



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:21 AM UTC

PDB ID : 8JJR / pdb_00008jjr
EMDB ID : EMD-36366
Title : Cryo-EM structure of Symbiodinium photosystem I
Authors : Zhao, L.S.; Wang, N.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on : 2023-05-31
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

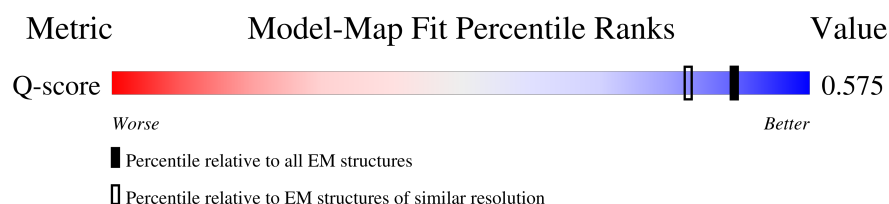
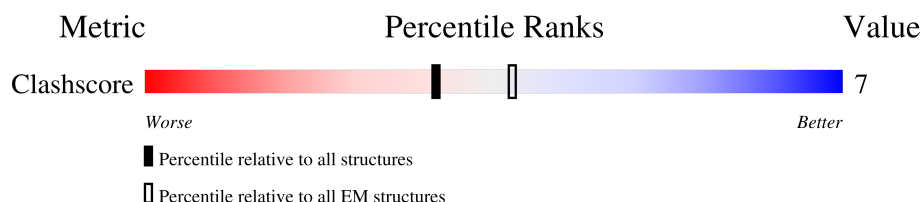
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

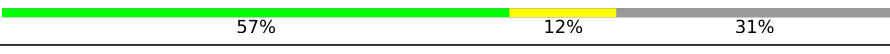
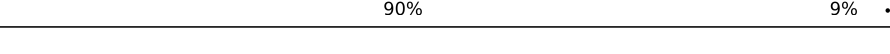
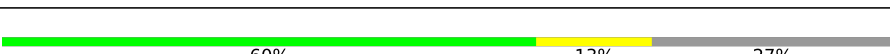
The reported resolution of this entry is 2.80 Å.

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



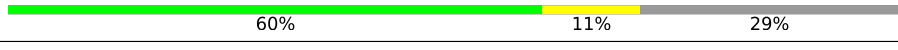
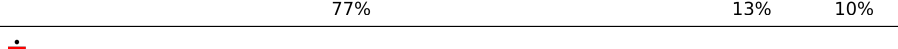
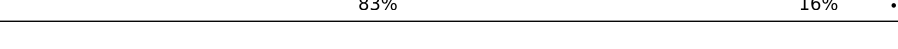
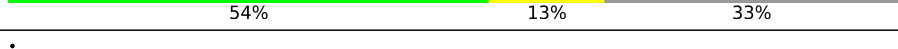
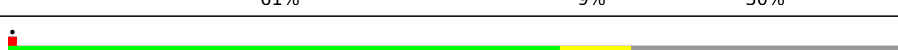
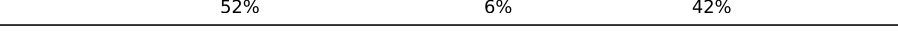
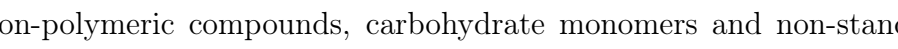
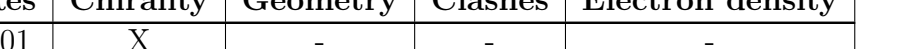
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	256	 65% 11% 24%
2	B	269	 57% 12% 31%
3	C	193	 90% 9% .
4	D	177	 86% 14%
5	E	253	 60% 13% 27%
6	F	286	 68% 10% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	G	228	
8	H	271	
9	I	246	
10	J	203	
11	K	226	
12	T	206	
13	U	137	
14	a	687	
15	b	669	
16	c	161	
17	d	295	
18	e	121	
19	f	279	
20	i	179	
21	j	141	
22	l	361	
23	m	142	
24	r	152	
25	x	121	
26	y	223	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	601	X	-	-	-
27	CLA	A	602	X	-	-	-
27	CLA	A	603	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	604	X	-	-	-
27	CLA	A	605	X	-	-	-
27	CLA	A	606	X	-	-	-
27	CLA	A	607	X	-	-	-
27	CLA	A	609	X	-	-	-
27	CLA	A	610	X	-	-	-
27	CLA	A	611	X	-	-	-
27	CLA	A	612	X	-	-	-
27	CLA	B	601	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	C	201	X	-	-	-
27	CLA	C	202	X	-	-	-
27	CLA	C	203	X	-	-	-
27	CLA	C	204	X	-	-	-
27	CLA	C	205	X	-	-	-
27	CLA	C	206	X	-	-	-
27	CLA	C	207	X	-	-	-
27	CLA	C	208	X	-	-	-
27	CLA	C	209	X	-	-	-
27	CLA	C	211	X	-	-	-
27	CLA	C	212	X	-	-	-
27	CLA	D	601	X	-	-	-
27	CLA	D	602	X	-	-	-
27	CLA	D	603	X	-	-	-
27	CLA	D	604	X	-	-	-
27	CLA	D	605	X	-	-	-
27	CLA	D	606	X	-	-	-
27	CLA	D	607	X	-	-	-
27	CLA	D	608	X	-	-	-
27	CLA	D	609	X	-	-	-
27	CLA	D	610	X	-	-	-
27	CLA	D	611	X	-	-	-
27	CLA	D	612	X	-	-	-
27	CLA	E	602	X	-	-	-
27	CLA	E	603	X	-	-	-
27	CLA	E	604	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	E	605	X	-	-	-
27	CLA	E	606	X	-	-	-
27	CLA	E	607	X	-	-	-
27	CLA	E	608	X	-	-	-
27	CLA	E	609	X	-	-	-
27	CLA	E	611	X	-	-	-
27	CLA	E	612	X	-	-	-
27	CLA	F	601	X	-	-	-
27	CLA	F	602	X	-	-	-
27	CLA	F	603	X	-	-	-
27	CLA	F	604	X	-	-	-
27	CLA	F	605	X	-	-	-
27	CLA	F	606	X	-	-	-
27	CLA	F	607	X	-	-	-
27	CLA	F	608	X	-	-	-
27	CLA	F	610	X	-	-	-
27	CLA	F	617	X	-	-	-
27	CLA	F	619	X	-	-	-
27	CLA	G	602	X	-	-	-
27	CLA	G	603	X	-	-	-
27	CLA	G	604	X	-	-	-
27	CLA	G	605	X	-	-	-
27	CLA	G	606	X	-	-	-
27	CLA	G	607	X	-	-	-
27	CLA	G	608	X	-	-	-
27	CLA	G	609	X	-	-	-
27	CLA	G	610	X	-	-	-
27	CLA	G	611	X	-	-	-
27	CLA	H	303	X	-	-	-
27	CLA	H	304	X	-	-	-
27	CLA	H	305	X	-	-	-
27	CLA	H	306	X	-	-	-
27	CLA	H	307	X	-	-	-
27	CLA	H	308	X	-	-	-
27	CLA	H	309	X	-	-	-
27	CLA	H	310	X	-	-	-
27	CLA	H	312	X	-	-	-
27	CLA	H	313	X	-	-	-
27	CLA	H	319	X	-	-	-
27	CLA	I	601	X	-	-	-
27	CLA	I	602	X	-	-	-
27	CLA	I	603	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	I	605	X	-	-	-
27	CLA	I	606	X	-	-	-
27	CLA	I	607	X	-	-	-
27	CLA	I	608	X	-	-	-
27	CLA	I	609	X	-	-	-
27	CLA	I	610	X	-	-	-
27	CLA	I	611	X	-	-	-
27	CLA	I	616	X	-	-	-
27	CLA	J	601	X	-	-	-
27	CLA	J	603	X	-	-	-
27	CLA	J	605	X	-	-	-
27	CLA	J	607	X	-	-	-
27	CLA	J	609	X	-	-	-
27	CLA	K	601	X	-	-	-
27	CLA	K	602	X	-	-	-
27	CLA	K	603	X	-	-	-
27	CLA	K	604	X	-	-	-
27	CLA	K	605	X	-	-	-
27	CLA	K	606	X	-	-	-
27	CLA	K	608	X	-	-	-
27	CLA	T	601	X	-	-	-
27	CLA	T	602	X	-	-	-
27	CLA	T	603	X	-	-	-
27	CLA	T	604	X	-	-	-
27	CLA	T	605	X	-	-	-
27	CLA	T	606	X	-	-	-
27	CLA	T	607	X	-	-	-
27	CLA	T	609	X	-	-	-
27	CLA	U	601	X	-	-	-
27	CLA	U	603	X	-	-	-
27	CLA	U	605	X	-	-	-
27	CLA	U	606	X	-	-	-
27	CLA	a	801	X	-	-	-
27	CLA	a	802	X	-	-	-
27	CLA	a	803	X	-	-	-
27	CLA	a	804	X	-	-	-
27	CLA	a	805	X	-	-	-
27	CLA	a	806	X	-	-	-
27	CLA	a	807	X	-	-	-
27	CLA	a	808	X	-	-	-
27	CLA	a	809	X	-	-	-
27	CLA	a	810	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	a	811	X	-	-	-
27	CLA	a	812	X	-	-	-
27	CLA	a	813	X	-	-	-
27	CLA	a	814	X	-	-	-
27	CLA	a	815	X	-	-	-
27	CLA	a	816	X	-	-	-
27	CLA	a	817	X	-	-	-
27	CLA	a	818	X	-	-	-
27	CLA	a	819	X	-	-	-
27	CLA	a	820	X	-	-	-
27	CLA	a	821	X	-	-	-
27	CLA	a	822	X	-	-	-
27	CLA	a	823	X	-	-	-
27	CLA	a	824	X	-	-	-
27	CLA	a	825	X	-	-	-
27	CLA	a	826	X	-	-	-
27	CLA	a	827	X	-	-	-
27	CLA	a	828	X	-	-	-
27	CLA	a	829	X	-	-	-
27	CLA	a	830	X	-	-	-
27	CLA	a	831	X	-	-	-
27	CLA	a	837	X	-	-	-
27	CLA	a	839	X	-	-	-
27	CLA	b	701	X	-	-	-
27	CLA	b	702	X	-	-	-
27	CLA	b	703	X	-	-	-
27	CLA	b	704	X	-	-	-
27	CLA	b	705	X	-	-	-
27	CLA	b	706	X	-	-	-
27	CLA	b	707	X	-	-	-
27	CLA	b	708	X	-	-	-
27	CLA	b	709	X	-	-	-
27	CLA	b	710	X	-	-	-
27	CLA	b	711	X	-	-	-
27	CLA	b	712	X	-	-	-
27	CLA	b	713	X	-	-	-
27	CLA	b	714	X	-	-	-
27	CLA	b	715	X	-	-	-
27	CLA	b	716	X	-	-	-
27	CLA	b	717	X	-	-	-
27	CLA	b	718	X	-	-	-
27	CLA	b	719	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	720	X	-	-	-
27	CLA	b	721	X	-	-	-
27	CLA	b	722	X	-	-	-
27	CLA	b	723	X	-	-	-
27	CLA	b	724	X	-	-	-
27	CLA	b	725	X	-	-	-
27	CLA	b	726	X	-	-	-
27	CLA	b	727	X	-	-	-
27	CLA	b	728	X	-	-	-
27	CLA	f	302	X	-	-	-
27	CLA	f	303	X	-	-	-
27	CLA	j	202	X	-	-	-
27	CLA	l	402	X	-	-	-
27	CLA	l	403	X	-	-	-
27	CLA	l	404	X	-	-	-
27	CLA	l	405	X	-	-	-
27	CLA	l	406	X	-	-	-
27	CLA	l	407	X	-	-	-
27	CLA	l	408	X	-	-	-
27	CLA	l	409	X	-	-	-
27	CLA	l	410	X	-	-	-
27	CLA	l	411	X	-	-	-
27	CLA	l	412	X	-	-	-
27	CLA	r	203	X	-	-	-
27	CLA	r	204	X	-	-	-
30	DD6	D	613	X	-	-	-
38	BCR	a	834	-	-	X	-
38	BCR	a	836	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 55980 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 PCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	194	Total	C	N	O	S	0	0
			1461	941	239	274	7		

- Molecule 2 is a protein called PCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	185	Total	C	N	O	S	0	0
			1412	900	237	264	11		

- Molecule 3 is a protein called PCP-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	192	Total	C	N	O	S	0	0
			1518	990	244	273	11		

- Molecule 4 is a protein called PCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	177	Total	C	N	O	S	0	0
			1375	893	226	245	11		

- Molecule 5 is a protein called PCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	184	Total	C	N	O	S	0	0
			1444	940	241	256	7		

- Molecule 6 is a protein called PCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1731	1118	282	314	17		

- Molecule 7 is a protein called PCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	173	Total	C	N	O	S	0	0
			1329	861	220	238	10		

- Molecule 8 is a protein called PCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	192	Total	C	N	O	S	0	0
			1458	948	241	261	8		

- Molecule 9 is a protein called PCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	221	Total	C	N	O	S	0	0
			1736	1138	272	315	11		

- Molecule 10 is a protein called PCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	173	Total	C	N	O	S	0	0
			1322	849	220	244	9		

- Molecule 11 is a protein called PCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	154	Total	C	N	O	S	0	0
			1134	718	194	211	11		

- Molecule 12 is a protein called PCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	140	Total	C	N	O	S	0	0
			1065	681	180	196	8		

- Molecule 13 is a protein called PCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	104	Total	C	N	O	S	0	0
			828	535	144	142	7		

- Molecule 14 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	665	Total	C	N	O	S	0	0
			5250	3443	877	904	26		

- Molecule 15 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	659	Total	C	N	O	S	0	0
			5220	3437	845	918	20		

- Molecule 16 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	c	86	Total	C	N	O	S	0	0
			651	402	109	131	9		

- Molecule 17 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	216	Total	C	N	O	S	0	0
			1765	1123	308	321	13		

- Molecule 18 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	e	73	Total	C	N	O	0	0
			590	386	101	103		

- Molecule 19 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	169	Total	C	N	O	S	0	0
			1349	859	238	246	6		

- Molecule 20 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	120	Total	C	N	O	S	0	0
			971	627	165	177	2		

- Molecule 21 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	j	99	Total	C	N	O	S	0	0
			791	507	130	153	1		

- Molecule 22 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	253	Total	C	N	O	S	0	0
			1974	1290	319	356	9		

- Molecule 23 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	79	Total	C	N	O	S	0	0
			598	391	102	104	1		

- Molecule 24 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	r	131	Total	C	N	O	S	0	0
			1082	714	168	194	6		

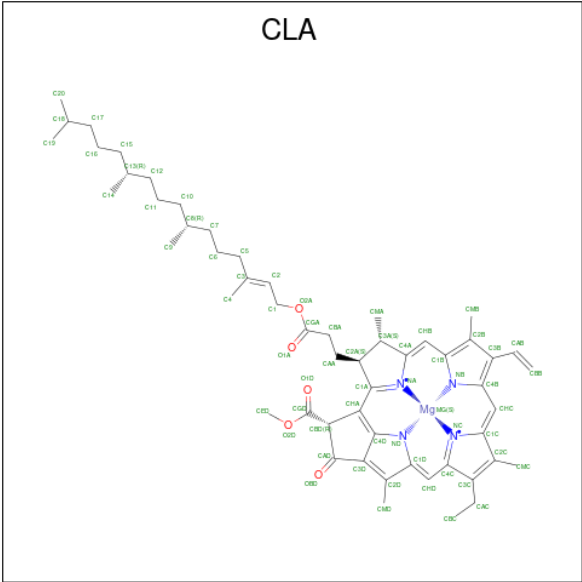
- Molecule 25 is a protein called PsaT.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	79	Total	C	N	O	S	0	0
			642	411	107	123	1		

- Molecule 26 is a protein called PsaU.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	130	Total	C	N	O	S	0	0
			1085	690	184	208	3		

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 47	C 37	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
27	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	F	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	H	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	I	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	J	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	J	1	Total 60	C 50	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
27	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	U	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	U	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

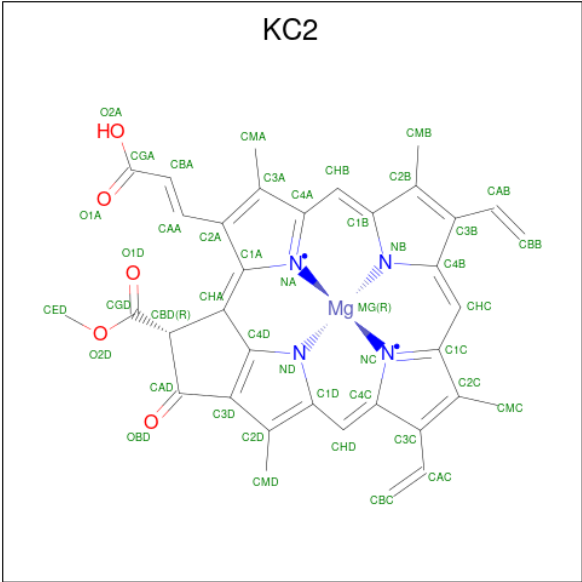
Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	f	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	f	1	Total 48	C 38	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
27	j	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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



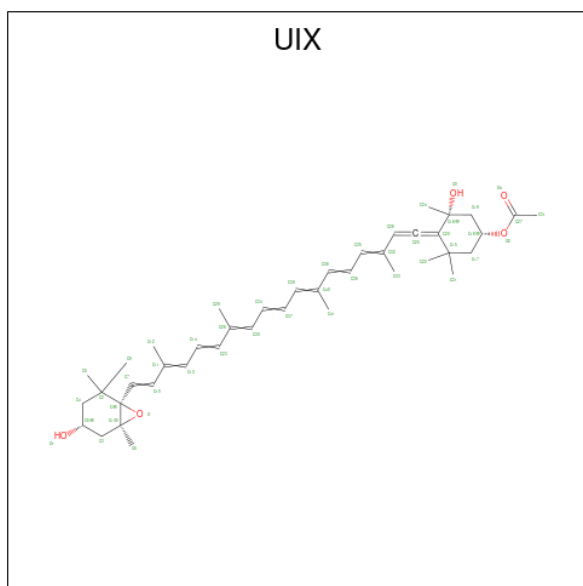
Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (CCD ID: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



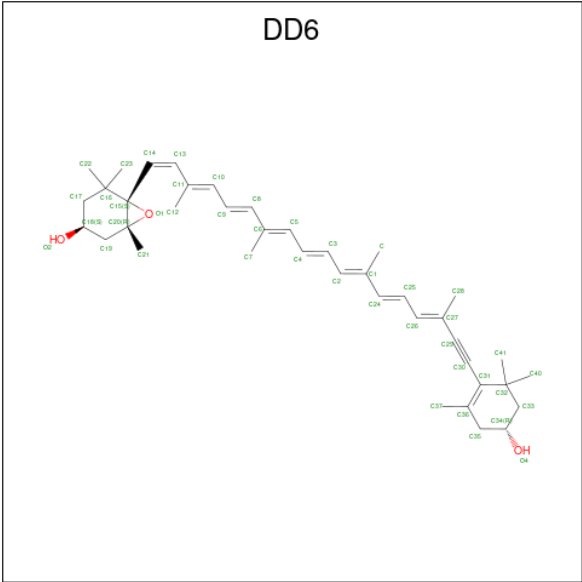
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			47	42	5	
29	A	1	Total	C	O	0
			47	42	5	
29	B	1	Total	C	O	0
			47	42	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			47	42	5	
29	C	1	Total	C	O	0
			47	42	5	
29	C	1	Total	C	O	0
			47	42	5	
29	D	1	Total	C	O	0
			47	42	5	
29	E	1	Total	C	O	0
			47	42	5	
29	F	1	Total	C	O	0
			47	42	5	
29	G	1	Total	C	O	0
			47	42	5	
29	H	1	Total	C	O	0
			47	42	5	
29	H	1	Total	C	O	0
			47	42	5	
29	I	1	Total	C	O	0
			47	42	5	
29	J	1	Total	C	O	0
			47	42	5	
29	T	1	Total	C	O	0
			47	42	5	
29	j	1	Total	C	O	0
			47	42	5	

- Molecule 30 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: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

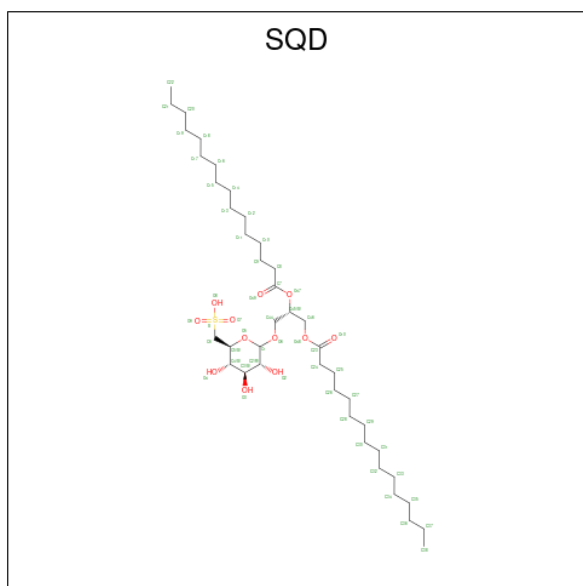
Mol	Chain	Residues	Atoms			AltConf
30	E	1	Total 43	C 40	O 3	0
30	E	1	Total 43	C 40	O 3	0
30	E	1	Total 43	C 40	O 3	0
30	F	1	Total 43	C 40	O 3	0
30	F	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	I	1	Total 43	C 40	O 3	0
30	I	1	Total 43	C 40	O 3	0
30	J	1	Total 43	C 40	O 3	0
30	K	1	Total 43	C 40	O 3	0
30	K	1	Total 43	C 40	O 3	0
30	K	1	Total 43	C 40	O 3	0
30	T	1	Total 43	C 40	O 3	0
30	T	1	Total 43	C 40	O 3	0

Continued on next page...

Continued from previous page...

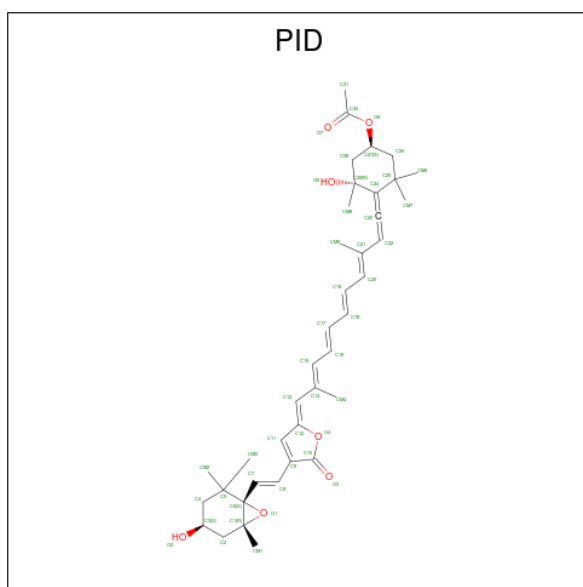
Mol	Chain	Residues	Atoms			AltConf
30	U	1	Total	C	O	0
			43	40	3	
30	b	1	Total	C	O	0
			43	40	3	
30	i	1	Total	C	O	0
			43	40	3	
30	r	1	Total	C	O	0
			43	40	3	
30	r	1	Total	C	O	0
			43	40	3	
30	r	1	Total	C	O	0
			43	40	3	

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



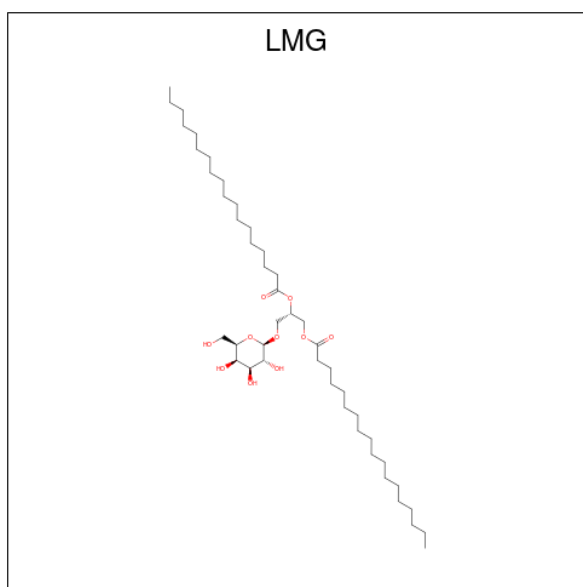
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	S	0
			28	15	12	1	
31	H	1	Total	C	O	S	0
			46	33	12	1	
31	y	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 32 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



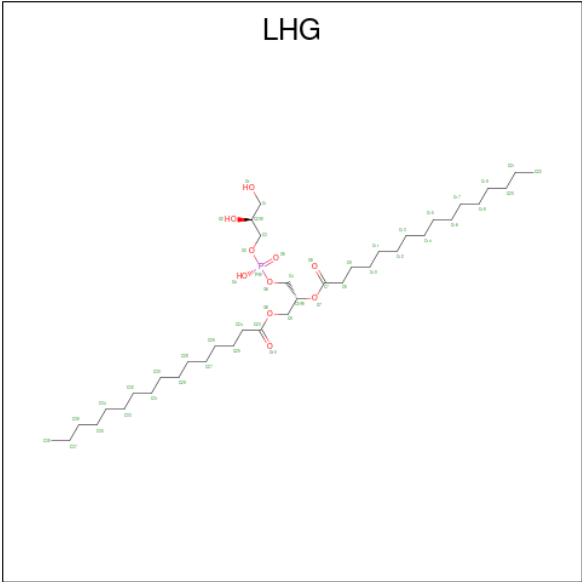
Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	I	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	K	1	Total	C	O	0
			46	39	7	
32	U	1	Total	C	O	0
			46	39	7	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



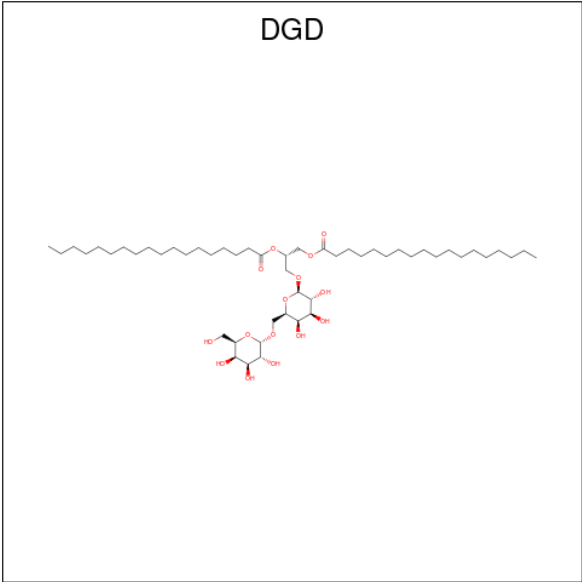
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			34	24	10	
33	D	1	Total	C	O	0
			35	25	10	
33	D	1	Total	C	O	0
			46	36	10	
33	F	1	Total	C	O	0
			46	36	10	
33	K	1	Total	C	O	0
			42	32	10	
33	b	1	Total	C	O	0
			55	45	10	
33	l	1	Total	C	O	0
			50	40	10	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



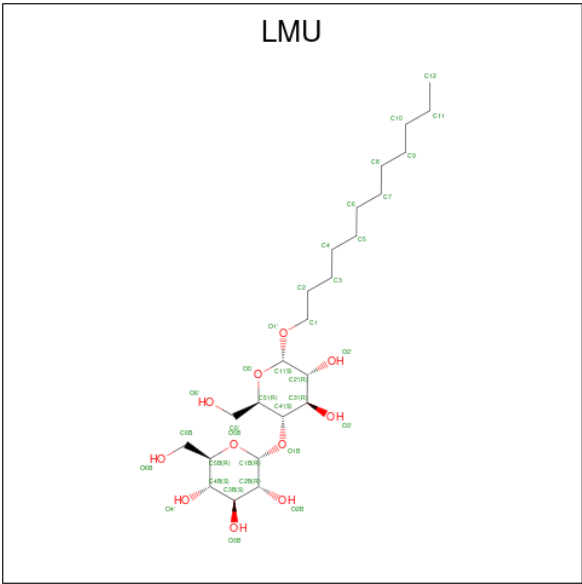
Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total	C	O	P	0
			46	35	10	1	
34	F	1	Total	C	O	P	0
			37	26	10	1	
34	G	1	Total	C	O	P	0
			34	23	10	1	
34	a	1	Total	C	O	P	0
			48	37	10	1	
34	j	1	Total	C	O	P	0
			37	26	10	1	
34	l	1	Total	C	O	P	0
			46	35	10	1	
34	r	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



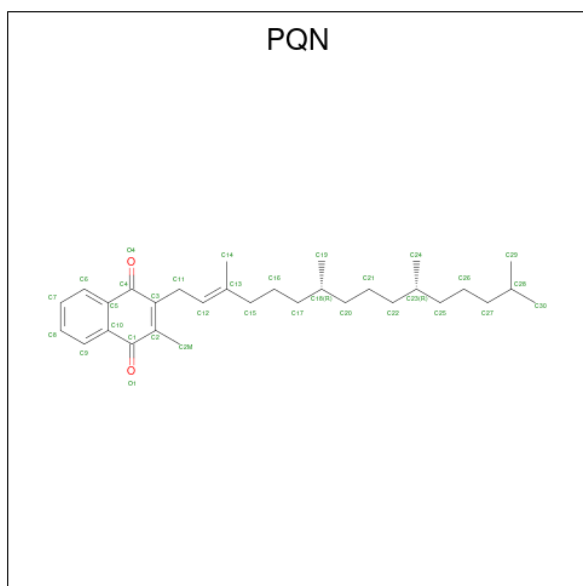
Mol	Chain	Residues	Atoms			AltConf
35	K	1	Total	C	O	0
			47	32	15	
35	f	1	Total	C	O	0
			52	37	15	
35	j	1	Total	C	O	0
			60	45	15	
35	l	1	Total	C	O	0
			55	40	15	

- Molecule 36 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



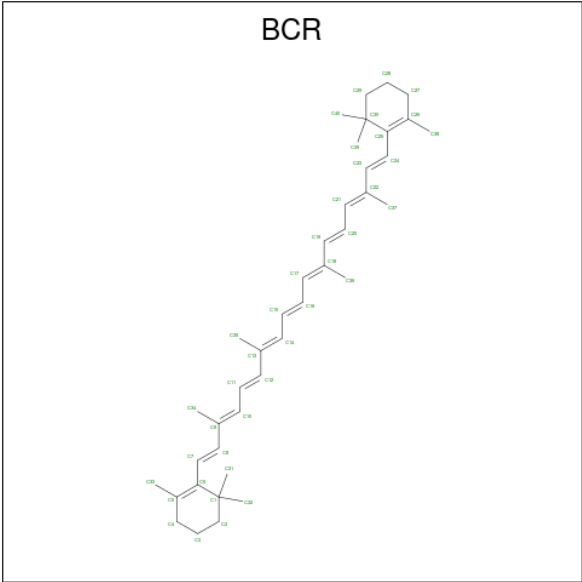
Mol	Chain	Residues	Atoms			AltConf
36	T	1	Total	C	O	0
			35	24	11	

- Molecule 37 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

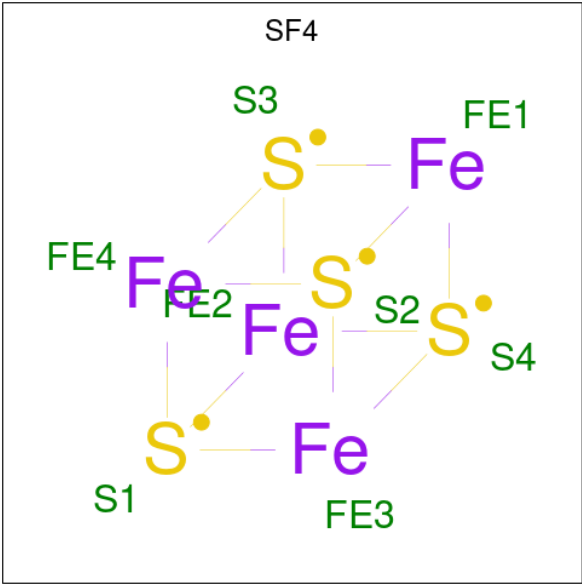
- Molecule 38 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
38	a	1	Total C 40 40	0
38	a	1	Total C 40 40	0
38	a	1	Total C 40 40	0
38	b	1	Total C 40 40	0
38	b	1	Total C 40 40	0
38	f	1	Total C 40 40	0
38	f	1	Total C 40 40	0
38	i	1	Total C 40 40	0
38	j	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	m	1	Total C 40 40	0

- Molecule 39 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as

"Ligand of Interest" by depositor).

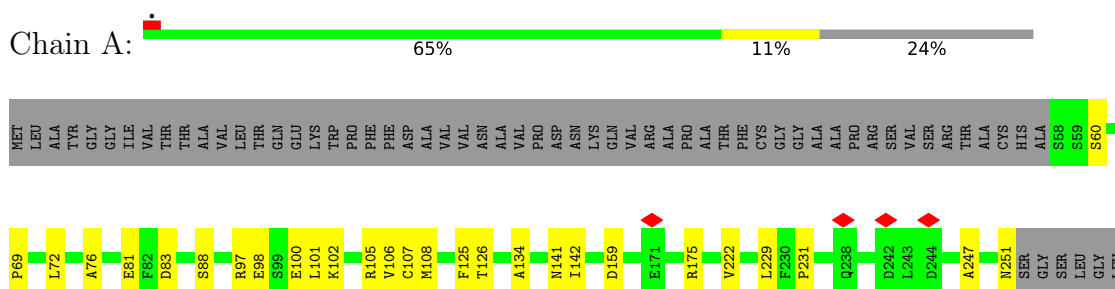


Mol	Chain	Residues	Atoms			AltConf
39	a	1	Total	Fe	S	0
			8	4	4	
39	c	1	Total	Fe	S	0
			8	4	4	
39	c	1	Total	Fe	S	0
			8	4	4	

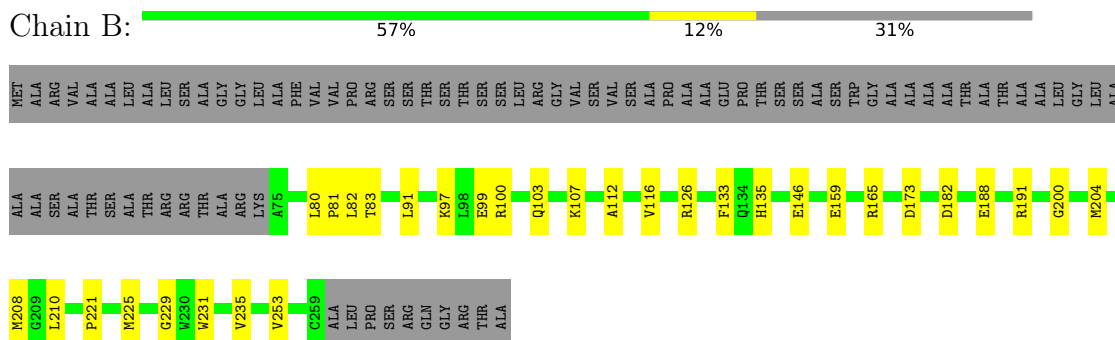
3 Residue-property plots

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

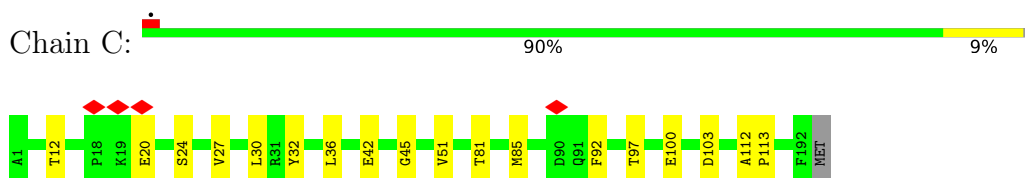
• Molecule 1: PCPI-7



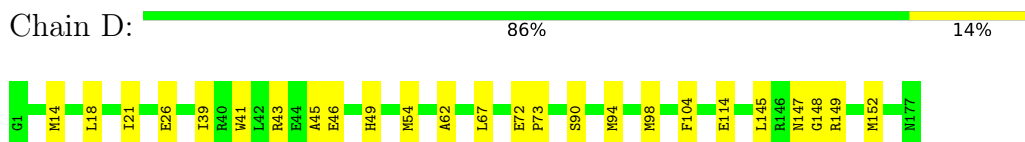
• Molecule 2: PCPI-1



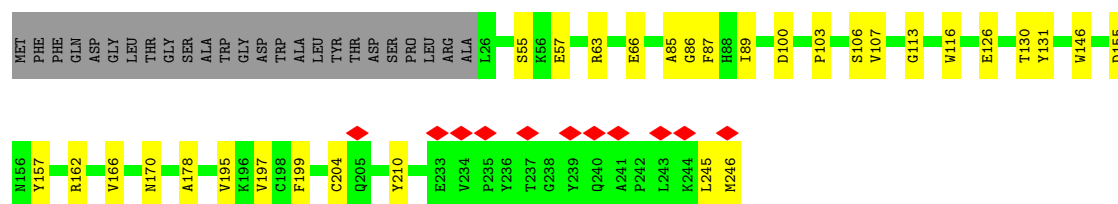
• Molecule 3: PCP-11



• Molecule 4: PCPI-6

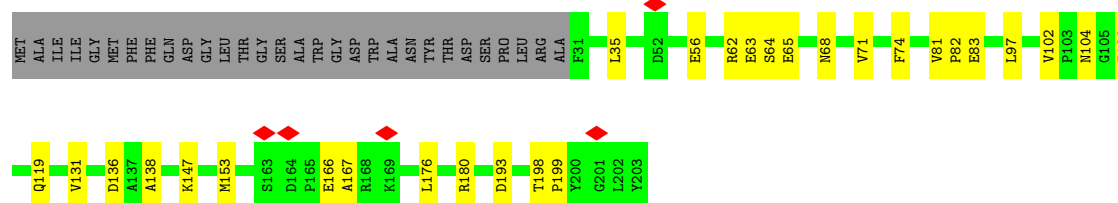


Chain I: 

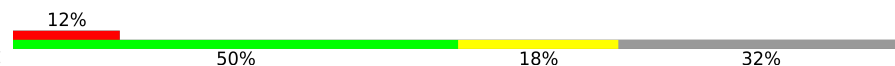


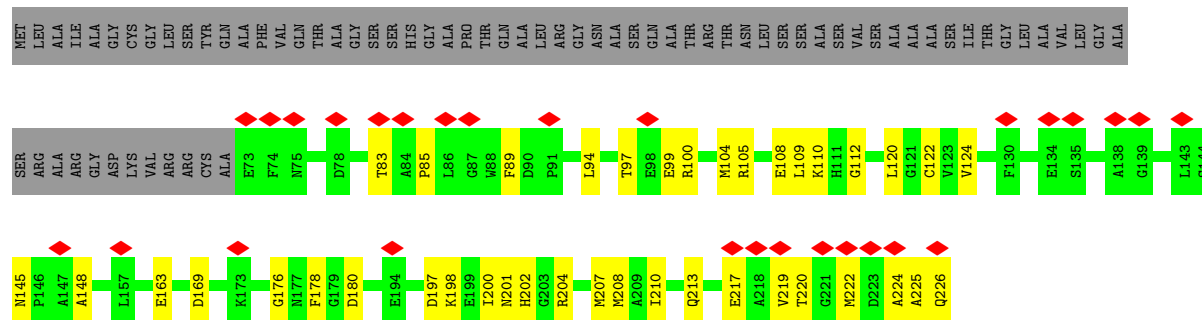
• Molecule 10: PCPI-9

Chain J: 



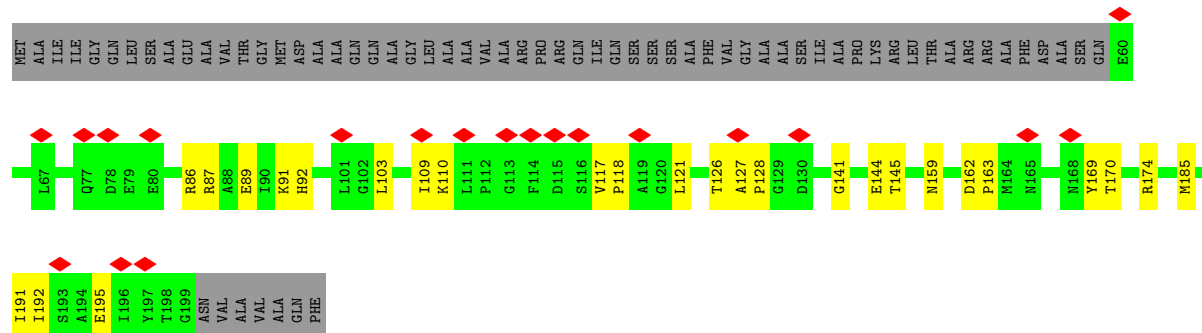
• Molecule 11: PCPI-13

Chain K: 

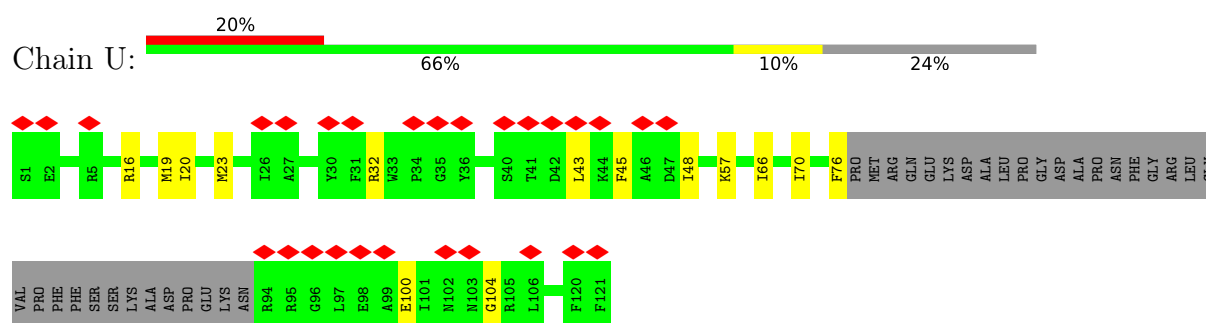


• Molecule 12: PCPI-12

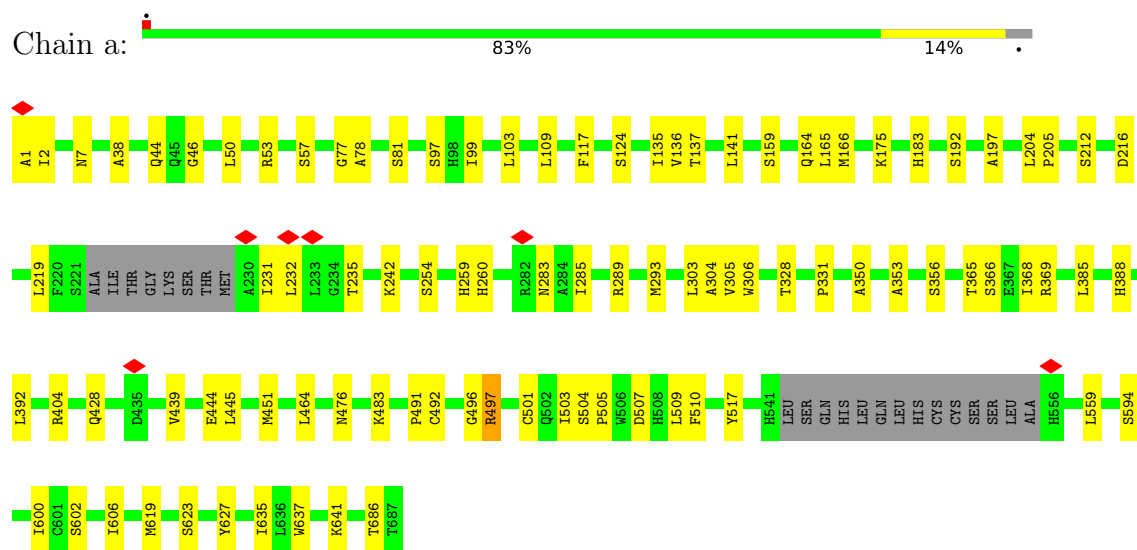
Chain T: 



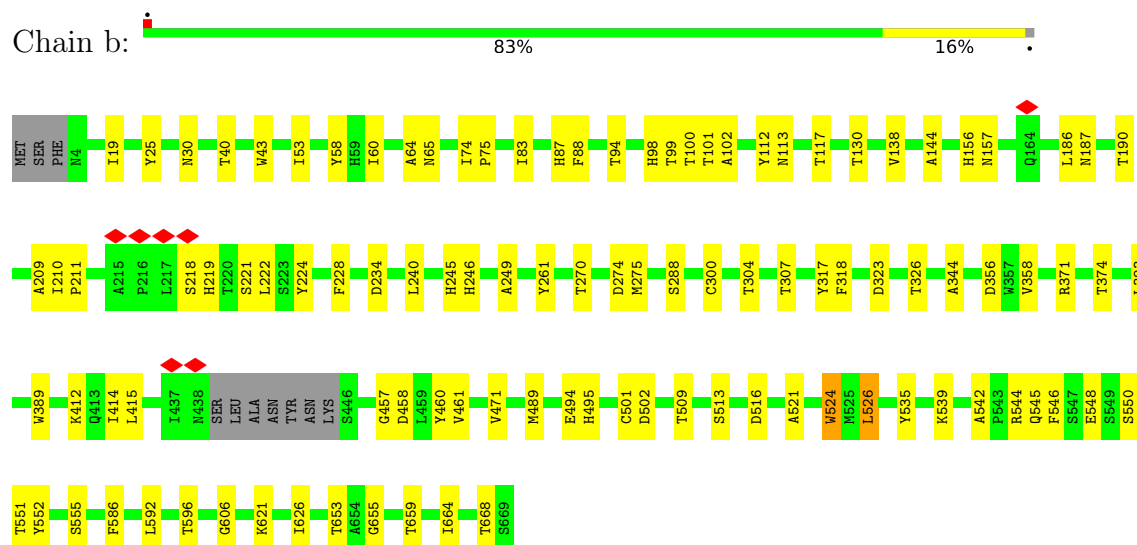
• Molecule 13: PCPI-2



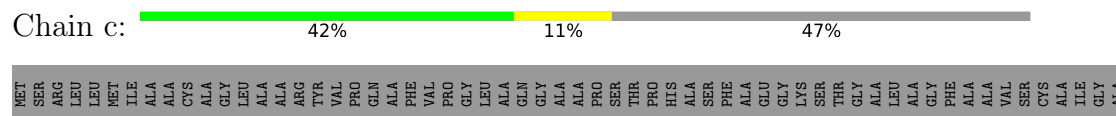
• Molecule 14: PsaA

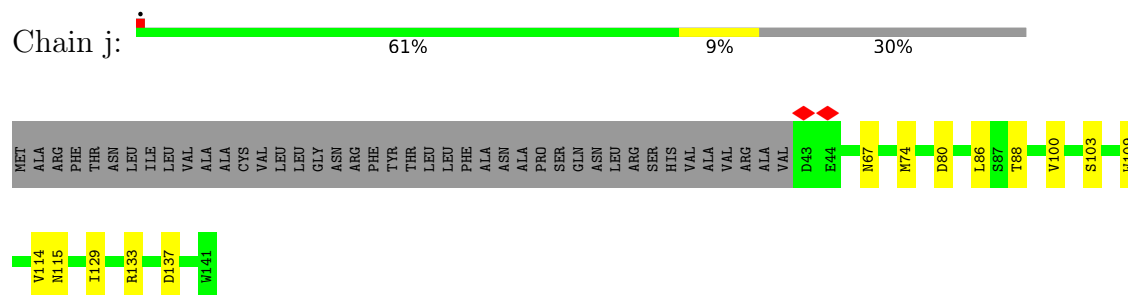


• Molecule 15: PsaB

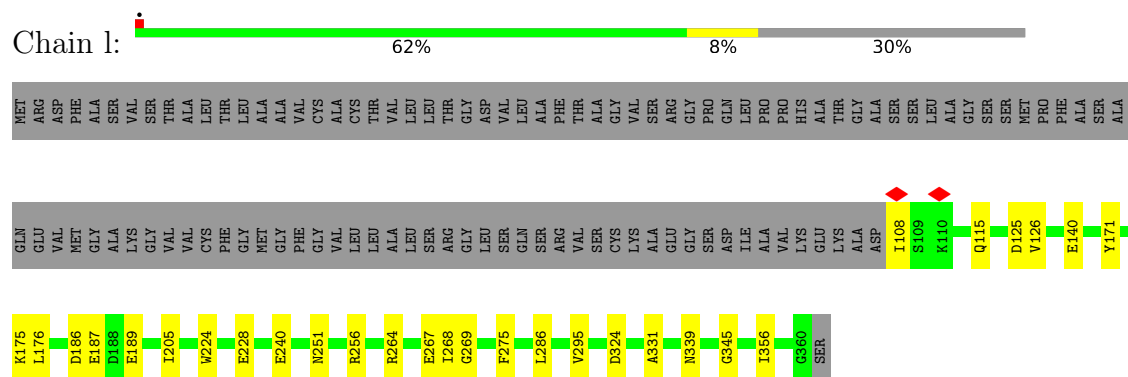


• Molecule 16: PsaC

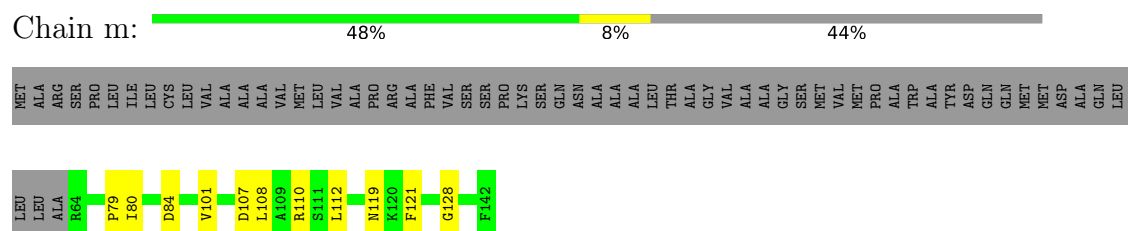




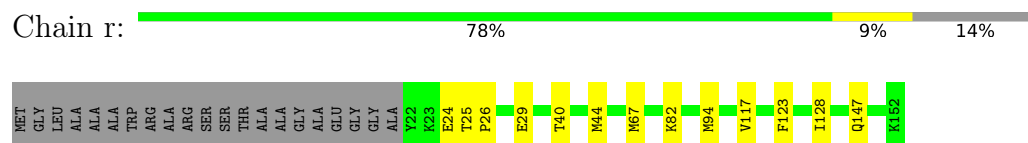
● Molecule 22: PsaL



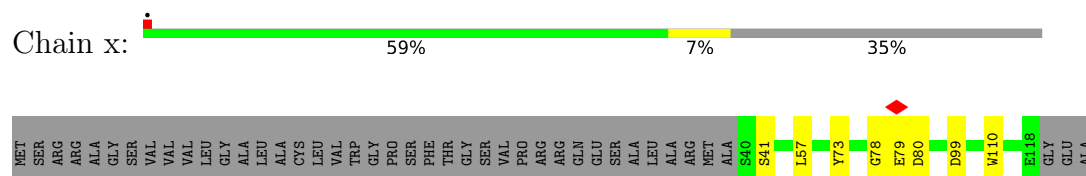
● Molecule 23: PsaM



● Molecule 24: PsaR

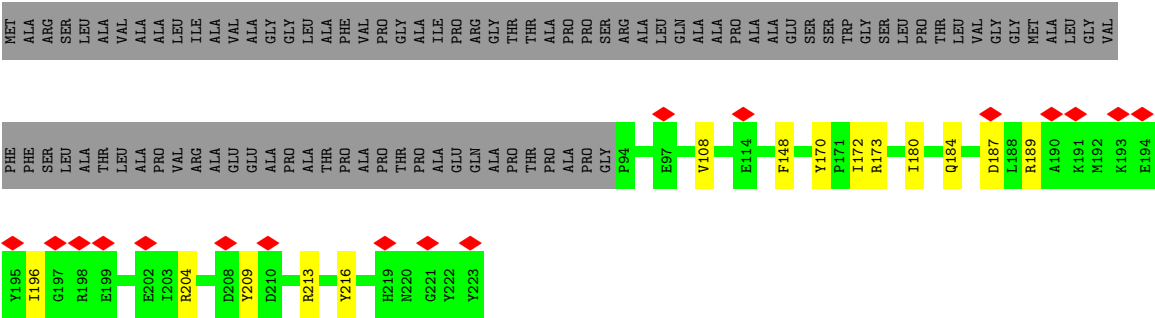


● Molecule 25: PsaT



● Molecule 26: PsaU





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.960	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.041	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, UIX, LHG, DGD, SQD, PID, SF4, PQN, LMU, KC2, CLA, DD6, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.15	0/1501	0.28	0/2037
2	B	0.28	0/1443	0.38	0/1954
3	C	0.14	0/1562	0.26	0/2114
4	D	0.15	0/1413	0.27	0/1912
5	E	0.19	0/1484	0.39	1/2006 (0.0%)
6	F	0.15	0/1785	0.31	1/2426 (0.0%)
7	G	0.32	0/1365	0.37	1/1841 (0.1%)
8	H	0.13	0/1499	0.29	0/2030
9	I	0.35	0/1794	0.42	1/2454 (0.0%)
10	J	0.25	0/1355	0.35	1/1835 (0.1%)
11	K	0.47	0/1162	0.52	0/1565
12	T	0.35	0/1090	0.39	0/1477
13	U	0.24	0/847	0.36	0/1140
14	a	0.19	0/5412	0.30	1/7363 (0.0%)
15	b	0.51	4/5390 (0.1%)	0.44	4/7368 (0.1%)
16	c	0.36	0/661	0.42	0/901
17	d	0.14	0/1803	0.29	0/2419
18	e	0.11	0/611	0.24	0/836
19	f	0.49	1/1384 (0.1%)	0.35	0/1873
20	i	0.14	0/1001	0.28	0/1357
21	j	0.14	0/808	0.26	0/1104
22	l	0.21	0/2031	0.31	0/2755
23	m	0.33	0/608	0.33	0/820
24	r	0.27	0/1118	0.33	0/1513
25	x	0.13	0/667	0.26	0/908
26	y	0.21	0/1119	0.40	1/1515 (0.1%)
All	All	0.30	5/40913 (0.0%)	0.35	11/55523 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	246	HIS	CA-C	-5.75	1.45	1.52
15	b	521	ALA	CA-C	-5.64	1.44	1.52
19	f	217	TRP	CA-C	-5.40	1.46	1.52
15	b	157	ASN	CA-C	-5.39	1.45	1.52
15	b	526	LEU	CA-C	-5.12	1.46	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	228	PHE	N-CA-C	-9.21	97.63	110.35
26	y	108	VAL	N-CA-C	8.17	119.16	111.48
5	E	77	ASN	N-CA-C	-8.16	98.39	110.23
9	I	89	ILE	N-CA-C	7.05	117.84	110.72
10	J	153	MET	CB-CA-C	-6.26	101.06	110.88
6	F	117	VAL	N-CA-C	6.23	122.29	109.34
15	b	586	PHE	N-CA-C	-5.58	106.47	113.28
15	b	524	TRP	N-CA-C	5.21	116.96	111.28
14	a	497	ARG	CB-CA-C	5.20	119.11	111.73
7	G	169	LYS	N-CA-C	-5.17	105.53	111.07
15	b	234	ASP	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1461	0	1420	18	0
2	B	1412	0	1384	22	0
3	C	1518	0	1491	16	0
4	D	1375	0	1359	19	0
5	E	1444	0	1418	24	0
6	F	1731	0	1691	24	0
7	G	1329	0	1301	23	0
8	H	1458	0	1426	20	0
9	I	1736	0	1687	25	0
10	J	1322	0	1296	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1134	0	1085	49	0
12	T	1065	0	1042	19	0
13	U	828	0	828	13	0
14	a	5250	0	5201	86	0
15	b	5220	0	5122	94	0
16	c	651	0	634	17	0
17	d	1765	0	1785	40	0
18	e	590	0	582	7	0
19	f	1349	0	1334	8	0
20	i	971	0	951	21	0
21	j	791	0	783	13	0
22	l	1974	0	1950	29	0
23	m	598	0	641	14	0
24	r	1082	0	1041	12	0
25	x	642	0	594	6	0
26	y	1085	0	1025	11	0
27	A	543	0	441	4	0
27	B	454	0	437	1	0
27	C	565	0	489	5	0
27	D	624	0	532	8	0
27	E	537	0	481	2	0
27	F	575	0	500	10	0
27	G	529	0	463	4	0
27	H	602	0	559	9	0
27	I	623	0	596	6	0
27	J	248	0	211	4	0
27	K	360	0	309	14	0
27	T	354	0	258	5	0
27	U	198	0	164	8	0
27	a	1927	0	1885	50	0
27	b	1717	0	1790	43	0
27	f	96	0	72	1	0
27	j	56	0	51	1	0
27	l	627	0	600	7	0
27	r	108	0	95	1	0
28	A	45	0	0	0	0
28	B	90	0	0	0	0
28	C	45	0	0	0	0
28	E	90	0	0	0	0
28	F	45	0	0	0	0
28	G	45	0	0	0	0
28	H	90	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	I	45	0	0	1	0
28	J	225	0	0	6	0
28	K	45	0	0	6	0
28	T	45	0	0	0	0
28	U	90	0	0	0	0
29	A	94	0	0	1	0
29	B	94	0	0	0	0
29	C	94	0	0	1	0
29	D	47	0	0	0	0
29	E	47	0	0	0	0
29	F	47	0	0	0	0
29	G	47	0	0	0	0
29	H	94	0	0	1	0
29	I	47	0	0	2	0
29	J	47	0	0	0	0
29	T	47	0	0	0	0
29	j	47	0	0	2	0
30	A	129	0	0	2	0
30	B	129	0	0	1	0
30	C	86	0	0	2	0
30	D	215	0	0	3	0
30	E	172	0	0	1	0
30	F	86	0	0	1	0
30	G	172	0	0	2	0
30	H	172	0	0	3	0
30	I	86	0	0	0	0
30	J	43	0	0	0	0
30	K	129	0	0	2	0
30	T	86	0	0	0	0
30	U	43	0	0	0	0
30	b	43	0	0	1	0
30	i	43	0	0	1	0
30	r	129	0	0	0	0
31	A	28	0	20	0	0
31	H	46	0	56	0	0
31	y	46	0	56	0	0
32	B	46	0	50	1	0
32	F	92	0	100	9	0
32	I	46	0	50	4	0
32	J	184	0	200	21	0
32	K	46	0	50	12	0
32	U	46	0	50	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	C	34	0	38	1	0
33	D	81	0	105	1	0
33	F	46	0	65	0	0
33	K	42	0	57	1	0
33	b	55	0	86	0	0
33	l	50	0	73	0	0
34	D	46	0	65	0	0
34	F	37	0	44	0	0
34	G	34	0	38	0	0
34	a	48	0	69	0	0
34	j	37	0	44	0	0
34	l	46	0	65	1	0
34	r	46	0	65	1	0
35	K	47	0	52	3	0
35	f	52	0	62	0	0
35	j	60	0	81	1	0
35	l	55	0	71	3	0
36	T	35	0	46	1	0
37	a	33	0	46	0	0
37	b	33	0	46	0	0
38	a	120	0	168	44	0
38	b	80	0	112	2	0
38	f	80	0	112	6	0
38	i	40	0	56	5	0
38	j	40	0	56	0	0
38	l	120	0	168	13	0
38	m	40	0	56	1	0
39	a	8	0	0	0	0
39	c	16	0	0	0	0
All	All	55980	0	51582	736	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:a:834:BCR:H362	38:a:836:BCR:C21	1.13	1.61
38:a:834:BCR:C36	38:a:836:BCR:H21C	0.99	1.45
3:C:12:THR:HG22	17:d:286:ASP:OD2	1.33	1.28
15:b:245:HIS:CD2	27:b:714:CLA:CBB	2.15	1.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:a:834:BCR:H372	38:a:836:BCR:C39	1.63	1.26
15:b:245:HIS:NE2	27:b:714:CLA:CBB	2.04	1.21
7:G:90:PHE:CE1	7:G:93:VAL:HG13	1.79	1.17
38:a:834:BCR:H362	38:a:836:BCR:C22	1.74	1.16
15:b:245:HIS:NE2	27:b:714:CLA:HBB2	1.59	1.13
38:a:834:BCR:C36	38:a:836:BCR:C21	1.86	1.11
38:a:834:BCR:H363	38:a:836:BCR:H21C	1.14	1.10
17:d:214:LEU:CD1	17:d:219:TYR:O	2.00	1.09
38:a:834:BCR:H372	38:a:836:BCR:H393	1.16	1.09
27:a:819:CLA:H2	38:a:836:BCR:HC7	1.39	1.05
22:l:205:ILE:HG12	22:l:224:TRP:HB2	1.35	1.03
11:K:120:LEU:HD12	27:K:603:CLA:HAC1	1.37	1.02
17:d:214:LEU:HD12	17:d:214:LEU:O	1.62	0.99
17:d:243:ASP:OD1	17:d:246:ASN:OD1	1.81	0.98
27:a:804:CLA:H143	38:a:836:BCR:H16C	1.43	0.97
11:K:120:LEU:CD1	27:K:603:CLA:HAC1	1.95	0.96
38:a:834:BCR:C37	38:a:836:BCR:H393	1.96	0.93
38:a:834:BCR:C36	38:a:836:BCR:C23	2.48	0.91
17:d:214:LEU:HD13	17:d:219:TYR:O	1.68	0.91
7:G:90:PHE:HE1	7:G:93:VAL:HG13	1.32	0.90
22:l:205:ILE:CG1	22:l:224:TRP:HB2	2.01	0.90
14:a:492:CYS:SG	14:a:501:CYS:HA	2.12	0.90
11:K:120:LEU:HD13	11:K:120:LEU:O	1.71	0.90
15:b:501:CYS:SG	15:b:509:THR:O	2.30	0.89
38:a:834:BCR:H361	38:a:836:BCR:H23C	1.56	0.87
1:A:76:ALA:O	1:A:97:ARG:NH2	2.07	0.87
6:F:188:TRP:O	30:F:612:DD6:O4	1.92	0.87
7:G:90:PHE:CE1	7:G:93:VAL:CG1	2.57	0.86
7:G:172:LYS:NZ	27:G:608:CLA:O1D	2.08	0.86
11:K:202:HIS:HE1	28:K:607:KC2:C4D	1.87	0.86
17:d:201:ARG:NH2	17:d:226:ALA:O	2.09	0.86
11:K:120:LEU:HD13	11:K:120:LEU:C	2.01	0.85
14:a:53:ARG:NH1	21:j:80:ASP:OD2	2.08	0.85
7:G:63:ARG:NH1	7:G:66:GLU:OE1	2.09	0.85
19:f:228:ASP:OD2	19:f:230:THR:OG1	1.94	0.85
15:b:245:HIS:HD2	27:b:714:CLA:CBB	1.91	0.84
2:B:165:ARG:NH1	2:B:173:ASP:OD2	2.11	0.84
38:a:834:BCR:H362	38:a:836:BCR:C23	2.08	0.84
15:b:19:ILE:O	15:b:25:TYR:OH	1.96	0.83
15:b:245:HIS:CD2	27:b:714:CLA:CAB	2.62	0.83
27:a:804:CLA:H143	38:a:836:BCR:H362	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:156:HIS:ND1	23:m:121:PHE:HA	1.94	0.82
27:a:819:CLA:C2	38:a:836:BCR:HC7	2.07	0.82
8:H:86:ILE:O	8:H:116:ARG:NH2	2.13	0.82
8:H:158:ASN:OD1	30:H:318:DD6:O2	1.96	0.82
10:J:65:GLU:OE2	10:J:180:ARG:NH1	2.13	0.81
16:c:135:ASP:OD2	18:e:66:SER:OG	1.97	0.81
27:a:804:CLA:C14	38:a:836:BCR:H362	2.10	0.81
11:K:198:LYS:O	11:K:202:HIS:CD2	2.34	0.81
5:E:143:SER:OG	5:E:145:GLU:OE1	1.99	0.81
3:C:24:SER:OG	3:C:45:GLY:O	1.97	0.81
5:E:106:GLU:OE2	35:l:416:DGD:O5E	1.98	0.80
35:K:614:DGD:O6E	35:K:614:DGD:O3D	1.98	0.80
11:K:197:ASP:OD1	11:K:201:ASN:ND2	2.15	0.80
14:a:2:ILE:O	14:a:164:GLN:NE2	2.14	0.80
32:I:614:PID:HM22	32:I:614:PID:H21	1.63	0.80
14:a:289:ARG:NH1	22:l:189:GLU:OE2	2.14	0.80
22:l:256:ARG:O	22:l:264:ARG:NH2	2.15	0.80
5:E:59:LEU:N	5:E:204:GLU:OE2	2.15	0.79
17:d:214:LEU:HD13	17:d:219:TYR:HB2	1.65	0.79
35:K:614:DGD:O5E	35:K:614:DGD:O4E	1.96	0.78
17:d:201:ARG:NH1	17:d:208:ASN:OD1	2.16	0.78
15:b:156:HIS:CE1	23:m:121:PHE:HA	2.18	0.78
18:e:112:GLU:N	18:e:112:GLU:OE1	2.16	0.78
8:H:116:ARG:NH1	8:H:119:GLU:OE2	2.16	0.78
15:b:245:HIS:HD2	27:b:714:CLA:HMB3	1.49	0.77
38:a:834:BCR:H372	38:a:836:BCR:H391	1.61	0.77
20:i:93:GLN:OE1	30:i:202:DD6:O2	2.02	0.77
3:C:12:THR:CG2	17:d:286:ASP:OD2	2.26	0.77
14:a:504:SER:OG	14:a:507:ASP:OD2	2.03	0.77
15:b:501:CYS:HG	15:b:509:THR:C	1.92	0.77
7:G:107:LEU:HD12	7:G:116:PRO:HG2	1.65	0.76
14:a:627:TYR:OH	27:a:802:CLA:OBD	2.02	0.76
38:a:834:BCR:C19	38:a:836:BCR:H382	2.15	0.76
30:C:216:DD6:O2	33:C:217:LMG:O10	2.03	0.76
14:a:353:ALA:HB2	14:a:509:LEU:CD1	2.16	0.76
38:l:413:BCR:H403	38:l:413:BCR:H23C	1.68	0.75
11:K:83:THR:HG22	11:K:85:PRO:HD2	1.69	0.75
22:l:339:ASN:ND2	27:l:410:CLA:O1D	2.20	0.75
14:a:212:SER:O	26:y:189:ARG:NH1	2.20	0.75
32:K:611:PID:H21	32:K:611:PID:HM22	1.68	0.75
32:J:614:PID:HM73	32:J:614:PID:HM51	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:248:ASP:OD1	6:F:249:ALA:N	2.19	0.74
28:J:604:KC2:O2A	34:r:202:LHG:O5	2.04	0.74
14:a:369:ARG:NH2	22:l:205:ILE:HD11	2.02	0.74
8:H:152:THR:OG1	8:H:155:GLU:OE1	2.06	0.74
9:I:63:ARG:NH1	9:I:66:GLU:OE1	2.21	0.73
15:b:659:THR:HG23	27:b:702:CLA:O1D	1.88	0.73
12:T:91:LYS:NZ	12:T:144:GLU:OE2	2.16	0.73
38:a:834:BCR:C36	38:a:836:BCR:H23C	2.14	0.73
15:b:187:ASN:ND2	15:b:261:TYR:O	2.20	0.73
6:F:261:LYS:NZ	27:F:608:CLA:O1D	2.22	0.73
8:H:260:GLN:O	8:H:264:THR:HG22	1.89	0.73
15:b:288:SER:OG	15:b:356:ASP:OD2	2.06	0.73
15:b:30:ASN:ND2	20:i:120:PHE:CE2	2.56	0.73
17:d:85:ARG:NH1	17:d:172:LYS:O	2.22	0.73
8:H:95:GLN:N	8:H:95:GLN:OE1	2.22	0.73
22:l:205:ILE:HG12	22:l:224:TRP:CB	2.16	0.73
15:b:371:ARG:O	15:b:374:THR:OG1	2.07	0.72
16:c:76:SER:O	16:c:144:GLN:NE2	2.21	0.72
7:G:34:ALA:O	7:G:63:ARG:NH2	2.22	0.72
38:a:834:BCR:C36	38:a:836:BCR:C22	2.50	0.72
11:K:120:LEU:CD1	27:K:603:CLA:CAC	2.67	0.72
21:j:109:TRP:O	21:j:115:ASN:ND2	2.23	0.72
14:a:641:LYS:NZ	19:f:265:VAL:O	2.23	0.72
27:J:609:CLA:HMB2	32:J:611:PID:HM13	1.72	0.71
32:J:613:PID:HM22	32:J:613:PID:H21	1.70	0.71
27:a:827:CLA:HBC2	27:a:827:CLA:HMC3	1.72	0.71
7:G:107:LEU:HD12	7:G:116:PRO:CG	2.20	0.71
11:K:97:THR:OG1	11:K:99:GLU:OE1	2.09	0.71
1:A:98:GLU:OE1	1:A:175:ARG:NH2	2.22	0.71
9:I:103:PRO:O	9:I:107:VAL:HG23	1.90	0.71
13:U:45:PHE:HA	27:U:603:CLA:HED1	1.73	0.71
19:f:122:LYS:O	19:f:182:LYS:NZ	2.23	0.71
12:T:141:GLY:O	12:T:145:THR:HG23	1.91	0.70
14:a:517:TYR:OH	27:a:801:CLA:HED3	1.90	0.70
7:G:68:LYS:NZ	27:G:606:CLA:O1D	2.25	0.70
15:b:412:LYS:HE3	21:j:137:ASP:OD1	1.91	0.69
11:K:120:LEU:HD12	27:K:603:CLA:CAC	2.20	0.69
28:I:604:KC2:CMC	38:l:413:BCR:H401	2.22	0.69
22:l:251:ASN:O	22:l:256:ARG:NH1	2.25	0.69
1:A:141:ASN:OD1	1:A:142:ILE:N	2.25	0.69
11:K:110:LYS:NZ	11:K:163:GLU:OE1	2.23	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:64:ALA:HB1	15:b:112:TYR:OH	1.92	0.69
16:c:83:ASP:OD2	18:e:85:LYS:NZ	2.23	0.69
22:l:175:LYS:O	35:l:416:DGD:O4D	2.11	0.68
11:K:105:ARG:NH1	11:K:108:GLU:OE1	2.26	0.68
15:b:53:ILE:HD11	38:b:731:BCR:H382	1.76	0.68
17:d:243:ASP:CG	17:d:246:ASN:OD1	2.37	0.67
38:a:834:BCR:H361	38:a:836:BCR:C23	2.19	0.67
27:a:804:CLA:H91	38:a:836:BCR:H12C	1.77	0.67
6:F:62:GLU:OE1	6:F:62:GLU:N	2.27	0.67
27:b:725:CLA:H41	38:l:414:BCR:H342	1.75	0.67
15:b:323:ASP:OD2	15:b:326:THR:OG1	2.12	0.66
2:B:135:HIS:O	30:B:612:DD6:O4	2.12	0.66
3:C:51:VAL:HG13	27:H:319:CLA:HMB2	1.77	0.66
15:b:245:HIS:HD2	27:b:714:CLA:CMB	2.07	0.66
16:c:76:SER:N	16:c:147:GLU:O	2.27	0.66
16:c:83:ASP:OD2	18:e:85:LYS:HD2	1.94	0.66
8:H:171:ASP:OD1	15:b:219:HIS:NE2	2.29	0.66
9:I:155:ASP:OD1	9:I:155:ASP:O	2.13	0.65
9:I:85:ALA:HB2	9:I:195:VAL:HG21	1.78	0.65
4:D:90:SER:OG	27:D:605:CLA:OBD	2.14	0.65
15:b:501:CYS:SG	15:b:502:ASP:N	2.70	0.65
1:A:83:ASP:OD2	1:A:88:SER:OG	2.11	0.65
9:I:146:TRP:NE1	27:I:606:CLA:O1A	2.29	0.64
14:a:369:ARG:HH22	22:l:205:ILE:CD1	2.10	0.64
17:d:137:ASN:N	17:d:141:ASN:OD1	2.30	0.64
1:A:247:ALA:O	1:A:251:ASN:ND2	2.30	0.64
32:K:611:PID:HM72	32:K:611:PID:H281	1.80	0.64
5:E:97:ASP:OD2	5:E:102:SER:OG	2.08	0.64
14:a:306:TRP:CD1	27:a:810:CLA:H42	2.32	0.64
15:b:156:HIS:HD2	23:m:128:GLY:N	1.96	0.64
20:i:141:GLU:O	20:i:145:GLU:HG2	1.98	0.63
11:K:120:LEU:CD1	11:K:120:LEU:C	2.70	0.63
32:J:611:PID:HM22	32:J:611:PID:H21	1.81	0.63
12:T:121:LEU:HD21	12:T:192:ILE:HG23	1.80	0.63
11:K:202:HIS:CE1	28:K:607:KC2:C4D	2.78	0.63
15:b:494:GLU:OE1	15:b:494:GLU:N	2.32	0.63
7:G:131:ARG:O	7:G:135:VAL:HG22	1.99	0.62
15:b:245:HIS:CD2	27:b:714:CLA:HBB1	2.31	0.62
15:b:100:THR:HG22	15:b:100:THR:O	2.00	0.62
11:K:202:HIS:CD2	27:K:605:CLA:HBB1	2.35	0.62
14:a:183:HIS:ND1	27:a:827:CLA:OBD	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:TYR:OH	3:C:42:GLU:O	2.18	0.62
14:a:353:ALA:HB2	14:a:509:LEU:HD13	1.82	0.62
9:I:85:ALA:HB2	9:I:195:VAL:CG2	2.30	0.61
32:I:614:PID:H282	32:I:614:PID:HM63	1.82	0.61
10:J:136:ASP:OD2	10:J:138:ALA:HB3	2.00	0.61
14:a:353:ALA:HB2	14:a:509:LEU:HD12	1.80	0.61
10:J:63:GLU:HG2	27:J:605:CLA:HED2	1.82	0.61
7:G:103:ALA:O	7:G:107:LEU:HD23	2.01	0.61
5:E:158:SER:O	26:y:213:ARG:NH2	2.33	0.61
16:c:136:PHE:HD2	17:d:205:ILE:HG21	1.65	0.61
13:U:23:MET:HB3	27:U:603:CLA:HBC2	1.82	0.61
3:C:103:ASP:OD2	30:C:216:DD6:O4	2.19	0.61
15:b:65:ASN:ND2	23:m:79:PRO:O	2.33	0.61
11:K:198:LYS:O	11:K:202:HIS:HD2	1.82	0.60
9:I:204:CYS:O	14:a:242:LYS:NZ	2.35	0.60
4:D:67:LEU:O	27:D:604:CLA:HMD2	2.00	0.60
22:l:125:ASP:OD1	22:l:126:VAL:N	2.35	0.60
3:C:27:VAL:HG23	3:C:27:VAL:O	2.01	0.60
14:a:491:PRO:O	14:a:492:CYS:SG	2.60	0.60
27:a:815:CLA:HBC2	38:a:836:BCR:H11C	1.84	0.59
32:J:615:PID:C8	32:J:615:PID:HM11	2.32	0.59
9:I:197:VAL:CG1	9:I:199:PHE:CE2	2.85	0.59
32:J:613:PID:HM82	32:J:613:PID:H262	1.83	0.59
38:a:834:BCR:H19C	38:a:836:BCR:H382	1.83	0.59
17:d:214:LEU:HD12	17:d:219:TYR:O	1.99	0.59
12:T:127:ALA:HB3	12:T:128:PRO:HD3	1.85	0.59
3:C:97:THR:OG1	3:C:100:GLU:OE1	2.21	0.59
14:a:350:ALA:HB2	27:a:820:CLA:HMC2	1.84	0.59
2:B:208:MET:HE2	2:B:208:MET:HA	1.83	0.59
15:b:501:CYS:SG	15:b:509:THR:C	2.82	0.59
15:b:101:THR:HG21	23:m:80:ILE:HD13	1.84	0.58
11:K:122:CYS:HB3	11:K:224:ALA:HB2	1.85	0.58
11:K:180:ASP:OD1	30:K:609:DD6:O2	2.21	0.58
1:A:101:LEU:O	1:A:105:ARG:HG3	2.04	0.58
23:m:84:ASP:OD1	23:m:84:ASP:N	2.36	0.58
23:m:107:ASP:OD1	23:m:110:ARG:NH2	2.36	0.58
3:C:20:GLU:N	3:C:20:GLU:OE1	2.36	0.58
14:a:635:ILE:HD13	27:a:830:CLA:HMD1	1.86	0.58
17:d:214:LEU:CD1	17:d:214:LEU:O	2.47	0.58
18:e:77:ASN:OD1	18:e:78:VAL:N	2.37	0.58
7:G:90:PHE:HE1	7:G:93:VAL:CG1	2.08	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:86:ARG:NH2	12:T:89:GLU:OE2	2.35	0.57
4:D:114:GLU:OE1	21:j:103:SER:OG	2.22	0.57
1:A:60:SER:OG	1:A:81:GLU:O	2.22	0.57
9:I:197:VAL:HG21	27:I:610:CLA:O1A	2.04	0.57
16:c:101:GLU:OE1	16:c:118:ARG:NH2	2.37	0.57
1:A:159:ASP:OD1	1:A:159:ASP:O	2.23	0.57
11:K:202:HIS:CE1	28:K:607:KC2:CHA	2.88	0.57
11:K:208:MET:SD	32:K:611:PID:H11	2.45	0.57
7:G:90:PHE:CZ	7:G:93:VAL:CG1	2.88	0.57
5:E:157:PHE:HA	5:E:161:THR:HG21	1.87	0.56
15:b:317:TYR:OH	27:b:718:CLA:OBD	2.09	0.56
15:b:274:ASP:HB3	24:r:67:MET:HE2	1.88	0.56
11:K:202:HIS:CE1	28:K:607:KC2:C1A	2.89	0.56
8:H:262:THR:HG21	27:H:313:CLA:O1D	2.05	0.56
14:a:369:ARG:HH22	22:l:205:ILE:HD11	1.65	0.56
10:J:147:LYS:NZ	28:J:608:KC2:O1A	2.38	0.56
27:a:819:CLA:NC	38:a:836:BCR:H322	2.21	0.56
14:a:619:MET:O	14:a:623:SER:OG	2.17	0.56
2:B:188:GLU:OE2	2:B:191:ARG:NH1	2.39	0.56
15:b:156:HIS:CD2	23:m:128:GLY:N	2.73	0.56
27:b:701:CLA:H41	27:b:701:CLA:C7	2.36	0.56
3:C:27:VAL:HG21	3:C:30:LEU:HD12	1.86	0.56
27:a:804:CLA:H143	38:a:836:BCR:C16	2.28	0.56
27:a:831:CLA:C1D	21:j:114:VAL:HG21	2.35	0.56
16:c:136:PHE:CD2	17:d:205:ILE:HG21	2.41	0.56
11:K:208:MET:SD	32:K:611:PID:C11	2.93	0.56
15:b:513:SER:OG	15:b:516:ASP:OD2	2.23	0.55
20:i:137:GLU:OE1	20:i:137:GLU:C	2.49	0.55
38:l:414:BCR:H392	38:l:414:BCR:H23C	1.87	0.55
2:B:107:LYS:NZ	2:B:159:GLU:OE2	2.23	0.55
3:C:112:ALA:HB3	3:C:113:PRO:HD3	1.88	0.55
8:H:125:ILE:HD12	27:H:308:CLA:HMD3	1.87	0.55
9:I:126:GLU:O	9:I:130:THR:HG22	2.06	0.55
14:a:385:LEU:HD11	27:a:823:CLA:HMB2	1.89	0.55
17:d:213:GLU:HG2	17:d:234:ILE:HG23	1.89	0.55
14:a:103:LEU:HD21	21:j:129:ILE:HG23	1.89	0.55
27:F:617:CLA:HED3	14:a:637:TRP:HH2	1.71	0.55
21:j:100:VAL:HG23	21:j:100:VAL:O	2.06	0.55
2:B:99:GLU:OE2	2:B:100:ARG:N	2.40	0.55
7:G:178:MET:HE3	27:G:602:CLA:HMC2	1.89	0.55
14:a:476:ASN:ND2	17:d:129:PRO:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:728:CLA:H142	38:f:304:BCR:H333	1.89	0.55
22:l:324:ASP:OD2	22:l:331:ALA:N	2.38	0.55
38:a:834:BCR:C22	38:a:836:BCR:H393	2.36	0.55
16:c:100:LEU:HD21	16:c:139:ILE:CD1	2.37	0.55
22:l:256:ARG:NH2	22:l:267:GLU:OE1	2.40	0.54
1:A:229:LEU:HD11	27:A:609:CLA:HMA1	1.89	0.54
27:a:816:CLA:H92	27:a:816:CLA:H52	1.88	0.54
27:b:704:CLA:H143	38:i:201:BCR:H332	1.89	0.54
14:a:1:ALA:N	14:a:164:GLN:O	2.40	0.54
14:a:464:LEU:HD21	27:a:824:CLA:HMB2	1.89	0.54
27:a:804:CLA:C9	38:a:836:BCR:H12C	2.37	0.54
15:b:358:VAL:HG13	17:d:213:GLU:OE1	2.07	0.54
15:b:552:TYR:O	15:b:555:SER:OG	2.24	0.54
25:x:80:ASP:OD1	25:x:80:ASP:O	2.25	0.54
15:b:596:THR:HG22	27:b:703:CLA:HMB1	1.88	0.54
11:K:219:VAL:HG12	11:K:220:THR:HG23	1.89	0.54
14:a:231:ILE:HG22	14:a:232:LEU:HD12	1.90	0.54
27:a:819:CLA:H2	38:a:836:BCR:C7	2.26	0.54
16:c:100:LEU:HD21	16:c:139:ILE:HD12	1.89	0.54
13:U:16:ARG:NH1	13:U:100:GLU:OE2	2.40	0.54
15:b:344:ALA:HB2	27:b:719:CLA:HMC2	1.89	0.54
38:i:201:BCR:H372	38:l:415:BCR:H403	1.90	0.54
7:G:168:MET:HE3	7:G:172:LYS:HG3	1.90	0.54
32:I:614:PID:HM22	32:I:614:PID:C2	2.36	0.54
11:K:225:ALA:O	11:K:226:GLN:HG3	2.08	0.54
20:i:134:ASP:OD1	20:i:135:ASP:N	2.41	0.54
27:a:811:CLA:CBB	38:a:836:BCR:H351	2.38	0.54
6:F:202:ILE:HG22	27:F:605:CLA:HED2	1.90	0.53
6:F:264:ARG:HA	6:F:267:MET:HE3	1.90	0.53
11:K:210:ILE:HG21	30:K:610:DD6:C24	2.37	0.53
38:i:201:BCR:H382	38:i:201:BCR:H23C	1.89	0.53
5:E:239:PHE:O	5:E:242:LEU:N	2.41	0.53
8:H:269:PRO:O	29:H:314:UIX:O1	2.27	0.53
14:a:369:ARG:NH2	22:l:205:ILE:CD1	2.69	0.53
14:a:285:ILE:HG22	14:a:285:ILE:O	2.07	0.53
15:b:249:ALA:HB1	27:r:203:CLA:HBC2	1.91	0.53
9:I:197:VAL:HG13	9:I:199:PHE:CE2	2.44	0.53
6:F:116:ASP:O	6:F:118:GLU:N	2.40	0.53
27:b:704:CLA:HMB2	27:b:705:CLA:HMB2	1.91	0.53
11:K:120:LEU:HD11	27:K:603:CLA:HAC1	1.87	0.53
32:J:613:PID:H312	32:J:614:PID:HM82	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:204:ARG:HA	11:K:207:MET:HE3	1.90	0.52
14:a:77:GLY:O	14:a:81:SER:OG	2.12	0.52
6:F:207:ILE:HG21	27:F:604:CLA:HBC3	1.90	0.52
14:a:517:TYR:HH	27:a:801:CLA:HED3	1.74	0.52
11:K:202:HIS:HE1	28:K:607:KC2:CHA	2.21	0.52
16:c:89:THR:HG22	16:c:102:MET:HG3	1.91	0.52
38:i:201:BCR:H402	38:l:415:BCR:H361	1.91	0.52
27:a:801:CLA:HMB3	27:a:826:CLA:OBD	2.10	0.52
15:b:221:SER:OG	15:b:222:LEU:N	2.42	0.52
20:i:75:THR:HG23	38:i:201:BCR:H333	1.91	0.52
27:b:709:CLA:HBB1	27:b:709:CLA:HMB1	1.92	0.52
17:d:126:PHE:CB	17:d:161:MET:HE1	2.40	0.52
16:c:83:ASP:OD2	18:e:85:LYS:CD	2.58	0.52
27:a:804:CLA:C4	38:a:836:BCR:H312	2.40	0.52
27:l:402:CLA:CBB	38:l:415:BCR:H342	2.40	0.52
15:b:592:LEU:O	15:b:596:THR:HG23	2.10	0.51
15:b:113:ASN:ND2	15:b:318:PHE:O	2.43	0.51
15:b:621:LYS:NZ	22:l:240:GLU:OE1	2.43	0.51
27:b:716:CLA:O1A	30:b:730:DD6:O2	2.28	0.51
32:F:614:PID:CM1	32:F:614:PID:C8	2.89	0.51
32:F:614:PID:C8	32:F:614:PID:HM21	2.39	0.51
9:I:199:PHE:CD2	38:a:833:BCR:H281	2.45	0.51
15:b:43:TRP:CB	15:b:144:ALA:HB2	2.40	0.51
22:l:286:LEU:HD12	22:l:295:VAL:HG21	1.91	0.51
14:a:192:SER:OG	14:a:260:HIS:O	2.27	0.51
14:a:219:LEU:HD21	26:y:196:ILE:HG13	1.92	0.51
27:a:827:CLA:HBC2	27:a:827:CLA:CMC	2.39	0.51
11:K:89:PHE:N	27:K:601:CLA:OBD	2.43	0.51
15:b:526:LEU:HD21	15:b:653:THR:HG23	1.92	0.51
17:d:235:LYS:O	17:d:238:VAL:HG22	2.11	0.51
8:H:173:THR:HG23	27:b:713:CLA:HED1	1.93	0.51
15:b:60:ILE:O	15:b:64:ALA:HB3	2.11	0.51
27:b:701:CLA:H41	27:b:701:CLA:H72	1.92	0.51
27:b:701:CLA:H42	27:b:701:CLA:C1C	2.41	0.51
24:r:40:THR:O	24:r:44:MET:HG3	2.11	0.51
2:B:146:GLU:N	2:B:146:GLU:OE1	2.40	0.51
14:a:350:ALA:HB2	27:a:820:CLA:CMC	2.40	0.51
7:G:90:PHE:CZ	7:G:93:VAL:HG11	2.45	0.51
17:d:181:HIS:HB3	17:d:182:PRO:HD3	1.92	0.51
19:f:211:THR:HG21	38:f:301:BCR:H342	1.93	0.51
4:D:26:GLU:OE2	30:D:615:DD6:O2	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:198:THR:HG22	10:J:199:PRO:HD2	1.92	0.50
10:J:35:LEU:O	10:J:62:ARG:NH2	2.42	0.50
14:a:78:ALA:HB2	14:a:141:LEU:HB3	1.93	0.50
15:b:358:VAL:HG22	17:d:213:GLU:OE1	2.11	0.50
8:H:261:ALA:HB2	8:H:271:LEU:C	2.36	0.50
15:b:300:CYS:O	15:b:304:THR:OG1	2.28	0.50
14:a:464:LEU:HD21	27:a:824:CLA:CMB	2.41	0.50
15:b:83:ILE:HD13	27:b:709:CLA:HMD2	1.93	0.50
8:H:118:ALA:O	8:H:122:HIS:ND1	2.41	0.50
28:J:608:KC2:CHC	32:J:611:PID:HM43	2.42	0.50
12:T:169:TYR:CD1	27:T:606:CLA:HED3	2.47	0.50
14:a:165:LEU:HD21	35:j:201:DGD:O2D	2.12	0.50
27:a:806:CLA:HBC2	27:a:806:CLA:CMC	2.42	0.50
17:d:235:LYS:O	17:d:239:MET:HG3	2.12	0.50
2:B:83:THR:OG1	34:l:401:LHG:O5	2.14	0.49
7:G:191:PHE:O	7:G:193:ALA:N	2.44	0.49
8:H:124:ARG:HA	8:H:127:MET:HE3	1.93	0.49
16:c:91:CYS:SG	16:c:100:LEU:HD22	2.52	0.49
14:a:328:THR:HG22	14:a:439:VAL:HG12	1.92	0.49
15:b:664:ILE:O	15:b:668:THR:OG1	2.27	0.49
11:K:100:ARG:NH1	12:T:162:ASP:O	2.45	0.49
14:a:7:ASN:HB3	21:j:100:VAL:HG23	1.93	0.49
38:a:834:BCR:H16C	38:a:836:BCR:H19C	1.93	0.49
15:b:489:MET:HE3	16:c:140:ARG:NH2	2.27	0.49
27:F:602:CLA:HMA3	32:F:614:PID:C18	2.42	0.49
27:I:616:CLA:HAC2	14:a:232:LEU:HD11	1.94	0.49
11:K:100:ARG:NH2	12:T:163:PRO:O	2.41	0.49
32:K:611:PID:HM72	32:K:611:PID:C28	2.43	0.49
14:a:235:THR:HG21	14:a:254:SER:OG	2.12	0.49
14:a:303:LEU:HD13	14:a:350:ALA:HB1	1.93	0.49
27:a:819:CLA:NB	38:a:836:BCR:HC31	2.28	0.49
24:r:117:VAL:HG21	24:r:123:PHE:CE1	2.48	0.49
13:U:70:ILE:HG21	27:U:605:CLA:CMC	2.43	0.49
20:i:159:LYS:NZ	24:r:24:GLU:OE2	2.43	0.49
22:l:186:ASP:OD1	22:l:187:GLU:N	2.42	0.49
11:K:202:HIS:HE1	28:K:607:KC2:ND	2.10	0.49
16:c:91:CYS:SG	16:c:92:VAL:N	2.85	0.49
32:J:615:PID:HM22	32:J:615:PID:H21	1.95	0.49
12:T:117:VAL:HG12	12:T:126:THR:HB	1.95	0.49
2:B:182:ASP:OD1	2:B:182:ASP:C	2.56	0.49
4:D:43:ARG:NH1	4:D:145:LEU:HD11	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:133:ASP:OD1	5:E:134:PHE:N	2.45	0.49
5:E:222:MET:HG2	30:E:614:DD6:C5	2.43	0.49
9:I:199:PHE:CE2	38:a:833:BCR:H281	2.48	0.49
17:d:83:ILE:HG21	17:d:171:LEU:HD21	1.93	0.49
4:D:41:TRP:NE1	27:D:603:CLA:O1A	2.43	0.48
4:D:62:ALA:HB1	4:D:67:LEU:HD23	1.95	0.48
6:F:156:GLU:OE2	6:F:233:ARG:NH2	2.46	0.48
14:a:385:LEU:HD11	27:a:823:CLA:CMB	2.43	0.48
32:K:611:PID:CM1	32:K:611:PID:C8	2.91	0.48
14:a:46:GLY:HA3	14:a:50:LEU:HD23	1.95	0.48
14:a:444:GLU:OE2	26:y:170:TYR:OH	2.26	0.48
15:b:218:SER:O	15:b:224:TYR:OH	2.29	0.48
13:U:43:LEU:CD2	13:U:48:ILE:HD11	2.44	0.48
27:U:603:CLA:HBC3	27:U:603:CLA:HHD	1.95	0.48
14:a:445:LEU:O	26:y:148:PHE:HZ	1.96	0.48
38:a:834:BCR:H362	38:a:836:BCR:H21C	0.68	0.48
2:B:231:TRP:HB3	2:B:235:VAL:HG23	1.95	0.48
8:H:263:LEU:CD1	27:H:312:CLA:HMD1	2.44	0.48
9:I:157:TYR:OH	14:a:283:ASN:OD1	2.30	0.48
27:a:826:CLA:HMD2	27:b:702:CLA:O1A	2.14	0.48
32:J:615:PID:HM11	32:J:615:PID:H8	1.96	0.48
11:K:112:GLY:CA	11:K:207:MET:HE2	2.44	0.48
27:a:804:CLA:H91	38:a:836:BCR:C12	2.44	0.48
27:a:820:CLA:H92	27:a:825:CLA:HED3	1.94	0.48
2:B:103:GLN:HG2	27:B:605:CLA:HED2	1.96	0.48
5:E:129:MET:CE	5:E:229:ILE:HD12	2.43	0.48
6:F:192:LEU:HD23	32:F:615:PID:HM23	1.96	0.48
27:J:609:CLA:CMB	32:J:611:PID:HM13	2.41	0.48
15:b:40:THR:CG2	23:m:108:LEU:HD11	2.43	0.48
4:D:54:MET:HE3	4:D:147:ASN:HB3	1.94	0.48
6:F:271:MET:HE1	27:F:601:CLA:C15	2.43	0.48
27:K:602:CLA:O1A	27:K:602:CLA:C2	2.62	0.48
14:a:57:SER:O	14:a:159:SER:OG	2.28	0.48
27:a:806:CLA:HBC2	27:a:806:CLA:HMC3	1.95	0.48
20:i:63:ASP:O	20:i:66:LYS:NZ	2.47	0.48
3:C:81:THR:CG2	27:C:205:CLA:HED1	2.43	0.48
33:D:619:LMG:O2	30:D:621:DD6:O4	2.31	0.48
13:U:48:ILE:HB	27:U:603:CLA:CED	2.43	0.48
14:a:503:ILE:HG23	15:b:606:GLY:HA3	1.95	0.48
15:b:245:HIS:CD2	27:b:714:CLA:HMB3	2.40	0.48
8:H:147:CYS:HA	8:H:159:ALA:HB1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:109:LEU:HD13	11:K:176:GLY:HA3	1.96	0.48
15:b:74:ILE:HB	15:b:75:PRO:HD3	1.95	0.48
25:x:41:SER:OG	25:x:57:LEU:O	2.32	0.48
9:I:86:GLY:O	9:I:87:PHE:C	2.55	0.47
32:K:611:PID:HM13	32:K:611:PID:H8	1.96	0.47
1:A:97:ARG:NH1	1:A:100:GLU:OE1	2.41	0.47
5:E:189:GLU:N	5:E:189:GLU:OE1	2.46	0.47
15:b:414:ILE:O	15:b:460:TYR:OH	2.25	0.47
17:d:270:GLN:OE1	17:d:271:GLU:N	2.47	0.47
20:i:141:GLU:HA	20:i:156:VAL:HG21	1.96	0.47
38:l:415:BCR:H23C	38:l:415:BCR:H392	1.94	0.47
28:J:604:KC2:CBC	32:J:613:PID:C17	2.93	0.47
27:J:605:CLA:HBC3	32:J:613:PID:HM21	1.97	0.47
14:a:293:MET:O	14:a:293:MET:HG2	2.13	0.47
25:x:78:GLY:O	25:x:79:GLU:HB3	2.14	0.47
4:D:54:MET:HE1	27:D:608:CLA:CAB	2.43	0.47
8:H:204:LYS:NZ	8:H:221:ASP:O	2.45	0.47
27:a:816:CLA:H92	27:a:816:CLA:C5	2.44	0.47
17:d:126:PHE:HB3	17:d:161:MET:HE1	1.95	0.47
32:F:614:PID:H21	32:F:614:PID:HM22	1.97	0.47
11:K:204:ARG:HB2	32:K:611:PID:HM23	1.96	0.47
2:B:253:VAL:HG12	15:b:100:THR:HG23	1.97	0.47
10:J:56:GLU:OE2	10:J:56:GLU:C	2.58	0.47
15:b:138:VAL:CG2	23:m:101:VAL:HG22	2.44	0.47
27:b:701:CLA:H42	27:b:701:CLA:NC	2.30	0.47
20:i:90:TYR:OH	20:i:96:ALA:O	2.29	0.47
1:A:222:VAL:HG13	1:A:231:PRO:HG3	1.97	0.47
27:I:605:CLA:HMB2	13:U:76:PHE:CZ	2.49	0.47
15:b:43:TRP:CE2	27:b:711:CLA:HED1	2.50	0.47
15:b:344:ALA:HB2	27:b:719:CLA:CMC	2.45	0.47
15:b:626:ILE:HG21	17:d:108:ARG:NH2	2.29	0.47
8:H:252:LEU:HD13	30:H:316:DD6:C26	2.44	0.47
5:E:219:ARG:HA	5:E:222:MET:HE3	1.96	0.47
10:J:166:GLU:OE1	10:J:167:ALA:N	2.48	0.47
27:j:202:CLA:C1A	27:j:202:CLA:CGA	2.94	0.46
30:D:615:DD6:O4	5:E:160:ALA:O	2.34	0.46
6:F:228:ILE:O	6:F:228:ILE:HG22	2.15	0.46
14:a:175:LYS:NZ	22:l:176:LEU:O	2.45	0.46
15:b:98:HIS:O	15:b:99:THR:OG1	2.29	0.46
20:i:90:TYR:CZ	20:i:96:ALA:O	2.68	0.46
2:B:210:LEU:HD23	2:B:221:PRO:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F:617:CLA:HBC2	27:b:722:CLA:HMC3	1.98	0.46
6:F:141:ASP:O	14:a:641:LYS:NZ	2.48	0.46
14:a:606:ILE:HD11	27:a:807:CLA:HMC2	1.97	0.46
20:i:177:LEU:HD11	25:x:110:TRP:HE3	1.79	0.46
10:J:176:LEU:O	10:J:180:ARG:HG3	2.16	0.46
32:J:611:PID:HM72	32:J:611:PID:HM51	1.97	0.46
32:J:614:PID:HM51	32:J:614:PID:CM7	2.44	0.46
15:b:270:THR:OG1	15:b:275:MET:HE2	2.15	0.46
16:c:128:CYS:SG	16:c:129:GLU:N	2.88	0.46
22:l:140:GLU:OE1	22:l:140:GLU:HA	2.16	0.46
9:I:162:ARG:O	9:I:166:VAL:HG23	2.16	0.46
11:K:178:PHE:HD2	27:K:605:CLA:HMD1	1.80	0.46
24:r:117:VAL:HG21	24:r:123:PHE:CZ	2.51	0.46
1:A:69:PRO:CG	1:A:72:LEU:HD21	2.46	0.46
27:F:617:CLA:HED3	14:a:637:TRP:CH2	2.51	0.46
27:H:319:CLA:H43	27:b:710:CLA:O1A	2.16	0.46
26:y:180:ILE:O	26:y:184:GLN:HG3	2.16	0.46
26:y:204:ARG:N	26:y:209:TYR:OH	2.39	0.46
4:D:14:MET:HG3	4:D:18:LEU:HD11	1.97	0.46
27:F:619:CLA:H62	27:F:619:CLA:H41	1.82	0.46
27:H:304:CLA:HAA1	27:H:304:CLA:CGD	2.46	0.46
11:K:145:ASN:OD1	11:K:148:ALA:N	2.45	0.46
14:a:99:ILE:HD11	14:a:117:PHE:CZ	2.51	0.46
22:l:205:ILE:CG1	22:l:224:TRP:CB	2.84	0.46
3:C:85:MET:HE3	29:C:215:UIX:C35	2.46	0.45
5:E:72:ILE:HG23	5:E:106:GLU:HB2	1.98	0.45
6:F:228:ILE:N	6:F:228:ILE:HD13	2.30	0.45
14:a:388:HIS:O	14:a:392:LEU:HG	2.16	0.45
19:f:166:ALA:O	19:f:170:ASN:OD1	2.33	0.45
2:B:200:GLY:O	2:B:204:MET:HG3	2.17	0.45
27:C:204:CLA:HED3	27:C:204:CLA:H141	1.99	0.45
27:a:837:CLA:OBD	27:b:702:CLA:HMB3	2.16	0.45
9:I:130:THR:HG23	9:I:131:TYR:CD2	2.52	0.45
12:T:159:ASN:OD1	27:T:606:CLA:HED2	2.16	0.45
3:C:51:VAL:HG13	27:H:319:CLA:CMB	2.44	0.45
7:G:107:LEU:HD12	7:G:116:PRO:HG3	1.97	0.45
14:a:559:LEU:HD11	26:y:172:ILE:CG1	2.47	0.45
15:b:655:GLY:O	15:b:659:THR:HG22	2.16	0.45
22:l:108:ILE:O	22:l:115:GLN:NE2	2.49	0.45
12:T:92:HIS:HB3	12:T:185:MET:HE2	1.97	0.45
15:b:156:HIS:HD2	23:m:128:GLY:CA	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:209:ALA:HB1	15:b:240:LEU:HD21	1.99	0.45
17:d:214:LEU:HD13	17:d:219:TYR:C	2.40	0.45
2:B:91:LEU:O	2:B:97:LYS:NZ	2.39	0.45
27:a:819:CLA:C4C	38:a:836:BCR:H322	2.46	0.45
15:b:415:LEU:HD22	15:b:551:THR:HG21	1.98	0.45
4:D:72:GLU:N	4:D:73:PRO:CD	2.79	0.45
27:D:611:CLA:OBD	26:y:216:TYR:OH	2.32	0.45
10:J:64:SER:O	10:J:68:ASN:ND2	2.45	0.45
13:U:20:ILE:HG22	27:U:603:CLA:CAB	2.47	0.45
14:a:365:THR:HG22	14:a:366:SER:H	1.81	0.45
14:a:216:ASP:HB3	14:a:219:LEU:HD23	1.99	0.45
4:D:46:GLU:OE2	4:D:149:ARG:NE	2.44	0.45
5:E:239:PHE:O	5:E:240:PRO:C	2.60	0.45
14:a:404:ARG:NH1	15:b:87:HIS:O	2.48	0.45
21:j:74:MET:HE1	21:j:86:LEU:HD11	1.99	0.45
27:b:704:CLA:H192	38:m:201:BCR:H362	1.99	0.44
4:D:94:MET:O	4:D:98:MET:HG2	2.17	0.44
32:K:611:PID:HM51	32:K:611:PID:HM83	1.97	0.44
22:l:228:GLU:OE2	25:x:73:TYR:OH	2.29	0.44
2:B:225:MET:O	2:B:229:GLY:N	2.50	0.44
6:F:121:CYS:HB3	6:F:125:LYS:O	2.18	0.44
6:F:183:TYR:CE2	6:F:203:VAL:HG23	2.52	0.44
7:G:105:ASN:OD1	30:G:616:DD6:O2	2.36	0.44
10:J:74:PHE:CD2	32:J:613:PID:HM11	2.51	0.44
12:T:118:PRO:CD	12:T:126:THR:HG21	2.47	0.44
15:b:458:ASP:OD1	15:b:539:LYS:NZ	2.50	0.44
20:i:98:TRP:CB	20:i:104:THR:HG21	2.48	0.44
14:a:38:ALA:O	14:a:44:GLN:NE2	2.51	0.44
38:a:834:BCR:H361	38:a:836:BCR:C21	2.23	0.44
15:b:58:TYR:HB2	15:b:130:THR:HG21	1.99	0.44
15:b:245:HIS:CD2	27:b:714:CLA:CMB	2.94	0.44
27:D:612:CLA:H61	27:D:612:CLA:H41	1.84	0.44
29:I:612:UIX:C19	27:l:412:CLA:HMC2	2.48	0.44
11:K:204:ARG:CB	32:K:611:PID:HM23	2.47	0.44
15:b:461:VAL:HG11	15:b:535:TYR:CG	2.53	0.44
10:J:71:VAL:HG22	32:J:613:PID:HM13	2.00	0.44
10:J:131:VAL:HG22	10:J:131:VAL:O	2.18	0.44
35:K:614:DGD:O5D	35:K:614:DGD:O4D	2.19	0.44
12:T:87:ARG:HG2	27:T:605:CLA:HED2	2.00	0.44
13:U:19:MET:SD	13:U:104:GLY:HA2	2.58	0.44
19:f:207:ILE:HG13	38:f:301:BCR:H313	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:l:275:PHE:CD1	22:l:275:PHE:C	2.95	0.44
27:A:605:CLA:H61	27:A:605:CLA:H41	1.89	0.44
5:E:216:LYS:HB3	27:E:609:CLA:HMD2	1.99	0.44
5:E:136:ARG:NH1	5:E:147:VAL:O	2.51	0.44
27:a:804:CLA:H143	38:a:836:BCR:C36	2.40	0.44
15:b:457:GLY:O	15:b:461:VAL:HG23	2.18	0.44
17:d:110:THR:O	17:d:113:ARG:NH2	2.50	0.44
8:H:186:LEU:HA	8:H:189:VAL:HG22	2.00	0.44
14:a:350:ALA:CB	27:a:820:CLA:HMC2	2.48	0.44
21:j:88:THR:O	21:j:88:THR:HG22	2.17	0.44
5:E:145:GLU:N	5:E:145:GLU:CD	2.76	0.43
6:F:95:VAL:HG21	32:F:615:PID:O7	2.18	0.43
14:a:594:SER:HB3	14:a:600:ILE:HD12	1.99	0.43
38:a:836:BCR:C8	38:a:836:BCR:H331	2.47	0.43
32:B:613:PID:H16	32:B:613:PID:HM41	1.78	0.43
10:J:81:VAL:HB	10:J:82:PRO:HD3	2.00	0.43
11:K:94:LEU:O	11:K:100:ARG:NE	2.43	0.43
12:T:191:ILE:O	12:T:195:GLU:HG2	2.18	0.43
1:A:107:CYS:SG	30:A:614:DD6:C2	3.07	0.43
7:G:69:HIS:HB3	7:G:178:MET:SD	2.57	0.43
9:I:113:GLY:HA2	9:I:116:TRP:CD1	2.54	0.43
14:a:259:HIS:HB2	27:a:814:CLA:CHB	2.48	0.43
17:d:236:ALA:HB1	24:r:40:THR:HG23	2.00	0.43
20:i:116:GLU:OE1	23:m:119:ASN:ND2	2.49	0.43
5:E:112:ARG:NH1	5:E:215:LEU:HD11	2.33	0.43
6:F:98:TRP:CZ3	6:F:228:ILE:HD11	2.54	0.43
27:H:303:CLA:HMC1	30:H:315:DD6:C9	2.48	0.43
11:K:213:GLN:O	11:K:217:GLU:HG3	2.18	0.43
14:a:428:GLN:O	26:y:173:ARG:NH1	2.48	0.43
15:b:40:THR:HB	23:m:112:LEU:HD21	2.00	0.43
27:b:727:CLA:H2A	27:b:727:CLA:O2A	2.17	0.43
18:e:93:ASP:OD1	18:e:93:ASP:N	2.51	0.43
27:f:302:CLA:HMB3	27:f:302:CLA:HBB1	2.00	0.43
14:a:135:ILE:HG21	14:a:141:LEU:HG	2.00	0.43
15:b:544:ARG:NH1	15:b:548:GLU:OE2	2.51	0.43
17:d:206:ARG:O	17:d:206:ARG:HG3	2.19	0.43
4:D:21:ILE:HD12	4:D:39:ILE:HG12	2.00	0.43
5:E:112:ARG:HD3	5:E:112:ARG:O	2.19	0.43
14:a:124:SER:CB	27:a:818:CLA:HED3	2.49	0.43
27:a:804:CLA:H61	27:a:804:CLA:H41	1.86	0.43
15:b:210:ILE:HB	15:b:211:PRO:HD3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:714:CLA:HMB3	27:b:714:CLA:HBB1	2.01	0.43
19:f:277:THR:OG1	19:f:278:GLN:N	2.51	0.43
22:l:269:GLY:O	22:l:345:GLY:HA2	2.19	0.43
4:D:18:LEU:HB2	27:D:602:CLA:HED1	2.00	0.43
9:I:100:ASP:O	9:I:106:SER:OG	2.30	0.43
11:K:120:LEU:HD11	11:K:124:VAL:HG21	2.01	0.43
15:b:186:LEU:O	15:b:190:THR:HG22	2.19	0.43
25:x:99:ASP:OD1	25:x:99:ASP:C	2.62	0.43
6:F:116:ASP:C	6:F:118:GLU:H	2.27	0.43
10:J:97:LEU:HD11	10:J:102:VAL:CG1	2.49	0.43
15:b:138:VAL:HG23	23:m:101:VAL:HG22	2.00	0.43
15:b:458:ASP:OD1	15:b:535:TYR:OH	2.23	0.43
17:d:270:GLN:C	17:d:270:GLN:CD	2.86	0.43
35:l:416:DGD:O5E	35:l:416:DGD:O4E	2.24	0.43
2:B:182:ASP:OD1	2:B:182:ASP:O	2.36	0.43
32:J:611:PID:O7	32:J:611:PID:C26	2.67	0.43
11:K:94:LEU:HD13	27:K:601:CLA:H2	2.01	0.43
12:T:109:ILE:HG22	12:T:110:LYS:N	2.34	0.43
38:a:836:BCR:H361	38:a:836:BCR:H20C	1.80	0.43
15:b:43:TRP:HB3	15:b:144:ALA:HB2	2.00	0.43
15:b:592:LEU:HD21	27:b:725:CLA:HBB2	2.01	0.43
26:y:187:ASP:OD1	26:y:187:ASP:C	2.62	0.43
30:A:615:DD6:C41	27:D:605:CLA:HED2	2.49	0.42
2:B:112:ALA:O	2:B:116:VAL:HG23	2.19	0.42
7:G:175:ARG:HB2	30:G:614:DD6:C41	2.49	0.42
8:H:232:ASP:OD1	8:H:233:GLU:N	2.52	0.42
14:a:304:ALA:HB3	27:l:411:CLA:HBB2	2.01	0.42
15:b:542:ALA:HB1	15:b:545:GLN:HB3	2.01	0.42
22:l:356:ILE:HG13	27:l:409:CLA:HED3	2.00	0.42
6:F:114:GLY:N	6:F:115:PRO:CD	2.82	0.42
27:K:601:CLA:HAC2	32:K:611:PID:HM22	2.01	0.42
27:b:708:CLA:CGA	27:b:708:CLA:C1A	2.97	0.42
2:B:80:LEU:N	2:B:81:PRO:HD2	2.34	0.42
5:E:68:GLU:OE1	21:j:67:ASN:ND2	2.53	0.42
27:F:602:CLA:HMD2	32:F:615:PID:H16	2.00	0.42
12:T:117:VAL:HG12	12:T:126:THR:CB	2.50	0.42
14:a:483:LYS:NZ	14:a:503:ILE:O	2.49	0.42
32:F:614:PID:H262	32:F:614:PID:H313	2.01	0.42
6:F:112:MET:HE1	6:F:151:VAL:HG22	2.01	0.42
9:I:55:SER:OG	9:I:57:GLU:OE1	2.28	0.42
9:I:178:ALA:CB	29:I:612:UIX:C13	2.98	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:245:LEU:O	9:I:246:MET:C	2.63	0.42
11:K:202:HIS:CD2	27:K:605:CLA:CBB	3.02	0.42
14:a:109:LEU:HD22	14:a:602:SER:HB3	2.01	0.42
14:a:356:SER:HB3	14:a:505:PRO:HB3	2.02	0.42
38:l:414:BCR:H24C	38:l:414:BCR:H371	1.89	0.42
24:r:128:ILE:HD12	24:r:128:ILE:H	1.84	0.42
10:J:119:GLN:OE1	28:J:604:KC2:ND	2.52	0.42
7:G:83:PRO:HA	7:G:86:PHE:O	2.20	0.42
10:J:166:GLU:C	10:J:166:GLU:CD	2.88	0.42
32:J:613:PID:HM22	32:J:613:PID:C2	2.44	0.42
15:b:117:THR:HG21	15:b:317:TYR:HD1	1.84	0.42
24:r:123:PHE:HB3	24:r:128:ILE:HD11	2.02	0.42
1:A:102:LYS:O	1:A:106:VAL:HG13	2.19	0.42
10:J:83:GLU:OE2	10:J:104:ASN:ND2	2.50	0.42
13:U:43:LEU:HD11	13:U:57:LYS:HD2	2.01	0.42
14:a:497:ARG:NH1	17:d:149:GLU:OE2	2.53	0.42
21:j:133:ARG:CD	29:j:204:UIX:O3	2.68	0.42
22:l:205:ILE:HG13	22:l:224:TRP:HB2	1.94	0.42
32:I:614:PID:H16	32:I:614:PID:HM41	1.96	0.42
11:K:120:LEU:HD11	27:K:603:CLA:CAC	2.47	0.42
38:l:413:BCR:C23	38:l:413:BCR:H392	2.49	0.42
27:C:205:CLA:H61	27:C:205:CLA:H41	1.94	0.42
5:E:72:ILE:HG21	22:l:171:TYR:CG	2.55	0.42
14:a:97:SER:OG	27:a:807:CLA:HED3	2.20	0.42
14:a:136:VAL:HG23	14:a:137:THR:HG23	2.02	0.42
2:B:82:LEU:HD21	27:l:410:CLA:HMB2	2.02	0.41
7:G:74:MET:HE3	7:G:174:GLY:HA2	2.01	0.41
27:H:319:CLA:H41	27:b:710:CLA:C1B	2.50	0.41
10:J:106:ILE:N	10:J:193:ASP:OD2	2.47	0.41
11:K:104:MET:HE1	27:K:602:CLA:O2A	2.20	0.41
16:c:157:LEU:HD23	17:d:106:MET:CG	2.50	0.41
20:i:94:GLU:OE1	20:i:94:GLU:C	2.63	0.41
4:D:148:GLY:O	4:D:152:MET:HG3	2.19	0.41
11:K:217:GLU:HG2	11:K:222:MET:O	2.20	0.41
15:b:489:MET:HE2	15:b:495:HIS:CD2	2.56	0.41
38:l:413:BCR:H24C	38:l:413:BCR:H371	1.84	0.41
38:l:413:BCR:H331	38:l:413:BCR:C8	2.50	0.41
1:A:97:ARG:HD2	1:A:101:LEU:CD2	2.49	0.41
14:a:365:THR:O	14:a:368:ILE:HG22	2.20	0.41
14:a:392:LEU:HB3	14:a:451:MET:HE3	2.01	0.41
20:i:137:GLU:OE2	20:i:141:GLU:OE2	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ARG:NH1	2:B:133:PHE:O	2.50	0.41
32:F:614:PID:H313	32:F:614:PID:C26	2.51	0.41
9:I:155:ASP:O	9:I:155:ASP:CG	2.63	0.41
27:T:603:CLA:CMC	27:T:603:CLA:HBC3	2.50	0.41
13:U:32:ARG:HH21	27:U:603:CLA:HED2	1.85	0.41
15:b:383:LEU:HD13	27:b:722:CLA:C3B	2.50	0.41
17:d:117:THR:CG2	17:d:142:LEU:HD13	2.50	0.41
38:f:301:BCR:H383	38:f:301:BCR:H23C	2.01	0.41
24:r:82:LYS:O	24:r:147:GLN:NE2	2.52	0.41
1:A:125:PHE:O	1:A:126:THR:C	2.64	0.41
14:a:204:LEU:HB2	14:a:205:PRO:HD3	2.01	0.41
15:b:245:HIS:HB3	27:b:714:CLA:HMB2	2.02	0.41
15:b:304:THR:HA	15:b:307:THR:HG22	2.02	0.41
3:C:36:LEU:HB2	27:C:203:CLA:HED1	2.02	0.41
11:K:200:ILE:O	11:K:204:ARG:HG3	2.21	0.41
14:a:496:GLY:O	14:a:497:ARG:HG2	2.20	0.41
15:b:344:ALA:HB2	27:b:719:CLA:C2C	2.51	0.41
20:i:88:VAL:HG21	38:l:414:BCR:H14C	2.02	0.41
20:i:98:TRP:HB3	20:i:104:THR:HG21	2.02	0.41
11:K:110:LYS:NZ	11:K:169:ASP:OD1	2.35	0.41
15:b:101:THR:HG22	15:b:102:ALA:N	2.36	0.41
38:b:731:BCR:H311	38:b:731:BCR:C8	2.51	0.41
1:A:134:ALA:HB1	27:A:604:CLA:HED3	2.03	0.41
14:a:197:ALA:HB2	27:a:812:CLA:CHC	2.51	0.41
17:d:157:GLN:CG	17:d:161:MET:HE3	2.50	0.41
2:B:99:GLU:OE2	2:B:99:GLU:C	2.64	0.41
3:C:92:PHE:CZ	27:C:201:CLA:HMD2	2.56	0.41
4:D:45:ALA:O	4:D:49:HIS:ND1	2.50	0.41
4:D:67:LEU:O	4:D:67:LEU:HG	2.20	0.41
5:E:132:PRO:HA	5:E:135:VAL:O	2.20	0.41
6:F:215:MET:HE2	24:r:94:MET:HE1	2.02	0.41
9:I:210:TYR:HE2	14:a:242:LYS:HZ1	1.67	0.41
12:T:103:LEU:HD13	12:T:191:ILE:HG21	2.01	0.41
13:U:20:ILE:HG23	27:U:603:CLA:HMC3	2.03	0.41
27:a:816:CLA:HMB2	27:a:824:CLA:HBA2	2.02	0.41
17:d:184:ASP:OD1	17:d:184:ASP:N	2.51	0.41
19:f:208:PHE:CD1	19:f:208:PHE:C	2.99	0.41
21:j:133:ARG:HD3	29:j:204:UIX:O3	2.21	0.41
28:J:604:KC2:CBC	32:J:613:PID:H17	2.51	0.41
32:J:613:PID:H11	32:J:614:PID:HM22	2.01	0.41
33:K:613:LMG:O5	33:K:613:LMG:O4	2.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:92:HIS:CD2	27:T:605:CLA:HMD2	2.56	0.41
14:a:331:PRO:HD3	14:a:686:THR:HG21	2.03	0.41
14:a:507:ASP:HA	14:a:510:PHE:HB3	2.03	0.41
15:b:88:PHE:CD1	15:b:94:THR:HG21	2.56	0.41
15:b:546:PHE:O	15:b:550:SER:OG	2.17	0.41
17:d:214:LEU:HD11	17:d:219:TYR:O	2.05	0.41
20:i:142:GLU:OE2	20:i:142:GLU:C	2.64	0.41
24:r:25:THR:O	24:r:29:GLU:HG3	2.21	0.41
6:F:199:PRO:HA	6:F:203:VAL:HG13	2.02	0.40
9:I:170:ASN:ND2	27:I:607:CLA:O1D	2.53	0.40
12:T:170:THR:O	12:T:174:ARG:HG3	2.22	0.40
27:a:826:CLA:H61	27:a:826:CLA:H41	1.87	0.40
38:a:836:BCR:H351	38:a:836:BCR:H15C	1.87	0.40
27:b:723:CLA:CGA	27:b:723:CLA:C1A	2.99	0.40
36:T:613:LMU:O3'	36:T:613:LMU:C1B	2.69	0.40
14:a:305:VAL:HG13	27:a:817:CLA:H41	2.03	0.40
38:a:834:BCR:H24C	38:a:834:BCR:H371	1.93	0.40
15:b:471:VAL:HG11	15:b:524:TRP:CE2	2.56	0.40
38:f:301:BCR:C8	38:f:301:BCR:H311	2.51	0.40
24:r:26:PRO:HA	24:r:29:GLU:HG3	2.03	0.40
32:K:611:PID:HM51	32:K:611:PID:CM8	2.51	0.40
38:f:301:BCR:H24C	38:f:301:BCR:H371	1.87	0.40
5:E:116:LEU:HD22	5:E:214:GLU:OE2	2.20	0.40
27:E:611:CLA:H43	27:G:605:CLA:H43	2.04	0.40
22:l:268:ILE:HD13	27:l:406:CLA:HMD1	2.03	0.40
1:A:108:MET:HE2	29:A:613:UIX:C39	2.51	0.40
27:A:601:CLA:CBC	4:D:104:PHE:CZ	3.05	0.40
6:F:248:ASP:OD1	6:F:248:ASP:C	2.64	0.40
27:I:603:CLA:O2A	27:I:603:CLA:C1A	2.69	0.40
13:U:66:ILE:O	13:U:70:ILE:HG12	2.22	0.40
14:a:53:ARG:HG3	14:a:166:MET:HB2	2.04	0.40
15:b:389:TRP:CZ2	27:b:723:CLA:HMC2	2.56	0.40
17:d:181:HIS:CB	17:d:182:PRO:HD3	2.51	0.40
20:i:104:THR:HG22	20:i:106:ARG:H	1.86	0.40
20:i:122:ASP:OD1	20:i:122:ASP:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

323 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	$\# Z > 2$
38	BCR	f	304	-	41,41,41	0.29	0	56,56,56	0.52	0
32	PID	J	615	-	43,49,49	1.60	7 (16%)	52,76,76	3.79	20 (38%)
38	BCR	f	301	-	41,41,41	0.30	0	56,56,56	0.73	0
27	CLA	T	604	12	45,49,73	2.17	10 (22%)	54,84,113	1.62	8 (14%)
27	CLA	l	405	22	65,69,73	1.77	9 (13%)	77,108,113	1.34	8 (10%)
27	CLA	a	806	-	59,63,73	1.84	9 (15%)	70,101,113	1.39	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	609	-	51,55,73	2.00	9 (17%)	60,91,113	1.48	8 (13%)
27	CLA	b	703	-	69,73,73	1.71	9 (13%)	82,113,113	1.31	11 (13%)
27	CLA	C	202	3	49,53,73	2.04	9 (18%)	58,89,113	1.54	8 (13%)
30	DD6	r	201	-	40,45,45	0.16	0	51,67,67	0.93	4 (7%)
30	DD6	C	216	-	40,45,45	0.15	0	51,67,67	0.77	2 (3%)
27	CLA	T	601	12	51,55,73	2.04	9 (17%)	60,91,113	1.55	8 (13%)
27	CLA	a	805	-	69,73,73	1.71	9 (13%)	82,113,113	1.30	8 (9%)
27	CLA	K	605	11	64,68,73	1.76	9 (14%)	76,107,113	1.32	7 (9%)
28	KC2	B	608	2	49,53,53	1.81	4 (8%)	60,89,89	1.15	4 (6%)
27	CLA	C	205	-	59,63,73	1.92	9 (15%)	70,101,113	1.58	8 (11%)
32	PID	J	611	-	43,49,49	1.64	7 (16%)	52,76,76	4.16	21 (40%)
27	CLA	K	601	11	61,65,73	1.83	9 (14%)	72,103,113	1.41	6 (8%)
30	DD6	F	612	-	40,45,45	0.16	0	51,67,67	0.52	0
33	LMG	K	613	-	42,42,55	0.54	0	50,50,63	0.65	0
27	CLA	T	606	12	49,53,73	2.05	9 (18%)	58,89,113	1.51	6 (10%)
27	CLA	l	409	-	69,73,73	1.69	9 (13%)	82,113,113	1.30	8 (9%)
27	CLA	D	610	4	51,55,73	1.99	9 (17%)	60,91,113	1.47	9 (15%)
33	LMG	D	619	-	46,46,55	0.53	0	54,54,63	0.70	1 (1%)
38	BCR	b	732	-	41,41,41	0.31	0	56,56,56	0.75	1 (1%)
30	DD6	i	202	-	40,45,45	0.19	0	51,67,67	0.81	2 (3%)
27	CLA	D	606	-	49,53,73	2.02	9 (18%)	58,89,113	1.51	8 (13%)
29	UIX	I	612	-	43,49,49	1.44	4 (9%)	53,74,74	2.15	19 (35%)
28	KC2	K	607	-	49,53,53	1.83	4 (8%)	60,89,89	1.16	4 (6%)
33	LMG	b	733	-	55,55,55	0.48	0	63,63,63	0.56	0
38	BCR	j	203	-	41,41,41	0.31	0	56,56,56	0.57	0
27	CLA	G	607	7	49,53,73	2.03	9 (18%)	58,89,113	1.60	8 (13%)
30	DD6	I	615	-	40,45,45	0.17	0	51,67,67	0.63	1 (1%)
27	CLA	I	605	9	59,63,73	1.82	9 (15%)	70,101,113	1.35	8 (11%)
27	CLA	B	601	-	64,68,73	1.76	9 (14%)	76,107,113	1.39	8 (10%)
27	CLA	A	607	-	49,53,73	2.05	9 (18%)	58,89,113	1.52	8 (13%)
27	CLA	A	605	1	59,63,73	1.84	9 (15%)	70,101,113	1.39	8 (11%)
27	CLA	a	814	-	59,63,73	1.84	9 (15%)	70,101,113	1.38	8 (11%)
28	KC2	T	608	-	49,53,53	1.83	4 (8%)	60,89,89	1.15	4 (6%)
27	CLA	U	603	-	54,58,73	2.00	9 (16%)	64,95,113	1.55	8 (12%)
28	KC2	G	601	-	49,53,53	1.81	4 (8%)	60,89,89	1.18	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	609	2	69,73,73	1.71	9 (13%)	82,113,113	1.28	9 (10%)
30	DD6	E	615	-	40,45,45	0.18	0	51,67,67	0.60	1 (1%)
27	CLA	b	704	-	69,73,73	1.69	9 (13%)	82,113,113	1.28	8 (9%)
32	PID	B	613	-	43,49,49	1.66	7 (16%)	52,76,76	3.65	23 (44%)
27	CLA	G	603	-	54,58,73	1.92	9 (16%)	64,95,113	1.46	9 (14%)
27	CLA	b	718	-	69,73,73	1.72	9 (13%)	82,113,113	1.41	10 (12%)
30	DD6	E	613	-	40,45,45	0.17	0	51,67,67	0.78	2 (3%)
29	UIX	C	213	-	43,49,49	1.36	5 (11%)	53,74,74	1.90	14 (26%)
27	CLA	B	603	-	69,73,73	1.76	9 (13%)	82,113,113	1.39	8 (9%)
27	CLA	a	802	-	59,63,73	1.84	9 (15%)	70,101,113	1.36	8 (11%)
38	BCR	a	836	-	41,41,41	0.82	2 (4%)	56,56,56	2.19	19 (33%)
27	CLA	C	212	-	51,55,73	2.02	9 (17%)	60,91,113	1.50	8 (13%)
27	CLA	D	612	-	59,63,73	1.87	9 (15%)	70,101,113	1.40	8 (11%)
30	DD6	G	613	-	40,45,45	0.16	0	51,67,67	0.70	2 (3%)
32	PID	J	613	-	43,49,49	1.75	8 (18%)	52,76,76	4.27	21 (40%)
27	CLA	l	404	-	59,63,73	1.85	9 (15%)	70,101,113	1.42	8 (11%)
27	CLA	T	607	-	49,53,73	2.05	9 (18%)	58,89,113	1.53	8 (13%)
27	CLA	C	209	-	49,53,73	2.06	9 (18%)	58,89,113	1.54	9 (15%)
27	CLA	b	707	-	69,73,73	1.70	9 (13%)	82,113,113	1.33	8 (9%)
27	CLA	r	204	-	64,68,73	1.77	9 (14%)	76,107,113	1.31	8 (10%)
27	CLA	a	822	-	64,68,73	1.78	9 (14%)	76,107,113	1.36	9 (11%)
30	DD6	K	610	-	40,45,45	0.17	0	51,67,67	0.77	2 (3%)
27	CLA	B	607	-	64,68,73	1.77	9 (14%)	76,107,113	1.32	9 (11%)
30	DD6	b	730	-	40,45,45	0.17	0	51,67,67	0.58	1 (1%)
28	KC2	J	608	-	49,53,53	1.83	4 (8%)	60,89,89	1.15	4 (6%)
34	LHG	D	620	-	45,45,48	0.53	0	48,51,54	0.51	0
27	CLA	l	411	22	52,56,73	1.97	9 (17%)	61,92,113	1.52	8 (13%)
27	CLA	l	403	-	69,73,73	1.72	9 (13%)	82,113,113	1.25	8 (9%)
30	DD6	D	621	-	40,45,45	0.18	0	51,67,67	0.77	2 (3%)
28	KC2	J	610	-	49,53,53	1.81	4 (8%)	60,89,89	1.15	4 (6%)
30	DD6	C	214	-	40,45,45	0.19	0	51,67,67	0.68	3 (5%)
27	CLA	F	602	-	60,64,73	1.87	9 (15%)	71,102,113	1.39	9 (12%)
27	CLA	a	826	-	59,63,73	1.83	9 (15%)	70,101,113	1.37	8 (11%)
32	PID	I	614	-	43,49,49	1.70	7 (16%)	52,76,76	3.91	24 (46%)
29	UIX	E	616	-	43,49,49	1.38	5 (11%)	53,74,74	1.99	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PQN	b	729	-	34,34,34	0.37	0	43,45,45	0.65	1 (2%)
27	CLA	a	803	27	54,58,73	1.93	9 (16%)	64,95,113	1.52	6 (9%)
35	DGD	j	201	-	61,61,67	0.92	4 (6%)	75,75,81	1.44	13 (17%)
29	UIX	F	613	-	43,49,49	1.33	4 (9%)	53,74,74	2.02	15 (28%)
33	LMG	D	618	-	35,35,55	0.55	0	43,43,63	0.77	1 (2%)
27	CLA	D	608	4	59,63,73	1.85	9 (15%)	70,101,113	1.43	8 (11%)
27	CLA	B	610	-	51,55,73	1.97	9 (17%)	60,91,113	1.52	8 (13%)
27	CLA	E	602	5	59,63,73	1.85	9 (15%)	70,101,113	1.41	9 (12%)
35	DGD	K	614	-	48,48,67	0.99	4 (8%)	62,62,81	1.42	10 (16%)
27	CLA	l	410	-	52,56,73	2.03	9 (17%)	61,92,113	1.54	8 (13%)
27	CLA	b	701	-	69,73,73	1.70	9 (13%)	82,113,113	1.27	8 (9%)
30	DD6	D	614	-	40,45,45	0.15	0	51,67,67	0.63	2 (3%)
30	DD6	J	612	-	40,45,45	0.18	0	51,67,67	0.59	1 (1%)
27	CLA	I	611	-	46,50,73	2.18	9 (19%)	53,85,113	1.69	9 (16%)
27	CLA	K	602	-	59,63,73	1.87	9 (15%)	70,101,113	1.39	8 (11%)
27	CLA	F	605	6	49,53,73	2.03	9 (18%)	58,89,113	1.56	9 (15%)
32	PID	J	614	-	43,49,49	1.63	6 (13%)	52,76,76	3.49	18 (34%)
28	KC2	A	608	-	49,53,53	1.81	4 (8%)	60,89,89	1.19	5 (8%)
27	CLA	C	203	3	69,73,73	1.71	9 (13%)	82,113,113	1.35	8 (9%)
27	CLA	E	605	5	49,53,73	2.08	9 (18%)	58,89,113	1.58	9 (15%)
27	CLA	F	601	6	64,68,73	1.79	9 (14%)	76,107,113	1.35	7 (9%)
27	CLA	H	310	-	49,53,73	2.10	9 (18%)	58,89,113	1.61	8 (13%)
30	DD6	H	316	-	40,45,45	0.20	0	51,67,67	0.73	2 (3%)
27	CLA	I	616	-	69,73,73	1.73	9 (13%)	82,113,113	1.25	9 (10%)
27	CLA	j	202	27	60,64,73	1.86	9 (15%)	71,102,113	1.32	8 (11%)
27	CLA	f	302	-	52,56,73	1.96	9 (17%)	61,92,113	1.47	9 (14%)
34	LHG	F	618	-	36,36,48	0.58	0	39,42,54	0.57	0
27	CLA	K	608	-	49,53,73	2.11	9 (18%)	58,89,113	1.52	9 (15%)
27	CLA	a	801	-	69,73,73	1.67	8 (11%)	82,113,113	1.20	9 (10%)
28	KC2	B	602	-	49,53,53	1.81	4 (8%)	60,89,89	1.11	4 (6%)
27	CLA	T	609	-	45,49,73	2.22	10 (22%)	54,84,113	1.66	8 (14%)
27	CLA	J	601	-	49,53,73	2.07	9 (18%)	58,89,113	1.60	6 (10%)
27	CLA	a	821	-	69,73,73	1.69	9 (13%)	82,113,113	1.28	8 (9%)
27	CLA	H	303	8	64,68,73	1.74	9 (14%)	76,107,113	1.35	10 (13%)
39	SF4	a	838	14	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	C	211	-	51,55,73	2.01	9 (17%)	60,91,113	1.45	8 (13%)
27	CLA	D	604	-	59,63,73	1.85	9 (15%)	70,101,113	1.43	8 (11%)
35	DGD	l	416	-	56,56,67	0.92	2 (3%)	70,70,81	1.39	8 (11%)
27	CLA	b	714	-	52,56,73	2.01	9 (17%)	61,92,113	1.59	7 (11%)
27	CLA	b	705	-	69,73,73	1.73	9 (13%)	82,113,113	1.38	7 (8%)
30	DD6	E	617	-	40,45,45	0.16	0	51,67,67	0.80	2 (3%)
27	CLA	J	607	-	46,50,73	2.12	9 (19%)	53,85,113	1.59	8 (15%)
27	CLA	K	603	-	49,53,73	2.05	9 (18%)	58,89,113	1.57	7 (12%)
30	DD6	A	615	-	40,45,45	0.17	0	51,67,67	0.72	1 (1%)
30	DD6	F	611	-	40,45,45	0.17	0	51,67,67	0.82	3 (5%)
27	CLA	a	817	-	59,63,73	1.86	9 (15%)	70,101,113	1.41	9 (12%)
27	CLA	G	608	-	64,68,73	1.82	9 (14%)	76,107,113	1.41	7 (9%)
27	CLA	a	820	-	69,73,73	1.74	9 (13%)	82,113,113	1.27	8 (9%)
27	CLA	b	723	-	69,73,73	1.71	9 (13%)	82,113,113	1.33	7 (8%)
30	DD6	I	613	-	40,45,45	0.18	0	51,67,67	0.78	2 (3%)
27	CLA	b	726	-	64,68,73	1.77	9 (14%)	76,107,113	1.32	9 (11%)
29	UIX	A	616	-	43,49,49	1.40	5 (11%)	53,74,74	1.98	18 (33%)
27	CLA	F	608	6	49,53,73	2.05	9 (18%)	58,89,113	1.53	8 (13%)
27	CLA	C	208	-	51,55,73	2.01	9 (17%)	60,91,113	1.49	8 (13%)
30	DD6	G	616	-	40,45,45	0.15	0	51,67,67	0.47	0
29	UIX	B	611	-	43,49,49	1.45	5 (11%)	53,74,74	2.02	21 (39%)
28	KC2	U	604	13	49,53,53	1.81	4 (8%)	60,89,89	1.12	4 (6%)
27	CLA	T	602	-	49,53,73	2.07	9 (18%)	58,89,113	1.52	8 (13%)
27	CLA	l	408	-	51,55,73	2.02	9 (17%)	60,91,113	1.55	7 (11%)
29	UIX	A	613	-	43,49,49	1.36	4 (9%)	53,74,74	1.88	16 (30%)
27	CLA	a	827	-	69,73,73	1.75	9 (13%)	82,113,113	1.42	8 (9%)
27	CLA	A	602	1	64,68,73	1.79	9 (14%)	76,107,113	1.37	9 (11%)
27	CLA	I	603	-	69,73,73	1.70	9 (13%)	82,113,113	1.34	8 (9%)
27	CLA	a	829	27	69,73,73	1.72	9 (13%)	82,113,113	1.29	8 (9%)
27	CLA	U	601	-	47,51,73	2.15	9 (19%)	55,86,113	1.72	7 (12%)
27	CLA	b	720	-	52,56,73	1.99	9 (17%)	61,92,113	1.48	8 (13%)
27	CLA	U	605	13	64,68,73	1.79	9 (14%)	76,107,113	1.29	7 (9%)
27	CLA	F	607	6	49,53,73	2.03	9 (18%)	58,89,113	1.57	7 (12%)
27	CLA	J	609	-	45,49,73	2.22	10 (22%)	54,84,113	1.69	8 (14%)
27	CLA	H	309	-	69,73,73	1.72	9 (13%)	82,113,113	1.31	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	716	-	69,73,73	1.73	9 (13%)	82,113,113	1.28	8 (9%)
27	CLA	a	808	14	59,63,73	1.90	9 (15%)	70,101,113	1.43	10 (14%)
30	DD6	K	612	-	40,45,45	0.17	0	51,67,67	0.72	4 (7%)
28	KC2	F	609	6	49,53,53	1.82	4 (8%)	60,89,89	1.13	4 (6%)
28	KC2	J	606	-	49,53,53	1.82	4 (8%)	60,89,89	1.11	4 (6%)
27	CLA	a	804	-	69,73,73	1.70	9 (13%)	82,113,113	1.37	11 (13%)
30	DD6	G	612	-	40,45,45	0.18	0	51,67,67	0.79	2 (3%)
30	DD6	G	614	-	40,45,45	0.16	0	51,67,67	0.56	1 (1%)
27	CLA	G	605	-	64,68,73	1.82	9 (14%)	76,107,113	1.44	9 (11%)
27	CLA	I	607	-	65,69,73	1.78	9 (13%)	77,108,113	1.33	8 (10%)
27	CLA	D	601	4	49,53,73	2.03	9 (18%)	58,89,113	1.50	8 (13%)
27	CLA	F	603	-	56,60,73	1.90	9 (16%)	65,97,113	1.44	8 (12%)
27	CLA	b	719	-	69,73,73	1.74	9 (13%)	82,113,113	1.27	8 (9%)
27	CLA	H	307	-	49,53,73	2.06	9 (18%)	58,89,113	1.50	8 (13%)
28	KC2	C	210	-	49,53,53	1.82	4 (8%)	60,89,89	1.13	4 (6%)
27	CLA	J	605	10	64,68,73	1.78	9 (14%)	76,107,113	1.28	7 (9%)
36	LMU	T	613	-	36,36,36	0.42	0	47,47,47	0.96	2 (4%)
35	DGD	f	305	-	53,53,67	0.97	3 (5%)	67,67,81	1.50	11 (16%)
30	DD6	A	614	-	40,45,45	0.16	0	51,67,67	0.72	3 (5%)
38	BCR	a	833	-	41,41,41	0.29	0	56,56,56	0.61	0
29	UIX	D	616	-	43,49,49	1.36	4 (9%)	53,74,74	2.08	17 (32%)
39	SF4	c	202	-	0,12,12	-	-	-	-	-
38	BCR	i	201	-	41,41,41	0.31	0	56,56,56	0.95	1 (1%)
30	DD6	H	301	-	40,45,45	0.19	0	51,67,67	0.72	2 (3%)
27	CLA	K	604	-	61,65,73	1.81	9 (14%)	72,103,113	1.35	7 (9%)
27	CLA	H	306	-	49,53,73	2.01	9 (18%)	58,89,113	1.51	8 (13%)
28	KC2	E	601	27	49,53,53	1.81	4 (8%)	60,89,89	1.16	4 (6%)
29	UIX	H	314	-	43,49,49	1.37	4 (9%)	53,74,74	1.96	20 (37%)
27	CLA	b	727	-	69,73,73	1.72	9 (13%)	82,113,113	1.35	9 (10%)
27	CLA	b	711	-	64,68,73	1.79	9 (14%)	76,107,113	1.36	8 (10%)
28	KC2	J	604	10	49,53,53	1.80	4 (8%)	60,89,89	1.14	4 (6%)
32	PID	F	614	-	43,49,49	1.69	6 (13%)	52,76,76	3.95	19 (36%)
27	CLA	H	305	-	64,68,73	1.80	9 (14%)	76,107,113	1.43	9 (11%)
27	CLA	B	604	2	51,55,73	2.06	9 (17%)	60,91,113	1.54	9 (15%)
27	CLA	E	609	28	49,53,73	2.05	9 (18%)	58,89,113	1.49	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	SF4	c	201	16	0,12,12	-	-	-		
27	CLA	r	203	-	52,56,73	2.02	9 (17%)	61,92,113	1.51	6 (9%)
30	DD6	H	318	28	40,45,45	0.15	0	51,67,67	0.56	2 (3%)
27	CLA	b	715	-	69,73,73	1.72	9 (13%)	82,113,113	1.40	10 (12%)
27	CLA	E	608	5	64,68,73	1.79	9 (14%)	76,107,113	1.36	7 (9%)
34	LHG	r	202	-	45,45,48	0.53	0	48,51,54	0.51	0
38	BCR	b	731	-	41,41,41	0.30	0	56,56,56	0.72	1 (1%)
27	CLA	b	710	-	59,63,73	1.89	9 (15%)	70,101,113	1.44	9 (12%)
27	CLA	a	812	-	54,58,73	2.01	9 (16%)	64,95,113	1.58	10 (15%)
27	CLA	I	610	-	59,63,73	1.88	9 (15%)	70,101,113	1.51	7 (10%)
27	CLA	a	811	-	52,56,73	2.01	9 (17%)	61,92,113	1.49	8 (13%)
27	CLA	H	313	-	64,68,73	1.80	9 (14%)	76,107,113	1.35	9 (11%)
27	CLA	I	606	9	59,63,73	1.86	9 (15%)	70,101,113	1.40	8 (11%)
27	CLA	l	406	-	69,73,73	1.70	9 (13%)	82,113,113	1.26	9 (10%)
27	CLA	C	206	-	51,55,73	1.96	9 (17%)	60,91,113	1.47	8 (13%)
27	CLA	G	610	7	51,55,73	1.99	9 (17%)	60,91,113	1.48	8 (13%)
30	DD6	B	612	-	40,45,45	0.17	0	51,67,67	0.61	2 (3%)
27	CLA	K	606	-	45,49,73	2.25	10 (22%)	54,84,113	1.72	8 (14%)
29	UIX	T	612	-	43,49,49	1.36	5 (11%)	53,74,74	2.03	21 (39%)
27	CLA	U	606	-	49,53,73	2.06	9 (18%)	58,89,113	1.53	8 (13%)
27	CLA	F	617	-	64,68,73	1.78	9 (14%)	76,107,113	1.34	8 (10%)
32	PID	K	611	-	43,49,49	1.76	6 (13%)	52,76,76	3.82	21 (40%)
27	CLA	F	610	6	51,55,73	2.03	9 (17%)	60,91,113	1.52	8 (13%)
27	CLA	b	702	-	69,73,73	1.66	9 (13%)	82,113,113	1.20	10 (12%)
29	UIX	J	616	-	43,49,49	1.36	4 (9%)	53,74,74	1.86	14 (26%)
27	CLA	a	831	-	59,63,73	1.85	9 (15%)	70,101,113	1.41	9 (12%)
30	DD6	E	614	-	40,45,45	0.16	0	51,67,67	0.51	0
31	SQD	H	320	-	44,46,54	1.19	3 (6%)	54,57,65	1.06	3 (5%)
27	CLA	A	610	-	59,63,73	1.84	9 (15%)	70,101,113	1.39	8 (11%)
27	CLA	T	605	12	49,53,73	2.00	9 (18%)	58,89,113	1.46	8 (13%)
33	LMG	C	217	-	34,34,55	0.58	0	42,42,63	0.71	1 (2%)
27	CLA	H	319	-	69,73,73	1.70	9 (13%)	82,113,113	1.29	8 (9%)
27	CLA	l	412	22	69,73,73	1.71	9 (13%)	82,113,113	1.32	9 (10%)
27	CLA	G	609	7	59,63,73	1.86	9 (15%)	70,101,113	1.39	10 (14%)
27	CLA	D	605	4	51,55,73	1.99	9 (17%)	60,91,113	1.44	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LHG	a	835	-	47,47,48	0.52	0	50,53,54	0.53	0
32	PID	F	615	-	43,49,49	1.63	7 (16%)	52,76,76	3.66	18 (34%)
27	CLA	b	713	-	69,73,73	1.71	9 (13%)	82,113,113	1.38	10 (12%)
28	KC2	H	302	30	49,53,53	1.81	4 (8%)	60,89,89	1.15	4 (6%)
27	CLA	a	815	-	64,68,73	1.75	9 (14%)	76,107,113	1.34	8 (10%)
27	CLA	f	303	19	52,56,73	2.01	9 (17%)	61,92,113	1.46	8 (13%)
27	CLA	H	312	-	46,50,73	2.09	9 (19%)	53,85,113	1.60	9 (16%)
30	DD6	B	616	-	40,45,45	0.15	0	51,67,67	0.53	0
27	CLA	b	712	-	52,56,73	2.01	9 (17%)	61,92,113	1.53	9 (14%)
30	DD6	D	617	-	40,45,45	0.18	0	51,67,67	0.62	2 (3%)
37	PQN	a	832	-	34,34,34	0.37	0	43,45,45	0.73	0
27	CLA	E	603	-	51,55,73	2.02	9 (17%)	60,91,113	1.49	8 (13%)
27	CLA	a	810	-	54,58,73	1.94	9 (16%)	64,95,113	1.47	9 (14%)
28	KC2	I	604	9	49,53,53	1.81	4 (8%)	60,89,89	1.14	4 (6%)
30	DD6	r	206	-	40,45,45	0.18	0	51,67,67	0.81	3 (5%)
27	CLA	B	606	-	69,73,73	1.74	9 (13%)	82,113,113	1.35	8 (9%)
29	UIX	H	317	-	43,49,49	1.32	5 (11%)	53,74,74	1.92	15 (28%)
38	BCR	l	414	-	41,41,41	0.34	0	56,56,56	0.83	0
27	CLA	b	725	-	69,73,73	1.69	9 (13%)	82,113,113	1.29	9 (10%)
27	CLA	b	708	-	69,73,73	1.67	9 (13%)	82,113,113	1.23	8 (9%)
27	CLA	I	608	9	64,68,73	1.78	9 (14%)	76,107,113	1.30	8 (10%)
27	CLA	C	207	3	64,68,73	1.78	9 (14%)	76,107,113	1.35	9 (11%)
27	CLA	A	611	27	49,53,73	2.04	9 (18%)	58,89,113	1.54	8 (13%)
27	CLA	a	825	-	69,73,73	1.72	9 (13%)	82,113,113	1.28	8 (9%)
27	CLA	a	809	-	51,55,73	2.04	9 (17%)	60,91,113	1.60	7 (11%)
30	DD6	U	607	-	40,45,45	0.14	0	51,67,67	0.63	1 (1%)
27	CLA	D	602	-	59,63,73	1.87	9 (15%)	70,101,113	1.44	8 (11%)
31	SQD	A	618	-	26,28,54	1.42	3 (11%)	36,39,65	1.25	3 (8%)
27	CLA	E	604	-	59,63,73	1.85	9 (15%)	70,101,113	1.41	9 (12%)
31	SQD	y	301	-	44,46,54	1.23	3 (6%)	54,57,65	1.03	3 (5%)
27	CLA	a	819	-	64,68,73	1.77	9 (14%)	76,107,113	1.32	8 (10%)
27	CLA	b	724	-	69,73,73	1.71	9 (13%)	82,113,113	1.29	8 (9%)
27	CLA	b	709	15	69,73,73	1.67	9 (13%)	82,113,113	1.25	9 (10%)
27	CLA	b	706	-	69,73,73	1.71	9 (13%)	82,113,113	1.28	9 (10%)
27	CLA	H	304	-	64,68,73	1.79	9 (14%)	76,107,113	1.41	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PID	U	608	-	43,49,49	1.65	8 (18%)	52,76,76	3.74	18 (34%)
27	CLA	D	609	-	49,53,73	2.05	9 (18%)	58,89,113	1.53	8 (13%)
27	CLA	a	837	-	69,73,73	1.68	9 (13%)	82,113,113	1.30	7 (8%)
34	LHG	l	401	-	45,45,48	0.52	0	48,51,54	0.47	0
34	LHG	j	205	-	36,36,48	0.58	0	39,42,54	0.54	0
27	CLA	b	721	-	54,58,73	1.97	9 (16%)	64,95,113	1.47	7 (10%)
33	LMG	l	417	-	50,50,55	0.50	0	58,58,63	0.61	0
27	CLA	a	839	-	65,69,73	1.76	9 (13%)	77,108,113	1.30	8 (10%)
27	CLA	l	407	-	52,56,73	2.01	9 (17%)	61,92,113	1.48	8 (13%)
27	CLA	A	603	-	59,63,73	1.85	9 (15%)	70,101,113	1.40	9 (12%)
27	CLA	a	830	-	69,73,73	1.71	9 (13%)	82,113,113	1.29	7 (8%)
27	CLA	D	611	-	64,68,73	1.78	9 (14%)	76,107,113	1.32	9 (11%)
30	DD6	T	611	-	40,45,45	0.18	0	51,67,67	0.65	2 (3%)
27	CLA	B	605	2	49,53,73	2.01	9 (18%)	58,89,113	1.52	9 (15%)
28	KC2	H	311	-	49,53,53	1.82	4 (8%)	60,89,89	1.15	4 (6%)
27	CLA	H	308	8	59,63,73	1.82	9 (15%)	70,101,113	1.36	8 (11%)
27	CLA	a	813	-	52,56,73	2.00	9 (17%)	61,92,113	1.49	8 (13%)
27	CLA	G	606	7	69,73,73	1.74	9 (13%)	82,113,113	1.36	9 (10%)
30	DD6	H	315	-	40,45,45	0.17	0	51,67,67	0.61	1 (1%)
30	DD6	B	614	-	40,45,45	0.40	0	51,67,67	0.77	1 (1%)
27	CLA	F	606	6	69,73,73	1.70	9 (13%)	82,113,113	1.29	8 (9%)
27	CLA	a	828	-	52,56,73	2.06	9 (17%)	61,92,113	1.59	7 (11%)
28	KC2	E	610	5	49,53,53	1.82	4 (8%)	60,89,89	1.13	4 (6%)
27	CLA	b	728	-	69,73,73	1.69	9 (13%)	82,113,113	1.27	9 (10%)
27	CLA	I	601	9	69,73,73	1.71	9 (13%)	82,113,113	1.30	7 (8%)
27	CLA	a	807	-	69,73,73	1.71	9 (13%)	82,113,113	1.33	10 (12%)
27	CLA	E	606	-	64,68,73	1.78	9 (14%)	76,107,113	1.36	8 (10%)
34	LHG	G	617	-	33,33,48	0.60	0	36,39,54	0.55	0
27	CLA	I	602	-	59,63,73	1.84	9 (15%)	70,101,113	1.34	8 (11%)
29	UIX	j	204	-	43,49,49	1.41	5 (11%)	53,74,74	2.02	18 (33%)
38	BCR	l	415	-	41,41,41	0.31	0	56,56,56	0.56	0
27	CLA	E	611	5	64,68,73	1.80	9 (14%)	76,107,113	1.39	8 (10%)
30	DD6	A	617	-	40,45,45	0.18	0	51,67,67	0.53	0
27	CLA	E	612	-	49,53,73	2.05	9 (18%)	58,89,113	1.50	8 (13%)
27	CLA	G	602	7	59,63,73	1.85	9 (15%)	70,101,113	1.39	7 (10%)
27	CLA	J	603	-	64,68,73	1.80	9 (14%)	76,107,113	1.35	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	a	824	-	69,73,73	1.72	9 (13%)	82,113,113	1.31	9 (10%)
30	DD6	D	613	-	40,45,45	0.42	0	51,67,67	0.72	2 (3%)
30	DD6	D	615	-	40,45,45	0.16	0	51,67,67	0.58	1 (1%)
29	UIX	G	615	-	43,49,49	1.38	4 (9%)	53,74,74	1.96	15 (28%)
27	CLA	F	604	-	49,53,73	1.97	9 (18%)	58,89,113	1.50	9 (15%)
30	DD6	K	609	-	40,45,45	0.17	0	51,67,67	0.56	1 (1%)
27	CLA	A	604	-	49,53,73	2.03	9 (18%)	58,89,113	1.52	8 (13%)
27	CLA	F	619	-	59,63,73	1.83	9 (15%)	70,101,113	1.38	8 (11%)
27	CLA	C	201	-	46,50,73	2.13	9 (19%)	53,85,113	1.62	10 (18%)
28	KC2	J	602	10	49,53,53	1.83	4 (8%)	60,89,89	1.13	4 (6%)
27	CLA	G	604	-	51,55,73	2.03	9 (17%)	60,91,113	1.56	6 (10%)
27	CLA	A	601	1	46,50,73	2.09	9 (19%)	53,85,113	1.59	9 (16%)
28	KC2	U	602	-	49,53,53	1.83	4 (8%)	60,89,89	1.14	4 (6%)
29	UIX	C	215	-	43,49,49	1.36	4 (9%)	53,74,74	2.14	22 (41%)
38	BCR	a	834	-	41,41,41	0.27	0	56,56,56	0.53	0
27	CLA	a	823	-	69,73,73	1.74	9 (13%)	82,113,113	1.37	8 (9%)
30	DD6	T	610	-	40,45,45	0.16	0	51,67,67	0.69	2 (3%)
27	CLA	C	204	-	69,73,73	1.73	9 (13%)	82,113,113	1.33	9 (10%)
27	CLA	l	402	-	64,68,73	1.78	9 (14%)	76,107,113	1.38	9 (11%)
38	BCR	m	201	-	41,41,41	0.30	0	56,56,56	0.69	0
27	CLA	D	607	4	64,68,73	1.78	9 (14%)	76,107,113	1.33	7 (9%)
27	CLA	I	609	9	49,53,73	2.05	9 (18%)	58,89,113	1.57	9 (15%)
27	CLA	b	722	-	52,56,73	1.98	9 (17%)	61,92,113	1.51	8 (13%)
29	UIX	B	615	-	43,49,49	1.38	5 (11%)	53,74,74	1.92	17 (32%)
27	CLA	T	603	-	49,53,73	2.03	9 (18%)	58,89,113	1.49	7 (12%)
27	CLA	A	606	1	51,55,73	1.99	9 (17%)	60,91,113	1.51	7 (11%)
27	CLA	D	603	-	59,63,73	1.88	9 (15%)	70,101,113	1.44	8 (11%)
30	DD6	r	205	-	40,45,45	0.19	0	51,67,67	0.79	2 (3%)
33	LMG	F	616	-	46,46,55	0.52	0	54,54,63	0.69	0
38	BCR	l	413	-	41,41,41	0.32	0	56,56,56	0.53	0
27	CLA	G	611	-	49,53,73	2.05	9 (18%)	58,89,113	1.50	8 (13%)
27	CLA	A	612	1	51,55,73	2.06	9 (17%)	60,91,113	1.71	10 (16%)
27	CLA	E	607	5	69,73,73	1.69	9 (13%)	82,113,113	1.22	8 (9%)
27	CLA	a	816	-	64,68,73	1.81	9 (14%)	76,107,113	1.36	8 (10%)
27	CLA	b	717	-	69,73,73	1.67	9 (13%)	82,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	a	818	-	59,63,73	1.85	9 (15%)	70,101,113	1.37	8 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	BCR	f	304	-	-	3/29/63/63	0/2/2/2
32	PID	J	615	-	-	6/24/93/93	0/4/4/4
38	BCR	f	301	-	-	9/29/63/63	0/2/2/2
27	CLA	T	604	12	1/1/10/20	2/10/86/115	-
27	CLA	l	405	22	1/1/14/20	3/35/111/115	-
27	CLA	a	806	-	1/1/13/20	3/27/103/115	-
27	CLA	A	609	-	1/1/11/20	1/18/94/115	-
27	CLA	b	703	-	1/1/15/20	5/39/115/115	-
27	CLA	C	202	3	1/1/11/20	2/15/91/115	-
30	DD6	r	201	-	-	1/26/80/80	0/3/3/3
30	DD6	C	216	-	-	1/26/80/80	0/3/3/3
27	CLA	T	601	12	1/1/11/20	2/18/94/115	-
27	CLA	a	805	-	1/1/15/20	8/39/115/115	-
27	CLA	K	605	11	1/1/14/20	8/33/109/115	-
28	KC2	B	608	2	-	4/15/71/71	-
27	CLA	C	205	-	1/1/13/20	6/27/103/115	-
32	PID	J	611	-	-	4/24/93/93	0/4/4/4
27	CLA	K	601	11	1/1/13/20	3/30/106/115	-
30	DD6	F	612	-	-	0/26/80/80	0/3/3/3
33	LMG	K	613	-	-	11/37/57/70	0/1/1/1
27	CLA	T	606	12	1/1/11/20	1/15/91/115	-
27	CLA	l	409	-	1/1/15/20	12/39/115/115	-
27	CLA	D	610	4	1/1/11/20	4/18/94/115	-
33	LMG	D	619	-	-	21/41/61/70	0/1/1/1
38	BCR	b	732	-	-	0/29/63/63	0/2/2/2
30	DD6	i	202	-	-	3/26/80/80	0/3/3/3
27	CLA	D	606	-	1/1/11/20	2/15/91/115	-
29	UIX	I	612	-	-	2/31/87/87	1/3/3/3
28	KC2	K	607	-	-	4/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	b	733	-	-	26/50/70/70	0/1/1/1
38	BCR	j	203	-	-	10/29/63/63	0/2/2/2
27	CLA	G	607	7	1/1/11/20	7/15/91/115	-
30	DD6	I	615	-	-	0/26/80/80	0/3/3/3
27	CLA	I	605	9	1/1/13/20	5/27/103/115	-
27	CLA	B	601	-	1/1/14/20	6/33/109/115	-
27	CLA	A	607	-	1/1/11/20	2/15/91/115	-
27	CLA	A	605	1	1/1/13/20	3/27/103/115	-
27	CLA	a	814	-	1/1/13/20	4/27/103/115	-
28	KC2	T	608	-	-	5/15/71/71	-
27	CLA	U	603	-	1/1/12/20	8/21/97/115	-
28	KC2	G	601	-	-	9/15/71/71	-
27	CLA	B	609	2	1/1/15/20	6/39/115/115	-
30	DD6	E	615	-	-	2/26/80/80	0/3/3/3
27	CLA	b	704	-	1/1/15/20	10/39/115/115	-
32	PID	B	613	-	-	3/24/93/93	0/4/4/4
27	CLA	G	603	-	1/1/12/20	4/21/97/115	-
27	CLA	b	718	-	1/1/15/20	7/39/115/115	-
30	DD6	E	613	-	-	1/26/80/80	0/3/3/3
29	UIX	C	213	-	-	2/31/87/87	0/3/3/3
27	CLA	B	603	-	1/1/15/20	8/39/115/115	-
27	CLA	a	802	-	1/1/13/20	1/27/103/115	-
38	BCR	a	836	-	-	14/29/63/63	0/2/2/2
27	CLA	C	212	-	1/1/11/20	2/18/94/115	-
27	CLA	D	612	-	1/1/13/20	6/27/103/115	-
30	DD6	G	613	-	-	2/26/80/80	0/3/3/3
32	PID	J	613	-	-	3/24/93/93	0/4/4/4
27	CLA	l	404	-	1/1/13/20	3/27/103/115	-
27	CLA	T	607	-	1/1/11/20	5/15/91/115	-
27	CLA	C	209	-	1/1/11/20	0/15/91/115	-
27	CLA	b	707	-	1/1/15/20	5/39/115/115	-
27	CLA	r	204	-	1/1/14/20	11/33/109/115	-
27	CLA	a	822	-	1/1/14/20	8/33/109/115	-
30	DD6	K	610	-	-	3/26/80/80	0/3/3/3
27	CLA	B	607	-	1/1/14/20	5/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DD6	b	730	-	-	0/26/80/80	0/3/3/3
28	KC2	J	608	-	-	4/15/71/71	-
34	LHG	D	620	-	-	22/50/50/53	-
27	CLA	l	411	22	1/1/11/20	3/19/95/115	-
27	CLA	l	403	-	1/1/15/20	9/39/115/115	-
30	DD6	D	621	-	-	5/26/80/80	0/3/3/3
28	KC2	J	610	-	-	8/15/71/71	-
30	DD6	C	214	-	-	1/26/80/80	0/3/3/3
27	CLA	F	602	-	1/1/13/20	5/29/105/115	-
27	CLA	a	826	-	1/1/13/20	4/27/103/115	-
32	PID	I	614	-	-	5/24/93/93	0/4/4/4
29	UIX	E	616	-	-	3/31/87/87	0/3/3/3
37	PQN	b	729	-	-	10/23/43/43	0/2/2/2
27	CLA	a	803	27	1/1/12/20	2/21/97/115	-
35	DGD	j	201	-	-	16/49/89/95	0/2/2/2
29	UIX	F	613	-	-	4/31/87/87	0/3/3/3
33	LMG	D	618	-	-	17/30/50/70	0/1/1/1
27	CLA	D	608	4	1/1/13/20	0/27/103/115	-
27	CLA	B	610	-	1/1/11/20	5/18/94/115	-
27	CLA	E	602	5	1/1/13/20	0/27/103/115	-
35	DGD	K	614	-	-	19/36/76/95	0/2/2/2
27	CLA	l	410	-	1/1/11/20	5/19/95/115	-
27	CLA	b	701	-	1/1/15/20	7/39/115/115	-
30	DD6	D	614	-	-	0/26/80/80	0/3/3/3
30	DD6	J	612	-	-	1/26/80/80	0/3/3/3
27	CLA	I	611	-	1/1/10/20	4/12/88/115	-
27	CLA	K	602	-	1/1/13/20	8/27/103/115	-
27	CLA	F	605	6	1/1/11/20	5/15/91/115	-
32	PID	J	614	-	-	0/24/93/93	0/4/4/4
28	KC2	A	608	-	-	7/15/71/71	-
27	CLA	C	203	3	1/1/15/20	2/39/115/115	-
27	CLA	E	605	5	1/1/11/20	6/15/91/115	-
27	CLA	F	601	6	1/1/14/20	2/33/109/115	-
27	CLA	H	310	-	1/1/11/20	4/15/91/115	-
30	DD6	H	316	-	-	1/26/80/80	0/3/3/3
27	CLA	I	616	-	1/1/15/20	1/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	j	202	27	1/1/13/20	3/29/105/115	-
27	CLA	f	302	-	1/1/11/20	1/19/95/115	-
34	LHG	F	618	-	-	21/41/41/53	-
27	CLA	K	608	-	1/1/11/20	3/15/91/115	-
27	CLA	a	801	-	1/1/15/20	3/39/115/115	-
28	KC2	B	602	-	-	3/15/71/71	-
27	CLA	T	609	-	1/1/10/20	0/10/86/115	-
27	CLA	J	601	-	1/1/11/20	4/15/91/115	-
27	CLA	a	821	-	1/1/15/20	9/39/115/115	-
27	CLA	H	303	8	1/1/14/20	2/33/109/115	-
39	SF4	a	838	14	-	-	0/6/5/5
27	CLA	C	211	-	1/1/11/20	0/18/94/115	-
27	CLA	D	604	-	1/1/13/20	7/27/103/115	-
35	DGD	l	416	-	-	17/44/84/95	0/2/2/2
27	CLA	b	714	-	1/1/11/20	5/19/95/115	-
27	CLA	b	705	-	1/1/15/20	9/39/115/115	-
30	DD6	E	617	-	-	2/26/80/80	0/3/3/3
27	CLA	J	607	-	1/1/10/20	2/12/88/115	-
27	CLA	K	603	-	1/1/11/20	5/15/91/115	-
30	DD6	A	615	-	-	2/26/80/80	0/3/3/3
30	DD6	F	611	-	-	3/26/80/80	0/3/3/3
27	CLA	a	817	-	1/1/13/20	2/27/103/115	-
27	CLA	G	608	-	1/1/14/20	5/33/109/115	-
27	CLA	a	820	-	1/1/15/20	8/39/115/115	-
27	CLA	b	723	-	1/1/15/20	4/39/115/115	-
30	DD6	I	613	-	-	1/26/80/80	0/3/3/3
27	CLA	b	726	-	1/1/14/20	5/33/109/115	-
29	UIX	A	616	-	-	6/31/87/87	0/3/3/3
27	CLA	F	608	6	1/1/11/20	3/15/91/115	-
27	CLA	C	208	-	1/1/11/20	0/18/94/115	-
30	DD6	G	616	-	-	1/26/80/80	0/3/3/3
29	UIX	B	611	-	-	2/31/87/87	0/3/3/3
28	KC2	U	604	13	-	8/15/71/71	-
27	CLA	T	602	-	1/1/11/20	4/15/91/115	-
27	CLA	l	408	-	1/1/11/20	3/18/94/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	UIX	A	613	-	-	2/31/87/87	0/3/3/3
27	CLA	a	827	-	1/1/15/20	14/39/115/115	-
27	CLA	A	602	1	1/1/14/20	0/33/109/115	-
27	CLA	I	603	-	1/1/15/20	9/39/115/115	-
27	CLA	a	829	27	1/1/15/20	14/39/115/115	-
27	CLA	U	601	-	1/1/10/20	1/13/89/115	-
27	CLA	b	720	-	1/1/11/20	4/19/95/115	-
27	CLA	U	605	13	1/1/14/20	6/33/109/115	-
27	CLA	F	607	6	1/1/11/20	7/15/91/115	-
27	CLA	J	609	-	1/1/10/20	4/10/86/115	-
27	CLA	H	309	-	1/1/15/20	5/39/115/115	-
27	CLA	b	716	-	1/1/15/20	4/39/115/115	-
27	CLA	a	808	14	1/1/13/20	4/27/103/115	-
30	DD6	K	612	-	-	5/26/80/80	0/3/3/3
28	KC2	F	609	6	-	6/15/71/71	-
28	KC2	J	606	-	-	6/15/71/71	-
27	CLA	a	804	-	1/1/15/20	11/39/115/115	-
30	DD6	G	612	-	-	0/26/80/80	0/3/3/3
30	DD6	G	614	-	-	2/26/80/80	0/3/3/3
27	CLA	G	605	-	1/1/14/20	0/33/109/115	-
27	CLA	I	607	-	1/1/14/20	3/35/111/115	-
27	CLA	D	601	4	1/1/11/20	3/15/91/115	-
27	CLA	F	603	-	1/1/12/20	4/24/100/115	-
27	CLA	b	719	-	1/1/15/20	6/39/115/115	-
27	CLA	H	307	-	1/1/11/20	5/15/91/115	-
28	KC2	C	210	-	-	7/15/71/71	-
27	CLA	J	605	10	1/1/14/20	4/33/109/115	-
36	LMU	T	613	-	-	5/21/61/61	0/2/2/2
35	DGD	f	305	-	-	17/41/81/95	0/2/2/2
30	DD6	A	614	-	-	1/26/80/80	0/3/3/3
38	BCR	a	833	-	-	7/29/63/63	0/2/2/2
29	UIX	D	616	-	-	5/31/87/87	0/3/3/3
39	SF4	c	202	-	-	-	0/6/5/5
38	BCR	i	201	-	-	6/29/63/63	0/2/2/2
30	DD6	H	301	-	-	3/26/80/80	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	K	604	-	1/1/13/20	5/30/106/115	-
27	CLA	H	306	-	1/1/11/20	5/15/91/115	-
28	KC2	E	601	27	-	10/15/71/71	-
29	UIX	H	314	-	-	2/31/87/87	0/3/3/3
27	CLA	b	727	-	1/1/15/20	10/39/115/115	-
27	CLA	b	711	-	1/1/14/20	4/33/109/115	-
28	KC2	J	604	10	-	4/15/71/71	-
32	PID	F	614	-	-	5/24/93/93	0/4/4/4
27	CLA	H	305	-	1/1/14/20	11/33/109/115	-
27	CLA	B	604	2	1/1/11/20	2/18/94/115	-
27	CLA	E	609	28	1/1/11/20	4/15/91/115	-
39	SF4	c	201	16	-	-	0/6/5/5
27	CLA	r	203	-	1/1/11/20	6/19/95/115	-
30	DD6	H	318	28	-	0/26/80/80	0/3/3/3
27	CLA	b	715	-	1/1/15/20	6/39/115/115	-
27	CLA	E	608	5	1/1/14/20	5/33/109/115	-
34	LHG	r	202	-	-	20/50/50/53	-
38	BCR	b	731	-	-	7/29/63/63	0/2/2/2
27	CLA	b	710	-	1/1/13/20	3/27/103/115	-
27	CLA	a	812	-	1/1/12/20	3/21/97/115	-
27	CLA	I	610	-	1/1/13/20	3/27/103/115	-
27	CLA	a	811	-	1/1/11/20	2/19/95/115	-
27	CLA	H	313	-	1/1/14/20	2/33/109/115	-
27	CLA	I	606	9	1/1/13/20	2/27/103/115	-
27	CLA	l	406	-	1/1/15/20	3/39/115/115	-
27	CLA	C	206	-	1/1/11/20	2/18/94/115	-
27	CLA	G	610	7	1/1/11/20	6/18/94/115	-
30	DD6	B	612	-	-	1/26/80/80	0/3/3/3
27	CLA	K	606	-	1/1/10/20	2/10/86/115	-
29	UIX	T	612	-	-	5/31/87/87	0/3/3/3
27	CLA	U	606	-	1/1/11/20	7/15/91/115	-
27	CLA	F	617	-	1/1/14/20	10/33/109/115	-
32	PID	K	611	-	-	6/24/93/93	1/4/4/4
27	CLA	F	610	6	1/1/11/20	5/18/94/115	-
27	CLA	b	702	-	1/1/15/20	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	UIX	J	616	-	-	3/31/87/87	0/3/3/3
27	CLA	a	831	-	1/1/13/20	2/27/103/115	-
30	DD6	E	614	-	-	0/26/80/80	0/3/3/3
31	SQD	H	320	-	-	14/41/61/69	0/1/1/1
27	CLA	A	610	-	1/1/13/20	4/27/103/115	-
27	CLA	T	605	12	1/1/11/20	0/15/91/115	-
33	LMG	C	217	-	-	13/29/49/70	0/1/1/1
27	CLA	H	319	-	1/1/15/20	8/39/115/115	-
27	CLA	l	412	22	1/1/15/20	12/39/115/115	-
27	CLA	G	609	7	1/1/13/20	4/27/103/115	-
27	CLA	D	605	4	1/1/11/20	2/18/94/115	-
34	LHG	a	835	-	-	20/52/52/53	-
32	PID	F	615	-	-	4/24/93/93	0/4/4/4
27	CLA	b	713	-	1/1/15/20	6/39/115/115	-
28	KC2	H	302	30	-	8/15/71/71	-
27	CLA	a	815	-	1/1/14/20	5/33/109/115	-
27	CLA	f	303	19	1/1/11/20	0/19/95/115	-
27	CLA	H	312	-	1/1/10/20	4/12/88/115	-
30	DD6	B	616	-	-	3/26/80/80	0/3/3/3
27	CLA	b	712	-	1/1/11/20	3/19/95/115	-
30	DD6	D	617	-	-	0/26/80/80	0/3/3/3
37	PQN	a	832	-	-	6/23/43/43	0/2/2/2
27	CLA	E	603	-	1/1/11/20	0/18/94/115	-
27	CLA	a	810	-	1/1/12/20	2/21/97/115	-
28	KC2	I	604	9	-	3/15/71/71	-
30	DD6	r	206	-	-	3/26/80/80	0/3/3/3
27	CLA	B	606	-	1/1/15/20	6/39/115/115	-
29	UIX	H	317	-	-	4/31/87/87	0/3/3/3
38	BCR	l	414	-	-	5/29/63/63	0/2/2/2
27	CLA	b	725	-	1/1/15/20	6/39/115/115	-
27	CLA	b	708	-	1/1/15/20	10/39/115/115	-
27	CLA	I	608	9	1/1/14/20	4/33/109/115	-
27	CLA	C	207	3	1/1/14/20	4/33/109/115	-
27	CLA	A	611	27	1/1/11/20	3/15/91/115	-
27	CLA	a	825	-	1/1/15/20	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	809	-	1/1/11/20	3/18/94/115	-
30	DD6	U	607	-	-	0/26/80/80	0/3/3/3
27	CLA	D	602	-	1/1/13/20	5/27/103/115	-
31	SQD	A	618	-	-	8/22/42/69	0/1/1/1
27	CLA	E	604	-	1/1/13/20	2/27/103/115	-
31	SQD	y	301	-	-	6/41/61/69	0/1/1/1
27	CLA	a	819	-	1/1/14/20	4/33/109/115	-
27	CLA	b	724	-	1/1/15/20	4/39/115/115	-
27	CLA	b	709	15	1/1/15/20	3/39/115/115	-
27	CLA	b	706	-	1/1/15/20	10/39/115/115	-
27	CLA	H	304	-	1/1/14/20	8/33/109/115	-
32	PID	U	608	-	-	4/24/93/93	1/4/4/4
27	CLA	D	609	-	1/1/11/20	2/15/91/115	-
27	CLA	a	837	-	1/1/15/20	3/39/115/115	-
34	LHG	l	401	-	-	22/50/50/53	-
34	LHG	j	205	-	-	15/41/41/53	-
27	CLA	b	721	-	1/1/12/20	2/21/97/115	-
33	LMG	l	417	-	-	21/45/65/70	0/1/1/1
27	CLA	a	839	-	1/1/14/20	5/35/111/115	-
27	CLA	l	407	-	1/1/11/20	3/19/95/115	-
27	CLA	A	603	-	1/1/13/20	2/27/103/115	-
27	CLA	a	830	-	1/1/15/20	11/39/115/115	-
27	CLA	D	611	-	1/1/14/20	4/33/109/115	-
30	DD6	T	611	-	-	2/26/80/80	0/3/3/3
27	CLA	B	605	2	1/1/11/20	5/15/91/115	-
28	KC2	H	311	-	-	10/15/71/71	-
27	CLA	H	308	8	1/1/13/20	2/27/103/115	-
27	CLA	a	813	-	1/1/11/20	5/19/95/115	-
27	CLA	G	606	7	1/1/15/20	7/39/115/115	-
30	DD6	H	315	-	-	0/26/80/80	0/3/3/3
30	DD6	B	614	-	-	5/26/80/80	0/3/3/3
27	CLA	F	606	6	1/1/15/20	13/39/115/115	-
27	CLA	a	828	-	1/1/11/20	4/19/95/115	-
28	KC2	E	610	5	-	7/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	728	-	1/1/15/20	8/39/115/115	-
27	CLA	I	601	9	1/1/15/20	7/39/115/115	-
27	CLA	a	807	-	1/1/15/20	10/39/115/115	-
27	CLA	E	606	-	1/1/14/20	7/33/109/115	-
34	LHG	G	617	-	-	22/38/38/53	-
27	CLA	I	602	-	1/1/13/20	6/27/103/115	-
29	UIX	j	204	-	-	6/31/87/87	0/3/3/3
38	BCR	l	415	-	-	13/29/63/63	0/2/2/2
27	CLA	E	611	5	1/1/14/20	4/33/109/115	-
30	DD6	A	617	-	-	4/26/80/80	0/3/3/3
27	CLA	E	612	-	1/1/11/20	2/15/91/115	-
27	CLA	G	602	7	1/1/13/20	4/27/103/115	-
27	CLA	J	603	-	1/1/14/20	5/33/109/115	-
27	CLA	a	824	-	1/1/15/20	8/39/115/115	-
30	DD6	D	613	-	1/1/12/24	2/26/80/80	0/3/3/3
30	DD6	D	615	-	-	2/26/80/80	0/3/3/3
29	UIX	G	615	-	-	4/31/87/87	0/3/3/3
27	CLA	F	604	-	1/1/11/20	4/15/91/115	-
30	DD6	K	609	-	-	4/26/80/80	0/3/3/3
27	CLA	A	604	-	1/1/11/20	2/15/91/115	-
27	CLA	F	619	-	1/1/13/20	3/27/103/115	-
27	CLA	C	201	-	1/1/10/20	4/12/88/115	-
28	KC2	J	602	10	-	5/15/71/71	-
27	CLA	G	604	-	1/1/11/20	2/18/94/115	-
27	CLA	A	601	1	1/1/10/20	4/12/88/115	-
28	KC2	U	602	-	-	4/15/71/71	-
29	UIX	C	215	-	-	3/31/87/87	0/3/3/3
38	BCR	a	834	-	-	5/29/63/63	0/2/2/2
27	CLA	a	823	-	1/1/15/20	12/39/115/115	-
30	DD6	T	610	-	-	3/26/80/80	0/3/3/3
27	CLA	C	204	-	1/1/15/20	4/39/115/115	-
27	CLA	l	402	-	1/1/14/20	3/33/109/115	-
38	BCR	m	201	-	-	10/29/63/63	0/2/2/2
27	CLA	D	607	4	1/1/14/20	5/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	I	609	9	1/1/11/20	2/15/91/115	-
27	CLA	b	722	-	1/1/11/20	5/19/95/115	-
29	UIX	B	615	-	-	3/31/87/87	1/3/3/3
27	CLA	T	603	-	1/1/11/20	4/15/91/115	-
27	CLA	A	606	1	1/1/11/20	2/18/94/115	-
27	CLA	D	603	-	1/1/13/20	3/27/103/115	-
30	DD6	r	205	-	-	4/26/80/80	0/3/3/3
33	LMG	F	616	-	-	14/41/61/70	0/1/1/1
38	BCR	l	413	-	-	3/29/63/63	0/2/2/2
27	CLA	G	611	-	1/1/11/20	0/15/91/115	-
27	CLA	A	612	1	1/1/11/20	4/18/94/115	-
27	CLA	E	607	5	1/1/15/20	10/39/115/115	-
27	CLA	a	816	-	1/1/14/20	8/33/109/115	-
27	CLA	b	717	-	1/1/15/20	7/39/115/115	-
27	CLA	a	818	-	1/1/13/20	6/27/103/115	-

All (2012) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	602	KC2	MG-ND	-10.18	1.85	2.05
28	J	606	KC2	MG-ND	-10.15	1.85	2.05
28	J	602	KC2	MG-ND	-10.14	1.85	2.05
28	B	608	KC2	MG-ND	-10.11	1.85	2.05
28	A	608	KC2	MG-ND	-10.11	1.85	2.05
28	U	602	KC2	MG-ND	-10.07	1.85	2.05
28	K	607	KC2	MG-ND	-10.03	1.85	2.05
28	J	608	KC2	MG-ND	-10.03	1.85	2.05
28	G	601	KC2	MG-ND	-10.02	1.85	2.05
28	E	610	KC2	MG-ND	-10.02	1.85	2.05
28	J	610	KC2	MG-ND	-10.01	1.85	2.05
28	H	302	KC2	MG-ND	-10.01	1.85	2.05
28	I	604	KC2	MG-ND	-10.01	1.85	2.05
28	H	311	KC2	MG-ND	-9.98	1.86	2.05
28	C	210	KC2	MG-ND	-9.94	1.86	2.05
28	F	609	KC2	MG-ND	-9.92	1.86	2.05
28	E	601	KC2	MG-ND	-9.91	1.86	2.05
28	T	608	KC2	MG-ND	-9.88	1.86	2.05
28	U	604	KC2	MG-ND	-9.80	1.86	2.05
28	J	604	KC2	MG-ND	-9.79	1.86	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	817	CLA	C1D-ND	7.05	1.47	1.37
27	a	831	CLA	C1D-ND	7.04	1.47	1.37
27	a	808	CLA	C1D-ND	7.03	1.47	1.37
27	I	616	CLA	C1D-ND	7.03	1.47	1.37
27	U	606	CLA	C1D-ND	6.99	1.47	1.37
27	F	610	CLA	C1D-ND	6.99	1.47	1.37
27	C	211	CLA	C1D-ND	6.99	1.47	1.37
27	T	604	CLA	C1D-ND	6.98	1.47	1.37
27	K	608	CLA	C1D-ND	6.98	1.47	1.37
27	U	603	CLA	C1D-ND	6.97	1.47	1.37
27	D	610	CLA	C1D-ND	6.97	1.47	1.37
27	G	609	CLA	C1D-ND	6.97	1.47	1.37
27	F	608	CLA	C1D-ND	6.95	1.47	1.37
27	a	810	CLA	C1D-ND	6.95	1.47	1.37
27	T	607	CLA	C1D-ND	6.93	1.47	1.37
27	K	602	CLA	C1D-ND	6.92	1.46	1.37
27	A	611	CLA	C1D-ND	6.91	1.46	1.37
27	J	607	CLA	C1D-ND	6.89	1.46	1.37
27	f	302	CLA	C1D-ND	6.89	1.46	1.37
27	T	603	CLA	C1D-ND	6.88	1.46	1.37
27	D	601	CLA	C1D-ND	6.87	1.46	1.37
27	I	608	CLA	C1D-ND	6.87	1.46	1.37
27	K	603	CLA	C1D-ND	6.87	1.46	1.37
27	G	610	CLA	C1D-ND	6.86	1.46	1.37
27	a	813	CLA	C1D-ND	6.86	1.46	1.37
27	D	611	CLA	C1D-ND	6.85	1.46	1.37
27	b	719	CLA	C1D-ND	6.84	1.46	1.37
27	G	607	CLA	C1D-ND	6.83	1.46	1.37
27	T	601	CLA	C1D-ND	6.82	1.46	1.37
27	E	612	CLA	C1D-ND	6.82	1.46	1.37
27	A	607	CLA	C1D-ND	6.81	1.46	1.37
27	E	604	CLA	C1D-ND	6.80	1.46	1.37
27	C	209	CLA	C1D-ND	6.80	1.46	1.37
27	b	726	CLA	C1D-ND	6.80	1.46	1.37
27	G	602	CLA	C1D-ND	6.79	1.46	1.37
27	C	202	CLA	C1D-ND	6.79	1.46	1.37
27	C	206	CLA	C1D-ND	6.79	1.46	1.37
27	a	806	CLA	C1D-ND	6.78	1.46	1.37
27	a	816	CLA	C1D-ND	6.78	1.46	1.37
27	B	604	CLA	C1D-ND	6.78	1.46	1.37
27	E	609	CLA	C1D-ND	6.77	1.46	1.37
27	B	607	CLA	C1D-ND	6.76	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	J	601	CLA	C1D-ND	6.76	1.46	1.37
27	T	609	CLA	C1D-ND	6.76	1.46	1.37
27	H	307	CLA	C1D-ND	6.76	1.46	1.37
27	A	609	CLA	C1D-ND	6.76	1.46	1.37
27	b	711	CLA	C1D-ND	6.75	1.46	1.37
27	I	611	CLA	C1D-ND	6.75	1.46	1.37
27	a	822	CLA	C1D-ND	6.74	1.46	1.37
27	T	602	CLA	C1D-ND	6.74	1.46	1.37
27	l	403	CLA	C1D-ND	6.74	1.46	1.37
27	B	610	CLA	C1D-ND	6.74	1.46	1.37
27	C	204	CLA	C1D-ND	6.74	1.46	1.37
27	A	604	CLA	C1D-ND	6.73	1.46	1.37
27	D	609	CLA	C1D-ND	6.73	1.46	1.37
27	K	601	CLA	C1D-ND	6.73	1.46	1.37
27	r	204	CLA	C1D-ND	6.71	1.46	1.37
27	E	606	CLA	C1D-ND	6.71	1.46	1.37
27	H	304	CLA	C1D-ND	6.71	1.46	1.37
27	F	617	CLA	C1D-ND	6.70	1.46	1.37
27	F	602	CLA	C1D-ND	6.70	1.46	1.37
27	G	604	CLA	C1D-ND	6.70	1.46	1.37
27	J	609	CLA	C1D-ND	6.70	1.46	1.37
27	a	828	CLA	C1D-ND	6.70	1.46	1.37
27	U	601	CLA	C1D-ND	6.69	1.46	1.37
27	C	212	CLA	C1D-ND	6.69	1.46	1.37
27	l	412	CLA	C1D-ND	6.68	1.46	1.37
27	H	312	CLA	C1D-ND	6.68	1.46	1.37
27	b	712	CLA	C1D-ND	6.68	1.46	1.37
27	U	605	CLA	C1D-ND	6.68	1.46	1.37
27	T	606	CLA	C1D-ND	6.68	1.46	1.37
27	D	612	CLA	C1D-ND	6.67	1.46	1.37
27	l	408	CLA	C1D-ND	6.67	1.46	1.37
27	F	601	CLA	C1D-ND	6.67	1.46	1.37
27	H	309	CLA	C1D-ND	6.67	1.46	1.37
27	F	605	CLA	C1D-ND	6.66	1.46	1.37
27	D	606	CLA	C1D-ND	6.66	1.46	1.37
27	E	602	CLA	C1D-ND	6.66	1.46	1.37
27	A	602	CLA	C1D-ND	6.65	1.46	1.37
27	C	201	CLA	C1D-ND	6.65	1.46	1.37
27	a	811	CLA	C1D-ND	6.65	1.46	1.37
27	J	603	CLA	C1D-ND	6.64	1.46	1.37
27	H	310	CLA	C1D-ND	6.64	1.46	1.37
27	K	606	CLA	C1D-ND	6.64	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	208	CLA	C1D-ND	6.64	1.46	1.37
27	b	710	CLA	C1D-ND	6.63	1.46	1.37
27	a	814	CLA	C1D-ND	6.63	1.46	1.37
27	E	608	CLA	C1D-ND	6.63	1.46	1.37
27	A	601	CLA	C1D-ND	6.62	1.46	1.37
27	a	815	CLA	C1D-ND	6.62	1.46	1.37
27	H	303	CLA	C1D-ND	6.62	1.46	1.37
27	b	720	CLA	C1D-ND	6.62	1.46	1.37
27	r	203	CLA	C1D-ND	6.62	1.46	1.37
27	a	819	CLA	C1D-ND	6.61	1.46	1.37
27	G	611	CLA	C1D-ND	6.61	1.46	1.37
27	G	603	CLA	C1D-ND	6.61	1.46	1.37
27	b	725	CLA	C1D-ND	6.61	1.46	1.37
27	a	804	CLA	C1D-ND	6.60	1.46	1.37
27	F	619	CLA	C1D-ND	6.60	1.46	1.37
27	F	607	CLA	C1D-ND	6.60	1.46	1.37
27	a	820	CLA	C1D-ND	6.59	1.46	1.37
27	b	722	CLA	C1D-ND	6.59	1.46	1.37
27	E	611	CLA	C1D-ND	6.59	1.46	1.37
27	b	701	CLA	C1D-ND	6.59	1.46	1.37
27	F	603	CLA	C1D-ND	6.59	1.46	1.37
27	H	313	CLA	C1D-ND	6.59	1.46	1.37
27	I	607	CLA	C1D-ND	6.59	1.46	1.37
27	H	319	CLA	C1D-ND	6.58	1.46	1.37
27	a	825	CLA	C1D-ND	6.58	1.46	1.37
27	A	603	CLA	C1D-ND	6.58	1.46	1.37
27	I	610	CLA	C1D-ND	6.58	1.46	1.37
27	I	606	CLA	C1D-ND	6.57	1.46	1.37
27	J	605	CLA	C1D-ND	6.57	1.46	1.37
27	B	609	CLA	C1D-ND	6.57	1.46	1.37
27	l	402	CLA	C1D-ND	6.57	1.46	1.37
27	b	721	CLA	C1D-ND	6.56	1.46	1.37
27	A	606	CLA	C1D-ND	6.56	1.46	1.37
27	G	608	CLA	C1D-ND	6.56	1.46	1.37
27	H	305	CLA	C1D-ND	6.55	1.46	1.37
27	b	728	CLA	C1D-ND	6.55	1.46	1.37
27	a	829	CLA	C1D-ND	6.55	1.46	1.37
27	A	610	CLA	C1D-ND	6.55	1.46	1.37
27	b	714	CLA	C1D-ND	6.54	1.46	1.37
27	A	605	CLA	C1D-ND	6.54	1.46	1.37
27	b	723	CLA	C1D-ND	6.54	1.46	1.37
27	l	406	CLA	C1D-ND	6.54	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	601	CLA	C1D-ND	6.53	1.46	1.37
27	I	603	CLA	C1D-ND	6.53	1.46	1.37
27	a	807	CLA	C1D-ND	6.53	1.46	1.37
27	I	609	CLA	C1D-ND	6.53	1.46	1.37
27	H	308	CLA	C1D-ND	6.53	1.46	1.37
27	D	605	CLA	C1D-ND	6.52	1.46	1.37
27	a	803	CLA	C1D-ND	6.51	1.46	1.37
27	I	605	CLA	C1D-ND	6.51	1.46	1.37
27	K	604	CLA	C1D-ND	6.51	1.46	1.37
27	b	706	CLA	C1D-ND	6.51	1.46	1.37
27	b	704	CLA	C1D-ND	6.51	1.46	1.37
27	j	202	CLA	C1D-ND	6.51	1.46	1.37
27	D	603	CLA	C1D-ND	6.50	1.46	1.37
27	a	805	CLA	C1D-ND	6.50	1.46	1.37
27	l	407	CLA	C1D-ND	6.50	1.46	1.37
27	F	606	CLA	C1D-ND	6.50	1.46	1.37
27	D	607	CLA	C1D-ND	6.50	1.46	1.37
27	T	605	CLA	C1D-ND	6.50	1.46	1.37
27	f	303	CLA	C1D-ND	6.49	1.46	1.37
27	H	306	CLA	C1D-ND	6.49	1.46	1.37
27	a	830	CLA	C1D-ND	6.49	1.46	1.37
27	l	409	CLA	C1D-ND	6.48	1.46	1.37
27	E	603	CLA	C1D-ND	6.48	1.46	1.37
27	b	724	CLA	C1D-ND	6.48	1.46	1.37
27	D	608	CLA	C1D-ND	6.48	1.46	1.37
27	a	824	CLA	C1D-ND	6.48	1.46	1.37
27	K	605	CLA	C1D-ND	6.47	1.46	1.37
27	B	601	CLA	C1D-ND	6.46	1.46	1.37
27	b	713	CLA	C1D-ND	6.46	1.46	1.37
27	B	603	CLA	C1D-ND	6.46	1.46	1.37
27	l	410	CLA	C1D-ND	6.46	1.46	1.37
27	B	606	CLA	C1D-ND	6.45	1.46	1.37
27	b	727	CLA	C1D-ND	6.45	1.46	1.37
27	b	716	CLA	C1D-ND	6.45	1.46	1.37
27	l	405	CLA	C1D-ND	6.44	1.46	1.37
27	a	812	CLA	C1D-ND	6.44	1.46	1.37
27	a	823	CLA	C1D-ND	6.44	1.46	1.37
27	D	602	CLA	C1D-ND	6.43	1.46	1.37
27	I	602	CLA	C1D-ND	6.43	1.46	1.37
27	E	605	CLA	C1D-ND	6.42	1.46	1.37
27	a	827	CLA	C1D-ND	6.42	1.46	1.37
27	C	207	CLA	C1D-ND	6.41	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	l	411	CLA	C1D-ND	6.40	1.46	1.37
27	a	839	CLA	C1D-ND	6.40	1.46	1.37
27	A	612	CLA	C1D-ND	6.39	1.46	1.37
27	a	818	CLA	C1D-ND	6.39	1.46	1.37
27	G	605	CLA	C1D-ND	6.37	1.46	1.37
27	B	605	CLA	C1D-ND	6.37	1.46	1.37
27	C	203	CLA	C1D-ND	6.35	1.46	1.37
27	b	705	CLA	C1D-ND	6.35	1.46	1.37
27	b	707	CLA	C1D-ND	6.33	1.46	1.37
27	a	821	CLA	C1D-ND	6.33	1.46	1.37
27	b	709	CLA	C1D-ND	6.33	1.46	1.37
27	b	717	CLA	C1D-ND	6.31	1.46	1.37
27	a	837	CLA	MG-ND	-6.31	1.93	2.05
27	a	826	CLA	C1D-ND	6.29	1.46	1.37
27	b	708	CLA	C1D-ND	6.27	1.46	1.37
27	b	715	CLA	C1D-ND	6.27	1.46	1.37
27	F	604	CLA	C1D-ND	6.25	1.46	1.37
27	b	718	CLA	C1D-ND	6.25	1.46	1.37
27	G	606	CLA	C1D-ND	6.24	1.46	1.37
27	E	607	CLA	C1D-ND	6.24	1.46	1.37
27	a	801	CLA	MG-ND	-6.22	1.93	2.05
27	a	809	CLA	C1D-ND	6.19	1.46	1.37
27	l	404	CLA	C1D-ND	6.18	1.46	1.37
27	b	703	CLA	C1D-ND	6.16	1.46	1.37
27	C	205	CLA	C1D-ND	6.14	1.45	1.37
27	D	604	CLA	C1D-ND	6.10	1.45	1.37
27	a	802	CLA	C1D-ND	6.01	1.45	1.37
27	b	702	CLA	C1D-ND	5.97	1.45	1.37
27	D	605	CLA	MG-ND	-5.96	1.94	2.05
27	b	702	CLA	MG-ND	-5.94	1.94	2.05
27	a	826	CLA	MG-ND	-5.90	1.94	2.05
27	l	404	CLA	MG-ND	-5.88	1.94	2.05
27	C	205	CLA	MG-NA	-5.87	1.92	2.06
27	b	703	CLA	MG-ND	-5.86	1.94	2.05
27	E	607	CLA	MG-ND	-5.83	1.94	2.05
27	E	605	CLA	MG-ND	-5.82	1.94	2.05
27	A	612	CLA	MG-NA	-5.82	1.92	2.06
27	a	812	CLA	MG-ND	-5.81	1.94	2.05
27	b	718	CLA	MG-ND	-5.81	1.94	2.05
27	a	837	CLA	C1D-ND	5.80	1.45	1.37
27	a	809	CLA	MG-NA	-5.78	1.92	2.06
27	a	828	CLA	MG-NA	-5.76	1.92	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	828	CLA	MG-NB	-5.76	1.94	2.05
27	a	802	CLA	MG-ND	-5.76	1.94	2.05
27	C	205	CLA	MG-ND	-5.75	1.94	2.05
27	G	605	CLA	MG-ND	-5.74	1.94	2.05
27	f	303	CLA	MG-ND	-5.73	1.94	2.05
27	C	205	CLA	MG-NB	-5.72	1.94	2.05
27	A	612	CLA	MG-ND	-5.72	1.94	2.05
27	a	818	CLA	MG-ND	-5.70	1.94	2.05
27	F	602	CLA	MG-ND	-5.70	1.94	2.05
27	b	706	CLA	MG-ND	-5.68	1.94	2.05
27	K	608	CLA	MG-NB	-5.68	1.94	2.05
27	a	812	CLA	MG-NA	-5.68	1.92	2.06
27	C	207	CLA	MG-ND	-5.67	1.94	2.05
27	T	605	CLA	MG-ND	-5.67	1.94	2.05
27	H	308	CLA	MG-ND	-5.66	1.94	2.05
27	a	837	CLA	MG-NB	-5.66	1.94	2.05
27	b	715	CLA	MG-NA	-5.66	1.92	2.06
28	T	608	KC2	C4B-NB	5.65	1.45	1.37
27	H	307	CLA	MG-ND	-5.65	1.94	2.05
27	K	604	CLA	MG-ND	-5.63	1.94	2.05
27	b	727	CLA	MG-ND	-5.63	1.94	2.05
27	b	708	CLA	MG-ND	-5.62	1.94	2.05
27	U	603	CLA	MG-ND	-5.62	1.94	2.05
27	a	811	CLA	MG-ND	-5.62	1.94	2.05
27	l	411	CLA	MG-ND	-5.62	1.94	2.05
27	a	809	CLA	MG-ND	-5.60	1.94	2.05
27	b	725	CLA	MG-ND	-5.60	1.94	2.05
27	a	805	CLA	MG-ND	-5.60	1.94	2.05
27	B	609	CLA	MG-ND	-5.60	1.94	2.05
27	b	717	CLA	MG-ND	-5.60	1.94	2.05
27	U	603	CLA	MG-NB	-5.60	1.94	2.05
27	G	611	CLA	MG-ND	-5.59	1.94	2.05
27	H	306	CLA	MG-ND	-5.59	1.94	2.05
27	H	310	CLA	MG-ND	-5.59	1.94	2.05
27	K	608	CLA	MG-ND	-5.59	1.94	2.05
27	b	720	CLA	MG-ND	-5.59	1.94	2.05
27	a	827	CLA	MG-ND	-5.59	1.94	2.05
27	H	304	CLA	MG-ND	-5.59	1.94	2.05
27	K	606	CLA	MG-NA	-5.59	1.93	2.06
27	C	204	CLA	MG-ND	-5.58	1.94	2.05
27	b	709	CLA	MG-ND	-5.58	1.94	2.05
27	l	409	CLA	MG-ND	-5.58	1.94	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	U	601	CLA	MG-NA	-5.58	1.93	2.06
27	D	607	CLA	MG-ND	-5.58	1.94	2.05
27	F	604	CLA	MG-ND	-5.57	1.94	2.05
27	l	407	CLA	MG-ND	-5.57	1.94	2.05
27	K	606	CLA	MG-ND	-5.57	1.94	2.05
27	A	612	CLA	MG-NB	-5.57	1.94	2.05
27	J	605	CLA	MG-ND	-5.56	1.94	2.05
27	D	606	CLA	MG-ND	-5.56	1.94	2.05
27	a	804	CLA	MG-ND	-5.56	1.94	2.05
27	a	823	CLA	MG-ND	-5.55	1.94	2.05
27	C	201	CLA	MG-ND	-5.55	1.94	2.05
27	K	606	CLA	MG-NB	-5.55	1.94	2.05
27	U	605	CLA	MG-ND	-5.55	1.94	2.05
27	F	606	CLA	MG-ND	-5.54	1.94	2.05
27	K	605	CLA	MG-ND	-5.54	1.94	2.05
27	H	312	CLA	MG-ND	-5.54	1.94	2.05
27	G	606	CLA	MG-ND	-5.54	1.94	2.05
27	I	605	CLA	MG-ND	-5.54	1.94	2.05
27	G	606	CLA	MG-NB	-5.54	1.94	2.05
27	G	605	CLA	MG-NA	-5.54	1.93	2.06
27	I	611	CLA	MG-NA	-5.54	1.93	2.06
27	F	617	CLA	MG-ND	-5.53	1.94	2.05
27	l	410	CLA	MG-NB	-5.53	1.94	2.05
27	b	714	CLA	MG-ND	-5.53	1.94	2.05
27	r	203	CLA	MG-NB	-5.53	1.94	2.05
27	I	608	CLA	MG-ND	-5.53	1.94	2.05
27	B	603	CLA	MG-NA	-5.53	1.93	2.06
27	F	605	CLA	MG-ND	-5.53	1.94	2.05
27	l	410	CLA	MG-ND	-5.53	1.94	2.05
27	a	829	CLA	MG-ND	-5.53	1.94	2.05
27	a	812	CLA	MG-NB	-5.53	1.94	2.05
27	I	602	CLA	MG-ND	-5.52	1.94	2.05
27	B	604	CLA	MG-NB	-5.52	1.94	2.05
27	a	820	CLA	MG-NA	-5.52	1.93	2.06
27	b	719	CLA	MG-NB	-5.52	1.94	2.05
27	A	605	CLA	MG-ND	-5.52	1.94	2.05
27	E	611	CLA	MG-ND	-5.51	1.94	2.05
27	I	611	CLA	MG-NB	-5.51	1.94	2.05
27	U	601	CLA	MG-NB	-5.51	1.94	2.05
27	H	310	CLA	MG-NB	-5.51	1.94	2.05
27	G	608	CLA	MG-NA	-5.51	1.93	2.06
27	D	604	CLA	MG-ND	-5.51	1.94	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	819	CLA	MG-ND	-5.51	1.94	2.05
27	l	403	CLA	MG-ND	-5.51	1.94	2.05
27	b	713	CLA	MG-ND	-5.50	1.94	2.05
27	A	610	CLA	MG-ND	-5.50	1.94	2.05
27	b	710	CLA	MG-NB	-5.50	1.94	2.05
27	a	815	CLA	MG-ND	-5.50	1.94	2.05
27	l	408	CLA	MG-ND	-5.50	1.94	2.05
27	j	202	CLA	MG-ND	-5.50	1.94	2.05
27	l	410	CLA	MG-NA	-5.50	1.93	2.06
27	H	305	CLA	MG-ND	-5.50	1.94	2.05
27	a	839	CLA	MG-ND	-5.50	1.94	2.05
27	B	605	CLA	MG-ND	-5.49	1.94	2.05
27	l	404	CLA	MG-NB	-5.49	1.94	2.05
27	B	606	CLA	MG-NA	-5.49	1.93	2.06
27	b	721	CLA	MG-ND	-5.49	1.94	2.05
27	a	820	CLA	MG-NB	-5.49	1.94	2.05
27	B	610	CLA	MG-ND	-5.49	1.94	2.05
27	a	821	CLA	MG-ND	-5.49	1.94	2.05
27	b	716	CLA	MG-NB	-5.49	1.94	2.05
27	l	405	CLA	MG-ND	-5.49	1.94	2.05
27	b	701	CLA	MG-ND	-5.49	1.94	2.05
27	B	603	CLA	MG-ND	-5.49	1.94	2.05
27	b	718	CLA	MG-NB	-5.49	1.94	2.05
27	H	310	CLA	MG-NA	-5.49	1.93	2.06
27	b	712	CLA	MG-NB	-5.48	1.94	2.05
27	I	609	CLA	MG-ND	-5.48	1.94	2.05
27	a	817	CLA	MG-ND	-5.48	1.94	2.05
27	A	603	CLA	MG-ND	-5.48	1.94	2.05
27	l	412	CLA	MG-ND	-5.47	1.94	2.05
27	B	606	CLA	MG-NB	-5.47	1.94	2.05
27	a	816	CLA	MG-ND	-5.47	1.94	2.05
27	I	607	CLA	MG-NB	-5.47	1.94	2.05
27	a	801	CLA	C1D-ND	5.47	1.45	1.37
27	G	603	CLA	MG-ND	-5.47	1.94	2.05
27	b	718	CLA	MG-NA	-5.47	1.93	2.06
27	b	726	CLA	MG-ND	-5.47	1.94	2.05
27	a	839	CLA	MG-NB	-5.47	1.95	2.05
27	I	610	CLA	MG-ND	-5.47	1.95	2.05
27	b	722	CLA	MG-ND	-5.46	1.95	2.05
27	a	823	CLA	MG-NA	-5.46	1.93	2.06
27	C	201	CLA	MG-NB	-5.46	1.95	2.05
27	E	608	CLA	MG-ND	-5.46	1.95	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	723	CLA	MG-ND	-5.46	1.95	2.05
27	E	603	CLA	MG-ND	-5.46	1.95	2.05
27	a	823	CLA	MG-NB	-5.46	1.95	2.05
27	b	710	CLA	MG-ND	-5.46	1.95	2.05
27	F	602	CLA	MG-NB	-5.45	1.95	2.05
27	J	609	CLA	MG-ND	-5.45	1.95	2.05
27	D	602	CLA	MG-ND	-5.45	1.95	2.05
27	E	605	CLA	MG-NB	-5.45	1.95	2.05
27	a	801	CLA	MG-NB	-5.45	1.95	2.05
27	T	602	CLA	MG-NB	-5.45	1.95	2.05
27	a	822	CLA	MG-ND	-5.45	1.95	2.05
27	H	307	CLA	MG-NB	-5.45	1.95	2.05
27	b	707	CLA	MG-ND	-5.45	1.95	2.05
27	D	603	CLA	MG-NB	-5.44	1.95	2.05
27	a	827	CLA	MG-NB	-5.44	1.95	2.05
27	b	711	CLA	MG-ND	-5.44	1.95	2.05
27	E	603	CLA	MG-NB	-5.44	1.95	2.05
27	H	303	CLA	MG-ND	-5.44	1.95	2.05
27	I	607	CLA	MG-ND	-5.44	1.95	2.05
27	D	601	CLA	MG-ND	-5.44	1.95	2.05
27	B	607	CLA	MG-ND	-5.44	1.95	2.05
27	G	608	CLA	MG-ND	-5.44	1.95	2.05
27	r	204	CLA	MG-ND	-5.44	1.95	2.05
27	T	607	CLA	MG-ND	-5.44	1.95	2.05
27	b	710	CLA	MG-NA	-5.43	1.93	2.06
27	b	721	CLA	MG-NB	-5.43	1.95	2.05
27	a	825	CLA	MG-ND	-5.43	1.95	2.05
27	D	602	CLA	MG-NB	-5.43	1.95	2.05
27	J	603	CLA	MG-ND	-5.43	1.95	2.05
27	a	807	CLA	MG-ND	-5.43	1.95	2.05
27	r	203	CLA	MG-ND	-5.43	1.95	2.05
27	A	602	CLA	MG-ND	-5.42	1.95	2.05
27	T	609	CLA	MG-ND	-5.42	1.95	2.05
27	T	601	CLA	MG-ND	-5.42	1.95	2.05
27	J	607	CLA	MG-ND	-5.42	1.95	2.05
27	b	714	CLA	MG-NA	-5.42	1.93	2.06
27	a	814	CLA	MG-ND	-5.42	1.95	2.05
27	b	719	CLA	MG-NA	-5.42	1.93	2.06
27	T	602	CLA	MG-ND	-5.42	1.95	2.05
27	H	319	CLA	MG-ND	-5.42	1.95	2.05
27	b	724	CLA	MG-ND	-5.42	1.95	2.05
27	b	705	CLA	MG-NA	-5.41	1.93	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	808	CLA	MG-ND	-5.41	1.95	2.05
27	D	603	CLA	MG-ND	-5.41	1.95	2.05
27	a	831	CLA	MG-ND	-5.41	1.95	2.05
27	a	813	CLA	MG-ND	-5.41	1.95	2.05
27	a	830	CLA	MG-ND	-5.41	1.95	2.05
27	G	606	CLA	MG-NA	-5.41	1.93	2.06
27	A	606	CLA	MG-ND	-5.41	1.95	2.05
27	K	602	CLA	MG-ND	-5.41	1.95	2.05
27	U	601	CLA	MG-ND	-5.41	1.95	2.05
28	E	601	KC2	C4B-NB	5.41	1.45	1.37
27	D	610	CLA	MG-ND	-5.41	1.95	2.05
27	B	604	CLA	MG-ND	-5.41	1.95	2.05
27	J	601	CLA	MG-ND	-5.40	1.95	2.05
27	a	820	CLA	MG-ND	-5.40	1.95	2.05
27	a	828	CLA	MG-ND	-5.40	1.95	2.05
27	J	609	CLA	MG-NA	-5.40	1.93	2.06
27	G	608	CLA	MG-NB	-5.40	1.95	2.05
27	a	803	CLA	MG-ND	-5.40	1.95	2.05
27	b	712	CLA	MG-ND	-5.40	1.95	2.05
27	G	609	CLA	MG-ND	-5.40	1.95	2.05
27	T	606	CLA	MG-ND	-5.40	1.95	2.05
27	C	203	CLA	MG-ND	-5.40	1.95	2.05
27	a	824	CLA	MG-NA	-5.40	1.93	2.06
27	C	206	CLA	MG-ND	-5.40	1.95	2.05
27	G	605	CLA	MG-NB	-5.40	1.95	2.05
27	B	603	CLA	MG-NB	-5.40	1.95	2.05
27	D	603	CLA	MG-NA	-5.40	1.93	2.06
27	C	212	CLA	MG-ND	-5.39	1.95	2.05
27	E	609	CLA	MG-ND	-5.39	1.95	2.05
28	U	604	KC2	C4B-NB	5.39	1.44	1.37
27	A	601	CLA	MG-ND	-5.39	1.95	2.05
27	a	827	CLA	MG-NA	-5.39	1.93	2.06
27	b	712	CLA	MG-NA	-5.39	1.93	2.06
27	T	609	CLA	MG-NA	-5.39	1.93	2.06
27	A	609	CLA	MG-ND	-5.39	1.95	2.05
27	I	601	CLA	MG-ND	-5.39	1.95	2.05
27	I	610	CLA	MG-NA	-5.39	1.93	2.06
27	J	601	CLA	MG-NB	-5.39	1.95	2.05
27	I	603	CLA	MG-NB	-5.39	1.95	2.05
27	H	309	CLA	MG-ND	-5.38	1.95	2.05
27	b	705	CLA	MG-NB	-5.38	1.95	2.05
27	a	802	CLA	MG-NA	-5.38	1.93	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	612	CLA	MG-ND	-5.38	1.95	2.05
27	D	604	CLA	MG-NB	-5.38	1.95	2.05
27	I	611	CLA	MG-ND	-5.38	1.95	2.05
27	I	603	CLA	MG-ND	-5.38	1.95	2.05
27	b	721	CLA	MG-NA	-5.37	1.93	2.06
27	C	202	CLA	MG-ND	-5.37	1.95	2.05
27	T	603	CLA	MG-ND	-5.37	1.95	2.05
27	E	605	CLA	MG-NA	-5.37	1.93	2.06
28	C	210	KC2	C4B-NB	5.37	1.44	1.37
28	F	609	KC2	C4B-NB	5.37	1.44	1.37
27	H	313	CLA	MG-ND	-5.37	1.95	2.05
27	J	605	CLA	MG-NB	-5.37	1.95	2.05
27	C	204	CLA	MG-NB	-5.37	1.95	2.05
27	H	305	CLA	MG-NB	-5.37	1.95	2.05
27	I	606	CLA	MG-NB	-5.37	1.95	2.05
27	F	603	CLA	MG-NB	-5.36	1.95	2.05
27	H	313	CLA	MG-NA	-5.36	1.93	2.06
27	B	601	CLA	MG-ND	-5.36	1.95	2.05
27	D	611	CLA	MG-ND	-5.36	1.95	2.05
27	I	616	CLA	MG-ND	-5.36	1.95	2.05
27	B	606	CLA	MG-ND	-5.36	1.95	2.05
27	b	728	CLA	MG-ND	-5.36	1.95	2.05
27	b	705	CLA	MG-ND	-5.36	1.95	2.05
27	E	611	CLA	MG-NA	-5.36	1.93	2.06
27	E	606	CLA	MG-ND	-5.36	1.95	2.05
27	G	602	CLA	MG-ND	-5.36	1.95	2.05
27	b	720	CLA	MG-NB	-5.36	1.95	2.05
27	l	408	CLA	MG-NA	-5.36	1.93	2.06
28	J	602	KC2	C4B-NB	5.35	1.44	1.37
27	D	608	CLA	MG-ND	-5.35	1.95	2.05
27	l	402	CLA	MG-ND	-5.35	1.95	2.05
27	b	716	CLA	MG-NA	-5.35	1.93	2.06
27	b	716	CLA	MG-ND	-5.35	1.95	2.05
27	B	604	CLA	MG-NA	-5.35	1.93	2.06
27	A	604	CLA	MG-ND	-5.35	1.95	2.05
27	C	209	CLA	MG-ND	-5.35	1.95	2.05
27	a	824	CLA	MG-ND	-5.34	1.95	2.05
27	A	607	CLA	MG-ND	-5.34	1.95	2.05
27	D	602	CLA	MG-NA	-5.34	1.93	2.06
27	b	719	CLA	MG-ND	-5.34	1.95	2.05
27	l	406	CLA	MG-ND	-5.34	1.95	2.05
27	A	601	CLA	MG-NB	-5.34	1.95	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	601	CLA	MG-NA	-5.34	1.93	2.06
27	F	619	CLA	MG-ND	-5.33	1.95	2.05
27	G	610	CLA	MG-ND	-5.33	1.95	2.05
28	H	311	KC2	C4B-NB	5.33	1.44	1.37
27	J	601	CLA	MG-NA	-5.33	1.93	2.06
27	a	808	CLA	MG-NB	-5.33	1.95	2.05
27	A	606	CLA	MG-NB	-5.33	1.95	2.05
27	K	601	CLA	MG-ND	-5.33	1.95	2.05
27	b	715	CLA	MG-ND	-5.33	1.95	2.05
27	K	603	CLA	C1B-NB	5.33	1.44	1.37
27	b	704	CLA	MG-ND	-5.33	1.95	2.05
27	a	802	CLA	MG-NB	-5.33	1.95	2.05
27	a	806	CLA	MG-ND	-5.33	1.95	2.05
27	f	302	CLA	MG-ND	-5.33	1.95	2.05
27	F	603	CLA	MG-NA	-5.33	1.93	2.06
27	b	727	CLA	MG-NA	-5.33	1.93	2.06
27	j	202	CLA	MG-NB	-5.33	1.95	2.05
27	E	602	CLA	MG-ND	-5.33	1.95	2.05
27	C	208	CLA	MG-ND	-5.32	1.95	2.05
27	C	211	CLA	MG-ND	-5.32	1.95	2.05
27	C	211	CLA	MG-NB	-5.32	1.95	2.05
27	A	603	CLA	MG-NB	-5.32	1.95	2.05
27	T	604	CLA	MG-ND	-5.32	1.95	2.05
27	l	407	CLA	MG-NB	-5.32	1.95	2.05
27	F	601	CLA	MG-ND	-5.32	1.95	2.05
28	J	604	KC2	C4B-NB	5.32	1.44	1.37
27	r	203	CLA	MG-NA	-5.32	1.93	2.06
27	a	809	CLA	MG-NB	-5.32	1.95	2.05
27	E	612	CLA	MG-ND	-5.32	1.95	2.05
27	H	312	CLA	MG-NB	-5.32	1.95	2.05
27	I	602	CLA	MG-NB	-5.32	1.95	2.05
27	l	405	CLA	MG-NA	-5.32	1.93	2.06
27	C	209	CLA	MG-NB	-5.31	1.95	2.05
27	G	604	CLA	MG-NA	-5.31	1.93	2.06
27	I	610	CLA	MG-NB	-5.31	1.95	2.05
27	D	609	CLA	MG-ND	-5.31	1.95	2.05
27	a	824	CLA	MG-NB	-5.31	1.95	2.05
27	a	807	CLA	MG-NA	-5.30	1.93	2.06
27	J	603	CLA	MG-NB	-5.30	1.95	2.05
27	I	611	CLA	C1B-NB	5.30	1.44	1.37
27	F	610	CLA	MG-NB	-5.30	1.95	2.05
27	H	305	CLA	MG-NA	-5.30	1.93	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	208	CLA	MG-NB	-5.30	1.95	2.05
27	A	609	CLA	MG-NB	-5.30	1.95	2.05
27	E	611	CLA	MG-NB	-5.30	1.95	2.05
27	T	603	CLA	MG-NB	-5.30	1.95	2.05
27	f	303	CLA	MG-NB	-5.29	1.95	2.05
27	U	606	CLA	C1B-NB	5.29	1.44	1.37
28	H	302	KC2	C4B-NB	5.29	1.44	1.37
27	B	604	CLA	C1B-NB	5.29	1.44	1.37
27	f	303	CLA	MG-NA	-5.29	1.93	2.06
27	D	605	CLA	MG-NB	-5.29	1.95	2.05
27	a	810	CLA	MG-ND	-5.29	1.95	2.05
27	C	203	CLA	MG-NA	-5.29	1.93	2.06
27	a	816	CLA	MG-NB	-5.29	1.95	2.05
27	G	604	CLA	MG-ND	-5.28	1.95	2.05
27	I	609	CLA	MG-NA	-5.28	1.93	2.06
27	a	813	CLA	MG-NB	-5.28	1.95	2.05
27	K	606	CLA	C1B-NB	5.28	1.44	1.37
27	T	609	CLA	C1B-NB	5.28	1.44	1.37
27	E	604	CLA	MG-ND	-5.28	1.95	2.05
27	l	405	CLA	MG-NB	-5.28	1.95	2.05
27	l	407	CLA	MG-NA	-5.28	1.93	2.06
27	l	404	CLA	MG-NA	-5.28	1.93	2.06
27	I	601	CLA	MG-NB	-5.28	1.95	2.05
27	b	702	CLA	MG-NB	-5.28	1.95	2.05
27	l	403	CLA	MG-NB	-5.27	1.95	2.05
28	J	608	KC2	C4B-NB	5.27	1.44	1.37
27	F	602	CLA	MG-NA	-5.27	1.93	2.06
27	D	611	CLA	MG-NB	-5.27	1.95	2.05
27	I	606	CLA	MG-ND	-5.27	1.95	2.05
27	a	828	CLA	C1B-NB	5.27	1.44	1.37
27	b	707	CLA	MG-NB	-5.27	1.95	2.05
27	H	313	CLA	MG-NB	-5.27	1.95	2.05
27	b	703	CLA	MG-NB	-5.27	1.95	2.05
27	a	816	CLA	MG-NA	-5.27	1.93	2.06
28	E	610	KC2	C4B-NB	5.27	1.44	1.37
27	F	603	CLA	MG-ND	-5.26	1.95	2.05
27	I	609	CLA	MG-NB	-5.26	1.95	2.05
27	J	609	CLA	MG-NB	-5.26	1.95	2.05
27	a	812	CLA	C1B-NB	5.26	1.44	1.37
27	F	601	CLA	MG-NB	-5.26	1.95	2.05
27	F	607	CLA	MG-ND	-5.26	1.95	2.05
27	a	818	CLA	MG-NA	-5.26	1.93	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	K	607	KC2	C4B-NB	5.26	1.44	1.37
27	a	825	CLA	MG-NB	-5.26	1.95	2.05
27	G	611	CLA	MG-NB	-5.25	1.95	2.05
27	K	603	CLA	MG-ND	-5.25	1.95	2.05
27	C	203	CLA	MG-NB	-5.25	1.95	2.05
27	D	606	CLA	MG-NB	-5.25	1.95	2.05
27	F	608	CLA	MG-ND	-5.25	1.95	2.05
27	K	608	CLA	C1B-NB	5.25	1.44	1.37
27	D	612	CLA	MG-NB	-5.25	1.95	2.05
27	b	727	CLA	MG-NB	-5.25	1.95	2.05
27	C	208	CLA	MG-NA	-5.25	1.93	2.06
27	U	605	CLA	MG-NB	-5.25	1.95	2.05
27	U	603	CLA	C1B-NB	5.24	1.44	1.37
27	b	709	CLA	MG-NB	-5.24	1.95	2.05
27	b	707	CLA	MG-NA	-5.24	1.93	2.06
27	F	605	CLA	MG-NB	-5.24	1.95	2.05
27	T	609	CLA	MG-NB	-5.24	1.95	2.05
27	b	703	CLA	MG-NA	-5.24	1.93	2.06
27	b	714	CLA	MG-NB	-5.24	1.95	2.05
27	B	609	CLA	MG-NB	-5.24	1.95	2.05
27	F	610	CLA	MG-ND	-5.24	1.95	2.05
27	T	607	CLA	MG-NB	-5.23	1.95	2.05
27	b	722	CLA	MG-NB	-5.23	1.95	2.05
27	D	609	CLA	MG-NB	-5.23	1.95	2.05
27	U	601	CLA	C1B-NB	5.23	1.44	1.37
27	C	209	CLA	C1B-NB	5.23	1.44	1.37
27	a	818	CLA	MG-NB	-5.23	1.95	2.05
27	G	604	CLA	MG-NB	-5.23	1.95	2.05
27	T	606	CLA	C1B-NB	5.23	1.44	1.37
27	a	830	CLA	MG-NB	-5.23	1.95	2.05
27	T	601	CLA	MG-NB	-5.23	1.95	2.05
27	A	611	CLA	MG-ND	-5.22	1.95	2.05
27	C	207	CLA	MG-NB	-5.22	1.95	2.05
27	b	711	CLA	MG-NB	-5.22	1.95	2.05
27	b	724	CLA	MG-NB	-5.22	1.95	2.05
27	F	608	CLA	C1B-NB	5.22	1.44	1.37
27	F	607	CLA	MG-NB	-5.22	1.95	2.05
27	T	607	CLA	C1B-NB	5.22	1.44	1.37
27	J	607	CLA	C1B-NB	5.22	1.44	1.37
27	E	604	CLA	MG-NB	-5.22	1.95	2.05
27	T	601	CLA	C1B-NB	5.22	1.44	1.37
27	b	713	CLA	MG-NB	-5.22	1.95	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	609	CLA	MG-NB	-5.21	1.95	2.05
27	E	607	CLA	MG-NB	-5.21	1.95	2.05
27	D	608	CLA	MG-NB	-5.21	1.95	2.05
27	K	604	CLA	MG-NB	-5.21	1.95	2.05
27	A	602	CLA	MG-NB	-5.21	1.95	2.05
27	C	201	CLA	C1B-NB	5.21	1.44	1.37
27	G	604	CLA	C1B-NB	5.21	1.44	1.37
27	E	603	CLA	MG-NA	-5.21	1.93	2.06
27	K	602	CLA	MG-NB	-5.21	1.95	2.05
27	U	606	CLA	MG-ND	-5.21	1.95	2.05
28	A	608	KC2	C4B-NB	5.21	1.44	1.37
27	l	408	CLA	MG-NB	-5.21	1.95	2.05
27	J	609	CLA	C1B-NB	5.20	1.44	1.37
27	F	610	CLA	C1B-NB	5.20	1.44	1.37
28	G	601	KC2	C4B-NB	5.20	1.44	1.37
27	E	608	CLA	MG-NB	-5.20	1.95	2.05
27	F	617	CLA	MG-NB	-5.20	1.95	2.05
27	a	829	CLA	MG-NA	-5.20	1.93	2.06
27	D	607	CLA	MG-NB	-5.20	1.95	2.05
27	A	607	CLA	MG-NB	-5.20	1.95	2.05
27	H	310	CLA	C1B-NB	5.20	1.44	1.37
27	a	811	CLA	MG-NB	-5.20	1.95	2.05
27	b	723	CLA	MG-NB	-5.20	1.95	2.05
27	C	212	CLA	MG-NB	-5.20	1.95	2.05
27	T	604	CLA	MG-NB	-5.19	1.95	2.05
27	J	603	CLA	MG-NA	-5.19	1.93	2.06
27	a	813	CLA	C1B-NB	5.19	1.44	1.37
27	D	608	CLA	MG-NA	-5.19	1.93	2.06
27	b	708	CLA	MG-NB	-5.19	1.95	2.05
27	l	412	CLA	MG-NB	-5.19	1.95	2.05
27	j	202	CLA	MG-NA	-5.19	1.93	2.06
27	F	607	CLA	MG-NA	-5.19	1.93	2.06
27	r	203	CLA	C1B-NB	5.19	1.44	1.37
27	l	407	CLA	C1B-NB	5.18	1.44	1.37
27	l	409	CLA	MG-NB	-5.18	1.95	2.05
27	l	403	CLA	MG-NA	-5.18	1.94	2.06
27	D	604	CLA	MG-NA	-5.18	1.94	2.06
27	b	715	CLA	MG-NB	-5.17	1.95	2.05
27	C	202	CLA	MG-NB	-5.17	1.95	2.05
27	A	607	CLA	C1B-NB	5.17	1.44	1.37
27	E	612	CLA	C1B-NB	5.17	1.44	1.37
27	b	713	CLA	MG-NA	-5.17	1.94	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	826	CLA	MG-NB	-5.17	1.95	2.05
27	C	212	CLA	C1B-NB	5.17	1.44	1.37
27	a	829	CLA	MG-NB	-5.16	1.95	2.05
27	A	611	CLA	C1B-NB	5.16	1.44	1.37
27	T	604	CLA	C1B-NB	5.16	1.44	1.37
27	D	601	CLA	MG-NB	-5.16	1.95	2.05
27	J	607	CLA	MG-NB	-5.16	1.95	2.05
27	l	402	CLA	C1B-NB	5.16	1.44	1.37
28	J	610	KC2	C4B-NB	5.16	1.44	1.37
27	E	612	CLA	MG-NB	-5.16	1.95	2.05
27	E	606	CLA	C1B-NB	5.16	1.44	1.37
27	G	607	CLA	MG-NB	-5.16	1.95	2.05
27	B	601	CLA	MG-NB	-5.15	1.95	2.05
27	H	309	CLA	MG-NB	-5.15	1.95	2.05
27	F	608	CLA	MG-NB	-5.15	1.95	2.05
27	I	608	CLA	MG-NB	-5.15	1.95	2.05
27	b	717	CLA	MG-NB	-5.15	1.95	2.05
28	U	602	KC2	C4B-NB	5.15	1.44	1.37
27	b	722	CLA	MG-NA	-5.15	1.94	2.06
27	F	605	CLA	C1B-NB	5.15	1.44	1.37
27	l	411	CLA	MG-NB	-5.15	1.95	2.05
27	T	602	CLA	C1B-NB	5.15	1.44	1.37
27	a	811	CLA	MG-NA	-5.15	1.94	2.06
27	K	608	CLA	MG-NA	-5.15	1.94	2.06
27	a	803	CLA	MG-NB	-5.14	1.95	2.05
27	b	726	CLA	MG-NB	-5.14	1.95	2.05
27	b	706	CLA	MG-NB	-5.14	1.95	2.05
27	G	607	CLA	MG-ND	-5.14	1.95	2.05
27	C	202	CLA	C1B-NB	5.14	1.44	1.37
27	D	610	CLA	C1B-NB	5.14	1.44	1.37
27	G	608	CLA	C1B-NB	5.14	1.44	1.37
27	b	724	CLA	MG-NA	-5.14	1.94	2.06
27	a	831	CLA	MG-NB	-5.14	1.95	2.05
27	a	806	CLA	MG-NB	-5.14	1.95	2.05
27	E	605	CLA	C1B-NB	5.14	1.44	1.37
27	r	204	CLA	MG-NB	-5.14	1.95	2.05
27	F	606	CLA	MG-NB	-5.13	1.95	2.05
27	I	605	CLA	MG-NB	-5.13	1.95	2.05
27	K	601	CLA	MG-NB	-5.13	1.95	2.05
27	a	803	CLA	C1B-NB	5.13	1.44	1.37
27	T	606	CLA	MG-NA	-5.13	1.94	2.06
27	F	610	CLA	MG-NA	-5.13	1.94	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	606	CLA	MG-NA	-5.13	1.94	2.06
27	T	605	CLA	MG-NB	-5.13	1.95	2.05
27	D	612	CLA	MG-NA	-5.13	1.94	2.06
27	C	209	CLA	MG-NA	-5.13	1.94	2.06
27	a	821	CLA	MG-NB	-5.13	1.95	2.05
28	B	608	KC2	C4B-NB	5.13	1.44	1.37
27	G	610	CLA	C1B-NB	5.13	1.44	1.37
27	U	605	CLA	C1B-NB	5.13	1.44	1.37
27	a	819	CLA	MG-NB	-5.12	1.95	2.05
27	a	839	CLA	MG-NA	-5.12	1.94	2.06
27	l	410	CLA	C1B-NB	5.12	1.44	1.37
27	H	319	CLA	MG-NB	-5.12	1.95	2.05
27	G	609	CLA	MG-NB	-5.12	1.95	2.05
28	I	604	KC2	C4B-NB	5.12	1.44	1.37
27	a	811	CLA	C1B-NB	5.11	1.44	1.37
27	C	212	CLA	MG-NA	-5.11	1.94	2.06
27	K	601	CLA	C1B-NB	5.11	1.44	1.37
27	F	619	CLA	MG-NB	-5.11	1.95	2.05
27	H	306	CLA	MG-NB	-5.11	1.95	2.05
27	H	313	CLA	C1B-NB	5.11	1.44	1.37
27	K	605	CLA	MG-NB	-5.11	1.95	2.05
27	B	601	CLA	MG-NA	-5.11	1.94	2.06
27	b	711	CLA	C1B-NB	5.11	1.44	1.37
27	A	602	CLA	C1B-NB	5.10	1.44	1.37
27	b	714	CLA	C1B-NB	5.10	1.44	1.37
27	b	728	CLA	MG-NB	-5.10	1.95	2.05
27	E	602	CLA	MG-NB	-5.10	1.95	2.05
27	B	605	CLA	MG-NB	-5.10	1.95	2.05
27	a	806	CLA	C1B-NB	5.10	1.44	1.37
27	a	821	CLA	MG-NA	-5.10	1.94	2.06
27	E	609	CLA	C1B-NB	5.10	1.44	1.37
28	B	602	KC2	C4B-NB	5.10	1.44	1.37
27	D	609	CLA	MG-NA	-5.10	1.94	2.06
27	T	606	CLA	MG-NB	-5.10	1.95	2.05
27	a	808	CLA	C1B-NB	5.10	1.44	1.37
27	E	606	CLA	MG-NB	-5.10	1.95	2.05
27	b	701	CLA	MG-NB	-5.10	1.95	2.05
27	A	610	CLA	MG-NB	-5.09	1.95	2.05
27	T	602	CLA	MG-NA	-5.09	1.94	2.06
27	a	805	CLA	MG-NB	-5.09	1.95	2.05
27	b	704	CLA	MG-NB	-5.09	1.95	2.05
27	G	611	CLA	C1B-NB	5.09	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	813	CLA	MG-NA	-5.09	1.94	2.06
27	b	723	CLA	MG-NA	-5.09	1.94	2.06
27	B	603	CLA	C1B-NB	5.09	1.44	1.37
27	H	309	CLA	C1B-NB	5.08	1.44	1.37
27	b	725	CLA	MG-NB	-5.08	1.95	2.05
27	j	202	CLA	C1B-NB	5.08	1.44	1.37
27	G	611	CLA	MG-NA	-5.08	1.94	2.06
27	l	412	CLA	MG-NA	-5.08	1.94	2.06
27	U	603	CLA	MG-NA	-5.08	1.94	2.06
27	a	805	CLA	MG-NA	-5.08	1.94	2.06
27	G	602	CLA	MG-NB	-5.08	1.95	2.05
27	a	807	CLA	MG-NB	-5.08	1.95	2.05
27	a	814	CLA	C1B-NB	5.08	1.44	1.37
27	G	602	CLA	C1B-NB	5.08	1.44	1.37
27	C	207	CLA	C1B-NB	5.08	1.44	1.37
27	D	609	CLA	C1B-NB	5.08	1.44	1.37
27	b	721	CLA	C1B-NB	5.07	1.44	1.37
27	B	607	CLA	MG-NB	-5.07	1.95	2.05
27	l	411	CLA	MG-NA	-5.07	1.94	2.06
27	b	720	CLA	C1B-NB	5.07	1.44	1.37
27	C	207	CLA	MG-NA	-5.07	1.94	2.06
27	a	808	CLA	MG-NA	-5.07	1.94	2.06
27	A	611	CLA	MG-NA	-5.07	1.94	2.06
27	l	405	CLA	C1B-NB	5.07	1.44	1.37
28	J	606	KC2	C4B-NB	5.07	1.44	1.37
27	a	804	CLA	MG-NB	-5.07	1.95	2.05
27	f	303	CLA	C1B-NB	5.06	1.44	1.37
27	a	830	CLA	MG-NA	-5.06	1.94	2.06
27	H	309	CLA	MG-NA	-5.06	1.94	2.06
27	H	306	CLA	C1B-NB	5.06	1.44	1.37
27	a	816	CLA	C1B-NB	5.06	1.44	1.37
27	H	308	CLA	MG-NB	-5.06	1.95	2.05
27	I	607	CLA	MG-NA	-5.06	1.94	2.06
27	I	603	CLA	MG-NA	-5.06	1.94	2.06
27	a	803	CLA	MG-NA	-5.05	1.94	2.06
27	A	604	CLA	MG-NB	-5.05	1.95	2.05
27	F	606	CLA	MG-NA	-5.05	1.94	2.06
27	G	603	CLA	MG-NB	-5.05	1.95	2.05
27	E	608	CLA	MG-NA	-5.05	1.94	2.06
27	b	704	CLA	MG-NA	-5.05	1.94	2.06
27	K	604	CLA	C1B-NB	5.05	1.44	1.37
27	l	406	CLA	MG-NA	-5.05	1.94	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	822	CLA	MG-NB	-5.05	1.95	2.05
27	a	809	CLA	C1B-NB	5.05	1.44	1.37
27	b	723	CLA	C1B-NB	5.05	1.44	1.37
27	l	402	CLA	MG-NA	-5.05	1.94	2.06
27	a	825	CLA	MG-NA	-5.05	1.94	2.06
27	l	402	CLA	MG-NB	-5.04	1.95	2.05
27	H	307	CLA	MG-NA	-5.04	1.94	2.06
27	F	601	CLA	C1B-NB	5.04	1.44	1.37
27	E	611	CLA	C1B-NB	5.04	1.44	1.37
27	a	810	CLA	MG-NA	-5.04	1.94	2.06
27	J	605	CLA	MG-NA	-5.04	1.94	2.06
27	D	607	CLA	MG-NA	-5.04	1.94	2.06
27	A	610	CLA	MG-NA	-5.04	1.94	2.06
27	C	201	CLA	MG-NA	-5.04	1.94	2.06
27	K	603	CLA	MG-NB	-5.04	1.95	2.05
27	D	607	CLA	C1B-NB	5.03	1.44	1.37
27	A	605	CLA	MG-NB	-5.03	1.95	2.05
27	J	607	CLA	MG-NA	-5.03	1.94	2.06
27	b	710	CLA	C1B-NB	5.03	1.44	1.37
27	E	602	CLA	C1B-NB	5.03	1.44	1.37
27	C	206	CLA	MG-NB	-5.03	1.95	2.05
27	G	605	CLA	C1B-NB	5.03	1.44	1.37
27	K	601	CLA	MG-NA	-5.03	1.94	2.06
27	a	825	CLA	C1B-NB	5.03	1.44	1.37
27	a	817	CLA	C1B-NB	5.02	1.44	1.37
27	G	609	CLA	C1B-NB	5.02	1.44	1.37
27	H	303	CLA	MG-NB	-5.02	1.95	2.05
27	I	606	CLA	C1B-NB	5.02	1.44	1.37
27	r	204	CLA	C1B-NB	5.02	1.44	1.37
27	G	603	CLA	MG-NA	-5.02	1.94	2.06
27	a	815	CLA	MG-NB	-5.02	1.95	2.05
27	I	610	CLA	C1B-NB	5.02	1.44	1.37
27	D	612	CLA	C1B-NB	5.02	1.44	1.37
27	B	610	CLA	C1B-NB	5.02	1.44	1.37
27	b	722	CLA	C1B-NB	5.01	1.44	1.37
27	A	601	CLA	MG-NA	-5.01	1.94	2.06
27	A	602	CLA	MG-NA	-5.01	1.94	2.06
27	A	605	CLA	C1B-NB	5.01	1.44	1.37
27	A	611	CLA	MG-NB	-5.01	1.95	2.05
27	b	715	CLA	C1B-NB	5.01	1.44	1.37
27	H	319	CLA	MG-NA	-5.01	1.94	2.06
27	D	601	CLA	C1B-NB	5.01	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	720	CLA	MG-NA	-5.01	1.94	2.06
27	b	706	CLA	MG-NA	-5.01	1.94	2.06
27	D	604	CLA	C1B-NB	5.00	1.44	1.37
27	J	601	CLA	C1B-NB	5.00	1.44	1.37
27	K	605	CLA	C1B-NB	5.00	1.44	1.37
27	G	607	CLA	C1B-NB	5.00	1.44	1.37
27	a	827	CLA	C1B-NB	5.00	1.44	1.37
27	b	701	CLA	C1B-NB	5.00	1.44	1.37
27	I	616	CLA	C1B-NB	5.00	1.44	1.37
27	b	708	CLA	MG-NA	-5.00	1.94	2.06
27	E	603	CLA	C1B-NB	5.00	1.44	1.37
27	f	302	CLA	C1B-NB	5.00	1.44	1.37
27	K	602	CLA	C1B-NB	5.00	1.44	1.37
27	a	815	CLA	MG-NA	-5.00	1.94	2.06
27	G	606	CLA	C1B-NB	5.00	1.44	1.37
27	E	609	CLA	MG-NA	-5.00	1.94	2.06
27	B	607	CLA	C1B-NB	5.00	1.44	1.37
27	A	605	CLA	MG-NA	-5.00	1.94	2.06
27	A	612	CLA	C1B-NB	5.00	1.44	1.37
27	F	607	CLA	C1B-NB	5.00	1.44	1.37
27	T	603	CLA	MG-NA	-5.00	1.94	2.06
27	B	606	CLA	C1B-NB	4.99	1.44	1.37
27	a	822	CLA	MG-NA	-4.99	1.94	2.06
27	E	612	CLA	MG-NA	-4.99	1.94	2.06
27	l	406	CLA	MG-NB	-4.99	1.95	2.05
27	J	603	CLA	C1B-NB	4.99	1.44	1.37
27	U	606	CLA	MG-NB	-4.99	1.95	2.05
27	a	829	CLA	C1B-NB	4.99	1.44	1.37
27	a	814	CLA	MG-NB	-4.99	1.95	2.05
27	T	603	CLA	C1B-NB	4.99	1.44	1.37
27	E	606	CLA	MG-NA	-4.99	1.94	2.06
27	C	208	CLA	C1B-NB	4.98	1.44	1.37
27	E	602	CLA	MG-NA	-4.98	1.94	2.06
27	b	713	CLA	C1B-NB	4.98	1.44	1.37
27	K	604	CLA	MG-NA	-4.98	1.94	2.06
27	C	211	CLA	C1B-NB	4.98	1.44	1.37
27	A	609	CLA	C1B-NB	4.98	1.44	1.37
27	A	609	CLA	MG-NA	-4.98	1.94	2.06
27	b	726	CLA	C1B-NB	4.98	1.44	1.37
27	U	606	CLA	MG-NA	-4.98	1.94	2.06
27	E	604	CLA	MG-NA	-4.98	1.94	2.06
27	b	711	CLA	MG-NA	-4.97	1.94	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	604	CLA	C1B-NB	4.97	1.44	1.37
27	F	617	CLA	MG-NA	-4.97	1.94	2.06
27	I	609	CLA	C1B-NB	4.97	1.44	1.37
27	H	307	CLA	C1B-NB	4.97	1.44	1.37
27	G	607	CLA	MG-NA	-4.97	1.94	2.06
27	A	606	CLA	MG-NA	-4.96	1.94	2.06
27	C	204	CLA	MG-NA	-4.96	1.94	2.06
27	G	610	CLA	MG-NB	-4.96	1.95	2.05
27	a	817	CLA	MG-NB	-4.96	1.96	2.05
27	b	705	CLA	C1B-NB	4.96	1.44	1.37
27	B	605	CLA	MG-NA	-4.96	1.94	2.06
27	C	205	CLA	C1B-NB	4.96	1.44	1.37
27	F	608	CLA	MG-NA	-4.96	1.94	2.06
27	A	601	CLA	C1B-NB	4.96	1.44	1.37
27	a	819	CLA	MG-NA	-4.96	1.94	2.06
27	r	204	CLA	MG-NA	-4.96	1.94	2.06
27	C	211	CLA	MG-NA	-4.96	1.94	2.06
27	b	724	CLA	C1B-NB	4.96	1.44	1.37
27	J	605	CLA	C1B-NB	4.95	1.44	1.37
27	F	601	CLA	MG-NA	-4.95	1.94	2.06
27	a	819	CLA	C1B-NB	4.95	1.44	1.37
27	C	202	CLA	MG-NA	-4.95	1.94	2.06
27	A	610	CLA	C1B-NB	4.95	1.44	1.37
27	b	727	CLA	C1B-NB	4.95	1.44	1.37
27	I	616	CLA	MG-NB	-4.95	1.96	2.05
27	U	605	CLA	MG-NA	-4.95	1.94	2.06
27	I	602	CLA	MG-NA	-4.95	1.94	2.06
27	b	709	CLA	MG-NA	-4.95	1.94	2.06
27	H	304	CLA	MG-NA	-4.95	1.94	2.06
27	a	822	CLA	C1B-NB	4.95	1.44	1.37
27	E	604	CLA	C1B-NB	4.95	1.44	1.37
27	A	606	CLA	C1B-NB	4.94	1.44	1.37
27	I	601	CLA	MG-NA	-4.94	1.94	2.06
27	a	805	CLA	C1B-NB	4.94	1.44	1.37
27	K	602	CLA	MG-NA	-4.94	1.94	2.06
27	H	306	CLA	MG-NA	-4.94	1.94	2.06
27	I	603	CLA	C1B-NB	4.94	1.44	1.37
27	b	717	CLA	MG-NA	-4.94	1.94	2.06
27	C	206	CLA	C1B-NB	4.94	1.44	1.37
27	F	604	CLA	MG-NB	-4.94	1.96	2.05
27	D	603	CLA	C1B-NB	4.94	1.44	1.37
27	A	604	CLA	MG-NA	-4.94	1.94	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	605	CLA	C1B-NB	4.94	1.44	1.37
27	D	608	CLA	C1B-NB	4.94	1.44	1.37
27	l	411	CLA	C1B-NB	4.94	1.44	1.37
27	H	312	CLA	MG-NA	-4.93	1.94	2.06
27	F	605	CLA	MG-NA	-4.93	1.94	2.06
27	D	605	CLA	C1B-NB	4.93	1.44	1.37
27	D	611	CLA	MG-NA	-4.93	1.94	2.06
27	F	619	CLA	MG-NA	-4.93	1.94	2.06
27	b	728	CLA	C1B-NB	4.93	1.44	1.37
27	a	823	CLA	C1B-NB	4.92	1.44	1.37
27	F	602	CLA	C1B-NB	4.92	1.44	1.37
27	a	830	CLA	C1B-NB	4.92	1.44	1.37
27	I	607	CLA	C1B-NB	4.92	1.44	1.37
27	D	610	CLA	MG-NB	-4.92	1.96	2.05
27	b	728	CLA	MG-NA	-4.92	1.94	2.06
27	C	204	CLA	C1B-NB	4.92	1.44	1.37
27	F	606	CLA	C1B-NB	4.91	1.44	1.37
27	l	408	CLA	C1B-NB	4.91	1.44	1.37
27	l	409	CLA	MG-NA	-4.91	1.94	2.06
32	J	615	PID	O6-C30	4.91	1.46	1.35
27	a	810	CLA	MG-NB	-4.91	1.96	2.05
29	F	613	UIX	O2-C27	4.91	1.46	1.35
32	U	608	PID	O6-C30	4.91	1.46	1.35
27	f	302	CLA	MG-NB	-4.91	1.96	2.05
27	I	605	CLA	C1B-NB	4.91	1.44	1.37
27	E	608	CLA	C1B-NB	4.90	1.44	1.37
27	H	312	CLA	C1B-NB	4.90	1.44	1.37
27	B	609	CLA	MG-NA	-4.90	1.94	2.06
27	A	607	CLA	MG-NA	-4.90	1.94	2.06
27	B	610	CLA	MG-NB	-4.90	1.96	2.05
27	a	824	CLA	C1B-NB	4.90	1.44	1.37
27	a	807	CLA	C1B-NB	4.90	1.44	1.37
27	H	319	CLA	C1B-NB	4.89	1.44	1.37
27	b	716	CLA	C1B-NB	4.89	1.44	1.37
27	D	606	CLA	C1B-NB	4.89	1.44	1.37
27	I	601	CLA	C1B-NB	4.89	1.44	1.37
27	H	308	CLA	MG-NA	-4.89	1.94	2.06
27	D	602	CLA	C1B-NB	4.89	1.44	1.37
27	a	810	CLA	C1B-NB	4.89	1.44	1.37
27	A	603	CLA	MG-NA	-4.89	1.94	2.06
27	F	619	CLA	C1B-NB	4.88	1.44	1.37
27	l	412	CLA	C1B-NB	4.88	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	603	CLA	MG-NA	-4.88	1.94	2.06
27	A	603	CLA	C1B-NB	4.88	1.44	1.37
27	a	839	CLA	C1B-NB	4.88	1.44	1.37
27	b	702	CLA	MG-NA	-4.88	1.94	2.06
27	a	814	CLA	MG-NA	-4.88	1.94	2.06
29	D	616	UIX	O2-C27	4.88	1.46	1.35
27	G	603	CLA	C1B-NB	4.88	1.44	1.37
27	b	725	CLA	C1B-NB	4.88	1.44	1.37
27	I	616	CLA	MG-NA	-4.88	1.94	2.06
27	b	719	CLA	C1B-NB	4.88	1.44	1.37
27	b	701	CLA	MG-NA	-4.88	1.94	2.06
32	B	613	PID	O6-C30	4.87	1.46	1.35
27	G	602	CLA	MG-NA	-4.87	1.94	2.06
27	E	607	CLA	MG-NA	-4.87	1.94	2.06
27	B	601	CLA	C1B-NB	4.87	1.44	1.37
27	b	712	CLA	C1B-NB	4.87	1.44	1.37
27	T	607	CLA	MG-NA	-4.87	1.94	2.06
27	a	806	CLA	MG-NA	-4.87	1.94	2.06
29	A	613	UIX	O2-C27	4.87	1.46	1.35
29	G	615	UIX	O2-C27	4.87	1.46	1.35
27	F	617	CLA	C1B-NB	4.87	1.44	1.37
27	I	602	CLA	C1B-NB	4.86	1.44	1.37
27	H	304	CLA	MG-NB	-4.86	1.96	2.05
27	T	605	CLA	C1B-NB	4.86	1.44	1.37
27	l	406	CLA	C1B-NB	4.86	1.44	1.37
27	K	605	CLA	MG-NA	-4.86	1.94	2.06
29	B	611	UIX	O2-C27	4.86	1.45	1.35
27	B	609	CLA	C1B-NB	4.86	1.44	1.37
29	B	615	UIX	O2-C27	4.86	1.45	1.35
29	J	616	UIX	O2-C27	4.86	1.45	1.35
27	H	305	CLA	C1B-NB	4.86	1.44	1.37
27	a	804	CLA	C1B-NB	4.85	1.44	1.37
27	l	409	CLA	C1B-NB	4.85	1.44	1.37
27	I	605	CLA	MG-NA	-4.85	1.94	2.06
27	D	601	CLA	MG-NA	-4.85	1.94	2.06
32	I	614	PID	O6-C30	4.85	1.45	1.35
29	E	616	UIX	O2-C27	4.85	1.45	1.35
27	a	818	CLA	C1B-NB	4.85	1.44	1.37
27	D	611	CLA	C1B-NB	4.84	1.44	1.37
29	j	204	UIX	O2-C27	4.84	1.45	1.35
27	H	308	CLA	C1B-NB	4.84	1.44	1.37
32	F	615	PID	O6-C30	4.84	1.45	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	837	CLA	MG-NA	-4.84	1.94	2.06
27	D	606	CLA	MG-NA	-4.84	1.94	2.06
27	F	603	CLA	C1B-NB	4.83	1.44	1.37
27	b	706	CLA	C1B-NB	4.83	1.44	1.37
29	A	616	UIX	O2-C27	4.83	1.45	1.35
27	b	704	CLA	C1B-NB	4.83	1.44	1.37
27	G	610	CLA	MG-NA	-4.83	1.94	2.06
27	l	403	CLA	C1B-NB	4.83	1.44	1.37
27	F	604	CLA	MG-NA	-4.83	1.94	2.06
29	C	215	UIX	O2-C27	4.83	1.45	1.35
27	E	607	CLA	C1B-NB	4.82	1.44	1.37
29	T	612	UIX	O2-C27	4.82	1.45	1.35
27	B	607	CLA	MG-NA	-4.82	1.94	2.06
27	a	826	CLA	MG-NA	-4.82	1.94	2.06
32	J	614	PID	O6-C30	4.82	1.45	1.35
27	b	725	CLA	MG-NA	-4.82	1.94	2.06
27	a	831	CLA	C1B-NB	4.81	1.44	1.37
27	F	604	CLA	C1B-NB	4.81	1.44	1.37
27	a	801	CLA	MG-NA	-4.80	1.94	2.06
27	C	203	CLA	C1B-NB	4.80	1.44	1.37
27	B	610	CLA	MG-NA	-4.80	1.94	2.06
27	b	726	CLA	MG-NA	-4.80	1.94	2.06
27	I	608	CLA	C1B-NB	4.80	1.44	1.37
29	H	314	UIX	O2-C27	4.79	1.45	1.35
27	a	804	CLA	MG-NA	-4.79	1.94	2.06
29	C	213	UIX	O2-C27	4.79	1.45	1.35
29	H	317	UIX	O2-C27	4.78	1.45	1.35
27	a	821	CLA	C1B-NB	4.78	1.44	1.37
27	H	303	CLA	C1B-NB	4.78	1.44	1.37
27	C	206	CLA	MG-NA	-4.78	1.94	2.06
27	a	831	CLA	MG-NA	-4.77	1.94	2.06
27	a	802	CLA	C1B-NB	4.76	1.44	1.37
32	F	614	PID	O6-C30	4.76	1.45	1.35
27	T	604	CLA	MG-NA	-4.76	1.95	2.06
32	K	611	PID	O6-C30	4.75	1.45	1.35
27	D	605	CLA	MG-NA	-4.74	1.95	2.06
32	J	613	PID	O6-C30	4.74	1.45	1.35
27	f	302	CLA	MG-NA	-4.74	1.95	2.06
27	H	304	CLA	C1B-NB	4.73	1.44	1.37
27	I	608	CLA	MG-NA	-4.73	1.95	2.06
27	T	605	CLA	MG-NA	-4.73	1.95	2.06
27	H	303	CLA	MG-NA	-4.73	1.95	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	815	CLA	C1B-NB	4.72	1.44	1.37
27	b	717	CLA	C1B-NB	4.71	1.44	1.37
27	a	817	CLA	MG-NA	-4.70	1.95	2.06
27	a	820	CLA	C1B-NB	4.69	1.44	1.37
27	b	703	CLA	C1B-NB	4.68	1.44	1.37
27	D	610	CLA	MG-NA	-4.67	1.95	2.06
32	J	611	PID	O6-C30	4.65	1.45	1.35
32	J	614	PID	C13-C12	4.65	1.49	1.36
32	F	615	PID	C13-C12	4.64	1.49	1.36
29	I	612	UIX	O2-C27	4.64	1.45	1.35
27	b	707	CLA	C1B-NB	4.61	1.43	1.37
32	I	614	PID	C13-C12	4.59	1.49	1.36
27	b	709	CLA	C1B-NB	4.58	1.43	1.37
29	j	204	UIX	C25-C20	-4.58	1.25	1.30
29	I	612	UIX	C25-C20	-4.57	1.25	1.30
32	K	611	PID	C13-C12	4.57	1.49	1.36
32	B	613	PID	C13-C12	4.56	1.49	1.36
27	G	609	CLA	MG-NA	-4.55	1.95	2.06
27	l	404	CLA	C1B-NB	4.54	1.43	1.37
27	a	801	CLA	C1B-NB	4.54	1.43	1.37
27	b	708	CLA	C1B-NB	4.54	1.43	1.37
32	K	611	PID	C23-C24	-4.54	1.25	1.30
32	J	615	PID	C13-C12	4.50	1.48	1.36
32	U	608	PID	C13-C12	4.49	1.48	1.36
32	F	614	PID	C13-C12	4.49	1.48	1.36
29	B	611	UIX	C25-C20	-4.47	1.25	1.30
32	J	613	PID	C23-C24	-4.46	1.25	1.30
31	y	301	SQD	O8-S	4.45	1.64	1.47
27	b	718	CLA	C1B-NB	4.43	1.43	1.37
27	a	826	CLA	C1B-NB	4.42	1.43	1.37
31	H	320	SQD	O8-S	4.42	1.63	1.47
31	A	618	SQD	O8-S	4.41	1.63	1.47
32	J	613	PID	C13-C12	4.36	1.48	1.36
27	a	837	CLA	C1B-NB	4.34	1.43	1.37
32	J	611	PID	C13-C12	4.31	1.48	1.36
31	y	301	SQD	O47-C7	4.29	1.46	1.34
31	y	301	SQD	O48-C23	4.28	1.45	1.33
31	H	320	SQD	O48-C23	4.24	1.45	1.33
27	b	702	CLA	C1B-NB	4.21	1.43	1.37
29	j	204	UIX	C25-C28	-4.17	1.25	1.31
29	C	215	UIX	C25-C20	-4.17	1.25	1.30
29	B	611	UIX	C25-C28	-4.17	1.25	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	614	PID	C23-C24	-4.16	1.25	1.30
32	K	611	PID	C23-C22	-4.10	1.25	1.31
29	I	612	UIX	C25-C28	-4.09	1.25	1.31
29	H	314	UIX	C25-C20	-4.09	1.25	1.30
27	U	606	CLA	C4B-NB	4.08	1.43	1.37
31	A	618	SQD	O47-C7	4.07	1.45	1.34
29	B	615	UIX	C25-C20	-4.04	1.25	1.30
32	U	608	PID	C23-C24	-4.04	1.25	1.30
32	J	613	PID	C23-C22	-4.04	1.25	1.31
29	T	612	UIX	C25-C20	-4.03	1.25	1.30
27	f	302	CLA	C4B-NB	4.03	1.43	1.37
29	J	616	UIX	C25-C20	-4.02	1.25	1.30
29	G	615	UIX	C25-C20	-4.01	1.25	1.30
29	A	616	UIX	C25-C20	-4.01	1.25	1.30
29	E	616	UIX	C25-C20	-4.00	1.25	1.30
32	B	613	PID	C23-C24	-3.99	1.25	1.30
27	I	616	CLA	C4B-NB	3.98	1.43	1.37
27	a	828	CLA	MG-NC	-3.97	1.96	2.06
32	I	614	PID	C23-C24	-3.97	1.26	1.30
29	A	613	UIX	C25-C20	-3.95	1.26	1.30
27	a	812	CLA	MG-NC	-3.94	1.96	2.06
31	H	320	SQD	O47-C7	3.94	1.45	1.34
27	F	608	CLA	C4B-NB	3.93	1.43	1.37
27	A	611	CLA	C4B-NB	3.92	1.43	1.37
27	a	811	CLA	C4B-NB	3.92	1.43	1.37
27	C	205	CLA	MG-NC	-3.91	1.97	2.06
27	K	603	CLA	C4B-NB	3.90	1.43	1.37
27	U	605	CLA	C4B-NB	3.90	1.43	1.37
27	G	610	CLA	C4B-NB	3.90	1.43	1.37
27	F	610	CLA	C4B-NB	3.90	1.43	1.37
27	U	601	CLA	MG-NC	-3.90	1.97	2.06
27	A	612	CLA	MG-NC	-3.89	1.97	2.06
27	I	611	CLA	MG-NC	-3.89	1.97	2.06
27	T	606	CLA	C4B-NB	3.89	1.43	1.37
27	T	607	CLA	C4B-NB	3.88	1.43	1.37
27	T	609	CLA	C4B-NB	3.88	1.43	1.37
32	J	611	PID	C23-C24	-3.88	1.26	1.30
29	F	613	UIX	C25-C20	-3.87	1.26	1.30
27	b	703	CLA	MG-NC	-3.87	1.97	2.06
27	D	609	CLA	C4B-NB	3.87	1.42	1.37
27	D	610	CLA	C4B-NB	3.87	1.42	1.37
27	J	607	CLA	C4B-NB	3.86	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	813	CLA	C4B-NB	3.86	1.42	1.37
27	j	202	CLA	C4B-NB	3.86	1.42	1.37
27	G	605	CLA	MG-NC	-3.85	1.97	2.06
27	C	202	CLA	C4B-NB	3.84	1.42	1.37
27	C	212	CLA	C4B-NB	3.84	1.42	1.37
27	A	604	CLA	C4B-NB	3.84	1.42	1.37
27	a	810	CLA	C4B-NB	3.84	1.42	1.37
27	a	814	CLA	C4B-NB	3.84	1.42	1.37
27	E	609	CLA	C4B-NB	3.84	1.42	1.37
27	G	604	CLA	C4B-NB	3.84	1.42	1.37
27	I	611	CLA	C4B-NB	3.84	1.42	1.37
27	B	606	CLA	MG-NC	-3.83	1.97	2.06
27	A	607	CLA	C4B-NB	3.83	1.42	1.37
27	A	605	CLA	C4B-NB	3.83	1.42	1.37
29	D	616	UIX	C25-C20	-3.83	1.26	1.30
27	T	604	CLA	C4B-NB	3.82	1.42	1.37
27	l	402	CLA	C4B-NB	3.82	1.42	1.37
27	H	313	CLA	MG-NC	-3.82	1.97	2.06
27	f	303	CLA	C4B-NB	3.81	1.42	1.37
27	a	809	CLA	MG-NC	-3.81	1.97	2.06
27	F	601	CLA	C4B-NB	3.81	1.42	1.37
27	a	808	CLA	C4B-NB	3.81	1.42	1.37
27	T	602	CLA	C4B-NB	3.80	1.42	1.37
27	K	606	CLA	C4B-NB	3.80	1.42	1.37
27	l	406	CLA	C4B-NB	3.80	1.42	1.37
27	B	610	CLA	C4B-NB	3.80	1.42	1.37
27	a	820	CLA	MG-NC	-3.80	1.97	2.06
27	E	612	CLA	C4B-NB	3.80	1.42	1.37
32	F	615	PID	C23-C24	-3.79	1.26	1.30
27	b	721	CLA	MG-NC	-3.79	1.97	2.06
27	B	604	CLA	MG-NC	-3.79	1.97	2.06
27	a	829	CLA	C4B-NB	3.79	1.42	1.37
27	a	823	CLA	MG-NC	-3.79	1.97	2.06
27	E	602	CLA	C4B-NB	3.78	1.42	1.37
29	C	215	UIX	C25-C28	-3.78	1.25	1.31
29	H	314	UIX	C25-C28	-3.78	1.25	1.31
27	b	724	CLA	C4B-NB	3.78	1.42	1.37
27	G	611	CLA	C4B-NB	3.78	1.42	1.37
27	C	209	CLA	C4B-NB	3.78	1.42	1.37
29	A	616	UIX	C25-C28	-3.77	1.25	1.31
27	a	817	CLA	C4B-NB	3.77	1.42	1.37
27	G	608	CLA	C4B-NB	3.77	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	H	310	CLA	MG-NC	-3.77	1.97	2.06
27	a	805	CLA	C4B-NB	3.77	1.42	1.37
27	K	602	CLA	C4B-NB	3.77	1.42	1.37
27	b	712	CLA	MG-NC	-3.77	1.97	2.06
27	I	610	CLA	MG-NC	-3.76	1.97	2.06
27	E	606	CLA	C4B-NB	3.76	1.42	1.37
29	G	615	UIX	C25-C28	-3.76	1.25	1.31
27	b	705	CLA	MG-NC	-3.76	1.97	2.06
27	J	609	CLA	C4B-NB	3.76	1.42	1.37
27	K	606	CLA	MG-NC	-3.76	1.97	2.06
27	l	410	CLA	C4B-NB	3.76	1.42	1.37
27	I	608	CLA	C4B-NB	3.75	1.42	1.37
27	l	410	CLA	MG-NC	-3.75	1.97	2.06
27	l	408	CLA	MG-NC	-3.75	1.97	2.06
27	B	603	CLA	MG-NC	-3.75	1.97	2.06
27	H	305	CLA	C4B-NB	3.75	1.42	1.37
27	K	605	CLA	C4B-NB	3.75	1.42	1.37
27	l	407	CLA	C4B-NB	3.75	1.42	1.37
27	F	617	CLA	C4B-NB	3.74	1.42	1.37
27	U	601	CLA	C4B-NB	3.74	1.42	1.37
27	T	601	CLA	MG-NC	-3.74	1.97	2.06
32	F	614	PID	C23-C22	-3.74	1.25	1.31
28	U	602	KC2	C1B-NB	3.74	1.42	1.37
27	G	608	CLA	MG-NC	-3.74	1.97	2.06
27	D	611	CLA	C4B-NB	3.74	1.42	1.37
27	D	612	CLA	C4B-NB	3.74	1.42	1.37
27	a	824	CLA	MG-NC	-3.74	1.97	2.06
27	K	608	CLA	C4B-NB	3.73	1.42	1.37
27	H	310	CLA	C4B-NB	3.73	1.42	1.37
27	G	609	CLA	C4B-NB	3.73	1.42	1.37
27	A	602	CLA	C4B-NB	3.73	1.42	1.37
29	T	612	UIX	C25-C28	-3.73	1.25	1.31
27	C	211	CLA	C4B-NB	3.73	1.42	1.37
27	H	309	CLA	C4B-NB	3.73	1.42	1.37
32	J	614	PID	C23-C24	-3.73	1.26	1.30
27	B	605	CLA	C4B-NB	3.73	1.42	1.37
27	b	714	CLA	MG-NC	-3.73	1.97	2.06
32	I	614	PID	C23-C22	-3.73	1.25	1.31
27	D	602	CLA	MG-NC	-3.73	1.97	2.06
27	b	715	CLA	MG-NC	-3.73	1.97	2.06
29	B	615	UIX	C25-C28	-3.73	1.25	1.31
27	T	601	CLA	C4B-NB	3.73	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	603	CLA	C4B-NB	3.72	1.42	1.37
27	j	202	CLA	MG-NC	-3.72	1.97	2.06
27	E	608	CLA	C4B-NB	3.72	1.42	1.37
27	B	607	CLA	C4B-NB	3.71	1.42	1.37
27	J	603	CLA	C4B-NB	3.71	1.42	1.37
27	b	716	CLA	C4B-NB	3.71	1.42	1.37
27	a	802	CLA	MG-NC	-3.71	1.97	2.06
27	F	607	CLA	C4B-NB	3.71	1.42	1.37
27	T	609	CLA	MG-NC	-3.71	1.97	2.06
27	B	609	CLA	C4B-NB	3.71	1.42	1.37
28	J	604	KC2	C1B-NB	3.71	1.42	1.37
27	a	825	CLA	C4B-NB	3.70	1.42	1.37
27	a	822	CLA	C4B-NB	3.70	1.42	1.37
27	H	313	CLA	C4B-NB	3.70	1.42	1.37
27	C	208	CLA	C4B-NB	3.70	1.42	1.37
27	K	604	CLA	C4B-NB	3.70	1.42	1.37
27	I	607	CLA	C4B-NB	3.70	1.42	1.37
27	b	728	CLA	C4B-NB	3.70	1.42	1.37
27	E	603	CLA	C4B-NB	3.70	1.42	1.37
27	l	404	CLA	MG-NC	-3.69	1.97	2.06
27	a	827	CLA	C4B-NB	3.69	1.42	1.37
27	J	609	CLA	C3A-C2A	-3.69	1.51	1.54
27	I	609	CLA	MG-NC	-3.69	1.97	2.06
27	B	604	CLA	C4B-NB	3.69	1.42	1.37
27	H	319	CLA	C4B-NB	3.69	1.42	1.37
27	b	718	CLA	MG-NC	-3.69	1.97	2.06
27	G	607	CLA	C4B-NB	3.69	1.42	1.37
27	b	719	CLA	MG-NC	-3.69	1.97	2.06
27	f	303	CLA	MG-NC	-3.69	1.97	2.06
27	D	603	CLA	MG-NC	-3.69	1.97	2.06
27	D	605	CLA	C4B-NB	3.68	1.42	1.37
29	A	613	UIX	C25-C28	-3.68	1.25	1.31
27	E	611	CLA	C4B-NB	3.68	1.42	1.37
27	G	606	CLA	C4B-NB	3.68	1.42	1.37
27	C	206	CLA	C4B-NB	3.68	1.42	1.37
27	b	704	CLA	C4B-NB	3.68	1.42	1.37
27	E	611	CLA	MG-NC	-3.68	1.97	2.06
27	b	716	CLA	MG-NC	-3.68	1.97	2.06
27	a	815	CLA	C4B-NB	3.68	1.42	1.37
27	a	807	CLA	MG-NC	-3.68	1.97	2.06
27	a	809	CLA	C4B-NB	3.68	1.42	1.37
27	C	207	CLA	C4B-NB	3.68	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	721	CLA	C4B-NB	3.67	1.42	1.37
27	T	605	CLA	C4B-NB	3.67	1.42	1.37
27	F	619	CLA	C4B-NB	3.67	1.42	1.37
27	a	808	CLA	MG-NC	-3.67	1.97	2.06
27	A	601	CLA	C4B-NB	3.67	1.42	1.37
27	a	828	CLA	C4B-NB	3.67	1.42	1.37
27	T	602	CLA	MG-NC	-3.67	1.97	2.06
27	a	806	CLA	C4B-NB	3.67	1.42	1.37
27	C	201	CLA	C4B-NB	3.66	1.42	1.37
27	b	701	CLA	C4B-NB	3.66	1.42	1.37
27	b	707	CLA	MG-NC	-3.66	1.97	2.06
27	G	604	CLA	MG-NC	-3.66	1.97	2.06
27	A	610	CLA	C4B-NB	3.66	1.42	1.37
27	a	807	CLA	C4B-NB	3.66	1.42	1.37
27	a	816	CLA	C4B-NB	3.66	1.42	1.37
27	K	601	CLA	C4B-NB	3.65	1.42	1.37
27	E	603	CLA	MG-NC	-3.65	1.97	2.06
27	C	209	CLA	MG-NC	-3.65	1.97	2.06
27	I	605	CLA	C4B-NB	3.65	1.42	1.37
27	C	203	CLA	MG-NC	-3.65	1.97	2.06
27	l	407	CLA	MG-NC	-3.65	1.97	2.06
27	b	726	CLA	C4B-NB	3.65	1.42	1.37
27	I	606	CLA	MG-NC	-3.64	1.97	2.06
27	b	720	CLA	C4B-NB	3.64	1.42	1.37
27	J	601	CLA	MG-NC	-3.64	1.97	2.06
27	I	601	CLA	C4B-NB	3.64	1.42	1.37
32	U	608	PID	O3-C10	3.64	1.28	1.21
27	r	203	CLA	MG-NC	-3.64	1.97	2.06
32	J	613	PID	O3-C10	3.64	1.28	1.21
27	H	305	CLA	MG-NC	-3.64	1.97	2.06
27	a	801	CLA	MG-NC	-3.64	1.97	2.06
28	K	607	KC2	C1B-NB	3.64	1.42	1.37
29	H	317	UIX	C25-C28	-3.64	1.26	1.31
27	D	601	CLA	C4B-NB	3.64	1.42	1.37
27	E	605	CLA	MG-NC	-3.63	1.97	2.06
32	J	615	PID	O3-C10	3.63	1.28	1.21
27	E	604	CLA	C4B-NB	3.63	1.42	1.37
27	r	204	CLA	C4B-NB	3.63	1.42	1.37
27	F	603	CLA	MG-NC	-3.63	1.97	2.06
27	b	710	CLA	MG-NC	-3.63	1.97	2.06
27	F	605	CLA	C4B-NB	3.63	1.42	1.37
27	G	606	CLA	MG-NC	-3.63	1.97	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	812	CLA	C4B-NB	3.63	1.42	1.37
27	G	603	CLA	C4B-NB	3.63	1.42	1.37
27	I	606	CLA	C4B-NB	3.63	1.42	1.37
27	a	819	CLA	C4B-NB	3.63	1.42	1.37
27	A	609	CLA	C4B-NB	3.63	1.42	1.37
29	E	616	UIX	C25-C28	-3.62	1.26	1.31
27	b	713	CLA	C4B-NB	3.62	1.42	1.37
27	H	304	CLA	C4B-NB	3.62	1.42	1.37
27	C	205	CLA	C4B-NB	3.62	1.42	1.37
27	r	203	CLA	C4B-NB	3.62	1.42	1.37
27	l	405	CLA	MG-NC	-3.62	1.97	2.06
28	F	609	KC2	C1B-NB	3.62	1.42	1.37
27	U	603	CLA	MG-NC	-3.62	1.97	2.06
27	I	607	CLA	MG-NC	-3.62	1.97	2.06
27	K	608	CLA	MG-NC	-3.62	1.97	2.06
27	A	606	CLA	C4B-NB	3.62	1.42	1.37
27	H	303	CLA	C4B-NB	3.62	1.42	1.37
27	b	712	CLA	C4B-NB	3.61	1.42	1.37
27	C	204	CLA	C4B-NB	3.61	1.42	1.37
27	E	605	CLA	C4B-NB	3.61	1.42	1.37
27	T	603	CLA	C4B-NB	3.61	1.42	1.37
27	a	804	CLA	C4B-NB	3.61	1.42	1.37
27	l	412	CLA	MG-NC	-3.61	1.97	2.06
27	G	602	CLA	C4B-NB	3.61	1.42	1.37
27	I	609	CLA	C4B-NB	3.61	1.42	1.37
27	a	820	CLA	C4B-NB	3.61	1.42	1.37
27	a	829	CLA	MG-NC	-3.61	1.97	2.06
29	D	616	UIX	C25-C28	-3.60	1.26	1.31
27	J	609	CLA	MG-NC	-3.60	1.97	2.06
27	b	711	CLA	C4B-NB	3.60	1.42	1.37
27	a	816	CLA	MG-NC	-3.60	1.97	2.06
32	U	608	PID	C23-C22	-3.60	1.26	1.31
27	D	607	CLA	C4B-NB	3.60	1.42	1.37
29	C	213	UIX	C25-C20	-3.60	1.26	1.30
29	H	317	UIX	C25-C20	-3.60	1.26	1.30
27	K	606	CLA	C3A-C2A	-3.60	1.51	1.54
29	J	616	UIX	C25-C28	-3.60	1.26	1.31
27	F	610	CLA	MG-NC	-3.60	1.97	2.06
27	I	602	CLA	C4B-NB	3.60	1.42	1.37
27	D	608	CLA	C4B-NB	3.59	1.42	1.37
27	F	604	CLA	C4B-NB	3.59	1.42	1.37
27	a	831	CLA	C4B-NB	3.59	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	710	CLA	C4B-NB	3.59	1.42	1.37
27	D	612	CLA	MG-NC	-3.59	1.97	2.06
27	D	604	CLA	C4B-NB	3.59	1.42	1.37
27	a	839	CLA	C4B-NB	3.59	1.42	1.37
32	F	615	PID	O3-C10	3.59	1.28	1.21
27	A	612	CLA	C4B-NB	3.59	1.42	1.37
27	D	608	CLA	MG-NC	-3.59	1.97	2.06
27	B	606	CLA	C4B-NB	3.58	1.42	1.37
28	C	210	KC2	C1B-NB	3.58	1.42	1.37
28	I	604	KC2	C4C-NC	3.58	1.43	1.37
27	C	203	CLA	C4B-NB	3.58	1.42	1.37
27	a	827	CLA	MG-NC	-3.58	1.97	2.06
27	F	606	CLA	C4B-NB	3.58	1.42	1.37
27	l	408	CLA	C4B-NB	3.58	1.42	1.37
27	F	602	CLA	MG-NC	-3.58	1.97	2.06
27	a	803	CLA	C4B-NB	3.58	1.42	1.37
27	F	602	CLA	C4B-NB	3.58	1.42	1.37
27	F	607	CLA	MG-NC	-3.57	1.97	2.06
27	H	306	CLA	C4B-NB	3.57	1.42	1.37
27	l	411	CLA	C4B-NB	3.57	1.42	1.37
27	b	723	CLA	C4B-NB	3.57	1.42	1.37
28	J	608	KC2	C1B-NB	3.57	1.42	1.37
27	J	605	CLA	C4B-NB	3.57	1.42	1.37
27	J	603	CLA	MG-NC	-3.57	1.97	2.06
32	J	614	PID	O3-C10	3.56	1.28	1.21
27	a	823	CLA	C4B-NB	3.56	1.42	1.37
28	U	604	KC2	C1B-NB	3.56	1.42	1.37
32	F	614	PID	O3-C10	3.56	1.28	1.21
27	D	606	CLA	C4B-NB	3.56	1.42	1.37
27	H	312	CLA	C4B-NB	3.56	1.42	1.37
27	C	204	CLA	MG-NC	-3.56	1.97	2.06
27	G	607	CLA	MG-NC	-3.56	1.97	2.06
27	E	607	CLA	C4B-NB	3.56	1.42	1.37
27	I	603	CLA	C4B-NB	3.56	1.42	1.37
27	b	706	CLA	C4B-NB	3.56	1.42	1.37
27	J	601	CLA	C4B-NB	3.56	1.42	1.37
28	E	610	KC2	C1B-NB	3.56	1.42	1.37
27	G	611	CLA	MG-NC	-3.56	1.97	2.06
27	G	605	CLA	C4B-NB	3.56	1.42	1.37
27	C	208	CLA	MG-NC	-3.55	1.97	2.06
27	b	705	CLA	C4B-NB	3.55	1.42	1.37
27	D	603	CLA	C4B-NB	3.55	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	602	CLA	MG-NC	-3.55	1.97	2.06
27	C	212	CLA	MG-NC	-3.55	1.97	2.06
27	A	603	CLA	C4B-NB	3.55	1.42	1.37
27	a	830	CLA	C4B-NB	3.55	1.42	1.37
27	D	609	CLA	MG-NC	-3.55	1.97	2.06
27	a	802	CLA	C4B-NB	3.55	1.42	1.37
27	l	405	CLA	C4B-NB	3.55	1.42	1.37
29	C	213	UIX	C25-C28	-3.54	1.26	1.31
27	b	722	CLA	C4B-NB	3.54	1.42	1.37
27	a	818	CLA	MG-NC	-3.54	1.97	2.06
27	a	811	CLA	MG-NC	-3.54	1.97	2.06
32	B	613	PID	C23-C22	-3.54	1.26	1.31
27	l	409	CLA	C4B-NB	3.54	1.42	1.37
27	b	711	CLA	MG-NC	-3.54	1.97	2.06
27	l	403	CLA	MG-NC	-3.54	1.97	2.06
27	H	307	CLA	C4B-NB	3.54	1.42	1.37
27	a	839	CLA	MG-NC	-3.53	1.97	2.06
27	b	727	CLA	MG-NC	-3.53	1.97	2.06
27	H	307	CLA	MG-NC	-3.53	1.97	2.06
32	B	613	PID	O3-C10	3.52	1.28	1.21
27	A	602	CLA	MG-NC	-3.52	1.97	2.06
32	I	614	PID	O3-C10	3.52	1.28	1.21
27	a	810	CLA	MG-NC	-3.52	1.97	2.06
27	J	607	CLA	MG-NC	-3.52	1.97	2.06
27	b	715	CLA	C4B-NB	3.52	1.42	1.37
27	l	402	CLA	MG-NC	-3.52	1.97	2.06
29	F	613	UIX	C25-C28	-3.52	1.26	1.31
27	D	604	CLA	MG-NC	-3.52	1.97	2.06
27	B	605	CLA	MG-NC	-3.52	1.97	2.06
27	b	702	CLA	C4B-NB	3.52	1.42	1.37
32	F	615	PID	C23-C22	-3.52	1.26	1.31
27	b	706	CLA	MG-NC	-3.52	1.97	2.06
27	a	825	CLA	MG-NC	-3.51	1.97	2.06
27	J	605	CLA	MG-NC	-3.51	1.97	2.06
28	H	302	KC2	C1B-NB	3.51	1.42	1.37
28	J	606	KC2	C4C-NC	3.51	1.43	1.37
27	H	308	CLA	C4B-NB	3.51	1.42	1.37
27	E	606	CLA	MG-NC	-3.51	1.97	2.06
27	A	603	CLA	MG-NC	-3.50	1.97	2.06
27	l	411	CLA	MG-NC	-3.50	1.97	2.06
27	b	727	CLA	C4B-NB	3.50	1.42	1.37
27	b	714	CLA	C4B-NB	3.50	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	604	CLA	MG-NC	-3.50	1.98	2.06
27	E	609	CLA	MG-NC	-3.49	1.98	2.06
27	b	704	CLA	MG-NC	-3.49	1.98	2.06
27	b	722	CLA	MG-NC	-3.49	1.98	2.06
27	H	304	CLA	MG-NC	-3.49	1.98	2.06
27	H	309	CLA	MG-NC	-3.49	1.98	2.06
27	b	713	CLA	MG-NC	-3.49	1.98	2.06
27	C	211	CLA	MG-NC	-3.49	1.98	2.06
27	E	608	CLA	MG-NC	-3.48	1.98	2.06
27	a	803	CLA	MG-NC	-3.48	1.98	2.06
27	C	201	CLA	MG-NC	-3.48	1.98	2.06
27	b	720	CLA	MG-NC	-3.48	1.98	2.06
27	A	605	CLA	MG-NC	-3.47	1.98	2.06
27	b	717	CLA	C4B-NB	3.47	1.42	1.37
27	C	207	CLA	MG-NC	-3.47	1.98	2.06
27	E	612	CLA	MG-NC	-3.47	1.98	2.06
27	G	603	CLA	MG-NC	-3.47	1.98	2.06
27	F	603	CLA	C4B-NB	3.47	1.42	1.37
27	D	602	CLA	C4B-NB	3.47	1.42	1.37
28	G	601	KC2	C1B-NB	3.47	1.42	1.37
27	A	607	CLA	MG-NC	-3.46	1.98	2.06
27	a	805	CLA	MG-NC	-3.46	1.98	2.06
27	T	606	CLA	MG-NC	-3.46	1.98	2.06
27	B	601	CLA	MG-NC	-3.46	1.98	2.06
28	H	311	KC2	C1B-NB	3.46	1.42	1.37
27	b	724	CLA	MG-NC	-3.46	1.98	2.06
32	J	615	PID	C23-C24	-3.46	1.26	1.30
27	r	204	CLA	MG-NC	-3.46	1.98	2.06
27	U	606	CLA	MG-NC	-3.45	1.98	2.06
27	A	611	CLA	MG-NC	-3.45	1.98	2.06
27	U	605	CLA	MG-NC	-3.45	1.98	2.06
27	b	707	CLA	C4B-NB	3.45	1.42	1.37
27	a	830	CLA	MG-NC	-3.45	1.98	2.06
27	l	406	CLA	MG-NC	-3.45	1.98	2.06
27	A	601	CLA	MG-NC	-3.45	1.98	2.06
27	D	611	CLA	MG-NC	-3.45	1.98	2.06
27	A	606	CLA	MG-NC	-3.45	1.98	2.06
27	A	609	CLA	MG-NC	-3.45	1.98	2.06
27	b	719	CLA	C4B-NB	3.44	1.42	1.37
27	I	601	CLA	MG-NC	-3.44	1.98	2.06
28	T	608	KC2	C4C-NC	3.44	1.43	1.37
32	J	614	PID	C23-C22	-3.44	1.26	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	822	CLA	MG-NC	-3.43	1.98	2.06
27	E	607	CLA	MG-NC	-3.43	1.98	2.06
27	B	601	CLA	C4B-NB	3.43	1.42	1.37
27	D	607	CLA	MG-NC	-3.43	1.98	2.06
27	b	723	CLA	MG-NC	-3.43	1.98	2.06
27	a	813	CLA	MG-NC	-3.42	1.98	2.06
27	K	601	CLA	MG-NC	-3.42	1.98	2.06
27	I	610	CLA	C4B-NB	3.42	1.42	1.37
28	K	607	KC2	C4C-NC	3.42	1.43	1.37
27	H	312	CLA	MG-NC	-3.42	1.98	2.06
27	a	821	CLA	MG-NC	-3.42	1.98	2.06
27	A	604	CLA	MG-NC	-3.42	1.98	2.06
27	I	616	CLA	MG-NC	-3.42	1.98	2.06
28	F	609	KC2	C4C-NC	3.42	1.43	1.37
28	J	602	KC2	C1B-NB	3.42	1.42	1.37
27	U	603	CLA	C4B-NB	3.42	1.42	1.37
27	K	603	CLA	MG-NC	-3.42	1.98	2.06
27	a	824	CLA	C4B-NB	3.42	1.42	1.37
27	C	202	CLA	MG-NC	-3.41	1.98	2.06
27	F	601	CLA	MG-NC	-3.41	1.98	2.06
28	C	210	KC2	C4C-NC	3.41	1.43	1.37
27	H	319	CLA	MG-NC	-3.41	1.98	2.06
27	l	412	CLA	C4B-NB	3.41	1.42	1.37
32	J	611	PID	O3-C10	3.40	1.28	1.21
27	T	607	CLA	MG-NC	-3.40	1.98	2.06
27	A	610	CLA	MG-NC	-3.39	1.98	2.06
27	F	617	CLA	MG-NC	-3.39	1.98	2.06
27	G	610	CLA	MG-NC	-3.39	1.98	2.06
27	a	821	CLA	C4B-NB	3.39	1.42	1.37
27	b	718	CLA	C4B-NB	3.39	1.42	1.37
27	F	608	CLA	MG-NC	-3.39	1.98	2.06
27	E	602	CLA	MG-NC	-3.39	1.98	2.06
32	J	611	PID	C23-C22	-3.39	1.26	1.31
27	B	609	CLA	MG-NC	-3.38	1.98	2.06
28	E	601	KC2	C1B-NB	3.38	1.42	1.37
27	a	826	CLA	MG-NC	-3.38	1.98	2.06
27	a	817	CLA	MG-NC	-3.38	1.98	2.06
27	b	728	CLA	MG-NC	-3.38	1.98	2.06
27	a	804	CLA	MG-NC	-3.38	1.98	2.06
27	I	602	CLA	MG-NC	-3.38	1.98	2.06
27	a	801	CLA	C4B-NB	3.37	1.42	1.37
28	I	604	KC2	C1B-NB	3.37	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	603	CLA	MG-NC	-3.37	1.98	2.06
27	F	606	CLA	MG-NC	-3.37	1.98	2.06
27	l	403	CLA	C4B-NB	3.37	1.42	1.37
28	J	608	KC2	C4C-NC	3.37	1.43	1.37
28	T	608	KC2	C1B-NB	3.37	1.42	1.37
28	J	610	KC2	C1B-NB	3.37	1.42	1.37
28	H	311	KC2	C4C-NC	3.37	1.43	1.37
28	E	601	KC2	C4C-NC	3.36	1.43	1.37
27	I	608	CLA	MG-NC	-3.36	1.98	2.06
27	a	831	CLA	MG-NC	-3.36	1.98	2.06
28	B	602	KC2	C1B-NB	3.35	1.42	1.37
27	b	709	CLA	C4B-NB	3.34	1.42	1.37
28	E	610	KC2	C4C-NC	3.34	1.43	1.37
27	b	725	CLA	C4B-NB	3.34	1.42	1.37
27	K	604	CLA	MG-NC	-3.34	1.98	2.06
27	F	619	CLA	MG-NC	-3.32	1.98	2.06
27	F	605	CLA	MG-NC	-3.32	1.98	2.06
28	J	606	KC2	C1B-NB	3.32	1.42	1.37
27	a	815	CLA	MG-NC	-3.32	1.98	2.06
28	U	604	KC2	C4C-NC	3.32	1.43	1.37
27	T	604	CLA	MG-NC	-3.31	1.98	2.06
27	T	603	CLA	MG-NC	-3.31	1.98	2.06
27	b	708	CLA	C4B-NB	3.31	1.42	1.37
27	B	607	CLA	MG-NC	-3.31	1.98	2.06
27	a	837	CLA	MG-NC	-3.30	1.98	2.06
27	b	726	CLA	MG-NC	-3.30	1.98	2.06
27	a	818	CLA	C4B-NB	3.30	1.42	1.37
28	J	610	KC2	C4C-NC	3.30	1.43	1.37
27	a	819	CLA	MG-NC	-3.30	1.98	2.06
27	b	701	CLA	MG-NC	-3.30	1.98	2.06
27	D	606	CLA	MG-NC	-3.29	1.98	2.06
27	b	702	CLA	MG-NC	-3.29	1.98	2.06
27	B	610	CLA	MG-NC	-3.29	1.98	2.06
27	b	708	CLA	MG-NC	-3.29	1.98	2.06
28	U	602	KC2	C4C-NC	3.29	1.43	1.37
27	b	703	CLA	C4B-NB	3.28	1.42	1.37
27	G	609	CLA	MG-NC	-3.28	1.98	2.06
27	b	717	CLA	MG-NC	-3.28	1.98	2.06
32	J	615	PID	C23-C22	-3.28	1.26	1.31
27	H	308	CLA	MG-NC	-3.28	1.98	2.06
28	J	604	KC2	C4C-NC	3.28	1.43	1.37
28	J	602	KC2	C4C-NC	3.27	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	601	CLA	MG-NC	-3.27	1.98	2.06
27	K	605	CLA	MG-NC	-3.27	1.98	2.06
27	H	306	CLA	MG-NC	-3.27	1.98	2.06
27	T	609	CLA	C3A-C2A	-3.27	1.51	1.54
27	f	302	CLA	MG-NC	-3.27	1.98	2.06
27	G	602	CLA	MG-NC	-3.26	1.98	2.06
28	H	302	KC2	C4C-NC	3.25	1.43	1.37
28	B	608	KC2	C1B-NB	3.25	1.42	1.37
28	G	601	KC2	C4C-NC	3.25	1.43	1.37
27	D	605	CLA	MG-NC	-3.24	1.98	2.06
27	a	814	CLA	MG-NC	-3.24	1.98	2.06
27	a	826	CLA	C4B-NB	3.23	1.42	1.37
27	l	409	CLA	MG-NC	-3.23	1.98	2.06
27	b	709	CLA	MG-NC	-3.23	1.98	2.06
28	B	608	KC2	C4C-NC	3.23	1.43	1.37
28	A	608	KC2	C4C-NC	3.22	1.43	1.37
27	F	604	CLA	MG-NC	-3.20	1.98	2.06
27	H	303	CLA	MG-NC	-3.19	1.98	2.06
27	I	605	CLA	MG-NC	-3.19	1.98	2.06
27	C	206	CLA	MG-NC	-3.18	1.98	2.06
27	b	725	CLA	MG-NC	-3.18	1.98	2.06
27	a	806	CLA	MG-NC	-3.18	1.98	2.06
32	K	611	PID	O3-C10	3.17	1.28	1.21
28	B	602	KC2	C4C-NC	3.17	1.43	1.37
28	A	608	KC2	C1B-NB	3.16	1.42	1.37
27	l	404	CLA	C4B-NB	3.16	1.42	1.37
27	D	610	CLA	MG-NC	-3.15	1.98	2.06
27	T	605	CLA	MG-NC	-3.14	1.98	2.06
27	T	604	CLA	C3A-C2A	-3.02	1.51	1.54
27	a	837	CLA	C4B-NB	2.83	1.41	1.37
32	J	613	PID	C11-C12	-2.82	1.38	1.44
32	K	611	PID	C25-C24	-2.75	1.49	1.54
29	A	616	UIX	O-C1	-2.62	1.42	1.46
31	A	618	SQD	O48-C23	2.62	1.46	1.33
32	J	613	PID	C25-C24	-2.54	1.50	1.54
32	J	611	PID	C11-C12	-2.53	1.39	1.44
29	C	215	UIX	O-C1	-2.51	1.43	1.46
29	I	612	UIX	C15-C20	-2.50	1.50	1.54
35	j	201	DGD	O2G-C2G	-2.50	1.40	1.46
29	C	213	UIX	C15-C20	-2.50	1.50	1.54
27	a	837	CLA	C3D-C4D	-2.49	1.38	1.44
29	B	611	UIX	C15-C20	-2.49	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	l	416	DGD	O2G-C2G	-2.47	1.40	1.46
32	J	611	PID	O1-C1	-2.45	1.43	1.46
29	D	616	UIX	O-C1	-2.44	1.43	1.46
29	B	615	UIX	O-C1	-2.44	1.43	1.46
38	a	836	BCR	C1-C6	-2.43	1.50	1.53
27	b	702	CLA	C1D-C2D	-2.42	1.40	1.45
35	l	416	DGD	O1G-C1G	-2.41	1.39	1.45
29	E	616	UIX	O-C1	-2.40	1.43	1.46
27	D	604	CLA	C1D-C2D	-2.38	1.40	1.45
29	H	314	UIX	O-C1	-2.38	1.43	1.46
35	f	305	DGD	O2G-C2G	-2.38	1.41	1.46
27	H	304	CLA	C1D-C2D	-2.37	1.40	1.45
27	K	605	CLA	C1D-C2D	-2.36	1.40	1.45
27	a	830	CLA	C1D-C2D	-2.36	1.40	1.45
35	j	201	DGD	O5D-C6D	-2.36	1.39	1.43
27	I	608	CLA	C1D-C2D	-2.35	1.40	1.45
29	B	611	UIX	O-C1	-2.35	1.43	1.46
27	G	606	CLA	C1D-C2D	-2.35	1.40	1.45
27	T	605	CLA	C1D-C2D	-2.34	1.40	1.45
27	I	602	CLA	C1D-C2D	-2.34	1.40	1.45
27	b	708	CLA	C1D-C2D	-2.33	1.40	1.45
27	a	827	CLA	C1D-C2D	-2.32	1.40	1.45
27	A	606	CLA	C1D-C2D	-2.32	1.40	1.45
27	a	839	CLA	C1D-C2D	-2.31	1.40	1.45
27	D	606	CLA	C1D-C2D	-2.31	1.40	1.45
27	a	817	CLA	C1D-C2D	-2.31	1.40	1.45
27	K	604	CLA	C1D-C2D	-2.31	1.40	1.45
29	J	616	UIX	O-C1	-2.31	1.43	1.46
27	D	610	CLA	C1D-C2D	-2.31	1.40	1.45
27	D	605	CLA	C1D-C2D	-2.30	1.40	1.45
29	A	613	UIX	O-C1	-2.30	1.43	1.46
27	C	204	CLA	C1D-C2D	-2.30	1.40	1.45
27	l	406	CLA	C1D-C2D	-2.30	1.40	1.45
27	a	801	CLA	C1D-C2D	-2.29	1.40	1.45
27	F	602	CLA	C1D-C2D	-2.29	1.40	1.45
27	a	822	CLA	C1D-C2D	-2.29	1.40	1.45
27	a	824	CLA	C3D-C4D	-2.29	1.39	1.44
27	a	804	CLA	C1D-C2D	-2.29	1.40	1.45
27	a	831	CLA	C1D-C2D	-2.29	1.40	1.45
27	a	826	CLA	C3D-C4D	-2.29	1.39	1.44
27	a	805	CLA	C1D-C2D	-2.29	1.40	1.45
27	a	818	CLA	C1D-C2D	-2.29	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	203	CLA	C3D-C4D	-2.28	1.39	1.44
27	E	603	CLA	C1D-C2D	-2.28	1.40	1.45
29	F	613	UIX	O-C1	-2.28	1.43	1.46
27	B	609	CLA	C1D-C2D	-2.28	1.40	1.45
27	B	607	CLA	C1D-C2D	-2.28	1.40	1.45
27	F	604	CLA	C1D-C2D	-2.28	1.40	1.45
29	E	616	UIX	C15-C20	-2.28	1.50	1.54
27	l	411	CLA	C1D-C2D	-2.28	1.40	1.45
27	G	609	CLA	C1D-C2D	-2.28	1.40	1.45
27	E	607	CLA	C1D-C2D	-2.28	1.40	1.45
27	a	821	CLA	C3D-C4D	-2.28	1.39	1.44
27	C	204	CLA	C3D-C4D	-2.28	1.39	1.44
27	H	305	CLA	C1D-C2D	-2.28	1.40	1.45
27	f	302	CLA	C1D-C2D	-2.28	1.40	1.45
27	b	717	CLA	C1D-C2D	-2.28	1.40	1.45
27	C	205	CLA	C1D-C2D	-2.28	1.40	1.45
35	K	614	DGD	O1G-C1G	-2.28	1.40	1.45
27	D	611	CLA	C1D-C2D	-2.27	1.40	1.45
27	A	603	CLA	C1D-C2D	-2.27	1.40	1.45
27	a	809	CLA	C1D-C2D	-2.27	1.40	1.45
27	F	617	CLA	C1D-C2D	-2.27	1.40	1.45
27	I	616	CLA	C1D-C2D	-2.27	1.40	1.45
27	a	802	CLA	C1D-C2D	-2.27	1.40	1.45
27	b	705	CLA	C1D-C2D	-2.27	1.40	1.45
27	a	826	CLA	C1D-C2D	-2.27	1.40	1.45
27	I	601	CLA	C1D-C2D	-2.27	1.40	1.45
27	j	202	CLA	C1D-C2D	-2.27	1.40	1.45
27	b	723	CLA	C1D-C2D	-2.27	1.40	1.45
27	D	603	CLA	C1D-C2D	-2.27	1.40	1.45
27	b	725	CLA	C1D-C2D	-2.27	1.40	1.45
27	l	411	CLA	C3D-C4D	-2.27	1.39	1.44
27	F	619	CLA	C1D-C2D	-2.27	1.40	1.45
27	G	603	CLA	C1D-C2D	-2.27	1.40	1.45
27	D	605	CLA	C3D-C4D	-2.26	1.39	1.44
27	b	727	CLA	C1D-C2D	-2.26	1.40	1.45
27	l	409	CLA	C1D-C2D	-2.26	1.40	1.45
27	a	803	CLA	C3D-C4D	-2.26	1.39	1.44
38	a	836	BCR	C30-C25	-2.26	1.50	1.53
27	a	823	CLA	C1D-C2D	-2.26	1.40	1.45
27	b	706	CLA	C1D-C2D	-2.26	1.40	1.45
27	l	403	CLA	C1D-C2D	-2.26	1.40	1.45
27	l	403	CLA	C3D-C4D	-2.26	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	706	CLA	C3D-C4D	-2.26	1.39	1.44
27	A	609	CLA	C1D-C2D	-2.26	1.40	1.45
27	b	703	CLA	C1D-C2D	-2.26	1.40	1.45
27	b	726	CLA	C1D-C2D	-2.26	1.40	1.45
27	E	603	CLA	C3D-C4D	-2.26	1.39	1.44
32	F	614	PID	C11-C12	-2.26	1.39	1.44
27	a	830	CLA	C3D-C4D	-2.26	1.39	1.44
27	l	408	CLA	C1D-C2D	-2.26	1.40	1.45
27	I	610	CLA	C3D-C4D	-2.26	1.39	1.44
27	b	715	CLA	C3D-C4D	-2.26	1.39	1.44
27	D	602	CLA	C1D-C2D	-2.25	1.40	1.45
27	b	718	CLA	C3D-C4D	-2.25	1.39	1.44
27	l	404	CLA	C3D-C4D	-2.25	1.39	1.44
29	G	615	UIX	O-C1	-2.25	1.43	1.46
27	G	602	CLA	C1D-C2D	-2.25	1.40	1.45
27	b	725	CLA	C3D-C4D	-2.25	1.39	1.44
27	H	307	CLA	C1D-C2D	-2.25	1.40	1.45
27	b	724	CLA	C1D-C2D	-2.25	1.40	1.45
32	U	608	PID	C25-C24	-2.25	1.50	1.54
27	C	212	CLA	C1D-C2D	-2.25	1.40	1.45
27	r	204	CLA	C1D-C2D	-2.25	1.40	1.45
27	E	609	CLA	C1D-C2D	-2.25	1.40	1.45
27	H	319	CLA	C1D-C2D	-2.25	1.40	1.45
27	B	604	CLA	C3D-C4D	-2.25	1.39	1.44
27	C	203	CLA	C1D-C2D	-2.25	1.40	1.45
27	K	602	CLA	C1D-C2D	-2.25	1.40	1.45
27	b	701	CLA	C1D-C2D	-2.25	1.40	1.45
27	I	606	CLA	C1D-C2D	-2.25	1.40	1.45
27	I	607	CLA	C1D-C2D	-2.25	1.40	1.45
27	a	810	CLA	C1D-C2D	-2.25	1.40	1.45
27	a	825	CLA	C3D-C4D	-2.25	1.39	1.44
27	a	820	CLA	C3D-C4D	-2.25	1.39	1.44
27	B	605	CLA	C1D-C2D	-2.25	1.40	1.45
27	b	710	CLA	C1D-C2D	-2.25	1.40	1.45
27	b	718	CLA	C1D-C2D	-2.25	1.40	1.45
27	A	602	CLA	C3D-C4D	-2.25	1.39	1.44
27	C	208	CLA	C1D-C2D	-2.24	1.40	1.45
27	B	601	CLA	C1D-C2D	-2.24	1.40	1.45
27	b	728	CLA	C1D-C2D	-2.24	1.40	1.45
27	G	606	CLA	C3D-C4D	-2.24	1.39	1.44
27	D	603	CLA	C3D-C4D	-2.24	1.39	1.44
27	F	601	CLA	C3D-C4D	-2.24	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	606	CLA	C3D-C4D	-2.24	1.39	1.44
27	D	612	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	825	CLA	C1D-C2D	-2.24	1.40	1.45
27	l	402	CLA	C3D-C4D	-2.24	1.39	1.44
27	A	602	CLA	C1D-C2D	-2.24	1.40	1.45
27	b	723	CLA	C3D-C4D	-2.24	1.39	1.44
27	D	601	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	814	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	829	CLA	C1D-C2D	-2.24	1.40	1.45
27	D	604	CLA	C3D-C4D	-2.24	1.39	1.44
32	J	614	PID	O1-C1	-2.24	1.43	1.46
27	b	707	CLA	C3D-C4D	-2.24	1.39	1.44
27	a	839	CLA	C3D-C4D	-2.24	1.39	1.44
27	b	709	CLA	C1D-C2D	-2.24	1.40	1.45
27	a	815	CLA	C1D-C2D	-2.24	1.40	1.45
27	H	319	CLA	C3D-C4D	-2.24	1.39	1.44
27	a	820	CLA	C1D-C2D	-2.24	1.40	1.45
27	C	211	CLA	C1D-C2D	-2.24	1.40	1.45
27	D	602	CLA	C3D-C4D	-2.24	1.39	1.44
27	a	813	CLA	C1D-C2D	-2.24	1.40	1.45
35	K	614	DGD	C4D-C5D	2.24	1.57	1.53
27	b	720	CLA	C1D-C2D	-2.24	1.40	1.45
27	H	307	CLA	C3D-C4D	-2.24	1.39	1.44
27	T	602	CLA	C1D-C2D	-2.23	1.40	1.45
27	l	406	CLA	C3D-C4D	-2.23	1.39	1.44
27	b	704	CLA	C1D-C2D	-2.23	1.40	1.45
27	A	610	CLA	C1D-C2D	-2.23	1.40	1.45
27	l	402	CLA	C1D-C2D	-2.23	1.40	1.45
27	I	603	CLA	C3D-C4D	-2.23	1.39	1.44
27	F	607	CLA	C1D-C2D	-2.23	1.40	1.45
27	I	606	CLA	C3D-C4D	-2.23	1.39	1.44
27	l	409	CLA	C3D-C4D	-2.23	1.39	1.44
27	A	604	CLA	C1D-C2D	-2.23	1.40	1.45
27	I	610	CLA	C1D-C2D	-2.23	1.40	1.45
27	F	601	CLA	C1D-C2D	-2.23	1.40	1.45
27	b	705	CLA	C3D-C4D	-2.23	1.39	1.44
27	b	722	CLA	C1D-C2D	-2.23	1.40	1.45
27	D	607	CLA	C3D-C4D	-2.23	1.39	1.44
27	H	303	CLA	C1D-C2D	-2.23	1.40	1.45
27	J	601	CLA	C1D-C2D	-2.23	1.40	1.45
27	l	407	CLA	C1D-C2D	-2.23	1.40	1.45
32	B	613	PID	O1-C1	-2.23	1.43	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	603	CLA	C1D-C2D	-2.23	1.40	1.45
29	T	612	UIX	O-C1	-2.23	1.43	1.46
27	D	608	CLA	C3D-C4D	-2.22	1.39	1.44
27	b	719	CLA	C3D-C4D	-2.22	1.39	1.44
27	J	605	CLA	C1D-C2D	-2.22	1.40	1.45
27	U	605	CLA	C1D-C2D	-2.22	1.40	1.45
27	a	809	CLA	C3D-C4D	-2.22	1.39	1.44
27	I	603	CLA	C1D-C2D	-2.22	1.40	1.45
27	H	310	CLA	C3D-C4D	-2.22	1.39	1.44
27	a	824	CLA	C1D-C2D	-2.22	1.40	1.45
27	b	711	CLA	C1D-C2D	-2.22	1.40	1.45
27	A	612	CLA	C3D-C4D	-2.22	1.39	1.44
27	b	716	CLA	C3D-C4D	-2.22	1.39	1.44
27	H	308	CLA	C1D-C2D	-2.22	1.40	1.45
27	b	719	CLA	C1D-C2D	-2.22	1.40	1.45
27	C	205	CLA	C3D-C4D	-2.22	1.39	1.44
27	I	602	CLA	C3D-C4D	-2.22	1.39	1.44
27	b	712	CLA	C3D-C4D	-2.22	1.39	1.44
27	A	601	CLA	C1D-C2D	-2.22	1.40	1.45
27	F	606	CLA	C1D-C2D	-2.22	1.40	1.45
27	H	312	CLA	C1D-C2D	-2.22	1.40	1.45
27	J	607	CLA	C1D-C2D	-2.22	1.40	1.45
27	C	201	CLA	C3D-C4D	-2.22	1.39	1.44
27	H	312	CLA	C3D-C4D	-2.22	1.39	1.44
27	E	611	CLA	C1D-C2D	-2.22	1.40	1.45
27	a	819	CLA	C1D-C2D	-2.22	1.40	1.45
27	l	404	CLA	C1D-C2D	-2.22	1.40	1.45
27	G	605	CLA	C1D-C2D	-2.22	1.40	1.45
27	H	303	CLA	C3D-C4D	-2.22	1.39	1.44
27	b	714	CLA	C3D-C4D	-2.22	1.39	1.44
27	C	201	CLA	C1D-C2D	-2.22	1.40	1.45
27	H	313	CLA	C3D-C4D	-2.22	1.39	1.44
27	G	608	CLA	C1D-C2D	-2.22	1.40	1.45
27	G	603	CLA	C3D-C4D	-2.21	1.39	1.44
27	b	728	CLA	C3D-C4D	-2.21	1.39	1.44
27	a	816	CLA	C1D-C2D	-2.21	1.41	1.45
27	r	203	CLA	C3D-C4D	-2.21	1.39	1.44
27	b	711	CLA	C3D-C4D	-2.21	1.39	1.44
27	b	713	CLA	C3D-C4D	-2.21	1.39	1.44
27	G	611	CLA	C1D-C2D	-2.21	1.41	1.45
27	K	608	CLA	C1D-C2D	-2.21	1.41	1.45
27	b	712	CLA	C1D-C2D	-2.21	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	l	412	CLA	C1D-C2D	-2.21	1.41	1.45
27	a	805	CLA	C3D-C4D	-2.21	1.39	1.44
27	F	619	CLA	C3D-C4D	-2.21	1.39	1.44
27	a	807	CLA	C1D-C2D	-2.21	1.41	1.45
27	l	405	CLA	C1D-C2D	-2.21	1.41	1.45
27	a	816	CLA	C3D-C4D	-2.21	1.39	1.44
27	b	721	CLA	C3D-C4D	-2.21	1.39	1.44
27	C	208	CLA	C3D-C4D	-2.21	1.39	1.44
27	a	812	CLA	C1D-C2D	-2.21	1.41	1.45
27	G	610	CLA	C1D-C2D	-2.21	1.41	1.45
27	A	606	CLA	C3D-C4D	-2.21	1.39	1.44
27	a	823	CLA	C3D-C4D	-2.21	1.39	1.44
27	b	720	CLA	C3D-C4D	-2.21	1.39	1.44
27	F	603	CLA	C1D-C2D	-2.21	1.41	1.45
27	E	602	CLA	C1D-C2D	-2.21	1.41	1.45
27	l	408	CLA	C3D-C4D	-2.21	1.39	1.44
27	b	714	CLA	C1D-C2D	-2.21	1.41	1.45
27	a	804	CLA	C3D-C4D	-2.21	1.39	1.44
27	I	605	CLA	C1D-C2D	-2.21	1.41	1.45
27	f	303	CLA	C1D-C2D	-2.21	1.41	1.45
27	a	810	CLA	C3D-C4D	-2.20	1.39	1.44
27	E	604	CLA	C1D-C2D	-2.20	1.41	1.45
27	E	608	CLA	C1D-C2D	-2.20	1.41	1.45
27	E	612	CLA	C1D-C2D	-2.20	1.41	1.45
27	G	611	CLA	C3D-C4D	-2.20	1.39	1.44
27	J	603	CLA	C3D-C4D	-2.20	1.39	1.44
27	G	604	CLA	C1D-C2D	-2.20	1.41	1.45
27	r	203	CLA	C1D-C2D	-2.20	1.41	1.45
27	b	724	CLA	C3D-C4D	-2.20	1.39	1.44
27	b	709	CLA	C3D-C4D	-2.20	1.39	1.44
27	C	202	CLA	C1D-C2D	-2.20	1.41	1.45
27	G	607	CLA	C1D-C2D	-2.20	1.41	1.45
27	D	611	CLA	C3D-C4D	-2.20	1.39	1.44
27	l	405	CLA	C3D-C4D	-2.20	1.39	1.44
27	a	811	CLA	C1D-C2D	-2.20	1.41	1.45
27	a	829	CLA	C3D-C4D	-2.20	1.39	1.44
27	E	611	CLA	C3D-C4D	-2.20	1.39	1.44
27	b	708	CLA	C3D-C4D	-2.20	1.39	1.44
27	l	410	CLA	C1D-C2D	-2.20	1.41	1.45
27	A	603	CLA	C3D-C4D	-2.20	1.39	1.44
27	a	828	CLA	C3D-C4D	-2.20	1.39	1.44
32	B	613	PID	C25-C24	-2.20	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	607	CLA	C1D-C2D	-2.20	1.41	1.45
27	H	306	CLA	C1D-C2D	-2.20	1.41	1.45
27	U	603	CLA	C1D-C2D	-2.20	1.41	1.45
27	G	605	CLA	C3D-C4D	-2.20	1.39	1.44
27	J	605	CLA	C3D-C4D	-2.20	1.39	1.44
27	E	605	CLA	C1D-C2D	-2.20	1.41	1.45
29	H	317	UIX	O-C1	-2.20	1.43	1.46
27	B	606	CLA	C3D-C4D	-2.20	1.39	1.44
27	b	717	CLA	C3D-C4D	-2.20	1.39	1.44
27	B	604	CLA	C1D-C2D	-2.20	1.41	1.45
27	K	603	CLA	C3D-C4D	-2.20	1.39	1.44
27	b	704	CLA	C3D-C4D	-2.20	1.39	1.44
32	I	614	PID	O1-C1	-2.20	1.43	1.46
27	T	603	CLA	C1D-C2D	-2.20	1.41	1.45
32	J	615	PID	O1-C1	-2.19	1.43	1.46
27	I	601	CLA	C3D-C4D	-2.19	1.39	1.44
27	D	612	CLA	C3D-C4D	-2.19	1.39	1.44
27	C	207	CLA	C1D-C2D	-2.19	1.41	1.45
27	C	209	CLA	C1D-C2D	-2.19	1.41	1.45
27	D	609	CLA	C1D-C2D	-2.19	1.41	1.45
27	B	609	CLA	C3D-C4D	-2.19	1.39	1.44
27	E	602	CLA	C3D-C4D	-2.19	1.39	1.44
27	a	821	CLA	C1D-C2D	-2.19	1.41	1.45
27	B	601	CLA	C3D-C4D	-2.19	1.39	1.44
27	b	727	CLA	C3D-C4D	-2.19	1.39	1.44
27	l	410	CLA	C3D-C4D	-2.19	1.39	1.44
27	b	701	CLA	C3D-C4D	-2.19	1.39	1.44
27	b	716	CLA	C1D-C2D	-2.19	1.41	1.45
27	A	612	CLA	C1D-C2D	-2.19	1.41	1.45
27	H	309	CLA	C3D-C4D	-2.19	1.39	1.44
29	C	213	UIX	O-C1	-2.19	1.43	1.46
27	F	603	CLA	C3D-C4D	-2.19	1.39	1.44
27	F	610	CLA	C1D-C2D	-2.19	1.41	1.45
27	H	313	CLA	C1D-C2D	-2.19	1.41	1.45
27	A	609	CLA	C3D-C4D	-2.19	1.39	1.44
27	T	601	CLA	C3D-C4D	-2.19	1.39	1.44
27	b	722	CLA	C3D-C4D	-2.19	1.39	1.44
27	T	604	CLA	C1D-C2D	-2.19	1.41	1.45
27	A	605	CLA	C1D-C2D	-2.19	1.41	1.45
27	a	806	CLA	C3D-C4D	-2.19	1.39	1.44
27	a	815	CLA	C3D-C4D	-2.19	1.39	1.44
27	b	710	CLA	C3D-C4D	-2.19	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	818	CLA	C3D-C4D	-2.19	1.39	1.44
27	J	603	CLA	C1D-C2D	-2.18	1.41	1.45
27	B	610	CLA	C3D-C4D	-2.18	1.39	1.44
27	K	601	CLA	C1D-C2D	-2.18	1.41	1.45
27	f	302	CLA	C3D-C4D	-2.18	1.39	1.44
27	H	310	CLA	C1D-C2D	-2.18	1.41	1.45
27	E	606	CLA	C3D-C4D	-2.18	1.39	1.44
27	G	607	CLA	C3D-C4D	-2.18	1.39	1.44
27	E	608	CLA	C3D-C4D	-2.18	1.39	1.44
27	A	605	CLA	C3D-C4D	-2.18	1.39	1.44
27	F	617	CLA	C3D-C4D	-2.18	1.39	1.44
27	I	609	CLA	C3D-C4D	-2.18	1.39	1.44
27	F	605	CLA	C1D-C2D	-2.18	1.41	1.45
27	a	808	CLA	C1D-C2D	-2.18	1.41	1.45
27	l	412	CLA	C3D-C4D	-2.18	1.39	1.44
27	E	605	CLA	C3D-C4D	-2.18	1.39	1.44
27	F	602	CLA	C3D-C4D	-2.18	1.39	1.44
27	K	606	CLA	C3D-C4D	-2.18	1.39	1.44
27	C	212	CLA	C3D-C4D	-2.18	1.39	1.44
27	A	601	CLA	C3D-C4D	-2.18	1.39	1.44
27	I	607	CLA	C3D-C4D	-2.18	1.39	1.44
27	H	309	CLA	C1D-C2D	-2.18	1.41	1.45
27	A	607	CLA	C3D-C4D	-2.17	1.39	1.44
27	b	721	CLA	C1D-C2D	-2.17	1.41	1.45
27	T	602	CLA	C3D-C4D	-2.17	1.39	1.44
27	B	610	CLA	C1D-C2D	-2.17	1.41	1.45
27	D	608	CLA	C1D-C2D	-2.17	1.41	1.45
27	l	407	CLA	C3D-C4D	-2.17	1.39	1.44
27	C	206	CLA	C1D-C2D	-2.17	1.41	1.45
27	K	604	CLA	C3D-C4D	-2.17	1.39	1.44
27	F	608	CLA	C1D-C2D	-2.17	1.41	1.45
27	A	604	CLA	C3D-C4D	-2.17	1.39	1.44
27	C	207	CLA	C3D-C4D	-2.17	1.39	1.44
27	K	601	CLA	C3D-C4D	-2.17	1.39	1.44
27	a	802	CLA	C3D-C4D	-2.17	1.39	1.44
27	a	837	CLA	C1D-C2D	-2.17	1.41	1.45
27	H	308	CLA	C3D-C4D	-2.17	1.39	1.44
27	C	206	CLA	C3D-C4D	-2.17	1.39	1.44
27	T	601	CLA	C1D-C2D	-2.17	1.41	1.45
27	T	606	CLA	C1D-C2D	-2.17	1.41	1.45
27	a	806	CLA	C1D-C2D	-2.17	1.41	1.45
27	U	603	CLA	C3D-C4D	-2.17	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	808	CLA	C3D-C4D	-2.17	1.39	1.44
27	K	602	CLA	C3D-C4D	-2.17	1.39	1.44
27	D	607	CLA	C1D-C2D	-2.17	1.41	1.45
27	a	827	CLA	C3D-C4D	-2.16	1.39	1.44
27	b	726	CLA	C3D-C4D	-2.16	1.39	1.44
32	U	608	PID	O1-C1	-2.16	1.43	1.46
27	E	606	CLA	C1D-C2D	-2.16	1.41	1.45
27	b	707	CLA	C1D-C2D	-2.16	1.41	1.45
27	F	604	CLA	C3D-C4D	-2.16	1.39	1.44
27	T	607	CLA	C1D-C2D	-2.16	1.41	1.45
27	T	607	CLA	C3D-C4D	-2.16	1.39	1.44
27	C	202	CLA	C3D-C4D	-2.16	1.39	1.44
27	C	209	CLA	C3D-C4D	-2.16	1.39	1.44
27	a	812	CLA	C3D-C4D	-2.16	1.39	1.44
27	G	602	CLA	C3D-C4D	-2.16	1.39	1.44
35	f	305	DGD	O1G-C1G	-2.16	1.40	1.45
27	D	609	CLA	C3D-C4D	-2.16	1.39	1.44
27	B	607	CLA	C3D-C4D	-2.16	1.39	1.44
27	I	605	CLA	C3D-C4D	-2.16	1.39	1.44
27	B	605	CLA	C3D-C4D	-2.16	1.39	1.44
27	E	604	CLA	C3D-C4D	-2.16	1.39	1.44
27	a	811	CLA	C3D-C4D	-2.16	1.39	1.44
27	F	607	CLA	C3D-C4D	-2.16	1.39	1.44
27	a	803	CLA	C1D-C2D	-2.16	1.41	1.45
27	a	814	CLA	C3D-C4D	-2.16	1.39	1.44
27	B	606	CLA	C1D-C2D	-2.16	1.41	1.45
27	r	204	CLA	C3D-C4D	-2.16	1.39	1.44
27	U	601	CLA	C1D-C2D	-2.16	1.41	1.45
27	G	604	CLA	C3D-C4D	-2.15	1.39	1.44
27	G	608	CLA	C3D-C4D	-2.15	1.39	1.44
27	J	609	CLA	C3D-C4D	-2.15	1.39	1.44
27	b	713	CLA	C1D-C2D	-2.15	1.41	1.45
27	E	607	CLA	C3D-C4D	-2.15	1.39	1.44
27	B	603	CLA	C3D-C4D	-2.15	1.39	1.44
27	U	606	CLA	C1D-C2D	-2.15	1.41	1.45
27	D	601	CLA	C3D-C4D	-2.15	1.39	1.44
27	H	306	CLA	C3D-C4D	-2.15	1.39	1.44
27	a	822	CLA	C3D-C4D	-2.15	1.39	1.44
27	a	831	CLA	C3D-C4D	-2.15	1.39	1.44
27	a	807	CLA	C3D-C4D	-2.15	1.39	1.44
27	F	605	CLA	C3D-C4D	-2.15	1.39	1.44
27	b	703	CLA	C3D-C4D	-2.15	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	I	614	PID	C25-C24	-2.15	1.50	1.54
32	U	608	PID	C11-C12	-2.15	1.40	1.44
27	E	612	CLA	C3D-C4D	-2.15	1.39	1.44
27	D	610	CLA	C3D-C4D	-2.15	1.39	1.44
27	I	611	CLA	C1D-C2D	-2.15	1.41	1.45
27	b	702	CLA	C3D-C4D	-2.15	1.39	1.44
27	U	605	CLA	C3D-C4D	-2.14	1.39	1.44
27	D	606	CLA	C3D-C4D	-2.14	1.39	1.44
27	I	609	CLA	C1D-C2D	-2.14	1.41	1.45
32	J	615	PID	C11-C12	-2.14	1.40	1.44
27	I	611	CLA	C3D-C4D	-2.14	1.39	1.44
27	J	601	CLA	C3D-C4D	-2.14	1.39	1.44
27	a	819	CLA	C3D-C4D	-2.14	1.39	1.44
27	E	609	CLA	C3D-C4D	-2.14	1.39	1.44
27	J	607	CLA	C3D-C4D	-2.14	1.39	1.44
27	A	610	CLA	C3D-C4D	-2.14	1.39	1.44
27	K	603	CLA	C1D-C2D	-2.14	1.41	1.45
27	U	601	CLA	C3D-C4D	-2.14	1.39	1.44
27	T	609	CLA	C1D-C2D	-2.14	1.41	1.45
27	H	305	CLA	C3D-C4D	-2.13	1.39	1.44
27	A	611	CLA	C1D-C2D	-2.13	1.41	1.45
27	C	211	CLA	C3D-C4D	-2.13	1.39	1.44
27	H	304	CLA	C3D-C4D	-2.13	1.39	1.44
27	K	605	CLA	C3D-C4D	-2.13	1.39	1.44
32	F	615	PID	O1-C1	-2.13	1.43	1.46
27	J	609	CLA	C1D-C2D	-2.13	1.41	1.45
27	K	606	CLA	C1D-C2D	-2.13	1.41	1.45
27	G	609	CLA	C3D-C4D	-2.13	1.39	1.44
29	j	204	UIX	C15-C20	-2.12	1.51	1.54
27	G	610	CLA	C3D-C4D	-2.12	1.39	1.44
27	T	604	CLA	C3D-C4D	-2.12	1.39	1.44
27	T	605	CLA	C3D-C4D	-2.12	1.39	1.44
27	a	817	CLA	C3D-C4D	-2.12	1.39	1.44
27	b	715	CLA	C1D-C2D	-2.11	1.41	1.45
27	F	610	CLA	C3D-C4D	-2.11	1.39	1.44
27	K	608	CLA	C3D-C4D	-2.11	1.39	1.44
27	F	608	CLA	C3D-C4D	-2.11	1.39	1.44
27	T	606	CLA	C3D-C4D	-2.10	1.39	1.44
27	a	813	CLA	C3D-C4D	-2.10	1.39	1.44
27	U	606	CLA	C3D-C4D	-2.10	1.39	1.44
27	I	616	CLA	C3D-C4D	-2.09	1.39	1.44
27	I	608	CLA	C3D-C4D	-2.09	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	615	UIX	C15-C20	-2.09	1.51	1.54
27	A	611	CLA	C3D-C4D	-2.08	1.39	1.44
27	T	609	CLA	C3D-C4D	-2.08	1.39	1.44
27	T	603	CLA	C3D-C4D	-2.08	1.39	1.44
35	j	201	DGD	O1G-C1G	-2.07	1.40	1.45
35	K	614	DGD	O2G-C2G	-2.07	1.41	1.46
27	a	828	CLA	C1D-C2D	-2.06	1.41	1.45
35	K	614	DGD	C4D-C3D	2.05	1.57	1.52
27	f	303	CLA	C3D-C4D	-2.05	1.39	1.44
32	F	615	PID	C11-C12	-2.04	1.40	1.44
29	A	616	UIX	C15-C20	-2.03	1.51	1.54
29	j	204	UIX	O-C1	-2.03	1.43	1.46
29	H	317	UIX	C15-C20	-2.02	1.51	1.54
35	j	201	DGD	O6D-C5D	-2.01	1.39	1.44
32	J	613	PID	O1-C1	-2.01	1.43	1.46
27	j	202	CLA	C3D-C4D	-2.01	1.39	1.44
35	f	305	DGD	C4E-C5E	2.00	1.57	1.53
29	T	612	UIX	C15-C20	-2.00	1.51	1.54

All (2317) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	613	PID	O4-C12-C11	17.74	117.47	107.39
32	J	615	PID	O4-C12-C11	17.60	117.39	107.39
32	J	611	PID	O4-C12-C11	17.60	117.39	107.39
32	U	608	PID	O4-C12-C11	17.23	117.17	107.39
32	F	614	PID	O4-C12-C11	17.17	117.14	107.39
32	F	615	PID	O4-C12-C11	17.05	117.07	107.39
32	I	614	PID	O4-C12-C11	16.88	116.97	107.39
32	B	613	PID	O4-C12-C11	16.71	116.88	107.39
32	K	611	PID	O4-C12-C11	16.64	116.84	107.39
32	J	614	PID	O4-C12-C11	16.45	116.73	107.39
32	J	613	PID	C12-O4-C10	-13.94	100.91	107.68
32	J	611	PID	C12-O4-C10	-13.57	101.09	107.68
32	J	615	PID	C12-O4-C10	-12.68	101.52	107.68
32	F	615	PID	C12-O4-C10	-12.59	101.56	107.68
32	F	614	PID	C12-O4-C10	-12.48	101.62	107.68
32	U	608	PID	C12-O4-C10	-12.32	101.70	107.68
32	K	611	PID	C12-O4-C10	-11.97	101.86	107.68
32	B	613	PID	C12-O4-C10	-11.78	101.96	107.68
32	I	614	PID	C12-O4-C10	-11.49	102.10	107.68
32	J	614	PID	C12-O4-C10	-11.32	102.18	107.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	613	PID	O1-C1-C2	9.17	122.09	113.49
32	I	614	PID	O1-C1-C2	8.82	121.76	113.49
32	F	614	PID	O1-C1-CM1	8.10	124.10	115.05
32	K	611	PID	O1-C1-C2	7.62	120.64	113.49
27	A	612	CLA	C4A-NA-C1A	-7.44	103.28	106.68
27	C	205	CLA	C4A-NA-C1A	-7.43	103.29	106.68
32	J	611	PID	CM1-C1-C6	-7.16	110.52	122.30
27	b	718	CLA	C4A-NA-C1A	-7.03	103.47	106.68
27	a	827	CLA	C4A-NA-C1A	-6.94	103.51	106.68
27	U	601	CLA	C4A-NA-C1A	-6.88	103.54	106.68
27	K	606	CLA	C4A-NA-C1A	-6.76	103.59	106.68
27	b	705	CLA	C4A-NA-C1A	-6.74	103.60	106.68
27	G	605	CLA	C4A-NA-C1A	-6.74	103.61	106.68
27	b	714	CLA	C4A-NA-C1A	-6.72	103.61	106.68
32	J	611	PID	O3-C10-C9	-6.69	124.08	131.04
27	a	809	CLA	C4A-NA-C1A	-6.68	103.63	106.68
27	a	812	CLA	C4A-NA-C1A	-6.61	103.66	106.68
27	B	603	CLA	C4A-NA-C1A	-6.61	103.67	106.68
27	J	609	CLA	C4A-NA-C1A	-6.53	103.70	106.68
27	H	310	CLA	C4A-NA-C1A	-6.52	103.70	106.68
27	I	610	CLA	C4A-NA-C1A	-6.51	103.71	106.68
27	G	607	CLA	C1D-ND-C4D	-6.48	101.77	106.31
32	F	615	PID	O3-C10-C9	-6.47	124.30	131.04
27	a	823	CLA	C4A-NA-C1A	-6.46	103.73	106.68
32	U	608	PID	CM1-C1-C2	6.45	121.49	114.24
29	E	616	UIX	C6-C1-C3	6.39	121.41	114.24
32	J	613	PID	O3-C10-C9	-6.38	124.40	131.04
27	K	603	CLA	C1D-ND-C4D	-6.36	101.85	106.31
32	J	613	PID	CM1-C1-C6	-6.35	111.84	122.30
32	J	611	PID	O1-C1-C2	6.35	119.44	113.49
27	B	604	CLA	C1D-ND-C4D	-6.31	101.88	106.31
27	b	727	CLA	C4A-NA-C1A	-6.31	103.80	106.68
27	E	605	CLA	C4A-NA-C1A	-6.30	103.80	106.68
27	T	607	CLA	C1D-ND-C4D	-6.29	101.90	106.31
27	H	305	CLA	C4A-NA-C1A	-6.29	103.81	106.68
27	b	711	CLA	C1D-ND-C4D	-6.29	101.90	106.31
27	a	828	CLA	C1D-ND-C4D	-6.27	101.91	106.31
27	U	603	CLA	C1D-ND-C4D	-6.27	101.92	106.31
27	G	604	CLA	C1D-ND-C4D	-6.26	101.92	106.31
27	F	610	CLA	C1D-ND-C4D	-6.25	101.93	106.31
27	E	606	CLA	C1D-ND-C4D	-6.25	101.93	106.31
27	C	204	CLA	C1D-ND-C4D	-6.24	101.93	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	604	CLA	C1D-ND-C4D	-6.24	101.94	106.31
27	a	803	CLA	C1D-ND-C4D	-6.23	101.94	106.31
27	F	608	CLA	C1D-ND-C4D	-6.23	101.94	106.31
27	b	723	CLA	C1D-ND-C4D	-6.23	101.94	106.31
27	H	309	CLA	C1D-ND-C4D	-6.23	101.94	106.31
27	G	608	CLA	C4A-NA-C1A	-6.22	103.84	106.68
27	C	209	CLA	C1D-ND-C4D	-6.22	101.95	106.31
27	l	402	CLA	C1D-ND-C4D	-6.21	101.95	106.31
27	a	828	CLA	C4A-NA-C1A	-6.21	103.85	106.68
27	U	606	CLA	C1D-ND-C4D	-6.21	101.96	106.31
27	I	603	CLA	C1D-ND-C4D	-6.20	101.96	106.31
27	J	603	CLA	C1D-ND-C4D	-6.19	101.97	106.31
27	H	313	CLA	C1D-ND-C4D	-6.18	101.98	106.31
27	F	607	CLA	C1D-ND-C4D	-6.18	101.98	106.31
27	E	611	CLA	C4A-NA-C1A	-6.18	103.86	106.68
27	C	202	CLA	C1D-ND-C4D	-6.18	101.98	106.31
27	K	602	CLA	C1D-ND-C4D	-6.18	101.98	106.31
27	D	612	CLA	C1D-ND-C4D	-6.17	101.98	106.31
27	A	604	CLA	C1D-ND-C4D	-6.17	101.98	106.31
27	b	719	CLA	C1D-ND-C4D	-6.17	101.98	106.31
27	C	212	CLA	C1D-ND-C4D	-6.17	101.98	106.31
27	b	712	CLA	C1D-ND-C4D	-6.17	101.98	106.31
27	A	602	CLA	C1D-ND-C4D	-6.16	101.99	106.31
27	I	607	CLA	C1D-ND-C4D	-6.16	101.99	106.31
27	A	601	CLA	C1D-ND-C4D	-6.16	101.99	106.31
27	D	608	CLA	C1D-ND-C4D	-6.16	101.99	106.31
27	T	602	CLA	C1D-ND-C4D	-6.16	101.99	106.31
27	a	810	CLA	C1D-ND-C4D	-6.16	101.99	106.31
27	a	808	CLA	C1D-ND-C4D	-6.16	101.99	106.31
27	D	603	CLA	C1D-ND-C4D	-6.15	101.99	106.31
27	a	813	CLA	C1D-ND-C4D	-6.15	101.99	106.31
27	H	312	CLA	C1D-ND-C4D	-6.15	102.00	106.31
27	l	404	CLA	C4A-NA-C1A	-6.15	103.87	106.68
27	I	606	CLA	C1D-ND-C4D	-6.15	102.00	106.31
27	b	715	CLA	C1D-ND-C4D	-6.15	102.00	106.31
27	A	609	CLA	C1D-ND-C4D	-6.14	102.00	106.31
27	b	715	CLA	C4A-NA-C1A	-6.14	103.88	106.68
27	A	607	CLA	C1D-ND-C4D	-6.14	102.00	106.31
27	I	611	CLA	C1D-ND-C4D	-6.14	102.00	106.31
27	G	602	CLA	C1D-ND-C4D	-6.14	102.00	106.31
27	U	601	CLA	C1D-ND-C4D	-6.14	102.00	106.31
27	B	610	CLA	C1D-ND-C4D	-6.14	102.01	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	606	CLA	C1D-ND-C4D	-6.13	102.01	106.31
27	b	713	CLA	C1D-ND-C4D	-6.13	102.01	106.31
27	b	713	CLA	C4A-NA-C1A	-6.13	103.88	106.68
27	K	601	CLA	C1D-ND-C4D	-6.13	102.01	106.31
27	F	603	CLA	C1D-ND-C4D	-6.12	102.02	106.31
27	D	609	CLA	C1D-ND-C4D	-6.12	102.02	106.31
27	a	806	CLA	C1D-ND-C4D	-6.12	102.02	106.31
27	A	611	CLA	C1D-ND-C4D	-6.11	102.02	106.31
27	E	602	CLA	C1D-ND-C4D	-6.11	102.02	106.31
27	F	605	CLA	C1D-ND-C4D	-6.11	102.02	106.31
27	G	610	CLA	C1D-ND-C4D	-6.11	102.02	106.31
27	a	817	CLA	C1D-ND-C4D	-6.11	102.02	106.31
27	T	603	CLA	C1D-ND-C4D	-6.11	102.03	106.31
27	I	611	CLA	C4A-NA-C1A	-6.11	103.89	106.68
27	C	208	CLA	C1D-ND-C4D	-6.10	102.03	106.31
27	E	604	CLA	C1D-ND-C4D	-6.10	102.03	106.31
27	C	203	CLA	C1D-ND-C4D	-6.10	102.03	106.31
27	D	611	CLA	C1D-ND-C4D	-6.10	102.03	106.31
27	F	601	CLA	C1D-ND-C4D	-6.10	102.03	106.31
27	E	612	CLA	C1D-ND-C4D	-6.10	102.03	106.31
27	I	610	CLA	C1D-ND-C4D	-6.09	102.04	106.31
27	r	203	CLA	C1D-ND-C4D	-6.09	102.04	106.31
27	b	716	CLA	C1D-ND-C4D	-6.09	102.04	106.31
32	J	611	PID	O1-C1-CM1	6.09	121.85	115.05
27	T	601	CLA	C1D-ND-C4D	-6.09	102.04	106.31
27	b	726	CLA	C1D-ND-C4D	-6.09	102.04	106.31
27	A	606	CLA	C1D-ND-C4D	-6.09	102.04	106.31
27	B	601	CLA	C1D-ND-C4D	-6.08	102.05	106.31
27	C	211	CLA	C1D-ND-C4D	-6.08	102.05	106.31
27	J	607	CLA	C1D-ND-C4D	-6.08	102.05	106.31
27	T	609	CLA	C4A-NA-C1A	-6.08	103.91	106.68
27	E	603	CLA	C1D-ND-C4D	-6.08	102.05	106.31
27	l	408	CLA	C4A-NA-C1A	-6.07	103.91	106.68
32	I	614	PID	CM1-C1-C6	-6.07	112.31	122.30
32	J	613	PID	C11-C12-C13	-6.07	114.91	128.34
27	I	601	CLA	C1D-ND-C4D	-6.07	102.05	106.31
27	K	608	CLA	C1D-ND-C4D	-6.07	102.05	106.31
27	a	816	CLA	C1D-ND-C4D	-6.07	102.05	106.31
27	b	707	CLA	C1D-ND-C4D	-6.06	102.06	106.31
27	F	619	CLA	C1D-ND-C4D	-6.06	102.06	106.31
27	a	822	CLA	C1D-ND-C4D	-6.06	102.06	106.31
27	H	303	CLA	C1D-ND-C4D	-6.06	102.06	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	825	CLA	C1D-ND-C4D	-6.05	102.06	106.31
32	J	615	PID	O3-C10-C9	-6.05	124.75	131.04
27	I	609	CLA	C4A-NA-C1A	-6.04	103.92	106.68
27	D	604	CLA	C1D-ND-C4D	-6.04	102.07	106.31
27	K	606	CLA	C1D-ND-C4D	-6.04	102.07	106.31
32	F	614	PID	O1-C1-C2	6.04	119.15	113.49
27	l	412	CLA	C1D-ND-C4D	-6.03	102.08	106.31
27	G	609	CLA	C1D-ND-C4D	-6.03	102.08	106.31
27	G	611	CLA	C1D-ND-C4D	-6.03	102.08	106.31
27	a	831	CLA	C1D-ND-C4D	-6.02	102.08	106.31
27	C	201	CLA	C1D-ND-C4D	-6.02	102.09	106.31
27	J	601	CLA	C4A-NA-C1A	-6.02	103.93	106.68
27	A	603	CLA	C1D-ND-C4D	-6.02	102.09	106.31
27	b	722	CLA	C1D-ND-C4D	-6.01	102.09	106.31
27	l	403	CLA	C1D-ND-C4D	-6.01	102.09	106.31
27	H	307	CLA	C1D-ND-C4D	-6.01	102.10	106.31
27	C	206	CLA	C1D-ND-C4D	-6.00	102.10	106.31
27	G	608	CLA	C1D-ND-C4D	-6.00	102.10	106.31
27	D	601	CLA	C1D-ND-C4D	-6.00	102.10	106.31
27	H	319	CLA	C1D-ND-C4D	-6.00	102.10	106.31
27	a	824	CLA	C1D-ND-C4D	-6.00	102.10	106.31
27	E	611	CLA	C1D-ND-C4D	-6.00	102.10	106.31
27	b	721	CLA	C1D-ND-C4D	-6.00	102.10	106.31
32	K	611	PID	O1-C1-CM1	6.00	121.75	115.05
27	l	408	CLA	C1D-ND-C4D	-5.99	102.11	106.31
27	T	609	CLA	C1D-ND-C4D	-5.99	102.11	106.31
27	b	725	CLA	C1D-ND-C4D	-5.99	102.11	106.31
27	l	410	CLA	C4A-NA-C1A	-5.99	103.95	106.68
27	D	606	CLA	C1D-ND-C4D	-5.99	102.11	106.31
27	l	411	CLA	C1D-ND-C4D	-5.99	102.11	106.31
27	E	609	CLA	C1D-ND-C4D	-5.99	102.11	106.31
27	G	606	CLA	C1D-ND-C4D	-5.99	102.11	106.31
27	D	610	CLA	C1D-ND-C4D	-5.98	102.11	106.31
27	b	710	CLA	C4A-NA-C1A	-5.98	103.95	106.68
27	J	601	CLA	C1D-ND-C4D	-5.98	102.11	106.31
27	a	814	CLA	C1D-ND-C4D	-5.98	102.11	106.31
27	E	608	CLA	C1D-ND-C4D	-5.98	102.12	106.31
32	U	608	PID	O3-C10-C9	-5.98	124.82	131.04
27	J	609	CLA	C1D-ND-C4D	-5.97	102.12	106.31
27	l	410	CLA	C1D-ND-C4D	-5.97	102.12	106.31
27	b	720	CLA	C1D-ND-C4D	-5.97	102.12	106.31
27	a	830	CLA	C1D-ND-C4D	-5.97	102.12	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	l	409	CLA	C1D-ND-C4D	-5.97	102.12	106.31
27	G	604	CLA	C4A-NA-C1A	-5.96	103.96	106.68
27	G	603	CLA	C1D-ND-C4D	-5.96	102.13	106.31
27	a	805	CLA	C1D-ND-C4D	-5.96	102.13	106.31
27	K	604	CLA	C1D-ND-C4D	-5.96	102.13	106.31
27	C	207	CLA	C4A-NA-C1A	-5.96	103.96	106.68
27	f	302	CLA	C1D-ND-C4D	-5.96	102.13	106.31
27	D	602	CLA	C4A-NA-C1A	-5.96	103.96	106.68
27	A	610	CLA	C1D-ND-C4D	-5.95	102.14	106.31
27	a	815	CLA	C1D-ND-C4D	-5.95	102.14	106.31
27	b	728	CLA	C1D-ND-C4D	-5.95	102.14	106.31
27	a	821	CLA	C1D-ND-C4D	-5.95	102.14	106.31
27	r	204	CLA	C1D-ND-C4D	-5.95	102.14	106.31
27	a	839	CLA	C1D-ND-C4D	-5.94	102.14	106.31
27	a	807	CLA	C1D-ND-C4D	-5.94	102.14	106.31
27	I	609	CLA	C1D-ND-C4D	-5.93	102.15	106.31
27	A	605	CLA	C1D-ND-C4D	-5.93	102.15	106.31
27	B	607	CLA	C1D-ND-C4D	-5.92	102.16	106.31
27	b	705	CLA	C1D-ND-C4D	-5.92	102.16	106.31
27	B	605	CLA	C1D-ND-C4D	-5.92	102.16	106.31
27	I	608	CLA	C1D-ND-C4D	-5.92	102.16	106.31
27	b	701	CLA	C1D-ND-C4D	-5.92	102.16	106.31
27	a	829	CLA	C1D-ND-C4D	-5.91	102.16	106.31
27	D	602	CLA	C1D-ND-C4D	-5.91	102.16	106.31
27	B	603	CLA	C1D-ND-C4D	-5.91	102.16	106.31
27	b	704	CLA	C1D-ND-C4D	-5.91	102.17	106.31
27	b	724	CLA	C1D-ND-C4D	-5.91	102.17	106.31
27	l	406	CLA	C1D-ND-C4D	-5.91	102.17	106.31
27	b	710	CLA	C1D-ND-C4D	-5.90	102.17	106.31
27	H	306	CLA	C1D-ND-C4D	-5.90	102.17	106.31
27	T	606	CLA	C1D-ND-C4D	-5.90	102.17	106.31
27	F	606	CLA	C1D-ND-C4D	-5.90	102.17	106.31
27	K	605	CLA	C1D-ND-C4D	-5.90	102.17	106.31
27	H	310	CLA	C1D-ND-C4D	-5.90	102.17	106.31
27	F	617	CLA	C1D-ND-C4D	-5.89	102.18	106.31
27	B	609	CLA	C1D-ND-C4D	-5.89	102.18	106.31
27	b	714	CLA	C1D-ND-C4D	-5.89	102.18	106.31
27	l	405	CLA	C1D-ND-C4D	-5.89	102.18	106.31
27	F	604	CLA	C1D-ND-C4D	-5.88	102.18	106.31
27	a	804	CLA	C1D-ND-C4D	-5.88	102.19	106.31
27	I	605	CLA	C1D-ND-C4D	-5.87	102.19	106.31
27	a	837	CLA	C1D-ND-C4D	-5.87	102.19	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	804	CLA	C4A-NA-C1A	-5.87	104.00	106.68
27	J	605	CLA	C1D-ND-C4D	-5.86	102.20	106.31
27	b	727	CLA	C1D-ND-C4D	-5.86	102.20	106.31
27	A	612	CLA	C1D-ND-C4D	-5.86	102.20	106.31
27	a	819	CLA	C1D-ND-C4D	-5.85	102.20	106.31
27	a	827	CLA	C1D-ND-C4D	-5.85	102.21	106.31
27	C	205	CLA	C1D-ND-C4D	-5.85	102.21	106.31
27	D	607	CLA	C1D-ND-C4D	-5.85	102.21	106.31
32	I	614	PID	O1-C1-CM1	5.85	121.58	115.05
27	I	616	CLA	C1D-ND-C4D	-5.84	102.21	106.31
27	H	308	CLA	C1D-ND-C4D	-5.84	102.21	106.31
27	l	407	CLA	C1D-ND-C4D	-5.84	102.22	106.31
27	b	706	CLA	C1D-ND-C4D	-5.83	102.22	106.31
27	B	606	CLA	C4A-NA-C1A	-5.83	104.02	106.68
27	T	601	CLA	C4A-NA-C1A	-5.83	104.02	106.68
27	b	707	CLA	C4A-NA-C1A	-5.83	104.02	106.68
27	I	602	CLA	C1D-ND-C4D	-5.82	102.23	106.31
27	a	811	CLA	C1D-ND-C4D	-5.81	102.23	106.31
27	a	823	CLA	C1D-ND-C4D	-5.80	102.24	106.31
27	a	820	CLA	C1D-ND-C4D	-5.80	102.24	106.31
32	J	613	PID	C8-C9-C10	5.79	134.93	123.60
27	F	602	CLA	C1D-ND-C4D	-5.78	102.26	106.31
27	H	305	CLA	C1D-ND-C4D	-5.78	102.26	106.31
27	G	605	CLA	C1D-ND-C4D	-5.77	102.26	106.31
27	r	203	CLA	C4A-NA-C1A	-5.77	104.05	106.68
27	E	605	CLA	C1D-ND-C4D	-5.76	102.27	106.31
32	B	613	PID	O3-C10-C9	-5.75	125.06	131.04
32	F	614	PID	O3-C10-C9	-5.73	125.07	131.04
27	C	201	CLA	C4A-NA-C1A	-5.73	104.06	106.68
27	b	717	CLA	C1D-ND-C4D	-5.73	102.30	106.31
27	b	709	CLA	C1D-ND-C4D	-5.72	102.30	106.31
27	U	605	CLA	C1D-ND-C4D	-5.71	102.31	106.31
27	a	809	CLA	C1D-ND-C4D	-5.70	102.31	106.31
27	E	608	CLA	C4A-NA-C1A	-5.70	104.08	106.68
27	D	605	CLA	C1D-ND-C4D	-5.69	102.32	106.31
27	a	812	CLA	C1D-ND-C4D	-5.69	102.32	106.31
27	T	605	CLA	C1D-ND-C4D	-5.69	102.32	106.31
27	a	811	CLA	C4A-NA-C1A	-5.69	104.08	106.68
27	a	818	CLA	C1D-ND-C4D	-5.67	102.33	106.31
27	B	604	CLA	C4A-NA-C1A	-5.66	104.10	106.68
27	b	722	CLA	C4A-NA-C1A	-5.66	104.10	106.68
27	C	207	CLA	C1D-ND-C4D	-5.65	102.35	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	837	CLA	C4A-NA-C1A	-5.65	104.10	106.68
32	J	614	PID	O3-C10-C9	-5.65	125.17	131.04
27	B	610	CLA	C4A-NA-C1A	-5.64	104.11	106.68
27	b	718	CLA	C1D-ND-C4D	-5.64	102.36	106.31
27	j	202	CLA	C1D-ND-C4D	-5.63	102.36	106.31
27	H	304	CLA	C1D-ND-C4D	-5.61	102.38	106.31
27	b	720	CLA	C4A-NA-C1A	-5.61	104.12	106.68
29	I	612	UIX	C6-C1-C3	5.60	120.53	114.24
27	l	404	CLA	C1D-ND-C4D	-5.60	102.39	106.31
27	a	826	CLA	C1D-ND-C4D	-5.59	102.39	106.31
29	G	615	UIX	C6-C1-C3	5.59	120.52	114.24
27	D	603	CLA	C4A-NA-C1A	-5.57	104.14	106.68
27	D	607	CLA	C4A-NA-C1A	-5.57	104.14	106.68
27	A	602	CLA	C4A-NA-C1A	-5.55	104.14	106.68
27	F	605	CLA	C4A-NA-C1A	-5.55	104.15	106.68
27	F	617	CLA	C4A-NA-C1A	-5.52	104.16	106.68
32	J	611	PID	C11-C12-C13	-5.52	116.14	128.34
27	C	203	CLA	C4A-NA-C1A	-5.52	104.16	106.68
27	l	411	CLA	C4A-NA-C1A	-5.51	104.16	106.68
27	a	803	CLA	C4A-NA-C1A	-5.51	104.17	106.68
27	K	601	CLA	C4A-NA-C1A	-5.48	104.18	106.68
27	b	708	CLA	C1D-ND-C4D	-5.48	102.47	106.31
27	I	606	CLA	C4A-NA-C1A	-5.47	104.19	106.68
32	K	611	PID	CM1-C1-C6	-5.46	113.31	122.30
27	l	402	CLA	C4A-NA-C1A	-5.44	104.19	106.68
27	f	303	CLA	C1D-ND-C4D	-5.44	102.49	106.31
27	b	721	CLA	C4A-NA-C1A	-5.43	104.20	106.68
27	F	606	CLA	C4A-NA-C1A	-5.42	104.20	106.68
27	A	605	CLA	C4A-NA-C1A	-5.42	104.21	106.68
27	F	602	CLA	C4A-NA-C1A	-5.42	104.21	106.68
27	H	319	CLA	C4A-NA-C1A	-5.41	104.21	106.68
27	a	806	CLA	C4A-NA-C1A	-5.40	104.21	106.68
27	l	407	CLA	C4A-NA-C1A	-5.40	104.22	106.68
27	l	405	CLA	C4A-NA-C1A	-5.40	104.22	106.68
27	a	829	CLA	C4A-NA-C1A	-5.37	104.23	106.68
32	I	614	PID	O3-C10-C9	-5.37	125.45	131.04
27	a	802	CLA	C1D-ND-C4D	-5.36	102.55	106.31
27	a	805	CLA	C4A-NA-C1A	-5.36	104.23	106.68
27	E	607	CLA	C1D-ND-C4D	-5.36	102.55	106.31
27	A	603	CLA	C4A-NA-C1A	-5.35	104.24	106.68
27	b	703	CLA	C1D-ND-C4D	-5.34	102.57	106.31
27	b	724	CLA	C4A-NA-C1A	-5.34	104.25	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	306	CLA	C4A-NA-C1A	-5.33	104.25	106.68
27	A	611	CLA	C4A-NA-C1A	-5.32	104.25	106.68
27	C	202	CLA	C4A-NA-C1A	-5.32	104.25	106.68
29	F	613	UIX	O2-C27-C31	5.31	120.56	111.09
27	f	303	CLA	C4A-NA-C1A	-5.31	104.26	106.68
27	l	409	CLA	C4A-NA-C1A	-5.30	104.26	106.68
27	J	603	CLA	C4A-NA-C1A	-5.30	104.26	106.68
27	D	608	CLA	C4A-NA-C1A	-5.30	104.26	106.68
27	a	825	CLA	C4A-NA-C1A	-5.27	104.27	106.68
27	F	607	CLA	C4A-NA-C1A	-5.26	104.28	106.68
27	E	603	CLA	C4A-NA-C1A	-5.25	104.28	106.68
27	K	603	CLA	C4A-NA-C1A	-5.25	104.28	106.68
27	B	601	CLA	C4A-NA-C1A	-5.25	104.28	106.68
27	a	815	CLA	C4A-NA-C1A	-5.24	104.29	106.68
32	K	611	PID	C8-C9-C10	5.23	133.85	123.60
27	F	601	CLA	C4A-NA-C1A	-5.23	104.29	106.68
27	U	603	CLA	C4A-NA-C1A	-5.23	104.29	106.68
27	b	723	CLA	C4A-NA-C1A	-5.22	104.30	106.68
27	a	816	CLA	C4A-NA-C1A	-5.22	104.30	106.68
27	D	609	CLA	C4A-NA-C1A	-5.22	104.30	106.68
27	E	602	CLA	C4A-NA-C1A	-5.21	104.30	106.68
32	F	614	PID	CM1-C1-C6	-5.19	113.76	122.30
27	a	814	CLA	C4A-NA-C1A	-5.19	104.31	106.68
27	F	610	CLA	C4A-NA-C1A	-5.19	104.31	106.68
27	a	802	CLA	C4A-NA-C1A	-5.19	104.31	106.68
27	T	606	CLA	C4A-NA-C1A	-5.18	104.32	106.68
32	J	611	PID	C8-C9-C10	5.17	133.73	123.60
27	C	204	CLA	C4A-NA-C1A	-5.17	104.32	106.68
27	l	412	CLA	C4A-NA-C1A	-5.17	104.32	106.68
27	J	607	CLA	C4A-NA-C1A	-5.17	104.32	106.68
27	E	606	CLA	C4A-NA-C1A	-5.16	104.33	106.68
27	H	312	CLA	C4A-NA-C1A	-5.16	104.33	106.68
27	F	604	CLA	C4A-NA-C1A	-5.15	104.33	106.68
27	G	609	CLA	C4A-NA-C1A	-5.14	104.33	106.68
27	C	208	CLA	C4A-NA-C1A	-5.14	104.33	106.68
27	b	701	CLA	C4A-NA-C1A	-5.14	104.33	106.68
27	a	819	CLA	C4A-NA-C1A	-5.13	104.34	106.68
27	C	209	CLA	C4A-NA-C1A	-5.11	104.35	106.68
27	a	817	CLA	C4A-NA-C1A	-5.11	104.35	106.68
27	C	212	CLA	C4A-NA-C1A	-5.11	104.35	106.68
27	H	309	CLA	C4A-NA-C1A	-5.11	104.35	106.68
27	A	607	CLA	C4A-NA-C1A	-5.10	104.35	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	612	CLA	C4A-NA-C1A	-5.10	104.35	106.68
27	b	711	CLA	C4A-NA-C1A	-5.10	104.35	106.68
27	a	821	CLA	C4A-NA-C1A	-5.10	104.35	106.68
27	K	608	CLA	C4A-NA-C1A	-5.08	104.36	106.68
27	A	610	CLA	C4A-NA-C1A	-5.08	104.36	106.68
27	a	826	CLA	C4A-NA-C1A	-5.08	104.36	106.68
27	D	604	CLA	C4A-NA-C1A	-5.07	104.36	106.68
27	a	831	CLA	C4A-NA-C1A	-5.07	104.36	106.68
27	a	808	CLA	C4A-NA-C1A	-5.07	104.36	106.68
27	K	604	CLA	C4A-NA-C1A	-5.07	104.37	106.68
29	F	613	UIX	C6-C1-C3	5.06	119.93	114.24
27	H	308	CLA	C4A-NA-C1A	-5.04	104.38	106.68
27	D	606	CLA	C4A-NA-C1A	-5.03	104.38	106.68
27	D	610	CLA	C4A-NA-C1A	-5.03	104.39	106.68
27	G	603	CLA	C4A-NA-C1A	-5.03	104.39	106.68
27	I	603	CLA	C4A-NA-C1A	-5.02	104.39	106.68
27	G	602	CLA	C4A-NA-C1A	-5.02	104.39	106.68
27	a	822	CLA	C4A-NA-C1A	-5.02	104.39	106.68
27	A	606	CLA	C4A-NA-C1A	-5.02	104.39	106.68
29	j	204	UIX	C6-C1-C3	5.01	119.87	114.24
32	U	608	PID	O6-C30-C31	5.00	120.01	111.09
27	a	818	CLA	C4A-NA-C1A	-4.98	104.41	106.68
32	F	615	PID	O6-C30-C31	4.98	119.97	111.09
27	A	609	CLA	C4A-NA-C1A	-4.98	104.41	106.68
27	F	608	CLA	C4A-NA-C1A	-4.98	104.41	106.68
27	F	603	CLA	C4A-NA-C1A	-4.98	104.41	106.68
29	A	616	UIX	C6-C1-C3	4.98	119.83	114.24
27	b	716	CLA	C4A-NA-C1A	-4.97	104.41	106.68
27	G	607	CLA	C4A-NA-C1A	-4.96	104.42	106.68
38	a	836	BCR	C15-C14-C13	-4.95	120.33	127.28
27	b	726	CLA	C4A-NA-C1A	-4.94	104.42	106.68
27	D	601	CLA	C4A-NA-C1A	-4.94	104.43	106.68
27	a	830	CLA	C4A-NA-C1A	-4.93	104.43	106.68
29	D	616	UIX	C14-C13-C11	-4.93	120.36	127.28
27	C	206	CLA	C4A-NA-C1A	-4.92	104.44	106.68
27	T	602	CLA	C4A-NA-C1A	-4.92	104.44	106.68
27	B	609	CLA	C4A-NA-C1A	-4.91	104.44	106.68
27	I	601	CLA	C4A-NA-C1A	-4.91	104.44	106.68
27	T	607	CLA	C4A-NA-C1A	-4.89	104.45	106.68
27	a	824	CLA	C4A-NA-C1A	-4.89	104.45	106.68
27	b	702	CLA	C1D-ND-C4D	-4.89	102.88	106.31
27	A	601	CLA	C4A-NA-C1A	-4.88	104.45	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	307	CLA	C4A-NA-C1A	-4.88	104.45	106.68
32	B	613	PID	O6-C30-C31	4.88	119.80	111.09
27	b	712	CLA	C4A-NA-C1A	-4.87	104.45	106.68
32	J	614	PID	C7-C8-C9	-4.87	119.92	126.06
27	I	607	CLA	C4A-NA-C1A	-4.86	104.46	106.68
32	J	615	PID	O6-C30-C31	4.85	119.74	111.09
27	H	303	CLA	C4A-NA-C1A	-4.84	104.47	106.68
27	E	609	CLA	C4A-NA-C1A	-4.84	104.47	106.68
27	b	706	CLA	C4A-NA-C1A	-4.84	104.47	106.68
27	F	619	CLA	C4A-NA-C1A	-4.84	104.47	106.68
27	U	606	CLA	C4A-NA-C1A	-4.84	104.47	106.68
27	H	304	CLA	C4A-NA-C1A	-4.80	104.49	106.68
27	a	807	CLA	C4A-NA-C1A	-4.80	104.49	106.68
29	H	317	UIX	C6-C1-C3	4.79	119.62	114.24
27	a	820	CLA	C4A-NA-C1A	-4.79	104.49	106.68
27	G	606	CLA	C4A-NA-C1A	-4.78	104.50	106.68
27	b	709	CLA	C4A-NA-C1A	-4.78	104.50	106.68
27	T	604	CLA	C4A-NA-C1A	-4.78	104.50	106.68
27	l	403	CLA	C4A-NA-C1A	-4.77	104.50	106.68
27	G	611	CLA	C4A-NA-C1A	-4.76	104.51	106.68
27	b	717	CLA	C4A-NA-C1A	-4.76	104.51	106.68
27	T	605	CLA	C4A-NA-C1A	-4.75	104.51	106.68
27	E	607	CLA	C4A-NA-C1A	-4.75	104.51	106.68
27	b	728	CLA	C4A-NA-C1A	-4.75	104.51	106.68
27	T	603	CLA	C4A-NA-C1A	-4.74	104.52	106.68
27	I	608	CLA	C4A-NA-C1A	-4.73	104.52	106.68
27	K	602	CLA	C4A-NA-C1A	-4.73	104.52	106.68
38	a	836	BCR	C11-C10-C9	-4.72	120.66	127.28
27	r	204	CLA	C4A-NA-C1A	-4.71	104.53	106.68
38	a	836	BCR	C20-C21-C22	-4.70	120.68	127.28
29	H	314	UIX	O2-C27-C31	4.70	119.46	111.09
29	C	215	UIX	O-C1-C3	-4.70	109.09	113.49
32	I	614	PID	O6-C30-C31	4.68	119.44	111.09
32	J	615	PID	CM1-C1-C2	4.67	119.49	114.24
32	F	614	PID	O6-C30-C31	4.66	119.41	111.09
29	G	615	UIX	O2-C27-C31	4.66	119.40	111.09
29	A	613	UIX	C6-C1-C3	4.66	119.48	114.24
32	J	613	PID	O1-C1-CM1	4.66	120.25	115.05
32	J	613	PID	C6-C7-C8	-4.65	116.15	125.99
29	B	615	UIX	O2-C27-C31	4.65	119.39	111.09
27	G	610	CLA	C4A-NA-C1A	-4.65	104.56	106.68
27	b	704	CLA	C4A-NA-C1A	-4.65	104.56	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	616	UIX	O2-C27-C31	4.64	119.36	111.09
27	A	604	CLA	C4A-NA-C1A	-4.64	104.56	106.68
27	D	605	CLA	C4A-NA-C1A	-4.62	104.57	106.68
32	B	613	PID	C7-C8-C9	-4.62	120.23	126.06
29	A	613	UIX	O2-C27-C31	4.62	119.33	111.09
29	I	612	UIX	O2-C27-C31	4.62	119.32	111.09
27	f	302	CLA	C4A-NA-C1A	-4.62	104.57	106.68
27	H	313	CLA	C4A-NA-C1A	-4.60	104.58	106.68
32	J	613	PID	O6-C30-C31	4.60	119.29	111.09
27	b	725	CLA	C4A-NA-C1A	-4.60	104.58	106.68
29	B	615	UIX	C6-C1-C3	4.60	119.41	114.24
27	E	612	CLA	C4A-NA-C1A	-4.60	104.58	106.68
29	j	204	UIX	O2-C27-C31	4.59	119.27	111.09
32	K	611	PID	C7-C8-C9	-4.59	120.27	126.06
27	a	810	CLA	C4A-NA-C1A	-4.59	104.59	106.68
29	C	213	UIX	O2-C27-C31	4.57	119.25	111.09
29	E	616	UIX	O2-C27-C31	4.57	119.25	111.09
29	C	213	UIX	C6-C1-C3	4.57	119.37	114.24
29	C	215	UIX	O2-C27-C31	4.57	119.23	111.09
27	I	602	CLA	C4A-NA-C1A	-4.57	104.60	106.68
27	B	605	CLA	C4A-NA-C1A	-4.56	104.60	106.68
27	J	605	CLA	C4A-NA-C1A	-4.56	104.60	106.68
29	D	616	UIX	O2-C27-C31	4.55	119.21	111.09
32	J	611	PID	O6-C30-C31	4.55	119.20	111.09
27	I	605	CLA	C4A-NA-C1A	-4.55	104.60	106.68
38	a	836	BCR	C24-C23-C22	-4.55	119.51	126.23
27	U	605	CLA	C4A-NA-C1A	-4.53	104.61	106.68
27	E	604	CLA	C4A-NA-C1A	-4.53	104.61	106.68
32	F	614	PID	C8-C9-C10	4.53	132.47	123.60
32	J	613	PID	C8-C9-C11	-4.52	118.44	127.28
29	T	612	UIX	O2-C27-C31	4.51	119.12	111.09
32	J	615	PID	C8-C9-C10	4.51	132.43	123.60
27	a	813	CLA	C4A-NA-C1A	-4.50	104.62	106.68
32	K	611	PID	O6-C30-C31	4.50	119.11	111.09
28	K	607	KC2	C1D-ND-C4D	4.49	109.46	106.31
29	J	616	UIX	O2-C27-C31	4.48	119.08	111.09
27	C	211	CLA	C4A-NA-C1A	-4.48	104.64	106.68
32	I	614	PID	C9-C11-C12	-4.48	103.00	108.75
29	H	314	UIX	C6-C1-C3	4.47	119.27	114.24
27	B	607	CLA	C4A-NA-C1A	-4.47	104.64	106.68
29	H	317	UIX	O2-C27-C31	4.47	119.06	111.09
32	J	615	PID	C9-C11-C12	-4.46	103.02	108.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	U	608	PID	C9-C11-C12	-4.39	103.11	108.75
27	b	703	CLA	C4A-NA-C1A	-4.37	104.69	106.68
29	H	314	UIX	O-C1-C6	-4.37	110.17	115.05
29	B	611	UIX	O2-C27-C31	4.36	118.87	111.09
27	a	801	CLA	C1D-ND-C4D	-4.36	103.25	106.31
27	l	406	CLA	C4A-NA-C1A	-4.36	104.69	106.68
27	D	611	CLA	C4A-NA-C1A	-4.36	104.69	106.68
27	b	708	CLA	C4A-NA-C1A	-4.35	104.69	106.68
27	j	202	CLA	C4A-NA-C1A	-4.35	104.69	106.68
38	a	836	BCR	C33-C5-C6	-4.35	119.74	124.48
32	U	608	PID	C8-C9-C10	4.34	132.11	123.60
28	A	608	KC2	C1D-ND-C4D	4.33	109.35	106.31
38	a	836	BCR	C16-C17-C18	-4.32	121.22	127.28
32	F	614	PID	C7-C8-C9	-4.31	120.62	126.06
32	J	614	PID	C9-C11-C12	-4.31	103.21	108.75
32	B	613	PID	C9-C11-C12	-4.31	103.22	108.75
27	b	719	CLA	C4A-NA-C1A	-4.29	104.72	106.68
35	f	305	DGD	O3G-C3G-C2G	-4.29	100.39	110.82
28	T	608	KC2	C1D-ND-C4D	4.28	109.32	106.31
32	J	614	PID	O6-C30-C31	4.27	118.70	111.09
29	D	616	UIX	C6-C1-C3	4.26	119.03	114.24
28	G	601	KC2	C1D-ND-C4D	4.25	109.30	106.31
28	J	610	KC2	C1D-ND-C4D	4.25	109.29	106.31
28	B	608	KC2	C1D-ND-C4D	4.25	109.29	106.31
28	J	608	KC2	C1D-ND-C4D	4.24	109.29	106.31
28	H	311	KC2	C1D-ND-C4D	4.24	109.29	106.31
28	J	602	KC2	C1D-ND-C4D	4.24	109.29	106.31
32	F	615	PID	C9-C11-C12	-4.24	103.30	108.75
32	F	614	PID	C11-C12-C13	-4.23	118.99	128.34
28	U	602	KC2	C1D-ND-C4D	4.20	109.26	106.31
29	G	615	UIX	C14-C13-C11	-4.20	121.39	127.28
29	D	616	UIX	O-C1-C6	-4.20	110.36	115.05
32	F	615	PID	CM1-C1-C2	4.18	118.94	114.24
32	J	611	PID	C9-C11-C12	-4.17	103.39	108.75
28	E	601	KC2	C1D-ND-C4D	4.16	109.23	106.31
28	F	609	KC2	C1D-ND-C4D	4.16	109.23	106.31
27	a	839	CLA	C4A-NA-C1A	-4.15	104.79	106.68
35	K	614	DGD	O3G-C3G-C2G	-4.15	100.74	110.82
28	H	302	KC2	C1D-ND-C4D	4.14	109.22	106.31
29	C	215	UIX	C12-C11-C10	4.14	124.41	118.09
32	I	614	PID	C7-C8-C9	-4.14	120.84	126.06
32	J	611	PID	C8-C9-C11	-4.13	119.20	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	616	UIX	O-C1-C3	-4.13	109.62	113.49
32	J	611	PID	C6-C7-C8	-4.13	117.26	125.99
27	I	616	CLA	C4A-NA-C1A	-4.12	104.80	106.68
32	K	611	PID	O3-C10-C9	-4.12	126.75	131.04
32	J	615	PID	C11-C12-C13	-4.12	119.22	128.34
28	B	602	KC2	C1D-ND-C4D	4.12	109.20	106.31
27	G	606	CLA	CAA-C2A-C1A	-4.11	98.52	111.97
29	J	616	UIX	C6-C1-C3	4.11	118.85	114.24
35	j	201	DGD	O3G-C3G-C2G	-4.10	100.84	110.82
32	F	615	PID	C8-C9-C10	4.10	131.63	123.60
30	E	617	DD6	C14-C13-C11	4.10	131.89	125.53
28	C	210	KC2	C1D-ND-C4D	4.09	109.19	106.31
28	J	604	KC2	C1D-ND-C4D	4.07	109.17	106.31
32	U	608	PID	C19-C20-C21	-4.06	121.58	127.28
32	F	615	PID	C7-C8-C9	-4.05	120.95	126.06
28	E	610	KC2	C1D-ND-C4D	4.04	109.15	106.31
28	J	606	KC2	C1D-ND-C4D	4.04	109.15	106.31
29	D	616	UIX	C34-C30-C26	-4.04	121.61	127.28
32	F	614	PID	C9-C11-C12	-4.04	103.57	108.75
29	E	616	UIX	C34-C30-C26	-4.02	121.64	127.28
28	U	604	KC2	C1D-ND-C4D	4.02	109.13	106.31
27	b	702	CLA	C4A-NA-C1A	-4.02	104.85	106.68
32	J	614	PID	CM1-C1-C2	4.01	118.75	114.24
35	l	416	DGD	O3G-C3G-C2G	-4.01	101.06	110.82
28	I	604	KC2	C1D-ND-C4D	4.00	109.12	106.31
32	I	614	PID	C19-C20-C21	-3.99	121.68	127.28
32	K	611	PID	C9-C11-C12	-3.99	103.63	108.75
29	T	612	UIX	C6-C1-C3	3.97	118.70	114.24
29	B	611	UIX	C12-C11-C10	3.96	124.14	118.09
32	J	611	PID	C19-C20-C21	-3.96	121.72	127.28
27	K	605	CLA	C4A-NA-C1A	-3.96	104.87	106.68
32	B	613	PID	C8-C9-C10	3.95	131.34	123.60
29	I	612	UIX	O-C1-C6	-3.94	110.64	115.05
32	F	615	PID	C11-C12-C13	-3.93	119.64	128.34
30	r	201	DD6	C14-C13-C11	3.93	131.62	125.53
32	U	608	PID	C11-C12-C13	-3.92	119.67	128.34
29	H	317	UIX	C34-C30-C26	-3.92	121.78	127.28
32	B	613	PID	C11-C12-C13	-3.91	119.69	128.34
30	K	610	DD6	C14-C13-C11	3.88	131.55	125.53
32	I	614	PID	C8-C9-C10	3.87	131.18	123.60
32	J	613	PID	C19-C20-C21	-3.86	121.86	127.28
27	a	801	CLA	C4A-NA-C1A	-3.85	104.92	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	611	UIX	C29-C26-C23	3.85	123.97	118.09
29	T	612	UIX	C34-C30-C26	-3.84	121.89	127.28
32	K	611	PID	C8-C9-C11	-3.84	119.79	127.28
32	K	611	PID	C19-C20-C21	-3.83	121.91	127.28
29	B	611	UIX	O-C1-C6	-3.82	110.78	115.05
32	J	615	PID	C7-C8-C9	-3.81	121.25	126.06
27	a	801	CLA	CHD-C1D-ND	-3.79	119.47	124.80
29	A	613	UIX	O-C1-C6	-3.78	110.82	115.05
29	B	611	UIX	C6-C1-C3	3.77	118.48	114.24
30	D	621	DD6	C14-C13-C11	3.77	131.37	125.53
32	J	614	PID	C8-C9-C10	3.76	130.97	123.60
30	A	615	DD6	C14-C13-C11	3.76	131.36	125.53
29	T	612	UIX	C29-C26-C23	3.75	123.81	118.09
32	J	613	PID	C9-C11-C12	-3.73	103.95	108.75
32	J	615	PID	C19-C20-C21	-3.73	122.04	127.28
29	C	215	UIX	C6-C1-C3	3.73	118.43	114.24
31	A	618	SQD	O47-C7-C8	3.72	119.54	111.48
29	A	616	UIX	C12-C11-C10	3.72	123.77	118.09
32	B	613	PID	C19-C20-C21	-3.72	122.06	127.28
32	U	608	PID	C7-C8-C9	-3.71	121.38	126.06
31	y	301	SQD	O47-C7-C8	3.70	119.49	111.48
29	H	317	UIX	O-C1-C6	-3.69	110.92	115.05
32	F	614	PID	C19-C20-C21	-3.69	122.10	127.28
29	j	204	UIX	C34-C30-C26	-3.68	122.11	127.28
27	U	603	CLA	CHD-C1D-ND	-3.67	119.64	124.80
29	J	616	UIX	O-C1-C6	-3.66	110.96	115.05
29	j	204	UIX	C14-C13-C11	-3.66	122.15	127.28
29	B	615	UIX	C12-C11-C10	3.65	123.66	118.09
29	C	215	UIX	C29-C26-C23	3.64	123.64	118.09
29	T	612	UIX	C12-C11-C10	3.62	123.62	118.09
29	E	616	UIX	C12-C11-C10	3.62	123.62	118.09
27	G	607	CLA	CHD-C1D-ND	-3.62	119.71	124.80
32	J	614	PID	C16-C15-C14	-3.61	122.22	127.28
27	T	601	CLA	CHD-C1D-ND	-3.60	119.74	124.80
29	A	613	UIX	C29-C26-C23	3.60	123.58	118.09
32	J	613	PID	C27-O6-C30	-3.60	111.49	117.85
38	a	836	BCR	C38-C26-C25	-3.60	120.56	124.48
27	b	703	CLA	CHD-C1D-ND	-3.60	119.74	124.80
29	C	215	UIX	O-C-C7	-3.60	106.58	116.88
27	G	605	CLA	CHD-C1D-ND	-3.59	119.75	124.80
29	H	317	UIX	C12-C11-C10	3.59	123.56	118.09
32	J	614	PID	C11-C12-C13	-3.58	120.41	128.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j	204	UIX	C41-C40-C38	3.58	123.56	118.09
27	a	837	CLA	CHD-C1D-ND	-3.58	119.76	124.80
27	b	707	CLA	CHD-C1D-ND	-3.58	119.77	124.80
32	F	614	PID	C29-C24-C25	3.57	123.24	119.70
29	E	616	UIX	C14-C13-C11	-3.57	122.28	127.28
30	G	613	DD6	C14-C13-C11	3.57	131.06	125.53
27	j	202	CLA	CHD-C1D-ND	-3.56	119.79	124.80
32	K	611	PID	C27-O6-C30	-3.56	111.55	117.85
32	J	611	PID	C17-C16-C15	-3.56	116.23	123.52
29	I	612	UIX	C41-C40-C38	3.56	123.53	118.09
27	B	603	CLA	CHD-C1D-ND	-3.56	119.79	124.80
27	b	713	CLA	CHD-C1D-ND	-3.56	119.80	124.80
27	a	824	CLA	CHD-C1D-ND	-3.55	119.80	124.80
27	b	721	CLA	CHD-C1D-ND	-3.55	119.81	124.80
27	B	604	CLA	CHD-C1D-ND	-3.54	119.81	124.80
27	H	309	CLA	CHD-C1D-ND	-3.54	119.82	124.80
27	B	605	CLA	CHD-C1D-ND	-3.54	119.82	124.80
27	a	808	CLA	CHD-C1D-ND	-3.54	119.82	124.80
29	G	615	UIX	C34-C30-C26	-3.54	122.31	127.28
27	B	606	CLA	CHD-C1D-ND	-3.54	119.82	124.80
27	a	818	CLA	CHD-C1D-ND	-3.54	119.82	124.80
27	E	603	CLA	CHD-C1D-ND	-3.54	119.83	124.80
27	l	404	CLA	CHD-C1D-ND	-3.54	119.83	124.80
27	b	714	CLA	CHD-C1D-ND	-3.54	119.83	124.80
27	f	303	CLA	CHD-C1D-ND	-3.54	119.83	124.80
27	I	610	CLA	CHD-C1D-ND	-3.53	119.83	124.80
30	i	202	DD6	O1-C20-C19	-3.53	110.18	113.49
29	H	314	UIX	C29-C26-C23	3.53	123.48	118.09
29	F	613	UIX	O-C1-C3	-3.53	110.18	113.49
27	b	705	CLA	CHD-C1D-ND	-3.53	119.83	124.80
27	A	612	CLA	CHD-C1D-ND	-3.53	119.83	124.80
27	I	611	CLA	CHD-C1D-ND	-3.53	119.83	124.80
27	l	412	CLA	CHD-C1D-ND	-3.53	119.83	124.80
27	D	608	CLA	CHD-C1D-ND	-3.53	119.84	124.80
29	C	213	UIX	C12-C11-C10	3.53	123.48	118.09
27	D	602	CLA	CHD-C1D-ND	-3.53	119.84	124.80
29	J	616	UIX	O-C1-C3	-3.53	110.19	113.49
27	a	812	CLA	CHD-C1D-ND	-3.52	119.84	124.80
29	D	616	UIX	C-C7-C10	-3.52	118.54	125.99
29	B	615	UIX	C29-C26-C23	3.52	123.47	118.09
27	K	608	CLA	CHD-C1D-ND	-3.52	119.84	124.80
29	C	213	UIX	C29-C26-C23	3.52	123.47	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	826	CLA	CHD-C1D-ND	-3.52	119.85	124.80
27	b	715	CLA	CHD-C1D-ND	-3.52	119.85	124.80
29	J	616	UIX	C12-C11-C10	3.52	123.46	118.09
27	E	607	CLA	CHD-C1D-ND	-3.51	119.86	124.80
27	U	601	CLA	CHD-C1D-ND	-3.51	119.86	124.80
27	K	603	CLA	CHD-C1D-ND	-3.51	119.86	124.80
27	a	809	CLA	CHD-C1D-ND	-3.51	119.86	124.80
32	J	615	PID	C8-C9-C11	-3.51	120.43	127.28
27	a	829	CLA	CHD-C1D-ND	-3.51	119.87	124.80
29	F	613	UIX	C29-C26-C23	3.50	123.44	118.09
27	b	719	CLA	CHD-C1D-ND	-3.50	119.87	124.80
27	l	411	CLA	CHD-C1D-ND	-3.50	119.87	124.80
29	T	612	UIX	C18-O2-C27	-3.50	111.66	117.85
27	G	604	CLA	CHD-C1D-ND	-3.50	119.88	124.80
27	I	607	CLA	CHD-C1D-ND	-3.50	119.88	124.80
27	l	406	CLA	CHD-C1D-ND	-3.50	119.88	124.80
27	a	804	CLA	CHD-C1D-ND	-3.50	119.88	124.80
27	b	711	CLA	CHD-C1D-ND	-3.50	119.88	124.80
30	G	612	DD6	C14-C13-C11	3.50	130.96	125.53
27	G	611	CLA	CHD-C1D-ND	-3.50	119.88	124.80
27	r	203	CLA	CHD-C1D-ND	-3.50	119.88	124.80
27	C	203	CLA	CHD-C1D-ND	-3.50	119.88	124.80
27	I	606	CLA	CHD-C1D-ND	-3.50	119.88	124.80
27	l	410	CLA	CHD-C1D-ND	-3.50	119.88	124.80
29	A	616	UIX	C34-C30-C26	-3.50	122.37	127.28
27	E	608	CLA	CHD-C1D-ND	-3.49	119.88	124.80
27	J	603	CLA	CHD-C1D-ND	-3.49	119.88	124.80
27	J	601	CLA	CHD-C1D-ND	-3.49	119.89	124.80
27	F	610	CLA	CHD-C1D-ND	-3.49	119.89	124.80
27	E	605	CLA	CHD-C1D-ND	-3.49	119.89	124.80
27	b	712	CLA	CHD-C1D-ND	-3.49	119.89	124.80
27	F	607	CLA	CHD-C1D-ND	-3.49	119.89	124.80
27	K	601	CLA	CHD-C1D-ND	-3.49	119.89	124.80
27	a	828	CLA	CHD-C1D-ND	-3.49	119.89	124.80
29	I	612	UIX	C34-C37-C39	-3.49	116.38	123.52
27	b	718	CLA	CHD-C1D-ND	-3.49	119.89	124.80
27	a	823	CLA	CHD-C1D-ND	-3.49	119.89	124.80
29	I	612	UIX	C14-C13-C11	-3.49	122.39	127.28
27	C	212	CLA	CHD-C1D-ND	-3.48	119.90	124.80
27	a	803	CLA	CHD-C1D-ND	-3.48	119.90	124.80
29	G	615	UIX	C36-C35-C32	-3.48	122.39	127.28
27	E	604	CLA	CHD-C1D-ND	-3.48	119.90	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	j	201	DGD	O6D-C1D-O3G	-3.48	101.82	110.04
32	B	613	PID	CM1-C1-C2	3.48	118.15	114.24
32	B	613	PID	C16-C15-C14	-3.48	122.40	127.28
29	H	314	UIX	C12-C11-C10	3.48	123.40	118.09
29	D	616	UIX	C10-C11-C13	3.48	124.48	119.01
27	a	816	CLA	CHD-C1D-ND	-3.48	119.91	124.80
27	b	716	CLA	CHD-C1D-ND	-3.48	119.91	124.80
27	E	602	CLA	CHD-C1D-ND	-3.48	119.91	124.80
27	I	609	CLA	CHD-C1D-ND	-3.47	119.91	124.80
27	T	607	CLA	CHD-C1D-ND	-3.47	119.91	124.80
27	b	722	CLA	CHD-C1D-ND	-3.47	119.91	124.80
29	F	613	UIX	C34-C30-C26	-3.47	122.41	127.28
27	K	606	CLA	CHD-C1D-ND	-3.47	119.92	124.80
27	T	606	CLA	CHD-C1D-ND	-3.47	119.92	124.80
27	A	602	CLA	CHD-C1D-ND	-3.47	119.92	124.80
27	A	610	CLA	CHD-C1D-ND	-3.47	119.92	124.80
30	r	206	DD6	C14-C13-C11	3.47	130.91	125.53
27	D	612	CLA	CHD-C1D-ND	-3.47	119.92	124.80
27	T	609	CLA	CHD-C1D-ND	-3.47	119.92	124.80
27	U	605	CLA	CHD-C1D-ND	-3.47	119.92	124.80
27	H	313	CLA	CHD-C1D-ND	-3.46	119.93	124.80
27	a	839	CLA	CHD-C1D-ND	-3.46	119.93	124.80
27	b	704	CLA	CHD-C1D-ND	-3.46	119.93	124.80
27	G	608	CLA	CHD-C1D-ND	-3.46	119.93	124.80
27	l	407	CLA	CHD-C1D-ND	-3.46	119.93	124.80
27	l	408	CLA	CHD-C1D-ND	-3.46	119.93	124.80
29	I	612	UIX	C34-C30-C26	-3.46	122.43	127.28
27	a	802	CLA	CHD-C1D-ND	-3.46	119.94	124.80
27	C	209	CLA	CHD-C1D-ND	-3.45	119.94	124.80
27	D	603	CLA	CHD-C1D-ND	-3.45	119.94	124.80
27	C	202	CLA	CHD-C1D-ND	-3.45	119.95	124.80
27	a	810	CLA	CHD-C1D-ND	-3.45	119.95	124.80
27	a	811	CLA	CHD-C1D-ND	-3.45	119.95	124.80
27	A	605	CLA	CHD-C1D-ND	-3.45	119.95	124.80
27	U	606	CLA	CHD-C1D-ND	-3.44	119.95	124.80
29	j	204	UIX	C29-C26-C23	3.44	123.35	118.09
29	C	213	UIX	C34-C30-C26	-3.44	122.45	127.28
27	U	603	CLA	C1-C2-C3	-3.44	121.19	126.76
27	D	611	CLA	CHD-C1D-ND	-3.44	119.96	124.80
30	C	216	DD6	C14-C13-C11	3.44	130.87	125.53
27	J	605	CLA	CHD-C1D-ND	-3.44	119.96	124.80
27	C	205	CLA	CHD-C1D-ND	-3.44	119.96	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	310	CLA	CHD-C1D-ND	-3.44	119.96	124.80
27	a	820	CLA	CHD-C1D-ND	-3.44	119.96	124.80
27	C	208	CLA	CHD-C1D-ND	-3.44	119.97	124.80
27	H	303	CLA	CHD-C1D-ND	-3.44	119.97	124.80
27	A	611	CLA	CHD-C1D-ND	-3.44	119.97	124.80
27	a	807	CLA	CHD-C1D-ND	-3.44	119.97	124.80
27	l	402	CLA	CHD-C1D-ND	-3.44	119.97	124.80
29	B	611	UIX	C-C7-C10	-3.43	118.73	125.99
27	J	609	CLA	CHD-C1D-ND	-3.43	119.97	124.80
27	b	710	CLA	CHD-C1D-ND	-3.43	119.97	124.80
27	F	617	CLA	CHD-C1D-ND	-3.43	119.97	124.80
27	I	601	CLA	CHD-C1D-ND	-3.43	119.97	124.80
27	D	609	CLA	CHD-C1D-ND	-3.43	119.98	124.80
27	E	609	CLA	CHD-C1D-ND	-3.42	119.98	124.80
27	F	619	CLA	CHD-C1D-ND	-3.42	119.98	124.80
27	C	204	CLA	CHD-C1D-ND	-3.42	119.99	124.80
27	l	405	CLA	CHD-C1D-ND	-3.42	119.99	124.80
27	F	601	CLA	CHD-C1D-ND	-3.42	119.99	124.80
27	b	727	CLA	CHD-C1D-ND	-3.42	119.99	124.80
27	B	609	CLA	CHD-C1D-ND	-3.42	119.99	124.80
27	D	607	CLA	CHD-C1D-ND	-3.42	119.99	124.80
27	H	319	CLA	CHD-C1D-ND	-3.42	119.99	124.80
27	A	606	CLA	CHD-C1D-ND	-3.42	120.00	124.80
27	a	821	CLA	CHD-C1D-ND	-3.42	120.00	124.80
29	A	616	UIX	C29-C26-C23	3.41	123.30	118.09
27	b	701	CLA	CHD-C1D-ND	-3.41	120.00	124.80
27	B	601	CLA	CHD-C1D-ND	-3.41	120.00	124.80
27	J	607	CLA	CHD-C1D-ND	-3.41	120.01	124.80
27	b	724	CLA	CHD-C1D-ND	-3.41	120.01	124.80
27	b	720	CLA	CHD-C1D-ND	-3.41	120.01	124.80
27	b	726	CLA	CHD-C1D-ND	-3.41	120.01	124.80
27	F	602	CLA	CHD-C1D-ND	-3.40	120.01	124.80
27	A	604	CLA	CHD-C1D-ND	-3.40	120.01	124.80
27	A	601	CLA	CHD-C1D-ND	-3.40	120.01	124.80
29	G	615	UIX	C29-C26-C23	3.40	123.28	118.09
27	E	612	CLA	CHD-C1D-ND	-3.40	120.02	124.80
27	C	207	CLA	CHD-C1D-ND	-3.40	120.02	124.80
27	G	602	CLA	CHD-C1D-ND	-3.40	120.02	124.80
29	T	612	UIX	O-C1-C3	-3.40	110.31	113.49
27	A	603	CLA	CHD-C1D-ND	-3.40	120.02	124.80
27	E	606	CLA	CHD-C1D-ND	-3.40	120.02	124.80
27	F	608	CLA	CHD-C1D-ND	-3.40	120.02	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	305	CLA	CHD-C1D-ND	-3.39	120.03	124.80
27	C	201	CLA	CHD-C1D-ND	-3.39	120.04	124.80
27	G	610	CLA	CHD-C1D-ND	-3.39	120.04	124.80
27	a	806	CLA	CHD-C1D-ND	-3.39	120.04	124.80
27	b	723	CLA	CHD-C1D-ND	-3.38	120.04	124.80
27	a	819	CLA	CHD-C1D-ND	-3.38	120.04	124.80
27	a	814	CLA	CHD-C1D-ND	-3.38	120.04	124.80
29	J	616	UIX	C14-C13-C11	-3.38	122.54	127.28
27	K	602	CLA	CHD-C1D-ND	-3.38	120.05	124.80
27	a	805	CLA	CHD-C1D-ND	-3.38	120.05	124.80
27	a	825	CLA	CHD-C1D-ND	-3.38	120.05	124.80
27	b	706	CLA	CHD-C1D-ND	-3.38	120.05	124.80
29	C	215	UIX	C34-C30-C26	-3.38	122.54	127.28
27	E	611	CLA	CHD-C1D-ND	-3.38	120.05	124.80
27	a	815	CLA	CHD-C1D-ND	-3.37	120.05	124.80
35	f	305	DGD	O6D-C1D-O3G	-3.37	102.07	110.04
27	C	211	CLA	CHD-C1D-ND	-3.37	120.06	124.80
27	a	830	CLA	CHD-C1D-ND	-3.37	120.06	124.80
27	a	827	CLA	CHD-C1D-ND	-3.37	120.06	124.80
27	b	728	CLA	CHD-C1D-ND	-3.37	120.06	124.80
27	a	831	CLA	CHD-C1D-ND	-3.36	120.07	124.80
27	a	813	CLA	CHD-C1D-ND	-3.36	120.07	124.80
27	l	403	CLA	CHD-C1D-ND	-3.36	120.07	124.80
32	I	614	PID	C27-O6-C30	-3.36	111.91	117.85
27	G	603	CLA	CHD-C1D-ND	-3.36	120.08	124.80
27	T	604	CLA	CHD-C1D-ND	-3.36	120.08	124.80
27	a	817	CLA	CHD-C1D-ND	-3.36	120.08	124.80
27	A	609	CLA	CHD-C1D-ND	-3.36	120.08	124.80
32	U	608	PID	C8-C9-C11	-3.36	120.72	127.28
29	T	612	UIX	C14-C13-C11	-3.36	122.57	127.28
30	E	613	DD6	C14-C13-C11	3.36	130.74	125.53
27	F	603	CLA	CHD-C1D-ND	-3.35	120.08	124.80
27	b	717	CLA	CHD-C1D-ND	-3.35	120.08	124.80
27	a	822	CLA	CHD-C1D-ND	-3.35	120.08	124.80
32	F	615	PID	C19-C20-C21	-3.35	122.58	127.28
29	I	612	UIX	O-C1-C3	-3.35	110.35	113.49
27	D	604	CLA	C1-C2-C3	-3.35	120.71	126.20
27	b	702	CLA	CHD-C1D-ND	-3.34	120.09	124.80
27	A	607	CLA	CHD-C1D-ND	-3.34	120.10	124.80
27	r	204	CLA	CHD-C1D-ND	-3.34	120.10	124.80
27	I	605	CLA	CHD-C1D-ND	-3.34	120.10	124.80
32	U	608	PID	C6-C7-C8	-3.34	118.94	125.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	606	CLA	CHD-C1D-ND	-3.34	120.11	124.80
27	H	307	CLA	CHD-C1D-ND	-3.33	120.11	124.80
27	b	703	CLA	C1-C2-C3	-3.33	120.74	126.20
27	C	206	CLA	CHD-C1D-ND	-3.33	120.12	124.80
27	f	302	CLA	CHD-C1D-ND	-3.33	120.12	124.80
27	I	603	CLA	CHD-C1D-ND	-3.32	120.12	124.80
29	F	613	UIX	C12-C11-C10	3.32	123.16	118.09
27	F	606	CLA	CHD-C1D-ND	-3.32	120.13	124.80
32	B	613	PID	O1-C1-CM1	-3.32	111.34	115.05
27	G	609	CLA	CHD-C1D-ND	-3.32	120.14	124.80
27	H	308	CLA	CHD-C1D-ND	-3.31	120.14	124.80
27	T	602	CLA	CHD-C1D-ND	-3.31	120.14	124.80
27	B	610	CLA	CHD-C1D-ND	-3.31	120.14	124.80
27	F	604	CLA	CHD-C1D-ND	-3.31	120.15	124.80
27	H	306	CLA	CHD-C1D-ND	-3.30	120.16	124.80
27	D	605	CLA	CHD-C1D-ND	-3.30	120.16	124.80
27	F	605	CLA	CHD-C1D-ND	-3.30	120.16	124.80
27	I	616	CLA	CHD-C1D-ND	-3.30	120.17	124.80
27	a	828	CLA	C3D-C4D-ND	3.29	115.34	109.99
27	T	603	CLA	CHD-C1D-ND	-3.29	120.17	124.80
29	I	612	UIX	C38-C40-C39	-3.29	113.83	119.01
27	B	607	CLA	CHD-C1D-ND	-3.29	120.17	124.80
27	D	606	CLA	CHD-C1D-ND	-3.29	120.17	124.80
30	B	614	DD6	O1-C20-C19	-3.28	110.41	113.49
27	b	715	CLA	C3D-C4D-ND	3.28	115.32	109.99
27	I	602	CLA	CHD-C1D-ND	-3.28	120.19	124.80
32	J	615	PID	C22-C23-C24	-3.28	173.80	177.66
27	D	601	CLA	CHD-C1D-ND	-3.27	120.20	124.80
27	b	709	CLA	CHD-C1D-ND	-3.27	120.20	124.80
27	G	607	CLA	C3D-C4D-ND	3.27	115.30	109.99
29	H	314	UIX	C34-C30-C26	-3.27	122.69	127.28
27	D	610	CLA	CHD-C1D-ND	-3.26	120.21	124.80
38	i	201	BCR	C24-C23-C22	-3.26	121.42	126.23
27	b	725	CLA	CHD-C1D-ND	-3.26	120.22	124.80
27	H	304	CLA	CHD-C1D-ND	-3.25	120.23	124.80
32	I	614	PID	C6-C7-C8	-3.25	119.12	125.99
29	E	616	UIX	C34-C37-C39	-3.25	116.87	123.52
29	j	204	UIX	C37-C39-C40	-3.24	122.73	127.28
29	D	616	UIX	C29-C26-C23	3.24	123.04	118.09
27	I	603	CLA	C1-C2-C3	-3.24	120.89	126.20
27	I	608	CLA	CHD-C1D-ND	-3.24	120.25	124.80
27	K	605	CLA	CHD-C1D-ND	-3.24	120.25	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	I	614	PID	C11-C12-C13	-3.24	121.18	128.34
29	A	616	UIX	C28-C25-C20	-3.24	173.84	177.66
27	a	837	CLA	C3D-C4D-ND	3.24	115.25	109.99
27	K	603	CLA	C3D-C4D-ND	3.23	115.24	109.99
29	H	317	UIX	C14-C13-C11	-3.23	122.75	127.28
27	a	803	CLA	C3D-C4D-ND	3.22	115.22	109.99
29	J	616	UIX	C36-C35-C32	-3.22	122.76	127.28
27	H	312	CLA	CHD-C1D-ND	-3.22	120.27	124.80
27	l	409	CLA	CHD-C1D-ND	-3.22	120.27	124.80
29	C	213	UIX	C18-O2-C27	-3.22	112.17	117.85
29	H	317	UIX	C29-C26-C23	3.19	122.96	118.09
27	K	604	CLA	CHD-C1D-ND	-3.19	120.31	124.80
27	D	608	CLA	C3D-C4D-ND	3.18	115.16	109.99
27	b	708	CLA	CHD-C1D-ND	-3.18	120.32	124.80
29	H	314	UIX	C-C7-C10	-3.18	119.27	125.99
27	G	604	CLA	C3D-C4D-ND	3.18	115.16	109.99
32	F	614	PID	C8-C9-C11	-3.18	121.07	127.28
27	B	606	CLA	C3D-C4D-ND	3.18	115.15	109.99
29	A	613	UIX	C12-C11-C10	3.17	122.93	118.09
29	C	213	UIX	C14-C13-C11	-3.17	122.84	127.28
27	I	606	CLA	C3D-C4D-ND	3.16	115.12	109.99
27	b	713	CLA	C3D-C4D-ND	3.15	115.11	109.99
32	B	613	PID	C27-O6-C30	-3.15	112.28	117.85
27	I	607	CLA	C3D-C4D-ND	3.15	115.11	109.99
27	H	309	CLA	C3D-C4D-ND	3.15	115.11	109.99
29	I	612	UIX	C18-O2-C27	-3.15	112.29	117.85
27	B	604	CLA	C3D-C4D-ND	3.15	115.10	109.99
27	b	723	CLA	C3D-C4D-ND	3.14	115.10	109.99
27	I	603	CLA	C3D-C4D-ND	3.14	115.09	109.99
27	l	402	CLA	C3D-C4D-ND	3.14	115.09	109.99
27	D	604	CLA	CHD-C1D-ND	-3.14	120.38	124.80
27	C	209	CLA	C3D-C4D-ND	3.14	115.08	109.99
27	T	602	CLA	C3D-C4D-ND	3.13	115.08	109.99
30	D	615	DD6	C14-C13-C11	3.13	130.38	125.53
27	b	716	CLA	C3D-C4D-ND	3.13	115.07	109.99
27	E	606	CLA	C3D-C4D-ND	3.12	115.06	109.99
27	I	611	CLA	C3D-C4D-ND	3.12	115.06	109.99
29	A	613	UIX	C-C7-C10	-3.12	119.40	125.99
27	b	707	CLA	C3D-C4D-ND	3.12	115.05	109.99
27	A	602	CLA	C3D-C4D-ND	3.11	115.05	109.99
27	A	601	CLA	C3D-C4D-ND	3.11	115.04	109.99
27	T	605	CLA	CHD-C1D-ND	-3.11	120.43	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	712	CLA	C3D-C4D-ND	3.11	115.04	109.99
29	H	317	UIX	C-C7-C10	-3.11	119.43	125.99
27	F	607	CLA	C3D-C4D-ND	3.10	115.03	109.99
27	F	610	CLA	C3D-C4D-ND	3.10	115.03	109.99
27	r	203	CLA	C3D-C4D-ND	3.10	115.03	109.99
27	D	604	CLA	C3D-C4D-ND	3.10	115.02	109.99
27	b	711	CLA	C3D-C4D-ND	3.10	115.02	109.99
27	U	601	CLA	C3D-C4D-ND	3.10	115.02	109.99
27	H	313	CLA	C3D-C4D-ND	3.09	115.02	109.99
27	E	604	CLA	C1-C2-C3	-3.09	121.13	126.20
29	B	611	UIX	C37-C34-C30	-3.09	117.19	123.52
27	C	204	CLA	C3D-C4D-ND	3.09	115.01	109.99
27	G	608	CLA	C3D-C4D-ND	3.09	115.01	109.99
27	C	203	CLA	C3D-C4D-ND	3.09	115.01	109.99
27	D	603	CLA	C3D-C4D-ND	3.09	115.01	109.99
27	F	605	CLA	C3D-C4D-ND	3.09	115.01	109.99
27	C	202	CLA	C3D-C4D-ND	3.09	115.00	109.99
38	a	836	BCR	C38-C26-C27	3.08	120.17	113.60
27	T	604	CLA	C3D-C4D-ND	3.08	114.99	109.99
27	C	212	CLA	C3D-C4D-ND	3.08	114.99	109.99
27	D	612	CLA	C3D-C4D-ND	3.08	114.99	109.99
27	U	603	CLA	C3D-C4D-ND	3.07	114.98	109.99
27	J	603	CLA	C3D-C4D-ND	3.07	114.98	109.99
27	a	813	CLA	C3D-C4D-ND	3.07	114.98	109.99
27	A	611	CLA	C3D-C4D-ND	3.07	114.97	109.99
27	G	602	CLA	C3D-C4D-ND	3.07	114.97	109.99
27	D	609	CLA	C3D-C4D-ND	3.07	114.97	109.99
27	E	602	CLA	C3D-C4D-ND	3.07	114.97	109.99
27	F	608	CLA	C3D-C4D-ND	3.07	114.97	109.99
27	b	719	CLA	C3D-C4D-ND	3.07	114.97	109.99
27	l	410	CLA	C3D-C4D-ND	3.06	114.97	109.99
27	F	603	CLA	C3D-C4D-ND	3.06	114.97	109.99
27	C	208	CLA	C3D-C4D-ND	3.06	114.96	109.99
27	U	606	CLA	C3D-C4D-ND	3.06	114.96	109.99
27	a	821	CLA	C3D-C4D-ND	3.06	114.96	109.99
27	B	610	CLA	C3D-C4D-ND	3.06	114.96	109.99
27	C	201	CLA	C3D-C4D-ND	3.06	114.96	109.99
35	K	614	DGD	O6D-C1D-O3G	-3.06	102.82	110.04
27	b	712	CLA	CAA-C2A-C1A	-3.06	101.96	111.97
27	I	609	CLA	C3D-C4D-ND	3.06	114.95	109.99
27	B	601	CLA	C3D-C4D-ND	3.05	114.95	109.99
27	E	604	CLA	C3D-C4D-ND	3.05	114.95	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	606	CLA	C3D-C4D-ND	3.05	114.95	109.99
27	A	604	CLA	C3D-C4D-ND	3.05	114.95	109.99
27	H	312	CLA	C3D-C4D-ND	3.05	114.95	109.99
27	A	607	CLA	C3D-C4D-ND	3.05	114.94	109.99
29	D	616	UIX	C34-C37-C39	-3.05	117.28	123.52
27	K	606	CLA	C3D-C4D-ND	3.05	114.94	109.99
27	b	722	CLA	C3D-C4D-ND	3.05	114.94	109.99
29	C	215	UIX	C18-O2-C27	-3.05	112.46	117.85
27	a	825	CLA	C3D-C4D-ND	3.05	114.94	109.99
27	A	609	CLA	C3D-C4D-ND	3.05	114.94	109.99
29	B	615	UIX	O-C1-C6	-3.05	111.64	115.05
27	K	601	CLA	C3D-C4D-ND	3.04	114.93	109.99
27	a	806	CLA	C3D-C4D-ND	3.04	114.93	109.99
27	E	612	CLA	C3D-C4D-ND	3.04	114.93	109.99
27	I	601	CLA	C3D-C4D-ND	3.04	114.93	109.99
27	H	319	CLA	C3D-C4D-ND	3.04	114.93	109.99
27	a	816	CLA	C3D-C4D-ND	3.03	114.92	109.99
30	r	201	DD6	O1-C15-C14	-3.03	108.19	116.88
27	B	605	CLA	C3D-C4D-ND	3.03	114.92	109.99
27	A	612	CLA	C3D-C4D-ND	3.03	114.92	109.99
27	b	721	CLA	C3D-C4D-ND	3.03	114.91	109.99
27	T	601	CLA	C3D-C4D-ND	3.03	114.91	109.99
27	J	609	CLA	C3D-C4D-ND	3.03	114.91	109.99
27	J	607	CLA	C3D-C4D-ND	3.03	114.91	109.99
27	G	606	CLA	C3D-C4D-ND	3.03	114.90	109.99
27	T	609	CLA	C3D-C4D-ND	3.02	114.90	109.99
27	D	607	CLA	C3D-C4D-ND	3.02	114.90	109.99
27	a	814	CLA	C3D-C4D-ND	3.02	114.90	109.99
27	I	610	CLA	C3D-C4D-ND	3.02	114.90	109.99
27	a	807	CLA	C3D-C4D-ND	3.02	114.90	109.99
27	F	619	CLA	C3D-C4D-ND	3.02	114.89	109.99
27	a	808	CLA	C3D-C4D-ND	3.02	114.89	109.99
29	I	612	UIX	C12-C11-C10	3.01	122.69	118.09
27	F	601	CLA	C3D-C4D-ND	3.01	114.88	109.99
38	a	836	BCR	C8-C7-C6	-3.01	118.96	127.00
27	a	807	CLA	CAA-C2A-C1A	-3.01	102.12	111.97
27	T	607	CLA	C3D-C4D-ND	3.01	114.88	109.99
27	G	611	CLA	C3D-C4D-ND	3.00	114.87	109.99
29	A	616	UIX	C38-C40-C39	-3.00	114.29	119.01
29	G	615	UIX	C18-O2-C27	-3.00	112.54	117.85
27	B	609	CLA	C3D-C4D-ND	3.00	114.86	109.99
27	C	205	CLA	C3D-C4D-ND	3.00	114.86	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	824	CLA	C3D-C4D-ND	3.00	114.86	109.99
27	a	839	CLA	C3D-C4D-ND	3.00	114.86	109.99
27	A	610	CLA	C3D-C4D-ND	3.00	114.86	109.99
27	F	606	CLA	C3D-C4D-ND	2.99	114.86	109.99
27	H	310	CLA	C3D-C4D-ND	2.99	114.86	109.99
27	l	409	CLA	C3D-C4D-ND	2.99	114.86	109.99
27	a	810	CLA	C3D-C4D-ND	2.99	114.85	109.99
27	l	412	CLA	C3D-C4D-ND	2.99	114.85	109.99
27	b	726	CLA	C3D-C4D-ND	2.99	114.85	109.99
27	H	306	CLA	C3D-C4D-ND	2.99	114.85	109.99
27	E	603	CLA	C3D-C4D-ND	2.99	114.85	109.99
27	H	303	CLA	C3D-C4D-ND	2.99	114.84	109.99
27	b	720	CLA	C3D-C4D-ND	2.99	114.84	109.99
27	a	822	CLA	C3D-C4D-ND	2.99	114.84	109.99
27	l	405	CLA	C3D-C4D-ND	2.99	114.84	109.99
27	A	605	CLA	C3D-C4D-ND	2.99	114.84	109.99
27	T	603	CLA	C3D-C4D-ND	2.98	114.84	109.99
27	D	611	CLA	C3D-C4D-ND	2.98	114.84	109.99
27	K	608	CLA	C3D-C4D-ND	2.98	114.84	109.99
27	l	408	CLA	C3D-C4D-ND	2.98	114.83	109.99
27	E	611	CLA	C3D-C4D-ND	2.98	114.83	109.99
27	b	724	CLA	C3D-C4D-ND	2.98	114.83	109.99
27	B	603	CLA	C3D-C4D-ND	2.98	114.83	109.99
27	a	829	CLA	C3D-C4D-ND	2.98	114.83	109.99
27	G	610	CLA	C3D-C4D-ND	2.98	114.83	109.99
32	F	615	PID	O1-C1-CM1	-2.98	111.72	115.05
27	A	603	CLA	C3D-C4D-ND	2.97	114.82	109.99
27	G	603	CLA	C3D-C4D-ND	2.97	114.82	109.99
27	b	727	CLA	C3D-C4D-ND	2.97	114.82	109.99
28	A	608	KC2	CHB-C4A-NA	2.97	128.84	124.23
32	J	611	PID	CM1-C1-C2	2.97	117.58	114.24
29	C	213	UIX	O-C1-C6	-2.97	111.73	115.05
27	I	605	CLA	C3D-C4D-ND	2.97	114.81	109.99
27	a	805	CLA	C3D-C4D-ND	2.97	114.81	109.99
27	C	206	CLA	C3D-C4D-ND	2.97	114.81	109.99
27	H	308	CLA	C3D-C4D-ND	2.97	114.81	109.99
27	K	602	CLA	C3D-C4D-ND	2.97	114.81	109.99
27	l	403	CLA	C3D-C4D-ND	2.97	114.81	109.99
27	l	411	CLA	C3D-C4D-ND	2.97	114.81	109.99
27	K	604	CLA	C3D-C4D-ND	2.96	114.81	109.99
27	a	815	CLA	C3D-C4D-ND	2.96	114.81	109.99
27	b	728	CLA	C3D-C4D-ND	2.96	114.81	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	616	UIX	C6-C1-C	-2.96	117.42	122.30
27	a	819	CLA	C3D-C4D-ND	2.96	114.80	109.99
32	J	614	PID	C18-C17-C16	-2.96	117.87	124.72
27	b	715	CLA	CAA-C2A-C1A	-2.96	102.27	111.97
27	E	608	CLA	C3D-C4D-ND	2.96	114.80	109.99
27	b	704	CLA	C3D-C4D-ND	2.96	114.80	109.99
27	E	609	CLA	C3D-C4D-ND	2.96	114.79	109.99
27	J	601	CLA	C3D-C4D-ND	2.96	114.79	109.99
32	F	615	PID	C8-C9-C11	-2.96	121.50	127.28
27	D	606	CLA	C3D-C4D-ND	2.96	114.79	109.99
27	b	725	CLA	C3D-C4D-ND	2.96	114.79	109.99
29	B	615	UIX	C34-C30-C26	-2.95	123.13	127.28
27	a	830	CLA	C3D-C4D-ND	2.95	114.79	109.99
27	b	714	CLA	C3D-C4D-ND	2.95	114.79	109.99
32	J	614	PID	O1-C1-CM1	-2.95	111.75	115.05
29	A	616	UIX	C34-C37-C39	-2.95	117.49	123.52
29	F	613	UIX	C-C7-C10	-2.95	119.76	125.99
27	T	606	CLA	C3D-C4D-ND	2.95	114.78	109.99
27	C	211	CLA	C3D-C4D-ND	2.95	114.77	109.99
27	a	812	CLA	C3D-C4D-ND	2.94	114.77	109.99
27	H	307	CLA	C3D-C4D-ND	2.94	114.77	109.99
27	b	705	CLA	C3D-C4D-ND	2.94	114.77	109.99
27	b	701	CLA	C3D-C4D-ND	2.94	114.77	109.99
29	j	204	UIX	O-C1-C3	-2.94	110.73	113.49
27	E	605	CLA	C3D-C4D-ND	2.94	114.77	109.99
27	J	605	CLA	C3D-C4D-ND	2.94	114.76	109.99
29	E	616	UIX	C29-C26-C23	2.94	122.57	118.09
27	l	407	CLA	C3D-C4D-ND	2.94	114.76	109.99
32	J	613	PID	C17-C16-C15	-2.93	117.51	123.52
27	a	824	CLA	CAA-C2A-C1A	-2.93	102.37	111.97
27	b	710	CLA	C3D-C4D-ND	2.93	114.75	109.99
27	F	604	CLA	C3D-C4D-ND	2.93	114.75	109.99
27	C	207	CLA	C3D-C4D-ND	2.93	114.75	109.99
27	b	709	CLA	C3D-C4D-ND	2.93	114.75	109.99
27	D	602	CLA	C3D-C4D-ND	2.93	114.75	109.99
29	B	615	UIX	C14-C13-C11	-2.92	123.18	127.28
29	j	204	UIX	C-C7-C10	-2.92	119.81	125.99
35	f	305	DGD	O6E-C5E-C4E	2.92	114.97	109.70
27	D	601	CLA	C3D-C4D-ND	2.92	114.74	109.99
27	r	204	CLA	C3D-C4D-ND	2.92	114.74	109.99
29	A	616	UIX	C35-C36-C38	-2.92	114.74	123.20
27	a	823	CLA	C3D-C4D-ND	2.92	114.73	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	809	CLA	C3D-C4D-ND	2.92	114.73	109.99
27	G	605	CLA	C3D-C4D-ND	2.92	114.73	109.99
27	l	406	CLA	C3D-C4D-ND	2.91	114.72	109.99
29	B	611	UIX	C34-C30-C26	-2.91	123.19	127.28
27	b	718	CLA	C3D-C4D-ND	2.91	114.72	109.99
29	G	615	UIX	C-C7-C10	-2.91	119.84	125.99
27	K	605	CLA	C3D-C4D-ND	2.91	114.72	109.99
27	a	831	CLA	C3D-C4D-ND	2.91	114.72	109.99
29	C	213	UIX	C-C7-C10	-2.91	119.84	125.99
29	E	616	UIX	C18-O2-C27	-2.90	112.72	117.85
28	G	601	KC2	CHB-C4A-NA	2.90	128.73	124.23
27	b	717	CLA	C3D-C4D-ND	2.90	114.71	109.99
27	b	702	CLA	CHB-C1B-NB	-2.90	119.70	124.05
27	a	817	CLA	C3D-C4D-ND	2.90	114.70	109.99
32	U	608	PID	C27-O6-C30	-2.90	112.72	117.85
29	A	613	UIX	C34-C30-C26	-2.89	123.22	127.28
27	B	607	CLA	C3D-C4D-ND	2.89	114.69	109.99
27	a	827	CLA	C3D-C4D-ND	2.89	114.69	109.99
27	l	404	CLA	C3D-C4D-ND	2.89	114.69	109.99
29	I	612	UIX	C35-C36-C38	-2.89	114.83	123.20
27	b	706	CLA	C3D-C4D-ND	2.89	114.68	109.99
35	l	416	DGD	O6D-C1D-O3G	-2.88	103.23	110.04
27	a	811	CLA	C3D-C4D-ND	2.88	114.67	109.99
27	a	820	CLA	C3D-C4D-ND	2.88	114.66	109.99
32	J	615	PID	C17-C16-C15	-2.87	117.64	123.52
27	I	602	CLA	C3D-C4D-ND	2.87	114.66	109.99
32	J	614	PID	C18-C19-C20	-2.87	117.64	123.52
29	D	616	UIX	C21-C15-C20	-2.87	107.90	110.47
27	F	602	CLA	C3D-C4D-ND	2.87	114.65	109.99
27	F	617	CLA	C3D-C4D-ND	2.87	114.65	109.99
29	B	615	UIX	C18-O2-C27	-2.87	112.78	117.85
29	H	314	UIX	C41-C40-C38	2.87	122.47	118.09
27	D	610	CLA	C3D-C4D-ND	2.86	114.64	109.99
29	j	204	UIX	C35-C36-C38	-2.86	114.91	123.20
29	F	613	UIX	C14-C13-C11	-2.86	123.26	127.28
32	J	615	PID	C27-O6-C30	-2.86	112.79	117.85
30	F	611	DD6	O1-C20-C19	-2.86	110.81	113.49
27	U	605	CLA	C3D-C4D-ND	2.86	114.63	109.99
27	a	818	CLA	C3D-C4D-ND	2.86	114.63	109.99
29	F	613	UIX	O-C1-C6	-2.86	111.86	115.05
27	a	826	CLA	C3D-C4D-ND	2.85	114.62	109.99
27	b	723	CLA	C1-C2-C3	-2.85	121.52	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	611	PID	C17-C18-C19	-2.85	118.13	124.72
29	J	616	UIX	C-C7-C10	-2.85	119.97	125.99
27	H	305	CLA	C3D-C4D-ND	2.85	114.62	109.99
27	f	302	CLA	C3D-C4D-ND	2.85	114.62	109.99
30	I	613	DD6	C14-C13-C11	2.85	129.95	125.53
29	A	613	UIX	C18-O2-C27	-2.84	112.82	117.85
27	a	802	CLA	C3D-C4D-ND	2.84	114.60	109.99
30	U	607	DD6	C14-C13-C11	2.84	129.93	125.53
27	G	609	CLA	C3D-C4D-ND	2.83	114.59	109.99
29	A	616	UIX	C14-C13-C11	-2.83	123.31	127.28
27	T	605	CLA	C3D-C4D-ND	2.83	114.59	109.99
38	a	836	BCR	C30-C25-C26	-2.82	118.78	122.64
29	I	612	UIX	C22-C15-C20	-2.82	107.95	110.47
32	B	613	PID	C8-C9-C11	-2.82	121.77	127.28
32	I	614	PID	CM6-C25-C24	-2.82	107.95	110.47
27	D	605	CLA	C3D-C4D-ND	2.82	114.57	109.99
30	r	205	DD6	C14-C13-C11	2.82	129.90	125.53
29	C	215	UIX	C38-C40-C39	-2.81	114.58	119.01
29	F	613	UIX	O2-C27-O4	-2.81	117.56	122.99
27	H	305	CLA	C1-C2-C3	-2.81	121.59	126.20
29	B	611	UIX	C21-C15-C20	-2.81	107.96	110.47
27	a	804	CLA	C3D-C4D-ND	2.81	114.55	109.99
29	H	314	UIX	C18-O2-C27	-2.81	112.89	117.85
29	T	612	UIX	C-C7-C10	-2.81	120.06	125.99
27	I	608	CLA	C3D-C4D-ND	2.80	114.55	109.99
29	C	215	UIX	C35-C36-C38	-2.80	115.09	123.20
27	b	713	CLA	C1-C2-C3	-2.79	121.62	126.20
29	H	317	UIX	C34-C37-C39	-2.79	117.81	123.52
32	I	614	PID	C8-C9-C11	-2.78	121.84	127.28
30	D	613	DD6	O1-C20-C19	-2.77	110.89	113.49
30	D	613	DD6	C14-C13-C11	2.77	129.83	125.53
27	j	202	CLA	C3D-C4D-ND	2.77	114.49	109.99
27	a	801	CLA	CHB-C1B-NB	-2.76	119.90	124.05
27	b	708	CLA	C3D-C4D-ND	2.76	114.48	109.99
27	b	703	CLA	C3D-C4D-ND	2.76	114.48	109.99
28	J	610	KC2	CHB-C4A-NA	2.76	128.51	124.23
27	I	616	CLA	C3D-C4D-ND	2.76	114.47	109.99
32	K	611	PID	C11-C12-C13	-2.76	122.24	128.34
30	r	205	DD6	C30-C29-C27	-2.76	166.86	176.23
29	B	615	UIX	C37-C34-C30	-2.76	117.88	123.52
29	C	215	UIX	C34-C37-C39	-2.75	117.88	123.52
28	H	302	KC2	CHB-C4A-NA	2.75	128.50	124.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	708	CLA	CHB-C1B-NB	-2.75	119.92	124.05
35	j	201	DGD	CDB-CCB-CBB	-2.75	100.49	114.37
35	f	305	DGD	C3D-C4D-C5D	-2.75	105.25	110.23
27	E	607	CLA	C3D-C4D-ND	2.74	114.45	109.99
29	j	204	UIX	O-C1-C6	-2.74	111.98	115.05
29	j	204	UIX	C38-C40-C39	-2.73	114.71	119.01
27	b	703	CLA	O2A-C1-C2	2.73	118.62	108.11
29	C	215	UIX	C-C7-C10	-2.73	120.22	125.99
32	I	614	PID	C26-C25-C24	2.72	111.86	109.21
27	f	303	CLA	C3D-C4D-ND	2.72	114.41	109.99
28	T	608	KC2	CHB-C4A-NA	2.72	128.44	124.23
27	a	830	CLA	C1-C2-C3	-2.72	121.75	126.20
27	C	204	CLA	C1-C2-C3	-2.72	121.75	126.20
29	j	204	UIX	C6-C1-C	-2.71	117.84	122.30
29	H	314	UIX	C35-C36-C38	-2.71	115.36	123.20
28	B	608	KC2	CHB-C4A-NA	2.71	128.43	124.23
28	H	311	KC2	CHB-C4A-NA	2.71	128.43	124.23
30	r	201	DD6	O1-C20-C19	-2.71	110.95	113.49
30	C	214	DD6	C14-C13-C11	2.71	129.73	125.53
29	B	615	UIX	C36-C35-C32	-2.70	123.50	127.28
28	E	601	KC2	CHB-C4A-NA	2.69	128.41	124.23
27	l	412	CLA	C1-C2-C3	-2.69	121.78	126.20
29	A	613	UIX	C14-C13-C11	-2.69	123.50	127.28
32	F	615	PID	O6-C30-O7	-2.69	117.80	122.99
29	B	611	UIX	C23-C26-C30	-2.68	114.79	119.01
29	j	204	UIX	C34-C37-C39	-2.68	118.04	123.52
32	J	614	PID	C8-C9-C11	-2.68	122.05	127.28
29	F	613	UIX	C17-C15-C20	2.68	111.81	109.21
29	T	612	UIX	C34-C37-C39	-2.68	118.05	123.52
27	B	603	CLA	C1-C2-C3	-2.67	121.81	126.20
30	G	614	DD6	C14-C13-C11	2.67	129.67	125.53
31	y	301	SQD	O48-C23-C24	2.67	119.97	111.83
27	C	203	CLA	C1-C2-C3	-2.67	121.83	126.20
27	a	816	CLA	CHB-C1B-NB	-2.67	120.05	124.05
30	F	611	DD6	O1-C15-C14	-2.66	109.25	116.88
29	C	215	UIX	C10-C11-C13	-2.66	114.83	119.01
27	a	801	CLA	CHA-C1A-NA	-2.66	120.37	126.39
35	f	305	DGD	CDB-CCB-CBB	-2.66	100.94	114.37
32	B	613	PID	C29-C24-C25	2.65	122.33	119.70
30	A	614	DD6	O1-C20-C19	-2.65	111.01	113.49
29	C	215	UIX	C16-C20-C15	2.65	122.32	119.70
29	B	615	UIX	O-C-C7	-2.64	109.30	116.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	613	PID	C6-C7-C8	-2.64	120.41	125.99
30	H	316	DD6	C14-C13-C11	2.64	129.62	125.53
32	J	615	PID	C17-C18-C19	-2.63	118.63	124.72
29	G	615	UIX	C22-C15-C20	-2.63	108.12	110.47
29	A	613	UIX	O-C1-C3	-2.63	111.03	113.49
28	E	610	KC2	CHB-C4A-NA	2.63	128.31	124.23
30	F	611	DD6	C14-C13-C11	2.63	129.61	125.53
31	A	618	SQD	O9-S-C6	2.63	110.68	106.76
27	E	605	CLA	CHB-C1B-NB	-2.62	120.11	124.05
35	K	614	DGD	C1E-O6E-C5E	2.62	118.84	113.72
31	y	301	SQD	O7-S-C6	2.62	110.67	106.76
29	B	611	UIX	C13-C14-C23	-2.61	115.63	123.20
37	b	729	PQN	C11-C3-C4	-2.61	115.83	118.58
27	I	605	CLA	CHB-C1B-NB	-2.61	120.13	124.05
28	C	210	KC2	CHB-C4A-NA	2.61	128.28	124.23
27	F	606	CLA	CHB-C1B-NB	-2.60	120.14	124.05
38	a	836	BCR	C2-C1-C6	-2.60	106.66	110.44
28	J	608	KC2	CHB-C4A-NA	2.60	128.26	124.23
29	H	317	UIX	C36-C35-C32	-2.60	123.63	127.28
32	F	614	PID	O1-C1-C6	-2.60	56.87	58.93
32	F	615	PID	C6-C7-C8	-2.60	120.50	125.99
32	U	608	PID	O6-C30-O7	-2.60	117.98	122.99
27	a	813	CLA	CHB-C1B-NB	-2.60	120.16	124.05
29	B	611	UIX	C10-C11-C13	-2.60	114.93	119.01
29	C	215	UIX	C22-C15-C20	-2.59	108.15	110.47
27	a	824	CLA	CHB-C1B-NB	-2.59	120.17	124.05
27	B	607	CLA	C2C-C1C-NC	2.58	112.69	109.98
30	i	202	DD6	C21-C20-C19	2.58	117.14	114.24
32	K	611	PID	C16-C15-C14	-2.58	123.66	127.28
32	J	615	PID	C6-C7-C8	-2.58	120.54	125.99
38	a	836	BCR	C7-C8-C9	-2.58	122.42	126.23
32	U	608	PID	C17-C18-C19	-2.58	118.76	124.72
27	a	820	CLA	CHB-C1B-NB	-2.58	120.18	124.05
32	B	613	PID	O6-C30-O7	-2.58	118.02	122.99
28	U	602	KC2	CHB-C4A-NA	2.58	128.23	124.23
27	H	304	CLA	C3D-C4D-ND	2.58	114.17	109.99
27	G	608	CLA	CHB-C1B-NB	-2.58	120.19	124.05
27	a	815	CLA	CHB-C1B-NB	-2.58	120.19	124.05
27	a	809	CLA	CHB-C1B-NB	-2.57	120.19	124.05
27	b	727	CLA	CHB-C1B-NB	-2.57	120.19	124.05
36	T	613	LMU	O1B-C4'-C3'	2.57	113.77	107.23
32	U	608	PID	C17-C16-C15	-2.57	118.26	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T	612	UIX	O-C1-C6	-2.57	112.17	115.05
27	b	706	CLA	CHB-C1B-NB	-2.57	120.20	124.05
29	F	613	UIX	C34-C37-C39	-2.57	118.27	123.52
29	C	215	UIX	C13-C14-C23	-2.56	115.78	123.20
30	I	615	DD6	C14-C13-C11	2.56	129.50	125.53
28	J	604	KC2	CHB-C4A-NA	2.56	128.20	124.23
29	C	215	UIX	C14-C13-C11	-2.56	123.69	127.28
32	J	611	PID	C7-C8-C9	-2.56	122.84	126.06
32	K	611	PID	O1-C1-C6	-2.55	56.91	58.93
27	b	719	CLA	CHB-C1B-NB	-2.55	120.23	124.05
29	B	611	UIX	C19-C18-C17	2.55	114.46	109.89
27	a	837	CLA	CHB-C1B-NB	-2.55	120.23	124.05
29	D	616	UIX	C29-C26-C30	-2.55	118.69	122.82
29	I	612	UIX	O2-C27-O4	-2.55	118.08	122.99
28	F	609	KC2	CHB-C4A-NA	2.54	128.18	124.23
27	C	207	CLA	CHB-C1B-NB	-2.54	120.23	124.05
27	a	812	CLA	CHB-C1B-NB	-2.54	120.23	124.05
38	a	836	BCR	C27-C26-C25	-2.54	119.27	122.70
27	a	817	CLA	C2C-C1C-NC	2.54	112.65	109.98
28	U	604	KC2	CHD-C1D-ND	-2.54	120.24	124.05
27	b	722	CLA	C2C-C1C-NC	2.54	112.64	109.98
29	B	615	UIX	C-C7-C10	-2.53	120.63	125.99
30	r	206	DD6	C21-C20-C19	2.53	117.08	114.24
27	b	713	CLA	CHB-C1B-NB	-2.53	120.25	124.05
27	f	302	CLA	CHB-C1B-NB	-2.53	120.25	124.05
29	C	213	UIX	C6-C1-C	-2.53	118.14	122.30
27	G	606	CLA	CHB-C1B-NB	-2.53	120.26	124.05
29	E	616	UIX	C35-C36-C38	-2.53	115.88	123.20
28	I	604	KC2	CHB-C4A-NA	2.53	128.15	124.23
29	j	204	UIX	C37-C34-C30	-2.52	118.35	123.52
27	b	717	CLA	CHB-C1B-NB	-2.52	120.26	124.05
30	H	301	DD6	C14-C13-C11	2.52	129.44	125.53
27	D	605	CLA	CHB-C1B-NB	-2.52	120.27	124.05
27	D	606	CLA	C2C-C1C-NC	2.52	112.63	109.98
27	a	807	CLA	CHB-C1B-NB	-2.52	120.28	124.05
27	f	303	CLA	CHB-C1B-NB	-2.52	120.28	124.05
27	a	823	CLA	C1-C2-C3	-2.51	122.08	126.20
29	I	612	UIX	C37-C39-C40	-2.51	123.75	127.28
30	T	610	DD6	O1-C15-C14	-2.51	109.67	116.88
29	F	613	UIX	C6-C1-C	-2.51	118.17	122.30
29	A	613	UIX	C37-C34-C30	-2.51	118.39	123.52
27	a	827	CLA	CHB-C1B-NB	-2.51	120.28	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	616	UIX	O-C-C7	-2.51	109.69	116.88
28	K	607	KC2	CHB-C4A-NA	2.51	128.12	124.23
29	E	616	UIX	C38-C40-C39	-2.51	115.06	119.01
27	l	409	CLA	CHB-C1B-NB	-2.51	120.29	124.05
28	J	604	KC2	CHD-C1D-ND	-2.51	120.29	124.05
29	H	314	UIX	C38-C40-C39	-2.51	115.07	119.01
27	H	303	CLA	CHB-C1B-NB	-2.51	120.29	124.05
27	b	704	CLA	C1-C2-C3	-2.50	122.09	126.20
30	A	614	DD6	C14-C13-C11	2.50	129.41	125.53
27	a	826	CLA	CHB-C1B-NB	-2.50	120.30	124.05
35	l	416	DGD	C3G-C2G-C1G	-2.50	105.95	111.78
27	b	708	CLA	C2C-C1C-NC	2.50	112.61	109.98
27	B	601	CLA	CHB-C1B-NB	-2.50	120.30	124.05
27	U	605	CLA	CHB-C1B-NB	-2.50	120.30	124.05
27	E	609	CLA	CHB-C1B-NB	-2.50	120.30	124.05
27	F	604	CLA	CHB-C1B-NB	-2.50	120.30	124.05
32	F	615	PID	O1-C1-C2	-2.50	111.15	113.49
35	j	201	DGD	O6E-C1E-O5D	-2.50	104.15	110.04
32	J	615	PID	O6-C30-O7	-2.49	118.17	122.99
27	b	707	CLA	CHB-C1B-NB	-2.49	120.31	124.05
30	D	617	DD6	C14-C13-C11	2.49	129.40	125.53
27	a	814	CLA	CHB-C1B-NB	-2.49	120.31	124.05
29	J	616	UIX	C34-C30-C26	-2.49	123.78	127.28
27	b	712	CLA	CHB-C1B-NB	-2.49	120.31	124.05
27	l	407	CLA	CHB-C1B-NB	-2.49	120.31	124.05
38	a	836	BCR	C28-C27-C26	-2.49	109.62	114.06
33	C	217	LMG	C8-O7-C10	2.49	123.75	117.80
27	K	605	CLA	CHB-C1B-NB	-2.49	120.32	124.05
27	a	808	CLA	C1-C2-C3	-2.49	122.12	126.20
27	G	603	CLA	CHB-C1B-NB	-2.48	120.33	124.05
29	H	314	UIX	C34-C37-C39	-2.48	118.44	123.52
30	K	612	DD6	C14-C13-C11	2.48	129.38	125.53
27	J	601	CLA	CHB-C1B-NB	-2.48	120.33	124.05
27	A	610	CLA	CHB-C1B-NB	-2.48	120.33	124.05
27	a	828	CLA	CHB-C1B-NB	-2.48	120.33	124.05
27	b	710	CLA	CHB-C1B-NB	-2.48	120.33	124.05
27	b	723	CLA	CHB-C1B-NB	-2.48	120.33	124.05
28	B	602	KC2	CHD-C1D-ND	-2.48	120.33	124.05
32	F	614	PID	O6-C30-O7	-2.48	118.21	122.99
27	E	607	CLA	CHB-C1B-NB	-2.48	120.33	124.05
27	l	402	CLA	CHB-C1B-NB	-2.48	120.34	124.05
27	l	403	CLA	CHB-C1B-NB	-2.47	120.34	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	I	410	CLA	CHB-C1B-NB	-2.47	120.34	124.05
29	T	612	UIX	O-C-C7	-2.47	109.79	116.88
32	B	613	PID	CM4-C14-C13	2.47	124.51	119.05
30	H	316	DD6	C21-C20-C19	2.47	117.02	114.24
27	a	839	CLA	CHB-C1B-NB	-2.47	120.34	124.05
28	J	602	KC2	CHB-C4A-NA	2.47	128.06	124.23
32	K	611	PID	C18-C17-C16	-2.47	119.01	124.72
27	H	304	CLA	C1-C2-C3	-2.47	122.15	126.20
32	J	611	PID	O4-C10-O3	2.47	124.79	120.17
27	I	609	CLA	CHB-C1B-NB	-2.47	120.35	124.05
28	U	602	KC2	CHD-C1D-ND	-2.47	120.35	124.05
27	C	203	CLA	CHB-C1B-NB	-2.47	120.35	124.05
27	a	802	CLA	CHB-C1B-NB	-2.47	120.35	124.05
27	b	722	CLA	CHB-C1B-NB	-2.46	120.35	124.05
27	J	607	CLA	CHB-C1B-NB	-2.46	120.36	124.05
27	a	805	CLA	CHB-C1B-NB	-2.46	120.36	124.05
28	C	210	KC2	CHD-C1D-ND	-2.46	120.36	124.05
27	H	313	CLA	CHB-C1B-NB	-2.46	120.36	124.05
27	b	701	CLA	CHB-C1B-NB	-2.46	120.36	124.05
27	F	602	CLA	CHB-C1B-NB	-2.46	120.36	124.05
29	B	611	UIX	C22-C15-C20	-2.46	108.27	110.47
27	E	606	CLA	CHB-C1B-NB	-2.46	120.36	124.05
27	a	804	CLA	CHB-C1B-NB	-2.46	120.36	124.05
32	J	615	PID	CM7-C25-C24	-2.46	108.27	110.47
28	K	607	KC2	CHD-C1D-ND	-2.46	120.36	124.05
27	B	607	CLA	CHB-C1B-NB	-2.46	120.36	124.05
27	H	306	CLA	CHB-C1B-NB	-2.46	120.36	124.05
27	a	831	CLA	CHB-C1B-NB	-2.45	120.37	124.05
27	a	818	CLA	CHB-C1B-NB	-2.45	120.37	124.05
28	E	610	KC2	CHD-C1D-ND	-2.45	120.37	124.05
28	J	606	KC2	CHD-C1D-ND	-2.45	120.37	124.05
32	J	613	PID	O6-C30-O7	-2.45	118.26	122.99
27	C	205	CLA	CHB-C1B-NB	-2.45	120.37	124.05
27	H	305	CLA	CHB-C1B-NB	-2.45	120.37	124.05
27	b	725	CLA	CHB-C1B-NB	-2.45	120.38	124.05
27	J	603	CLA	CHB-C1B-NB	-2.45	120.38	124.05
27	K	608	CLA	CHB-C1B-NB	-2.45	120.38	124.05
27	H	319	CLA	CHB-C1B-NB	-2.45	120.38	124.05
28	F	609	KC2	CHD-C1D-ND	-2.45	120.38	124.05
28	H	302	KC2	CHD-C1D-ND	-2.45	120.38	124.05
27	H	308	CLA	CHB-C1B-NB	-2.45	120.38	124.05
27	I	610	CLA	CHB-C1B-NB	-2.44	120.38	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	615	UIX	C10-C11-C13	2.44	122.85	119.01
27	B	603	CLA	CHB-C1B-NB	-2.44	120.39	124.05
27	a	811	CLA	CHB-C1B-NB	-2.44	120.39	124.05
28	J	608	KC2	CHD-C1D-ND	-2.44	120.39	124.05
27	G	611	CLA	CHB-C1B-NB	-2.44	120.39	124.05
27	a	830	CLA	CHB-C1B-NB	-2.44	120.39	124.05
27	b	709	CLA	CHB-C1B-NB	-2.44	120.39	124.05
27	j	202	CLA	CHB-C1B-NB	-2.44	120.39	124.05
29	J	616	UIX	C37-C34-C30	-2.44	118.53	123.52
27	b	725	CLA	C2C-C1C-NC	2.44	112.55	109.98
32	U	608	PID	CM1-C1-C6	-2.44	118.29	122.30
32	F	614	PID	C17-C16-C15	-2.44	118.53	123.52
28	E	601	KC2	CHD-C1D-ND	-2.44	120.39	124.05
27	a	808	CLA	CHB-C1B-NB	-2.44	120.39	124.05
29	E	616	UIX	C-C7-C10	-2.44	120.84	125.99
27	I	607	CLA	CHB-C1B-NB	-2.44	120.39	124.05
27	a	822	CLA	CHB-C1B-NB	-2.44	120.39	124.05
27	l	412	CLA	C2C-C1C-NC	2.44	112.54	109.98
27	H	307	CLA	CHB-C1B-NB	-2.43	120.40	124.05
27	I	616	CLA	CHB-C1B-NB	-2.43	120.40	124.05
27	U	606	CLA	CHB-C1B-NB	-2.43	120.40	124.05
35	K	614	DGD	C6D-O5D-C1E	2.43	119.01	113.80
27	I	608	CLA	C2C-C1C-NC	2.43	112.54	109.98
27	F	608	CLA	CHB-C1B-NB	-2.43	120.40	124.05
27	a	801	CLA	C4D-CHA-C1A	-2.43	118.35	121.24
27	C	209	CLA	CHB-C1B-NB	-2.43	120.41	124.05
27	b	724	CLA	CHB-C1B-NB	-2.43	120.41	124.05
29	I	612	UIX	C-C7-C10	-2.43	120.86	125.99
27	T	602	CLA	CHB-C1B-NB	-2.43	120.41	124.05
27	T	606	CLA	CHB-C1B-NB	-2.43	120.41	124.05
27	l	411	CLA	CHB-C1B-NB	-2.43	120.41	124.05
27	D	607	CLA	CHB-C1B-NB	-2.43	120.41	124.05
27	H	310	CLA	CHB-C1B-NB	-2.43	120.41	124.05
27	B	609	CLA	C1-C2-C3	-2.42	122.22	126.20
27	I	611	CLA	CAA-C2A-C1A	-2.42	106.77	112.14
27	J	605	CLA	CHB-C1B-NB	-2.42	120.41	124.05
30	H	315	DD6	C14-C13-C11	2.42	129.29	125.53
27	F	601	CLA	CHB-C1B-NB	-2.42	120.42	124.05
28	T	608	KC2	CHD-C1D-ND	-2.42	120.42	124.05
29	C	215	UIX	C17-C15-C20	2.42	111.56	109.21
27	I	608	CLA	CHB-C1B-NB	-2.42	120.42	124.05
31	H	320	SQD	O47-C7-C8	2.42	116.71	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	I	602	CLA	CHB-C1B-NB	-2.42	120.42	124.05
27	K	601	CLA	CHB-C1B-NB	-2.42	120.42	124.05
27	b	716	CLA	CHB-C1B-NB	-2.42	120.42	124.05
27	A	611	CLA	CHB-C1B-NB	-2.42	120.42	124.05
28	H	311	KC2	CHD-C1D-ND	-2.42	120.42	124.05
29	G	615	UIX	O2-C27-O4	-2.42	118.33	122.99
28	G	601	KC2	CHD-C1D-ND	-2.42	120.42	124.05
27	l	408	CLA	CHB-C1B-NB	-2.41	120.43	124.05
28	J	602	KC2	CHD-C1D-ND	-2.41	120.43	124.05
27	I	605	CLA	C2C-C1C-NC	2.41	112.52	109.98
32	B	613	PID	C17-C16-C15	-2.41	118.58	123.52
32	I	614	PID	C16-C15-C14	-2.41	123.90	127.28
27	D	603	CLA	CHB-C1B-NB	-2.41	120.43	124.05
27	b	704	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	b	718	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	C	205	CLA	C3A-C2A-C1A	-2.41	97.73	101.34
27	D	612	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	E	602	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	I	611	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	K	604	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	T	603	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	D	609	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	C	202	CLA	CHB-C1B-NB	-2.41	120.44	124.05
28	I	604	KC2	CHD-C1D-ND	-2.41	120.44	124.05
27	D	608	CLA	C1-C2-C3	-2.41	122.25	126.20
27	D	610	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	E	603	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	G	602	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	C	208	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	C	212	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	b	715	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	E	612	CLA	CHB-C1B-NB	-2.41	120.44	124.05
27	B	605	CLA	CHB-C1B-NB	-2.40	120.44	124.05
27	C	211	CLA	CHB-C1B-NB	-2.40	120.44	124.05
27	C	206	CLA	C2C-C1C-NC	2.40	112.51	109.98
27	l	412	CLA	CHB-C1B-NB	-2.40	120.44	124.05
27	a	801	CLA	CHD-C1D-C2D	2.40	130.49	125.49
27	T	609	CLA	CHB-C1B-NB	-2.40	120.44	124.05
27	F	619	CLA	CHB-C1B-NB	-2.40	120.45	124.05
27	b	711	CLA	CHB-C1B-NB	-2.40	120.45	124.05
28	J	610	KC2	CHD-C1D-ND	-2.40	120.45	124.05
27	E	608	CLA	CHB-C1B-NB	-2.40	120.45	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	609	CLA	CHB-C1B-NB	-2.40	120.45	124.05
27	b	721	CLA	CHB-C1B-NB	-2.40	120.45	124.05
32	I	614	PID	O6-C30-O7	-2.40	118.36	122.99
27	D	611	CLA	CHB-C1B-NB	-2.40	120.45	124.05
27	E	606	CLA	C2C-C1C-NC	2.40	112.50	109.98
32	K	611	PID	O6-C30-O7	-2.40	118.36	122.99
27	G	610	CLA	CHB-C1B-NB	-2.40	120.45	124.05
29	J	616	UIX	C29-C26-C23	2.40	121.75	118.09
27	H	304	CLA	C4D-CHA-C1A	-2.40	118.38	121.24
27	H	307	CLA	C2C-C1C-NC	2.40	112.50	109.98
27	A	601	CLA	CHB-C1B-NB	-2.40	120.45	124.05
35	K	614	DGD	O5D-C6D-C5D	-2.40	104.02	109.42
29	j	204	UIX	C13-C14-C23	-2.40	116.26	123.20
27	f	302	CLA	C2C-C1C-NC	2.40	112.50	109.98
27	B	609	CLA	CHB-C1B-NB	-2.39	120.46	124.05
27	T	607	CLA	CHB-C1B-NB	-2.39	120.46	124.05
27	b	714	CLA	CHB-C1B-NB	-2.39	120.46	124.05
27	F	610	CLA	CHB-C1B-NB	-2.39	120.46	124.05
27	D	606	CLA	CHB-C1B-NB	-2.39	120.46	124.05
27	a	831	CLA	C2C-C1C-NC	2.39	112.50	109.98
27	I	601	CLA	CHB-C1B-NB	-2.39	120.46	124.05
27	K	606	CLA	CHB-C1B-NB	-2.39	120.46	124.05
29	T	612	UIX	C36-C35-C32	-2.39	123.93	127.28
27	B	604	CLA	CHB-C1B-NB	-2.39	120.47	124.05
27	b	728	CLA	CHB-C1B-NB	-2.39	120.47	124.05
32	B	613	PID	C17-C18-C19	-2.39	119.20	124.72
29	C	213	UIX	C34-C37-C39	-2.39	118.64	123.52
27	A	607	CLA	CHB-C1B-NB	-2.38	120.47	124.05
29	T	612	UIX	O2-C27-O4	-2.38	118.39	122.99
27	D	601	CLA	CHB-C1B-NB	-2.38	120.47	124.05
29	B	611	UIX	C14-C13-C11	-2.38	123.94	127.28
29	A	616	UIX	O2-C27-O4	-2.38	118.39	122.99
27	E	604	CLA	CHB-C1B-NB	-2.38	120.48	124.05
27	a	831	CLA	CHC-C1C-C2C	-2.38	120.18	126.95
27	F	603	CLA	CHB-C1B-NB	-2.38	120.48	124.05
31	H	320	SQD	O47-C45-C44	2.38	116.88	108.34
27	a	821	CLA	CHB-C1B-NB	-2.38	120.48	124.05
27	I	602	CLA	C2C-C1C-NC	2.38	112.48	109.98
27	l	405	CLA	CHB-C1B-NB	-2.38	120.48	124.05
27	r	204	CLA	CHB-C1B-NB	-2.38	120.48	124.05
28	B	608	KC2	CHD-C1D-ND	-2.38	120.48	124.05
27	B	607	CLA	CHC-C1C-C2C	-2.38	120.19	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	604	CLA	CHB-C1B-NB	-2.38	120.48	124.05
27	D	608	CLA	CHB-C1B-NB	-2.38	120.48	124.05
28	E	610	KC2	CHD-C4C-NC	2.38	127.89	124.31
27	a	810	CLA	CHC-C1C-C2C	-2.38	120.20	126.95
29	A	616	UIX	C-C7-C10	-2.37	120.97	125.99
27	l	406	CLA	CHB-C1B-NB	-2.37	120.49	124.05
27	a	817	CLA	CHC-C1C-C2C	-2.37	120.20	126.95
28	B	602	KC2	CHB-C4A-NA	2.37	127.91	124.23
27	a	806	CLA	CHB-C1B-NB	-2.37	120.49	124.05
27	T	605	CLA	CHB-C1B-NB	-2.37	120.49	124.05
27	C	206	CLA	CHB-C1B-NB	-2.37	120.49	124.05
35	j	201	DGD	C3G-C2G-C1G	-2.37	106.26	111.78
27	D	606	CLA	CHC-C1C-C2C	-2.37	120.22	126.95
28	A	608	KC2	CHD-C1D-ND	-2.37	120.50	124.05
29	C	213	UIX	O2-C27-O4	-2.37	118.42	122.99
27	F	607	CLA	CHB-C1B-NB	-2.37	120.50	124.05
27	b	703	CLA	CHB-C1B-NB	-2.37	120.50	124.05
27	b	728	CLA	C1-C2-C3	-2.37	122.32	126.20
29	E	616	UIX	O2-C27-O4	-2.37	118.42	122.99
27	A	606	CLA	CHB-C1B-NB	-2.36	120.50	124.05
27	A	609	CLA	CHB-C1B-NB	-2.36	120.50	124.05
27	B	606	CLA	CHB-C1B-NB	-2.36	120.50	124.05
27	E	606	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
30	H	318	DD6	C14-C13-C11	2.36	129.19	125.53
27	C	204	CLA	CHB-C1B-NB	-2.36	120.51	124.05
27	a	819	CLA	CHB-C1B-NB	-2.36	120.51	124.05
29	A	616	UIX	C18-O2-C27	-2.36	113.68	117.85
29	H	314	UIX	C13-C14-C23	-2.36	116.36	123.20
29	H	314	UIX	C37-C39-C40	-2.36	123.97	127.28
29	H	314	UIX	O2-C27-O4	-2.36	118.44	122.99
27	C	201	CLA	CHB-C1B-NB	-2.36	120.51	124.05
27	K	603	CLA	CHB-C1B-NB	-2.36	120.51	124.05
30	A	614	DD6	O1-C15-C14	-2.36	110.12	116.88
27	b	726	CLA	CHB-C1B-NB	-2.36	120.51	124.05
27	a	810	CLA	CHB-C1B-NB	-2.36	120.51	124.05
27	a	820	CLA	C2C-C1C-NC	2.36	112.46	109.98
27	l	412	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
28	U	604	KC2	CHB-C4A-NA	2.35	127.88	124.23
27	A	612	CLA	C2A-C3A-C4A	-2.35	98.07	101.87
29	D	616	UIX	C17-C15-C20	2.35	111.50	109.21
28	U	604	KC2	CHD-C4C-NC	2.35	127.86	124.31
27	K	602	CLA	CHB-C1B-NB	-2.35	120.52	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	610	CLA	CHC-C1C-C2C	-2.35	120.26	126.95
28	H	302	KC2	CHD-C4C-NC	2.35	127.85	124.31
30	C	216	DD6	O1-C15-C14	-2.35	110.14	116.88
35	K	614	DGD	C3G-C2G-C1G	-2.35	106.31	111.78
27	A	612	CLA	CHB-C1B-NB	-2.35	120.53	124.05
27	I	616	CLA	C2C-C1C-NC	2.35	112.45	109.98
27	A	605	CLA	CHB-C1B-NB	-2.35	120.53	124.05
27	T	601	CLA	CHB-C1B-NB	-2.34	120.53	124.05
29	B	615	UIX	O2-C27-O4	-2.34	118.47	122.99
29	H	317	UIX	C18-O2-C27	-2.34	113.71	117.85
27	C	206	CLA	CHC-C1C-C2C	-2.34	120.29	126.95
27	A	602	CLA	CHB-C1B-NB	-2.34	120.53	124.05
35	f	305	DGD	C1E-O6E-C5E	2.34	118.29	113.72
27	A	603	CLA	CHB-C1B-NB	-2.34	120.54	124.05
35	l	416	DGD	O5D-C6D-C5D	-2.34	104.15	109.42
29	H	314	UIX	O-C1-C3	-2.34	111.30	113.49
27	a	817	CLA	CHB-C1B-NB	-2.34	120.54	124.05
29	I	612	UIX	C19-C18-C17	2.34	114.08	109.89
27	F	605	CLA	CHB-C1B-NB	-2.34	120.55	124.05
27	b	725	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
30	r	206	DD6	O1-C20-C19	-2.34	111.30	113.49
27	H	312	CLA	CHB-C1B-NB	-2.33	120.55	124.05
27	a	829	CLA	CHB-C1B-NB	-2.33	120.55	124.05
27	l	404	CLA	CHB-C1B-NB	-2.33	120.55	124.05
27	U	606	CLA	C2C-C1C-NC	2.33	112.43	109.98
27	I	610	CLA	C1-C2-C3	-2.33	122.37	126.20
28	J	604	KC2	CHD-C4C-NC	2.33	127.83	124.31
27	G	605	CLA	CHB-C1B-NB	-2.33	120.55	124.05
27	U	601	CLA	CHB-C1B-NB	-2.33	120.55	124.05
27	a	803	CLA	CHB-C1B-NB	-2.33	120.55	124.05
28	A	608	KC2	CHD-C4C-NC	2.33	127.82	124.31
27	b	722	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
27	a	825	CLA	CHB-C1B-NB	-2.33	120.55	124.05
29	H	317	UIX	O2-C27-O4	-2.33	118.49	122.99
30	C	214	DD6	O1-C15-C14	-2.33	110.20	116.88
27	a	820	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
27	f	302	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
27	E	609	CLA	C2C-C1C-NC	2.33	112.43	109.98
27	F	608	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
27	H	309	CLA	CHB-C1B-NB	-2.33	120.56	124.05
27	a	805	CLA	C2C-C1C-NC	2.33	112.42	109.98
27	r	203	CLA	CHB-C1B-NB	-2.33	120.56	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	604	CLA	CHB-C1B-NB	-2.32	120.56	124.05
27	B	610	CLA	CHB-C1B-NB	-2.32	120.57	124.05
27	b	702	CLA	C3D-C4D-ND	2.32	113.76	109.99
29	G	615	UIX	C34-C37-C39	-2.32	118.77	123.52
27	F	617	CLA	CHB-C1B-NB	-2.32	120.57	124.05
32	J	613	PID	O1-C1-C6	-2.32	57.09	58.93
27	b	705	CLA	CHB-C1B-NB	-2.32	120.57	124.05
29	B	615	UIX	O-C1-C3	-2.32	111.32	113.49
28	F	609	KC2	CHD-C4C-NC	2.32	127.80	124.31
30	D	614	DD6	C14-C13-C11	2.32	129.12	125.53
27	T	605	CLA	C2C-C1C-NC	2.32	112.41	109.98
27	a	827	CLA	CHA-C1A-NA	-2.31	121.15	126.39
27	D	611	CLA	C1-C2-C3	-2.31	122.41	126.20
27	a	813	CLA	C2C-C1C-NC	2.31	112.41	109.98
32	J	611	PID	O1-C1-C6	-2.31	57.10	58.93
27	B	610	CLA	C2C-C1C-NC	2.31	112.41	109.98
29	T	612	UIX	C38-C40-C39	-2.31	115.38	119.01
27	G	603	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
28	B	608	KC2	CHD-C4C-NC	2.31	127.79	124.31
27	I	606	CLA	CHB-C1B-NB	-2.31	120.59	124.05
28	H	311	KC2	CHD-C4C-NC	2.31	127.78	124.31
27	H	307	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
32	F	615	PID	O4-C10-O3	2.31	124.49	120.17
27	b	708	CLA	CHC-C1C-C2C	-2.31	120.40	126.95
27	a	810	CLA	C2C-C1C-NC	2.31	112.40	109.98
27	D	604	CLA	CHB-C1B-NB	-2.30	120.59	124.05
27	I	603	CLA	CHB-C1B-NB	-2.30	120.59	124.05
27	a	822	CLA	C2C-C1C-NC	2.30	112.40	109.98
27	a	804	CLA	O2A-C1-C2	2.30	116.97	108.11
27	A	611	CLA	C2C-C1C-NC	2.30	112.40	109.98
27	r	204	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
27	a	808	CLA	C2C-C1C-NC	2.30	112.40	109.98
32	J	613	PID	C17-C18-C19	-2.30	119.40	124.72
27	D	601	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
29	B	615	UIX	C37-C39-C40	-2.30	124.05	127.28
27	a	815	CLA	C2C-C1C-NC	2.30	112.40	109.98
29	C	215	UIX	C23-C26-C30	-2.30	115.39	119.01
27	U	603	CLA	CHB-C1B-NB	-2.30	120.60	124.05
27	a	804	CLA	CHA-C1A-NA	-2.30	121.19	126.39
27	F	606	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
27	I	608	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
27	T	605	CLA	CHC-C1C-C2C	-2.30	120.42	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	602	CLA	CHB-C1B-NB	-2.30	120.60	124.05
38	b	731	BCR	C8-C9-C10	-2.30	115.40	119.01
27	B	606	CLA	CAA-C2A-C1A	-2.30	104.45	111.97
32	J	613	PID	O4-C10-O3	2.30	124.47	120.17
27	a	827	CLA	C1-C2-C3	-2.29	122.44	126.20
27	a	808	CLA	CHC-C1C-C2C	-2.29	120.43	126.95
27	a	837	CLA	CHD-C1D-C2D	2.29	130.26	125.49
29	T	612	UIX	C16-C20-C15	2.29	121.97	119.70
29	j	204	UIX	C23-C26-C30	-2.29	115.40	119.01
27	K	602	CLA	C2C-C1C-NC	2.29	112.39	109.98
27	D	601	CLA	C2C-C1C-NC	2.29	112.39	109.98
27	G	610	CLA	C2C-C1C-NC	2.29	112.39	109.98
27	l	405	CLA	C2C-C1C-NC	2.29	112.39	109.98
27	I	605	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
29	C	215	UIX	O2-C27-O4	-2.29	118.57	122.99
27	A	611	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
27	b	726	CLA	C2C-C1C-NC	2.29	112.38	109.98
27	b	720	CLA	CHB-C1B-NB	-2.28	120.62	124.05
27	F	606	CLA	C2C-C1C-NC	2.28	112.38	109.98
27	H	304	CLA	C2C-C1C-NC	2.28	112.38	109.98
27	H	308	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
29	j	204	UIX	O2-C27-O4	-2.28	118.58	122.99
27	G	604	CLA	CHB-C1B-NB	-2.28	120.62	124.05
27	C	202	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
27	H	312	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
28	C	210	KC2	CHD-C4C-NC	2.28	127.75	124.31
27	b	703	CLA	CHB-C4A-NA	2.28	127.69	124.40
27	a	805	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
27	a	801	CLA	C3D-C4D-ND	2.28	113.70	109.99
27	a	815	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
29	A	616	UIX	C3-C5-C4	2.28	115.06	110.79
27	G	609	CLA	CHB-C1B-NB	-2.28	120.62	124.05
27	E	609	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
27	F	608	CLA	C2C-C1C-NC	2.28	112.38	109.98
27	b	706	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
29	H	317	UIX	C6-C1-C	-2.28	118.55	122.30
27	b	703	CLA	CHD-C1D-C2D	2.28	130.23	125.49
27	G	607	CLA	CHB-C1B-NB	-2.28	120.63	124.05
27	E	611	CLA	CHB-C1B-NB	-2.28	120.63	124.05
28	G	601	KC2	CHD-C4C-NC	2.28	127.74	124.31
27	b	719	CLA	CHC-C1C-C2C	-2.28	120.48	126.95
32	J	611	PID	C28-C27-C26	-2.28	105.80	109.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	605	CLA	CHD-C1D-C2D	2.28	130.22	125.49
27	T	607	CLA	CHC-C1C-C2C	-2.27	120.48	126.95
32	J	614	PID	C6-C7-C8	-2.27	121.18	125.99
27	l	411	CLA	C2C-C1C-NC	2.27	112.37	109.98
27	F	601	CLA	C1-C2-C3	-2.27	122.47	126.20
29	H	314	UIX	C10-C11-C13	-2.27	115.44	119.01
27	a	826	CLA	CHA-C1A-NA	-2.27	121.25	126.39
27	a	824	CLA	CHD-C1D-C2D	2.27	130.21	125.49
28	K	607	KC2	CHD-C4C-NC	2.27	127.73	124.31
27	l	404	CLA	CHD-C1D-C2D	2.27	130.20	125.49
27	I	616	CLA	CHC-C1C-C2C	-2.27	120.51	126.95
29	D	616	UIX	O-C-C7	-2.27	110.39	116.88
30	T	611	DD6	C21-C20-C19	2.27	116.79	114.24
35	j	201	DGD	O5D-C6D-C5D	-2.27	104.31	109.42
31	A	618	SQD	O7-S-C6	2.27	110.14	106.76
27	b	726	CLA	CHC-C1C-C2C	-2.26	120.51	126.95
27	C	202	CLA	C2C-C1C-NC	2.26	112.36	109.98
27	T	604	CLA	C2C-C1C-NC	2.26	112.36	109.98
28	E	601	KC2	CHD-C4C-NC	2.26	127.72	124.31
27	b	702	CLA	CHA-C1A-NA	-2.26	121.27	126.39
27	b	707	CLA	CHD-C1D-C2D	2.26	130.19	125.49
29	D	616	UIX	C35-C36-C38	-2.26	116.64	123.20
27	K	604	CLA	CHC-C1C-C2C	-2.26	120.53	126.95
32	I	614	PID	O1-C1-C6	-2.26	57.14	58.93
27	G	609	CLA	C2C-C1C-NC	2.26	112.35	109.98
27	b	725	CLA	C1-C2-C3	-2.26	122.50	126.20
27	b	706	CLA	C2C-C1C-NC	2.26	112.35	109.98
27	C	204	CLA	C2C-C1C-NC	2.25	112.35	109.98
27	D	605	CLA	C2C-C1C-NC	2.25	112.35	109.98
27	a	823	CLA	CHB-C1B-NB	-2.25	120.67	124.05
27	B	609	CLA	C2C-C1C-NC	2.25	112.35	109.98
27	T	607	CLA	C2C-C1C-NC	2.25	112.35	109.98
27	a	812	CLA	CHD-C1D-C2D	2.25	130.17	125.49
33	D	618	LMG	C8-O7-C10	2.25	123.19	117.80
38	a	836	BCR	C30-C25-C24	2.25	121.76	115.65
28	B	602	KC2	CHD-C4C-NC	2.25	127.70	124.31
29	C	215	UIX	C37-C34-C30	-2.25	118.91	123.52
29	B	611	UIX	C37-C39-C40	-2.25	124.12	127.28
27	U	603	CLA	CHA-C1A-NA	-2.25	121.30	126.39
32	J	613	PID	C18-C19-C20	-2.25	118.92	123.52
27	I	601	CLA	C1-C2-C3	-2.25	122.51	126.20
28	J	602	KC2	CHD-C4C-NC	2.25	127.70	124.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	706	CLA	C1-C2-C3	-2.25	122.51	126.20
27	H	304	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
27	U	606	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
29	I	612	UIX	C6-C1-C	-2.25	118.60	122.30
27	T	601	CLA	CHD-C1D-C2D	2.25	130.16	125.49
27	f	303	CLA	CHD-C1D-C2D	2.25	130.16	125.49
27	b	727	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
27	a	807	CLA	CHC-C1C-C2C	-2.25	120.57	126.95
27	B	605	CLA	CAA-C2A-C1A	-2.25	104.62	111.97
27	a	816	CLA	CHC-C1C-C2C	-2.25	120.57	126.95
27	l	405	CLA	CHC-C1C-C2C	-2.24	120.57	126.95
27	A	607	CLA	CHC-C1C-C2C	-2.24	120.57	126.95
27	G	603	CLA	C2C-C1C-NC	2.24	112.34	109.98
29	T	612	UIX	C37-C34-C30	-2.24	118.93	123.52
35	K	614	DGD	O2D-C2D-C1D	-2.24	104.73	110.08
29	I	612	UIX	C28-C25-C20	-2.24	175.02	177.66
27	b	721	CLA	CHD-C1D-C2D	2.24	130.15	125.49
27	F	602	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
27	D	605	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
27	A	601	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
27	a	813	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
27	A	601	CLA	CAA-C2A-C1A	-2.24	107.19	112.14
27	a	818	CLA	CHD-C1D-C2D	2.24	130.14	125.49
27	a	808	CLA	CHD-C1D-C2D	2.24	130.14	125.49
27	I	602	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
27	l	411	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
27	U	603	CLA	CHD-C1D-C2D	2.24	130.14	125.49
27	b	719	CLA	CHD-C1D-C2D	2.24	130.14	125.49
27	E	612	CLA	C2C-C1C-NC	2.24	112.33	109.98
30	B	612	DD6	C14-C13-C11	2.24	129.00	125.53
27	b	713	CLA	CHD-C1D-C2D	2.23	130.13	125.49
27	A	601	CLA	C2C-C1C-NC	2.23	112.33	109.98
27	a	816	CLA	C2C-C1C-NC	2.23	112.33	109.98
27	F	604	CLA	CHC-C1C-C2C	-2.23	120.60	126.95
27	b	714	CLA	CHD-C1D-C2D	2.23	130.13	125.49
27	F	605	CLA	CHC-C1C-C2C	-2.23	120.60	126.95
27	A	612	CLA	CHD-C1D-C2D	2.23	130.13	125.49
27	a	828	CLA	CHD-C1D-C2D	2.23	130.13	125.49
27	b	709	CLA	C2C-C1C-NC	2.23	112.33	109.98
27	G	610	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
27	G	607	CLA	CHD-C1D-C2D	2.23	130.13	125.49
27	a	822	CLA	C1-C2-C3	-2.23	122.54	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	607	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
27	H	313	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
27	I	610	CLA	CHD-C1D-C2D	2.23	130.12	125.49
27	A	609	CLA	C2C-C1C-NC	2.23	112.32	109.98
27	b	719	CLA	C2C-C1C-NC	2.23	112.32	109.98
35	l	416	DGD	CDB-CCB-CBB	-2.23	103.11	114.37
27	G	611	CLA	CHC-C1C-C2C	-2.23	120.62	126.95
27	a	822	CLA	CHC-C1C-C2C	-2.23	120.62	126.95
27	b	718	CLA	CHD-C1D-C2D	2.23	130.12	125.49
27	C	204	CLA	CHC-C1C-C2C	-2.22	120.62	126.95
32	B	613	PID	CM4-C14-C15	-2.22	119.21	122.82
27	E	605	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
27	E	605	CLA	CHD-C1D-C2D	2.22	130.11	125.49
27	H	312	CLA	C2C-C1C-NC	2.22	112.32	109.98
38	a	836	BCR	C20-C19-C18	-2.22	120.27	126.36
27	B	603	CLA	CHD-C1D-C2D	2.22	130.11	125.49
27	l	412	CLA	CHD-C1D-C2D	2.22	130.11	125.49
27	a	826	CLA	CHD-C1D-C2D	2.22	130.11	125.49
27	K	608	CLA	C2C-C1C-NC	2.22	112.31	109.98
32	J	614	PID	C22-C23-C24	-2.22	175.04	177.66
27	E	607	CLA	CHD-C1D-C2D	2.22	130.10	125.49
27	U	605	CLA	CHD-C1D-C2D	2.22	130.10	125.49
29	A	616	UIX	C13-C14-C23	-2.22	116.77	123.20
27	j	202	CLA	CHD-C1D-C2D	2.22	130.10	125.49
27	I	611	CLA	CHD-C1D-C2D	2.22	130.10	125.49
27	b	709	CLA	CHC-C1C-C2C	-2.22	120.65	126.95
27	l	410	CLA	CHD-C1D-C2D	2.22	130.10	125.49
29	B	611	UIX	C35-C36-C38	-2.22	116.78	123.20
27	B	606	CLA	CHD-C1D-C2D	2.22	130.10	125.49
27	K	602	CLA	CHC-C1C-C2C	-2.22	120.65	126.95
27	l	406	CLA	C1-C2-C3	-2.22	122.57	126.20
27	b	712	CLA	CHC-C1C-C2C	-2.22	120.65	126.95
28	J	610	KC2	CHD-C4C-NC	2.21	127.65	124.31
29	G	615	UIX	C6-C1-C	-2.21	118.66	122.30
27	b	715	CLA	CHC-C1C-C2C	-2.21	120.66	126.95
32	J	613	PID	O4-C12-C13	2.21	127.61	122.89
27	K	603	CLA	CHD-C1D-C2D	2.21	130.09	125.49
27	b	712	CLA	CHD-C1D-C2D	2.21	130.09	125.49
27	A	609	CLA	CHC-C1C-C2C	-2.21	120.66	126.95
27	H	304	CLA	CHB-C1B-NB	-2.21	120.73	124.05
32	U	608	PID	O4-C10-O3	2.21	124.31	120.17
27	D	609	CLA	C2C-C1C-NC	2.21	112.30	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	605	CLA	CHD-C1D-C2D	2.21	130.08	125.49
27	B	609	CLA	CHC-C1C-C2C	-2.21	120.67	126.95
27	A	607	CLA	C2C-C1C-NC	2.21	112.30	109.98
27	r	204	CLA	C2C-C1C-NC	2.21	112.30	109.98
27	b	705	CLA	CHD-C1D-C2D	2.21	130.08	125.49
27	B	604	CLA	CHD-C1D-C2D	2.21	130.08	125.49
27	a	823	CLA	CHD-C1D-C2D	2.21	130.08	125.49
27	B	607	CLA	C1-C2-C3	-2.21	122.58	126.20
27	b	715	CLA	CHD-C1D-C2D	2.21	130.08	125.49
27	D	610	CLA	C2C-C1C-NC	2.21	112.30	109.98
29	A	613	UIX	O2-C27-O4	-2.21	118.73	122.99
27	D	612	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
27	D	609	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
27	A	605	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
30	E	615	DD6	C21-C20-C19	2.20	116.72	114.24
27	I	609	CLA	CHD-C1D-C2D	2.20	130.07	125.49
27	D	610	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
27	F	603	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
32	J	615	PID	O4-C10-O3	2.20	124.30	120.17
27	b	702	CLA	C2C-C1C-NC	2.20	112.30	109.98
27	G	604	CLA	CHD-C1D-C2D	2.20	130.07	125.49
27	J	601	CLA	CHD-C1D-C2D	2.20	130.07	125.49
27	l	407	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
27	a	839	CLA	C2C-C1C-NC	2.20	112.29	109.98
27	K	601	CLA	CHD-C1D-C2D	2.20	130.06	125.49
27	B	605	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
28	T	608	KC2	CHD-C4C-NC	2.20	127.62	124.31
28	J	606	KC2	CHB-C4A-NA	2.20	127.64	124.23
35	K	614	DGD	C5B-C4B-C3B	-2.20	103.25	114.37
27	a	809	CLA	CHD-C1D-C2D	2.20	130.06	125.49
27	D	602	CLA	CHD-C1D-C2D	2.20	130.06	125.49
27	D	608	CLA	CHD-C1D-C2D	2.20	130.06	125.49
29	D	616	UIX	O2-C27-O4	-2.20	118.75	122.99
27	a	816	CLA	CHD-C1D-C2D	2.20	130.06	125.49
27	D	611	CLA	C2C-C1C-NC	2.20	112.29	109.98
27	E	602	CLA	CHD-C1D-C2D	2.20	130.05	125.49
27	b	722	CLA	CHD-C1D-C2D	2.20	130.05	125.49
29	C	215	UIX	O-C1-C6	-2.19	112.59	115.05
27	G	611	CLA	CHD-C1D-C2D	2.19	130.05	125.49
27	F	605	CLA	CAA-C2A-C1A	-2.19	104.78	111.97
27	E	612	CLA	CHC-C1C-C2C	-2.19	120.71	126.95
27	T	602	CLA	CHC-C1C-C2C	-2.19	120.71	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	609	CLA	CHC-C1C-C2C	-2.19	120.71	126.95
27	G	609	CLA	CHD-C4C-C3C	-2.19	121.58	124.77
27	D	612	CLA	C2C-C1C-NC	2.19	112.29	109.98
27	a	804	CLA	CHD-C1D-C2D	2.19	130.05	125.49
27	a	824	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
27	H	309	CLA	CHD-C1D-C2D	2.19	130.05	125.49
27	J	607	CLA	C2C-C1C-NC	2.19	112.28	109.98
27	J	603	CLA	CHD-C1D-C2D	2.19	130.04	125.49
28	J	608	KC2	CHD-C4C-NC	2.19	127.61	124.31
27	E	604	CLA	CHD-C1D-C2D	2.19	130.04	125.49
29	B	611	UIX	C18-O2-C27	-2.19	113.98	117.85
27	F	610	CLA	CHD-C1D-C2D	2.19	130.04	125.49
27	U	601	CLA	CHD-C1D-C2D	2.19	130.04	125.49
27	r	203	CLA	CHD-C1D-C2D	2.19	130.04	125.49
32	I	614	PID	C17-C16-C15	-2.19	119.04	123.52
38	a	836	BCR	C33-C5-C4	2.19	118.26	113.60
29	G	615	UIX	C37-C39-C40	-2.19	124.21	127.28
27	a	829	CLA	CHD-C1D-C2D	2.19	130.04	125.49
27	l	406	CLA	CHD-C1D-C2D	2.19	130.04	125.49
27	a	807	CLA	C2C-C1C-NC	2.19	112.28	109.98
27	H	310	CLA	CHD-C1D-C2D	2.19	130.04	125.49
27	b	709	CLA	C1-C2-C3	-2.19	122.61	126.20
30	T	610	DD6	O1-C20-C15	-2.19	57.20	58.93
27	l	403	CLA	CHC-C1C-C2C	-2.19	120.73	126.95
27	F	602	CLA	C2C-C1C-NC	2.19	112.28	109.98
27	I	606	CLA	CHD-C1D-C2D	2.19	130.03	125.49
27	E	607	CLA	CHA-C1A-NA	-2.19	121.44	126.39
27	l	404	CLA	CHA-C1A-NA	-2.19	121.44	126.39
27	H	303	CLA	C1-C2-C3	-2.18	122.62	126.20
27	a	825	CLA	CHC-C1C-C2C	-2.18	120.74	126.95
30	H	301	DD6	O1-C20-C19	-2.18	111.44	113.49
27	A	610	CLA	CHC-C1C-C2C	-2.18	120.74	126.95
27	T	609	CLA	CHC-C1C-C2C	-2.18	120.74	126.95
27	b	703	CLA	CHA-C1A-NA	-2.18	121.45	126.39
27	a	824	CLA	C2C-C1C-NC	2.18	112.28	109.98
27	G	608	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
27	T	604	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
27	E	603	CLA	CHD-C1D-C2D	2.18	130.03	125.49
27	G	608	CLA	CHD-C1D-C2D	2.18	130.03	125.49
27	C	207	CLA	CHD-C1D-C2D	2.18	130.02	125.49
27	l	408	CLA	CHD-C1D-C2D	2.18	130.02	125.49
27	B	605	CLA	C2C-C1C-NC	2.18	112.27	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	608	CLA	CHD-C1D-C2D	2.18	130.02	125.49
38	a	836	BCR	C15-C16-C17	-2.18	119.06	123.52
28	U	602	KC2	CHD-C4C-NC	2.18	127.59	124.31
27	A	603	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
27	A	610	CLA	CHD-C1D-C2D	2.18	130.02	125.49
27	a	810	CLA	CHD-C1D-C2D	2.18	130.02	125.49
27	l	409	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
27	T	606	CLA	CHD-C1D-C2D	2.18	130.02	125.49
27	a	803	CLA	CHD-C1D-C2D	2.18	130.02	125.49
27	C	201	CLA	C2C-C1C-NC	2.18	112.27	109.98
27	H	319	CLA	C2C-C1C-NC	2.18	112.27	109.98
27	a	831	CLA	C1-C2-C3	-2.18	122.63	126.20
27	b	710	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
27	T	609	CLA	CHD-C1D-C2D	2.18	130.02	125.49
29	T	612	UIX	C21-C15-C20	-2.18	108.52	110.47
27	I	607	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
29	H	314	UIX	C22-C15-C20	-2.18	108.52	110.47
27	C	203	CLA	CHD-C1D-C2D	2.18	130.01	125.49
27	b	711	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
27	l	411	CLA	CHD-C1D-C2D	2.18	130.01	125.49
27	C	209	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
27	K	606	CLA	CHC-C1C-C2C	-2.18	120.77	126.95
27	H	319	CLA	CHC-C1C-C2C	-2.18	120.77	126.95
27	B	609	CLA	CHD-C1D-C2D	2.18	130.01	125.49
27	D	607	CLA	CHD-C1D-C2D	2.18	130.01	125.49
27	b	704	CLA	CHD-C1D-C2D	2.17	130.01	125.49
27	J	609	CLA	CHD-C1D-C2D	2.17	130.01	125.49
27	K	608	CLA	CHC-C1C-C2C	-2.17	120.77	126.95
27	C	212	CLA	CHD-C1D-C2D	2.17	130.01	125.49
27	U	606	CLA	CHD-C1D-C2D	2.17	130.00	125.49
27	D	611	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
27	A	605	CLA	CHD-C1D-C2D	2.17	130.00	125.49
27	b	716	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
27	a	820	CLA	CHD-C1D-C2D	2.17	130.00	125.49
27	l	407	CLA	CHD-C1D-C2D	2.17	130.00	125.49
27	H	306	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
27	b	710	CLA	CHD-C1D-C2D	2.17	130.00	125.49
27	a	821	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
27	E	608	CLA	CHD-C1D-C2D	2.17	130.00	125.49
27	b	711	CLA	CHD-C1D-C2D	2.17	130.00	125.49
27	a	839	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
27	F	610	CLA	CHC-C1C-C2C	-2.17	120.78	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	f	305	DGD	O5D-C6D-C5D	-2.17	104.53	109.42
27	A	602	CLA	CHD-C1D-C2D	2.17	130.00	125.49
27	K	604	CLA	C2C-C1C-NC	2.17	112.26	109.98
27	G	605	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
27	a	810	CLA	C1-C2-C3	-2.17	123.25	126.76
27	b	718	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
27	C	205	CLA	CHD-C1D-C2D	2.17	130.00	125.49
27	I	608	CLA	CHA-C1A-NA	-2.17	121.48	126.39
27	a	829	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
27	J	605	CLA	CHD-C1D-C2D	2.17	129.99	125.49
27	I	609	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
27	a	819	CLA	CHD-C1D-C2D	2.17	129.99	125.49
27	D	607	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
27	A	603	CLA	C2C-C1C-NC	2.17	112.26	109.98
27	a	811	CLA	CHD-C1D-C2D	2.16	129.99	125.49
27	A	610	CLA	C2C-C1C-NC	2.16	112.25	109.98
27	G	609	CLA	CHA-C1A-NA	-2.16	121.49	126.39
27	C	212	CLA	CHC-C1C-C2C	-2.16	120.80	126.95
27	b	702	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
27	G	611	CLA	C2C-C1C-NC	2.16	112.25	109.98
27	C	208	CLA	CHD-C1D-C2D	2.16	129.98	125.49
27	B	604	CLA	CHC-C1C-C2C	-2.16	120.80	126.95
29	H	317	UIX	O-C1-C3	-2.16	111.47	113.49
27	b	718	CLA	C1-C2-C3	-2.16	122.66	126.20
27	H	303	CLA	C2C-C1C-NC	2.16	112.25	109.98
27	a	819	CLA	CHC-C1C-C2C	-2.16	120.81	126.95
27	b	701	CLA	CHD-C1D-C2D	2.16	129.98	125.49
38	a	836	BCR	C23-C24-C25	-2.16	121.23	127.00
27	D	612	CLA	CHD-C1D-C2D	2.16	129.98	125.49
27	F	607	CLA	CHD-C1D-C2D	2.16	129.98	125.49
32	B	613	PID	CM7-C25-C24	-2.16	108.54	110.47
27	H	313	CLA	CHD-C1D-C2D	2.16	129.98	125.49
27	a	821	CLA	CHD-C1D-C2D	2.16	129.97	125.49
35	f	305	DGD	O2D-C2D-C1D	-2.16	104.94	110.08
27	H	303	CLA	CHD-C1D-C2D	2.16	129.97	125.49
29	E	616	UIX	C6-C1-C	-2.16	118.75	122.30
27	C	209	CLA	CHD-C1D-C2D	2.16	129.97	125.49
30	G	612	DD6	C21-C20-C19	2.16	116.66	114.24
27	H	319	CLA	CHD-C1D-C2D	2.15	129.97	125.49
27	a	807	CLA	CHD-C1D-C2D	2.15	129.97	125.49
27	l	408	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
27	A	611	CLA	CHD-C1D-C2D	2.15	129.97	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	716	CLA	CHD-C1D-C2D	2.15	129.97	125.49
27	l	406	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
29	B	611	UIX	O-C1-C3	-2.15	111.47	113.49
27	b	724	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	l	405	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	G	609	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
27	C	202	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	a	839	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	b	720	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	l	402	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	K	606	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	H	304	CLA	CHA-C1A-NA	-2.15	121.52	126.39
29	F	613	UIX	O-C-C7	-2.15	110.72	116.88
27	C	201	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	D	609	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	T	607	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	b	724	CLA	C1-C2-C3	-2.15	122.67	126.20
29	D	616	UIX	C38-C40-C39	-2.15	115.63	119.01
27	l	402	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
32	F	614	PID	C16-C15-C14	-2.15	124.26	127.28
27	b	701	CLA	C2C-C1C-NC	2.15	112.24	109.98
27	E	612	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	F	602	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	a	806	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	b	727	CLA	CHD-C1D-C2D	2.15	129.96	125.49
27	I	606	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
27	F	619	CLA	CHD-C1D-C2D	2.15	129.95	125.49
29	T	612	UIX	C35-C36-C38	-2.15	116.98	123.20
32	I	614	PID	C18-C17-C16	-2.15	119.76	124.72
27	b	702	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
27	I	603	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
27	l	402	CLA	C2C-C1C-NC	2.15	112.23	109.98
27	a	814	CLA	CHD-C1D-C2D	2.14	129.95	125.49
27	a	815	CLA	CHD-C1D-C2D	2.14	129.95	125.49
27	b	706	CLA	CHD-C1D-C2D	2.14	129.95	125.49
30	I	613	DD6	O1-C20-C15	-2.14	57.23	58.93
27	E	611	CLA	CHC-C1C-C2C	-2.14	120.85	126.95
27	b	703	CLA	CHC-C1C-C2C	-2.14	120.85	126.95
27	H	308	CLA	C2C-C1C-NC	2.14	112.23	109.98
27	I	601	CLA	CHD-C1D-C2D	2.14	129.94	125.49
30	B	612	DD6	O1-C15-C14	-2.14	110.74	116.88
32	J	611	PID	O6-C27-C26	2.14	113.12	107.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J	616	UIX	O2-C27-O4	-2.14	118.86	122.99
32	J	615	PID	O1-C6-C7	-2.14	110.74	116.88
27	b	707	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
27	J	607	CLA	CHD-C1D-C2D	2.14	129.94	125.49
27	F	604	CLA	C2C-C1C-NC	2.14	112.23	109.98
28	A	608	KC2	CHB-C4A-C3A	-2.14	121.65	125.03
27	D	603	CLA	CHD-C1D-C2D	2.14	129.94	125.49
27	F	602	CLA	CHA-C1A-NA	-2.14	121.55	126.39
27	F	601	CLA	CHD-C1D-C2D	2.14	129.94	125.49
27	G	602	CLA	CHD-C1D-C2D	2.14	129.94	125.49
27	C	207	CLA	CHC-C1C-C2C	-2.14	120.87	126.95
27	H	310	CLA	CHC-C1C-C2C	-2.14	120.87	126.95
27	l	403	CLA	C2C-C1C-NC	2.14	112.23	109.98
27	E	611	CLA	CHD-C1D-C2D	2.14	129.93	125.49
27	f	303	CLA	CHC-C1C-C2C	-2.14	120.87	126.95
27	A	604	CLA	CHD-C1D-C2D	2.14	129.93	125.49
27	E	609	CLA	CHD-C1D-C2D	2.14	129.93	125.49
27	b	726	CLA	CHD-C1D-C2D	2.14	129.93	125.49
27	I	607	CLA	C2C-C1C-NC	2.14	112.23	109.98
27	T	602	CLA	C2C-C1C-NC	2.14	112.23	109.98
27	F	617	CLA	CHD-C1D-C2D	2.14	129.93	125.49
27	b	728	CLA	CHC-C1C-C2C	-2.14	120.88	126.95
27	D	611	CLA	CHD-C1D-C2D	2.13	129.93	125.49
29	B	615	UIX	C13-C14-C23	-2.13	117.02	123.20
27	a	802	CLA	CHD-C1D-C2D	2.13	129.93	125.49
27	a	837	CLA	CHA-C1A-NA	-2.13	121.56	126.39
27	E	603	CLA	CHC-C1C-C2C	-2.13	120.89	126.95
27	B	601	CLA	CHD-C1D-C2D	2.13	129.92	125.49
27	C	204	CLA	CHD-C1D-C2D	2.13	129.92	125.49
31	H	320	SQD	O48-C23-C24	2.13	118.34	111.83
27	U	601	CLA	CHA-C1A-NA	-2.13	121.56	126.39
27	b	716	CLA	C2C-C1C-NC	2.13	112.22	109.98
27	C	201	CLA	CHC-C1C-C2C	-2.13	120.89	126.95
27	I	603	CLA	CHD-C1D-C2D	2.13	129.92	125.49
27	I	607	CLA	CHD-C1D-C2D	2.13	129.92	125.49
28	I	604	KC2	CHC-C1C-NC	2.13	127.54	124.23
27	A	612	CLA	CHC-C1C-C2C	-2.13	120.90	126.95
27	H	305	CLA	CHD-C1D-C2D	2.13	129.91	125.49
35	j	201	DGD	C4E-C3E-C2E	-2.13	107.09	110.83
27	I	606	CLA	C2C-C1C-NC	2.13	112.22	109.98
27	B	606	CLA	CHC-C1C-C2C	-2.13	120.90	126.95
27	J	603	CLA	CHC-C1C-C2C	-2.13	120.90	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	825	CLA	CHD-C1D-C2D	2.13	129.91	125.49
27	D	603	CLA	CHC-C1C-C2C	-2.13	120.90	126.95
27	C	211	CLA	CHD-C1D-C2D	2.13	129.91	125.49
27	H	308	CLA	CHD-C1D-C2D	2.13	129.91	125.49
30	K	612	DD6	O1-C15-C14	-2.13	110.78	116.88
27	b	715	CLA	C1-C2-C3	-2.13	122.71	126.20
32	J	614	PID	O6-C30-O7	-2.13	118.89	122.99
27	D	605	CLA	CHD-C1D-C2D	2.13	129.91	125.49
27	a	819	CLA	C2C-C1C-NC	2.13	112.22	109.98
27	b	727	CLA	CHA-C1A-NA	-2.13	121.58	126.39
30	J	612	DD6	C14-C13-C11	2.13	128.83	125.53
27	C	205	CLA	CHA-C1A-NA	-2.13	121.58	126.39
27	l	403	CLA	CHD-C1D-C2D	2.12	129.91	125.49
27	b	717	CLA	CHD-C1D-C2D	2.12	129.91	125.49
27	C	206	CLA	CHD-C1D-C2D	2.12	129.90	125.49
27	a	821	CLA	C2C-C1C-NC	2.12	112.21	109.98
30	D	614	DD6	O1-C15-C14	-2.12	110.80	116.88
27	b	713	CLA	C2C-C1C-NC	2.12	112.21	109.98
29	G	615	UIX	C37-C34-C30	-2.12	119.18	123.52
27	E	605	CLA	CHA-C1A-NA	-2.12	121.59	126.39
27	G	610	CLA	CHD-C1D-C2D	2.12	129.90	125.49
27	E	604	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
27	E	605	CLA	C2C-C1C-NC	2.12	112.21	109.98
27	b	723	CLA	CHD-C1D-C2D	2.12	129.90	125.49
27	C	211	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
27	F	608	CLA	CHD-C1D-C2D	2.12	129.90	125.49
27	a	805	CLA	CHD-C1D-C2D	2.12	129.90	125.49
38	b	732	BCR	C29-C30-C25	2.12	113.52	110.44
32	K	611	PID	C18-C19-C20	-2.12	119.18	123.52
27	a	811	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
27	a	817	CLA	CHA-C1A-NA	-2.12	121.59	126.39
27	a	804	CLA	CHB-C4A-NA	2.12	127.46	124.40
32	F	614	PID	C28-C27-C26	-2.12	106.08	109.89
27	T	604	CLA	CHD-C1D-C2D	2.12	129.89	125.49
27	b	713	CLA	CHC-C1C-C2C	-2.12	120.93	126.95
29	A	613	UIX	C6-C1-C	-2.12	118.82	122.30
27	H	305	CLA	CHA-C1A-NA	-2.12	121.60	126.39
27	b	701	CLA	CHC-C1C-C2C	-2.12	120.93	126.95
27	C	211	CLA	C2C-C1C-NC	2.12	112.20	109.98
27	b	707	CLA	C2C-C1C-NC	2.12	112.20	109.98
27	a	814	CLA	CHC-C1C-C2C	-2.12	120.94	126.95
27	E	606	CLA	CHD-C1D-C2D	2.12	129.89	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	812	CLA	CHC-C1C-C2C	-2.11	120.94	126.95
27	A	603	CLA	CHD-C1D-C2D	2.11	129.88	125.49
27	b	728	CLA	CHD-C1D-C2D	2.11	129.88	125.49
27	F	617	CLA	CHC-C1C-C2C	-2.11	120.94	126.95
27	U	605	CLA	CHC-C1C-C2C	-2.11	120.94	126.95
27	a	807	CLA	CHB-C4A-NA	2.11	127.45	124.40
27	C	207	CLA	CHA-C1A-NA	-2.11	121.61	126.39
27	H	310	CLA	CHA-C1A-NA	-2.11	121.61	126.39
35	j	201	DGD	CFB-CEB-CDB	-2.11	103.69	114.37
27	a	811	CLA	CHA-C1A-NA	-2.11	121.61	126.39
27	a	812	CLA	CHA-C1A-NA	-2.11	121.61	126.39
32	K	611	PID	C17-C18-C19	-2.11	119.84	124.72
27	A	612	CLA	CHA-C1A-NA	-2.11	121.61	126.39
27	I	605	CLA	CHD-C1D-C2D	2.11	129.88	125.49
27	A	609	CLA	CHD-C1D-C2D	2.11	129.88	125.49
27	a	831	CLA	CHD-C1D-C2D	2.11	129.88	125.49
35	l	416	DGD	CAB-C9B-C8B	-2.11	103.71	114.37
30	K	609	DD6	O1-C20-C15	-2.11	57.26	58.93
35	f	305	DGD	CBB-CAB-C9B	-2.11	103.71	114.37
27	K	602	CLA	CHD-C1D-C2D	2.11	129.87	125.49
27	b	724	CLA	CHC-C1C-C2C	-2.11	120.96	126.95
27	b	727	CLA	C2C-C1C-NC	2.11	112.19	109.98
29	J	616	UIX	C37-C39-C40	-2.11	124.32	127.28
27	K	605	CLA	C2C-C1C-NC	2.11	112.19	109.98
27	j	202	CLA	CHC-C1C-C2C	-2.11	120.96	126.95
27	A	604	CLA	CHC-C1C-C2C	-2.11	120.97	126.95
27	a	814	CLA	C2C-C1C-NC	2.11	112.19	109.98
27	a	813	CLA	CHD-C1D-C2D	2.10	129.86	125.49
27	A	602	CLA	C1-C2-C3	-2.10	122.75	126.20
27	F	610	CLA	C2C-C1C-NC	2.10	112.19	109.98
27	f	302	CLA	CHD-C1D-C2D	2.10	129.86	125.49
27	F	605	CLA	C2C-C1C-NC	2.10	112.19	109.98
27	b	714	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
27	B	603	CLA	CHA-C1A-NA	-2.10	121.63	126.39
27	F	607	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
32	K	611	PID	C17-C16-C15	-2.10	119.22	123.52
27	b	710	CLA	C2C-C1C-NC	2.10	112.19	109.98
27	F	619	CLA	CHC-C1C-C2C	-2.10	120.99	126.95
27	b	721	CLA	CHC-C1C-C2C	-2.10	120.99	126.95
27	D	603	CLA	C1-C2-C3	-2.10	122.76	126.20
27	A	601	CLA	CHD-C1D-C2D	2.10	129.85	125.49
27	b	702	CLA	CHD-C1D-C2D	2.10	129.85	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	612	DD6	O1-C20-C15	-2.10	57.27	58.93
27	B	610	CLA	CHD-C1D-C2D	2.10	129.85	125.49
27	F	606	CLA	CHD-C1D-C2D	2.10	129.85	125.49
35	f	305	DGD	CAB-C9B-C8B	-2.10	103.78	114.37
27	r	204	CLA	CHD-C1D-C2D	2.09	129.84	125.49
27	b	712	CLA	C2C-C1C-NC	2.09	112.18	109.98
29	B	611	UIX	C38-C40-C39	-2.09	115.72	119.01
27	a	822	CLA	CHD-C1D-C2D	2.09	129.84	125.49
27	a	827	CLA	CHD-C1D-C2D	2.09	129.84	125.49
27	a	828	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
27	l	410	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
27	a	830	CLA	CHD-C1D-C2D	2.09	129.84	125.49
35	j	201	DGD	CAB-C9B-C8B	-2.09	103.80	114.37
27	I	611	CLA	CHC-C1C-C2C	-2.09	121.01	126.95
29	F	613	UIX	C13-C14-C23	-2.09	117.14	123.20
27	A	602	CLA	CHC-C1C-C2C	-2.09	121.01	126.95
27	J	605	CLA	CHC-C1C-C2C	-2.09	121.01	126.95
27	a	823	CLA	CHC-C1C-C2C	-2.09	121.01	126.95
27	C	209	CLA	CAA-C2A-C1A	-2.09	105.13	111.97
27	H	304	CLA	CHB-C4A-NA	2.09	127.42	124.40
27	A	607	CLA	CHD-C1D-C2D	2.09	129.83	125.49
32	B	613	PID	O1-C1-C2	-2.09	111.53	113.49
32	I	614	PID	C17-C18-C19	-2.09	119.89	124.72
27	J	603	CLA	C2C-C1C-NC	2.09	112.17	109.98
27	b	718	CLA	C2C-C1C-NC	2.09	112.17	109.98
27	F	603	CLA	CHD-C1D-C2D	2.09	129.83	125.49
27	G	605	CLA	C2C-C1C-NC	2.09	112.17	109.98
27	C	208	CLA	CHC-C1C-C2C	-2.09	121.02	126.95
29	A	613	UIX	C35-C36-C38	-2.08	117.16	123.20
33	D	619	LMG	C3-C4-C5	-2.08	106.45	110.23
27	a	829	CLA	C2C-C1C-NC	2.08	112.17	109.98
27	a	817	CLA	CHD-C1D-C2D	2.08	129.82	125.49
30	E	613	DD6	O1-C20-C15	-2.08	57.28	58.93
30	H	318	DD6	O1-C20-C15	-2.08	57.28	58.93
27	F	605	CLA	CHD-C1D-C2D	2.08	129.82	125.49
29	C	213	UIX	C19-C18-C17	2.08	113.62	109.89
27	H	307	CLA	CHD-C1D-C2D	2.08	129.81	125.49
27	H	313	CLA	C2C-C1C-NC	2.08	112.17	109.98
27	b	720	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
27	H	304	CLA	C2A-C1A-CHA	2.08	127.48	123.87
27	G	606	CLA	CHD-C1D-C2D	2.08	129.81	125.49
27	G	606	CLA	CBA-CAA-C2A	2.08	119.98	113.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	605	CLA	CHA-C1A-NA	-2.08	121.69	126.39
27	D	601	CLA	CHD-C1D-C2D	2.08	129.81	125.49
28	G	601	KC2	CHB-C4A-C3A	-2.08	121.75	125.03
27	E	602	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
27	T	601	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
29	B	611	UIX	O2-C27-O4	-2.08	118.98	122.99
27	H	306	CLA	CHD-C1D-C2D	2.08	129.80	125.49
27	H	303	CLA	CMC-C2C-C1C	2.07	128.28	125.03
35	j	201	DGD	CBB-CAB-C9B	-2.07	103.88	114.37
35	j	201	DGD	O6D-C5D-C6D	-2.07	102.58	106.69
27	C	212	CLA	C2C-C1C-NC	2.07	112.16	109.98
27	j	202	CLA	C2C-C1C-NC	2.07	112.16	109.98
27	D	608	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
27	D	604	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
27	G	603	CLA	CHD-C1D-C2D	2.07	129.80	125.49
27	G	607	CLA	CAA-C2A-C1A	-2.07	105.18	111.97
27	T	602	CLA	CHD-C1D-C2D	2.07	129.80	125.49
28	J	606	KC2	CHD-C4C-NC	2.07	127.43	124.31
29	J	616	UIX	C18-O2-C27	-2.07	114.19	117.85
29	A	616	UIX	C10-C11-C13	-2.07	115.75	119.01
27	b	718	CLA	CHA-C1A-NA	-2.07	121.71	126.39
27	b	728	CLA	C2C-C1C-NC	2.07	112.16	109.98
27	b	709	CLA	CHD-C1D-C2D	2.07	129.79	125.49
27	E	604	CLA	C2C-C1C-NC	2.07	112.15	109.98
27	b	710	CLA	CHA-C1A-NA	-2.07	121.71	126.39
27	f	303	CLA	CHA-C1A-NA	-2.07	121.71	126.39
27	D	606	CLA	CHD-C1D-C2D	2.06	129.78	125.49
30	D	621	DD6	O1-C15-C14	-2.06	110.96	116.88
27	F	619	CLA	C2C-C1C-NC	2.06	112.15	109.98
29	A	613	UIX	O-C-C7	-2.06	110.97	116.88
30	C	214	DD6	O1-C20-C15	-2.06	57.29	58.93
27	a	802	CLA	CHC-C1C-C2C	-2.06	121.08	126.95
35	j	201	DGD	C1D-C2D-C3D	-2.06	105.67	110.01
27	G	609	CLA	CHD-C1D-C2D	2.06	129.78	125.49
27	a	812	CLA	C3A-C2A-C1A	-2.06	98.25	101.34
27	C	207	CLA	C2C-C1C-NC	2.06	112.15	109.98
27	D	605	CLA	CHA-C1A-NA	-2.06	121.72	126.39
27	a	804	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
27	C	209	CLA	C2C-C1C-NC	2.06	112.14	109.98
27	I	616	CLA	CHD-C1D-C2D	2.06	129.77	125.49
29	A	613	UIX	C13-C14-C23	-2.06	117.24	123.20
27	T	603	CLA	CHC-C1C-C2C	-2.06	121.10	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	T	612	UIX	C13-C14-C23	-2.06	117.24	123.20
27	A	606	CLA	CHD-C1D-C2D	2.06	129.76	125.49
27	H	303	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
27	B	604	CLA	C2C-C1C-NC	2.06	112.14	109.98
27	D	610	CLA	CHD-C1D-C2D	2.06	129.76	125.49
27	K	605	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
27	a	826	CLA	CHB-C4A-NA	2.06	127.37	124.40
27	b	711	CLA	C2C-C1C-NC	2.06	112.14	109.98
27	F	617	CLA	C2C-C1C-NC	2.05	112.14	109.98
30	D	617	DD6	O1-C20-C15	-2.05	57.30	58.93
27	l	402	CLA	C1-C2-C3	-2.05	122.83	126.20
30	K	612	DD6	O1-C20-C19	-2.05	111.57	113.49
32	F	615	PID	CM1-C1-C6	-2.05	118.92	122.30
27	G	606	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
27	H	305	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
27	B	607	CLA	CHD-C1D-C2D	2.05	129.75	125.49
27	K	608	CLA	CHA-C1A-NA	-2.05	121.75	126.39
27	b	717	CLA	C2C-C1C-NC	2.05	112.14	109.98
27	E	602	CLA	C2C-C1C-NC	2.05	112.13	109.98
27	l	409	CLA	C2C-C1C-NC	2.05	112.13	109.98
27	l	404	CLA	CHC-C1C-C2C	-2.05	121.13	126.95
36	T	613	LMU	O5B-C5B-C4B	2.05	113.39	109.70
35	K	614	DGD	C7B-C6B-C5B	-2.05	104.02	114.37
27	F	603	CLA	C2C-C1C-NC	2.05	112.13	109.98
30	E	617	DD6	O1-C15-C14	-2.05	111.01	116.88
27	G	602	CLA	CMC-C2C-C1C	2.05	128.23	125.03
27	a	825	CLA	C2C-C1C-NC	2.05	112.13	109.98
27	K	606	CLA	CHA-C1A-NA	-2.05	121.76	126.39
27	A	602	CLA	C2C-C1C-NC	2.04	112.13	109.98
27	F	604	CLA	CHD-C1D-C2D	2.04	129.74	125.49
27	b	725	CLA	CHD-C1D-C2D	2.04	129.74	125.49
27	C	203	CLA	CHC-C1C-C2C	-2.04	121.15	126.95
27	a	801	CLA	CHC-C1C-C2C	-2.04	121.15	126.95
27	a	802	CLA	CHA-C1A-NA	-2.04	121.77	126.39
27	a	818	CLA	C1-C2-C3	-2.04	122.85	126.20
27	A	604	CLA	C2C-C1C-NC	2.04	112.12	109.98
27	B	601	CLA	CAA-C2A-C1A	-2.04	105.29	111.97
35	f	305	DGD	C5B-C4B-C3B	-2.04	104.06	114.37
29	H	317	UIX	C38-C40-C39	-2.04	115.80	119.01
35	j	201	DGD	C1E-O6E-C5E	2.04	117.70	113.72
27	I	609	CLA	CHA-C1A-NA	-2.04	121.78	126.39
27	H	309	CLA	CHC-C1C-C2C	-2.04	121.16	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	I	602	CLA	CHD-C1D-C2D	2.04	129.72	125.49
27	I	611	CLA	CHA-C1A-NA	-2.04	121.78	126.39
27	E	611	CLA	CHA-C1A-NA	-2.04	121.78	126.39
27	A	612	CLA	C3A-C2A-C1A	-2.04	98.29	101.34
27	l	409	CLA	CHD-C1D-C2D	2.04	129.72	125.49
35	l	416	DGD	O2D-C2D-C1D	-2.03	105.23	110.08
27	l	407	CLA	C2C-C1C-NC	2.03	112.12	109.98
27	D	610	CLA	CHA-C1A-NA	-2.03	121.79	126.39
27	E	607	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
27	C	201	CLA	CAA-C2A-C1A	-2.03	107.64	112.14
30	T	611	DD6	C14-C13-C11	2.03	128.68	125.53
27	H	312	CLA	CAA-C2A-C1A	-2.03	107.64	112.14
27	K	603	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
27	T	603	CLA	CHD-C1D-C2D	2.03	129.71	125.49
27	T	601	CLA	CHA-C1A-NA	-2.03	121.79	126.39
29	B	615	UIX	C23-C26-C30	-2.03	115.82	119.01
27	D	604	CLA	C2C-C1C-NC	2.03	112.11	109.98
27	C	201	CLA	CHA-C1A-NA	-2.03	121.80	126.39
27	a	808	CLA	CHA-C1A-NA	-2.03	121.80	126.39
27	E	602	CLA	C1-C2-C3	-2.03	122.88	126.20
27	f	302	CLA	CHA-C1A-NA	-2.03	121.80	126.39
27	a	809	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
27	E	603	CLA	C2C-C1C-NC	2.03	112.11	109.98
27	T	609	CLA	C2C-C1C-NC	2.02	112.11	109.98
27	H	312	CLA	CHD-C1D-C2D	2.02	129.70	125.49
29	H	314	UIX	C37-C34-C30	-2.02	119.38	123.52
27	a	806	CLA	CHC-C1C-C2C	-2.02	121.20	126.95
29	T	612	UIX	C10-C11-C13	-2.02	115.83	119.01
27	A	603	CLA	CHA-C1A-NA	-2.02	121.81	126.39
27	F	604	CLA	CHA-C1A-NA	-2.02	121.81	126.39
30	b	730	DD6	O1-C20-C15	-2.02	57.33	58.93
27	I	609	CLA	C2C-C1C-NC	2.02	112.11	109.98
27	a	804	CLA	C2C-C1C-NC	2.02	112.11	109.98
27	l	410	CLA	C2C-C1C-NC	2.02	112.11	109.98
35	l	416	DGD	O3E-C3E-C2E	-2.02	105.61	110.38
27	C	208	CLA	C2C-C1C-NC	2.02	112.10	109.98
30	K	610	DD6	O1-C20-C15	-2.02	57.33	58.93
27	H	306	CLA	CHB-C4A-NA	2.02	127.31	124.40
29	C	213	UIX	C37-C34-C30	-2.02	119.39	123.52
27	a	812	CLA	C1-C2-C3	-2.02	123.50	126.76
27	T	605	CLA	CHA-C1A-NA	-2.02	121.82	126.39
27	l	406	CLA	C2C-C1C-NC	2.02	112.10	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	313	CLA	C1-C2-C3	-2.02	122.89	126.20
32	F	615	PID	C18-C17-C16	-2.02	120.06	124.72
27	b	704	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
27	G	603	CLA	C1-C2-C3	-2.02	123.50	126.76
27	A	606	CLA	CHD-C4C-C3C	-2.01	121.84	124.77
27	A	605	CLA	C2C-C1C-NC	2.01	112.10	109.98
27	b	708	CLA	CHD-C1D-C2D	2.01	129.67	125.49
32	I	614	PID	CM7-C25-C24	-2.01	108.67	110.47
27	b	720	CLA	CHA-C1A-NA	-2.01	121.84	126.39
27	a	818	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
27	B	601	CLA	CHD-C4C-C3C	-2.01	121.84	124.77
27	E	608	CLA	CHA-C1A-NA	-2.01	121.84	126.39
27	H	304	CLA	CHD-C1D-C2D	2.01	129.67	125.49
27	H	309	CLA	C2C-C1C-NC	2.01	112.09	109.98
29	H	314	UIX	C14-C13-C11	-2.01	124.46	127.28
27	I	616	CLA	CHA-C1A-NA	-2.01	121.84	126.39
35	K	614	DGD	C4E-C3E-C2E	-2.01	107.31	110.83
30	r	201	DD6	O1-C20-C15	-2.01	57.34	58.93
27	b	715	CLA	CHC-C1C-NC	2.01	127.33	124.31
27	J	609	CLA	C2C-C1C-NC	2.01	112.09	109.98
27	b	713	CLA	CHA-C1A-NA	-2.01	121.85	126.39
30	G	613	DD6	O1-C20-C15	-2.00	57.34	58.93
32	J	614	PID	O4-C10-O3	2.00	123.93	120.17
27	b	726	CLA	CHA-C1A-NA	-2.00	121.85	126.39
27	D	602	CLA	CHA-C1A-NA	-2.00	121.86	126.39
27	G	607	CLA	CHD-C4C-C3C	-2.00	121.86	124.77
27	B	604	CLA	CHA-C1A-NA	-2.00	121.86	126.39
27	D	602	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
27	b	705	CLA	CHC-C1C-C2C	-2.00	121.26	126.95

All (197) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	601	CLA	ND
27	A	602	CLA	ND
27	A	603	CLA	ND
27	A	604	CLA	ND
27	A	605	CLA	ND
27	A	606	CLA	ND
27	A	607	CLA	ND
27	A	609	CLA	ND
27	A	610	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
27	A	611	CLA	ND
27	A	612	CLA	ND
27	B	601	CLA	ND
27	B	603	CLA	ND
27	B	604	CLA	ND
27	B	605	CLA	ND
27	B	606	CLA	ND
27	B	607	CLA	ND
27	B	609	CLA	ND
27	B	610	CLA	ND
27	C	201	CLA	ND
27	C	202	CLA	ND
27	C	203	CLA	ND
27	C	204	CLA	ND
27	C	205	CLA	ND
27	C	206	CLA	ND
27	C	207	CLA	ND
27	C	208	CLA	ND
27	C	209	CLA	ND
27	C	211	CLA	ND
27	C	212	CLA	ND
27	D	601	CLA	ND
27	D	602	CLA	ND
27	D	603	CLA	ND
27	D	604	CLA	ND
27	D	605	CLA	ND
27	D	606	CLA	ND
27	D	607	CLA	ND
27	D	608	CLA	ND
27	D	609	CLA	ND
27	D	610	CLA	ND
27	D	611	CLA	ND
27	D	612	CLA	ND
27	E	602	CLA	ND
27	E	603	CLA	ND
27	E	604	CLA	ND
27	E	605	CLA	ND
27	E	606	CLA	ND
27	E	607	CLA	ND
27	E	608	CLA	ND
27	E	609	CLA	ND
27	E	611	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
27	E	612	CLA	ND
27	F	601	CLA	ND
27	F	602	CLA	ND
27	F	603	CLA	ND
27	F	604	CLA	ND
27	F	605	CLA	ND
27	F	606	CLA	ND
27	F	607	CLA	ND
27	F	608	CLA	ND
27	F	610	CLA	ND
27	F	617	CLA	ND
27	F	619	CLA	ND
27	G	602	CLA	ND
27	G	603	CLA	ND
27	G	604	CLA	ND
27	G	605	CLA	ND
27	G	606	CLA	ND
27	G	607	CLA	ND
27	G	608	CLA	ND
27	G	609	CLA	ND
27	G	610	CLA	ND
27	G	611	CLA	ND
27	H	303	CLA	ND
27	H	304	CLA	ND
27	H	305	CLA	ND
27	H	306	CLA	ND
27	H	307	CLA	ND
27	H	308	CLA	ND
27	H	309	CLA	ND
27	H	310	CLA	ND
27	H	312	CLA	ND
27	H	313	CLA	ND
27	H	319	CLA	ND
27	I	601	CLA	ND
27	I	602	CLA	ND
27	I	603	CLA	ND
27	I	605	CLA	ND
27	I	606	CLA	ND
27	I	607	CLA	ND
27	I	608	CLA	ND
27	I	609	CLA	ND
27	I	610	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
27	I	611	CLA	ND
27	I	616	CLA	ND
27	J	601	CLA	ND
27	J	603	CLA	ND
27	J	605	CLA	ND
27	J	607	CLA	ND
27	J	609	CLA	ND
27	K	601	CLA	ND
27	K	602	CLA	ND
27	K	603	CLA	ND
27	K	604	CLA	ND
27	K	605	CLA	ND
27	K	606	CLA	ND
27	K	608	CLA	ND
27	T	601	CLA	ND
27	T	602	CLA	ND
27	T	603	CLA	ND
27	T	604	CLA	ND
27	T	605	CLA	ND
27	T	606	CLA	ND
27	T	607	CLA	ND
27	T	609	CLA	ND
27	U	601	CLA	ND
27	U	603	CLA	ND
27	U	605	CLA	ND
27	U	606	CLA	ND
27	a	801	CLA	ND
27	a	802	CLA	ND
27	a	803	CLA	ND
27	a	804	CLA	ND
27	a	805	CLA	ND
27	a	806	CLA	ND
27	a	807	CLA	ND
27	a	808	CLA	ND
27	a	809	CLA	ND
27	a	810	CLA	ND
27	a	811	CLA	ND
27	a	812	CLA	ND
27	a	813	CLA	ND
27	a	814	CLA	ND
27	a	815	CLA	ND
27	a	816	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
27	a	817	CLA	ND
27	a	818	CLA	ND
27	a	819	CLA	ND
27	a	820	CLA	ND
27	a	821	CLA	ND
27	a	822	CLA	ND
27	a	823	CLA	ND
27	a	824	CLA	ND
27	a	825	CLA	ND
27	a	826	CLA	ND
27	a	827	CLA	ND
27	a	828	CLA	ND
27	a	829	CLA	ND
27	a	830	CLA	ND
27	a	831	CLA	ND
27	a	837	CLA	ND
27	a	839	CLA	ND
27	b	701	CLA	ND
27	b	702	CLA	ND
27	b	703	CLA	ND
27	b	704	CLA	ND
27	b	705	CLA	ND
27	b	706	CLA	ND
27	b	707	CLA	ND
27	b	708	CLA	ND
27	b	709	CLA	ND
27	b	710	CLA	ND
27	b	711	CLA	ND
27	b	712	CLA	ND
27	b	713	CLA	ND
27	b	714	CLA	ND
27	b	715	CLA	ND
27	b	716	CLA	ND
27	b	717	CLA	ND
27	b	718	CLA	ND
27	b	719	CLA	ND
27	b	720	CLA	ND
27	b	721	CLA	ND
27	b	722	CLA	ND
27	b	723	CLA	ND
27	b	724	CLA	ND
27	b	725	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
27	b	726	CLA	ND
27	b	727	CLA	ND
27	b	728	CLA	ND
27	f	302	CLA	ND
27	f	303	CLA	ND
27	j	202	CLA	ND
27	l	402	CLA	ND
27	l	403	CLA	ND
27	l	404	CLA	ND
27	l	405	CLA	ND
27	l	406	CLA	ND
27	l	407	CLA	ND
27	l	408	CLA	ND
27	l	409	CLA	ND
27	l	410	CLA	ND
27	l	411	CLA	ND
27	l	412	CLA	ND
27	r	203	CLA	ND
27	r	204	CLA	ND
30	D	613	DD6	C20

All (1685) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	601	CLA	C1A-C2A-CAA-CBA
27	A	601	CLA	C2B-C3B-CAB-CBB
27	A	601	CLA	C4B-C3B-CAB-CBB
27	A	604	CLA	C1A-C2A-CAA-CBA
27	A	606	CLA	C1A-C2A-CAA-CBA
27	A	606	CLA	C3A-C2A-CAA-CBA
27	A	612	CLA	C1A-C2A-CAA-CBA
27	B	601	CLA	C3A-C2A-CAA-CBA
27	B	604	CLA	C2B-C3B-CAB-CBB
27	B	604	CLA	C4B-C3B-CAB-CBB
27	B	605	CLA	C1A-C2A-CAA-CBA
27	B	605	CLA	C3A-C2A-CAA-CBA
27	C	201	CLA	C3A-C2A-CAA-CBA
27	C	206	CLA	CHA-CBD-CGD-O1D
27	C	206	CLA	CHA-CBD-CGD-O2D
27	D	606	CLA	CHA-CBD-CGD-O1D
27	D	606	CLA	CHA-CBD-CGD-O2D
27	D	610	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	D	610	CLA	CHA-CBD-CGD-O2D
27	F	602	CLA	C1A-C2A-CAA-CBA
27	F	602	CLA	C2-C3-C5-C6
27	F	602	CLA	C4-C3-C5-C6
27	F	603	CLA	CAD-CBD-CGD-O1D
27	F	603	CLA	CAD-CBD-CGD-O2D
27	F	605	CLA	C1A-C2A-CAA-CBA
27	F	607	CLA	C3A-C2A-CAA-CBA
27	F	607	CLA	C2B-C3B-CAB-CBB
27	F	607	CLA	C4B-C3B-CAB-CBB
27	F	610	CLA	C1A-C2A-CAA-CBA
27	G	602	CLA	C2B-C3B-CAB-CBB
27	G	602	CLA	C4B-C3B-CAB-CBB
27	G	603	CLA	CHA-CBD-CGD-O1D
27	G	603	CLA	CHA-CBD-CGD-O2D
27	G	607	CLA	C3A-C2A-CAA-CBA
27	G	607	CLA	CHA-CBD-CGD-O1D
27	G	607	CLA	CHA-CBD-CGD-O2D
27	G	610	CLA	CHA-CBD-CGD-O1D
27	G	610	CLA	CHA-CBD-CGD-O2D
27	H	307	CLA	CHA-CBD-CGD-O1D
27	H	307	CLA	CHA-CBD-CGD-O2D
27	H	310	CLA	C3A-C2A-CAA-CBA
27	I	602	CLA	CAD-CBD-CGD-O1D
27	I	602	CLA	CAD-CBD-CGD-O2D
27	I	608	CLA	CHA-CBD-CGD-O1D
27	I	608	CLA	CHA-CBD-CGD-O2D
27	I	611	CLA	C1A-C2A-CAA-CBA
27	I	611	CLA	CHA-CBD-CGD-O1D
27	I	611	CLA	CHA-CBD-CGD-O2D
27	J	601	CLA	C1A-C2A-CAA-CBA
27	J	601	CLA	C3A-C2A-CAA-CBA
27	J	601	CLA	C4B-C3B-CAB-CBB
27	J	609	CLA	CAD-CBD-CGD-O2D
27	K	601	CLA	C2B-C3B-CAB-CBB
27	K	601	CLA	C4B-C3B-CAB-CBB
27	K	605	CLA	C1A-C2A-CAA-CBA
27	K	605	CLA	C3A-C2A-CAA-CBA
27	T	604	CLA	C2B-C3B-CAB-CBB
27	T	604	CLA	C4B-C3B-CAB-CBB
27	U	606	CLA	CAD-CBD-CGD-O1D
27	U	606	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	803	CLA	C1A-C2A-CAA-CBA
27	a	803	CLA	C3A-C2A-CAA-CBA
27	a	804	CLA	C6-C7-C8-C9
27	a	807	CLA	C1A-C2A-CAA-CBA
27	a	807	CLA	CHA-CBD-CGD-O1D
27	a	807	CLA	CHA-CBD-CGD-O2D
27	a	809	CLA	C1A-C2A-CAA-CBA
27	a	812	CLA	C1A-C2A-CAA-CBA
27	a	813	CLA	C3A-C2A-CAA-CBA
27	a	820	CLA	C1A-C2A-CAA-CBA
27	a	820	CLA	C3A-C2A-CAA-CBA
27	a	820	CLA	CHA-CBD-CGD-O1D
27	a	820	CLA	CHA-CBD-CGD-O2D
27	a	822	CLA	C3A-C2A-CAA-CBA
27	a	822	CLA	CHA-CBD-CGD-O1D
27	a	822	CLA	CHA-CBD-CGD-O2D
27	a	823	CLA	CAD-CBD-CGD-O2D
27	a	824	CLA	C14-C13-C15-C16
27	a	825	CLA	C1A-C2A-CAA-CBA
27	a	825	CLA	C3A-C2A-CAA-CBA
27	a	826	CLA	C2B-C3B-CAB-CBB
27	a	826	CLA	C4B-C3B-CAB-CBB
27	a	829	CLA	C1A-C2A-CAA-CBA
27	a	829	CLA	C14-C13-C15-C16
27	a	831	CLA	CHA-CBD-CGD-O1D
27	a	831	CLA	CHA-CBD-CGD-O2D
27	a	839	CLA	C1A-C2A-CAA-CBA
27	a	839	CLA	C3A-C2A-CAA-CBA
27	b	703	CLA	C2-C1-O2A-CGA
27	b	704	CLA	C2B-C3B-CAB-CBB
27	b	704	CLA	C4B-C3B-CAB-CBB
27	b	705	CLA	C1A-C2A-CAA-CBA
27	b	705	CLA	C3A-C2A-CAA-CBA
27	b	708	CLA	C1A-C2A-CAA-CBA
27	b	708	CLA	C4B-C3B-CAB-CBB
27	b	708	CLA	CHA-CBD-CGD-O1D
27	b	708	CLA	CHA-CBD-CGD-O2D
27	b	713	CLA	C1A-C2A-CAA-CBA
27	b	713	CLA	C3A-C2A-CAA-CBA
27	b	714	CLA	C1A-C2A-CAA-CBA
27	b	717	CLA	C3A-C2A-CAA-CBA
27	b	718	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	b	720	CLA	C2B-C3B-CAB-CBB
27	b	720	CLA	C4B-C3B-CAB-CBB
27	b	721	CLA	CHA-CBD-CGD-O1D
27	b	721	CLA	CHA-CBD-CGD-O2D
27	b	725	CLA	C2B-C3B-CAB-CBB
27	b	725	CLA	C4B-C3B-CAB-CBB
27	b	727	CLA	C1A-C2A-CAA-CBA
27	j	202	CLA	CAD-CBD-CGD-O1D
27	j	202	CLA	CAD-CBD-CGD-O2D
27	l	403	CLA	C2B-C3B-CAB-CBB
27	l	403	CLA	C4B-C3B-CAB-CBB
27	l	403	CLA	CHA-CBD-CGD-O1D
27	l	403	CLA	CHA-CBD-CGD-O2D
27	l	404	CLA	C2B-C3B-CAB-CBB
27	l	404	CLA	C4B-C3B-CAB-CBB
27	l	410	CLA	C4B-C3B-CAB-CBB
27	l	412	CLA	C2B-C3B-CAB-CBB
27	l	412	CLA	C4B-C3B-CAB-CBB
27	l	412	CLA	CHA-CBD-CGD-O1D
27	l	412	CLA	CHA-CBD-CGD-O2D
27	r	203	CLA	C1A-C2A-CAA-CBA
27	r	204	CLA	CAD-CBD-CGD-O1D
27	r	204	CLA	CAD-CBD-CGD-O2D
28	A	608	KC2	CHA-CBD-CGD-O1D
28	A	608	KC2	CHA-CBD-CGD-O2D
28	B	608	KC2	C3A-C2A-CAA-CBA
28	B	608	KC2	CHA-CBD-CGD-O1D
28	B	608	KC2	CHA-CBD-CGD-O2D
28	C	210	KC2	C2C-C3C-CAC-CBC
28	C	210	KC2	C4C-C3C-CAC-CBC
28	C	210	KC2	CHA-CBD-CGD-O1D
28	C	210	KC2	CHA-CBD-CGD-O2D
28	E	601	KC2	CHA-CBD-CGD-O1D
28	E	601	KC2	CHA-CBD-CGD-O2D
28	G	601	KC2	C3A-C2A-CAA-CBA
28	G	601	KC2	C2B-C3B-CAB-CBB
28	G	601	KC2	CHA-CBD-CGD-O1D
28	G	601	KC2	CHA-CBD-CGD-O2D
28	H	302	KC2	C3A-C2A-CAA-CBA
28	H	302	KC2	C2B-C3B-CAB-CBB
28	H	302	KC2	CHA-CBD-CGD-O1D
28	H	302	KC2	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	H	311	KC2	C1A-C2A-CAA-CBA
28	I	604	KC2	C2B-C3B-CAB-CBB
28	J	602	KC2	C3A-C2A-CAA-CBA
28	J	604	KC2	C3A-C2A-CAA-CBA
28	J	604	KC2	C2C-C3C-CAC-CBC
28	J	604	KC2	C4C-C3C-CAC-CBC
28	J	606	KC2	C1A-C2A-CAA-CBA
28	U	602	KC2	C2B-C3B-CAB-CBB
28	U	604	KC2	C3A-C2A-CAA-CBA
28	U	604	KC2	C2C-C3C-CAC-CBC
29	A	613	UIX	C31-C27-O2-C18
29	A	616	UIX	C2-C-C7-C10
29	B	615	UIX	C1-C-C7-C10
29	B	615	UIX	C31-C27-O2-C18
29	C	213	UIX	C31-C27-O2-C18
29	C	215	UIX	C1-C-C7-C10
29	C	215	UIX	C31-C27-O2-C18
29	D	616	UIX	C31-C27-O2-C18
29	E	616	UIX	C2-C-C7-C10
29	F	613	UIX	O4-C27-O2-C18
29	F	613	UIX	C31-C27-O2-C18
29	H	314	UIX	C31-C27-O2-C18
29	I	612	UIX	C31-C27-O2-C18
29	J	616	UIX	C31-C27-O2-C18
29	T	612	UIX	C1-C-C7-C10
29	T	612	UIX	C31-C27-O2-C18
29	j	204	UIX	O-C-C7-C10
29	j	204	UIX	C31-C27-O2-C18
30	A	617	DD6	C10-C11-C13-C14
30	A	617	DD6	C13-C14-C15-C20
30	B	614	DD6	C13-C14-C15-C20
30	B	616	DD6	C13-C14-C15-C20
30	B	616	DD6	C13-C14-C15-O1
30	D	613	DD6	C13-C14-C15-O1
30	D	621	DD6	C11-C10-C9-C8
30	H	301	DD6	C13-C14-C15-C20
30	H	316	DD6	C13-C14-C15-O1
30	K	609	DD6	C10-C11-C13-C14
30	K	609	DD6	C13-C14-C15-C20
30	K	612	DD6	C10-C11-C13-C14
30	K	612	DD6	C12-C11-C13-C14
30	K	612	DD6	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	K	612	DD6	C13-C14-C15-C20
30	K	612	DD6	C13-C14-C15-O1
30	T	610	DD6	C10-C11-C13-C14
30	T	610	DD6	C13-C14-C15-C20
30	T	611	DD6	C13-C14-C15-C16
30	i	202	DD6	C13-C14-C15-C16
30	i	202	DD6	C5-C6-C8-C9
30	r	201	DD6	C13-C14-C15-C20
30	r	205	DD6	C13-C14-C15-O1
31	A	618	SQD	O5-C5-C6-S
31	A	618	SQD	C5-C6-S-O7
31	A	618	SQD	C5-C6-S-O8
31	A	618	SQD	C5-C6-S-O9
32	B	613	PID	O1-C6-C7-C8
32	B	613	PID	C31-C30-O6-C27
32	F	614	PID	C31-C30-O6-C27
32	F	615	PID	C31-C30-O6-C27
32	F	615	PID	O7-C30-O6-C27
32	I	614	PID	O1-C6-C7-C8
32	I	614	PID	C31-C30-O6-C27
32	J	613	PID	O1-C6-C7-C8
32	J	613	PID	C31-C30-O6-C27
32	J	615	PID	C1-C6-C7-C8
32	J	615	PID	C31-C30-O6-C27
32	J	615	PID	O7-C30-O6-C27
32	K	611	PID	C1-C6-C7-C8
32	K	611	PID	C31-C30-O6-C27
32	K	611	PID	O7-C30-O6-C27
32	U	608	PID	C31-C30-O6-C27
32	U	608	PID	O7-C30-O6-C27
33	C	217	LMG	C11-C10-O7-C8
33	D	618	LMG	C2-C1-O1-C7
33	D	618	LMG	O6-C1-O1-C7
33	D	619	LMG	O6-C1-O1-C7
33	D	619	LMG	O9-C10-O7-C8
33	F	616	LMG	C2-C1-O1-C7
33	F	616	LMG	O6-C1-O1-C7
33	F	616	LMG	C11-C10-O7-C8
33	K	613	LMG	O7-C8-C9-O8
33	b	733	LMG	C11-C10-O7-C8
33	l	417	LMG	O1-C7-C8-O7
33	l	417	LMG	O9-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	D	620	LHG	C3-O3-P-O4
34	D	620	LHG	C3-O3-P-O6
34	D	620	LHG	C4-O6-P-O3
34	D	620	LHG	C4-O6-P-O5
34	D	620	LHG	O7-C5-C6-O8
34	F	618	LHG	O1-C1-C2-C3
34	F	618	LHG	C3-O3-P-O5
34	F	618	LHG	C4-O6-P-O3
34	F	618	LHG	C8-C7-O7-C5
34	G	617	LHG	C3-O3-P-O6
34	G	617	LHG	C4-O6-P-O5
34	G	617	LHG	C8-C7-O7-C5
34	a	835	LHG	O2-C2-C3-O3
34	a	835	LHG	C3-O3-P-O4
34	a	835	LHG	C3-O3-P-O6
34	j	205	LHG	C4-O6-P-O5
34	j	205	LHG	C8-C7-O7-C5
34	l	401	LHG	C4-O6-P-O4
34	r	202	LHG	C3-O3-P-O4
34	r	202	LHG	C3-O3-P-O6
34	r	202	LHG	O7-C5-C6-O8
35	f	305	DGD	O1G-C1G-C2G-O2G
35	j	201	DGD	C2B-C1B-O2G-C2G
35	j	201	DGD	O1B-C1B-O2G-C2G
35	l	416	DGD	C2B-C1B-O2G-C2G
35	l	416	DGD	O1B-C1B-O2G-C2G
38	a	833	BCR	C19-C20-C21-C22
38	a	833	BCR	C21-C22-C23-C24
38	a	833	BCR	C37-C22-C23-C24
38	a	833	BCR	C23-C24-C25-C26
38	a	833	BCR	C23-C24-C25-C30
38	a	836	BCR	C7-C8-C9-C10
38	a	836	BCR	C21-C22-C23-C24
38	a	836	BCR	C37-C22-C23-C24
38	a	836	BCR	C23-C24-C25-C26
38	f	301	BCR	C11-C12-C13-C14
38	f	301	BCR	C11-C12-C13-C35
38	f	301	BCR	C17-C18-C19-C20
38	i	201	BCR	C17-C18-C19-C20
38	i	201	BCR	C36-C18-C19-C20
38	i	201	BCR	C21-C22-C23-C24
38	i	201	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	i	201	BCR	C23-C24-C25-C30
38	j	203	BCR	C17-C18-C19-C20
38	j	203	BCR	C36-C18-C19-C20
38	l	414	BCR	C7-C8-C9-C10
38	l	415	BCR	C5-C6-C7-C8
38	l	415	BCR	C11-C12-C13-C14
38	l	415	BCR	C17-C18-C19-C20
38	l	415	BCR	C23-C24-C25-C26
38	l	415	BCR	C23-C24-C25-C30
38	m	201	BCR	C11-C12-C13-C14
38	m	201	BCR	C11-C12-C13-C35
38	m	201	BCR	C17-C18-C19-C20
27	a	827	CLA	C4C-C3C-CAC-CBC
29	A	613	UIX	O4-C27-O2-C18
29	A	616	UIX	C31-C27-O2-C18
29	C	215	UIX	O4-C27-O2-C18
29	E	616	UIX	C31-C27-O2-C18
29	G	615	UIX	C31-C27-O2-C18
29	H	314	UIX	O4-C27-O2-C18
29	H	317	UIX	C31-C27-O2-C18
29	I	612	UIX	O4-C27-O2-C18
32	B	613	PID	O7-C30-O6-C27
32	I	614	PID	O7-C30-O6-C27
27	a	827	CLA	C2C-C3C-CAC-CBC
29	B	615	UIX	O4-C27-O2-C18
29	C	213	UIX	O4-C27-O2-C18
29	D	616	UIX	O4-C27-O2-C18
29	J	616	UIX	O4-C27-O2-C18
29	T	612	UIX	O4-C27-O2-C18
32	J	611	PID	C31-C30-O6-C27
32	J	613	PID	O7-C30-O6-C27
35	K	614	DGD	O1A-C1A-O1G-C1G
32	F	614	PID	O7-C30-O6-C27
29	D	616	UIX	C19-C18-O2-C27
29	F	613	UIX	C19-C18-O2-C27
29	J	616	UIX	C17-C18-O2-C27
29	j	204	UIX	C19-C18-O2-C27
32	F	614	PID	C28-C27-O6-C30
32	J	611	PID	C26-C27-O6-C30
32	K	611	PID	C26-C27-O6-C30
32	U	608	PID	C28-C27-O6-C30
27	a	806	CLA	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	C	217	LMG	C29-C28-O8-C9
33	C	217	LMG	O10-C28-O8-C9
33	D	619	LMG	O10-C28-O8-C9
33	F	616	LMG	O10-C28-O8-C9
34	G	617	LHG	O10-C23-O8-C6
35	l	416	DGD	C4E-C5E-C6E-O5E
29	A	616	UIX	O4-C27-O2-C18
29	E	616	UIX	O4-C27-O2-C18
29	j	204	UIX	O4-C27-O2-C18
36	T	613	LMU	O5B-C1B-O1B-C4'
27	a	806	CLA	C2C-C3C-CAC-CBC
33	C	217	LMG	O9-C10-O7-C8
33	F	616	LMG	O9-C10-O7-C8
34	G	617	LHG	O9-C7-O7-C5
34	j	205	LHG	O9-C7-O7-C5
32	J	615	PID	C28-C27-O6-C30
27	A	603	CLA	C3-C5-C6-C7
27	E	606	CLA	C3-C5-C6-C7
27	a	818	CLA	C3-C5-C6-C7
27	a	839	CLA	C3-C5-C6-C7
27	b	706	CLA	C3-C5-C6-C7
27	l	403	CLA	C3-C5-C6-C7
27	r	204	CLA	C3-C5-C6-C7
33	F	616	LMG	C29-C28-O8-C9
34	G	617	LHG	C24-C23-O8-C6
29	B	611	UIX	C31-C27-O2-C18
33	D	619	LMG	C11-C10-O7-C8
33	l	417	LMG	C11-C10-O7-C8
29	H	317	UIX	O4-C27-O2-C18
29	G	615	UIX	O4-C27-O2-C18
28	J	606	KC2	CAA-CBA-CGA-O1A
28	J	606	KC2	CAA-CBA-CGA-O2A
28	U	602	KC2	CAA-CBA-CGA-O1A
28	U	602	KC2	CAA-CBA-CGA-O2A
27	C	205	CLA	C4-C3-C5-C6
27	D	612	CLA	C4-C3-C5-C6
27	E	608	CLA	C4-C3-C5-C6
27	E	611	CLA	C4-C3-C5-C6
27	F	619	CLA	C4-C3-C5-C6
27	G	609	CLA	C4-C3-C5-C6
27	I	607	CLA	C4-C3-C5-C6
27	K	602	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	804	CLA	C4-C3-C5-C6
27	a	807	CLA	C4-C3-C5-C6
27	a	824	CLA	C4-C3-C5-C6
27	a	826	CLA	C4-C3-C5-C6
27	b	708	CLA	C4-C3-C5-C6
27	C	205	CLA	C2-C3-C5-C6
27	D	612	CLA	C2-C3-C5-C6
27	E	611	CLA	C2-C3-C5-C6
27	F	619	CLA	C2-C3-C5-C6
27	I	607	CLA	C2-C3-C5-C6
27	K	602	CLA	C2-C3-C5-C6
27	a	804	CLA	C2-C3-C5-C6
27	a	807	CLA	C2-C3-C5-C6
27	a	826	CLA	C2-C3-C5-C6
27	C	204	CLA	C2A-CAA-CBA-CGA
27	I	607	CLA	C2A-CAA-CBA-CGA
34	D	620	LHG	O10-C23-O8-C6
27	D	602	CLA	C3-C5-C6-C7
27	F	617	CLA	C3-C5-C6-C7
27	a	814	CLA	C3-C5-C6-C7
27	a	825	CLA	C3-C5-C6-C7
27	j	202	CLA	C3-C5-C6-C7
33	D	619	LMG	C29-C28-O8-C9
33	l	417	LMG	C29-C28-O8-C9
34	r	202	LHG	O10-C23-O8-C6
33	b	733	LMG	O9-C10-O7-C8
34	F	618	LHG	O9-C7-O7-C5
27	T	603	CLA	C2C-C3C-CAC-CBC
27	G	608	CLA	C3-C5-C6-C7
37	a	832	PQN	C13-C15-C16-C17
34	G	617	LHG	O2-C2-C3-O3
34	D	620	LHG	C24-C23-O8-C6
35	l	416	DGD	O6E-C5E-C6E-O5E
33	l	417	LMG	O10-C28-O8-C9
33	C	217	LMG	O6-C5-C6-O5
33	D	619	LMG	O6-C5-C6-O5
33	D	618	LMG	C11-C10-O7-C8
34	r	202	LHG	C8-C7-O7-C5
32	I	614	PID	C26-C27-O6-C30
27	B	609	CLA	C3-C5-C6-C7
34	r	202	LHG	C24-C23-O8-C6
35	K	614	DGD	C2A-C1A-O1G-C1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	T	613	LMU	C3'-C4'-O1B-C1B
27	E	608	CLA	C2-C3-C5-C6
27	a	824	CLA	C2-C3-C5-C6
33	D	618	LMG	O9-C10-O7-C8
27	a	809	CLA	C2A-CAA-CBA-CGA
35	K	614	DGD	O6D-C1D-O3G-C3G
35	f	305	DGD	O6E-C1E-O5D-C6D
35	j	201	DGD	O6D-C1D-O3G-C3G
33	b	733	LMG	C29-C28-O8-C9
27	F	604	CLA	C2C-C3C-CAC-CBC
32	J	611	PID	O7-C30-O6-C27
28	A	608	KC2	CAA-CBA-CGA-O2A
33	D	618	LMG	O6-C5-C6-O5
35	f	305	DGD	O6E-C5E-C6E-O5E
33	C	217	LMG	C4-C5-C6-O5
33	b	733	LMG	O10-C28-O8-C9
34	G	617	LHG	C1-C2-C3-O3
34	a	835	LHG	C1-C2-C3-O3
27	I	603	CLA	CBA-CGA-O2A-C1
27	a	804	CLA	CBA-CGA-O2A-C1
32	I	614	PID	C28-C27-O6-C30
33	D	618	LMG	C4-C5-C6-O5
33	D	619	LMG	C4-C5-C6-O5
33	l	417	LMG	C4-C5-C6-O5
28	A	608	KC2	CAA-CBA-CGA-O1A
28	E	601	KC2	CAA-CBA-CGA-O1A
28	J	610	KC2	CAA-CBA-CGA-O1A
28	J	610	KC2	CAA-CBA-CGA-O2A
28	U	604	KC2	CAA-CBA-CGA-O2A
27	D	607	CLA	C4-C3-C5-C6
27	I	603	CLA	C4-C3-C5-C6
27	D	607	CLA	C2-C3-C5-C6
27	G	609	CLA	C2-C3-C5-C6
27	I	603	CLA	C2-C3-C5-C6
27	b	708	CLA	C2-C3-C5-C6
27	H	305	CLA	C3-C5-C6-C7
27	F	606	CLA	C6-C7-C8-C9
27	F	617	CLA	C6-C7-C8-C9
27	H	319	CLA	C14-C13-C15-C16
27	K	605	CLA	C11-C10-C8-C9
27	a	804	CLA	C11-C10-C8-C9
27	a	816	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	821	CLA	C11-C10-C8-C9
27	a	825	CLA	C6-C7-C8-C9
27	a	827	CLA	C6-C7-C8-C9
27	a	827	CLA	C11-C12-C13-C14
27	b	708	CLA	C6-C7-C8-C9
27	l	409	CLA	C11-C12-C13-C14
37	a	832	PQN	C21-C22-C23-C24
37	b	729	PQN	C21-C22-C23-C24
33	D	619	LMG	C2-C1-O1-C7
35	K	614	DGD	C2D-C1D-O3G-C3G
35	j	201	DGD	C2D-C1D-O3G-C3G
27	U	603	CLA	CBD-CGD-O2D-CED
29	D	616	UIX	C7-C10-C11-C12
29	G	615	UIX	C7-C10-C11-C12
30	A	615	DD6	C12-C11-C13-C14
30	D	615	DD6	C12-C11-C13-C14
30	D	621	DD6	C12-C11-C13-C14
30	D	621	DD6	C7-C6-C8-C9
30	E	617	DD6	C12-C11-C13-C14
30	F	611	DD6	C12-C11-C13-C14
30	G	614	DD6	C12-C11-C13-C14
30	K	609	DD6	C12-C11-C13-C14
30	T	610	DD6	C12-C11-C13-C14
30	r	205	DD6	C12-C11-C13-C14
30	r	206	DD6	C12-C11-C13-C14
38	a	833	BCR	C36-C18-C19-C20
38	a	834	BCR	C11-C12-C13-C35
38	a	836	BCR	C7-C8-C9-C34
38	b	731	BCR	C7-C8-C9-C34
38	f	301	BCR	C36-C18-C19-C20
38	j	203	BCR	C7-C8-C9-C34
38	l	413	BCR	C36-C18-C19-C20
38	l	414	BCR	C7-C8-C9-C34
38	l	415	BCR	C11-C12-C13-C35
38	l	415	BCR	C36-C18-C19-C20
38	m	201	BCR	C36-C18-C19-C20
29	D	616	UIX	C7-C10-C11-C13
29	G	615	UIX	C7-C10-C11-C13
30	A	615	DD6	C10-C11-C13-C14
30	D	615	DD6	C10-C11-C13-C14
30	D	621	DD6	C10-C11-C13-C14
30	D	621	DD6	C5-C6-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	E	617	DD6	C10-C11-C13-C14
30	F	611	DD6	C10-C11-C13-C14
30	G	614	DD6	C10-C11-C13-C14
30	r	205	DD6	C10-C11-C13-C14
30	r	206	DD6	C10-C11-C13-C14
38	a	833	BCR	C17-C18-C19-C20
38	j	203	BCR	C7-C8-C9-C10
38	m	201	BCR	C21-C22-C23-C24
35	f	305	DGD	C4E-C5E-C6E-O5E
34	r	202	LHG	O9-C7-O7-C5
28	C	210	KC2	CAA-CBA-CGA-O1A
28	E	601	KC2	CAA-CBA-CGA-O2A
28	J	602	KC2	CAA-CBA-CGA-O1A
28	J	602	KC2	CAA-CBA-CGA-O2A
28	T	608	KC2	CAA-CBA-CGA-O2A
28	U	604	KC2	CAA-CBA-CGA-O1A
35	K	614	DGD	O1G-C1G-C2G-O2G
27	b	703	CLA	CBA-CGA-O2A-C1
27	K	602	CLA	C2-C1-O2A-CGA
27	a	821	CLA	C10-C11-C12-C13
27	a	824	CLA	C5-C6-C7-C8
27	b	701	CLA	C5-C6-C7-C8
34	l	401	LHG	O1-C1-C2-O2
27	b	719	CLA	C10-C11-C12-C13
27	G	606	CLA	C11-C12-C13-C15
28	C	210	KC2	CAA-CBA-CGA-O2A
28	T	608	KC2	CAA-CBA-CGA-O1A
27	A	605	CLA	C4-C3-C5-C6
33	K	613	LMG	C10-C11-C12-C13
38	a	836	BCR	C9-C10-C11-C12
32	U	608	PID	C26-C27-O6-C30
27	I	603	CLA	C13-C15-C16-C17
34	j	205	LHG	C7-C8-C9-C10
27	a	807	CLA	C8-C10-C11-C12
37	b	729	PQN	C25-C26-C27-C28
27	F	610	CLA	C2A-CAA-CBA-CGA
27	a	807	CLA	C2A-CAA-CBA-CGA
27	a	818	CLA	C2A-CAA-CBA-CGA
28	H	311	KC2	CAA-CBA-CGA-O1A
27	a	823	CLA	C10-C11-C12-C13
33	b	733	LMG	C10-C11-C12-C13
27	I	603	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	b	704	CLA	C3-C5-C6-C7
29	B	611	UIX	O4-C27-O2-C18
33	l	417	LMG	O6-C5-C6-O5
27	G	606	CLA	C15-C16-C17-C18
27	a	820	CLA	C15-C16-C17-C18
27	a	830	CLA	C8-C10-C11-C12
27	b	718	CLA	C10-C11-C12-C13
27	b	725	CLA	C5-C6-C7-C8
34	F	618	LHG	C9-C10-C11-C12
33	b	733	LMG	C28-C29-C30-C31
27	a	839	CLA	C8-C10-C11-C12
27	a	823	CLA	C3-C5-C6-C7
27	I	601	CLA	C10-C11-C12-C13
27	b	716	CLA	C8-C10-C11-C12
28	H	311	KC2	CAA-CBA-CGA-O2A
27	H	306	CLA	C2C-C3C-CAC-CBC
27	b	703	CLA	C8-C10-C11-C12
27	l	412	CLA	C13-C15-C16-C17
27	l	407	CLA	O2A-C1-C2-C3
27	b	702	CLA	CBD-CGD-O2D-CED
37	b	729	PQN	C15-C16-C17-C18
27	F	606	CLA	C2A-CAA-CBA-CGA
31	H	320	SQD	C24-C23-O48-C46
32	J	615	PID	C26-C27-O6-C30
27	D	607	CLA	C5-C6-C7-C8
27	H	309	CLA	C10-C11-C12-C13
27	a	818	CLA	C5-C6-C7-C8
27	l	406	CLA	C10-C11-C12-C13
27	l	409	CLA	C5-C6-C7-C8
27	K	602	CLA	C5-C6-C7-C8
27	a	804	CLA	C13-C15-C16-C17
37	a	832	PQN	C18-C20-C21-C22
27	T	603	CLA	C4C-C3C-CAC-CBC
27	B	603	CLA	C8-C10-C11-C12
37	b	729	PQN	C18-C20-C21-C22
32	F	615	PID	C28-C27-O6-C30
27	A	605	CLA	C2-C3-C5-C6
27	a	829	CLA	C15-C16-C17-C18
27	b	722	CLA	O2A-C1-C2-C3
27	f	302	CLA	O2A-C1-C2-C3
27	r	203	CLA	O2A-C1-C2-C3
35	f	305	DGD	C2E-C1E-O5D-C6D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	b	706	CLA	C15-C16-C17-C18
35	f	305	DGD	C1B-C2B-C3B-C4B
32	F	615	PID	C26-C27-O6-C30
27	G	606	CLA	C5-C6-C7-C8
27	a	804	CLA	O1A-CGA-O2A-C1
27	H	304	CLA	C3-C5-C6-C7
29	j	204	UIX	C7-C10-C11-C12
30	A	617	DD6	C12-C11-C13-C14
30	B	614	DD6	C12-C11-C13-C14
30	G	613	DD6	C12-C11-C13-C14
30	K	610	DD6	C12-C11-C13-C14
34	G	617	LHG	C2-C3-O3-P
38	a	836	BCR	C11-C12-C13-C35
38	j	203	BCR	C37-C22-C23-C24
38	l	415	BCR	C37-C22-C23-C24
38	m	201	BCR	C37-C22-C23-C24
36	T	613	LMU	C5'-C4'-O1B-C1B
29	j	204	UIX	C7-C10-C11-C13
30	G	613	DD6	C10-C11-C13-C14
30	K	610	DD6	C10-C11-C13-C14
38	a	834	BCR	C11-C12-C13-C14
38	a	836	BCR	C11-C12-C13-C14
38	b	731	BCR	C7-C8-C9-C10
38	l	415	BCR	C21-C22-C23-C24
27	b	703	CLA	O1A-CGA-O2A-C1
31	H	320	SQD	O10-C23-O48-C46
27	T	603	CLA	C2A-CAA-CBA-CGA
27	a	819	CLA	C2A-CAA-CBA-CGA
27	b	712	CLA	C2A-CAA-CBA-CGA
27	b	704	CLA	C5-C6-C7-C8
34	j	205	LHG	O1-C1-C2-C3
34	l	401	LHG	O1-C1-C2-C3
33	C	217	LMG	C7-C8-O7-C10
33	D	618	LMG	C9-C8-O7-C10
34	D	620	LHG	C29-C30-C31-C32
27	B	607	CLA	C3-C5-C6-C7
27	I	610	CLA	C3-C5-C6-C7
27	J	605	CLA	C3-C5-C6-C7
27	a	816	CLA	C3-C5-C6-C7
27	D	611	CLA	C5-C6-C7-C8
28	G	601	KC2	CAA-CBA-CGA-O1A
28	G	601	KC2	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	b	713	CLA	C5-C6-C7-C8
27	l	409	CLA	C10-C11-C12-C13
34	G	617	LHG	C23-C24-C25-C26
27	G	606	CLA	C3-C5-C6-C7
27	F	604	CLA	C4C-C3C-CAC-CBC
37	b	729	PQN	C26-C27-C28-C29
29	A	616	UIX	C17-C18-O2-C27
33	K	613	LMG	C20-C21-C22-C23
35	l	416	DGD	C4B-C5B-C6B-C7B
33	D	618	LMG	C17-C18-C19-C20
34	D	620	LHG	C12-C13-C14-C15
27	a	827	CLA	C5-C6-C7-C8
33	K	613	LMG	C17-C18-C19-C20
31	H	320	SQD	C24-C25-C26-C27
33	D	619	LMG	C21-C22-C23-C24
33	b	733	LMG	C34-C35-C36-C37
33	l	417	LMG	C21-C22-C23-C24
34	G	617	LHG	C10-C11-C12-C13
30	C	214	DD6	C27-C29-C30-C31
30	D	613	DD6	C27-C29-C30-C31
33	D	619	LMG	C11-C12-C13-C14
27	C	201	CLA	C4B-C3B-CAB-CBB
27	D	612	CLA	C4B-C3B-CAB-CBB
27	E	605	CLA	C4B-C3B-CAB-CBB
27	H	306	CLA	C4B-C3B-CAB-CBB
27	K	606	CLA	C4B-C3B-CAB-CBB
27	U	603	CLA	C4B-C3B-CAB-CBB
27	a	814	CLA	C4B-C3B-CAB-CBB
34	r	202	LHG	C23-C24-C25-C26
35	f	305	DGD	C1A-C2A-C3A-C4A
29	F	613	UIX	C17-C18-O2-C27
35	K	614	DGD	C6B-C7B-C8B-C9B
27	D	603	CLA	C6-C7-C8-C9
27	D	603	CLA	C6-C7-C8-C10
27	b	707	CLA	C16-C17-C18-C19
27	F	605	CLA	C2C-C3C-CAC-CBC
33	l	417	LMG	C17-C18-C19-C20
37	a	832	PQN	C20-C21-C22-C23
27	b	706	CLA	C11-C10-C8-C7
27	l	403	CLA	C6-C7-C8-C10
33	D	619	LMG	C22-C23-C24-C25
35	f	305	DGD	C5B-C6B-C7B-C8B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	j	201	DGD	C4A-C5A-C6A-C7A
27	D	603	CLA	C3-C5-C6-C7
27	E	611	CLA	C3-C5-C6-C7
27	A	611	CLA	C3A-C2A-CAA-CBA
27	C	205	CLA	C3A-C2A-CAA-CBA
27	E	605	CLA	C3A-C2A-CAA-CBA
27	F	610	CLA	C3A-C2A-CAA-CBA
27	T	602	CLA	C3A-C2A-CAA-CBA
27	a	805	CLA	C3A-C2A-CAA-CBA
27	a	808	CLA	C3A-C2A-CAA-CBA
27	a	812	CLA	C3A-C2A-CAA-CBA
27	a	821	CLA	C3A-C2A-CAA-CBA
27	b	708	CLA	C3A-C2A-CAA-CBA
34	r	202	LHG	C28-C29-C30-C31
35	K	614	DGD	C4E-C5E-C6E-O5E
34	a	835	LHG	C4-C5-C6-O8
34	a	835	LHG	C24-C25-C26-C27
27	H	308	CLA	C3-C5-C6-C7
33	K	613	LMG	C12-C13-C14-C15
34	r	202	LHG	C24-C25-C26-C27
34	a	835	LHG	C11-C10-C9-C8
27	r	204	CLA	C10-C11-C12-C13
37	b	729	PQN	C26-C27-C28-C30
27	D	612	CLA	C2B-C3B-CAB-CBB
27	E	605	CLA	C2B-C3B-CAB-CBB
27	E	607	CLA	C2B-C3B-CAB-CBB
27	J	601	CLA	C2B-C3B-CAB-CBB
27	b	708	CLA	C2B-C3B-CAB-CBB
27	l	410	CLA	C2B-C3B-CAB-CBB
38	a	836	BCR	C23-C24-C25-C30
38	b	731	BCR	C1-C6-C7-C8
38	f	301	BCR	C1-C6-C7-C8
38	j	203	BCR	C23-C24-C25-C26
38	l	415	BCR	C1-C6-C7-C8
33	l	417	LMG	C13-C14-C15-C16
34	r	202	LHG	C27-C28-C29-C30
34	a	835	LHG	C24-C23-O8-C6
27	l	409	CLA	C3-C5-C6-C7
27	K	602	CLA	C2A-CAA-CBA-CGA
27	F	606	CLA	C13-C15-C16-C17
33	b	733	LMG	C31-C32-C33-C34
34	a	835	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	C	217	LMG	C15-C16-C17-C18
33	D	618	LMG	C13-C14-C15-C16
33	D	619	LMG	C12-C13-C14-C15
33	D	619	LMG	C16-C17-C18-C19
33	F	616	LMG	C23-C24-C25-C26
34	j	205	LHG	C25-C26-C27-C28
34	F	618	LHG	C24-C23-O8-C6
27	C	207	CLA	C11-C10-C8-C9
27	G	608	CLA	C11-C10-C8-C9
27	b	725	CLA	C11-C12-C13-C14
31	y	301	SQD	C10-C11-C12-C13
34	D	620	LHG	C18-C19-C20-C21
33	D	618	LMG	C14-C15-C16-C17
33	b	733	LMG	C19-C20-C21-C22
35	j	201	DGD	CCB-CDB-CEB-CFB
35	l	416	DGD	CEB-CFB-CGB-CHB
35	K	614	DGD	C2E-C1E-O5D-C6D
33	C	217	LMG	C14-C15-C16-C17
31	H	320	SQD	C8-C7-O47-C45
34	D	620	LHG	C8-C7-O7-C5
35	f	305	DGD	O1B-C1B-O2G-C2G
38	l	413	BCR	C17-C18-C19-C20
35	f	305	DGD	C5D-C6D-O5D-C1E
31	y	301	SQD	C25-C26-C27-C28
27	b	702	CLA	C5-C6-C7-C8
27	b	707	CLA	C16-C17-C18-C20
28	A	608	KC2	C2B-C3B-CAB-CBB
28	E	601	KC2	C2B-C3B-CAB-CBB
28	E	601	KC2	C2C-C3C-CAC-CBC
28	F	609	KC2	C2B-C3B-CAB-CBB
28	H	311	KC2	C2B-C3B-CAB-CBB
28	H	311	KC2	C2C-C3C-CAC-CBC
28	J	608	KC2	C2C-C3C-CAC-CBC
28	J	610	KC2	C2B-C3B-CAB-CBB
28	J	610	KC2	C2C-C3C-CAC-CBC
34	r	202	LHG	C9-C10-C11-C12
32	F	614	PID	C26-C27-O6-C30
34	l	401	LHG	C28-C29-C30-C31
35	K	614	DGD	C4B-C5B-C6B-C7B
35	j	201	DGD	C2A-C3A-C4A-C5A
27	J	603	CLA	C5-C6-C7-C8
33	D	618	LMG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	T	613	LMU	O5B-C5B-C6B-O6B
33	b	733	LMG	C35-C36-C37-C38
27	b	705	CLA	C5-C6-C7-C8
27	b	718	CLA	C13-C15-C16-C17
27	l	412	CLA	C10-C11-C12-C13
28	I	604	KC2	C4B-C3B-CAB-CBB
28	U	604	KC2	C4C-C3C-CAC-CBC
27	D	604	CLA	C6-C7-C8-C9
29	A	616	UIX	C19-C18-O2-C27
27	B	606	CLA	C13-C15-C16-C17
27	F	601	CLA	C8-C10-C11-C12
27	a	804	CLA	C10-C11-C12-C13
34	r	202	LHG	C18-C19-C20-C21
35	K	614	DGD	C7B-C8B-C9B-CAB
33	b	733	LMG	C36-C37-C38-C39
35	f	305	DGD	C8B-C9B-CAB-CBB
35	j	201	DGD	O6E-C5E-C6E-O5E
34	l	401	LHG	C11-C10-C9-C8
31	y	301	SQD	C11-C12-C13-C14
31	H	320	SQD	O49-C7-O47-C45
34	D	620	LHG	O9-C7-O7-C5
27	b	717	CLA	C10-C11-C12-C13
27	H	306	CLA	C4C-C3C-CAC-CBC
27	b	713	CLA	C2A-CAA-CBA-CGA
27	b	726	CLA	C2A-CAA-CBA-CGA
27	U	605	CLA	C10-C11-C12-C13
27	b	727	CLA	C8-C10-C11-C12
35	l	416	DGD	C9B-CAB-CBB-CCB
34	F	618	LHG	O1-C1-C2-O2
34	a	835	LHG	O10-C23-O8-C6
34	F	618	LHG	C26-C27-C28-C29
27	A	605	CLA	C1A-C2A-CAA-CBA
27	A	611	CLA	C1A-C2A-CAA-CBA
27	B	601	CLA	C1A-C2A-CAA-CBA
27	C	205	CLA	C1A-C2A-CAA-CBA
27	D	601	CLA	C1A-C2A-CAA-CBA
27	D	612	CLA	C1A-C2A-CAA-CBA
27	F	607	CLA	C1A-C2A-CAA-CBA
27	F	608	CLA	C1A-C2A-CAA-CBA
27	G	607	CLA	C1A-C2A-CAA-CBA
27	H	310	CLA	C1A-C2A-CAA-CBA
27	K	603	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	T	602	CLA	C1A-C2A-CAA-CBA
27	T	607	CLA	C1A-C2A-CAA-CBA
27	a	805	CLA	C1A-C2A-CAA-CBA
27	a	808	CLA	C1A-C2A-CAA-CBA
27	a	813	CLA	C1A-C2A-CAA-CBA
27	a	821	CLA	C1A-C2A-CAA-CBA
27	a	822	CLA	C1A-C2A-CAA-CBA
27	b	717	CLA	C1A-C2A-CAA-CBA
27	b	724	CLA	C1A-C2A-CAA-CBA
27	G	608	CLA	C5-C6-C7-C8
36	T	613	LMU	O5'-C5'-C6'-O6'
33	F	616	LMG	C30-C31-C32-C33
27	H	313	CLA	C3-C5-C6-C7
27	H	319	CLA	C6-C7-C8-C10
27	I	601	CLA	C11-C12-C13-C15
27	U	605	CLA	C11-C10-C8-C7
27	a	823	CLA	C11-C12-C13-C15
27	a	827	CLA	C6-C7-C8-C10
27	l	409	CLA	C11-C12-C13-C15
27	l	412	CLA	C11-C12-C13-C15
34	F	618	LHG	C12-C13-C14-C15
34	G	617	LHG	C11-C10-C9-C8
27	I	611	CLA	C3A-C2A-CAA-CBA
27	a	816	CLA	C4-C3-C5-C6
34	F	618	LHG	O10-C23-O8-C6
33	D	618	LMG	C28-C29-C30-C31
27	B	606	CLA	C2A-CAA-CBA-CGA
27	b	724	CLA	C2A-CAA-CBA-CGA
27	l	406	CLA	C2A-CAA-CBA-CGA
27	H	319	CLA	C6-C7-C8-C9
27	l	412	CLA	C11-C12-C13-C14
34	D	620	LHG	C14-C15-C16-C17
27	I	605	CLA	CBA-CGA-O2A-C1
27	K	605	CLA	CBA-CGA-O2A-C1
31	H	320	SQD	O6-C44-C45-C46
33	l	417	LMG	O1-C7-C8-C9
34	D	620	LHG	C4-C5-C6-O8
34	l	401	LHG	C4-C5-C6-O8
35	f	305	DGD	O1G-C1G-C2G-C3G
27	a	805	CLA	C8-C10-C11-C12
27	b	713	CLA	C8-C10-C11-C12
33	l	417	LMG	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	K	614	DGD	O6E-C5E-C6E-O5E
27	E	606	CLA	C8-C10-C11-C12
27	a	830	CLA	C4-C3-C5-C6
27	a	816	CLA	C2-C3-C5-C6
27	a	830	CLA	C2-C3-C5-C6
38	m	201	BCR	C7-C8-C9-C34
33	K	613	LMG	O6-C5-C6-O5
38	f	301	BCR	C7-C8-C9-C10
38	m	201	BCR	C7-C8-C9-C10
27	K	604	CLA	C2C-C3C-CAC-CBC
27	B	607	CLA	C8-C10-C11-C12
27	a	825	CLA	C15-C16-C17-C18
35	l	416	DGD	CBB-CCB-CDB-CEB
27	H	306	CLA	C2A-CAA-CBA-CGA
27	E	607	CLA	CBA-CGA-O2A-C1
27	K	602	CLA	CBA-CGA-O2A-C1
27	b	724	CLA	O2A-C1-C2-C3
31	H	320	SQD	C44-C45-O47-C7
34	a	835	LHG	C16-C17-C18-C19
34	r	202	LHG	C31-C32-C33-C34
27	l	406	CLA	C8-C10-C11-C12
38	f	301	BCR	C9-C10-C11-C12
37	b	729	PQN	C13-C15-C16-C17
34	l	401	LHG	C18-C19-C20-C21
33	K	613	LMG	C24-C25-C26-C27
27	D	602	CLA	C6-C7-C8-C10
31	H	320	SQD	C25-C26-C27-C28
34	a	835	LHG	O7-C5-C6-O8
34	D	620	LHG	C19-C20-C21-C22
31	H	320	SQD	C27-C28-C29-C30
34	r	202	LHG	C11-C10-C9-C8
35	f	305	DGD	CDB-CEB-CFB-CGB
27	H	304	CLA	C8-C10-C11-C12
27	U	603	CLA	C2-C1-O2A-CGA
35	j	201	DGD	CFB-CGB-CHB-CIB
27	b	717	CLA	CBA-CGA-O2A-C1
34	j	205	LHG	C13-C14-C15-C16
33	l	417	LMG	C10-C11-C12-C13
27	B	606	CLA	C5-C6-C7-C8
27	E	604	CLA	C4-C3-C5-C6
27	F	606	CLA	C4-C3-C5-C6
35	f	305	DGD	C2A-C1A-O1G-C1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	F	618	LHG	C24-C25-C26-C27
30	B	614	DD6	C27-C29-C30-C31
30	E	613	DD6	C27-C29-C30-C31
30	G	616	DD6	C27-C29-C30-C31
30	I	613	DD6	C27-C29-C30-C31
30	K	610	DD6	C27-C29-C30-C31
34	G	617	LHG	O1-C1-C2-O2
27	B	603	CLA	C14-C13-C15-C16
27	I	601	CLA	C11-C12-C13-C14
27	U	605	CLA	C11-C10-C8-C9
27	a	823	CLA	C11-C12-C13-C14
27	l	403	CLA	C6-C7-C8-C9
37	b	729	PQN	C24-C23-C25-C26
33	F	616	LMG	C18-C19-C20-C21
27	b	706	CLA	C10-C11-C12-C13
27	D	607	CLA	C4B-C3B-CAB-CBB
27	E	607	CLA	C4B-C3B-CAB-CBB
27	E	609	CLA	C4B-C3B-CAB-CBB
27	F	606	CLA	C4B-C3B-CAB-CBB
27	G	604	CLA	C4B-C3B-CAB-CBB
27	I	602	CLA	C4B-C3B-CAB-CBB
27	J	607	CLA	C4B-C3B-CAB-CBB
27	K	608	CLA	C4B-C3B-CAB-CBB
27	T	607	CLA	C4B-C3B-CAB-CBB
27	U	606	CLA	C4B-C3B-CAB-CBB
27	a	821	CLA	C4B-C3B-CAB-CBB
27	b	705	CLA	C4B-C3B-CAB-CBB
27	b	707	CLA	C4B-C3B-CAB-CBB
33	l	417	LMG	C29-C30-C31-C32
35	K	614	DGD	C3B-C4B-C5B-C6B
35	l	416	DGD	C3B-C4B-C5B-C6B
31	A	618	SQD	C2-C1-O6-C44
34	G	617	LHG	O6-C4-C5-C6
34	r	202	LHG	O6-C4-C5-C6
34	l	401	LHG	C19-C20-C21-C22
35	l	416	DGD	C4A-C5A-C6A-C7A
27	B	603	CLA	C12-C13-C15-C16
27	B	606	CLA	C12-C13-C15-C16
27	H	319	CLA	C12-C13-C15-C16
27	a	804	CLA	C6-C7-C8-C10
27	a	820	CLA	C6-C7-C8-C10
27	a	824	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	829	CLA	C12-C13-C15-C16
27	b	701	CLA	C11-C12-C13-C15
27	b	723	CLA	C11-C10-C8-C7
27	b	727	CLA	C11-C12-C13-C15
27	b	728	CLA	C12-C13-C15-C16
37	a	832	PQN	C21-C22-C23-C25
27	F	605	CLA	C4C-C3C-CAC-CBC
33	b	733	LMG	C14-C15-C16-C17
27	A	610	CLA	C3A-C2A-CAA-CBA
27	F	603	CLA	C4-C3-C5-C6
27	F	605	CLA	C3A-C2A-CAA-CBA
27	K	608	CLA	C3A-C2A-CAA-CBA
27	a	807	CLA	C3A-C2A-CAA-CBA
27	b	725	CLA	C4-C3-C5-C6
27	l	412	CLA	C3A-C2A-CAA-CBA
27	a	821	CLA	C8-C10-C11-C12
27	b	715	CLA	C5-C6-C7-C8
27	E	604	CLA	C2-C3-C5-C6
27	F	603	CLA	C2-C3-C5-C6
27	H	305	CLA	C5-C6-C7-C8
38	b	731	BCR	C9-C10-C11-C12
38	m	201	BCR	C9-C10-C11-C12
38	f	301	BCR	C7-C8-C9-C34
35	l	416	DGD	O1A-C1A-O1G-C1G
33	D	618	LMG	C12-C13-C14-C15
35	K	614	DGD	C2A-C3A-C4A-C5A
27	a	811	CLA	O2A-C1-C2-C3
31	A	618	SQD	C44-C45-C46-O48
33	D	618	LMG	O1-C7-C8-C9
33	D	619	LMG	O1-C7-C8-C9
33	K	613	LMG	C7-C8-C9-O8
34	G	617	LHG	C4-C5-C6-O8
34	r	202	LHG	C4-C5-C6-O8
35	K	614	DGD	O1G-C1G-C2G-C3G
27	a	823	CLA	C8-C10-C11-C12
33	F	616	LMG	C31-C32-C33-C34
34	j	205	LHG	C11-C10-C9-C8
27	a	829	CLA	C4-C3-C5-C6
27	F	606	CLA	C2-C3-C5-C6
27	b	725	CLA	C2-C3-C5-C6
27	J	609	CLA	C2C-C3C-CAC-CBC
27	b	705	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	a	834	BCR	C1-C6-C7-C8
38	a	836	BCR	C1-C6-C7-C8
38	f	301	BCR	C5-C6-C7-C8
38	i	201	BCR	C23-C24-C25-C26
32	K	611	PID	C28-C27-O6-C30
27	I	605	CLA	C3-C5-C6-C7
27	b	715	CLA	C8-C10-C11-C12
34	l	401	LHG	C12-C13-C14-C15
27	I	602	CLA	C2A-CAA-CBA-CGA
33	D	618	LMG	O1-C7-C8-O7
33	D	619	LMG	O1-C7-C8-O7
33	b	733	LMG	O1-C7-C8-O7
35	j	201	DGD	O1G-C1G-C2G-O2G
34	G	617	LHG	C14-C15-C16-C17
27	B	606	CLA	C14-C13-C15-C16
27	H	313	CLA	C6-C7-C8-C9
27	a	819	CLA	C11-C10-C8-C9
27	a	820	CLA	C6-C7-C8-C9
27	a	824	CLA	C11-C12-C13-C14
27	b	727	CLA	C11-C12-C13-C14
27	b	728	CLA	C14-C13-C15-C16
31	A	618	SQD	O5-C1-O6-C44
27	E	606	CLA	C5-C6-C7-C8
27	D	604	CLA	C6-C7-C8-C10
27	U	603	CLA	O1D-CGD-O2D-CED
27	b	714	CLA	O2A-C1-C2-C3
33	l	417	LMG	C18-C19-C20-C21
27	H	312	CLA	C1A-C2A-CAA-CBA
35	K	614	DGD	O6D-C5D-C6D-O5D
33	C	217	LMG	C11-C12-C13-C14
27	F	606	CLA	CBA-CGA-O2A-C1
27	a	828	CLA	CAA-CBA-CGA-O2A
33	b	733	LMG	C4-C5-C6-O5
27	K	605	CLA	O1A-CGA-O2A-C1
35	l	416	DGD	CFB-CGB-CHB-CIB
27	E	607	CLA	C12-C13-C15-C16
27	a	815	CLA	C6-C7-C8-C10
27	a	821	CLA	C11-C10-C8-C7
27	b	727	CLA	C6-C7-C8-C10
27	l	409	CLA	C11-C10-C8-C7
38	j	203	BCR	C21-C22-C23-C24
29	T	612	UIX	C19-C18-O2-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	H	320	SQD	C7-C8-C9-C10
27	H	305	CLA	C4-C3-C5-C6
27	I	605	CLA	O1A-CGA-O2A-C1
35	f	305	DGD	O1A-C1A-O1G-C1G
28	E	610	KC2	C2C-C3C-CAC-CBC
28	F	609	KC2	C2C-C3C-CAC-CBC
28	H	302	KC2	C2C-C3C-CAC-CBC
28	K	607	KC2	C2C-C3C-CAC-CBC
28	U	604	KC2	C2B-C3B-CAB-CBB
33	l	417	LMG	C34-C35-C36-C37
27	I	610	CLA	O2A-C1-C2-C3
33	l	417	LMG	C9-C8-O7-C10
27	D	602	CLA	C6-C7-C8-C9
27	D	611	CLA	C11-C12-C13-C14
27	K	602	CLA	O1A-CGA-O2A-C1
27	b	706	CLA	C5-C6-C7-C8
34	G	617	LHG	O6-C4-C5-O7
33	b	733	LMG	C23-C24-C25-C26
28	A	608	KC2	C4B-C3B-CAB-CBB
28	E	610	KC2	C4C-C3C-CAC-CBC
28	G	601	KC2	C4B-C3B-CAB-CBB
28	H	302	KC2	C4B-C3B-CAB-CBB
28	H	311	KC2	C4C-C3C-CAC-CBC
28	J	608	KC2	C4C-C3C-CAC-CBC
28	K	607	KC2	C4C-C3C-CAC-CBC
28	U	602	KC2	C4B-C3B-CAB-CBB
34	a	835	LHG	C31-C32-C33-C34
27	I	608	CLA	C4-C3-C5-C6
33	K	613	LMG	C15-C16-C17-C18
27	E	607	CLA	O1A-CGA-O2A-C1
33	D	619	LMG	C30-C31-C32-C33
31	A	618	SQD	O47-C45-C46-O48
27	I	616	CLA	C11-C12-C13-C14
27	a	820	CLA	C14-C13-C15-C16
27	a	823	CLA	C6-C7-C8-C9
27	b	723	CLA	C11-C10-C8-C9
34	a	835	LHG	C15-C16-C17-C18
35	j	201	DGD	C6B-C7B-C8B-C9B
33	D	619	LMG	C31-C32-C33-C34
33	l	417	LMG	C12-C13-C14-C15
29	T	612	UIX	C17-C18-O2-C27
27	H	304	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	b	728	CLA	C2-C1-O2A-CGA
27	a	813	CLA	O2A-C1-C2-C3
27	a	829	CLA	C16-C17-C18-C19
27	H	319	CLA	C15-C16-C17-C18
33	b	733	LMG	C20-C21-C22-C23
27	B	607	CLA	C4-C3-C5-C6
27	a	819	CLA	C4-C3-C5-C6
27	b	726	CLA	C4-C3-C5-C6
35	K	614	DGD	C1B-C2B-C3B-C4B
27	a	829	CLA	C2-C3-C5-C6
27	J	605	CLA	C5-C6-C7-C8
27	B	603	CLA	C2A-CAA-CBA-CGA
27	b	716	CLA	C16-C17-C18-C20
33	b	733	LMG	C13-C14-C15-C16
30	r	206	DD6	C27-C29-C30-C31
27	I	602	CLA	C3-C5-C6-C7
27	A	607	CLA	C4B-C3B-CAB-CBB
27	A	610	CLA	C4B-C3B-CAB-CBB
27	C	202	CLA	C4B-C3B-CAB-CBB
27	C	212	CLA	C4B-C3B-CAB-CBB
27	D	601	CLA	C4B-C3B-CAB-CBB
27	D	605	CLA	C4B-C3B-CAB-CBB
27	E	605	CLA	C1A-C2A-CAA-CBA
27	E	612	CLA	C4B-C3B-CAB-CBB
27	F	608	CLA	C4B-C3B-CAB-CBB
27	G	609	CLA	C4B-C3B-CAB-CBB
27	G	610	CLA	C4B-C3B-CAB-CBB
27	H	307	CLA	C4B-C3B-CAB-CBB
27	H	319	CLA	C4B-C3B-CAB-CBB
27	K	603	CLA	C4B-C3B-CAB-CBB
27	U	606	CLA	C1A-C2A-CAA-CBA
27	a	825	CLA	C4B-C3B-CAB-CBB
27	b	707	CLA	C1A-C2A-CAA-CBA
27	r	204	CLA	C4B-C3B-CAB-CBB
27	F	617	CLA	C4-C3-C5-C6
27	b	706	CLA	C4-C3-C5-C6
27	b	711	CLA	C4-C3-C5-C6
30	B	614	DD6	C10-C11-C13-C14
27	r	204	CLA	C5-C6-C7-C8
34	D	620	LHG	O6-C4-C5-C6
34	l	401	LHG	C26-C27-C28-C29
27	F	606	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	807	CLA	C6-C7-C8-C10
27	b	719	CLA	C11-C12-C13-C15
27	l	405	CLA	C6-C7-C8-C10
34	j	205	LHG	C27-C28-C29-C30
27	E	607	CLA	C4-C3-C5-C6
27	b	718	CLA	C3A-C2A-CAA-CBA
34	D	620	LHG	O6-C4-C5-O7
34	r	202	LHG	O6-C4-C5-O7
27	b	719	CLA	C3-C5-C6-C7
27	E	607	CLA	C14-C13-C15-C16
27	F	606	CLA	C11-C10-C8-C9
27	a	829	CLA	C11-C12-C13-C14
27	b	701	CLA	C11-C12-C13-C14
27	b	724	CLA	C11-C12-C13-C14
27	b	727	CLA	C6-C7-C8-C9
27	l	409	CLA	C11-C10-C8-C9
35	j	201	DGD	C3A-C4A-C5A-C6A
28	E	601	KC2	C1A-C2A-CAA-CBA
28	E	601	KC2	C3A-C2A-CAA-CBA
28	H	311	KC2	C3A-C2A-CAA-CBA
28	J	602	KC2	C1A-C2A-CAA-CBA
28	J	604	KC2	C1A-C2A-CAA-CBA
28	J	606	KC2	C3A-C2A-CAA-CBA
27	K	604	CLA	C4C-C3C-CAC-CBC
31	H	320	SQD	O6-C44-C45-O47
34	G	617	LHG	O7-C5-C6-O8
34	l	401	LHG	O7-C5-C6-O8
34	D	620	LHG	C1-C2-C3-O3
27	a	828	CLA	O2A-C1-C2-C3
34	a	835	LHG	C27-C28-C29-C30
28	J	608	KC2	CAA-CBA-CGA-O2A
33	b	733	LMG	C22-C23-C24-C25
33	b	733	LMG	O1-C7-C8-C9
35	j	201	DGD	O1G-C1G-C2G-C3G
35	l	416	DGD	O1G-C1G-C2G-C3G
27	a	817	CLA	C4-C3-C5-C6
27	B	607	CLA	C2-C3-C5-C6
27	a	801	CLA	CBD-CGD-O2D-CED
27	B	603	CLA	CAD-CBD-CGD-O2D
27	B	610	CLA	CAD-CBD-CGD-O2D
27	C	205	CLA	CAD-CBD-CGD-O2D
27	D	604	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	F	610	CLA	CAD-CBD-CGD-O2D
27	H	305	CLA	CAD-CBD-CGD-O2D
27	H	312	CLA	CAD-CBD-CGD-O2D
27	I	603	CLA	CAD-CBD-CGD-O2D
27	K	603	CLA	CAD-CBD-CGD-O2D
27	T	601	CLA	CAD-CBD-CGD-O2D
27	b	704	CLA	CAD-CBD-CGD-O2D
27	l	407	CLA	CAD-CBD-CGD-O2D
28	E	610	KC2	CAD-CBD-CGD-O2D
27	l	405	CLA	C10-C11-C12-C13
27	b	717	CLA	O1A-CGA-O2A-C1
27	H	304	CLA	CBA-CGA-O2A-C1
33	b	733	LMG	C38-C39-C40-C41
27	a	823	CLA	C5-C6-C7-C8
27	U	601	CLA	C2A-CAA-CBA-CGA
27	A	611	CLA	CHA-CBD-CGD-O1D
27	B	603	CLA	CAD-CBD-CGD-O1D
27	B	610	CLA	CAD-CBD-CGD-O1D
27	C	201	CLA	CAD-CBD-CGD-O1D
27	C	205	CLA	CAD-CBD-CGD-O1D
27	D	604	CLA	CAD-CBD-CGD-O1D
27	F	610	CLA	CAD-CBD-CGD-O1D
27	H	305	CLA	CAD-CBD-CGD-O1D
27	H	312	CLA	CAD-CBD-CGD-O1D
27	I	603	CLA	CAD-CBD-CGD-O1D
27	J	609	CLA	CAD-CBD-CGD-O1D
27	K	603	CLA	CAD-CBD-CGD-O1D
27	T	601	CLA	CAD-CBD-CGD-O1D
27	a	810	CLA	CHA-CBD-CGD-O1D
27	a	810	CLA	CHA-CBD-CGD-O2D
27	a	823	CLA	CAD-CBD-CGD-O1D
27	b	704	CLA	CAD-CBD-CGD-O1D
27	b	720	CLA	CHA-CBD-CGD-O1D
27	b	720	CLA	CHA-CBD-CGD-O2D
27	b	723	CLA	CHA-CBD-CGD-O1D
27	l	407	CLA	CAD-CBD-CGD-O1D
27	l	411	CLA	CHA-CBD-CGD-O1D
27	l	411	CLA	CHA-CBD-CGD-O2D
28	B	602	KC2	CHA-CBD-CGD-O2D
28	E	610	KC2	CAD-CBD-CGD-O1D
28	H	311	KC2	CHA-CBD-CGD-O1D
28	H	311	KC2	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	J	606	KC2	CHA-CBD-CGD-O1D
28	J	606	KC2	CHA-CBD-CGD-O2D
28	J	610	KC2	CHA-CBD-CGD-O1D
28	J	610	KC2	CHA-CBD-CGD-O2D
28	K	607	KC2	CHA-CBD-CGD-O1D
34	D	620	LHG	C4-O6-P-O4
34	F	618	LHG	C4-O6-P-O5
34	G	617	LHG	C3-O3-P-O5
34	l	401	LHG	C4-O6-P-O3
34	l	401	LHG	C4-O6-P-O5
38	a	836	BCR	C13-C14-C15-C16
38	j	203	BCR	C15-C16-C17-C18
28	J	608	KC2	CAA-CBA-CGA-O1A
27	D	604	CLA	C4-C3-C5-C6
27	b	704	CLA	C4-C3-C5-C6
27	C	201	CLA	C2B-C3B-CAB-CBB
27	C	212	CLA	C2B-C3B-CAB-CBB
27	G	604	CLA	C2B-C3B-CAB-CBB
27	G	610	CLA	C2B-C3B-CAB-CBB
27	H	306	CLA	C2B-C3B-CAB-CBB
27	K	606	CLA	C2B-C3B-CAB-CBB
27	U	603	CLA	C2B-C3B-CAB-CBB
27	a	814	CLA	C2B-C3B-CAB-CBB
27	a	825	CLA	C2B-C3B-CAB-CBB
27	D	604	CLA	C2-C3-C5-C6
27	I	608	CLA	C2-C3-C5-C6
27	b	726	CLA	C2-C3-C5-C6
35	j	201	DGD	O6D-C5D-C6D-O5D
27	b	728	CLA	C13-C15-C16-C17
34	j	205	LHG	C2-C3-O3-P
27	C	203	CLA	C16-C17-C18-C20
27	G	608	CLA	C11-C12-C13-C15
28	F	609	KC2	CAA-CBA-CGA-O1A
28	F	609	KC2	CAA-CBA-CGA-O2A
29	H	317	UIX	C17-C18-O2-C27
33	D	618	LMG	C16-C17-C18-C19
34	a	835	LHG	O1-C1-C2-C3
27	b	709	CLA	C10-C11-C12-C13
38	a	834	BCR	C9-C10-C11-C12
38	a	836	BCR	C19-C20-C21-C22
27	b	704	CLA	C15-C16-C17-C18
33	l	417	LMG	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	l	402	CLA	C10-C11-C12-C13
27	C	207	CLA	C6-C7-C8-C9
27	a	829	CLA	C11-C10-C8-C9
27	a	830	CLA	C11-C10-C8-C9
27	a	830	CLA	C14-C13-C15-C16
27	b	706	CLA	C11-C10-C8-C9
27	a	825	CLA	C11-C12-C13-C15
34	a	835	LHG	C25-C26-C27-C28
27	G	602	CLA	C6-C7-C8-C9
27	G	602	CLA	C6-C7-C8-C10
27	a	829	CLA	C16-C17-C18-C20
27	H	305	CLA	CBA-CGA-O2A-C1
33	b	733	LMG	C17-C18-C19-C20
27	C	207	CLA	C4-C3-C5-C6
27	C	203	CLA	C16-C17-C18-C19
27	D	611	CLA	C11-C12-C13-C15
34	a	835	LHG	C18-C19-C20-C21
38	l	414	BCR	C15-C16-C17-C18
27	b	727	CLA	CAA-CBA-CGA-O2A
27	l	409	CLA	C4-C3-C5-C6
27	E	607	CLA	C13-C15-C16-C17
33	D	619	LMG	C13-C14-C15-C16
27	b	728	CLA	C15-C16-C17-C18
27	F	605	CLA	C2A-CAA-CBA-CGA
33	K	613	LMG	C22-C23-C24-C25
34	a	835	LHG	C13-C14-C15-C16
35	K	614	DGD	O6E-C1E-O5D-C6D
34	D	620	LHG	O2-C2-C3-O3
34	l	401	LHG	O2-C2-C3-O3
27	C	207	CLA	C2-C3-C5-C6
27	E	607	CLA	C2-C3-C5-C6
27	F	617	CLA	C2-C3-C5-C6
27	b	706	CLA	C2-C3-C5-C6
27	U	603	CLA	C2C-C3C-CAC-CBC
29	H	317	UIX	C19-C18-O2-C27
30	J	612	DD6	C27-C29-C30-C31
34	l	401	LHG	C1-C2-C3-O3
27	F	602	CLA	CAA-CBA-CGA-O2A
27	U	603	CLA	CBA-CGA-O2A-C1
27	b	702	CLA	C13-C15-C16-C17
27	B	601	CLA	C4B-C3B-CAB-CBB
27	I	605	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	816	CLA	C4B-C3B-CAB-CBB
27	a	827	CLA	C4B-C3B-CAB-CBB
31	y	301	SQD	C28-C29-C30-C31
27	F	606	CLA	O1A-CGA-O2A-C1
27	b	701	CLA	C3-C5-C6-C7
35	j	201	DGD	O1A-C1A-O1G-C1G
27	B	605	CLA	C2A-CAA-CBA-CGA
27	a	837	CLA	C4-C3-C5-C6
27	a	813	CLA	CAA-CBA-CGA-O2A
27	H	305	CLA	C2-C3-C5-C6
27	a	817	CLA	C2-C3-C5-C6
34	F	618	LHG	O6-C4-C5-O7
28	E	601	KC2	C4B-C3B-CAB-CBB
28	E	601	KC2	C4C-C3C-CAC-CBC
28	F	609	KC2	C4B-C3B-CAB-CBB
28	H	302	KC2	C4C-C3C-CAC-CBC
28	H	311	KC2	C4B-C3B-CAB-CBB
28	J	610	KC2	C4B-C3B-CAB-CBB
28	J	610	KC2	C4C-C3C-CAC-CBC
28	T	608	KC2	C4B-C3B-CAB-CBB
27	b	719	CLA	C8-C10-C11-C12
34	r	202	LHG	C11-C12-C13-C14
27	a	801	CLA	C5-C6-C7-C8
34	l	401	LHG	C10-C11-C12-C13
33	C	217	LMG	O7-C8-C9-O8
34	F	618	LHG	O7-C5-C6-O8
35	l	416	DGD	O1G-C1G-C2G-O2G
27	A	604	CLA	C3A-C2A-CAA-CBA
27	A	612	CLA	C3A-C2A-CAA-CBA
27	B	603	CLA	C3A-C2A-CAA-CBA
27	F	602	CLA	C3A-C2A-CAA-CBA
27	H	304	CLA	C4-C3-C5-C6
27	H	305	CLA	C3A-C2A-CAA-CBA
27	a	805	CLA	C4-C3-C5-C6
27	a	827	CLA	C3A-C2A-CAA-CBA
27	a	828	CLA	C3A-C2A-CAA-CBA
27	b	710	CLA	C3A-C2A-CAA-CBA
27	b	714	CLA	C3A-C2A-CAA-CBA
27	b	727	CLA	C3A-C2A-CAA-CBA
27	a	819	CLA	C2-C3-C5-C6
27	b	711	CLA	C2-C3-C5-C6
27	b	705	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	f	304	BCR	C35-C13-C14-C15
38	l	415	BCR	C11-C10-C9-C34
27	l	410	CLA	C2-C1-O2A-CGA
38	l	414	BCR	C19-C20-C21-C22
34	F	618	LHG	C28-C29-C30-C31
38	b	731	BCR	C36-C18-C19-C20
27	l	412	CLA	C4-C3-C5-C6
27	H	304	CLA	CAA-CBA-CGA-O2A
27	b	704	CLA	C2-C3-C5-C6
27	B	601	CLA	C2A-CAA-CBA-CGA
28	E	610	KC2	CAA-CBA-CGA-O1A
27	b	718	CLA	C8-C10-C11-C12
27	F	604	CLA	CAA-CBA-CGA-O2A
27	B	601	CLA	C6-C7-C8-C9
27	C	204	CLA	C6-C7-C8-C9
27	a	807	CLA	C6-C7-C8-C9
27	b	715	CLA	C14-C13-C15-C16
27	J	609	CLA	C4C-C3C-CAC-CBC
27	B	605	CLA	CAA-CBA-CGA-O1A
33	b	733	LMG	C9-C8-O7-C10
34	F	618	LHG	C4-C5-O7-C7
27	a	837	CLA	C2-C3-C5-C6
27	l	409	CLA	C2-C3-C5-C6
27	B	605	CLA	CAA-CBA-CGA-O2A
27	I	606	CLA	C2A-CAA-CBA-CGA
27	A	609	CLA	C1A-C2A-CAA-CBA
27	A	610	CLA	C1A-C2A-CAA-CBA
27	I	601	CLA	C1A-C2A-CAA-CBA
27	a	814	CLA	C1A-C2A-CAA-CBA
27	l	412	CLA	C1A-C2A-CAA-CBA
38	f	304	BCR	C12-C13-C14-C15
38	l	415	BCR	C11-C10-C9-C8
27	E	605	CLA	CAA-CBA-CGA-O2A
27	H	303	CLA	C5-C6-C7-C8
27	A	607	CLA	C2B-C3B-CAB-CBB
27	A	610	CLA	C2B-C3B-CAB-CBB
27	C	202	CLA	C2B-C3B-CAB-CBB
27	D	601	CLA	C2B-C3B-CAB-CBB
27	D	605	CLA	C2B-C3B-CAB-CBB
27	E	609	CLA	C2B-C3B-CAB-CBB
27	E	612	CLA	C2B-C3B-CAB-CBB
27	F	606	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	F	608	CLA	C2B-C3B-CAB-CBB
27	G	609	CLA	C2B-C3B-CAB-CBB
27	H	309	CLA	C2B-C3B-CAB-CBB
27	H	319	CLA	C2B-C3B-CAB-CBB
27	I	605	CLA	C2B-C3B-CAB-CBB
27	J	603	CLA	C2B-C3B-CAB-CBB
27	J	607	CLA	C2B-C3B-CAB-CBB
27	K	603	CLA	C2B-C3B-CAB-CBB
27	T	607	CLA	C2B-C3B-CAB-CBB
27	U	606	CLA	C2B-C3B-CAB-CBB
27	a	816	CLA	C2B-C3B-CAB-CBB
27	a	821	CLA	C2B-C3B-CAB-CBB
27	a	827	CLA	C2B-C3B-CAB-CBB
27	a	830	CLA	C2B-C3B-CAB-CBB
27	b	707	CLA	C2B-C3B-CAB-CBB
27	r	204	CLA	C2B-C3B-CAB-CBB
38	a	834	BCR	C5-C6-C7-C8
38	a	836	BCR	C5-C6-C7-C8
38	f	304	BCR	C23-C24-C25-C30
38	j	203	BCR	C1-C6-C7-C8
38	j	203	BCR	C23-C24-C25-C30
38	l	413	BCR	C23-C24-C25-C30
38	l	414	BCR	C5-C6-C7-C8
38	m	201	BCR	C5-C6-C7-C8
27	b	702	CLA	CBA-CGA-O2A-C1
33	K	613	LMG	C19-C20-C21-C22
34	D	620	LHG	C11-C12-C13-C14
34	j	205	LHG	C28-C29-C30-C31
27	E	605	CLA	CAA-CBA-CGA-O1A
27	E	606	CLA	C4-C3-C5-C6
27	G	606	CLA	C4-C3-C5-C6
27	H	308	CLA	C4-C3-C5-C6
27	a	815	CLA	C4-C3-C5-C6
27	a	805	CLA	C2-C3-C5-C6
27	l	412	CLA	C2-C3-C5-C6
27	B	609	CLA	C11-C12-C13-C15
27	F	606	CLA	C11-C10-C8-C7
27	K	605	CLA	C11-C10-C8-C7
27	a	816	CLA	C6-C7-C8-C10
27	a	829	CLA	C11-C12-C13-C15
27	a	830	CLA	C11-C10-C8-C7
27	b	708	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	j	205	LHG	C10-C11-C12-C13
27	F	617	CLA	C11-C12-C13-C15
27	G	607	CLA	C2A-CAA-CBA-CGA
27	I	603	CLA	C2A-CAA-CBA-CGA
27	a	837	CLA	C2A-CAA-CBA-CGA
27	b	701	CLA	C2A-CAA-CBA-CGA
27	b	704	CLA	C2A-CAA-CBA-CGA
34	l	401	LHG	C23-C24-C25-C26
33	b	733	LMG	C37-C38-C39-C40
35	l	416	DGD	C1A-C2A-C3A-C4A
27	b	718	CLA	C15-C16-C17-C18
27	B	603	CLA	C16-C17-C18-C20
33	D	619	LMG	C17-C18-C19-C20
27	H	309	CLA	C4-C3-C5-C6
27	U	605	CLA	C4-C3-C5-C6
27	b	723	CLA	C4-C3-C5-C6
27	b	727	CLA	C4-C3-C5-C6
33	D	618	LMG	C15-C16-C17-C18
27	B	606	CLA	CAA-CBA-CGA-O2A
27	U	605	CLA	C2-C3-C5-C6
27	F	606	CLA	C2-C1-O2A-CGA
27	l	409	CLA	C4C-C3C-CAC-CBC
27	b	718	CLA	C11-C10-C8-C9
27	F	604	CLA	CAA-CBA-CGA-O1A
27	H	307	CLA	CAA-CBA-CGA-O2A
28	E	610	KC2	CAA-CBA-CGA-O2A
27	B	609	CLA	C4-C3-C5-C6
27	J	605	CLA	C4-C3-C5-C6
27	b	715	CLA	C4-C3-C5-C6
27	l	402	CLA	C4-C3-C5-C6
37	b	729	PQN	C14-C13-C15-C16
27	b	713	CLA	C15-C16-C17-C18
33	F	616	LMG	C15-C16-C17-C18
34	l	401	LHG	C30-C31-C32-C33
27	H	304	CLA	C2-C3-C5-C6
34	F	618	LHG	C4-C5-C6-O8
27	H	305	CLA	O1A-CGA-O2A-C1
27	b	710	CLA	C2A-CAA-CBA-CGA
27	b	701	CLA	C8-C10-C11-C12
30	A	614	DD6	C27-C29-C30-C31
30	E	615	DD6	C27-C29-C30-C31
30	F	611	DD6	C27-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	H	301	DD6	C27-C29-C30-C31
27	l	409	CLA	C2C-C3C-CAC-CBC
27	H	307	CLA	CAA-CBA-CGA-O1A
27	U	606	CLA	CAA-CBA-CGA-O2A
27	l	408	CLA	C2-C1-O2A-CGA
27	F	617	CLA	C4B-C3B-CAB-CBB
27	J	603	CLA	C4B-C3B-CAB-CBB
27	a	812	CLA	C4B-C3B-CAB-CBB
27	a	813	CLA	C4B-C3B-CAB-CBB
27	a	830	CLA	C4B-C3B-CAB-CBB
27	r	203	CLA	C4B-C3B-CAB-CBB
27	H	304	CLA	O1A-CGA-O2A-C1
27	I	609	CLA	CAA-CBA-CGA-O2A
27	a	801	CLA	CAA-CBA-CGA-O2A
27	T	602	CLA	CAA-CBA-CGA-O2A
27	U	606	CLA	CAA-CBA-CGA-O1A
27	a	827	CLA	C16-C17-C18-C19
35	f	305	DGD	C2B-C3B-C4B-C5B
34	F	618	LHG	O6-C4-C5-C6
27	a	828	CLA	CAA-CBA-CGA-O1A
27	E	609	CLA	CAA-CBA-CGA-O1A
34	l	401	LHG	C16-C17-C18-C19
27	E	611	CLA	C10-C11-C12-C13
27	T	602	CLA	CAA-CBA-CGA-O1A
27	T	607	CLA	CAA-CBA-CGA-O2A
27	b	702	CLA	C14-C13-C15-C16
27	b	705	CLA	C11-C10-C8-C9
27	r	204	CLA	C6-C7-C8-C9
27	B	610	CLA	C2C-C3C-CAC-CBC
27	D	604	CLA	C2A-CAA-CBA-CGA
27	b	728	CLA	C2A-CAA-CBA-CGA
27	F	617	CLA	C2-C1-O2A-CGA
27	H	305	CLA	C2-C1-O2A-CGA
27	a	815	CLA	C2-C1-O2A-CGA
27	a	839	CLA	C2-C1-O2A-CGA
27	b	709	CLA	C2-C1-O2A-CGA
33	D	619	LMG	C28-C29-C30-C31
27	a	829	CLA	C3A-C2A-CAA-CBA
27	b	722	CLA	C3A-C2A-CAA-CBA
27	l	410	CLA	C3A-C2A-CAA-CBA
27	E	609	CLA	CAA-CBA-CGA-O2A
27	b	715	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	l	402	CLA	C2-C3-C5-C6
28	B	602	KC2	C2C-C3C-CAC-CBC
28	J	602	KC2	C2B-C3B-CAB-CBB
27	a	822	CLA	O2A-C1-C2-C3
27	b	701	CLA	O2A-C1-C2-C3
27	D	611	CLA	C10-C11-C12-C13
27	F	607	CLA	CAA-CBA-CGA-O2A
27	r	204	CLA	CBA-CGA-O2A-C1
29	A	616	UIX	O-C-C7-C10
30	C	216	DD6	C13-C14-C15-O1
30	H	301	DD6	C13-C14-C15-O1
30	T	611	DD6	C13-C14-C15-O1
30	i	202	DD6	C13-C14-C15-O1
32	F	614	PID	O1-C6-C7-C8
32	K	611	PID	O1-C6-C7-C8
27	I	609	CLA	CAA-CBA-CGA-O1A
33	l	417	LMG	C33-C34-C35-C36
34	j	205	LHG	C24-C25-C26-C27
35	K	614	DGD	C1G-C2G-C3G-O3G
27	U	603	CLA	O1A-CGA-O2A-C1
27	D	602	CLA	C5-C6-C7-C8
28	B	602	KC2	C4C-C3C-CAC-CBC
28	F	609	KC2	C4C-C3C-CAC-CBC
28	T	608	KC2	C4C-C3C-CAC-CBC
28	U	604	KC2	C4B-C3B-CAB-CBB
27	T	607	CLA	CAA-CBA-CGA-O1A
35	l	416	DGD	C2A-C3A-C4A-C5A
27	a	825	CLA	C2A-CAA-CBA-CGA
34	G	617	LHG	C24-C25-C26-C27
27	K	605	CLA	C5-C6-C7-C8
27	b	711	CLA	CAA-CBA-CGA-O2A
35	K	614	DGD	O2G-C2G-C3G-O3G
27	b	717	CLA	C14-C13-C15-C16
27	b	719	CLA	C6-C7-C8-C9
27	b	719	CLA	C11-C12-C13-C14
27	a	822	CLA	CAA-CBA-CGA-O2A
27	b	705	CLA	CAA-CBA-CGA-O2A
33	D	619	LMG	C15-C16-C17-C18
27	b	727	CLA	C3-C5-C6-C7
27	E	608	CLA	C5-C6-C7-C8
27	a	808	CLA	CAA-CBA-CGA-O2A
35	l	416	DGD	O1G-C1A-C2A-C3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	E	606	CLA	C2-C3-C5-C6
27	F	607	CLA	CAA-CBA-CGA-O1A
27	T	606	CLA	C2A-CAA-CBA-CGA
27	a	805	CLA	C6-C7-C8-C10
27	a	825	CLA	C6-C7-C8-C10
27	a	827	CLA	C11-C10-C8-C7
27	a	827	CLA	C11-C12-C13-C15
27	r	204	CLA	C11-C10-C8-C7
37	a	832	PQN	C16-C17-C18-C20
37	b	729	PQN	C21-C22-C23-C25
34	l	401	LHG	C11-C12-C13-C14
27	B	601	CLA	C2B-C3B-CAB-CBB
27	B	609	CLA	C2B-C3B-CAB-CBB
27	D	607	CLA	C2B-C3B-CAB-CBB
27	F	617	CLA	C2B-C3B-CAB-CBB
27	H	310	CLA	C2B-C3B-CAB-CBB
27	I	602	CLA	C2B-C3B-CAB-CBB
27	K	608	CLA	C2B-C3B-CAB-CBB
27	a	811	CLA	C2B-C3B-CAB-CBB
27	r	203	CLA	C2B-C3B-CAB-CBB
38	b	731	BCR	C5-C6-C7-C8
34	a	835	LHG	C17-C18-C19-C20
27	a	804	CLA	CAA-CBA-CGA-O2A
27	D	602	CLA	C2-C1-O2A-CGA
27	F	619	CLA	C2-C1-O2A-CGA
27	a	818	CLA	C2-C1-O2A-CGA
27	a	830	CLA	C2-C1-O2A-CGA
27	r	203	CLA	C2-C1-O2A-CGA
27	a	823	CLA	CAA-CBA-CGA-O2A
32	J	611	PID	C28-C27-O6-C30
33	l	417	LMG	C16-C17-C18-C19
27	H	312	CLA	C2C-C3C-CAC-CBC
27	F	617	CLA	CBA-CGA-O2A-C1
27	K	604	CLA	C5-C6-C7-C8
33	F	616	LMG	C10-C11-C12-C13
27	a	805	CLA	CAA-CBA-CGA-O2A
27	G	607	CLA	CAA-CBA-CGA-O1A
27	a	821	CLA	C13-C15-C16-C17
34	r	202	LHG	C32-C33-C34-C35
27	l	404	CLA	C5-C6-C7-C8
35	f	305	DGD	O6D-C5D-C6D-O5D
27	C	204	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	I	601	CLA	CAA-CBA-CGA-O2A
27	a	830	CLA	C15-C16-C17-C18
27	b	710	CLA	C4-C3-C5-C6
34	F	618	LHG	C29-C30-C31-C32
27	G	603	CLA	CAA-CBA-CGA-O2A
27	b	722	CLA	CAA-CBA-CGA-O2A
27	l	408	CLA	CAA-CBA-CGA-O2A
27	a	816	CLA	C5-C6-C7-C8
27	a	824	CLA	C10-C11-C12-C13
27	G	606	CLA	C2-C3-C5-C6
35	j	201	DGD	CAB-CBB-CCB-CDB
27	B	609	CLA	CAA-CBA-CGA-O2A
30	B	612	DD6	C27-C29-C30-C31
27	a	829	CLA	C13-C15-C16-C17
33	F	616	LMG	C19-C20-C21-C22
27	E	607	CLA	C11-C10-C8-C9
27	l	405	CLA	C6-C7-C8-C9
27	D	610	CLA	CAA-CBA-CGA-O2A
27	b	706	CLA	CAA-CBA-CGA-O2A
31	H	320	SQD	C13-C14-C15-C16
27	A	603	CLA	C4B-C3B-CAB-CBB
27	A	612	CLA	C4B-C3B-CAB-CBB
27	B	610	CLA	C4B-C3B-CAB-CBB
27	G	606	CLA	C1A-C2A-CAA-CBA
27	H	309	CLA	C4B-C3B-CAB-CBB
27	H	310	CLA	C4B-C3B-CAB-CBB
27	a	818	CLA	C4B-C3B-CAB-CBB
27	a	822	CLA	C4B-C3B-CAB-CBB
27	a	823	CLA	C4B-C3B-CAB-CBB
27	b	716	CLA	C4B-C3B-CAB-CBB
27	b	722	CLA	C1A-C2A-CAA-CBA
27	l	410	CLA	C1A-C2A-CAA-CBA
34	l	401	LHG	C7-C8-C9-C10
27	H	319	CLA	C4-C3-C5-C6
27	a	818	CLA	C4-C3-C5-C6
27	l	403	CLA	C4-C3-C5-C6
27	B	610	CLA	C4C-C3C-CAC-CBC
27	G	610	CLA	CAA-CBA-CGA-O2A
27	b	703	CLA	CAA-CBA-CGA-O2A
27	b	712	CLA	CAA-CBA-CGA-O2A
34	j	205	LHG	O7-C7-C8-C9
27	D	609	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	806	CLA	C6-C7-C8-C10
27	E	606	CLA	CAA-CBA-CGA-O2A
27	b	714	CLA	CAA-CBA-CGA-O2A
27	a	829	CLA	C10-C11-C12-C13
27	a	827	CLA	C2-C1-O2A-CGA
27	b	702	CLA	C2-C1-O2A-CGA
27	F	617	CLA	C6-C7-C8-C10
27	K	601	CLA	C11-C10-C8-C7
27	a	824	CLA	C12-C13-C15-C16
27	b	702	CLA	C11-C10-C8-C7
27	b	726	CLA	C11-C10-C8-C7
27	l	403	CLA	C11-C12-C13-C15
27	J	603	CLA	C10-C11-C12-C13
27	D	612	CLA	O2A-C1-C2-C3
33	b	733	LMG	C7-C8-O7-C10
34	G	617	LHG	C6-C5-O7-C7
34	l	401	LHG	C6-C5-O7-C7
34	F	618	LHG	O2-C2-C3-O3
27	b	728	CLA	CAA-CBA-CGA-O2A
38	a	836	BCR	C15-C16-C17-C18
27	H	305	CLA	C2A-CAA-CBA-CGA
27	a	815	CLA	C2A-CAA-CBA-CGA
27	a	830	CLA	C2A-CAA-CBA-CGA
27	a	805	CLA	CAA-CBA-CGA-O1A
27	a	808	CLA	CAA-CBA-CGA-O1A
34	G	617	LHG	C5-C4-O6-P
27	G	607	CLA	CAA-CBA-CGA-O2A
27	G	608	CLA	C3A-C2A-CAA-CBA
27	a	809	CLA	C3A-C2A-CAA-CBA
27	a	823	CLA	C3A-C2A-CAA-CBA
27	r	203	CLA	C3A-C2A-CAA-CBA
27	r	204	CLA	C8-C10-C11-C12
27	I	610	CLA	C6-C7-C8-C10
33	C	217	LMG	C10-C11-C12-C13
27	b	722	CLA	CAA-CBA-CGA-O1A
27	I	603	CLA	CAA-CBA-CGA-O2A
27	b	717	CLA	CAA-CBA-CGA-O2A
33	C	217	LMG	O7-C10-C11-C12
31	y	301	SQD	C24-C25-C26-C27
27	b	715	CLA	C2A-CAA-CBA-CGA
27	a	815	CLA	C6-C7-C8-C9
27	b	709	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	b	733	LMG	C18-C19-C20-C21
38	l	415	BCR	C13-C14-C15-C16
27	l	409	CLA	C8-C10-C11-C12
27	I	601	CLA	CAA-CBA-CGA-O1A
27	b	711	CLA	CAA-CBA-CGA-O1A
27	A	601	CLA	C4C-C3C-CAC-CBC
27	F	601	CLA	CAA-CBA-CGA-O2A
28	B	608	KC2	C1A-C2A-CAA-CBA
28	C	210	KC2	C1A-C2A-CAA-CBA
28	E	610	KC2	C1A-C2A-CAA-CBA
28	G	601	KC2	C1A-C2A-CAA-CBA
28	H	302	KC2	C1A-C2A-CAA-CBA
28	I	604	KC2	C1A-C2A-CAA-CBA
28	U	604	KC2	C1A-C2A-CAA-CBA
30	A	617	DD6	C13-C14-C15-C16
30	B	614	DD6	C13-C14-C15-C16
30	B	616	DD6	C13-C14-C15-C16
30	E	615	DD6	C13-C14-C15-C16
30	K	609	DD6	C13-C14-C15-C16
30	r	205	DD6	C13-C14-C15-C16
31	H	320	SQD	O5-C5-C6-S
31	y	301	SQD	O5-C5-C6-S
32	J	615	PID	C5-C6-C7-C8
27	b	702	CLA	O1A-CGA-O2A-C1
33	F	616	LMG	C24-C25-C26-C27
27	B	607	CLA	C10-C11-C12-C13
27	H	303	CLA	C10-C11-C12-C13
31	H	320	SQD	O47-C7-C8-C9
38	b	731	BCR	C17-C18-C19-C20
27	l	408	CLA	CAA-CBA-CGA-O1A
27	B	609	CLA	CAA-CBA-CGA-O1A
27	E	606	CLA	CAA-CBA-CGA-O1A
27	a	822	CLA	CAA-CBA-CGA-O1A
34	D	620	LHG	C24-C25-C26-C27
27	a	804	CLA	CAA-CBA-CGA-O1A
27	b	706	CLA	CAA-CBA-CGA-O1A
27	b	712	CLA	CAA-CBA-CGA-O1A
27	b	714	CLA	CAA-CBA-CGA-O1A
28	A	608	KC2	C2C-C3C-CAC-CBC
28	G	601	KC2	C2C-C3C-CAC-CBC
28	T	608	KC2	C2C-C3C-CAC-CBC
27	D	609	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	C	204	CLA	CAA-CBA-CGA-O1A
27	b	705	CLA	CAA-CBA-CGA-O1A
33	b	733	LMG	C33-C34-C35-C36
27	A	612	CLA	CAD-CBD-CGD-O2D
27	F	607	CLA	CAD-CBD-CGD-O2D
27	I	601	CLA	CAD-CBD-CGD-O2D
27	J	603	CLA	CAD-CBD-CGD-O2D
27	K	602	CLA	CAD-CBD-CGD-O2D
27	T	603	CLA	CAD-CBD-CGD-O2D
27	a	827	CLA	CAD-CBD-CGD-O2D
27	b	716	CLA	CAD-CBD-CGD-O2D
27	b	726	CLA	CAD-CBD-CGD-O2D
27	l	411	CLA	CAD-CBD-CGD-O2D
28	K	607	KC2	CAD-CBD-CGD-O2D
27	J	605	CLA	CAA-CBA-CGA-O2A
27	G	603	CLA	CAA-CBA-CGA-O1A
27	K	605	CLA	C2-C1-O2A-CGA
27	U	605	CLA	C2-C1-O2A-CGA
27	b	728	CLA	CAA-CBA-CGA-O1A
34	j	205	LHG	O9-C7-C8-C9
27	H	309	CLA	CAA-CBA-CGA-O2A
27	K	604	CLA	CAA-CBA-CGA-O2A
27	E	608	CLA	C11-C12-C13-C15
27	a	802	CLA	C6-C7-C8-C9
27	I	606	CLA	CAA-CBA-CGA-O2A
27	E	608	CLA	C8-C10-C11-C12
27	D	610	CLA	CAA-CBA-CGA-O1A
27	G	610	CLA	CAA-CBA-CGA-O1A
27	K	604	CLA	CAA-CBA-CGA-O1A

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	K	611	PID	C24-C25-C26-C27-C28-C29
29	B	615	UIX	C15-C16-C17-C18-C19-C20
29	I	612	UIX	C15-C16-C17-C18-C19-C20
32	U	608	PID	C24-C25-C26-C27-C28-C29

158 monomers are involved in 306 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	f	304	BCR	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	J	615	PID	3	0
38	f	301	BCR	5	0
27	a	806	CLA	2	0
27	A	609	CLA	1	0
27	b	703	CLA	1	0
30	C	216	DD6	2	0
27	K	605	CLA	3	0
27	C	205	CLA	2	0
32	J	611	PID	6	0
27	K	601	CLA	3	0
30	F	612	DD6	1	0
33	K	613	LMG	1	0
27	T	606	CLA	2	0
27	l	409	CLA	1	0
33	D	619	LMG	1	0
30	i	202	DD6	1	0
29	I	612	UIX	2	0
28	K	607	KC2	6	0
27	I	605	CLA	1	0
27	A	605	CLA	1	0
27	a	814	CLA	1	0
27	U	603	CLA	7	0
27	b	704	CLA	3	0
32	B	613	PID	1	0
27	b	718	CLA	1	0
27	a	802	CLA	1	0
38	a	836	BCR	41	0
27	D	612	CLA	1	0
32	J	613	PID	10	0
30	K	610	DD6	1	0
30	b	730	DD6	1	0
28	J	608	KC2	2	0
27	l	411	CLA	1	0
30	D	621	DD6	1	0
27	F	602	CLA	2	0
27	a	826	CLA	3	0
32	I	614	PID	4	0
35	j	201	DGD	1	0
27	D	608	CLA	1	0
35	K	614	DGD	3	0
27	l	410	CLA	2	0
27	b	701	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	K	602	CLA	2	0
27	F	605	CLA	1	0
32	J	614	PID	4	0
27	C	203	CLA	1	0
27	F	601	CLA	1	0
30	H	316	DD6	1	0
27	I	616	CLA	1	0
27	j	202	CLA	1	0
27	f	302	CLA	1	0
27	a	801	CLA	3	0
27	H	303	CLA	1	0
27	D	604	CLA	1	0
35	l	416	DGD	3	0
27	b	714	CLA	12	0
27	b	705	CLA	1	0
27	K	603	CLA	6	0
30	A	615	DD6	1	0
27	a	817	CLA	1	0
27	G	608	CLA	1	0
27	a	820	CLA	4	0
27	b	723	CLA	2	0
27	F	608	CLA	1	0
30	G	616	DD6	1	0
29	A	613	UIX	1	0
27	a	827	CLA	3	0
27	I	603	CLA	1	0
27	U	605	CLA	1	0
27	J	609	CLA	2	0
27	b	716	CLA	1	0
27	a	804	CLA	10	0
30	G	614	DD6	1	0
27	G	605	CLA	1	0
27	I	607	CLA	1	0
27	b	719	CLA	3	0
27	J	605	CLA	2	0
36	T	613	LMU	1	0
30	A	614	DD6	1	0
38	a	833	BCR	2	0
38	i	201	BCR	5	0
29	H	314	UIX	1	0
27	b	727	CLA	1	0
27	b	711	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	J	604	KC2	4	0
32	F	614	PID	6	0
27	E	609	CLA	1	0
27	r	203	CLA	1	0
30	H	318	DD6	1	0
34	r	202	LHG	1	0
38	b	731	BCR	2	0
27	b	710	CLA	2	0
27	a	812	CLA	1	0
27	I	610	CLA	1	0
27	a	811	CLA	1	0
27	H	313	CLA	1	0
27	I	606	CLA	1	0
27	l	406	CLA	1	0
30	B	612	DD6	1	0
27	F	617	CLA	3	0
32	K	611	PID	12	0
27	b	702	CLA	3	0
27	a	831	CLA	1	0
30	E	614	DD6	1	0
27	T	605	CLA	2	0
33	C	217	LMG	1	0
27	H	319	CLA	4	0
27	l	412	CLA	1	0
27	D	605	CLA	2	0
32	F	615	PID	3	0
27	b	713	CLA	1	0
27	a	815	CLA	1	0
27	H	312	CLA	1	0
27	a	810	CLA	1	0
28	I	604	KC2	1	0
38	l	414	BCR	4	0
27	b	725	CLA	2	0
27	b	708	CLA	1	0
27	a	825	CLA	1	0
27	D	602	CLA	1	0
27	a	819	CLA	6	0
27	b	709	CLA	2	0
27	H	304	CLA	1	0
27	a	837	CLA	1	0
34	l	401	LHG	1	0
27	a	830	CLA	1	0

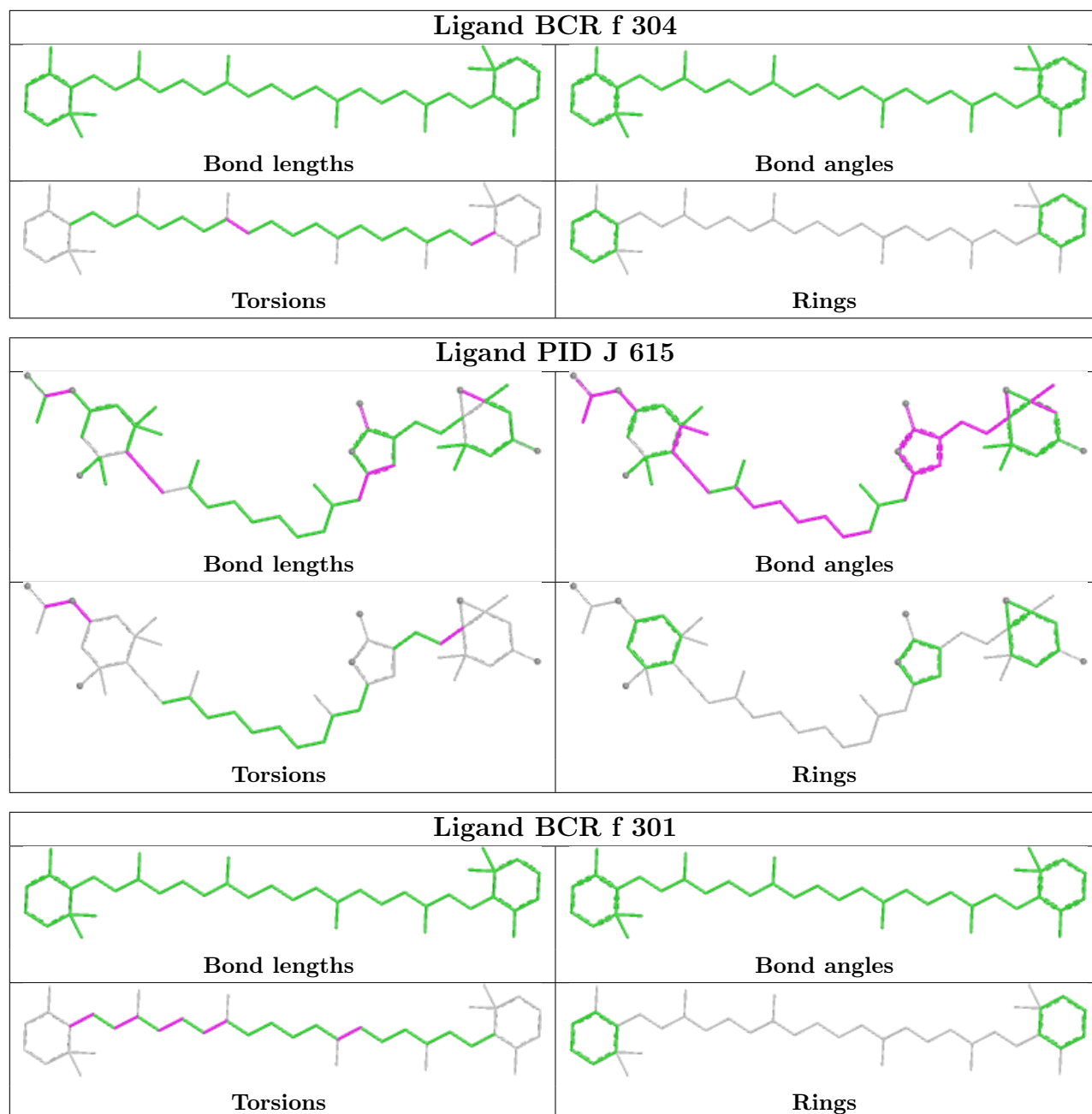
Continued on next page...

Continued from previous page...

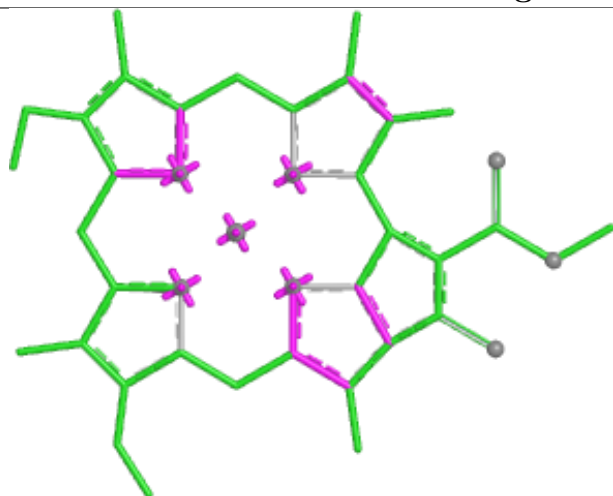
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	611	CLA	1	0
27	B	605	CLA	1	0
27	H	308	CLA	1	0
27	G	606	CLA	1	0
30	H	315	DD6	1	0
27	b	728	CLA	1	0
27	a	807	CLA	2	0
29	j	204	UIX	2	0
38	l	415	BCR	4	0
27	E	611	CLA	1	0
27	G	602	CLA	1	0
27	a	824	CLA	3	0
30	D	615	DD6	2	0
27	F	604	CLA	1	0
30	K	609	DD6	1	0
27	A	604	CLA	1	0
27	F	619	CLA	1	0
27	C	201	CLA	1	0
27	A	601	CLA	1	0
29	C	215	UIX	1	0
38	a	834	BCR	22	0
27	a	823	CLA	2	0
27	C	204	CLA	1	0
27	l	402	CLA	1	0
38	m	201	BCR	1	0
27	b	722	CLA	2	0
27	T	603	CLA	1	0
27	D	603	CLA	1	0
38	l	413	BCR	5	0
27	a	816	CLA	3	0
27	a	818	CLA	1	0

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

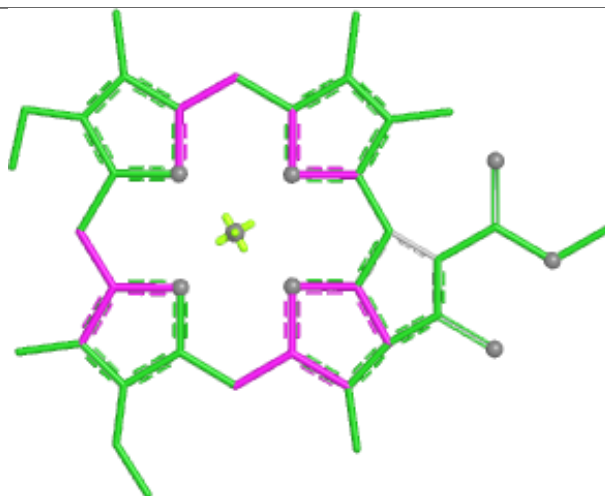
equivalents in the CSD to analyse the geometry.



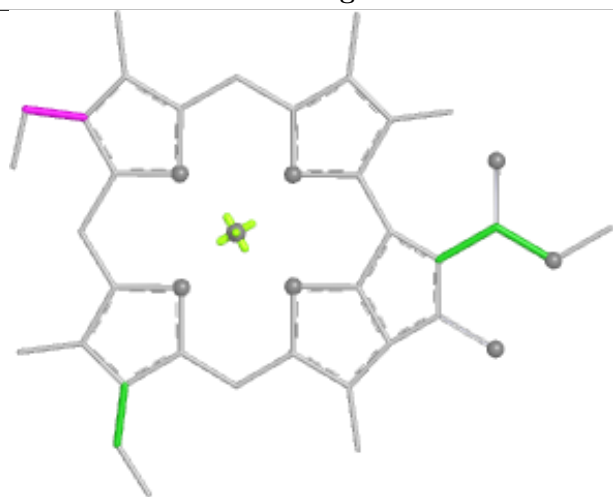
Ligand CLA T 604



Bond lengths



Bond angles

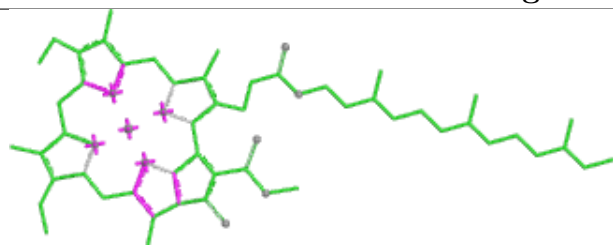


Torsions

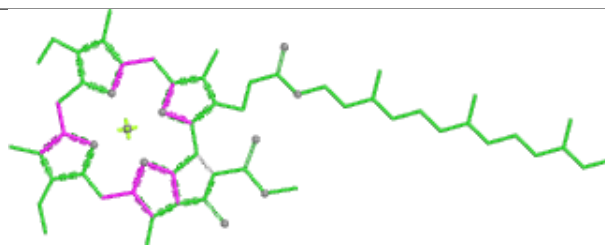


Rings

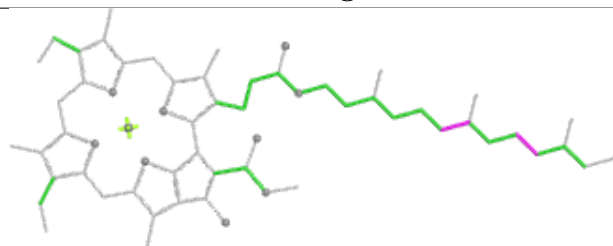
Ligand CLA I 405



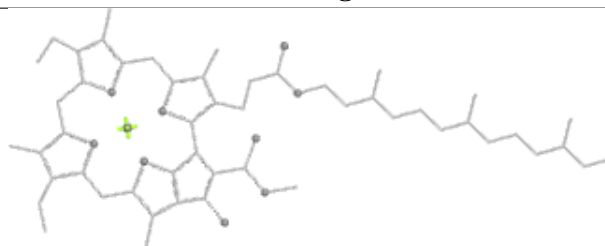
Bond lengths



Bond angles

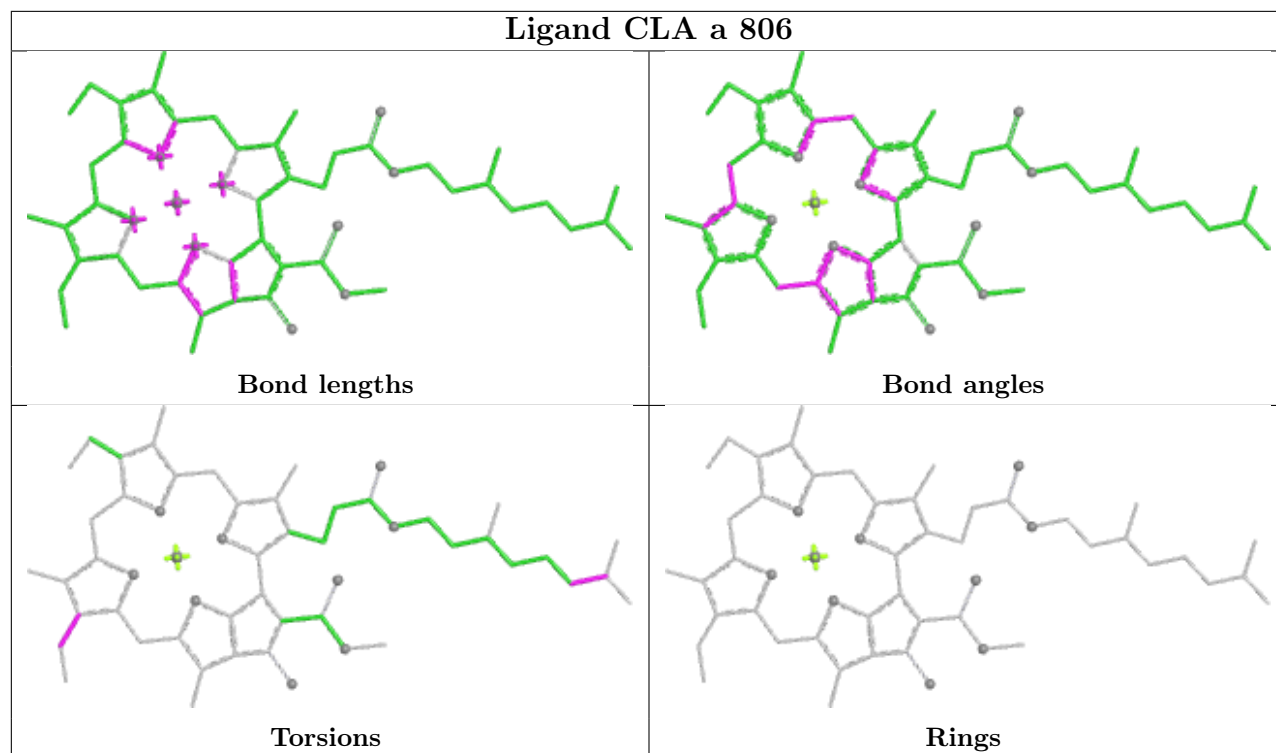


Torsions

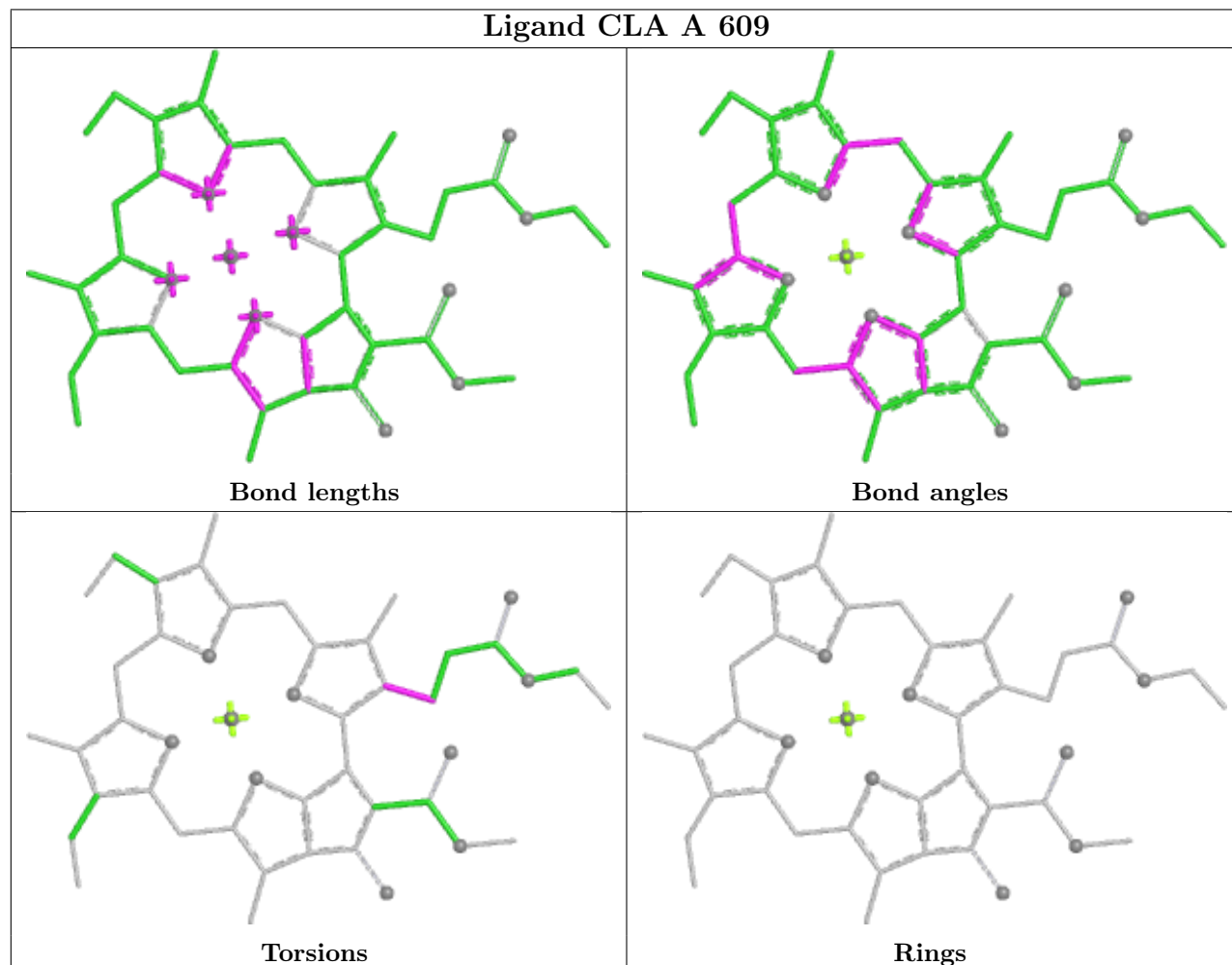


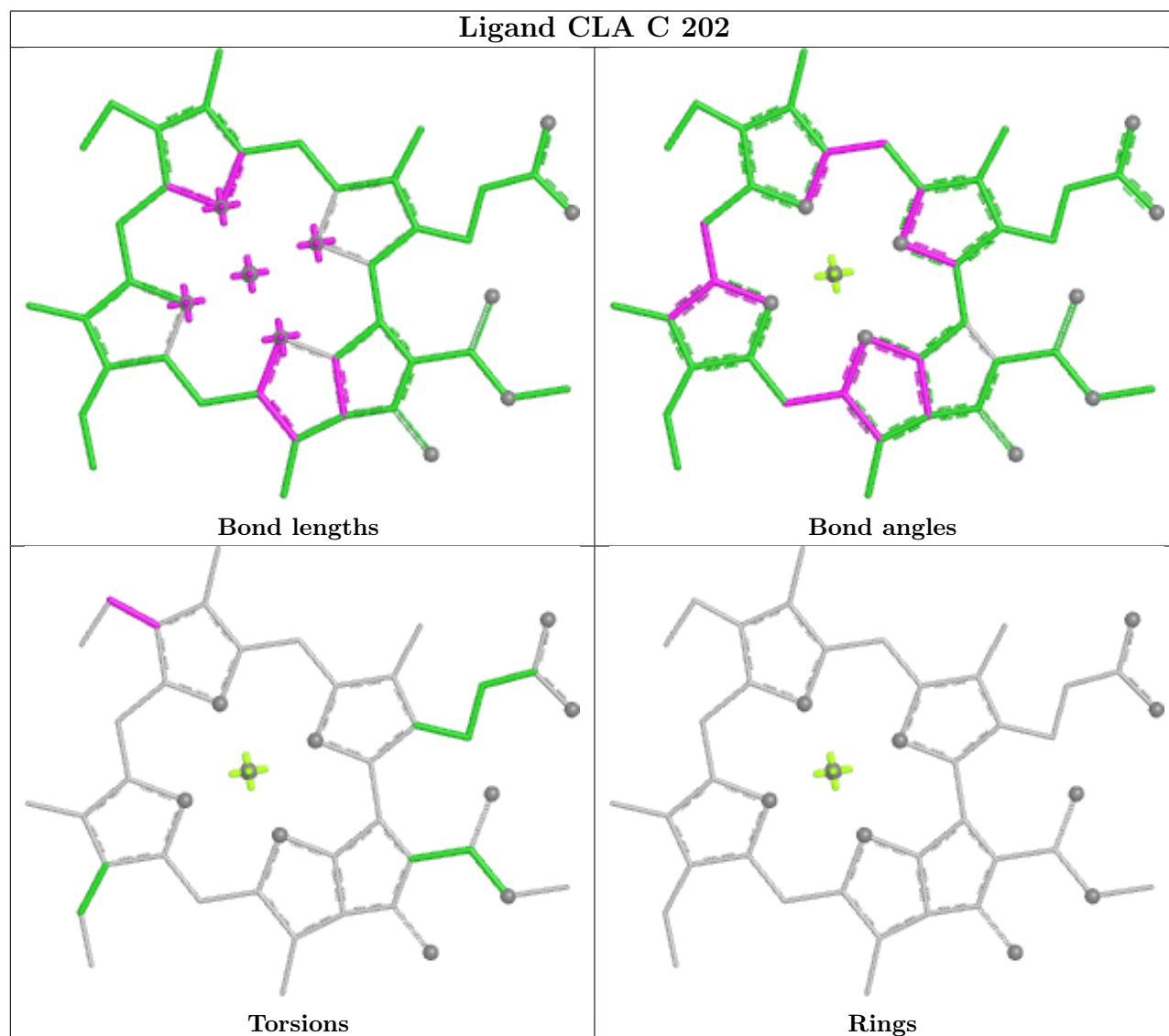
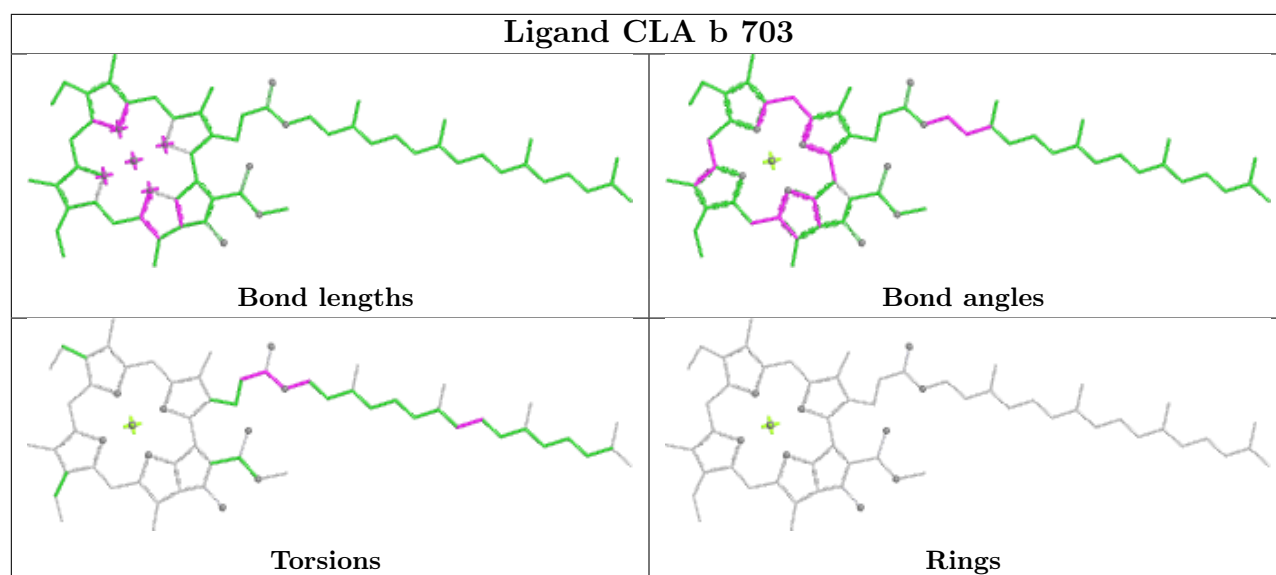
Rings

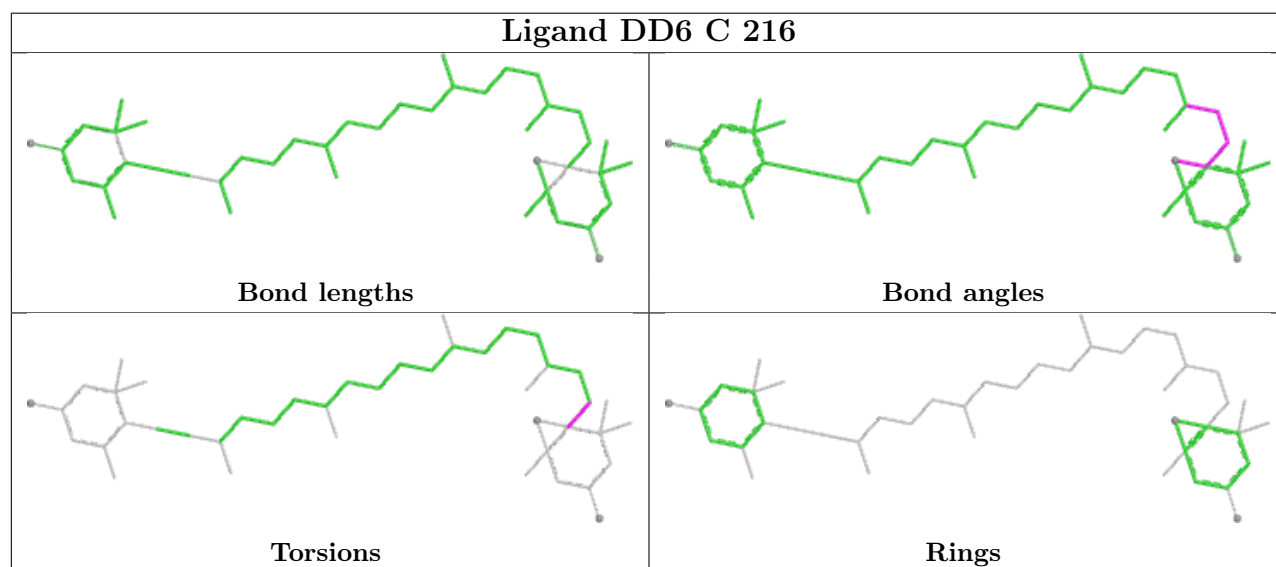
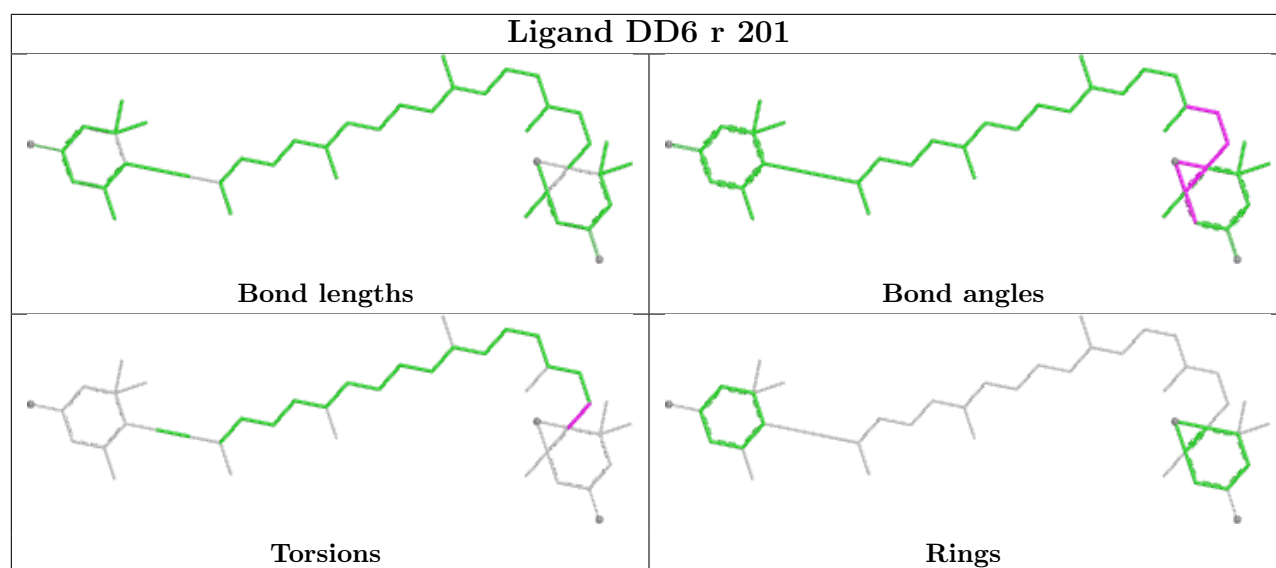
Ligand CLA a 806



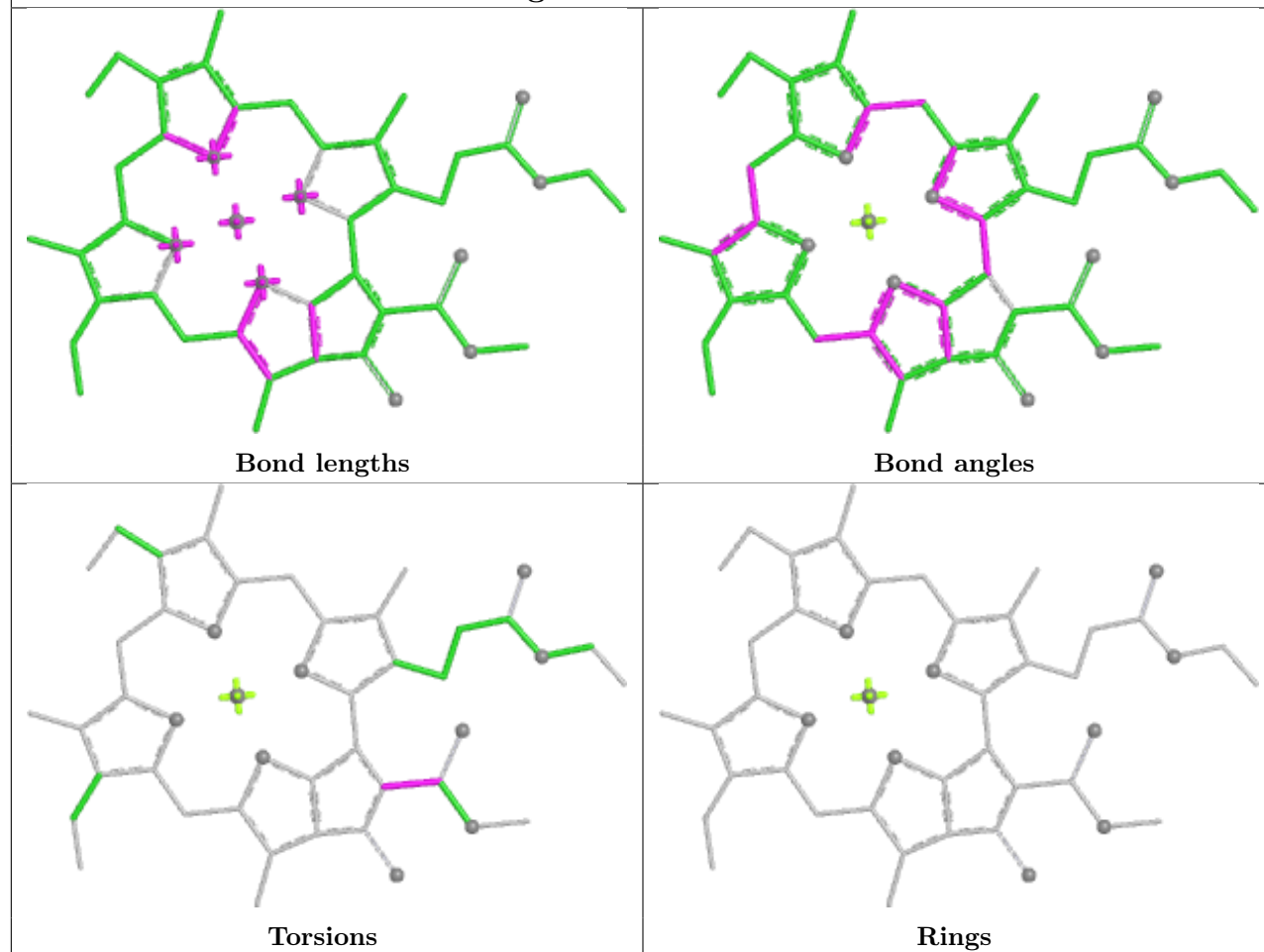
Ligand CLA A 609



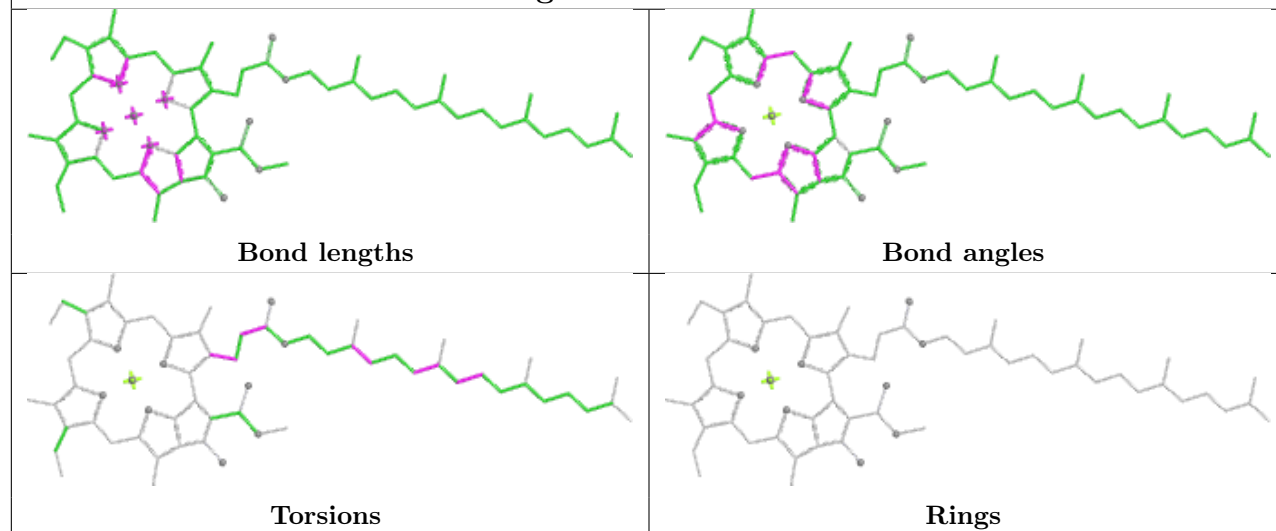


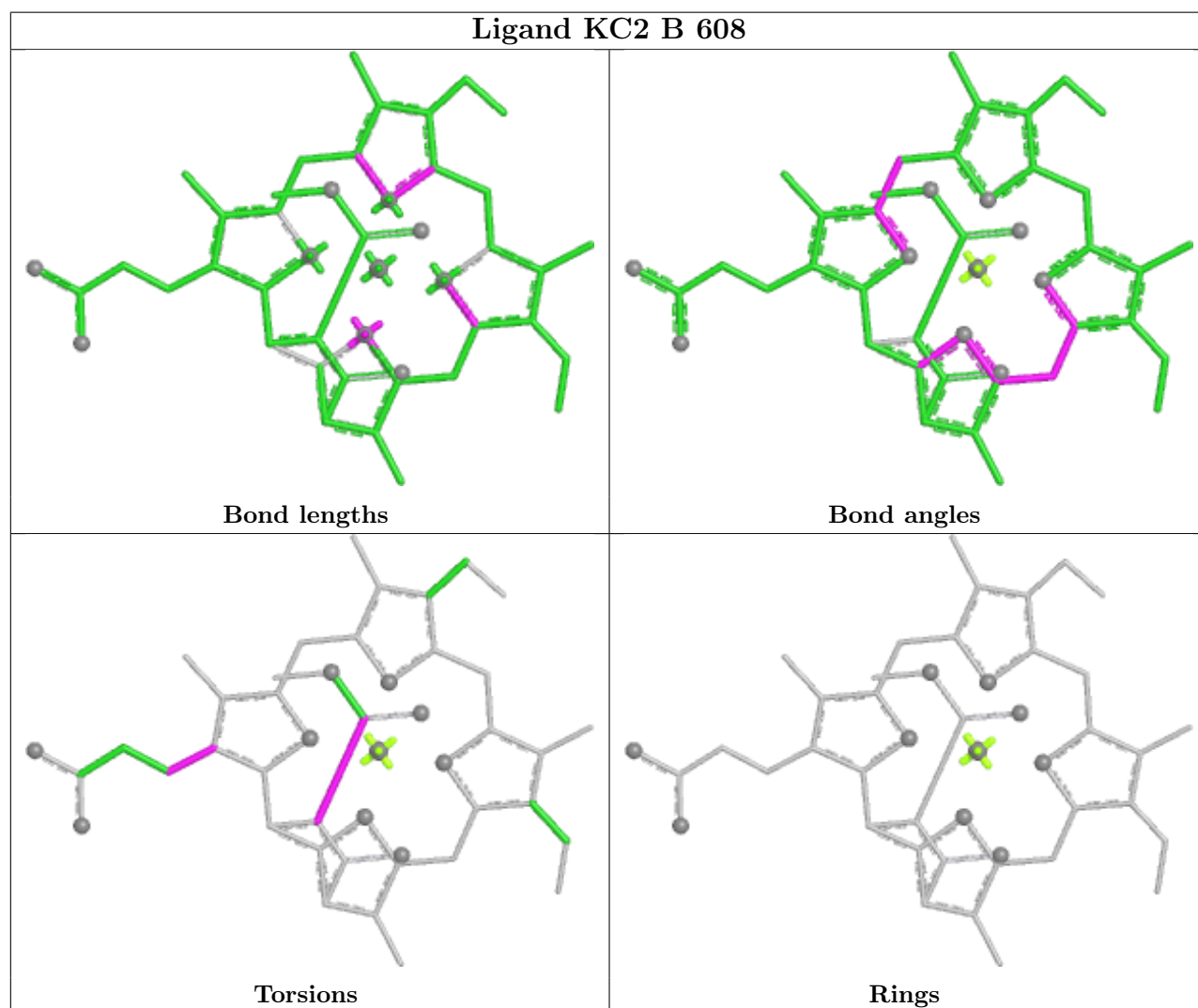
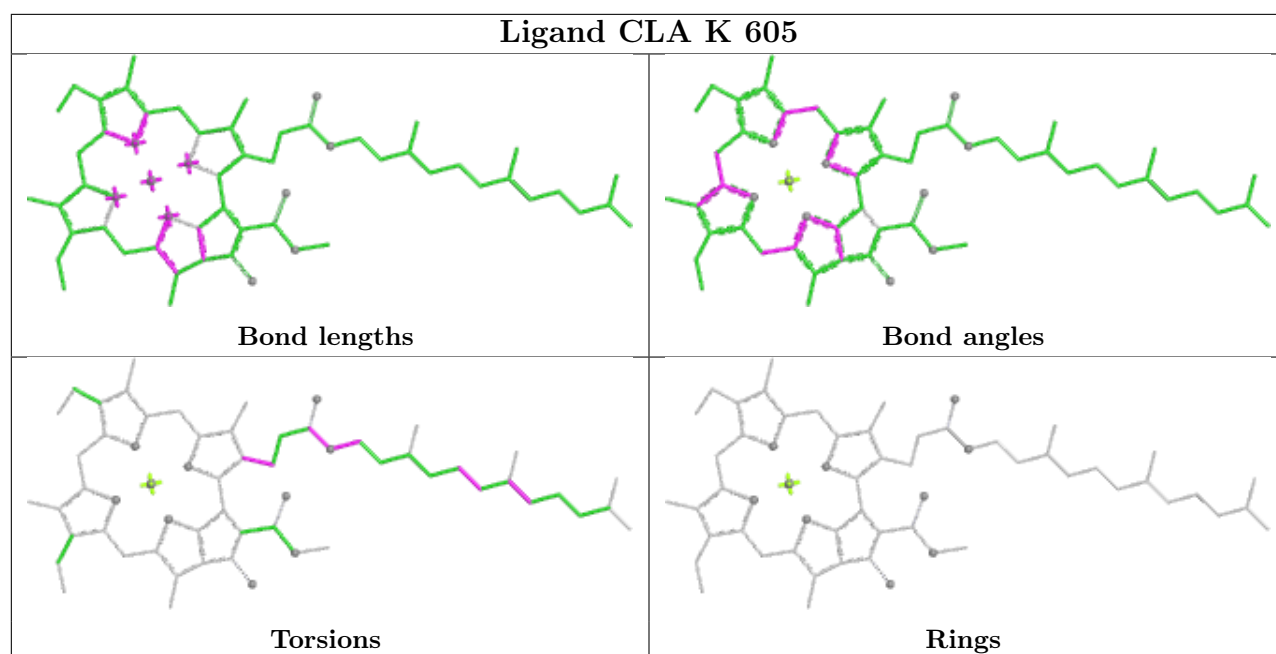


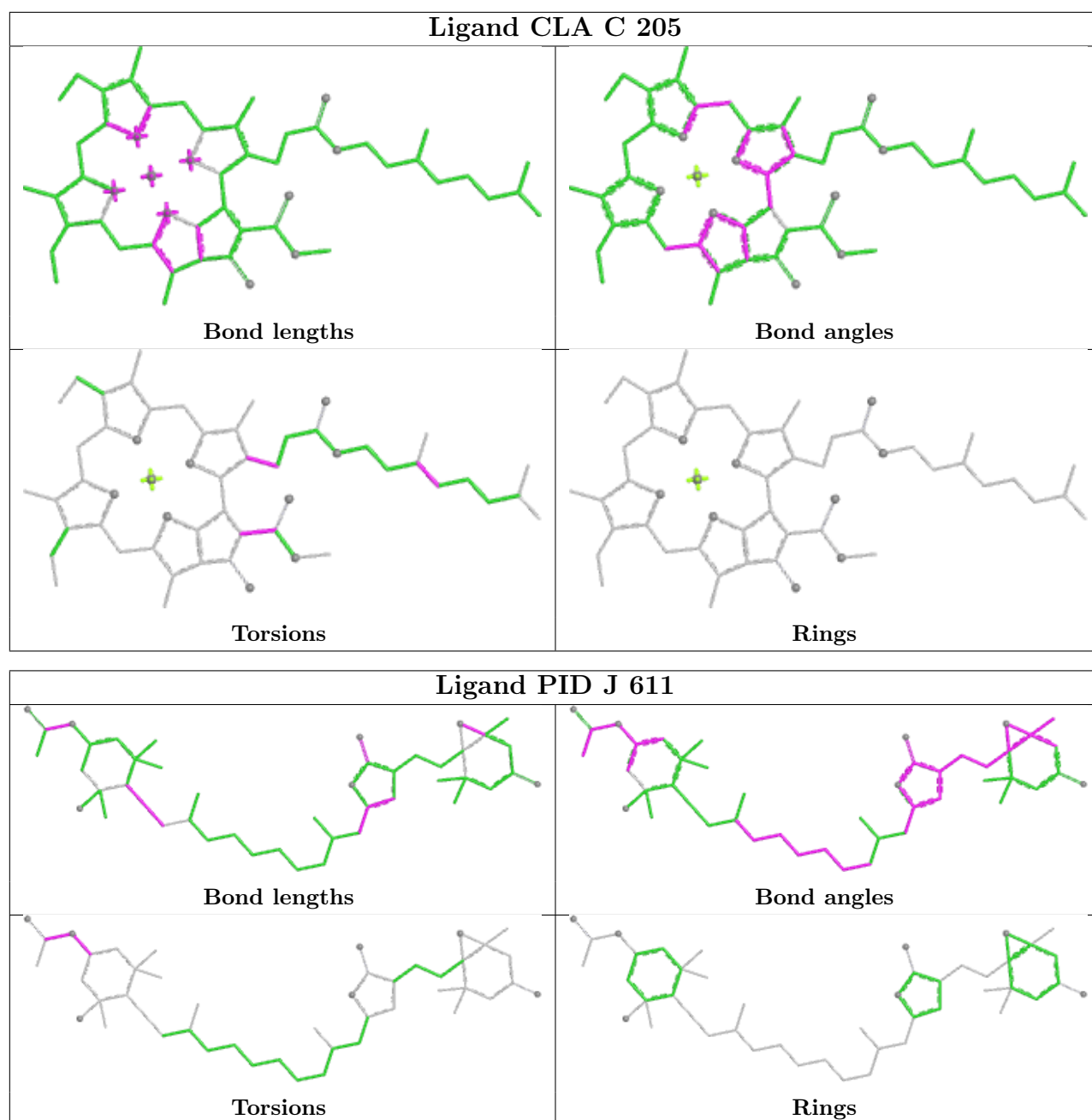
Ligand CLA T 601

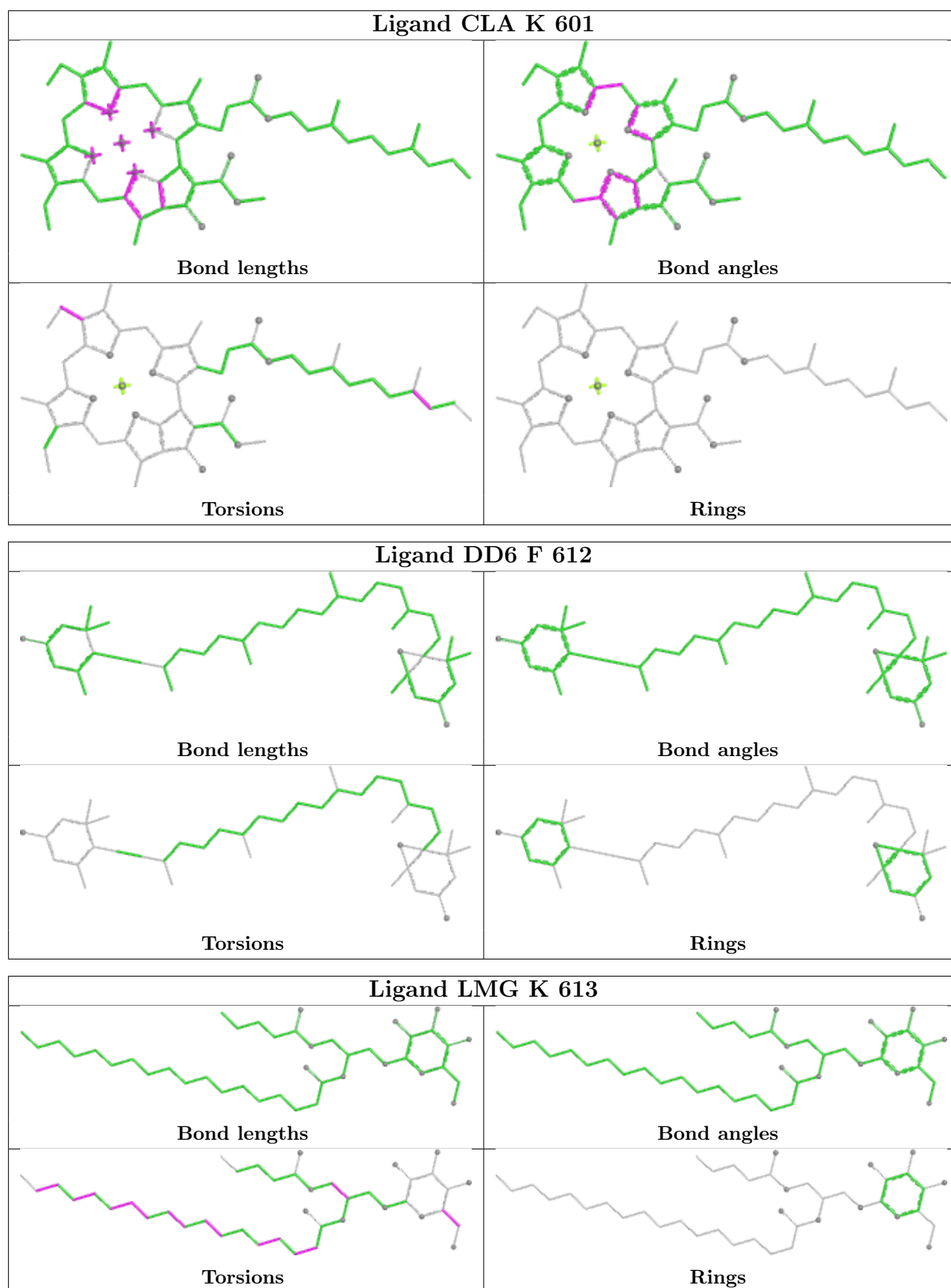


Ligand CLA a 805

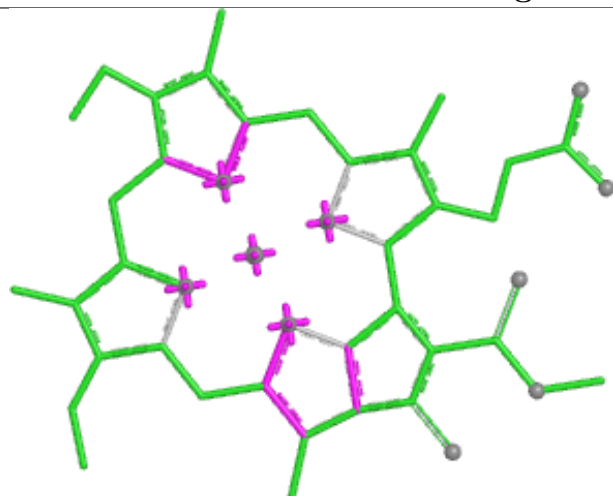




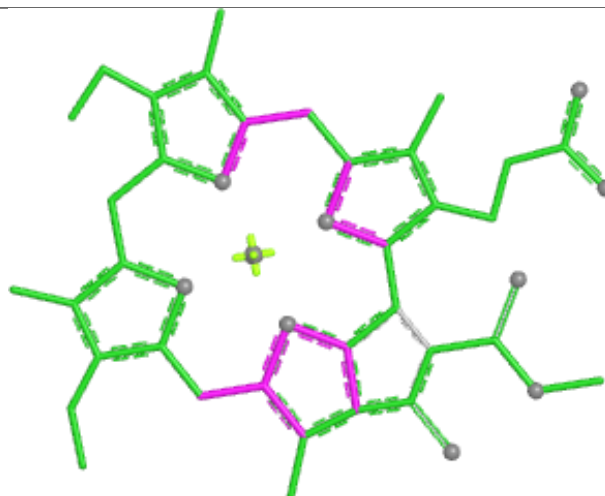




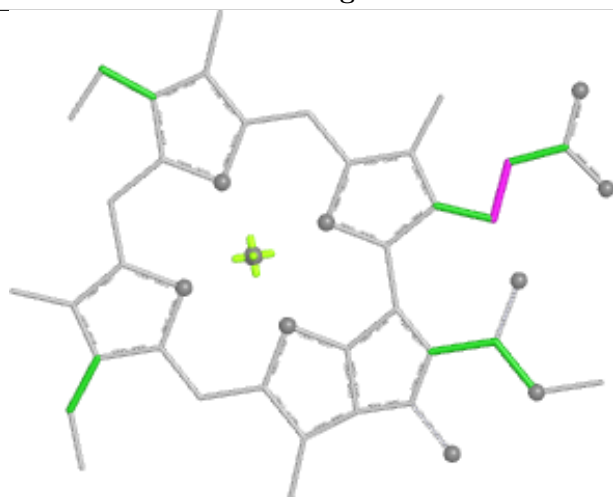
Ligand CLA T 606



Bond lengths



Bond angles

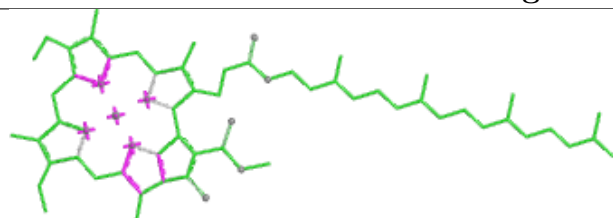


Torsions

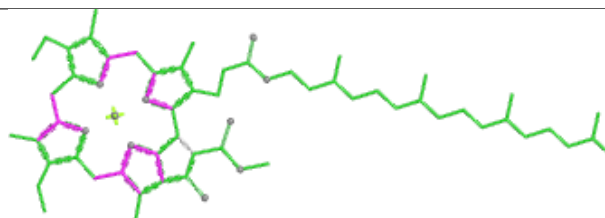


Rings

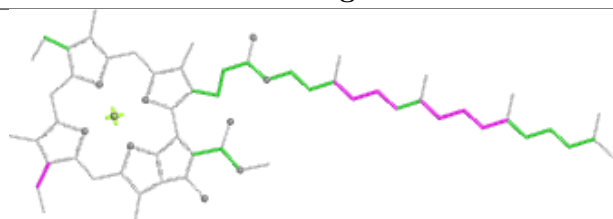
Ligand CLA I 409



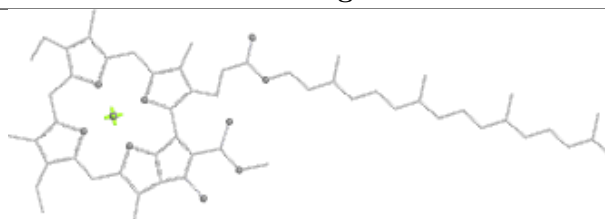
Bond lengths



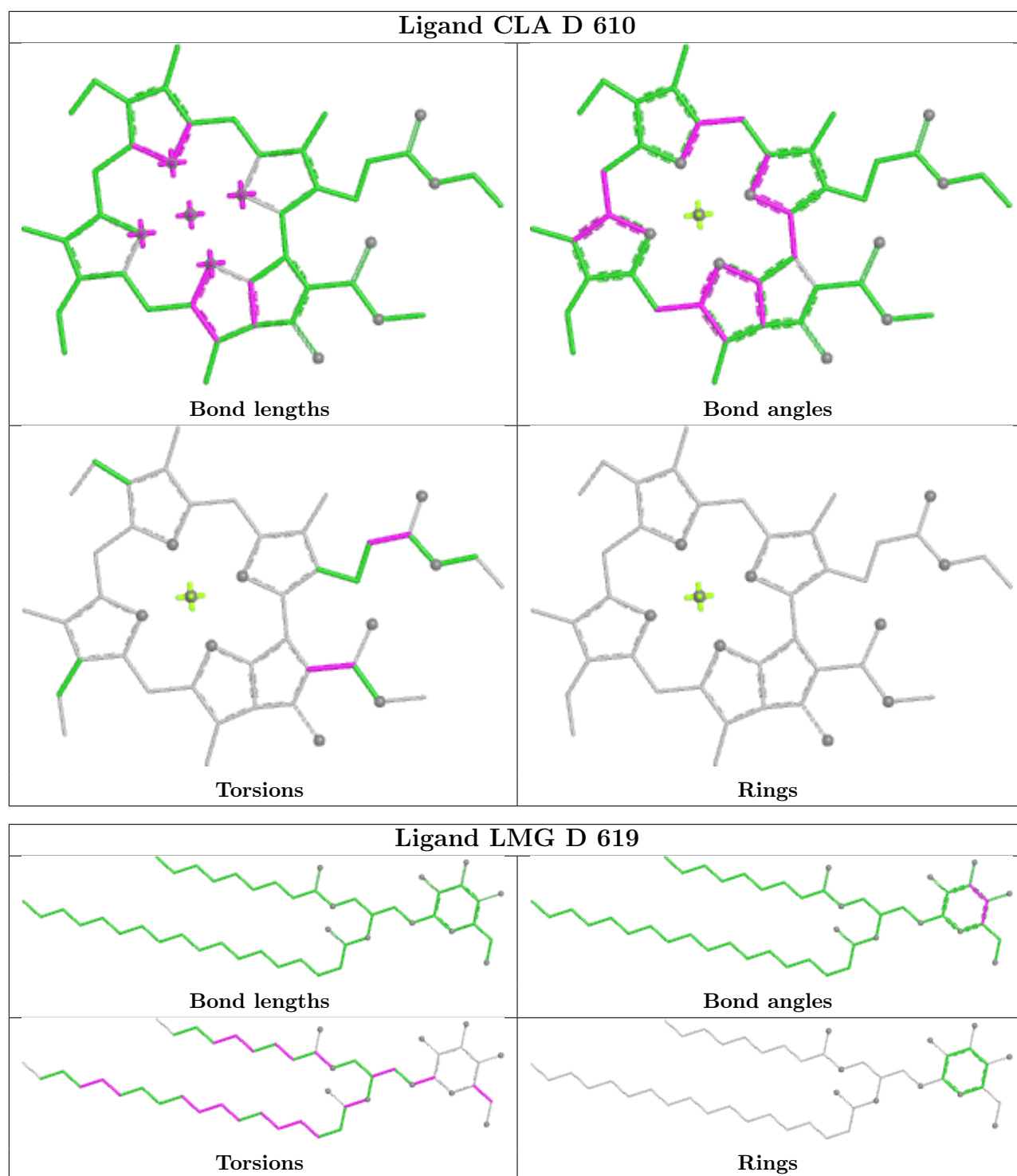
Bond angles

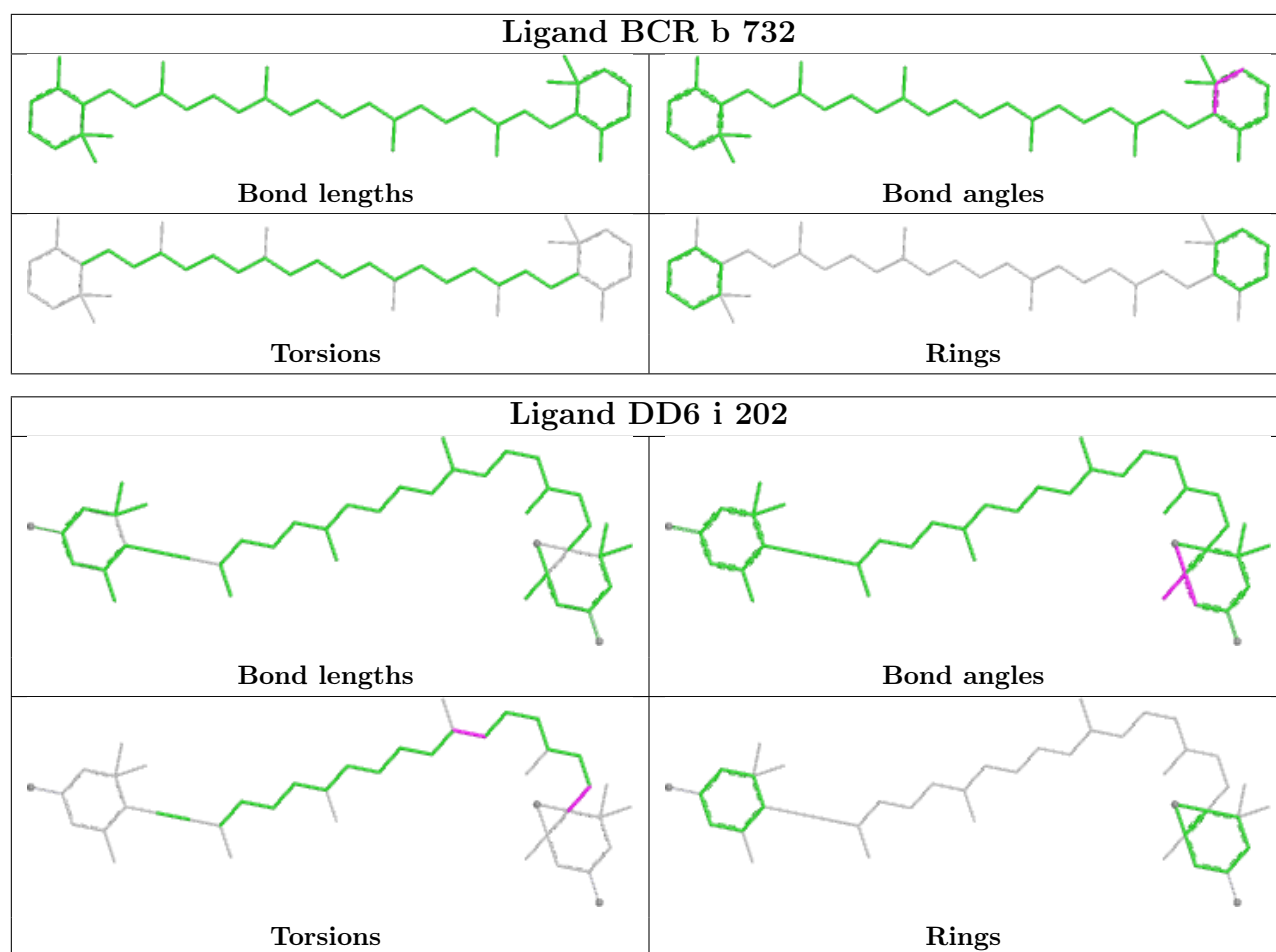


Torsions

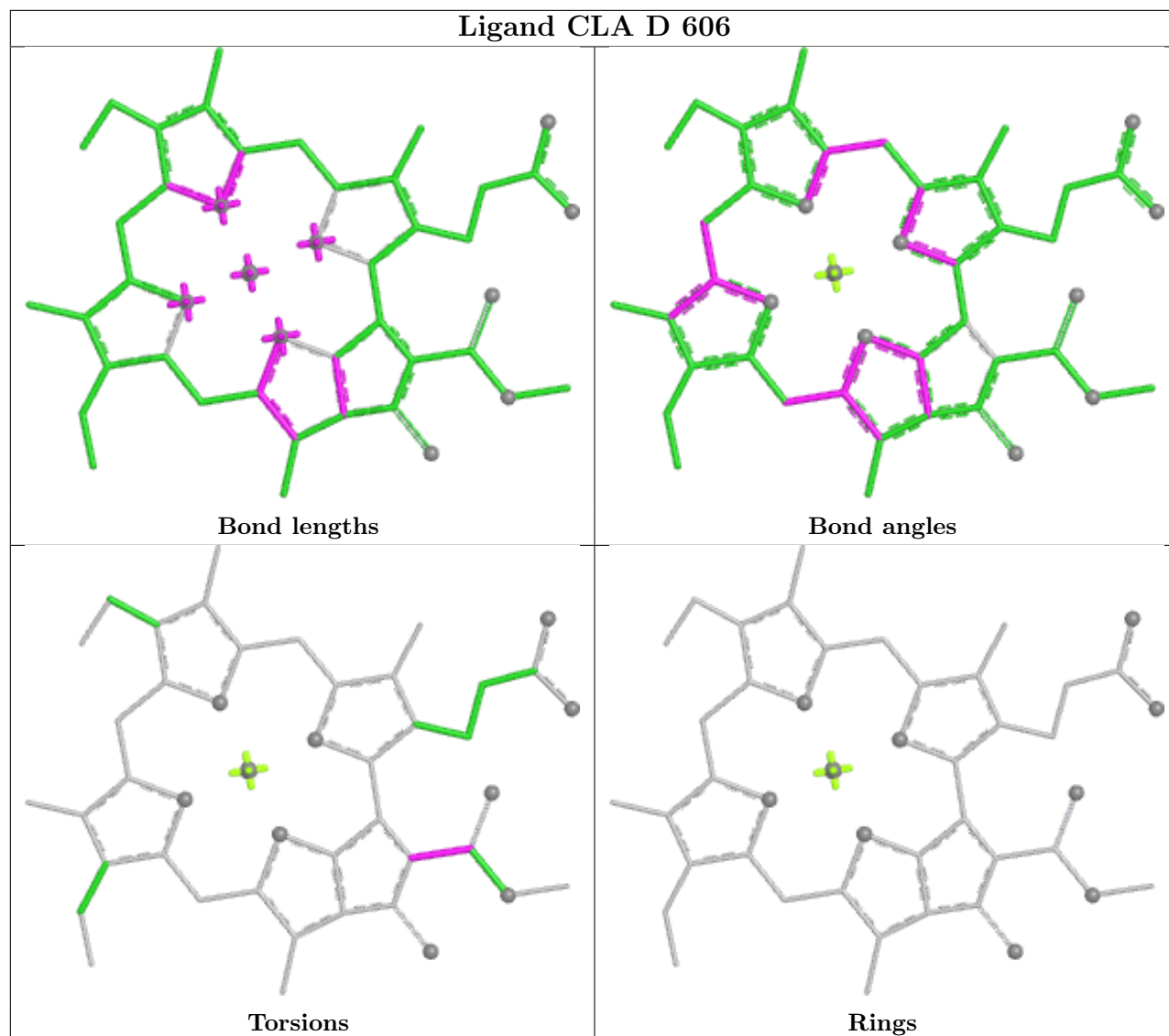


Rings

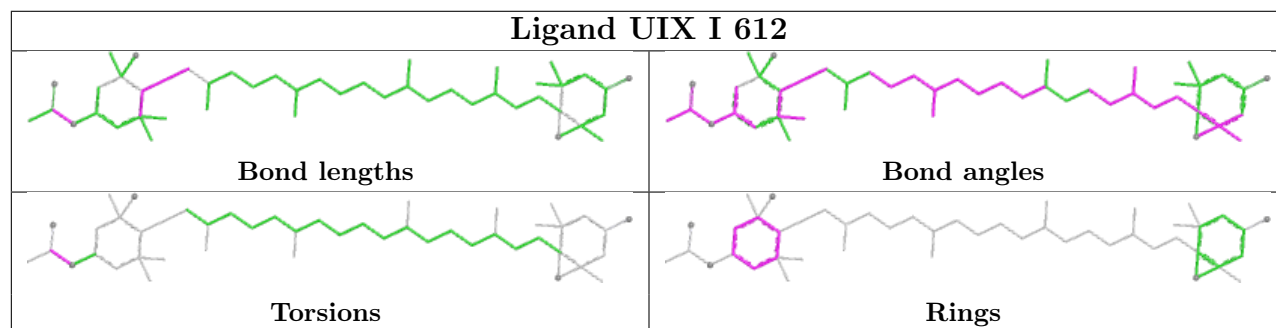




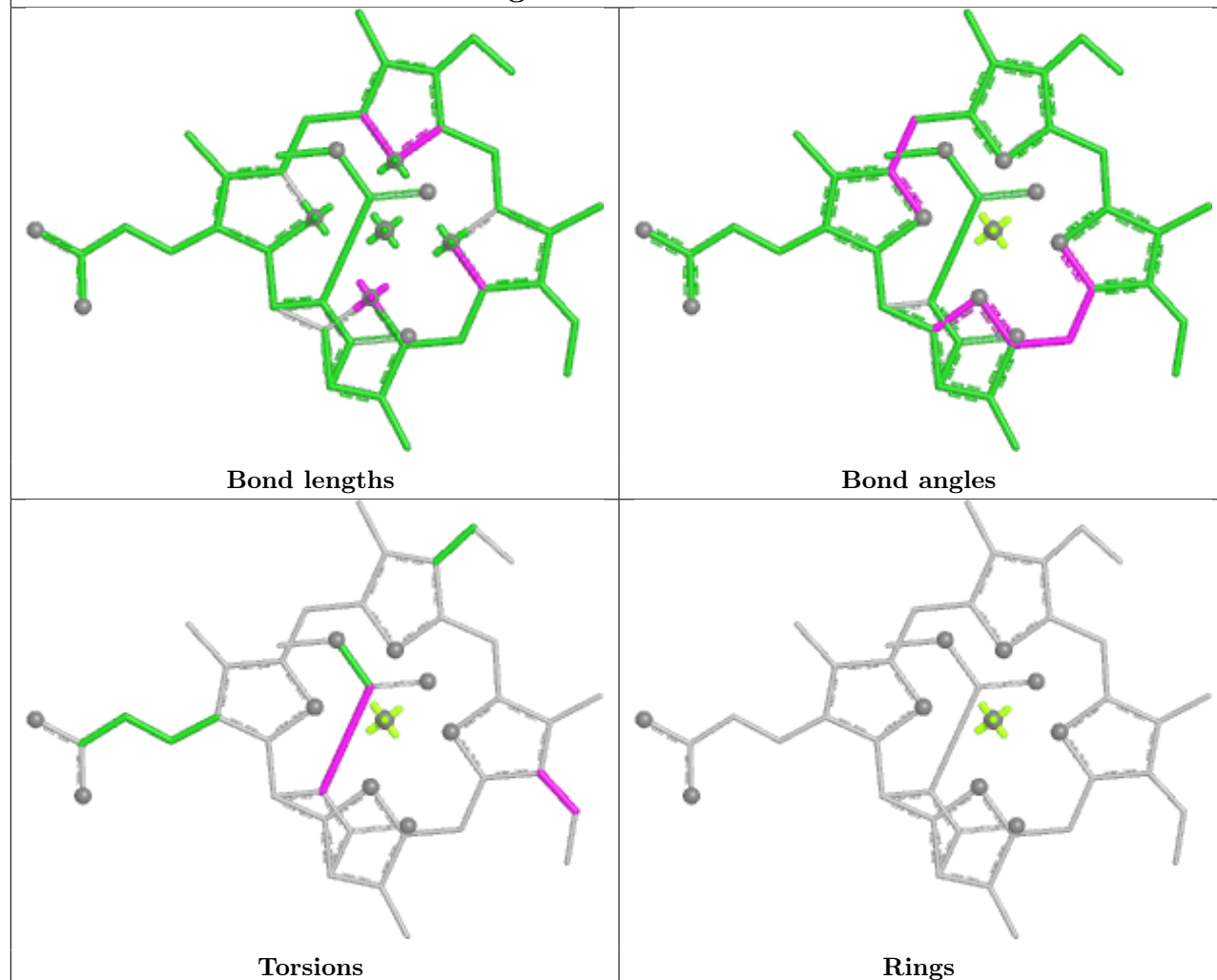
Ligand CLA D 606



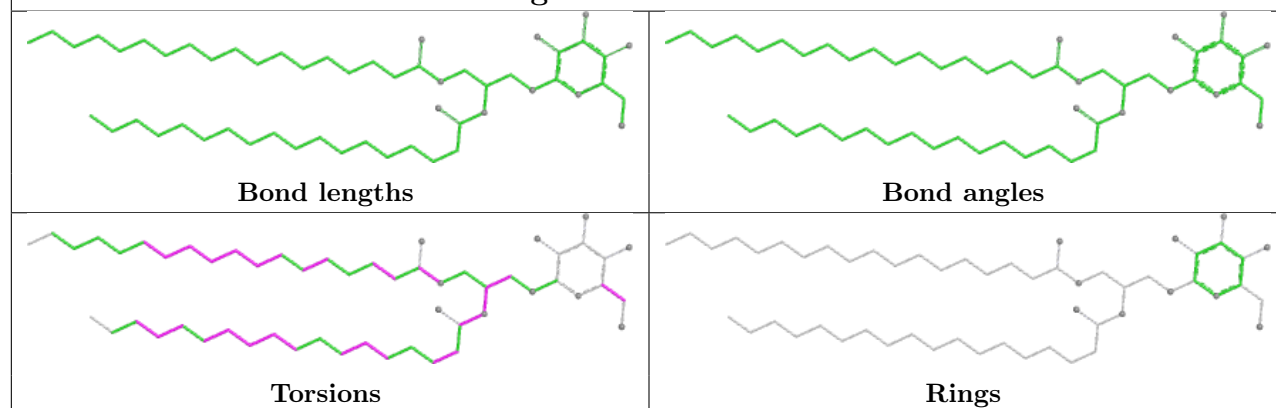
Ligand UIX I 612

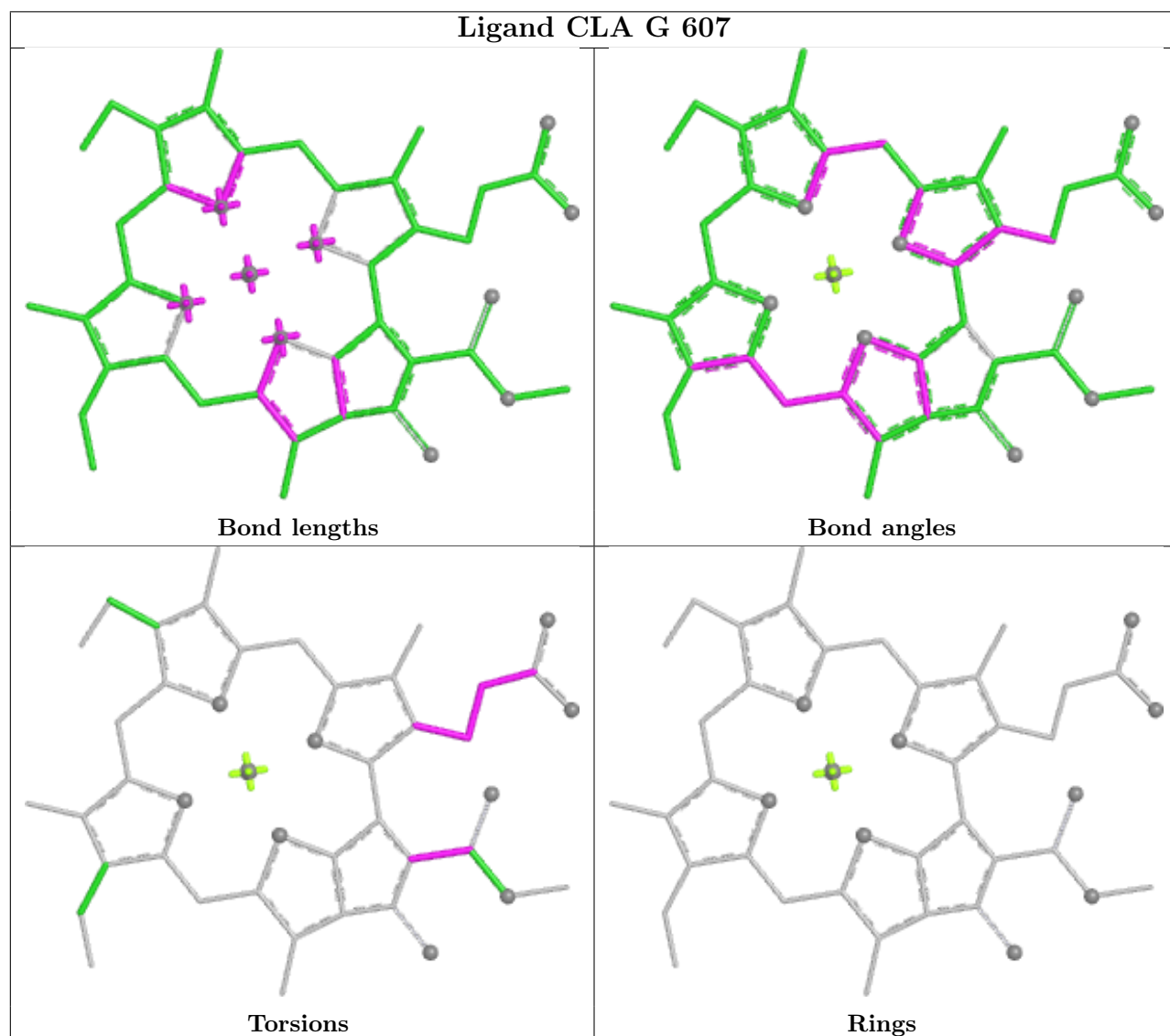
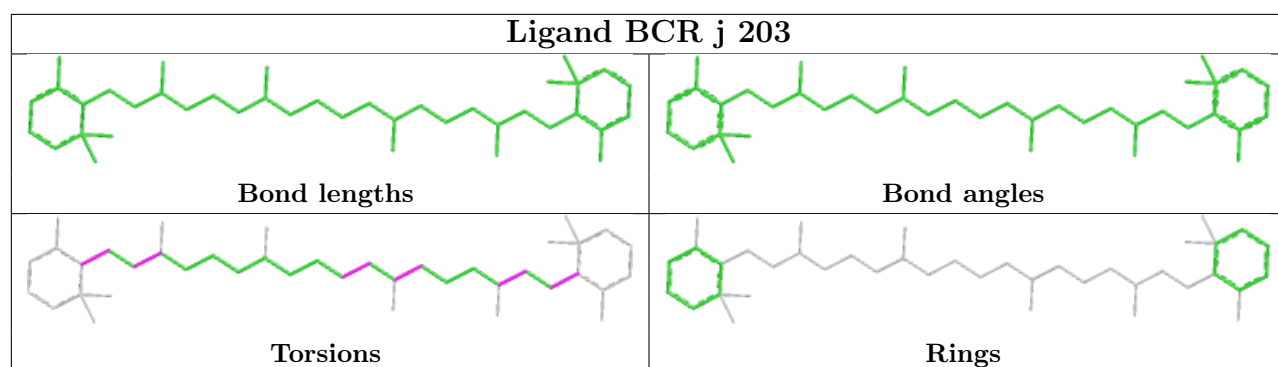


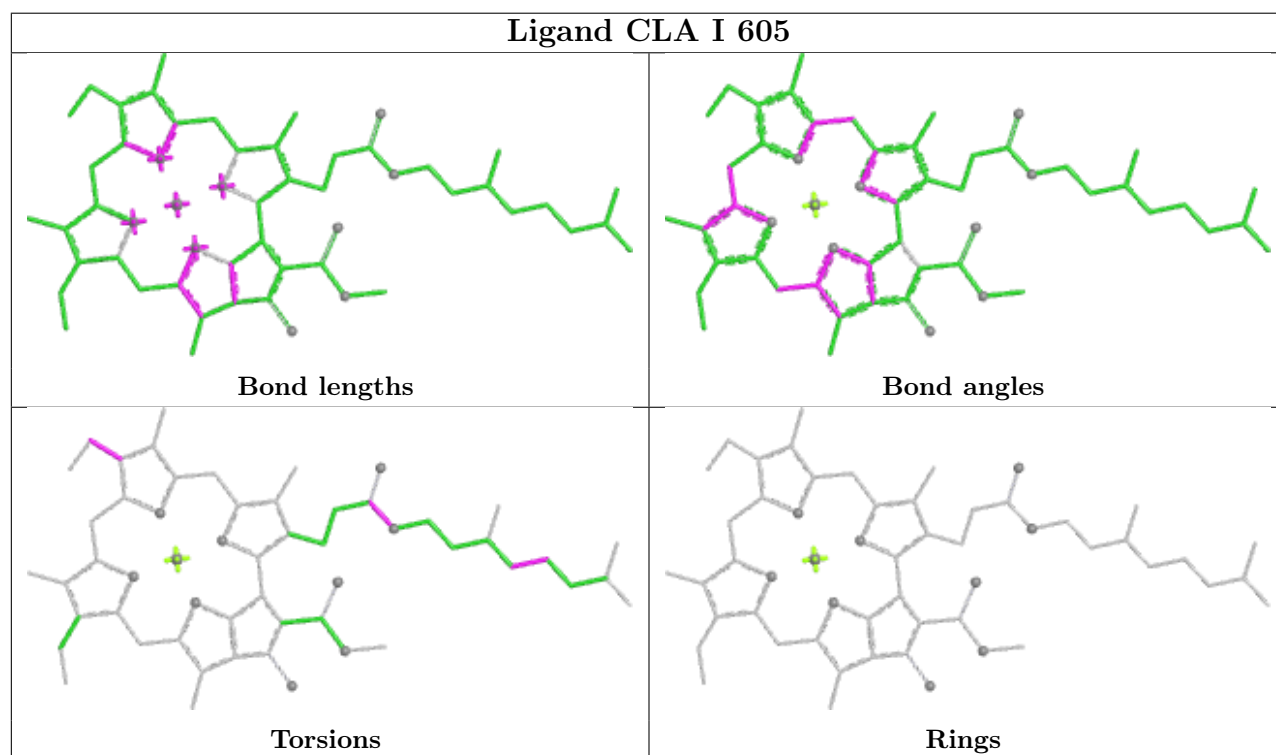
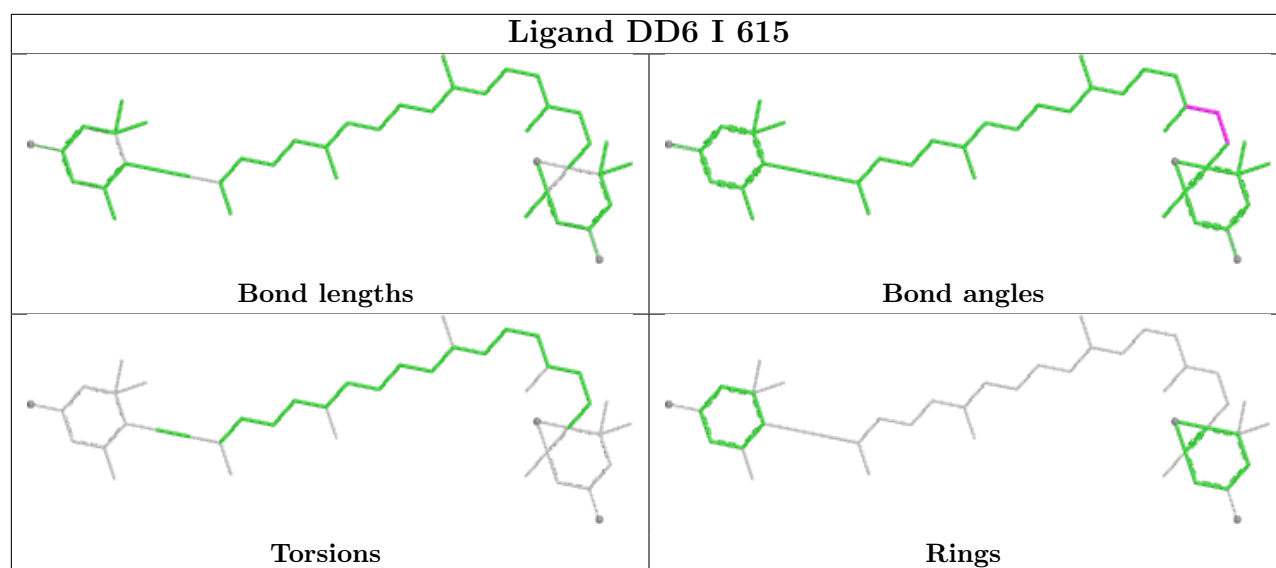
Ligand KC2 K 607



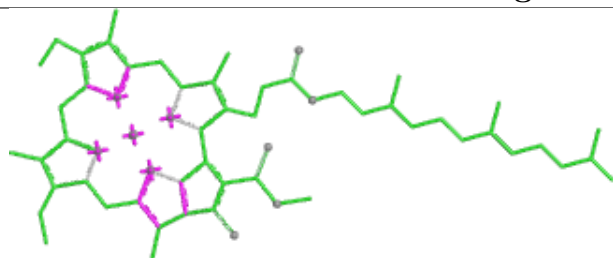
Ligand LMG b 733



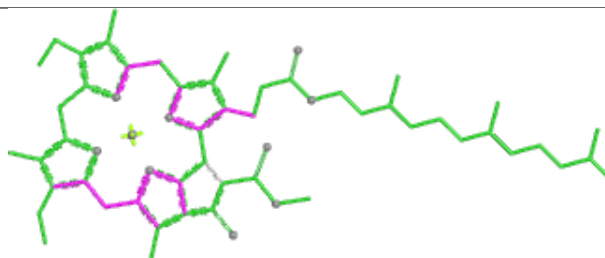




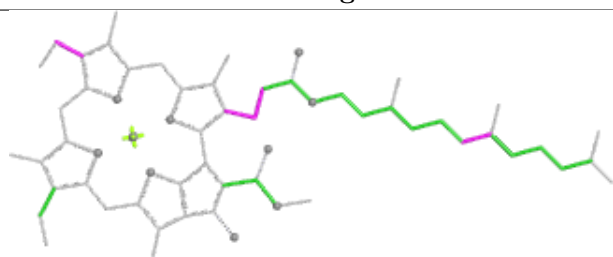
Ligand CLA B 601



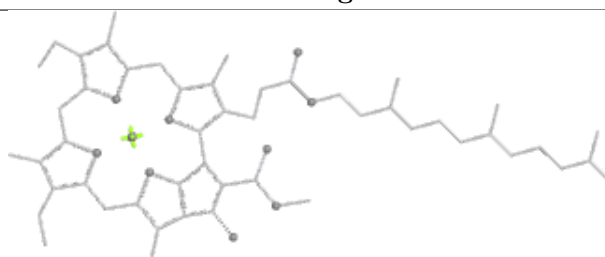
Bond lengths



Bond angles

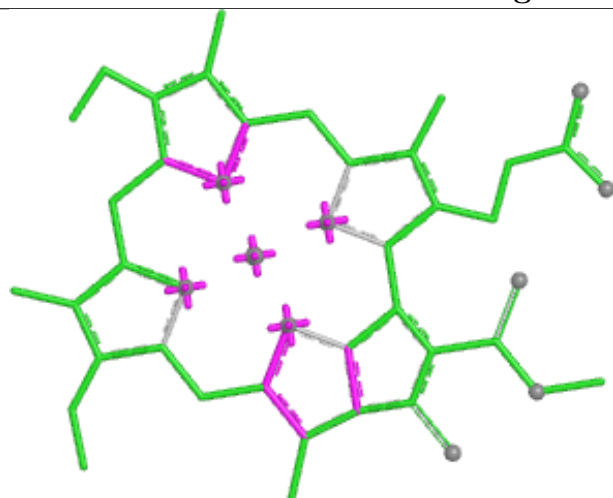


Torsions

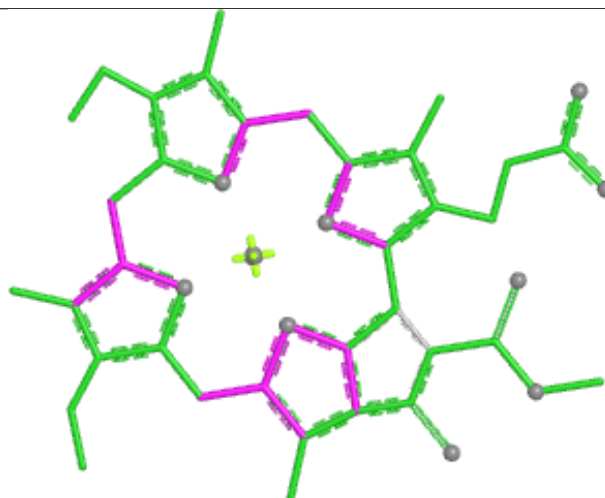


Rings

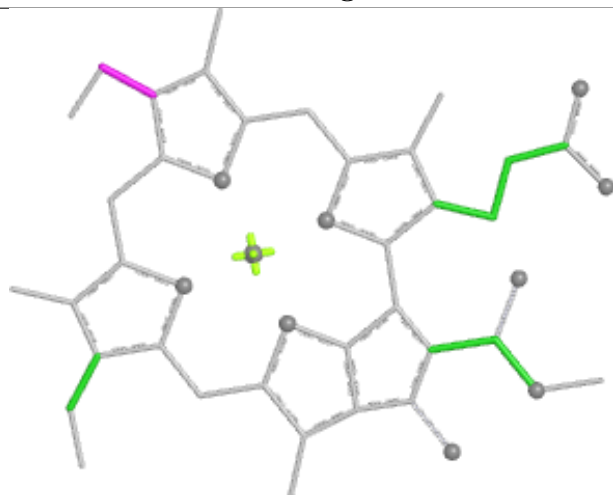
Ligand CLA A 607



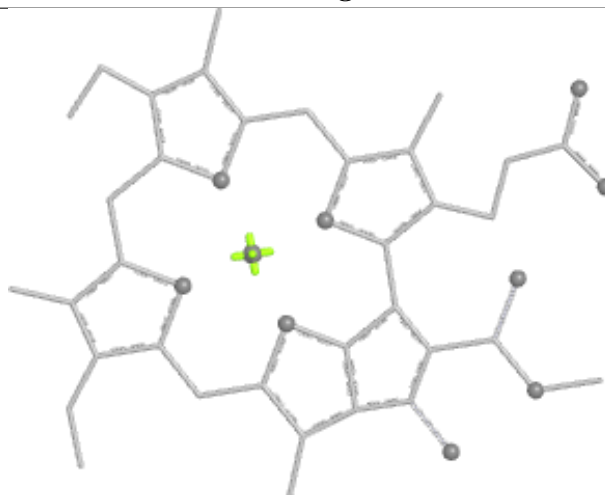
Bond lengths



Bond angles

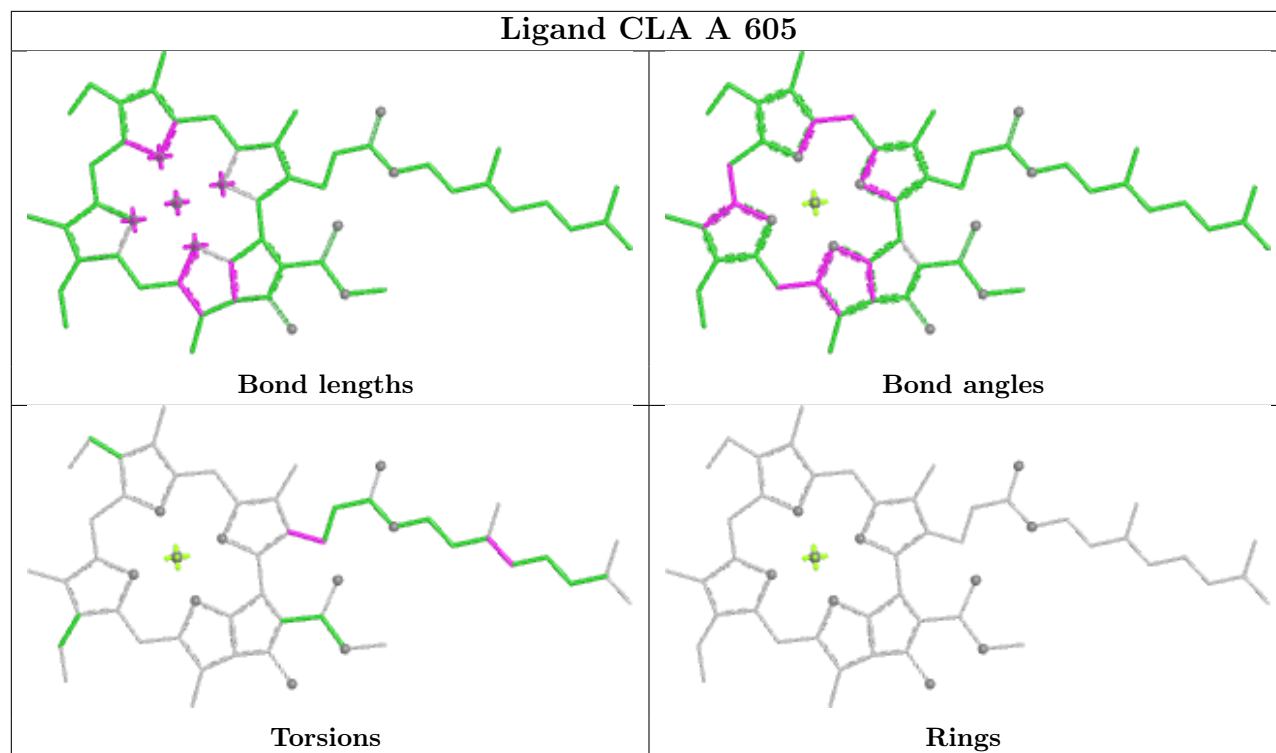


Torsions

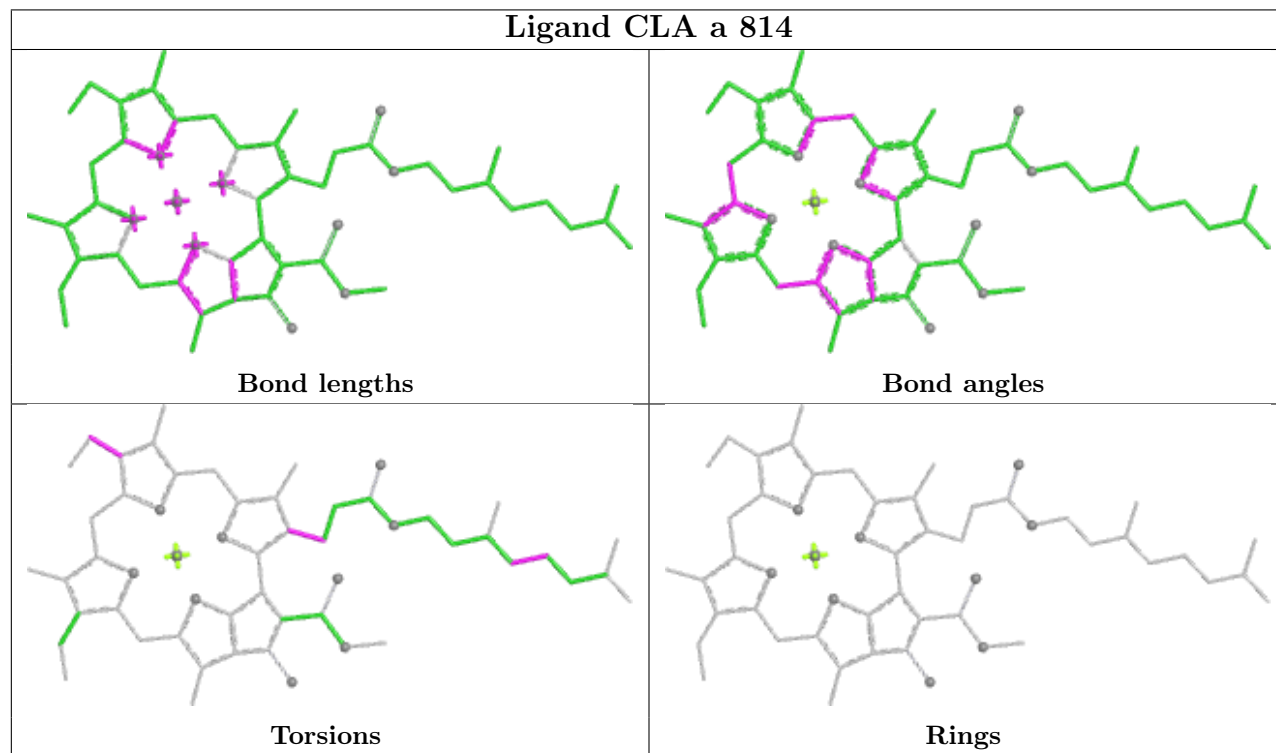


Rings

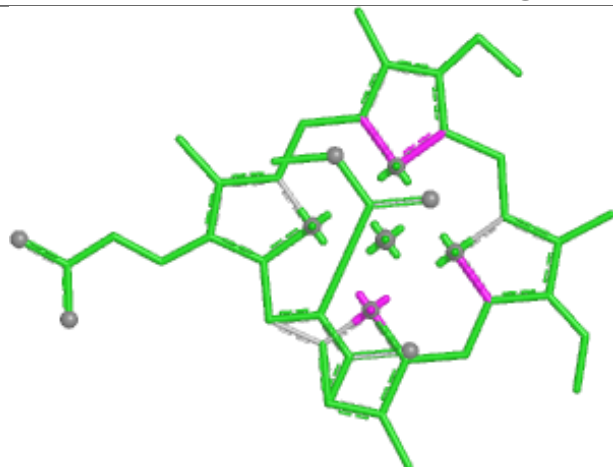
Ligand CLA A 605



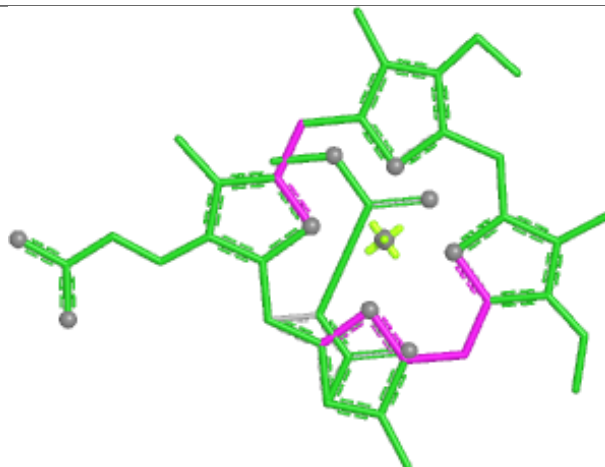
Ligand CLA a 814



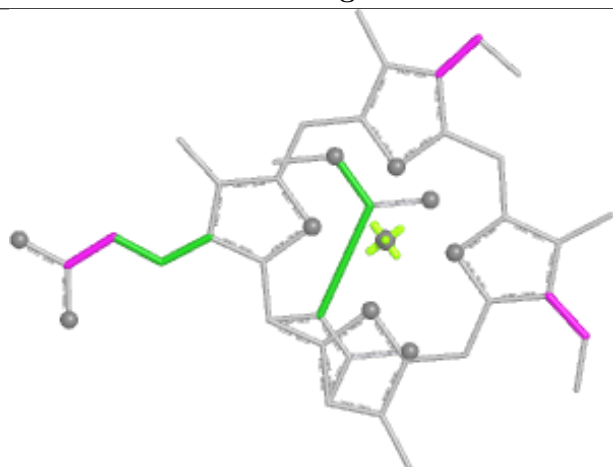
Ligand KC2 T 608



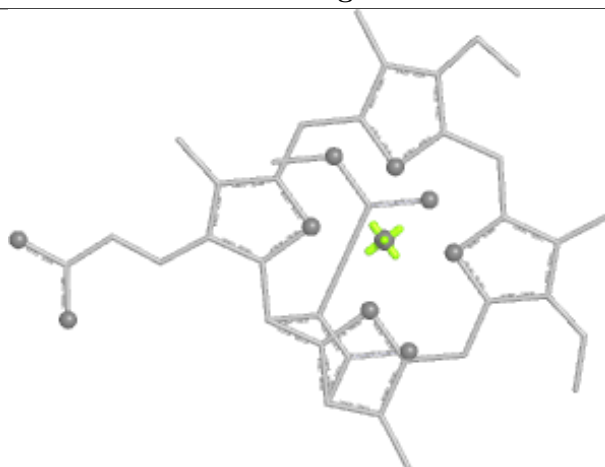
Bond lengths



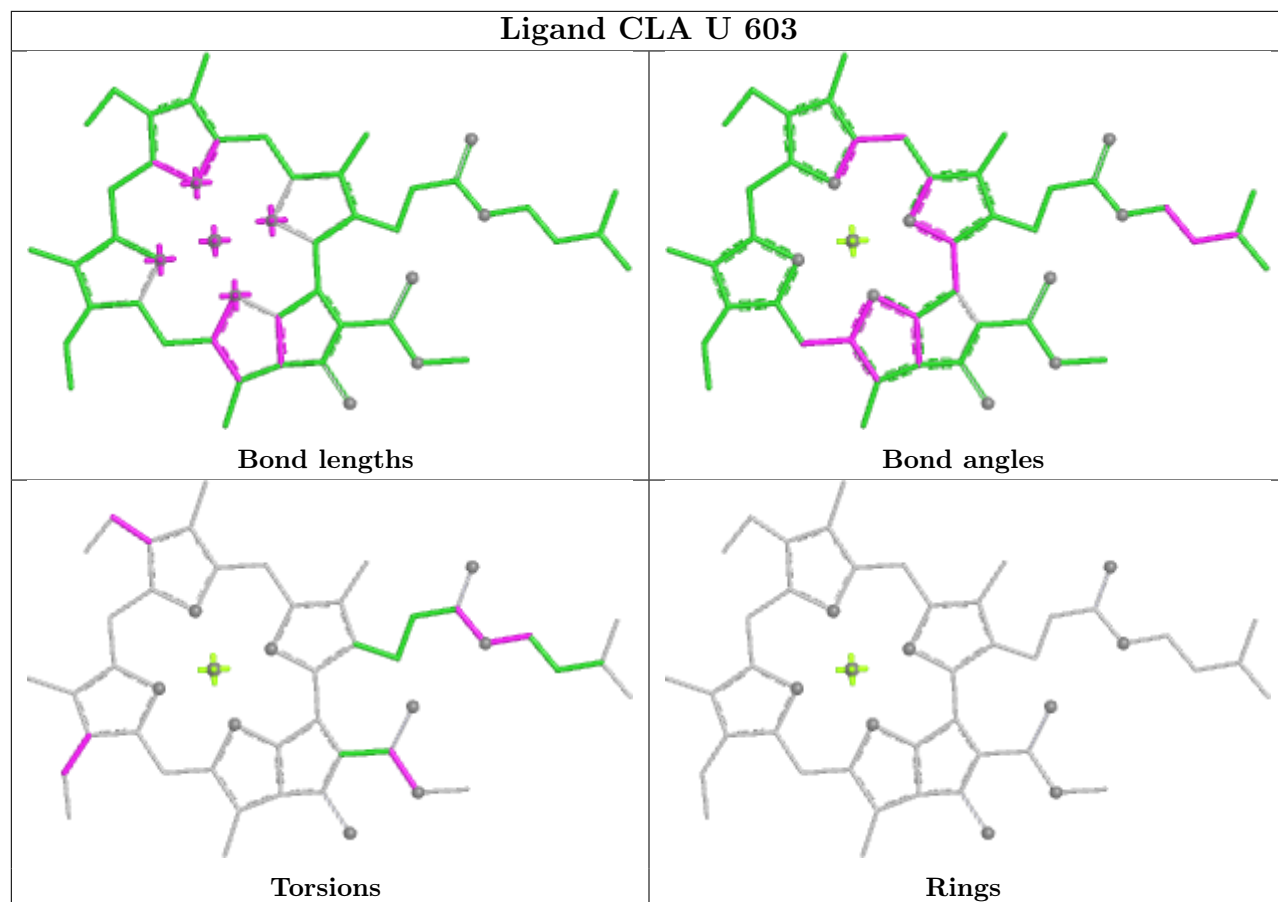
Bond angles



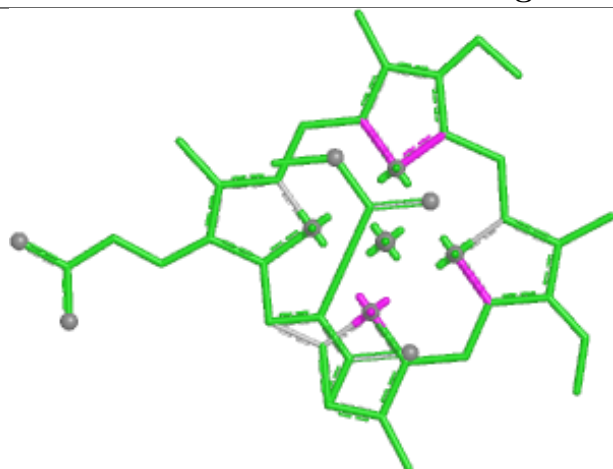
Torsions



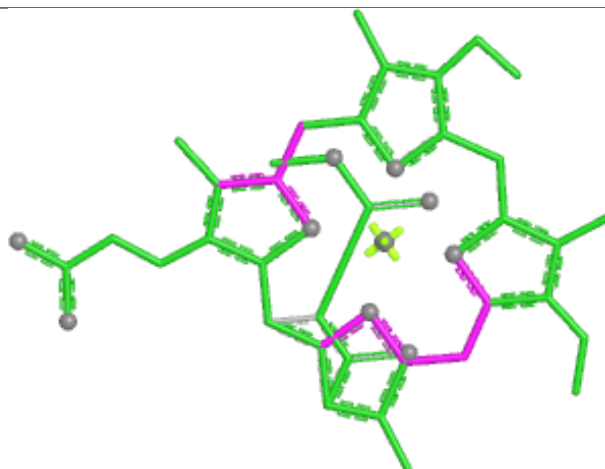
Rings



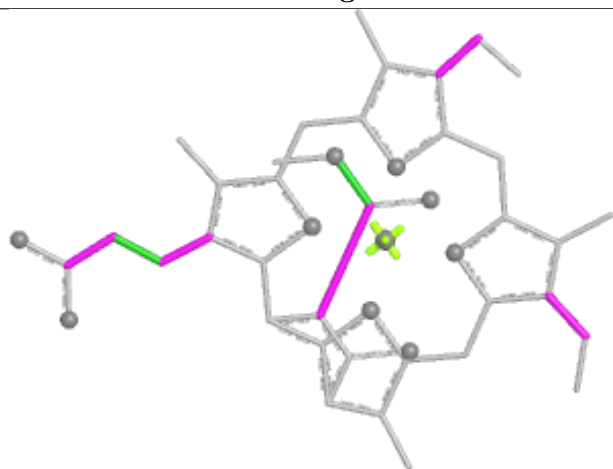
Ligand KC2 G 601



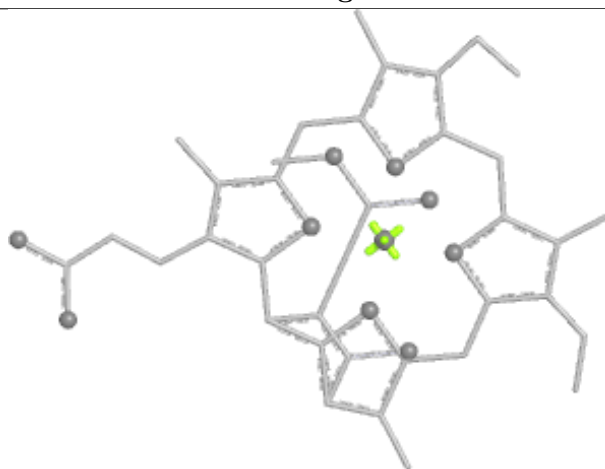
Bond lengths



Bond angles

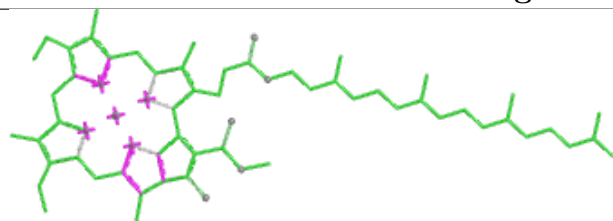


Torsions

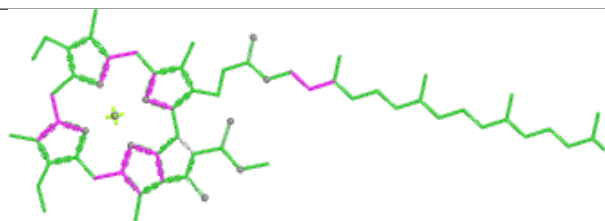


Rings

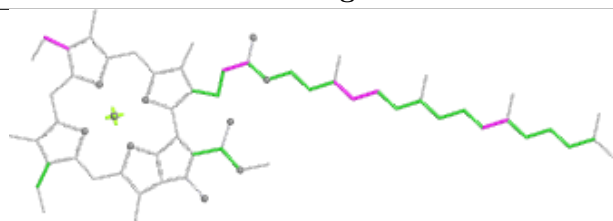
Ligand CLA B 609



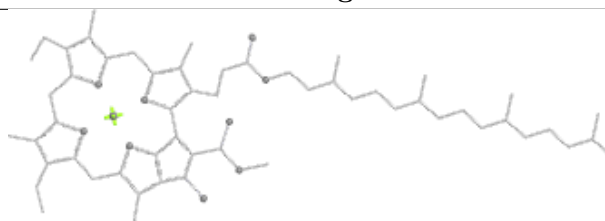
Bond lengths



Bond angles

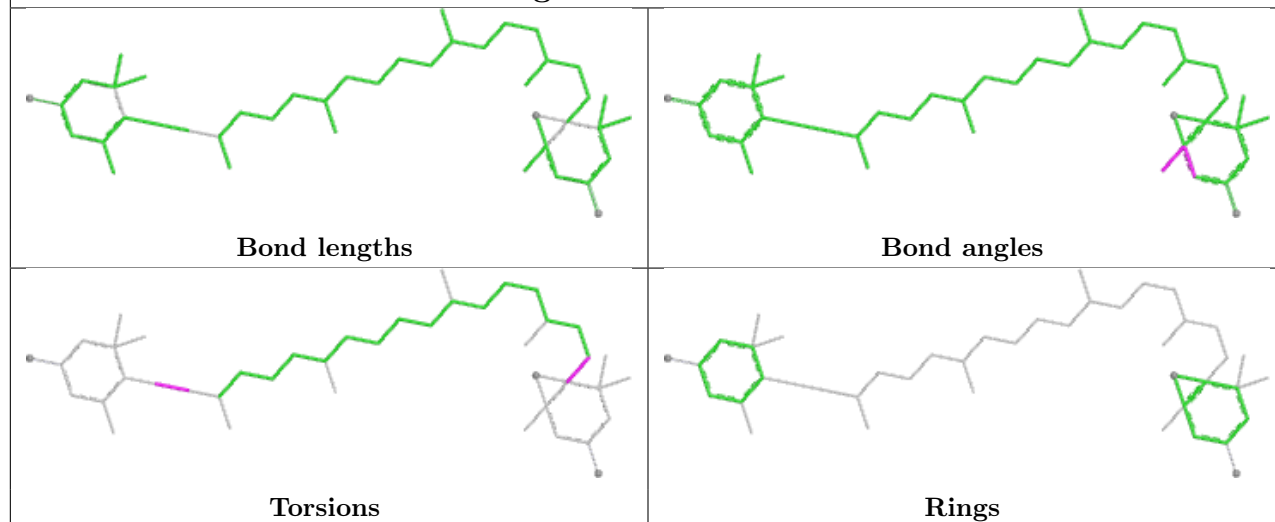


Torsions

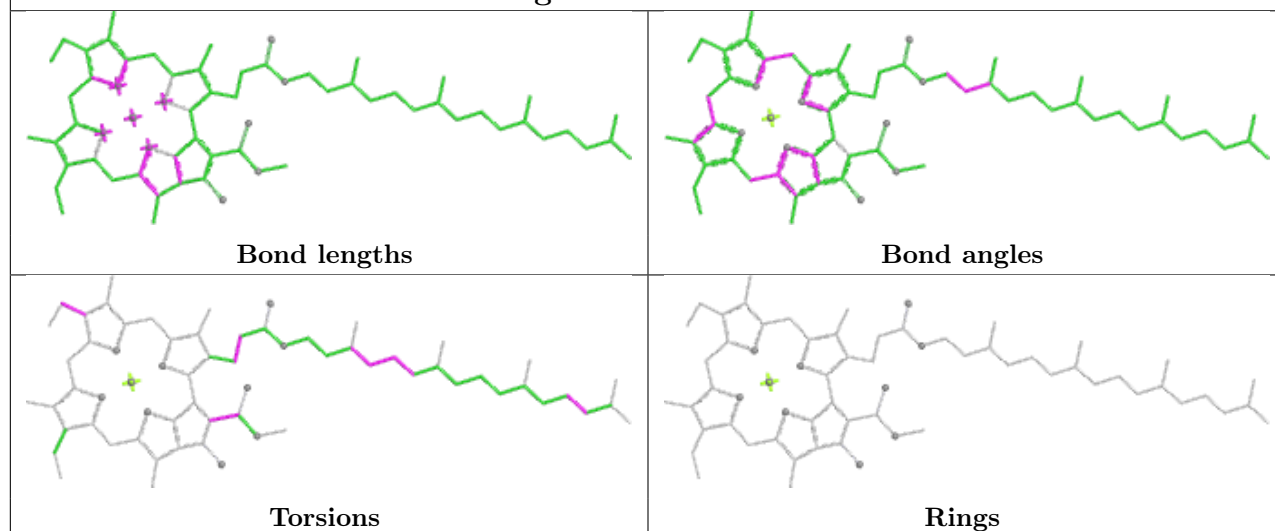


Rings

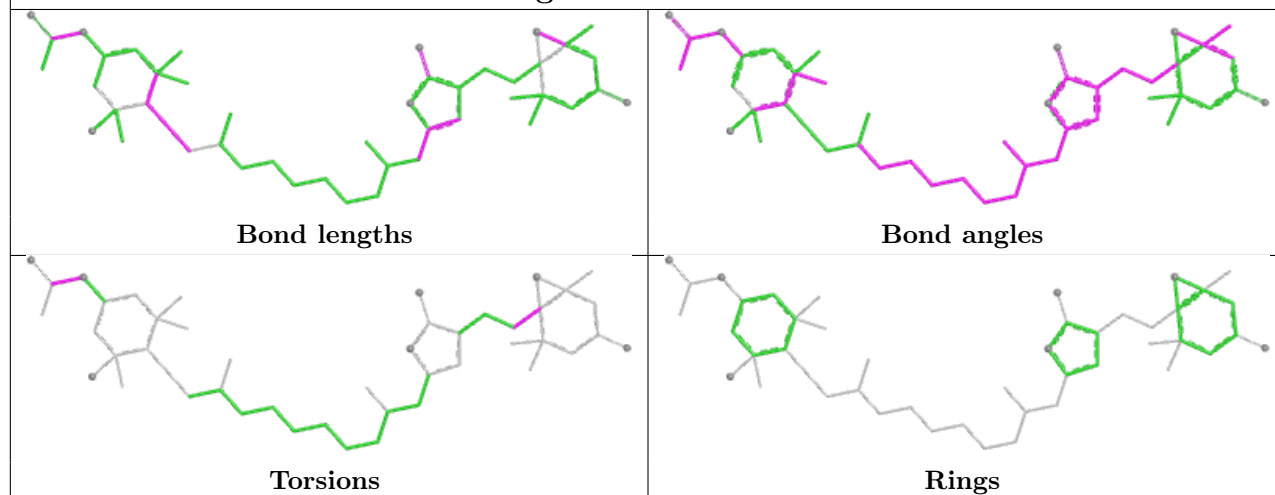
Ligand DD6 E 615



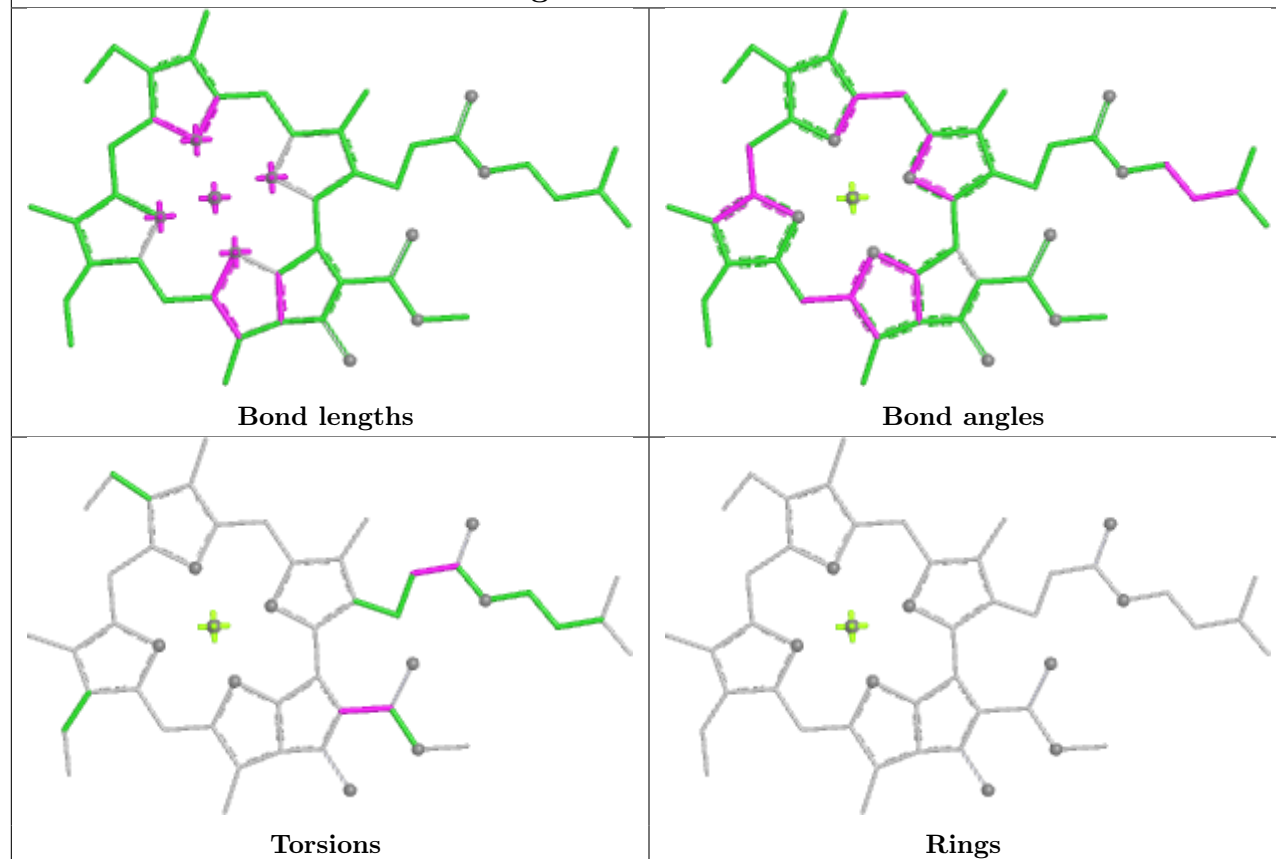
Ligand CLA b 704



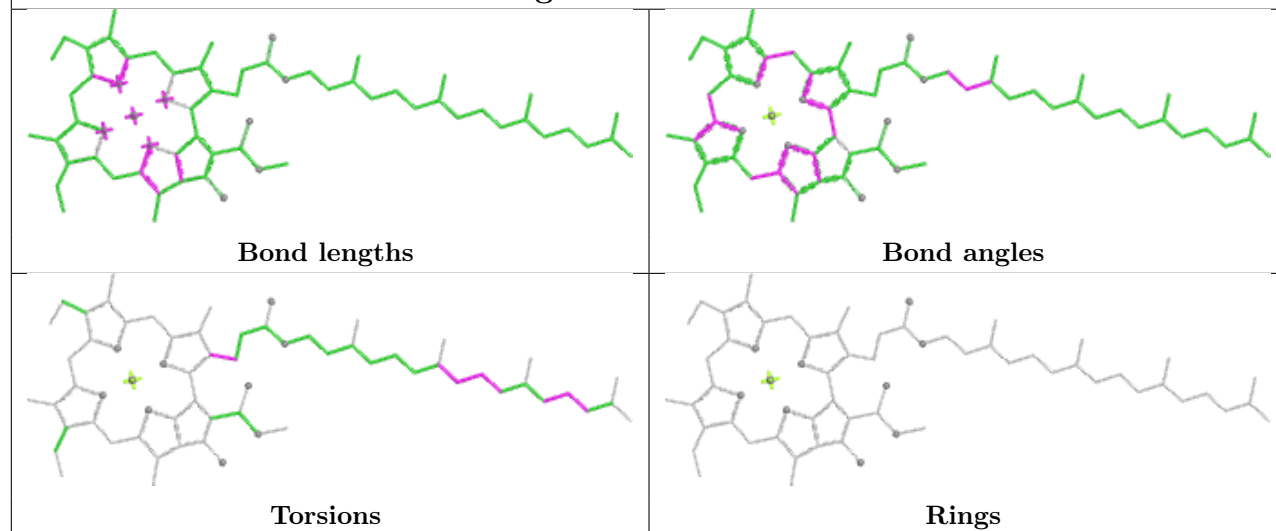
Ligand PID B 613

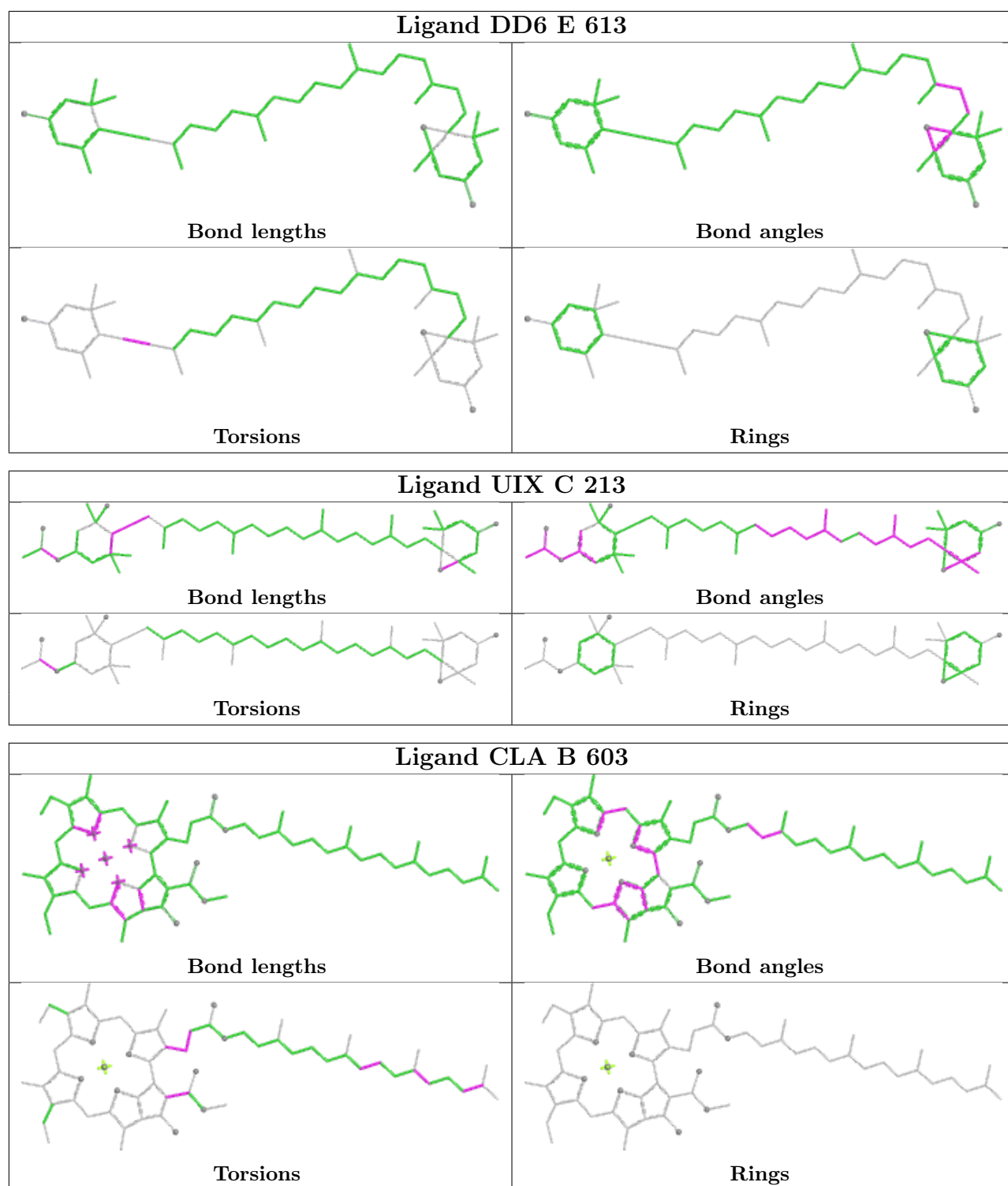


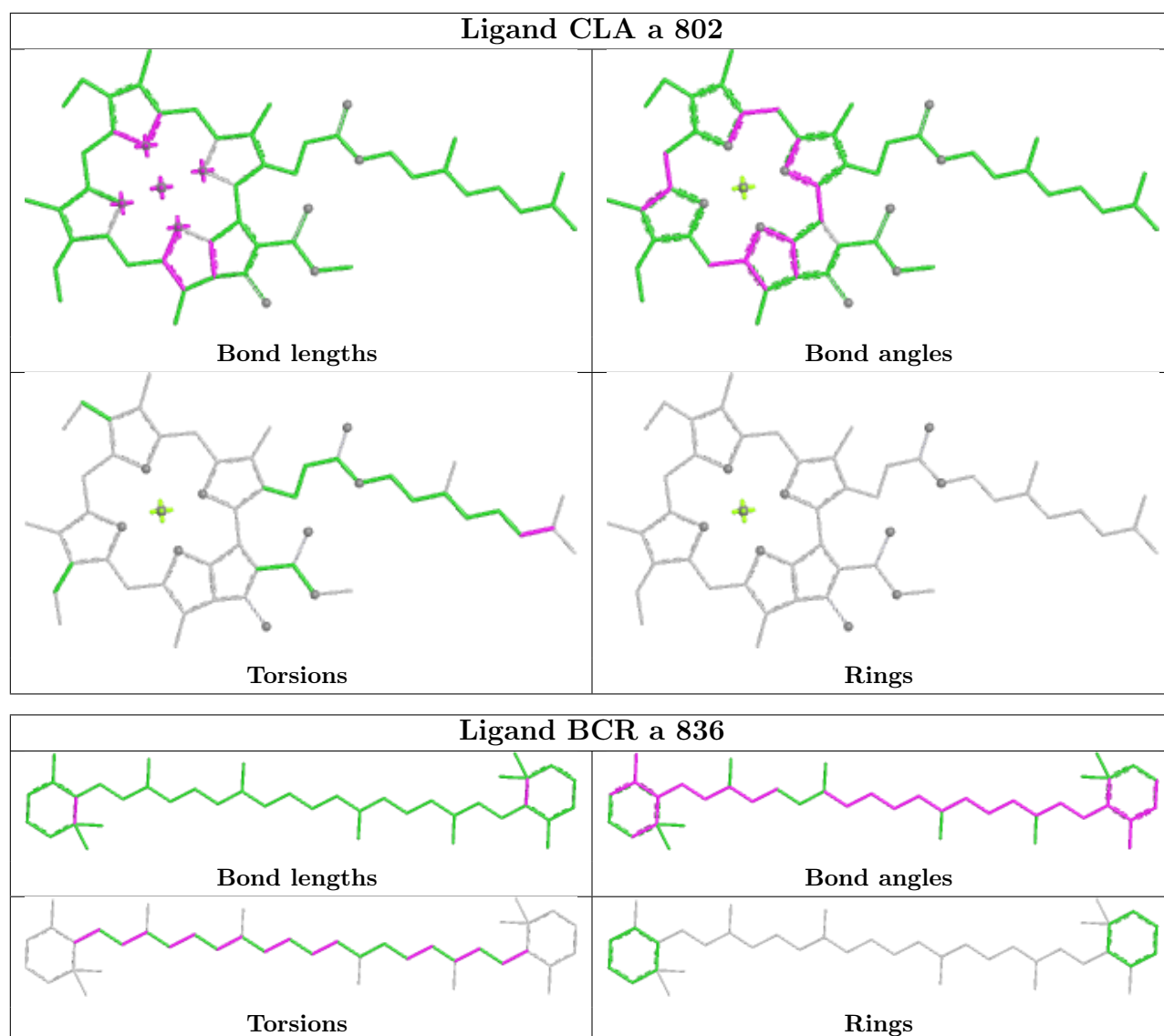
Ligand CLA G 603



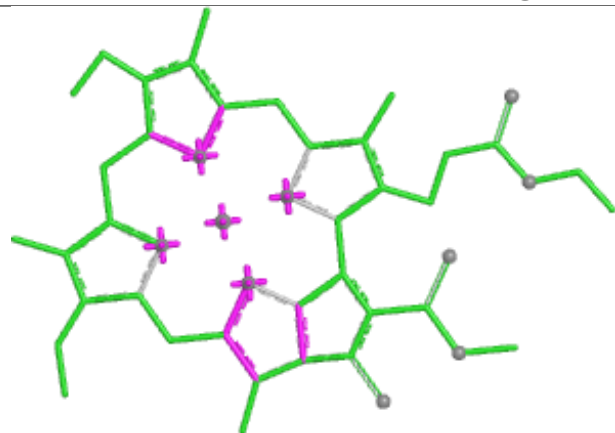
Ligand CLA b 718



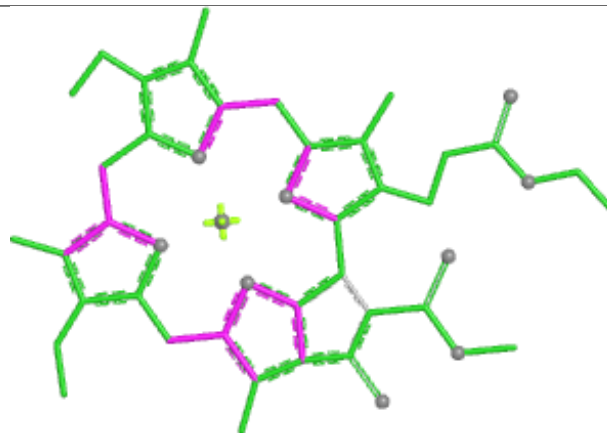




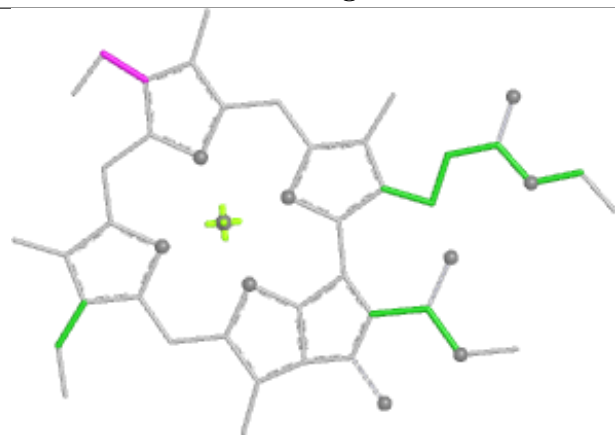
Ligand CLA C 212



Bond lengths



Bond angles

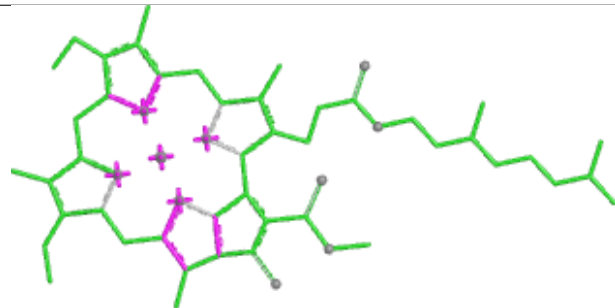


Torsions

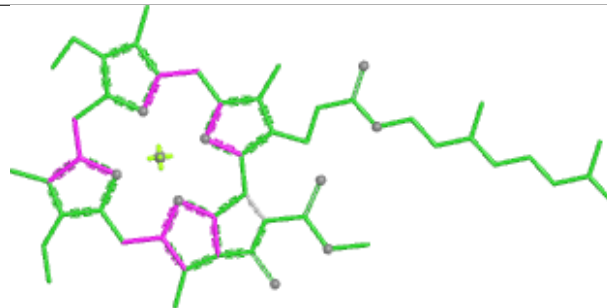


Rings

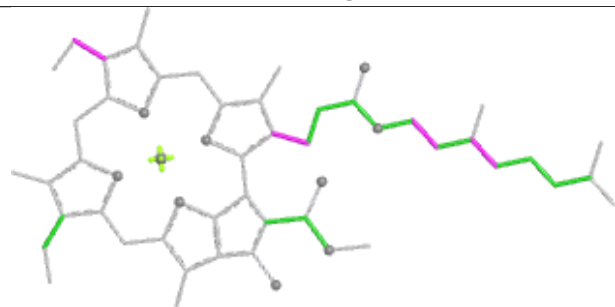
Ligand CLA D 612



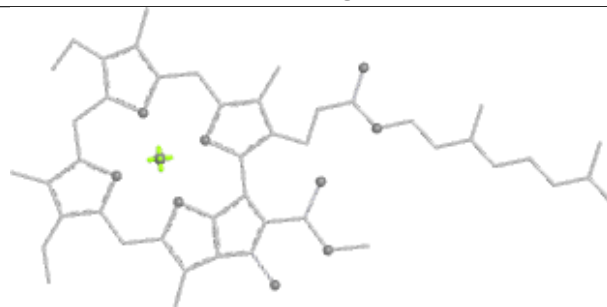
Bond lengths



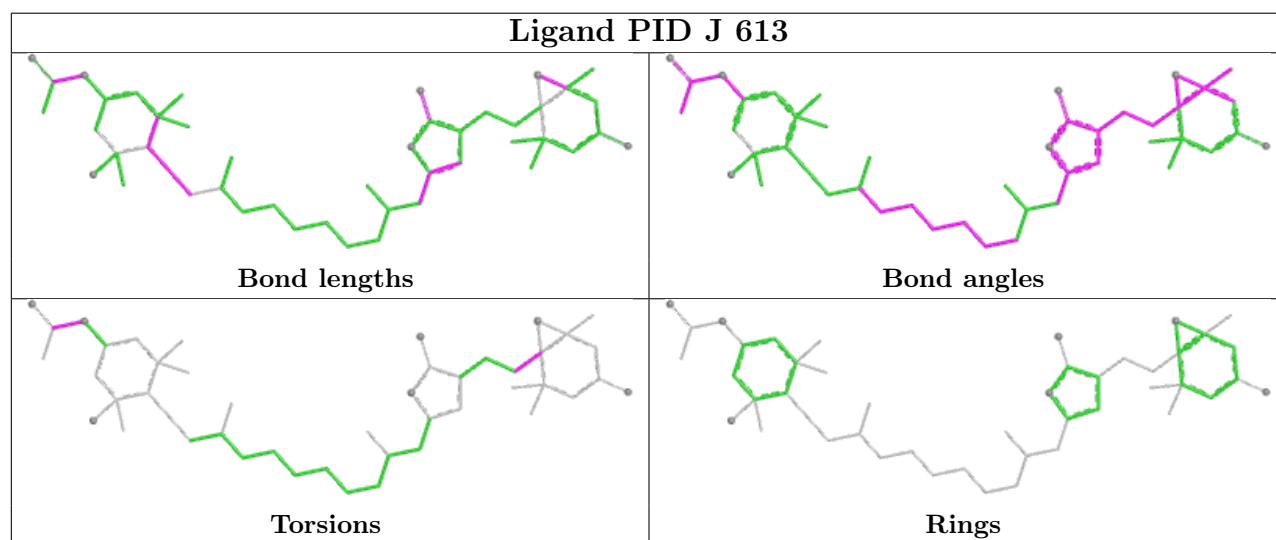
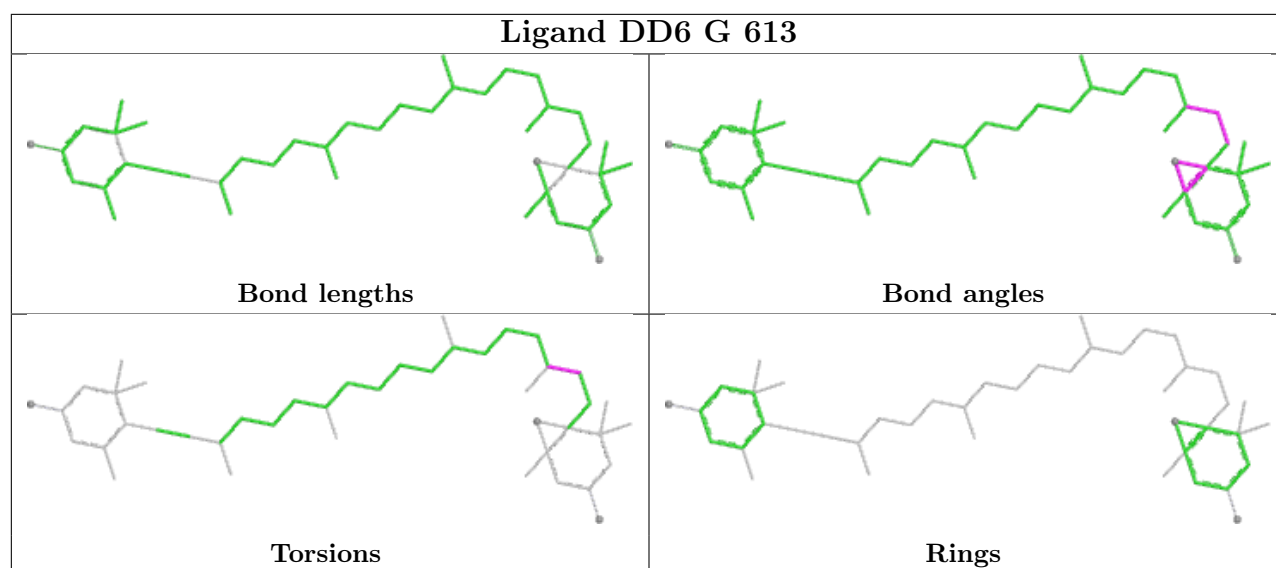
Bond angles

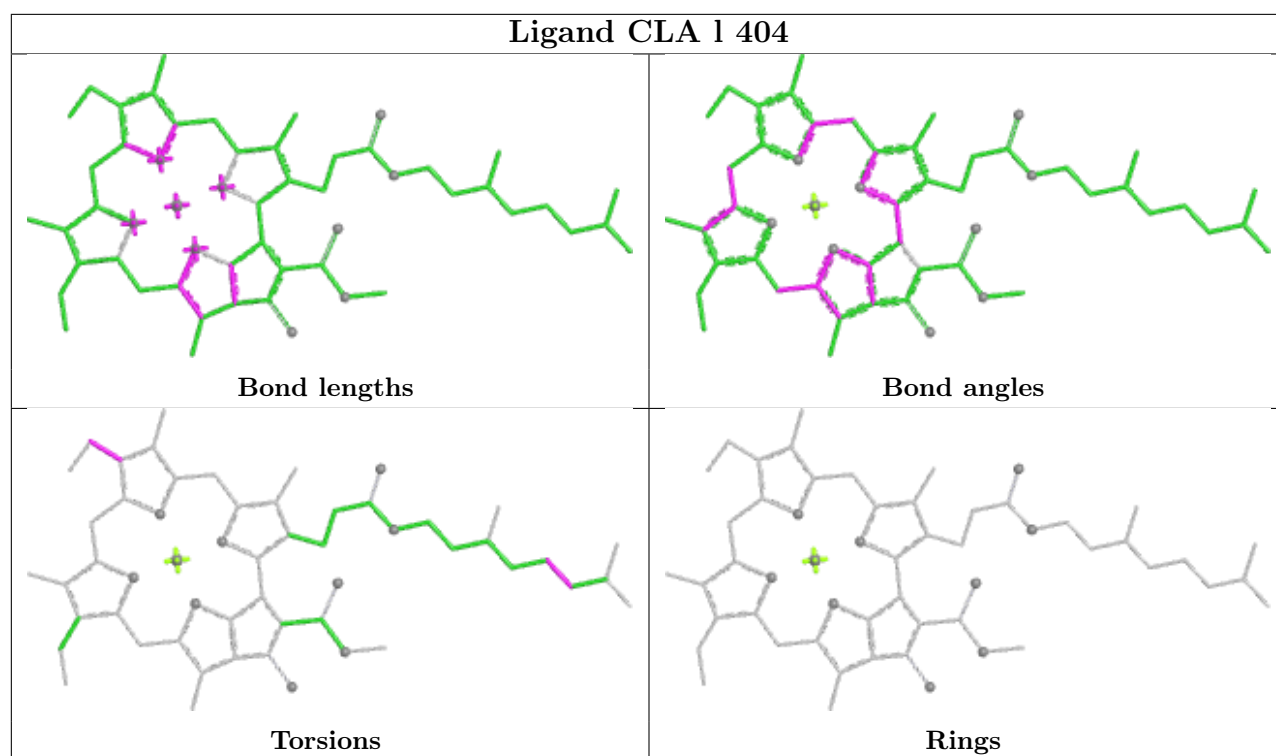


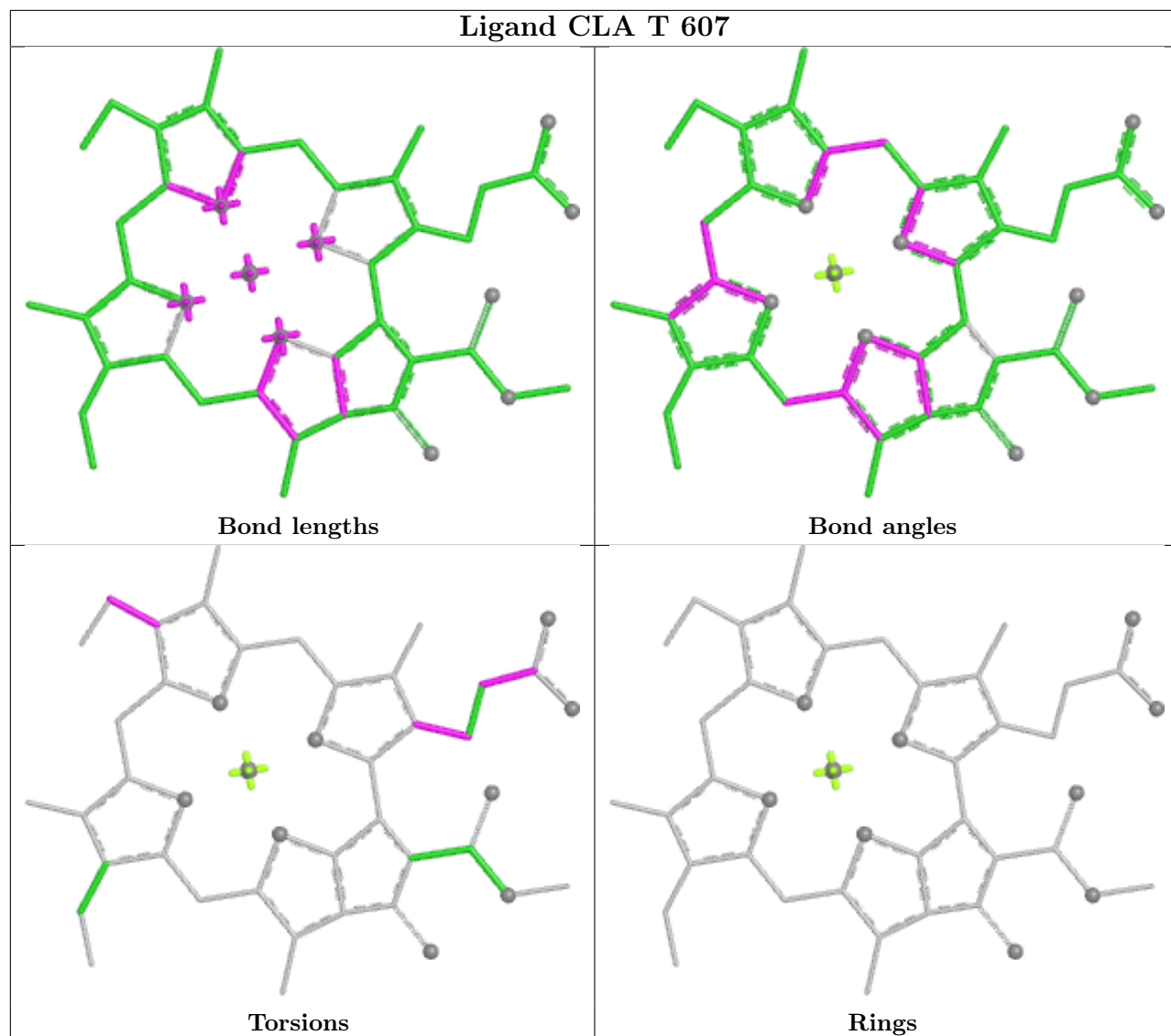
Torsions



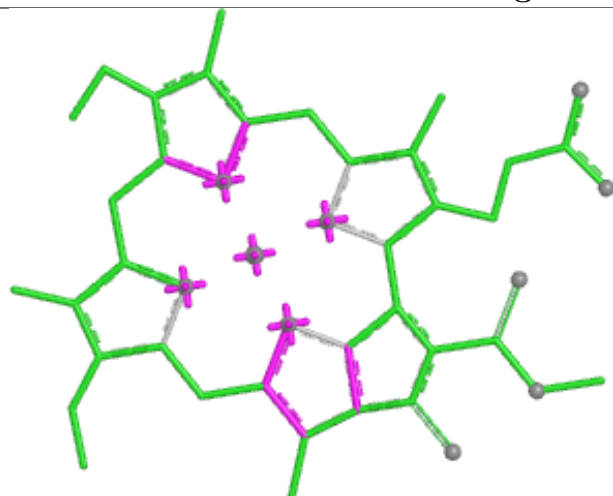
Rings



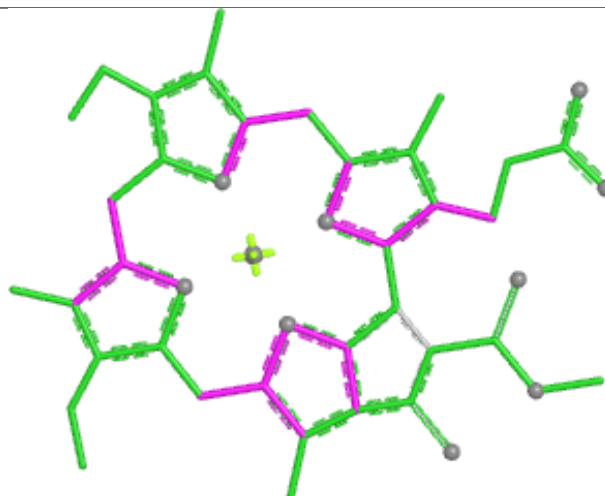




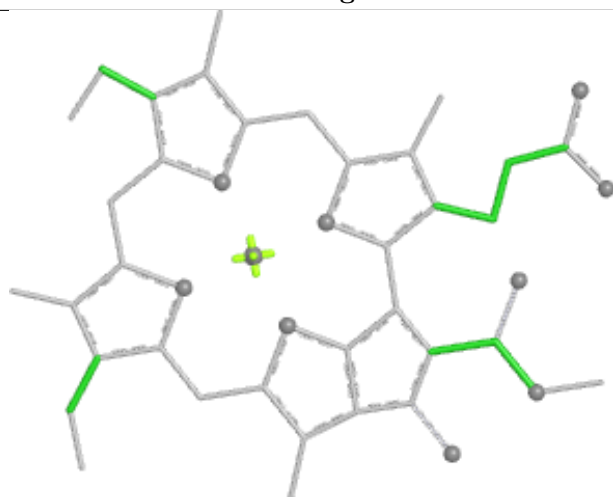
Ligand CLA C 209



Bond lengths



Bond angles

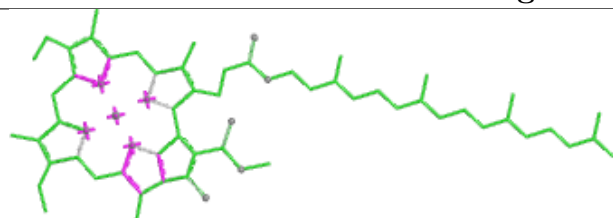


Torsions

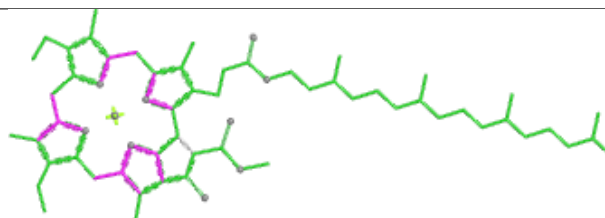


Rings

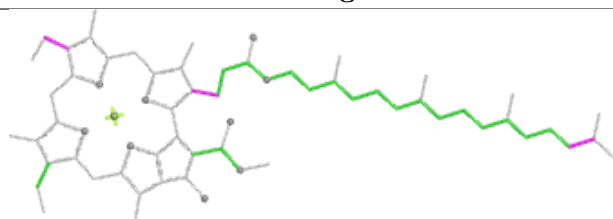
Ligand CLA b 707



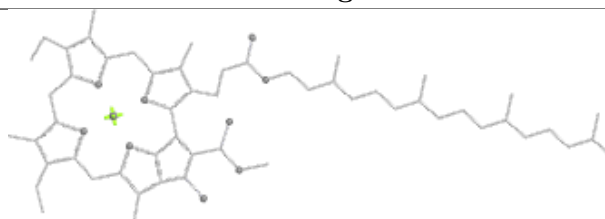
Bond lengths



Bond angles

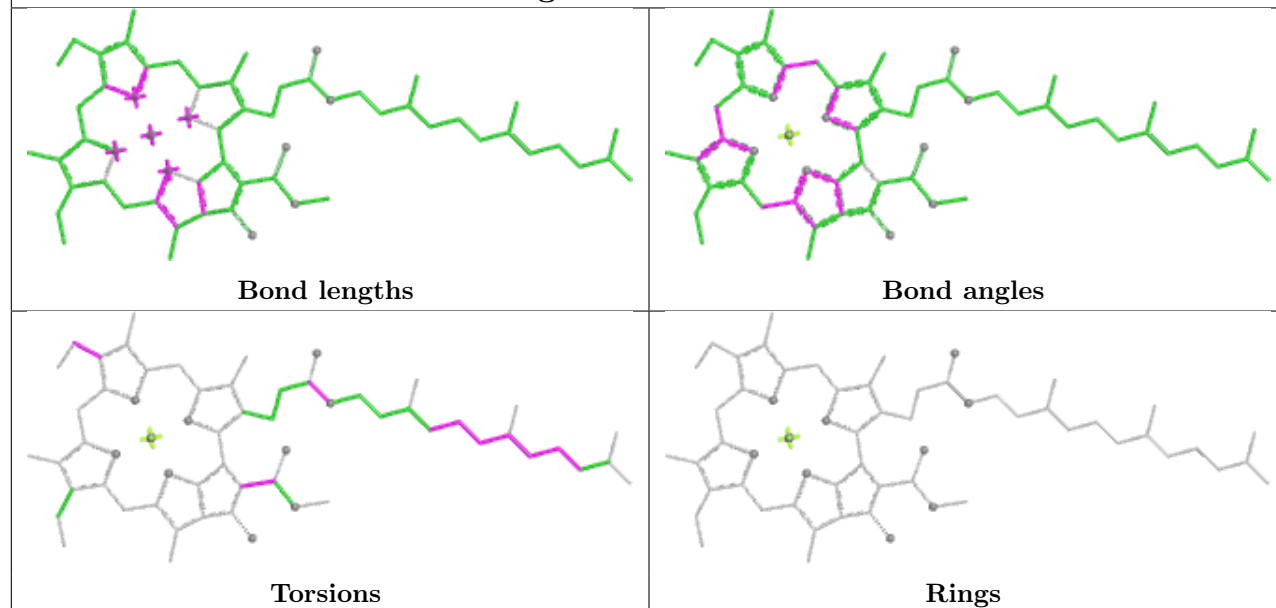


Torsions

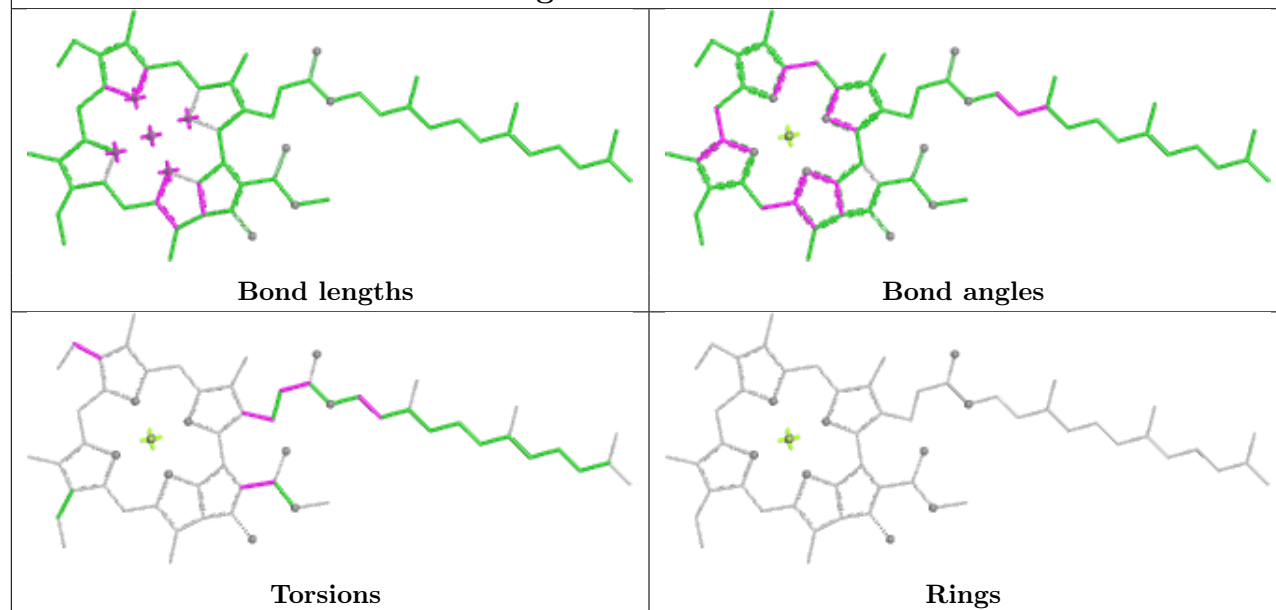


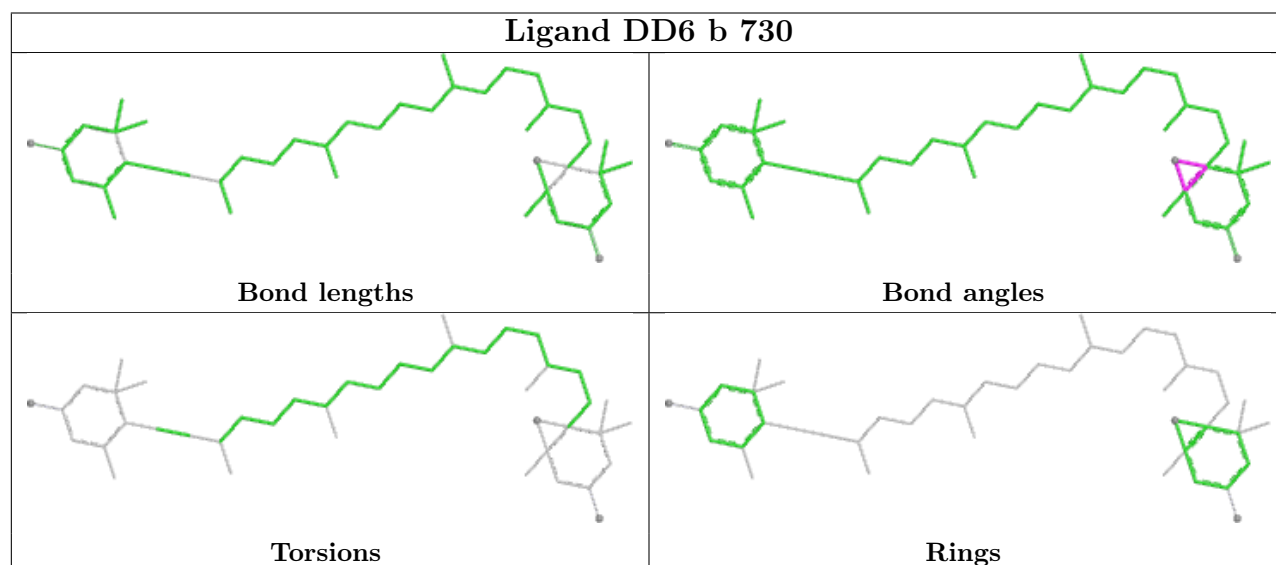
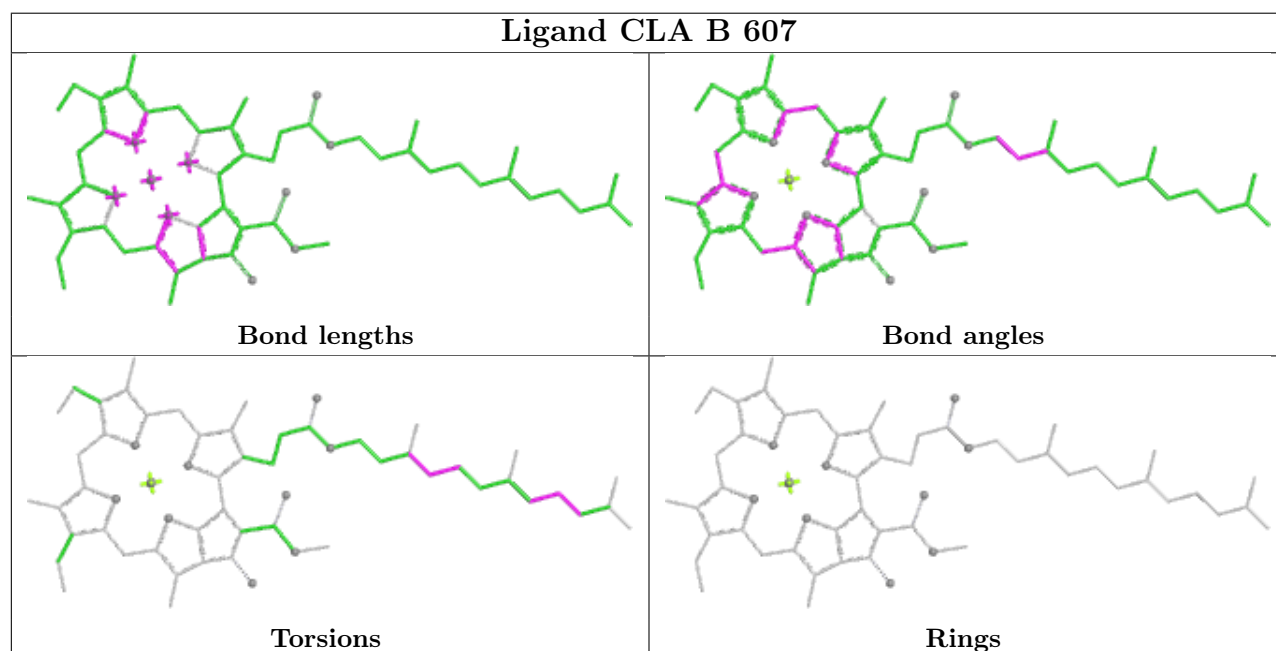
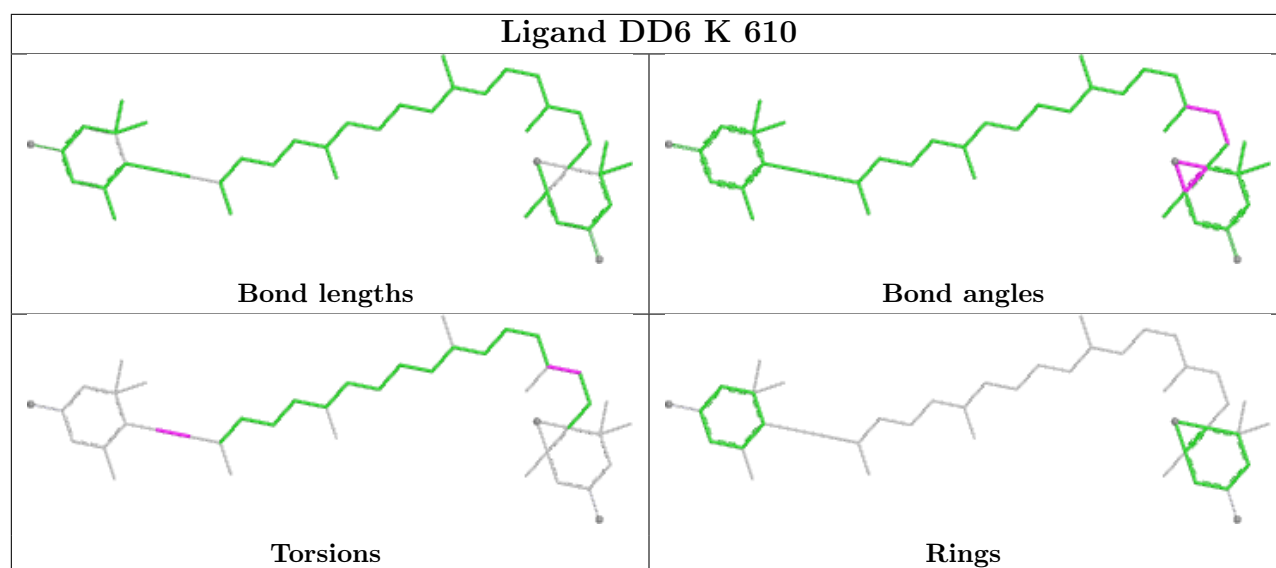
Rings

Ligand CLA r 204

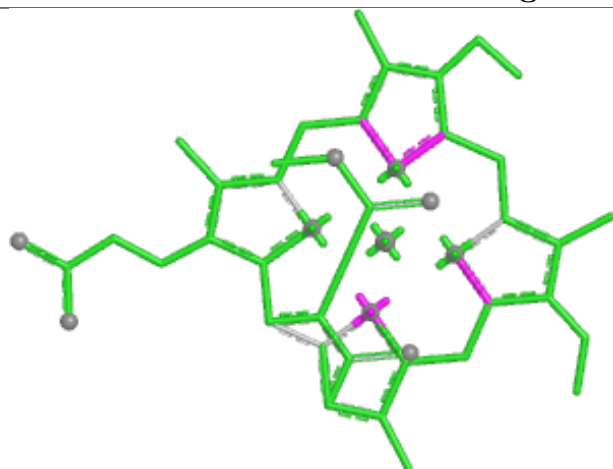


Ligand CLA a 822

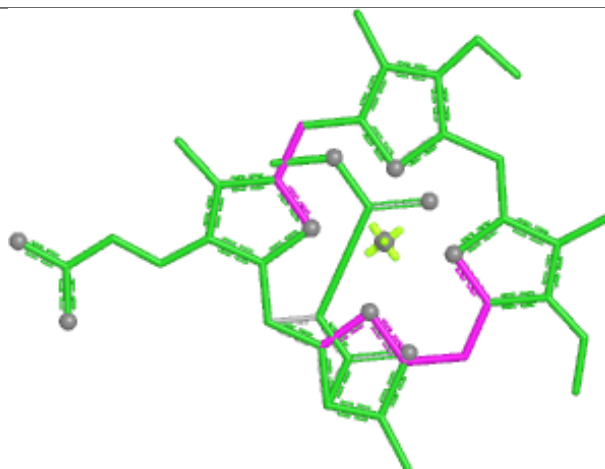




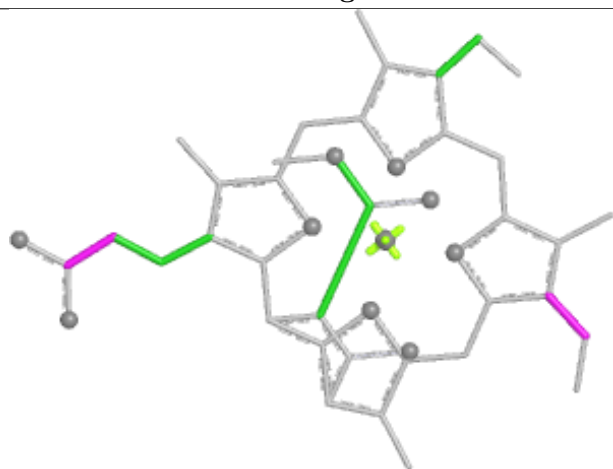
Ligand KC2 J 608



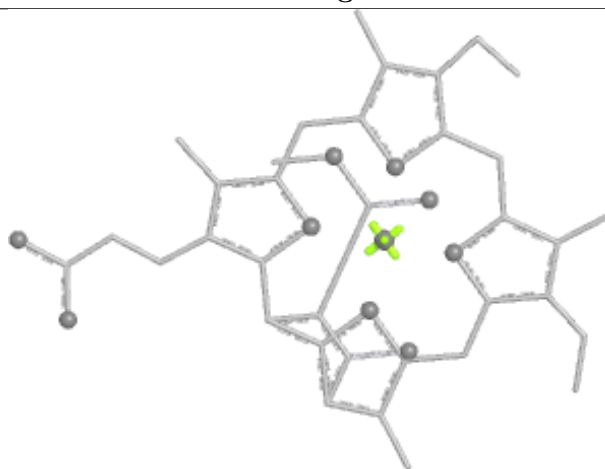
Bond lengths



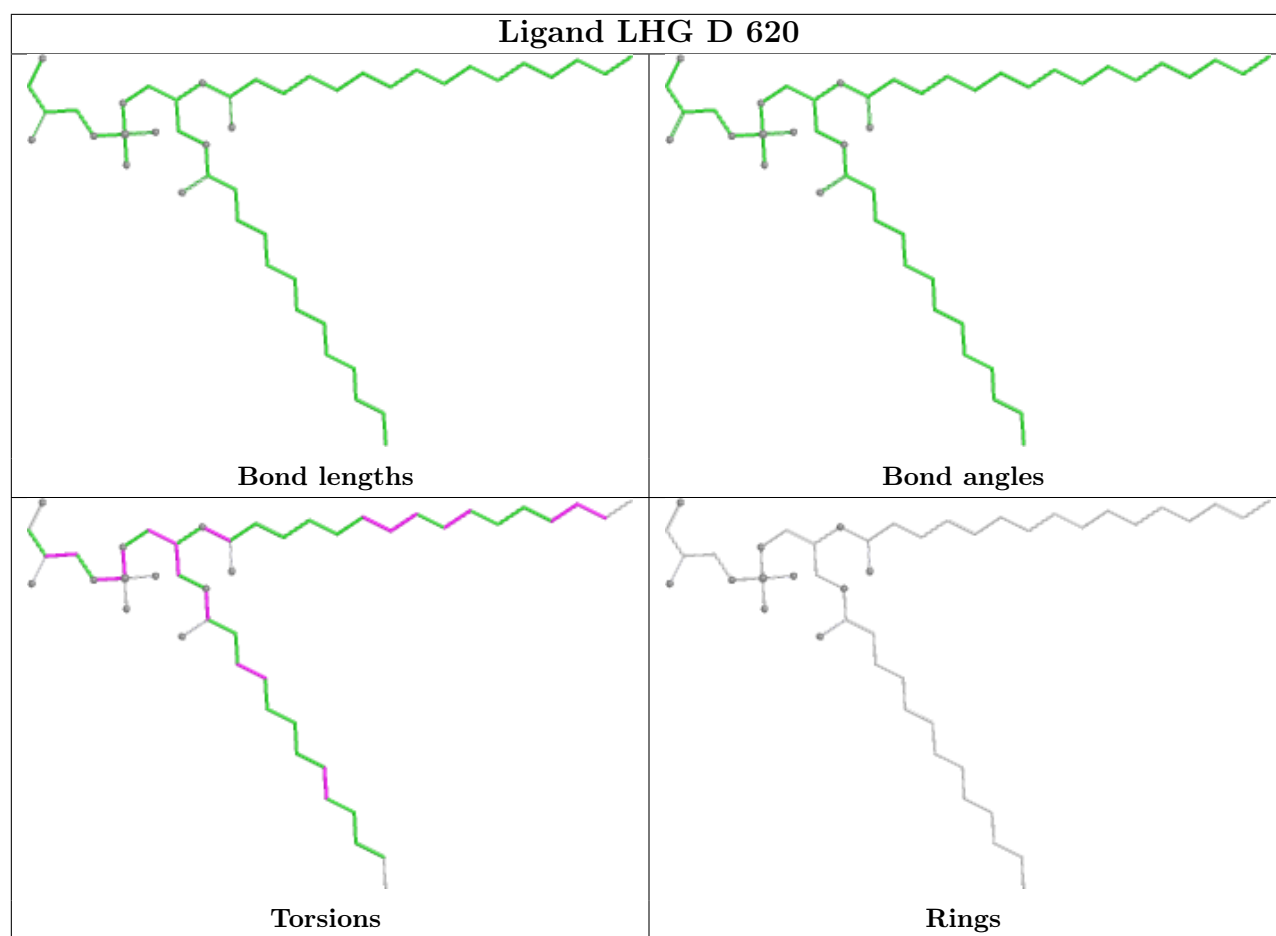
Bond angles



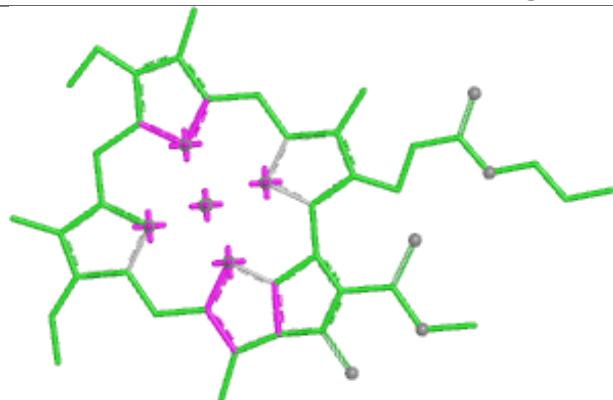
Torsions



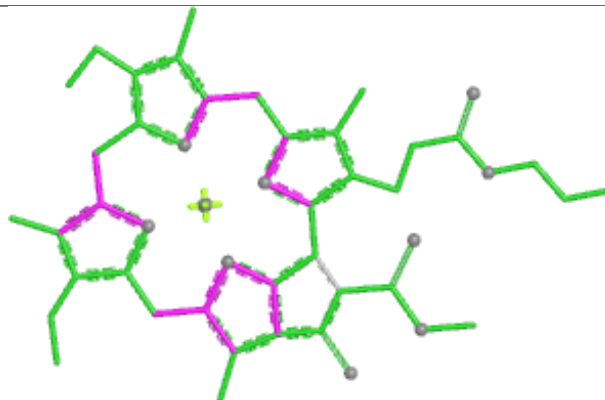
Rings



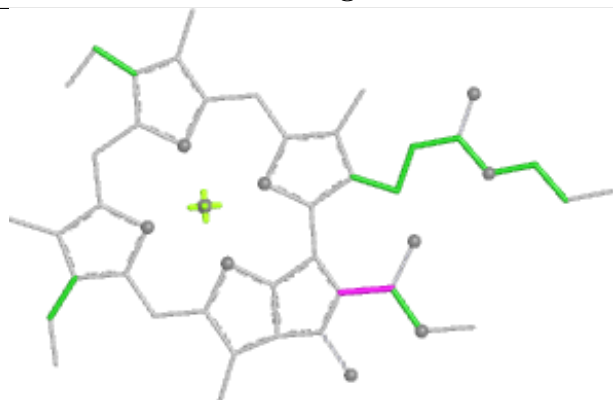
Ligand CLA 1 411



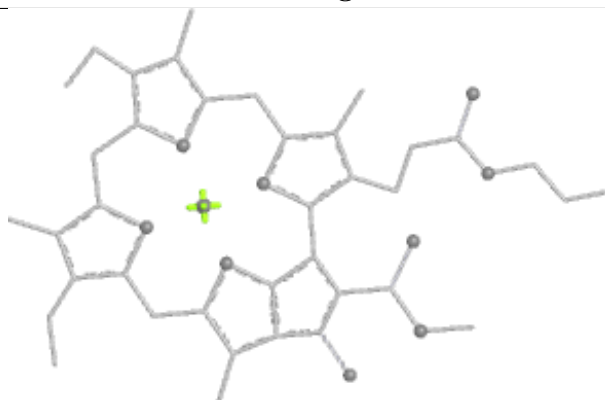
Bond lengths



Bond angles

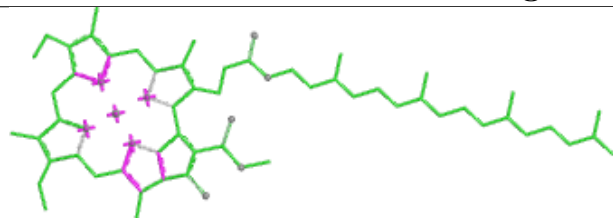


Torsions

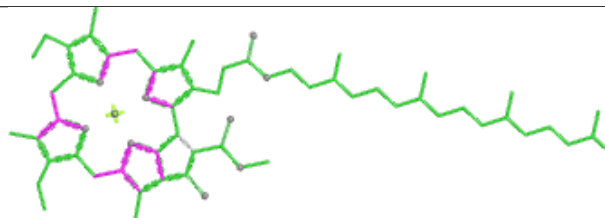


Rings

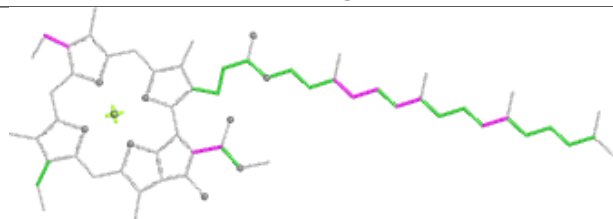
Ligand CLA 1 403



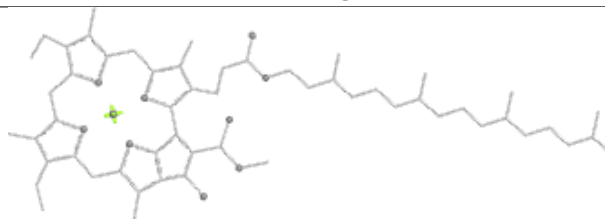
Bond lengths



Bond angles

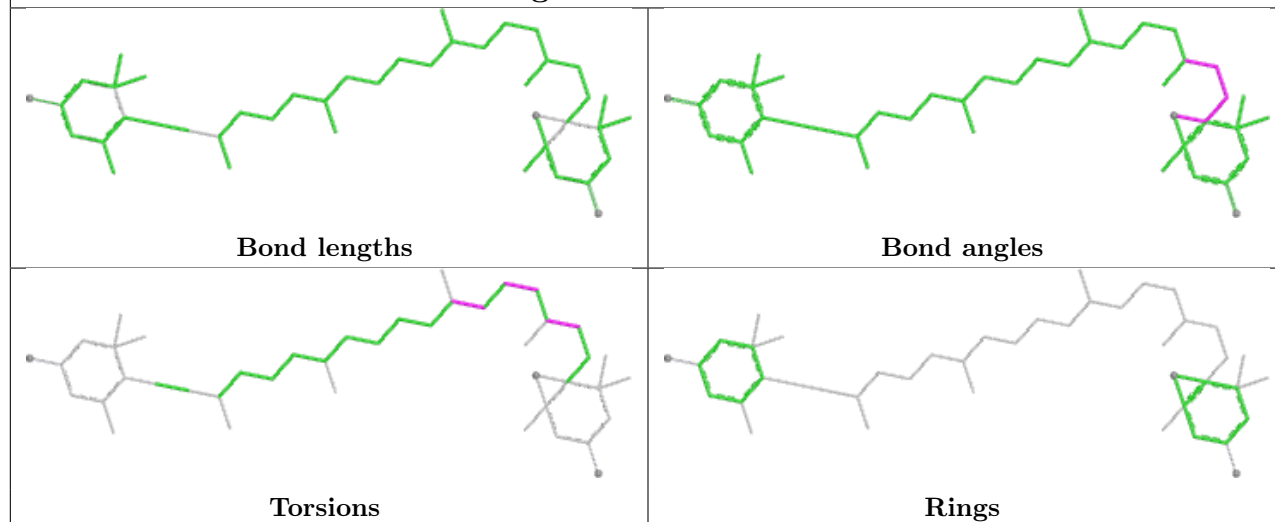


Torsions

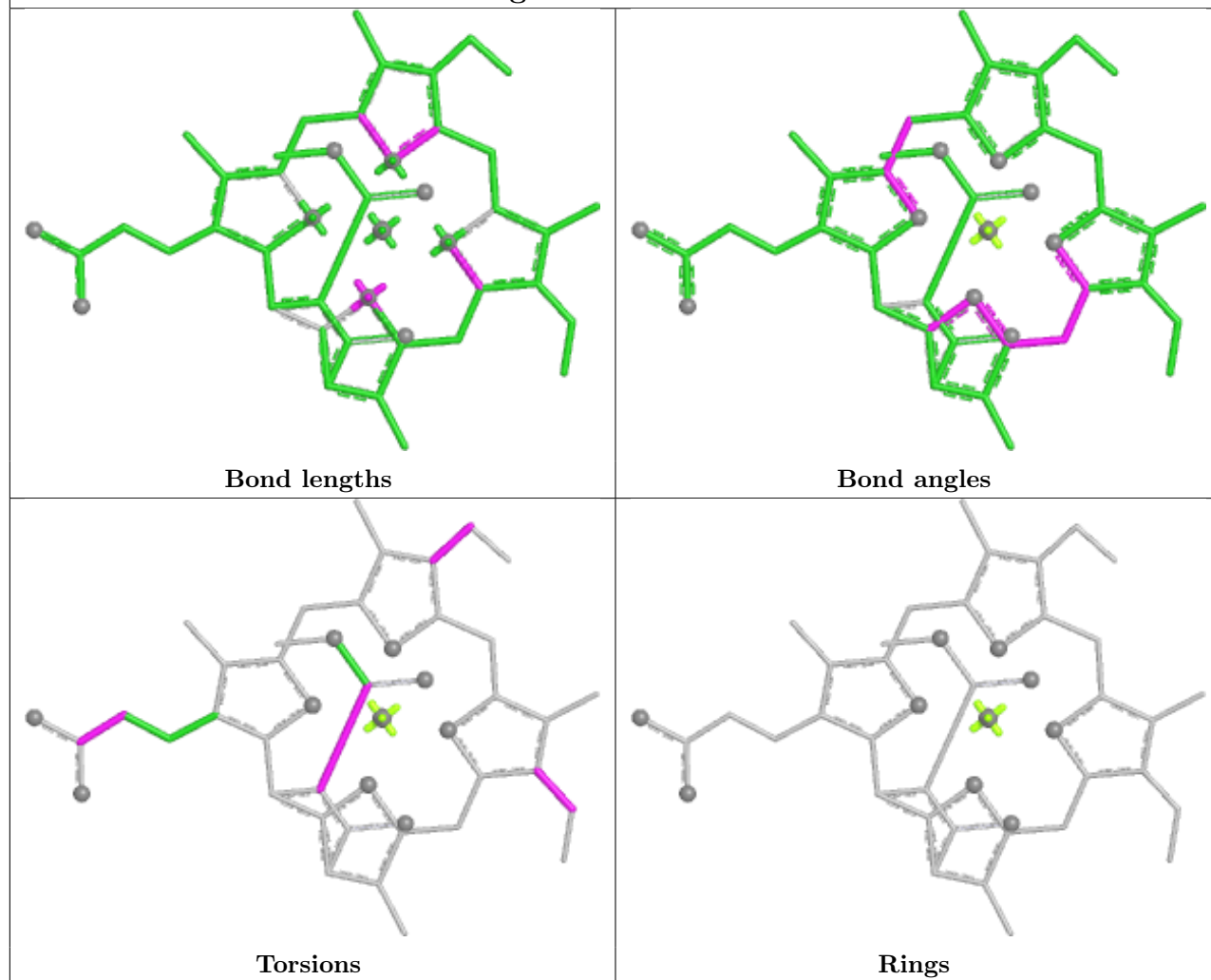


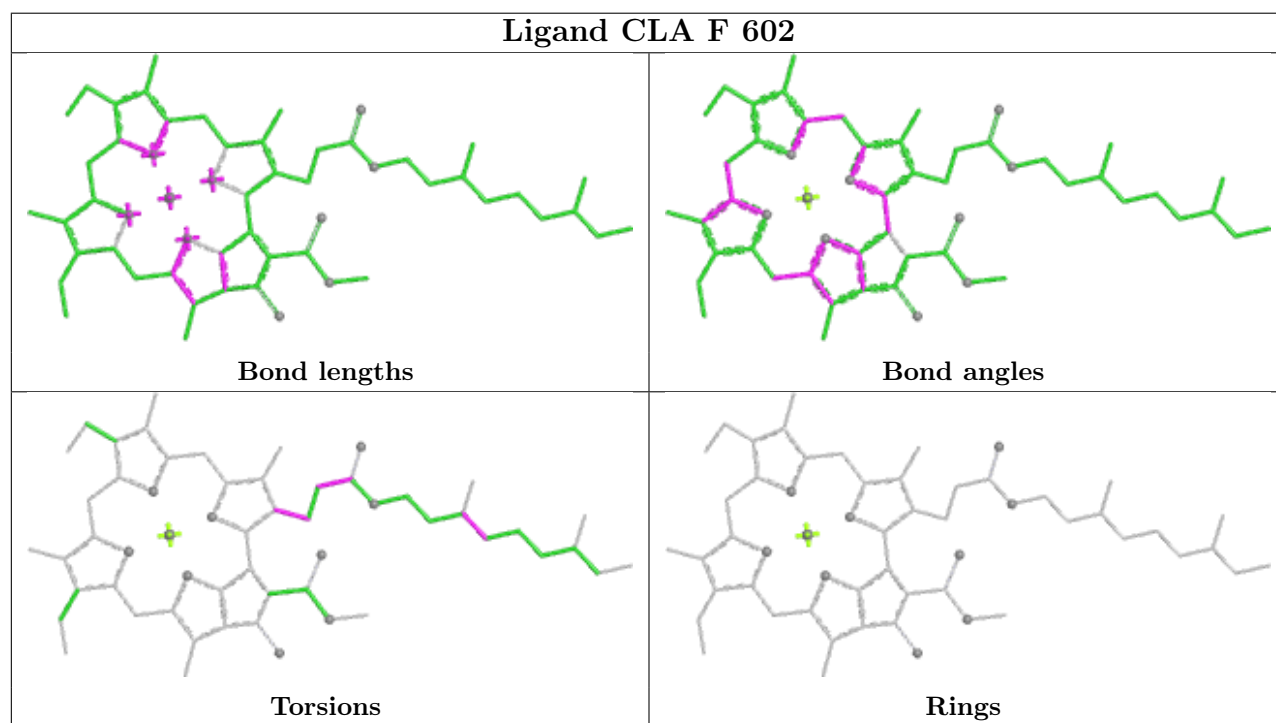
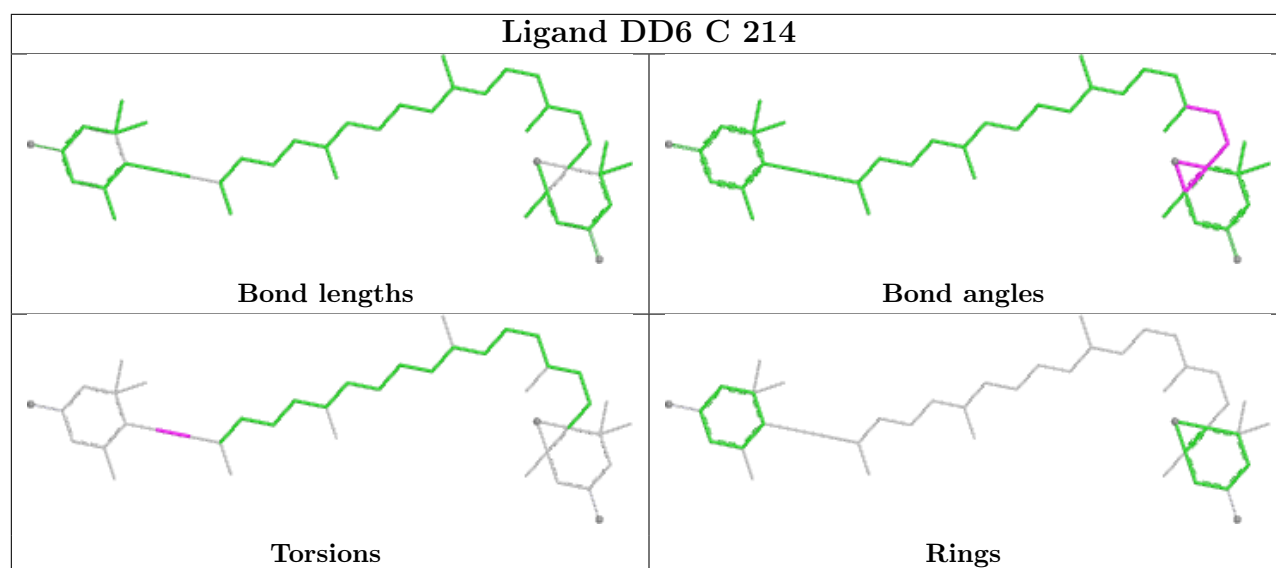
Rings

Ligand DD6 D 621

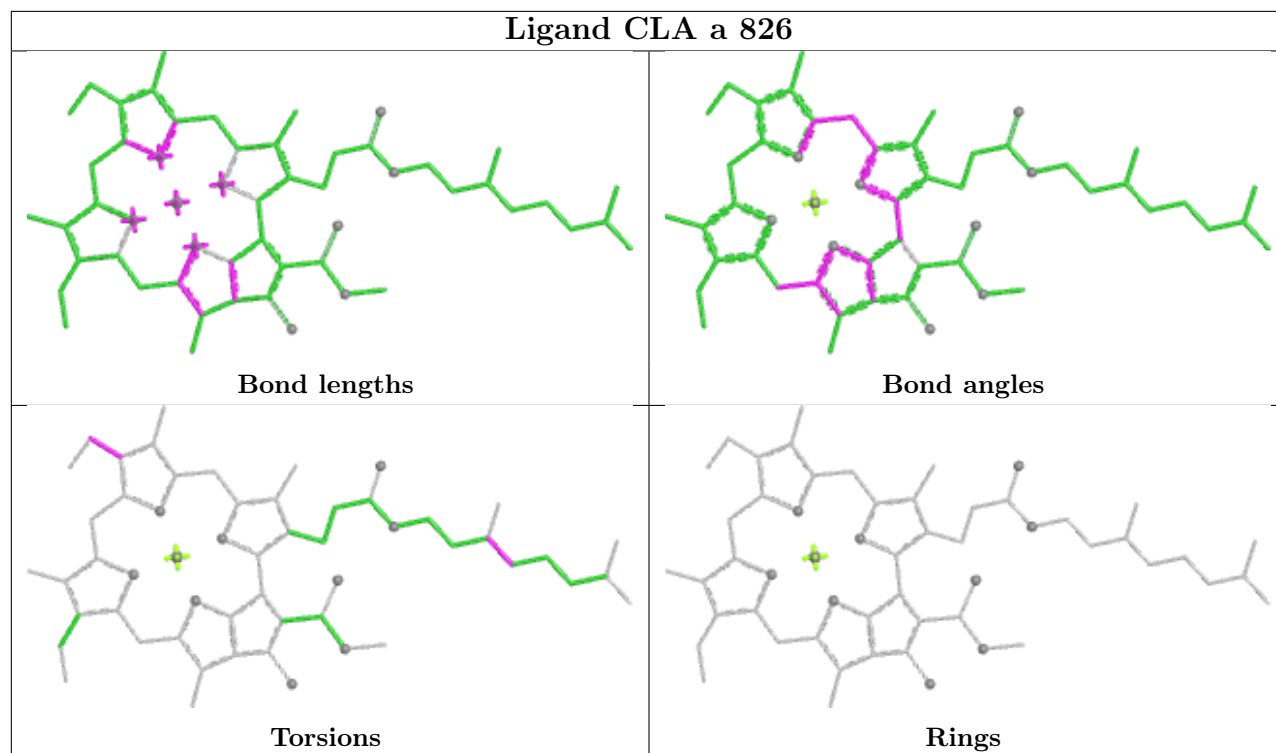


Ligand KC2 J 610

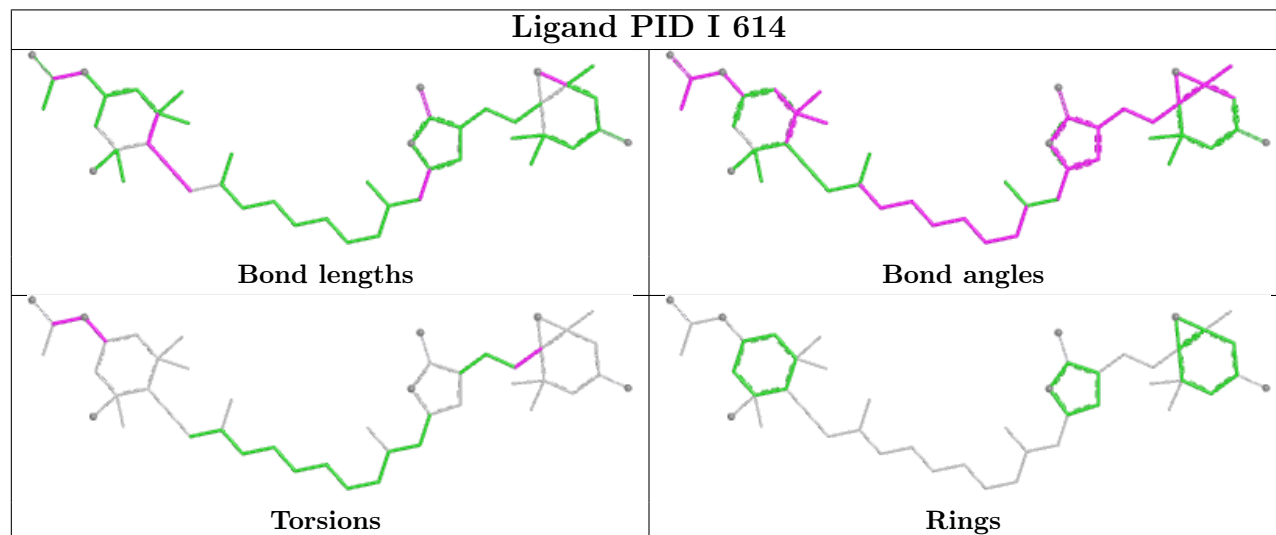




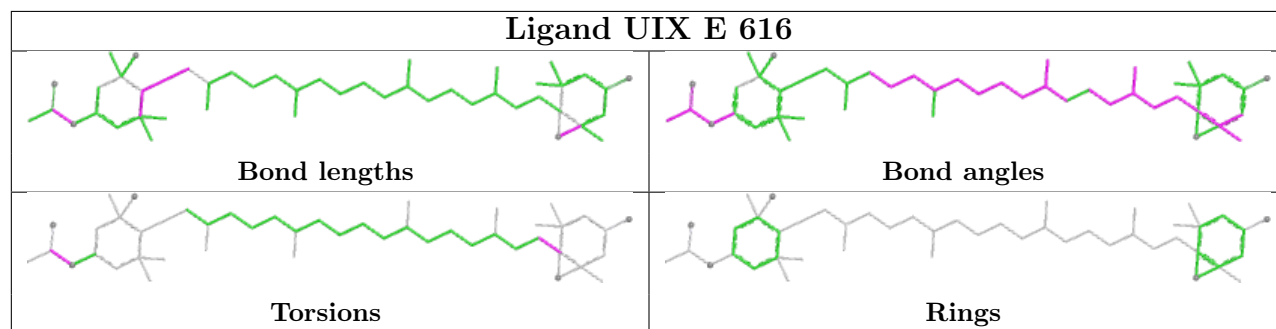
Ligand CLA a 826

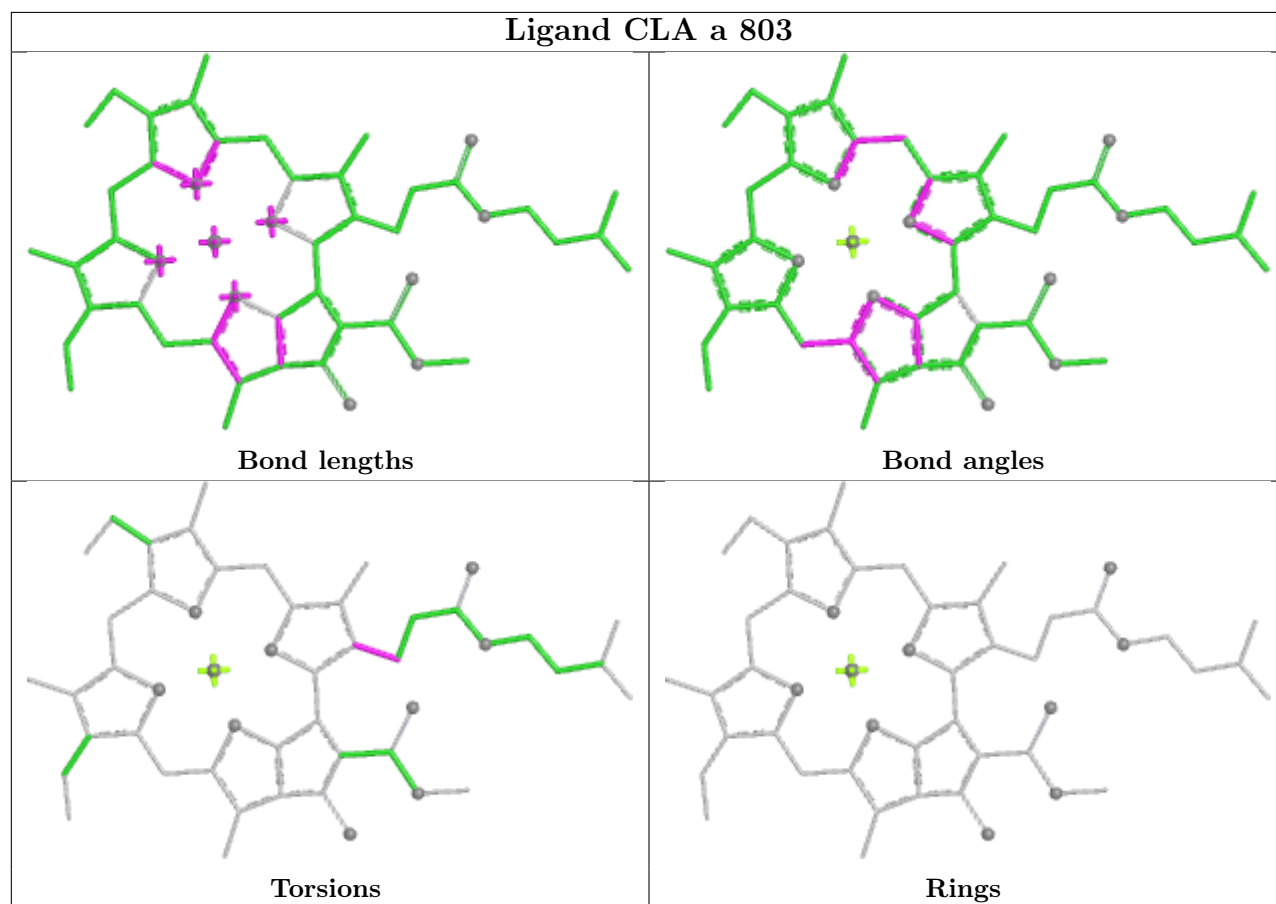
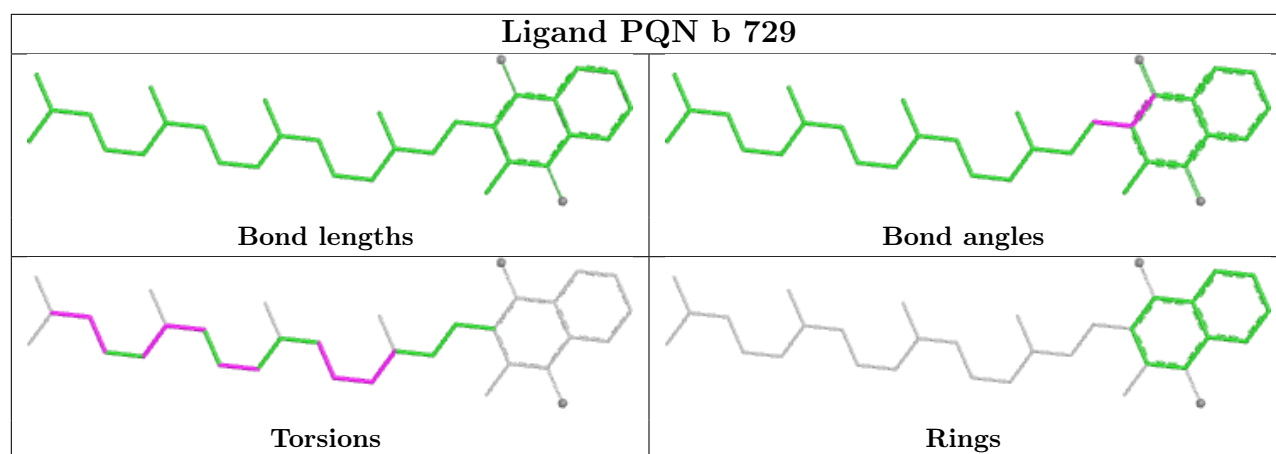


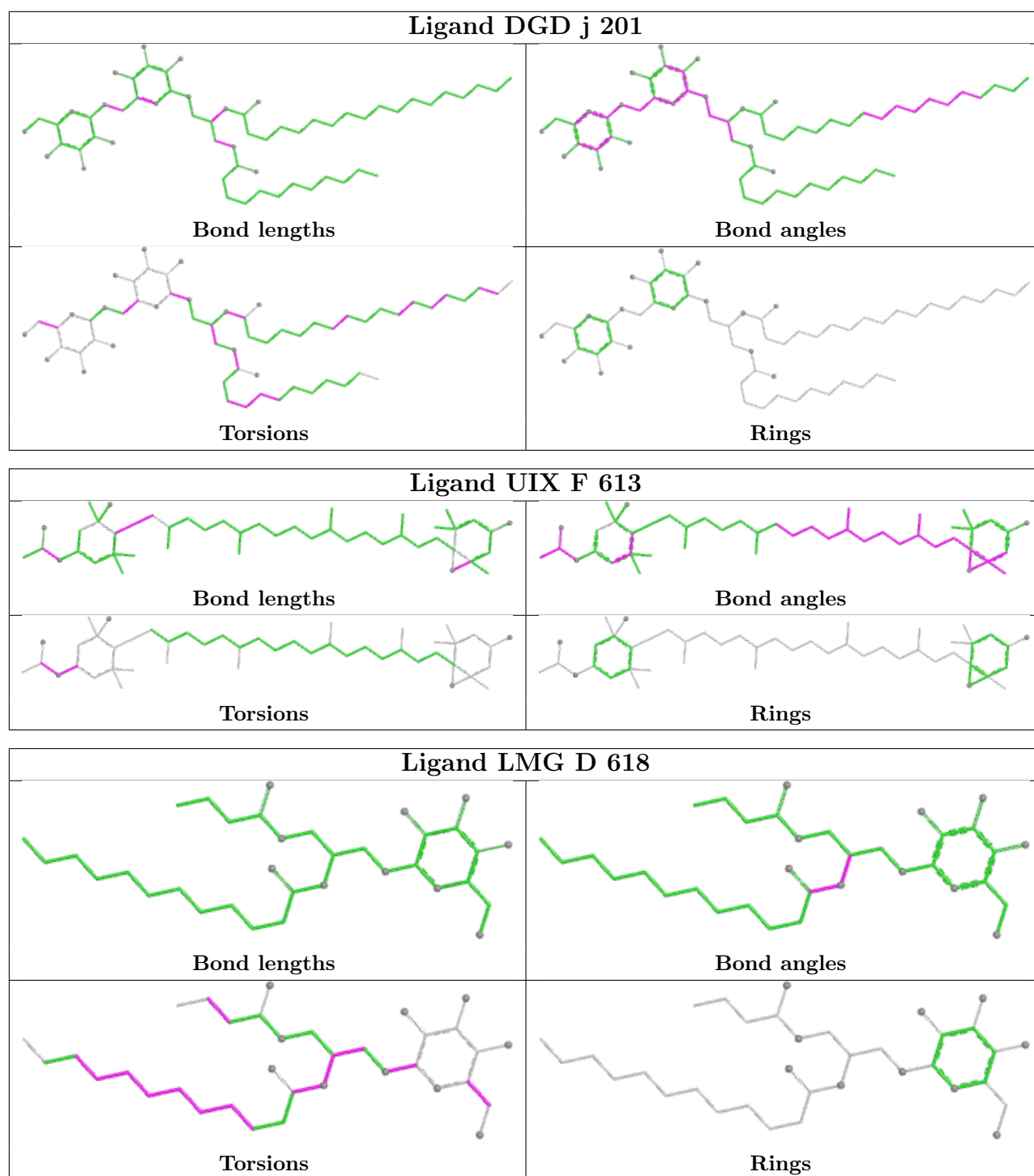
Ligand PID I 614



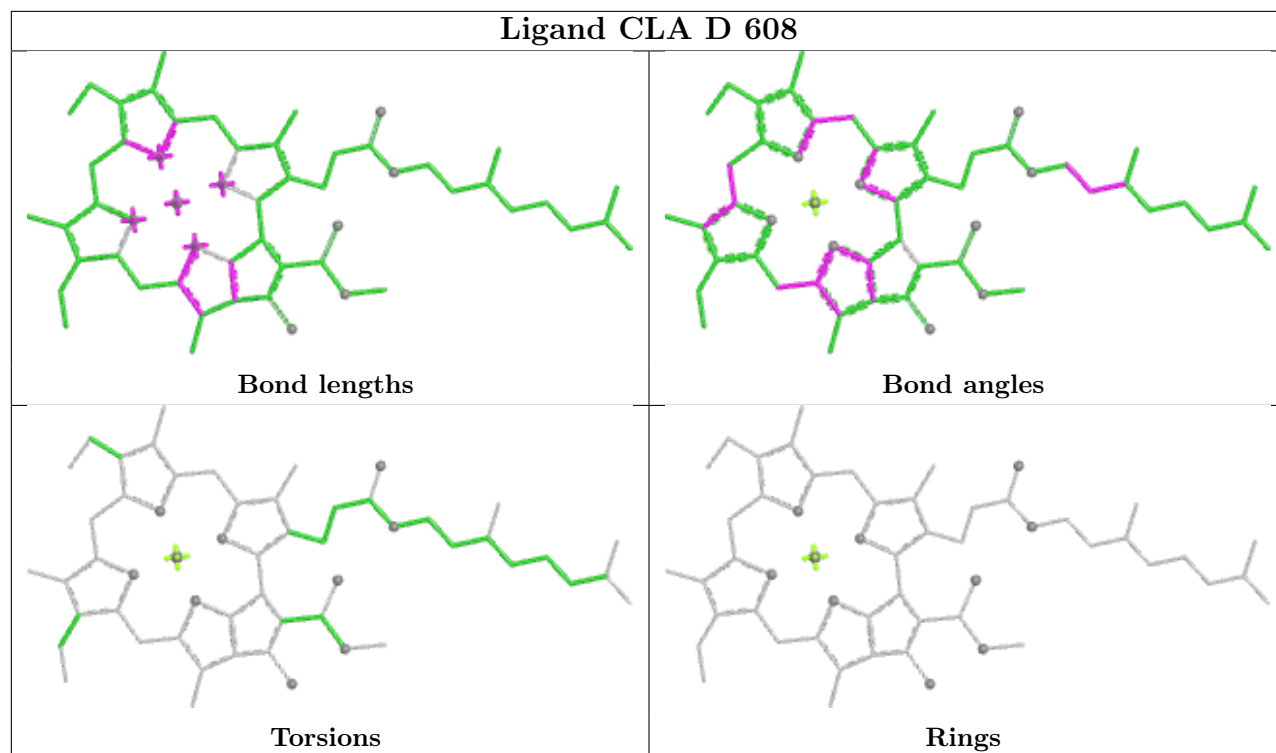
Ligand UIX E 616



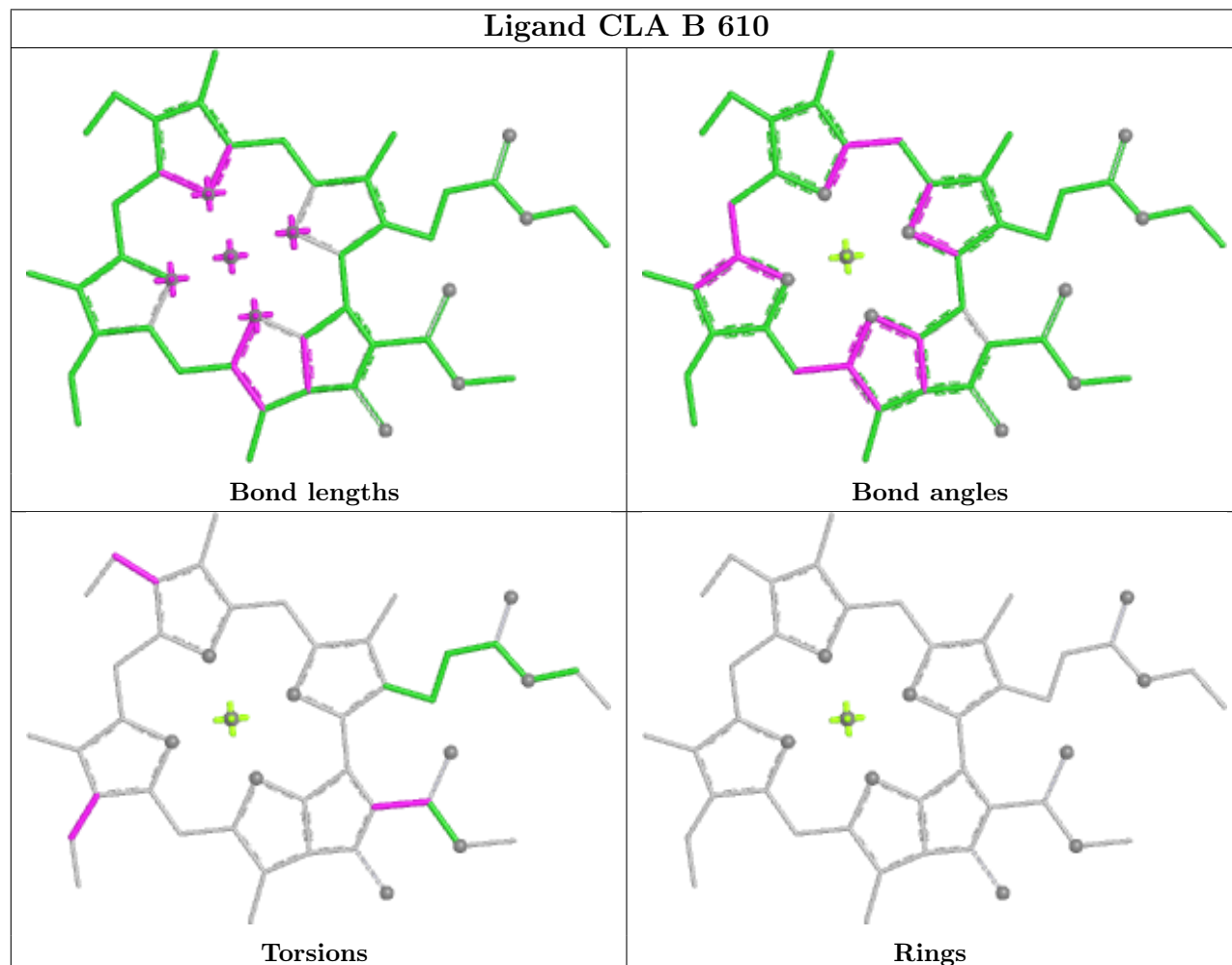




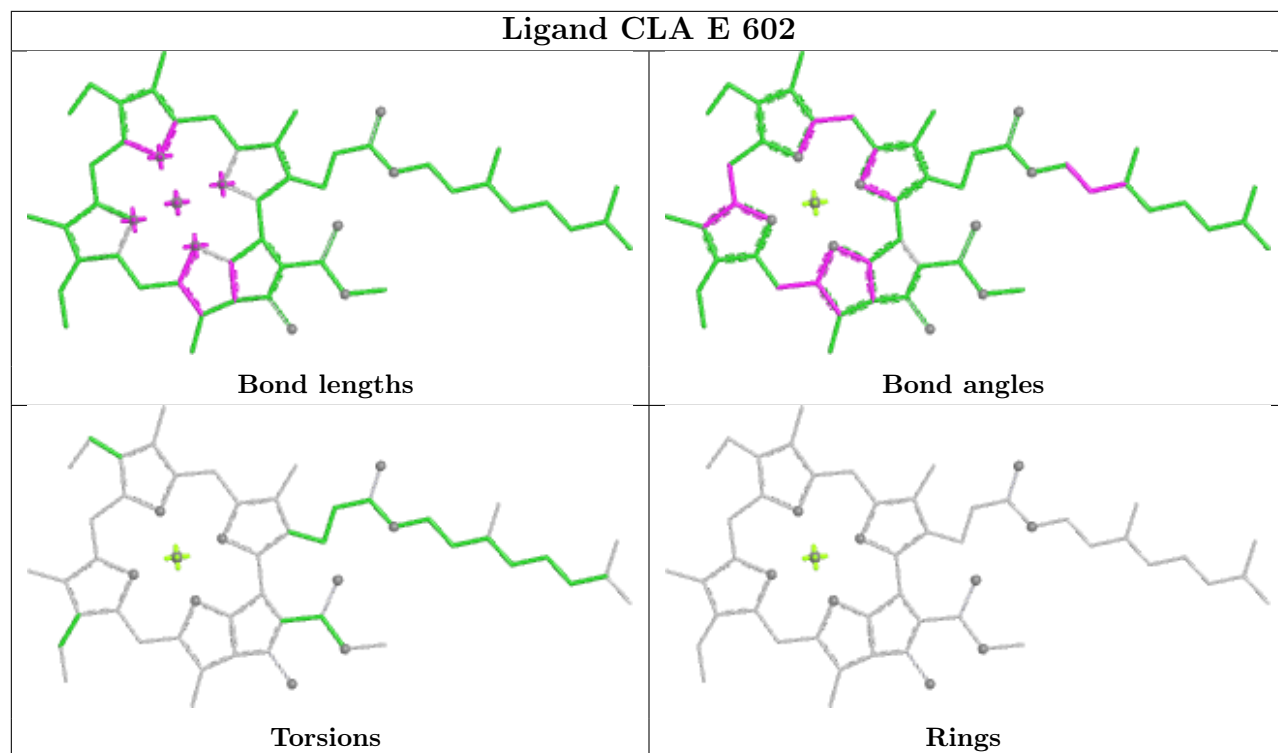
Ligand CLA D 608



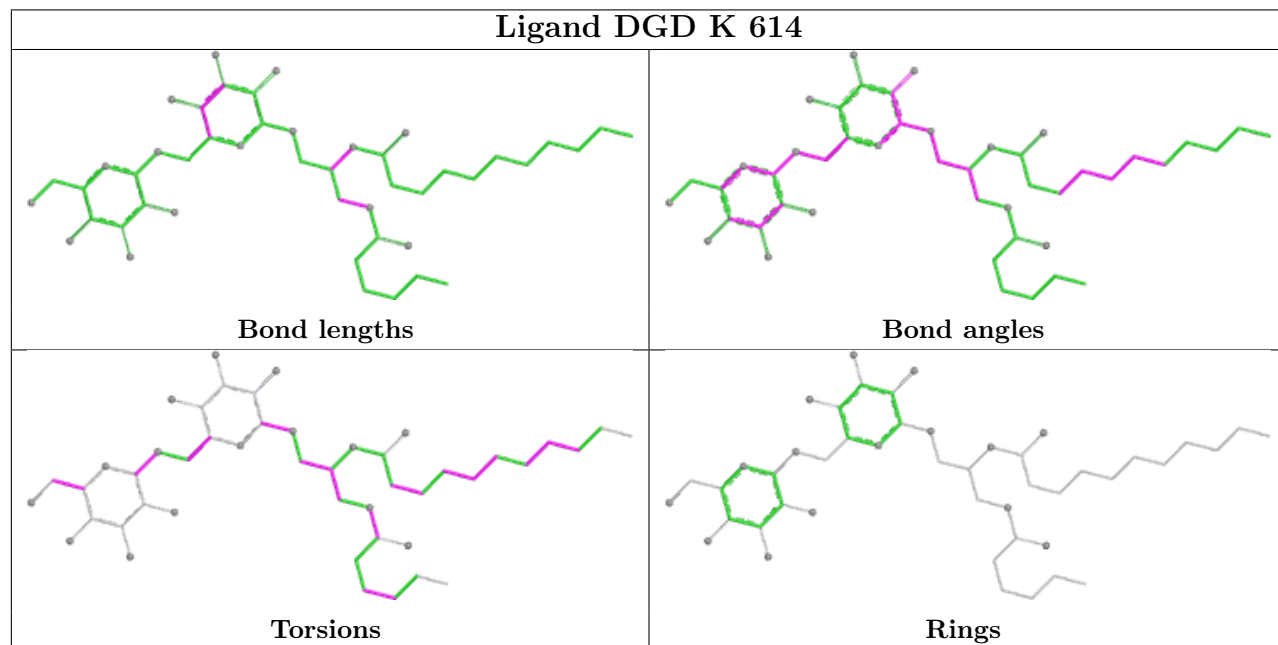
Ligand CLA B 610



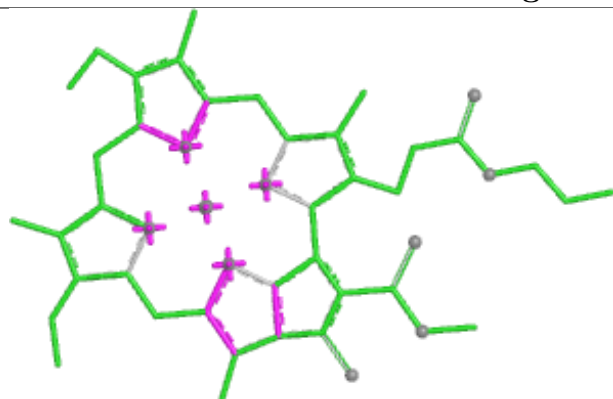
Ligand CLA E 602



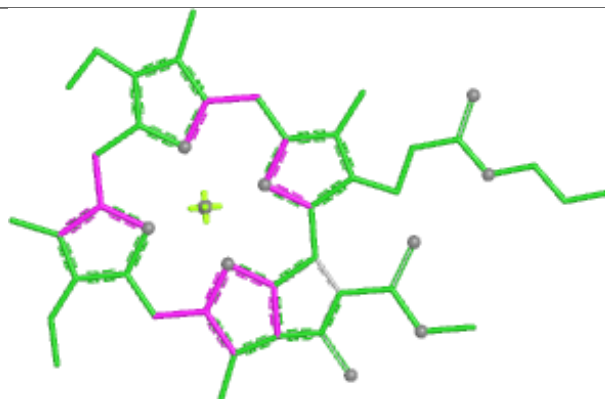
Ligand DGD K 614



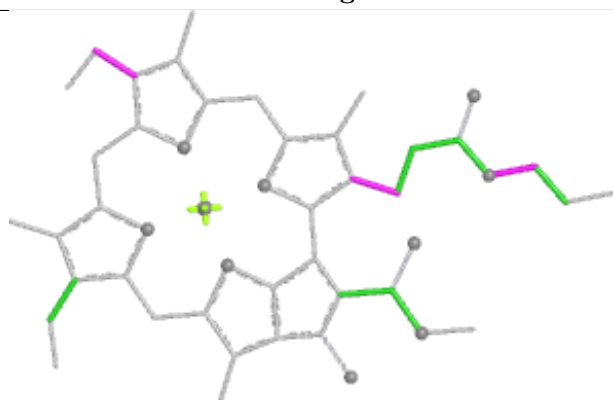
Ligand CLA l 410



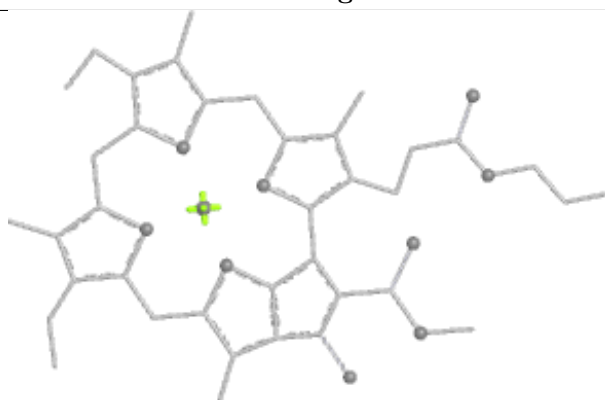
Bond lengths



Bond angles

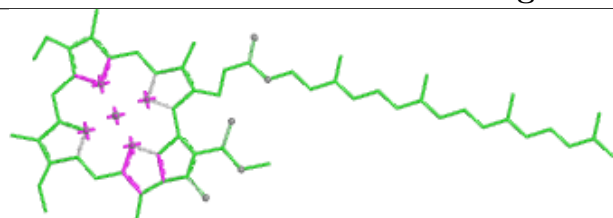


Torsions

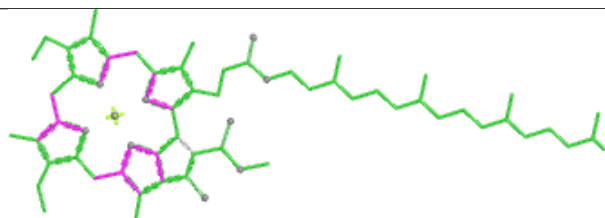


Rings

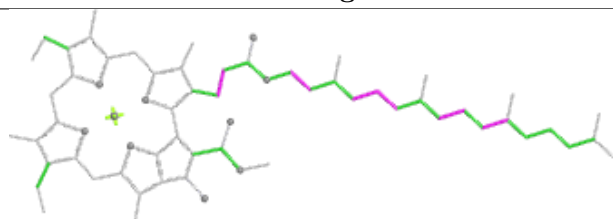
Ligand CLA b 701



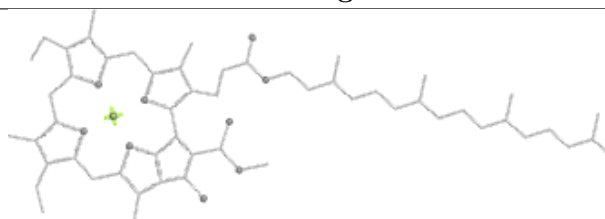
Bond lengths



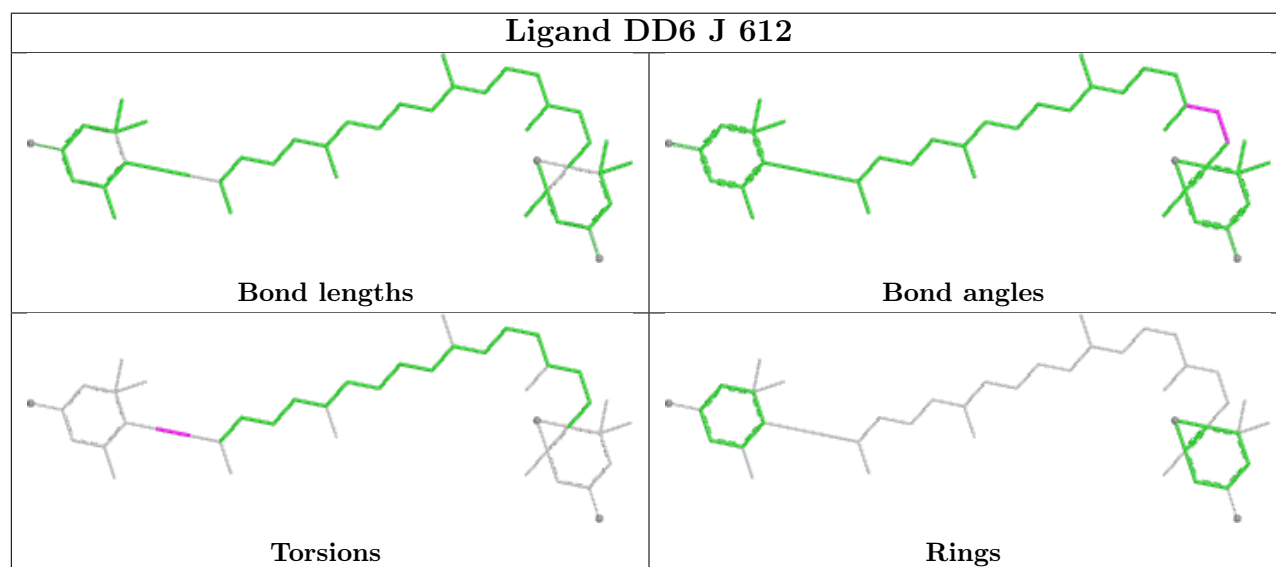
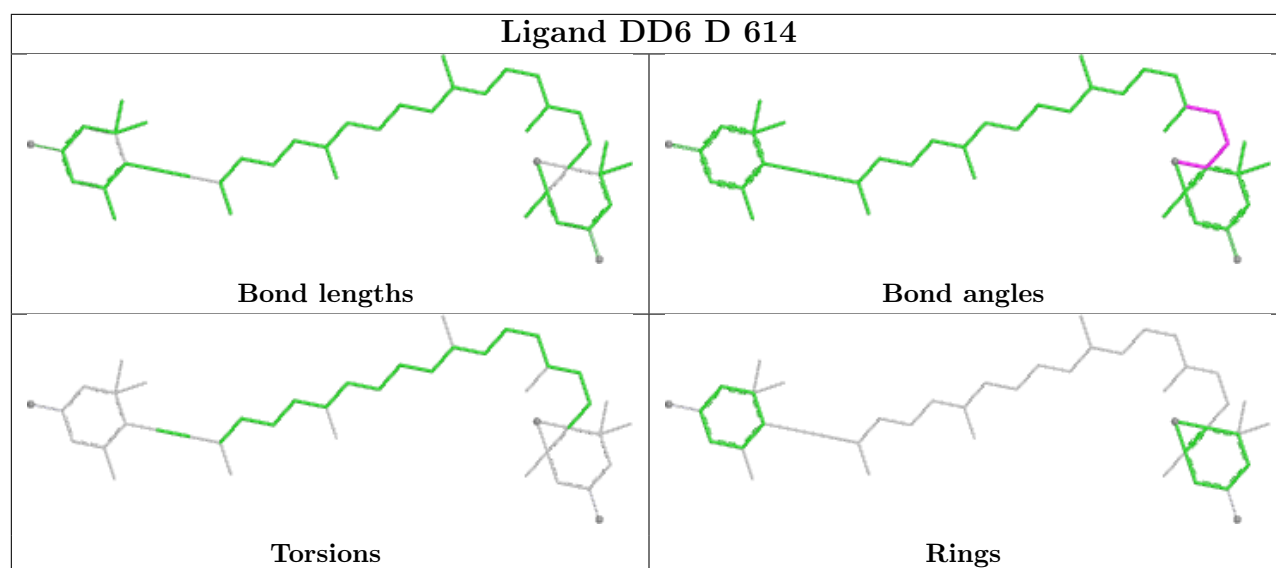
Bond angles



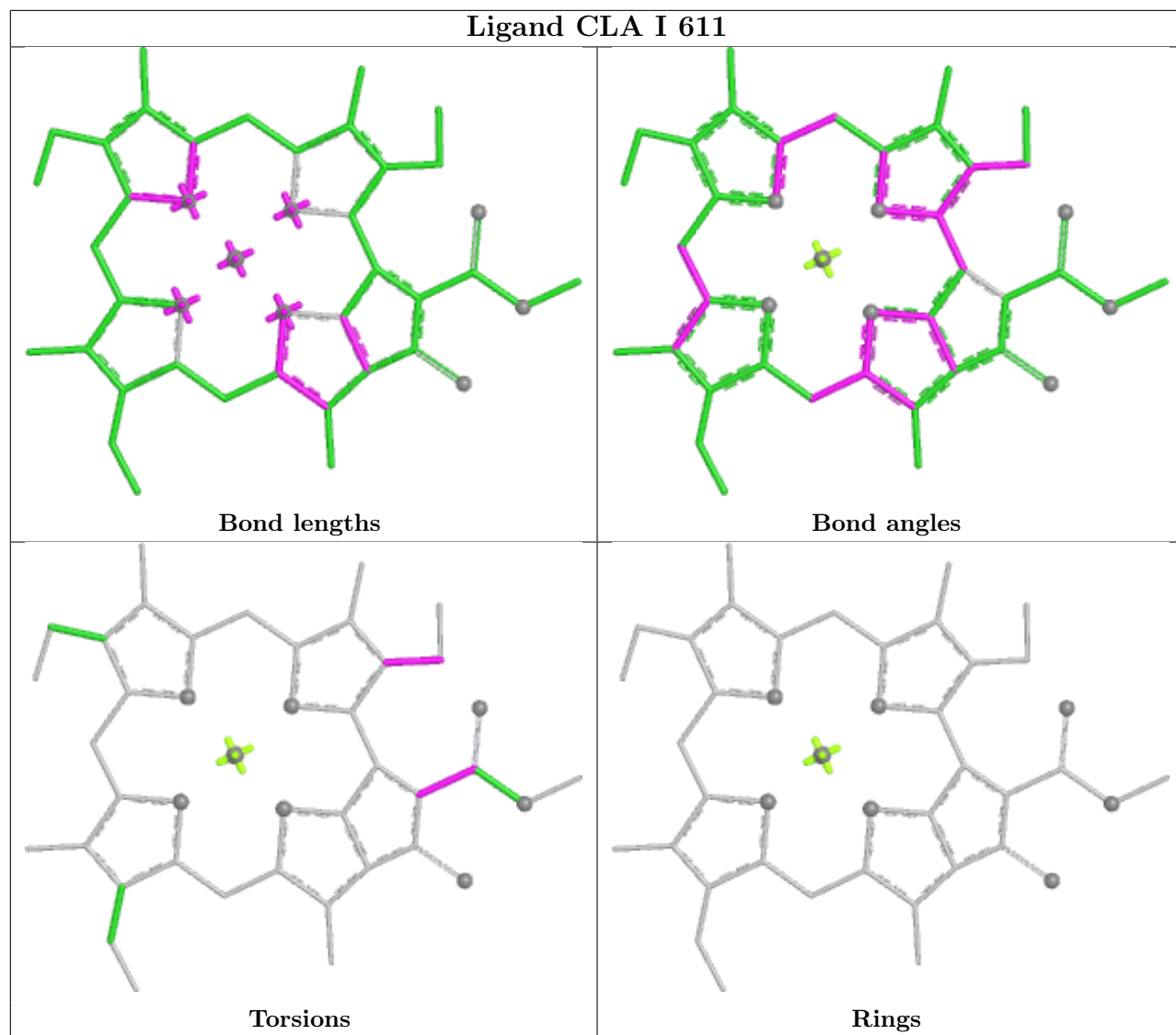
Torsions

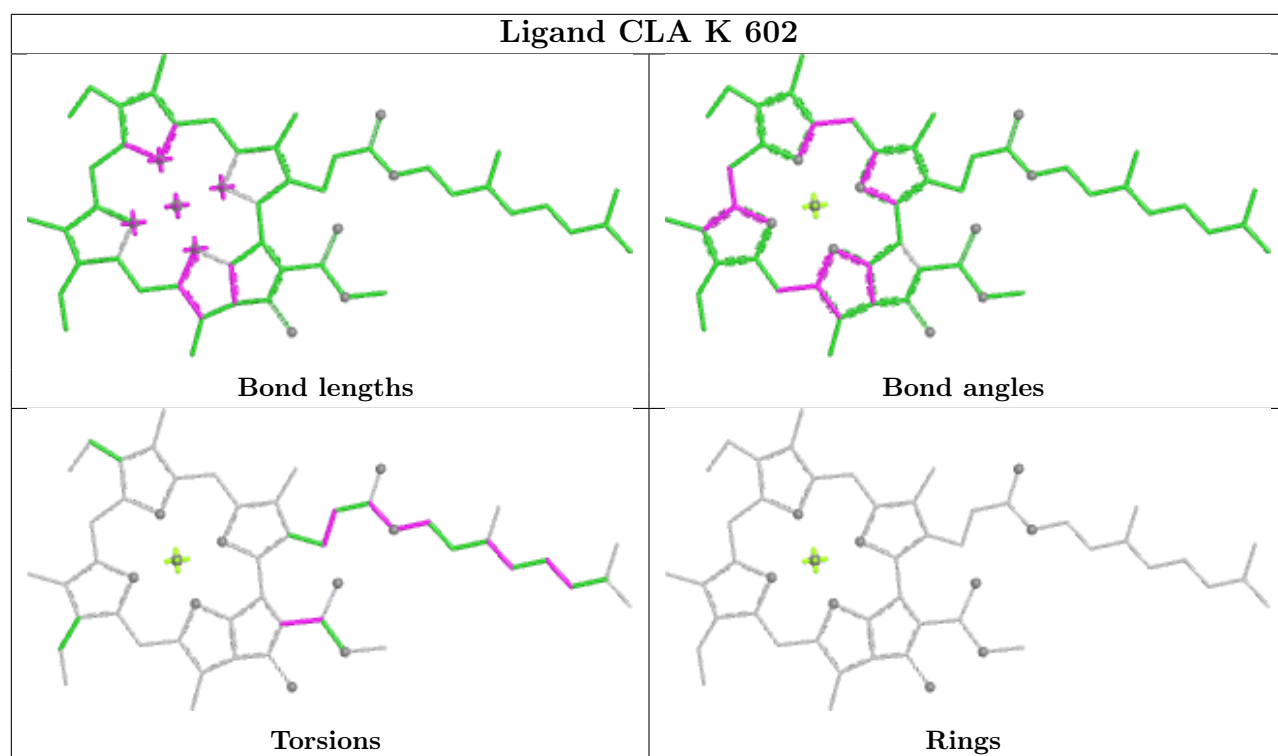


Rings

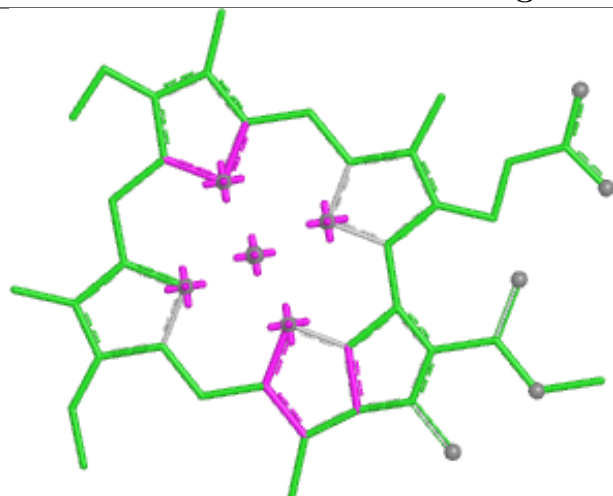


Ligand CLA I 611

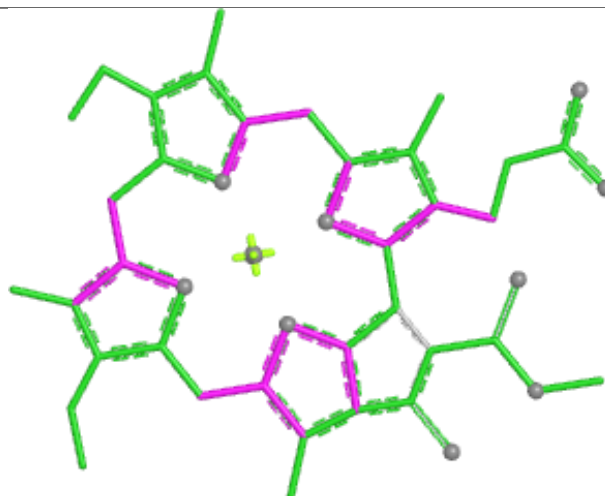




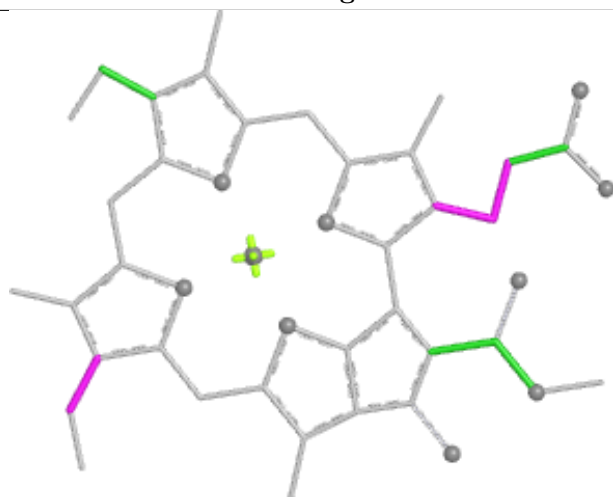
Ligand CLA F 605



Bond lengths



Bond angles

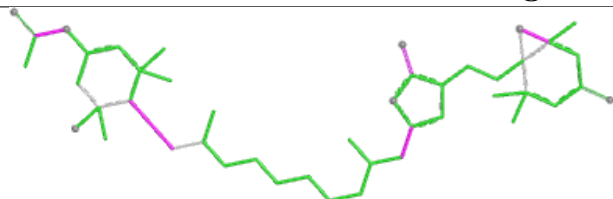


Torsions

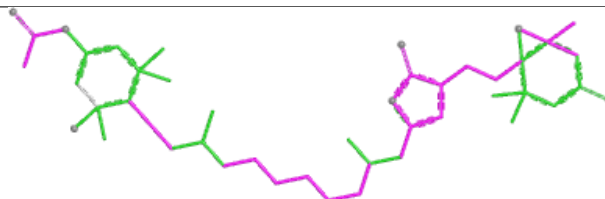


Rings

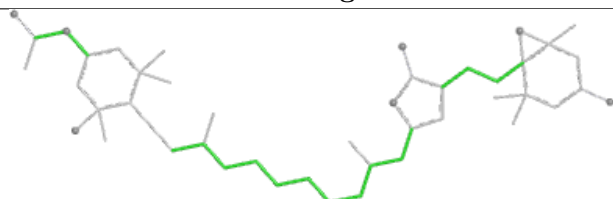
Ligand PID J 614



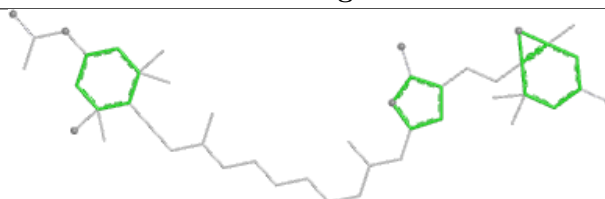
Bond lengths



Bond angles

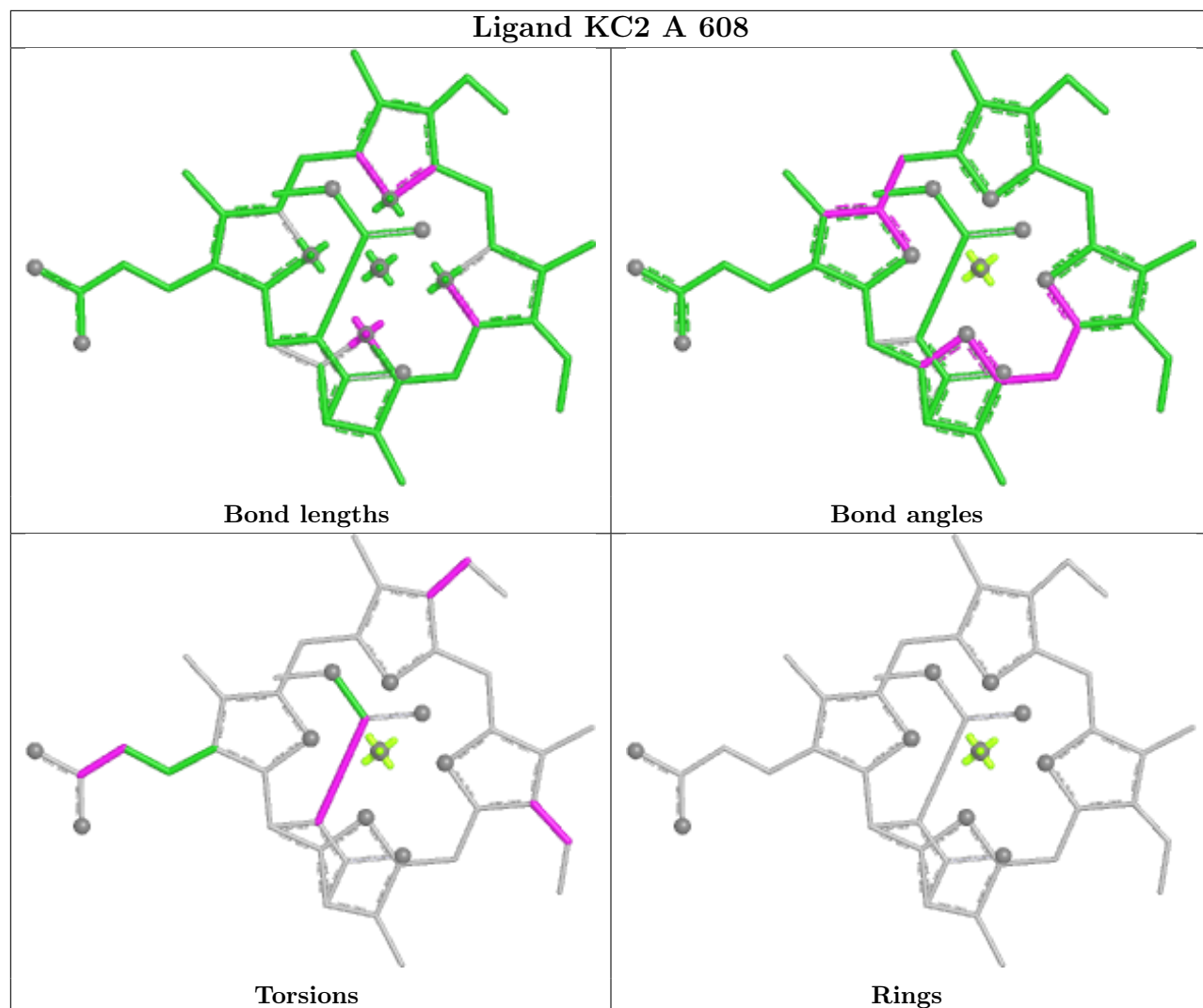


Torsions

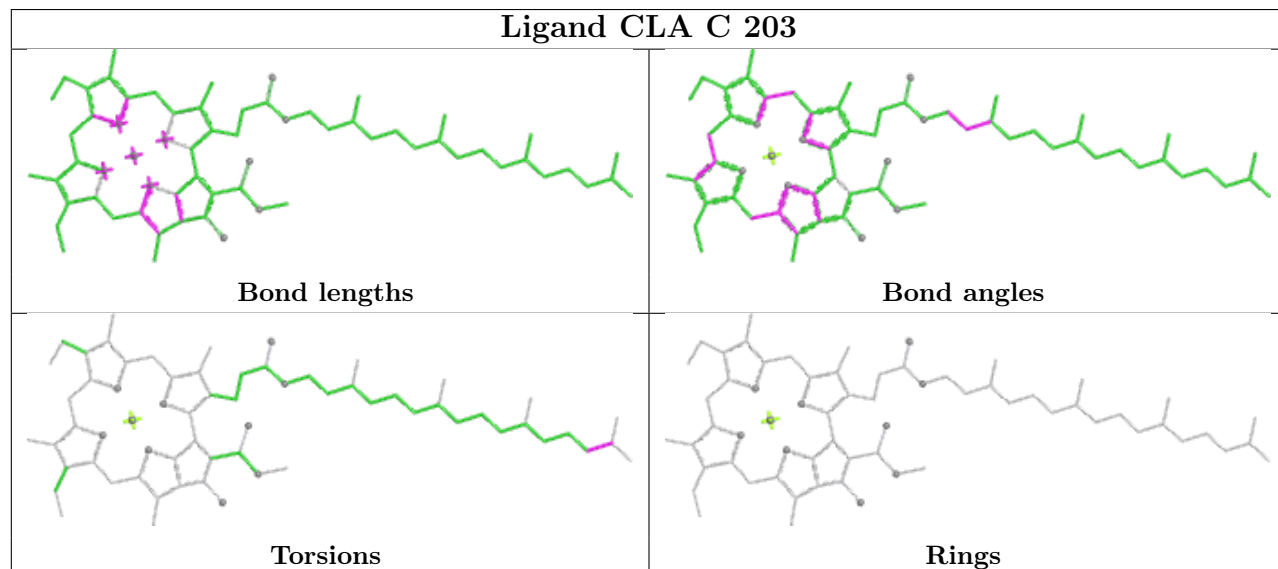


Rings

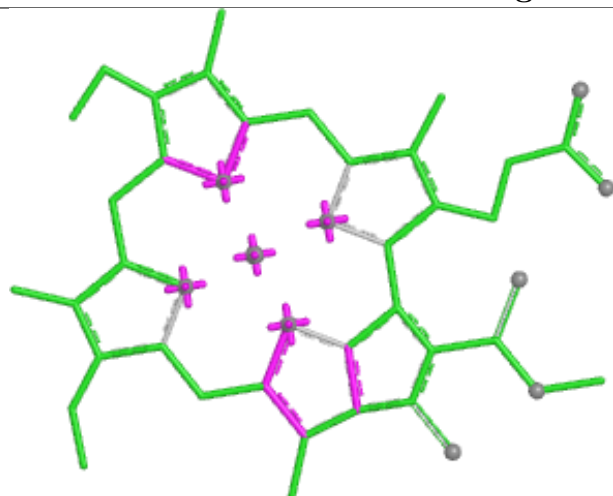
Ligand KC2 A 608



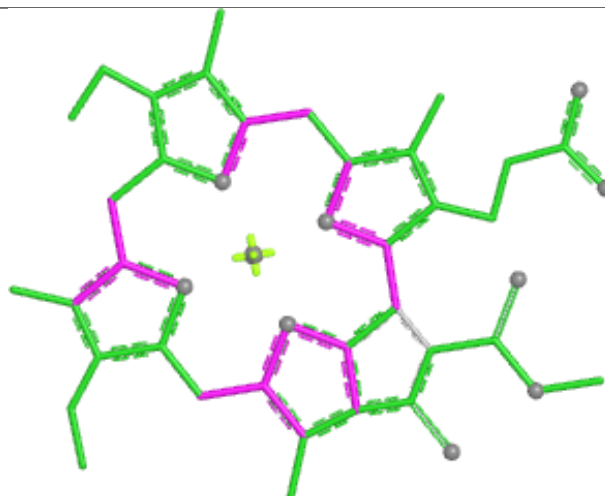
Ligand CLA C 203



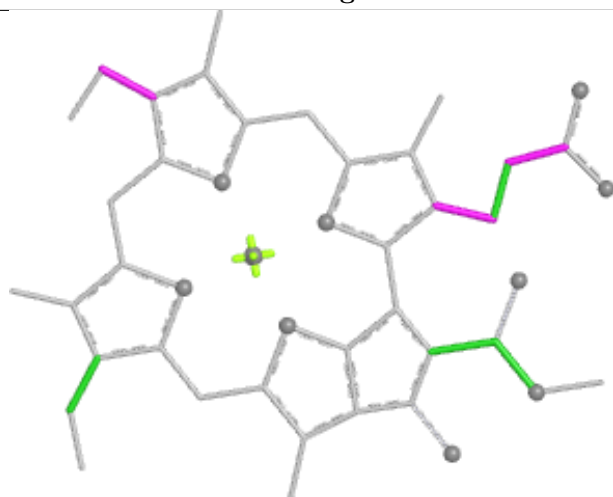
Ligand CLA E 605



Bond lengths



Bond angles

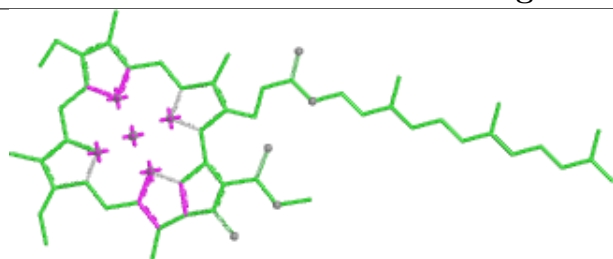


Torsions

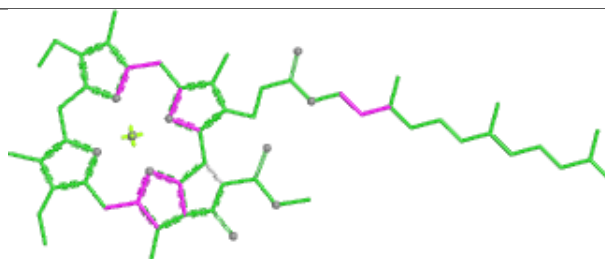


Rings

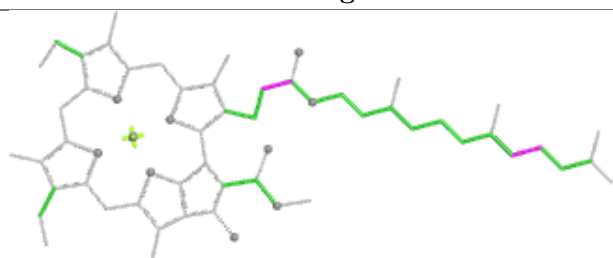
Ligand CLA F 601



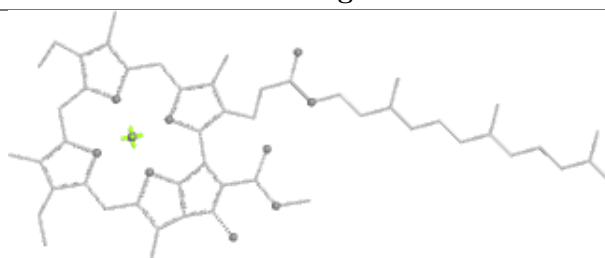
Bond lengths



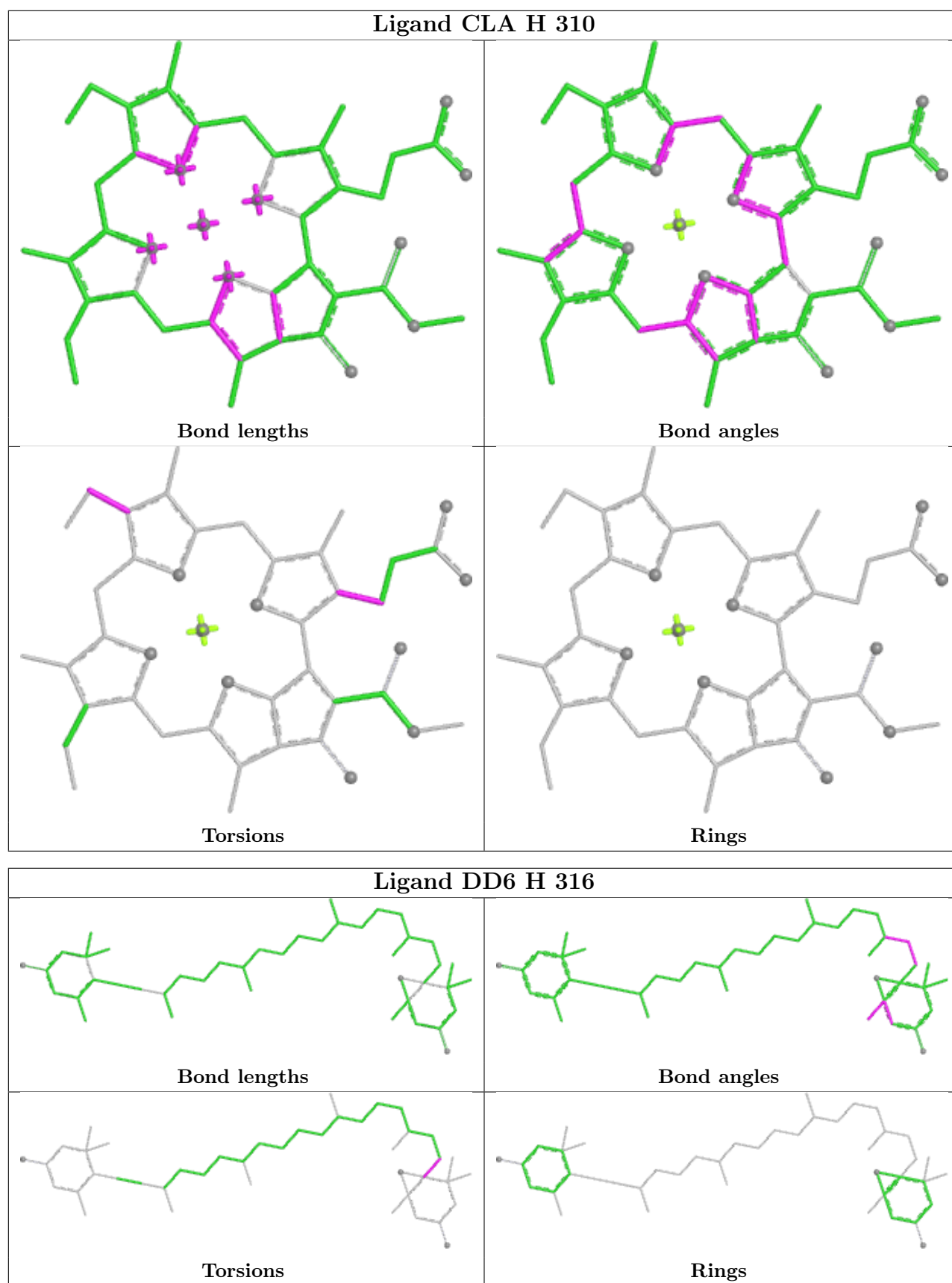
Bond angles

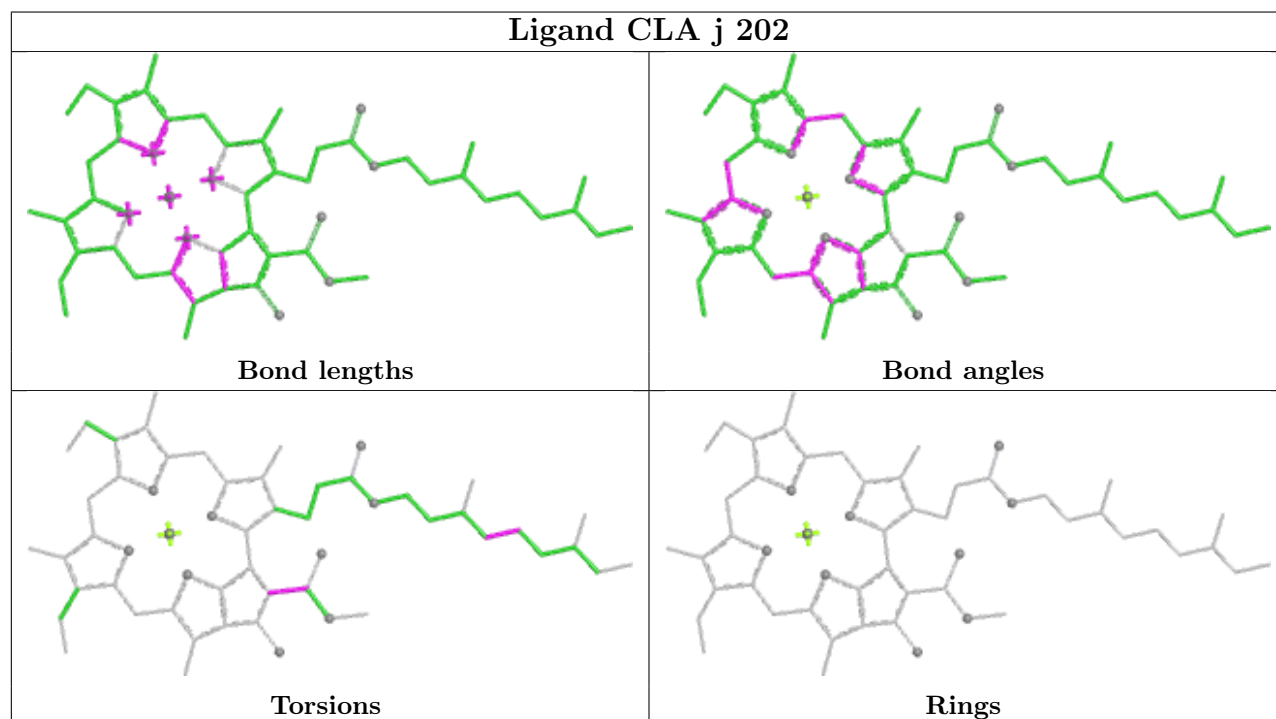
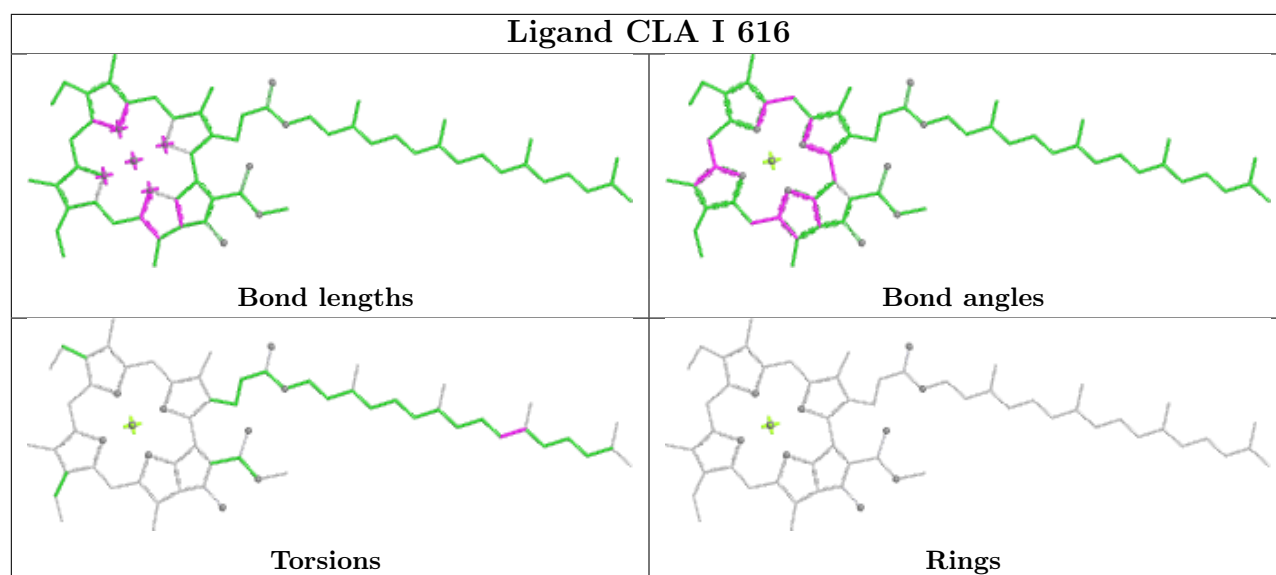


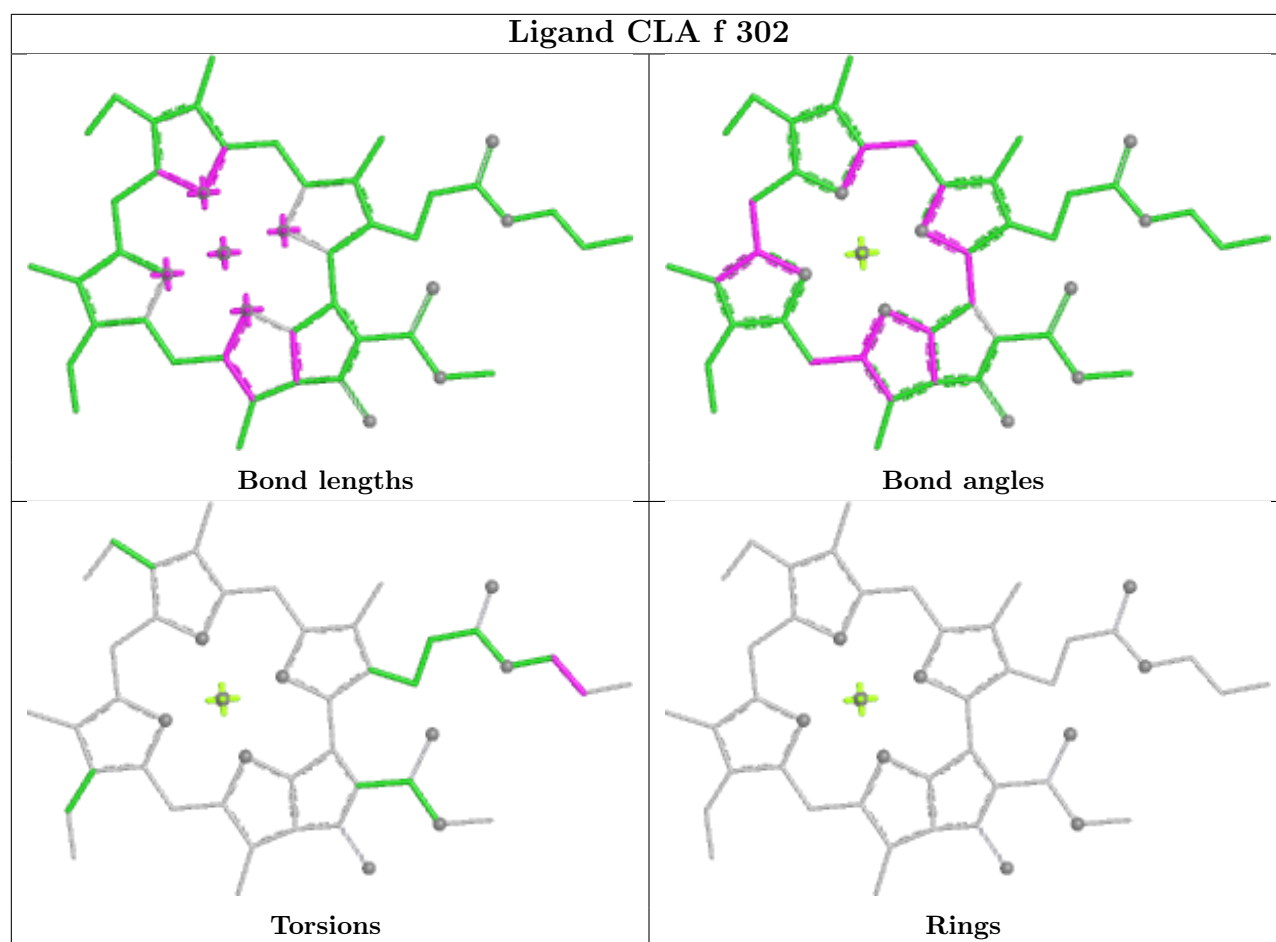
Torsions

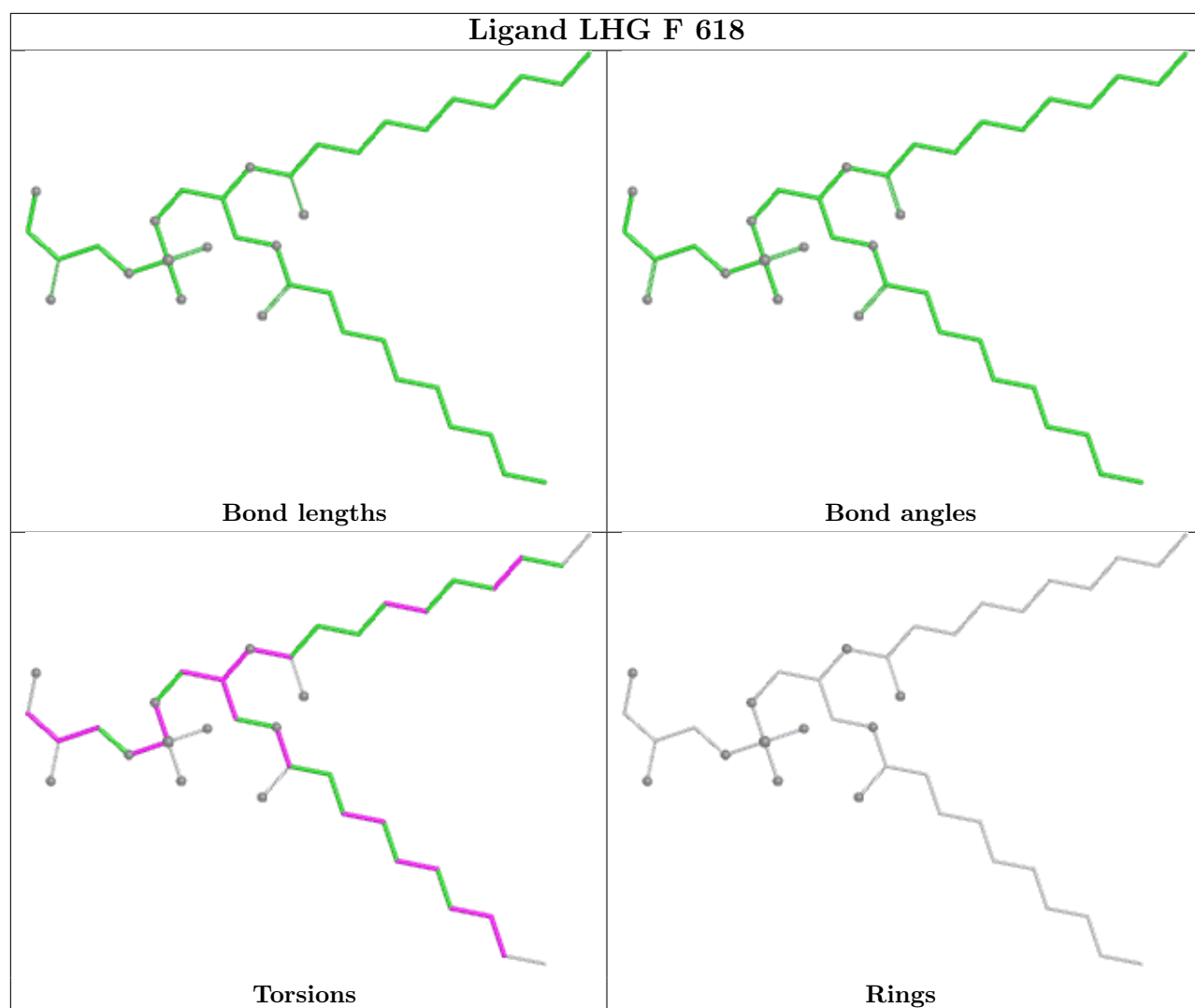


Rings

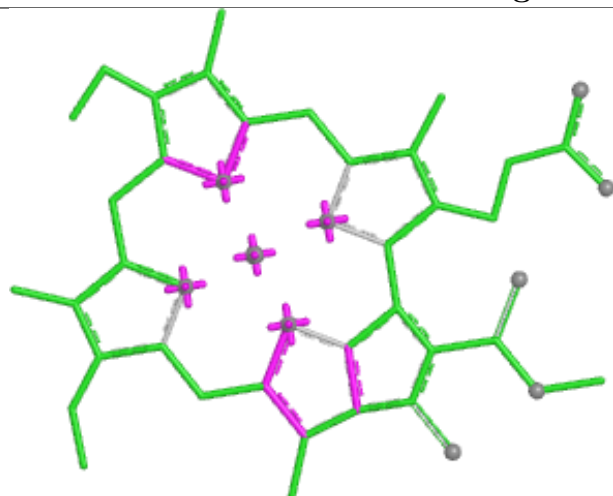




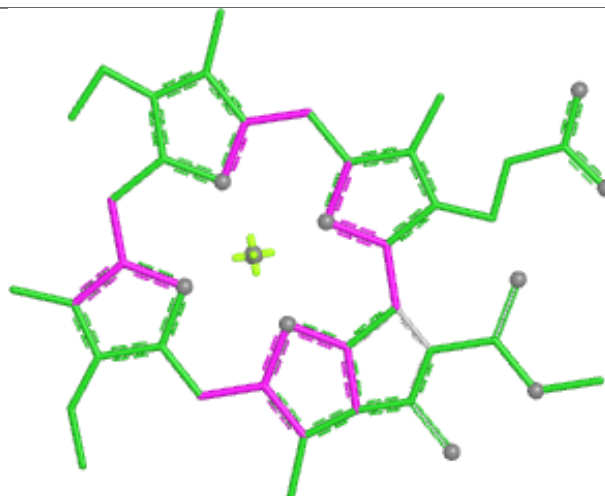




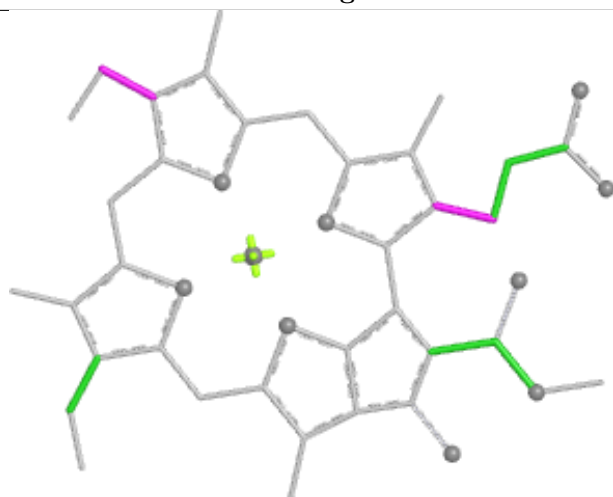
Ligand CLA K 608



Bond lengths



Bond angles

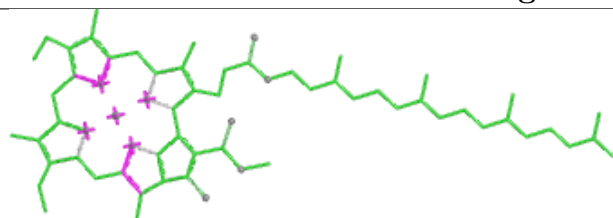


Torsions

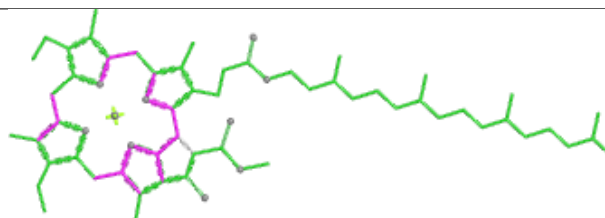


Rings

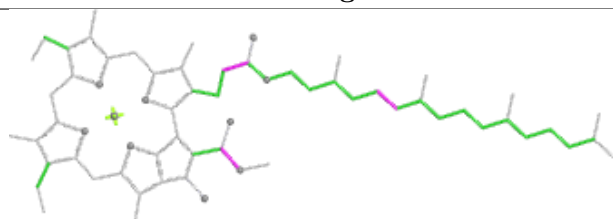
Ligand CLA a 801



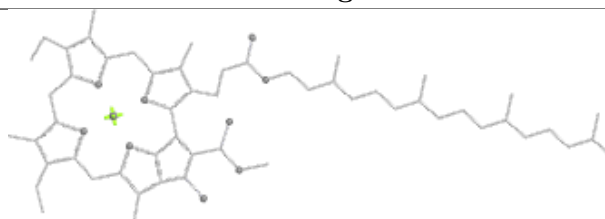
Bond lengths



Bond angles

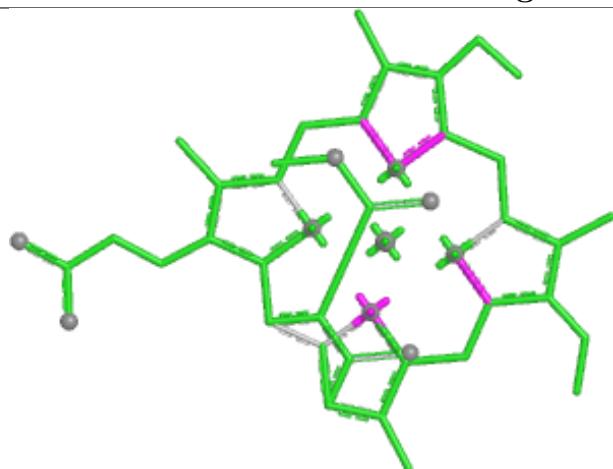


Torsions

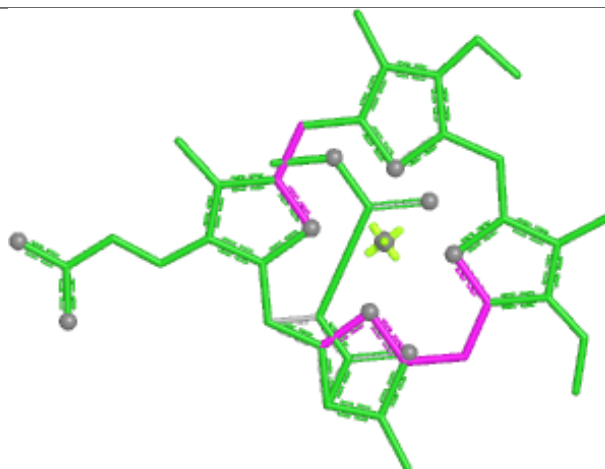


Rings

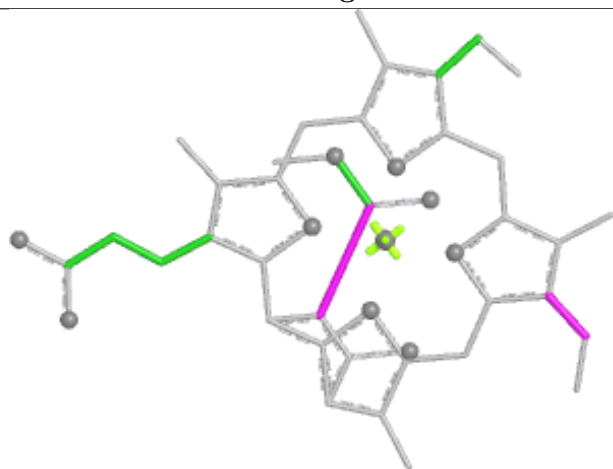
Ligand KC2 B 602



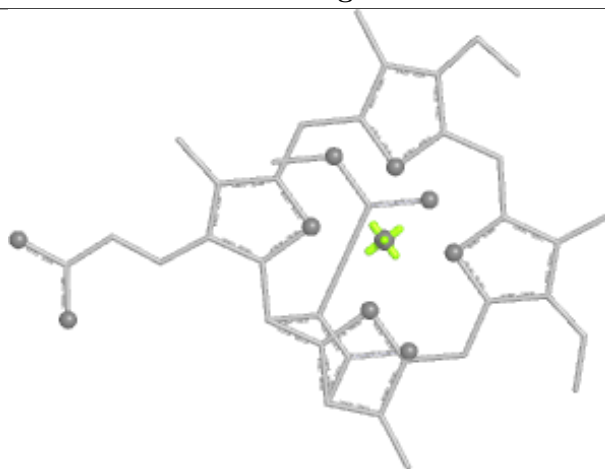
Bond lengths



Bond angles

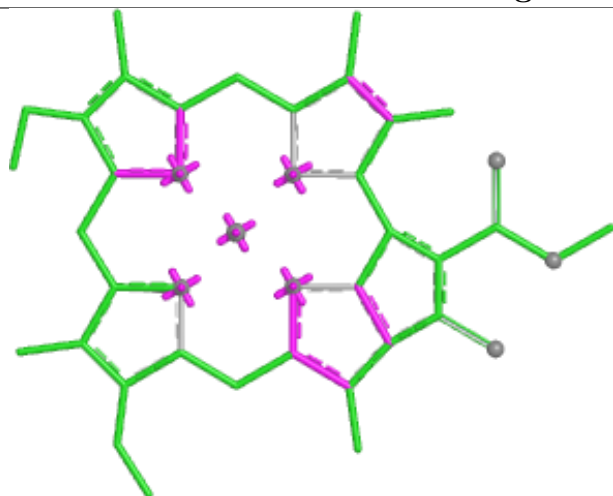


Torsions

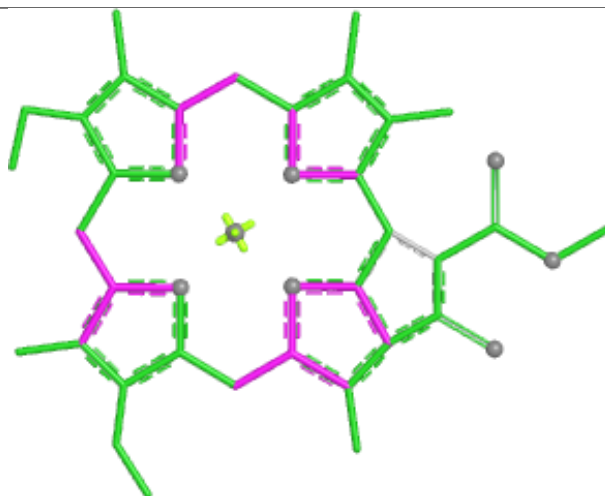


Rings

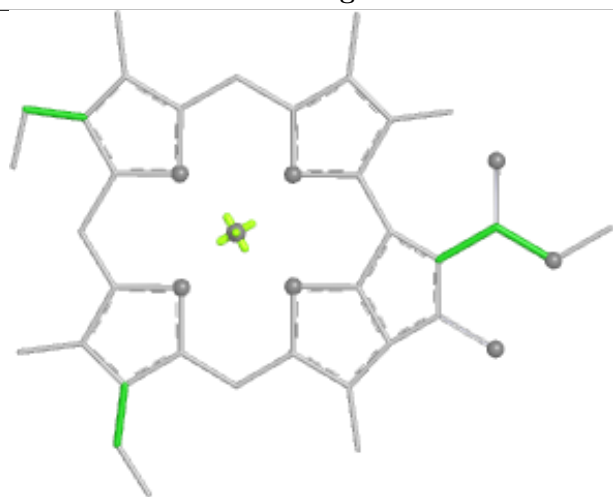
Ligand CLA T 609



Bond lengths



Bond angles

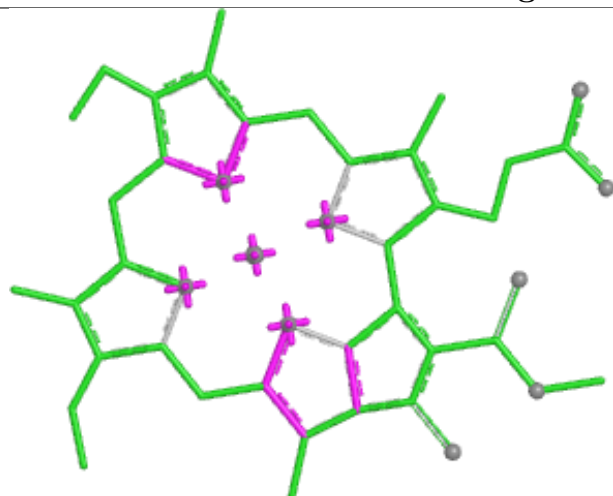


Torsions

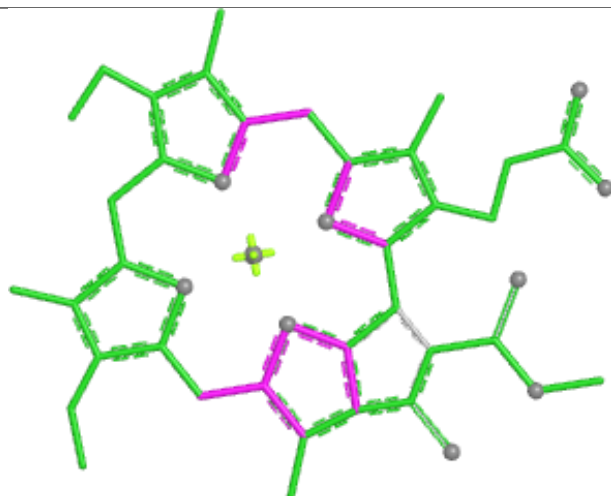


Rings

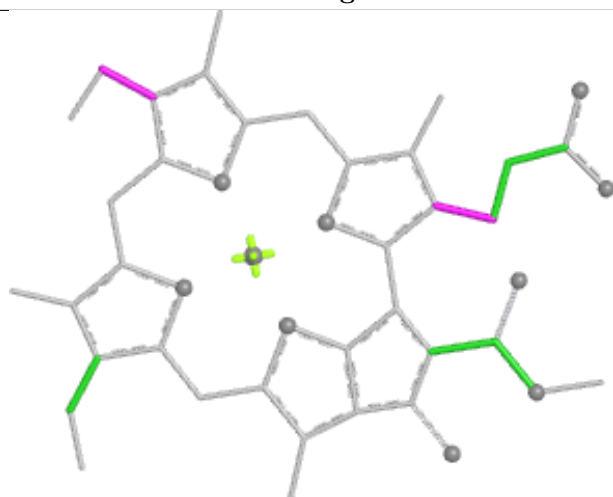
Ligand CLA J 601



Bond lengths



Bond angles

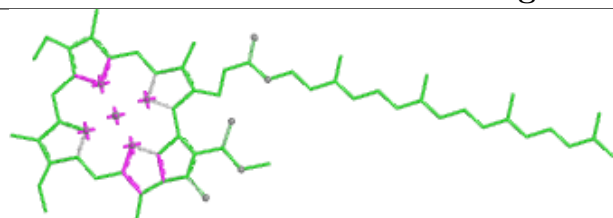


Torsions

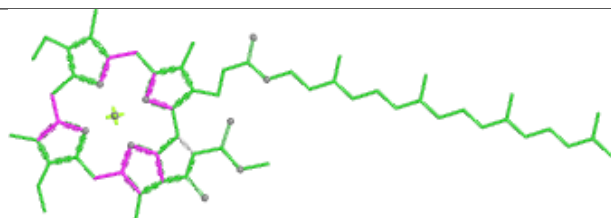


Rings

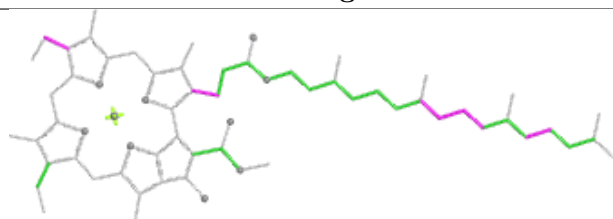
Ligand CLA a 821



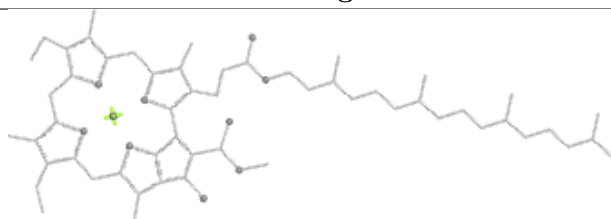
Bond lengths



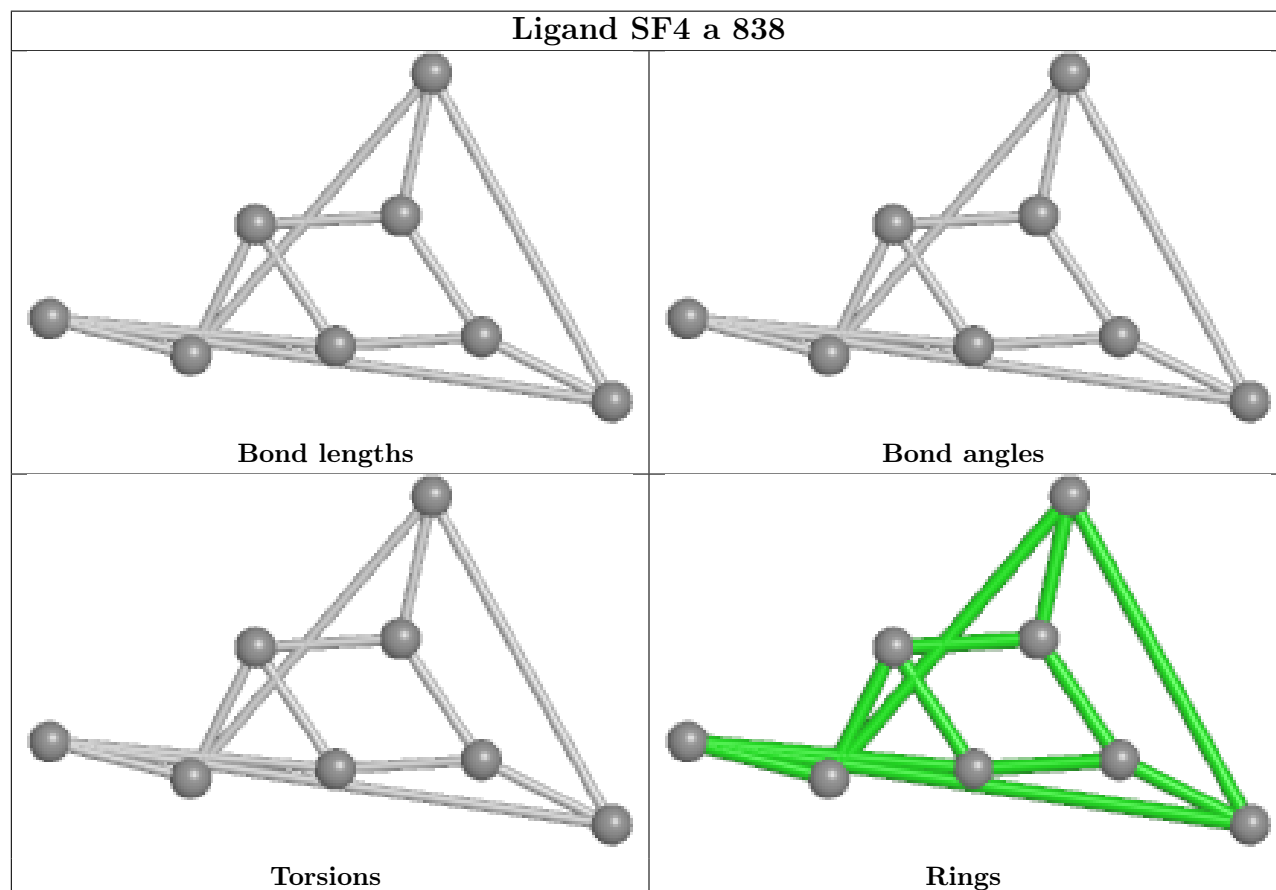
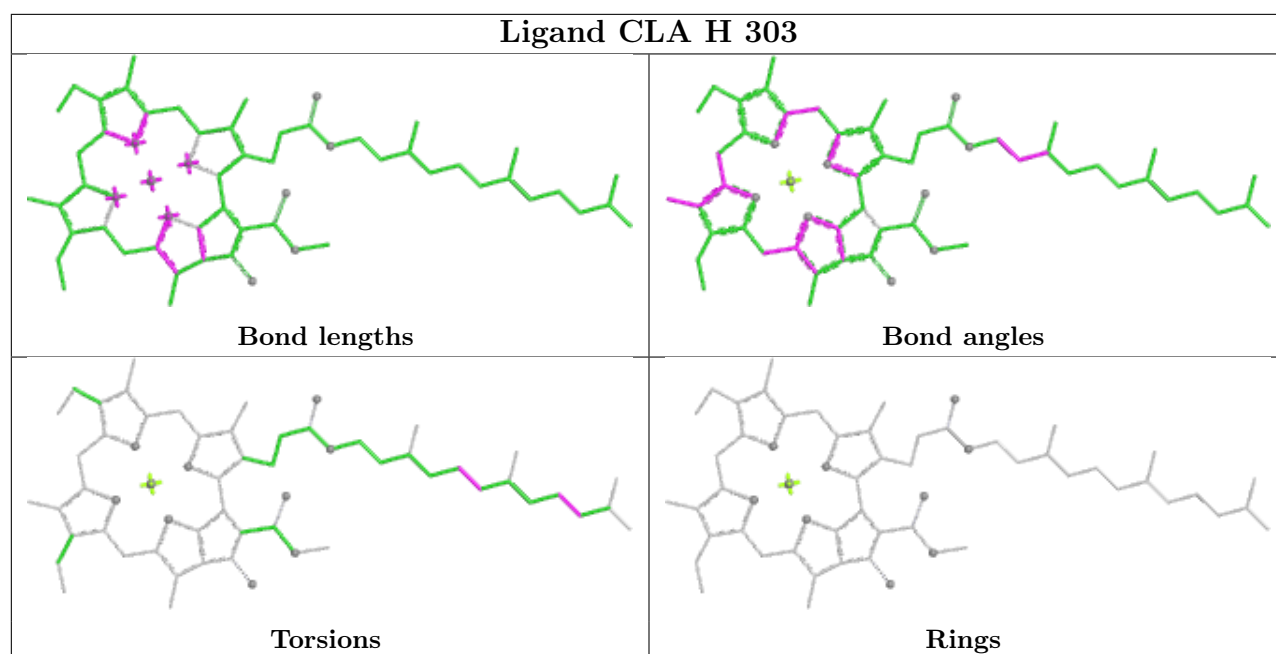
Bond angles



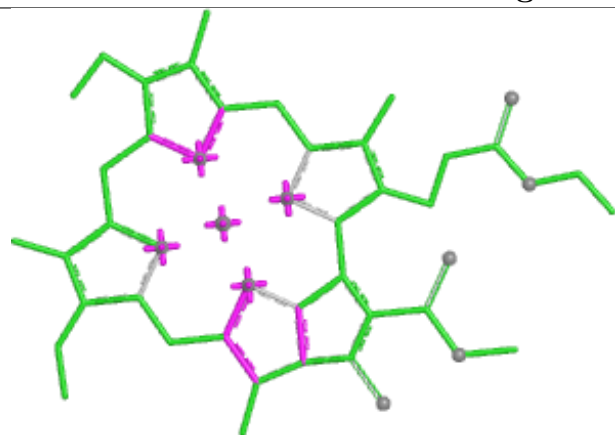
Torsions



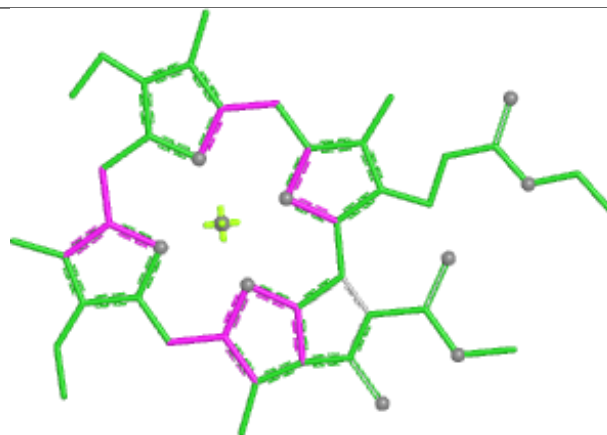
Rings



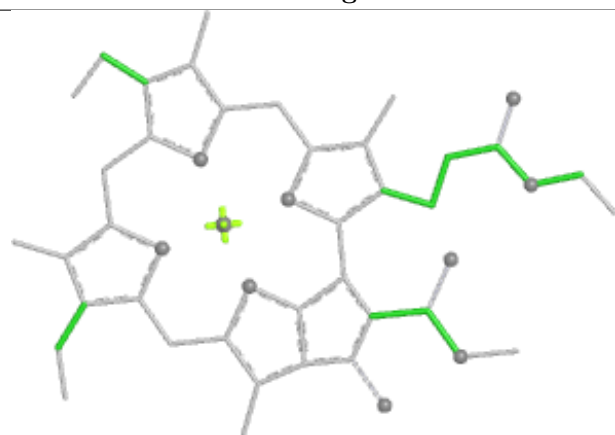
Ligand CLA C 211



Bond lengths



Bond angles

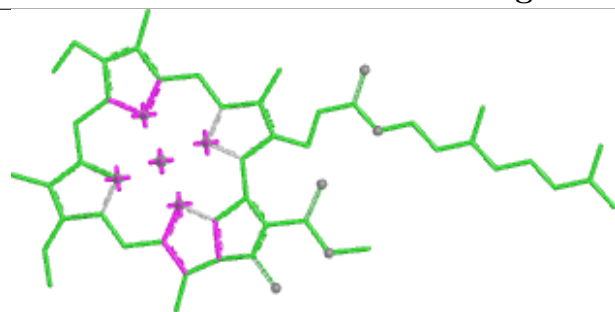


Torsions

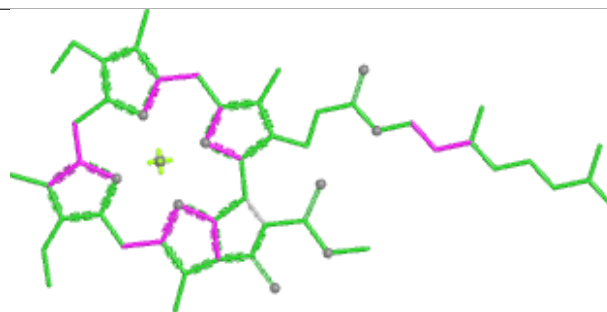


Rings

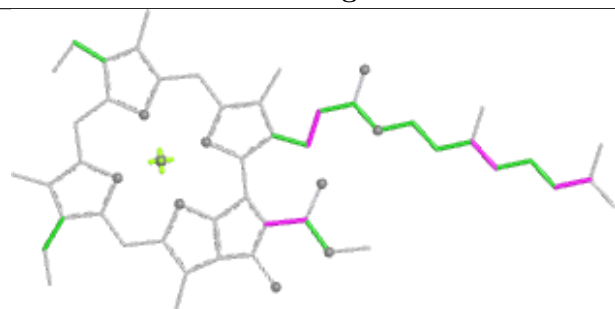
Ligand CLA D 604



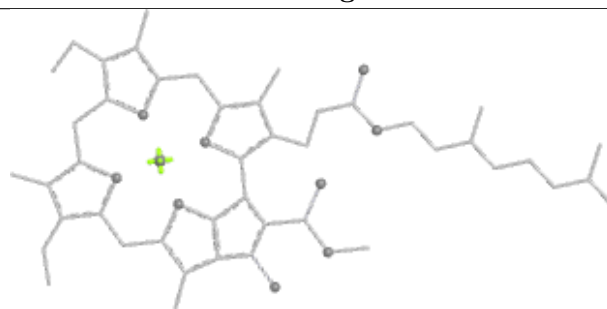
Bond lengths



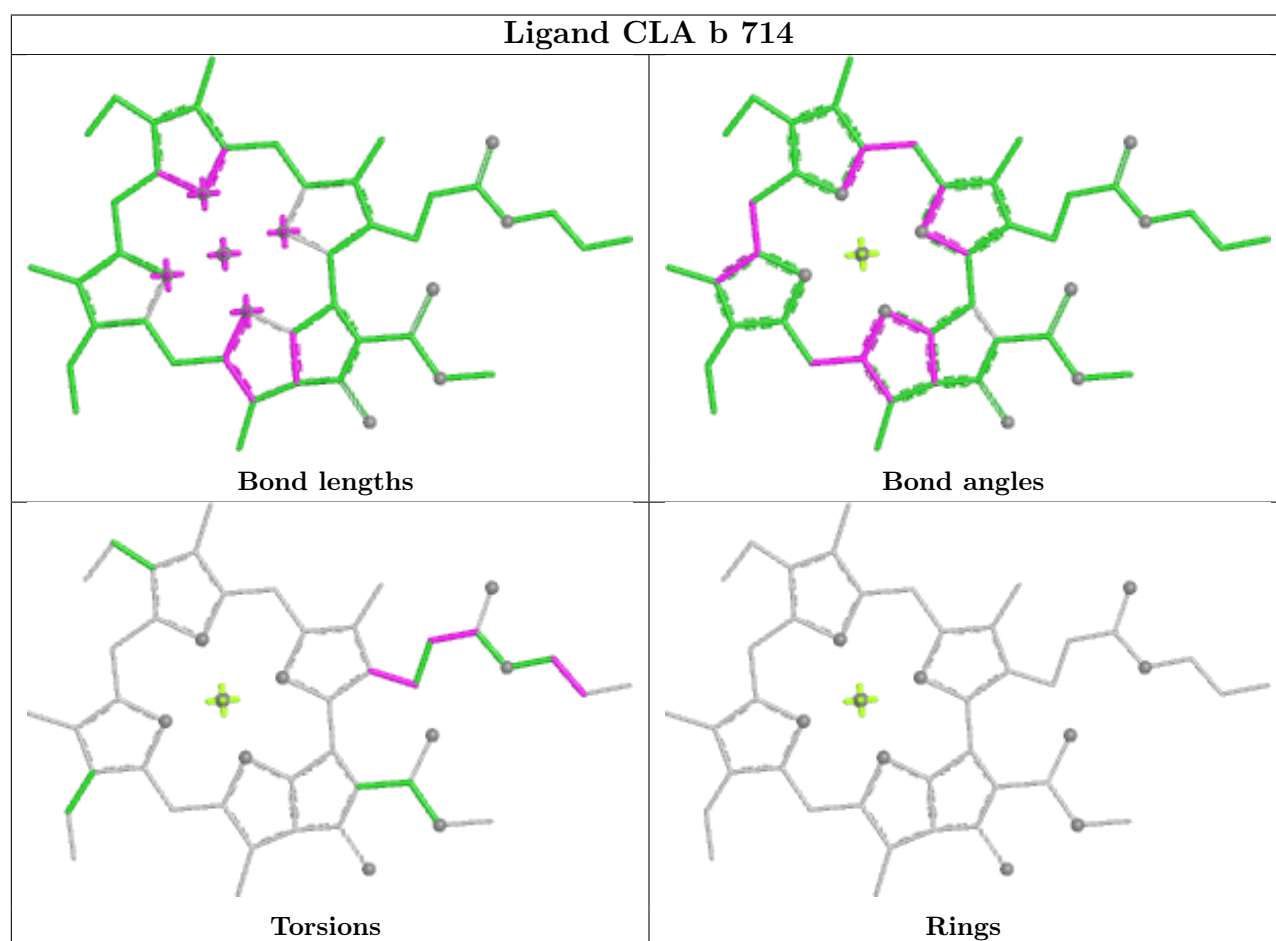
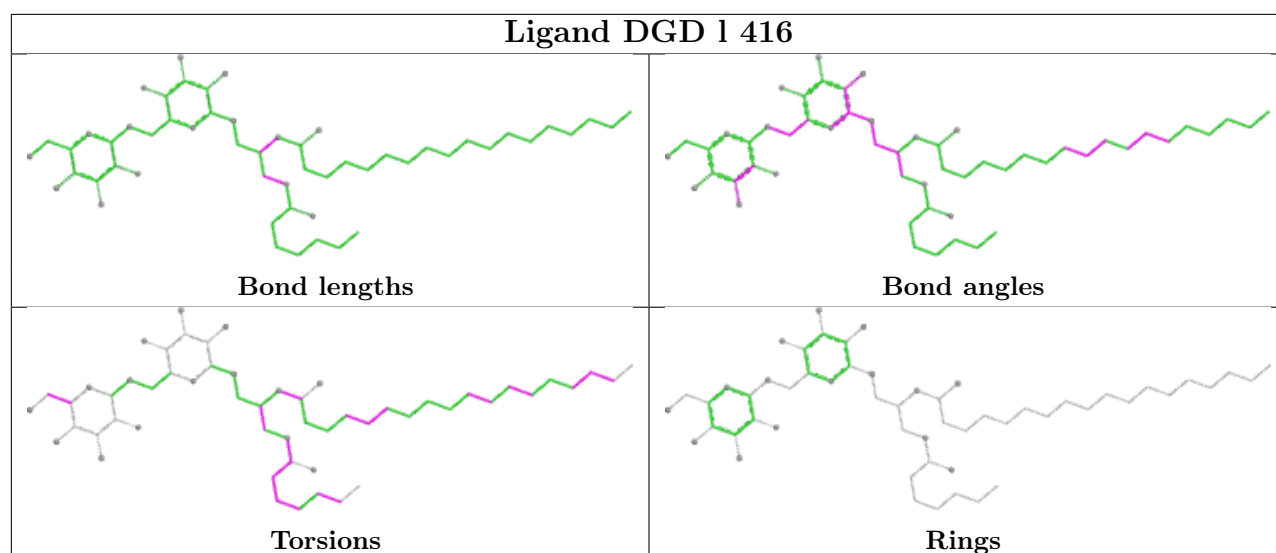
Bond angles

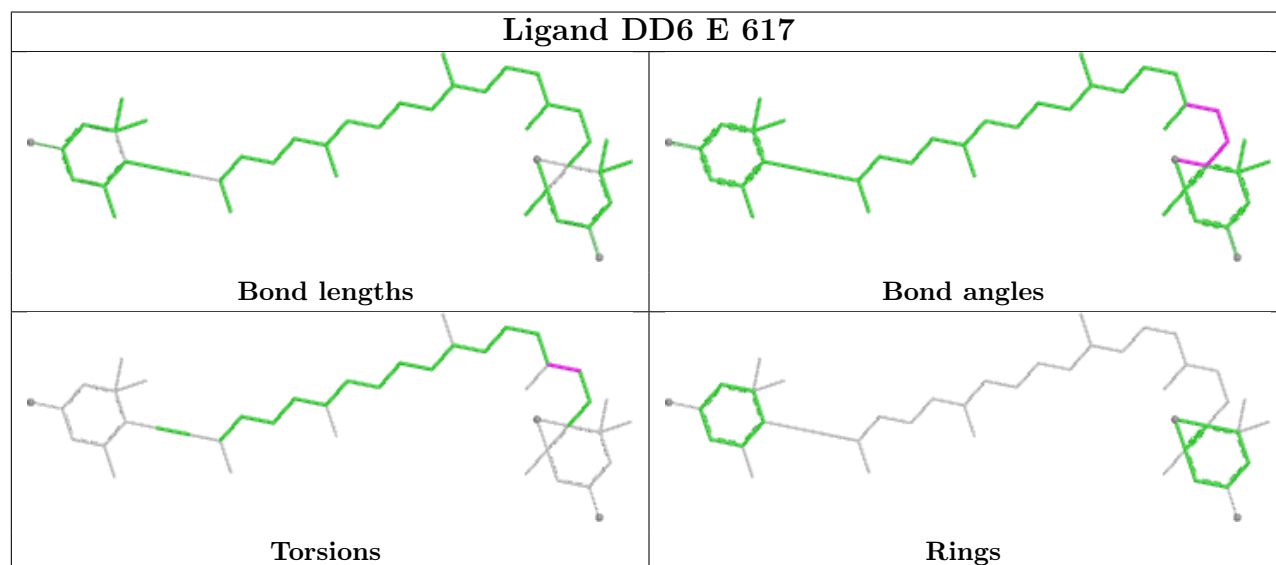
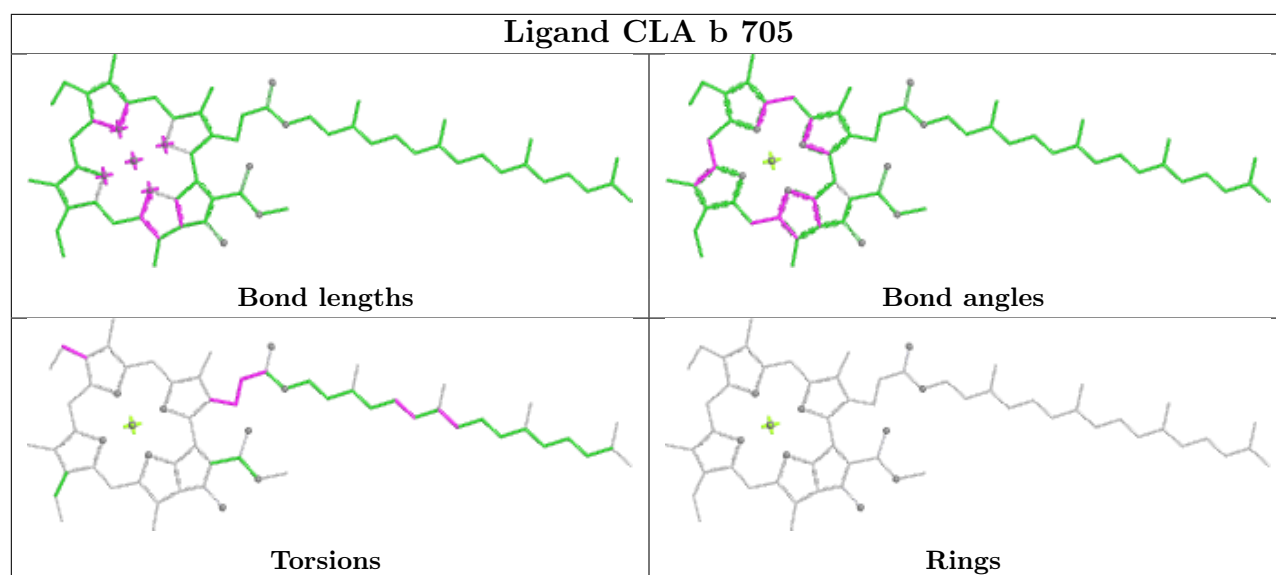


Torsions

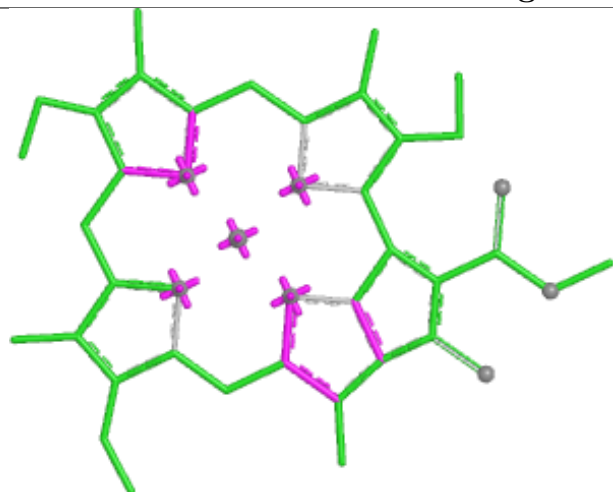


Rings

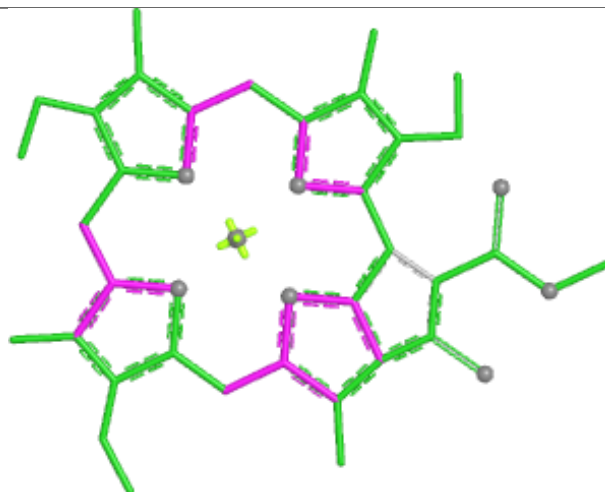




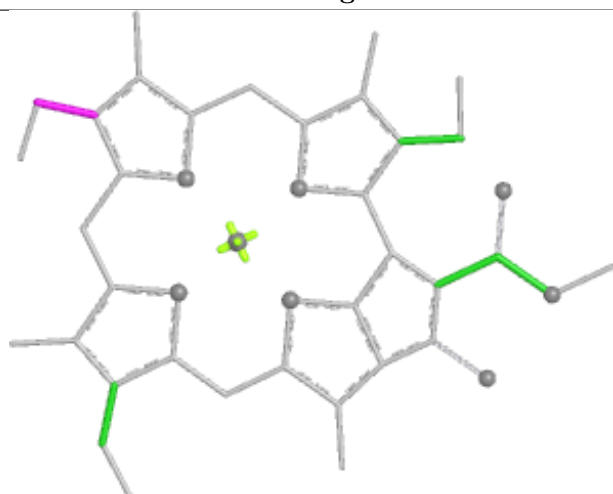
Ligand CLA J 607



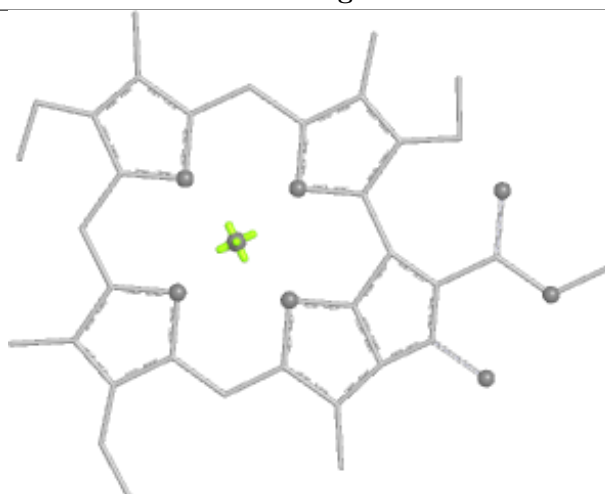
Bond lengths



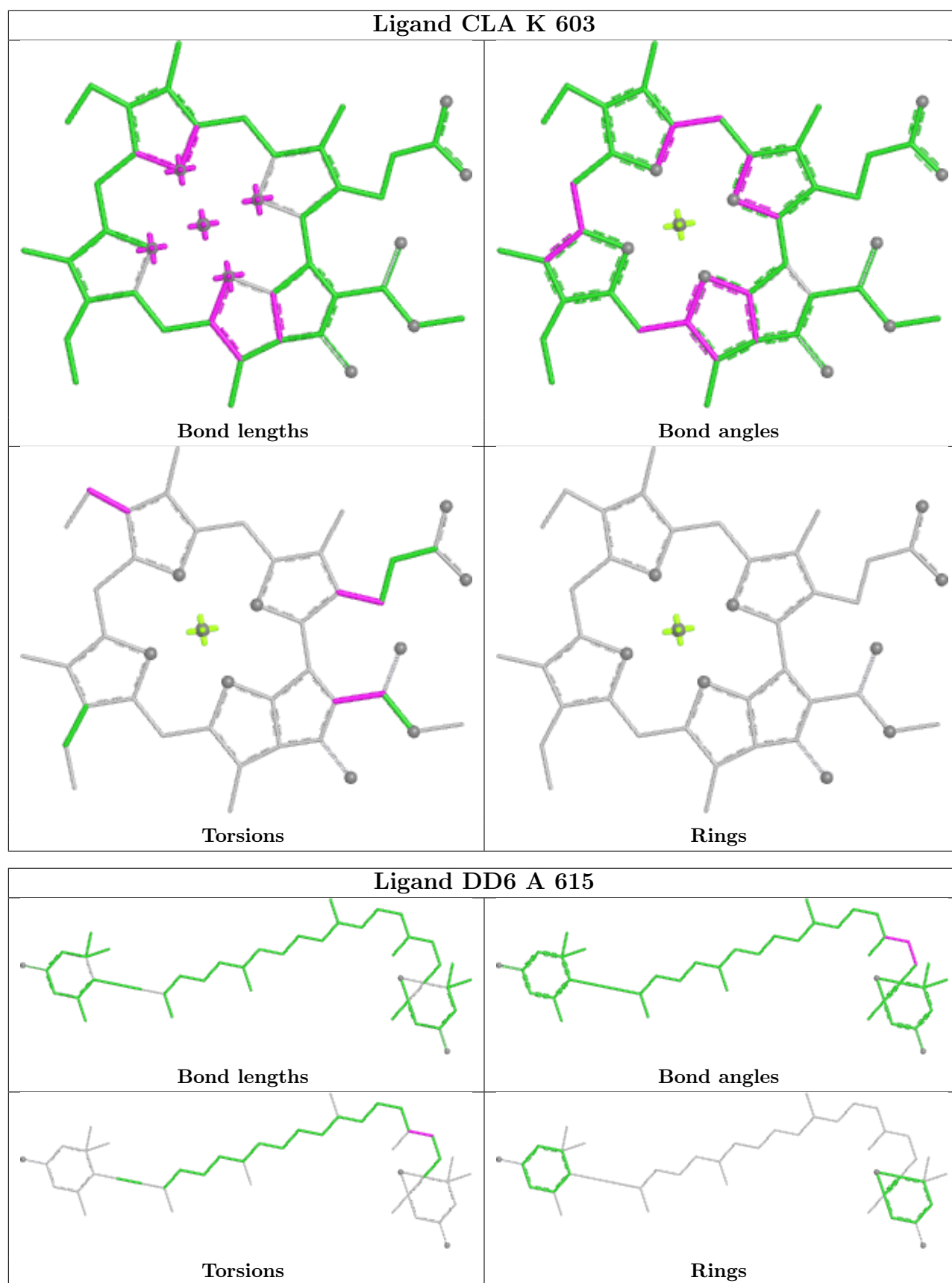
Bond angles

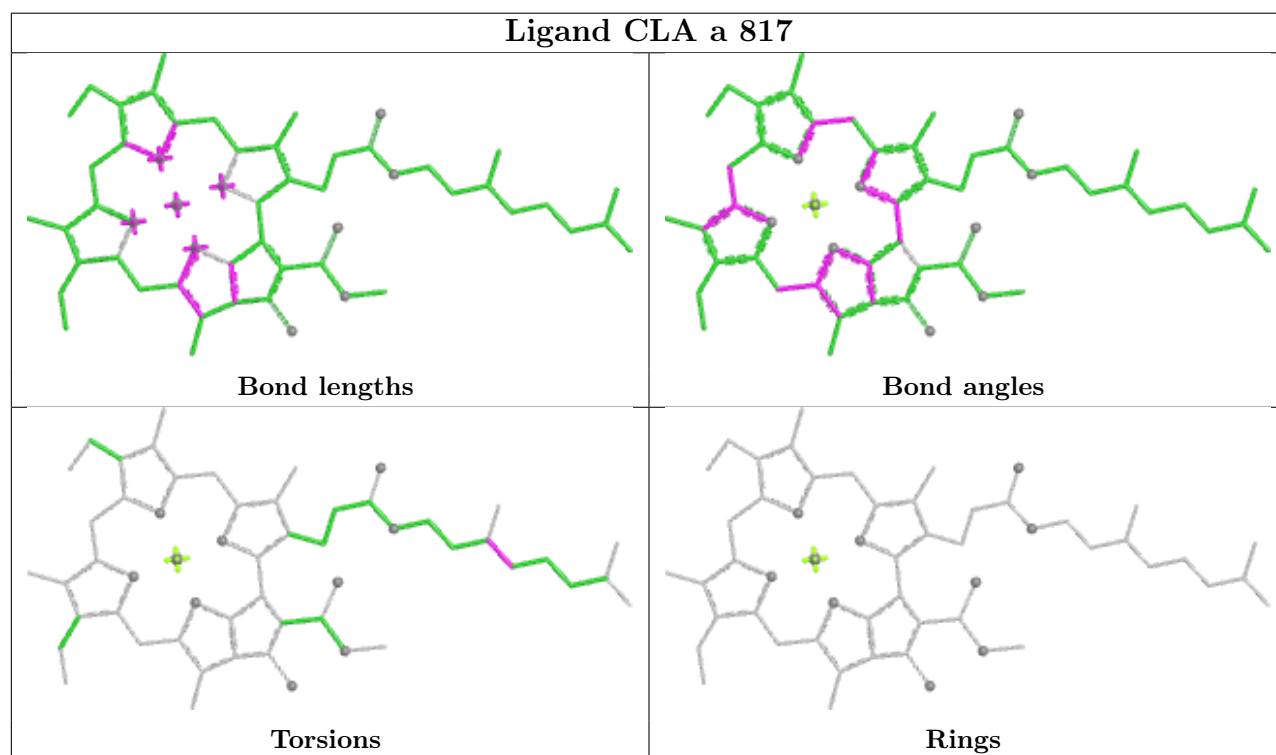
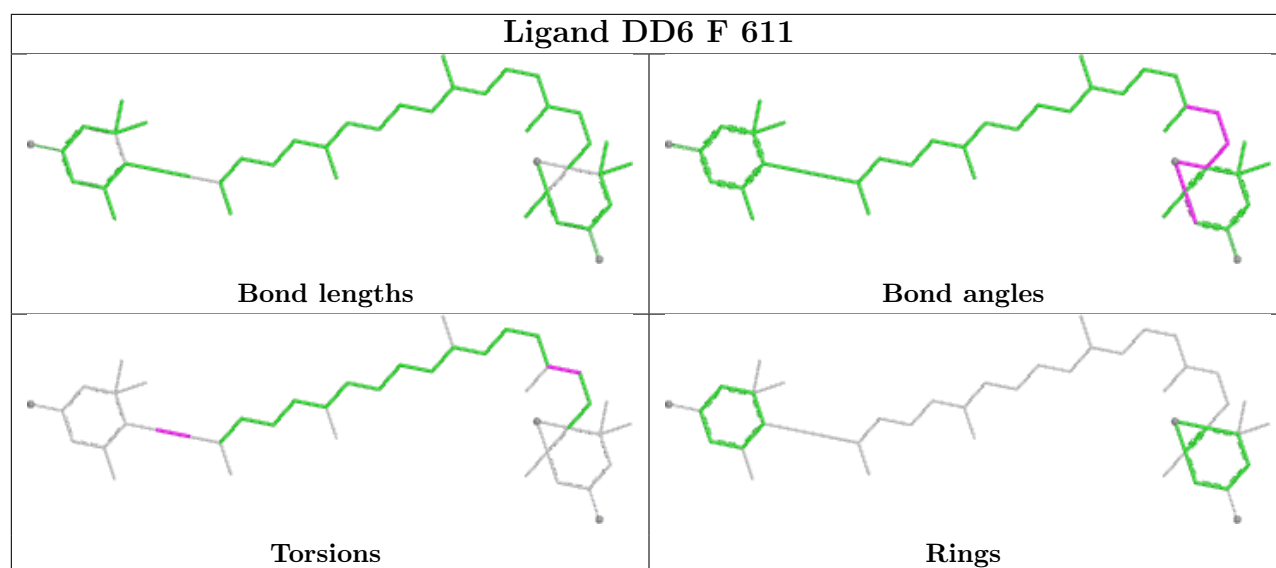


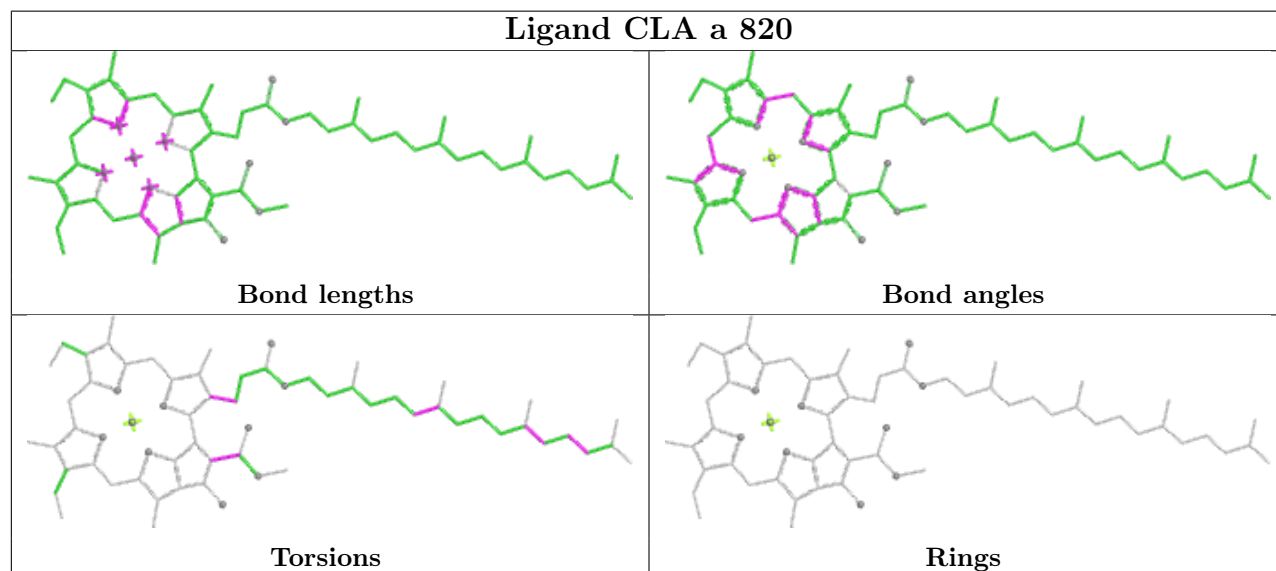
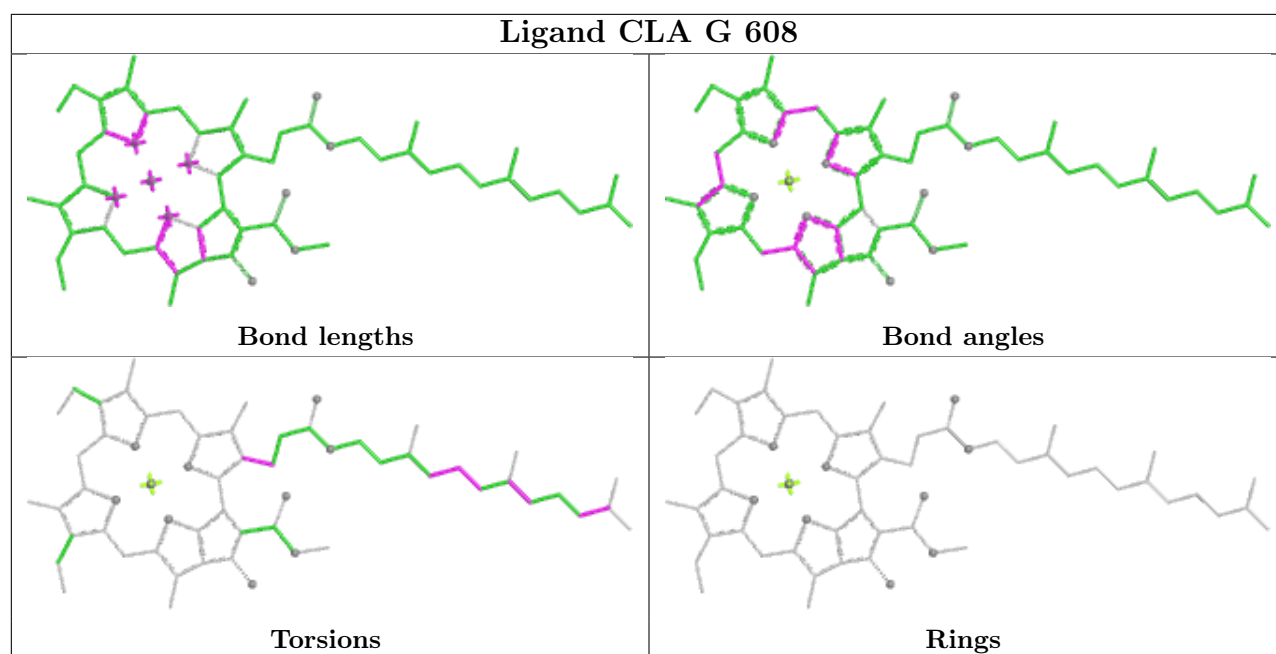
Torsions

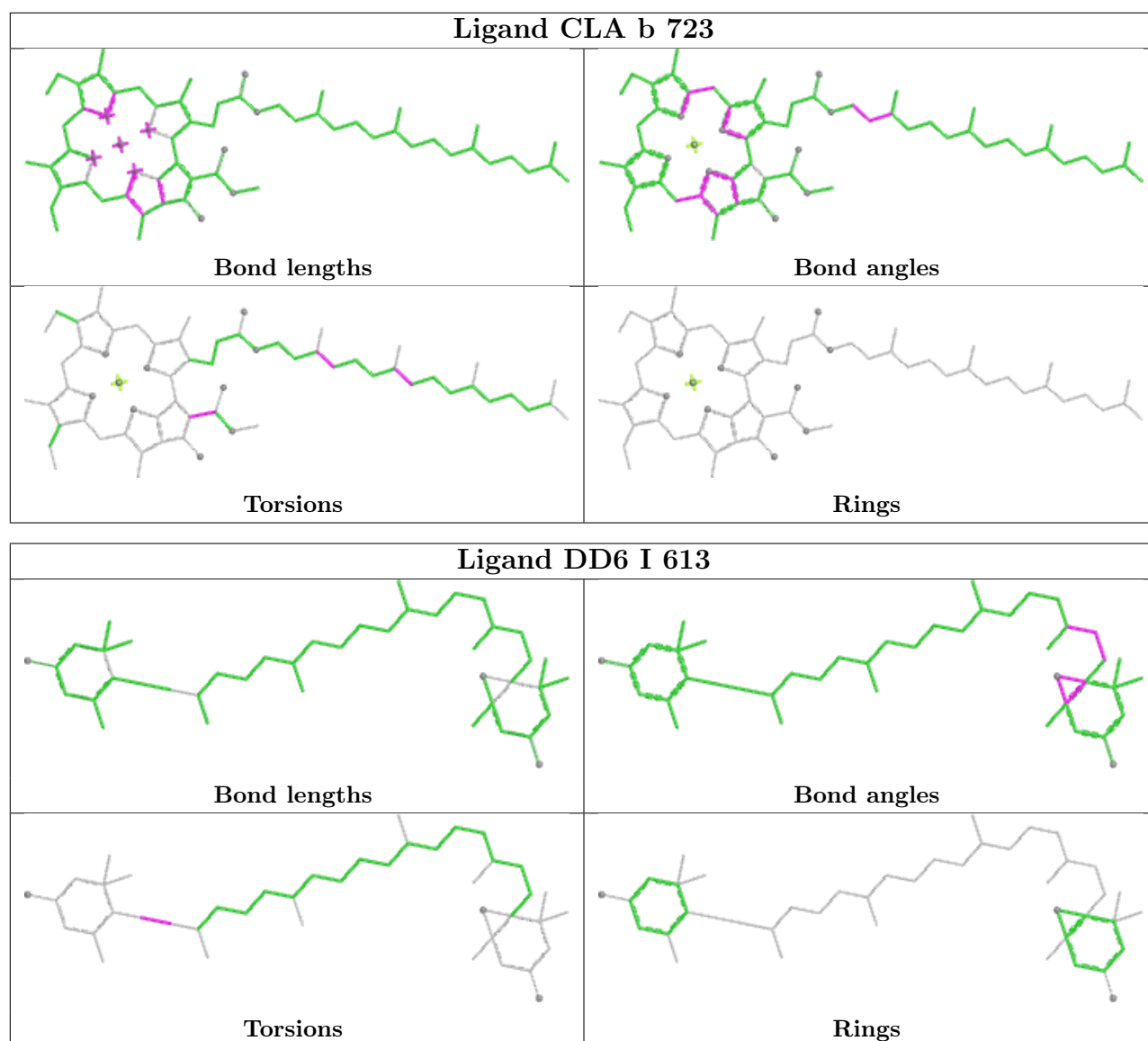


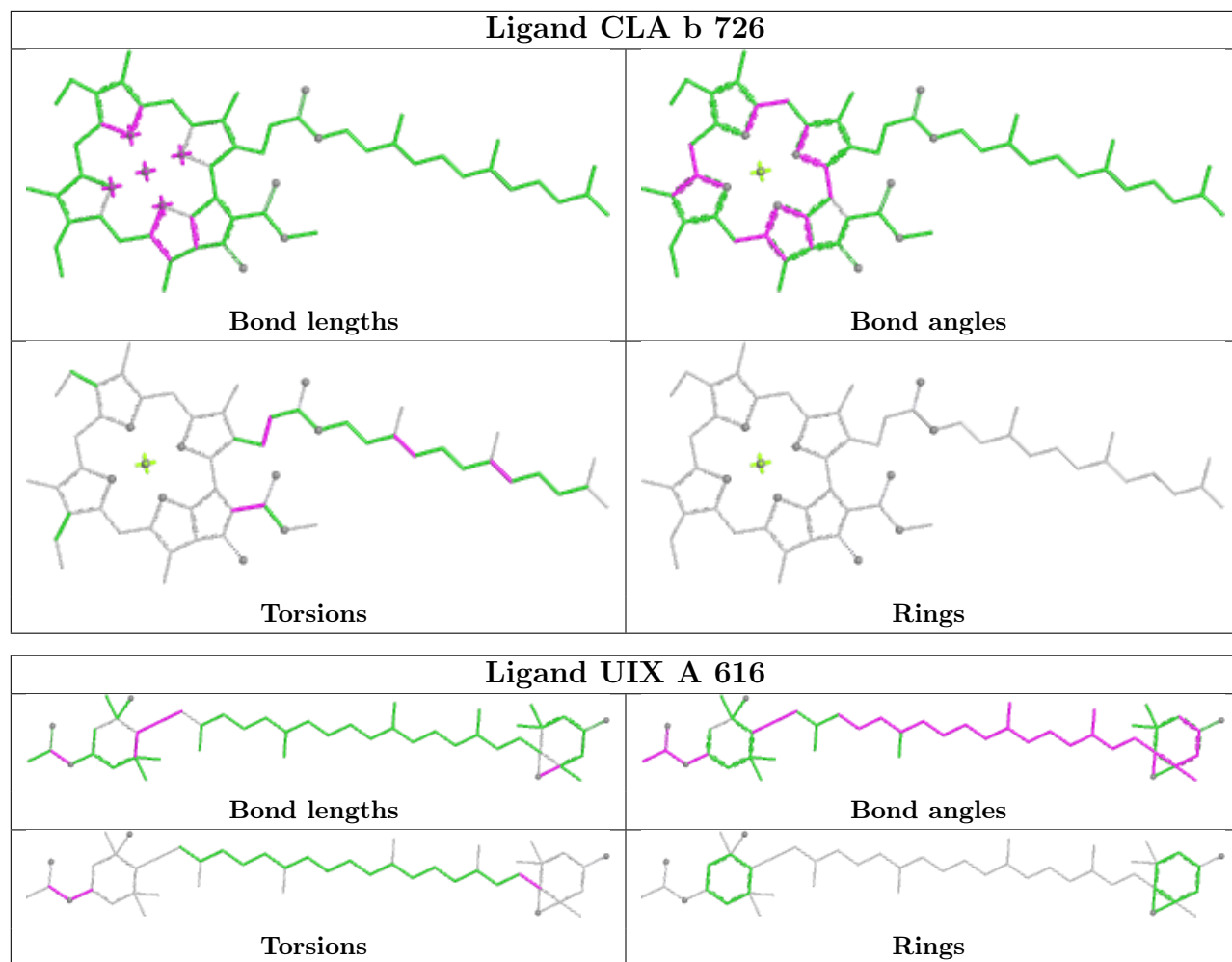
Rings



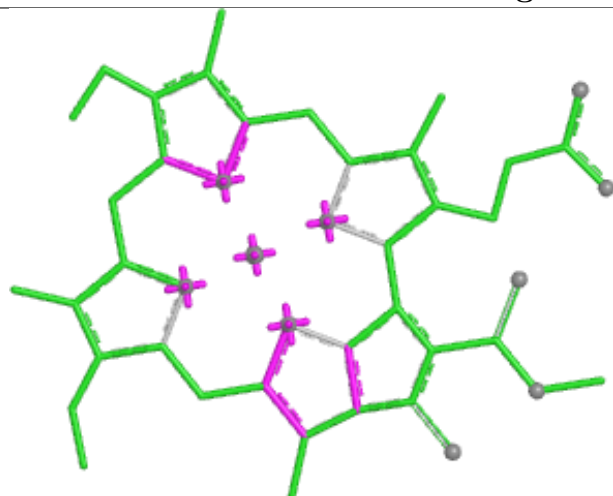




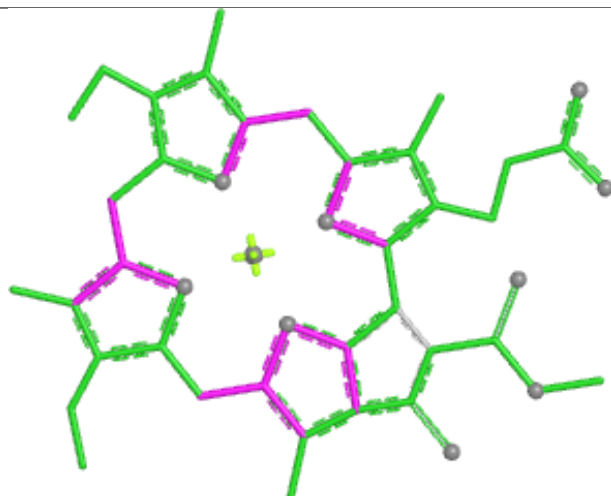




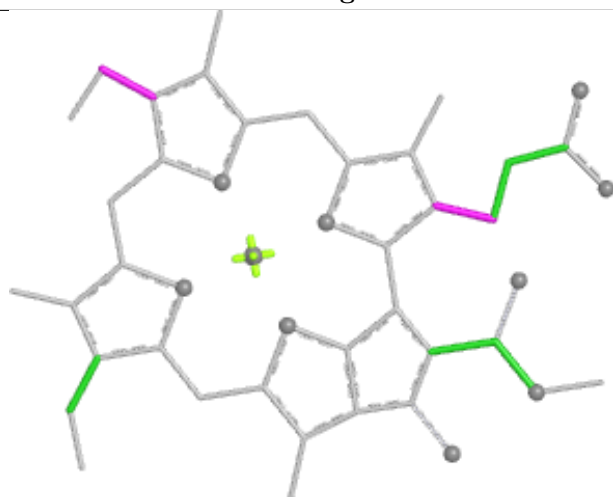
Ligand CLA F 608



Bond lengths



Bond angles

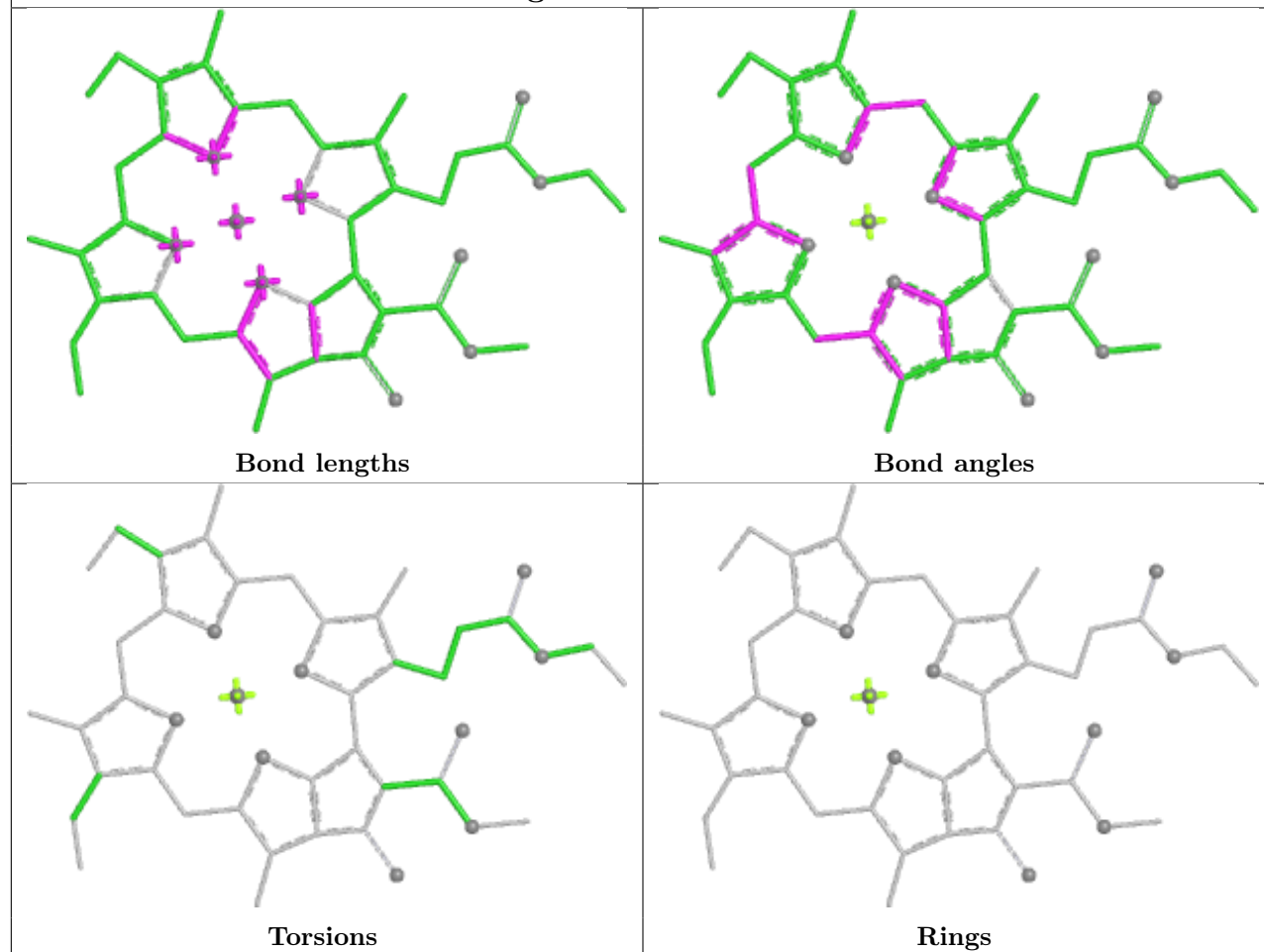


Torsions

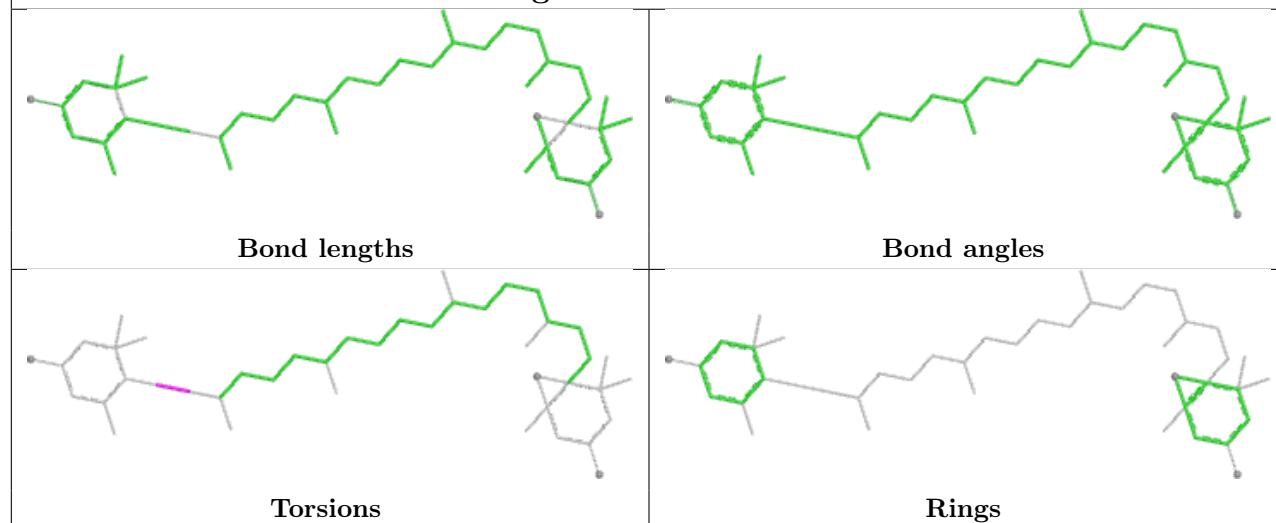


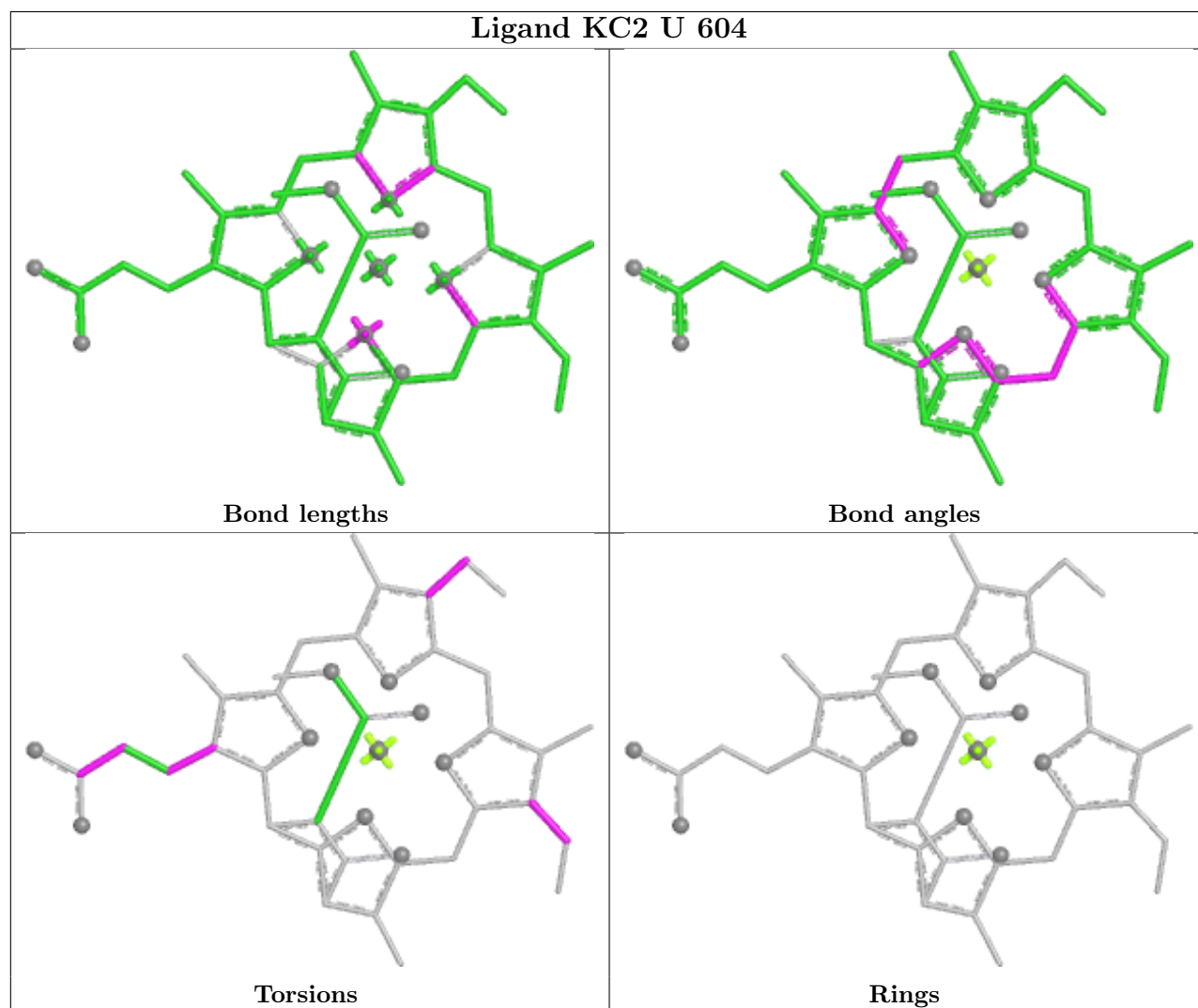
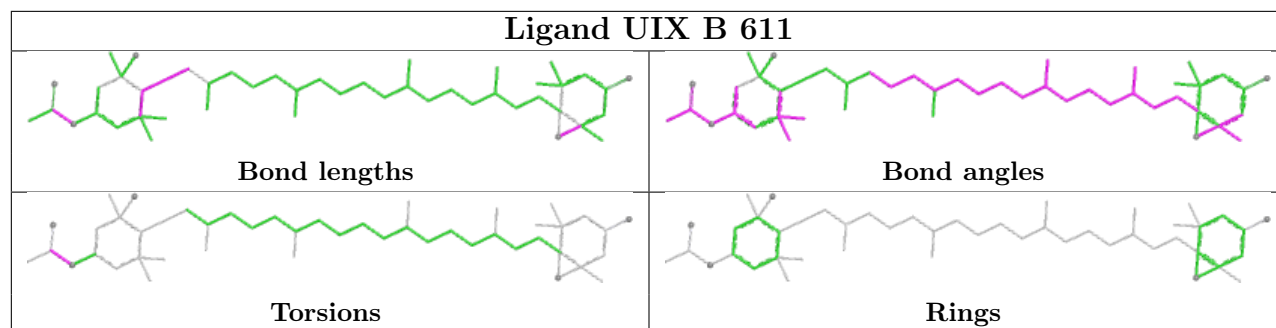
Rings

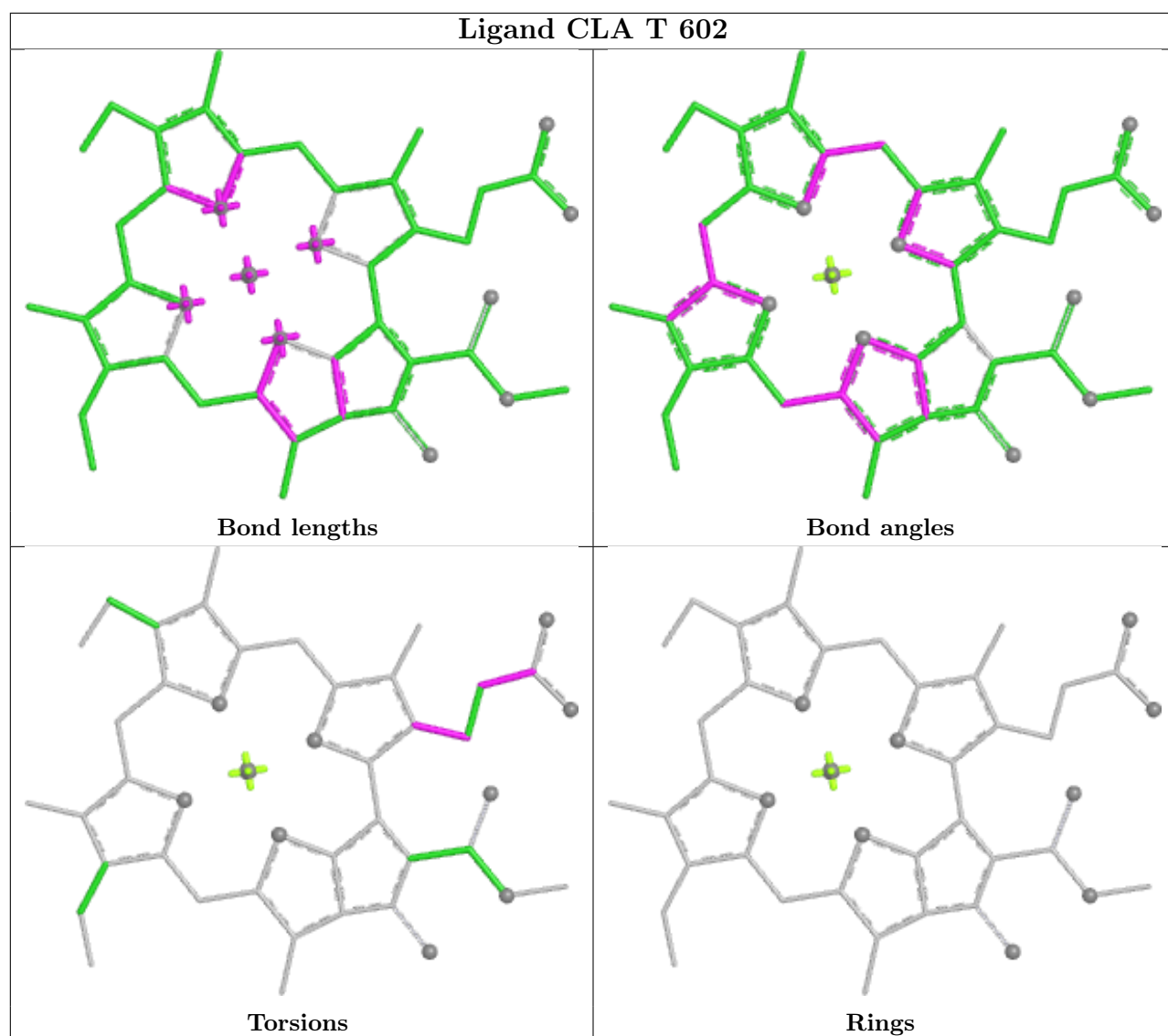
Ligand CLA C 208



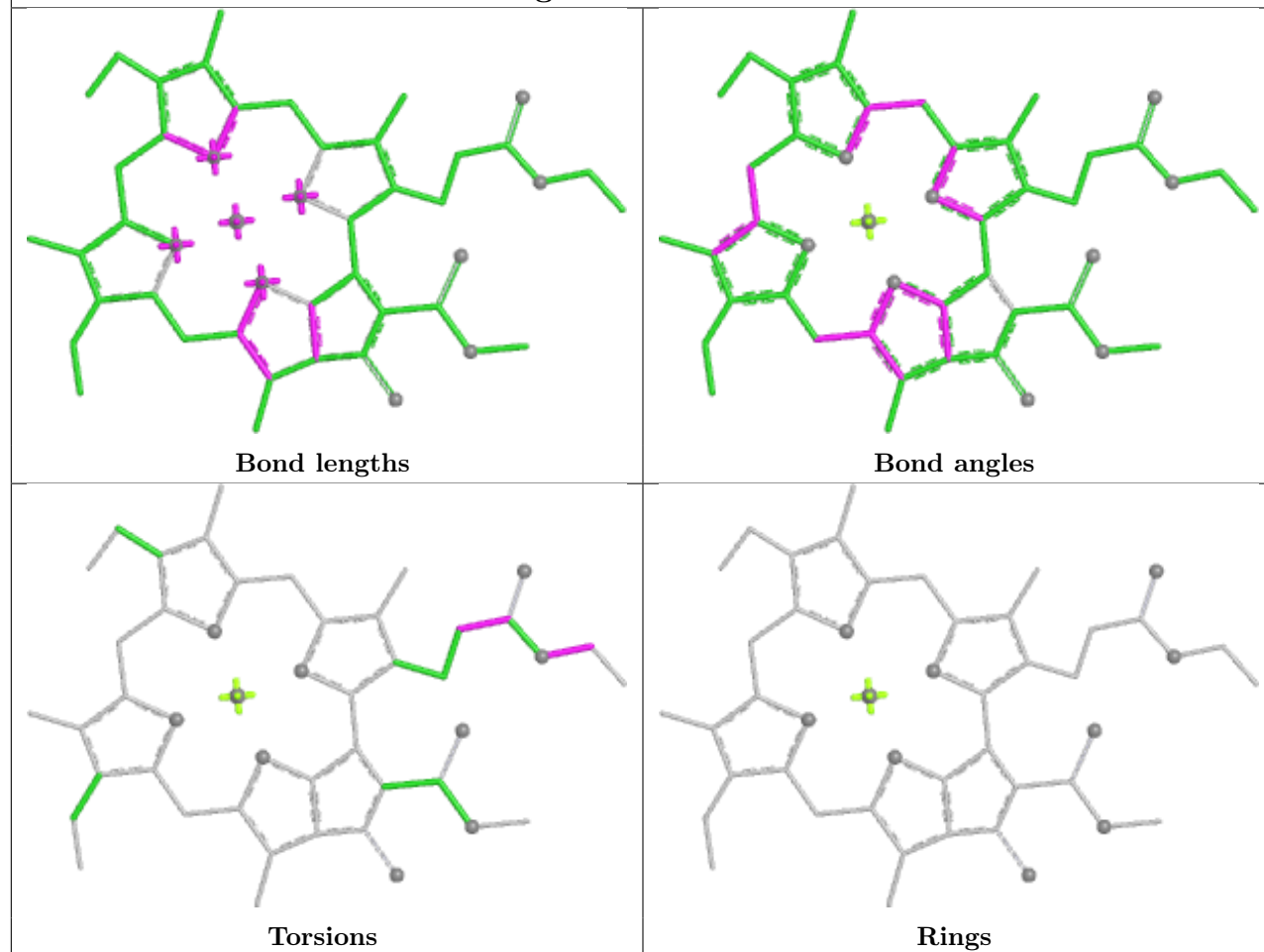
Ligand DD6 G 616



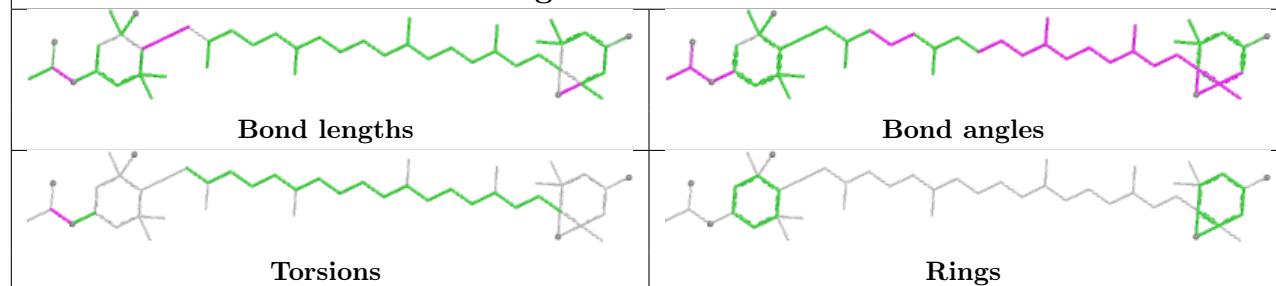


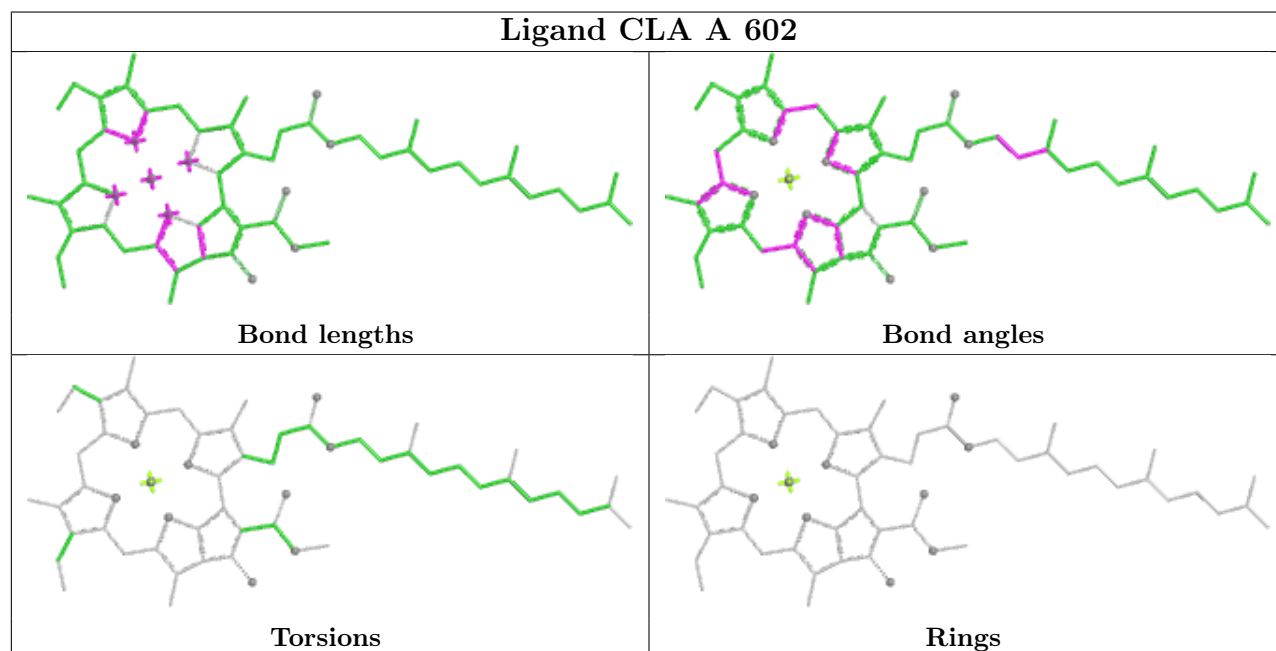
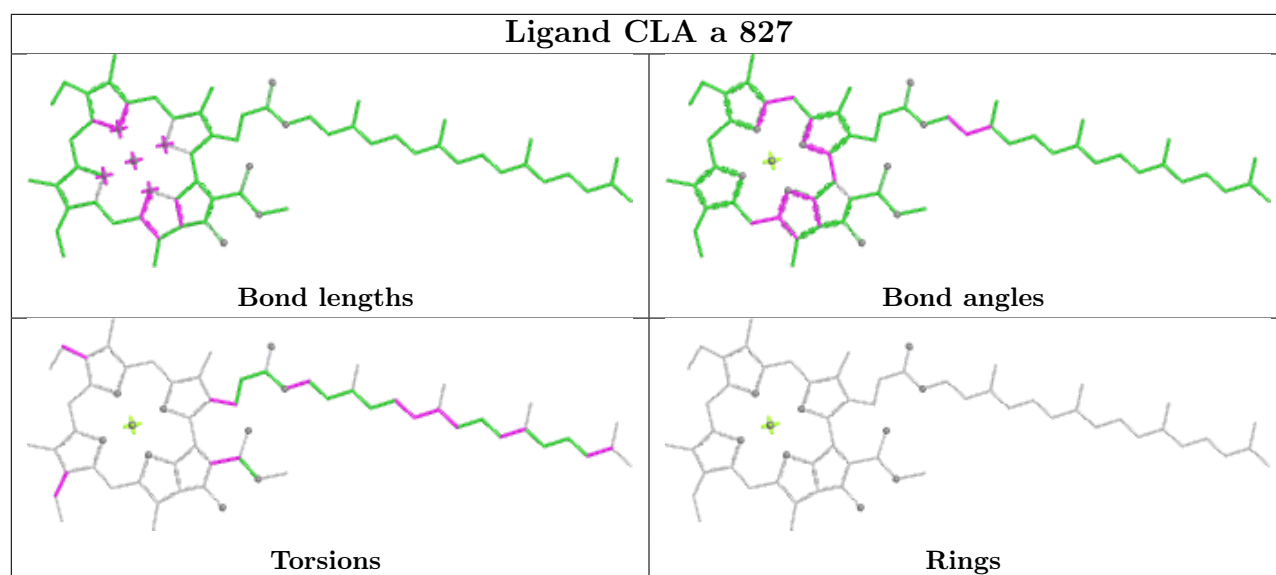


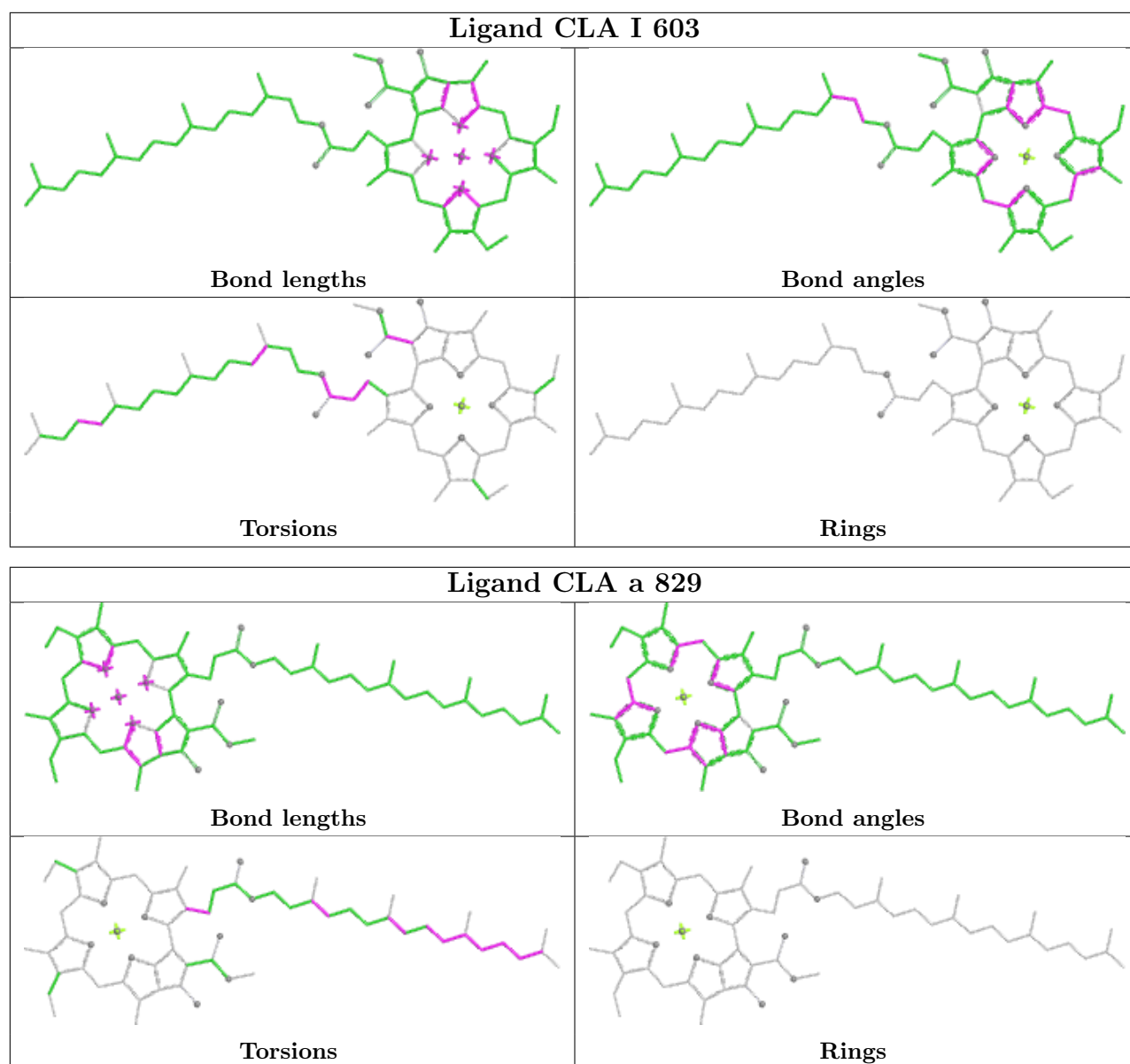
Ligand CLA 1 408

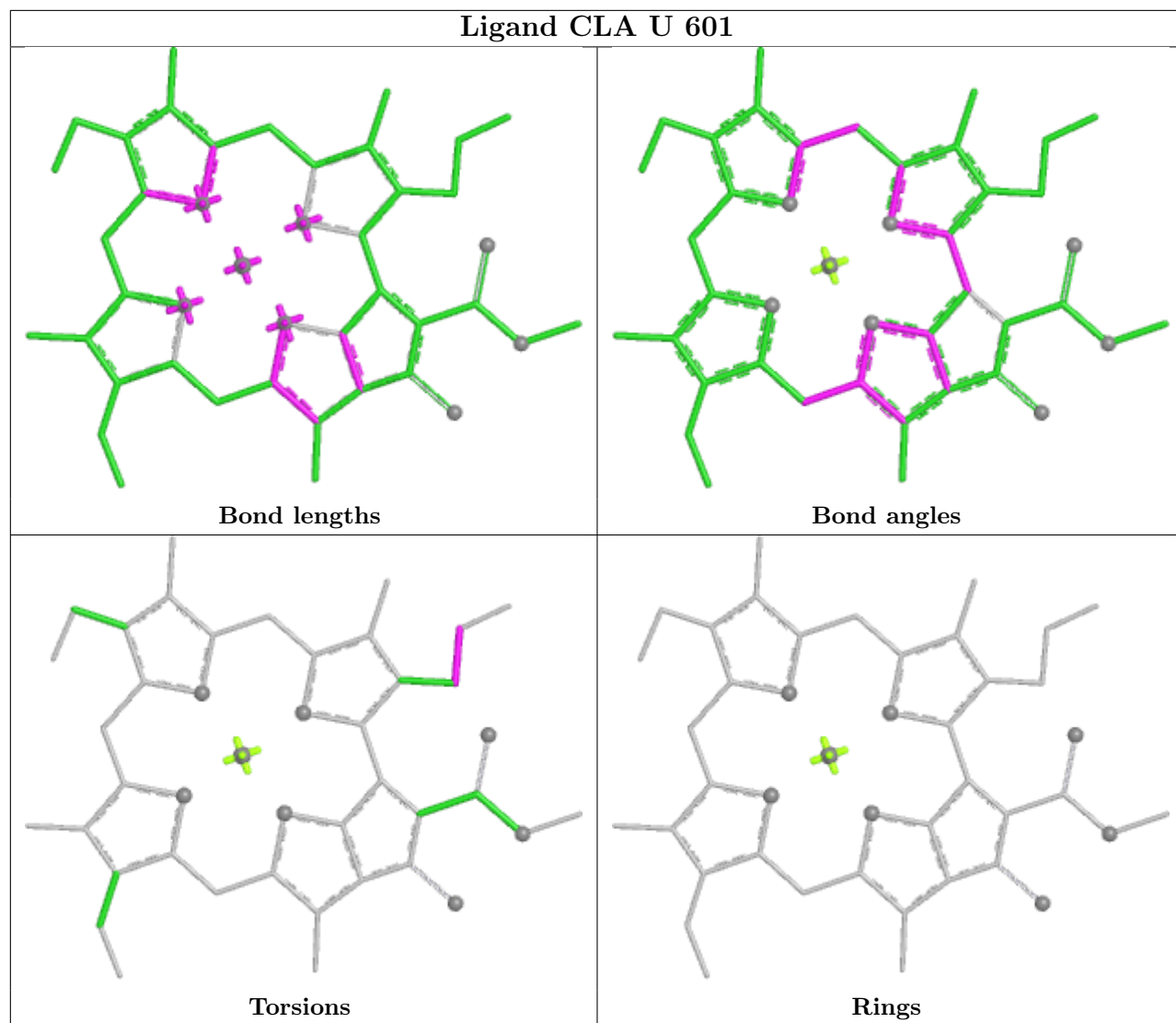


Ligand UIX A 613

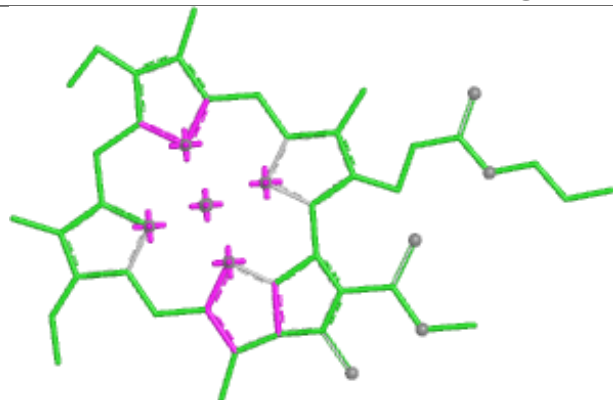




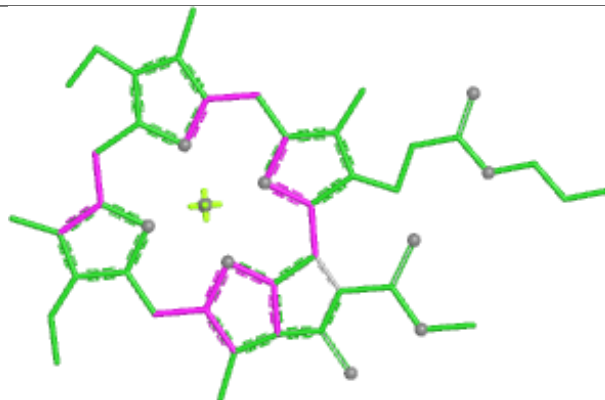




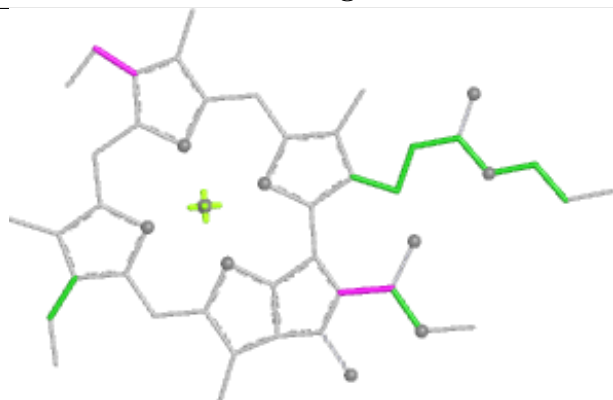
Ligand CLA b 720



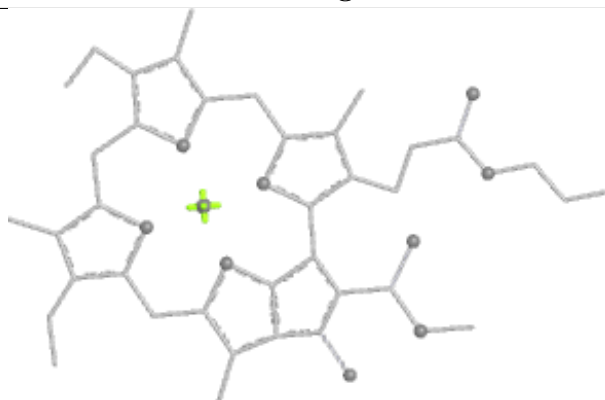
Bond lengths



Bond angles

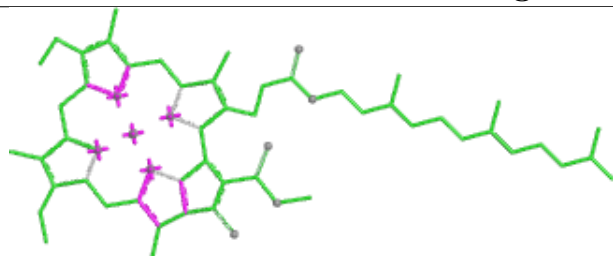


Torsions

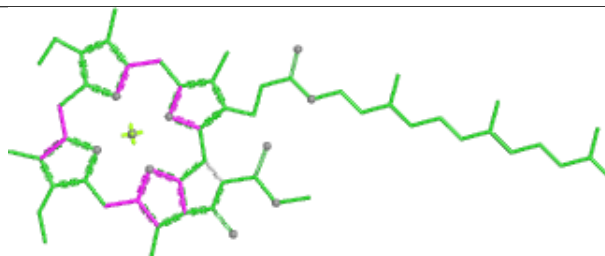


Rings

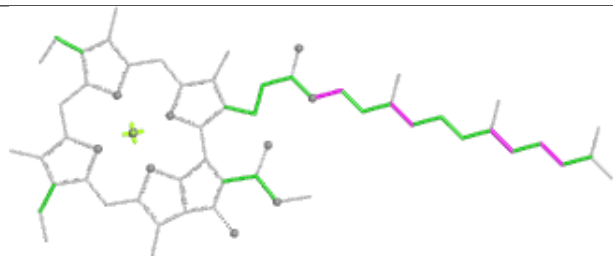
Ligand CLA U 605



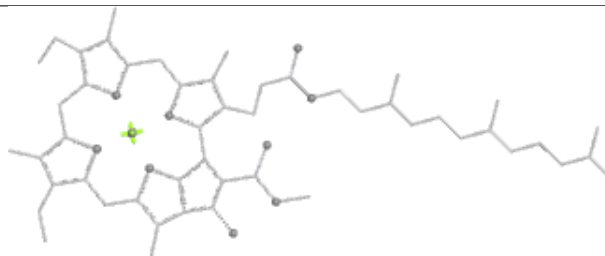
Bond lengths



Bond angles

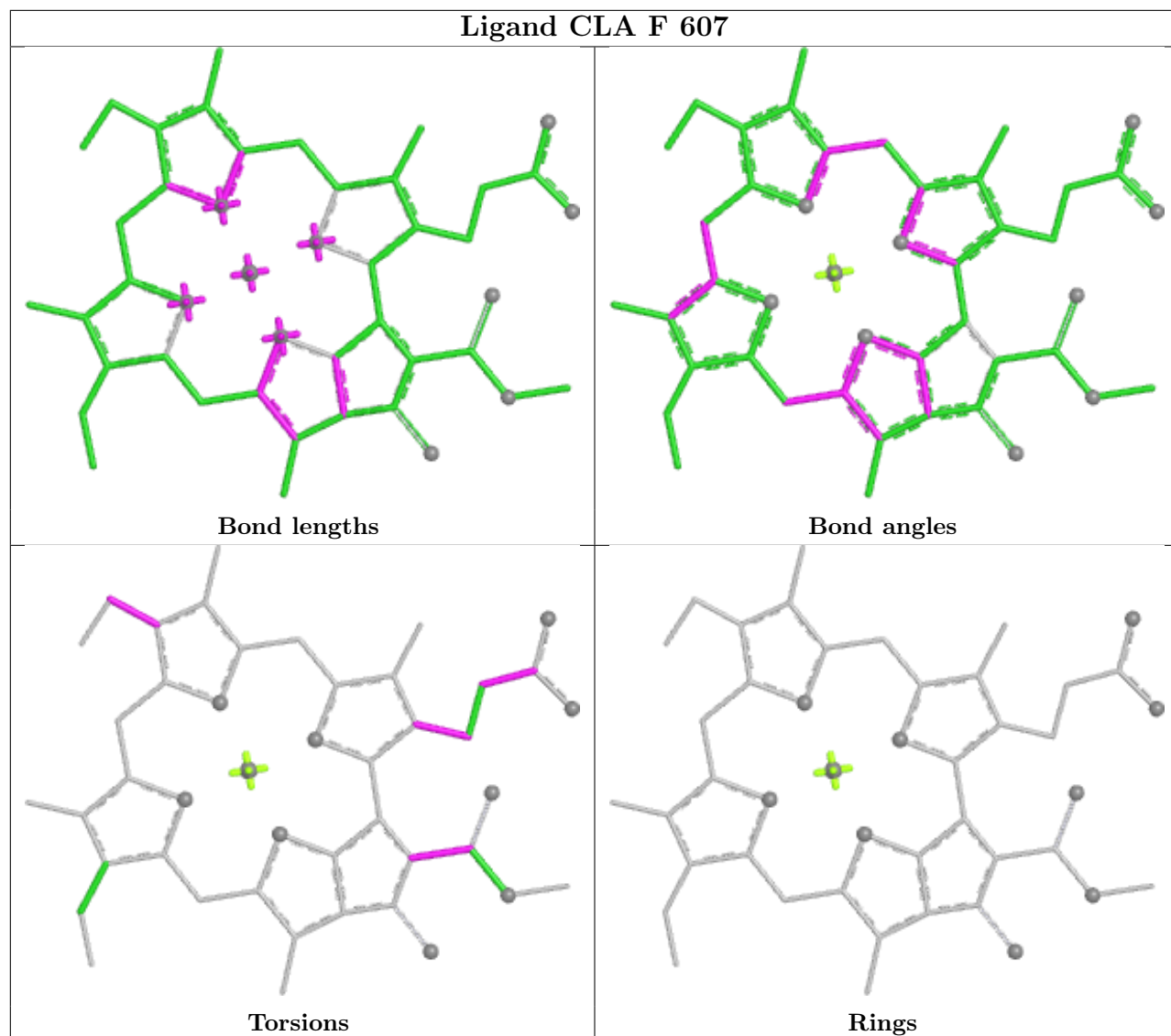


Torsions

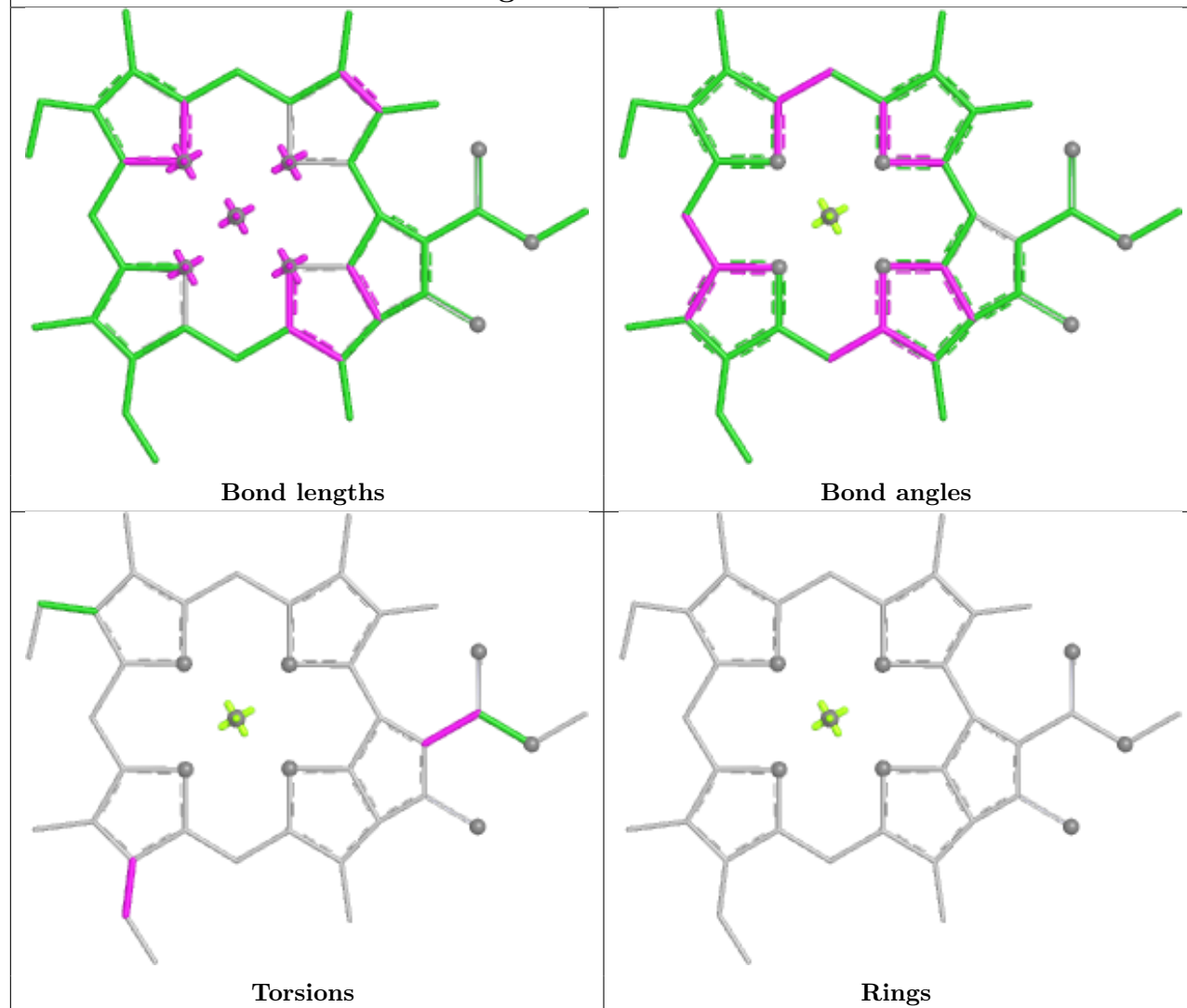


Rings

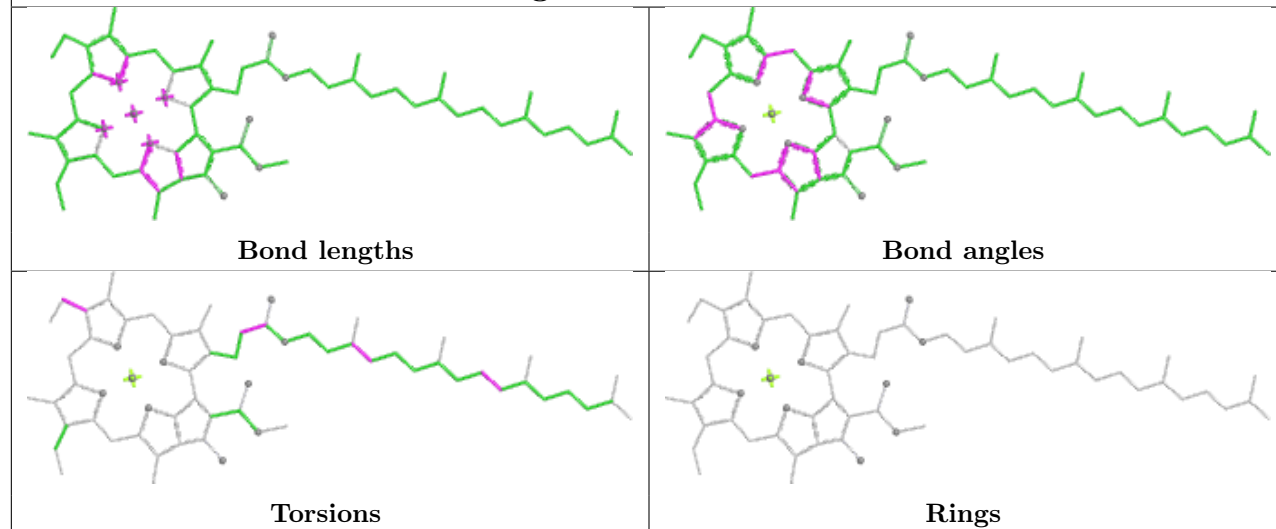
Ligand CLA F 607

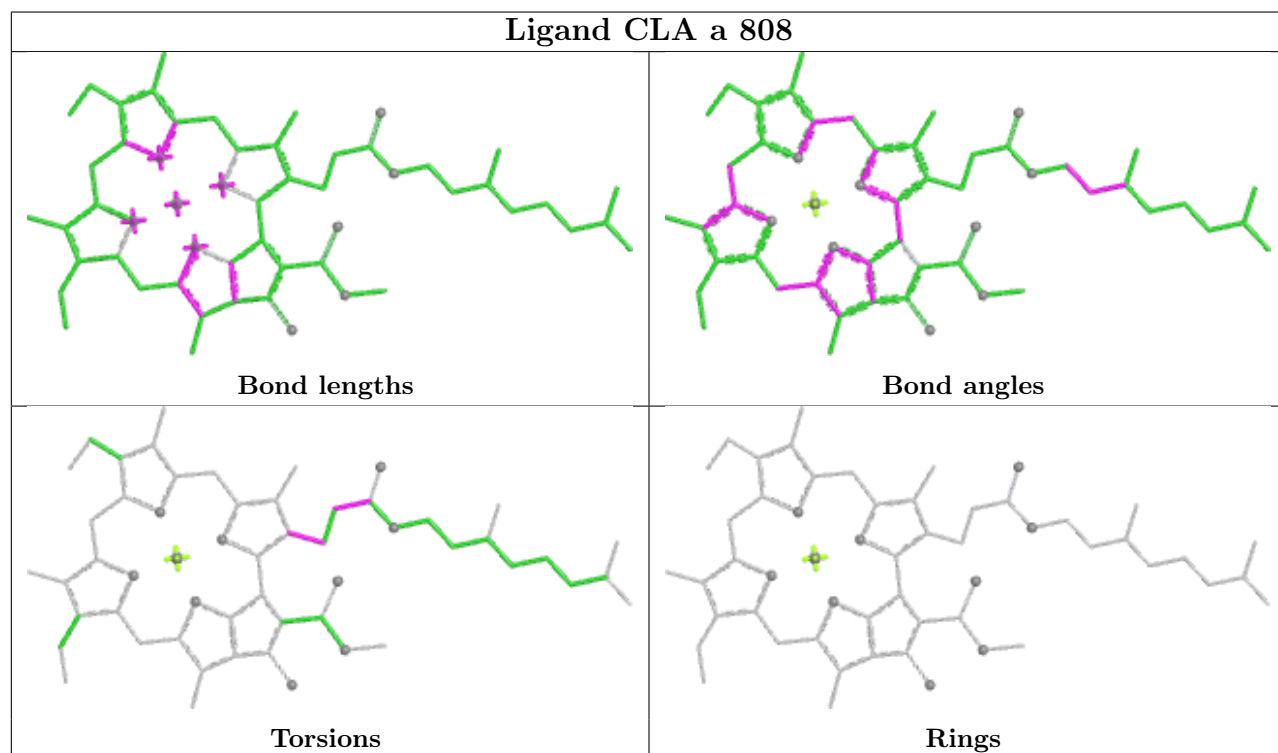
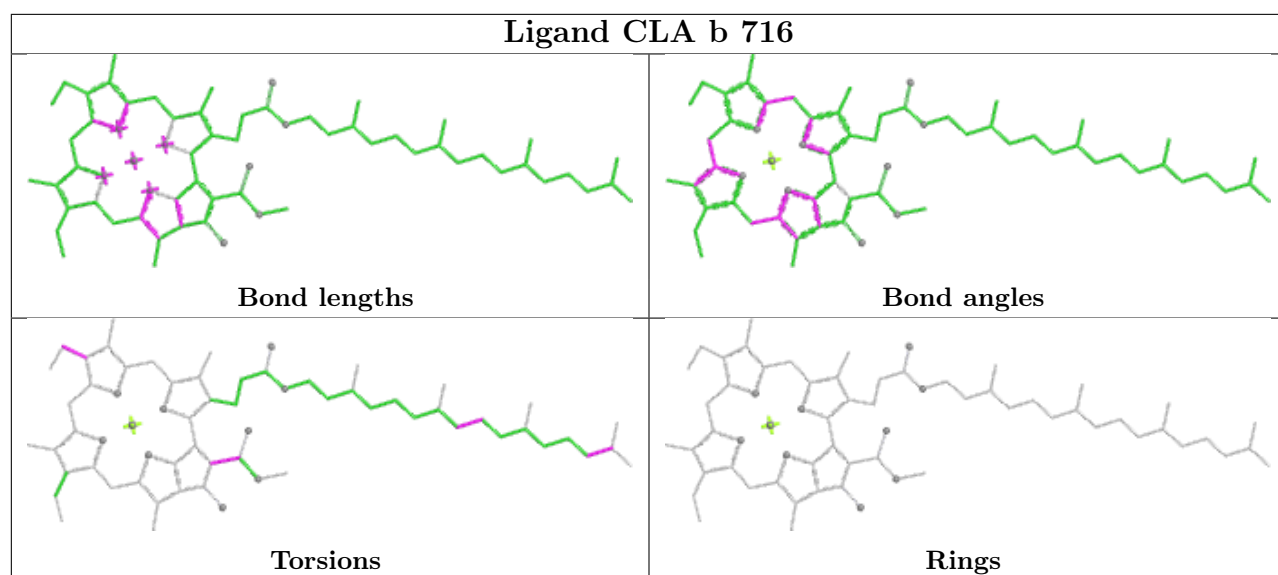


Ligand CLA J 609

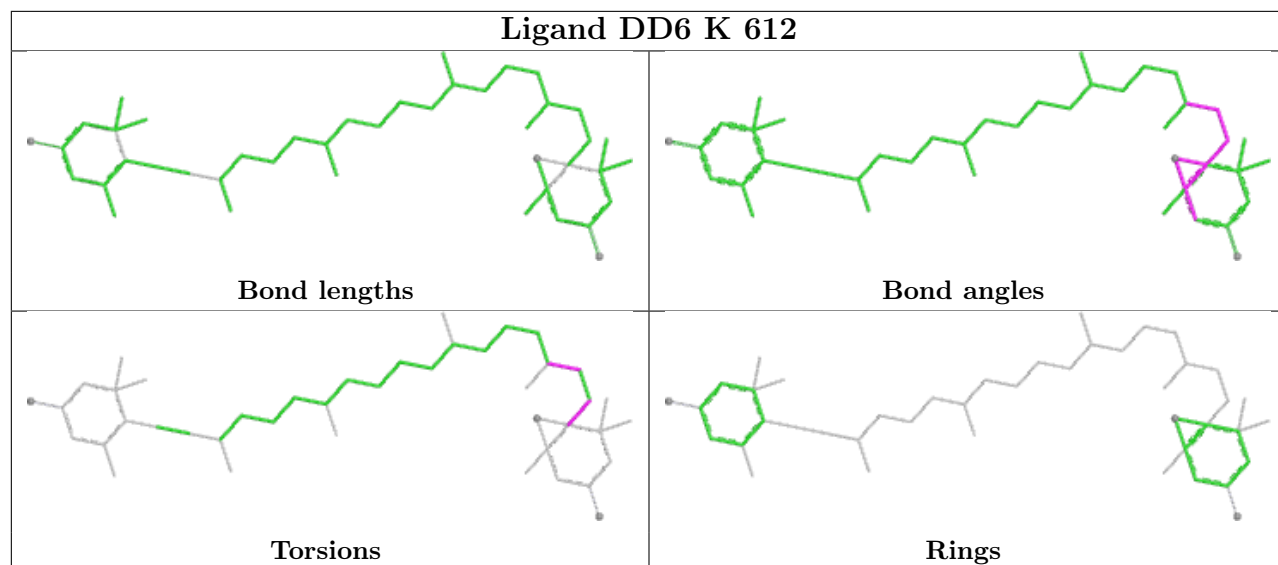


Ligand CLA H 309

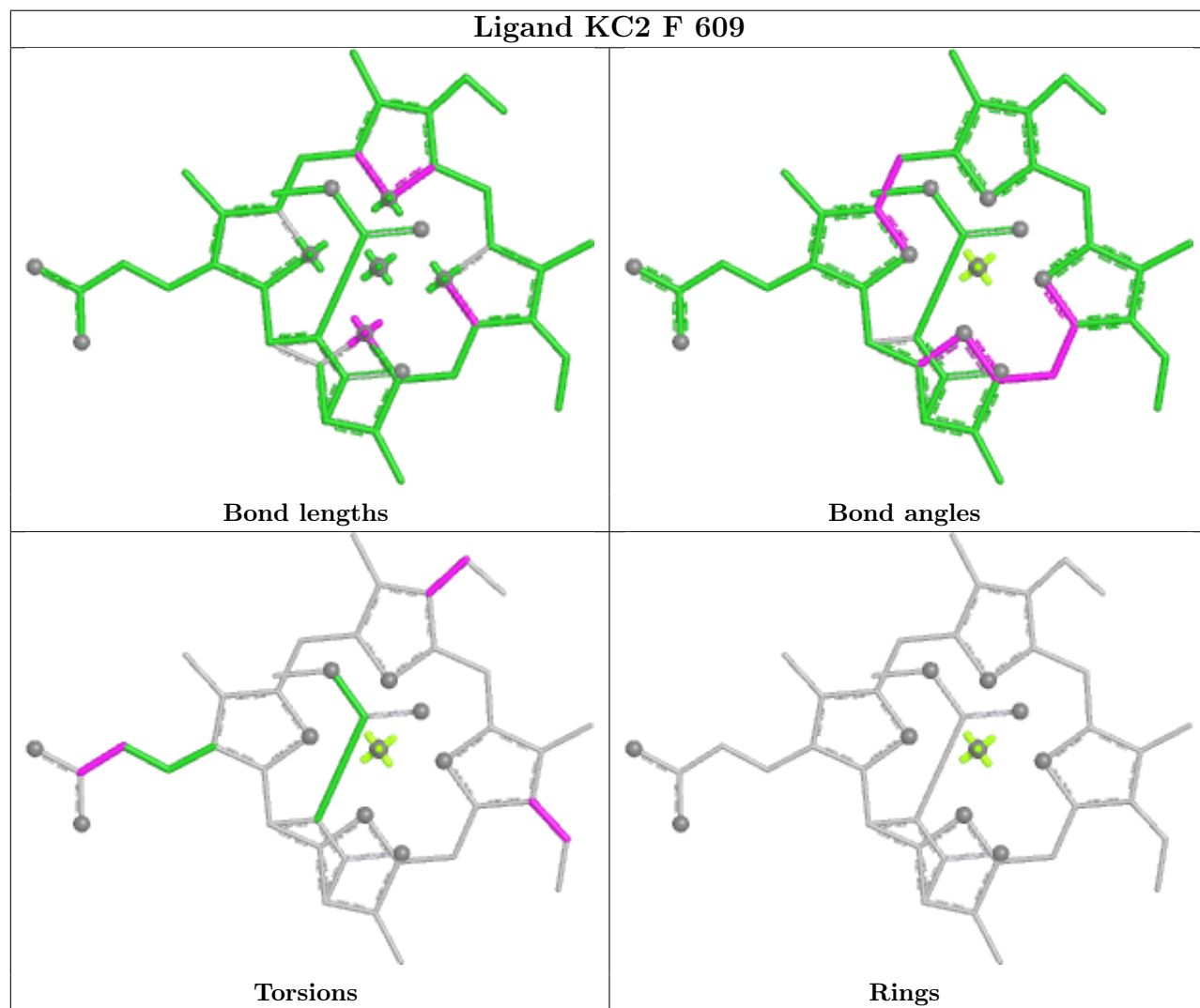




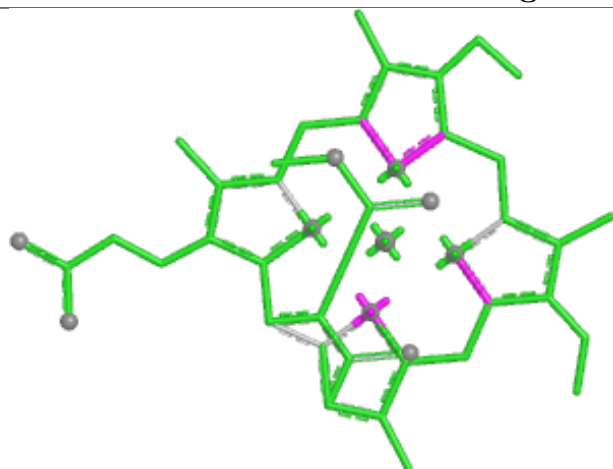
Ligand DD6 K 612



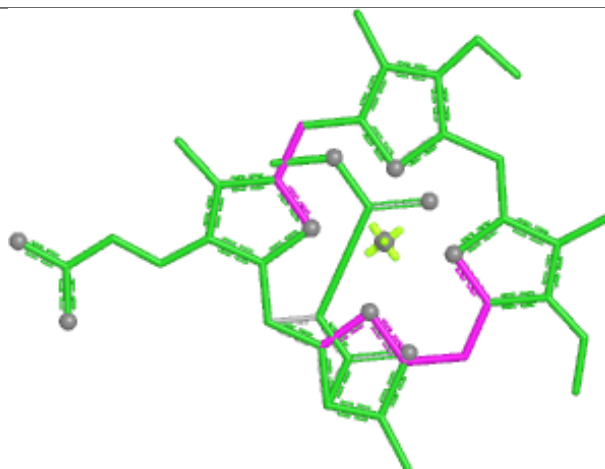
Ligand KC2 F 609



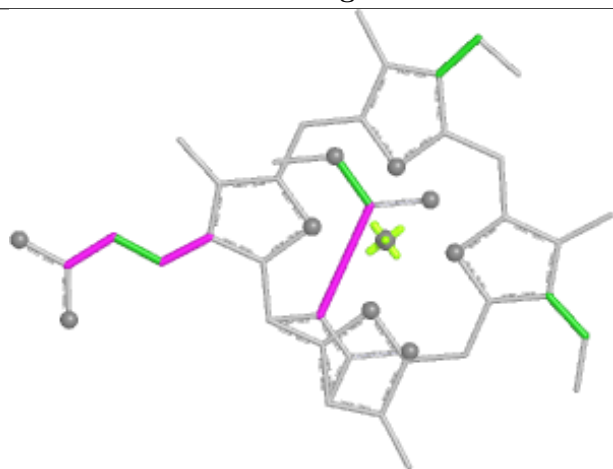
Ligand KC2 J 606



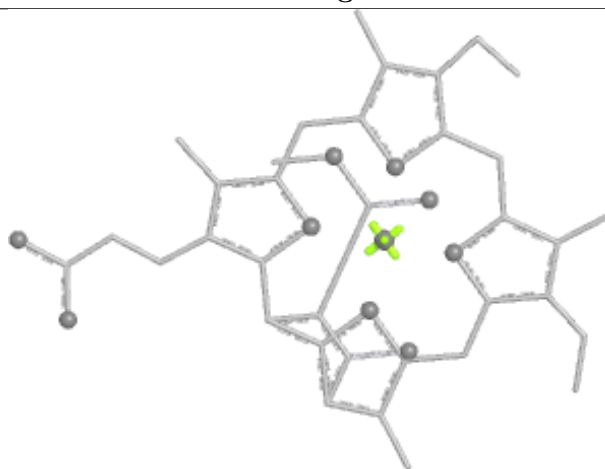
Bond lengths



Bond angles

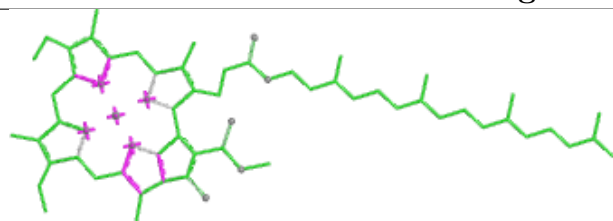


Torsions

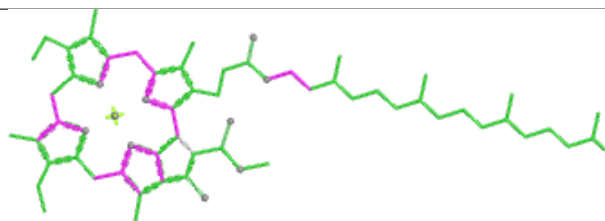


Rings

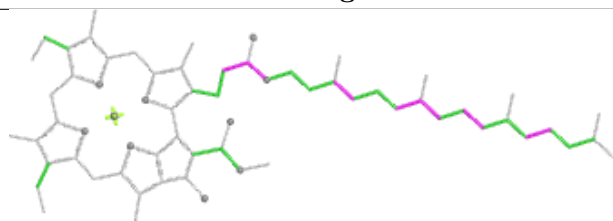
Ligand CLA a 804



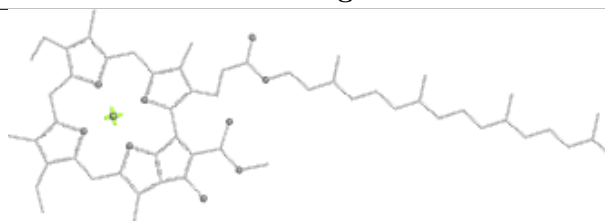
Bond lengths



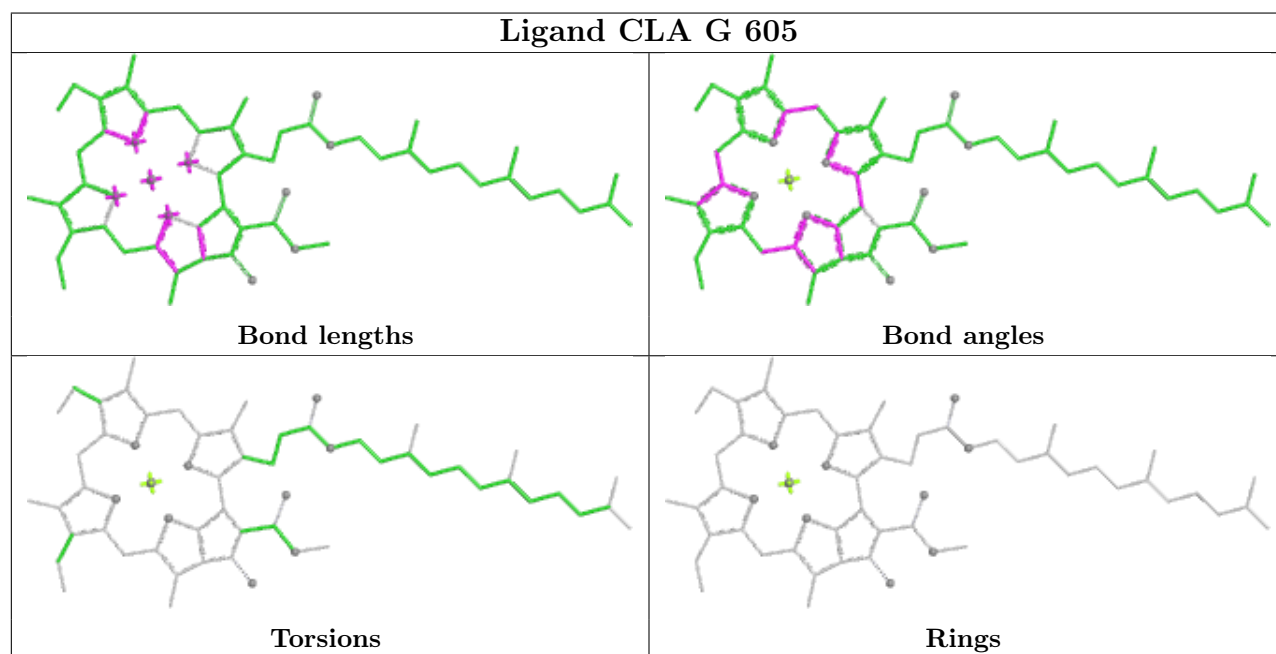
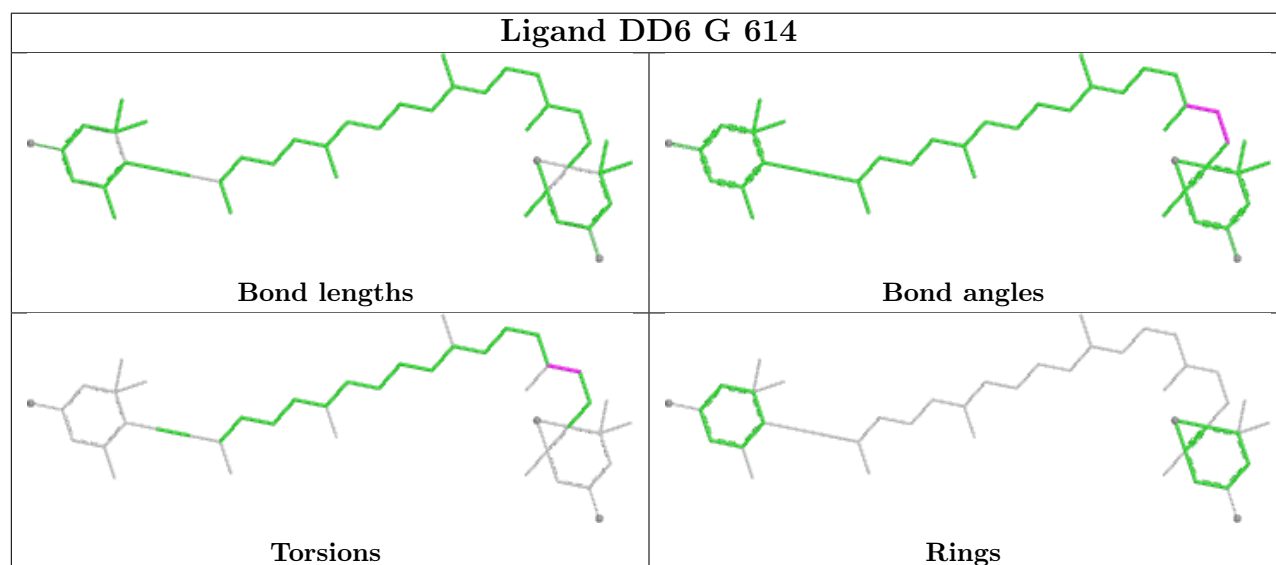
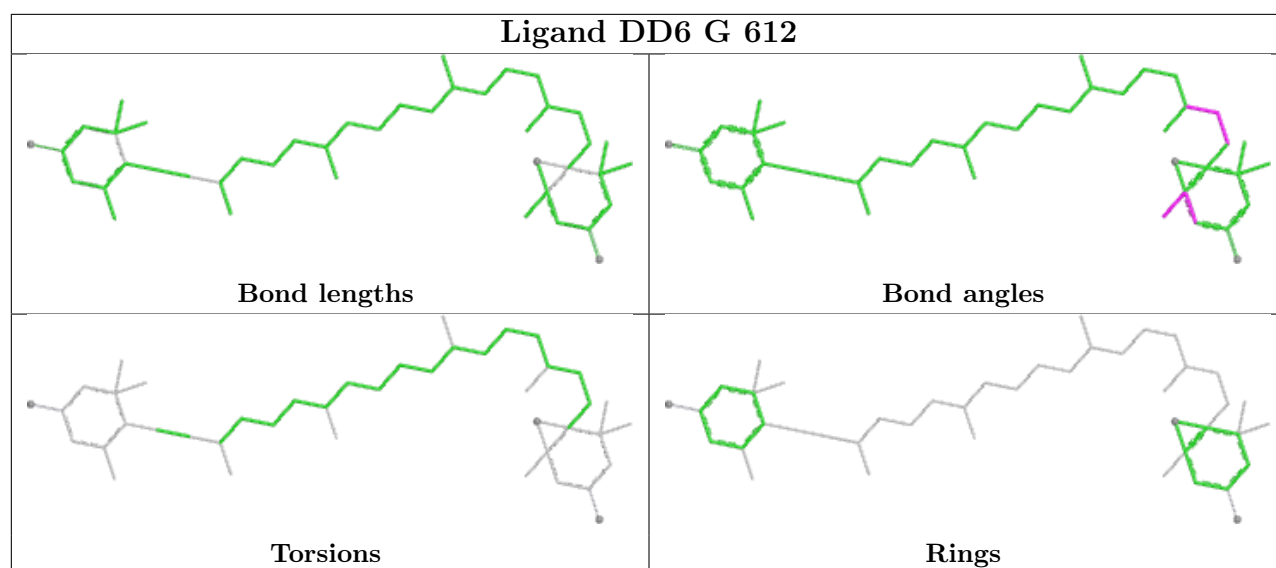
Bond angles



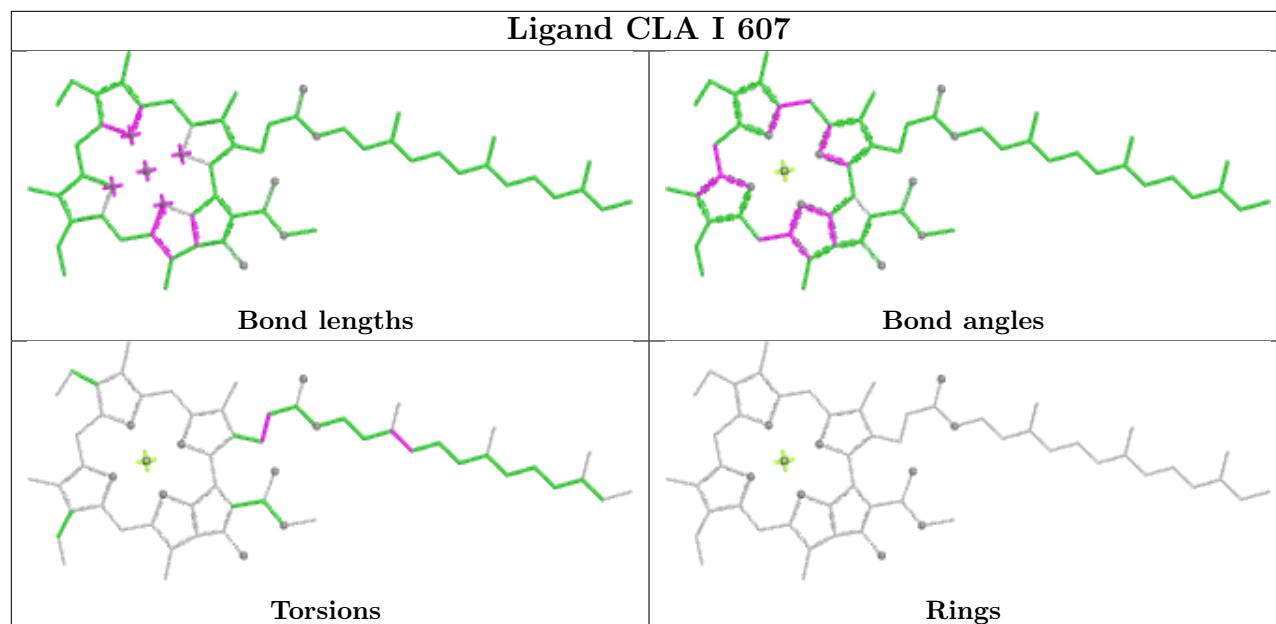
Torsions



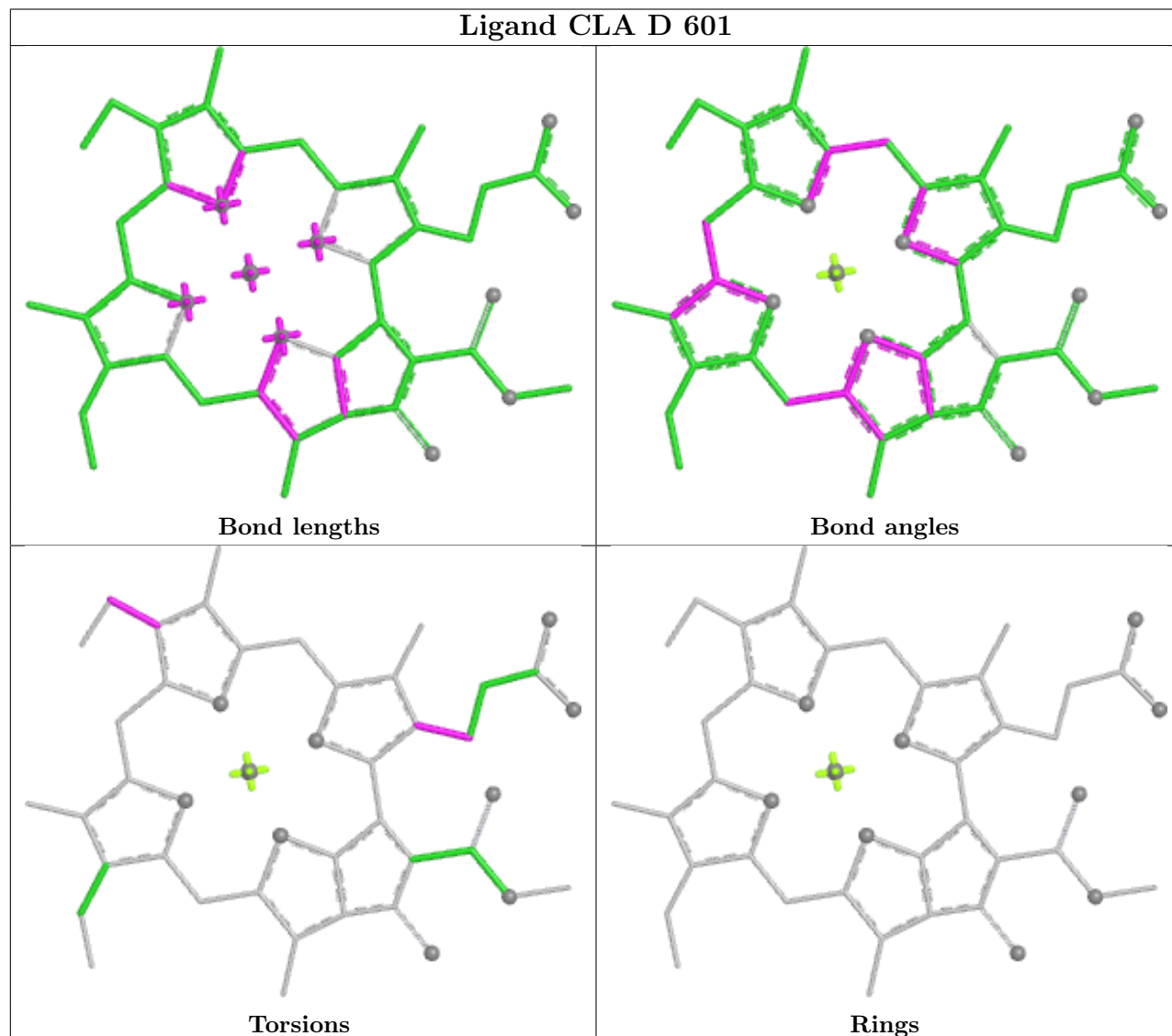
Rings

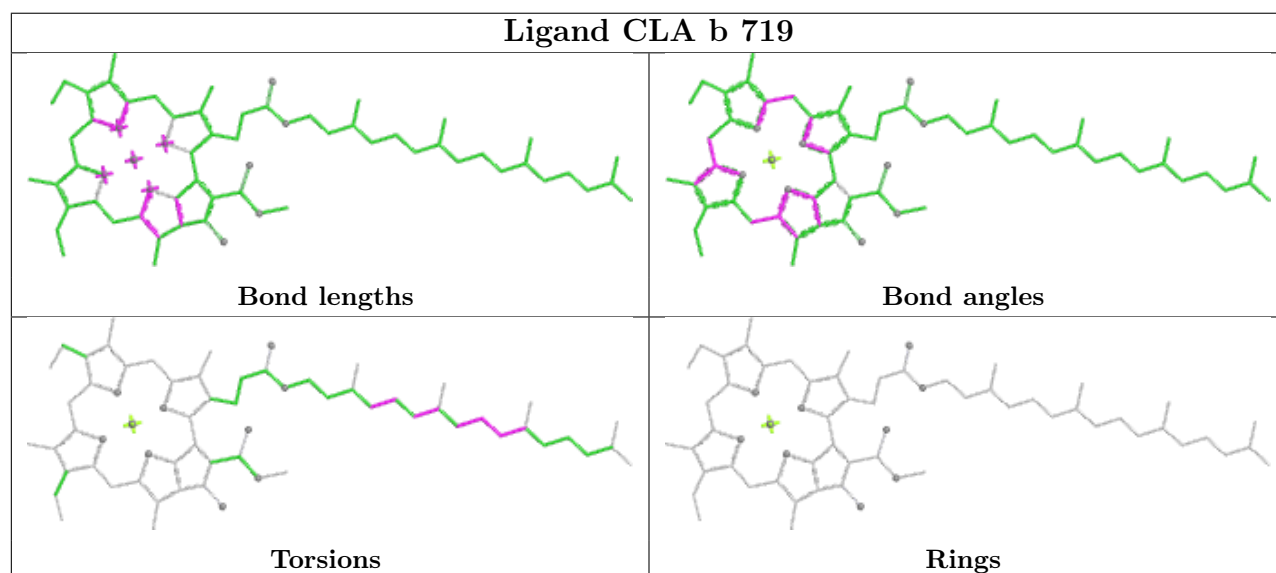
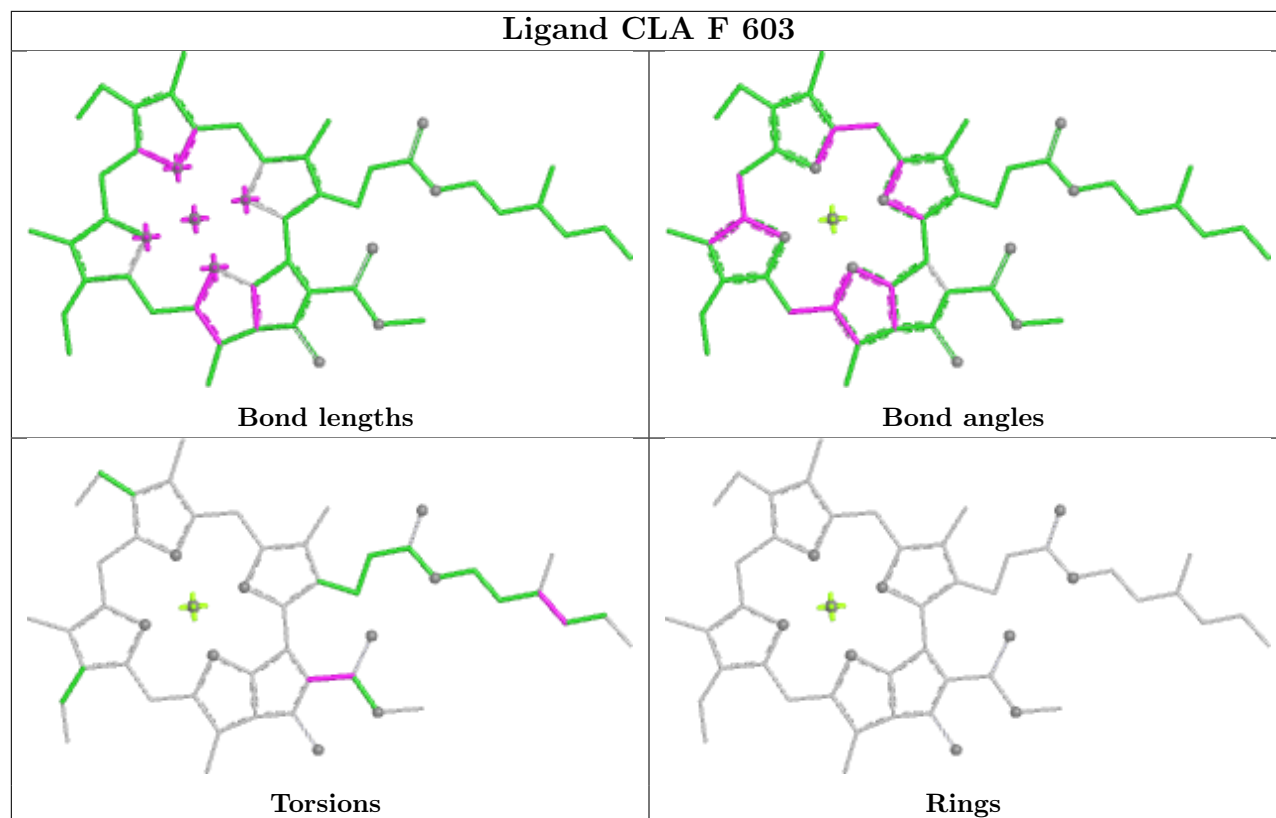


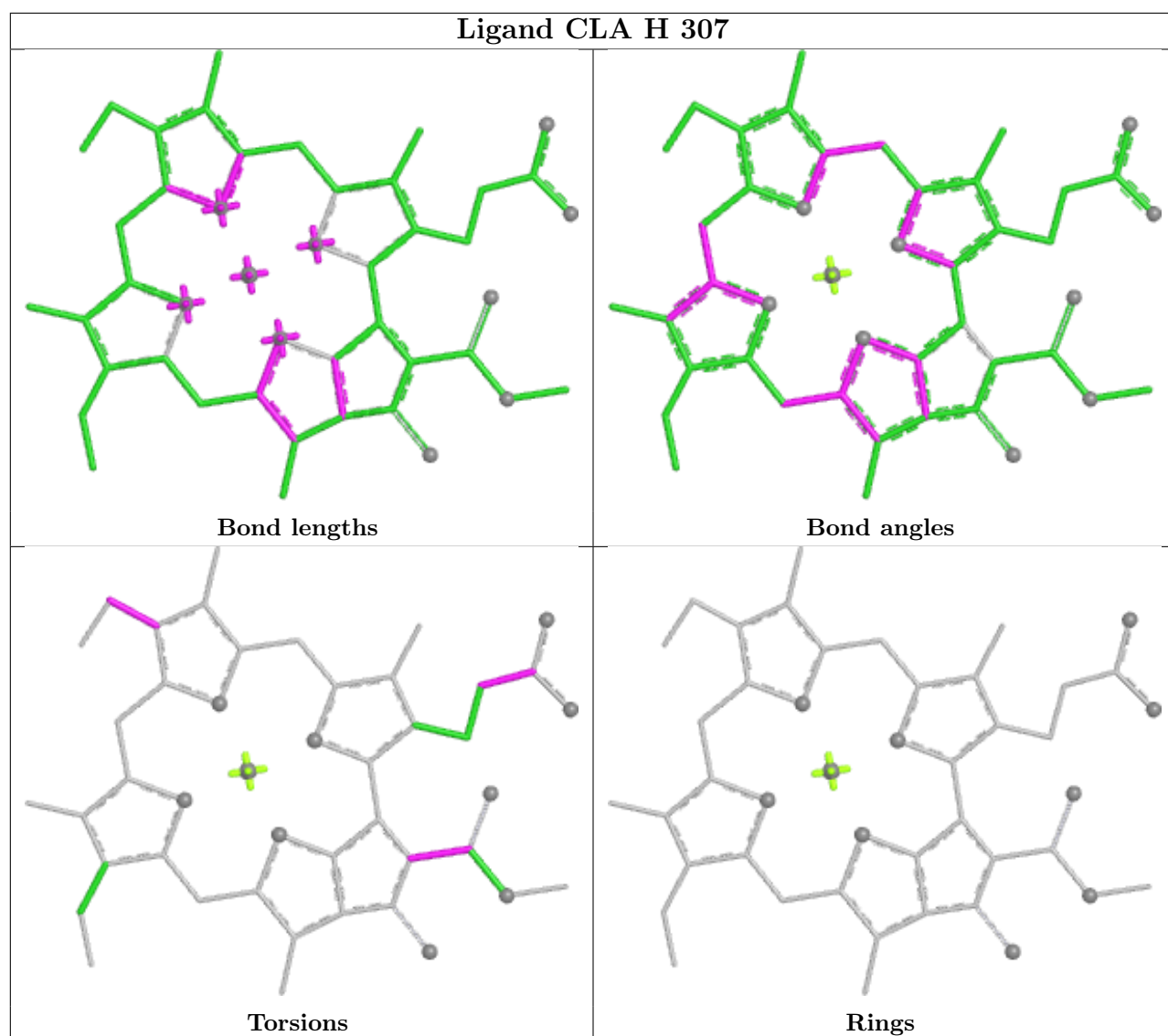
Ligand CLA I 607



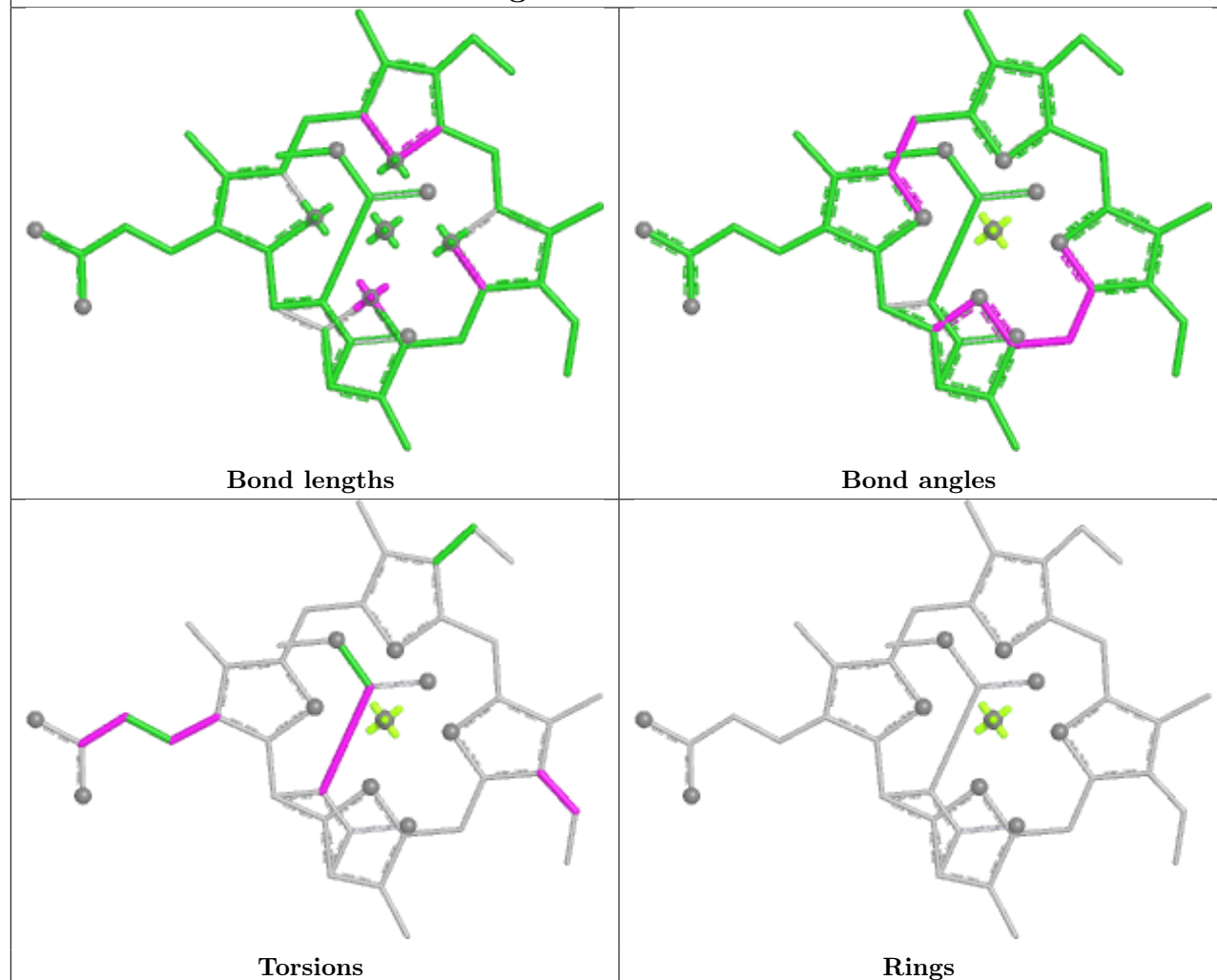
Ligand CLA D 601



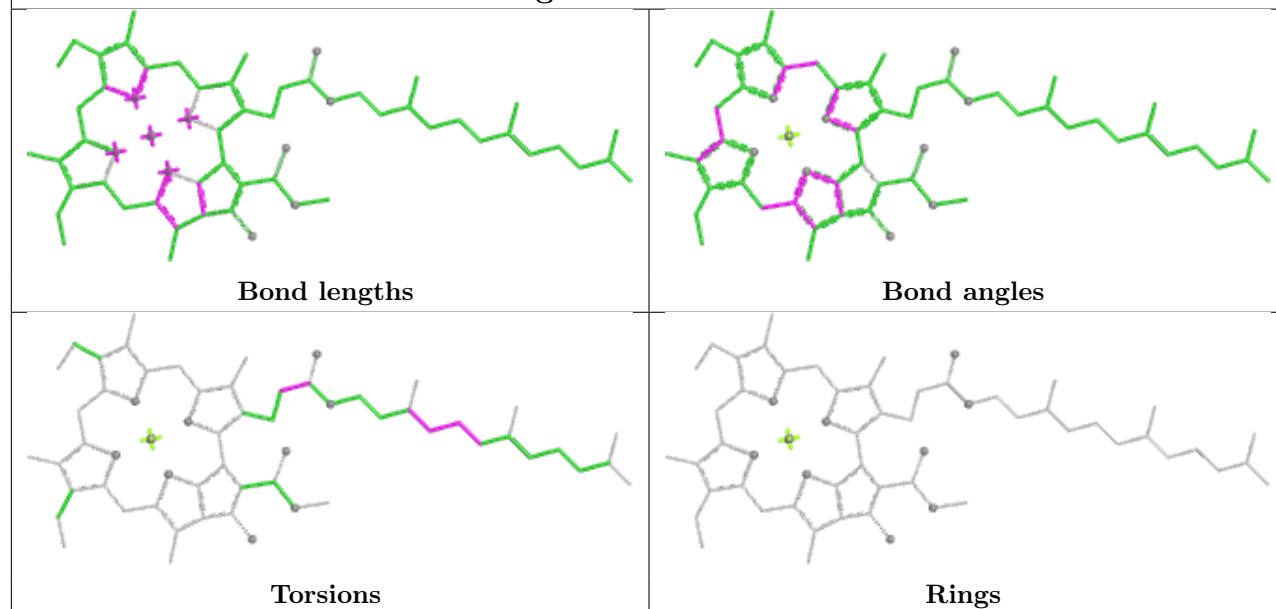


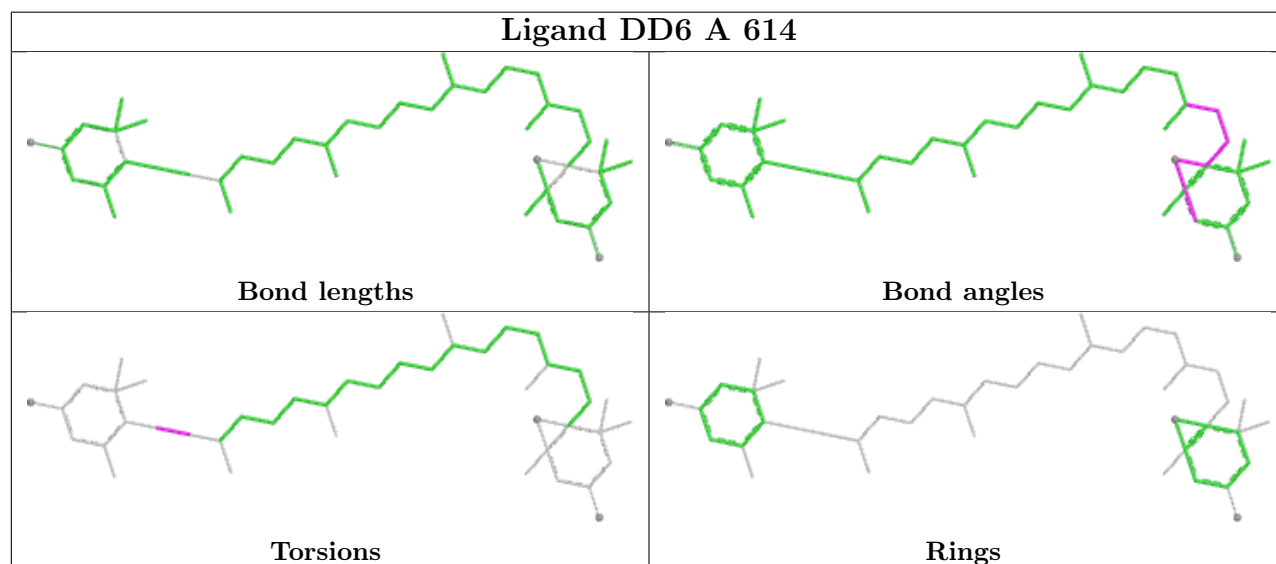
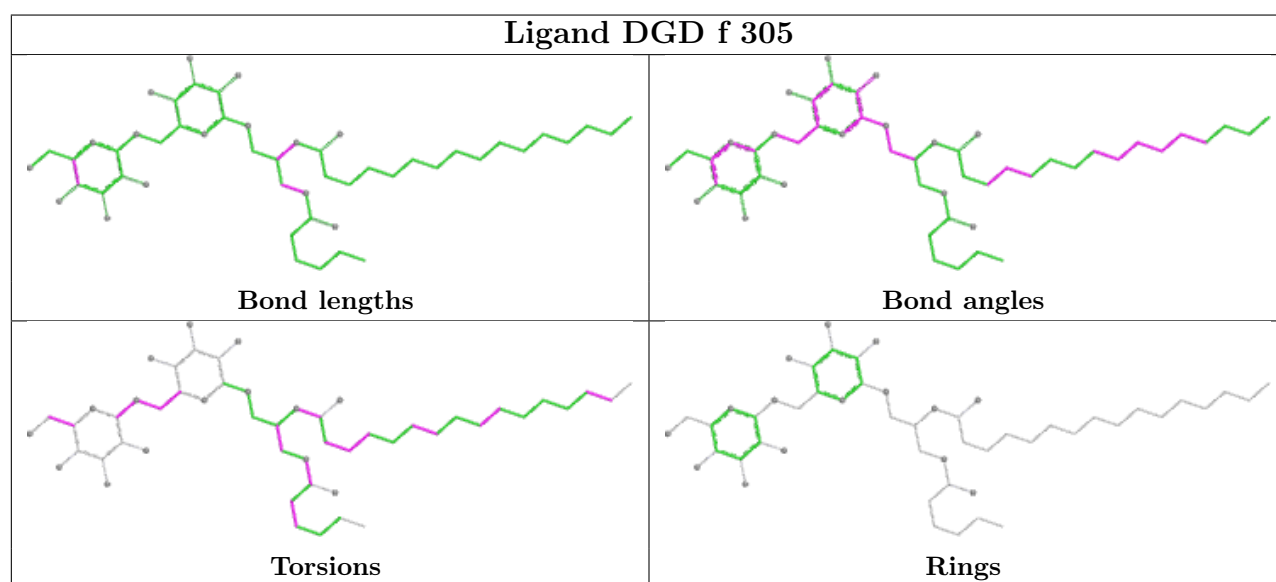
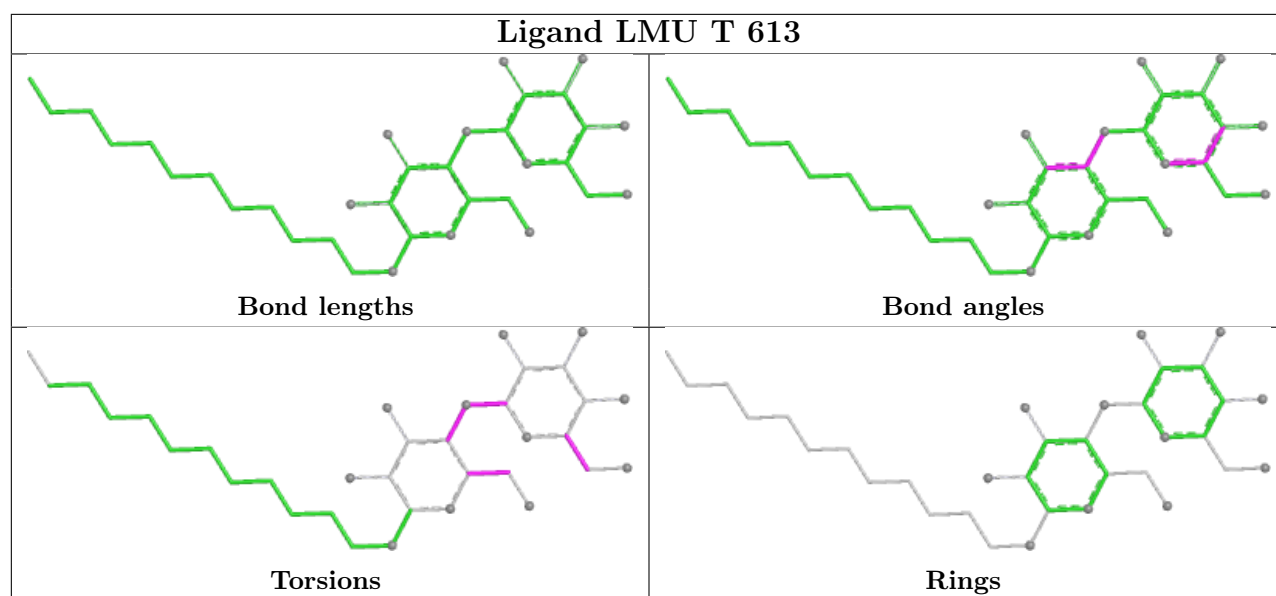


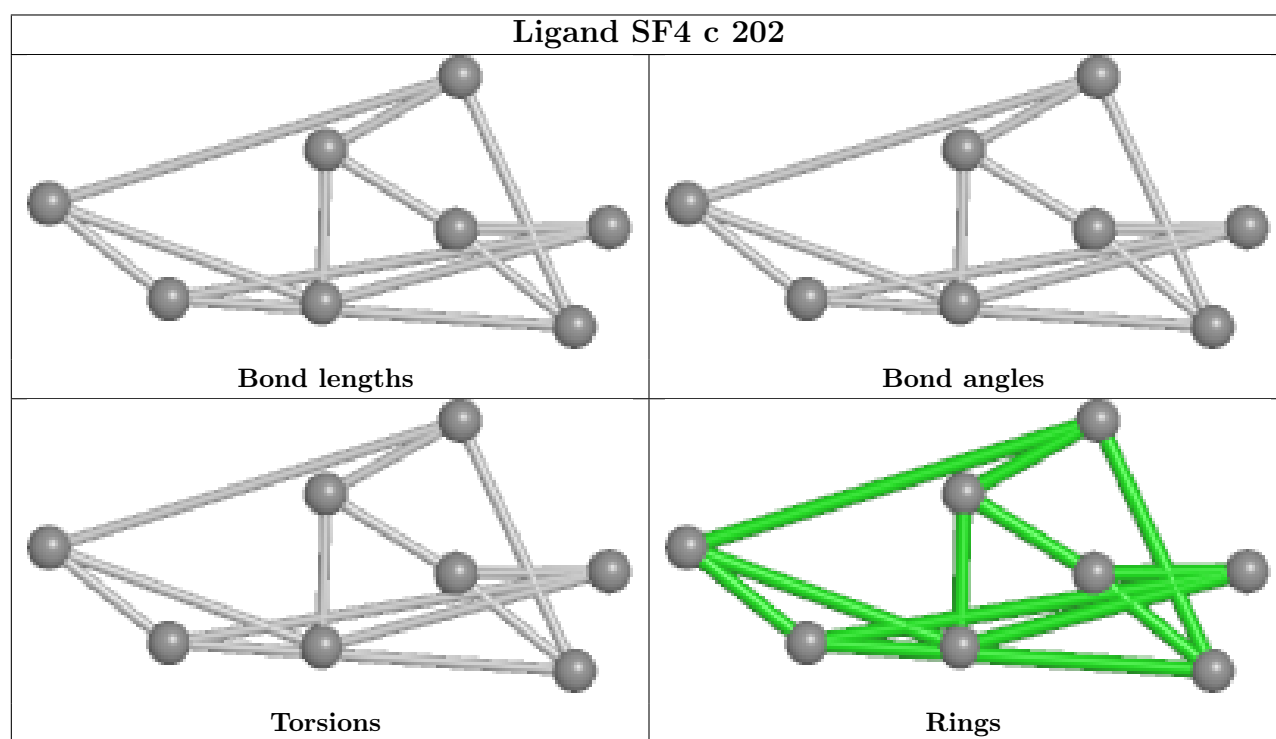
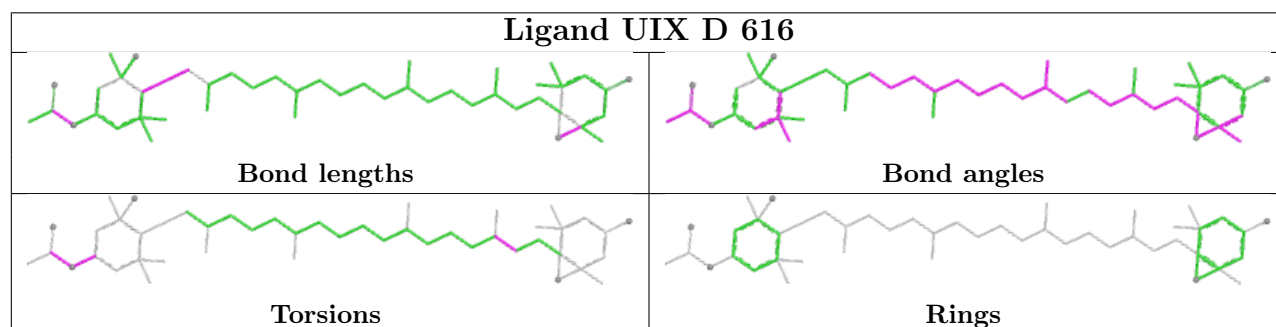
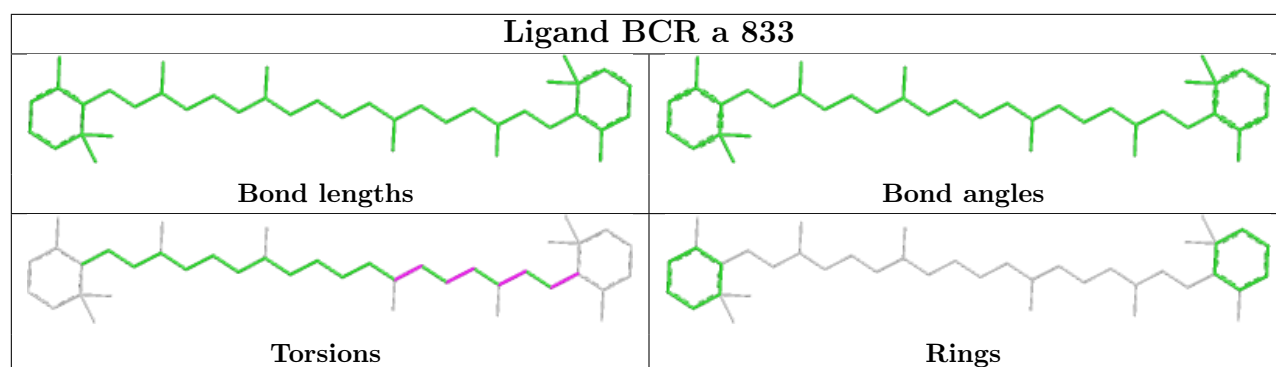
Ligand KC2 C 210

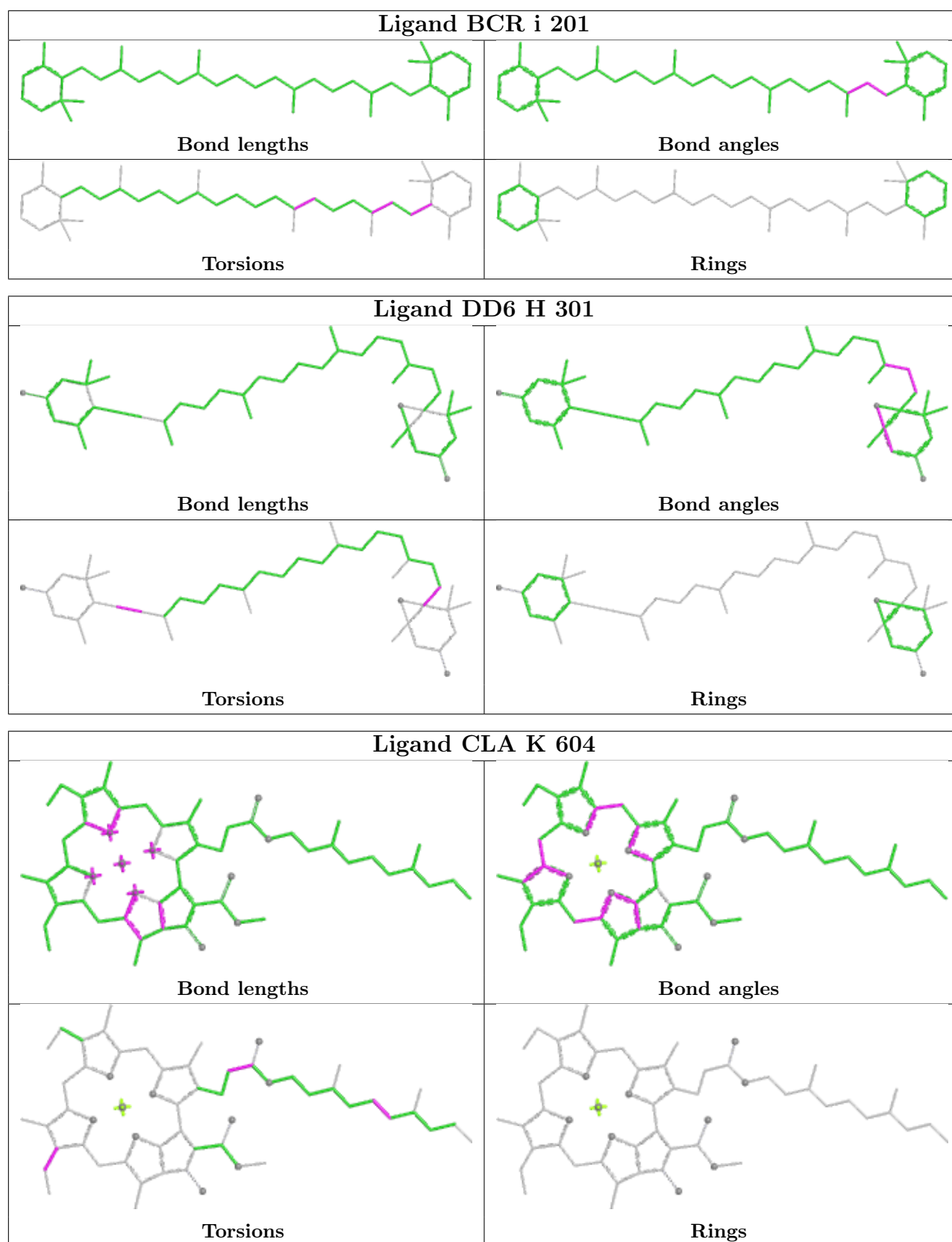


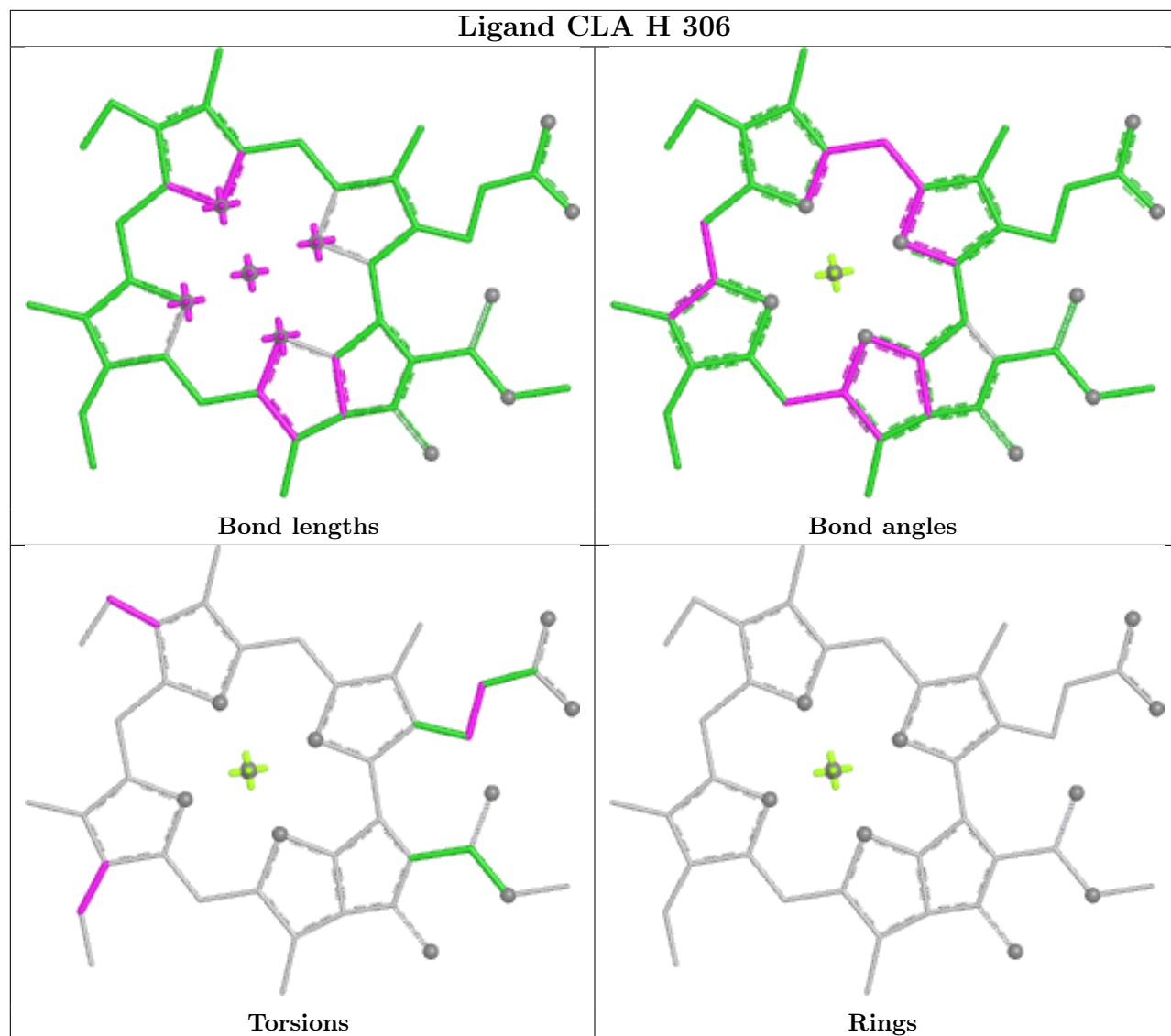
Ligand CLA J 605



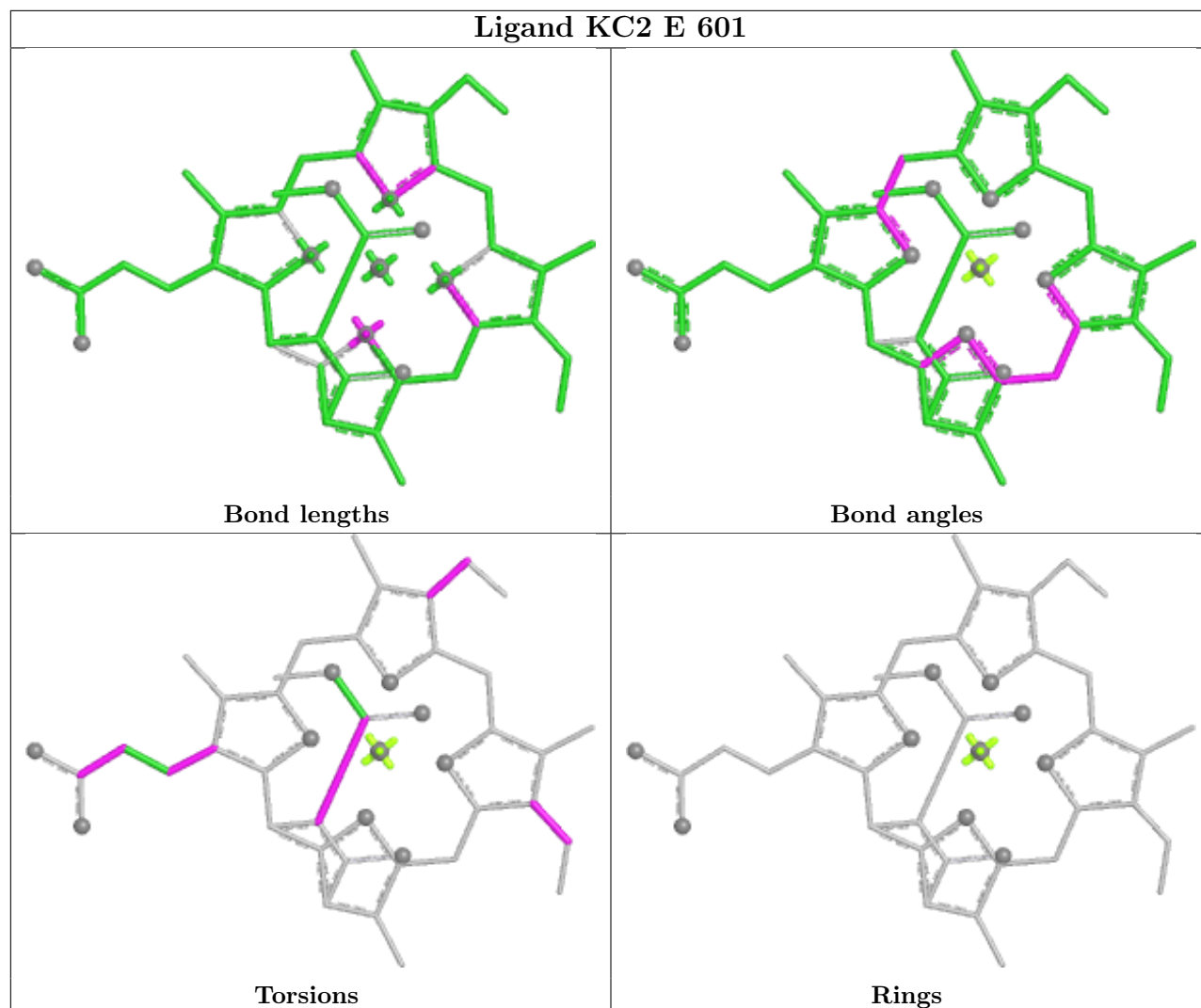




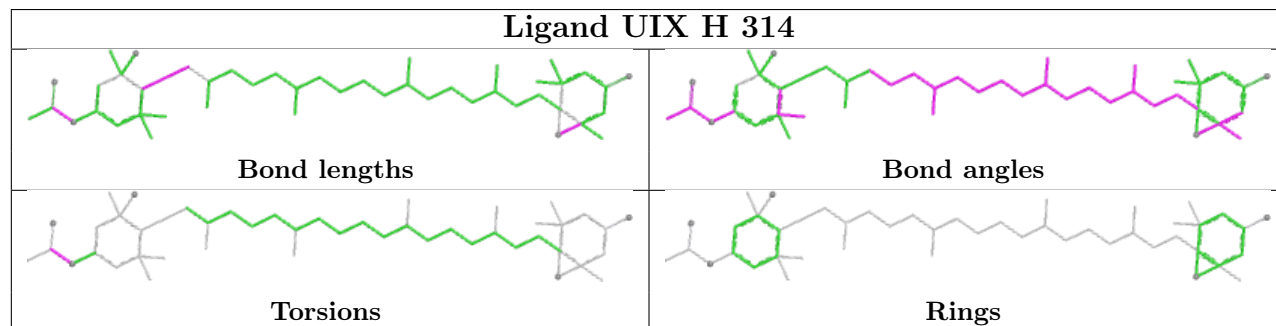


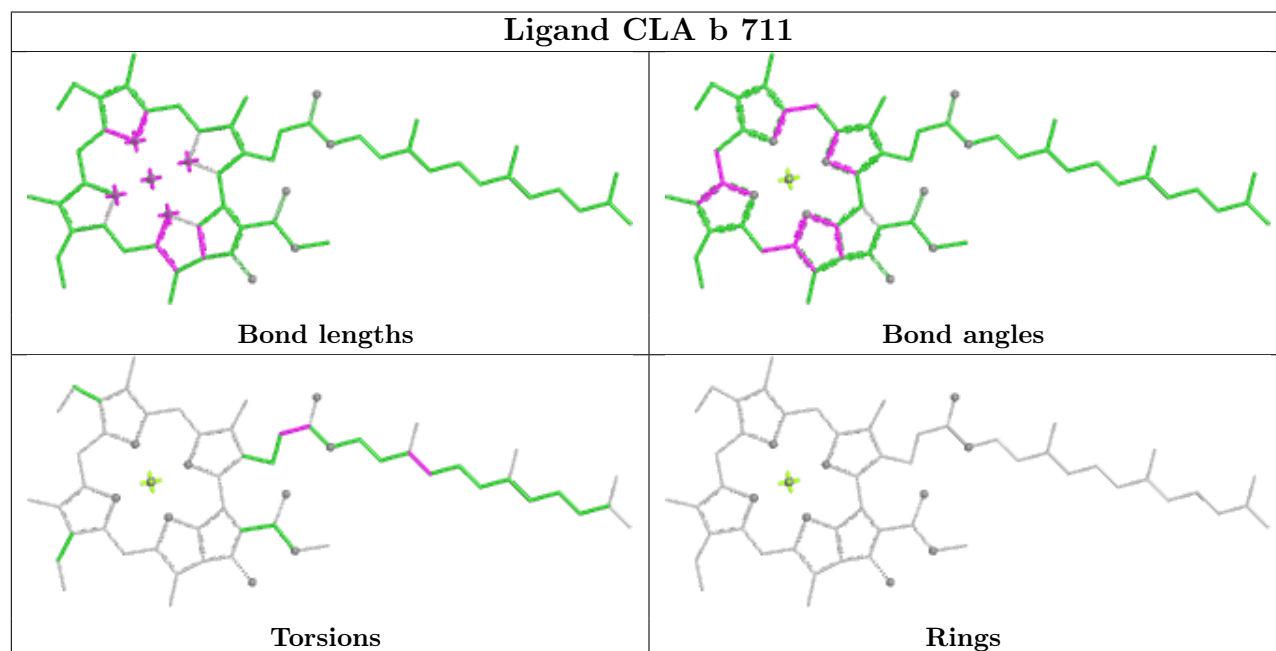
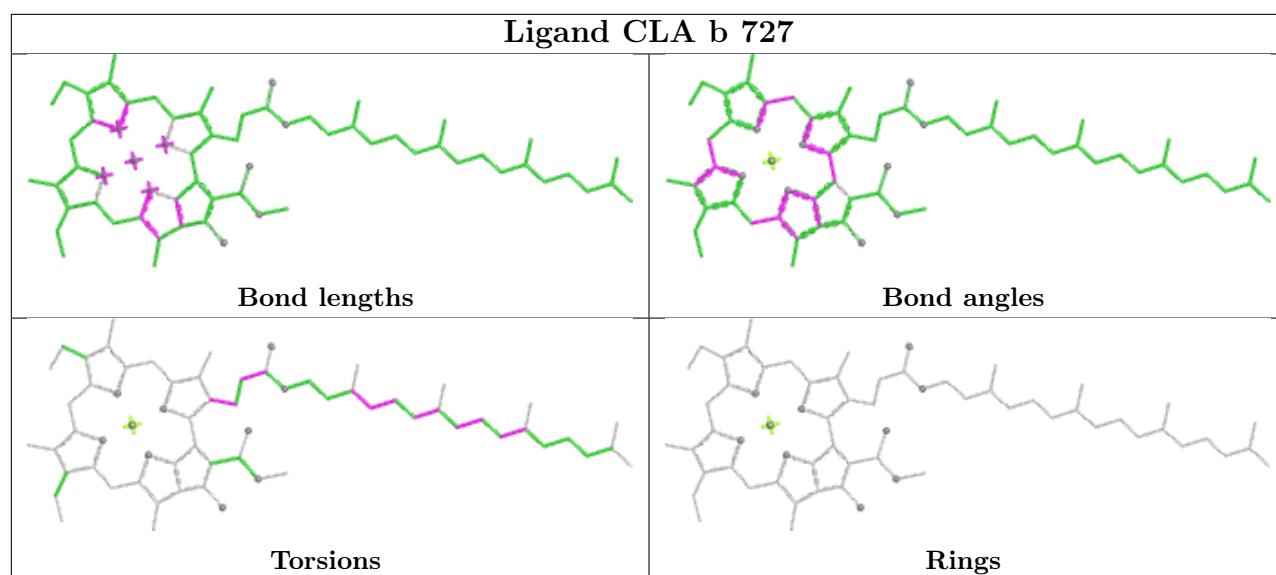


Ligand KC2 E 601

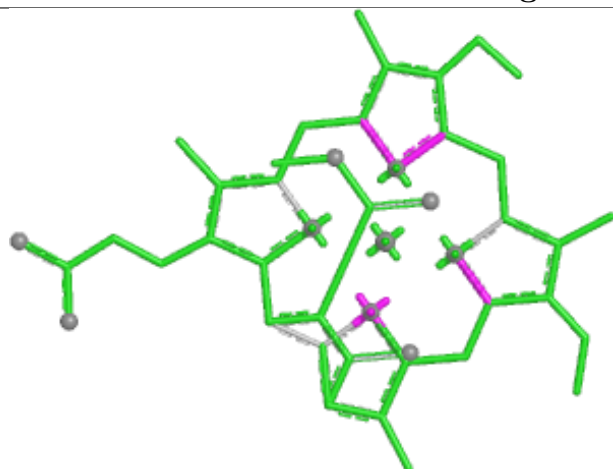


Ligand UIX H 314

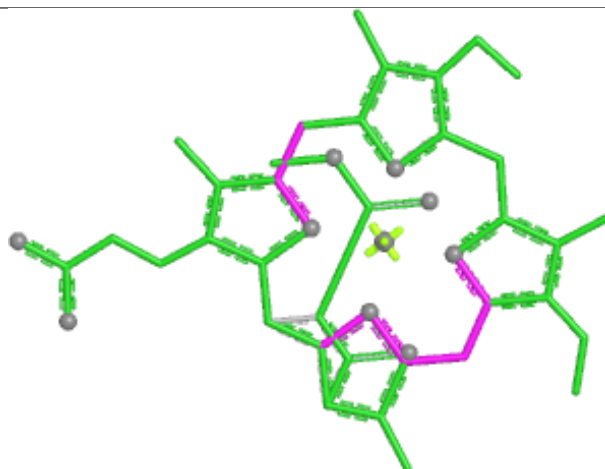




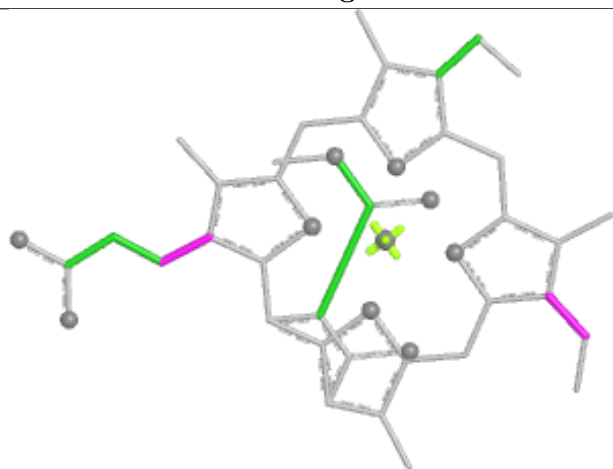
Ligand KC2 J 604



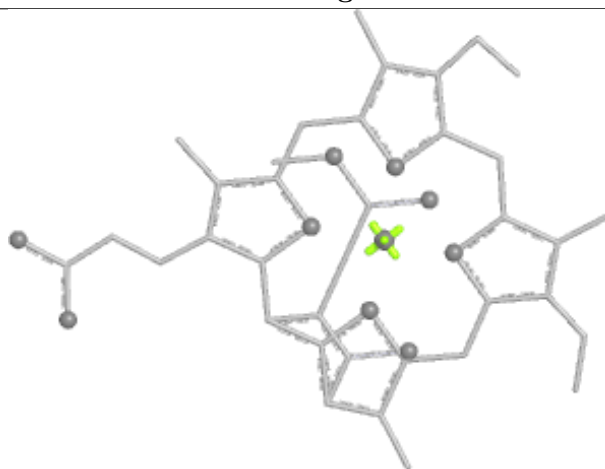
Bond lengths



Bond angles

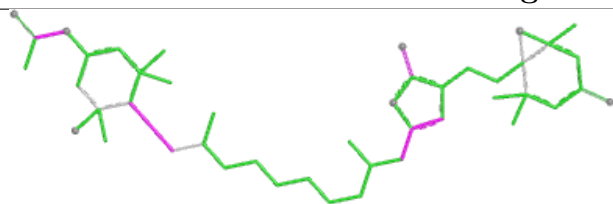


Torsions

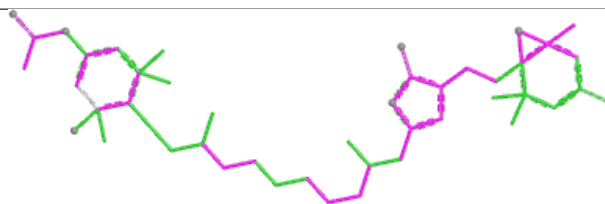


Rings

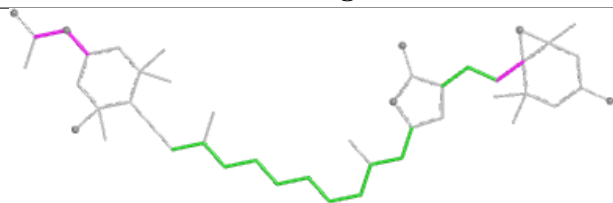
Ligand PID F 614



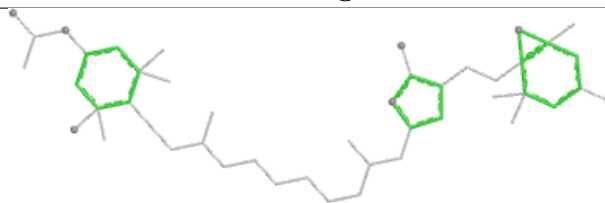
Bond lengths



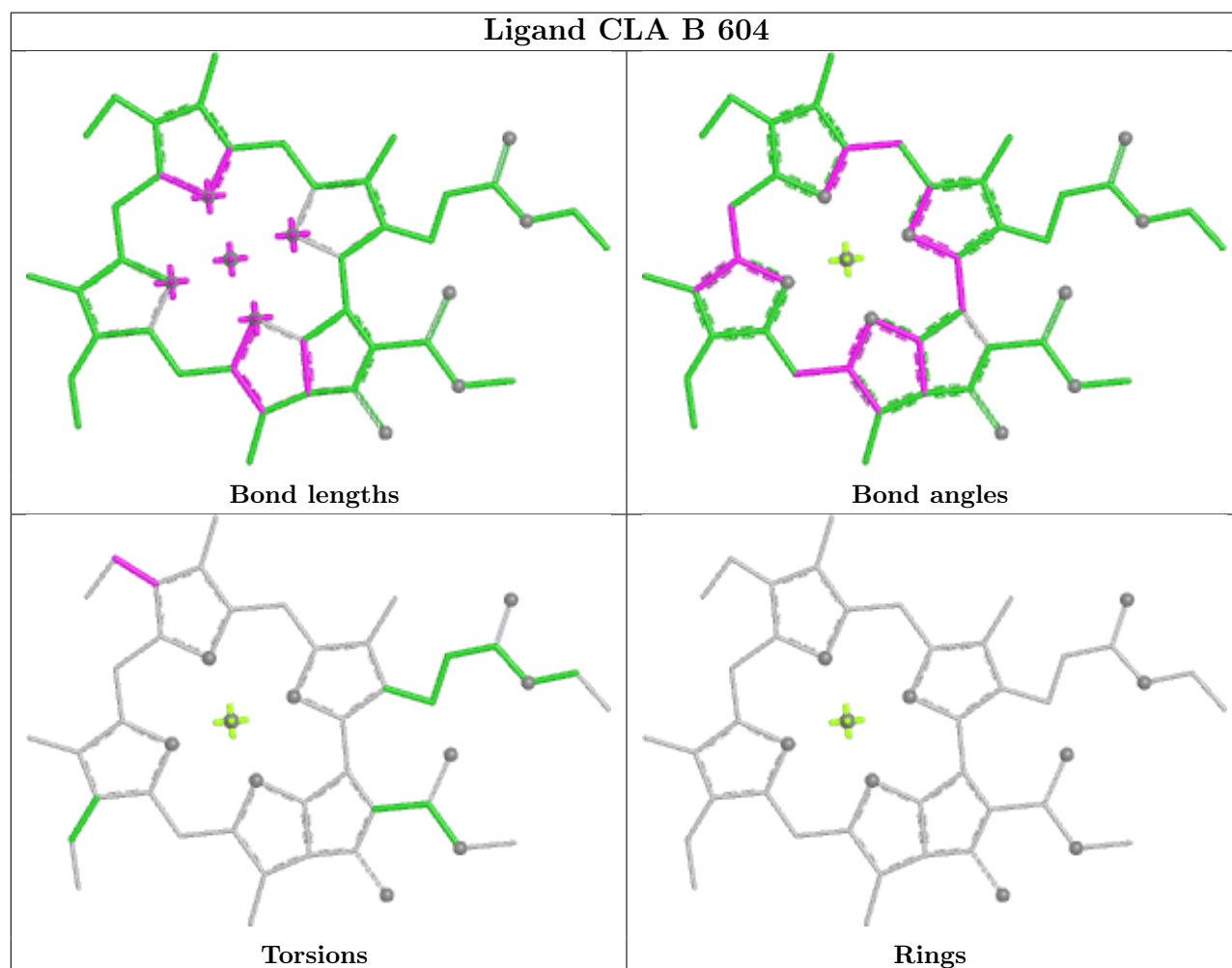
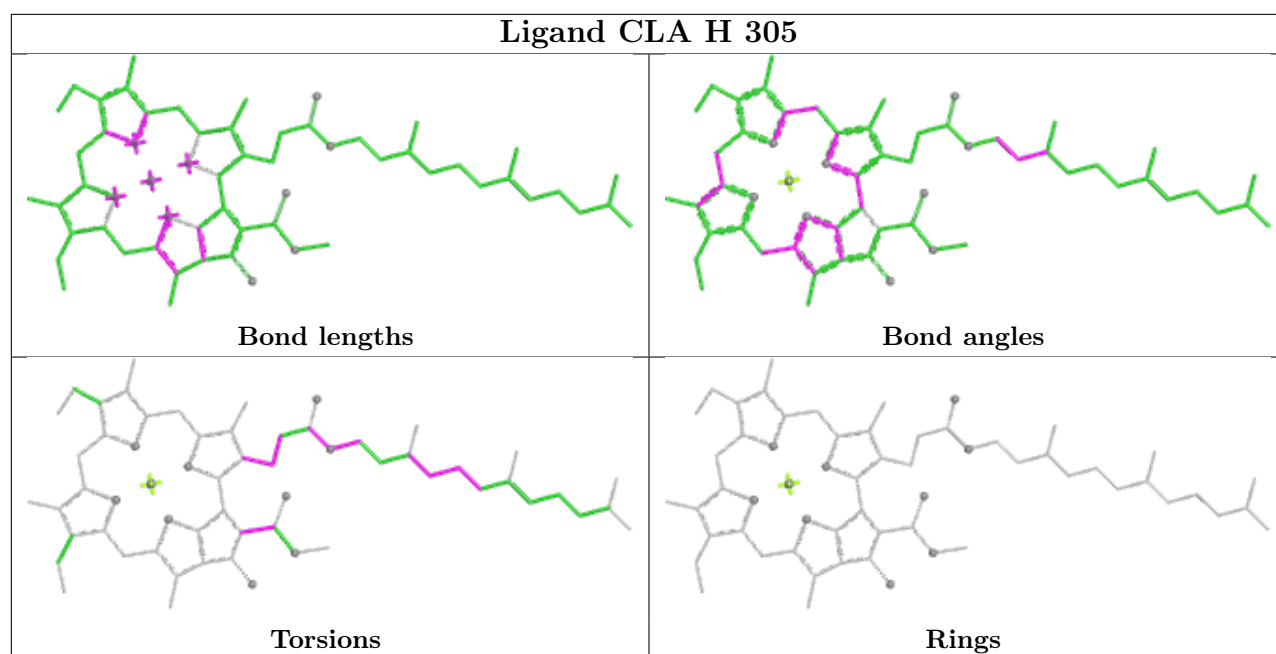
Bond angles



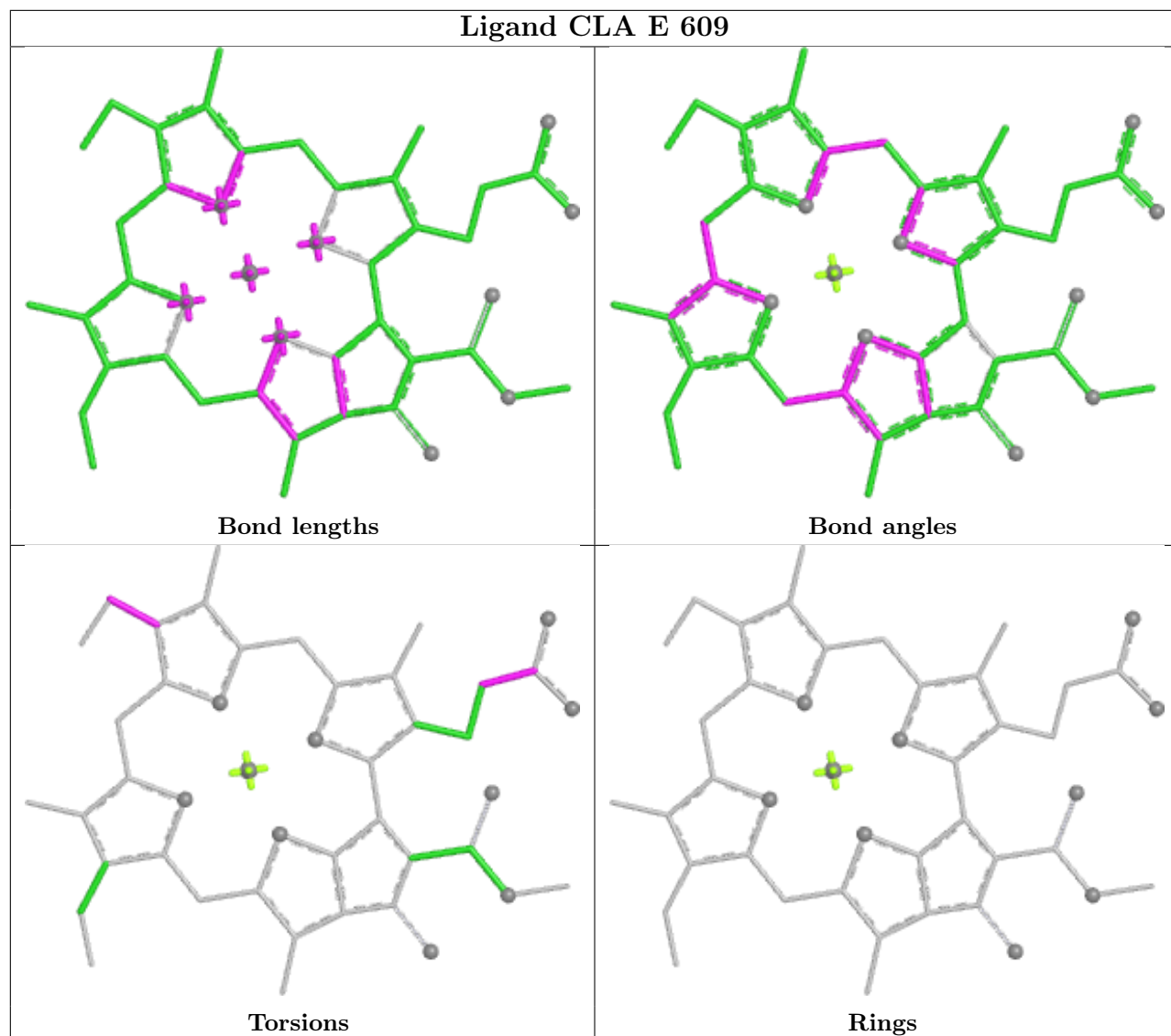
Torsions

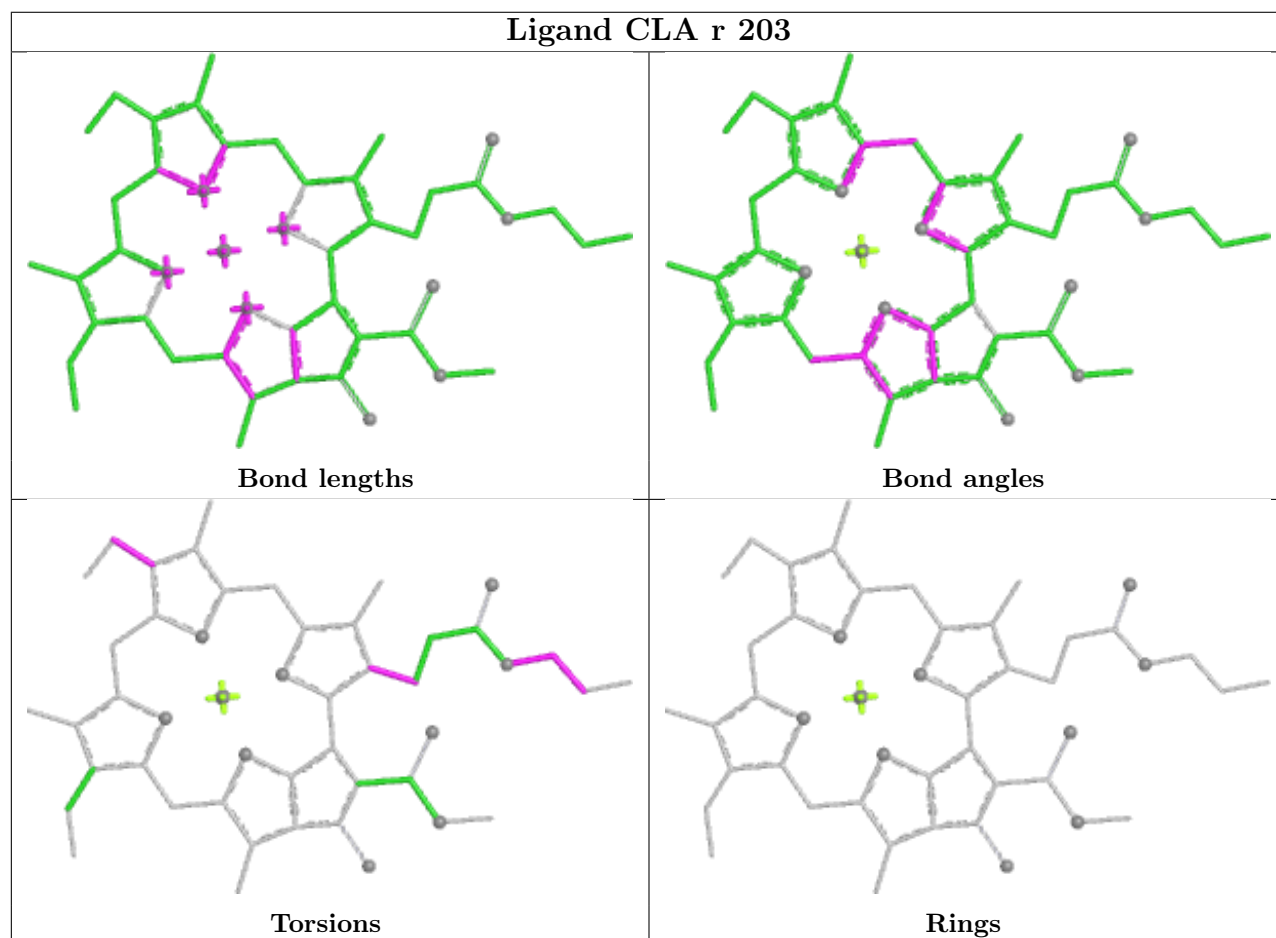
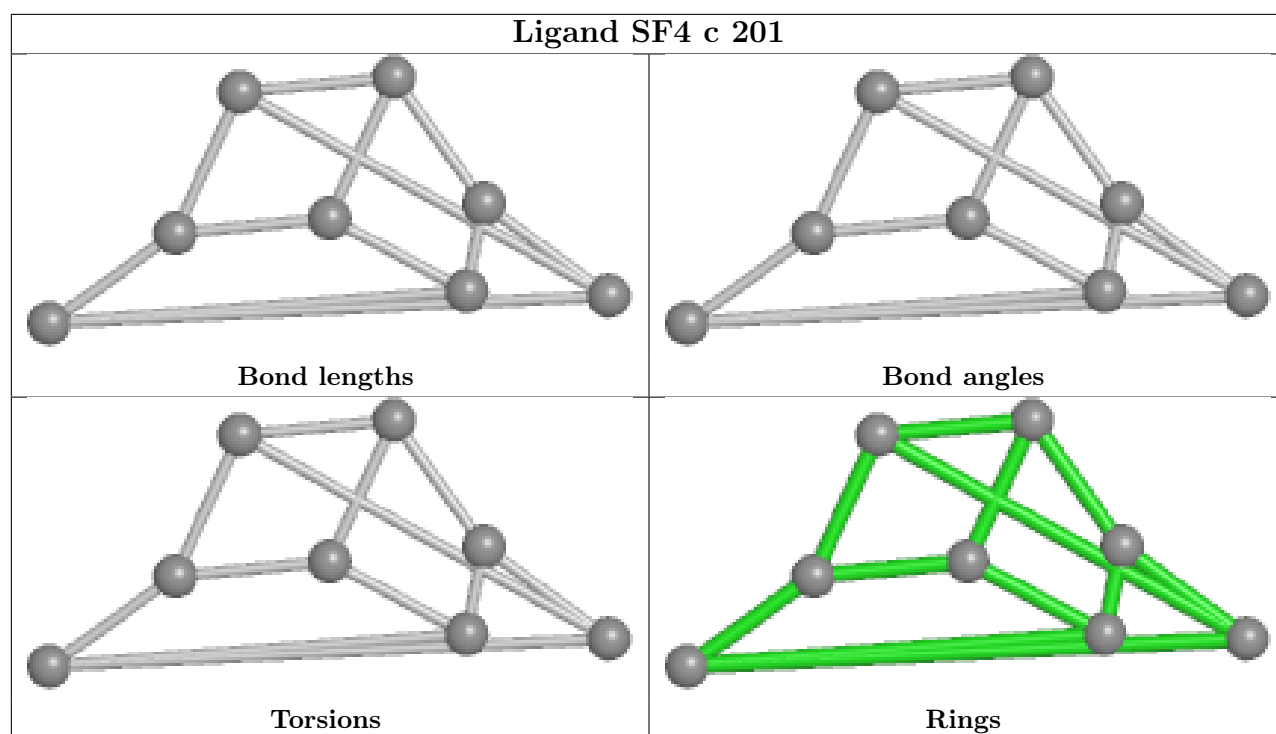


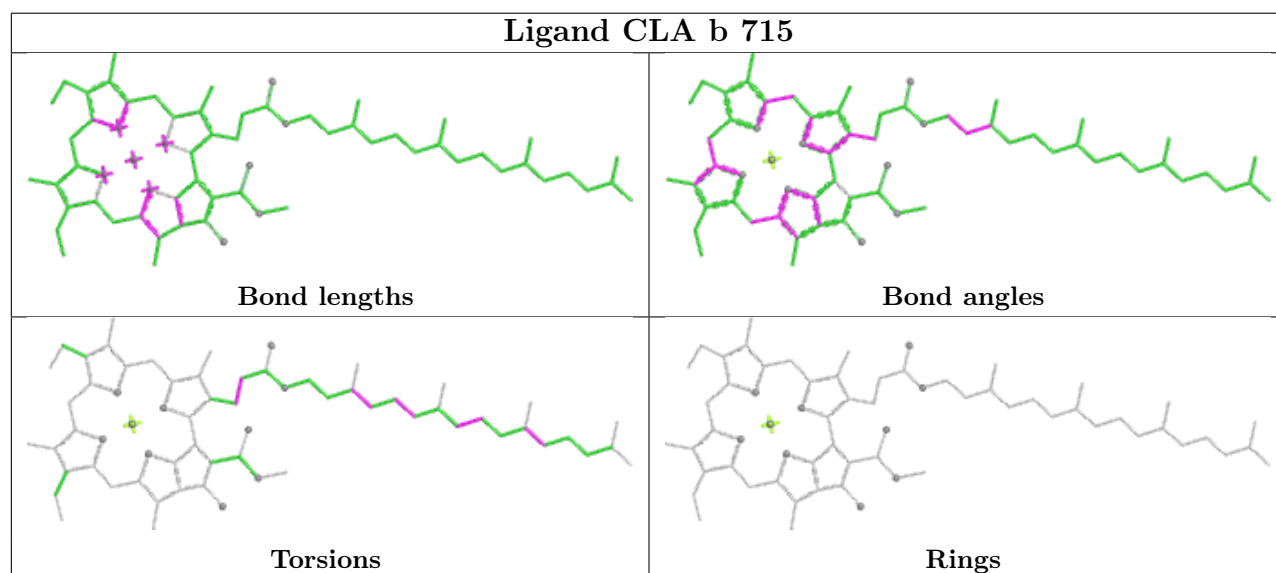
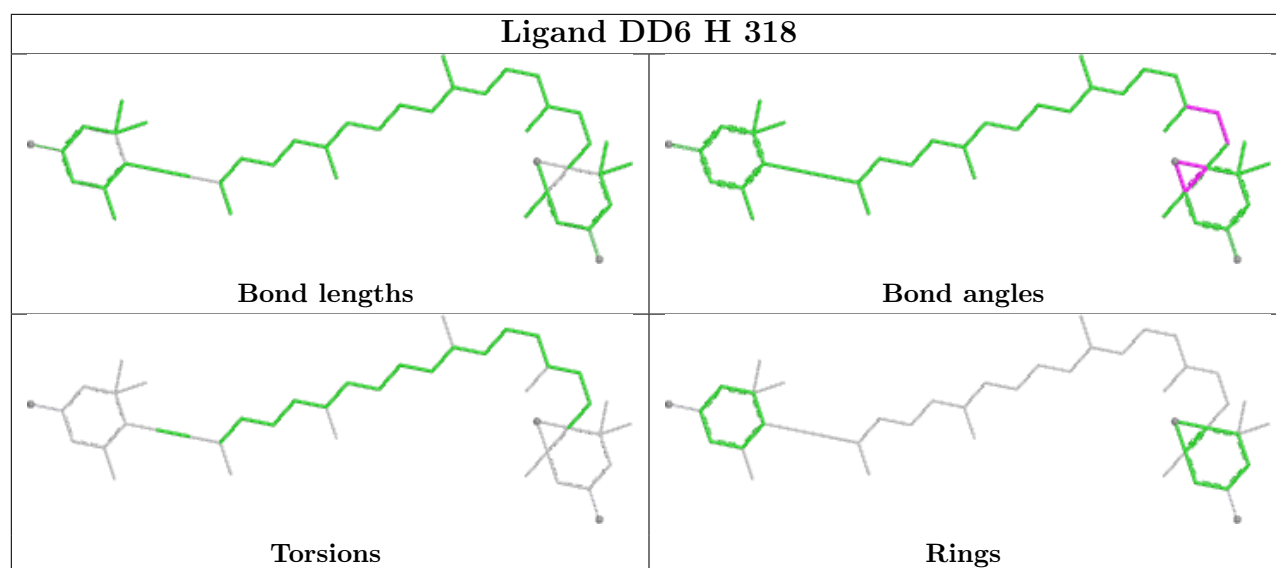
Rings



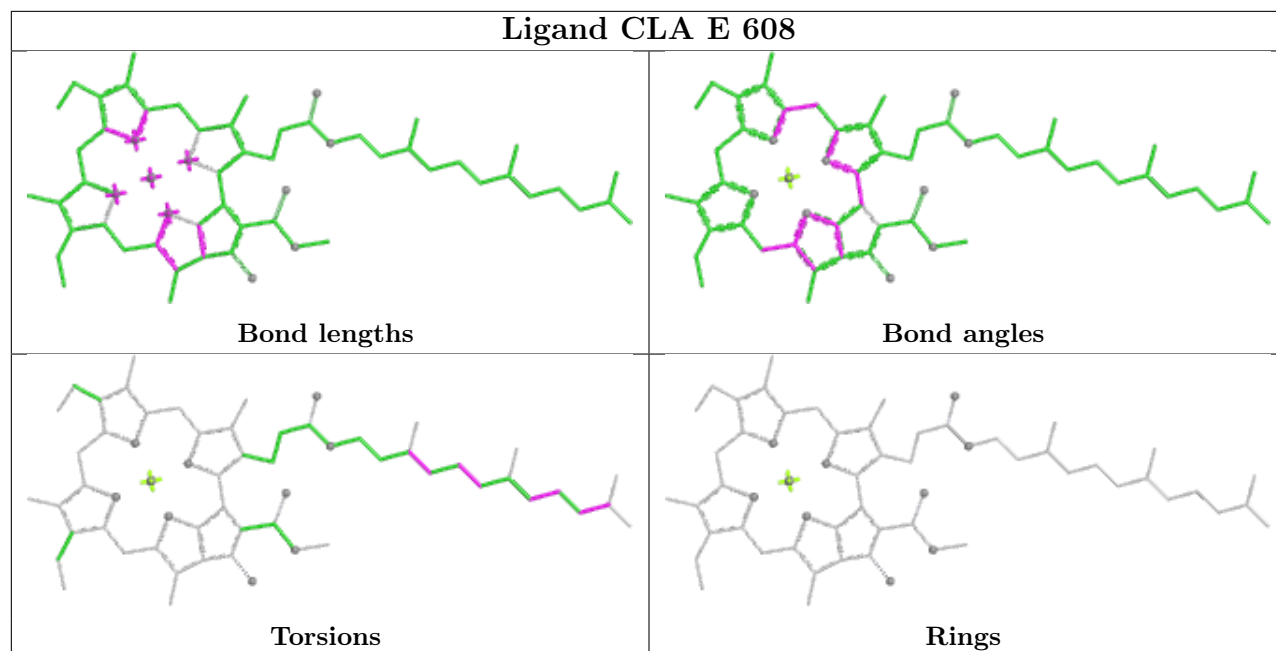
Ligand CLA E 609



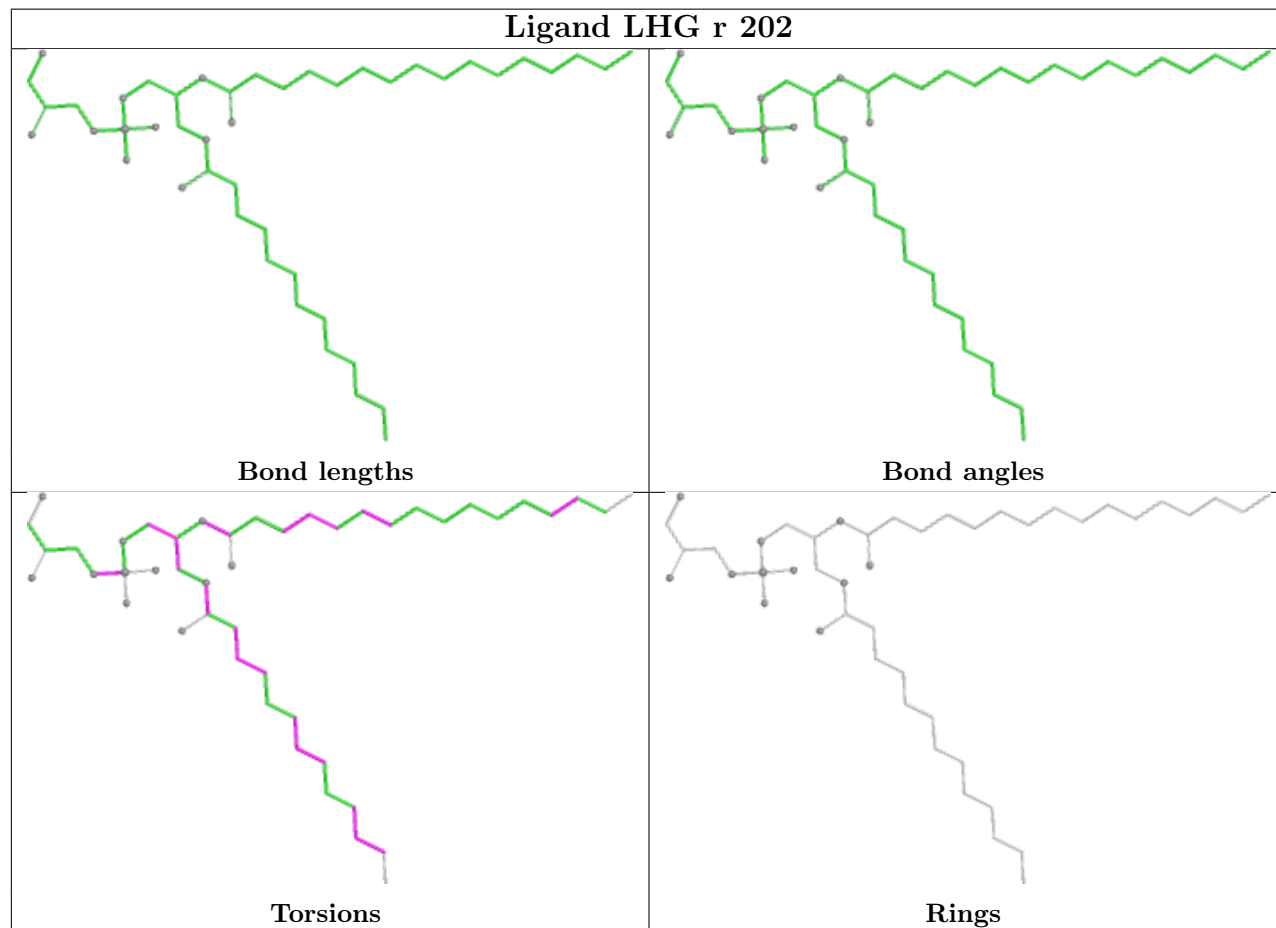


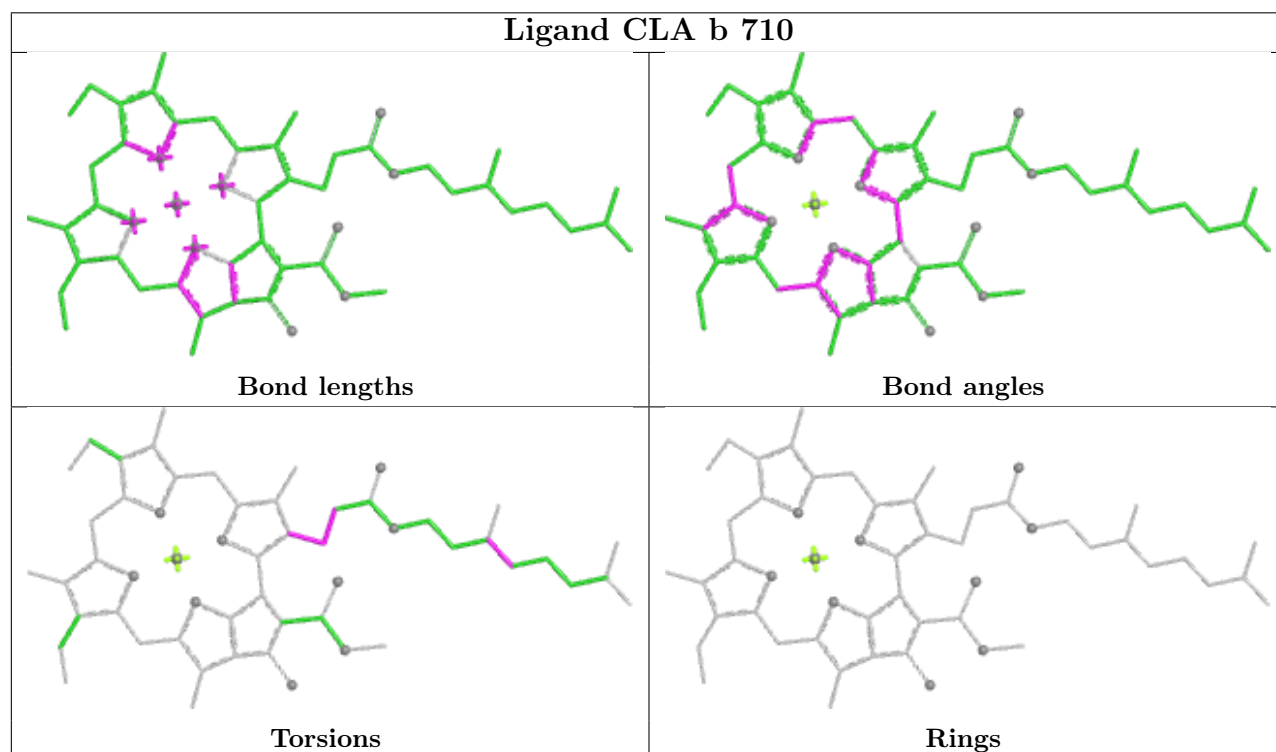
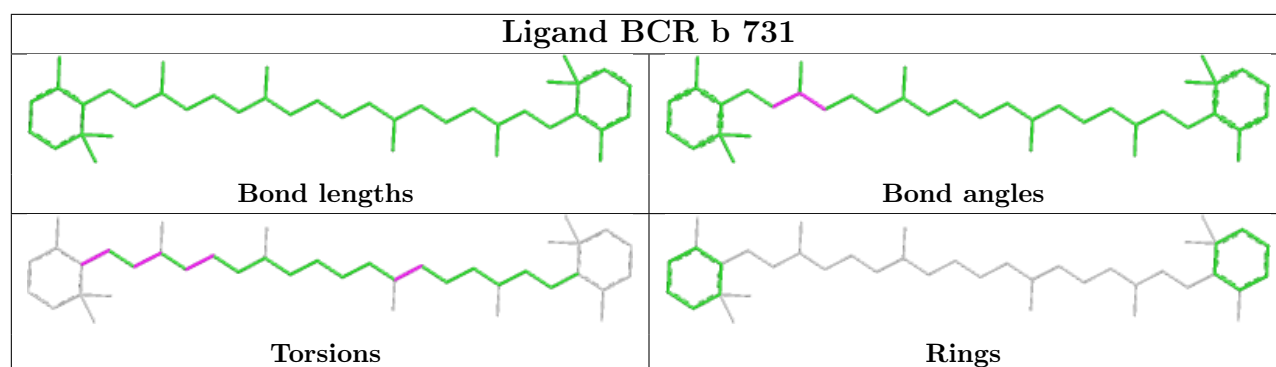


Ligand CLA E 608

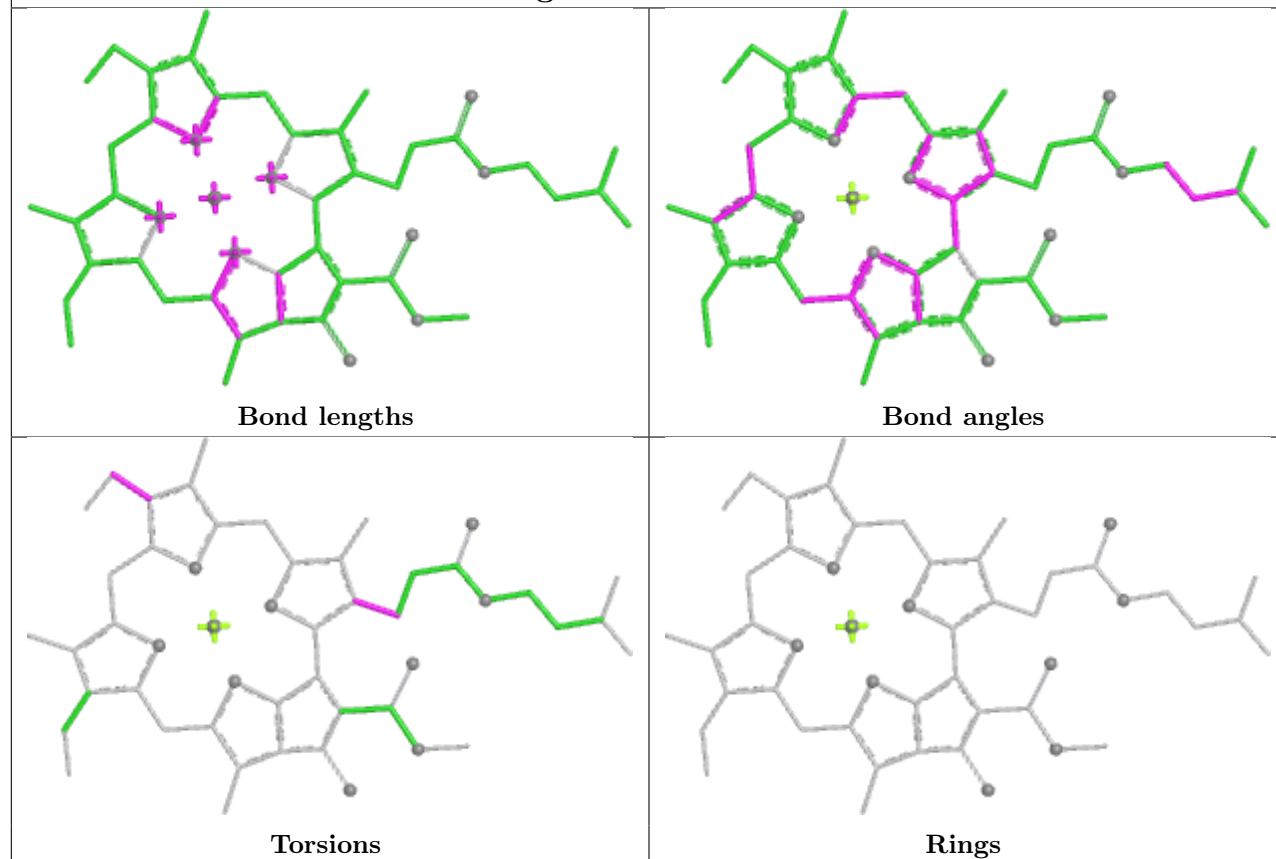


Ligand LHG r 202

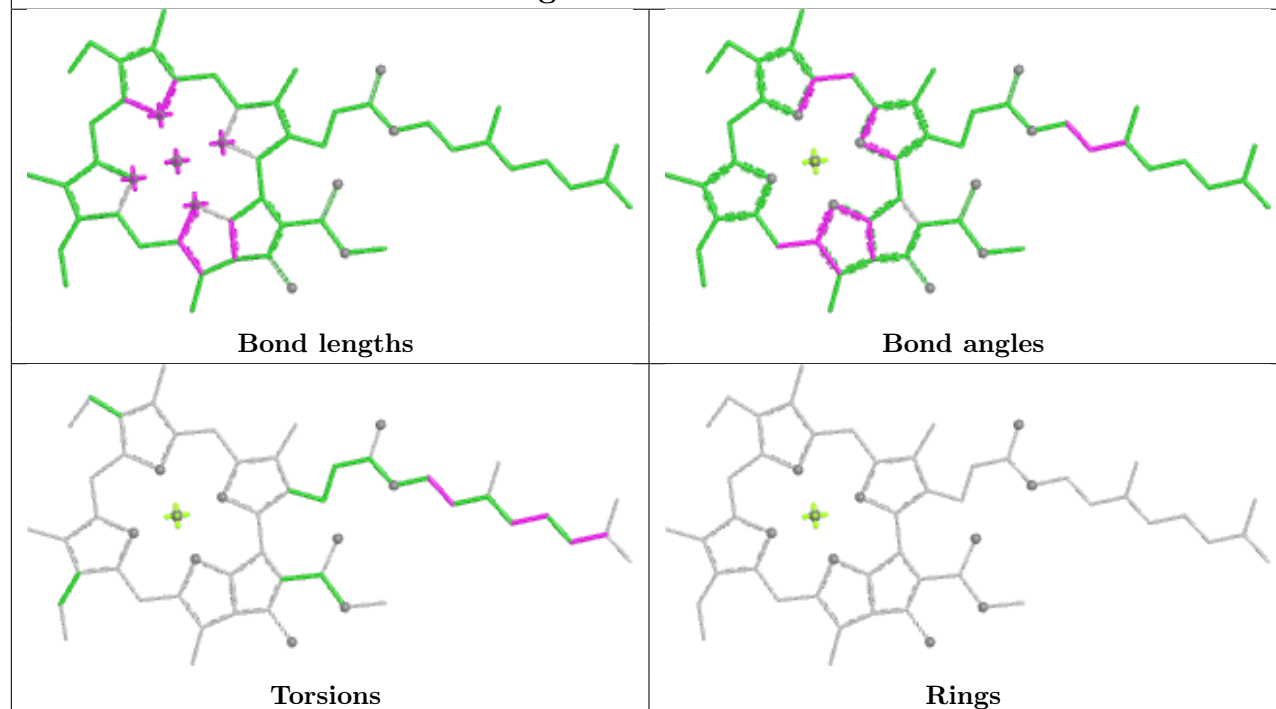




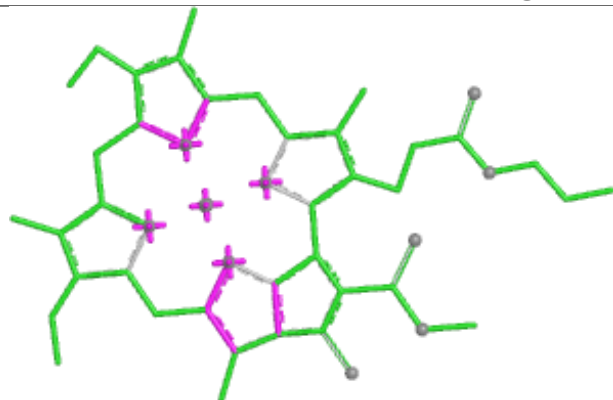
Ligand CLA a 812



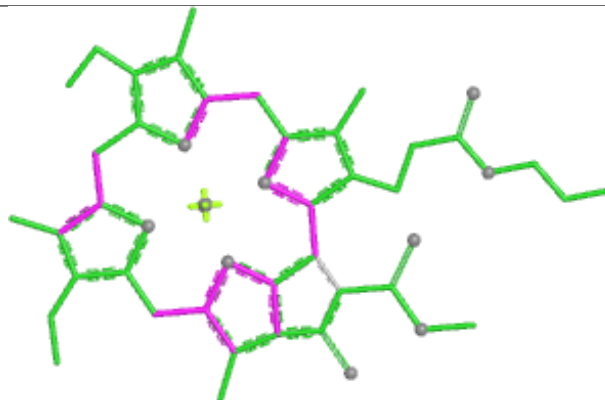
Ligand CLA I 610



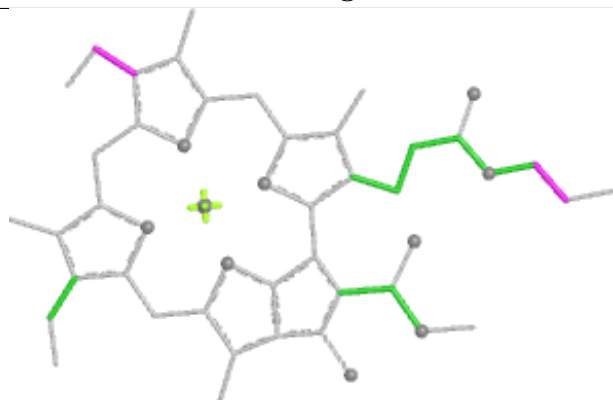
Ligand CLA a 811



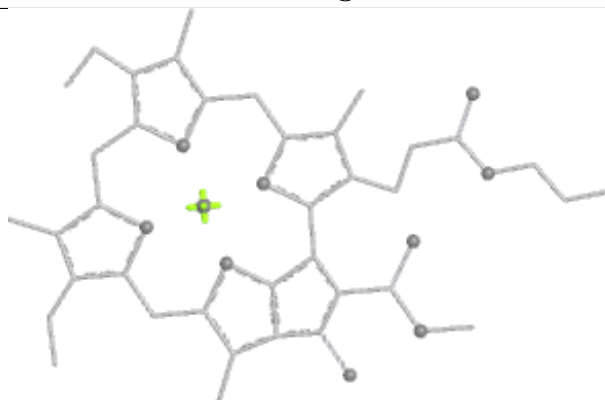
Bond lengths



Bond angles

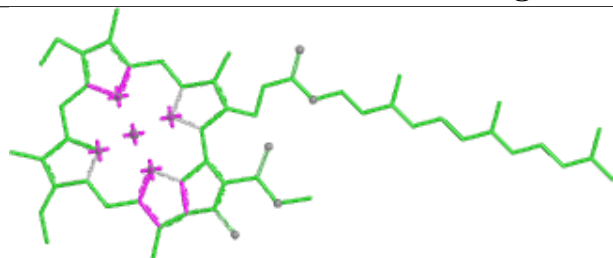


Torsions

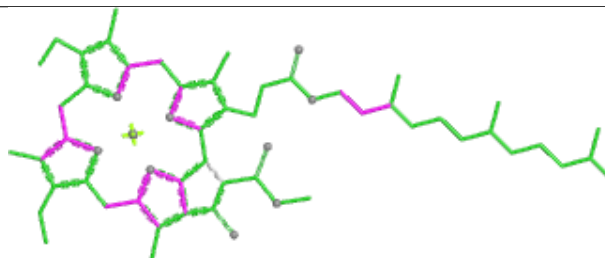


Rings

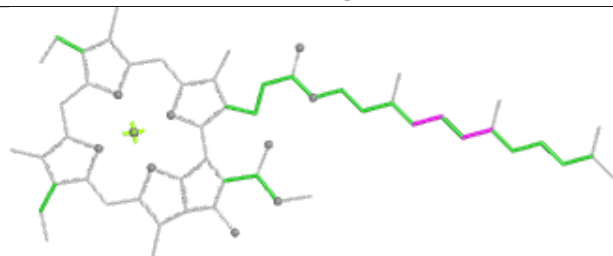
Ligand CLA H 313



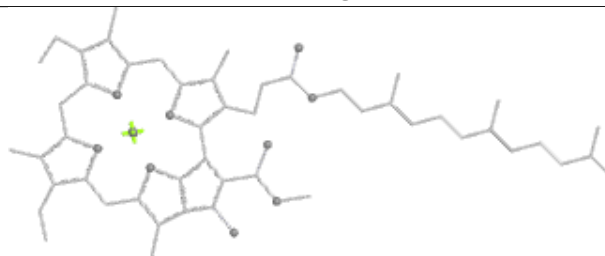
Bond lengths



Bond angles

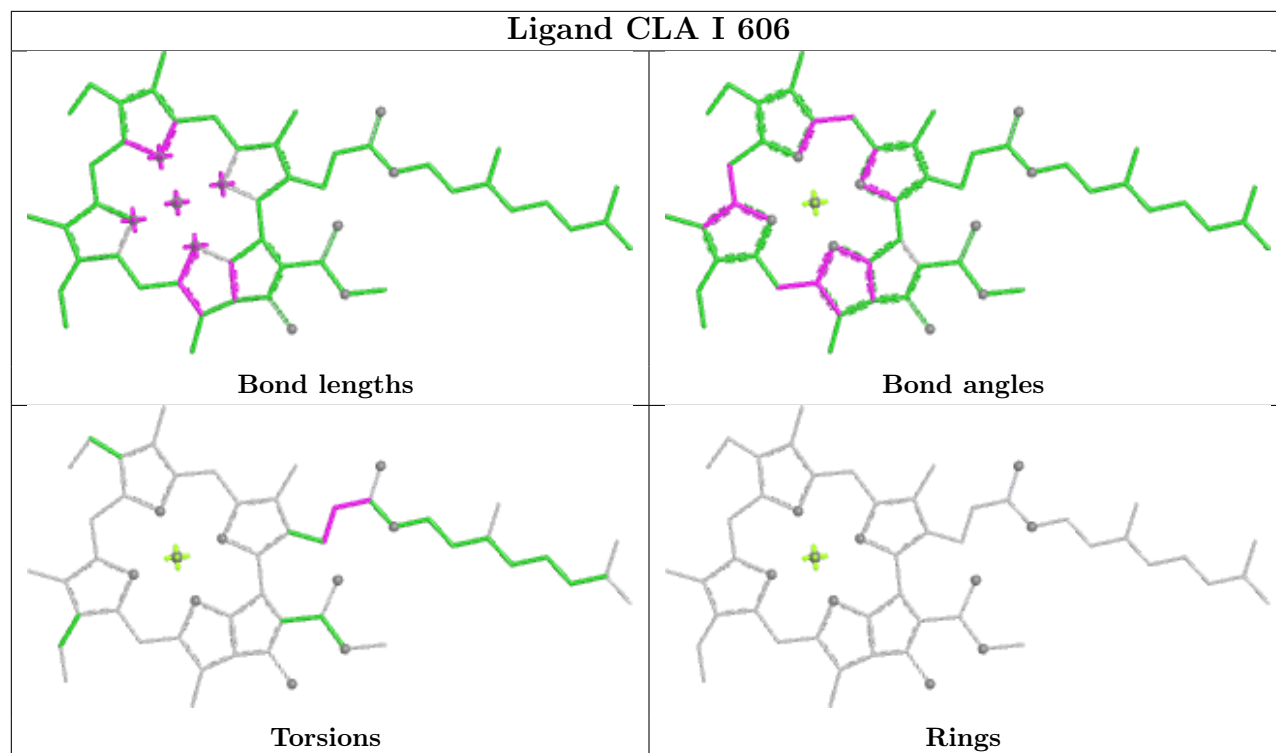


Torsions

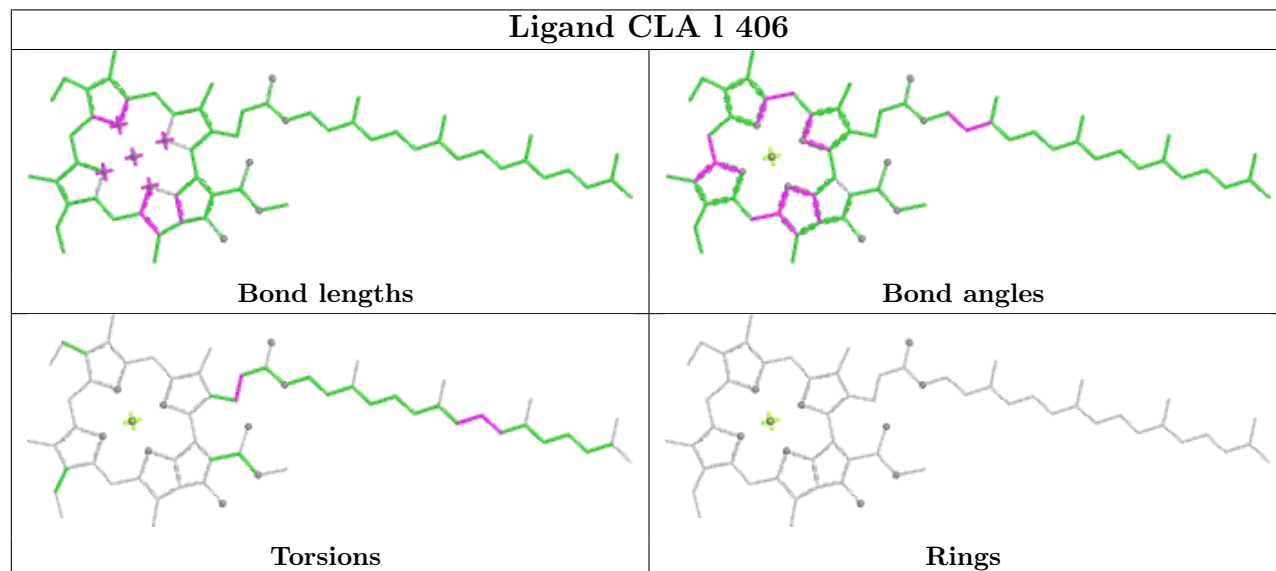


Rings

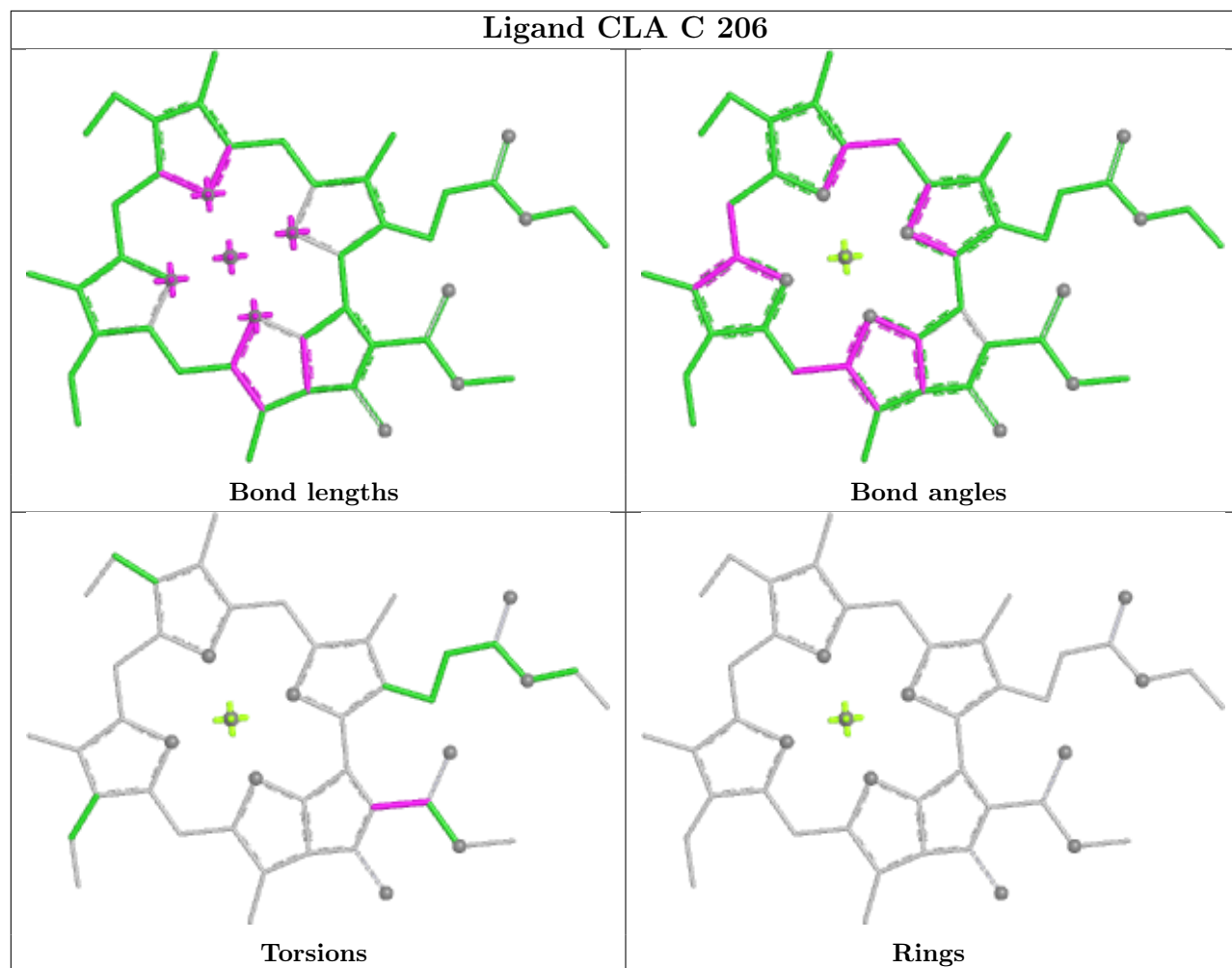
Ligand CLA I 606

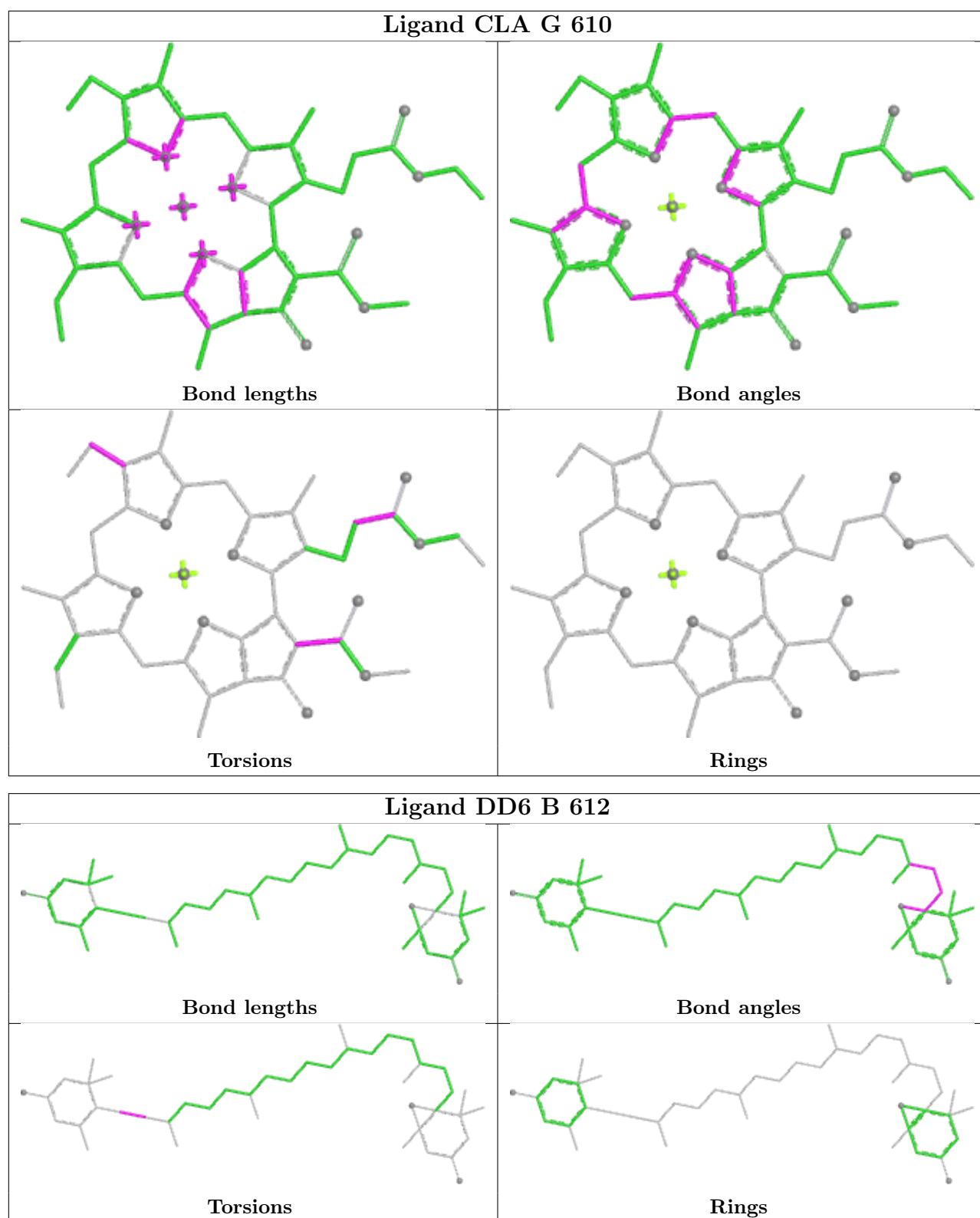


Ligand CLA I 406

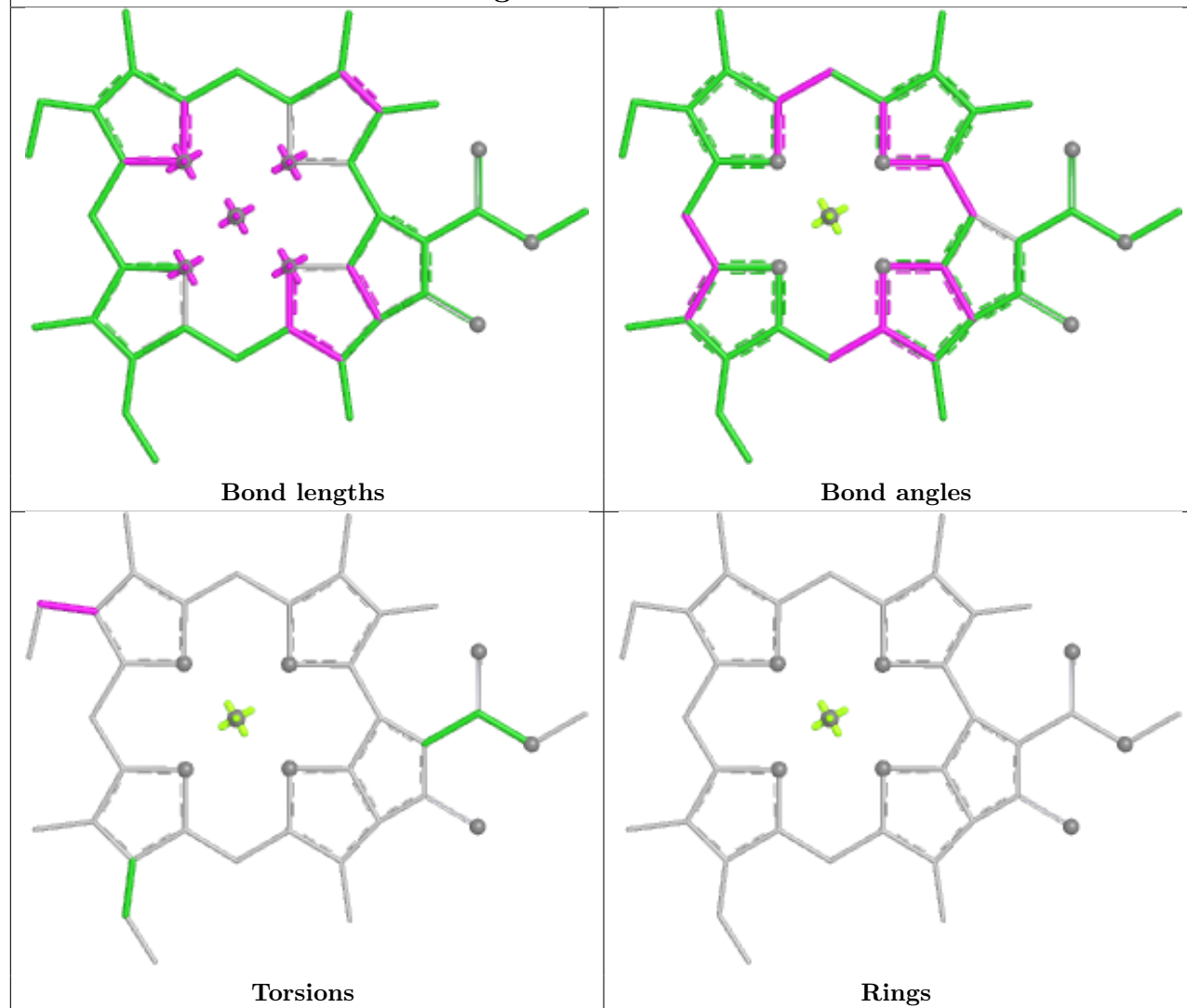


Ligand CLA C 206

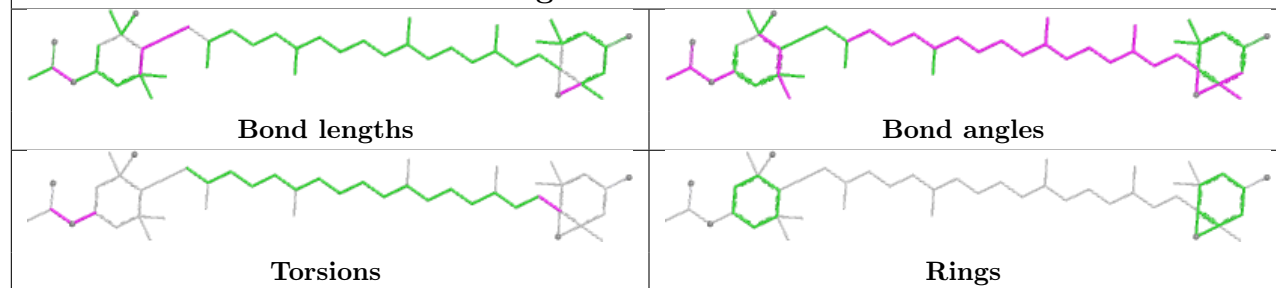




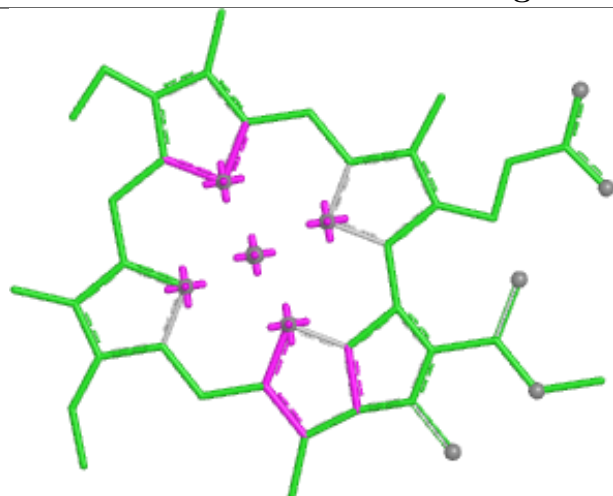
Ligand CLA K 606



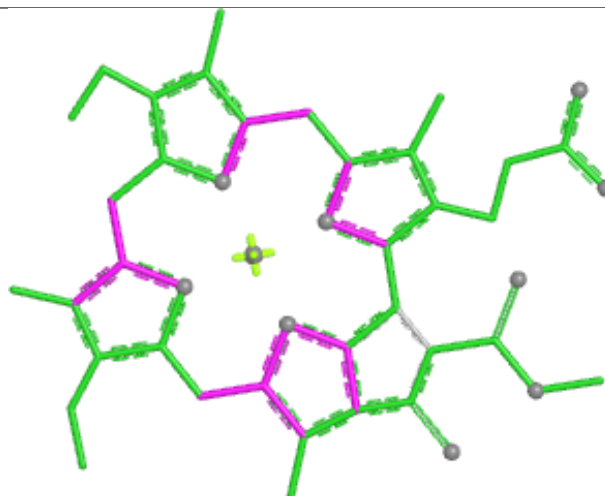
Ligand UIX T 612



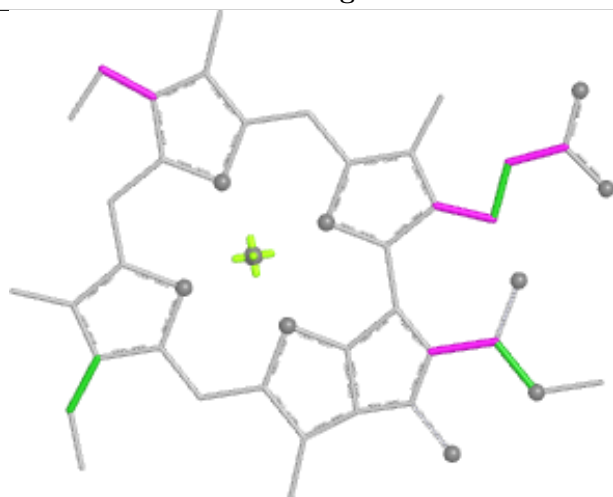
Ligand CLA U 606



Bond lengths



Bond angles

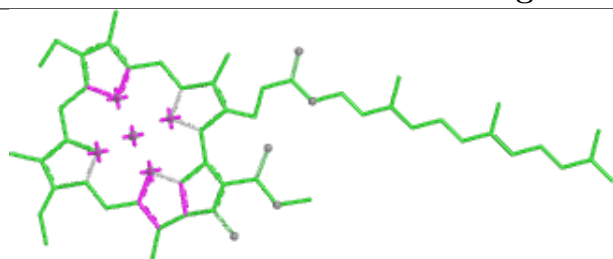


Torsions

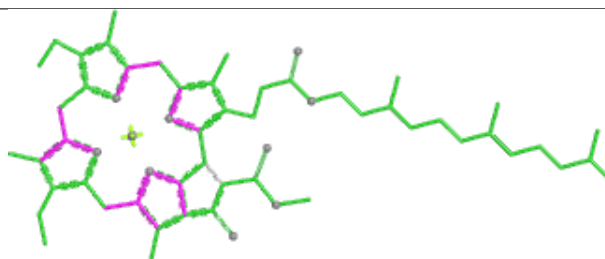


Rings

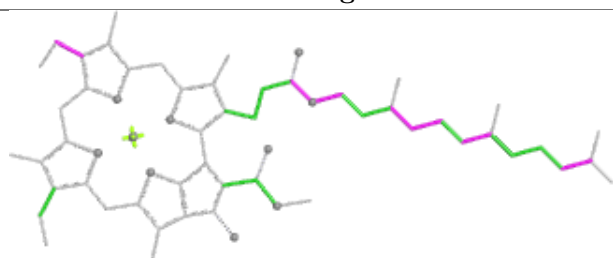
Ligand CLA F 617



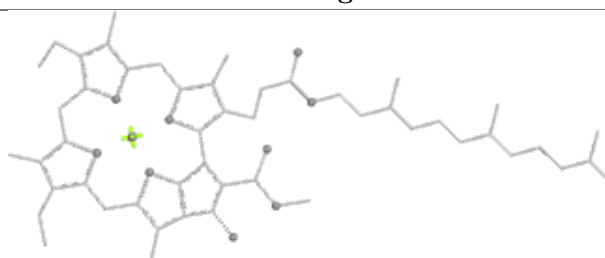
Bond lengths



Bond angles

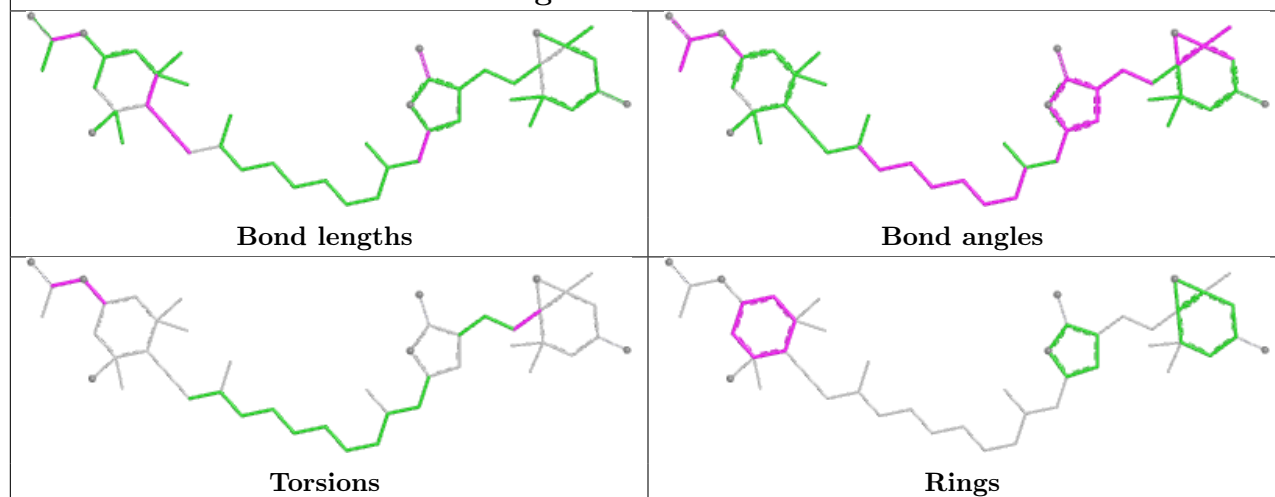


Torsions

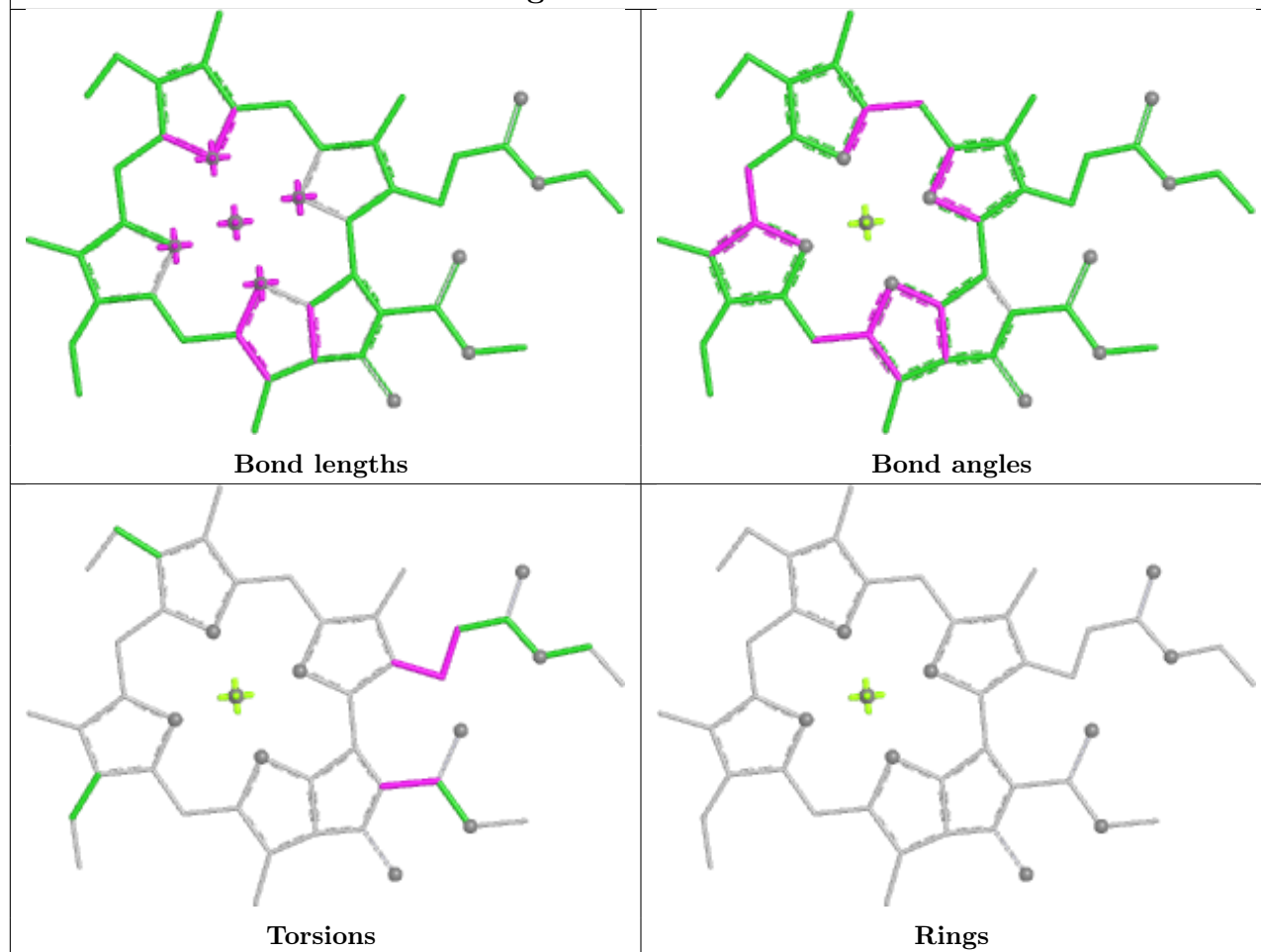


Rings

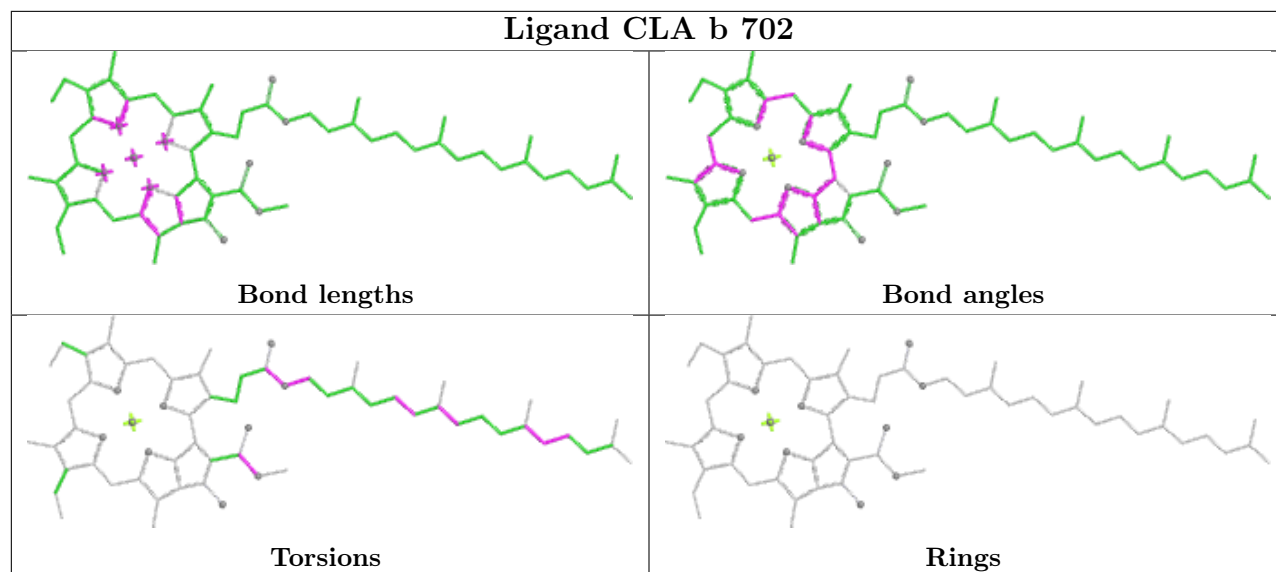
Ligand PID K 611



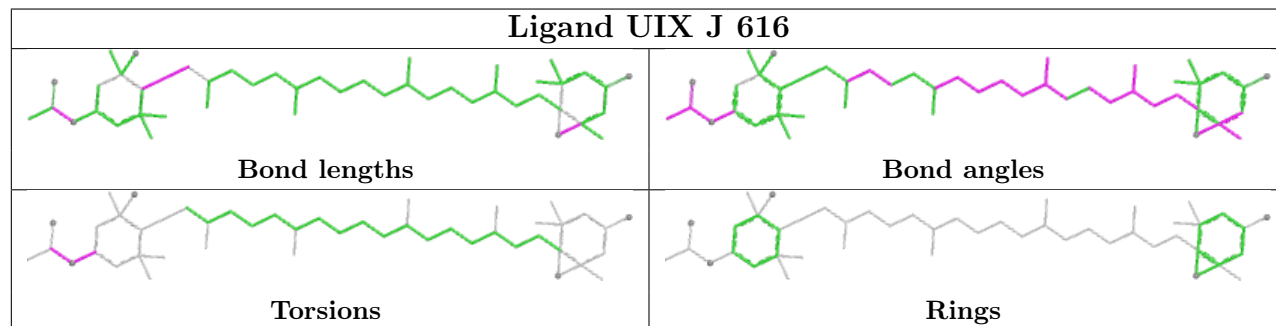
Ligand CLA F 610



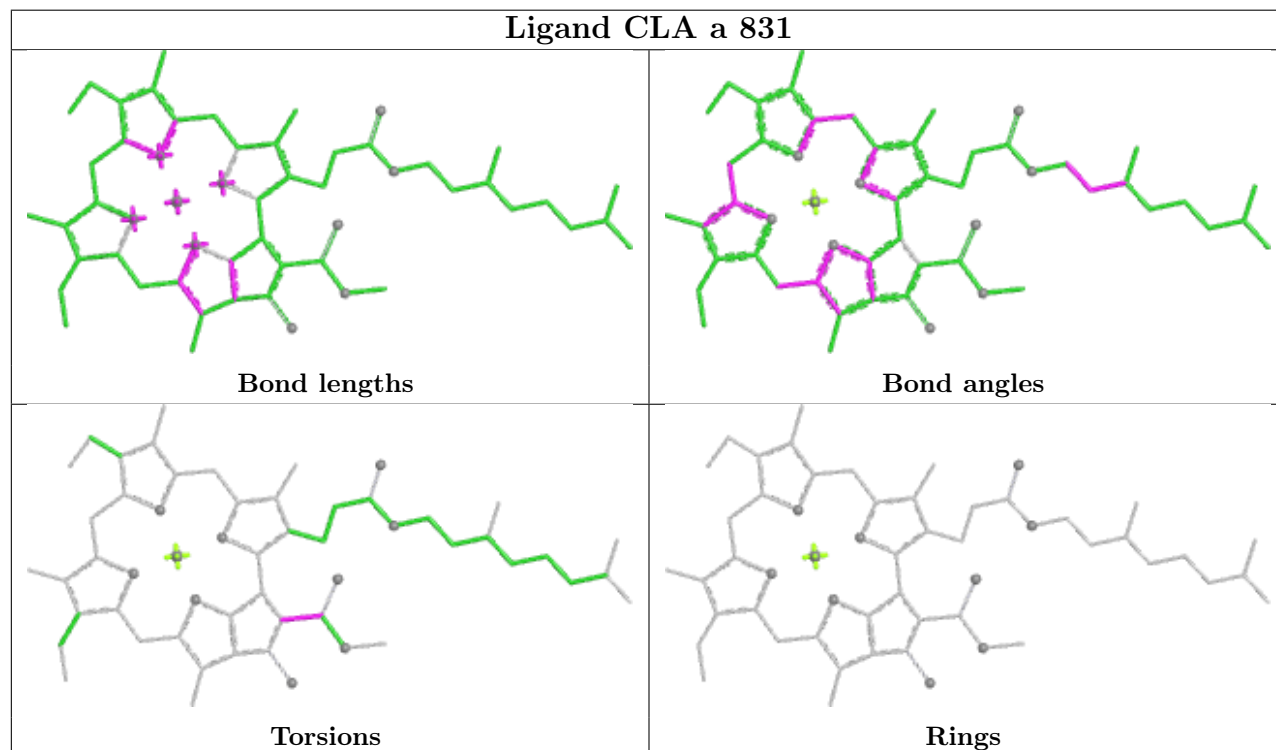
Ligand CLA b 702

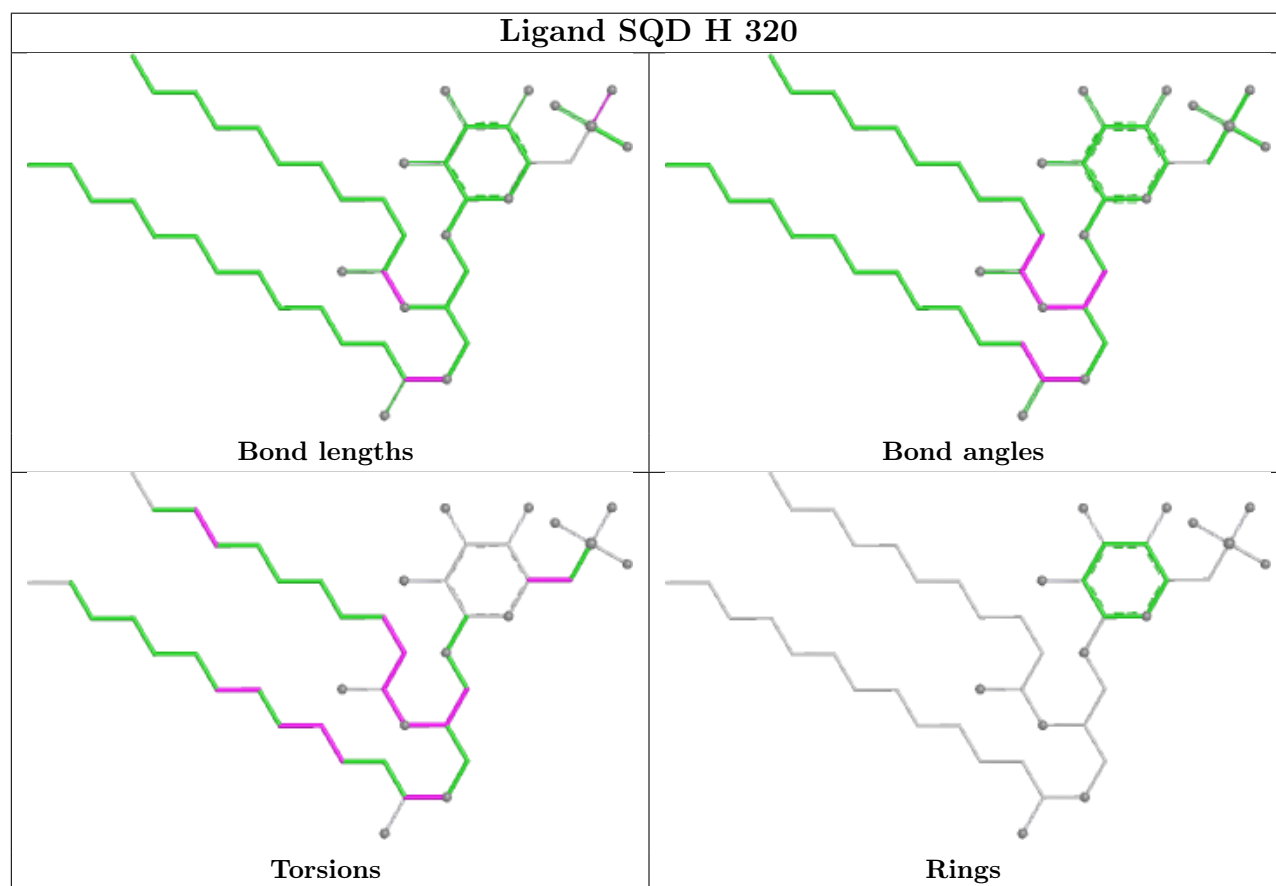
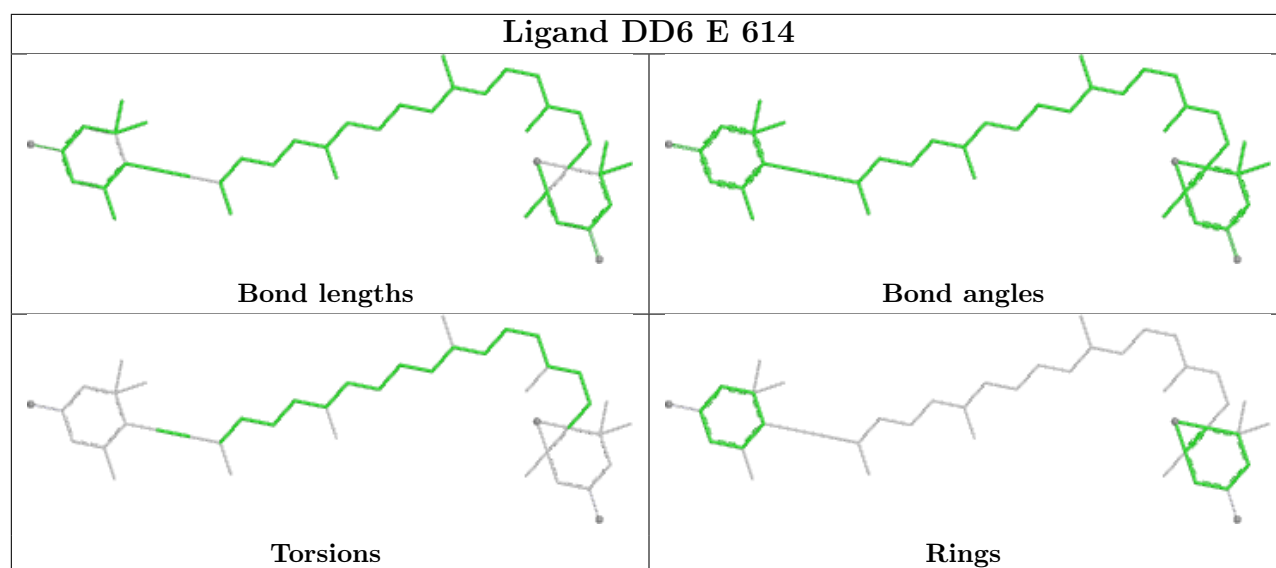


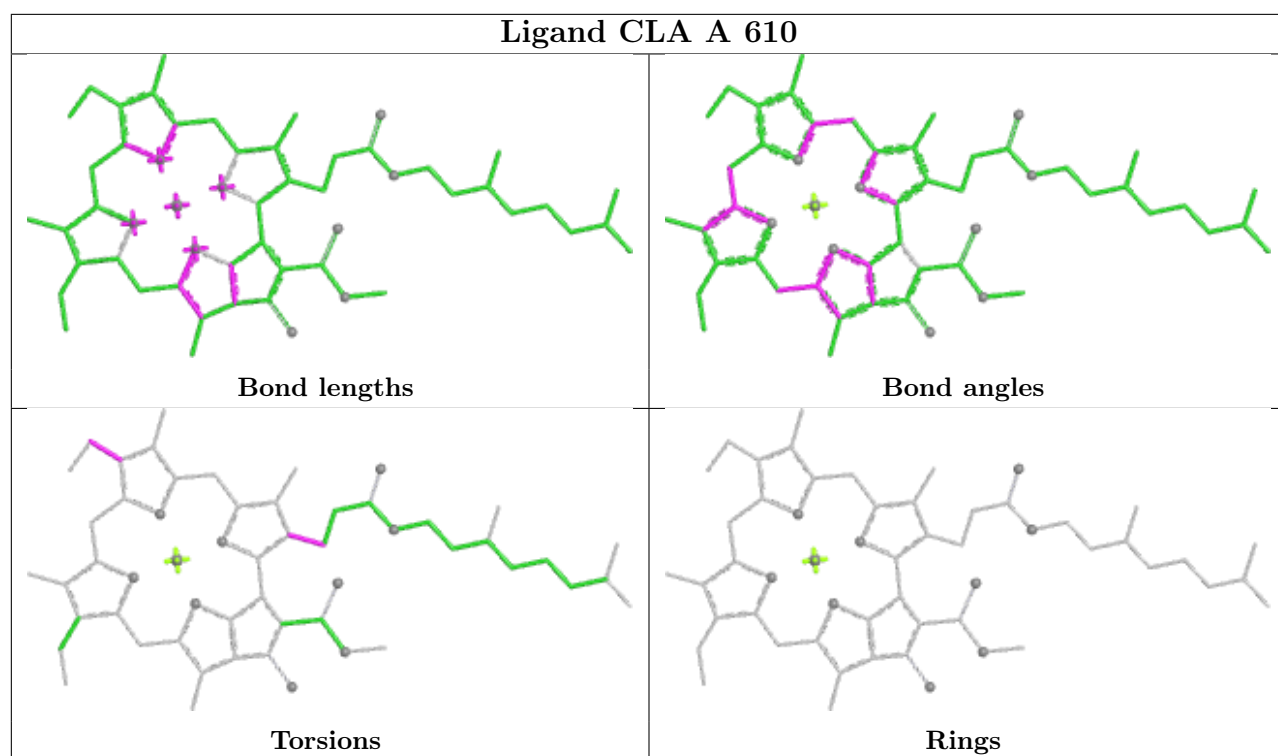
Ligand UIX J 616



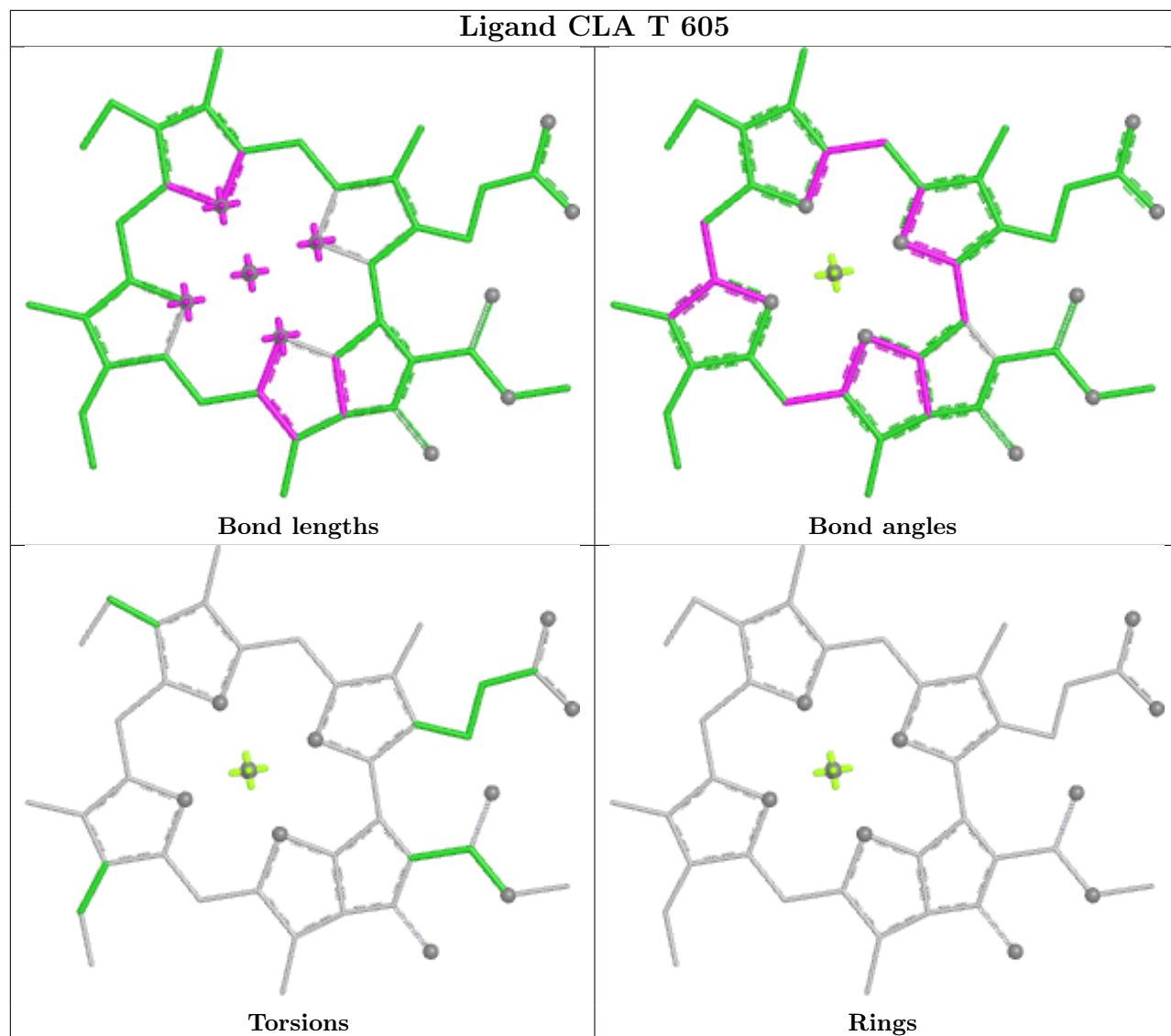
Ligand CLA a 831



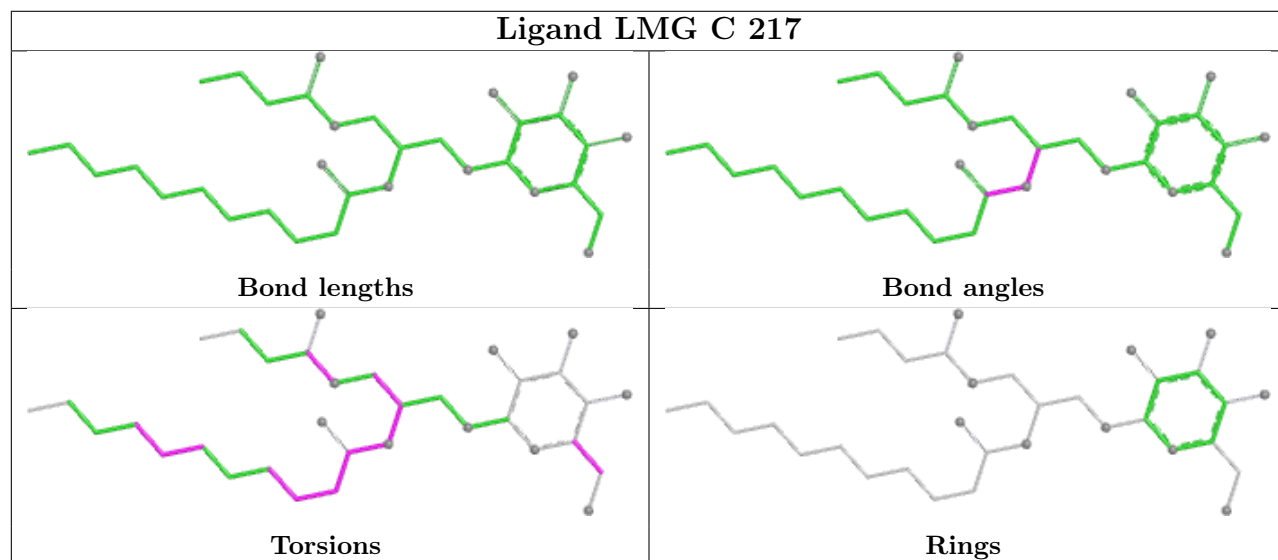


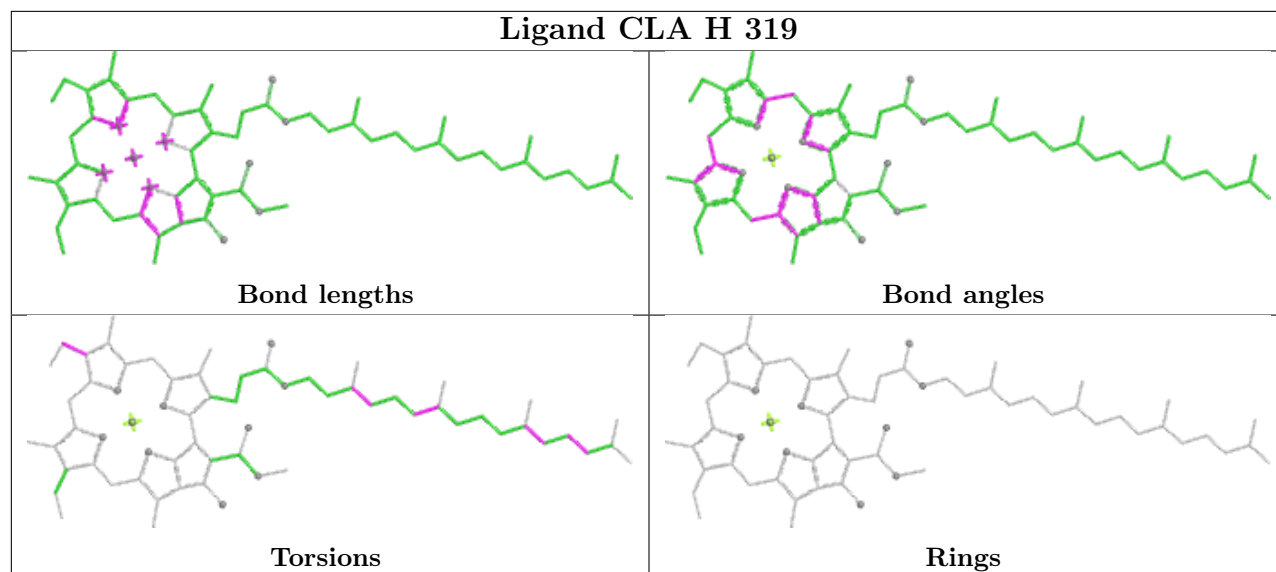
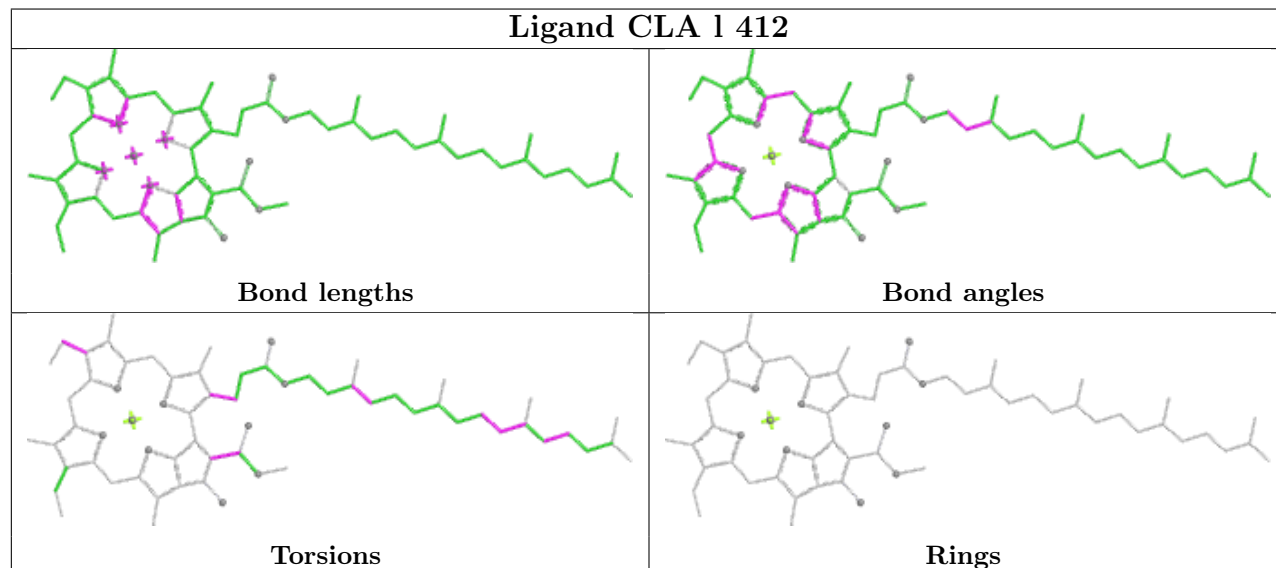


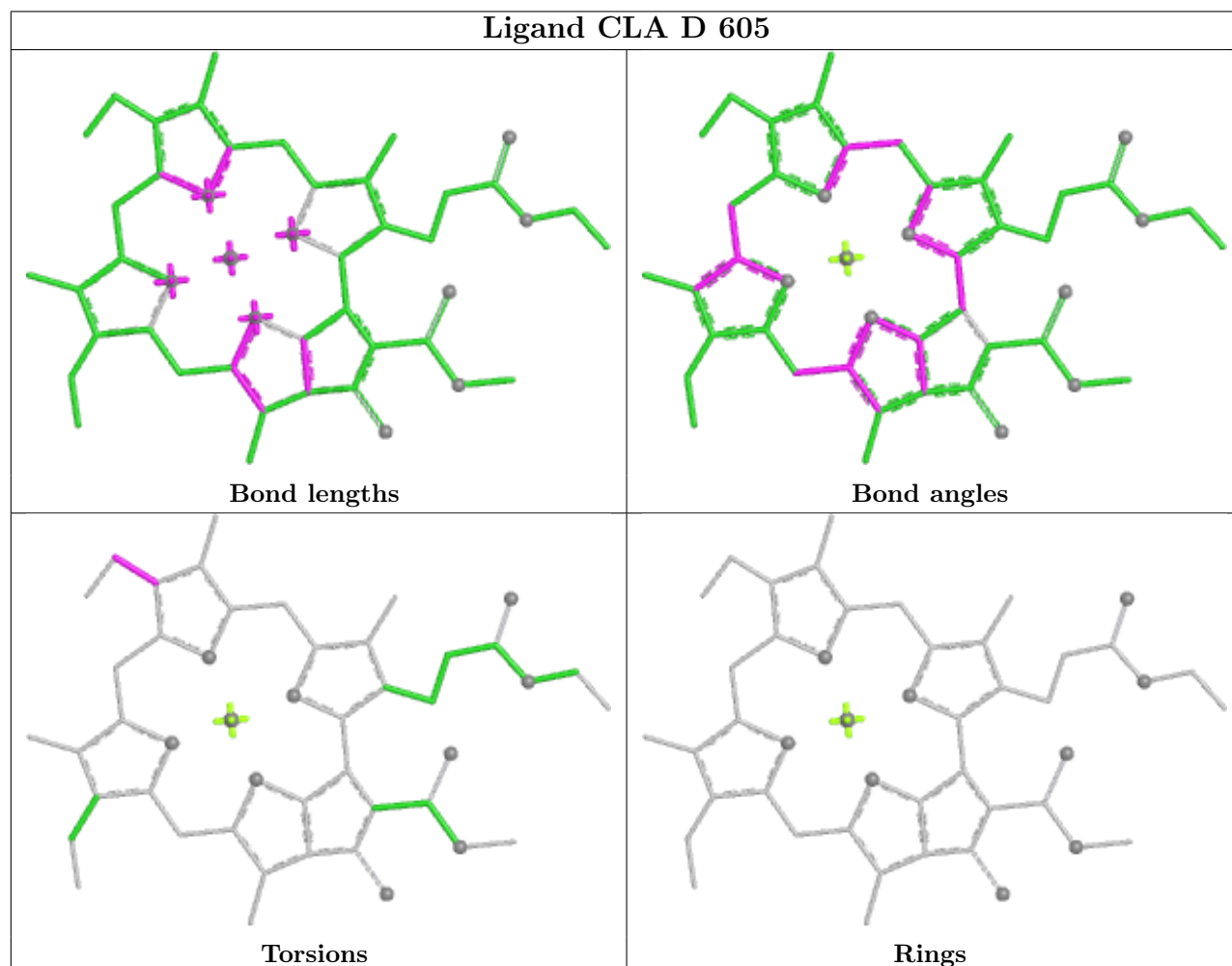
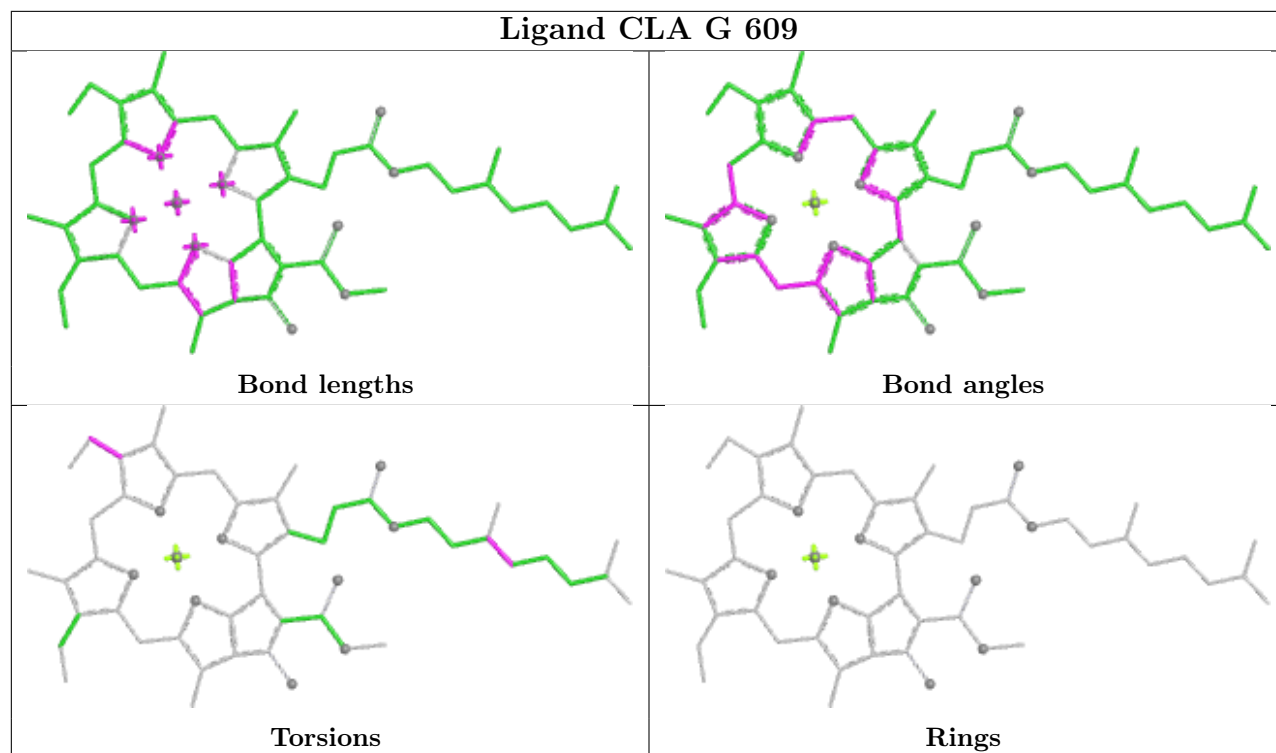
Ligand CLA T 605

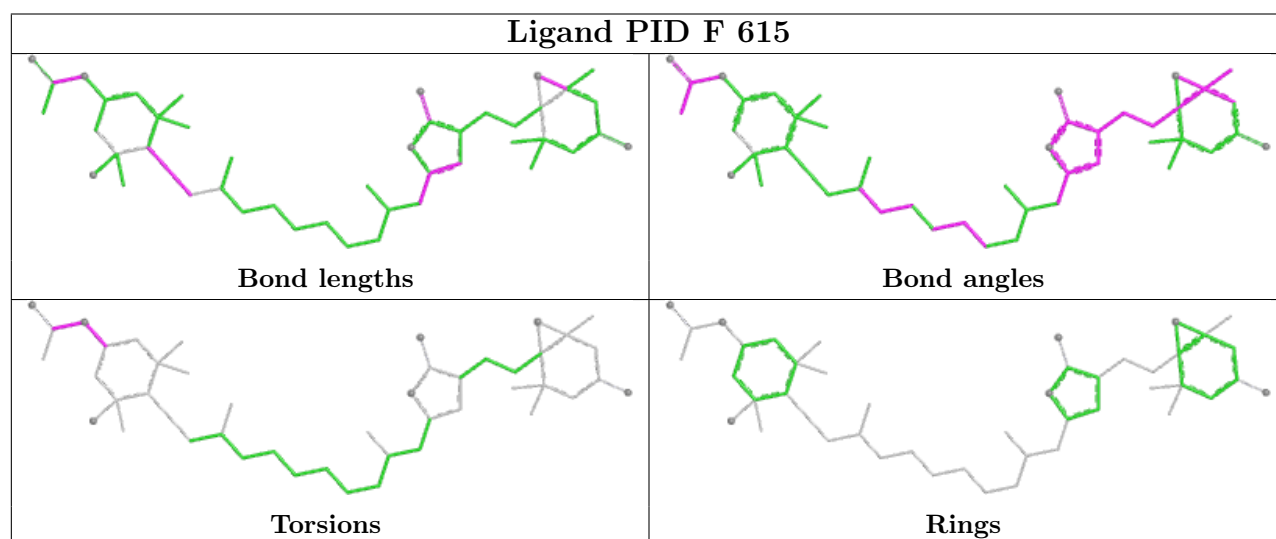
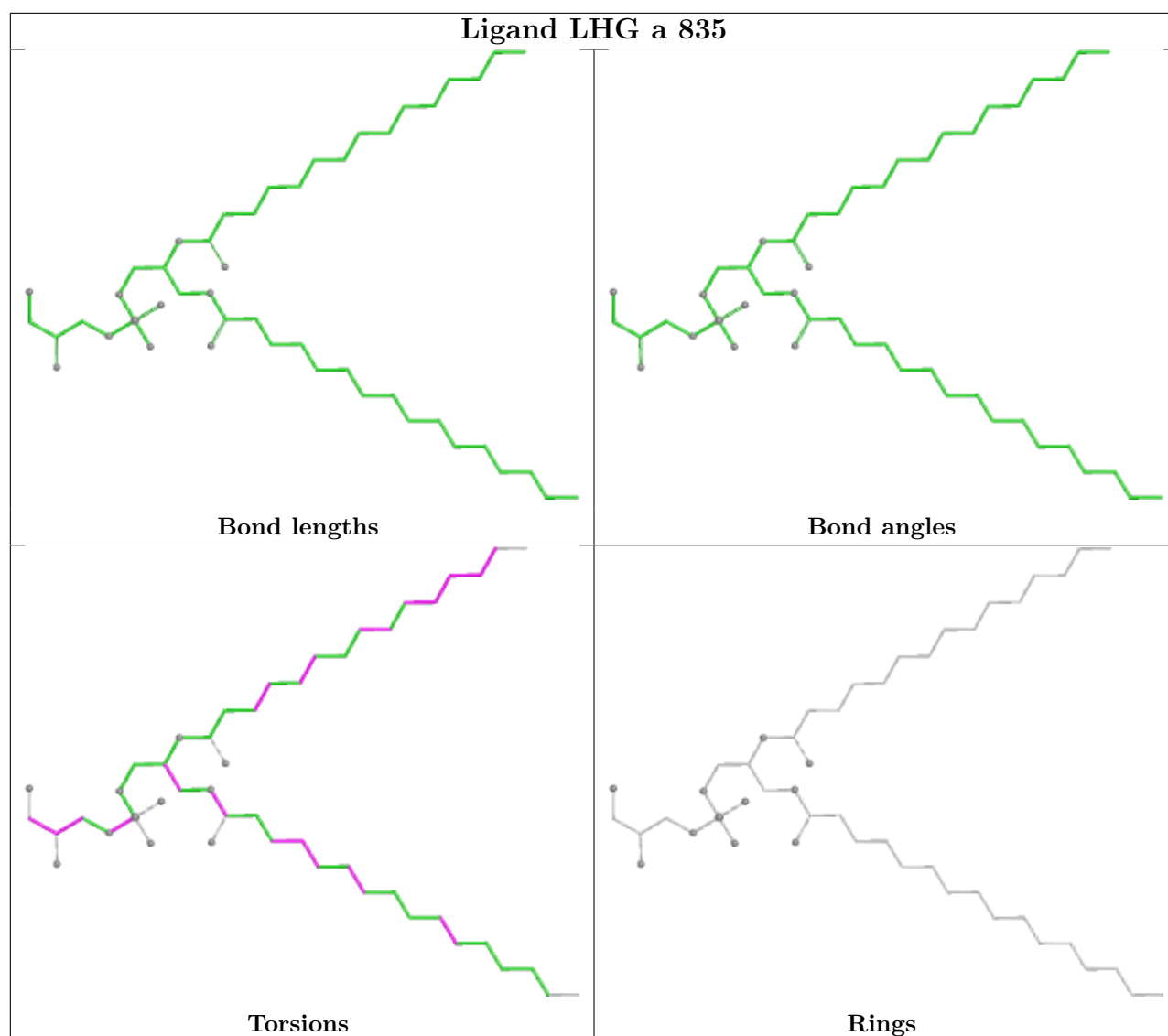


Ligand LMG C 217

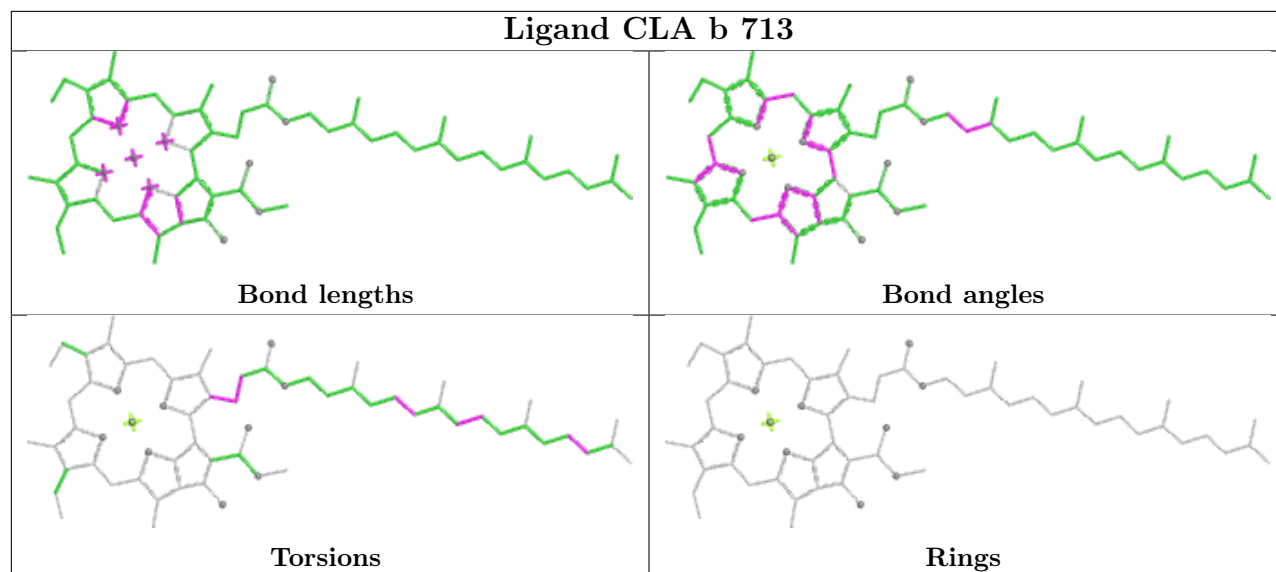


Ligand CLA H 319**Ligand CLA I 412**

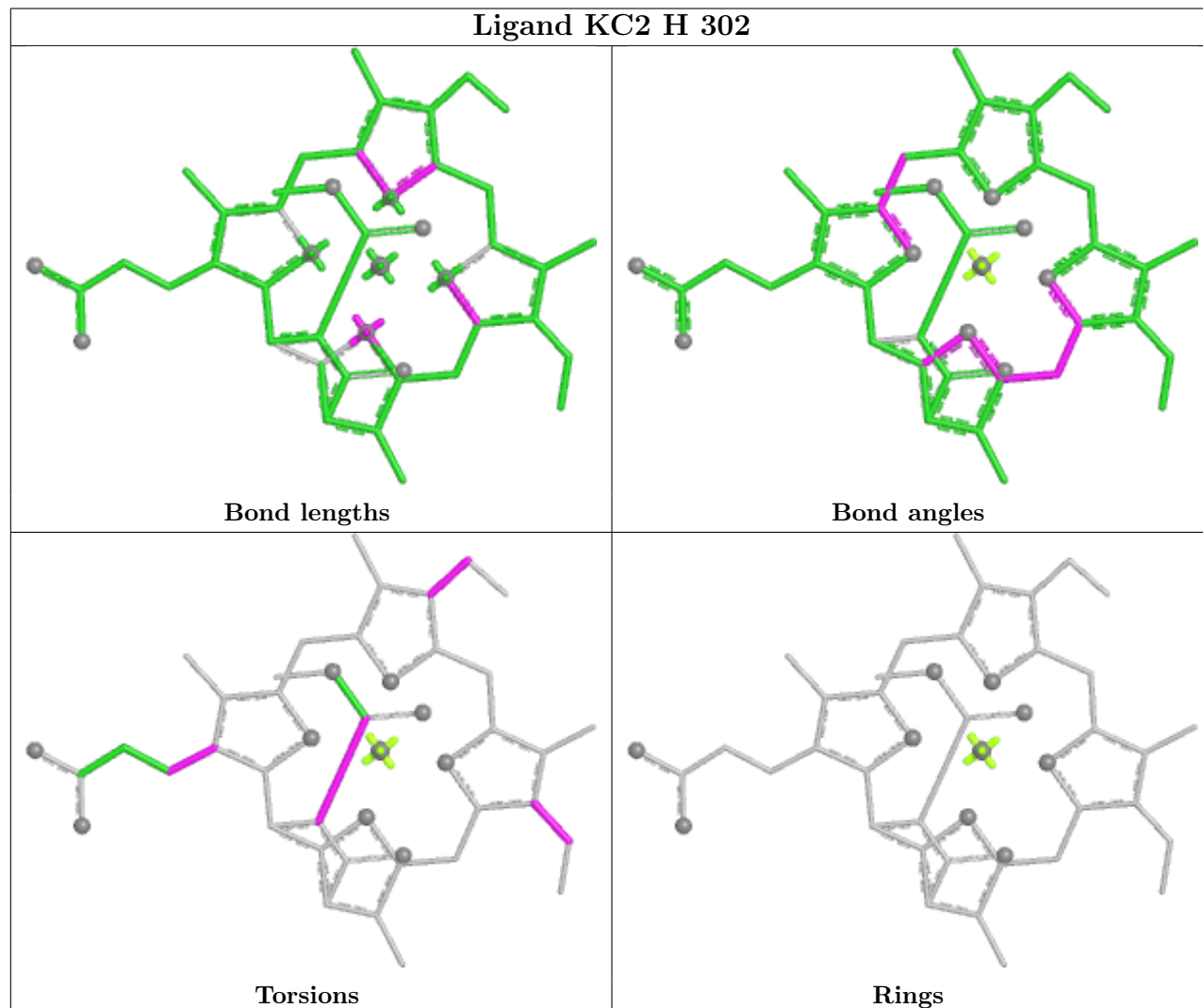




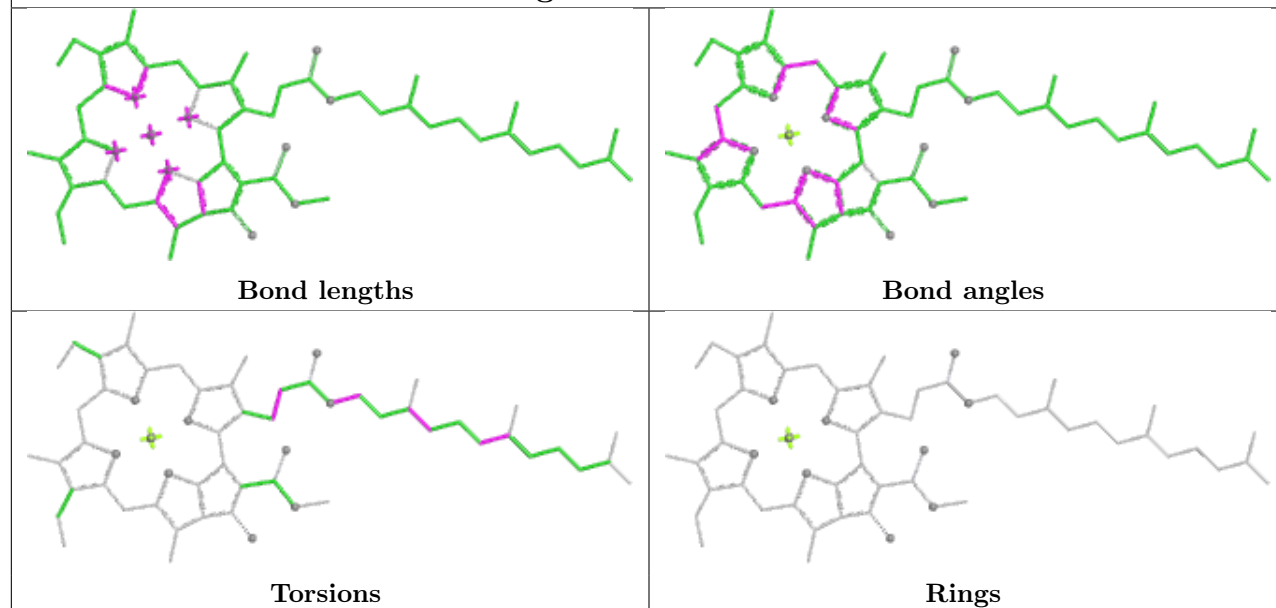
Ligand CLA b 713



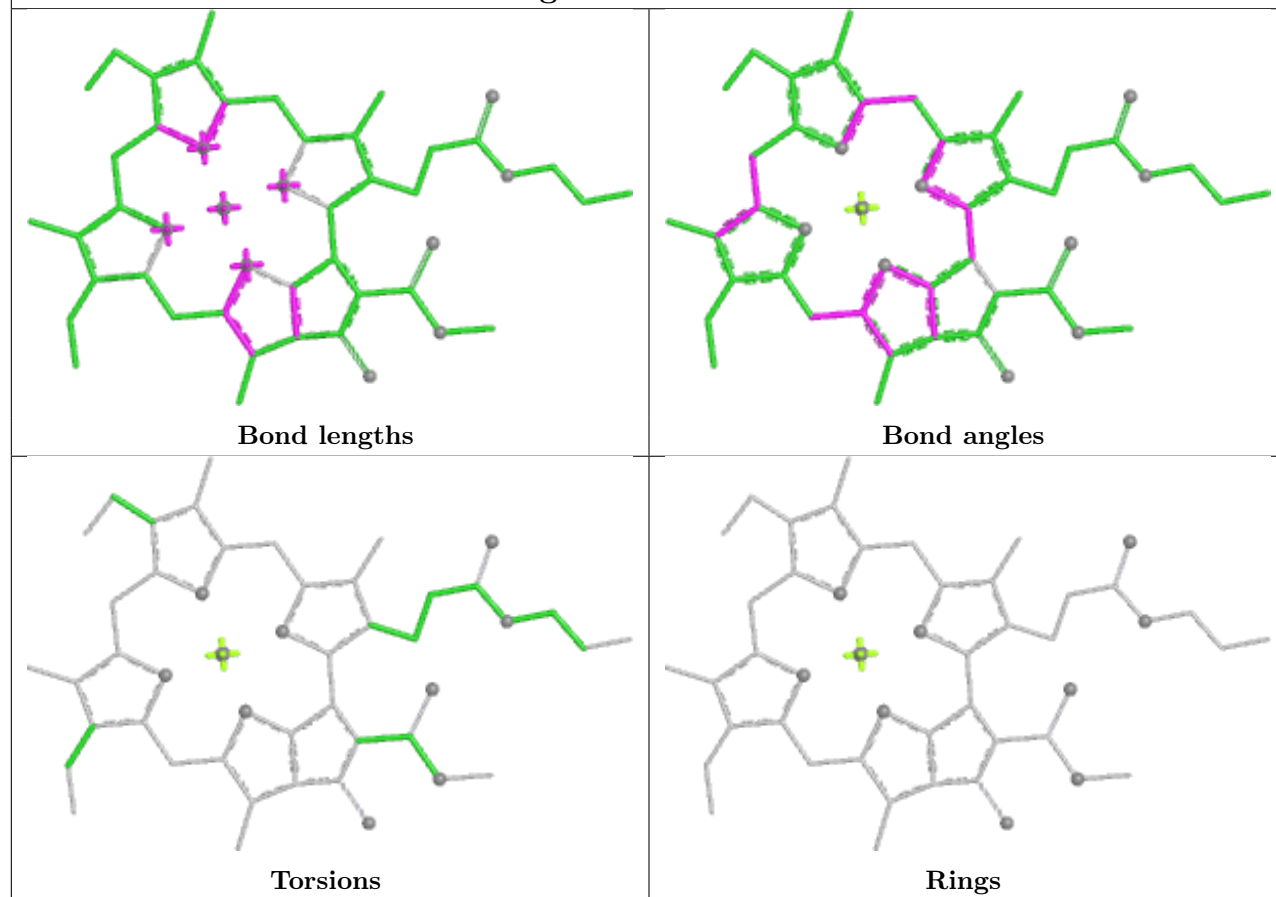
Ligand KC2 H 302



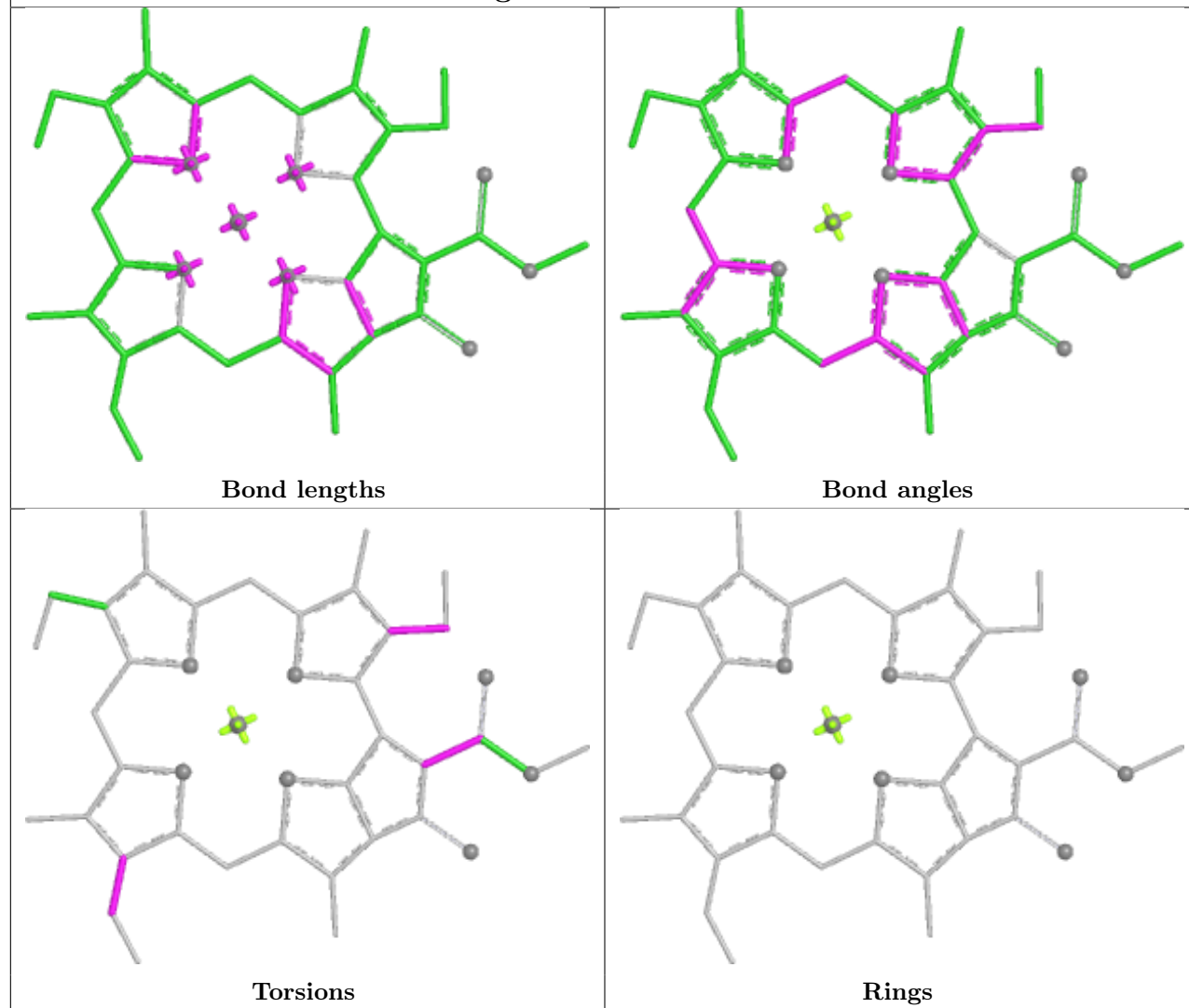
Ligand CLA a 815



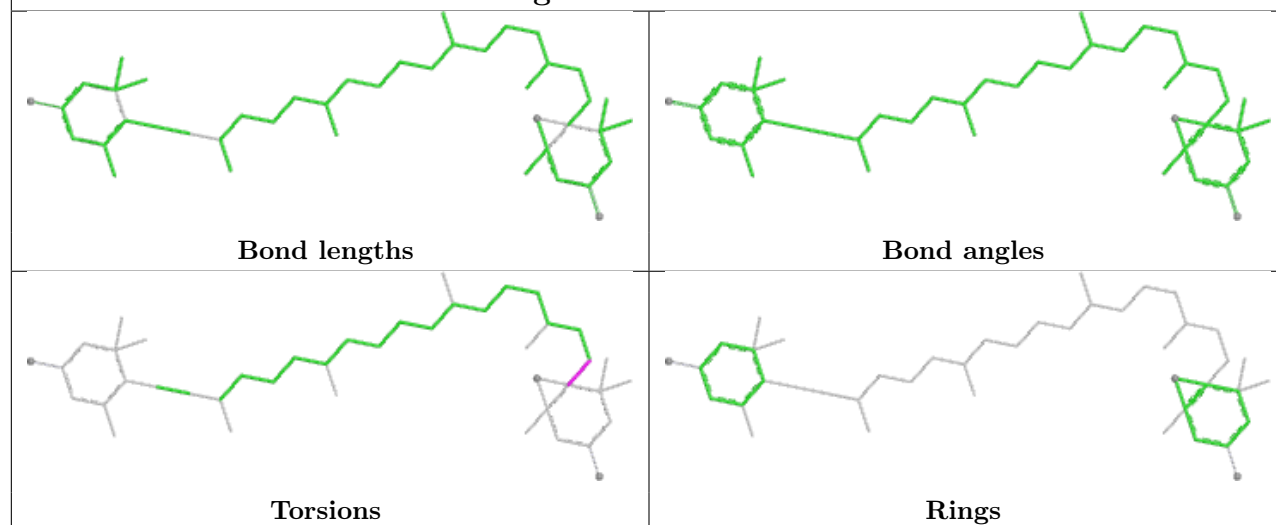
Ligand CLA f 303



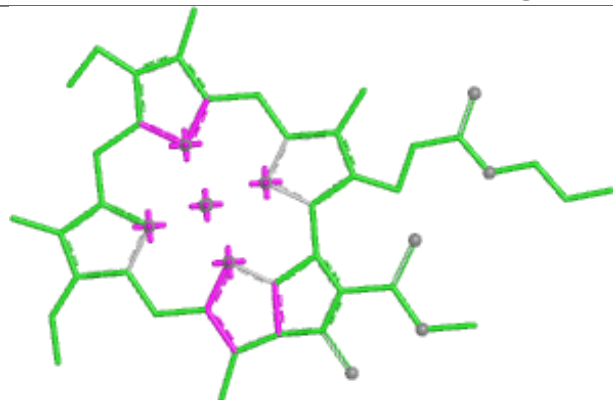
Ligand CLA H 312



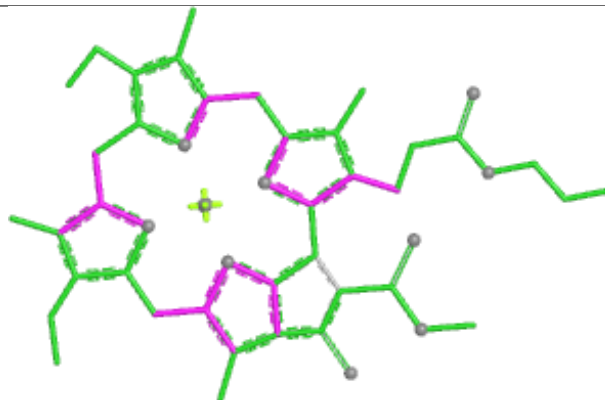
Ligand DD6 B 616



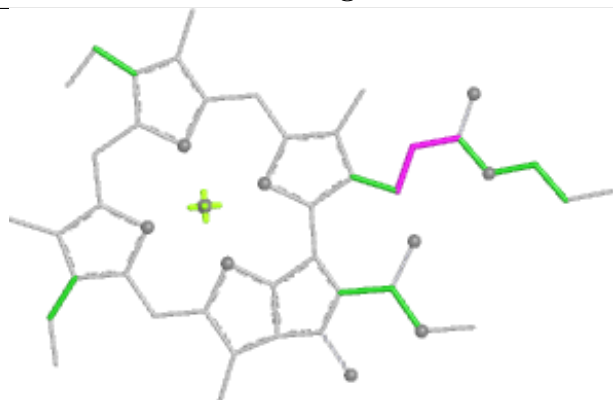
Ligand CLA b 712



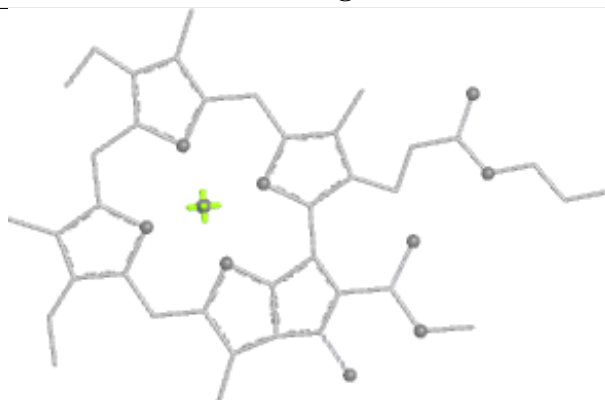
Bond lengths



Bond angles

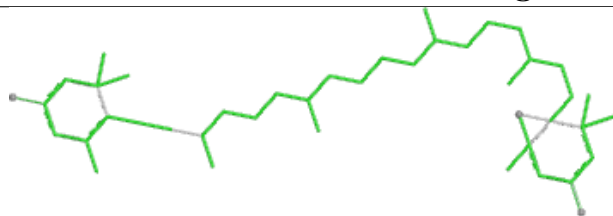


Torsions

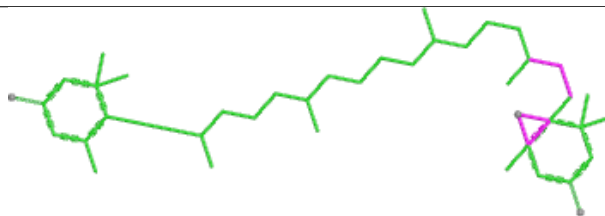


Rings

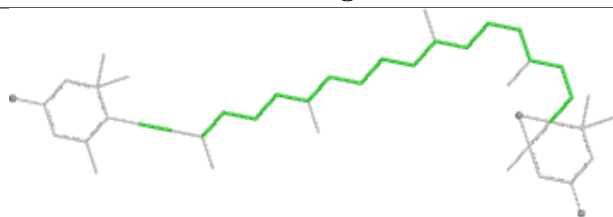
Ligand DD6 D 617



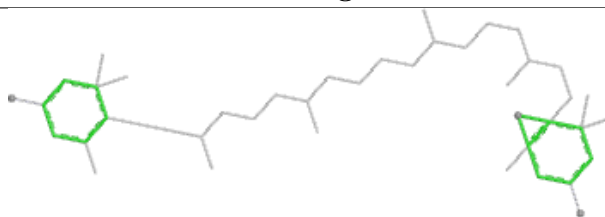
Bond lengths



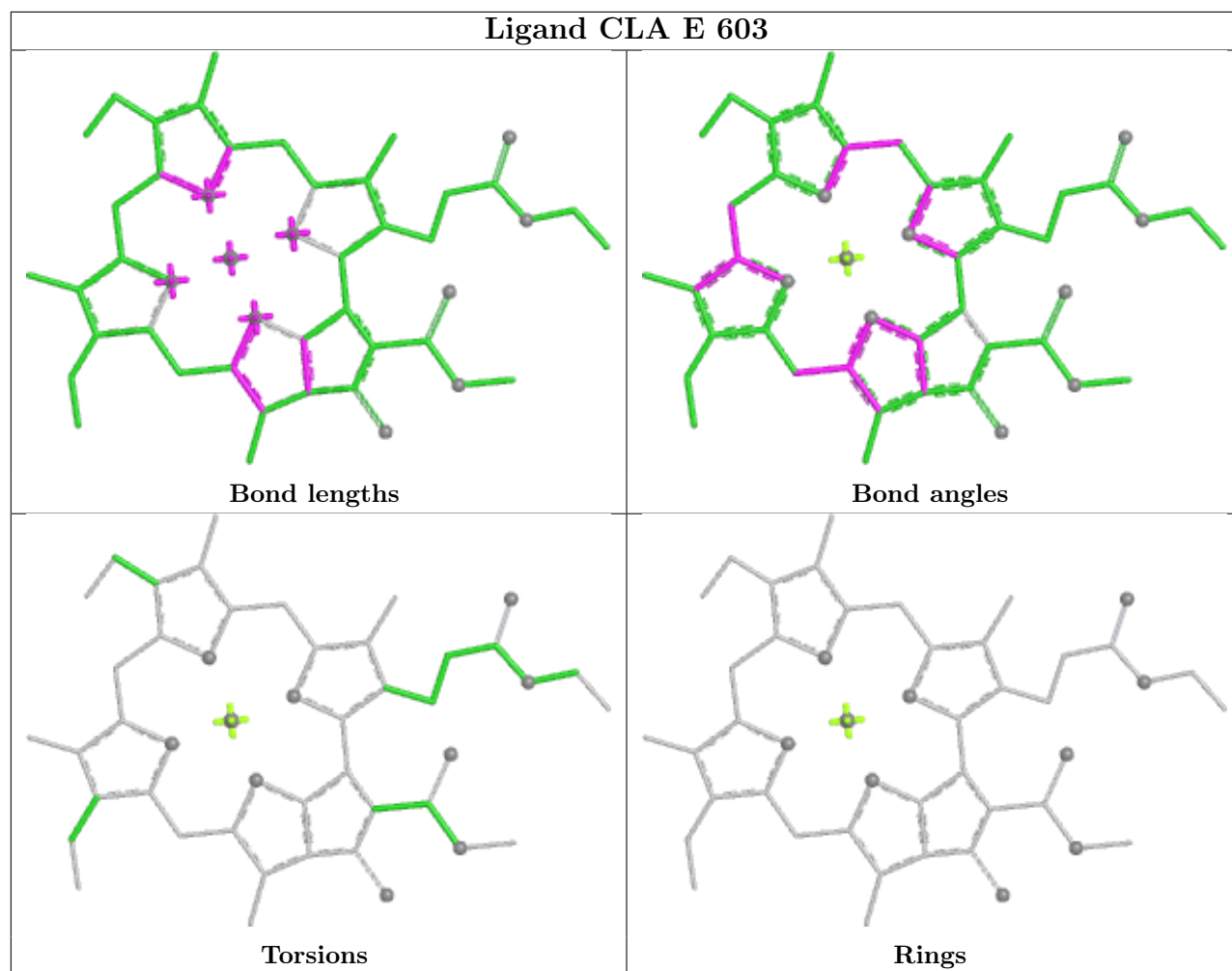
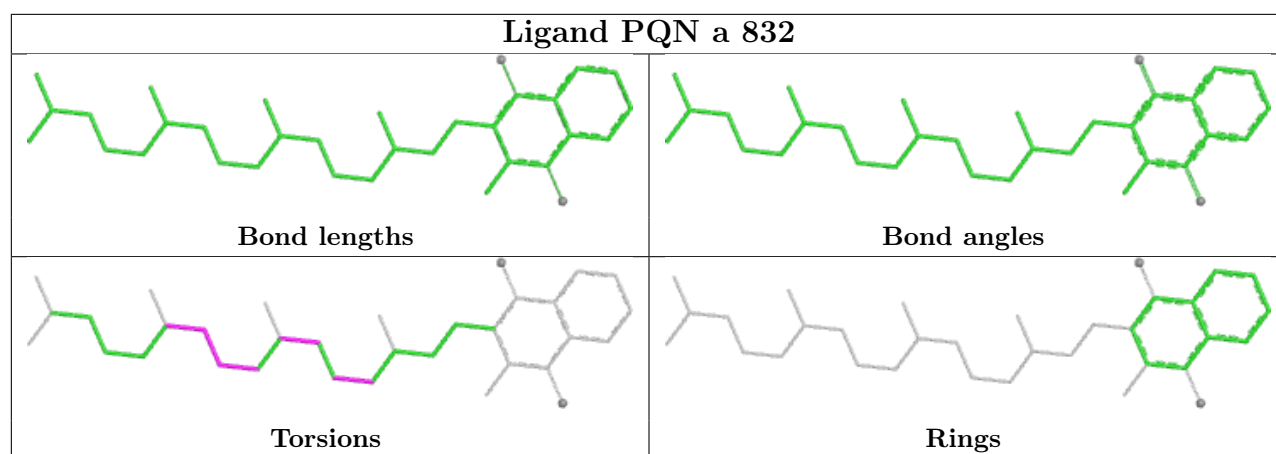
Bond angles

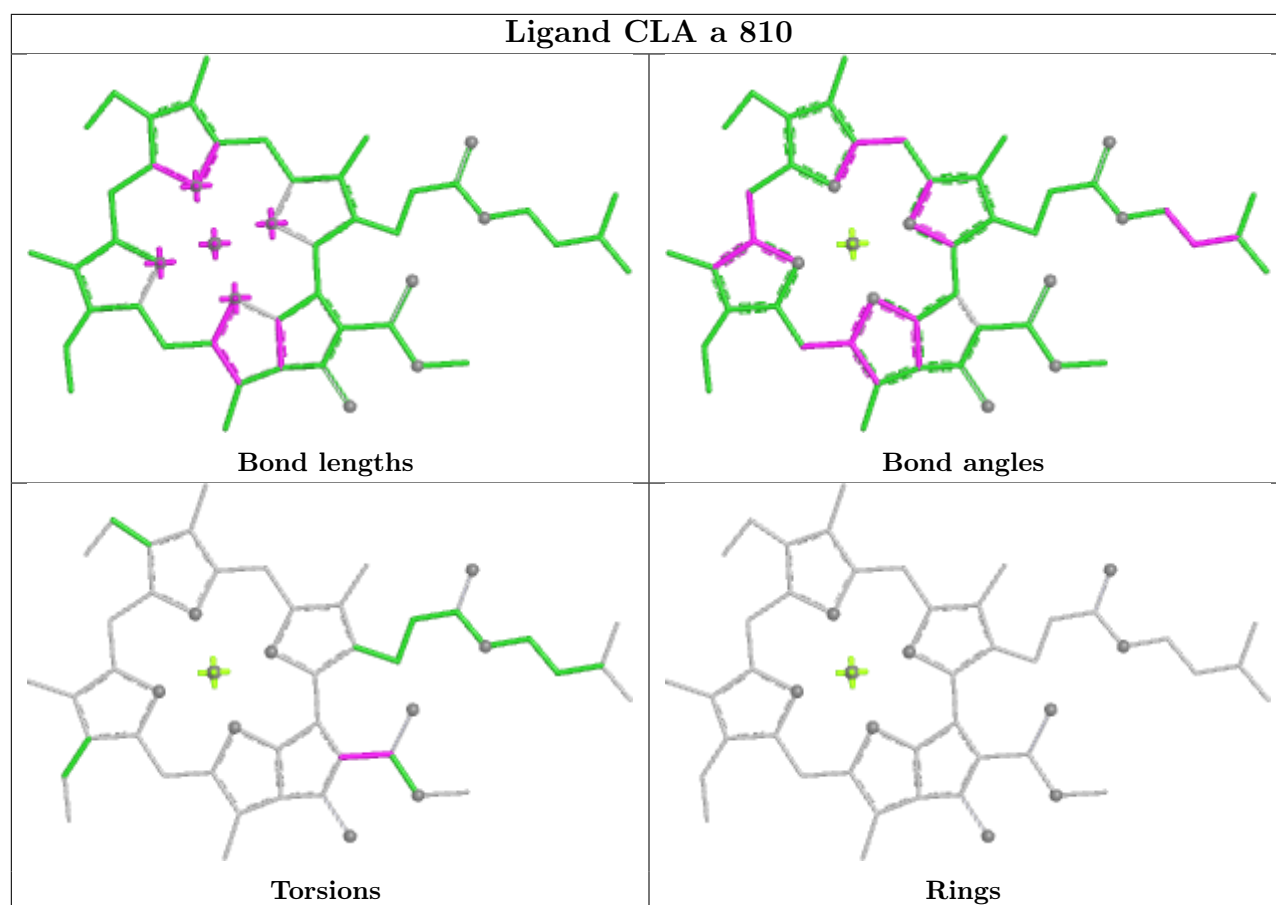


Torsions

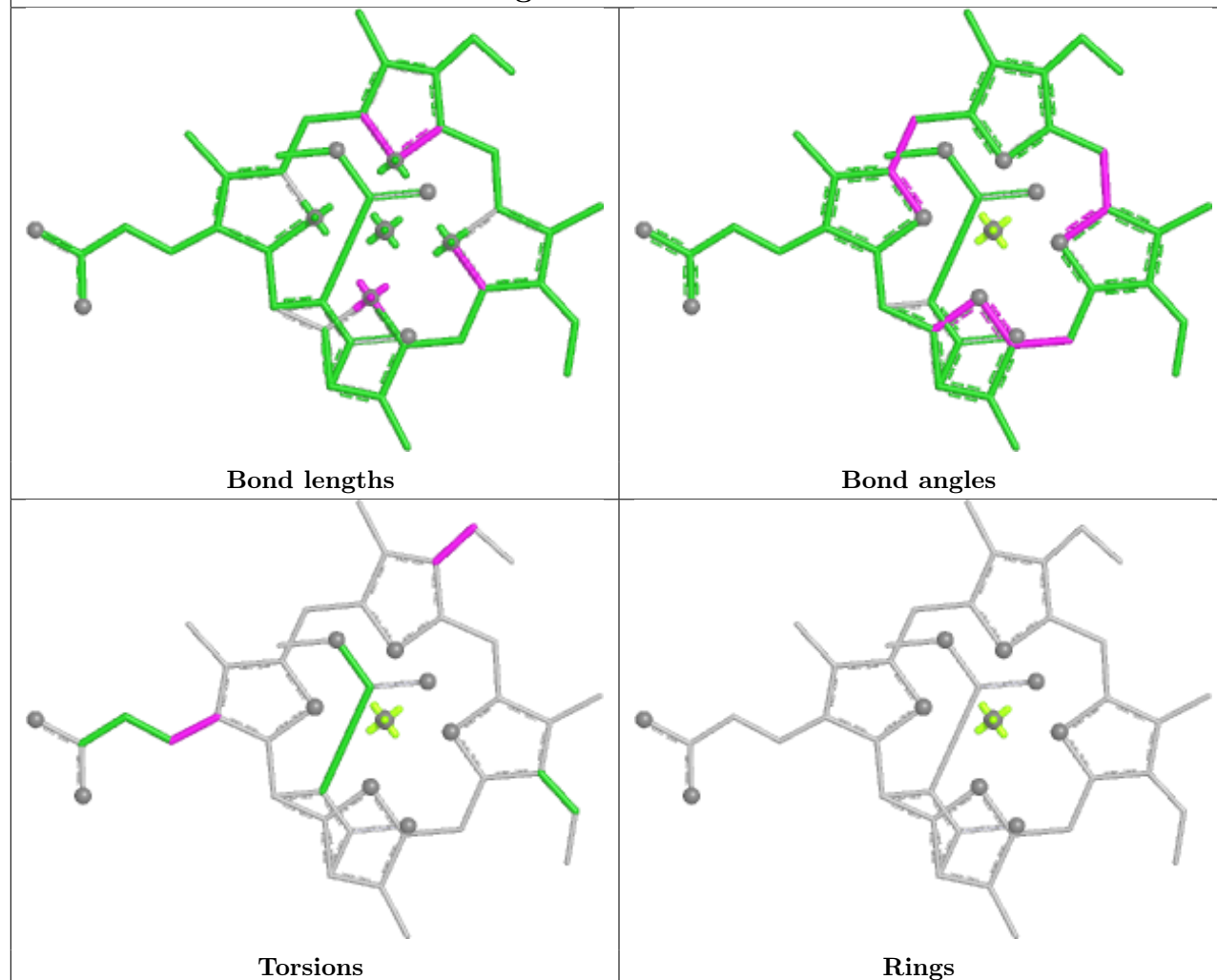


Rings

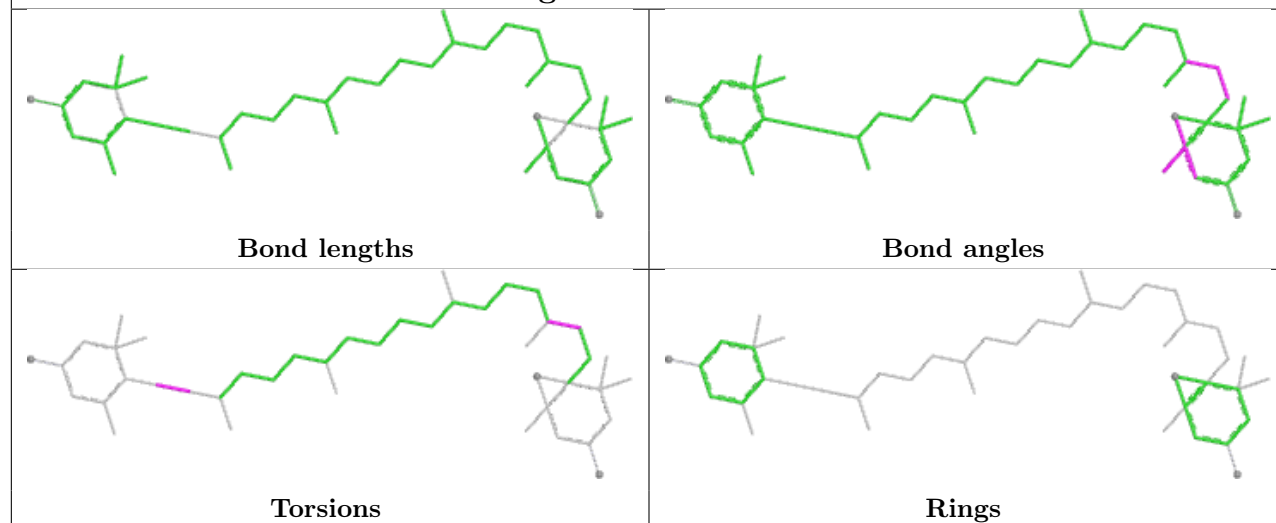


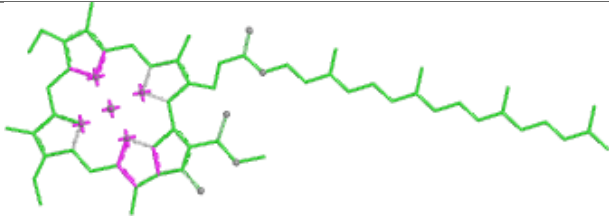
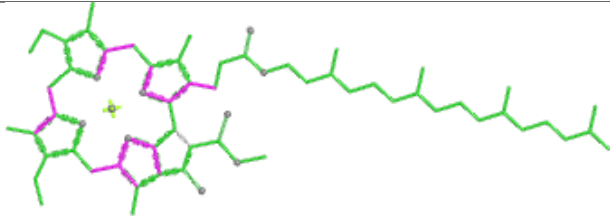
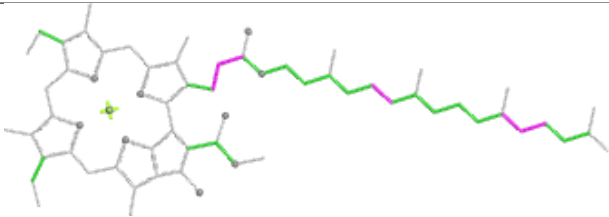
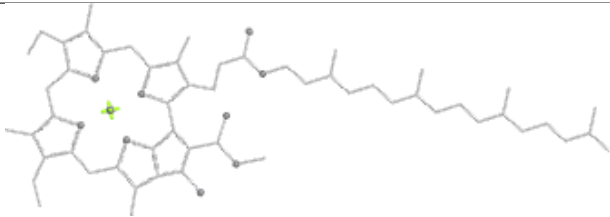


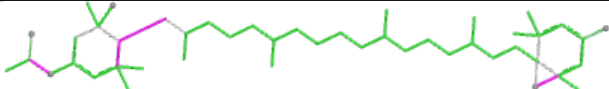
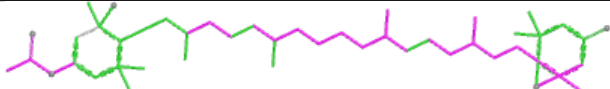
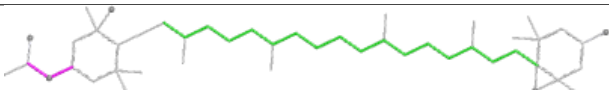
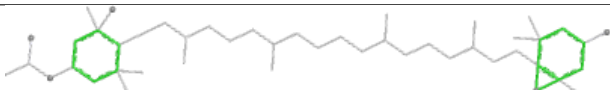
Ligand KC2 I 604

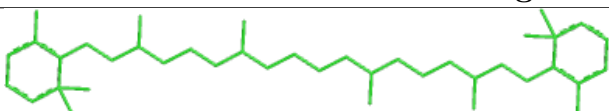
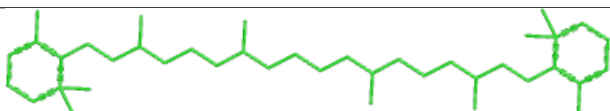
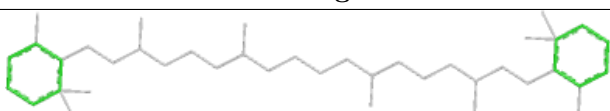


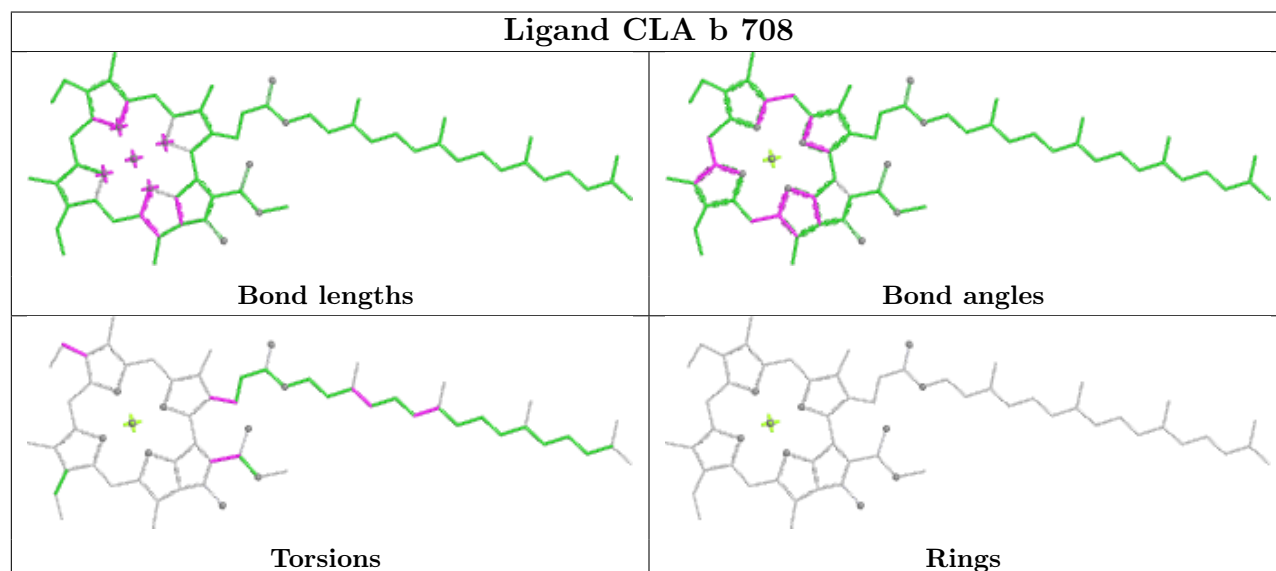
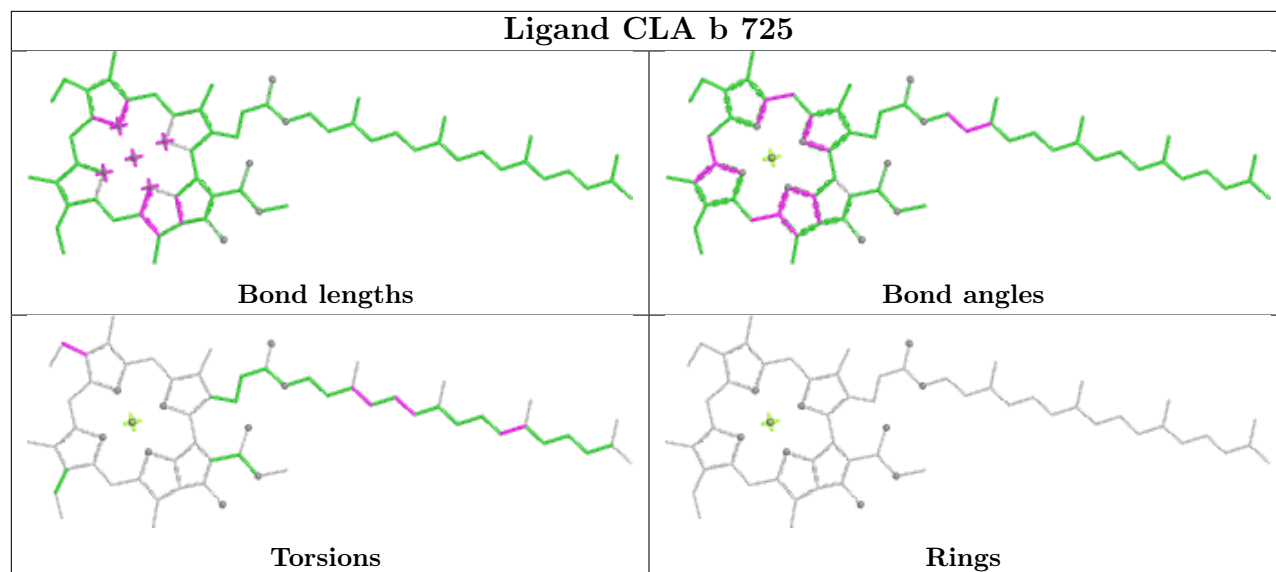
Ligand DD6 r 206

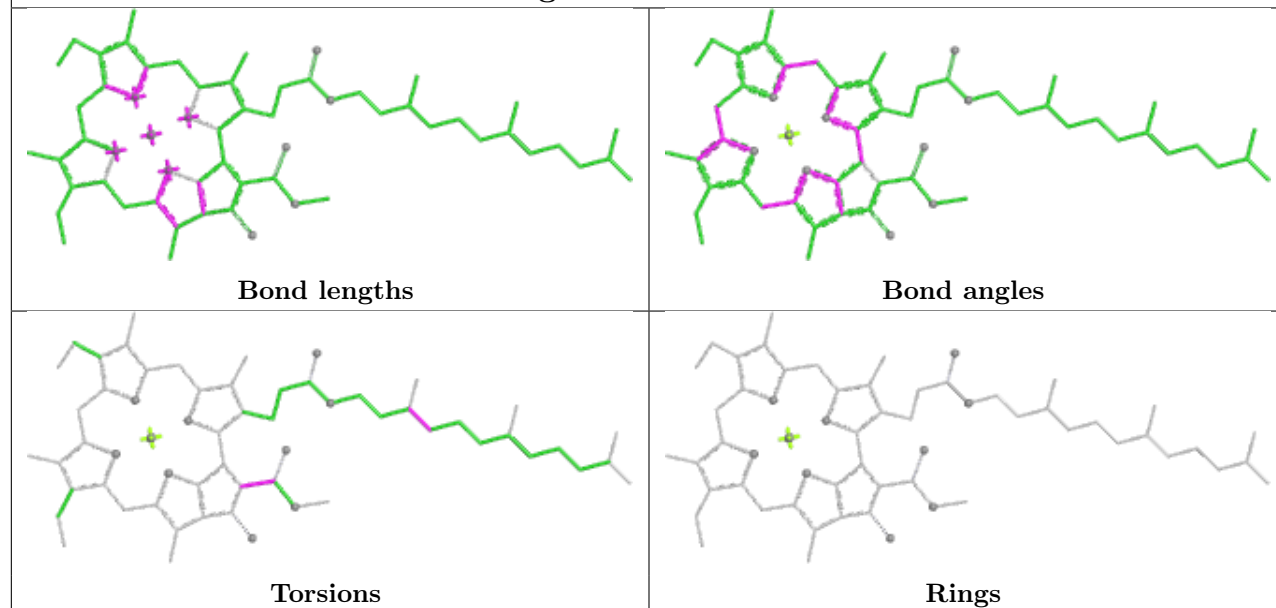
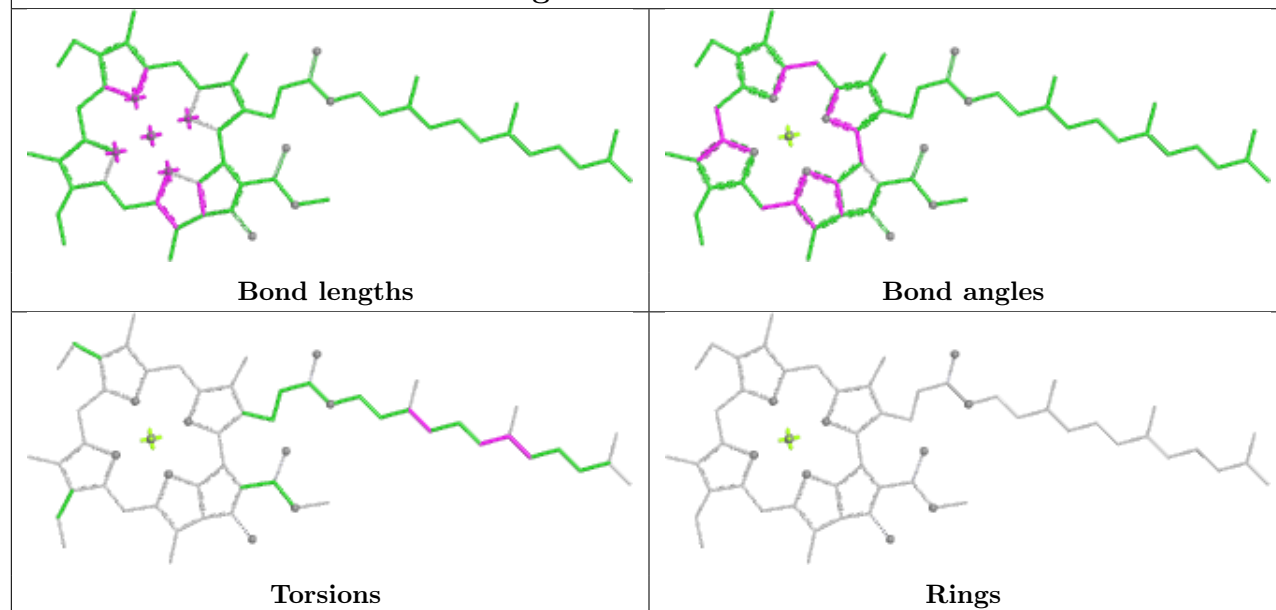


Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

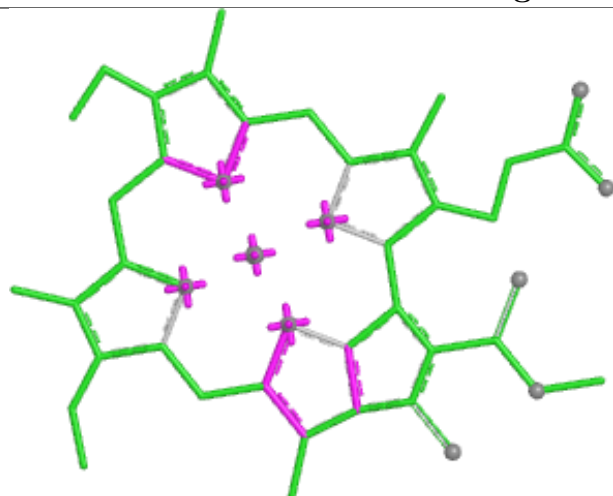
Ligand UIX H 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 1 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

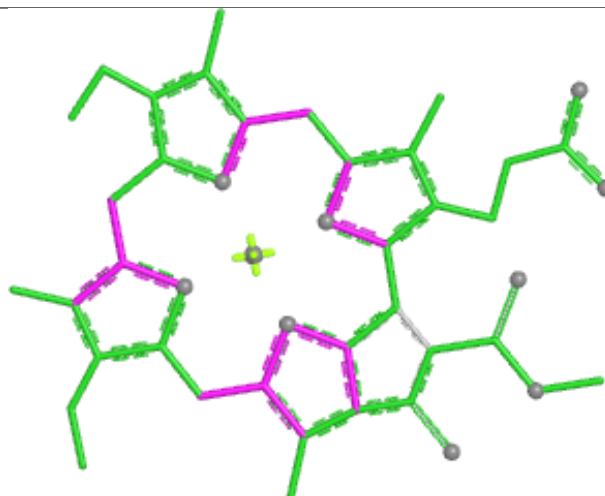


Ligand CLA I 608**Ligand CLA C 207**

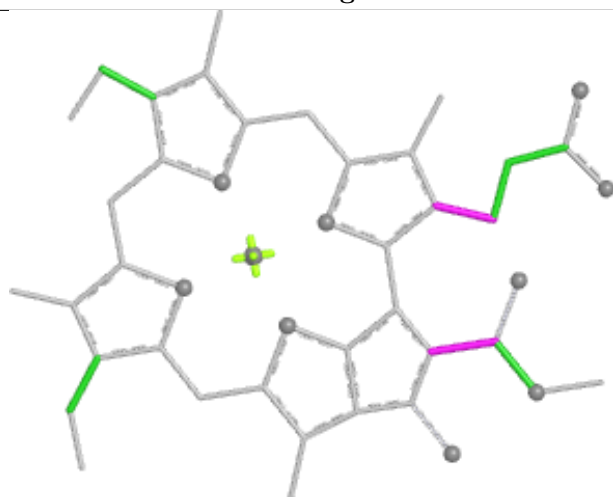
Ligand CLA A 611



Bond lengths



Bond angles

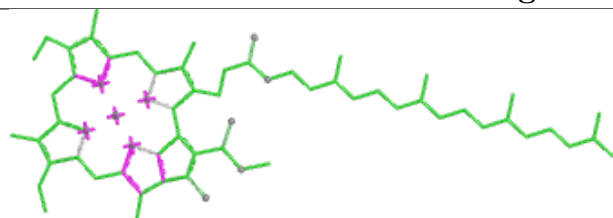


Torsions

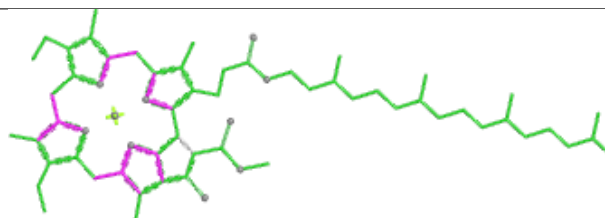


Rings

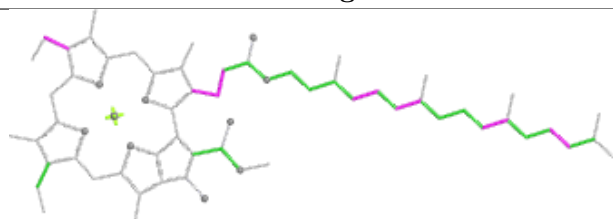
Ligand CLA a 825



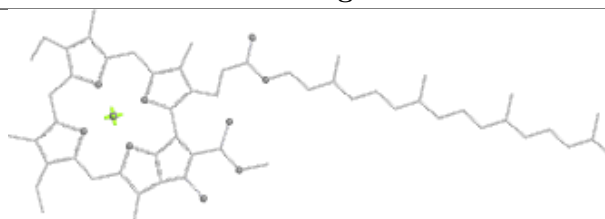
Bond lengths



Bond angles

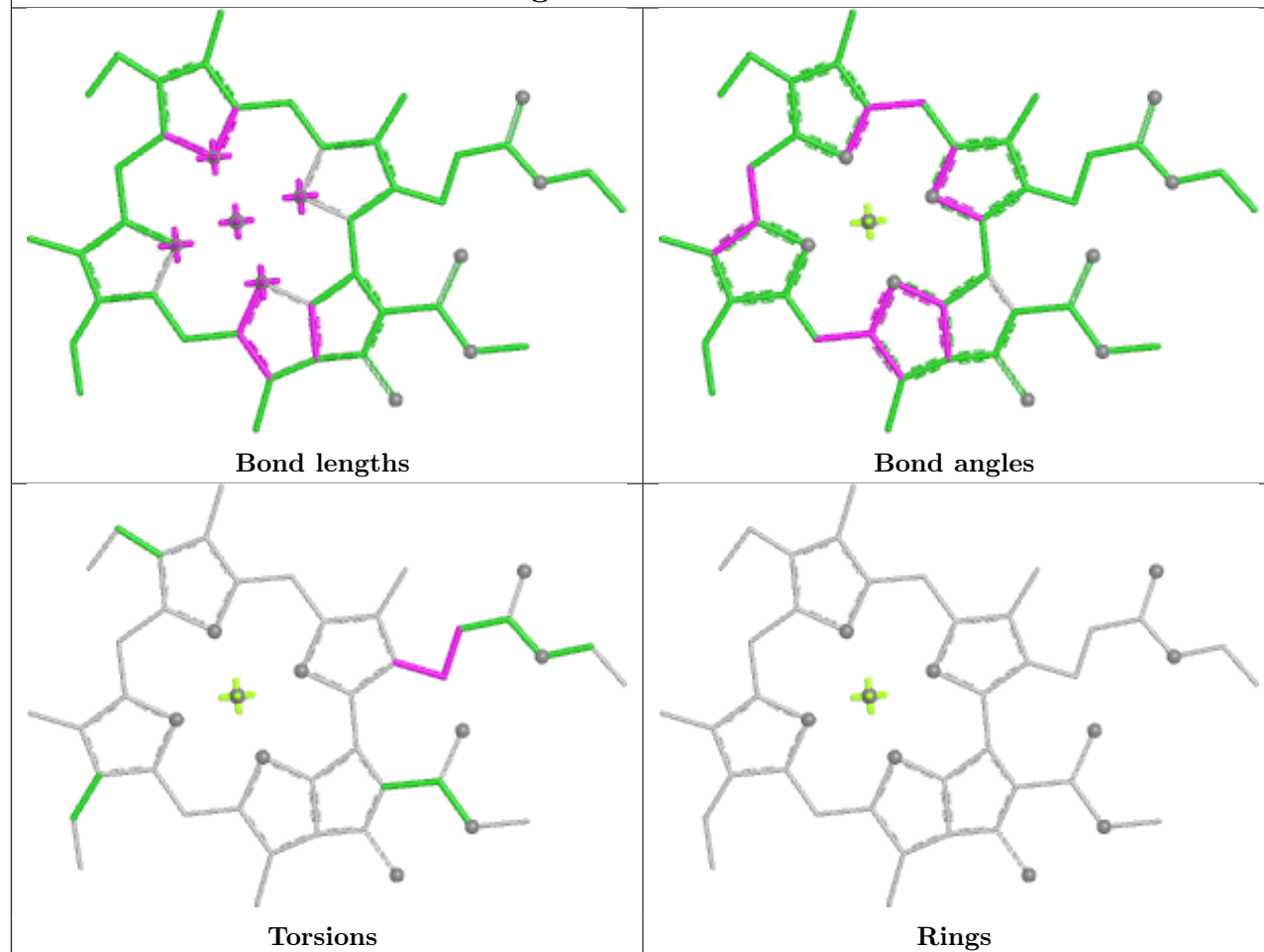


Torsions

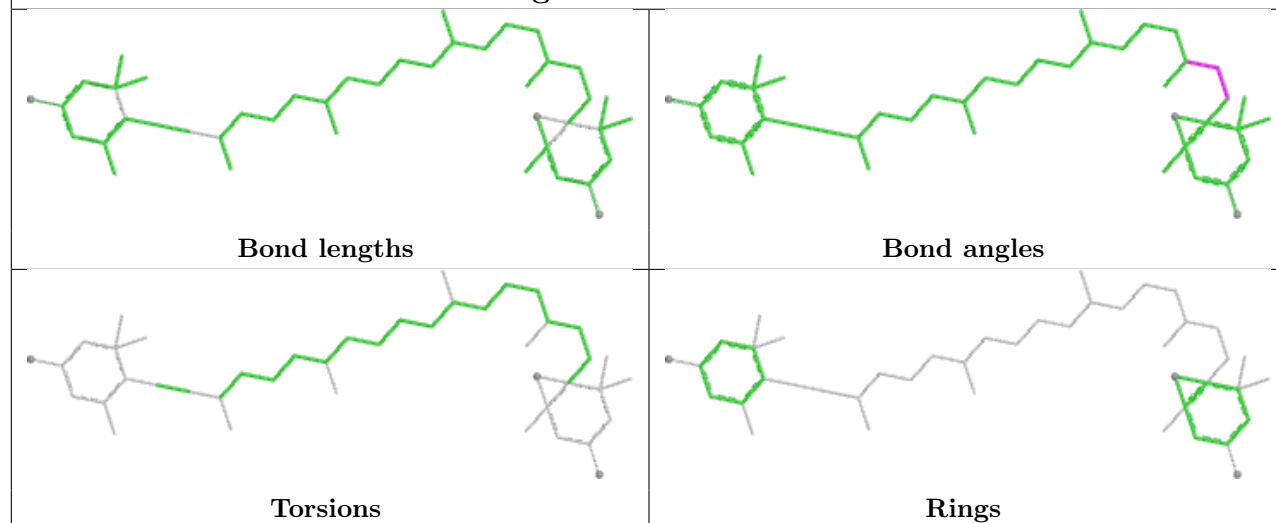


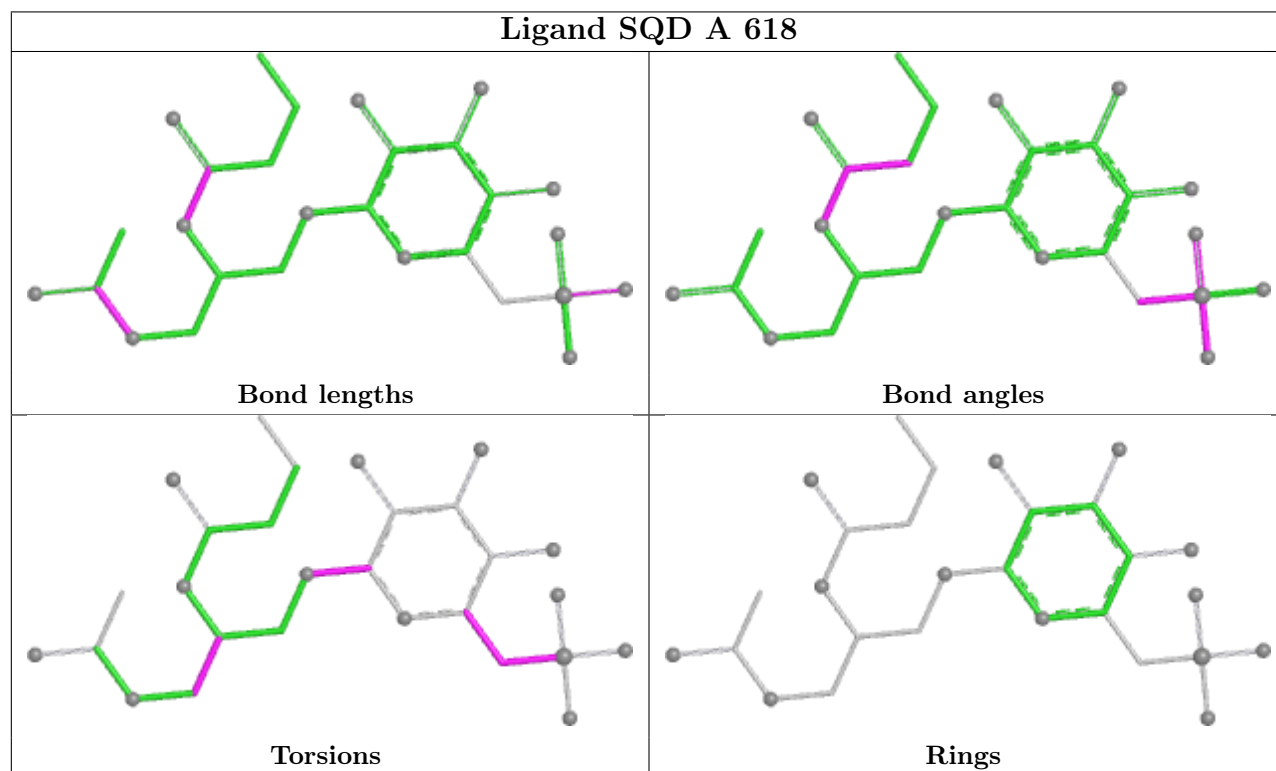
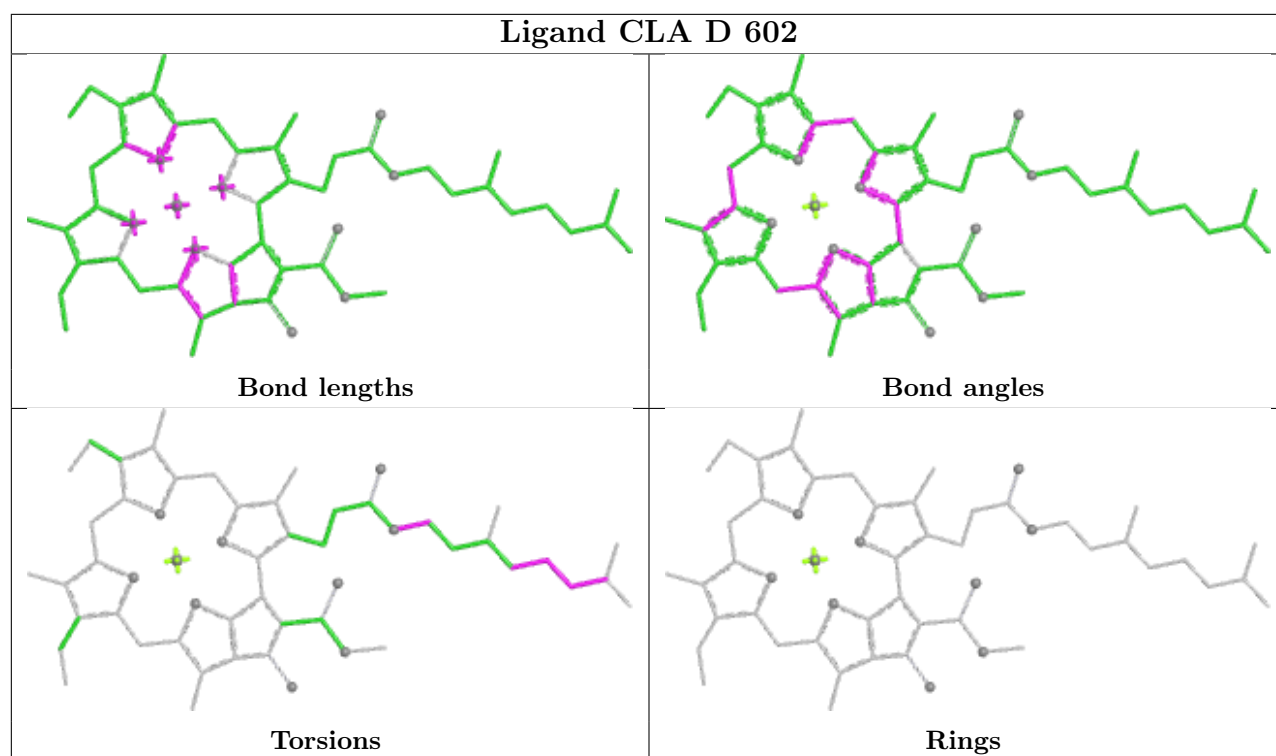
Rings

Ligand CLA a 809

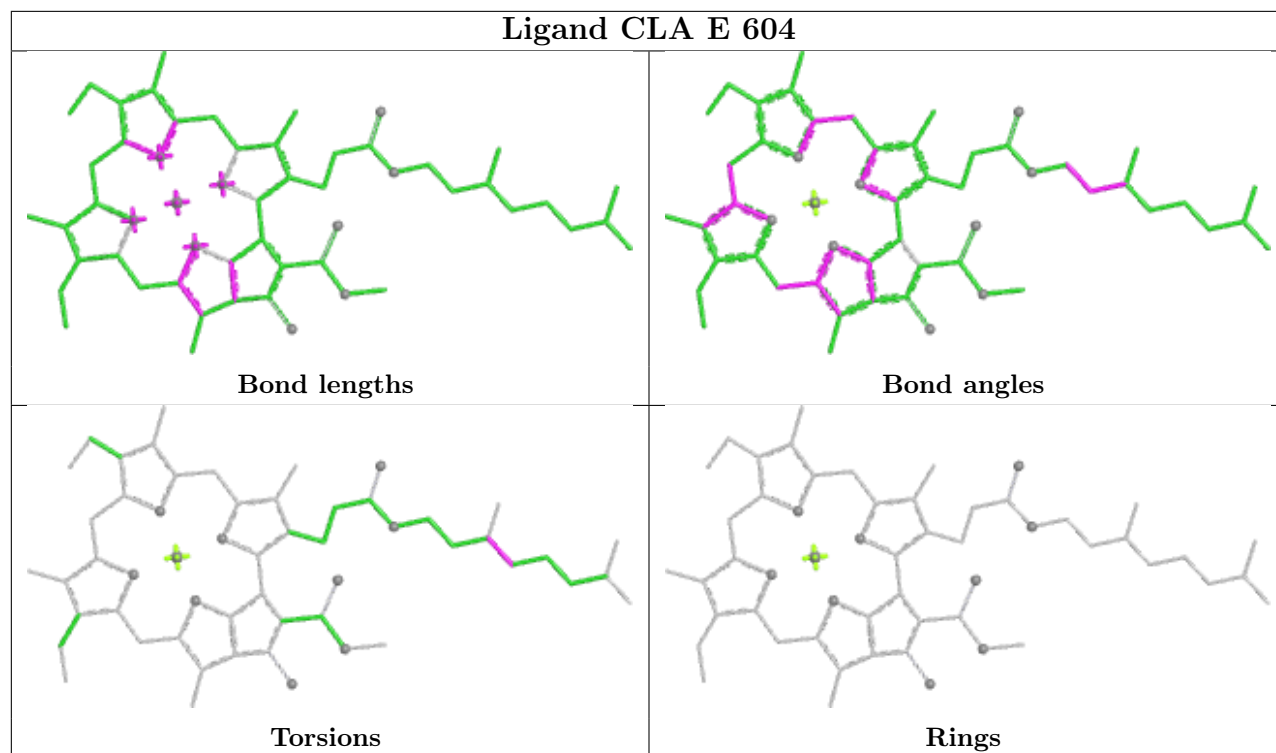


Ligand DD6 U 607

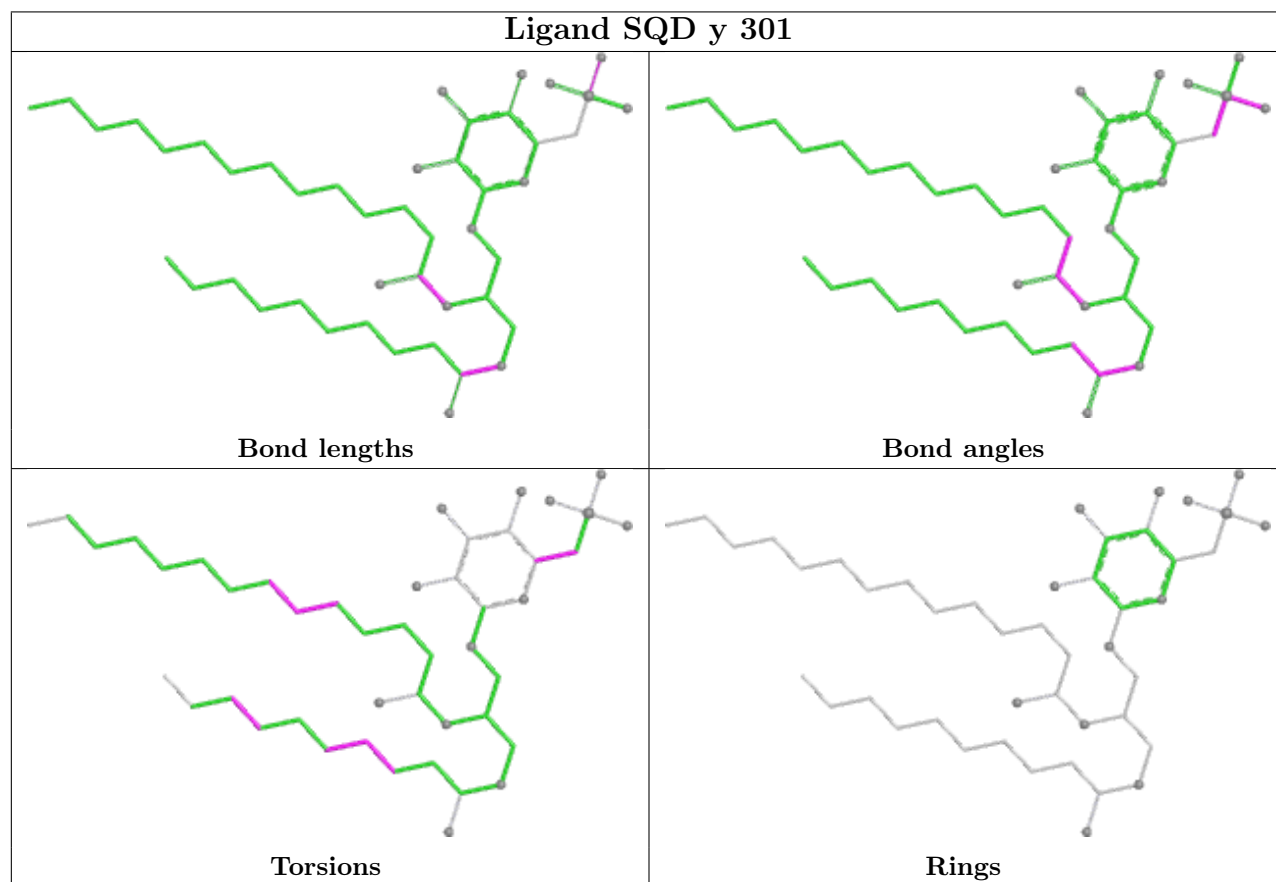




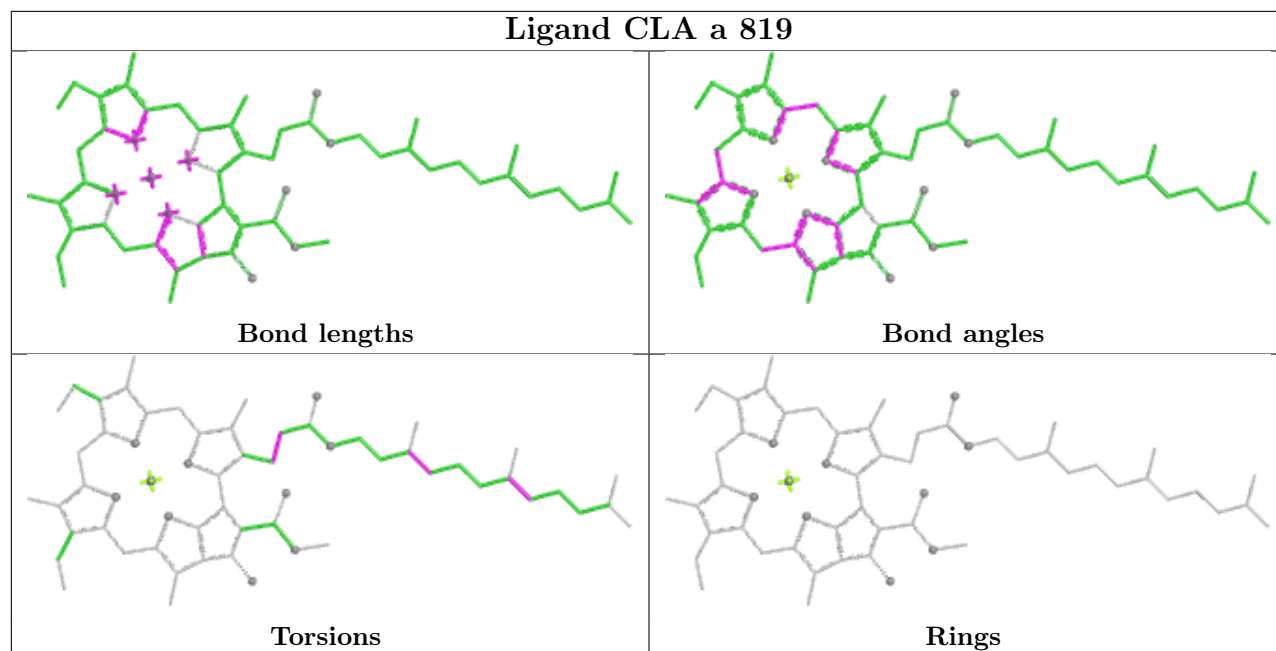
Ligand CLA E 604



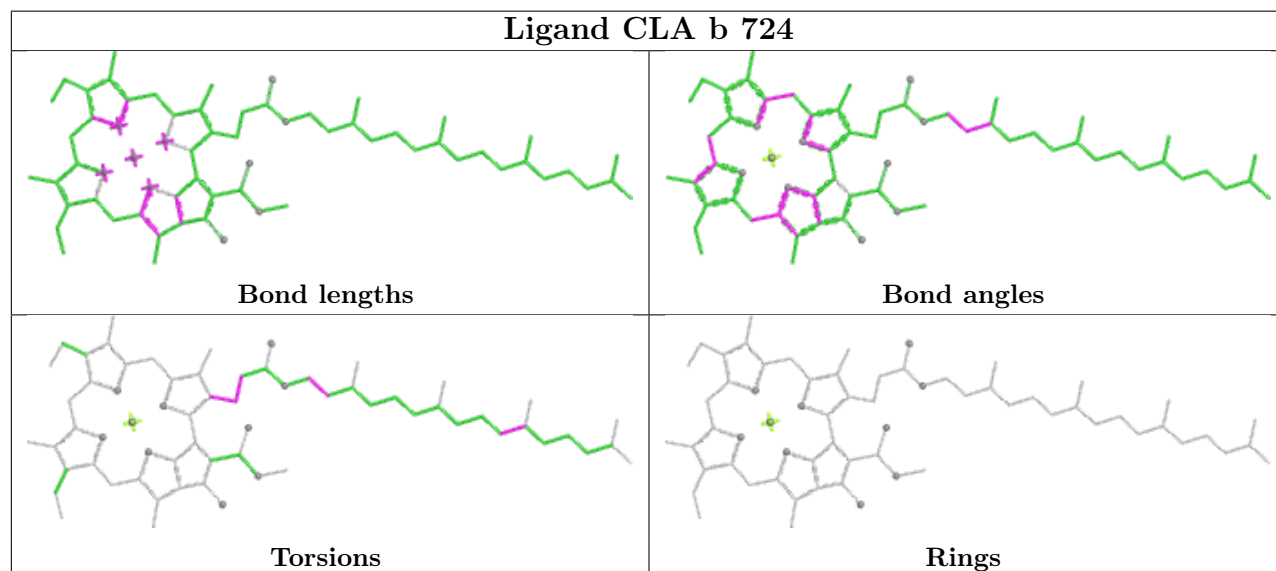
Ligand SQD y 301

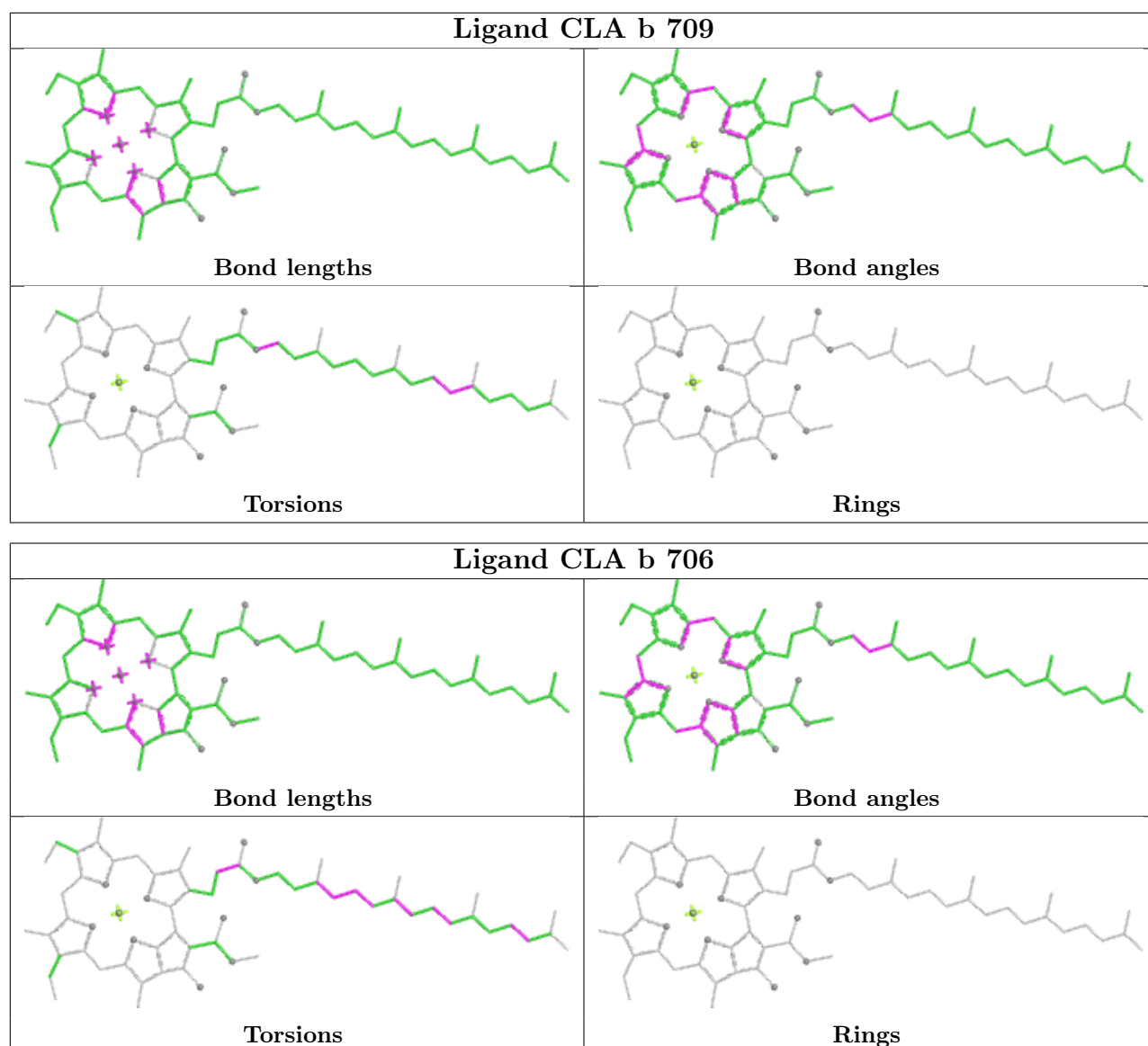


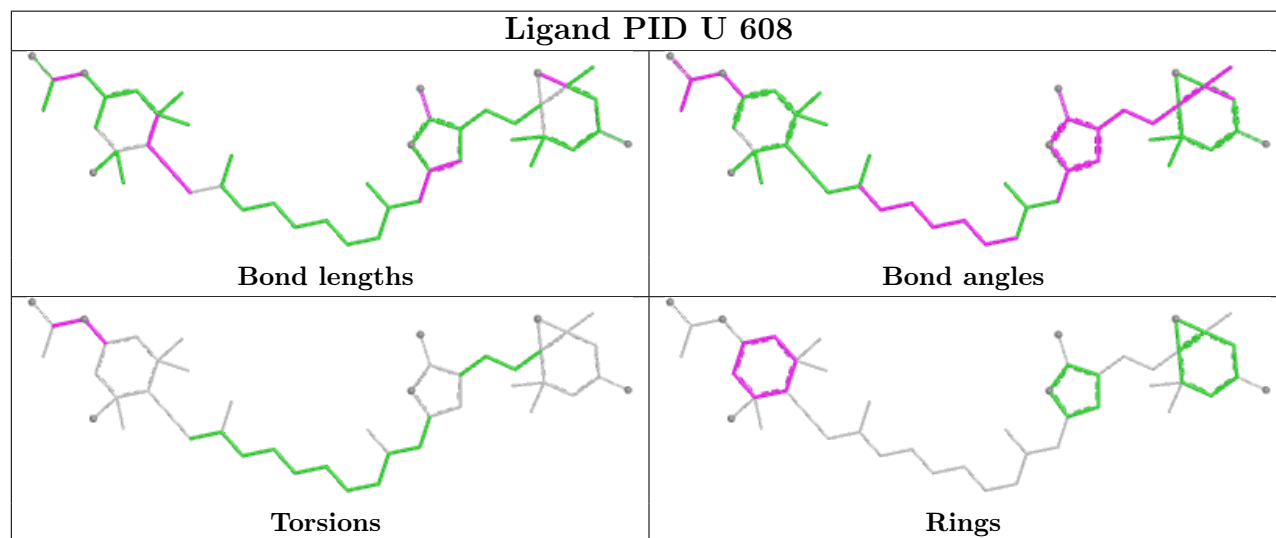
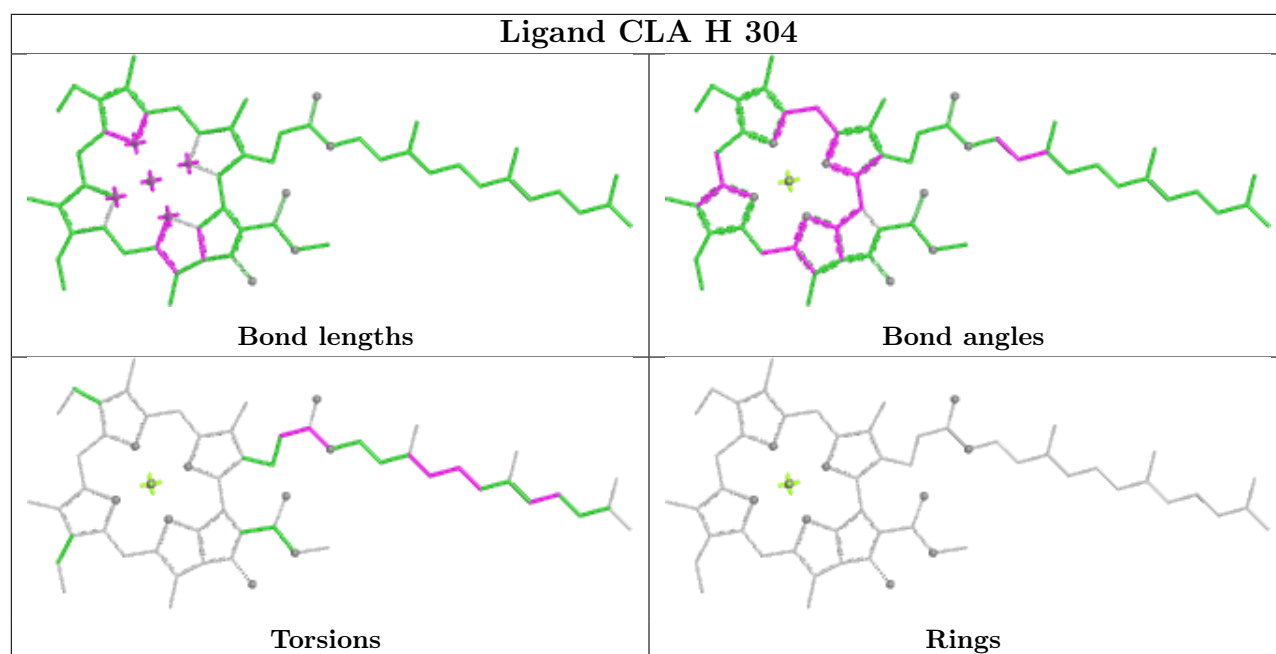
Ligand CLA a 819



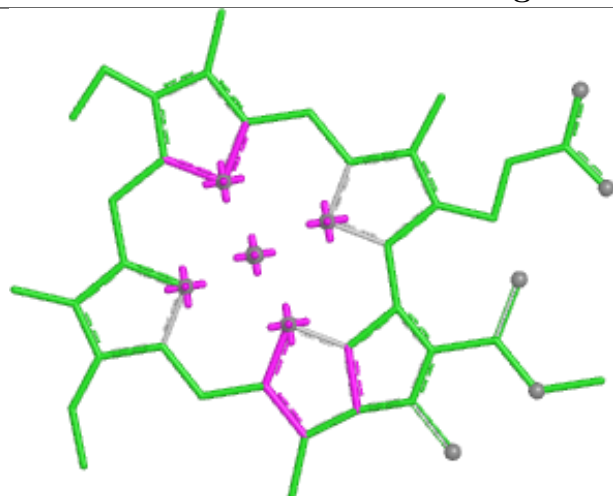
Ligand CLA b 724



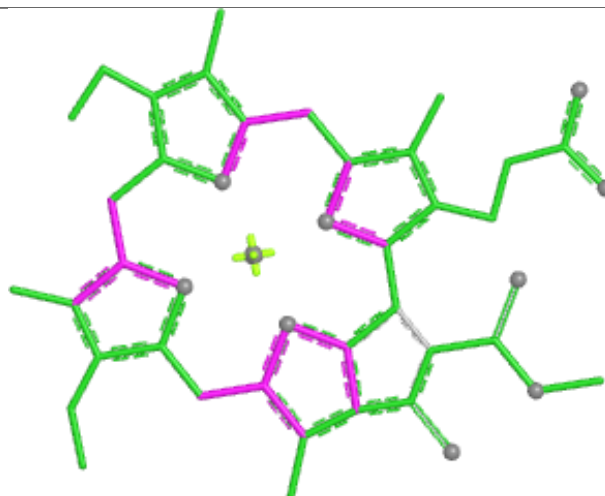




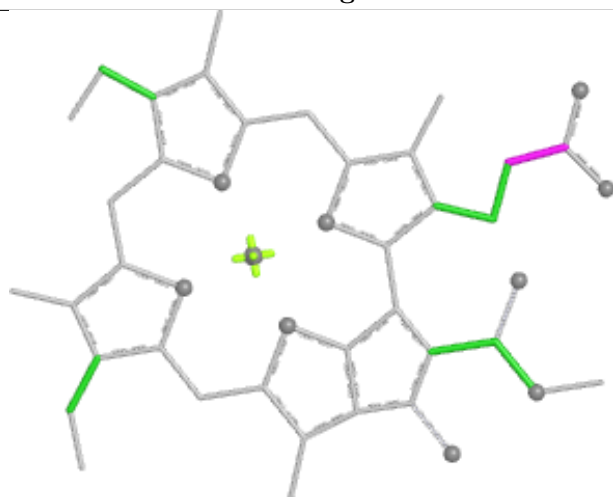
Ligand CLA D 609



Bond lengths



Bond angles

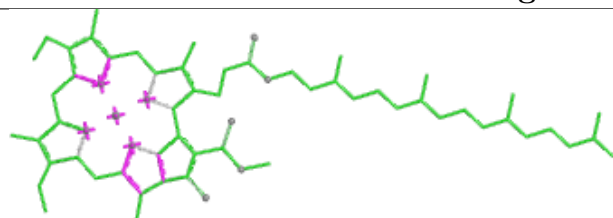


Torsions

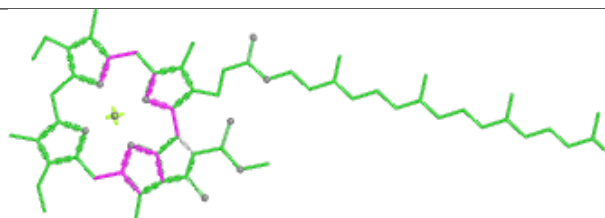


Rings

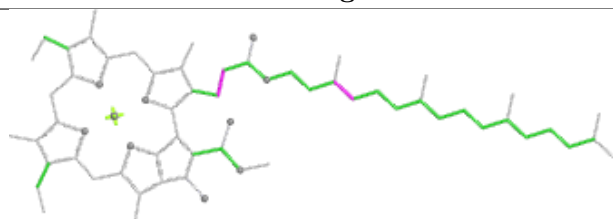
Ligand CLA a 837



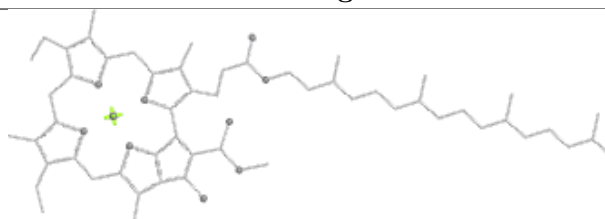
Bond lengths



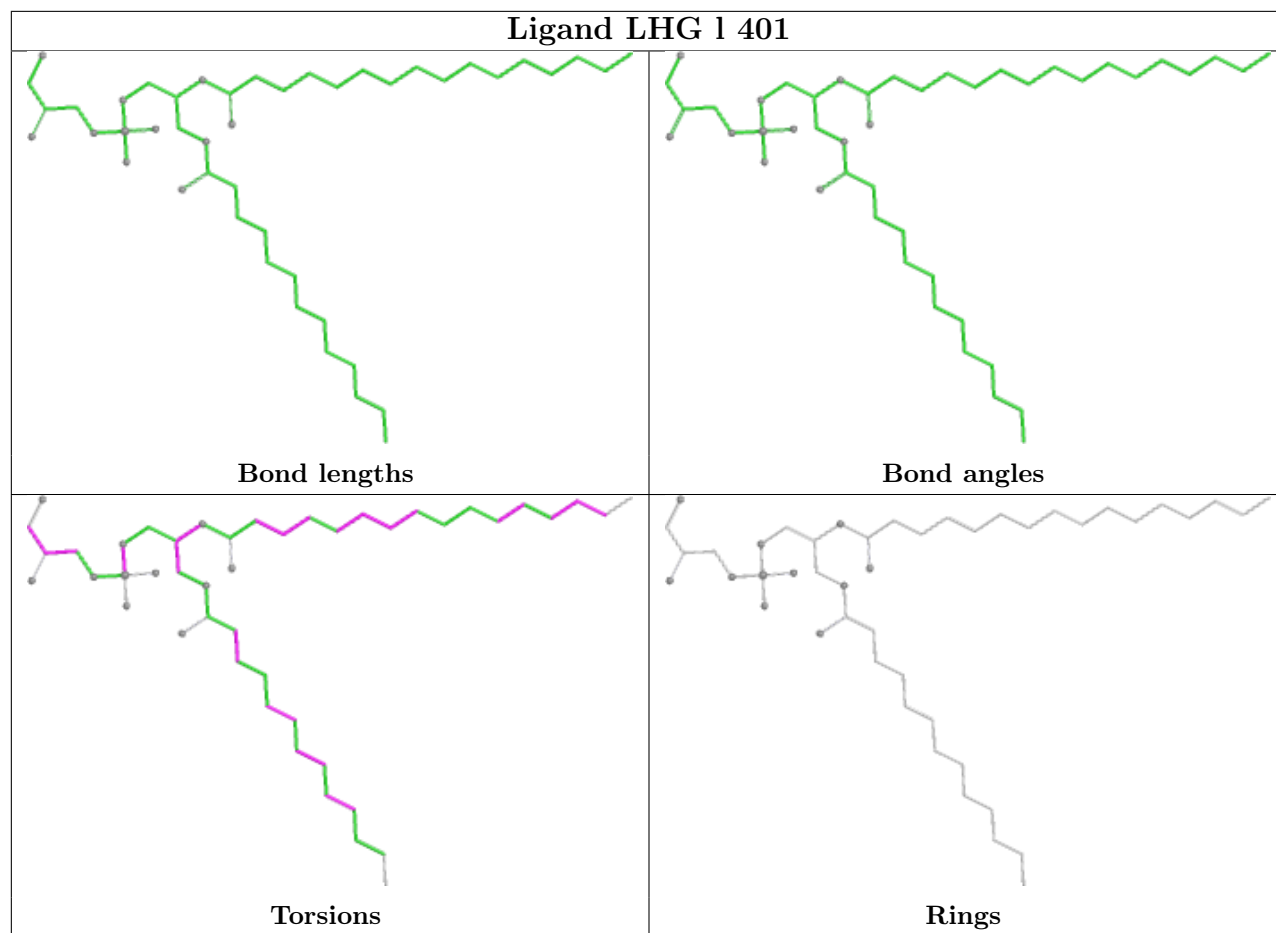
Bond angles

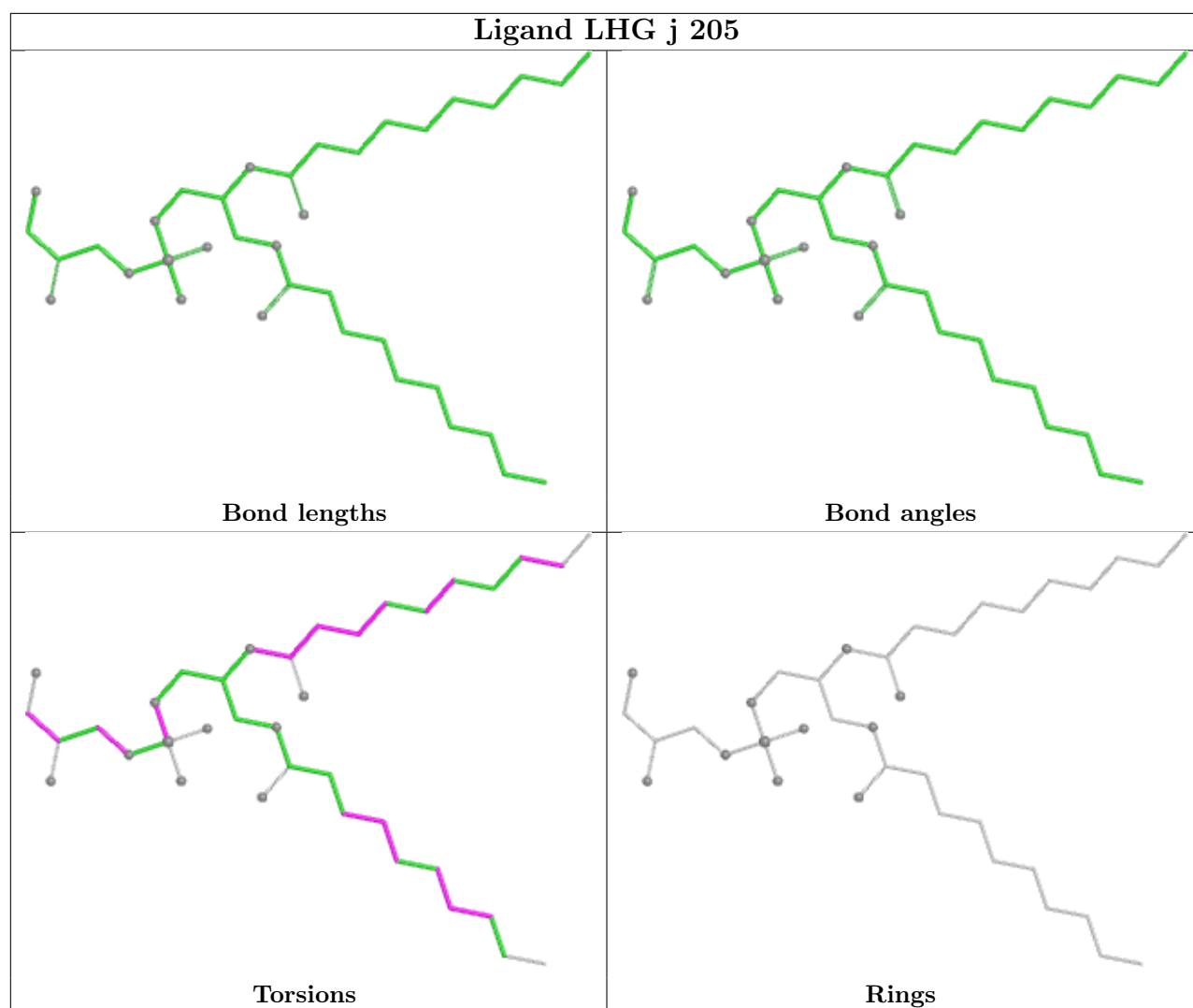


Torsions

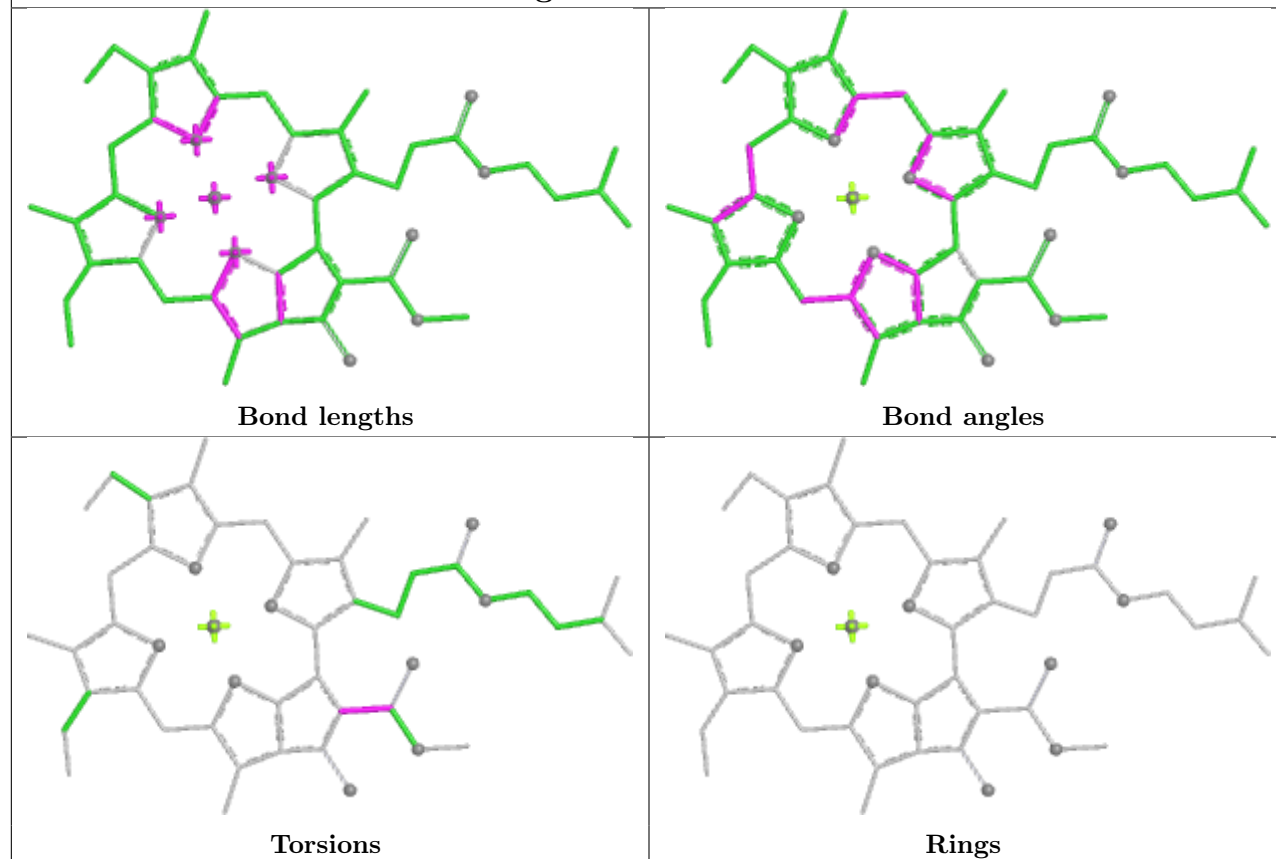


Rings





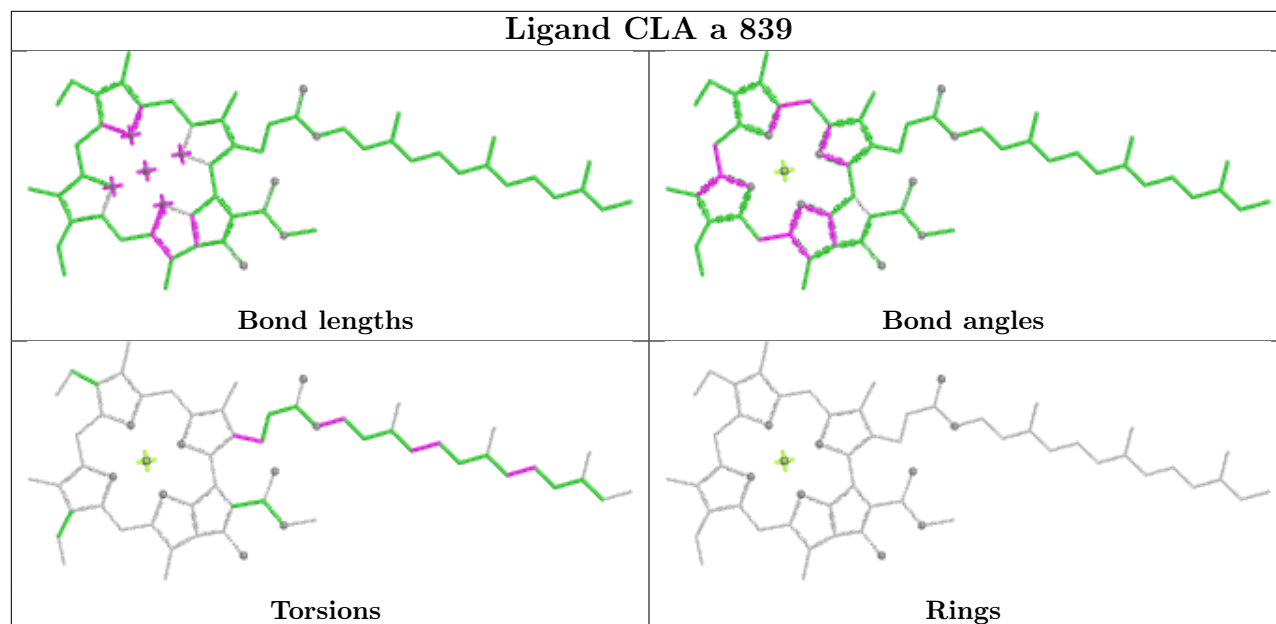
Ligand CLA b 721



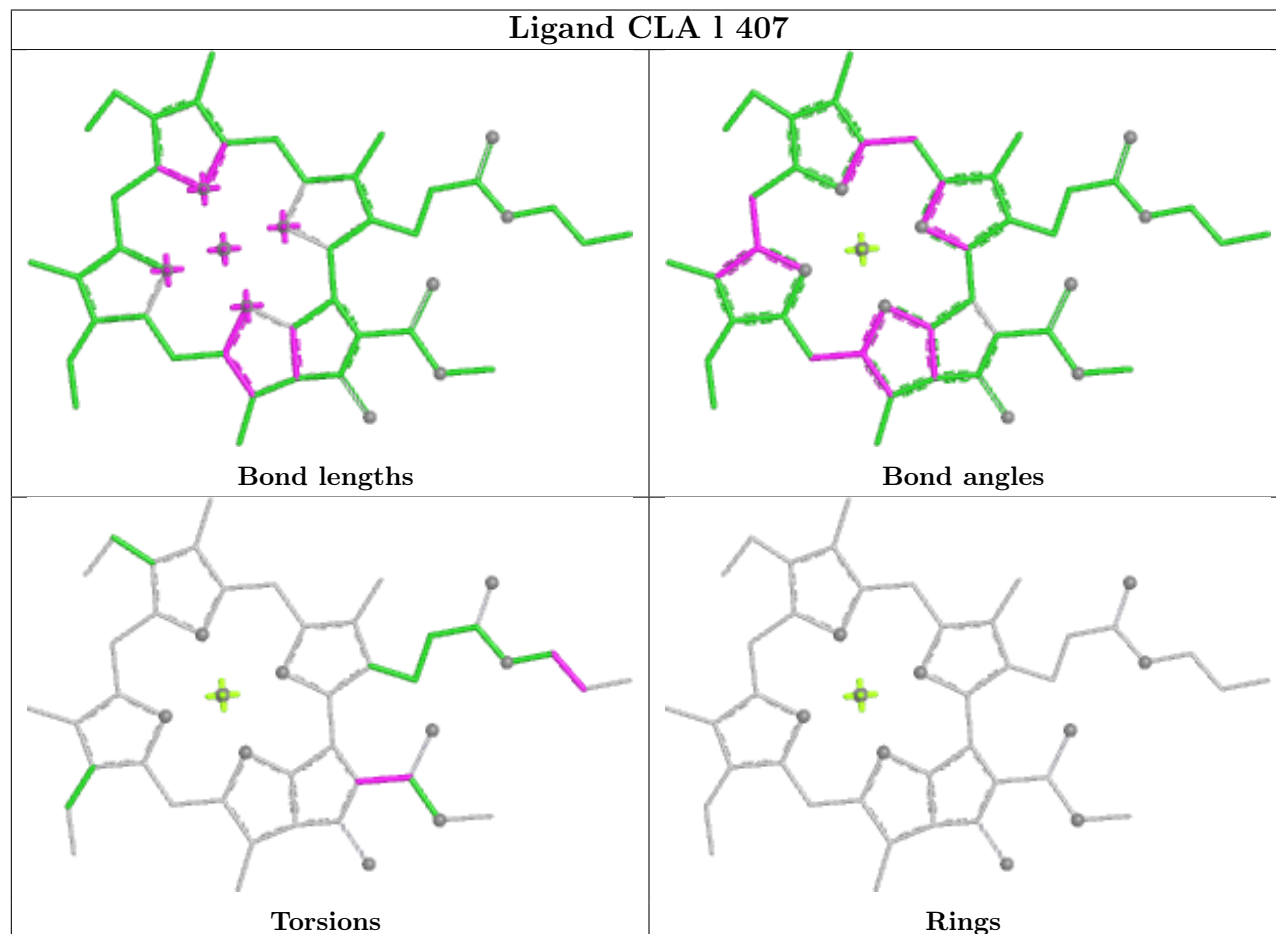
Ligand LMG 1 417



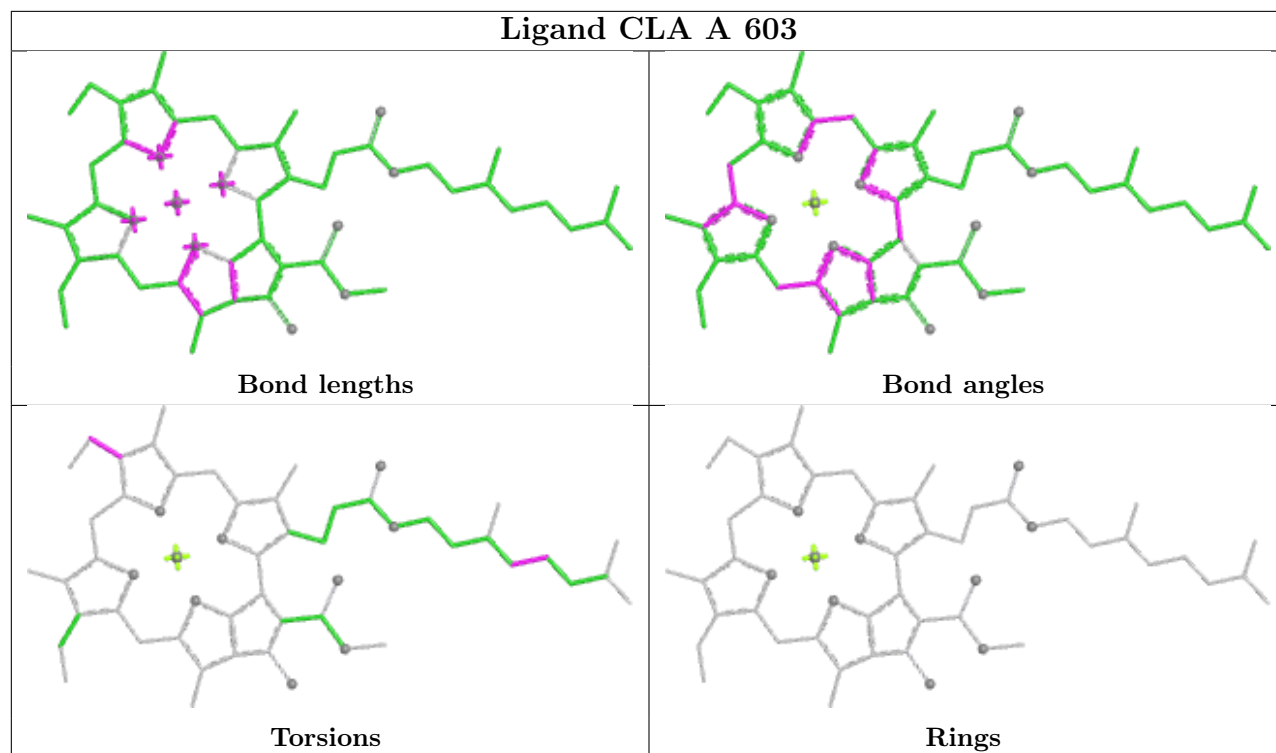
Ligand CLA a 839



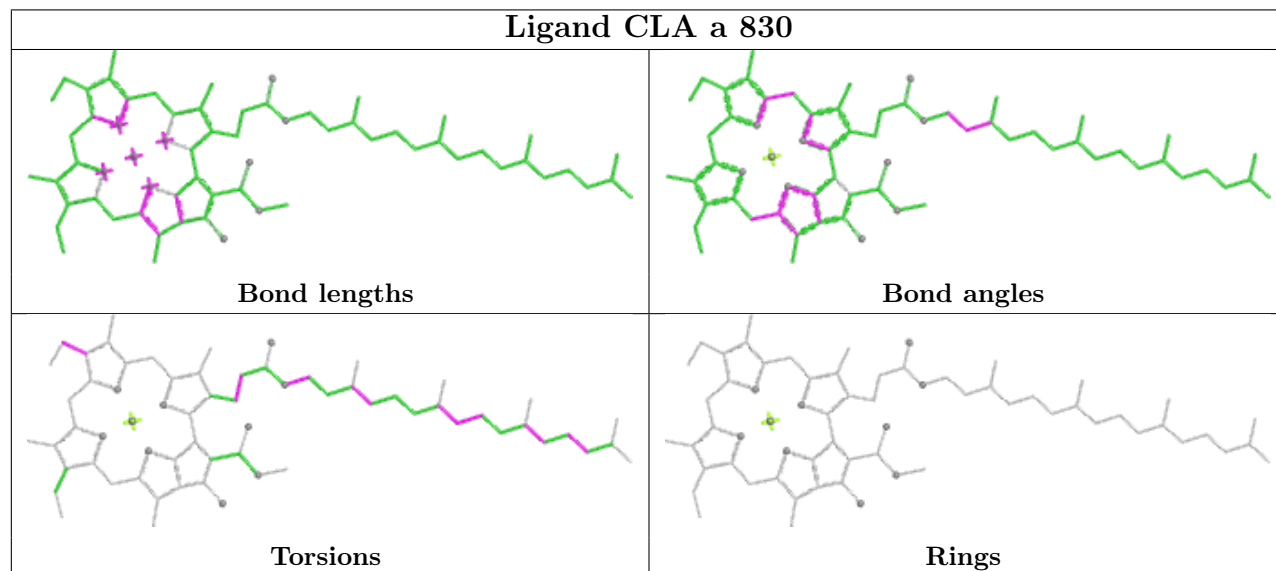
Ligand CLA l 407

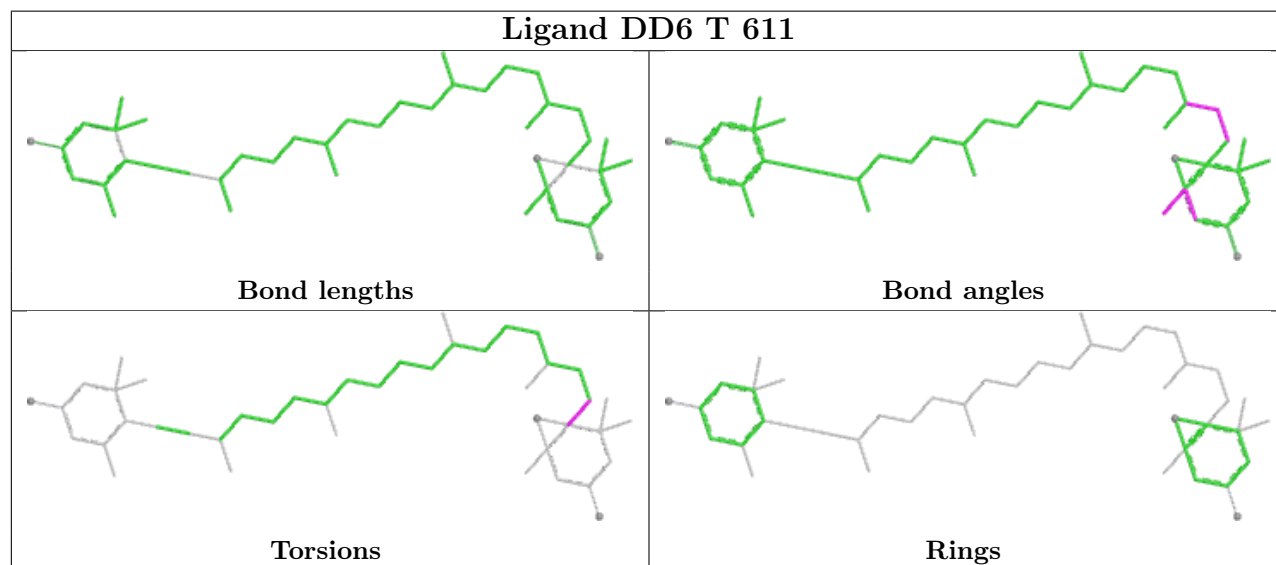
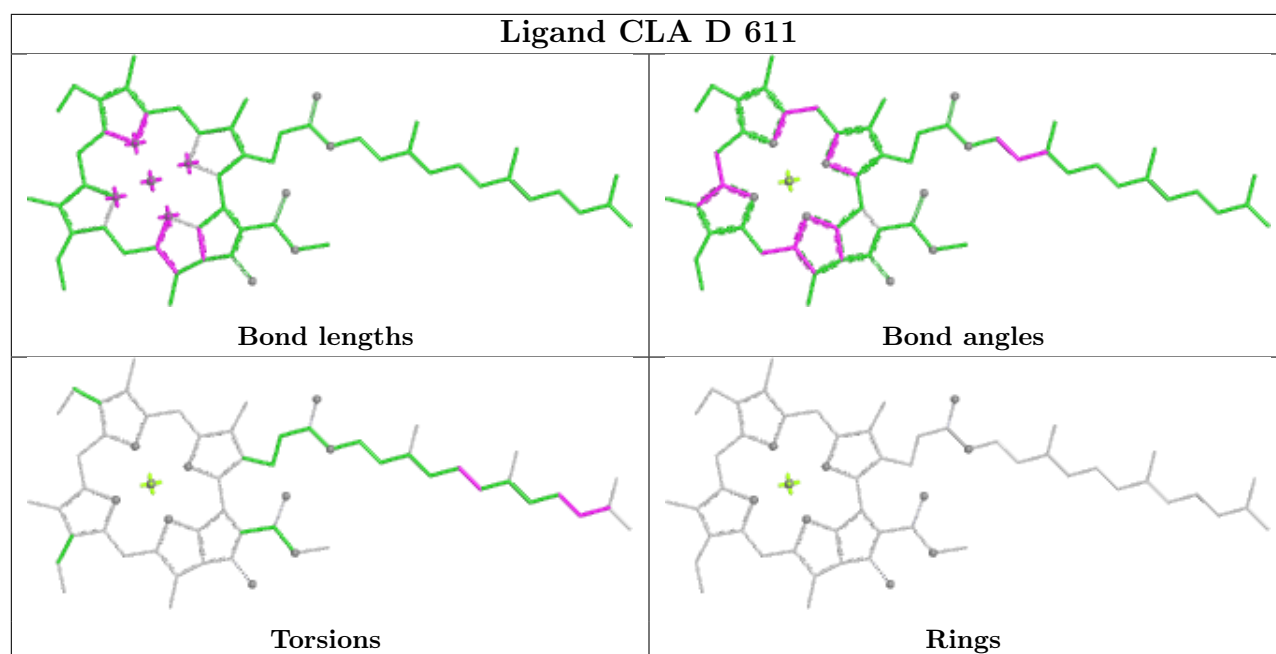


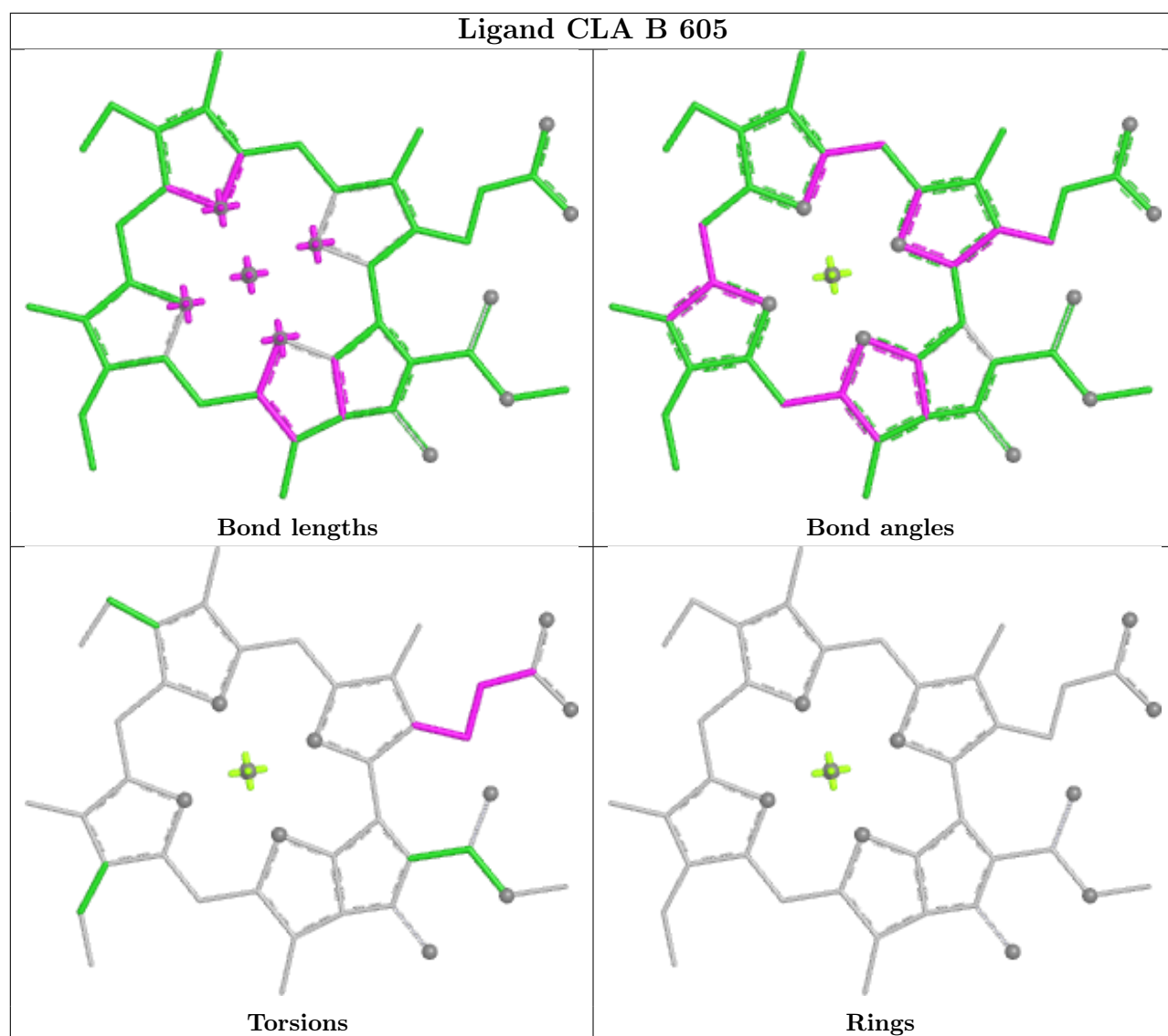
Ligand CLA A 603



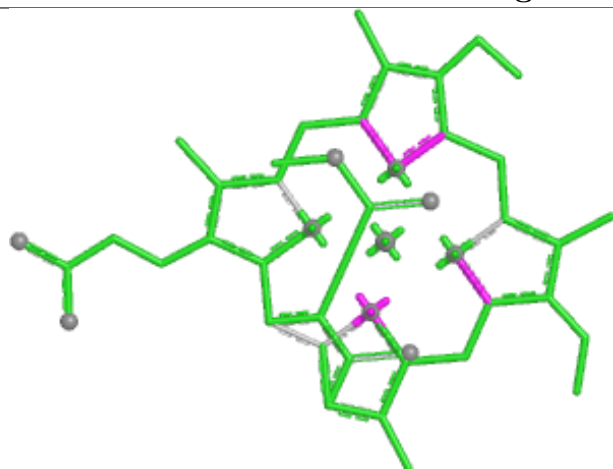
Ligand CLA a 830



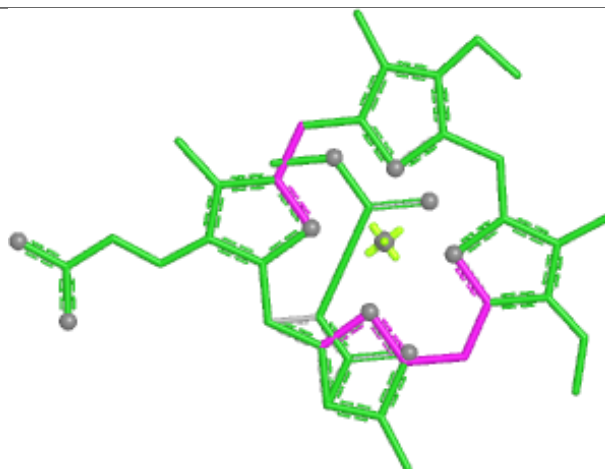




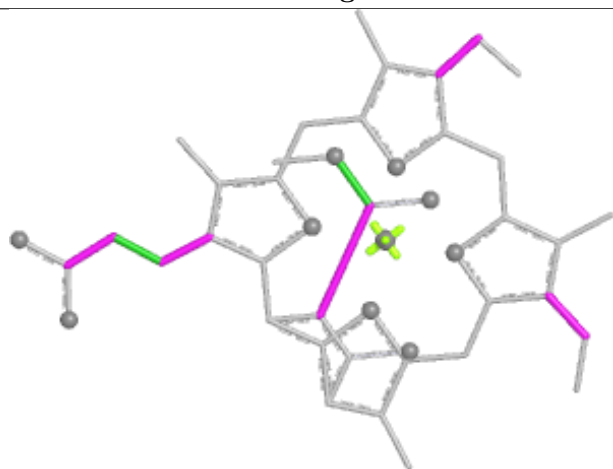
Ligand KC2 H 311



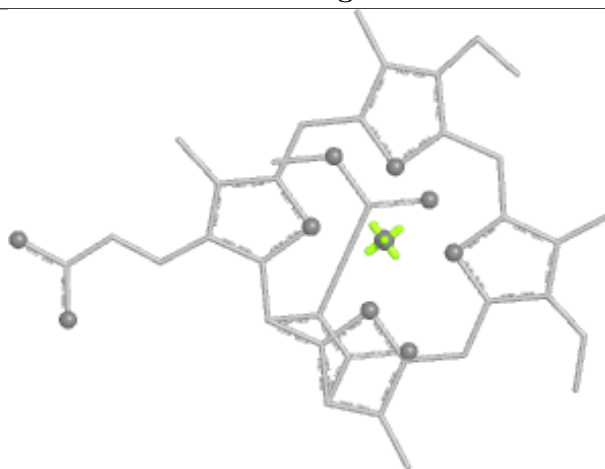
Bond lengths



Bond angles

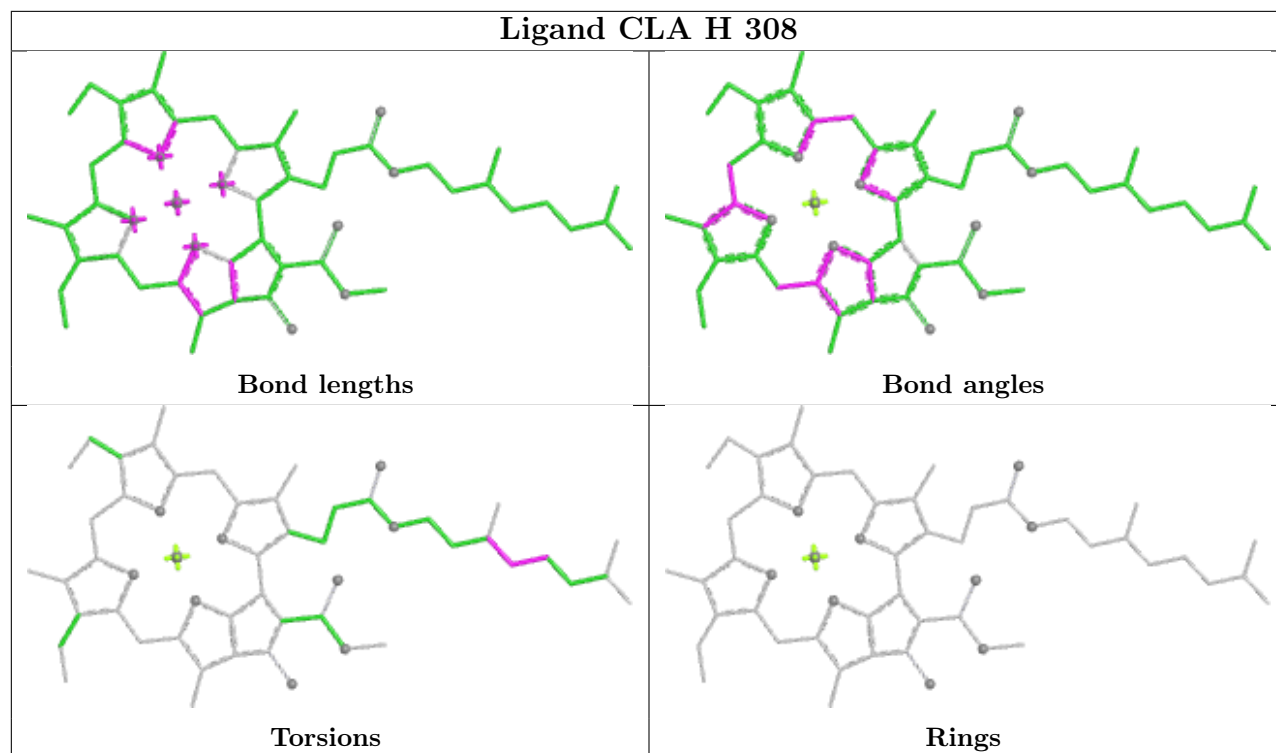


Torsions

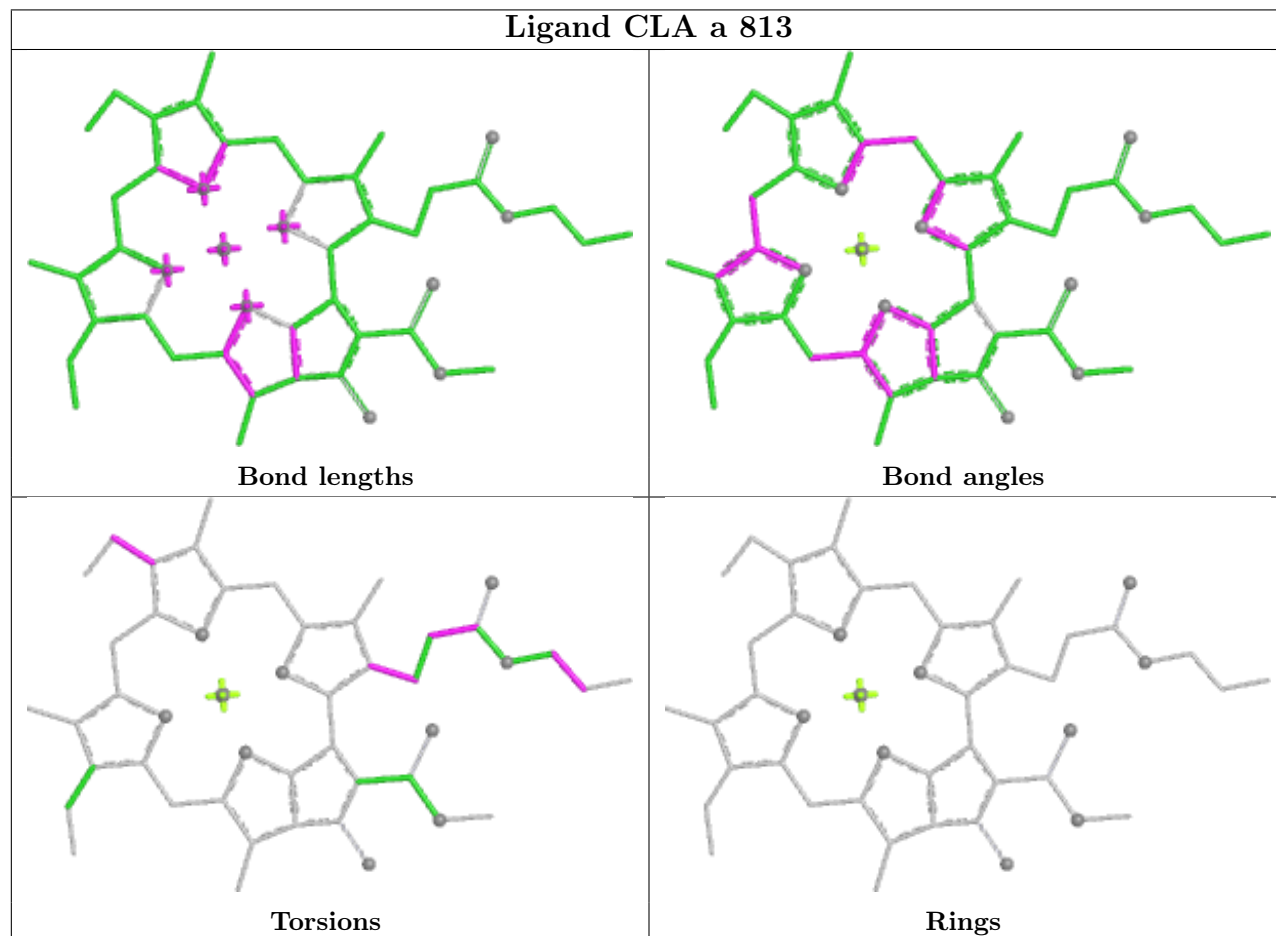


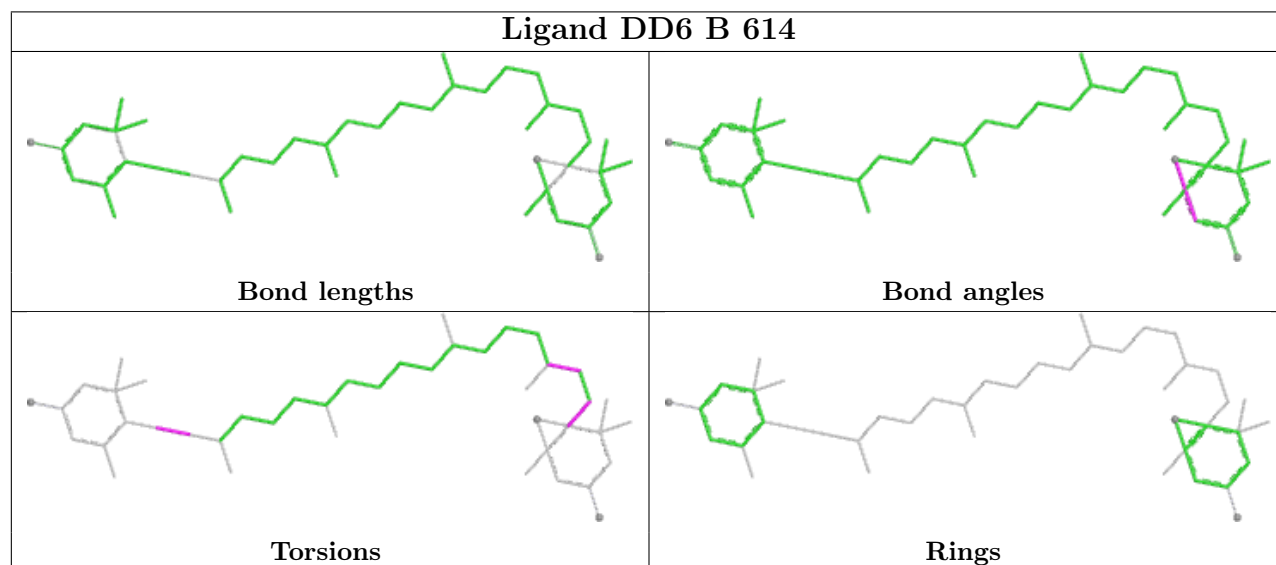
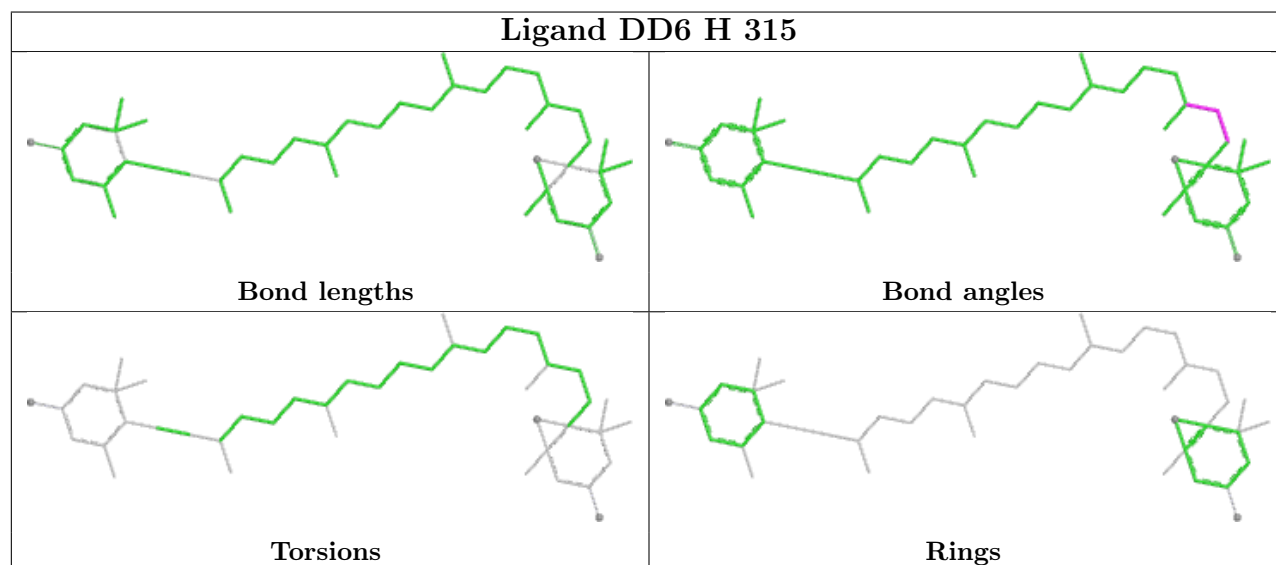
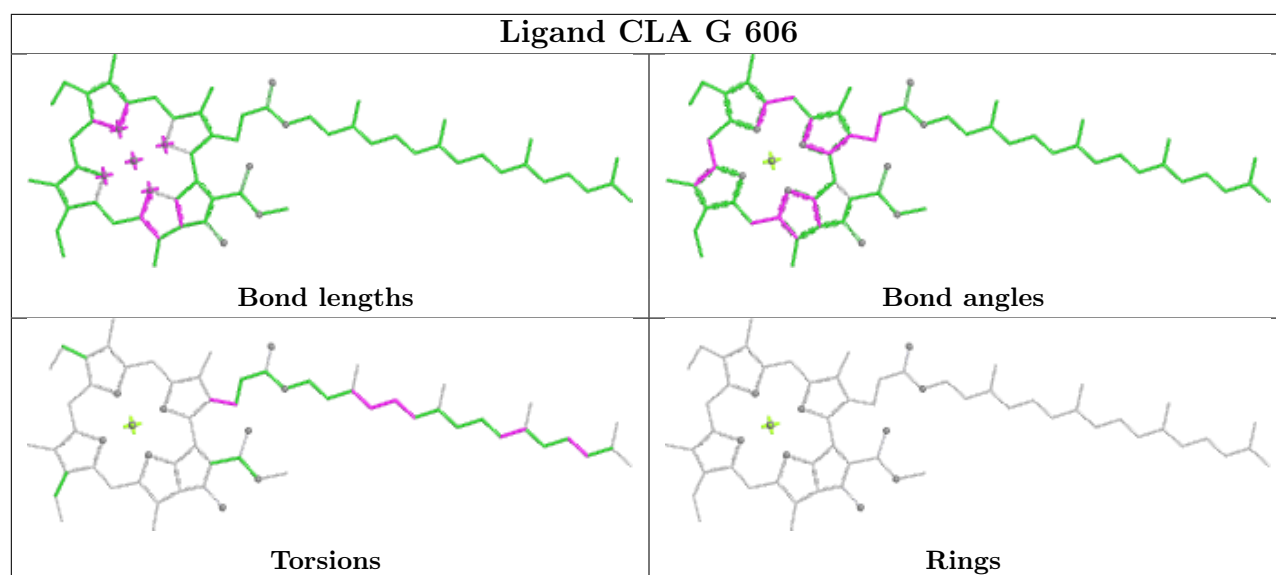
Rings

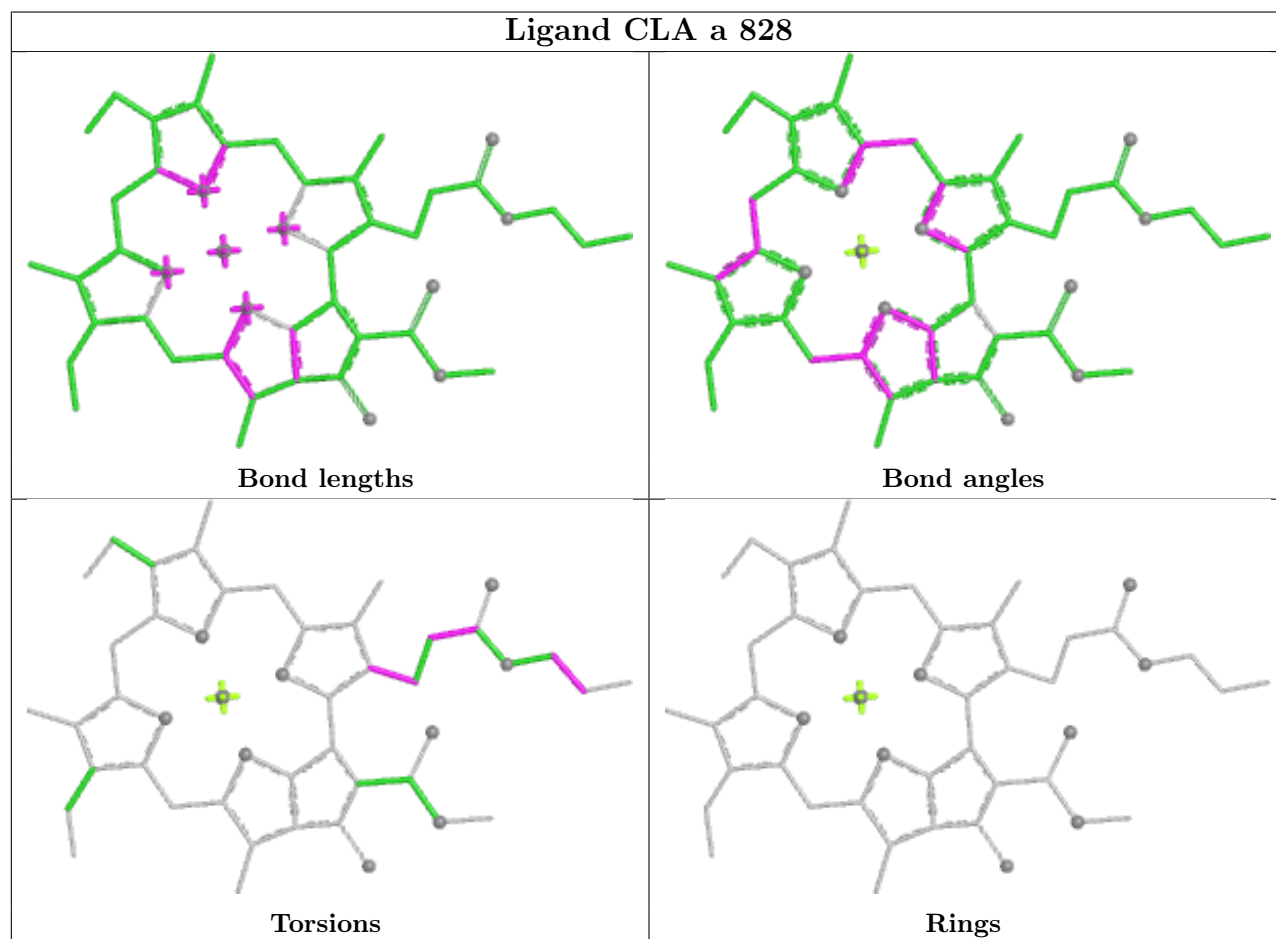
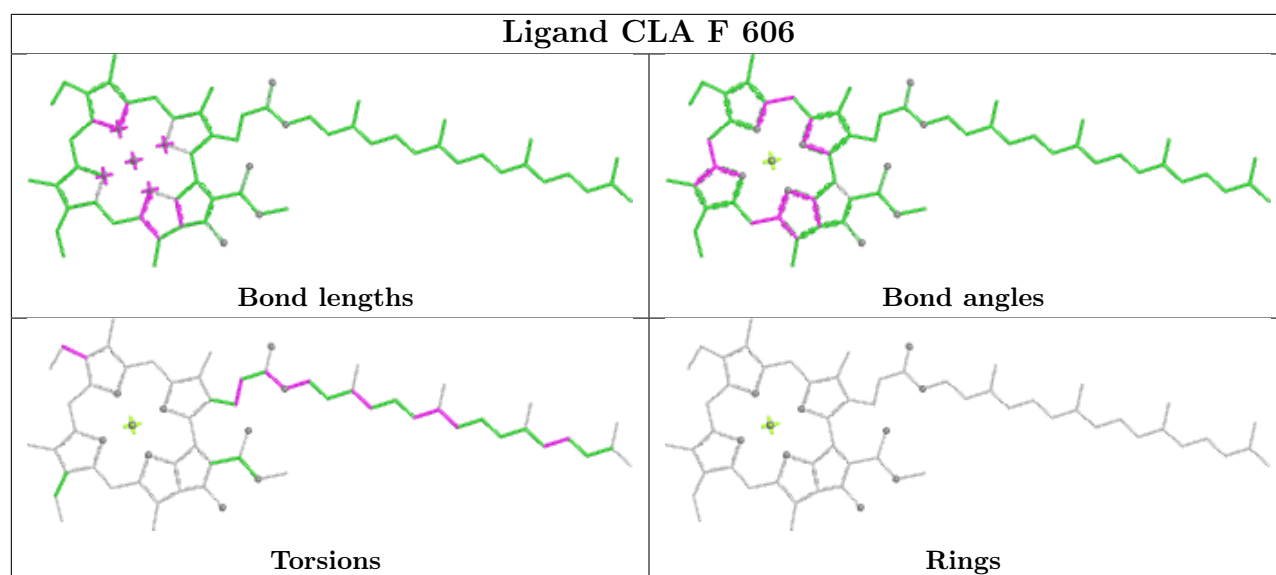
Ligand CLA H 308



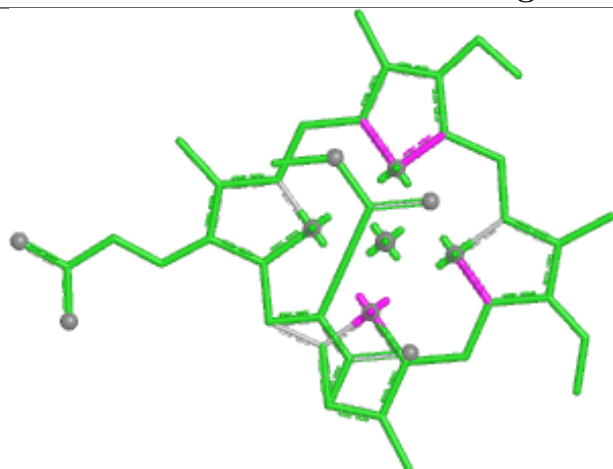
Ligand CLA a 813



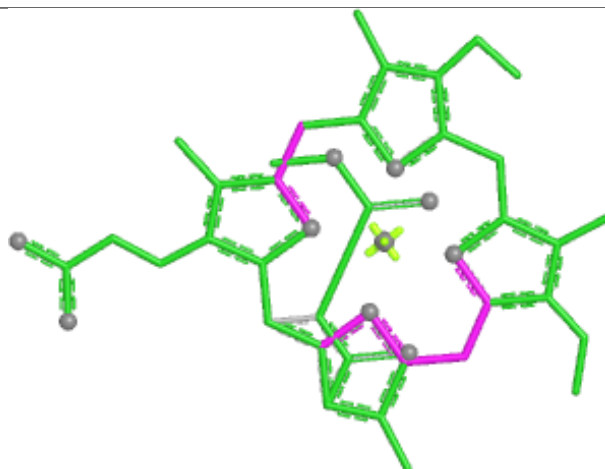




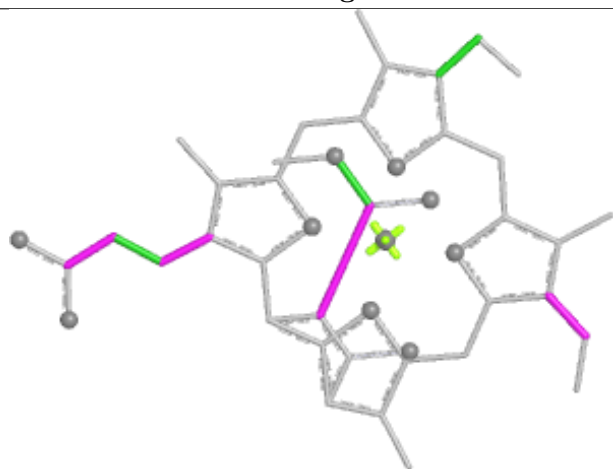
Ligand KC2 E 610



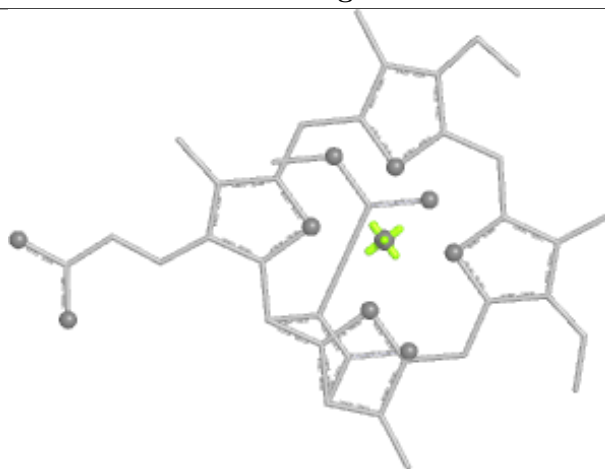
Bond lengths



Bond angles

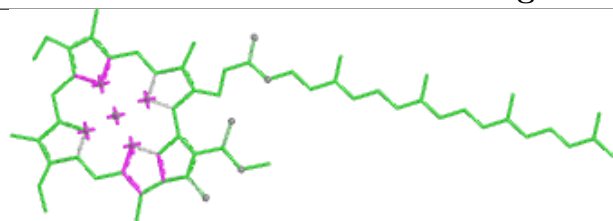


Torsions

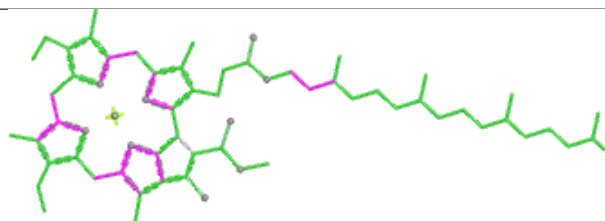


Rings

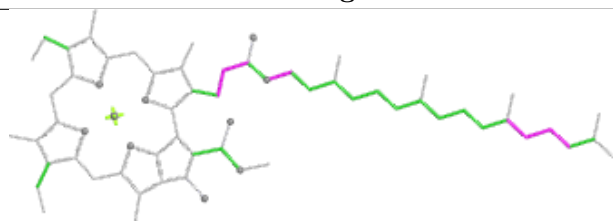
Ligand CLA b 728



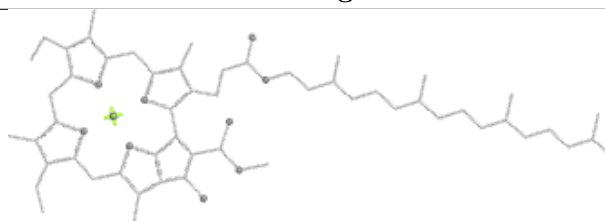
Bond lengths



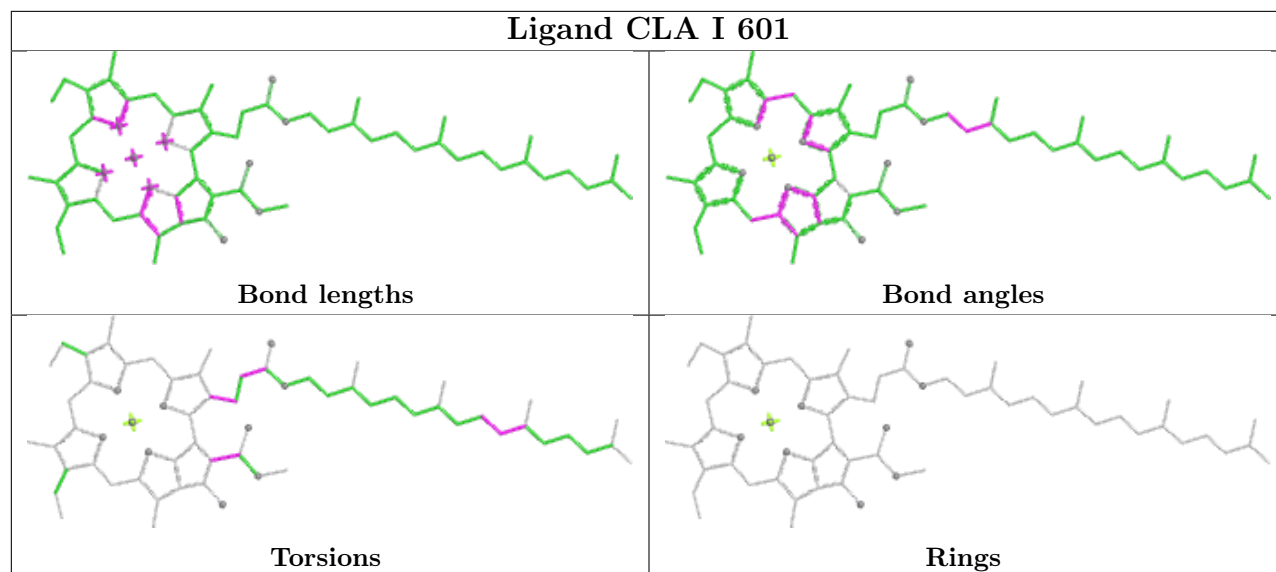
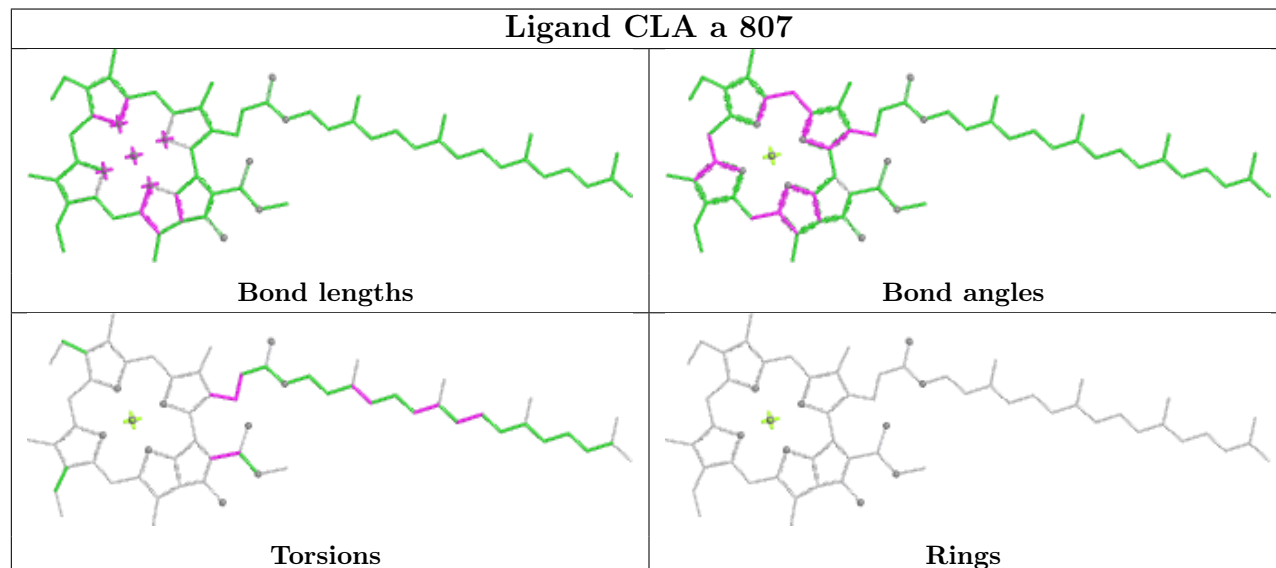
Bond angles



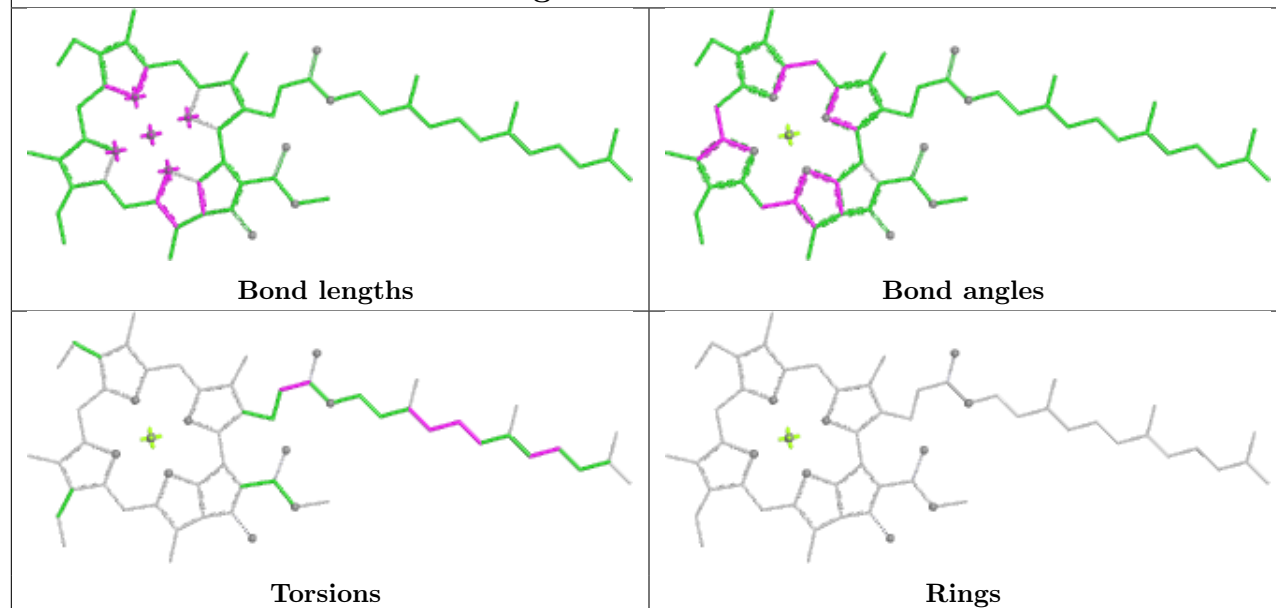
Torsions



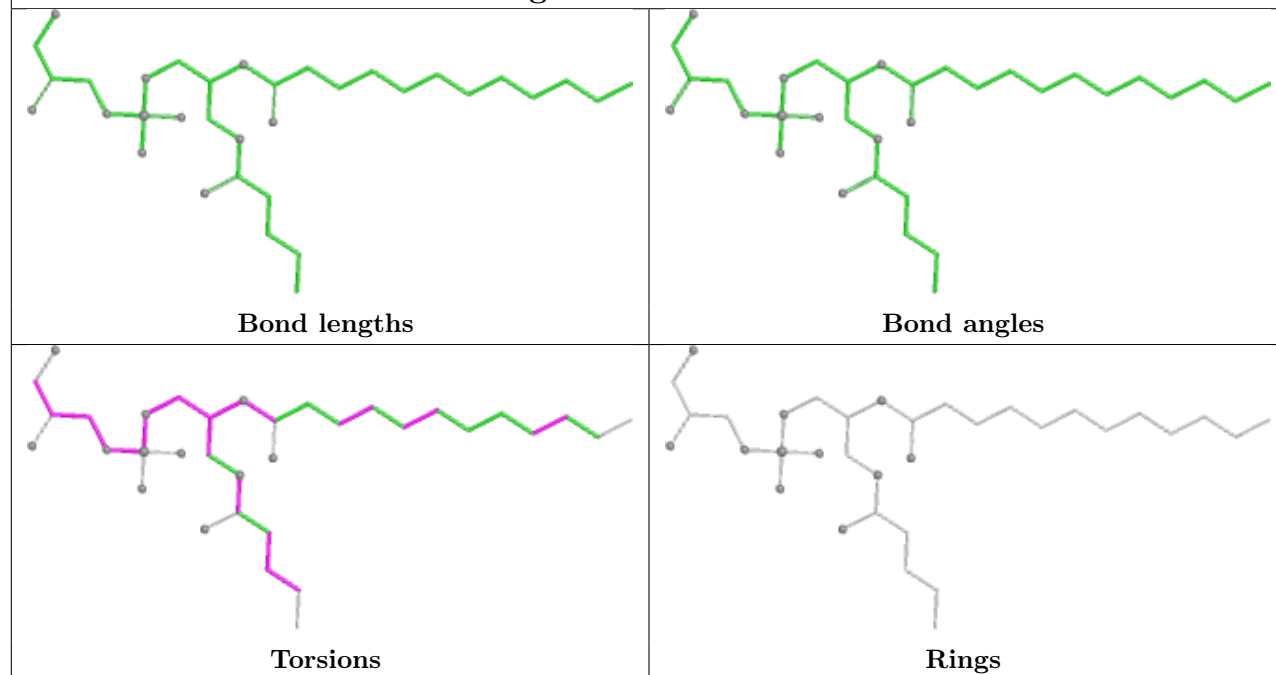
Rings

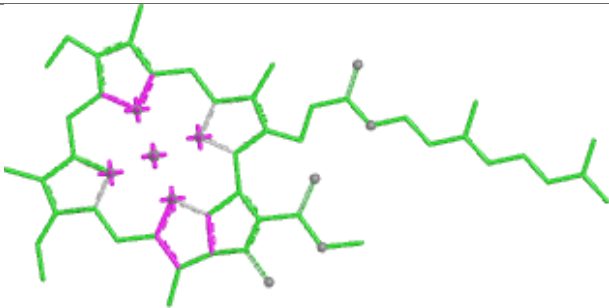
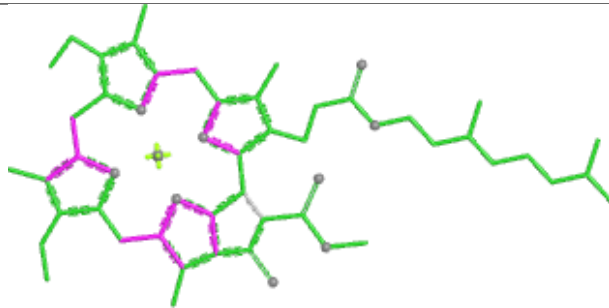
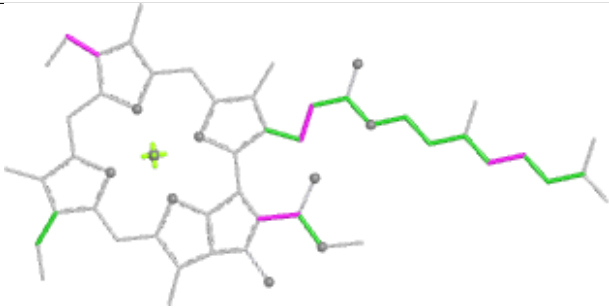
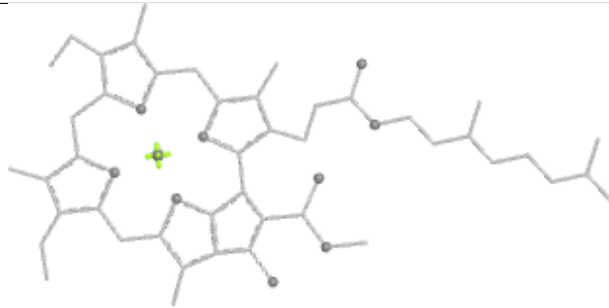
Ligand CLA I 601**Ligand CLA a 807**

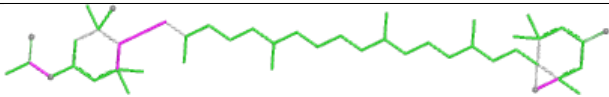
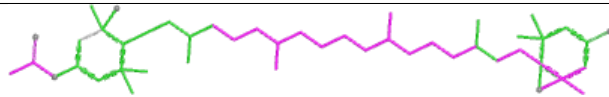
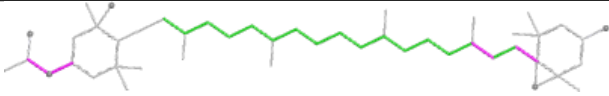
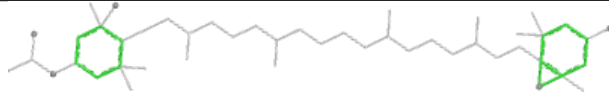
Ligand CLA E 606

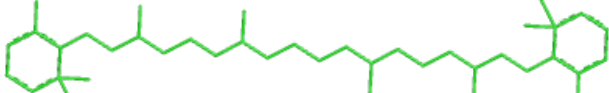
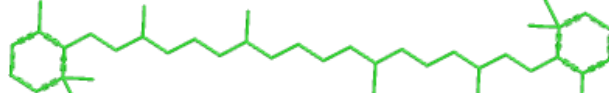
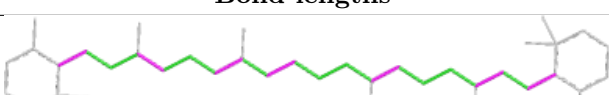
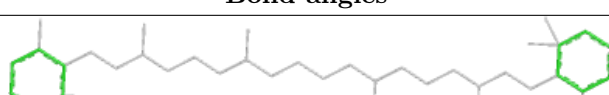


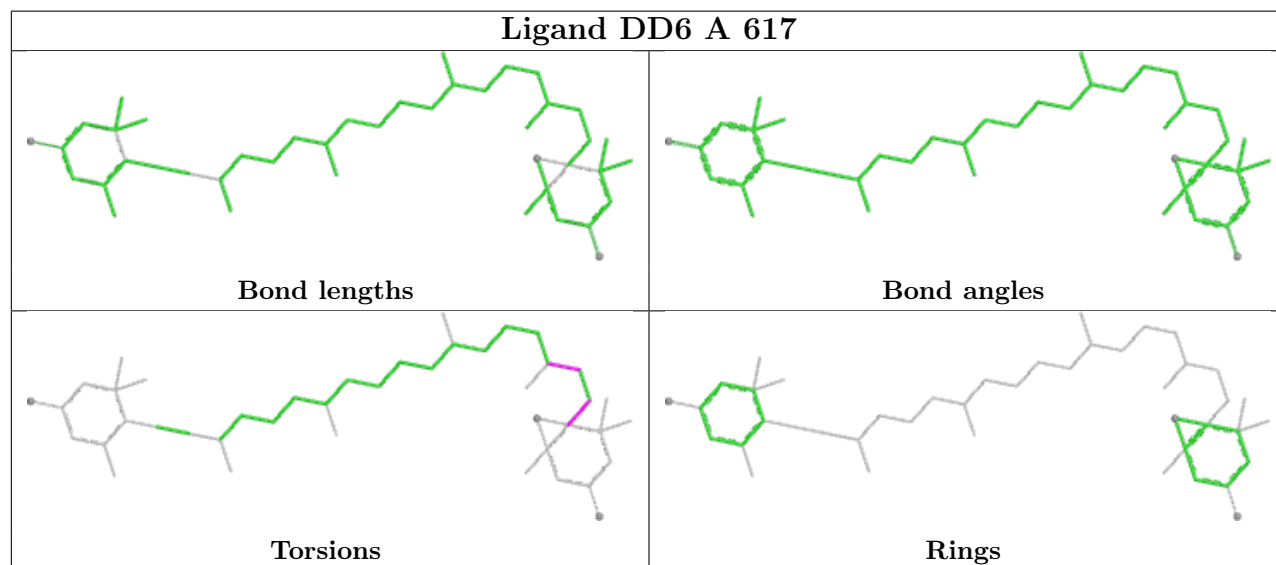
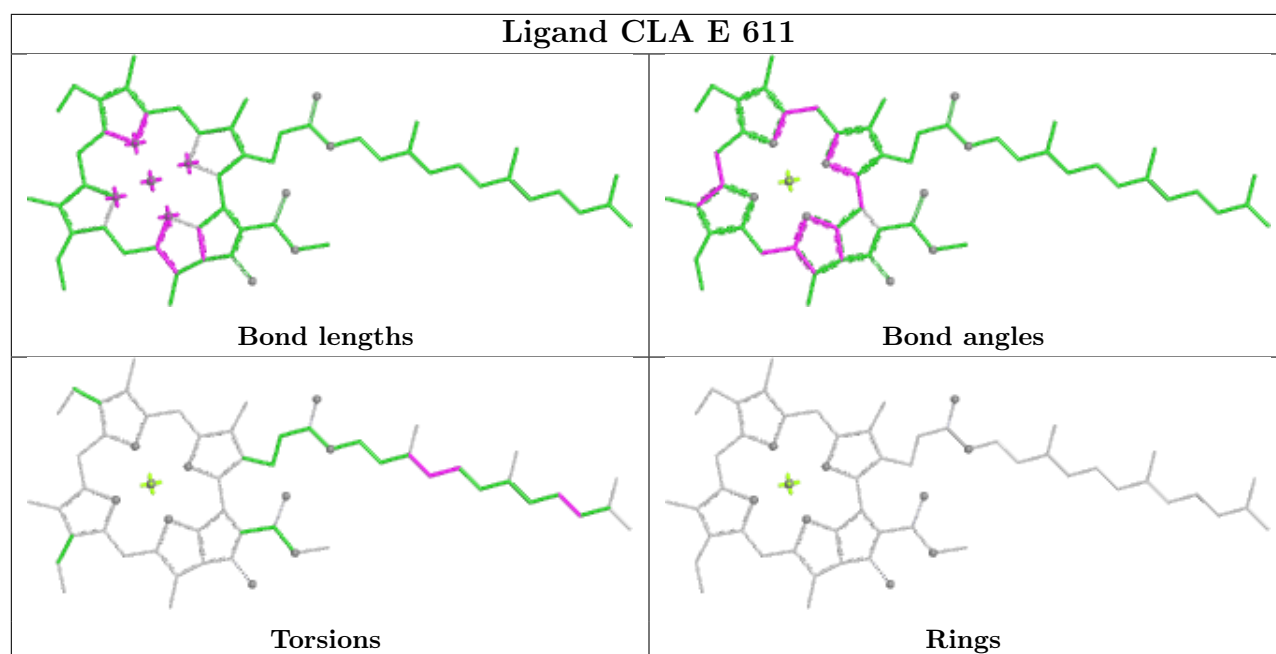
Ligand LHG G 617



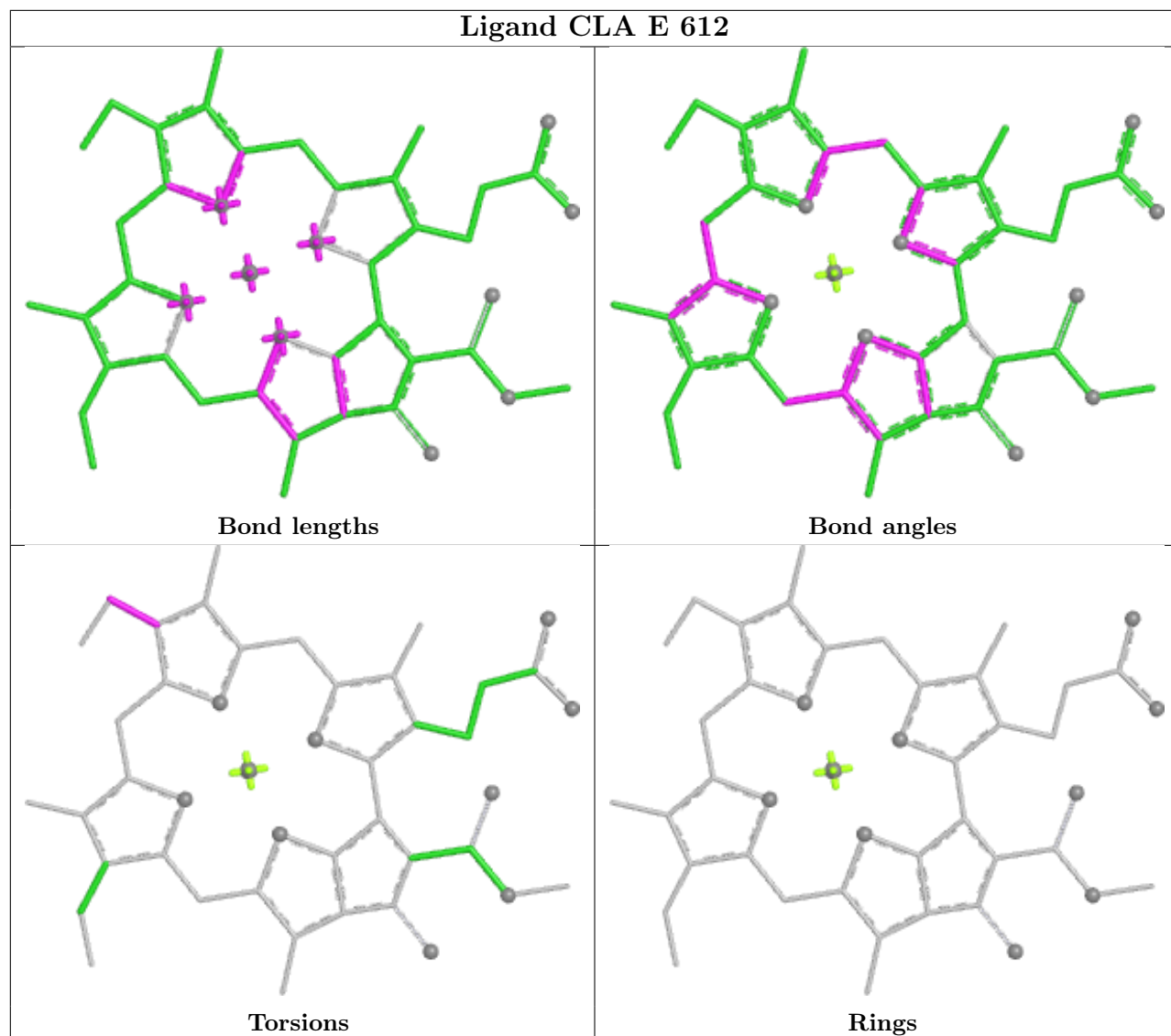
Ligand CLA I 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UIX j 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

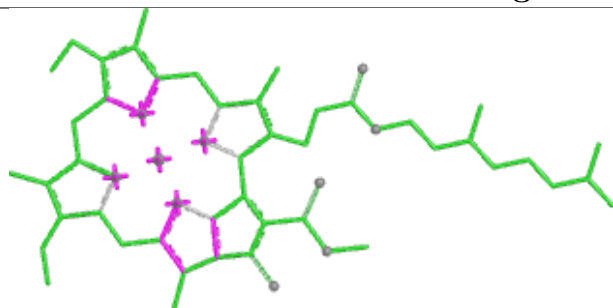
Ligand BCR 1 415	
	
Bond lengths	Bond angles
	
Torsions	Rings



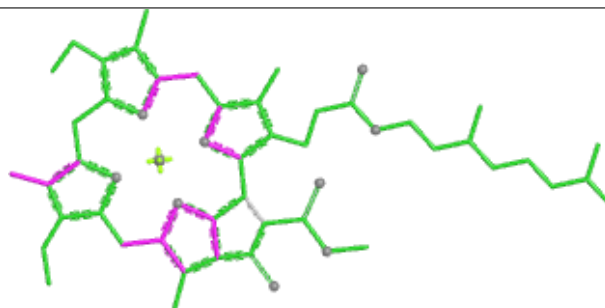
Ligand CLA E 612



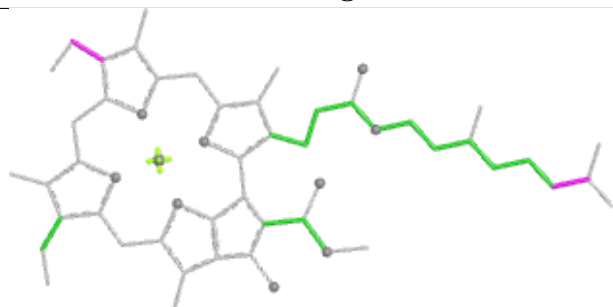
Ligand CLA G 602



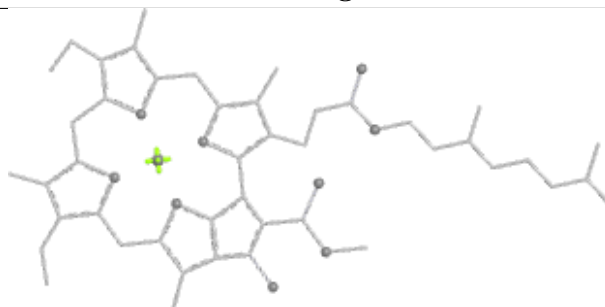
Bond lengths



Bond angles

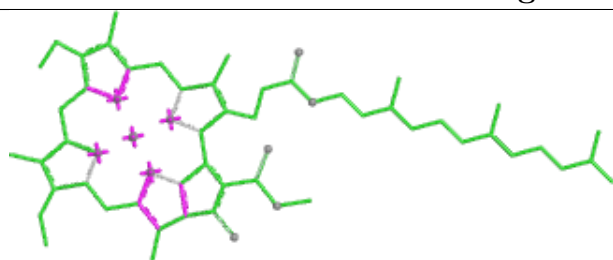


Torsions

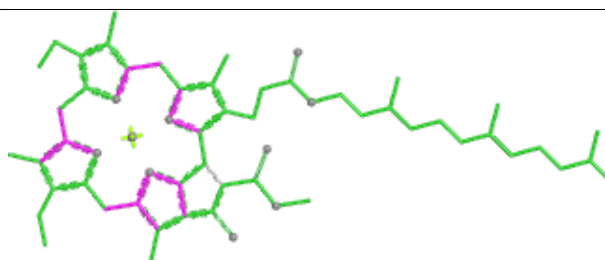


Rings

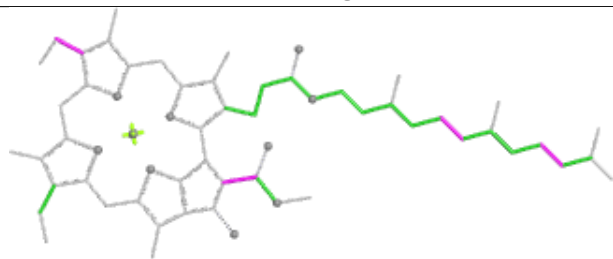
Ligand CLA J 603



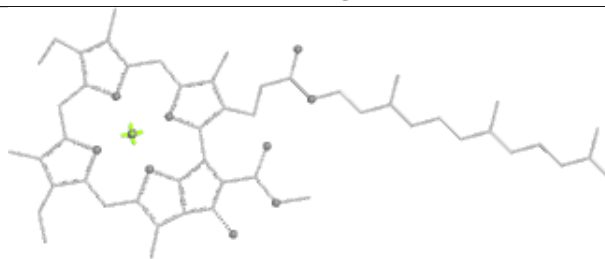
Bond lengths



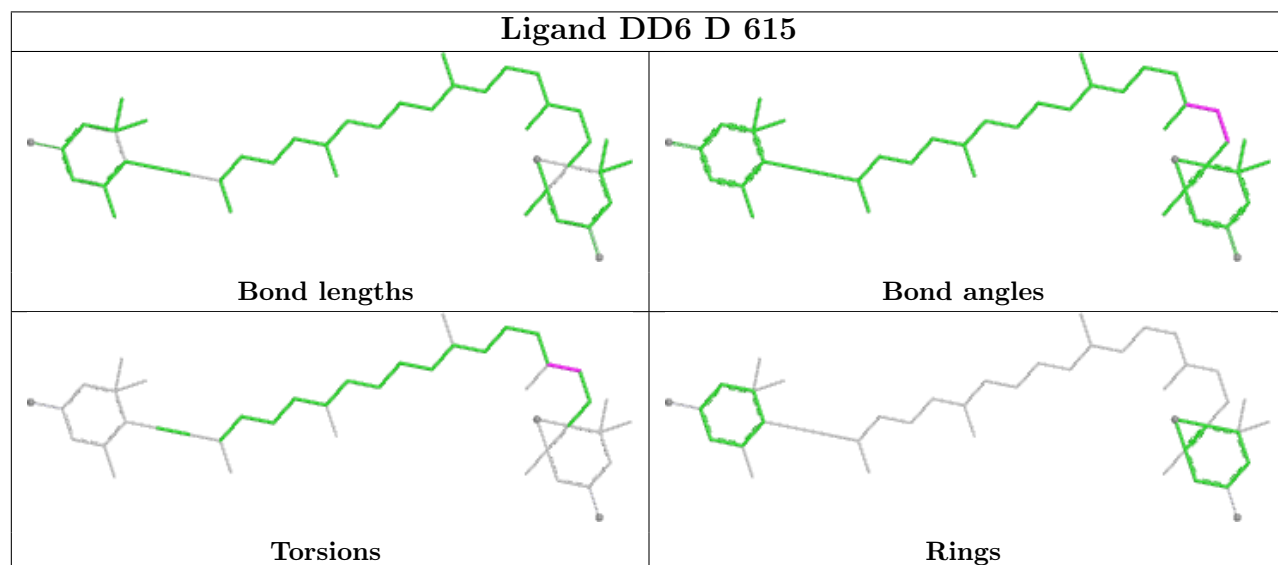
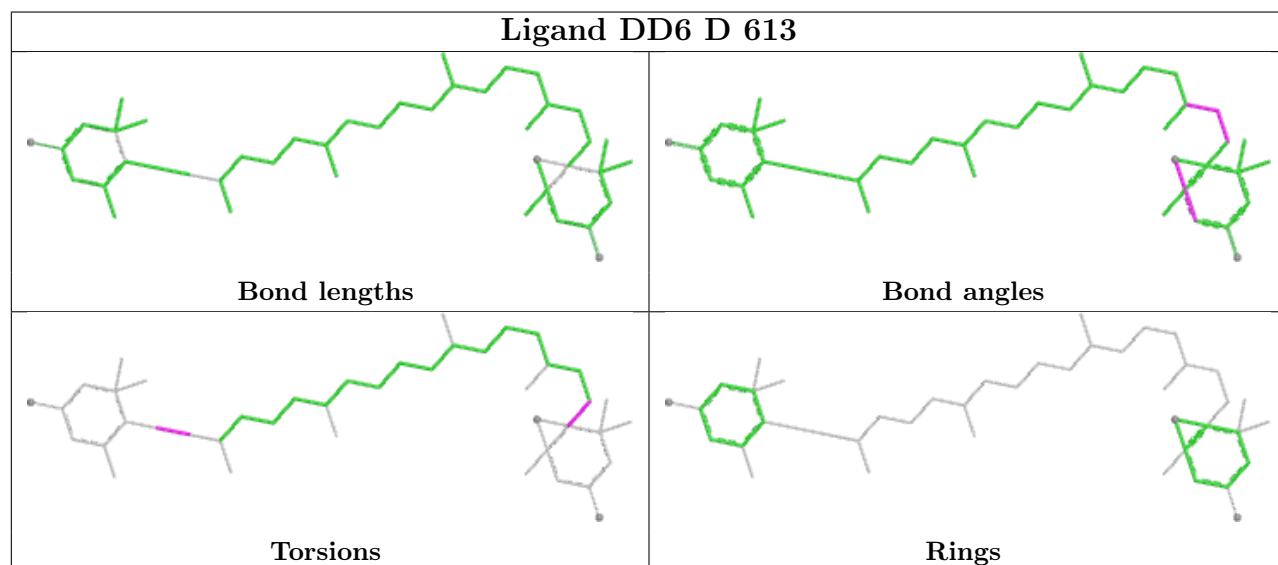
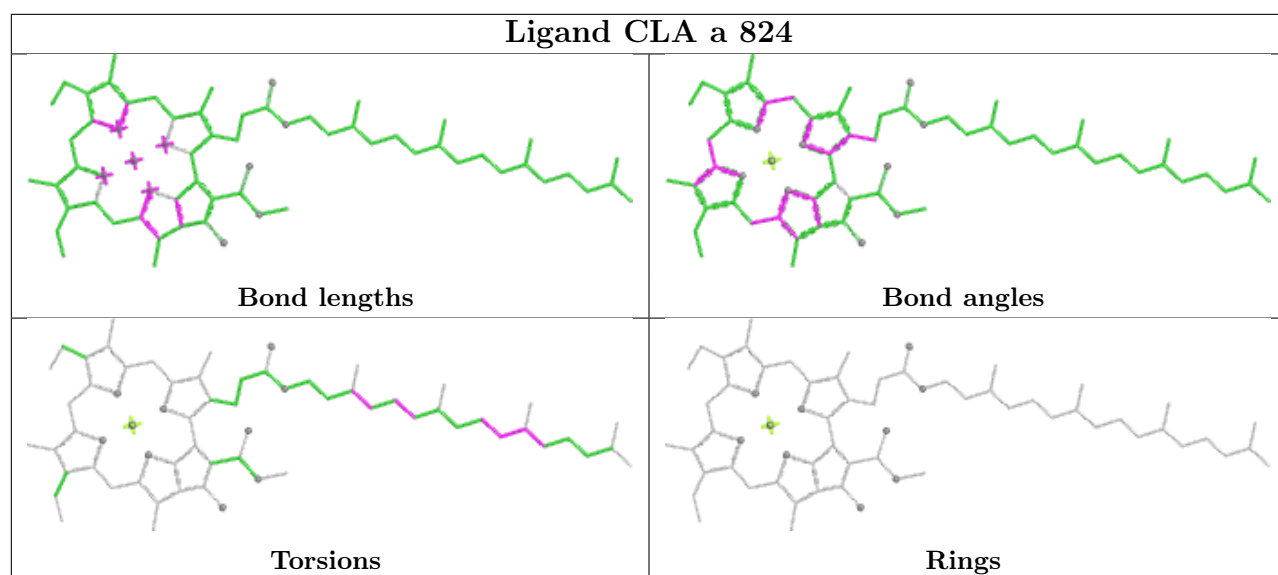
Bond angles

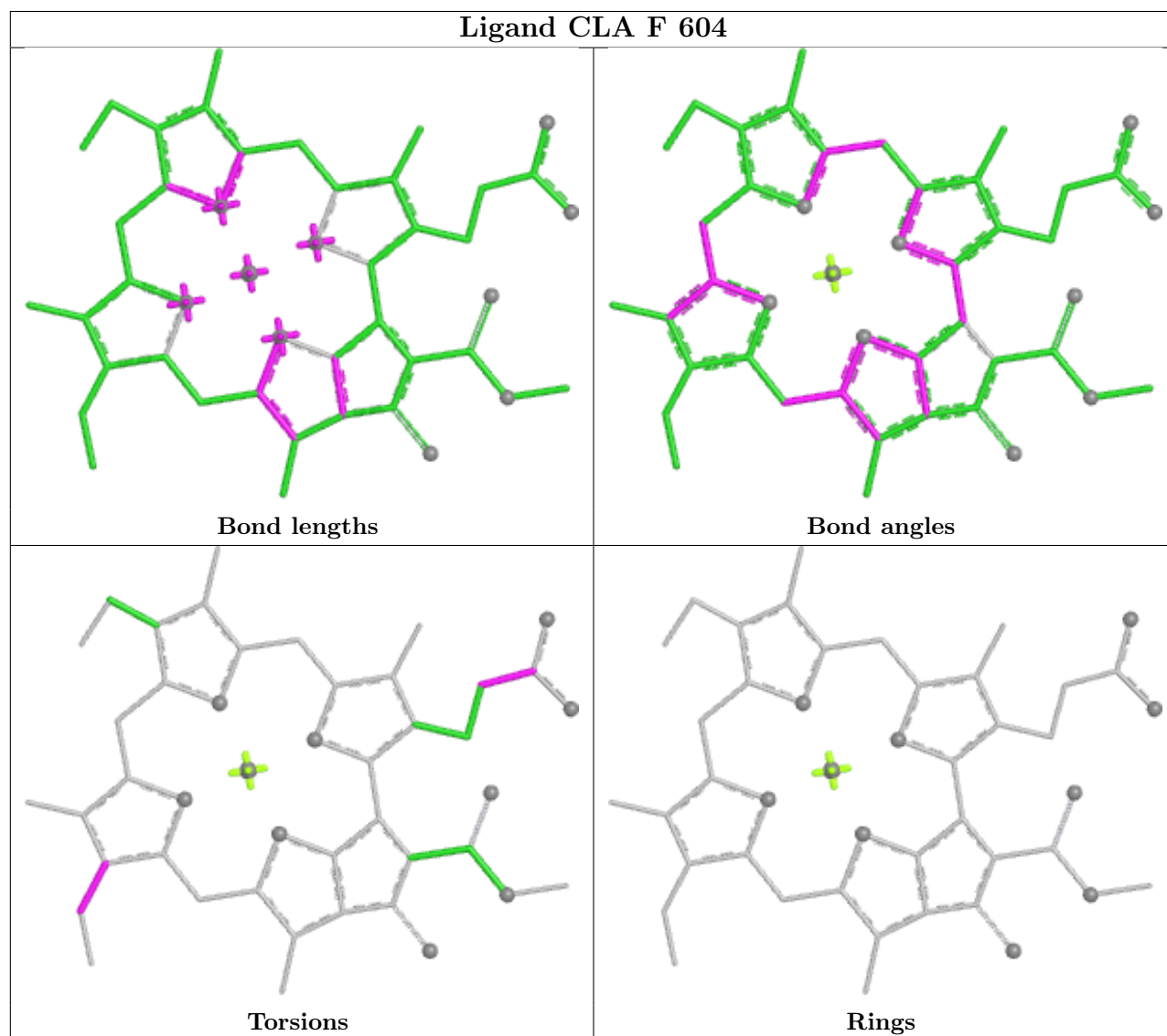
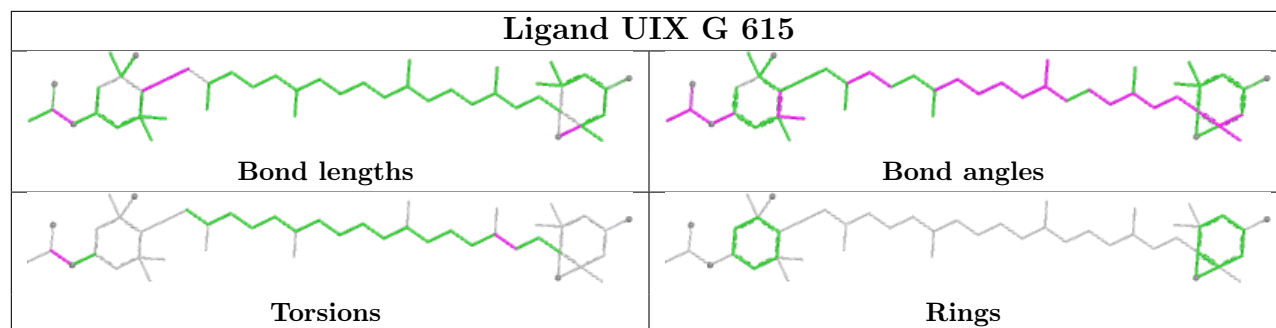


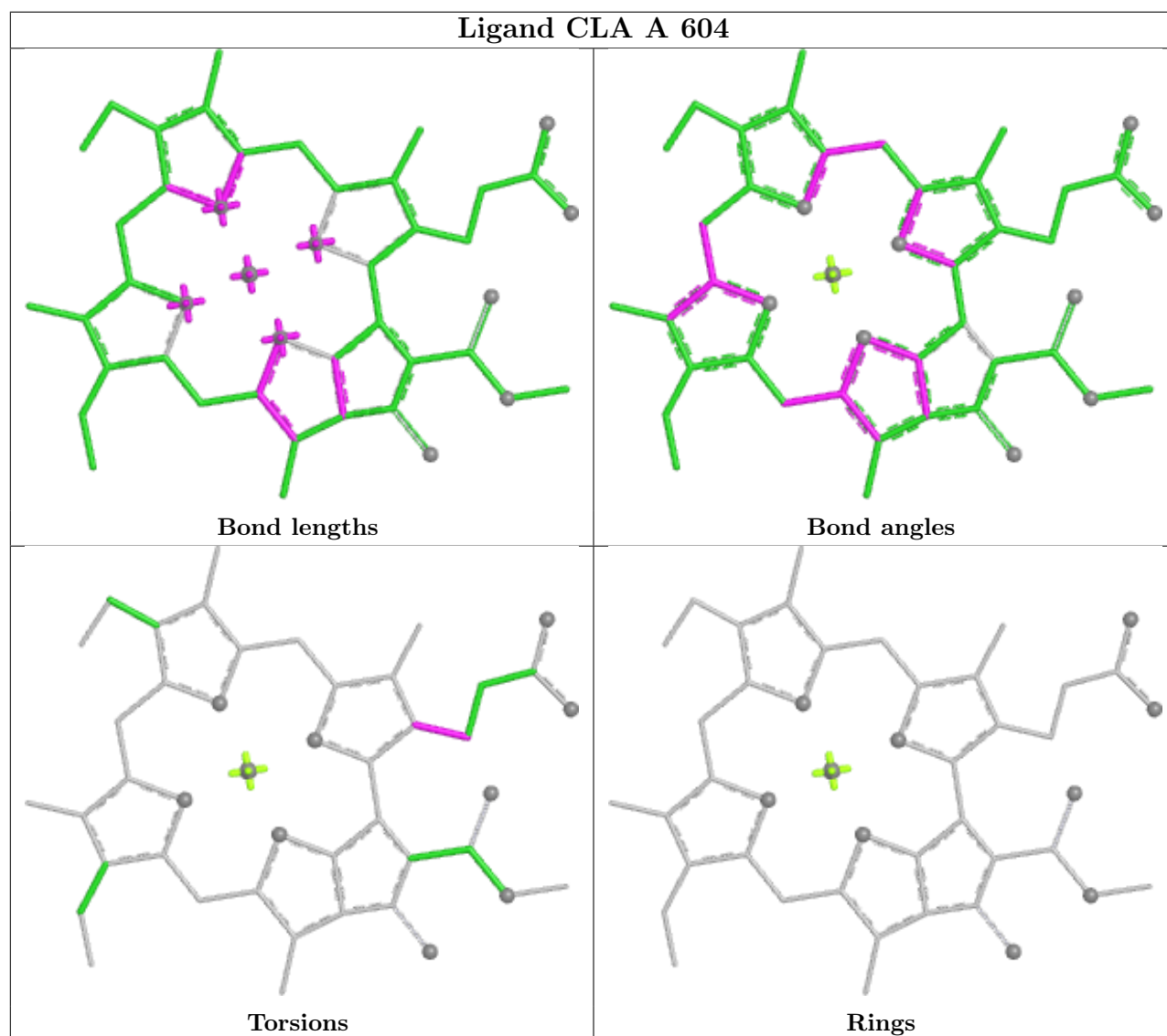
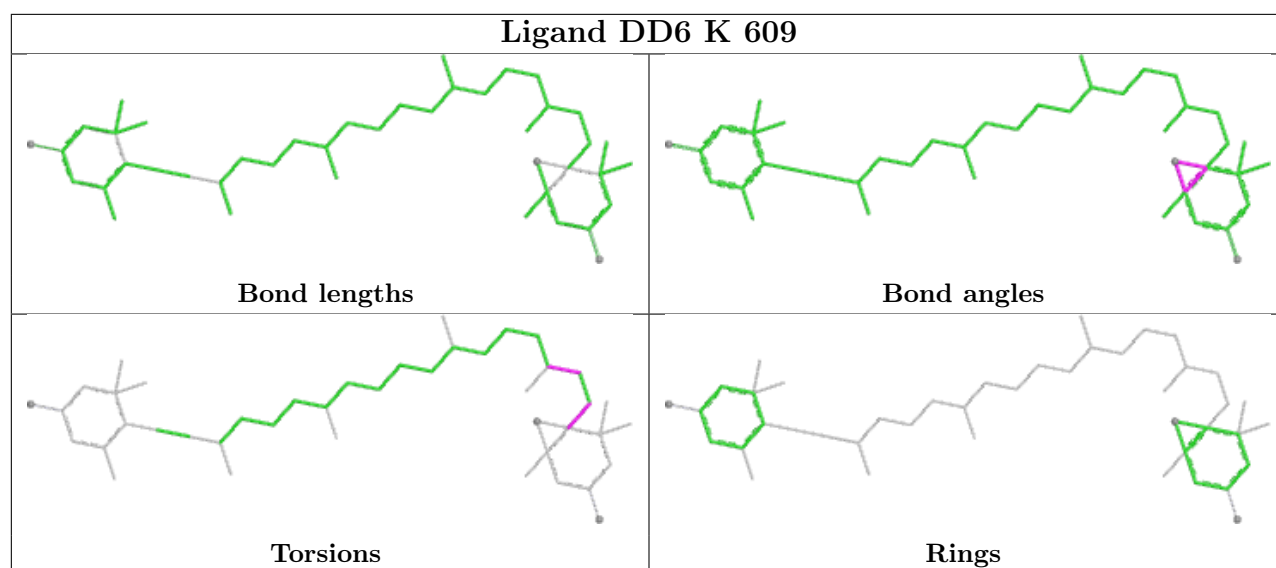
Torsions

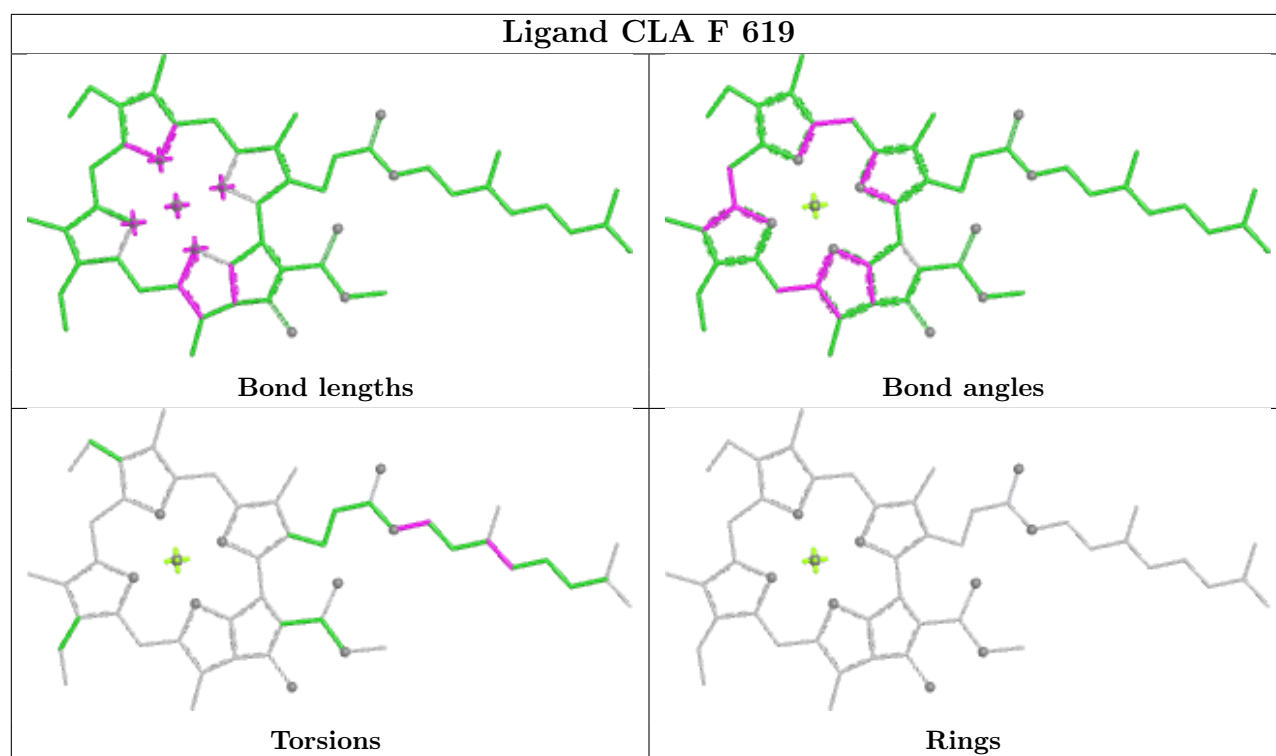


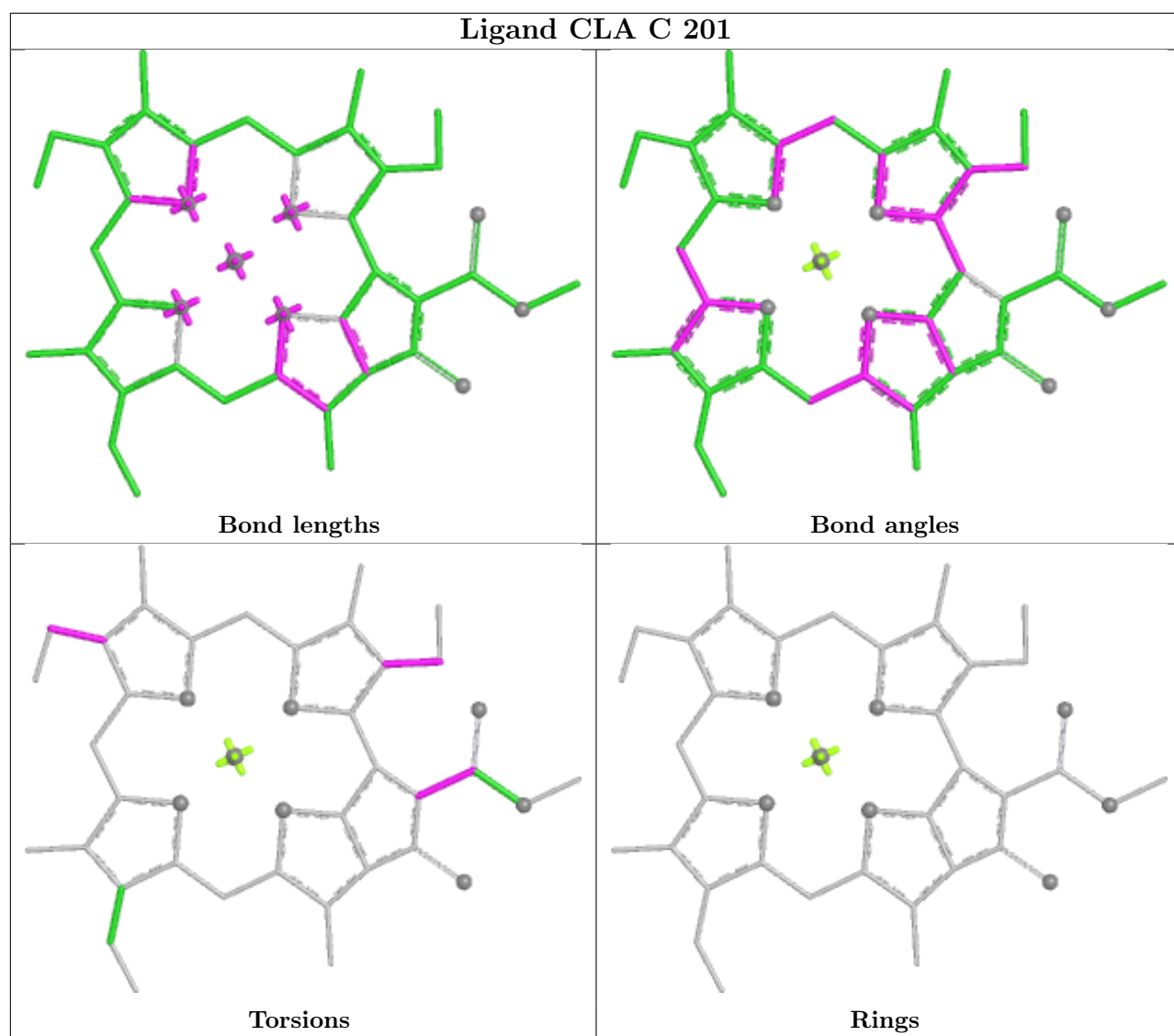
Rings



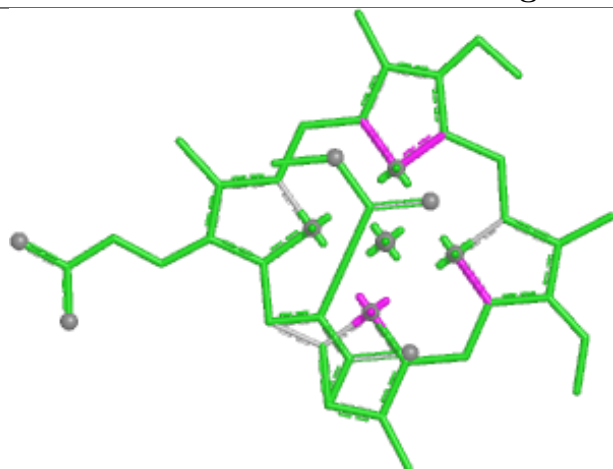




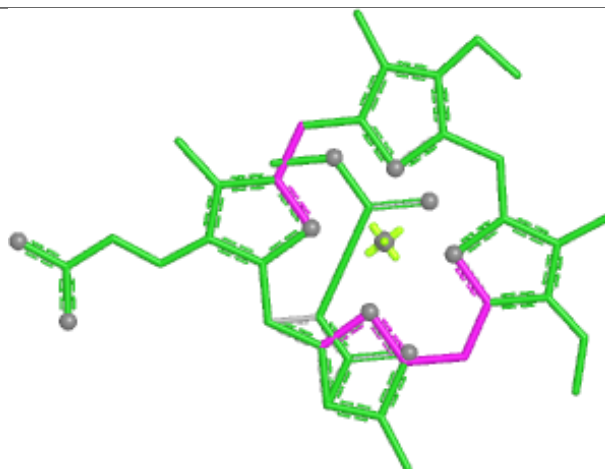




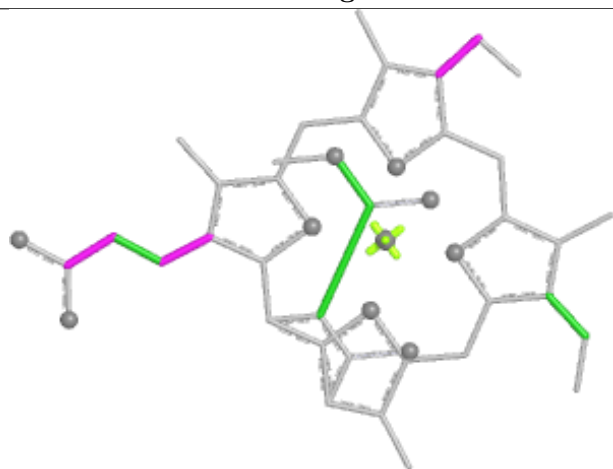
Ligand KC2 J 602



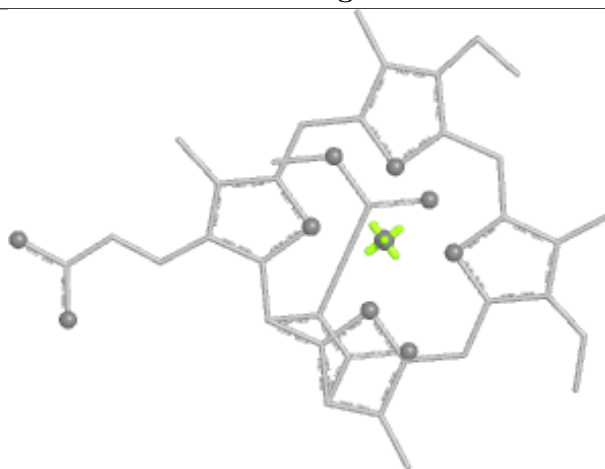
Bond lengths



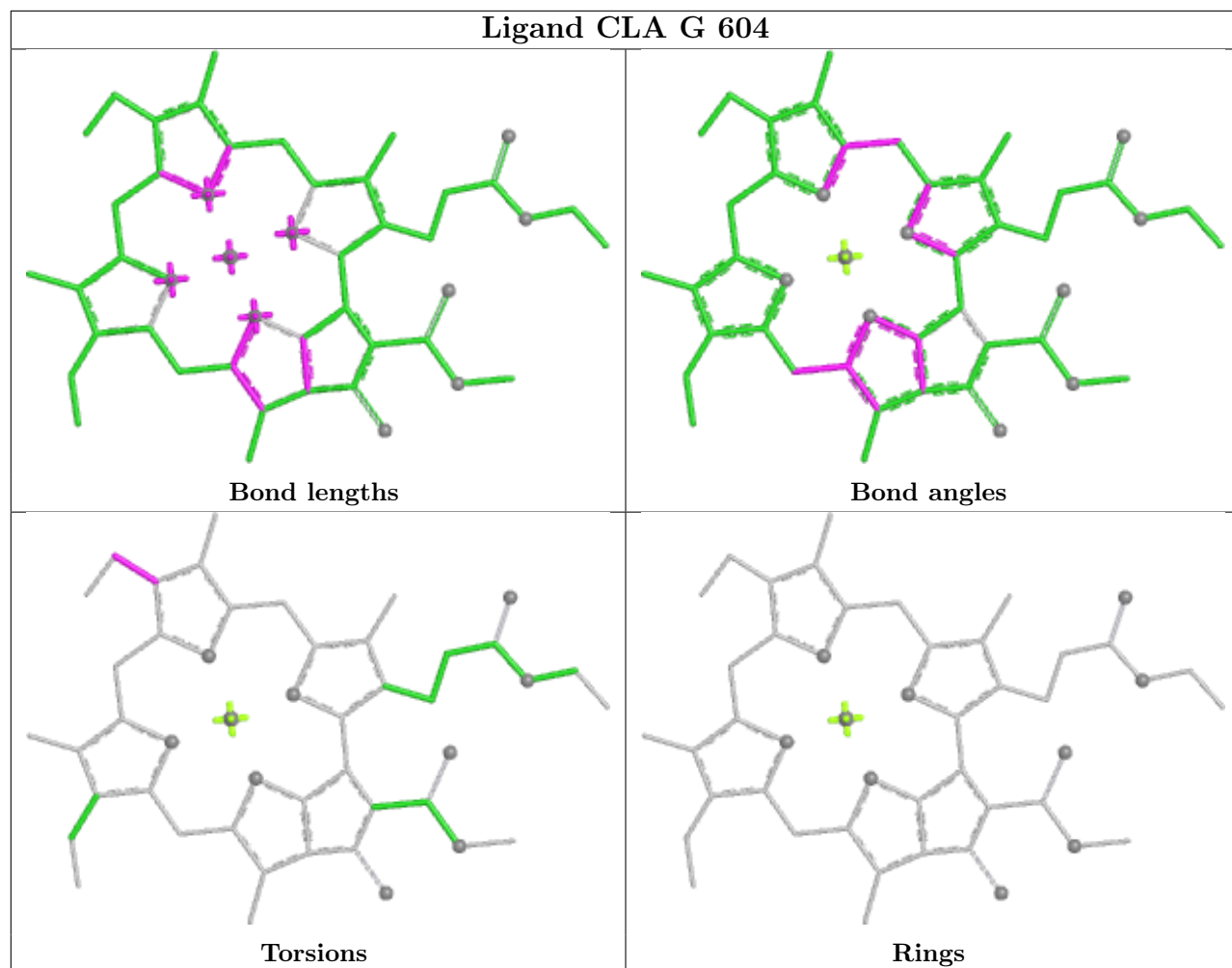
Bond angles

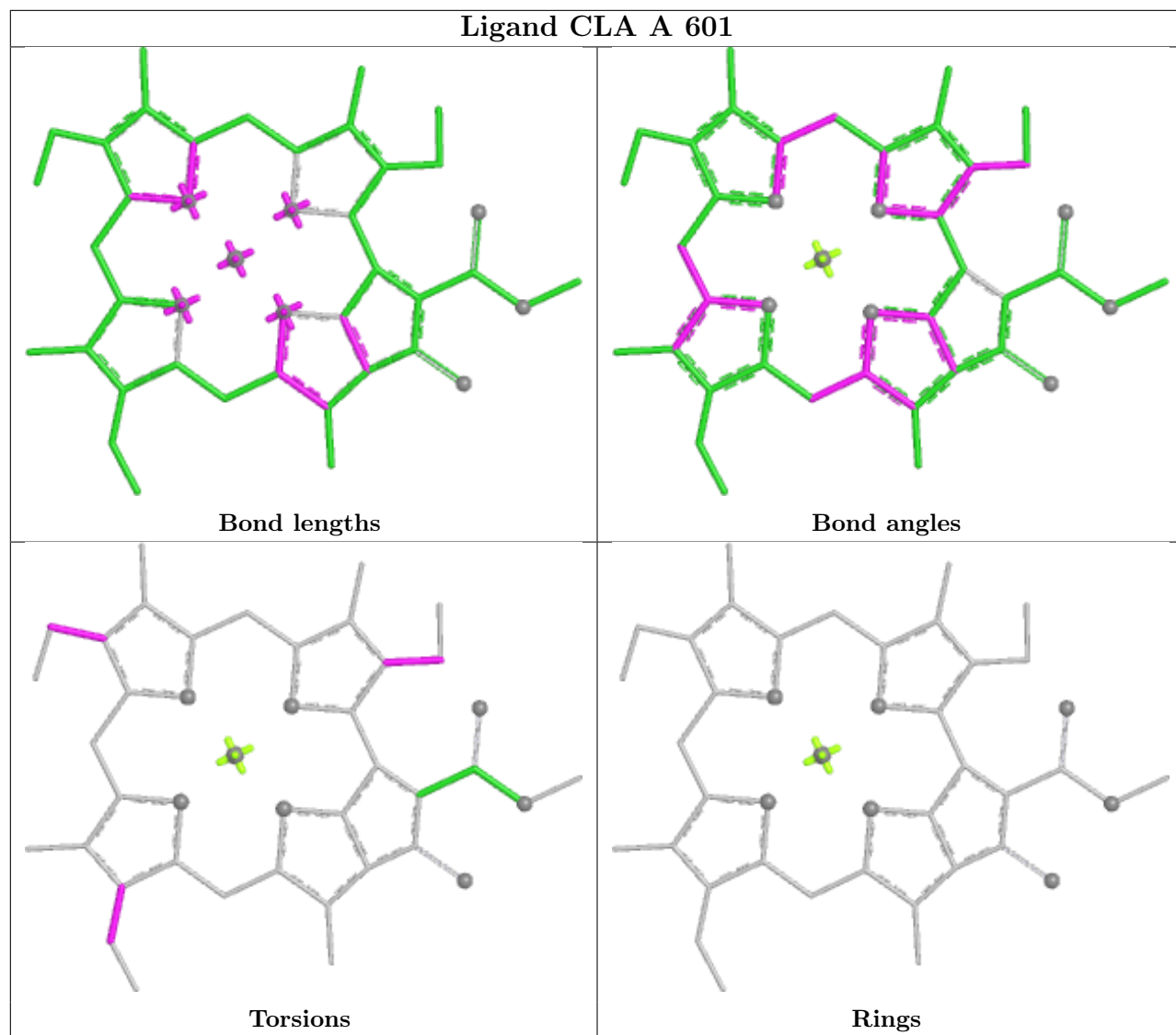


Torsions

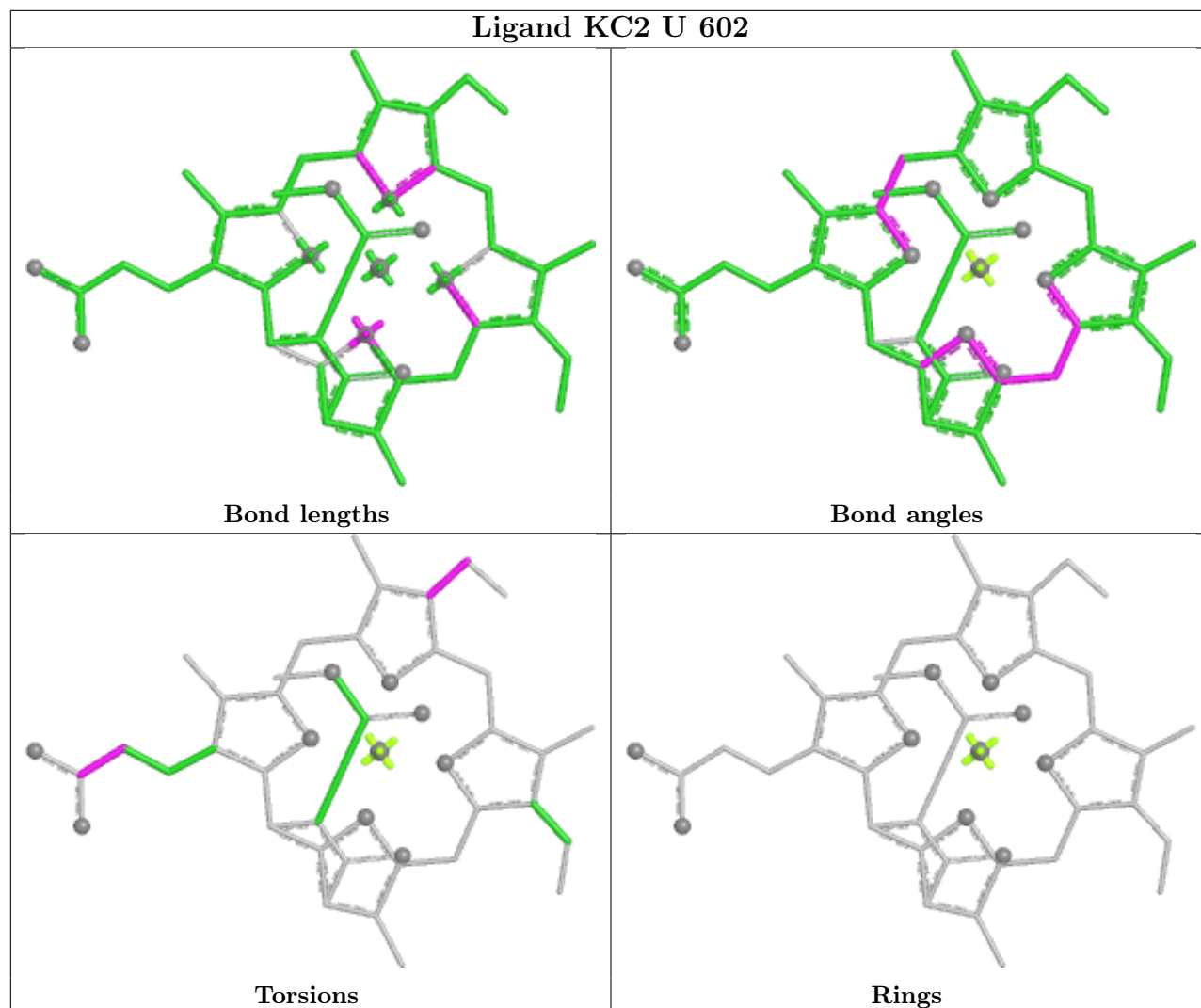


Rings

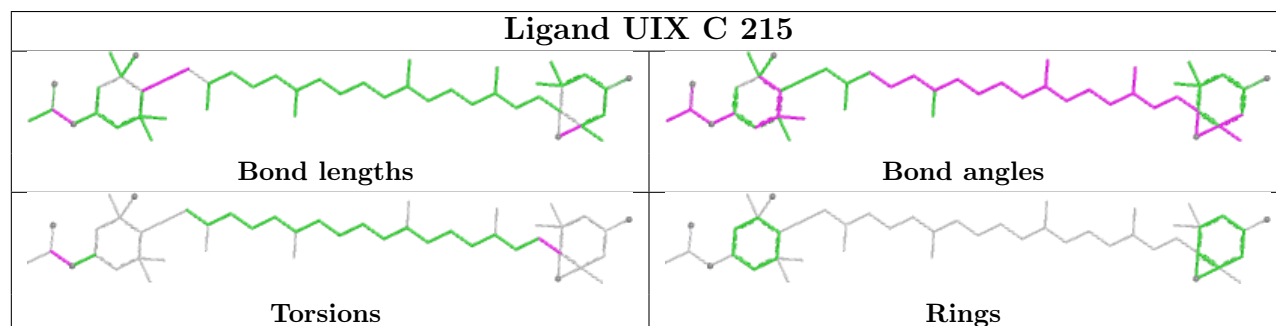




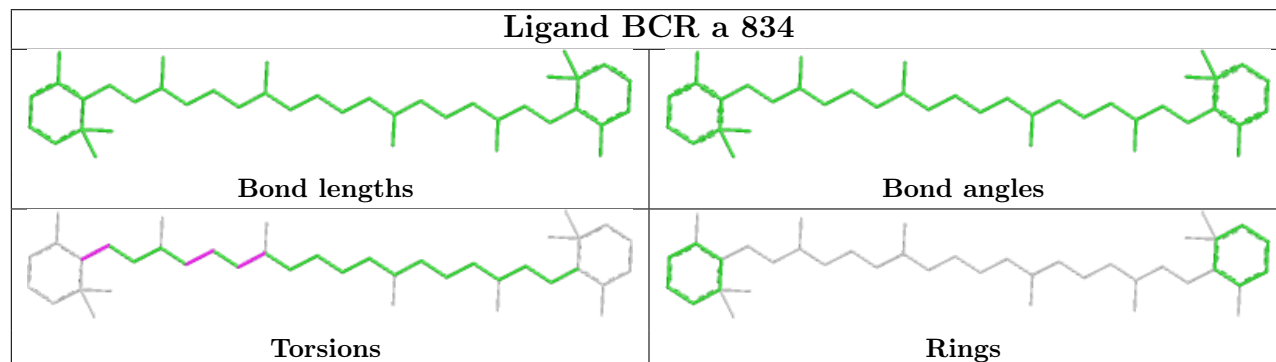
Ligand KC2 U 602

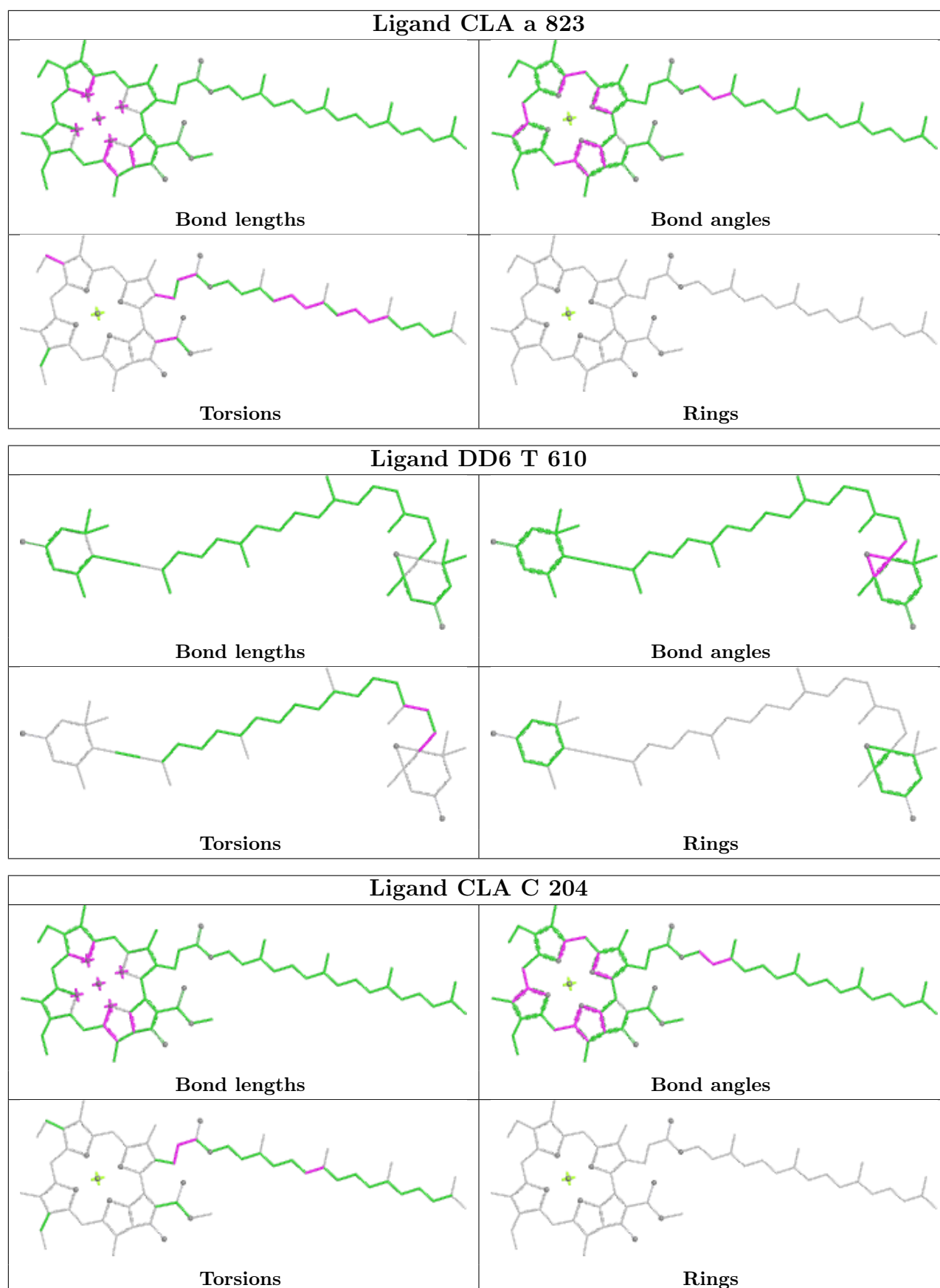


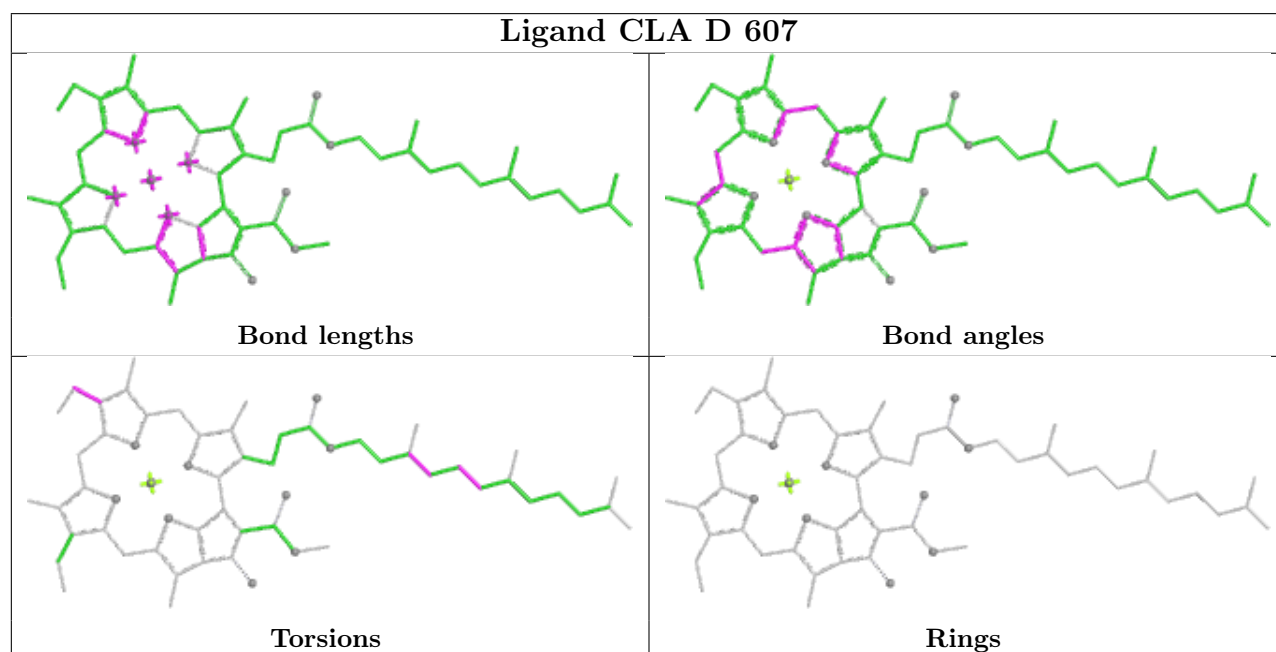
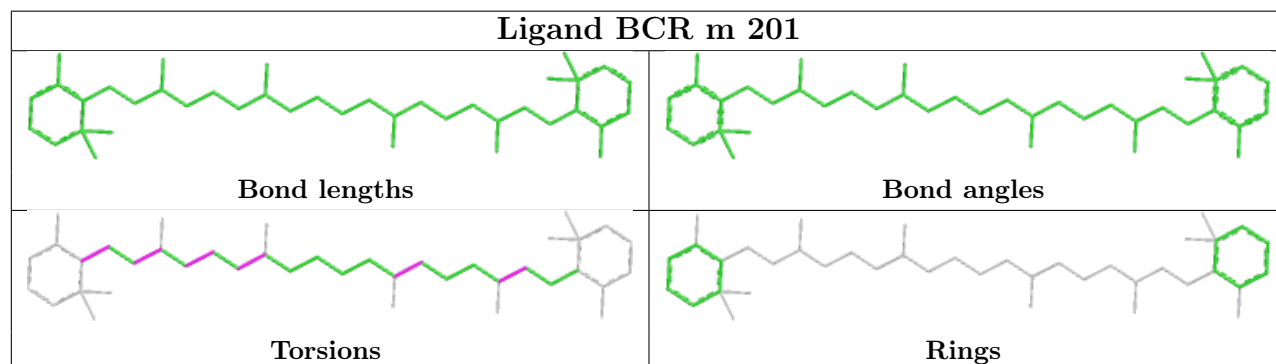
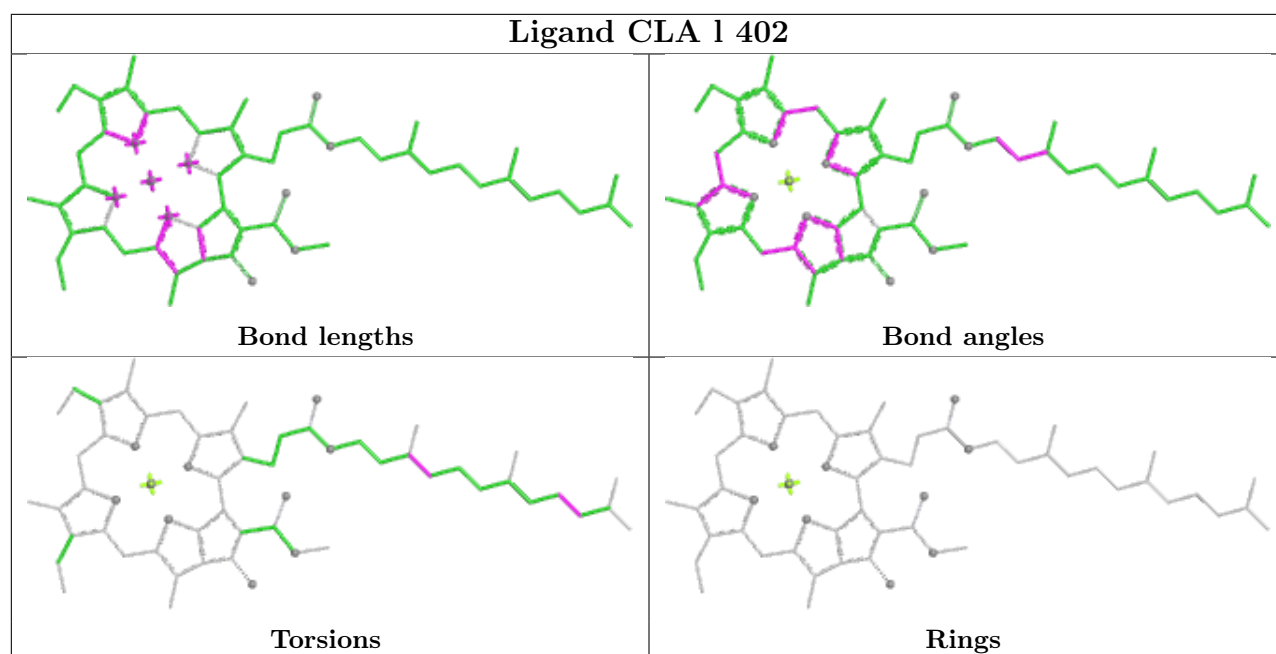
Ligand UIX C 215



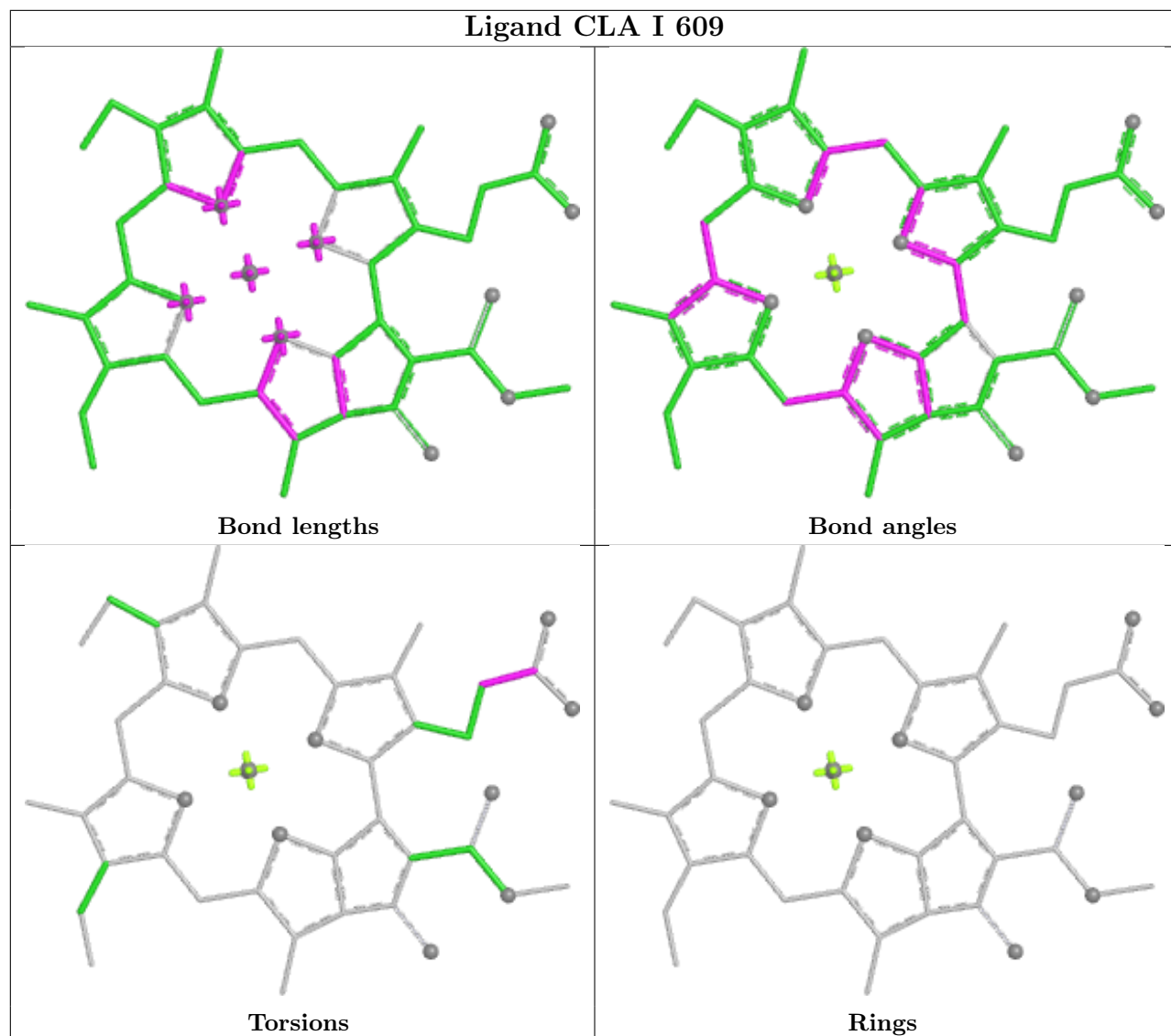
Ligand BCR a 834



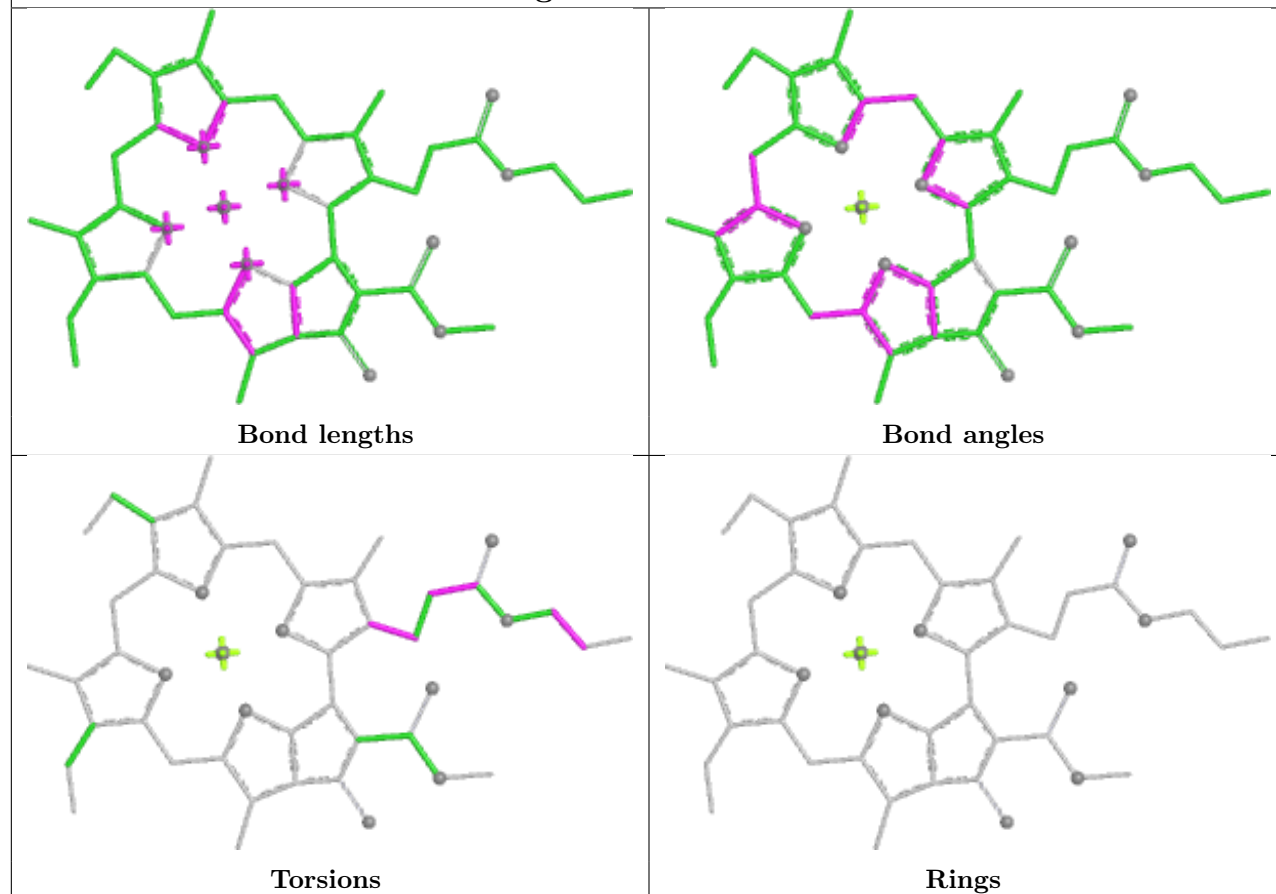




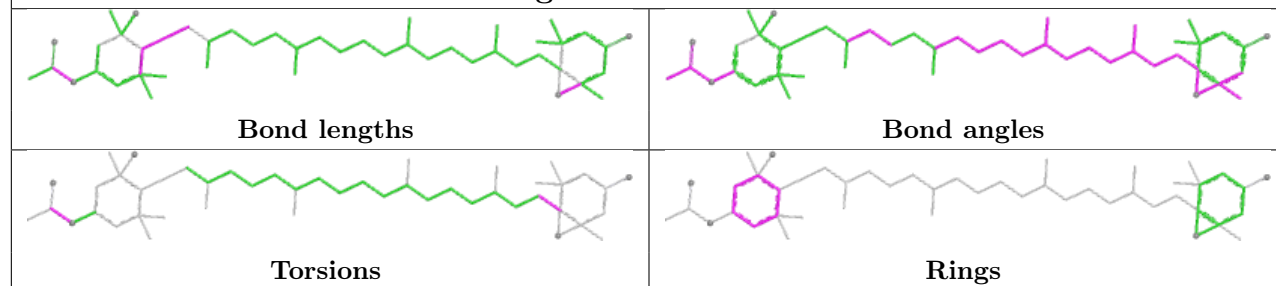
Ligand CLA I 609

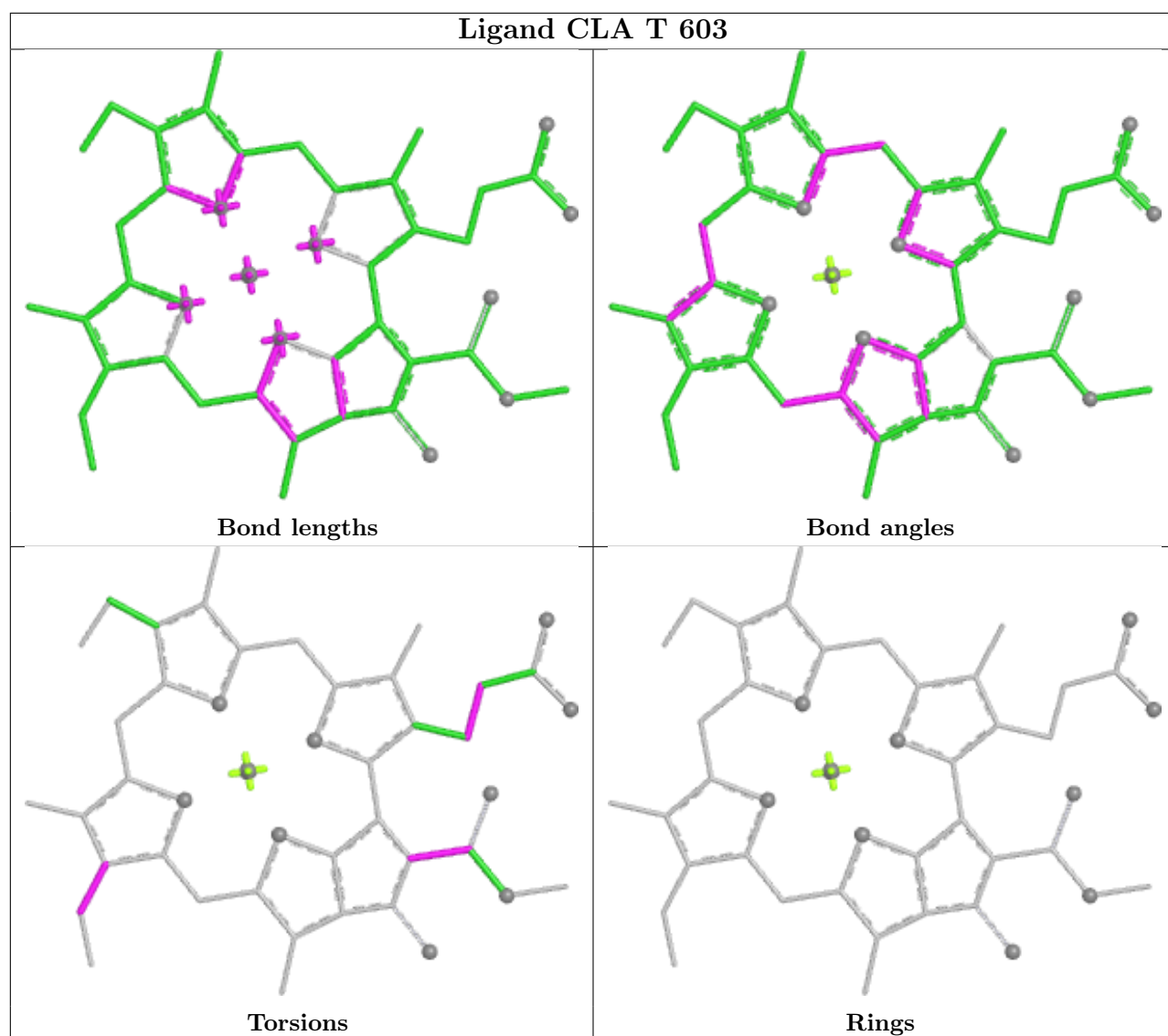


Ligand CLA b 722

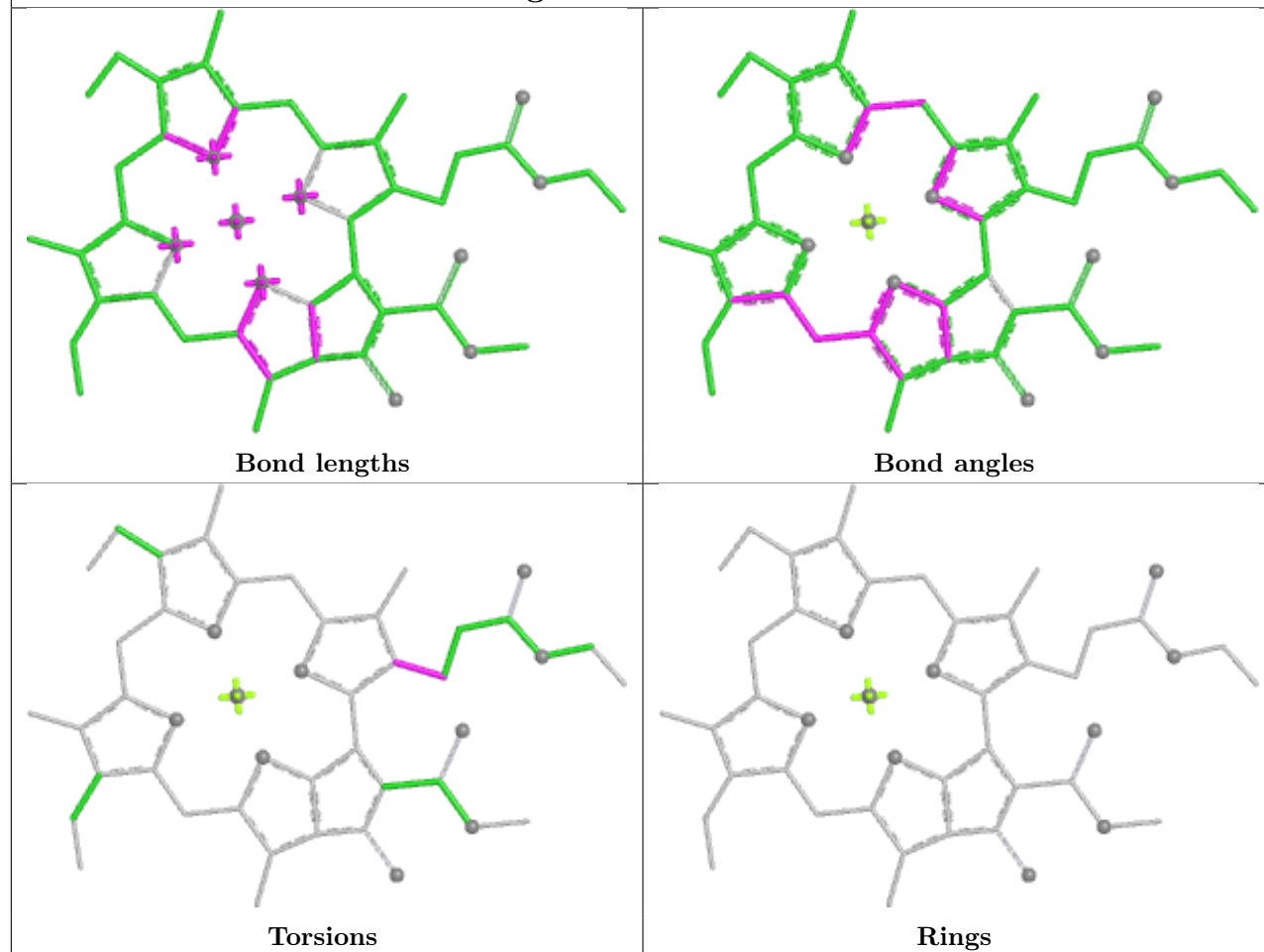


Ligand UIX B 615

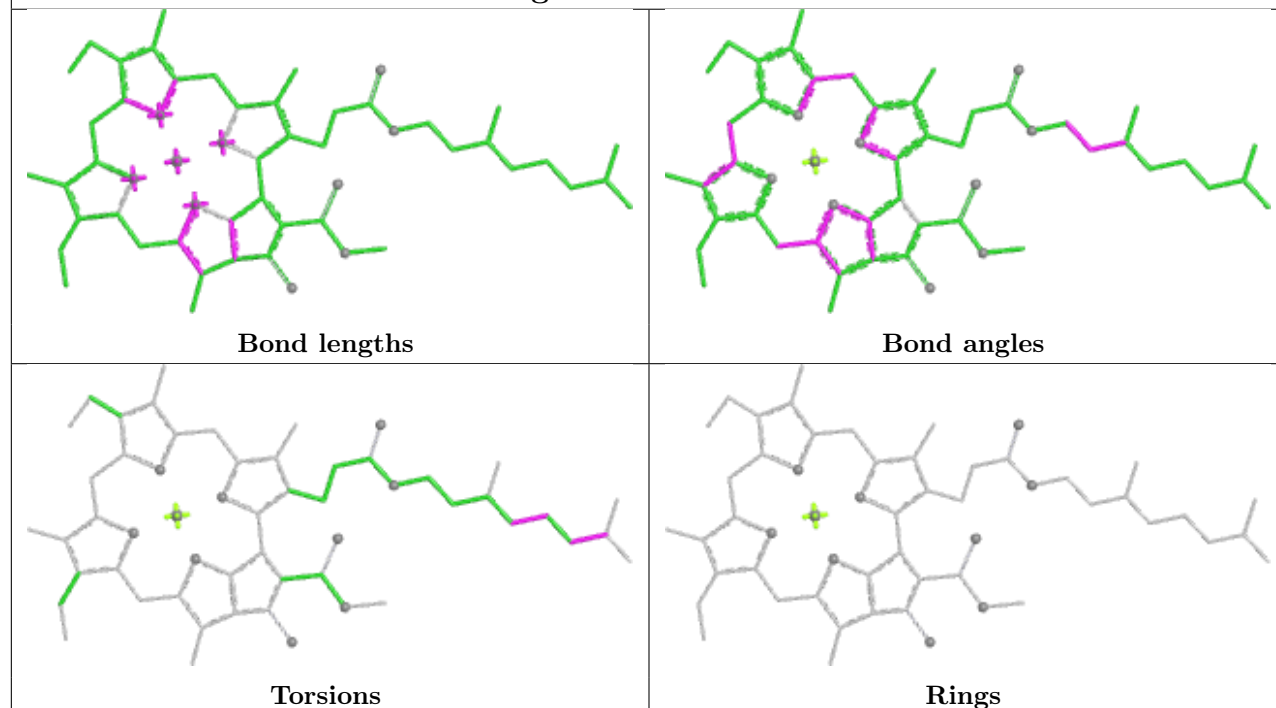


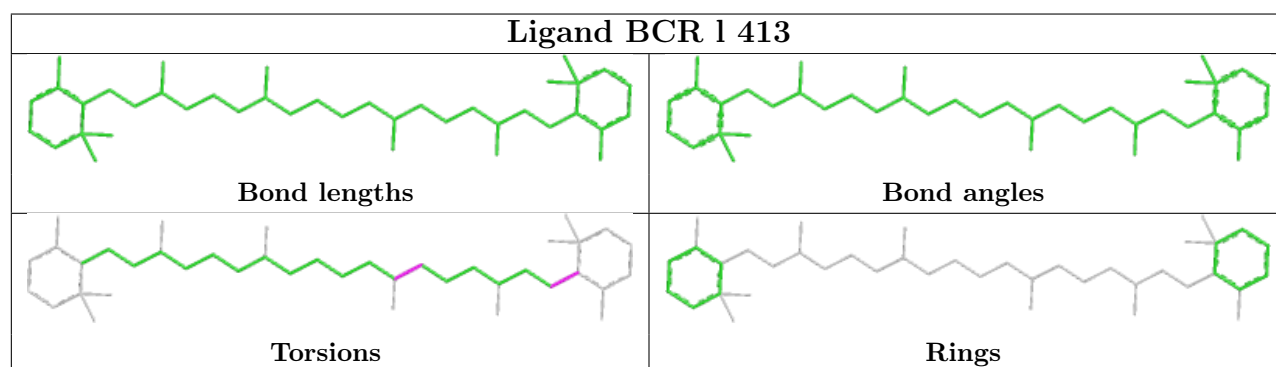
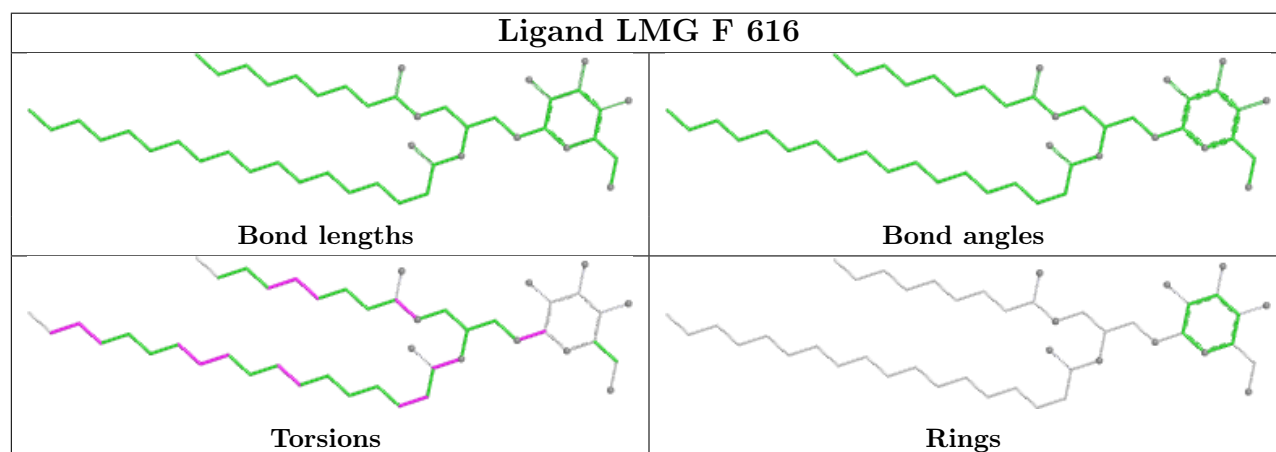
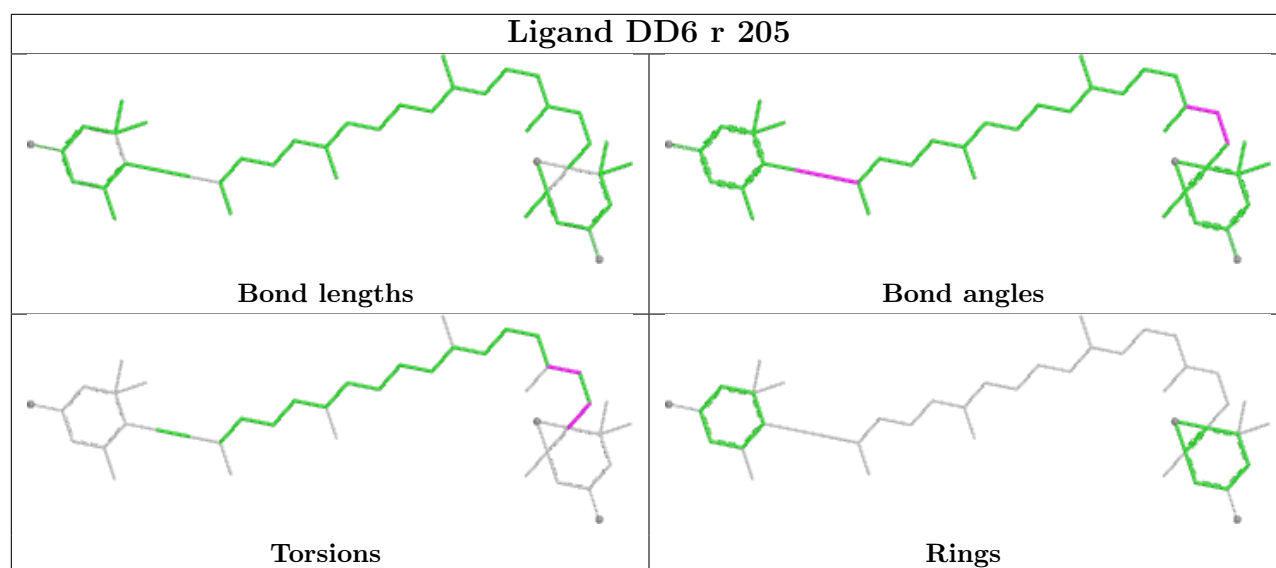


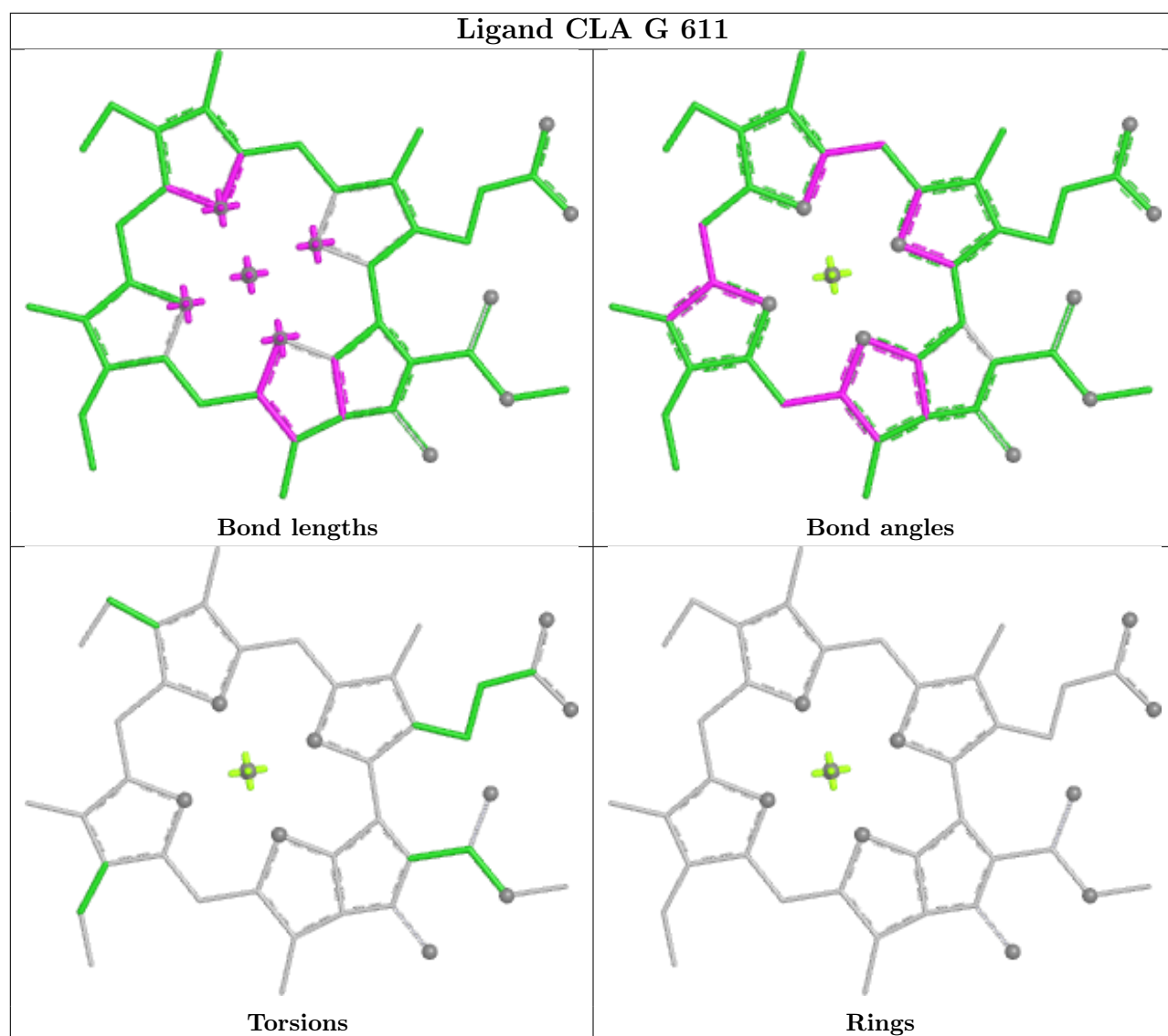
Ligand CLA A 606



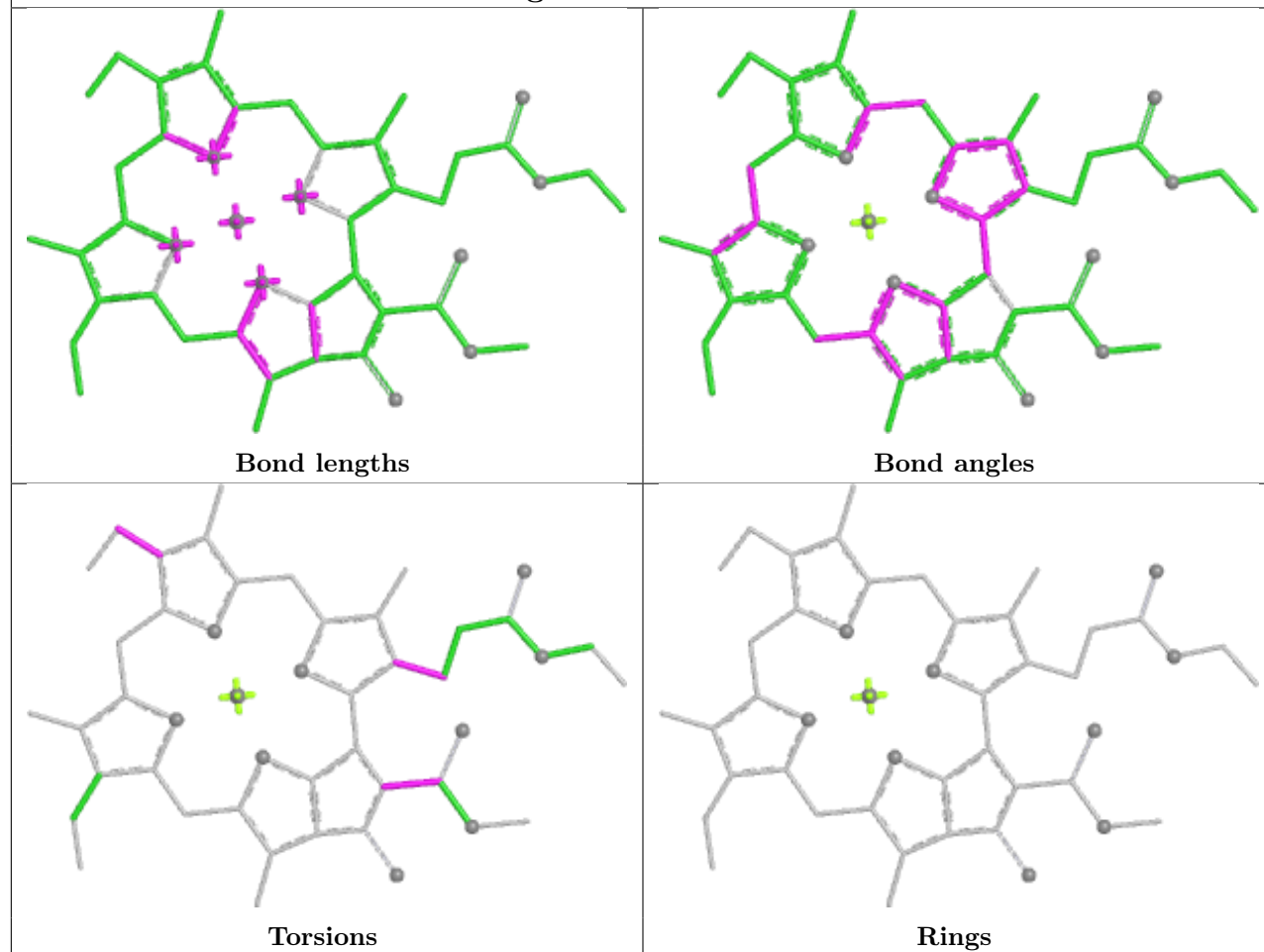
Ligand CLA D 603



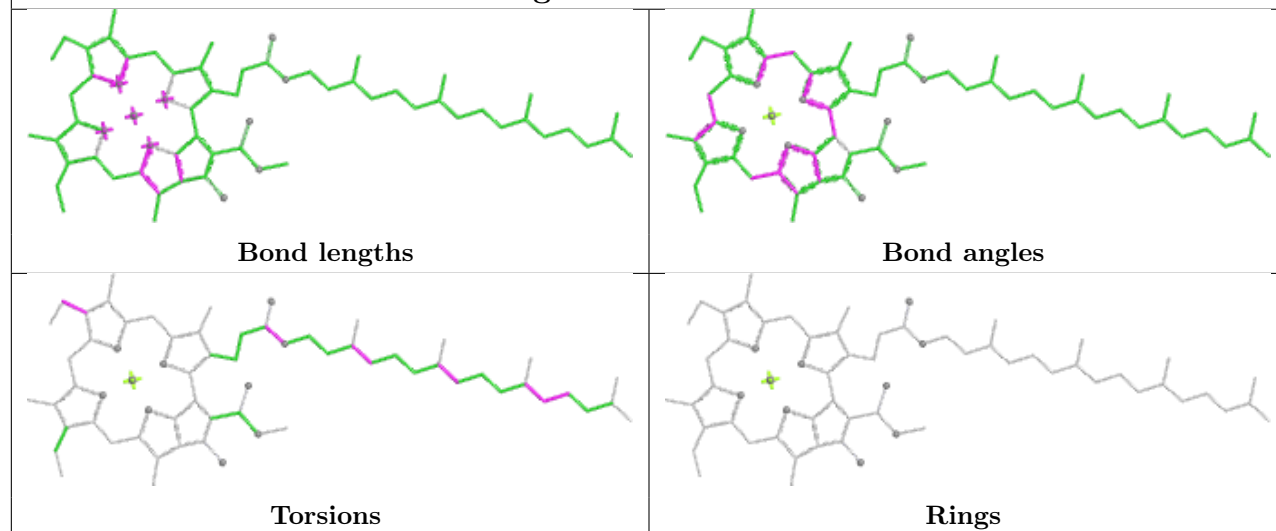




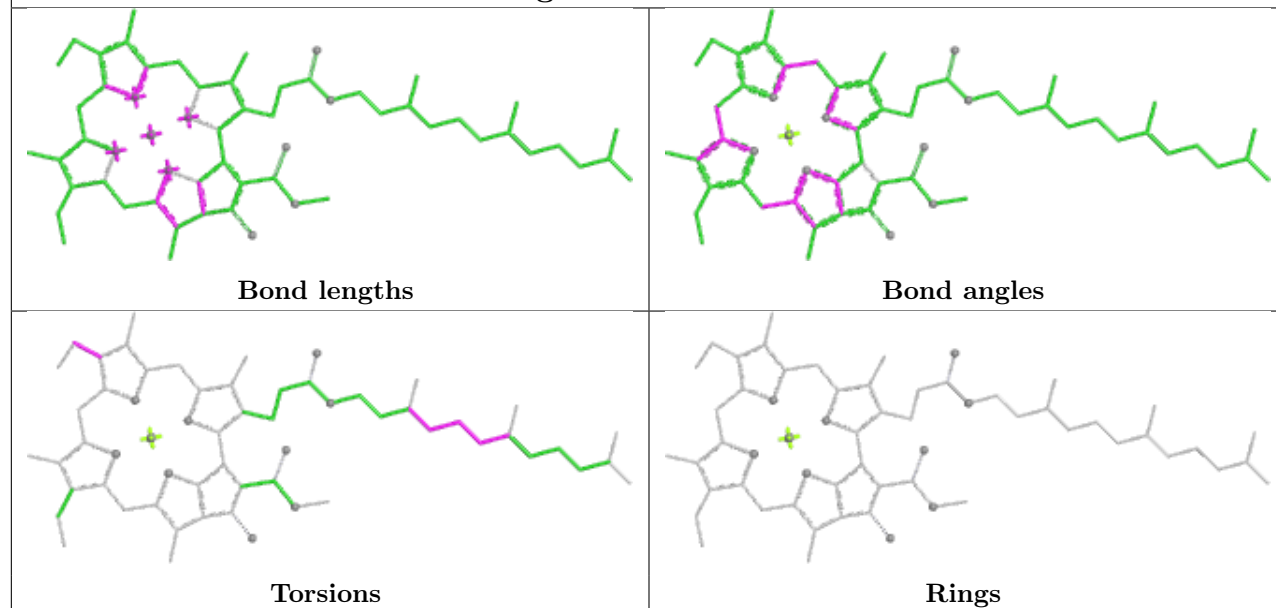
Ligand CLA A 612



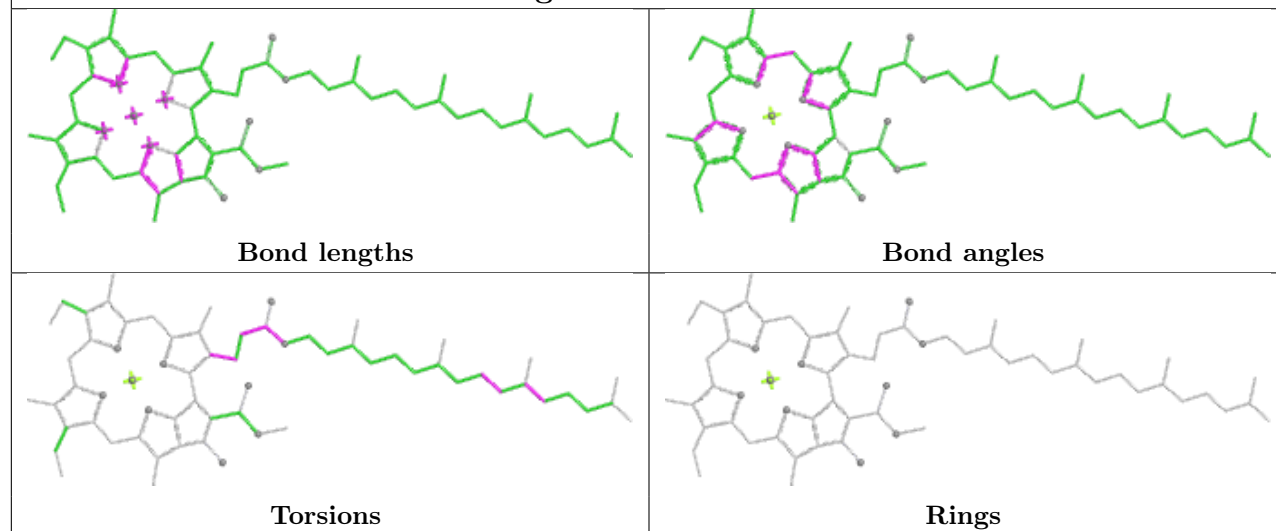
Ligand CLA E 607

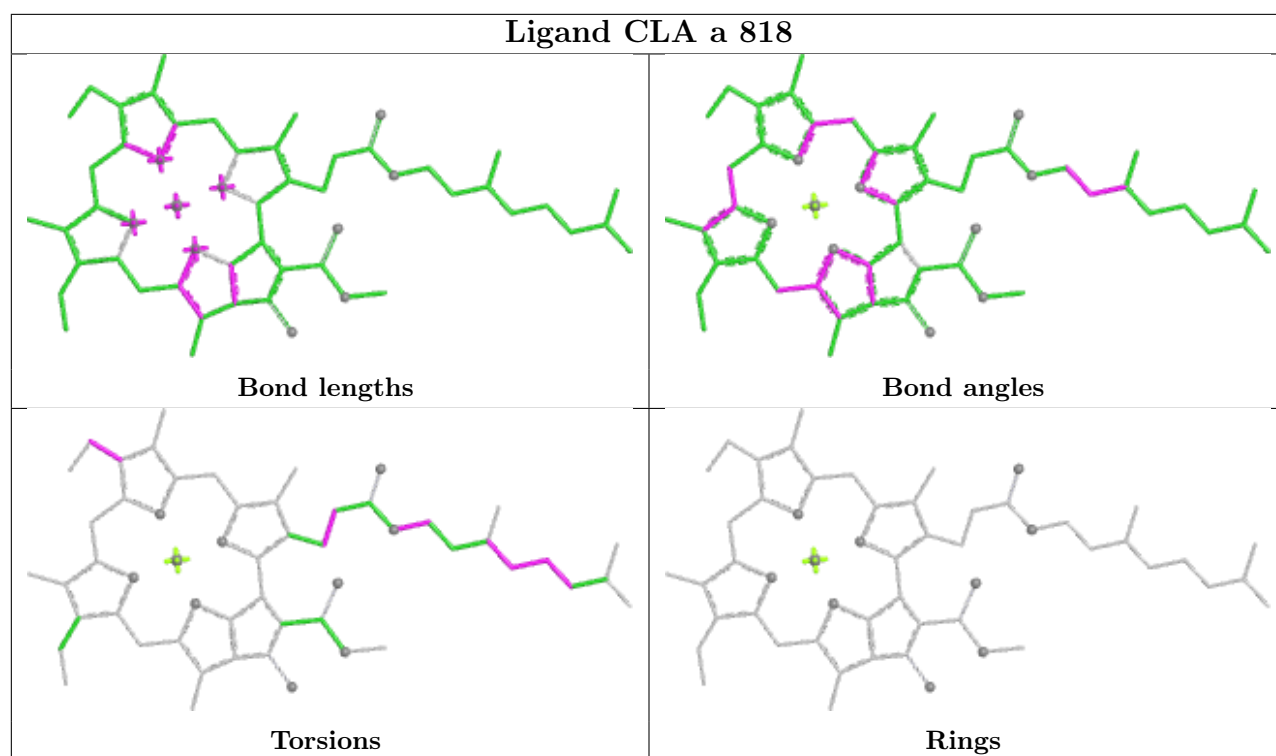


Ligand CLA a 816



Ligand CLA b 717





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

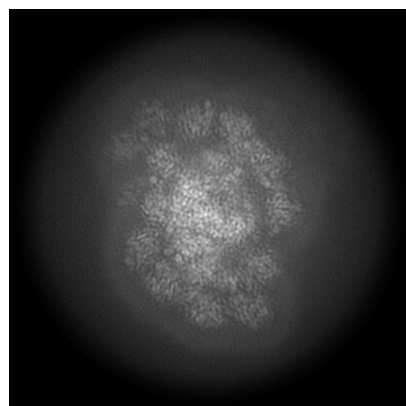
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36366. These allow visual inspection of the internal detail of the map and identification of artifacts.

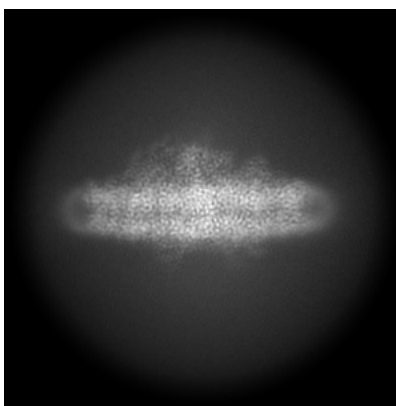
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

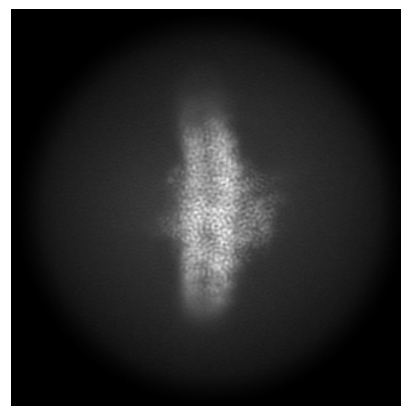
6.1.1 Primary map



X

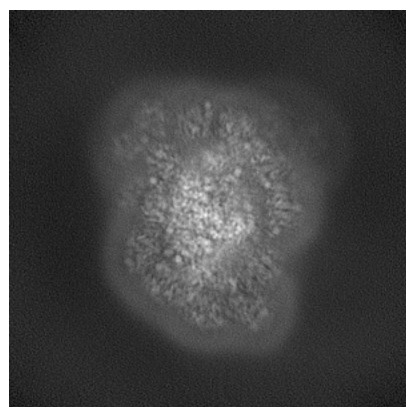


Y

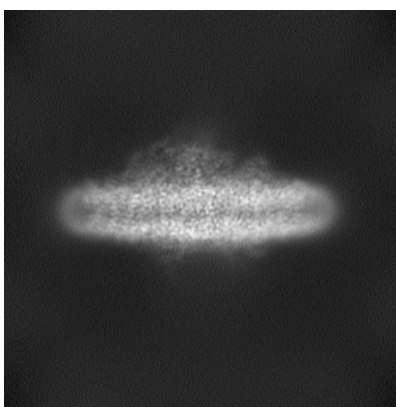


Z

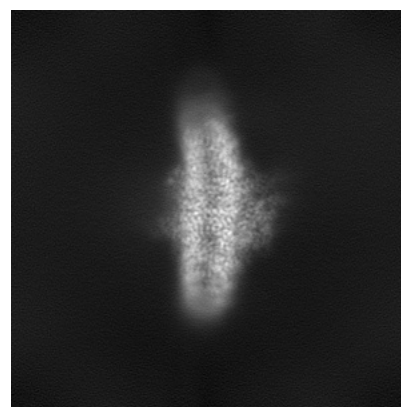
6.1.2 Raw map



X



Y

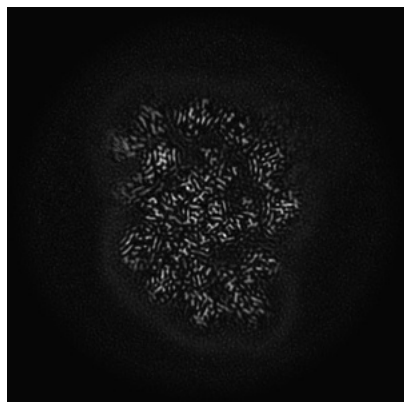


Z

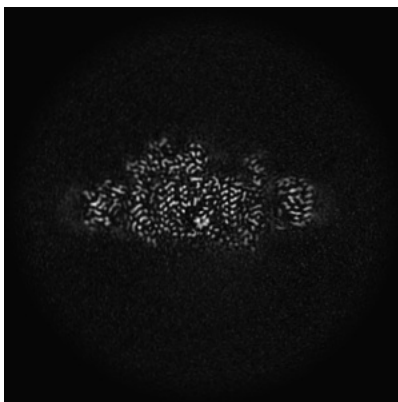
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

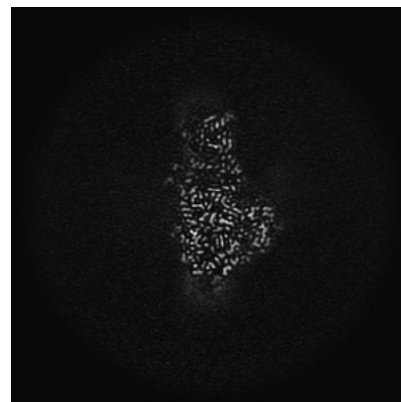
6.2.1 Primary map



X Index: 160

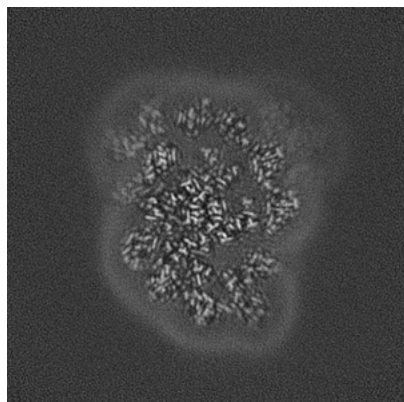


Y Index: 160

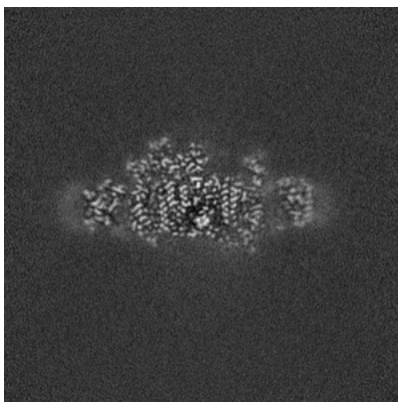


Z Index: 160

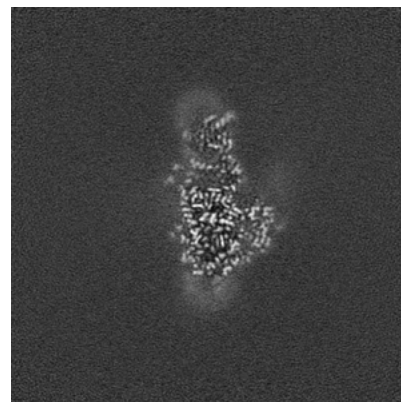
6.2.2 Raw map



X Index: 160



Y Index: 160

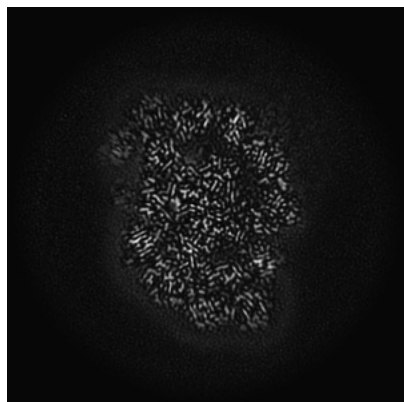


Z Index: 160

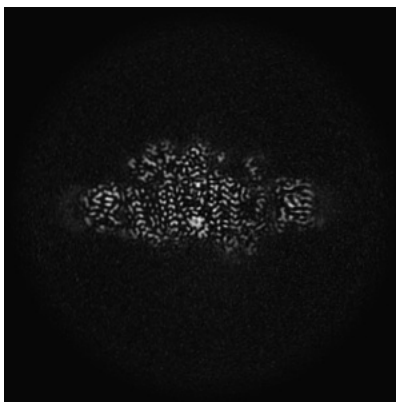
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

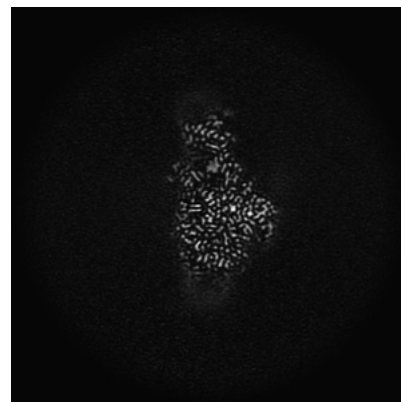
6.3.1 Primary map



X Index: 167

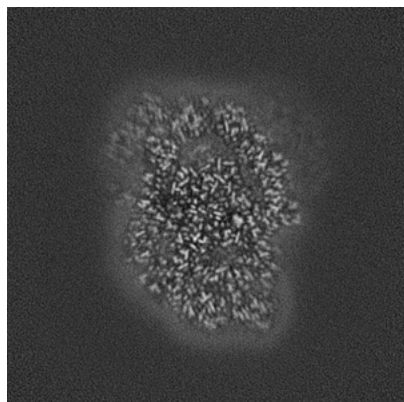


Y Index: 157

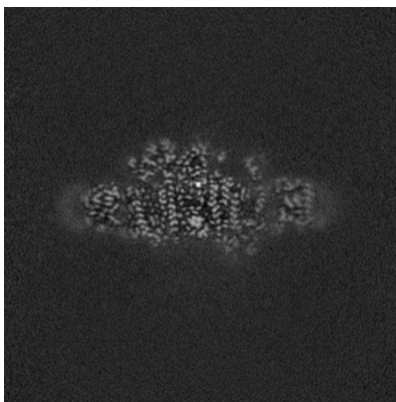


Z Index: 155

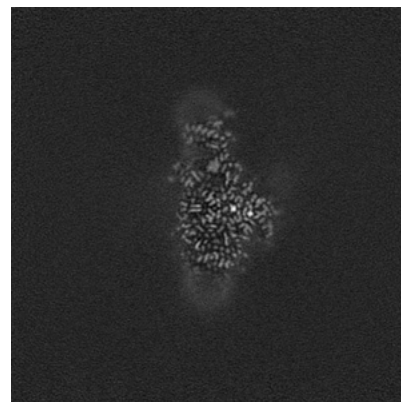
6.3.2 Raw map



X Index: 170



Y Index: 157

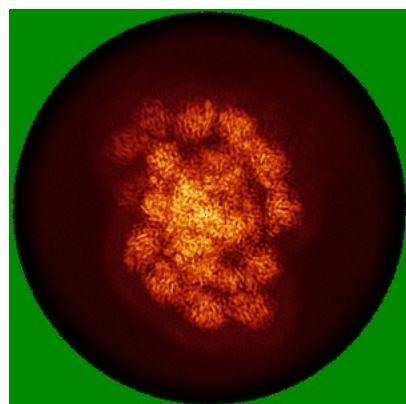


Z Index: 155

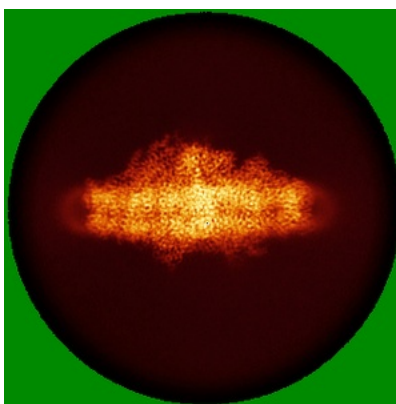
The images above show the largest variance slices of the map in three orthogonal directions.

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

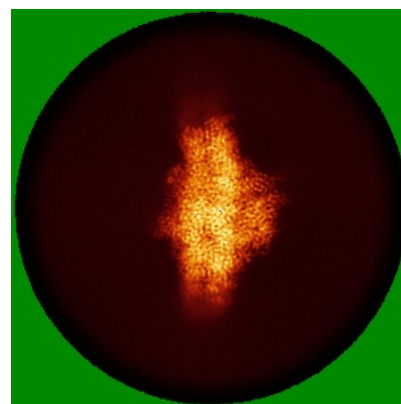
6.4.1 Primary map



X

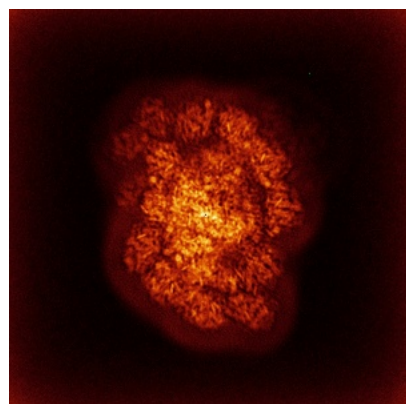


Y

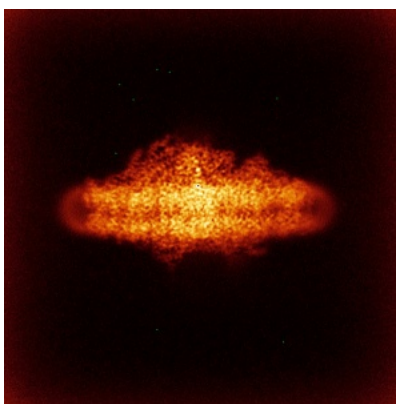


Z

6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

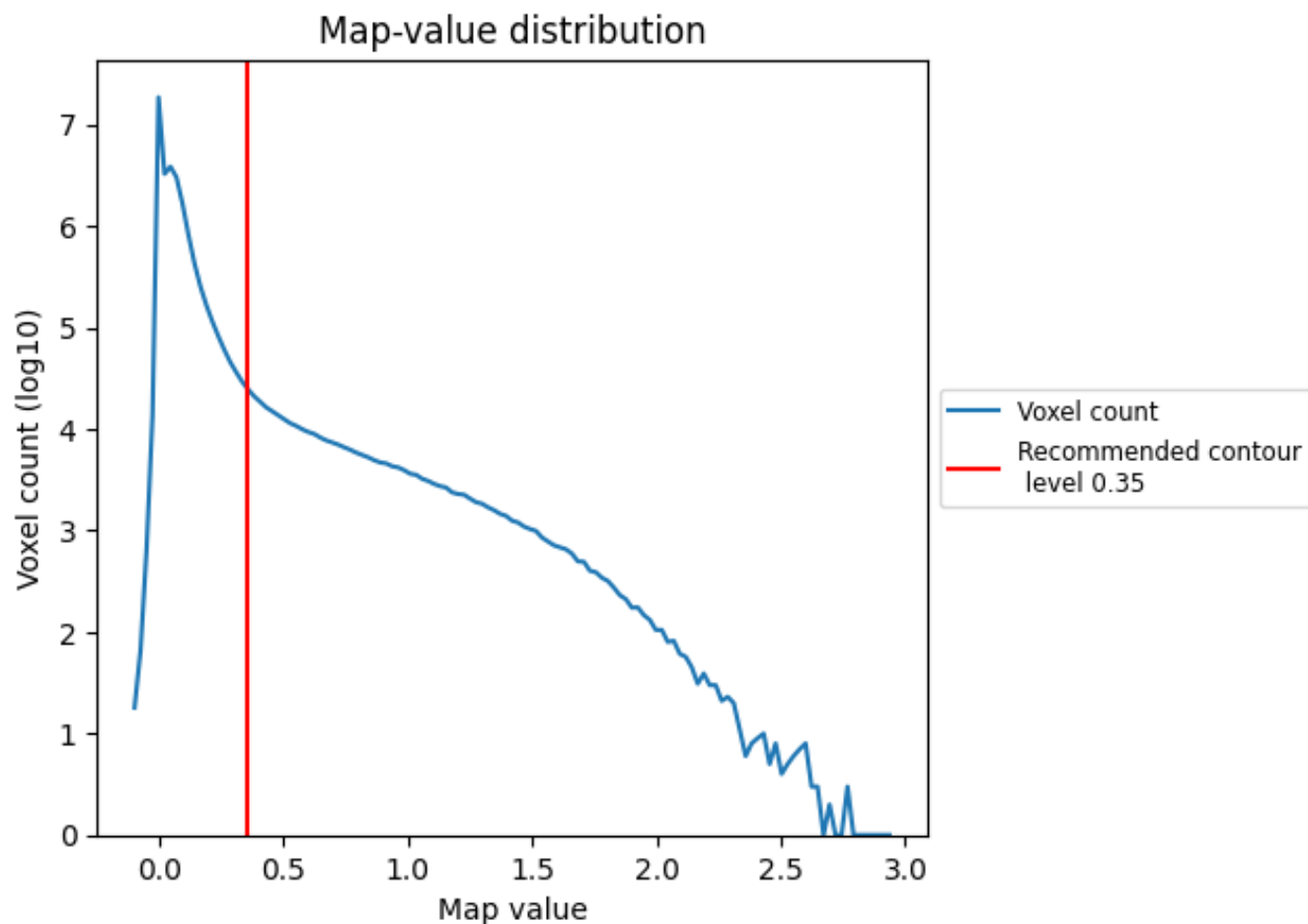
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

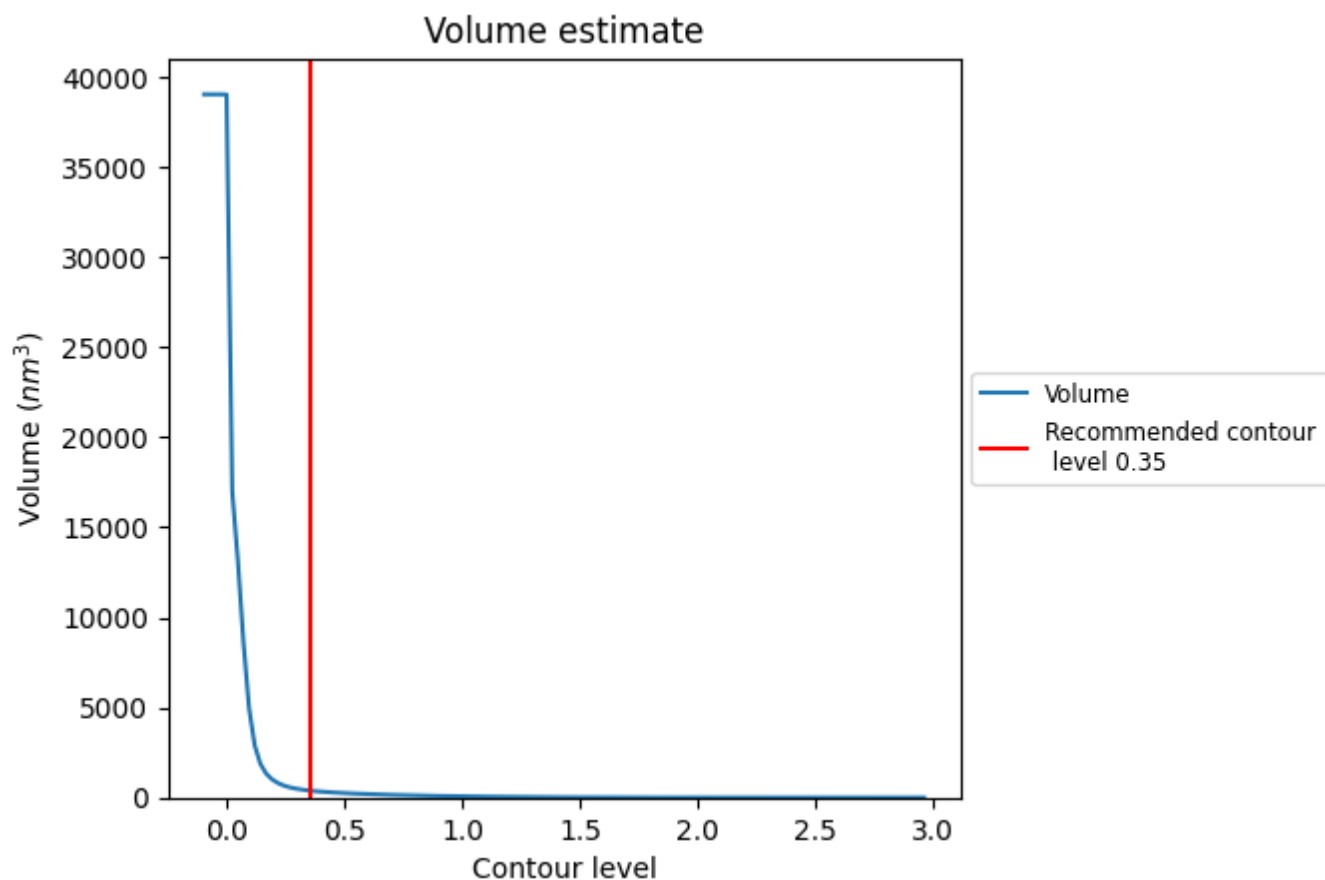
This section contains the results of statistical analysis of the map.

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.

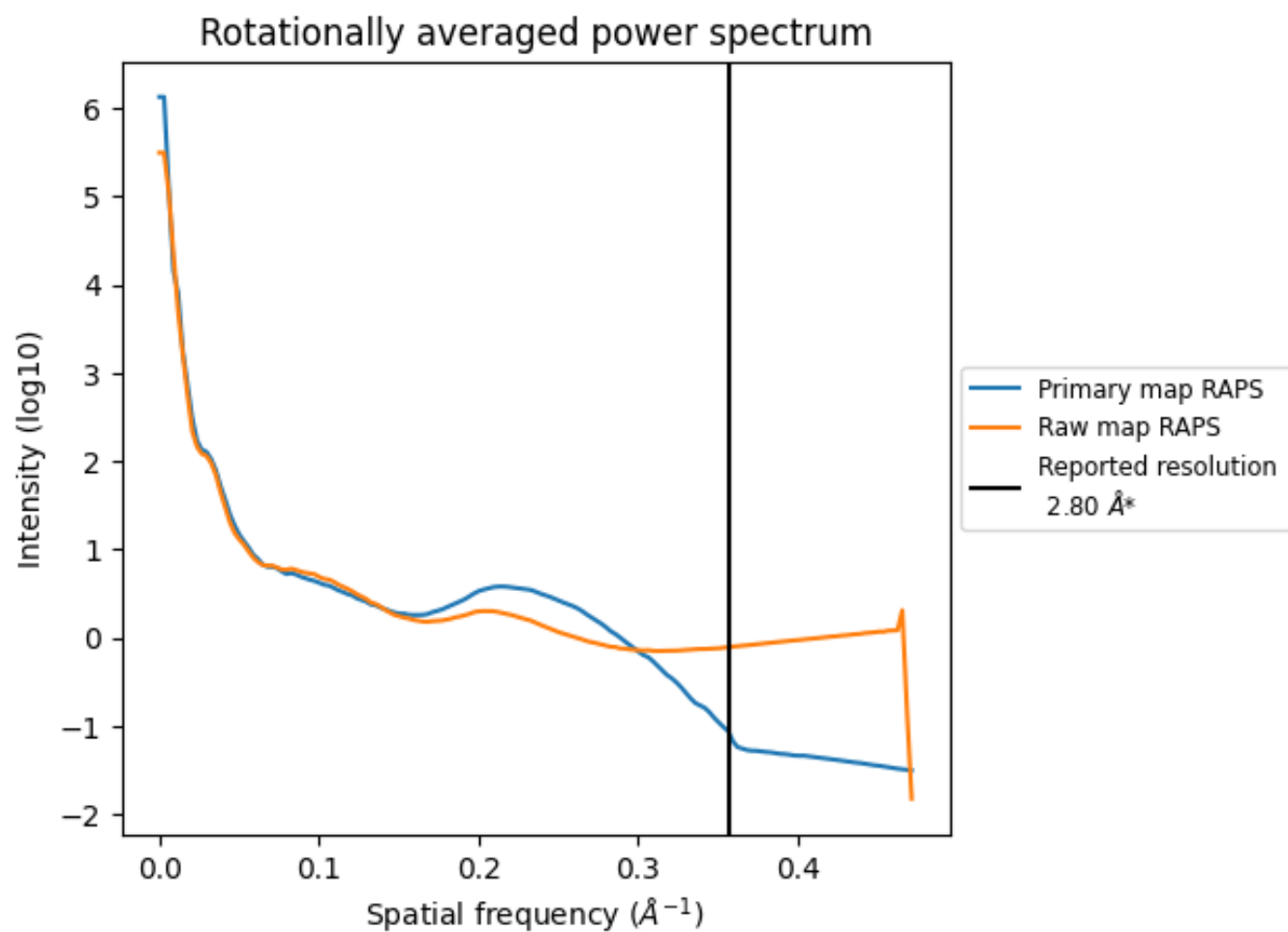
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 386 nm³; this corresponds to an approximate mass of 349 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 ⓘ

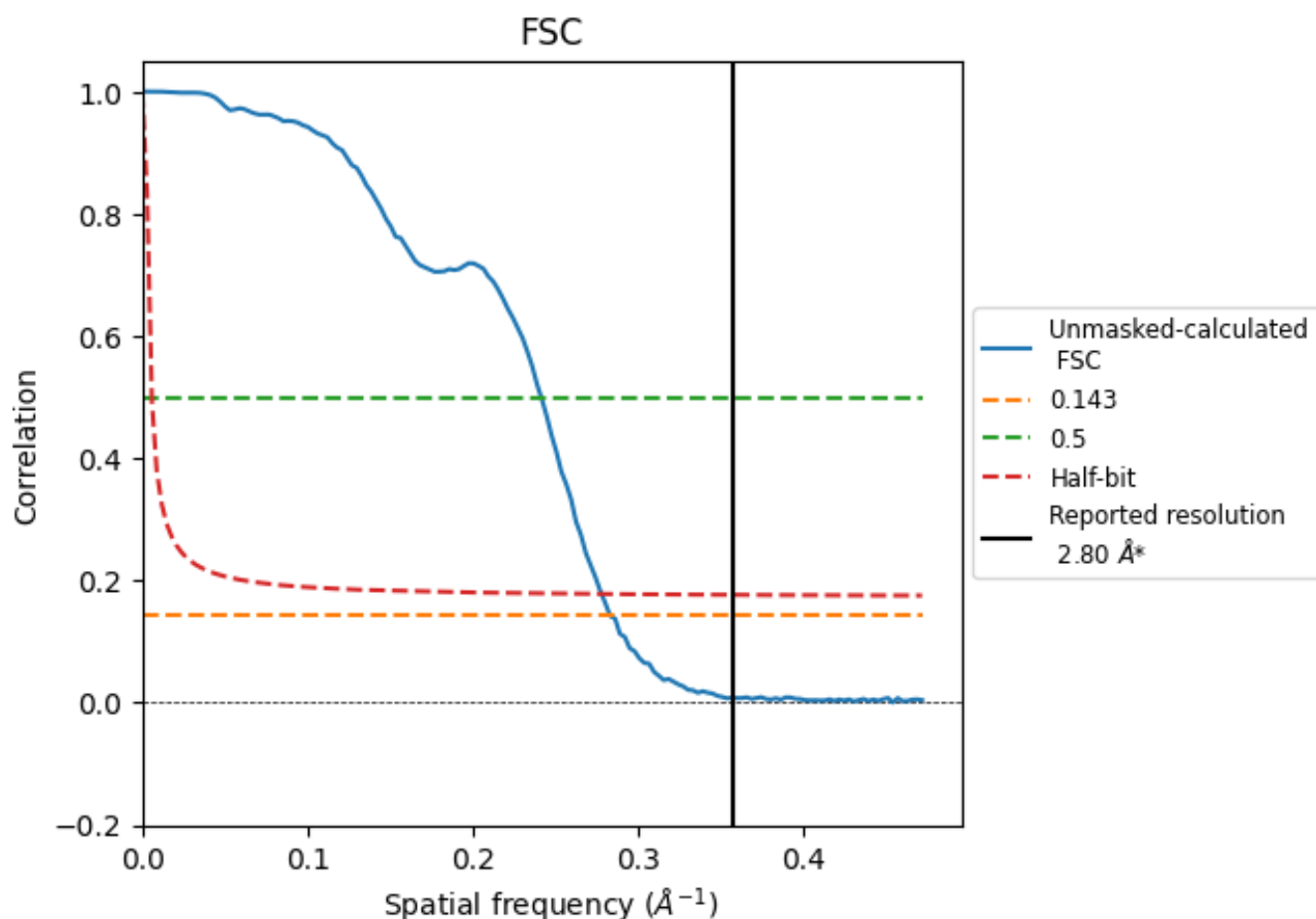


*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

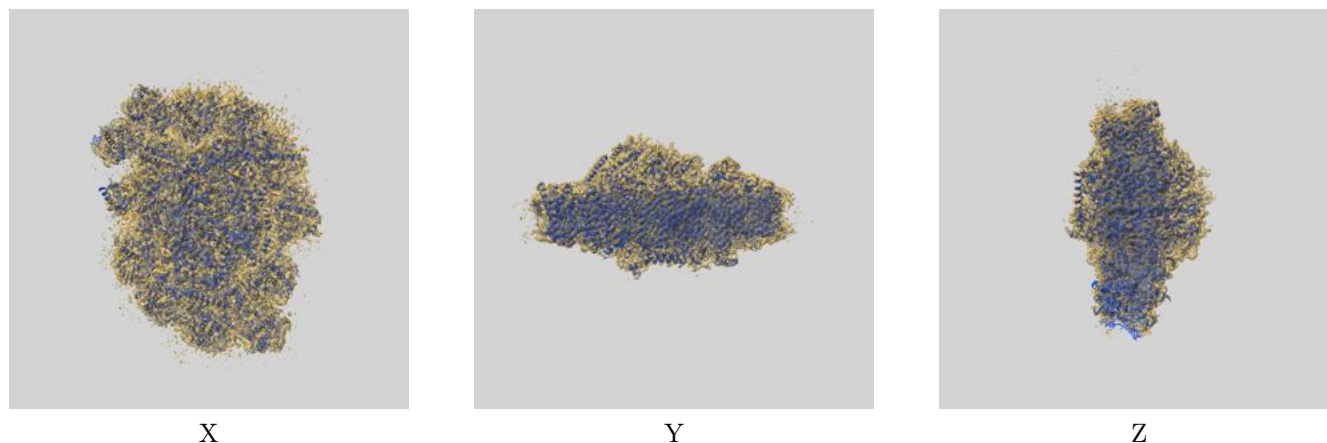
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	4.14	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

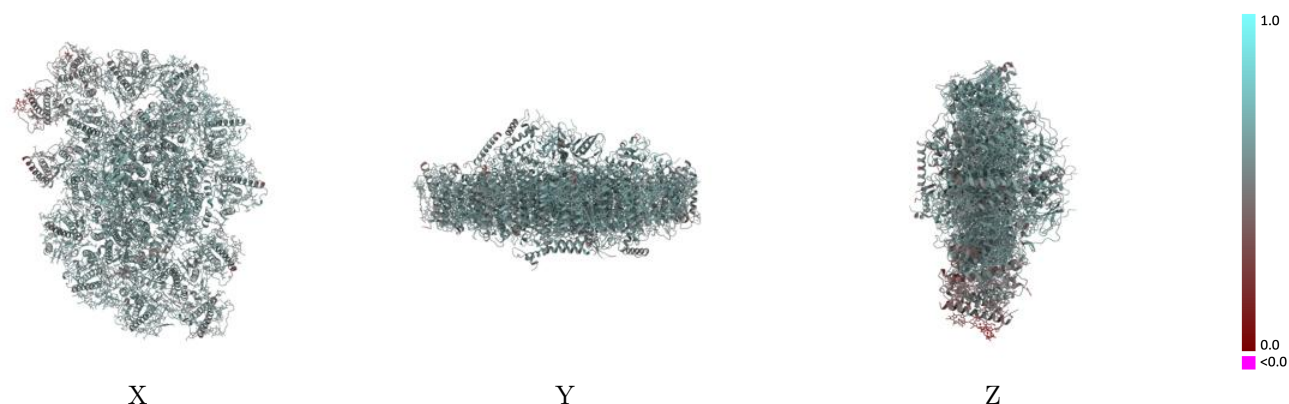
This section contains information regarding the fit between EMDB map EMD-36366 and PDB model 8JJR. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

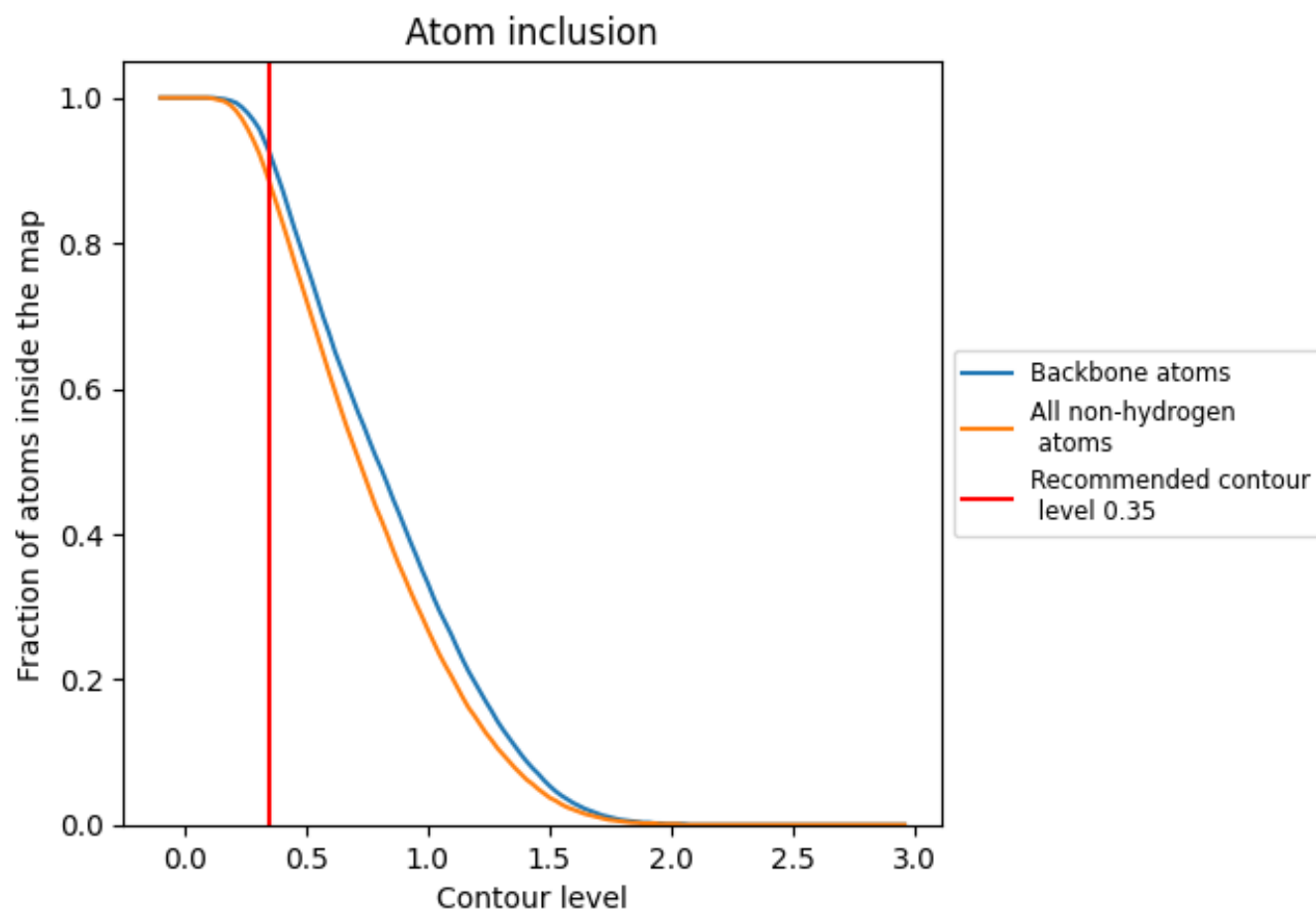


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.5750
A	 0.8810	 0.5710
B	 0.9160	 0.5810
C	 0.8970	 0.5880
D	 0.9220	 0.6000
E	 0.9190	 0.5760
F	 0.8660	 0.5680
G	 0.8660	 0.5410
H	 0.9040	 0.5730
I	 0.8900	 0.5700
J	 0.8410	 0.5450
K	 0.6670	 0.4810
T	 0.6320	 0.4260
U	 0.6680	 0.4840
a	 0.9250	 0.6020
b	 0.9490	 0.6130
c	 0.9760	 0.6000
d	 0.9020	 0.5800
e	 0.9500	 0.6090
f	 0.8320	 0.5850
i	 0.8890	 0.5790
j	 0.8380	 0.5740
l	 0.9350	 0.6010
m	 0.9130	 0.6000
r	 0.9290	 0.5780
x	 0.9140	 0.5860
y	 0.7230	 0.5400

