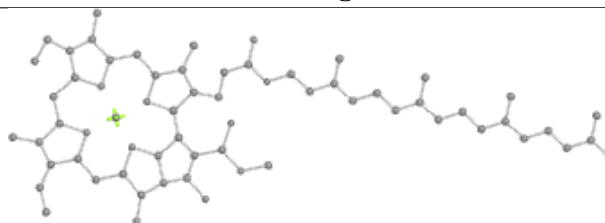
Bond lengths



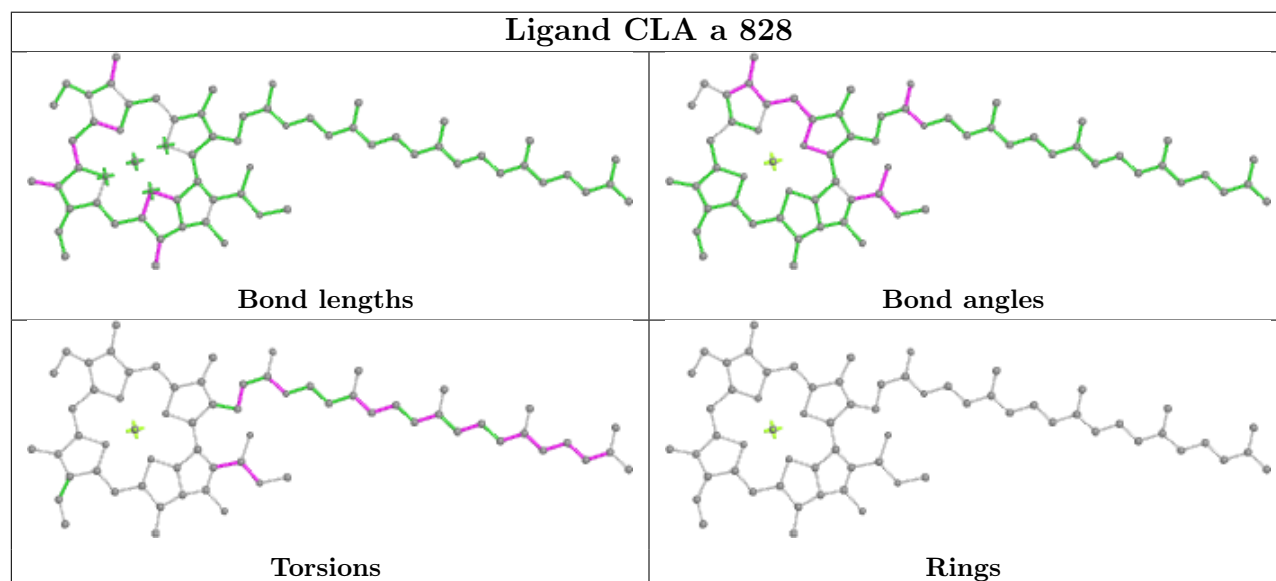
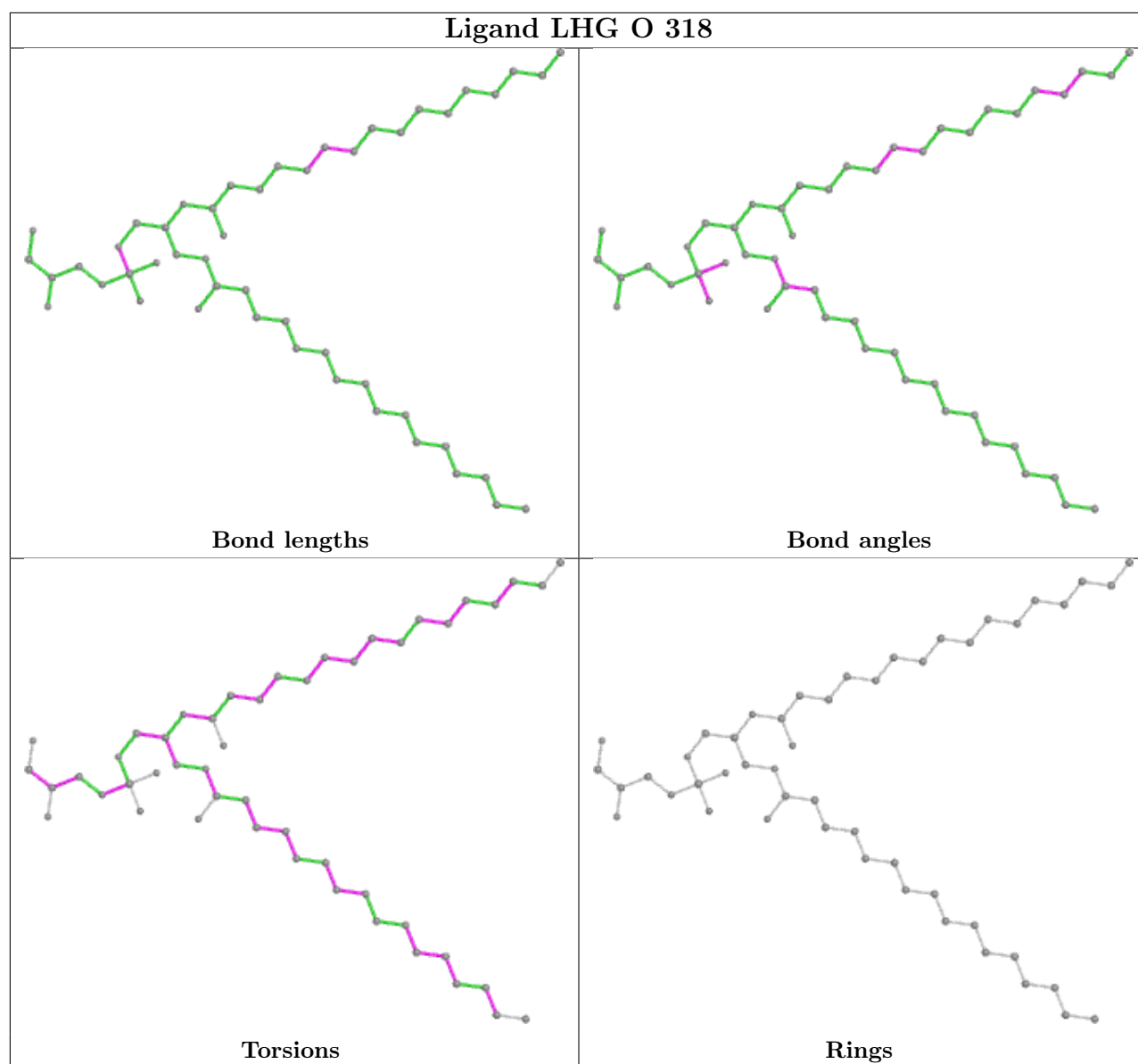
Bond angles



Torsions

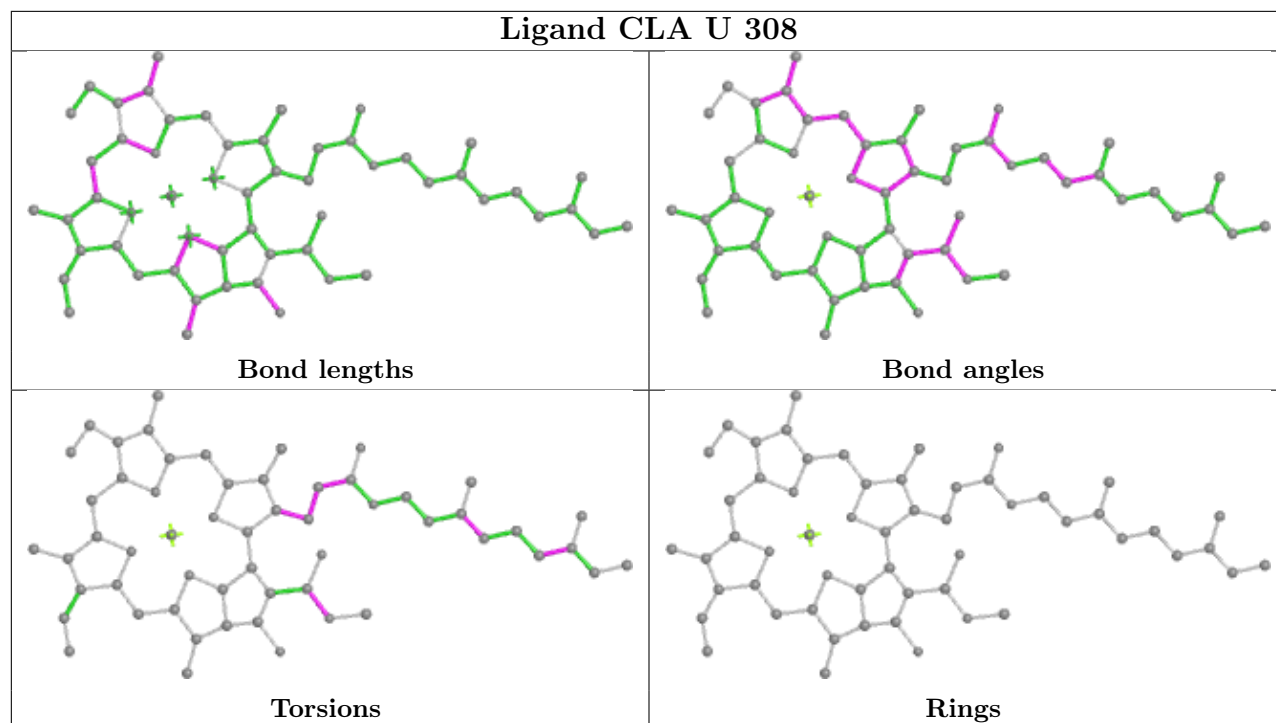


Rings

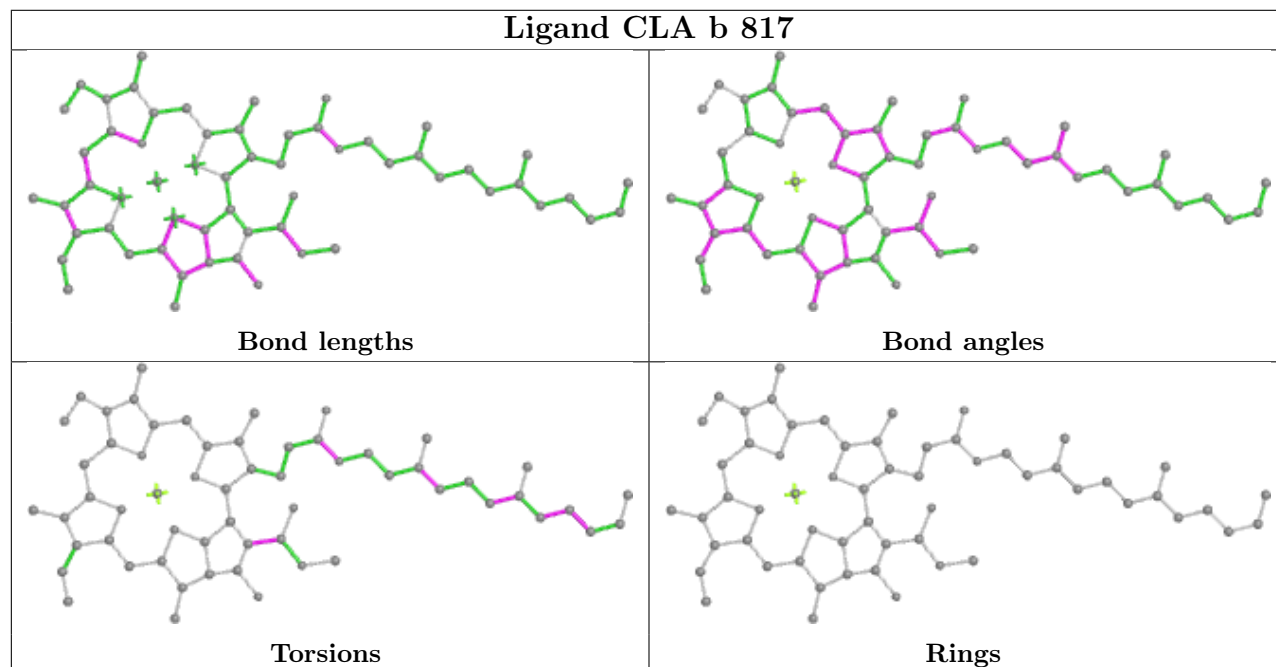


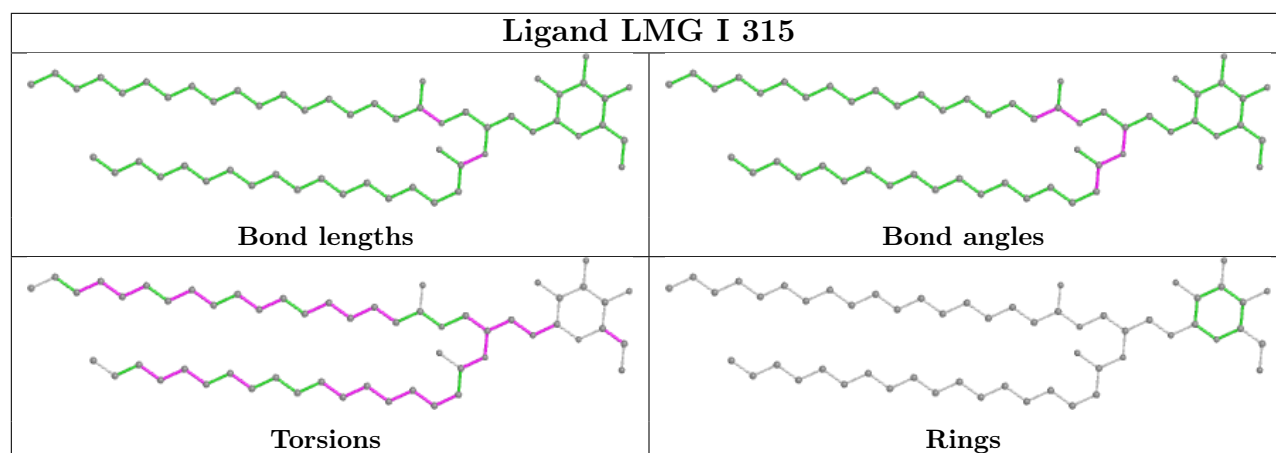
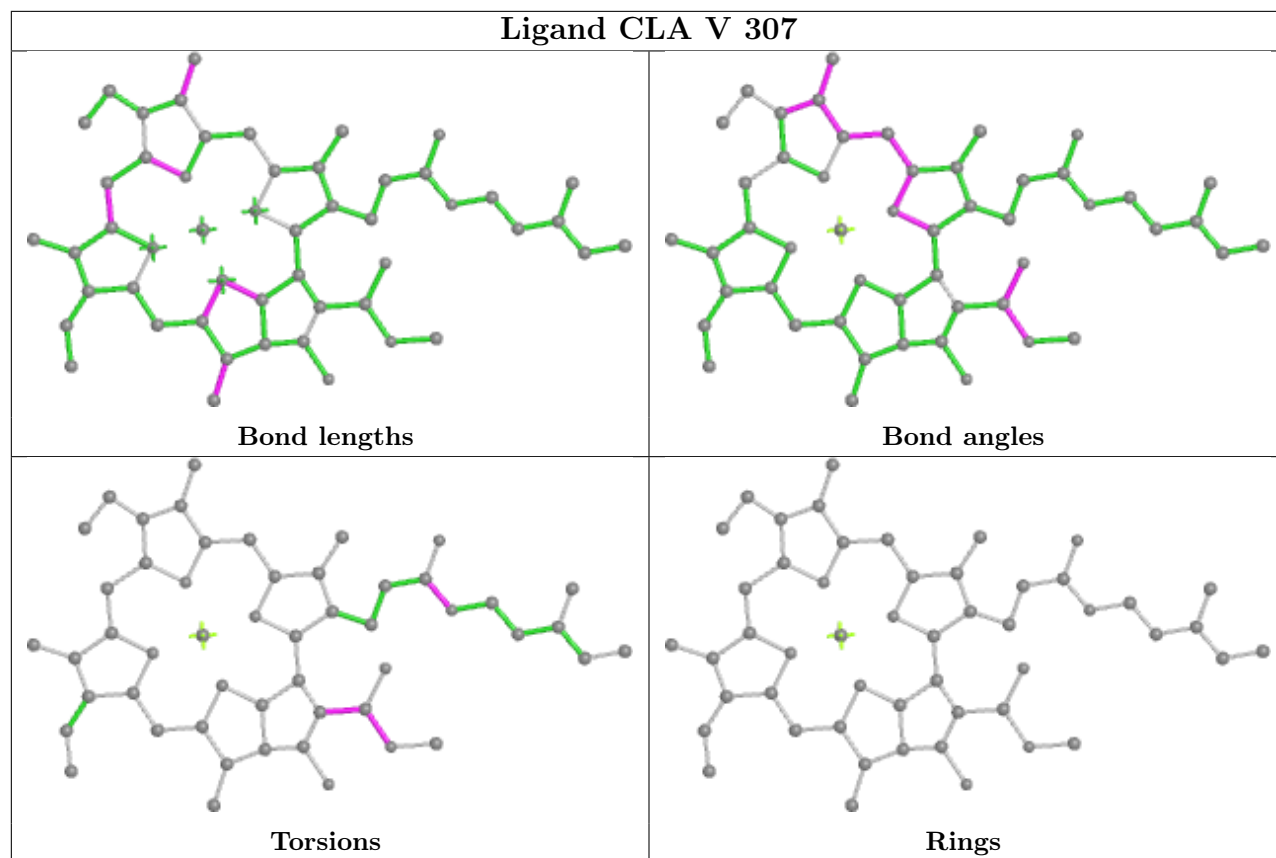


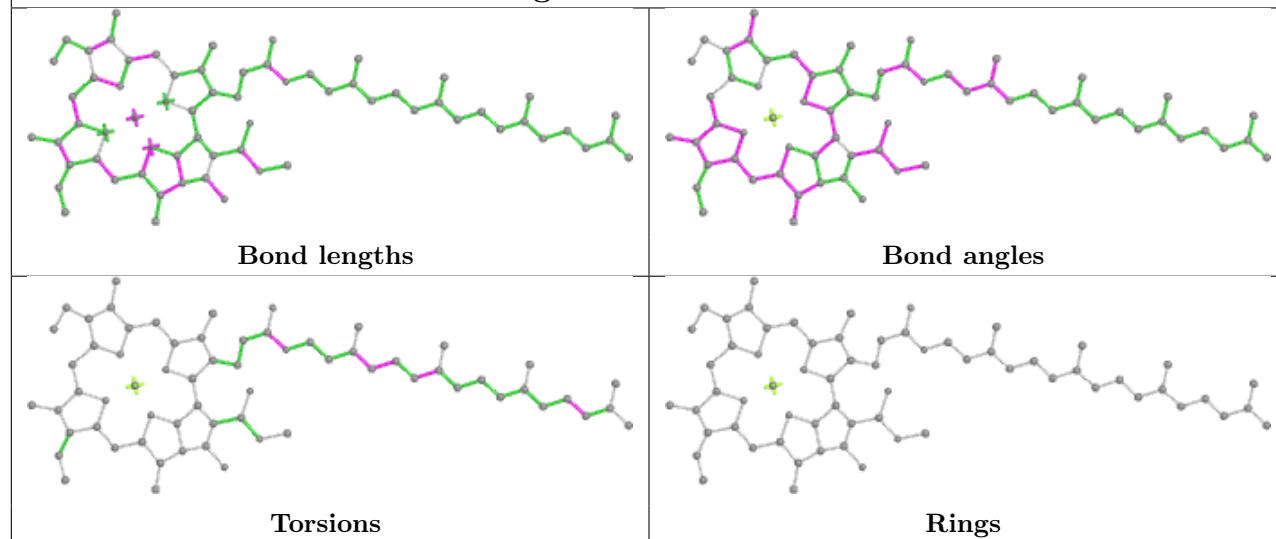
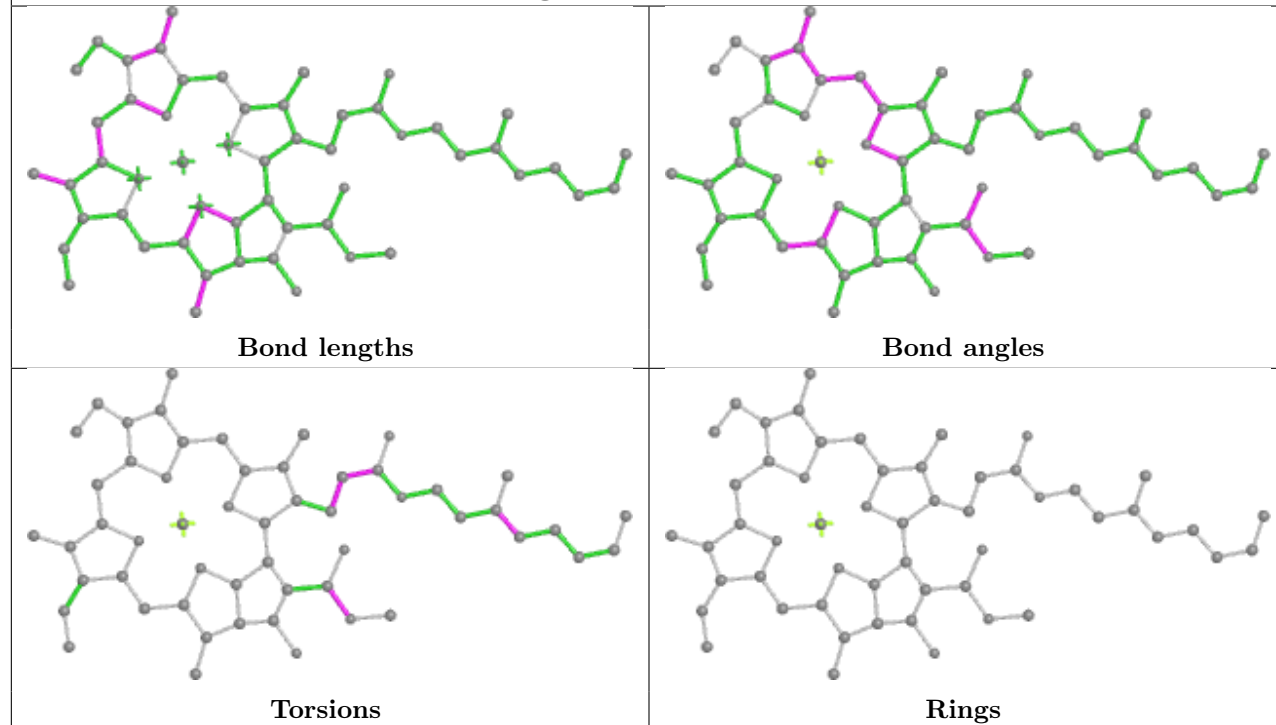
## Ligand CLA U 308

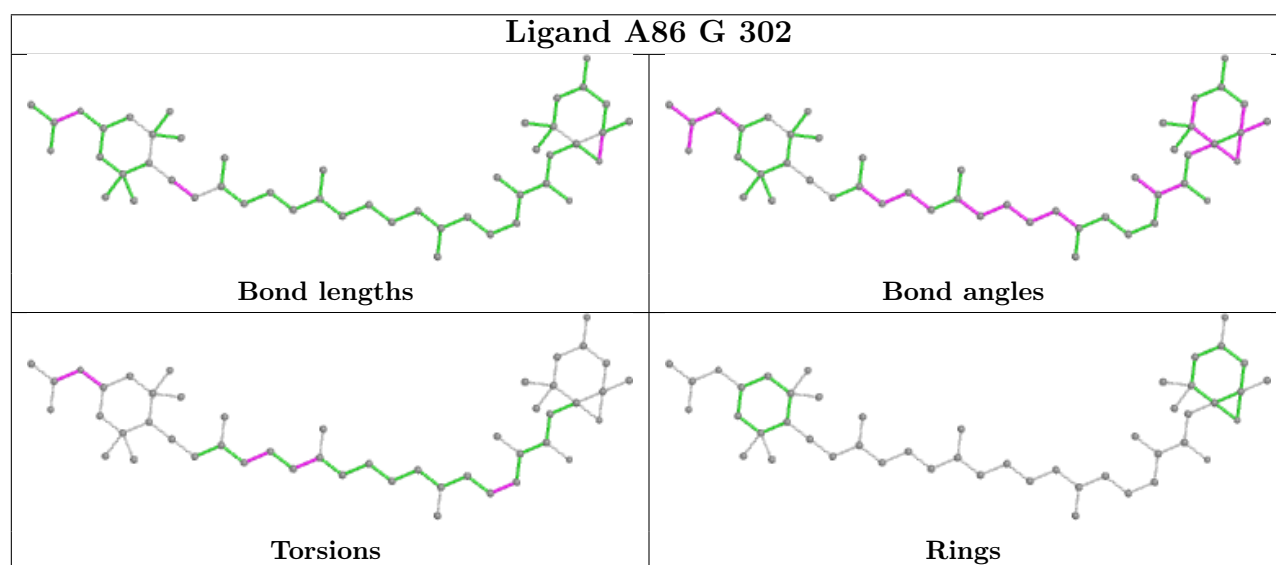
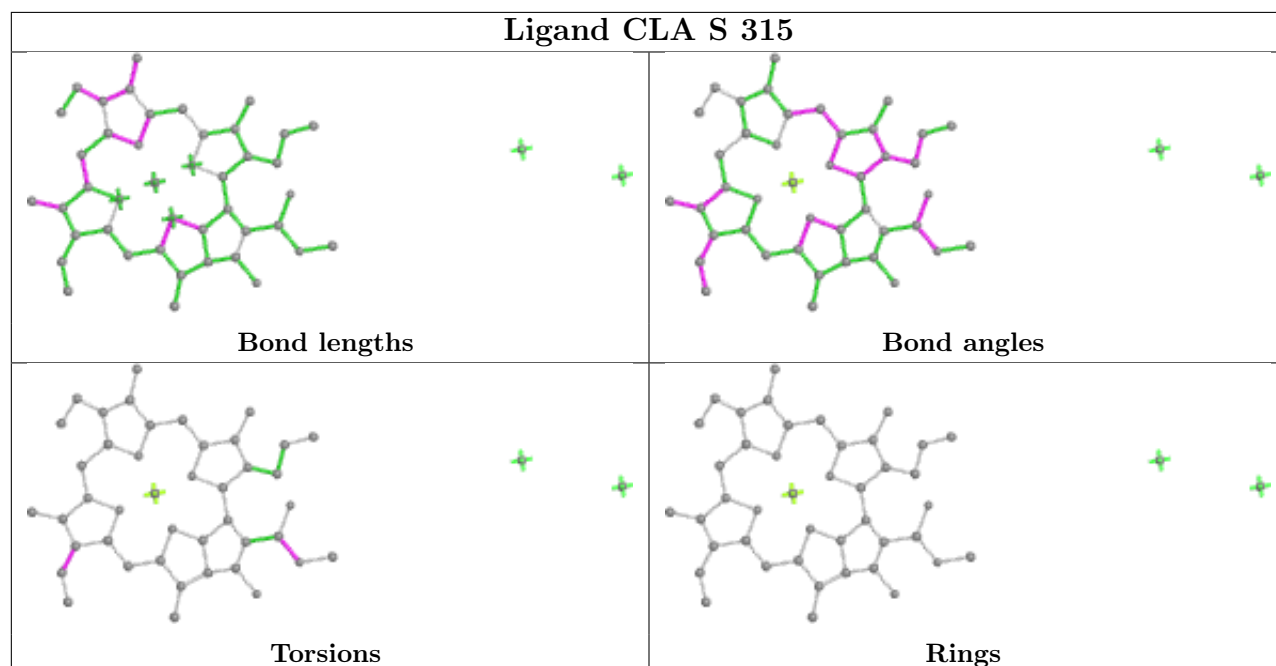
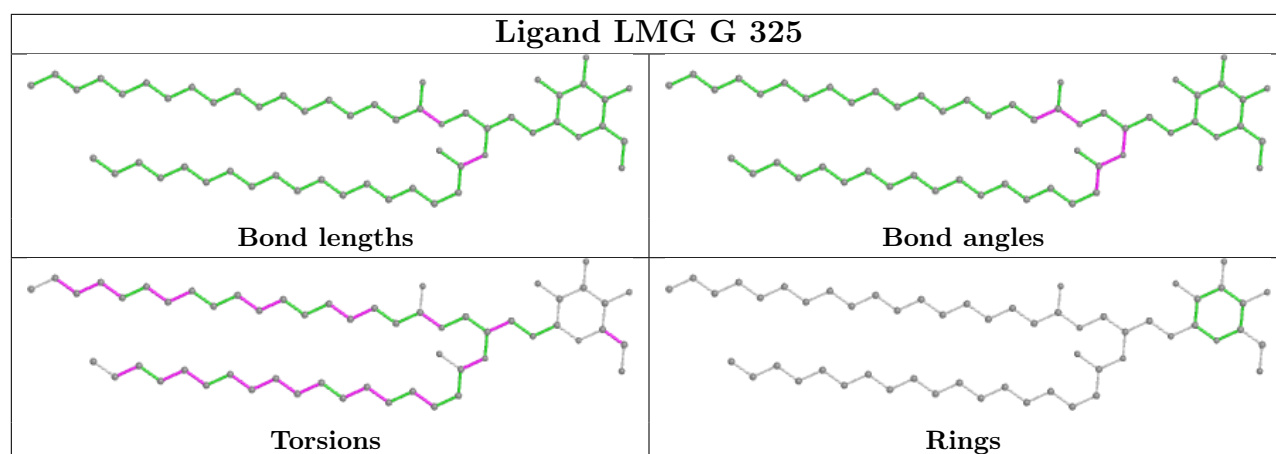


## Ligand CLA b 817

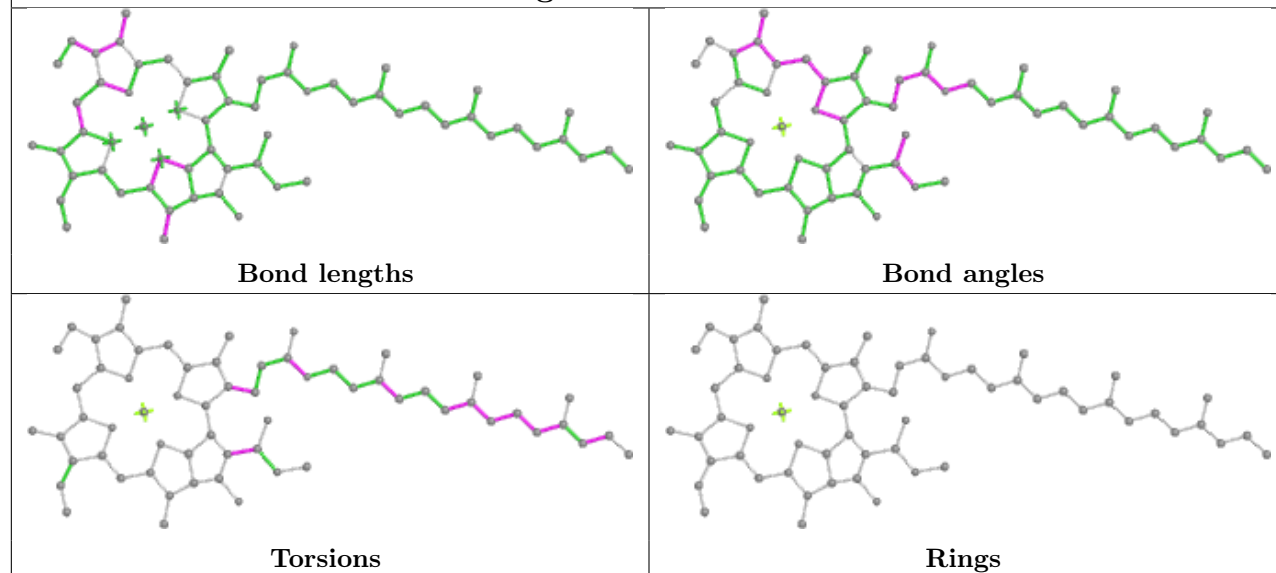




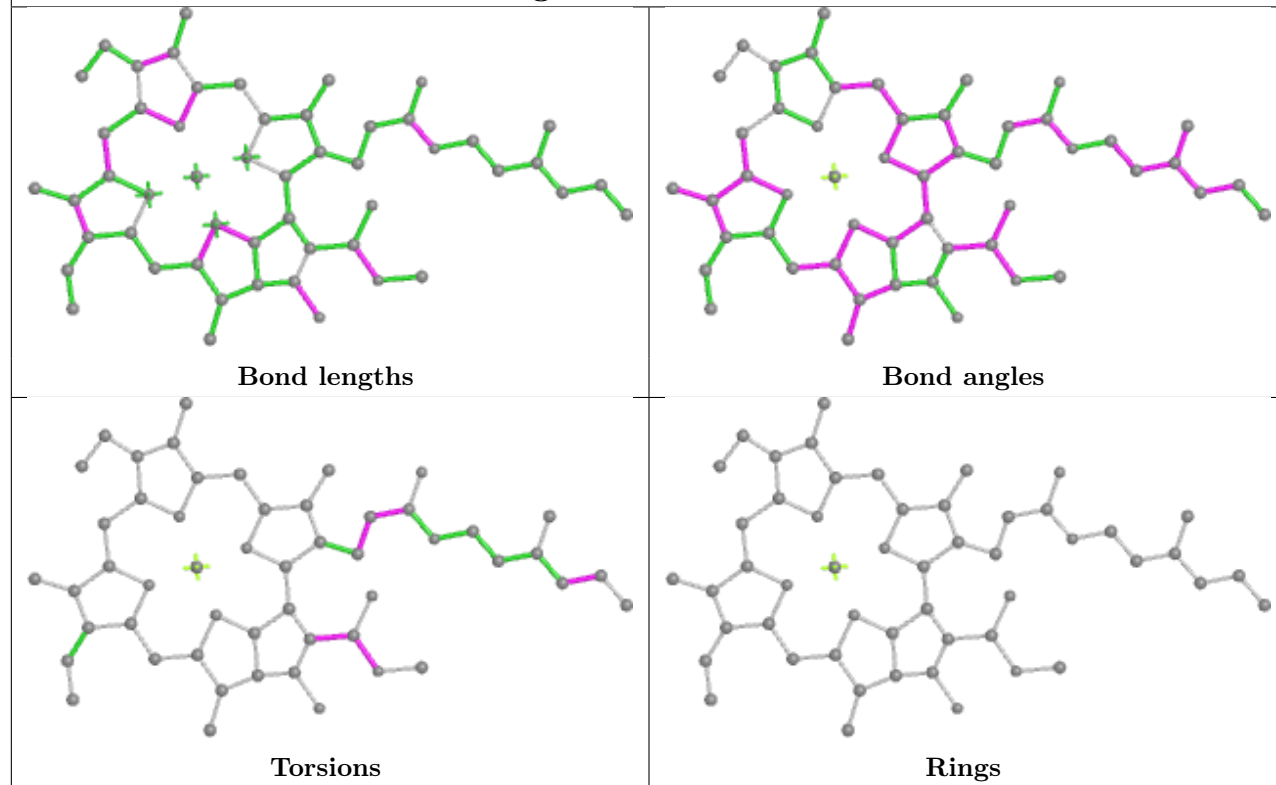
**Ligand CLA E 313****Ligand CLA a 811**

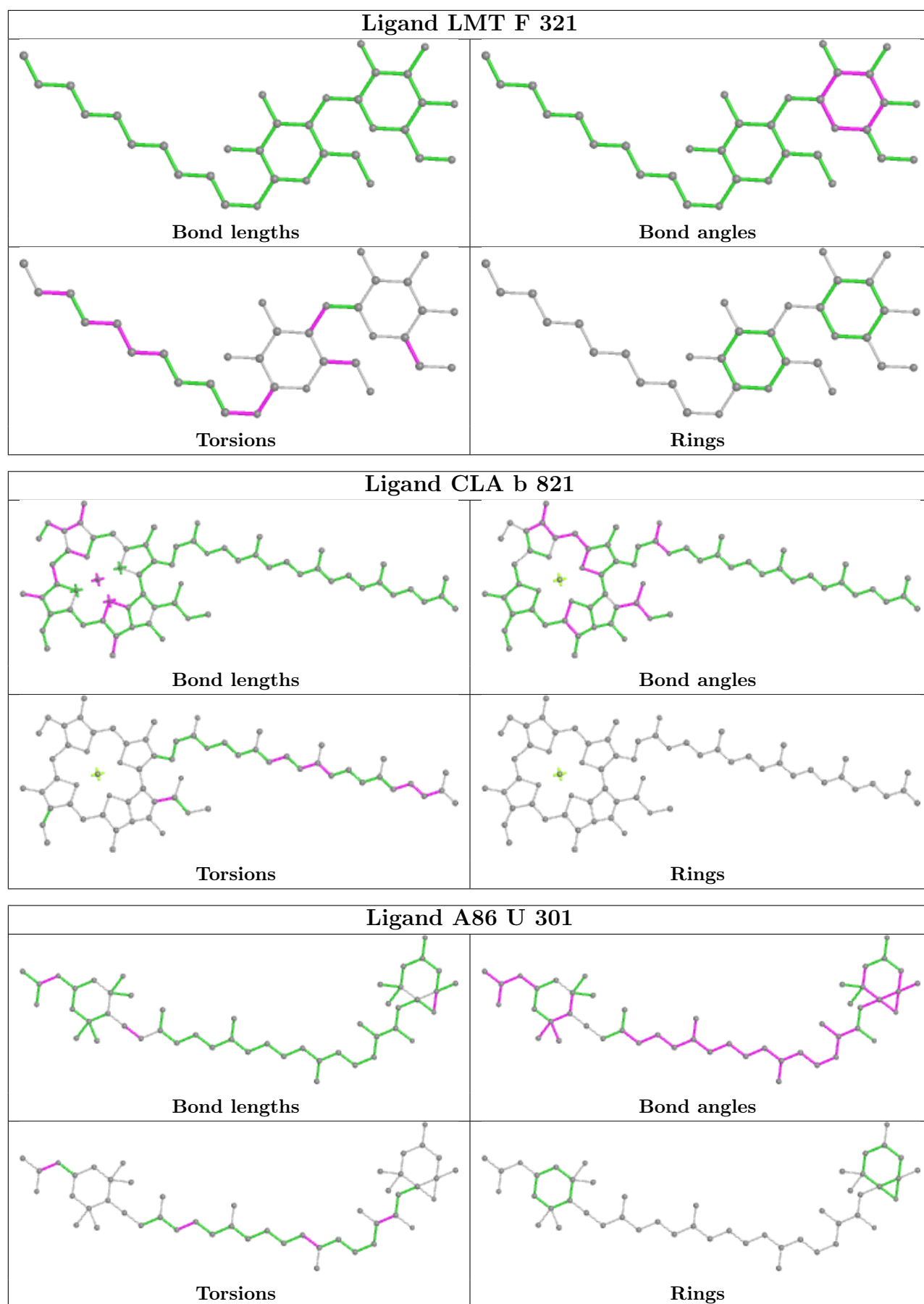


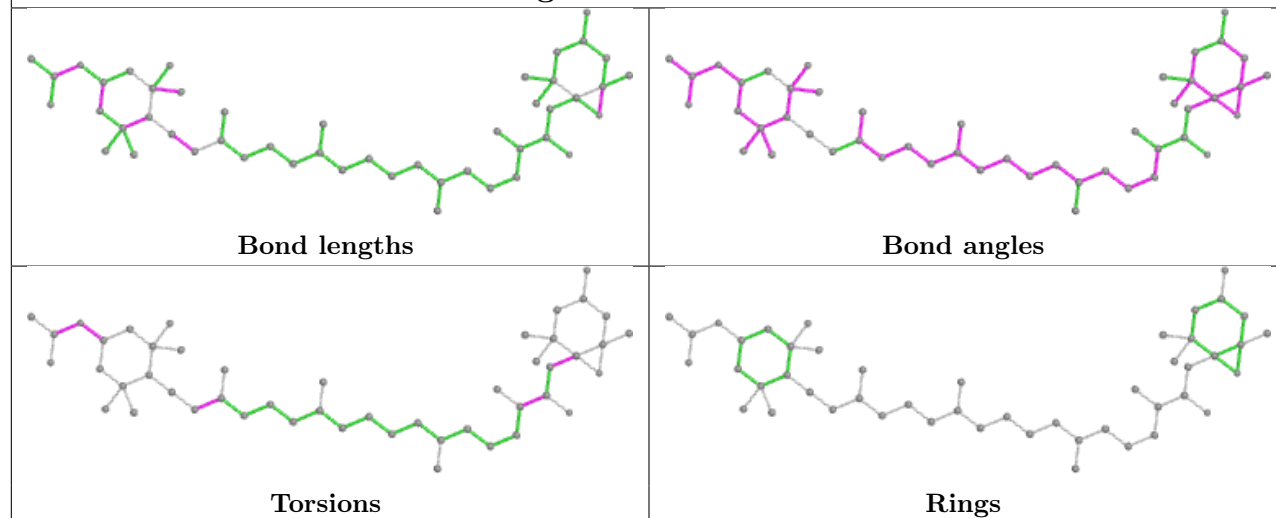
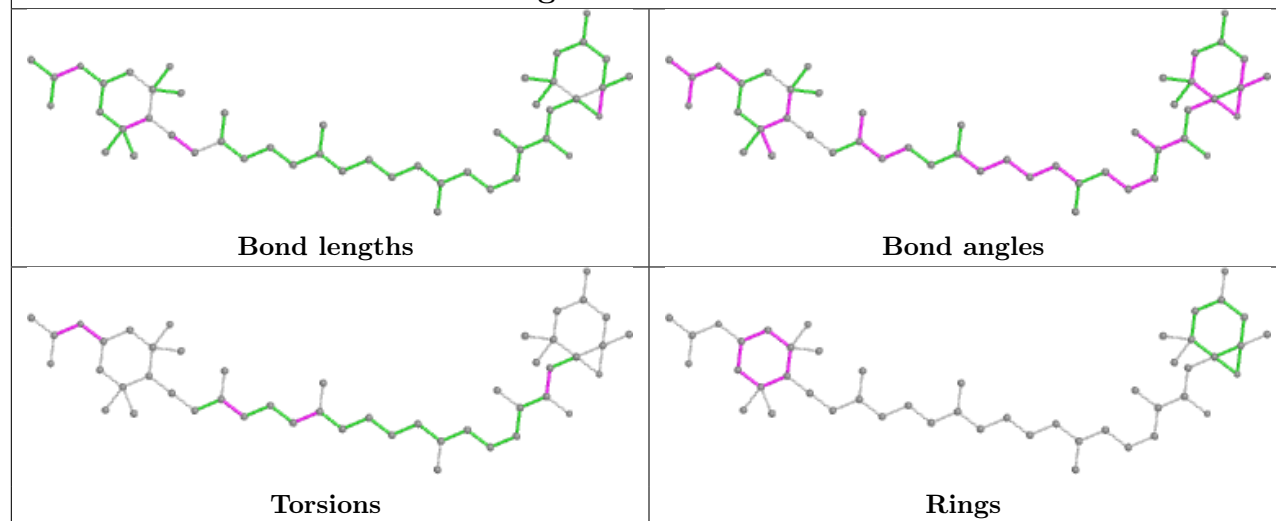
## Ligand CLA a 810



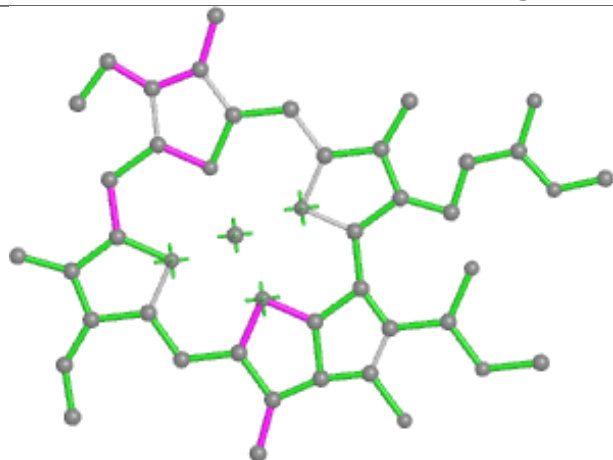
## Ligand CLA B 309



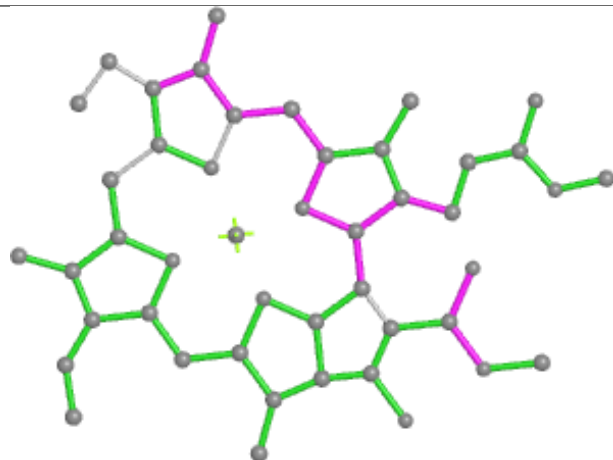


**Ligand A86 N 320****Ligand A86 C 203**

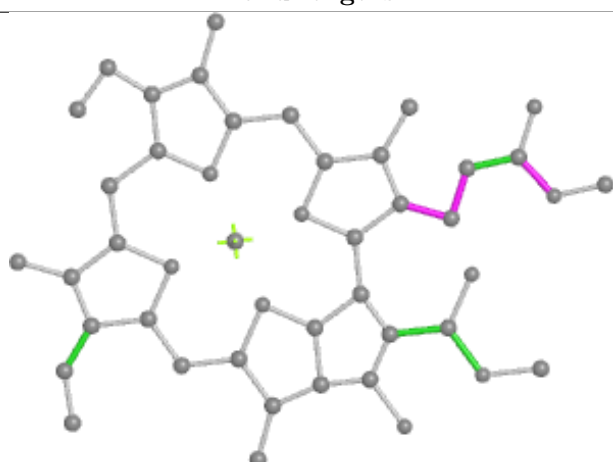
## Ligand CLA B 307



Bond lengths



Bond angles

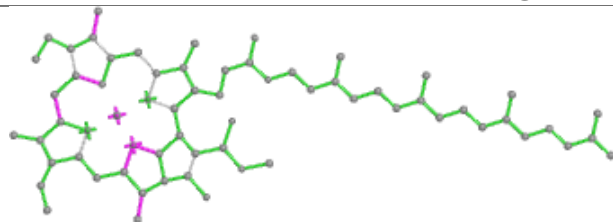


Torsions

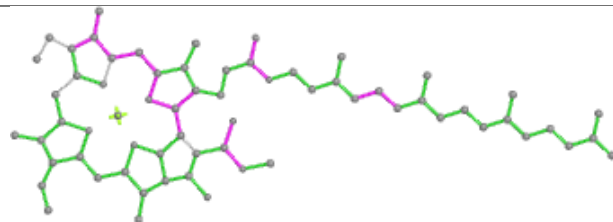


Rings

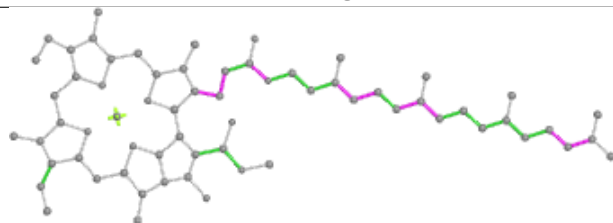
## Ligand CLA F 314



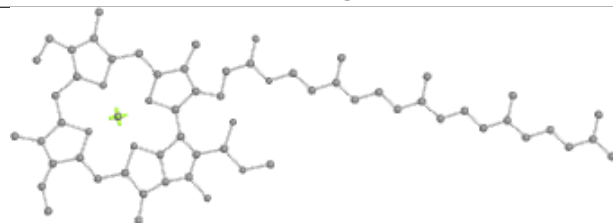
Bond lengths



Bond angles



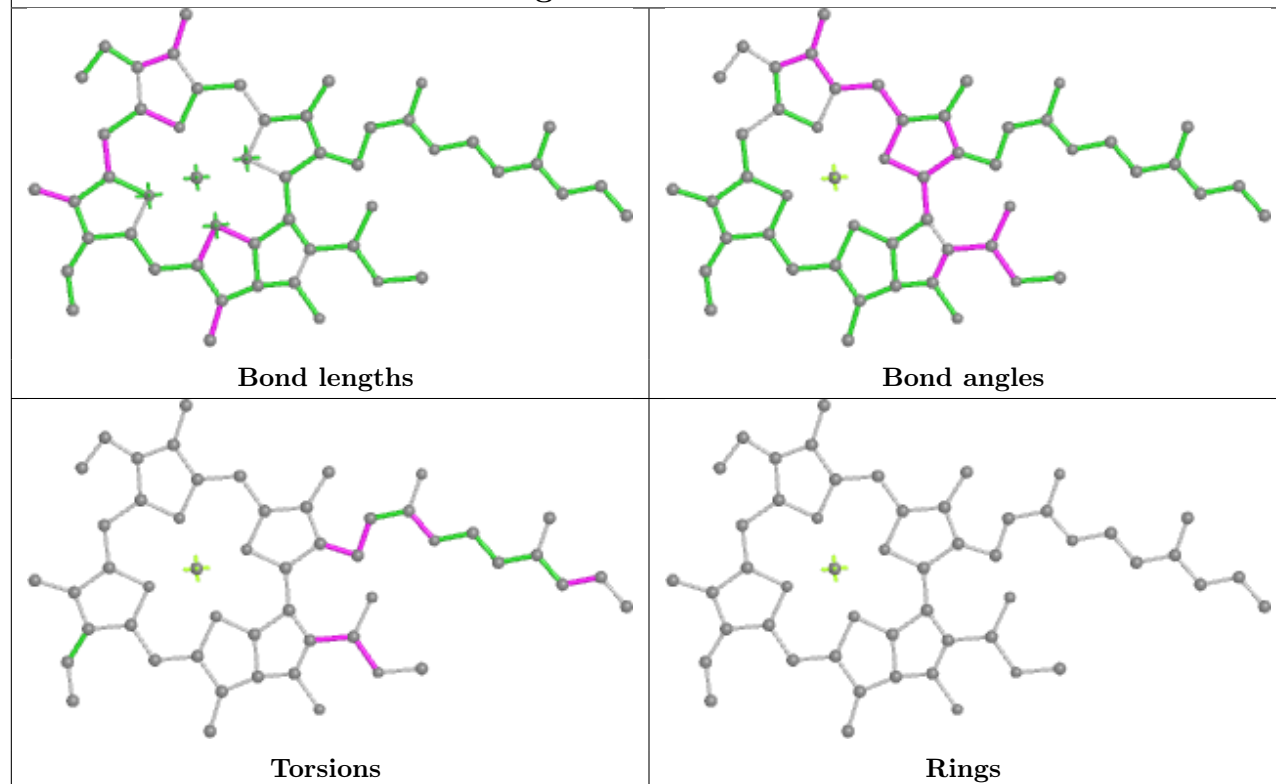
Torsions



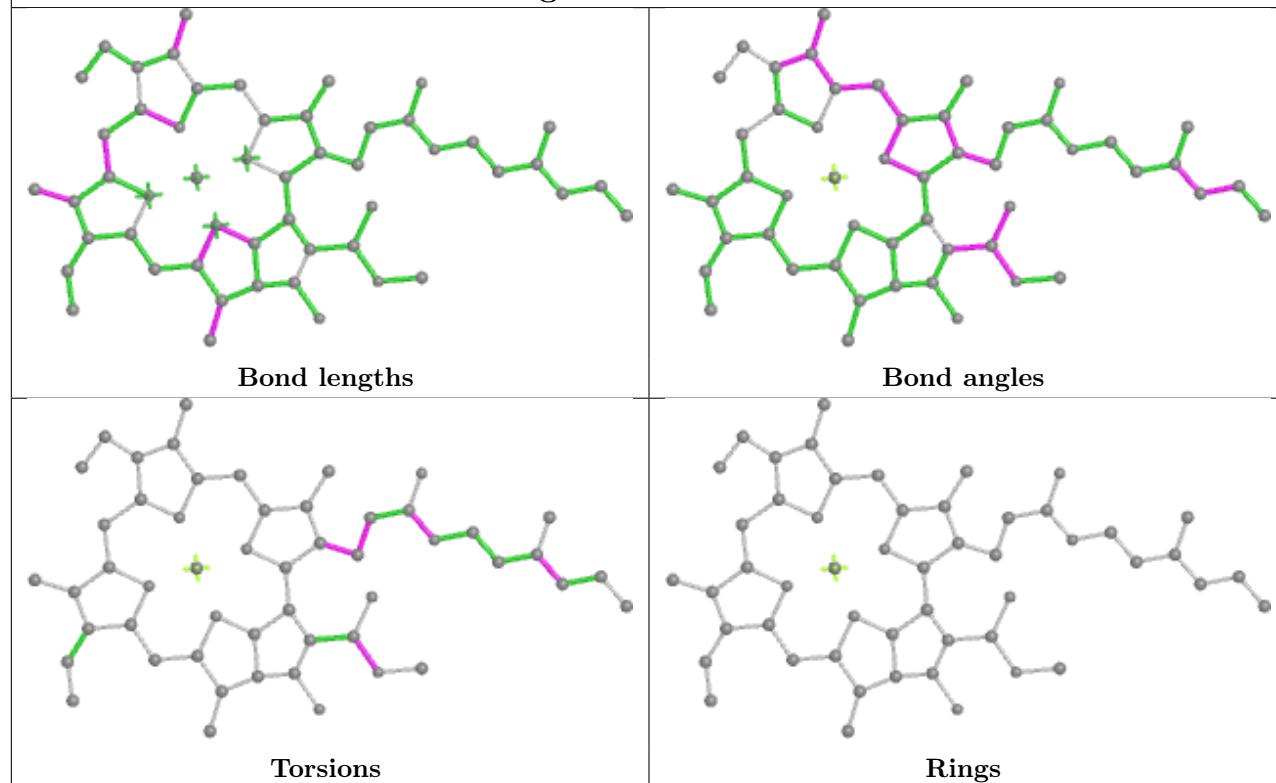
Rings

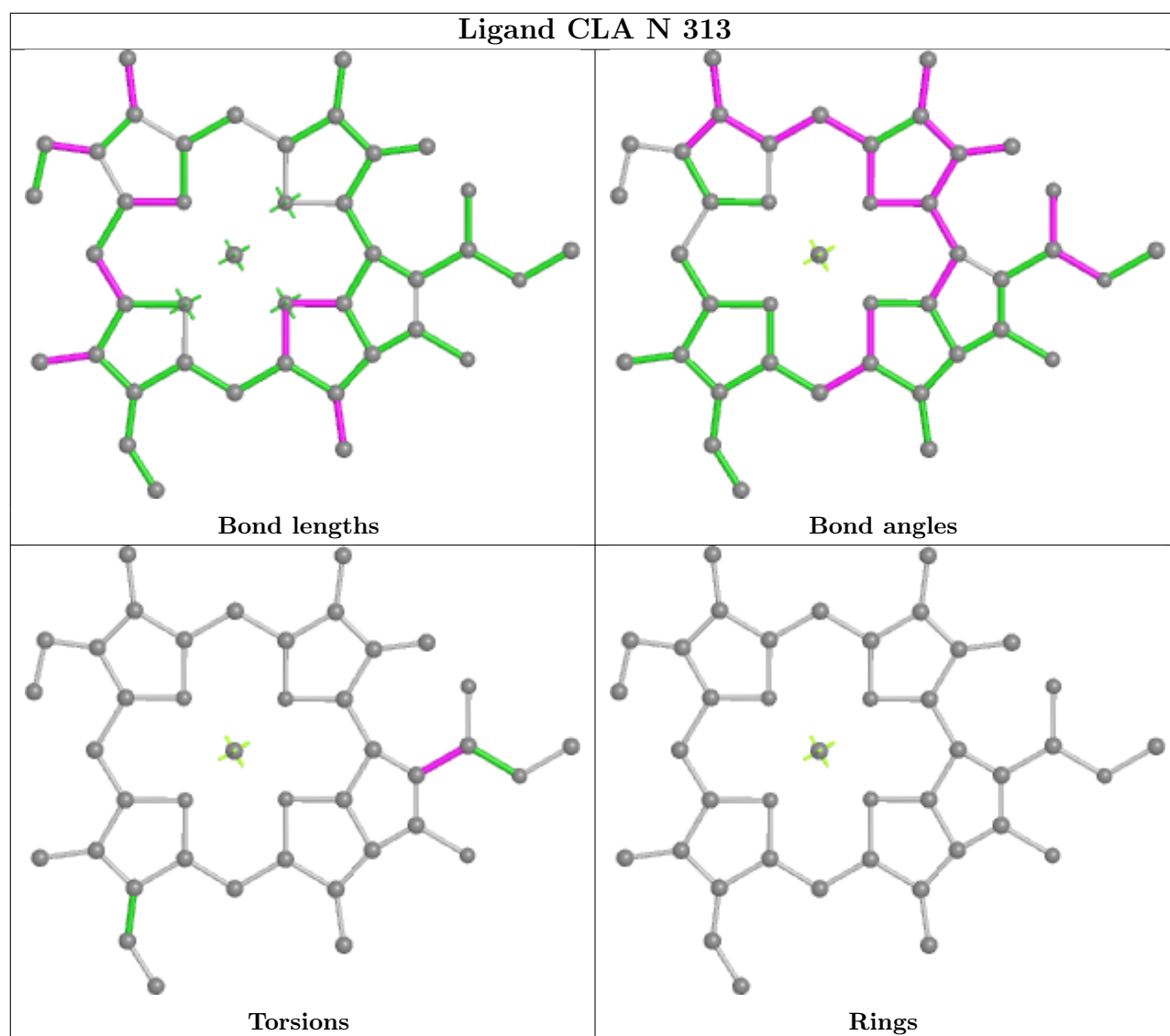


## Ligand CLA S 321

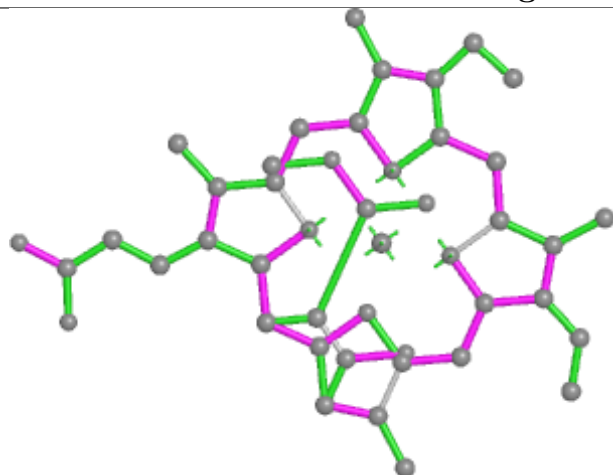


## Ligand CLA f 805

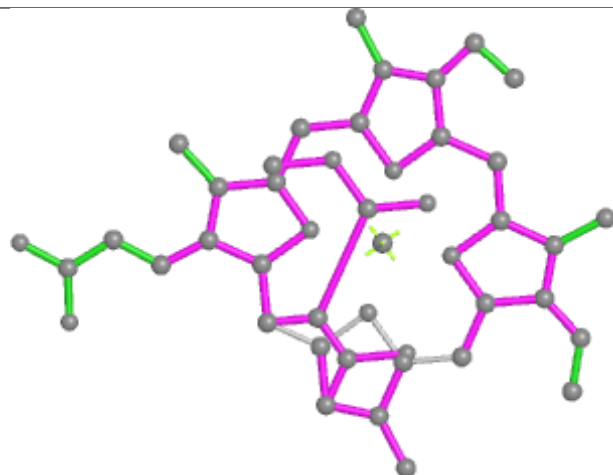




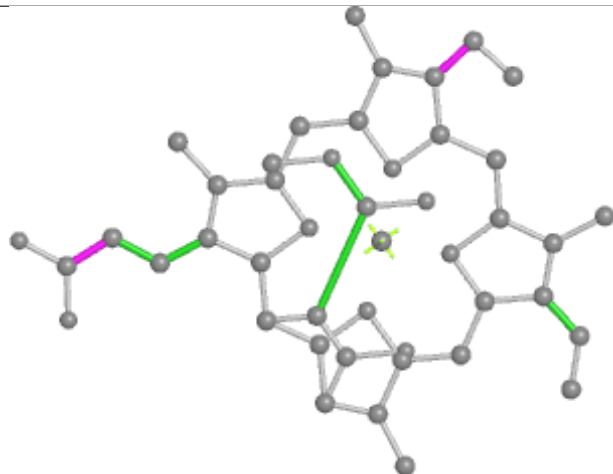
## Ligand KC1 L 317



Bond lengths



Bond angles

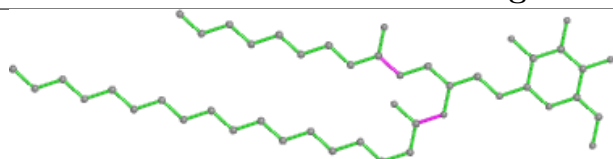


Torsions

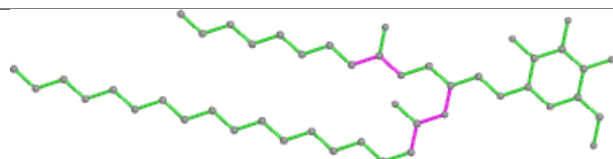


Rings

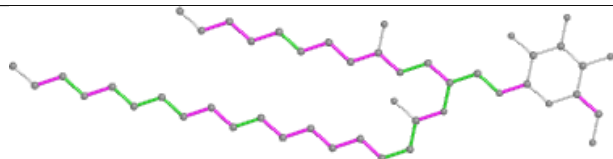
## Ligand LMG V 316



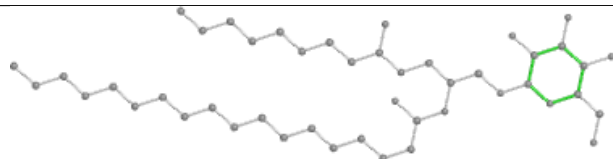
Bond lengths



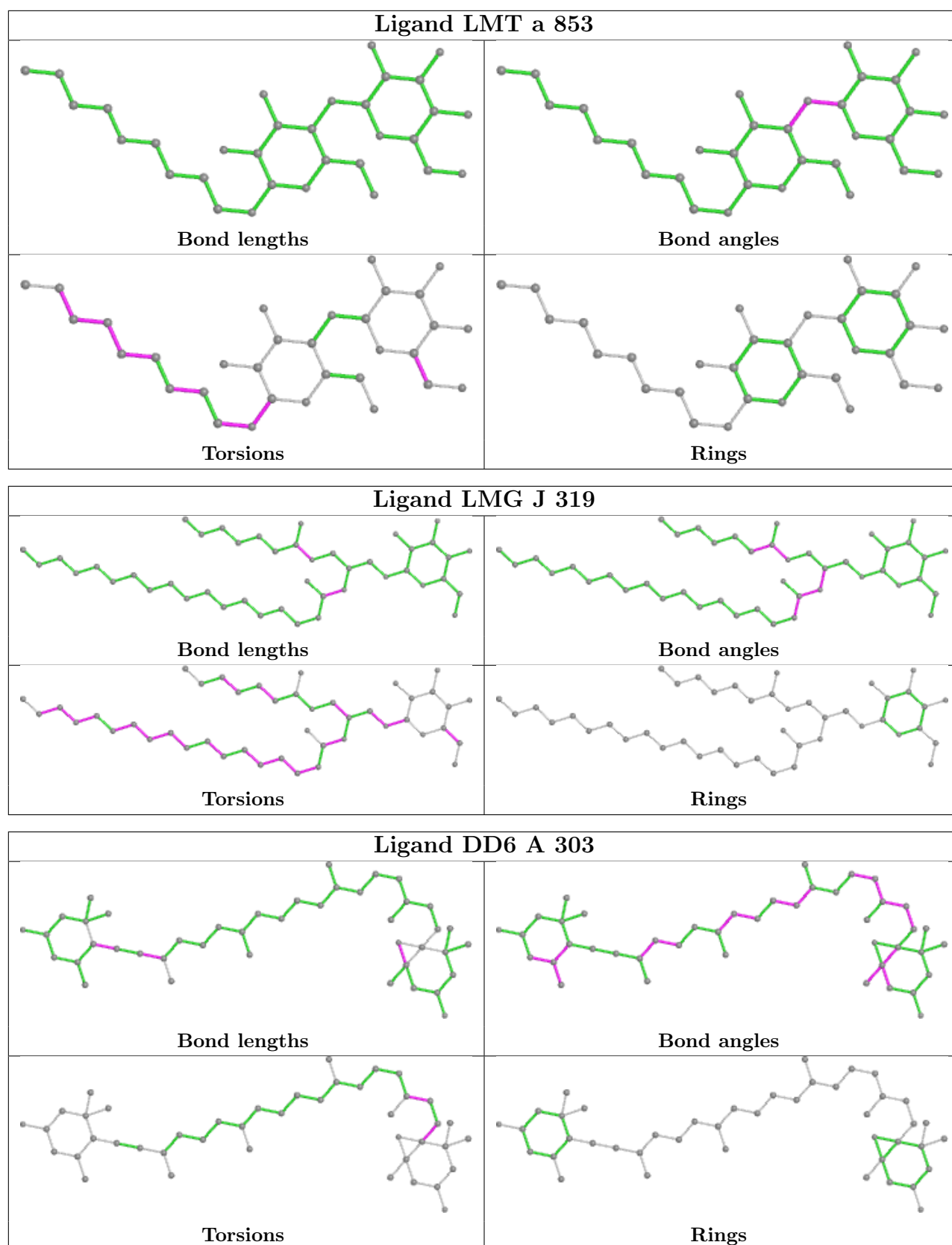
Bond angles



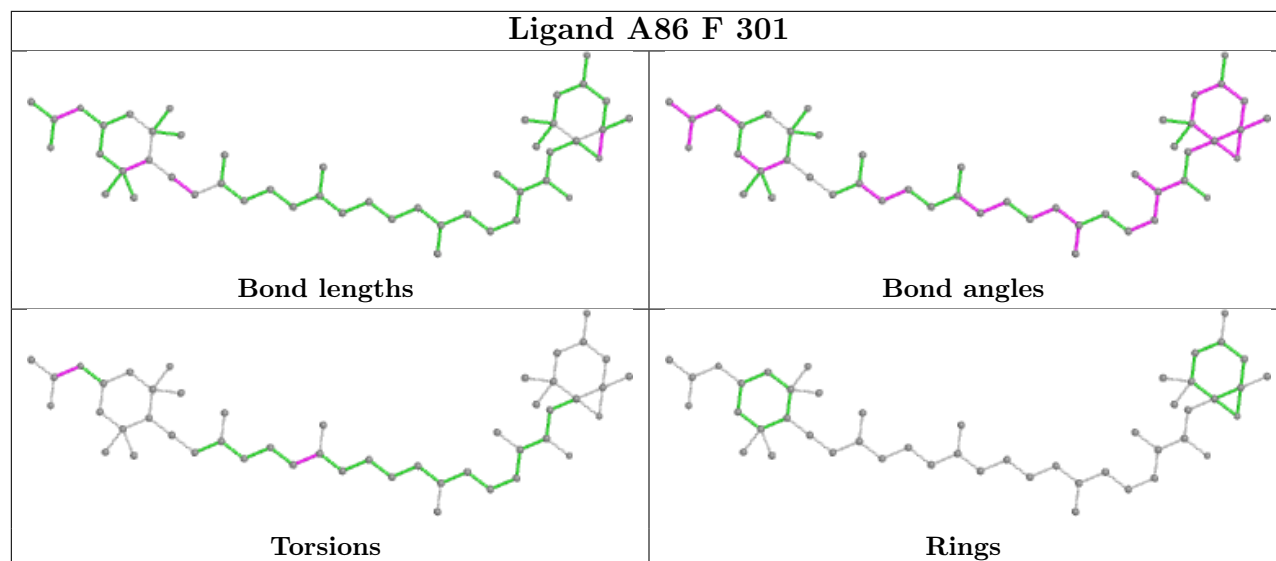
Torsions



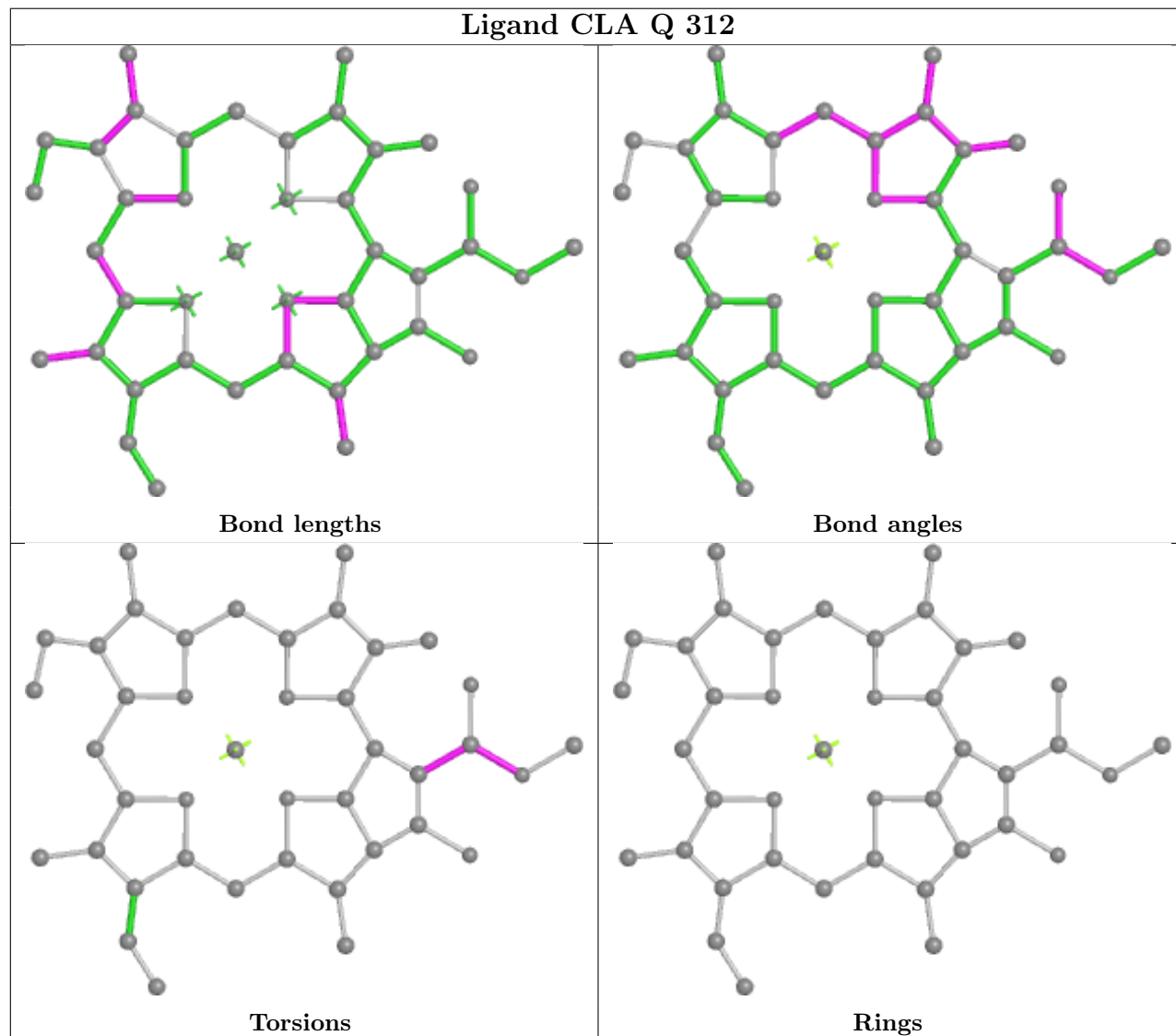
Rings

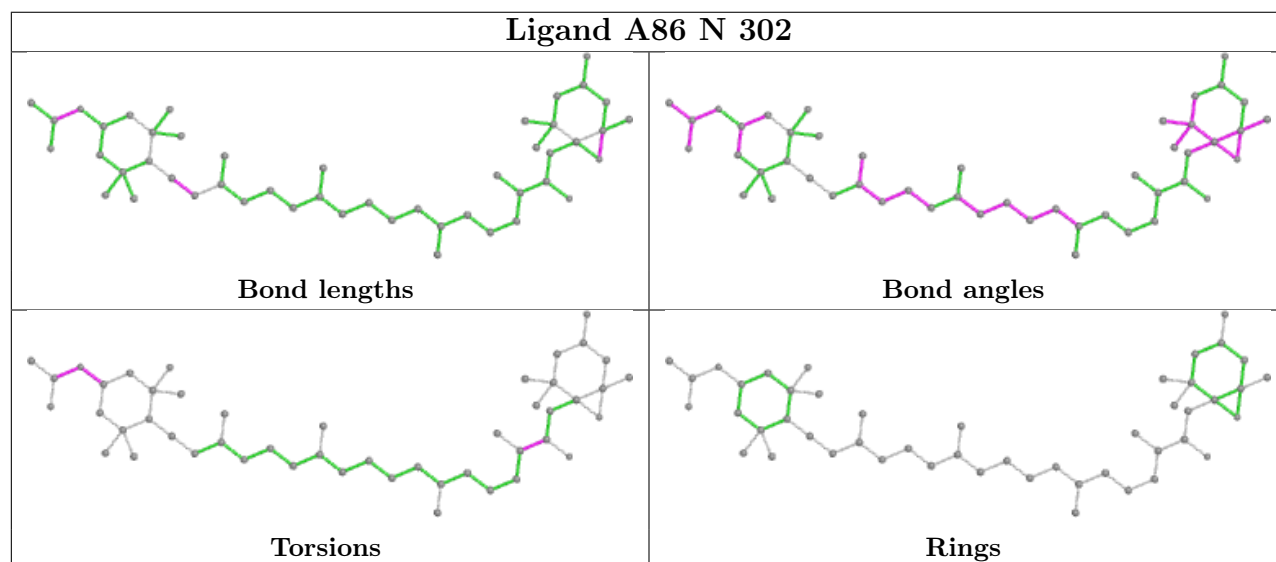
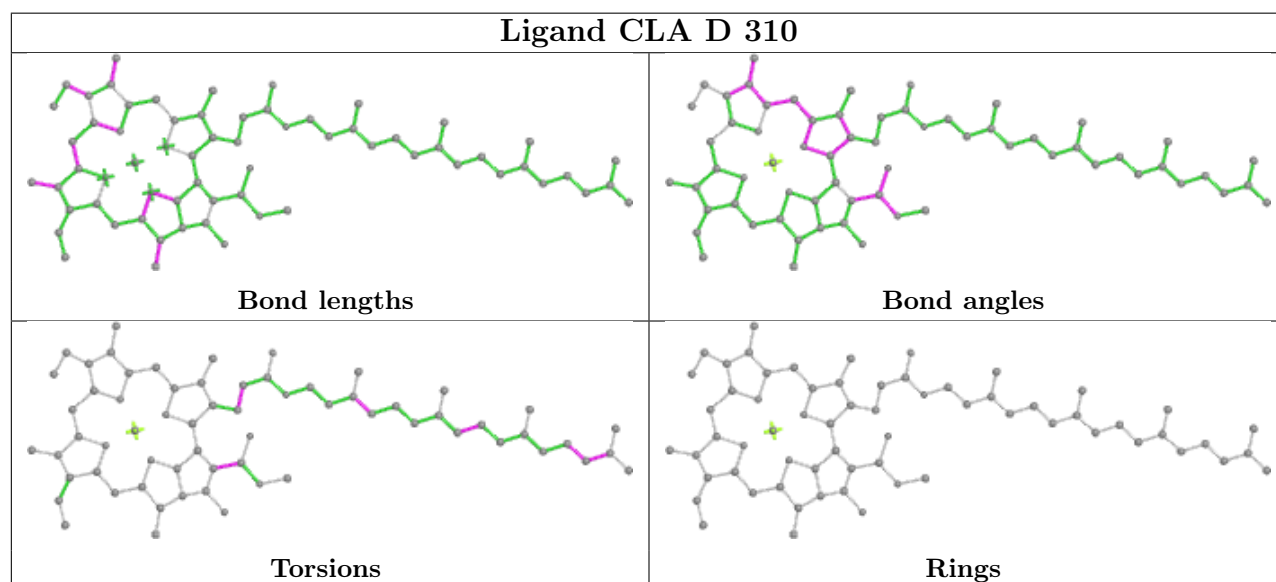
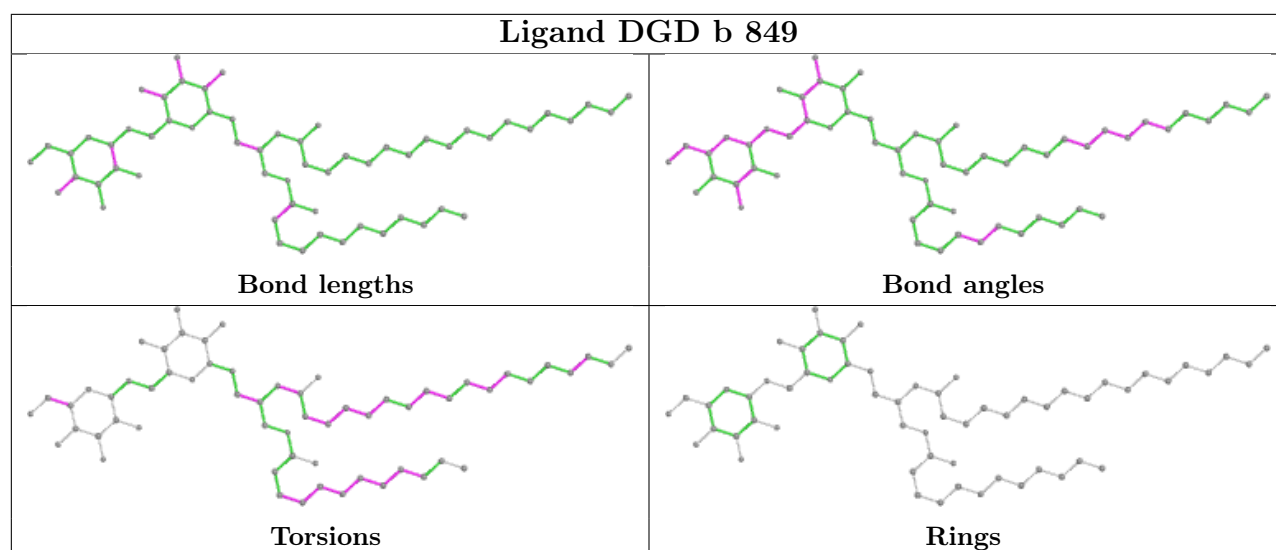


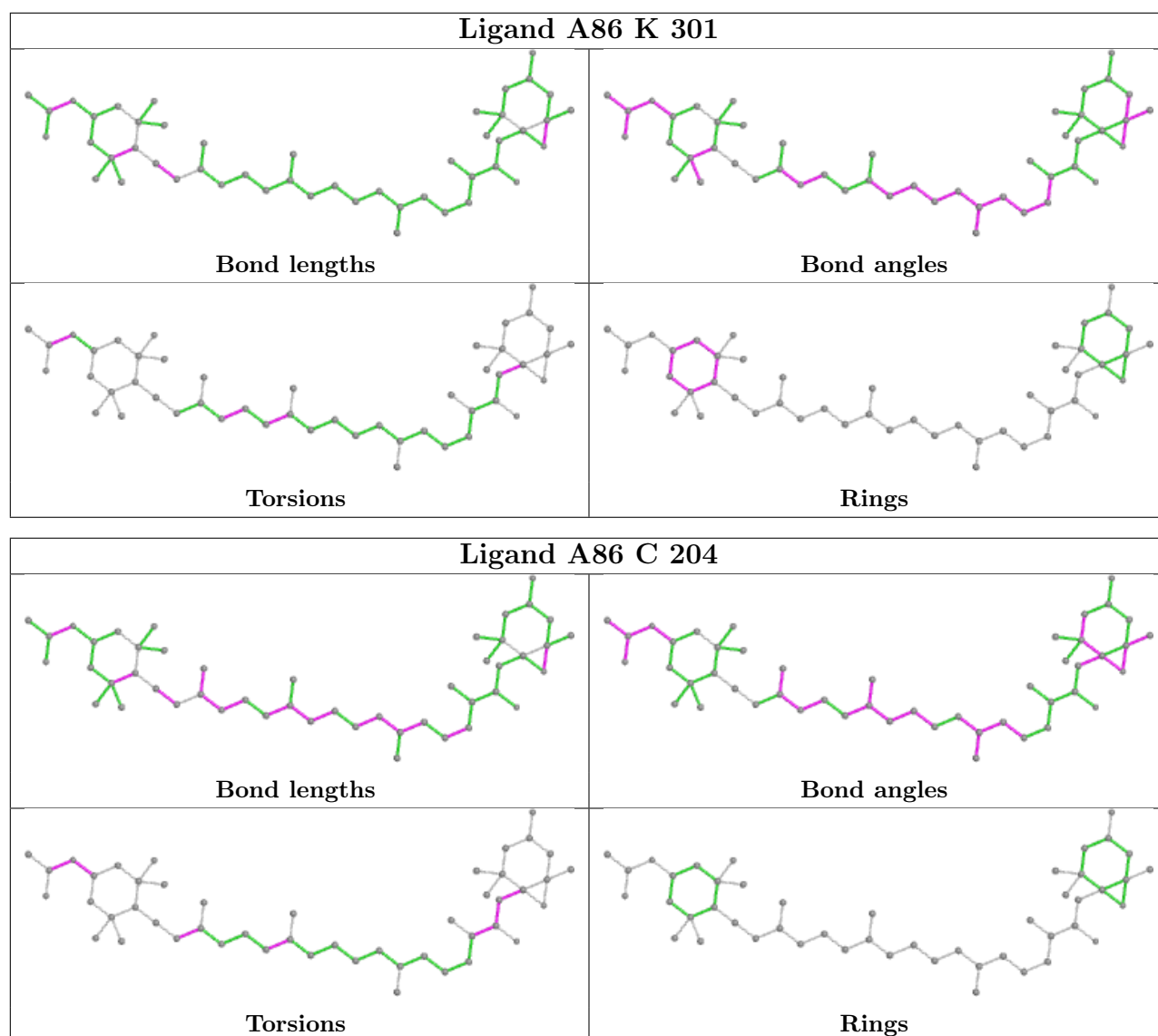
## Ligand A86 F 301



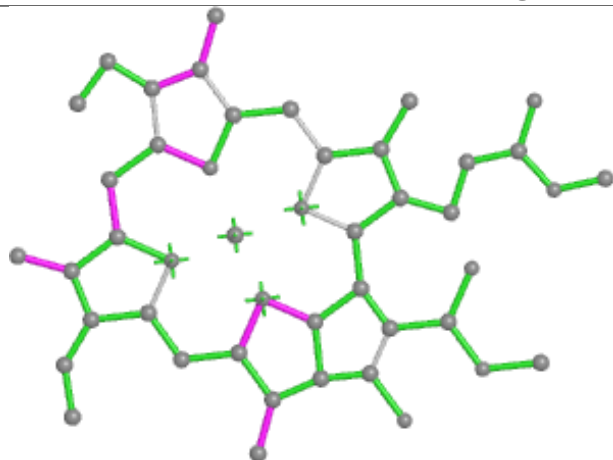
## Ligand CLA Q 312



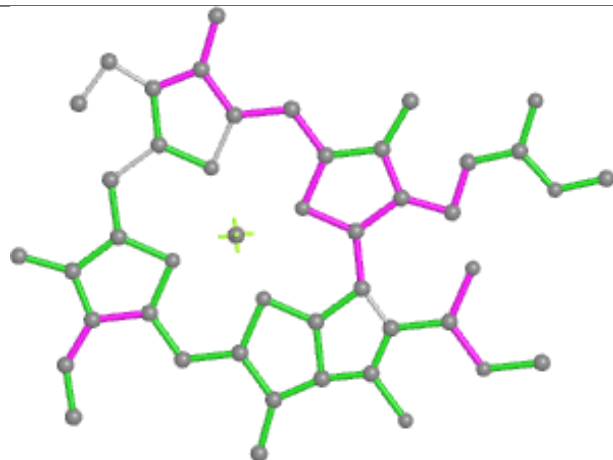




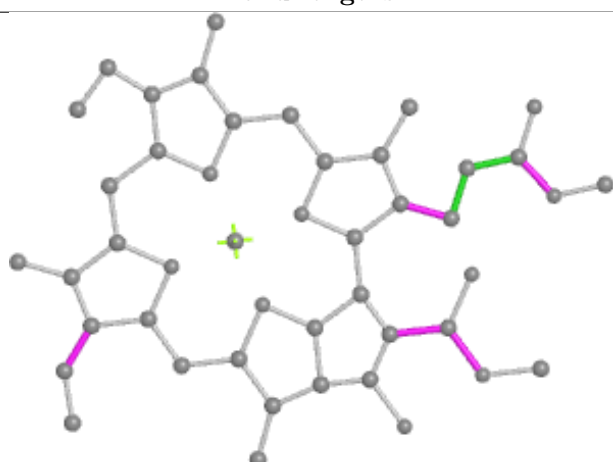
## Ligand CLA R 314



Bond lengths



Bond angles

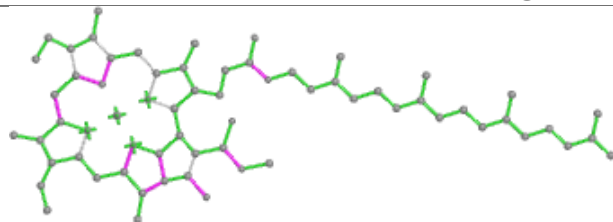


Torsions

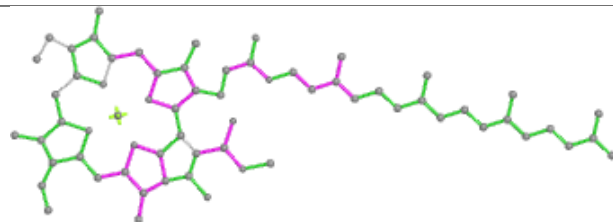


Rings

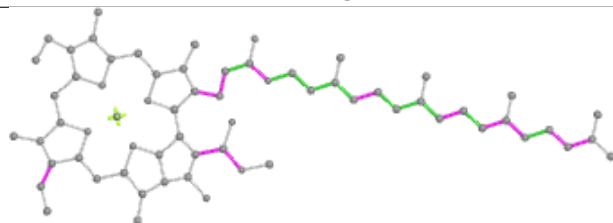
## Ligand CLA a 816



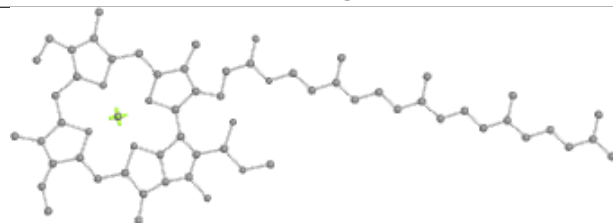
Bond lengths



Bond angles



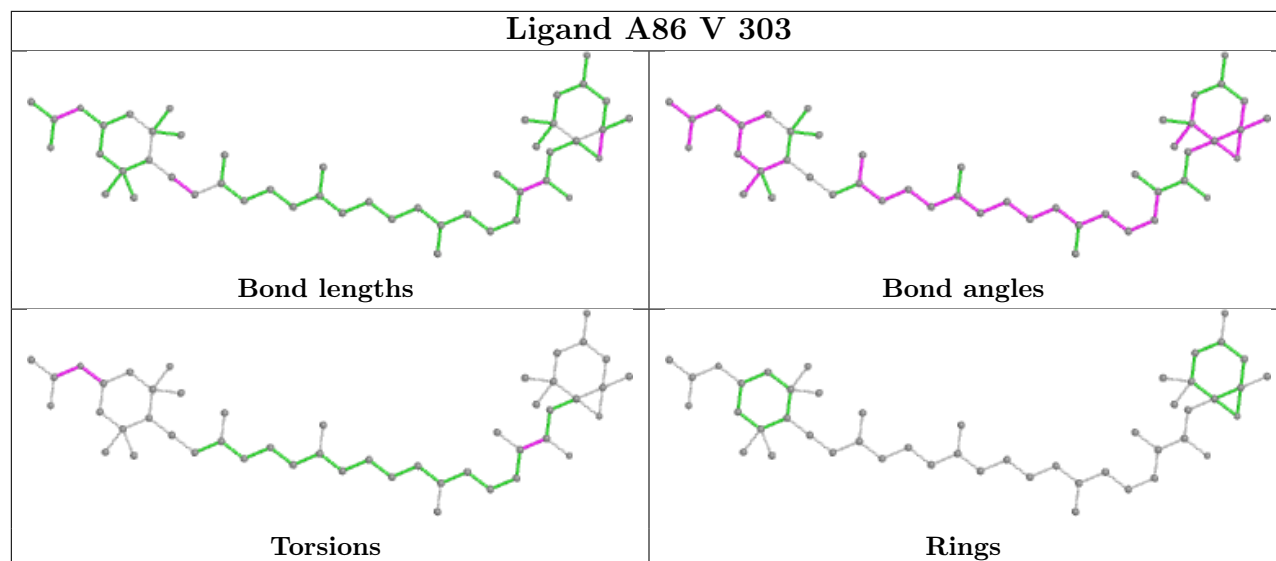
Torsions



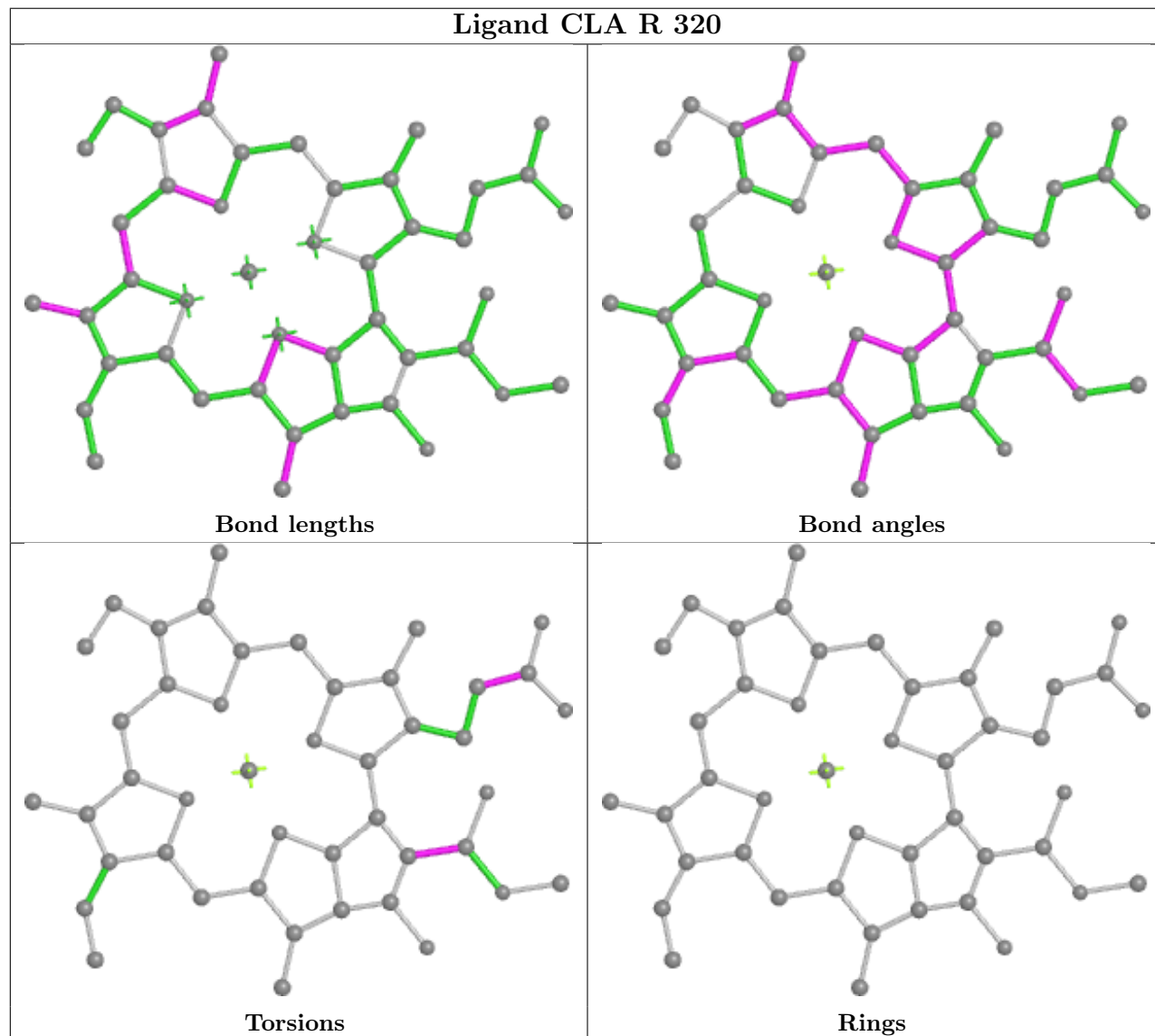
Rings



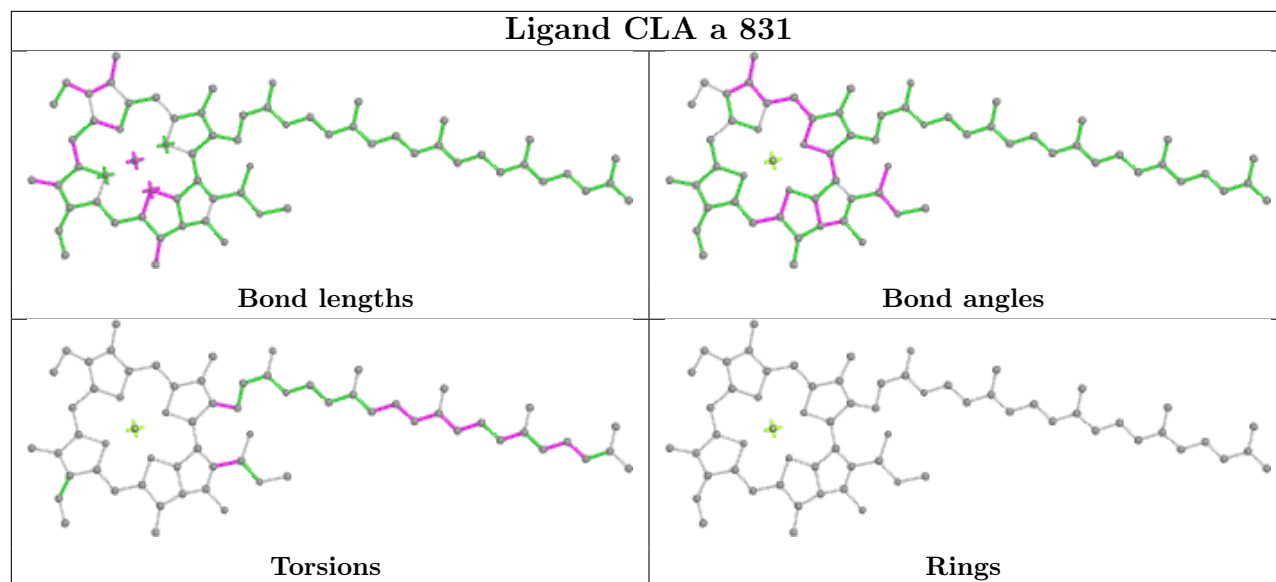
## Ligand A86 V 303



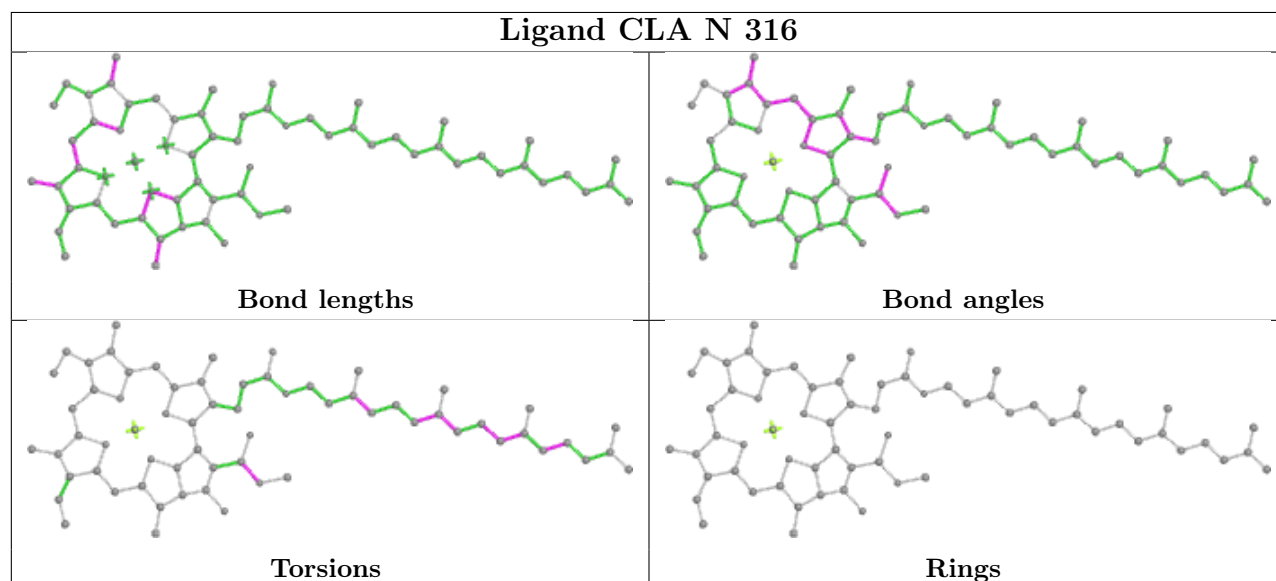
## Ligand CLA R 320



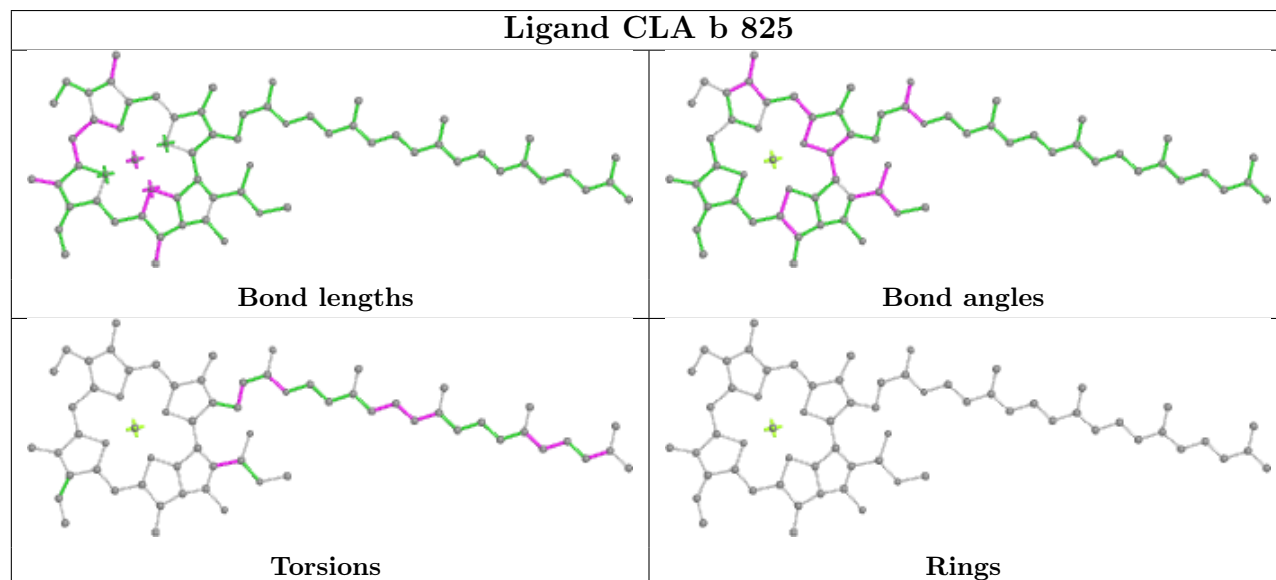
## Ligand CLA a 831



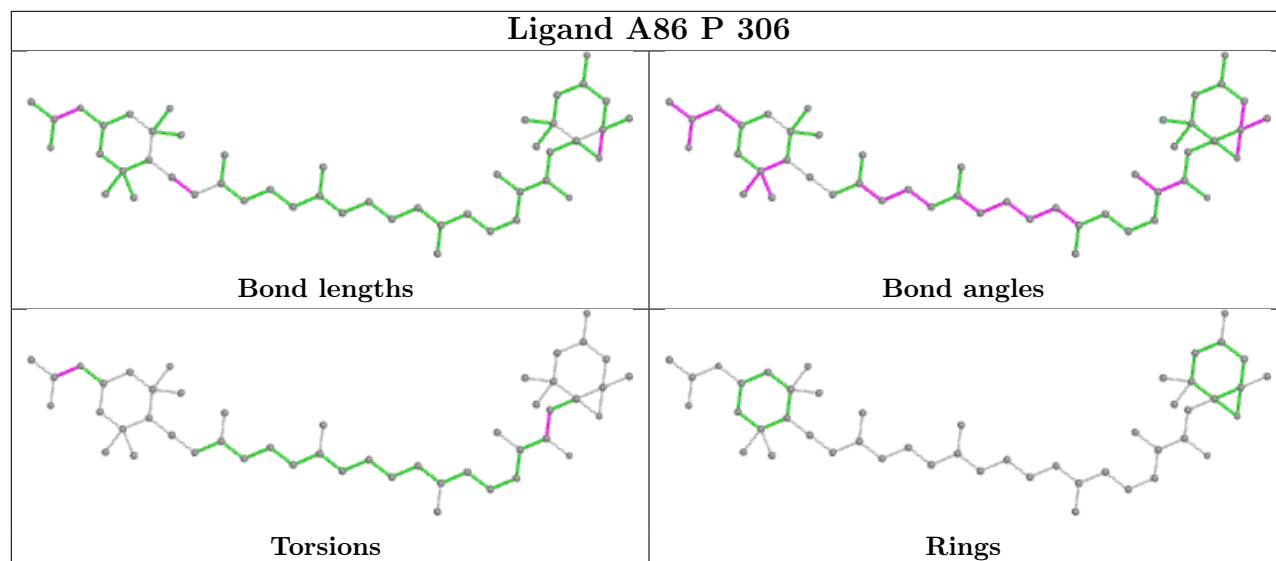
## Ligand CLA N 316



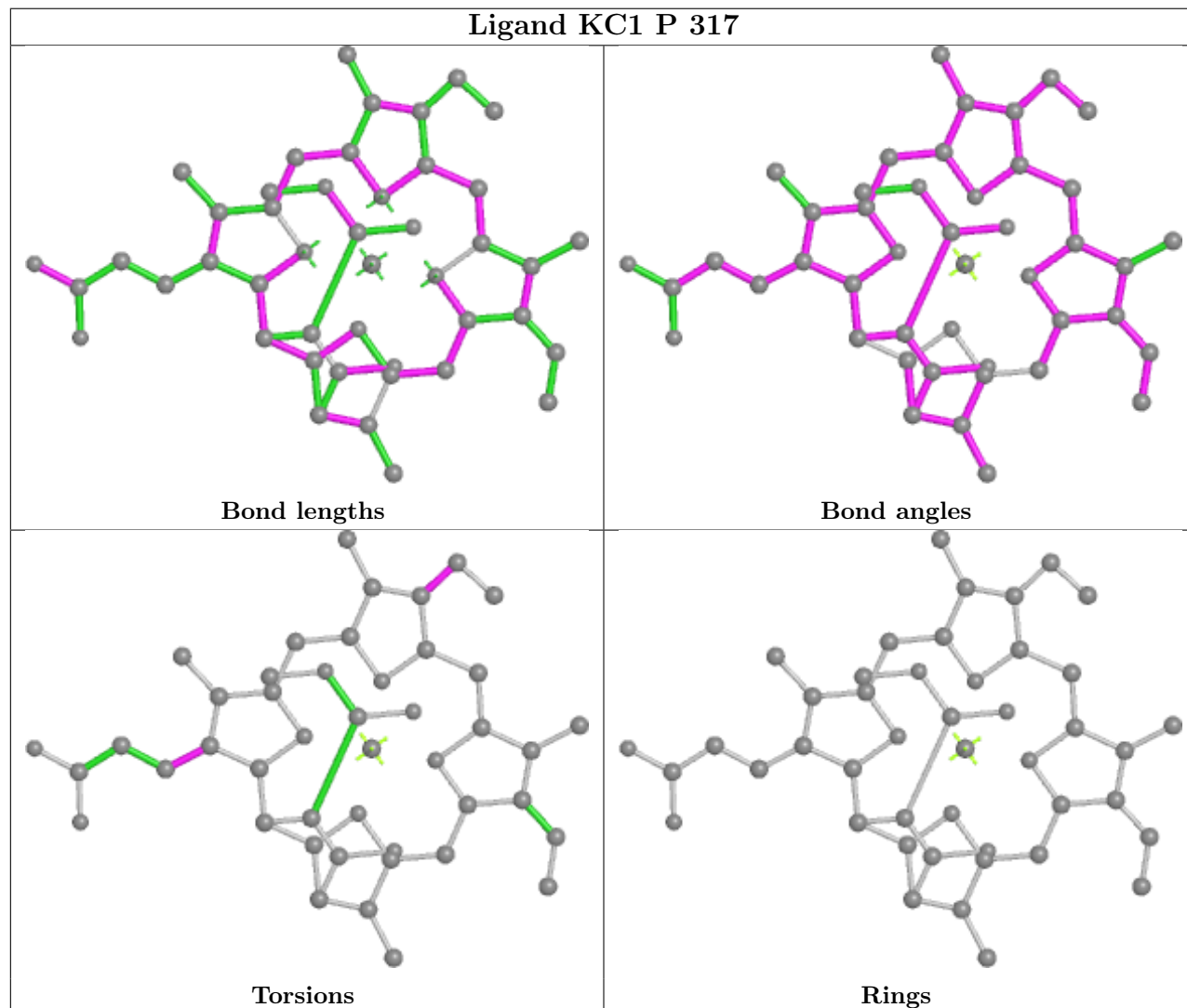
## Ligand CLA b 825

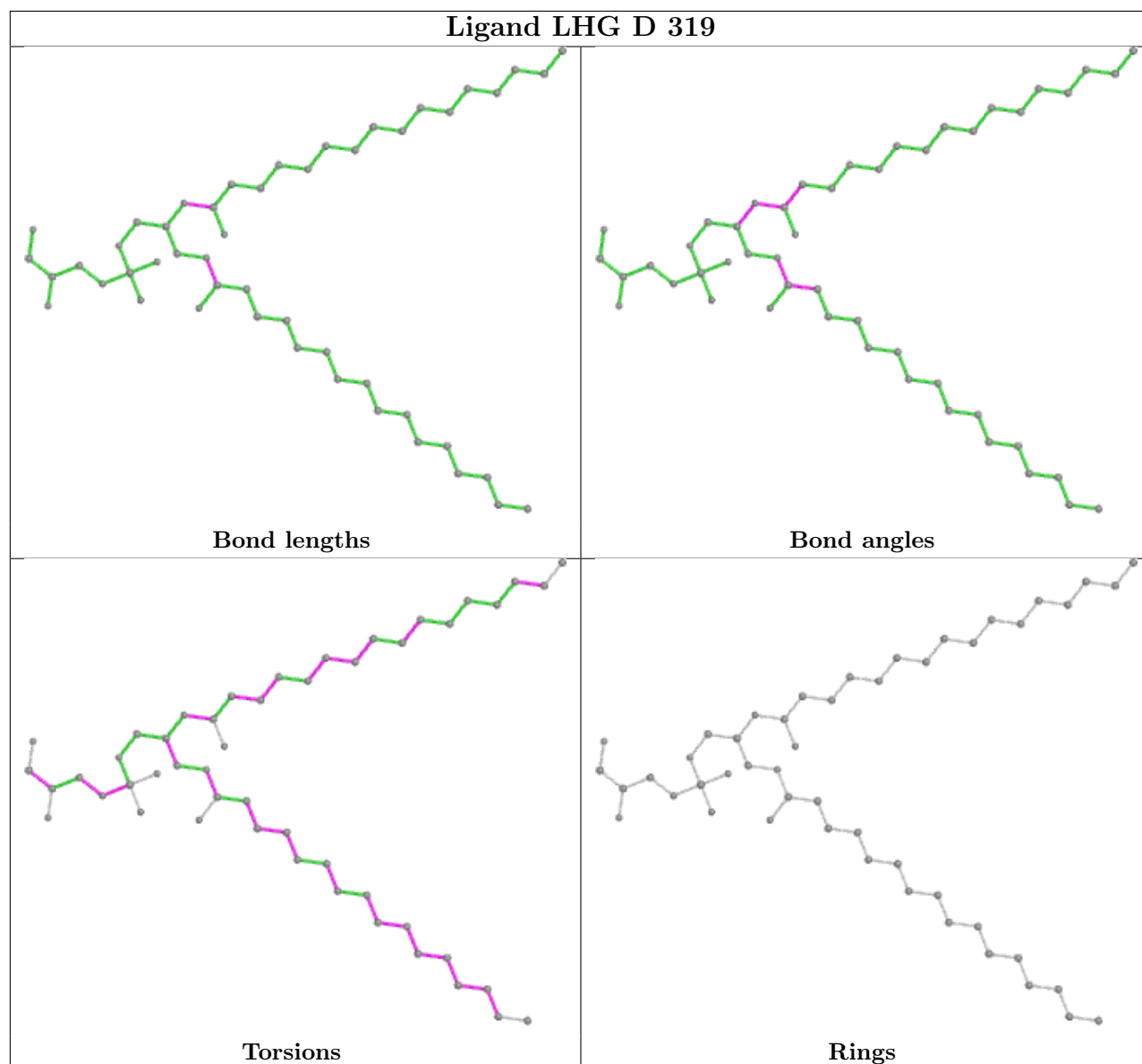
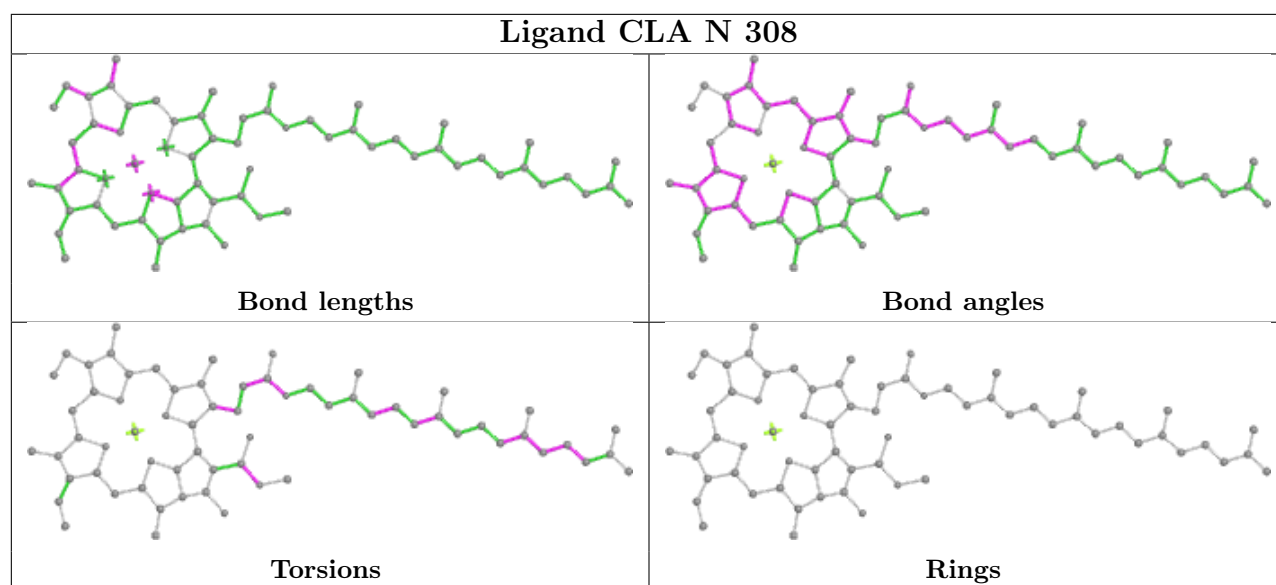


## Ligand A86 P 306

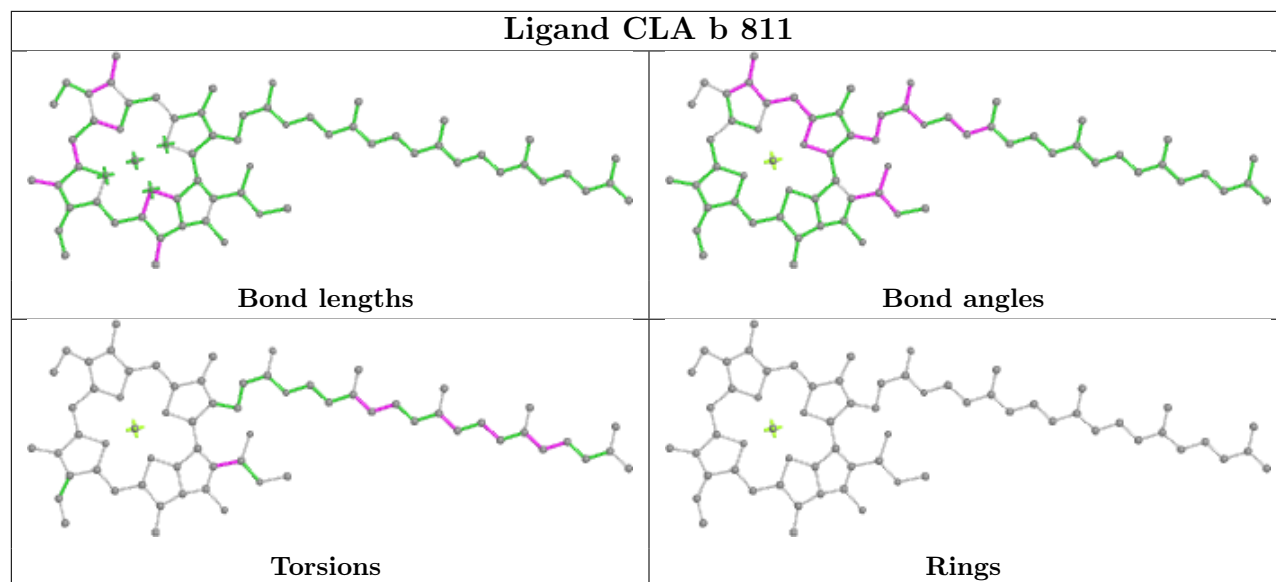


## Ligand KC1 P 317

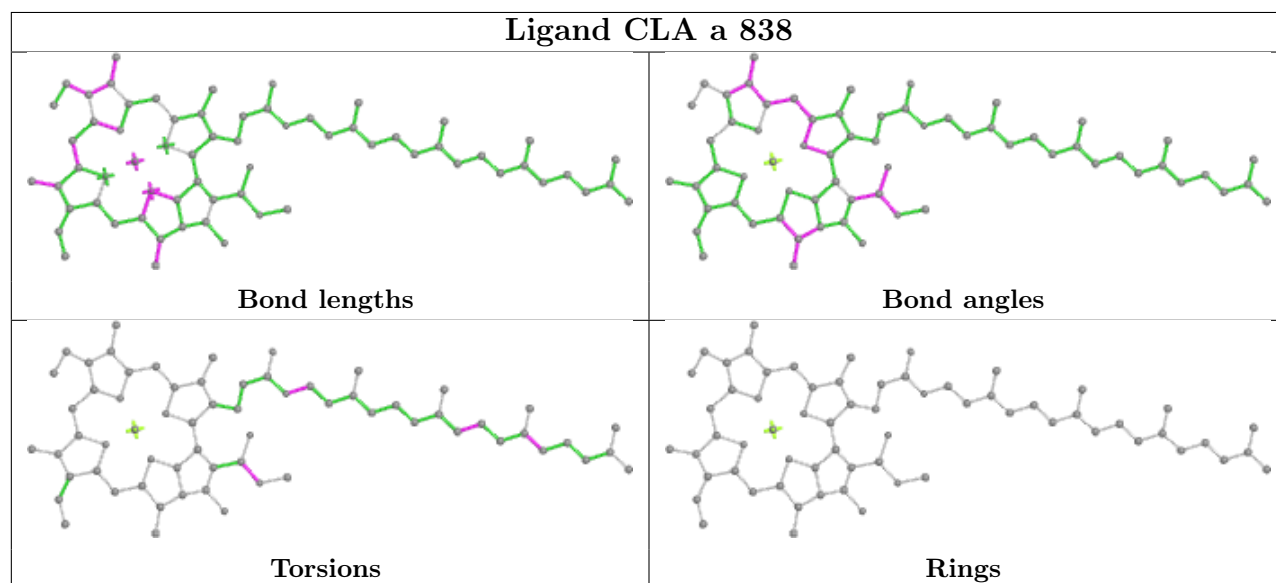




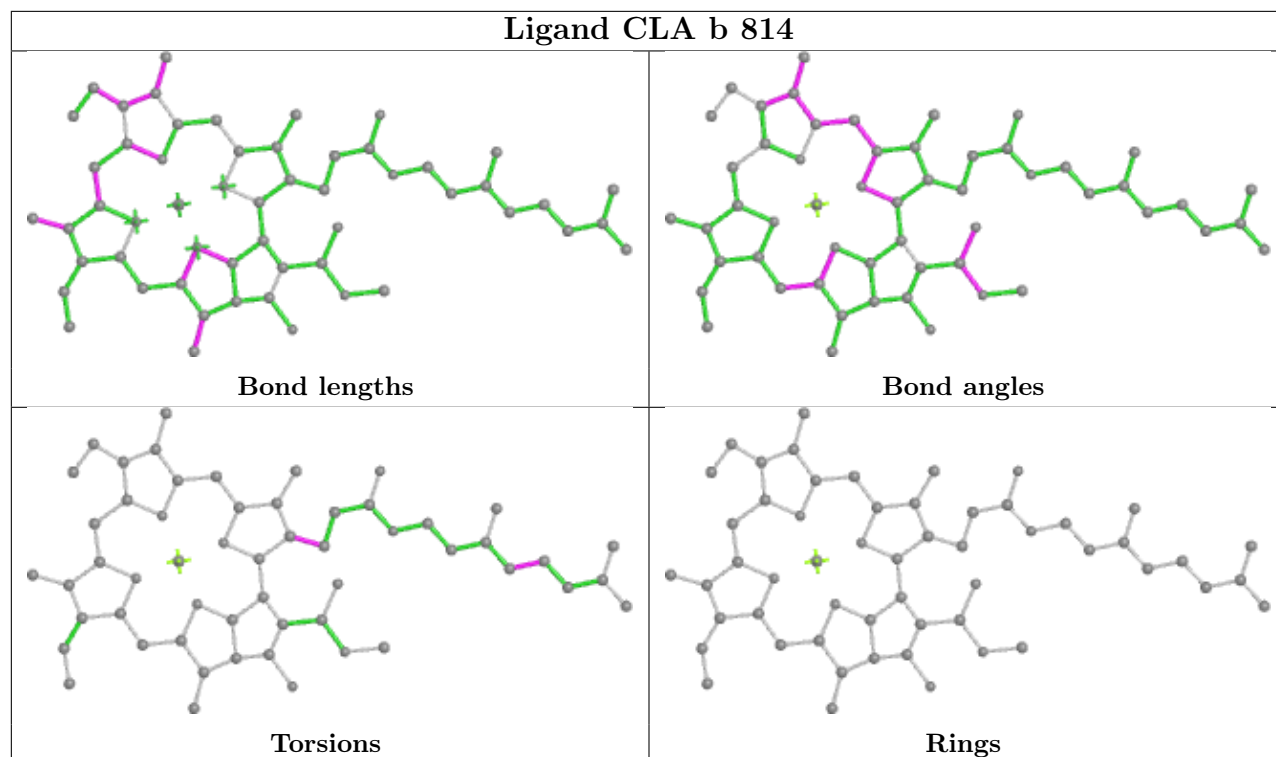
## Ligand CLA b 811



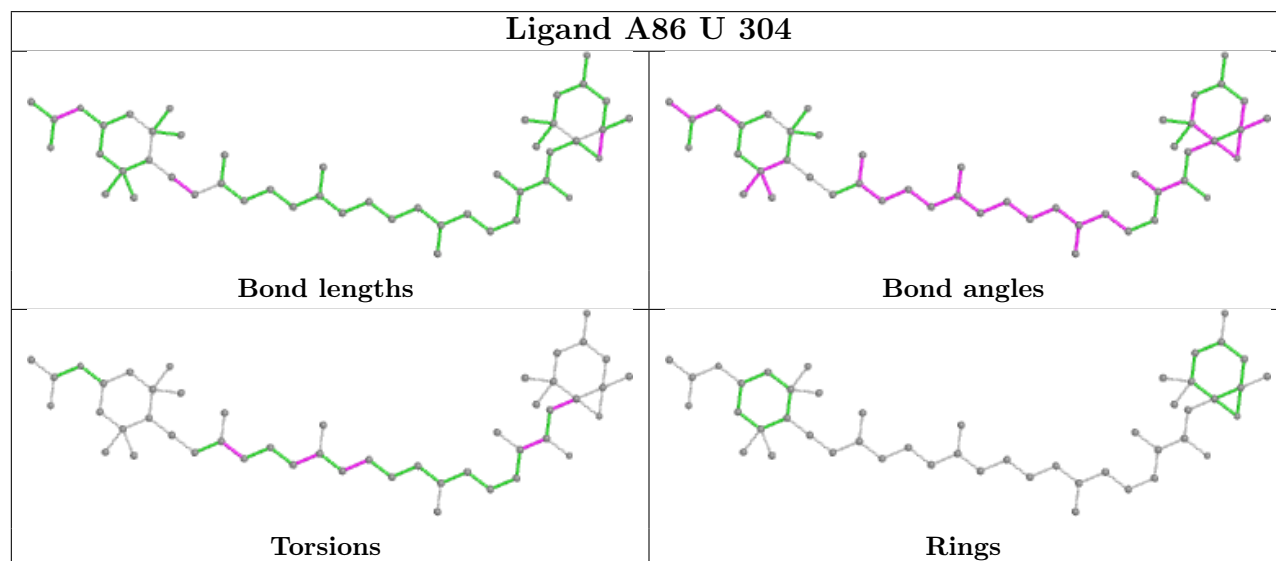
## Ligand CLA a 838



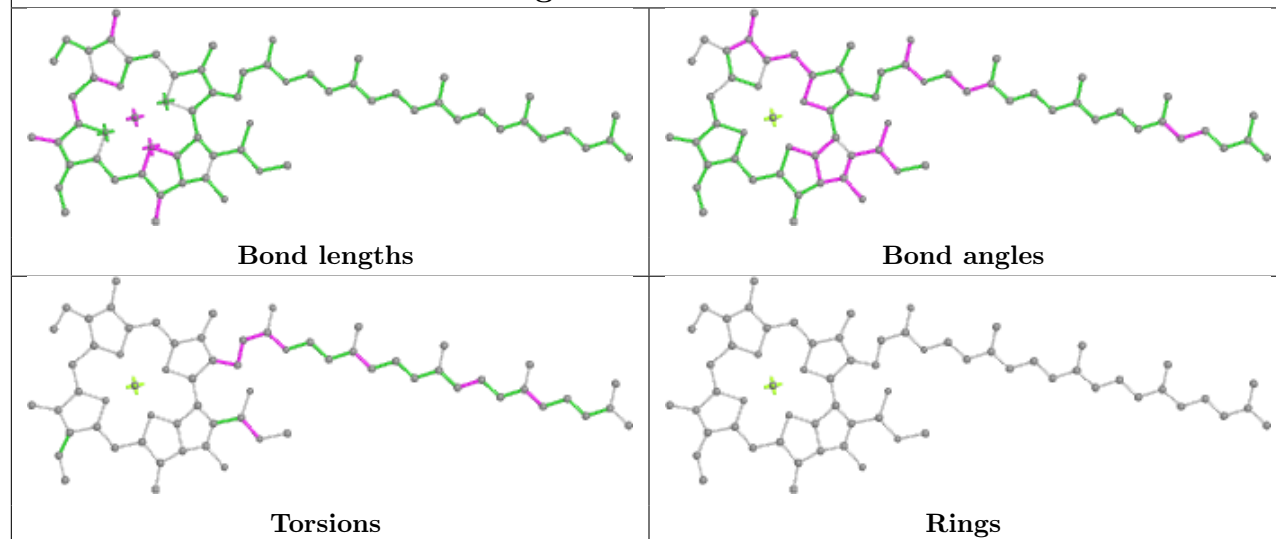
## Ligand CLA b 814



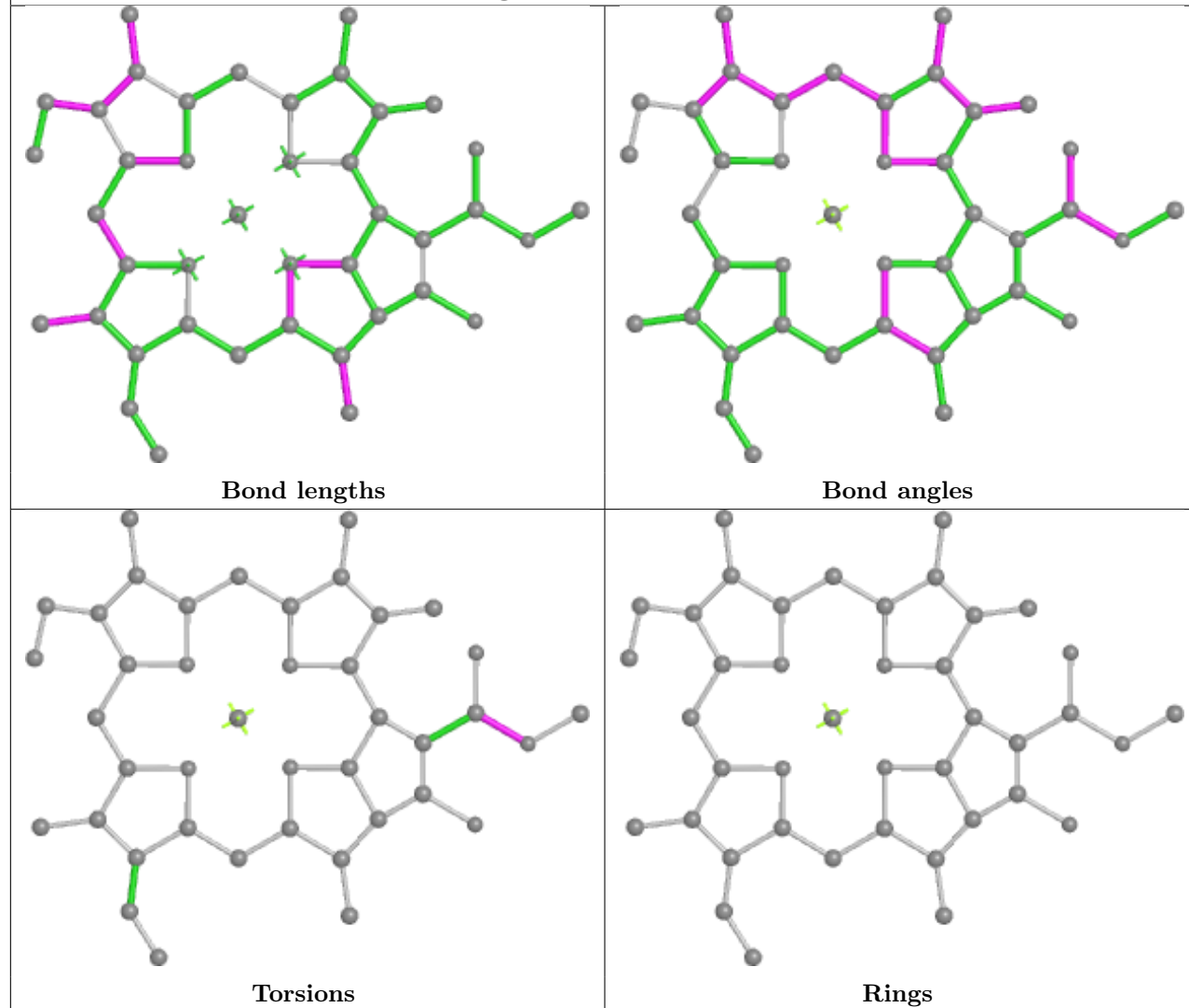
## Ligand A86 U 304

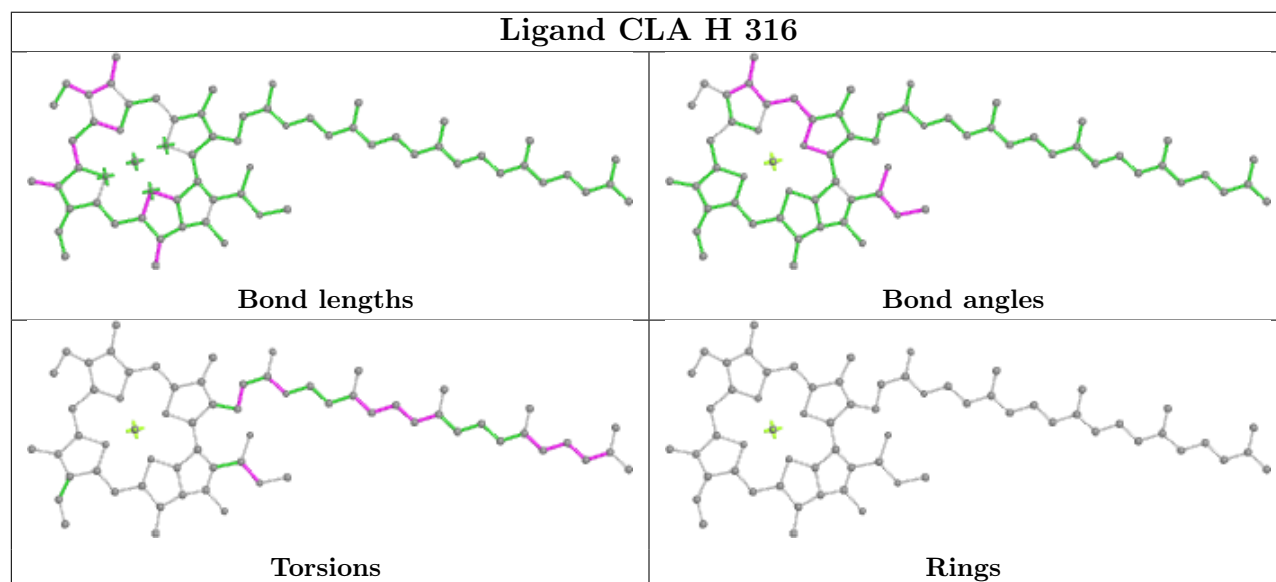
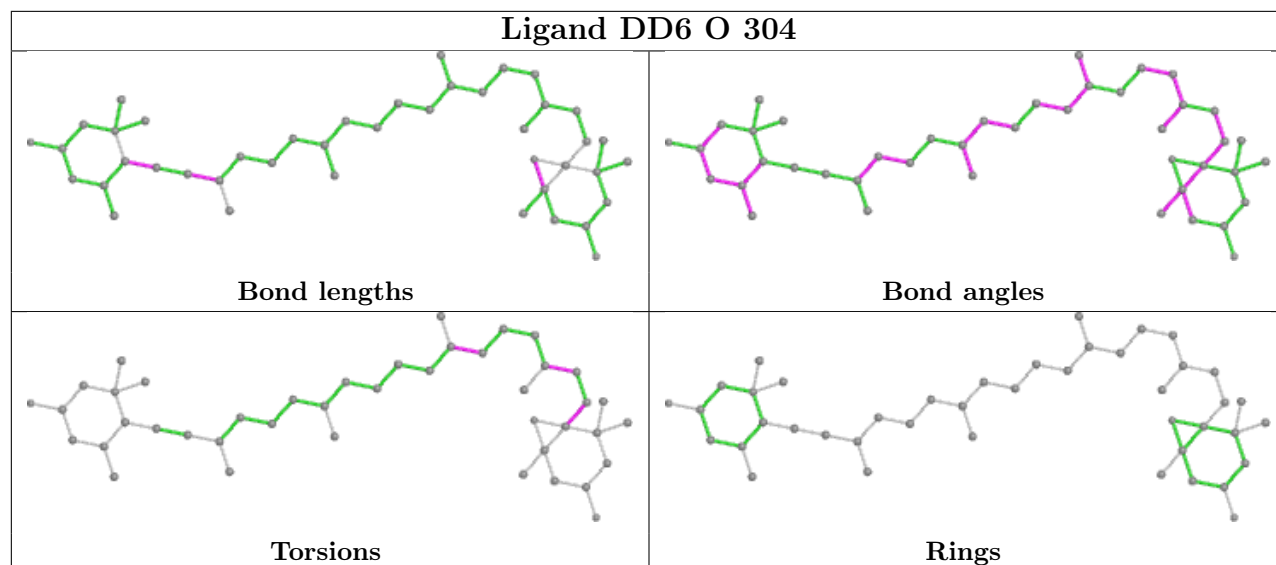


## Ligand CLA b 828



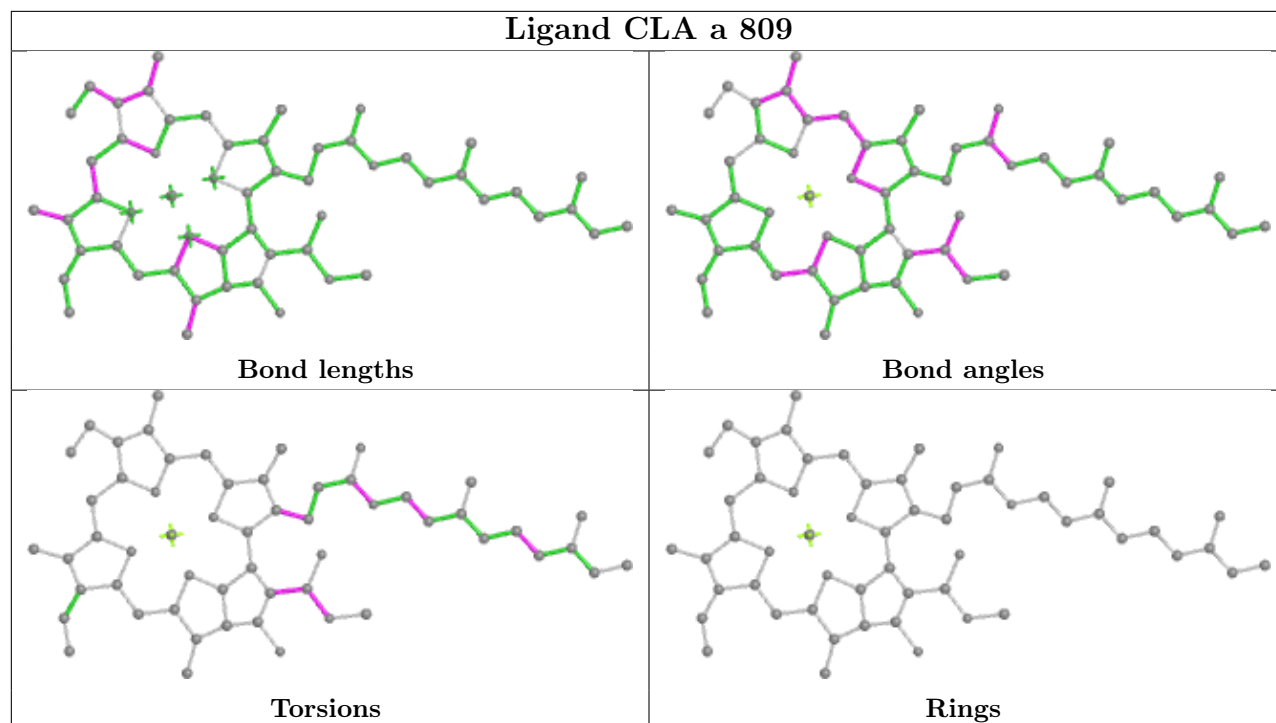
## Ligand CLA C 214



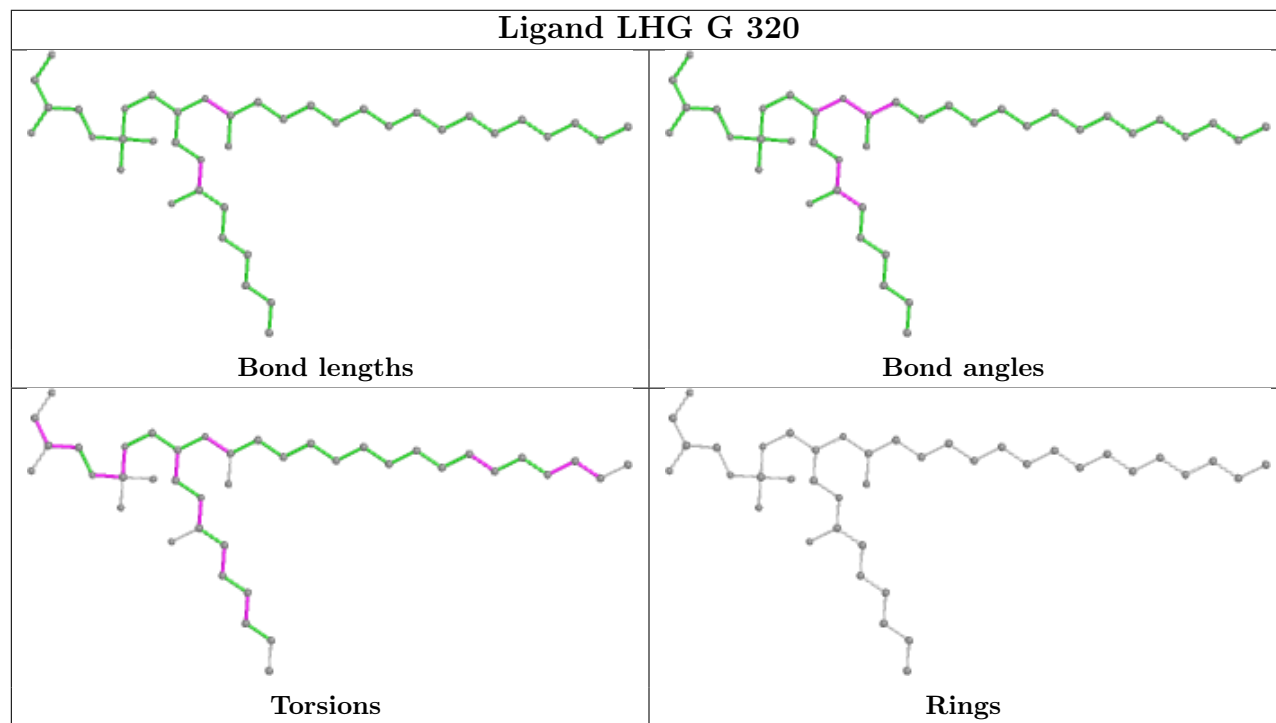


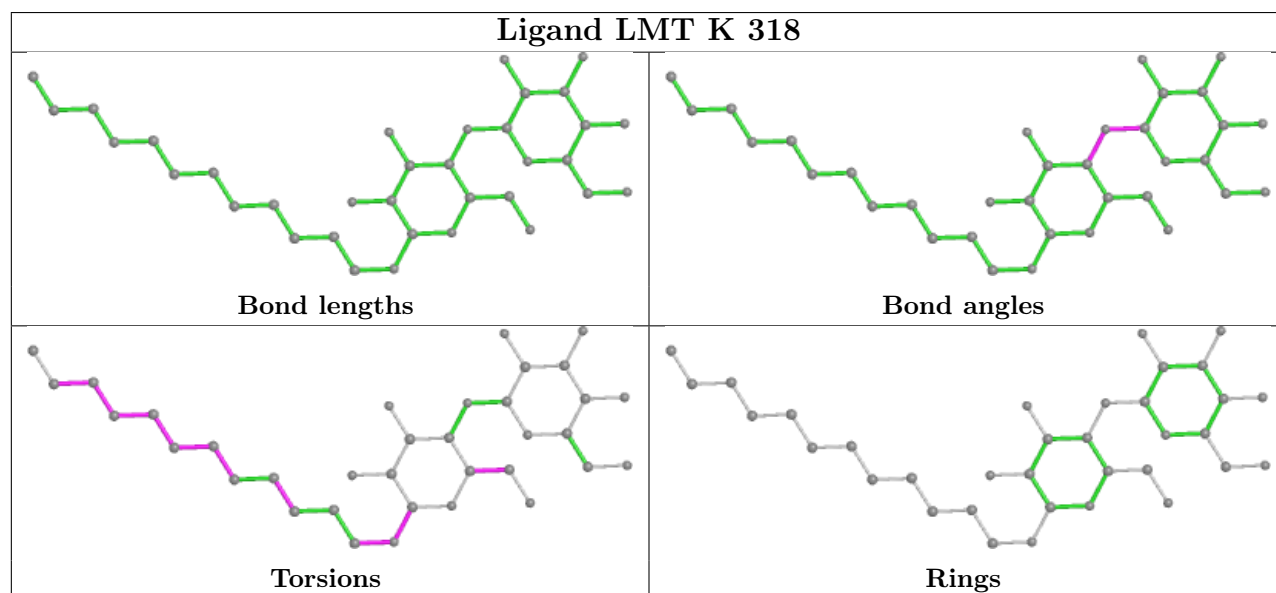
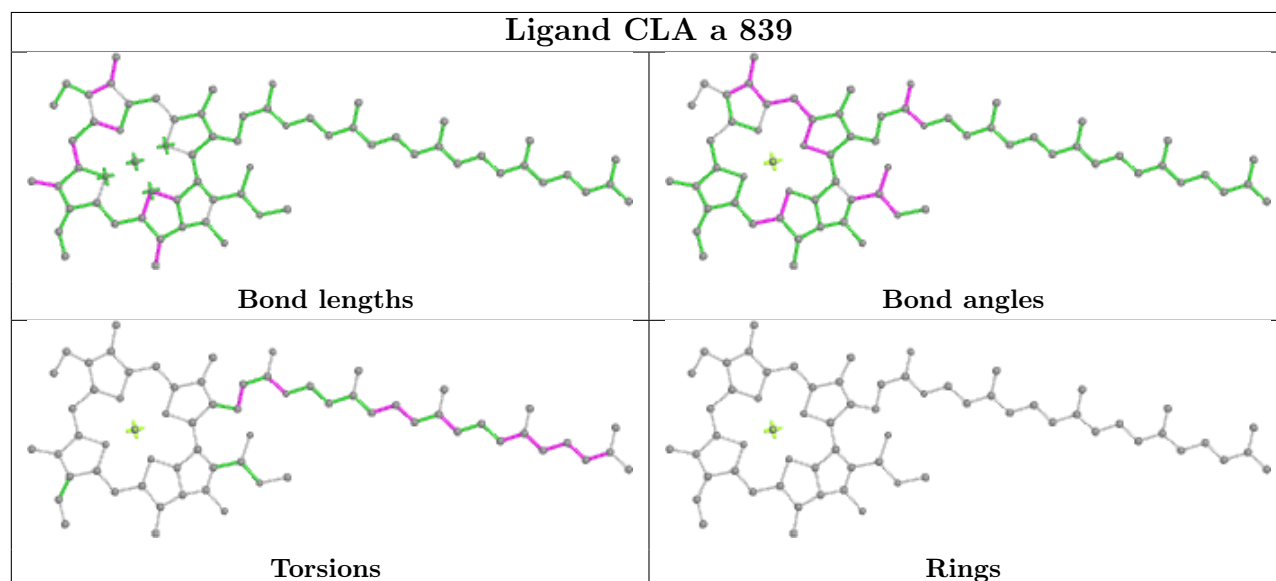
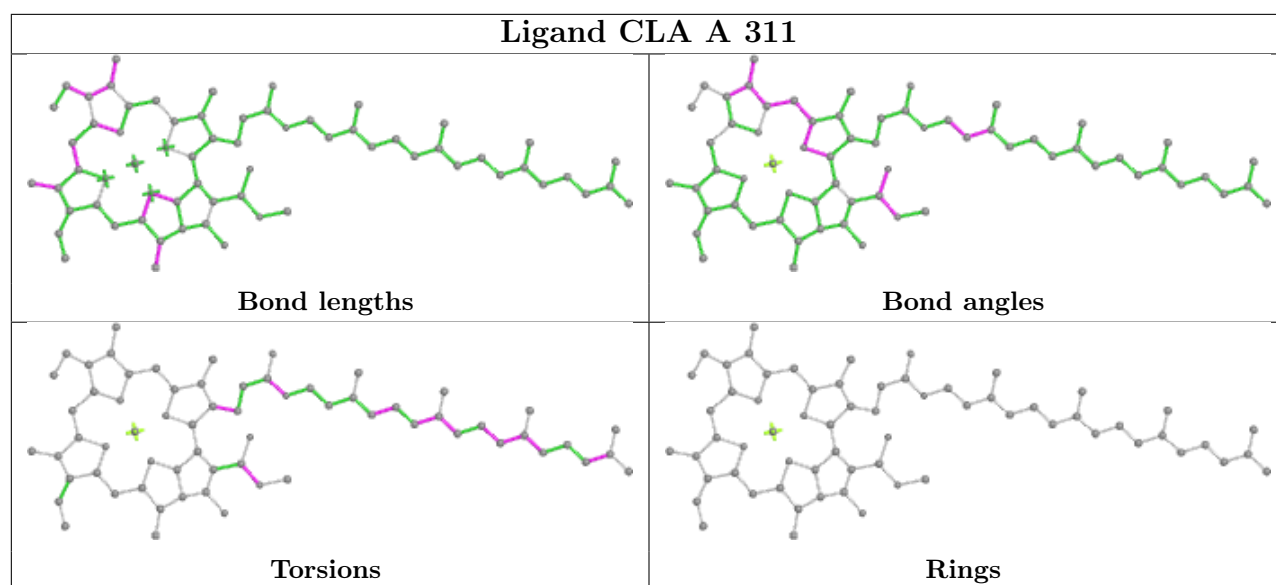


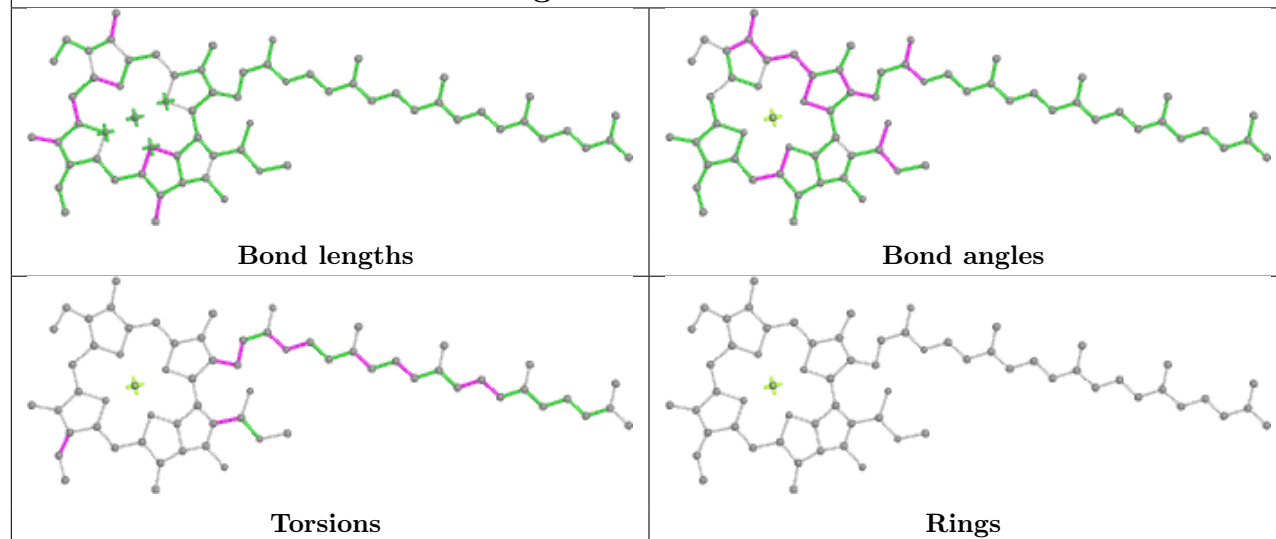
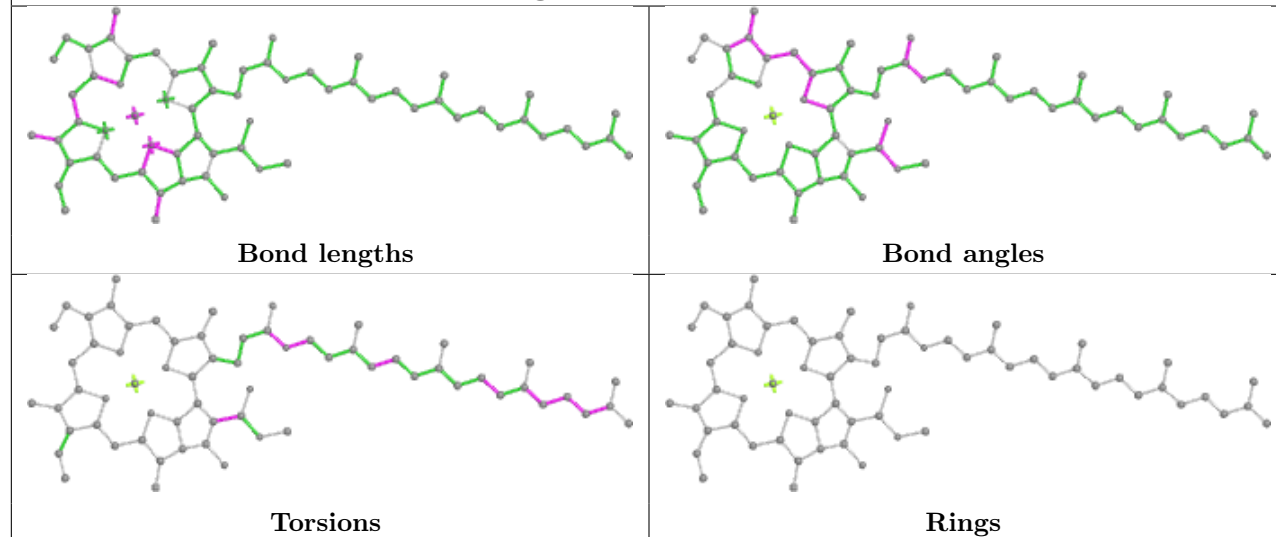
## Ligand CLA a 809



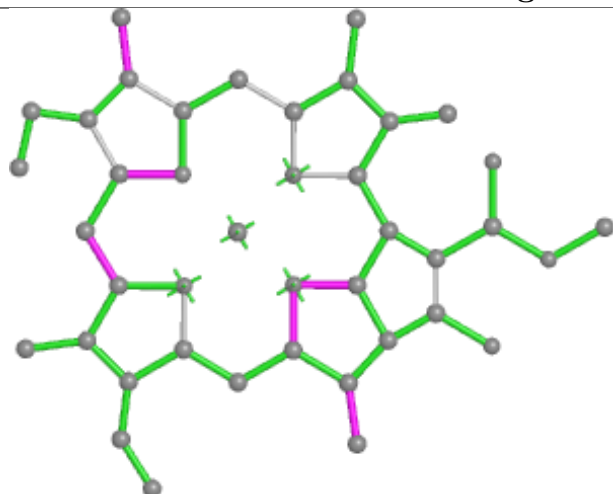
## Ligand LHG G 320



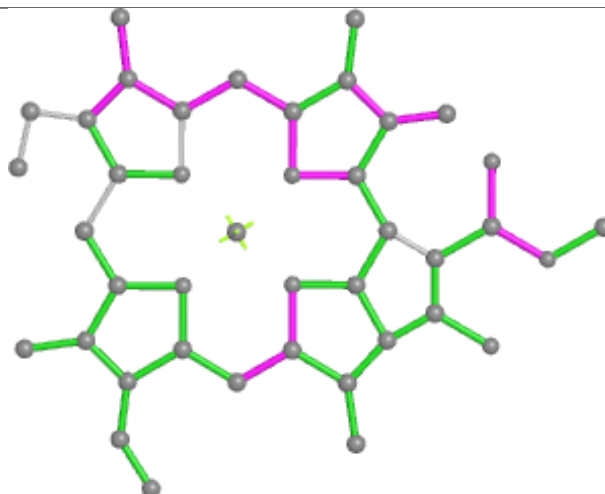


**Ligand CLA E 312****Ligand CLA A 310**

## Ligand CLA S 317



Bond lengths



Bond angles

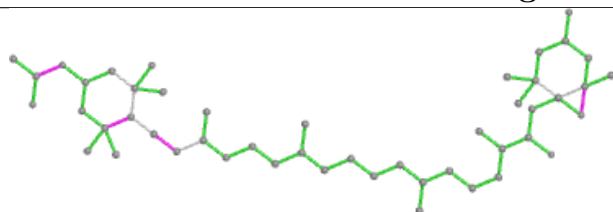


Torsions

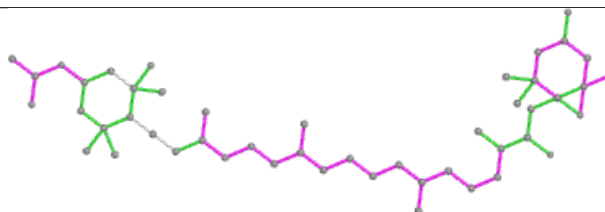


Rings

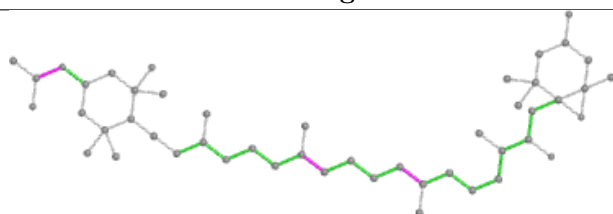
## Ligand A86 G 306



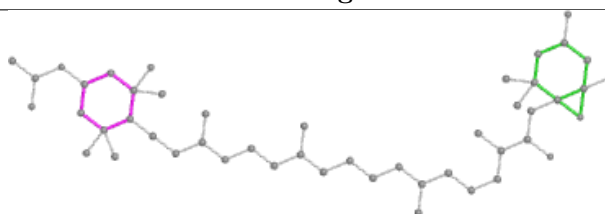
Bond lengths



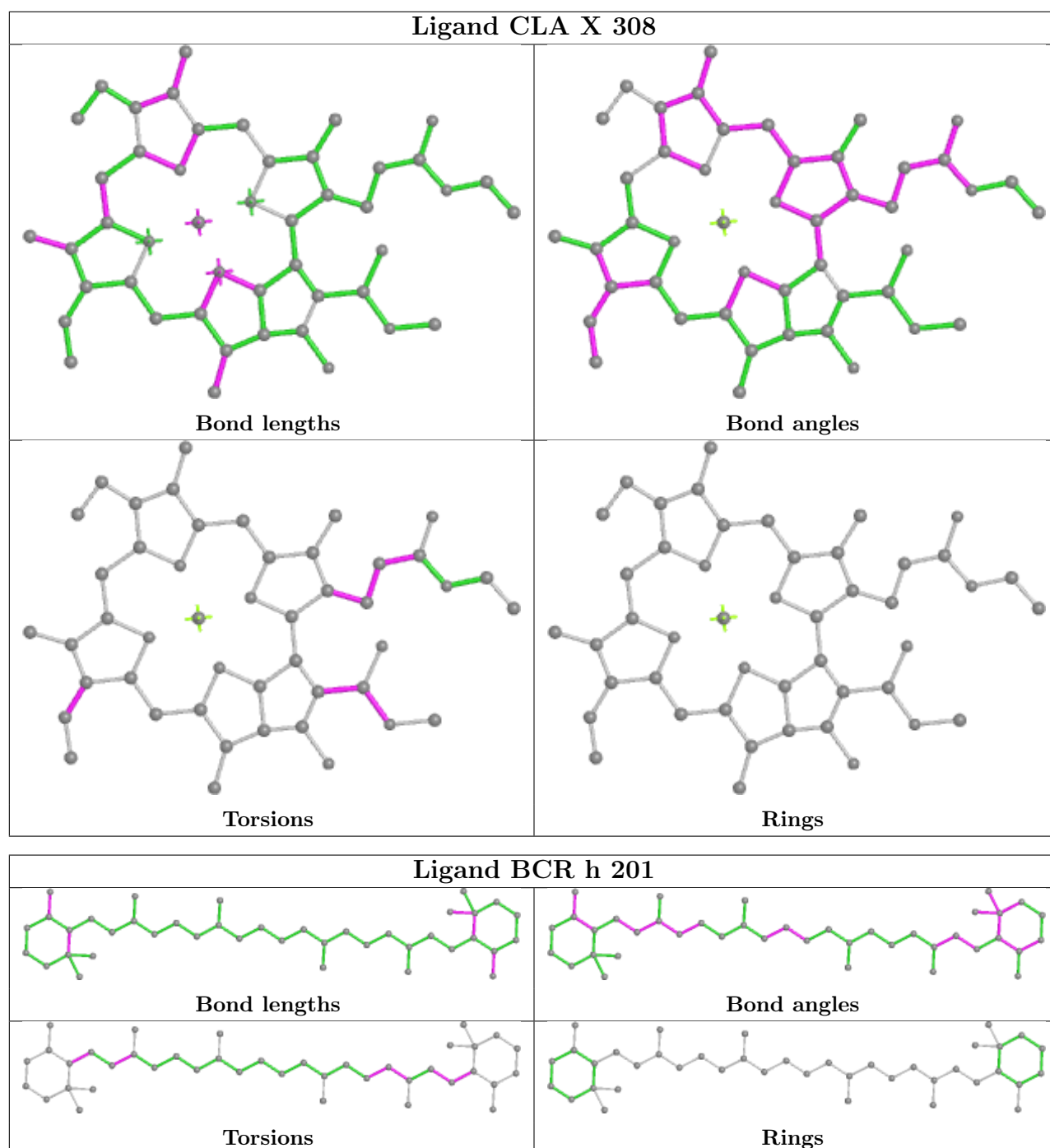
Bond angles

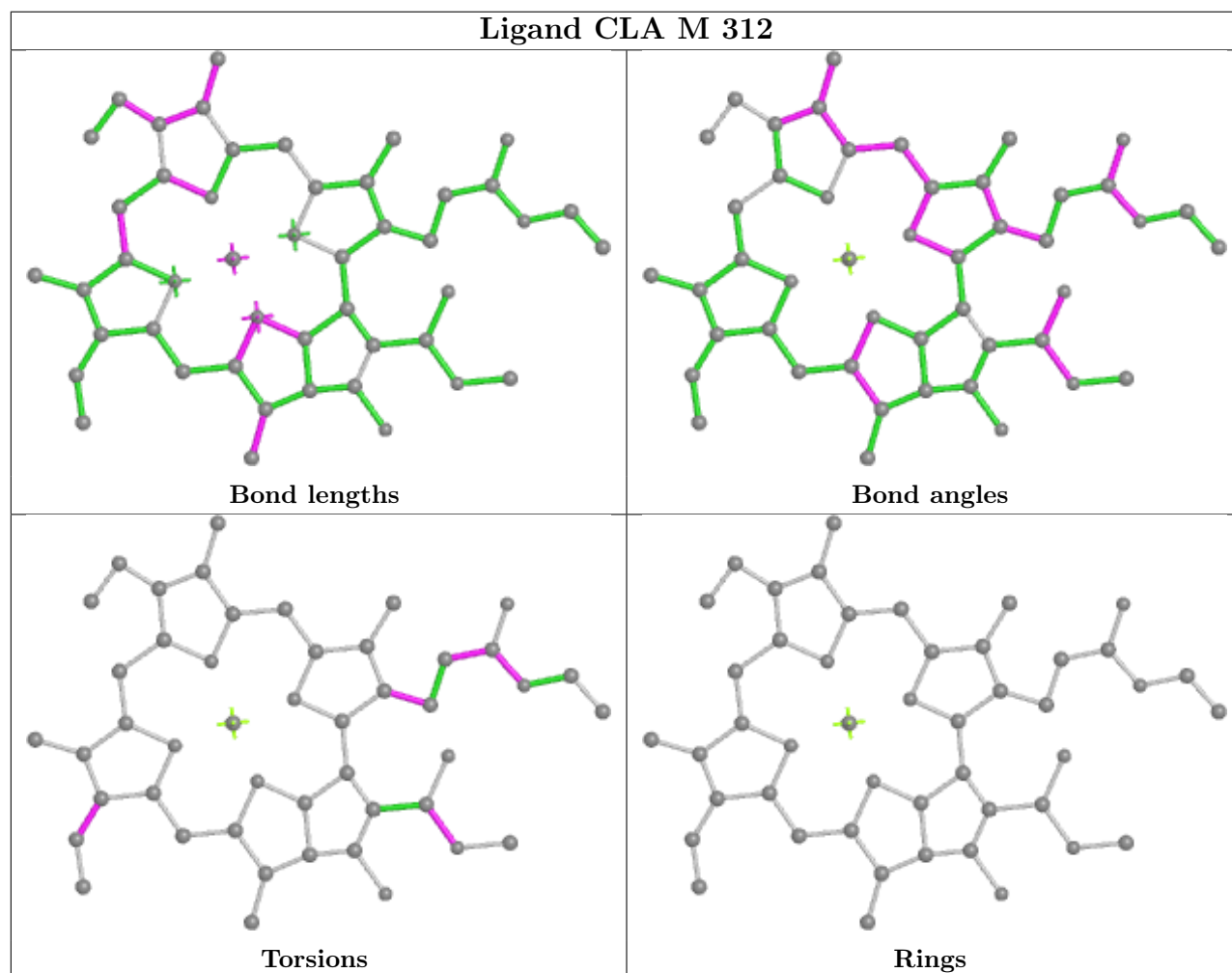
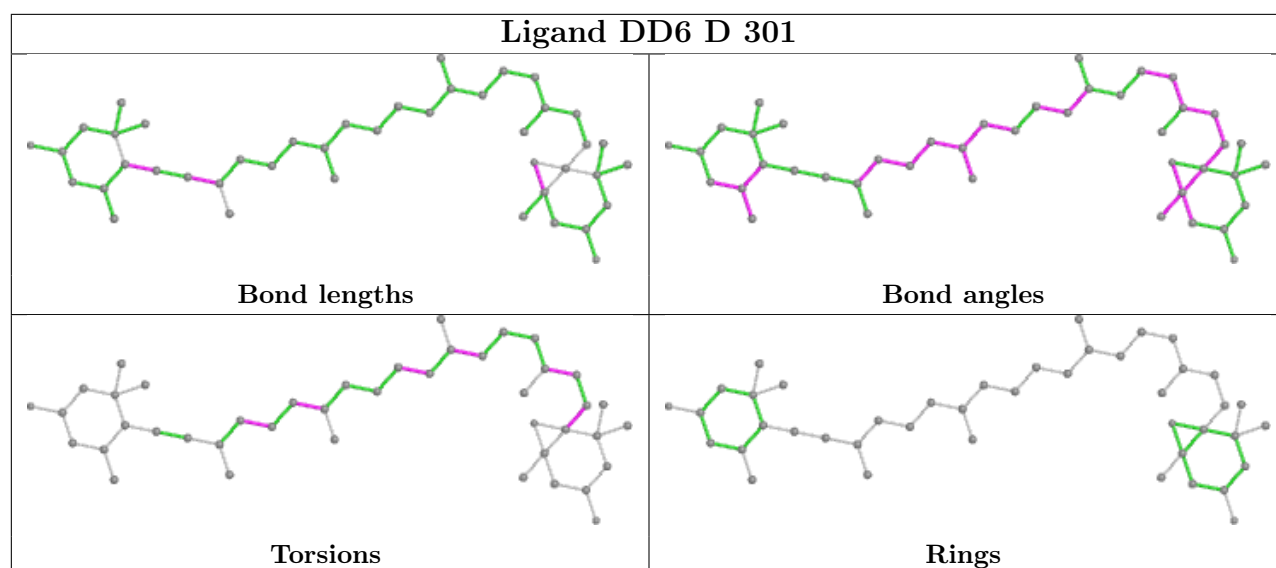


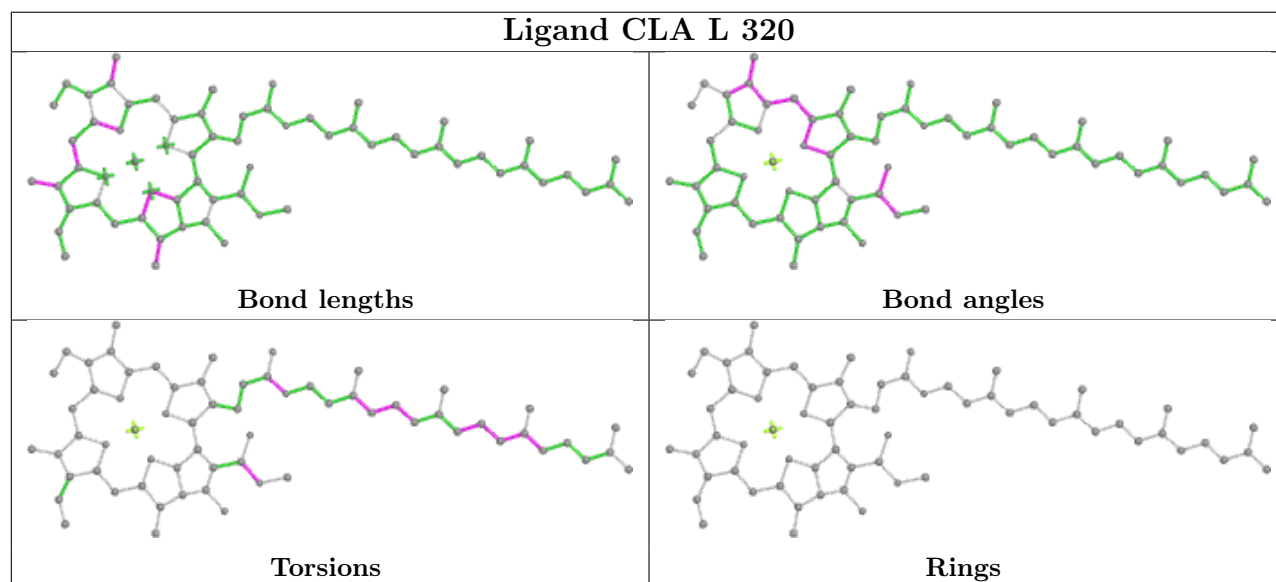
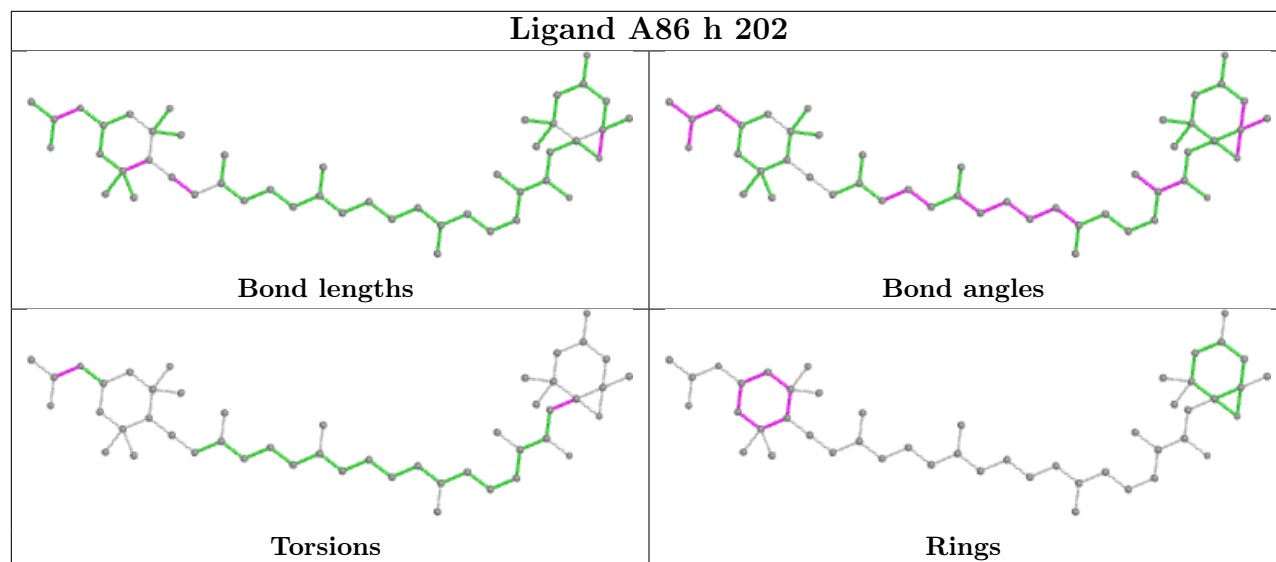
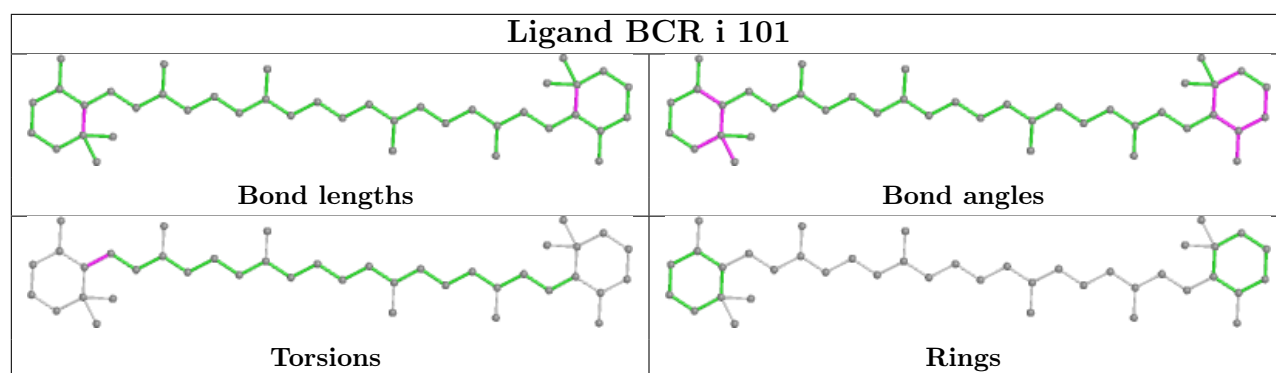
Torsions



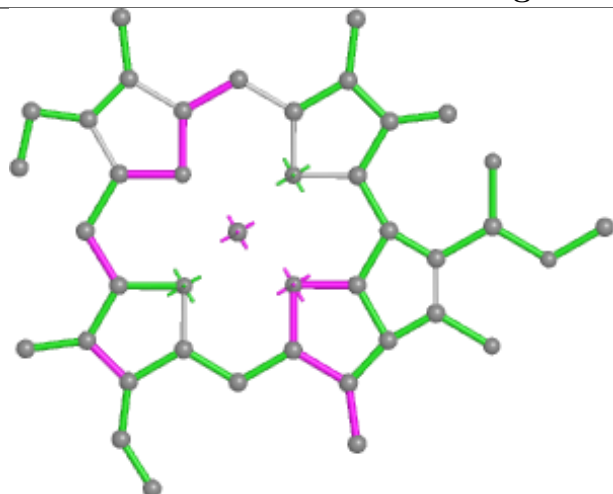
Rings



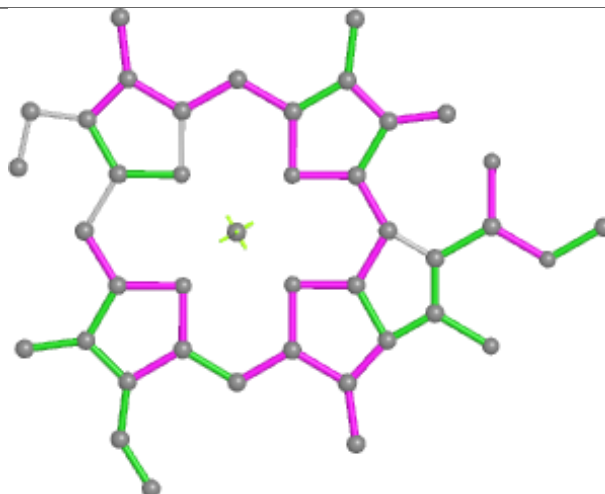




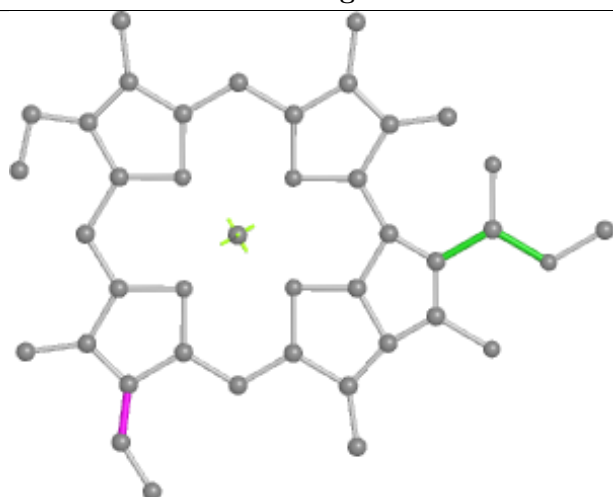
## Ligand CLA N 310



Bond lengths



Bond angles

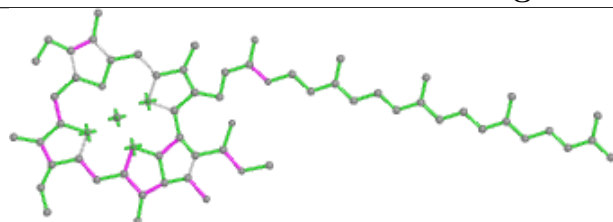


Torsions

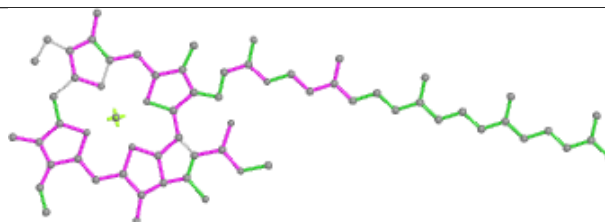


Rings

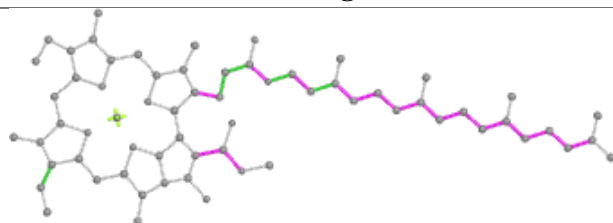
## Ligand CLA O 316



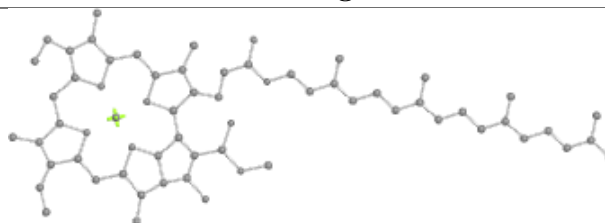
Bond lengths



Bond angles



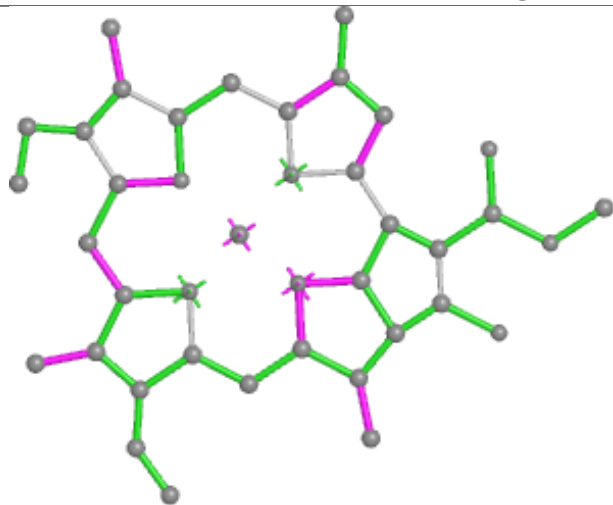
Torsions



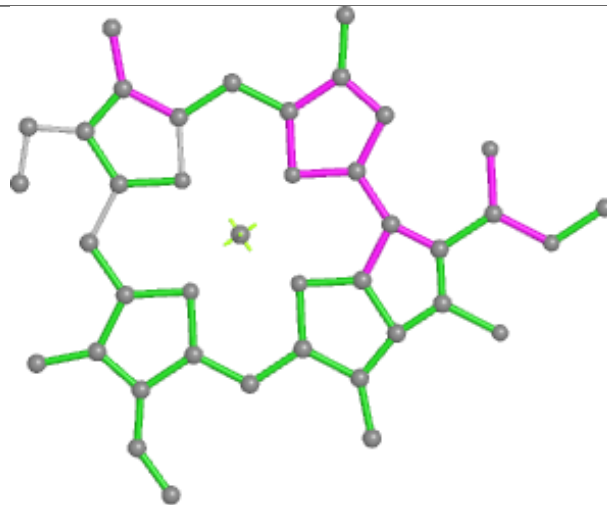
Rings



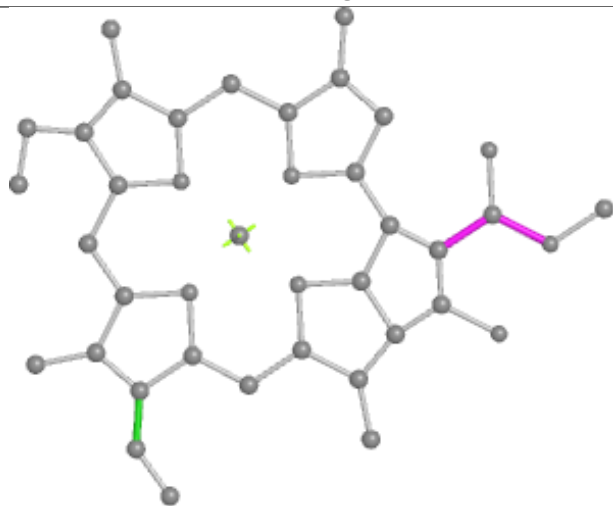
## Ligand CLA O 312



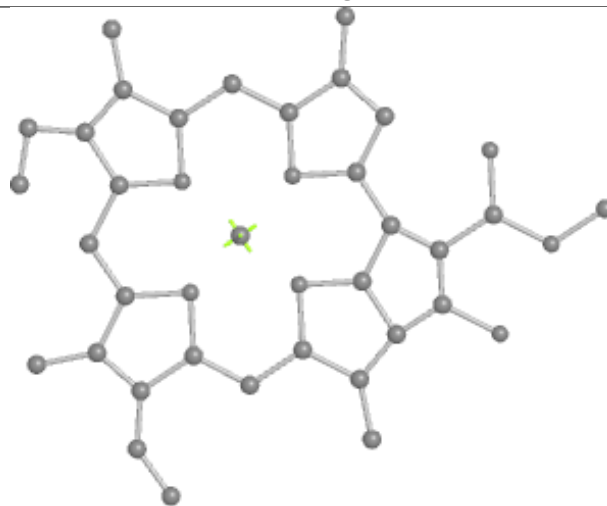
Bond lengths



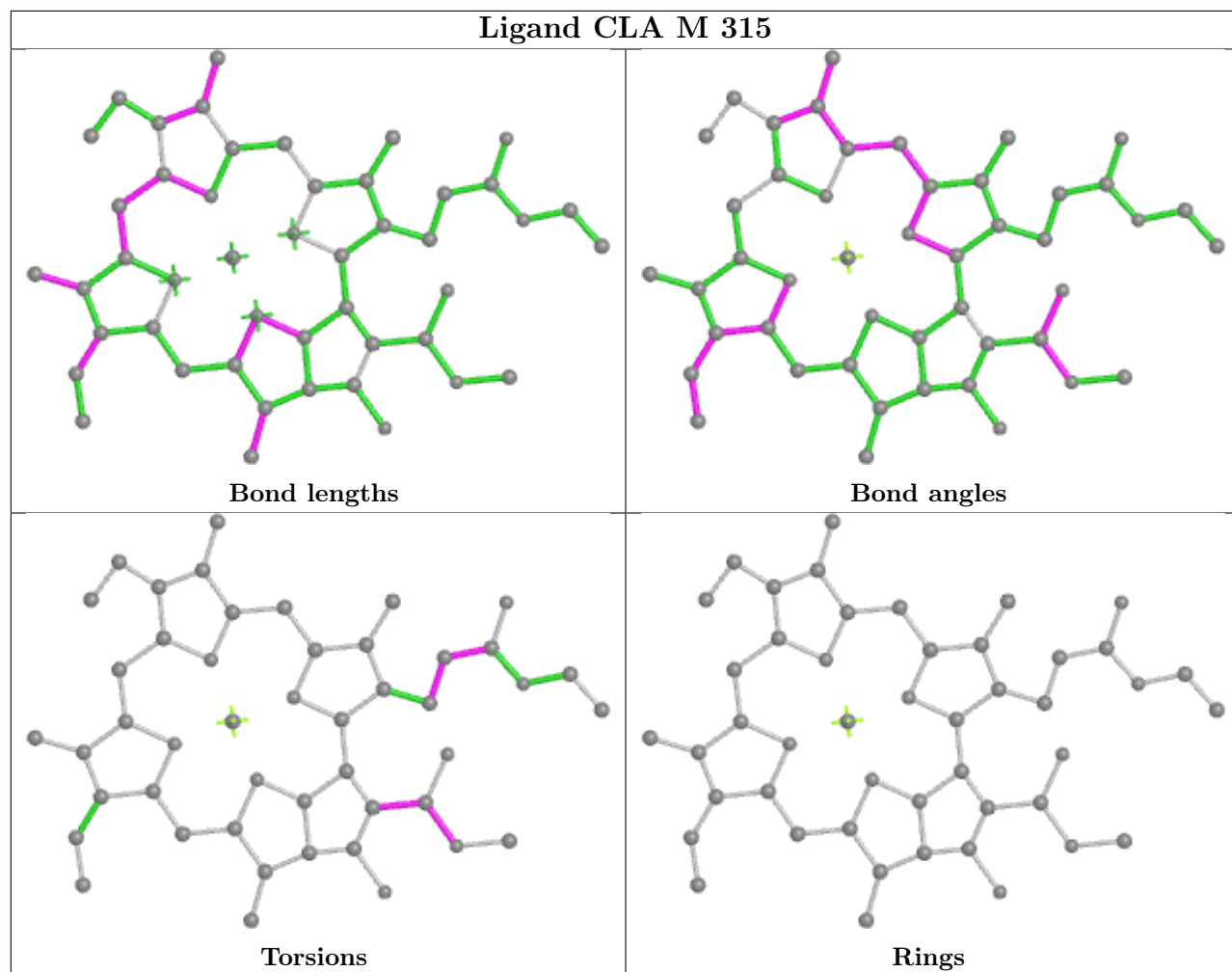
Bond angles

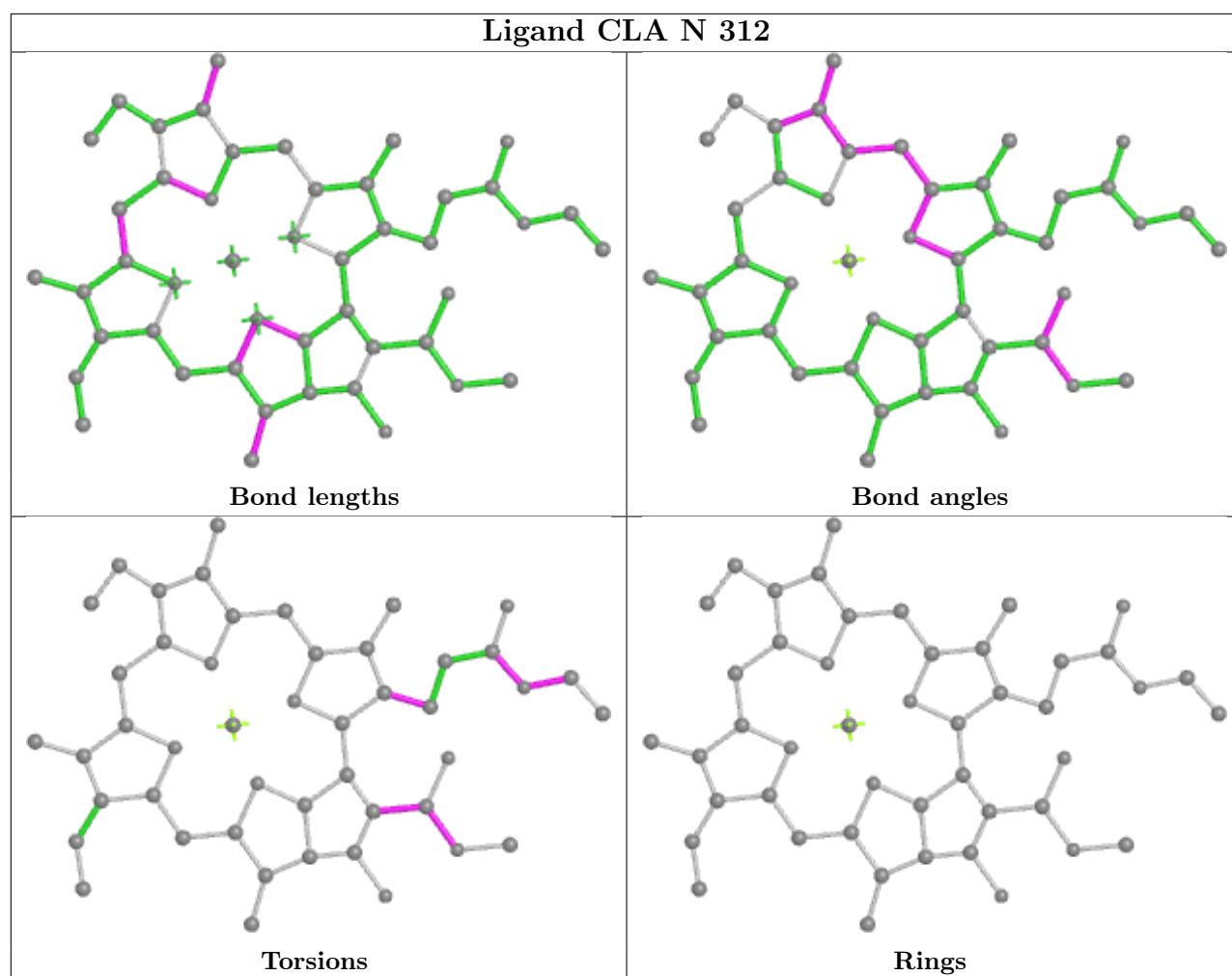


Torsions

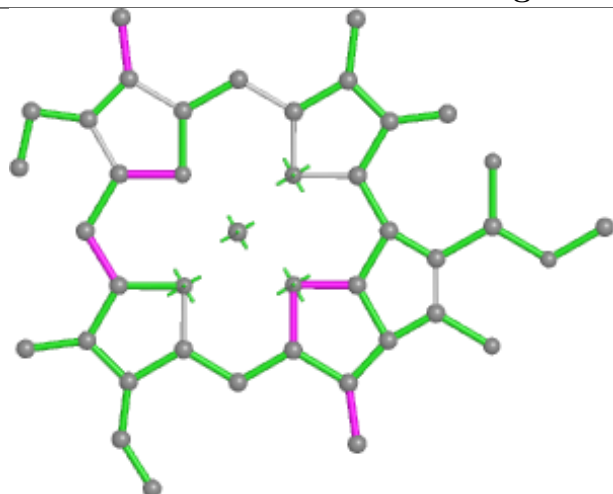


Rings

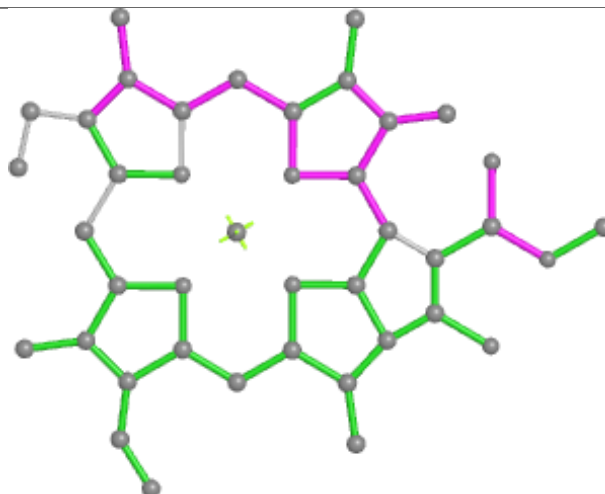




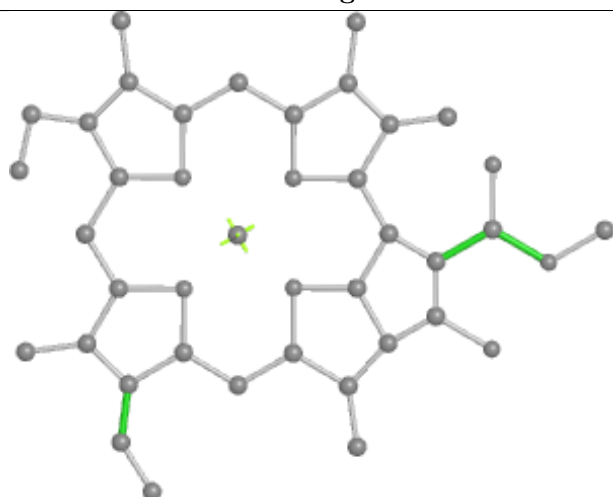
## Ligand CLA N 315



Bond lengths



Bond angles

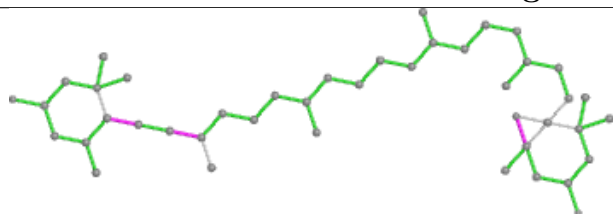


Torsions

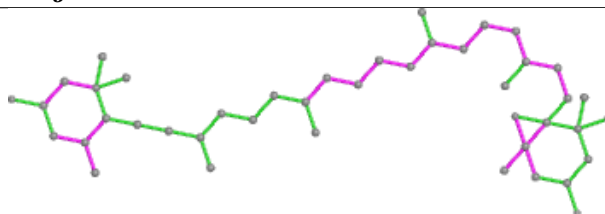


Rings

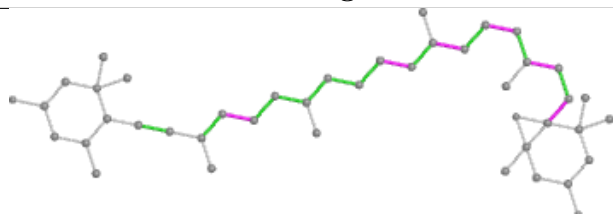
## Ligand DD6 j 103



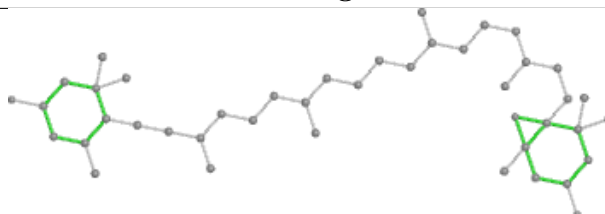
Bond lengths



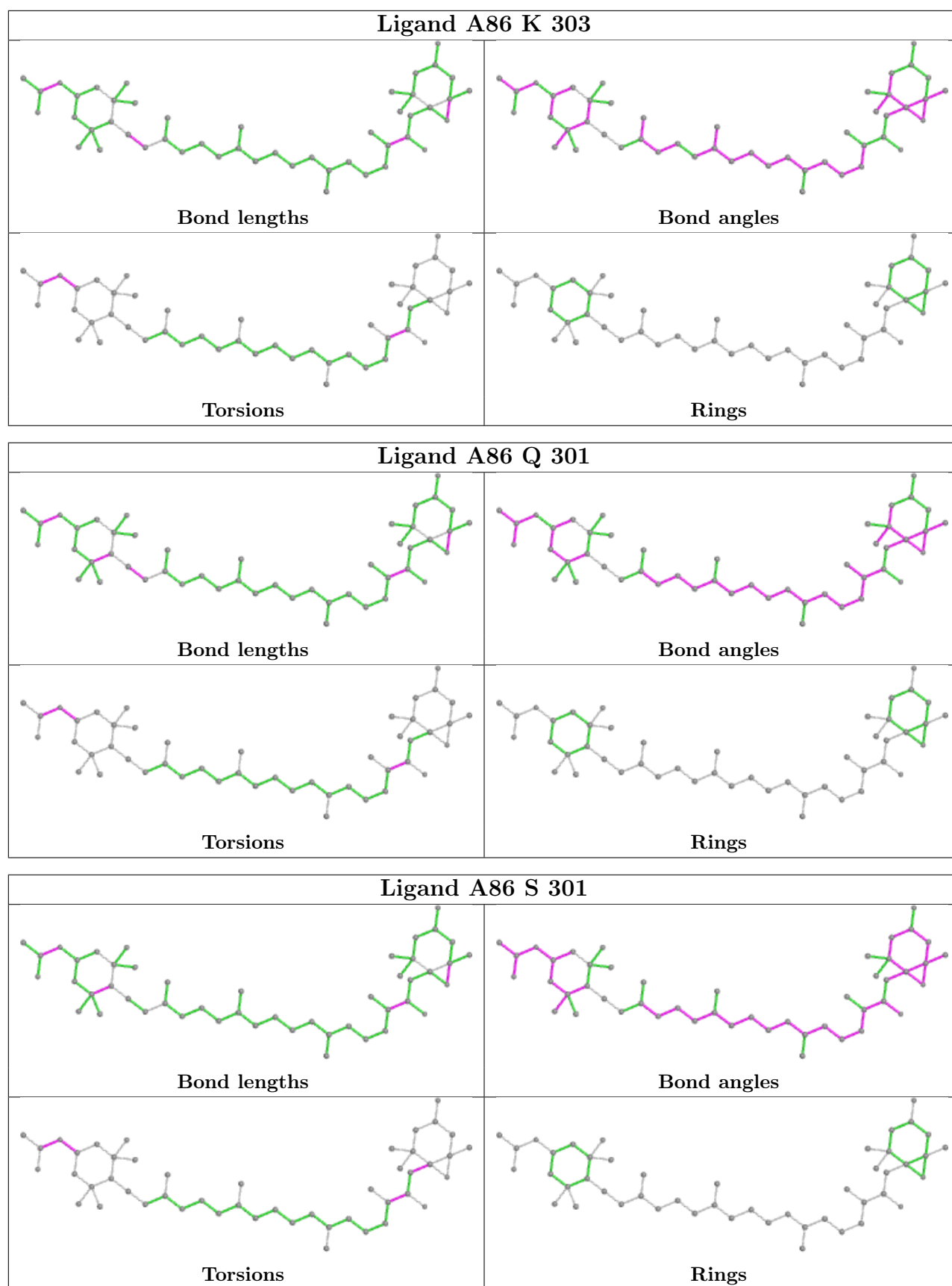
Bond angles

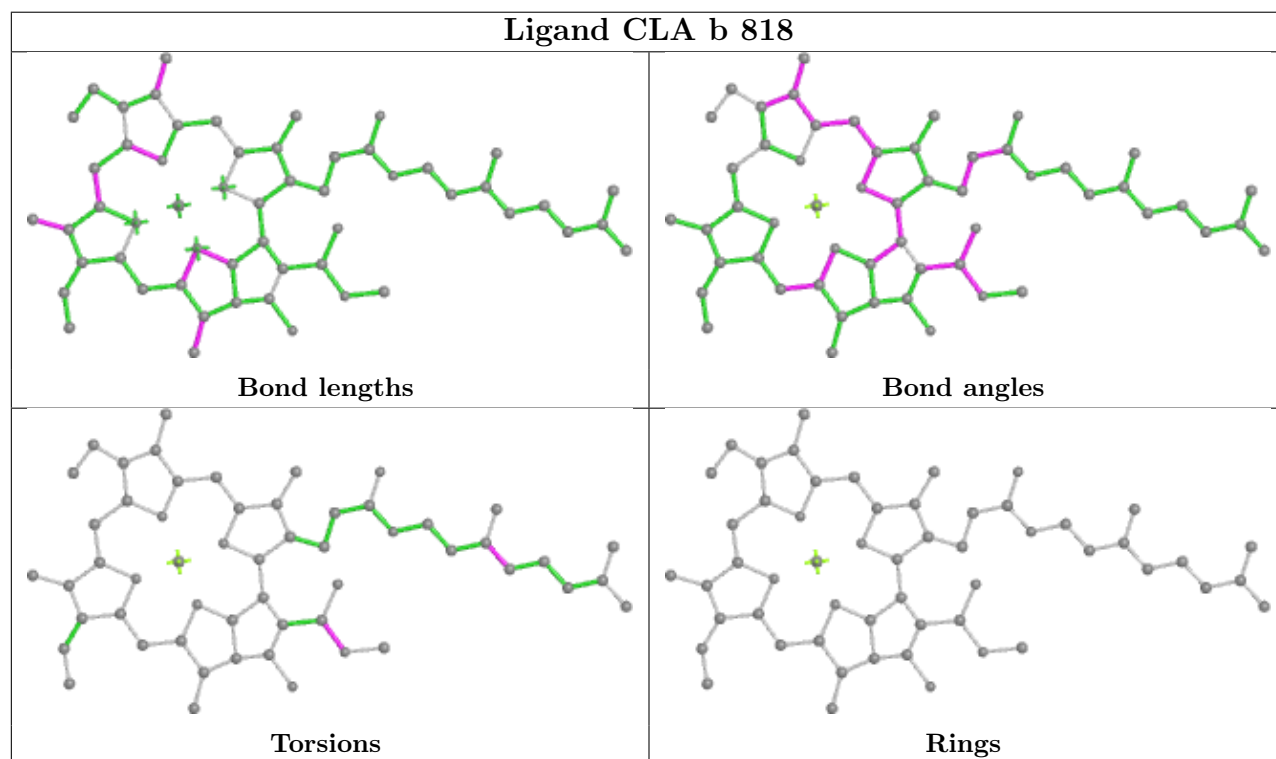
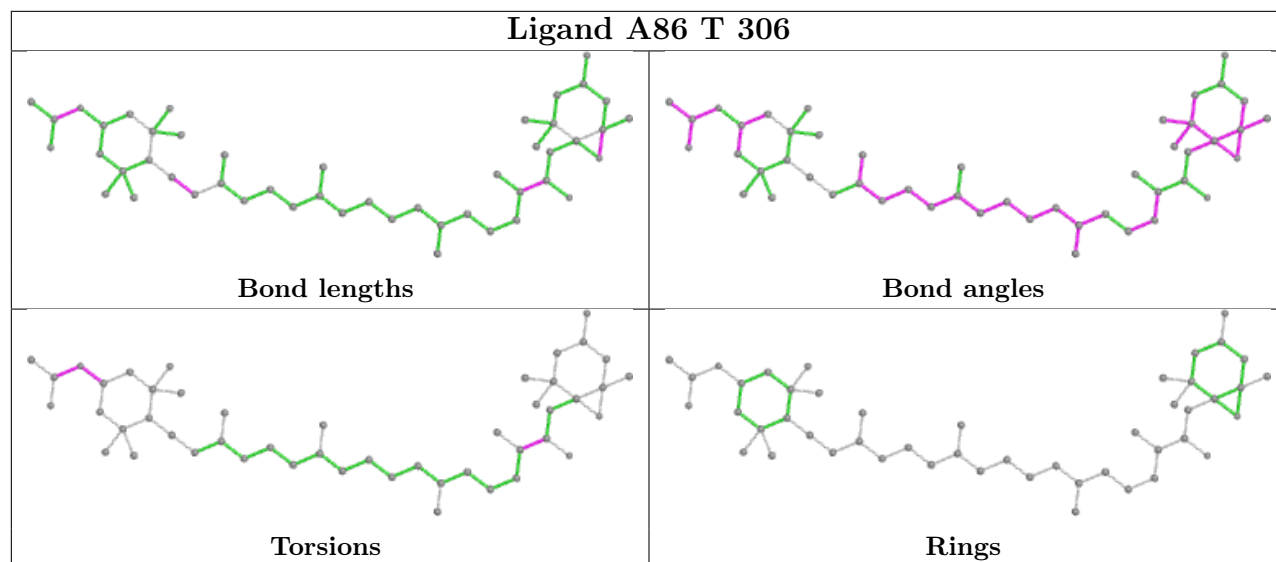
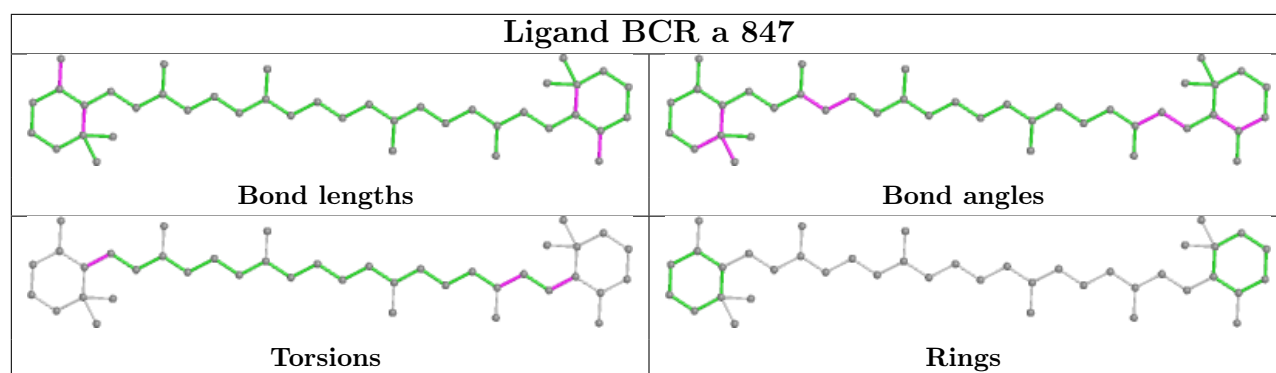


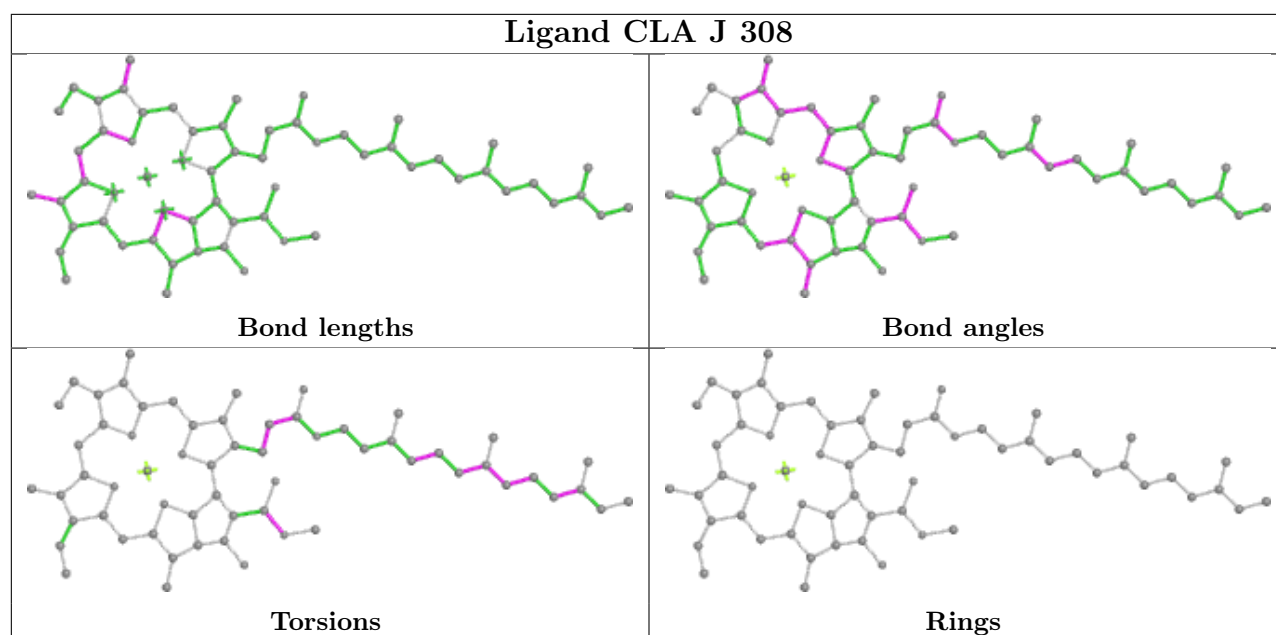
Torsions

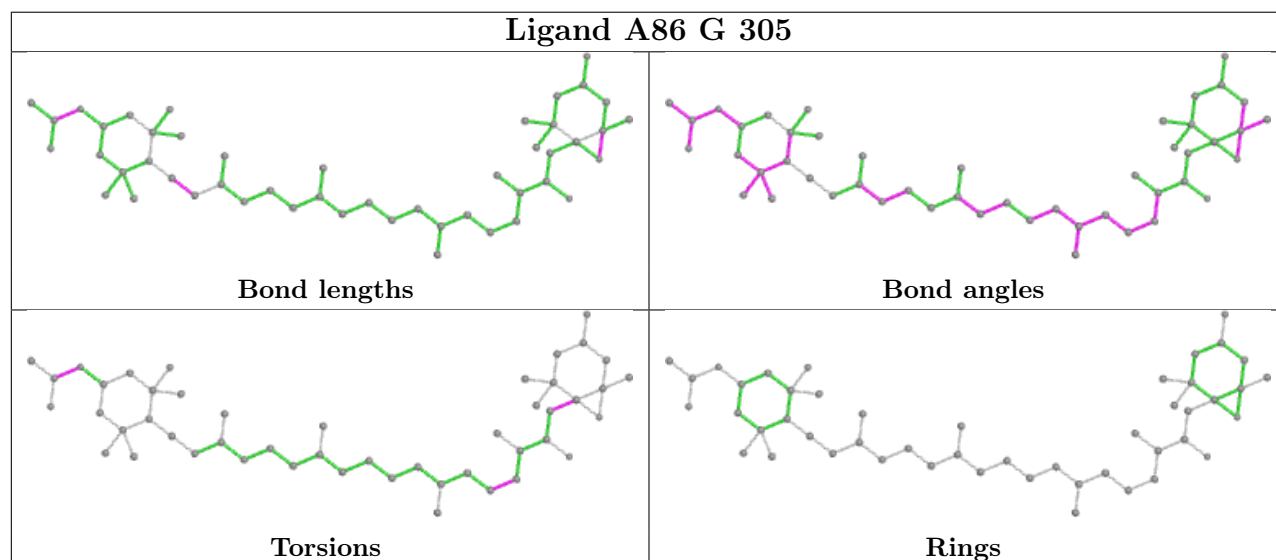
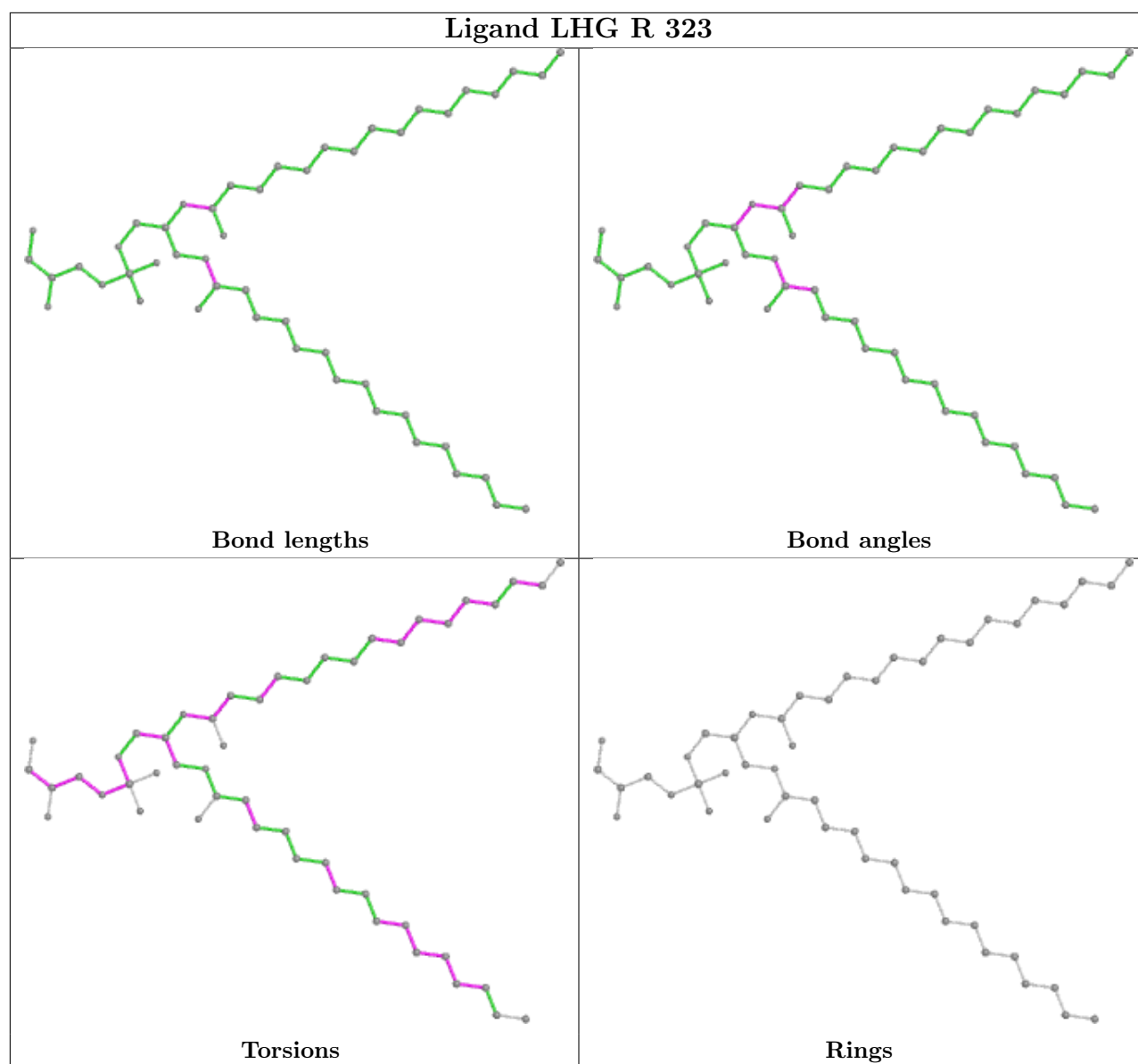


Rings



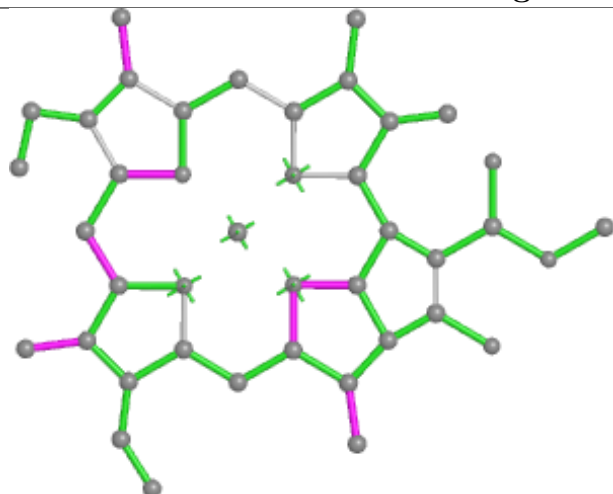




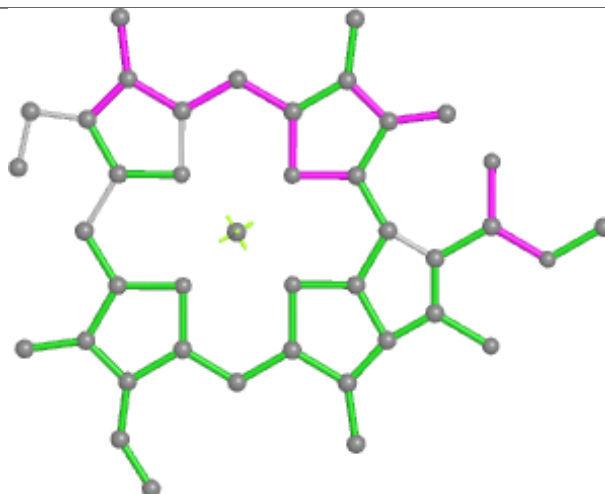




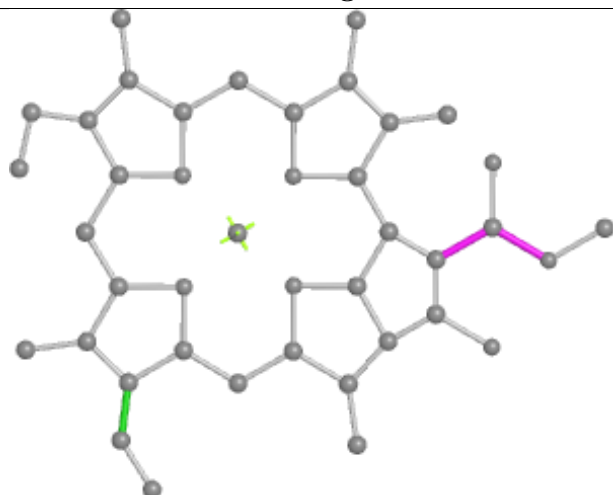
## Ligand CLA K 315



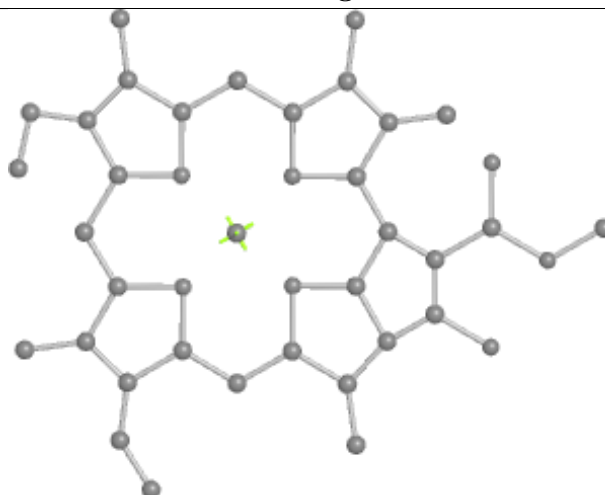
Bond lengths



Bond angles

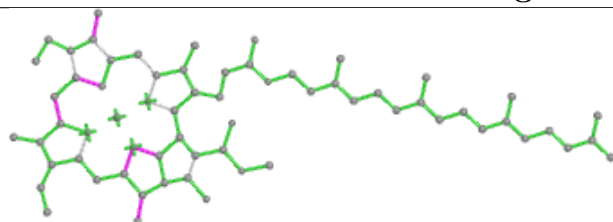


Torsions

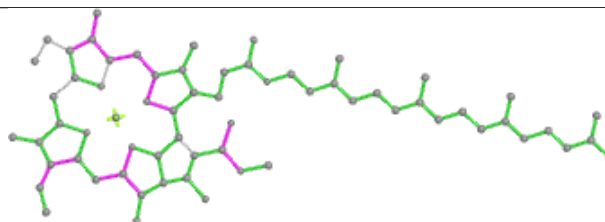


Rings

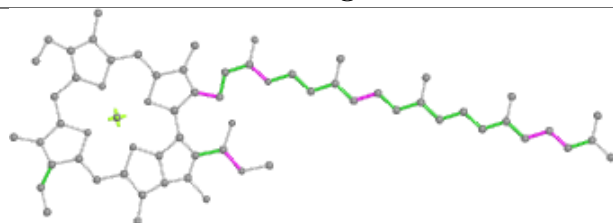
## Ligand CLA T 313



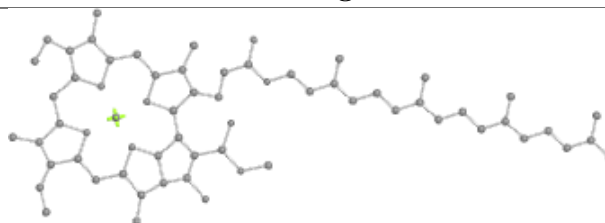
Bond lengths



Bond angles

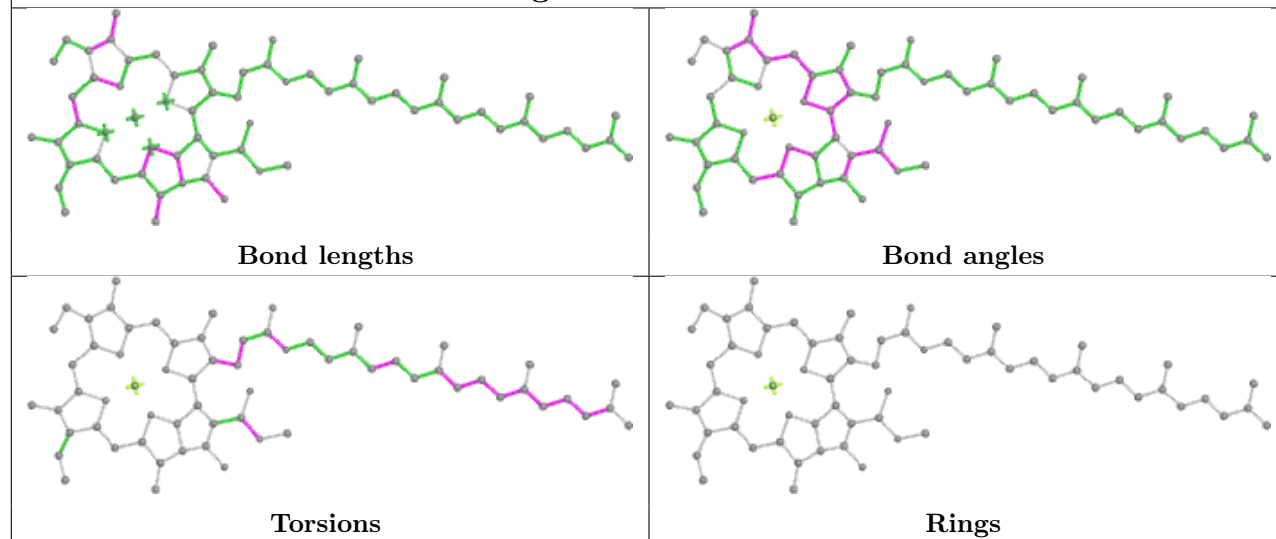


Torsions

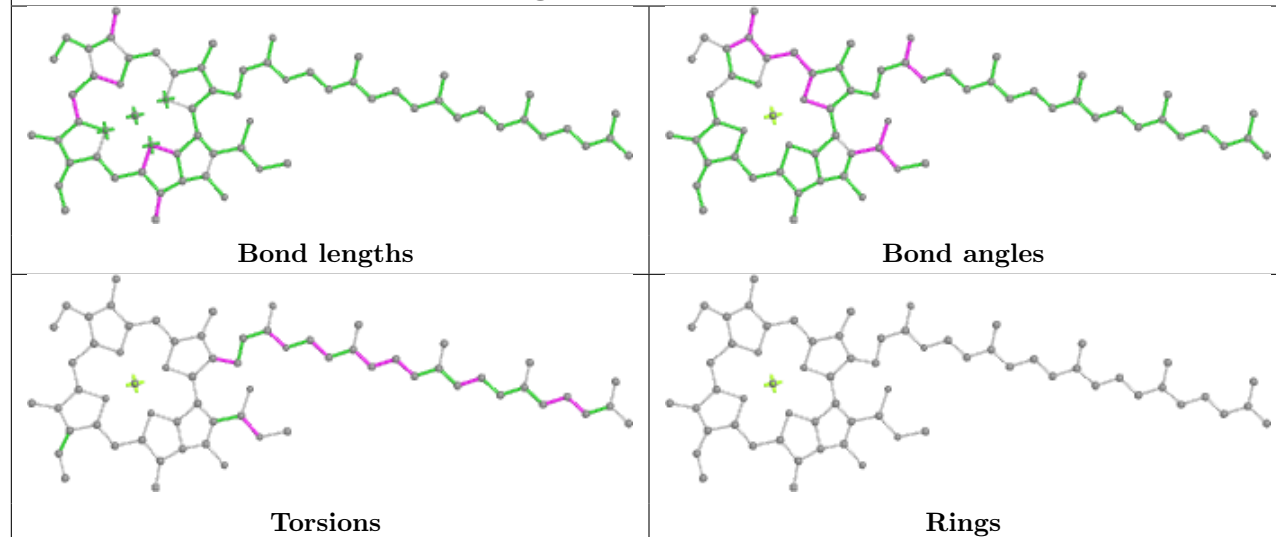


Rings

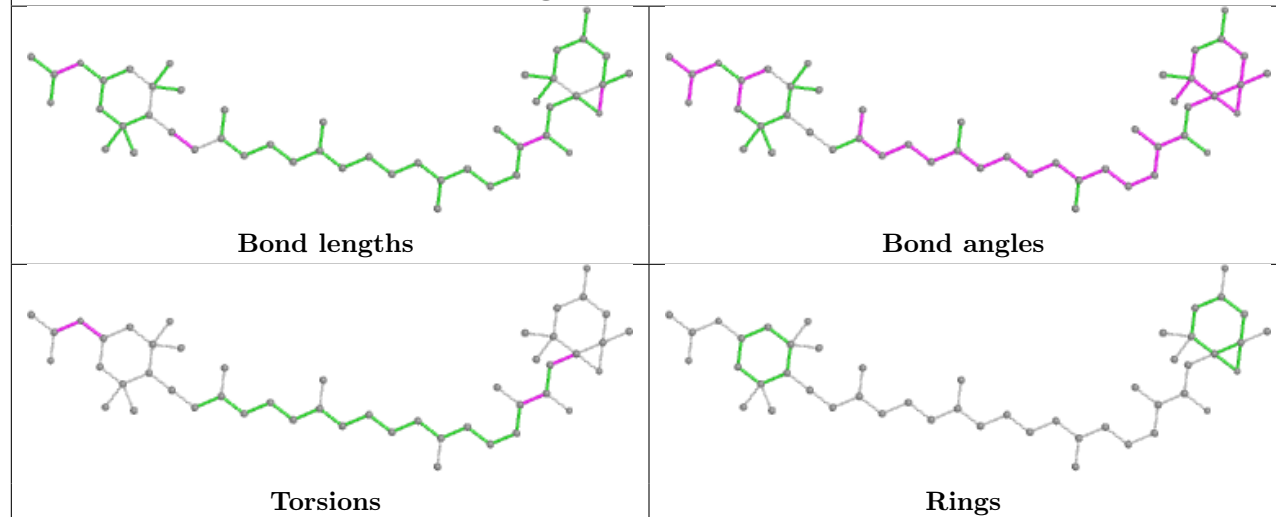
## Ligand CLA A 314

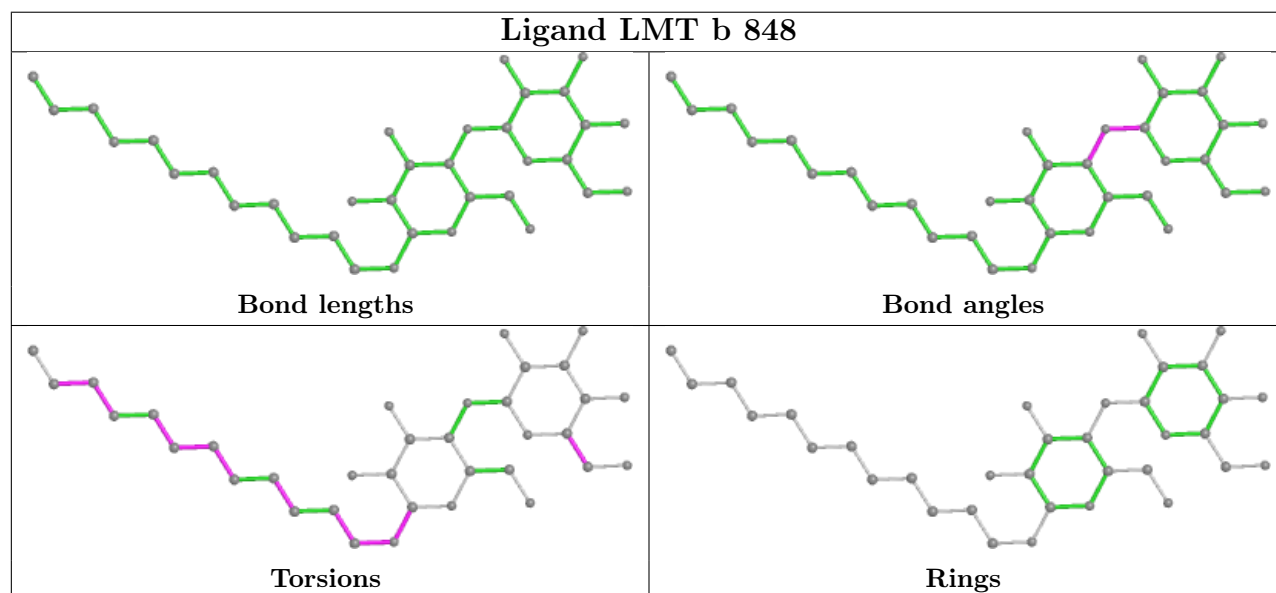
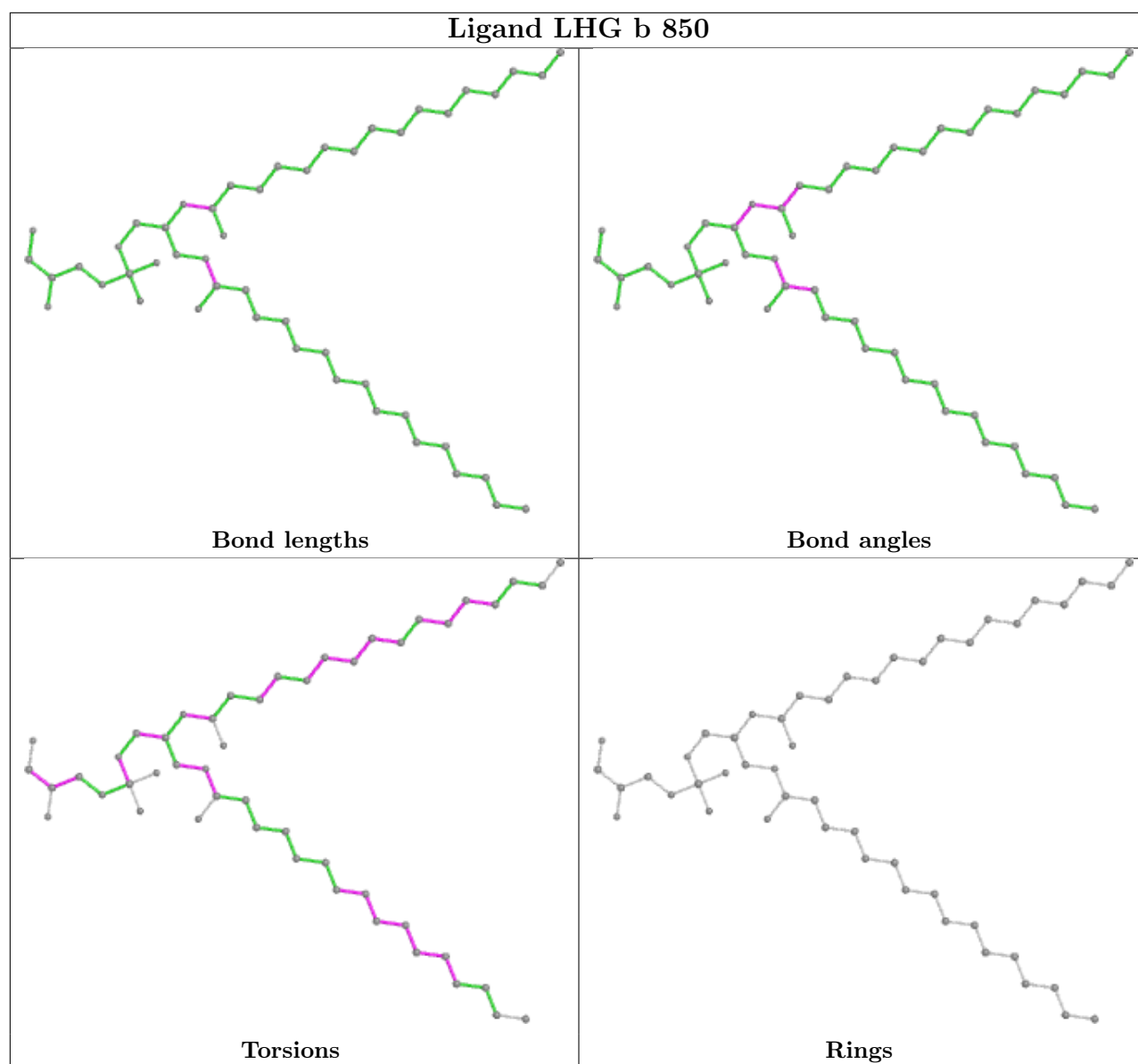


## Ligand CLA R 311

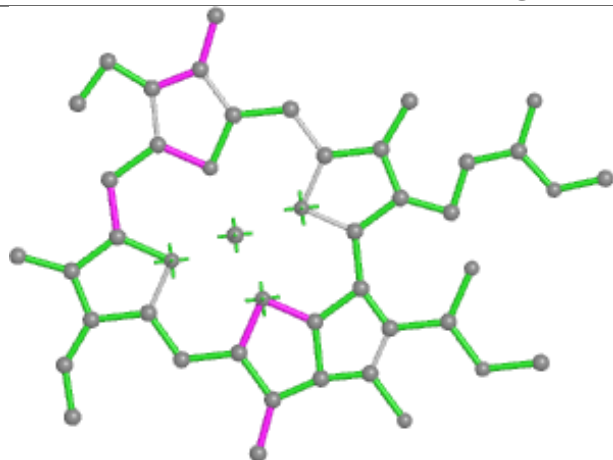


## Ligand A86 X 305

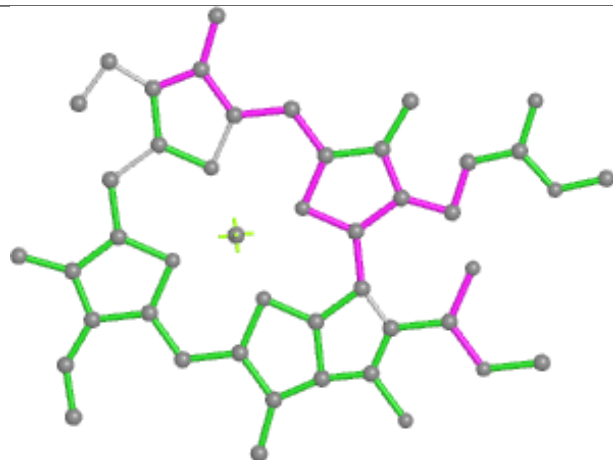




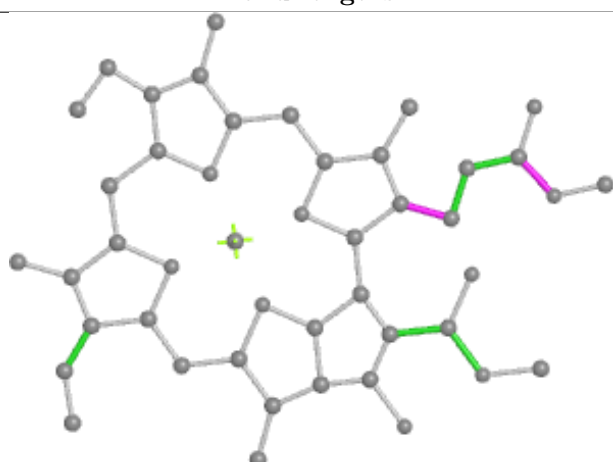
## Ligand CLA U 309



Bond lengths



Bond angles

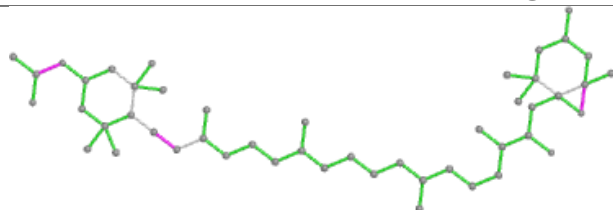


Torsions

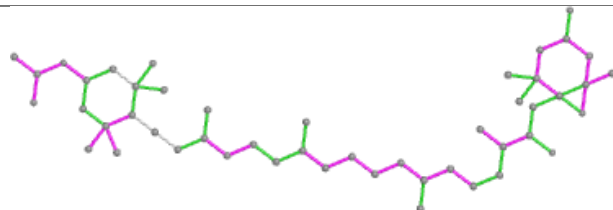


Rings

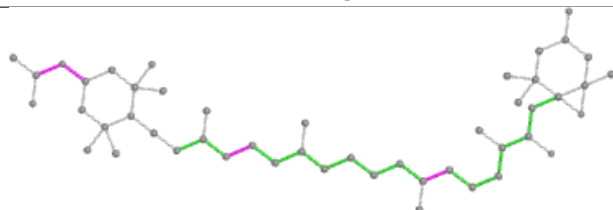
## Ligand A86 J 305



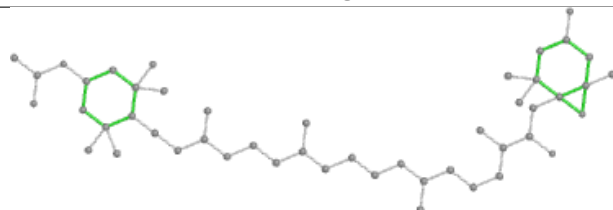
Bond lengths



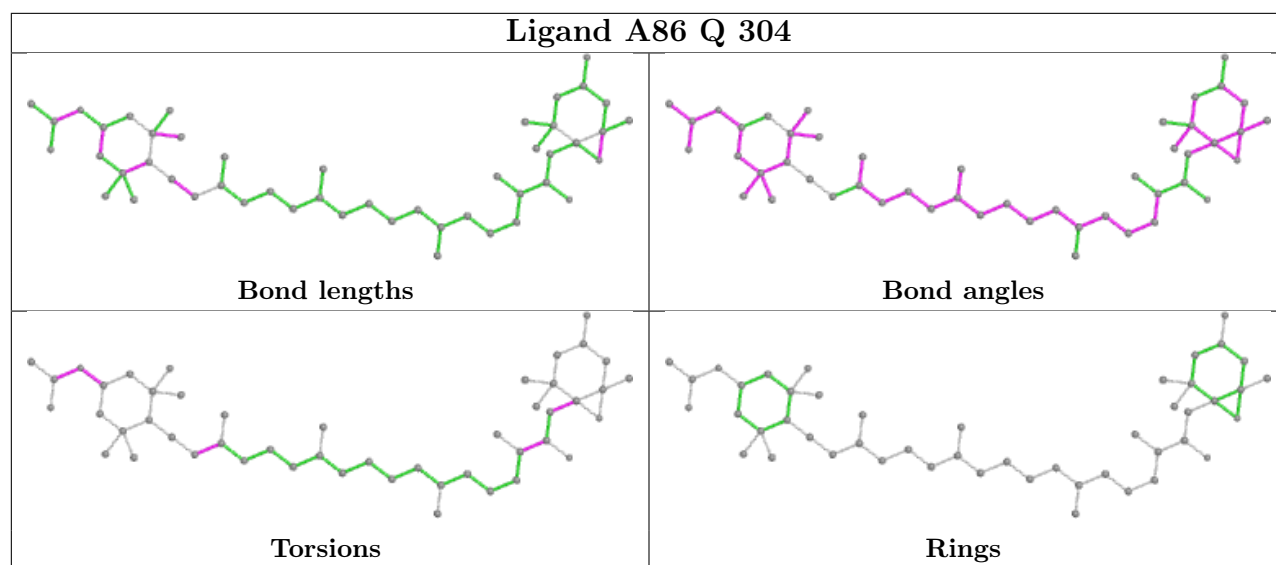
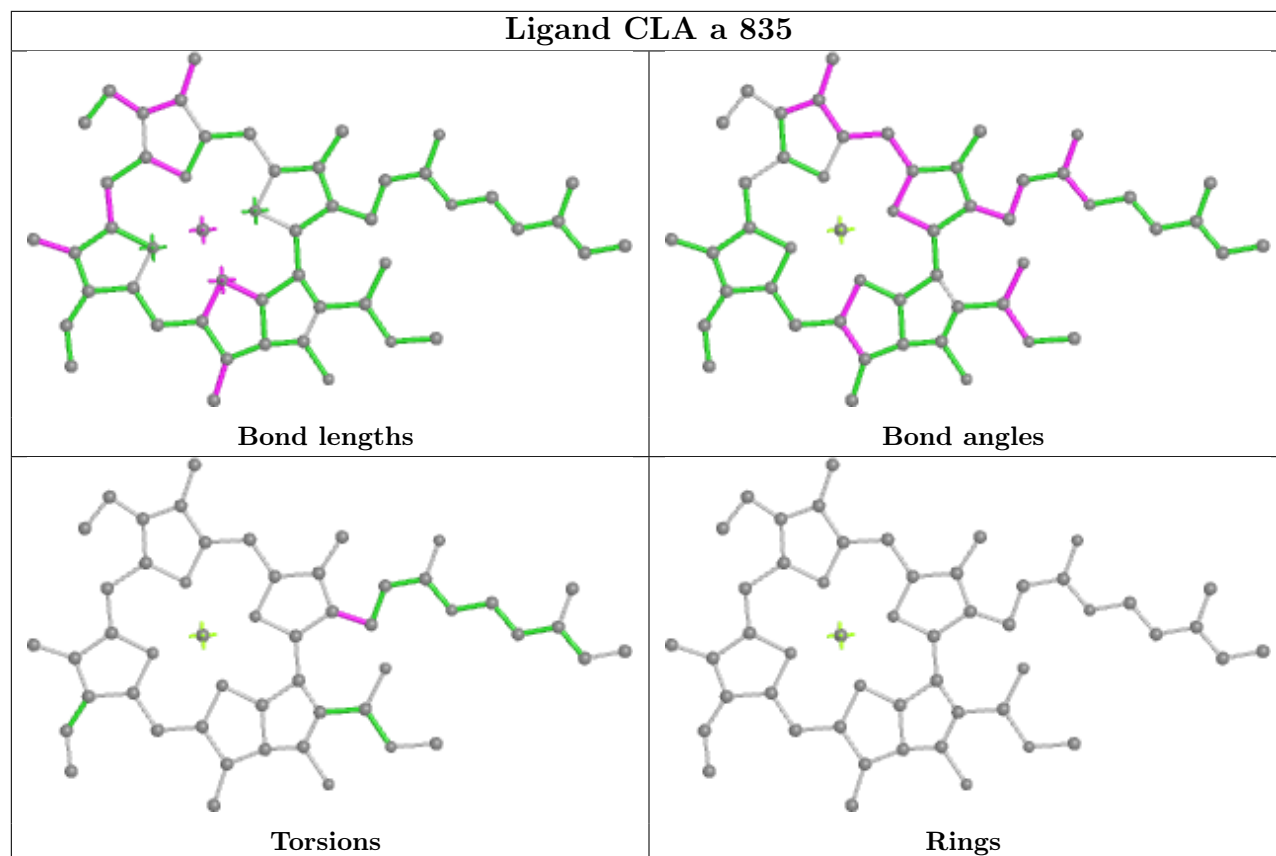
Bond angles

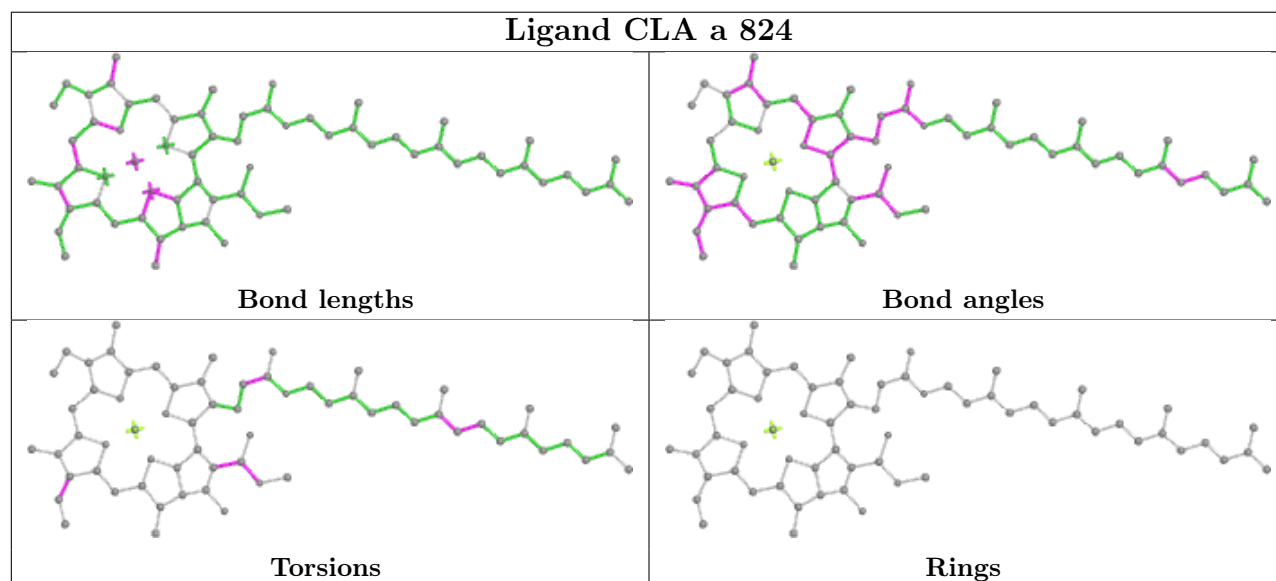
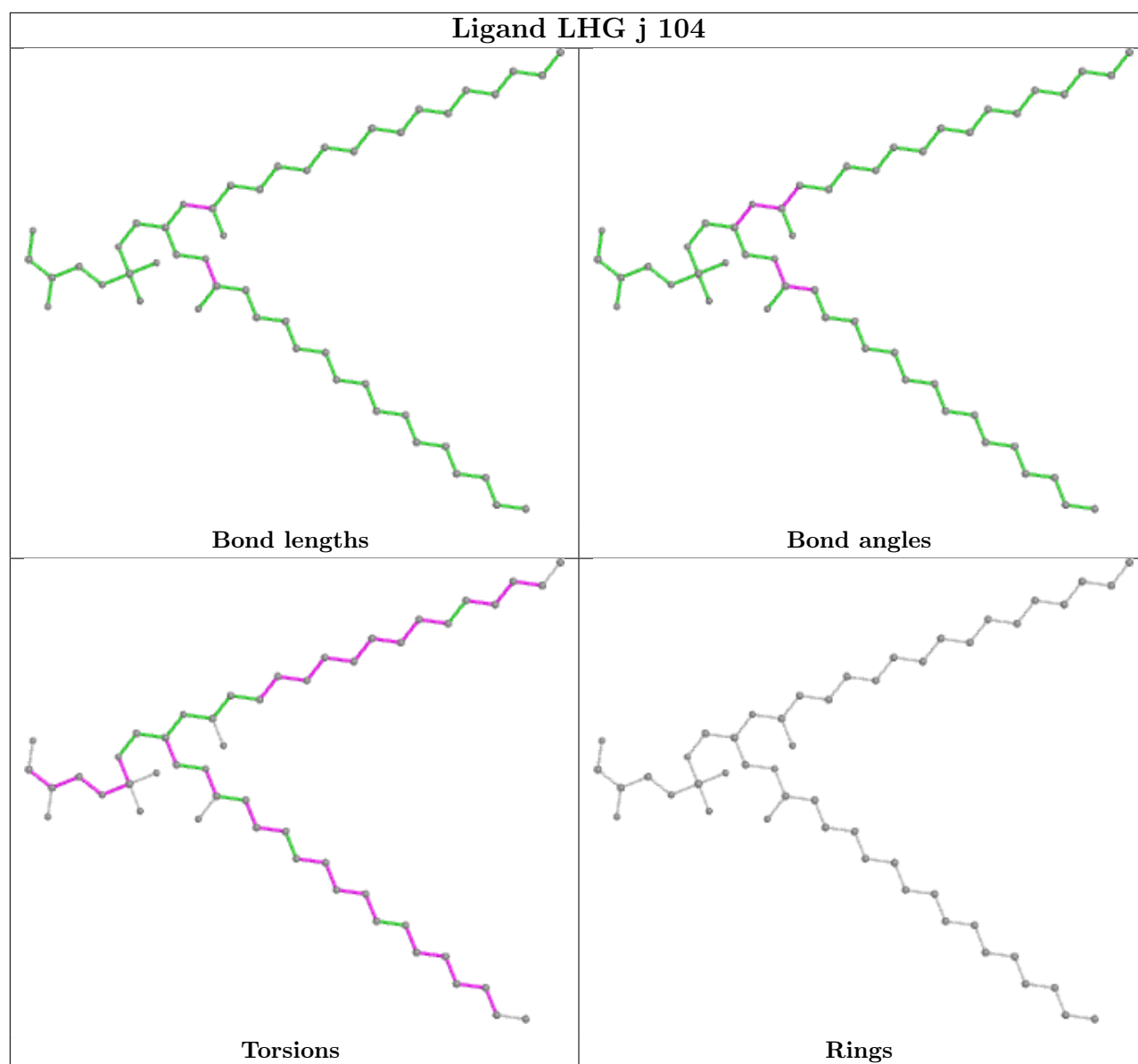


Torsions

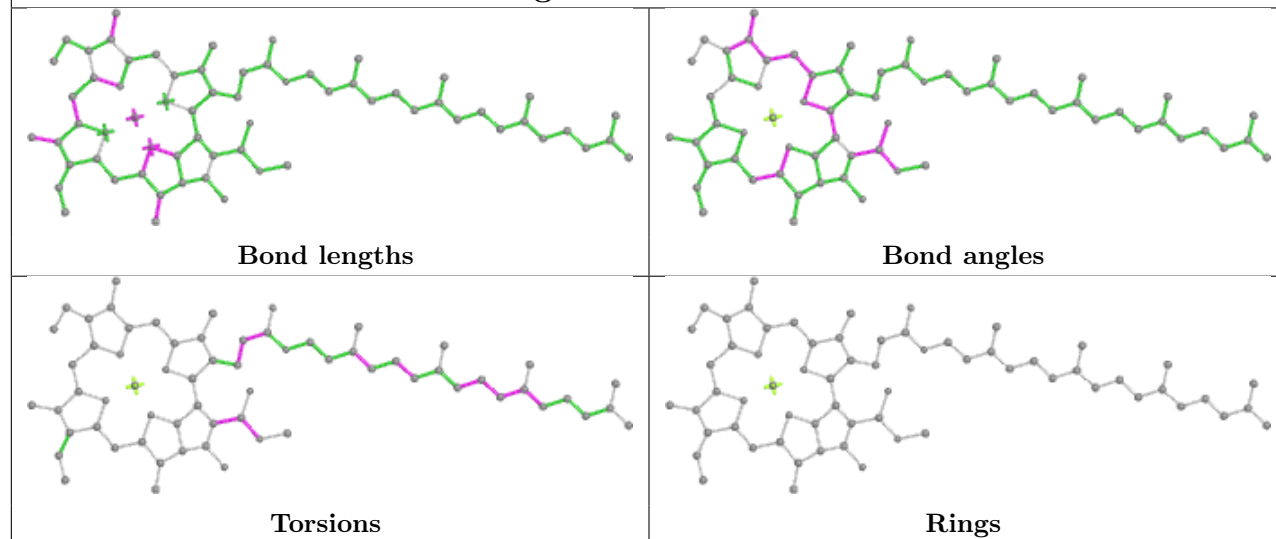


Rings

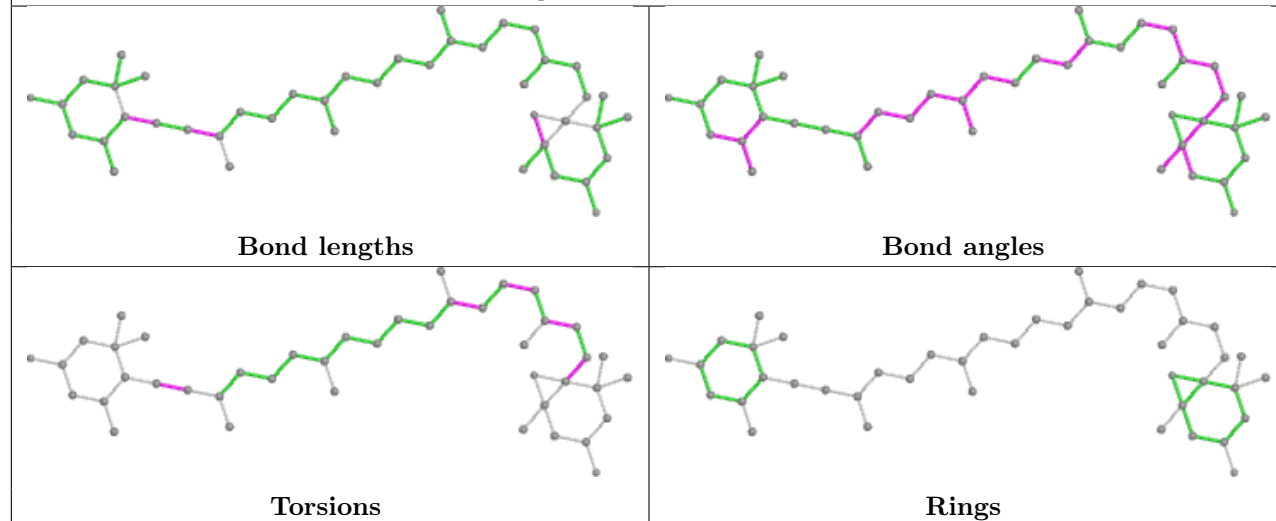




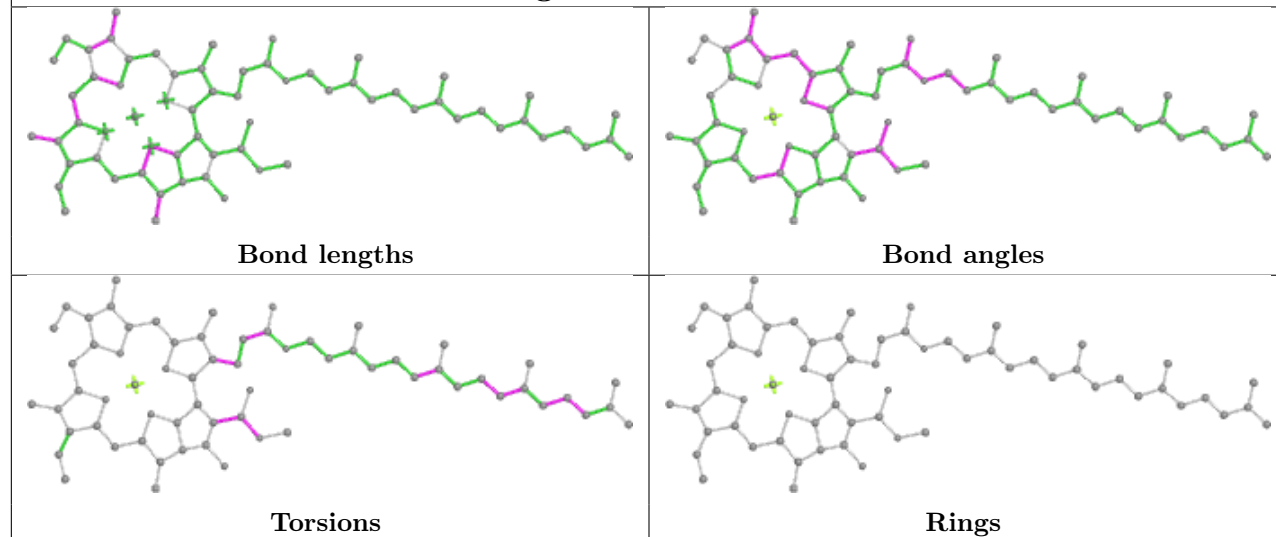
## Ligand CLA L 311

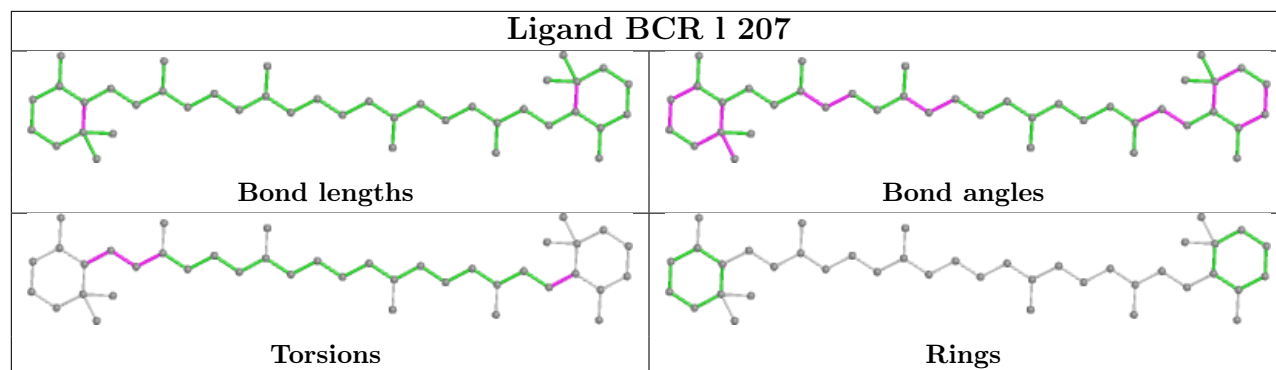
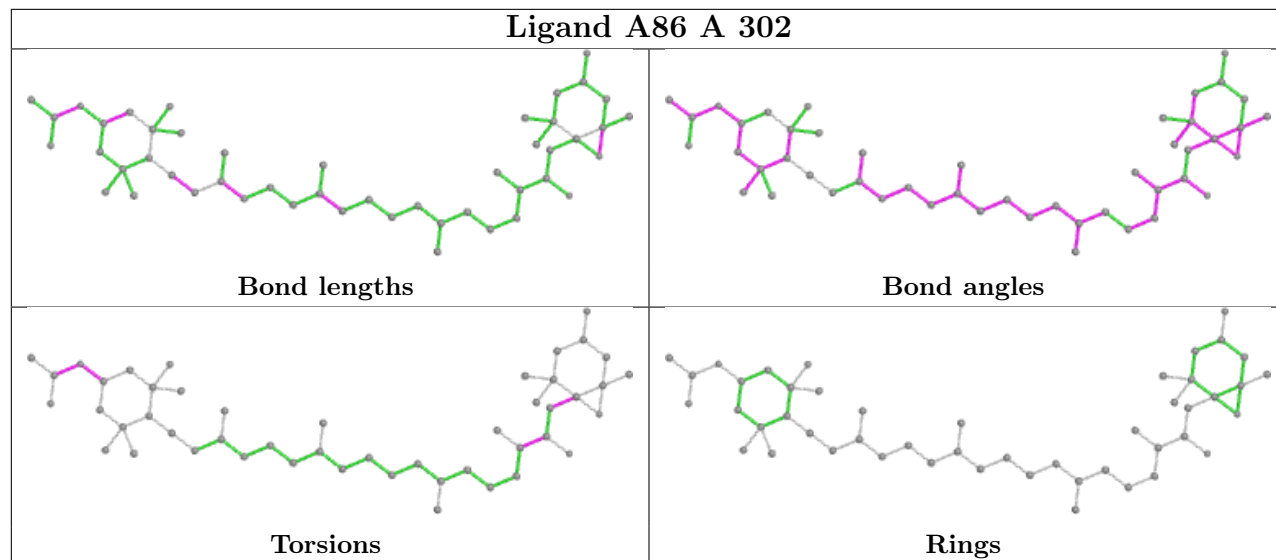
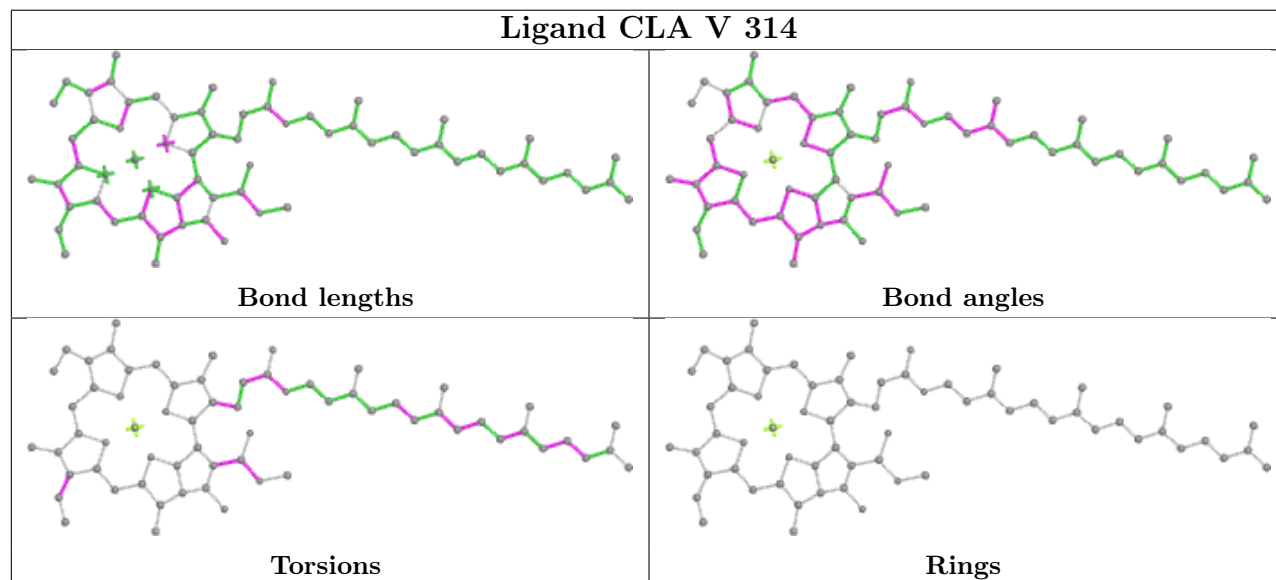


## Ligand DD6 D 304



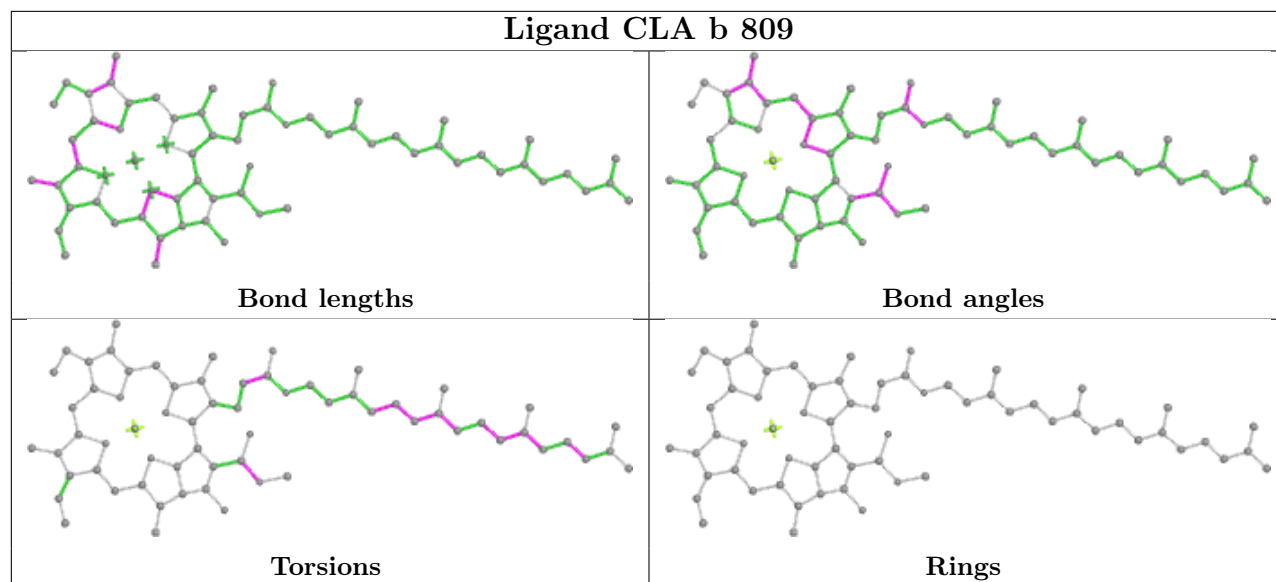
## Ligand CLA b 808



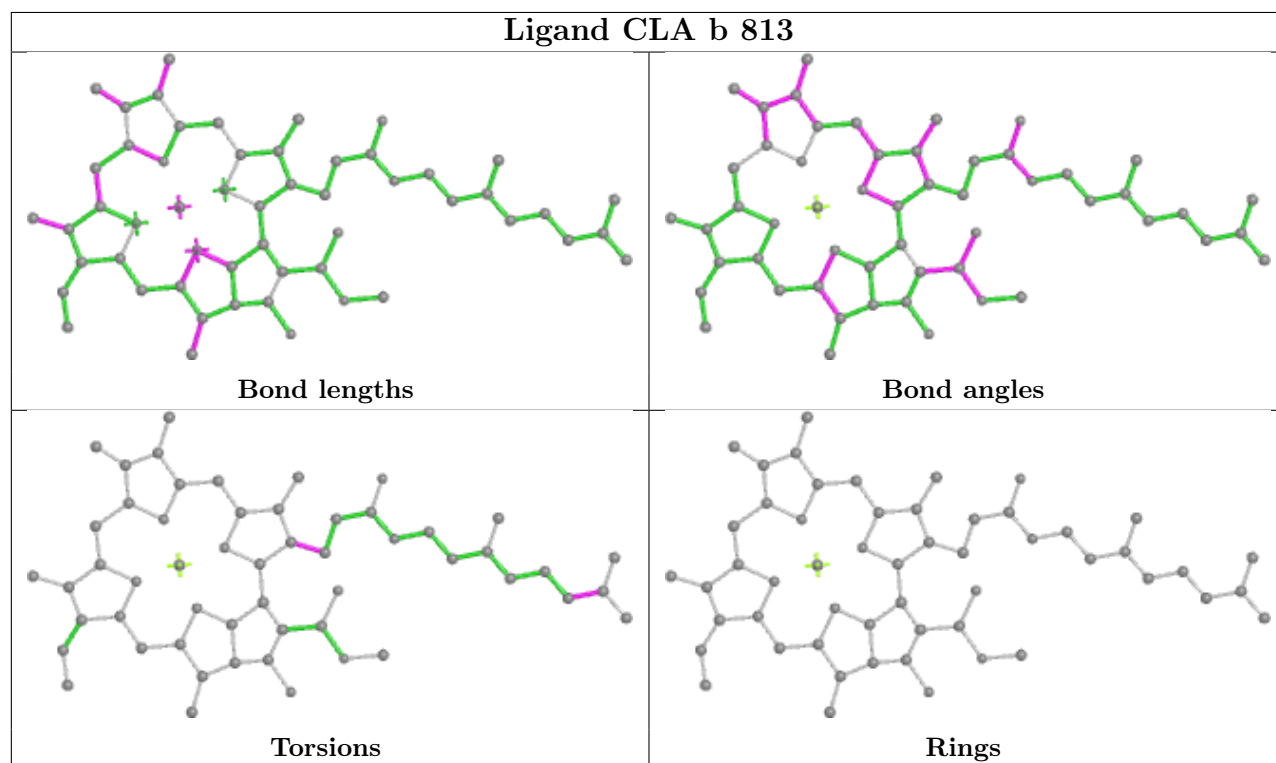
**Ligand BCR 1 207****Ligand A86 A 302****Ligand CLA V 314**



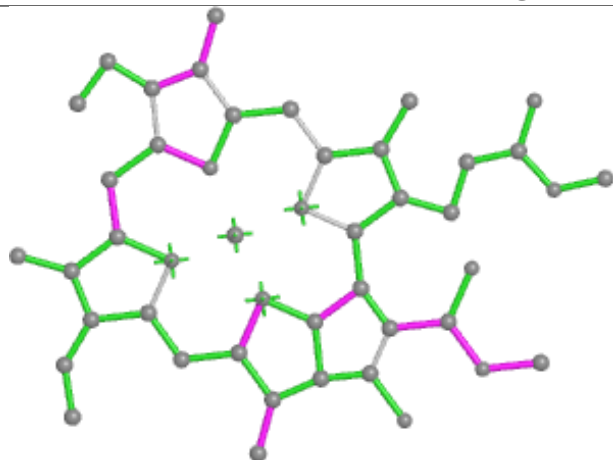
## Ligand CLA b 809



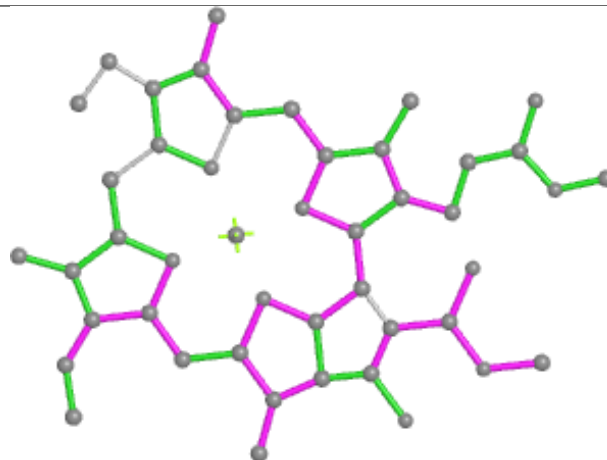
## Ligand CLA b 813



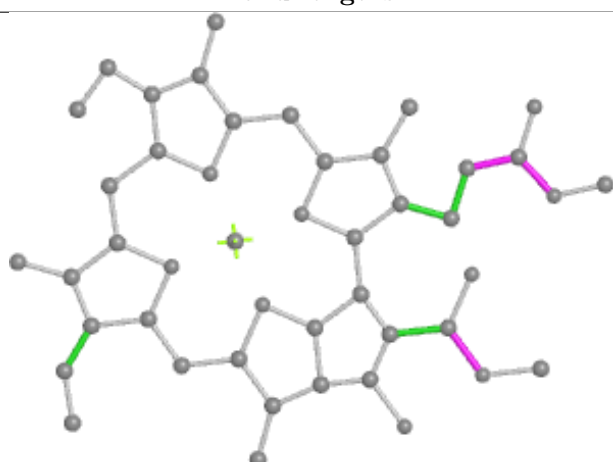
## Ligand CLA H 310



Bond lengths



Bond angles

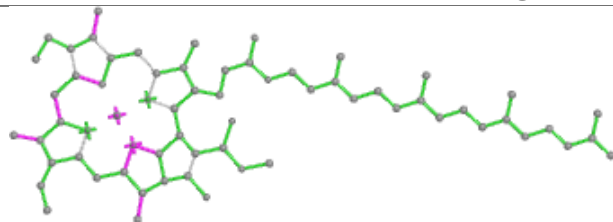


Torsions

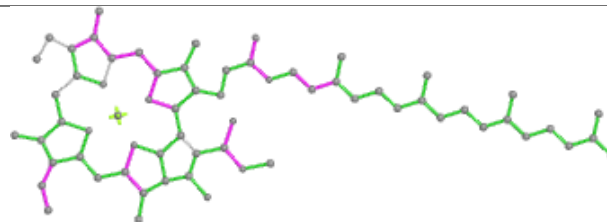


Rings

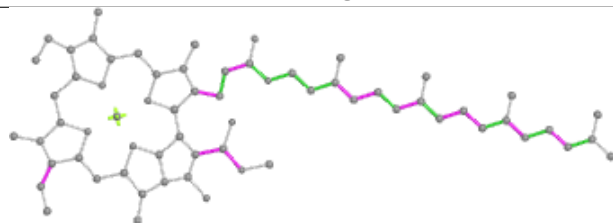
## Ligand CLA O 309



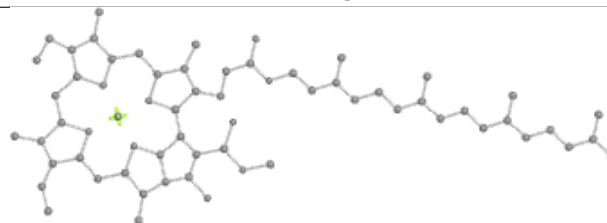
Bond lengths



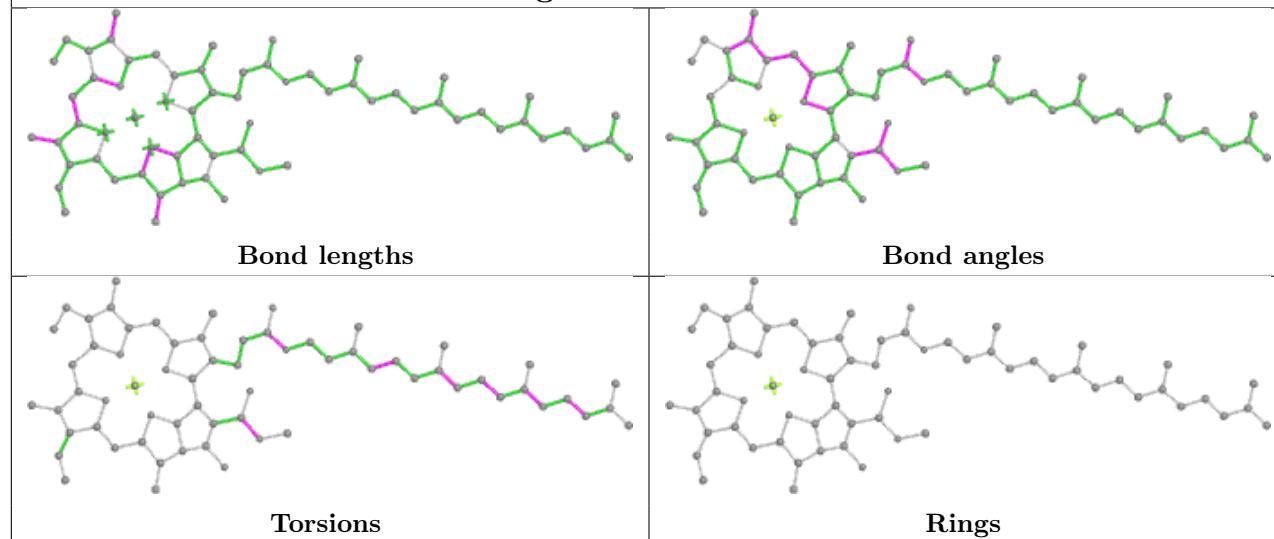
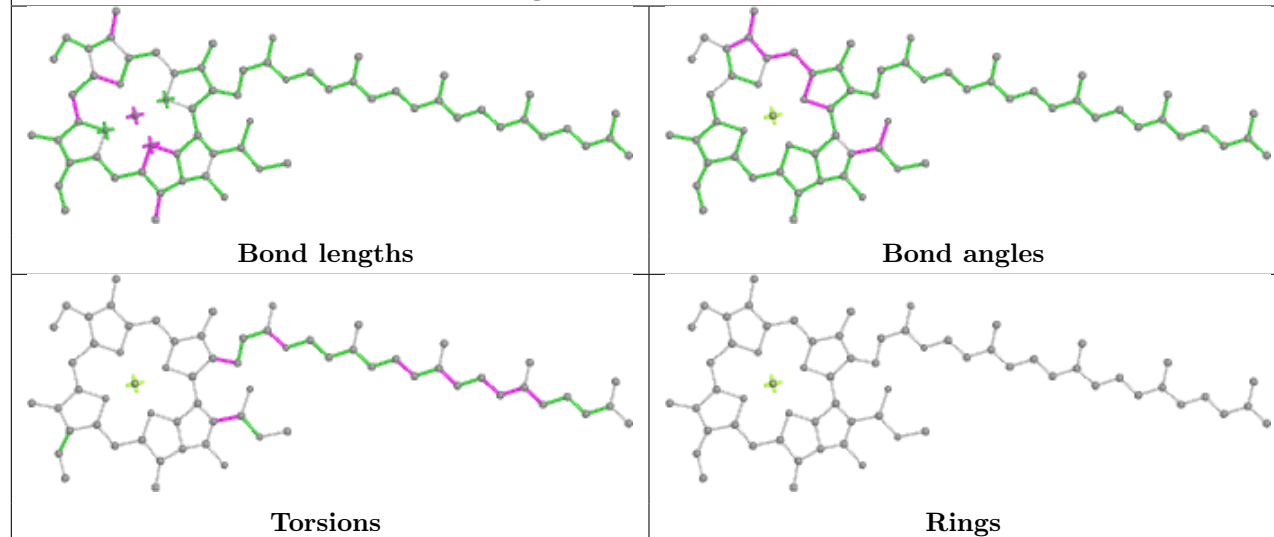
Bond angles

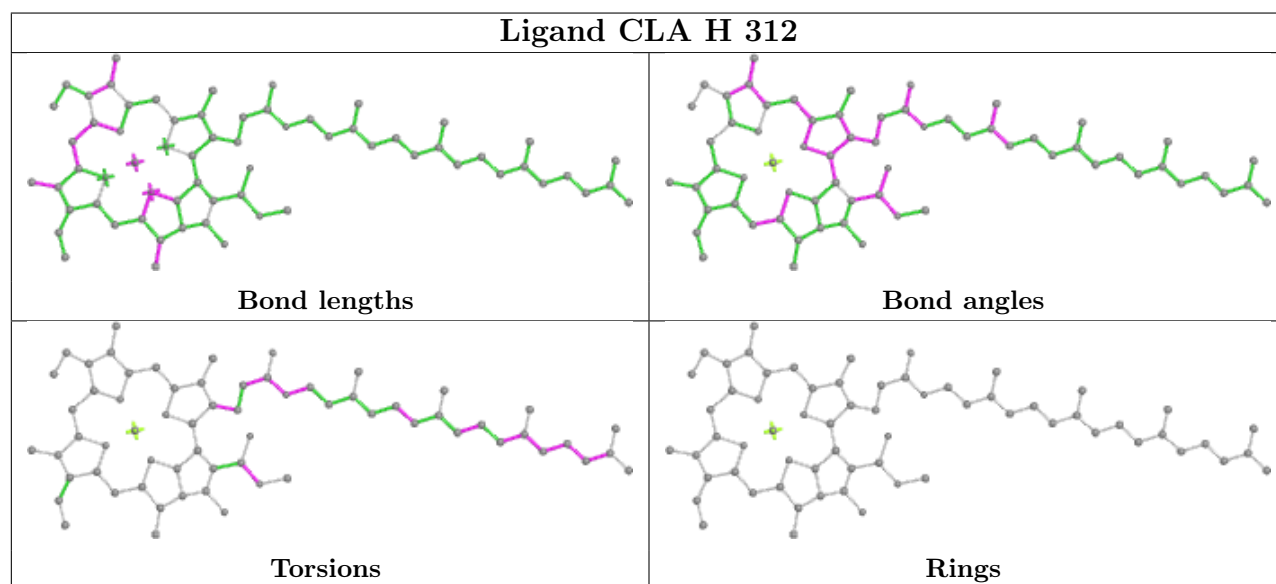
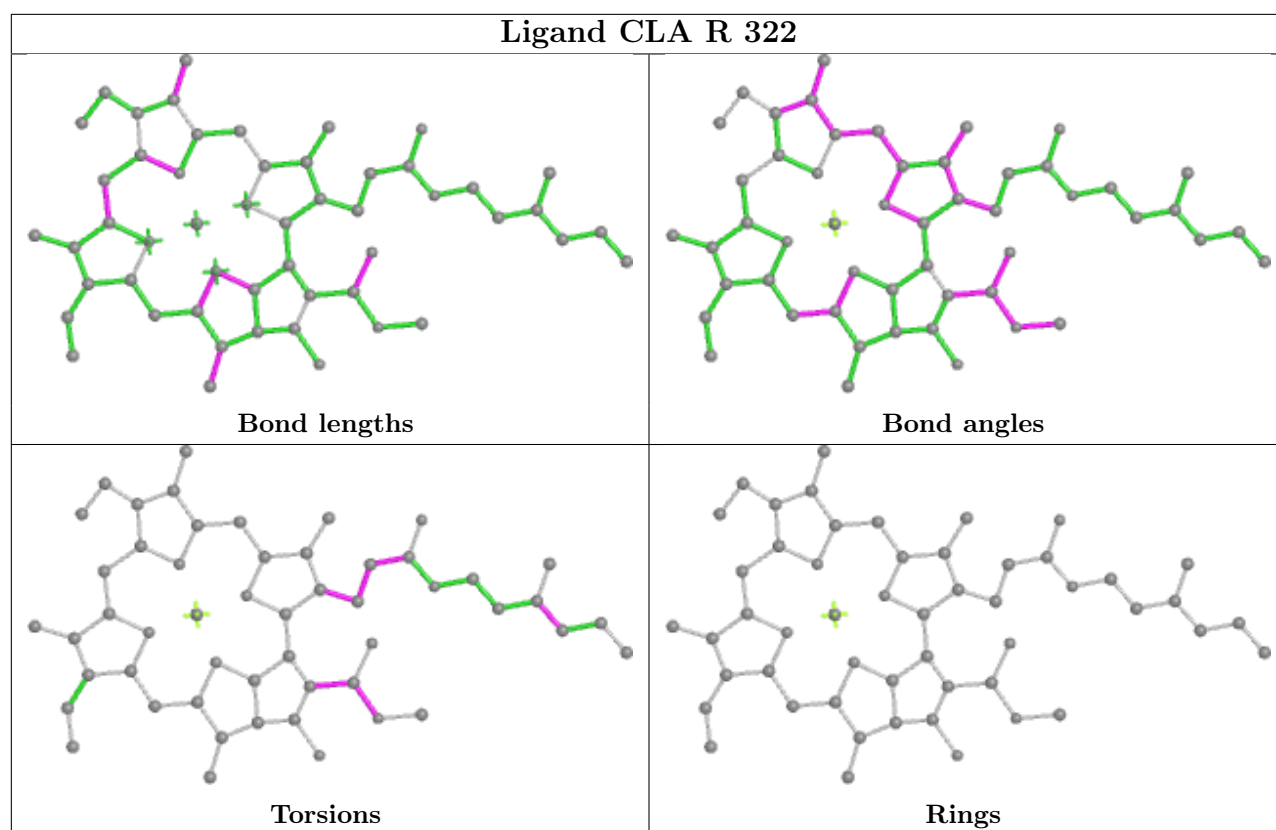


Torsions

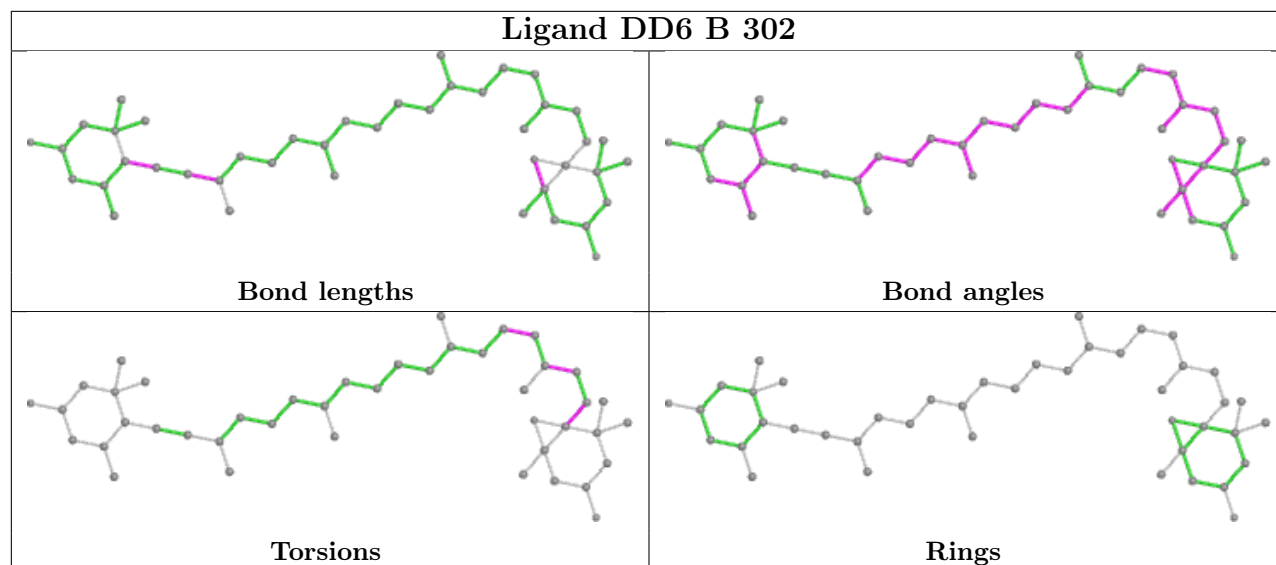


Rings

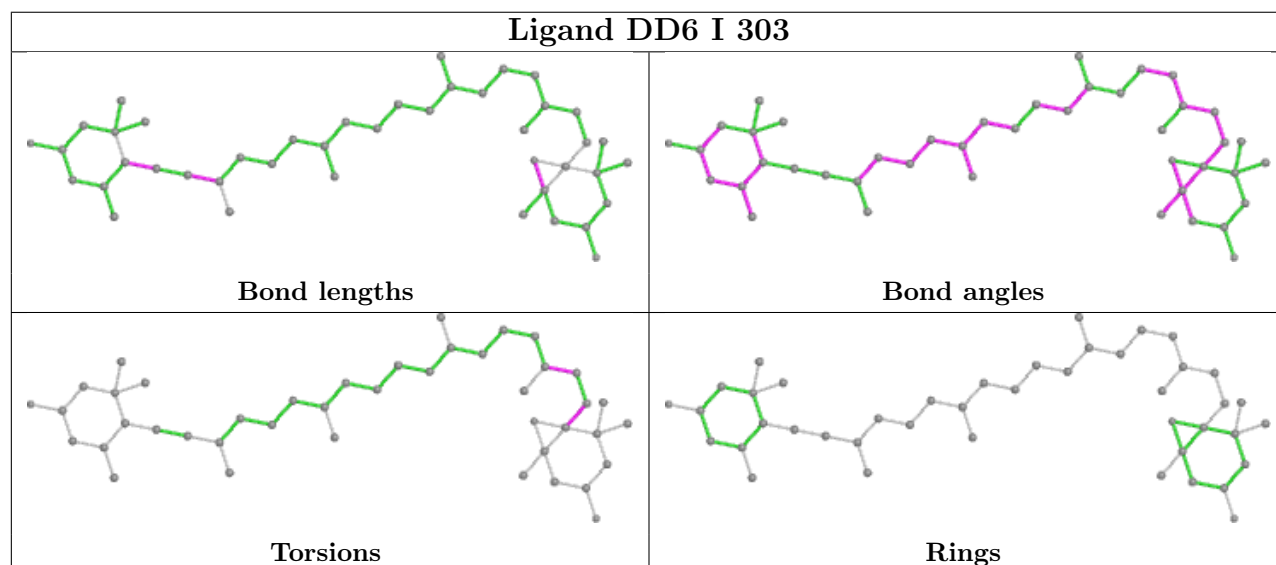
**Ligand CLA J 312****Ligand CLA M 311**



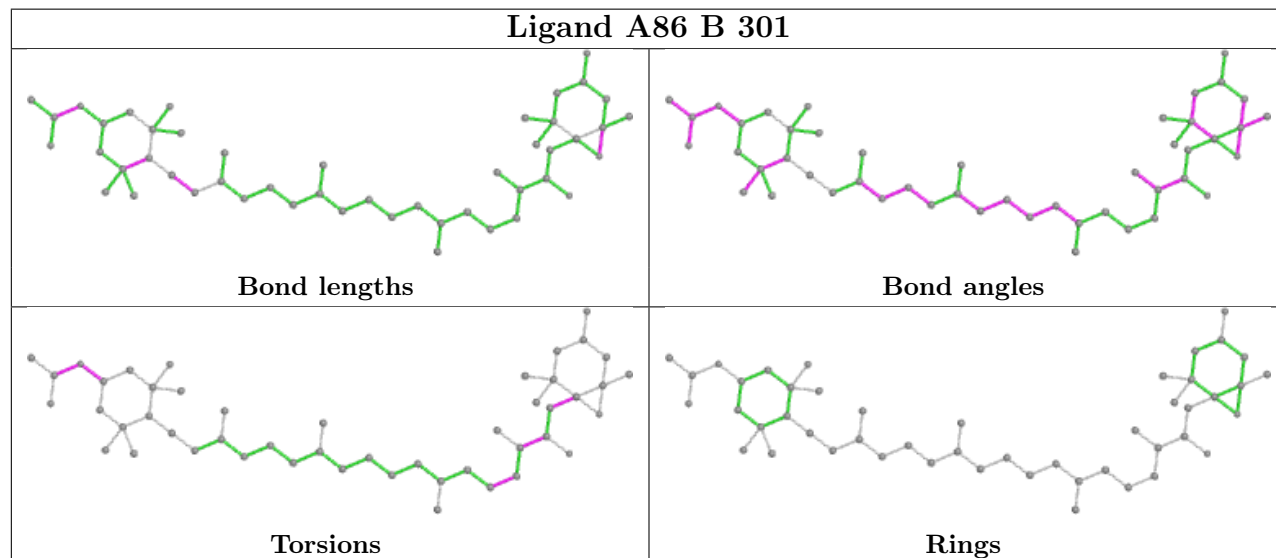
## Ligand DD6 B 302



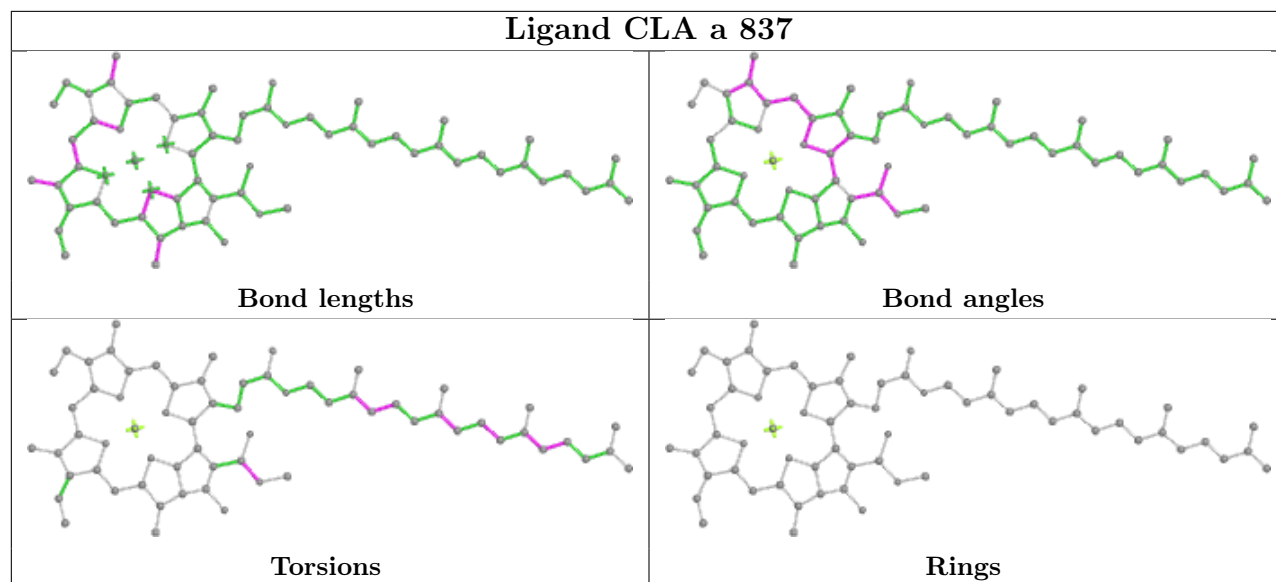
## Ligand DD6 I 303



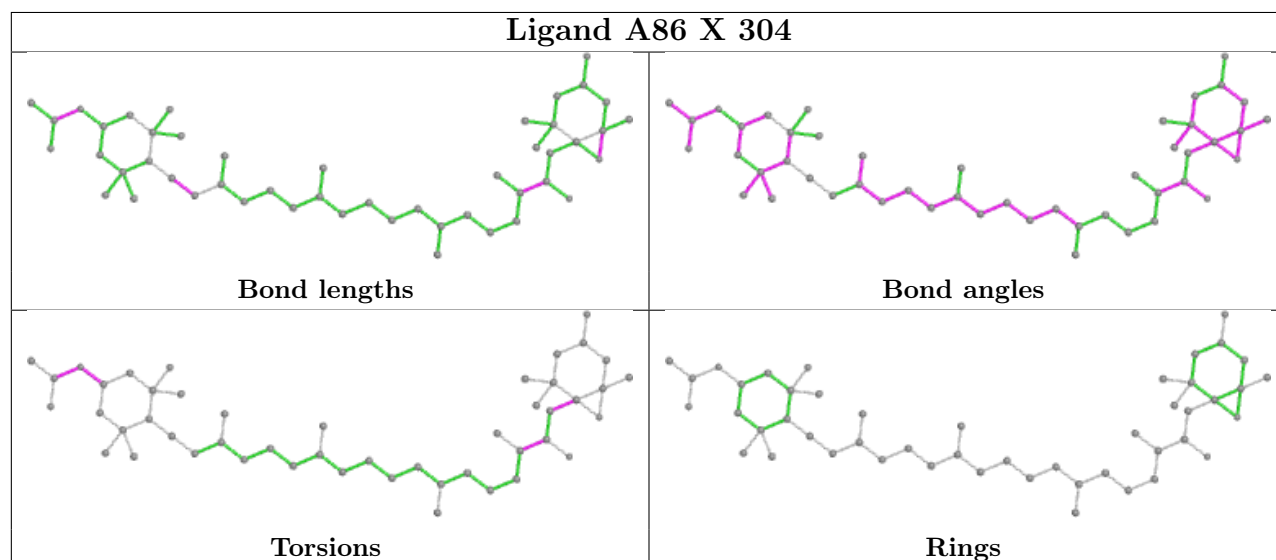
## Ligand A86 B 301



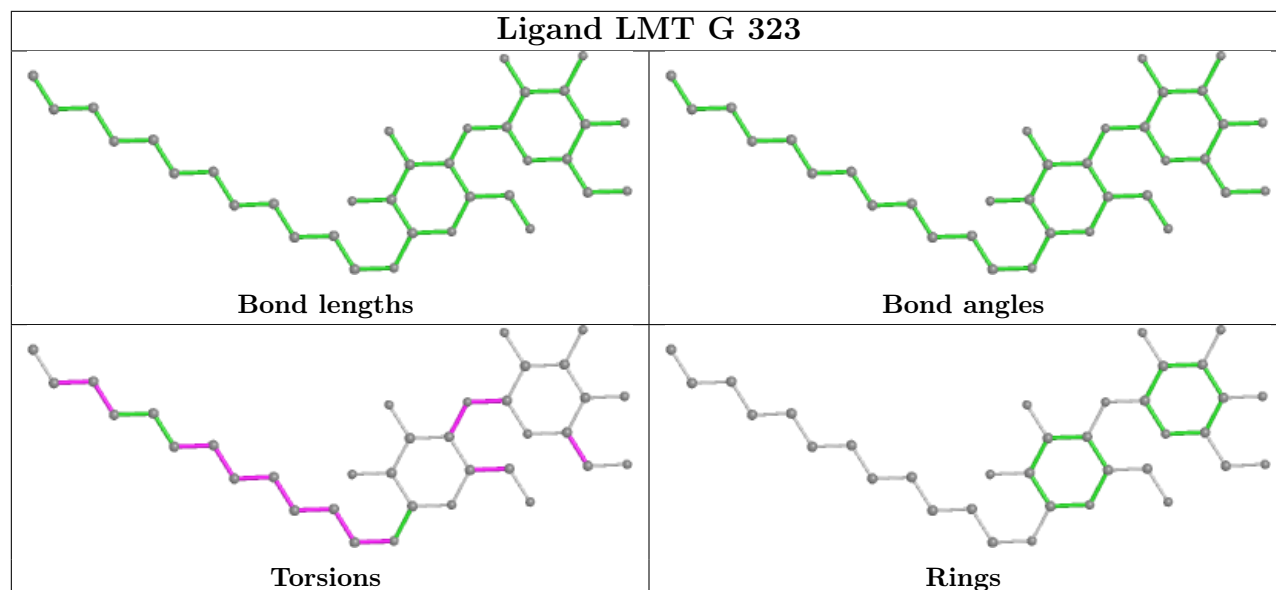
## Ligand CLA a 837

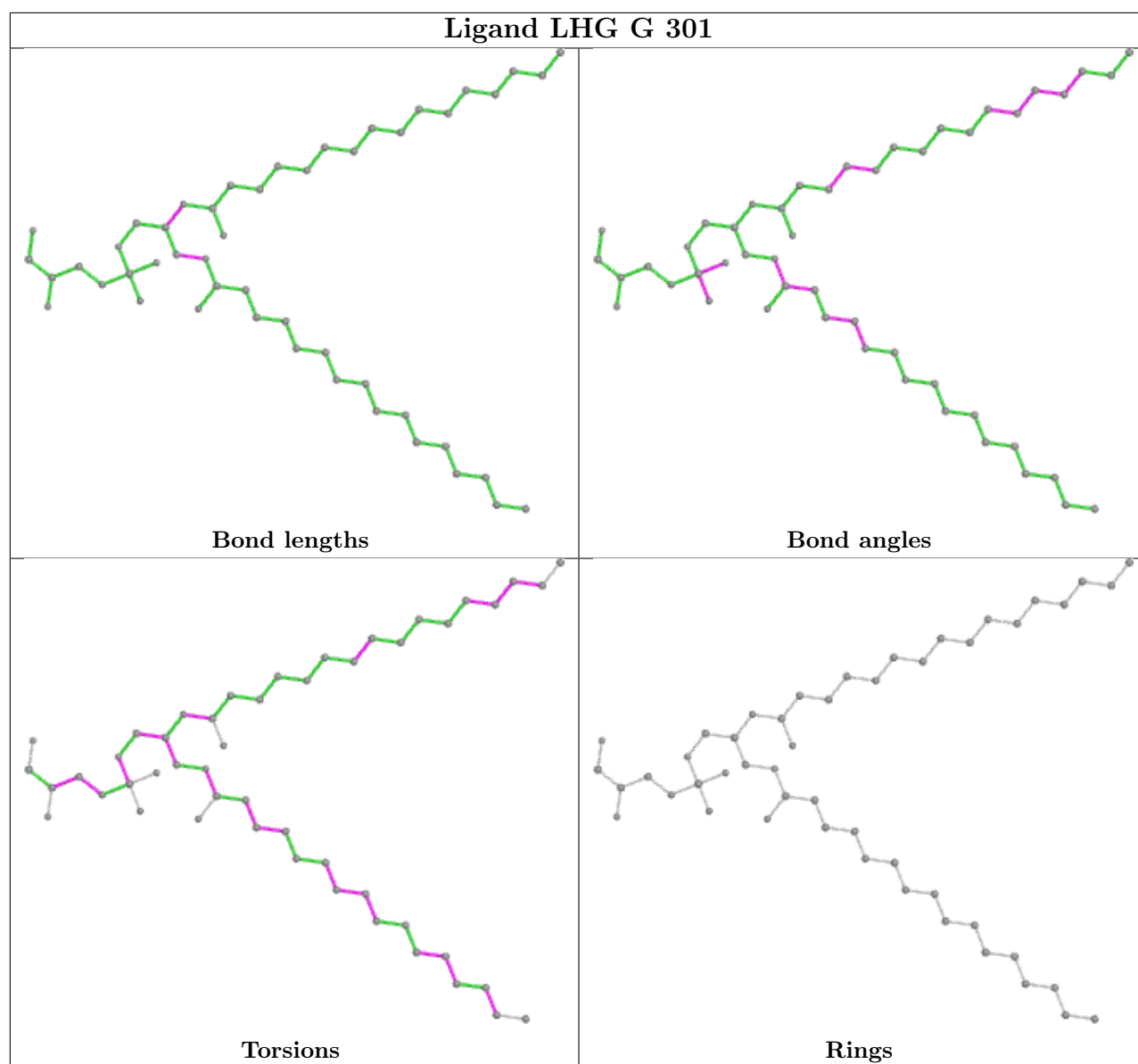


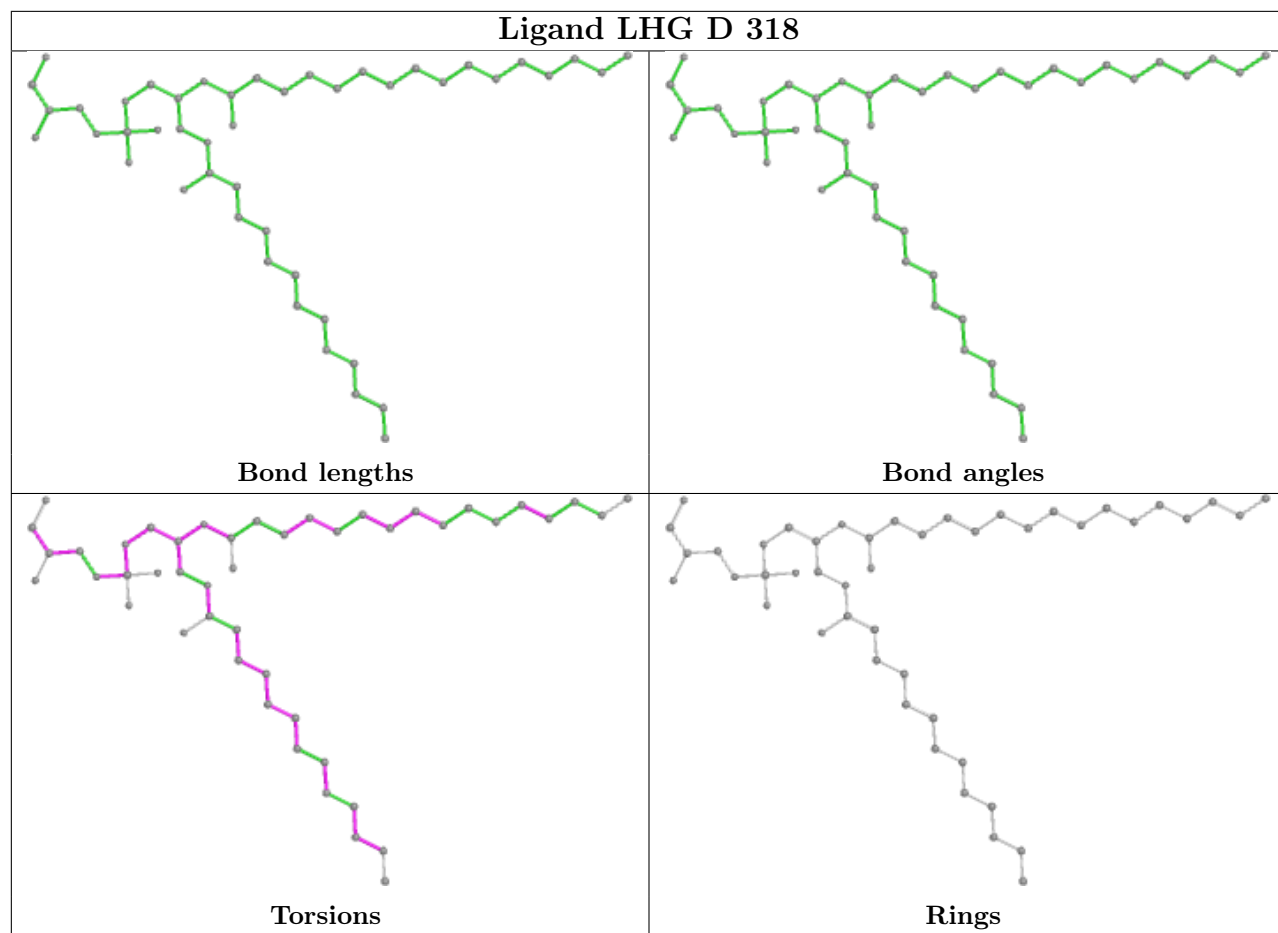
## Ligand A86 X 304



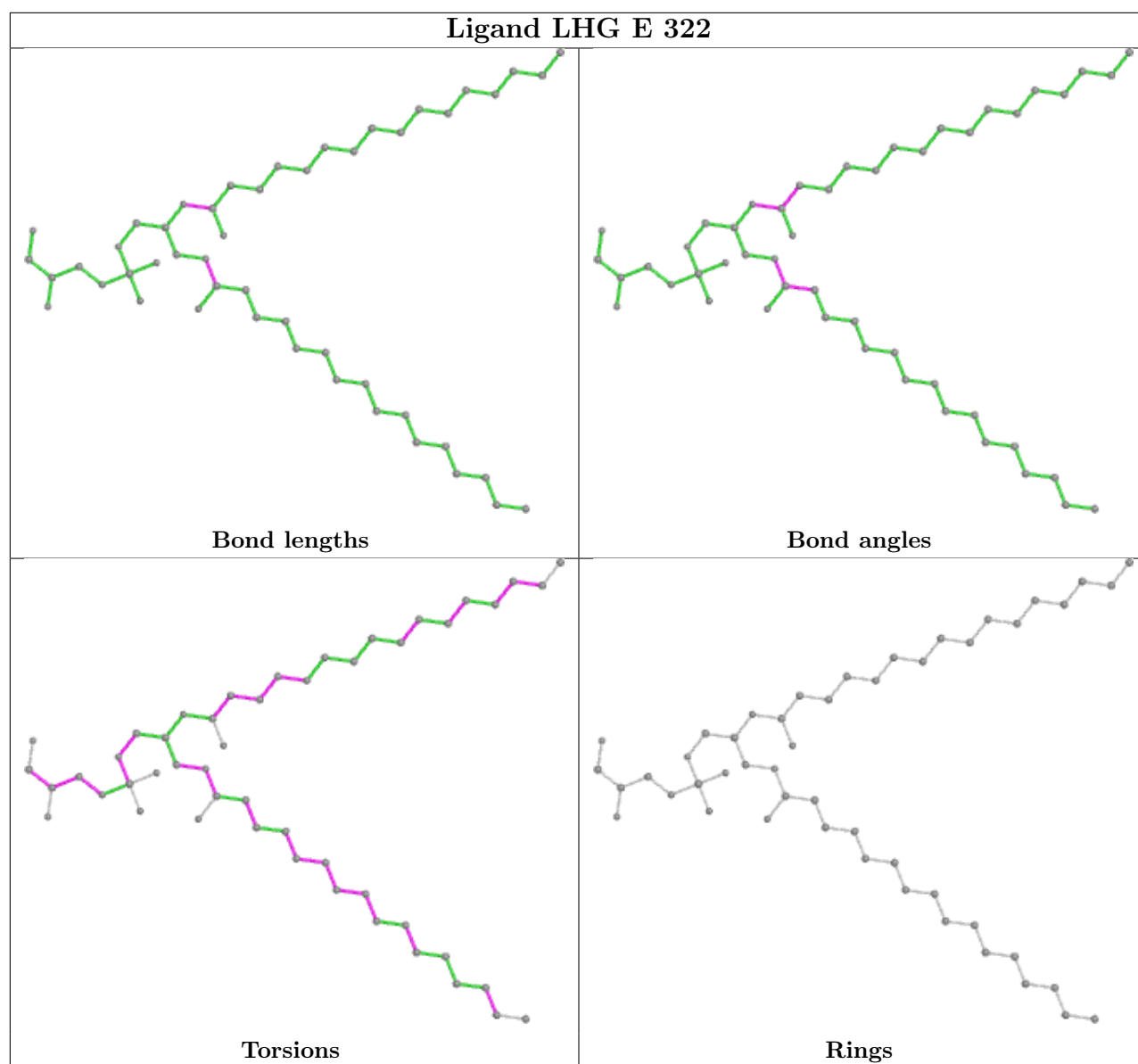
## Ligand LMT G 323



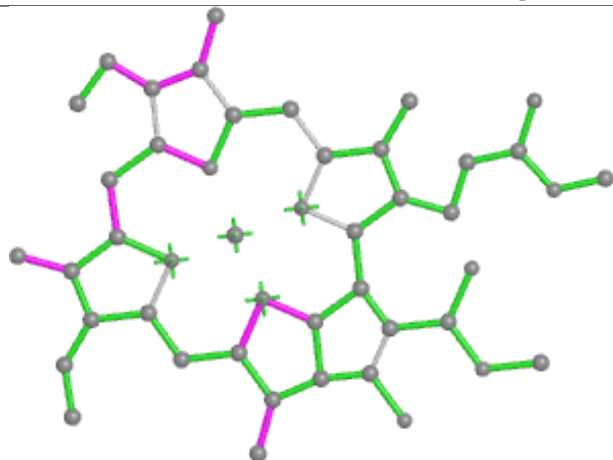




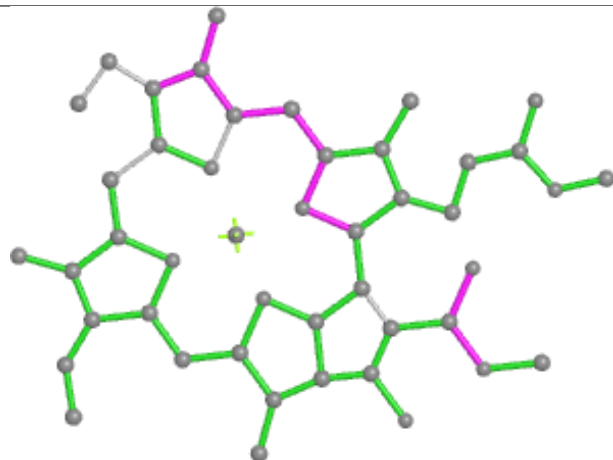




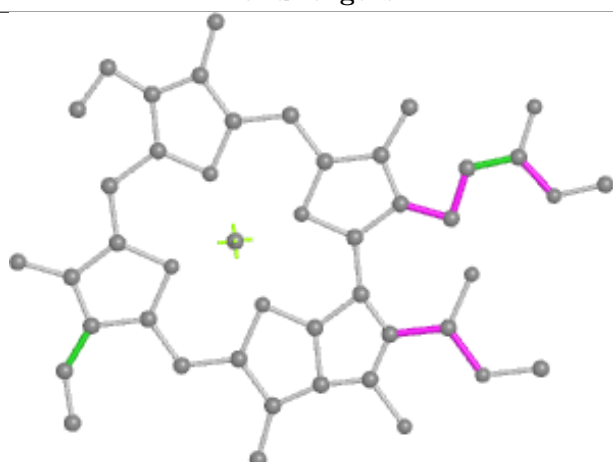
## Ligand CLA A 309



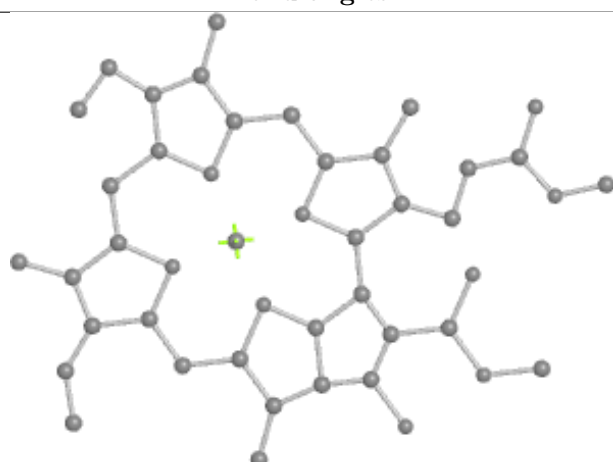
Bond lengths



Bond angles

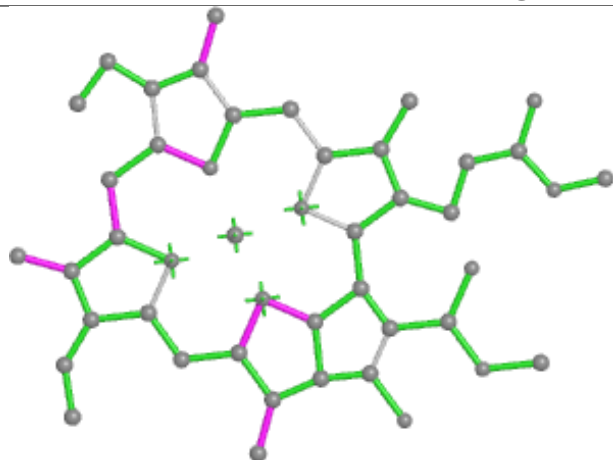


Torsions

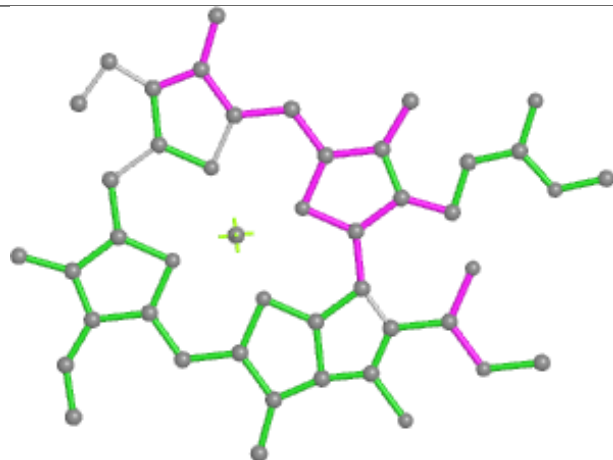


Rings

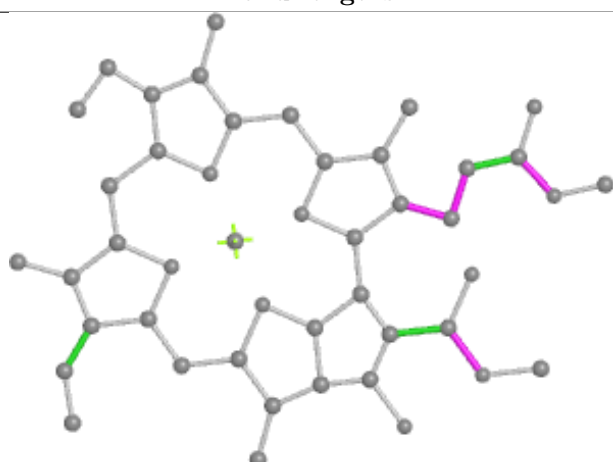
## Ligand CLA K 311



Bond lengths



Bond angles

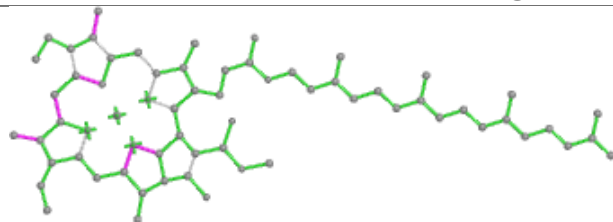


Torsions

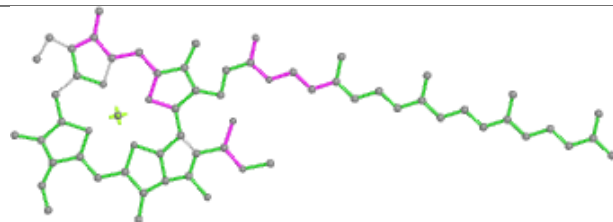


Rings

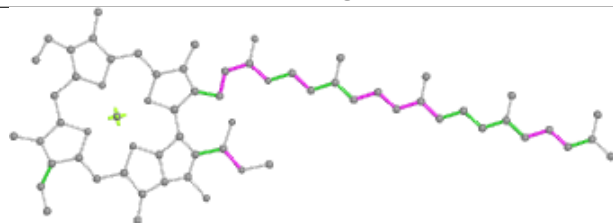
## Ligand CLA W 207



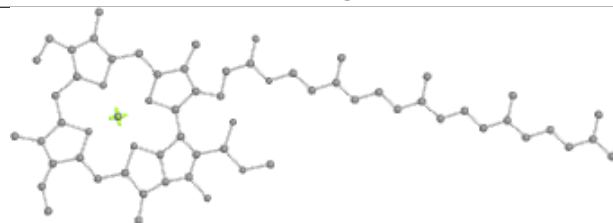
Bond lengths



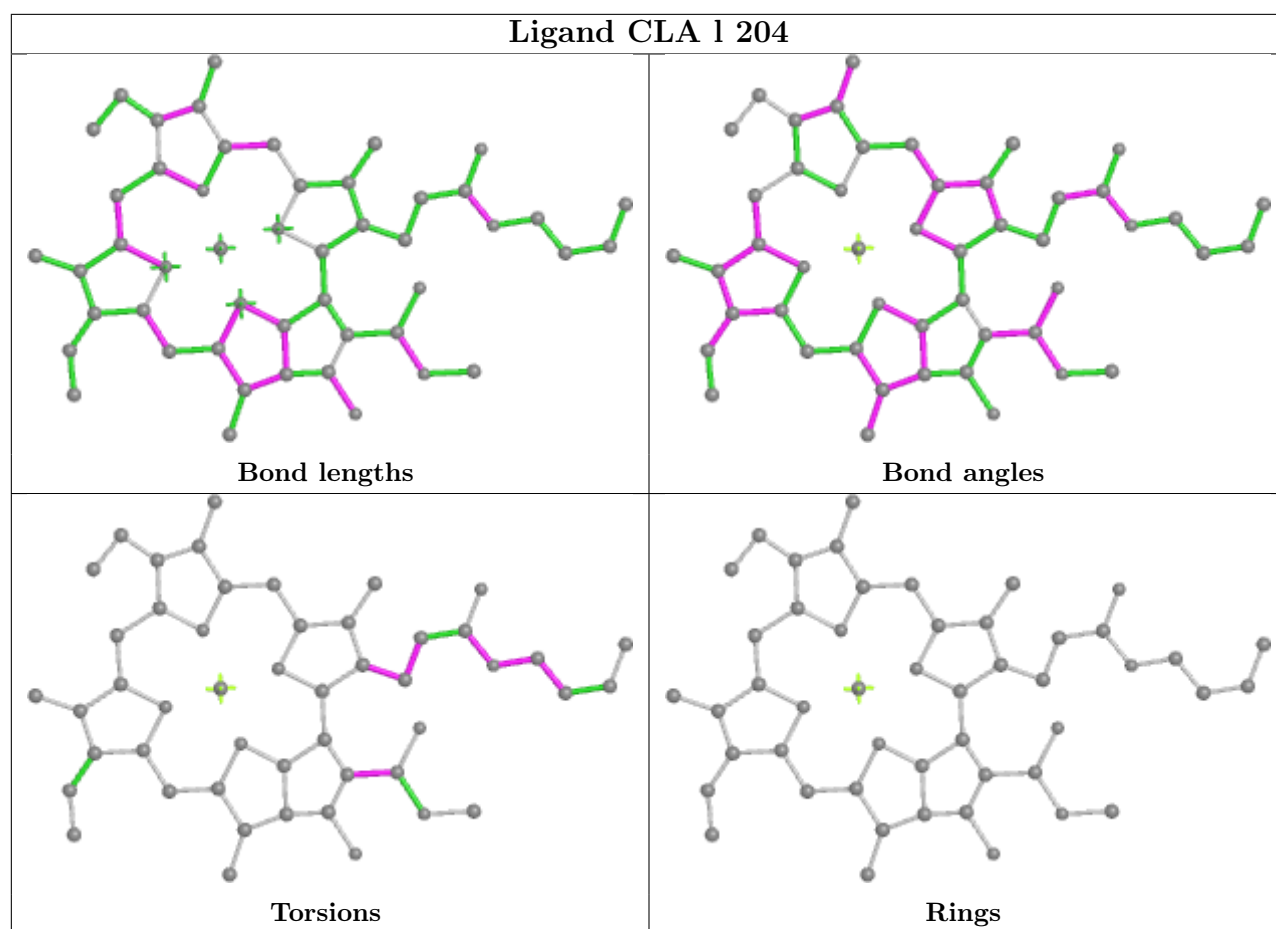
Bond angles



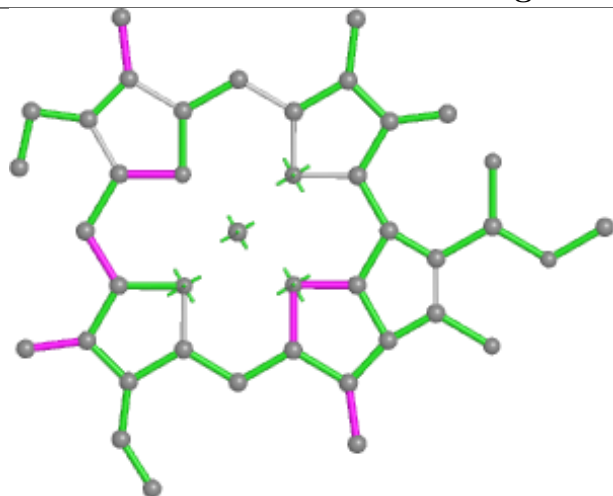
Torsions



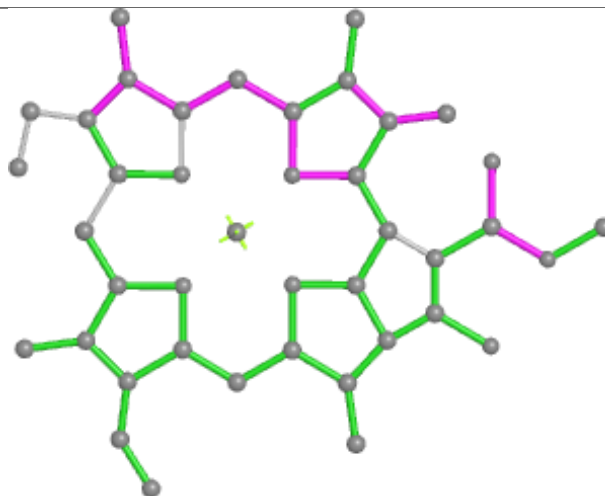
Rings



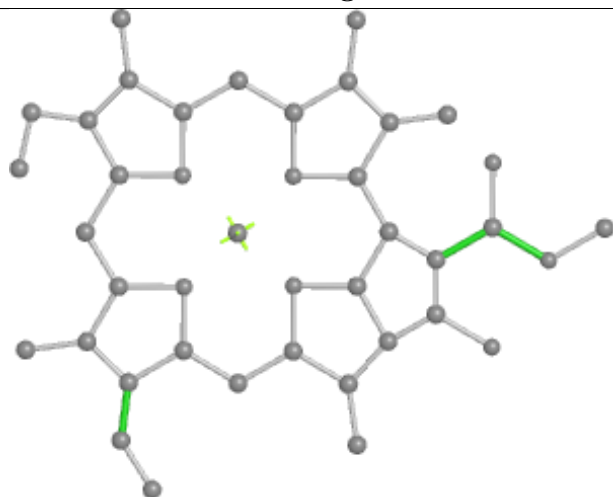
## Ligand CLA T 316



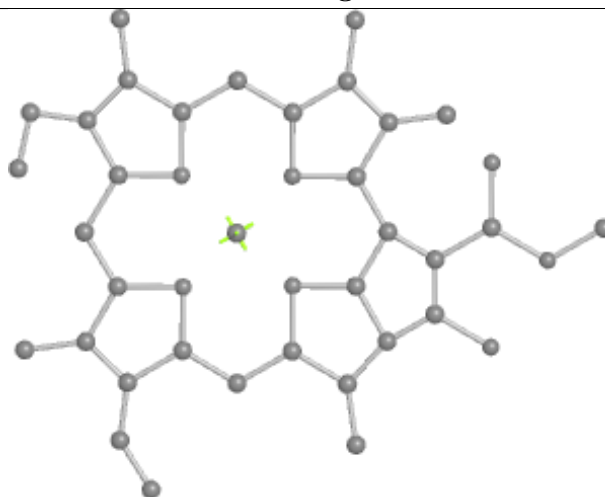
Bond lengths



Bond angles

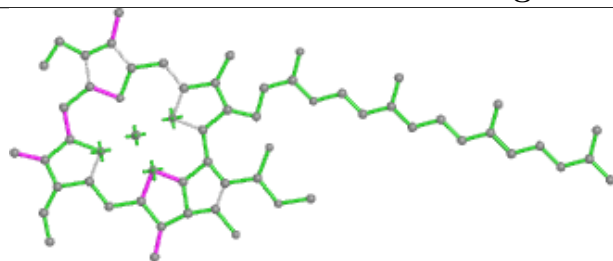


Torsions

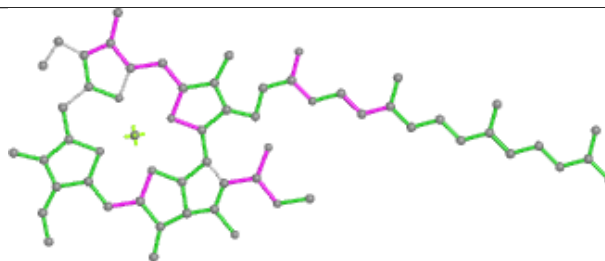


Rings

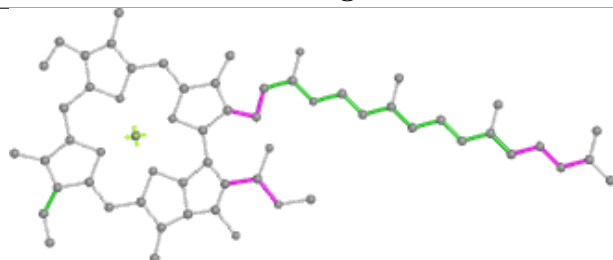
## Ligand CLA A 307



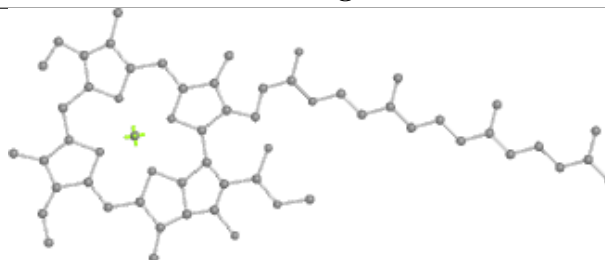
Bond lengths



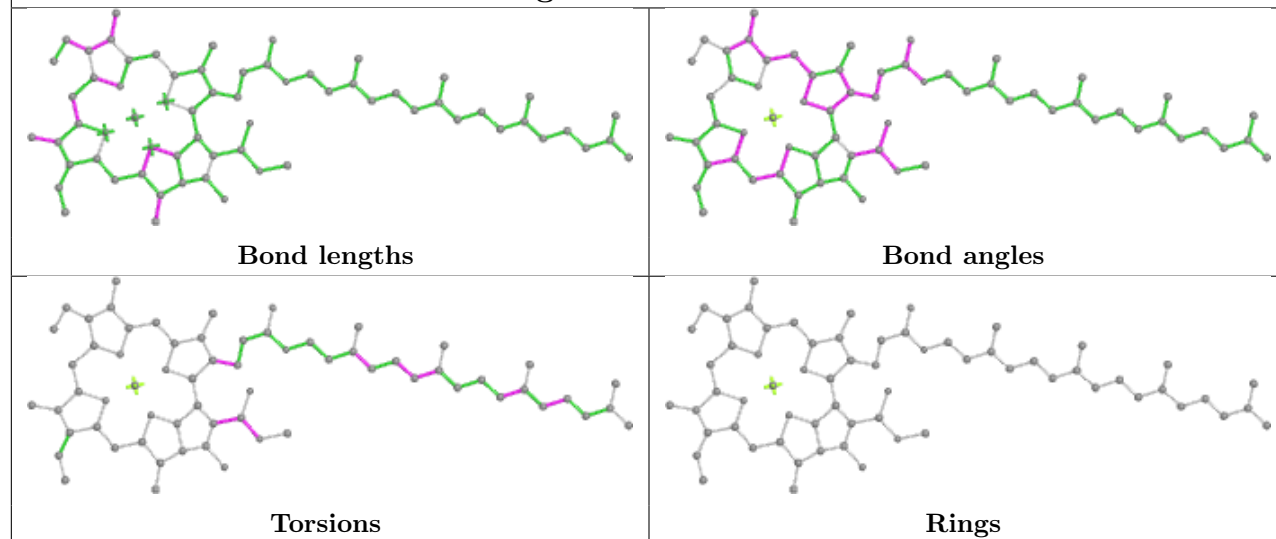
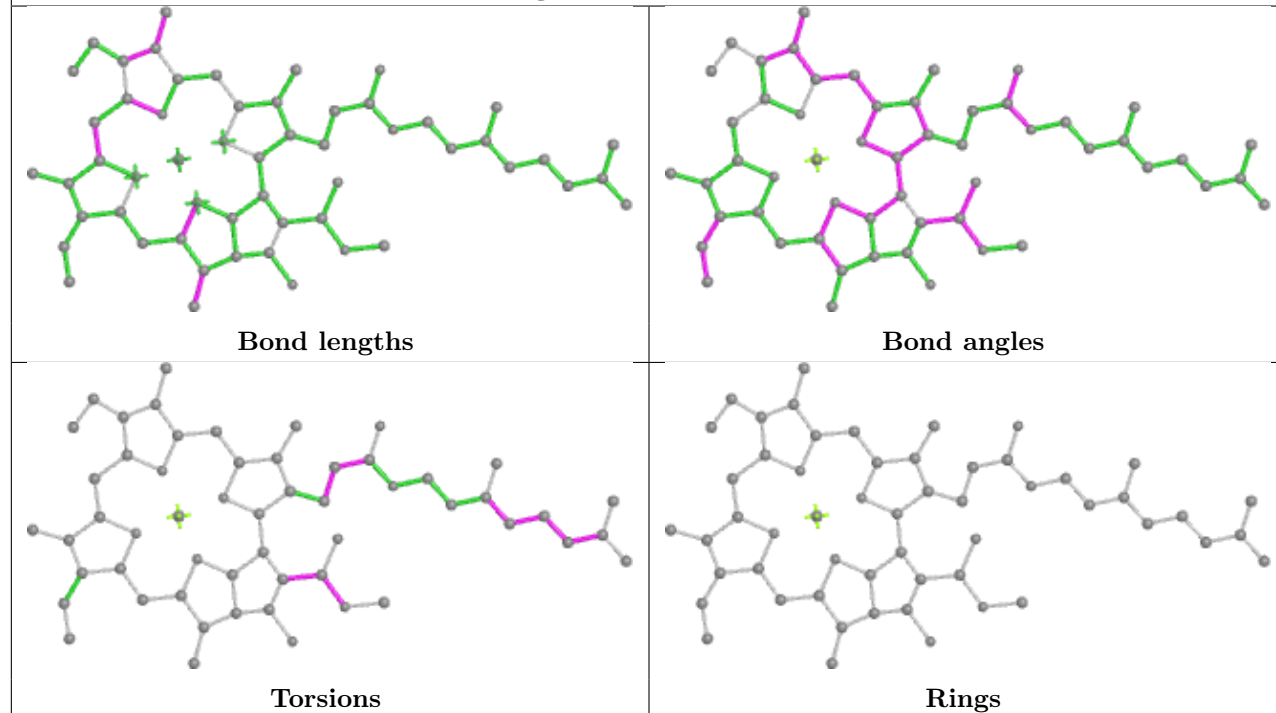
Bond angles

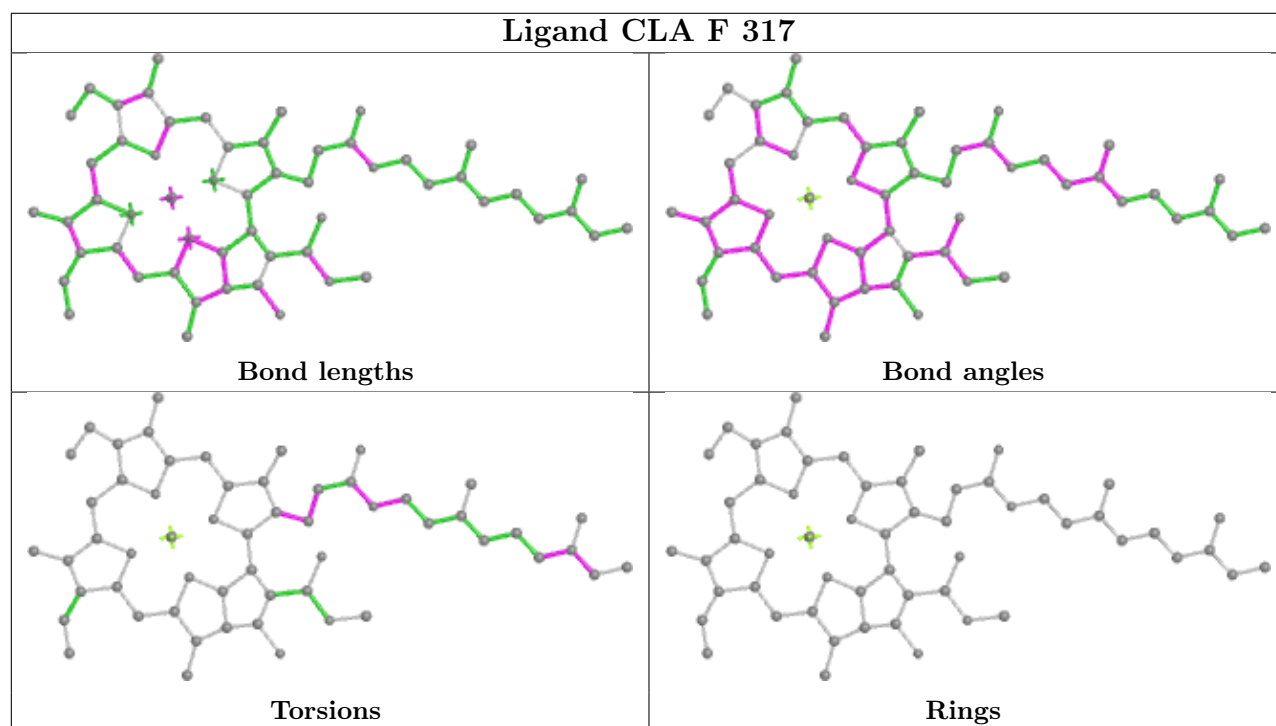
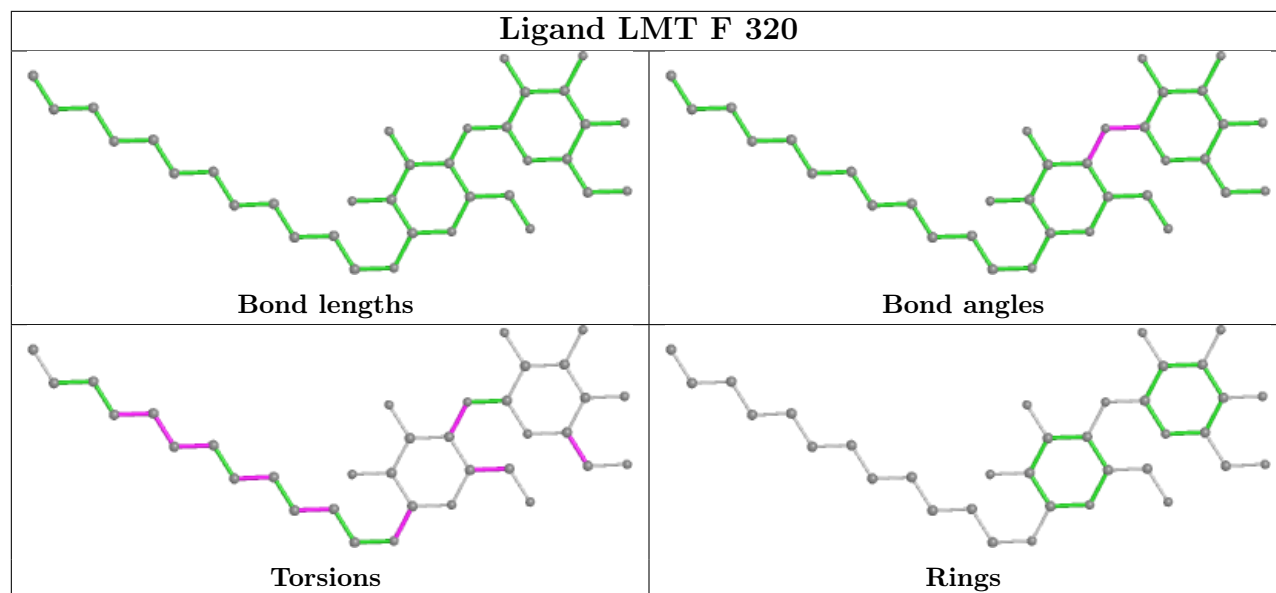


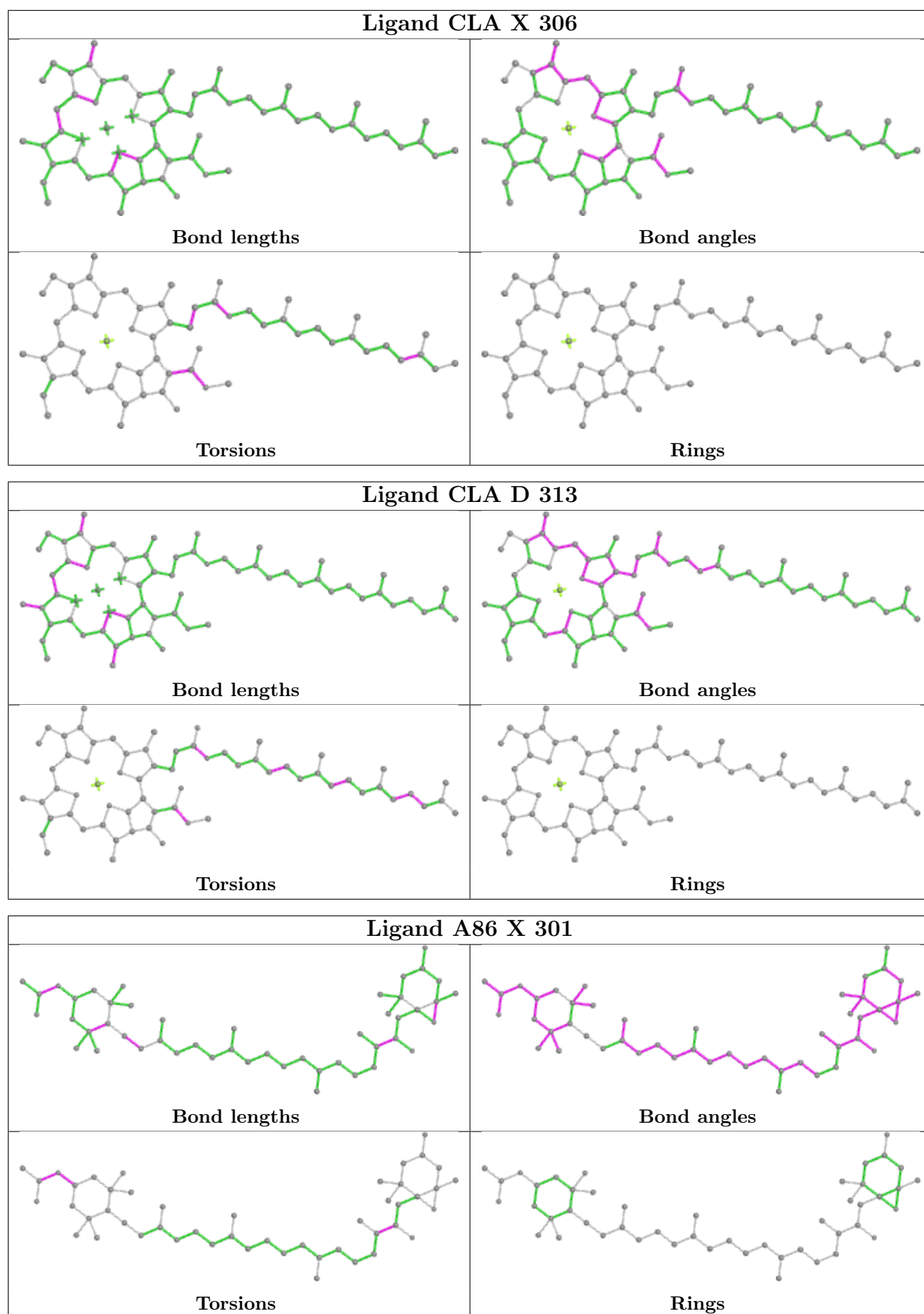
Torsions



Rings

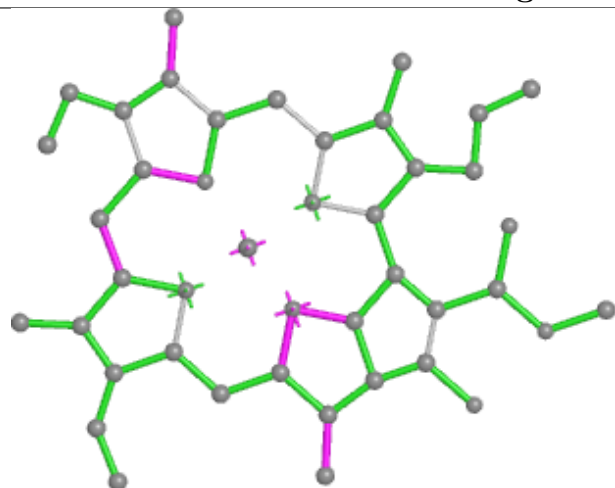
**Ligand CLA a 832****Ligand CLA B 311**



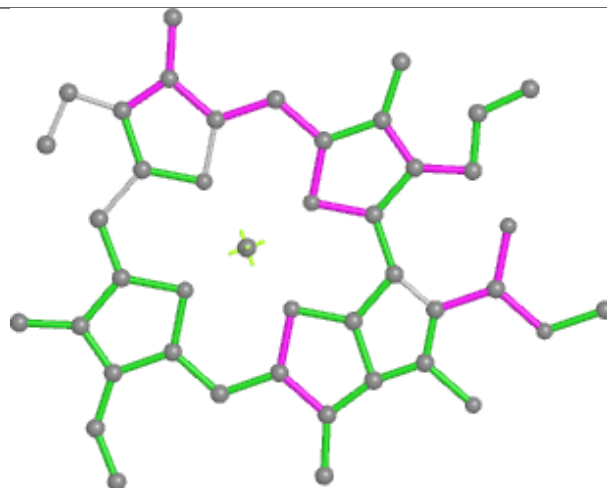




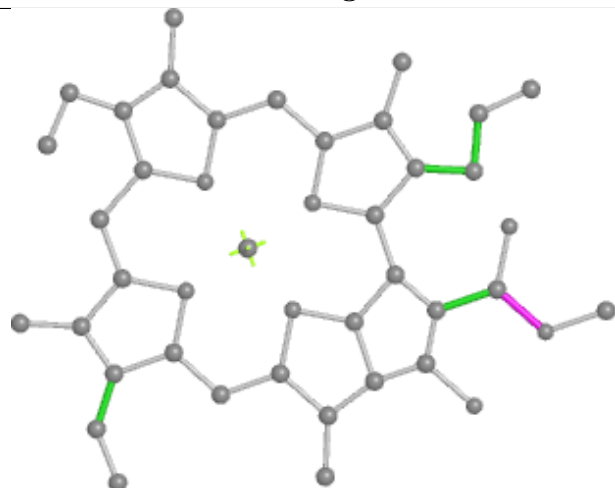
## Ligand CLA C 205



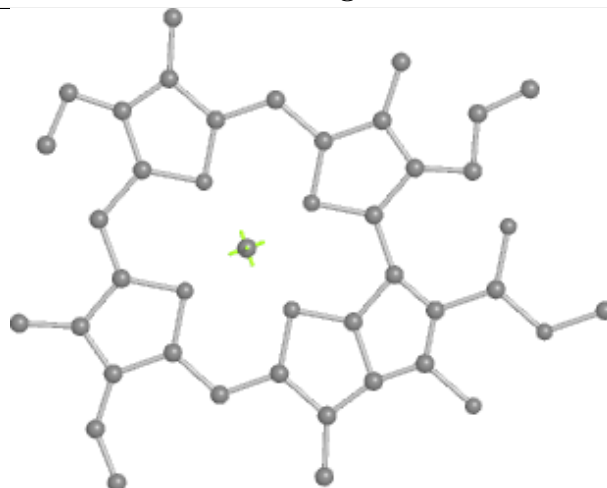
Bond lengths



Bond angles

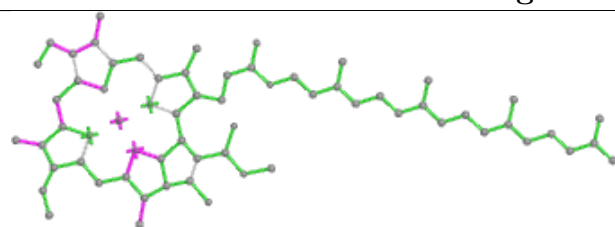


Torsions

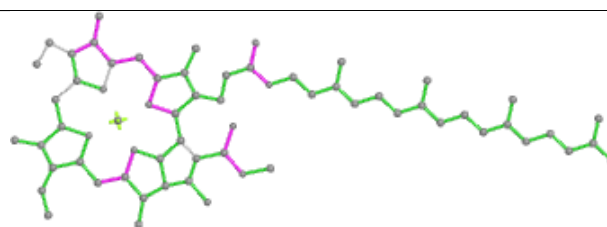


Rings

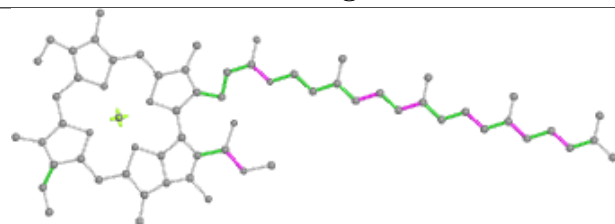
## Ligand CLA C 211



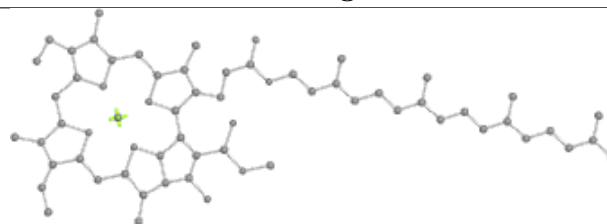
Bond lengths



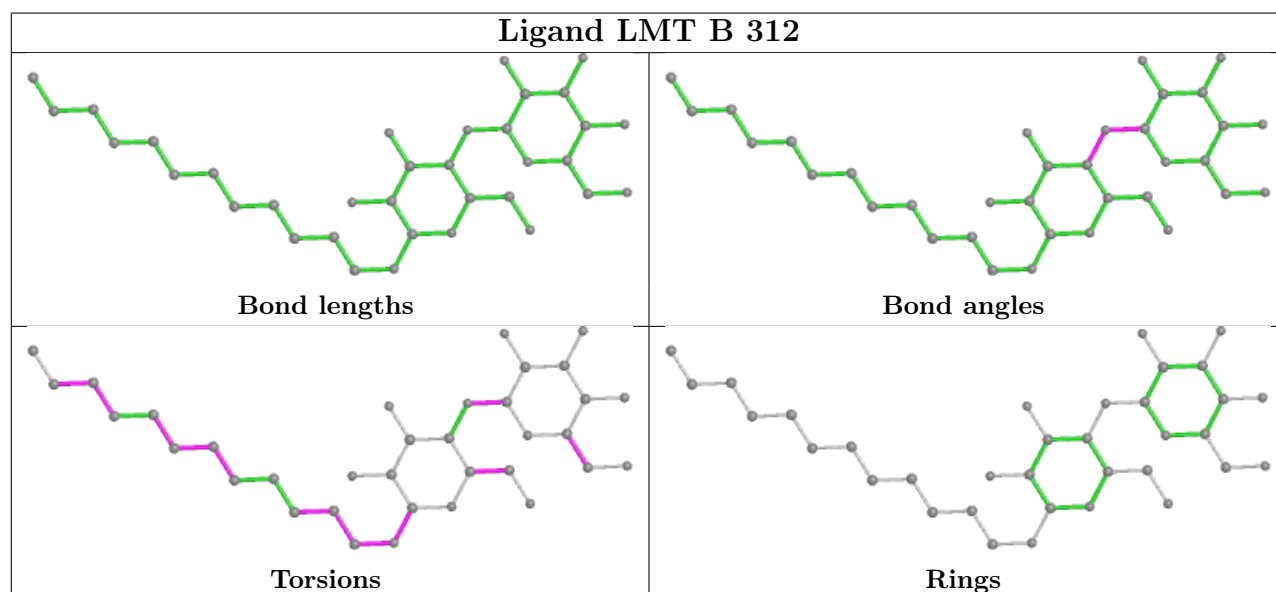
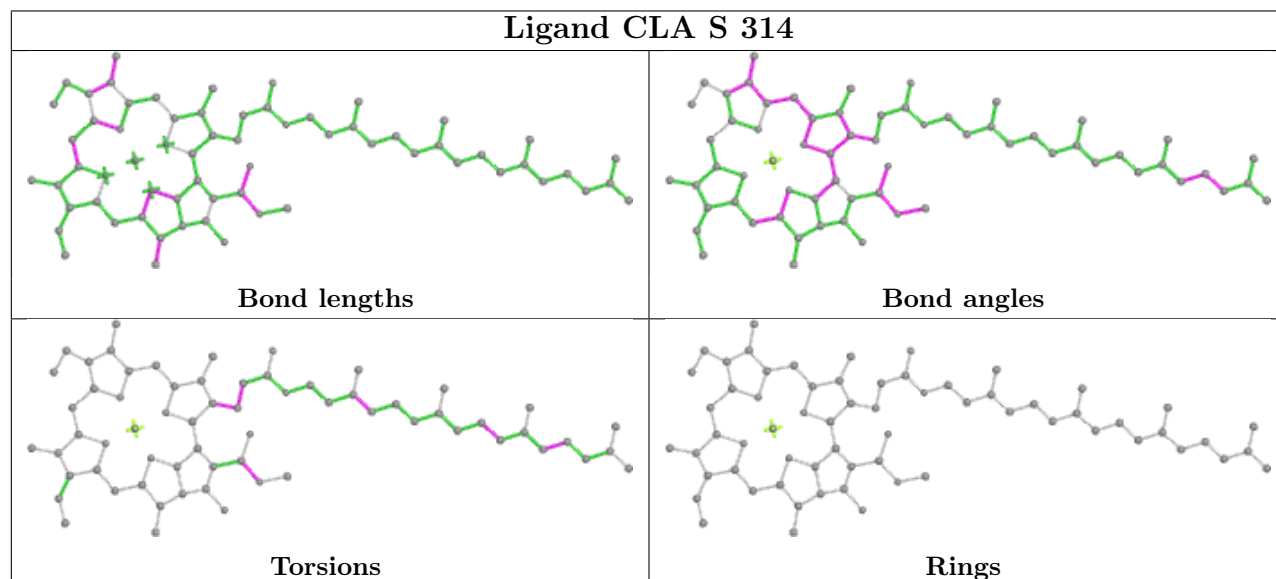
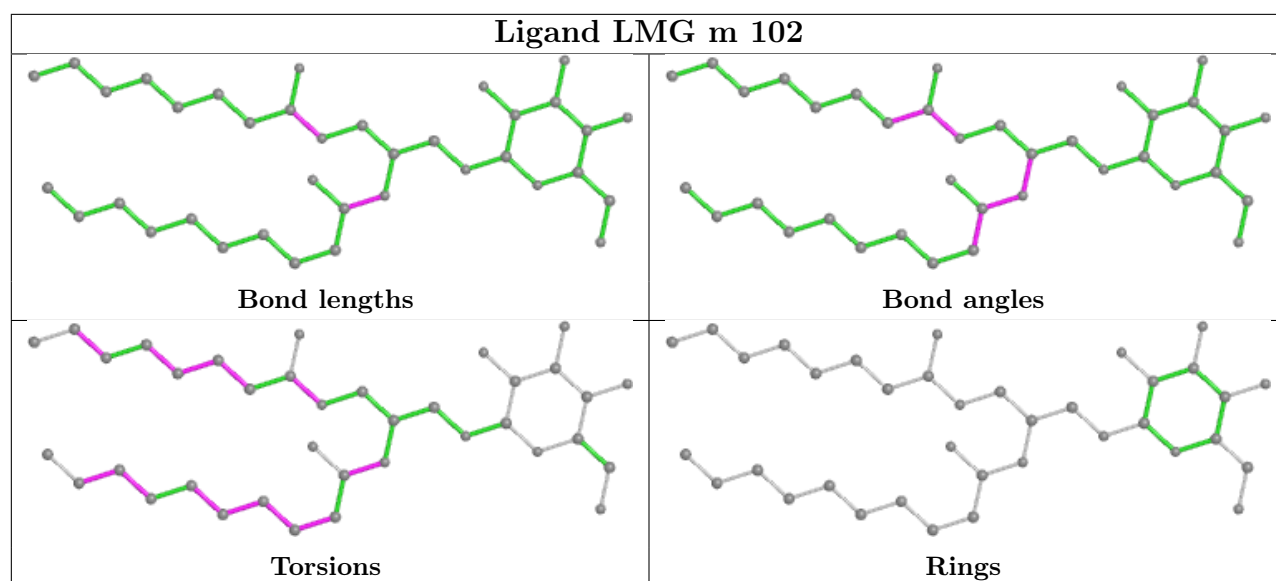
Bond angles

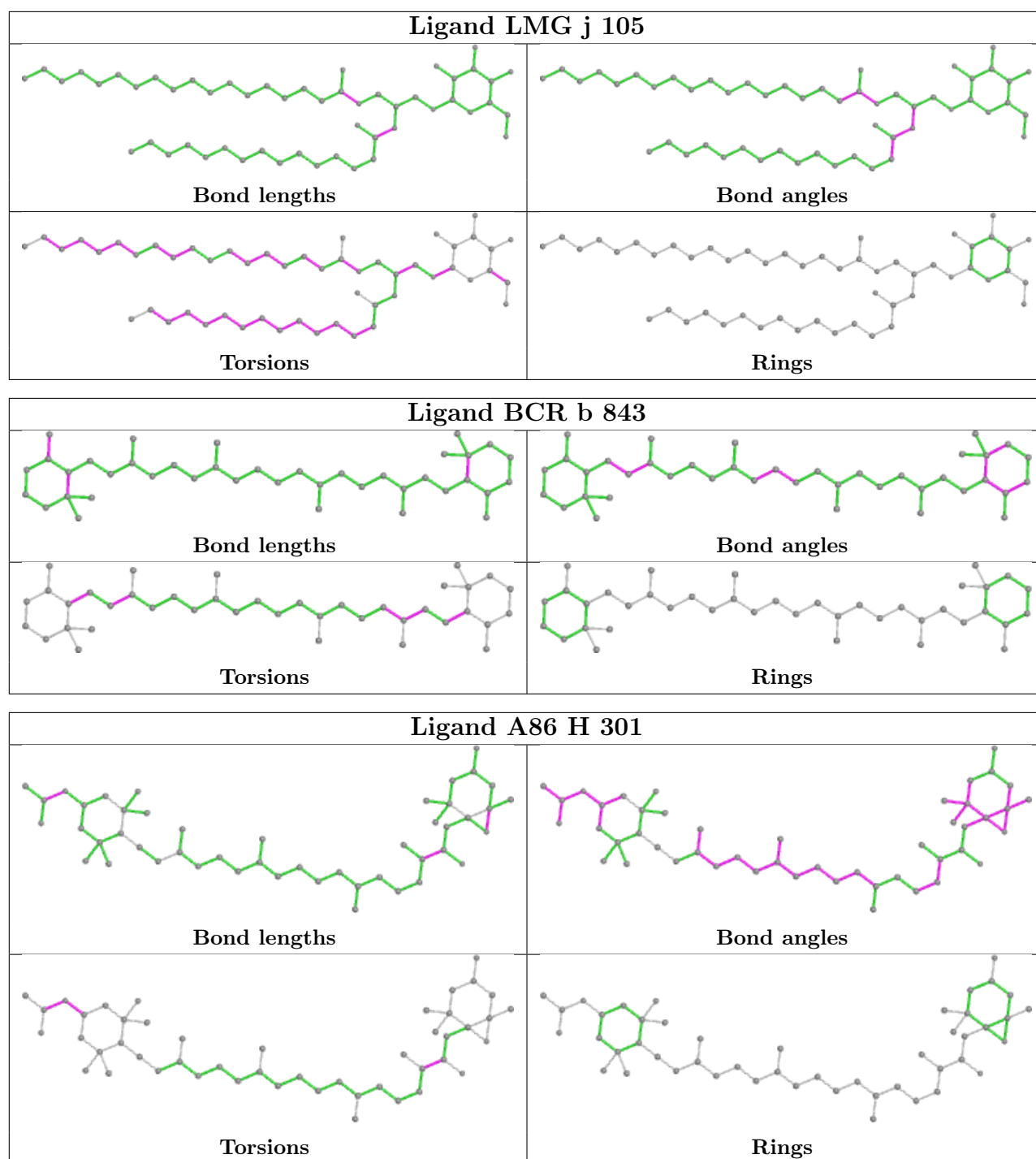


Torsions

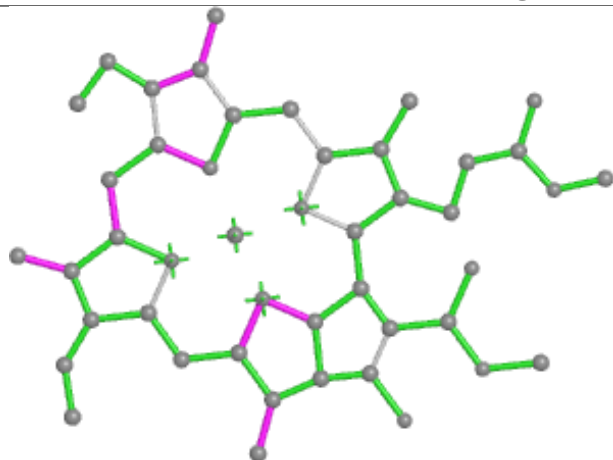


Rings

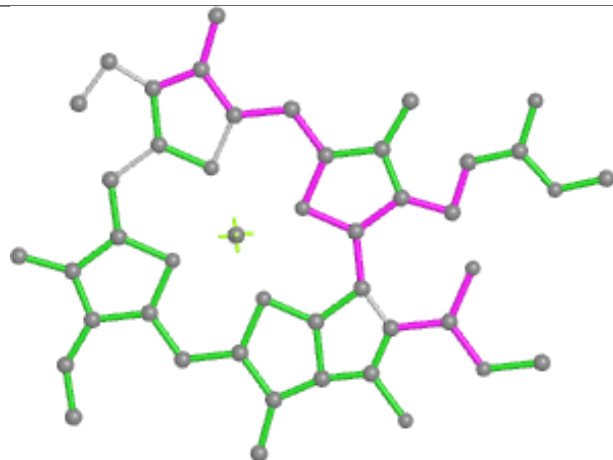




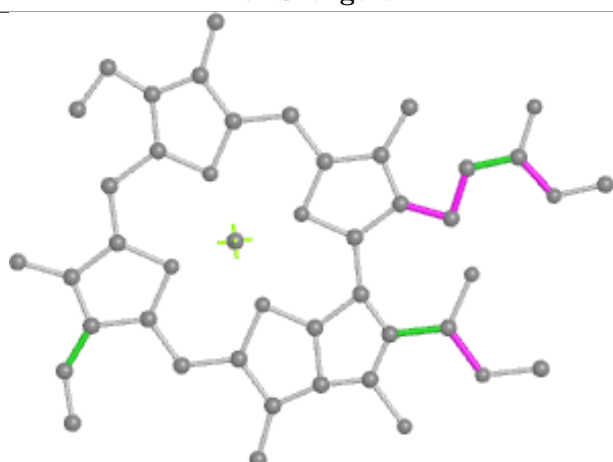
## Ligand CLA O 310



Bond lengths



Bond angles

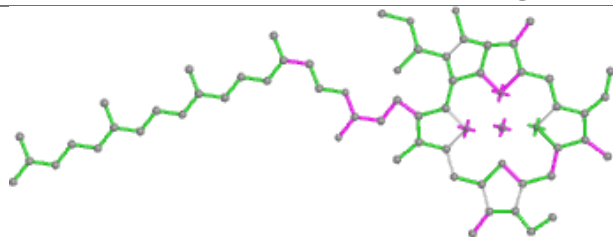


Torsions

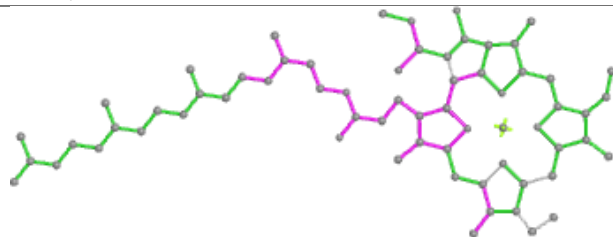


Rings

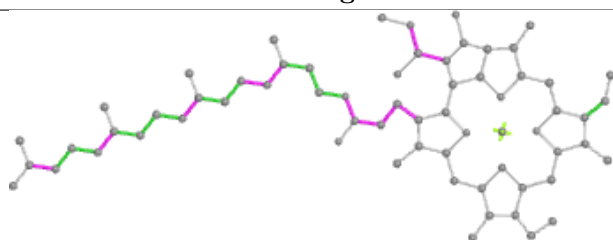
## Ligand CLA Q 310



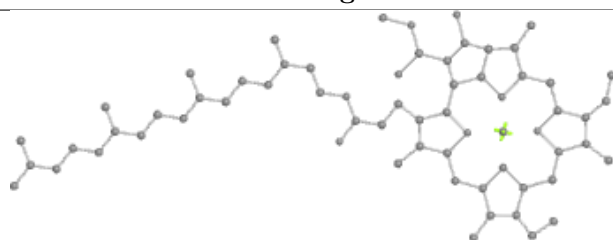
Bond lengths



Bond angles

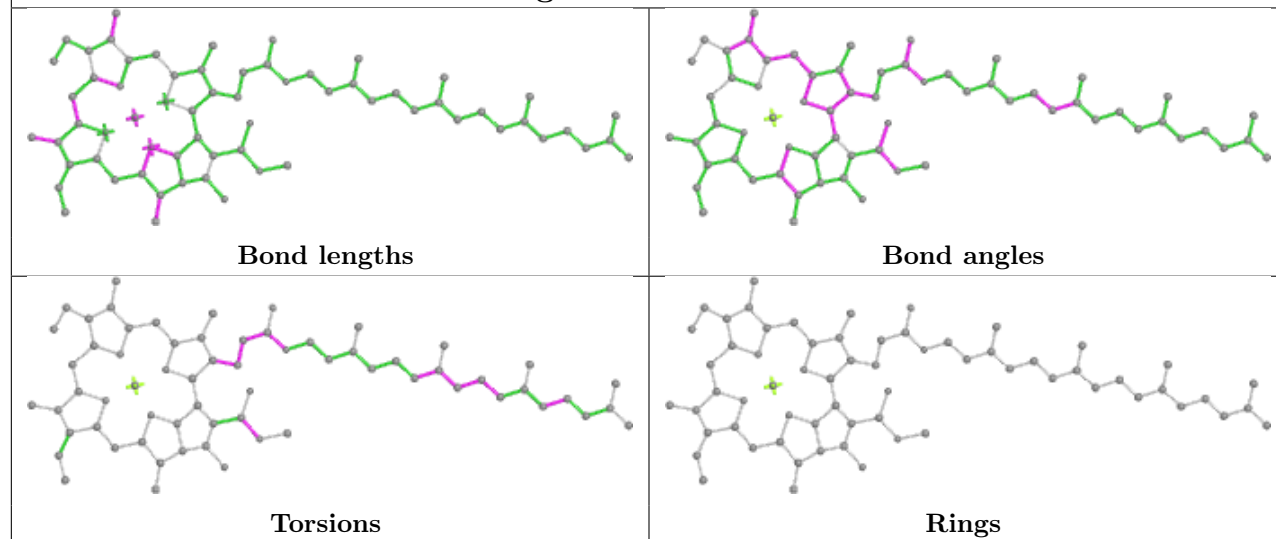


Torsions

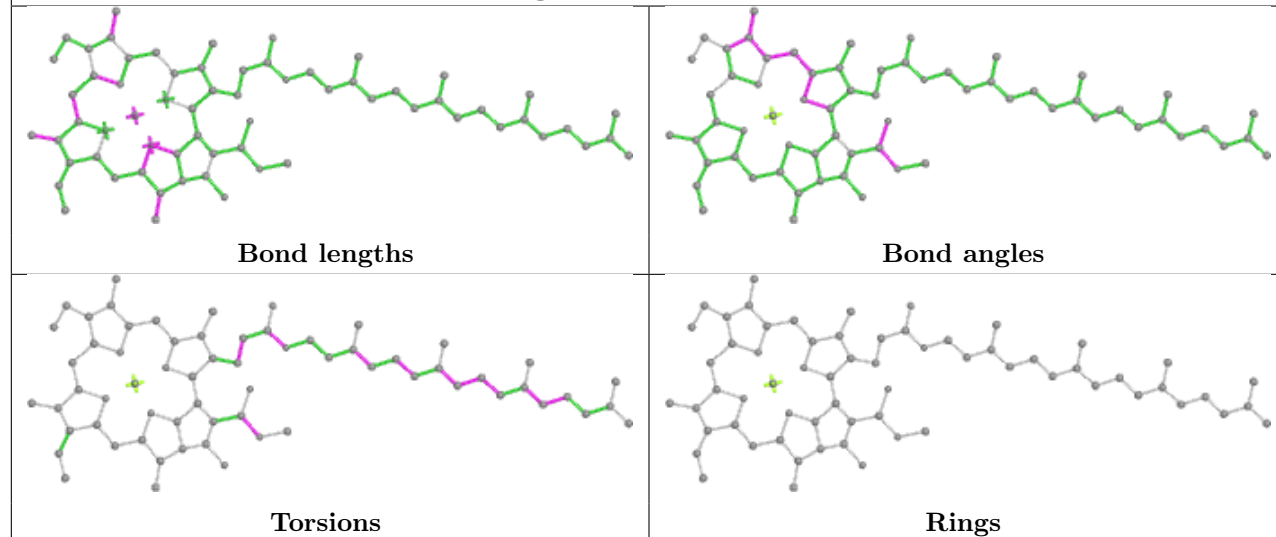


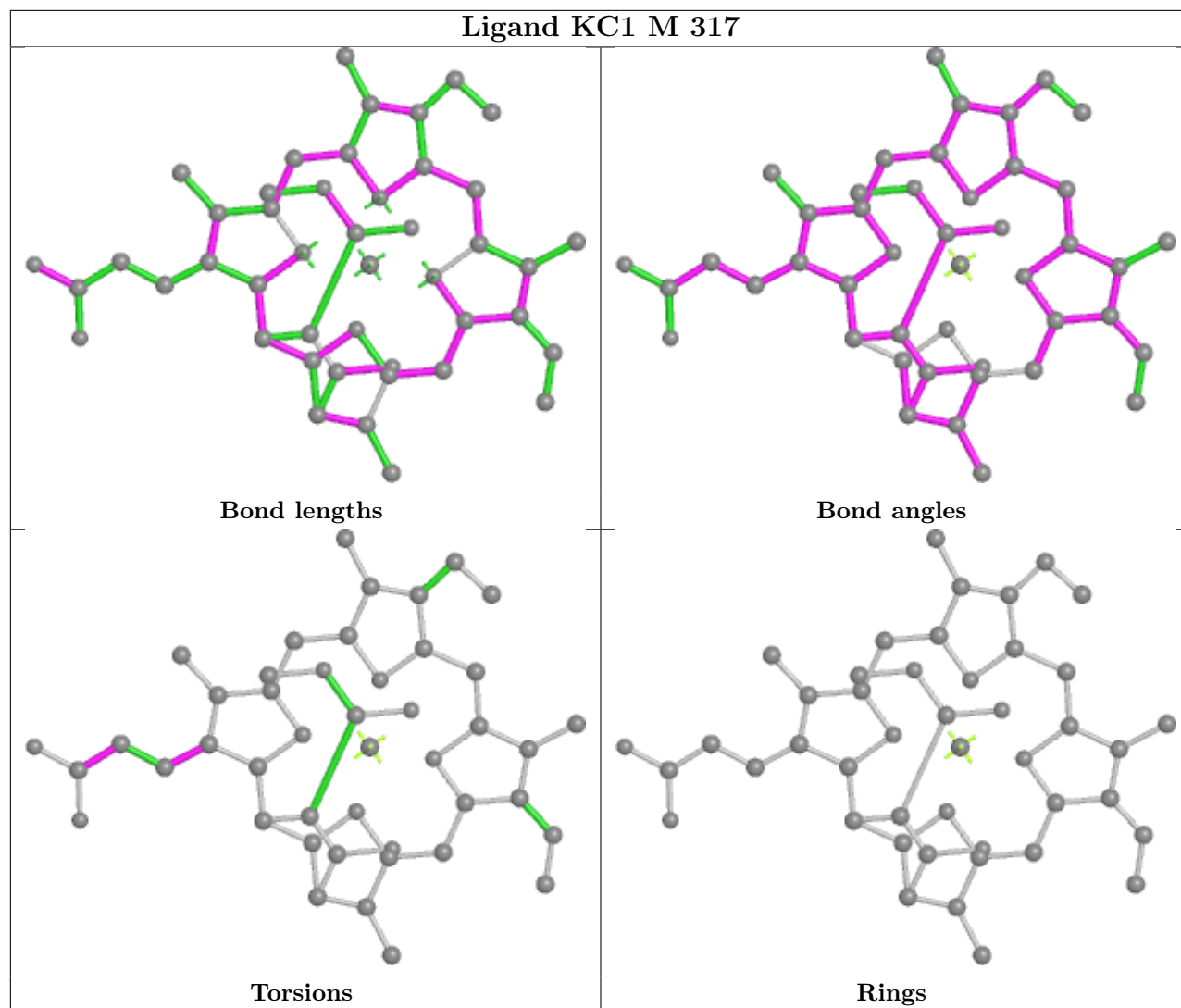
Rings

## Ligand CLA a 817

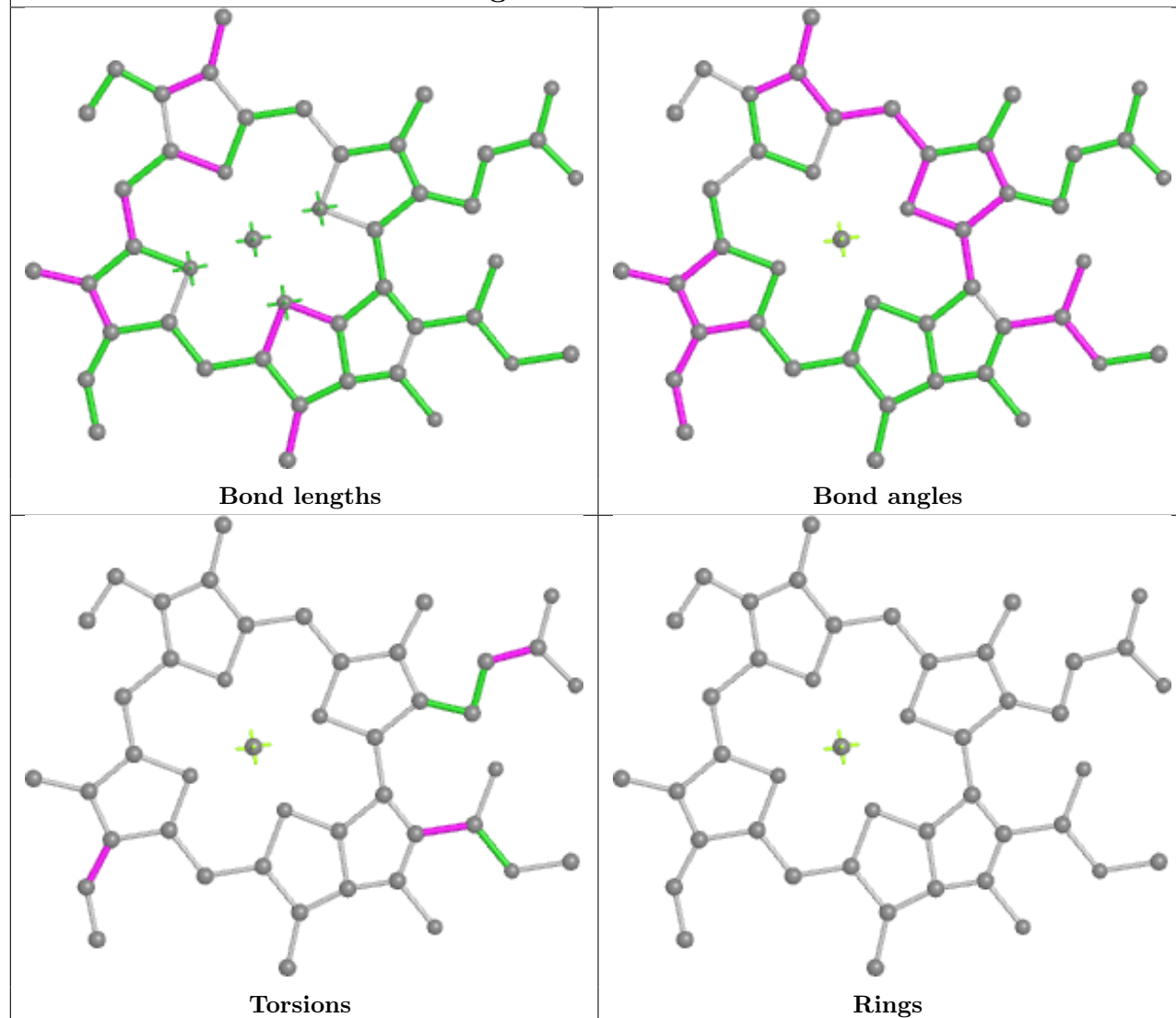


## Ligand CLA O 307

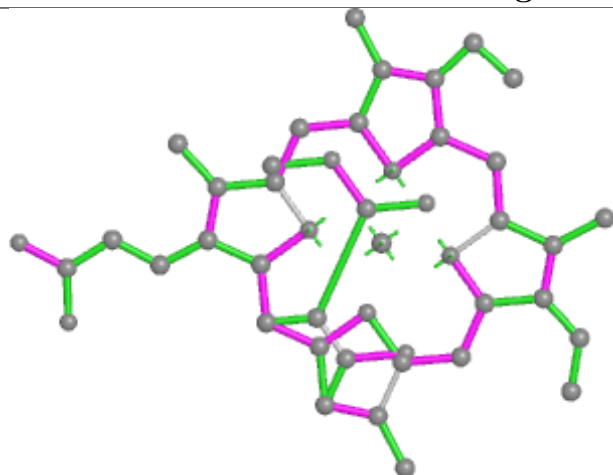




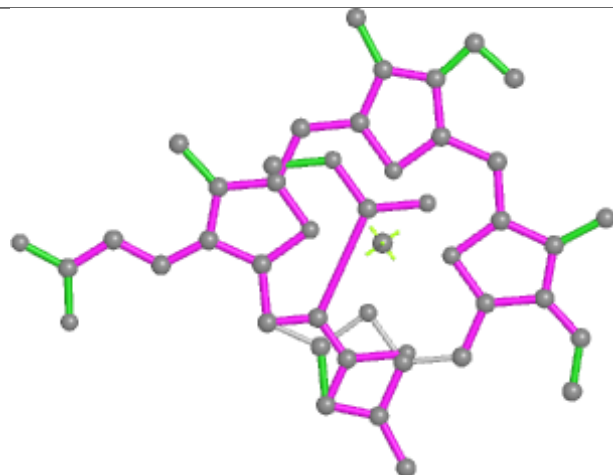
## Ligand CLA R 319



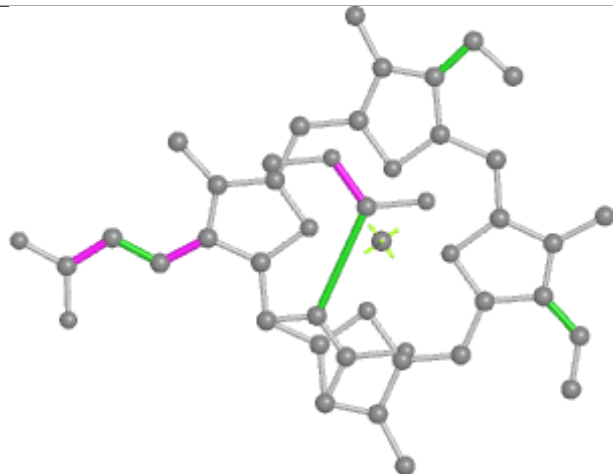
## Ligand KC1 H 313



Bond lengths



Bond angles

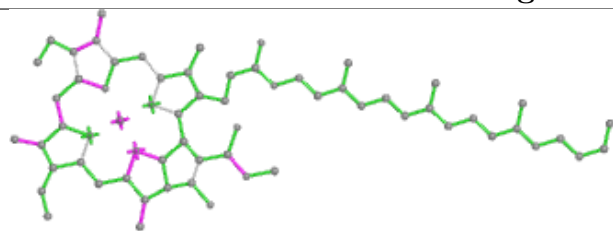


Torsions

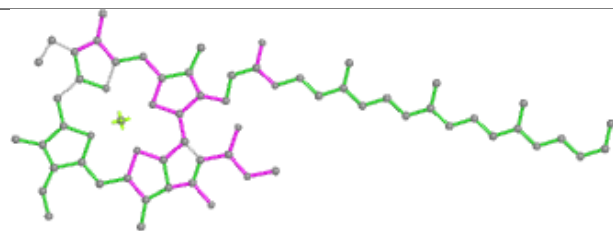


Rings

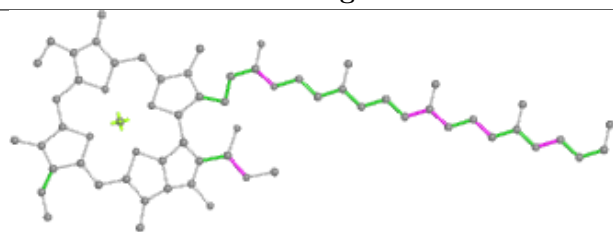
## Ligand CLA b 826



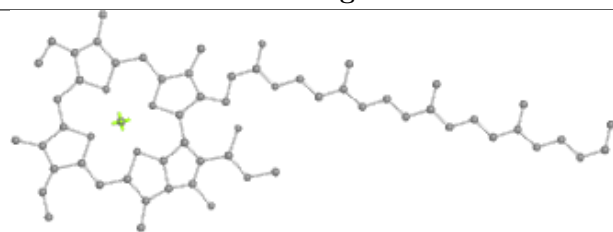
Bond lengths



Bond angles



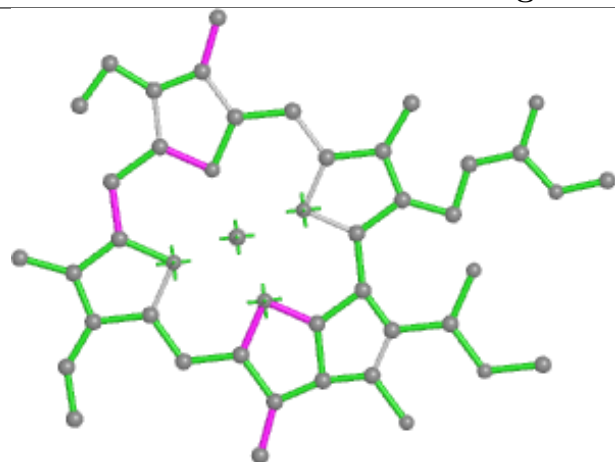
Torsions



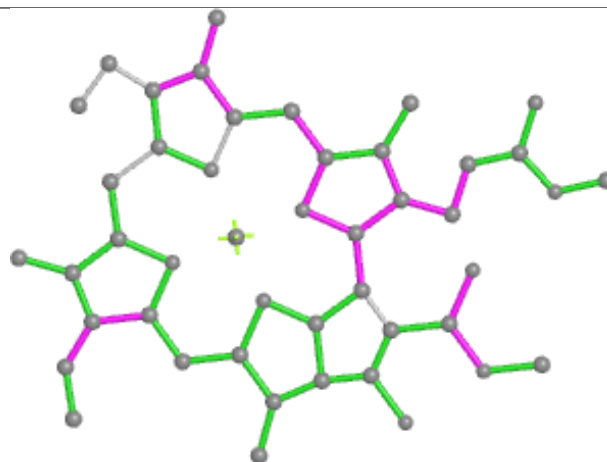
Rings



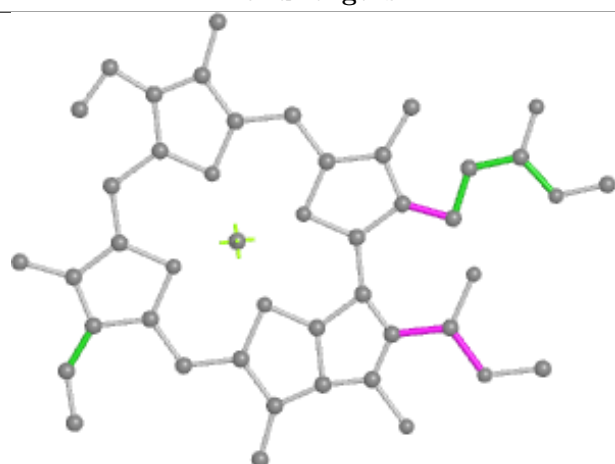
## Ligand CLA T 312



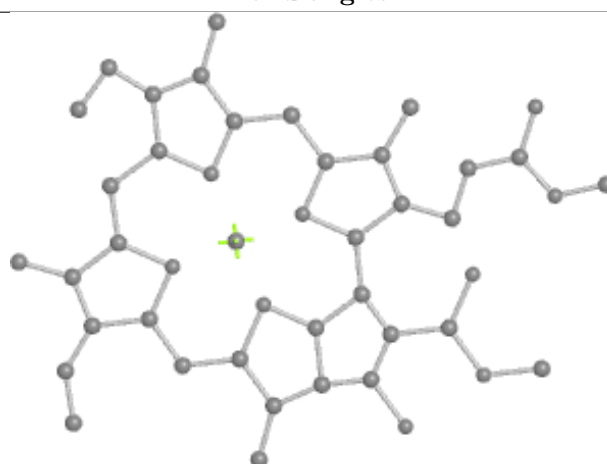
Bond lengths



Bond angles

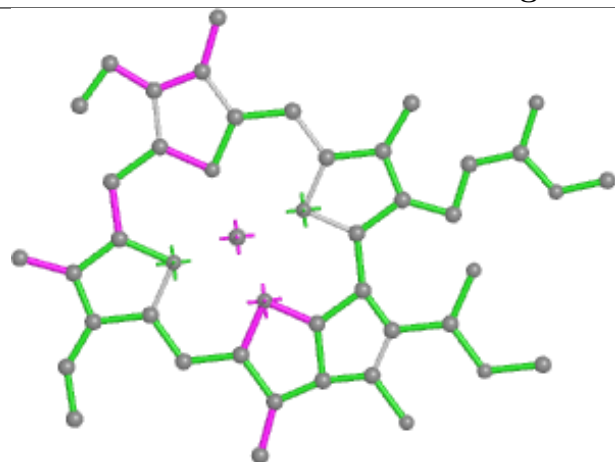


Torsions

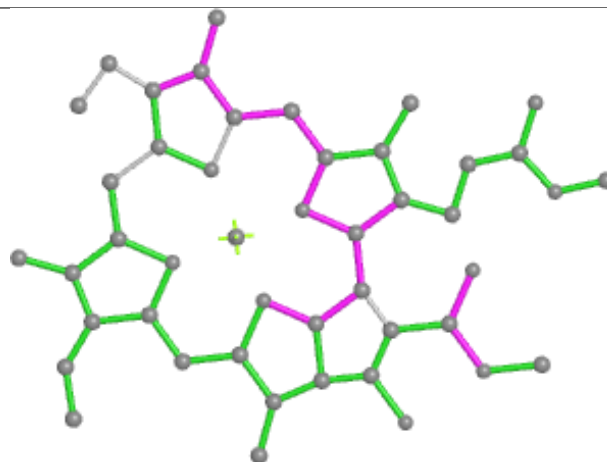


Rings

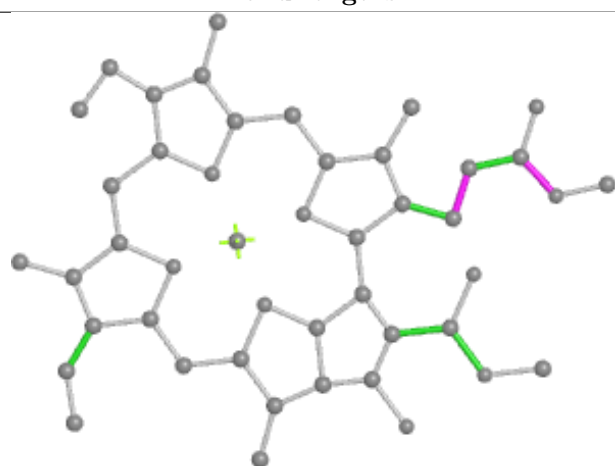
## Ligand CLA J 311



Bond lengths



Bond angles

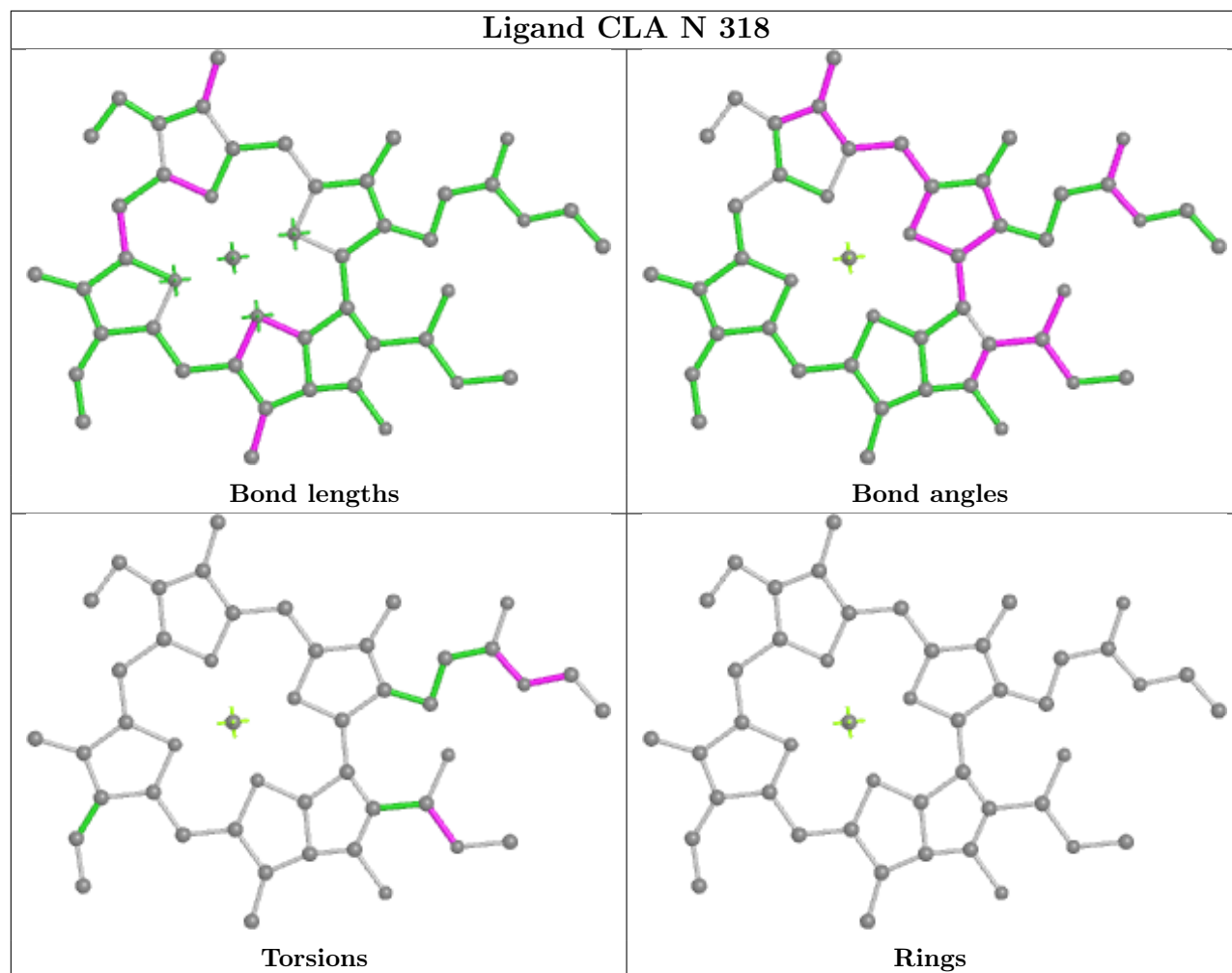


Torsions

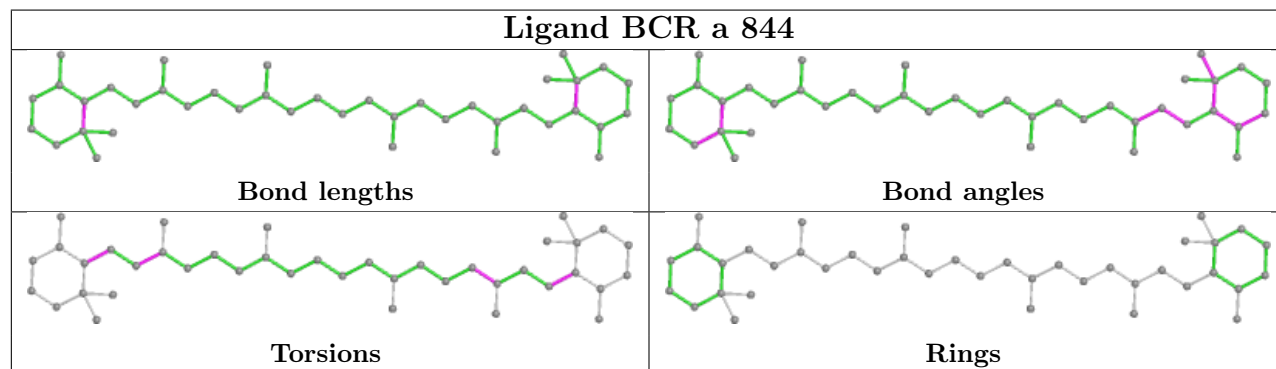


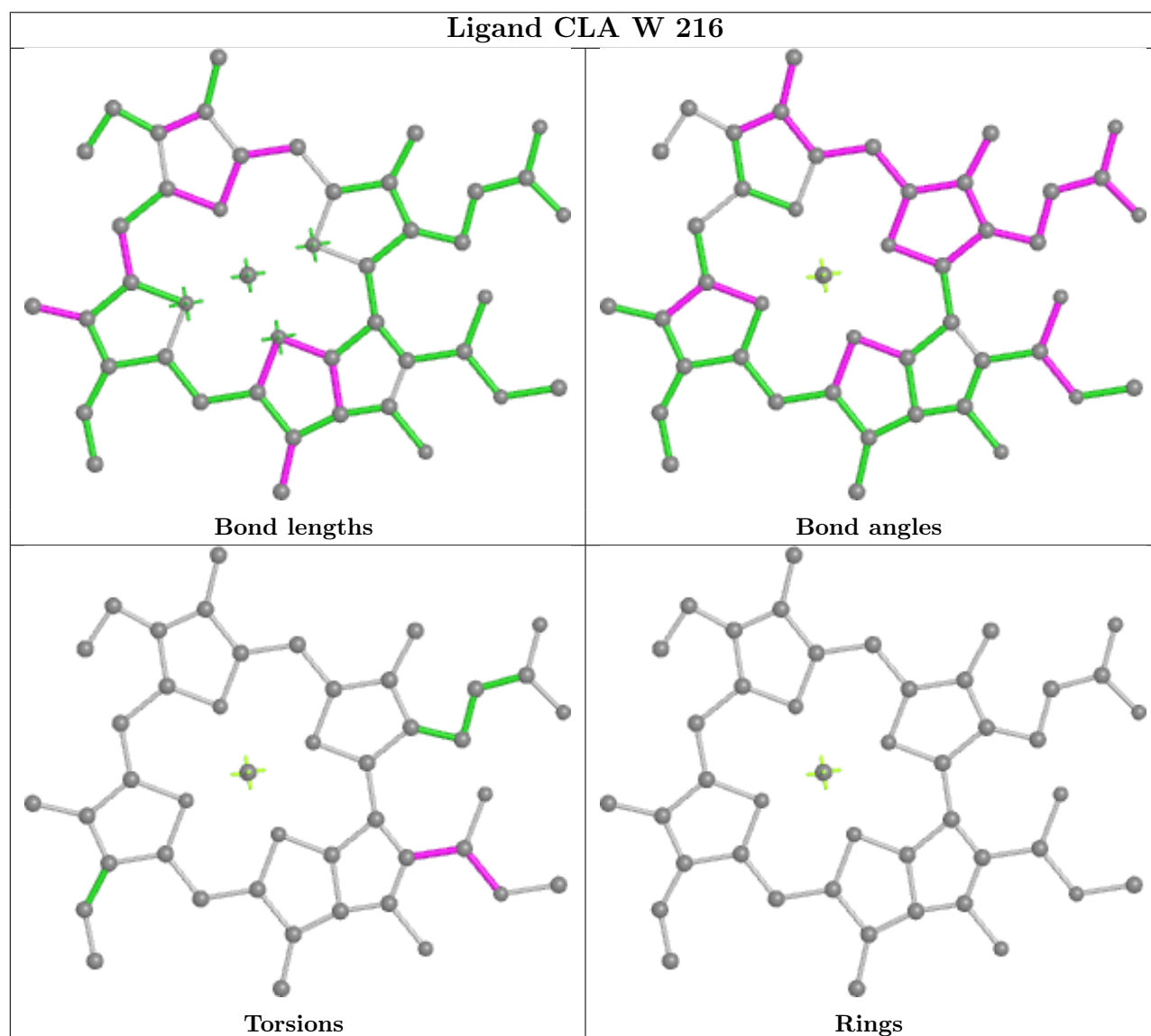
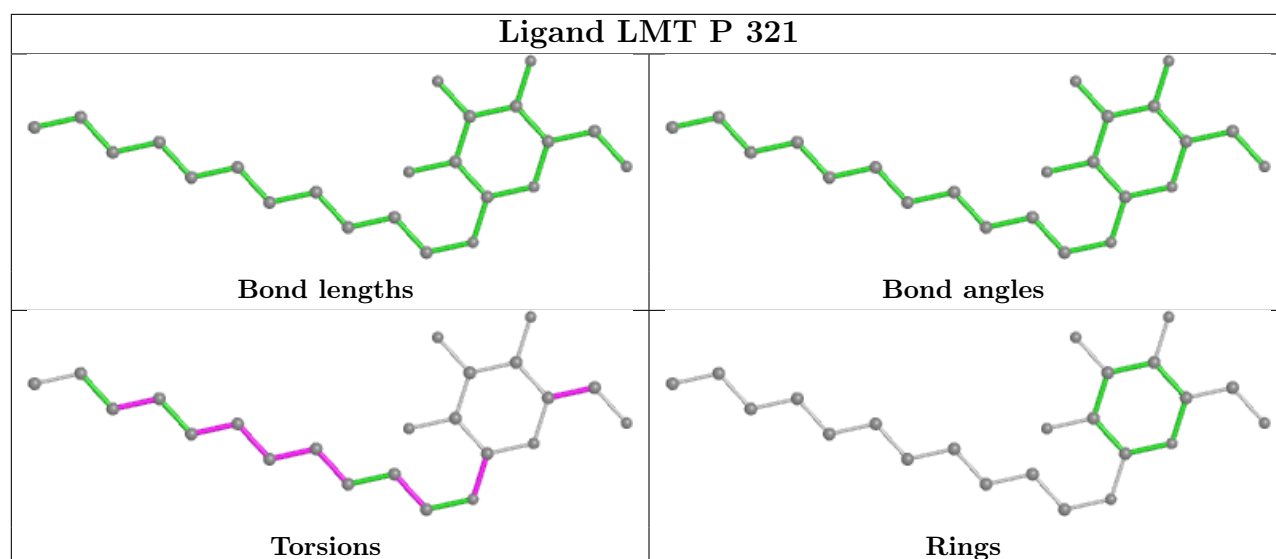
Rings

## Ligand CLA N 318

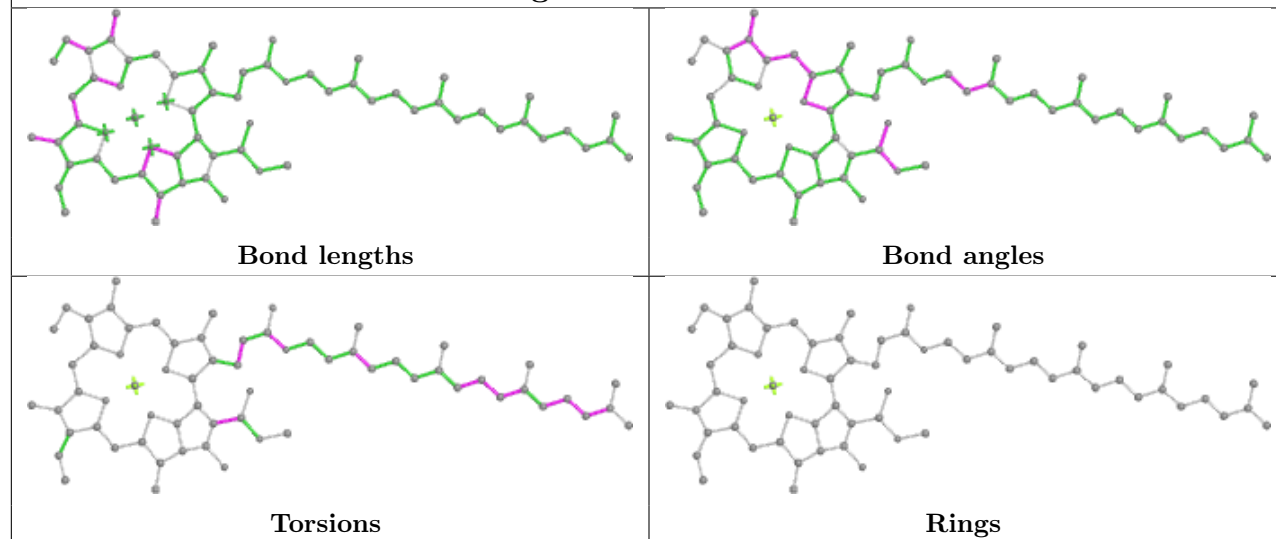


## Ligand BCR a 844

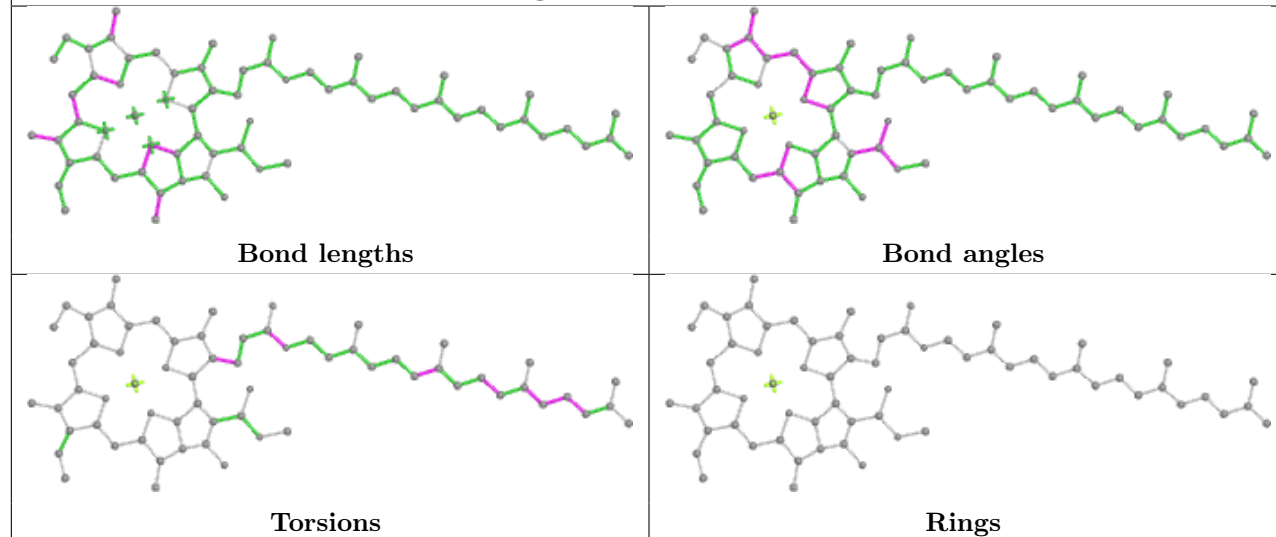




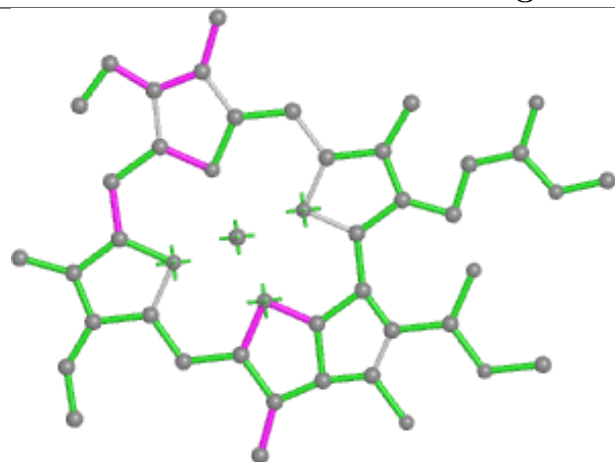
## Ligand CLA H 309



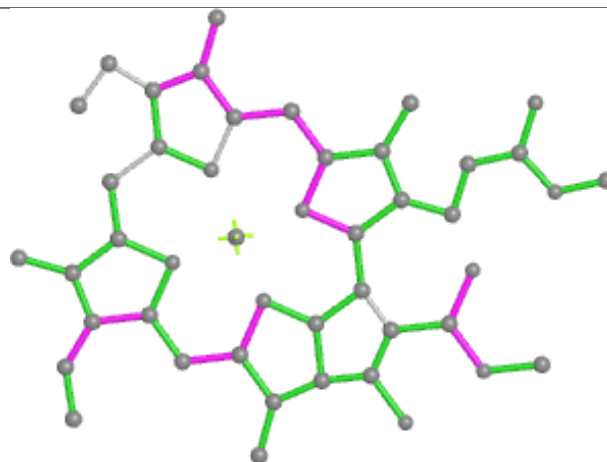
## Ligand CLA H 311



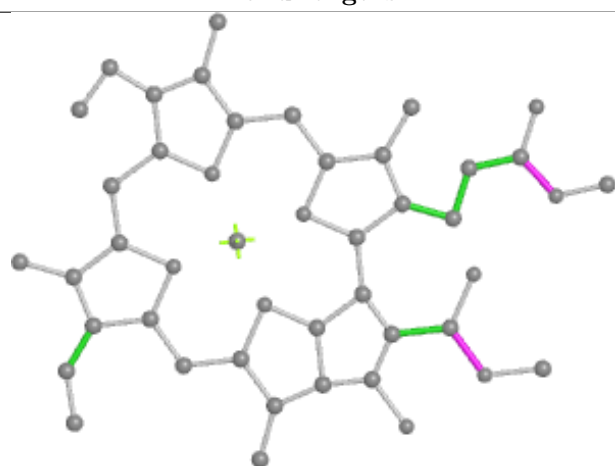
## Ligand CLA B 306



Bond lengths



Bond angles

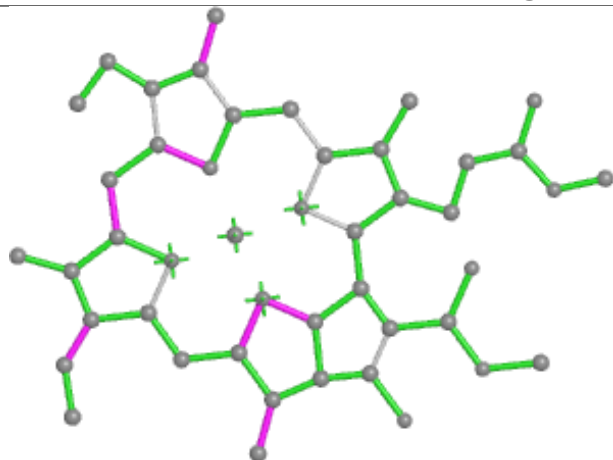


Torsions

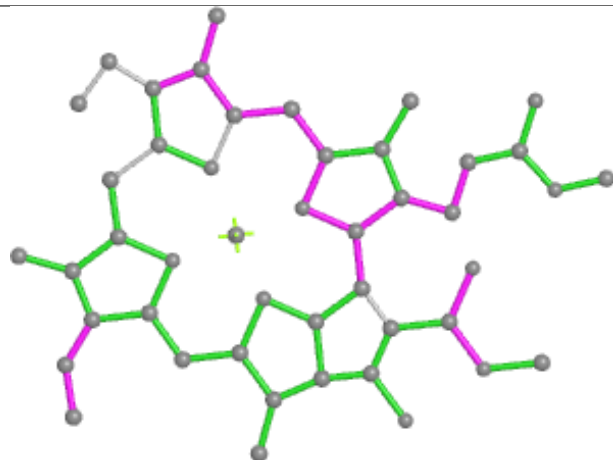


Rings

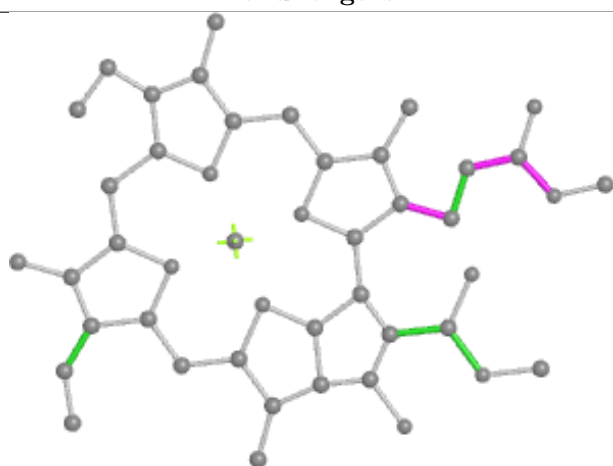
## Ligand CLA I 309



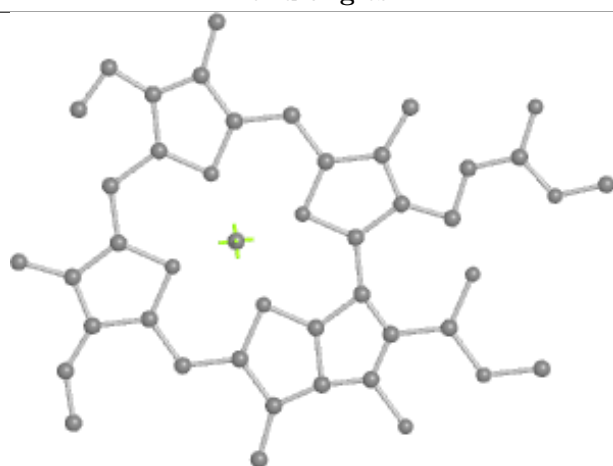
Bond lengths



Bond angles

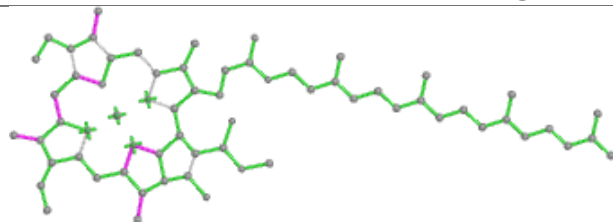


Torsions

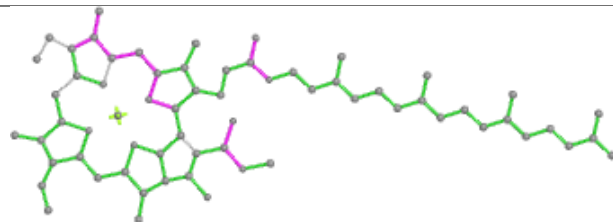


Rings

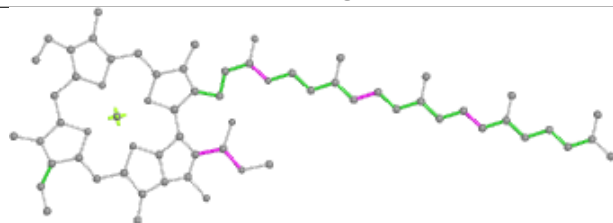
## Ligand CLA V 310



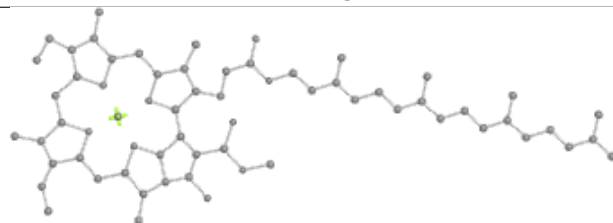
Bond lengths



Bond angles

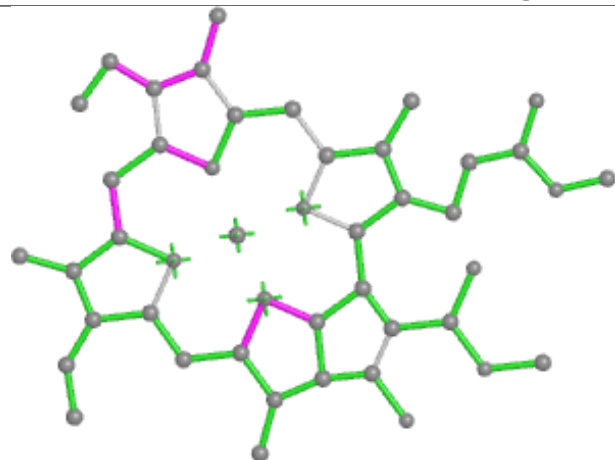


Torsions

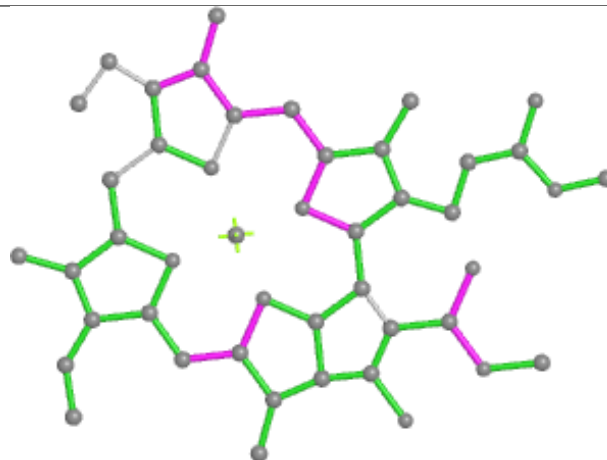


Rings

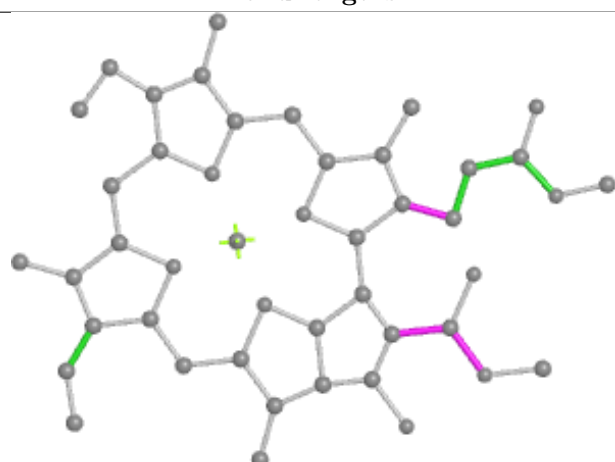
## Ligand CLA E 317



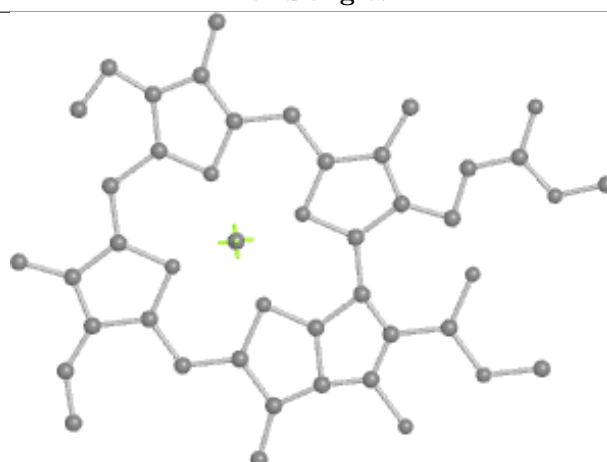
Bond lengths



Bond angles

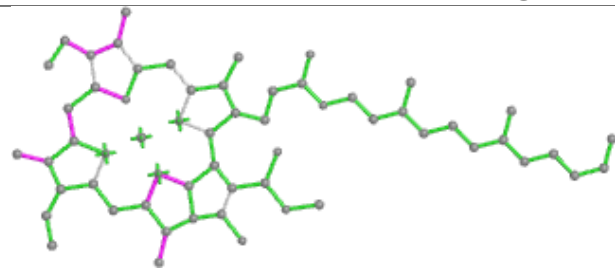


Torsions

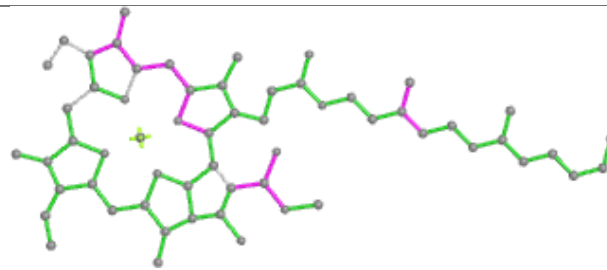


Rings

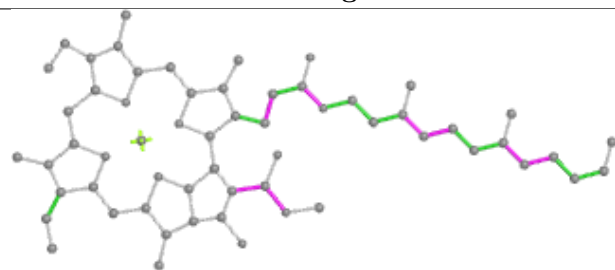
## Ligand CLA K 309



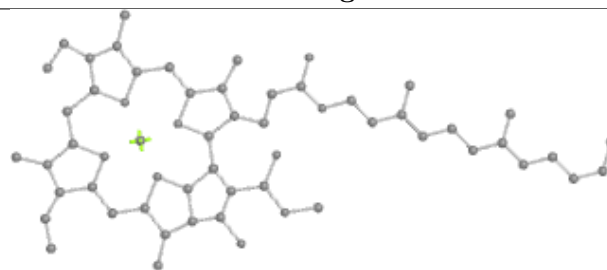
Bond lengths



Bond angles

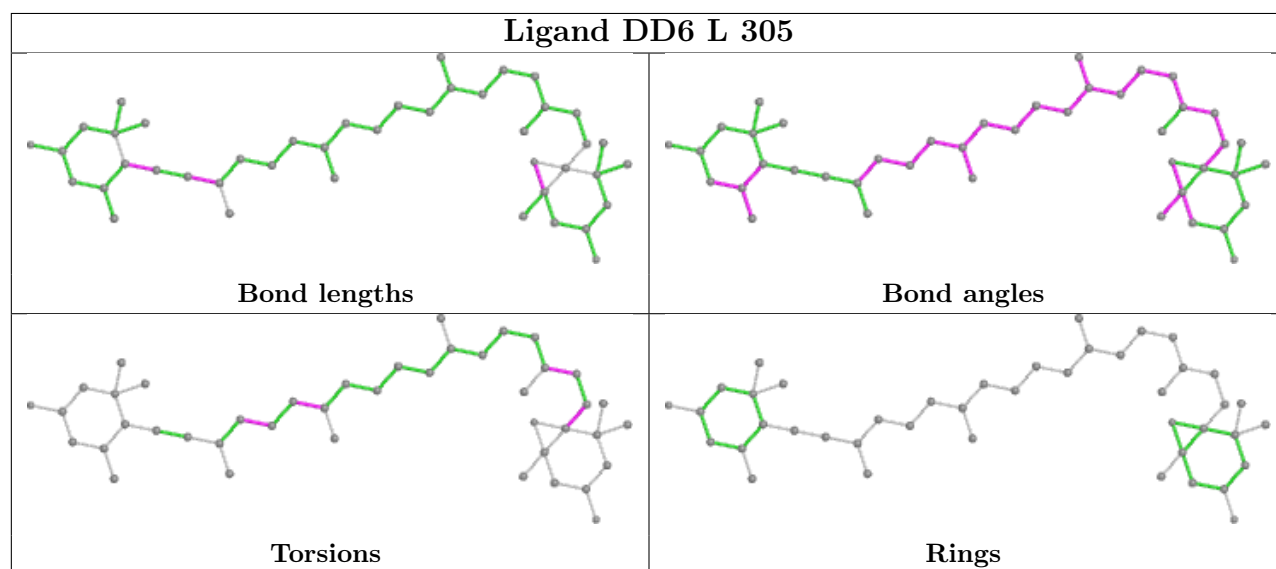
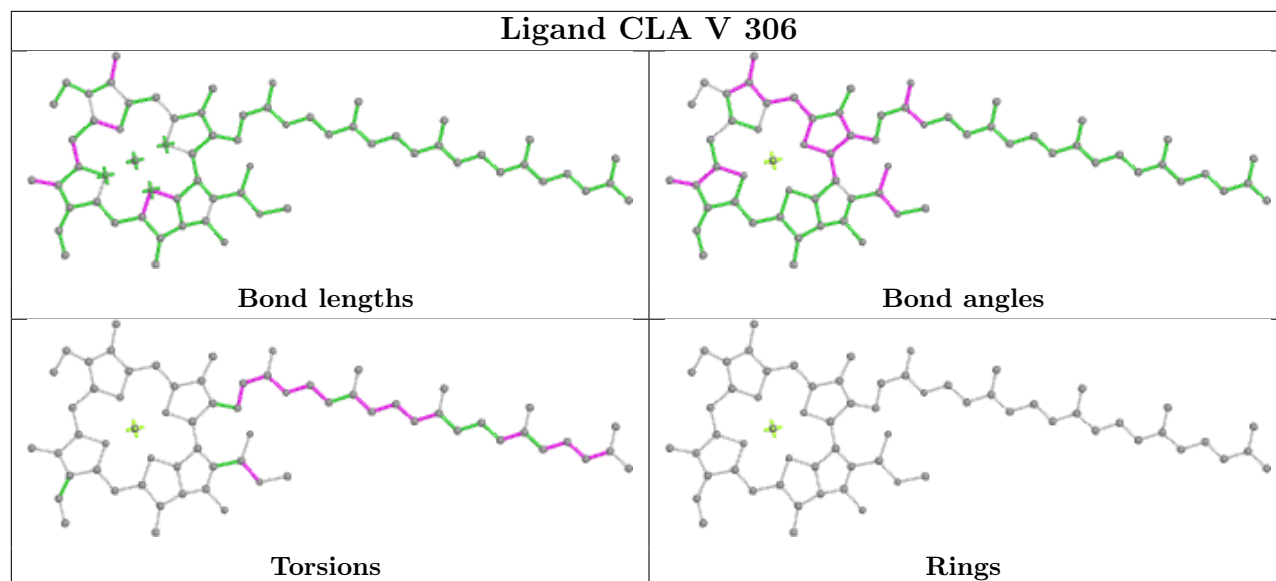
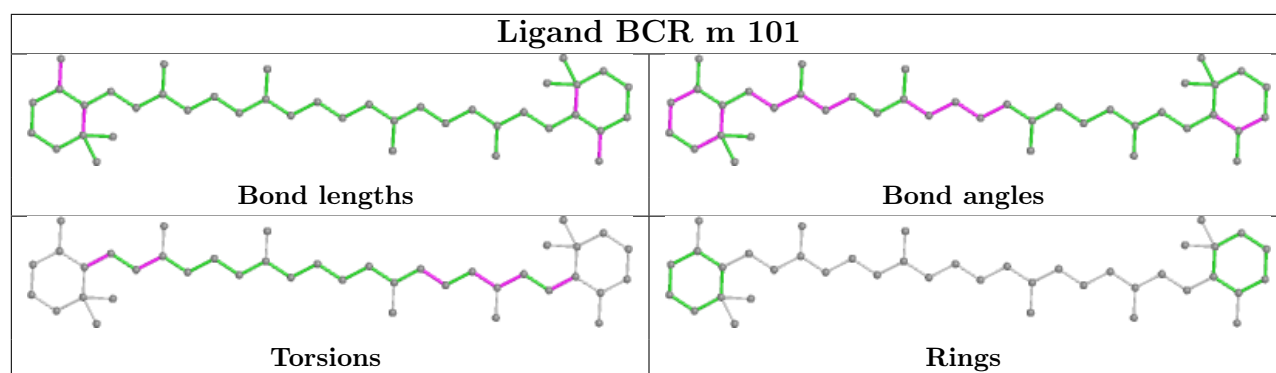


Torsions

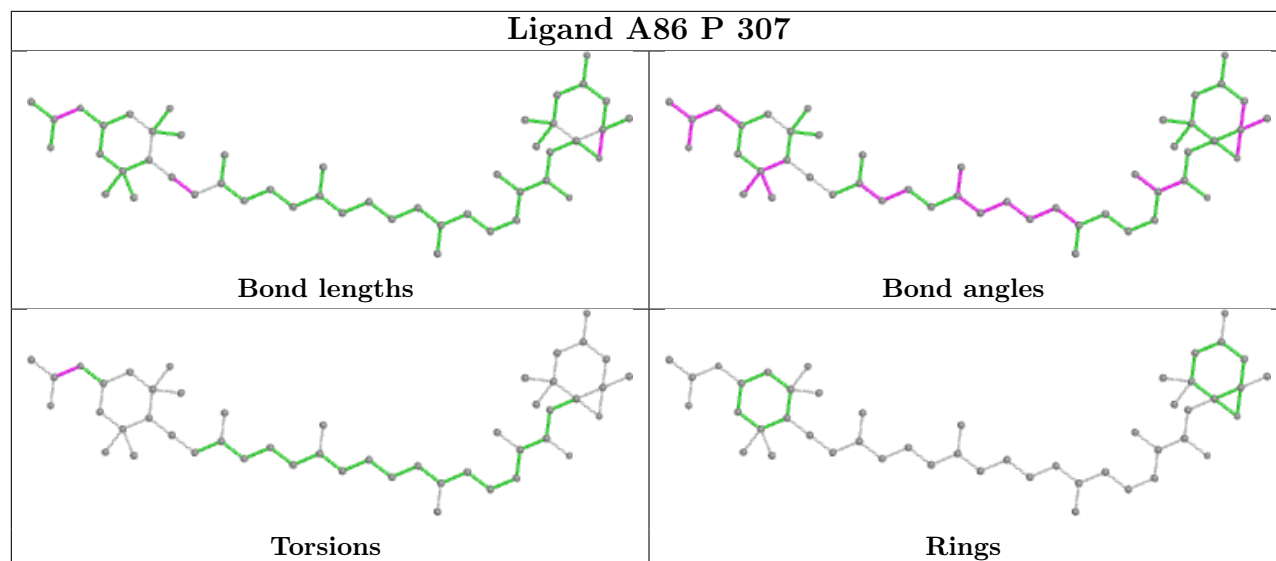


Rings

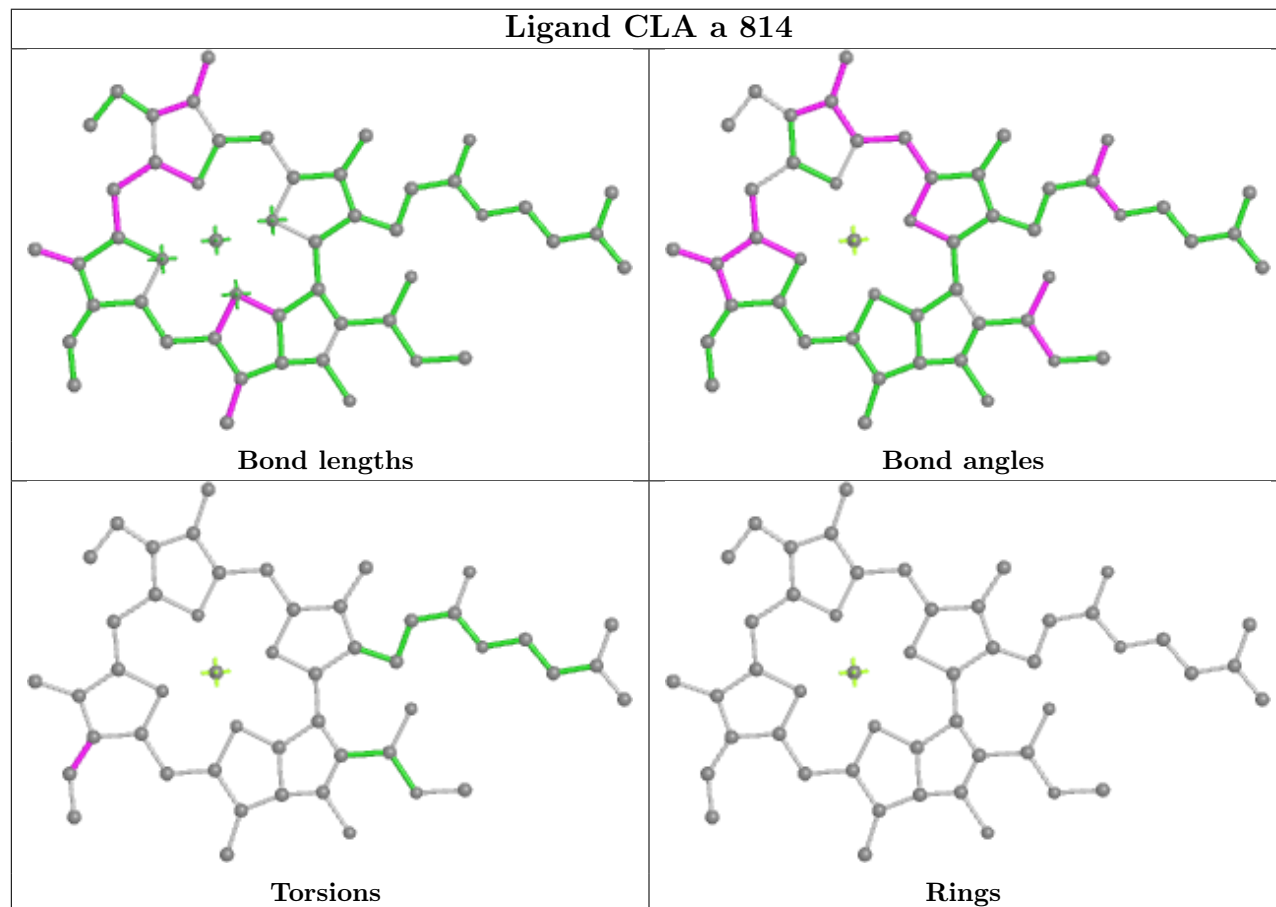


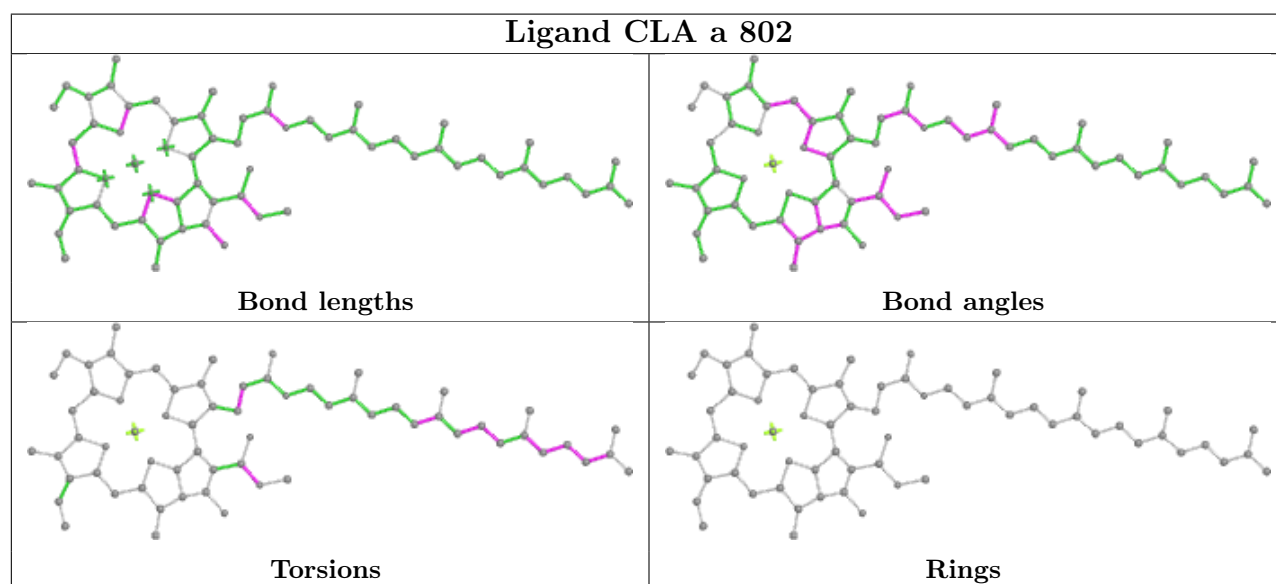
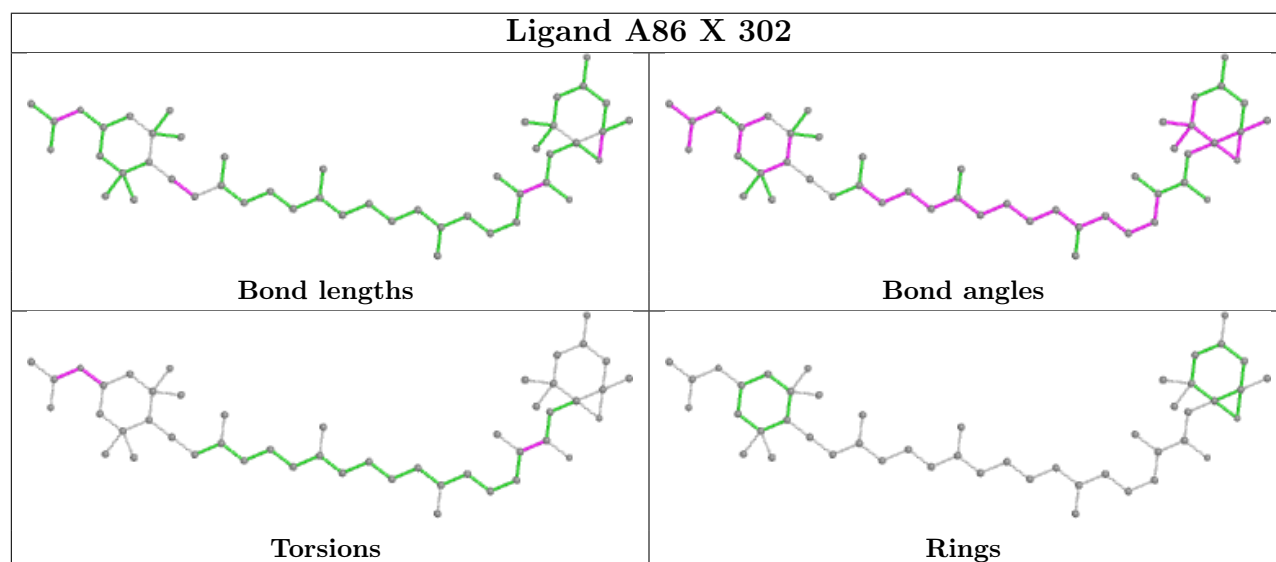
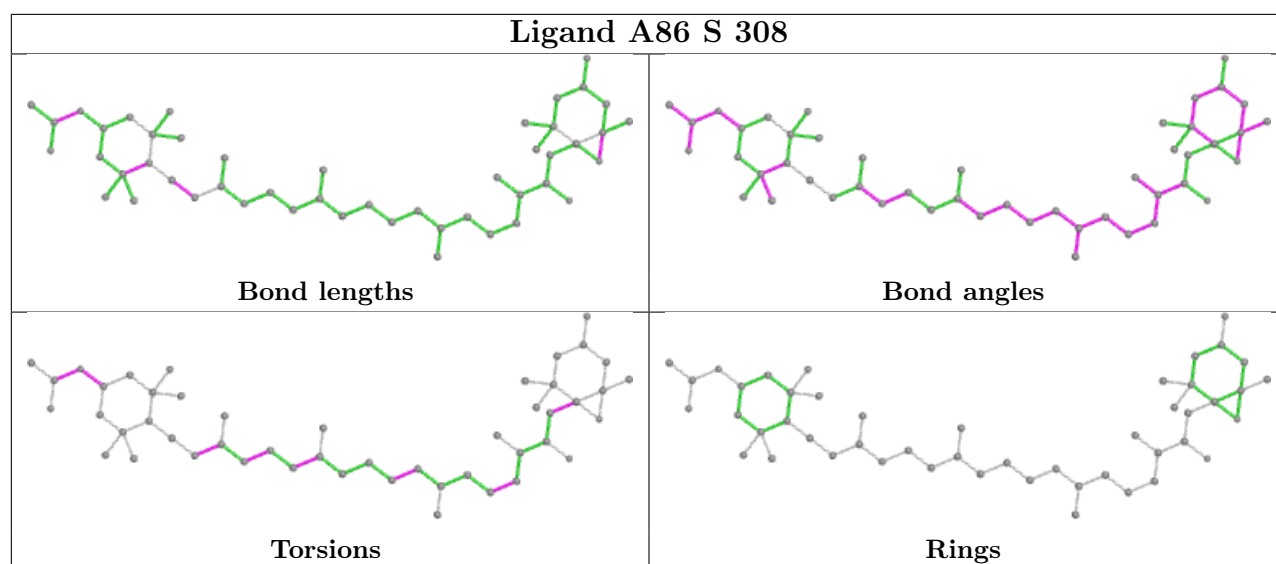


## Ligand A86 P 307

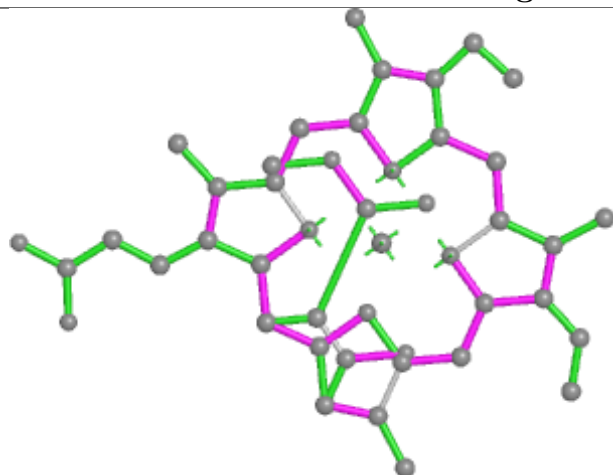


## Ligand CLA a 814

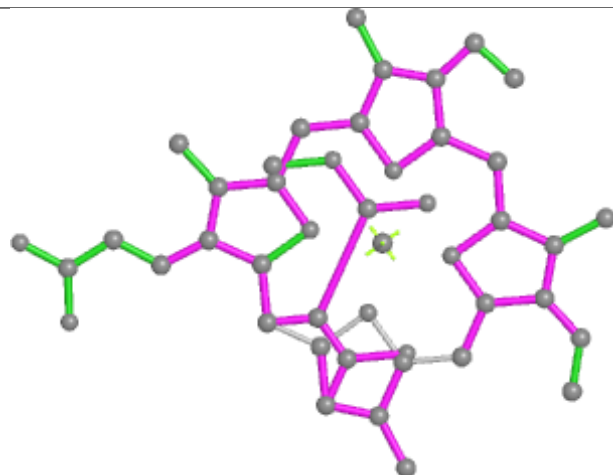




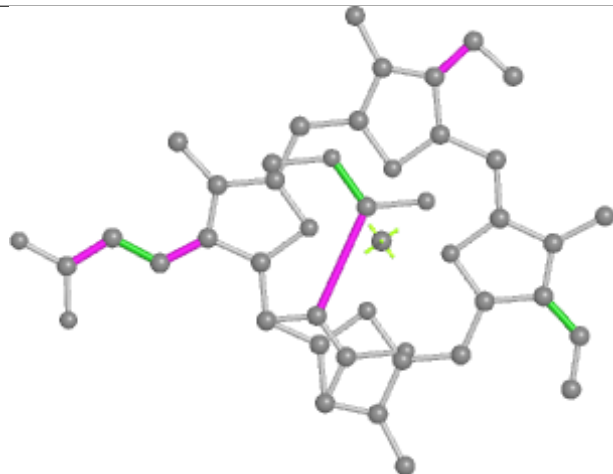
## Ligand KC1 C 213



Bond lengths



Bond angles

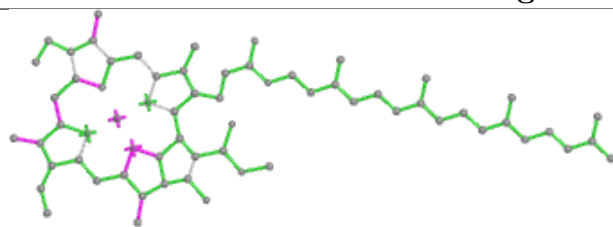


Torsions

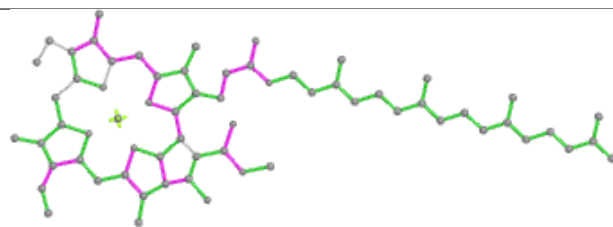


Rings

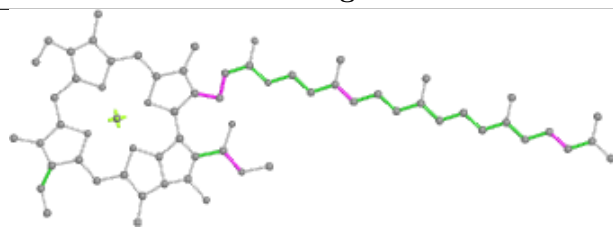
## Ligand CLA b 801



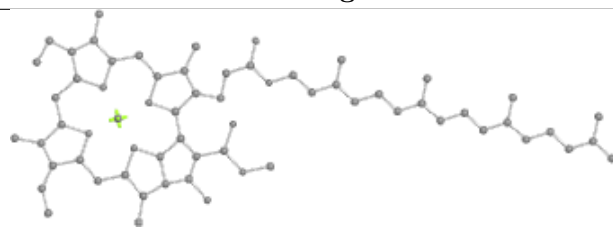
Bond lengths



Bond angles

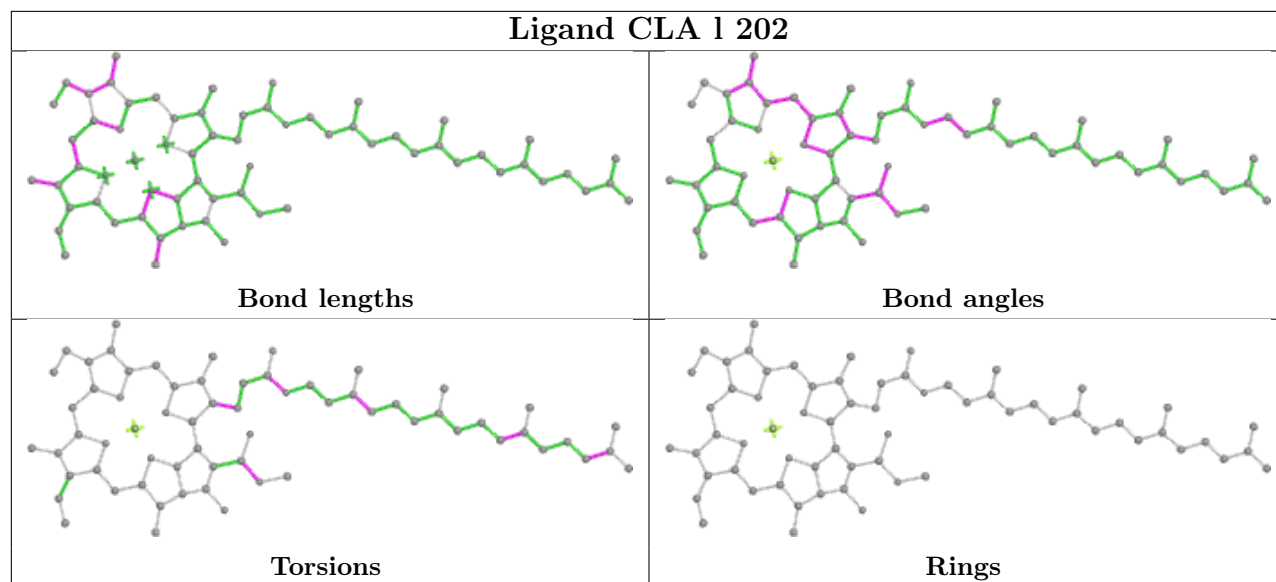


Torsions

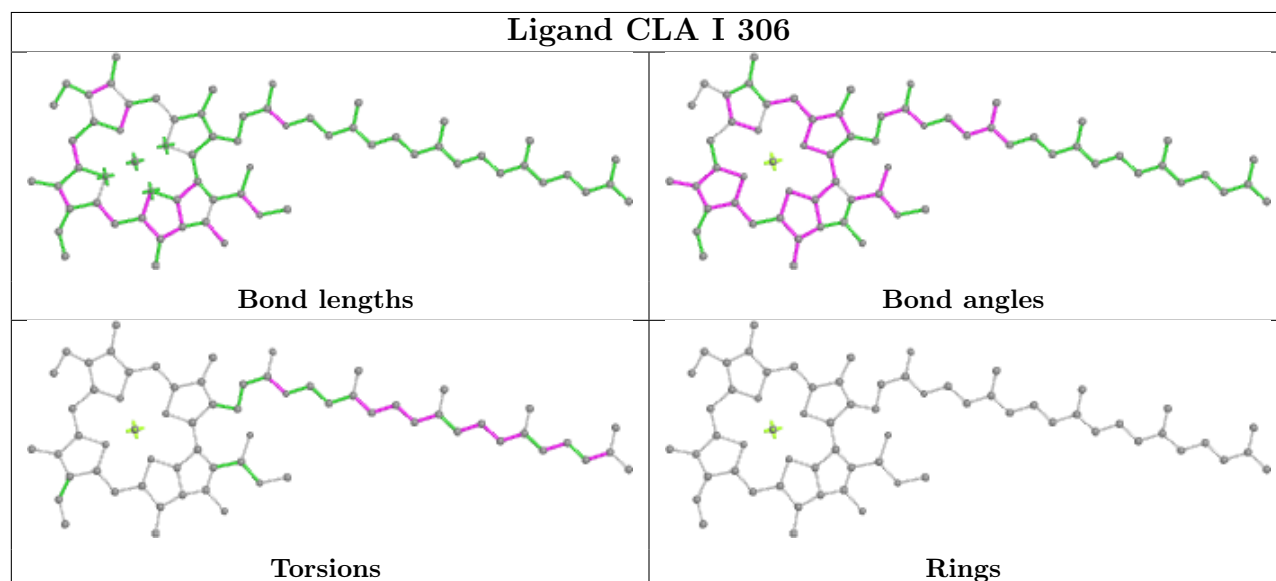


Rings

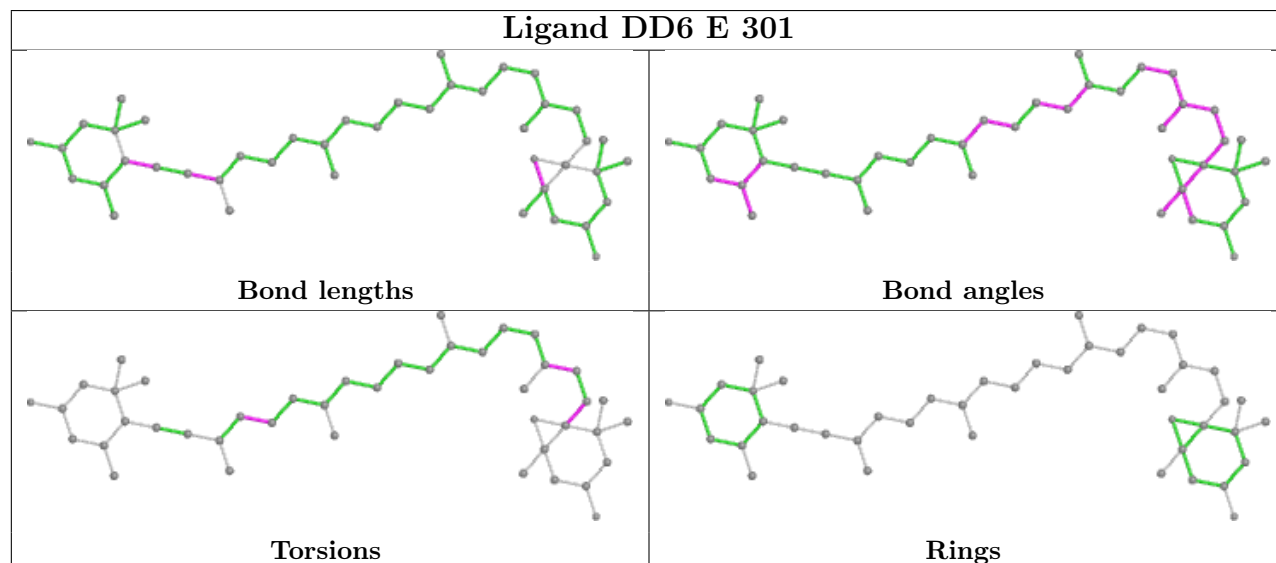
## Ligand CLA I 202

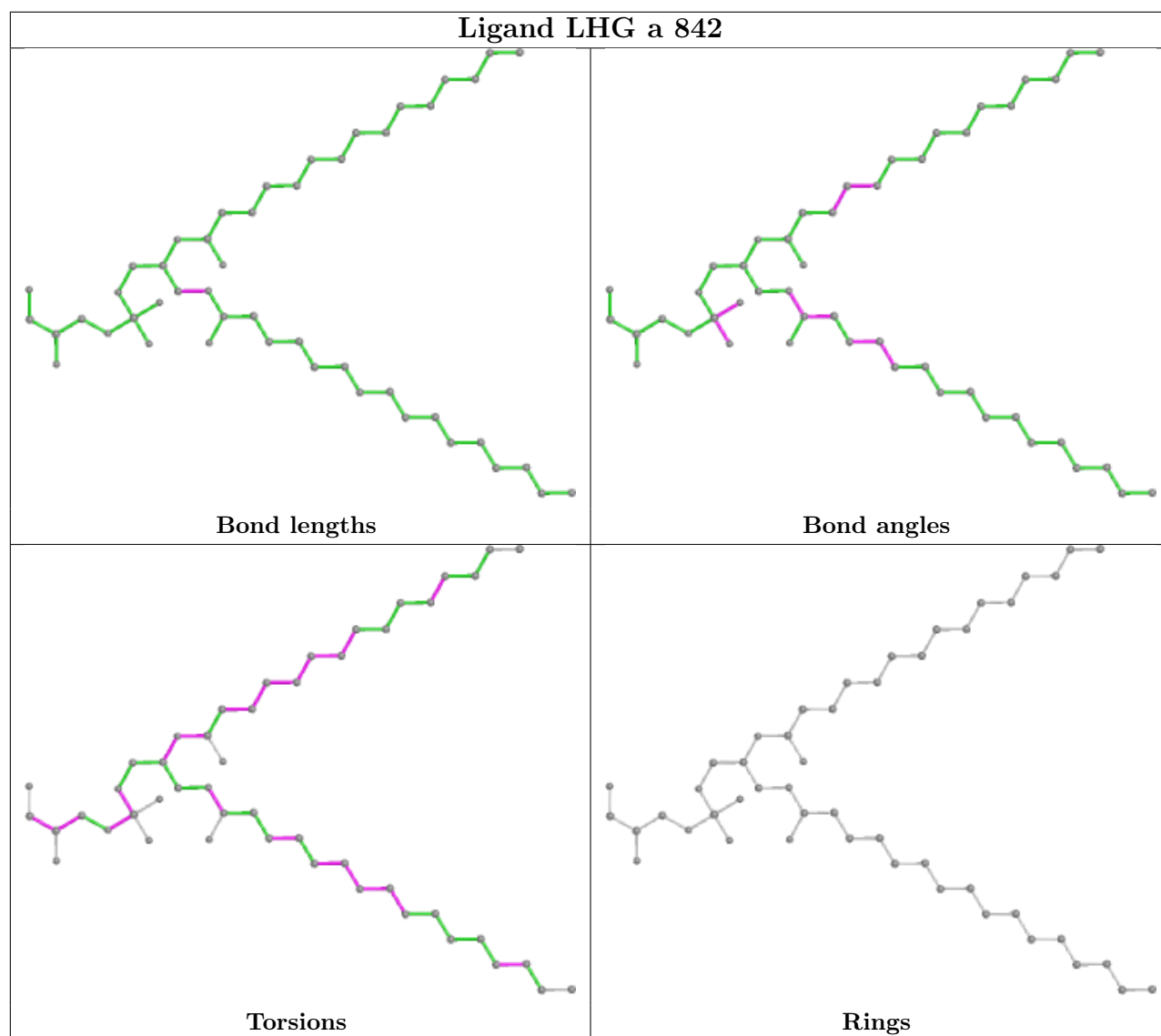
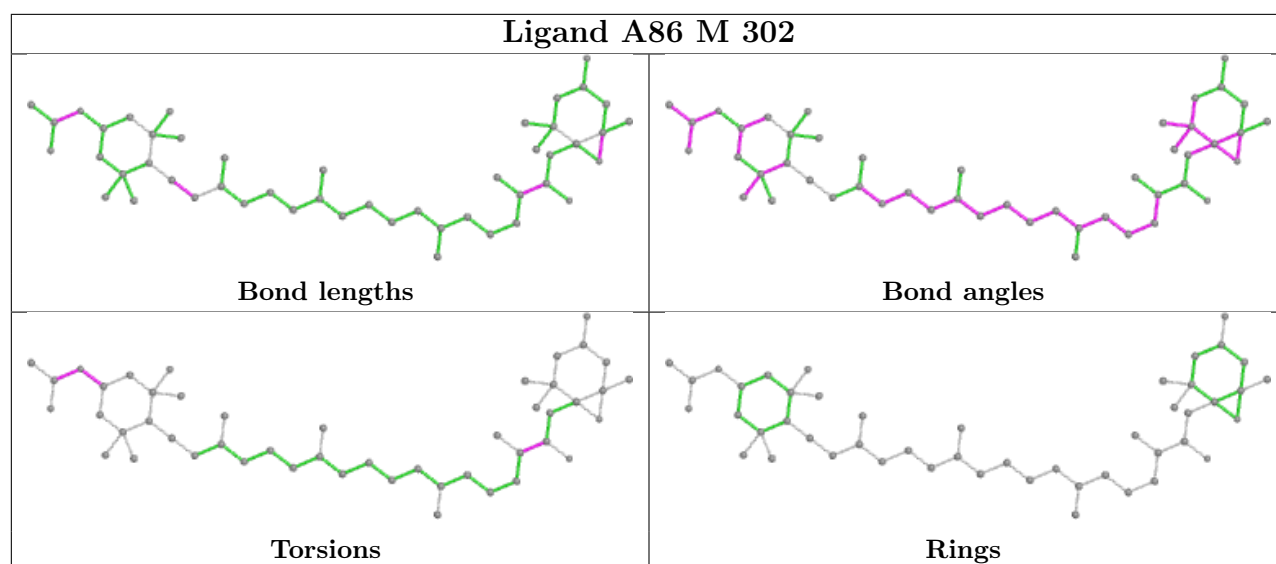


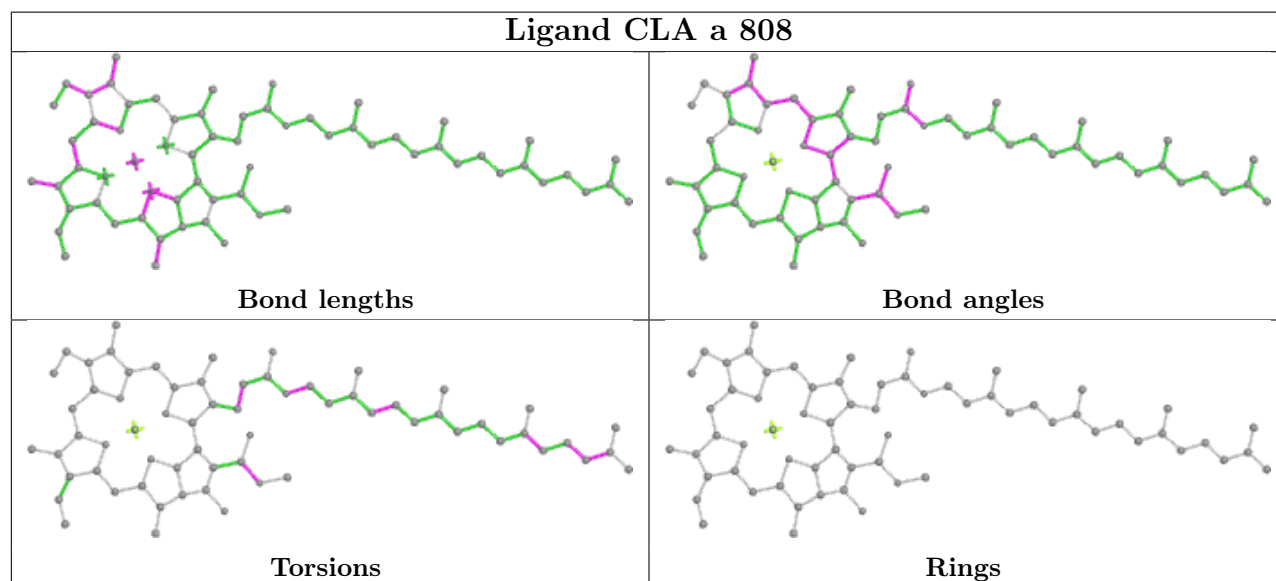
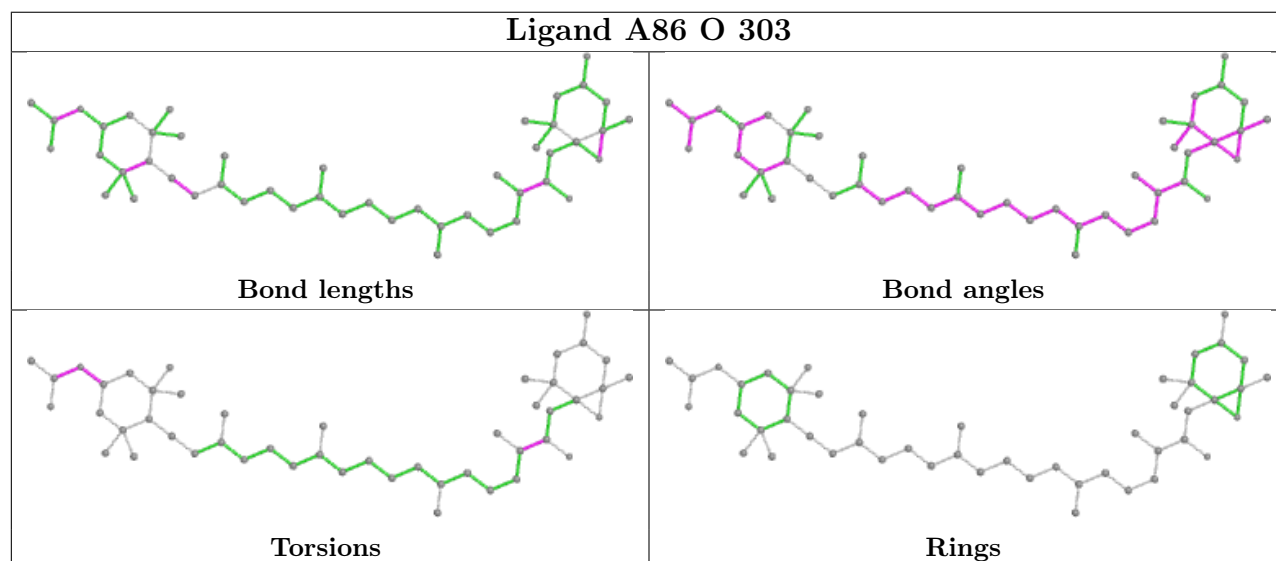
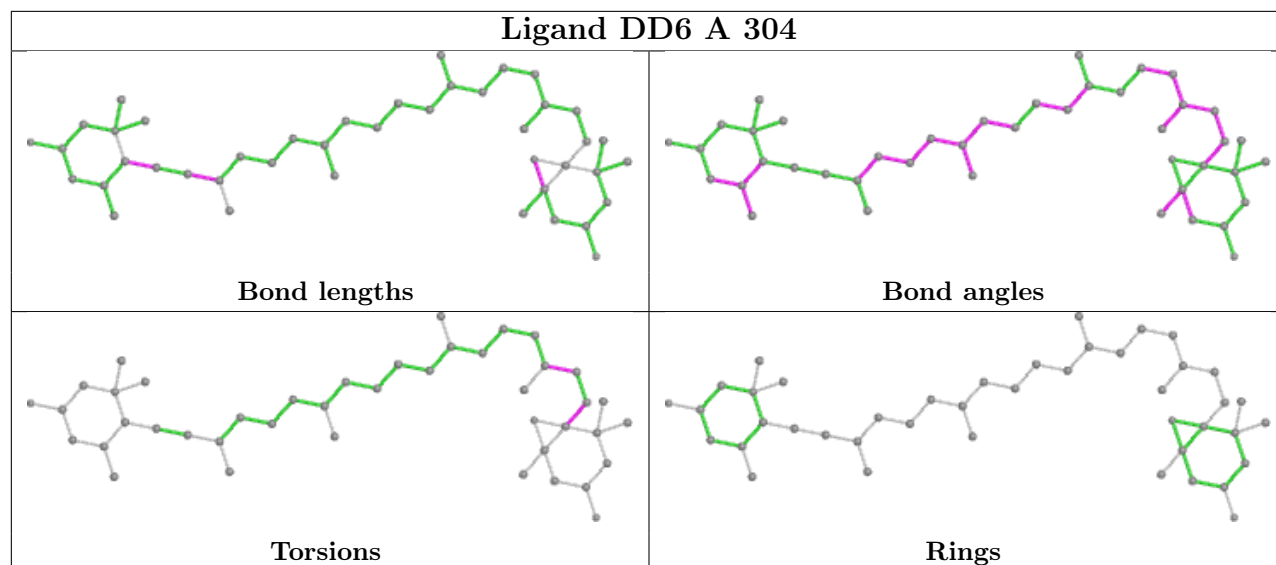
## Ligand CLA I 306



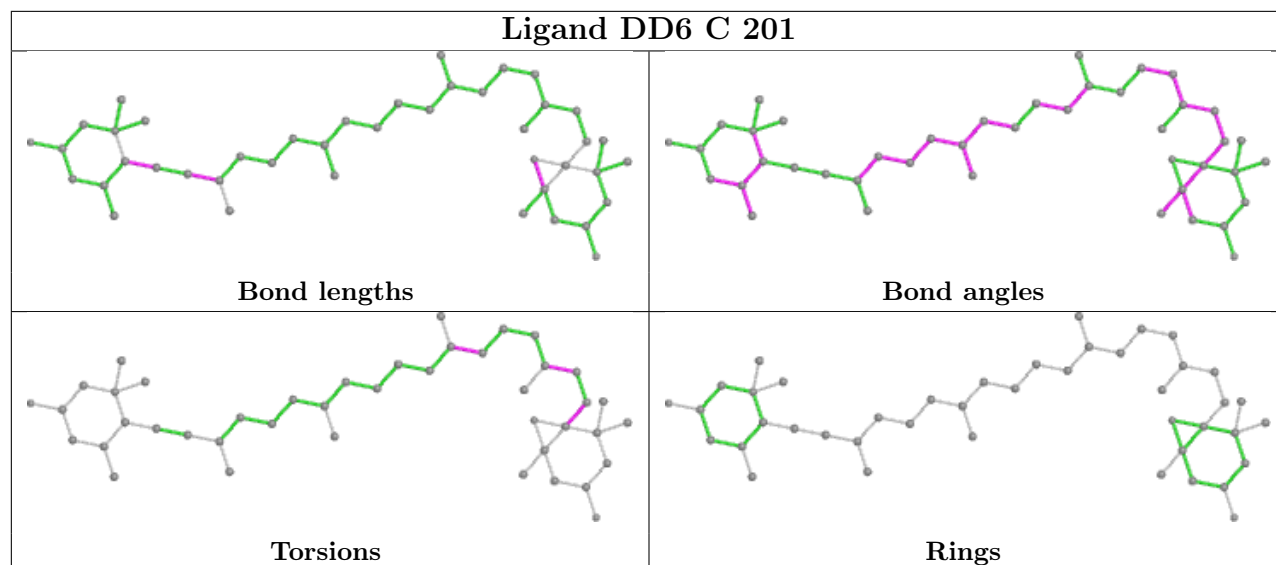
## Ligand DD6 E 301



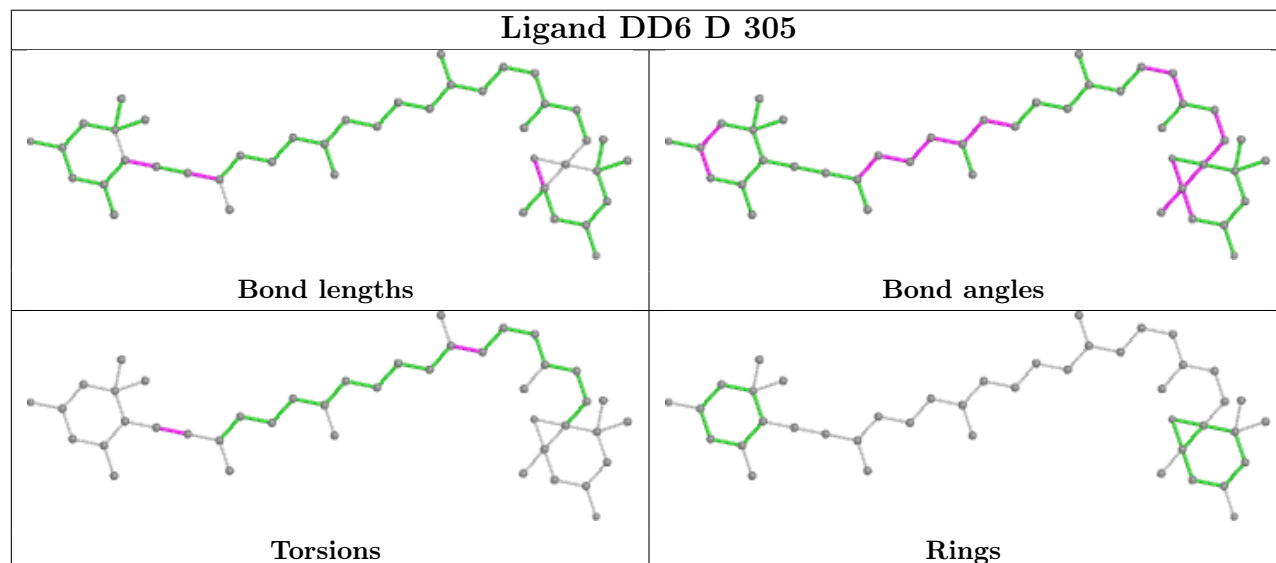




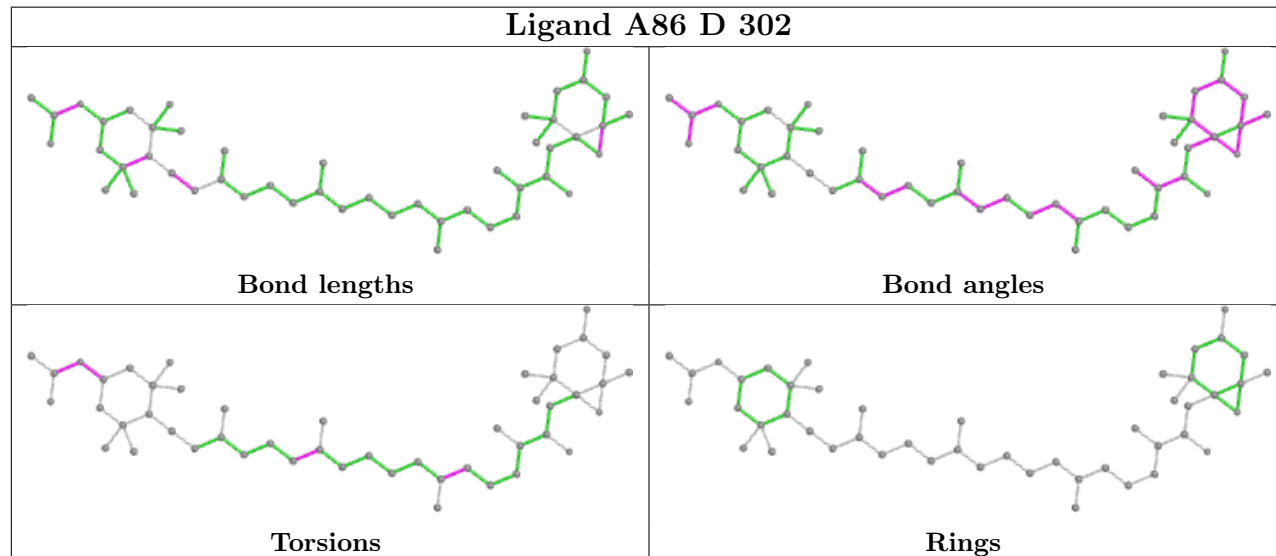
## Ligand DD6 C 201



## Ligand DD6 D 305

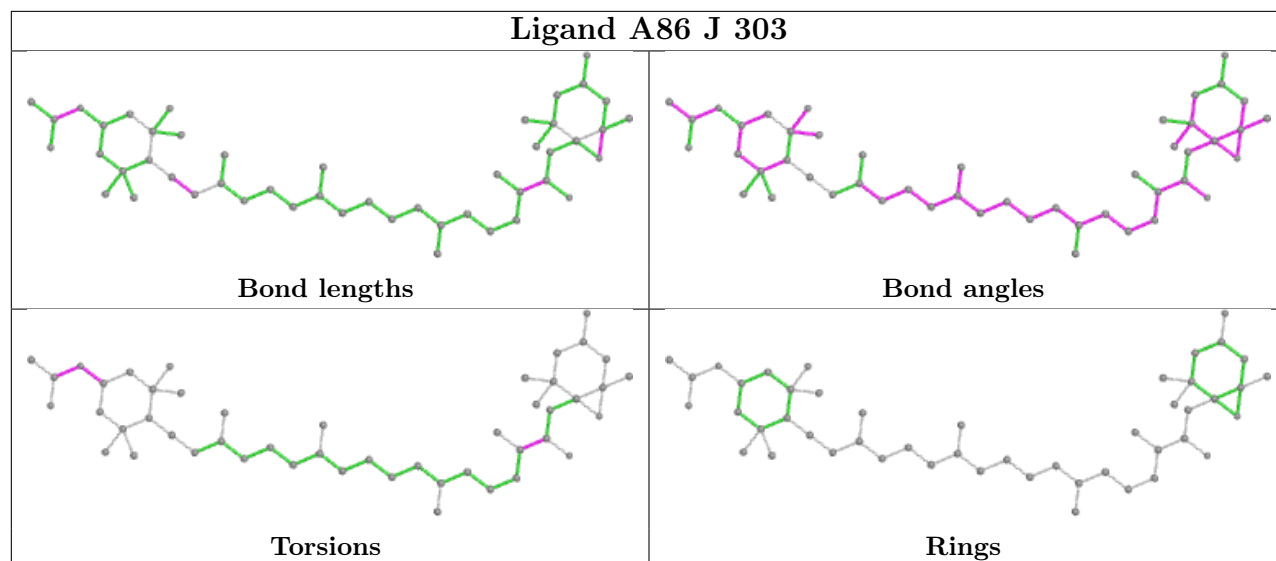


## Ligand A86 D 302

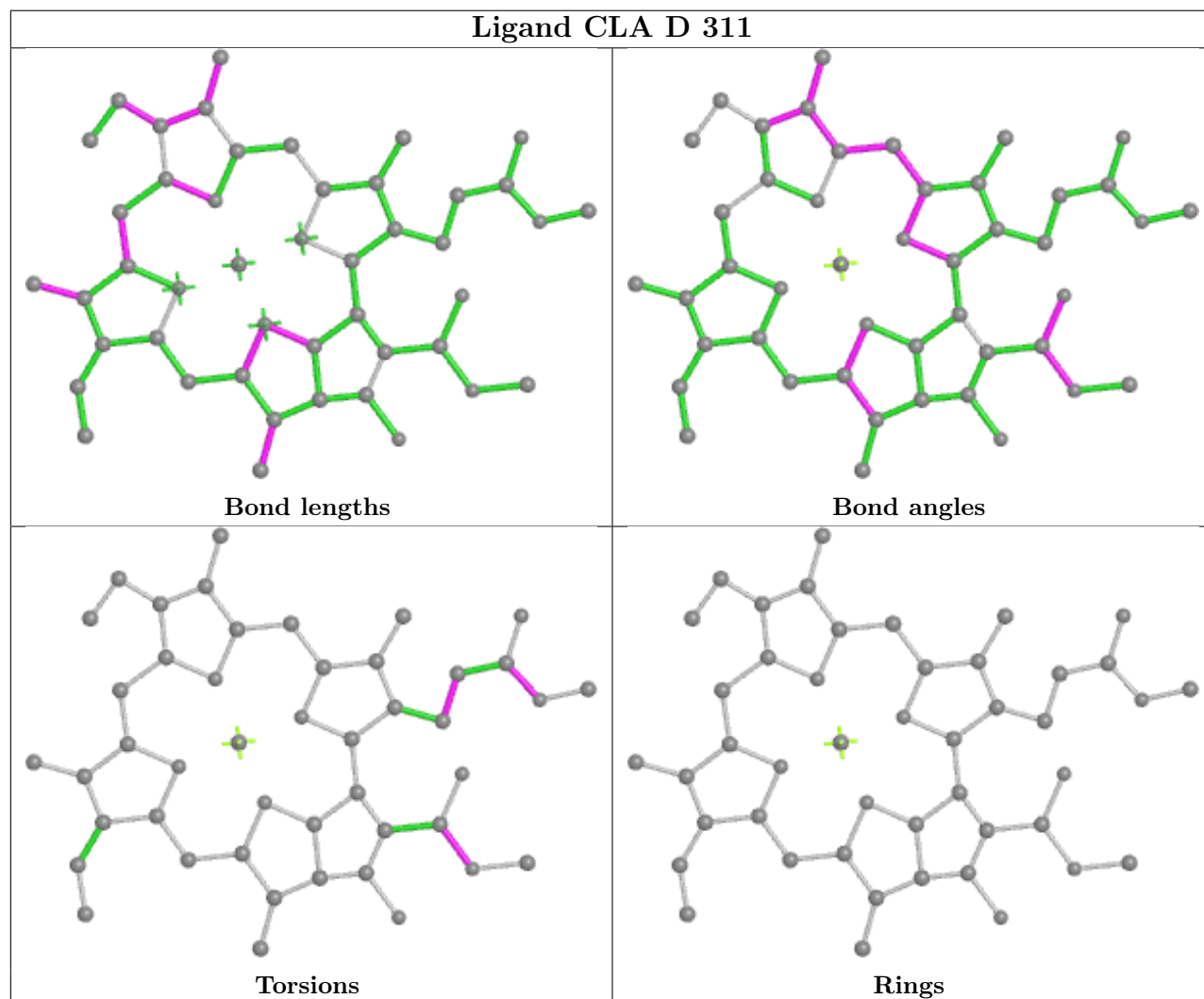




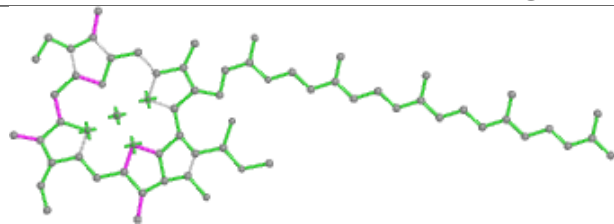
## Ligand A86 J 303



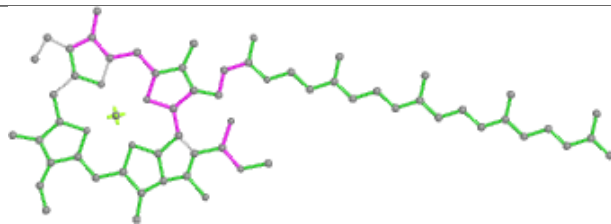
## Ligand CLA D 311



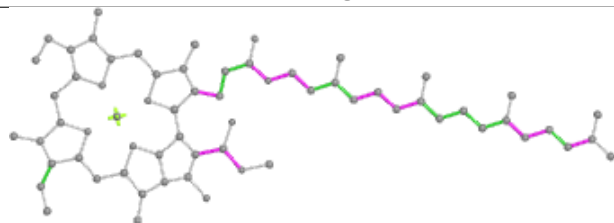
## Ligand CLA i 102



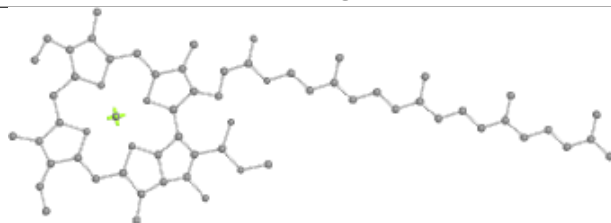
Bond lengths



Bond angles

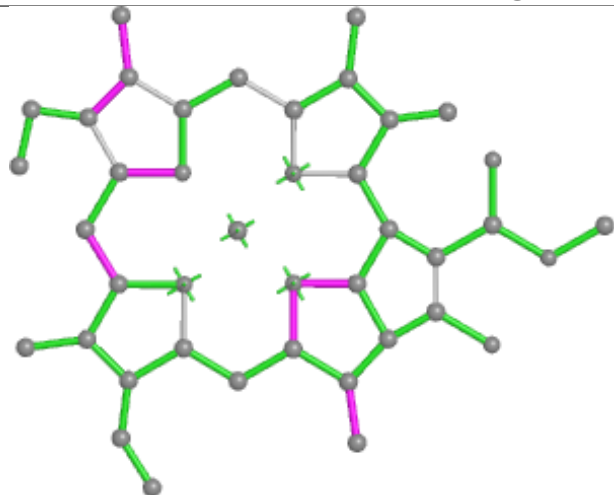


Torsions

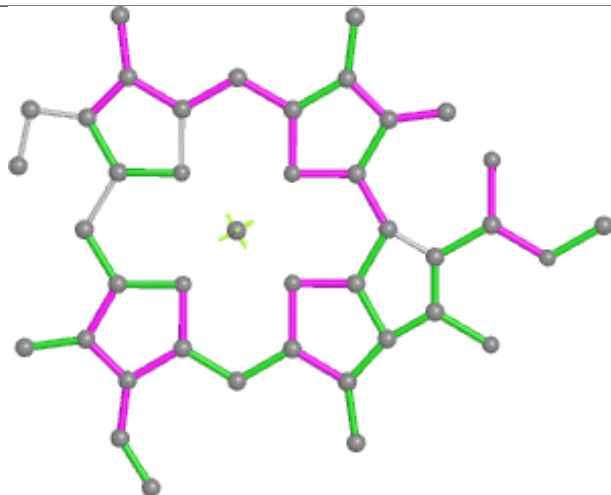


Rings

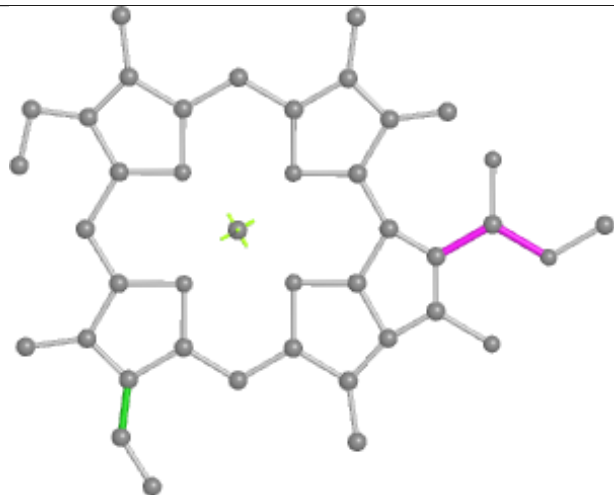
## Ligand CLA W 214



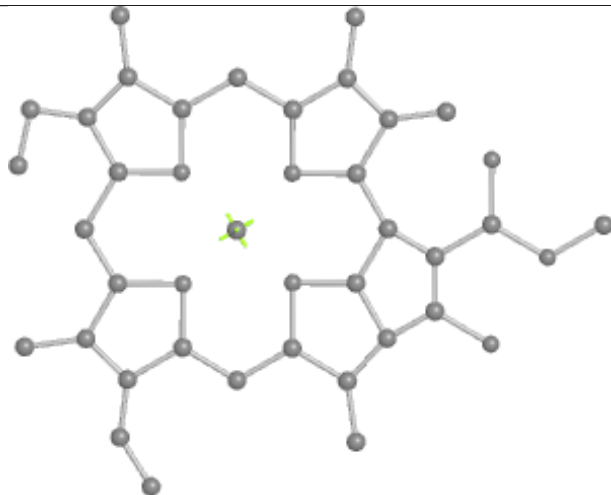
Bond lengths



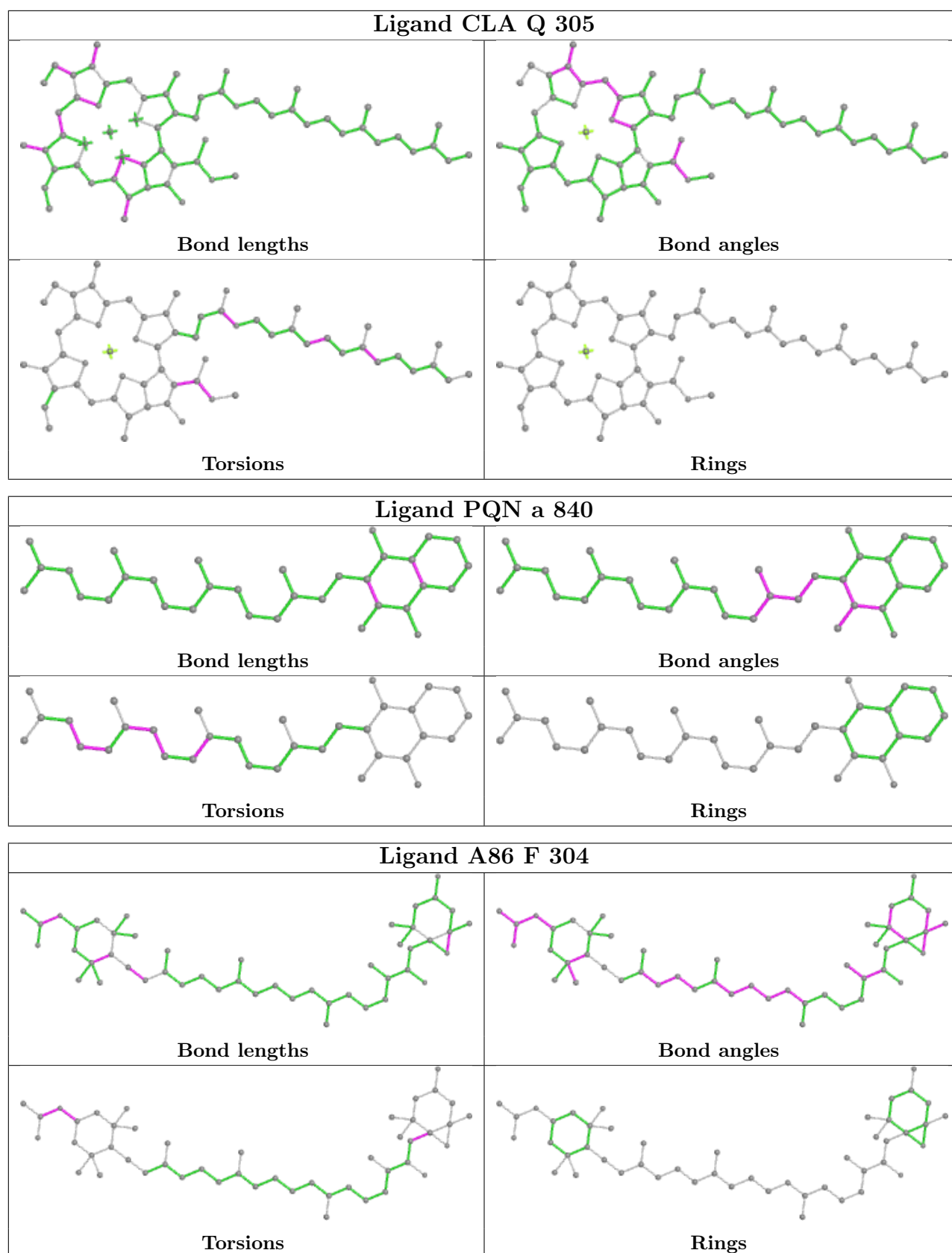
Bond angles

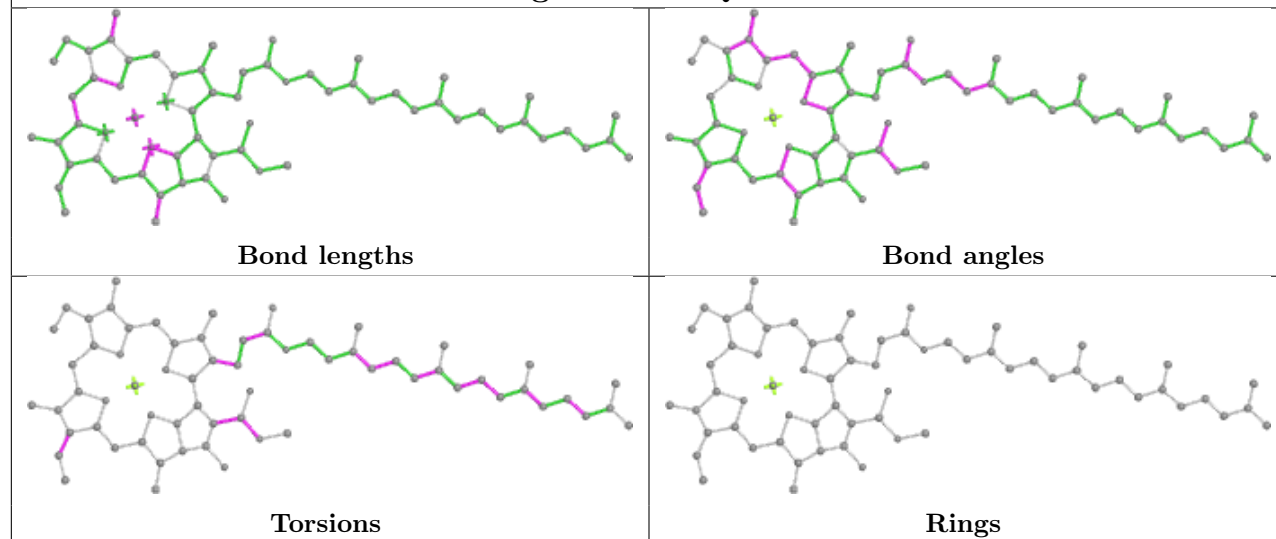
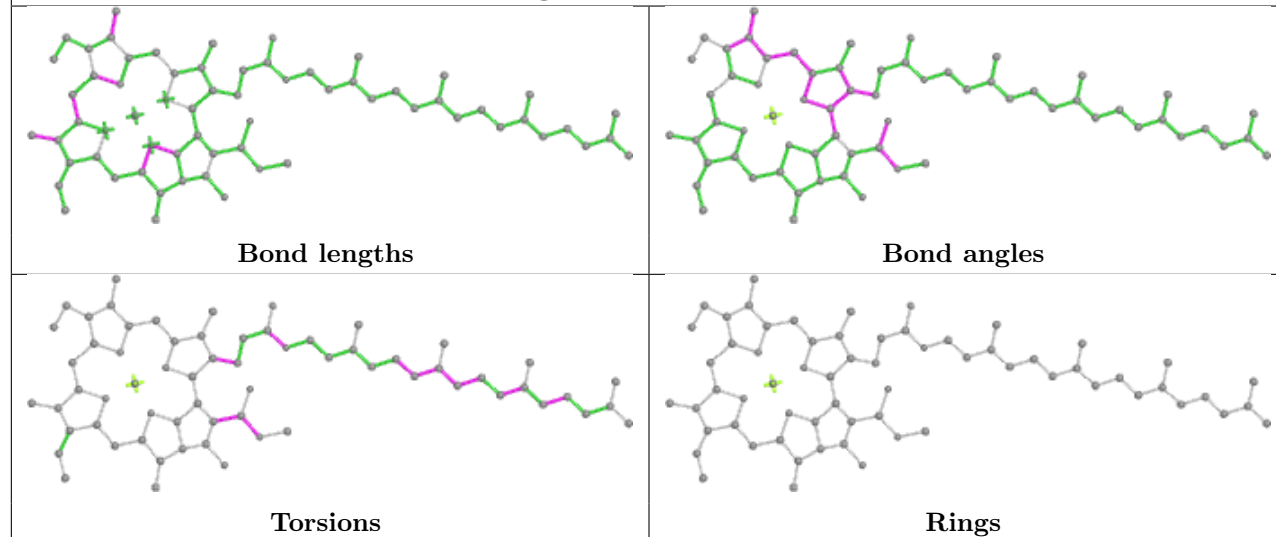


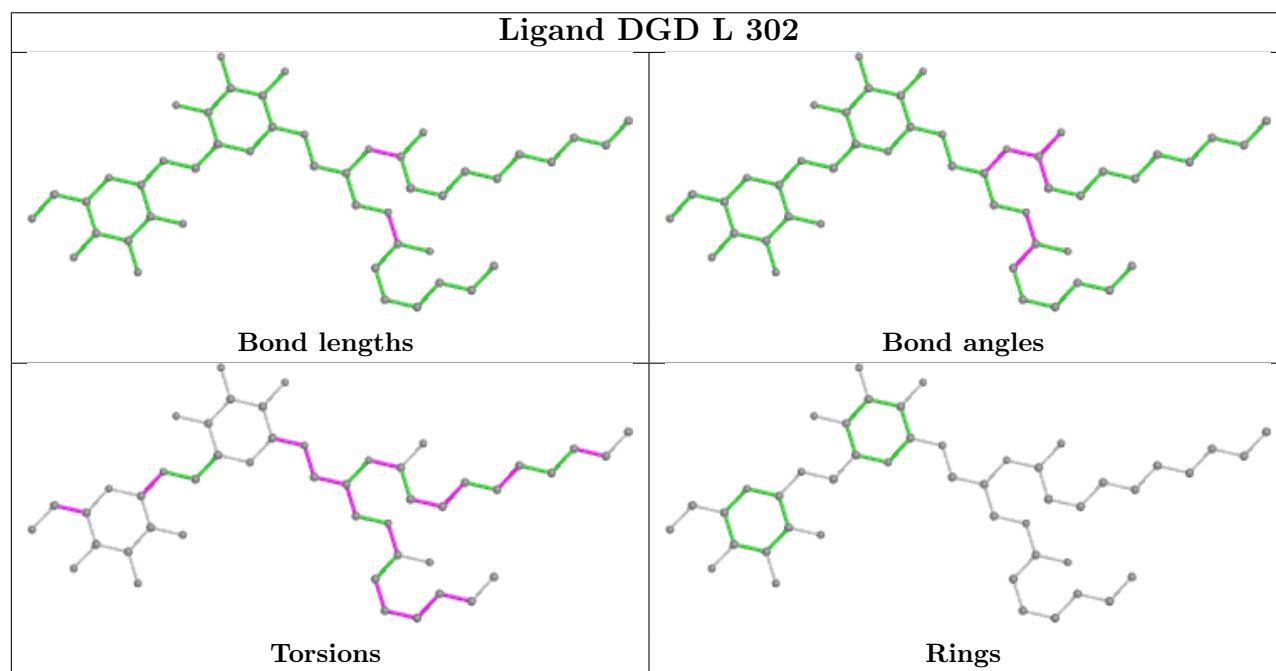
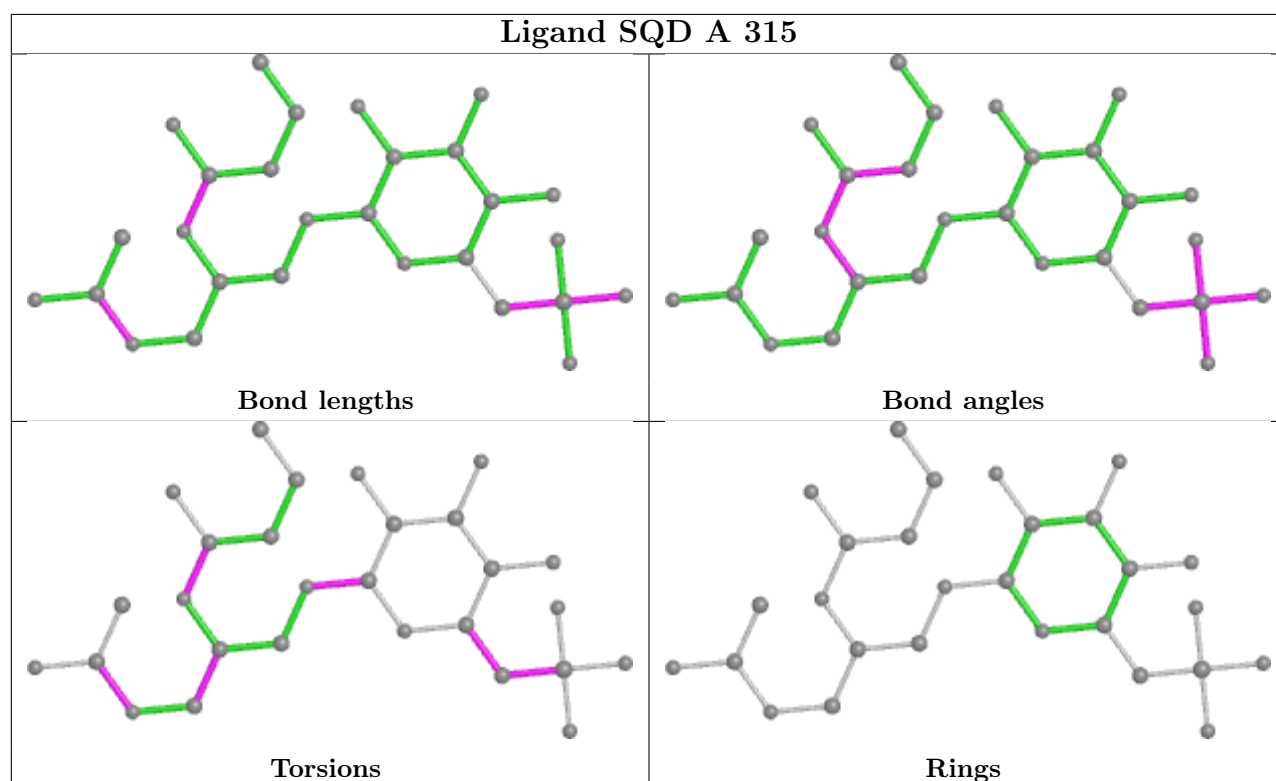
Torsions



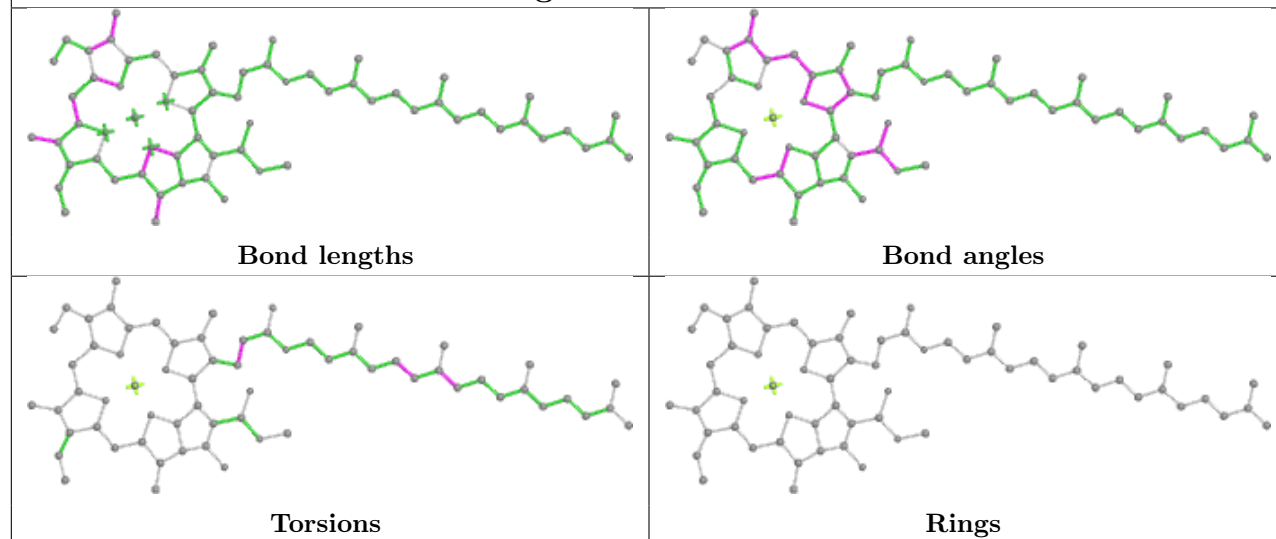
Rings



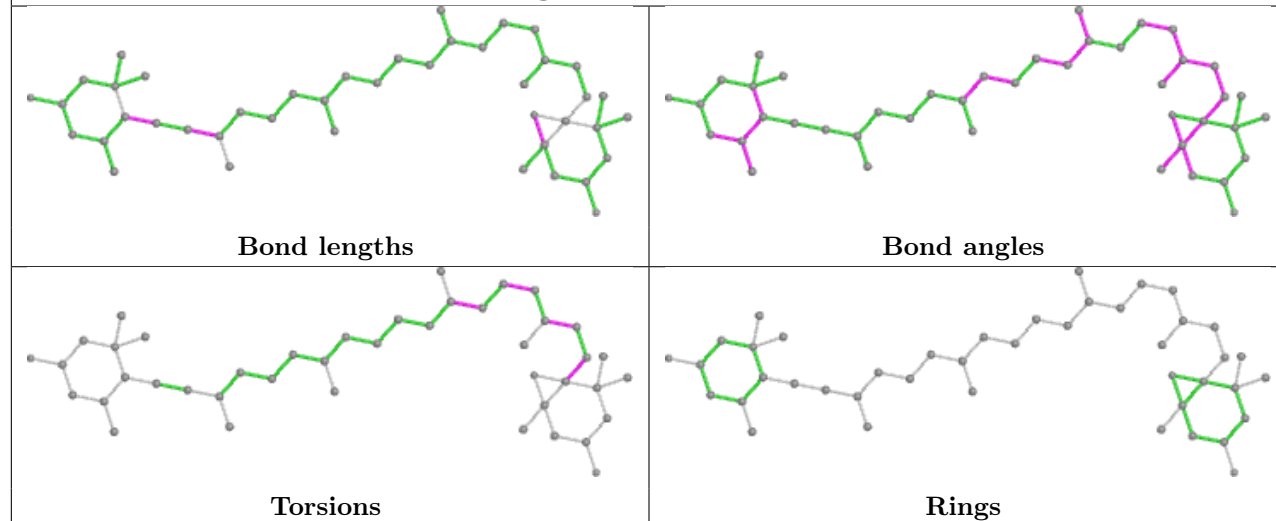
**Ligand CLA Q 308****Ligand CLA S 320**



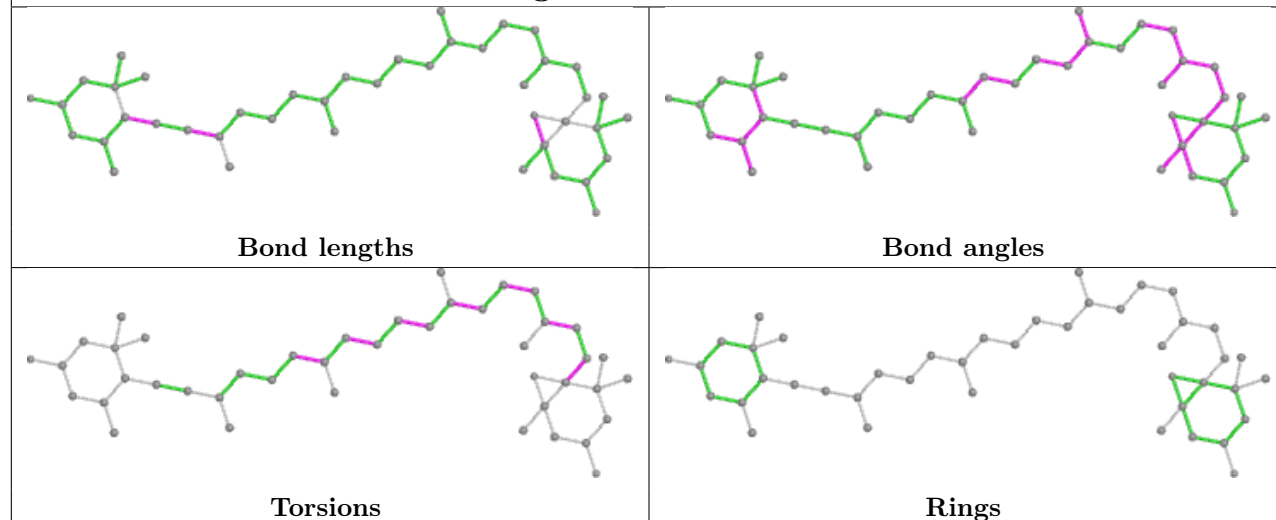
## Ligand CLA b 839



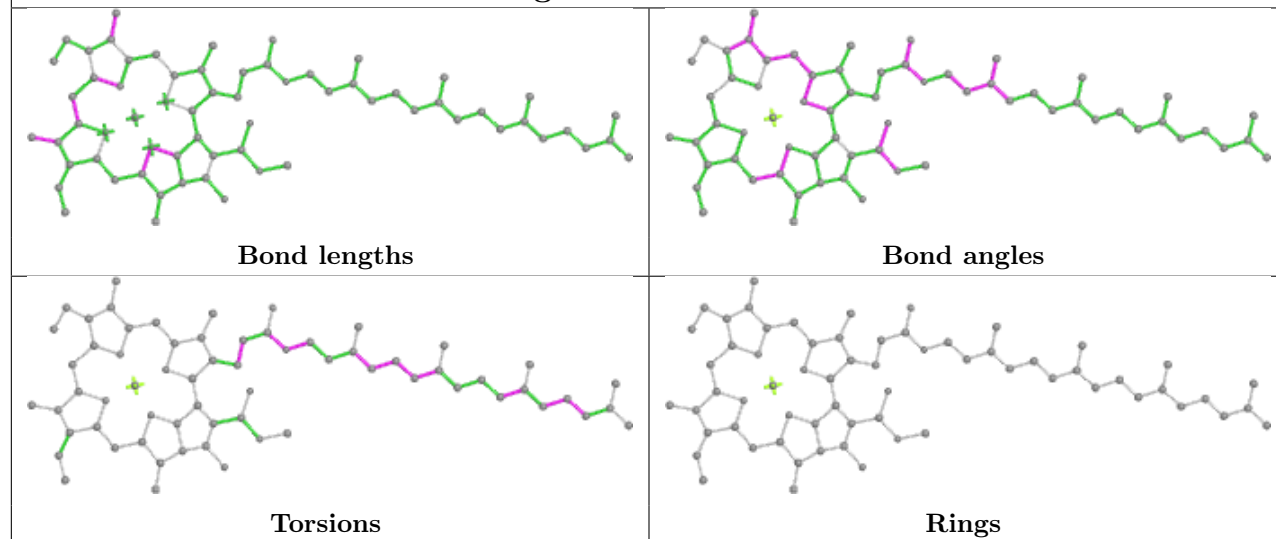
## Ligand DD6 F 303



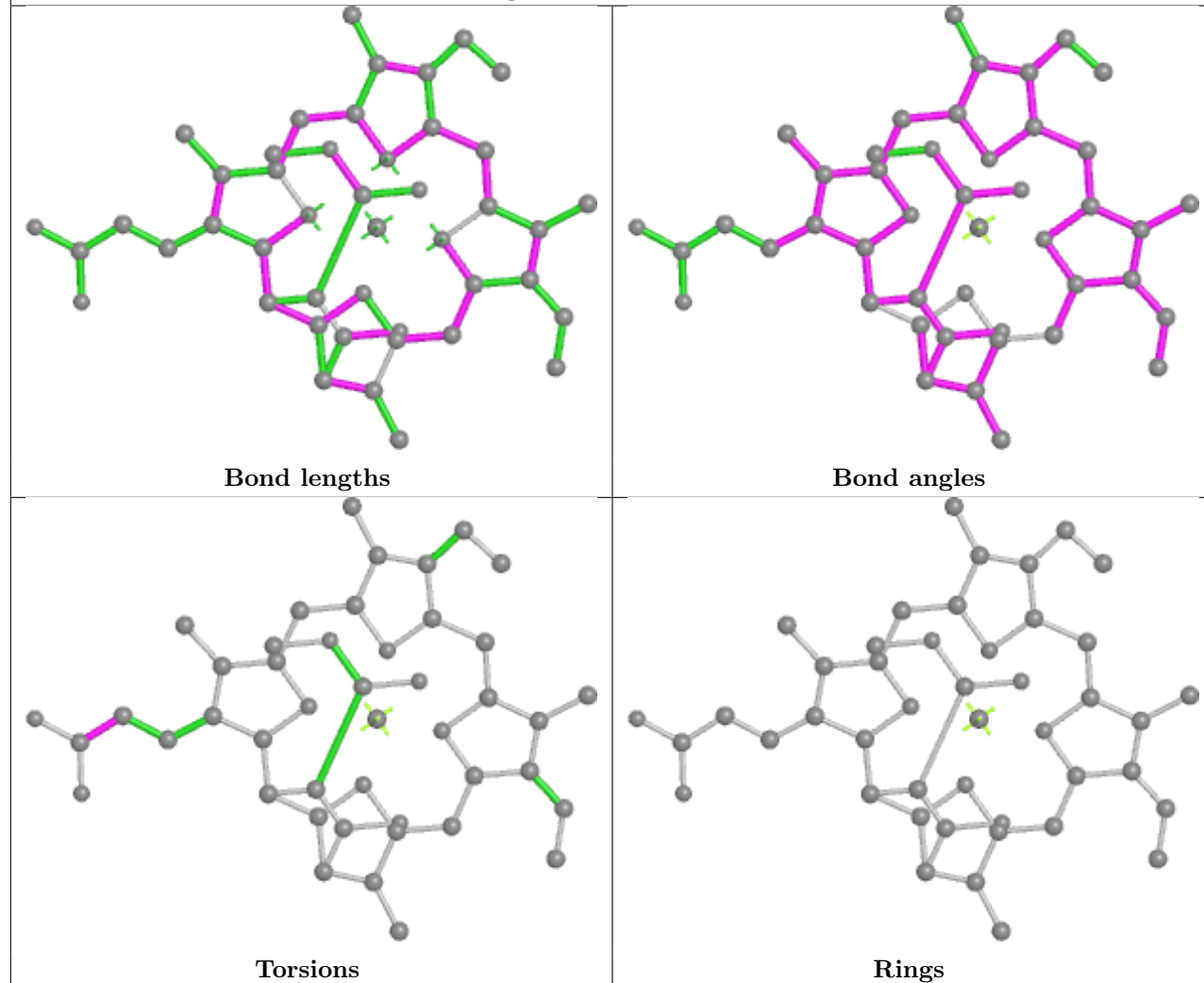
## Ligand DD6 R 308

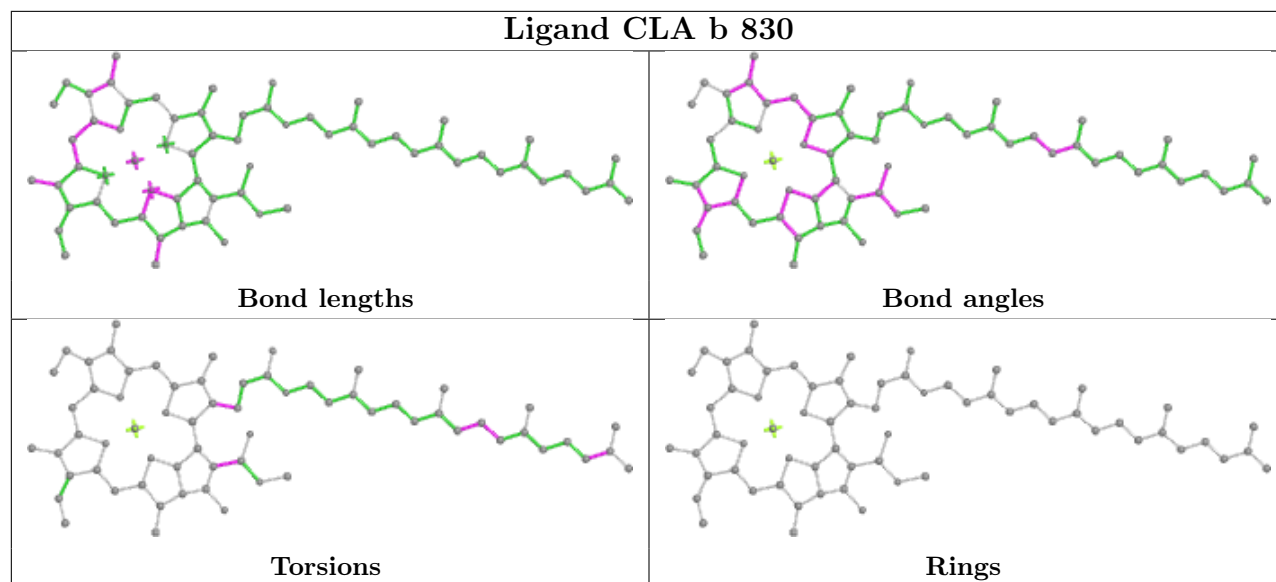
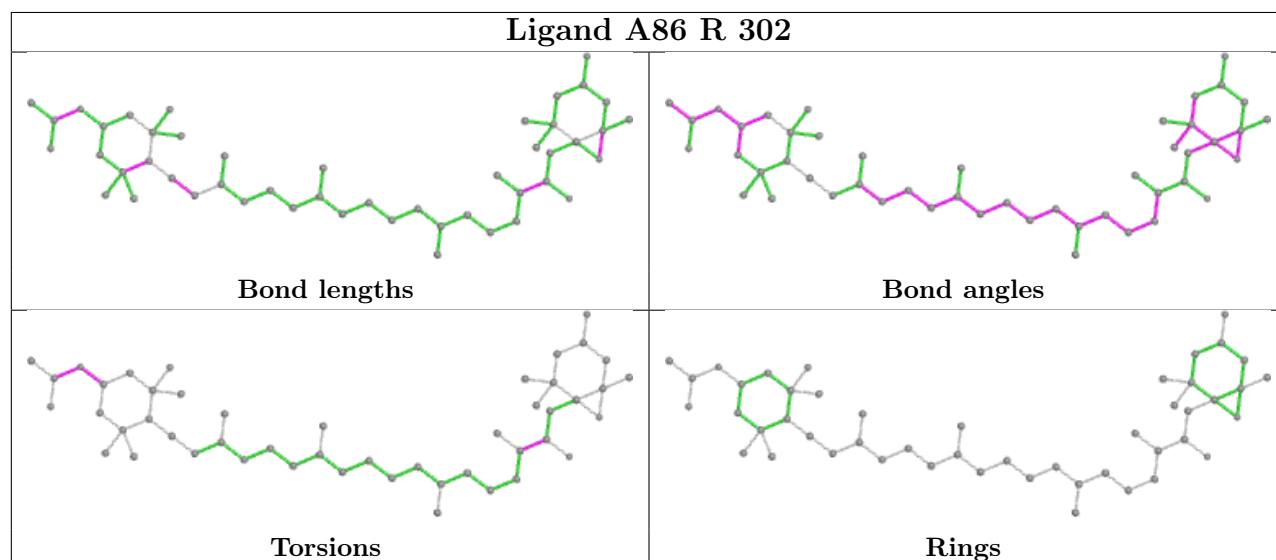


## Ligand CLA F 309



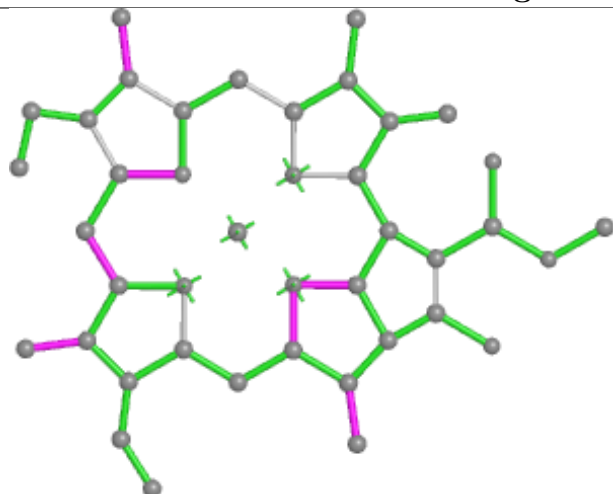
## Ligand KC1 A 312



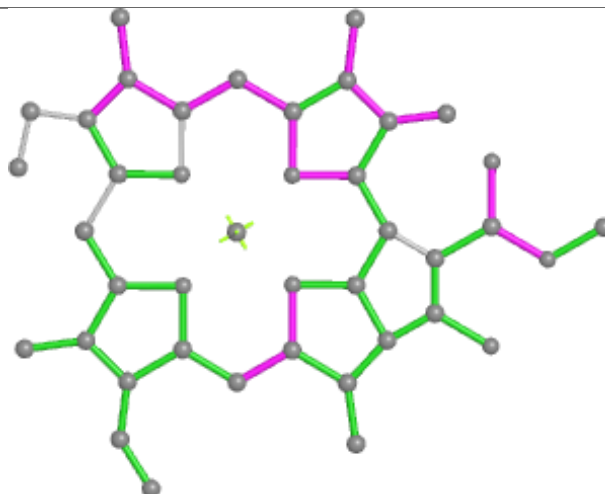
**Ligand CLA b 830****Ligand A86 R 302**



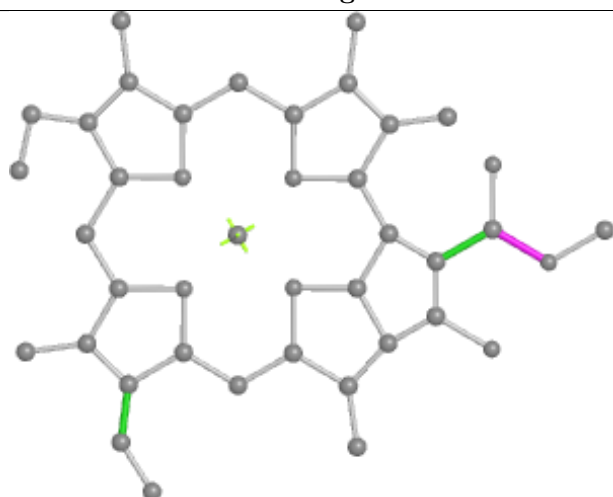
## Ligand CLA R 318



Bond lengths



Bond angles

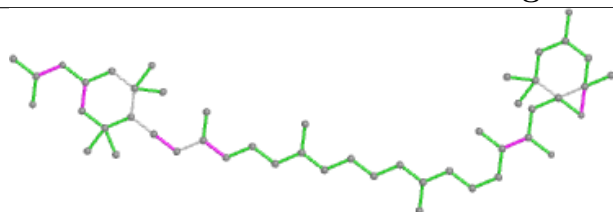


Torsions

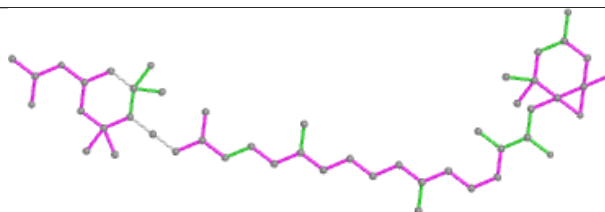


Rings

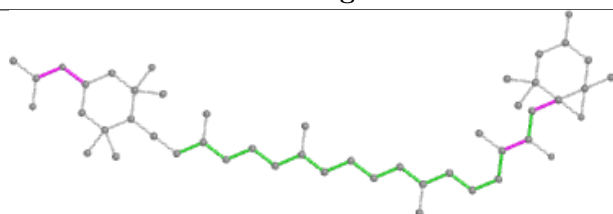
## Ligand A86 L 319



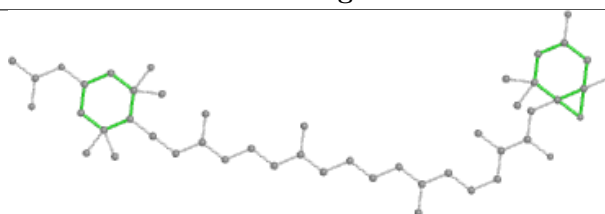
Bond lengths



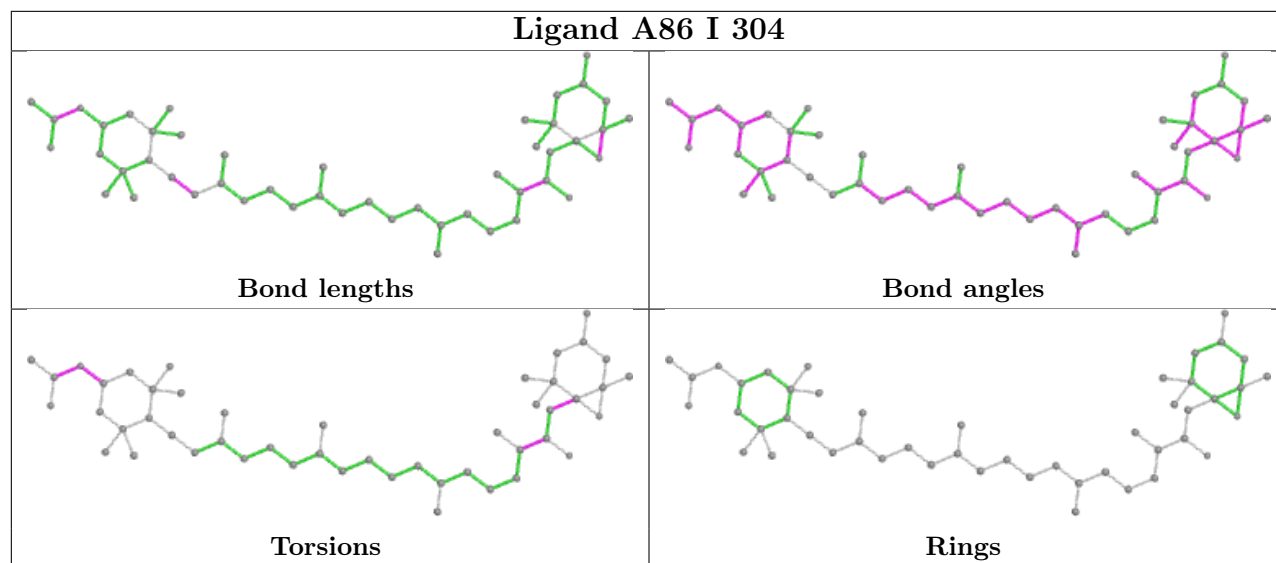
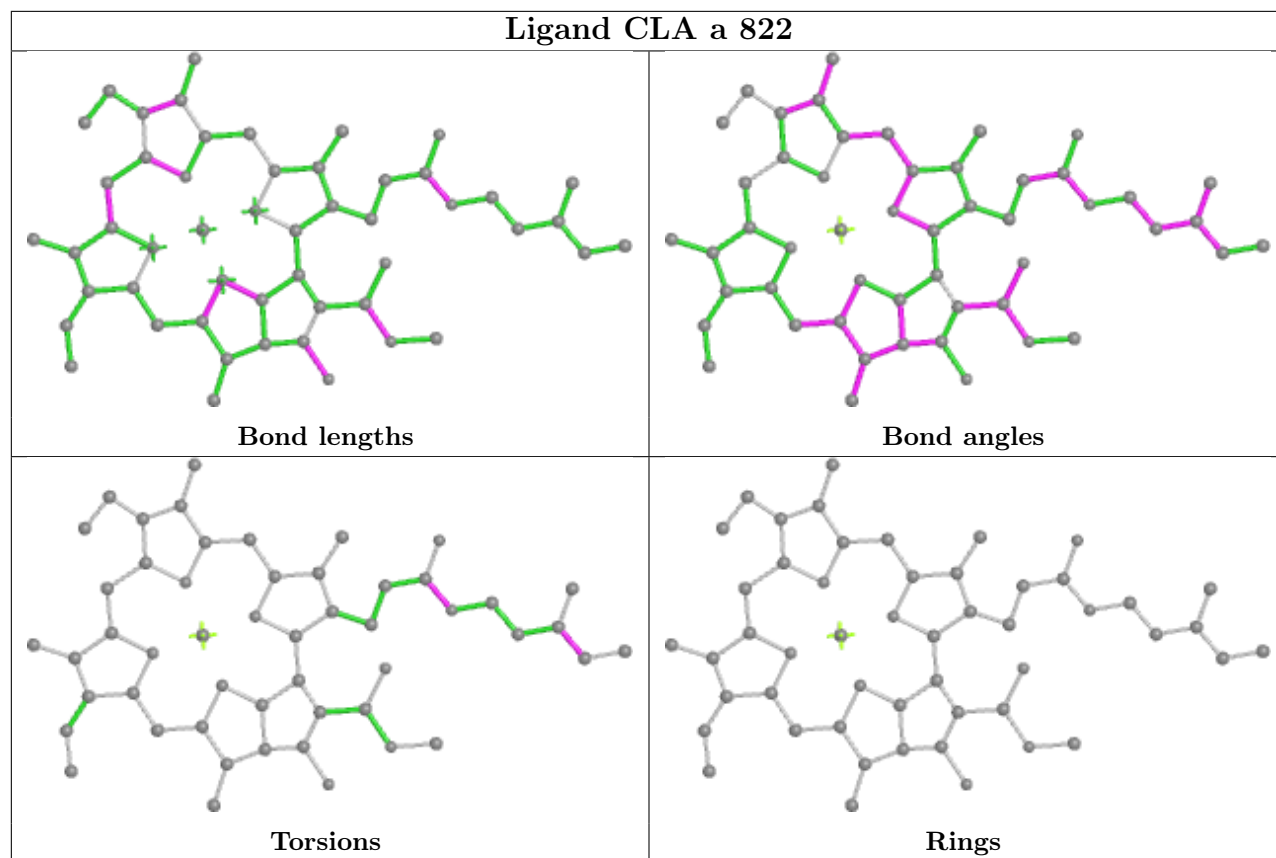
Bond angles

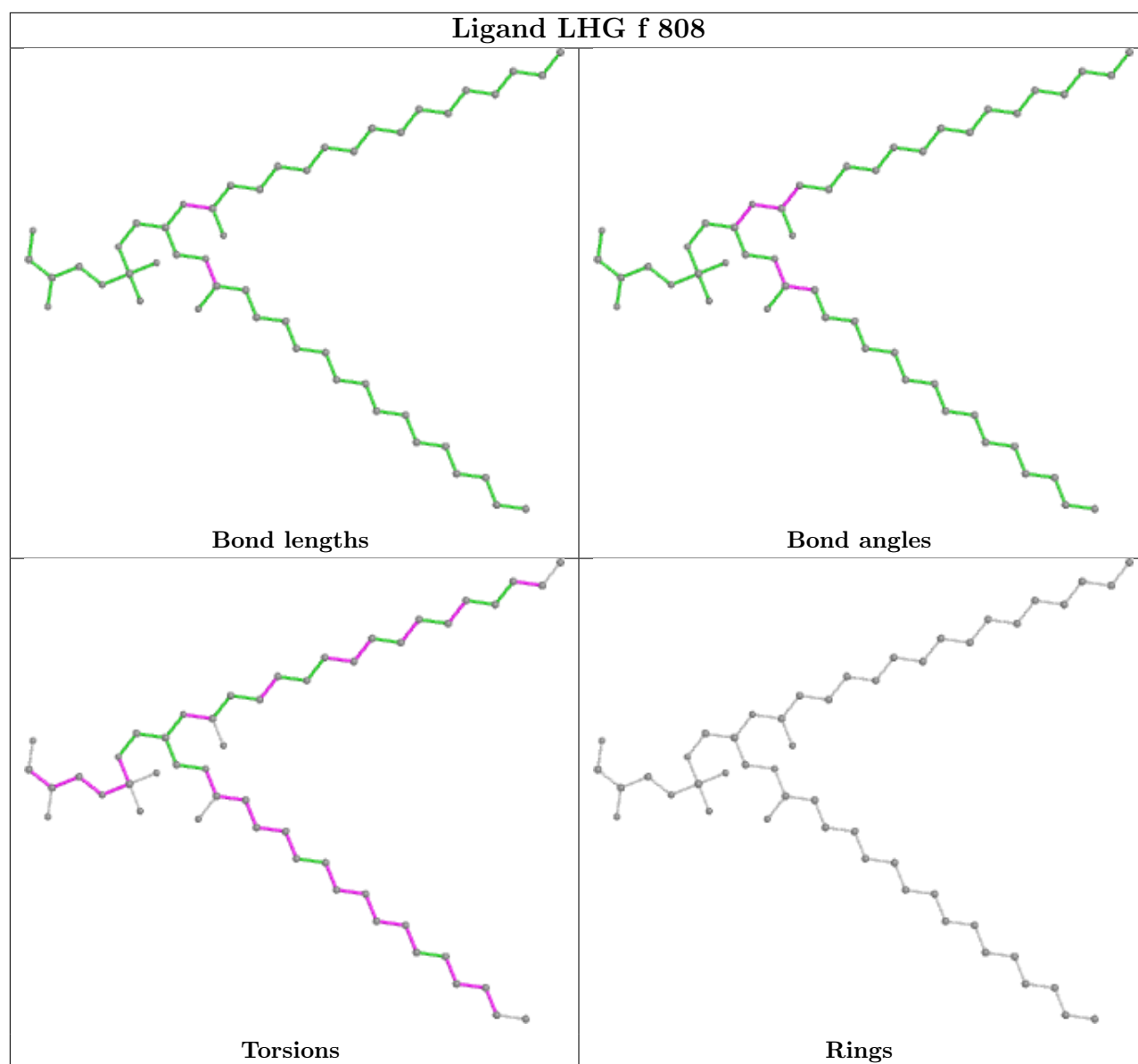


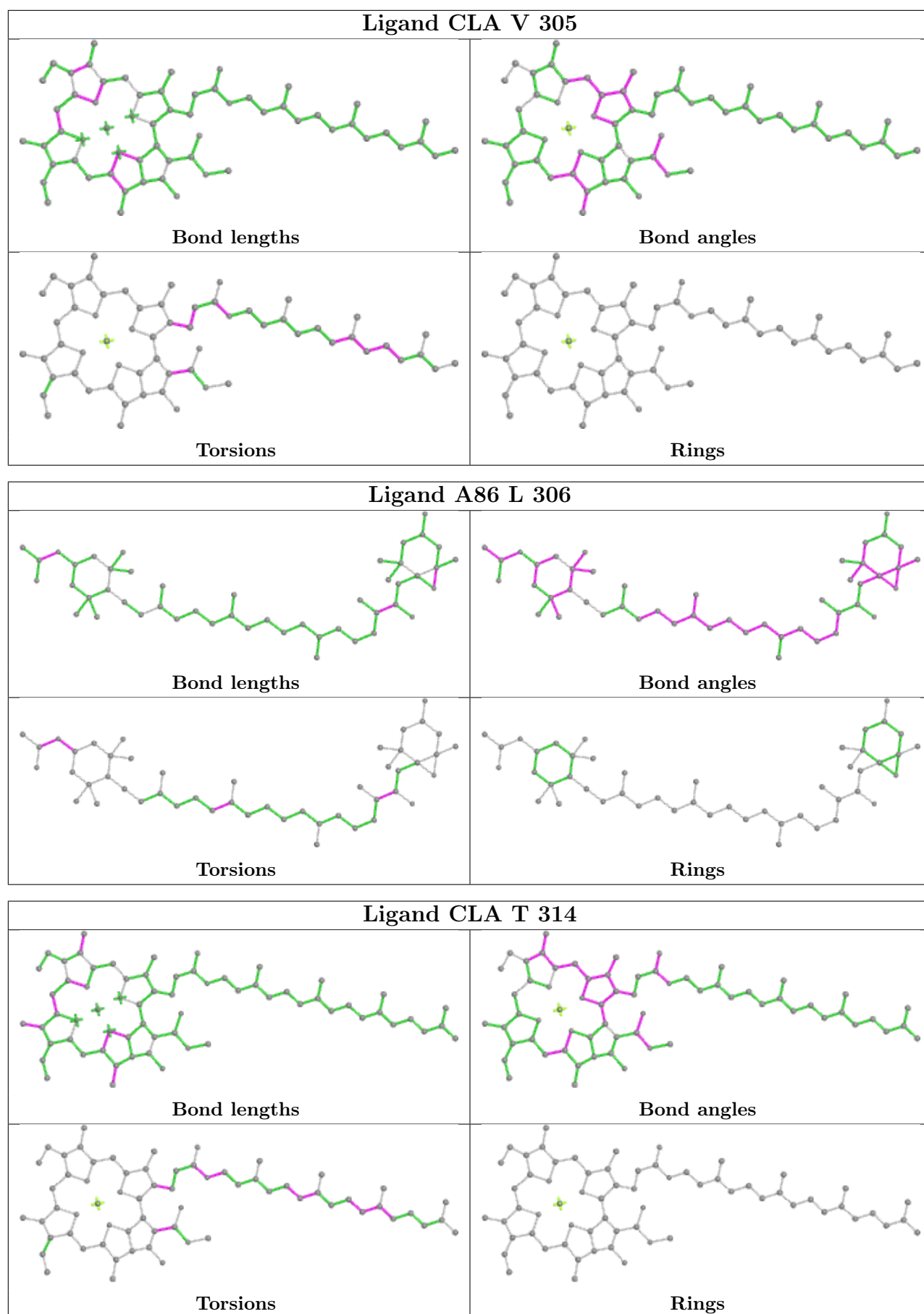
Torsions



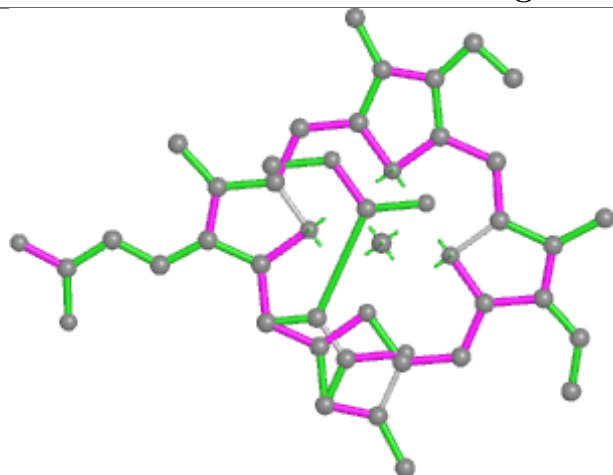
Rings



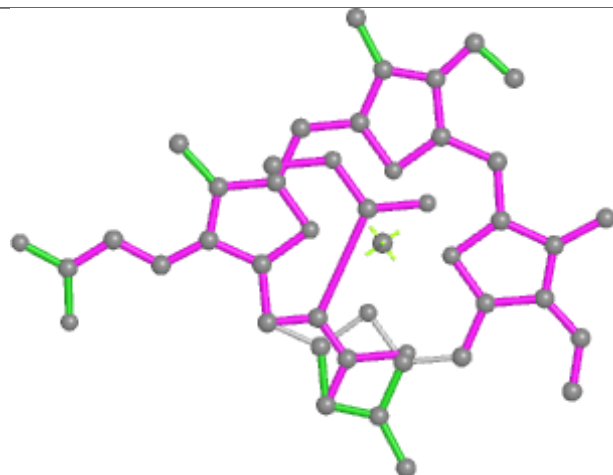




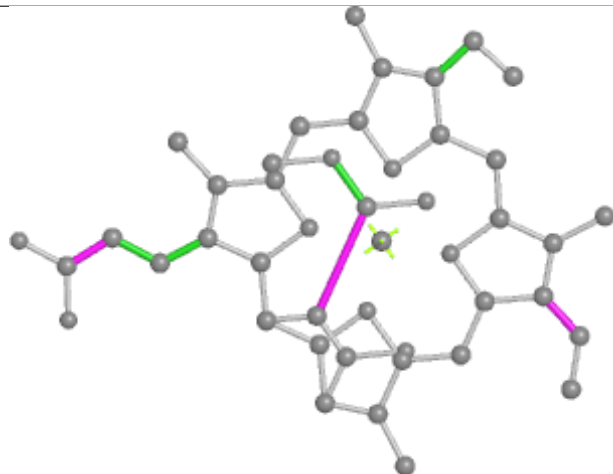
## Ligand KC1 G 318



Bond lengths



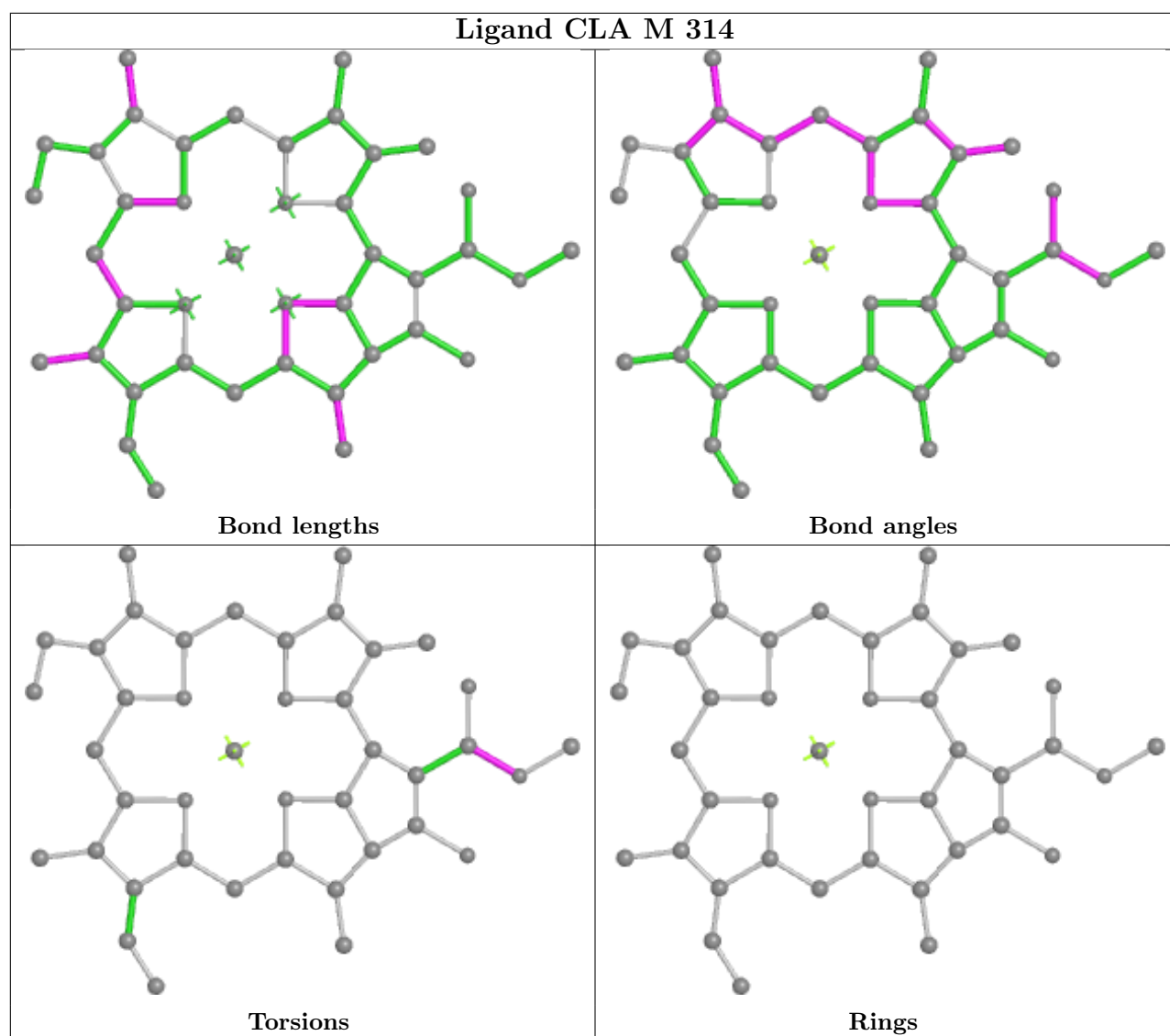
Bond angles



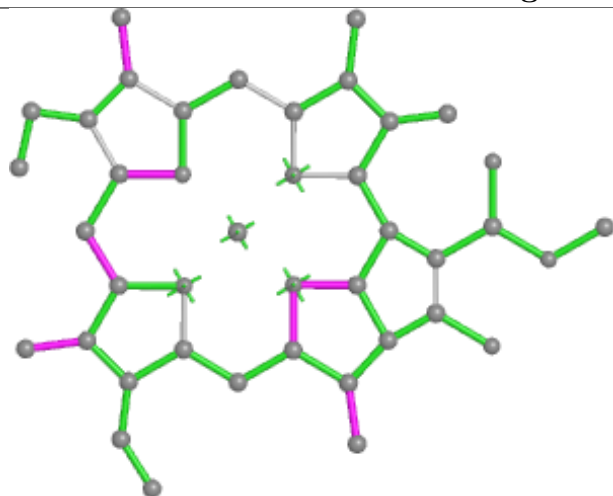
Torsions



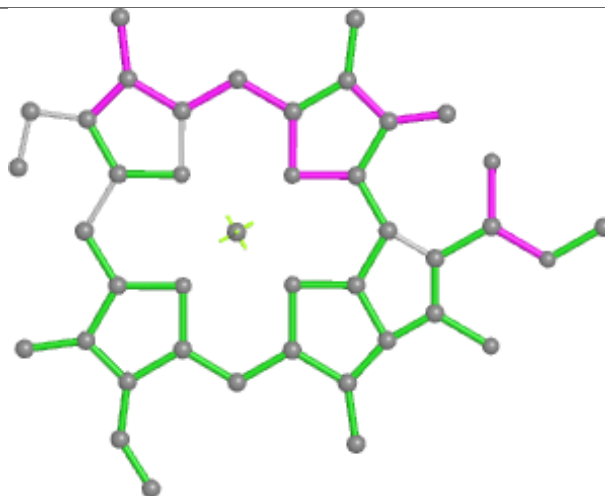
Rings



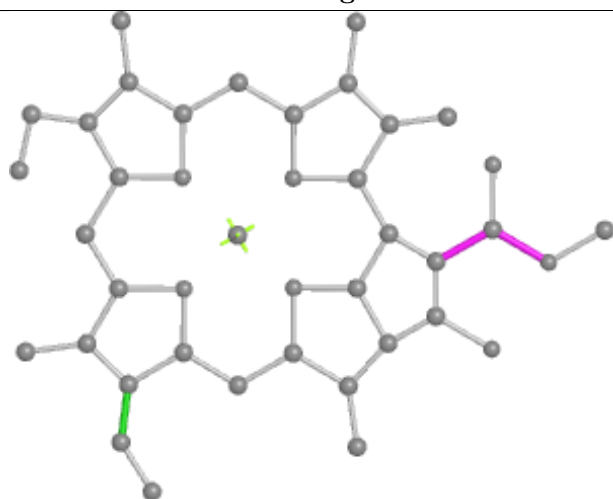
## Ligand CLA I 313



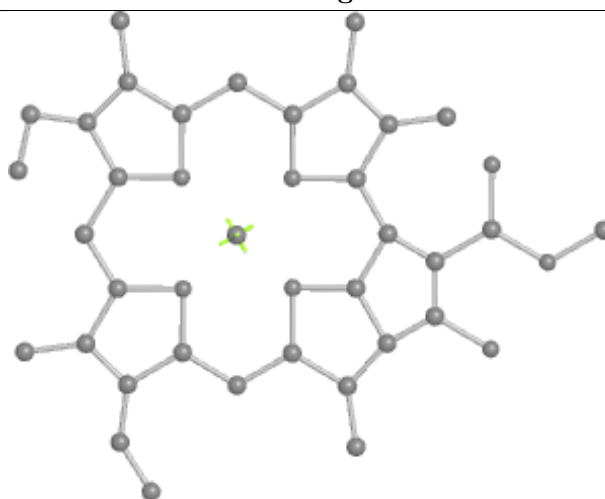
Bond lengths



Bond angles

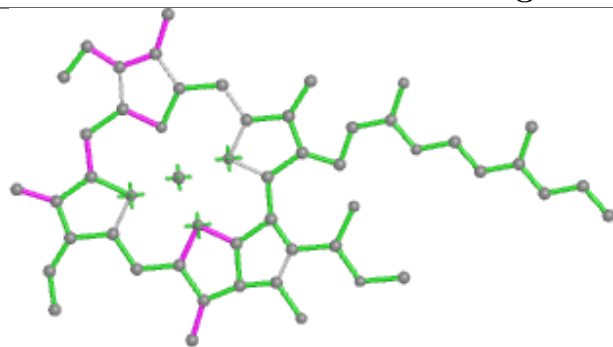


Torsions

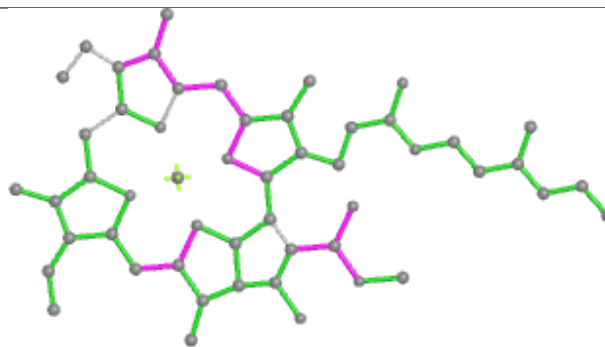


Rings

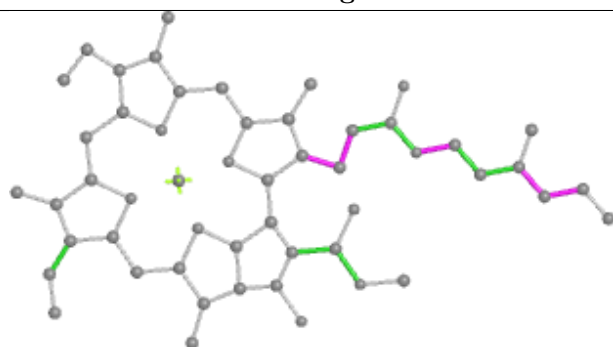
## Ligand CLA F 313



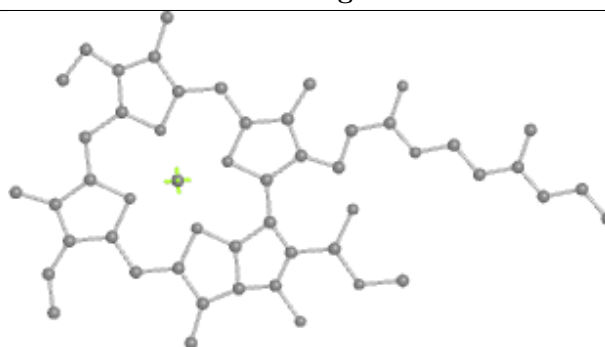
Bond lengths



Bond angles

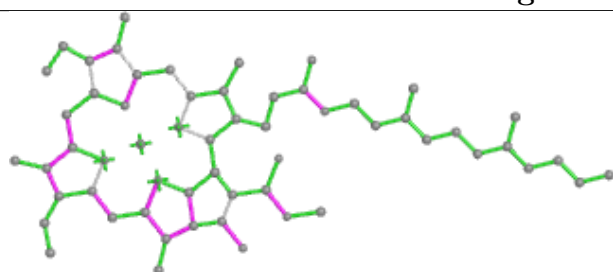


Torsions

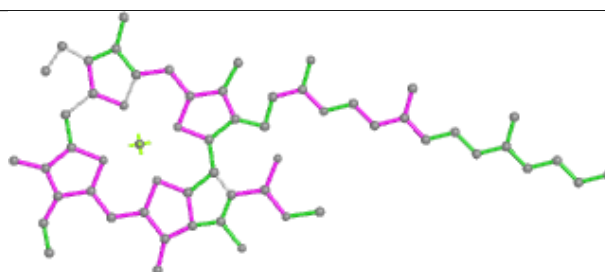


Rings

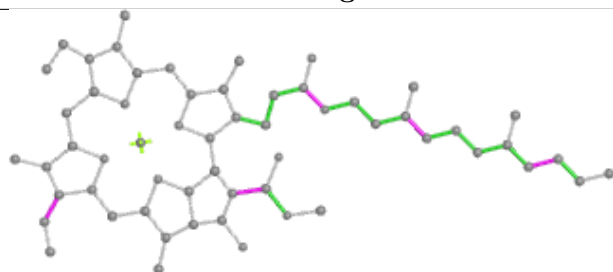
## Ligand CLA b 836



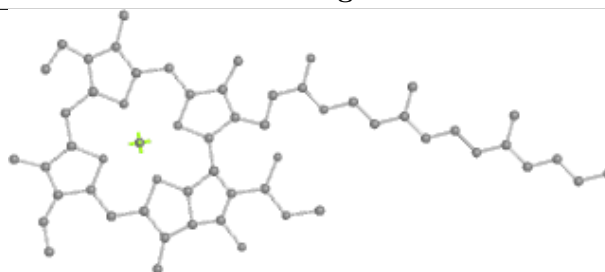
Bond lengths



Bond angles

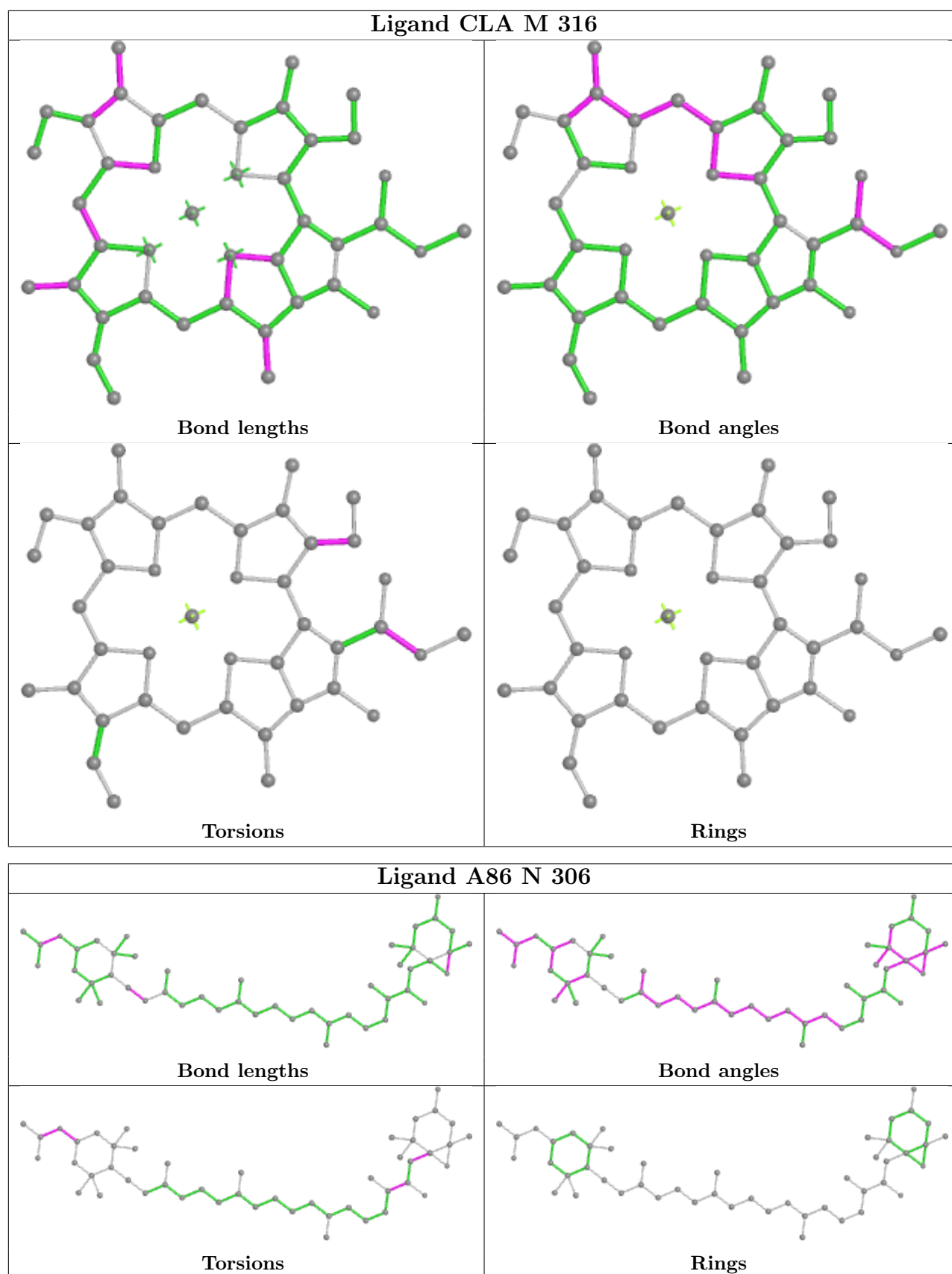


Torsions

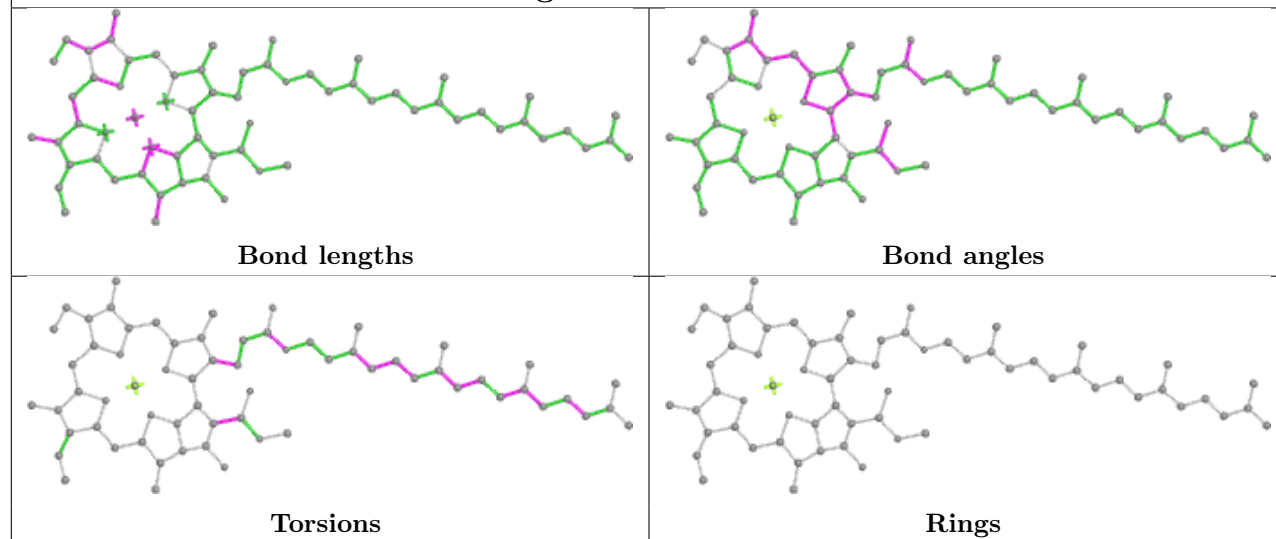


Rings

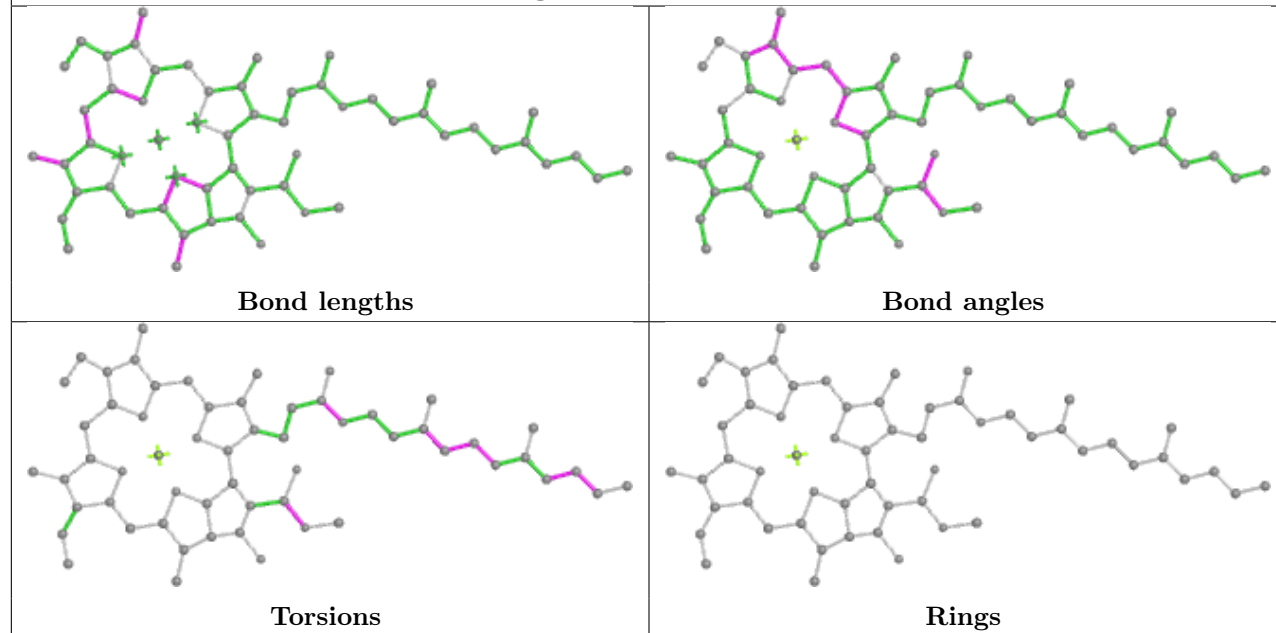




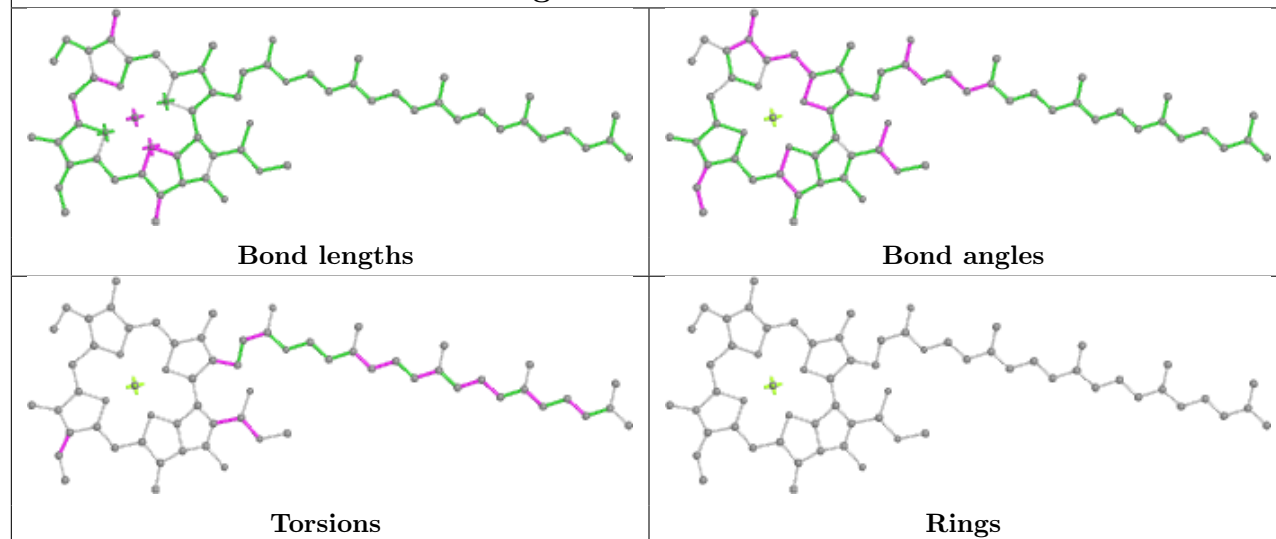
## Ligand CLA a 805



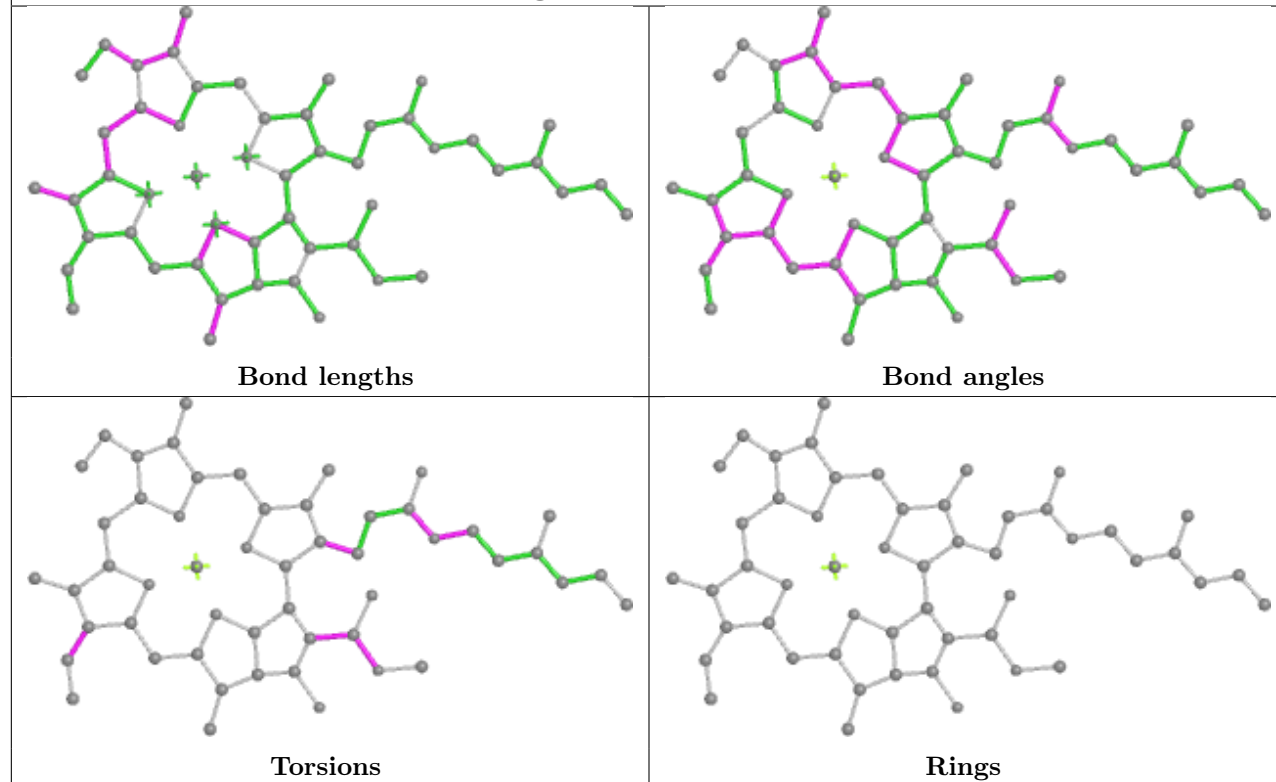
## Ligand CLA O 311

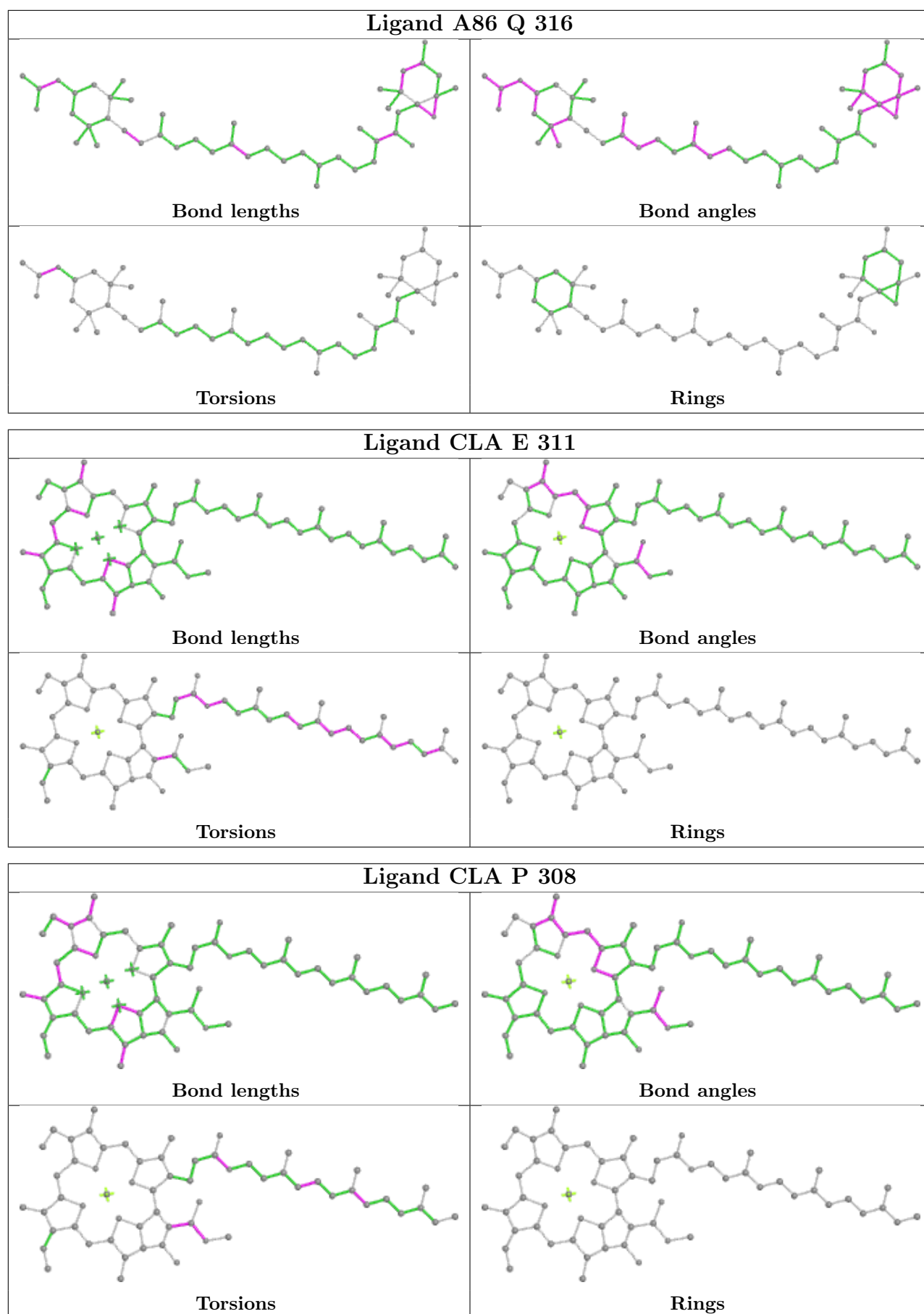


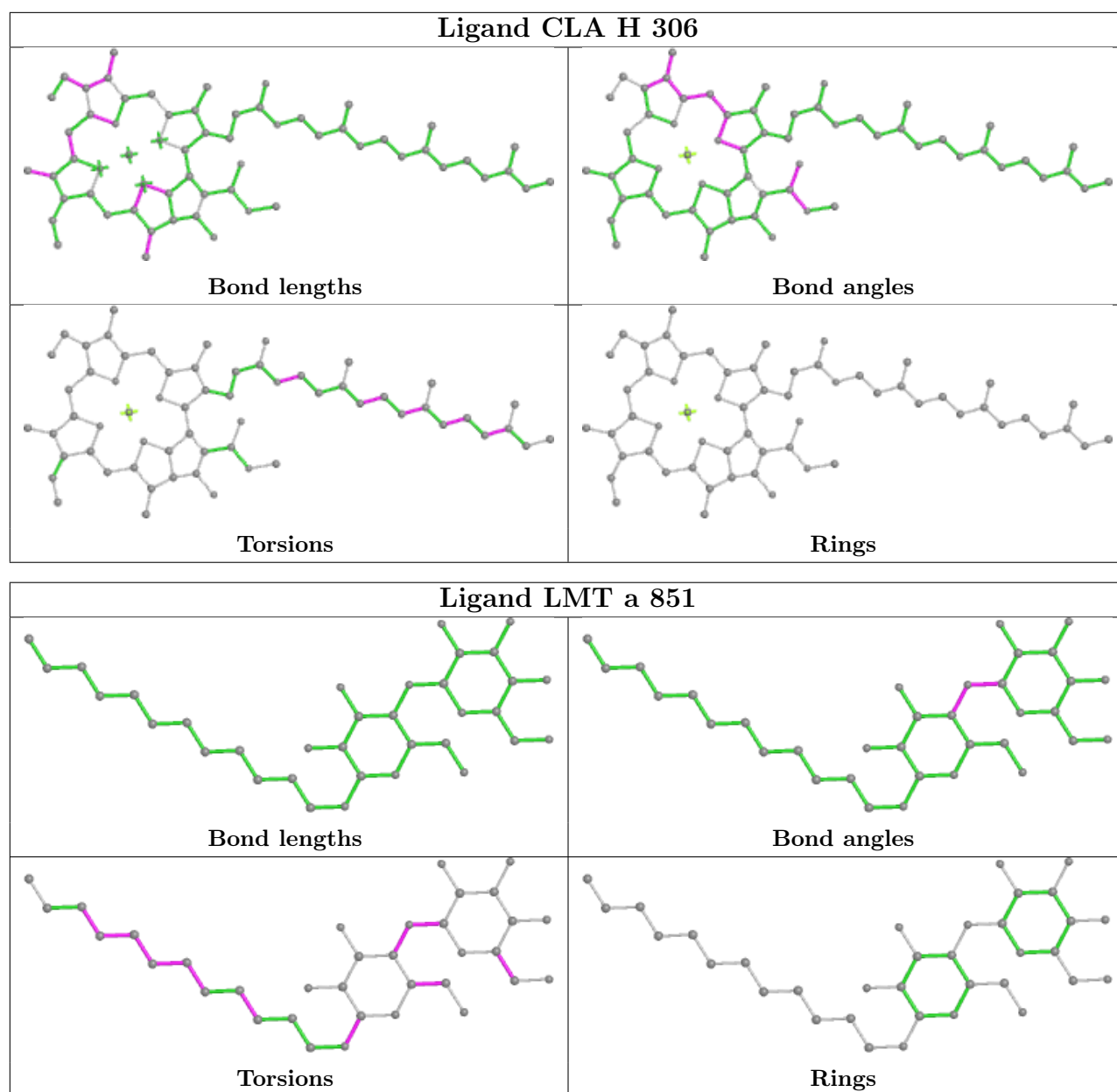
## Ligand CLA P 311



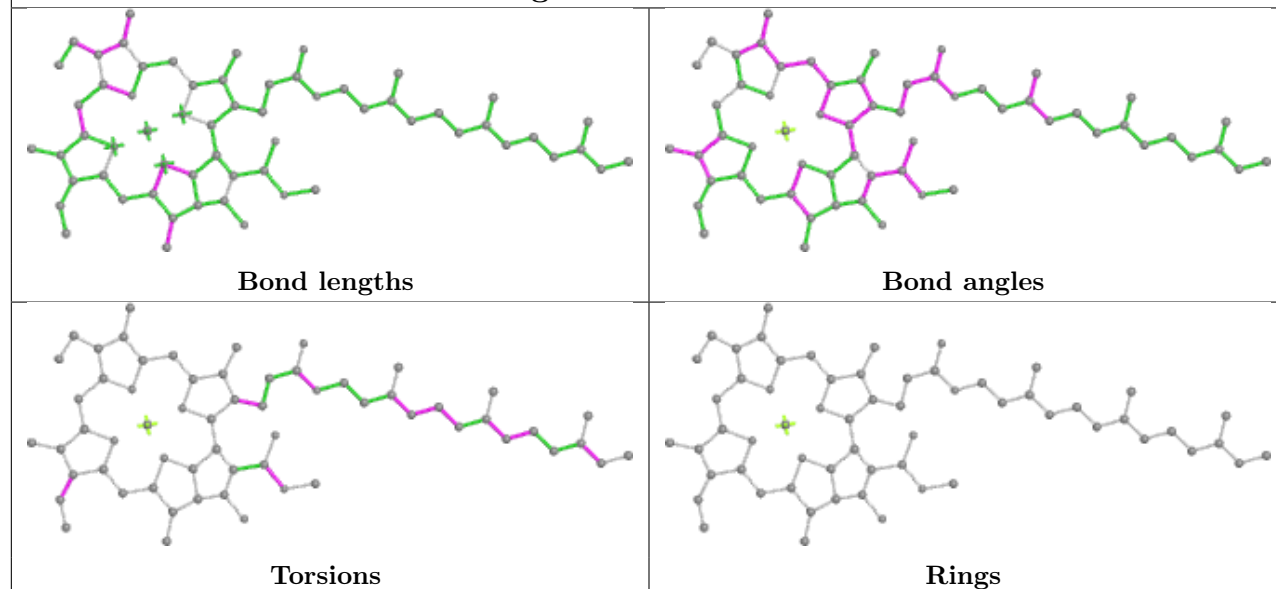
## Ligand CLA D 316



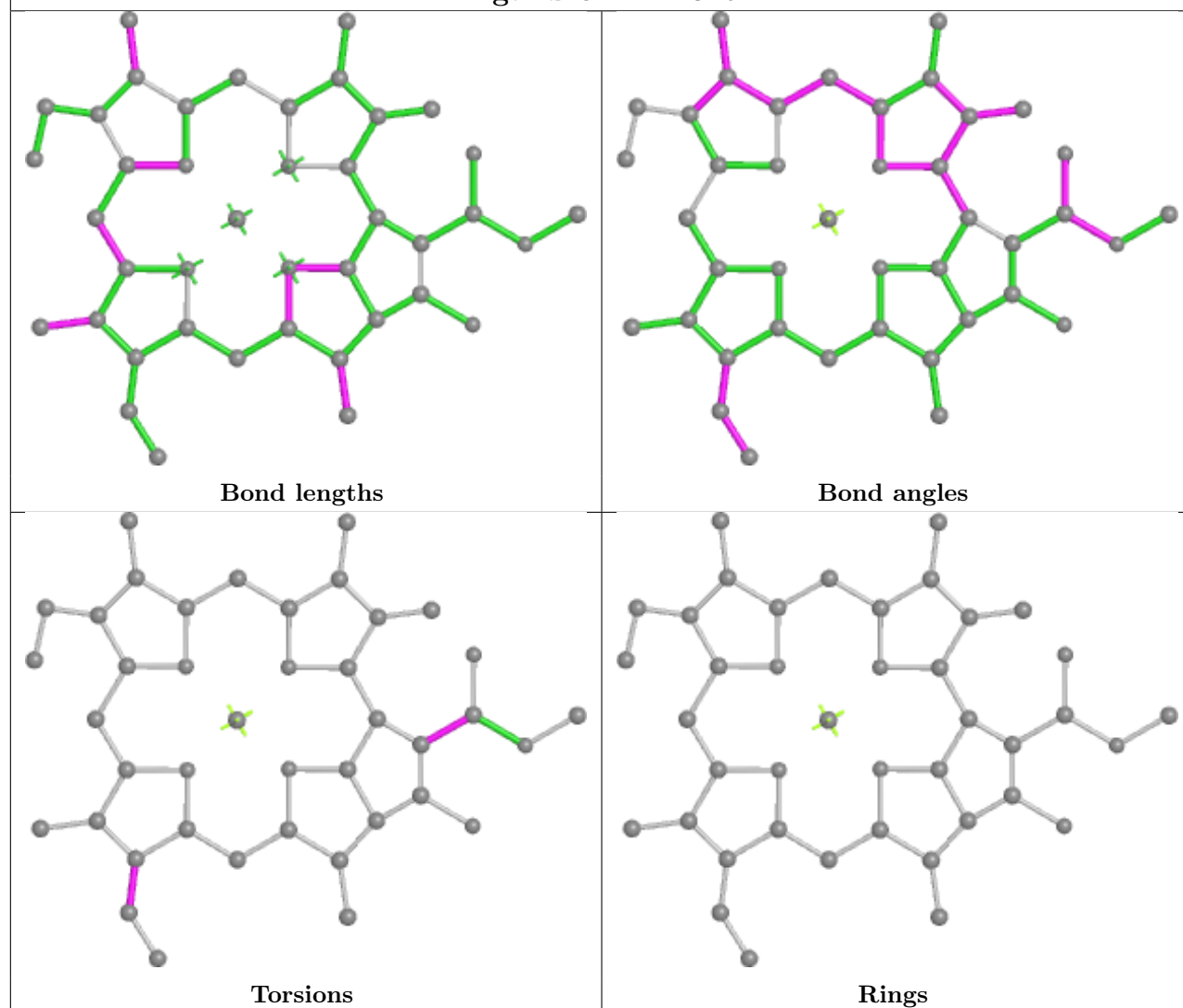


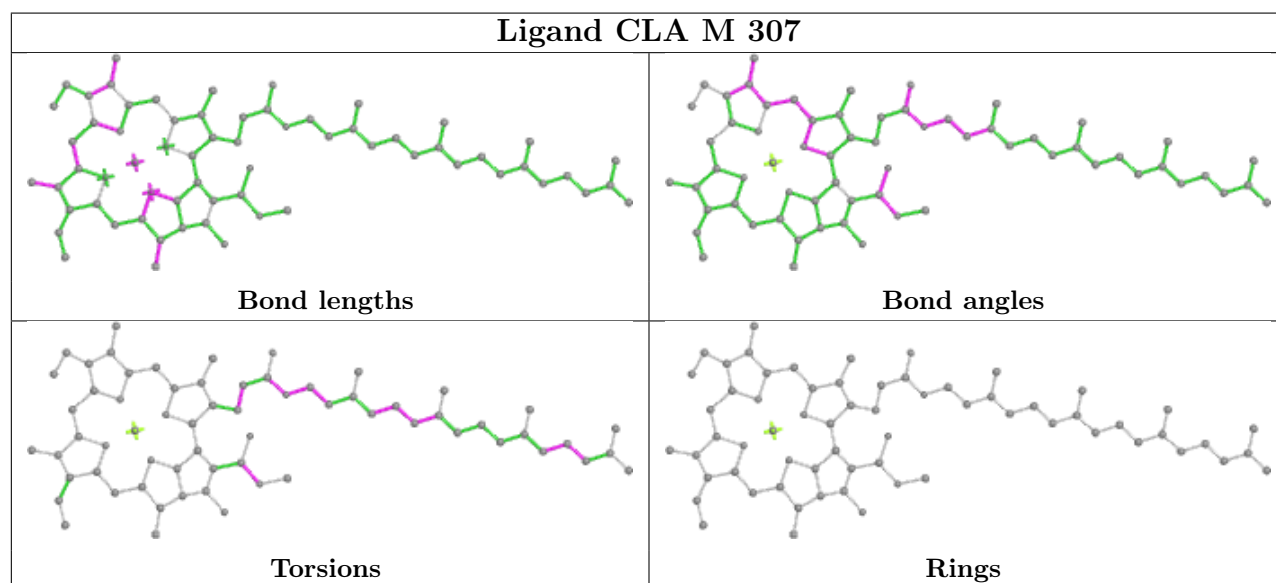
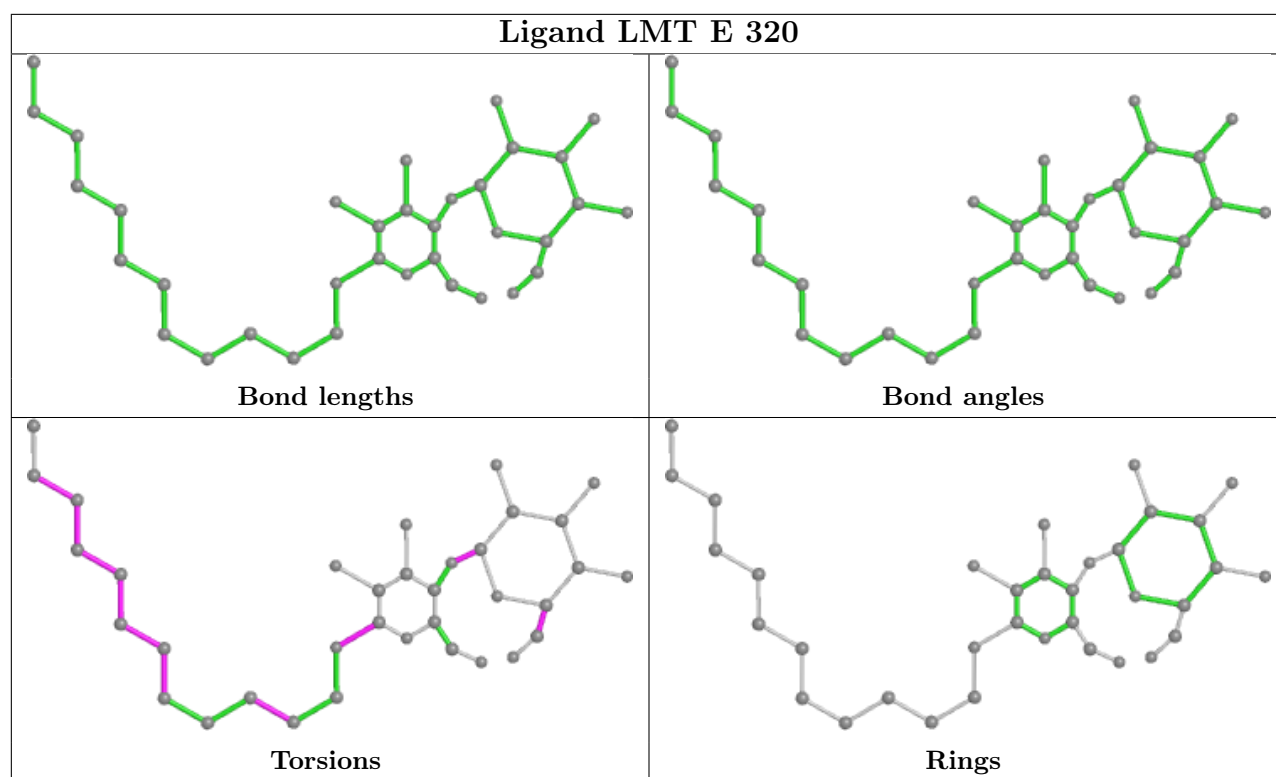


## Ligand CLA D 307

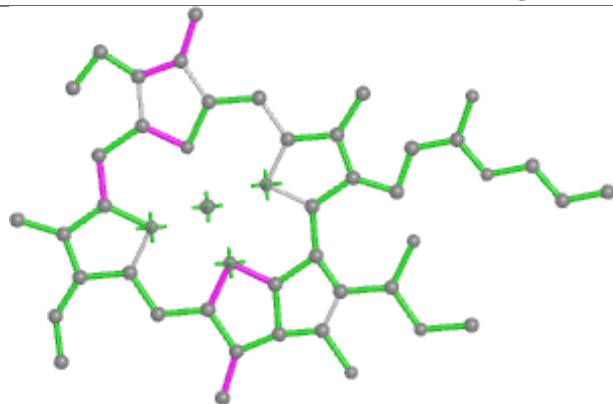


## Ligand CLA D 315

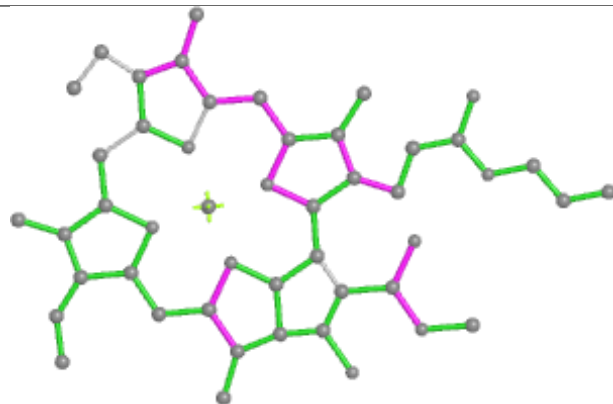




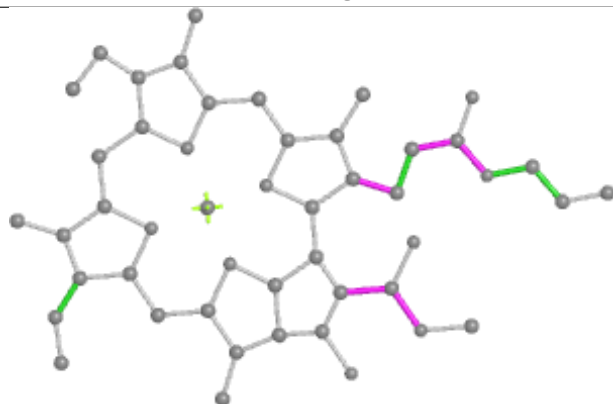
## Ligand CLA H 305



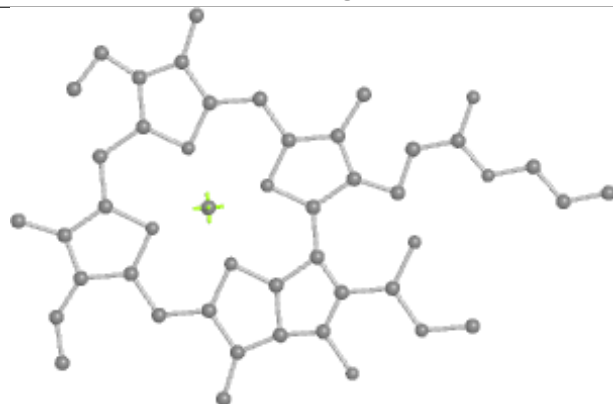
Bond lengths



Bond angles

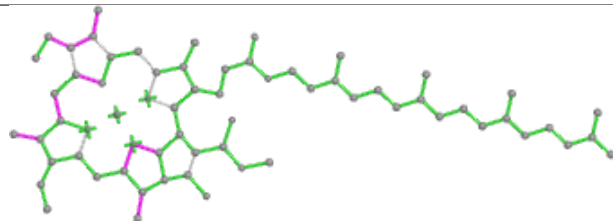


Torsions

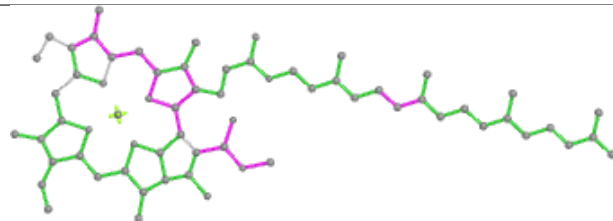


Rings

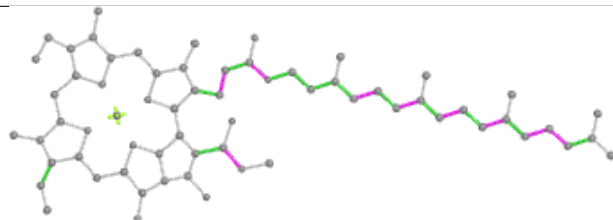
## Ligand CLA R 312



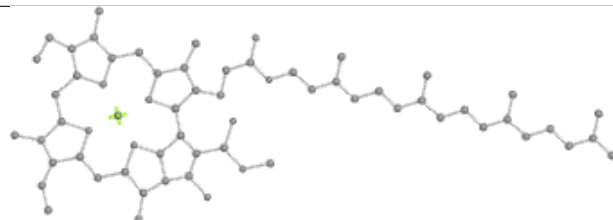
Bond lengths



Bond angles

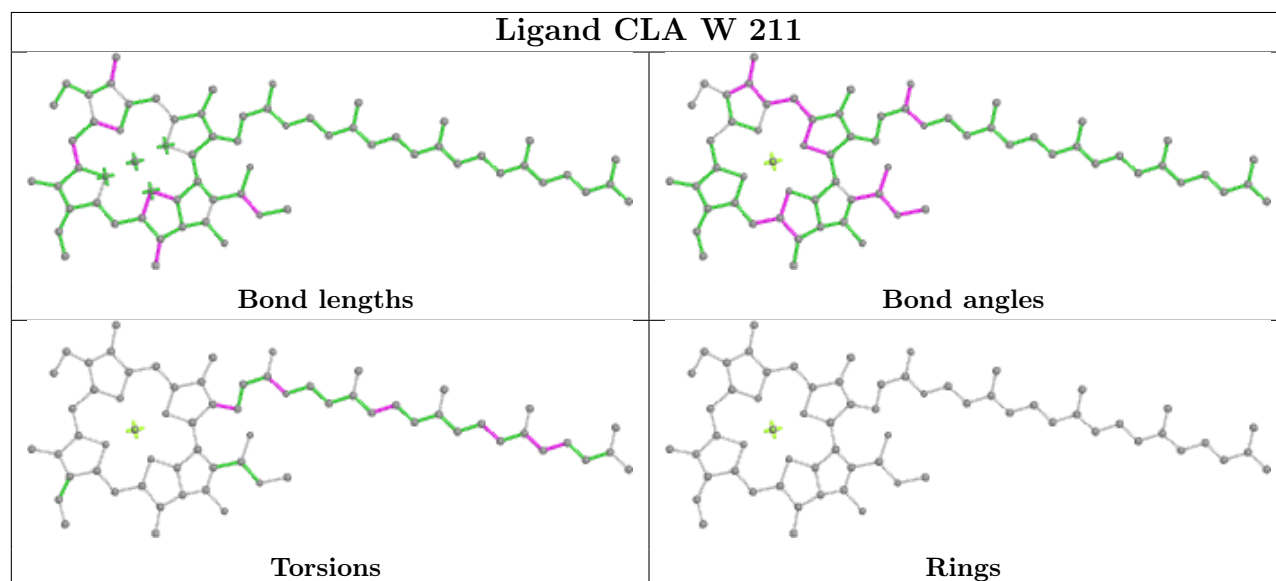
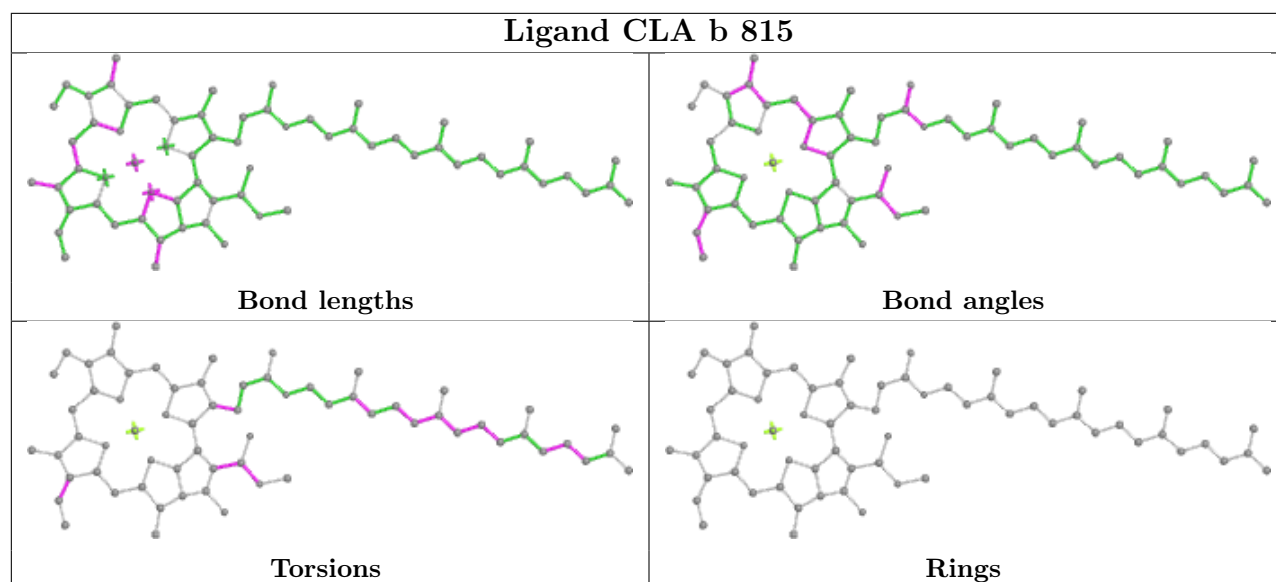
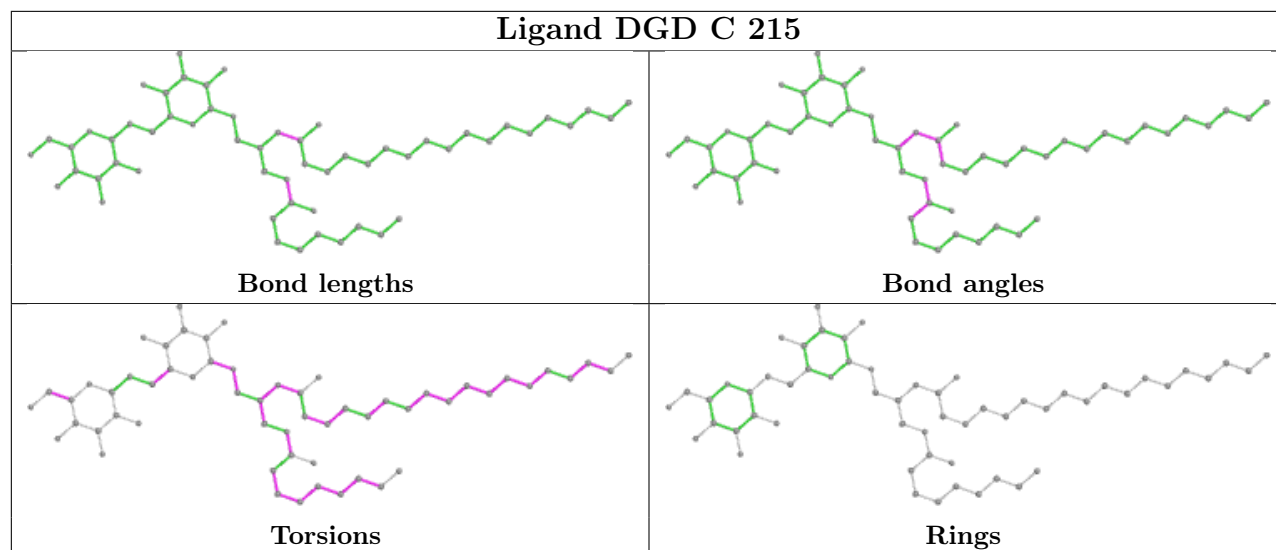


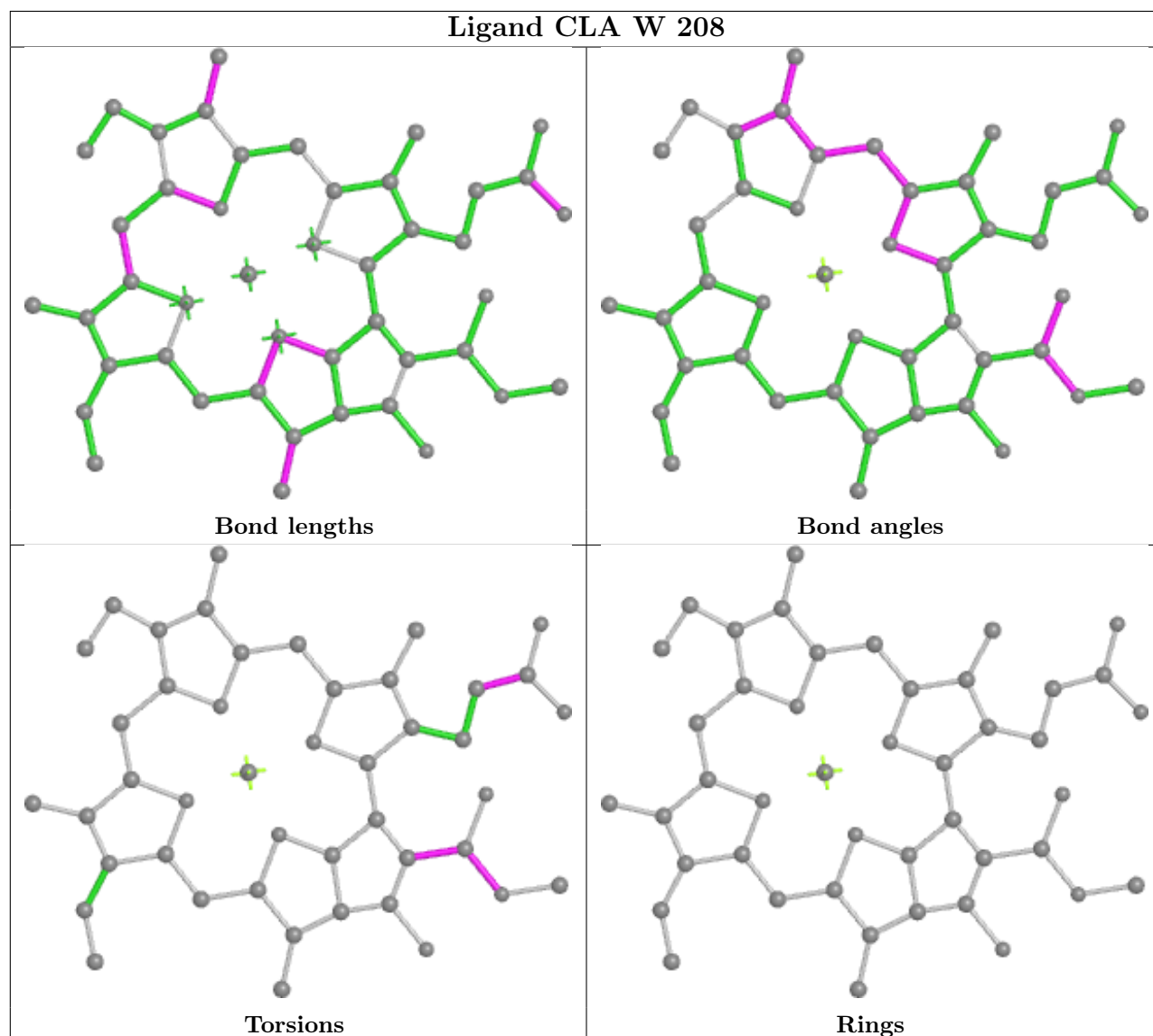
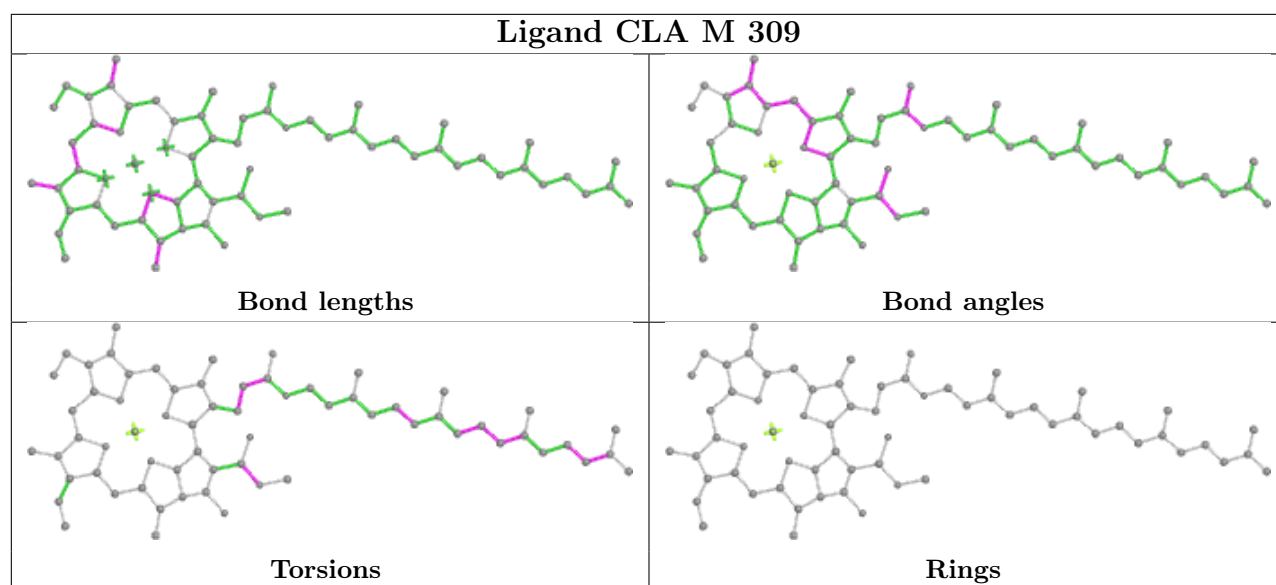
Torsions



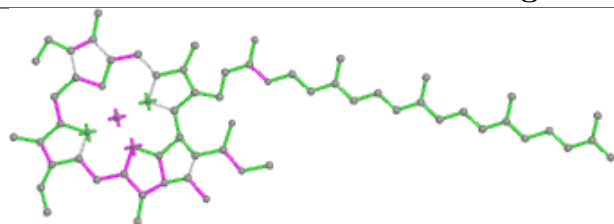
Rings



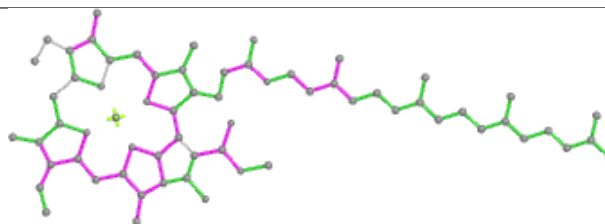




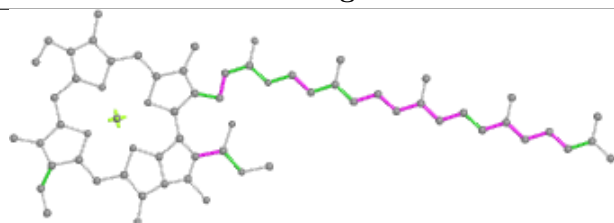
## Ligand CLA I 308



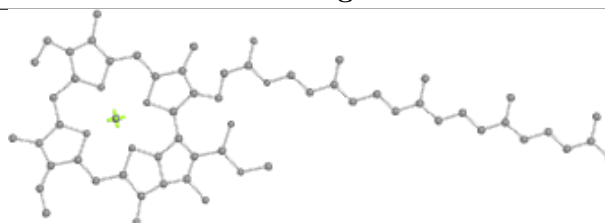
Bond lengths



Bond angles

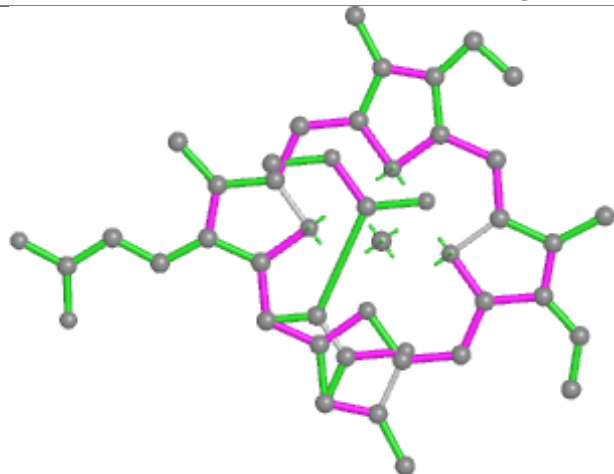


Torsions

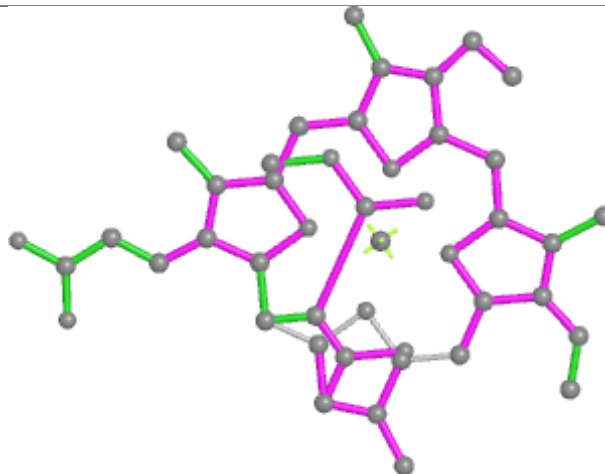


Rings

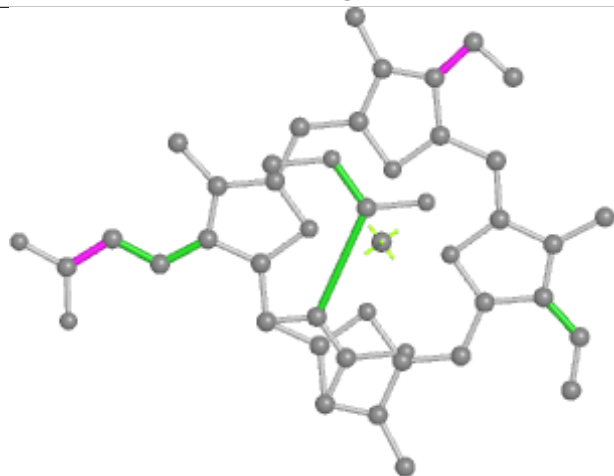
## Ligand KC1 R 317



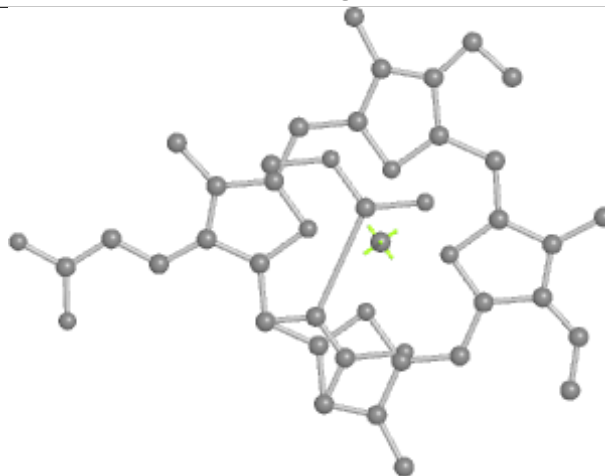
Bond lengths



Bond angles

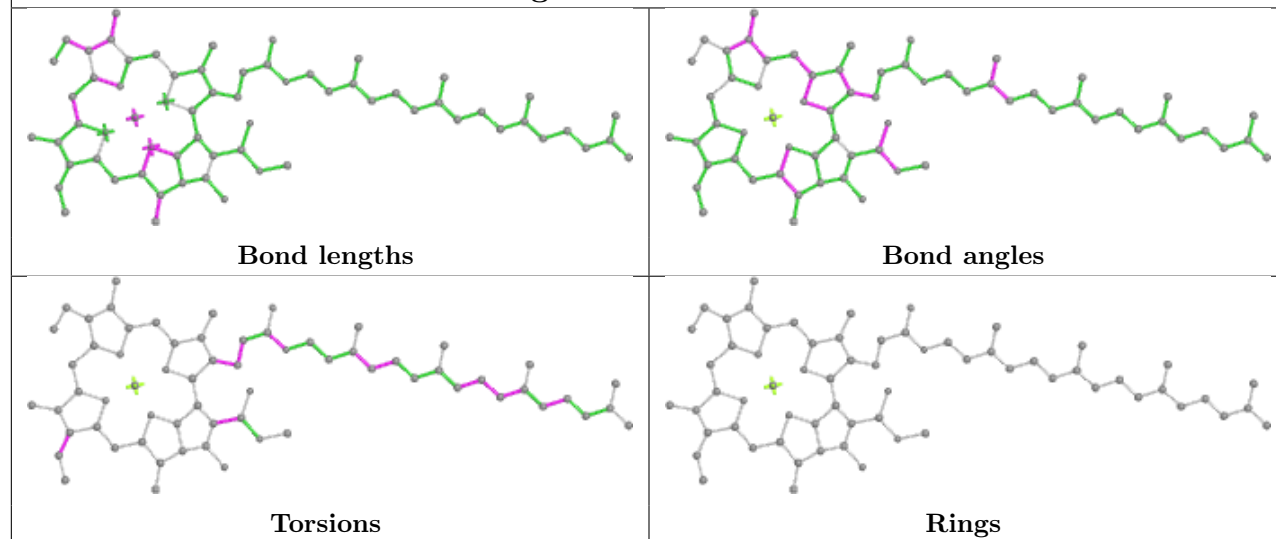


Torsions

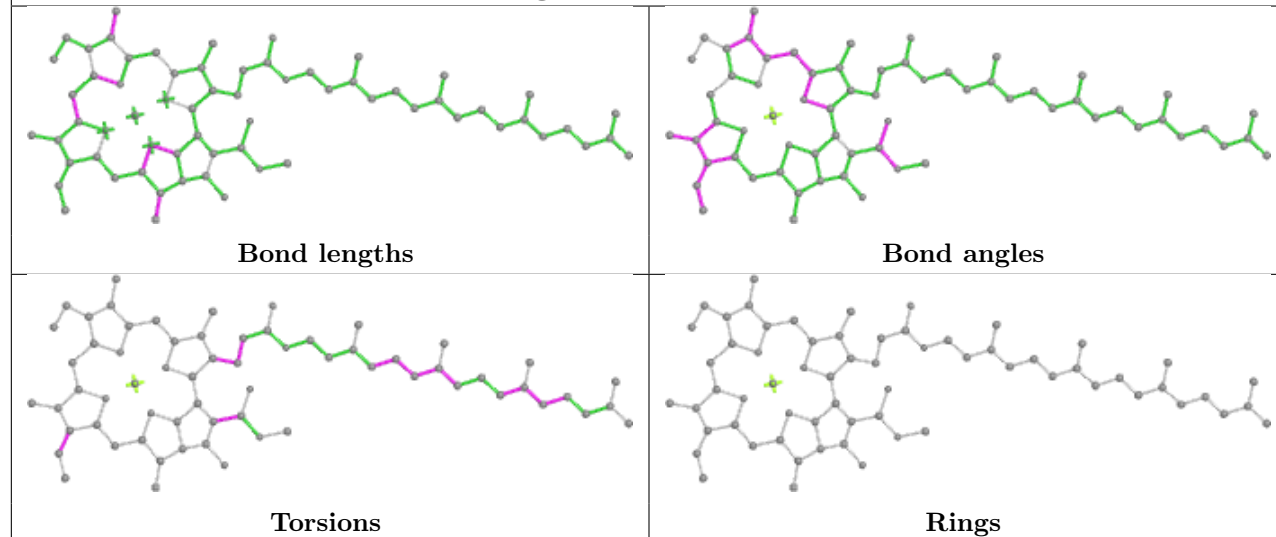


Rings

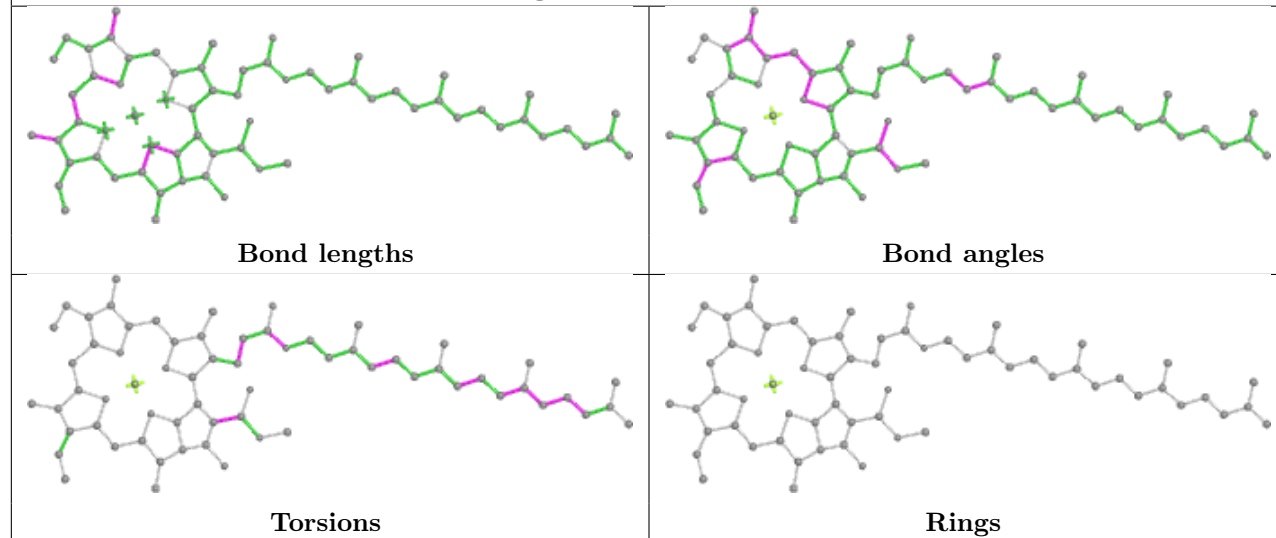
## Ligand CLA G 311



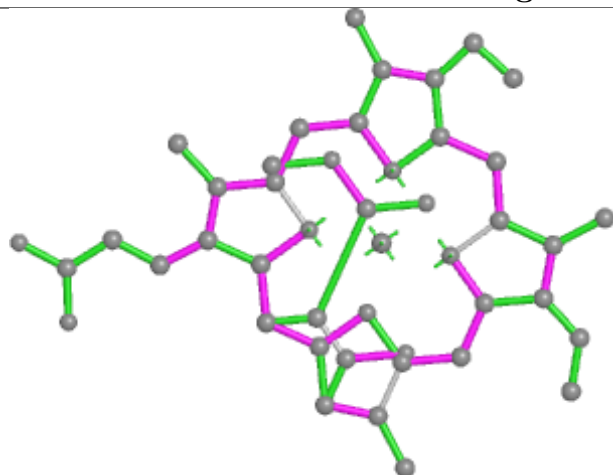
## Ligand CLA E 316



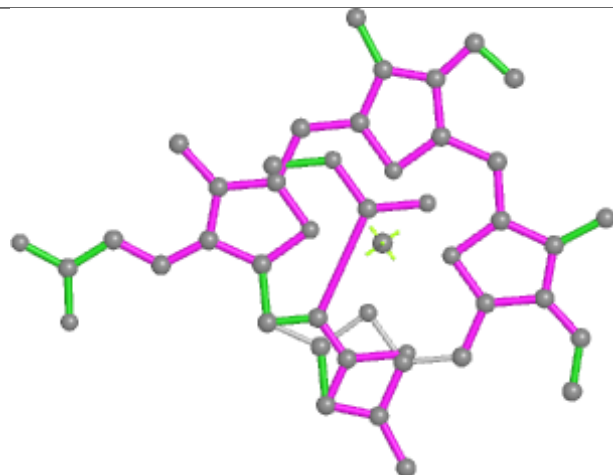
## Ligand CLA K 308



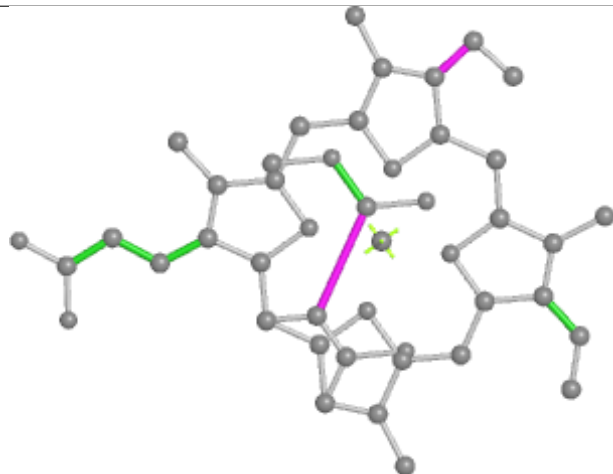
## Ligand KC1 O 315



Bond lengths



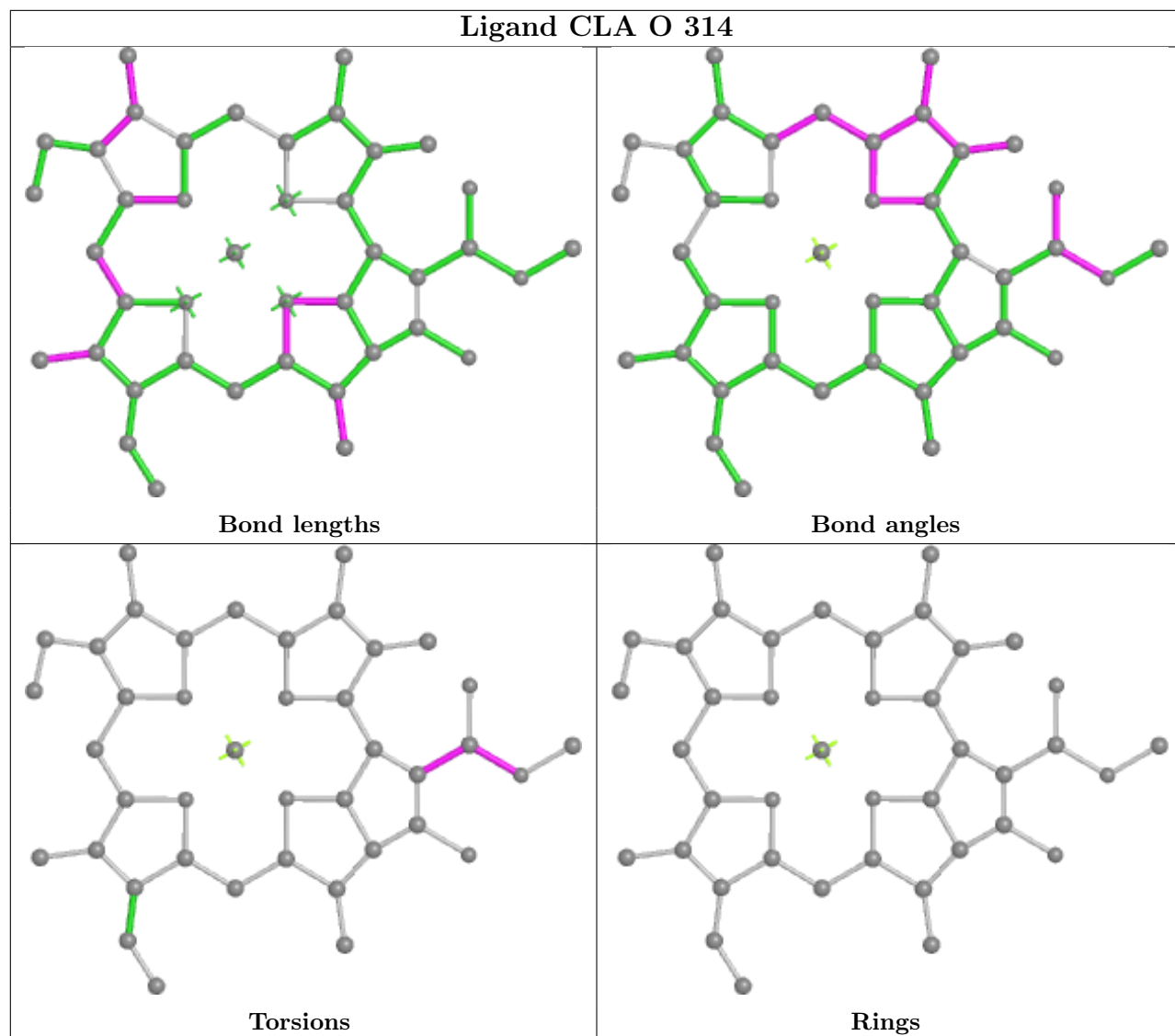
Bond angles



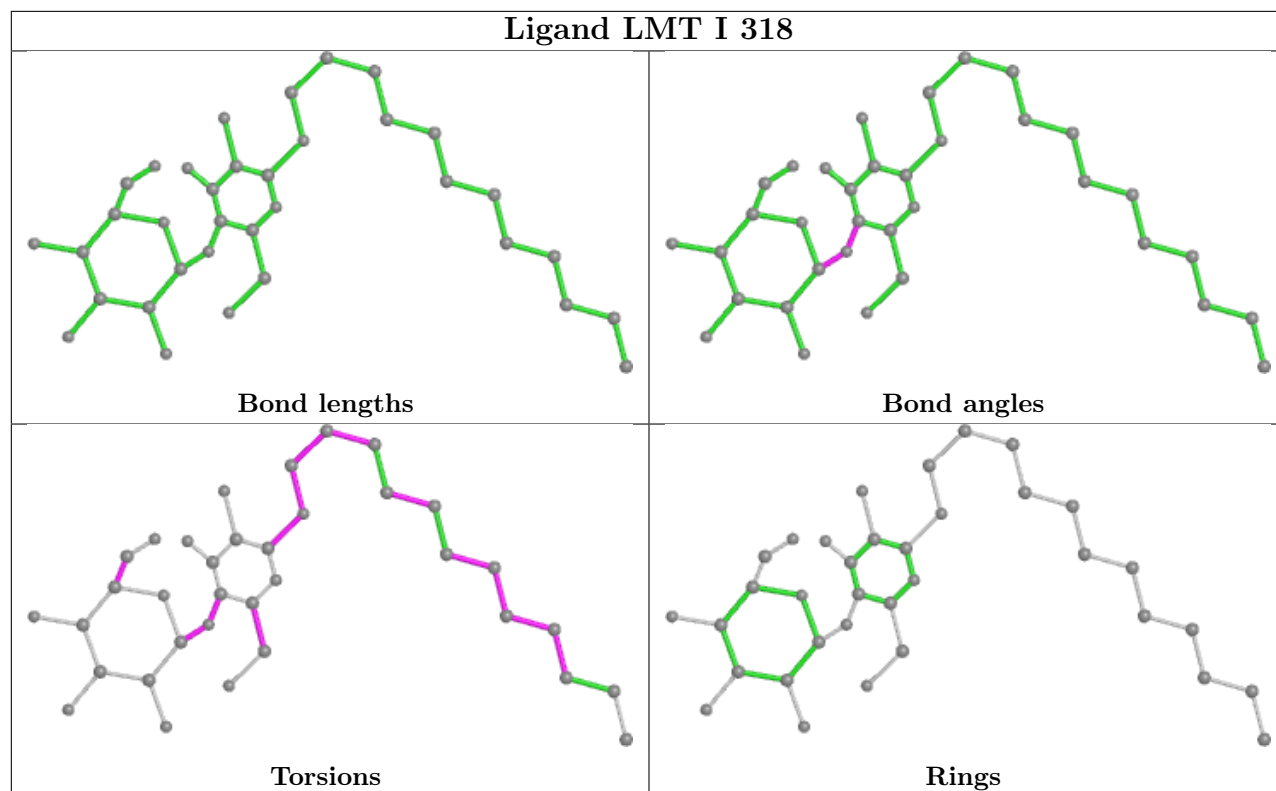
Torsions



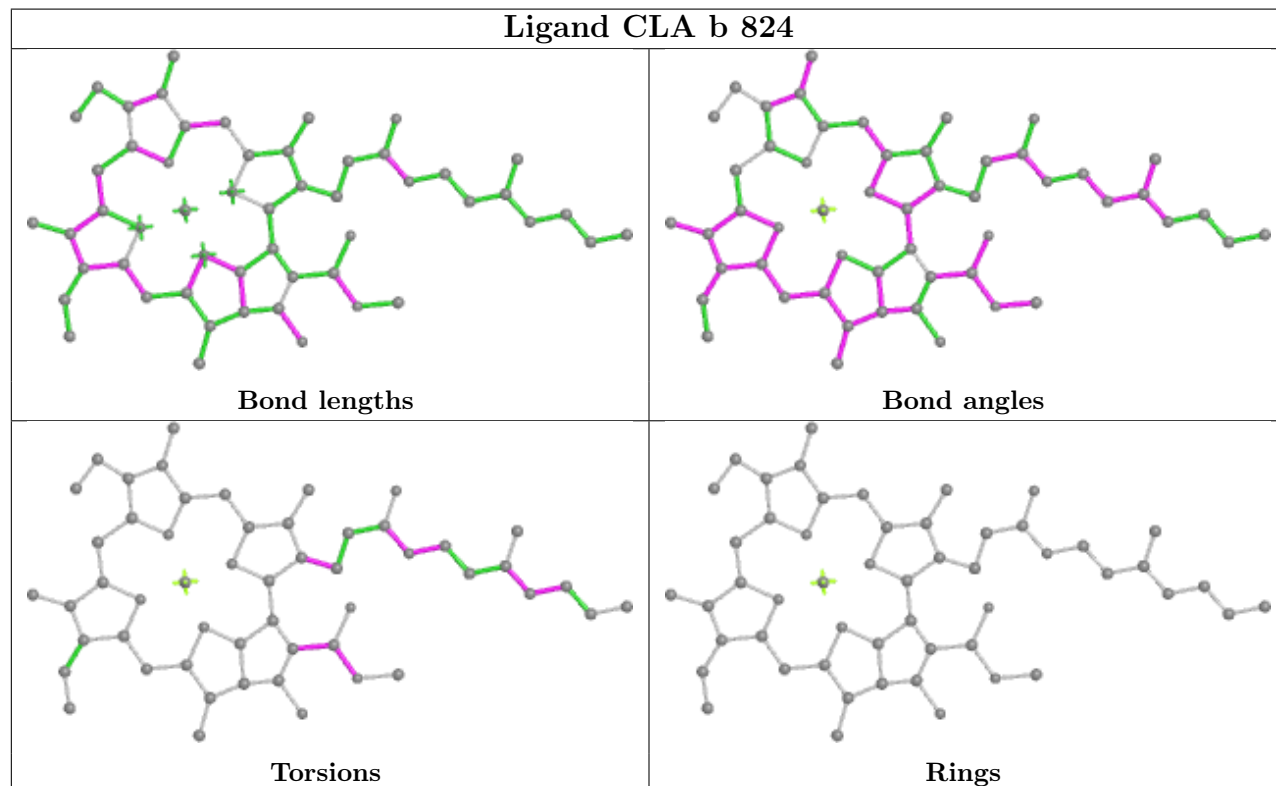
Rings

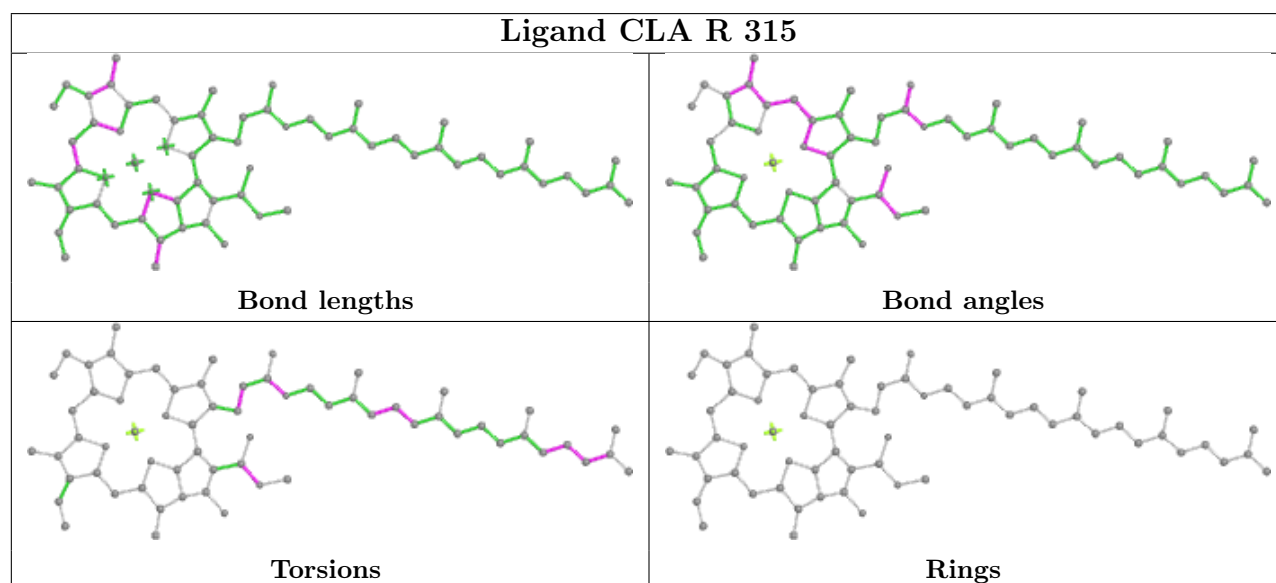
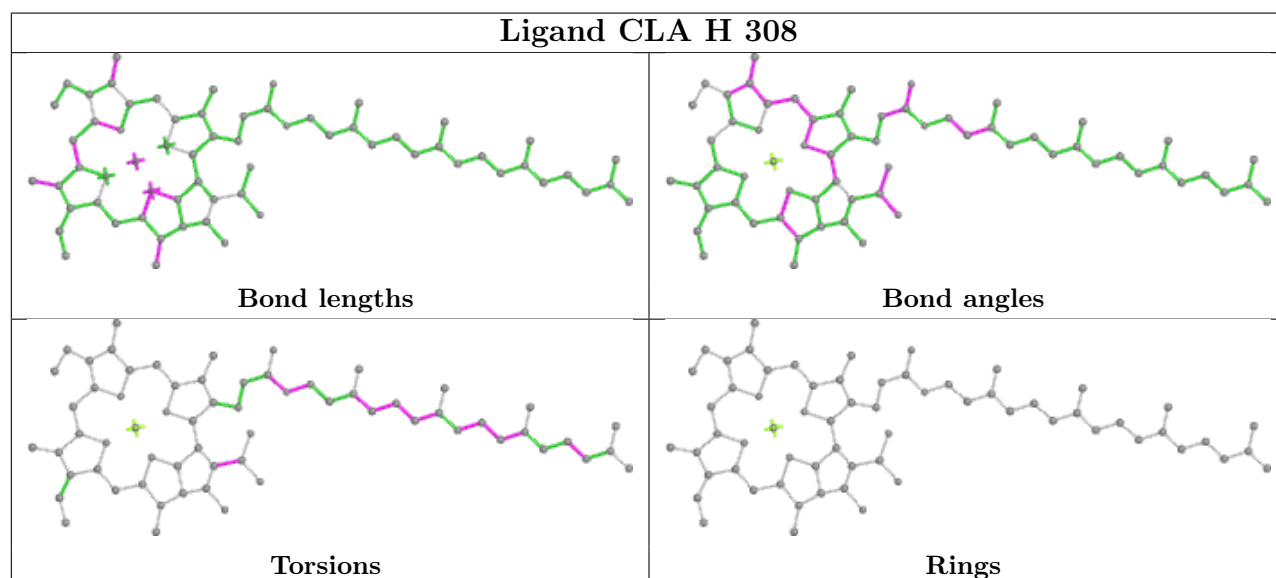
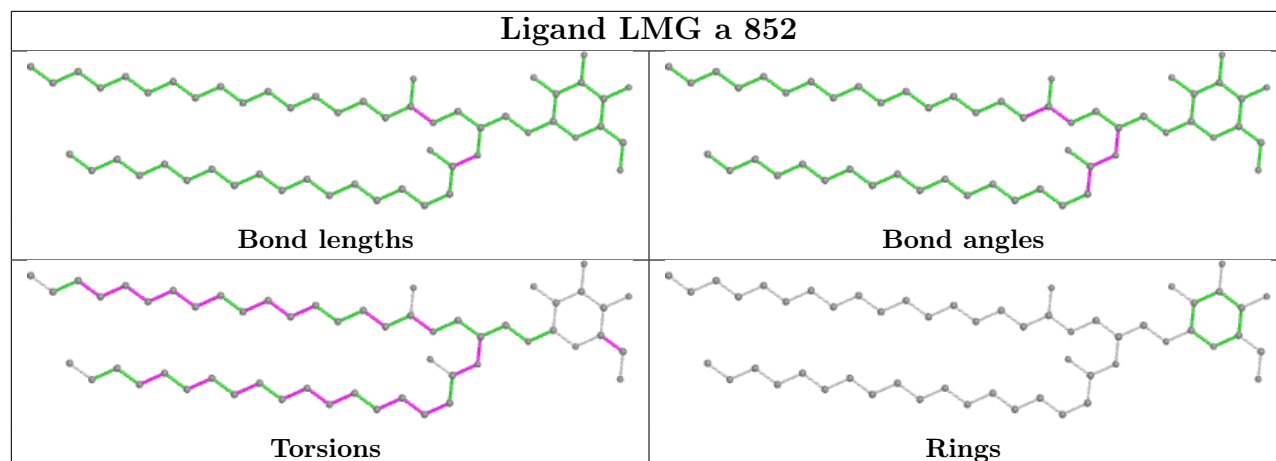


## Ligand LMT I 318



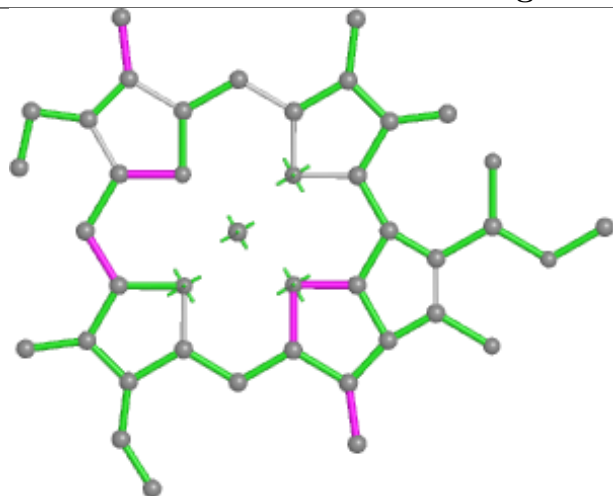
## Ligand CLA b 824



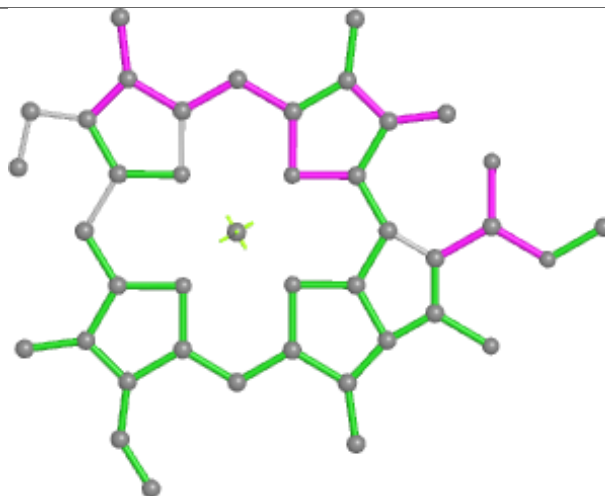




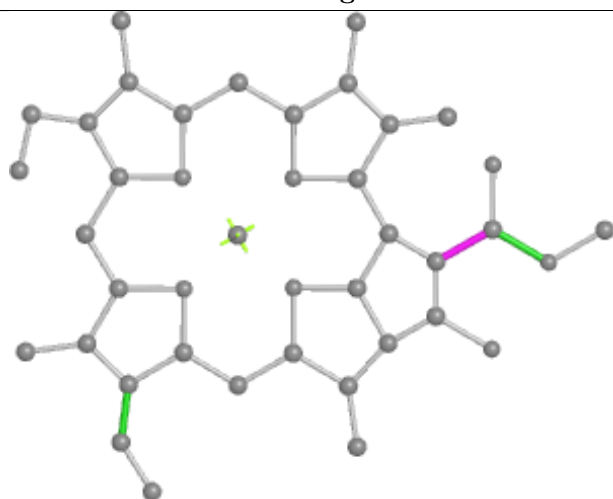
## Ligand CLA L 316



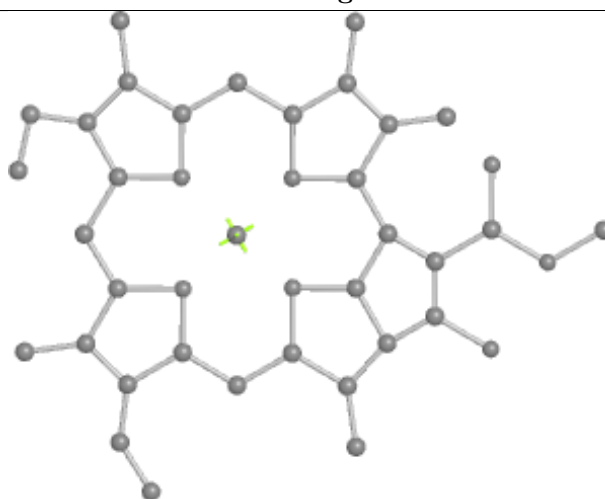
Bond lengths



Bond angles

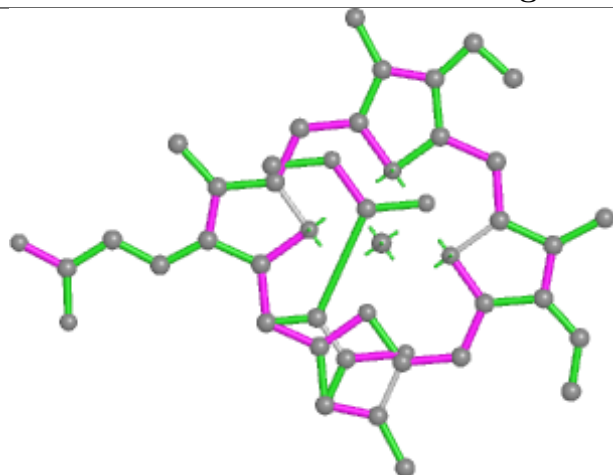


Torsions

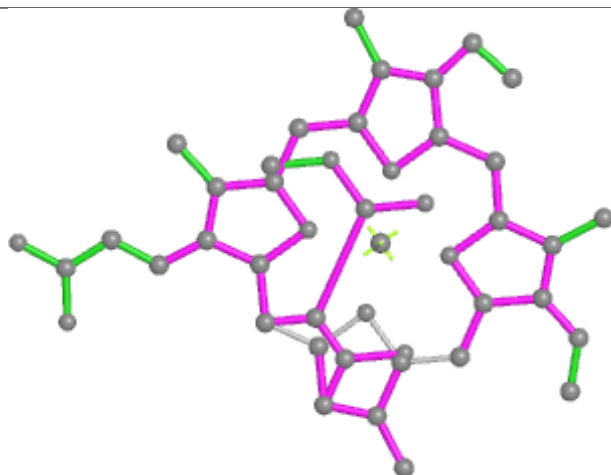


Rings

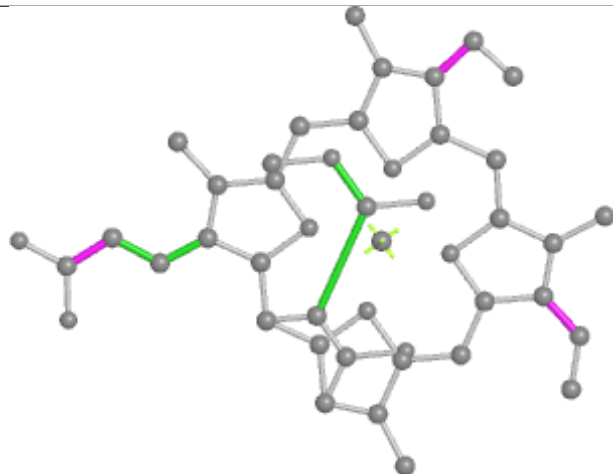
## Ligand KC1 J 314



Bond lengths



Bond angles

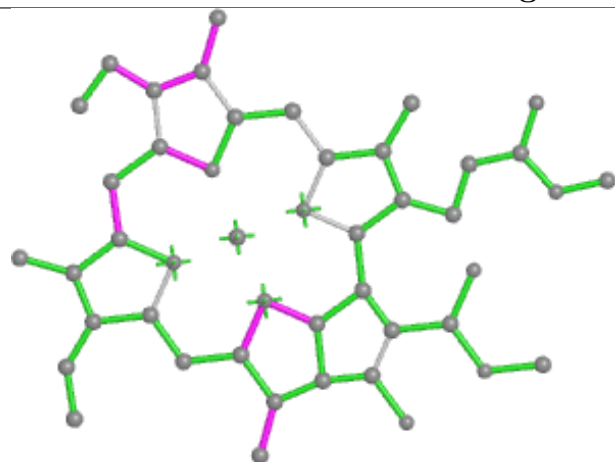


Torsions

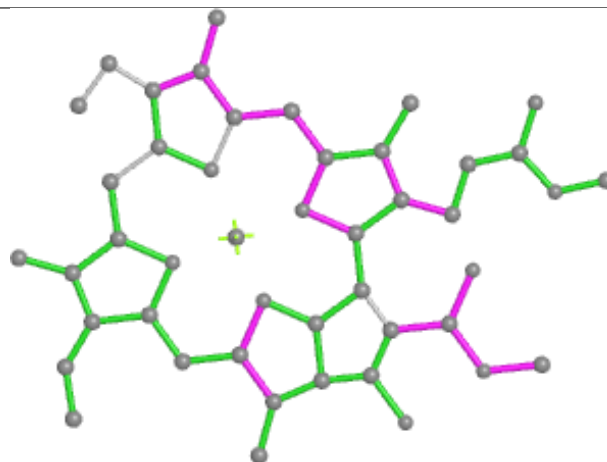


Rings

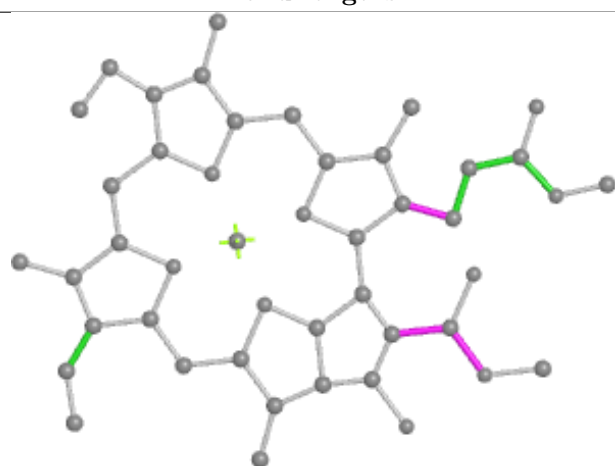
## Ligand CLA b 822



Bond lengths



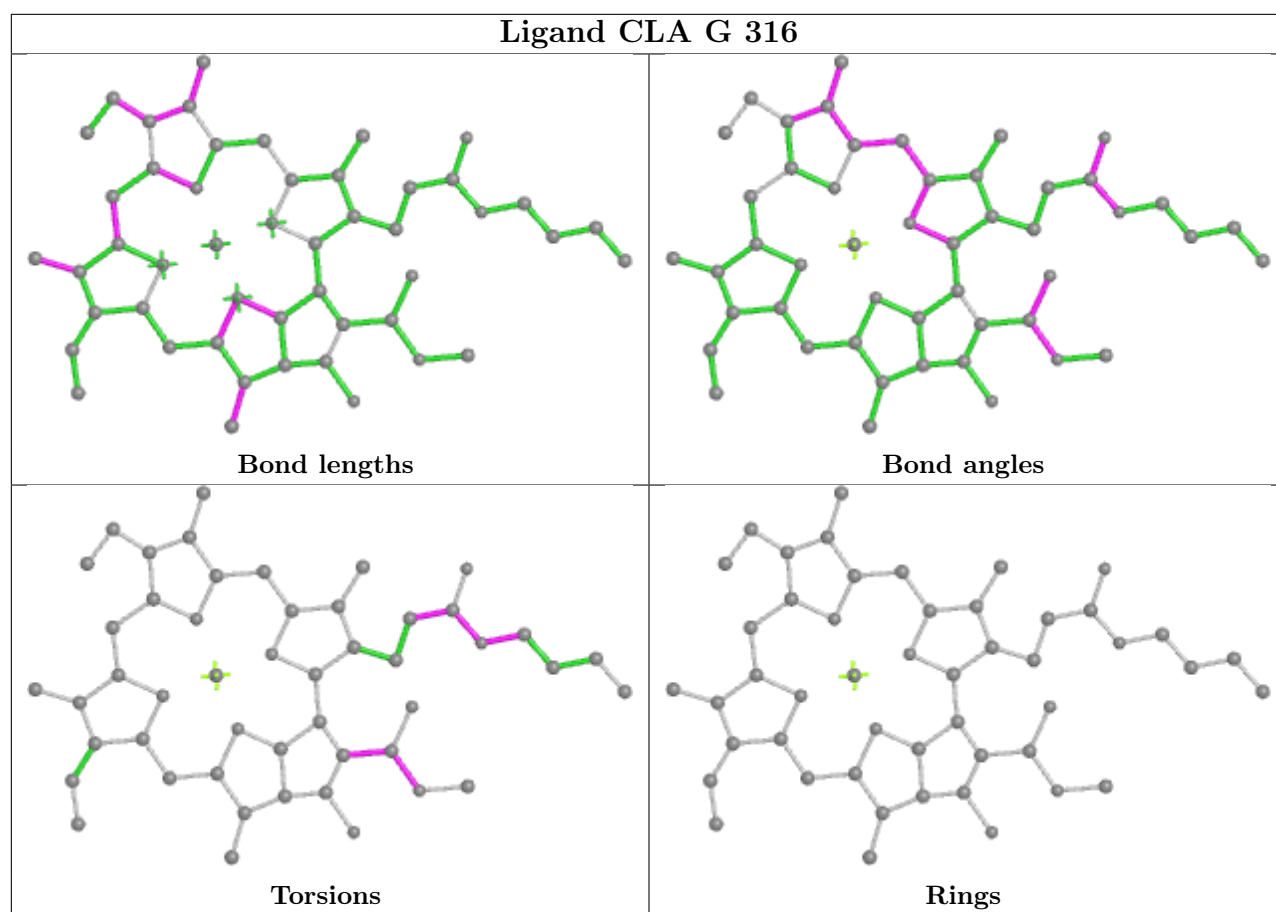
Bond angles



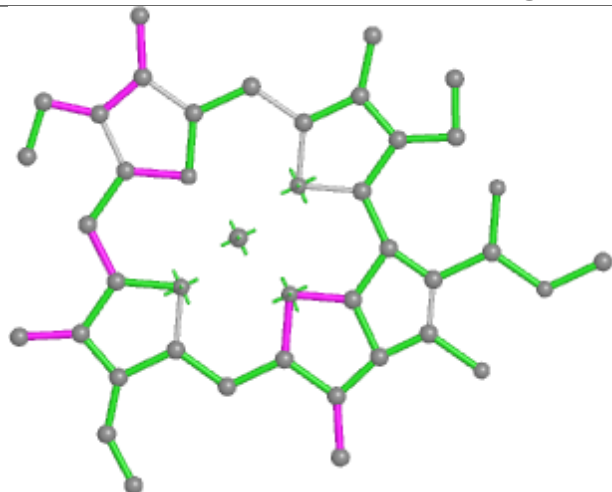
Torsions



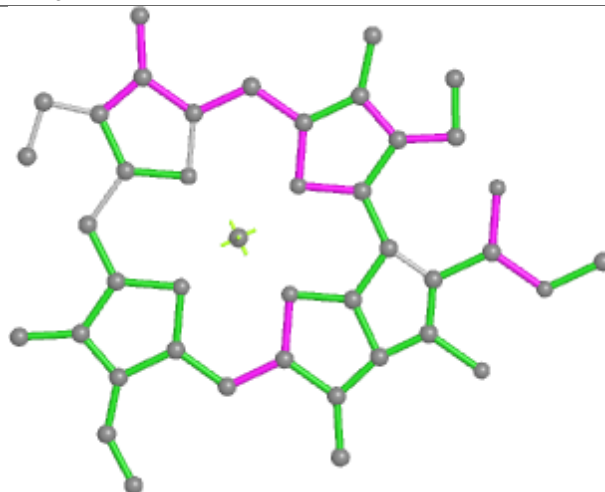
Rings



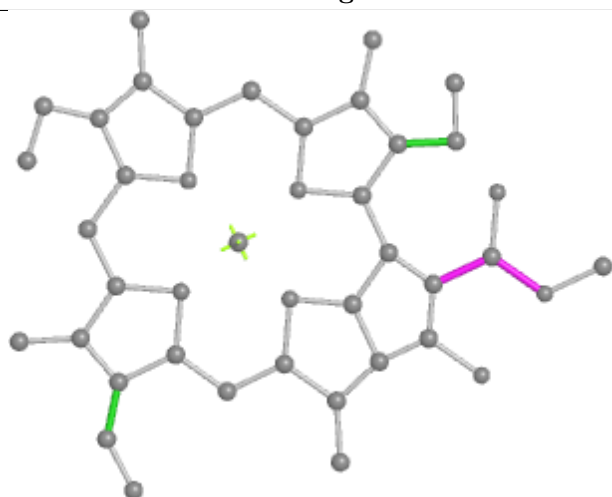
## Ligand CLA j 106



Bond lengths



Bond angles

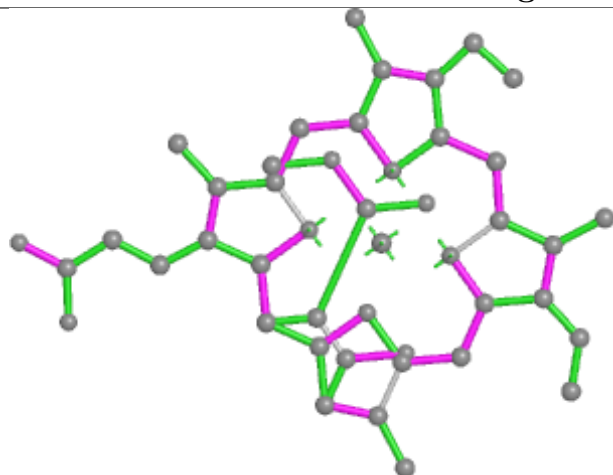


Torsions

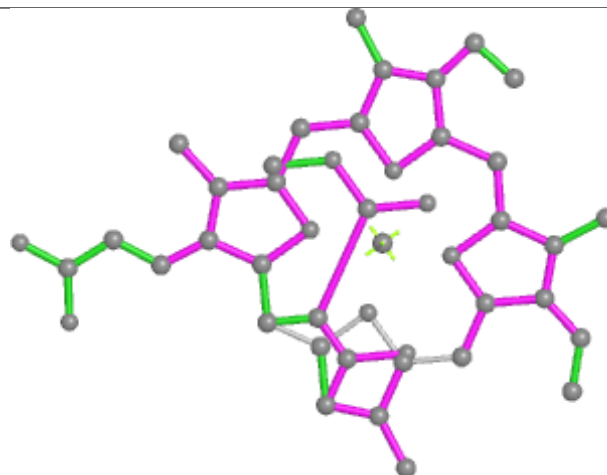


Rings

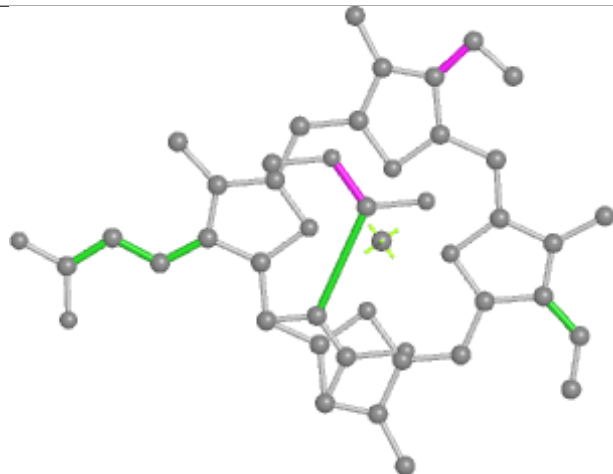
## Ligand KC1 F 315



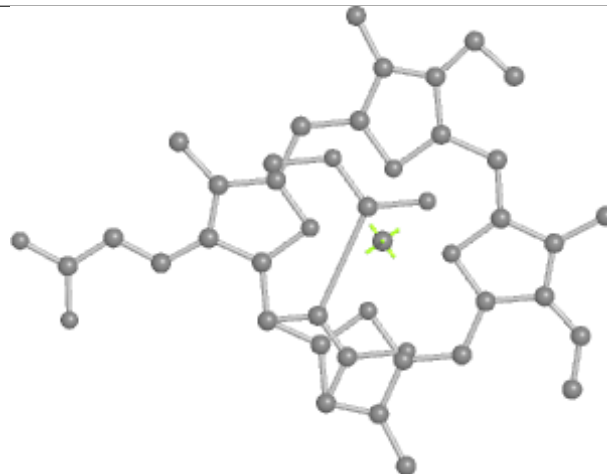
Bond lengths



Bond angles

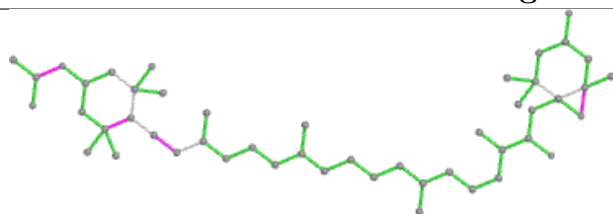


Torsions

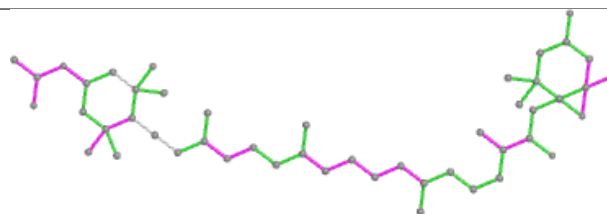


Rings

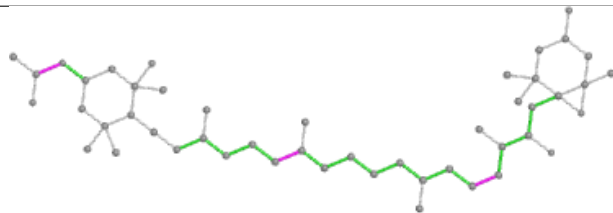
## Ligand A86 R 305



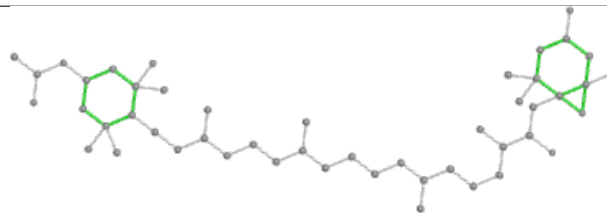
Bond lengths



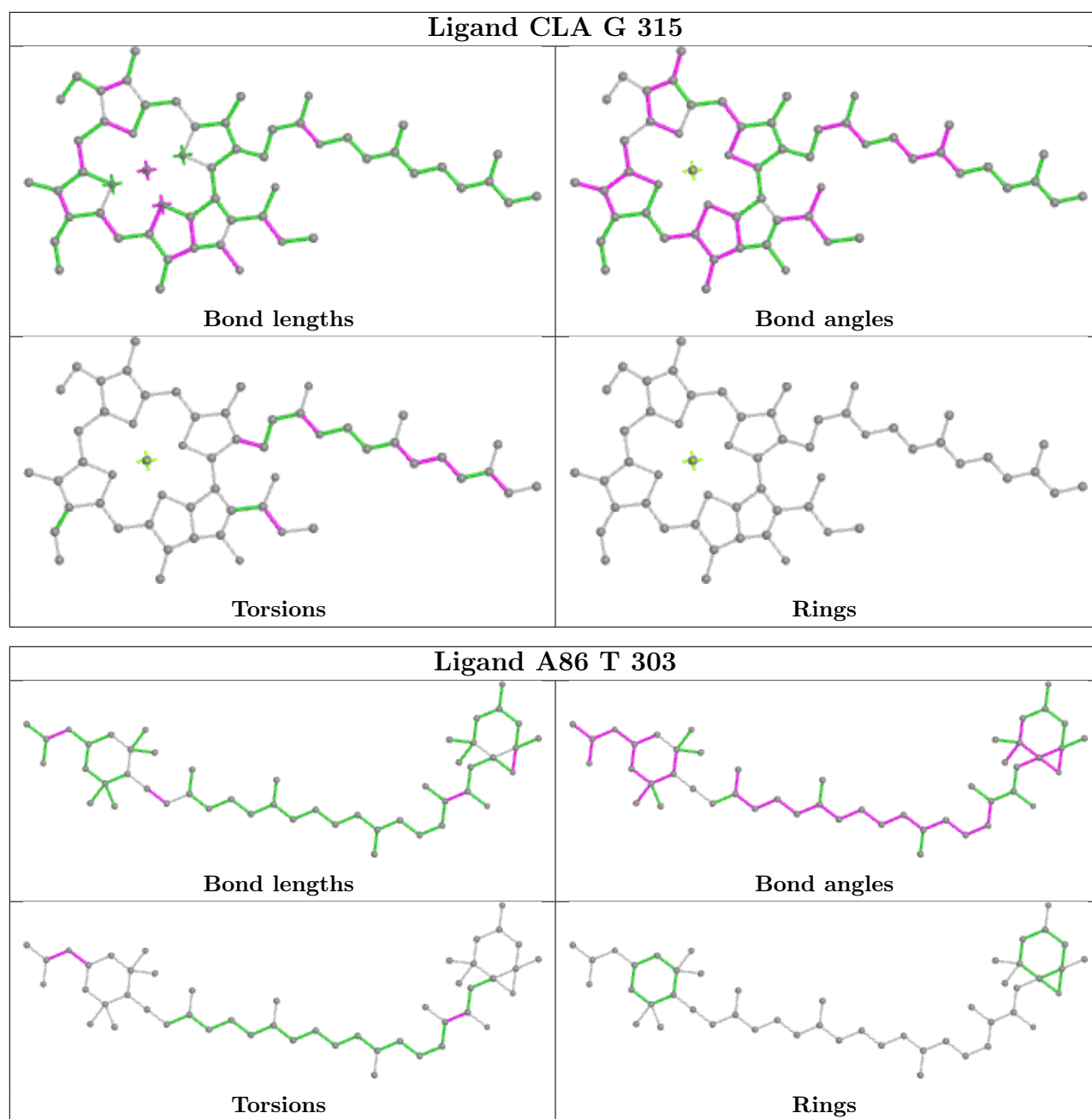
Bond angles



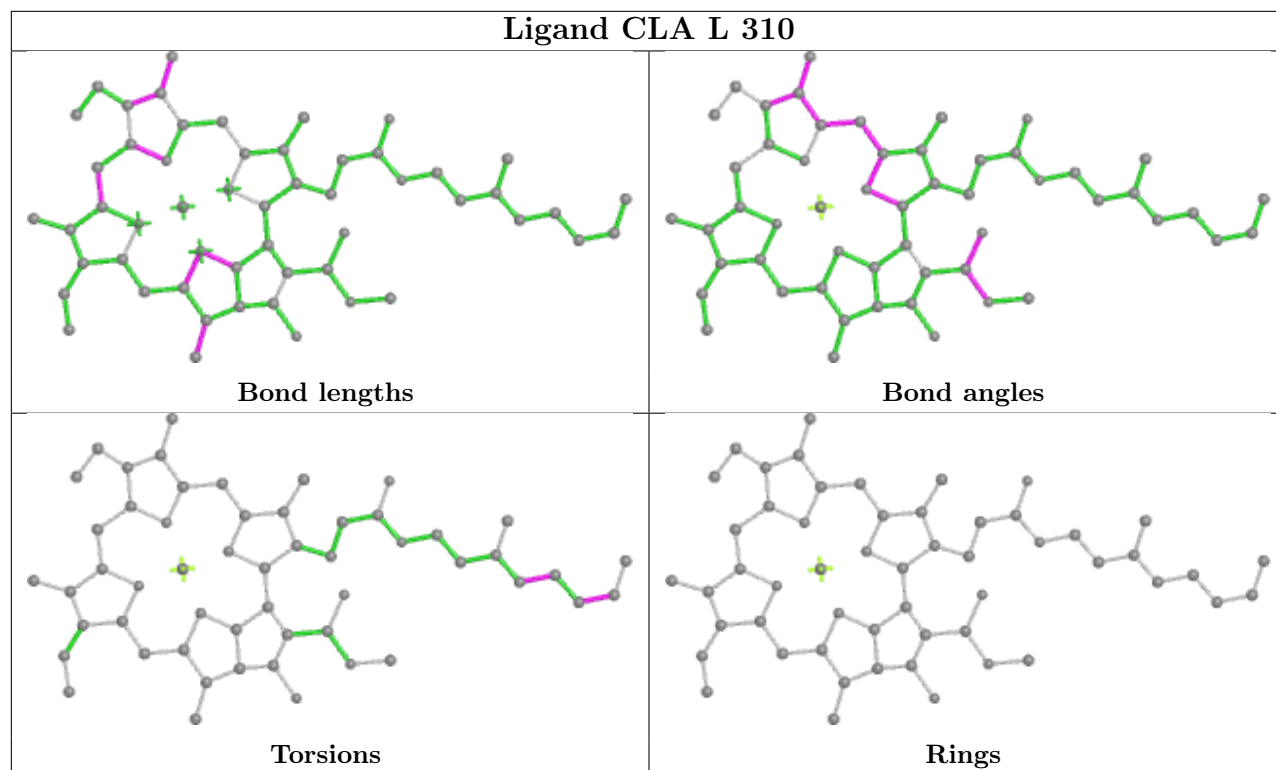
Torsions



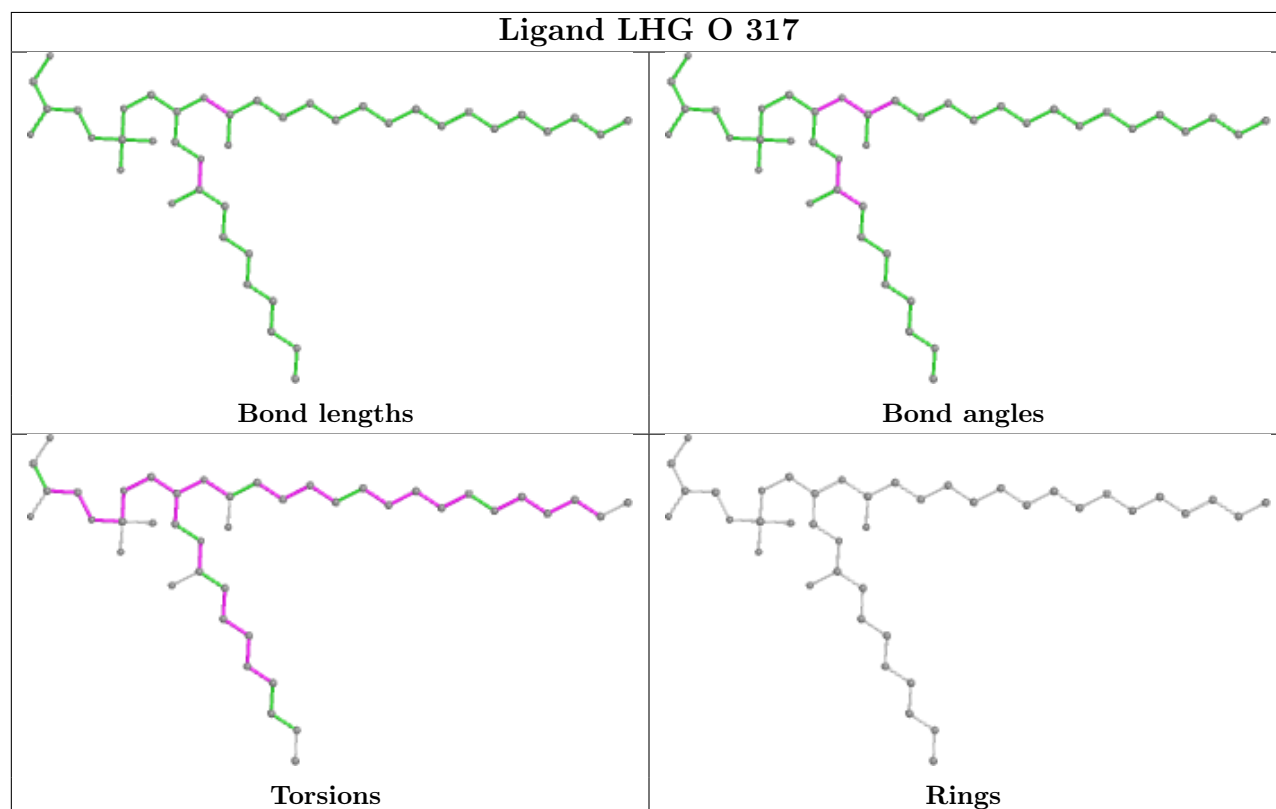
Rings



## Ligand CLA L 310

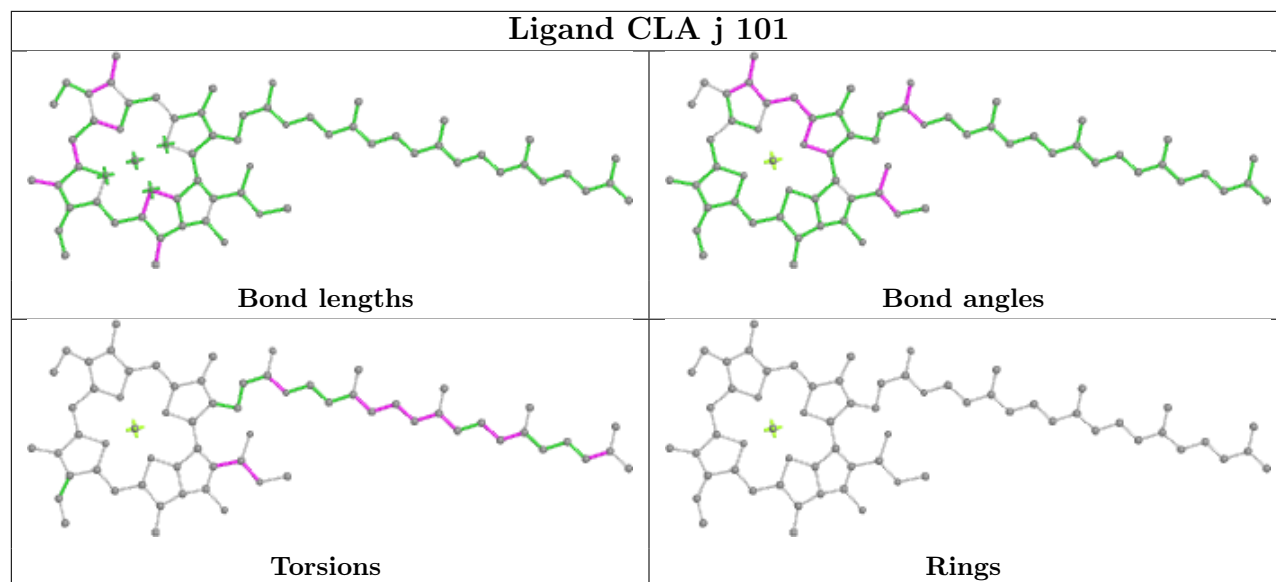


## Ligand LHG O 317

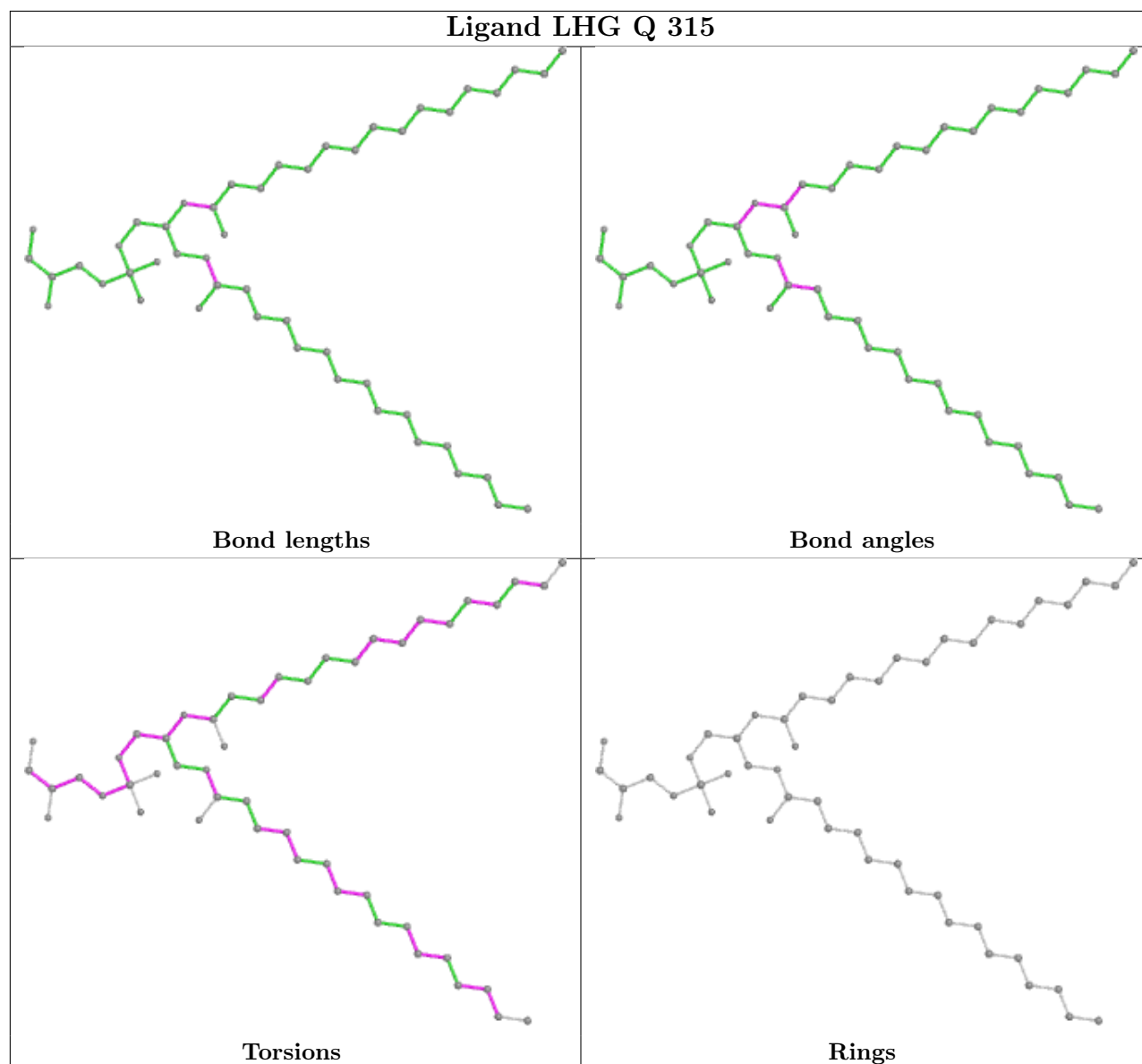




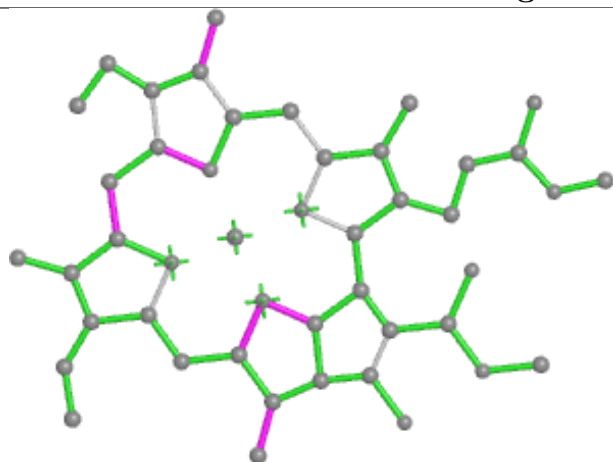
## Ligand CLA j 101



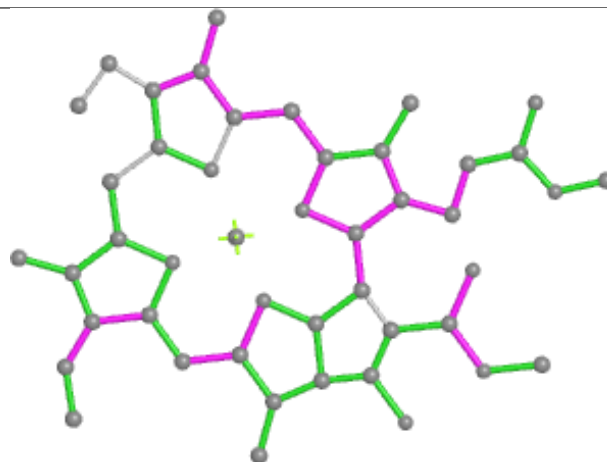
## Ligand LHG Q 315



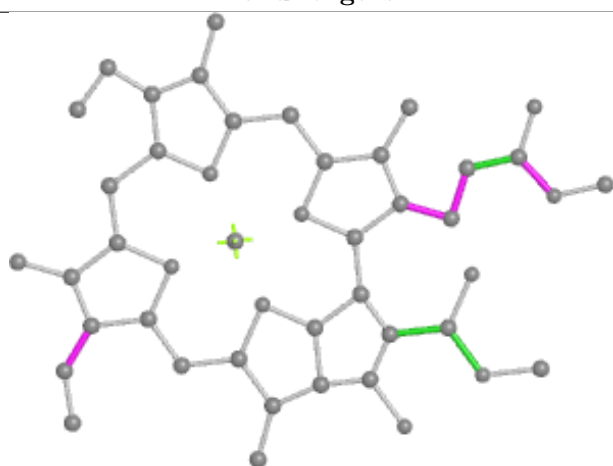
## Ligand CLA S 313



Bond lengths



Bond angles

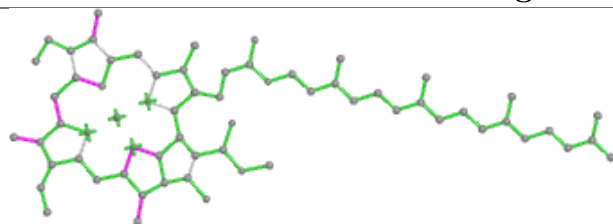


Torsions

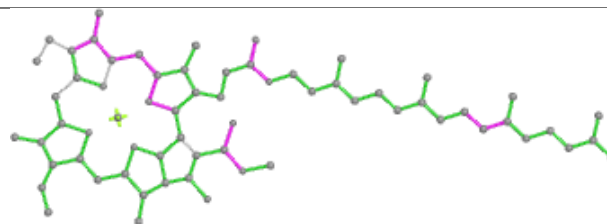


Rings

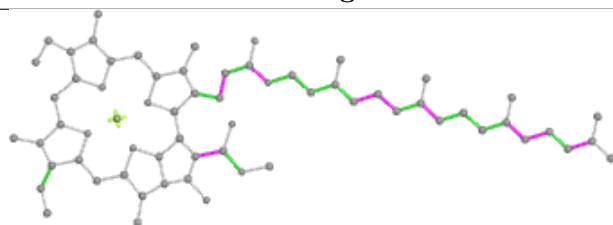
## Ligand CLA P 310



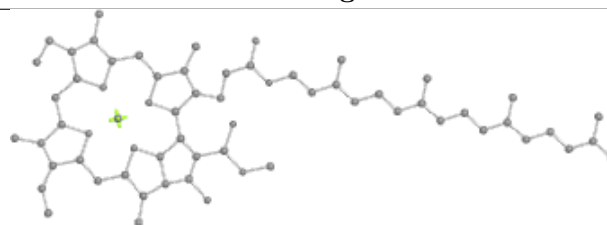
Bond lengths



Bond angles

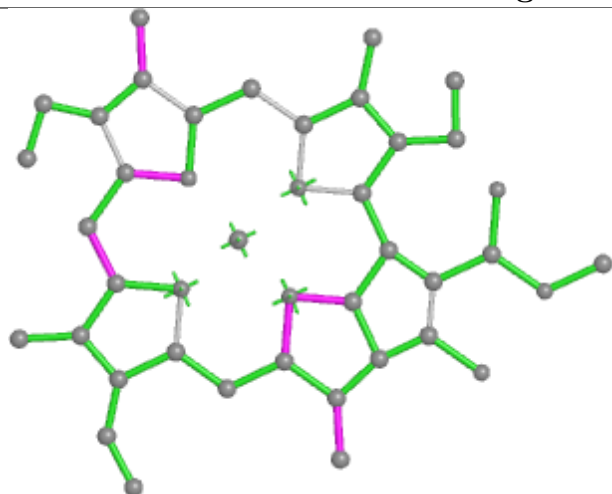


Torsions

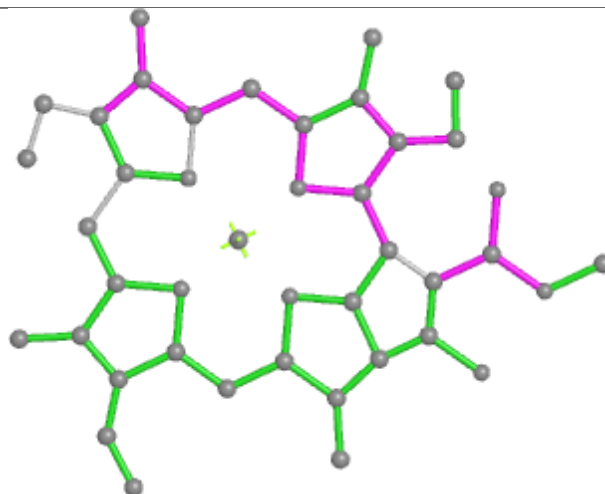


Rings

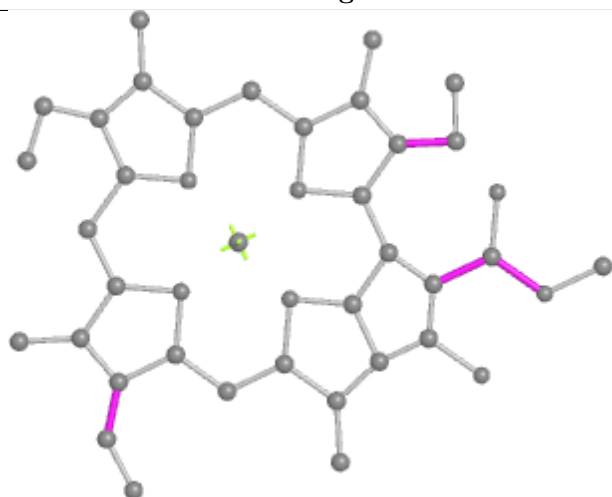
## Ligand CLA S 318



Bond lengths



Bond angles

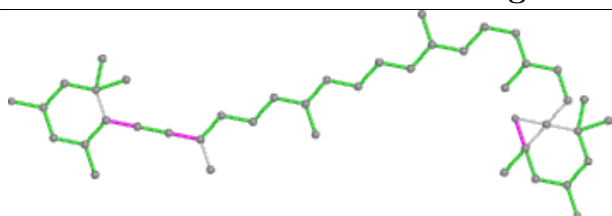


Torsions

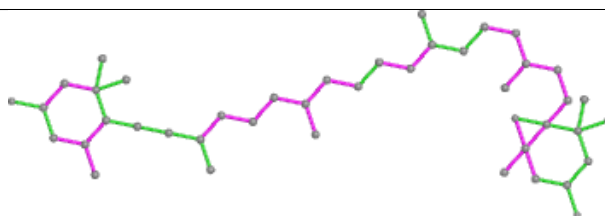


Rings

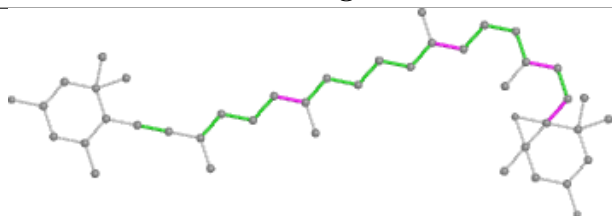
## Ligand DD6 W 205



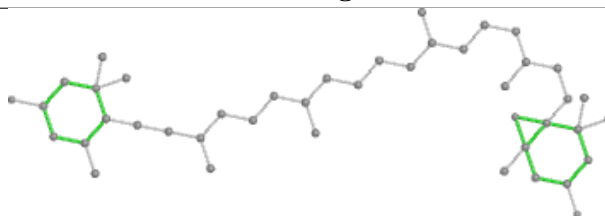
Bond lengths



Bond angles

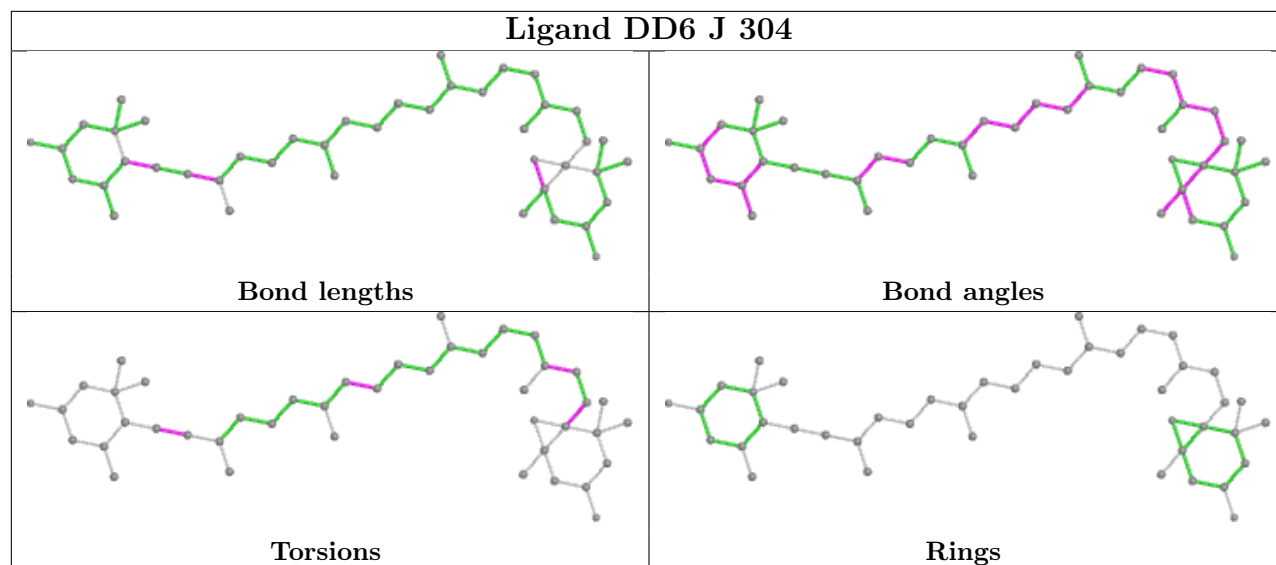


Torsions

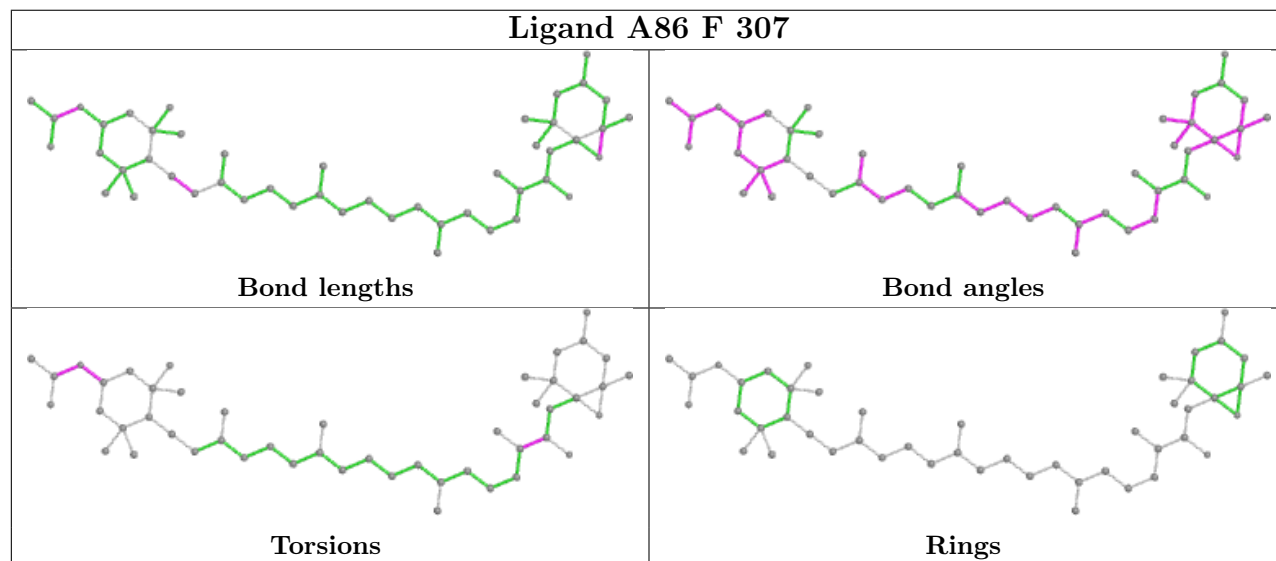


Rings

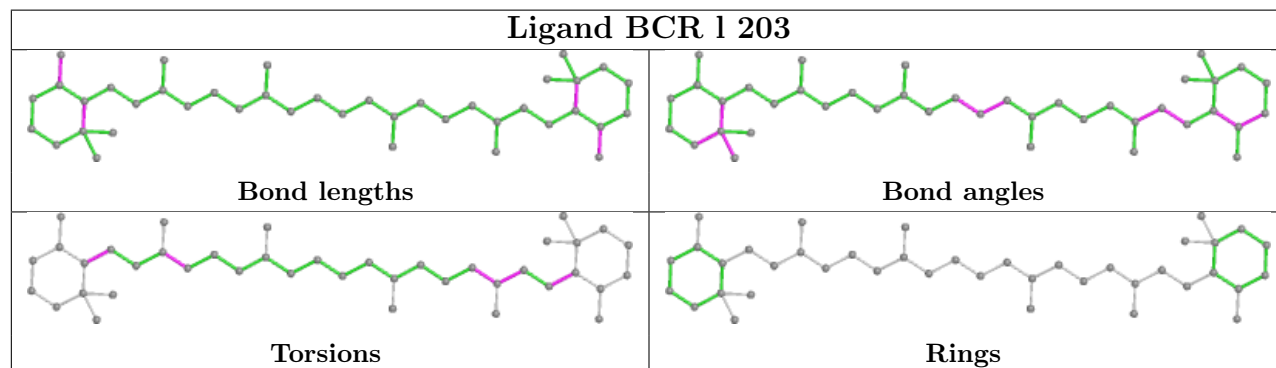
## Ligand DD6 J 304

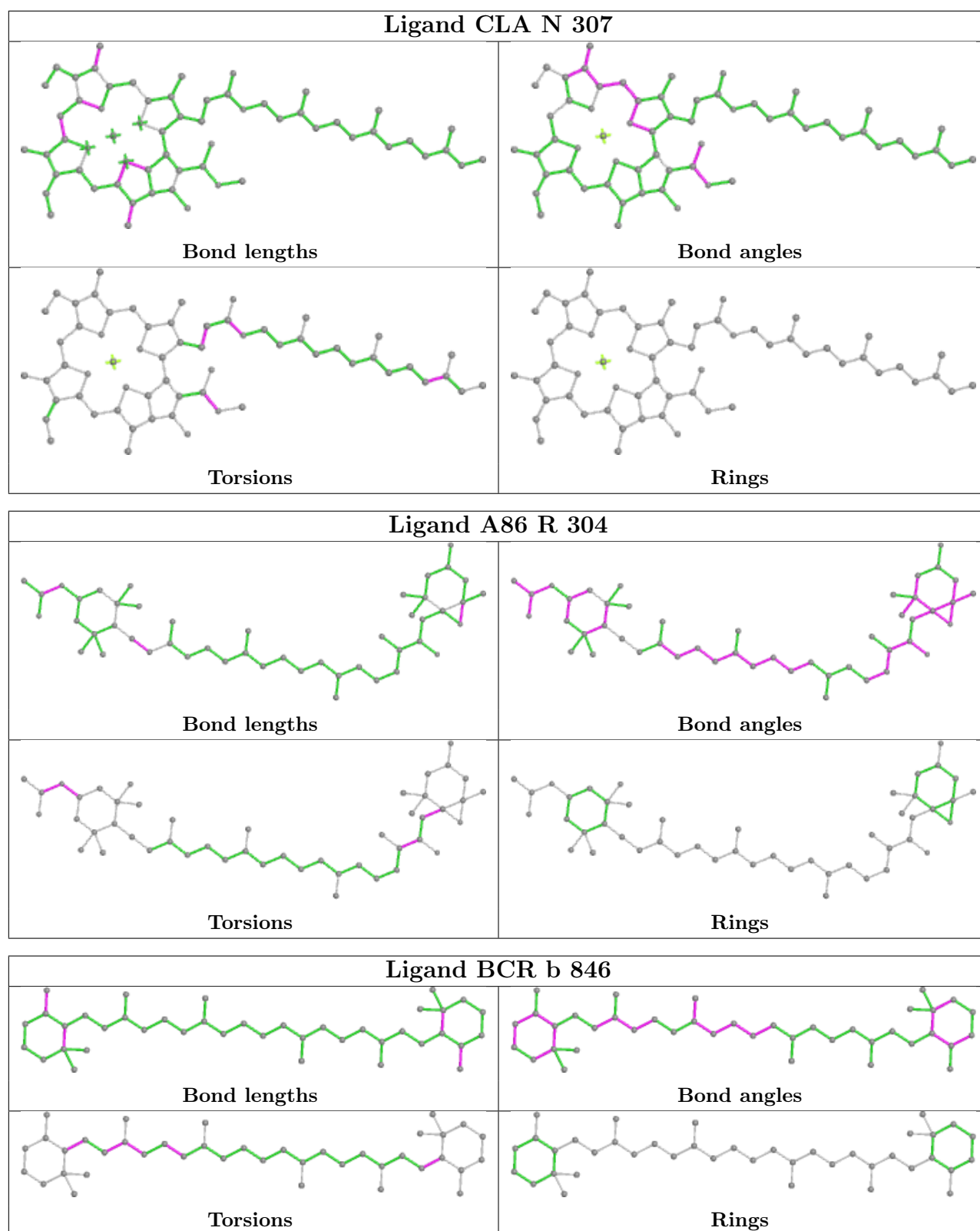


## Ligand A86 F 307

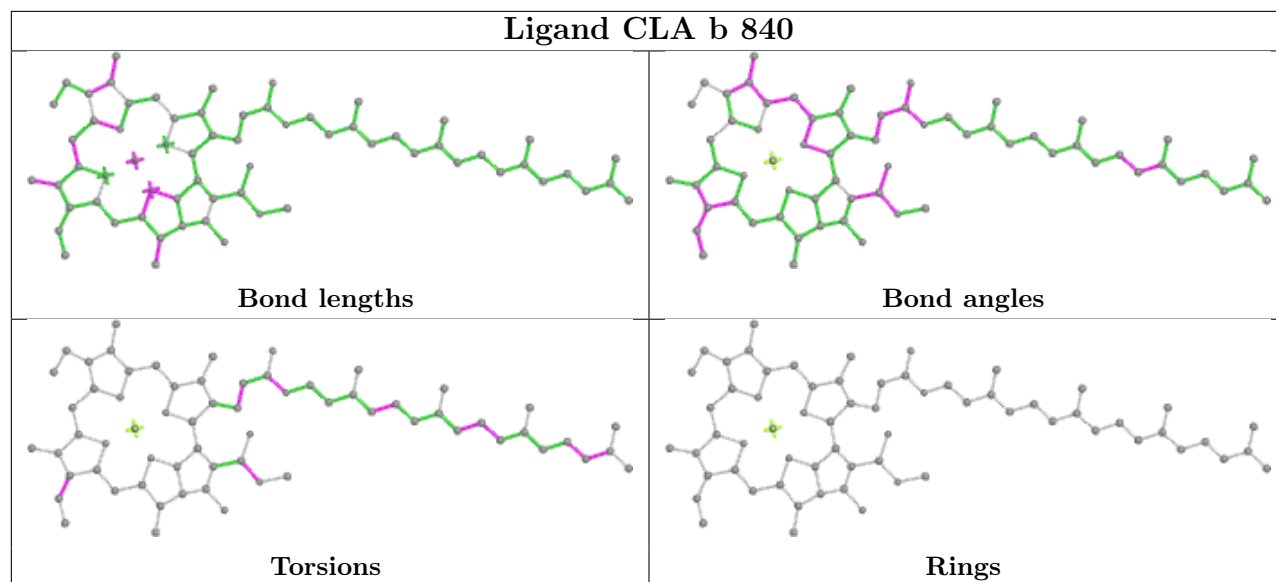


## Ligand BCR I 203

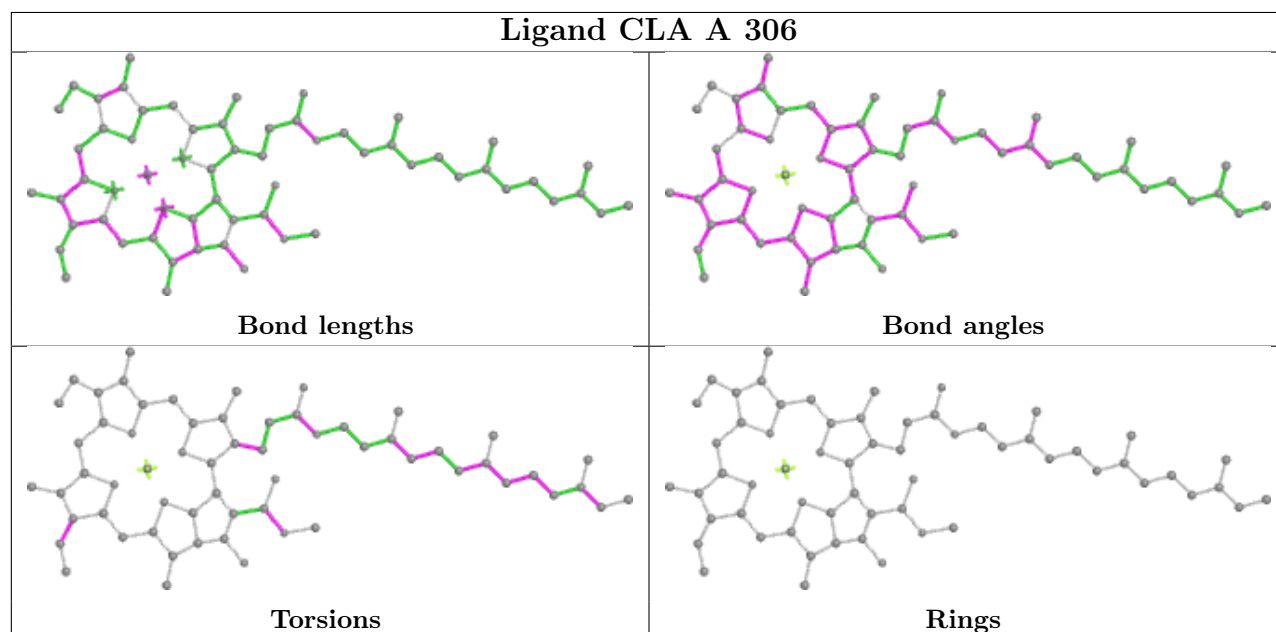




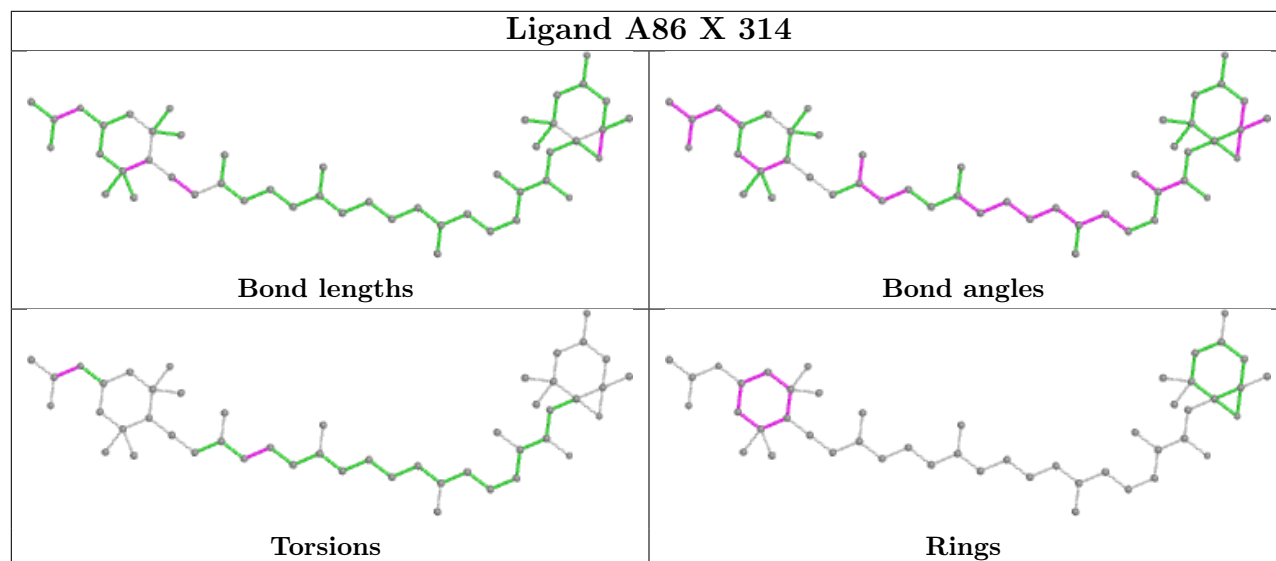
## Ligand CLA b 840



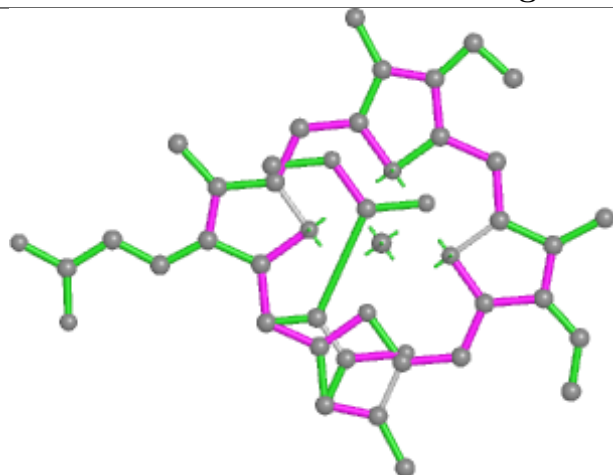
## Ligand CLA A 306



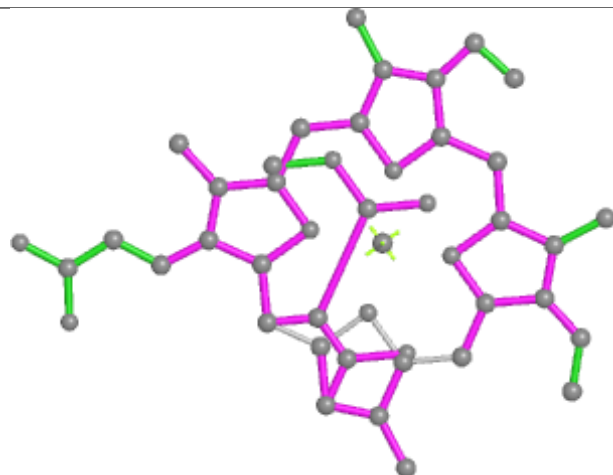
## Ligand A86 X 314



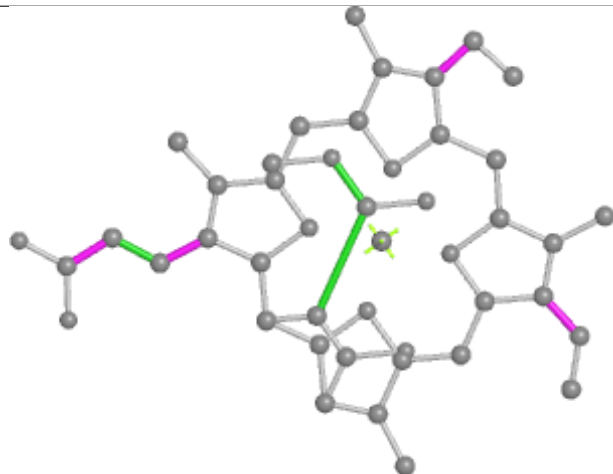
## Ligand KC1 S 316



Bond lengths



Bond angles

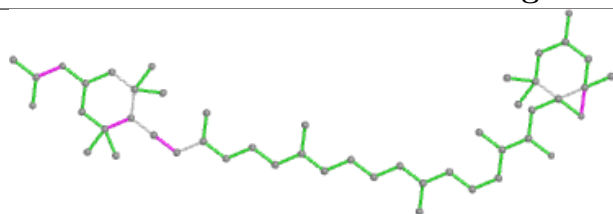


Torsions

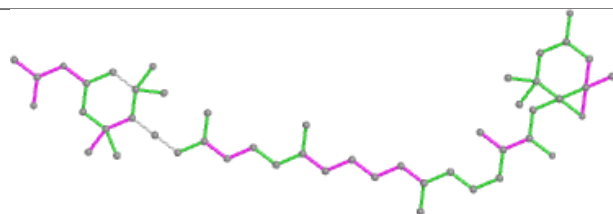


Rings

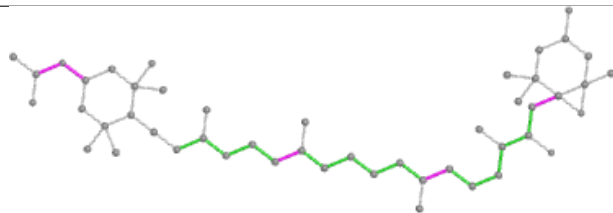
## Ligand A86 F 302



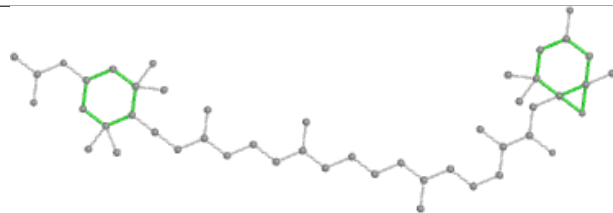
Bond lengths



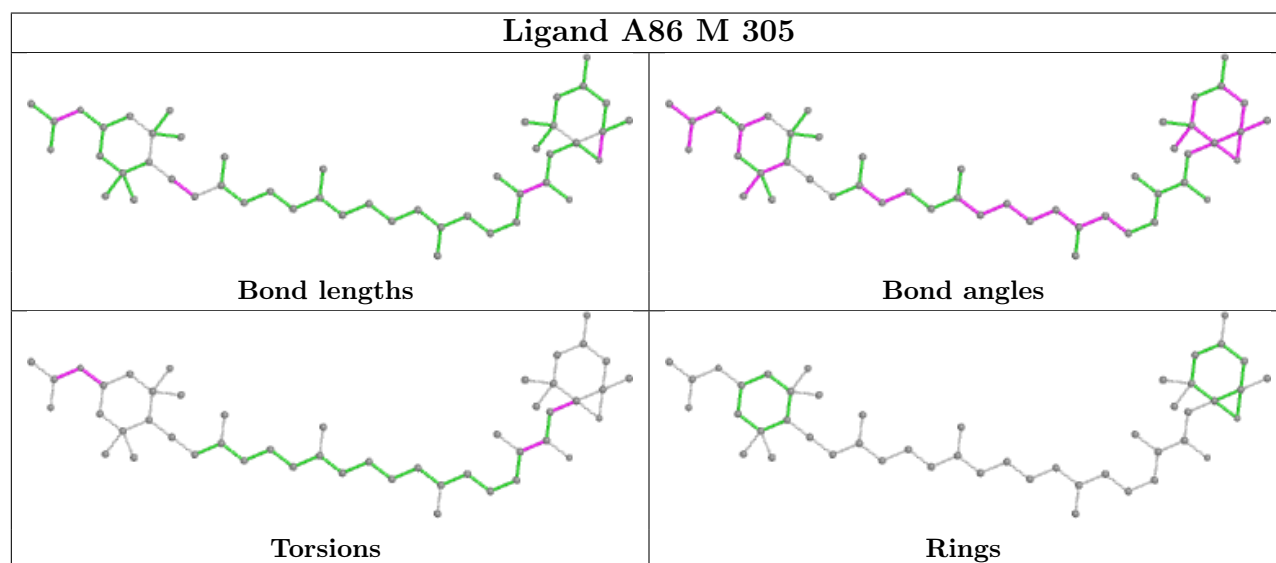
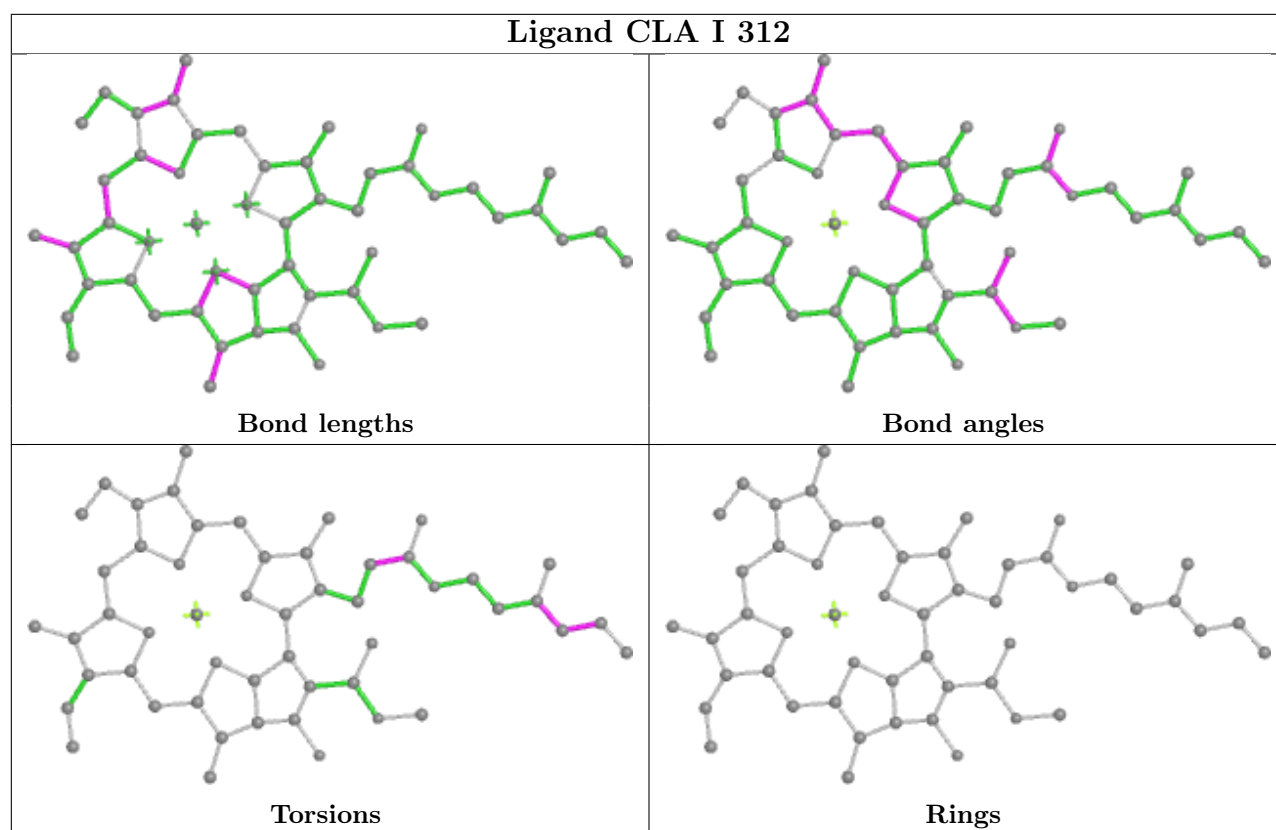
Bond angles



Torsions

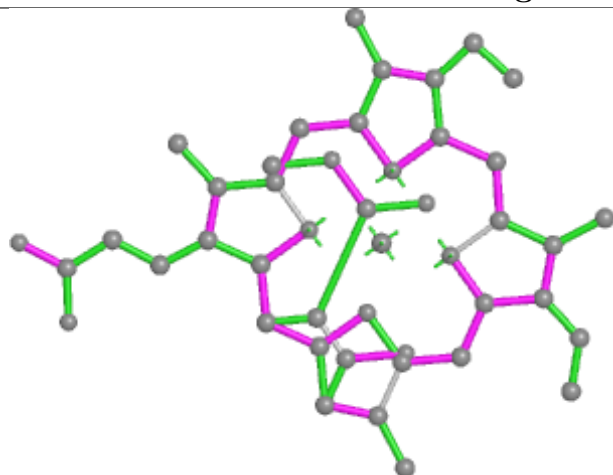


Rings

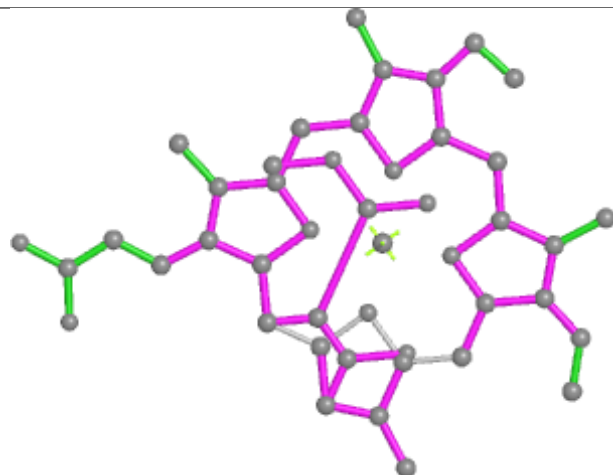




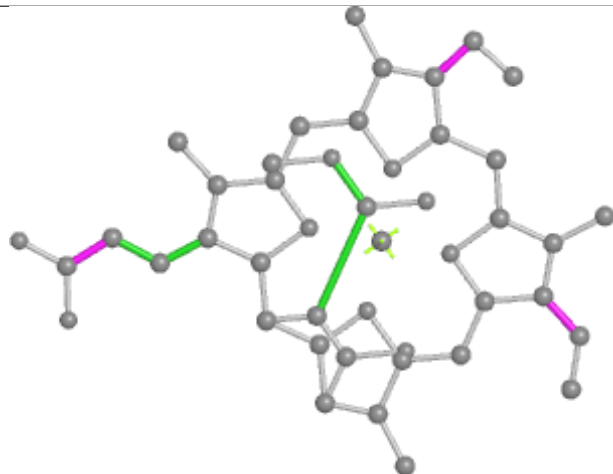
## Ligand KC1 G 308



Bond lengths



Bond angles

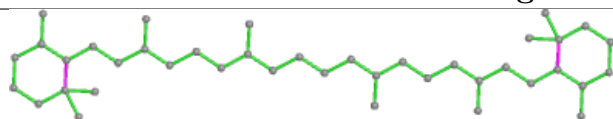


Torsions

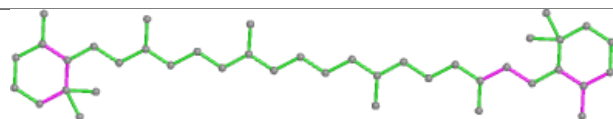


Rings

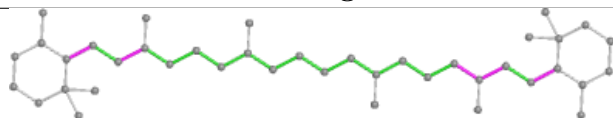
## Ligand BCR a 845



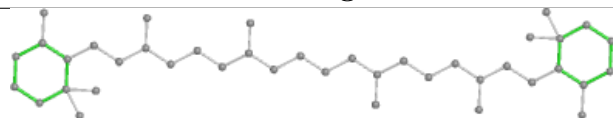
Bond lengths



Bond angles

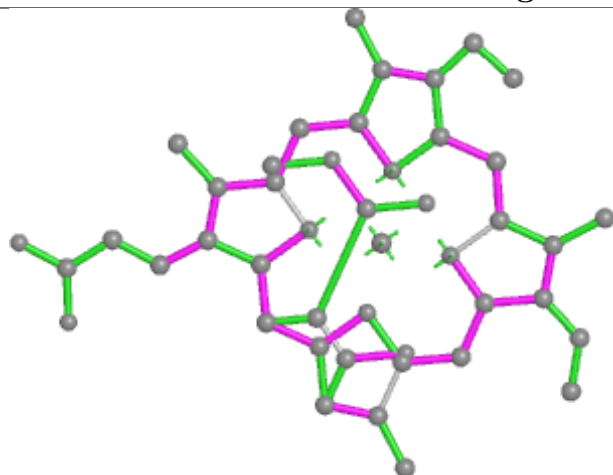


Torsions

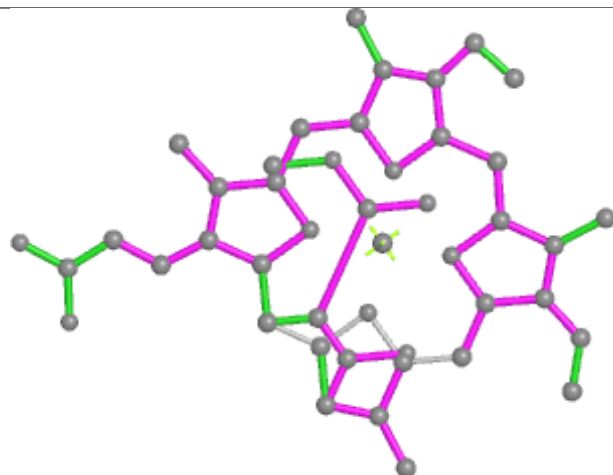


Rings

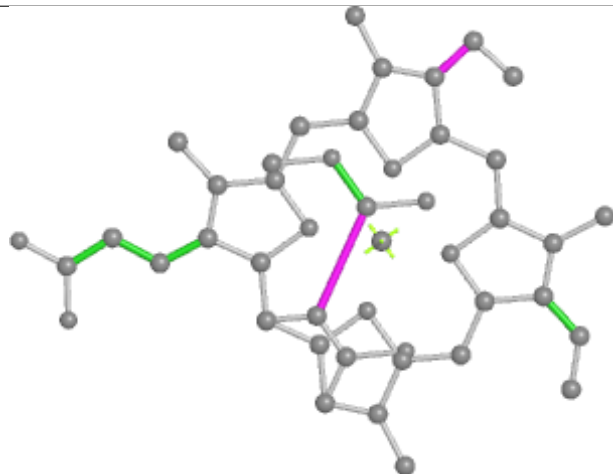
## Ligand KC1 P 315



Bond lengths



Bond angles

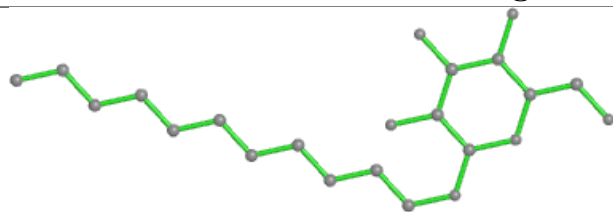


Torsions

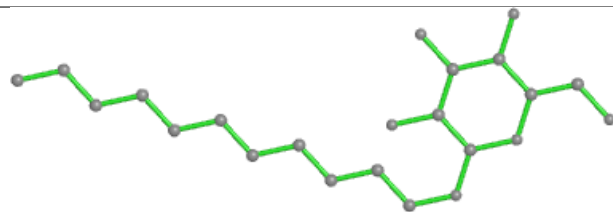


Rings

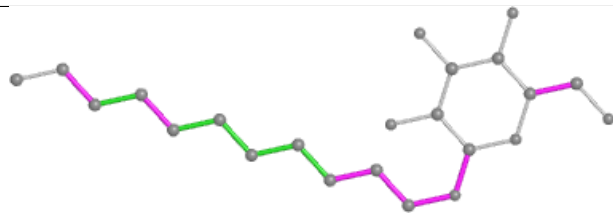
## Ligand LMT P 320



Bond lengths



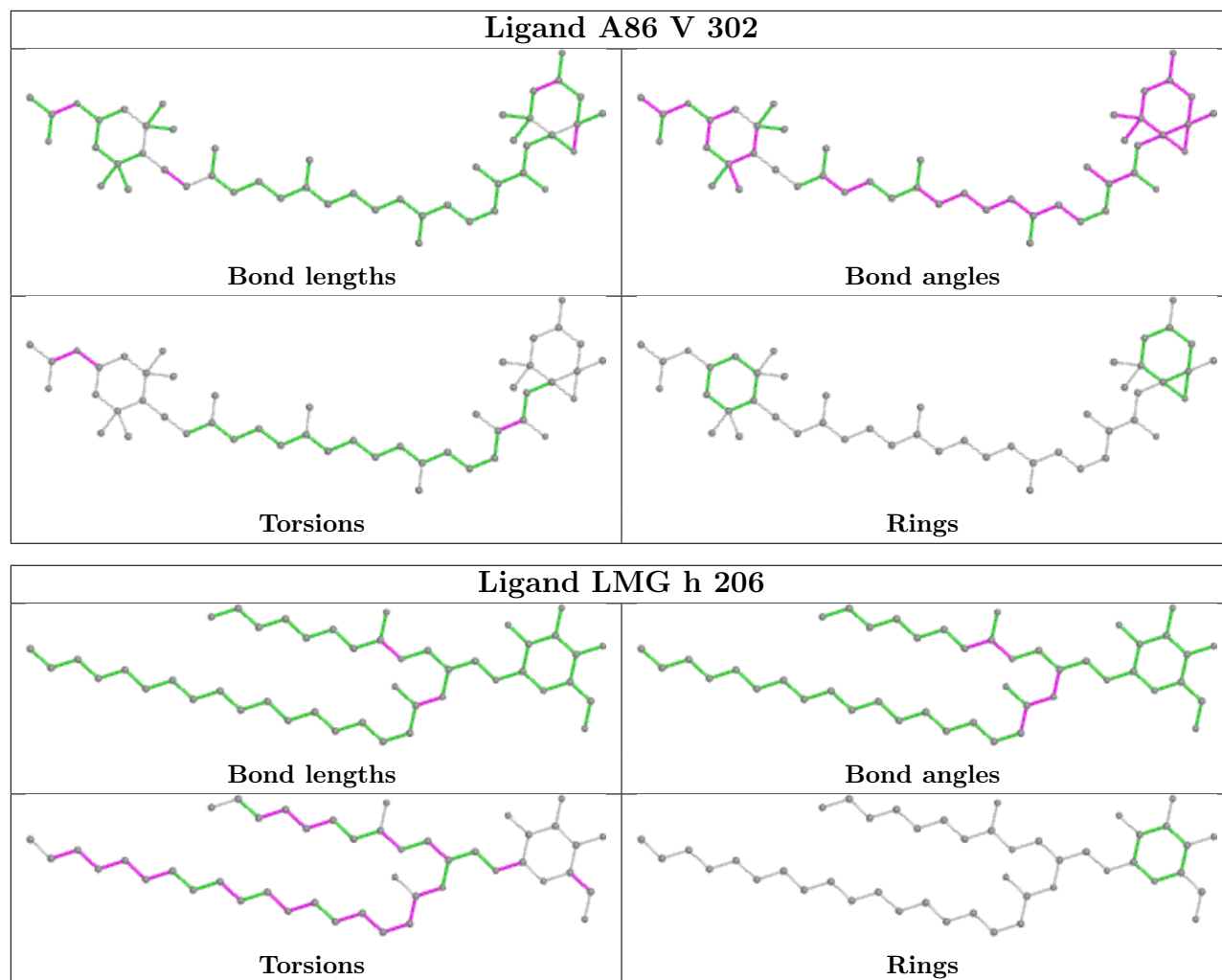
Bond angles



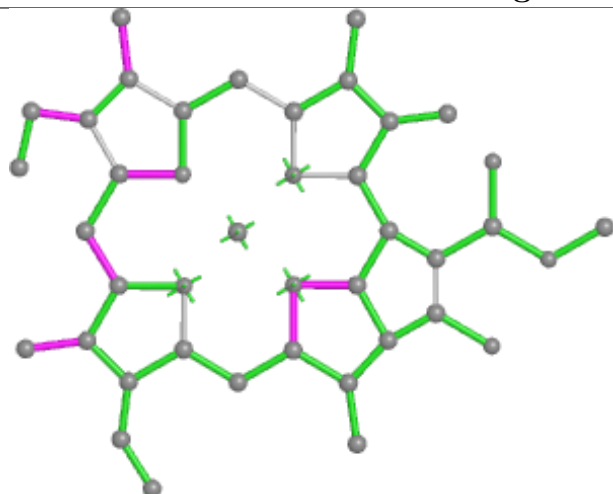
Torsions



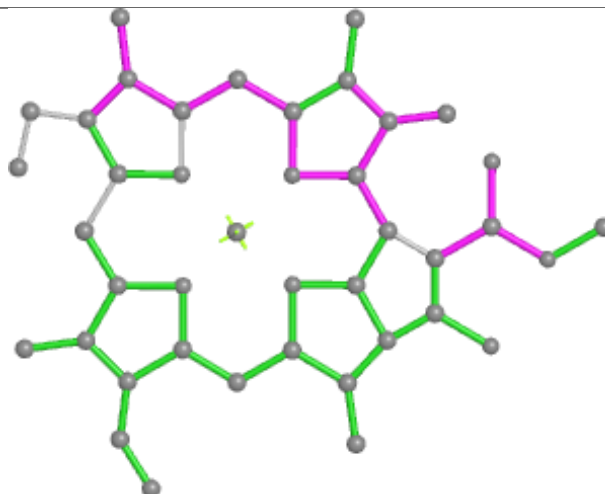
Rings



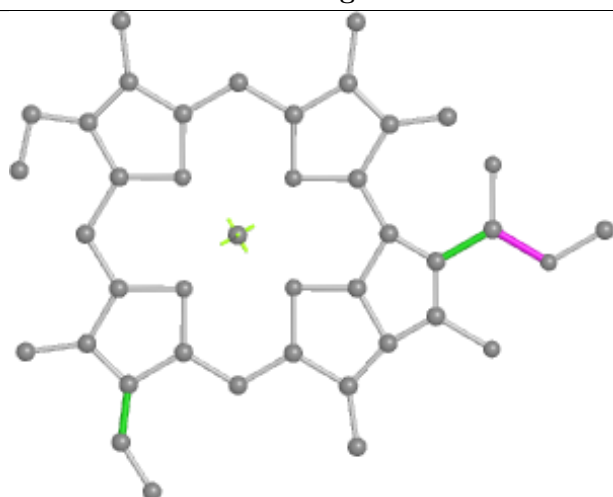
## Ligand CLA U 313



Bond lengths



Bond angles

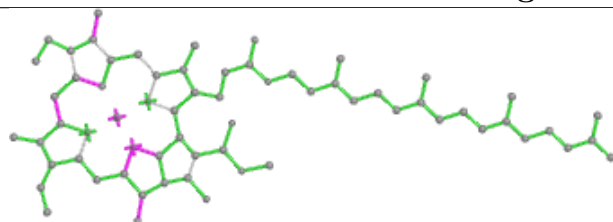


Torsions

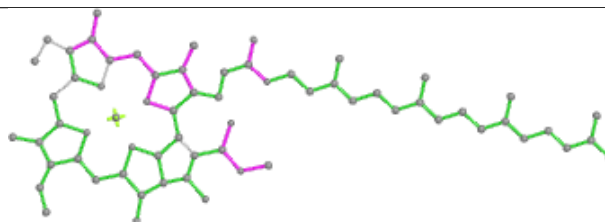


Rings

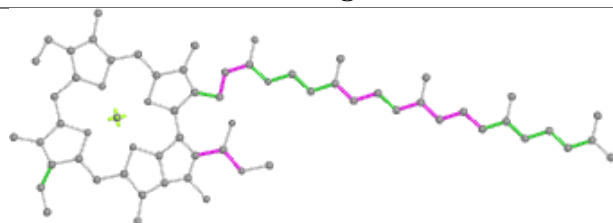
## Ligand CLA S 312



Bond lengths



Bond angles

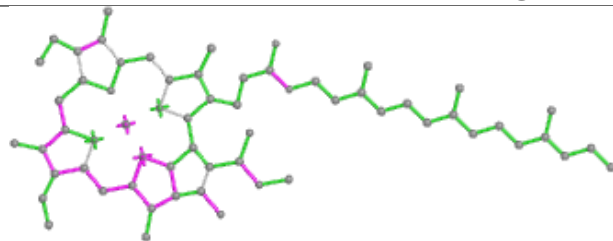


Torsions

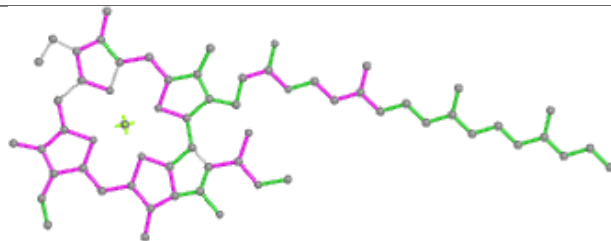


Rings

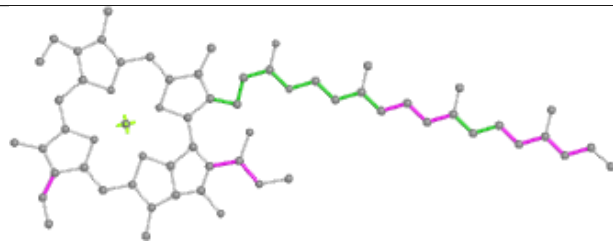
## Ligand CLA K 310



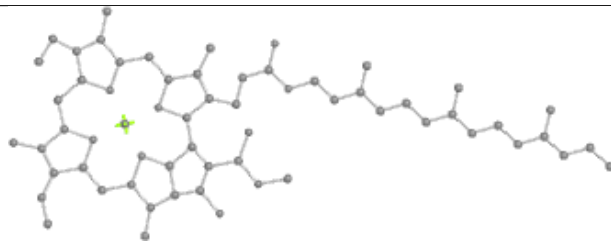
Bond lengths



Bond angles

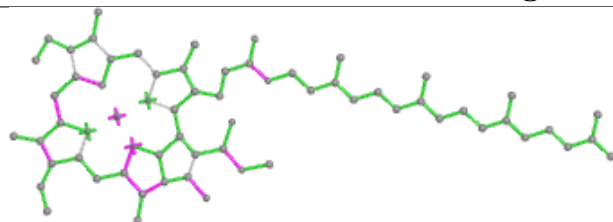


Torsions

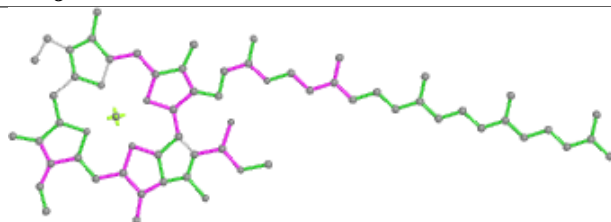


Rings

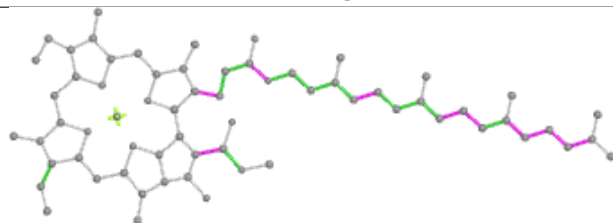
## Ligand CLA j 102



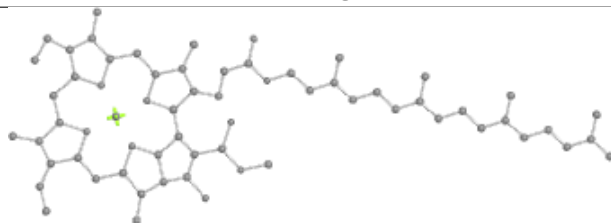
Bond lengths



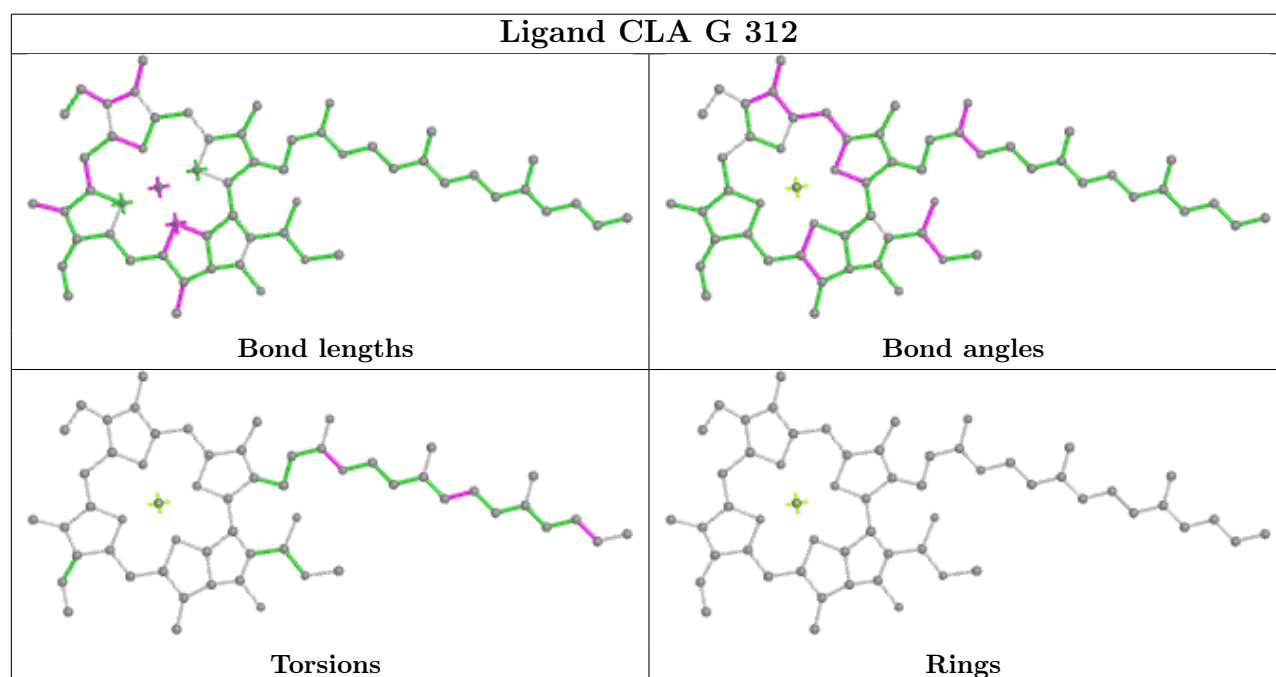
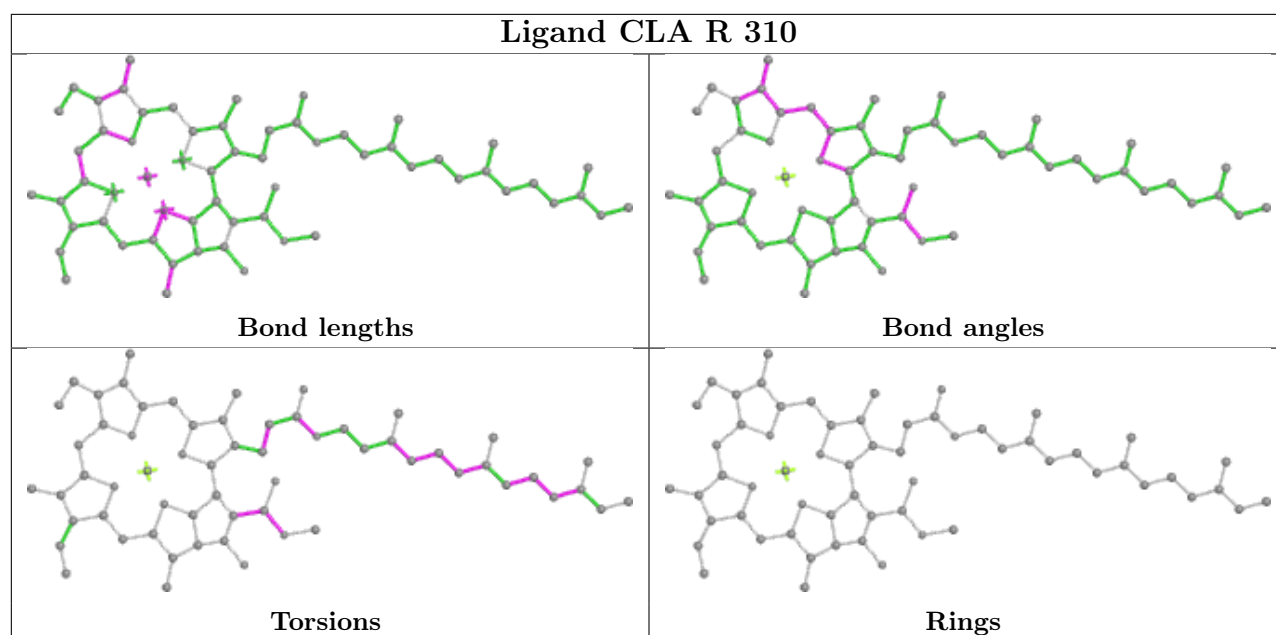
Bond angles



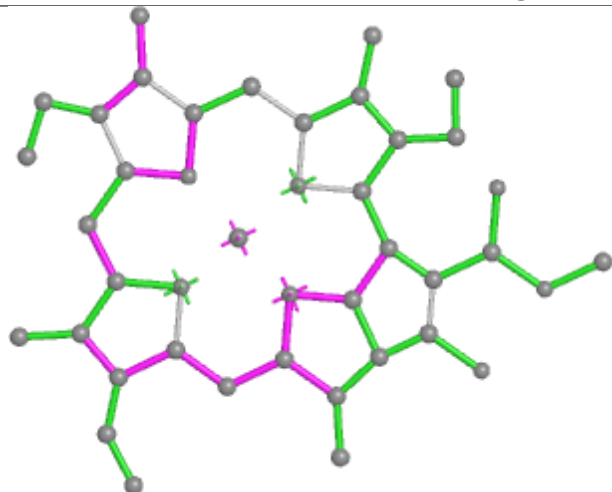
Torsions



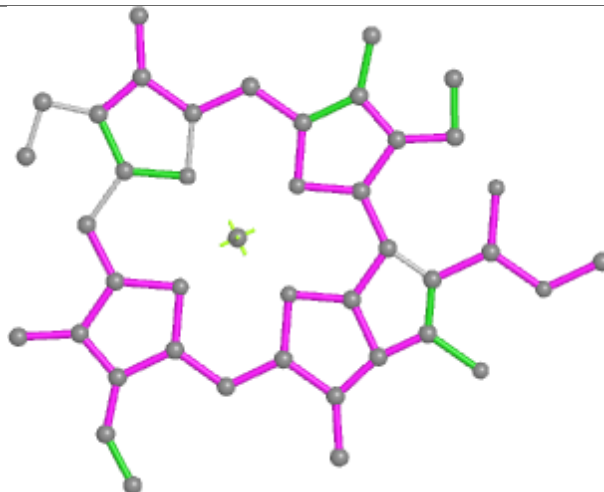
Rings



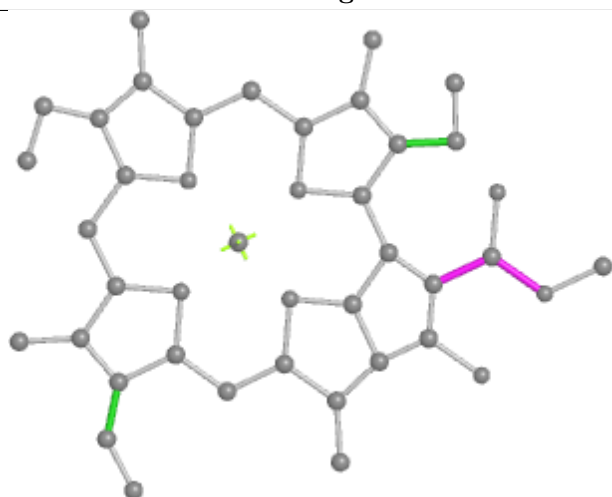
## Ligand CLA N 319



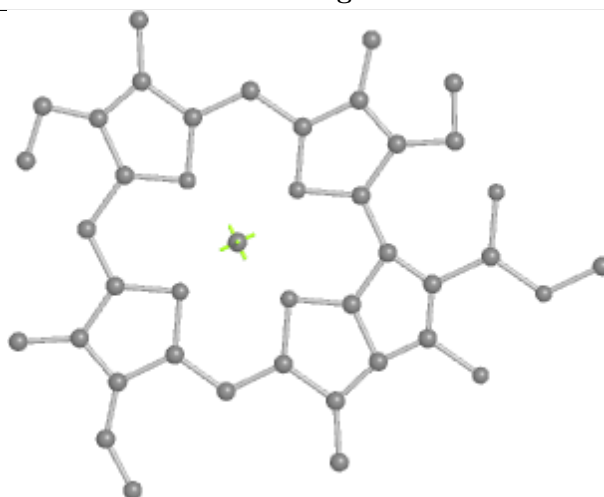
Bond lengths



Bond angles

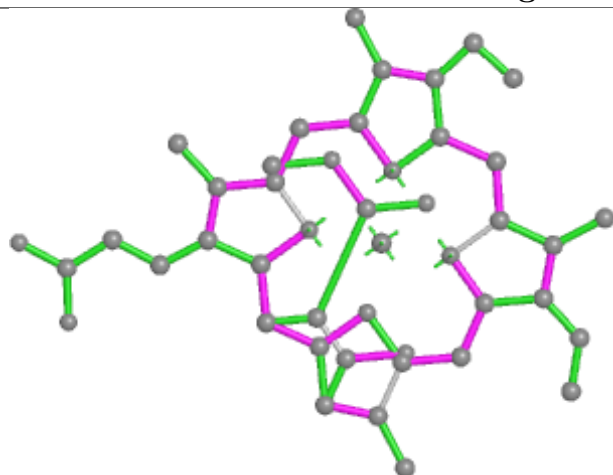


Torsions

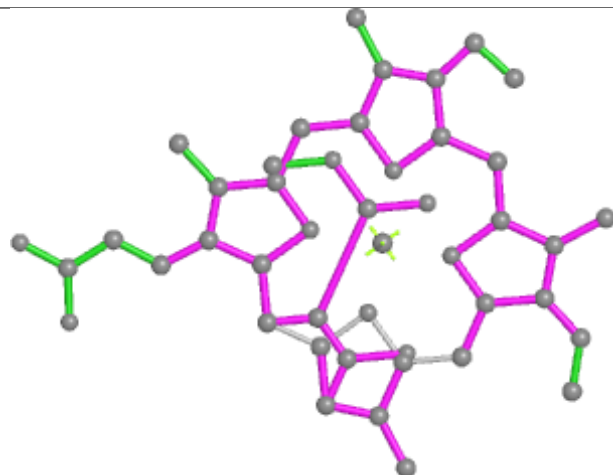


Rings

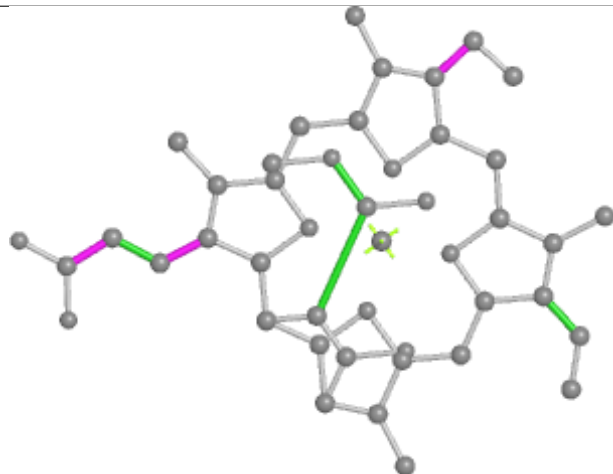
## Ligand KC1 L 315



Bond lengths



Bond angles

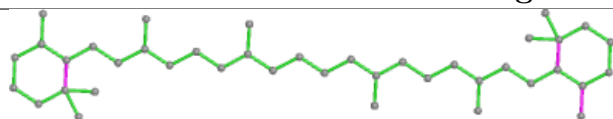


Torsions

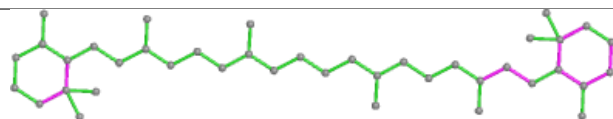


Rings

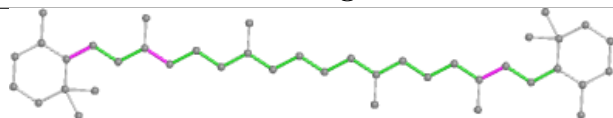
## Ligand BCR b 844



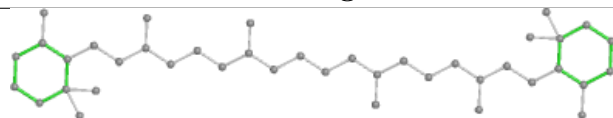
Bond lengths



Bond angles



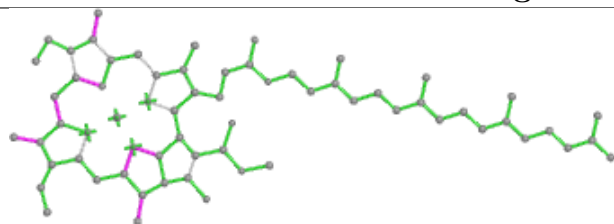
Torsions



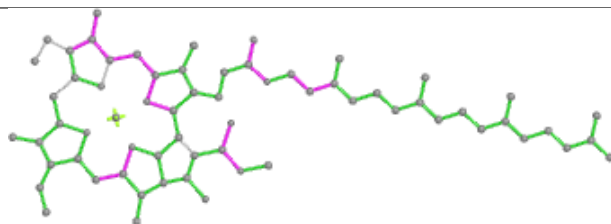
Rings



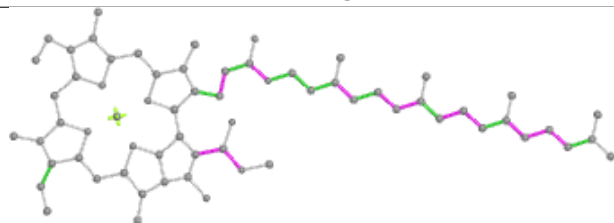
## Ligand CLA V 308



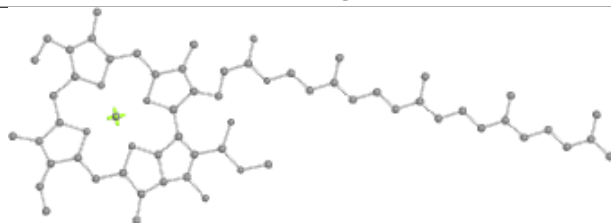
Bond lengths



Bond angles

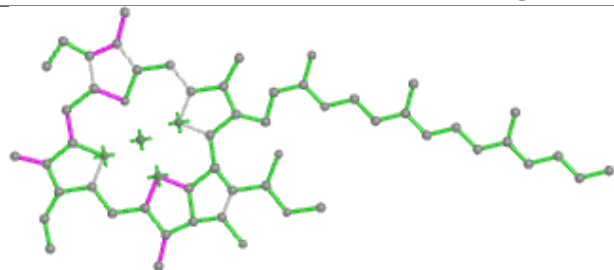


Torsions

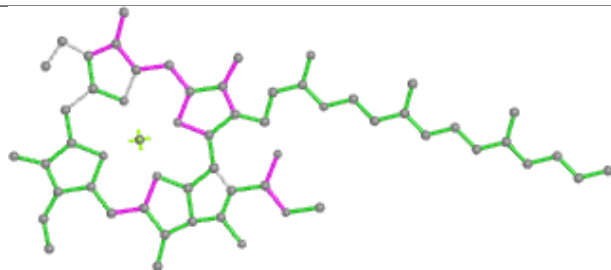


Rings

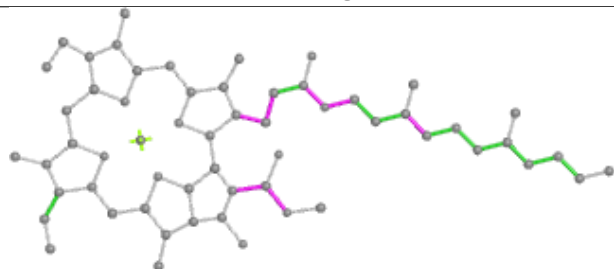
## Ligand CLA D 317



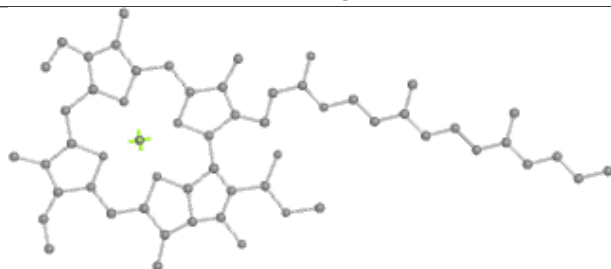
Bond lengths



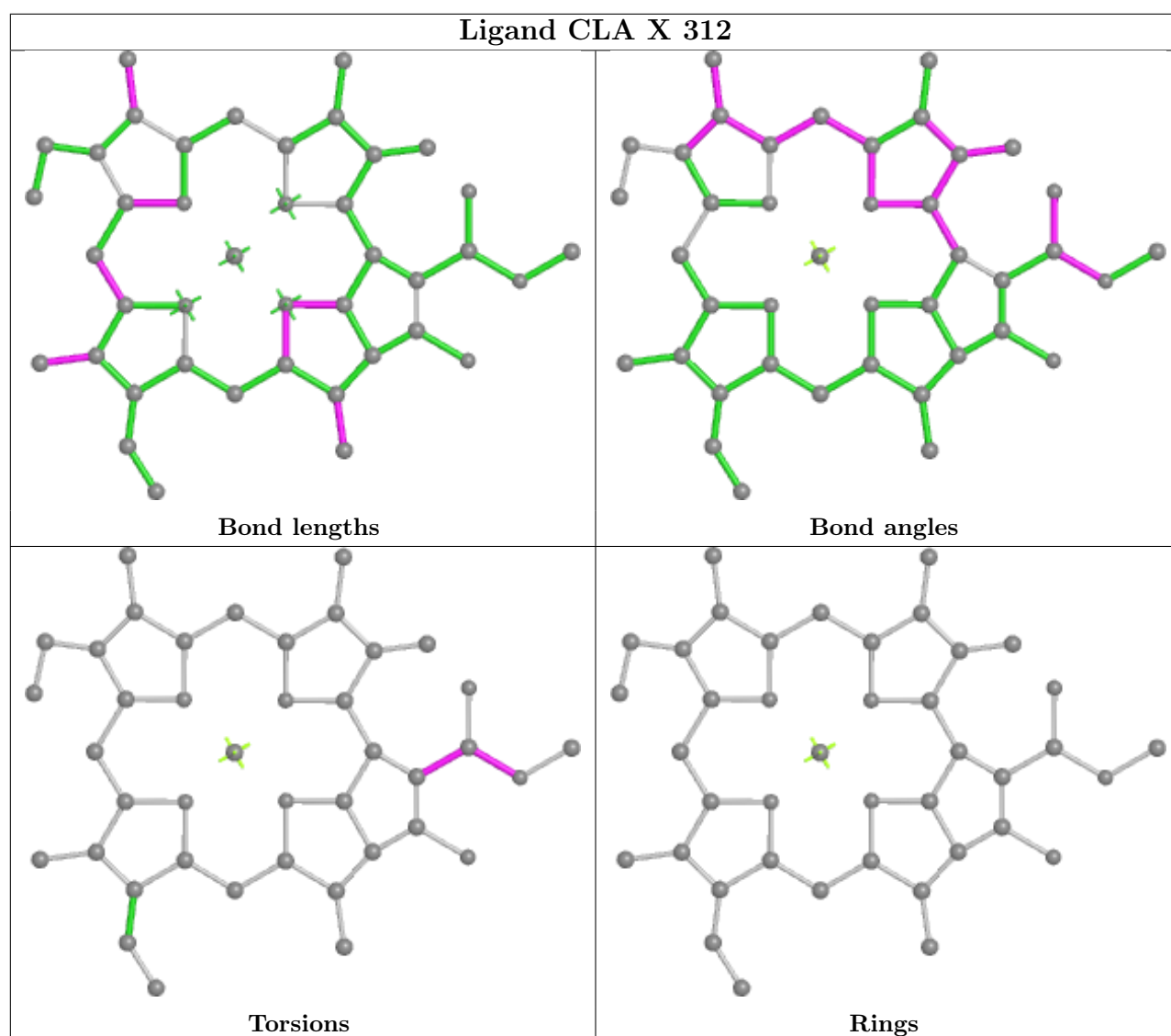
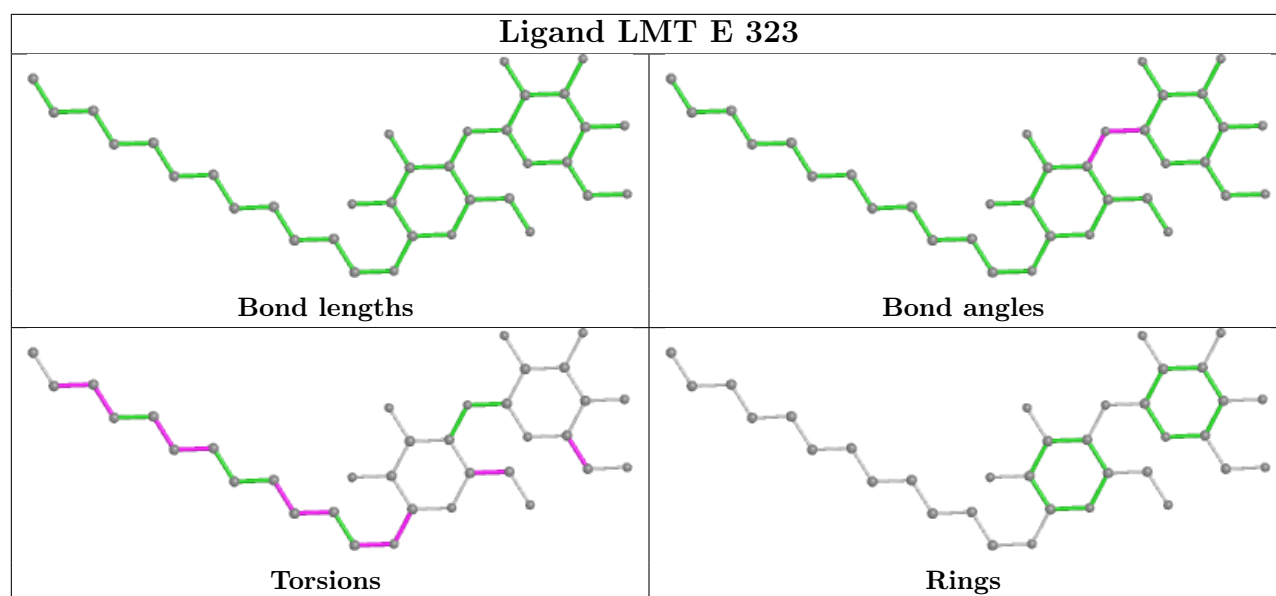
Bond angles

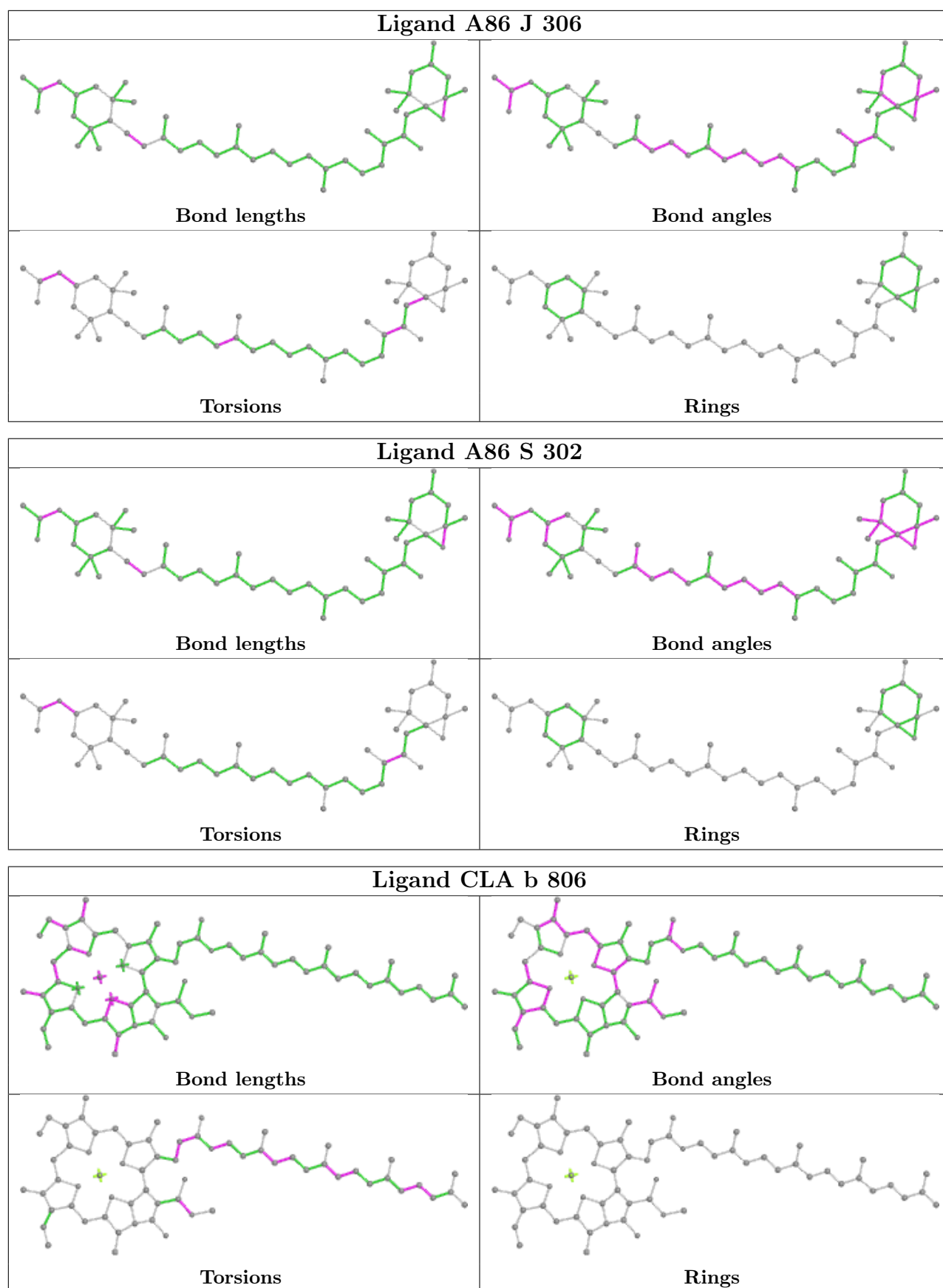


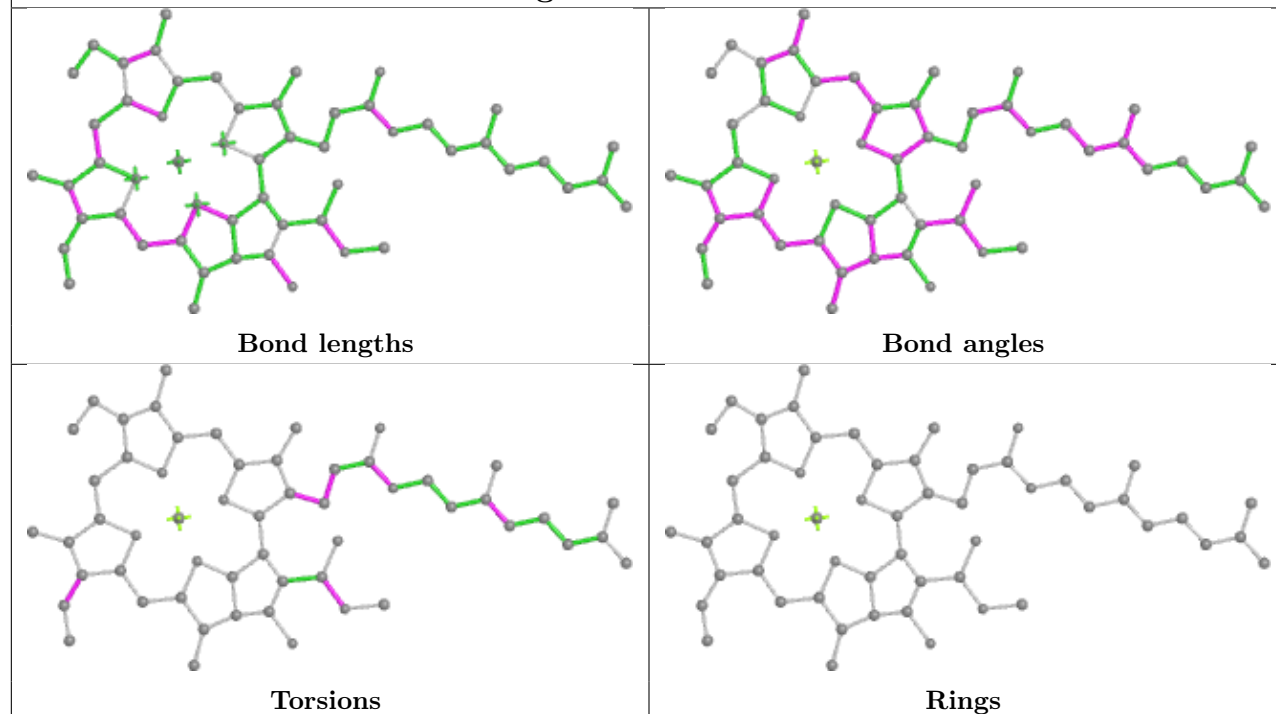
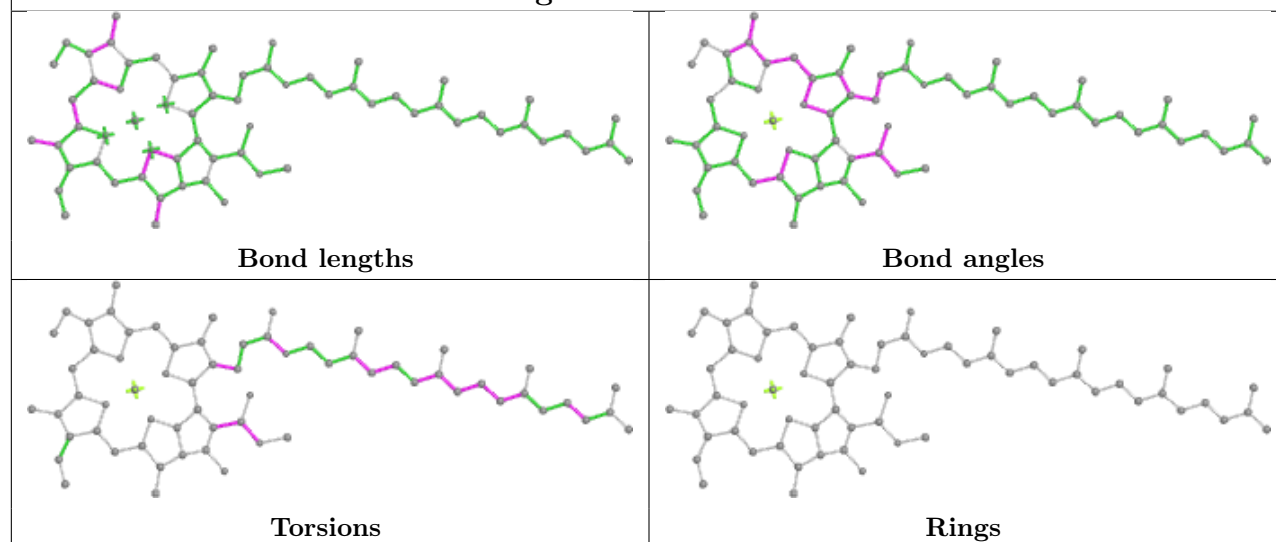
Torsions

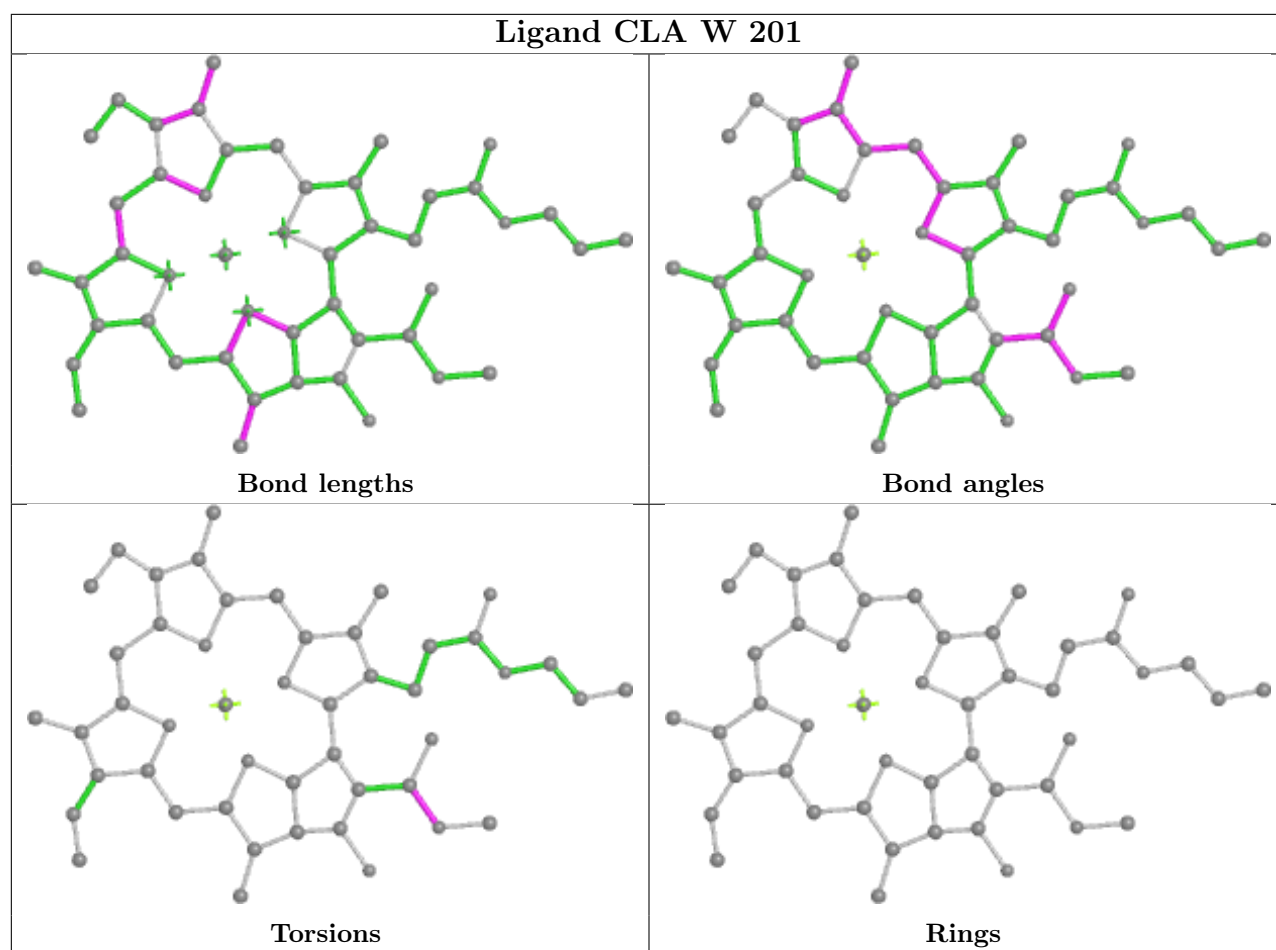


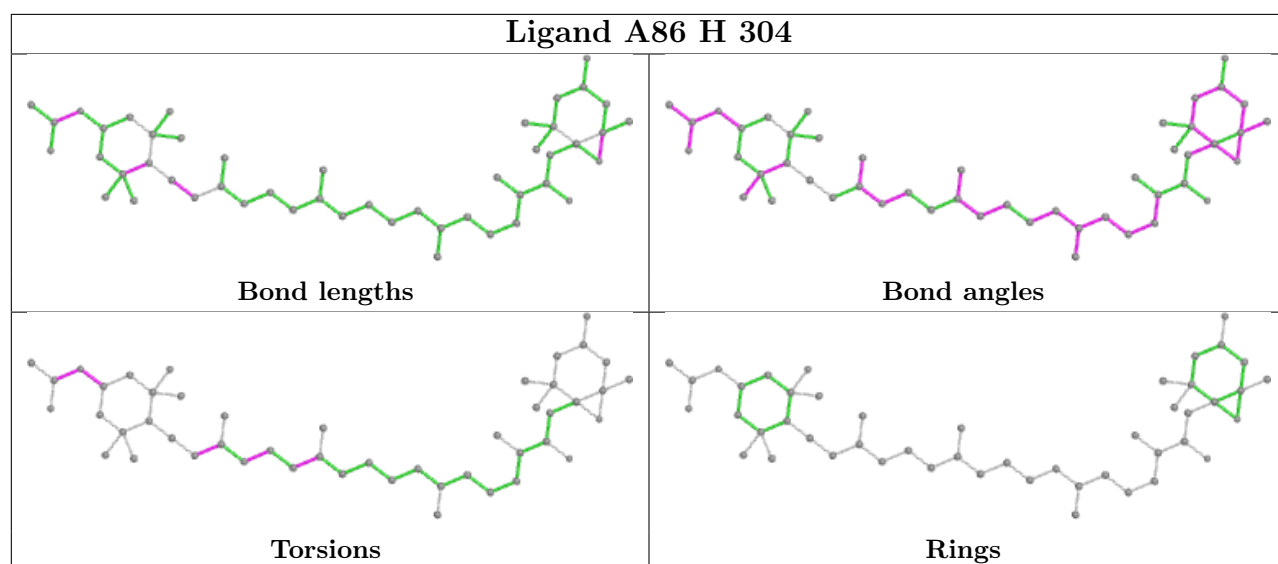
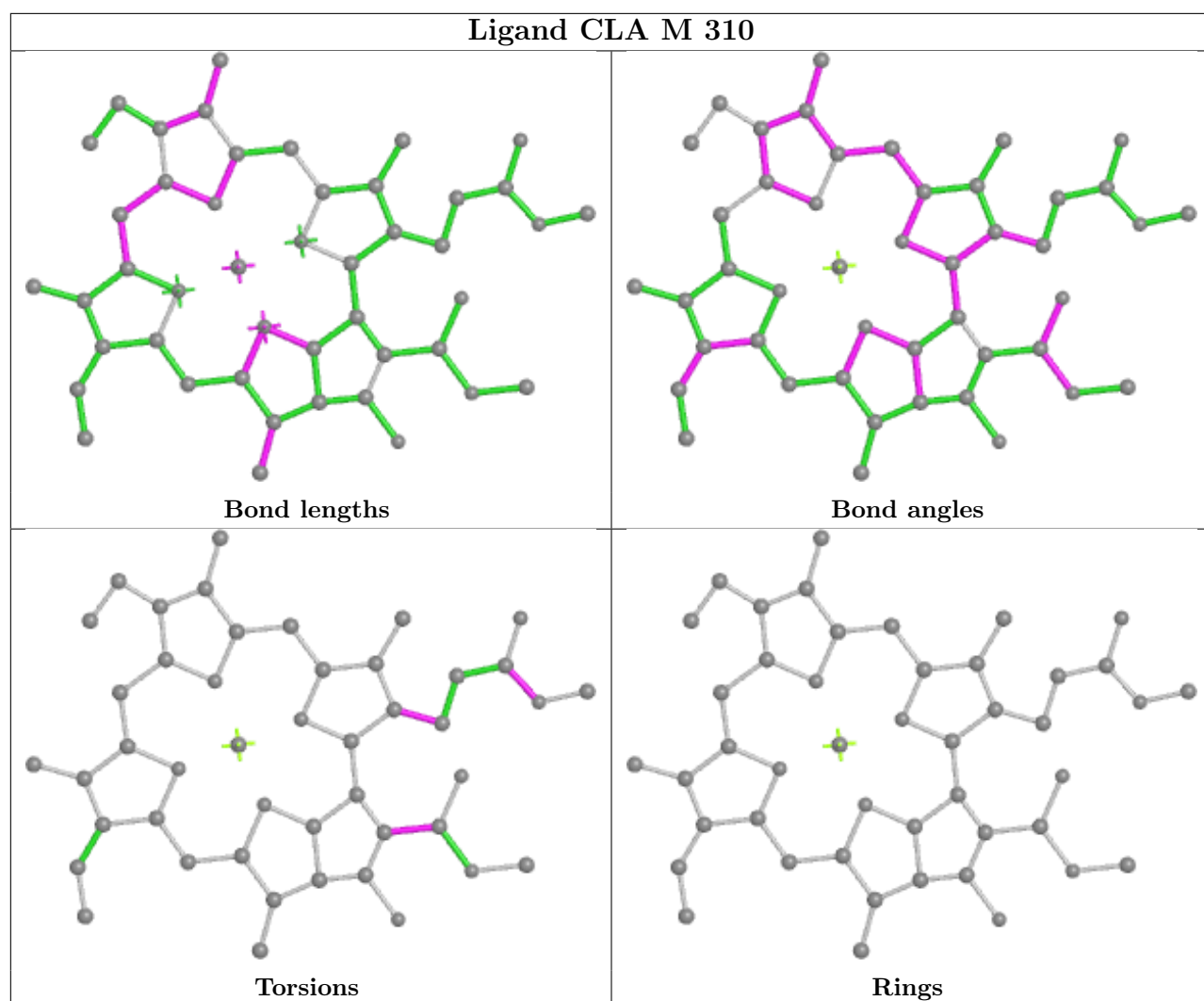
Rings



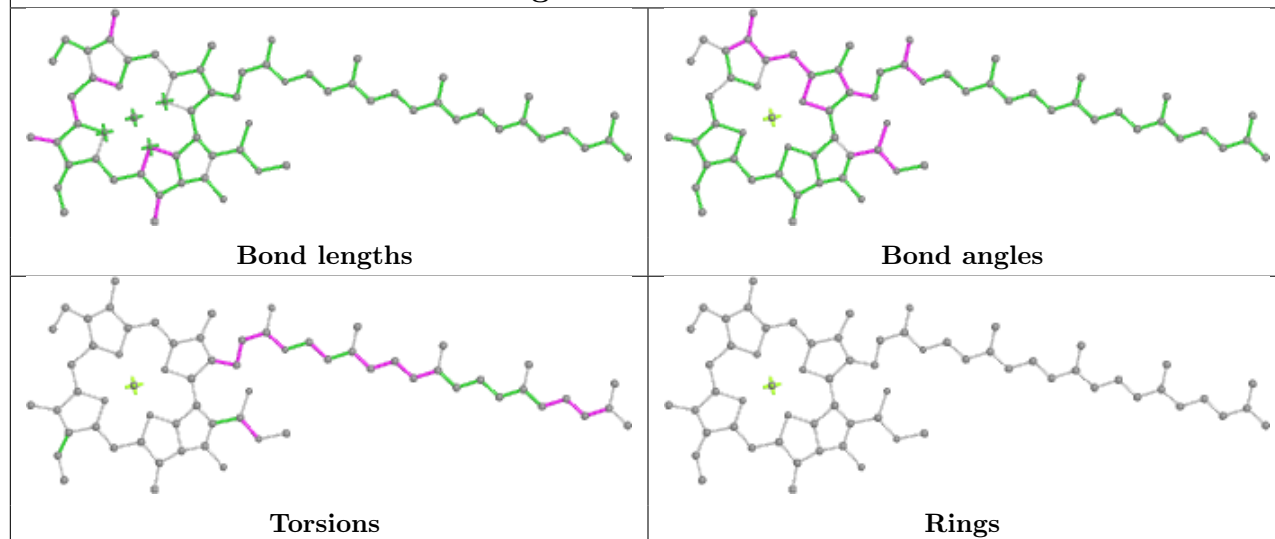


**Ligand CLA a 823****Ligand CLA h 203**

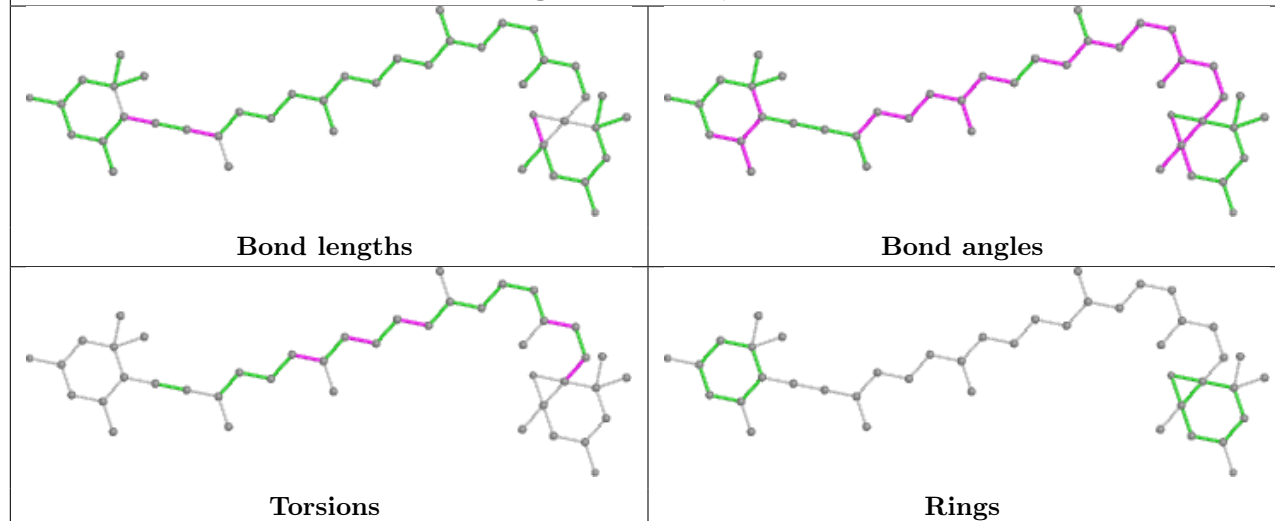




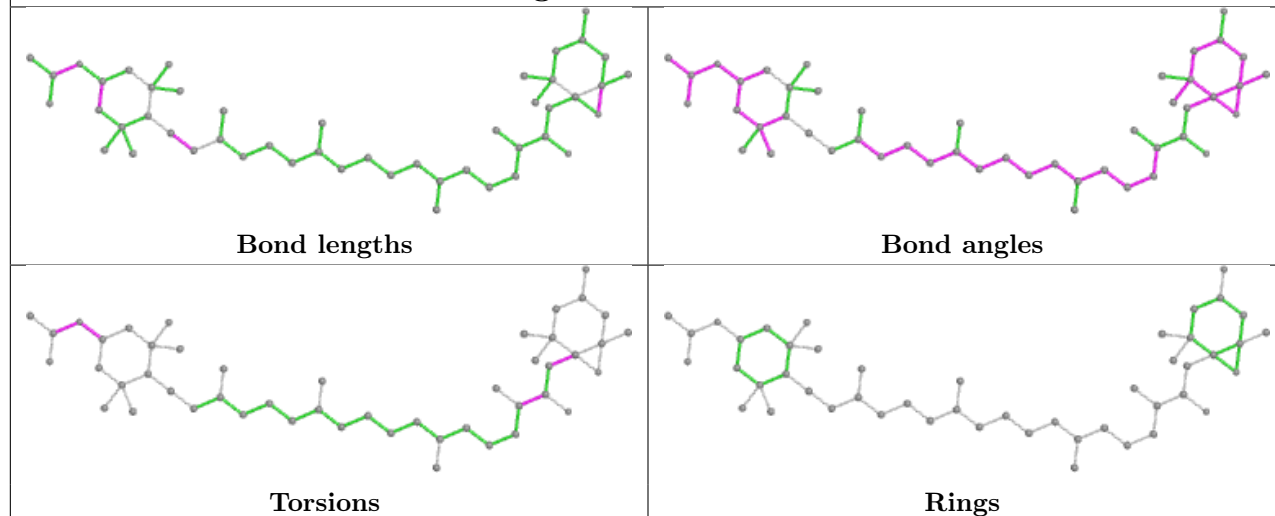
## Ligand CLA T 309



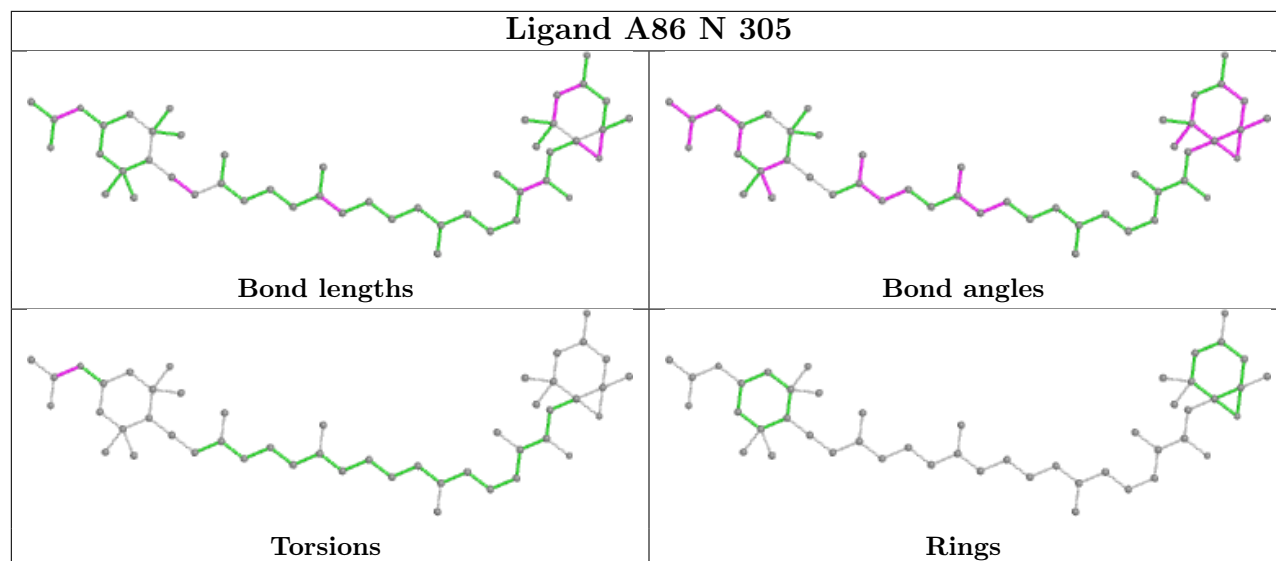
## Ligand DD6 Q 302



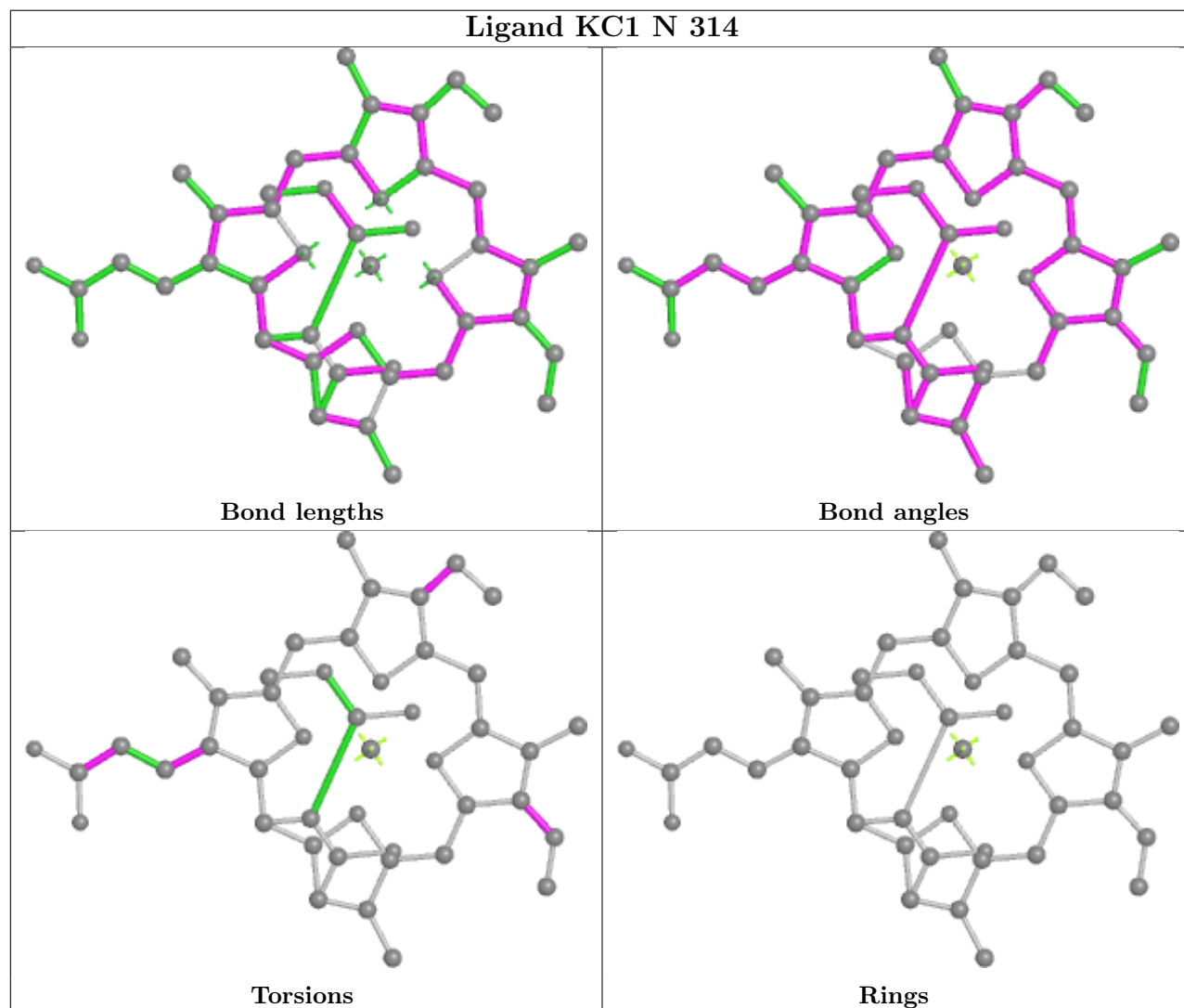
## Ligand A86 M 301



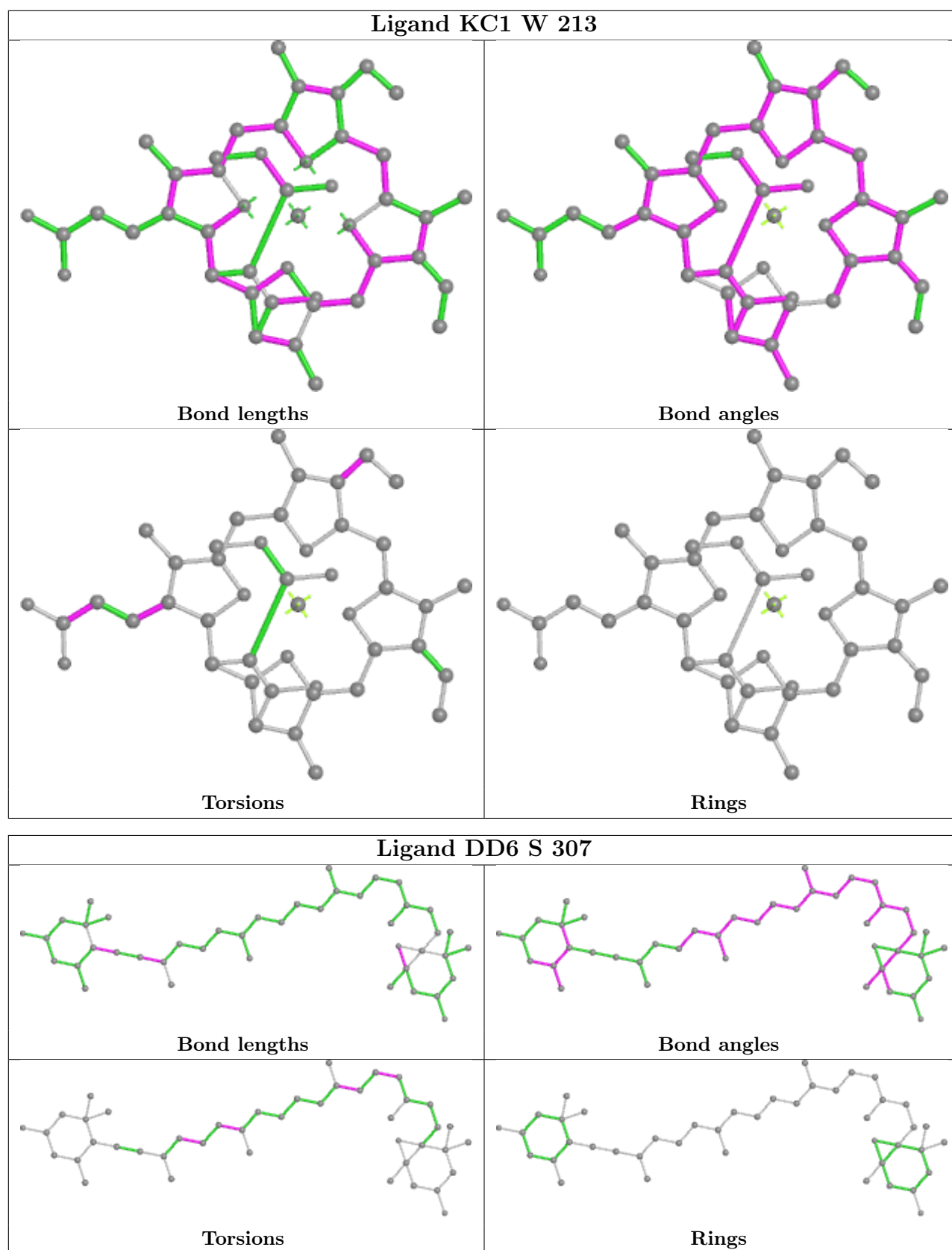
## Ligand A86 N 305



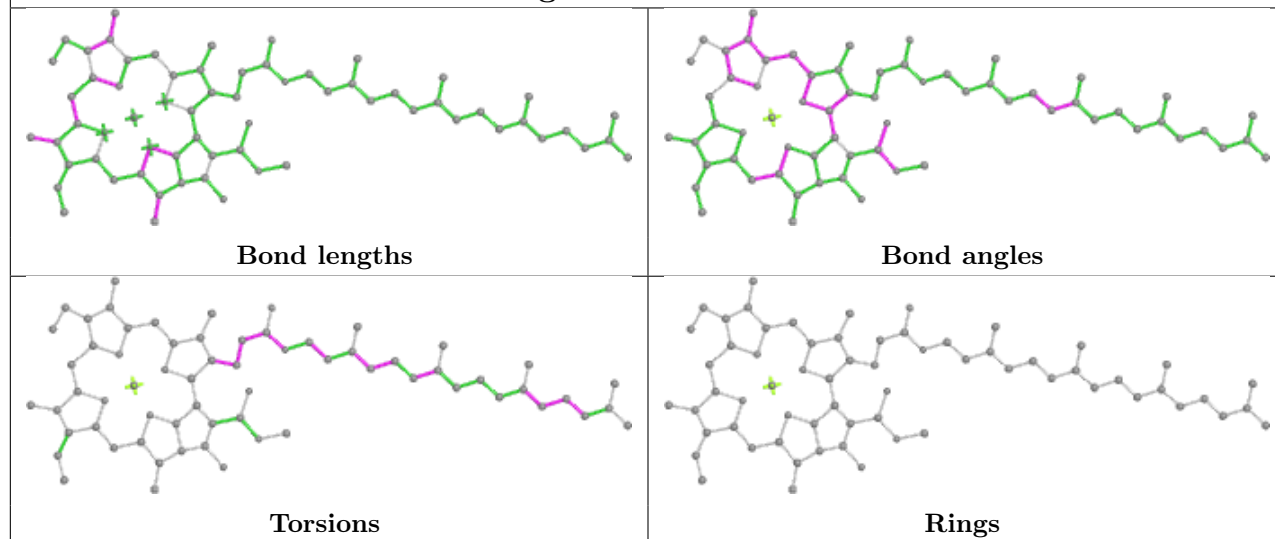
## Ligand KC1 N 314



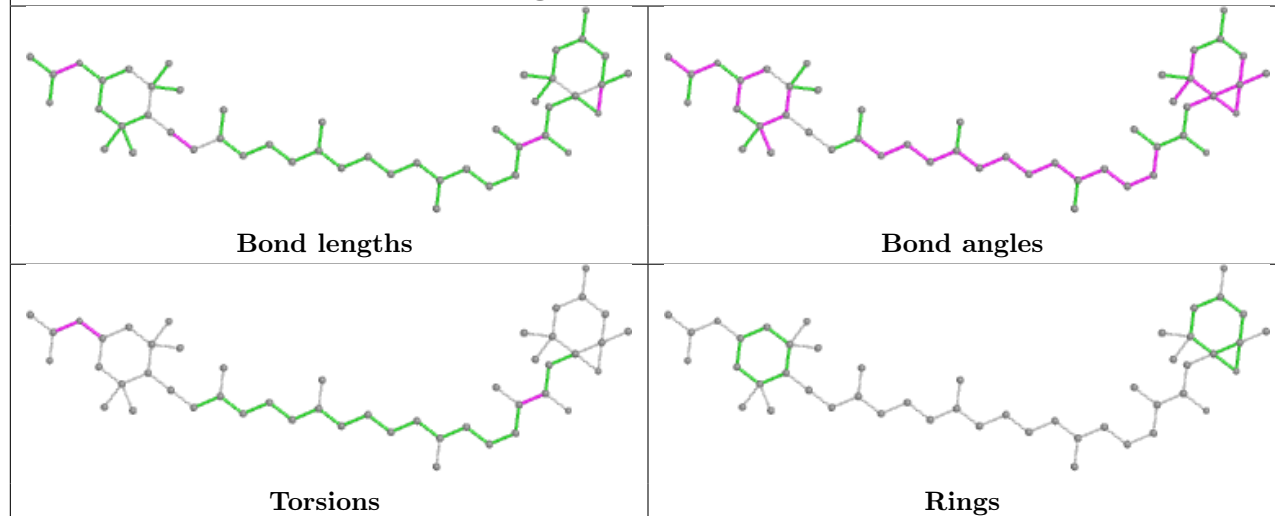




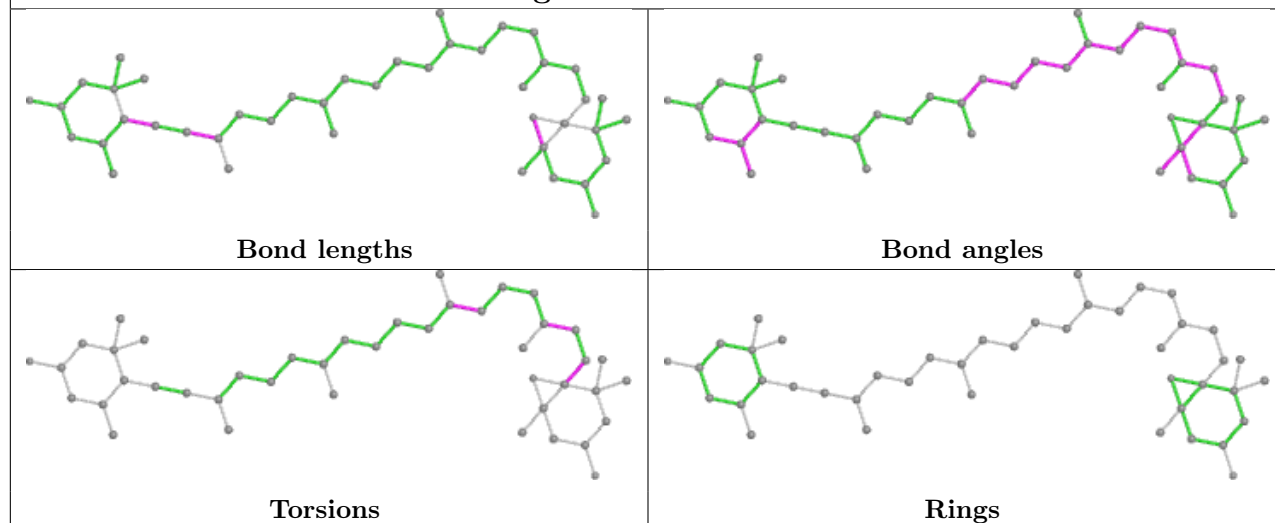
## Ligand CLA f 802

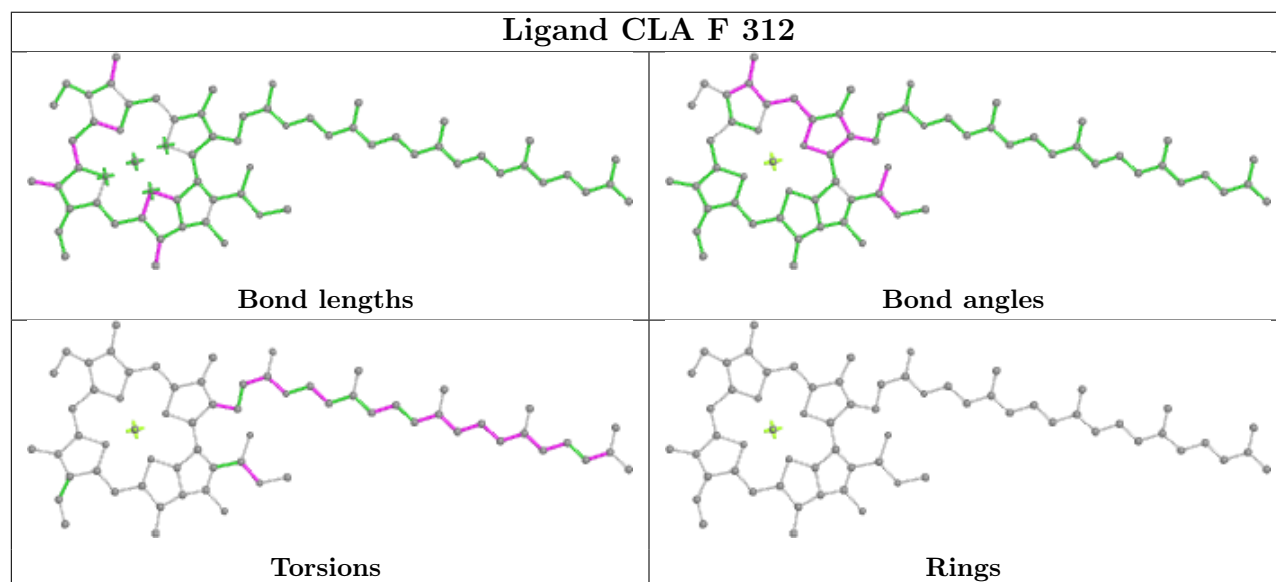
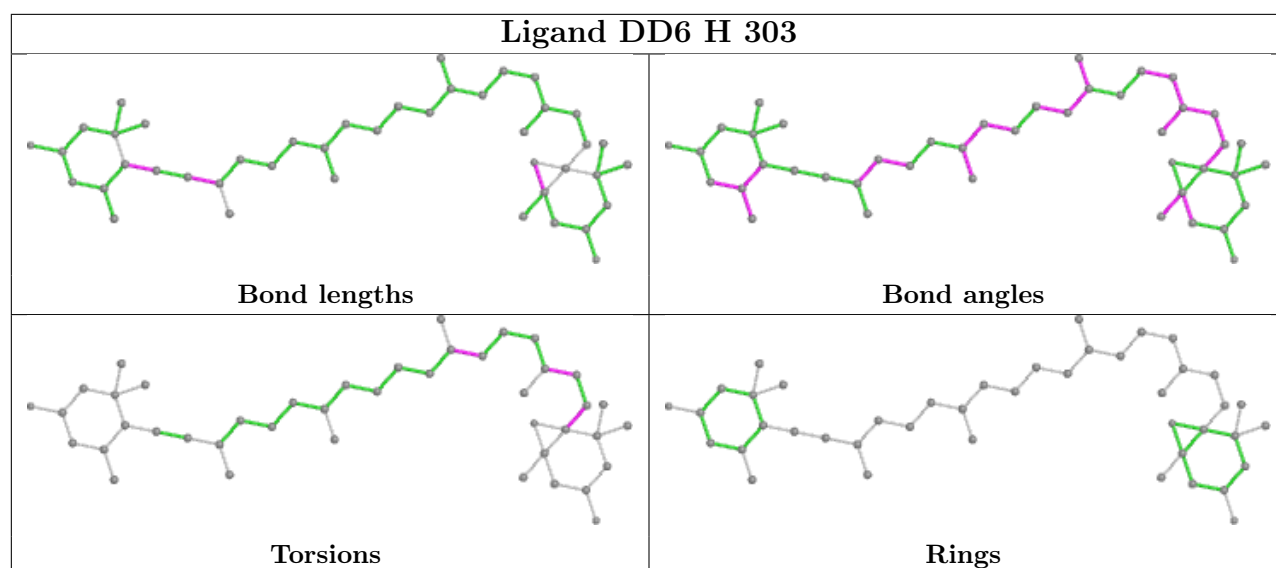


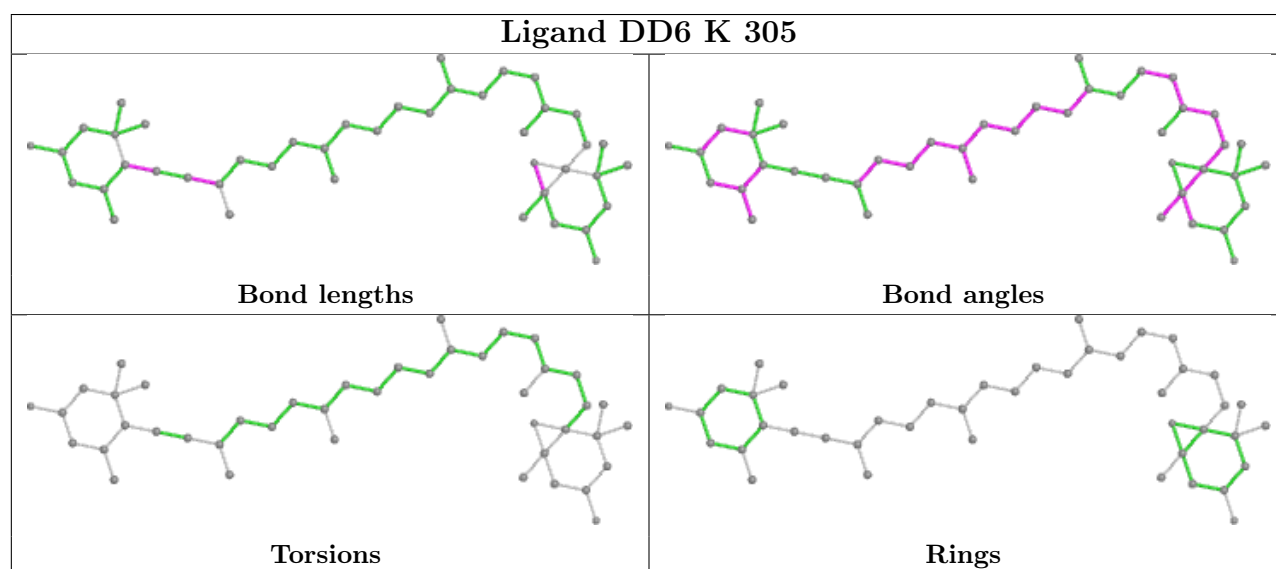
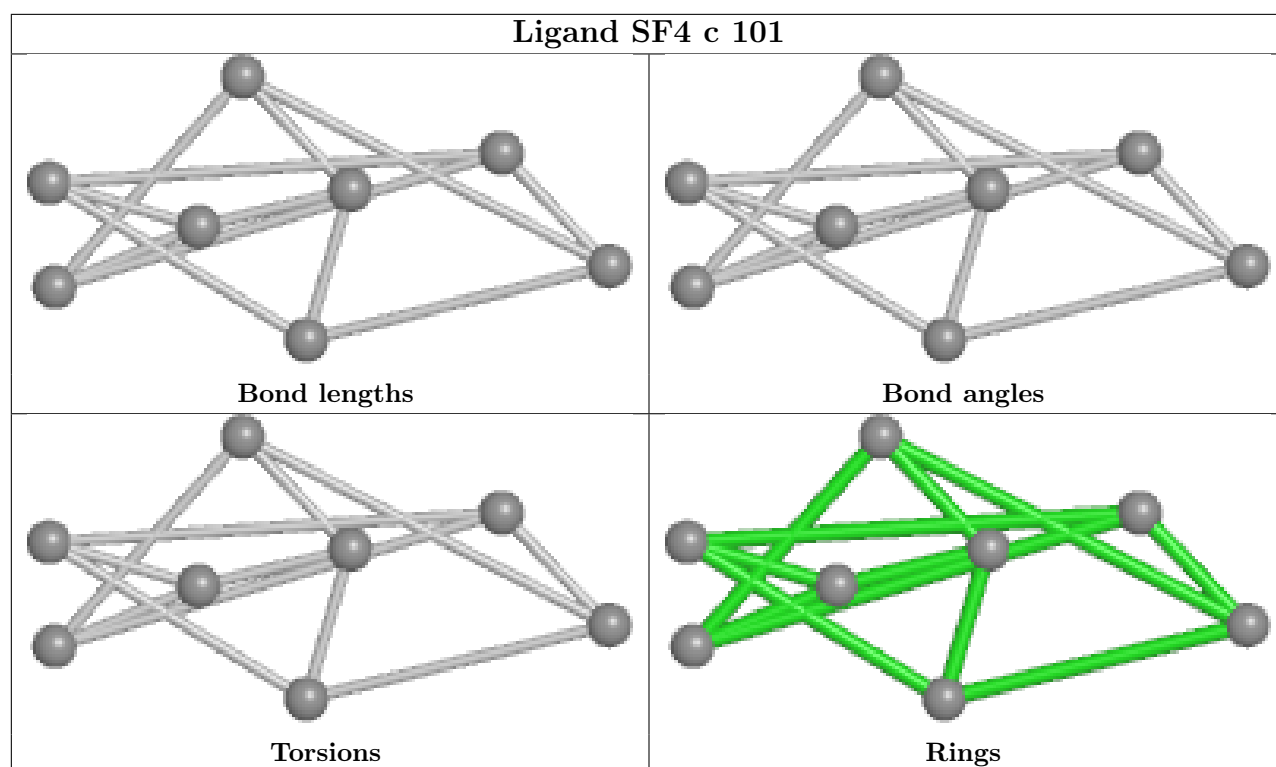
## Ligand A86 W 203

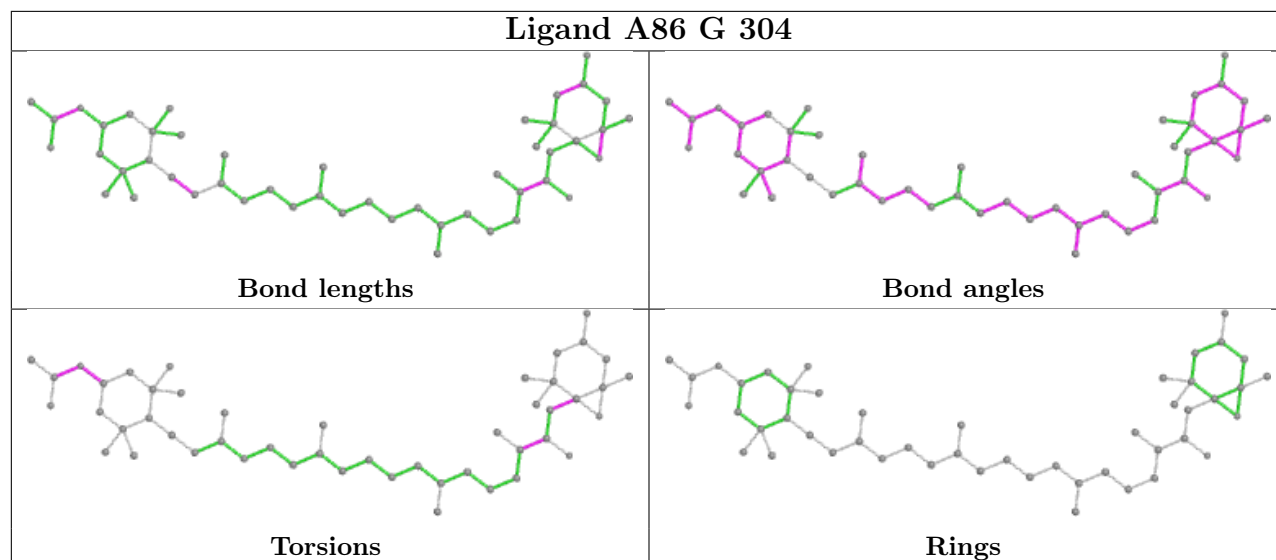
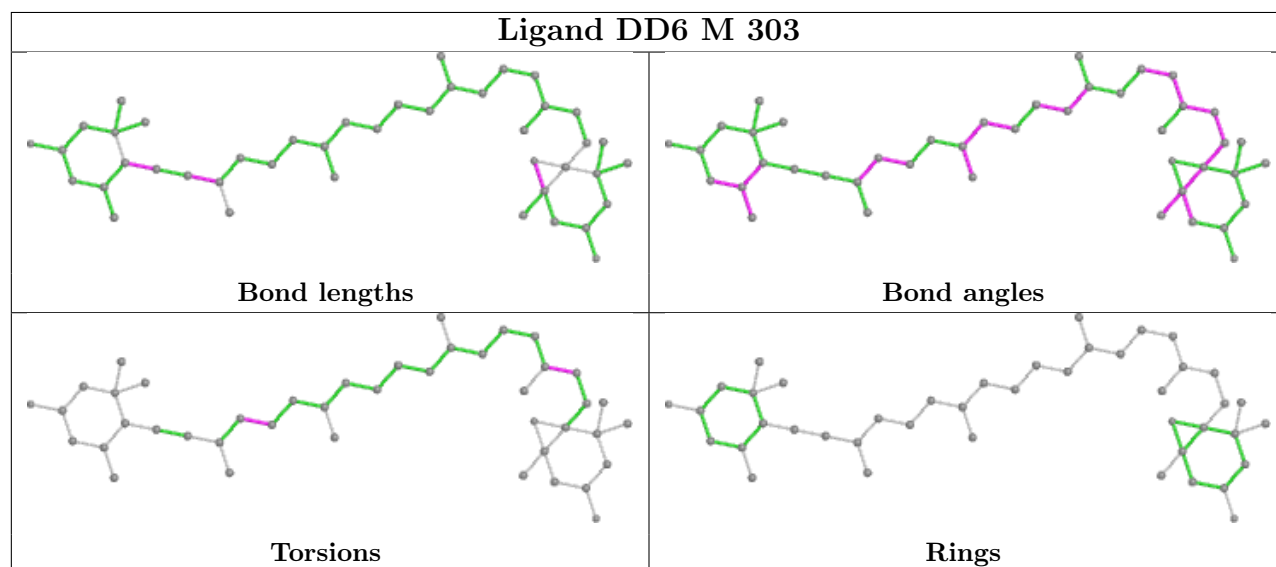
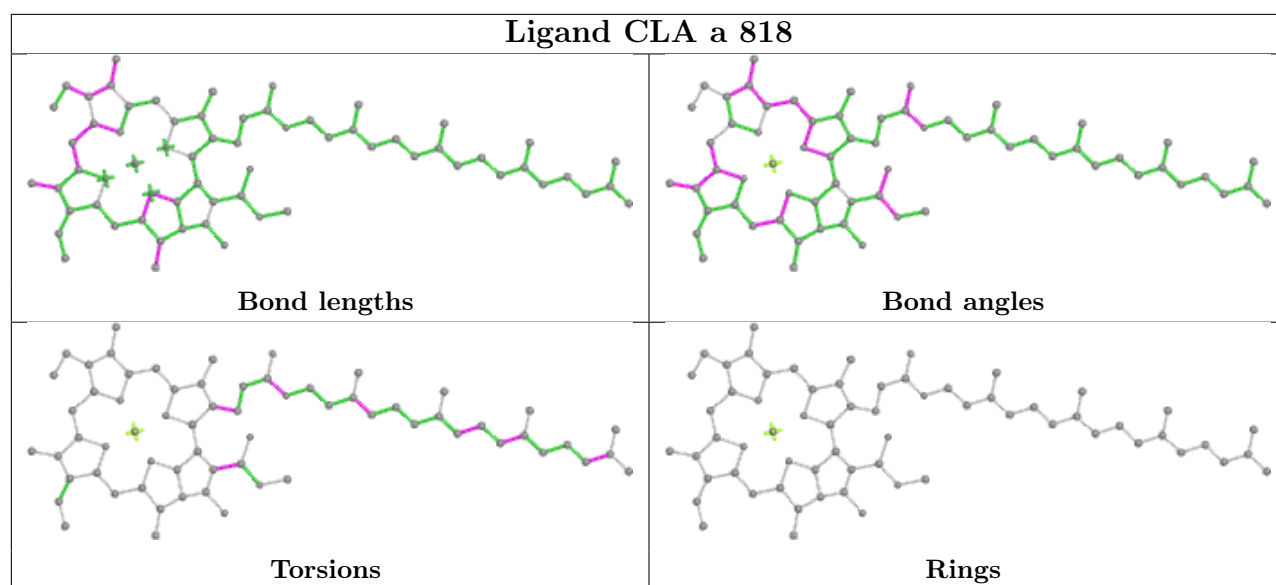


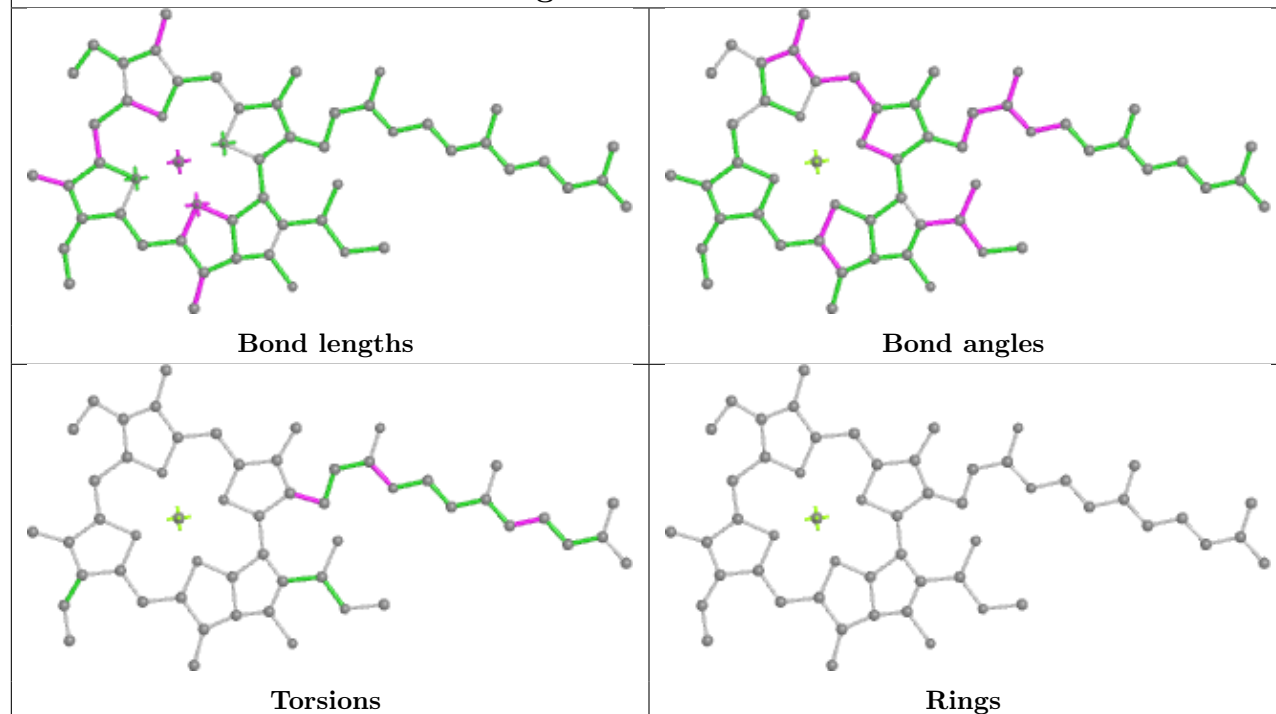
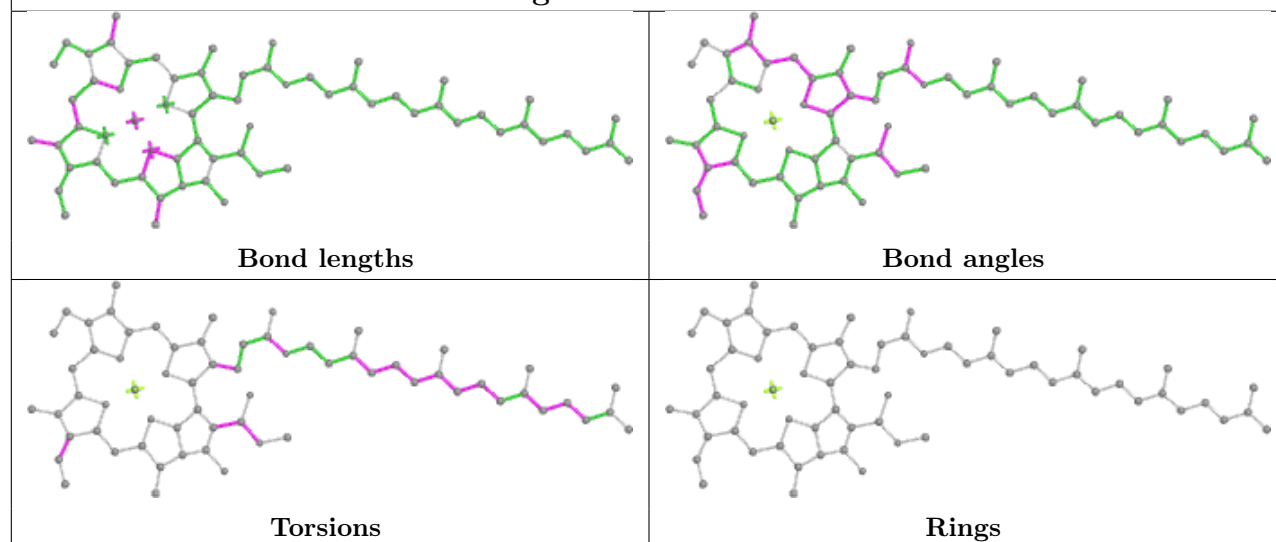
## Ligand DD6 E 303

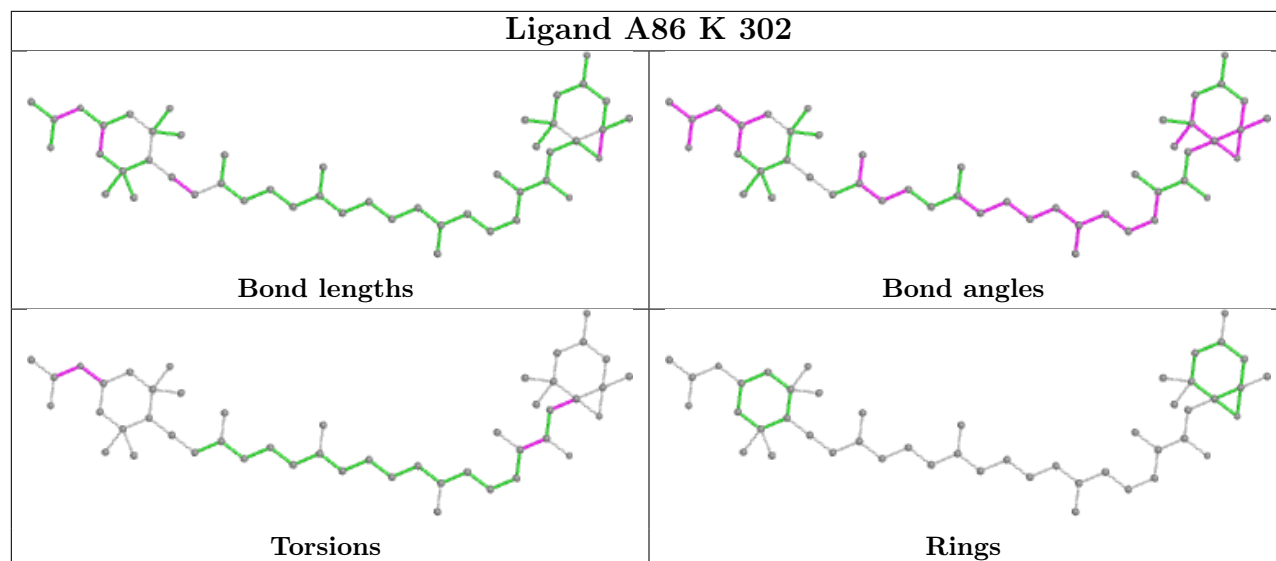
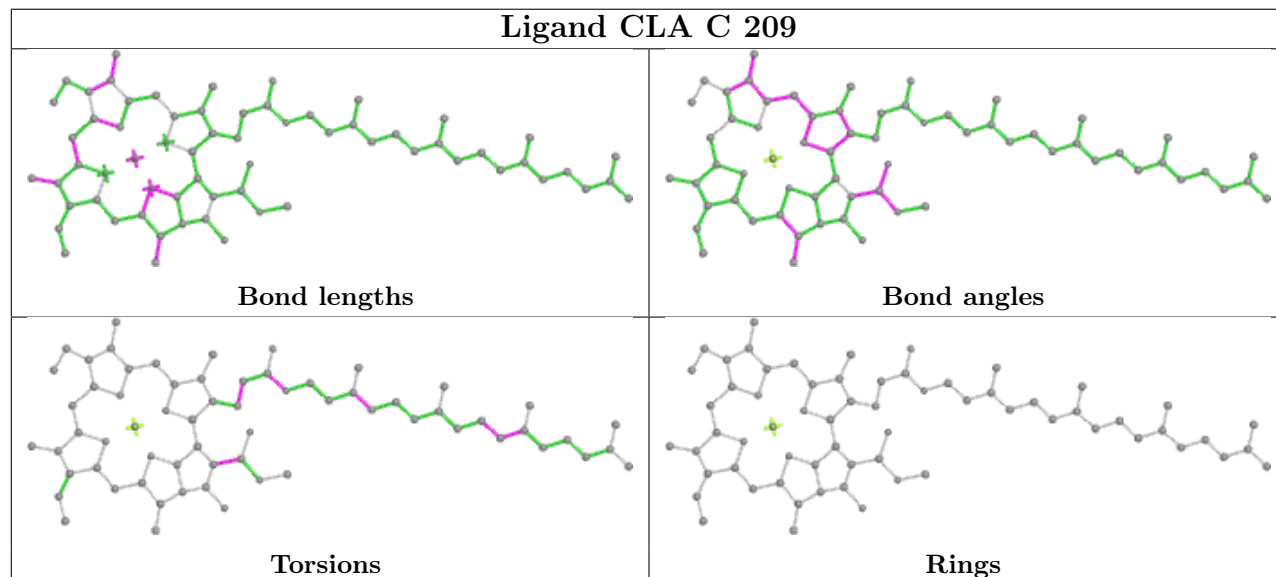
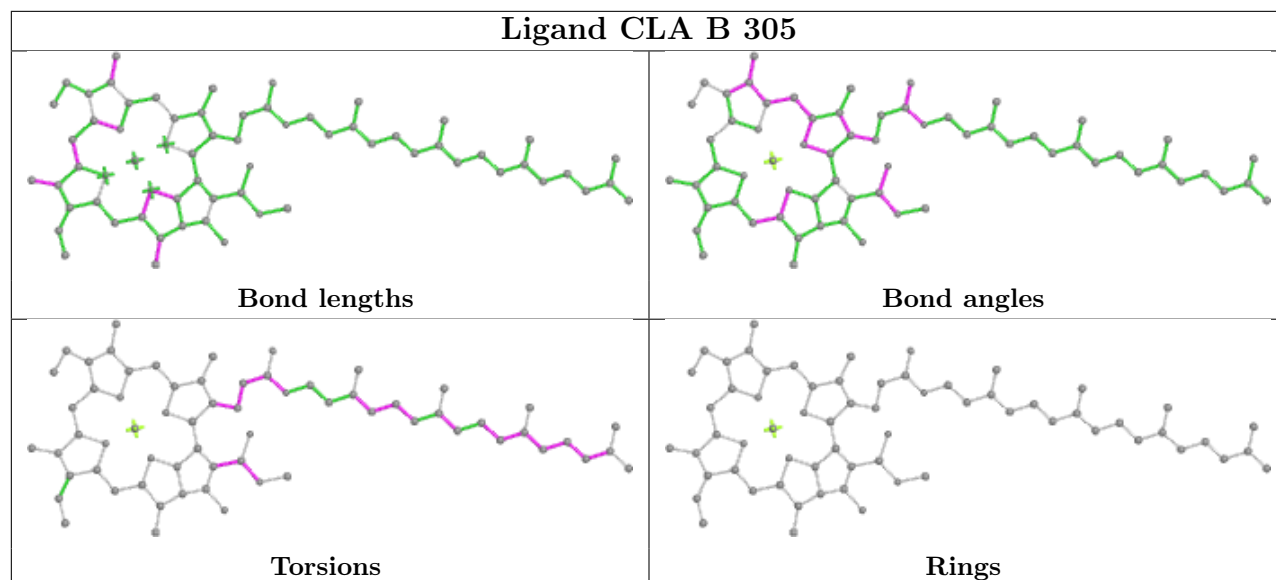




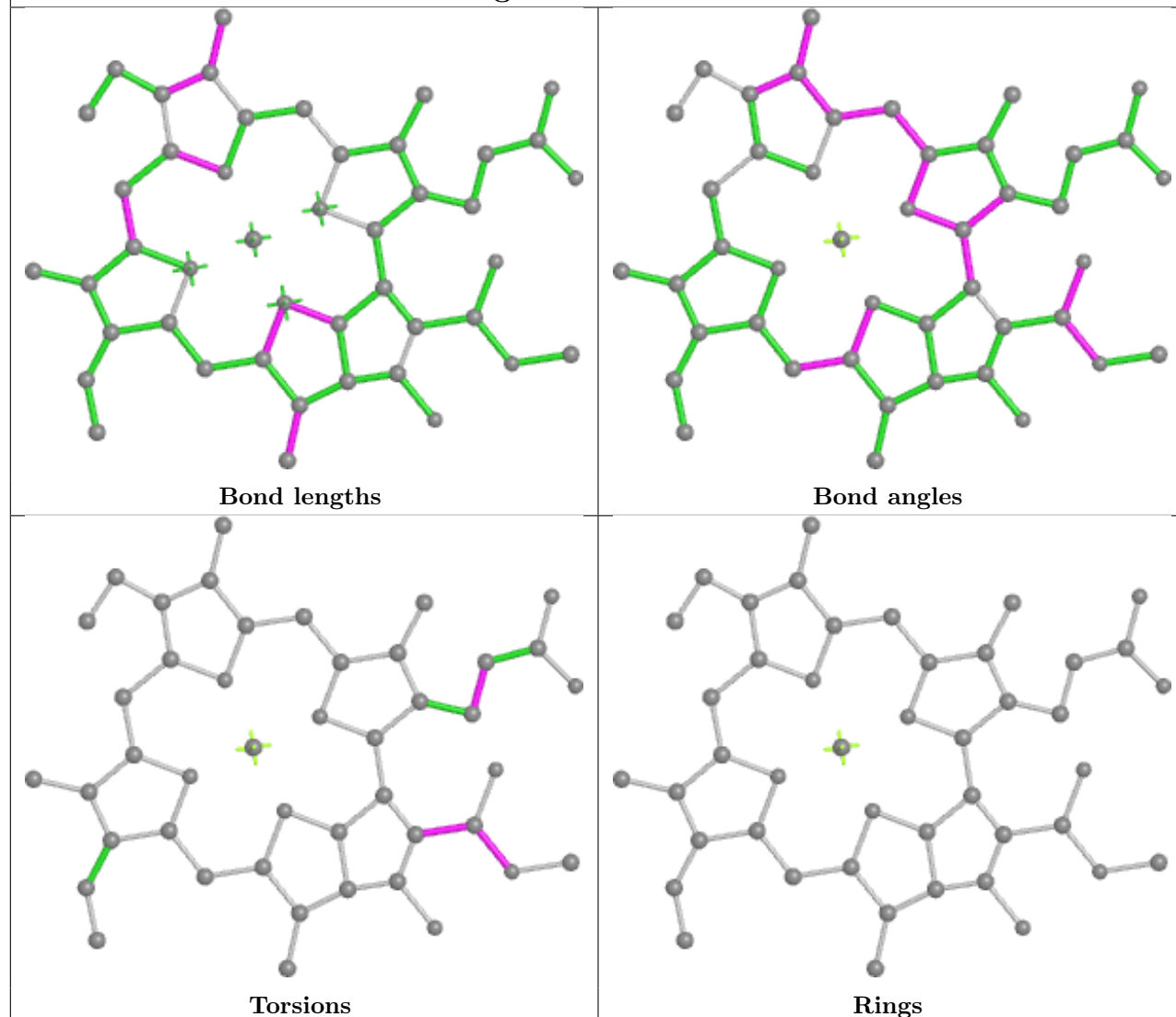




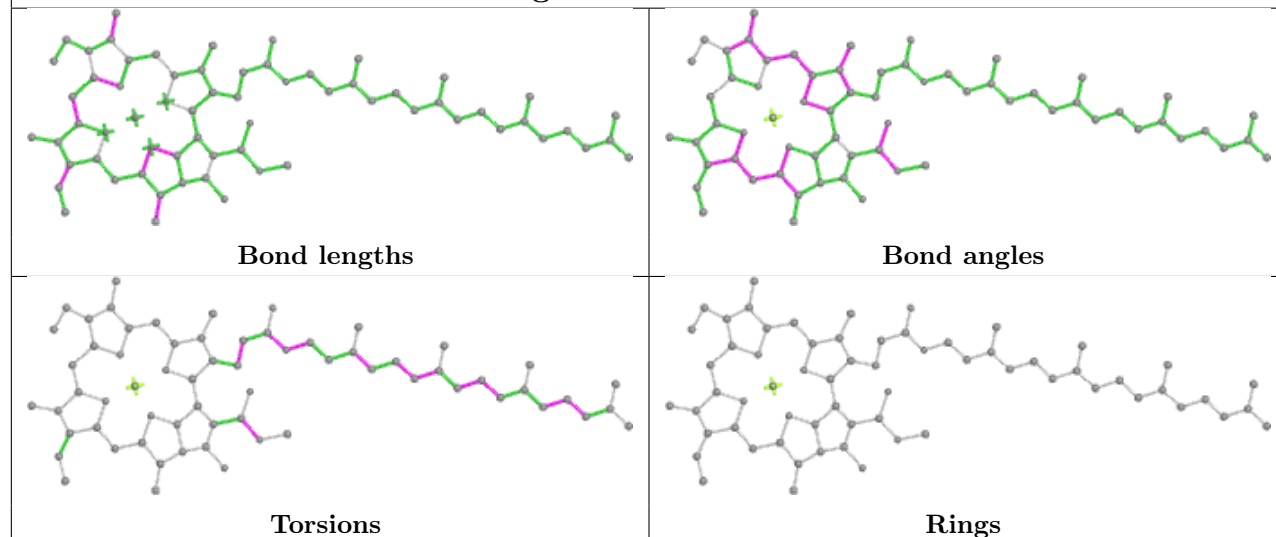
**Ligand CLA a 803****Ligand CLA C 212**

**Ligand A86 K 302****Ligand CLA C 209****Ligand CLA B 305**

## Ligand CLA a 834

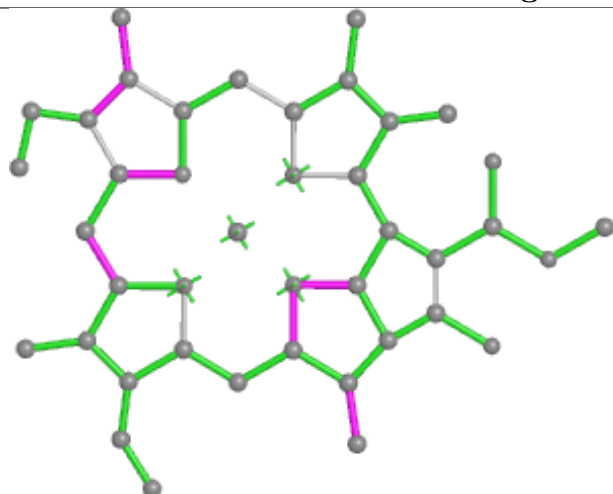


## Ligand CLA B 308

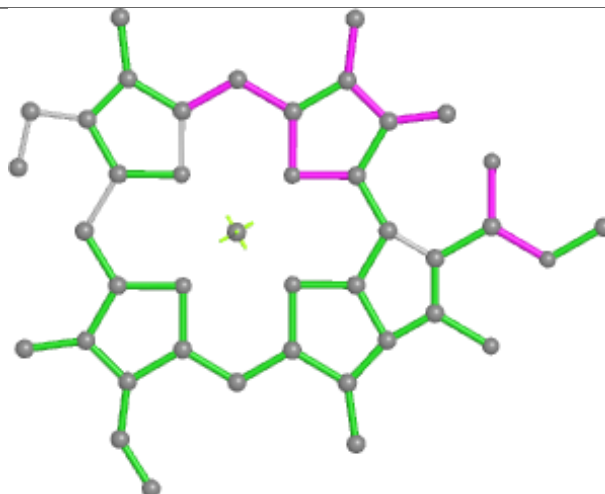




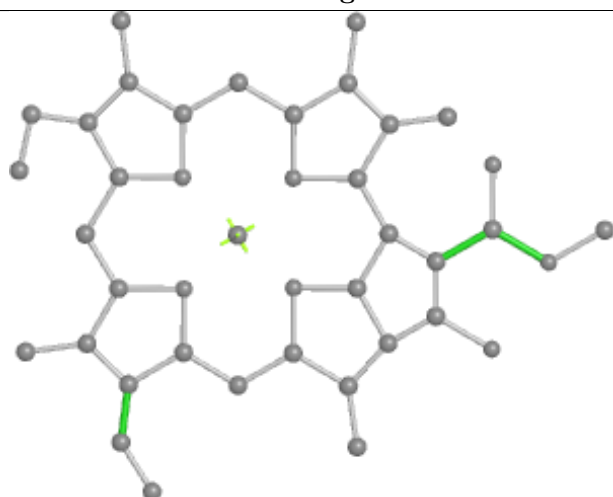
## Ligand CLA I 314



Bond lengths



Bond angles

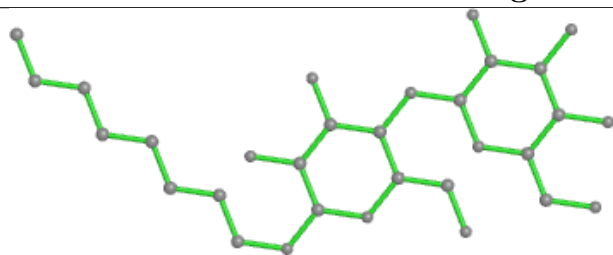


Torsions

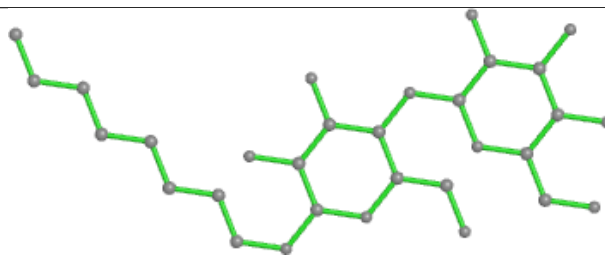


Rings

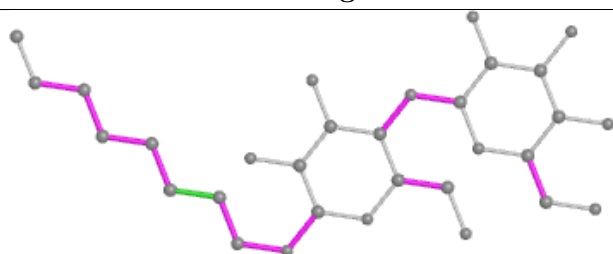
## Ligand LMT K 317



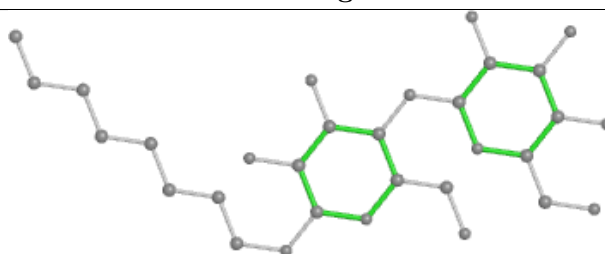
Bond lengths



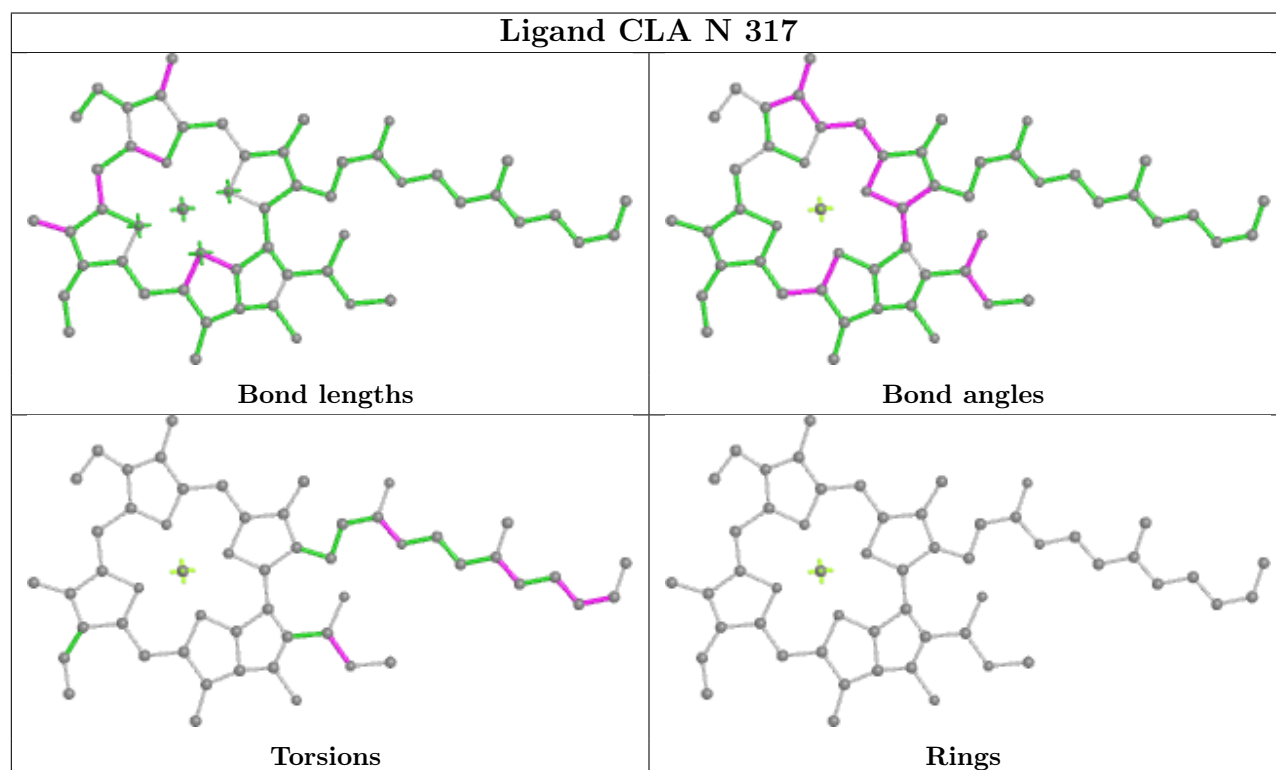
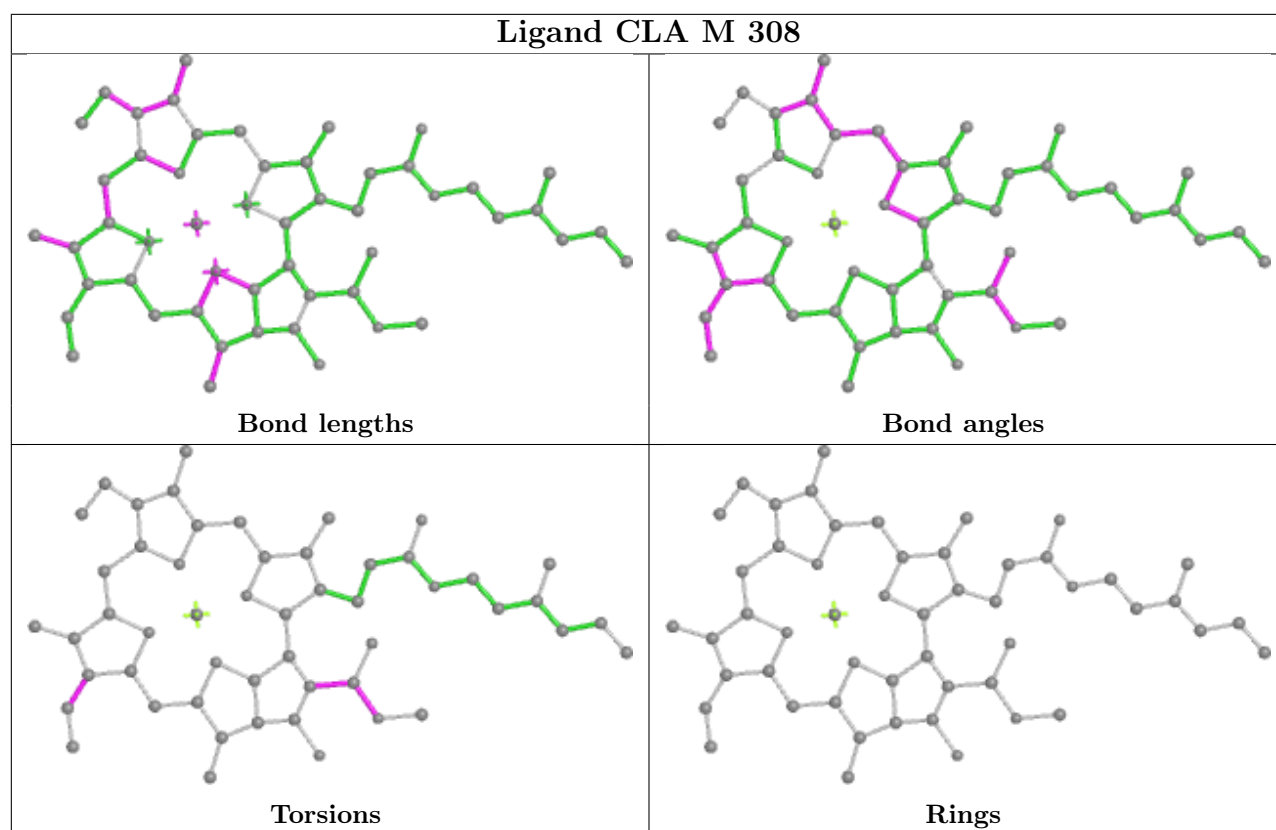
Bond angles

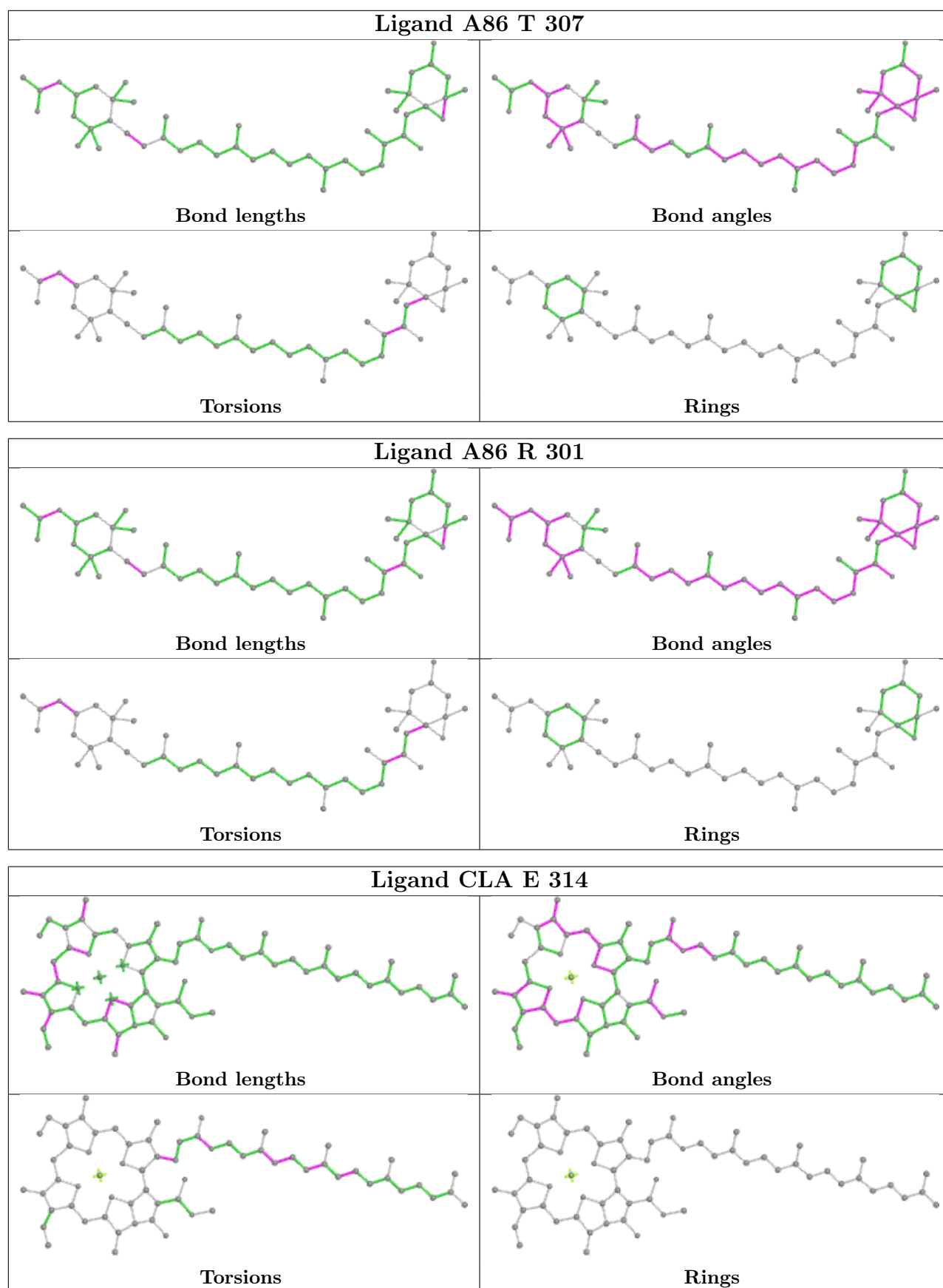


Torsions

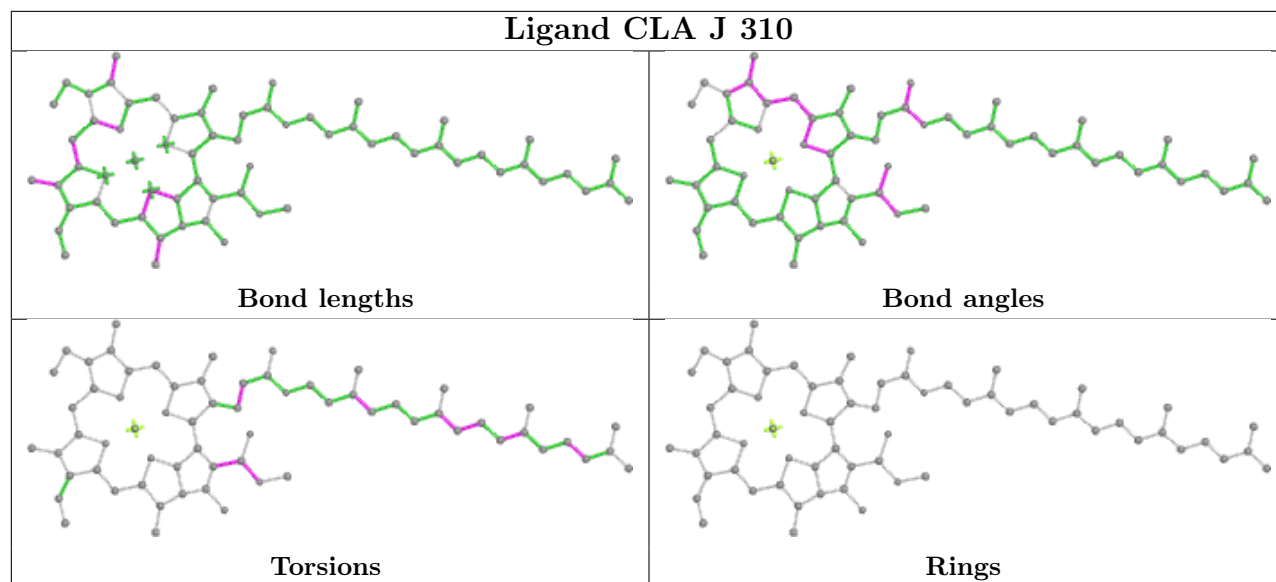


Rings

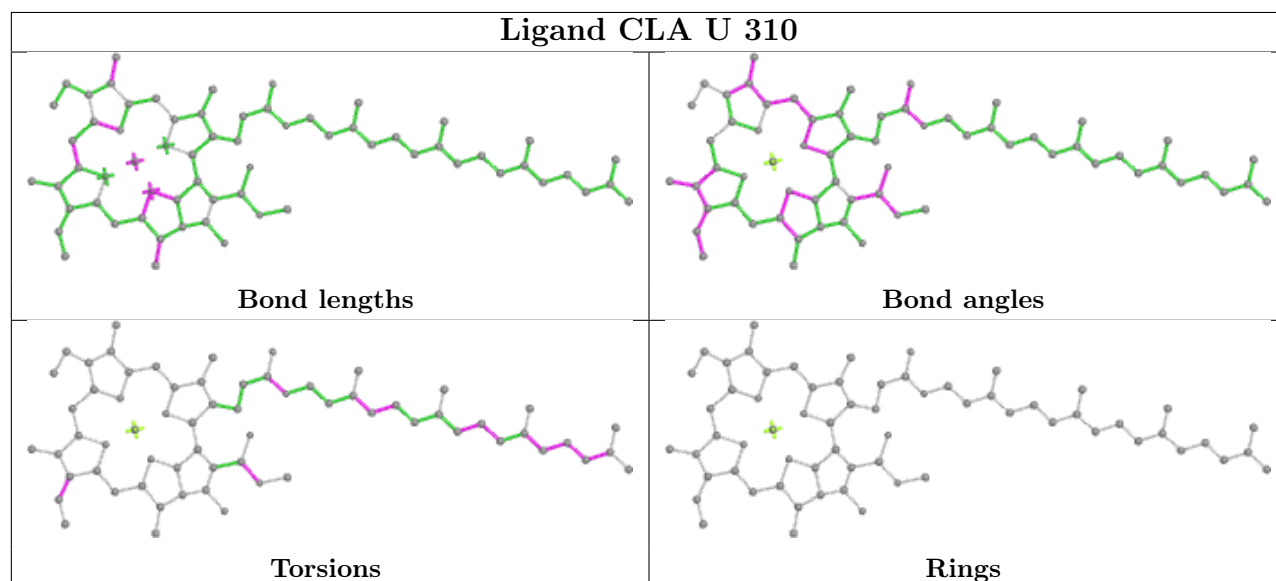




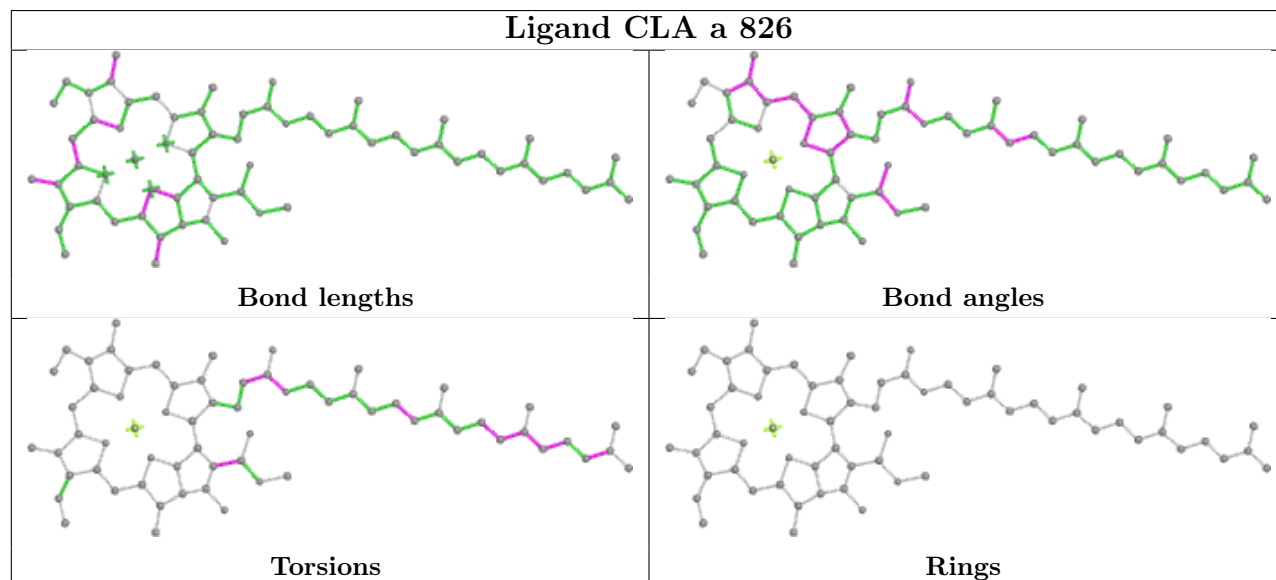
## Ligand CLA J 310



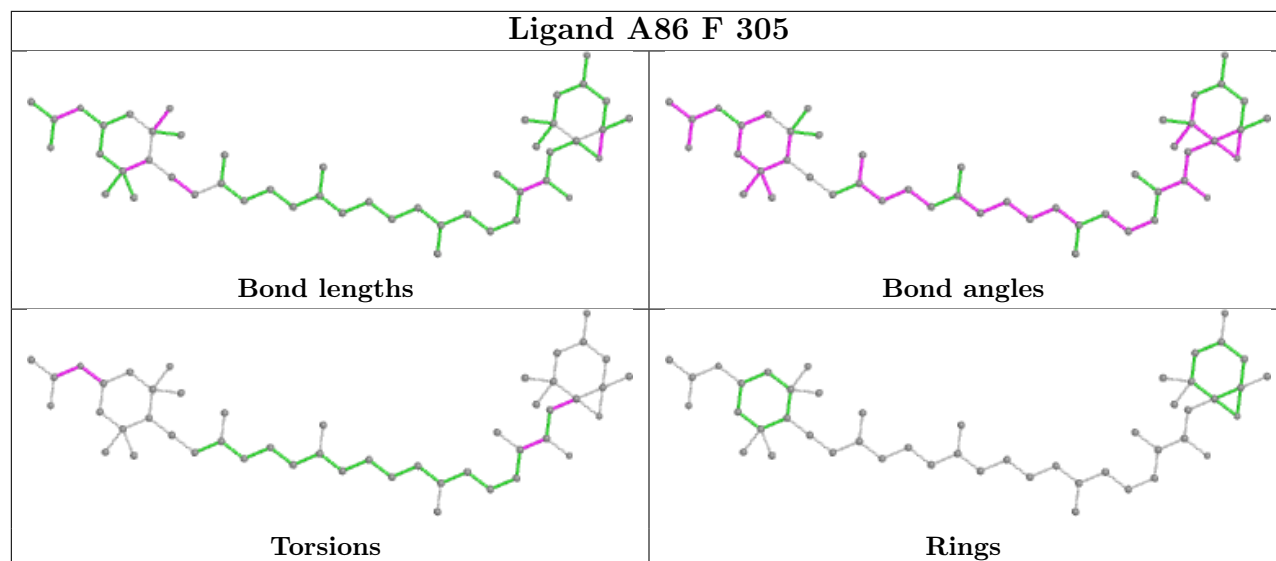
## Ligand CLA U 310



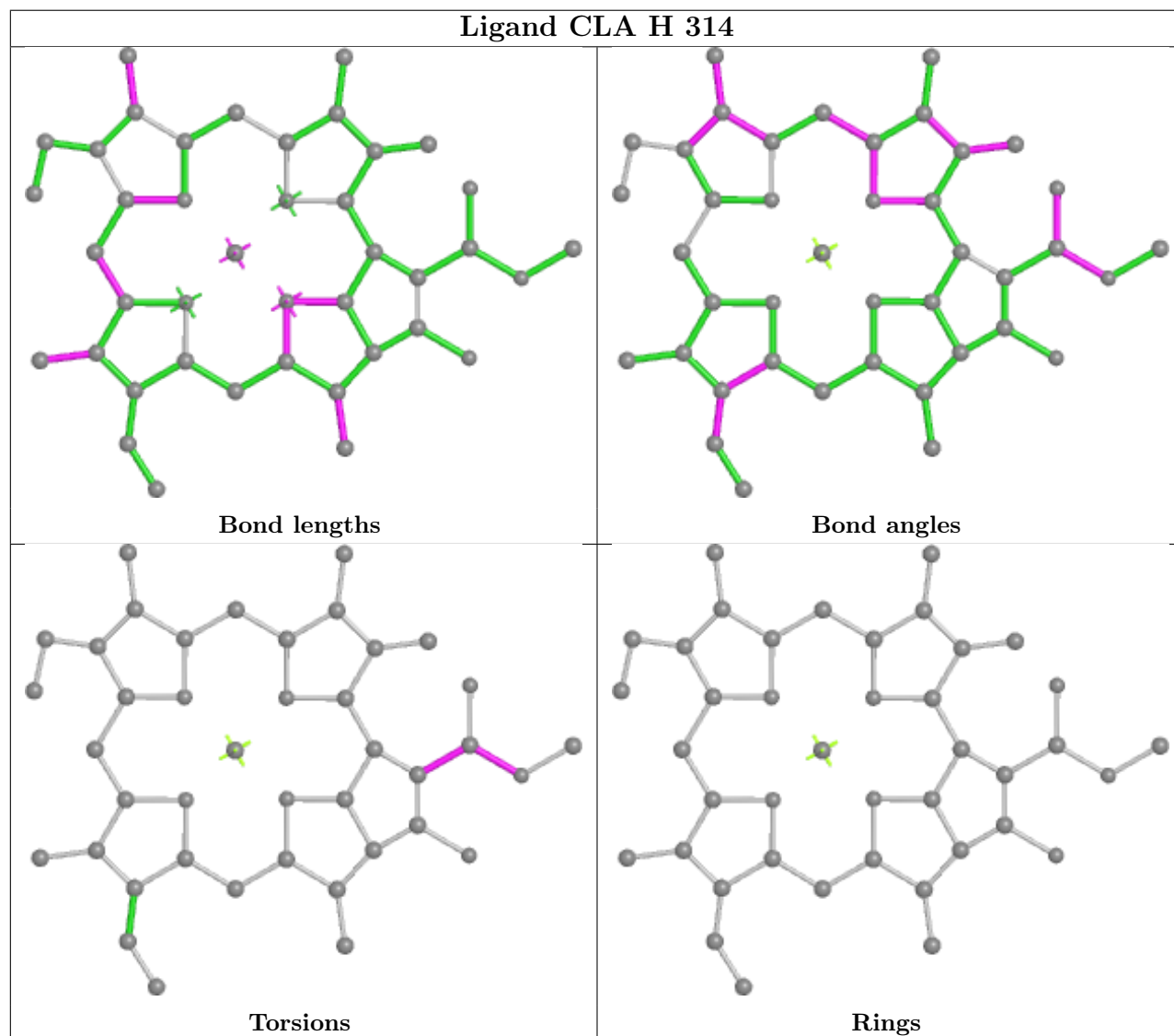
## Ligand CLA a 826

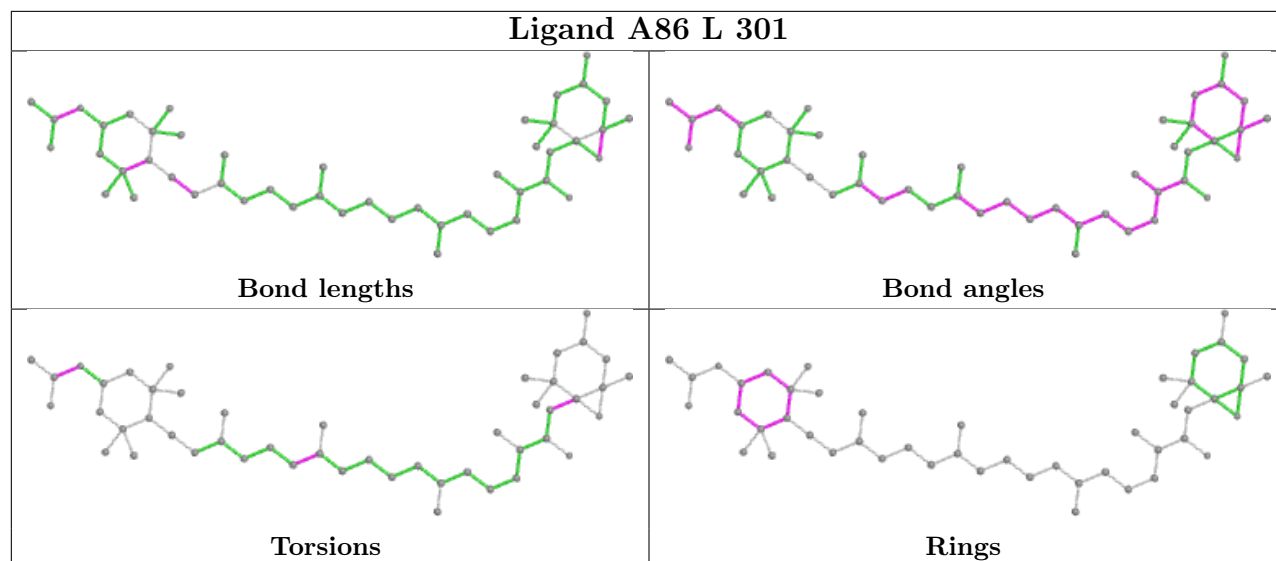
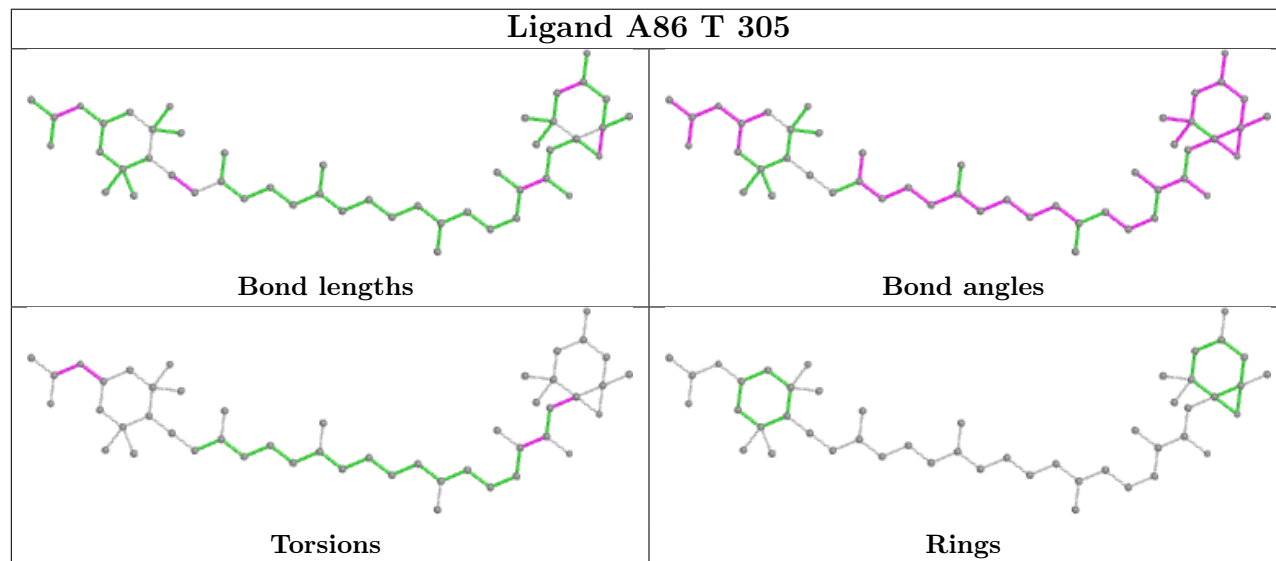


## Ligand A86 F 305

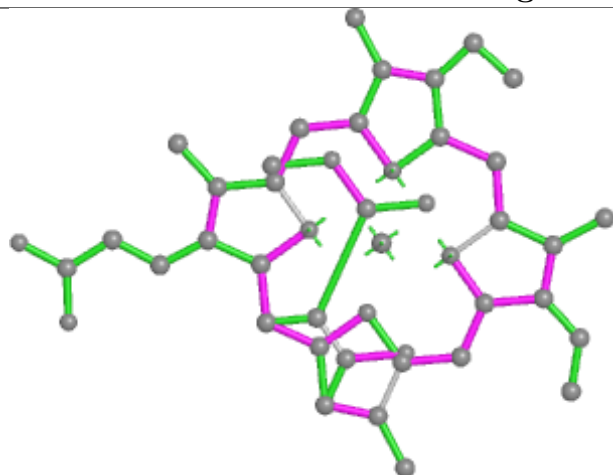


## Ligand CLA H 314

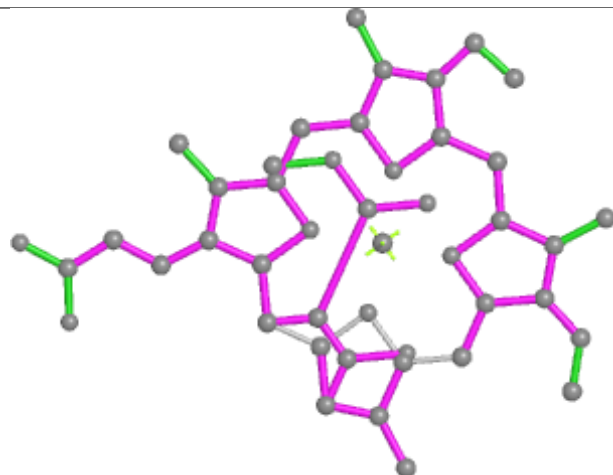


**Ligand A86 L 301****Ligand A86 T 305**

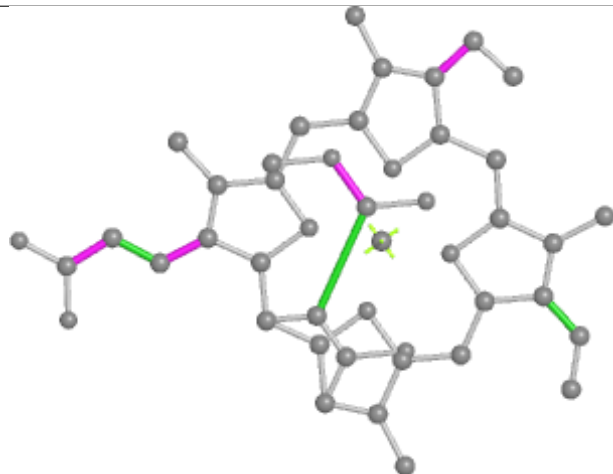
## Ligand KC1 T 315



Bond lengths



Bond angles

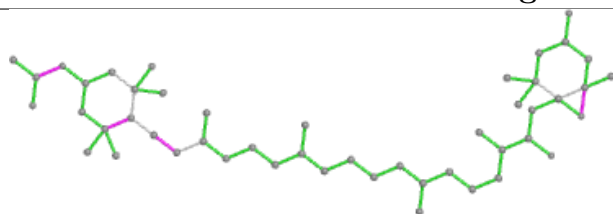


Torsions

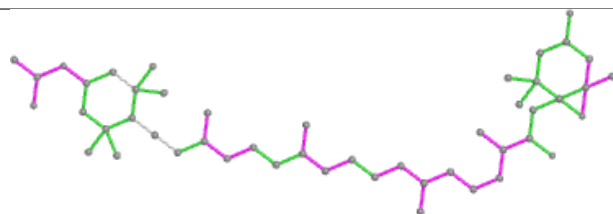


Rings

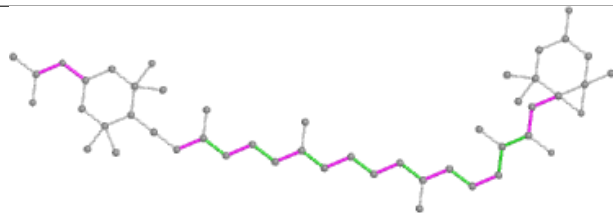
## Ligand A86 U 303



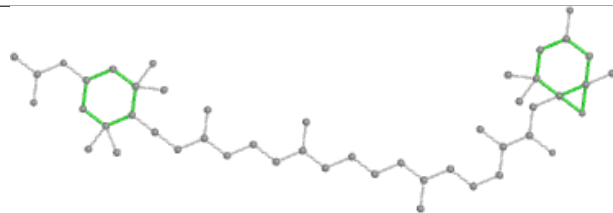
Bond lengths



Bond angles

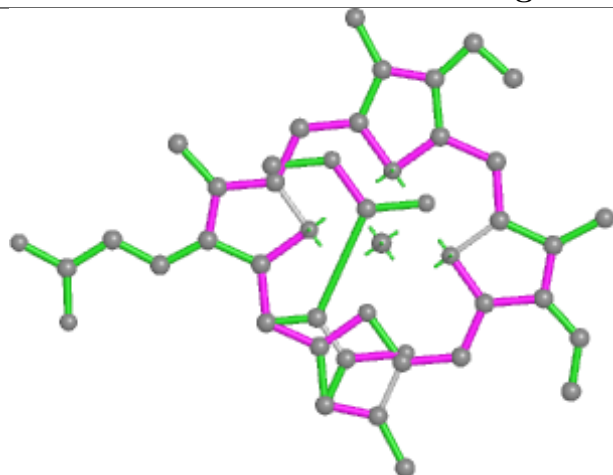


Torsions

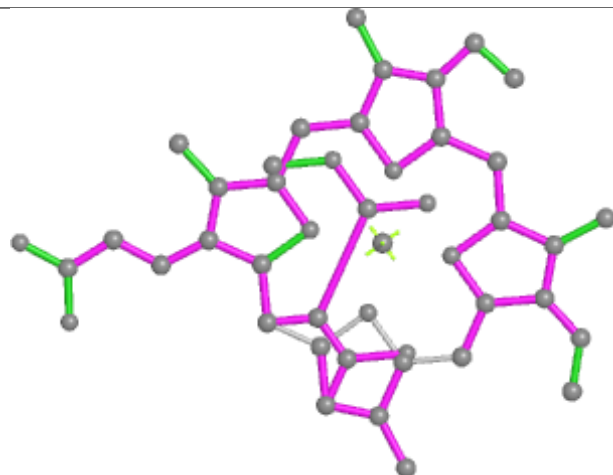


Rings

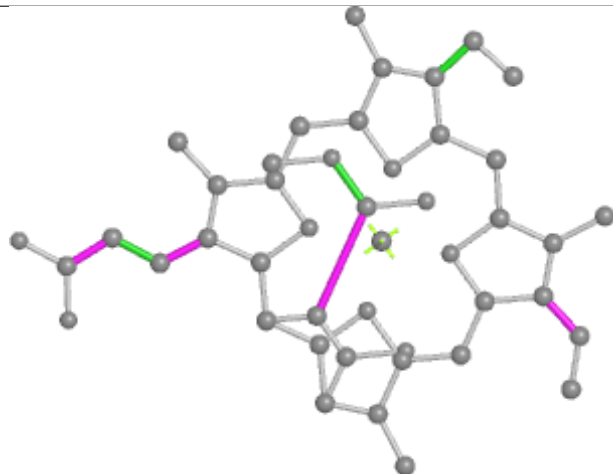
## Ligand KC1 V 312



Bond lengths



Bond angles

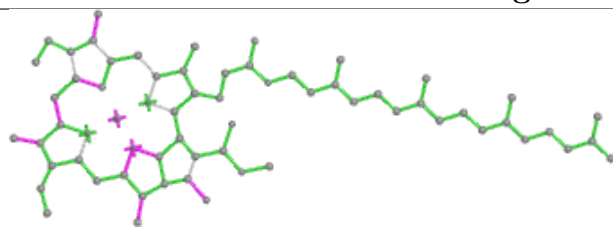


Torsions

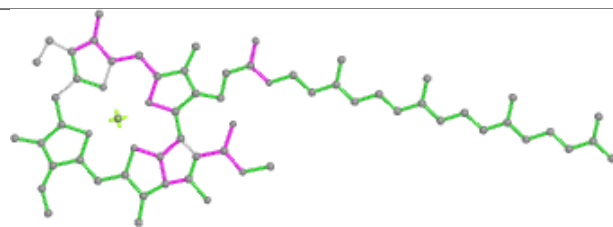


Rings

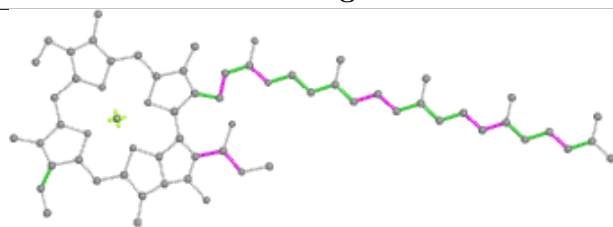
## Ligand CLA K 313



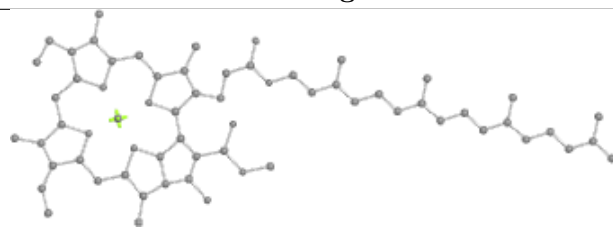
Bond lengths



Bond angles



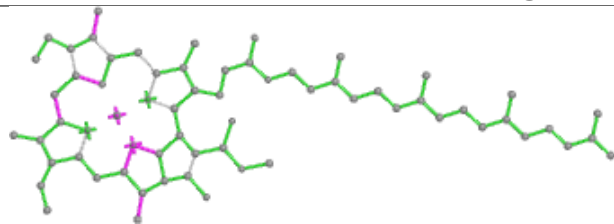
Torsions



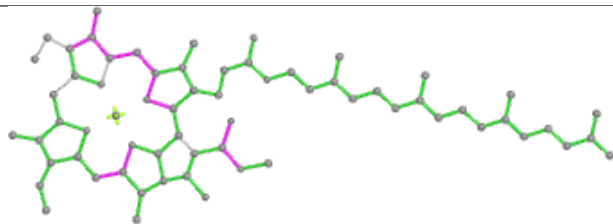
Rings



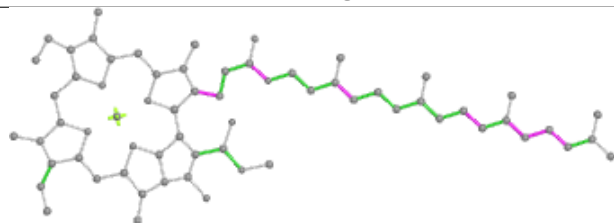
## Ligand CLA I 310



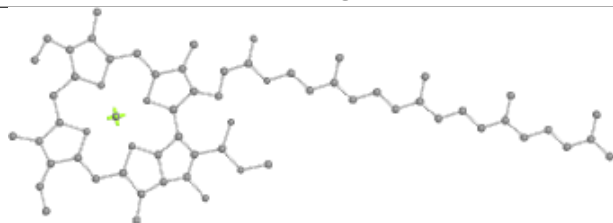
Bond lengths



Bond angles

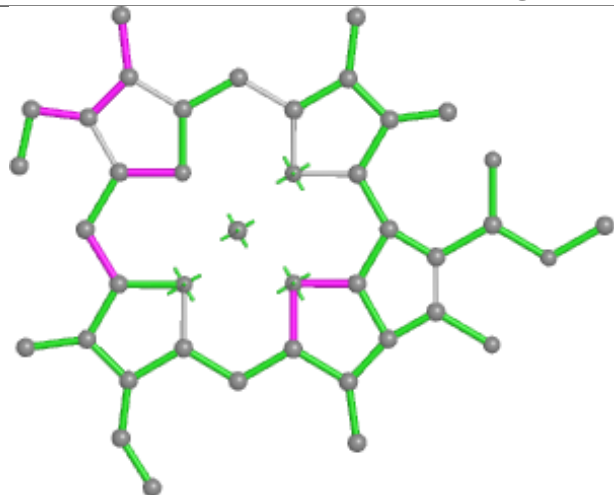


Torsions

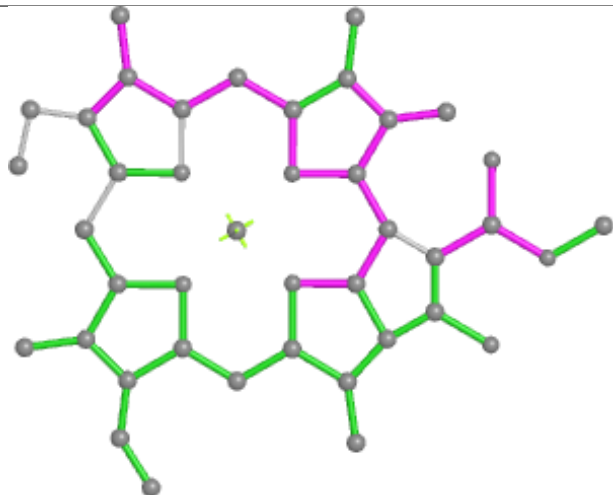


Rings

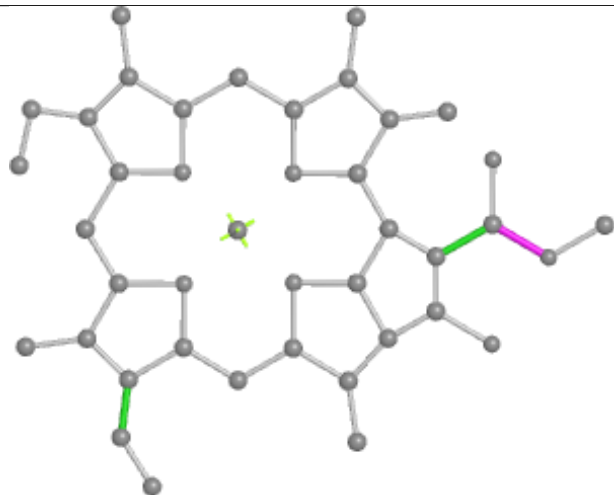
## Ligand CLA X 310



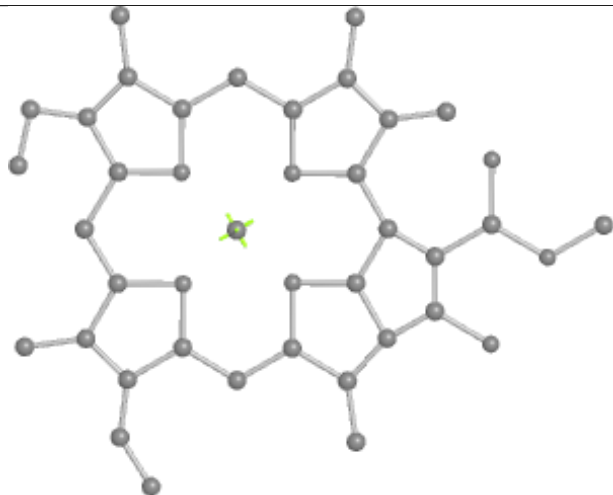
Bond lengths



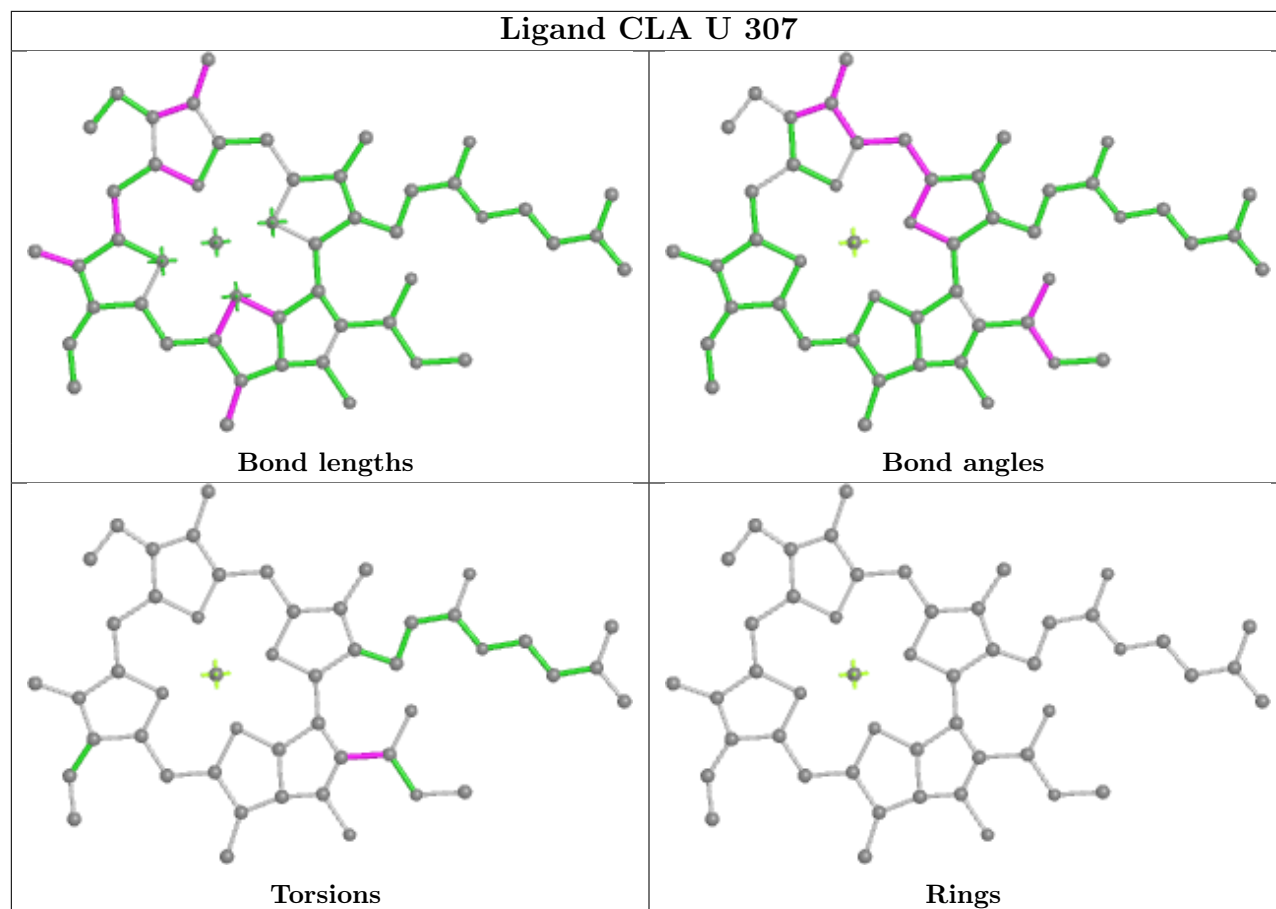
Bond angles

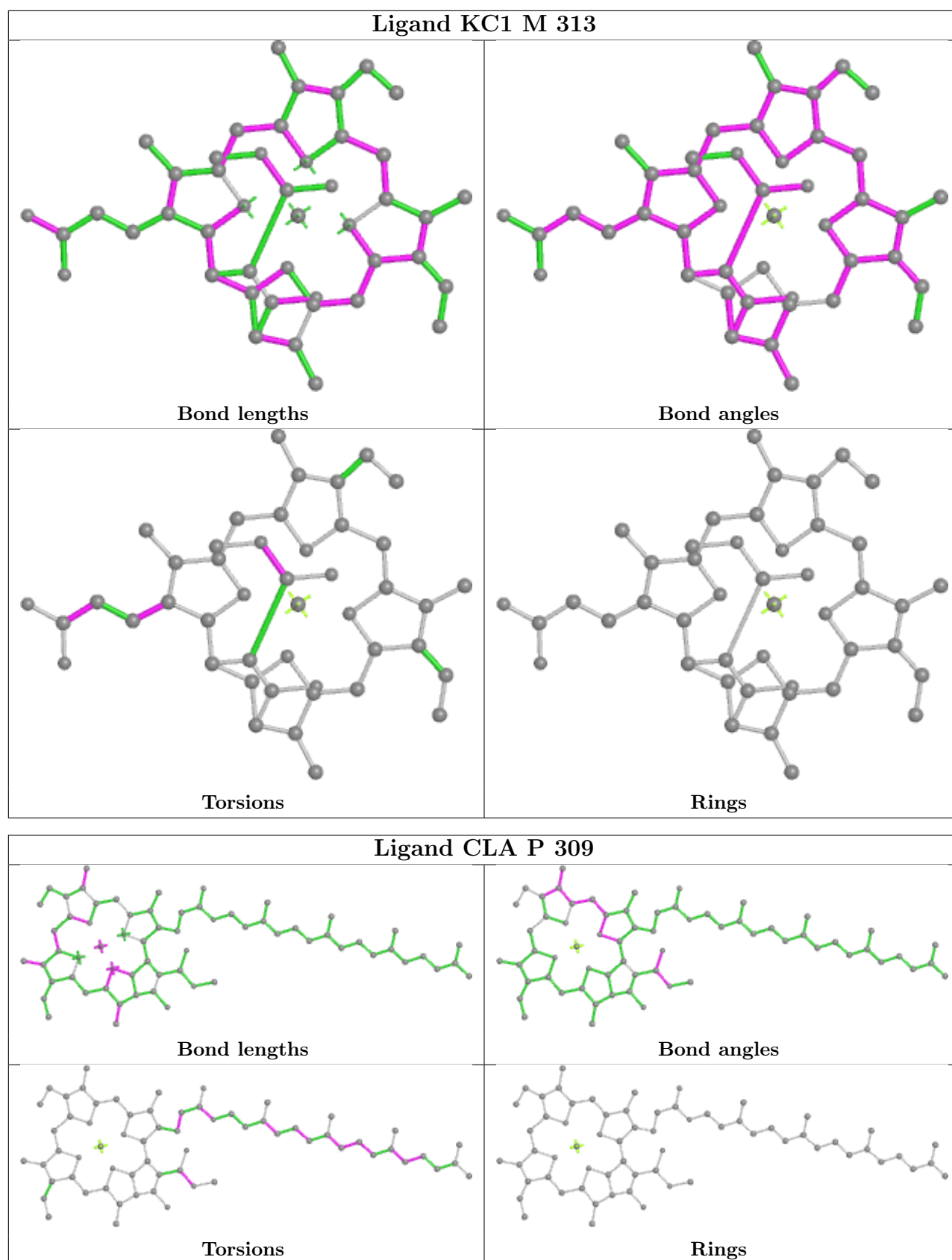


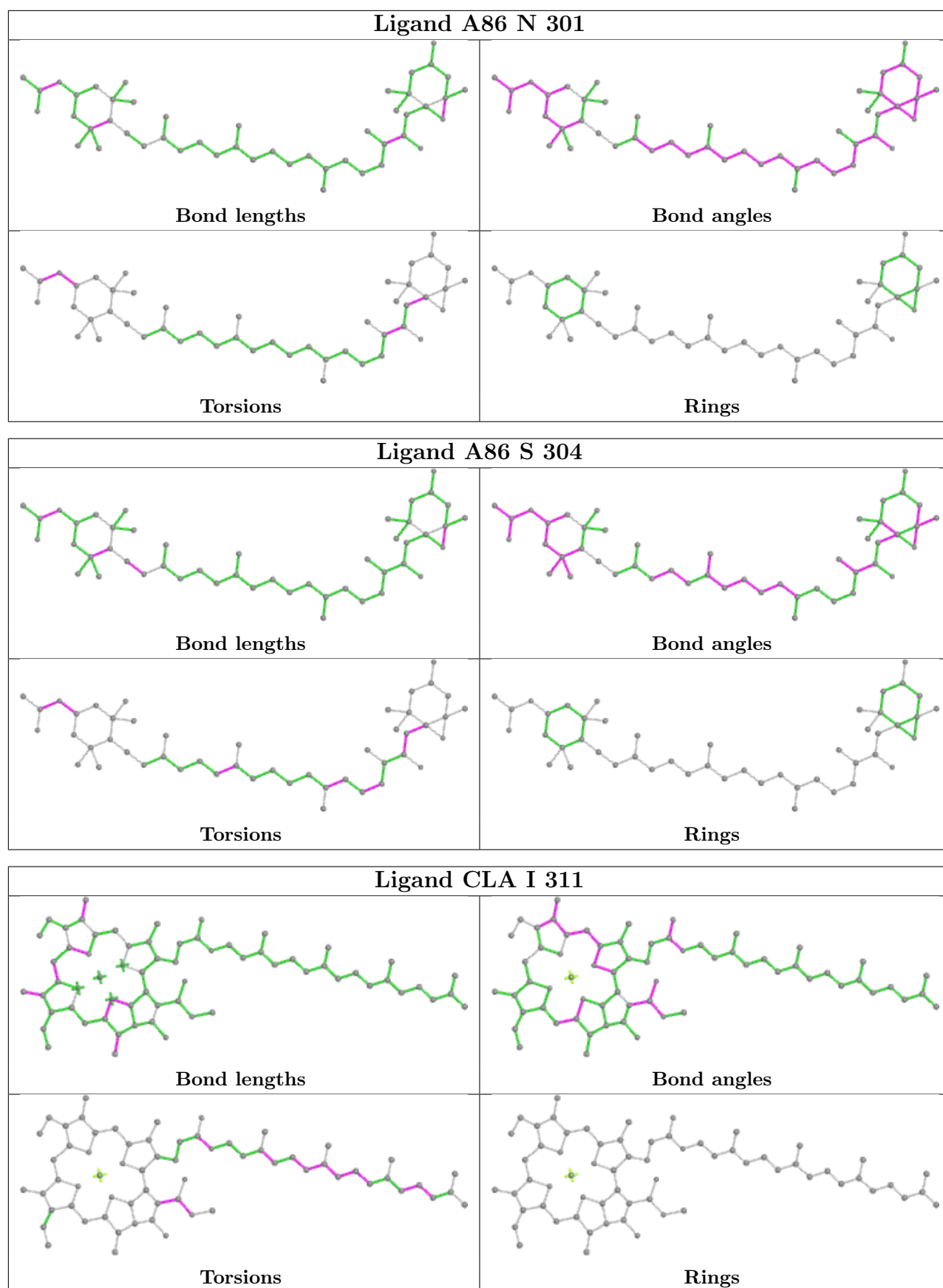
Torsions

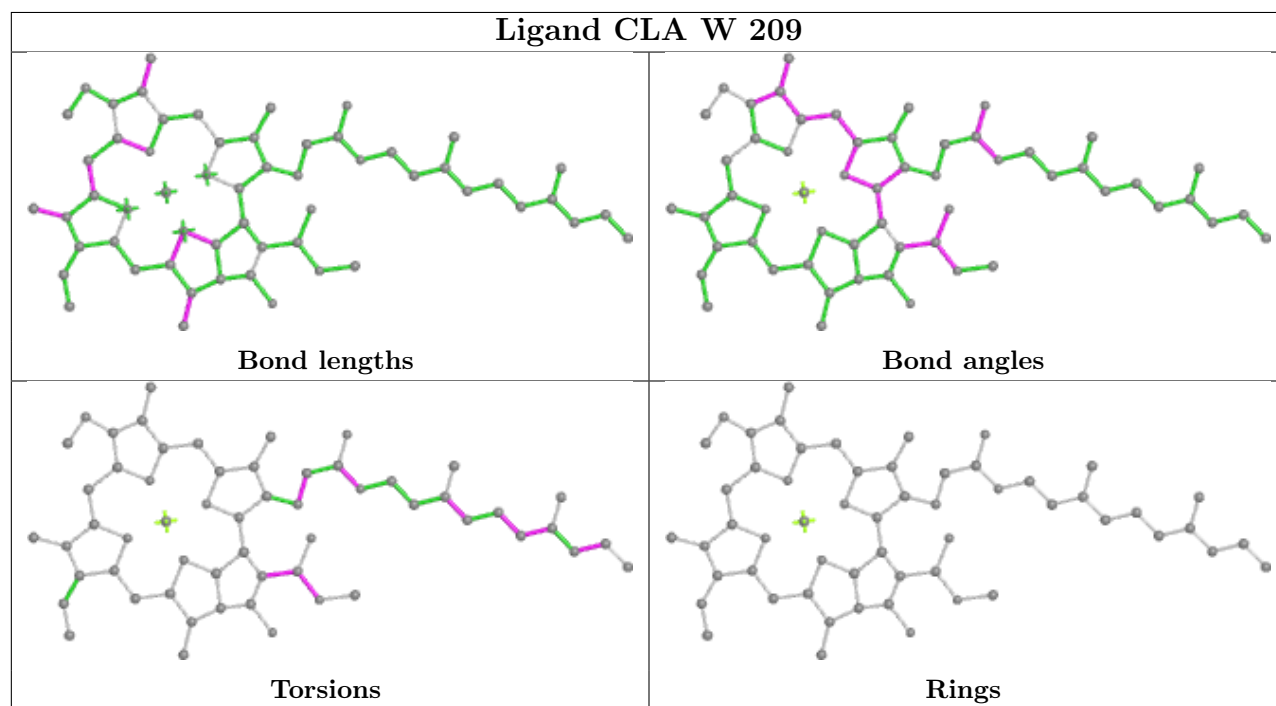
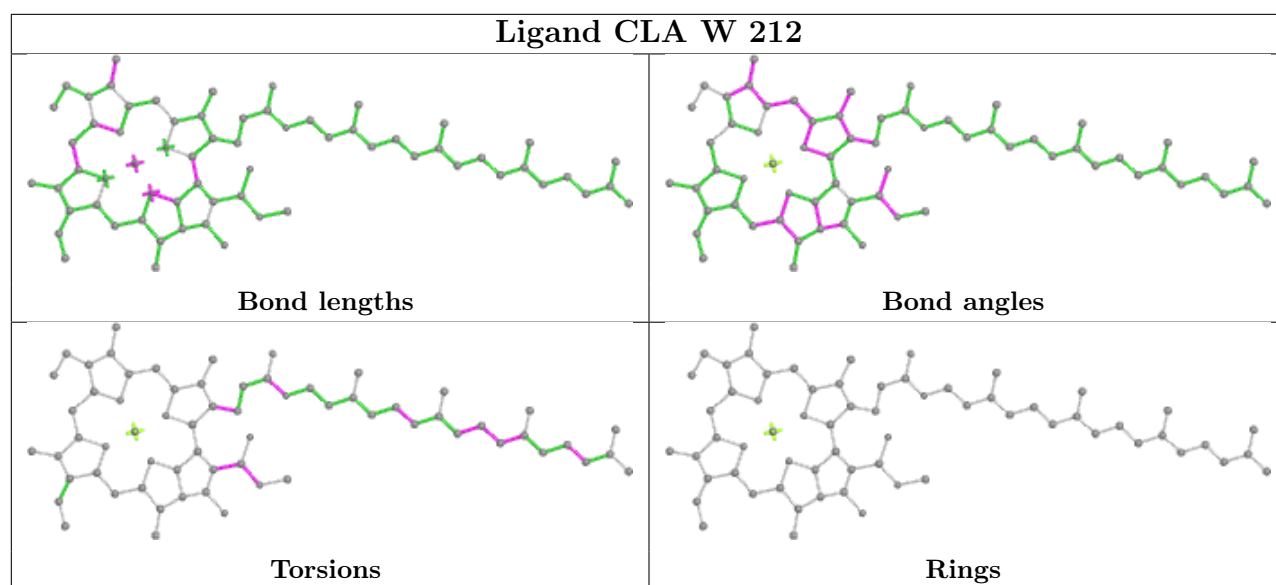


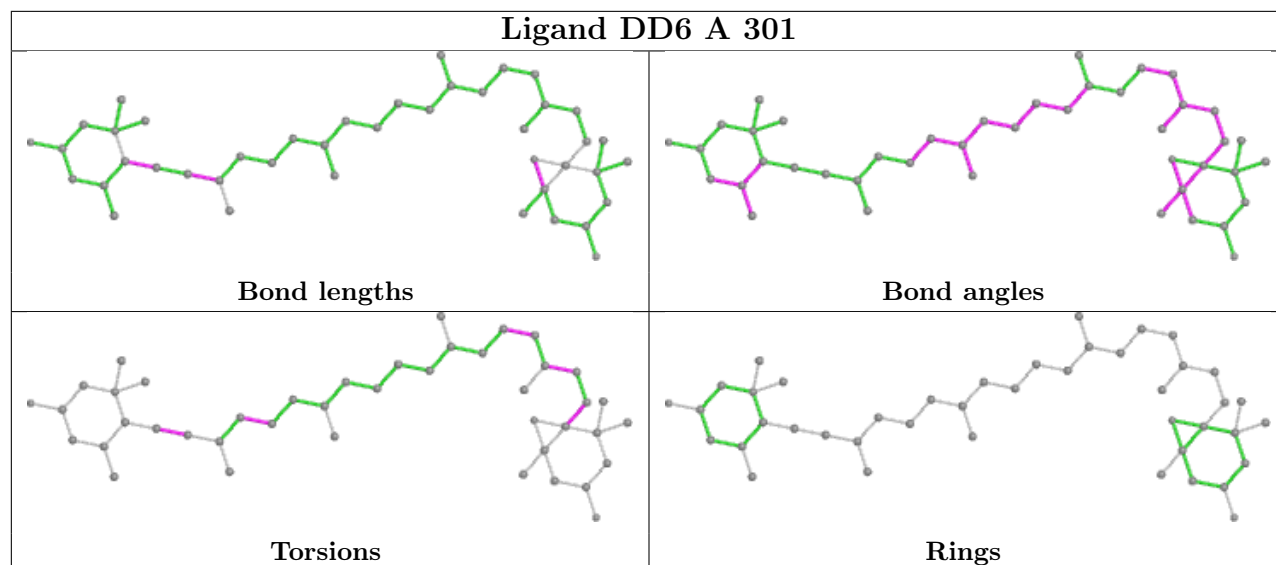
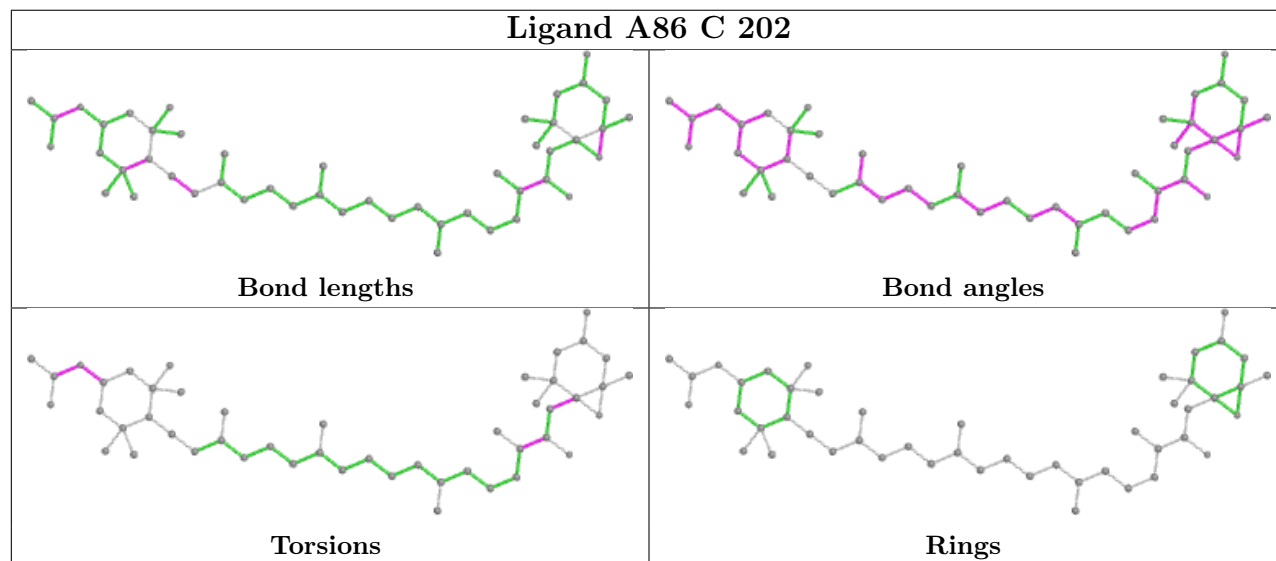
Rings

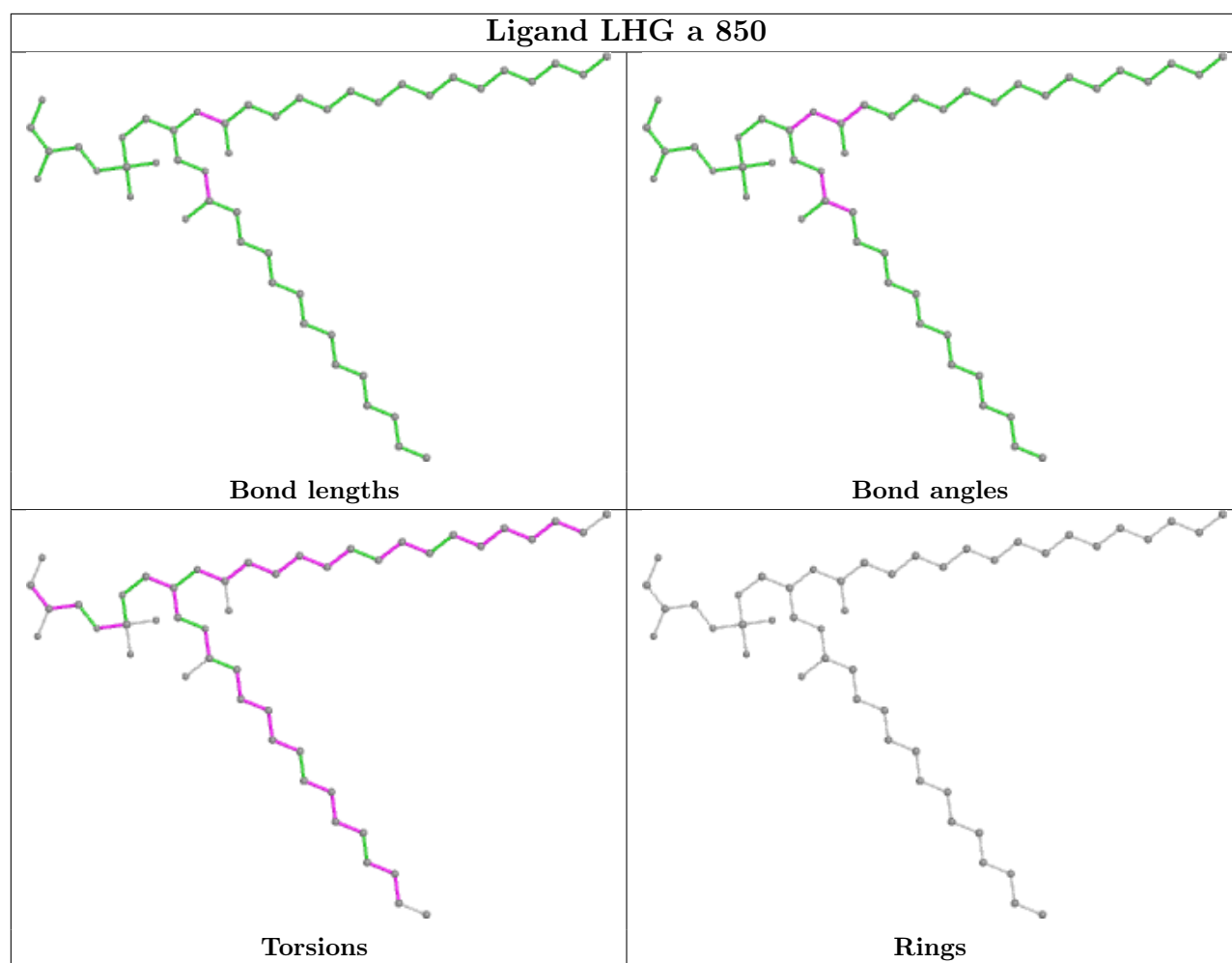




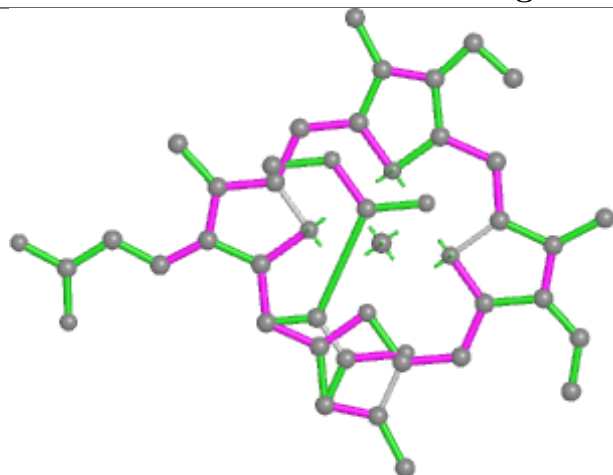




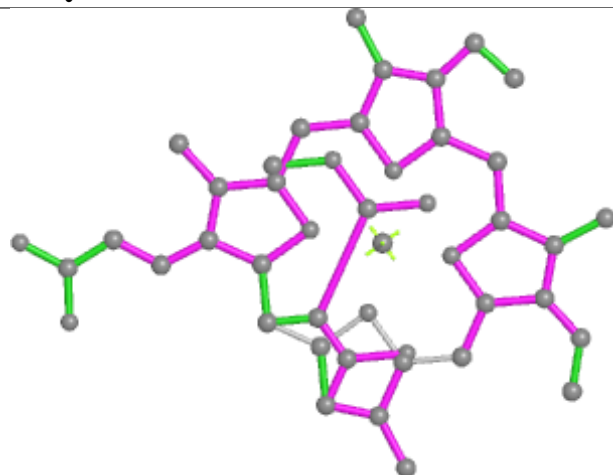
**Ligand DD6 A 301****Ligand A86 C 202**



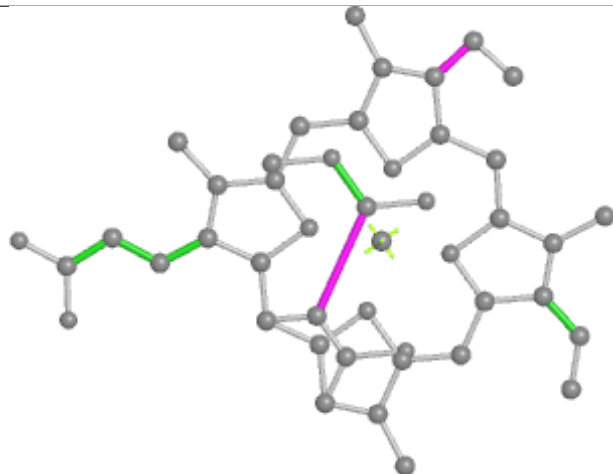
## Ligand KC1 Q 311



Bond lengths



Bond angles

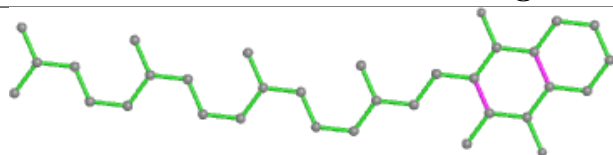


Torsions

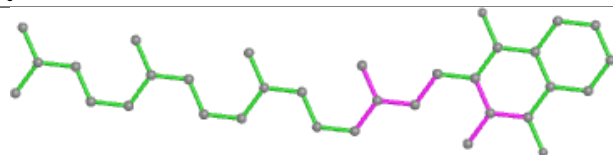


Rings

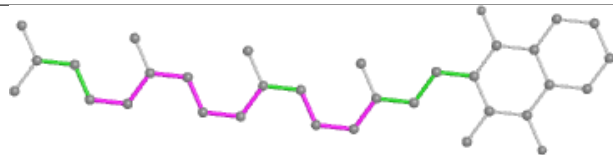
## Ligand PQN b 842



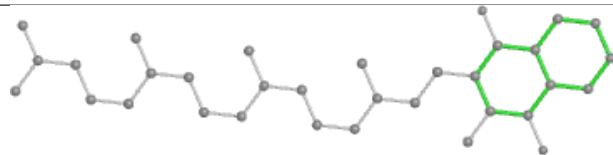
Bond lengths



Bond angles



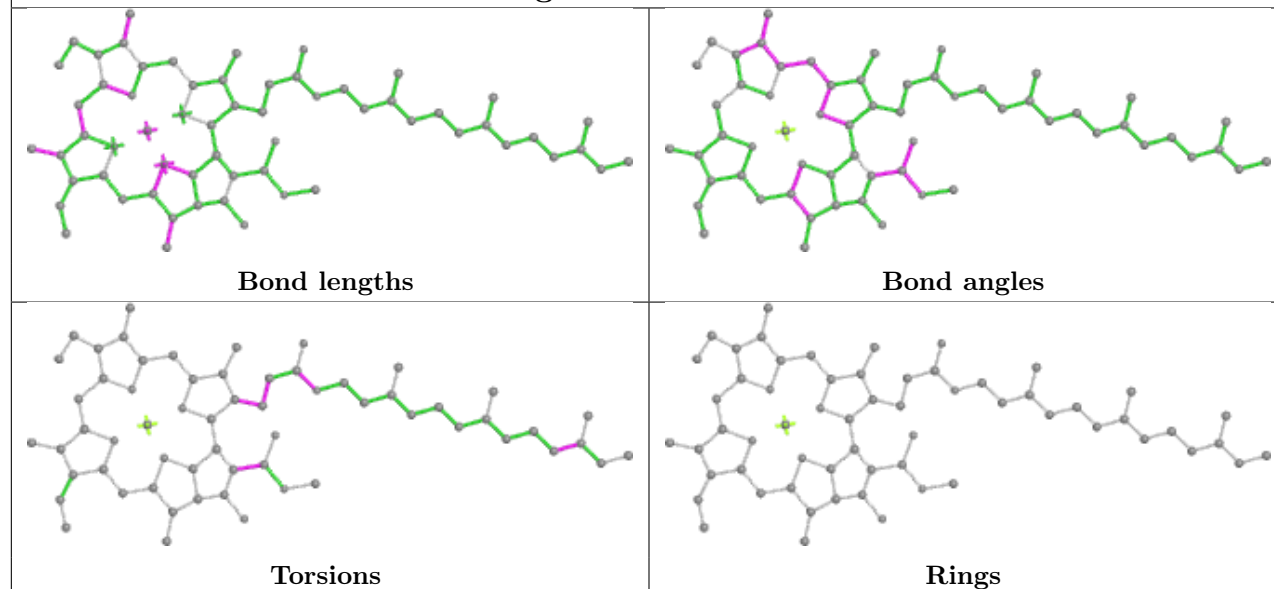
Torsions



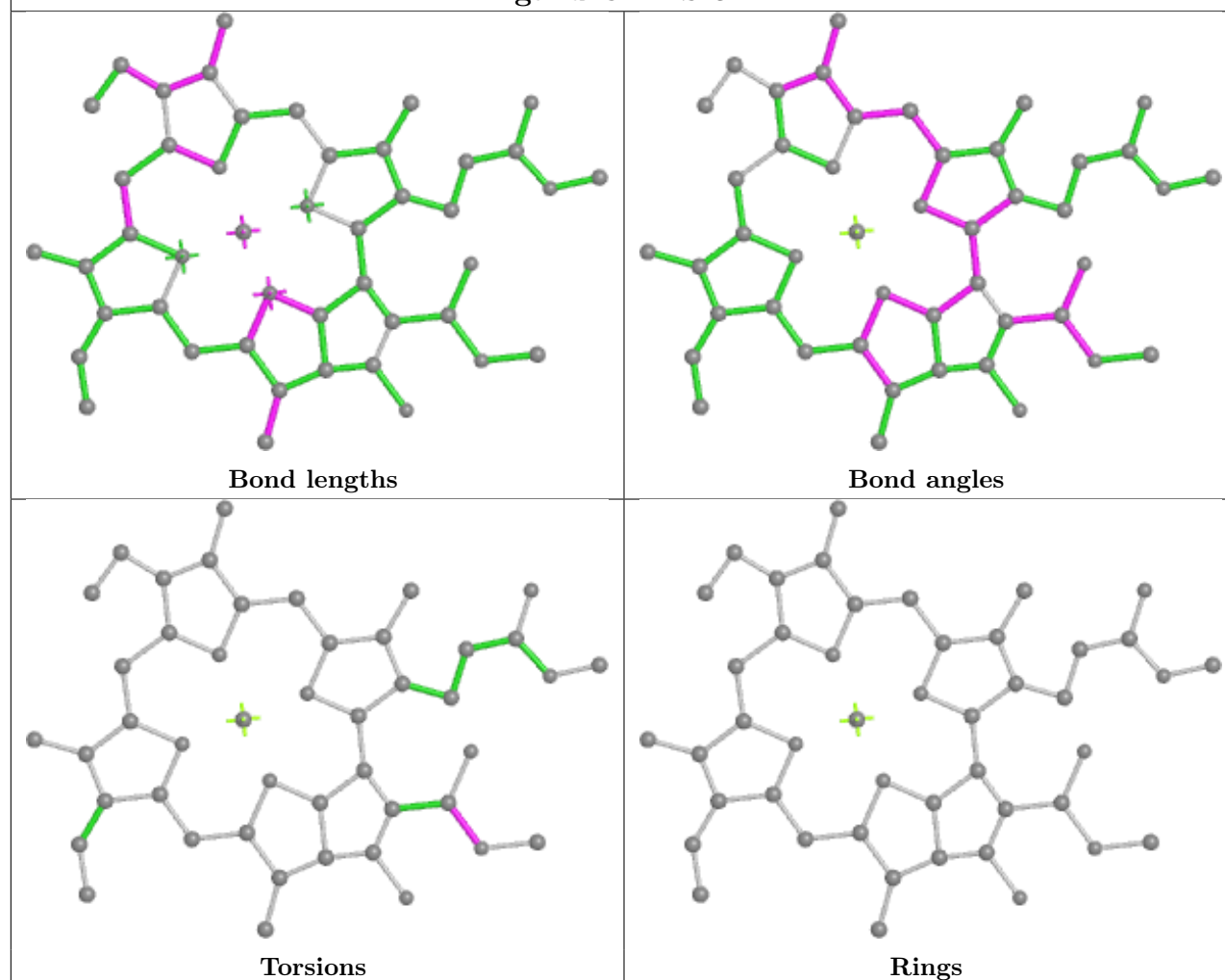
Rings

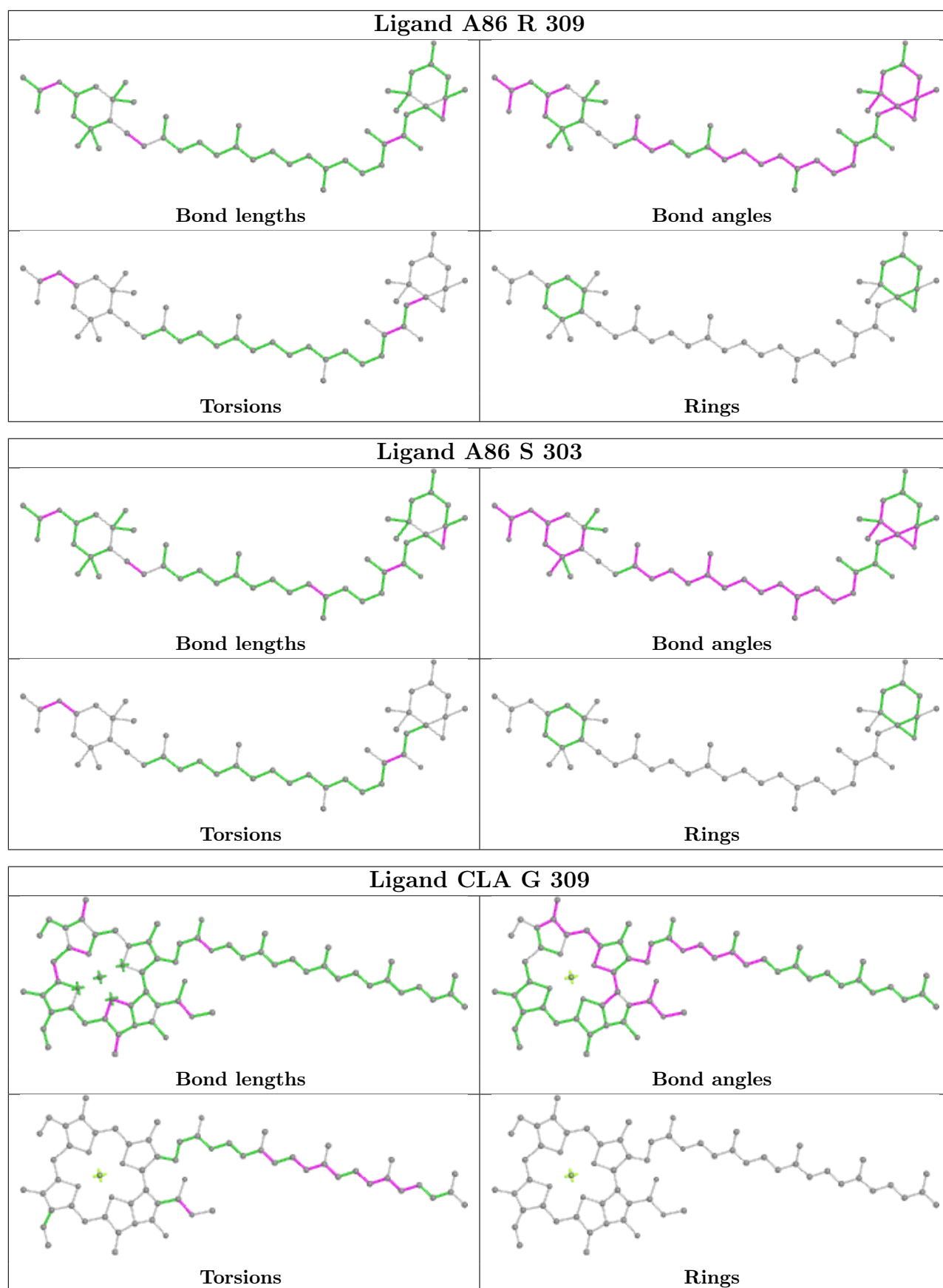


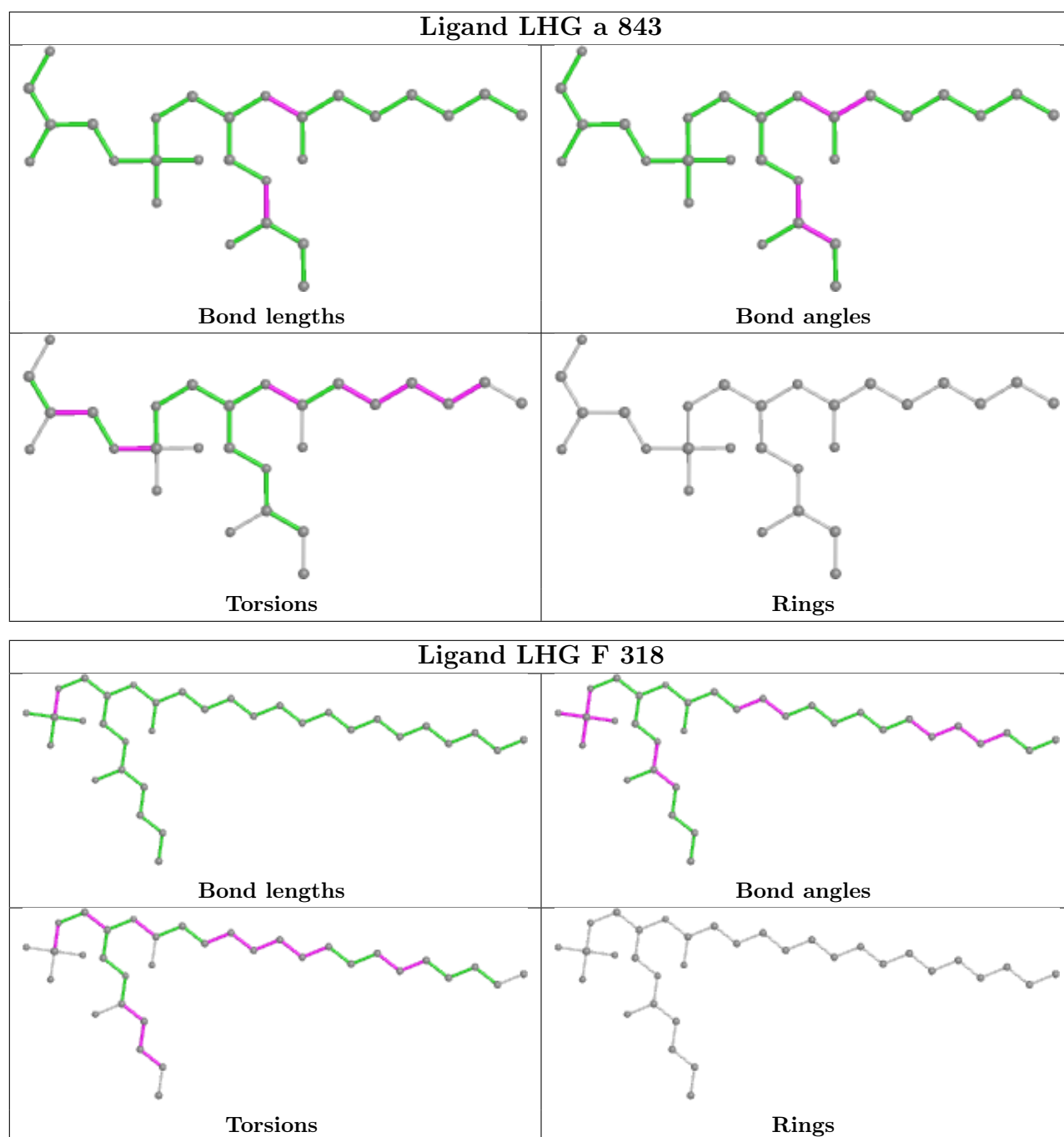
## Ligand CLA S 309



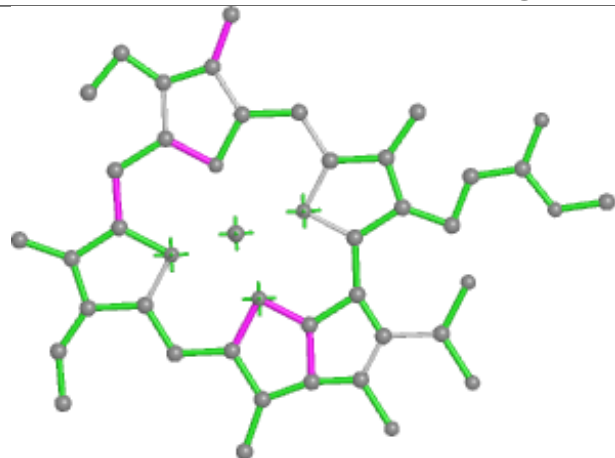
## Ligand CLA S 311



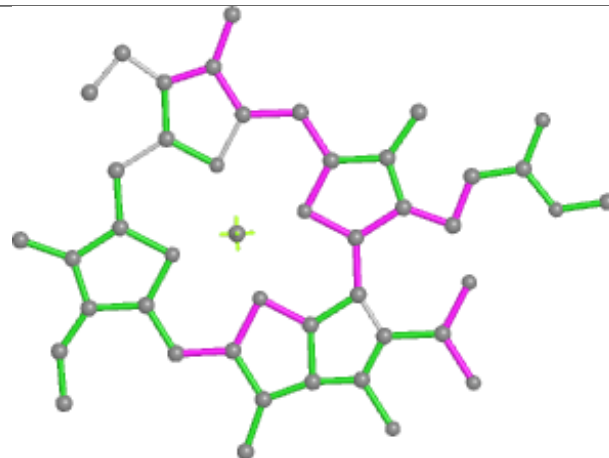




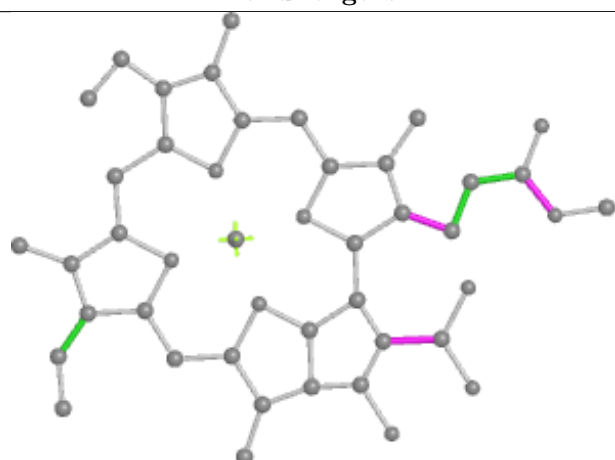
## Ligand CLA X 309



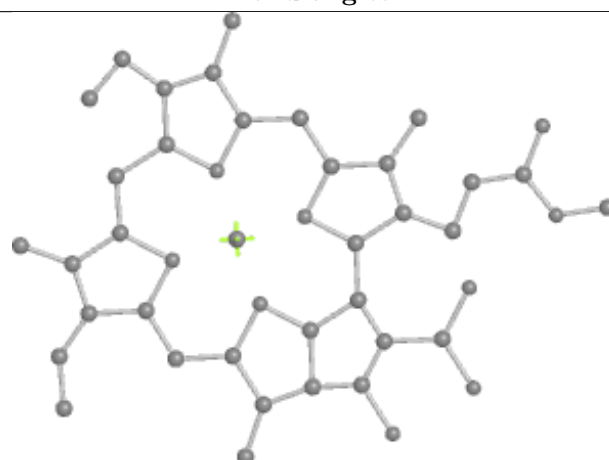
Bond lengths



Bond angles

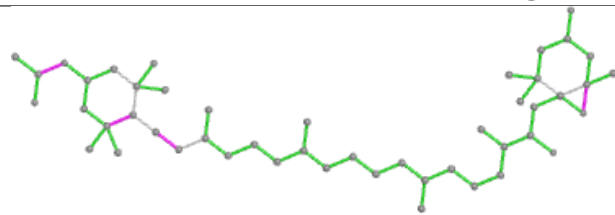


Torsions

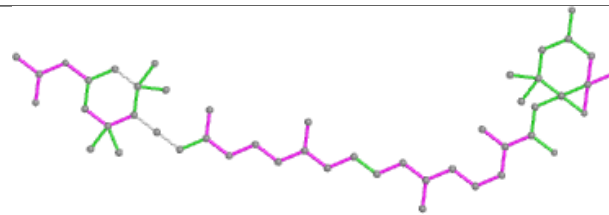


Rings

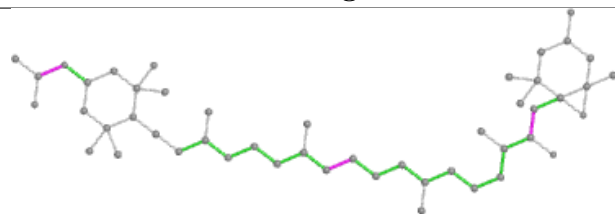
## Ligand A86 T 301



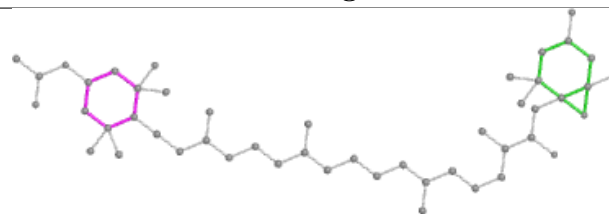
Bond lengths



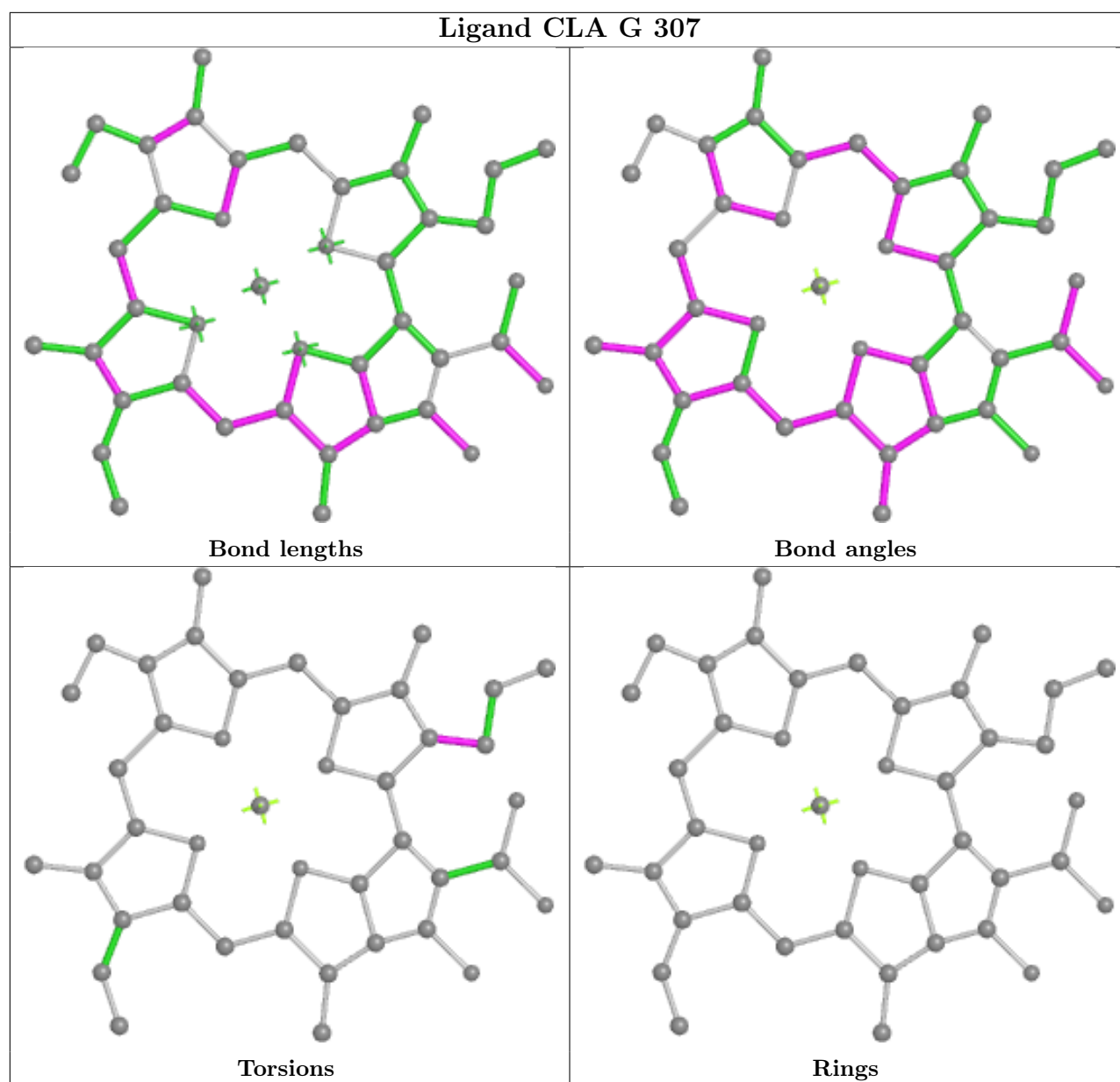
Bond angles

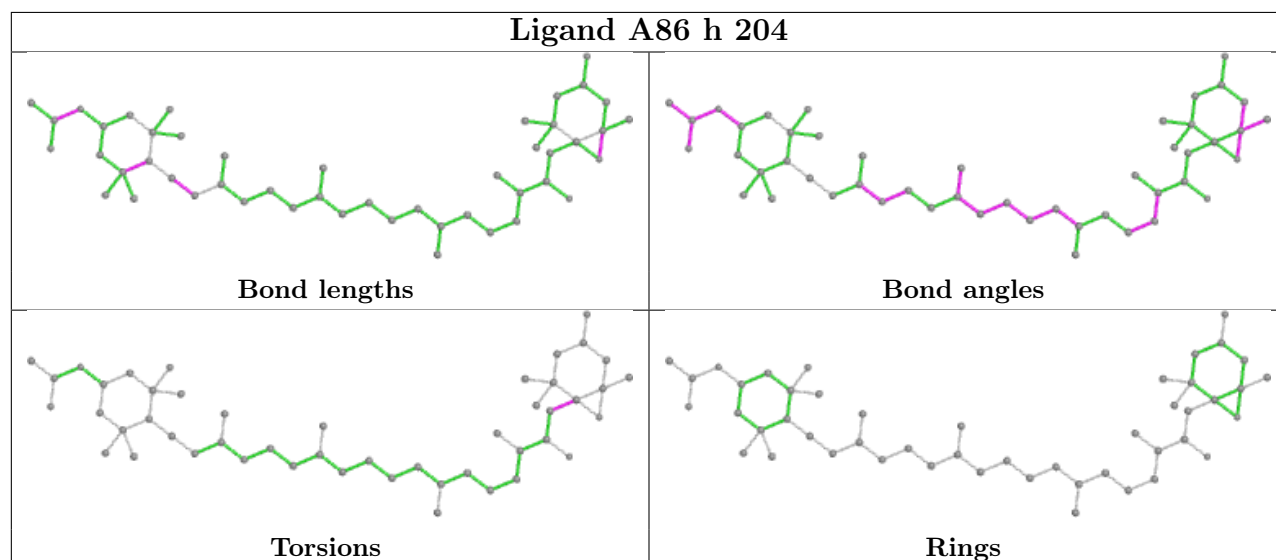
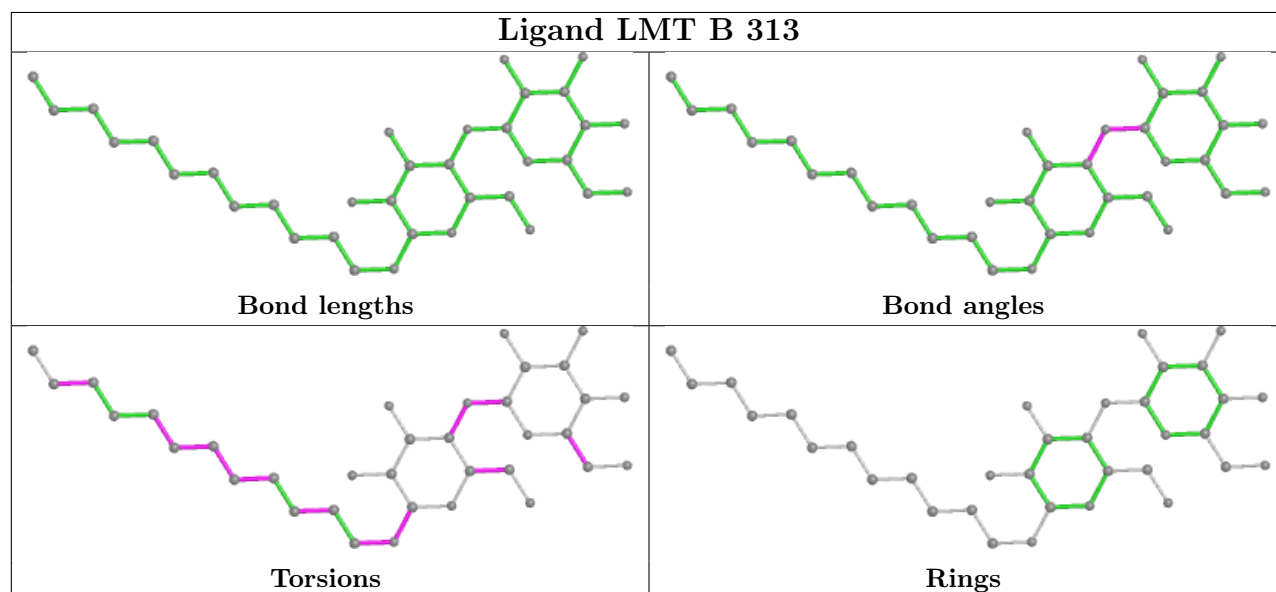
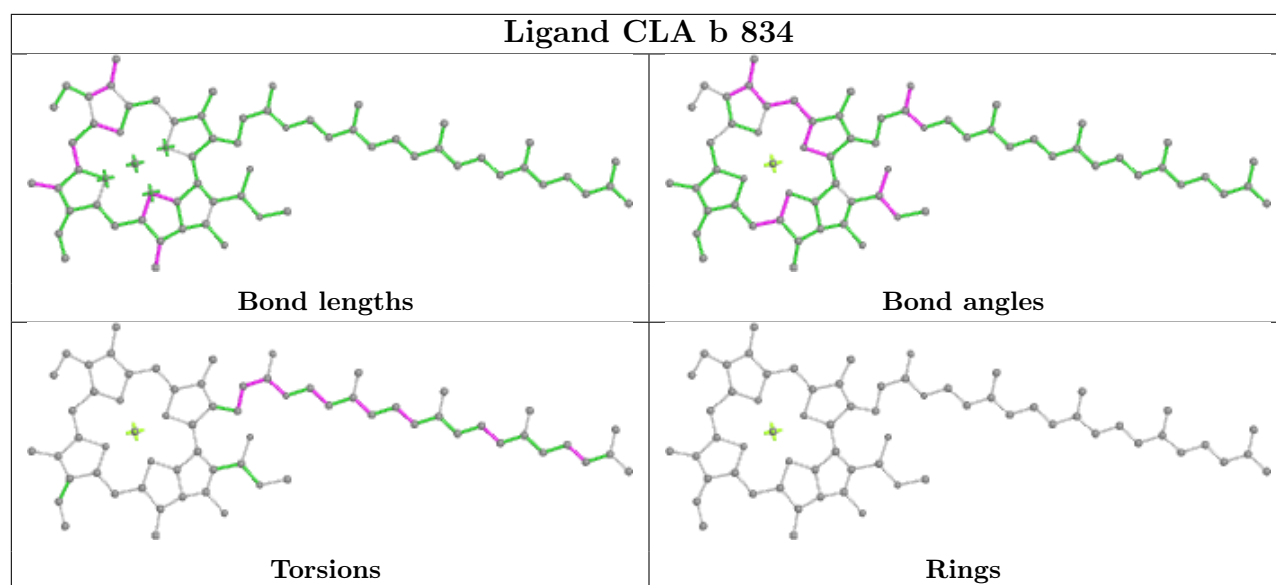


Torsions

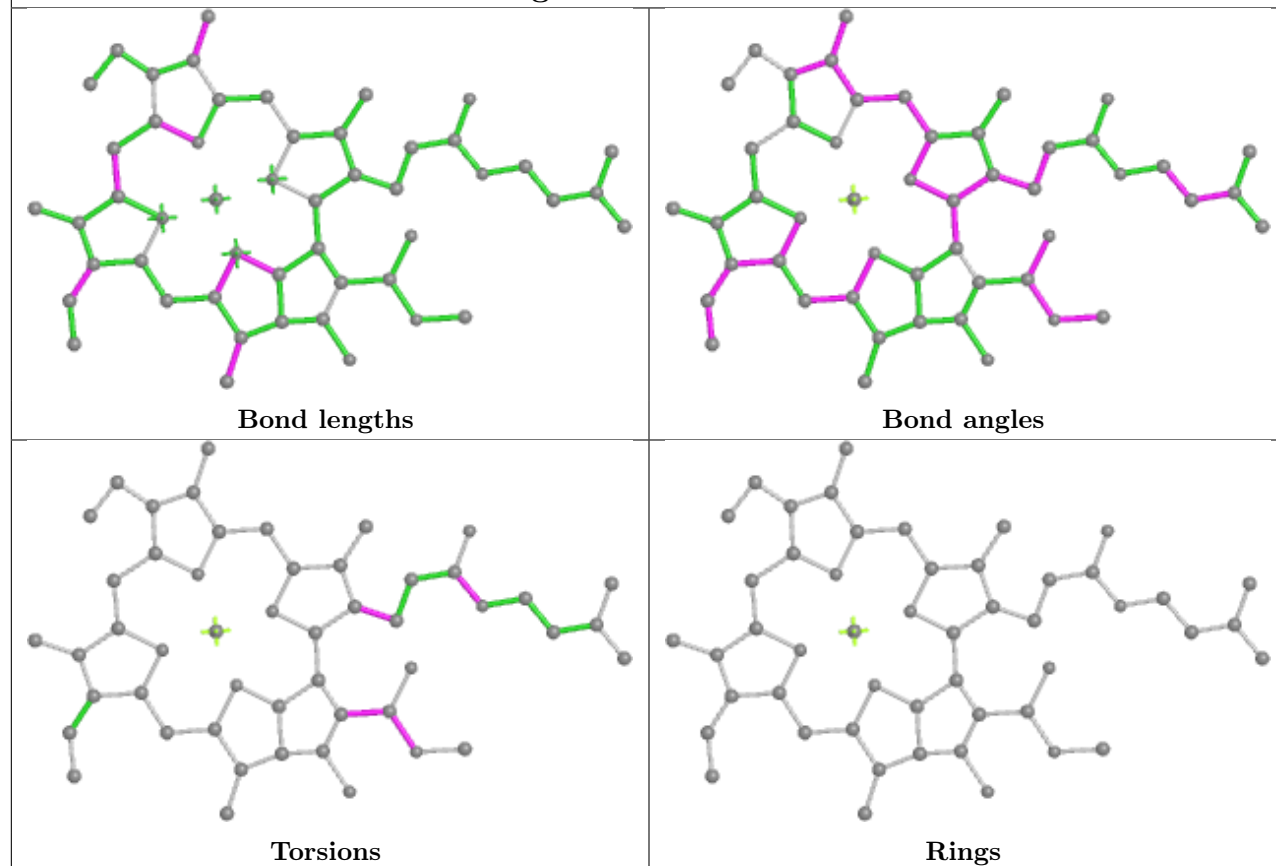


Rings

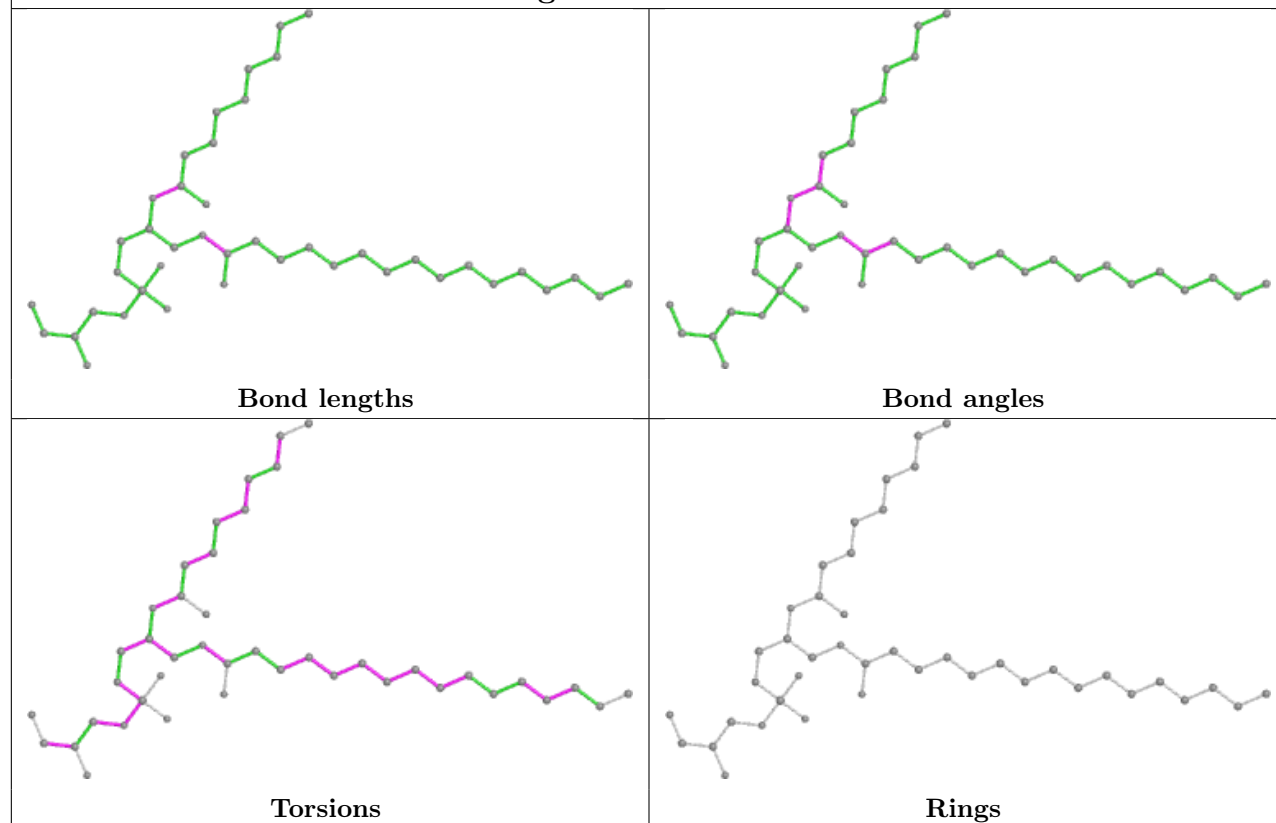


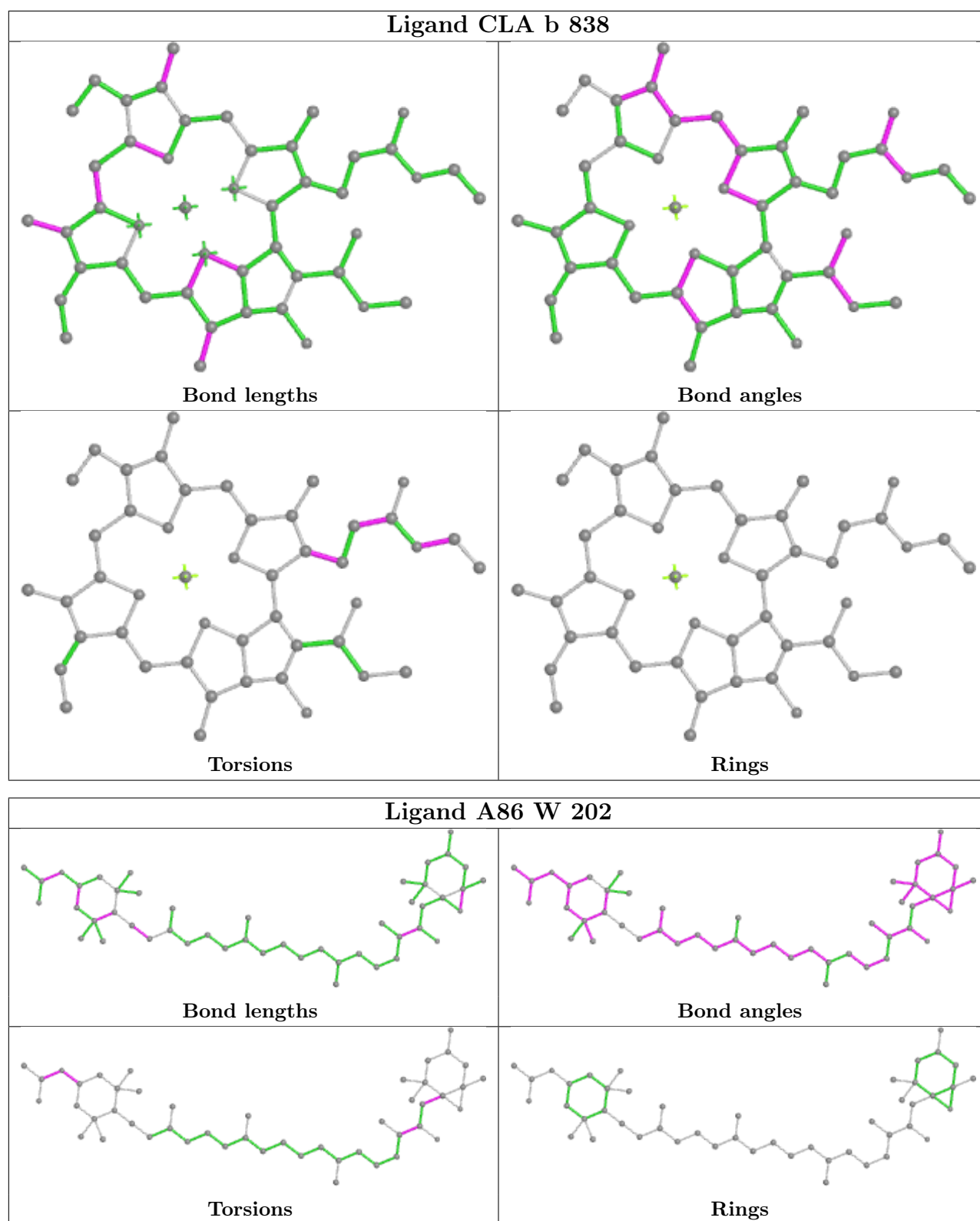


## Ligand CLA X 307



## Ligand LHG f 809





## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

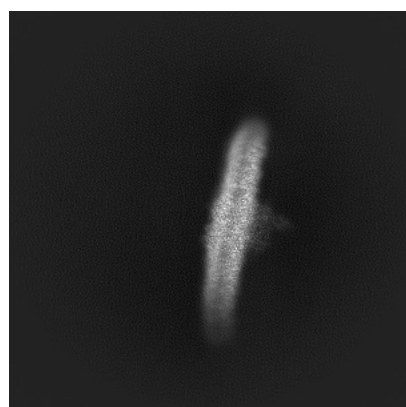
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30012. These allow visual inspection of the internal detail of the map and identification of artifacts.

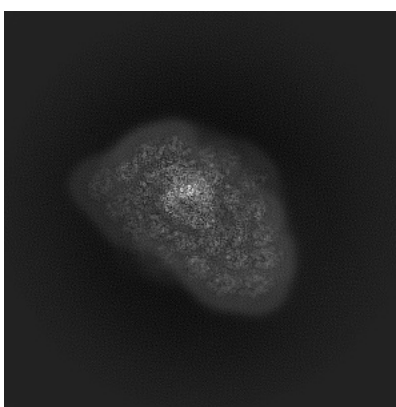
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

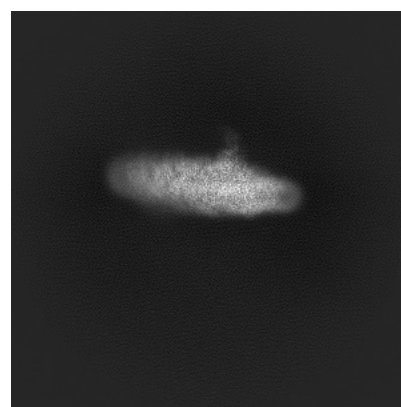
#### 6.1.1 Primary map



X



Y

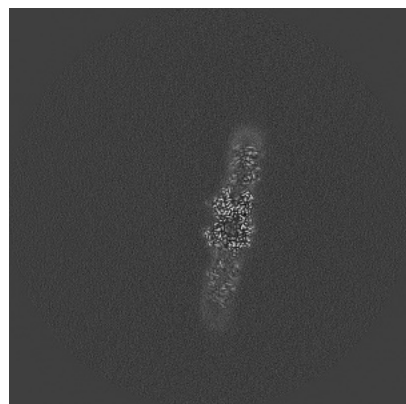


Z

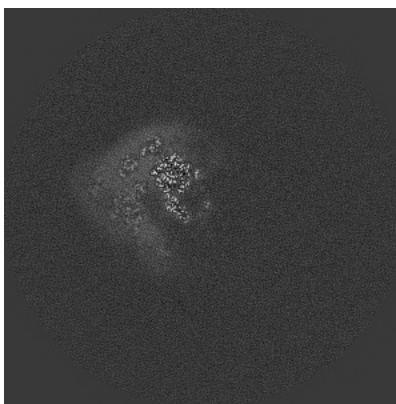
The images above show the map projected in three orthogonal directions.

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

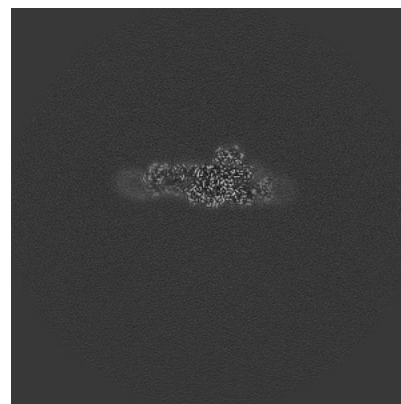
#### 6.2.1 Primary map



X Index: 260



Y Index: 260



Z Index: 260

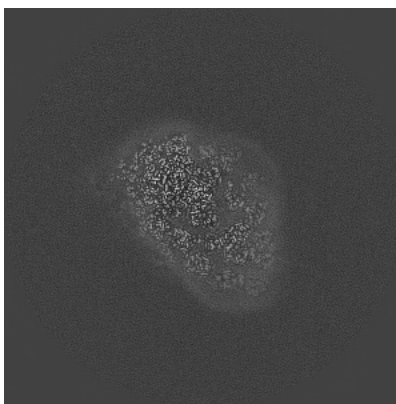
The images above show central slices of the map in three orthogonal directions.

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

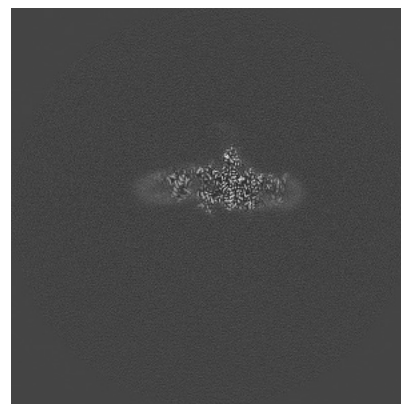
### 6.3.1 Primary map



X Index: 278



Y Index: 294

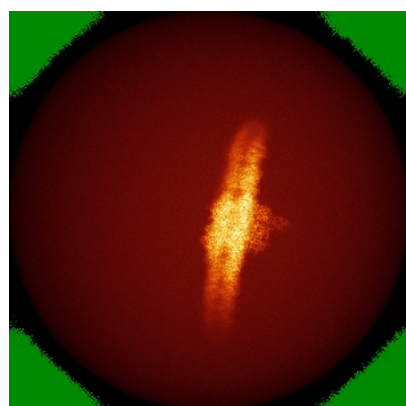


Z Index: 231

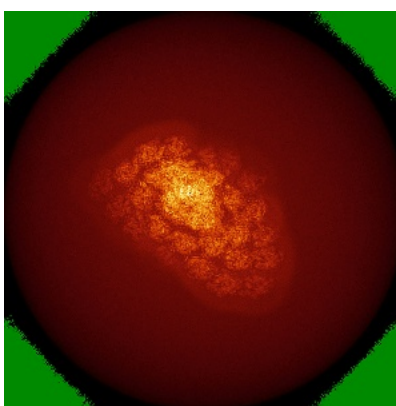
The images above show the largest variance slices of the map in three orthogonal directions.

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

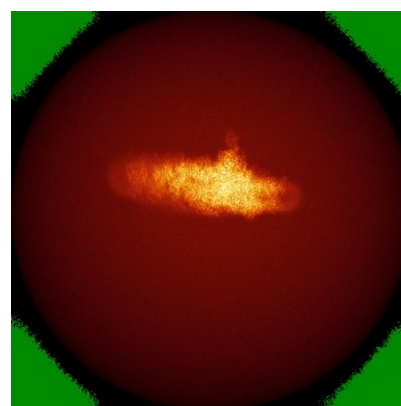
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

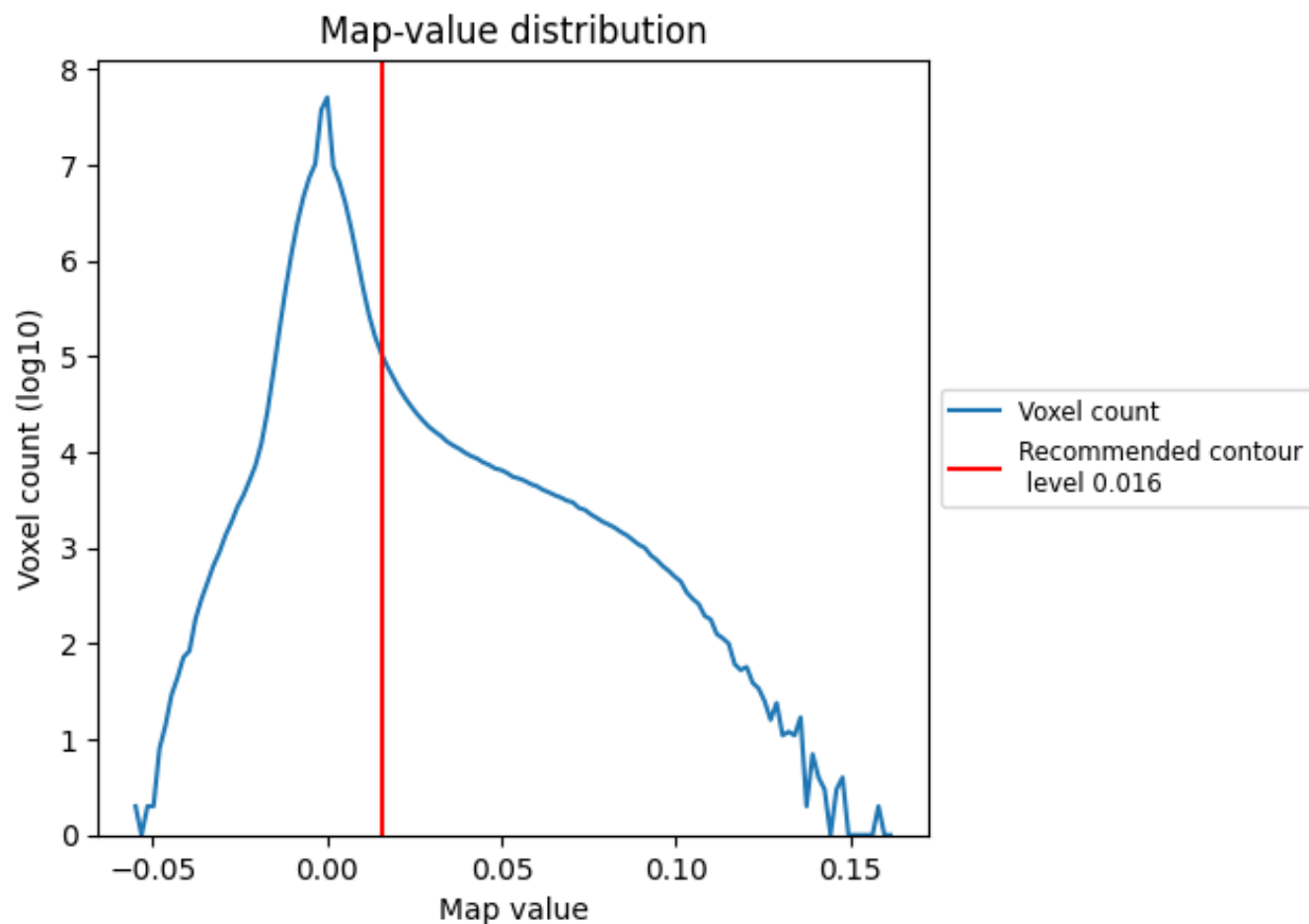
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

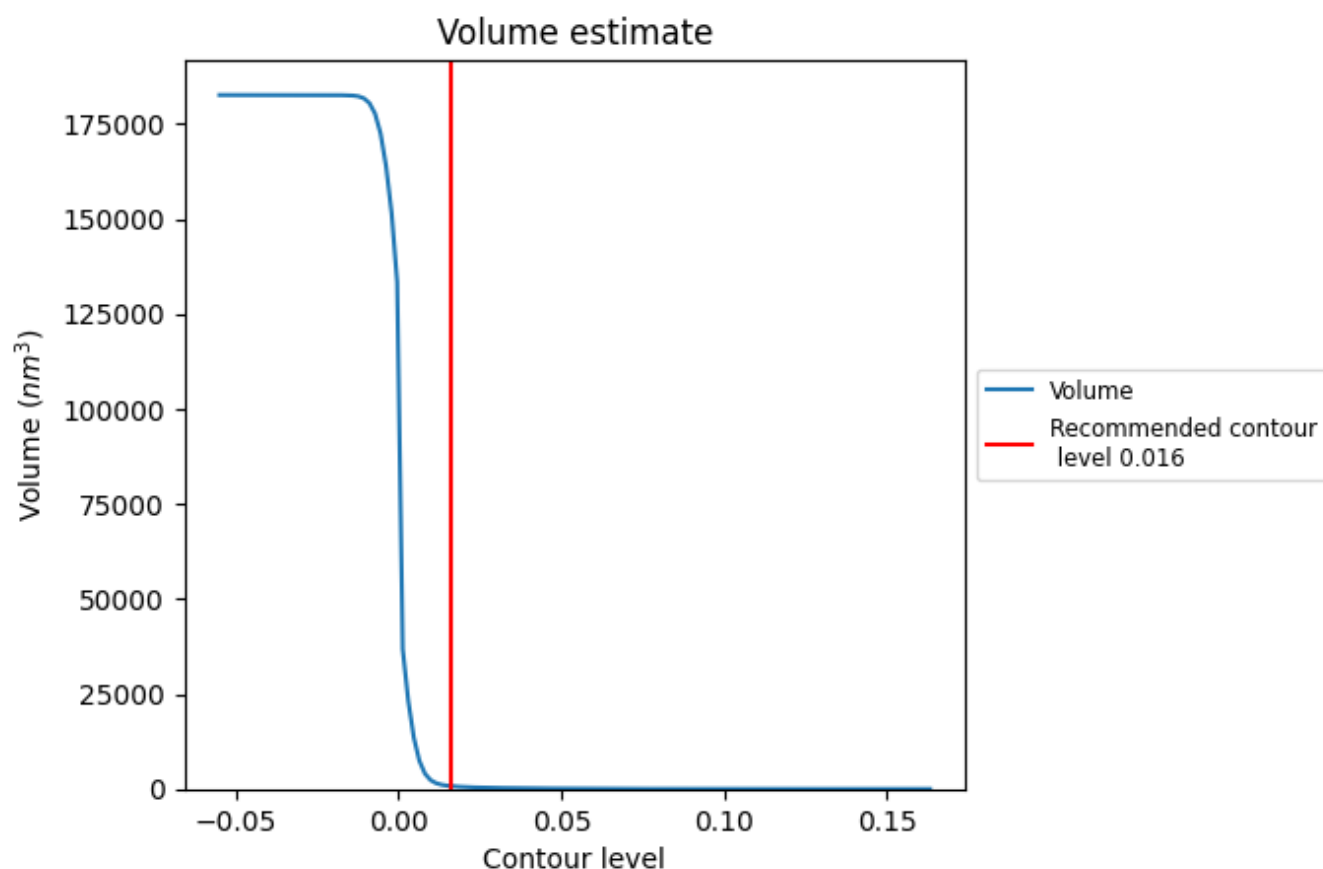
This section contains the results of statistical analysis of the map.

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



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

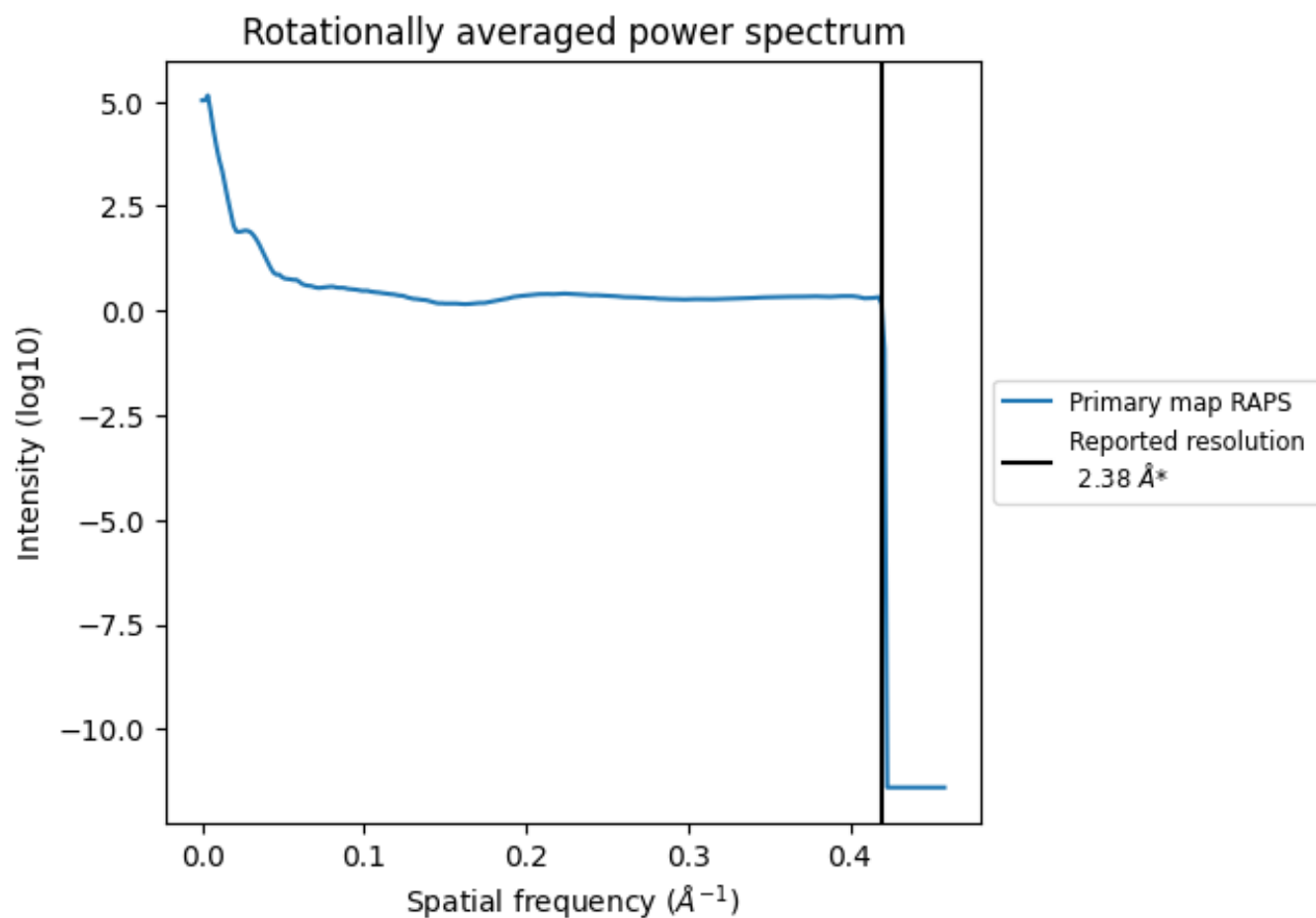
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $778 \text{ nm}^3$ ; this corresponds to an approximate mass of 703 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 0.420  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.



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

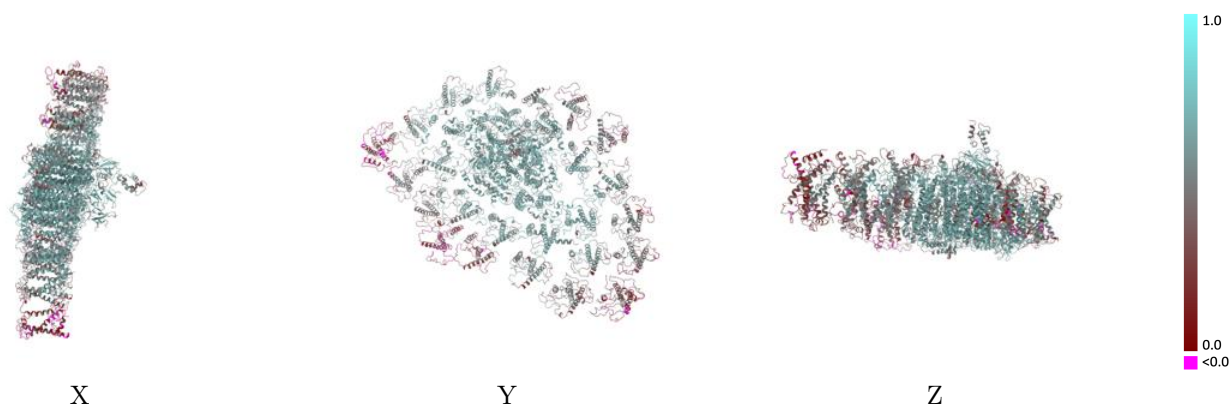
This section contains information regarding the fit between EMDB map EMD-30012 and PDB model 6LY5. Per-residue inclusion information can be found in section [3](#) on page [52](#).

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



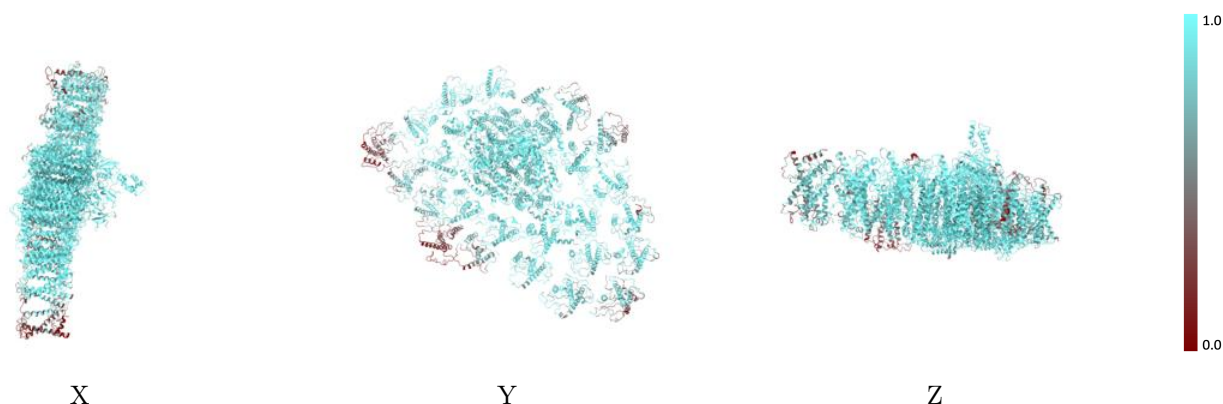
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



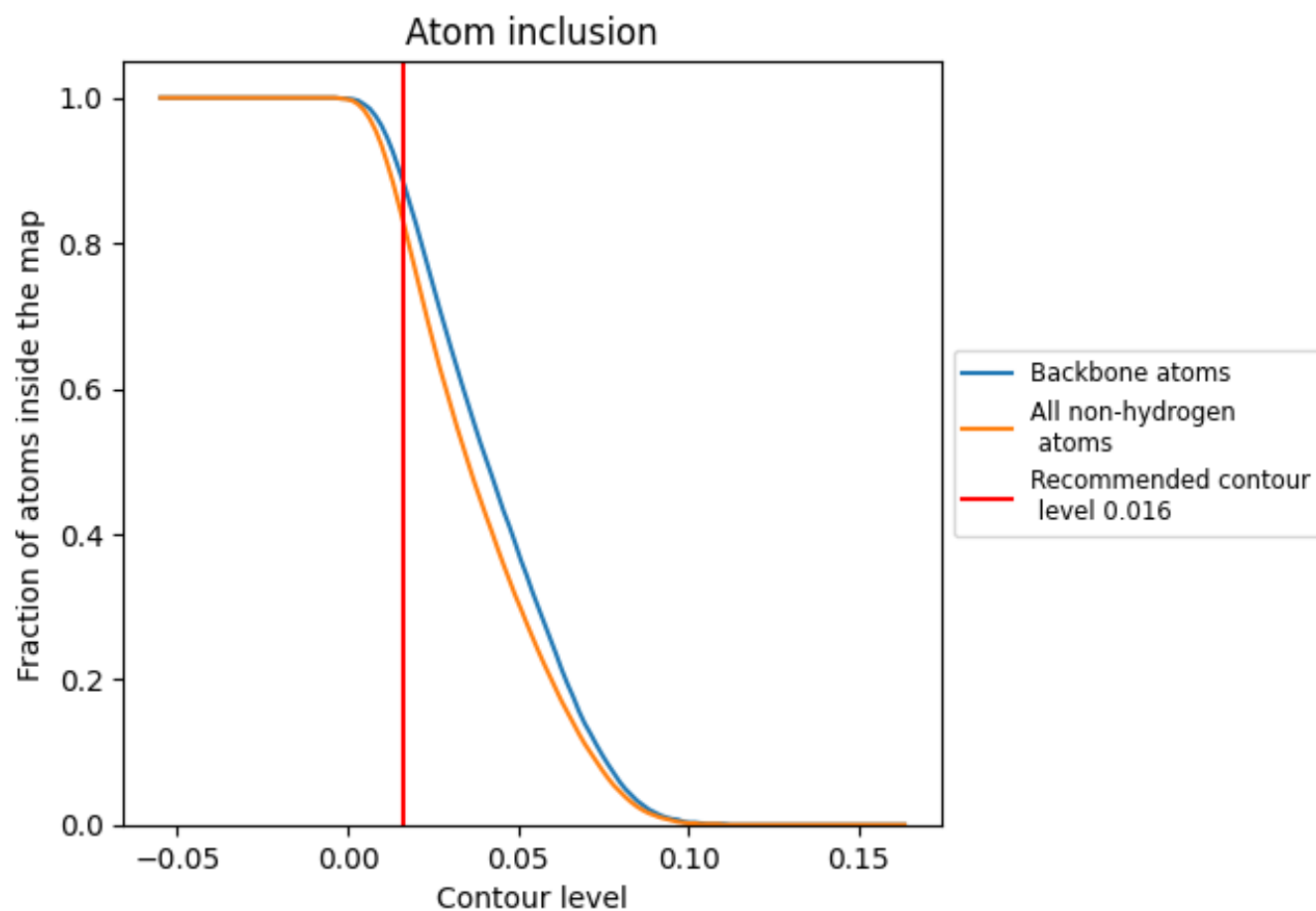
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.5170
A	 0.9410	 0.5810
B	 0.8370	 0.4930
C	 0.8980	 0.5340
D	 0.9340	 0.5870
E	 0.9530	 0.6050
F	 0.9430	 0.5960
G	 0.9570	 0.6150
H	 0.8900	 0.5450
I	 0.9240	 0.5640
J	 0.9060	 0.5400
K	 0.8890	 0.5170
L	 0.8050	 0.4220
M	 0.8700	 0.4820
N	 0.3040	 0.1740
O	 0.6670	 0.4100
P	 0.8980	 0.5260
Q	 0.7760	 0.3880
R	 0.7930	 0.4220
S	 0.5670	 0.2610
T	 0.6280	 0.3920
U	 0.6600	 0.3880
V	 0.7550	 0.4470
W	 0.4970	 0.2640
X	 0.1530	 0.1400
a	 0.9830	 0.6690
b	 0.9910	 0.6730
c	 0.9770	 0.6620
d	 0.9460	 0.6200
e	 0.9210	 0.5940
f	 0.9320	 0.6150
g	 0.8870	 0.4480
h	 0.9690	 0.6040
i	 0.9430	 0.6250
j	 0.9380	 0.6250



*Continued on next page...*

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Chain	Atom inclusion	Q-score
l	 0.9580	 0.6310
m	 0.9420	 0.6140