



## Full wwPDB EM Validation Report ⓘ

Feb 18, 2024 – 07:39 PM JST

PDB ID : 8JW0  
EMDB ID : EMD-36678  
Title : PSI-AcpPCI supercomplex from *Amphidinium carterae*  
Authors : Li, Z.H.; Li, X.Y.; Wang, W.D.  
Deposited on : 2023-06-28  
Resolution : 2.90 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

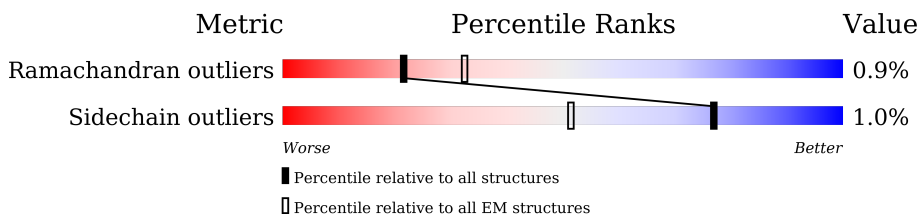
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.90 Å.

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



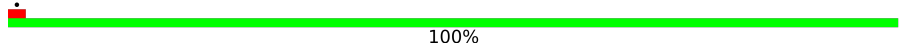
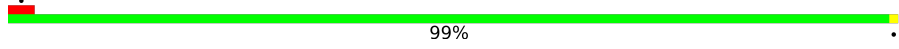
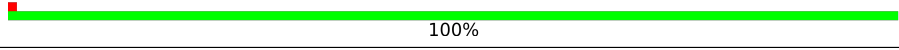
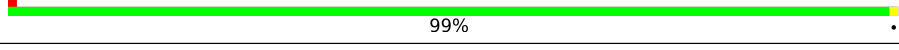
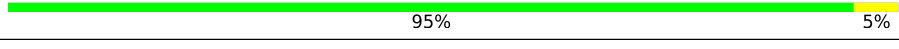
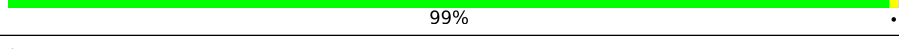
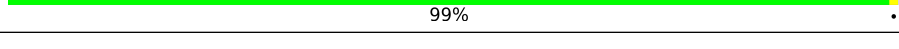
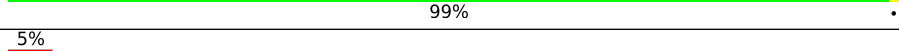
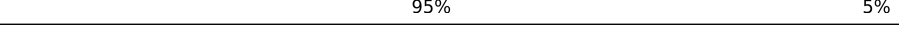
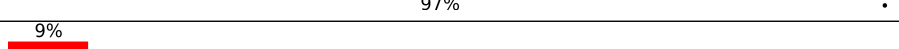
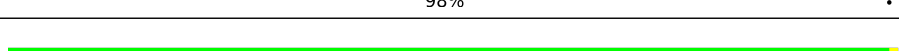
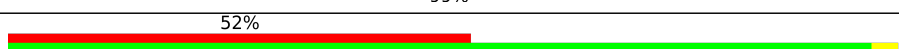

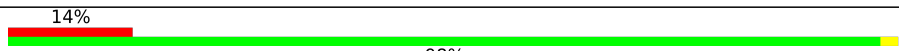
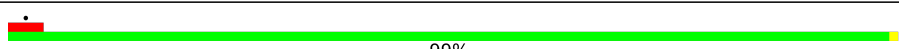
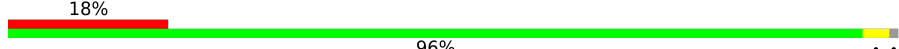
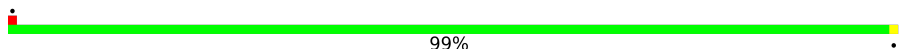
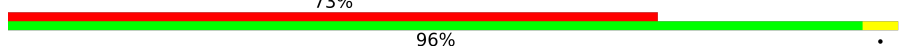
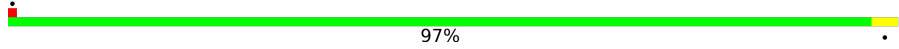

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	a	645	5% 99%
2	b	617	99%
3	c	86	100%
4	d	257	99%
5	e	74	100%
6	f	185	100%
7	h	132	95% 5%
8	i	126	98%
9	j	70	97%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	l	253	 100%
11	m	89	 99%
12	A	180	 100%
13	G	215	 99%
14	I	194	 95% 5%
15	K	172	 99%
16	F	176	 99%
17	J	165	 99%
18	M	168	 95% 5% 5%
19	L	185	 97%
20	D	160	 98% 9%
21	B	172	 99%
22	H	160	 97% 52%
23	N	160	 96% 39%
24	O	161	 98% 14%
25	C	160	 99%
25	T	160	 96% 18%
26	Q	162	 99%
27	P	160	 96% 73%
28	E	142	 97%

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
29	CLA	A	206	X	-	-	-
29	CLA	A	207	X	-	-	-
29	CLA	A	208	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	209	X	-	-	-
29	CLA	A	210	X	-	-	-
29	CLA	A	211	X	-	-	-
29	CLA	A	212	X	-	-	-
29	CLA	A	214	X	-	-	-
29	CLA	A	215	X	-	-	-
29	CLA	A	216	X	-	-	-
29	CLA	A	217	X	-	-	-
29	CLA	A	218	X	-	-	-
29	CLA	B	306	X	-	-	-
29	CLA	B	307	X	-	-	-
29	CLA	B	308	X	-	-	-
29	CLA	B	309	X	-	-	-
29	CLA	B	310	X	-	-	-
29	CLA	B	311	X	-	-	-
29	CLA	B	312	X	-	-	-
29	CLA	B	314	X	-	-	-
29	CLA	B	315	X	-	-	-
29	CLA	B	316	X	-	-	-
29	CLA	C	308	X	-	-	-
29	CLA	C	309	X	-	-	-
29	CLA	C	311	X	-	-	-
29	CLA	C	313	X	-	-	-
29	CLA	C	314	X	-	-	-
29	CLA	C	316	X	-	-	-
29	CLA	D	308	X	-	-	-
29	CLA	D	309	X	-	-	-
29	CLA	D	311	X	-	-	-
29	CLA	D	312	X	-	-	-
29	CLA	D	313	X	-	-	-
29	CLA	D	314	X	-	-	-
29	CLA	D	316	X	-	-	-
29	CLA	E	305	X	-	-	-
29	CLA	E	306	X	-	-	-
29	CLA	E	308	X	-	-	-
29	CLA	E	309	X	-	-	-
29	CLA	E	310	X	-	-	-
29	CLA	E	311	X	-	-	-
29	CLA	E	313	X	-	-	-
29	CLA	E	315	X	-	-	-
29	CLA	F	307	X	-	-	-
29	CLA	F	308	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	F	310	X	-	-	-
29	CLA	F	311	X	-	-	-
29	CLA	F	312	X	-	-	-
29	CLA	F	313	X	-	-	-
29	CLA	F	315	X	-	-	-
29	CLA	F	316	X	-	-	-
29	CLA	G	301	X	-	-	-
29	CLA	G	302	X	-	-	-
29	CLA	G	304	X	-	-	-
29	CLA	G	311	X	-	-	-
29	CLA	G	312	X	-	-	-
29	CLA	G	313	X	-	-	-
29	CLA	G	314	X	-	-	-
29	CLA	G	316	X	-	-	-
29	CLA	G	317	X	-	-	-
29	CLA	G	319	X	-	-	-
29	CLA	H	307	X	-	-	-
29	CLA	H	308	X	-	-	-
29	CLA	H	310	X	-	-	-
29	CLA	H	312	X	-	-	-
29	CLA	H	313	X	-	-	-
29	CLA	H	315	X	-	-	-
29	CLA	I	201	X	-	-	-
29	CLA	I	207	X	-	-	-
29	CLA	I	208	X	-	-	-
29	CLA	I	209	X	-	-	-
29	CLA	I	210	X	-	-	-
29	CLA	I	211	X	-	-	-
29	CLA	I	212	X	-	-	-
29	CLA	I	213	X	-	-	-
29	CLA	I	214	X	-	-	-
29	CLA	I	216	X	-	-	-
29	CLA	I	217	X	-	-	-
29	CLA	J	305	X	-	-	-
29	CLA	J	306	X	-	-	-
29	CLA	J	307	X	-	-	-
29	CLA	J	308	X	-	-	-
29	CLA	J	309	X	-	-	-
29	CLA	J	310	X	-	-	-
29	CLA	J	311	X	-	-	-
29	CLA	J	313	X	-	-	-
29	CLA	K	207	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	K	208	X	-	-	-
29	CLA	K	209	X	-	-	-
29	CLA	K	210	X	-	-	-
29	CLA	K	211	X	-	-	-
29	CLA	K	212	X	-	-	-
29	CLA	K	213	X	-	-	-
29	CLA	K	214	X	-	-	-
29	CLA	K	216	X	-	-	-
29	CLA	K	217	X	-	-	-
29	CLA	K	218	X	-	-	-
29	CLA	L	307	X	-	-	-
29	CLA	L	308	X	-	-	-
29	CLA	L	309	X	-	-	-
29	CLA	L	310	X	-	-	-
29	CLA	L	311	X	-	-	-
29	CLA	L	312	X	-	-	-
29	CLA	L	313	X	-	-	-
29	CLA	L	315	X	-	-	-
29	CLA	L	316	X	-	-	-
29	CLA	L	317	X	-	-	-
29	CLA	M	306	X	-	-	-
29	CLA	M	307	X	-	-	-
29	CLA	M	308	X	-	-	-
29	CLA	M	309	X	-	-	-
29	CLA	M	310	X	-	-	-
29	CLA	M	311	X	-	-	-
29	CLA	M	313	X	-	-	-
29	CLA	M	314	X	-	-	-
29	CLA	M	315	X	-	-	-
29	CLA	N	308	X	-	-	-
29	CLA	N	309	X	-	-	-
29	CLA	N	311	X	-	-	-
29	CLA	N	313	X	-	-	-
29	CLA	N	314	X	-	-	-
29	CLA	N	316	X	-	-	-
29	CLA	O	308	X	-	-	-
29	CLA	O	311	X	-	-	-
29	CLA	O	313	X	-	-	-
29	CLA	O	316	X	-	-	-
29	CLA	P	209	X	-	-	-
29	CLA	P	210	X	-	-	-
29	CLA	P	212	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	P	214	X	-	-	-
29	CLA	P	215	X	-	-	-
29	CLA	P	217	X	-	-	-
29	CLA	Q	307	X	-	-	-
29	CLA	Q	308	X	-	-	-
29	CLA	Q	310	X	-	-	-
29	CLA	Q	312	X	-	-	-
29	CLA	Q	313	X	-	-	-
29	CLA	Q	315	X	-	-	-
29	CLA	T	308	X	-	-	-
29	CLA	T	309	X	-	-	-
29	CLA	T	311	X	-	-	-
29	CLA	T	313	X	-	-	-
29	CLA	T	314	X	-	-	-
29	CLA	T	316	X	-	-	-
29	CLA	a	801	X	-	-	-
29	CLA	a	802	X	-	-	-
29	CLA	a	803	X	-	-	-
29	CLA	a	804	X	-	-	-
29	CLA	a	805	X	-	-	-
29	CLA	a	806	X	-	-	-
29	CLA	a	807	X	-	-	-
29	CLA	a	808	X	-	-	-
29	CLA	a	809	X	-	-	-
29	CLA	a	810	X	-	-	-
29	CLA	a	811	X	-	-	-
29	CLA	a	812	X	-	-	-
29	CLA	a	813	X	-	-	-
29	CLA	a	814	X	-	-	-
29	CLA	a	815	X	-	-	-
29	CLA	a	816	X	-	-	-
29	CLA	a	817	X	-	-	-
29	CLA	a	818	X	-	-	-
29	CLA	a	819	X	-	-	-
29	CLA	a	820	X	-	-	-
29	CLA	a	821	X	-	-	-
29	CLA	a	822	X	-	-	-
29	CLA	a	823	X	-	-	-
29	CLA	a	824	X	-	-	-
29	CLA	a	825	X	-	-	-
29	CLA	a	826	X	-	-	-
29	CLA	a	827	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	a	828	X	-	-	-
29	CLA	a	829	X	-	-	-
29	CLA	a	830	X	-	-	-
29	CLA	a	831	X	-	-	-
29	CLA	a	837	X	-	-	-
29	CLA	b	701	X	-	-	-
29	CLA	b	702	X	-	-	-
29	CLA	b	703	X	-	-	-
29	CLA	b	704	X	-	-	-
29	CLA	b	705	X	-	-	-
29	CLA	b	706	X	-	-	-
29	CLA	b	707	X	-	-	-
29	CLA	b	708	X	-	-	-
29	CLA	b	709	X	-	-	-
29	CLA	b	710	X	-	-	-
29	CLA	b	711	X	-	-	-
29	CLA	b	712	X	-	-	-
29	CLA	b	713	X	-	-	-
29	CLA	b	714	X	-	-	-
29	CLA	b	715	X	-	-	-
29	CLA	b	716	X	-	-	-
29	CLA	b	717	X	-	-	-
29	CLA	b	718	X	-	-	-
29	CLA	b	719	X	-	-	-
29	CLA	b	720	X	-	-	-
29	CLA	b	721	X	-	-	-
29	CLA	b	722	X	-	-	-
29	CLA	b	723	X	-	-	-
29	CLA	b	724	X	-	-	-
29	CLA	b	725	X	-	-	-
29	CLA	b	726	X	-	-	-
29	CLA	b	731	X	-	-	-
29	CLA	b	736	X	-	-	-
29	CLA	f	802	X	-	-	-
29	CLA	f	803	X	-	-	-
29	CLA	f	805	X	-	-	-
29	CLA	h	201	X	-	-	-
29	CLA	i	201	X	-	-	-
29	CLA	i	202	X	-	-	-
29	CLA	i	203	X	-	-	-
29	CLA	j	104	X	-	-	-
29	CLA	l	501	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
29	CLA	1	502	X	-	-	-
29	CLA	1	503	X	-	-	-
29	CLA	1	504	X	-	-	-
29	CLA	1	505	X	-	-	-
29	CLA	1	508	X	-	-	-
29	CLA	1	509	X	-	-	-
29	CLA	1	510	X	-	-	-

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 63119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	645	Total	C	N	O	S	0	0
			4980	3267	825	874	14		

- Molecule 2 is a protein called Photosystem I PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	617	Total	C	N	O	S	0	0
			4813	3185	765	848	15		

- Molecule 3 is a protein called Photosystem I PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	86	Total	C	N	O	S	0	0
			647	401	109	128	9		

- Molecule 4 is a protein called Photosystem I PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	257	Total	C	N	O	S	0	0
			1985	1259	340	375	11		

- Molecule 5 is a protein called Photosystem I PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	e	74	Total	C	N	O	0	0
			607	392	102	113		

- Molecule 6 is a protein called Photosystem I PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	185	Total	C	N	O	S	0	0
			1455	926	257	263	9		

- Molecule 7 is a protein called Photosystem I PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	h	132	1056	693	167	191	5	0	0

- Molecule 8 is a protein called Photosystem I PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	i	126	1001	651	164	183	3	0	0

- Molecule 9 is a protein called Photosystem I PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	j	70	549	362	86	100	1	0	0

- Molecule 10 is a protein called Photosystem I PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	l	253	1961	1274	321	355	11	0	0

- Molecule 11 is a protein called Photosystem I PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	m	89	679	438	109	131	1	0	0

- Molecule 12 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A	180	1358	882	221	245	10	0	0

- Molecule 13 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	215	1675	1086	278	299	12	0	0

- Molecule 14 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	I	194	1455	946	244	253	12	0	0

- Molecule 15 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	172	1325	857	222	234	12	0	0

- Molecule 16 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	F	176	1356	869	226	249	12	0	0

- Molecule 17 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	J	165	1282	828	207	239	8	0	0

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	M	168	1346	885	224	232	5	0	0

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	L	185	1453	942	242	263	6	0	0

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	D	160	1198	761	200	230	7	0	0

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	B	172	1371	888	226	245	12	0	0

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	H	160	1202	769	198	228	7	0	0

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	N	160	1203	767	200	229	7	0	0

- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	O	161	1226	789	204	226	7	0	0

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	T	159	1189	756	199	226	8	0	0
25	C	160	1200	765	200	227	8	0	0

- Molecule 26 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-17, acpPCI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Q	162	1219	787	204	219	9	0	0

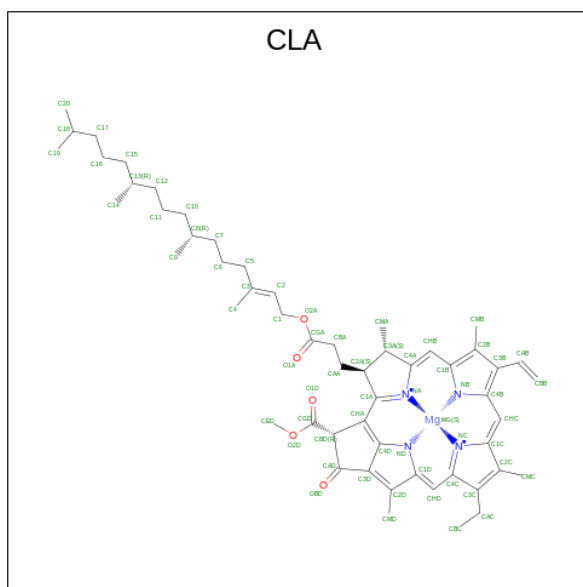
- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	P	160	1218	778	204	228	8	0	0

- Molecule 28 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-1, acpPCI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	E	142	1071	684	178	201	8	0	0

- Molecule 29 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	a	1	65	55	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	65	55	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	a	1	55	45	1	4	5	0
29	a	1	55	45	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	51	41	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	55	45	1	4	5	0
29	a	1	56	46	1	4	5	0
29	a	1	60	50	1	4	5	0
29	a	1	51	41	1	4	5	0
29	a	1	46	36	1	4	5	0
29	a	1	45	35	1	4	5	0
29	a	1	46	36	1	4	5	0
29	a	1	45	35	1	4	5	0
29	a	1	47	37	1	4	5	0
29	a	1	57	47	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	47	37	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	58	48	1	4	5	0
29	a	1	65	55	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	a	1	65	55	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	46	36	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	56	46	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	55	45	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	52	42	1	4	5	0
29	b	1	60	50	1	4	5	0
29	b	1	46	36	1	4	5	0
29	b	1	58	48	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	53	43	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	b	1	64	54	1	4	5	0
29	b	1	46	36	1	4	5	0
29	b	1	53	43	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	50	40	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	58	48	1	4	5	0
29	b	1	58	48	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	47	37	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	56	46	1	4	5	0
29	b	1	65	55	1	4	5	0
29	f	1	46	36	1	4	5	0
29	f	1	46	36	1	4	5	0
29	f	1	60	50	1	4	5	0
29	h	1	60	50	1	4	5	0
29	i	1	65	55	1	4	5	0
29	i	1	65	55	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	i	1	55	45	1	4	5	0
29	j	1	52	42	1	4	5	0
29	l	1	60	50	1	4	5	0
29	l	1	65	55	1	4	5	0
29	l	1	65	55	1	4	5	0
29	l	1	65	55	1	4	5	0
29	l	1	65	55	1	4	5	0
29	l	1	41	33	1	4	3	0
29	l	1	41	33	1	4	3	0
29	l	1	45	35	1	4	5	0
29	A	1	45	35	1	4	5	0
29	A	1	55	45	1	4	5	0
29	A	1	55	45	1	4	5	0
29	A	1	65	55	1	4	5	0
29	A	1	46	36	1	4	5	0
29	A	1	55	45	1	4	5	0
29	A	1	55	45	1	4	5	0
29	A	1	41	33	1	4	3	0
29	A	1	47	37	1	4	5	0
29	A	1	41	33	1	4	3	0
29	A	1	51	41	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	A	1	60	50	1	4	5	0
29	G	1	49	39	1	4	5	0
29	G	1	65	55	1	4	5	0
29	G	1	61	51	1	4	5	0
29	G	1	51	41	1	4	5	0
29	G	1	65	55	1	4	5	0
29	G	1	55	45	1	4	5	0
29	G	1	60	50	1	4	5	0
29	G	1	65	55	1	4	5	0
29	G	1	53	43	1	4	5	0
29	G	1	41	33	1	4	3	0
29	I	1	45	35	1	4	5	0
29	I	1	49	39	1	4	5	0
29	I	1	46	36	1	4	5	0
29	I	1	60	50	1	4	5	0
29	I	1	55	45	1	4	5	0
29	I	1	65	55	1	4	5	0
29	I	1	55	45	1	4	5	0
29	I	1	65	55	1	4	5	0
29	I	1	55	45	1	4	5	0
29	I	1	52	42	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	I	1	55	45	1	4	5	0
29	K	1	49	39	1	4	5	0
29	K	1	46	36	1	4	5	0
29	K	1	54	44	1	4	5	0
29	K	1	50	40	1	4	5	0
29	K	1	55	45	1	4	5	0
29	K	1	52	42	1	4	5	0
29	K	1	48	38	1	4	5	0
29	K	1	55	45	1	4	5	0
29	K	1	41	33	1	4	3	0
29	K	1	46	36	1	4	5	0
29	K	1	45	35	1	4	5	0
29	F	1	46	36	1	4	5	0
29	F	1	46	36	1	4	5	0
29	F	1	46	36	1	4	5	0
29	F	1	46	36	1	4	5	0
29	F	1	46	36	1	4	5	0
29	F	1	46	36	1	4	5	0
29	F	1	41	33	1	4	3	0
29	F	1	41	33	1	4	3	0
29	J	1	46	36	1	4	5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	J	1	65	55	1	4	5	0
29	J	1	46	36	1	4	5	0
29	J	1	56	46	1	4	5	0
29	J	1	46	36	1	4	5	0
29	J	1	47	37	1	4	5	0
29	J	1	53	43	1	4	5	0
29	J	1	41	33	1	4	3	0
29	M	1	53	43	1	4	5	0
29	M	1	55	45	1	4	5	0
29	M	1	48	38	1	4	5	0
29	M	1	46	36	1	4	5	0
29	M	1	48	38	1	4	5	0
29	M	1	46	36	1	4	5	0
29	M	1	41	33	1	4	3	0
29	M	1	52	42	1	4	5	0
29	M	1	46	36	1	4	5	0
29	L	1	50	40	1	4	5	0
29	L	1	53	43	1	4	5	0
29	L	1	55	45	1	4	5	0
29	L	1	55	45	1	4	5	0
29	L	1	46	36	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	L	1	55	45	1	4	5	0
29	L	1	53	43	1	4	5	0
29	L	1	41	33	1	4	3	0
29	L	1	52	42	1	4	5	0
29	L	1	46	36	1	4	5	0
29	D	1	47	37	1	4	5	0
29	D	1	46	36	1	4	5	0
29	D	1	46	36	1	4	5	0
29	D	1	46	36	1	4	5	0
29	D	1	45	35	1	4	5	0
29	D	1	47	37	1	4	5	0
29	D	1	41	33	1	4	3	0
29	B	1	49	39	1	4	5	0
29	B	1	45	35	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	55	45	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	51	41	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	41	33	1	4	3	0
29	B	1	46	36	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	B	1	45	35	1	4	5	0
29	H	1	47	37	1	4	5	0
29	H	1	65	55	1	4	5	0
29	H	1	51	41	1	4	5	0
29	H	1	46	36	1	4	5	0
29	H	1	47	37	1	4	5	0
29	H	1	41	33	1	4	3	0
29	N	1	47	37	1	4	5	0
29	N	1	65	55	1	4	5	0
29	N	1	51	41	1	4	5	0
29	N	1	46	36	1	4	5	0
29	N	1	47	37	1	4	5	0
29	N	1	41	33	1	4	3	0
29	O	1	47	37	1	4	5	0
29	O	1	65	55	1	4	5	0
29	O	1	51	41	1	4	5	0
29	O	1	46	36	1	4	5	0
29	O	1	47	37	1	4	5	0
29	O	1	41	33	1	4	3	0
29	T	1	47	37	1	4	5	0
29	T	1	46	36	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

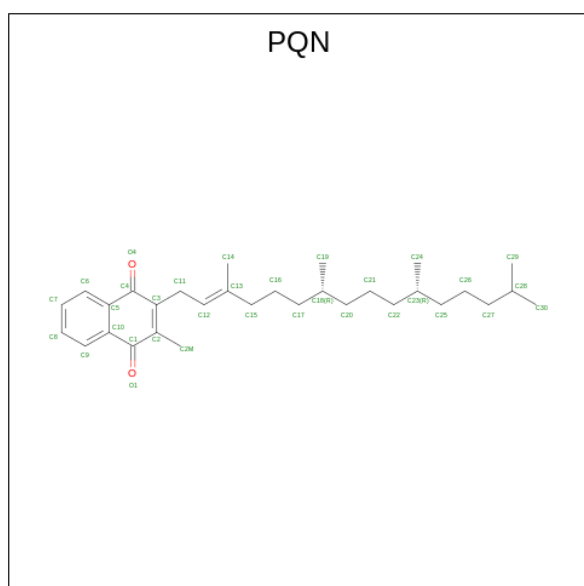
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	T	1	46	36	1	4	5	0
29	T	1	46	36	1	4	5	0
29	T	1	47	37	1	4	5	0
29	T	1	41	33	1	4	3	0
29	Q	1	47	37	1	4	5	0
29	Q	1	65	55	1	4	5	0
29	Q	1	65	55	1	4	5	0
29	Q	1	46	36	1	4	5	0
29	Q	1	47	37	1	4	5	0
29	Q	1	41	33	1	4	3	0
29	C	1	47	37	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	51	41	1	4	5	0
29	C	1	46	36	1	4	5	0
29	C	1	47	37	1	4	5	0
29	C	1	41	33	1	4	3	0
29	P	1	47	37	1	4	5	0
29	P	1	65	55	1	4	5	0
29	P	1	51	41	1	4	5	0
29	P	1	46	36	1	4	5	0
29	P	1	47	37	1	4	5	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	E	1	Total 61	C 51	Mg 1	N 4	O 5	0
29	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	E	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	E	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	E	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	E	1	Total 48	C 38	Mg 1	N 4	O 5	0
29	E	1	Total 57	C 47	Mg 1	N 4	O 5	0

- Molecule 30 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



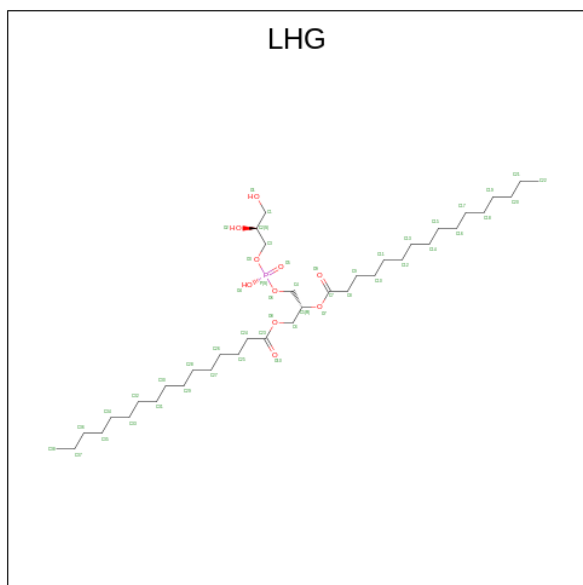
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	a	1	Total 33	C 31	O 2	0

Continued on next page...

Continued from previous page...

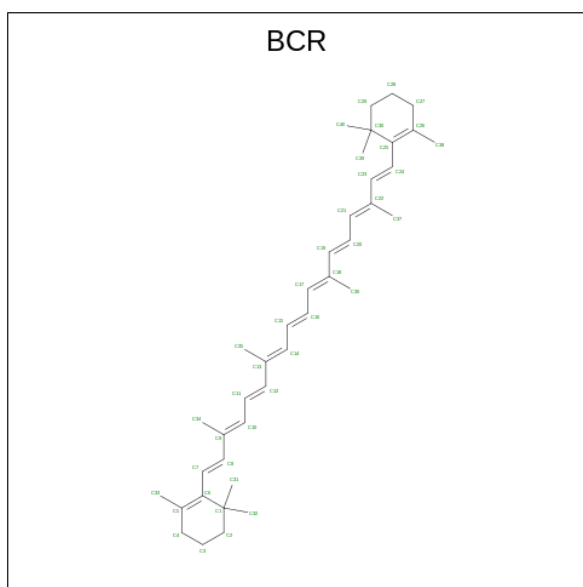
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	b	1	33	31	2	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
31	a	1	48	37	10	1	0

- Molecule 32 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



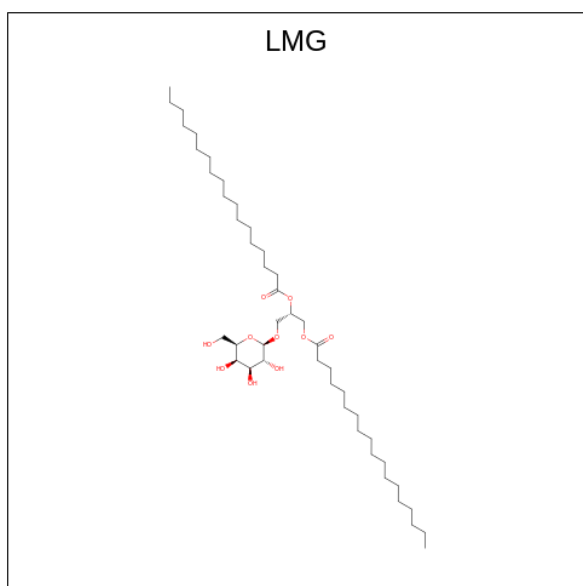
Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	i	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	m	1	Total C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

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

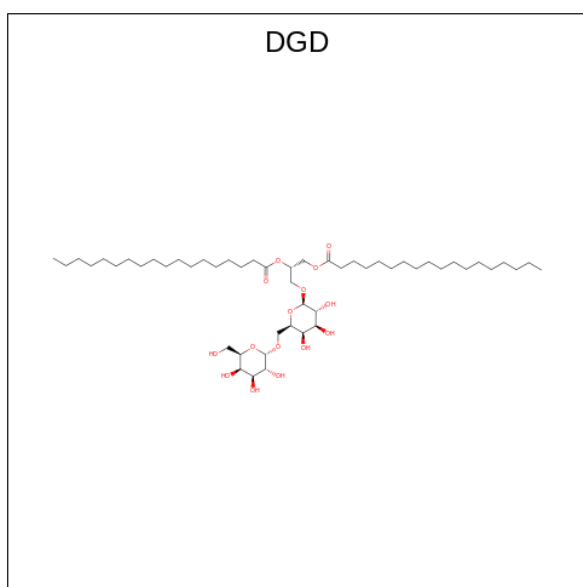
- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).





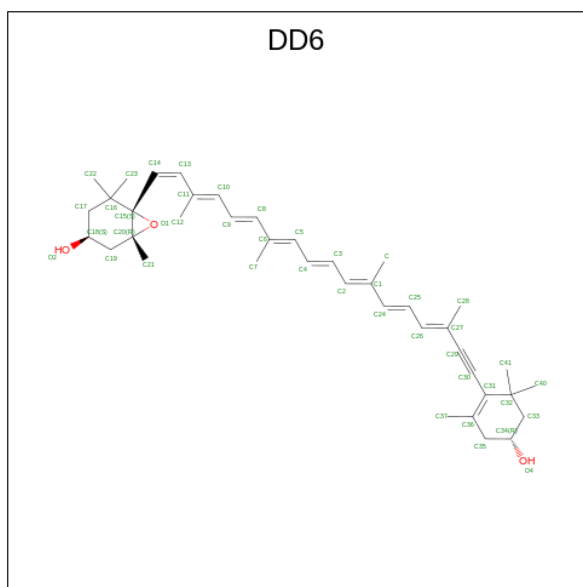
Mol	Chain	Residues	Atoms			AltConf
34	b	1	Total	C	O	0
			46	36	10	
34	b	1	Total	C	O	0
			44	34	10	
34	b	1	Total	C	O	0
			40	30	10	
34	h	1	Total	C	O	0
			28	18	10	
34	j	1	Total	C	O	0
			43	33	10	
34	A	1	Total	C	O	0
			37	27	10	
34	K	1	Total	C	O	0
			43	33	10	
34	K	1	Total	C	O	0
			35	25	10	
34	K	1	Total	C	O	0
			36	26	10	
34	P	1	Total	C	O	0
			27	17	10	
34	E	1	Total	C	O	0
			32	22	10	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	b	1	Total	C	O	0
			57	42	15	
35	h	1	Total	C	O	0
			54	39	15	
35	j	1	Total	C	O	0
			43	28	15	
35	j	1	Total	C	O	0
			41	26	15	
35	j	1	Total	C	O	0
			49	34	15	
35	m	1	Total	C	O	0
			66	51	15	
35	G	1	Total	C	O	0
			45	30	15	
35	B	1	Total	C	O	0
			45	30	15	

- Molecule 36 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
36	h	1	Total	C	O	0
			43	40	3	
36	m	1	Total	C	O	0
			43	40	3	
36	A	1	Total	C	O	0
			43	40	3	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	A	1	43	40	3	0
36	A	1	43	40	3	0
36	G	1	43	40	3	0
36	G	1	43	40	3	0
36	G	1	43	40	3	0
36	G	1	43	40	3	0
36	I	1	43	40	3	0
36	I	1	43	40	3	0
36	I	1	43	40	3	0
36	I	1	43	40	3	0
36	I	1	43	40	3	0
36	K	1	43	40	3	0
36	K	1	43	40	3	0
36	K	1	43	40	3	0
36	K	1	43	40	3	0
36	K	1	43	40	3	0
36	K	1	43	40	3	0
36	F	1	43	40	3	0
36	F	1	43	40	3	0
36	J	1	43	40	3	0
36	J	1	43	40	3	0

*Continued on next page...*

*Continued from previous page...*

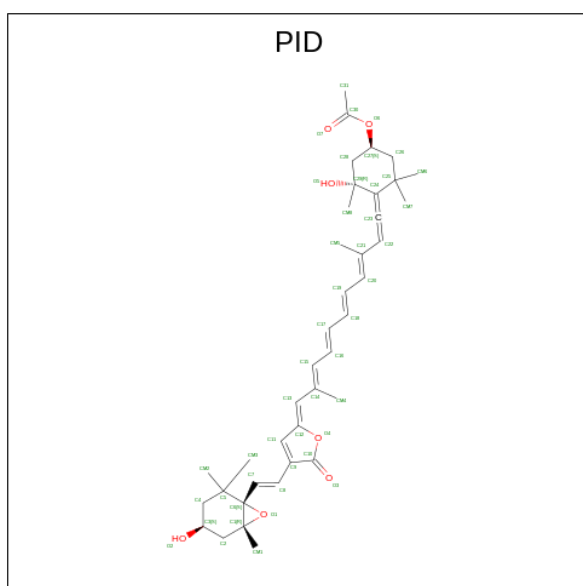
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	J	1	43	40	3	0
36	M	1	43	40	3	0
36	M	1	43	40	3	0
36	M	1	43	40	3	0
36	M	1	43	40	3	0
36	L	1	43	40	3	0
36	L	1	43	40	3	0
36	L	1	43	40	3	0
36	L	1	43	40	3	0
36	D	1	43	40	3	0
36	D	1	43	40	3	0
36	B	1	42	39	3	0
36	B	1	43	40	3	0
36	B	1	43	40	3	0
36	B	1	43	40	3	0
36	B	1	43	40	3	0
36	H	1	43	40	3	0
36	N	1	43	40	3	0
36	O	1	43	40	3	0
36	T	1	43	40	3	0
36	Q	1	43	40	3	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
36	C	1	Total	C	O	0
			43	40	3	
36	P	1	Total	C	O	0
			43	40	3	
36	E	1	Total	C	O	0
			43	40	3	
36	E	1	Total	C	O	0
			43	40	3	

- Molecule 37 is PERIDININ (three-letter code: PID) (formula: C<sub>39</sub>H<sub>50</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	h	1	Total	C	O	0
			46	39	7	
37	j	1	Total	C	O	0
			46	39	7	
37	G	1	Total	C	O	0
			46	39	7	
37	G	1	Total	C	O	0
			46	39	7	
37	G	1	Total	C	O	0
			46	39	7	
37	F	1	Total	C	O	0
			46	39	7	
37	F	1	Total	C	O	0
			46	39	7	

Continued on next page...

*Continued from previous page...*

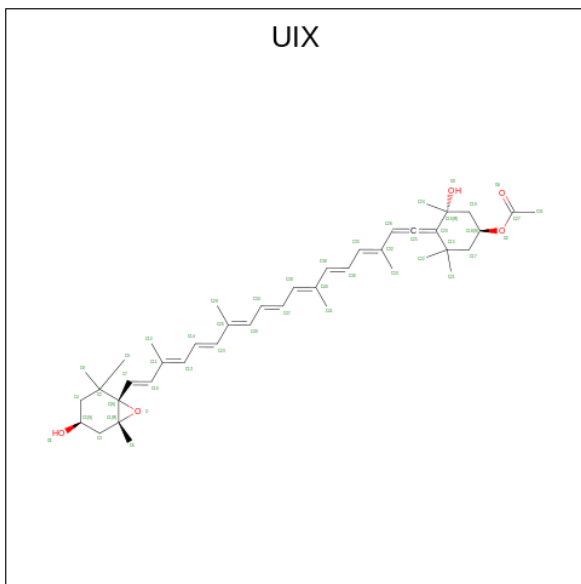
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	F	1	46	39	7	0
37	D	1	46	39	7	0
37	D	1	46	39	7	0
37	D	1	46	39	7	0
37	D	1	46	39	7	0
37	D	1	46	39	7	0
37	H	1	46	39	7	0
37	H	1	46	39	7	0
37	H	1	46	39	7	0
37	H	1	46	39	7	0
37	H	1	46	39	7	0
37	H	1	46	39	7	0
37	N	1	46	39	7	0
37	N	1	46	39	7	0
37	N	1	46	39	7	0
37	N	1	46	39	7	0
37	N	1	46	39	7	0
37	N	1	46	39	7	0
37	O	1	46	39	7	0
37	O	1	46	39	7	0
37	O	1	46	39	7	0
37	O	1	46	39	7	0
37	O	1	46	39	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	T	1	46	39	7	0
37	T	1	46	39	7	0
37	T	1	46	39	7	0
37	T	1	46	39	7	0
37	T	1	46	39	7	0
37	T	1	46	39	7	0
37	T	1	46	39	7	0
37	Q	1	46	39	7	0
37	Q	1	46	39	7	0
37	Q	1	46	39	7	0
37	Q	1	46	39	7	0
37	C	1	46	39	7	0
37	C	1	46	39	7	0
37	C	1	46	39	7	0
37	C	1	46	39	7	0
37	C	1	46	39	7	0
37	P	1	46	39	7	0
37	P	1	46	39	7	0
37	P	1	46	39	7	0
37	P	1	46	39	7	0
37	P	1	46	39	7	0
37	E	1	46	39	7	0

- Molecule 38 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 (three-letter code: UIX) (formula: C<sub>42</sub>H<sub>58</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			47	42	5	
38	F	1	Total	C	O	0
			47	42	5	
38	J	1	Total	C	O	0
			47	42	5	
38	L	1	Total	C	O	0
			47	42	5	
38	B	1	Total	C	O	0
			47	42	5	
38	N	1	Total	C	O	0
			47	42	5	
38	O	1	Total	C	O	0
			47	42	5	
38	T	1	Total	C	O	0
			47	42	5	
38	Q	1	Total	C	O	0
			47	42	5	
38	C	1	Total	C	O	0
			47	42	5	
38	P	1	Total	C	O	0
			47	42	5	

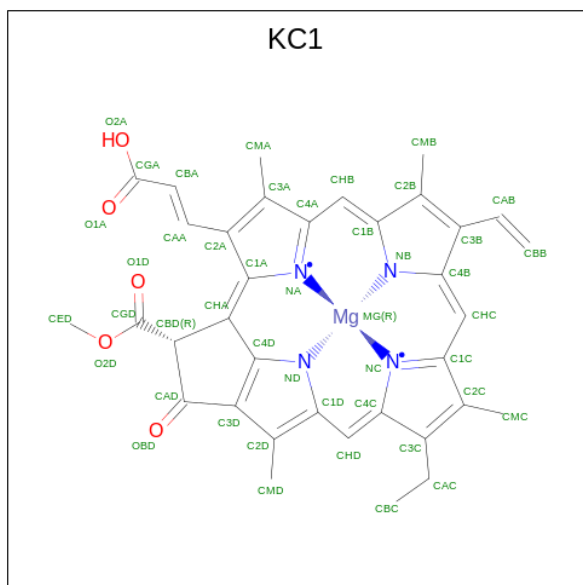
*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
38	E	1	47	42	5	0

- Molecule 39 is Chlorophyll c1 (three-letter code: KC1) (formula:  $C_{35}H_{30}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
39	A	1	45	35	1	4	5	0
39	A	1	45	35	1	4	5	0
39	G	1	45	35	1	4	5	0
39	G	1	45	35	1	4	5	0
39	I	1	45	35	1	4	5	0
39	K	1	45	35	1	4	5	0
39	F	1	45	35	1	4	5	0
39	F	1	45	35	1	4	5	0
39	J	1	45	35	1	4	5	0
39	M	1	45	35	1	4	5	0

Continued on next page...

*Continued from previous page...*

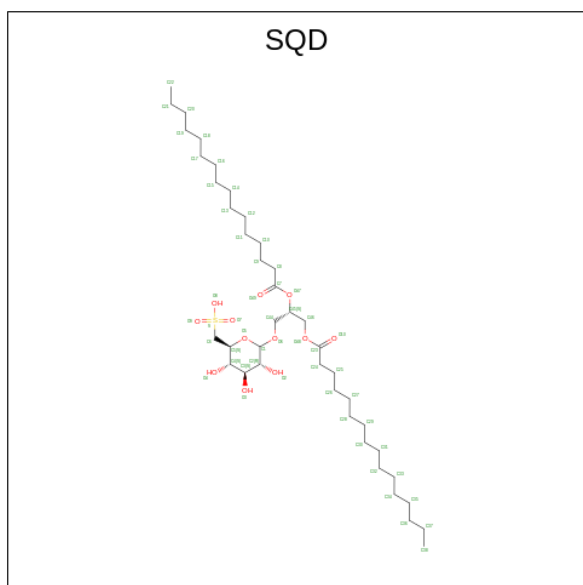
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
39	M	1	45	35	1	4	5	0
39	L	1	45	35	1	4	5	0
39	L	1	45	35	1	4	5	0
39	D	1	45	35	1	4	5	0
39	D	1	45	35	1	4	5	0
39	B	1	45	35	1	4	5	0
39	H	1	45	35	1	4	5	0
39	H	1	45	35	1	4	5	0
39	H	1	45	35	1	4	5	0
39	N	1	45	35	1	4	5	0
39	N	1	45	35	1	4	5	0
39	N	1	45	35	1	4	5	0
39	O	1	45	35	1	4	5	0
39	O	1	45	35	1	4	5	0
39	O	1	45	35	1	4	5	0
39	T	1	45	35	1	4	5	0
39	T	1	45	35	1	4	5	0
39	T	1	45	35	1	4	5	0
39	Q	1	45	35	1	4	5	0
39	Q	1	45	35	1	4	5	0
39	Q	1	45	35	1	4	5	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S) (labeled as "Ligand of Interest" by depositor).

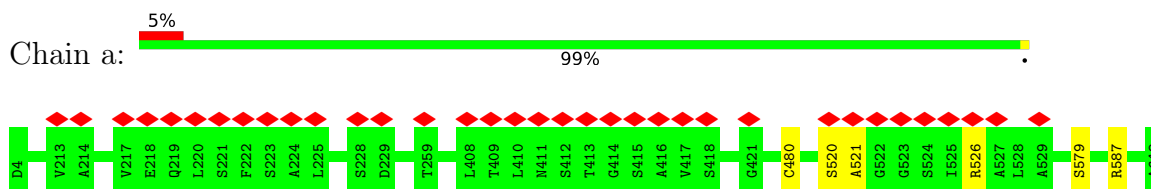


Mol	Chain	Residues	Atoms			AltConf	
40	J	1	Total	C	O	S	0
			45	32	12	1	
40	B	1	Total	C	O	S	0
			42	29	12	1	

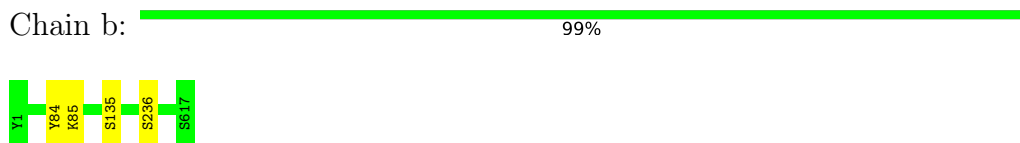
### 3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem I PsaA



- Molecule 2: Photosystem I PsaB

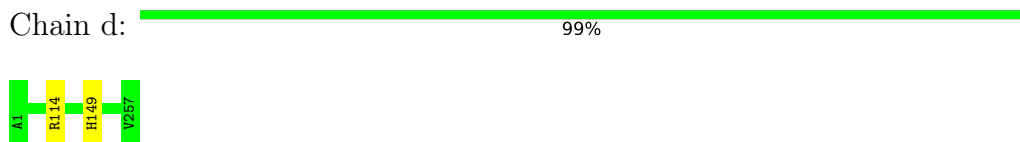


- Molecule 3: Photosystem I PsaC

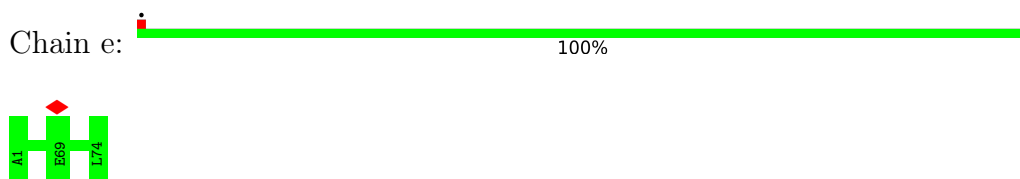


There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem I PsaD



- Molecule 5: Photosystem I PsaE



- Molecule 6: Photosystem I PsaF

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Photosystem I PsaR

Chain h:  95% 5%



- Molecule 8: Photosystem I PsaI

Chain i:  98%



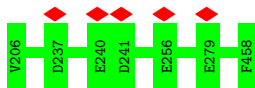
- Molecule 9: Photosystem I PsaJ

Chain j:  97%



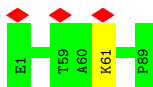
- Molecule 10: Photosystem I PsaL

Chain l:  100%



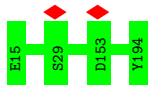
- Molecule 11: Photosystem I PsaM

Chain m:  99%



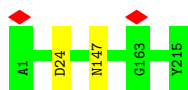
- Molecule 12: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10

Chain A:  100%



- Molecule 13: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8

Chain G:  99%



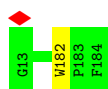
- Molecule 14: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7

Chain I:  95%



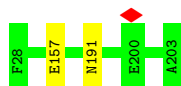
- Molecule 15: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6

Chain K:  99%



- Molecule 16: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2

Chain F:  99%



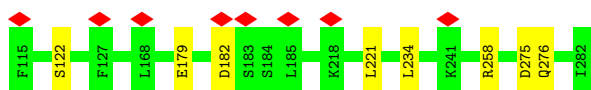
- Molecule 17: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3

Chain J:  99%

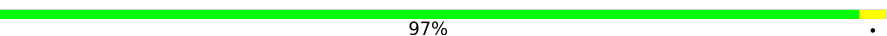


- Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4

Chain M:  95%

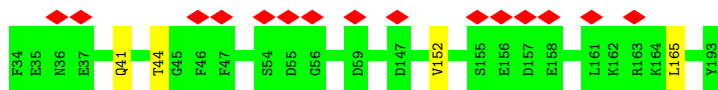


- Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5

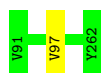
Chain L:  97%



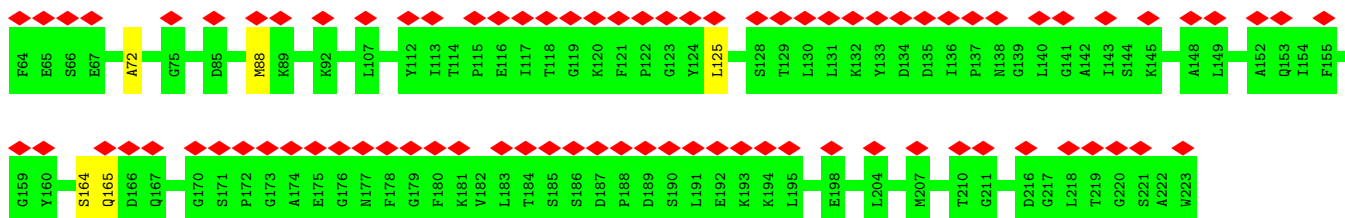
- Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9



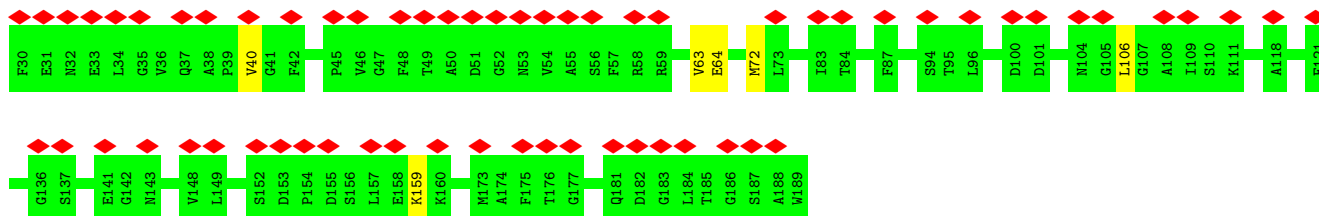
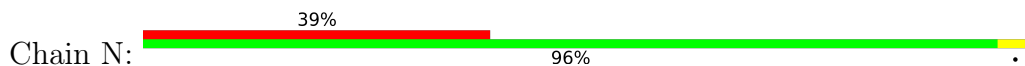
- Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11



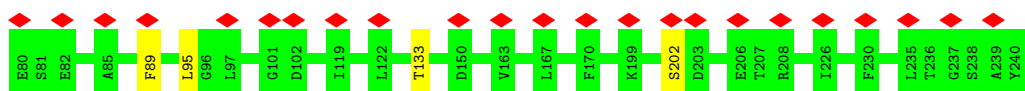
- Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12



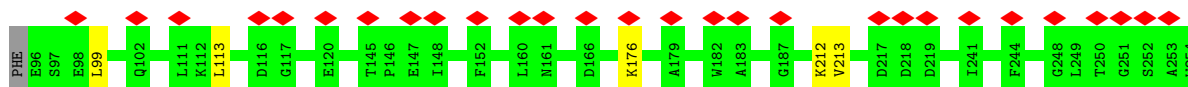
- Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13



- Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15

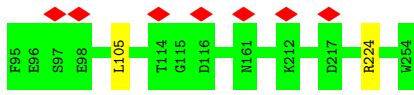


- Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16



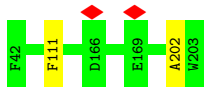
- Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16

Chain C:  99%

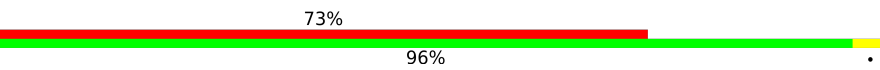


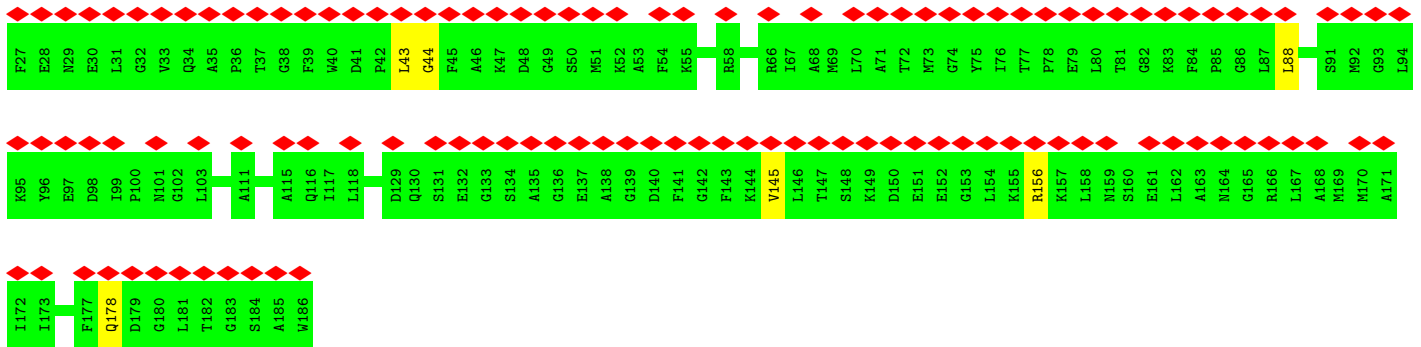
- Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-17, acpPCI-17

Chain Q:  99%



- Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14

Chain P:  96%



- Molecule 28: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-1, acpPCI-1

Chain E:  97%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	356838	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)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.883	Depositor
Minimum map value	-0.563	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.22	Depositor
Map size ( $\text{\AA}$ )	665.6, 665.6, 665.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3, 1.3, 1.3	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, SQD, KC1, UIX, LMG, DD6, PID, DGD, PQN, LHG, SF4, CLA

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	0.33	0/5133	0.46	0/7019
2	b	0.35	0/4968	0.46	0/6804
3	c	0.31	0/657	0.50	0/897
4	d	0.30	0/2034	0.50	0/2766
5	e	0.30	0/624	0.43	0/851
6	f	0.28	0/1484	0.48	0/1998
7	h	0.31	0/1089	0.46	0/1479
8	i	0.30	0/1030	0.44	0/1394
9	j	0.36	0/566	0.52	0/774
10	l	0.28	0/2014	0.46	0/2737
11	m	0.30	0/694	0.48	0/939
12	A	0.28	0/1395	0.45	0/1892
13	G	0.30	0/1730	0.43	0/2348
14	I	0.31	0/1499	0.47	0/2037
15	K	0.29	0/1358	0.48	0/1838
16	F	0.29	0/1395	0.50	0/1886
17	J	0.27	0/1317	0.46	0/1795
18	M	0.27	0/1395	0.49	0/1888
19	L	0.28	0/1490	0.52	0/2021
20	D	0.27	0/1223	0.51	0/1650
21	B	0.30	0/1404	0.49	0/1891
22	H	0.28	0/1232	0.49	0/1665
23	N	0.27	0/1233	0.50	0/1671
24	O	0.28	0/1260	0.50	0/1709
25	C	0.26	0/1226	0.50	0/1653
25	T	0.27	0/1214	0.50	0/1637
26	Q	0.28	0/1251	0.50	0/1690
27	P	0.28	0/1245	0.49	0/1673
28	E	0.28	0/1093	0.52	0/1473
All	All	0.30	0/44253	0.48	0/60075

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	643/645 (100%)	594 (92%)	47 (7%)	2 (0%)	41	71
2	b	615/617 (100%)	581 (94%)	34 (6%)	0	100	100
3	c	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
4	d	255/257 (99%)	239 (94%)	15 (6%)	1 (0%)	34	66
5	e	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
6	f	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
7	h	130/132 (98%)	121 (93%)	6 (5%)	3 (2%)	6	23
8	i	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
9	j	68/70 (97%)	60 (88%)	8 (12%)	0	100	100
10	l	251/253 (99%)	231 (92%)	20 (8%)	0	100	100
11	m	87/89 (98%)	79 (91%)	8 (9%)	0	100	100
12	A	178/180 (99%)	163 (92%)	15 (8%)	0	100	100
13	G	213/215 (99%)	189 (89%)	23 (11%)	1 (0%)	29	61
14	I	192/194 (99%)	165 (86%)	21 (11%)	6 (3%)	4	16
15	K	170/172 (99%)	153 (90%)	16 (9%)	1 (1%)	25	58
16	F	174/176 (99%)	154 (88%)	19 (11%)	1 (1%)	25	58

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	J	163/165 (99%)	144 (88%)	18 (11%)	1 (1%)	25	58
18	M	166/168 (99%)	134 (81%)	26 (16%)	6 (4%)	3	14
19	L	183/185 (99%)	152 (83%)	26 (14%)	5 (3%)	5	19
20	D	158/160 (99%)	142 (90%)	15 (10%)	1 (1%)	25	58
21	B	170/172 (99%)	153 (90%)	17 (10%)	0	100	100
22	H	158/160 (99%)	135 (85%)	19 (12%)	4 (2%)	5	21
23	N	158/160 (99%)	126 (80%)	31 (20%)	1 (1%)	25	58
24	O	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8	28
25	C	158/160 (99%)	146 (92%)	11 (7%)	1 (1%)	25	58
25	T	157/160 (98%)	142 (90%)	11 (7%)	4 (2%)	5	21
26	Q	160/162 (99%)	138 (86%)	20 (12%)	2 (1%)	12	37
27	P	158/160 (99%)	139 (88%)	16 (10%)	3 (2%)	8	28
28	E	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	7	26
All	All	5527/5586 (99%)	4986 (90%)	492 (9%)	49 (1%)	21	48

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	520	SER
4	d	149	HIS
14	I	116	SER
14	I	135	LYS
14	I	186	VAL
15	K	182	TRP
18	M	179	GLU
18	M	182	ASP
19	L	195	ASN
20	D	152	VAL
22	H	72	ALA
23	N	106	LEU
24	O	95	LEU
25	T	213	VAL
26	Q	202	ALA
27	P	88	LEU
27	P	145	VAL
28	E	101	ALA
28	E	116	GLU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
28	E	186	GLU
1	a	521	ALA
7	h	42	PRO
14	I	64	ILE
14	I	65	GLY
18	M	122	SER
19	L	235	ARG
19	L	265	ALA
22	H	88	MET
22	H	125	LEU
26	Q	111	PHE
18	M	276	GLN
25	T	99	LEU
25	T	212	LYS
25	C	105	LEU
27	P	44	GLY
13	G	147	ASN
16	F	157	GLU
19	L	117	PHE
7	h	38	ARG
19	L	118	ALA
22	H	164	SER
24	O	202	SER
25	T	113	LEU
7	h	41	ASN
18	M	221	LEU
18	M	275	ASP
24	O	89	PHE
14	I	68	PRO
17	J	103	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	531/535 (99%)	527 (99%)	4 (1%)	81 94

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	502/504 (100%)	498 (99%)	4 (1%)	81	94
3	c	73/74 (99%)	73 (100%)	0	100	100
4	d	213/222 (96%)	212 (100%)	1 (0%)	88	96
5	e	65/66 (98%)	65 (100%)	0	100	100
6	f	151/151 (100%)	151 (100%)	0	100	100
7	h	109/109 (100%)	106 (97%)	3 (3%)	43	76
8	i	106/106 (100%)	103 (97%)	3 (3%)	43	76
9	j	60/60 (100%)	58 (97%)	2 (3%)	38	72
10	l	200/203 (98%)	200 (100%)	0	100	100
11	m	72/72 (100%)	71 (99%)	1 (1%)	67	89
12	A	136/141 (96%)	136 (100%)	0	100	100
13	G	171/171 (100%)	170 (99%)	1 (1%)	86	96
14	I	141/156 (90%)	138 (98%)	3 (2%)	53	81
15	K	133/138 (96%)	133 (100%)	0	100	100
16	F	140/140 (100%)	139 (99%)	1 (1%)	84	95
17	J	136/136 (100%)	135 (99%)	1 (1%)	84	95
18	M	128/128 (100%)	126 (98%)	2 (2%)	62	86
19	L	145/145 (100%)	144 (99%)	1 (1%)	84	95
20	D	123/123 (100%)	120 (98%)	3 (2%)	49	79
21	B	146/146 (100%)	145 (99%)	1 (1%)	84	95
22	H	123/123 (100%)	122 (99%)	1 (1%)	81	94
23	N	124/124 (100%)	119 (96%)	5 (4%)	31	65
24	O	124/124 (100%)	123 (99%)	1 (1%)	81	94
25	C	121/121 (100%)	120 (99%)	1 (1%)	81	94
25	T	120/121 (99%)	119 (99%)	1 (1%)	81	94
26	Q	120/120 (100%)	120 (100%)	0	100	100
27	P	123/123 (100%)	120 (98%)	3 (2%)	49	79
28	E	108/108 (100%)	107 (99%)	1 (1%)	78	93
All	All	4444/4490 (99%)	4400 (99%)	44 (1%)	77	92

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	480	CYS
1	a	526	ARG
1	a	579	SER
1	a	587	ARG
2	b	84	TYR
2	b	85	LYS
2	b	135	SER
2	b	236	SER
4	d	114	ARG
7	h	35	ILE
7	h	37	ARG
7	h	40	PHE
8	i	142	LYS
8	i	144	LEU
8	i	154	LYS
9	j	25	ILE
9	j	27	THR
11	m	61	LYS
13	G	24	ASP
14	I	67	TYR
14	I	71	GLU
14	I	72	MET
16	F	191	ASN
17	J	229	SER
18	M	234	LEU
18	M	258	ARG
19	L	179	TYR
20	D	41	GLN
20	D	44	THR
20	D	165	LEU
21	B	97	VAL
22	H	165	GLN
23	N	40	VAL
23	N	63	VAL
23	N	64	GLU
23	N	72	MET
23	N	159	LYS
24	O	133	THR
25	T	176	LYS
25	C	224	ARG
27	P	43	LEU
27	P	156	ARG
27	P	178	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
28	E	112	LEU

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

Mol	Chain	Res	Type
1	a	627	HIS
13	G	64	ASN
16	F	176	ASN
17	J	227	ASN
18	M	191	HIS
22	H	71	GLN
24	O	218	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

411 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	$\# Z  > 2$
39	KC1	G	315	-	48,53,53	1.54	7 (14%)	55,89,89	1.90	11 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	PID	P	208	-	41,49,49	1.37	4 (9%)	49,76,76	2.42	7 (14%)
32	BCR	m	103	-	41,41,41	0.82	1 (2%)	56,56,56	2.35	18 (32%)
36	DD6	B	303	-	39,45,45	2.04	3 (7%)	52,67,67	1.80	14 (26%)
29	CLA	b	719	-	50,58,73	1.69	6 (12%)	58,95,113	1.60	10 (17%)
29	CLA	A	206	39	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
29	CLA	a	827	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	8 (10%)
29	CLA	a	829	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
36	DD6	I	206	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	12 (23%)
29	CLA	G	316	-	65,73,73	1.50	8 (12%)	76,113,113	4.94	11 (14%)
29	CLA	F	308	-	46,54,73	1.74	7 (15%)	53,90,113	1.52	6 (11%)
29	CLA	G	302	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
32	BCR	l	506	-	41,41,41	0.75	0	56,56,56	1.93	14 (25%)
29	CLA	M	314	-	52,60,73	1.65	5 (9%)	60,97,113	1.49	7 (11%)
32	BCR	b	735	-	41,41,41	0.77	0	56,56,56	2.04	17 (30%)
39	KC1	E	312	28	48,53,53	1.56	7 (14%)	55,89,89	1.84	12 (21%)
29	CLA	a	807	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	9 (11%)
29	CLA	I	210	-	55,63,73	1.58	6 (10%)	64,101,113	1.47	7 (10%)
29	CLA	A	209	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
37	PID	N	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.49	5 (10%)
39	KC1	A	213	-	48,53,53	1.53	7 (14%)	55,89,89	1.84	11 (20%)
39	KC1	O	310	-	48,53,53	1.53	7 (14%)	55,89,89	1.86	12 (21%)
36	DD6	J	303	-	39,45,45	2.10	3 (7%)	52,67,67	2.11	18 (34%)
36	DD6	N	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	12 (23%)
29	CLA	P	215	-	47,55,73	1.77	5 (10%)	54,91,113	1.70	9 (16%)
29	CLA	C	313	25	46,54,73	1.73	6 (13%)	53,90,113	1.53	6 (11%)
29	CLA	h	201	-	60,68,73	1.51	7 (11%)	70,107,113	1.46	8 (11%)
29	CLA	A	208	-	55,63,73	1.58	7 (12%)	64,101,113	1.50	7 (10%)
36	DD6	I	205	-	39,45,45	2.45	5 (12%)	52,67,67	2.18	17 (32%)
29	CLA	G	314	-	60,68,73	1.52	7 (11%)	70,107,113	1.49	8 (11%)
29	CLA	D	313	20	45,53,73	1.76	6 (13%)	52,89,113	1.55	6 (11%)
36	DD6	G	308	-	39,45,45	2.01	2 (5%)	52,67,67	2.12	15 (28%)
36	DD6	h	202	-	39,45,45	2.19	5 (12%)	52,67,67	2.33	19 (36%)
29	CLA	b	701	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
37	PID	T	305	-	41,49,49	1.32	4 (9%)	49,76,76	1.52	7 (14%)
29	CLA	T	308	-	47,55,73	1.75	6 (12%)	54,91,113	1.52	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	a	809	1	65,73,73	1.46	7 (10%)	76,113,113	1.41	8 (10%)
37	PID	T	317	-	41,49,49	1.33	4 (9%)	49,76,76	1.70	9 (18%)
39	KC1	H	314	-	48,53,53	1.51	7 (14%)	55,89,89	1.86	10 (18%)
29	CLA	B	312	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
38	UIX	E	304	-	41,49,49	1.30	4 (9%)	52,74,74	2.43	18 (34%)
29	CLA	f	803	6	46,54,73	1.73	6 (13%)	53,90,113	1.56	6 (11%)
29	CLA	L	309	-	55,63,73	1.59	6 (10%)	64,101,113	1.48	7 (10%)
29	CLA	a	806	1	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
29	CLA	a	801	-	65,73,73	1.44	10 (15%)	76,113,113	1.40	7 (9%)
29	CLA	l	509	-	41,49,73	1.83	7 (17%)	47,84,113	1.65	8 (17%)
32	BCR	l	507	-	41,41,41	0.75	0	56,56,56	1.99	16 (28%)
29	CLA	E	308	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
29	CLA	P	214	27	46,54,73	1.77	6 (13%)	53,90,113	1.55	6 (11%)
29	CLA	B	315	-	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	O	314	-	47,55,73	1.78	7 (14%)	54,91,113	1.58	8 (14%)
29	CLA	H	312	22	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	K	216	-	41,49,73	1.81	7 (17%)	47,84,113	1.74	7 (14%)
29	CLA	B	310	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	7 (9%)
39	KC1	C	315	25	48,53,53	1.52	7 (14%)	55,89,89	1.82	10 (18%)
36	DD6	I	202	-	39,45,45	2.03	3 (7%)	52,67,67	1.92	14 (26%)
39	KC1	C	310	-	48,53,53	1.54	7 (14%)	55,89,89	1.89	10 (18%)
39	KC1	A	205	29	48,53,53	1.53	7 (14%)	55,89,89	1.87	13 (23%)
29	CLA	F	311	-	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
39	KC1	D	315	-	48,53,53	1.52	7 (14%)	55,89,89	1.84	8 (14%)
32	BCR	a	835	-	41,41,41	0.79	0	56,56,56	2.12	16 (28%)
29	CLA	b	721	-	58,66,73	1.56	8 (13%)	67,104,113	1.48	9 (13%)
29	CLA	b	702	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
29	CLA	C	316	-	41,49,73	1.82	6 (14%)	47,84,113	1.73	7 (14%)
36	DD6	L	305	-	39,45,45	2.05	3 (7%)	52,67,67	1.95	14 (26%)
29	CLA	b	706	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	7 (9%)
29	CLA	l	502	10	65,73,73	1.49	9 (13%)	76,113,113	1.39	9 (11%)
29	CLA	L	310	-	55,63,73	1.60	6 (10%)	64,101,113	1.48	7 (10%)
39	KC1	K	215	-	48,53,53	1.56	7 (14%)	55,89,89	1.89	13 (23%)
29	CLA	D	316	-	41,49,73	1.84	6 (14%)	47,84,113	1.71	7 (14%)
37	PID	O	301	-	41,49,49	1.32	4 (9%)	49,76,76	1.62	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	T	309	25	46,54,73	1.74	7 (15%)	53,90,113	1.58	7 (13%)
29	CLA	b	723	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	8 (10%)
36	DD6	F	303	-	39,45,45	2.11	3 (7%)	52,67,67	2.09	13 (25%)
29	CLA	a	802	-	65,73,73	1.47	6 (9%)	76,113,113	1.47	9 (11%)
36	DD6	K	221	-	39,45,45	2.14	4 (10%)	52,67,67	2.24	15 (28%)
29	CLA	F	312	16	46,54,73	1.73	6 (13%)	53,90,113	1.53	6 (11%)
37	PID	D	303	-	41,49,49	1.37	4 (9%)	49,76,76	1.51	8 (16%)
39	KC1	H	309	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
36	DD6	G	307	-	39,45,45	2.71	10 (25%)	52,67,67	2.55	19 (36%)
29	CLA	A	212	-	55,63,73	1.56	7 (12%)	64,101,113	1.47	8 (12%)
38	UIX	L	302	-	41,49,49	1.26	3 (7%)	52,74,74	2.41	17 (32%)
29	CLA	T	316	-	41,49,73	1.84	6 (14%)	47,84,113	1.67	7 (14%)
29	CLA	b	722	-	58,66,73	1.53	7 (12%)	67,104,113	1.50	7 (10%)
29	CLA	b	731	-	56,64,73	1.57	6 (10%)	65,102,113	1.47	9 (13%)
29	CLA	K	210	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)
39	KC1	D	310	-	48,53,53	1.51	7 (14%)	55,89,89	1.84	9 (16%)
36	DD6	J	301	-	39,45,45	2.06	3 (7%)	52,67,67	2.26	17 (32%)
34	LMG	K	201	-	43,43,55	0.79	0	51,51,63	1.32	5 (9%)
38	UIX	N	306	-	41,49,49	1.26	4 (9%)	52,74,74	2.60	20 (38%)
29	CLA	F	310	-	46,54,73	1.70	7 (15%)	53,90,113	1.63	7 (13%)
29	CLA	I	216	-	52,60,73	1.64	7 (13%)	60,97,113	1.58	9 (15%)
29	CLA	K	218	-	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
29	CLA	L	316	-	52,60,73	1.68	7 (13%)	60,97,113	1.48	8 (13%)
29	CLA	b	736	-	65,73,73	1.48	9 (13%)	76,113,113	6.29	12 (15%)
29	CLA	a	812	-	60,68,73	1.51	7 (11%)	70,107,113	1.50	7 (10%)
29	CLA	A	207	-	55,63,73	1.60	7 (12%)	64,101,113	1.48	7 (10%)
37	PID	C	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.52	6 (12%)
29	CLA	B	309	-	55,63,73	1.58	6 (10%)	64,101,113	1.49	7 (10%)
29	CLA	L	313	-	53,61,73	1.61	6 (11%)	61,98,113	1.52	8 (13%)
34	LMG	b	734	-	40,40,55	0.81	0	48,48,63	1.29	6 (12%)
29	CLA	i	203	-	55,63,73	1.56	6 (10%)	64,101,113	1.51	8 (12%)
29	CLA	a	822	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
29	CLA	K	207	15	49,57,73	1.70	6 (12%)	55,93,113	1.54	8 (14%)
37	PID	F	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.67	6 (12%)
29	CLA	C	314	-	47,55,73	1.74	6 (12%)	54,91,113	1.64	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	J	305	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	7 (13%)
31	LHG	a	833	-	47,47,48	0.28	0	50,53,54	0.31	0
35	DGD	b	733	-	58,58,67	0.94	3 (5%)	72,72,81	1.25	7 (9%)
37	PID	O	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.50	6 (12%)
29	CLA	F	315	-	41,49,73	1.84	5 (12%)	47,84,113	1.71	8 (17%)
29	CLA	J	306	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	7 (9%)
39	KC1	H	311	-	48,53,53	1.52	7 (14%)	55,89,89	1.82	10 (18%)
29	CLA	D	314	-	47,55,73	1.72	7 (14%)	54,91,113	1.65	7 (12%)
29	CLA	N	309	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
37	PID	T	307	-	41,49,49	1.33	4 (9%)	49,76,76	1.58	8 (16%)
29	CLA	b	725	-	65,73,73	1.47	8 (12%)	76,113,113	1.35	7 (9%)
29	CLA	E	315	-	57,65,73	1.60	6 (10%)	66,103,113	1.45	8 (12%)
29	CLA	J	308	-	56,64,73	1.57	6 (10%)	65,102,113	1.49	8 (12%)
36	DD6	G	306	-	39,45,45	2.12	3 (7%)	52,67,67	2.19	13 (25%)
37	PID	h	204	-	41,49,49	1.35	4 (9%)	49,76,76	1.40	6 (12%)
29	CLA	f	802	-	46,54,73	1.73	7 (15%)	53,90,113	1.54	6 (11%)
29	CLA	l	503	10	65,73,73	1.48	8 (12%)	76,113,113	1.40	8 (10%)
29	CLA	M	311	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	8 (15%)
36	DD6	F	301	-	39,45,45	2.11	4 (10%)	52,67,67	1.99	14 (26%)
36	DD6	K	206	-	39,45,45	2.05	3 (7%)	52,67,67	2.01	14 (26%)
29	CLA	J	313	-	41,49,73	1.83	6 (14%)	47,84,113	1.67	8 (17%)
38	UIX	P	207	-	41,49,49	1.27	3 (7%)	52,74,74	2.56	19 (36%)
29	CLA	b	720	-	65,73,73	1.49	8 (12%)	76,113,113	1.36	6 (7%)
29	CLA	a	814	-	46,54,73	1.74	7 (15%)	53,90,113	1.53	6 (11%)
37	PID	N	305	-	41,49,49	1.37	4 (9%)	49,76,76	1.36	4 (8%)
36	DD6	M	303	-	39,45,45	2.11	4 (10%)	52,67,67	2.03	14 (26%)
29	CLA	a	803	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	6 (7%)
38	UIX	B	304	-	41,49,49	1.27	3 (7%)	52,74,74	2.45	16 (30%)
37	PID	O	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.42	7 (14%)
29	CLA	J	311	-	53,61,73	1.64	9 (16%)	61,98,113	1.48	7 (11%)
29	CLA	l	508	-	41,49,73	1.82	7 (17%)	47,84,113	1.66	7 (14%)
29	CLA	N	311	-	51,59,73	1.67	5 (9%)	59,96,113	1.53	7 (11%)
37	PID	j	101	-	41,49,49	1.37	4 (9%)	49,76,76	1.46	9 (18%)
36	DD6	A	201	-	39,45,45	2.02	3 (7%)	52,67,67	2.02	16 (30%)
37	PID	H	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.40	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	b	704	-	65,73,73	1.47	8 (12%)	76,113,113	3.99	8 (10%)
29	CLA	b	715	-	46,54,73	1.75	7 (15%)	53,90,113	1.55	7 (13%)
29	CLA	l	501	-	60,68,73	1.54	6 (10%)	70,107,113	1.48	7 (10%)
39	KC1	P	211	-	48,53,53	1.54	7 (14%)	55,89,89	1.86	13 (23%)
29	CLA	H	308	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	9 (11%)
36	DD6	O	303	-	39,45,45	2.10	4 (10%)	52,67,67	2.19	17 (32%)
29	CLA	E	310	28	46,54,73	1.72	6 (13%)	53,90,113	1.57	6 (11%)
37	PID	D	306	-	41,49,49	1.36	4 (9%)	49,76,76	1.42	8 (16%)
29	CLA	I	214	-	55,63,73	1.57	7 (12%)	64,101,113	1.48	8 (12%)
29	CLA	L	315	-	41,49,73	1.87	7 (17%)	47,84,113	1.63	7 (14%)
39	KC1	O	315	-	48,53,53	1.51	6 (12%)	55,89,89	1.87	10 (18%)
29	CLA	B	316	-	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
35	DGD	j	105	-	42,42,67	1.03	2 (4%)	56,56,81	1.07	5 (8%)
29	CLA	A	210	12	46,54,73	1.77	7 (15%)	53,90,113	1.51	7 (13%)
29	CLA	G	304	-	59,67,73	1.54	8 (13%)	68,105,113	1.51	7 (10%)
29	CLA	K	214	-	55,63,73	1.62	9 (16%)	64,101,113	1.45	9 (14%)
37	PID	G	303	-	41,49,49	1.37	4 (9%)	49,76,76	1.33	5 (10%)
29	CLA	I	209	-	60,68,73	1.52	7 (11%)	70,107,113	5.16	11 (15%)
29	CLA	a	813	-	51,59,73	1.69	7 (13%)	59,96,113	1.50	7 (11%)
32	BCR	i	204	-	41,41,41	0.76	0	56,56,56	2.35	15 (26%)
29	CLA	b	726	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	8 (10%)
36	DD6	L	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.97	11 (21%)
37	PID	P	202	-	41,49,49	1.32	4 (9%)	49,76,76	1.37	8 (16%)
37	PID	Q	304	-	41,49,49	1.33	4 (9%)	49,76,76	1.54	6 (12%)
29	CLA	b	711	-	58,66,73	1.56	7 (12%)	67,104,113	1.44	8 (11%)
29	CLA	F	316	16	41,49,73	1.82	6 (14%)	47,84,113	1.68	7 (14%)
29	CLA	I	213	14	65,73,73	1.48	6 (9%)	76,113,113	4.10	12 (15%)
29	CLA	C	308	-	47,55,73	1.73	6 (12%)	54,91,113	1.52	7 (12%)
29	CLA	a	831	-	65,73,73	1.46	7 (10%)	76,113,113	4.96	9 (11%)
29	CLA	B	314	21	41,49,73	1.80	7 (17%)	47,84,113	1.72	7 (14%)
29	CLA	C	309	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	6 (7%)
36	DD6	A	204	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	15 (28%)
37	PID	C	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	6 (12%)
29	CLA	K	208	-	46,54,73	1.74	7 (15%)	53,90,113	1.52	6 (11%)
29	CLA	b	707	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	a	805	-	55,63,73	1.59	7 (12%)	64,101,113	1.50	6 (9%)
29	CLA	b	703	-	65,73,73	1.48	7 (10%)	76,113,113	1.34	6 (7%)
29	CLA	K	213	-	48,56,73	1.71	7 (14%)	55,92,113	1.51	8 (14%)
34	LMG	A	219	-	37,37,55	0.85	0	45,45,63	1.31	5 (11%)
29	CLA	A	216	-	41,49,73	1.83	7 (17%)	47,84,113	1.66	7 (14%)
29	CLA	a	830	-	56,64,73	1.56	6 (10%)	65,102,113	5.34	10 (15%)
29	CLA	b	718	-	65,73,73	1.47	7 (10%)	76,113,113	1.48	8 (10%)
37	PID	Q	303	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	6 (12%)
29	CLA	M	315	-	46,54,73	1.73	6 (13%)	53,90,113	1.53	6 (11%)
36	DD6	M	302	-	39,45,45	2.11	4 (10%)	52,67,67	2.09	14 (26%)
39	KC1	F	309	-	48,53,53	1.53	7 (14%)	55,89,89	1.88	11 (20%)
29	CLA	Q	307	-	47,55,73	1.74	6 (12%)	54,91,113	1.52	7 (12%)
32	BCR	a	838	-	41,41,41	0.76	0	56,56,56	2.12	18 (32%)
29	CLA	P	210	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
37	PID	G	309	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	5 (10%)
39	KC1	I	215	14	48,53,53	1.54	7 (14%)	55,89,89	1.87	11 (20%)
29	CLA	L	307	39	50,58,73	1.68	7 (14%)	58,95,113	5.67	10 (17%)
29	CLA	b	709	-	60,68,73	1.52	7 (11%)	70,107,113	1.43	8 (11%)
29	CLA	l	505	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
29	CLA	P	209	-	47,55,73	1.75	5 (10%)	54,91,113	1.53	7 (12%)
34	LMG	E	316	-	32,32,55	0.99	1 (3%)	40,40,63	1.27	2 (5%)
29	CLA	G	301	-	49,57,73	1.69	7 (14%)	55,93,113	1.57	7 (12%)
29	CLA	I	208	-	46,54,73	1.74	6 (13%)	53,90,113	5.89	8 (15%)
38	UIX	A	203	-	41,49,49	1.27	4 (9%)	52,74,74	2.39	21 (40%)
37	PID	C	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.59	6 (12%)
29	CLA	a	828	-	46,54,73	1.75	7 (15%)	53,90,113	1.54	6 (11%)
29	CLA	M	313	-	41,49,73	1.85	7 (17%)	47,84,113	1.69	7 (14%)
32	BCR	a	834	-	41,41,41	0.74	0	56,56,56	2.05	16 (28%)
29	CLA	i	201	-	65,73,73	1.43	6 (9%)	76,113,113	1.42	7 (9%)
38	UIX	F	305	-	41,49,49	1.27	3 (7%)	52,74,74	2.89	19 (36%)
29	CLA	a	826	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	8 (10%)
29	CLA	N	308	-	47,55,73	1.75	6 (12%)	54,91,113	1.53	7 (12%)
29	CLA	T	313	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	6 (11%)
37	PID	P	206	-	41,49,49	1.36	4 (9%)	49,76,76	1.79	8 (16%)
37	PID	T	304	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	5 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	b	717	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	9 (11%)
29	CLA	a	818	-	47,55,73	1.74	6 (12%)	54,91,113	1.53	8 (14%)
29	CLA	a	820	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	7 (9%)
29	CLA	a	837	-	55,63,73	1.60	6 (10%)	64,101,113	1.40	7 (10%)
29	CLA	a	815	-	45,53,73	1.75	7 (15%)	52,89,113	1.63	8 (15%)
37	PID	O	307	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	7 (14%)
29	CLA	D	311	-	46,54,73	1.72	6 (13%)	53,90,113	1.58	7 (13%)
39	KC1	M	305	-	48,53,53	1.52	7 (14%)	55,89,89	1.89	12 (21%)
29	CLA	a	821	-	47,55,73	1.73	6 (12%)	54,91,113	1.53	7 (12%)
29	CLA	M	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	7 (13%)
29	CLA	Q	312	-	46,54,73	1.74	6 (13%)	53,90,113	1.54	7 (13%)
29	CLA	I	201	29	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
39	KC1	T	310	-	48,53,53	1.53	7 (14%)	55,89,89	1.79	10 (18%)
40	SQD	B	317	-	41,42,54	0.44	1 (2%)	50,53,65	0.50	0
32	BCR	b	728	-	41,41,41	0.78	1 (2%)	56,56,56	2.04	15 (26%)
29	CLA	P	217	-	41,49,73	1.84	6 (14%)	47,84,113	1.74	7 (14%)
32	BCR	f	804	-	41,41,41	0.74	0	56,56,56	1.98	16 (28%)
29	CLA	L	311	19	46,54,73	1.75	6 (13%)	53,90,113	1.49	7 (13%)
30	PQN	b	727	-	34,34,34	1.54	2 (5%)	42,45,45	1.19	3 (7%)
29	CLA	A	215	-	47,55,73	1.72	7 (14%)	54,91,113	1.55	6 (11%)
29	CLA	b	713	-	53,61,73	1.65	5 (9%)	61,98,113	1.45	6 (9%)
39	KC1	T	315	25	48,53,53	1.51	7 (14%)	55,89,89	1.83	10 (18%)
29	CLA	a	824	-	65,73,73	1.46	7 (10%)	76,113,113	1.37	7 (9%)
29	CLA	M	310	18	48,56,73	1.71	6 (12%)	55,92,113	1.55	7 (12%)
29	CLA	F	313	16	46,54,73	1.75	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	N	313	23	46,54,73	1.72	6 (13%)	53,90,113	4.81	10 (18%)
36	DD6	Q	302	-	39,45,45	1.99	3 (7%)	52,67,67	1.86	12 (23%)
29	CLA	a	808	-	51,59,73	1.67	8 (15%)	59,96,113	1.50	8 (13%)
29	CLA	I	212	-	55,63,73	1.61	6 (10%)	64,101,113	6.83	13 (20%)
36	DD6	B	302	-	39,45,45	2.06	3 (7%)	52,67,67	1.92	13 (25%)
37	PID	P	203	-	41,49,49	1.36	4 (9%)	49,76,76	1.45	8 (16%)
29	CLA	A	218	12	60,68,73	1.52	7 (11%)	70,107,113	1.46	8 (11%)
36	DD6	E	303	-	39,45,45	2.02	3 (7%)	52,67,67	1.74	10 (19%)
36	DD6	G	305	-	39,45,45	2.20	3 (7%)	52,67,67	2.96	17 (32%)
29	CLA	G	312	13	65,73,73	1.47	8 (12%)	76,113,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	PID	N	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.41	5 (10%)
36	DD6	B	305	-	39,45,45	2.02	3 (7%)	52,67,67	1.91	16 (30%)
37	PID	O	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.59	7 (14%)
29	CLA	E	314	28	48,56,73	1.72	7 (14%)	55,92,113	1.54	7 (12%)
36	DD6	C	303	-	39,45,45	2.07	3 (7%)	52,67,67	2.04	15 (28%)
29	CLA	b	716	-	53,61,73	1.62	7 (13%)	61,98,113	1.53	8 (13%)
36	DD6	B	319	-	39,45,45	2.09	3 (7%)	52,67,67	2.26	16 (30%)
37	PID	D	307	-	41,49,49	1.35	4 (9%)	49,76,76	1.59	7 (14%)
37	PID	F	306	-	41,49,49	1.35	4 (9%)	49,76,76	1.47	6 (12%)
29	CLA	a	810	1	55,63,73	1.61	7 (12%)	64,101,113	1.46	8 (12%)
36	DD6	M	304	-	39,45,45	2.05	3 (7%)	52,67,67	1.76	13 (25%)
37	PID	Q	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.47	6 (12%)
29	CLA	a	825	-	65,73,73	1.49	8 (12%)	76,113,113	1.48	9 (11%)
37	PID	P	205	-	41,49,49	1.34	4 (9%)	49,76,76	1.54	6 (12%)
29	CLA	a	811	-	56,64,73	1.62	6 (10%)	65,102,113	1.43	7 (10%)
37	PID	F	304	-	41,49,49	1.61	5 (12%)	49,76,76	1.57	7 (14%)
29	CLA	H	315	-	41,49,73	1.84	6 (14%)	47,84,113	1.66	8 (17%)
29	CLA	P	212	-	51,59,73	1.68	6 (11%)	59,96,113	1.50	8 (13%)
38	UIX	J	304	-	41,49,49	1.26	3 (7%)	52,74,74	2.40	13 (25%)
29	CLA	b	708	2	52,60,73	1.66	7 (13%)	60,97,113	1.55	8 (13%)
36	DD6	J	302	-	39,45,45	2.08	2 (5%)	52,67,67	2.19	17 (32%)
29	CLA	J	309	17	46,54,73	1.72	6 (13%)	53,90,113	1.61	6 (11%)
35	DGD	h	203	-	55,55,67	0.90	2 (3%)	69,69,81	0.98	3 (4%)
29	CLA	B	306	21	49,57,73	1.70	6 (12%)	55,93,113	1.55	8 (14%)
29	CLA	H	310	-	51,59,73	1.69	6 (11%)	59,96,113	1.54	8 (13%)
29	CLA	G	311	13	51,59,73	1.64	6 (11%)	59,96,113	1.50	7 (11%)
29	CLA	F	307	-	46,54,73	1.74	6 (13%)	53,90,113	1.56	7 (13%)
29	CLA	b	724	-	47,55,73	1.73	9 (19%)	54,91,113	1.54	8 (14%)
29	CLA	L	317	-	46,54,73	1.75	6 (13%)	53,90,113	1.55	6 (11%)
37	PID	Q	306	-	41,49,49	1.33	4 (9%)	49,76,76	1.52	6 (12%)
29	CLA	a	804	-	55,63,73	1.62	7 (12%)	64,101,113	1.54	9 (14%)
30	PQN	a	832	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
39	KC1	B	313	21	48,53,53	1.53	7 (14%)	55,89,89	1.86	12 (21%)
37	PID	G	310	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	7 (14%)
39	KC1	N	310	-	48,53,53	1.52	7 (14%)	55,89,89	1.86	10 (18%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	LMG	h	205	-	28,28,55	1.02	1 (3%)	36,36,63	1.27	4 (11%)
29	CLA	T	314	-	47,55,73	1.73	5 (10%)	54,91,113	1.66	9 (16%)
29	CLA	D	308	-	47,55,73	1.73	6 (12%)	54,91,113	1.55	7 (12%)
35	DGD	j	106	-	50,50,67	0.97	2 (4%)	64,64,81	1.04	4 (6%)
34	LMG	b	732	-	44,44,55	0.80	1 (2%)	52,52,63	1.32	6 (11%)
39	KC1	Q	314	26	48,53,53	1.54	7 (14%)	55,89,89	1.87	10 (18%)
39	KC1	Q	309	-	48,53,53	1.54	7 (14%)	55,89,89	1.88	11 (20%)
39	KC1	P	216	-	48,53,53	1.51	7 (14%)	55,89,89	1.84	9 (16%)
39	KC1	P	213	27	48,53,53	1.52	7 (14%)	55,89,89	1.78	12 (21%)
35	DGD	m	102	-	67,67,67	0.83	2 (2%)	81,81,81	0.91	4 (4%)
29	CLA	O	309	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	6 (7%)
29	CLA	G	317	-	53,61,73	1.62	7 (13%)	61,98,113	1.47	6 (9%)
29	CLA	E	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.56	7 (13%)
29	CLA	a	816	-	46,54,73	1.73	7 (15%)	53,90,113	1.56	7 (13%)
29	CLA	I	211	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	8 (10%)
29	CLA	G	319	13	41,49,73	1.81	6 (14%)	47,84,113	1.69	7 (14%)
29	CLA	K	212	-	52,60,73	1.69	7 (13%)	60,97,113	1.50	9 (15%)
37	PID	H	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.63	5 (10%)
29	CLA	Q	310	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
29	CLA	Q	308	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	8 (10%)
29	CLA	Q	313	-	47,55,73	1.73	6 (12%)	54,91,113	1.53	7 (12%)
39	KC1	N	315	-	48,53,53	1.50	6 (12%)	55,89,89	1.81	10 (18%)
29	CLA	H	313	-	47,55,73	1.74	6 (12%)	54,91,113	1.64	8 (14%)
29	CLA	O	316	-	41,49,73	1.85	6 (14%)	47,84,113	1.68	7 (14%)
35	DGD	G	320	-	46,46,67	1.01	2 (4%)	60,60,81	0.98	3 (5%)
29	CLA	K	209	-	54,62,73	1.61	7 (12%)	62,99,113	1.50	9 (14%)
29	CLA	N	316	-	41,49,73	1.85	6 (14%)	47,84,113	1.66	7 (14%)
29	CLA	A	217	-	51,59,73	1.66	6 (11%)	59,96,113	1.49	8 (13%)
29	CLA	O	308	-	47,55,73	1.76	6 (12%)	54,91,113	1.55	7 (12%)
29	CLA	b	710	-	46,54,73	1.74	7 (15%)	53,90,113	1.53	7 (13%)
29	CLA	a	823	-	58,66,73	1.54	7 (12%)	67,104,113	1.48	8 (11%)
29	CLA	l	510	-	45,53,73	1.80	6 (13%)	52,89,113	1.54	8 (15%)
32	BCR	b	729	-	41,41,41	0.79	1 (2%)	56,56,56	1.88	20 (35%)
37	PID	C	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	6 (12%)
29	CLA	E	305	-	61,69,73	1.54	6 (9%)	71,108,113	1.45	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	DD6	E	302	-	39,45,45	2.11	3 (7%)	52,67,67	2.26	18 (34%)
38	UIX	T	306	-	41,49,49	1.29	4 (9%)	52,74,74	2.77	24 (46%)
39	KC1	C	312	-	48,53,53	1.54	7 (14%)	55,89,89	1.87	12 (21%)
37	PID	D	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.45	5 (10%)
37	PID	N	307	-	41,49,49	1.36	4 (9%)	49,76,76	1.59	9 (18%)
38	UIX	C	306	-	41,49,49	1.27	4 (9%)	52,74,74	2.55	22 (42%)
29	CLA	I	207	14	49,57,73	1.68	7 (14%)	55,93,113	1.59	7 (12%)
39	KC1	L	314	-	48,53,53	1.55	7 (14%)	55,89,89	1.86	11 (20%)
29	CLA	N	314	-	47,55,73	1.72	7 (14%)	54,91,113	1.61	7 (12%)
29	CLA	D	309	-	46,54,73	1.74	6 (13%)	53,90,113	1.57	6 (11%)
35	DGD	B	318	-	46,46,67	1.00	2 (4%)	60,60,81	1.32	10 (16%)
29	CLA	a	817	-	45,53,73	1.80	6 (13%)	52,89,113	1.55	7 (13%)
29	CLA	M	307	-	55,63,73	1.60	7 (12%)	64,101,113	1.44	7 (10%)
36	DD6	D	304	-	39,45,45	2.09	4 (10%)	52,67,67	2.14	15 (28%)
33	SF4	c	102	3	0,12,12	-	-	-	-	-
29	CLA	E	306	28	65,73,73	1.47	7 (10%)	76,113,113	1.38	7 (9%)
39	KC1	E	307	-	48,53,53	1.52	7 (14%)	55,89,89	1.87	11 (20%)
29	CLA	L	312	-	55,63,73	1.58	6 (10%)	64,101,113	1.45	7 (10%)
39	KC1	O	312	-	48,53,53	1.48	7 (14%)	55,89,89	1.98	11 (20%)
29	CLA	f	805	-	60,68,73	1.53	6 (10%)	70,107,113	1.40	7 (10%)
36	DD6	A	202	-	39,45,45	1.97	3 (7%)	52,67,67	1.81	10 (19%)
37	PID	C	305	-	41,49,49	1.36	4 (9%)	49,76,76	1.95	9 (18%)
29	CLA	K	217	-	46,54,73	1.76	8 (17%)	53,90,113	1.55	6 (11%)
36	DD6	I	204	-	39,45,45	2.19	5 (12%)	52,67,67	2.08	16 (30%)
36	DD6	M	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.85	15 (28%)
39	KC1	G	318	-	48,53,53	1.56	7 (14%)	55,89,89	1.83	10 (18%)
29	CLA	E	311	-	65,73,73	1.46	7 (10%)	76,113,113	1.43	9 (11%)
34	LMG	K	219	-	35,35,55	0.92	1 (2%)	43,43,63	1.19	4 (9%)
36	DD6	H	303	-	39,45,45	1.94	3 (7%)	52,67,67	1.98	14 (26%)
37	PID	T	302	-	41,49,49	1.38	4 (9%)	49,76,76	1.51	8 (16%)
37	PID	D	305	-	41,49,49	1.32	4 (9%)	49,76,76	1.48	7 (14%)
29	CLA	J	307	-	46,54,73	1.73	7 (15%)	53,90,113	1.52	6 (11%)
29	CLA	M	306	-	53,61,73	1.62	6 (11%)	61,98,113	1.51	7 (11%)
29	CLA	A	214	12	41,49,73	1.83	6 (14%)	47,84,113	1.62	7 (14%)
29	CLA	M	308	-	48,56,73	1.71	7 (14%)	55,92,113	1.52	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	b	714	-	64,72,73	1.47	7 (10%)	74,111,113	1.40	9 (12%)
36	DD6	P	204	-	39,45,45	1.99	3 (7%)	52,67,67	2.19	15 (28%)
29	CLA	L	308	-	53,61,73	1.62	6 (11%)	61,98,113	5.52	10 (16%)
32	BCR	f	801	-	41,41,41	0.71	0	56,56,56	2.03	17 (30%)
33	SF4	c	101	3	0,12,12	-	-	-	-	-
36	DD6	L	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.98	17 (32%)
29	CLA	O	311	-	51,59,73	1.67	6 (11%)	59,96,113	1.52	7 (11%)
39	KC1	M	312	-	48,53,53	1.53	7 (14%)	55,89,89	1.89	11 (20%)
29	CLA	K	211	-	55,63,73	1.58	7 (12%)	64,101,113	1.51	10 (15%)
38	UIX	Q	305	-	41,49,49	1.26	4 (9%)	52,74,74	2.78	22 (42%)
29	CLA	B	307	-	45,53,73	1.78	6 (13%)	52,89,113	1.58	7 (13%)
29	CLA	G	313	-	55,63,73	1.57	6 (10%)	64,101,113	1.50	7 (10%)
29	CLA	I	217	-	55,63,73	1.61	6 (10%)	64,101,113	1.45	7 (10%)
29	CLA	j	104	29	52,60,73	1.64	7 (13%)	60,97,113	1.57	7 (11%)
33	SF4	a	836	2,1	0,12,12	-	-	-	-	-
39	KC1	T	312	-	48,53,53	1.50	7 (14%)	55,89,89	1.84	10 (18%)
29	CLA	O	313	24	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	C	311	-	51,59,73	1.65	6 (11%)	59,96,113	1.54	8 (13%)
36	DD6	B	301	-	38,44,45	2.03	3 (7%)	50,65,67	2.00	14 (28%)
29	CLA	i	202	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	8 (10%)
39	KC1	J	312	17	48,53,53	1.52	7 (14%)	55,89,89	1.84	10 (18%)
36	DD6	L	303	-	39,45,45	2.06	3 (7%)	52,67,67	1.73	13 (25%)
37	PID	H	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	5 (10%)
29	CLA	b	705	-	65,73,73	1.45	8 (12%)	76,113,113	1.45	7 (9%)
36	DD6	I	203	-	39,45,45	2.29	3 (7%)	52,67,67	2.41	17 (32%)
29	CLA	Q	315	-	41,49,73	1.84	7 (17%)	47,84,113	1.69	7 (14%)
37	PID	T	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.49	5 (10%)
34	LMG	b	730	-	46,46,55	0.81	2 (4%)	54,54,63	1.32	5 (9%)
37	PID	H	305	-	41,49,49	1.33	4 (9%)	49,76,76	1.75	8 (16%)
37	PID	E	301	-	41,49,49	1.39	4 (9%)	49,76,76	1.95	9 (18%)
29	CLA	l	504	-	65,73,73	1.46	6 (9%)	76,113,113	4.11	11 (14%)
34	LMG	K	220	-	36,36,55	0.86	1 (2%)	44,44,63	1.23	4 (9%)
29	CLA	T	311	-	46,54,73	1.74	5 (10%)	53,90,113	1.56	7 (13%)
36	DD6	K	203	-	39,45,45	2.04	3 (7%)	52,67,67	1.90	13 (25%)
29	CLA	B	308	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	DGD	j	103	-	44,44,67	0.99	2 (4%)	58,58,81	1.32	9 (15%)
37	PID	H	306	-	41,49,49	1.31	4 (9%)	49,76,76	1.46	6 (12%)
34	LMG	P	201	-	27,27,55	0.98	0	35,35,63	1.29	5 (14%)
29	CLA	D	312	20	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
39	KC1	N	312	23	48,53,53	1.52	7 (14%)	55,89,89	1.86	12 (21%)
39	KC1	F	314	-	48,53,53	1.50	7 (14%)	55,89,89	1.87	10 (18%)
36	DD6	D	301	-	39,45,45	2.08	3 (7%)	52,67,67	2.07	15 (28%)
36	DD6	K	202	-	39,45,45	2.15	3 (7%)	52,67,67	3.00	16 (30%)
36	DD6	T	303	-	39,45,45	1.98	3 (7%)	52,67,67	1.97	15 (28%)
36	DD6	K	205	-	39,45,45	2.05	3 (7%)	52,67,67	1.91	17 (32%)
38	UIX	O	306	-	41,49,49	1.25	3 (7%)	52,74,74	2.70	21 (40%)
29	CLA	H	307	-	47,55,73	1.74	6 (12%)	54,91,113	1.52	7 (12%)
29	CLA	a	819	-	57,65,73	1.58	7 (12%)	66,103,113	1.44	9 (13%)
37	PID	N	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	5 (10%)
29	CLA	A	211	-	55,63,73	1.57	6 (10%)	64,101,113	1.45	7 (10%)
29	CLA	J	310	-	47,55,73	1.71	6 (12%)	54,91,113	1.59	7 (12%)
40	SQD	J	314	-	44,45,54	0.42	1 (2%)	53,56,65	0.61	2 (3%)
29	CLA	E	313	-	41,49,73	1.85	6 (14%)	47,84,113	1.67	7 (14%)
39	KC1	L	306	29	48,53,53	1.55	7 (14%)	55,89,89	1.90	14 (25%)
36	DD6	K	204	-	39,45,45	2.08	3 (7%)	52,67,67	1.95	18 (34%)
34	LMG	j	102	-	43,43,55	0.78	0	51,51,63	1.29	5 (9%)
29	CLA	B	311	21	51,59,73	1.66	7 (13%)	59,96,113	1.52	7 (11%)
39	KC1	Q	311	-	48,53,53	1.53	7 (14%)	55,89,89	1.85	11 (20%)
36	DD6	m	101	-	39,45,45	2.04	3 (7%)	52,67,67	2.04	16 (30%)
29	CLA	b	712	-	65,73,73	1.47	7 (10%)	76,113,113	4.09	11 (14%)

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
39	KC1	G	315	-	-	6/15/71/71	-
37	PID	P	208	-	-	4/24/93/93	0/4/4/4
32	BCR	m	103	-	-	5/29/63/63	0/2/2/2
36	DD6	B	303	-	-	0/26/80/80	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	719	-	1/1/12/20	10/19/97/115	-
29	CLA	A	206	39	1/1/11/20	3/13/91/115	-
29	CLA	a	827	-	1/1/15/20	12/37/115/115	-
29	CLA	a	829	-	1/1/15/20	16/37/115/115	-
36	DD6	I	206	-	-	2/26/80/80	0/3/3/3
29	CLA	G	316	-	1/1/15/20	12/37/115/115	-
29	CLA	F	308	-	1/1/11/20	3/15/93/115	-
29	CLA	G	302	-	1/1/15/20	15/37/115/115	-
32	BCR	l	506	-	-	9/29/63/63	0/2/2/2
29	CLA	M	314	-	1/1/12/20	7/22/100/115	-
32	BCR	b	735	-	-	4/29/63/63	0/2/2/2
39	KC1	E	312	28	-	7/15/71/71	-
29	CLA	a	807	-	1/1/15/20	16/37/115/115	-
29	CLA	I	210	-	1/1/13/20	6/25/103/115	-
29	CLA	A	209	-	1/1/15/20	20/37/115/115	-
37	PID	N	301	-	-	4/24/93/93	0/4/4/4
39	KC1	A	213	-	-	7/15/71/71	-
39	KC1	O	310	-	-	6/15/71/71	-
36	DD6	J	303	-	-	2/26/80/80	0/3/3/3
36	DD6	N	303	-	-	1/26/80/80	0/3/3/3
29	CLA	P	215	-	1/1/11/20	7/16/94/115	-
29	CLA	C	313	25	1/1/11/20	5/15/93/115	-
29	CLA	h	201	-	1/1/14/20	7/31/109/115	-
29	CLA	A	208	-	1/1/13/20	3/25/103/115	-
36	DD6	I	205	-	-	6/26/80/80	0/3/3/3
29	CLA	G	314	-	1/1/14/20	8/31/109/115	-
29	CLA	D	313	20	1/1/11/20	4/13/91/115	-
36	DD6	G	308	-	-	1/26/80/80	0/3/3/3
36	DD6	h	202	-	-	2/26/80/80	0/3/3/3
29	CLA	b	701	-	1/1/15/20	13/37/115/115	-
37	PID	T	305	-	-	0/24/93/93	0/4/4/4
29	CLA	T	308	-	1/1/11/20	2/16/94/115	-
29	CLA	a	809	1	1/1/15/20	17/37/115/115	-
37	PID	T	317	-	-	10/24/93/93	1/4/4/4
39	KC1	H	314	-	-	6/15/71/71	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	312	-	1/1/15/20	10/37/115/115	-
38	UIX	E	304	-	-	2/31/87/87	0/3/3/3
29	CLA	f	803	6	1/1/11/20	8/15/93/115	-
29	CLA	L	309	-	1/1/13/20	2/25/103/115	-
29	CLA	a	806	1	1/1/15/20	16/37/115/115	-
29	CLA	a	801	-	1/1/15/20	10/37/115/115	-
29	CLA	l	509	-	1/1/10/20	2/8/86/115	-
32	BCR	l	507	-	-	5/29/63/63	0/2/2/2
29	CLA	E	308	-	1/1/15/20	10/37/115/115	-
29	CLA	P	214	27	1/1/11/20	7/15/93/115	-
29	CLA	B	315	-	1/1/11/20	3/15/93/115	-
29	CLA	O	314	-	-	6/16/94/115	-
29	CLA	H	312	22	1/1/11/20	7/15/93/115	-
29	CLA	K	216	-	1/1/10/20	3/8/86/115	-
29	CLA	B	310	-	1/1/15/20	16/37/115/115	-
39	KC1	C	315	25	-	8/15/71/71	-
36	DD6	I	202	-	-	5/26/80/80	0/3/3/3
39	KC1	C	310	-	-	9/15/71/71	-
39	KC1	A	205	29	-	6/15/71/71	-
29	CLA	F	311	-	1/1/11/20	3/15/93/115	-
39	KC1	D	315	-	-	6/15/71/71	-
32	BCR	a	835	-	-	2/29/63/63	0/2/2/2
29	CLA	b	721	-	1/1/13/20	10/29/107/115	-
29	CLA	b	702	-	1/1/15/20	17/37/115/115	-
29	CLA	C	316	-	1/1/10/20	6/8/86/115	-
36	DD6	L	305	-	-	4/26/80/80	0/3/3/3
29	CLA	b	706	-	1/1/15/20	11/37/115/115	-
29	CLA	l	502	10	1/1/15/20	13/37/115/115	-
29	CLA	L	310	-	1/1/13/20	9/25/103/115	-
39	KC1	K	215	-	-	6/15/71/71	-
29	CLA	D	316	-	1/1/10/20	5/8/86/115	-
37	PID	O	301	-	-	3/24/93/93	0/4/4/4
29	CLA	T	309	25	1/1/11/20	4/15/93/115	-
29	CLA	b	723	-	1/1/15/20	5/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DD6	F	303	-	-	0/26/80/80	0/3/3/3
29	CLA	a	802	-	1/1/15/20	10/37/115/115	-
36	DD6	K	221	-	-	5/26/80/80	0/3/3/3
29	CLA	F	312	16	1/1/11/20	5/15/93/115	-
37	PID	D	303	-	-	1/24/93/93	0/4/4/4
39	KC1	H	309	-	-	8/15/71/71	-
36	DD6	G	307	-	-	2/26/80/80	0/3/3/3
29	CLA	A	212	-	1/1/13/20	10/25/103/115	-
38	UIX	L	302	-	-	2/31/87/87	0/3/3/3
29	CLA	T	316	-	1/1/10/20	6/8/86/115	-
29	CLA	b	722	-	1/1/13/20	8/29/107/115	-
29	CLA	b	731	-	1/1/13/20	3/27/105/115	-
29	CLA	K	210	-	1/1/12/20	6/19/97/115	-
39	KC1	D	310	-	-	5/15/71/71	-
36	DD6	J	301	-	-	3/26/80/80	0/3/3/3
34	LMG	K	201	-	-	17/38/58/70	0/1/1/1
38	UIX	N	306	-	-	9/31/87/87	0/3/3/3
29	CLA	F	310	-	1/1/11/20	8/15/93/115	-
29	CLA	I	216	-	1/1/12/20	4/22/100/115	-
29	CLA	K	218	-	1/1/11/20	7/13/91/115	-
29	CLA	L	316	-	1/1/12/20	11/22/100/115	-
29	CLA	b	736	-	1/1/15/20	16/37/115/115	-
29	CLA	a	812	-	1/1/14/20	15/31/109/115	-
29	CLA	A	207	-	1/1/13/20	5/25/103/115	-
37	PID	C	307	-	-	2/24/93/93	0/4/4/4
29	CLA	B	309	-	1/1/13/20	6/25/103/115	-
29	CLA	L	313	-	1/1/12/20	8/23/101/115	-
34	LMG	b	734	-	-	10/35/55/70	0/1/1/1
29	CLA	i	203	-	1/1/13/20	12/25/103/115	-
29	CLA	a	822	-	1/1/15/20	8/37/115/115	-
29	CLA	K	207	15	1/1/11/20	6/18/96/115	-
37	PID	F	302	-	-	3/24/93/93	0/4/4/4
29	CLA	C	314	-	1/1/11/20	7/16/94/115	-
29	CLA	J	305	-	1/1/11/20	2/15/93/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	a	833	-	-	8/52/52/53	-
35	DGD	b	733	-	-	24/46/86/95	0/2/2/2
37	PID	O	304	-	-	3/24/93/93	0/4/4/4
29	CLA	F	315	-	1/1/10/20	3/8/86/115	-
29	CLA	J	306	-	1/1/15/20	17/37/115/115	-
39	KC1	H	311	-	-	6/15/71/71	-
29	CLA	D	314	-	1/1/11/20	7/16/94/115	-
29	CLA	N	309	-	1/1/15/20	15/37/115/115	-
37	PID	T	307	-	-	4/24/93/93	0/4/4/4
29	CLA	b	725	-	1/1/15/20	9/37/115/115	-
29	CLA	E	315	-	1/1/13/20	6/28/106/115	-
29	CLA	J	308	-	1/1/13/20	8/27/105/115	-
36	DD6	G	306	-	-	1/26/80/80	0/3/3/3
37	PID	h	204	-	-	2/24/93/93	1/4/4/4
29	CLA	f	802	-	1/1/11/20	4/15/93/115	-
29	CLA	l	503	10	1/1/15/20	15/37/115/115	-
29	CLA	M	311	-	1/1/11/20	8/15/93/115	-
36	DD6	F	301	-	-	8/26/80/80	0/3/3/3
36	DD6	K	206	-	-	1/26/80/80	0/3/3/3
29	CLA	J	313	-	1/1/10/20	2/8/86/115	-
38	UIX	P	207	-	-	6/31/87/87	0/3/3/3
29	CLA	b	720	-	1/1/15/20	15/37/115/115	-
29	CLA	a	814	-	1/1/11/20	6/15/93/115	-
37	PID	N	305	-	-	19/24/93/93	0/4/4/4
36	DD6	M	303	-	-	6/26/80/80	0/3/3/3
29	CLA	a	803	-	1/1/15/20	8/37/115/115	-
38	UIX	B	304	-	-	2/31/87/87	0/3/3/3
37	PID	O	302	-	-	2/24/93/93	0/4/4/4
29	CLA	J	311	-	1/1/12/20	8/23/101/115	-
29	CLA	l	508	-	1/1/10/20	2/8/86/115	-
29	CLA	N	311	-	1/1/12/20	6/21/99/115	-
37	PID	j	101	-	-	2/24/93/93	0/4/4/4
36	DD6	A	201	-	-	3/26/80/80	0/3/3/3
37	PID	H	302	-	-	2/24/93/93	0/4/4/4

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	704	-	1/1/15/20	10/37/115/115	-
29	CLA	b	715	-	1/1/11/20	7/15/93/115	-
29	CLA	l	501	-	1/1/14/20	13/31/109/115	-
39	KC1	P	211	-	-	7/15/71/71	-
29	CLA	H	308	-	1/1/15/20	9/37/115/115	-
36	DD6	O	303	-	-	4/26/80/80	0/3/3/3
29	CLA	E	310	28	1/1/11/20	4/15/93/115	-
37	PID	D	306	-	-	3/24/93/93	0/4/4/4
29	CLA	I	214	-	1/1/13/20	5/25/103/115	-
29	CLA	L	315	-	1/1/10/20	4/8/86/115	-
39	KC1	O	315	-	-	9/15/71/71	-
29	CLA	B	316	-	1/1/11/20	4/13/91/115	-
35	DGD	j	105	-	-	0/30/70/95	0/2/2/2
29	CLA	A	210	12	1/1/11/20	6/15/93/115	-
29	CLA	G	304	-	1/1/13/20	12/30/108/115	-
29	CLA	K	214	-	1/1/13/20	8/25/103/115	-
37	PID	G	303	-	-	6/24/93/93	0/4/4/4
29	CLA	I	209	-	1/1/14/20	14/31/109/115	-
29	CLA	a	813	-	1/1/12/20	10/21/99/115	-
32	BCR	i	204	-	-	4/29/63/63	0/2/2/2
29	CLA	b	726	-	1/1/15/20	6/37/115/115	-
36	DD6	L	301	-	-	4/26/80/80	0/3/3/3
37	PID	P	202	-	-	4/24/93/93	0/4/4/4
37	PID	Q	304	-	-	2/24/93/93	0/4/4/4
29	CLA	b	711	-	1/1/13/20	11/29/107/115	-
29	CLA	F	316	16	1/1/10/20	4/8/86/115	-
29	CLA	I	213	14	1/1/15/20	13/37/115/115	-
29	CLA	C	308	-	1/1/11/20	7/16/94/115	-
29	CLA	a	831	-	1/1/15/20	14/37/115/115	-
29	CLA	B	314	21	1/1/10/20	6/8/86/115	-
29	CLA	C	309	-	1/1/15/20	10/37/115/115	-
36	DD6	A	204	-	-	2/26/80/80	0/3/3/3
37	PID	C	304	-	-	3/24/93/93	0/4/4/4
29	CLA	K	208	-	1/1/11/20	5/15/93/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	707	-	1/1/15/20	11/37/115/115	-
29	CLA	a	805	-	1/1/13/20	6/25/103/115	-
29	CLA	b	703	-	1/1/15/20	13/37/115/115	-
29	CLA	K	213	-	1/1/11/20	5/17/95/115	-
34	LMG	A	219	-	-	17/32/52/70	0/1/1/1
29	CLA	A	216	-	1/1/10/20	0/8/86/115	-
29	CLA	a	830	-	1/1/13/20	5/27/105/115	-
29	CLA	b	718	-	1/1/15/20	14/37/115/115	-
37	PID	Q	303	-	-	0/24/93/93	0/4/4/4
29	CLA	M	315	-	1/1/11/20	5/15/93/115	-
36	DD6	M	302	-	-	1/26/80/80	0/3/3/3
39	KC1	F	309	-	-	7/15/71/71	-
29	CLA	Q	307	-	1/1/11/20	1/16/94/115	-
32	BCR	a	838	-	-	6/29/63/63	0/2/2/2
29	CLA	P	210	-	1/1/15/20	10/37/115/115	-
37	PID	G	309	-	-	2/24/93/93	0/4/4/4
39	KC1	I	215	14	-	10/15/71/71	-
29	CLA	L	307	39	1/1/12/20	9/19/97/115	-
29	CLA	b	709	-	1/1/14/20	17/31/109/115	-
29	CLA	l	505	-	1/1/15/20	12/37/115/115	-
29	CLA	P	209	-	1/1/11/20	8/16/94/115	-
34	LMG	E	316	-	-	10/27/47/70	0/1/1/1
29	CLA	G	301	-	1/1/11/20	6/18/96/115	-
29	CLA	I	208	-	1/1/11/20	7/15/93/115	-
38	UIX	A	203	-	-	4/31/87/87	0/3/3/3
37	PID	C	301	-	-	4/24/93/93	0/4/4/4
29	CLA	a	828	-	1/1/11/20	8/15/93/115	-
29	CLA	M	313	-	1/1/10/20	2/8/86/115	-
32	BCR	a	834	-	-	0/29/63/63	0/2/2/2
29	CLA	i	201	-	1/1/15/20	16/37/115/115	-
38	UIX	F	305	-	-	12/31/87/87	0/3/3/3
29	CLA	a	826	-	1/1/15/20	10/37/115/115	-
29	CLA	N	308	-	1/1/11/20	7/16/94/115	-
29	CLA	T	313	-	1/1/11/20	7/15/93/115	-
37	PID	P	206	-	-	8/24/93/93	0/4/4/4

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	T	304	-	-	1/24/93/93	0/4/4/4
29	CLA	b	717	-	1/1/15/20	14/37/115/115	-
29	CLA	a	818	-	1/1/11/20	4/16/94/115	-
29	CLA	a	820	-	1/1/15/20	10/37/115/115	-
29	CLA	a	837	-	1/1/13/20	12/25/103/115	-
29	CLA	a	815	-	1/1/11/20	4/13/91/115	-
37	PID	O	307	-	-	4/24/93/93	0/4/4/4
29	CLA	D	311	-	1/1/11/20	12/15/93/115	-
39	KC1	M	305	-	-	5/15/71/71	-
29	CLA	a	821	-	1/1/11/20	9/16/94/115	-
29	CLA	M	309	-	1/1/11/20	6/15/93/115	-
29	CLA	Q	312	-	1/1/11/20	3/15/93/115	-
29	CLA	I	201	29	1/1/11/20	4/13/91/115	-
39	KC1	T	310	-	-	5/15/71/71	-
40	SQD	B	317	-	-	4/37/57/69	0/1/1/1
32	BCR	b	728	-	-	7/29/63/63	0/2/2/2
29	CLA	P	217	-	1/1/10/20	3/8/86/115	-
32	BCR	f	804	-	-	2/29/63/63	0/2/2/2
29	CLA	L	311	19	1/1/11/20	7/15/93/115	-
30	PQN	b	727	-	-	4/23/43/43	0/2/2/2
29	CLA	A	215	-	1/1/11/20	4/16/94/115	-
29	CLA	b	713	-	1/1/12/20	4/23/101/115	-
39	KC1	T	315	25	-	5/15/71/71	-
29	CLA	a	824	-	1/1/15/20	9/37/115/115	-
29	CLA	M	310	18	1/1/11/20	5/17/95/115	-
29	CLA	F	313	16	1/1/11/20	6/15/93/115	-
29	CLA	N	313	23	1/1/11/20	9/15/93/115	-
36	DD6	Q	302	-	-	1/26/80/80	0/3/3/3
29	CLA	a	808	-	1/1/12/20	4/21/99/115	-
29	CLA	I	212	-	1/1/13/20	10/25/103/115	-
36	DD6	B	302	-	-	2/26/80/80	0/3/3/3
37	PID	P	203	-	-	3/24/93/93	0/4/4/4
29	CLA	A	218	12	1/1/14/20	10/31/109/115	-
36	DD6	E	303	-	-	1/26/80/80	0/3/3/3
36	DD6	G	305	-	-	7/26/80/80	0/3/3/3

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	312	13	1/1/15/20	16/37/115/115	-
37	PID	N	302	-	-	2/24/93/93	0/4/4/4
36	DD6	B	305	-	-	2/26/80/80	0/3/3/3
37	PID	O	305	-	-	7/24/93/93	0/4/4/4
29	CLA	E	314	28	-	5/17/95/115	-
36	DD6	C	303	-	-	0/26/80/80	0/3/3/3
29	CLA	b	716	-	1/1/12/20	7/23/101/115	-
36	DD6	B	319	-	-	9/26/80/80	0/3/3/3
37	PID	D	307	-	-	4/24/93/93	0/4/4/4
37	PID	F	306	-	-	0/24/93/93	0/4/4/4
29	CLA	a	810	1	1/1/13/20	10/25/103/115	-
36	DD6	M	304	-	-	3/26/80/80	0/3/3/3
37	PID	Q	301	-	-	2/24/93/93	0/4/4/4
29	CLA	a	825	-	1/1/15/20	13/37/115/115	-
37	PID	P	205	-	-	1/24/93/93	0/4/4/4
29	CLA	a	811	-	1/1/13/20	6/27/105/115	-
37	PID	F	304	-	-	15/24/93/93	1/4/4/4
29	CLA	H	315	-	1/1/10/20	3/8/86/115	-
29	CLA	P	212	-	1/1/12/20	8/21/99/115	-
38	UIX	J	304	-	-	3/31/87/87	0/3/3/3
29	CLA	b	708	2	1/1/12/20	5/22/100/115	-
36	DD6	J	302	-	-	2/26/80/80	0/3/3/3
29	CLA	J	309	17	1/1/11/20	5/15/93/115	-
35	DGD	h	203	-	-	8/43/83/95	0/2/2/2
29	CLA	B	306	21	1/1/11/20	5/18/96/115	-
29	CLA	H	310	-	1/1/12/20	9/21/99/115	-
29	CLA	G	311	13	1/1/12/20	7/21/99/115	-
29	CLA	F	307	-	1/1/11/20	2/15/93/115	-
29	CLA	b	724	-	1/1/11/20	2/16/94/115	-
29	CLA	L	317	-	1/1/11/20	5/15/93/115	-
37	PID	Q	306	-	-	3/24/93/93	0/4/4/4
29	CLA	a	804	-	1/1/13/20	1/25/103/115	-
30	PQN	a	832	-	-	6/23/43/43	0/2/2/2
39	KC1	B	313	21	-	8/15/71/71	-
37	PID	G	310	-	-	2/24/93/93	0/4/4/4

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	KC1	N	310	-	-	6/15/71/71	-
34	LMG	h	205	-	-	3/23/43/70	0/1/1/1
29	CLA	T	314	-	1/1/11/20	7/16/94/115	-
29	CLA	D	308	-	1/1/11/20	5/16/94/115	-
35	DGD	j	106	-	-	16/38/78/95	0/2/2/2
34	LMG	b	732	-	-	20/39/59/70	0/1/1/1
39	KC1	Q	314	26	-	8/15/71/71	-
39	KC1	Q	309	-	-	7/15/71/71	-
39	KC1	P	216	-	-	6/15/71/71	-
39	KC1	P	213	27	-	5/15/71/71	-
35	DGD	m	102	-	-	8/55/95/95	0/2/2/2
29	CLA	O	309	-	-	10/37/115/115	-
29	CLA	G	317	-	1/1/12/20	8/23/101/115	-
29	CLA	E	309	-	1/1/11/20	8/15/93/115	-
29	CLA	a	816	-	1/1/11/20	8/15/93/115	-
29	CLA	I	211	-	1/1/15/20	8/37/115/115	-
29	CLA	G	319	13	1/1/10/20	3/8/86/115	-
29	CLA	K	212	-	1/1/12/20	5/22/100/115	-
37	PID	H	304	-	-	0/24/93/93	0/4/4/4
29	CLA	Q	310	-	1/1/15/20	13/37/115/115	-
29	CLA	Q	308	-	1/1/15/20	21/37/115/115	-
29	CLA	Q	313	-	1/1/11/20	6/16/94/115	-
39	KC1	N	315	-	-	9/15/71/71	-
29	CLA	H	313	-	1/1/11/20	8/16/94/115	-
29	CLA	O	316	-	1/1/10/20	5/8/86/115	-
35	DGD	G	320	-	-	9/34/74/95	0/2/2/2
29	CLA	K	209	-	1/1/12/20	10/24/102/115	-
29	CLA	N	316	-	1/1/10/20	5/8/86/115	-
29	CLA	A	217	-	1/1/12/20	7/21/99/115	-
29	CLA	O	308	-	1/1/11/20	6/16/94/115	-
29	CLA	b	710	-	1/1/11/20	7/15/93/115	-
29	CLA	a	823	-	1/1/13/20	11/29/107/115	-
29	CLA	l	510	-	1/1/11/20	5/13/91/115	-
32	BCR	b	729	-	-	6/29/63/63	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	C	302	-	-	2/24/93/93	0/4/4/4
29	CLA	E	305	-	1/1/14/20	14/33/111/115	-
36	DD6	E	302	-	-	2/26/80/80	0/3/3/3
38	UIX	T	306	-	-	4/31/87/87	0/3/3/3
39	KC1	C	312	-	-	8/15/71/71	-
37	PID	D	302	-	-	1/24/93/93	0/4/4/4
37	PID	N	307	-	-	6/24/93/93	0/4/4/4
38	UIX	C	306	-	-	6/31/87/87	0/3/3/3
29	CLA	I	207	14	1/1/11/20	6/18/96/115	-
39	KC1	L	314	-	-	7/15/71/71	-
29	CLA	N	314	-	1/1/11/20	7/16/94/115	-
29	CLA	D	309	-	1/1/11/20	2/15/93/115	-
35	DGD	B	318	-	-	9/34/74/95	0/2/2/2
29	CLA	a	817	-	1/1/11/20	4/13/91/115	-
29	CLA	M	307	-	1/1/13/20	6/25/103/115	-
36	DD6	D	304	-	-	6/26/80/80	0/3/3/3
33	SF4	c	102	3	-	-	0/6/5/5
29	CLA	E	306	28	1/1/15/20	14/37/115/115	-
39	KC1	E	307	-	-	6/15/71/71	-
29	CLA	L	312	-	1/1/13/20	11/25/103/115	-
39	KC1	O	312	-	-	4/15/71/71	-
29	CLA	f	805	-	1/1/14/20	10/31/109/115	-
36	DD6	A	202	-	-	1/26/80/80	0/3/3/3
37	PID	C	305	-	-	9/24/93/93	0/4/4/4
29	CLA	K	217	-	1/1/11/20	4/15/93/115	-
36	DD6	I	204	-	-	3/26/80/80	0/3/3/3
36	DD6	M	301	-	-	2/26/80/80	0/3/3/3
39	KC1	G	318	-	-	5/15/71/71	-
29	CLA	E	311	-	1/1/15/20	11/37/115/115	-
34	LMG	K	219	-	-	16/30/50/70	0/1/1/1
36	DD6	H	303	-	-	1/26/80/80	0/3/3/3
37	PID	T	302	-	-	1/24/93/93	0/4/4/4
37	PID	D	305	-	-	5/24/93/93	0/4/4/4
29	CLA	J	307	-	1/1/11/20	3/15/93/115	-
29	CLA	M	306	-	1/1/12/20	6/23/101/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	214	12	1/1/10/20	4/8/86/115	-
29	CLA	M	308	-	1/1/11/20	9/17/95/115	-
29	CLA	b	714	-	1/1/14/20	6/36/114/115	-
36	DD6	P	204	-	-	2/26/80/80	0/3/3/3
29	CLA	L	308	-	1/1/12/20	10/23/101/115	-
32	BCR	f	801	-	-	5/29/63/63	0/2/2/2
33	SF4	c	101	3	-	-	0/6/5/5
36	DD6	L	304	-	-	2/26/80/80	0/3/3/3
29	CLA	O	311	-	1/1/12/20	3/21/99/115	-
39	KC1	M	312	-	-	6/15/71/71	-
29	CLA	K	211	-	1/1/13/20	7/25/103/115	-
38	UIX	Q	305	-	-	5/31/87/87	0/3/3/3
29	CLA	B	307	-	1/1/11/20	2/13/91/115	-
29	CLA	G	313	-	1/1/13/20	3/25/103/115	-
29	CLA	I	217	-	1/1/13/20	9/25/103/115	-
29	CLA	j	104	29	1/1/12/20	4/22/100/115	-
33	SF4	a	836	2,1	-	-	0/6/5/5
39	KC1	T	312	-	-	5/15/71/71	-
29	CLA	O	313	24	1/1/11/20	5/15/93/115	-
29	CLA	C	311	-	1/1/12/20	7/21/99/115	-
36	DD6	B	301	-	-	4/24/78/80	0/3/3/3
29	CLA	i	202	-	1/1/15/20	12/37/115/115	-
39	KC1	J	312	17	-	5/15/71/71	-
36	DD6	L	303	-	-	0/26/80/80	0/3/3/3
37	PID	H	301	-	-	2/24/93/93	0/4/4/4
29	CLA	b	705	-	1/1/15/20	12/37/115/115	-
36	DD6	I	203	-	-	7/26/80/80	0/3/3/3
29	CLA	Q	315	-	1/1/10/20	6/8/86/115	-
37	PID	T	301	-	-	2/24/93/93	0/4/4/4
34	LMG	b	730	-	-	19/41/61/70	0/1/1/1
37	PID	H	305	-	-	3/24/93/93	0/4/4/4
37	PID	E	301	-	-	6/24/93/93	0/4/4/4
29	CLA	l	504	-	1/1/15/20	10/37/115/115	-
34	LMG	K	220	-	-	13/31/51/70	0/1/1/1
29	CLA	T	311	-	1/1/11/20	10/15/93/115	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DD6	K	203	-	-	6/26/80/80	0/3/3/3
29	CLA	B	308	-	1/1/15/20	13/37/115/115	-
35	DGD	j	103	-	-	10/32/72/95	0/2/2/2
37	PID	H	306	-	-	4/24/93/93	0/4/4/4
34	LMG	P	201	-	-	6/22/42/70	0/1/1/1
29	CLA	D	312	20	1/1/11/20	5/15/93/115	-
39	KC1	N	312	23	-	6/15/71/71	-
39	KC1	F	314	-	-	6/15/71/71	-
36	DD6	D	301	-	-	8/26/80/80	0/3/3/3
36	DD6	K	202	-	-	8/26/80/80	0/3/3/3
36	DD6	T	303	-	-	7/26/80/80	0/3/3/3
36	DD6	K	205	-	-	1/26/80/80	0/3/3/3
38	UIX	O	306	-	-	6/31/87/87	0/3/3/3
29	CLA	H	307	-	1/1/11/20	5/16/94/115	-
29	CLA	a	819	-	1/1/13/20	6/28/106/115	-
37	PID	N	304	-	-	1/24/93/93	0/4/4/4
29	CLA	A	211	-	1/1/13/20	5/25/103/115	-
29	CLA	J	310	-	1/1/11/20	6/16/94/115	-
40	SQD	J	314	-	-	9/40/60/69	0/1/1/1
29	CLA	E	313	-	1/1/10/20	2/8/86/115	-
39	KC1	L	306	29	-	5/15/71/71	-
36	DD6	K	204	-	-	5/26/80/80	0/3/3/3
34	LMG	j	102	-	-	24/38/58/70	0/1/1/1
29	CLA	B	311	21	1/1/12/20	4/21/99/115	-
39	KC1	Q	311	-	-	6/15/71/71	-
36	DD6	m	101	-	-	1/26/80/80	0/3/3/3
29	CLA	b	712	-	1/1/15/20	12/37/115/115	-

All (2170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	307	DD6	C29-C27	-9.45	1.24	1.42
36	I	203	DD6	C29-C27	-9.14	1.25	1.42
36	K	202	DD6	C29-C27	-9.12	1.25	1.42
36	G	306	DD6	C29-C27	-9.01	1.25	1.42
36	K	221	DD6	C29-C27	-8.93	1.25	1.42
36	G	305	DD6	C29-C27	-8.85	1.25	1.42

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	302	DD6	C29-C27	-8.85	1.25	1.42
36	B	302	DD6	C29-C27	-8.84	1.25	1.42
36	J	303	DD6	C29-C27	-8.82	1.25	1.42
36	I	204	DD6	C29-C27	-8.81	1.25	1.42
36	D	301	DD6	C29-C27	-8.80	1.25	1.42
36	E	302	DD6	C29-C27	-8.79	1.25	1.42
36	B	319	DD6	C29-C27	-8.78	1.25	1.42
36	M	302	DD6	C29-C27	-8.77	1.25	1.42
36	K	206	DD6	C29-C27	-8.77	1.25	1.42
36	M	303	DD6	C29-C27	-8.77	1.25	1.42
36	I	205	DD6	C29-C27	-8.76	1.25	1.42
36	L	305	DD6	C29-C27	-8.75	1.25	1.42
36	M	304	DD6	C29-C27	-8.75	1.25	1.42
36	I	206	DD6	C29-C27	-8.74	1.25	1.42
36	L	303	DD6	C29-C27	-8.73	1.25	1.42
36	F	303	DD6	C29-C27	-8.72	1.25	1.42
36	F	301	DD6	C29-C27	-8.72	1.25	1.42
36	m	101	DD6	C29-C27	-8.71	1.25	1.42
36	K	204	DD6	C29-C27	-8.71	1.25	1.42
36	J	301	DD6	C29-C27	-8.69	1.25	1.42
36	K	205	DD6	C29-C27	-8.68	1.25	1.42
36	B	303	DD6	C29-C27	-8.66	1.25	1.42
36	B	305	DD6	C29-C27	-8.66	1.25	1.42
36	I	202	DD6	C29-C27	-8.65	1.25	1.42
36	A	204	DD6	C29-C27	-8.65	1.25	1.42
36	h	202	DD6	C29-C27	-8.64	1.25	1.42
36	D	304	DD6	C29-C27	-8.64	1.25	1.42
36	K	203	DD6	C29-C27	-8.63	1.25	1.42
36	C	303	DD6	C29-C27	-8.63	1.25	1.42
36	G	307	DD6	C30-C31	-8.59	1.24	1.42
36	L	304	DD6	C29-C27	-8.58	1.26	1.42
36	A	201	DD6	C29-C27	-8.58	1.26	1.42
36	B	301	DD6	C29-C27	-8.58	1.26	1.42
36	G	308	DD6	C29-C27	-8.57	1.26	1.42
36	E	303	DD6	C29-C27	-8.56	1.26	1.42
36	O	303	DD6	C29-C27	-8.54	1.26	1.42
36	L	301	DD6	C29-C27	-8.52	1.26	1.42
36	P	204	DD6	C29-C27	-8.49	1.26	1.42
36	Q	302	DD6	C29-C27	-8.48	1.26	1.42
36	T	303	DD6	C29-C27	-8.48	1.26	1.42
36	A	202	DD6	C29-C27	-8.43	1.26	1.42
36	M	301	DD6	C29-C27	-8.41	1.26	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	203	DD6	C30-C31	-8.37	1.24	1.42
36	N	303	DD6	C29-C27	-8.33	1.26	1.42
36	H	303	DD6	C29-C27	-8.32	1.26	1.42
36	G	305	DD6	C30-C31	-8.16	1.25	1.42
36	K	202	DD6	C30-C31	-8.15	1.25	1.42
36	J	303	DD6	C30-C31	-8.10	1.25	1.42
36	J	302	DD6	C30-C31	-8.08	1.25	1.42
36	E	302	DD6	C30-C31	-8.06	1.25	1.42
36	K	221	DD6	C30-C31	-8.04	1.25	1.42
36	h	202	DD6	C30-C31	-8.04	1.25	1.42
36	F	301	DD6	C30-C31	-8.03	1.25	1.42
36	I	204	DD6	C30-C31	-8.03	1.25	1.42
36	G	306	DD6	C30-C31	-8.00	1.25	1.42
36	M	302	DD6	C30-C31	-7.99	1.25	1.42
36	K	204	DD6	C30-C31	-7.98	1.25	1.42
36	M	303	DD6	C30-C31	-7.98	1.25	1.42
36	B	319	DD6	C30-C31	-7.97	1.25	1.42
36	L	303	DD6	C30-C31	-7.97	1.25	1.42
36	C	303	DD6	C30-C31	-7.95	1.25	1.42
36	F	303	DD6	C30-C31	-7.94	1.25	1.42
36	K	206	DD6	C30-C31	-7.94	1.25	1.42
36	L	305	DD6	C30-C31	-7.94	1.25	1.42
36	I	205	DD6	C30-C31	-7.91	1.25	1.42
36	K	205	DD6	C30-C31	-7.91	1.25	1.42
36	K	203	DD6	C30-C31	-7.89	1.25	1.42
36	m	101	DD6	C30-C31	-7.88	1.25	1.42
36	B	302	DD6	C30-C31	-7.87	1.25	1.42
36	D	304	DD6	C30-C31	-7.87	1.25	1.42
36	M	304	DD6	C30-C31	-7.86	1.25	1.42
36	B	303	DD6	C30-C31	-7.86	1.26	1.42
36	J	301	DD6	C30-C31	-7.85	1.26	1.42
36	G	308	DD6	C30-C31	-7.85	1.26	1.42
36	O	303	DD6	C30-C31	-7.83	1.26	1.42
36	B	305	DD6	C30-C31	-7.82	1.26	1.42
36	I	206	DD6	C30-C31	-7.80	1.26	1.42
36	A	204	DD6	C30-C31	-7.79	1.26	1.42
36	A	201	DD6	C30-C31	-7.79	1.26	1.42
36	D	301	DD6	C30-C31	-7.78	1.26	1.42
36	E	303	DD6	C30-C31	-7.78	1.26	1.42
36	L	301	DD6	C30-C31	-7.75	1.26	1.42
36	M	301	DD6	C30-C31	-7.73	1.26	1.42
36	B	301	DD6	C30-C31	-7.72	1.26	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P	215	CLA	C4B-NB	7.71	1.42	1.35
36	P	204	DD6	C30-C31	-7.70	1.26	1.42
36	I	202	DD6	C30-C31	-7.70	1.26	1.42
36	Q	302	DD6	C30-C31	-7.68	1.26	1.42
29	L	316	CLA	C4B-NB	7.66	1.42	1.35
36	L	304	DD6	C30-C31	-7.66	1.26	1.42
36	T	303	DD6	C30-C31	-7.65	1.26	1.42
29	L	315	CLA	C4B-NB	7.59	1.42	1.35
29	O	308	CLA	C4B-NB	7.59	1.42	1.35
36	N	303	DD6	C30-C31	-7.58	1.26	1.42
29	a	804	CLA	C4B-NB	7.58	1.42	1.35
36	A	202	DD6	C30-C31	-7.58	1.26	1.42
29	H	313	CLA	C4B-NB	7.57	1.42	1.35
29	P	214	CLA	C4B-NB	7.57	1.42	1.35
29	E	309	CLA	C4B-NB	7.55	1.41	1.35
29	O	309	CLA	C4B-NB	7.54	1.41	1.35
29	I	510	CLA	C4B-NB	7.54	1.41	1.35
29	O	314	CLA	C4B-NB	7.54	1.41	1.35
29	C	314	CLA	C4B-NB	7.54	1.41	1.35
29	P	209	CLA	C4B-NB	7.53	1.41	1.35
29	O	316	CLA	C4B-NB	7.53	1.41	1.35
29	H	310	CLA	C4B-NB	7.53	1.41	1.35
29	a	817	CLA	C4B-NB	7.52	1.41	1.35
29	N	308	CLA	C4B-NB	7.52	1.41	1.35
36	H	303	DD6	C30-C31	-7.51	1.26	1.42
29	T	308	CLA	C4B-NB	7.50	1.41	1.35
29	H	315	CLA	C4B-NB	7.49	1.41	1.35
29	N	309	CLA	C4B-NB	7.48	1.41	1.35
29	a	813	CLA	C4B-NB	7.48	1.41	1.35
29	N	316	CLA	C4B-NB	7.47	1.41	1.35
29	K	218	CLA	C4B-NB	7.46	1.41	1.35
29	a	811	CLA	C4B-NB	7.46	1.41	1.35
29	b	713	CLA	C4B-NB	7.46	1.41	1.35
29	E	315	CLA	C4B-NB	7.46	1.41	1.35
29	a	818	CLA	C4B-NB	7.45	1.41	1.35
29	Q	307	CLA	C4B-NB	7.45	1.41	1.35
29	K	212	CLA	C4B-NB	7.45	1.41	1.35
29	T	316	CLA	C4B-NB	7.45	1.41	1.35
29	H	307	CLA	C4B-NB	7.45	1.41	1.35
29	D	308	CLA	C4B-NB	7.44	1.41	1.35
29	b	720	CLA	C4B-NB	7.44	1.41	1.35
29	I	217	CLA	C4B-NB	7.44	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T	313	CLA	C4B-NB	7.43	1.41	1.35
29	F	315	CLA	C4B-NB	7.43	1.41	1.35
29	E	313	CLA	C4B-NB	7.43	1.41	1.35
29	F	307	CLA	C4B-NB	7.43	1.41	1.35
29	K	208	CLA	C4B-NB	7.42	1.41	1.35
29	T	314	CLA	C4B-NB	7.42	1.41	1.35
29	P	212	CLA	C4B-NB	7.42	1.41	1.35
29	J	305	CLA	C4B-NB	7.41	1.41	1.35
29	D	316	CLA	C4B-NB	7.41	1.41	1.35
29	M	313	CLA	C4B-NB	7.41	1.41	1.35
29	K	217	CLA	C4B-NB	7.41	1.41	1.35
29	a	828	CLA	C4B-NB	7.41	1.41	1.35
29	Q	315	CLA	C4B-NB	7.40	1.41	1.35
29	C	308	CLA	C4B-NB	7.40	1.41	1.35
29	I	509	CLA	C4B-NB	7.40	1.41	1.35
29	L	311	CLA	C4B-NB	7.39	1.41	1.35
29	N	313	CLA	C4B-NB	7.39	1.41	1.35
29	O	311	CLA	C4B-NB	7.38	1.41	1.35
29	b	708	CLA	C4B-NB	7.37	1.41	1.35
29	M	311	CLA	C4B-NB	7.37	1.41	1.35
29	A	214	CLA	C4B-NB	7.37	1.41	1.35
29	a	821	CLA	C4B-NB	7.37	1.41	1.35
29	B	307	CLA	C4B-NB	7.37	1.41	1.35
29	Q	308	CLA	C4B-NB	7.37	1.41	1.35
29	D	312	CLA	C4B-NB	7.36	1.41	1.35
29	T	309	CLA	C4B-NB	7.36	1.41	1.35
29	J	313	CLA	C4B-NB	7.36	1.41	1.35
29	G	316	CLA	C4B-NB	7.36	1.41	1.35
29	P	217	CLA	C4B-NB	7.36	1.41	1.35
29	N	314	CLA	C4B-NB	7.35	1.41	1.35
29	T	311	CLA	C4B-NB	7.35	1.41	1.35
29	L	307	CLA	C4B-NB	7.35	1.41	1.35
29	K	207	CLA	C4B-NB	7.34	1.41	1.35
29	G	301	CLA	C4B-NB	7.34	1.41	1.35
29	M	309	CLA	C4B-NB	7.34	1.41	1.35
30	b	727	PQN	C3-C2	7.34	1.48	1.35
29	b	710	CLA	C4B-NB	7.33	1.41	1.35
29	N	311	CLA	C4B-NB	7.33	1.41	1.35
29	F	316	CLA	C4B-NB	7.33	1.41	1.35
29	L	317	CLA	C4B-NB	7.33	1.41	1.35
29	B	316	CLA	C4B-NB	7.33	1.41	1.35
29	f	805	CLA	C4B-NB	7.32	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	M	310	CLA	C4B-NB	7.32	1.41	1.35
29	b	707	CLA	C4B-NB	7.32	1.41	1.35
29	A	210	CLA	C4B-NB	7.31	1.41	1.35
29	A	217	CLA	C4B-NB	7.31	1.41	1.35
29	I	207	CLA	C4B-NB	7.31	1.41	1.35
29	l	501	CLA	C4B-NB	7.31	1.41	1.35
29	E	305	CLA	C4B-NB	7.31	1.41	1.35
29	I	212	CLA	C4B-NB	7.30	1.41	1.35
29	b	703	CLA	C4B-NB	7.30	1.41	1.35
29	M	315	CLA	C4B-NB	7.30	1.41	1.35
29	a	807	CLA	C4B-NB	7.30	1.41	1.35
29	a	810	CLA	C4B-NB	7.29	1.41	1.35
29	B	306	CLA	C4B-NB	7.29	1.41	1.35
29	l	508	CLA	C4B-NB	7.29	1.41	1.35
29	a	825	CLA	C4B-NB	7.29	1.41	1.35
29	a	803	CLA	C4B-NB	7.29	1.41	1.35
29	G	304	CLA	C4B-NB	7.28	1.41	1.35
29	D	309	CLA	C4B-NB	7.28	1.41	1.35
29	a	837	CLA	C4B-NB	7.28	1.41	1.35
29	D	314	CLA	C4B-NB	7.28	1.41	1.35
29	E	308	CLA	C4B-NB	7.28	1.41	1.35
29	E	314	CLA	C4B-NB	7.28	1.41	1.35
29	A	216	CLA	C4B-NB	7.28	1.41	1.35
29	M	308	CLA	C4B-NB	7.28	1.41	1.35
30	a	832	PQN	C3-C2	7.27	1.48	1.35
29	b	706	CLA	C4B-NB	7.27	1.41	1.35
29	I	201	CLA	C4B-NB	7.27	1.41	1.35
29	O	313	CLA	C4B-NB	7.27	1.41	1.35
29	I	216	CLA	C4B-NB	7.27	1.41	1.35
29	B	315	CLA	C4B-NB	7.27	1.41	1.35
29	Q	310	CLA	C4B-NB	7.26	1.41	1.35
29	b	724	CLA	C4B-NB	7.26	1.41	1.35
29	A	206	CLA	C4B-NB	7.26	1.41	1.35
29	H	308	CLA	C4B-NB	7.26	1.41	1.35
29	j	104	CLA	C4B-NB	7.26	1.41	1.35
29	A	207	CLA	C4B-NB	7.26	1.41	1.35
29	I	213	CLA	C4B-NB	7.26	1.41	1.35
29	E	306	CLA	C4B-NB	7.26	1.41	1.35
29	H	312	CLA	C4B-NB	7.25	1.41	1.35
29	b	736	CLA	C4B-NB	7.25	1.41	1.35
29	C	316	CLA	C4B-NB	7.25	1.41	1.35
29	b	719	CLA	C4B-NB	7.25	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	815	CLA	C4B-NB	7.24	1.41	1.35
29	a	816	CLA	C4B-NB	7.24	1.41	1.35
29	C	309	CLA	C4B-NB	7.24	1.41	1.35
29	Q	313	CLA	C4B-NB	7.24	1.41	1.35
29	A	215	CLA	C4B-NB	7.24	1.41	1.35
29	Q	312	CLA	C4B-NB	7.24	1.41	1.35
29	b	712	CLA	C4B-NB	7.24	1.41	1.35
29	K	213	CLA	C4B-NB	7.23	1.41	1.35
29	a	814	CLA	C4B-NB	7.23	1.41	1.35
29	P	210	CLA	C4B-NB	7.22	1.41	1.35
29	f	802	CLA	C4B-NB	7.22	1.41	1.35
29	b	726	CLA	C4B-NB	7.22	1.41	1.35
29	F	311	CLA	C4B-NB	7.22	1.41	1.35
29	M	314	CLA	C4B-NB	7.22	1.41	1.35
29	F	308	CLA	C4B-NB	7.22	1.41	1.35
29	C	313	CLA	C4B-NB	7.22	1.41	1.35
29	a	819	CLA	C4B-NB	7.21	1.41	1.35
29	b	717	CLA	C4B-NB	7.21	1.41	1.35
29	l	505	CLA	C4B-NB	7.21	1.41	1.35
29	l	503	CLA	C4B-NB	7.20	1.41	1.35
29	a	812	CLA	C4B-NB	7.20	1.41	1.35
29	L	310	CLA	C4B-NB	7.20	1.41	1.35
29	B	311	CLA	C4B-NB	7.20	1.41	1.35
29	b	709	CLA	C4B-NB	7.20	1.41	1.35
29	a	826	CLA	C4B-NB	7.19	1.41	1.35
29	L	309	CLA	C4B-NB	7.19	1.41	1.35
29	b	715	CLA	C4B-NB	7.19	1.41	1.35
29	E	310	CLA	C4B-NB	7.18	1.41	1.35
29	a	827	CLA	C4B-NB	7.18	1.41	1.35
29	I	208	CLA	C4B-NB	7.18	1.41	1.35
29	J	311	CLA	C4B-NB	7.18	1.41	1.35
29	a	802	CLA	C4B-NB	7.18	1.41	1.35
29	a	805	CLA	C4B-NB	7.18	1.41	1.35
29	G	302	CLA	C4B-NB	7.17	1.41	1.35
29	M	307	CLA	C4B-NB	7.17	1.41	1.35
29	F	313	CLA	C4B-NB	7.17	1.41	1.35
29	A	209	CLA	C4B-NB	7.16	1.41	1.35
29	K	216	CLA	C4B-NB	7.16	1.41	1.35
29	l	504	CLA	C4B-NB	7.16	1.41	1.35
29	B	314	CLA	C4B-NB	7.15	1.41	1.35
29	B	310	CLA	C4B-NB	7.15	1.41	1.35
29	C	311	CLA	C4B-NB	7.15	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	218	CLA	C4B-NB	7.15	1.41	1.35
29	D	313	CLA	C4B-NB	7.15	1.41	1.35
29	f	803	CLA	C4B-NB	7.15	1.41	1.35
29	a	808	CLA	C4B-NB	7.15	1.41	1.35
29	B	308	CLA	C4B-NB	7.15	1.41	1.35
29	b	702	CLA	C4B-NB	7.14	1.41	1.35
29	a	831	CLA	C4B-NB	7.14	1.41	1.35
29	b	716	CLA	C4B-NB	7.14	1.41	1.35
29	K	214	CLA	C4B-NB	7.13	1.41	1.35
29	J	310	CLA	C4B-NB	7.13	1.41	1.35
29	M	306	CLA	C4B-NB	7.13	1.41	1.35
29	b	718	CLA	C4B-NB	7.13	1.41	1.35
29	a	829	CLA	C4B-NB	7.12	1.41	1.35
29	D	311	CLA	C4B-NB	7.12	1.41	1.35
29	K	209	CLA	C4B-NB	7.12	1.41	1.35
29	K	210	CLA	C4B-NB	7.12	1.41	1.35
29	a	824	CLA	C4B-NB	7.12	1.41	1.35
29	b	714	CLA	C4B-NB	7.11	1.41	1.35
29	G	317	CLA	C4B-NB	7.11	1.41	1.35
29	b	723	CLA	C4B-NB	7.11	1.41	1.35
29	l	502	CLA	C4B-NB	7.11	1.41	1.35
29	F	312	CLA	C4B-NB	7.11	1.41	1.35
29	b	721	CLA	C4B-NB	7.11	1.41	1.35
29	G	314	CLA	C4B-NB	7.10	1.41	1.35
29	a	820	CLA	C4B-NB	7.09	1.41	1.35
29	G	319	CLA	C4B-NB	7.09	1.41	1.35
29	J	309	CLA	C4B-NB	7.09	1.41	1.35
29	b	701	CLA	C4B-NB	7.08	1.41	1.35
29	A	208	CLA	C4B-NB	7.08	1.41	1.35
29	b	731	CLA	C4B-NB	7.08	1.41	1.35
29	J	307	CLA	C4B-NB	7.08	1.41	1.35
29	a	809	CLA	C4B-NB	7.08	1.41	1.35
29	L	312	CLA	C4B-NB	7.07	1.41	1.35
29	G	313	CLA	C4B-NB	7.07	1.41	1.35
29	G	312	CLA	C4B-NB	7.07	1.41	1.35
29	b	704	CLA	C4B-NB	7.07	1.41	1.35
29	I	211	CLA	C4B-NB	7.07	1.41	1.35
29	G	311	CLA	C4B-NB	7.06	1.41	1.35
29	B	309	CLA	C4B-NB	7.05	1.41	1.35
29	F	310	CLA	C4B-NB	7.05	1.41	1.35
29	I	210	CLA	C4B-NB	7.05	1.41	1.35
29	h	201	CLA	C4B-NB	7.05	1.41	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	830	CLA	C4B-NB	7.04	1.41	1.35
29	b	711	CLA	C4B-NB	7.04	1.41	1.35
29	J	306	CLA	C4B-NB	7.04	1.41	1.35
29	L	308	CLA	C4B-NB	7.04	1.41	1.35
29	E	311	CLA	C4B-NB	7.04	1.41	1.35
29	a	822	CLA	C4B-NB	7.04	1.41	1.35
29	a	823	CLA	C4B-NB	7.04	1.41	1.35
29	b	725	CLA	C4B-NB	7.04	1.41	1.35
29	b	722	CLA	C4B-NB	7.03	1.41	1.35
29	a	806	CLA	C4B-NB	7.02	1.41	1.35
29	L	313	CLA	C4B-NB	7.02	1.41	1.35
29	K	211	CLA	C4B-NB	7.01	1.41	1.35
39	L	306	KC1	C4D-CHA	-7.00	1.36	1.45
29	J	308	CLA	C4B-NB	6.99	1.41	1.35
39	G	318	KC1	C4D-CHA	-6.99	1.36	1.45
29	I	209	CLA	C4B-NB	6.97	1.41	1.35
29	A	211	CLA	C4B-NB	6.95	1.41	1.35
29	b	705	CLA	C4B-NB	6.95	1.41	1.35
29	I	214	CLA	C4B-NB	6.95	1.41	1.35
29	A	212	CLA	C4B-NB	6.95	1.41	1.35
29	B	312	CLA	C4B-NB	6.93	1.41	1.35
29	i	202	CLA	C4B-NB	6.92	1.41	1.35
39	P	211	KC1	C4D-CHA	-6.91	1.36	1.45
36	I	205	DD6	C19-C20	6.90	1.61	1.52
39	I	215	KC1	C4D-CHA	-6.89	1.36	1.45
29	i	203	CLA	C4B-NB	6.89	1.41	1.35
39	L	314	KC1	C4D-CHA	-6.89	1.36	1.45
39	E	312	KC1	C4D-CHA	-6.87	1.36	1.45
29	i	201	CLA	C4B-NB	6.85	1.41	1.35
39	O	310	KC1	C4D-CHA	-6.83	1.36	1.45
39	K	215	KC1	C4D-CHA	-6.83	1.36	1.45
39	Q	309	KC1	C4D-CHA	-6.83	1.36	1.45
39	A	213	KC1	C4D-CHA	-6.81	1.36	1.45
39	A	205	KC1	C4D-CHA	-6.77	1.36	1.45
39	H	309	KC1	C4D-CHA	-6.75	1.36	1.45
39	B	313	KC1	C4D-CHA	-6.74	1.36	1.45
39	M	312	KC1	C4D-CHA	-6.71	1.36	1.45
39	Q	314	KC1	C4D-CHA	-6.71	1.36	1.45
39	O	315	KC1	C4D-CHA	-6.69	1.36	1.45
39	N	310	KC1	C4D-CHA	-6.66	1.36	1.45
39	F	309	KC1	C4D-CHA	-6.66	1.36	1.45
39	H	314	KC1	C4D-CHA	-6.65	1.36	1.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	310	KC1	C4D-CHA	-6.64	1.36	1.45
39	D	315	KC1	C4D-CHA	-6.63	1.36	1.45
39	C	312	KC1	C4D-CHA	-6.62	1.36	1.45
39	J	312	KC1	C4D-CHA	-6.61	1.36	1.45
39	H	311	KC1	C4D-CHA	-6.61	1.36	1.45
39	T	310	KC1	C4D-CHA	-6.61	1.36	1.45
39	E	307	KC1	C4D-CHA	-6.59	1.36	1.45
39	T	315	KC1	C4D-CHA	-6.59	1.36	1.45
39	M	305	KC1	C4D-CHA	-6.57	1.36	1.45
39	P	216	KC1	C4D-CHA	-6.57	1.36	1.45
39	N	315	KC1	C4D-CHA	-6.55	1.36	1.45
39	N	312	KC1	C4D-CHA	-6.54	1.36	1.45
29	a	801	CLA	C4B-NB	6.52	1.41	1.35
39	C	315	KC1	C4D-CHA	-6.50	1.36	1.45
39	F	314	KC1	C4D-CHA	-6.49	1.37	1.45
39	D	310	KC1	C4D-CHA	-6.47	1.37	1.45
39	P	213	KC1	C4D-CHA	-6.46	1.37	1.45
39	T	312	KC1	C4D-CHA	-6.34	1.37	1.45
39	Q	311	KC1	C4D-CHA	-6.26	1.37	1.45
39	G	315	KC1	C4D-CHA	-6.18	1.37	1.45
37	D	303	PID	C13-C14	-5.81	1.34	1.45
37	F	304	PID	O1-C1	-5.77	1.37	1.46
37	N	302	PID	C13-C14	-5.71	1.34	1.45
37	G	303	PID	C13-C14	-5.71	1.34	1.45
37	P	203	PID	C13-C14	-5.71	1.34	1.45
39	O	312	KC1	C4D-CHA	-5.70	1.37	1.45
37	H	305	PID	C13-C14	-5.69	1.34	1.45
37	D	306	PID	C13-C14	-5.66	1.34	1.45
37	F	304	PID	C13-C14	-5.66	1.34	1.45
37	O	302	PID	C13-C14	-5.66	1.34	1.45
37	h	204	PID	C13-C14	-5.64	1.34	1.45
37	G	310	PID	C13-C14	-5.63	1.34	1.45
37	H	302	PID	C13-C14	-5.61	1.34	1.45
37	T	317	PID	C13-C14	-5.59	1.34	1.45
37	N	305	PID	C13-C14	-5.57	1.34	1.45
37	F	306	PID	C13-C14	-5.57	1.34	1.45
37	Q	303	PID	C13-C14	-5.52	1.34	1.45
37	C	305	PID	C13-C14	-5.52	1.34	1.45
37	G	309	PID	C13-C14	-5.50	1.34	1.45
37	j	101	PID	C13-C14	-5.46	1.35	1.45
37	N	301	PID	C13-C14	-5.45	1.35	1.45
37	T	307	PID	C13-C14	-5.43	1.35	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	T	301	PID	C13-C14	-5.42	1.35	1.45
37	Q	301	PID	C13-C14	-5.42	1.35	1.45
37	T	302	PID	C13-C14	-5.42	1.35	1.45
37	C	304	PID	C13-C14	-5.42	1.35	1.45
37	F	302	PID	C13-C14	-5.41	1.35	1.45
37	D	302	PID	C13-C14	-5.41	1.35	1.45
37	T	305	PID	C13-C14	-5.40	1.35	1.45
37	O	307	PID	C13-C14	-5.40	1.35	1.45
37	E	301	PID	C13-C14	-5.39	1.35	1.45
37	C	301	PID	C13-C14	-5.39	1.35	1.45
37	Q	304	PID	C13-C14	-5.38	1.35	1.45
37	Q	306	PID	C13-C14	-5.38	1.35	1.45
37	O	304	PID	C13-C14	-5.38	1.35	1.45
37	D	305	PID	C13-C14	-5.37	1.35	1.45
37	N	304	PID	C13-C14	-5.34	1.35	1.45
37	H	301	PID	C13-C14	-5.33	1.35	1.45
37	C	307	PID	C13-C14	-5.31	1.35	1.45
37	O	305	PID	C13-C14	-5.30	1.35	1.45
37	D	307	PID	C13-C14	-5.30	1.35	1.45
37	C	302	PID	C13-C14	-5.29	1.35	1.45
37	N	307	PID	C13-C14	-5.28	1.35	1.45
37	P	205	PID	C13-C14	-5.24	1.35	1.45
37	P	202	PID	C13-C14	-5.24	1.35	1.45
36	G	307	DD6	C19-C20	5.23	1.59	1.52
37	O	301	PID	C13-C14	-5.21	1.35	1.45
37	H	304	PID	C13-C14	-5.19	1.35	1.45
37	T	304	PID	C13-C14	-5.18	1.35	1.45
36	G	307	DD6	C21-C20	-5.16	1.43	1.51
37	P	206	PID	C13-C14	-5.14	1.35	1.45
37	H	306	PID	C13-C14	-5.10	1.35	1.45
37	P	208	PID	C13-C14	-5.08	1.35	1.45
39	G	315	KC1	MG-NB	-4.93	1.96	2.05
39	Q	311	KC1	MG-NB	-4.86	1.96	2.05
38	B	304	UIX	O2-C27	4.81	1.46	1.35
39	P	213	KC1	MG-NB	-4.80	1.96	2.05
39	C	312	KC1	MG-NB	-4.79	1.96	2.05
39	C	310	KC1	MG-NB	-4.79	1.96	2.05
39	T	310	KC1	MG-NB	-4.78	1.96	2.05
39	C	315	KC1	MG-NB	-4.78	1.96	2.05
38	T	306	UIX	O2-C27	4.77	1.46	1.35
39	O	312	KC1	MG-NB	-4.77	1.96	2.05
39	Q	314	KC1	MG-NB	-4.76	1.96	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	D	310	KC1	MG-NB	-4.76	1.96	2.05
39	K	215	KC1	MG-NB	-4.76	1.96	2.05
38	N	306	UIX	O2-C27	4.74	1.45	1.35
38	C	306	UIX	O2-C27	4.74	1.45	1.35
38	P	207	UIX	O2-C27	4.73	1.45	1.35
39	E	312	KC1	MG-NB	-4.73	1.96	2.05
38	Q	305	UIX	O2-C27	4.72	1.45	1.35
38	L	302	UIX	O2-C27	4.72	1.45	1.35
39	D	315	KC1	MG-NB	-4.72	1.96	2.05
39	H	311	KC1	MG-NB	-4.72	1.96	2.05
39	Q	309	KC1	MG-NB	-4.72	1.96	2.05
30	b	727	PQN	C10-C5	4.71	1.48	1.40
39	M	312	KC1	MG-NB	-4.71	1.96	2.05
39	N	315	KC1	MG-NB	-4.70	1.96	2.05
39	G	318	KC1	MG-NB	-4.70	1.96	2.05
38	E	304	UIX	O2-C27	4.70	1.45	1.35
39	H	314	KC1	MG-NB	-4.70	1.96	2.05
39	O	315	KC1	MG-NB	-4.70	1.96	2.05
39	N	310	KC1	MG-NB	-4.70	1.96	2.05
39	E	307	KC1	MG-NB	-4.70	1.96	2.05
38	O	306	UIX	O2-C27	4.69	1.45	1.35
39	T	312	KC1	MG-NB	-4.69	1.96	2.05
39	M	305	KC1	MG-NB	-4.68	1.96	2.05
39	F	314	KC1	MG-NB	-4.68	1.96	2.05
39	J	312	KC1	MG-NB	-4.67	1.96	2.05
39	N	312	KC1	MG-NB	-4.66	1.96	2.05
39	O	310	KC1	MG-NB	-4.65	1.96	2.05
39	F	309	KC1	MG-NB	-4.65	1.96	2.05
39	H	309	KC1	MG-NB	-4.65	1.96	2.05
39	L	306	KC1	MG-NB	-4.65	1.96	2.05
39	I	215	KC1	MG-NB	-4.64	1.96	2.05
39	B	313	KC1	MG-NB	-4.64	1.96	2.05
39	A	213	KC1	MG-NB	-4.63	1.96	2.05
39	A	205	KC1	MG-NB	-4.62	1.96	2.05
38	A	203	UIX	O2-C27	4.62	1.45	1.35
39	T	315	KC1	MG-NB	-4.62	1.96	2.05
39	P	216	KC1	MG-NB	-4.62	1.96	2.05
38	F	305	UIX	O2-C27	4.62	1.45	1.35
39	P	211	KC1	MG-NB	-4.62	1.96	2.05
30	a	832	PQN	C10-C5	4.59	1.48	1.40
39	L	314	KC1	MG-NB	-4.58	1.96	2.05
36	I	203	DD6	C19-C20	4.57	1.58	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	J	304	UIX	O2-C27	4.36	1.45	1.35
35	b	733	DGD	O2G-C1B	4.27	1.46	1.34
35	B	318	DGD	O1G-C1A	4.26	1.45	1.33
35	j	106	DGD	O1G-C1A	4.23	1.45	1.33
35	G	320	DGD	O1G-C1A	4.22	1.45	1.33
37	E	301	PID	C20-C21	4.20	1.41	1.35
35	m	102	DGD	O1G-C1A	4.18	1.45	1.33
35	j	105	DGD	O1G-C1A	4.16	1.45	1.33
35	b	733	DGD	O1G-C1A	4.15	1.45	1.33
35	h	203	DGD	O1G-C1A	4.11	1.45	1.33
35	G	320	DGD	O2G-C1B	4.10	1.45	1.34
35	j	106	DGD	O2G-C1B	4.07	1.45	1.34
35	j	103	DGD	O1G-C1A	4.06	1.45	1.33
35	j	105	DGD	O2G-C1B	4.03	1.45	1.34
35	h	203	DGD	O2G-C1B	4.02	1.45	1.34
29	P	217	CLA	C1D-ND	4.00	1.42	1.37
35	B	318	DGD	O2G-C1B	3.99	1.45	1.34
29	O	314	CLA	C1D-ND	3.94	1.42	1.37
29	P	209	CLA	C1D-ND	3.93	1.42	1.37
29	O	316	CLA	C1D-ND	3.92	1.42	1.37
29	F	315	CLA	C1D-ND	3.92	1.42	1.37
29	E	314	CLA	C1D-ND	3.91	1.42	1.37
35	m	102	DGD	O2G-C1B	3.90	1.45	1.34
29	T	316	CLA	C1D-ND	3.89	1.42	1.37
29	O	308	CLA	C1D-ND	3.89	1.42	1.37
29	O	311	CLA	C1D-ND	3.89	1.42	1.37
29	M	309	CLA	C1D-ND	3.89	1.42	1.37
29	P	215	CLA	C1D-ND	3.88	1.42	1.37
29	D	316	CLA	C1D-ND	3.88	1.42	1.37
29	E	313	CLA	C1D-ND	3.88	1.42	1.37
35	j	103	DGD	O2G-C1B	3.88	1.45	1.34
29	N	316	CLA	C1D-ND	3.87	1.42	1.37
29	O	309	CLA	C1D-ND	3.87	1.42	1.37
29	H	315	CLA	C1D-ND	3.87	1.42	1.37
29	N	308	CLA	C1D-ND	3.86	1.42	1.37
29	P	212	CLA	C1D-ND	3.86	1.42	1.37
29	L	316	CLA	C1D-ND	3.84	1.42	1.37
29	T	313	CLA	C1D-ND	3.84	1.42	1.37
29	J	308	CLA	C1D-ND	3.84	1.42	1.37
29	G	319	CLA	C1D-ND	3.84	1.42	1.37
29	J	313	CLA	C1D-ND	3.83	1.42	1.37
29	a	817	CLA	C1D-ND	3.83	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	819	CLA	C1D-ND	3.82	1.42	1.37
36	I	205	DD6	C21-C20	-3.82	1.45	1.51
37	P	208	PID	C20-C21	3.82	1.40	1.35
29	A	210	CLA	C1D-ND	3.82	1.42	1.37
29	E	310	CLA	C1D-ND	3.82	1.42	1.37
29	a	813	CLA	C1D-ND	3.81	1.42	1.37
29	b	721	CLA	C1D-ND	3.81	1.42	1.37
29	H	307	CLA	C1D-ND	3.81	1.42	1.37
29	D	312	CLA	C1D-ND	3.80	1.42	1.37
29	C	316	CLA	C1D-ND	3.80	1.42	1.37
29	P	214	CLA	C1D-ND	3.80	1.42	1.37
29	J	305	CLA	C1D-ND	3.80	1.42	1.37
29	M	314	CLA	C1D-ND	3.80	1.42	1.37
29	F	316	CLA	C1D-ND	3.80	1.42	1.37
29	M	313	CLA	C1D-ND	3.79	1.42	1.37
29	E	305	CLA	C1D-ND	3.79	1.42	1.37
29	A	206	CLA	C1D-ND	3.79	1.42	1.37
29	H	312	CLA	C1D-ND	3.79	1.42	1.37
29	b	715	CLA	C1D-ND	3.79	1.42	1.37
29	B	306	CLA	C1D-ND	3.78	1.42	1.37
29	T	308	CLA	C1D-ND	3.78	1.42	1.37
29	N	311	CLA	C1D-ND	3.77	1.42	1.37
29	E	309	CLA	C1D-ND	3.77	1.42	1.37
29	a	821	CLA	C1D-ND	3.77	1.42	1.37
29	G	317	CLA	C1D-ND	3.77	1.42	1.37
29	H	310	CLA	C1D-ND	3.77	1.42	1.37
29	l	502	CLA	C1D-ND	3.77	1.42	1.37
29	M	306	CLA	C1D-ND	3.76	1.42	1.37
29	L	311	CLA	C1D-ND	3.76	1.42	1.37
29	B	307	CLA	C1D-ND	3.76	1.42	1.37
29	b	713	CLA	C1D-ND	3.76	1.42	1.37
29	D	309	CLA	C1D-ND	3.76	1.42	1.37
29	L	315	CLA	C1D-ND	3.75	1.42	1.37
38	A	203	UIX	C25-C28	-3.75	1.25	1.32
29	Q	307	CLA	C1D-ND	3.75	1.42	1.37
29	M	308	CLA	C1D-ND	3.74	1.42	1.37
29	a	804	CLA	C1D-ND	3.74	1.42	1.37
29	P	210	CLA	C1D-ND	3.74	1.42	1.37
29	T	311	CLA	C1D-ND	3.74	1.42	1.37
29	N	314	CLA	C1D-ND	3.74	1.42	1.37
29	B	312	CLA	C1D-ND	3.74	1.42	1.37
29	E	315	CLA	C1D-ND	3.74	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	311	CLA	C1D-ND	3.73	1.42	1.37
29	F	312	CLA	C1D-ND	3.73	1.42	1.37
29	b	720	CLA	C1D-ND	3.73	1.42	1.37
29	Q	315	CLA	C1D-ND	3.73	1.42	1.37
29	M	311	CLA	C1D-ND	3.73	1.42	1.37
29	l	508	CLA	C1D-ND	3.73	1.42	1.37
29	K	207	CLA	C1D-ND	3.72	1.42	1.37
29	l	505	CLA	C1D-ND	3.72	1.42	1.37
29	K	212	CLA	C1D-ND	3.72	1.42	1.37
29	a	816	CLA	C1D-ND	3.72	1.42	1.37
29	C	309	CLA	C1D-ND	3.72	1.42	1.37
38	E	304	UIX	C25-C28	-3.72	1.25	1.32
29	M	307	CLA	C1D-ND	3.72	1.42	1.37
29	L	308	CLA	C1D-ND	3.71	1.42	1.37
29	D	308	CLA	C1D-ND	3.71	1.42	1.37
29	a	811	CLA	C1D-ND	3.71	1.42	1.37
29	I	208	CLA	C1D-ND	3.71	1.42	1.37
29	L	310	CLA	C1D-ND	3.71	1.42	1.37
29	C	314	CLA	C1D-ND	3.71	1.42	1.37
29	h	201	CLA	C1D-ND	3.70	1.42	1.37
29	a	829	CLA	C1D-ND	3.70	1.42	1.37
29	C	308	CLA	C1D-ND	3.70	1.42	1.37
37	T	302	PID	C20-C21	3.70	1.40	1.35
29	I	201	CLA	C1D-ND	3.70	1.42	1.37
29	D	314	CLA	C1D-ND	3.70	1.42	1.37
29	j	104	CLA	C1D-ND	3.70	1.42	1.37
29	T	309	CLA	C1D-ND	3.70	1.42	1.37
29	B	315	CLA	C1D-ND	3.70	1.42	1.37
29	F	308	CLA	C1D-ND	3.69	1.42	1.37
38	J	304	UIX	C25-C28	-3.69	1.25	1.32
29	a	809	CLA	C1D-ND	3.69	1.42	1.37
29	M	315	CLA	C1D-ND	3.69	1.42	1.37
29	L	313	CLA	C1D-ND	3.69	1.42	1.37
29	M	310	CLA	C1D-ND	3.69	1.42	1.37
29	G	316	CLA	C1D-ND	3.69	1.42	1.37
29	K	216	CLA	C1D-ND	3.69	1.42	1.37
29	T	314	CLA	C1D-ND	3.69	1.42	1.37
29	F	313	CLA	C1D-ND	3.69	1.42	1.37
29	B	309	CLA	C1D-ND	3.68	1.42	1.37
29	D	311	CLA	C1D-ND	3.68	1.42	1.37
29	a	818	CLA	C1D-ND	3.68	1.42	1.37
29	Q	308	CLA	C1D-ND	3.68	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	803	CLA	C1D-ND	3.68	1.42	1.37
29	F	311	CLA	C1D-ND	3.68	1.42	1.37
29	J	310	CLA	C1D-ND	3.68	1.42	1.37
29	Q	313	CLA	C1D-ND	3.68	1.42	1.37
29	l	510	CLA	C1D-ND	3.68	1.42	1.37
29	J	309	CLA	C1D-ND	3.68	1.42	1.37
29	H	308	CLA	C1D-ND	3.67	1.42	1.37
29	I	216	CLA	C1D-ND	3.67	1.42	1.37
29	f	803	CLA	C1D-ND	3.67	1.42	1.37
29	K	210	CLA	C1D-ND	3.67	1.42	1.37
38	B	304	UIX	C25-C28	-3.67	1.25	1.32
29	K	214	CLA	C1D-ND	3.66	1.42	1.37
29	K	217	CLA	C1D-ND	3.66	1.42	1.37
29	b	719	CLA	C1D-ND	3.66	1.42	1.37
29	a	822	CLA	C1D-ND	3.66	1.42	1.37
29	a	826	CLA	C1D-ND	3.66	1.42	1.37
29	F	307	CLA	C1D-ND	3.65	1.42	1.37
29	b	712	CLA	C1D-ND	3.65	1.42	1.37
29	L	309	CLA	C1D-ND	3.65	1.42	1.37
29	L	317	CLA	C1D-ND	3.65	1.42	1.37
29	Q	310	CLA	C1D-ND	3.65	1.42	1.37
29	b	706	CLA	C1D-ND	3.65	1.42	1.37
29	I	217	CLA	C1D-ND	3.65	1.42	1.37
29	N	309	CLA	C1D-ND	3.65	1.42	1.37
29	Q	312	CLA	C1D-ND	3.65	1.42	1.37
29	b	702	CLA	C1D-ND	3.64	1.42	1.37
29	I	209	CLA	C1D-ND	3.64	1.42	1.37
29	A	211	CLA	C1D-ND	3.64	1.42	1.37
29	A	209	CLA	C1D-ND	3.64	1.42	1.37
29	J	307	CLA	C1D-ND	3.64	1.42	1.37
29	K	213	CLA	C1D-ND	3.64	1.42	1.37
29	I	211	CLA	C1D-ND	3.64	1.42	1.37
29	a	815	CLA	C1D-ND	3.64	1.42	1.37
29	B	308	CLA	C1D-ND	3.64	1.42	1.37
29	A	207	CLA	C1D-ND	3.64	1.42	1.37
29	a	814	CLA	C1D-ND	3.63	1.42	1.37
29	a	823	CLA	C1D-ND	3.63	1.42	1.37
29	E	311	CLA	C1D-ND	3.63	1.42	1.37
29	l	501	CLA	C1D-ND	3.63	1.42	1.37
29	A	208	CLA	C1D-ND	3.63	1.42	1.37
29	b	724	CLA	C1D-ND	3.63	1.42	1.37
29	B	316	CLA	C1D-ND	3.63	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	O	306	UIX	C25-C28	-3.63	1.25	1.32
29	G	301	CLA	C1D-ND	3.63	1.42	1.37
29	a	807	CLA	C1D-ND	3.63	1.42	1.37
29	b	716	CLA	C1D-ND	3.63	1.42	1.37
29	L	307	CLA	C1D-ND	3.63	1.42	1.37
29	a	830	CLA	C1D-ND	3.62	1.42	1.37
29	a	828	CLA	C1D-ND	3.62	1.42	1.37
29	A	216	CLA	C1D-ND	3.62	1.42	1.37
29	K	209	CLA	C1D-ND	3.62	1.42	1.37
29	b	722	CLA	C1D-ND	3.62	1.42	1.37
38	F	305	UIX	C25-C28	-3.62	1.25	1.32
37	P	206	PID	C20-C21	3.62	1.40	1.35
29	b	709	CLA	C1D-ND	3.62	1.42	1.37
29	B	311	CLA	C1D-ND	3.61	1.42	1.37
29	i	201	CLA	C1D-ND	3.61	1.42	1.37
29	K	211	CLA	C1D-ND	3.61	1.42	1.37
29	A	215	CLA	C1D-ND	3.61	1.42	1.37
29	G	314	CLA	C1D-ND	3.61	1.42	1.37
29	a	831	CLA	C1D-ND	3.61	1.42	1.37
29	b	707	CLA	C1D-ND	3.61	1.42	1.37
29	i	202	CLA	C1D-ND	3.60	1.42	1.37
29	a	808	CLA	C1D-ND	3.60	1.42	1.37
29	a	827	CLA	C1D-ND	3.60	1.42	1.37
29	B	314	CLA	C1D-ND	3.59	1.42	1.37
29	G	312	CLA	C1D-ND	3.59	1.42	1.37
29	I	213	CLA	C1D-ND	3.59	1.42	1.37
29	G	311	CLA	C1D-ND	3.59	1.42	1.37
29	G	302	CLA	C1D-ND	3.59	1.42	1.37
29	b	736	CLA	C1D-ND	3.58	1.42	1.37
38	T	306	UIX	C25-C28	-3.58	1.26	1.32
38	P	207	UIX	C25-C28	-3.58	1.26	1.32
29	l	509	CLA	C1D-ND	3.58	1.42	1.37
29	I	207	CLA	C1D-ND	3.58	1.42	1.37
29	J	311	CLA	C1D-ND	3.58	1.42	1.37
29	I	212	CLA	C1D-ND	3.58	1.42	1.37
29	b	701	CLA	C1D-ND	3.58	1.42	1.37
29	H	313	CLA	C1D-ND	3.58	1.42	1.37
36	O	303	DD6	C19-C20	3.58	1.57	1.52
29	b	710	CLA	C1D-ND	3.57	1.42	1.37
29	f	802	CLA	C1D-ND	3.57	1.42	1.37
29	C	313	CLA	C1D-ND	3.57	1.42	1.37
29	b	708	CLA	C1D-ND	3.57	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	805	CLA	C1D-ND	3.57	1.42	1.37
29	a	825	CLA	C1D-ND	3.56	1.42	1.37
29	a	805	CLA	C1D-ND	3.56	1.42	1.37
29	a	820	CLA	C1D-ND	3.56	1.42	1.37
29	b	726	CLA	C1D-ND	3.56	1.42	1.37
29	E	308	CLA	C1D-ND	3.56	1.42	1.37
29	b	725	CLA	C1D-ND	3.55	1.42	1.37
29	i	203	CLA	C1D-ND	3.55	1.42	1.37
29	O	313	CLA	C1D-ND	3.55	1.42	1.37
29	L	312	CLA	C1D-ND	3.55	1.42	1.37
29	A	212	CLA	C1D-ND	3.55	1.42	1.37
29	K	208	CLA	C1D-ND	3.55	1.42	1.37
29	D	313	CLA	C1D-ND	3.54	1.42	1.37
38	L	302	UIX	C25-C28	-3.54	1.26	1.32
38	N	306	UIX	C25-C28	-3.54	1.26	1.32
29	G	313	CLA	C1D-ND	3.54	1.42	1.37
29	b	723	CLA	C1D-ND	3.54	1.42	1.37
29	b	731	CLA	C1D-ND	3.53	1.42	1.37
29	K	218	CLA	C1D-ND	3.53	1.42	1.37
29	a	810	CLA	C1D-ND	3.53	1.42	1.37
37	N	307	PID	C20-C21	3.53	1.40	1.35
29	a	812	CLA	C1D-ND	3.52	1.42	1.37
29	A	218	CLA	C1D-ND	3.52	1.42	1.37
29	I	210	CLA	C1D-ND	3.51	1.42	1.37
29	b	703	CLA	C1D-ND	3.50	1.42	1.37
37	D	307	PID	C20-C21	3.50	1.40	1.35
38	Q	305	UIX	C25-C28	-3.50	1.26	1.32
29	a	837	CLA	C1D-ND	3.50	1.42	1.37
29	b	711	CLA	C1D-ND	3.49	1.42	1.37
29	a	802	CLA	C1D-ND	3.49	1.42	1.37
29	a	806	CLA	C1D-ND	3.49	1.42	1.37
36	G	307	DD6	C36-C31	-3.48	1.31	1.34
37	j	101	PID	C20-C21	3.47	1.40	1.35
29	G	304	CLA	C1D-ND	3.47	1.42	1.37
29	I	214	CLA	C1D-ND	3.46	1.42	1.37
38	C	306	UIX	C25-C28	-3.46	1.26	1.32
37	P	205	PID	C20-C21	3.46	1.40	1.35
29	b	714	CLA	C1D-ND	3.46	1.42	1.37
37	N	305	PID	C20-C21	3.45	1.40	1.35
29	l	503	CLA	C1D-ND	3.45	1.42	1.37
29	J	306	CLA	C1D-ND	3.45	1.42	1.37
37	T	304	PID	C20-C21	3.44	1.40	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	310	CLA	C1D-ND	3.43	1.42	1.37
29	l	504	CLA	C1D-ND	3.43	1.42	1.37
37	O	305	PID	C20-C21	3.41	1.40	1.35
29	O	314	CLA	CHC-C1C	3.40	1.43	1.35
29	b	704	CLA	C1D-ND	3.40	1.42	1.37
29	a	801	CLA	C4D-ND	-3.40	1.33	1.37
29	A	217	CLA	C1D-ND	3.40	1.42	1.37
29	b	717	CLA	C1D-ND	3.40	1.42	1.37
29	b	718	CLA	C1D-ND	3.39	1.41	1.37
37	C	305	PID	C20-C21	3.39	1.40	1.35
29	a	824	CLA	C1D-ND	3.38	1.41	1.37
29	F	310	CLA	C1D-ND	3.37	1.41	1.37
37	H	306	PID	C20-C21	3.36	1.40	1.35
29	A	214	CLA	C1D-ND	3.36	1.41	1.37
37	C	302	PID	C20-C21	3.36	1.40	1.35
37	H	304	PID	C20-C21	3.35	1.40	1.35
37	N	304	PID	C20-C21	3.34	1.40	1.35
37	C	301	PID	C20-C21	3.33	1.40	1.35
37	H	302	PID	C20-C21	3.33	1.40	1.35
29	a	801	CLA	C1D-ND	3.33	1.41	1.37
29	E	306	CLA	C1D-ND	3.33	1.41	1.37
37	P	202	PID	C20-C21	3.32	1.40	1.35
29	a	802	CLA	CHC-C1C	3.32	1.43	1.35
29	N	313	CLA	C1D-ND	3.32	1.41	1.37
37	C	307	PID	C20-C21	3.31	1.40	1.35
29	b	705	CLA	C1D-ND	3.30	1.41	1.37
29	J	308	CLA	C4D-ND	-3.29	1.33	1.37
37	D	302	PID	C20-C21	3.29	1.40	1.35
37	H	301	PID	C20-C21	3.29	1.40	1.35
37	O	301	PID	C20-C21	3.28	1.40	1.35
29	b	711	CLA	C4D-ND	-3.26	1.33	1.37
37	N	301	PID	C20-C21	3.25	1.40	1.35
37	O	302	PID	C20-C21	3.25	1.40	1.35
29	K	214	CLA	C4D-ND	-3.25	1.33	1.37
37	Q	301	PID	C20-C21	3.24	1.40	1.35
29	N	309	CLA	CHC-C1C	3.24	1.43	1.35
29	H	312	CLA	CHC-C1C	3.24	1.43	1.35
29	b	719	CLA	CHC-C1C	3.24	1.43	1.35
29	M	311	CLA	C4D-ND	-3.21	1.33	1.37
29	a	803	CLA	C4D-ND	-3.21	1.33	1.37
37	T	301	PID	C20-C21	3.21	1.40	1.35
29	b	726	CLA	C4D-ND	-3.21	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	313	CLA	C4D-ND	-3.20	1.33	1.37
29	G	302	CLA	CHC-C1C	3.20	1.43	1.35
29	K	209	CLA	C4D-ND	-3.19	1.33	1.37
29	K	209	CLA	CHC-C1C	3.19	1.43	1.35
29	I	209	CLA	C4D-ND	-3.19	1.33	1.37
37	G	303	PID	C20-C21	3.19	1.40	1.35
29	Q	308	CLA	CHC-C1C	3.19	1.43	1.35
29	b	716	CLA	C4D-ND	-3.19	1.33	1.37
29	a	808	CLA	CHC-C1C	3.19	1.43	1.35
29	O	316	CLA	CHC-C1C	3.19	1.43	1.35
37	C	304	PID	C20-C21	3.19	1.40	1.35
29	P	214	CLA	CHC-C1C	3.18	1.43	1.35
29	B	308	CLA	C4D-ND	-3.18	1.33	1.37
29	M	311	CLA	CHC-C1C	3.18	1.43	1.35
29	J	310	CLA	C4D-ND	-3.18	1.33	1.37
29	M	313	CLA	CHC-C1C	3.18	1.43	1.35
29	P	215	CLA	CHC-C1C	3.18	1.43	1.35
29	J	310	CLA	CHC-C1C	3.18	1.43	1.35
29	h	201	CLA	CHC-C1C	3.17	1.43	1.35
29	M	307	CLA	CHC-C1C	3.17	1.43	1.35
29	P	212	CLA	CHC-C1C	3.17	1.43	1.35
29	b	714	CLA	CHC-C1C	3.17	1.43	1.35
29	T	313	CLA	CHC-C1C	3.17	1.43	1.35
29	a	823	CLA	CHC-C1C	3.17	1.43	1.35
29	L	315	CLA	CHC-C1C	3.17	1.43	1.35
29	b	703	CLA	CHC-C1C	3.17	1.43	1.35
29	K	210	CLA	CHC-C1C	3.17	1.43	1.35
29	I	210	CLA	C4D-ND	-3.17	1.33	1.37
29	a	823	CLA	C4D-ND	-3.17	1.33	1.37
29	b	723	CLA	CHC-C1C	3.17	1.43	1.35
29	I	201	CLA	CHC-C1C	3.17	1.43	1.35
37	Q	304	PID	C20-C21	3.17	1.40	1.35
29	L	308	CLA	C4D-ND	-3.17	1.33	1.37
29	b	705	CLA	CHC-C1C	3.16	1.43	1.35
29	I	210	CLA	CHC-C1C	3.16	1.43	1.35
29	E	311	CLA	CHC-C1C	3.16	1.43	1.35
29	b	717	CLA	C4D-ND	-3.16	1.33	1.37
29	b	724	CLA	CHC-C1C	3.16	1.43	1.35
29	E	313	CLA	CHC-C1C	3.16	1.43	1.35
29	K	213	CLA	CHC-C1C	3.16	1.43	1.35
29	O	314	CLA	C4D-ND	-3.15	1.33	1.37
29	D	311	CLA	CHC-C1C	3.15	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	211	CLA	CHC-C1C	3.15	1.43	1.35
29	D	313	CLA	CHC-C1C	3.15	1.43	1.35
37	O	304	PID	C20-C21	3.15	1.40	1.35
29	a	806	CLA	CHC-C1C	3.15	1.43	1.35
29	K	214	CLA	CHC-C1C	3.15	1.43	1.35
29	I	213	CLA	CHC-C1C	3.15	1.43	1.35
29	Q	315	CLA	CHC-C1C	3.15	1.43	1.35
29	E	314	CLA	CHC-C1C	3.15	1.43	1.35
37	D	306	PID	C20-C21	3.15	1.40	1.35
29	a	837	CLA	CHC-C1C	3.14	1.43	1.35
29	O	309	CLA	CHC-C1C	3.14	1.43	1.35
29	M	309	CLA	CHC-C1C	3.14	1.43	1.35
29	L	312	CLA	CHC-C1C	3.14	1.43	1.35
29	N	316	CLA	CHC-C1C	3.14	1.43	1.35
29	O	311	CLA	CHC-C1C	3.14	1.43	1.35
29	b	706	CLA	C4D-ND	-3.14	1.33	1.37
29	a	825	CLA	CMB-C2B	-3.14	1.45	1.51
29	b	736	CLA	CHC-C1C	3.14	1.43	1.35
29	a	821	CLA	CHC-C1C	3.14	1.43	1.35
29	a	824	CLA	CHC-C1C	3.14	1.43	1.35
29	F	307	CLA	CHC-C1C	3.14	1.43	1.35
29	a	812	CLA	C4D-ND	-3.14	1.33	1.37
29	M	310	CLA	CHC-C1C	3.14	1.43	1.35
29	F	310	CLA	CHC-C1C	3.14	1.43	1.35
29	a	818	CLA	CHC-C1C	3.14	1.43	1.35
29	i	202	CLA	C4D-ND	-3.14	1.33	1.37
29	F	308	CLA	C4D-ND	-3.14	1.33	1.37
29	A	208	CLA	C4D-ND	-3.13	1.33	1.37
29	A	217	CLA	CHC-C1C	3.13	1.43	1.35
29	J	305	CLA	CHC-C1C	3.13	1.43	1.35
29	b	711	CLA	CHC-C1C	3.13	1.43	1.35
29	l	504	CLA	CHC-C1C	3.13	1.43	1.35
29	G	317	CLA	CHC-C1C	3.13	1.43	1.35
29	E	308	CLA	CHC-C1C	3.13	1.43	1.35
37	F	306	PID	C20-C21	3.13	1.39	1.35
29	H	315	CLA	CHC-C1C	3.13	1.43	1.35
29	O	308	CLA	CHC-C1C	3.13	1.43	1.35
29	a	824	CLA	C4D-ND	-3.13	1.33	1.37
39	K	215	KC1	C4B-NB	-3.13	1.33	1.37
29	L	317	CLA	CHC-C1C	3.13	1.43	1.35
29	H	310	CLA	CHC-C1C	3.13	1.43	1.35
29	L	313	CLA	CHC-C1C	3.13	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T	309	CLA	C4D-ND	-3.13	1.33	1.37
29	a	805	CLA	CHC-C1C	3.13	1.43	1.35
37	F	302	PID	C20-C21	3.13	1.39	1.35
29	K	218	CLA	CHC-C1C	3.13	1.43	1.35
29	G	301	CLA	CHC-C1C	3.13	1.43	1.35
29	D	309	CLA	CHC-C1C	3.13	1.43	1.35
29	b	709	CLA	CHC-C1C	3.13	1.43	1.35
29	A	211	CLA	CHC-C1C	3.13	1.43	1.35
29	Q	312	CLA	CHC-C1C	3.13	1.43	1.35
29	b	724	CLA	C4D-ND	-3.13	1.33	1.37
29	A	208	CLA	CHC-C1C	3.13	1.43	1.35
29	C	311	CLA	CHC-C1C	3.13	1.43	1.35
29	B	310	CLA	CHC-C1C	3.13	1.43	1.35
29	b	736	CLA	C4D-ND	-3.12	1.33	1.37
29	G	312	CLA	CHC-C1C	3.12	1.43	1.35
29	b	731	CLA	CHC-C1C	3.12	1.43	1.35
29	l	501	CLA	CHC-C1C	3.12	1.43	1.35
29	A	207	CLA	CHC-C1C	3.12	1.43	1.35
29	B	311	CLA	CHC-C1C	3.12	1.43	1.35
29	l	508	CLA	CHC-C1C	3.12	1.43	1.35
29	D	308	CLA	CHC-C1C	3.12	1.43	1.35
29	C	308	CLA	CHC-C1C	3.12	1.43	1.35
29	A	209	CLA	CHC-C1C	3.12	1.43	1.35
29	l	503	CLA	CHC-C1C	3.12	1.43	1.35
29	A	218	CLA	CHC-C1C	3.12	1.43	1.35
29	b	720	CLA	CHC-C1C	3.12	1.43	1.35
29	J	313	CLA	CHC-C1C	3.12	1.43	1.35
29	F	316	CLA	CHC-C1C	3.12	1.43	1.35
29	A	207	CLA	C4D-ND	-3.12	1.33	1.37
29	A	212	CLA	C4D-ND	-3.12	1.33	1.37
29	F	315	CLA	CHC-C1C	3.12	1.43	1.35
29	I	216	CLA	CHC-C1C	3.12	1.43	1.35
29	L	308	CLA	CHC-C1C	3.12	1.43	1.35
29	H	313	CLA	CHC-C1C	3.12	1.43	1.35
29	a	813	CLA	CHC-C1C	3.11	1.43	1.35
29	b	710	CLA	CHC-C1C	3.11	1.43	1.35
29	E	310	CLA	CHC-C1C	3.11	1.43	1.35
29	P	209	CLA	CHC-C1C	3.11	1.43	1.35
29	a	807	CLA	CHC-C1C	3.11	1.42	1.35
29	O	313	CLA	CHC-C1C	3.11	1.42	1.35
29	T	311	CLA	CHC-C1C	3.11	1.42	1.35
29	b	707	CLA	CHC-C1C	3.11	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T	316	CLA	CHC-C1C	3.11	1.42	1.35
29	K	207	CLA	CHC-C1C	3.11	1.42	1.35
29	I	214	CLA	C4D-ND	-3.11	1.33	1.37
29	A	212	CLA	CHC-C1C	3.11	1.42	1.35
29	A	214	CLA	CHC-C1C	3.11	1.42	1.35
29	a	807	CLA	C4D-ND	-3.11	1.33	1.37
37	P	203	PID	C20-C21	3.11	1.39	1.35
29	a	817	CLA	CHC-C1C	3.11	1.42	1.35
29	T	309	CLA	CHC-C1C	3.11	1.42	1.35
29	M	315	CLA	CHC-C1C	3.11	1.42	1.35
29	b	714	CLA	C4D-ND	-3.11	1.33	1.37
29	N	313	CLA	CHC-C1C	3.11	1.42	1.35
29	C	309	CLA	CHC-C1C	3.11	1.42	1.35
29	C	313	CLA	CHC-C1C	3.11	1.42	1.35
29	L	310	CLA	CHC-C1C	3.11	1.42	1.35
29	H	308	CLA	CHC-C1C	3.11	1.42	1.35
29	H	307	CLA	CHC-C1C	3.11	1.42	1.35
29	N	308	CLA	CHC-C1C	3.11	1.42	1.35
29	L	311	CLA	CHC-C1C	3.11	1.42	1.35
29	a	802	CLA	C4D-ND	-3.11	1.33	1.37
29	a	814	CLA	C4D-ND	-3.11	1.33	1.37
29	G	311	CLA	CHC-C1C	3.10	1.42	1.35
29	K	216	CLA	CHC-C1C	3.10	1.42	1.35
29	G	316	CLA	C4D-ND	-3.10	1.33	1.37
29	N	311	CLA	CHC-C1C	3.10	1.42	1.35
29	M	309	CLA	C4D-ND	-3.10	1.33	1.37
29	Q	310	CLA	CHC-C1C	3.10	1.42	1.35
29	B	312	CLA	C4D-ND	-3.10	1.33	1.37
29	a	827	CLA	CHC-C1C	3.10	1.42	1.35
29	D	314	CLA	CHC-C1C	3.10	1.42	1.35
29	A	218	CLA	C4D-ND	-3.10	1.33	1.37
29	a	812	CLA	CHC-C1C	3.10	1.42	1.35
29	K	211	CLA	CHC-C1C	3.10	1.42	1.35
36	I	205	DD6	O1-C20	-3.10	1.41	1.46
29	B	308	CLA	CHC-C1C	3.10	1.42	1.35
29	N	314	CLA	CHC-C1C	3.10	1.42	1.35
29	E	308	CLA	C4D-ND	-3.10	1.33	1.37
29	E	311	CLA	C4D-ND	-3.10	1.33	1.37
29	a	826	CLA	CHC-C1C	3.10	1.42	1.35
29	Q	307	CLA	CHC-C1C	3.10	1.42	1.35
29	b	701	CLA	CHC-C1C	3.10	1.42	1.35
29	a	827	CLA	C4D-ND	-3.10	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	809	CLA	CHC-C1C	3.10	1.42	1.35
37	T	307	PID	C20-C21	3.10	1.39	1.35
29	B	312	CLA	CHC-C1C	3.10	1.42	1.35
29	b	715	CLA	C4D-ND	-3.09	1.33	1.37
29	J	307	CLA	CHC-C1C	3.09	1.42	1.35
29	M	307	CLA	C4D-ND	-3.09	1.33	1.37
29	Q	310	CLA	C4D-ND	-3.09	1.33	1.37
29	Q	313	CLA	CHC-C1C	3.09	1.42	1.35
37	O	307	PID	C20-C21	3.09	1.39	1.35
29	G	313	CLA	CHC-C1C	3.09	1.42	1.35
29	J	308	CLA	CHC-C1C	3.09	1.42	1.35
29	a	831	CLA	CHC-C1C	3.09	1.42	1.35
29	I	214	CLA	CHC-C1C	3.09	1.42	1.35
29	F	308	CLA	CHC-C1C	3.09	1.42	1.35
29	T	308	CLA	CHC-C1C	3.09	1.42	1.35
29	b	708	CLA	C4D-ND	-3.09	1.33	1.37
29	b	725	CLA	C4D-ND	-3.09	1.33	1.37
29	a	816	CLA	CHC-C1C	3.09	1.42	1.35
29	a	830	CLA	CHC-C1C	3.09	1.42	1.35
29	E	309	CLA	CHC-C1C	3.09	1.42	1.35
29	a	820	CLA	CHC-C1C	3.09	1.42	1.35
29	a	808	CLA	C4D-ND	-3.09	1.33	1.37
29	f	805	CLA	CHC-C1C	3.09	1.42	1.35
29	E	306	CLA	CHC-C1C	3.09	1.42	1.35
29	M	306	CLA	CHC-C1C	3.09	1.42	1.35
29	L	309	CLA	CHC-C1C	3.09	1.42	1.35
29	L	313	CLA	C4D-ND	-3.09	1.33	1.37
29	a	828	CLA	CHC-C1C	3.09	1.42	1.35
29	J	306	CLA	CHC-C1C	3.09	1.42	1.35
29	D	316	CLA	CHC-C1C	3.09	1.42	1.35
29	E	315	CLA	CHC-C1C	3.09	1.42	1.35
29	a	814	CLA	CHC-C1C	3.09	1.42	1.35
29	B	316	CLA	CHC-C1C	3.09	1.42	1.35
29	B	309	CLA	CHC-C1C	3.09	1.42	1.35
29	b	721	CLA	CHC-C1C	3.08	1.42	1.35
29	B	307	CLA	CHC-C1C	3.08	1.42	1.35
29	b	717	CLA	CHC-C1C	3.08	1.42	1.35
29	A	216	CLA	CHC-C1C	3.08	1.42	1.35
29	P	210	CLA	CHC-C1C	3.08	1.42	1.35
29	G	319	CLA	CHC-C1C	3.08	1.42	1.35
29	a	806	CLA	C4D-ND	-3.08	1.33	1.37
29	l	502	CLA	C4D-ND	-3.08	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	713	CLA	CHC-C1C	3.08	1.42	1.35
29	I	208	CLA	CHC-C1C	3.08	1.42	1.35
29	G	304	CLA	CHC-C1C	3.08	1.42	1.35
29	a	826	CLA	C4D-ND	-3.08	1.33	1.37
29	l	504	CLA	C4D-ND	-3.08	1.33	1.37
29	l	509	CLA	CHC-C1C	3.08	1.42	1.35
29	J	311	CLA	C4D-ND	-3.08	1.33	1.37
29	l	505	CLA	CHC-C1C	3.08	1.42	1.35
29	B	315	CLA	CHC-C1C	3.07	1.42	1.35
29	l	502	CLA	CHC-C1C	3.07	1.42	1.35
29	a	815	CLA	CHC-C1C	3.07	1.42	1.35
29	a	822	CLA	CHC-C1C	3.07	1.42	1.35
29	a	811	CLA	CHC-C1C	3.07	1.42	1.35
29	a	811	CLA	C4D-ND	-3.07	1.33	1.37
29	F	311	CLA	CHC-C1C	3.07	1.42	1.35
29	a	830	CLA	C4D-ND	-3.07	1.33	1.37
29	b	722	CLA	CHC-C1C	3.07	1.42	1.35
29	Q	313	CLA	C4D-ND	-3.07	1.33	1.37
37	h	204	PID	C20-C21	3.07	1.39	1.35
29	Q	308	CLA	C4D-ND	-3.07	1.33	1.37
29	b	703	CLA	C4D-ND	-3.07	1.33	1.37
29	B	314	CLA	CHC-C1C	3.07	1.42	1.35
29	K	210	CLA	C4D-ND	-3.07	1.33	1.37
29	C	309	CLA	C4D-ND	-3.07	1.33	1.37
29	I	209	CLA	CHC-C1C	3.07	1.42	1.35
29	b	731	CLA	C4D-ND	-3.06	1.33	1.37
29	a	819	CLA	CHC-C1C	3.06	1.42	1.35
29	G	312	CLA	C4D-ND	-3.06	1.33	1.37
29	P	217	CLA	CHC-C1C	3.06	1.42	1.35
29	A	206	CLA	CHC-C1C	3.06	1.42	1.35
29	J	311	CLA	CHC-C1C	3.06	1.42	1.35
29	l	510	CLA	CHC-C1C	3.06	1.42	1.35
29	K	208	CLA	CHC-C1C	3.06	1.42	1.35
29	I	216	CLA	C4D-ND	-3.06	1.33	1.37
29	L	309	CLA	C4D-ND	-3.06	1.33	1.37
29	K	213	CLA	C4D-ND	-3.06	1.33	1.37
29	K	212	CLA	C4D-ND	-3.06	1.33	1.37
29	I	212	CLA	C4D-ND	-3.06	1.33	1.37
29	b	723	CLA	C4D-ND	-3.05	1.33	1.37
39	Q	311	KC1	C4B-NB	-3.05	1.34	1.37
29	K	208	CLA	C4D-ND	-3.05	1.33	1.37
29	i	203	CLA	C4D-ND	-3.05	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	210	CLA	CHC-C1C	3.05	1.42	1.35
29	D	312	CLA	CHC-C1C	3.05	1.42	1.35
29	a	829	CLA	C4D-ND	-3.05	1.33	1.37
29	b	716	CLA	CHC-C1C	3.05	1.42	1.35
29	a	831	CLA	C4D-ND	-3.05	1.33	1.37
29	J	309	CLA	CHC-C1C	3.05	1.42	1.35
29	a	804	CLA	CHC-C1C	3.05	1.42	1.35
29	f	803	CLA	CHC-C1C	3.04	1.42	1.35
29	D	313	CLA	C4D-ND	-3.04	1.33	1.37
29	f	803	CLA	C4D-ND	-3.04	1.33	1.37
29	i	201	CLA	CHC-C1C	3.04	1.42	1.35
29	G	317	CLA	C4D-ND	-3.04	1.33	1.37
29	a	803	CLA	CHC-C1C	3.04	1.42	1.35
29	f	802	CLA	CHC-C1C	3.04	1.42	1.35
29	b	726	CLA	CHC-C1C	3.04	1.42	1.35
29	f	802	CLA	C4D-ND	-3.04	1.33	1.37
37	F	304	PID	C20-C21	3.04	1.39	1.35
29	b	704	CLA	CHC-C1C	3.04	1.42	1.35
29	b	712	CLA	CHC-C1C	3.04	1.42	1.35
29	i	203	CLA	CHC-C1C	3.04	1.42	1.35
29	L	307	CLA	CHC-C1C	3.04	1.42	1.35
29	h	201	CLA	C4D-ND	-3.04	1.33	1.37
29	N	311	CLA	C4D-ND	-3.04	1.33	1.37
29	I	212	CLA	CHC-C1C	3.04	1.42	1.35
37	Q	306	PID	C20-C21	3.04	1.39	1.35
29	B	306	CLA	CHC-C1C	3.04	1.42	1.35
37	T	305	PID	C20-C21	3.04	1.39	1.35
29	F	312	CLA	CHC-C1C	3.04	1.42	1.35
29	b	718	CLA	CMB-C2B	-3.04	1.45	1.51
29	K	217	CLA	CHC-C1C	3.04	1.42	1.35
29	b	712	CLA	C4D-ND	-3.03	1.33	1.37
29	K	211	CLA	C4D-ND	-3.03	1.33	1.37
29	D	312	CLA	C4D-ND	-3.03	1.33	1.37
29	G	314	CLA	CHC-C1C	3.03	1.42	1.35
29	b	725	CLA	CHC-C1C	3.03	1.42	1.35
29	T	314	CLA	CHC-C1C	3.03	1.42	1.35
29	C	314	CLA	CHC-C1C	3.03	1.42	1.35
29	b	722	CLA	C4D-ND	-3.03	1.33	1.37
29	b	702	CLA	CHC-C1C	3.03	1.42	1.35
29	E	315	CLA	C4D-ND	-3.03	1.33	1.37
29	b	705	CLA	C4D-ND	-3.03	1.33	1.37
29	b	719	CLA	C4D-ND	-3.03	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	837	CLA	C4D-ND	-3.03	1.33	1.37
29	b	709	CLA	C4D-ND	-3.02	1.33	1.37
29	j	104	CLA	CHC-C1C	3.02	1.42	1.35
29	B	309	CLA	C4D-ND	-3.02	1.33	1.37
29	b	710	CLA	C4D-ND	-3.02	1.33	1.37
29	I	207	CLA	C4D-ND	-3.02	1.33	1.37
29	A	209	CLA	C4D-ND	-3.02	1.33	1.37
29	L	316	CLA	C4D-ND	-3.02	1.33	1.37
29	a	810	CLA	CHC-C1C	3.02	1.42	1.35
29	B	316	CLA	C4D-ND	-3.02	1.33	1.37
29	M	308	CLA	CHC-C1C	3.02	1.42	1.35
37	D	303	PID	C20-C21	3.02	1.39	1.35
29	b	713	CLA	C4D-ND	-3.02	1.33	1.37
29	L	316	CLA	CHC-C1C	3.02	1.42	1.35
29	a	829	CLA	CHC-C1C	3.02	1.42	1.35
29	G	301	CLA	C4D-ND	-3.02	1.33	1.37
29	F	313	CLA	C4D-ND	-3.02	1.33	1.37
37	Q	303	PID	C20-C21	3.02	1.39	1.35
29	J	307	CLA	C4D-ND	-3.01	1.33	1.37
29	J	313	CLA	C4D-ND	-3.01	1.33	1.37
29	a	819	CLA	C4D-ND	-3.01	1.33	1.37
29	J	305	CLA	C4D-ND	-3.01	1.33	1.37
29	B	311	CLA	C4D-ND	-3.01	1.33	1.37
29	E	305	CLA	CHC-C1C	3.01	1.42	1.35
29	I	208	CLA	C4D-ND	-3.01	1.33	1.37
29	l	501	CLA	C4D-ND	-3.01	1.33	1.37
29	l	503	CLA	C4D-ND	-3.01	1.33	1.37
29	M	314	CLA	CHC-C1C	3.01	1.42	1.35
29	b	701	CLA	C4D-ND	-3.01	1.33	1.37
29	E	306	CLA	C4D-ND	-3.01	1.33	1.37
29	i	202	CLA	CHC-C1C	3.01	1.42	1.35
29	K	212	CLA	CHC-C1C	3.01	1.42	1.35
29	C	311	CLA	C4D-ND	-3.01	1.33	1.37
29	L	311	CLA	C4D-ND	-3.01	1.33	1.37
29	b	720	CLA	C4D-ND	-3.00	1.33	1.37
29	a	818	CLA	C4D-ND	-3.00	1.33	1.37
29	a	805	CLA	C4D-ND	-3.00	1.33	1.37
29	P	210	CLA	C4D-ND	-3.00	1.33	1.37
29	b	721	CLA	C4D-ND	-3.00	1.33	1.37
29	A	217	CLA	C4D-ND	-3.00	1.33	1.37
29	M	313	CLA	C4D-ND	-3.00	1.33	1.37
29	B	307	CLA	C4D-ND	-2.99	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	718	CLA	C4D-ND	-2.99	1.33	1.37
29	I	213	CLA	C4D-ND	-2.99	1.33	1.37
29	O	309	CLA	C4D-ND	-2.99	1.33	1.37
29	K	218	CLA	C4D-ND	-2.99	1.33	1.37
29	M	314	CLA	C4D-ND	-2.99	1.33	1.37
29	N	314	CLA	C4D-ND	-2.99	1.33	1.37
29	l	505	CLA	C4D-ND	-2.99	1.33	1.37
29	H	308	CLA	C4D-ND	-2.99	1.33	1.37
29	O	313	CLA	C4D-ND	-2.99	1.33	1.37
29	I	217	CLA	CHC-C1C	2.99	1.42	1.35
29	A	211	CLA	C4D-ND	-2.99	1.33	1.37
29	a	809	CLA	C4D-ND	-2.99	1.33	1.37
29	M	310	CLA	C4D-ND	-2.99	1.33	1.37
29	L	317	CLA	C4D-ND	-2.99	1.33	1.37
29	a	813	CLA	C4D-ND	-2.98	1.33	1.37
29	L	315	CLA	C4D-ND	-2.98	1.33	1.37
29	E	310	CLA	C4D-ND	-2.98	1.33	1.37
29	a	822	CLA	C4D-ND	-2.98	1.33	1.37
29	K	217	CLA	C4D-ND	-2.98	1.33	1.37
29	E	313	CLA	C4D-ND	-2.98	1.33	1.37
29	A	215	CLA	C4D-ND	-2.98	1.33	1.37
29	G	316	CLA	CHC-C1C	2.98	1.42	1.35
29	Q	307	CLA	C4D-ND	-2.98	1.33	1.37
29	C	316	CLA	CHC-C1C	2.98	1.42	1.35
29	b	704	CLA	C4D-ND	-2.98	1.33	1.37
29	I	207	CLA	CHC-C1C	2.98	1.42	1.35
29	I	217	CLA	C4D-ND	-2.97	1.33	1.37
29	B	306	CLA	C4D-ND	-2.97	1.33	1.37
29	a	825	CLA	C4D-ND	-2.97	1.33	1.37
29	M	308	CLA	C4D-ND	-2.97	1.33	1.37
29	B	310	CLA	C4D-ND	-2.97	1.33	1.37
29	P	212	CLA	C4D-ND	-2.97	1.33	1.37
29	a	810	CLA	C4D-ND	-2.97	1.33	1.37
29	a	820	CLA	C4D-ND	-2.97	1.33	1.37
29	G	313	CLA	C4D-ND	-2.97	1.33	1.37
29	C	308	CLA	C4D-ND	-2.97	1.33	1.37
29	A	215	CLA	CHC-C1C	2.97	1.42	1.35
29	G	304	CLA	C4D-ND	-2.97	1.33	1.37
29	I	201	CLA	C4D-ND	-2.97	1.33	1.37
29	T	311	CLA	C4D-ND	-2.97	1.33	1.37
37	G	309	PID	C20-C21	2.97	1.39	1.35
29	J	306	CLA	C4D-ND	-2.97	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	702	CLA	C4D-ND	-2.97	1.33	1.37
29	K	207	CLA	C4D-ND	-2.97	1.33	1.37
29	L	310	CLA	C4D-ND	-2.97	1.33	1.37
29	H	310	CLA	C4D-ND	-2.96	1.33	1.37
29	l	509	CLA	C4D-ND	-2.96	1.33	1.37
29	D	311	CLA	C4D-ND	-2.96	1.33	1.37
29	O	311	CLA	C4D-ND	-2.96	1.33	1.37
29	E	314	CLA	C4D-ND	-2.96	1.33	1.37
29	F	313	CLA	CHC-C1C	2.96	1.42	1.35
29	G	314	CLA	C4D-ND	-2.96	1.33	1.37
39	G	315	KC1	C4B-NB	-2.96	1.34	1.37
29	E	305	CLA	C4D-ND	-2.96	1.33	1.37
37	N	302	PID	C20-C21	2.96	1.39	1.35
29	J	309	CLA	C4D-ND	-2.96	1.33	1.37
29	D	309	CLA	C4D-ND	-2.96	1.33	1.37
29	I	211	CLA	C4D-ND	-2.95	1.33	1.37
29	E	309	CLA	C4D-ND	-2.95	1.33	1.37
39	G	318	KC1	C4B-NB	-2.95	1.34	1.37
29	M	315	CLA	C4D-ND	-2.95	1.33	1.37
29	i	201	CLA	C4D-ND	-2.95	1.33	1.37
29	b	715	CLA	CHC-C1C	2.95	1.42	1.35
29	D	314	CLA	C4D-ND	-2.95	1.33	1.37
29	O	308	CLA	C4D-ND	-2.95	1.33	1.37
29	b	718	CLA	CHC-C1C	2.95	1.42	1.35
29	A	216	CLA	C4D-ND	-2.94	1.33	1.37
29	b	708	CLA	CHC-C1C	2.94	1.42	1.35
29	T	308	CLA	C4D-ND	-2.94	1.33	1.37
29	a	828	CLA	C4D-ND	-2.94	1.33	1.37
29	K	216	CLA	C4D-ND	-2.94	1.33	1.37
29	A	214	CLA	C4D-ND	-2.94	1.33	1.37
29	a	817	CLA	C4D-ND	-2.94	1.33	1.37
29	G	311	CLA	C4D-ND	-2.94	1.33	1.37
29	B	314	CLA	C4D-ND	-2.94	1.33	1.37
29	F	312	CLA	C4D-ND	-2.94	1.33	1.37
29	b	707	CLA	C4D-ND	-2.94	1.33	1.37
29	D	316	CLA	C4D-ND	-2.94	1.33	1.37
37	T	317	PID	C20-C21	2.94	1.39	1.35
39	L	314	KC1	C4B-NB	-2.94	1.34	1.37
29	a	801	CLA	CHC-C1C	2.94	1.42	1.35
29	G	319	CLA	C4D-ND	-2.93	1.33	1.37
29	A	210	CLA	C4D-ND	-2.93	1.33	1.37
39	G	315	KC1	CBA-CGA	-2.93	1.41	1.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T	314	CLA	C4D-ND	-2.93	1.33	1.37
29	Q	312	CLA	C4D-ND	-2.93	1.33	1.37
29	B	315	CLA	C4D-ND	-2.93	1.33	1.37
39	H	309	KC1	CBA-CGA	-2.92	1.41	1.48
29	F	310	CLA	C4D-ND	-2.92	1.33	1.37
29	N	313	CLA	C4D-ND	-2.92	1.33	1.37
29	a	816	CLA	C4D-ND	-2.92	1.33	1.37
29	G	302	CLA	C4D-ND	-2.92	1.33	1.37
29	a	804	CLA	C4D-ND	-2.92	1.33	1.37
36	I	204	DD6	O1-C20	-2.92	1.42	1.46
29	T	313	CLA	C4D-ND	-2.92	1.33	1.37
29	l	510	CLA	C4D-ND	-2.91	1.33	1.37
37	D	305	PID	C20-C21	2.91	1.39	1.35
29	L	312	CLA	C4D-ND	-2.91	1.33	1.37
29	M	306	CLA	C4D-ND	-2.91	1.33	1.37
29	F	316	CLA	C4D-ND	-2.91	1.33	1.37
29	b	706	CLA	CHC-C1C	2.91	1.42	1.35
29	H	307	CLA	C4D-ND	-2.91	1.33	1.37
39	C	312	KC1	C4B-NB	-2.90	1.34	1.37
29	F	311	CLA	C4D-ND	-2.90	1.33	1.37
29	H	315	CLA	C4D-ND	-2.90	1.33	1.37
29	N	316	CLA	C4D-ND	-2.90	1.33	1.37
29	Q	315	CLA	C4D-ND	-2.90	1.33	1.37
29	a	821	CLA	C4D-ND	-2.89	1.33	1.37
29	O	316	CLA	C4D-ND	-2.89	1.33	1.37
29	C	314	CLA	C4D-ND	-2.89	1.33	1.37
39	T	310	KC1	CBA-CGA	-2.89	1.41	1.48
29	a	815	CLA	C4D-ND	-2.88	1.33	1.37
29	C	313	CLA	C4D-ND	-2.88	1.33	1.37
39	F	309	KC1	CBA-CGA	-2.88	1.41	1.48
39	T	312	KC1	C4B-NB	-2.88	1.34	1.37
29	F	307	CLA	C4D-ND	-2.88	1.33	1.37
29	P	217	CLA	C4D-ND	-2.88	1.33	1.37
29	l	508	CLA	C4D-ND	-2.88	1.33	1.37
29	a	825	CLA	CHC-C1C	2.88	1.42	1.35
39	C	315	KC1	C4B-NB	-2.88	1.34	1.37
29	f	805	CLA	C4D-ND	-2.88	1.33	1.37
39	O	312	KC1	C4B-NB	-2.87	1.34	1.37
29	N	308	CLA	C4D-ND	-2.87	1.33	1.37
39	C	310	KC1	C4B-NB	-2.87	1.34	1.37
34	E	316	LMG	C4-C5	2.87	1.59	1.53
29	D	308	CLA	C4D-ND	-2.87	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	312	CLA	C4D-ND	-2.87	1.33	1.37
29	C	316	CLA	C4D-ND	-2.86	1.33	1.37
39	K	215	KC1	CBA-CGA	-2.86	1.41	1.48
39	P	213	KC1	C4B-NB	-2.86	1.34	1.37
38	T	306	UIX	O-C1	-2.86	1.42	1.46
29	A	206	CLA	C4D-ND	-2.86	1.33	1.37
29	P	214	CLA	C4D-ND	-2.86	1.33	1.37
39	E	312	KC1	C4B-NB	-2.86	1.34	1.37
39	C	312	KC1	CBA-CGA	-2.86	1.41	1.48
38	P	207	UIX	O-C1	-2.86	1.42	1.46
39	M	312	KC1	C4B-NB	-2.85	1.34	1.37
29	L	307	CLA	C4D-ND	-2.85	1.33	1.37
39	E	307	KC1	CBA-CGA	-2.85	1.41	1.48
29	P	209	CLA	C4D-ND	-2.85	1.33	1.37
39	T	315	KC1	CBA-CGA	-2.85	1.41	1.48
39	I	215	KC1	CBA-CGA	-2.84	1.41	1.48
39	G	318	KC1	CBA-CGA	-2.84	1.41	1.48
39	Q	309	KC1	CBA-CGA	-2.84	1.41	1.48
39	M	305	KC1	C4B-NB	-2.84	1.34	1.37
29	N	309	CLA	C4D-ND	-2.84	1.33	1.37
37	P	208	PID	C13-C12	2.84	1.44	1.36
39	L	306	KC1	CBA-CGA	-2.83	1.42	1.48
39	N	315	KC1	CBA-CGA	-2.83	1.42	1.48
39	E	312	KC1	CBA-CGA	-2.83	1.42	1.48
29	j	104	CLA	C4D-ND	-2.83	1.33	1.37
39	B	313	KC1	C4B-NB	-2.83	1.34	1.37
39	E	307	KC1	C4B-NB	-2.83	1.34	1.37
29	G	316	CLA	CMB-C2B	-2.83	1.45	1.51
39	Q	314	KC1	CBA-CGA	-2.83	1.42	1.48
39	A	213	KC1	CBA-CGA	-2.83	1.42	1.48
39	Q	311	KC1	CBA-CGA	-2.82	1.42	1.48
39	P	211	KC1	CBA-CGA	-2.82	1.42	1.48
39	O	310	KC1	CBA-CGA	-2.82	1.42	1.48
39	T	310	KC1	C4B-NB	-2.82	1.34	1.37
39	Q	309	KC1	C4B-NB	-2.82	1.34	1.37
29	T	316	CLA	C4D-ND	-2.82	1.33	1.37
39	D	315	KC1	CBA-CGA	-2.81	1.42	1.48
39	A	213	KC1	C4B-NB	-2.81	1.34	1.37
39	H	311	KC1	C4B-NB	-2.81	1.34	1.37
29	b	708	CLA	CMB-C2B	-2.81	1.45	1.51
39	P	216	KC1	CBA-CGA	-2.81	1.42	1.48
39	F	309	KC1	C4B-NB	-2.80	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	N	310	KC1	CBA-CGA	-2.80	1.42	1.48
39	H	309	KC1	C4B-NB	-2.80	1.34	1.37
39	F	314	KC1	C4B-NB	-2.80	1.34	1.37
39	F	314	KC1	CBA-CGA	-2.80	1.42	1.48
39	J	312	KC1	CBA-CGA	-2.79	1.42	1.48
39	A	205	KC1	CBA-CGA	-2.79	1.42	1.48
39	I	215	KC1	C4B-NB	-2.79	1.34	1.37
39	Q	314	KC1	C4B-NB	-2.79	1.34	1.37
39	N	312	KC1	C4B-NB	-2.79	1.34	1.37
39	B	313	KC1	CBA-CGA	-2.79	1.42	1.48
39	O	315	KC1	CBA-CGA	-2.79	1.42	1.48
39	N	312	KC1	CBA-CGA	-2.79	1.42	1.48
39	J	312	KC1	C4B-NB	-2.79	1.34	1.37
29	F	315	CLA	C4D-ND	-2.78	1.33	1.37
39	D	310	KC1	C4B-NB	-2.78	1.34	1.37
29	P	215	CLA	C4D-ND	-2.77	1.33	1.37
39	D	315	KC1	C4B-NB	-2.76	1.34	1.37
39	P	216	KC1	C4B-NB	-2.76	1.34	1.37
39	D	310	KC1	CBA-CGA	-2.76	1.42	1.48
39	P	213	KC1	CBA-CGA	-2.76	1.42	1.48
39	M	312	KC1	CBA-CGA	-2.76	1.42	1.48
39	C	310	KC1	CBA-CGA	-2.76	1.42	1.48
36	D	304	DD6	C19-C20	2.76	1.56	1.52
37	H	305	PID	C20-C21	2.76	1.39	1.35
39	L	314	KC1	CBA-CGA	-2.76	1.42	1.48
39	N	315	KC1	C4B-NB	-2.75	1.34	1.37
38	C	306	UIX	O-C1	-2.75	1.42	1.46
37	P	206	PID	C13-C12	2.75	1.44	1.36
29	K	212	CLA	CMB-C2B	-2.75	1.45	1.51
39	M	305	KC1	CBA-CGA	-2.75	1.42	1.48
39	H	314	KC1	CBA-CGA	-2.75	1.42	1.48
39	A	205	KC1	C4B-NB	-2.75	1.34	1.37
39	O	312	KC1	CBA-CGA	-2.74	1.42	1.48
37	G	310	PID	C8-C9	-2.74	1.39	1.46
39	H	311	KC1	CBA-CGA	-2.74	1.42	1.48
39	C	315	KC1	CBA-CGA	-2.74	1.42	1.48
37	N	302	PID	C8-C9	-2.74	1.39	1.46
36	K	221	DD6	C19-C20	2.74	1.56	1.52
39	G	315	KC1	C1B-NB	-2.73	1.34	1.37
37	Q	303	PID	C8-C9	-2.73	1.39	1.46
37	O	305	PID	C13-C12	2.73	1.44	1.36
37	H	304	PID	C13-C12	2.72	1.44	1.36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	O	315	KC1	C4B-NB	-2.72	1.34	1.37
39	T	315	KC1	C4B-NB	-2.71	1.34	1.37
39	L	306	KC1	C4B-NB	-2.71	1.34	1.37
37	H	306	PID	C13-C12	2.71	1.44	1.36
37	P	205	PID	C13-C12	2.71	1.44	1.36
29	l	503	CLA	CMB-C2B	-2.70	1.46	1.51
37	P	203	PID	C8-C9	-2.70	1.39	1.46
29	a	811	CLA	CMB-C2B	-2.69	1.46	1.51
39	N	310	KC1	C4B-NB	-2.69	1.34	1.37
37	G	310	PID	C20-C21	2.69	1.39	1.35
36	I	204	DD6	C21-C20	-2.69	1.47	1.51
29	b	717	CLA	CMB-C2B	-2.68	1.46	1.51
37	T	317	PID	C8-C9	-2.68	1.39	1.46
29	A	217	CLA	CMB-C2B	-2.68	1.46	1.51
37	F	306	PID	C8-C9	-2.68	1.39	1.46
36	G	305	DD6	C36-C31	-2.68	1.31	1.34
37	Q	301	PID	C8-C9	-2.68	1.39	1.46
37	G	309	PID	C8-C9	-2.67	1.39	1.46
37	N	304	PID	C8-C9	-2.67	1.39	1.46
29	J	309	CLA	CMB-C2B	-2.67	1.46	1.51
37	O	301	PID	C13-C12	2.67	1.43	1.36
37	N	307	PID	C13-C12	2.67	1.43	1.36
39	H	314	KC1	C4B-NB	-2.67	1.34	1.37
29	E	305	CLA	CMB-C2B	-2.67	1.46	1.51
37	D	306	PID	C8-C9	-2.67	1.39	1.46
37	D	303	PID	C8-C9	-2.66	1.39	1.46
37	T	307	PID	C8-C9	-2.66	1.39	1.46
29	b	706	CLA	CMB-C2B	-2.66	1.46	1.51
29	b	705	CLA	CMB-C2B	-2.66	1.46	1.51
37	O	304	PID	C8-C9	-2.65	1.39	1.46
37	T	301	PID	C8-C9	-2.65	1.39	1.46
29	a	810	CLA	CMB-C2B	-2.65	1.46	1.51
37	C	302	PID	C8-C9	-2.65	1.39	1.46
29	A	210	CLA	CMB-C2B	-2.65	1.46	1.51
37	C	307	PID	C13-C12	2.65	1.43	1.36
37	h	204	PID	C8-C9	-2.65	1.39	1.46
37	C	304	PID	C8-C9	-2.65	1.39	1.46
37	T	305	PID	C8-C9	-2.64	1.39	1.46
29	l	502	CLA	CMB-C2B	-2.64	1.46	1.51
29	K	217	CLA	CMB-C2B	-2.64	1.46	1.51
29	l	501	CLA	CMB-C2B	-2.64	1.46	1.51
39	O	310	KC1	C4B-NB	-2.63	1.34	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	T	302	PID	C13-C12	2.63	1.43	1.36
29	b	712	CLA	CMB-C2B	-2.63	1.46	1.51
36	h	202	DD6	O1-C20	-2.63	1.42	1.46
29	a	829	CLA	CMB-C2B	-2.63	1.46	1.51
37	D	305	PID	C13-C12	2.63	1.43	1.36
39	T	312	KC1	CBA-CGA	-2.63	1.42	1.48
37	G	303	PID	C8-C9	-2.62	1.39	1.46
37	D	307	PID	C13-C12	2.62	1.43	1.36
29	J	311	CLA	CMB-C2B	-2.62	1.46	1.51
29	a	801	CLA	CMB-C2B	-2.62	1.46	1.51
29	M	309	CLA	CMB-C2B	-2.62	1.46	1.51
37	T	304	PID	C13-C12	2.62	1.43	1.36
37	Q	306	PID	C13-C12	2.61	1.43	1.36
29	b	725	CLA	CMB-C2B	-2.61	1.46	1.51
37	F	302	PID	C8-C9	-2.61	1.39	1.46
36	D	301	DD6	O1-C20	-2.60	1.42	1.46
37	H	301	PID	C13-C12	2.60	1.43	1.36
29	b	726	CLA	CMB-C2B	-2.60	1.46	1.51
37	D	302	PID	C13-C12	2.60	1.43	1.36
37	P	202	PID	C13-C12	2.60	1.43	1.36
37	O	307	PID	C8-C9	-2.60	1.39	1.46
29	O	313	CLA	CMB-C2B	-2.60	1.46	1.51
29	b	702	CLA	CMB-C2B	-2.60	1.46	1.51
37	H	304	PID	C8-C9	-2.60	1.39	1.46
37	j	101	PID	C13-C12	2.60	1.43	1.36
37	C	301	PID	C13-C12	2.60	1.43	1.36
37	O	304	PID	C13-C12	2.60	1.43	1.36
36	G	307	DD6	O1-C20	-2.59	1.42	1.46
39	P	211	KC1	C4B-NB	-2.59	1.34	1.37
39	C	310	KC1	C1B-NB	-2.59	1.34	1.37
29	a	803	CLA	CMB-C2B	-2.59	1.46	1.51
29	A	216	CLA	CMB-C2B	-2.59	1.46	1.51
37	T	304	PID	C8-C9	-2.59	1.39	1.46
37	F	302	PID	C13-C12	2.59	1.43	1.36
37	Q	306	PID	C8-C9	-2.58	1.39	1.46
29	b	711	CLA	CMB-C2B	-2.58	1.46	1.51
29	I	212	CLA	CMB-C2B	-2.58	1.46	1.51
37	C	302	PID	C13-C12	2.58	1.43	1.36
29	I	210	CLA	CMB-C2B	-2.57	1.46	1.51
29	E	315	CLA	CMB-C2B	-2.57	1.46	1.51
37	H	301	PID	C8-C9	-2.57	1.39	1.46
38	Q	305	UIX	O-C1	-2.57	1.42	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	H	302	PID	C8-C9	-2.57	1.39	1.46
29	F	313	CLA	CMB-C2B	-2.57	1.46	1.51
37	N	304	PID	C13-C12	2.57	1.43	1.36
29	a	802	CLA	CMB-C2B	-2.57	1.46	1.51
29	B	306	CLA	CMB-C2B	-2.57	1.46	1.51
37	C	305	PID	C8-C9	-2.57	1.39	1.46
29	a	820	CLA	CMB-C2B	-2.57	1.46	1.51
29	b	720	CLA	CMB-C2B	-2.57	1.46	1.51
38	L	302	UIX	O-C1	-2.57	1.42	1.46
29	B	315	CLA	CMB-C2B	-2.56	1.46	1.51
29	K	218	CLA	CMB-C2B	-2.56	1.46	1.51
36	M	303	DD6	C19-C20	2.56	1.55	1.52
29	b	724	CLA	CMB-C2B	-2.56	1.46	1.51
37	N	301	PID	C8-C9	-2.56	1.39	1.46
37	F	304	PID	C8-C9	-2.56	1.39	1.46
37	C	301	PID	C8-C9	-2.56	1.39	1.46
29	K	208	CLA	CMB-C2B	-2.56	1.46	1.51
29	a	808	CLA	CMB-C2B	-2.56	1.46	1.51
38	F	305	UIX	O-C1	-2.56	1.42	1.46
37	O	302	PID	C8-C9	-2.55	1.39	1.46
29	l	509	CLA	CMB-C2B	-2.55	1.46	1.51
29	Q	313	CLA	CMB-C2B	-2.55	1.46	1.51
29	b	715	CLA	CMB-C2B	-2.55	1.46	1.51
37	T	301	PID	C13-C12	2.55	1.43	1.36
29	D	313	CLA	CMB-C2B	-2.55	1.46	1.51
37	D	302	PID	C8-C9	-2.55	1.40	1.46
29	a	824	CLA	CMB-C2B	-2.55	1.46	1.51
29	b	707	CLA	CMB-C2B	-2.55	1.46	1.51
29	B	316	CLA	CMB-C2B	-2.54	1.46	1.51
29	D	314	CLA	CMB-C2B	-2.54	1.46	1.51
29	I	217	CLA	CMB-C2B	-2.54	1.46	1.51
29	b	713	CLA	CMB-C2B	-2.54	1.46	1.51
37	N	301	PID	C13-C12	2.54	1.43	1.36
29	K	214	CLA	CMB-C2B	-2.54	1.46	1.51
29	E	314	CLA	CMB-C2B	-2.54	1.46	1.51
29	I	213	CLA	CMB-C2B	-2.54	1.46	1.51
37	C	304	PID	C13-C12	2.53	1.43	1.36
29	l	505	CLA	CMB-C2B	-2.53	1.46	1.51
37	F	306	PID	C13-C12	2.53	1.43	1.36
29	a	826	CLA	CMB-C2B	-2.53	1.46	1.51
29	a	817	CLA	CMB-C2B	-2.53	1.46	1.51
29	b	719	CLA	CMB-C2B	-2.53	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Q	314	KC1	C1B-NB	-2.53	1.34	1.37
29	I	209	CLA	CMB-C2B	-2.53	1.46	1.51
29	L	312	CLA	CMB-C2B	-2.53	1.46	1.51
29	I	214	CLA	CMB-C2B	-2.53	1.46	1.51
29	a	809	CLA	CMB-C2B	-2.53	1.46	1.51
39	Q	311	KC1	C1B-NB	-2.53	1.34	1.37
29	M	314	CLA	CMB-C2B	-2.53	1.46	1.51
37	Q	304	PID	C8-C9	-2.53	1.40	1.46
29	b	721	CLA	CMB-C2B	-2.53	1.46	1.51
37	Q	304	PID	C13-C12	2.53	1.43	1.36
29	a	827	CLA	CMB-C2B	-2.53	1.46	1.51
38	O	306	UIX	O-C1	-2.53	1.42	1.46
29	b	736	CLA	CMB-C2B	-2.53	1.46	1.51
29	L	310	CLA	CMB-C2B	-2.52	1.46	1.51
29	a	819	CLA	CMB-C2B	-2.52	1.46	1.51
29	b	714	CLA	CMB-C2B	-2.52	1.46	1.51
39	O	312	KC1	C1B-NB	-2.52	1.34	1.37
29	a	818	CLA	CMB-C2B	-2.52	1.46	1.51
29	T	314	CLA	CMB-C2B	-2.52	1.46	1.51
37	O	307	PID	C13-C12	2.52	1.43	1.36
37	E	301	PID	C13-C12	2.52	1.43	1.36
29	l	510	CLA	CMB-C2B	-2.52	1.46	1.51
29	M	311	CLA	CMB-C2B	-2.52	1.46	1.51
37	N	305	PID	C8-C9	-2.52	1.40	1.46
29	F	312	CLA	CMB-C2B	-2.52	1.46	1.51
29	i	201	CLA	CMB-C2B	-2.52	1.46	1.51
37	D	305	PID	C8-C9	-2.52	1.40	1.46
37	T	305	PID	C13-C12	2.52	1.43	1.36
29	A	209	CLA	CMB-C2B	-2.52	1.46	1.51
29	G	312	CLA	CMB-C2B	-2.52	1.46	1.51
36	M	302	DD6	C19-C20	2.51	1.55	1.52
38	B	304	UIX	O-C1	-2.51	1.42	1.46
37	O	301	PID	C8-C9	-2.51	1.40	1.46
29	A	215	CLA	CMB-C2B	-2.51	1.46	1.51
29	b	710	CLA	CMB-C2B	-2.51	1.46	1.51
29	L	307	CLA	CMB-C2B	-2.51	1.46	1.51
37	Q	301	PID	C13-C12	2.51	1.43	1.36
38	E	304	UIX	O-C1	-2.51	1.42	1.46
37	P	206	PID	C8-C9	-2.51	1.40	1.46
29	A	218	CLA	CMB-C2B	-2.51	1.46	1.51
29	E	311	CLA	CMB-C2B	-2.51	1.46	1.51
37	N	305	PID	C13-C12	2.51	1.43	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	310	CLA	CMD-C2D	-2.51	1.45	1.50
29	a	804	CLA	CMB-C2B	-2.50	1.46	1.51
29	b	716	CLA	CMB-C2B	-2.50	1.46	1.51
29	f	805	CLA	CMB-C2B	-2.50	1.46	1.51
29	L	311	CLA	CMB-C2B	-2.50	1.46	1.51
29	a	813	CLA	CMB-C2B	-2.50	1.46	1.51
29	f	803	CLA	CMB-C2B	-2.50	1.46	1.51
29	G	301	CLA	CMB-C2B	-2.50	1.46	1.51
29	K	207	CLA	CMB-C2B	-2.50	1.46	1.51
29	J	307	CLA	CMB-C2B	-2.50	1.46	1.51
29	b	703	CLA	CMB-C2B	-2.50	1.46	1.51
29	I	208	CLA	CMB-C2B	-2.50	1.46	1.51
29	I	207	CLA	CMB-C2B	-2.50	1.46	1.51
29	A	211	CLA	CMB-C2B	-2.50	1.46	1.51
29	a	814	CLA	CMB-C2B	-2.49	1.46	1.51
39	E	312	KC1	C1B-NB	-2.49	1.34	1.37
29	a	812	CLA	CMB-C2B	-2.49	1.46	1.51
37	C	305	PID	C13-C12	2.49	1.43	1.36
29	F	308	CLA	CMB-C2B	-2.49	1.46	1.51
39	C	315	KC1	C1B-NB	-2.49	1.34	1.37
29	F	311	CLA	CMB-C2B	-2.49	1.46	1.51
29	B	309	CLA	CMB-C2B	-2.49	1.46	1.51
29	a	816	CLA	CMB-C2B	-2.49	1.46	1.51
37	P	202	PID	C8-C9	-2.49	1.40	1.46
29	M	307	CLA	CMB-C2B	-2.49	1.46	1.51
39	K	215	KC1	C1B-NB	-2.49	1.34	1.37
39	C	312	KC1	C1B-NB	-2.49	1.34	1.37
29	b	731	CLA	CMB-C2B	-2.49	1.46	1.51
29	L	313	CLA	CMB-C2B	-2.49	1.46	1.51
29	f	802	CLA	CMB-C2B	-2.49	1.46	1.51
29	K	213	CLA	CMB-C2B	-2.49	1.46	1.51
37	T	307	PID	C13-C12	2.49	1.43	1.36
29	a	806	CLA	CMB-C2B	-2.49	1.46	1.51
29	l	508	CLA	CMB-C2B	-2.48	1.46	1.51
29	Q	310	CLA	CMB-C2B	-2.48	1.46	1.51
39	F	309	KC1	C1B-NB	-2.48	1.34	1.37
37	G	309	PID	C13-C12	2.48	1.43	1.36
37	Q	303	PID	C13-C12	2.48	1.43	1.36
37	H	305	PID	C13-C12	2.48	1.43	1.36
29	b	709	CLA	CMB-C2B	-2.48	1.46	1.51
29	l	504	CLA	CMB-C2B	-2.48	1.46	1.51
29	J	305	CLA	CMB-C2B	-2.48	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	P	205	PID	C8-C9	-2.48	1.40	1.46
29	a	805	CLA	CMB-C2B	-2.48	1.46	1.51
29	a	822	CLA	CMB-C2B	-2.48	1.46	1.51
29	a	828	CLA	CMB-C2B	-2.48	1.46	1.51
39	G	315	KC1	C4A-C3A	-2.48	1.39	1.44
29	A	206	CLA	CMB-C2B	-2.48	1.46	1.51
29	L	316	CLA	CMB-C2B	-2.48	1.46	1.51
29	H	313	CLA	CMB-C2B	-2.47	1.46	1.51
29	i	203	CLA	CMB-C2B	-2.47	1.46	1.51
29	G	304	CLA	CMB-C2B	-2.47	1.46	1.51
29	K	211	CLA	CMB-C2B	-2.47	1.46	1.51
29	L	315	CLA	CMB-C2B	-2.47	1.46	1.51
29	Q	312	CLA	CMB-C2B	-2.47	1.46	1.51
29	C	313	CLA	CMB-C2B	-2.47	1.46	1.51
29	E	306	CLA	CMB-C2B	-2.47	1.46	1.51
29	G	317	CLA	CMB-C2B	-2.47	1.46	1.51
29	B	307	CLA	CMB-C2B	-2.47	1.46	1.51
29	L	309	CLA	CMB-C2B	-2.47	1.46	1.51
37	E	301	PID	C8-C9	-2.47	1.40	1.46
29	a	830	CLA	CMB-C2B	-2.47	1.46	1.51
29	L	317	CLA	CMB-C2B	-2.47	1.46	1.51
29	I	211	CLA	CMB-C2B	-2.47	1.46	1.51
29	C	314	CLA	CMB-C2B	-2.47	1.46	1.51
39	T	312	KC1	CHD-C4C	2.47	1.41	1.35
37	H	302	PID	C13-C12	2.47	1.43	1.36
36	h	202	DD6	C10-C11	-2.47	1.32	1.35
29	A	212	CLA	CMB-C2B	-2.47	1.46	1.51
29	Q	308	CLA	CMB-C2B	-2.47	1.46	1.51
29	I	216	CLA	CMB-C2B	-2.47	1.46	1.51
29	M	308	CLA	CMB-C2B	-2.46	1.46	1.51
29	L	308	CLA	CMB-C2B	-2.46	1.46	1.51
29	A	207	CLA	CMB-C2B	-2.46	1.46	1.51
29	F	310	CLA	CMB-C2B	-2.46	1.46	1.51
29	G	319	CLA	CMB-C2B	-2.46	1.46	1.51
29	h	201	CLA	CMB-C2B	-2.46	1.46	1.51
29	A	214	CLA	CMD-C2D	-2.46	1.45	1.50
29	b	718	CLA	CMD-C2D	-2.46	1.45	1.50
29	a	807	CLA	CMB-C2B	-2.46	1.46	1.51
29	J	308	CLA	CMB-C2B	-2.46	1.46	1.51
29	a	837	CLA	CMB-C2B	-2.46	1.46	1.51
29	F	316	CLA	CMB-C2B	-2.46	1.46	1.51
29	T	308	CLA	CMB-C2B	-2.46	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	704	CLA	CMB-C2B	-2.46	1.46	1.51
29	B	308	CLA	CMB-C2B	-2.46	1.46	1.51
29	A	214	CLA	CMB-C2B	-2.45	1.46	1.51
29	K	216	CLA	CMB-C2B	-2.45	1.46	1.51
29	J	310	CLA	CMB-C2B	-2.45	1.46	1.51
29	C	316	CLA	CMB-C2B	-2.45	1.46	1.51
29	b	722	CLA	CMB-C2B	-2.45	1.46	1.51
29	G	311	CLA	CMB-C2B	-2.45	1.46	1.51
29	G	313	CLA	CMB-C2B	-2.45	1.46	1.51
29	B	311	CLA	CMB-C2B	-2.45	1.46	1.51
29	b	723	CLA	CMB-C2B	-2.45	1.46	1.51
29	a	815	CLA	CMB-C2B	-2.45	1.46	1.51
29	j	104	CLA	CMB-C2B	-2.45	1.46	1.51
29	Q	307	CLA	CMB-C2B	-2.44	1.46	1.51
29	H	308	CLA	CMB-C2B	-2.44	1.46	1.51
39	M	312	KC1	C1B-NB	-2.44	1.34	1.37
39	T	315	KC1	C1B-NB	-2.44	1.34	1.37
37	T	302	PID	C8-C9	-2.44	1.40	1.46
37	D	306	PID	C13-C12	2.44	1.43	1.36
29	O	309	CLA	CMB-C2B	-2.44	1.46	1.51
37	D	307	PID	C8-C9	-2.44	1.40	1.46
37	j	101	PID	C8-C9	-2.44	1.40	1.46
29	G	314	CLA	CMB-C2B	-2.44	1.46	1.51
29	I	201	CLA	CMB-C2B	-2.44	1.46	1.51
29	K	209	CLA	CMB-C2B	-2.44	1.46	1.51
29	T	309	CLA	CMB-C2B	-2.43	1.46	1.51
29	P	210	CLA	CMB-C2B	-2.43	1.46	1.51
29	b	701	CLA	CMB-C2B	-2.43	1.46	1.51
29	F	307	CLA	CMB-C2B	-2.43	1.46	1.51
37	C	307	PID	C8-C9	-2.43	1.40	1.46
29	P	214	CLA	CMB-C2B	-2.43	1.46	1.51
29	E	308	CLA	CMB-C2B	-2.43	1.46	1.51
39	P	211	KC1	C1B-NB	-2.43	1.34	1.37
29	A	208	CLA	CMB-C2B	-2.43	1.46	1.51
29	O	314	CLA	CMB-C2B	-2.43	1.46	1.51
38	J	304	UIX	O-C1	-2.43	1.42	1.46
39	Q	311	KC1	CHD-C4C	2.43	1.41	1.35
29	i	202	CLA	CMB-C2B	-2.43	1.46	1.51
39	O	312	KC1	C4A-C3A	-2.43	1.39	1.44
39	I	215	KC1	C1B-NB	-2.43	1.34	1.37
29	J	306	CLA	CMB-C2B	-2.43	1.46	1.51
29	b	719	CLA	CMD-C2D	-2.42	1.45	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	T	317	PID	C13-C12	2.42	1.43	1.36
39	L	314	KC1	C1B-NB	-2.42	1.34	1.37
29	a	821	CLA	CMB-C2B	-2.42	1.46	1.51
39	D	315	KC1	C1B-NB	-2.42	1.34	1.37
39	Q	309	KC1	C1B-NB	-2.42	1.34	1.37
37	O	302	PID	C13-C12	2.42	1.43	1.36
39	O	310	KC1	C1B-NB	-2.42	1.34	1.37
29	a	831	CLA	CMB-C2B	-2.42	1.46	1.51
29	O	308	CLA	CMB-C2B	-2.42	1.46	1.51
29	B	312	CLA	CMB-C2B	-2.42	1.46	1.51
29	D	312	CLA	CMB-C2B	-2.42	1.46	1.51
29	C	308	CLA	CMB-C2B	-2.42	1.46	1.51
39	T	310	KC1	CHD-C4C	2.42	1.41	1.35
39	J	312	KC1	C1B-NB	-2.42	1.34	1.37
39	A	205	KC1	C1B-NB	-2.42	1.34	1.37
29	H	307	CLA	CMB-C2B	-2.42	1.46	1.51
29	M	306	CLA	CMB-C2B	-2.42	1.46	1.51
29	M	313	CLA	CMB-C2B	-2.41	1.46	1.51
29	J	313	CLA	CMB-C2B	-2.41	1.46	1.51
29	O	311	CLA	CMB-C2B	-2.41	1.46	1.51
29	F	315	CLA	CMB-C2B	-2.41	1.46	1.51
29	G	302	CLA	CMB-C2B	-2.41	1.46	1.51
29	C	311	CLA	CMB-C2B	-2.41	1.46	1.51
29	P	215	CLA	CMB-C2B	-2.41	1.46	1.51
39	E	312	KC1	CHD-C4C	2.41	1.41	1.35
39	C	312	KC1	CHD-C4C	2.41	1.41	1.35
29	M	310	CLA	CMB-C2B	-2.41	1.46	1.51
39	N	310	KC1	C1B-NB	-2.41	1.34	1.37
37	h	204	PID	C13-C12	2.41	1.43	1.36
29	B	314	CLA	CMB-C2B	-2.41	1.46	1.51
39	E	307	KC1	C1B-NB	-2.41	1.34	1.37
29	N	309	CLA	CMB-C2B	-2.41	1.46	1.51
29	D	311	CLA	CMB-C2B	-2.40	1.46	1.51
39	D	315	KC1	CHD-C4C	2.40	1.41	1.35
29	B	310	CLA	CMB-C2B	-2.40	1.46	1.51
29	E	309	CLA	CMB-C2B	-2.40	1.46	1.51
39	L	314	KC1	CHD-C4C	2.40	1.41	1.35
39	H	309	KC1	C1B-NB	-2.40	1.34	1.37
29	P	209	CLA	CMB-C2B	-2.40	1.46	1.51
29	a	823	CLA	CMB-C2B	-2.40	1.46	1.51
29	D	309	CLA	CMB-C2B	-2.40	1.46	1.51
29	C	309	CLA	CMB-C2B	-2.40	1.46	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	M	305	KC1	CHD-C4C	2.40	1.41	1.35
39	D	310	KC1	CHD-C4C	2.40	1.41	1.35
39	C	310	KC1	CHD-C4C	2.40	1.41	1.35
29	N	314	CLA	CMB-C2B	-2.40	1.46	1.51
39	B	313	KC1	C1B-NB	-2.39	1.34	1.37
29	H	310	CLA	CMB-C2B	-2.39	1.46	1.51
29	N	308	CLA	CMB-C2B	-2.39	1.46	1.51
29	Q	315	CLA	CMB-C2B	-2.39	1.46	1.51
36	B	319	DD6	O1-C20	-2.39	1.42	1.46
39	P	213	KC1	CHD-C4C	2.39	1.41	1.35
39	H	314	KC1	C1B-NB	-2.39	1.34	1.37
29	N	316	CLA	CMB-C2B	-2.39	1.46	1.51
39	A	213	KC1	C1B-NB	-2.39	1.34	1.37
39	N	315	KC1	CHD-C4C	2.39	1.41	1.35
29	M	315	CLA	CMB-C2B	-2.39	1.46	1.51
39	H	311	KC1	CHD-C4C	2.39	1.41	1.35
36	O	303	DD6	O1-C20	-2.39	1.42	1.46
39	M	305	KC1	C1B-NB	-2.39	1.34	1.37
29	T	311	CLA	CMB-C2B	-2.39	1.46	1.51
29	E	313	CLA	CMB-C2B	-2.39	1.46	1.51
39	T	310	KC1	C1B-NB	-2.38	1.34	1.37
29	O	316	CLA	CMB-C2B	-2.38	1.46	1.51
29	K	210	CLA	CMB-C2B	-2.38	1.46	1.51
29	D	316	CLA	CMB-C2B	-2.38	1.46	1.51
29	K	214	CLA	C3B-C2B	-2.38	1.37	1.40
29	N	313	CLA	CMB-C2B	-2.38	1.46	1.51
39	N	312	KC1	C1B-NB	-2.38	1.34	1.37
39	J	312	KC1	CHD-C4C	2.38	1.41	1.35
29	N	311	CLA	CMB-C2B	-2.38	1.46	1.51
36	I	204	DD6	C19-C20	2.38	1.55	1.52
39	P	213	KC1	C1B-NB	-2.38	1.34	1.37
29	E	310	CLA	CMB-C2B	-2.37	1.46	1.51
39	P	216	KC1	C1B-NB	-2.37	1.34	1.37
37	N	302	PID	C13-C12	2.37	1.43	1.36
39	N	312	KC1	CHD-C4C	2.37	1.41	1.35
39	G	318	KC1	C1B-NB	-2.37	1.34	1.37
38	N	306	UIX	O-C1	-2.37	1.42	1.46
36	M	303	DD6	O1-C20	-2.37	1.42	1.46
29	P	212	CLA	CMB-C2B	-2.37	1.46	1.51
39	O	315	KC1	C1B-NB	-2.37	1.34	1.37
29	D	313	CLA	CMD-C2D	-2.37	1.45	1.50
29	H	315	CLA	CMB-C2B	-2.37	1.46	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	T	313	CLA	CMB-C2B	-2.37	1.46	1.51
37	G	310	PID	C13-C12	2.36	1.43	1.36
39	C	315	KC1	CHD-C4C	2.36	1.41	1.35
37	G	303	PID	C13-C12	2.36	1.43	1.36
37	F	304	PID	C13-C12	2.36	1.43	1.36
36	C	303	DD6	O1-C20	-2.36	1.42	1.46
29	b	704	CLA	CMD-C2D	-2.36	1.45	1.50
29	T	316	CLA	CMB-C2B	-2.36	1.46	1.51
29	b	736	CLA	CMC-C2C	-2.36	1.45	1.50
39	P	211	KC1	CHD-C4C	2.36	1.41	1.35
37	N	307	PID	C8-C9	-2.35	1.40	1.46
29	D	308	CLA	CMB-C2B	-2.35	1.46	1.51
37	P	203	PID	C13-C12	2.35	1.43	1.36
39	D	310	KC1	C1B-NB	-2.35	1.34	1.37
39	H	311	KC1	C1B-NB	-2.35	1.34	1.37
34	h	205	LMG	O7-C8	-2.35	1.40	1.46
29	l	505	CLA	CMD-C2D	-2.35	1.45	1.50
37	D	303	PID	C13-C12	2.34	1.43	1.36
29	P	217	CLA	CMB-C2B	-2.34	1.46	1.51
39	H	314	KC1	CHD-C4C	2.34	1.41	1.35
39	A	205	KC1	C4A-C3A	-2.34	1.40	1.44
39	N	310	KC1	CHD-C4C	2.34	1.41	1.35
39	T	312	KC1	C1B-NB	-2.34	1.34	1.37
29	F	310	CLA	CMD-C2D	-2.34	1.45	1.50
39	Q	309	KC1	CHD-C4C	2.34	1.41	1.35
39	L	306	KC1	C1B-NB	-2.33	1.34	1.37
29	f	805	CLA	CMD-C2D	-2.33	1.45	1.50
39	T	315	KC1	CHD-C4C	2.33	1.40	1.35
39	A	213	KC1	CHD-C4C	2.33	1.40	1.35
39	O	312	KC1	CHD-C4C	2.33	1.40	1.35
29	H	312	CLA	CMB-C2B	-2.33	1.46	1.51
39	P	216	KC1	CHD-C4C	2.33	1.40	1.35
39	A	205	KC1	CHD-C4C	2.32	1.40	1.35
39	G	318	KC1	CHD-C4C	2.32	1.40	1.35
37	P	208	PID	C8-C9	-2.32	1.40	1.46
39	H	309	KC1	CHD-C4C	2.32	1.40	1.35
39	M	312	KC1	CHD-C4C	2.31	1.40	1.35
36	E	303	DD6	O1-C20	-2.31	1.42	1.46
39	E	307	KC1	CHD-C4C	2.31	1.40	1.35
39	F	314	KC1	CHD-C4C	2.31	1.40	1.35
39	Q	314	KC1	CHD-C4C	2.31	1.40	1.35
36	K	204	DD6	O1-C20	-2.30	1.42	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	306	DD6	O1-C20	-2.30	1.42	1.46
39	F	314	KC1	C1B-NB	-2.29	1.35	1.37
34	K	219	LMG	O7-C8	-2.29	1.40	1.46
38	A	203	UIX	O-C1	-2.29	1.42	1.46
39	B	313	KC1	CHD-C4C	2.29	1.40	1.35
39	O	315	KC1	CHD-C4C	2.29	1.40	1.35
36	A	204	DD6	O1-C20	-2.28	1.42	1.46
36	B	303	DD6	O1-C20	-2.28	1.42	1.46
39	F	309	KC1	CHD-C4C	2.28	1.40	1.35
39	B	313	KC1	C4A-C3A	-2.28	1.40	1.44
36	J	303	DD6	O1-C20	-2.27	1.43	1.46
39	L	306	KC1	CHD-C4C	2.27	1.40	1.35
39	N	315	KC1	C1B-NB	-2.27	1.35	1.37
29	a	837	CLA	CMD-C2D	-2.27	1.46	1.50
39	F	309	KC1	C4A-C3A	-2.27	1.40	1.44
29	A	217	CLA	CMD-C2D	-2.26	1.46	1.50
36	B	301	DD6	O1-C20	-2.26	1.43	1.46
39	O	310	KC1	CHD-C4C	2.26	1.40	1.35
39	O	310	KC1	C4A-C3A	-2.26	1.40	1.44
38	E	304	UIX	C15-C20	-2.26	1.50	1.54
36	K	202	DD6	C21-C20	-2.26	1.48	1.51
39	E	307	KC1	C4A-C3A	-2.26	1.40	1.44
29	a	812	CLA	CMD-C2D	-2.26	1.46	1.50
39	K	215	KC1	CHD-C4C	2.25	1.40	1.35
36	H	303	DD6	O1-C20	-2.25	1.43	1.46
29	A	215	CLA	CMD-C2D	-2.25	1.46	1.50
39	I	215	KC1	CHD-C4C	2.25	1.40	1.35
29	a	820	CLA	CMD-C2D	-2.25	1.46	1.50
36	G	307	DD6	C-C1	-2.25	1.46	1.50
39	Q	311	KC1	C4A-C3A	-2.24	1.40	1.44
39	E	312	KC1	C4A-C3A	-2.24	1.40	1.44
36	N	303	DD6	O1-C20	-2.24	1.43	1.46
36	m	101	DD6	O1-C20	-2.24	1.43	1.46
36	E	302	DD6	O1-C20	-2.24	1.43	1.46
38	A	203	UIX	C15-C20	-2.24	1.50	1.54
32	m	103	BCR	C30-C25	-2.23	1.50	1.53
29	a	801	CLA	CMD-C2D	-2.23	1.46	1.50
34	b	730	LMG	O8-C9	-2.23	1.40	1.45
39	C	310	KC1	C4A-C3A	-2.23	1.40	1.44
39	N	310	KC1	C4A-C3A	-2.23	1.40	1.44
29	b	725	CLA	CMD-C2D	-2.22	1.46	1.50
29	A	218	CLA	CMC-C2C	-2.22	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	M	312	KC1	C4A-C3A	-2.22	1.40	1.44
39	I	215	KC1	C4A-C3A	-2.22	1.40	1.44
29	b	711	CLA	C3B-CAB	-2.22	1.43	1.47
36	A	202	DD6	O1-C20	-2.21	1.43	1.46
29	E	306	CLA	CMD-C2D	-2.21	1.46	1.50
29	h	201	CLA	CMC-C2C	-2.21	1.46	1.50
29	C	313	CLA	CMD-C2D	-2.21	1.46	1.50
36	P	204	DD6	O1-C20	-2.21	1.43	1.46
39	A	213	KC1	C4A-C3A	-2.21	1.40	1.44
29	a	827	CLA	C3B-C2B	-2.21	1.37	1.40
36	B	305	DD6	O1-C20	-2.21	1.43	1.46
37	O	305	PID	C8-C9	-2.21	1.40	1.46
39	T	312	KC1	C4A-C3A	-2.21	1.40	1.44
39	C	312	KC1	C4A-C3A	-2.21	1.40	1.44
36	K	203	DD6	O1-C20	-2.21	1.43	1.46
39	Q	314	KC1	C4A-C3A	-2.21	1.40	1.44
29	K	212	CLA	CMD-C2D	-2.21	1.46	1.50
29	I	214	CLA	CMD-C2D	-2.21	1.46	1.50
29	a	831	CLA	CMD-C2D	-2.21	1.46	1.50
36	M	301	DD6	O1-C20	-2.20	1.43	1.46
36	L	303	DD6	O1-C20	-2.20	1.43	1.46
29	L	316	CLA	CMD-C2D	-2.20	1.46	1.50
29	a	810	CLA	CMD-C2D	-2.20	1.46	1.50
36	L	305	DD6	O1-C20	-2.20	1.43	1.46
29	a	802	CLA	CMD-C2D	-2.20	1.46	1.50
34	b	732	LMG	O7-C8	-2.20	1.41	1.46
29	G	313	CLA	CMD-C2D	-2.20	1.46	1.50
39	L	314	KC1	C4A-C3A	-2.20	1.40	1.44
29	K	212	CLA	C3B-C2B	-2.20	1.37	1.40
29	f	803	CLA	CMD-C2D	-2.20	1.46	1.50
39	K	215	KC1	C4A-C3A	-2.20	1.40	1.44
36	L	304	DD6	O1-C20	-2.19	1.43	1.46
29	l	504	CLA	CMD-C2D	-2.19	1.46	1.50
37	H	305	PID	C8-C9	-2.19	1.40	1.46
29	N	313	CLA	CMD-C2D	-2.19	1.46	1.50
29	a	806	CLA	CMD-C2D	-2.19	1.46	1.50
36	I	202	DD6	O1-C20	-2.19	1.43	1.46
29	F	310	CLA	CMC-C2C	-2.19	1.46	1.50
36	K	205	DD6	O1-C20	-2.19	1.43	1.46
29	K	218	CLA	CMD-C2D	-2.19	1.46	1.50
36	K	206	DD6	O1-C20	-2.19	1.43	1.46
29	a	824	CLA	CMD-C2D	-2.18	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	M	305	KC1	C4A-C3A	-2.18	1.40	1.44
39	J	312	KC1	C4A-C3A	-2.18	1.40	1.44
29	i	203	CLA	CMD-C2D	-2.18	1.46	1.50
29	J	306	CLA	CMD-C2D	-2.18	1.46	1.50
29	b	705	CLA	CMC-C2C	-2.18	1.46	1.50
29	K	213	CLA	CMD-C2D	-2.18	1.46	1.50
39	L	306	KC1	C4A-C3A	-2.17	1.40	1.44
29	a	808	CLA	CMD-C2D	-2.17	1.46	1.50
29	L	312	CLA	CMD-C2D	-2.17	1.46	1.50
29	G	302	CLA	CMD-C2D	-2.17	1.46	1.50
29	a	826	CLA	CMD-C2D	-2.17	1.46	1.50
40	B	317	SQD	O8-S	2.17	1.55	1.47
39	P	211	KC1	C4A-C3A	-2.17	1.40	1.44
29	b	723	CLA	CMD-C2D	-2.17	1.46	1.50
39	F	314	KC1	C4A-C3A	-2.17	1.40	1.44
36	Q	302	DD6	O1-C20	-2.16	1.43	1.46
29	b	703	CLA	CMD-C2D	-2.16	1.46	1.50
29	a	808	CLA	C3B-CAB	-2.16	1.43	1.47
29	a	805	CLA	CMD-C2D	-2.16	1.46	1.50
29	b	714	CLA	CMD-C2D	-2.16	1.46	1.50
34	b	730	LMG	O7-C8	-2.15	1.41	1.46
29	K	216	CLA	CMD-C2D	-2.15	1.46	1.50
36	I	206	DD6	O1-C20	-2.15	1.43	1.46
29	B	314	CLA	CMD-C2D	-2.15	1.46	1.50
39	G	315	KC1	CHD-C4C	2.15	1.40	1.35
29	b	706	CLA	CMC-C2C	-2.15	1.46	1.50
29	b	705	CLA	CMD-C2D	-2.15	1.46	1.50
29	B	311	CLA	CMC-C2C	-2.15	1.46	1.50
36	G	307	DD6	C19-C18	-2.15	1.49	1.52
29	l	502	CLA	CMC-C2C	-2.15	1.46	1.50
29	b	724	CLA	CMD-C2D	-2.14	1.46	1.50
39	D	310	KC1	C4A-C3A	-2.14	1.40	1.44
29	b	715	CLA	CMD-C2D	-2.14	1.46	1.50
29	G	316	CLA	C3B-C2B	-2.14	1.37	1.40
29	P	217	CLA	CMC-C2C	-2.14	1.46	1.50
29	J	311	CLA	C3B-C2B	-2.14	1.37	1.40
29	b	717	CLA	CMD-C2D	-2.14	1.46	1.50
32	b	729	BCR	C30-C25	-2.14	1.50	1.53
34	K	220	LMG	O7-C8	-2.14	1.41	1.46
29	Q	312	CLA	CMD-C2D	-2.14	1.46	1.50
29	b	710	CLA	CMD-C2D	-2.14	1.46	1.50
29	a	814	CLA	CMC-C2C	-2.14	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	T	303	DD6	O1-C20	-2.14	1.43	1.46
29	A	218	CLA	CMD-C2D	-2.13	1.46	1.50
29	G	316	CLA	CMD-C2D	-2.13	1.46	1.50
29	O	313	CLA	CMD-C2D	-2.13	1.46	1.50
29	l	502	CLA	C3B-C2B	-2.13	1.37	1.40
29	G	312	CLA	CMD-C2D	-2.13	1.46	1.50
29	M	311	CLA	CMD-C2D	-2.13	1.46	1.50
29	D	316	CLA	CMC-C2C	-2.13	1.46	1.50
29	f	802	CLA	CMD-C2D	-2.13	1.46	1.50
29	M	315	CLA	CMD-C2D	-2.13	1.46	1.50
29	L	316	CLA	CMC-C2C	-2.13	1.46	1.50
29	B	311	CLA	CMD-C2D	-2.13	1.46	1.50
29	b	701	CLA	CMD-C2D	-2.13	1.46	1.50
29	A	211	CLA	CMD-C2D	-2.13	1.46	1.50
29	a	803	CLA	CMD-C2D	-2.13	1.46	1.50
29	a	807	CLA	CMD-C2D	-2.13	1.46	1.50
29	b	722	CLA	CMD-C2D	-2.13	1.46	1.50
29	b	726	CLA	CMD-C2D	-2.13	1.46	1.50
29	a	823	CLA	CMC-C2C	-2.13	1.46	1.50
39	H	309	KC1	C4A-C3A	-2.12	1.40	1.44
29	i	201	CLA	CMD-C2D	-2.12	1.46	1.50
29	b	722	CLA	CMC-C2C	-2.12	1.46	1.50
29	K	209	CLA	CMD-C2D	-2.12	1.46	1.50
29	K	211	CLA	CMD-C2D	-2.12	1.46	1.50
38	Q	305	UIX	C15-C20	-2.12	1.51	1.54
39	G	318	KC1	C4A-C3A	-2.12	1.40	1.44
40	J	314	SQD	O8-S	2.12	1.55	1.47
29	a	804	CLA	CMC-C2C	-2.12	1.46	1.50
29	D	308	CLA	CMD-C2D	-2.12	1.46	1.50
29	a	825	CLA	C3B-C2B	-2.12	1.37	1.40
29	J	311	CLA	CMD-C2D	-2.12	1.46	1.50
37	H	306	PID	C8-C9	-2.12	1.41	1.46
29	I	201	CLA	CMD-C2D	-2.12	1.46	1.50
29	b	736	CLA	C3B-C2B	-2.12	1.37	1.40
39	P	213	KC1	C4A-C3A	-2.12	1.40	1.44
29	G	314	CLA	CMD-C2D	-2.12	1.46	1.50
29	I	207	CLA	CMD-C2D	-2.12	1.46	1.50
29	E	308	CLA	CMD-C2D	-2.12	1.46	1.50
29	l	502	CLA	CMD-C2D	-2.11	1.46	1.50
29	G	314	CLA	CMC-C2C	-2.11	1.46	1.50
29	F	308	CLA	CMD-C2D	-2.11	1.46	1.50
29	B	316	CLA	CMD-C2D	-2.11	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	Q	309	KC1	C4A-C3A	-2.11	1.40	1.44
29	a	823	CLA	CMD-C2D	-2.11	1.46	1.50
29	a	825	CLA	CMC-C2C	-2.11	1.46	1.50
29	Q	310	CLA	CMD-C2D	-2.11	1.46	1.50
36	F	301	DD6	C19-C20	2.11	1.55	1.52
29	G	311	CLA	CMD-C2D	-2.11	1.46	1.50
29	b	715	CLA	CMC-C2C	-2.11	1.46	1.50
29	A	208	CLA	CMD-C2D	-2.11	1.46	1.50
29	K	208	CLA	CMD-C2D	-2.11	1.46	1.50
29	i	202	CLA	CMD-C2D	-2.11	1.46	1.50
29	I	213	CLA	CMD-C2D	-2.11	1.46	1.50
29	J	310	CLA	CMD-C2D	-2.11	1.46	1.50
29	b	703	CLA	CMC-C2C	-2.11	1.46	1.50
29	L	308	CLA	CMD-C2D	-2.11	1.46	1.50
29	b	716	CLA	CMD-C2D	-2.11	1.46	1.50
29	K	217	CLA	CMD-C2D	-2.11	1.46	1.50
29	C	309	CLA	CMD-C2D	-2.11	1.46	1.50
29	K	217	CLA	C3B-C2B	-2.11	1.37	1.40
36	M	302	DD6	O1-C20	-2.10	1.43	1.46
29	F	312	CLA	CMD-C2D	-2.10	1.46	1.50
29	K	211	CLA	CMC-C2C	-2.10	1.46	1.50
29	L	309	CLA	CMD-C2D	-2.10	1.46	1.50
29	M	307	CLA	CMD-C2D	-2.10	1.46	1.50
29	A	207	CLA	CMD-C2D	-2.10	1.46	1.50
29	E	305	CLA	CMD-C2D	-2.10	1.46	1.50
29	I	212	CLA	CMD-C2D	-2.10	1.46	1.50
29	b	702	CLA	CMD-C2D	-2.10	1.46	1.50
39	H	314	KC1	C4A-C3A	-2.10	1.40	1.44
29	b	706	CLA	CMD-C2D	-2.10	1.46	1.50
39	N	312	KC1	C4A-C3A	-2.10	1.40	1.44
29	G	304	CLA	CMD-C2D	-2.10	1.46	1.50
29	b	711	CLA	CMD-C2D	-2.10	1.46	1.50
29	F	307	CLA	CMD-C2D	-2.10	1.46	1.50
29	J	307	CLA	CMD-C2D	-2.10	1.46	1.50
29	b	724	CLA	CMC-C2C	-2.10	1.46	1.50
29	B	315	CLA	CMD-C2D	-2.10	1.46	1.50
29	A	216	CLA	CMD-C2D	-2.10	1.46	1.50
29	B	306	CLA	CMD-C2D	-2.10	1.46	1.50
29	N	314	CLA	CMC-C2C	-2.10	1.46	1.50
29	b	708	CLA	CMC-C2C	-2.09	1.46	1.50
38	C	306	UIX	C15-C20	-2.09	1.51	1.54
36	D	304	DD6	O1-C20	-2.09	1.43	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	302	DD6	O1-C20	-2.09	1.43	1.46
29	M	313	CLA	CMC-C2C	-2.09	1.46	1.50
39	T	310	KC1	C4A-C3A	-2.09	1.40	1.44
39	T	315	KC1	C4A-C3A	-2.09	1.40	1.44
29	a	806	CLA	CMC-C2C	-2.09	1.46	1.50
36	A	201	DD6	O1-C20	-2.09	1.43	1.46
29	l	501	CLA	CMD-C2D	-2.09	1.46	1.50
29	H	312	CLA	CMD-C2D	-2.09	1.46	1.50
29	G	301	CLA	CMD-C2D	-2.09	1.46	1.50
29	b	707	CLA	CMD-C2D	-2.09	1.46	1.50
29	M	310	CLA	CMD-C2D	-2.09	1.46	1.50
29	F	316	CLA	CMD-C2D	-2.09	1.46	1.50
29	a	824	CLA	CMC-C2C	-2.09	1.46	1.50
29	a	830	CLA	CMD-C2D	-2.09	1.46	1.50
36	F	303	DD6	O1-C20	-2.09	1.43	1.46
29	O	309	CLA	CMD-C2D	-2.09	1.46	1.50
29	a	829	CLA	CMD-C2D	-2.08	1.46	1.50
29	B	309	CLA	CMD-C2D	-2.08	1.46	1.50
29	a	807	CLA	CMC-C2C	-2.08	1.46	1.50
29	K	210	CLA	CMD-C2D	-2.08	1.46	1.50
29	K	207	CLA	CMD-C2D	-2.08	1.46	1.50
29	a	820	CLA	C3B-CAB	-2.08	1.43	1.47
29	b	720	CLA	CMD-C2D	-2.08	1.46	1.50
29	b	718	CLA	CMC-C2C	-2.08	1.46	1.50
29	B	307	CLA	CMD-C2D	-2.08	1.46	1.50
29	l	503	CLA	C3B-C2B	-2.08	1.37	1.40
29	I	208	CLA	CMD-C2D	-2.08	1.46	1.50
29	H	307	CLA	CMD-C2D	-2.08	1.46	1.50
29	l	503	CLA	CMC-C2C	-2.08	1.46	1.50
29	G	317	CLA	CMD-C2D	-2.08	1.46	1.50
29	K	213	CLA	CMC-C2C	-2.08	1.46	1.50
36	K	221	DD6	O1-C20	-2.08	1.43	1.46
29	L	315	CLA	CMC-C2C	-2.08	1.46	1.50
29	T	309	CLA	CMC-C2C	-2.08	1.46	1.50
29	a	801	CLA	C3B-C2B	-2.08	1.37	1.40
29	I	209	CLA	CMD-C2D	-2.08	1.46	1.50
29	b	726	CLA	CMC-C2C	-2.08	1.46	1.50
29	l	509	CLA	CMD-C2D	-2.08	1.46	1.50
29	B	314	CLA	CMC-C2C	-2.08	1.46	1.50
29	a	827	CLA	CMD-C2D	-2.08	1.46	1.50
29	L	317	CLA	CMD-C2D	-2.08	1.46	1.50
29	Q	315	CLA	CMD-C2D	-2.08	1.46	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	308	CLA	CMD-C2D	-2.07	1.46	1.50
29	b	736	CLA	CMD-C2D	-2.07	1.46	1.50
29	I	217	CLA	CMD-C2D	-2.07	1.46	1.50
29	a	822	CLA	CMD-C2D	-2.07	1.46	1.50
39	C	315	KC1	C4A-C3A	-2.07	1.40	1.44
29	a	801	CLA	CMC-C2C	-2.07	1.46	1.50
29	b	709	CLA	CMD-C2D	-2.07	1.46	1.50
29	h	201	CLA	CMD-C2D	-2.07	1.46	1.50
29	A	210	CLA	CMD-C2D	-2.07	1.46	1.50
29	l	510	CLA	CMD-C2D	-2.07	1.46	1.50
29	O	314	CLA	CMC-C2C	-2.07	1.46	1.50
29	b	712	CLA	CMD-C2D	-2.07	1.46	1.50
29	b	701	CLA	CMC-C2C	-2.07	1.46	1.50
29	F	313	CLA	CMD-C2D	-2.07	1.46	1.50
29	L	311	CLA	CMD-C2D	-2.07	1.46	1.50
29	I	210	CLA	CMD-C2D	-2.07	1.46	1.50
29	A	209	CLA	CMD-C2D	-2.07	1.46	1.50
29	a	814	CLA	CMD-C2D	-2.07	1.46	1.50
39	D	315	KC1	C4A-C3A	-2.07	1.40	1.44
29	B	312	CLA	CMD-C2D	-2.07	1.46	1.50
29	j	104	CLA	CMD-C2D	-2.07	1.46	1.50
29	L	307	CLA	CMD-C2D	-2.07	1.46	1.50
29	O	314	CLA	CMD-C2D	-2.07	1.46	1.50
29	P	214	CLA	CMD-C2D	-2.07	1.46	1.50
29	b	721	CLA	CMD-C2D	-2.06	1.46	1.50
29	A	212	CLA	CMD-C2D	-2.06	1.46	1.50
29	J	307	CLA	C3B-CAB	-2.06	1.43	1.47
29	a	812	CLA	CMC-C2C	-2.06	1.46	1.50
29	L	315	CLA	CMD-C2D	-2.06	1.46	1.50
29	N	309	CLA	CMD-C2D	-2.06	1.46	1.50
29	a	818	CLA	CMD-C2D	-2.06	1.46	1.50
29	A	206	CLA	CMD-C2D	-2.06	1.46	1.50
29	J	308	CLA	CMD-C2D	-2.06	1.46	1.50
39	P	216	KC1	C4A-C3A	-2.06	1.40	1.44
29	b	714	CLA	CMC-C2C	-2.06	1.46	1.50
29	a	810	CLA	C3B-C2B	-2.06	1.37	1.40
29	C	311	CLA	CMD-C2D	-2.06	1.46	1.50
29	b	705	CLA	C3B-CAB	-2.06	1.43	1.47
29	H	308	CLA	CMD-C2D	-2.06	1.46	1.50
29	G	319	CLA	CMD-C2D	-2.06	1.46	1.50
36	F	301	DD6	C21-C20	2.06	1.55	1.51
29	I	211	CLA	CMD-C2D	-2.06	1.46	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	815	CLA	CMC-C2C	-2.06	1.46	1.50
36	J	301	DD6	O1-C20	-2.06	1.43	1.46
29	b	704	CLA	CMC-C2C	-2.06	1.46	1.50
29	b	716	CLA	CMC-C2C	-2.06	1.46	1.50
29	J	305	CLA	CMD-C2D	-2.06	1.46	1.50
29	I	216	CLA	CMD-C2D	-2.06	1.46	1.50
29	Q	313	CLA	CMD-C2D	-2.06	1.46	1.50
36	G	307	DD6	C10-C11	-2.06	1.33	1.35
29	M	307	CLA	CMC-C2C	-2.06	1.46	1.50
29	C	314	CLA	CMD-C2D	-2.06	1.46	1.50
36	G	307	DD6	C2-C1	-2.05	1.33	1.35
29	a	811	CLA	CMD-C2D	-2.05	1.46	1.50
29	E	311	CLA	CMD-C2D	-2.05	1.46	1.50
29	a	827	CLA	CMC-C2C	-2.05	1.46	1.50
29	Q	307	CLA	CMD-C2D	-2.05	1.46	1.50
29	F	308	CLA	CMC-C2C	-2.05	1.46	1.50
29	b	707	CLA	CMC-C2C	-2.05	1.46	1.50
29	Q	308	CLA	CMD-C2D	-2.05	1.46	1.50
29	b	710	CLA	CMC-C2C	-2.05	1.46	1.50
29	a	825	CLA	CMD-C2D	-2.05	1.46	1.50
29	C	316	CLA	CMD-C2D	-2.05	1.46	1.50
29	D	314	CLA	CMC-C2C	-2.05	1.46	1.50
29	a	809	CLA	CMD-C2D	-2.05	1.46	1.50
29	a	815	CLA	CMD-C2D	-2.05	1.46	1.50
29	F	311	CLA	CMD-C2D	-2.05	1.46	1.50
29	J	309	CLA	CMD-C2D	-2.05	1.46	1.50
29	a	805	CLA	CMC-C2C	-2.05	1.46	1.50
35	b	733	DGD	O3G-C1D	2.05	1.43	1.40
29	b	725	CLA	CMC-C2C	-2.05	1.46	1.50
29	b	731	CLA	CMD-C2D	-2.05	1.46	1.50
29	E	306	CLA	CMC-C2C	-2.05	1.46	1.50
39	H	311	KC1	C4A-C3A	-2.05	1.40	1.44
29	b	709	CLA	CMC-C2C	-2.05	1.46	1.50
29	i	202	CLA	CMC-C2C	-2.05	1.46	1.50
29	K	216	CLA	CMC-C2C	-2.05	1.46	1.50
29	D	312	CLA	CMD-C2D	-2.05	1.46	1.50
29	E	309	CLA	CMD-C2D	-2.05	1.46	1.50
29	L	310	CLA	CMD-C2D	-2.05	1.46	1.50
29	A	210	CLA	C3B-C2B	-2.05	1.37	1.40
29	a	821	CLA	CMD-C2D	-2.04	1.46	1.50
29	a	804	CLA	CMD-C2D	-2.04	1.46	1.50
29	f	802	CLA	CMC-C2C	-2.04	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	E	314	CLA	CMD-C2D	-2.04	1.46	1.50
29	I	211	CLA	CMC-C2C	-2.04	1.46	1.50
29	D	311	CLA	CMD-C2D	-2.04	1.46	1.50
29	D	314	CLA	CMD-C2D	-2.04	1.46	1.50
29	E	313	CLA	CMD-C2D	-2.04	1.46	1.50
29	B	308	CLA	CMC-C2C	-2.04	1.46	1.50
29	a	813	CLA	CMD-C2D	-2.04	1.46	1.50
29	O	311	CLA	CMC-C2C	-2.04	1.46	1.50
29	T	316	CLA	CMD-C2D	-2.04	1.46	1.50
29	M	306	CLA	CMD-C2D	-2.04	1.46	1.50
29	Q	315	CLA	CMC-C2C	-2.04	1.46	1.50
29	b	736	CLA	C3B-CAB	-2.04	1.43	1.47
29	a	801	CLA	MG-ND	-2.04	2.01	2.05
29	J	306	CLA	CMC-C2C	-2.04	1.46	1.50
29	a	816	CLA	CMC-C2C	-2.03	1.46	1.50
29	a	816	CLA	CMD-C2D	-2.03	1.46	1.50
29	A	208	CLA	CMC-C2C	-2.03	1.46	1.50
29	G	304	CLA	CMC-C2C	-2.03	1.46	1.50
29	a	819	CLA	CMD-C2D	-2.03	1.46	1.50
29	l	503	CLA	CMD-C2D	-2.03	1.46	1.50
29	M	308	CLA	CMC-C2C	-2.03	1.46	1.50
29	l	502	CLA	C3B-CAB	-2.03	1.43	1.47
36	L	301	DD6	O1-C20	-2.03	1.43	1.46
29	O	308	CLA	CMD-C2D	-2.03	1.46	1.50
29	G	317	CLA	CMC-C2C	-2.03	1.46	1.50
29	K	208	CLA	CMC-C2C	-2.03	1.46	1.50
29	M	313	CLA	CMD-C2D	-2.03	1.46	1.50
29	A	207	CLA	CMC-C2C	-2.03	1.46	1.50
29	K	214	CLA	CMD-C2D	-2.03	1.46	1.50
29	G	312	CLA	CMC-C2C	-2.03	1.46	1.50
29	H	315	CLA	CMD-C2D	-2.03	1.46	1.50
29	M	308	CLA	CMD-C2D	-2.03	1.46	1.50
29	L	313	CLA	CMC-C2C	-2.03	1.46	1.50
29	H	313	CLA	CMC-C2C	-2.03	1.46	1.50
29	b	721	CLA	C3B-C2B	-2.03	1.37	1.40
29	a	817	CLA	CMD-C2D	-2.02	1.46	1.50
29	b	724	CLA	C3B-C2B	-2.02	1.37	1.40
29	b	721	CLA	CMC-C2C	-2.02	1.46	1.50
29	E	315	CLA	CMD-C2D	-2.02	1.46	1.50
29	A	215	CLA	CMC-C2C	-2.02	1.46	1.50
29	a	801	CLA	C3B-CAB	-2.02	1.43	1.47
29	M	309	CLA	CMD-C2D	-2.02	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	813	CLA	CMC-C2C	-2.02	1.46	1.50
29	b	708	CLA	CMD-C2D	-2.02	1.46	1.50
29	a	828	CLA	CMD-C2D	-2.02	1.46	1.50
29	O	316	CLA	CMC-C2C	-2.02	1.46	1.50
29	l	508	CLA	CMC-C2C	-2.02	1.46	1.50
29	K	214	CLA	CMC-C2C	-2.02	1.46	1.50
29	a	808	CLA	C3B-C2B	-2.02	1.37	1.40
29	I	207	CLA	CMC-C2C	-2.02	1.46	1.50
29	E	310	CLA	CMD-C2D	-2.02	1.46	1.50
29	I	214	CLA	CMC-C2C	-2.02	1.46	1.50
29	a	828	CLA	CMC-C2C	-2.02	1.46	1.50
29	l	508	CLA	CMD-C2D	-2.02	1.46	1.50
29	j	104	CLA	CMC-C2C	-2.02	1.46	1.50
29	E	311	CLA	CMC-C2C	-2.02	1.46	1.50
29	l	509	CLA	CMC-C2C	-2.02	1.46	1.50
36	M	304	DD6	O1-C20	-2.02	1.43	1.46
29	b	720	CLA	C3B-C2B	-2.02	1.37	1.40
29	E	314	CLA	CMC-C2C	-2.01	1.46	1.50
29	a	820	CLA	CMC-C2C	-2.01	1.46	1.50
29	P	210	CLA	CMD-C2D	-2.01	1.46	1.50
29	J	311	CLA	CMC-C2C	-2.01	1.46	1.50
29	I	209	CLA	CMC-C2C	-2.01	1.46	1.50
29	N	314	CLA	CMD-C2D	-2.01	1.46	1.50
29	B	312	CLA	CMC-C2C	-2.01	1.46	1.50
29	b	723	CLA	CMC-C2C	-2.01	1.46	1.50
29	K	209	CLA	CMC-C2C	-2.01	1.46	1.50
29	a	827	CLA	C3B-CAB	-2.01	1.43	1.47
29	b	720	CLA	CMC-C2C	-2.01	1.46	1.50
29	J	313	CLA	CMD-C2D	-2.01	1.46	1.50
29	K	217	CLA	CMC-C2C	-2.01	1.46	1.50
29	N	308	CLA	CMD-C2D	-2.01	1.46	1.50
29	a	831	CLA	CMC-C2C	-2.01	1.46	1.50
29	J	311	CLA	C3B-CAB	-2.01	1.43	1.47
29	D	309	CLA	CMD-C2D	-2.01	1.46	1.50
29	T	313	CLA	CMD-C2D	-2.01	1.46	1.50
29	a	803	CLA	CMC-C2C	-2.01	1.46	1.50
29	A	212	CLA	CMC-C2C	-2.01	1.46	1.50
29	I	216	CLA	CMC-C2C	-2.01	1.46	1.50
29	C	308	CLA	CMD-C2D	-2.01	1.46	1.50
29	A	216	CLA	CMC-C2C	-2.01	1.46	1.50
29	Q	308	CLA	CMC-C2C	-2.01	1.46	1.50
29	G	312	CLA	C3B-C2B	-2.01	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	728	BCR	C1-C6	-2.01	1.51	1.53
29	b	724	CLA	C3B-CAB	-2.01	1.43	1.47
29	T	309	CLA	CMD-C2D	-2.00	1.46	1.50
29	P	212	CLA	CMD-C2D	-2.00	1.46	1.50
29	a	809	CLA	CMC-C2C	-2.00	1.46	1.50
29	L	307	CLA	CMC-C2C	-2.00	1.46	1.50
29	H	310	CLA	CMD-C2D	-2.00	1.46	1.50
29	b	704	CLA	C3B-C2B	-2.00	1.37	1.40
29	b	725	CLA	C3B-C2B	-2.00	1.37	1.40
29	a	819	CLA	CMC-C2C	-2.00	1.46	1.50
29	a	829	CLA	CMC-C2C	-2.00	1.46	1.50
29	b	712	CLA	CMC-C2C	-2.00	1.46	1.50
29	G	301	CLA	CMC-C2C	-2.00	1.46	1.50
29	N	316	CLA	CMD-C2D	-2.00	1.46	1.50
29	B	310	CLA	CMC-C2C	-2.00	1.46	1.50
29	K	214	CLA	C3B-CAB	-2.00	1.43	1.47
38	T	306	UIX	C15-C20	-2.00	1.51	1.54
29	T	308	CLA	CMD-C2D	-2.00	1.46	1.50
36	h	202	DD6	C-C1	-2.00	1.46	1.50
29	G	316	CLA	CMC-C2C	-2.00	1.46	1.50
29	G	304	CLA	C3B-CAB	-2.00	1.43	1.47
38	N	306	UIX	C15-C20	-2.00	1.51	1.54

All (3687) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	308	CLA	O2D-CGD-CBD	26.55	158.46	111.27
29	b	736	CLA	O2D-CGD-CBD	26.54	158.43	111.27
29	I	209	CLA	O2D-CGD-CBD	26.47	158.31	111.27
29	I	212	CLA	O2D-CGD-CBD	26.29	157.99	111.27
29	a	831	CLA	O2D-CGD-CBD	26.25	157.91	111.27
29	L	307	CLA	O2D-CGD-CBD	26.21	157.84	111.27
29	a	830	CLA	O2D-CGD-CBD	26.14	157.72	111.27
29	I	208	CLA	O2D-CGD-CBD	25.92	157.32	111.27
29	G	316	CLA	O2D-CGD-CBD	25.79	157.10	111.27
29	I	209	CLA	O2D-CGD-O1D	-25.63	73.74	123.84
29	L	308	CLA	O2D-CGD-O1D	-25.60	73.79	123.84
29	a	831	CLA	O2D-CGD-O1D	-25.53	73.93	123.84
29	I	208	CLA	O2D-CGD-O1D	-25.48	74.02	123.84
29	L	307	CLA	O2D-CGD-O1D	-25.44	74.09	123.84
29	I	212	CLA	O2D-CGD-O1D	-25.39	74.19	123.84
29	b	736	CLA	O2D-CGD-O1D	-25.39	74.20	123.84

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	830	CLA	O2D-CGD-O1D	-25.39	74.20	123.84
29	G	316	CLA	O2D-CGD-O1D	-24.98	75.00	123.84
29	b	712	CLA	C4-C3-C5	-22.62	77.21	115.27
29	b	736	CLA	C4-C3-C5	-22.61	77.23	115.27
29	I	213	CLA	C4-C3-C5	-22.44	77.52	115.27
29	l	504	CLA	C4-C3-C5	-22.41	77.57	115.27
29	I	212	CLA	C4-C3-C5	-22.38	77.62	115.27
29	G	316	CLA	O1D-CGD-CBD	-20.71	82.11	124.48
29	N	313	CLA	O2D-CGD-O1D	-20.59	83.57	123.84
29	b	704	CLA	O2D-CGD-O1D	-20.50	83.76	123.84
29	I	208	CLA	O1D-CGD-CBD	-20.12	83.31	124.48
29	a	830	CLA	O1D-CGD-CBD	-20.02	83.53	124.48
29	L	307	CLA	O1D-CGD-CBD	-19.91	83.75	124.48
29	I	212	CLA	O1D-CGD-CBD	-19.88	83.80	124.48
29	a	831	CLA	O1D-CGD-CBD	-19.79	83.98	124.48
29	b	736	CLA	O1D-CGD-CBD	-19.67	84.23	124.48
29	I	209	CLA	O1D-CGD-CBD	-19.50	84.58	124.48
29	L	308	CLA	O1D-CGD-CBD	-19.46	84.67	124.48
29	I	212	CLA	C5-C3-C2	19.34	160.26	121.12
29	I	213	CLA	C5-C3-C2	19.31	160.18	121.12
29	l	504	CLA	C5-C3-C2	19.21	159.99	121.12
29	N	313	CLA	O1D-CGD-CBD	19.20	163.76	124.48
29	b	736	CLA	C5-C3-C2	19.14	159.84	121.12
29	b	712	CLA	C5-C3-C2	19.12	159.81	121.12
29	b	704	CLA	O1D-CGD-CBD	18.85	163.06	124.48
29	b	704	CLA	O2D-CGD-CBD	-17.90	79.46	111.27
29	N	313	CLA	O2D-CGD-CBD	-17.44	80.27	111.27
29	l	504	CLA	C4-C3-C2	-16.08	82.42	123.68
29	b	712	CLA	C4-C3-C2	-16.01	82.59	123.68
29	b	736	CLA	C4-C3-C2	-16.00	82.62	123.68
29	I	212	CLA	C4-C3-C2	-15.99	82.65	123.68
29	I	213	CLA	C4-C3-C2	-15.99	82.67	123.68
36	K	202	DD6	C21-C20-C19	11.94	127.71	114.28
38	F	305	UIX	O-C1-C3	10.77	121.47	113.38
36	G	305	DD6	C21-C20-C19	10.48	126.07	114.28
37	P	208	PID	C18-C19-C20	10.14	144.25	123.47
36	K	202	DD6	C21-C20-C15	-9.67	106.05	122.26
38	J	304	UIX	O-C1-C3	9.62	120.61	113.38
38	L	302	UIX	O-C1-C3	8.03	119.42	113.38
38	E	304	UIX	O-C1-C3	7.90	119.32	113.38
37	C	305	PID	C17-C16-C15	7.87	139.60	123.47
37	E	301	PID	C17-C16-C15	7.82	139.49	123.47

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	B	304	UIX	O-C1-C3	7.72	119.18	113.38
36	G	305	DD6	C21-C20-C15	-7.54	109.62	122.26
36	I	203	DD6	O1-C20-C19	7.44	118.97	113.38
29	P	215	CLA	C4A-NA-C1A	7.44	110.05	106.71
36	G	305	DD6	C3-C2-C1	-7.38	116.78	127.31
36	J	301	DD6	C3-C2-C1	-7.28	116.92	127.31
29	b	706	CLA	C4A-NA-C1A	7.22	109.95	106.71
29	H	313	CLA	C4A-NA-C1A	7.18	109.94	106.71
29	a	801	CLA	C4A-NA-C1A	7.13	109.91	106.71
38	L	302	UIX	C6-C1-C	-7.12	110.33	122.26
29	a	810	CLA	C4A-NA-C1A	7.12	109.91	106.71
29	j	104	CLA	C4A-NA-C1A	7.08	109.89	106.71
36	M	302	DD6	C3-C2-C1	-7.06	117.23	127.31
38	Q	305	UIX	C14-C13-C11	-7.05	117.25	127.31
29	G	304	CLA	C4A-NA-C1A	7.03	109.86	106.71
29	i	201	CLA	C4A-NA-C1A	7.01	109.86	106.71
38	A	203	UIX	C6-C1-C	-7.01	110.51	122.26
29	L	307	CLA	C4A-NA-C1A	7.00	109.85	106.71
29	P	217	CLA	C4A-NA-C1A	6.98	109.84	106.71
29	F	311	CLA	C4A-NA-C1A	6.98	109.84	106.71
29	F	310	CLA	C4A-NA-C1A	6.97	109.84	106.71
36	K	202	DD6	O1-C20-C19	-6.96	108.15	113.38
38	B	304	UIX	C6-C1-C	-6.96	110.59	122.26
29	N	313	CLA	C4A-NA-C1A	6.96	109.83	106.71
29	C	314	CLA	C4A-NA-C1A	6.96	109.83	106.71
29	b	736	CLA	C4A-NA-C1A	6.95	109.83	106.71
29	b	721	CLA	C4A-NA-C1A	6.95	109.83	106.71
38	E	304	UIX	C6-C1-C	-6.95	110.61	122.26
37	P	208	PID	C17-C16-C15	6.94	137.68	123.47
38	F	305	UIX	C34-C30-C26	-6.93	117.42	127.31
29	I	207	CLA	C4A-NA-C1A	6.92	109.82	106.71
29	T	309	CLA	C4A-NA-C1A	6.89	109.81	106.71
36	F	301	DD6	C9-C10-C11	-6.87	117.50	127.31
29	C	316	CLA	C4A-NA-C1A	6.84	109.78	106.71
29	F	315	CLA	C4A-NA-C1A	6.84	109.78	106.71
29	G	314	CLA	C4A-NA-C1A	6.83	109.78	106.71
36	h	202	DD6	C21-C20-C19	6.81	121.94	114.28
39	K	215	KC1	CHC-C4B-NB	6.80	130.70	124.45
29	F	316	CLA	C4A-NA-C1A	6.80	109.76	106.71
29	D	316	CLA	C4A-NA-C1A	6.80	109.76	106.71
29	l	504	CLA	C4A-NA-C1A	6.77	109.75	106.71
29	a	825	CLA	C4A-NA-C1A	6.77	109.75	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	314	CLA	C4A-NA-C1A	6.77	109.75	106.71
29	a	804	CLA	C4A-NA-C1A	6.76	109.75	106.71
29	A	206	CLA	C4A-NA-C1A	6.76	109.75	106.71
29	B	311	CLA	C4A-NA-C1A	6.76	109.75	106.71
29	T	314	CLA	C4A-NA-C1A	6.76	109.74	106.71
29	a	812	CLA	C4A-NA-C1A	6.76	109.74	106.71
29	I	216	CLA	C4A-NA-C1A	6.75	109.74	106.71
29	E	309	CLA	C4A-NA-C1A	6.74	109.74	106.71
29	l	501	CLA	C4A-NA-C1A	6.74	109.74	106.71
36	G	307	DD6	C3-C2-C1	-6.74	117.69	127.31
29	I	208	CLA	C4A-NA-C1A	6.74	109.73	106.71
29	J	309	CLA	C4A-NA-C1A	6.73	109.73	106.71
29	P	214	CLA	C4A-NA-C1A	6.73	109.73	106.71
29	b	701	CLA	C4A-NA-C1A	6.72	109.73	106.71
38	J	304	UIX	C6-C1-C	-6.72	111.00	122.26
29	b	702	CLA	C4A-NA-C1A	6.72	109.73	106.71
29	F	313	CLA	C4A-NA-C1A	6.72	109.73	106.71
29	Q	315	CLA	C4A-NA-C1A	6.72	109.73	106.71
38	T	306	UIX	C14-C13-C11	-6.72	117.72	127.31
29	B	314	CLA	C4A-NA-C1A	6.72	109.72	106.71
29	l	502	CLA	C4A-NA-C1A	6.71	109.72	106.71
29	I	201	CLA	C4A-NA-C1A	6.71	109.72	106.71
29	B	312	CLA	C4A-NA-C1A	6.71	109.72	106.71
29	Q	313	CLA	C4A-NA-C1A	6.71	109.72	106.71
29	L	310	CLA	C4A-NA-C1A	6.70	109.72	106.71
29	a	807	CLA	C4A-NA-C1A	6.70	109.72	106.71
29	B	307	CLA	C4A-NA-C1A	6.70	109.72	106.71
29	C	311	CLA	C4A-NA-C1A	6.70	109.72	106.71
38	Q	305	UIX	C6-C1-C	-6.69	111.05	122.26
29	C	313	CLA	C4A-NA-C1A	6.69	109.71	106.71
29	J	311	CLA	C4A-NA-C1A	6.68	109.71	106.71
29	a	815	CLA	C4A-NA-C1A	6.67	109.71	106.71
29	a	827	CLA	C4A-NA-C1A	6.67	109.71	106.71
29	L	313	CLA	C4A-NA-C1A	6.67	109.71	106.71
29	b	709	CLA	C4A-NA-C1A	6.67	109.70	106.71
29	E	308	CLA	C4A-NA-C1A	6.67	109.70	106.71
36	B	319	DD6	C3-C2-C1	-6.67	117.79	127.31
29	J	306	CLA	C4A-NA-C1A	6.66	109.70	106.71
29	M	313	CLA	C4A-NA-C1A	6.66	109.70	106.71
29	a	831	CLA	C4A-NA-C1A	6.66	109.70	106.71
29	a	828	CLA	C4A-NA-C1A	6.66	109.70	106.71
38	A	203	UIX	O-C1-C3	6.65	118.38	113.38

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	805	CLA	C4A-NA-C1A	6.65	109.69	106.71
29	D	308	CLA	C4A-NA-C1A	6.64	109.69	106.71
29	a	824	CLA	C4A-NA-C1A	6.63	109.69	106.71
29	b	722	CLA	C4A-NA-C1A	6.63	109.69	106.71
39	P	211	KC1	CHB-C1B-NB	6.63	130.54	124.45
29	A	215	CLA	C4A-NA-C1A	6.63	109.69	106.71
29	A	214	CLA	C4A-NA-C1A	6.62	109.68	106.71
29	M	308	CLA	C4A-NA-C1A	6.62	109.68	106.71
29	K	216	CLA	C4A-NA-C1A	6.62	109.68	106.71
29	I	217	CLA	C4A-NA-C1A	6.62	109.68	106.71
29	Q	310	CLA	C4A-NA-C1A	6.62	109.68	106.71
29	D	311	CLA	C4A-NA-C1A	6.61	109.68	106.71
29	J	308	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	N	311	CLA	C4A-NA-C1A	6.60	109.67	106.71
39	H	314	KC1	CHB-C1B-NB	6.60	130.52	124.45
29	b	705	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	a	806	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	A	207	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	H	310	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	a	817	CLA	C4A-NA-C1A	6.59	109.67	106.71
29	a	816	CLA	C4A-NA-C1A	6.59	109.67	106.71
29	K	217	CLA	C4A-NA-C1A	6.59	109.67	106.71
29	L	317	CLA	C4A-NA-C1A	6.58	109.67	106.71
29	b	707	CLA	C4A-NA-C1A	6.58	109.66	106.71
29	A	208	CLA	C4A-NA-C1A	6.58	109.66	106.71
29	K	207	CLA	C4A-NA-C1A	6.57	109.66	106.71
29	L	309	CLA	C4A-NA-C1A	6.57	109.66	106.71
29	F	307	CLA	C4A-NA-C1A	6.57	109.66	106.71
29	I	211	CLA	C4A-NA-C1A	6.55	109.65	106.71
29	E	305	CLA	C4A-NA-C1A	6.55	109.65	106.71
29	a	809	CLA	C4A-NA-C1A	6.54	109.65	106.71
29	h	201	CLA	C4A-NA-C1A	6.54	109.65	106.71
29	f	802	CLA	C4A-NA-C1A	6.54	109.65	106.71
29	i	203	CLA	C4A-NA-C1A	6.54	109.65	106.71
29	N	308	CLA	C4A-NA-C1A	6.54	109.65	106.71
29	M	306	CLA	C4A-NA-C1A	6.53	109.64	106.71
29	N	314	CLA	C4A-NA-C1A	6.53	109.64	106.71
29	Q	307	CLA	C4A-NA-C1A	6.53	109.64	106.71
29	B	316	CLA	C4A-NA-C1A	6.53	109.64	106.71
29	O	311	CLA	C4A-NA-C1A	6.53	109.64	106.71
29	I	214	CLA	C4A-NA-C1A	6.53	109.64	106.71
29	O	308	CLA	C4A-NA-C1A	6.53	109.64	106.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	713	CLA	C4A-NA-C1A	6.52	109.64	106.71
39	Q	314	KC1	CHB-C1B-NB	6.52	130.45	124.45
29	a	823	CLA	C4A-NA-C1A	6.52	109.64	106.71
29	P	212	CLA	C4A-NA-C1A	6.52	109.64	106.71
29	M	310	CLA	C4A-NA-C1A	6.51	109.64	106.71
32	i	204	BCR	C24-C23-C22	-6.51	116.40	126.23
36	G	308	DD6	C14-C13-C11	-6.51	115.43	125.53
29	G	316	CLA	C4A-NA-C1A	6.51	109.63	106.71
29	L	316	CLA	C4A-NA-C1A	6.51	109.63	106.71
29	A	212	CLA	C4A-NA-C1A	6.50	109.63	106.71
29	C	309	CLA	C4A-NA-C1A	6.50	109.63	106.71
29	K	218	CLA	C4A-NA-C1A	6.50	109.63	106.71
29	G	301	CLA	C4A-NA-C1A	6.50	109.63	106.71
29	C	308	CLA	C4A-NA-C1A	6.49	109.63	106.71
29	G	311	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	f	803	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	a	829	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	M	315	CLA	C4A-NA-C1A	6.48	109.62	106.71
29	H	307	CLA	C4A-NA-C1A	6.48	109.62	106.71
36	O	303	DD6	O1-C20-C19	6.48	118.25	113.38
29	K	210	CLA	C4A-NA-C1A	6.48	109.62	106.71
29	E	306	CLA	C4A-NA-C1A	6.48	109.62	106.71
29	a	818	CLA	C4A-NA-C1A	6.47	109.62	106.71
29	l	503	CLA	C4A-NA-C1A	6.47	109.62	106.71
39	N	312	KC1	CHC-C4B-NB	6.47	130.40	124.45
36	K	221	DD6	C9-C10-C11	-6.47	118.07	127.31
36	K	221	DD6	O1-C20-C19	6.46	118.24	113.38
29	T	316	CLA	C4A-NA-C1A	6.46	109.61	106.71
29	a	813	CLA	C4A-NA-C1A	6.46	109.61	106.71
29	i	202	CLA	C4A-NA-C1A	6.46	109.61	106.71
29	b	710	CLA	C4A-NA-C1A	6.46	109.61	106.71
29	N	316	CLA	C4A-NA-C1A	6.45	109.61	106.71
29	D	309	CLA	C4A-NA-C1A	6.45	109.61	106.71
36	I	205	DD6	O1-C20-C21	6.45	122.78	115.06
29	D	312	CLA	C4A-NA-C1A	6.45	109.61	106.71
29	O	316	CLA	C4A-NA-C1A	6.45	109.61	106.71
29	Q	312	CLA	C4A-NA-C1A	6.45	109.61	106.71
29	G	313	CLA	C4A-NA-C1A	6.45	109.60	106.71
36	J	301	DD6	C9-C10-C11	-6.44	118.11	127.31
29	A	218	CLA	C4A-NA-C1A	6.44	109.60	106.71
29	Q	308	CLA	C4A-NA-C1A	6.44	109.60	106.71
29	G	319	CLA	C4A-NA-C1A	6.44	109.60	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	308	CLA	C4A-NA-C1A	6.44	109.60	106.71
39	N	310	KC1	CHB-C1B-NB	6.44	130.37	124.45
29	K	209	CLA	C4A-NA-C1A	6.44	109.60	106.71
39	H	311	KC1	CHC-C4B-NB	6.44	130.37	124.45
29	l	508	CLA	C4A-NA-C1A	6.43	109.60	106.71
32	m	103	BCR	C15-C14-C13	-6.43	118.13	127.31
39	G	318	KC1	CHC-C4B-NB	6.43	130.36	124.45
29	P	210	CLA	C4A-NA-C1A	6.43	109.60	106.71
39	M	312	KC1	CHB-C1B-NB	6.43	130.36	124.45
29	A	216	CLA	C4A-NA-C1A	6.43	109.59	106.71
39	L	306	KC1	CHC-C4B-NB	6.42	130.36	124.45
39	A	213	KC1	CHB-C1B-NB	6.41	130.35	124.45
29	A	209	CLA	C4A-NA-C1A	6.41	109.59	106.71
29	T	308	CLA	C4A-NA-C1A	6.41	109.59	106.71
38	O	306	UIX	C14-C13-C11	-6.41	118.17	127.31
29	a	826	CLA	C4A-NA-C1A	6.40	109.58	106.71
29	F	312	CLA	C4A-NA-C1A	6.40	109.58	106.71
29	E	315	CLA	C4A-NA-C1A	6.39	109.58	106.71
29	J	313	CLA	C4A-NA-C1A	6.39	109.58	106.71
39	E	312	KC1	CHB-C1B-NB	6.39	130.33	124.45
29	G	312	CLA	C4A-NA-C1A	6.39	109.58	106.71
29	E	313	CLA	C4A-NA-C1A	6.39	109.58	106.71
39	H	309	KC1	CHB-C1B-NB	6.39	130.32	124.45
37	T	317	PID	C17-C16-C15	6.38	136.55	123.47
29	b	725	CLA	C4A-NA-C1A	6.38	109.57	106.71
29	B	315	CLA	C4A-NA-C1A	6.38	109.57	106.71
29	T	311	CLA	C4A-NA-C1A	6.38	109.57	106.71
36	E	302	DD6	C14-C13-C11	-6.38	115.63	125.53
39	O	315	KC1	CHB-C1B-NB	6.38	130.32	124.45
29	b	714	CLA	C4A-NA-C1A	6.37	109.57	106.71
29	a	821	CLA	C4A-NA-C1A	6.37	109.57	106.71
29	b	716	CLA	C4A-NA-C1A	6.36	109.56	106.71
29	L	308	CLA	C4A-NA-C1A	6.36	109.56	106.71
39	A	205	KC1	CHB-C1B-NB	6.36	130.30	124.45
29	L	315	CLA	C4A-NA-C1A	6.36	109.56	106.71
29	b	708	CLA	C4A-NA-C1A	6.35	109.56	106.71
39	H	309	KC1	CHC-C4B-NB	6.35	130.29	124.45
29	L	312	CLA	C4A-NA-C1A	6.35	109.56	106.71
39	E	307	KC1	CHC-C4B-NB	6.35	130.29	124.45
29	l	509	CLA	C4A-NA-C1A	6.35	109.56	106.71
29	f	805	CLA	C4A-NA-C1A	6.34	109.56	106.71
29	b	712	CLA	C4A-NA-C1A	6.34	109.56	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	308	CLA	C4A-NA-C1A	6.34	109.56	106.71
29	B	309	CLA	C4A-NA-C1A	6.34	109.56	106.71
39	C	310	KC1	CHB-C1B-NB	6.34	130.28	124.45
29	b	731	CLA	C4A-NA-C1A	6.33	109.55	106.71
29	B	306	CLA	C4A-NA-C1A	6.33	109.55	106.71
39	B	313	KC1	CHB-C1B-NB	6.33	130.27	124.45
29	B	310	CLA	C4A-NA-C1A	6.33	109.55	106.71
38	O	306	UIX	C6-C1-C	-6.33	111.66	122.26
29	T	313	CLA	C4A-NA-C1A	6.33	109.55	106.71
32	m	103	BCR	C7-C8-C9	-6.33	116.68	126.23
29	a	830	CLA	C4A-NA-C1A	6.32	109.55	106.71
29	b	720	CLA	C4A-NA-C1A	6.32	109.55	106.71
29	D	313	CLA	C4A-NA-C1A	6.32	109.55	106.71
29	b	715	CLA	C4A-NA-C1A	6.32	109.55	106.71
39	T	312	KC1	CHC-C4B-NB	6.32	130.26	124.45
29	b	726	CLA	C4A-NA-C1A	6.31	109.55	106.71
29	K	208	CLA	C4A-NA-C1A	6.31	109.54	106.71
29	J	305	CLA	C4A-NA-C1A	6.31	109.54	106.71
29	B	308	CLA	C4A-NA-C1A	6.31	109.54	106.71
39	O	312	KC1	O2D-CGD-CBD	6.31	122.47	111.27
39	C	312	KC1	CHC-C4B-NB	6.30	130.25	124.45
29	G	302	CLA	C4A-NA-C1A	6.30	109.54	106.71
32	a	838	BCR	C16-C17-C18	-6.30	118.32	127.31
29	b	718	CLA	C4A-NA-C1A	6.29	109.54	106.71
39	F	309	KC1	CHC-C4B-NB	6.29	130.23	124.45
39	J	312	KC1	CHB-C1B-NB	6.29	130.23	124.45
39	Q	309	KC1	CHC-C4B-NB	6.28	130.23	124.45
39	I	215	KC1	CHB-C1B-NB	6.27	130.22	124.45
29	I	212	CLA	C4A-NA-C1A	6.27	109.53	106.71
29	P	209	CLA	C4A-NA-C1A	6.26	109.52	106.71
29	E	310	CLA	C4A-NA-C1A	6.26	109.52	106.71
29	E	311	CLA	C4A-NA-C1A	6.26	109.52	106.71
29	H	312	CLA	C4A-NA-C1A	6.25	109.51	106.71
29	a	822	CLA	C4A-NA-C1A	6.24	109.51	106.71
39	L	314	KC1	CHB-C1B-NB	6.24	130.19	124.45
29	I	213	CLA	C4A-NA-C1A	6.24	109.51	106.71
39	L	306	KC1	CHB-C1B-NB	6.24	130.19	124.45
39	N	312	KC1	CHB-C1B-NB	6.24	130.19	124.45
29	a	814	CLA	C4A-NA-C1A	6.24	109.51	106.71
39	D	310	KC1	CHB-C1B-NB	6.24	130.19	124.45
29	b	723	CLA	C4A-NA-C1A	6.23	109.51	106.71
29	K	211	CLA	C4A-NA-C1A	6.23	109.51	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Q	309	KC1	CHB-C1B-NB	6.23	130.18	124.45
39	D	315	KC1	CHB-C1B-NB	6.23	130.18	124.45
29	l	510	CLA	C4A-NA-C1A	6.23	109.50	106.71
29	H	315	CLA	C4A-NA-C1A	6.22	109.50	106.71
39	C	315	KC1	CHB-C1B-NB	6.22	130.17	124.45
39	P	216	KC1	CHB-C1B-NB	6.22	130.17	124.45
39	Q	314	KC1	CHC-C4B-NB	6.22	130.17	124.45
38	F	305	UIX	C6-C1-C	-6.22	111.84	122.26
39	F	309	KC1	CHB-C1B-NB	6.21	130.16	124.45
39	F	314	KC1	CHC-C4B-NB	6.21	130.16	124.45
29	I	209	CLA	C4A-NA-C1A	6.20	109.49	106.71
29	K	212	CLA	C4A-NA-C1A	6.20	109.49	106.71
32	l	507	BCR	C15-C14-C13	-6.20	118.46	127.31
29	a	811	CLA	C4A-NA-C1A	6.20	109.49	106.71
38	Q	305	UIX	C7-C10-C11	-6.20	115.92	125.53
39	P	216	KC1	CHC-C4B-NB	6.20	130.15	124.45
39	O	310	KC1	CHB-C1B-NB	6.19	130.15	124.45
29	G	317	CLA	C4A-NA-C1A	6.19	109.49	106.71
39	N	310	KC1	CHC-C4B-NB	6.18	130.14	124.45
29	K	213	CLA	C4A-NA-C1A	6.18	109.48	106.71
39	M	312	KC1	CHC-C4B-NB	6.18	130.13	124.45
39	B	313	KC1	CHC-C4B-NB	6.18	130.13	124.45
39	D	310	KC1	CHC-C4B-NB	6.17	130.13	124.45
29	a	837	CLA	C4A-NA-C1A	6.17	109.48	106.71
36	G	307	DD6	C-C1-C2	-6.17	114.28	122.92
39	A	205	KC1	CHC-C4B-NB	6.17	130.12	124.45
29	a	808	CLA	C4A-NA-C1A	6.16	109.47	106.71
29	I	210	CLA	C4A-NA-C1A	6.16	109.47	106.71
29	M	307	CLA	C4A-NA-C1A	6.16	109.47	106.71
29	O	309	CLA	C4A-NA-C1A	6.16	109.47	106.71
39	F	314	KC1	CHB-C1B-NB	6.16	130.11	124.45
39	H	314	KC1	CHC-C4B-NB	6.14	130.10	124.45
39	M	305	KC1	CHB-C1B-NB	6.14	130.10	124.45
39	T	315	KC1	CHB-C1B-NB	6.14	130.10	124.45
39	N	315	KC1	CHB-C1B-NB	6.14	130.09	124.45
39	C	310	KC1	CHC-C4B-NB	6.13	130.09	124.45
36	C	303	DD6	C4-C5-C6	-6.13	118.56	127.31
39	G	315	KC1	CHB-C1B-NB	6.13	130.09	124.45
29	a	819	CLA	C4A-NA-C1A	6.12	109.46	106.71
29	A	211	CLA	C4A-NA-C1A	6.12	109.46	106.71
39	G	318	KC1	CHB-C1B-NB	6.12	130.08	124.45
39	Q	311	KC1	CHC-C4B-NB	6.12	130.08	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	302	DD6	C4-C5-C6	-6.12	118.58	127.31
39	O	315	KC1	CHC-C4B-NB	6.11	130.07	124.45
39	T	310	KC1	CHB-C1B-NB	6.11	130.07	124.45
39	T	315	KC1	CHC-C4B-NB	6.11	130.07	124.45
37	P	206	PID	C17-C16-C15	6.10	135.97	123.47
38	C	306	UIX	C14-C13-C11	-6.10	118.61	127.31
29	b	717	CLA	C4A-NA-C1A	6.10	109.45	106.71
39	O	310	KC1	CHC-C4B-NB	6.10	130.06	124.45
39	A	213	KC1	CHC-C4B-NB	6.09	130.05	124.45
29	J	307	CLA	C4A-NA-C1A	6.09	109.44	106.71
39	E	307	KC1	CHB-C1B-NB	6.09	130.05	124.45
38	P	207	UIX	O-C1-C3	6.09	117.96	113.38
39	D	315	KC1	CHC-C4B-NB	6.09	130.05	124.45
29	A	217	CLA	C4A-NA-C1A	6.09	109.44	106.71
29	N	309	CLA	C4A-NA-C1A	6.09	109.44	106.71
39	M	305	KC1	CHC-C4B-NB	6.08	130.04	124.45
39	I	215	KC1	CHC-C4B-NB	6.08	130.04	124.45
29	a	820	CLA	C4A-NA-C1A	6.08	109.44	106.71
29	b	719	CLA	C4A-NA-C1A	6.08	109.44	106.71
39	H	311	KC1	CHB-C1B-NB	6.08	130.04	124.45
39	C	312	KC1	CHB-C1B-NB	6.07	130.03	124.45
29	L	311	CLA	C4A-NA-C1A	6.07	109.43	106.71
39	C	315	KC1	CHC-C4B-NB	6.07	130.03	124.45
29	O	313	CLA	C4A-NA-C1A	6.05	109.43	106.71
38	Q	305	UIX	O-C1-C6	6.05	122.31	115.06
29	J	310	CLA	C4A-NA-C1A	6.05	109.42	106.71
39	P	213	KC1	CHC-C4B-NB	6.04	130.01	124.45
39	T	312	KC1	CHB-C1B-NB	6.03	130.00	124.45
29	M	314	CLA	C4A-NA-C1A	6.03	109.42	106.71
29	M	311	CLA	C4A-NA-C1A	6.01	109.41	106.71
39	O	312	KC1	CHC-C4B-NB	6.00	129.97	124.45
29	b	724	CLA	C4A-NA-C1A	5.99	109.40	106.71
38	T	306	UIX	C6-C1-C	-5.99	112.22	122.26
36	G	308	DD6	C9-C10-C11	-5.99	118.76	127.31
29	K	214	CLA	C4A-NA-C1A	5.99	109.40	106.71
29	E	314	CLA	C4A-NA-C1A	5.99	109.40	106.71
39	L	314	KC1	CHC-C4B-NB	5.98	129.95	124.45
39	K	215	KC1	CHB-C1B-NB	5.97	129.94	124.45
36	P	204	DD6	O1-C20-C19	-5.96	108.90	113.38
38	N	306	UIX	C6-C1-C	-5.95	112.29	122.26
39	N	315	KC1	CHC-C4B-NB	5.94	129.92	124.45
29	b	704	CLA	C4A-NA-C1A	5.94	109.38	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	J	303	DD6	C9-C10-C11	-5.94	118.84	127.31
36	P	204	DD6	C4-C5-C6	-5.94	118.84	127.31
38	N	306	UIX	O-C1-C3	5.93	117.84	113.38
39	O	312	KC1	CHB-C1B-NB	5.91	129.89	124.45
38	C	306	UIX	C6-C1-C	-5.91	112.36	122.26
32	i	204	BCR	C20-C21-C22	-5.90	118.89	127.31
36	D	301	DD6	C3-C2-C1	-5.90	118.89	127.31
37	F	302	PID	C18-C19-C20	5.88	135.52	123.47
39	T	310	KC1	CHC-C4B-NB	5.88	129.86	124.45
38	C	306	UIX	O-C1-C3	5.88	117.80	113.38
29	l	505	CLA	C4A-NA-C1A	5.88	109.35	106.71
39	P	213	KC1	CHB-C1B-NB	5.87	129.85	124.45
38	P	207	UIX	C14-C13-C11	-5.86	118.94	127.31
29	A	210	CLA	C4A-NA-C1A	5.86	109.34	106.71
39	G	315	KC1	CHC-C4B-NB	5.84	129.82	124.45
29	a	803	CLA	C4A-NA-C1A	5.83	109.33	106.71
39	J	312	KC1	CHC-C4B-NB	5.83	129.81	124.45
29	a	802	CLA	C4A-NA-C1A	5.82	109.32	106.71
29	b	711	CLA	C4A-NA-C1A	5.82	109.32	106.71
37	H	304	PID	C17-C16-C15	5.81	135.38	123.47
29	b	703	CLA	C4A-NA-C1A	5.81	109.32	106.71
32	m	103	BCR	C11-C10-C9	-5.81	119.03	127.31
39	E	312	KC1	CHC-C4B-NB	5.80	129.78	124.45
38	T	306	UIX	C36-C35-C32	-5.79	119.05	127.31
39	P	211	KC1	CHC-C4B-NB	5.77	129.76	124.45
36	O	303	DD6	C4-C5-C6	-5.76	119.09	127.31
36	G	306	DD6	C9-C10-C11	-5.75	119.10	127.31
36	T	303	DD6	C9-C10-C11	-5.75	119.11	127.31
32	b	728	BCR	C24-C23-C22	-5.75	117.55	126.23
39	Q	311	KC1	CHB-C1B-NB	5.74	129.73	124.45
29	M	309	CLA	C4A-NA-C1A	5.72	109.28	106.71
36	A	201	DD6	C9-C10-C11	-5.70	119.17	127.31
37	P	208	PID	C17-C18-C19	5.70	137.50	124.81
32	i	204	BCR	C16-C17-C18	-5.69	119.19	127.31
36	J	303	DD6	C3-C2-C1	-5.67	119.22	127.31
38	P	207	UIX	C6-C1-C	-5.65	112.80	122.26
37	T	307	PID	C18-C19-C20	5.64	135.03	123.47
38	N	306	UIX	C37-C39-C40	-5.62	119.29	127.31
38	O	306	UIX	C37-C39-C40	-5.62	119.29	127.31
38	O	306	UIX	C7-C10-C11	-5.62	116.81	125.53
38	T	306	UIX	C7-C10-C11	-5.62	116.82	125.53
36	D	304	DD6	C4-C5-C6	-5.61	119.30	127.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	301	PID	C18-C19-C20	5.59	134.92	123.47
36	F	303	DD6	C4-C5-C6	-5.58	119.35	127.31
37	C	301	PID	C17-C16-C15	5.57	134.88	123.47
32	f	801	BCR	C20-C21-C22	-5.55	119.39	127.31
37	O	301	PID	C17-C16-C15	5.54	134.83	123.47
29	O	314	CLA	C4A-NA-C1A	5.54	109.19	106.71
32	f	801	BCR	C15-C14-C13	-5.52	119.43	127.31
38	T	306	UIX	C37-C39-C40	-5.52	119.44	127.31
37	H	305	PID	C17-C16-C15	5.50	134.75	123.47
36	K	206	DD6	C3-C2-C1	-5.50	119.46	127.31
36	G	307	DD6	C9-C10-C11	-5.49	119.48	127.31
32	b	728	BCR	C20-C21-C22	-5.48	119.49	127.31
38	F	305	UIX	C14-C13-C11	-5.48	119.49	127.31
38	T	306	UIX	C34-C30-C26	-5.47	119.50	127.31
38	T	306	UIX	O-C1-C3	5.46	117.49	113.38
36	I	204	DD6	C3-C2-C1	-5.46	119.52	127.31
36	F	303	DD6	O1-C20-C19	5.46	117.48	113.38
36	D	304	DD6	C3-C2-C1	-5.45	119.53	127.31
37	O	301	PID	CM4-C14-C15	-5.45	115.29	122.92
32	f	804	BCR	C15-C14-C13	-5.45	119.53	127.31
36	G	307	DD6	C4-C5-C6	-5.45	119.53	127.31
38	Q	305	UIX	C34-C30-C26	-5.43	119.55	127.31
36	M	303	DD6	C9-C10-C11	-5.42	119.57	127.31
38	C	306	UIX	C7-C10-C11	-5.40	117.15	125.53
36	K	202	DD6	C3-C2-C1	-5.39	119.61	127.31
37	T	317	PID	CM4-C14-C15	-5.38	115.38	122.92
38	O	306	UIX	O-C1-C6	5.37	121.49	115.06
36	G	306	DD6	C3-C2-C1	-5.36	119.67	127.31
37	H	304	PID	CM4-C14-C15	-5.36	115.42	122.92
36	I	203	DD6	C3-C2-C1	-5.35	119.67	127.31
39	G	315	KC1	O2D-CGD-CBD	5.34	120.76	111.27
36	K	203	DD6	C9-C10-C11	-5.29	119.75	127.31
32	i	204	BCR	C7-C8-C9	-5.29	118.24	126.23
38	N	306	UIX	C34-C30-C26	-5.28	119.77	127.31
36	I	205	DD6	C4-C5-C6	-5.27	119.78	127.31
36	B	319	DD6	C21-C20-C19	5.27	120.21	114.28
36	m	101	DD6	C3-C2-C1	-5.27	119.79	127.31
37	P	208	PID	CM4-C14-C15	-5.26	115.56	122.92
37	P	205	PID	C17-C16-C15	5.25	134.23	123.47
36	L	305	DD6	C21-C20-C19	5.23	120.17	114.28
39	F	309	KC1	O2D-CGD-CBD	5.23	120.55	111.27
36	B	305	DD6	C3-C2-C1	-5.22	119.86	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	P	204	DD6	C21-C20-C19	5.19	120.12	114.28
36	I	205	DD6	C3-C2-C1	-5.18	119.92	127.31
37	O	304	PID	CM4-C14-C15	-5.18	115.67	122.92
37	C	301	PID	CM4-C14-C15	-5.18	115.67	122.92
32	a	834	BCR	C16-C17-C18	-5.18	119.92	127.31
36	J	302	DD6	C21-C20-C15	-5.18	113.59	122.26
39	Q	311	KC1	O2D-CGD-CBD	5.18	120.46	111.27
36	G	305	DD6	C4-C5-C6	-5.17	119.93	127.31
37	F	304	PID	CM4-C14-C15	-5.17	115.68	122.92
36	L	304	DD6	C3-C2-C1	-5.16	119.95	127.31
38	N	306	UIX	C14-C13-C11	-5.15	119.96	127.31
36	A	204	DD6	C21-C20-C19	5.12	120.04	114.28
36	M	301	DD6	C3-C2-C1	-5.12	120.00	127.31
36	M	303	DD6	C4-C5-C6	-5.12	120.01	127.31
36	M	303	DD6	C3-C2-C1	-5.11	120.02	127.31
39	C	310	KC1	O2D-CGD-CBD	5.11	120.34	111.27
32	a	834	BCR	C15-C14-C13	-5.09	120.05	127.31
38	T	306	UIX	O-C1-C6	5.07	121.13	115.06
36	T	303	DD6	C4-C5-C6	-5.07	120.07	127.31
36	A	201	DD6	C3-C2-C1	-5.07	120.08	127.31
36	I	205	DD6	C9-C10-C11	-5.05	120.11	127.31
32	a	835	BCR	C15-C14-C13	-5.04	120.11	127.31
36	D	304	DD6	C21-C20-C19	5.03	119.94	114.28
36	m	101	DD6	C21-C20-C19	5.02	119.93	114.28
38	Q	305	UIX	C6-C1-C3	5.02	119.92	114.28
38	F	305	UIX	C36-C35-C32	-5.01	120.15	127.31
36	K	206	DD6	C21-C20-C19	5.01	119.91	114.28
36	K	221	DD6	C4-C5-C6	-5.01	120.17	127.31
36	K	221	DD6	C3-C2-C1	-5.00	120.18	127.31
37	N	304	PID	CM4-C14-C15	-4.99	115.93	122.92
37	P	205	PID	CM4-C14-C15	-4.99	115.93	122.92
36	J	302	DD6	C21-C20-C19	4.99	119.89	114.28
36	B	302	DD6	C21-C20-C19	4.99	119.89	114.28
38	P	207	UIX	C34-C30-C26	-4.99	120.19	127.31
36	A	201	DD6	C21-C20-C19	4.98	119.88	114.28
36	h	202	DD6	C4-C5-C6	-4.97	120.21	127.31
37	O	304	PID	C17-C16-C15	4.97	133.65	123.47
32	b	735	BCR	C24-C23-C22	-4.97	118.73	126.23
36	I	202	DD6	C3-C2-C1	-4.97	120.22	127.31
36	B	301	DD6	C21-C20-C19	4.97	119.87	114.28
37	Q	304	PID	C18-C19-C20	4.96	133.64	123.47
38	B	304	UIX	O2-C27-C31	4.96	120.22	111.09

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	D	315	KC1	O2D-CGD-CBD	4.96	120.08	111.27
36	J	302	DD6	C3-C2-C1	-4.96	120.24	127.31
36	I	204	DD6	C9-C10-C11	-4.96	120.24	127.31
37	T	305	PID	C18-C19-C20	4.95	133.62	123.47
36	E	302	DD6	C9-C10-C11	-4.95	120.25	127.31
32	i	204	BCR	C11-C10-C9	-4.94	120.26	127.31
36	H	303	DD6	C4-C5-C6	-4.94	120.26	127.31
38	E	304	UIX	O2-C27-C31	4.93	120.17	111.09
37	H	301	PID	CM4-C14-C15	-4.93	116.02	122.92
36	I	202	DD6	C21-C20-C19	4.93	119.82	114.28
39	L	314	KC1	O2D-CGD-CBD	4.92	120.02	111.27
38	P	207	UIX	O-C1-C6	4.92	120.95	115.06
38	C	306	UIX	C37-C39-C40	-4.91	120.30	127.31
39	C	312	KC1	O2D-CGD-CBD	4.91	120.00	111.27
39	K	215	KC1	O2D-CGD-CBD	4.91	120.00	111.27
36	G	305	DD6	C9-C10-C11	-4.91	120.31	127.31
32	a	835	BCR	C20-C21-C22	-4.90	120.31	127.31
39	J	312	KC1	O2D-CGD-CBD	4.90	119.97	111.27
36	A	202	DD6	C21-C20-C19	4.90	119.79	114.28
39	M	305	KC1	O2D-CGD-CBD	4.90	119.97	111.27
39	Q	314	KC1	O2D-CGD-CBD	4.89	119.96	111.27
39	I	215	KC1	O2D-CGD-CBD	4.89	119.96	111.27
39	D	310	KC1	O2D-CGD-CBD	4.89	119.95	111.27
39	P	216	KC1	O2D-CGD-CBD	4.89	119.95	111.27
37	T	304	PID	CM4-C14-C15	-4.89	116.08	122.92
36	B	305	DD6	C21-C20-C19	4.88	119.77	114.28
36	G	305	DD6	C24-C1-C2	4.88	126.43	118.94
36	L	301	DD6	C21-C20-C19	4.88	119.77	114.28
39	P	211	KC1	O2D-CGD-CBD	4.88	119.93	111.27
32	a	835	BCR	C16-C17-C18	-4.88	120.35	127.31
36	L	305	DD6	C4-C5-C6	-4.87	120.36	127.31
36	K	202	DD6	C4-C5-C6	-4.87	120.36	127.31
39	T	312	KC1	O2D-CGD-CBD	4.86	119.91	111.27
29	a	802	CLA	CMB-C2B-C1B	-4.86	120.99	128.46
37	N	301	PID	C17-C16-C15	4.86	133.43	123.47
29	b	718	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
36	T	303	DD6	C21-C20-C19	4.85	119.74	114.28
39	O	310	KC1	O2D-CGD-CBD	4.85	119.89	111.27
38	F	305	UIX	C7-C10-C11	-4.85	118.00	125.53
37	Q	303	PID	CM4-C14-C15	-4.85	116.14	122.92
36	K	205	DD6	C21-C20-C19	4.84	119.72	114.28
39	M	312	KC1	O2D-CGD-CBD	4.84	119.86	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	301	PID	CM4-C14-C15	-4.83	116.16	122.92
38	N	306	UIX	O-C1-C6	4.82	120.83	115.06
39	H	314	KC1	O2D-CGD-CBD	4.81	119.81	111.27
38	C	306	UIX	O-C1-C6	4.80	120.81	115.06
38	L	302	UIX	C34-C30-C26	-4.80	120.46	127.31
37	C	304	PID	C17-C16-C15	4.80	133.30	123.47
37	H	301	PID	C17-C16-C15	4.80	133.30	123.47
36	K	204	DD6	C9-C10-C11	-4.78	120.48	127.31
36	K	203	DD6	C21-C20-C19	4.78	119.65	114.28
36	D	304	DD6	C9-C10-C11	-4.78	120.50	127.31
36	F	303	DD6	C3-C2-C1	-4.77	120.50	127.31
39	Q	309	KC1	O2D-CGD-CBD	4.77	119.75	111.27
37	C	304	PID	CM4-C14-C15	-4.77	116.24	122.92
36	J	302	DD6	C4-C5-C6	-4.76	120.52	127.31
36	G	306	DD6	C4-C5-C6	-4.75	120.53	127.31
36	L	301	DD6	C3-C2-C1	-4.75	120.53	127.31
38	N	306	UIX	C36-C35-C32	-4.75	120.53	127.31
37	Q	303	PID	C17-C16-C15	4.75	133.20	123.47
32	b	728	BCR	C16-C17-C18	-4.73	120.55	127.31
37	Q	306	PID	CM4-C14-C15	-4.73	116.29	122.92
36	B	301	DD6	C3-C2-C1	-4.73	120.56	127.31
38	F	305	UIX	C37-C39-C40	-4.73	120.56	127.31
38	P	207	UIX	C37-C39-C40	-4.73	120.56	127.31
39	A	213	KC1	O2D-CGD-CBD	4.73	119.67	111.27
39	N	310	KC1	O2D-CGD-CBD	4.73	119.67	111.27
32	l	506	BCR	C28-C27-C26	-4.73	105.63	114.08
36	D	301	DD6	C14-C13-C11	4.73	132.87	125.53
36	L	304	DD6	C9-C10-C11	-4.72	120.57	127.31
39	N	312	KC1	O2D-CGD-CBD	4.72	119.65	111.27
37	G	309	PID	CM4-C14-C15	-4.71	116.32	122.92
32	a	838	BCR	C15-C14-C13	-4.71	120.59	127.31
36	I	203	DD6	C9-C10-C11	-4.71	120.59	127.31
36	I	203	DD6	C21-C20-C19	4.71	119.58	114.28
36	G	306	DD6	C21-C20-C19	4.71	119.58	114.28
36	B	303	DD6	C21-C20-C19	4.70	119.57	114.28
38	Q	305	UIX	C37-C39-C40	-4.70	120.60	127.31
32	b	729	BCR	C3-C4-C5	-4.68	105.72	114.08
37	P	203	PID	C18-C19-C20	4.68	133.05	123.47
36	N	303	DD6	C21-C20-C19	4.68	119.54	114.28
39	G	318	KC1	O2D-CGD-CBD	4.67	119.57	111.27
39	B	313	KC1	O2D-CGD-CBD	4.67	119.57	111.27
39	T	315	KC1	O2D-CGD-CBD	4.67	119.57	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	N	315	KC1	O2D-CGD-CBD	4.67	119.57	111.27
35	B	318	DGD	O2G-C1B-C2B	4.67	121.56	111.50
36	I	206	DD6	C3-C2-C1	-4.66	120.65	127.31
36	I	206	DD6	C21-C20-C19	4.66	119.53	114.28
38	O	306	UIX	O-C1-C3	4.66	116.88	113.38
36	G	308	DD6	C3-C2-C1	-4.65	120.67	127.31
38	Q	305	UIX	C36-C35-C32	-4.65	120.67	127.31
36	K	202	DD6	C15-C14-C13	-4.65	116.17	125.99
29	O	313	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
38	A	203	UIX	O-C1-C6	4.64	120.62	115.06
35	b	733	DGD	O2G-C1B-C2B	4.64	121.50	111.50
32	f	804	BCR	C11-C10-C9	-4.64	120.69	127.31
36	B	302	DD6	C4-C5-C6	-4.64	120.69	127.31
38	O	306	UIX	C34-C30-C26	-4.64	120.69	127.31
38	T	306	UIX	O2-C27-C31	4.63	119.61	111.09
37	D	307	PID	C17-C16-C15	4.62	132.95	123.47
37	T	301	PID	CM4-C14-C15	-4.62	116.45	122.92
36	O	303	DD6	O1-C20-C21	4.62	120.59	115.06
36	Q	302	DD6	C21-C20-C19	4.62	119.47	114.28
32	b	728	BCR	C33-C5-C6	-4.61	119.35	124.53
37	N	304	PID	C17-C16-C15	4.61	132.93	123.47
36	Q	302	DD6	C4-C5-C6	-4.61	120.73	127.31
38	P	207	UIX	C7-C10-C11	-4.60	118.39	125.53
37	G	303	PID	C17-C16-C15	4.60	132.91	123.47
37	F	302	PID	CM4-C14-C15	-4.60	116.48	122.92
37	D	307	PID	C18-C19-C20	4.60	132.90	123.47
32	m	103	BCR	C16-C17-C18	-4.60	120.75	127.31
39	L	306	KC1	O2D-CGD-CBD	4.59	119.42	111.27
36	M	304	DD6	C3-C2-C1	-4.58	120.77	127.31
39	E	307	KC1	O2D-CGD-CBD	4.58	119.41	111.27
36	I	206	DD6	O1-C20-C19	-4.58	109.94	113.38
37	O	305	PID	CM4-C14-C15	-4.58	116.51	122.92
38	O	306	UIX	O2-C27-C31	4.58	119.51	111.09
37	E	301	PID	C16-C15-C14	4.58	133.84	127.31
36	I	203	DD6	C4-C5-C6	-4.57	120.78	127.31
38	O	306	UIX	C6-C1-C3	4.57	119.42	114.28
36	E	303	DD6	C21-C20-C19	4.57	119.42	114.28
36	D	301	DD6	O1-C20-C21	-4.56	109.59	115.06
38	C	306	UIX	C34-C30-C26	-4.56	120.80	127.31
38	J	304	UIX	C14-C23-C26	-4.56	113.61	126.42
37	T	301	PID	C18-C19-C20	4.56	132.81	123.47
38	C	306	UIX	O2-C27-C31	4.55	119.46	111.09

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	307	PID	CM4-C14-C15	-4.55	116.55	122.92
36	A	201	DD6	C14-C13-C11	-4.55	118.48	125.53
37	G	310	PID	C18-C19-C20	4.54	132.78	123.47
39	C	315	KC1	O2D-CGD-CBD	4.53	119.32	111.27
37	C	302	PID	CM4-C14-C15	-4.53	116.58	122.92
36	h	202	DD6	C3-C2-C1	-4.52	120.86	127.31
38	J	304	UIX	C34-C30-C26	-4.52	120.86	127.31
37	O	305	PID	C6-C7-C8	4.52	135.54	125.99
37	H	305	PID	C6-C7-C8	4.52	135.54	125.99
37	Q	301	PID	CM4-C14-C15	-4.51	116.60	122.92
39	F	314	KC1	O2D-CGD-CBD	4.51	119.29	111.27
39	T	310	KC1	O2D-CGD-CBD	4.51	119.29	111.27
38	E	304	UIX	C34-C30-C26	-4.51	120.88	127.31
36	I	203	DD6	C37-C36-C31	-4.49	118.24	124.35
39	A	205	KC1	O2D-CGD-CBD	4.49	119.25	111.27
37	H	305	PID	CM4-C14-C15	-4.49	116.63	122.92
36	O	303	DD6	C9-C10-C11	-4.49	120.90	127.31
29	I	211	CLA	CMB-C2B-C1B	-4.48	121.57	128.46
38	A	203	UIX	O2-C27-C31	4.48	119.33	111.09
37	Q	306	PID	C17-C16-C15	4.48	132.64	123.47
36	H	303	DD6	C21-C20-C19	4.47	119.31	114.28
29	a	812	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
38	Q	305	UIX	O2-C27-C31	4.47	119.31	111.09
39	H	309	KC1	O2D-CGD-CBD	4.47	119.20	111.27
36	C	303	DD6	C9-C10-C11	-4.47	120.94	127.31
36	B	301	DD6	O1-C20-C19	-4.46	110.03	113.38
32	f	801	BCR	C24-C23-C22	-4.46	119.49	126.23
37	F	306	PID	CM4-C14-C15	-4.46	116.67	122.92
36	F	301	DD6	O1-C20-C19	4.45	116.72	113.38
37	D	302	PID	C18-C19-C20	4.42	132.53	123.47
37	D	305	PID	CM4-C14-C15	-4.42	116.73	122.92
37	N	302	PID	C18-C19-C20	4.42	132.53	123.47
37	C	302	PID	C18-C19-C20	4.42	132.52	123.47
38	P	207	UIX	O2-C27-C31	4.42	119.21	111.09
38	N	306	UIX	O2-C27-C31	4.41	119.21	111.09
36	J	303	DD6	C4-C5-C6	-4.41	121.02	127.31
38	N	306	UIX	C6-C1-C3	4.41	119.24	114.28
36	K	205	DD6	C37-C36-C31	-4.41	118.36	124.35
29	J	310	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
32	b	735	BCR	C16-C17-C18	-4.40	121.02	127.31
36	G	305	DD6	C-C1-C2	-4.39	116.77	122.92
36	L	301	DD6	C4-C5-C6	-4.39	121.05	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	P	202	PID	CM4-C14-C15	-4.38	116.78	122.92
37	O	307	PID	CM4-C14-C15	-4.38	116.79	122.92
36	D	301	DD6	C21-C20-C19	4.37	119.20	114.28
29	A	208	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
32	a	835	BCR	C24-C23-C22	-4.37	119.63	126.23
37	P	208	PID	C12-O4-C10	4.37	109.92	107.65
37	H	306	PID	CM4-C14-C15	-4.37	116.81	122.92
37	C	305	PID	C16-C15-C14	4.36	133.54	127.31
37	G	309	PID	C17-C16-C15	4.36	132.41	123.47
36	K	204	DD6	C3-C2-C1	-4.36	121.09	127.31
38	L	302	UIX	O2-C27-C31	4.36	119.11	111.09
37	P	206	PID	CM4-C14-C15	-4.36	116.82	122.92
36	L	305	DD6	C3-C2-C1	-4.35	121.10	127.31
36	I	204	DD6	C4-C5-C6	-4.35	121.10	127.31
36	L	303	DD6	C21-C20-C19	4.35	119.17	114.28
35	j	105	DGD	O2G-C1B-C2B	4.34	120.85	111.50
37	O	302	PID	C18-C19-C20	4.33	132.35	123.47
29	b	723	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
36	L	304	DD6	C21-C20-C19	4.33	119.15	114.28
36	P	204	DD6	C15-C14-C13	-4.33	116.85	125.99
36	M	302	DD6	C9-C10-C11	-4.33	121.14	127.31
37	T	301	PID	C17-C16-C15	4.33	132.34	123.47
36	B	302	DD6	C3-C2-C1	-4.32	121.14	127.31
38	F	305	UIX	O2-C27-C31	4.32	119.03	111.09
36	L	304	DD6	C15-C14-C13	-4.31	116.87	125.99
32	m	103	BCR	C20-C21-C22	-4.31	121.16	127.31
29	h	201	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
37	H	306	PID	C18-C19-C20	4.31	132.30	123.47
37	N	305	PID	CM4-C14-C15	-4.30	116.90	122.92
37	C	307	PID	CM4-C14-C15	-4.30	116.90	122.92
29	K	210	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
32	l	506	BCR	C3-C4-C5	-4.30	106.41	114.08
37	T	307	PID	CM4-C14-C15	-4.29	116.91	122.92
37	T	305	PID	CM4-C14-C15	-4.29	116.91	122.92
39	P	213	KC1	O2D-CGD-CBD	4.29	118.89	111.27
29	T	314	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
37	D	302	PID	CM4-C14-C15	-4.28	116.93	122.92
37	P	208	PID	C19-C20-C21	4.27	133.40	127.31
29	a	825	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
36	J	301	DD6	C4-C5-C6	-4.27	121.22	127.31
29	a	823	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
36	L	301	DD6	C9-C10-C11	-4.26	121.23	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	O	315	KC1	O2D-CGD-CBD	4.25	118.82	111.27
35	j	106	DGD	O2G-C1B-C2B	4.25	120.66	111.50
36	H	303	DD6	C3-C2-C1	-4.24	121.26	127.31
36	B	319	DD6	C14-C13-C11	-4.24	118.95	125.53
37	Q	301	PID	C18-C19-C20	4.24	132.15	123.47
36	A	204	DD6	C3-C2-C1	-4.24	121.26	127.31
29	H	312	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
38	E	304	UIX	O-C1-C6	4.23	120.12	115.06
37	Q	304	PID	CM4-C14-C15	-4.23	117.00	122.92
36	B	319	DD6	C20-C19-C18	-4.23	104.39	112.75
29	b	719	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
36	h	202	DD6	C37-C36-C31	-4.22	118.61	124.35
37	T	302	PID	C18-C19-C20	4.22	132.11	123.47
38	A	203	UIX	C6-C1-C3	4.22	119.02	114.28
36	P	204	DD6	C3-C2-C1	-4.21	121.30	127.31
36	B	319	DD6	C37-C36-C31	-4.21	118.63	124.35
29	E	311	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
38	O	306	UIX	C36-C35-C32	-4.21	121.31	127.31
39	E	312	KC1	O2D-CGD-CBD	4.20	118.74	111.27
37	H	304	PID	C12-O4-C10	4.20	109.84	107.65
36	B	303	DD6	C3-C2-C1	-4.20	121.32	127.31
36	K	202	DD6	C37-C36-C31	-4.20	118.64	124.35
36	G	306	DD6	O1-C20-C19	-4.20	110.23	113.38
32	i	204	BCR	C15-C14-C13	-4.20	121.32	127.31
32	l	507	BCR	C3-C4-C5	-4.19	106.59	114.08
36	M	304	DD6	C21-C20-C19	4.19	119.00	114.28
32	a	834	BCR	C11-C10-C9	-4.19	121.33	127.31
37	N	307	PID	CM4-C14-C15	-4.18	117.06	122.92
37	O	301	PID	C12-O4-C10	4.18	109.83	107.65
37	T	304	PID	C17-C16-C15	4.18	132.04	123.47
29	B	315	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
37	H	302	PID	C18-C19-C20	4.17	132.02	123.47
38	B	304	UIX	O-C1-C6	4.17	120.05	115.06
38	N	306	UIX	C7-C10-C11	-4.17	119.06	125.53
29	a	803	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
29	G	301	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
37	C	307	PID	C18-C19-C20	4.15	131.98	123.47
36	K	203	DD6	C37-C36-C31	-4.15	118.71	124.35
37	G	310	PID	CM4-C14-C15	-4.15	117.11	122.92
29	J	308	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
29	I	210	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
29	B	309	CLA	CMB-C2B-C1B	-4.14	122.10	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	E	310	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
36	J	302	DD6	C15-C14-C13	-4.13	117.25	125.99
39	H	311	KC1	O2D-CGD-CBD	4.13	118.61	111.27
36	C	303	DD6	C3-C2-C1	-4.13	121.42	127.31
36	m	101	DD6	O1-C20-C19	-4.13	110.28	113.38
29	L	309	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
29	M	309	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
35	h	203	DGD	O2G-C1B-C2B	4.12	120.39	111.50
37	C	301	PID	C12-O4-C10	4.12	109.79	107.65
37	D	305	PID	C17-C16-C15	4.12	131.91	123.47
36	E	302	DD6	C3-C2-C1	-4.12	121.44	127.31
29	O	314	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
38	P	207	UIX	C16-C20-C15	4.11	123.77	119.70
29	b	708	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
29	b	722	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
29	D	314	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
37	P	206	PID	C18-C19-C20	4.10	131.88	123.47
32	l	506	BCR	C7-C8-C9	-4.10	120.05	126.23
39	O	312	KC1	C3D-CAD-CBD	-4.09	102.21	107.61
37	C	305	PID	C17-C18-C19	4.09	133.92	124.81
29	G	313	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
29	A	218	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
29	a	831	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
36	A	202	DD6	C3-C2-C1	-4.08	121.49	127.31
36	K	205	DD6	C41-C32-C31	-4.08	103.99	110.47
36	L	304	DD6	C37-C36-C31	-4.08	118.81	124.35
29	E	314	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
29	a	830	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
35	m	102	DGD	O2G-C1B-C2B	4.06	120.25	111.50
36	M	301	DD6	C21-C20-C19	4.06	118.84	114.28
29	a	829	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
29	A	211	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
32	a	835	BCR	C11-C10-C9	-4.05	121.53	127.31
36	G	307	DD6	O1-C20-C15	-4.04	55.61	58.96
29	b	716	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
36	B	319	DD6	C9-C10-C11	-4.04	121.55	127.31
38	L	302	UIX	C-C7-C10	-4.04	117.45	125.99
29	N	313	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
36	K	221	DD6	C14-C13-C11	-4.03	119.27	125.53
36	D	304	DD6	C14-C13-C11	-4.03	119.27	125.53
36	K	202	DD6	C9-C10-C11	-4.03	121.56	127.31
29	b	703	CLA	CMB-C2B-C1B	-4.03	122.28	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	J	302	DD6	C9-C10-C11	-4.02	121.57	127.31
32	b	735	BCR	C28-C27-C26	-4.02	106.89	114.08
36	H	303	DD6	C9-C10-C11	-4.02	121.57	127.31
37	j	101	PID	C18-C19-C20	4.02	131.71	123.47
36	G	306	DD6	C37-C36-C31	-4.01	118.89	124.35
29	B	310	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
29	B	312	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
37	T	302	PID	CM4-C14-C15	-4.01	117.31	122.92
32	f	804	BCR	C7-C8-C9	-4.01	120.17	126.23
36	G	307	DD6	C24-C1-C2	4.01	125.09	118.94
36	P	204	DD6	C9-C10-C11	-4.01	121.59	127.31
29	G	317	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
36	Q	302	DD6	C9-C10-C11	-4.00	121.60	127.31
29	a	815	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
36	M	303	DD6	C14-C13-C11	-3.99	119.34	125.53
29	A	217	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
36	h	202	DD6	C20-C19-C18	-3.99	104.86	112.75
38	B	304	UIX	C37-C39-C40	-3.99	121.62	127.31
36	K	203	DD6	C14-C13-C11	-3.98	119.35	125.53
36	K	206	DD6	C9-C10-C11	-3.98	121.63	127.31
37	h	204	PID	CM4-C14-C15	-3.98	117.35	122.92
36	I	204	DD6	C37-C36-C31	-3.98	118.94	124.35
29	N	314	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
29	M	310	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
29	a	802	CLA	CMB-C2B-C3B	3.97	132.11	124.68
37	N	305	PID	C17-C16-C15	3.97	131.61	123.47
37	F	306	PID	C18-C19-C20	3.97	131.60	123.47
36	J	302	DD6	O1-C20-C21	3.97	119.81	115.06
37	F	304	PID	O1-C1-CM1	3.97	119.81	115.06
36	M	303	DD6	C37-C36-C31	-3.96	118.96	124.35
36	F	303	DD6	C37-C36-C31	-3.96	118.97	124.35
29	b	701	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
37	N	301	PID	C12-O4-C10	3.96	109.71	107.65
37	C	305	PID	C6-C7-C8	3.96	134.36	125.99
36	L	303	DD6	C37-C36-C31	-3.95	118.98	124.35
29	B	308	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
32	b	729	BCR	C16-C17-C18	-3.95	121.67	127.31
29	K	211	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
29	K	216	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
36	J	302	DD6	C37-C36-C31	-3.95	118.98	124.35
36	M	304	DD6	C15-C14-C13	-3.95	117.65	125.99
29	Q	308	CLA	CMB-C2B-C1B	-3.94	122.40	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	319	DD6	O1-C20-C19	-3.94	110.42	113.38
36	G	305	DD6	C9-C8-C6	-3.94	115.34	126.42
29	E	313	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
29	i	201	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
29	b	711	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
36	G	308	DD6	C21-C20-C19	3.94	118.71	114.28
29	A	207	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
29	M	314	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
36	H	303	DD6	O1-C20-C19	-3.93	110.43	113.38
37	F	304	PID	C18-C19-C20	3.93	131.53	123.47
38	E	304	UIX	C-C7-C10	-3.93	117.68	125.99
29	G	302	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
29	a	807	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
37	P	205	PID	C12-O4-C10	3.92	109.69	107.65
36	M	302	DD6	C4-C5-C6	-3.92	121.71	127.31
32	b	735	BCR	C20-C21-C22	-3.92	121.71	127.31
32	l	507	BCR	C11-C10-C9	-3.92	121.71	127.31
36	m	101	DD6	C15-C14-C13	-3.91	117.72	125.99
29	a	806	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
32	f	801	BCR	C16-C17-C18	-3.91	121.72	127.31
37	Q	306	PID	C12-O4-C10	3.91	109.69	107.65
37	P	206	PID	C12-O4-C10	3.91	109.69	107.65
29	i	203	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
38	L	302	UIX	O-C1-C6	3.91	119.74	115.06
29	J	309	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
36	I	204	DD6	O1-C20-C21	3.91	119.73	115.06
36	C	303	DD6	C37-C36-C31	-3.90	119.05	124.35
36	I	203	DD6	C14-C13-C11	-3.90	119.48	125.53
29	G	319	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
29	A	212	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
36	M	302	DD6	C37-C36-C31	-3.89	119.06	124.35
29	O	311	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
36	G	305	DD6	C37-C36-C31	-3.89	119.06	124.35
37	F	302	PID	C12-O4-C10	3.89	109.68	107.65
35	G	320	DGD	O2G-C1B-C2B	3.89	119.89	111.50
32	i	204	BCR	C3-C4-C5	-3.89	107.13	114.08
36	B	302	DD6	C37-C36-C31	-3.89	119.06	124.35
37	D	307	PID	C12-O4-C10	3.89	109.67	107.65
29	a	809	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
36	G	307	DD6	O1-C20-C19	3.88	116.30	113.38
32	a	835	BCR	C33-C5-C6	-3.88	120.17	124.53
29	M	307	CLA	CMB-C2B-C1B	-3.88	122.50	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	720	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
29	D	311	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
36	E	303	DD6	C3-C2-C1	-3.88	121.77	127.31
36	L	303	DD6	C3-C2-C1	-3.87	121.78	127.31
37	H	306	PID	C17-C16-C15	3.87	131.41	123.47
37	O	307	PID	C17-C16-C15	3.87	131.41	123.47
29	l	501	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
29	b	709	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
29	I	216	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
38	L	302	UIX	C6-C1-C3	3.87	118.64	114.28
38	C	306	UIX	C6-C1-C3	3.87	118.64	114.28
37	H	301	PID	C12-O4-C10	3.87	109.66	107.65
29	I	209	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
29	O	316	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
38	E	304	UIX	C37-C39-C40	-3.86	121.79	127.31
29	B	314	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
35	j	103	DGD	C2G-O2G-C1B	-3.86	108.29	117.79
36	h	202	DD6	C32-C33-C34	-3.86	104.93	113.64
29	K	209	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
29	H	315	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
37	G	303	PID	CM4-C14-C15	-3.85	117.53	122.92
29	N	309	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
29	a	805	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
35	j	103	DGD	C1E-O6E-C5E	3.84	121.23	113.69
29	b	717	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
37	N	302	PID	CM4-C14-C15	-3.84	117.55	122.92
34	E	316	LMG	O6-C5-C4	3.83	116.65	109.69
37	P	202	PID	C12-O4-C10	3.83	109.64	107.65
29	f	805	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
32	i	204	BCR	C33-C5-C6	-3.83	120.23	124.53
29	C	314	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
36	B	301	DD6	C15-C14-C13	-3.82	117.91	125.99
29	Q	315	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
29	D	309	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
29	l	508	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
29	D	316	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
29	L	313	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
29	H	310	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
36	K	204	DD6	C4-C5-C6	-3.81	121.88	127.31
36	I	203	DD6	C25-C26-C27	-3.80	115.56	126.58
37	C	302	PID	C12-O4-C10	3.80	109.63	107.65
29	b	731	CLA	CMB-C2B-C1B	-3.79	122.63	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	302	DD6	C9-C10-C11	-3.79	121.90	127.31
29	l	503	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
29	i	202	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
35	j	103	DGD	O2G-C1B-C2B	3.79	119.66	111.50
29	N	316	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
29	b	726	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
37	T	304	PID	C12-O4-C10	3.78	109.62	107.65
29	M	313	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
29	l	505	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
37	O	305	PID	C12-O4-C10	3.77	109.61	107.65
32	a	838	BCR	C3-C4-C5	-3.77	107.34	114.08
29	l	504	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
36	L	304	DD6	C4-C5-C6	-3.77	121.93	127.31
29	I	201	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
36	N	303	DD6	C4-C5-C6	-3.77	121.94	127.31
36	L	305	DD6	C37-C36-C31	-3.77	119.23	124.35
29	L	312	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
36	I	202	DD6	C37-C36-C31	-3.76	119.24	124.35
29	A	209	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
37	N	304	PID	C12-O4-C10	3.75	109.60	107.65
37	C	304	PID	C12-O4-C10	3.75	109.60	107.65
29	L	310	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
32	a	835	BCR	C7-C8-C9	-3.75	120.58	126.23
37	C	307	PID	C12-O4-C10	3.74	109.60	107.65
29	a	823	CLA	CMB-C2B-C3B	3.74	131.68	124.68
37	F	306	PID	C17-C16-C15	3.74	131.14	123.47
30	b	727	PQN	C11-C12-C13	-3.74	120.56	126.79
37	Q	304	PID	C12-O4-C10	3.74	109.60	107.65
38	Q	305	UIX	C1-C3-C5	-3.74	105.35	112.75
37	D	306	PID	CM4-C14-C15	-3.74	117.69	122.92
29	O	313	CLA	CMB-C2B-C3B	3.74	131.67	124.68
29	G	314	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
29	D	313	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
37	F	302	PID	C17-C16-C15	3.74	131.13	123.47
29	J	306	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
29	L	308	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
29	J	310	CLA	CMB-C2B-C3B	3.73	131.67	124.68
32	l	506	BCR	C16-C17-C18	-3.73	121.98	127.31
32	b	735	BCR	C3-C4-C5	-3.73	107.42	114.08
36	F	301	DD6	C37-C36-C31	-3.73	119.28	124.35
29	K	208	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
29	C	309	CLA	CMB-C2B-C1B	-3.72	122.74	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	T	305	PID	C12-O4-C10	3.72	109.59	107.65
29	C	311	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
29	b	712	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
29	I	214	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
36	A	201	DD6	C4-C5-C6	-3.72	122.00	127.31
29	T	311	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
38	B	304	UIX	C34-C30-C26	-3.72	122.01	127.31
29	j	104	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	F	315	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	N	311	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	B	311	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
36	L	303	DD6	C4-C5-C6	-3.71	122.02	127.31
38	B	304	UIX	C6-C1-C3	3.70	118.45	114.28
37	H	302	PID	CM4-C14-C15	-3.70	117.73	122.92
29	b	705	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
29	F	310	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
36	E	303	DD6	C37-C36-C31	-3.70	119.32	124.35
29	P	217	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
32	a	838	BCR	C28-C27-C26	-3.70	107.47	114.08
36	G	306	DD6	C15-C14-C13	-3.70	118.17	125.99
38	P	207	UIX	C36-C35-C32	-3.70	122.03	127.31
37	T	307	PID	CM5-C21-C20	-3.70	117.74	122.92
29	L	307	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
37	T	301	PID	C12-O4-C10	3.70	109.57	107.65
29	Q	310	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
32	b	729	BCR	C15-C14-C13	-3.69	122.04	127.31
36	F	303	DD6	C15-C14-C13	-3.69	118.18	125.99
29	a	812	CLA	CMB-C2B-C3B	3.69	131.59	124.68
36	M	301	DD6	C37-C36-C31	-3.69	119.33	124.35
29	a	821	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
29	P	210	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
36	J	303	DD6	C37-C36-C31	-3.69	119.34	124.35
36	D	301	DD6	C12-C11-C13	3.69	123.89	118.08
29	A	208	CLA	CMB-C2B-C3B	3.69	131.58	124.68
36	B	301	DD6	C9-C10-C11	-3.69	122.05	127.31
29	I	211	CLA	CMB-C2B-C3B	3.69	131.57	124.68
36	H	303	DD6	C15-C14-C13	-3.68	118.20	125.99
29	a	819	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
29	J	313	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
32	a	838	BCR	C20-C21-C22	-3.68	122.05	127.31
29	T	313	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
37	D	305	PID	C12-O4-C10	3.68	109.57	107.65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	302	DD6	C37-C36-C31	-3.68	119.35	124.35
37	C	305	PID	CM5-C21-C20	-3.68	117.77	122.92
36	I	204	DD6	C20-C19-C18	-3.68	105.48	112.75
37	Q	303	PID	C12-O4-C10	3.67	109.56	107.65
38	T	306	UIX	C6-C1-C3	3.67	118.41	114.28
37	D	303	PID	CM4-C14-C15	-3.67	117.78	122.92
36	J	301	DD6	C25-C24-C1	-3.67	116.10	126.42
29	M	315	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
36	I	202	DD6	C4-C5-C6	-3.67	122.07	127.31
29	O	309	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
29	H	308	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
29	b	719	CLA	CMB-C2B-C3B	3.67	131.54	124.68
32	a	834	BCR	C38-C26-C25	-3.66	120.41	124.53
36	G	305	DD6	C14-C13-C11	-3.66	119.85	125.53
29	l	509	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
36	K	205	DD6	C15-C14-C13	-3.66	118.25	125.99
29	C	316	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
37	D	302	PID	C12-O4-C10	3.66	109.56	107.65
29	A	216	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
32	m	103	BCR	C24-C23-C22	-3.66	120.71	126.23
29	f	803	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
37	N	307	PID	C17-C16-C15	3.65	130.95	123.47
29	b	723	CLA	CMB-C2B-C3B	3.65	131.50	124.68
36	J	301	DD6	C37-C36-C31	-3.65	119.39	124.35
37	N	305	PID	C18-C19-C20	3.65	130.95	123.47
39	F	314	KC1	C3D-CAD-CBD	-3.65	102.80	107.61
36	G	308	DD6	C37-C36-C31	-3.65	119.39	124.35
29	f	802	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
32	a	838	BCR	C24-C23-C22	-3.64	120.73	126.23
36	K	203	DD6	C4-C5-C6	-3.64	122.11	127.31
32	f	804	BCR	C16-C17-C18	-3.64	122.11	127.31
29	I	207	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
29	G	312	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
37	D	306	PID	C18-C19-C20	3.64	130.93	123.47
29	a	814	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
29	H	313	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
38	L	302	UIX	C34-C37-C39	-3.64	116.02	123.47
32	f	804	BCR	C20-C21-C22	-3.63	122.12	127.31
29	T	316	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
36	B	319	DD6	C4-C5-C6	-3.63	122.13	127.31
29	P	215	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
29	h	201	CLA	CMB-C2B-C3B	3.62	131.46	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	213	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
29	D	308	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
32	b	735	BCR	C15-C14-C13	-3.62	122.14	127.31
37	G	309	PID	C12-O4-C10	3.62	109.53	107.65
32	a	838	BCR	C7-C8-C9	-3.62	120.77	126.23
36	J	301	DD6	C21-C20-C19	3.62	118.35	114.28
37	Q	301	PID	C12-O4-C10	3.62	109.53	107.65
32	m	103	BCR	C38-C26-C27	3.61	120.56	113.62
29	a	803	CLA	CMB-C2B-C3B	3.61	131.44	124.68
36	K	206	DD6	C15-C14-C13	-3.61	118.36	125.99
29	a	824	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
29	b	710	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
29	I	212	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
37	O	307	PID	C12-O4-C10	3.59	109.52	107.65
29	a	811	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
37	T	317	PID	C12-O4-C10	3.59	109.52	107.65
37	O	304	PID	C12-O4-C10	3.59	109.52	107.65
29	a	816	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
29	K	210	CLA	CMB-C2B-C3B	3.59	131.40	124.68
37	H	305	PID	C12-O4-C10	3.59	109.52	107.65
37	Q	306	PID	C18-C19-C20	3.59	130.82	123.47
36	M	301	DD6	C4-C5-C6	-3.59	122.19	127.31
29	a	804	CLA	O2D-CGD-O1D	-3.59	116.83	123.84
36	B	303	DD6	C15-C14-C13	-3.59	118.41	125.99
29	M	311	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
36	C	303	DD6	C15-C14-C13	-3.58	118.42	125.99
37	j	101	PID	CM4-C14-C15	-3.58	117.90	122.92
36	L	305	DD6	C15-C14-C13	-3.58	118.42	125.99
37	O	305	PID	C17-C16-C15	3.58	130.81	123.47
29	b	724	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
37	F	302	PID	CM5-C21-C20	-3.58	117.91	122.92
36	M	302	DD6	C15-C14-C13	-3.58	118.43	125.99
36	G	307	DD6	C21-C20-C19	3.58	118.30	114.28
29	T	314	CLA	CMB-C2B-C3B	3.57	131.36	124.68
37	N	307	PID	C12-O4-C10	3.57	109.51	107.65
29	T	309	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
36	A	204	DD6	C37-C36-C31	-3.57	119.50	124.35
38	F	305	UIX	C6-C1-C3	3.57	118.30	114.28
29	H	312	CLA	CMB-C2B-C3B	3.57	131.36	124.68
36	T	303	DD6	C15-C14-C13	-3.57	118.45	125.99
36	L	301	DD6	C37-C36-C31	-3.57	119.50	124.35
39	M	305	KC1	C3D-CAD-CBD	-3.57	102.91	107.61

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	m	103	BCR	C27-C26-C25	-3.56	117.56	122.73
29	a	804	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
36	K	221	DD6	C37-C36-C31	-3.56	119.51	124.35
29	F	308	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
38	B	304	UIX	C14-C13-C11	-3.56	122.23	127.31
29	F	312	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
37	F	306	PID	C12-O4-C10	3.56	109.50	107.65
36	m	101	DD6	C9-C10-C11	-3.56	122.23	127.31
29	b	718	CLA	CMB-C2B-C3B	3.56	131.33	124.68
36	h	202	DD6	C15-C14-C13	-3.55	118.48	125.99
29	b	707	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
29	F	316	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
37	N	307	PID	CM2-C5-C4	-3.55	102.82	108.98
38	J	304	UIX	C35-C36-C38	-3.55	112.15	123.22
37	H	305	PID	C17-C18-C19	3.55	132.70	124.81
29	M	306	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
37	h	204	PID	C12-O4-C10	3.54	109.50	107.65
29	b	702	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
36	Q	302	DD6	C3-C2-C1	-3.54	122.25	127.31
37	P	203	PID	CM4-C14-C15	-3.54	117.96	122.92
29	B	306	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
29	b	714	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
37	N	307	PID	C18-C19-C20	3.53	130.71	123.47
29	E	308	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
36	A	202	DD6	C37-C36-C31	-3.53	119.55	124.35
36	G	305	DD6	C32-C33-C34	-3.53	105.67	113.64
36	F	301	DD6	O1-C20-C21	3.53	119.28	115.06
29	b	716	CLA	CMB-C2B-C3B	3.53	131.28	124.68
29	G	316	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
37	C	305	PID	C12-O4-C10	3.52	109.48	107.65
38	E	304	UIX	C6-C1-C3	3.52	118.24	114.28
36	K	203	DD6	C3-C2-C1	-3.52	122.28	127.31
36	K	204	DD6	C14-C13-C11	-3.52	120.07	125.53
32	a	834	BCR	C33-C5-C6	-3.52	120.57	124.53
36	A	202	DD6	C4-C5-C6	-3.52	122.29	127.31
36	B	303	DD6	C37-C36-C31	-3.52	119.57	124.35
36	M	302	DD6	C-C1-C2	-3.52	118.00	122.92
29	F	307	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
38	J	304	UIX	O-C1-C6	3.51	119.26	115.06
32	a	834	BCR	C7-C8-C9	-3.50	120.94	126.23
29	a	822	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
36	G	308	DD6	C4-C5-C6	-3.50	122.31	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	837	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
29	L	316	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
36	A	201	DD6	C37-C36-C31	-3.50	119.59	124.35
29	a	830	CLA	CMB-C2B-C3B	3.50	131.23	124.68
37	T	302	PID	C12-O4-C10	3.50	109.47	107.65
37	O	302	PID	CM4-C14-C15	-3.50	118.03	122.92
36	J	303	DD6	C25-C24-C1	-3.49	116.60	126.42
29	M	311	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
37	E	301	PID	C12-O4-C10	3.49	109.47	107.65
29	J	307	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
36	E	303	DD6	C4-C5-C6	-3.49	122.33	127.31
32	f	804	BCR	C38-C26-C25	-3.49	120.61	124.53
29	F	313	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
29	K	218	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
29	E	315	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
29	J	305	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
29	B	309	CLA	CMB-C2B-C3B	3.48	131.20	124.68
36	M	304	DD6	C37-C36-C31	-3.48	119.61	124.35
29	P	214	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
37	C	307	PID	C17-C16-C15	3.48	130.60	123.47
29	E	311	CLA	CMB-C2B-C3B	3.48	131.19	124.68
36	I	206	DD6	C37-C36-C31	-3.48	119.62	124.35
29	E	310	CLA	CMB-C2B-C3B	3.48	131.19	124.68
36	A	204	DD6	C15-C14-C13	-3.47	118.65	125.99
29	C	313	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
29	G	301	CLA	CMB-C2B-C3B	3.47	131.17	124.68
29	b	703	CLA	CMB-C2B-C3B	3.47	131.17	124.68
29	P	212	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
38	J	304	UIX	O2-C27-C31	3.47	117.47	111.09
36	m	101	DD6	C4-C5-C6	-3.47	122.36	127.31
29	b	736	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
38	J	304	UIX	C6-C1-C3	3.46	118.18	114.28
29	A	214	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
29	A	218	CLA	CMB-C2B-C3B	3.46	131.16	124.68
32	l	507	BCR	C24-C23-C22	-3.46	121.01	126.23
29	G	311	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
32	a	838	BCR	C11-C10-C9	-3.46	122.38	127.31
29	L	317	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
36	K	204	DD6	C37-C36-C31	-3.46	119.65	124.35
32	l	506	BCR	C38-C26-C25	-3.45	120.65	124.53
37	Q	301	PID	C17-C16-C15	3.45	130.55	123.47
29	a	808	CLA	CMB-C2B-C1B	-3.45	123.16	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	307	DD6	C14-C13-C11	-3.45	120.17	125.53
29	L	309	CLA	CMB-C2B-C3B	3.45	131.14	124.68
36	B	305	DD6	C15-C14-C13	-3.45	118.70	125.99
29	K	213	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
29	M	308	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
29	E	306	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
29	I	217	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
29	G	304	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
38	O	306	UIX	C1-C3-C5	-3.44	105.94	112.75
36	I	203	DD6	O1-C20-C15	-3.44	56.11	58.96
35	b	733	DGD	O1G-C1A-C2A	3.44	122.70	111.91
29	B	316	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
32	a	834	BCR	C20-C21-C22	-3.43	122.41	127.31
29	a	820	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
29	Q	312	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
29	A	206	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
36	O	303	DD6	C21-C20-C15	-3.43	116.51	122.26
29	b	722	CLA	CMB-C2B-C3B	3.43	131.10	124.68
29	O	308	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
36	B	302	DD6	C15-C14-C13	-3.43	118.74	125.99
29	I	210	CLA	CMB-C2B-C3B	3.42	131.09	124.68
29	a	826	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
29	a	828	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
36	A	202	DD6	C15-C14-C13	-3.42	118.76	125.99
37	H	302	PID	C12-O4-C10	3.42	109.43	107.65
29	B	308	CLA	CMB-C2B-C3B	3.42	131.07	124.68
36	B	305	DD6	O1-C20-C19	-3.42	110.82	113.38
37	Q	304	PID	CM5-C21-C20	-3.42	118.14	122.92
32	b	728	BCR	C8-C7-C6	-3.41	117.62	127.20
37	T	305	PID	CM5-C21-C20	-3.41	118.15	122.92
39	O	315	KC1	C3D-CAD-CBD	-3.41	103.12	107.61
29	J	308	CLA	CMB-C2B-C3B	3.41	131.05	124.68
29	A	210	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
29	P	209	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
29	a	813	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
29	B	307	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
29	F	311	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
29	O	314	CLA	CMB-C2B-C3B	3.40	131.04	124.68
29	D	314	CLA	CMB-C2B-C3B	3.40	131.04	124.68
29	K	207	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
29	E	305	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
36	E	302	DD6	O1-C20-C21	3.40	119.12	115.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	215	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
39	G	315	KC1	C3D-CAD-CBD	-3.39	103.14	107.61
29	G	313	CLA	CMB-C2B-C3B	3.39	131.02	124.68
36	Q	302	DD6	C37-C36-C31	-3.39	119.74	124.35
37	G	310	PID	C12-O4-C10	3.39	109.41	107.65
29	A	211	CLA	CMB-C2B-C3B	3.39	131.02	124.68
29	a	818	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
36	B	301	DD6	C37-C36-C31	-3.39	119.75	124.35
36	I	202	DD6	C15-C14-C13	-3.38	118.84	125.99
29	E	309	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
36	G	306	DD6	C14-C13-C11	-3.38	120.28	125.53
36	I	203	DD6	C21-C20-C15	-3.38	116.60	122.26
29	B	312	CLA	CMB-C2B-C3B	3.38	131.00	124.68
29	b	715	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
29	E	314	CLA	CMB-C2B-C3B	3.38	130.99	124.68
29	T	308	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
39	K	215	KC1	CHC-C4B-C3B	-3.38	119.48	125.26
29	a	831	CLA	CMB-C2B-C3B	3.37	130.99	124.68
38	A	203	UIX	C34-C30-C26	-3.37	122.50	127.31
29	I	216	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
36	G	307	DD6	C19-C18-C17	-3.37	104.27	110.77
29	a	806	CLA	CMB-C2B-C3B	3.37	130.98	124.68
29	C	308	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
36	J	301	DD6	C25-C26-C27	-3.37	116.80	126.58
29	a	807	CLA	CMB-C2B-C3B	3.37	130.98	124.68
29	B	315	CLA	CMB-C2B-C3B	3.37	130.98	124.68
29	K	211	CLA	O2D-CGD-O1D	-3.37	117.26	123.84
37	T	301	PID	CM5-C21-C20	-3.36	118.21	122.92
29	D	312	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
36	K	206	DD6	O1-C20-C19	-3.36	110.86	113.38
29	i	203	CLA	CMB-C2B-C3B	3.36	130.97	124.68
29	H	307	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
29	A	206	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
36	N	303	DD6	C15-C14-C13	-3.36	118.89	125.99
29	G	302	CLA	CMB-C2B-C3B	3.36	130.96	124.68
37	G	310	PID	CM5-C21-C20	-3.36	118.22	122.92
37	D	303	PID	C6-C7-C8	-3.36	118.90	125.99
32	l	507	BCR	C38-C26-C25	-3.35	120.76	124.53
36	I	205	DD6	C37-C36-C31	-3.35	119.79	124.35
29	Q	307	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
39	D	315	KC1	C3D-CAD-CBD	-3.35	103.19	107.61
38	A	203	UIX	C37-C39-C40	-3.35	122.53	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	825	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
36	K	206	DD6	C37-C36-C31	-3.35	119.80	124.35
36	J	301	DD6	O1-C20-C21	-3.35	111.05	115.06
29	A	215	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
29	L	311	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
32	b	728	BCR	C15-C14-C13	-3.35	122.53	127.31
37	D	302	PID	CM5-C21-C20	-3.35	118.24	122.92
29	B	310	CLA	CMB-C2B-C3B	3.34	130.94	124.68
39	J	312	KC1	C3D-CAD-CBD	-3.34	103.21	107.61
36	m	101	DD6	C37-C36-C31	-3.34	119.81	124.35
32	f	801	BCR	C11-C10-C9	-3.34	122.54	127.31
29	I	208	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
29	K	211	CLA	CMB-C2B-C3B	3.34	130.92	124.68
36	E	302	DD6	C21-C20-C19	3.34	118.03	114.28
29	i	201	CLA	CMB-C2B-C3B	3.34	130.92	124.68
29	K	217	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
29	G	317	CLA	CMB-C2B-C3B	3.33	130.92	124.68
29	M	314	CLA	CMB-C2B-C3B	3.33	130.92	124.68
36	K	202	DD6	C3-C4-C5	-3.33	116.64	123.47
29	a	815	CLA	CMB-C2B-C3B	3.33	130.91	124.68
36	F	301	DD6	C3-C2-C1	-3.33	122.56	127.31
36	h	202	DD6	C9-C10-C11	-3.33	122.56	127.31
29	b	701	CLA	CMB-C2B-C3B	3.33	130.90	124.68
29	a	817	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
29	i	203	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
37	h	204	PID	C18-C19-C20	3.32	130.28	123.47
39	M	312	KC1	C3D-CAD-CBD	-3.32	103.23	107.61
29	L	315	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
29	M	310	CLA	CMB-C2B-C3B	3.32	130.88	124.68
36	B	303	DD6	C4-C5-C6	-3.31	122.58	127.31
32	f	804	BCR	C24-C23-C22	-3.31	121.23	126.23
29	G	319	CLA	CMB-C2B-C3B	3.31	130.88	124.68
29	N	313	CLA	CMB-C2B-C3B	3.31	130.87	124.68
29	O	314	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
29	J	306	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
29	E	313	CLA	CMB-C2B-C3B	3.31	130.87	124.68
32	f	804	BCR	C33-C5-C6	-3.30	120.82	124.53
37	D	302	PID	C17-C16-C15	3.30	130.24	123.47
29	M	309	CLA	CMB-C2B-C3B	3.30	130.85	124.68
29	b	711	CLA	CMB-C2B-C3B	3.30	130.85	124.68
36	T	303	DD6	C37-C36-C31	-3.30	119.86	124.35
36	E	303	DD6	C15-C14-C13	-3.30	119.02	125.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	305	DD6	C25-C24-C1	-3.30	117.16	126.42
36	H	303	DD6	C37-C36-C31	-3.29	119.87	124.35
37	D	306	PID	C12-O4-C10	3.29	109.36	107.65
29	A	212	CLA	CMB-C2B-C3B	3.29	130.84	124.68
29	A	207	CLA	CMB-C2B-C3B	3.29	130.84	124.68
35	B	318	DGD	O6E-C5E-C4E	3.29	115.67	109.69
37	O	302	PID	C12-O4-C10	3.29	109.36	107.65
38	A	203	UIX	C-C7-C10	-3.29	119.04	125.99
29	l	501	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
29	E	315	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
29	N	308	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
29	l	502	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
38	P	207	UIX	C6-C1-C3	3.29	117.98	114.28
29	K	216	CLA	CMB-C2B-C3B	3.28	130.82	124.68
29	H	315	CLA	CMB-C2B-C3B	3.28	130.82	124.68
29	J	308	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
36	K	204	DD6	O1-C20-C21	3.28	118.99	115.06
29	Q	308	CLA	CMB-C2B-C3B	3.28	130.82	124.68
32	l	507	BCR	C20-C21-C22	-3.28	122.63	127.31
29	a	805	CLA	CMB-C2B-C3B	3.28	130.81	124.68
29	K	209	CLA	CMB-C2B-C3B	3.28	130.81	124.68
29	a	809	CLA	CMB-C2B-C3B	3.28	130.81	124.68
29	b	721	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
39	C	310	KC1	C3D-CAD-CBD	-3.27	103.30	107.61
37	T	307	PID	C12-O4-C10	3.27	109.35	107.65
37	D	303	PID	C18-C19-C20	3.27	130.17	123.47
37	N	304	PID	C18-C19-C20	3.27	130.17	123.47
37	j	101	PID	C12-O4-C10	3.27	109.35	107.65
38	B	304	UIX	C-C7-C10	-3.26	119.09	125.99
36	F	303	DD6	O1-C20-C21	3.26	118.97	115.06
29	F	310	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
29	b	707	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
36	K	205	DD6	C3-C2-C1	-3.26	122.66	127.31
37	P	203	PID	C12-O4-C10	3.26	109.35	107.65
29	I	216	CLA	CMB-C2B-C3B	3.26	130.77	124.68
29	D	311	CLA	CMB-C2B-C3B	3.25	130.77	124.68
36	D	304	DD6	C37-C36-C31	-3.25	119.93	124.35
29	O	316	CLA	CMB-C2B-C3B	3.25	130.76	124.68
29	O	311	CLA	CMB-C2B-C3B	3.25	130.76	124.68
29	N	314	CLA	CMB-C2B-C3B	3.25	130.75	124.68
37	C	307	PID	CM2-C5-C4	-3.25	103.34	108.98
37	E	301	PID	CM4-C14-C15	-3.24	118.38	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	309	CLA	CMB-C2B-C3B	3.24	130.75	124.68
37	F	306	PID	CM5-C21-C20	-3.24	118.38	122.92
36	O	303	DD6	C3-C2-C1	-3.24	122.69	127.31
29	B	314	CLA	CMB-C2B-C3B	3.24	130.74	124.68
36	D	301	DD6	C4-C5-C6	-3.24	122.69	127.31
29	I	211	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
37	N	302	PID	CM5-C21-C20	-3.24	118.39	122.92
29	J	311	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
36	h	202	DD6	C21-C20-C15	-3.23	116.84	122.26
32	f	801	BCR	C33-C5-C6	-3.23	120.90	124.53
37	N	302	PID	C12-O4-C10	3.23	109.33	107.65
29	H	310	CLA	CMB-C2B-C3B	3.23	130.72	124.68
29	G	314	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
36	M	304	DD6	C9-C10-C11	-3.23	122.71	127.31
36	N	303	DD6	C37-C36-C31	-3.22	119.97	124.35
36	O	303	DD6	C15-C14-C13	-3.22	119.18	125.99
38	J	304	UIX	C34-C37-C39	-3.22	116.87	123.47
29	M	307	CLA	CMB-C2B-C3B	3.22	130.71	124.68
36	I	204	DD6	C24-C1-C2	3.22	123.88	118.94
37	H	306	PID	CM5-C21-C20	-3.22	118.42	122.92
29	C	314	CLA	CMB-C2B-C3B	3.22	130.69	124.68
29	b	709	CLA	CMB-C2B-C3B	3.21	130.69	124.68
29	a	802	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
36	N	303	DD6	C9-C10-C11	-3.21	122.73	127.31
32	l	506	BCR	C20-C21-C22	-3.21	122.73	127.31
36	I	206	DD6	C4-C5-C6	-3.21	122.73	127.31
29	F	310	CLA	CMB-C2B-C3B	3.21	130.68	124.68
29	B	314	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
36	L	303	DD6	O1-C20-C21	-3.21	111.22	115.06
29	b	713	CLA	CMB-C2B-C1B	-3.21	123.54	128.46
29	b	716	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
37	H	302	PID	CM5-C21-C20	-3.21	118.43	122.92
36	B	305	DD6	C37-C36-C31	-3.20	119.99	124.35
29	a	829	CLA	CMB-C2B-C3B	3.20	130.67	124.68
36	E	302	DD6	C21-C20-C15	-3.20	116.89	122.26
29	l	508	CLA	CMB-C2B-C3B	3.20	130.67	124.68
29	N	309	CLA	CMB-C2B-C3B	3.20	130.67	124.68
36	K	205	DD6	O1-C20-C19	-3.20	110.98	113.38
37	C	307	PID	CM5-C21-C20	-3.20	118.44	122.92
36	J	303	DD6	C14-C13-C11	-3.20	120.57	125.53
36	J	303	DD6	C20-C19-C18	-3.20	106.42	112.75
29	I	209	CLA	CMB-C2B-C3B	3.20	130.66	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	313	CLA	CMB-C2B-C3B	3.20	130.66	124.68
29	l	501	CLA	CMB-C2B-C3B	3.20	130.66	124.68
30	a	832	PQN	C2M-C2-C3	-3.19	119.19	124.40
29	K	214	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
36	I	206	DD6	C15-C14-C13	-3.19	119.24	125.99
36	F	303	DD6	C21-C20-C15	-3.19	116.91	122.26
29	Q	313	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
39	T	310	KC1	C3D-CAD-CBD	-3.19	103.41	107.61
37	Q	301	PID	CM5-C21-C20	-3.19	118.46	122.92
30	a	832	PQN	C11-C12-C13	-3.19	121.49	126.79
35	b	733	DGD	C1D-C2D-C3D	3.18	116.63	110.00
29	Q	315	CLA	CMB-C2B-C3B	3.18	130.63	124.68
36	D	301	DD6	C10-C9-C8	-3.18	113.29	123.22
29	L	312	CLA	CMB-C2B-C3B	3.18	130.63	124.68
29	i	202	CLA	CMB-C2B-C3B	3.18	130.63	124.68
29	C	314	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
36	M	301	DD6	O1-C20-C21	-3.17	111.26	115.06
29	T	311	CLA	CMB-C2B-C3B	3.17	130.61	124.68
36	E	303	DD6	O1-C20-C21	-3.17	111.26	115.06
29	K	216	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
29	a	826	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
37	Q	306	PID	CM5-C21-C20	-3.17	118.49	122.92
29	a	827	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
29	a	809	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
29	l	504	CLA	CMB-C2B-C3B	3.16	130.59	124.68
30	a	832	PQN	C14-C13-C15	3.16	120.59	115.27
29	j	104	CLA	CMB-C2B-C3B	3.16	130.59	124.68
29	b	731	CLA	CMB-C2B-C3B	3.16	130.59	124.68
29	K	214	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
29	a	829	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
29	J	306	CLA	CMB-C2B-C3B	3.16	130.58	124.68
38	Q	305	UIX	O-C1-C3	3.15	115.75	113.38
29	J	309	CLA	CMB-C2B-C3B	3.15	130.58	124.68
36	T	303	DD6	C3-C2-C1	-3.15	122.81	127.31
29	Q	310	CLA	CMB-C2B-C3B	3.15	130.58	124.68
32	l	506	BCR	C23-C24-C25	-3.15	118.35	127.20
29	D	314	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
29	F	307	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
29	N	316	CLA	CMB-C2B-C3B	3.15	130.56	124.68
29	C	311	CLA	CMB-C2B-C3B	3.15	130.56	124.68
29	G	314	CLA	CMB-C2B-C3B	3.15	130.56	124.68
39	C	315	KC1	C3D-CAD-CBD	-3.14	103.47	107.61

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	827	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
29	D	316	CLA	CMB-C2B-C3B	3.14	130.56	124.68
29	L	316	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
29	T	314	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
29	I	214	CLA	CMB-C2B-C3B	3.14	130.55	124.68
37	O	302	PID	CM5-C21-C20	-3.14	118.53	122.92
29	b	705	CLA	CMB-C2B-C3B	3.14	130.55	124.68
29	b	724	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
37	N	307	PID	CM5-C21-C20	-3.14	118.53	122.92
32	b	735	BCR	C33-C5-C6	-3.14	121.00	124.53
39	O	312	KC1	O1D-CGD-CBD	-3.14	118.07	124.48
29	b	725	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
29	b	717	CLA	CMB-C2B-C3B	3.14	130.54	124.68
36	K	204	DD6	C20-C19-C18	-3.14	106.55	112.75
29	I	201	CLA	CMB-C2B-C3B	3.13	130.54	124.68
29	E	311	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
36	N	303	DD6	C3-C2-C1	-3.13	122.84	127.31
29	K	212	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
39	N	315	KC1	C3D-CAD-CBD	-3.13	103.48	107.61
29	A	209	CLA	CMB-C2B-C3B	3.13	130.54	124.68
29	l	504	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
29	b	721	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
29	G	312	CLA	CMB-C2B-C3B	3.13	130.53	124.68
29	N	311	CLA	CMB-C2B-C3B	3.13	130.53	124.68
38	P	207	UIX	C22-C15-C20	-3.13	107.67	110.47
29	f	805	CLA	CMB-C2B-C3B	3.13	130.53	124.68
29	N	314	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
37	C	302	PID	CM5-C21-C20	-3.12	118.55	122.92
29	L	308	CLA	CMB-C2B-C3B	3.12	130.52	124.68
29	P	210	CLA	CMB-C2B-C3B	3.12	130.52	124.68
39	O	312	KC1	O2D-CGD-O1D	-3.12	117.73	123.84
37	P	203	PID	CM5-C21-C20	-3.12	118.55	122.92
39	T	315	KC1	C3D-CAD-CBD	-3.12	103.50	107.61
29	A	217	CLA	CMB-C2B-C3B	3.12	130.51	124.68
29	l	509	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
36	K	206	DD6	C4-C5-C6	-3.12	122.86	127.31
29	M	313	CLA	CMB-C2B-C3B	3.12	130.51	124.68
29	a	819	CLA	CMB-C2B-C3B	3.12	130.51	124.68
29	C	309	CLA	CMB-C2B-C3B	3.11	130.50	124.68
36	B	303	DD6	C33-C34-C35	-3.11	106.04	110.30
32	a	838	BCR	C33-C5-C6	-3.11	121.04	124.53
38	F	305	UIX	C18-O2-C27	-3.11	112.11	117.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	m	101	DD6	C3-C4-C5	-3.11	117.11	123.47
29	b	708	CLA	CMB-C2B-C3B	3.10	130.49	124.68
36	L	305	DD6	O1-C20-C19	-3.10	111.05	113.38
29	b	706	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
29	T	313	CLA	CMB-C2B-C3B	3.10	130.48	124.68
29	O	309	CLA	CMB-C2B-C3B	3.10	130.47	124.68
36	I	205	DD6	C25-C24-C1	-3.09	117.72	126.42
29	C	311	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
29	E	305	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
29	b	714	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
29	F	311	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
36	Q	302	DD6	C15-C14-C13	-3.09	119.45	125.99
36	I	206	DD6	C9-C10-C11	-3.09	122.90	127.31
37	F	304	PID	C17-C16-C15	3.09	129.80	123.47
36	h	202	DD6	C14-C13-C11	-3.09	120.74	125.53
37	C	301	PID	C18-C19-C20	3.09	129.80	123.47
29	b	718	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
29	J	311	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
32	a	834	BCR	C3-C4-C5	-3.08	108.57	114.08
37	H	306	PID	C12-O4-C10	3.08	109.25	107.65
29	l	505	CLA	CMB-C2B-C3B	3.08	130.44	124.68
29	F	315	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
29	l	509	CLA	CMB-C2B-C3B	3.08	130.44	124.68
32	b	728	BCR	C33-C5-C4	3.08	119.53	113.62
29	K	208	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
38	O	306	UIX	C16-C20-C15	3.08	122.75	119.70
29	L	310	CLA	CMB-C2B-C3B	3.08	130.44	124.68
36	M	302	DD6	C21-C20-C19	3.08	117.74	114.28
36	G	308	DD6	C21-C20-C15	-3.08	117.11	122.26
29	J	313	CLA	CMB-C2B-C3B	3.08	130.43	124.68
29	b	711	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
29	M	315	CLA	CMB-C2B-C3B	3.08	130.43	124.68
29	T	311	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
29	F	315	CLA	CMB-C2B-C3B	3.07	130.43	124.68
36	D	301	DD6	C37-C36-C31	-3.07	120.17	124.35
39	E	312	KC1	C3D-CAD-CBD	-3.07	103.56	107.61
29	a	824	CLA	CMB-C2B-C3B	3.07	130.42	124.68
29	l	502	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
36	L	303	DD6	C15-C14-C13	-3.07	119.51	125.99
37	H	301	PID	C18-C19-C20	3.07	129.76	123.47
36	J	301	DD6	C37-C36-C35	3.07	120.04	114.36
29	L	307	CLA	CMB-C2B-C3B	3.07	130.41	124.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	305	PID	CM4-C14-C15	-3.06	118.63	122.92
36	B	319	DD6	C-C1-C2	-3.06	118.63	122.92
29	B	311	CLA	CMB-C2B-C3B	3.06	130.41	124.68
36	A	204	DD6	C9-C10-C11	-3.06	122.94	127.31
29	P	217	CLA	CMB-C2B-C3B	3.06	130.41	124.68
29	a	806	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
29	l	503	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
29	P	215	CLA	CMB-C2B-C3B	3.06	130.40	124.68
29	Q	312	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
29	a	821	CLA	CMB-C2B-C3B	3.05	130.39	124.68
29	b	715	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
36	h	202	DD6	C28-C27-C29	3.05	122.89	116.84
29	G	313	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
29	E	306	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
29	D	313	CLA	CMB-C2B-C3B	3.05	130.38	124.68
29	H	308	CLA	CMB-C2B-C3B	3.05	130.38	124.68
37	D	306	PID	CM5-C21-C20	-3.05	118.65	122.92
36	L	301	DD6	C14-C13-C11	-3.05	120.80	125.53
29	a	815	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
29	J	307	CLA	CMB-C2B-C3B	3.05	130.38	124.68
29	b	719	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
29	I	201	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
29	P	215	CLA	CHB-C4A-NA	3.05	128.72	124.51
32	m	103	BCR	C23-C24-C25	-3.05	118.65	127.20
29	f	802	CLA	CMB-C2B-C3B	3.05	130.38	124.68
29	f	803	CLA	CMB-C2B-C3B	3.05	130.38	124.68
32	a	834	BCR	C28-C27-C26	-3.04	108.64	114.08
29	b	708	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
32	a	835	BCR	C38-C26-C25	-3.04	121.11	124.53
37	N	301	PID	C18-C19-C20	3.04	129.71	123.47
29	M	306	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	b	726	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	l	503	CLA	CMB-C2B-C3B	3.04	130.36	124.68
32	m	103	BCR	C30-C25-C26	-3.04	118.33	122.61
29	T	316	CLA	CMB-C2B-C3B	3.04	130.36	124.68
29	K	207	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
37	D	307	PID	CM5-C21-C20	-3.03	118.67	122.92
29	b	702	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
29	a	814	CLA	CMB-C2B-C3B	3.03	130.35	124.68
29	b	710	CLA	CMB-C2B-C3B	3.03	130.35	124.68
29	B	306	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
29	E	308	CLA	CMB-C2B-C3B	3.03	130.35	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	816	CLA	CMB-C2B-C3B	3.03	130.35	124.68
36	G	307	DD6	C37-C36-C31	-3.03	120.23	124.35
29	a	825	CLA	CMB-C2B-C3B	3.03	130.34	124.68
32	l	507	BCR	C2-C1-C6	3.03	115.14	110.48
36	D	304	DD6	C-C1-C2	-3.03	118.68	122.92
29	b	712	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
39	N	312	KC1	CHC-C4B-C3B	-3.02	120.08	125.26
29	b	724	CLA	CMB-C2B-C3B	3.02	130.34	124.68
29	O	309	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
29	B	308	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
29	N	309	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
29	b	726	CLA	CMB-C2B-C3B	3.02	130.33	124.68
37	C	302	PID	C17-C16-C15	3.02	129.66	123.47
29	J	313	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
37	N	305	PID	CM5-C21-C20	-3.02	118.69	122.92
36	L	305	DD6	C9-C8-C6	-3.02	117.93	126.42
36	M	301	DD6	C9-C10-C11	-3.02	123.00	127.31
29	f	803	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
36	D	301	DD6	C-C1-C2	-3.02	118.69	122.92
38	T	306	UIX	C16-C20-C15	3.02	122.69	119.70
36	Q	302	DD6	C33-C34-C35	-3.02	106.17	110.30
29	F	316	CLA	CMB-C2B-C3B	3.02	130.32	124.68
29	b	712	CLA	CMB-C2B-C3B	3.01	130.32	124.68
29	D	308	CLA	CMB-C2B-C3B	3.01	130.32	124.68
29	O	316	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
37	G	309	PID	CM5-C21-C20	-3.01	118.70	122.92
29	a	813	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
36	h	202	DD6	C24-C1-C2	3.01	123.56	118.94
29	h	201	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
29	P	217	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
29	K	210	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
38	P	207	UIX	C18-O2-C27	-3.01	112.29	117.90
32	l	507	BCR	C15-C16-C17	-3.01	117.32	123.47
37	T	304	PID	C18-C19-C20	3.00	129.63	123.47
37	P	206	PID	C26-C25-C24	3.00	112.13	109.21
32	f	801	BCR	C3-C4-C5	-3.00	108.72	114.08
32	i	204	BCR	C28-C27-C26	-3.00	108.72	114.08
29	l	508	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
29	K	213	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
29	f	802	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
29	H	315	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
29	b	714	CLA	CMB-C2B-C3B	3.00	130.29	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	312	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
29	b	723	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
29	b	731	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
29	T	309	CLA	CMB-C2B-C3B	3.00	130.29	124.68
29	F	312	CLA	CMB-C2B-C3B	3.00	130.29	124.68
38	Q	305	UIX	C14-C23-C26	-3.00	118.00	126.42
36	G	305	DD6	C25-C26-C27	-3.00	117.88	126.58
29	b	703	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
29	P	214	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
36	O	303	DD6	C37-C36-C31	-2.99	120.28	124.35
35	j	106	DGD	O1G-C1A-C2A	2.99	121.30	111.91
32	l	507	BCR	C7-C8-C9	-2.99	121.71	126.23
37	T	317	PID	C16-C15-C14	-2.99	123.04	127.31
29	M	311	CLA	CMB-C2B-C3B	2.99	130.28	124.68
39	G	318	KC1	CHC-C4B-C3B	-2.99	120.14	125.26
29	P	212	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
29	a	805	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
29	a	808	CLA	CMB-C2B-C3B	2.99	130.27	124.68
29	b	720	CLA	CMB-C2B-C3B	2.99	130.27	124.68
36	G	307	DD6	C15-C14-C13	-2.99	119.68	125.99
36	J	301	DD6	C14-C13-C11	-2.99	120.90	125.53
39	T	312	KC1	CHC-C4B-C3B	-2.99	120.15	125.26
29	Q	315	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
32	m	103	BCR	C28-C27-C26	-2.99	108.75	114.08
29	a	819	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
29	A	207	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
29	Q	307	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
36	L	303	DD6	C10-C9-C8	-2.98	113.91	123.22
38	N	306	UIX	C22-C15-C20	-2.98	107.80	110.47
36	M	303	DD6	C21-C20-C19	2.98	117.64	114.28
36	I	202	DD6	C9-C10-C11	-2.98	123.05	127.31
29	C	316	CLA	CMB-C2B-C3B	2.98	130.26	124.68
36	h	202	DD6	C33-C34-C35	-2.98	106.22	110.30
37	F	304	PID	O1-C1-C2	2.98	115.62	113.38
36	E	302	DD6	C4-C3-C2	-2.98	117.37	123.47
29	F	307	CLA	CMB-C2B-C3B	2.98	130.25	124.68
29	Q	308	CLA	C1-C2-C3	-2.98	120.89	126.04
29	a	812	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
29	G	301	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
29	b	702	CLA	CMB-C2B-C3B	2.97	130.24	124.68
29	G	304	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
37	H	301	PID	CM5-C21-C20	-2.97	118.76	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	301	PID	CM5-C21-C20	-2.97	118.76	122.92
39	H	311	KC1	CHC-C4B-C3B	-2.97	120.18	125.26
29	G	319	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
29	A	209	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
29	K	212	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
29	B	312	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
29	a	803	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
29	a	810	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
36	A	202	DD6	C33-C34-C35	-2.97	106.25	110.30
36	D	304	DD6	C20-C19-C18	-2.96	106.88	112.75
38	A	203	UIX	C18-O2-C27	-2.96	112.37	117.90
32	b	735	BCR	C29-C30-C25	2.96	115.04	110.48
29	A	208	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
36	F	301	DD6	C15-C14-C13	-2.96	119.74	125.99
29	b	703	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
39	C	312	KC1	CHC-C4B-C3B	-2.96	120.20	125.26
29	B	309	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
35	B	318	DGD	C3D-C4D-C5D	2.96	115.51	110.24
29	M	306	CLA	CMB-C2B-C3B	2.96	130.21	124.68
37	N	301	PID	CM5-C21-C20	-2.96	118.78	122.92
38	N	306	UIX	C16-C20-C15	2.95	122.63	119.70
29	F	308	CLA	CMB-C2B-C3B	2.95	130.20	124.68
37	H	304	PID	C17-C18-C19	2.95	131.38	124.81
37	h	204	PID	CM5-C21-C20	-2.95	118.79	122.92
39	H	314	KC1	C3D-CAD-CBD	-2.95	103.72	107.61
29	G	302	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	Q	308	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	M	313	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	E	308	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
29	I	207	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
29	A	216	CLA	CMB-C2B-C3B	2.95	130.19	124.68
29	b	705	CLA	CAC-C3C-C4C	2.95	128.63	124.81
36	G	305	DD6	C20-C19-C18	-2.95	106.92	112.75
29	B	315	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
36	Q	302	DD6	O1-C20-C19	-2.94	111.17	113.38
29	J	310	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
36	B	305	DD6	C4-C5-C6	-2.94	123.11	127.31
29	G	311	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
29	a	822	CLA	CMB-C2B-C3B	2.94	130.19	124.68
39	Q	314	KC1	CHC-C4B-C3B	-2.94	120.22	125.26
29	I	217	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
36	J	303	DD6	C25-C26-C27	-2.94	118.03	126.58

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	317	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
36	F	301	DD6	C4-C5-C6	-2.94	123.11	127.31
29	H	313	CLA	CMB-C2B-C3B	2.94	130.18	124.68
38	B	304	UIX	C16-C20-C15	2.94	122.61	119.70
29	B	310	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
39	F	309	KC1	CHC-C4B-C3B	-2.94	120.23	125.26
29	a	818	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
29	Q	313	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
29	K	217	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
29	I	210	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
29	T	316	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
39	P	216	KC1	CHC-C4B-C3B	-2.93	120.24	125.26
37	D	303	PID	C12-O4-C10	2.93	109.18	107.65
32	f	804	BCR	C28-C27-C26	-2.93	108.84	114.08
29	H	308	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
36	L	305	DD6	C9-C10-C11	-2.93	123.13	127.31
39	H	314	KC1	CHC-C4B-C3B	-2.93	120.25	125.26
29	A	218	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	K	209	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
36	K	204	DD6	C12-C11-C10	-2.93	118.82	122.92
38	O	306	UIX	C12-C11-C13	-2.93	118.83	122.92
36	P	204	DD6	C37-C36-C31	-2.93	120.37	124.35
29	a	803	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
29	G	304	CLA	CMB-C2B-C3B	2.92	130.15	124.68
37	O	301	PID	CM5-C21-C20	-2.92	118.83	122.92
39	L	306	KC1	CHC-C4B-C3B	-2.92	120.26	125.26
29	a	824	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
36	I	204	DD6	C12-C11-C10	-2.92	118.83	122.92
39	Q	309	KC1	C3D-CAD-CBD	-2.92	103.76	107.61
36	K	204	DD6	C25-C24-C1	-2.92	118.21	126.42
36	I	202	DD6	C37-C36-C35	2.92	119.76	114.36
32	i	204	BCR	C16-C15-C14	-2.92	117.50	123.47
29	L	313	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
32	a	835	BCR	C3-C4-C5	-2.92	108.87	114.08
38	B	304	UIX	C18-O2-C27	-2.92	112.46	117.90
29	D	311	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
29	D	312	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
39	P	211	KC1	CHB-C1B-C2B	-2.92	119.36	125.48
29	C	316	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
36	L	305	DD6	C21-C20-C15	-2.91	117.38	122.26
39	E	307	KC1	CHC-C4B-C3B	-2.91	120.27	125.26
29	D	316	CLA	O2D-CGD-O1D	-2.91	118.14	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	303	DD6	C9-C10-C11	-2.91	123.16	127.31
39	P	216	KC1	C3D-CAD-CBD	-2.91	103.77	107.61
29	L	310	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
35	B	318	DGD	C2G-O2G-C1B	-2.91	110.64	117.79
36	A	204	DD6	C4-C5-C6	-2.91	123.16	127.31
29	H	313	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
29	Q	310	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
29	a	808	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
29	E	310	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
29	a	801	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
32	l	507	BCR	C16-C17-C18	-2.90	123.17	127.31
29	B	316	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
29	I	207	CLA	CMB-C2B-C3B	2.90	130.11	124.68
36	I	205	DD6	C7-C6-C5	-2.90	118.86	122.92
37	P	206	PID	CM5-C21-C20	-2.90	118.86	122.92
29	a	823	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
37	N	304	PID	CM5-C21-C20	-2.90	118.86	122.92
32	m	103	BCR	C11-C12-C13	-2.90	118.27	126.42
29	b	713	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
29	F	313	CLA	CMB-C2B-C3B	2.90	130.10	124.68
32	m	103	BCR	C15-C16-C17	-2.90	117.54	123.47
29	b	717	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
29	P	212	CLA	CMB-C2B-C3B	2.90	130.10	124.68
37	O	304	PID	C18-C19-C20	2.90	129.41	123.47
37	T	317	PID	CM5-C21-C20	-2.90	118.87	122.92
36	L	301	DD6	C33-C34-C35	-2.90	106.34	110.30
29	b	736	CLA	CMB-C2B-C3B	2.89	130.09	124.68
29	G	311	CLA	CMB-C2B-C3B	2.89	130.09	124.68
29	a	820	CLA	CMB-C2B-C3B	2.89	130.09	124.68
29	A	212	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
29	L	315	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
29	C	313	CLA	CMB-C2B-C3B	2.89	130.09	124.68
39	L	314	KC1	CHC-C4B-C3B	-2.89	120.31	125.26
29	N	316	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
32	f	801	BCR	C36-C18-C17	-2.89	118.88	122.92
29	b	720	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
29	O	313	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
36	G	307	DD6	C32-C31-C36	-2.89	118.56	122.63
29	l	505	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
29	a	837	CLA	CMB-C2B-C3B	2.89	130.08	124.68
38	N	306	UIX	C1-C3-C5	-2.88	107.04	112.75
29	b	707	CLA	CMB-C2B-C3B	2.88	130.07	124.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	715	CLA	CMB-C2B-C3B	2.88	130.07	124.68
34	j	102	LMG	O6-C1-O1	-2.88	103.15	109.97
29	I	213	CLA	CMB-C2B-C3B	2.88	130.07	124.68
29	K	208	CLA	CMB-C2B-C3B	2.88	130.07	124.68
29	E	306	CLA	CMB-C2B-C3B	2.88	130.07	124.68
29	b	709	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	E	313	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
39	H	309	KC1	CHC-C4B-C3B	-2.88	120.33	125.26
38	E	304	UIX	C36-C35-C32	-2.88	123.20	127.31
29	l	510	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	E	309	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	b	716	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
29	K	218	CLA	CMB-C2B-C3B	2.88	130.06	124.68
38	T	306	UIX	C22-C15-C20	-2.88	107.90	110.47
29	B	307	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	I	213	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
29	i	202	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
39	A	213	KC1	C3D-CAD-CBD	-2.87	103.82	107.61
29	b	705	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	Q	312	CLA	CMB-C2B-C3B	2.87	130.05	124.68
29	a	804	CLA	O2D-CGD-CBD	2.87	116.37	111.27
29	L	315	CLA	CAA-C2A-C3A	-2.87	109.40	116.10
35	j	106	DGD	C2G-O2G-C1B	-2.87	110.73	117.79
37	G	309	PID	C18-C19-C20	2.87	129.35	123.47
29	C	308	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	F	308	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	l	506	BCR	C11-C10-C9	-2.87	123.22	127.31
29	J	309	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	a	807	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
29	N	308	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
39	M	312	KC1	CHC-C4B-C3B	-2.86	120.36	125.26
36	T	303	DD6	C9-C8-C6	-2.86	118.37	126.42
29	a	837	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
37	P	202	PID	C17-C18-C19	2.86	131.18	124.81
36	C	303	DD6	C21-C20-C19	2.86	117.50	114.28
32	a	835	BCR	C33-C5-C4	2.86	119.11	113.62
38	F	305	UIX	O-C1-C6	2.86	118.48	115.06
37	D	305	PID	CM5-C21-C20	-2.86	118.92	122.92
37	O	307	PID	CM5-C21-C20	-2.86	118.92	122.92
38	Q	305	UIX	C12-C11-C13	-2.86	118.92	122.92
39	O	315	KC1	CHC-C4B-C3B	-2.86	120.37	125.26
38	F	305	UIX	C34-C37-C39	-2.86	117.62	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	L	314	KC1	C3D-CAD-CBD	-2.85	103.85	107.61
36	I	205	DD6	C24-C1-C2	2.85	123.32	118.94
38	C	306	UIX	C12-C11-C13	-2.85	118.93	122.92
29	A	215	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
36	E	303	DD6	C10-C9-C8	-2.85	114.32	123.22
37	G	303	PID	C12-O4-C10	2.85	109.13	107.65
29	L	311	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	O	311	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
32	b	729	BCR	C20-C21-C22	-2.85	123.24	127.31
37	Q	304	PID	C17-C16-C15	2.85	129.31	123.47
29	P	209	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	P	210	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	J	303	DD6	C24-C1-C2	2.85	123.31	118.94
29	a	816	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	P	214	CLA	CMB-C2B-C3B	2.85	130.00	124.68
29	b	722	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	L	312	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	H	310	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
37	T	304	PID	CM5-C21-C20	-2.84	118.94	122.92
29	b	706	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	J	307	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	P	217	CLA	CAA-C2A-C3A	-2.84	109.46	116.10
39	H	314	KC1	CHB-C1B-C2B	-2.84	119.52	125.48
39	F	314	KC1	CHC-C4B-C3B	-2.84	120.40	125.26
29	B	306	CLA	CMB-C2B-C3B	2.84	129.99	124.68
29	A	210	CLA	CMB-C2B-C3B	2.84	129.99	124.68
35	h	203	DGD	C2G-O2G-C1B	-2.84	110.81	117.79
29	K	216	CLA	CAA-C2A-C3A	-2.84	109.48	116.10
29	a	826	CLA	CMB-C2B-C3B	2.84	129.98	124.68
36	A	202	DD6	C21-C20-C15	-2.84	117.51	122.26
29	K	218	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	K	213	CLA	CMB-C2B-C3B	2.83	129.98	124.68
36	F	301	DD6	C37-C36-C35	2.83	119.60	114.36
29	L	317	CLA	CMB-C2B-C3B	2.83	129.98	124.68
34	K	220	LMG	O6-C1-O1	-2.83	103.27	109.97
36	L	301	DD6	O1-C20-C19	-2.83	111.26	113.38
29	M	308	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
36	O	303	DD6	C37-C36-C35	2.83	119.60	114.36
37	j	101	PID	CM5-C21-C20	-2.83	118.96	122.92
38	A	203	UIX	C35-C36-C38	-2.83	114.39	123.22
29	B	316	CLA	CMB-C2B-C3B	2.83	129.97	124.68
29	H	312	CLA	O2D-CGD-O1D	-2.83	118.31	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Q	311	KC1	C4B-CHC-C1C	-2.83	119.96	126.06
36	K	205	DD6	C3-C4-C5	-2.83	117.68	123.47
29	L	309	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
38	B	304	UIX	C36-C35-C32	-2.83	123.28	127.31
29	L	317	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
39	G	318	KC1	C3D-CAD-CBD	-2.82	103.89	107.61
36	I	204	DD6	C-C1-C2	-2.82	118.97	122.92
32	f	801	BCR	C7-C8-C9	-2.82	121.97	126.23
29	a	810	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
38	T	306	UIX	C14-C23-C26	-2.82	118.49	126.42
29	D	313	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
39	B	313	KC1	CHC-C4B-C3B	-2.82	120.43	125.26
36	A	204	DD6	C25-C26-C27	-2.82	118.39	126.58
29	a	818	CLA	CMB-C2B-C3B	2.82	129.96	124.68
32	f	801	BCR	C28-C27-C26	-2.82	109.04	114.08
29	b	725	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
39	B	313	KC1	C3D-CAD-CBD	-2.82	103.89	107.61
36	I	202	DD6	C25-C26-C27	-2.82	118.40	126.58
39	T	315	KC1	CHC-C4B-C3B	-2.82	120.44	125.26
32	l	507	BCR	C28-C27-C26	-2.82	109.05	114.08
29	C	309	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
29	l	510	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
29	H	307	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
29	P	209	CLA	CMB-C2B-C3B	2.81	129.94	124.68
29	M	315	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
29	T	308	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
29	F	311	CLA	CMB-C2B-C3B	2.81	129.94	124.68
29	b	705	CLA	CHB-C4A-NA	2.81	128.40	124.51
29	T	313	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
29	E	315	CLA	CMB-C2B-C3B	2.81	129.94	124.68
37	C	305	PID	C19-C20-C21	2.81	131.32	127.31
32	a	834	BCR	C23-C24-C25	-2.81	119.31	127.20
32	a	834	BCR	C38-C26-C27	2.81	119.02	113.62
32	b	728	BCR	C28-C27-C26	-2.81	109.06	114.08
36	h	202	DD6	C26-C25-C24	-2.81	114.45	123.22
32	b	735	BCR	C8-C7-C6	-2.81	119.32	127.20
29	I	212	CLA	CMB-C2B-C3B	2.81	129.93	124.68
38	N	306	UIX	C18-O2-C27	-2.81	112.67	117.90
29	M	308	CLA	CMB-C2B-C3B	2.80	129.93	124.68
29	E	314	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
36	B	319	DD6	C32-C33-C34	-2.80	107.31	113.64
29	J	305	CLA	CMB-C2B-C3B	2.80	129.92	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	204	BCR	C33-C5-C4	2.80	119.00	113.62
29	O	308	CLA	CMB-C2B-C3B	2.80	129.92	124.68
29	a	811	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
37	O	301	PID	C18-C19-C20	2.80	129.21	123.47
39	L	314	KC1	CHB-C1B-C2B	-2.80	119.61	125.48
29	a	823	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	O	308	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
38	E	304	UIX	C22-C15-C20	-2.80	107.97	110.47
29	T	309	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
39	A	213	KC1	CHC-C4B-C3B	-2.79	120.48	125.26
29	a	820	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	a	834	BCR	C24-C23-C22	-2.79	122.01	126.23
29	b	710	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
39	Q	309	KC1	CHC-C4B-C3B	-2.79	120.48	125.26
29	F	313	CLA	CHB-C4A-NA	2.79	128.37	124.51
39	Q	311	KC1	C3D-CAD-CBD	-2.79	103.93	107.61
38	C	306	UIX	C1-C3-C5	-2.79	107.23	112.75
36	A	202	DD6	C9-C10-C11	-2.79	123.33	127.31
32	b	729	BCR	C10-C11-C12	-2.79	114.51	123.22
36	B	305	DD6	C9-C10-C11	-2.79	123.33	127.31
29	D	308	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
36	K	205	DD6	C37-C36-C35	2.79	119.52	114.36
36	A	204	DD6	C33-C34-C35	-2.79	106.49	110.30
29	a	822	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
29	A	214	CLA	CMB-C2B-C3B	2.79	129.89	124.68
39	O	310	KC1	CHC-C4B-C3B	-2.78	120.50	125.26
39	G	315	KC1	C4B-CHC-C1C	-2.78	120.05	126.06
29	G	304	CLA	CHB-C4A-NA	2.78	128.36	124.51
36	J	303	DD6	C12-C11-C10	-2.78	119.02	122.92
37	T	302	PID	CM5-C21-C20	-2.78	119.02	122.92
39	Q	311	KC1	CHC-C4B-C3B	-2.78	120.50	125.26
29	M	314	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
29	N	311	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	O	314	CLA	O2D-CGD-CBD	2.78	116.21	111.27
37	D	303	PID	CM5-C21-C20	-2.78	119.03	122.92
39	M	312	KC1	CHB-C1B-C2B	-2.78	119.64	125.48
29	a	804	CLA	CMB-C2B-C3B	2.78	129.88	124.68
29	B	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
39	N	310	KC1	CHC-C4B-C3B	-2.78	120.50	125.26
35	j	103	DGD	O1G-C1A-C2A	2.78	120.63	111.91
29	a	811	CLA	CMB-C2B-C3B	2.78	129.87	124.68
32	l	506	BCR	C33-C5-C6	-2.77	121.41	124.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	303	DD6	C-C1-C2	-2.77	119.04	122.92
29	A	211	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
29	M	307	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	a	805	CLA	CHB-C4A-NA	2.77	128.35	124.51
36	N	303	DD6	C21-C20-C15	-2.77	117.61	122.26
29	j	104	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
39	A	213	KC1	CHB-C1B-C2B	-2.77	119.67	125.48
39	D	310	KC1	C3D-CAD-CBD	-2.77	103.96	107.61
36	h	202	DD6	C10-C9-C8	-2.77	114.58	123.22
39	L	306	KC1	C3D-CAD-CBD	-2.77	103.96	107.61
29	b	701	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
29	E	309	CLA	CMB-C2B-C3B	2.77	129.85	124.68
37	O	304	PID	CM5-C21-C20	-2.77	119.05	122.92
29	T	308	CLA	CMB-C2B-C3B	2.77	129.85	124.68
36	L	303	DD6	C12-C11-C13	2.77	122.43	118.08
39	C	310	KC1	CHC-C4B-C3B	-2.77	120.53	125.26
29	C	313	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
36	J	301	DD6	C-C1-C2	-2.76	119.05	122.92
38	J	304	UIX	C7-C10-C11	-2.76	121.24	125.53
29	a	813	CLA	CMB-C2B-C3B	2.76	129.84	124.68
29	a	817	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
32	f	801	BCR	C20-C19-C18	-2.76	118.67	126.42
29	a	814	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	I	217	CLA	CMB-C2B-C3B	2.76	129.84	124.68
35	h	203	DGD	O1G-C1A-C2A	2.76	120.56	111.91
32	b	735	BCR	C38-C26-C25	-2.76	121.43	124.53
39	O	312	KC1	C4B-CHC-C1C	-2.75	120.12	126.06
36	E	302	DD6	C9-C8-C6	-2.75	118.68	126.42
36	K	206	DD6	C21-C20-C15	-2.75	117.65	122.26
36	H	303	DD6	C33-C34-C35	-2.75	106.54	110.30
29	I	214	CLA	CHB-C4A-NA	2.75	128.32	124.51
29	Q	307	CLA	CMB-C2B-C3B	2.75	129.82	124.68
29	J	305	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	F	312	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
39	E	312	KC1	O1D-CGD-CBD	-2.75	118.86	124.48
34	b	730	LMG	O6-C1-O1	-2.75	103.47	109.97
38	T	306	UIX	C12-C11-C13	-2.75	119.08	122.92
29	a	828	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
39	A	205	KC1	CHB-C1B-C2B	-2.75	119.72	125.48
36	F	301	DD6	C25-C26-C27	-2.74	118.61	126.58
37	P	205	PID	CM5-C21-C20	-2.74	119.08	122.92
37	T	302	PID	C18-C17-C16	2.74	130.92	124.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	503	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
36	P	204	DD6	C37-C36-C35	2.74	119.44	114.36
34	b	734	LMG	O6-C1-O1	-2.74	103.48	109.97
36	L	305	DD6	C14-C13-C11	-2.74	121.28	125.53
36	J	301	DD6	C3-C4-C5	-2.74	117.86	123.47
29	K	207	CLA	CMB-C2B-C3B	2.74	129.80	124.68
36	L	301	DD6	C15-C14-C13	-2.74	120.20	125.99
29	A	215	CLA	CMB-C2B-C3B	2.74	129.80	124.68
29	D	309	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	T	316	CLA	CAA-C2A-C3A	-2.74	109.71	116.10
32	a	838	BCR	C38-C26-C25	-2.74	121.45	124.53
39	C	315	KC1	CHC-C4B-C3B	-2.74	120.58	125.26
29	A	206	CLA	CMB-C2B-C3B	2.74	129.80	124.68
39	P	213	KC1	O1D-CGD-CBD	-2.73	118.89	124.48
29	a	828	CLA	CMB-C2B-C3B	2.73	129.79	124.68
29	K	214	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
32	f	801	BCR	C38-C26-C25	-2.73	121.46	124.53
29	C	308	CLA	CMB-C2B-C3B	2.73	129.79	124.68
29	l	502	CLA	CMB-C2B-C3B	2.73	129.79	124.68
39	P	213	KC1	C4B-CHC-C1C	-2.73	120.17	126.06
37	E	301	PID	CM5-C21-C20	-2.73	119.10	122.92
39	D	310	KC1	CHC-C4B-C3B	-2.73	120.59	125.26
36	K	206	DD6	C25-C24-C1	-2.73	118.75	126.42
39	Q	314	KC1	CHB-C1B-C2B	-2.73	119.75	125.48
39	I	215	KC1	CHC-C4B-C3B	-2.73	120.59	125.26
37	C	304	PID	C18-C19-C20	2.73	129.06	123.47
29	A	216	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
39	M	305	KC1	O1D-CGD-CBD	-2.73	118.91	124.48
29	F	313	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
29	A	217	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
39	N	310	KC1	CHB-C1B-C2B	-2.72	119.77	125.48
29	L	315	CLA	CMB-C2B-C3B	2.72	129.77	124.68
29	J	306	CLA	C1-C2-C3	-2.72	121.34	126.04
36	J	302	DD6	C25-C24-C1	-2.72	118.78	126.42
29	B	311	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
29	D	314	CLA	CHB-C4A-NA	2.72	128.27	124.51
29	I	208	CLA	CMB-C2B-C3B	2.72	129.76	124.68
39	O	312	KC1	CHC-C4B-C3B	-2.72	120.61	125.26
38	Q	305	UIX	C16-C20-C15	2.72	122.39	119.70
30	b	727	PQN	C2M-C2-C3	-2.72	119.97	124.40
36	J	303	DD6	C-C1-C2	-2.72	119.12	122.92
37	C	304	PID	CM5-C21-C20	-2.72	119.12	122.92

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	E	312	KC1	CHB-C1B-C2B	-2.72	119.78	125.48
38	O	306	UIX	C14-C23-C26	-2.72	118.79	126.42
37	E	301	PID	C17-C18-C19	2.71	130.85	124.81
37	F	304	PID	CM5-C21-C20	-2.71	119.12	122.92
32	b	735	BCR	C38-C26-C27	2.71	118.83	113.62
36	I	203	DD6	C15-C14-C13	-2.71	120.26	125.99
29	a	806	CLA	CHB-C4A-NA	2.71	128.26	124.51
36	M	301	DD6	C33-C34-C35	-2.71	106.59	110.30
39	A	205	KC1	CHC-C4B-C3B	-2.71	120.62	125.26
32	m	103	BCR	C3-C4-C5	-2.71	109.24	114.08
36	O	303	DD6	C25-C24-C1	-2.71	118.80	126.42
29	D	312	CLA	CMB-C2B-C3B	2.71	129.74	124.68
36	B	302	DD6	C14-C13-C11	-2.71	121.33	125.53
34	K	201	LMG	O6-C1-O1	-2.71	103.57	109.97
29	F	310	CLA	CHB-C4A-NA	2.71	128.25	124.51
36	G	307	DD6	C23-C16-C22	2.70	111.36	107.37
35	j	105	DGD	C2G-O2G-C1B	-2.70	111.13	117.79
29	b	719	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
29	F	311	CLA	CHB-C4A-NA	2.70	128.25	124.51
29	a	821	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
29	A	210	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
36	K	203	DD6	C21-C20-C15	-2.70	117.73	122.26
37	D	306	PID	C17-C16-C15	2.70	129.01	123.47
32	b	729	BCR	C23-C24-C25	-2.70	119.62	127.20
37	H	304	PID	CM5-C21-C20	-2.70	119.14	122.92
29	H	307	CLA	CMB-C2B-C3B	2.70	129.72	124.68
36	A	204	DD6	C21-C20-C15	-2.70	117.74	122.26
29	I	214	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
29	L	311	CLA	CMB-C2B-C3B	2.69	129.72	124.68
29	K	214	CLA	CHB-C4A-NA	2.69	128.24	124.51
39	I	215	KC1	CHB-C1B-C2B	-2.69	119.83	125.48
36	A	202	DD6	O1-C20-C19	-2.69	111.36	113.38
39	B	313	KC1	CHB-C1B-C2B	-2.69	119.83	125.48
36	B	305	DD6	C33-C34-C35	-2.69	106.62	110.30
36	G	306	DD6	C3-C4-C5	-2.69	117.96	123.47
39	O	315	KC1	O1D-CGD-CBD	-2.69	118.98	124.48
38	O	306	UIX	C22-C15-C20	-2.69	108.06	110.47
36	C	303	DD6	C33-C34-C35	-2.69	106.62	110.30
37	O	305	PID	C19-C20-C21	2.69	131.15	127.31
38	F	305	UIX	C36-C38-C40	-2.69	118.87	126.42
29	C	314	CLA	CHB-C4A-NA	2.69	128.22	124.51
29	N	308	CLA	CMB-C2B-C3B	2.68	129.70	124.68

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	727	PQN	C14-C13-C15	2.68	119.78	115.27
36	O	303	DD6	C14-C13-C11	-2.68	121.37	125.53
29	A	216	CLA	CAA-C2A-C3A	-2.68	109.85	116.10
29	J	313	CLA	CAA-C2A-C3A	-2.68	109.86	116.10
29	K	214	CLA	CMB-C2B-C3B	2.67	129.68	124.68
29	b	707	CLA	CHB-C4A-NA	2.67	128.21	124.51
38	P	207	UIX	C36-C38-C40	-2.67	118.90	126.42
36	I	203	DD6	C37-C36-C35	2.67	119.31	114.36
37	O	307	PID	CM3-C5-C4	-2.67	104.34	108.98
29	a	809	CLA	CHB-C4A-NA	2.67	128.21	124.51
29	a	817	CLA	CMB-C2B-C3B	2.67	129.67	124.68
29	b	721	CLA	CMB-C2B-C3B	2.67	129.67	124.68
38	L	302	UIX	C14-C13-C11	-2.67	123.50	127.31
32	i	204	BCR	C20-C19-C18	-2.67	118.92	126.42
29	G	304	CLA	C1-C2-C3	-2.67	121.43	126.04
39	P	216	KC1	CHB-C1B-C2B	-2.67	119.89	125.48
39	N	312	KC1	CHB-C1B-C2B	-2.67	119.89	125.48
36	J	301	DD6	C9-C8-C6	-2.67	118.93	126.42
29	i	201	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
29	M	309	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
29	P	215	CLA	O2D-CGD-CBD	2.66	116.00	111.27
29	E	314	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
39	E	307	KC1	CBD-CHA-C1A	2.66	133.85	128.88
29	D	309	CLA	CHB-C4A-NA	2.66	128.20	124.51
39	N	315	KC1	CHC-C4B-C3B	-2.66	120.70	125.26
39	Q	309	KC1	O1D-CGD-CBD	-2.66	119.03	124.48
39	C	312	KC1	C4B-CHC-C1C	-2.66	120.31	126.06
29	i	202	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
38	P	207	UIX	C14-C23-C26	-2.66	118.94	126.42
38	L	302	UIX	C36-C35-C32	-2.66	123.51	127.31
39	C	310	KC1	CHB-C1B-C2B	-2.66	119.90	125.48
36	K	221	DD6	C12-C11-C10	-2.66	119.20	122.92
32	l	507	BCR	C35-C13-C14	-2.66	119.20	122.92
37	P	202	PID	CM5-C21-C20	-2.66	119.20	122.92
29	J	311	CLA	CMB-C2B-C3B	2.66	129.65	124.68
29	G	302	CLA	CHB-C4A-NA	2.66	128.19	124.51
39	F	309	KC1	CHB-C1B-C2B	-2.66	119.91	125.48
39	H	309	KC1	CHB-C1B-C2B	-2.66	119.91	125.48
39	O	310	KC1	CHB-C1B-C2B	-2.65	119.91	125.48
32	a	838	BCR	C20-C19-C18	-2.65	118.96	126.42
29	F	316	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
38	T	306	UIX	C36-C38-C40	-2.65	118.96	126.42

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	K	206	DD6	C14-C13-C11	-2.65	121.41	125.53
37	T	307	PID	CM2-C5-C4	-2.65	104.37	108.98
36	F	303	DD6	C4-C3-C2	-2.65	118.04	123.47
36	M	302	DD6	C3-C4-C5	-2.65	118.04	123.47
36	B	319	DD6	C4-C3-C2	-2.65	118.04	123.47
36	T	303	DD6	C33-C34-C35	-2.65	106.68	110.30
29	a	801	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
39	C	315	KC1	C4B-CHC-C1C	-2.65	120.35	126.06
39	P	213	KC1	CHC-C4B-C3B	-2.65	120.73	125.26
36	h	202	DD6	O1-C20-C21	2.65	118.23	115.06
39	J	312	KC1	CHB-C1B-C2B	-2.65	119.93	125.48
29	A	214	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
39	D	315	KC1	CHC-C4B-C3B	-2.64	120.73	125.26
29	A	210	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
29	M	314	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
36	H	303	DD6	C9-C8-C6	-2.64	118.99	126.42
29	F	315	CLA	CAA-C2A-C3A	-2.64	109.93	116.10
29	a	820	CLA	CHB-C4A-NA	2.64	128.16	124.51
39	L	306	KC1	CHB-C1B-C2B	-2.64	119.94	125.48
29	L	307	CLA	C1-C2-C3	-2.64	122.48	126.75
39	E	312	KC1	O2D-CGD-O1D	-2.64	118.68	123.84
29	L	317	CLA	CHB-C4A-NA	2.64	128.16	124.51
38	C	306	UIX	C22-C15-C20	-2.64	108.11	110.47
38	B	304	UIX	C7-C10-C11	-2.64	121.44	125.53
36	E	302	DD6	C37-C36-C35	2.64	119.24	114.36
38	A	203	UIX	C21-C15-C20	-2.64	108.11	110.47
29	Q	315	CLA	CAA-C2A-C3A	-2.64	109.95	116.10
35	G	320	DGD	O1G-C1A-C2A	2.63	120.18	111.91
36	N	303	DD6	C33-C34-C35	-2.63	106.70	110.30
35	m	102	DGD	O1G-C1A-C2A	2.63	120.17	111.91
38	Q	305	UIX	C22-C15-C20	-2.63	108.11	110.47
29	L	307	CLA	CHB-C4A-NA	2.63	128.15	124.51
39	N	312	KC1	C3D-CAD-CBD	-2.63	104.14	107.61
38	Q	305	UIX	C18-O2-C27	-2.63	112.99	117.90
36	F	301	DD6	C14-C13-C11	-2.63	121.45	125.53
29	C	316	CLA	CAA-C2A-C3A	-2.63	109.96	116.10
36	h	202	DD6	C-C1-C2	-2.63	119.24	122.92
38	O	306	UIX	C36-C38-C40	-2.63	119.03	126.42
39	P	211	KC1	C3D-CAD-CBD	-2.62	104.15	107.61
39	O	315	KC1	C4B-CHC-C1C	-2.62	120.40	126.06
36	K	205	DD6	C4-C5-C6	-2.62	123.56	127.31
29	a	827	CLA	CMB-C2B-C3B	2.62	129.58	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	303	DD6	C9-C8-C6	-2.62	119.05	126.42
36	A	204	DD6	O1-C20-C19	-2.62	111.41	113.38
36	L	301	DD6	C21-C20-C15	-2.62	117.87	122.26
29	b	736	CLA	CHB-C4A-NA	2.62	128.13	124.51
29	Q	313	CLA	CMB-C2B-C3B	2.62	129.58	124.68
39	M	305	KC1	CHC-C4B-C3B	-2.62	120.78	125.26
39	T	315	KC1	CHB-C1B-C2B	-2.62	119.99	125.48
29	E	308	CLA	CHB-C4A-NA	2.61	128.13	124.51
29	M	310	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
29	a	819	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
32	f	804	BCR	C3-C4-C5	-2.61	109.41	114.08
36	M	301	DD6	C41-C32-C31	-2.61	106.32	110.47
29	E	305	CLA	CMB-C2B-C3B	2.61	129.56	124.68
29	j	104	CLA	CHB-C4A-NA	2.61	128.12	124.51
36	B	301	DD6	C8-C6-C5	-2.61	119.00	124.81
37	G	303	PID	CM5-C21-C20	-2.61	119.27	122.92
32	a	835	BCR	C28-C27-C26	-2.61	109.42	114.08
39	K	215	KC1	CHB-C1B-C2B	-2.61	120.01	125.48
36	K	204	DD6	C24-C1-C2	2.61	122.94	118.94
36	I	205	DD6	C25-C26-C27	-2.61	119.01	126.58
36	m	101	DD6	C37-C36-C35	2.61	119.18	114.36
37	Q	303	PID	CM5-C21-C20	-2.61	119.27	122.92
37	P	206	PID	C29-C24-C25	2.61	122.28	119.70
39	O	310	KC1	CBD-CHA-C1A	2.61	133.74	128.88
39	I	215	KC1	O1D-CGD-CBD	-2.61	119.15	124.48
29	b	704	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
39	D	315	KC1	CHB-C1B-C2B	-2.60	120.02	125.48
29	f	805	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
36	Q	302	DD6	C14-C13-C11	-2.60	121.49	125.53
36	I	203	DD6	C25-C24-C1	-2.60	119.11	126.42
39	G	318	KC1	CHB-C1B-C2B	-2.60	120.02	125.48
35	m	102	DGD	C2G-O2G-C1B	-2.60	111.39	117.79
29	E	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
32	a	838	BCR	C23-C24-C25	-2.60	119.90	127.20
34	b	732	LMG	C1-C2-C3	-2.60	104.58	110.00
32	b	729	BCR	C39-C30-C25	-2.60	106.08	110.30
29	A	206	CLA	CHB-C4A-NA	2.60	128.10	124.51
36	B	301	DD6	O1-C20-C21	-2.59	111.95	115.06
36	D	301	DD6	C24-C1-C2	2.59	122.92	118.94
29	B	314	CLA	CAA-C2A-C3A	-2.59	110.05	116.10
36	O	303	DD6	C20-C19-C18	-2.59	107.62	112.75
36	A	201	DD6	C21-C20-C15	-2.59	117.92	122.26

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	316	CLA	CMB-C2B-C3B	2.59	129.53	124.68
39	C	315	KC1	CHB-C1B-C2B	-2.59	120.05	125.48
39	H	309	KC1	CBD-CHA-C1A	2.59	133.71	128.88
39	T	312	KC1	C4B-CHC-C1C	-2.59	120.47	126.06
29	i	201	CLA	CHB-C4A-NA	2.59	128.09	124.51
29	N	316	CLA	CAA-C2A-C3A	-2.59	110.06	116.10
36	G	307	DD6	C37-C36-C35	2.59	119.15	114.36
29	L	316	CLA	CMB-C2B-C3B	2.59	129.52	124.68
39	H	311	KC1	C4B-CHC-C1C	-2.59	120.48	126.06
29	a	807	CLA	CHB-C4A-NA	2.59	128.09	124.51
39	F	314	KC1	CHB-C1B-C2B	-2.59	120.06	125.48
29	F	316	CLA	CAA-C2A-C3A	-2.59	110.06	116.10
39	H	309	KC1	O1D-CGD-CBD	-2.59	119.19	124.48
29	K	207	CLA	CHB-C4A-NA	2.59	128.09	124.51
29	D	316	CLA	CAA-C2A-C3A	-2.58	110.07	116.10
37	P	205	PID	C17-C18-C19	2.58	130.56	124.81
29	a	804	CLA	CHB-C4A-NA	2.58	128.08	124.51
29	b	725	CLA	CMB-C2B-C3B	2.58	129.51	124.68
29	I	211	CLA	O2D-CGD-CBD	2.58	115.86	111.27
39	P	211	KC1	CHC-C4B-C3B	-2.58	120.84	125.26
29	G	312	CLA	CHB-C4A-NA	2.58	128.08	124.51
29	M	306	CLA	CHB-C4A-NA	2.58	128.08	124.51
39	O	310	KC1	C2A-C3A-C4A	2.58	108.40	106.49
39	M	312	KC1	C4B-CHC-C1C	-2.58	120.49	126.06
29	F	316	CLA	CHB-C4A-NA	2.58	128.08	124.51
39	H	311	KC1	CBD-CHA-C1A	2.58	133.69	128.88
29	b	701	CLA	CHB-C4A-NA	2.58	128.07	124.51
36	J	303	DD6	C37-C36-C35	2.58	119.13	114.36
38	E	304	UIX	O2-C27-O4	-2.57	117.85	122.96
29	K	212	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
29	G	319	CLA	CAA-C2A-C3A	-2.57	110.09	116.10
37	T	305	PID	C17-C16-C15	2.57	128.75	123.47
32	l	506	BCR	C2-C1-C6	2.57	114.44	110.48
29	G	314	CLA	C1-C2-C3	-2.57	121.59	126.04
36	L	305	DD6	C25-C26-C27	-2.57	119.11	126.58
36	J	301	DD6	C12-C11-C10	-2.57	119.32	122.92
36	O	303	DD6	C32-C31-C36	-2.57	119.00	122.63
36	M	302	DD6	C14-C13-C11	-2.57	121.54	125.53
38	E	304	UIX	C14-C13-C11	-2.57	123.64	127.31
39	O	315	KC1	CHB-C1B-C2B	-2.57	120.09	125.48
39	E	307	KC1	C2A-C3A-C4A	2.57	108.39	106.49
36	K	206	DD6	C25-C26-C27	-2.57	119.13	126.58

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	T	312	KC1	CHB-C1B-C2B	-2.57	120.10	125.48
39	F	314	KC1	C4B-CHC-C1C	-2.57	120.52	126.06
32	b	735	BCR	C33-C5-C4	2.57	118.55	113.62
39	D	315	KC1	C4B-CHC-C1C	-2.57	120.52	126.06
39	O	312	KC1	CHB-C1B-C2B	-2.57	120.10	125.48
39	D	310	KC1	CHB-C1B-C2B	-2.57	120.10	125.48
39	F	309	KC1	C4B-CHC-C1C	-2.56	120.53	126.06
39	M	305	KC1	CHB-C1B-C2B	-2.56	120.10	125.48
29	H	308	CLA	CHB-C4A-NA	2.56	128.06	124.51
36	B	302	DD6	C21-C20-C15	-2.56	117.96	122.26
36	L	305	DD6	C37-C36-C35	2.56	119.11	114.36
29	T	314	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
29	A	215	CLA	CHB-C4A-NA	2.56	128.06	124.51
39	E	307	KC1	C4B-CHC-C1C	-2.56	120.53	126.06
29	b	717	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
38	L	302	UIX	C18-O2-C27	-2.56	113.12	117.90
39	Q	309	KC1	C2A-C3A-C4A	2.56	108.39	106.49
29	D	311	CLA	CHB-C4A-NA	2.56	128.05	124.51
39	J	312	KC1	C4B-CHC-C1C	-2.56	120.54	126.06
29	l	501	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
36	G	308	DD6	C12-C11-C10	-2.56	119.34	122.92
29	l	510	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
29	G	314	CLA	CHB-C4A-NA	2.56	128.05	124.51
29	K	217	CLA	CMB-C2B-C3B	2.56	129.46	124.68
29	b	701	CLA	C1-C2-C3	-2.56	121.62	126.04
29	a	828	CLA	CHB-C4A-NA	2.56	128.05	124.51
39	N	310	KC1	C3D-CAD-CBD	-2.55	104.24	107.61
29	T	314	CLA	CHB-C4A-NA	2.55	128.04	124.51
35	j	103	DGD	O6E-C5E-C4E	2.55	114.33	109.69
29	G	301	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
29	H	312	CLA	CHB-C4A-NA	2.55	128.04	124.51
29	H	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
29	a	827	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
39	Q	311	KC1	O1D-CGD-CBD	-2.55	119.26	124.48
36	K	221	DD6	C37-C36-C35	2.55	119.08	114.36
29	b	736	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
29	I	214	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
29	C	311	CLA	CHB-C4A-NA	2.55	128.04	124.51
37	O	305	PID	C17-C18-C19	2.55	130.48	124.81
38	O	306	UIX	C18-O2-C27	-2.55	113.14	117.90
39	T	315	KC1	C4B-CHC-C1C	-2.55	120.56	126.06
29	b	725	CLA	O2A-CGA-O1A	-2.55	117.16	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	h	204	PID	C17-C16-C15	2.55	128.70	123.47
37	P	203	PID	C18-C17-C16	2.55	130.48	124.81
36	L	304	DD6	C21-C20-C15	-2.55	117.99	122.26
36	T	303	DD6	C21-C20-C15	-2.55	117.99	122.26
39	C	315	KC1	O1D-CGD-CBD	-2.55	119.28	124.48
39	F	309	KC1	CBD-CHA-C1A	2.55	133.63	128.88
34	h	205	LMG	O6-C1-O1	-2.54	103.95	109.97
29	I	207	CLA	CHB-C4A-NA	2.54	128.03	124.51
36	M	304	DD6	C21-C20-C15	-2.54	118.00	122.26
29	K	218	CLA	CHB-C4A-NA	2.54	128.03	124.51
32	l	506	BCR	C10-C11-C12	-2.54	115.28	123.22
29	H	308	CLA	C1-C2-C3	-2.54	121.65	126.04
39	J	312	KC1	CHC-C4B-C3B	-2.54	120.91	125.26
29	a	802	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
39	A	205	KC1	C3D-CAD-CBD	-2.54	104.26	107.61
36	C	303	DD6	O1-C20-C21	2.54	118.10	115.06
29	a	820	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
29	a	812	CLA	CHB-C4A-NA	2.54	128.02	124.51
39	L	306	KC1	CBD-CHA-C1A	2.54	133.61	128.88
29	B	308	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
29	b	722	CLA	CHB-C4A-NA	2.54	128.02	124.51
29	E	308	CLA	CHD-C1D-ND	-2.54	122.12	124.45
29	B	311	CLA	CHB-C4A-NA	2.54	128.02	124.51
39	H	311	KC1	CHB-C1B-C2B	-2.54	120.16	125.48
36	I	204	DD6	C25-C24-C1	-2.54	119.29	126.42
29	b	721	CLA	CHB-C4A-NA	2.54	128.02	124.51
29	N	314	CLA	CHB-C4A-NA	2.53	128.02	124.51
36	I	205	DD6	C37-C36-C35	2.53	119.05	114.36
39	H	311	KC1	O1D-CGD-CBD	-2.53	119.30	124.48
36	N	303	DD6	C14-C13-C11	-2.53	121.60	125.53
29	C	314	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
29	a	827	CLA	CHB-C4A-NA	2.53	128.01	124.51
39	N	315	KC1	CHB-C1B-C2B	-2.53	120.17	125.48
29	b	718	CLA	C2D-C1D-ND	-2.53	108.24	110.10
35	j	105	DGD	O1G-C1A-C2A	2.53	119.85	111.91
29	L	315	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	Q	310	CLA	CHB-C4A-NA	2.53	128.01	124.51
36	M	303	DD6	C9-C8-C6	-2.53	119.31	126.42
32	b	735	BCR	C10-C11-C12	-2.53	115.32	123.22
29	O	311	CLA	CHB-C4A-NA	2.53	128.01	124.51
29	G	312	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
36	K	202	DD6	C37-C36-C35	2.53	119.04	114.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	303	DD6	C37-C36-C35	2.53	119.04	114.36
36	H	303	DD6	C14-C13-C11	-2.53	121.61	125.53
32	b	729	BCR	C15-C16-C17	-2.53	118.30	123.47
29	K	211	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
29	h	201	CLA	CHB-C4A-NA	2.53	128.00	124.51
29	T	311	CLA	CHB-C4A-NA	2.53	128.00	124.51
29	b	705	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
29	b	706	CLA	CHB-C4A-NA	2.52	128.00	124.51
39	Q	309	KC1	CHB-C1B-C2B	-2.52	120.19	125.48
39	C	312	KC1	CHB-C1B-C2B	-2.52	120.19	125.48
29	b	713	CLA	CMB-C2B-C3B	2.52	129.40	124.68
36	B	301	DD6	C28-C27-C29	2.52	121.83	116.84
29	A	216	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	G	313	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	F	315	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	a	815	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	K	216	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	P	217	CLA	CHB-C4A-NA	2.52	128.00	124.51
36	I	205	DD6	C-C1-C2	-2.52	119.39	122.92
38	P	207	UIX	C12-C11-C13	-2.52	119.39	122.92
29	M	310	CLA	CHB-C4A-NA	2.52	128.00	124.51
39	L	306	KC1	O1D-CGD-CBD	-2.52	119.33	124.48
39	N	310	KC1	C4B-CHC-C1C	-2.52	120.63	126.06
29	A	212	CLA	CHB-C4A-NA	2.52	127.99	124.51
37	P	202	PID	C18-C17-C16	2.52	130.41	124.81
29	b	704	CLA	C1B-CHB-C4A	-2.52	125.14	130.12
29	G	311	CLA	CHB-C4A-NA	2.51	127.99	124.51
36	I	202	DD6	C21-C20-C15	-2.51	118.05	122.26
29	b	731	CLA	CHB-C4A-NA	2.51	127.99	124.51
39	Q	309	KC1	C4B-CHC-C1C	-2.51	120.64	126.06
37	T	317	PID	C15-C14-C13	2.51	123.88	117.00
29	M	311	CLA	O2D-CGD-CBD	2.51	115.73	111.27
39	Q	309	KC1	O2D-CGD-O1D	-2.51	118.93	123.84
39	D	310	KC1	C4B-CHC-C1C	-2.51	120.64	126.06
29	T	313	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	b	715	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
37	H	305	PID	CM5-C21-C20	-2.51	119.41	122.92
29	Q	313	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	a	832	PQN	C2M-C2-C1	2.51	120.43	116.27
29	J	311	CLA	CHB-C4A-NA	2.51	127.98	124.51
39	C	312	KC1	O1D-CGD-CBD	-2.51	119.35	124.48
29	G	319	CLA	CHB-C4A-NA	2.51	127.98	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	301	PID	C19-C20-C21	2.51	130.89	127.31
39	M	305	KC1	C4B-CHC-C1C	-2.51	120.65	126.06
36	B	302	DD6	C28-C27-C29	2.51	121.80	116.84
29	C	316	CLA	CHB-C4A-NA	2.50	127.97	124.51
38	B	304	UIX	C22-C15-C20	-2.50	108.23	110.47
29	L	310	CLA	CHB-C4A-NA	2.50	127.97	124.51
38	C	306	UIX	C18-O2-C27	-2.50	113.23	117.90
36	K	221	DD6	C-C1-C2	-2.50	119.42	122.92
29	b	709	CLA	CHB-C4A-NA	2.50	127.97	124.51
29	J	306	CLA	CHB-C4A-NA	2.50	127.97	124.51
39	K	215	KC1	CBD-CHA-C1A	2.50	133.54	128.88
29	I	216	CLA	CHB-C4A-NA	2.50	127.97	124.51
36	G	306	DD6	C25-C24-C1	-2.50	119.39	126.42
29	C	309	CLA	CHB-C4A-NA	2.50	127.97	124.51
36	M	302	DD6	C32-C33-C34	-2.50	108.00	113.64
32	l	506	BCR	C38-C26-C27	2.50	118.41	113.62
29	l	502	CLA	CHB-C4A-NA	2.50	127.96	124.51
29	B	312	CLA	CHB-C4A-NA	2.50	127.96	124.51
29	P	210	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
35	B	318	DGD	O1G-C1A-C2A	2.50	119.74	111.91
29	N	308	CLA	CHB-C4A-NA	2.50	127.96	124.51
29	a	801	CLA	CMB-C2B-C3B	2.50	129.35	124.68
29	l	501	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	B	309	CLA	CHB-C4A-NA	2.49	127.96	124.51
32	f	804	BCR	C15-C16-C17	-2.49	118.36	123.47
39	L	314	KC1	CAC-C3C-C4C	2.49	128.05	124.81
39	N	312	KC1	C4B-CHC-C1C	-2.49	120.68	126.06
36	m	101	DD6	C25-C24-C1	-2.49	119.41	126.42
29	l	503	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	T	316	CLA	CHB-C4A-NA	2.49	127.96	124.51
36	M	304	DD6	C25-C26-C27	-2.49	119.34	126.58
38	C	306	UIX	C16-C20-C15	2.49	122.17	119.70
39	H	314	KC1	C4B-CHC-C1C	-2.49	120.68	126.06
29	J	309	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	L	312	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	N	309	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	J	311	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
36	M	304	DD6	C37-C36-C35	2.49	118.97	114.36
39	I	215	KC1	CBD-CHA-C1A	2.49	133.53	128.88
36	N	303	DD6	O1-C20-C21	-2.49	112.07	115.06
29	L	313	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	b	724	CLA	C1B-CHB-C4A	-2.49	125.18	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	315	KC1	CHB-C1B-C2B	-2.49	120.25	125.48
36	B	303	DD6	C10-C9-C8	-2.49	115.44	123.22
39	T	310	KC1	CHB-C1B-C2B	-2.49	120.25	125.48
29	b	708	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
29	l	504	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	N	313	CLA	CHB-C4A-NA	2.49	127.96	124.51
38	E	304	UIX	C35-C36-C38	-2.49	115.44	123.22
29	I	217	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
29	T	309	CLA	CHB-C4A-NA	2.49	127.95	124.51
39	A	205	KC1	C2A-C3A-C4A	2.49	108.33	106.49
29	a	818	CLA	CHB-C4A-NA	2.49	127.95	124.51
37	Q	303	PID	CM2-C5-C4	-2.49	104.66	108.98
29	I	208	CLA	CHB-C4A-NA	2.49	127.95	124.51
29	B	316	CLA	CHB-C4A-NA	2.49	127.95	124.51
37	G	310	PID	C28-C27-C26	2.49	114.22	109.88
29	B	307	CLA	CHB-C4A-NA	2.49	127.95	124.51
39	H	309	KC1	O2D-CGD-O1D	-2.49	118.97	123.84
36	M	304	DD6	C25-C24-C1	-2.49	119.43	126.42
29	E	311	CLA	CHB-C4A-NA	2.49	127.95	124.51
29	L	311	CLA	CHB-C4A-NA	2.49	127.95	124.51
29	O	314	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
39	C	310	KC1	C4B-CHC-C1C	-2.49	120.69	126.06
32	a	838	BCR	C38-C26-C27	2.49	118.39	113.62
36	K	221	DD6	O1-C20-C21	2.49	118.03	115.06
37	D	303	PID	C26-C25-C24	2.48	111.63	109.21
29	A	218	CLA	CHB-C4A-NA	2.48	127.95	124.51
29	Q	315	CLA	CHB-C4A-NA	2.48	127.95	124.51
39	T	310	KC1	O1D-CGD-CBD	-2.48	119.40	124.48
36	B	305	DD6	C25-C24-C1	-2.48	119.44	126.42
29	T	309	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
39	P	216	KC1	C4B-CHC-C1C	-2.48	120.70	126.06
29	a	813	CLA	CHB-C4A-NA	2.48	127.95	124.51
29	J	307	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
39	L	306	KC1	C4B-CHC-C1C	-2.48	120.70	126.06
29	b	702	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	b	719	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	B	306	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	I	213	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	P	214	CLA	CHB-C4A-NA	2.48	127.94	124.51
36	M	301	DD6	C15-C14-C13	-2.48	120.75	125.99
36	K	206	DD6	C33-C34-C35	-2.48	106.91	110.30
39	G	315	KC1	O2D-CGD-O1D	-2.48	118.99	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Q	311	KC1	O2D-CGD-O1D	-2.48	118.99	123.84
39	C	312	KC1	CBD-CHA-C1A	2.48	133.51	128.88
29	K	213	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
29	I	201	CLA	CHB-C4A-NA	2.48	127.94	124.51
36	P	204	DD6	C34-C35-C36	-2.48	106.92	111.85
39	Q	314	KC1	CBD-CHA-C1A	2.48	133.50	128.88
39	A	205	KC1	O1D-CGD-CBD	-2.48	119.41	124.48
36	B	305	DD6	C21-C20-C15	-2.48	118.11	122.26
36	J	303	DD6	C13-C11-C10	2.48	122.74	118.94
29	i	203	CLA	CHB-C4A-NA	2.48	127.94	124.51
36	M	303	DD6	O1-C20-C21	2.48	118.03	115.06
29	E	306	CLA	CHB-C4A-NA	2.48	127.94	124.51
36	G	306	DD6	O1-C20-C21	-2.48	112.09	115.06
29	a	825	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	B	314	CLA	CHB-C4A-NA	2.47	127.93	124.51
39	T	310	KC1	CHC-C4B-C3B	-2.47	121.03	125.26
29	b	706	CLA	CMB-C2B-C3B	2.47	129.30	124.68
39	E	312	KC1	CHC-C4B-C3B	-2.47	121.03	125.26
29	H	315	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
29	M	313	CLA	CHB-C4A-NA	2.47	127.93	124.51
29	O	308	CLA	CHB-C4A-NA	2.47	127.93	124.51
39	A	205	KC1	C4B-CHC-C1C	-2.47	120.73	126.06
39	T	310	KC1	C4B-CHC-C1C	-2.47	120.73	126.06
29	a	807	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
38	B	304	UIX	O2-C27-O4	-2.47	118.06	122.96
39	B	313	KC1	O1D-CGD-CBD	-2.47	119.44	124.48
29	P	209	CLA	CHB-C4A-NA	2.46	127.92	124.51
29	J	306	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
36	I	205	DD6	C12-C11-C10	-2.46	119.47	122.92
29	F	307	CLA	CHB-C4A-NA	2.46	127.92	124.51
39	K	215	KC1	C4B-CHC-C1C	-2.46	120.75	126.06
34	b	734	LMG	O1-C7-C8	-2.46	104.96	110.90
37	F	302	PID	C17-C18-C19	2.46	130.29	124.81
29	H	310	CLA	CHB-C4A-NA	2.46	127.92	124.51
29	b	720	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
36	I	206	DD6	C21-C20-C15	-2.46	118.14	122.26
29	K	212	CLA	CMB-C2B-C3B	2.46	129.28	124.68
29	a	826	CLA	CHB-C4A-NA	2.46	127.91	124.51
36	A	201	DD6	C25-C26-C27	-2.46	119.44	126.58
39	A	213	KC1	C4B-CHC-C1C	-2.46	120.75	126.06
29	H	307	CLA	CHB-C4A-NA	2.46	127.91	124.51
29	b	714	CLA	C1B-CHB-C4A	-2.46	125.25	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	311	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
39	H	309	KC1	C4B-CHC-C1C	-2.46	120.76	126.06
37	j	101	PID	C16-C15-C14	2.46	130.82	127.31
39	T	312	KC1	O1D-CGD-CBD	-2.46	119.46	124.48
36	D	304	DD6	C33-C34-C35	-2.46	106.94	110.30
29	a	817	CLA	CHB-C4A-NA	2.46	127.91	124.51
29	A	209	CLA	CHB-C4A-NA	2.46	127.91	124.51
29	l	501	CLA	O2D-CGD-CBD	2.46	115.63	111.27
36	K	205	DD6	C21-C20-C15	-2.46	118.14	122.26
38	A	203	UIX	C1-C3-C5	-2.45	107.89	112.75
29	a	816	CLA	CHB-C4A-NA	2.45	127.91	124.51
29	E	313	CLA	CAA-C2A-C3A	-2.45	110.37	116.10
29	Q	310	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
39	E	307	KC1	CHB-C1B-C2B	-2.45	120.34	125.48
29	a	825	CLA	O2D-CGD-CBD	2.45	115.63	111.27
29	P	215	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
29	D	316	CLA	CHB-C4A-NA	2.45	127.90	124.51
36	D	301	DD6	C25-C24-C1	-2.45	119.53	126.42
29	a	802	CLA	C1-C2-C3	-2.45	121.80	126.04
32	a	835	BCR	C8-C7-C6	-2.45	120.32	127.20
37	P	206	PID	C6-C7-C8	-2.45	120.81	125.99
29	D	308	CLA	CHB-C4A-NA	2.45	127.90	124.51
29	E	315	CLA	CHB-C4A-NA	2.45	127.90	124.51
29	b	713	CLA	CHB-C4A-NA	2.45	127.90	124.51
29	b	714	CLA	CHB-C4A-NA	2.45	127.90	124.51
29	j	104	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
29	H	310	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
38	J	304	UIX	C37-C39-C40	-2.45	123.82	127.31
36	B	301	DD6	C37-C36-C35	2.45	118.89	114.36
39	A	205	KC1	C1A-C2A-C3A	-2.45	105.17	107.11
39	N	315	KC1	O1D-CGD-CBD	-2.45	119.48	124.48
29	K	217	CLA	CHB-C4A-NA	2.45	127.89	124.51
39	G	315	KC1	CHC-C4B-C3B	-2.45	121.07	125.26
29	C	313	CLA	CHB-C4A-NA	2.45	127.89	124.51
39	O	315	KC1	C2A-C3A-C4A	2.45	108.30	106.49
39	C	310	KC1	C2A-C3A-C4A	2.45	108.30	106.49
38	T	306	UIX	C33-C32-C35	-2.45	119.50	122.92
29	T	308	CLA	CHB-C4A-NA	2.44	127.89	124.51
39	M	305	KC1	O2D-CGD-O1D	-2.44	119.06	123.84
36	P	204	DD6	C21-C20-C15	-2.44	118.17	122.26
32	b	729	BCR	C8-C7-C6	-2.44	120.34	127.20
29	J	313	CLA	CHB-C4A-NA	2.44	127.89	124.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	301	DD6	C8-C9-C10	-2.44	118.47	123.47
29	K	210	CLA	CHB-C4A-NA	2.44	127.89	124.51
39	L	314	KC1	CBD-CHA-C1A	2.44	133.44	128.88
39	T	312	KC1	CBD-CHA-C1A	2.44	133.44	128.88
38	T	306	UIX	C18-O2-C27	-2.44	113.35	117.90
29	O	309	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
36	L	304	DD6	C3-C4-C5	-2.44	118.48	123.47
29	M	313	CLA	CAA-C2A-C3A	-2.44	110.41	116.10
36	P	204	DD6	C9-C8-C6	-2.44	119.56	126.42
32	b	735	BCR	C37-C22-C21	-2.44	119.51	122.92
29	b	726	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
29	l	508	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
34	P	201	LMG	O3-C3-C2	-2.44	104.71	110.35
29	K	209	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
29	K	211	CLA	O2D-CGD-CBD	2.44	115.60	111.27
37	T	307	PID	C17-C16-C15	2.43	128.46	123.47
39	N	315	KC1	C4B-CHC-C1C	-2.43	120.81	126.06
29	J	307	CLA	CHB-C4A-NA	2.43	127.88	124.51
32	a	835	BCR	C38-C26-C27	2.43	118.29	113.62
34	P	201	LMG	O6-C1-O1	-2.43	104.21	109.97
29	J	310	CLA	CHB-C4A-NA	2.43	127.88	124.51
29	l	508	CLA	CAA-C2A-C3A	-2.43	110.42	116.10
29	b	701	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
37	P	202	PID	C17-C16-C15	2.43	128.46	123.47
29	b	711	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
29	O	316	CLA	CAA-C2A-C3A	-2.43	110.42	116.10
36	G	305	DD6	C7-C6-C5	-2.43	119.52	122.92
29	Q	312	CLA	CHB-C4A-NA	2.43	127.87	124.51
39	I	215	KC1	C3D-CAD-CBD	-2.43	104.40	107.61
36	E	302	DD6	C20-C19-C18	-2.43	107.94	112.75
29	D	312	CLA	CHB-C4A-NA	2.43	127.87	124.51
37	D	306	PID	C6-C7-C8	-2.43	120.86	125.99
29	O	316	CLA	CHB-C4A-NA	2.43	127.87	124.51
36	K	221	DD6	C24-C1-C2	2.43	122.67	118.94
36	E	302	DD6	C33-C34-C35	-2.43	106.98	110.30
29	K	211	CLA	C1-C2-C3	-2.43	121.84	126.04
29	f	803	CLA	CHB-C4A-NA	2.43	127.87	124.51
29	M	311	CLA	CHB-C4A-NA	2.43	127.87	124.51
29	G	314	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
36	G	308	DD6	C13-C11-C10	2.43	122.67	118.94
39	B	313	KC1	C4B-CHC-C1C	-2.43	120.83	126.06
29	D	313	CLA	CHB-C4A-NA	2.42	127.86	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	311	CLA	CHB-C4A-NA	2.42	127.86	124.51
39	M	305	KC1	C2A-C3A-C4A	2.42	108.28	106.49
39	P	213	KC1	C3D-CAD-CBD	-2.42	104.41	107.61
29	K	213	CLA	CHB-C4A-NA	2.42	127.86	124.51
37	P	205	PID	C18-C19-C20	2.42	128.44	123.47
29	a	822	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
38	A	203	UIX	C37-C34-C30	-2.42	118.51	123.47
39	P	211	KC1	C2A-C3A-C4A	2.42	108.28	106.49
29	N	309	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
29	l	510	CLA	CHB-C4A-NA	2.42	127.86	124.51
39	P	211	KC1	CBD-CHA-C1A	2.42	133.40	128.88
38	Q	305	UIX	C10-C11-C13	2.42	122.66	118.94
29	a	808	CLA	CHB-C4A-NA	2.42	127.86	124.51
29	M	315	CLA	CHB-C4A-NA	2.42	127.86	124.51
39	F	314	KC1	O2D-CGD-O1D	-2.42	119.11	123.84
36	C	303	DD6	C14-C13-C11	-2.42	121.78	125.53
39	Q	314	KC1	C4B-CHC-C1C	-2.42	120.84	126.06
29	B	310	CLA	CHB-C4A-NA	2.42	127.86	124.51
35	j	103	DGD	O6E-C1E-C2E	2.42	115.47	110.35
36	I	204	DD6	C14-C13-C11	-2.42	121.78	125.53
32	b	729	BCR	C21-C20-C19	-2.42	115.67	123.22
39	E	312	KC1	C4B-CHC-C1C	-2.42	120.84	126.06
36	I	204	DD6	O1-C20-C15	-2.42	56.96	58.96
37	P	203	PID	CM4-C14-C13	2.42	124.63	119.05
29	b	710	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
36	M	304	DD6	C4-C5-C6	-2.42	123.86	127.31
39	G	318	KC1	CBD-CHA-C1A	2.42	133.38	128.88
38	C	306	UIX	C36-C35-C32	-2.41	123.86	127.31
36	F	301	DD6	C9-C8-C6	-2.41	119.64	126.42
36	F	301	DD6	C12-C11-C10	-2.41	119.54	122.92
39	K	215	KC1	C3D-CAD-CBD	-2.41	104.43	107.61
39	F	314	KC1	C2A-C3A-C4A	2.41	108.28	106.49
29	b	711	CLA	CHB-C4A-NA	2.41	127.85	124.51
29	A	208	CLA	CHB-C4A-NA	2.41	127.85	124.51
39	F	314	KC1	O1D-CGD-CBD	-2.41	119.55	124.48
39	O	310	KC1	C4B-CHC-C1C	-2.41	120.86	126.06
39	I	215	KC1	O2D-CGD-O1D	-2.41	119.12	123.84
36	M	302	DD6	C33-C34-C35	-2.41	107.00	110.30
36	I	205	DD6	C14-C13-C11	-2.41	121.79	125.53
36	M	302	DD6	O1-C20-C19	2.41	115.19	113.38
32	b	729	BCR	C2-C1-C6	2.41	114.19	110.48
34	K	219	LMG	O6-C1-O1	-2.41	104.27	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	219	LMG	O1-C7-C8	-2.41	105.08	110.90
39	G	318	KC1	C4B-CHC-C1C	-2.41	120.86	126.06
29	F	315	CLA	O2D-CGD-CBD	2.41	115.55	111.27
29	l	502	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
39	L	306	KC1	C2A-C3A-C4A	2.41	108.27	106.49
29	a	805	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
29	a	822	CLA	CHB-C4A-NA	2.41	127.84	124.51
34	b	730	LMG	C40-C39-C38	-2.41	102.21	114.42
37	H	306	PID	C1-C2-C3	-2.41	107.99	112.75
36	E	302	DD6	C-C1-C2	-2.41	119.55	122.92
29	C	311	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
39	Q	314	KC1	C3D-CAD-CBD	-2.41	104.44	107.61
29	Q	307	CLA	CHB-C4A-NA	2.40	127.84	124.51
29	F	308	CLA	CHB-C4A-NA	2.40	127.84	124.51
36	L	303	DD6	C37-C36-C35	2.40	118.81	114.36
29	b	712	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
36	D	304	DD6	C37-C36-C35	2.40	118.81	114.36
29	I	217	CLA	CHB-C4A-NA	2.40	127.83	124.51
36	K	205	DD6	C9-C10-C11	-2.40	123.88	127.31
38	C	306	UIX	C14-C23-C26	-2.40	119.67	126.42
29	a	806	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
38	A	203	UIX	C14-C13-C11	-2.40	123.89	127.31
29	A	214	CLA	CAA-C2A-C3A	-2.40	110.50	116.10
29	G	302	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
29	a	802	CLA	CHB-C4A-NA	2.40	127.83	124.51
38	A	203	UIX	C19-C18-C17	2.40	114.06	109.88
29	A	210	CLA	CHD-C1D-ND	-2.40	122.25	124.45
29	b	721	CLA	O2D-CGD-CBD	2.40	115.53	111.27
29	M	311	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
35	b	733	DGD	O2D-C2D-C3D	-2.40	104.81	110.35
39	T	315	KC1	O1D-CGD-CBD	-2.40	119.58	124.48
37	H	302	PID	C17-C16-C15	2.40	128.38	123.47
29	a	821	CLA	CHB-C4A-NA	2.40	127.83	124.51
36	K	203	DD6	C37-C36-C35	2.40	118.80	114.36
39	E	312	KC1	C2A-C3A-C4A	2.40	108.26	106.49
39	M	312	KC1	O1D-CGD-CBD	-2.40	119.58	124.48
29	K	214	CLA	CHD-C1D-ND	-2.40	122.25	124.45
36	F	301	DD6	C25-C24-C1	-2.39	119.69	126.42
29	a	811	CLA	CHB-C4A-NA	2.39	127.82	124.51
32	b	728	BCR	C11-C10-C9	-2.39	123.89	127.31
29	A	212	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
36	m	101	DD6	C21-C20-C15	-2.39	118.25	122.26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	316	CLA	CHB-C4A-NA	2.39	127.82	124.51
29	a	826	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
29	I	209	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
39	O	315	KC1	O2D-CGD-O1D	-2.39	119.16	123.84
29	P	212	CLA	CHB-C4A-NA	2.39	127.82	124.51
39	I	215	KC1	C4B-CHC-C1C	-2.39	120.90	126.06
29	M	308	CLA	CHB-C4A-NA	2.39	127.82	124.51
29	E	313	CLA	CHB-C4A-NA	2.39	127.82	124.51
32	m	103	BCR	C38-C26-C25	-2.39	121.84	124.53
29	I	213	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
38	F	305	UIX	C22-C15-C20	-2.39	108.33	110.47
29	a	825	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
29	b	718	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
29	A	214	CLA	CHB-C4A-NA	2.39	127.81	124.51
36	B	319	DD6	C19-C18-C17	-2.39	106.17	110.77
29	l	509	CLA	CAA-C2A-C3A	-2.39	110.53	116.10
29	J	305	CLA	CHB-C4A-NA	2.39	127.81	124.51
36	K	204	DD6	C19-C18-C17	-2.39	106.17	110.77
29	a	837	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
29	N	311	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
29	E	308	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
37	G	303	PID	C17-C18-C19	2.38	130.12	124.81
36	m	101	DD6	C33-C34-C35	-2.38	107.04	110.30
37	O	307	PID	C18-C19-C20	2.38	128.36	123.47
29	K	211	CLA	CHB-C4A-NA	2.38	127.81	124.51
36	E	302	DD6	C34-C35-C36	-2.38	107.11	111.85
29	K	209	CLA	CHB-C4A-NA	2.38	127.80	124.51
32	b	728	BCR	C20-C19-C18	-2.38	119.73	126.42
34	b	732	LMG	O6-C1-O1	-2.38	104.34	109.97
34	j	102	LMG	O3-C3-C2	-2.38	104.85	110.35
38	O	306	UIX	C10-C11-C13	2.38	122.59	118.94
39	Q	314	KC1	C2A-C3A-C4A	2.38	108.25	106.49
29	b	725	CLA	CHB-C4A-NA	2.37	127.80	124.51
29	E	310	CLA	CHB-C4A-NA	2.37	127.80	124.51
36	L	304	DD6	C13-C11-C10	2.37	122.58	118.94
29	H	308	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
36	A	201	DD6	C9-C8-C6	-2.37	119.75	126.42
29	N	314	CLA	O2D-CGD-CBD	2.37	115.48	111.27
29	G	316	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	M	310	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
38	A	203	UIX	C16-C20-C15	2.37	122.05	119.70
36	B	303	DD6	O1-C20-C19	-2.37	111.60	113.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	316	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	a	830	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	b	701	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
32	b	729	BCR	C33-C5-C6	-2.37	121.86	124.53
29	a	809	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
36	G	307	DD6	C9-C8-C6	-2.37	119.75	126.42
29	b	702	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	K	218	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	J	310	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	N	314	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	F	312	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	A	209	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	Q	312	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	E	305	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
38	A	203	UIX	O2-C27-O4	-2.37	118.25	122.96
29	a	830	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	E	313	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	b	710	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	a	831	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	b	718	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	b	712	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
37	O	302	PID	C16-C15-C14	2.37	130.69	127.31
29	C	308	CLA	CHB-C4A-NA	2.37	127.78	124.51
29	I	211	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
36	G	308	DD6	C33-C34-C35	-2.37	107.06	110.30
37	D	307	PID	C26-C25-C24	2.37	111.51	109.21
29	a	810	CLA	CHB-C4A-NA	2.37	127.78	124.51
29	L	308	CLA	CHB-C4A-NA	2.37	127.78	124.51
32	b	729	BCR	C38-C26-C25	-2.37	121.87	124.53
36	Q	302	DD6	C9-C8-C6	-2.37	119.77	126.42
36	J	301	DD6	C24-C1-C2	2.36	122.57	118.94
29	f	802	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
29	E	311	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	l	503	CLA	CHD-C1D-ND	-2.36	122.28	124.45
38	O	306	UIX	C41-C40-C39	-2.36	119.61	122.92
29	a	808	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	K	212	CLA	CHB-C4A-NA	2.36	127.78	124.51
39	C	310	KC1	O2D-CGD-O1D	-2.36	119.22	123.84
29	L	313	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
39	F	309	KC1	C3D-CAD-CBD	-2.36	104.50	107.61
29	b	715	CLA	CHB-C4A-NA	2.36	127.78	124.51
29	i	201	CLA	C1B-CHB-C4A	-2.36	125.44	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	P	211	KC1	C4B-CHC-C1C	-2.36	120.97	126.06
29	b	704	CLA	CMB-C2B-C3B	2.36	129.09	124.68
29	J	308	CLA	CHB-C4A-NA	2.36	127.78	124.51
36	B	303	DD6	C21-C20-C15	-2.36	118.31	122.26
36	Q	302	DD6	C21-C20-C15	-2.36	118.31	122.26
29	D	314	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
37	O	302	PID	CM4-C14-C13	2.36	124.49	119.05
39	B	313	KC1	O2D-CGD-O1D	-2.36	119.23	123.84
29	a	818	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
39	J	312	KC1	O2D-CGD-O1D	-2.36	119.23	123.84
34	K	201	LMG	O1-C1-C2	-2.36	104.62	108.30
29	O	313	CLA	CHB-C4A-NA	2.36	127.77	124.51
29	G	314	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
29	E	315	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
29	b	723	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
36	K	204	DD6	C33-C34-C35	-2.36	107.08	110.30
29	L	316	CLA	CHB-C4A-NA	2.36	127.77	124.51
36	B	301	DD6	C5-C4-C3	-2.35	119.57	124.81
29	l	505	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
29	A	207	CLA	CHB-C4A-NA	2.35	127.77	124.51
38	N	306	UIX	C33-C32-C35	-2.35	119.62	122.92
29	a	814	CLA	CHB-C4A-NA	2.35	127.77	124.51
29	E	306	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
29	H	313	CLA	CHD-C1D-ND	-2.35	122.29	124.45
37	T	302	PID	C17-C16-C15	2.35	128.29	123.47
29	b	720	CLA	CHB-C4A-NA	2.35	127.77	124.51
29	a	811	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
29	a	824	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
29	L	312	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
35	b	733	DGD	O1G-C1A-O1A	-2.35	117.66	123.59
29	A	208	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
29	L	309	CLA	CHB-C4A-NA	2.35	127.76	124.51
39	L	314	KC1	C4B-CHC-C1C	-2.35	120.99	126.06
38	N	306	UIX	C12-C11-C13	-2.35	119.63	122.92
29	A	211	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
29	I	209	CLA	CHB-C4A-NA	2.35	127.76	124.51
35	B	318	DGD	O6D-C1D-C2D	-2.35	105.38	110.35
37	D	305	PID	C18-C19-C20	2.35	128.28	123.47
29	l	505	CLA	CHB-C4A-NA	2.35	127.76	124.51
29	H	315	CLA	CHB-C4A-NA	2.35	127.76	124.51
29	B	315	CLA	CHB-C4A-NA	2.35	127.76	124.51
29	F	308	CLA	C1B-CHB-C4A	-2.35	125.47	130.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	K	221	DD6	O1-C20-C15	-2.35	57.02	58.96
34	K	201	LMG	O2-C2-C1	-2.35	104.35	110.05
29	P	210	CLA	CHB-C4A-NA	2.35	127.76	124.51
29	L	316	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
29	Q	308	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
39	N	310	KC1	CBD-CHA-C1A	2.34	133.25	128.88
32	b	735	BCR	C16-C15-C14	-2.34	118.67	123.47
29	b	726	CLA	CHB-C4A-NA	2.34	127.75	124.51
32	a	838	BCR	C16-C15-C14	-2.34	118.67	123.47
36	M	303	DD6	C32-C33-C34	-2.34	108.35	113.64
34	b	730	LMG	C38-C37-C36	-2.34	102.54	114.42
32	l	506	BCR	C33-C5-C4	2.34	118.11	113.62
36	O	303	DD6	C9-C8-C6	-2.34	119.84	126.42
34	A	219	LMG	O6-C1-O1	-2.34	104.43	109.97
38	O	306	UIX	O2-C27-O4	-2.34	118.31	122.96
36	G	307	DD6	C23-C16-C15	-2.34	103.73	110.05
32	b	729	BCR	C28-C27-C26	-2.34	109.90	114.08
29	I	210	CLA	CHB-C4A-NA	2.34	127.75	124.51
29	I	211	CLA	CHB-C4A-NA	2.34	127.75	124.51
29	a	813	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
38	F	305	UIX	C29-C26-C30	-2.34	119.65	122.92
38	L	302	UIX	C37-C39-C40	-2.34	123.97	127.31
39	A	205	KC1	CBD-CHA-C1A	2.34	133.24	128.88
29	b	719	CLA	C2D-C1D-ND	-2.34	108.38	110.10
29	I	210	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
36	K	202	DD6	C10-C9-C8	-2.34	115.93	123.22
37	D	305	PID	CM2-C5-C4	-2.34	104.92	108.98
29	a	812	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
29	P	209	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
29	K	210	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
34	b	732	LMG	O1-C7-C8	-2.33	105.27	110.90
29	B	308	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
37	G	310	PID	C17-C16-C15	2.33	128.25	123.47
30	a	832	PQN	C11-C3-C4	2.33	121.00	118.50
32	f	801	BCR	C37-C22-C21	-2.33	119.66	122.92
32	f	804	BCR	C23-C24-C25	-2.33	120.65	127.20
38	P	207	UIX	C3-C5-C4	-2.33	106.27	110.77
34	K	201	LMG	O1-C7-C8	-2.33	105.28	110.90
29	F	313	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
29	K	208	CLA	CHB-C4A-NA	2.33	127.73	124.51
38	C	306	UIX	O2-C27-O4	-2.33	118.33	122.96
29	G	301	CLA	CHB-C4A-NA	2.33	127.73	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	304	DD6	C34-C35-C36	-2.33	107.22	111.85
36	A	201	DD6	C15-C14-C13	-2.33	121.07	125.99
34	b	730	LMG	O3-C3-C2	-2.33	104.97	110.35
39	M	312	KC1	C2A-C3A-C4A	2.33	108.21	106.49
39	C	310	KC1	O1D-CGD-CBD	-2.33	119.72	124.48
36	I	204	DD6	O1-C20-C19	2.33	115.13	113.38
29	J	305	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
38	T	306	UIX	C29-C26-C30	-2.33	119.67	122.92
38	T	306	UIX	O2-C27-O4	-2.32	118.34	122.96
39	K	215	KC1	O2A-CGA-O1A	-2.32	117.84	122.67
39	J	312	KC1	O1D-CGD-CBD	-2.32	119.73	124.48
38	L	302	UIX	C41-C40-C38	2.32	121.74	118.08
29	l	508	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	Q	308	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	A	216	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
37	T	317	PID	C28-C27-C26	2.32	113.93	109.88
29	a	824	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	b	723	CLA	CHB-C4A-NA	2.32	127.72	124.51
39	P	213	KC1	CHB-C1B-C2B	-2.32	120.61	125.48
29	h	201	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
38	N	306	UIX	C14-C23-C26	-2.32	119.90	126.42
36	H	303	DD6	C28-C27-C29	2.32	121.43	116.84
29	a	837	CLA	CHB-C4A-NA	2.32	127.72	124.51
36	L	301	DD6	C37-C36-C35	2.32	118.65	114.36
34	A	219	LMG	C38-C37-C36	-2.32	102.66	114.42
29	G	304	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
29	G	319	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
34	b	734	LMG	O3-C3-C2	-2.32	104.99	110.35
29	M	313	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
36	H	303	DD6	C21-C20-C15	-2.32	118.38	122.26
29	D	309	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
29	C	313	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
32	f	804	BCR	C38-C26-C27	2.31	118.06	113.62
36	D	304	DD6	O1-C20-C15	-2.31	57.04	58.96
29	G	317	CLA	CHB-C4A-NA	2.31	127.71	124.51
34	K	220	LMG	O3-C3-C2	-2.31	105.00	110.35
36	M	304	DD6	C20-C19-C18	2.31	117.33	112.75
29	b	719	CLA	C1-C2-C3	-2.31	123.01	126.75
36	M	303	DD6	C12-C11-C10	-2.31	119.69	122.92
29	b	716	CLA	CHD-C1D-ND	-2.31	122.33	124.45
39	L	306	KC1	C1A-C2A-C3A	-2.31	105.28	107.11
36	M	301	DD6	C3-C4-C5	-2.31	118.74	123.47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	319	DD6	O1-C20-C15	-2.31	57.05	58.96
29	a	804	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
36	I	206	DD6	C37-C36-C35	2.31	118.64	114.36
29	l	509	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
37	D	303	PID	O4-C12-C13	2.31	127.82	122.89
29	I	212	CLA	CHB-C4A-NA	2.31	127.70	124.51
29	K	214	CLA	O2D-CGD-CBD	2.31	115.37	111.27
36	B	305	DD6	C25-C26-C27	-2.31	119.88	126.58
38	Q	305	UIX	C21-C15-C20	-2.31	108.41	110.47
29	B	312	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
39	F	309	KC1	O1D-CGD-CBD	-2.31	119.76	124.48
39	C	312	KC1	O2D-CGD-O1D	-2.31	119.33	123.84
29	A	218	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
29	a	823	CLA	CHB-C4A-NA	2.31	127.70	124.51
29	L	310	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
36	M	303	DD6	C25-C24-C1	-2.31	119.94	126.42
29	O	309	CLA	CHB-C4A-NA	2.30	127.70	124.51
37	N	302	PID	CM4-C14-C13	2.30	124.36	119.05
39	K	215	KC1	O1D-CGD-CBD	-2.30	119.77	124.48
29	l	505	CLA	C2D-C1D-ND	-2.30	108.41	110.10
29	L	308	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
36	I	202	DD6	C3-C4-C5	-2.30	118.76	123.47
37	j	101	PID	C18-C17-C16	2.30	129.94	124.81
38	Q	305	UIX	C33-C32-C35	-2.30	119.70	122.92
36	F	301	DD6	C21-C20-C15	-2.30	118.40	122.26
29	B	306	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
29	T	311	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
36	M	304	DD6	C3-C4-C5	-2.30	118.76	123.47
32	b	729	BCR	C33-C5-C4	2.30	118.03	113.62
29	F	316	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
29	b	707	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
36	G	308	DD6	O1-C20-C21	-2.30	112.30	115.06
29	L	317	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
36	K	206	DD6	C3-C4-C5	-2.30	118.77	123.47
29	H	313	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
36	G	305	DD6	C28-C27-C29	2.30	121.39	116.84
29	M	309	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
39	O	310	KC1	O1D-CGD-CBD	-2.30	119.78	124.48
29	a	823	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
37	T	317	PID	C18-C19-C20	2.30	128.18	123.47
29	l	510	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
29	K	208	CLA	C1B-CHB-C4A	-2.30	125.57	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	i	202	CLA	C1-C2-C3	-2.30	122.07	126.04
32	m	103	BCR	C20-C19-C18	-2.30	119.97	126.42
39	P	216	KC1	C2A-C3A-C4A	2.30	108.19	106.49
39	G	315	KC1	C2A-C3A-C4A	2.29	108.19	106.49
29	C	309	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
38	F	305	UIX	C16-C20-C15	2.29	121.97	119.70
38	E	304	UIX	C13-C14-C23	-2.29	116.06	123.22
29	H	315	CLA	CAA-C2A-C3A	-2.29	110.75	116.10
29	b	712	CLA	CHB-C4A-NA	2.29	127.68	124.51
39	H	311	KC1	C3D-CAD-CBD	-2.29	104.59	107.61
29	b	708	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	l	509	CLA	CHB-C4A-NA	2.29	127.68	124.51
36	F	303	DD6	C33-C34-C35	-2.29	107.17	110.30
39	Q	311	KC1	CHB-C1B-C2B	-2.29	120.67	125.48
29	B	308	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	B	310	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
34	h	205	LMG	O2-C2-C1	-2.29	104.48	110.05
29	b	731	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
39	E	307	KC1	O1D-CGD-CBD	-2.29	119.80	124.48
29	b	709	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
29	F	307	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
29	E	305	CLA	CHB-C4A-NA	2.29	127.68	124.51
32	b	728	BCR	C7-C8-C9	-2.29	122.78	126.23
39	G	315	KC1	O1D-CGD-CBD	-2.29	119.80	124.48
36	B	301	DD6	C21-C20-C15	-2.29	118.43	122.26
39	C	315	KC1	O2D-CGD-O1D	-2.29	119.37	123.84
29	P	214	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
29	B	316	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
36	I	205	DD6	C33-C34-C35	-2.29	107.17	110.30
39	P	213	KC1	O2D-CGD-O1D	-2.29	119.37	123.84
32	a	838	BCR	C33-C5-C4	2.29	118.01	113.62
36	G	307	DD6	C12-C11-C10	-2.29	119.72	122.92
29	B	311	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
29	O	316	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
29	T	313	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
39	N	310	KC1	C2A-C3A-C4A	2.28	108.18	106.49
29	f	805	CLA	CHB-C4A-NA	2.28	127.67	124.51
36	B	302	DD6	C26-C25-C24	-2.28	116.09	123.22
35	B	318	DGD	C1E-O6E-C5E	2.28	118.17	113.69
29	a	801	CLA	CHB-C4A-NA	2.28	127.67	124.51
29	H	312	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
39	L	306	KC1	O2D-CGD-O1D	-2.28	119.38	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	310	PID	CM4-C14-C13	2.28	124.31	119.05
29	b	724	CLA	CHB-C4A-NA	2.28	127.67	124.51
36	M	301	DD6	C14-C13-C11	-2.28	121.99	125.53
39	D	310	KC1	O1D-CGD-CBD	-2.28	119.82	124.48
29	A	207	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
36	B	319	DD6	C10-C9-C8	-2.28	116.10	123.22
29	L	309	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
29	D	316	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
29	G	302	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
36	D	304	DD6	C9-C8-C6	-2.28	120.02	126.42
36	E	303	DD6	C25-C26-C27	-2.28	119.97	126.58
29	i	203	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
29	a	810	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
29	a	828	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
39	O	310	KC1	C3D-CAD-CBD	-2.28	104.61	107.61
38	Q	305	UIX	C29-C26-C30	-2.28	119.73	122.92
36	h	202	DD6	C37-C36-C35	2.28	118.57	114.36
29	P	215	CLA	CED-O2D-CGD	2.28	121.08	115.94
39	N	312	KC1	CBD-CHA-C1A	2.27	133.12	128.88
36	M	301	DD6	C37-C36-C35	2.27	118.57	114.36
36	O	303	DD6	C7-C6-C5	-2.27	119.74	122.92
29	D	313	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
39	T	315	KC1	C2A-C3A-C4A	2.27	108.17	106.49
29	I	212	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
29	A	206	CLA	O2D-CGD-CBD	2.27	115.31	111.27
36	K	203	DD6	C12-C11-C10	-2.27	119.74	122.92
39	A	213	KC1	O1D-CGD-CBD	-2.27	119.83	124.48
29	J	308	CLA	O2D-CGD-CBD	2.27	115.31	111.27
36	J	302	DD6	C9-C8-C6	-2.27	120.03	126.42
29	J	309	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
29	M	307	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
36	L	305	DD6	C4-C3-C2	-2.27	118.82	123.47
29	M	307	CLA	CHB-C4A-NA	2.27	127.65	124.51
37	O	307	PID	C6-C7-C8	2.27	130.79	125.99
38	Q	305	UIX	O2-C27-O4	-2.27	118.45	122.96
29	b	722	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
29	T	308	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
29	A	217	CLA	CHB-C4A-NA	2.27	127.65	124.51
36	M	302	DD6	C37-C36-C35	2.27	118.56	114.36
38	E	304	UIX	C34-C37-C39	-2.27	118.83	123.47
35	B	318	DGD	O2G-C1B-O1B	-2.27	118.22	123.70
29	K	207	CLA	CHD-C1D-ND	-2.27	122.37	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	211	CLA	CHB-C4A-NA	2.27	127.64	124.51
39	T	312	KC1	C3D-CAD-CBD	-2.27	104.62	107.61
39	E	307	KC1	C3D-CAD-CBD	-2.27	104.62	107.61
29	f	802	CLA	CHB-C4A-NA	2.26	127.64	124.51
29	I	216	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
36	G	305	DD6	C12-C11-C10	-2.26	119.75	122.92
29	K	212	CLA	C2D-C1D-ND	-2.26	108.44	110.10
29	O	313	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
39	H	311	KC1	O2D-CGD-O1D	-2.26	119.41	123.84
34	K	219	LMG	O3-C3-C2	-2.26	105.12	110.35
38	O	306	UIX	C29-C26-C30	-2.26	119.76	122.92
36	O	303	DD6	O1-C20-C15	-2.26	57.09	58.96
29	K	216	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
29	A	210	CLA	CHB-C4A-NA	2.26	127.64	124.51
36	H	303	DD6	C7-C6-C5	-2.26	119.76	122.92
39	N	310	KC1	O1D-CGD-CBD	-2.26	119.86	124.48
32	f	804	BCR	C11-C12-C13	-2.26	120.07	126.42
37	T	317	PID	C17-C18-C19	2.26	129.83	124.81
36	M	301	DD6	C25-C24-C1	-2.26	120.08	126.42
29	N	313	CLA	CMD-C2D-C1D	-2.26	120.74	124.71
29	l	510	CLA	CMB-C2B-C3B	2.26	128.90	124.68
38	N	306	UIX	O2-C27-O4	-2.26	118.48	122.96
29	a	829	CLA	CHB-C4A-NA	2.25	127.63	124.51
29	a	804	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
36	N	303	DD6	C37-C36-C35	2.25	118.53	114.36
29	j	104	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
29	C	316	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
29	G	313	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
29	K	217	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
29	T	316	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
29	a	816	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
29	O	308	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
29	i	202	CLA	CHB-C4A-NA	2.25	127.62	124.51
29	I	216	CLA	C1-C2-C3	-2.25	122.15	126.04
36	A	201	DD6	C12-C11-C10	-2.25	119.77	122.92
29	a	817	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
29	C	308	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
29	P	217	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
39	P	211	KC1	O1D-CGD-CBD	-2.25	119.88	124.48
39	N	315	KC1	O2D-CGD-O1D	-2.25	119.44	123.84
29	E	314	CLA	CHB-C4A-NA	2.25	127.62	124.51
37	j	101	PID	C6-C7-C8	-2.25	121.24	125.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	P	203	PID	C16-C15-C14	2.25	130.52	127.31
37	O	302	PID	C18-C17-C16	2.25	129.81	124.81
29	a	830	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
29	a	801	CLA	C1-C2-C3	-2.25	122.16	126.04
32	l	507	BCR	C38-C26-C27	2.25	117.93	113.62
29	a	810	CLA	CMB-C2B-C3B	2.25	128.88	124.68
36	T	303	DD6	C4-C3-C2	-2.25	118.87	123.47
29	Q	312	CLA	O1D-CGD-CBD	2.25	129.08	124.48
29	L	315	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
36	K	206	DD6	C37-C36-C35	2.25	118.52	114.36
39	D	310	KC1	C2A-C3A-C4A	2.25	108.15	106.49
29	D	314	CLA	O2D-CGD-CBD	2.25	115.26	111.27
29	I	213	CLA	C1-C2-C3	-2.25	122.16	126.04
35	B	318	DGD	O6D-C5D-C4D	2.25	113.77	109.69
29	b	721	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
29	G	317	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
36	E	303	DD6	C37-C36-C35	2.24	118.51	114.36
36	K	205	DD6	C14-C13-C11	-2.24	122.05	125.53
36	P	204	DD6	C33-C32-C31	2.24	114.17	109.62
29	E	305	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
29	a	829	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
39	C	315	KC1	C2A-C3A-C4A	2.24	108.15	106.49
29	F	315	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
36	J	303	DD6	C9-C8-C6	-2.24	120.12	126.42
37	T	307	PID	C18-C17-C16	2.24	129.80	124.81
29	B	309	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
36	K	202	DD6	C-C1-C2	-2.24	119.78	122.92
38	P	207	UIX	O2-C27-O4	-2.24	118.51	122.96
39	D	315	KC1	O1D-CGD-CBD	-2.24	119.90	124.48
29	E	309	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
37	N	307	PID	O1-C1-C2	-2.24	111.70	113.38
29	I	209	CLA	C1-C2-C3	-2.24	122.17	126.04
37	D	303	PID	CM4-C14-C13	2.24	124.21	119.05
29	a	819	CLA	C1-C2-C3	-2.24	122.17	126.04
39	P	216	KC1	O1D-CGD-CBD	-2.24	119.91	124.48
29	D	311	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
36	J	302	DD6	C32-C33-C34	-2.24	108.59	113.64
29	b	725	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
29	b	721	CLA	C1-C2-C3	-2.24	122.18	126.04
29	G	312	CLA	CHD-C1D-ND	-2.24	122.40	124.45
36	B	303	DD6	O1-C20-C21	-2.24	112.38	115.06
29	b	724	CLA	O2A-CGA-O1A	-2.23	117.95	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	315	KC1	CMD-C2D-C1D	-2.23	125.03	128.46
36	I	205	DD6	C19-C18-C17	-2.23	106.46	110.77
36	C	303	DD6	C4-C3-C2	-2.23	118.90	123.47
34	b	732	LMG	O2-C2-C1	-2.23	104.62	110.05
29	a	815	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
29	a	821	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
38	T	306	UIX	C3-C5-C4	-2.23	106.46	110.77
32	m	103	BCR	C35-C13-C14	-2.23	119.80	122.92
39	B	313	KC1	C2A-C3A-C4A	2.23	108.14	106.49
32	a	838	BCR	C8-C7-C6	-2.23	120.93	127.20
36	C	303	DD6	C7-C6-C5	-2.23	119.80	122.92
29	K	207	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
29	J	313	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
34	K	201	LMG	O3-C3-C2	-2.23	105.19	110.35
29	I	208	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
36	M	303	DD6	C-C1-C2	-2.23	119.80	122.92
29	A	217	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
29	J	308	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
36	K	204	DD6	C13-C11-C10	2.23	122.36	118.94
36	I	202	DD6	O1-C20-C21	-2.23	112.38	115.06
29	l	504	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
29	P	212	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
29	Q	307	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
29	A	215	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
39	N	312	KC1	C1A-C2A-C3A	-2.23	105.35	107.11
29	Q	315	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
34	h	205	LMG	O3-C3-C2	-2.23	105.20	110.35
29	I	217	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
29	b	716	CLA	CHB-C4A-NA	2.23	127.59	124.51
34	h	205	LMG	O7-C10-O9	-2.23	118.32	123.70
29	B	308	CLA	CHD-C1D-ND	-2.23	122.41	124.45
39	H	314	KC1	O1D-CGD-CBD	-2.23	119.93	124.48
38	F	305	UIX	O2-C27-O4	-2.22	118.54	122.96
38	L	302	UIX	C13-C14-C23	-2.22	116.28	123.22
39	L	314	KC1	C2A-C3A-C4A	2.22	108.14	106.49
29	B	307	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
36	D	301	DD6	C37-C36-C35	2.22	118.47	114.36
36	T	303	DD6	C37-C36-C35	2.22	118.47	114.36
36	B	302	DD6	C4-C3-C2	-2.22	118.92	123.47
29	I	212	CLA	CHD-C1D-ND	-2.22	122.41	124.45
29	B	306	CLA	CHD-C1D-ND	-2.22	122.41	124.45
29	a	831	CLA	C1B-CHB-C4A	-2.22	125.72	130.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	308	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
36	M	303	DD6	C7-C6-C5	-2.22	119.81	122.92
29	M	306	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
29	f	803	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
29	G	311	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
37	H	305	PID	C19-C20-C21	2.22	130.48	127.31
32	b	728	BCR	C16-C15-C14	-2.22	118.93	123.47
36	G	306	DD6	C25-C26-C27	-2.22	120.14	126.58
29	F	311	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
29	I	213	CLA	CHD-C1D-ND	-2.22	122.42	124.45
29	N	316	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
39	P	213	KC1	CBD-CHA-C1A	2.22	133.01	128.88
38	N	306	UIX	C29-C26-C30	-2.22	119.82	122.92
29	O	314	CLA	CHD-C1D-ND	-2.22	122.42	124.45
39	C	312	KC1	C3D-CAD-CBD	-2.22	104.69	107.61
40	J	314	SQD	O6-C1-C2	2.22	111.76	108.30
29	b	731	CLA	CHD-C1D-ND	-2.22	122.42	124.45
29	K	214	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
36	K	202	DD6	C25-C24-C1	-2.21	120.19	126.42
29	a	812	CLA	CHD-C1D-ND	-2.21	122.42	124.45
29	Q	313	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
34	j	102	LMG	O1-C1-C2	-2.21	104.85	108.30
29	a	810	CLA	C1-C2-C3	-2.21	122.21	126.04
29	K	212	CLA	CHD-C1D-ND	-2.21	122.42	124.45
29	C	314	CLA	O2D-CGD-CBD	2.21	115.20	111.27
39	Q	314	KC1	O1D-CGD-CBD	-2.21	119.96	124.48
29	M	308	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
38	N	306	UIX	C41-C40-C39	-2.21	119.83	122.92
29	H	307	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
37	j	101	PID	C17-C16-C15	2.21	128.00	123.47
39	K	215	KC1	C2A-C3A-C4A	2.21	108.12	106.49
29	L	311	CLA	CHD-C1D-ND	-2.21	122.42	124.45
29	N	313	CLA	CMD-C2D-C3D	2.21	132.69	127.61
37	D	306	PID	CM4-C14-C13	2.21	124.14	119.05
29	I	201	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
29	O	311	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
38	L	302	UIX	C35-C36-C38	-2.21	116.33	123.22
36	I	202	DD6	O1-C20-C19	-2.21	111.72	113.38
34	A	219	LMG	O3-C3-C2	-2.21	105.25	110.35
29	I	207	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
36	L	304	DD6	C25-C24-C1	-2.21	120.22	126.42
38	A	203	UIX	C13-C14-C23	-2.20	116.34	123.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	G	308	DD6	C3-C4-C5	-2.20	118.96	123.47
36	A	202	DD6	C14-C13-C11	-2.20	122.11	125.53
37	N	307	PID	CM1-C1-C6	-2.20	118.57	122.26
29	N	308	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
39	T	312	KC1	C2A-C3A-C4A	2.20	108.12	106.49
37	O	304	PID	CM2-C5-C4	-2.20	105.16	108.98
34	b	734	LMG	O1-C1-C2	-2.20	104.87	108.30
29	D	312	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
36	K	203	DD6	O1-C20-C21	-2.20	112.42	115.06
39	M	305	KC1	C1A-C2A-C3A	-2.20	105.37	107.11
29	A	206	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
29	E	315	CLA	O2D-CGD-CBD	2.20	115.17	111.27
29	G	312	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
29	b	708	CLA	CHD-C1D-ND	-2.20	122.43	124.45
39	A	213	KC1	O2D-CGD-O1D	-2.20	119.54	123.84
29	a	819	CLA	CHB-C4A-NA	2.20	127.55	124.51
29	H	310	CLA	C1-C2-C3	-2.20	122.25	126.04
29	B	314	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
29	l	505	CLA	CHD-C1D-ND	-2.19	122.44	124.45
39	N	315	KC1	C2A-C3A-C4A	2.19	108.11	106.49
36	A	201	DD6	C25-C24-C1	-2.19	120.26	126.42
38	T	306	UIX	C41-C40-C39	-2.19	119.85	122.92
32	f	804	BCR	C35-C13-C14	-2.19	119.85	122.92
36	B	305	DD6	C37-C36-C35	2.19	118.42	114.36
36	C	303	DD6	C34-C35-C36	-2.19	107.49	111.85
29	a	814	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
36	P	204	DD6	C7-C6-C5	-2.19	119.86	122.92
36	L	304	DD6	C37-C36-C35	2.19	118.41	114.36
36	K	203	DD6	C9-C8-C6	-2.19	120.27	126.42
35	b	733	DGD	O6D-C5D-C6D	2.19	111.08	106.67
29	b	716	CLA	O2D-CGD-CBD	2.19	115.16	111.27
36	L	304	DD6	C-C1-C2	-2.19	119.86	122.92
37	D	305	PID	O1-C1-C2	-2.19	111.74	113.38
29	M	309	CLA	CHB-C4A-NA	2.19	127.53	124.51
39	A	205	KC1	O2D-CGD-O1D	-2.19	119.56	123.84
34	b	730	LMG	O2-C2-C1	-2.19	104.74	110.05
29	a	823	CLA	CHD-C1D-ND	-2.19	122.45	124.45
38	A	203	UIX	C7-C10-C11	-2.18	122.14	125.53
39	A	205	KC1	O2A-CGA-O1A	-2.18	118.13	122.67
36	B	305	DD6	C3-C4-C5	-2.18	119.00	123.47
36	D	301	DD6	C15-C14-C13	2.18	130.61	125.99
36	I	203	DD6	C32-C33-C34	-2.18	108.71	113.64

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	713	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
29	J	310	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
29	L	307	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
37	C	304	PID	C17-C18-C19	2.18	129.66	124.81
36	K	221	DD6	C7-C6-C5	-2.18	119.87	122.92
36	J	303	DD6	C7-C6-C5	-2.18	119.87	122.92
36	B	305	DD6	C-C1-C2	-2.18	119.87	122.92
36	H	303	DD6	C-C1-C2	-2.18	119.87	122.92
29	L	313	CLA	CHD-C1D-ND	-2.18	122.45	124.45
36	D	304	DD6	C7-C6-C5	-2.18	119.87	122.92
39	L	306	KC1	O2A-CGA-O1A	-2.18	118.14	122.67
29	E	310	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
32	b	729	BCR	C7-C8-C9	-2.18	122.94	126.23
37	T	305	PID	CM4-C14-C13	2.18	124.07	119.05
36	A	204	DD6	C10-C9-C8	-2.18	116.42	123.22
29	M	315	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
39	N	312	KC1	O1D-CGD-CBD	-2.18	120.03	124.48
36	I	205	DD6	O1-C20-C19	2.18	115.02	113.38
38	F	305	UIX	C14-C23-C26	-2.18	120.30	126.42
29	F	312	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
37	F	304	PID	C28-C27-C26	2.18	113.67	109.88
32	a	835	BCR	C15-C16-C17	-2.18	119.02	123.47
36	B	319	DD6	C37-C36-C35	2.17	118.38	114.36
34	b	734	LMG	O2-C2-C1	-2.17	104.77	110.05
36	J	302	DD6	C37-C36-C35	2.17	118.38	114.36
36	I	203	DD6	C3-C4-C5	-2.17	119.02	123.47
36	J	303	DD6	O1-C20-C21	2.17	117.66	115.06
32	a	834	BCR	C33-C5-C4	2.17	117.79	113.62
29	A	214	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
36	J	302	DD6	C3-C4-C5	-2.17	119.03	123.47
36	A	201	DD6	O1-C20-C21	-2.17	112.45	115.06
29	I	213	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
37	Q	303	PID	C17-C18-C19	2.17	129.64	124.81
35	G	320	DGD	C2G-O2G-C1B	-2.17	112.45	117.79
29	B	312	CLA	CHD-C1D-ND	-2.17	122.46	124.45
32	a	835	BCR	C37-C22-C21	-2.17	119.88	122.92
36	O	303	DD6	C4-C3-C2	-2.17	119.03	123.47
29	P	212	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
39	L	314	KC1	O1D-CGD-CBD	-2.17	120.05	124.48
34	K	219	LMG	O2-C2-C1	-2.17	104.79	110.05
36	D	304	DD6	C15-C14-C13	-2.17	121.42	125.99
38	J	304	UIX	C-C7-C10	-2.17	121.42	125.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	L	304	DD6	C32-C33-C34	-2.17	108.75	113.64
37	C	301	PID	C15-C14-C13	2.16	122.93	117.00
32	f	801	BCR	C19-C18-C17	2.16	122.26	118.94
32	b	729	BCR	C34-C9-C8	2.16	121.49	118.08
29	K	212	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
29	I	207	CLA	CHD-C1D-ND	-2.16	122.47	124.45
36	E	302	DD6	C7-C6-C5	-2.16	119.89	122.92
39	I	215	KC1	C2A-C3A-C4A	2.16	108.09	106.49
39	J	312	KC1	C2A-C3A-C4A	2.16	108.09	106.49
29	F	310	CLA	O2D-CGD-CBD	2.16	115.11	111.27
39	F	309	KC1	C2A-C3A-C4A	2.16	108.09	106.49
36	D	301	DD6	C32-C33-C34	-2.16	108.76	113.64
37	P	203	PID	O4-C12-C13	2.16	127.50	122.89
36	B	303	DD6	C3-C4-C5	-2.16	119.05	123.47
29	a	801	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
32	f	801	BCR	C2-C1-C6	2.16	113.80	110.48
29	b	726	CLA	CHD-C1D-ND	-2.16	122.47	124.45
36	m	101	DD6	C28-C27-C29	2.16	121.11	116.84
29	b	736	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
32	l	506	BCR	C35-C13-C12	2.16	121.47	118.08
36	J	301	DD6	C7-C6-C5	-2.16	119.90	122.92
29	b	707	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
36	G	307	DD6	O1-C20-C21	2.15	117.64	115.06
37	T	302	PID	C28-C27-C26	2.15	113.64	109.88
32	i	204	BCR	C10-C11-C12	-2.15	116.50	123.22
37	H	305	PID	C26-C25-C24	2.15	111.30	109.21
29	a	807	CLA	CHD-C1D-ND	-2.15	122.48	124.45
29	P	215	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
29	I	209	CLA	CHD-C1D-ND	-2.15	122.48	124.45
29	b	723	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
34	K	220	LMG	O2-C2-C1	-2.15	104.83	110.05
29	H	308	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
29	b	711	CLA	CHD-C1D-ND	-2.15	122.48	124.45
38	L	302	UIX	O2-C27-O4	-2.15	118.70	122.96
36	I	204	DD6	C37-C36-C35	2.15	118.33	114.36
29	b	709	CLA	CHD-C1D-ND	-2.15	122.48	124.45
36	M	302	DD6	O1-C20-C15	-2.15	57.18	58.96
39	N	312	KC1	C2A-C3A-C4A	2.15	108.08	106.49
36	T	303	DD6	C25-C24-C1	-2.15	120.39	126.42
36	N	303	DD6	C9-C8-C6	-2.15	120.39	126.42
29	Q	310	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
34	A	219	LMG	O2-C2-C1	-2.14	104.84	110.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	K	205	DD6	C10-C9-C8	-2.14	116.53	123.22
37	T	307	PID	CM4-C14-C13	2.14	123.99	119.05
29	P	212	CLA	CHD-C1D-ND	-2.14	122.48	124.45
38	P	207	UIX	C29-C26-C30	-2.14	119.92	122.92
29	E	306	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
29	N	311	CLA	CHD-C1D-ND	-2.14	122.49	124.45
39	C	312	KC1	C2A-C3A-C4A	2.14	108.07	106.49
38	E	304	UIX	C18-O2-C27	-2.14	113.91	117.90
39	B	313	KC1	CBD-CHA-C1A	2.14	132.87	128.88
29	a	818	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
29	b	717	CLA	CHB-C4A-NA	2.14	127.47	124.51
36	K	221	DD6	C21-C20-C19	2.14	116.69	114.28
34	j	102	LMG	O2-C2-C1	-2.14	104.85	110.05
29	a	815	CLA	CHD-C1D-ND	-2.14	122.49	124.45
39	C	312	KC1	C1A-C2A-C3A	-2.14	105.42	107.11
29	h	201	CLA	CHD-C1D-ND	-2.14	122.49	124.45
32	m	103	BCR	C33-C5-C6	-2.14	122.13	124.53
36	h	202	DD6	C4-C3-C2	-2.14	119.10	123.47
39	O	312	KC1	C2A-C3A-C4A	2.14	108.07	106.49
36	M	304	DD6	O1-C20-C21	-2.13	112.50	115.06
29	A	211	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
36	F	303	DD6	C7-C6-C5	-2.13	119.94	122.92
38	C	306	UIX	C41-C40-C39	-2.13	119.94	122.92
29	L	316	CLA	O2D-CGD-CBD	2.13	115.06	111.27
39	H	314	KC1	C2A-C3A-C4A	2.13	108.07	106.49
39	F	309	KC1	O2D-CGD-O1D	-2.13	119.67	123.84
36	T	303	DD6	C12-C11-C10	-2.13	119.94	122.92
38	C	306	UIX	C29-C26-C30	-2.13	119.94	122.92
38	T	306	UIX	C10-C11-C13	2.13	122.21	118.94
36	I	206	DD6	C14-C13-C11	-2.13	122.23	125.53
29	b	707	CLA	O1D-CGD-CBD	2.13	128.84	124.48
34	P	201	LMG	O1-C7-C8	-2.13	105.77	110.90
29	a	826	CLA	O2D-CGD-CBD	2.13	115.05	111.27
29	a	809	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
29	L	313	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
29	M	314	CLA	CHB-C4A-NA	2.13	127.45	124.51
29	J	311	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
29	H	310	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
32	b	735	BCR	C34-C9-C8	2.13	121.43	118.08
29	B	315	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
37	P	202	PID	C19-C20-C21	2.13	130.34	127.31
34	b	732	LMG	C38-C37-C36	-2.12	103.64	114.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	805	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
38	C	306	UIX	C10-C11-C13	2.12	122.20	118.94
29	M	311	CLA	CHD-C1D-ND	-2.12	122.50	124.45
29	O	311	CLA	CHD-C1D-ND	-2.12	122.50	124.45
36	E	302	DD6	C26-C25-C24	-2.12	116.59	123.22
29	B	308	CLA	C1-C2-C3	-2.12	122.37	126.04
29	a	804	CLA	C1-C2-C3	-2.12	122.37	126.04
32	a	834	BCR	C36-C18-C17	-2.12	119.95	122.92
29	a	822	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
36	K	203	DD6	C15-C14-C13	-2.12	121.51	125.99
37	h	204	PID	CM4-C14-C13	2.12	123.94	119.05
32	b	728	BCR	C36-C18-C17	-2.12	119.95	122.92
29	a	821	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
29	N	313	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
36	J	302	DD6	C33-C34-C35	-2.12	107.40	110.30
39	E	312	KC1	CAC-C3C-C4C	2.12	127.56	124.81
29	b	719	CLA	CHD-C1D-ND	-2.12	122.51	124.45
29	C	311	CLA	CHD-C1D-ND	-2.12	122.51	124.45
36	I	206	DD6	C10-C9-C8	-2.12	116.61	123.22
29	E	311	CLA	CHD-C1D-ND	-2.12	122.51	124.45
29	K	210	CLA	C1-C2-C3	-2.12	123.33	126.75
39	A	213	KC1	C2A-C3A-C4A	2.12	108.06	106.49
37	Q	306	PID	CM2-C5-C4	-2.12	105.31	108.98
37	P	202	PID	CM4-C14-C13	2.12	123.93	119.05
32	b	728	BCR	C1-C6-C7	2.12	121.76	115.78
39	Q	311	KC1	C2A-C3A-C4A	2.11	108.06	106.49
37	O	301	PID	C17-C18-C19	2.11	129.52	124.81
37	j	101	PID	CM4-C14-C13	2.11	123.93	119.05
29	b	722	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
36	J	303	DD6	C19-C18-C17	-2.11	106.69	110.77
36	L	304	DD6	C7-C6-C5	-2.11	119.96	122.92
32	f	801	BCR	C35-C13-C14	-2.11	119.96	122.92
37	N	307	PID	CM3-C5-C4	-2.11	105.31	108.98
29	K	209	CLA	CHD-C1D-ND	-2.11	122.51	124.45
37	E	301	PID	CM3-C5-C4	-2.11	105.31	108.98
36	A	201	DD6	C37-C36-C35	2.11	118.27	114.36
34	b	732	LMG	O3-C3-C2	-2.11	105.47	110.35
32	a	834	BCR	C8-C7-C6	-2.11	121.27	127.20
34	P	201	LMG	O2-C2-C1	-2.11	104.92	110.05
39	O	310	KC1	CMD-C2D-C1D	-2.11	125.22	128.46
29	b	706	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
35	j	103	DGD	O2G-C1B-O1B	-2.11	118.61	123.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	504	CLA	C1-C2-C3	-2.11	122.40	126.04
29	a	827	CLA	O2D-CGD-CBD	2.11	115.02	111.27
29	I	214	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
32	i	204	BCR	C29-C30-C25	2.11	113.73	110.48
39	M	312	KC1	O2D-CGD-O1D	-2.11	119.72	123.84
29	a	818	CLA	CHD-C1D-ND	-2.11	122.52	124.45
29	l	503	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
36	K	204	DD6	C37-C36-C35	2.11	118.26	114.36
29	b	723	CLA	CHD-C1D-ND	-2.11	122.52	124.45
36	K	221	DD6	C3-C4-C5	-2.11	119.16	123.47
29	A	209	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
36	B	305	DD6	C10-C9-C8	-2.10	116.65	123.22
29	K	210	CLA	CHD-C1D-ND	-2.10	122.52	124.45
36	J	302	DD6	C20-C19-C18	-2.10	108.59	112.75
37	H	302	PID	CM4-C14-C13	2.10	123.90	119.05
29	Q	307	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
29	b	717	CLA	CHD-C1D-ND	-2.10	122.52	124.45
29	a	809	CLA	C1-C2-C3	-2.10	122.41	126.04
29	B	310	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
29	i	202	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
36	A	201	DD6	C-C1-C2	-2.10	119.98	122.92
29	a	810	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
36	I	202	DD6	C10-C9-C8	-2.10	116.67	123.22
39	H	309	KC1	C3D-CAD-CBD	-2.10	104.84	107.61
29	E	308	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
38	F	305	UIX	C-C7-C10	-2.10	121.56	125.99
29	A	209	CLA	CHD-C1D-ND	-2.10	122.53	124.45
29	A	212	CLA	CHD-C1D-ND	-2.10	122.53	124.45
29	G	313	CLA	CHD-C1D-ND	-2.10	122.53	124.45
29	L	310	CLA	CHD-C1D-ND	-2.10	122.53	124.45
39	H	309	KC1	C2A-C3A-C4A	2.10	108.04	106.49
36	I	205	DD6	O1-C20-C15	-2.10	57.22	58.96
29	a	825	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
39	H	314	KC1	O2D-CGD-O1D	-2.10	119.74	123.84
29	a	803	CLA	CHD-C1D-ND	-2.10	122.53	124.45
39	P	211	KC1	C1A-C2A-C3A	-2.10	105.45	107.11
36	C	303	DD6	C-C1-C2	-2.10	119.99	122.92
36	G	308	DD6	C37-C36-C35	2.09	118.23	114.36
36	K	202	DD6	C24-C1-C2	2.09	122.15	118.94
29	I	216	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
29	N	308	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
29	b	714	CLA	O2D-CGD-CBD	2.09	114.99	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	K	205	DD6	C32-C33-C34	-2.09	108.92	113.64
36	K	202	DD6	C7-C6-C5	-2.09	119.99	122.92
29	K	209	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
34	P	201	LMG	O7-C10-O9	-2.09	118.65	123.70
29	A	218	CLA	CHD-C1D-ND	-2.09	122.53	124.45
29	l	502	CLA	C1-C2-C3	-2.09	122.43	126.04
32	l	507	BCR	C23-C24-C25	-2.09	121.33	127.20
36	m	101	DD6	C7-C6-C8	2.09	121.37	118.08
36	L	304	DD6	C19-C18-C17	2.09	114.81	110.77
36	D	301	DD6	C12-C11-C10	-2.09	120.00	122.92
32	b	728	BCR	C10-C11-C12	-2.09	116.70	123.22
37	P	208	PID	C15-C14-C13	2.09	122.72	117.00
29	b	706	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
36	M	301	DD6	C-C1-C2	-2.09	120.00	122.92
36	A	204	DD6	C25-C24-C1	-2.09	120.55	126.42
29	a	807	CLA	C1-C2-C3	-2.09	122.43	126.04
29	Q	313	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
29	A	212	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
29	M	314	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
29	a	802	CLA	CHD-C1D-ND	-2.09	122.54	124.45
29	b	731	CLA	C1-C2-C3	-2.08	122.44	126.04
39	M	305	KC1	O2A-CGA-O1A	-2.08	118.34	122.67
32	a	838	BCR	C10-C11-C12	-2.08	116.72	123.22
29	T	308	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
29	a	819	CLA	CHD-C1D-ND	-2.08	122.54	124.45
29	a	827	CLA	CHD-C1D-ND	-2.08	122.54	124.45
29	D	311	CLA	CHD-C1D-ND	-2.08	122.54	124.45
39	G	318	KC1	C1A-C2A-C3A	-2.08	105.46	107.11
29	a	819	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
36	J	303	DD6	C33-C34-C35	-2.08	107.46	110.30
36	F	303	DD6	C32-C33-C34	-2.08	108.95	113.64
39	Q	311	KC1	CAC-C3C-C4C	2.08	127.51	124.81
29	b	707	CLA	CHD-C1D-ND	-2.08	122.54	124.45
29	A	217	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
34	K	219	LMG	O7-C10-O9	-2.08	118.68	123.70
29	A	209	CLA	C1-C2-C3	-2.08	122.45	126.04
29	H	308	CLA	CHD-C1D-ND	-2.08	122.55	124.45
39	P	213	KC1	C2A-C3A-C4A	2.08	108.03	106.49
29	a	837	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
36	K	202	DD6	C32-C33-C34	-2.08	108.95	113.64
29	L	307	CLA	O2A-CGA-O1A	-2.08	118.36	123.59
36	K	205	DD6	C28-C27-C29	2.07	120.95	116.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	306	PID	O4-C12-C13	2.07	127.31	122.89
36	L	304	DD6	C20-C19-C18	2.07	116.85	112.75
29	Q	310	CLA	CHD-C1D-ND	-2.07	122.55	124.45
32	a	838	BCR	C29-C30-C25	2.07	113.67	110.48
36	A	204	DD6	C3-C4-C5	-2.07	119.23	123.47
29	C	311	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
29	a	820	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
39	T	310	KC1	O2D-CGD-O1D	-2.07	119.79	123.84
39	P	211	KC1	O2D-CGD-O1D	-2.07	119.79	123.84
29	I	210	CLA	CHD-C1D-ND	-2.07	122.55	124.45
29	C	308	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
29	P	210	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
32	b	735	BCR	C27-C26-C25	-2.07	119.72	122.73
29	i	201	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	B	309	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
36	I	204	DD6	C7-C6-C5	-2.07	120.03	122.92
36	L	304	DD6	C12-C11-C10	-2.07	120.03	122.92
29	L	308	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	a	826	CLA	CHD-C1D-ND	-2.07	122.55	124.45
37	O	305	PID	CM5-C21-C20	-2.07	120.03	122.92
36	T	303	DD6	O1-C20-C21	-2.07	112.58	115.06
29	E	315	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
29	N	309	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
32	i	204	BCR	C37-C22-C21	-2.07	120.03	122.92
29	a	822	CLA	C1-C2-C3	-2.07	122.47	126.04
29	H	315	CLA	CHD-C1D-ND	-2.07	122.56	124.45
29	K	211	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
29	O	308	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
38	E	304	UIX	C37-C34-C30	-2.07	119.24	123.47
34	j	102	LMG	O1-C7-C8	-2.07	105.91	110.90
29	D	308	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
29	N	309	CLA	CHD-C1D-ND	-2.07	122.56	124.45
29	b	708	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
29	f	805	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
29	H	307	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
29	b	711	CLA	O2D-CGD-CBD	2.06	114.94	111.27
35	j	105	DGD	O2G-C1B-O1B	-2.06	118.71	123.70
29	M	306	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
39	A	213	KC1	CBD-CHA-C1A	2.06	132.73	128.88
36	B	319	DD6	C24-C1-C2	2.06	122.11	118.94
32	a	834	BCR	C15-C16-C17	-2.06	119.25	123.47
36	K	204	DD6	O1-C20-C15	-2.06	57.25	58.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	308	CLA	CHD-C1D-ND	-2.06	122.56	124.45
29	b	715	CLA	O2D-CGD-CBD	2.06	114.93	111.27
36	J	302	DD6	C23-C16-C22	2.06	110.41	107.37
39	T	315	KC1	O2D-CGD-O1D	-2.06	119.81	123.84
37	Q	301	PID	CM4-C14-C13	2.06	123.81	119.05
36	P	204	DD6	C4-C3-C2	-2.06	119.25	123.47
36	G	308	DD6	O1-C20-C19	2.06	114.93	113.38
36	M	303	DD6	O1-C20-C15	-2.06	57.25	58.96
29	A	218	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
34	b	734	LMG	O7-C10-O9	-2.06	118.73	123.70
36	B	301	DD6	C25-C26-C27	-2.06	120.60	126.58
39	T	310	KC1	C2A-C3A-C4A	2.06	108.01	106.49
38	C	306	UIX	C21-C15-C20	-2.06	108.63	110.47
32	l	507	BCR	C34-C9-C10	-2.06	120.04	122.92
29	a	808	CLA	CHD-C1D-ND	-2.06	122.56	124.45
38	J	304	UIX	C41-C40-C38	2.06	121.32	118.08
36	B	303	DD6	C34-C35-C36	-2.06	107.76	111.85
29	b	714	CLA	C1-C2-C3	-2.06	122.49	126.04
29	a	807	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
36	A	204	DD6	C14-C13-C11	-2.06	122.34	125.53
29	I	214	CLA	CHD-C1D-ND	-2.06	122.56	124.45
37	D	307	PID	C17-C18-C19	2.06	129.38	124.81
29	b	717	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
29	E	311	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
29	b	731	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
29	K	213	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
36	J	302	DD6	C19-C18-C17	-2.05	106.81	110.77
29	a	817	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	G	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	B	313	KC1	C1A-C2A-C3A	-2.05	105.48	107.11
37	Q	304	PID	CM4-C14-C13	2.05	123.79	119.05
29	b	710	CLA	CHD-C1D-ND	-2.05	122.57	124.45
36	L	303	DD6	C25-C26-C27	-2.05	120.62	126.58
29	L	316	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
29	P	209	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
29	E	309	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	G	318	KC1	O1D-CGD-CBD	-2.05	120.28	124.48
29	b	703	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
36	I	203	DD6	C9-C8-C6	-2.05	120.66	126.42
35	B	318	DGD	C3E-C4E-C5E	2.05	113.90	110.24
29	G	316	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	I	211	CLA	O2A-CGA-O1A	-2.05	118.42	123.59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	806	CLA	CHD-C1D-ND	-2.05	122.57	124.45
32	f	801	BCR	C11-C12-C13	-2.05	120.66	126.42
29	l	504	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
38	A	203	UIX	C29-C26-C23	2.05	121.31	118.08
37	T	305	PID	C26-C25-C24	2.05	111.20	109.21
29	Q	308	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	l	510	CLA	CHD-C1D-ND	-2.05	122.57	124.45
39	O	312	KC1	CAC-C3C-C4C	2.05	127.47	124.81
29	H	313	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
29	M	309	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	E	314	CLA	CHD-C1D-ND	-2.05	122.57	124.45
35	m	102	DGD	O2G-C1B-O1B	-2.05	118.76	123.70
29	I	209	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
36	K	204	DD6	C-C1-C2	-2.05	120.06	122.92
36	A	201	DD6	C3-C4-C5	-2.05	119.28	123.47
36	m	101	DD6	C34-C35-C36	-2.05	107.78	111.85
32	a	835	BCR	C20-C19-C18	-2.05	120.67	126.42
29	F	310	CLA	C1B-CHB-C4A	-2.04	126.07	130.12
36	B	302	DD6	C-C1-C24	2.04	121.30	118.08
29	T	309	CLA	CHD-C1D-ND	-2.04	122.58	124.45
29	i	203	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
32	b	729	BCR	C38-C26-C27	2.04	117.54	113.62
36	K	205	DD6	C7-C6-C8	2.04	121.30	118.08
29	a	831	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
29	T	311	CLA	CHD-C1D-ND	-2.04	122.58	124.45
36	G	306	DD6	C10-C9-C8	-2.04	116.84	123.22
29	T	314	CLA	CED-O2D-CGD	2.04	120.55	115.94
29	G	316	CLA	C1-C2-C3	-2.04	122.51	126.04
36	L	305	DD6	C25-C24-C1	-2.04	120.69	126.42
32	b	729	BCR	C16-C15-C14	-2.04	119.30	123.47
39	L	306	KC1	CHD-C4C-NC	2.04	127.30	124.20
36	Q	302	DD6	O1-C20-C21	-2.04	112.61	115.06
36	E	302	DD6	C-C1-C24	2.04	121.29	118.08
29	J	313	CLA	CHD-C1D-ND	-2.04	122.58	124.45
39	K	215	KC1	CAA-CBA-CGA	-2.04	116.78	127.26
36	B	303	DD6	C37-C36-C35	2.04	118.13	114.36
36	B	305	DD6	C14-C13-C11	-2.04	122.37	125.53
38	T	306	UIX	C1-C3-C5	-2.04	108.72	112.75
29	C	314	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
32	l	507	BCR	C11-C12-C13	-2.04	120.69	126.42
29	K	209	CLA	C1-C2-C3	-2.04	122.52	126.04
37	T	302	PID	CM4-C14-C13	2.04	123.75	119.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	502	CLA	O2D-CGD-CBD	2.04	114.89	111.27
29	l	502	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
36	A	204	DD6	O1-C20-C21	-2.03	112.62	115.06
29	b	717	CLA	C1-C2-C3	-2.03	122.52	126.04
29	A	217	CLA	C1-C2-C3	-2.03	122.52	126.04
29	A	208	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
29	G	301	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
38	A	203	UIX	C41-C40-C38	2.03	121.28	118.08
38	Q	305	UIX	C41-C40-C39	-2.03	120.07	122.92
36	L	303	DD6	C21-C20-C15	-2.03	118.85	122.26
29	T	314	CLA	O2D-CGD-CBD	2.03	114.88	111.27
29	M	310	CLA	CHD-C1D-ND	-2.03	122.59	124.45
39	E	307	KC1	O2D-CGD-O1D	-2.03	119.86	123.84
36	K	204	DD6	C7-C6-C5	-2.03	120.08	122.92
38	E	304	UIX	C12-C11-C10	2.03	121.28	118.08
29	a	816	CLA	CHD-C1D-ND	-2.03	122.59	124.45
35	j	105	DGD	O6D-C5D-C6D	2.03	110.77	106.67
37	C	302	PID	CM4-C14-C13	2.03	123.73	119.05
36	K	205	DD6	C33-C34-C35	-2.03	107.52	110.30
36	B	302	DD6	C3-C4-C5	-2.03	119.31	123.47
29	T	314	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
29	I	216	CLA	CHD-C1D-ND	-2.03	122.59	124.45
29	a	815	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
35	j	103	DGD	O3G-C3G-C2G	-2.03	106.01	110.90
29	A	207	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
39	N	312	KC1	O2D-CGD-O1D	-2.03	119.87	123.84
29	I	212	CLA	C1-C2-C3	-2.03	122.54	126.04
29	E	311	CLA	O2D-CGD-CBD	2.03	114.87	111.27
29	J	305	CLA	CHD-C1D-ND	-2.03	122.59	124.45
29	a	802	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
36	K	203	DD6	C4-C3-C2	-2.03	119.33	123.47
37	F	306	PID	C6-C7-C8	-2.02	121.71	125.99
36	B	303	DD6	C12-C11-C13	2.02	121.27	118.08
29	L	312	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
35	j	106	DGD	O2G-C1B-O1B	-2.02	118.81	123.70
29	b	709	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
34	E	316	LMG	C1-O6-C5	2.02	117.66	113.69
37	C	305	PID	CM4-C14-C13	2.02	123.71	119.05
39	P	211	KC1	CHD-C4C-NC	2.02	127.27	124.20
39	P	213	KC1	C1A-C2A-C3A	-2.02	105.51	107.11
32	b	729	BCR	C35-C13-C12	2.02	121.26	118.08
29	i	203	CLA	O2D-CGD-CBD	2.02	114.86	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	721	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
29	b	704	CLA	CHB-C4A-NA	2.02	127.31	124.51
36	L	303	DD6	C25-C24-C1	-2.02	120.74	126.42
36	L	303	DD6	C3-C4-C5	-2.02	119.34	123.47
29	B	307	CLA	CHD-C1D-ND	-2.02	122.60	124.45
29	a	829	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	h	201	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	G	316	CLA	CHD-C1D-ND	-2.02	122.60	124.45
36	I	202	DD6	C14-C13-C11	-2.02	122.40	125.53
29	O	314	CLA	CHB-C4A-NA	2.02	127.30	124.51
39	K	215	KC1	CMD-C2D-C1D	-2.02	125.36	128.46
29	M	307	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	a	824	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	K	207	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
35	b	733	DGD	O6D-C5D-C4D	-2.02	106.03	109.69
29	b	726	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	K	211	CLA	CHD-C1D-ND	-2.02	122.60	124.45
29	b	718	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
39	Q	309	KC1	CBD-CHA-C1A	2.02	132.64	128.88
36	J	301	DD6	C13-C11-C10	2.02	122.03	118.94
29	b	712	CLA	CHD-C1D-ND	-2.02	122.60	124.45
29	b	701	CLA	CHD-C1D-ND	-2.01	122.60	124.45
39	E	312	KC1	C1A-C2A-C3A	-2.01	105.52	107.11
39	M	312	KC1	CAA-CBA-CGA	-2.01	116.91	127.26
34	K	220	LMG	O1-C7-C8	-2.01	106.04	110.90
29	a	808	CLA	C1-C2-C3	-2.01	122.56	126.04
36	G	308	DD6	C9-C8-C6	-2.01	120.77	126.42
36	I	204	DD6	C13-C11-C10	2.01	122.03	118.94
38	B	304	UIX	C37-C34-C30	-2.01	119.36	123.47
29	F	307	CLA	O2D-CGD-CBD	2.01	114.84	111.27
36	E	303	DD6	C21-C20-C15	-2.01	118.89	122.26
29	K	213	CLA	CHD-C1D-ND	-2.01	122.61	124.45
29	B	308	CLA	O2D-CGD-CBD	2.01	114.84	111.27
36	I	206	DD6	C4-C3-C2	-2.01	119.36	123.47
38	T	306	UIX	C21-C15-C20	-2.01	108.67	110.47
29	b	714	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
36	K	204	DD6	C21-C20-C19	2.01	116.54	114.28
36	T	303	DD6	C7-C6-C5	-2.01	120.11	122.92
29	a	830	CLA	CHD-C1D-ND	-2.01	122.61	124.45
40	J	314	SQD	O8-S-C6	-2.01	102.54	105.74
36	P	204	DD6	C8-C6-C5	2.01	122.02	118.94
36	m	101	DD6	C14-C13-C11	-2.01	122.42	125.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	306	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
29	L	309	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
32	f	804	BCR	C34-C9-C10	-2.00	120.12	122.92
39	O	310	KC1	C1A-C2A-C3A	-2.00	105.52	107.11
29	a	811	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	l	509	CLA	CHD-C1D-ND	-2.00	122.61	124.45
38	C	306	UIX	C3-C5-C4	-2.00	106.91	110.77
36	M	301	DD6	C10-C9-C8	-2.00	116.97	123.22
38	L	302	UIX	C7-C10-C11	-2.00	122.42	125.53
29	b	724	CLA	O2D-CGD-CBD	2.00	114.83	111.27
29	B	311	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	J	308	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	a	813	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	b	719	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
29	a	825	CLA	C1-C2-C3	-2.00	122.58	126.04
35	j	103	DGD	O1G-C1A-O1A	-2.00	118.54	123.59
36	I	203	DD6	C33-C34-C35	-2.00	107.57	110.30

All (220) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	a	801	CLA	ND
29	a	802	CLA	ND
29	a	803	CLA	ND
29	a	804	CLA	ND
29	a	805	CLA	ND
29	a	806	CLA	ND
29	a	807	CLA	ND
29	a	808	CLA	ND
29	a	809	CLA	ND
29	a	810	CLA	ND
29	a	811	CLA	ND
29	a	812	CLA	ND
29	a	813	CLA	ND
29	a	814	CLA	ND
29	a	815	CLA	ND
29	a	816	CLA	ND
29	a	817	CLA	ND
29	a	818	CLA	ND
29	a	819	CLA	ND
29	a	820	CLA	ND
29	a	821	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
29	a	822	CLA	ND
29	a	823	CLA	ND
29	a	824	CLA	ND
29	a	825	CLA	ND
29	a	826	CLA	ND
29	a	827	CLA	ND
29	a	828	CLA	ND
29	a	829	CLA	ND
29	a	830	CLA	ND
29	a	831	CLA	ND
29	a	837	CLA	ND
29	b	701	CLA	ND
29	b	702	CLA	ND
29	b	703	CLA	ND
29	b	704	CLA	ND
29	b	705	CLA	ND
29	b	706	CLA	ND
29	b	707	CLA	ND
29	b	708	CLA	ND
29	b	709	CLA	ND
29	b	710	CLA	ND
29	b	711	CLA	ND
29	b	712	CLA	ND
29	b	713	CLA	ND
29	b	714	CLA	ND
29	b	715	CLA	ND
29	b	716	CLA	ND
29	b	717	CLA	ND
29	b	718	CLA	ND
29	b	719	CLA	ND
29	b	720	CLA	ND
29	b	721	CLA	ND
29	b	722	CLA	ND
29	b	723	CLA	ND
29	b	724	CLA	ND
29	b	725	CLA	ND
29	b	726	CLA	ND
29	b	731	CLA	ND
29	b	736	CLA	ND
29	f	802	CLA	ND
29	f	803	CLA	ND
29	f	805	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
29	h	201	CLA	ND
29	i	201	CLA	ND
29	i	202	CLA	ND
29	i	203	CLA	ND
29	j	104	CLA	ND
29	l	501	CLA	ND
29	l	502	CLA	ND
29	l	503	CLA	ND
29	l	504	CLA	ND
29	l	505	CLA	ND
29	l	508	CLA	ND
29	l	509	CLA	ND
29	l	510	CLA	ND
29	A	206	CLA	ND
29	A	207	CLA	ND
29	A	208	CLA	ND
29	A	209	CLA	ND
29	A	210	CLA	ND
29	A	211	CLA	ND
29	A	212	CLA	ND
29	A	214	CLA	ND
29	A	215	CLA	ND
29	A	216	CLA	ND
29	A	217	CLA	ND
29	A	218	CLA	ND
29	G	301	CLA	ND
29	G	302	CLA	ND
29	G	304	CLA	ND
29	G	311	CLA	ND
29	G	312	CLA	ND
29	G	313	CLA	ND
29	G	314	CLA	ND
29	G	316	CLA	ND
29	G	317	CLA	ND
29	G	319	CLA	ND
29	I	201	CLA	ND
29	I	207	CLA	ND
29	I	208	CLA	ND
29	I	209	CLA	ND
29	I	210	CLA	ND
29	I	211	CLA	ND
29	I	212	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
29	I	213	CLA	ND
29	I	214	CLA	ND
29	I	216	CLA	ND
29	I	217	CLA	ND
29	K	207	CLA	ND
29	K	208	CLA	ND
29	K	209	CLA	ND
29	K	210	CLA	ND
29	K	211	CLA	ND
29	K	212	CLA	ND
29	K	213	CLA	ND
29	K	214	CLA	ND
29	K	216	CLA	ND
29	K	217	CLA	ND
29	K	218	CLA	ND
29	F	307	CLA	ND
29	F	308	CLA	ND
29	F	310	CLA	ND
29	F	311	CLA	ND
29	F	312	CLA	ND
29	F	313	CLA	ND
29	F	315	CLA	ND
29	F	316	CLA	ND
29	J	305	CLA	ND
29	J	306	CLA	ND
29	J	307	CLA	ND
29	J	308	CLA	ND
29	J	309	CLA	ND
29	J	310	CLA	ND
29	J	311	CLA	ND
29	J	313	CLA	ND
29	M	306	CLA	ND
29	M	307	CLA	ND
29	M	308	CLA	ND
29	M	309	CLA	ND
29	M	310	CLA	ND
29	M	311	CLA	ND
29	M	313	CLA	ND
29	M	314	CLA	ND
29	M	315	CLA	ND
29	L	307	CLA	ND
29	L	308	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
29	L	309	CLA	ND
29	L	310	CLA	ND
29	L	311	CLA	ND
29	L	312	CLA	ND
29	L	313	CLA	ND
29	L	315	CLA	ND
29	L	316	CLA	ND
29	L	317	CLA	ND
29	D	308	CLA	ND
29	D	309	CLA	ND
29	D	311	CLA	ND
29	D	312	CLA	ND
29	D	313	CLA	ND
29	D	314	CLA	ND
29	D	316	CLA	ND
29	B	306	CLA	ND
29	B	307	CLA	ND
29	B	308	CLA	ND
29	B	309	CLA	ND
29	B	310	CLA	ND
29	B	311	CLA	ND
29	B	312	CLA	ND
29	B	314	CLA	ND
29	B	315	CLA	ND
29	B	316	CLA	ND
29	H	307	CLA	ND
29	H	308	CLA	ND
29	H	310	CLA	ND
29	H	312	CLA	ND
29	H	313	CLA	ND
29	H	315	CLA	ND
29	N	308	CLA	ND
29	N	309	CLA	ND
29	N	311	CLA	ND
29	N	313	CLA	ND
29	N	314	CLA	ND
29	N	316	CLA	ND
29	O	308	CLA	ND
29	O	311	CLA	ND
29	O	313	CLA	ND
29	O	316	CLA	ND
29	T	308	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
29	T	309	CLA	ND
29	T	311	CLA	ND
29	T	313	CLA	ND
29	T	314	CLA	ND
29	T	316	CLA	ND
29	Q	307	CLA	ND
29	Q	308	CLA	ND
29	Q	310	CLA	ND
29	Q	312	CLA	ND
29	Q	313	CLA	ND
29	Q	315	CLA	ND
29	C	308	CLA	ND
29	C	309	CLA	ND
29	C	311	CLA	ND
29	C	313	CLA	ND
29	C	314	CLA	ND
29	C	316	CLA	ND
29	P	209	CLA	ND
29	P	210	CLA	ND
29	P	212	CLA	ND
29	P	214	CLA	ND
29	P	215	CLA	ND
29	P	217	CLA	ND
29	E	305	CLA	ND
29	E	306	CLA	ND
29	E	308	CLA	ND
29	E	309	CLA	ND
29	E	310	CLA	ND
29	E	311	CLA	ND
29	E	313	CLA	ND
29	E	315	CLA	ND

All (2704) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	a	801	CLA	CHA-CBD-CGD-O1D
29	a	801	CLA	CHA-CBD-CGD-O2D
29	a	801	CLA	CBD-CGD-O2D-CED
29	a	805	CLA	C1A-C2A-CAA-CBA
29	a	805	CLA	C3A-C2A-CAA-CBA
29	a	805	CLA	CBD-CGD-O2D-CED
29	a	807	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	a	809	CLA	C1A-C2A-CAA-CBA
29	a	809	CLA	C3A-C2A-CAA-CBA
29	a	811	CLA	C1A-C2A-CAA-CBA
29	a	812	CLA	C1A-C2A-CAA-CBA
29	a	813	CLA	C1A-C2A-CAA-CBA
29	a	813	CLA	C3A-C2A-CAA-CBA
29	a	814	CLA	CBA-CGA-O2A-C1
29	a	815	CLA	C1A-C2A-CAA-CBA
29	a	815	CLA	C3A-C2A-CAA-CBA
29	a	816	CLA	CHA-CBD-CGD-O1D
29	a	816	CLA	CHA-CBD-CGD-O2D
29	a	818	CLA	C3A-C2A-CAA-CBA
29	a	819	CLA	C1A-C2A-CAA-CBA
29	a	819	CLA	C3A-C2A-CAA-CBA
29	a	821	CLA	C3A-C2A-CAA-CBA
29	a	821	CLA	CBD-CGD-O2D-CED
29	a	823	CLA	CBD-CGD-O2D-CED
29	a	825	CLA	CHA-CBD-CGD-O1D
29	a	825	CLA	CHA-CBD-CGD-O2D
29	a	825	CLA	C2-C3-C5-C6
29	a	825	CLA	C4-C3-C5-C6
29	a	826	CLA	C1A-C2A-CAA-CBA
29	a	826	CLA	C3A-C2A-CAA-CBA
29	a	828	CLA	CBD-CGD-O2D-CED
29	a	837	CLA	C1A-C2A-CAA-CBA
29	a	837	CLA	C3A-C2A-CAA-CBA
29	b	704	CLA	C2-C3-C5-C6
29	b	704	CLA	C4-C3-C5-C6
29	b	705	CLA	C1A-C2A-CAA-CBA
29	b	705	CLA	C3A-C2A-CAA-CBA
29	b	705	CLA	CBD-CGD-O2D-CED
29	b	706	CLA	C1A-C2A-CAA-CBA
29	b	706	CLA	C2-C3-C5-C6
29	b	706	CLA	C4-C3-C5-C6
29	b	707	CLA	CBD-CGD-O2D-CED
29	b	710	CLA	C1A-C2A-CAA-CBA
29	b	710	CLA	C3A-C2A-CAA-CBA
29	b	712	CLA	C3A-C2A-CAA-CBA
29	b	713	CLA	C3A-C2A-CAA-CBA
29	b	714	CLA	CHA-CBD-CGD-O1D
29	b	714	CLA	CHA-CBD-CGD-O2D
29	b	715	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	b	715	CLA	C3A-C2A-CAA-CBA
29	b	715	CLA	C2A-CAA-CBA-CGA
29	b	715	CLA	CBA-CGA-O2A-C1
29	b	717	CLA	C1A-C2A-CAA-CBA
29	b	717	CLA	C4-C3-C5-C6
29	b	718	CLA	C2-C3-C5-C6
29	b	718	CLA	C4-C3-C5-C6
29	b	719	CLA	C1A-C2A-CAA-CBA
29	b	719	CLA	C3A-C2A-CAA-CBA
29	b	720	CLA	CBD-CGD-O2D-CED
29	b	721	CLA	C6-C7-C8-C9
29	b	722	CLA	CBD-CGD-O2D-CED
29	b	722	CLA	C2-C3-C5-C6
29	b	722	CLA	C4-C3-C5-C6
29	b	725	CLA	CHA-CBD-CGD-O1D
29	b	725	CLA	CHA-CBD-CGD-O2D
29	b	726	CLA	C11-C12-C13-C14
29	b	731	CLA	CBD-CGD-O2D-CED
29	b	736	CLA	CBD-CGD-O2D-CED
29	f	803	CLA	CHA-CBD-CGD-O1D
29	f	803	CLA	CHA-CBD-CGD-O2D
29	f	805	CLA	C1A-C2A-CAA-CBA
29	h	201	CLA	C1A-C2A-CAA-CBA
29	h	201	CLA	C3A-C2A-CAA-CBA
29	h	201	CLA	C2-C3-C5-C6
29	h	201	CLA	C4-C3-C5-C6
29	i	202	CLA	C6-C7-C8-C9
29	i	203	CLA	CHA-CBD-CGD-O1D
29	i	203	CLA	CHA-CBD-CGD-O2D
29	l	501	CLA	C1A-C2A-CAA-CBA
29	l	501	CLA	C3A-C2A-CAA-CBA
29	l	502	CLA	CHA-CBD-CGD-O1D
29	l	502	CLA	CHA-CBD-CGD-O2D
29	l	504	CLA	CBD-CGD-O2D-CED
29	l	510	CLA	C1A-C2A-CAA-CBA
29	A	209	CLA	CHA-CBD-CGD-O1D
29	A	209	CLA	CHA-CBD-CGD-O2D
29	A	210	CLA	CHA-CBD-CGD-O1D
29	A	210	CLA	CHA-CBD-CGD-O2D
29	A	210	CLA	CBD-CGD-O2D-CED
29	A	212	CLA	C2-C3-C5-C6
29	A	212	CLA	C4-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	A	214	CLA	CHA-CBD-CGD-O1D
29	A	214	CLA	CHA-CBD-CGD-O2D
29	A	217	CLA	CHA-CBD-CGD-O1D
29	A	217	CLA	CBD-CGD-O2D-CED
29	G	302	CLA	C1A-C2A-CAA-CBA
29	G	302	CLA	C4-C3-C5-C6
29	G	304	CLA	C1A-C2A-CAA-CBA
29	G	304	CLA	C3A-C2A-CAA-CBA
29	G	304	CLA	CBD-CGD-O2D-CED
29	G	304	CLA	O1D-CGD-O2D-CED
29	G	314	CLA	CBD-CGD-O2D-CED
29	G	316	CLA	CBD-CGD-O2D-CED
29	I	208	CLA	C1A-C2A-CAA-CBA
29	I	208	CLA	C3A-C2A-CAA-CBA
29	I	208	CLA	CBA-CGA-O2A-C1
29	I	208	CLA	O1A-CGA-O2A-C1
29	I	212	CLA	C1A-C2A-CAA-CBA
29	I	212	CLA	O2A-C1-C2-C3
29	I	216	CLA	CAD-CBD-CGD-O1D
29	I	216	CLA	CAD-CBD-CGD-O2D
29	I	217	CLA	CHA-CBD-CGD-O1D
29	I	217	CLA	CHA-CBD-CGD-O2D
29	I	217	CLA	CBD-CGD-O2D-CED
29	K	207	CLA	C1A-C2A-CAA-CBA
29	K	207	CLA	C3A-C2A-CAA-CBA
29	K	207	CLA	CHA-CBD-CGD-O1D
29	K	207	CLA	CHA-CBD-CGD-O2D
29	K	209	CLA	O1A-CGA-O2A-C1
29	K	209	CLA	CHA-CBD-CGD-O1D
29	K	209	CLA	CHA-CBD-CGD-O2D
29	K	209	CLA	C2-C3-C5-C6
29	K	209	CLA	C4-C3-C5-C6
29	K	213	CLA	CBD-CGD-O2D-CED
29	K	216	CLA	CBD-CGD-O2D-CED
29	K	217	CLA	CBA-CGA-O2A-C1
29	K	218	CLA	C1A-C2A-CAA-CBA
29	K	218	CLA	C3A-C2A-CAA-CBA
29	K	218	CLA	CBD-CGD-O2D-CED
29	F	310	CLA	C1A-C2A-CAA-CBA
29	F	310	CLA	CHA-CBD-CGD-O1D
29	F	310	CLA	CHA-CBD-CGD-O2D
29	F	313	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	F	313	CLA	C3A-C2A-CAA-CBA
29	F	313	CLA	CBA-CGA-O2A-C1
29	F	313	CLA	CBD-CGD-O2D-CED
29	F	313	CLA	O1D-CGD-O2D-CED
29	F	316	CLA	CHA-CBD-CGD-O1D
29	F	316	CLA	CHA-CBD-CGD-O2D
29	J	305	CLA	CBD-CGD-O2D-CED
29	J	306	CLA	C1A-C2A-CAA-CBA
29	J	306	CLA	C3A-C2A-CAA-CBA
29	J	306	CLA	CBD-CGD-O2D-CED
29	J	306	CLA	C2-C3-C5-C6
29	J	306	CLA	C4-C3-C5-C6
29	J	309	CLA	CBA-CGA-O2A-C1
29	J	310	CLA	C1A-C2A-CAA-CBA
29	J	311	CLA	CHA-CBD-CGD-O1D
29	J	311	CLA	CHA-CBD-CGD-O2D
29	J	311	CLA	C4-C3-C5-C6
29	J	313	CLA	CBD-CGD-O2D-CED
29	M	309	CLA	CBA-CGA-O2A-C1
29	M	311	CLA	CHA-CBD-CGD-O1D
29	M	311	CLA	CHA-CBD-CGD-O2D
29	M	315	CLA	C1A-C2A-CAA-CBA
29	M	315	CLA	C3A-C2A-CAA-CBA
29	M	315	CLA	CBD-CGD-O2D-CED
29	M	315	CLA	O1D-CGD-O2D-CED
29	L	307	CLA	C1A-C2A-CAA-CBA
29	L	307	CLA	C3A-C2A-CAA-CBA
29	L	307	CLA	CBD-CGD-O2D-CED
29	L	311	CLA	C1A-C2A-CAA-CBA
29	L	311	CLA	C3A-C2A-CAA-CBA
29	L	312	CLA	C1A-C2A-CAA-CBA
29	L	312	CLA	C3A-C2A-CAA-CBA
29	L	313	CLA	CHA-CBD-CGD-O1D
29	L	313	CLA	CHA-CBD-CGD-O2D
29	L	315	CLA	CHA-CBD-CGD-O1D
29	L	315	CLA	CHA-CBD-CGD-O2D
29	L	315	CLA	CBD-CGD-O2D-CED
29	L	317	CLA	CBA-CGA-O2A-C1
29	D	308	CLA	CBD-CGD-O2D-CED
29	D	309	CLA	CBD-CGD-O2D-CED
29	D	311	CLA	CBD-CGD-O2D-CED
29	D	312	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	D	312	CLA	O1A-CGA-O2A-C1
29	D	313	CLA	CBD-CGD-O2D-CED
29	D	314	CLA	CBD-CGD-O2D-CED
29	D	316	CLA	CHA-CBD-CGD-O1D
29	D	316	CLA	CHA-CBD-CGD-O2D
29	B	306	CLA	CHA-CBD-CGD-O1D
29	B	306	CLA	CHA-CBD-CGD-O2D
29	B	307	CLA	CBD-CGD-O2D-CED
29	B	310	CLA	C1A-C2A-CAA-CBA
29	B	310	CLA	C3A-C2A-CAA-CBA
29	B	314	CLA	CAD-CBD-CGD-O1D
29	B	314	CLA	CAD-CBD-CGD-O2D
29	H	307	CLA	CHA-CBD-CGD-O1D
29	H	307	CLA	CHA-CBD-CGD-O2D
29	H	310	CLA	CBD-CGD-O2D-CED
29	H	310	CLA	C2-C3-C5-C6
29	H	310	CLA	C4-C3-C5-C6
29	H	312	CLA	C1A-C2A-CAA-CBA
29	H	312	CLA	C3A-C2A-CAA-CBA
29	H	312	CLA	CBD-CGD-O2D-CED
29	H	313	CLA	CBD-CGD-O2D-CED
29	H	315	CLA	CBD-CGD-O2D-CED
29	N	308	CLA	CHA-CBD-CGD-O1D
29	N	308	CLA	CHA-CBD-CGD-O2D
29	N	313	CLA	C1A-C2A-CAA-CBA
29	N	313	CLA	C3A-C2A-CAA-CBA
29	N	314	CLA	CBD-CGD-O2D-CED
29	O	308	CLA	CHA-CBD-CGD-O1D
29	O	313	CLA	CBD-CGD-O2D-CED
29	O	314	CLA	CBD-CGD-O2D-CED
29	O	314	CLA	O1D-CGD-O2D-CED
29	O	316	CLA	CAD-CBD-CGD-O1D
29	O	316	CLA	CAD-CBD-CGD-O2D
29	T	308	CLA	CBD-CGD-O2D-CED
29	T	311	CLA	CHA-CBD-CGD-O1D
29	T	311	CLA	CHA-CBD-CGD-O2D
29	T	311	CLA	CAD-CBD-CGD-O1D
29	T	311	CLA	CAD-CBD-CGD-O2D
29	T	311	CLA	CBD-CGD-O2D-CED
29	T	313	CLA	CHA-CBD-CGD-O1D
29	T	313	CLA	CBD-CGD-O2D-CED
29	T	314	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	T	314	CLA	O1D-CGD-O2D-CED
29	T	316	CLA	CAD-CBD-CGD-O1D
29	T	316	CLA	CAD-CBD-CGD-O2D
29	Q	308	CLA	C1A-C2A-CAA-CBA
29	Q	308	CLA	C3A-C2A-CAA-CBA
29	Q	308	CLA	C4-C3-C5-C6
29	Q	310	CLA	C2-C3-C5-C6
29	Q	310	CLA	C4-C3-C5-C6
29	Q	312	CLA	CBA-CGA-O2A-C1
29	Q	313	CLA	C1A-C2A-CAA-CBA
29	Q	315	CLA	CAD-CBD-CGD-O1D
29	Q	315	CLA	CAD-CBD-CGD-O2D
29	C	309	CLA	CHA-CBD-CGD-O1D
29	C	311	CLA	CAD-CBD-CGD-O1D
29	C	311	CLA	CAD-CBD-CGD-O2D
29	C	311	CLA	CBD-CGD-O2D-CED
29	C	313	CLA	CBA-CGA-O2A-C1
29	C	313	CLA	CBD-CGD-O2D-CED
29	C	314	CLA	CBD-CGD-O2D-CED
29	C	316	CLA	CHA-CBD-CGD-O1D
29	C	316	CLA	CHA-CBD-CGD-O2D
29	C	316	CLA	CAD-CBD-CGD-O1D
29	C	316	CLA	CAD-CBD-CGD-O2D
29	P	209	CLA	O1A-CGA-O2A-C1
29	P	209	CLA	CHA-CBD-CGD-O1D
29	P	209	CLA	CHA-CBD-CGD-O2D
29	P	214	CLA	C1A-C2A-CAA-CBA
29	P	214	CLA	C3A-C2A-CAA-CBA
29	P	214	CLA	CBD-CGD-O2D-CED
29	P	215	CLA	CBD-CGD-O2D-CED
29	E	305	CLA	CBD-CGD-O2D-CED
29	E	305	CLA	C2-C3-C5-C6
29	E	305	CLA	C4-C3-C5-C6
29	E	308	CLA	CHA-CBD-CGD-O1D
29	E	308	CLA	CHA-CBD-CGD-O2D
29	E	308	CLA	CAD-CBD-CGD-O1D
29	E	309	CLA	C1A-C2A-CAA-CBA
29	E	309	CLA	CHA-CBD-CGD-O1D
29	E	309	CLA	CHA-CBD-CGD-O2D
29	E	310	CLA	CBD-CGD-O2D-CED
29	E	313	CLA	CHA-CBD-CGD-O1D
29	E	313	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	E	314	CLA	CHA-CBD-CGD-O1D
29	E	314	CLA	CHA-CBD-CGD-O2D
29	E	315	CLA	C1A-C2A-CAA-CBA
29	E	315	CLA	C3A-C2A-CAA-CBA
32	a	838	BCR	C7-C8-C9-C10
32	a	838	BCR	C7-C8-C9-C34
32	b	729	BCR	C1-C6-C7-C8
32	i	204	BCR	C21-C22-C23-C24
32	i	204	BCR	C37-C22-C23-C24
32	l	506	BCR	C1-C6-C7-C8
32	l	507	BCR	C7-C8-C9-C10
32	l	507	BCR	C7-C8-C9-C34
32	m	103	BCR	C7-C8-C9-C10
32	m	103	BCR	C7-C8-C9-C34
32	m	103	BCR	C21-C22-C23-C24
32	m	103	BCR	C37-C22-C23-C24
34	b	734	LMG	O7-C8-C9-O8
34	h	205	LMG	O9-C10-O7-C8
34	A	219	LMG	C2-C1-O1-C7
34	A	219	LMG	O6-C1-O1-C7
34	A	219	LMG	O9-C10-O7-C8
34	A	219	LMG	C11-C10-O7-C8
34	K	219	LMG	C2-C1-O1-C7
34	K	219	LMG	O6-C1-O1-C7
34	K	219	LMG	C11-C10-O7-C8
34	E	316	LMG	C8-C7-O1-C1
35	b	733	DGD	C2B-C1B-O2G-C2G
35	b	733	DGD	O6D-C1D-O3G-C3G
35	j	103	DGD	C2B-C1B-O2G-C2G
35	j	103	DGD	O6E-C1E-O5D-C6D
36	A	201	DD6	C5-C6-C8-C9
36	A	201	DD6	C7-C6-C8-C9
36	A	202	DD6	C27-C29-C30-C31
36	G	305	DD6	C10-C11-C13-C14
36	G	305	DD6	C12-C11-C13-C14
36	G	305	DD6	C5-C6-C8-C9
36	G	305	DD6	C7-C6-C8-C9
36	I	202	DD6	C-C1-C24-C25
36	I	202	DD6	C13-C14-C15-O1
36	I	203	DD6	C5-C6-C8-C9
36	I	203	DD6	C7-C6-C8-C9
36	I	205	DD6	C5-C6-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
36	I	205	DD6	C7-C6-C8-C9
36	I	206	DD6	C13-C14-C15-O1
36	K	202	DD6	C1-C2-C3-C4
36	K	202	DD6	C5-C6-C8-C9
36	K	202	DD6	C7-C6-C8-C9
36	K	203	DD6	C13-C14-C15-O1
36	K	204	DD6	C10-C11-C13-C14
36	K	204	DD6	C12-C11-C13-C14
36	K	204	DD6	C13-C14-C15-C20
36	K	221	DD6	C11-C10-C9-C8
36	K	221	DD6	C5-C6-C8-C9
36	K	221	DD6	C7-C6-C8-C9
36	F	301	DD6	C1-C2-C3-C4
36	F	301	DD6	C24-C25-C26-C27
36	F	301	DD6	C5-C6-C8-C9
36	J	301	DD6	C10-C11-C13-C14
36	J	301	DD6	C12-C11-C13-C14
36	M	301	DD6	C10-C11-C13-C14
36	M	301	DD6	C12-C11-C13-C14
36	M	303	DD6	C7-C6-C8-C9
36	M	304	DD6	C10-C11-C13-C14
36	M	304	DD6	C12-C11-C13-C14
36	L	301	DD6	C13-C14-C15-O1
36	L	305	DD6	C5-C6-C8-C9
36	L	305	DD6	C7-C6-C8-C9
36	D	301	DD6	C10-C11-C13-C14
36	D	301	DD6	C12-C11-C13-C14
36	D	301	DD6	C5-C6-C8-C9
36	D	301	DD6	C7-C6-C8-C9
36	D	304	DD6	C10-C11-C13-C14
36	D	304	DD6	C12-C11-C13-C14
36	B	319	DD6	C5-C6-C8-C9
36	B	319	DD6	C7-C6-C8-C9
36	O	303	DD6	C1-C2-C3-C4
36	T	303	DD6	C13-C14-C15-O1
37	j	101	PID	C31-C30-O6-C27
37	G	303	PID	C13-C14-C15-C16
37	G	303	PID	CM4-C14-C15-C16
37	G	309	PID	O7-C30-O6-C27
37	F	302	PID	O7-C30-O6-C27
37	F	304	PID	C1-C6-C7-C8
37	F	304	PID	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
37	F	304	PID	C6-C7-C8-C9
37	F	304	PID	C7-C8-C9-C10
37	F	304	PID	C7-C8-C9-C11
37	F	304	PID	O4-C12-C13-C14
37	F	304	PID	C18-C19-C20-C21
37	F	304	PID	C19-C20-C21-C22
37	F	304	PID	C19-C20-C21-CM5
37	F	304	PID	C20-C21-C22-C23
37	F	304	PID	C31-C30-O6-C27
37	D	303	PID	C26-C27-O6-C30
37	D	305	PID	C19-C20-C21-C22
37	D	305	PID	C19-C20-C21-CM5
37	D	305	PID	C20-C21-C22-C23
37	D	305	PID	CM5-C21-C22-C23
37	D	307	PID	O1-C6-C7-C8
37	H	301	PID	O7-C30-O6-C27
37	H	305	PID	O7-C30-O6-C27
37	H	306	PID	C1-C6-C7-C8
37	H	306	PID	C5-C6-C7-C8
37	N	301	PID	O1-C6-C7-C8
37	N	301	PID	O7-C30-O6-C27
37	N	304	PID	O4-C12-C13-C14
37	N	305	PID	C1-C6-C7-C8
37	N	305	PID	O1-C6-C7-C8
37	N	305	PID	C6-C7-C8-C9
37	N	305	PID	C7-C8-C9-C10
37	N	305	PID	C7-C8-C9-C11
37	N	305	PID	O4-C12-C13-C14
37	N	305	PID	C13-C14-C15-C16
37	N	305	PID	CM4-C14-C15-C16
37	N	305	PID	C15-C16-C17-C18
37	N	305	PID	C17-C18-C19-C20
37	N	305	PID	C19-C20-C21-C22
37	N	305	PID	C19-C20-C21-CM5
37	N	305	PID	C26-C27-O6-C30
37	N	305	PID	C31-C30-O6-C27
37	N	305	PID	O7-C30-O6-C27
37	N	307	PID	C1-C6-C7-C8
37	N	307	PID	C5-C6-C7-C8
37	N	307	PID	O1-C6-C7-C8
37	N	307	PID	C6-C7-C8-C9
37	O	301	PID	O1-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
37	O	301	PID	O7-C30-O6-C27
37	O	302	PID	O7-C30-O6-C27
37	O	304	PID	O4-C12-C13-C14
37	O	305	PID	C6-C7-C8-C9
37	O	305	PID	C19-C20-C21-C22
37	O	305	PID	C19-C20-C21-CM5
37	O	305	PID	O7-C30-O6-C27
37	O	307	PID	C1-C6-C7-C8
37	O	307	PID	C5-C6-C7-C8
37	T	301	PID	O1-C6-C7-C8
37	T	301	PID	O4-C12-C13-C14
37	T	302	PID	C26-C27-O6-C30
37	T	304	PID	O1-C6-C7-C8
37	T	307	PID	C7-C8-C9-C10
37	T	307	PID	C7-C8-C9-C11
37	T	307	PID	O7-C30-O6-C27
37	T	317	PID	C1-C6-C7-C8
37	T	317	PID	C7-C8-C9-C10
37	T	317	PID	C7-C8-C9-C11
37	T	317	PID	O4-C12-C13-C14
37	T	317	PID	C31-C30-O6-C27
37	Q	304	PID	O7-C30-O6-C27
37	Q	306	PID	O1-C6-C7-C8
37	C	301	PID	O7-C30-O6-C27
37	C	302	PID	O7-C30-O6-C27
37	C	304	PID	O4-C12-C13-C14
37	C	304	PID	C19-C20-C21-C22
37	C	304	PID	C19-C20-C21-CM5
37	C	305	PID	C1-C6-C7-C8
37	C	305	PID	C5-C6-C7-C8
37	C	305	PID	O1-C6-C7-C8
37	C	305	PID	C6-C7-C8-C9
37	C	305	PID	O7-C30-O6-C27
37	C	307	PID	O7-C30-O6-C27
37	P	202	PID	O1-C6-C7-C8
37	P	202	PID	O7-C30-O6-C27
37	P	203	PID	O7-C30-O6-C27
37	P	206	PID	C19-C20-C21-C22
37	P	206	PID	C19-C20-C21-CM5
37	P	206	PID	O7-C30-O6-C27
37	P	208	PID	O1-C6-C7-C8
37	P	208	PID	O7-C30-O6-C27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
37	E	301	PID	O1-C6-C7-C8
37	E	301	PID	C14-C15-C16-C17
37	E	301	PID	C18-C19-C20-C21
37	E	301	PID	C20-C21-C22-C23
38	F	305	UIX	C7-C10-C11-C12
38	F	305	UIX	C14-C23-C26-C29
38	F	305	UIX	C14-C23-C26-C30
38	F	305	UIX	C31-C27-O2-C18
38	F	305	UIX	C25-C28-C32-C33
38	F	305	UIX	C25-C28-C32-C35
38	F	305	UIX	C36-C38-C40-C39
38	F	305	UIX	C36-C38-C40-C41
38	J	304	UIX	C11-C13-C14-C23
38	J	304	UIX	C14-C23-C26-C29
38	J	304	UIX	C14-C23-C26-C30
38	L	302	UIX	C31-C27-O2-C18
38	N	306	UIX	C36-C38-C40-C39
38	N	306	UIX	C36-C38-C40-C41
38	O	306	UIX	C25-C28-C32-C33
38	O	306	UIX	C25-C28-C32-C35
38	Q	305	UIX	C25-C28-C32-C33
38	Q	305	UIX	C25-C28-C32-C35
38	C	306	UIX	C31-C27-O2-C18
38	C	306	UIX	C25-C28-C32-C33
38	C	306	UIX	C25-C28-C32-C35
38	C	306	UIX	C36-C38-C40-C39
38	C	306	UIX	C36-C38-C40-C41
38	P	207	UIX	C31-C27-O2-C18
39	A	205	KC1	C2B-C3B-CAB-CBB
39	A	205	KC1	C4B-C3B-CAB-CBB
39	A	213	KC1	C2B-C3B-CAB-CBB
39	A	213	KC1	C4B-C3B-CAB-CBB
39	A	213	KC1	C2A-CAA-CBA-CGA
39	A	213	KC1	CAA-CBA-CGA-O2A
39	G	315	KC1	C1A-C2A-CAA-CBA
39	G	315	KC1	C2B-C3B-CAB-CBB
39	G	318	KC1	C2B-C3B-CAB-CBB
39	G	318	KC1	C2A-CAA-CBA-CGA
39	I	215	KC1	C1A-C2A-CAA-CBA
39	I	215	KC1	C2B-C3B-CAB-CBB
39	I	215	KC1	C4B-C3B-CAB-CBB
39	I	215	KC1	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
39	I	215	KC1	CHA-CBD-CGD-O2D
39	I	215	KC1	CBD-CGD-O2D-CED
39	K	215	KC1	C1A-C2A-CAA-CBA
39	F	309	KC1	C3A-C2A-CAA-CBA
39	F	309	KC1	C2B-C3B-CAB-CBB
39	F	309	KC1	C4B-C3B-CAB-CBB
39	F	309	KC1	CHA-CBD-CGD-O1D
39	F	309	KC1	CHA-CBD-CGD-O2D
39	F	314	KC1	C2B-C3B-CAB-CBB
39	F	314	KC1	C4B-C3B-CAB-CBB
39	F	314	KC1	CBD-CGD-O2D-CED
39	F	314	KC1	O1D-CGD-O2D-CED
39	J	312	KC1	C2B-C3B-CAB-CBB
39	J	312	KC1	C4B-C3B-CAB-CBB
39	J	312	KC1	C2A-CAA-CBA-CGA
39	M	305	KC1	C2B-C3B-CAB-CBB
39	M	305	KC1	C4B-C3B-CAB-CBB
39	M	312	KC1	C1A-C2A-CAA-CBA
39	M	312	KC1	C3A-C2A-CAA-CBA
39	M	312	KC1	C2B-C3B-CAB-CBB
39	M	312	KC1	C4B-C3B-CAB-CBB
39	M	312	KC1	CBD-CGD-O2D-CED
39	M	312	KC1	O1D-CGD-O2D-CED
39	L	306	KC1	C2B-C3B-CAB-CBB
39	L	306	KC1	C4B-C3B-CAB-CBB
39	L	314	KC1	C1A-C2A-CAA-CBA
39	L	314	KC1	C3A-C2A-CAA-CBA
39	L	314	KC1	CBD-CGD-O2D-CED
39	L	314	KC1	O1D-CGD-O2D-CED
39	D	310	KC1	C1A-C2A-CAA-CBA
39	D	310	KC1	C3A-C2A-CAA-CBA
39	D	310	KC1	C2B-C3B-CAB-CBB
39	D	310	KC1	C4B-C3B-CAB-CBB
39	D	315	KC1	C1A-C2A-CAA-CBA
39	D	315	KC1	C3A-C2A-CAA-CBA
39	D	315	KC1	C2B-C3B-CAB-CBB
39	D	315	KC1	C4B-C3B-CAB-CBB
39	D	315	KC1	CBD-CGD-O2D-CED
39	D	315	KC1	O1D-CGD-O2D-CED
39	B	313	KC1	C2B-C3B-CAB-CBB
39	B	313	KC1	C4B-C3B-CAB-CBB
39	B	313	KC1	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
39	B	313	KC1	CBD-CGD-O2D-CED
39	H	309	KC1	C1A-C2A-CAA-CBA
39	H	309	KC1	C2B-C3B-CAB-CBB
39	H	309	KC1	C4B-C3B-CAB-CBB
39	H	311	KC1	C2B-C3B-CAB-CBB
39	H	311	KC1	C4B-C3B-CAB-CBB
39	H	311	KC1	CBD-CGD-O2D-CED
39	H	314	KC1	C1A-C2A-CAA-CBA
39	H	314	KC1	C3A-C2A-CAA-CBA
39	H	314	KC1	CBD-CGD-O2D-CED
39	H	314	KC1	O1D-CGD-O2D-CED
39	N	310	KC1	C1A-C2A-CAA-CBA
39	N	310	KC1	C3A-C2A-CAA-CBA
39	N	310	KC1	C2B-C3B-CAB-CBB
39	N	312	KC1	C2B-C3B-CAB-CBB
39	N	312	KC1	C4B-C3B-CAB-CBB
39	N	312	KC1	CBD-CGD-O2D-CED
39	N	315	KC1	C1A-C2A-CAA-CBA
39	N	315	KC1	C3A-C2A-CAA-CBA
39	N	315	KC1	CBD-CGD-O2D-CED
39	N	315	KC1	O1D-CGD-O2D-CED
39	O	310	KC1	C3A-C2A-CAA-CBA
39	O	312	KC1	C2B-C3B-CAB-CBB
39	O	315	KC1	C3A-C2A-CAA-CBA
39	O	315	KC1	C2A-CAA-CBA-CGA
39	T	310	KC1	C1A-C2A-CAA-CBA
39	T	310	KC1	C3A-C2A-CAA-CBA
39	T	310	KC1	C2B-C3B-CAB-CBB
39	T	310	KC1	C4B-C3B-CAB-CBB
39	T	312	KC1	C1A-C2A-CAA-CBA
39	T	312	KC1	C2B-C3B-CAB-CBB
39	T	312	KC1	C4B-C3B-CAB-CBB
39	T	315	KC1	C3A-C2A-CAA-CBA
39	Q	309	KC1	C1A-C2A-CAA-CBA
39	Q	309	KC1	C2B-C3B-CAB-CBB
39	Q	309	KC1	C4B-C3B-CAB-CBB
39	Q	309	KC1	CHA-CBD-CGD-O2D
39	Q	311	KC1	C2B-C3B-CAB-CBB
39	Q	311	KC1	C4B-C3B-CAB-CBB
39	Q	314	KC1	C3A-C2A-CAA-CBA
39	Q	314	KC1	CBD-CGD-O2D-CED
39	Q	314	KC1	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
39	C	310	KC1	C1A-C2A-CAA-CBA
39	C	310	KC1	C3A-C2A-CAA-CBA
39	C	310	KC1	C2B-C3B-CAB-CBB
39	C	310	KC1	CHA-CBD-CGD-O1D
39	C	310	KC1	CHA-CBD-CGD-O2D
39	C	312	KC1	C2B-C3B-CAB-CBB
39	C	312	KC1	CHA-CBD-CGD-O1D
39	C	315	KC1	C3A-C2A-CAA-CBA
39	C	315	KC1	CBD-CGD-O2D-CED
39	P	211	KC1	C1A-C2A-CAA-CBA
39	P	211	KC1	C3A-C2A-CAA-CBA
39	P	211	KC1	C2A-CAA-CBA-CGA
39	P	213	KC1	C2B-C3B-CAB-CBB
39	P	213	KC1	CHA-CBD-CGD-O2D
39	P	216	KC1	C3A-C2A-CAA-CBA
39	P	216	KC1	C2A-CAA-CBA-CGA
39	E	307	KC1	C3A-C2A-CAA-CBA
39	E	307	KC1	C2B-C3B-CAB-CBB
39	E	307	KC1	C4B-C3B-CAB-CBB
39	E	312	KC1	C1A-C2A-CAA-CBA
39	E	312	KC1	C2B-C3B-CAB-CBB
39	E	312	KC1	C4B-C3B-CAB-CBB
40	B	317	SQD	O5-C1-O6-C44
37	h	204	PID	O7-C30-O6-C27
37	G	309	PID	C31-C30-O6-C27
37	F	302	PID	C31-C30-O6-C27
37	D	306	PID	O7-C30-O6-C27
37	H	302	PID	O7-C30-O6-C27
37	H	305	PID	C31-C30-O6-C27
37	H	306	PID	O7-C30-O6-C27
37	O	301	PID	C31-C30-O6-C27
37	O	302	PID	C31-C30-O6-C27
37	O	305	PID	C31-C30-O6-C27
37	Q	304	PID	C31-C30-O6-C27
37	C	302	PID	C31-C30-O6-C27
37	C	305	PID	C31-C30-O6-C27
37	P	203	PID	C31-C30-O6-C27
37	P	206	PID	C31-C30-O6-C27
37	P	208	PID	C31-C30-O6-C27
38	B	304	UIX	O4-C27-O2-C18
38	N	306	UIX	C31-C27-O2-C18
38	O	306	UIX	C31-C27-O2-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
38	T	306	UIX	C31-C27-O2-C18
38	Q	305	UIX	C31-C27-O2-C18
29	b	731	CLA	O1D-CGD-O2D-CED
29	b	736	CLA	O1D-CGD-O2D-CED
29	A	217	CLA	O1D-CGD-O2D-CED
29	G	311	CLA	O1D-CGD-O2D-CED
29	G	316	CLA	O1D-CGD-O2D-CED
29	M	308	CLA	O1D-CGD-O2D-CED
29	L	307	CLA	O1D-CGD-O2D-CED
29	L	315	CLA	O1D-CGD-O2D-CED
29	D	309	CLA	O1D-CGD-O2D-CED
29	D	313	CLA	O1D-CGD-O2D-CED
29	D	316	CLA	O1D-CGD-O2D-CED
29	N	314	CLA	O1D-CGD-O2D-CED
29	O	316	CLA	O1D-CGD-O2D-CED
29	T	313	CLA	O1D-CGD-O2D-CED
29	E	310	CLA	O1D-CGD-O2D-CED
39	C	315	KC1	O1D-CGD-O2D-CED
37	h	204	PID	C31-C30-O6-C27
37	D	306	PID	C31-C30-O6-C27
37	H	301	PID	C31-C30-O6-C27
37	H	302	PID	C31-C30-O6-C27
37	H	306	PID	C31-C30-O6-C27
37	N	301	PID	C31-C30-O6-C27
37	T	307	PID	C31-C30-O6-C27
37	T	317	PID	O7-C30-O6-C27
37	C	301	PID	C31-C30-O6-C27
37	C	307	PID	C31-C30-O6-C27
37	P	202	PID	C31-C30-O6-C27
38	A	203	UIX	C31-C27-O2-C18
38	F	305	UIX	O4-C27-O2-C18
38	L	302	UIX	O4-C27-O2-C18
38	B	304	UIX	C31-C27-O2-C18
29	a	801	CLA	O1D-CGD-O2D-CED
29	a	803	CLA	O1D-CGD-O2D-CED
29	a	812	CLA	O1D-CGD-O2D-CED
29	a	817	CLA	O1D-CGD-O2D-CED
29	a	830	CLA	O1D-CGD-O2D-CED
29	a	831	CLA	O1D-CGD-O2D-CED
29	b	708	CLA	O1D-CGD-O2D-CED
29	A	210	CLA	O1D-CGD-O2D-CED
29	I	208	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	I	212	CLA	O1D-CGD-O2D-CED
29	F	312	CLA	O1D-CGD-O2D-CED
29	L	310	CLA	O1D-CGD-O2D-CED
29	H	312	CLA	O1D-CGD-O2D-CED
29	N	313	CLA	O1D-CGD-O2D-CED
29	N	316	CLA	O1D-CGD-O2D-CED
29	Q	310	CLA	O1D-CGD-O2D-CED
29	Q	315	CLA	O1D-CGD-O2D-CED
29	C	313	CLA	O1D-CGD-O2D-CED
29	C	316	CLA	O1D-CGD-O2D-CED
29	P	214	CLA	O1D-CGD-O2D-CED
29	P	215	CLA	O1D-CGD-O2D-CED
29	E	305	CLA	O1D-CGD-O2D-CED
39	I	215	KC1	O1D-CGD-O2D-CED
39	B	313	KC1	O1D-CGD-O2D-CED
29	a	803	CLA	CBD-CGD-O2D-CED
29	a	812	CLA	CBD-CGD-O2D-CED
29	a	813	CLA	CBD-CGD-O2D-CED
29	a	817	CLA	CBD-CGD-O2D-CED
29	a	819	CLA	CBD-CGD-O2D-CED
29	a	820	CLA	CBD-CGD-O2D-CED
29	a	827	CLA	CBD-CGD-O2D-CED
29	a	830	CLA	CBD-CGD-O2D-CED
29	a	831	CLA	CBD-CGD-O2D-CED
29	b	702	CLA	CBD-CGD-O2D-CED
29	b	704	CLA	CBD-CGD-O2D-CED
29	b	708	CLA	CBD-CGD-O2D-CED
29	b	719	CLA	CBD-CGD-O2D-CED
29	f	802	CLA	CBD-CGD-O2D-CED
29	l	502	CLA	CBD-CGD-O2D-CED
29	A	212	CLA	CBD-CGD-O2D-CED
29	G	311	CLA	CBD-CGD-O2D-CED
29	I	201	CLA	CBD-CGD-O2D-CED
29	I	208	CLA	CBD-CGD-O2D-CED
29	I	210	CLA	CBD-CGD-O2D-CED
29	I	212	CLA	CBD-CGD-O2D-CED
29	I	216	CLA	CBD-CGD-O2D-CED
29	F	310	CLA	CBD-CGD-O2D-CED
29	F	312	CLA	CBD-CGD-O2D-CED
29	M	306	CLA	CBD-CGD-O2D-CED
29	M	308	CLA	CBD-CGD-O2D-CED
29	L	310	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	L	312	CLA	CBD-CGD-O2D-CED
29	D	316	CLA	CBD-CGD-O2D-CED
29	B	316	CLA	CBD-CGD-O2D-CED
29	N	309	CLA	CBD-CGD-O2D-CED
29	N	311	CLA	CBD-CGD-O2D-CED
29	N	313	CLA	CBD-CGD-O2D-CED
29	N	316	CLA	CBD-CGD-O2D-CED
29	O	316	CLA	CBD-CGD-O2D-CED
29	T	309	CLA	CBD-CGD-O2D-CED
29	Q	310	CLA	CBD-CGD-O2D-CED
29	Q	315	CLA	CBD-CGD-O2D-CED
29	C	316	CLA	CBD-CGD-O2D-CED
29	P	209	CLA	CBD-CGD-O2D-CED
29	E	306	CLA	CBD-CGD-O2D-CED
39	O	315	KC1	CBD-CGD-O2D-CED
29	a	806	CLA	O1A-CGA-O2A-C1
29	a	813	CLA	O1A-CGA-O2A-C1
29	b	707	CLA	O1A-CGA-O2A-C1
29	b	709	CLA	O1A-CGA-O2A-C1
29	f	805	CLA	O1A-CGA-O2A-C1
29	I	209	CLA	O1A-CGA-O2A-C1
29	I	213	CLA	O1A-CGA-O2A-C1
29	J	310	CLA	O1A-CGA-O2A-C1
29	Q	313	CLA	O1A-CGA-O2A-C1
29	a	814	CLA	O1A-CGA-O2A-C1
29	a	816	CLA	O1A-CGA-O2A-C1
29	b	715	CLA	O1A-CGA-O2A-C1
29	K	217	CLA	O1A-CGA-O2A-C1
29	F	313	CLA	O1A-CGA-O2A-C1
29	M	309	CLA	O1A-CGA-O2A-C1
29	Q	312	CLA	O1A-CGA-O2A-C1
38	T	306	UIX	O4-C27-O2-C18
29	a	813	CLA	O1D-CGD-O2D-CED
29	a	823	CLA	O1D-CGD-O2D-CED
29	b	702	CLA	O1D-CGD-O2D-CED
29	b	704	CLA	O1D-CGD-O2D-CED
29	l	502	CLA	O1D-CGD-O2D-CED
29	l	504	CLA	O1D-CGD-O2D-CED
29	I	210	CLA	O1D-CGD-O2D-CED
29	K	213	CLA	O1D-CGD-O2D-CED
29	D	314	CLA	O1D-CGD-O2D-CED
29	B	307	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	B	316	CLA	O1D-CGD-O2D-CED
29	N	309	CLA	O1D-CGD-O2D-CED
29	N	311	CLA	O1D-CGD-O2D-CED
29	a	816	CLA	CBA-CGA-O2A-C1
37	N	307	PID	C31-C30-O6-C27
29	a	828	CLA	O1D-CGD-O2D-CED
29	b	705	CLA	O1D-CGD-O2D-CED
29	I	209	CLA	O1D-CGD-O2D-CED
29	I	217	CLA	O1D-CGD-O2D-CED
29	K	216	CLA	O1D-CGD-O2D-CED
29	K	218	CLA	O1D-CGD-O2D-CED
29	J	305	CLA	O1D-CGD-O2D-CED
29	J	306	CLA	O1D-CGD-O2D-CED
29	L	308	CLA	O1D-CGD-O2D-CED
29	D	308	CLA	O1D-CGD-O2D-CED
29	H	310	CLA	O1D-CGD-O2D-CED
29	H	313	CLA	O1D-CGD-O2D-CED
29	H	315	CLA	O1D-CGD-O2D-CED
29	C	314	CLA	O1D-CGD-O2D-CED
29	a	806	CLA	CBA-CGA-O2A-C1
29	b	707	CLA	CBA-CGA-O2A-C1
29	b	709	CLA	CBA-CGA-O2A-C1
29	f	805	CLA	CBA-CGA-O2A-C1
29	I	209	CLA	CBA-CGA-O2A-C1
29	J	310	CLA	CBA-CGA-O2A-C1
29	Q	313	CLA	CBA-CGA-O2A-C1
34	K	219	LMG	C29-C28-O8-C9
29	a	802	CLA	CBD-CGD-O2D-CED
29	a	814	CLA	CBD-CGD-O2D-CED
29	a	816	CLA	CBD-CGD-O2D-CED
29	a	826	CLA	CBD-CGD-O2D-CED
29	a	837	CLA	CBD-CGD-O2D-CED
29	b	717	CLA	CBD-CGD-O2D-CED
29	i	202	CLA	CBD-CGD-O2D-CED
29	i	203	CLA	CBD-CGD-O2D-CED
29	l	503	CLA	CBD-CGD-O2D-CED
29	A	209	CLA	CBD-CGD-O2D-CED
29	I	209	CLA	CBD-CGD-O2D-CED
29	F	308	CLA	CBD-CGD-O2D-CED
29	J	310	CLA	CBD-CGD-O2D-CED
29	M	313	CLA	CBD-CGD-O2D-CED
29	L	308	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	L	317	CLA	CBD-CGD-O2D-CED
29	E	311	CLA	CBD-CGD-O2D-CED
39	Q	309	KC1	CBD-CGD-O2D-CED
39	P	213	KC1	CBD-CGD-O2D-CED
37	N	307	PID	O7-C30-O6-C27
38	O	306	UIX	O4-C27-O2-C18
29	b	702	CLA	O1A-CGA-O2A-C1
29	l	504	CLA	O1A-CGA-O2A-C1
29	M	310	CLA	O1A-CGA-O2A-C1
29	D	314	CLA	O1A-CGA-O2A-C1
29	B	306	CLA	O1A-CGA-O2A-C1
29	N	308	CLA	O1A-CGA-O2A-C1
29	N	314	CLA	O1A-CGA-O2A-C1
29	O	308	CLA	O1A-CGA-O2A-C1
29	T	314	CLA	O1A-CGA-O2A-C1
29	C	308	CLA	O1A-CGA-O2A-C1
29	C	314	CLA	O1A-CGA-O2A-C1
29	P	215	CLA	O1A-CGA-O2A-C1
29	E	305	CLA	O1A-CGA-O2A-C1
34	b	732	LMG	O10-C28-O8-C9
34	K	219	LMG	O10-C28-O8-C9
34	E	316	LMG	O10-C28-O8-C9
35	j	106	DGD	O1A-C1A-O1G-C1G
29	C	313	CLA	O1A-CGA-O2A-C1
29	a	805	CLA	O1D-CGD-O2D-CED
29	a	821	CLA	O1D-CGD-O2D-CED
29	b	707	CLA	O1D-CGD-O2D-CED
29	b	720	CLA	O1D-CGD-O2D-CED
29	b	722	CLA	O1D-CGD-O2D-CED
29	G	314	CLA	O1D-CGD-O2D-CED
29	J	313	CLA	O1D-CGD-O2D-CED
29	D	311	CLA	O1D-CGD-O2D-CED
29	O	313	CLA	O1D-CGD-O2D-CED
29	T	311	CLA	O1D-CGD-O2D-CED
38	N	306	UIX	O4-C27-O2-C18
29	T	308	CLA	O1D-CGD-O2D-CED
29	C	311	CLA	O1D-CGD-O2D-CED
39	N	312	KC1	O1D-CGD-O2D-CED
29	b	721	CLA	CBD-CGD-O2D-CED
29	M	310	CLA	CBD-CGD-O2D-CED
29	B	312	CLA	CBD-CGD-O2D-CED
39	E	312	KC1	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	P	201	LMG	O9-C10-O7-C8
35	b	733	DGD	O1B-C1B-O2G-C2G
35	j	103	DGD	O1B-C1B-O2G-C2G
29	a	828	CLA	CBA-CGA-O2A-C1
29	F	310	CLA	CBA-CGA-O2A-C1
29	F	312	CLA	CBA-CGA-O2A-C1
38	C	306	UIX	O4-C27-O2-C18
29	f	803	CLA	O1A-CGA-O2A-C1
29	T	313	CLA	O1A-CGA-O2A-C1
29	P	214	CLA	O1A-CGA-O2A-C1
29	a	829	CLA	C3-C5-C6-C7
29	b	703	CLA	C3-C5-C6-C7
29	b	706	CLA	C3-C5-C6-C7
29	b	711	CLA	C3-C5-C6-C7
29	b	713	CLA	C3-C5-C6-C7
29	b	716	CLA	C3-C5-C6-C7
29	b	717	CLA	C3-C5-C6-C7
29	f	805	CLA	C3-C5-C6-C7
29	i	201	CLA	C3-C5-C6-C7
29	A	211	CLA	C3-C5-C6-C7
29	A	212	CLA	C3-C5-C6-C7
29	A	218	CLA	C3-C5-C6-C7
29	G	317	CLA	C3-C5-C6-C7
29	I	210	CLA	C3-C5-C6-C7
29	I	213	CLA	C3-C5-C6-C7
29	J	311	CLA	C3-C5-C6-C7
29	L	312	CLA	C3-C5-C6-C7
29	B	309	CLA	C3-C5-C6-C7
29	a	813	CLA	CBA-CGA-O2A-C1
29	b	702	CLA	CBA-CGA-O2A-C1
29	I	213	CLA	CBA-CGA-O2A-C1
29	K	209	CLA	CBA-CGA-O2A-C1
29	N	308	CLA	CBA-CGA-O2A-C1
29	N	314	CLA	CBA-CGA-O2A-C1
29	O	308	CLA	CBA-CGA-O2A-C1
29	T	314	CLA	CBA-CGA-O2A-C1
29	C	314	CLA	CBA-CGA-O2A-C1
29	P	209	CLA	CBA-CGA-O2A-C1
34	b	732	LMG	C29-C28-O8-C9
34	E	316	LMG	C29-C28-O8-C9
37	F	304	PID	O7-C30-O6-C27
38	P	207	UIX	O4-C27-O2-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	h	205	LMG	C11-C10-O7-C8
29	a	819	CLA	O1D-CGD-O2D-CED
29	F	310	CLA	O1D-CGD-O2D-CED
29	b	709	CLA	CBD-CGD-O2D-CED
29	C	308	CLA	CBD-CGD-O2D-CED
29	P	210	CLA	CBD-CGD-O2D-CED
37	j	101	PID	O7-C30-O6-C27
29	H	307	CLA	O1A-CGA-O2A-C1
29	F	310	CLA	O1A-CGA-O2A-C1
29	F	312	CLA	O1A-CGA-O2A-C1
37	G	310	PID	C31-C30-O6-C27
39	B	313	KC1	CAA-CBA-CGA-O1A
29	f	802	CLA	CBA-CGA-O2A-C1
29	f	803	CLA	CBA-CGA-O2A-C1
29	T	313	CLA	CBA-CGA-O2A-C1
29	P	214	CLA	CBA-CGA-O2A-C1
29	M	314	CLA	C3-C5-C6-C7
38	Q	305	UIX	O4-C27-O2-C18
29	a	823	CLA	C4-C3-C5-C6
29	b	716	CLA	C4-C3-C5-C6
29	L	313	CLA	C4-C3-C5-C6
29	H	308	CLA	C4-C3-C5-C6
29	C	309	CLA	C4-C3-C5-C6
29	J	311	CLA	C2-C3-C5-C6
29	L	313	CLA	C2-C3-C5-C6
29	Q	308	CLA	C2-C3-C5-C6
29	b	712	CLA	CBD-CGD-O2D-CED
29	K	210	CLA	CBD-CGD-O2D-CED
29	M	314	CLA	CBD-CGD-O2D-CED
29	P	217	CLA	CBD-CGD-O2D-CED
29	E	309	CLA	CBD-CGD-O2D-CED
29	a	813	CLA	C2A-CAA-CBA-CGA
29	b	719	CLA	C2A-CAA-CBA-CGA
29	b	725	CLA	C2A-CAA-CBA-CGA
29	b	736	CLA	C2A-CAA-CBA-CGA
29	h	201	CLA	C2A-CAA-CBA-CGA
29	A	215	CLA	C2A-CAA-CBA-CGA
29	G	301	CLA	C2A-CAA-CBA-CGA
29	I	209	CLA	C2A-CAA-CBA-CGA
29	M	314	CLA	C2A-CAA-CBA-CGA
29	D	308	CLA	C2A-CAA-CBA-CGA
29	A	215	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	E	306	CLA	O1D-CGD-O2D-CED
29	a	828	CLA	O1A-CGA-O2A-C1
29	b	722	CLA	C3-C5-C6-C7
29	b	736	CLA	C3-C5-C6-C7
29	i	203	CLA	C3-C5-C6-C7
29	l	505	CLA	C3-C5-C6-C7
29	H	308	CLA	C3-C5-C6-C7
30	b	727	PQN	C13-C15-C16-C17
29	a	819	CLA	CBA-CGA-O2A-C1
29	l	504	CLA	CBA-CGA-O2A-C1
29	A	217	CLA	CBA-CGA-O2A-C1
29	M	306	CLA	CBA-CGA-O2A-C1
29	M	310	CLA	CBA-CGA-O2A-C1
29	L	316	CLA	CBA-CGA-O2A-C1
29	D	314	CLA	CBA-CGA-O2A-C1
29	B	306	CLA	CBA-CGA-O2A-C1
29	C	308	CLA	CBA-CGA-O2A-C1
29	P	215	CLA	CBA-CGA-O2A-C1
29	E	305	CLA	CBA-CGA-O2A-C1
35	j	106	DGD	C2A-C1A-O1G-C1G
29	b	705	CLA	C2C-C3C-CAC-CBC
29	C	314	CLA	C2-C1-O2A-CGA
29	O	309	CLA	CBD-CGD-O2D-CED
29	f	802	CLA	O1D-CGD-O2D-CED
29	A	212	CLA	O1D-CGD-O2D-CED
29	I	216	CLA	O1D-CGD-O2D-CED
29	T	309	CLA	O1D-CGD-O2D-CED
29	P	209	CLA	O1D-CGD-O2D-CED
29	a	819	CLA	O1A-CGA-O2A-C1
29	b	712	CLA	O1A-CGA-O2A-C1
29	A	217	CLA	O1A-CGA-O2A-C1
29	L	313	CLA	O1A-CGA-O2A-C1
29	L	316	CLA	O1A-CGA-O2A-C1
34	A	219	LMG	O10-C28-O8-C9
29	J	309	CLA	O1A-CGA-O2A-C1
29	L	317	CLA	O1A-CGA-O2A-C1
29	b	719	CLA	O1D-CGD-O2D-CED
36	I	203	DD6	C1-C2-C3-C4
36	K	202	DD6	C3-C4-C5-C6
36	L	305	DD6	C11-C10-C9-C8
36	D	304	DD6	C3-C4-C5-C6
36	O	303	DD6	C24-C25-C26-C27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
37	G	303	PID	C14-C15-C16-C17
37	N	305	PID	C14-C15-C16-C17
37	C	305	PID	C14-C15-C16-C17
37	P	208	PID	C18-C19-C20-C21
34	j	102	LMG	O6-C5-C6-O5
34	K	201	LMG	O6-C5-C6-O5
35	b	733	DGD	O6E-C5E-C6E-O5E
38	E	304	UIX	C31-C27-O2-C18
29	b	710	CLA	CBD-CGD-O2D-CED
29	b	711	CLA	CBD-CGD-O2D-CED
29	K	214	CLA	CBD-CGD-O2D-CED
29	F	315	CLA	CBD-CGD-O2D-CED
29	L	316	CLA	CBD-CGD-O2D-CED
29	N	308	CLA	CBD-CGD-O2D-CED
29	P	212	CLA	CBD-CGD-O2D-CED
39	C	310	KC1	CBD-CGD-O2D-CED
29	M	306	CLA	O1D-CGD-O2D-CED
29	L	312	CLA	O1D-CGD-O2D-CED
29	a	801	CLA	C3-C5-C6-C7
29	a	804	CLA	C3-C5-C6-C7
29	a	837	CLA	C3-C5-C6-C7
29	b	704	CLA	C3-C5-C6-C7
29	b	709	CLA	C3-C5-C6-C7
29	b	718	CLA	C3-C5-C6-C7
29	G	313	CLA	C3-C5-C6-C7
29	a	820	CLA	CBA-CGA-O2A-C1
29	b	720	CLA	CBA-CGA-O2A-C1
29	l	505	CLA	CBA-CGA-O2A-C1
29	A	215	CLA	CBA-CGA-O2A-C1
29	I	207	CLA	CBA-CGA-O2A-C1
29	H	307	CLA	CBA-CGA-O2A-C1
34	b	730	LMG	C29-C28-O8-C9
34	A	219	LMG	C29-C28-O8-C9
37	N	302	PID	C31-C30-O6-C27
38	E	304	UIX	O4-C27-O2-C18
29	M	306	CLA	O1A-CGA-O2A-C1
29	a	820	CLA	O1D-CGD-O2D-CED
34	P	201	LMG	C11-C10-O7-C8
37	N	302	PID	O7-C30-O6-C27
29	K	208	CLA	CBA-CGA-O2A-C1
29	E	309	CLA	CBA-CGA-O2A-C1
29	M	311	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	L	311	CLA	CBD-CGD-O2D-CED
29	O	311	CLA	CBD-CGD-O2D-CED
39	H	309	KC1	CBD-CGD-O2D-CED
34	A	219	LMG	O6-C5-C6-O5
29	f	802	CLA	O1A-CGA-O2A-C1
29	I	201	CLA	O1D-CGD-O2D-CED
38	A	203	UIX	O4-C27-O2-C18
29	A	206	CLA	CBD-CGD-O2D-CED
29	F	316	CLA	CBD-CGD-O2D-CED
29	b	712	CLA	CBA-CGA-O2A-C1
29	L	313	CLA	CBA-CGA-O2A-C1
29	E	306	CLA	CBA-CGA-O2A-C1
34	E	316	LMG	O6-C5-C6-O5
39	C	310	KC1	CAA-CBA-CGA-O2A
29	a	820	CLA	O1A-CGA-O2A-C1
29	b	720	CLA	O1A-CGA-O2A-C1
29	l	505	CLA	O1A-CGA-O2A-C1
34	b	730	LMG	O10-C28-O8-C9
29	M	308	CLA	O2A-C1-C2-C3
29	a	820	CLA	C4-C3-C5-C6
29	b	711	CLA	C4-C3-C5-C6
29	i	201	CLA	C4-C3-C5-C6
29	G	312	CLA	C4-C3-C5-C6
29	L	308	CLA	C4-C3-C5-C6
29	N	309	CLA	C4-C3-C5-C6
29	a	820	CLA	C2-C3-C5-C6
29	b	711	CLA	C2-C3-C5-C6
29	b	716	CLA	C2-C3-C5-C6
29	b	717	CLA	C2-C3-C5-C6
29	i	201	CLA	C2-C3-C5-C6
29	G	302	CLA	C2-C3-C5-C6
29	G	312	CLA	C2-C3-C5-C6
29	L	308	CLA	C2-C3-C5-C6
29	N	309	CLA	C2-C3-C5-C6
29	E	306	CLA	C2A-CAA-CBA-CGA
29	a	827	CLA	O1D-CGD-O2D-CED
34	K	220	LMG	O6-C5-C6-O5
29	I	207	CLA	O1A-CGA-O2A-C1
29	E	306	CLA	O1A-CGA-O2A-C1
35	G	320	DGD	O6E-C1E-O5D-C6D
29	a	824	CLA	CBA-CGA-O2A-C1
29	L	312	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	B	311	CLA	CBA-CGA-O2A-C1
34	j	102	LMG	C29-C28-O8-C9
35	b	733	DGD	C2A-C1A-O1G-C1G
29	M	311	CLA	CBA-CGA-O2A-C1
29	E	310	CLA	CBA-CGA-O2A-C1
34	b	730	LMG	C11-C10-O7-C8
34	K	219	LMG	C4-C5-C6-O5
35	b	733	DGD	C4E-C5E-C6E-O5E
29	a	814	CLA	O1D-CGD-O2D-CED
29	l	503	CLA	O1D-CGD-O2D-CED
29	H	313	CLA	C2-C1-O2A-CGA
29	a	826	CLA	O1D-CGD-O2D-CED
29	L	312	CLA	O1A-CGA-O2A-C1
29	b	721	CLA	C3-C5-C6-C7
29	B	315	CLA	CBA-CGA-O2A-C1
29	a	807	CLA	CBA-CGA-O2A-C1
29	a	811	CLA	CBA-CGA-O2A-C1
29	a	829	CLA	CBA-CGA-O2A-C1
29	a	830	CLA	CBA-CGA-O2A-C1
29	b	724	CLA	CBA-CGA-O2A-C1
29	j	104	CLA	CBA-CGA-O2A-C1
29	G	304	CLA	CBA-CGA-O2A-C1
29	G	317	CLA	CBA-CGA-O2A-C1
29	K	214	CLA	CBA-CGA-O2A-C1
29	L	308	CLA	CBA-CGA-O2A-C1
29	O	314	CLA	CBA-CGA-O2A-C1
29	b	718	CLA	CBD-CGD-O2D-CED
34	K	220	LMG	C4-C5-C6-O5
29	E	309	CLA	O1A-CGA-O2A-C1
29	a	837	CLA	O1D-CGD-O2D-CED
29	i	202	CLA	O1D-CGD-O2D-CED
36	I	203	DD6	C11-C10-C9-C8
36	F	301	DD6	C3-C4-C5-C6
36	T	303	DD6	C24-C25-C26-C27
38	F	305	UIX	C11-C13-C14-C23
38	P	207	UIX	C34-C37-C39-C40
29	l	504	CLA	C13-C15-C16-C17
34	j	102	LMG	C4-C5-C6-O5
37	G	303	PID	C31-C30-O6-C27
39	A	213	KC1	CAA-CBA-CGA-O1A
39	K	215	KC1	CAA-CBA-CGA-O2A
39	L	314	KC1	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
39	H	309	KC1	CAA-CBA-CGA-O2A
39	C	312	KC1	CAA-CBA-CGA-O1A
39	E	307	KC1	CAA-CBA-CGA-O2A
29	K	208	CLA	O1A-CGA-O2A-C1
34	K	201	LMG	C4-C5-C6-O5
29	a	829	CLA	C15-C16-C17-C18
29	i	201	CLA	C10-C11-C12-C13
29	l	502	CLA	C8-C10-C11-C12
35	b	733	DGD	C2D-C1D-O3G-C3G
40	J	314	SQD	C2-C1-O6-C44
34	b	730	LMG	O7-C8-C9-O8
29	b	724	CLA	O1A-CGA-O2A-C1
29	G	317	CLA	O1A-CGA-O2A-C1
29	a	831	CLA	C4-C3-C5-C6
29	H	308	CLA	C2-C3-C5-C6
29	a	807	CLA	C11-C10-C8-C9
29	a	807	CLA	C11-C12-C13-C14
29	a	823	CLA	C6-C7-C8-C9
29	a	824	CLA	C6-C7-C8-C9
29	a	829	CLA	C6-C7-C8-C9
29	a	829	CLA	C11-C12-C13-C14
29	a	829	CLA	C14-C13-C15-C16
29	b	704	CLA	C6-C7-C8-C9
29	b	705	CLA	C14-C13-C15-C16
29	l	505	CLA	C6-C7-C8-C9
29	A	218	CLA	C6-C7-C8-C9
29	I	213	CLA	C11-C12-C13-C14
29	B	310	CLA	C6-C7-C8-C9
29	Q	308	CLA	C6-C7-C8-C9
29	A	209	CLA	O1D-CGD-O2D-CED
29	M	313	CLA	O1D-CGD-O2D-CED
29	L	317	CLA	O1D-CGD-O2D-CED
29	B	310	CLA	C5-C6-C7-C8
32	a	838	BCR	C37-C22-C23-C24
32	b	728	BCR	C36-C18-C19-C20
32	f	801	BCR	C7-C8-C9-C34
32	l	506	BCR	C37-C22-C23-C24
32	l	507	BCR	C11-C12-C13-C35
36	h	202	DD6	C12-C11-C13-C14
36	G	307	DD6	C12-C11-C13-C14
36	I	203	DD6	C-C1-C24-C25
36	F	301	DD6	C12-C11-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
36	F	301	DD6	C7-C6-C8-C9
36	M	303	DD6	C12-C11-C13-C14
36	L	301	DD6	C12-C11-C13-C14
36	L	304	DD6	C12-C11-C13-C14
36	B	301	DD6	C12-C11-C13-C14
36	B	319	DD6	C-C1-C24-C25
36	E	302	DD6	C12-C11-C13-C14
32	l	506	BCR	C21-C22-C23-C24
36	G	307	DD6	C10-C11-C13-C14
36	I	203	DD6	C2-C1-C24-C25
36	K	202	DD6	C10-C11-C13-C14
36	F	301	DD6	C10-C11-C13-C14
36	M	303	DD6	C10-C11-C13-C14
36	M	303	DD6	C5-C6-C8-C9
36	L	301	DD6	C10-C11-C13-C14
36	L	304	DD6	C10-C11-C13-C14
36	B	301	DD6	C10-C11-C13-C14
36	B	319	DD6	C2-C1-C24-C25
36	E	302	DD6	C10-C11-C13-C14
38	F	305	UIX	C7-C10-C11-C13
34	K	201	LMG	C11-C10-O7-C8
29	a	811	CLA	O1A-CGA-O2A-C1
29	a	830	CLA	O1A-CGA-O2A-C1
29	K	214	CLA	O1A-CGA-O2A-C1
29	L	308	CLA	O1A-CGA-O2A-C1
29	O	314	CLA	O1A-CGA-O2A-C1
29	a	829	CLA	C13-C15-C16-C17
29	a	816	CLA	O1D-CGD-O2D-CED
39	H	311	KC1	O1D-CGD-O2D-CED
29	J	307	CLA	CBA-CGA-O2A-C1
39	A	205	KC1	CAA-CBA-CGA-O2A
39	M	305	KC1	CAA-CBA-CGA-O2A
39	Q	311	KC1	CAA-CBA-CGA-O2A
39	C	312	KC1	CAA-CBA-CGA-O2A
29	F	308	CLA	O1D-CGD-O2D-CED
29	l	501	CLA	C3-C5-C6-C7
29	l	504	CLA	C3-C5-C6-C7
29	l	501	CLA	CBA-CGA-O2A-C1
29	l	503	CLA	CBA-CGA-O2A-C1
29	Q	308	CLA	CBA-CGA-O2A-C1
29	a	824	CLA	C13-C15-C16-C17
29	b	702	CLA	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	b	707	CLA	C8-C10-C11-C12
29	b	707	CLA	C15-C16-C17-C18
29	b	718	CLA	C8-C10-C11-C12
29	b	725	CLA	C15-C16-C17-C18
29	l	504	CLA	C10-C11-C12-C13
34	K	219	LMG	O6-C5-C6-O5
34	b	732	LMG	C10-C11-C12-C13
34	E	316	LMG	C28-C29-C30-C31
29	J	310	CLA	O1D-CGD-O2D-CED
29	b	701	CLA	C8-C10-C11-C12
29	b	709	CLA	C5-C6-C7-C8
29	i	202	CLA	C5-C6-C7-C8
29	G	312	CLA	C5-C6-C7-C8
29	J	306	CLA	C8-C10-C11-C12
29	E	306	CLA	C13-C15-C16-C17
29	j	104	CLA	O1A-CGA-O2A-C1
34	b	732	LMG	C28-C29-C30-C31
35	j	103	DGD	C1B-C2B-C3B-C4B
34	b	730	LMG	O6-C5-C6-O5
29	a	807	CLA	C5-C6-C7-C8
29	b	703	CLA	C10-C11-C12-C13
29	a	802	CLA	O1D-CGD-O2D-CED
29	b	717	CLA	O1D-CGD-O2D-CED
39	L	306	KC1	CAA-CBA-CGA-O2A
39	B	313	KC1	CAA-CBA-CGA-O2A
39	O	310	KC1	CAA-CBA-CGA-O2A
39	O	315	KC1	CAA-CBA-CGA-O2A
29	b	703	CLA	C13-C15-C16-C17
29	G	312	CLA	C10-C11-C12-C13
29	B	310	CLA	C10-C11-C12-C13
35	m	102	DGD	C4D-C5D-C6D-O5D
35	h	203	DGD	C1B-C2B-C3B-C4B
35	j	106	DGD	C1B-C2B-C3B-C4B
29	K	213	CLA	O2A-C1-C2-C3
29	a	823	CLA	C6-C7-C8-C10
29	a	829	CLA	C11-C12-C13-C15
29	b	703	CLA	C11-C10-C8-C7
29	b	706	CLA	C6-C7-C8-C10
29	b	736	CLA	C6-C7-C8-C10
29	E	308	CLA	C11-C10-C8-C7
30	a	832	PQN	C13-C15-C16-C17
29	a	829	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	G	304	CLA	O1A-CGA-O2A-C1
36	I	202	DD6	C24-C25-C26-C27
36	I	203	DD6	C24-C25-C26-C27
36	F	301	DD6	C11-C10-C9-C8
36	B	319	DD6	C1-C2-C3-C4
36	B	319	DD6	C3-C4-C5-C6
38	P	207	UIX	C32-C35-C36-C38
29	b	702	CLA	C2A-CAA-CBA-CGA
29	b	717	CLA	C2A-CAA-CBA-CGA
29	K	209	CLA	C2A-CAA-CBA-CGA
29	L	307	CLA	C2A-CAA-CBA-CGA
29	N	313	CLA	C2A-CAA-CBA-CGA
29	b	721	CLA	O1D-CGD-O2D-CED
29	i	203	CLA	O1D-CGD-O2D-CED
29	M	310	CLA	O1D-CGD-O2D-CED
29	B	312	CLA	O1D-CGD-O2D-CED
29	E	311	CLA	O1D-CGD-O2D-CED
29	a	806	CLA	C15-C16-C17-C18
29	b	718	CLA	C5-C6-C7-C8
29	i	201	CLA	C5-C6-C7-C8
29	l	505	CLA	C5-C6-C7-C8
29	I	210	CLA	C5-C6-C7-C8
29	E	311	CLA	C5-C6-C7-C8
29	E	315	CLA	C5-C6-C7-C8
37	G	310	PID	O7-C30-O6-C27
39	M	305	KC1	CAA-CBA-CGA-O1A
29	a	807	CLA	O1A-CGA-O2A-C1
29	Q	308	CLA	O1A-CGA-O2A-C1
34	K	201	LMG	O6-C1-O1-C7
29	l	501	CLA	C10-C11-C12-C13
35	b	733	DGD	C1A-C2A-C3A-C4A
35	j	106	DGD	C1A-C2A-C3A-C4A
29	E	311	CLA	C3-C5-C6-C7
29	b	718	CLA	C10-C11-C12-C13
29	i	201	CLA	C15-C16-C17-C18
29	I	211	CLA	C5-C6-C7-C8
29	I	213	CLA	C13-C15-C16-C17
29	K	211	CLA	C5-C6-C7-C8
29	a	808	CLA	CBA-CGA-O2A-C1
29	A	212	CLA	CBA-CGA-O2A-C1
29	D	308	CLA	CBA-CGA-O2A-C1
29	b	705	CLA	C4C-C3C-CAC-CBC

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	J	311	CLA	CBD-CGD-O2D-CED
29	a	824	CLA	O1A-CGA-O2A-C1
29	B	311	CLA	O1A-CGA-O2A-C1
35	b	733	DGD	O1A-C1A-O1G-C1G
29	a	807	CLA	C10-C11-C12-C13
29	I	209	CLA	C10-C11-C12-C13
29	I	213	CLA	C15-C16-C17-C18
29	L	312	CLA	C5-C6-C7-C8
29	B	308	CLA	C5-C6-C7-C8
29	C	308	CLA	O1D-CGD-O2D-CED
29	P	210	CLA	O1D-CGD-O2D-CED
29	M	307	CLA	CBD-CGD-O2D-CED
39	T	315	KC1	CAA-CBA-CGA-O2A
29	a	826	CLA	C15-C16-C17-C18
29	b	736	CLA	C15-C16-C17-C18
29	A	209	CLA	C8-C10-C11-C12
29	G	312	CLA	C13-C15-C16-C17
29	G	316	CLA	C13-C15-C16-C17
29	E	306	CLA	C15-C16-C17-C18
29	a	810	CLA	C3-C5-C6-C7
29	K	211	CLA	C3-C5-C6-C7
29	E	305	CLA	C3-C5-C6-C7
29	I	211	CLA	CBA-CGA-O2A-C1
29	J	306	CLA	CBA-CGA-O2A-C1
34	P	201	LMG	C29-C28-O8-C9
29	B	310	CLA	C15-C16-C17-C18
29	E	305	CLA	C10-C11-C12-C13
35	m	102	DGD	O6D-C5D-C6D-O5D
29	b	709	CLA	O1D-CGD-O2D-CED
29	C	309	CLA	C2-C3-C5-C6
29	b	723	CLA	C5-C6-C7-C8
29	l	503	CLA	C8-C10-C11-C12
29	a	809	CLA	C2A-CAA-CBA-CGA
29	a	823	CLA	C2A-CAA-CBA-CGA
29	I	211	CLA	C2A-CAA-CBA-CGA
29	L	308	CLA	C2A-CAA-CBA-CGA
29	l	502	CLA	C16-C17-C18-C20
37	P	202	PID	C16-C17-C18-C19
39	G	318	KC1	CAA-CBA-CGA-O2A
29	a	809	CLA	CBA-CGA-O2A-C1
29	a	826	CLA	CBA-CGA-O2A-C1
29	b	736	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	K	210	CLA	O1D-CGD-O2D-CED
36	G	305	DD6	C1-C2-C3-C4
36	G	305	DD6	C3-C4-C5-C6
36	D	304	DD6	C1-C2-C3-C4
38	F	305	UIX	C32-C35-C36-C38
38	O	306	UIX	C26-C30-C34-C37
38	O	306	UIX	C32-C35-C36-C38
34	b	730	LMG	C38-C39-C40-C41
29	M	314	CLA	O1D-CGD-O2D-CED
29	M	309	CLA	CBD-CGD-O2D-CED
37	O	304	PID	C19-C20-C21-CM5
37	Q	306	PID	C19-C20-C21-CM5
29	a	827	CLA	C3-C5-C6-C7
29	N	309	CLA	C3-C5-C6-C7
34	b	732	LMG	C32-C33-C34-C35
34	K	220	LMG	C30-C31-C32-C33
35	j	103	DGD	C2B-C3B-C4B-C5B
29	l	501	CLA	O1A-CGA-O2A-C1
29	P	217	CLA	O1D-CGD-O2D-CED
39	K	215	KC1	C2A-CAA-CBA-CGA
39	D	310	KC1	C2A-CAA-CBA-CGA
39	H	309	KC1	C2A-CAA-CBA-CGA
39	N	315	KC1	C2A-CAA-CBA-CGA
29	I	212	CLA	C6-C7-C8-C10
29	L	312	CLA	C6-C7-C8-C10
29	N	309	CLA	C16-C17-C18-C19
35	b	733	DGD	C9B-CAB-CBB-CCB
35	G	320	DGD	C2A-C3A-C4A-C5A
29	O	309	CLA	O1D-CGD-O2D-CED
29	E	309	CLA	O1D-CGD-O2D-CED
34	K	219	LMG	O9-C10-O7-C8
39	I	215	KC1	CAA-CBA-CGA-O2A
39	N	315	KC1	CAA-CBA-CGA-O2A
34	K	220	LMG	C28-C29-C30-C31
29	b	712	CLA	O1D-CGD-O2D-CED
35	b	733	DGD	C7B-C8B-C9B-CAB
35	b	733	DGD	O6D-C5D-C6D-O5D
29	N	308	CLA	O1D-CGD-O2D-CED
29	b	717	CLA	C5-C6-C7-C8
29	L	311	CLA	CBA-CGA-O2A-C1
34	b	732	LMG	C33-C34-C35-C36
34	K	201	LMG	C2-C1-O1-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
37	O	304	PID	C19-C20-C21-C22
37	Q	306	PID	C19-C20-C21-C22
29	L	307	CLA	CBA-CGA-O2A-C1
34	j	102	LMG	C18-C19-C20-C21
29	a	825	CLA	C13-C15-C16-C17
29	b	736	CLA	O1A-CGA-O2A-C1
29	l	503	CLA	O1A-CGA-O2A-C1
34	j	102	LMG	O10-C28-O8-C9
29	a	810	CLA	C6-C7-C8-C10
29	G	314	CLA	C11-C12-C13-C15
29	I	210	CLA	C6-C7-C8-C9
29	H	308	CLA	C16-C17-C18-C20
29	P	210	CLA	C16-C17-C18-C20
29	F	315	CLA	O1D-CGD-O2D-CED
29	a	823	CLA	C2-C3-C5-C6
29	a	824	CLA	C14-C13-C15-C16
29	b	709	CLA	C11-C10-C8-C9
29	l	503	CLA	C6-C7-C8-C9
29	P	210	CLA	C14-C13-C15-C16
29	E	311	CLA	C11-C12-C13-C14
34	b	730	LMG	C36-C37-C38-C39
34	b	732	LMG	C31-C32-C33-C34
34	K	201	LMG	C34-C35-C36-C37
29	b	706	CLA	C8-C10-C11-C12
39	J	312	KC1	CAA-CBA-CGA-O2A
39	L	306	KC1	CAA-CBA-CGA-O1A
39	Q	311	KC1	CAA-CBA-CGA-O1A
39	C	315	KC1	CAA-CBA-CGA-O2A
39	E	307	KC1	CAA-CBA-CGA-O1A
29	a	837	CLA	C2A-CAA-CBA-CGA
29	l	510	CLA	C2A-CAA-CBA-CGA
29	I	211	CLA	O1A-CGA-O2A-C1
32	b	728	BCR	C37-C22-C23-C24
32	l	506	BCR	C7-C8-C9-C34
36	I	205	DD6	C12-C11-C13-C14
36	K	202	DD6	C12-C11-C13-C14
36	J	302	DD6	C12-C11-C13-C14
36	J	303	DD6	C12-C11-C13-C14
34	K	201	LMG	C31-C32-C33-C34
32	b	728	BCR	C21-C22-C23-C24
36	I	205	DD6	C10-C11-C13-C14
36	J	302	DD6	C10-C11-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
36	J	303	DD6	C10-C11-C13-C14
29	i	202	CLA	C3-C5-C6-C7
29	G	302	CLA	C3-C5-C6-C7
29	I	211	CLA	C3-C5-C6-C7
29	b	714	CLA	C5-C6-C7-C8
29	K	212	CLA	CBD-CGD-O2D-CED
39	A	205	KC1	CBD-CGD-O2D-CED
34	b	730	LMG	C14-C15-C16-C17
34	b	734	LMG	C18-C19-C20-C21
29	b	717	CLA	C16-C17-C18-C19
29	b	717	CLA	C16-C17-C18-C20
29	I	212	CLA	C6-C7-C8-C9
29	L	312	CLA	C6-C7-C8-C9
29	P	210	CLA	C16-C17-C18-C19
29	P	210	CLA	C5-C6-C7-C8
34	A	219	LMG	C30-C31-C32-C33
35	j	106	DGD	C2A-C3A-C4A-C5A
29	E	314	CLA	CBD-CGD-O2D-CED
34	b	732	LMG	O6-C5-C6-O5
39	A	205	KC1	CAA-CBA-CGA-O1A
39	K	215	KC1	CAA-CBA-CGA-O1A
29	a	809	CLA	O1A-CGA-O2A-C1
29	a	826	CLA	O1A-CGA-O2A-C1
34	j	102	LMG	C17-C18-C19-C20
29	E	310	CLA	O1A-CGA-O2A-C1
29	a	821	CLA	CBA-CGA-O2A-C1
29	b	711	CLA	CBA-CGA-O2A-C1
29	B	308	CLA	CBA-CGA-O2A-C1
29	b	710	CLA	O1D-CGD-O2D-CED
29	a	806	CLA	C3A-C2A-CAA-CBA
29	a	811	CLA	C3A-C2A-CAA-CBA
29	a	812	CLA	C3A-C2A-CAA-CBA
29	a	828	CLA	C3A-C2A-CAA-CBA
29	b	706	CLA	C3A-C2A-CAA-CBA
29	b	717	CLA	C3A-C2A-CAA-CBA
29	f	803	CLA	C3A-C2A-CAA-CBA
29	F	310	CLA	C3A-C2A-CAA-CBA
29	L	316	CLA	C3A-C2A-CAA-CBA
29	D	314	CLA	C3A-C2A-CAA-CBA
29	H	313	CLA	C3A-C2A-CAA-CBA
29	N	314	CLA	C3A-C2A-CAA-CBA
29	T	314	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	Q	313	CLA	C3A-C2A-CAA-CBA
29	C	314	CLA	C3A-C2A-CAA-CBA
29	P	215	CLA	C3A-C2A-CAA-CBA
29	a	803	CLA	C15-C16-C17-C18
29	b	704	CLA	C13-C15-C16-C17
29	b	712	CLA	C5-C6-C7-C8
34	b	734	LMG	C11-C12-C13-C14
29	N	313	CLA	CBA-CGA-O2A-C1
29	b	711	CLA	O1D-CGD-O2D-CED
29	L	316	CLA	O1D-CGD-O2D-CED
29	A	212	CLA	O1A-CGA-O2A-C1
29	D	308	CLA	O1A-CGA-O2A-C1
29	a	810	CLA	C6-C7-C8-C9
29	N	309	CLA	C16-C17-C18-C20
34	K	219	LMG	C32-C33-C34-C35
29	M	310	CLA	O2A-C1-C2-C3
29	P	212	CLA	O1D-CGD-O2D-CED
34	K	201	LMG	C17-C18-C19-C20
35	m	102	DGD	C6A-C7A-C8A-C9A
37	P	206	PID	C17-C18-C19-C20
35	b	733	DGD	C1B-C2B-C3B-C4B
34	K	220	LMG	C14-C15-C16-C17
29	a	808	CLA	O1A-CGA-O2A-C1
29	b	702	CLA	C5-C6-C7-C8
29	G	314	CLA	C4-C3-C5-C6
29	a	827	CLA	CBA-CGA-O2A-C1
29	b	719	CLA	CBA-CGA-O2A-C1
29	B	315	CLA	O1A-CGA-O2A-C1
29	G	314	CLA	C2-C3-C5-C6
34	K	220	LMG	C11-C10-O7-C8
39	C	310	KC1	CAA-CBA-CGA-O1A
29	O	314	CLA	C2-C1-O2A-CGA
37	Q	301	PID	C26-C27-O6-C30
37	Q	301	PID	C28-C27-O6-C30
29	a	803	CLA	C2A-CAA-CBA-CGA
29	b	711	CLA	C2A-CAA-CBA-CGA
34	j	102	LMG	C31-C32-C33-C34
29	J	306	CLA	O1A-CGA-O2A-C1
29	G	314	CLA	C11-C12-C13-C14
29	H	308	CLA	C16-C17-C18-C19
29	M	311	CLA	O1A-CGA-O2A-C1
34	b	734	LMG	C17-C18-C19-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	b	730	LMG	O9-C10-O7-C8
29	a	806	CLA	C2-C1-O2A-CGA
34	b	730	LMG	C37-C38-C39-C40
29	a	812	CLA	C8-C10-C11-C12
29	G	316	CLA	C5-C6-C7-C8
34	j	102	LMG	C34-C35-C36-C37
35	G	320	DGD	C1A-C2A-C3A-C4A
32	a	838	BCR	C23-C24-C25-C26
32	a	838	BCR	C23-C24-C25-C30
32	b	729	BCR	C5-C6-C7-C8
32	b	735	BCR	C1-C6-C7-C8
32	b	735	BCR	C5-C6-C7-C8
32	l	506	BCR	C5-C6-C7-C8
32	l	506	BCR	C23-C24-C25-C26
32	l	506	BCR	C23-C24-C25-C30
37	N	305	PID	C16-C17-C18-C19
29	a	805	CLA	CBA-CGA-O2A-C1
29	l	502	CLA	CBA-CGA-O2A-C1
29	J	309	CLA	C2C-C3C-CAC-CBC
29	L	307	CLA	O1A-CGA-O2A-C1
29	a	807	CLA	C8-C10-C11-C12
29	l	503	CLA	C5-C6-C7-C8
29	I	213	CLA	C10-C11-C12-C13
29	a	809	CLA	C4-C3-C5-C6
29	G	304	CLA	C4-C3-C5-C6
29	M	314	CLA	C4-C3-C5-C6
29	a	807	CLA	C11-C12-C13-C15
29	a	807	CLA	C12-C13-C15-C16
29	a	809	CLA	C2-C3-C5-C6
29	a	812	CLA	C11-C10-C8-C7
29	a	825	CLA	C12-C13-C15-C16
29	a	829	CLA	C12-C13-C15-C16
29	b	702	CLA	C6-C7-C8-C10
29	b	709	CLA	C11-C10-C8-C7
29	i	202	CLA	C6-C7-C8-C10
29	l	503	CLA	C6-C7-C8-C10
29	l	505	CLA	C6-C7-C8-C10
29	A	209	CLA	C11-C12-C13-C15
29	G	312	CLA	C6-C7-C8-C10
29	J	306	CLA	C12-C13-C15-C16
29	B	310	CLA	C6-C7-C8-C10
29	P	210	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	E	311	CLA	C11-C12-C13-C15
29	L	313	CLA	C3-C5-C6-C7
29	Q	308	CLA	C3-C5-C6-C7
29	a	821	CLA	O1A-CGA-O2A-C1
29	a	827	CLA	O1A-CGA-O2A-C1
29	b	711	CLA	O1A-CGA-O2A-C1
29	b	719	CLA	O1A-CGA-O2A-C1
29	B	308	CLA	O1A-CGA-O2A-C1
29	b	709	CLA	C8-C10-C11-C12
29	A	212	CLA	C5-C6-C7-C8
29	I	217	CLA	C5-C6-C7-C8
36	D	301	DD6	C24-C25-C26-C27
39	C	312	KC1	CBD-CGD-O2D-CED
37	N	305	PID	C28-C27-O6-C30
29	K	214	CLA	O1D-CGD-O2D-CED
29	F	316	CLA	O1D-CGD-O2D-CED
29	O	311	CLA	O1D-CGD-O2D-CED
29	J	307	CLA	O1A-CGA-O2A-C1
29	G	302	CLA	CBA-CGA-O2A-C1
29	G	312	CLA	CBA-CGA-O2A-C1
29	H	313	CLA	CBA-CGA-O2A-C1
31	a	833	LHG	C24-C23-O8-C6
29	b	713	CLA	C2A-CAA-CBA-CGA
29	G	312	CLA	C2A-CAA-CBA-CGA
29	J	308	CLA	C2A-CAA-CBA-CGA
29	L	317	CLA	C2A-CAA-CBA-CGA
29	B	310	CLA	C2A-CAA-CBA-CGA
29	P	214	CLA	C2A-CAA-CBA-CGA
29	b	736	CLA	C10-C11-C12-C13
35	h	203	DGD	CAB-CBB-CCB-CDB
34	K	219	LMG	C30-C31-C32-C33
37	F	304	PID	C16-C17-C18-C19
34	j	102	LMG	C28-C29-C30-C31
29	L	311	CLA	O1D-CGD-O2D-CED
39	N	315	KC1	C2B-C3B-CAB-CBB
39	O	310	KC1	C2B-C3B-CAB-CBB
29	i	202	CLA	C16-C17-C18-C20
29	I	210	CLA	C6-C7-C8-C10
29	E	308	CLA	C16-C17-C18-C19
29	J	306	CLA	C13-C15-C16-C17
37	G	303	PID	O7-C30-O6-C27
35	G	320	DGD	C2B-C1B-O2G-C2G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
39	G	315	KC1	C4B-C3B-CAB-CBB
39	G	318	KC1	C4B-C3B-CAB-CBB
39	N	310	KC1	C4B-C3B-CAB-CBB
39	O	312	KC1	C4B-C3B-CAB-CBB
39	C	310	KC1	C4B-C3B-CAB-CBB
39	C	312	KC1	C4B-C3B-CAB-CBB
39	P	213	KC1	C4B-C3B-CAB-CBB
29	G	312	CLA	C8-C10-C11-C12
35	j	106	DGD	C3A-C4A-C5A-C6A
34	K	201	LMG	O9-C10-O7-C8
29	E	314	CLA	O2A-C1-C2-C3
34	K	219	LMG	O7-C8-C9-O8
29	a	810	CLA	CBD-CGD-O2D-CED
29	l	502	CLA	C16-C17-C18-C19
34	K	201	LMG	C33-C34-C35-C36
29	b	722	CLA	C8-C10-C11-C12
29	A	218	CLA	C5-C6-C7-C8
29	I	209	CLA	C4-C3-C5-C6
29	A	210	CLA	CBA-CGA-O2A-C1
29	F	307	CLA	CBA-CGA-O2A-C1
34	A	219	LMG	C28-C29-C30-C31
29	a	831	CLA	C2-C3-C5-C6
36	A	204	DD6	C27-C29-C30-C31
36	I	204	DD6	C27-C29-C30-C31
36	M	304	DD6	C27-C29-C30-C31
36	L	301	DD6	C27-C29-C30-C31
36	L	305	DD6	C27-C29-C30-C31
36	B	305	DD6	C27-C29-C30-C31
36	H	303	DD6	C27-C29-C30-C31
36	N	303	DD6	C27-C29-C30-C31
36	O	303	DD6	C27-C29-C30-C31
36	Q	302	DD6	C27-C29-C30-C31
36	P	204	DD6	C27-C29-C30-C31
34	b	730	LMG	C34-C35-C36-C37
29	a	802	CLA	C11-C12-C13-C14
29	a	812	CLA	C11-C10-C8-C9
29	a	825	CLA	C14-C13-C15-C16
29	b	703	CLA	C11-C10-C8-C9
29	b	712	CLA	C14-C13-C15-C16
29	b	736	CLA	C6-C7-C8-C9
29	b	736	CLA	C11-C12-C13-C14
29	A	209	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	G	312	CLA	C6-C7-C8-C9
29	G	316	CLA	C14-C13-C15-C16
29	J	306	CLA	C14-C13-C15-C16
29	b	726	CLA	C3-C5-C6-C7
34	P	201	LMG	O6-C5-C6-O5
36	I	204	DD6	C12-C11-C13-C14
36	K	203	DD6	C12-C11-C13-C14
36	I	204	DD6	C10-C11-C13-C14
36	K	203	DD6	C10-C11-C13-C14
29	a	805	CLA	O1A-CGA-O2A-C1
29	l	502	CLA	O1A-CGA-O2A-C1
29	a	806	CLA	C1A-C2A-CAA-CBA
29	a	818	CLA	C1A-C2A-CAA-CBA
29	a	820	CLA	C1A-C2A-CAA-CBA
29	a	821	CLA	C1A-C2A-CAA-CBA
29	a	828	CLA	C1A-C2A-CAA-CBA
29	b	712	CLA	C1A-C2A-CAA-CBA
29	b	713	CLA	C1A-C2A-CAA-CBA
29	b	720	CLA	C1A-C2A-CAA-CBA
29	b	721	CLA	C1A-C2A-CAA-CBA
29	f	803	CLA	C1A-C2A-CAA-CBA
29	A	212	CLA	C1A-C2A-CAA-CBA
29	G	316	CLA	C1A-C2A-CAA-CBA
29	I	217	CLA	C1A-C2A-CAA-CBA
29	F	308	CLA	C1A-C2A-CAA-CBA
29	L	316	CLA	C1A-C2A-CAA-CBA
29	D	314	CLA	C1A-C2A-CAA-CBA
29	H	313	CLA	C1A-C2A-CAA-CBA
29	N	314	CLA	C1A-C2A-CAA-CBA
29	T	309	CLA	C1A-C2A-CAA-CBA
29	T	314	CLA	C1A-C2A-CAA-CBA
29	C	314	CLA	C1A-C2A-CAA-CBA
29	P	215	CLA	C1A-C2A-CAA-CBA
29	i	202	CLA	C16-C17-C18-C19
35	j	106	DGD	C2B-C1B-O2G-C2G
39	H	309	KC1	CAA-CBA-CGA-O1A
39	H	311	KC1	CAA-CBA-CGA-O2A
36	O	303	DD6	C3-C4-C5-C6
29	a	820	CLA	C13-C15-C16-C17
29	T	316	CLA	CBD-CGD-O2D-CED
29	L	308	CLA	C3-C5-C6-C7
31	a	833	LHG	C2-C3-O3-P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	G	302	CLA	O1A-CGA-O2A-C1
29	Q	310	CLA	C10-C11-C12-C13
34	E	316	LMG	C29-C30-C31-C32
29	T	311	CLA	CBA-CGA-O2A-C1
29	E	308	CLA	C16-C17-C18-C20
34	b	730	LMG	C11-C12-C13-C14
29	b	723	CLA	CBA-CGA-O2A-C1
29	I	212	CLA	CBA-CGA-O2A-C1
29	J	308	CLA	C5-C6-C7-C8
29	P	215	CLA	C2-C1-O2A-CGA
34	b	732	LMG	C14-C15-C16-C17
34	A	219	LMG	C31-C32-C33-C34
35	b	733	DGD	C2B-C3B-C4B-C5B
29	H	313	CLA	O1A-CGA-O2A-C1
35	h	203	DGD	C7B-C8B-C9B-CAB
35	h	203	DGD	C9B-CAB-CBB-CCB
29	J	306	CLA	C16-C17-C18-C20
29	b	718	CLA	O1D-CGD-O2D-CED
29	M	311	CLA	O1D-CGD-O2D-CED
39	O	315	KC1	O1D-CGD-O2D-CED
35	j	103	DGD	C4D-C5D-C6D-O5D
34	b	734	LMG	C7-C8-C9-O8
34	K	201	LMG	C7-C8-C9-O8
34	E	316	LMG	O1-C7-C8-C9
35	j	103	DGD	C1G-C2G-C3G-O3G
29	G	312	CLA	O1A-CGA-O2A-C1
34	K	220	LMG	O10-C28-O8-C9
40	B	317	SQD	C45-C44-O6-C1
29	A	206	CLA	O1D-CGD-O2D-CED
29	b	703	CLA	C8-C10-C11-C12
29	b	716	CLA	C5-C6-C7-C8
34	b	732	LMG	C38-C39-C40-C41
29	l	505	CLA	CAA-CBA-CGA-O2A
35	b	733	DGD	C4B-C5B-C6B-C7B
29	a	802	CLA	C13-C15-C16-C17
40	J	314	SQD	C8-C7-O47-C45
29	l	501	CLA	C8-C10-C11-C12
29	I	209	CLA	C8-C10-C11-C12
29	O	309	CLA	C13-C15-C16-C17
29	b	701	CLA	C4-C3-C5-C6
29	A	209	CLA	C4-C3-C5-C6
29	K	211	CLA	C4-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	K	220	LMG	C32-C33-C34-C35
35	h	203	DGD	C8B-C9B-CAB-CBB
29	b	701	CLA	C2-C3-C5-C6
39	N	310	KC1	C2A-CAA-CBA-CGA
29	a	837	CLA	C6-C7-C8-C9
29	C	309	CLA	C16-C17-C18-C19
29	A	207	CLA	CBA-CGA-O2A-C1
29	B	312	CLA	CBA-CGA-O2A-C1
29	J	309	CLA	C4C-C3C-CAC-CBC
29	Q	310	CLA	C8-C10-C11-C12
30	a	832	PQN	C23-C25-C26-C27
29	G	304	CLA	C11-C12-C13-C14
34	P	201	LMG	C9-C8-O7-C10
29	J	309	CLA	C2A-CAA-CBA-CGA
29	a	829	CLA	C2-C1-O2A-CGA
34	j	102	LMG	C14-C15-C16-C17
34	b	734	LMG	C29-C28-O8-C9
29	E	314	CLA	O1D-CGD-O2D-CED
29	b	702	CLA	C16-C17-C18-C20
29	i	201	CLA	C8-C10-C11-C12
34	b	730	LMG	C32-C33-C34-C35
29	l	503	CLA	C10-C11-C12-C13
37	T	317	PID	C19-C20-C21-C22
40	B	317	SQD	C2-C1-O6-C44
29	a	837	CLA	C5-C6-C7-C8
34	K	219	LMG	C28-C29-C30-C31
29	a	803	CLA	C4-C3-C5-C6
34	b	732	LMG	C37-C38-C39-C40
34	j	102	LMG	C30-C31-C32-C33
29	a	802	CLA	C11-C10-C8-C7
29	a	803	CLA	C2-C3-C5-C6
29	a	829	CLA	C6-C7-C8-C10
29	a	829	CLA	C11-C10-C8-C7
29	b	706	CLA	C12-C13-C15-C16
29	b	712	CLA	C12-C13-C15-C16
29	b	736	CLA	C11-C12-C13-C15
29	i	202	CLA	C11-C10-C8-C7
29	l	504	CLA	C6-C7-C8-C10
29	A	209	CLA	C2-C3-C5-C6
29	A	209	CLA	C12-C13-C15-C16
29	G	316	CLA	C12-C13-C15-C16
29	I	211	CLA	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	J	308	CLA	C6-C7-C8-C10
29	B	312	CLA	C11-C10-C8-C7
29	N	309	CLA	C11-C12-C13-C15
29	E	306	CLA	C6-C7-C8-C10
29	E	308	CLA	C11-C12-C13-C15
29	E	315	CLA	C11-C10-C8-C7
30	a	832	PQN	C22-C23-C25-C26
29	I	212	CLA	O1A-CGA-O2A-C1
34	j	102	LMG	C19-C20-C21-C22
29	a	802	CLA	C11-C10-C8-C9
29	a	806	CLA	C6-C7-C8-C9
29	a	827	CLA	C6-C7-C8-C9
29	a	829	CLA	C11-C10-C8-C9
29	b	705	CLA	C11-C10-C8-C9
29	b	711	CLA	C11-C10-C8-C9
29	b	718	CLA	C11-C12-C13-C14
29	A	209	CLA	C14-C13-C15-C16
29	A	218	CLA	C11-C10-C8-C9
29	B	312	CLA	C11-C10-C8-C9
29	N	309	CLA	C11-C12-C13-C14
29	Q	308	CLA	C11-C10-C8-C9
29	E	306	CLA	C6-C7-C8-C9
29	E	308	CLA	C11-C12-C13-C14
29	E	315	CLA	C11-C10-C8-C9
30	b	727	PQN	C21-C22-C23-C24
37	D	305	PID	C17-C18-C19-C20
37	P	206	PID	C15-C16-C17-C18
29	a	816	CLA	C2A-CAA-CBA-CGA
29	b	720	CLA	C2A-CAA-CBA-CGA
29	I	201	CLA	C2A-CAA-CBA-CGA
39	L	314	KC1	C2C-C3C-CAC-CBC
29	M	309	CLA	O1D-CGD-O2D-CED
29	b	723	CLA	O1A-CGA-O2A-C1
29	b	701	CLA	CBD-CGD-O2D-CED
29	J	308	CLA	CBD-CGD-O2D-CED
36	K	203	DD6	C7-C6-C8-C9
29	J	306	CLA	C16-C17-C18-C19
29	C	309	CLA	C16-C17-C18-C20
34	b	730	LMG	C17-C18-C19-C20
39	E	312	KC1	C2C-C3C-CAC-CBC
36	I	202	DD6	C2-C1-C24-C25
34	j	102	LMG	C33-C34-C35-C36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	G	320	DGD	O1B-C1B-O2G-C2G
34	A	219	LMG	C34-C35-C36-C37
29	L	311	CLA	O1A-CGA-O2A-C1
29	a	826	CLA	C13-C15-C16-C17
39	G	318	KC1	CAA-CBA-CGA-O1A
39	O	315	KC1	CAA-CBA-CGA-O1A
34	j	102	LMG	O7-C10-C11-C12
29	A	207	CLA	O1A-CGA-O2A-C1
29	A	207	CLA	CBD-CGD-O2D-CED
34	b	732	LMG	C36-C37-C38-C39
35	b	733	DGD	CAB-CBB-CCB-CDB
29	A	209	CLA	C13-C15-C16-C17
29	l	505	CLA	C4-C3-C5-C6
29	K	211	CLA	C2-C3-C5-C6
35	b	733	DGD	C7A-C8A-C9A-CAA
35	h	203	DGD	C2A-C3A-C4A-C5A
29	M	307	CLA	O1D-CGD-O2D-CED
29	b	721	CLA	C5-C6-C7-C8
39	N	315	KC1	CAA-CBA-CGA-O1A
39	O	310	KC1	CAA-CBA-CGA-O1A
29	a	837	CLA	C6-C7-C8-C10
29	M	311	CLA	C2A-CAA-CBA-CGA
34	K	220	LMG	C29-C28-O8-C9
29	a	824	CLA	CBD-CGD-O2D-CED
29	J	311	CLA	O1D-CGD-O2D-CED
29	a	807	CLA	C3A-C2A-CAA-CBA
29	b	721	CLA	C3A-C2A-CAA-CBA
29	i	203	CLA	C3A-C2A-CAA-CBA
29	G	302	CLA	C3A-C2A-CAA-CBA
29	I	212	CLA	C3A-C2A-CAA-CBA
29	J	310	CLA	C3A-C2A-CAA-CBA
29	D	311	CLA	C3A-C2A-CAA-CBA
29	H	310	CLA	C3A-C2A-CAA-CBA
29	a	825	CLA	C15-C16-C17-C18
36	G	305	DD6	C11-C10-C9-C8
36	G	306	DD6	C11-C10-C9-C8
36	D	301	DD6	C11-C10-C9-C8
38	N	306	UIX	C34-C37-C39-C40
29	A	218	CLA	C8-C10-C11-C12
29	B	310	CLA	C8-C10-C11-C12
39	T	315	KC1	CAA-CBA-CGA-O1A
29	a	822	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	b	730	LMG	O1-C7-C8-C9
34	b	730	LMG	C7-C8-C9-O8
34	K	219	LMG	C7-C8-C9-O8
35	j	106	DGD	C1G-C2G-C3G-O3G
35	b	733	DGD	C4D-C5D-C6D-O5D
29	G	302	CLA	CAA-CBA-CGA-O2A
29	P	210	CLA	C3-C5-C6-C7
29	a	807	CLA	C4-C3-C5-C6
29	a	812	CLA	C4-C3-C5-C6
35	B	318	DGD	C4D-C5D-C6D-O5D
39	Q	314	KC1	CAA-CBA-CGA-O2A
35	B	318	DGD	C2B-C3B-C4B-C5B
29	K	212	CLA	O1D-CGD-O2D-CED
34	A	219	LMG	C4-C5-C6-O5
29	K	218	CLA	C2A-CAA-CBA-CGA
29	O	309	CLA	C15-C16-C17-C18
29	a	812	CLA	CBA-CGA-O2A-C1
29	A	211	CLA	CBA-CGA-O2A-C1
29	B	312	CLA	O1A-CGA-O2A-C1
31	a	833	LHG	O10-C23-O8-C6
39	F	314	KC1	C3A-C2A-CAA-CBA
39	Q	309	KC1	C3A-C2A-CAA-CBA
34	K	201	LMG	C18-C19-C20-C21
34	b	730	LMG	O1-C7-C8-O7
34	E	316	LMG	O1-C7-C8-O7
35	j	103	DGD	O2G-C2G-C3G-O3G
35	j	106	DGD	O1G-C1G-C2G-O2G
37	P	206	PID	C14-C15-C16-C17
29	b	702	CLA	C16-C17-C18-C19
29	J	306	CLA	C15-C16-C17-C18
34	K	219	LMG	C33-C34-C35-C36
39	F	309	KC1	CAA-CBA-CGA-O1A
29	a	822	CLA	C2-C1-O2A-CGA
29	b	716	CLA	C2-C1-O2A-CGA
29	b	718	CLA	C2-C1-O2A-CGA
29	I	209	CLA	C2-C1-O2A-CGA
29	M	314	CLA	C2-C1-O2A-CGA
34	P	201	LMG	O10-C28-O8-C9
29	a	809	CLA	C14-C13-C15-C16
29	b	701	CLA	C11-C10-C8-C9
29	b	701	CLA	C11-C12-C13-C14
29	b	706	CLA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	b	706	CLA	C14-C13-C15-C16
29	b	718	CLA	C11-C10-C8-C9
29	i	202	CLA	C11-C10-C8-C9
29	B	308	CLA	C6-C7-C8-C9
29	B	310	CLA	C11-C10-C8-C9
29	H	308	CLA	C11-C12-C13-C14
39	O	310	KC1	C1A-C2A-CAA-CBA
39	O	312	KC1	C1A-C2A-CAA-CBA
39	Q	314	KC1	C1A-C2A-CAA-CBA
39	E	307	KC1	C1A-C2A-CAA-CBA
29	a	812	CLA	C2A-CAA-CBA-CGA
29	i	201	CLA	C2A-CAA-CBA-CGA
29	l	503	CLA	C2A-CAA-CBA-CGA
32	b	729	BCR	C23-C24-C25-C26
32	b	729	BCR	C23-C24-C25-C30
32	i	204	BCR	C5-C6-C7-C8
29	b	736	CLA	C8-C10-C11-C12
34	b	732	LMG	C17-C18-C19-C20
36	T	303	DD6	C-C1-C24-C25
32	a	838	BCR	C21-C22-C23-C24
32	b	728	BCR	C17-C18-C19-C20
32	f	801	BCR	C7-C8-C9-C10
32	l	506	BCR	C7-C8-C9-C10
36	h	202	DD6	C10-C11-C13-C14
35	j	106	DGD	O1B-C1B-O2G-C2G
37	F	304	PID	C17-C18-C19-C20
34	b	732	LMG	C13-C14-C15-C16
29	I	217	CLA	C6-C7-C8-C9
39	P	216	KC1	CAA-CBA-CGA-O2A
35	m	102	DGD	CCA-CDA-CEA-CFA
29	b	725	CLA	CBD-CGD-O2D-CED
29	a	802	CLA	C12-C13-C15-C16
29	a	806	CLA	C6-C7-C8-C10
29	a	807	CLA	C11-C10-C8-C7
29	a	809	CLA	C11-C10-C8-C7
29	a	809	CLA	C12-C13-C15-C16
29	a	820	CLA	C11-C10-C8-C7
29	a	822	CLA	C11-C12-C13-C15
29	a	827	CLA	C6-C7-C8-C10
29	b	701	CLA	C11-C10-C8-C7
29	b	704	CLA	C6-C7-C8-C10
29	b	705	CLA	C11-C10-C8-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	b	711	CLA	C11-C10-C8-C7
29	b	718	CLA	C11-C12-C13-C15
29	b	720	CLA	C11-C10-C8-C7
29	A	218	CLA	C11-C10-C8-C7
29	G	312	CLA	C11-C12-C13-C15
29	B	308	CLA	C6-C7-C8-C10
29	B	310	CLA	C11-C10-C8-C7
29	H	308	CLA	C11-C12-C13-C15
29	Q	308	CLA	C11-C10-C8-C7
29	Q	310	CLA	C11-C10-C8-C7
29	E	306	CLA	C11-C12-C13-C15
30	b	727	PQN	C21-C22-C23-C25
36	K	202	DD6	C11-C10-C9-C8
36	M	303	DD6	C11-C10-C9-C8
29	a	810	CLA	C2A-CAA-CBA-CGA
29	b	714	CLA	C8-C10-C11-C12
37	D	306	PID	CM4-C14-C15-C16
37	T	317	PID	C19-C20-C21-CM5
35	B	318	DGD	O6D-C5D-C6D-O5D
39	C	312	KC1	C2A-CAA-CBA-CGA
29	i	201	CLA	C13-C15-C16-C17
29	G	302	CLA	C15-C16-C17-C18
29	i	203	CLA	CBA-CGA-O2A-C1
35	b	733	DGD	C8A-C9A-CAA-CBA
29	a	822	CLA	CAD-CBD-CGD-O2D
29	a	827	CLA	CAD-CBD-CGD-O2D
29	b	720	CLA	CAD-CBD-CGD-O2D
29	b	721	CLA	CAD-CBD-CGD-O2D
29	f	805	CLA	CAD-CBD-CGD-O2D
29	i	201	CLA	CAD-CBD-CGD-O2D
29	l	505	CLA	CAD-CBD-CGD-O2D
29	I	201	CLA	CAD-CBD-CGD-O2D
29	I	209	CLA	CAD-CBD-CGD-O2D
29	K	211	CLA	CAD-CBD-CGD-O2D
29	F	311	CLA	CAD-CBD-CGD-O2D
29	J	307	CLA	CAD-CBD-CGD-O2D
29	D	313	CLA	CAD-CBD-CGD-O2D
29	D	314	CLA	CAD-CBD-CGD-O2D
29	H	313	CLA	CAD-CBD-CGD-O2D
29	N	309	CLA	CAD-CBD-CGD-O2D
29	O	313	CLA	CAD-CBD-CGD-O2D
29	T	309	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	C	313	CLA	CAD-CBD-CGD-O2D
35	b	733	DGD	C3G-C2G-O2G-C1B
37	F	304	PID	CM5-C21-C22-C23
37	P	206	PID	CM5-C21-C22-C23
37	E	301	PID	CM5-C21-C22-C23
38	N	306	UIX	C25-C28-C32-C33
38	T	306	UIX	C25-C28-C32-C33
39	F	314	KC1	CAD-CBD-CGD-O2D
39	L	306	KC1	CAD-CBD-CGD-O2D
39	H	314	KC1	C2B-C3B-CAB-CBB
39	O	315	KC1	C2B-C3B-CAB-CBB
39	T	315	KC1	C2B-C3B-CAB-CBB
39	Q	314	KC1	C2B-C3B-CAB-CBB
39	C	315	KC1	C2B-C3B-CAB-CBB
39	P	211	KC1	C2B-C3B-CAB-CBB
29	M	307	CLA	C3-C5-C6-C7
29	a	810	CLA	O1D-CGD-O2D-CED
29	b	712	CLA	C4-C3-C5-C6
29	L	310	CLA	C4-C3-C5-C6
29	a	812	CLA	C11-C12-C13-C15
29	L	310	CLA	C2-C3-C5-C6
35	G	320	DGD	C1G-C2G-C3G-O3G
37	G	303	PID	C12-C13-C14-CM4
29	a	829	CLA	C5-C6-C7-C8
29	I	207	CLA	O2A-C1-C2-C3
29	K	207	CLA	O2A-C1-C2-C3
39	N	315	KC1	C4B-C3B-CAB-CBB
39	O	310	KC1	C4B-C3B-CAB-CBB
29	b	725	CLA	C16-C17-C18-C20
34	j	102	LMG	C32-C33-C34-C35
29	T	316	CLA	O1D-CGD-O2D-CED
29	a	809	CLA	CHA-CBD-CGD-O1D
29	a	809	CLA	CHA-CBD-CGD-O2D
29	a	828	CLA	CHA-CBD-CGD-O1D
29	b	702	CLA	CHA-CBD-CGD-O1D
29	b	702	CLA	CHA-CBD-CGD-O2D
29	b	709	CLA	CHA-CBD-CGD-O1D
29	b	709	CLA	CHA-CBD-CGD-O2D
29	b	719	CLA	CHA-CBD-CGD-O1D
29	b	719	CLA	CHA-CBD-CGD-O2D
29	l	501	CLA	CHA-CBD-CGD-O1D
29	l	501	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	l	508	CLA	CHA-CBD-CGD-O1D
29	l	508	CLA	CHA-CBD-CGD-O2D
29	l	509	CLA	CHA-CBD-CGD-O1D
29	l	509	CLA	CHA-CBD-CGD-O2D
29	A	217	CLA	CHA-CBD-CGD-O2D
29	G	302	CLA	CHA-CBD-CGD-O1D
29	G	302	CLA	CHA-CBD-CGD-O2D
29	I	207	CLA	CHA-CBD-CGD-O1D
29	I	207	CLA	CHA-CBD-CGD-O2D
29	J	308	CLA	CHA-CBD-CGD-O1D
29	J	308	CLA	CHA-CBD-CGD-O2D
29	D	311	CLA	CHA-CBD-CGD-O1D
29	D	311	CLA	CHA-CBD-CGD-O2D
29	N	313	CLA	CHA-CBD-CGD-O1D
29	N	316	CLA	CHA-CBD-CGD-O1D
29	O	308	CLA	CHA-CBD-CGD-O2D
29	O	309	CLA	CHA-CBD-CGD-O1D
29	O	309	CLA	CHA-CBD-CGD-O2D
29	T	313	CLA	CHA-CBD-CGD-O2D
29	Q	313	CLA	CHA-CBD-CGD-O1D
29	C	309	CLA	CHA-CBD-CGD-O2D
29	P	212	CLA	CHA-CBD-CGD-O1D
29	P	212	CLA	CHA-CBD-CGD-O2D
29	E	305	CLA	CHA-CBD-CGD-O1D
39	A	205	KC1	CHA-CBD-CGD-O2D
39	K	215	KC1	CHA-CBD-CGD-O1D
39	N	312	KC1	CHA-CBD-CGD-O2D
39	T	310	KC1	CHA-CBD-CGD-O1D
39	C	312	KC1	CHA-CBD-CGD-O2D
29	K	209	CLA	C3-C5-C6-C7
34	b	732	LMG	O7-C8-C9-O8
34	K	201	LMG	O7-C8-C9-O8
35	j	106	DGD	O2G-C2G-C3G-O3G
29	a	822	CLA	O1A-CGA-O2A-C1
29	A	211	CLA	O1A-CGA-O2A-C1
29	Q	310	CLA	C3-C5-C6-C7
29	b	702	CLA	C4-C3-C5-C6
29	I	213	CLA	C4-C3-C5-C6
29	O	309	CLA	C4-C3-C5-C6
29	M	314	CLA	C2-C3-C5-C6
36	m	101	DD6	C27-C29-C30-C31
36	A	201	DD6	C27-C29-C30-C31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
36	I	202	DD6	C27-C29-C30-C31
36	I	206	DD6	C27-C29-C30-C31
36	K	203	DD6	C27-C29-C30-C31
36	K	204	DD6	C27-C29-C30-C31
36	K	205	DD6	C27-C29-C30-C31
36	J	301	DD6	C27-C29-C30-C31
36	D	301	DD6	C27-C29-C30-C31
36	B	301	DD6	C27-C29-C30-C31
36	B	302	DD6	C27-C29-C30-C31
36	T	303	DD6	C27-C29-C30-C31
34	b	734	LMG	C16-C17-C18-C19
34	K	220	LMG	O9-C10-O7-C8
29	a	802	CLA	C14-C13-C15-C16
29	a	820	CLA	C11-C10-C8-C9
29	b	707	CLA	C6-C7-C8-C9
29	i	201	CLA	C6-C7-C8-C9
29	A	209	CLA	C11-C10-C8-C9
29	G	312	CLA	C11-C12-C13-C14
29	E	306	CLA	C11-C12-C13-C14
29	E	311	CLA	C11-C10-C8-C9
29	N	313	CLA	O1A-CGA-O2A-C1
29	a	831	CLA	C5-C6-C7-C8
29	b	707	CLA	C16-C17-C18-C20
29	A	209	CLA	C16-C17-C18-C20
29	K	211	CLA	C2A-CAA-CBA-CGA
29	D	312	CLA	C2A-CAA-CBA-CGA
29	a	812	CLA	O1A-CGA-O2A-C1
29	i	203	CLA	O1A-CGA-O2A-C1
32	a	835	BCR	C7-C8-C9-C34
32	b	728	BCR	C7-C8-C9-C34
36	K	221	DD6	C12-C11-C13-C14
36	T	303	DD6	C12-C11-C13-C14
29	G	319	CLA	CBD-CGD-O2D-CED
36	K	221	DD6	C10-C11-C13-C14
36	T	303	DD6	C10-C11-C13-C14
29	b	731	CLA	C3-C5-C6-C7
40	B	317	SQD	C12-C13-C14-C15
29	b	711	CLA	C1A-C2A-CAA-CBA
29	i	203	CLA	C1A-C2A-CAA-CBA
29	I	214	CLA	C1A-C2A-CAA-CBA
29	M	311	CLA	C1A-C2A-CAA-CBA
29	B	312	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	G	312	CLA	C16-C17-C18-C20
36	B	319	DD6	C11-C10-C9-C8
37	O	305	PID	C18-C19-C20-C21
29	a	807	CLA	C2-C3-C5-C6
29	G	304	CLA	C2-C3-C5-C6
29	I	209	CLA	C2-C3-C5-C6
40	J	314	SQD	C23-C24-C25-C26
40	J	314	SQD	O5-C1-O6-C44
29	a	806	CLA	C13-C15-C16-C17
35	h	203	DGD	CBB-CCB-CDB-CEB
29	P	212	CLA	C2A-CAA-CBA-CGA
29	l	502	CLA	C3-C5-C6-C7
29	A	207	CLA	O1D-CGD-O2D-CED
29	A	212	CLA	C6-C7-C8-C10
34	K	201	LMG	C14-C15-C16-C17
29	b	703	CLA	CAD-CBD-CGD-O1D
29	A	209	CLA	CAD-CBD-CGD-O1D
29	A	214	CLA	CAD-CBD-CGD-O1D
29	G	311	CLA	C2-C3-C5-C6
29	G	314	CLA	CAD-CBD-CGD-O1D
29	K	216	CLA	CAD-CBD-CGD-O1D
29	D	311	CLA	CAD-CBD-CGD-O1D
29	D	316	CLA	CAD-CBD-CGD-O1D
29	B	311	CLA	C2-C3-C5-C6
29	H	315	CLA	CAD-CBD-CGD-O1D
29	N	316	CLA	CAD-CBD-CGD-O1D
29	P	212	CLA	CAD-CBD-CGD-O1D
38	N	306	UIX	C25-C28-C32-C35
35	G	320	DGD	O6D-C5D-C6D-O5D
40	J	314	SQD	O49-C7-O47-C45
29	b	723	CLA	CBD-CGD-O2D-CED
29	b	707	CLA	C6-C7-C8-C10
29	i	201	CLA	C6-C7-C8-C10
29	l	501	CLA	C6-C7-C8-C10
29	l	502	CLA	C12-C13-C15-C16
29	A	209	CLA	C11-C10-C8-C7
29	B	312	CLA	C12-C13-C15-C16
29	E	309	CLA	C3A-C2A-CAA-CBA
29	E	311	CLA	C11-C10-C8-C7
34	K	220	LMG	C10-C11-C12-C13
29	b	725	CLA	O1D-CGD-O2D-CED
29	b	701	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	N	309	CLA	C2A-CAA-CBA-CGA
29	T	311	CLA	C2A-CAA-CBA-CGA
29	E	311	CLA	C2A-CAA-CBA-CGA
29	I	217	CLA	C6-C7-C8-C10
34	E	316	LMG	C31-C32-C33-C34
29	J	306	CLA	C3-C5-C6-C7
29	M	315	CLA	CAA-CBA-CGA-O2A
34	b	732	LMG	C7-C8-C9-O8
34	j	102	LMG	C7-C8-C9-O8
35	B	318	DGD	C1G-C2G-C3G-O3G
37	D	307	PID	O4-C12-C13-C14
37	N	301	PID	O4-C12-C13-C14
37	C	301	PID	O4-C12-C13-C14
37	P	205	PID	O4-C12-C13-C14
29	F	307	CLA	O1A-CGA-O2A-C1
34	j	102	LMG	O7-C8-C9-O8
35	G	320	DGD	O2G-C2G-C3G-O3G
35	B	318	DGD	O2G-C2G-C3G-O3G
34	b	730	LMG	C16-C17-C18-C19
35	j	106	DGD	C2G-C3G-O3G-C1D
29	A	210	CLA	O1A-CGA-O2A-C1
29	f	805	CLA	C5-C6-C7-C8
29	D	311	CLA	CBA-CGA-O2A-C1
29	J	308	CLA	O1D-CGD-O2D-CED
29	b	736	CLA	C4-C3-C5-C6
29	a	818	CLA	CAA-CBA-CGA-O2A
29	K	212	CLA	CAA-CBA-CGA-O2A
29	a	809	CLA	C11-C10-C8-C9
29	a	822	CLA	C11-C12-C13-C14
29	a	831	CLA	C11-C12-C13-C14
29	b	714	CLA	C11-C10-C8-C9
29	b	718	CLA	C6-C7-C8-C9
29	l	505	CLA	C11-C10-C8-C9
29	G	304	CLA	C11-C10-C8-C9
29	Q	310	CLA	C11-C10-C8-C9
29	E	305	CLA	C6-C7-C8-C9
29	A	209	CLA	C16-C17-C18-C19
29	b	701	CLA	O1D-CGD-O2D-CED
37	E	301	PID	C7-C8-C9-C11
29	b	707	CLA	C16-C17-C18-C19
29	T	311	CLA	O1A-CGA-O2A-C1
29	a	824	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
39	G	315	KC1	CAA-CBA-CGA-O2A
31	a	833	LHG	C14-C15-C16-C17
29	a	801	CLA	C16-C17-C18-C19
29	G	301	CLA	C1-C2-C3-C4
29	a	818	CLA	C2A-CAA-CBA-CGA
29	b	703	CLA	C2A-CAA-CBA-CGA
29	j	104	CLA	C2A-CAA-CBA-CGA
29	A	209	CLA	C2A-CAA-CBA-CGA
29	L	310	CLA	C2A-CAA-CBA-CGA
29	Q	310	CLA	CBA-CGA-O2A-C1
29	a	823	CLA	C2-C1-O2A-CGA
29	a	826	CLA	C2-C1-O2A-CGA
29	i	203	CLA	C2-C1-O2A-CGA
29	K	210	CLA	C2-C1-O2A-CGA
29	Q	310	CLA	O1A-CGA-O2A-C1
34	K	219	LMG	C34-C35-C36-C37
29	B	314	CLA	CBD-CGD-O2D-CED
29	A	211	CLA	C5-C6-C7-C8
32	i	204	BCR	C1-C6-C7-C8
32	m	103	BCR	C23-C24-C25-C26
29	i	203	CLA	CAA-CBA-CGA-O2A
35	h	203	DGD	C4B-C5B-C6B-C7B
35	G	320	DGD	C4D-C5D-C6D-O5D
29	N	311	CLA	C2A-CAA-CBA-CGA
31	a	833	LHG	C3-O3-P-O6
35	B	318	DGD	C1A-C2A-C3A-C4A
29	f	805	CLA	C11-C12-C13-C15
29	b	723	CLA	O1D-CGD-O2D-CED
29	b	720	CLA	C4-C3-C5-C6
35	b	733	DGD	C8B-C9B-CAB-CBB
29	b	720	CLA	C2-C3-C5-C6
29	A	218	CLA	C6-C7-C8-C10
29	Q	308	CLA	C11-C12-C13-C15
29	E	305	CLA	C6-C7-C8-C10
34	E	316	LMG	C30-C31-C32-C33
29	a	825	CLA	C6-C7-C8-C9
29	b	725	CLA	C6-C7-C8-C9
29	l	501	CLA	C6-C7-C8-C9
29	J	308	CLA	C6-C7-C8-C9
29	E	308	CLA	C11-C10-C8-C9
36	I	205	DD6	C11-C10-C9-C8
29	b	726	CLA	C16-C17-C18-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	i	202	CLA	C2A-CAA-CBA-CGA
34	b	732	LMG	C35-C36-C37-C38
29	G	311	CLA	O1A-CGA-O2A-C1
34	A	219	LMG	C33-C34-C35-C36
29	b	716	CLA	CBA-CGA-O2A-C1
29	a	825	CLA	C5-C6-C7-C8
29	G	319	CLA	O1D-CGD-O2D-CED
29	b	704	CLA	CAA-CBA-CGA-O2A
29	l	505	CLA	C2-C3-C5-C6
29	a	825	CLA	CBA-CGA-O2A-C1
29	G	301	CLA	CBA-CGA-O2A-C1
29	G	311	CLA	CBA-CGA-O2A-C1
29	K	213	CLA	CBA-CGA-O2A-C1
29	b	716	CLA	O1A-CGA-O2A-C1
39	I	215	KC1	CAA-CBA-CGA-O1A
29	i	202	CLA	C15-C16-C17-C18
32	l	507	BCR	C9-C10-C11-C12
36	B	301	DD6	C24-C25-C26-C27
36	E	303	DD6	C24-C25-C26-C27
38	N	306	UIX	C26-C30-C34-C37
29	K	213	CLA	O1A-CGA-O2A-C1
29	M	308	CLA	CBA-CGA-O2A-C1
31	a	833	LHG	C9-C10-C11-C12
29	I	213	CLA	C16-C17-C18-C20
39	H	314	KC1	C4B-C3B-CAB-CBB
39	P	211	KC1	C4B-C3B-CAB-CBB
29	l	504	CLA	C4-C3-C5-C6
29	G	317	CLA	C4-C3-C5-C6
29	M	307	CLA	C4-C3-C5-C6
29	b	709	CLA	C2-C3-C5-C6
29	a	825	CLA	O1A-CGA-O2A-C1
34	K	220	LMG	C31-C32-C33-C34
29	b	705	CLA	C2-C1-O2A-CGA
29	j	104	CLA	C2-C1-O2A-CGA
29	B	308	CLA	C2-C1-O2A-CGA
29	B	310	CLA	C2-C1-O2A-CGA
29	a	801	CLA	C5-C6-C7-C8
29	f	805	CLA	C2A-CAA-CBA-CGA
29	A	207	CLA	C2A-CAA-CBA-CGA
29	I	208	CLA	C2A-CAA-CBA-CGA
29	H	308	CLA	C2A-CAA-CBA-CGA
29	H	310	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	K	220	LMG	O1-C7-C8-O7
35	b	733	DGD	O2G-C2G-C3G-O3G
35	B	318	DGD	C2A-C3A-C4A-C5A
37	T	317	PID	C28-C27-O6-C30
35	m	102	DGD	CAA-CBA-CCA-CDA
29	b	708	CLA	C3A-C2A-CAA-CBA
29	l	510	CLA	C3A-C2A-CAA-CBA
29	M	309	CLA	C3A-C2A-CAA-CBA
29	O	313	CLA	C3A-C2A-CAA-CBA
29	B	306	CLA	O2A-C1-C2-C3
32	f	801	BCR	C15-C16-C17-C18
29	a	810	CLA	C5-C6-C7-C8
29	l	510	CLA	CAA-CBA-CGA-O1A
29	b	709	CLA	C4-C3-C5-C6
29	L	316	CLA	C2C-C3C-CAC-CBC
29	a	803	CLA	C6-C7-C8-C9
29	b	701	CLA	C14-C13-C15-C16
29	b	725	CLA	C11-C12-C13-C14
29	b	736	CLA	C11-C10-C8-C9
29	C	309	CLA	C6-C7-C8-C9
29	E	306	CLA	C14-C13-C15-C16
30	a	832	PQN	C19-C18-C20-C21
29	b	704	CLA	C16-C17-C18-C19
35	m	102	DGD	C5B-C6B-C7B-C8B
32	b	735	BCR	C20-C21-C22-C37
32	f	801	BCR	C16-C17-C18-C36
32	f	804	BCR	C35-C13-C14-C15
35	j	106	DGD	O1G-C1G-C2G-C3G
29	D	311	CLA	C2A-CAA-CBA-CGA
29	M	308	CLA	O1A-CGA-O2A-C1
31	a	833	LHG	C11-C10-C9-C8
29	a	801	CLA	C16-C17-C18-C20
29	b	736	CLA	O2A-C1-C2-C3
32	b	729	BCR	C37-C22-C23-C24
38	A	203	UIX	C14-C23-C26-C29
34	b	732	LMG	C16-C17-C18-C19
34	A	219	LMG	C7-C8-O7-C10
29	a	808	CLA	C1A-C2A-CAA-CBA
29	a	816	CLA	C1A-C2A-CAA-CBA
29	b	708	CLA	C1A-C2A-CAA-CBA
29	b	709	CLA	C1A-C2A-CAA-CBA
29	G	317	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	K	214	CLA	C1A-C2A-CAA-CBA
29	D	311	CLA	C1A-C2A-CAA-CBA
29	O	313	CLA	C1A-C2A-CAA-CBA
29	a	802	CLA	C11-C12-C13-C15
29	a	811	CLA	C6-C7-C8-C10
29	G	302	CLA	C12-C13-C15-C16
29	B	310	CLA	C12-C13-C15-C16
29	Q	308	CLA	C6-C7-C8-C10
29	Q	308	CLA	C12-C13-C15-C16
29	H	308	CLA	C15-C16-C17-C18
32	l	506	BCR	C13-C14-C15-C16
29	G	301	CLA	O1A-CGA-O2A-C1
29	a	829	CLA	C2A-CAA-CBA-CGA
29	G	314	CLA	C2A-CAA-CBA-CGA
29	J	311	CLA	C2A-CAA-CBA-CGA
29	L	313	CLA	C2A-CAA-CBA-CGA
29	T	313	CLA	C2A-CAA-CBA-CGA
29	T	314	CLA	C2A-CAA-CBA-CGA
29	C	309	CLA	C2A-CAA-CBA-CGA
35	j	106	DGD	O6D-C5D-C6D-O5D
34	b	734	LMG	C31-C32-C33-C34
34	h	205	LMG	C11-C12-C13-C14
39	G	315	KC1	C3A-C2A-CAA-CBA
39	H	309	KC1	C3A-C2A-CAA-CBA
39	T	312	KC1	C3A-C2A-CAA-CBA
39	E	312	KC1	C3A-C2A-CAA-CBA
29	l	510	CLA	CAA-CBA-CGA-O2A
29	N	314	CLA	C2-C1-O2A-CGA
29	l	503	CLA	C4-C3-C5-C6
29	I	212	CLA	C4-C3-C5-C6
29	Q	308	CLA	C10-C11-C12-C13
34	b	734	LMG	C12-C13-C14-C15
29	a	830	CLA	C3-C5-C6-C7
32	b	735	BCR	C20-C21-C22-C23
32	f	801	BCR	C16-C17-C18-C19
32	f	804	BCR	C12-C13-C14-C15
36	K	202	DD6	C24-C25-C26-C27
36	P	204	DD6	C24-C25-C26-C27
29	B	314	CLA	O1D-CGD-O2D-CED
29	a	806	CLA	C5-C6-C7-C8
29	a	827	CLA	C13-C15-C16-C17
39	C	315	KC1	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	b	714	CLA	C2-C1-O2A-CGA
29	a	822	CLA	C14-C13-C15-C16
29	l	505	CLA	CAA-CBA-CGA-O1A
29	G	311	CLA	C4-C3-C5-C6
29	B	311	CLA	C4-C3-C5-C6
39	A	213	KC1	C1A-C2A-CAA-CBA
39	F	309	KC1	C1A-C2A-CAA-CBA
39	J	312	KC1	C1A-C2A-CAA-CBA
39	M	305	KC1	C1A-C2A-CAA-CBA
39	B	313	KC1	C1A-C2A-CAA-CBA
39	H	311	KC1	C1A-C2A-CAA-CBA
39	Q	311	KC1	C1A-C2A-CAA-CBA
39	C	315	KC1	C1A-C2A-CAA-CBA
39	P	216	KC1	C1A-C2A-CAA-CBA
29	i	203	CLA	C2A-CAA-CBA-CGA
29	I	214	CLA	C2A-CAA-CBA-CGA
29	L	316	CLA	C2A-CAA-CBA-CGA
29	I	214	CLA	C6-C7-C8-C9
32	b	728	BCR	C1-C6-C7-C8
34	j	102	LMG	O1-C7-C8-C9
36	D	304	DD6	C24-C25-C26-C27
38	T	306	UIX	C34-C37-C39-C40
29	I	217	CLA	C4-C3-C5-C6
29	K	212	CLA	C4-C3-C5-C6
29	B	308	CLA	C4-C3-C5-C6
32	a	835	BCR	C7-C8-C9-C10
36	K	203	DD6	C5-C6-C8-C9
36	T	303	DD6	C2-C1-C24-C25
34	b	732	LMG	C4-C5-C6-O5
35	B	318	DGD	C5D-C6D-O5D-C1E
29	L	316	CLA	C4C-C3C-CAC-CBC
29	I	213	CLA	C16-C17-C18-C19
29	B	308	CLA	C3-C5-C6-C7
29	G	311	CLA	C2A-CAA-CBA-CGA
29	I	207	CLA	C2A-CAA-CBA-CGA
29	K	207	CLA	C2A-CAA-CBA-CGA
29	H	312	CLA	C2A-CAA-CBA-CGA
29	O	314	CLA	C2A-CAA-CBA-CGA
29	a	801	CLA	CAA-CBA-CGA-O2A
29	a	825	CLA	C3-C5-C6-C7
29	b	702	CLA	C3-C5-C6-C7
29	O	308	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	b	734	LMG	C30-C31-C32-C33
29	N	309	CLA	C10-C11-C12-C13
29	a	801	CLA	C6-C7-C8-C10
29	a	812	CLA	C2-C3-C5-C6
29	b	703	CLA	C6-C7-C8-C10
29	f	803	CLA	CBD-CGD-O2D-CED
36	B	319	DD6	C24-C25-C26-C27
37	N	305	PID	C18-C19-C20-C21
29	L	309	CLA	CAA-CBA-CGA-O2A
39	N	310	KC1	CAA-CBA-CGA-O2A
39	P	211	KC1	CAA-CBA-CGA-O2A
29	a	821	CLA	CAA-CBA-CGA-O2A
29	b	706	CLA	C2A-CAA-CBA-CGA
29	a	809	CLA	C10-C11-C12-C13
29	N	309	CLA	C15-C16-C17-C18
37	D	307	PID	C19-C20-C21-CM5
37	C	305	PID	C19-C20-C21-CM5
29	b	703	CLA	CAA-CBA-CGA-O2A
35	j	106	DGD	O1G-C1A-C2A-C3A
29	B	308	CLA	CBD-CGD-O2D-CED
29	a	806	CLA	C4-C3-C5-C6
29	M	306	CLA	C4-C3-C5-C6
29	B	309	CLA	C4-C3-C5-C6
29	E	311	CLA	C4-C3-C5-C6
30	b	727	PQN	C14-C13-C15-C16
29	b	702	CLA	C2-C3-C5-C6
29	l	503	CLA	C2-C3-C5-C6
29	O	309	CLA	C2-C3-C5-C6
29	f	803	CLA	O1D-CGD-O2D-CED
39	Q	314	KC1	C2A-CAA-CBA-CGA
29	A	208	CLA	CAA-CBA-CGA-O2A
29	b	720	CLA	C11-C10-C8-C9
29	b	726	CLA	C11-C10-C8-C9
29	l	502	CLA	C14-C13-C15-C16
29	l	503	CLA	C11-C10-C8-C9
29	I	213	CLA	C6-C7-C8-C9
29	B	308	CLA	C14-C13-C15-C16
29	B	310	CLA	C14-C13-C15-C16
29	B	312	CLA	C6-C7-C8-C9
29	B	312	CLA	C14-C13-C15-C16
29	N	309	CLA	C14-C13-C15-C16
29	C	309	CLA	C11-C10-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
30	a	832	PQN	C24-C23-C25-C26
29	f	805	CLA	C3A-C2A-CAA-CBA
29	I	209	CLA	CAA-CBA-CGA-O2A
29	B	316	CLA	CAA-CBA-CGA-O2A
29	a	808	CLA	CAD-CBD-CGD-O2D
29	a	821	CLA	CAD-CBD-CGD-O2D
29	a	826	CLA	CAD-CBD-CGD-O2D
29	a	831	CLA	CAD-CBD-CGD-O2D
29	b	705	CLA	CAD-CBD-CGD-O2D
29	b	718	CLA	CAD-CBD-CGD-O2D
29	h	201	CLA	CAD-CBD-CGD-O2D
29	A	206	CLA	CAD-CBD-CGD-O2D
29	A	208	CLA	CAD-CBD-CGD-O2D
29	G	301	CLA	CAD-CBD-CGD-O2D
29	I	213	CLA	CAD-CBD-CGD-O2D
29	I	214	CLA	CAD-CBD-CGD-O2D
29	F	315	CLA	CAD-CBD-CGD-O2D
29	M	307	CLA	CAD-CBD-CGD-O2D
29	L	308	CLA	CAD-CBD-CGD-O2D
29	B	310	CLA	CAD-CBD-CGD-O2D
29	H	312	CLA	CAD-CBD-CGD-O2D
29	N	311	CLA	CAD-CBD-CGD-O2D
29	Q	313	CLA	CAD-CBD-CGD-O2D
38	P	207	UIX	C25-C28-C32-C33
39	G	315	KC1	CAD-CBD-CGD-O2D
39	O	312	KC1	CAD-CBD-CGD-O2D
39	O	315	KC1	CAD-CBD-CGD-O2D
39	T	312	KC1	CAD-CBD-CGD-O2D
39	P	216	KC1	C2B-C3B-CAB-CBB
29	K	209	CLA	C6-C7-C8-C9
30	a	832	PQN	C15-C16-C17-C18
29	b	721	CLA	C2-C1-O2A-CGA
29	D	313	CLA	C4C-C3C-CAC-CBC
29	b	720	CLA	CAA-CBA-CGA-O2A
29	L	316	CLA	CAA-CBA-CGA-O2A
35	m	102	DGD	C2B-C3B-C4B-C5B
29	a	810	CLA	C4-C3-C5-C6
29	E	311	CLA	C2-C3-C5-C6
29	b	710	CLA	CAA-CBA-CGA-O2A
29	G	313	CLA	CAA-CBA-CGA-O2A
29	K	210	CLA	CAA-CBA-CGA-O2A
29	K	217	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	F	311	CLA	CAA-CBA-CGA-O2A
35	j	103	DGD	O1G-C1A-C2A-C3A
32	l	507	BCR	C11-C12-C13-C14
38	A	203	UIX	C14-C23-C26-C30
36	A	204	DD6	C13-C14-C15-O1
36	G	308	DD6	C13-C14-C15-O1
36	I	205	DD6	C13-C14-C15-O1
36	K	204	DD6	C13-C14-C15-O1
36	K	206	DD6	C13-C14-C15-O1
36	M	303	DD6	C13-C14-C15-O1
36	D	304	DD6	C13-C14-C15-O1
36	B	302	DD6	C13-C14-C15-O1
36	B	305	DD6	C13-C14-C15-O1
36	B	319	DD6	C13-C14-C15-O1
37	D	302	PID	O1-C6-C7-C8
37	O	307	PID	O1-C6-C7-C8
37	C	301	PID	O1-C6-C7-C8
37	P	203	PID	O1-C6-C7-C8
29	a	817	CLA	CAA-CBA-CGA-O2A
29	a	809	CLA	C13-C15-C16-C17
35	b	733	DGD	O2G-C1B-C2B-C3B
29	O	309	CLA	C16-C17-C18-C20
29	a	817	CLA	CAA-CBA-CGA-O1A
29	l	502	CLA	C15-C16-C17-C18
29	E	308	CLA	C10-C11-C12-C13
29	a	837	CLA	O2A-C1-C2-C3
29	b	712	CLA	O2A-C1-C2-C3
29	b	720	CLA	O2A-C1-C2-C3
29	b	726	CLA	O2A-C1-C2-C3
29	G	302	CLA	O2A-C1-C2-C3
29	G	312	CLA	O2A-C1-C2-C3
29	K	210	CLA	O2A-C1-C2-C3
29	B	310	CLA	O2A-C1-C2-C3
29	E	306	CLA	O2A-C1-C2-C3
39	O	315	KC1	C4B-C3B-CAB-CBB
39	T	315	KC1	C4B-C3B-CAB-CBB
39	Q	314	KC1	C4B-C3B-CAB-CBB
39	C	315	KC1	C4B-C3B-CAB-CBB
39	P	216	KC1	C4B-C3B-CAB-CBB
29	Q	310	CLA	C2A-CAA-CBA-CGA
29	h	201	CLA	C8-C10-C11-C12
29	P	210	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	G	302	CLA	CAA-CBA-CGA-O1A
29	b	717	CLA	O1A-CGA-O2A-C1
29	I	214	CLA	C6-C7-C8-C10
29	a	814	CLA	CHA-CBD-CGD-O1D
29	a	815	CLA	CHA-CBD-CGD-O1D
29	a	815	CLA	CHA-CBD-CGD-O2D
29	a	823	CLA	CHA-CBD-CGD-O1D
29	a	823	CLA	CHA-CBD-CGD-O2D
29	a	828	CLA	CHA-CBD-CGD-O2D
29	a	831	CLA	CHA-CBD-CGD-O1D
29	a	837	CLA	CHA-CBD-CGD-O1D
29	a	837	CLA	CHA-CBD-CGD-O2D
29	b	701	CLA	CHA-CBD-CGD-O1D
29	b	701	CLA	CHA-CBD-CGD-O2D
29	b	710	CLA	CHA-CBD-CGD-O1D
29	A	218	CLA	CHA-CBD-CGD-O1D
29	A	218	CLA	CHA-CBD-CGD-O2D
29	G	316	CLA	CHA-CBD-CGD-O2D
29	G	317	CLA	CHA-CBD-CGD-O1D
29	G	317	CLA	CHA-CBD-CGD-O2D
29	K	208	CLA	CHA-CBD-CGD-O1D
29	K	208	CLA	CHA-CBD-CGD-O2D
29	K	214	CLA	CHA-CBD-CGD-O1D
29	K	214	CLA	CHA-CBD-CGD-O2D
29	M	308	CLA	CHA-CBD-CGD-O1D
29	M	308	CLA	CHA-CBD-CGD-O2D
29	L	308	CLA	CHA-CBD-CGD-O1D
29	L	310	CLA	CHA-CBD-CGD-O1D
29	L	311	CLA	CHA-CBD-CGD-O2D
29	L	312	CLA	CHA-CBD-CGD-O2D
29	B	308	CLA	CHA-CBD-CGD-O2D
29	B	309	CLA	CHA-CBD-CGD-O1D
29	B	309	CLA	CHA-CBD-CGD-O2D
29	B	314	CLA	CHA-CBD-CGD-O1D
29	B	314	CLA	CHA-CBD-CGD-O2D
29	N	316	CLA	CHA-CBD-CGD-O2D
29	O	311	CLA	CHA-CBD-CGD-O1D
29	O	316	CLA	CHA-CBD-CGD-O2D
29	T	316	CLA	CHA-CBD-CGD-O1D
29	T	316	CLA	CHA-CBD-CGD-O2D
29	Q	308	CLA	CHA-CBD-CGD-O1D
29	Q	308	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	Q	310	CLA	CHA-CBD-CGD-O1D
29	Q	315	CLA	CHA-CBD-CGD-O1D
29	Q	315	CLA	CHA-CBD-CGD-O2D
29	C	308	CLA	CHA-CBD-CGD-O1D
29	C	308	CLA	CHA-CBD-CGD-O2D
29	C	311	CLA	CHA-CBD-CGD-O2D
29	E	305	CLA	CHA-CBD-CGD-O2D
39	I	215	KC1	CHA-CBD-CGD-O1D
39	K	215	KC1	CHA-CBD-CGD-O2D
39	N	312	KC1	CHA-CBD-CGD-O1D
39	Q	311	KC1	CHA-CBD-CGD-O2D
39	P	211	KC1	CHA-CBD-CGD-O2D
39	P	213	KC1	CHA-CBD-CGD-O1D
39	E	312	KC1	CHA-CBD-CGD-O1D
29	b	701	CLA	C13-C15-C16-C17
29	B	316	CLA	CAA-CBA-CGA-O1A
29	D	311	CLA	CAA-CBA-CGA-O2A
29	a	806	CLA	C2-C3-C5-C6
37	D	307	PID	C19-C20-C21-C22
37	C	305	PID	C19-C20-C21-C22
29	E	306	CLA	C16-C17-C18-C20
29	L	307	CLA	CAA-CBA-CGA-O2A
34	K	201	LMG	C30-C31-C32-C33
34	j	102	LMG	O1-C7-C8-O7
29	I	211	CLA	C13-C15-C16-C17
29	D	311	CLA	O1A-CGA-O2A-C1
29	a	806	CLA	CAA-CBA-CGA-O2A
29	a	831	CLA	CAA-CBA-CGA-O2A
29	b	709	CLA	CAA-CBA-CGA-O2A
29	l	501	CLA	CAA-CBA-CGA-O2A
29	H	310	CLA	CAA-CBA-CGA-O2A
29	a	802	CLA	C2A-CAA-CBA-CGA
29	a	812	CLA	C11-C12-C13-C14
29	b	717	CLA	CAA-CBA-CGA-O2A
29	D	312	CLA	CAA-CBA-CGA-O2A
34	b	730	LMG	C40-C41-C42-C43
35	B	318	DGD	C4B-C5B-C6B-C7B
29	a	806	CLA	C11-C12-C13-C15
29	b	721	CLA	C6-C7-C8-C10
29	l	503	CLA	C11-C10-C8-C7
29	G	316	CLA	C11-C12-C13-C15
29	C	309	CLA	C11-C10-C8-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	a	833	LHG	C24-C25-C26-C27
29	b	707	CLA	C13-C15-C16-C17
34	j	102	LMG	O8-C28-C29-C30
29	a	831	CLA	O1A-CGA-O2A-C1
29	a	811	CLA	C6-C7-C8-C9
29	b	703	CLA	C6-C7-C8-C9
29	l	504	CLA	C6-C7-C8-C9
29	G	316	CLA	C11-C12-C13-C14
29	Q	308	CLA	C14-C13-C15-C16
34	j	102	LMG	O9-C10-C11-C12
37	O	305	PID	C14-C15-C16-C17
29	G	301	CLA	O2A-C1-C2-C3
37	F	302	PID	C15-C16-C17-C18
34	K	201	LMG	C10-C11-C12-C13
40	J	314	SQD	C4-C5-C6-S
29	a	821	CLA	CAA-CBA-CGA-O1A
29	b	703	CLA	CAA-CBA-CGA-O1A
35	b	733	DGD	O1B-C1B-C2B-C3B
29	b	717	CLA	CBA-CGA-O2A-C1
29	K	217	CLA	CAA-CBA-CGA-O1A
29	O	309	CLA	C16-C17-C18-C19
29	A	211	CLA	C4-C3-C5-C6
29	P	212	CLA	CAA-CBA-CGA-O2A
29	b	710	CLA	CAA-CBA-CGA-O1A
34	j	102	LMG	C11-C12-C13-C14
29	a	831	CLA	CBA-CGA-O2A-C1
29	a	831	CLA	C1A-C2A-CAA-CBA
29	b	703	CLA	C1A-C2A-CAA-CBA
29	b	722	CLA	C1A-C2A-CAA-CBA
29	A	215	CLA	C1A-C2A-CAA-CBA
29	A	217	CLA	C1A-C2A-CAA-CBA
29	I	209	CLA	C1A-C2A-CAA-CBA
29	K	212	CLA	C1A-C2A-CAA-CBA
29	F	312	CLA	C1A-C2A-CAA-CBA
29	M	309	CLA	C1A-C2A-CAA-CBA
29	B	308	CLA	C1A-C2A-CAA-CBA
29	H	310	CLA	C1A-C2A-CAA-CBA
29	Q	312	CLA	C1A-C2A-CAA-CBA
29	A	208	CLA	CAA-CBA-CGA-O1A
29	I	209	CLA	CAA-CBA-CGA-O1A
29	L	316	CLA	CAA-CBA-CGA-O1A
34	A	219	LMG	O9-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	j	106	DGD	O1A-C1A-C2A-C3A
34	K	201	LMG	O1-C7-C8-C9
29	C	311	CLA	C2A-CAA-CBA-CGA
29	O	308	CLA	CBD-CGD-O2D-CED
29	I	211	CLA	C16-C17-C18-C19
34	b	732	LMG	C30-C31-C32-C33
40	J	314	SQD	C9-C10-C11-C12
29	H	307	CLA	O1D-CGD-O2D-CED
29	L	309	CLA	CAA-CBA-CGA-O1A
29	D	311	CLA	CAA-CBA-CGA-O1A
34	j	102	LMG	O10-C28-C29-C30
29	G	302	CLA	C8-C10-C11-C12
36	D	301	DD6	C11-C13-C14-C15
37	H	305	PID	C6-C7-C8-C9
37	O	307	PID	C6-C7-C8-C9
37	T	317	PID	C6-C7-C8-C9
35	j	103	DGD	O1A-C1A-C2A-C3A
40	J	314	SQD	C13-C14-C15-C16
29	a	813	CLA	CAA-CBA-CGA-O2A
29	b	719	CLA	CAA-CBA-CGA-O2A
29	B	309	CLA	CAA-CBA-CGA-O2A
34	A	219	LMG	O7-C10-C11-C12
29	B	315	CLA	C4C-C3C-CAC-CBC
29	b	709	CLA	CAA-CBA-CGA-O1A
29	K	210	CLA	CAA-CBA-CGA-O1A
29	G	316	CLA	C8-C10-C11-C12
29	E	305	CLA	C8-C10-C11-C12
29	K	209	CLA	CAA-CBA-CGA-O2A
29	a	807	CLA	C15-C16-C17-C18
29	A	209	CLA	C15-C16-C17-C18
29	a	806	CLA	CAA-CBA-CGA-O1A
29	b	720	CLA	CAA-CBA-CGA-O1A
29	B	308	CLA	O1D-CGD-O2D-CED
29	M	307	CLA	C2-C3-C5-C6
29	a	813	CLA	C2-C3-C5-C6
29	a	814	CLA	CAD-CBD-CGD-O1D
29	a	827	CLA	CAD-CBD-CGD-O1D
29	b	722	CLA	CAD-CBD-CGD-O1D
29	G	304	CLA	CAD-CBD-CGD-O1D
29	G	312	CLA	CAD-CBD-CGD-O1D
29	G	316	CLA	CAD-CBD-CGD-O1D
29	G	319	CLA	CAD-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	K	208	CLA	CAD-CBD-CGD-O1D
29	K	214	CLA	CAD-CBD-CGD-O1D
29	J	306	CLA	CAD-CBD-CGD-O1D
29	M	306	CLA	CAD-CBD-CGD-O1D
29	L	310	CLA	CAD-CBD-CGD-O1D
29	Q	307	CLA	CAD-CBD-CGD-O1D
29	Q	308	CLA	CAD-CBD-CGD-O1D
29	C	308	CLA	CAD-CBD-CGD-O1D
29	P	210	CLA	CAD-CBD-CGD-O1D
29	P	217	CLA	CAD-CBD-CGD-O1D
29	E	315	CLA	CAD-CBD-CGD-O1D
34	A	219	LMG	C9-C8-O7-C10
38	P	207	UIX	C25-C28-C32-C35
39	Q	309	KC1	CAD-CBD-CGD-O1D
40	J	314	SQD	O5-C5-C6-S
29	b	715	CLA	CBD-CGD-O2D-CED
29	G	313	CLA	CAA-CBA-CGA-O1A
29	F	311	CLA	CAA-CBA-CGA-O1A
29	D	312	CLA	CAA-CBA-CGA-O1A
29	N	311	CLA	CAA-CBA-CGA-O2A
34	K	219	LMG	O8-C28-C29-C30
29	a	806	CLA	C11-C12-C13-C14
29	a	807	CLA	C14-C13-C15-C16
29	b	702	CLA	C6-C7-C8-C9
29	b	712	CLA	C11-C10-C8-C9
29	b	720	CLA	C6-C7-C8-C9
29	i	201	CLA	C14-C13-C15-C16
29	b	715	CLA	O1D-CGD-O2D-CED
29	K	218	CLA	CAA-CBA-CGA-O2A
29	H	310	CLA	CAA-CBA-CGA-O1A
29	l	503	CLA	CAA-CBA-CGA-O2A
29	H	312	CLA	CAA-CBA-CGA-O2A
39	L	314	KC1	CAA-CBA-CGA-O2A
29	M	308	CLA	CAA-CBA-CGA-O2A
29	B	309	CLA	C5-C6-C7-C8
29	a	831	CLA	CAA-CBA-CGA-O1A
29	l	501	CLA	CAA-CBA-CGA-O1A
29	L	307	CLA	CAA-CBA-CGA-O1A
29	P	212	CLA	CAA-CBA-CGA-O1A
29	Q	308	CLA	C16-C17-C18-C20
29	a	803	CLA	C11-C10-C8-C7
29	a	822	CLA	C12-C13-C15-C16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
29	a	823	CLA	C11-C10-C8-C7
29	a	824	CLA	C6-C7-C8-C10
29	a	831	CLA	C11-C12-C13-C15
29	b	705	CLA	C12-C13-C15-C16
29	b	726	CLA	C11-C12-C13-C15
29	i	201	CLA	C12-C13-C15-C16
29	G	304	CLA	C11-C10-C8-C7
29	G	317	CLA	C2-C3-C5-C6
29	I	213	CLA	C11-C12-C13-C15
35	m	102	DGD	C1B-C2B-C3B-C4B
29	a	810	CLA	CAA-CBA-CGA-O1A
29	a	809	CLA	CAA-CBA-CGA-O2A
29	a	810	CLA	CAA-CBA-CGA-O2A
29	a	812	CLA	CAA-CBA-CGA-O2A
29	a	827	CLA	CAA-CBA-CGA-O2A
29	i	201	CLA	CAA-CBA-CGA-O2A
29	A	209	CLA	CAA-CBA-CGA-O2A
29	L	310	CLA	CAA-CBA-CGA-O2A
29	N	308	CLA	CAA-CBA-CGA-O2A
29	P	209	CLA	CAA-CBA-CGA-O2A
29	E	305	CLA	CAA-CBA-CGA-O2A
32	b	728	BCR	C7-C8-C9-C10
32	b	729	BCR	C21-C22-C23-C24
38	Q	305	UIX	C7-C10-C11-C13
29	L	310	CLA	CAA-CBA-CGA-O1A
36	M	302	DD6	C3-C4-C5-C6
38	N	306	UIX	C32-C35-C36-C38
29	b	708	CLA	CAA-CBA-CGA-O2A
29	N	313	CLA	CAA-CBA-CGA-O2A
29	T	311	CLA	CAA-CBA-CGA-O2A
29	Q	308	CLA	CAA-CBA-CGA-O2A
29	C	311	CLA	CAA-CBA-CGA-O2A
34	j	102	LMG	O6-C1-O1-C7
29	A	214	CLA	O1D-CGD-O2D-CED
29	N	309	CLA	C2C-C3C-CAC-CBC
29	a	813	CLA	CAA-CBA-CGA-O1A
29	a	827	CLA	CAA-CBA-CGA-O1A
29	i	201	CLA	CAA-CBA-CGA-O1A
29	N	311	CLA	CAA-CBA-CGA-O1A
29	P	209	CLA	CAA-CBA-CGA-O1A
29	f	805	CLA	C8-C10-C11-C12
29	b	702	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

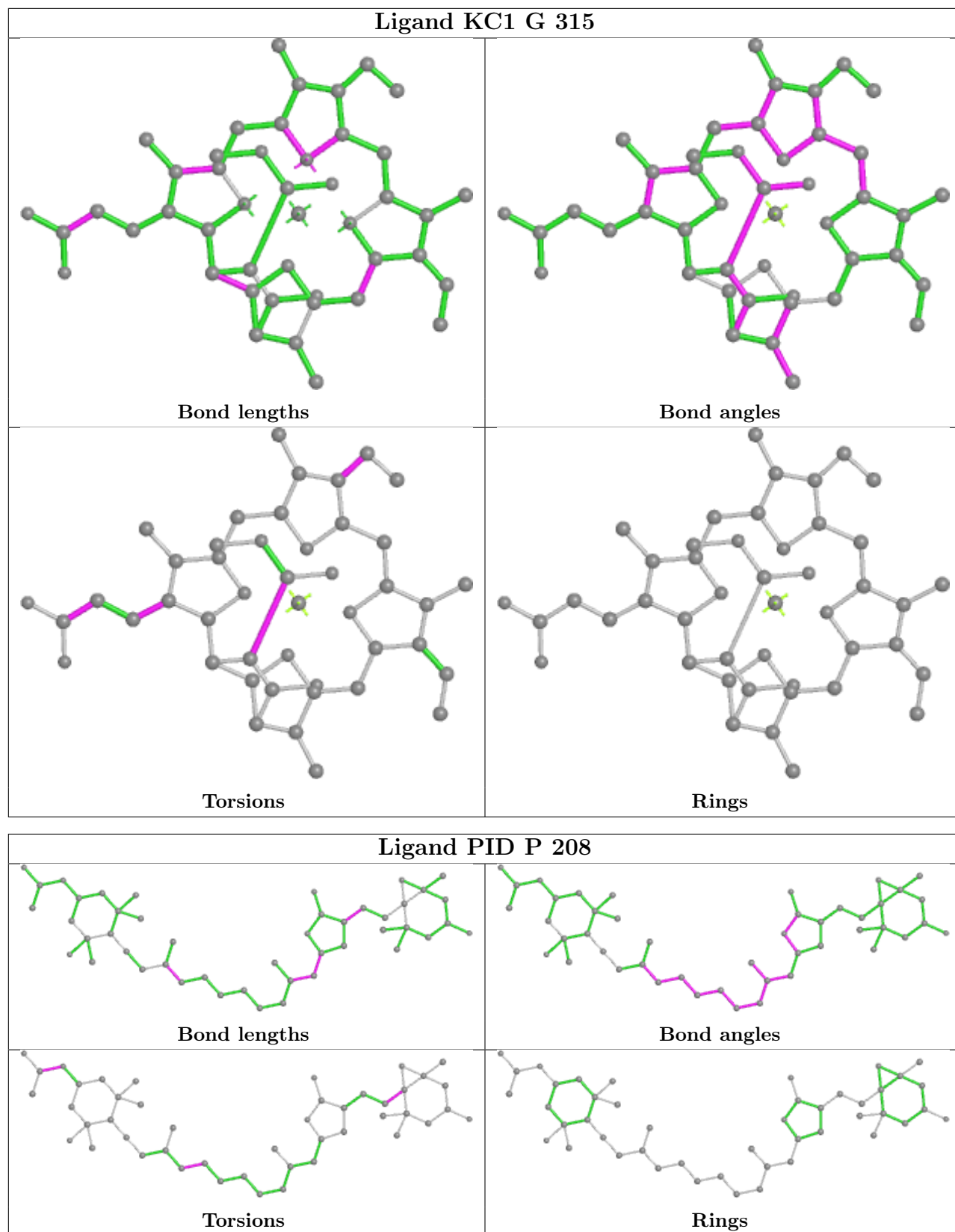
Mol	Chain	Res	Type	Atoms
29	A	218	CLA	CAA-CBA-CGA-O2A
29	K	211	CLA	CAA-CBA-CGA-O2A
29	a	809	CLA	CAA-CBA-CGA-O1A
29	a	824	CLA	C2A-CAA-CBA-CGA
29	b	709	CLA	C2A-CAA-CBA-CGA
29	Q	308	CLA	C2A-CAA-CBA-CGA
39	A	213	KC1	C4C-C3C-CAC-CBC
29	M	308	CLA	CAA-CBA-CGA-O1A
29	K	218	CLA	CAA-CBA-CGA-O1A

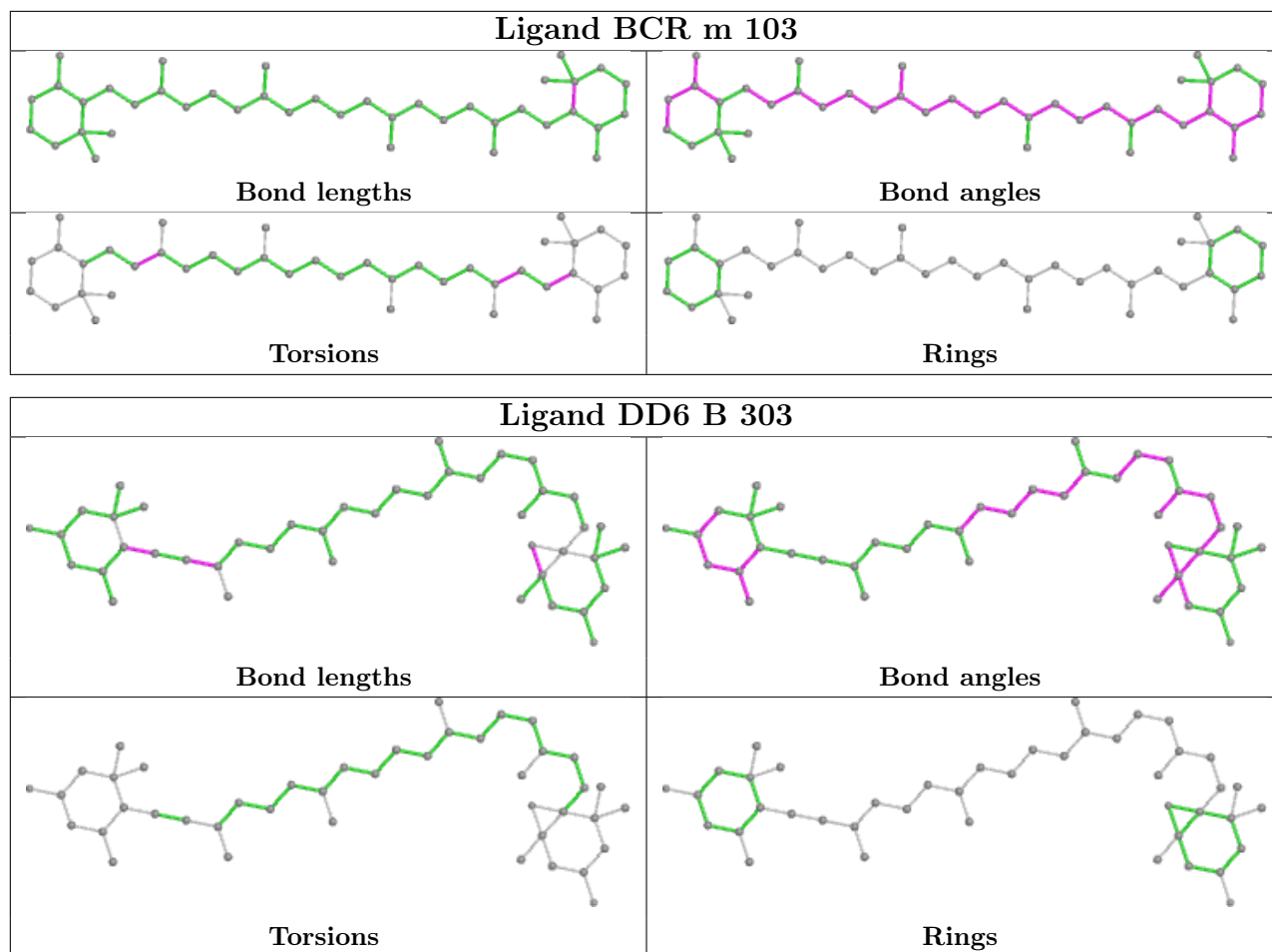
All (3) ring outliers are listed below:

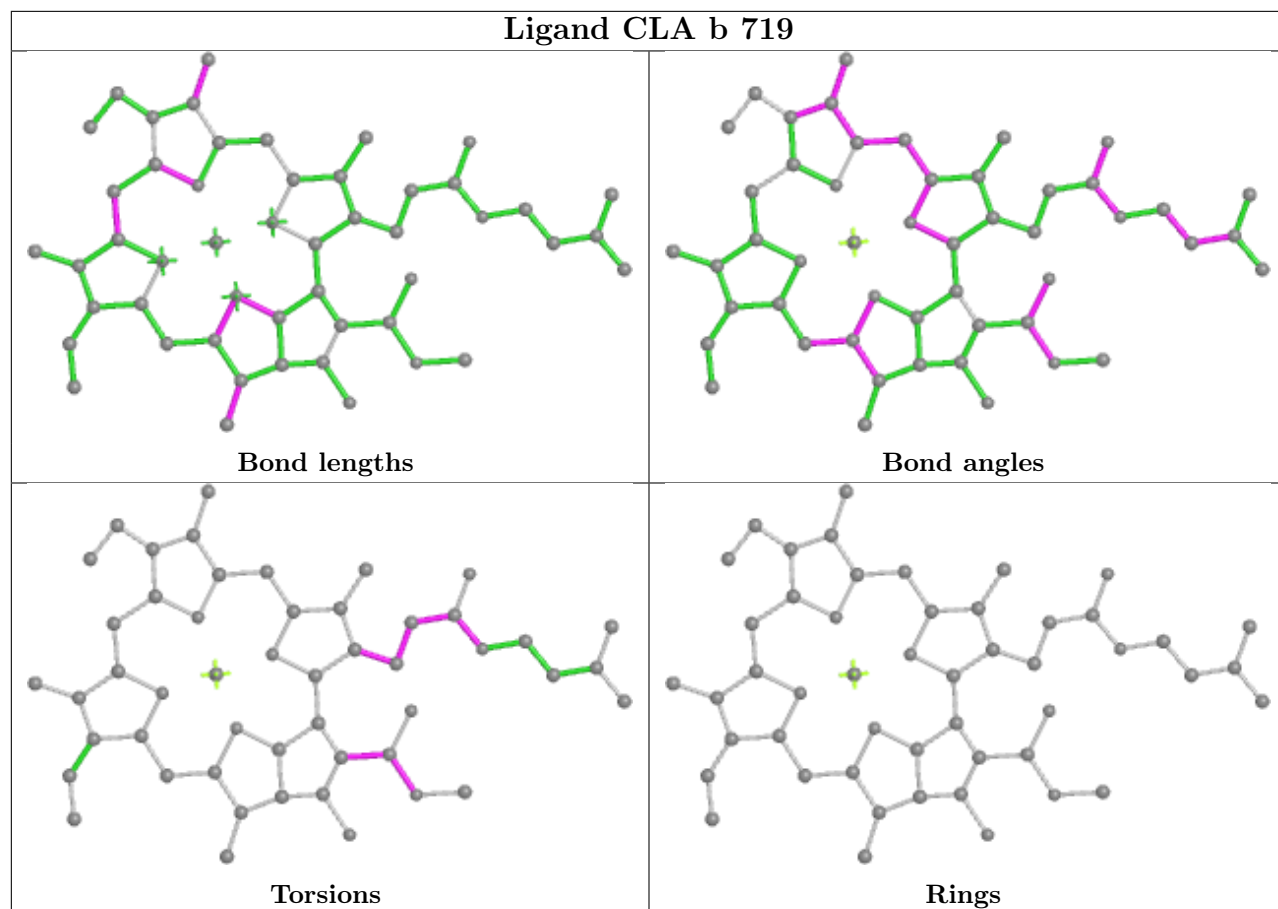
Mol	Chain	Res	Type	Atoms
37	h	204	PID	C24-C25-C26-C27-C28-C29
37	T	317	PID	C24-C25-C26-C27-C28-C29
37	F	304	PID	C24-C25-C26-C27-C28-C29

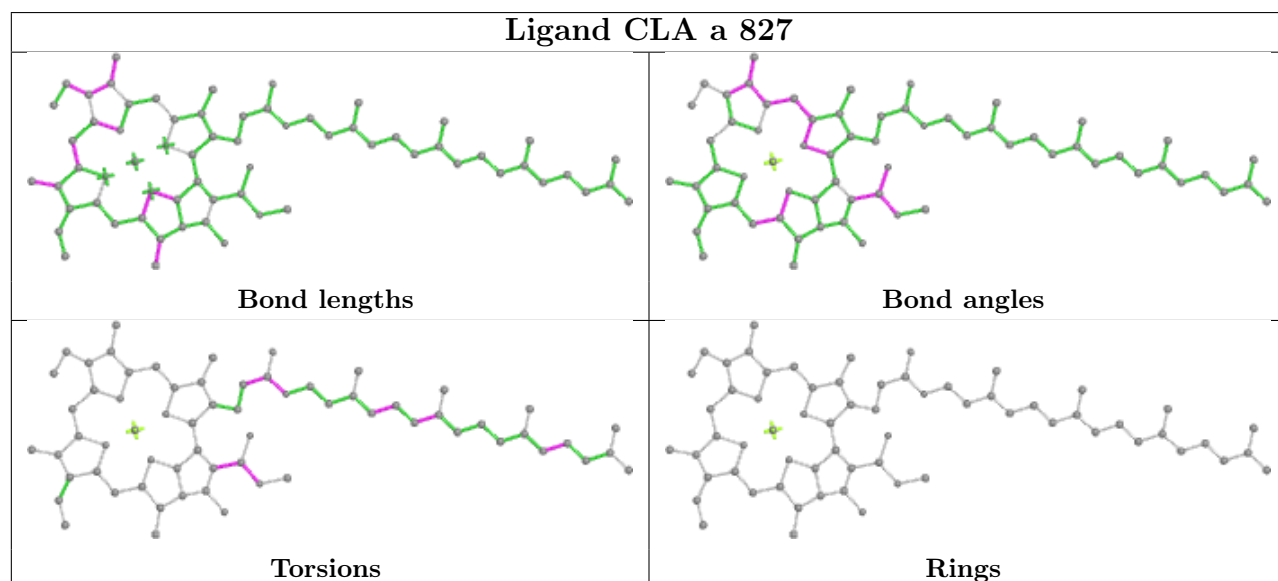
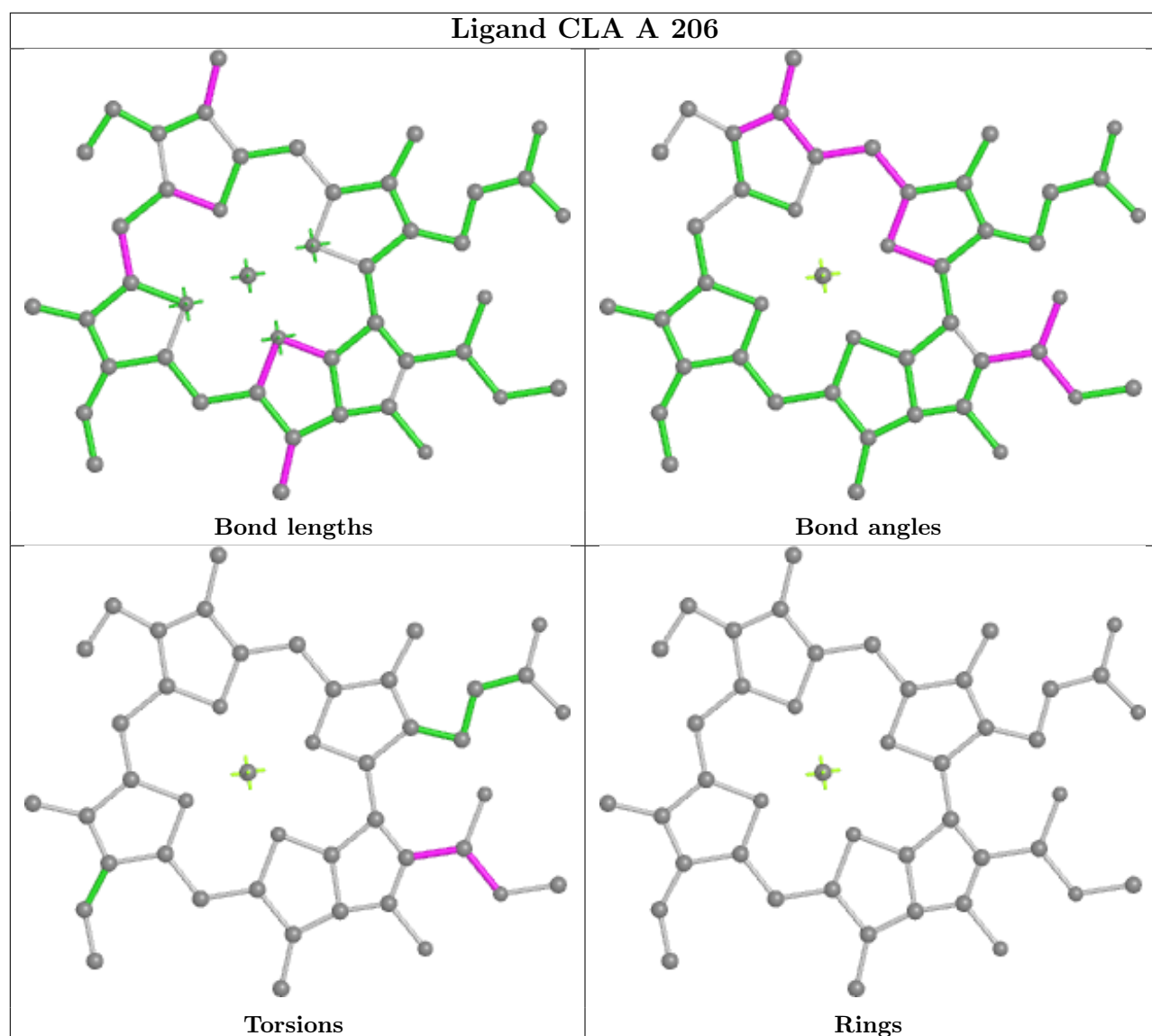
No monomer is involved in short contacts.

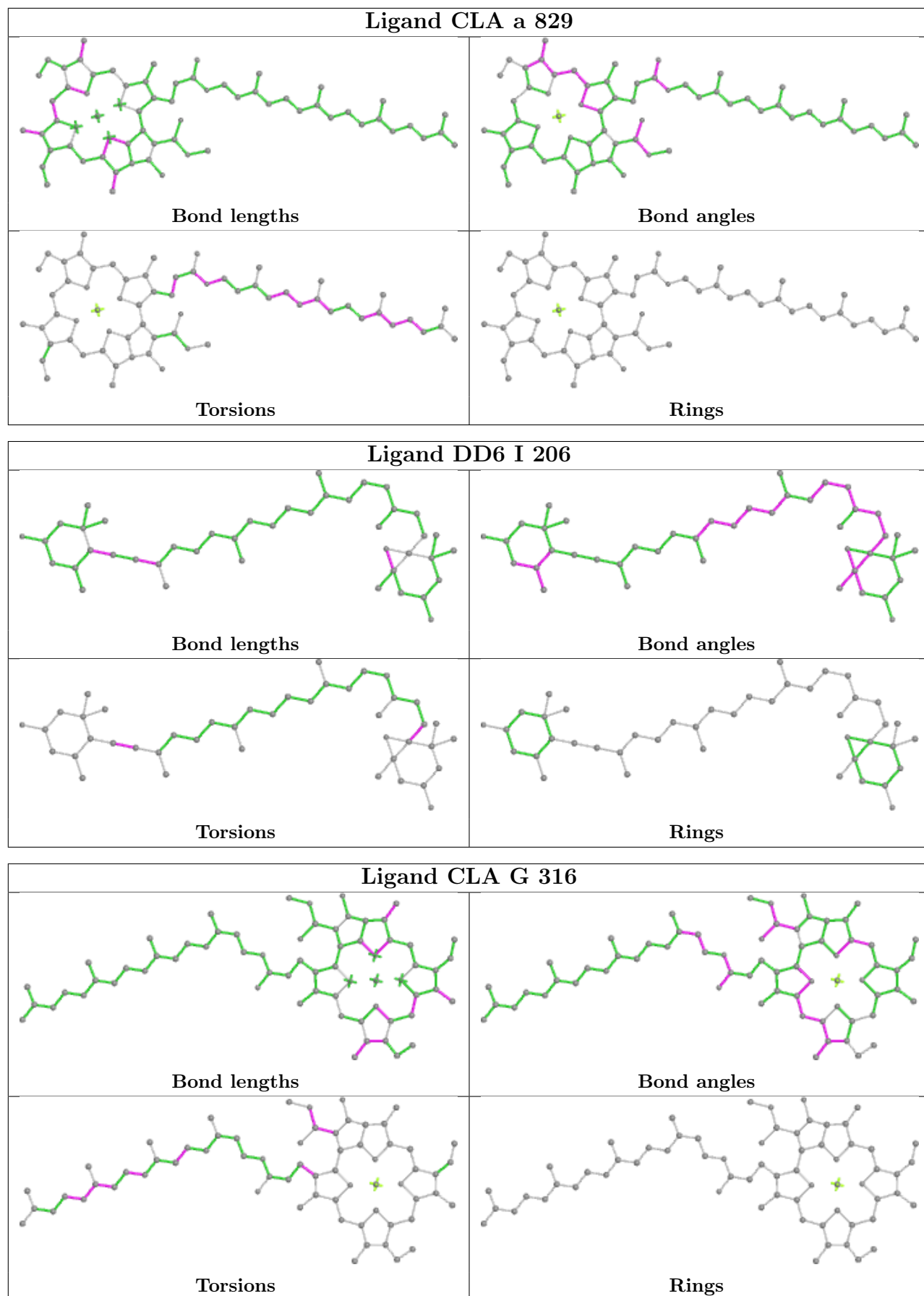
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

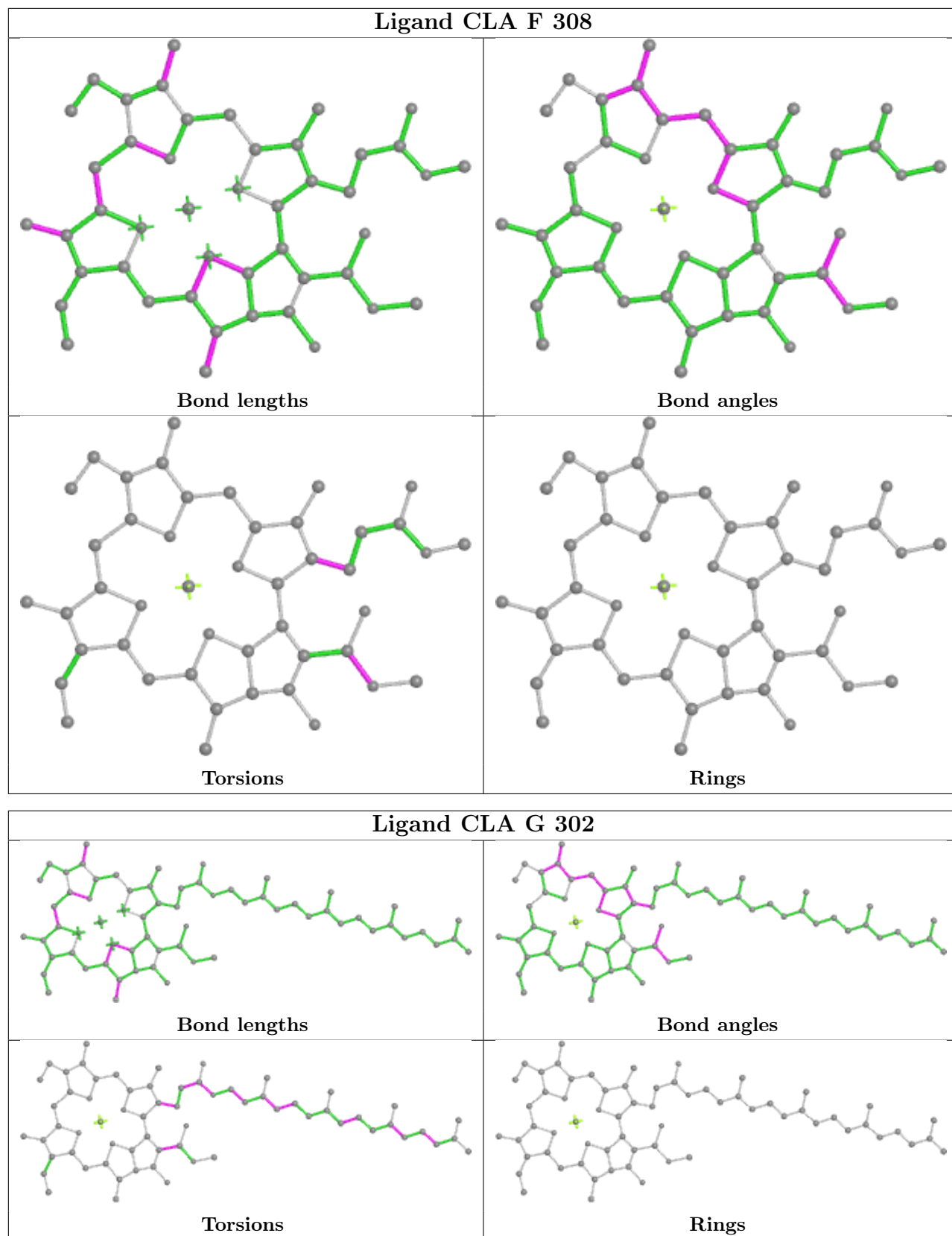




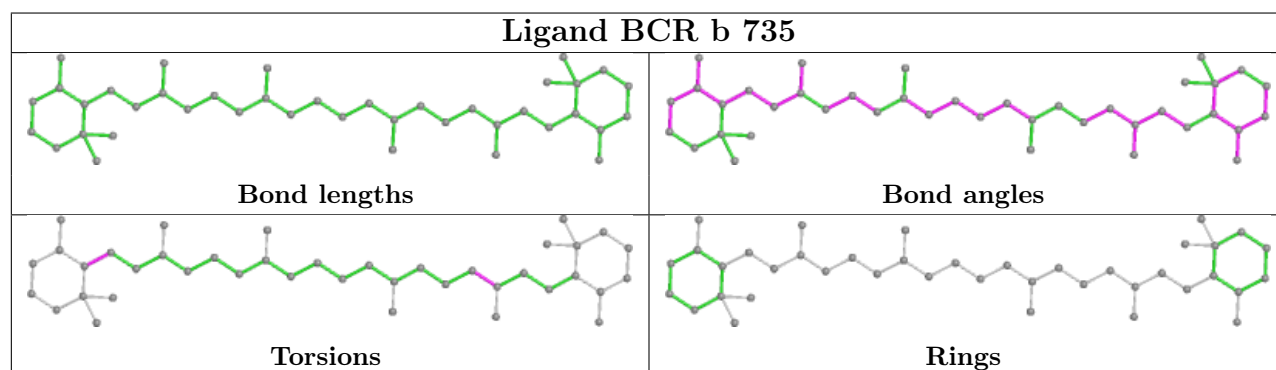
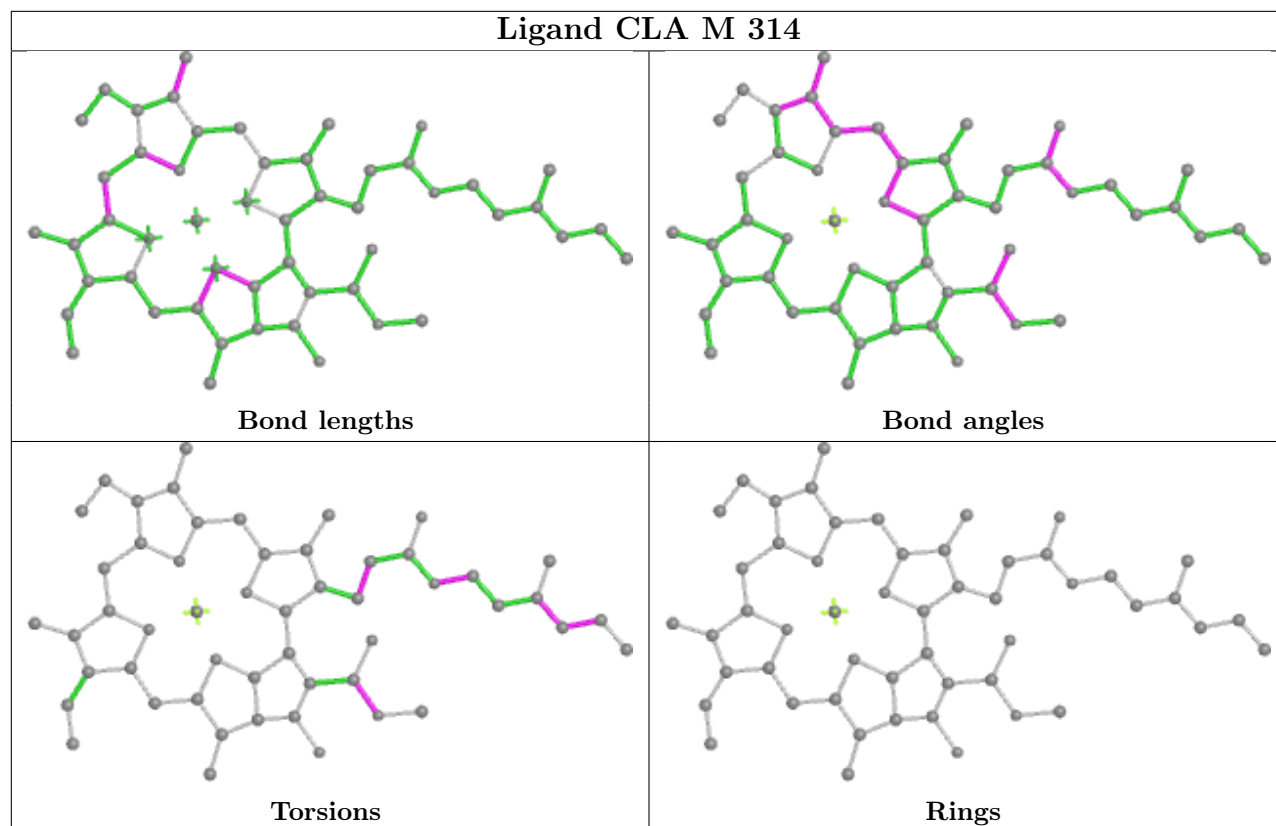
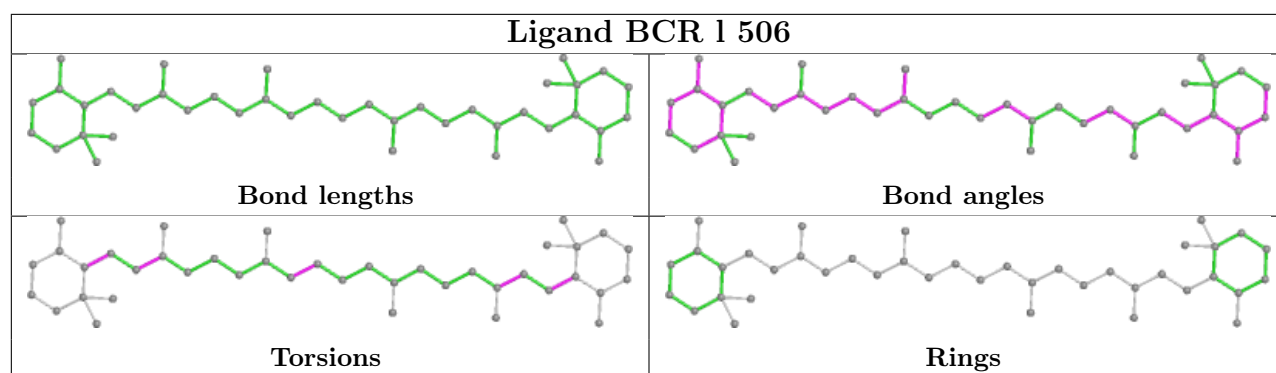


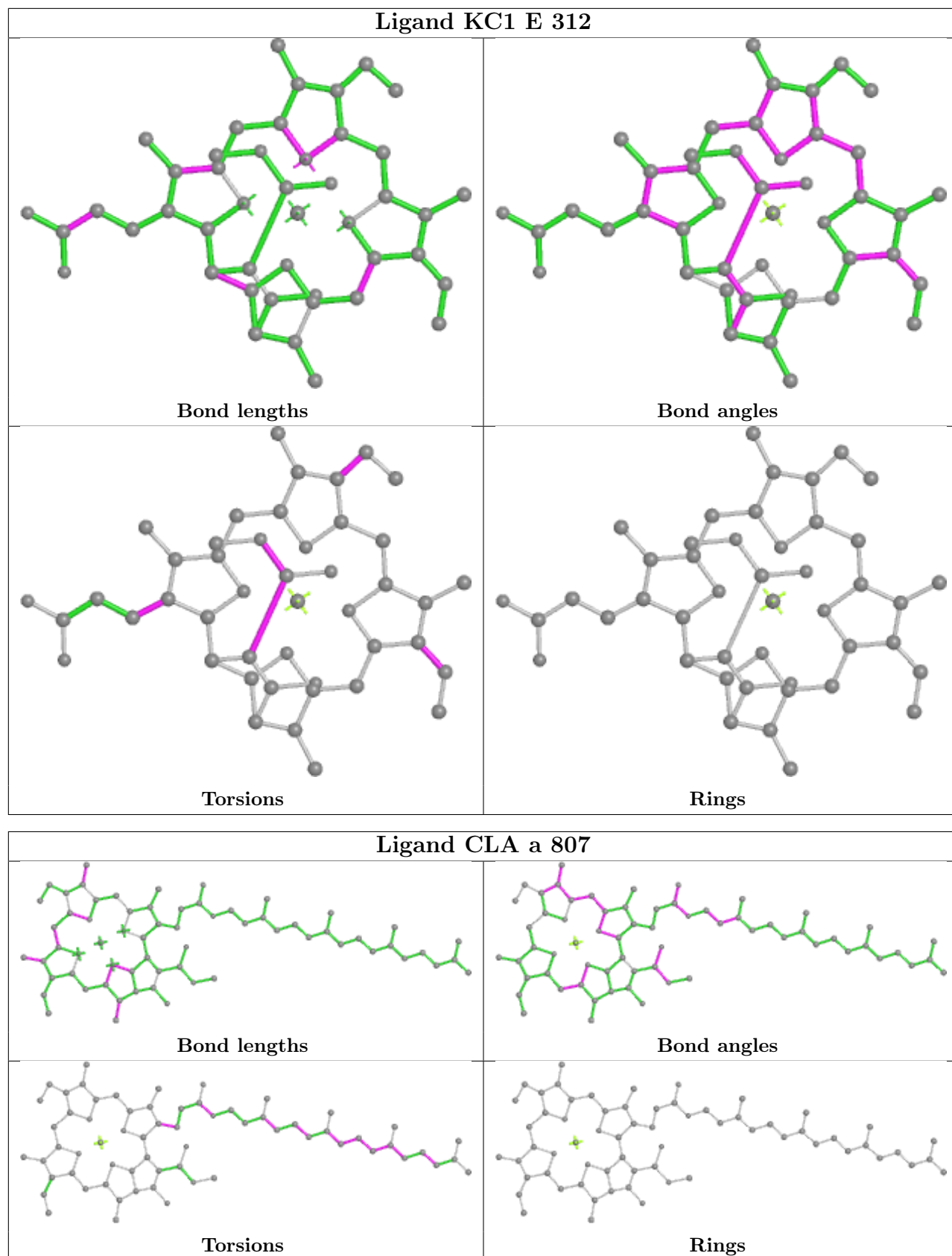


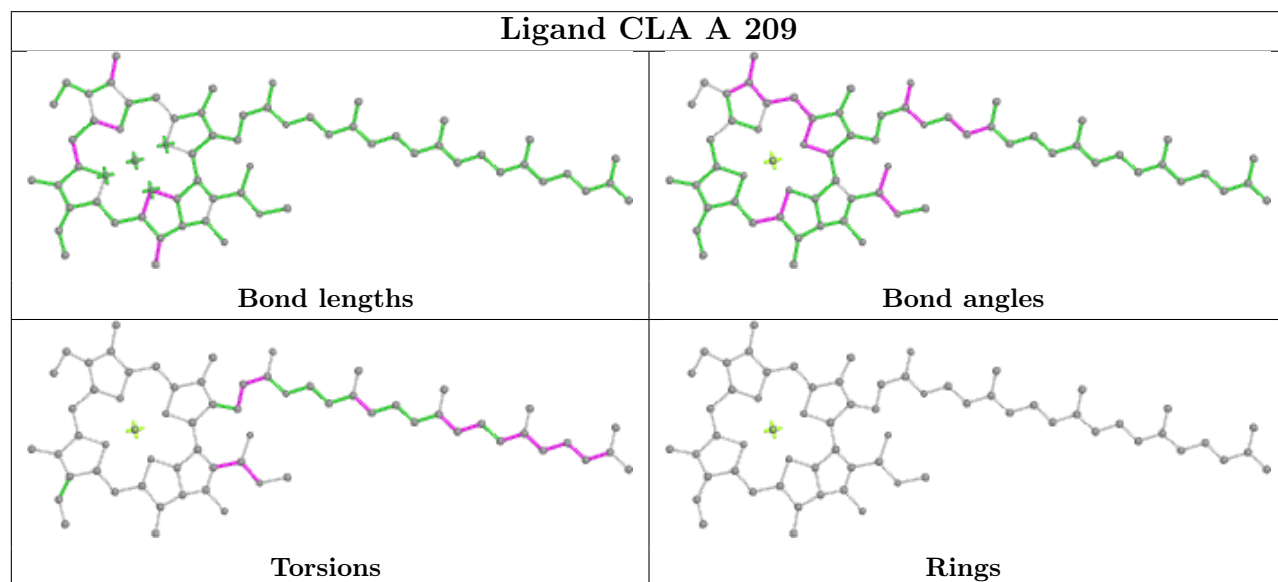
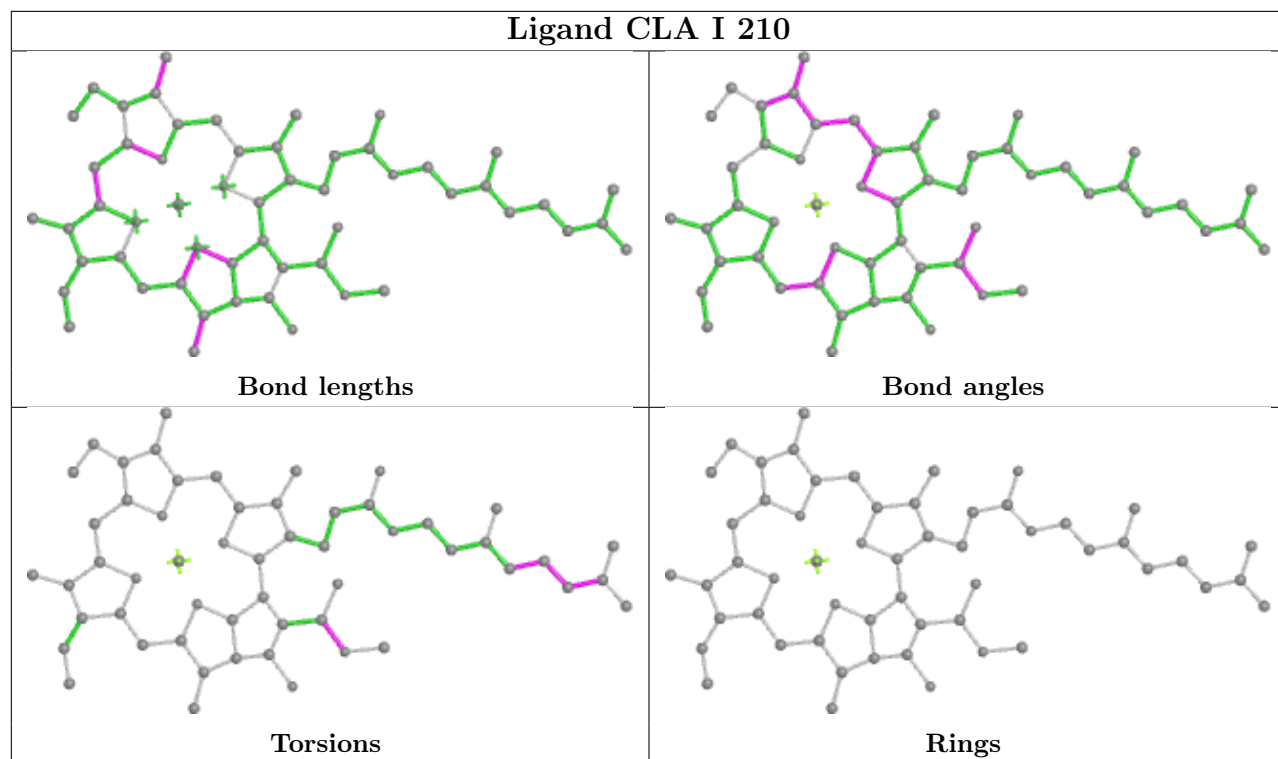


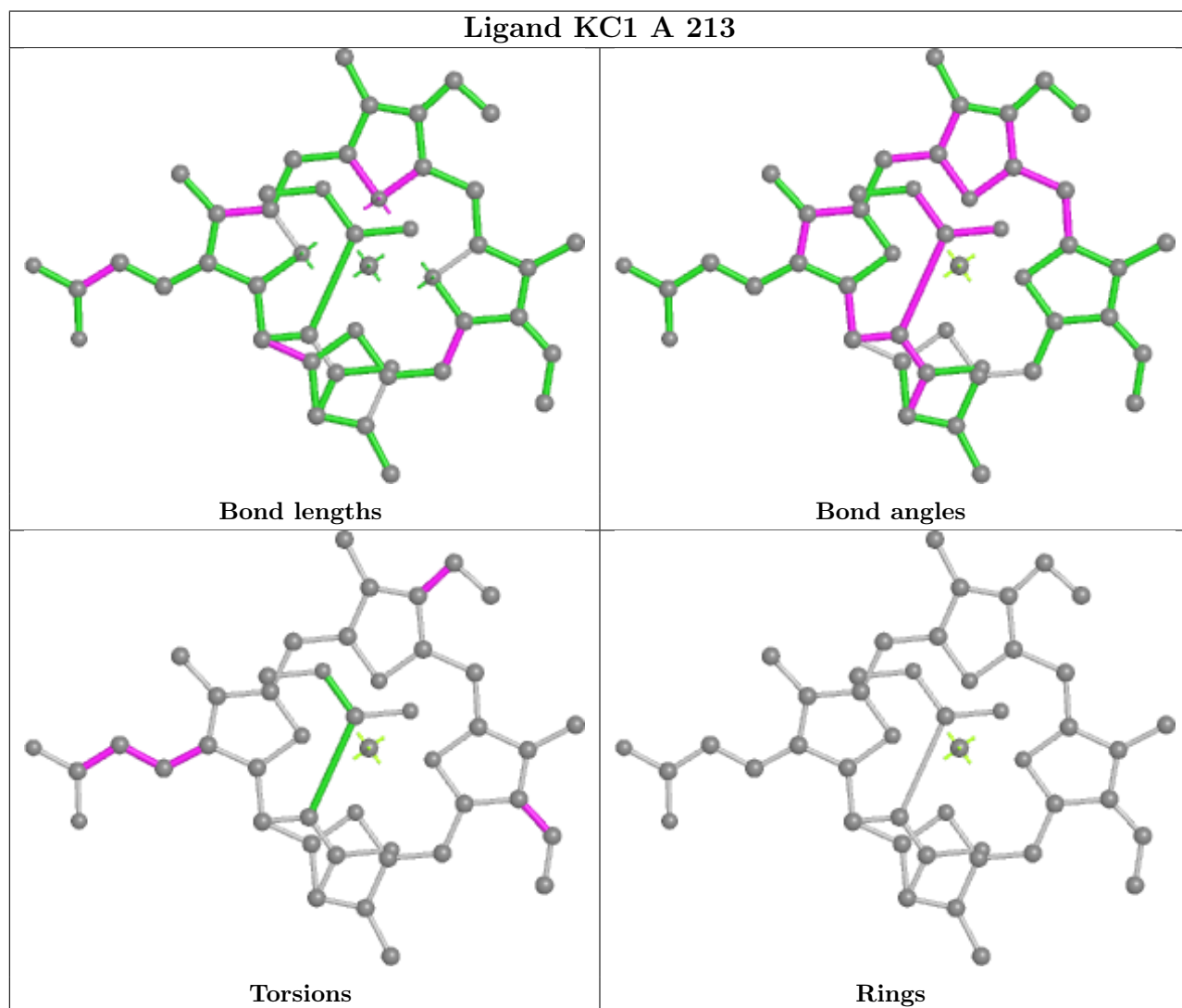
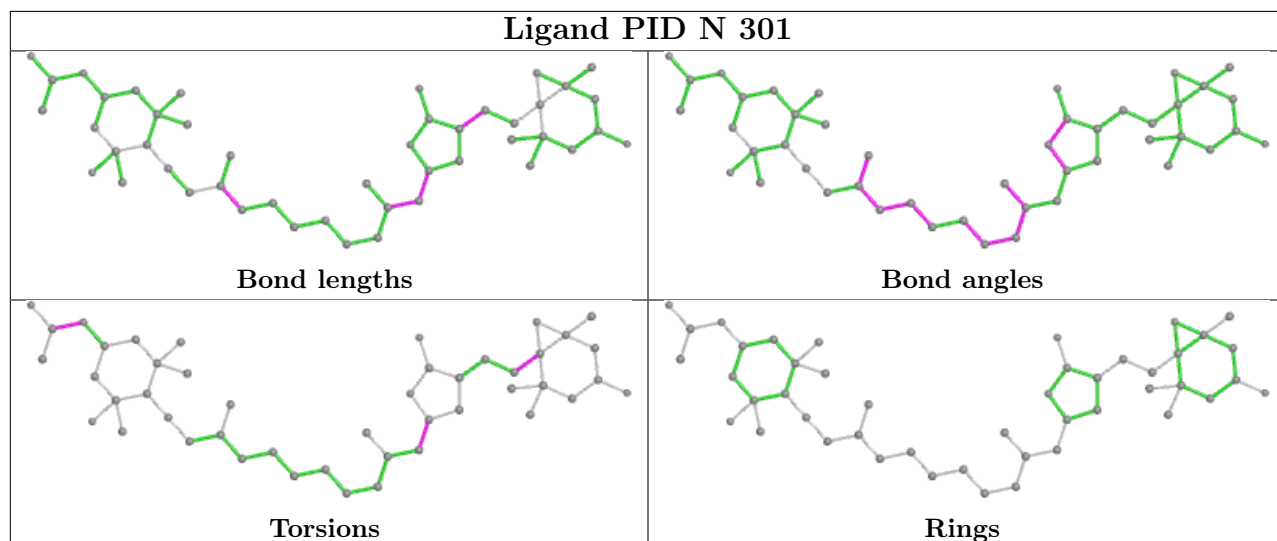


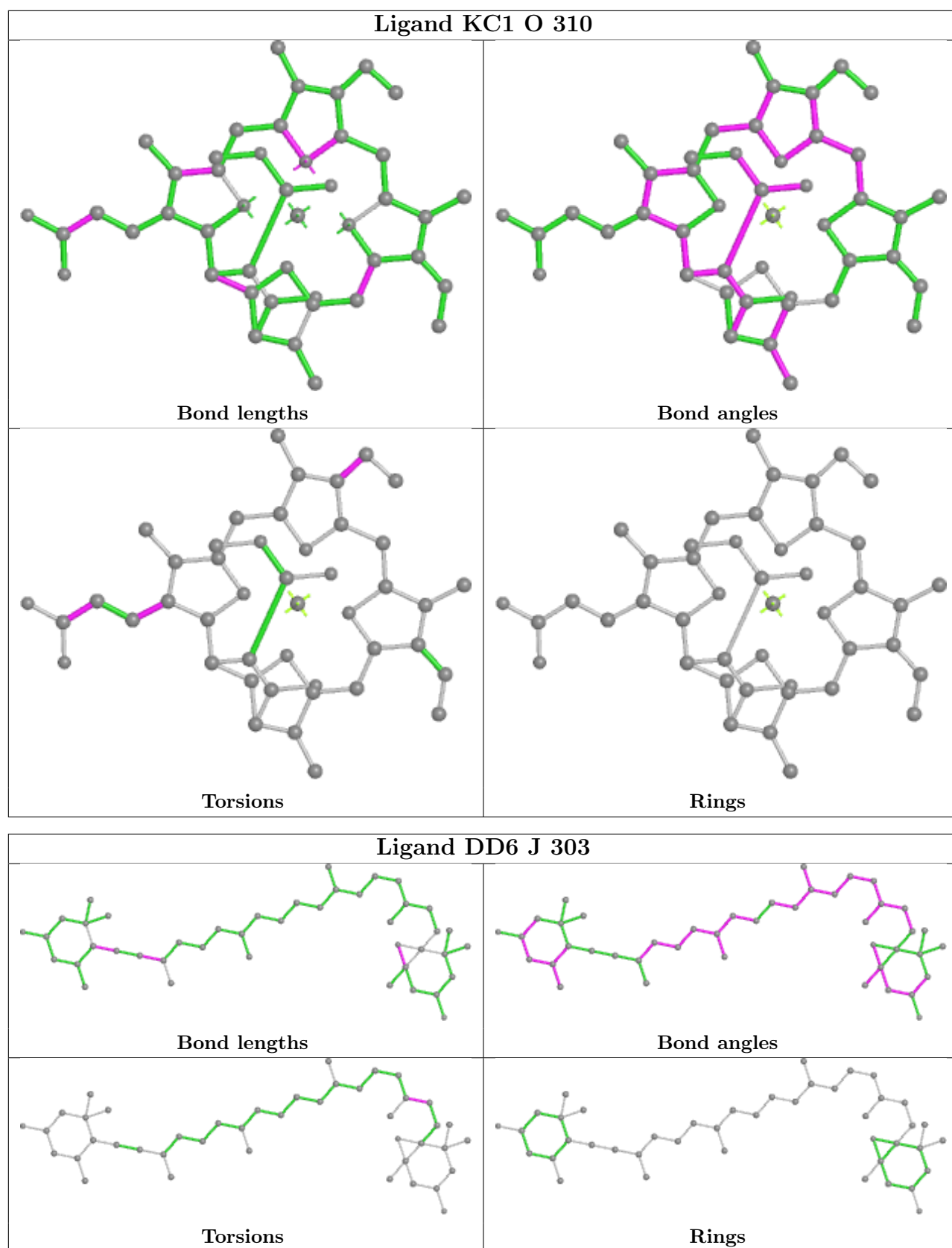


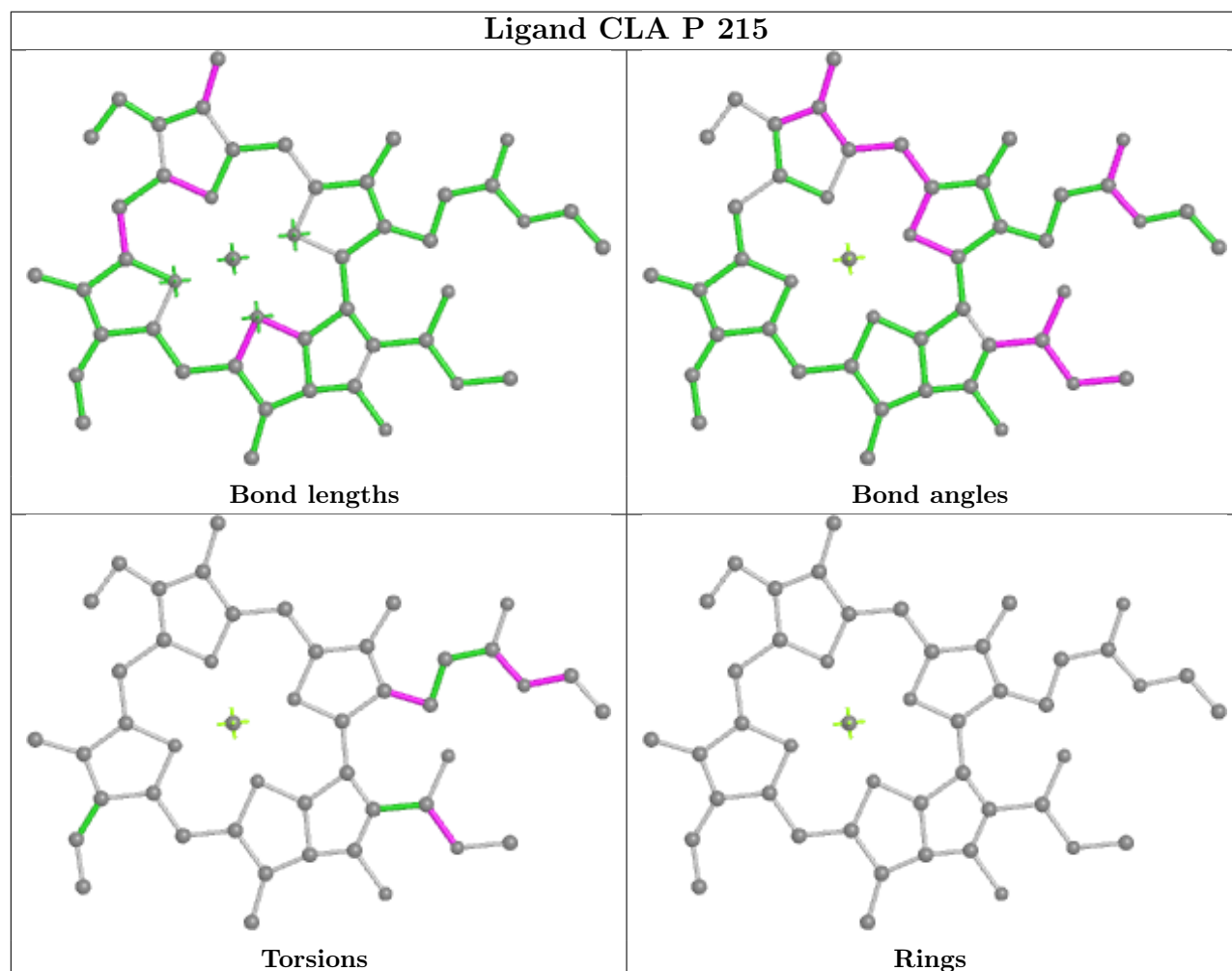
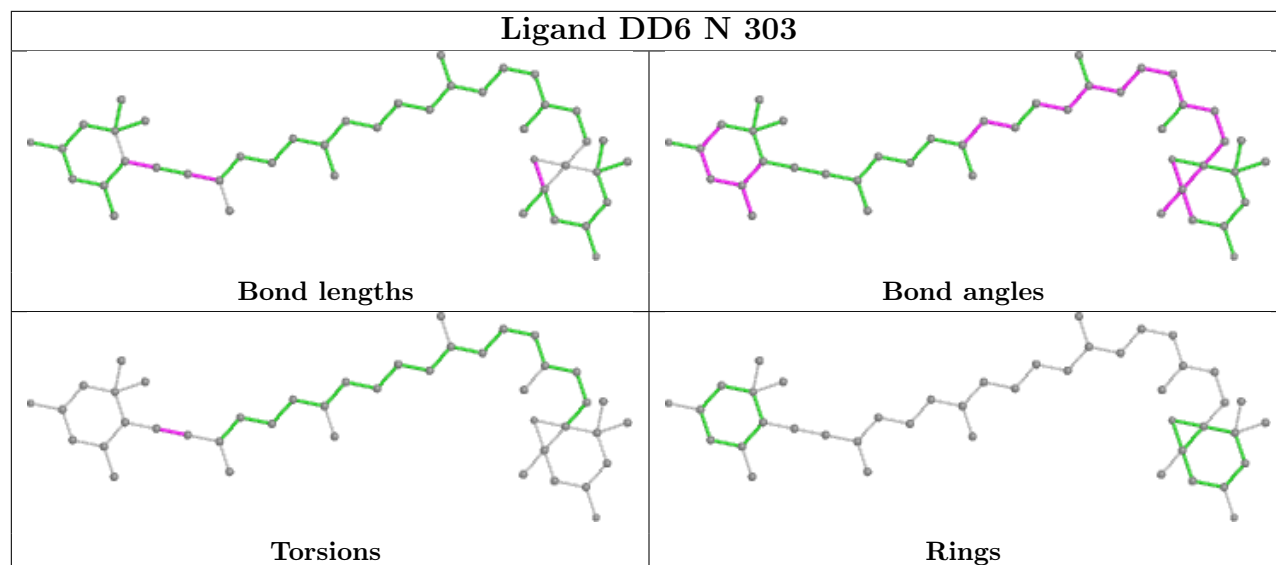


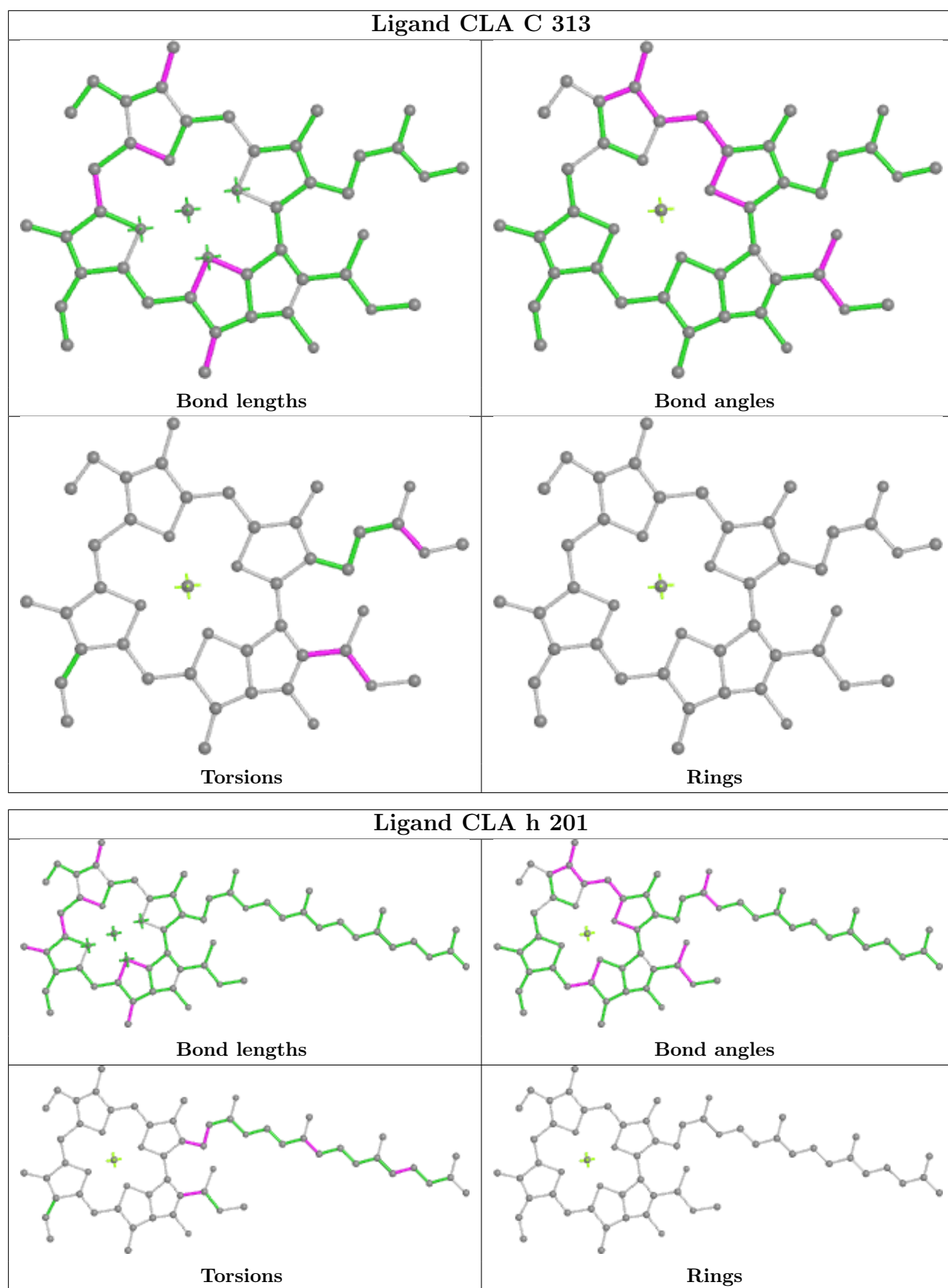


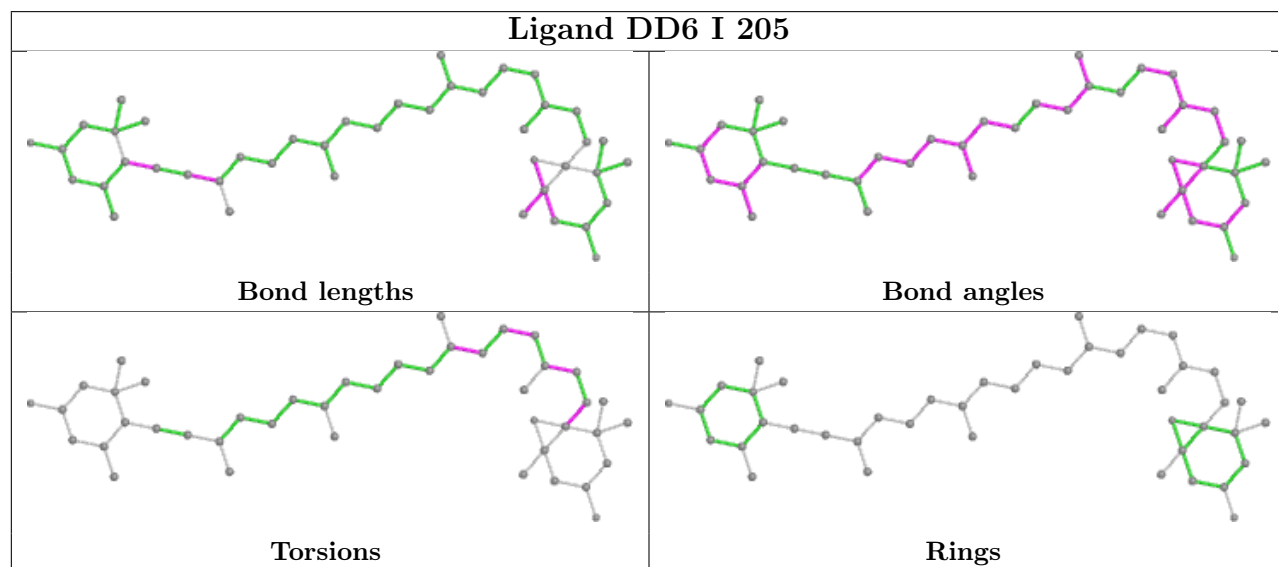
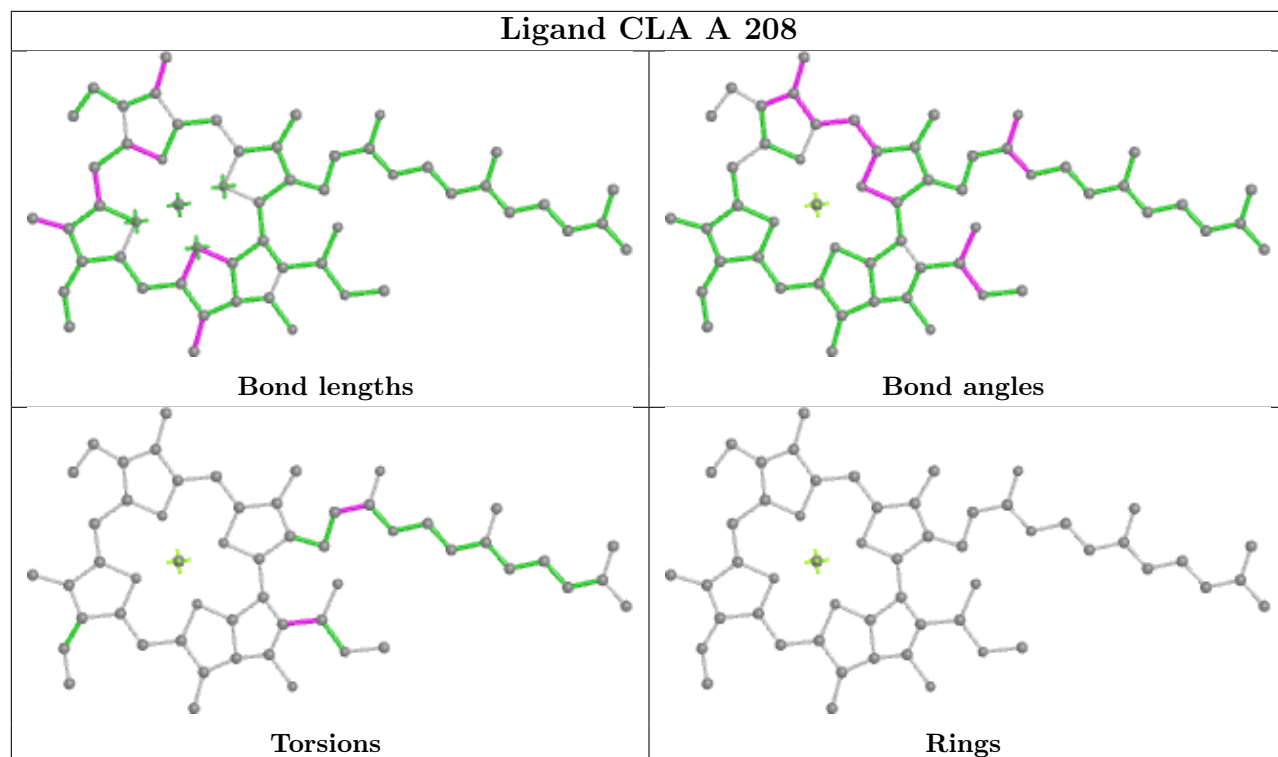




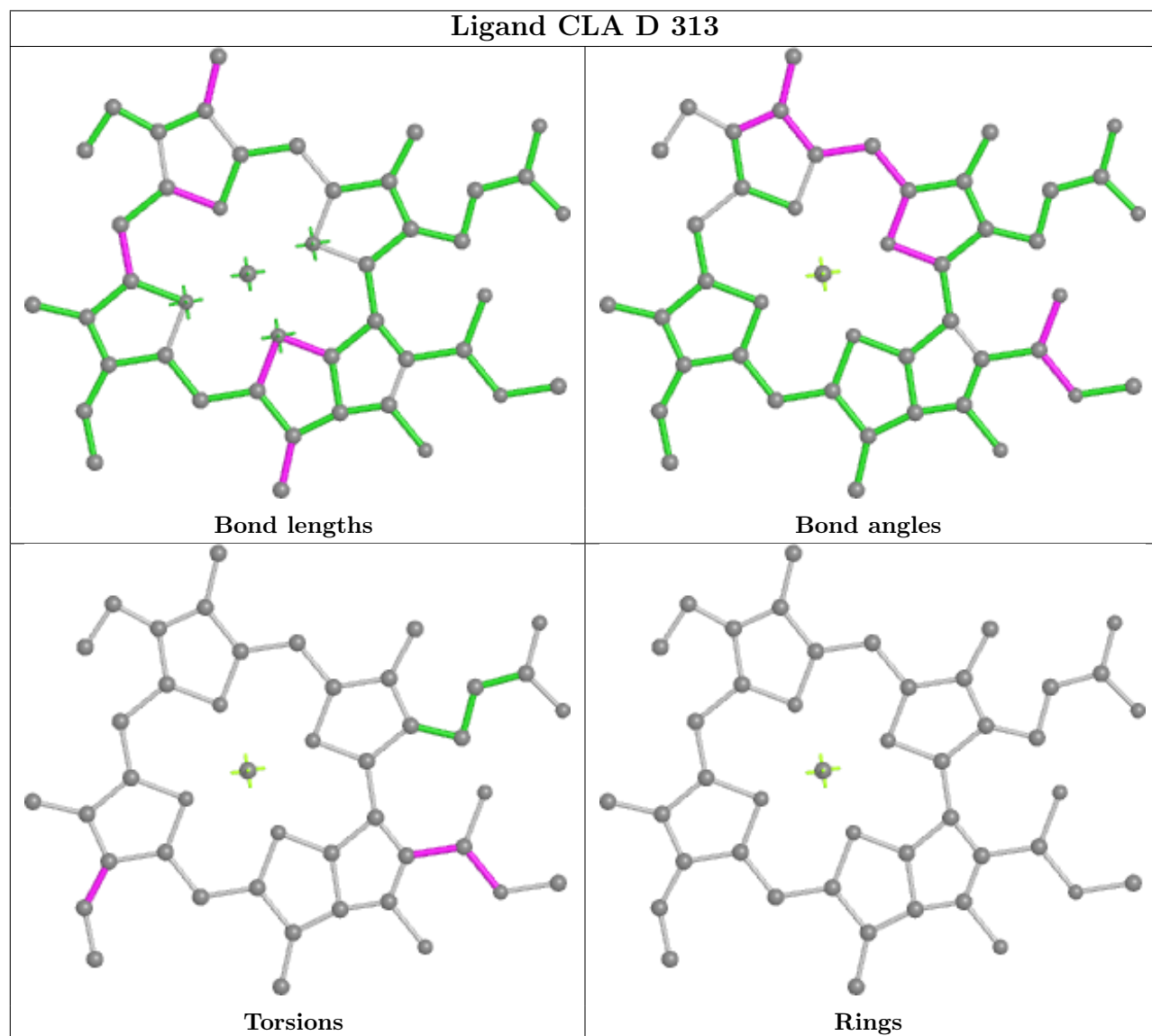
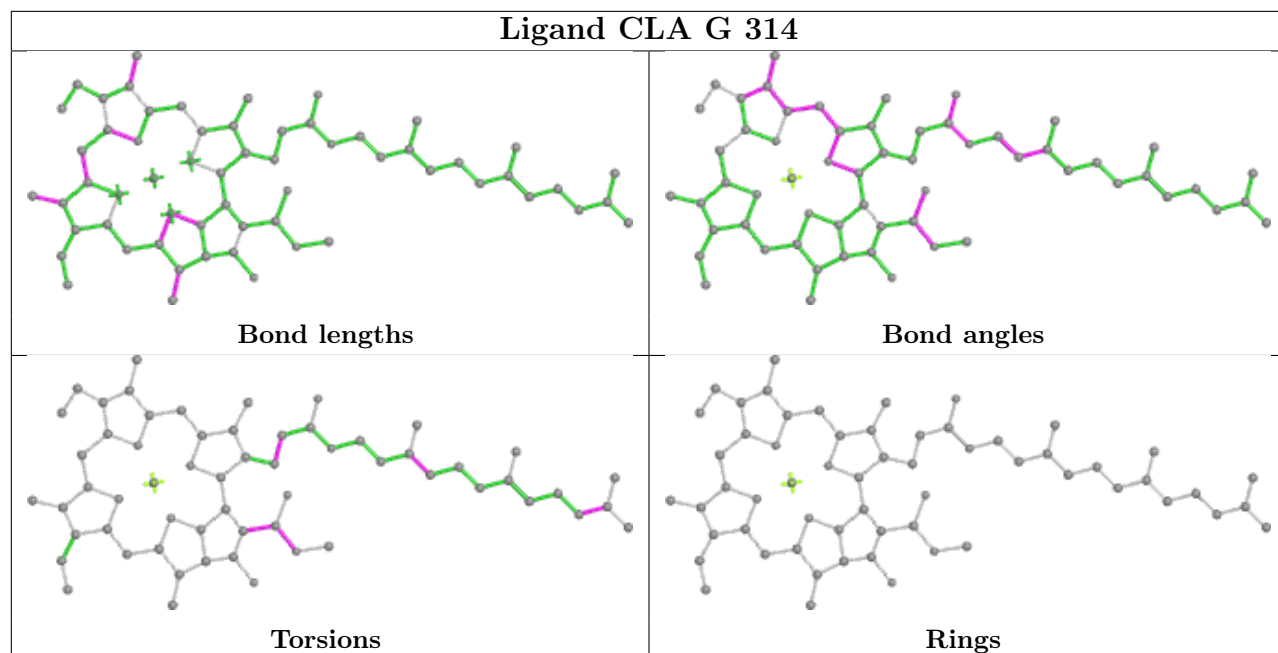


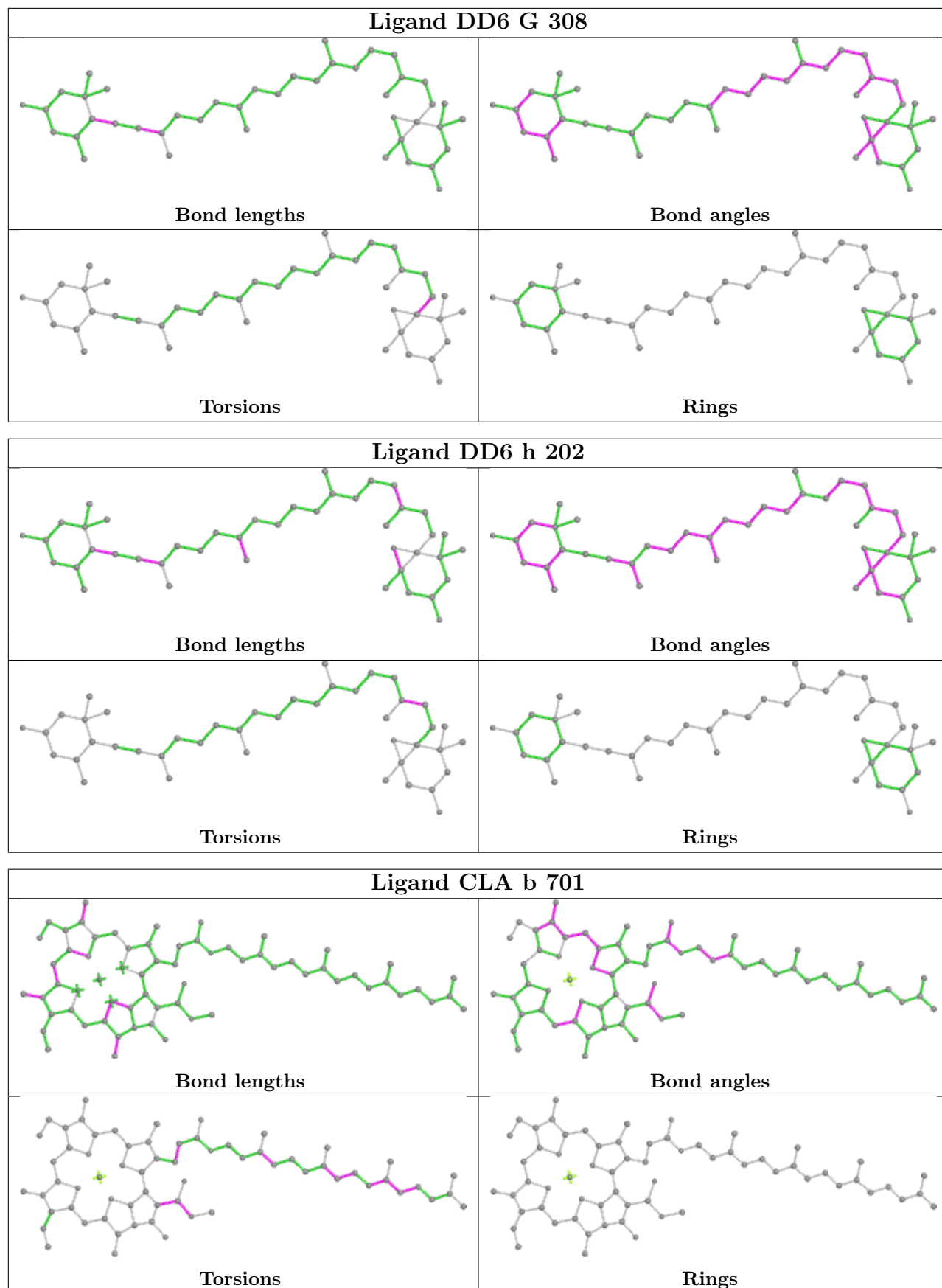


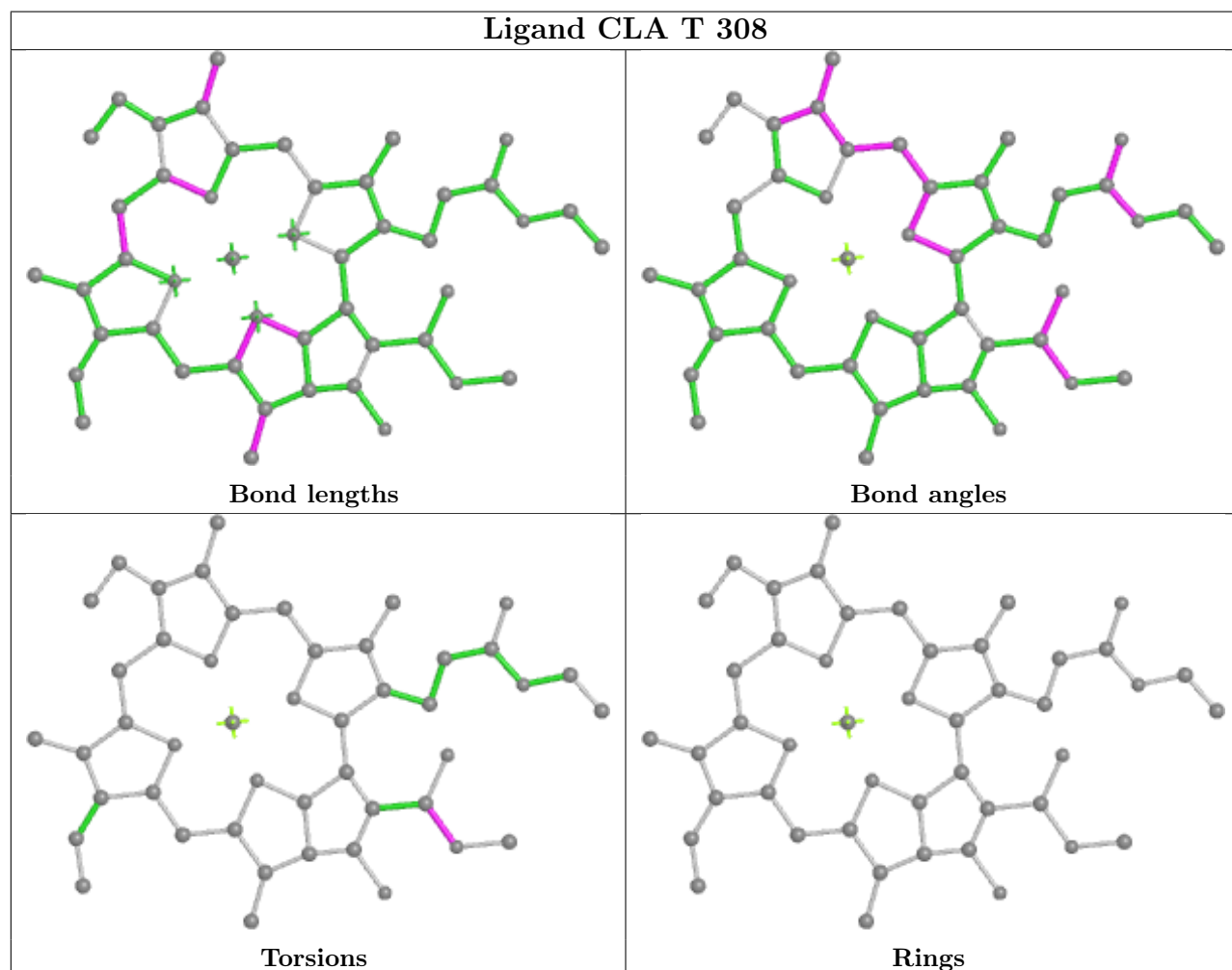
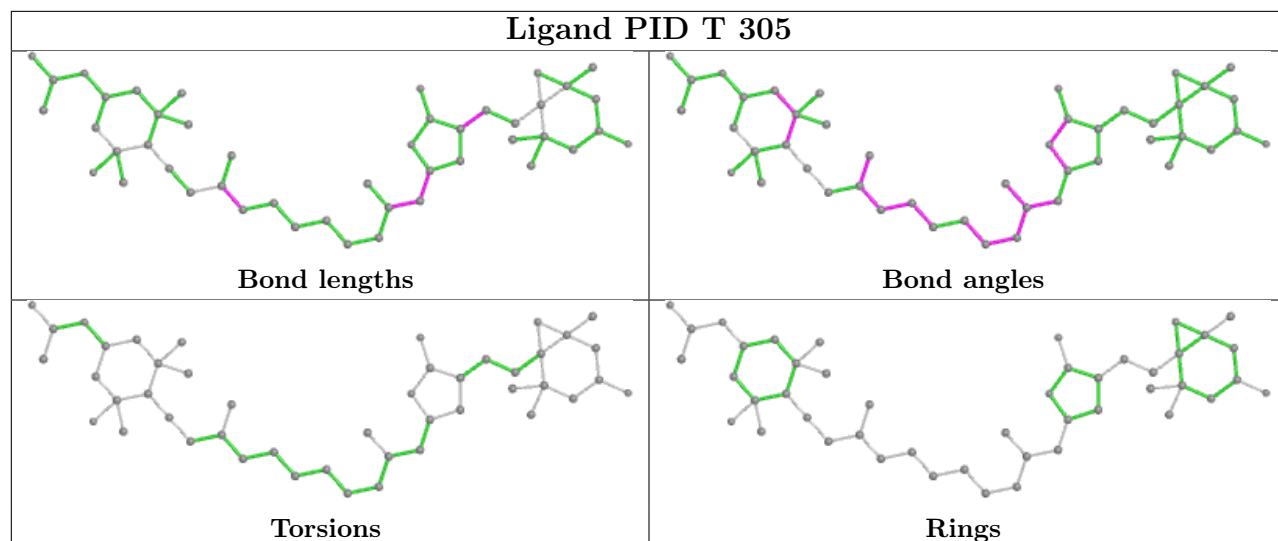


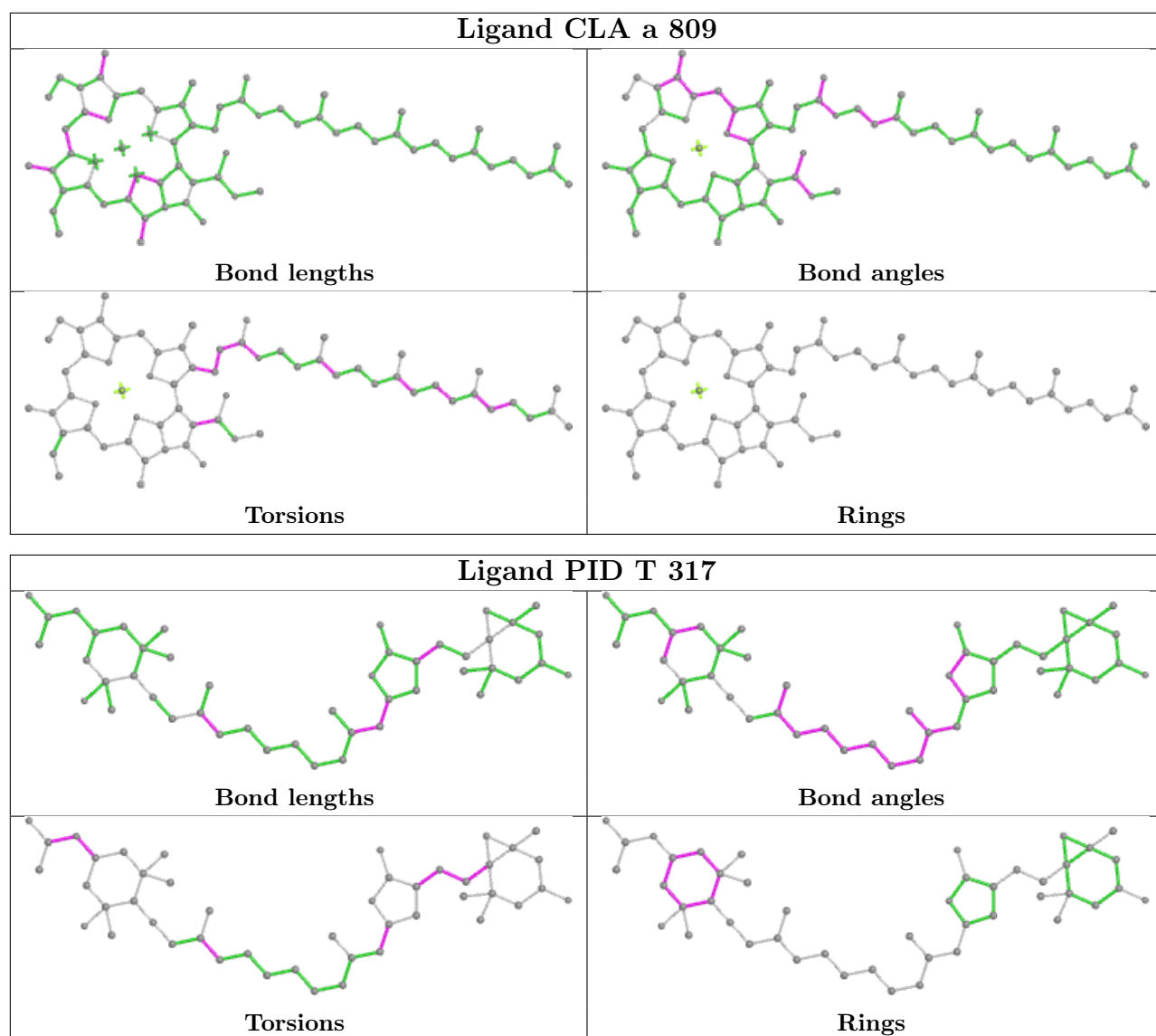


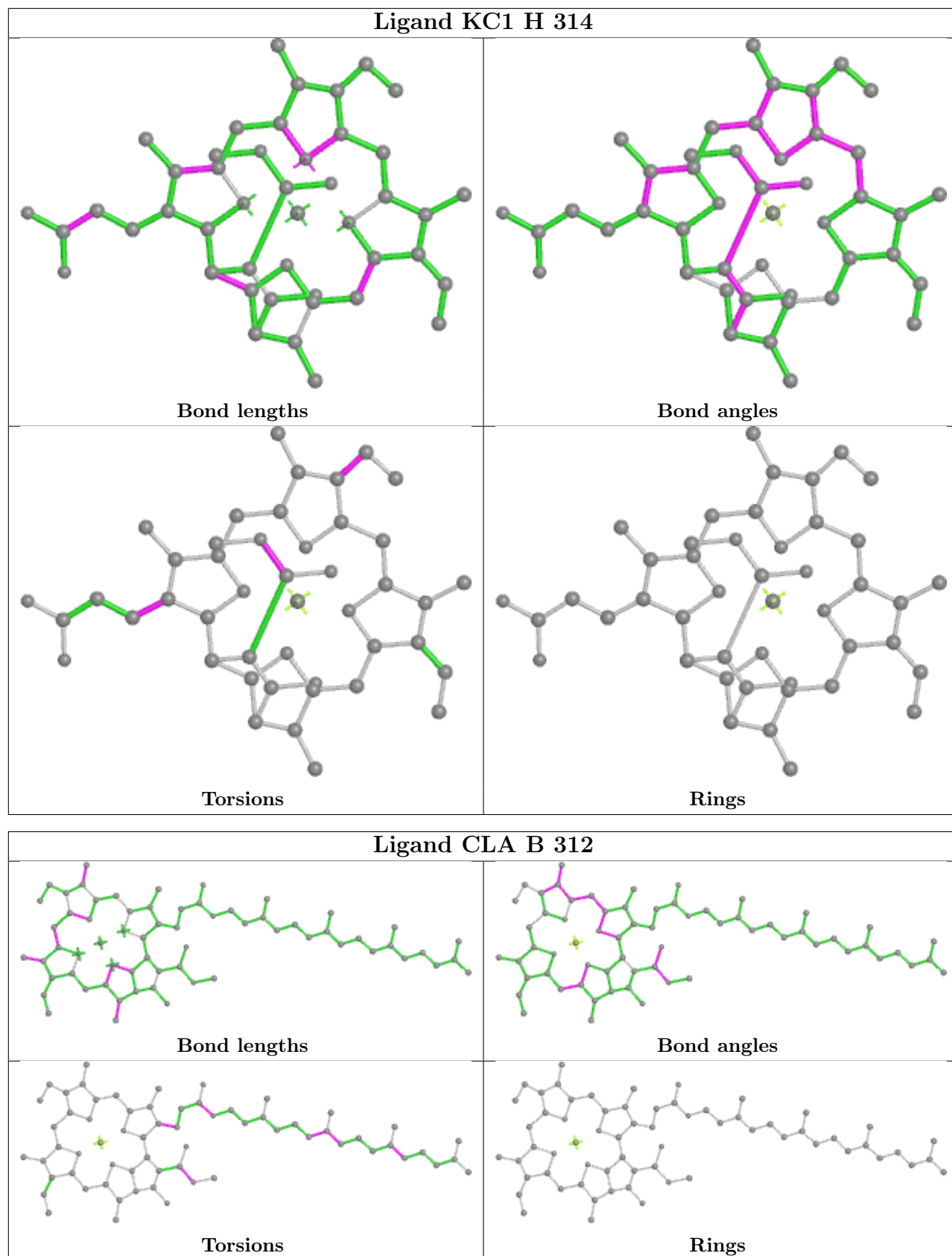


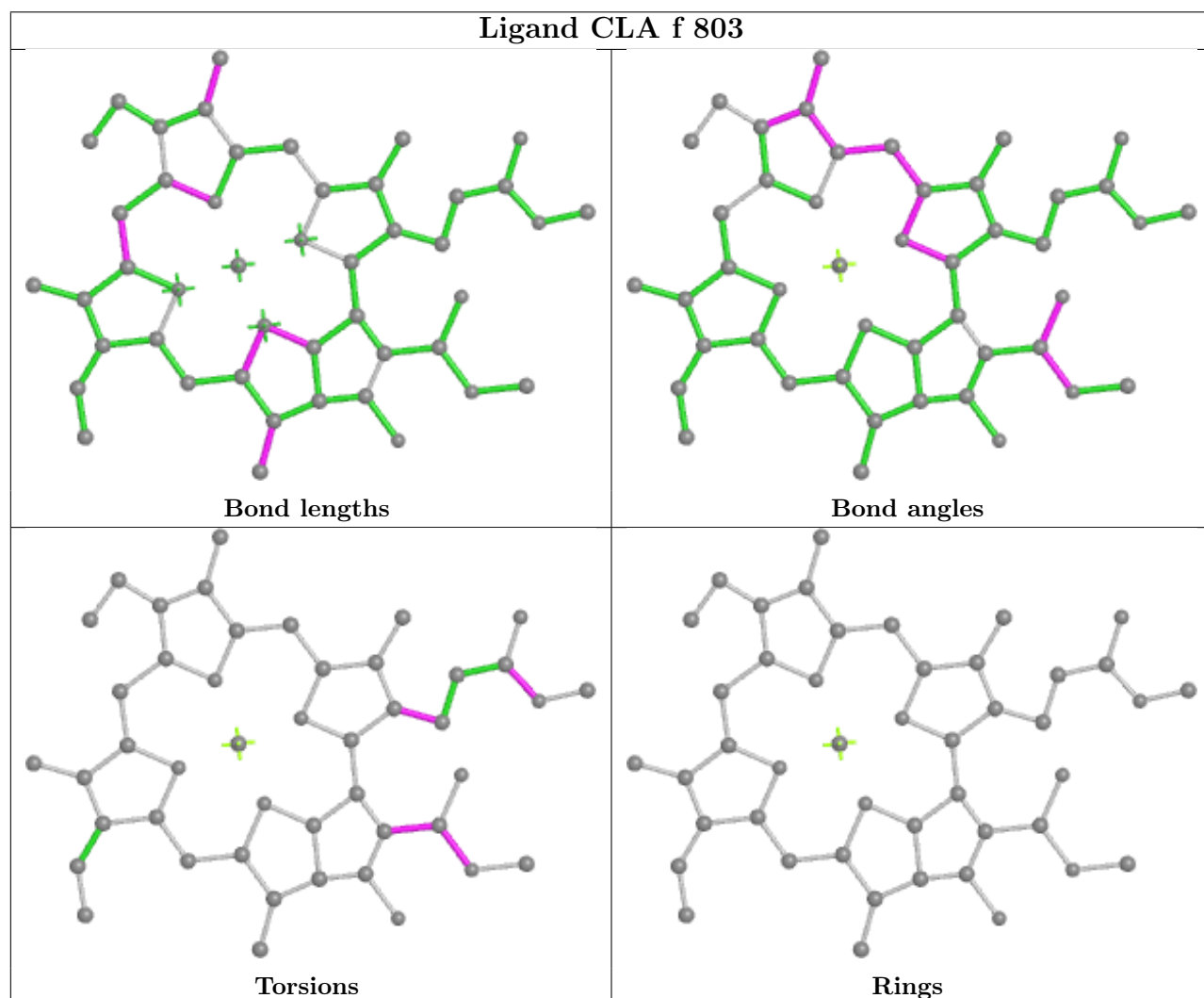
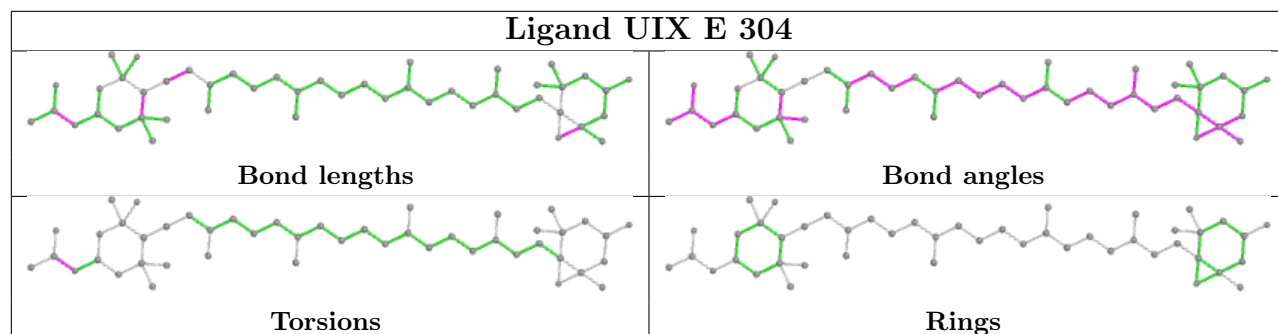




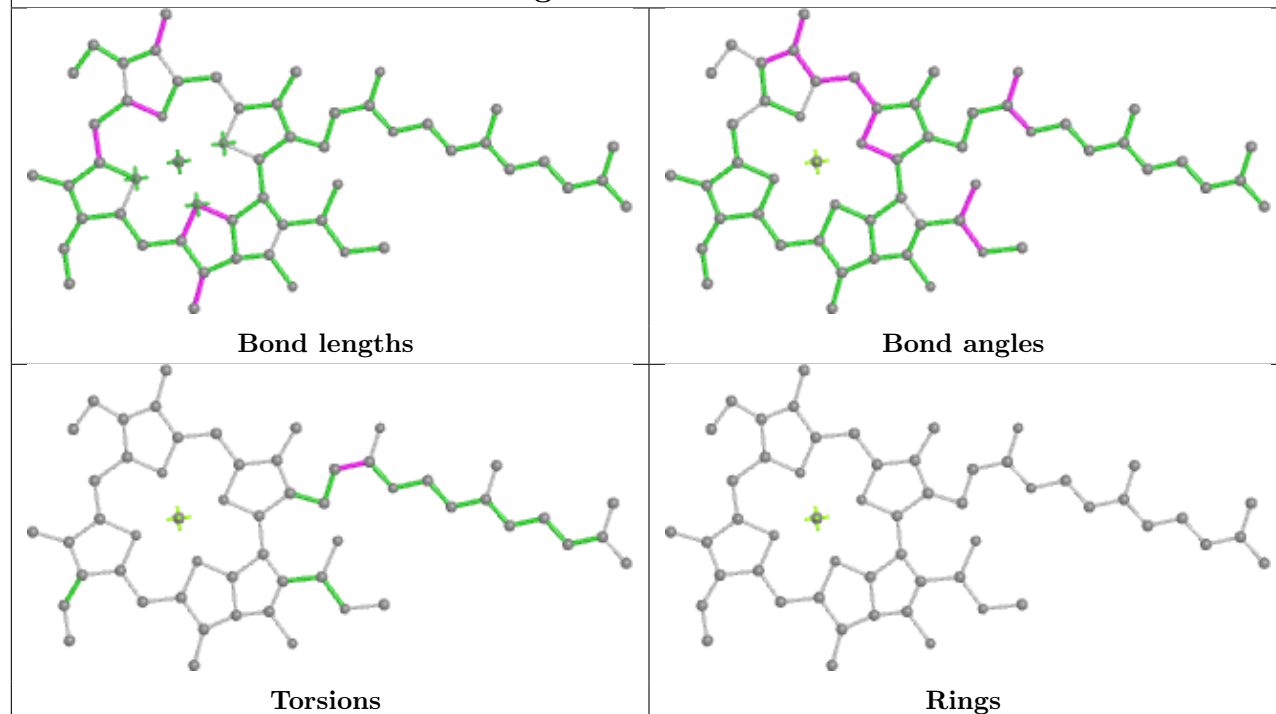




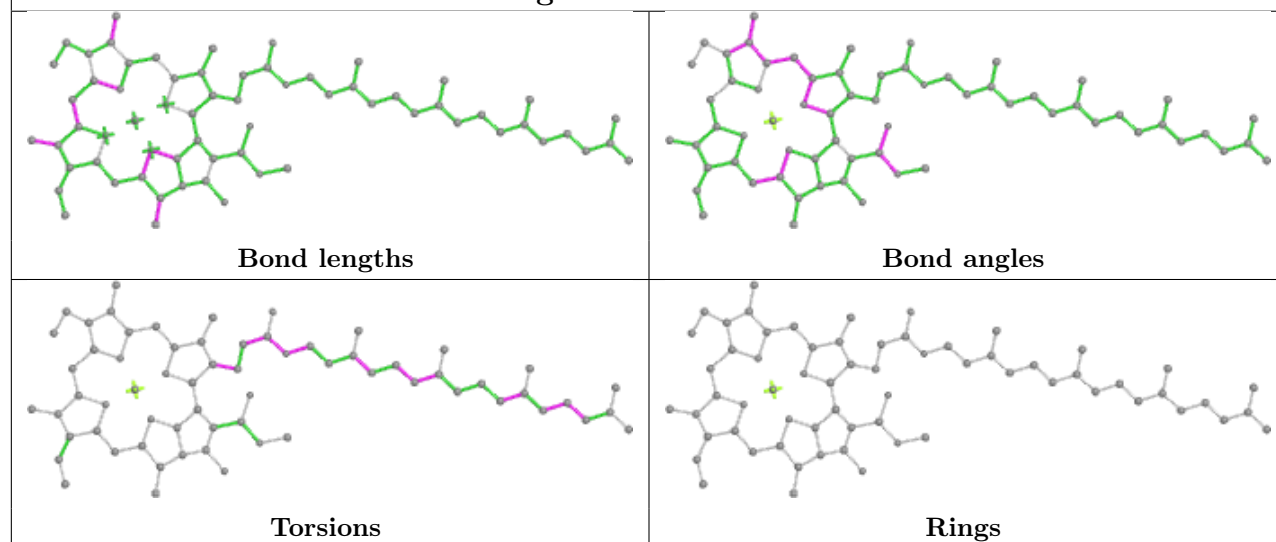


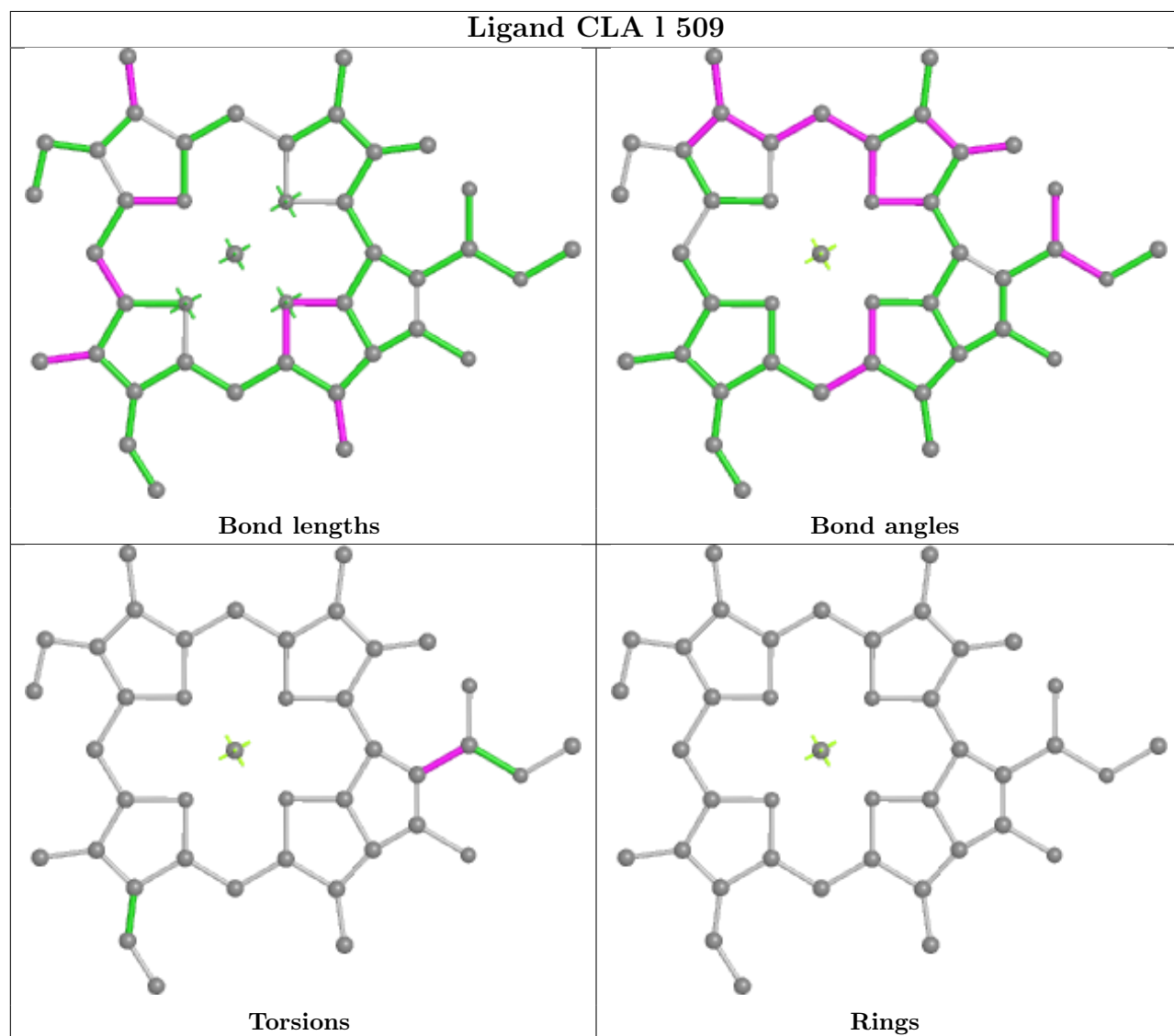
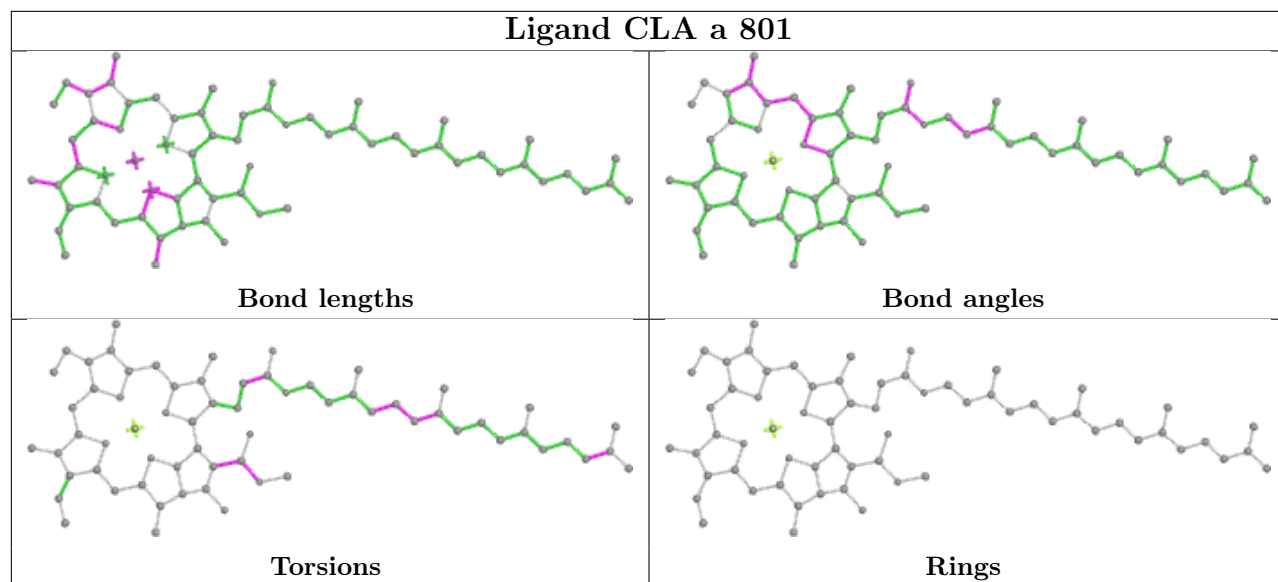


## Ligand CLA L 309

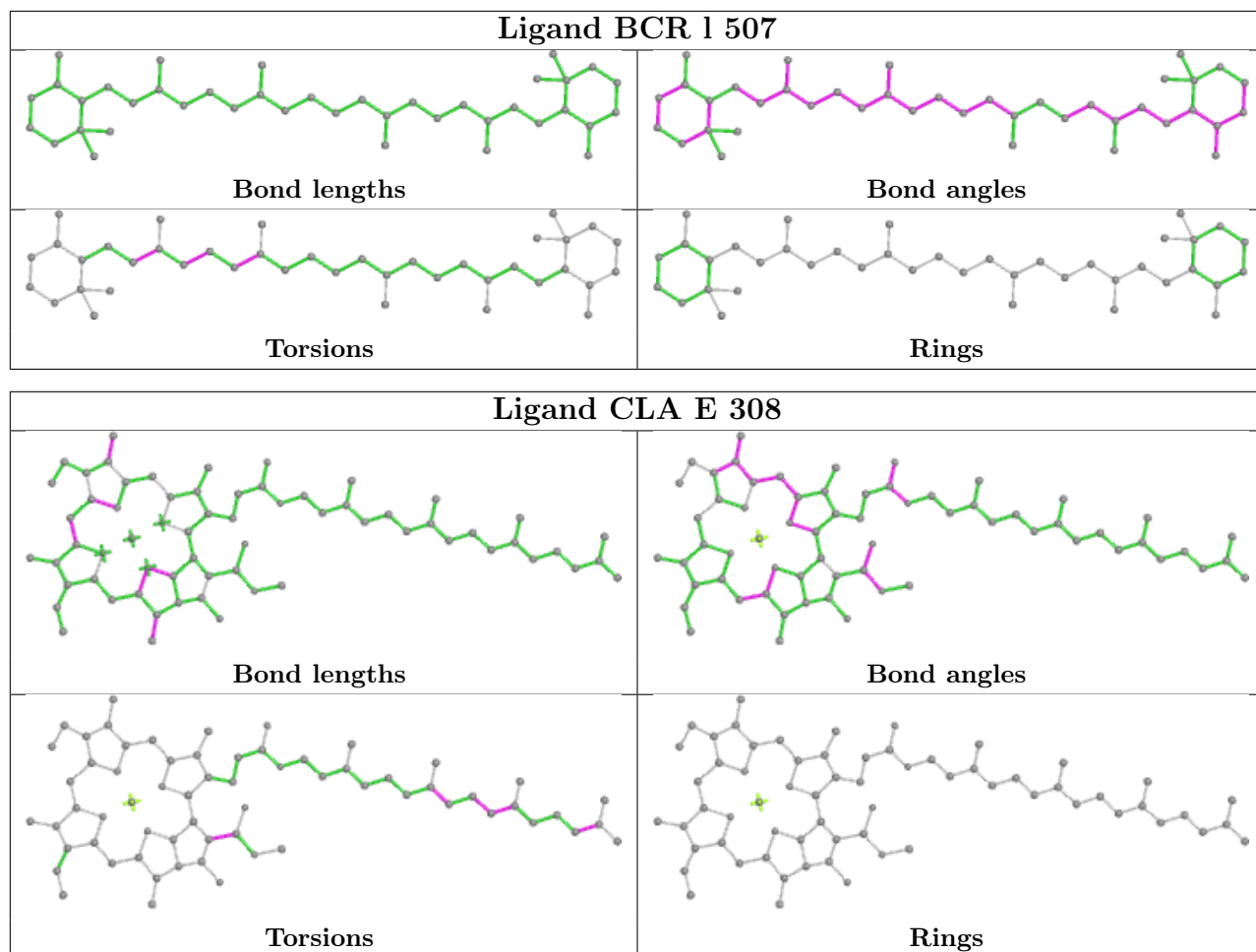


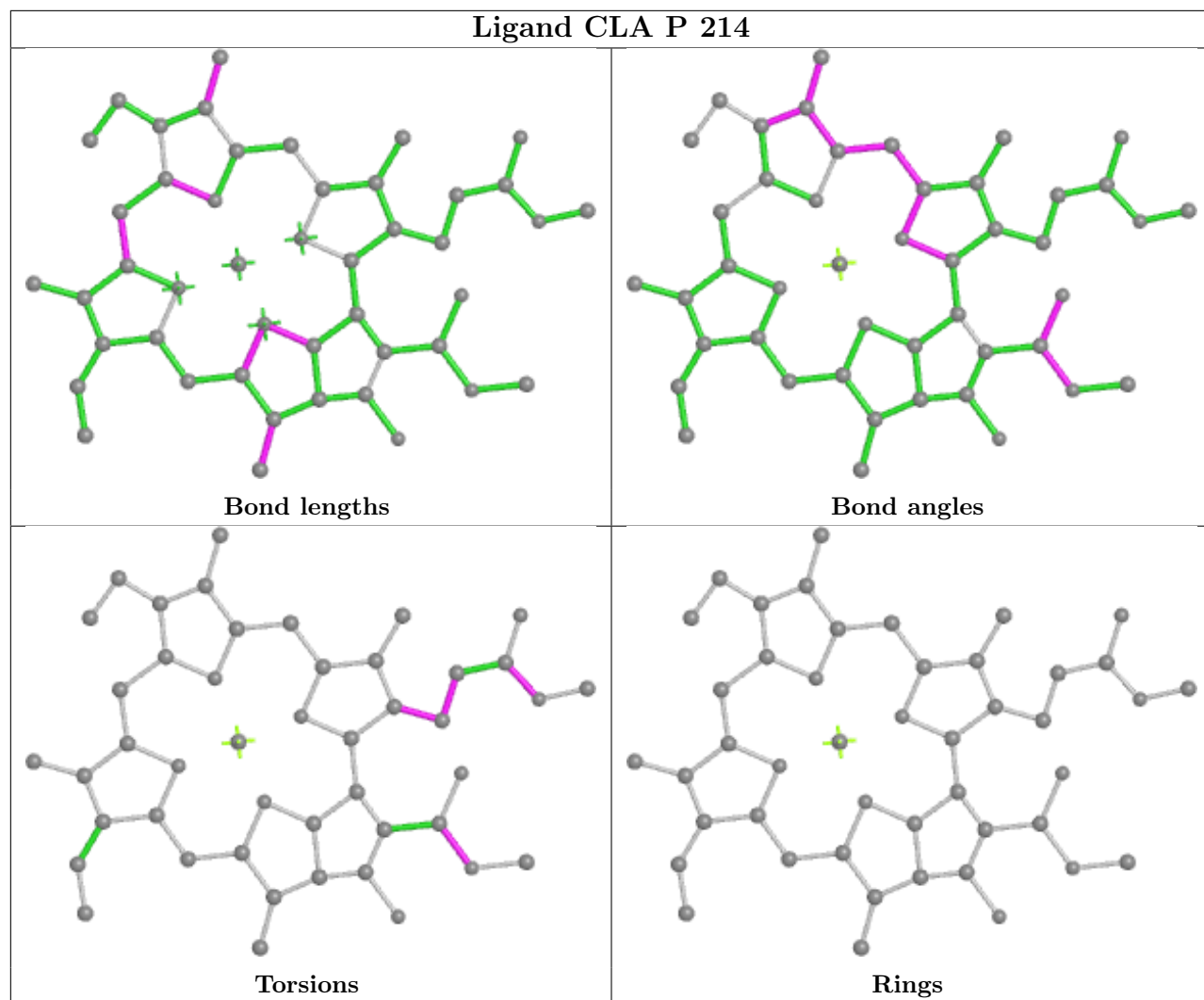
## Ligand CLA a 806

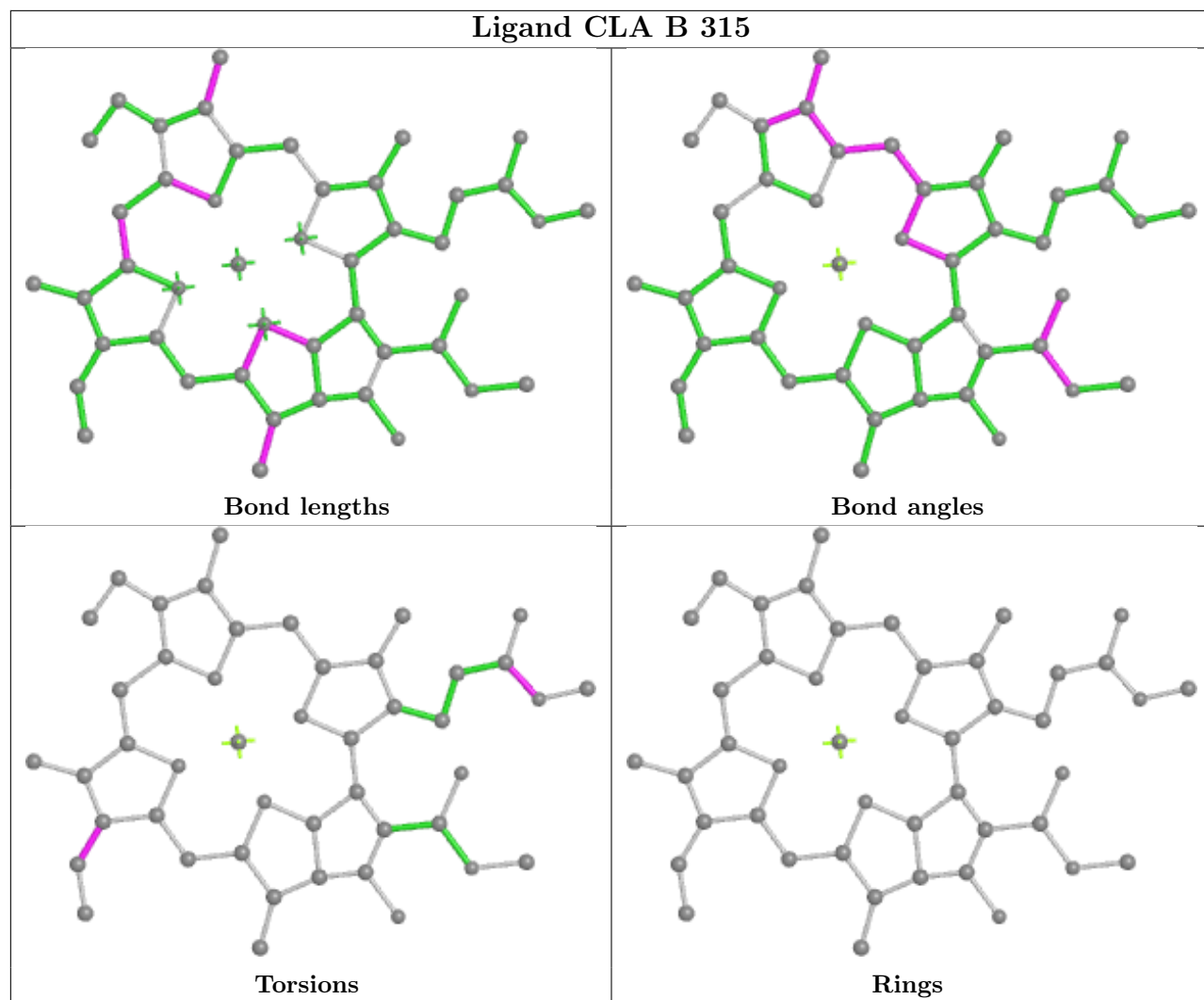


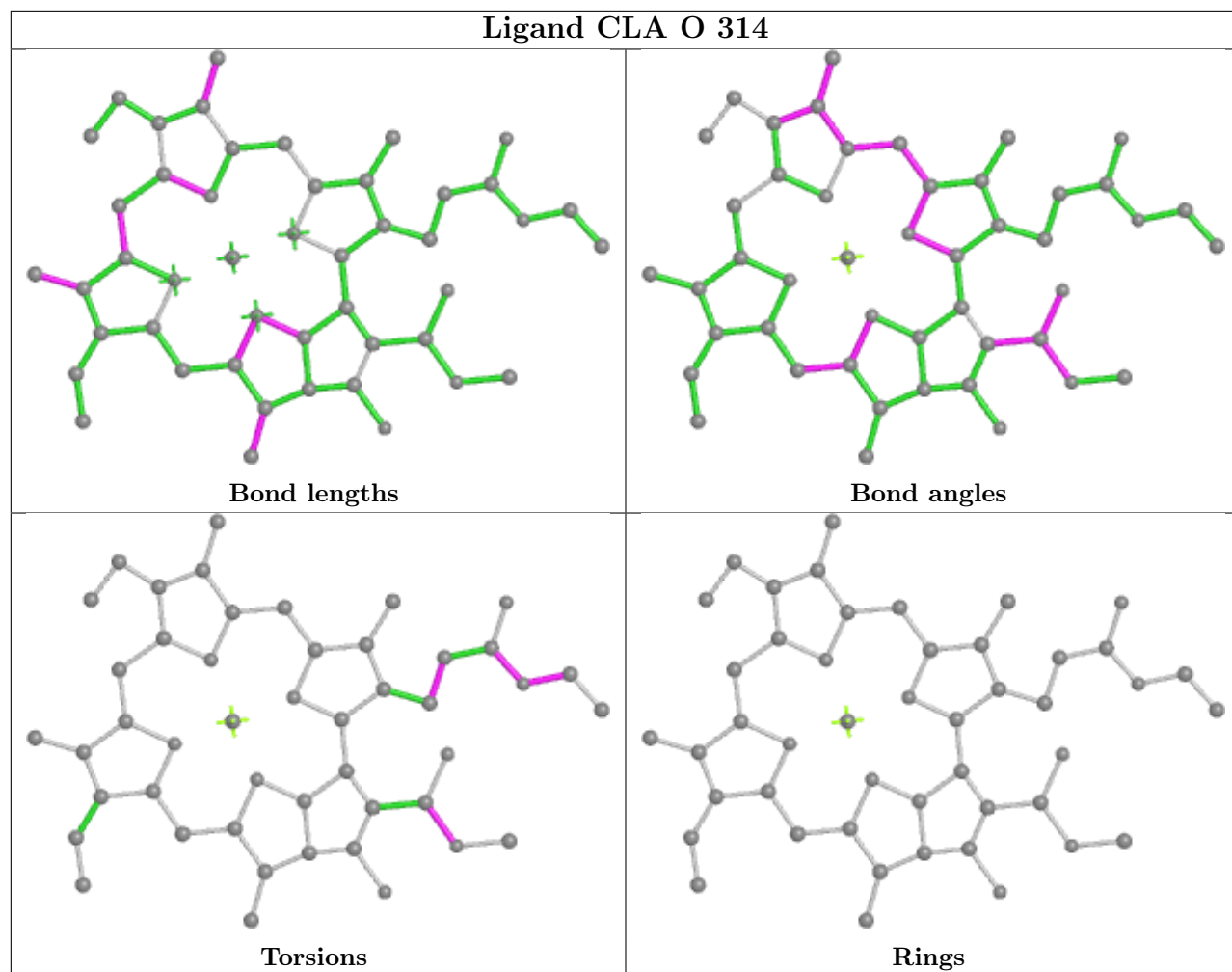


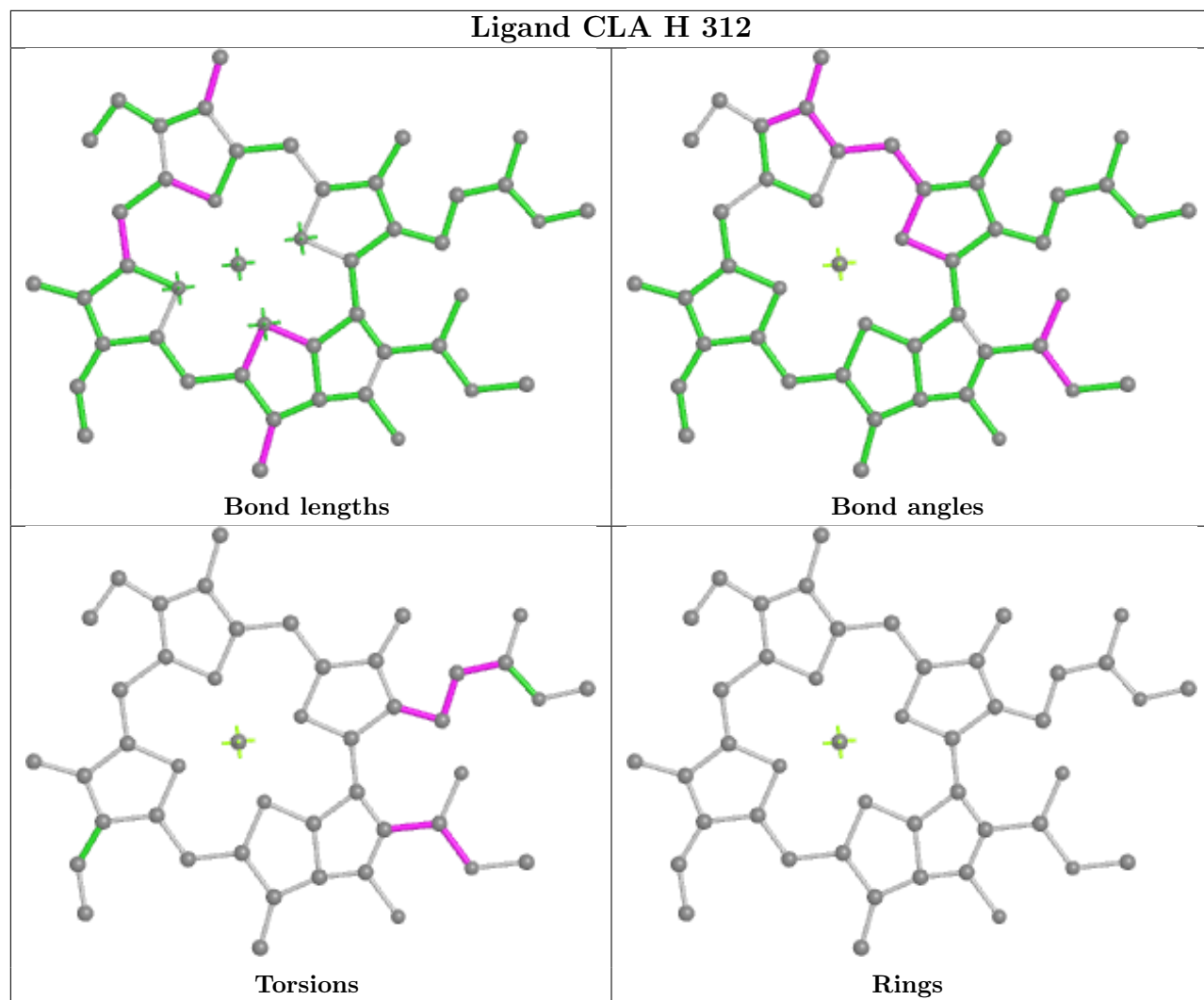


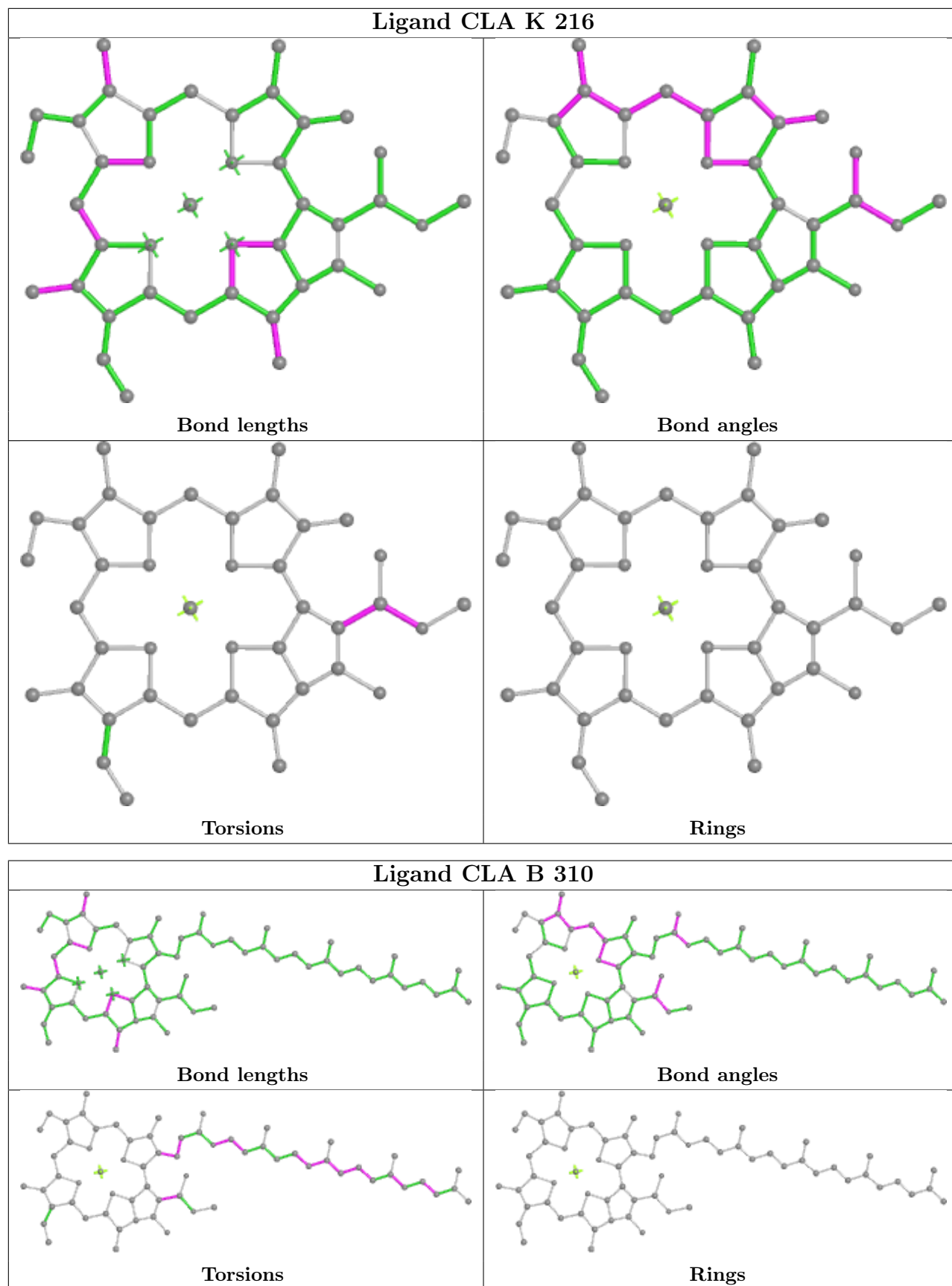


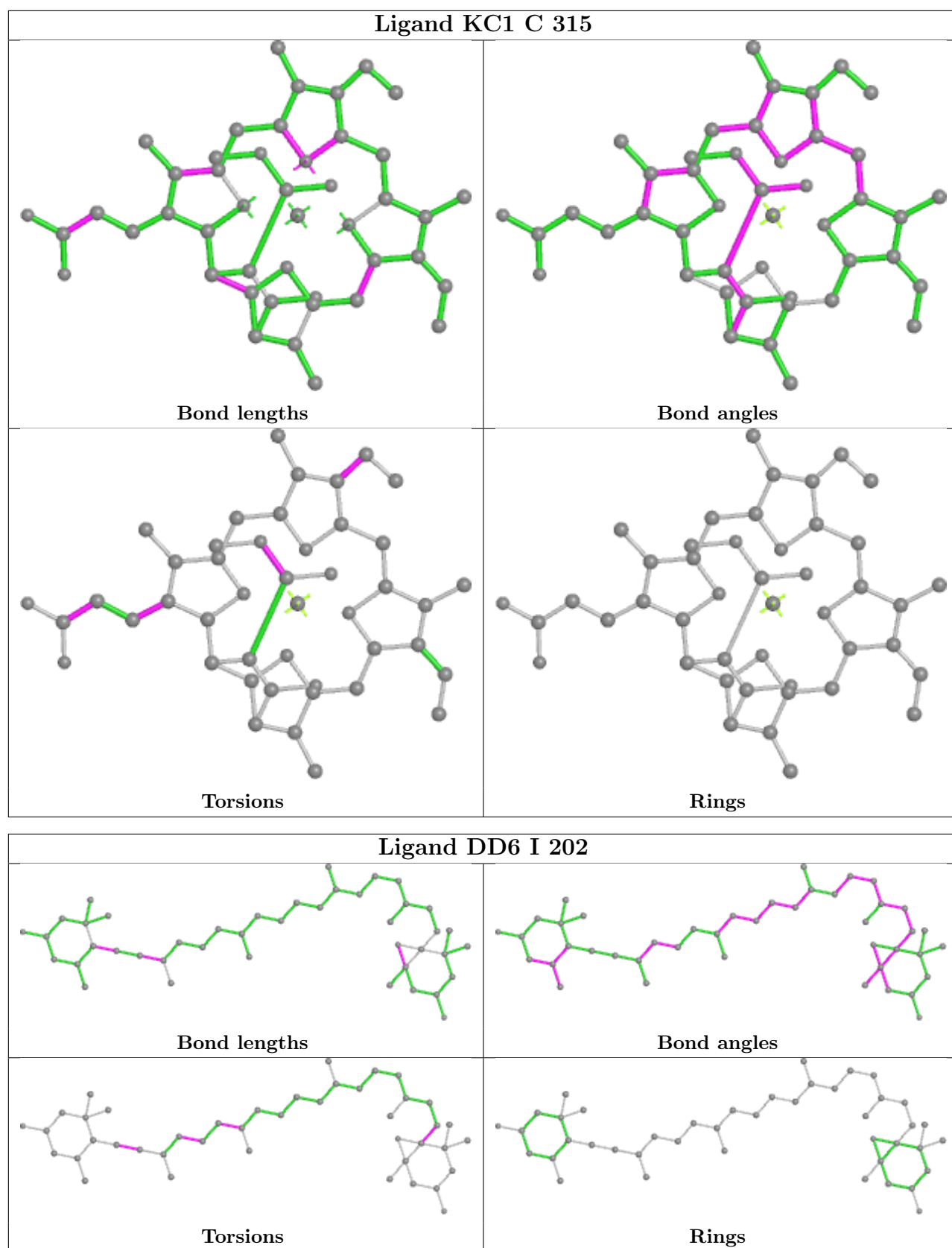


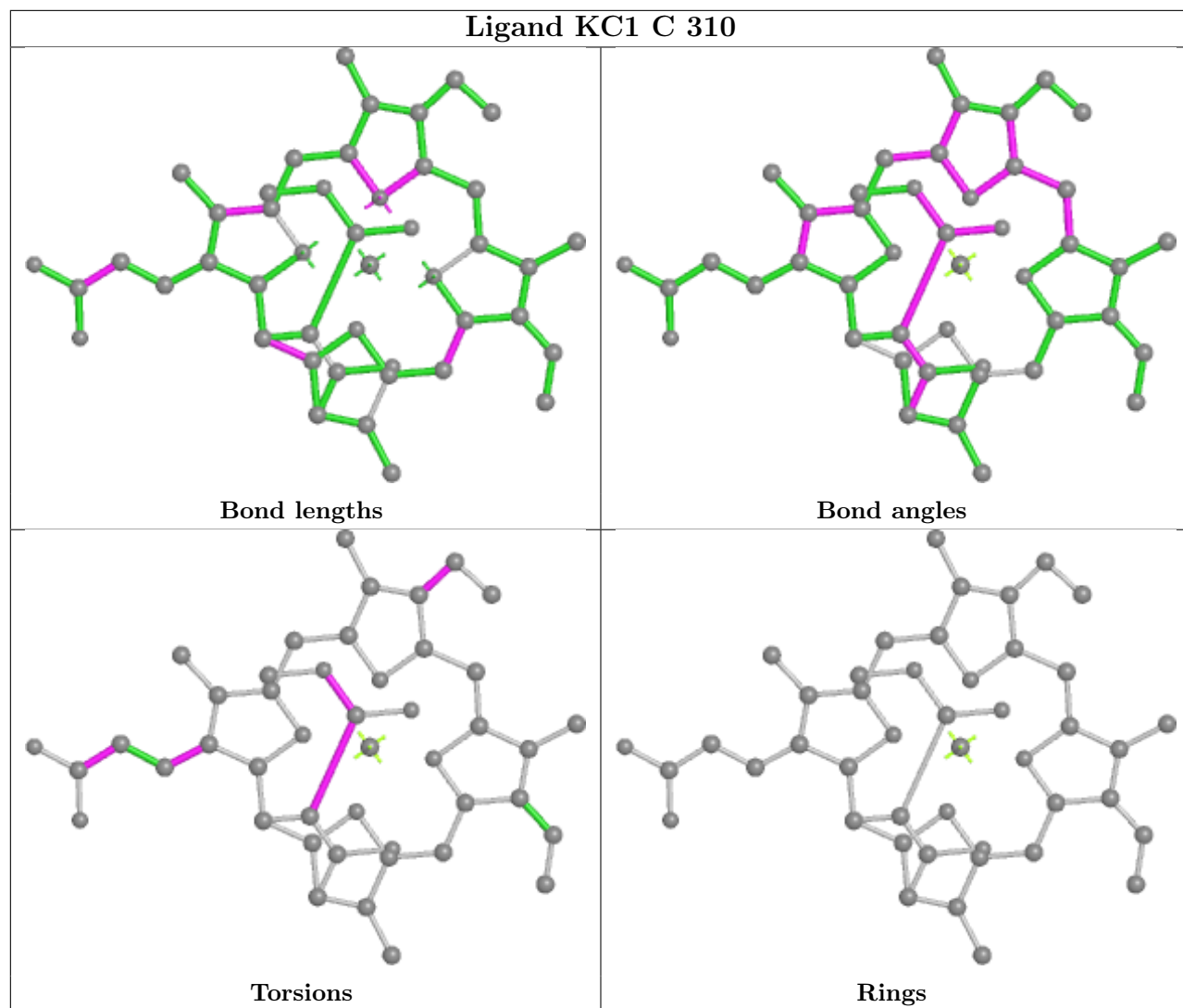




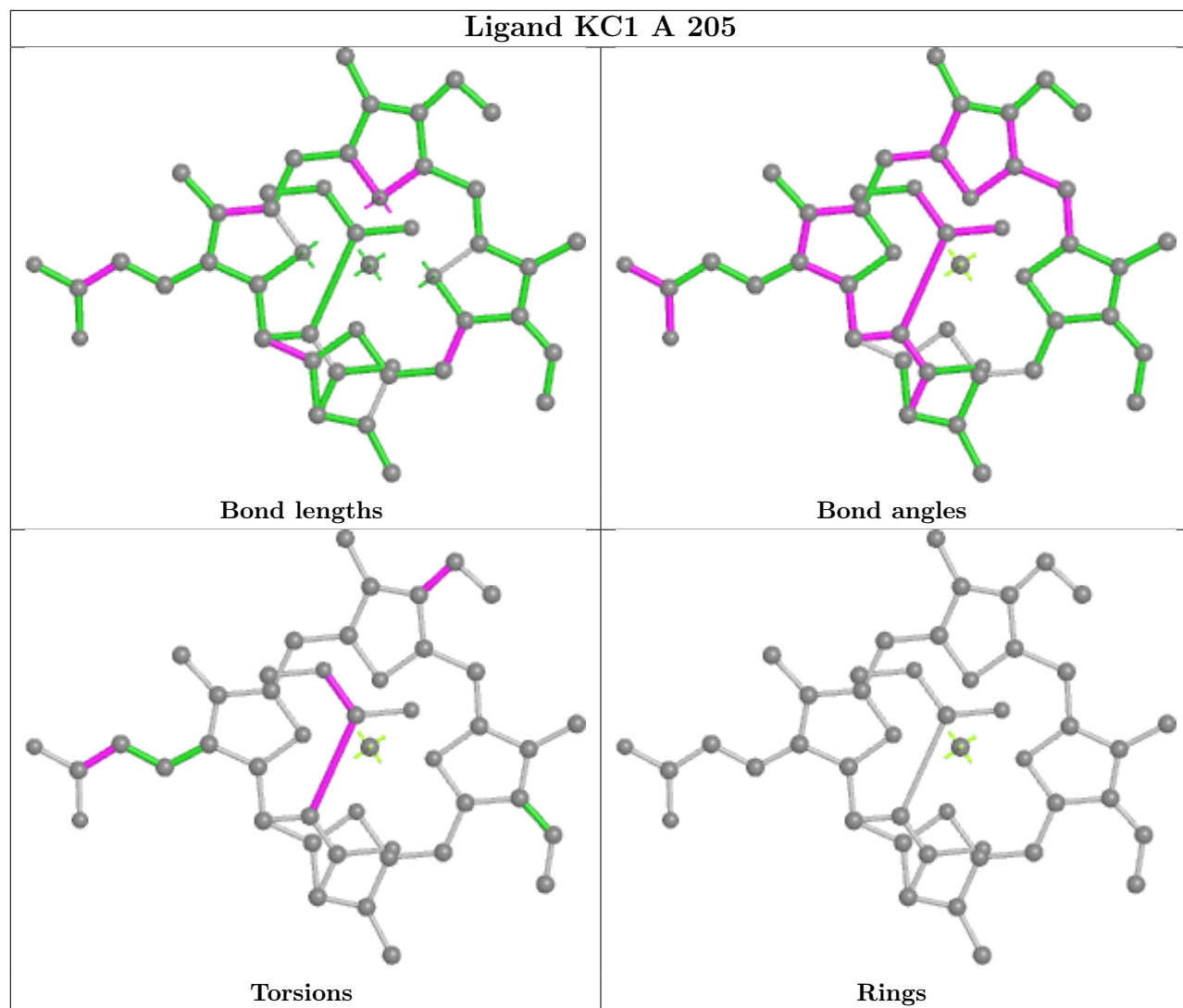


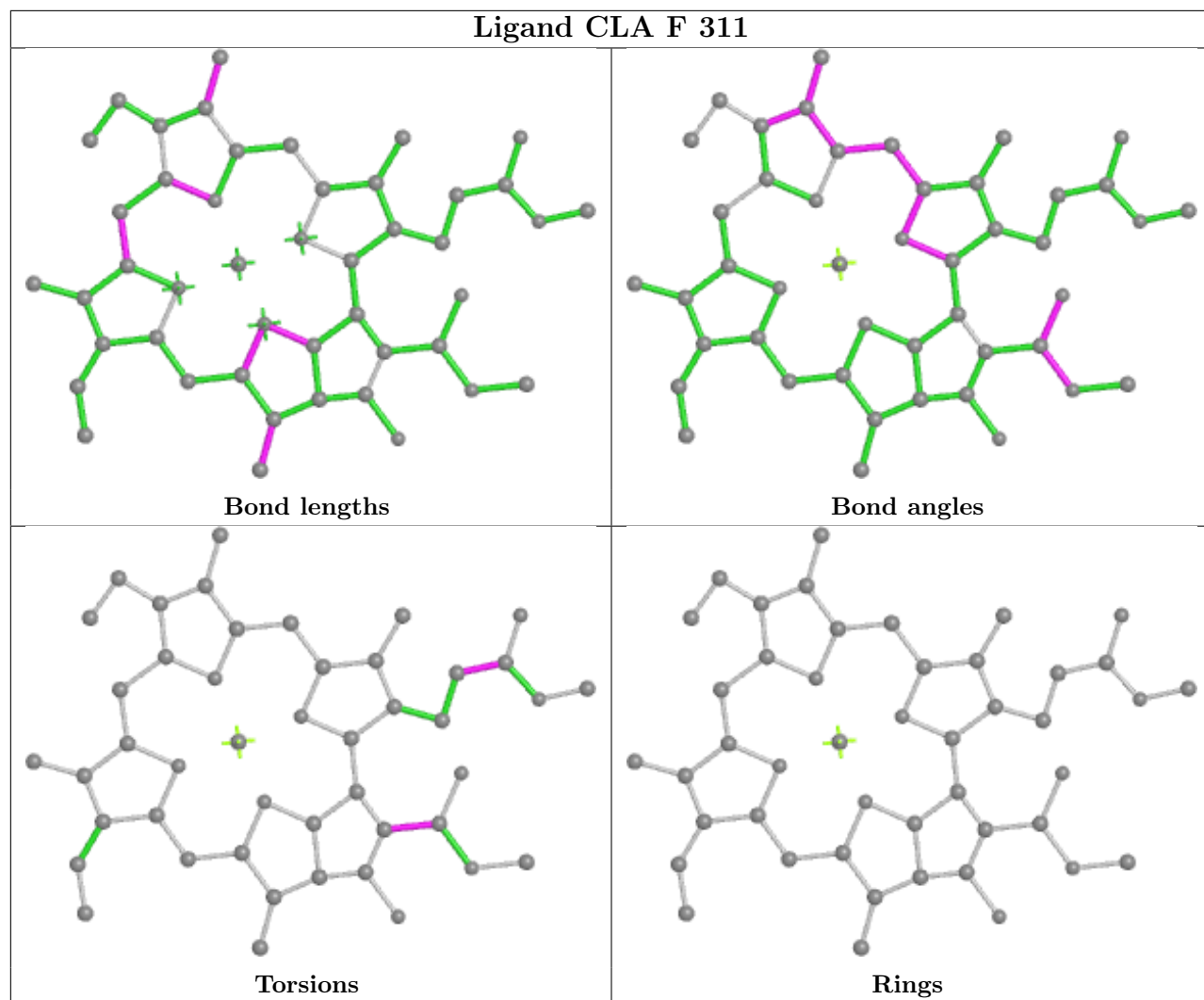


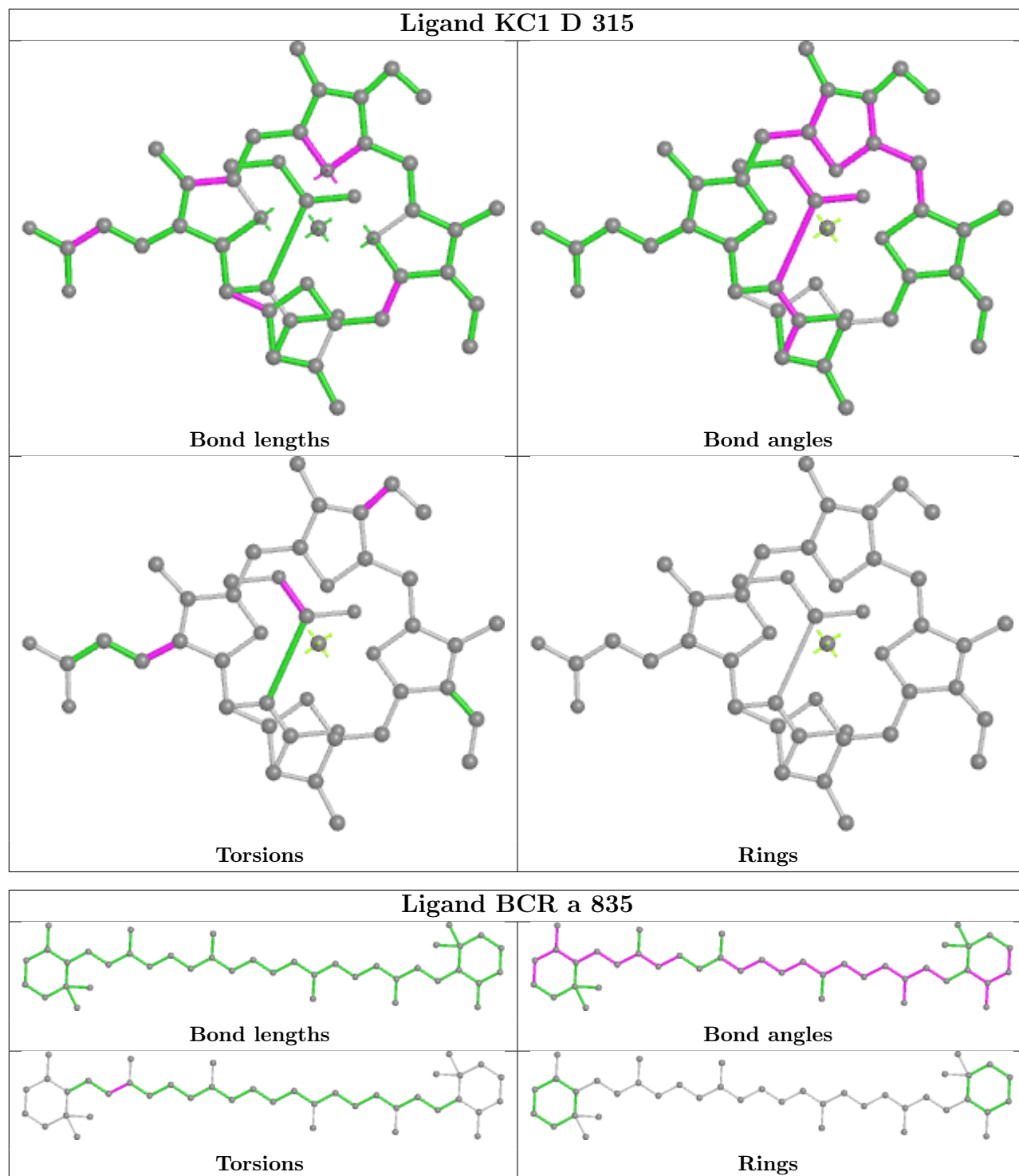


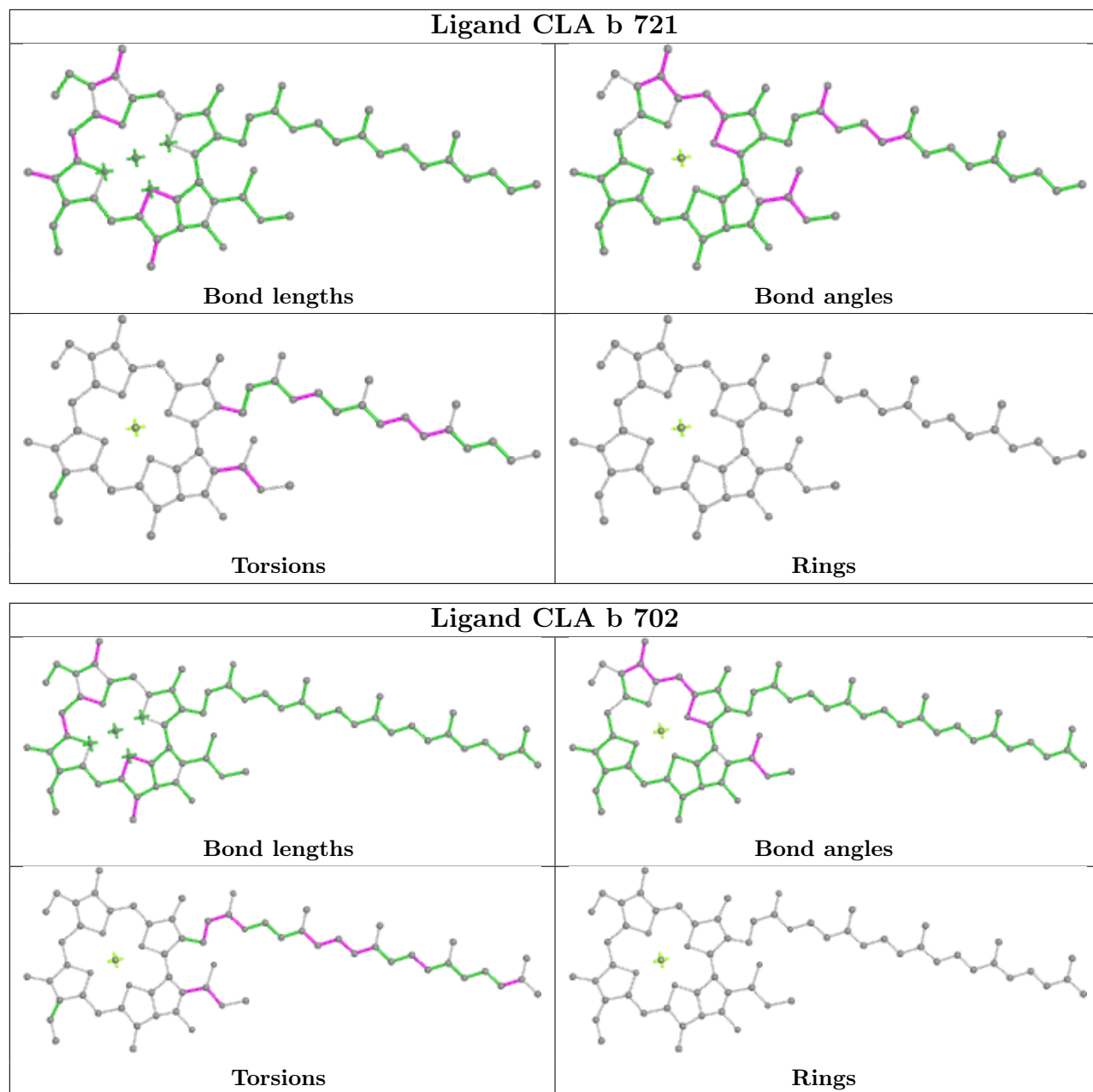


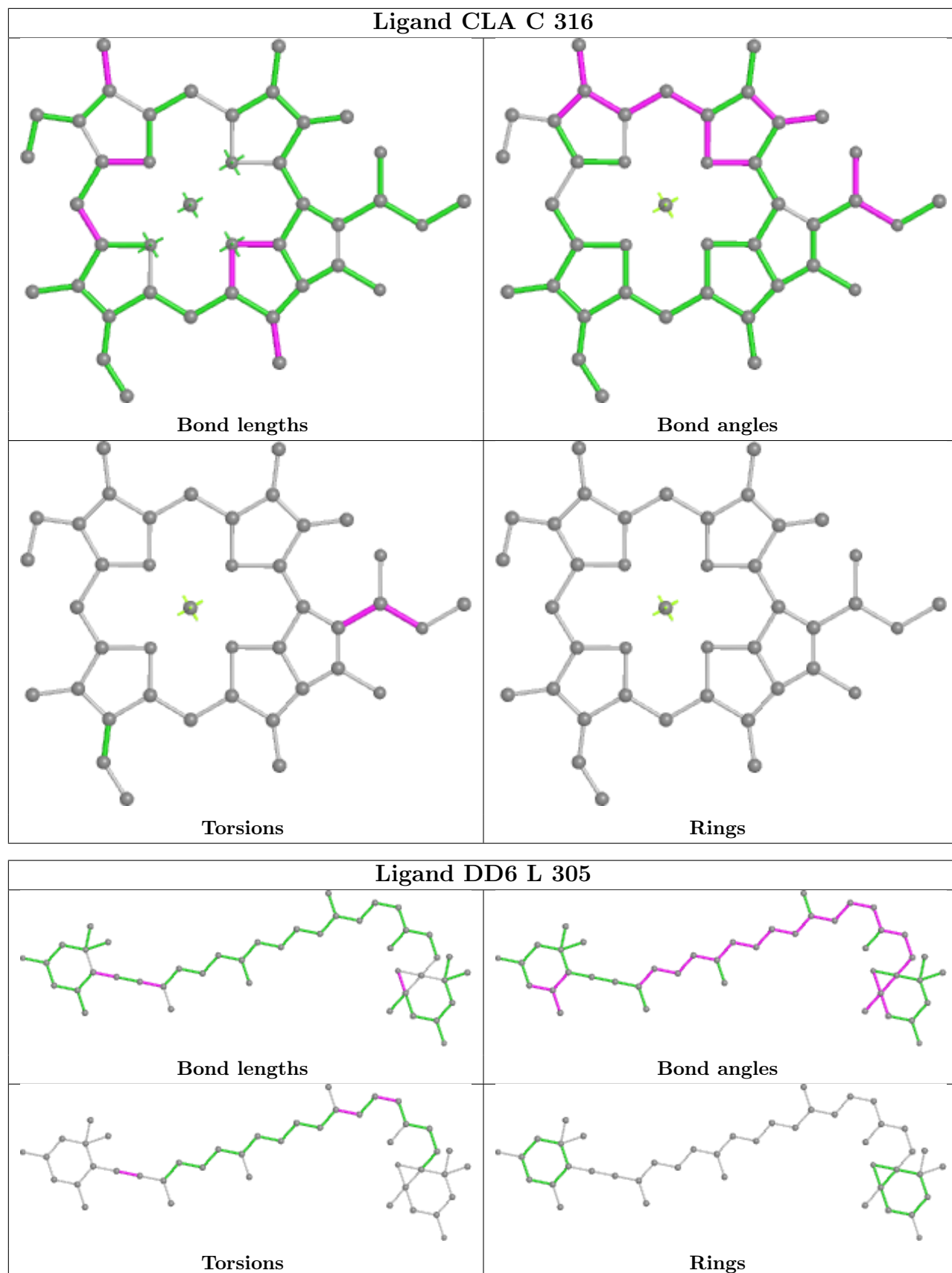


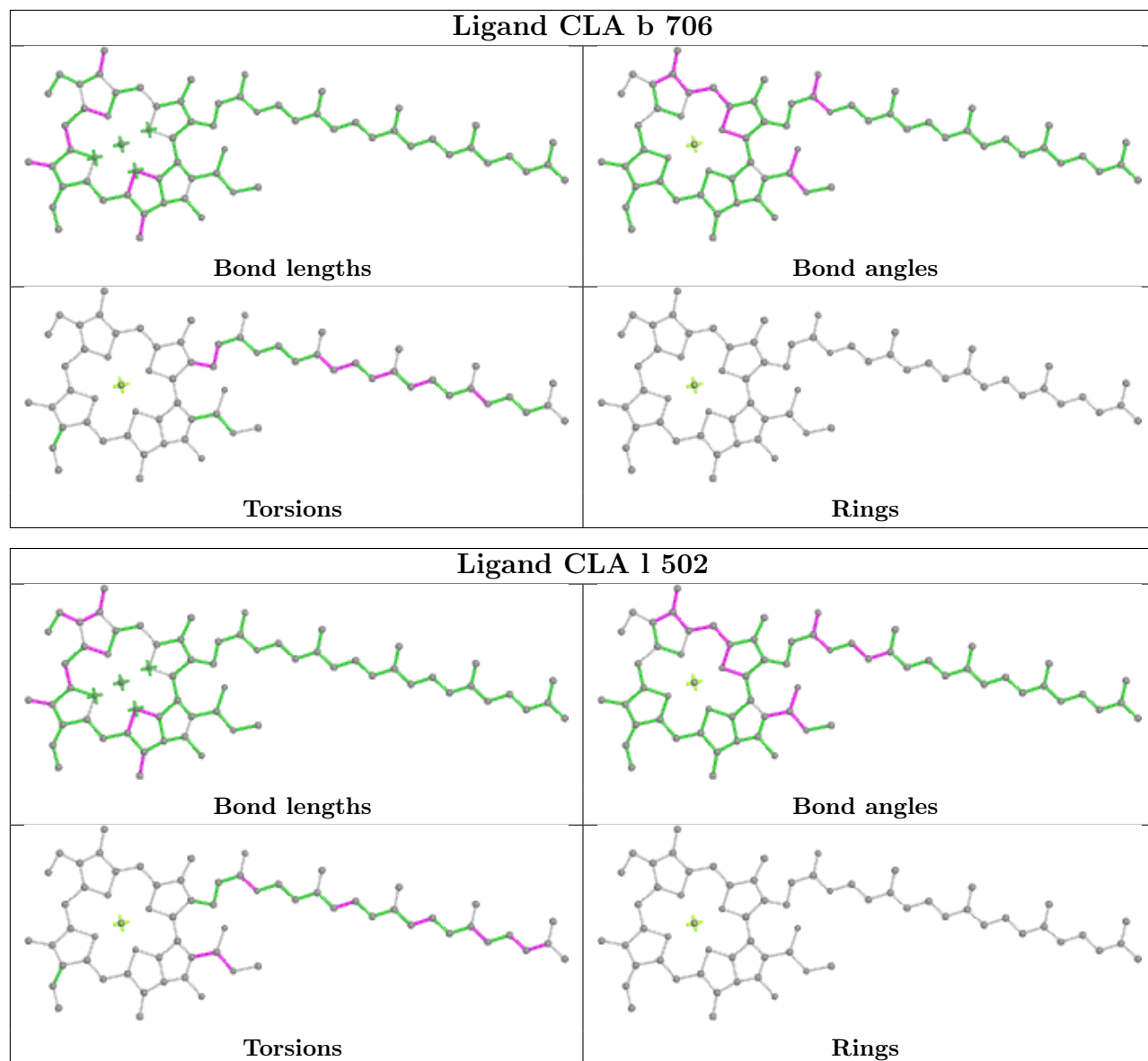


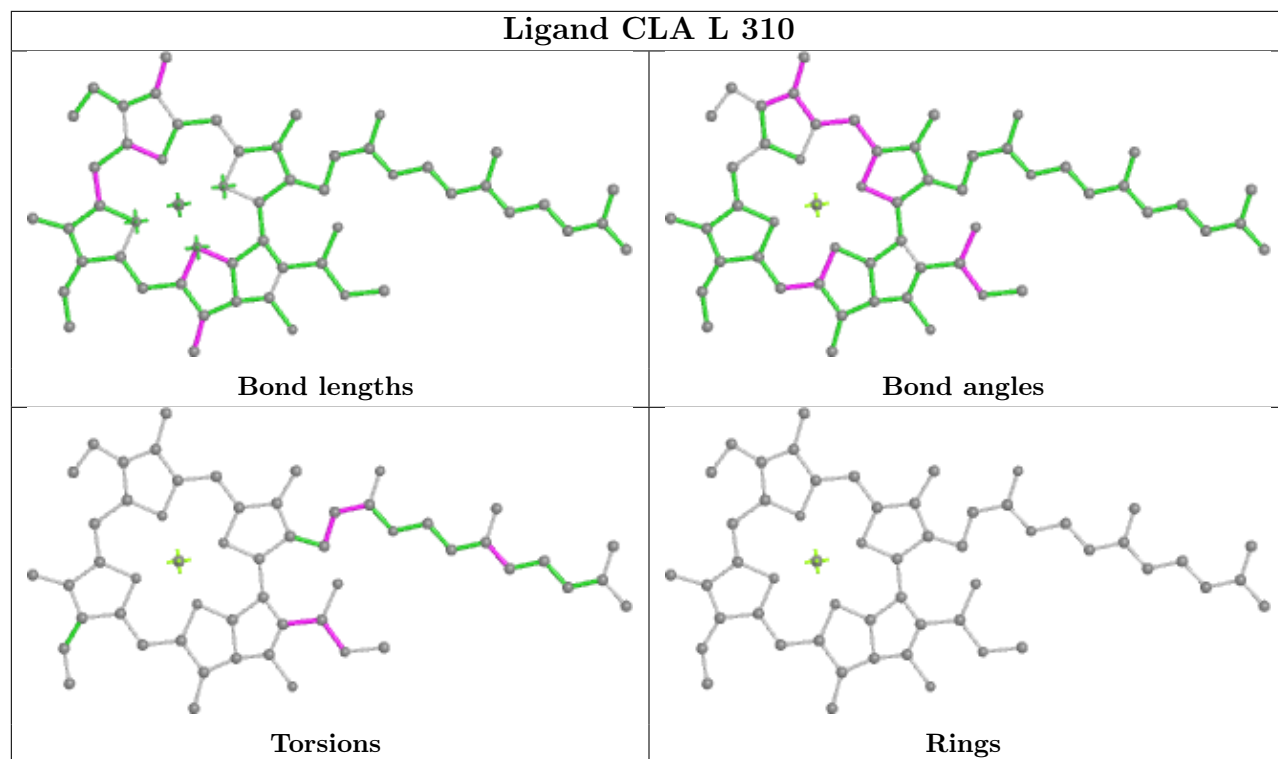


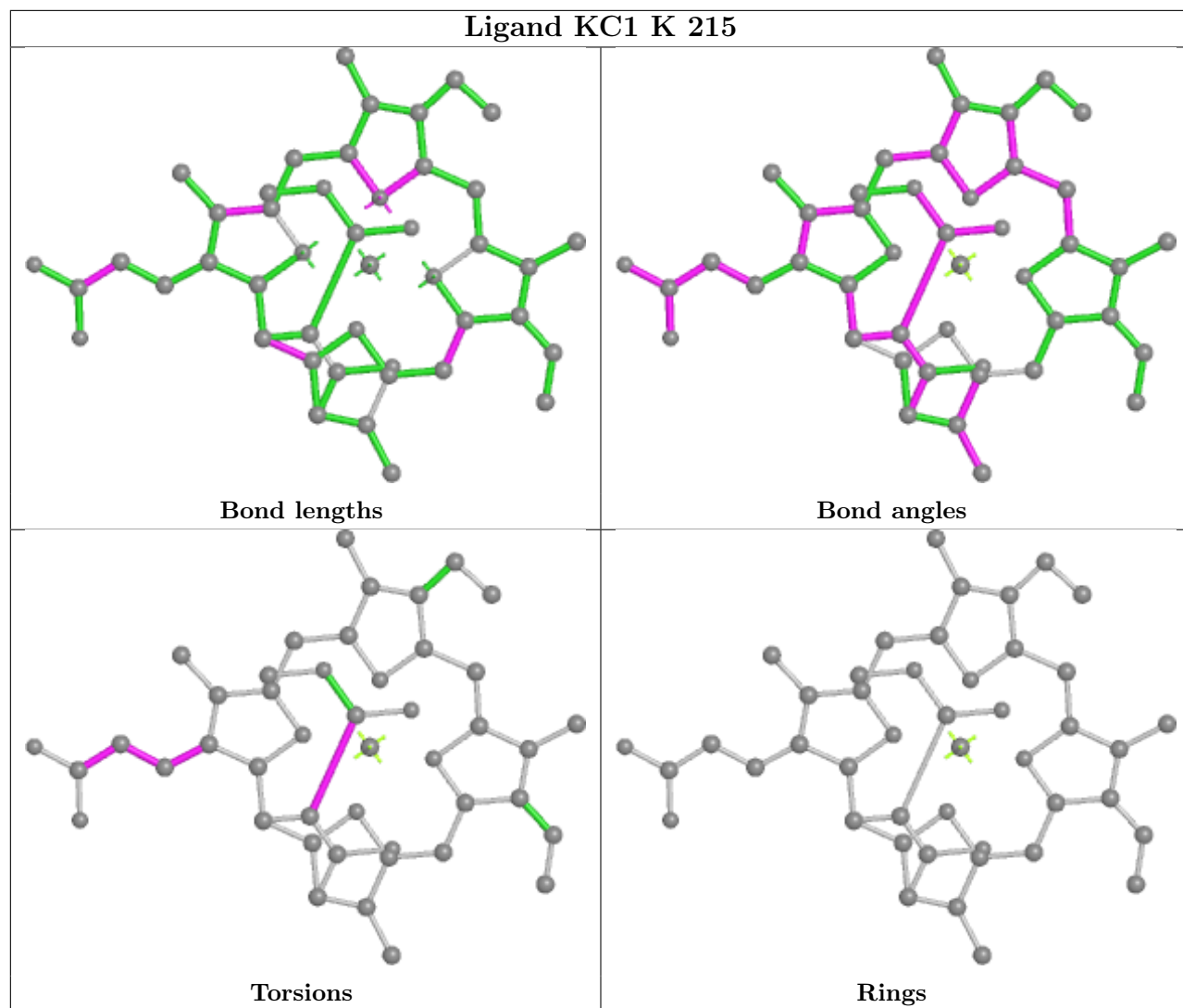




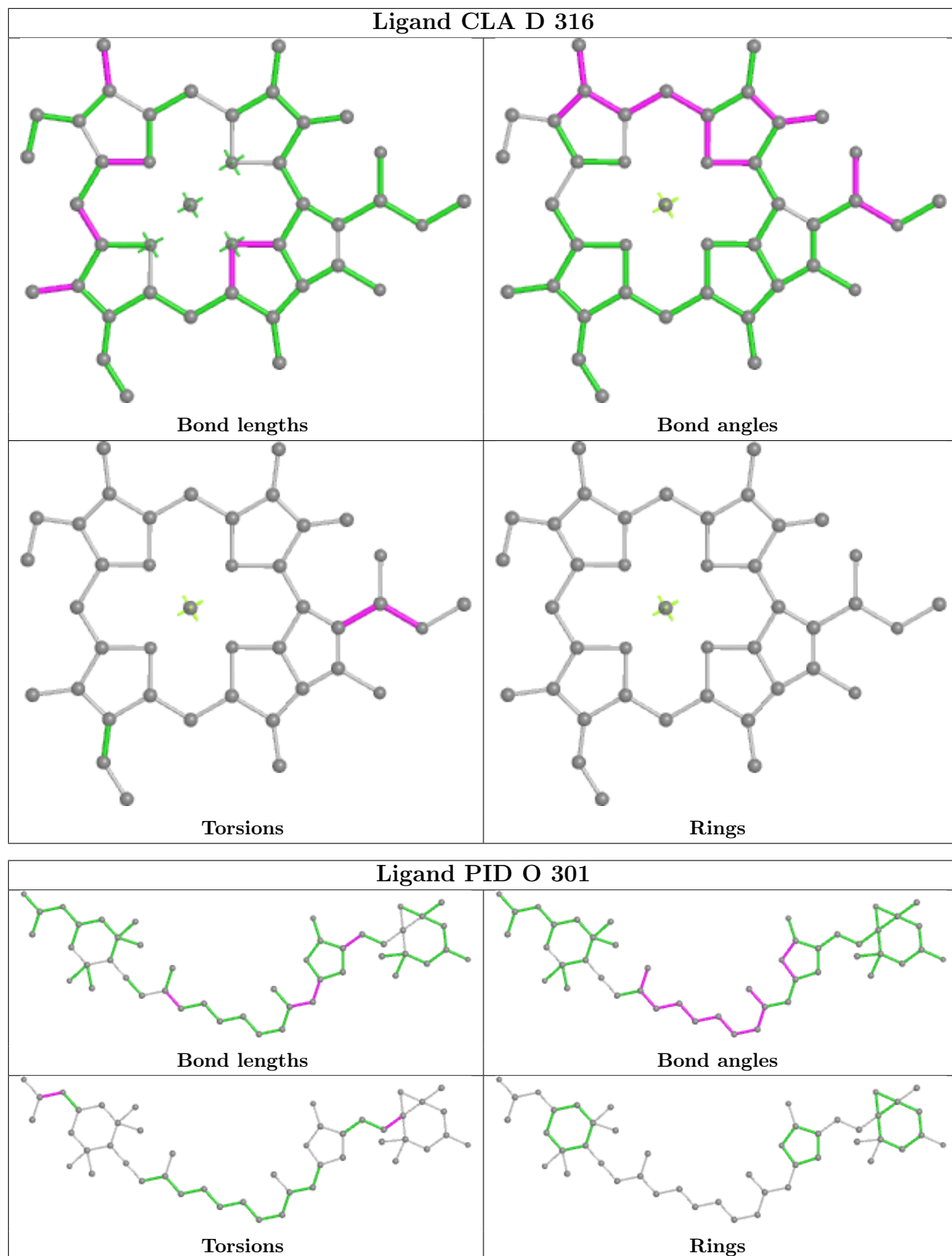


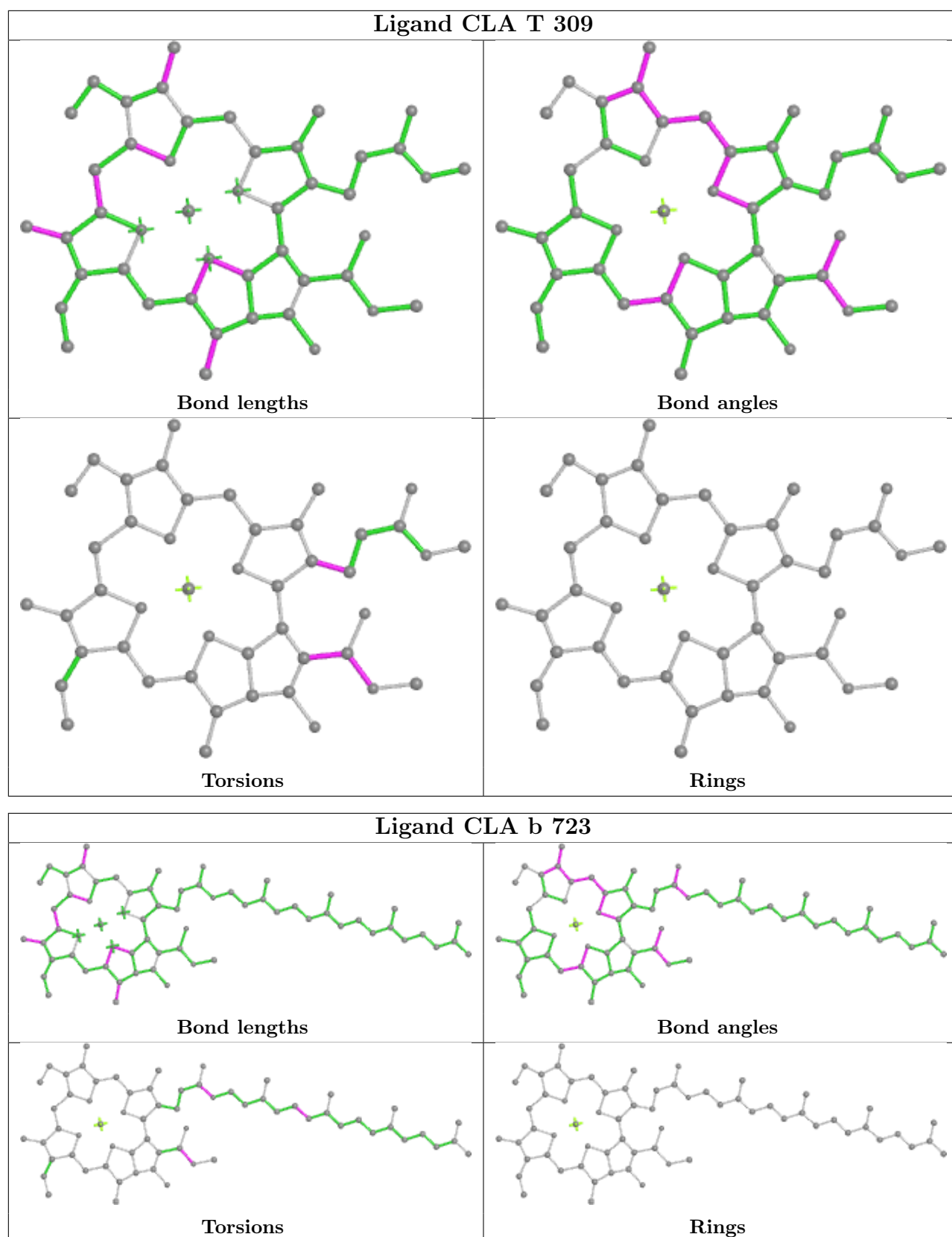


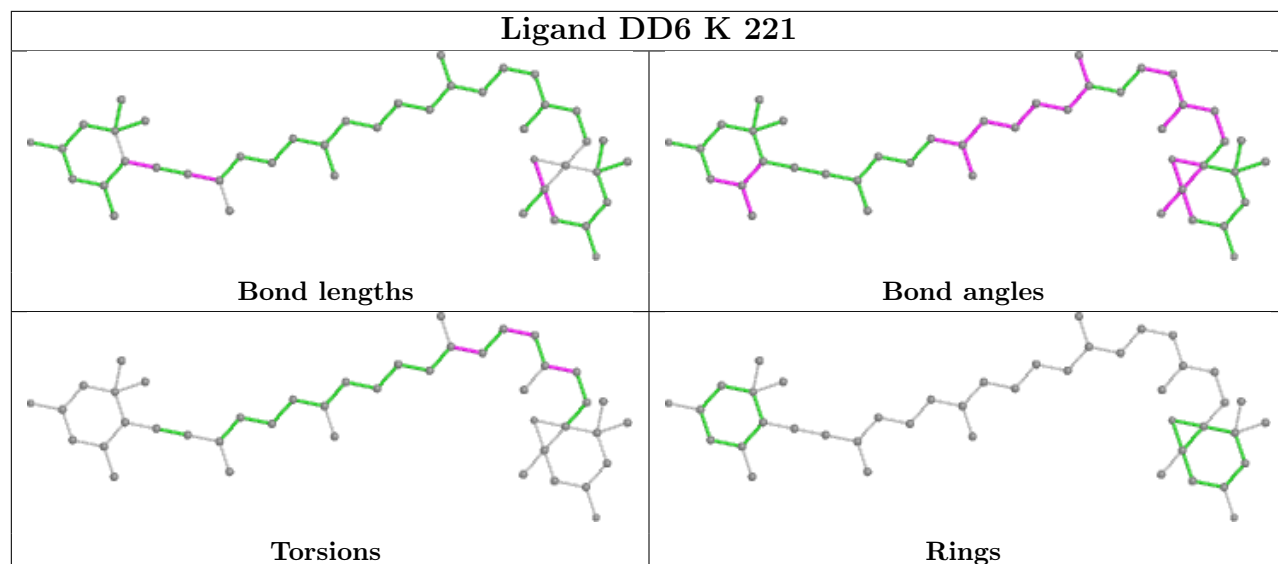
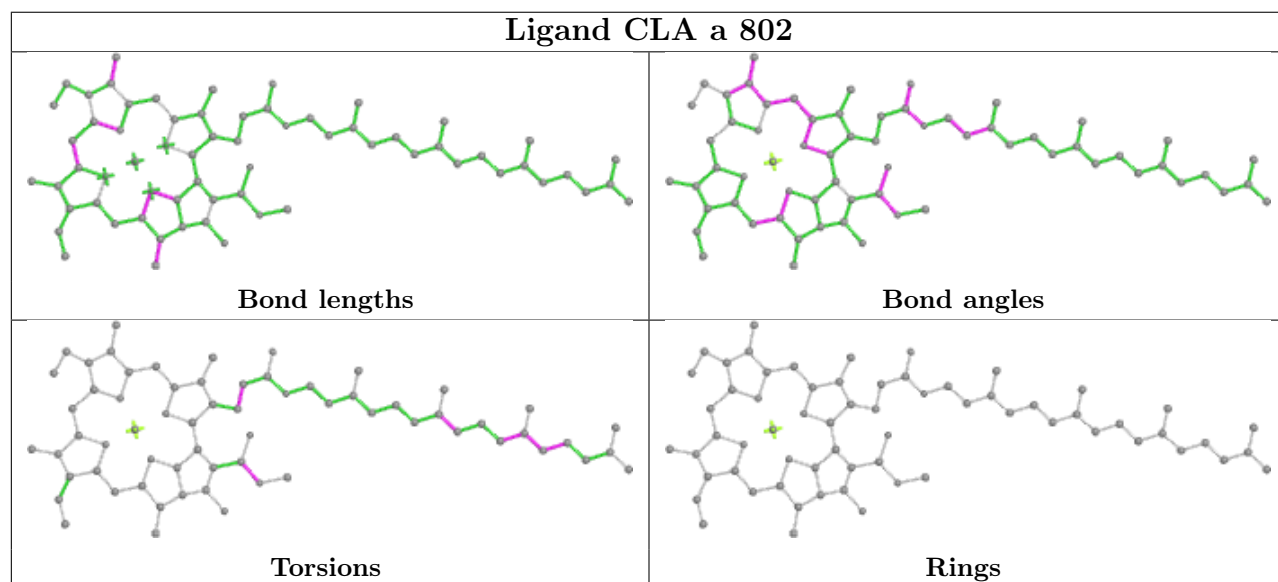
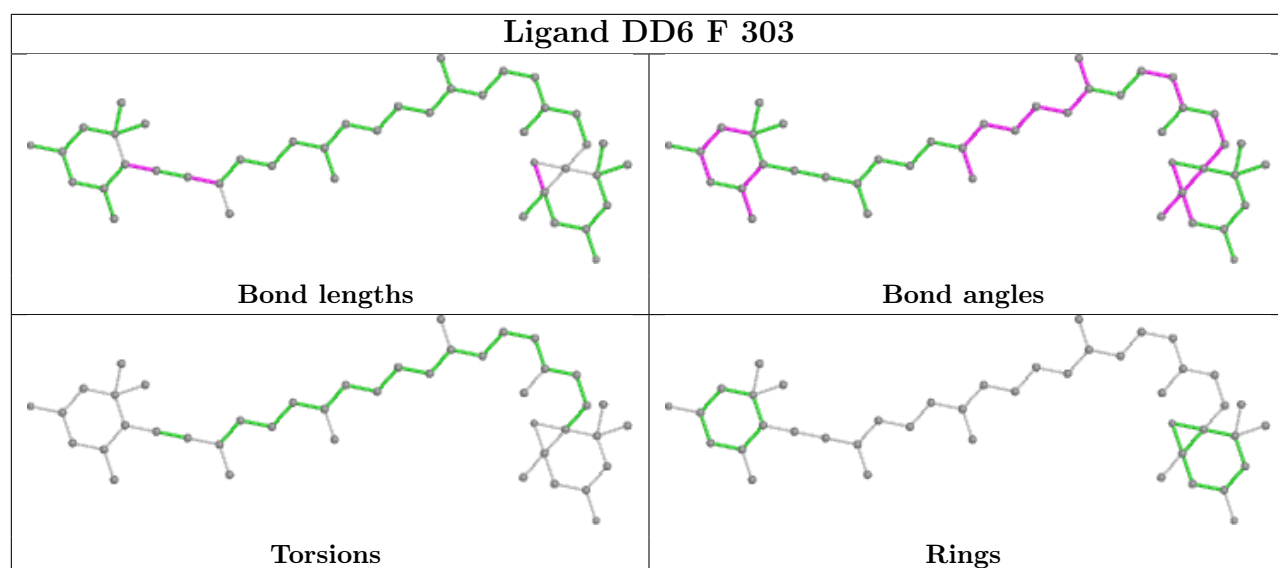


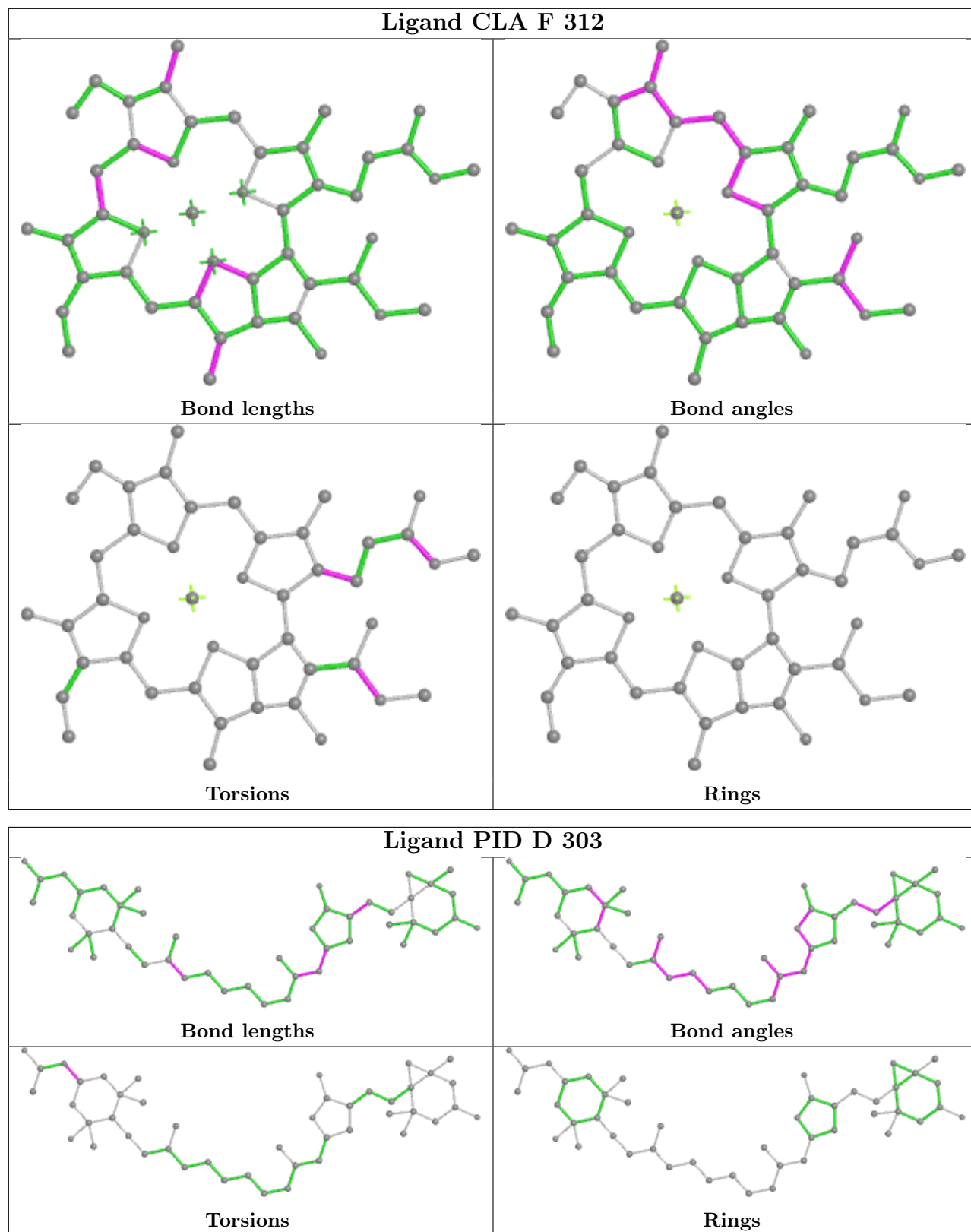


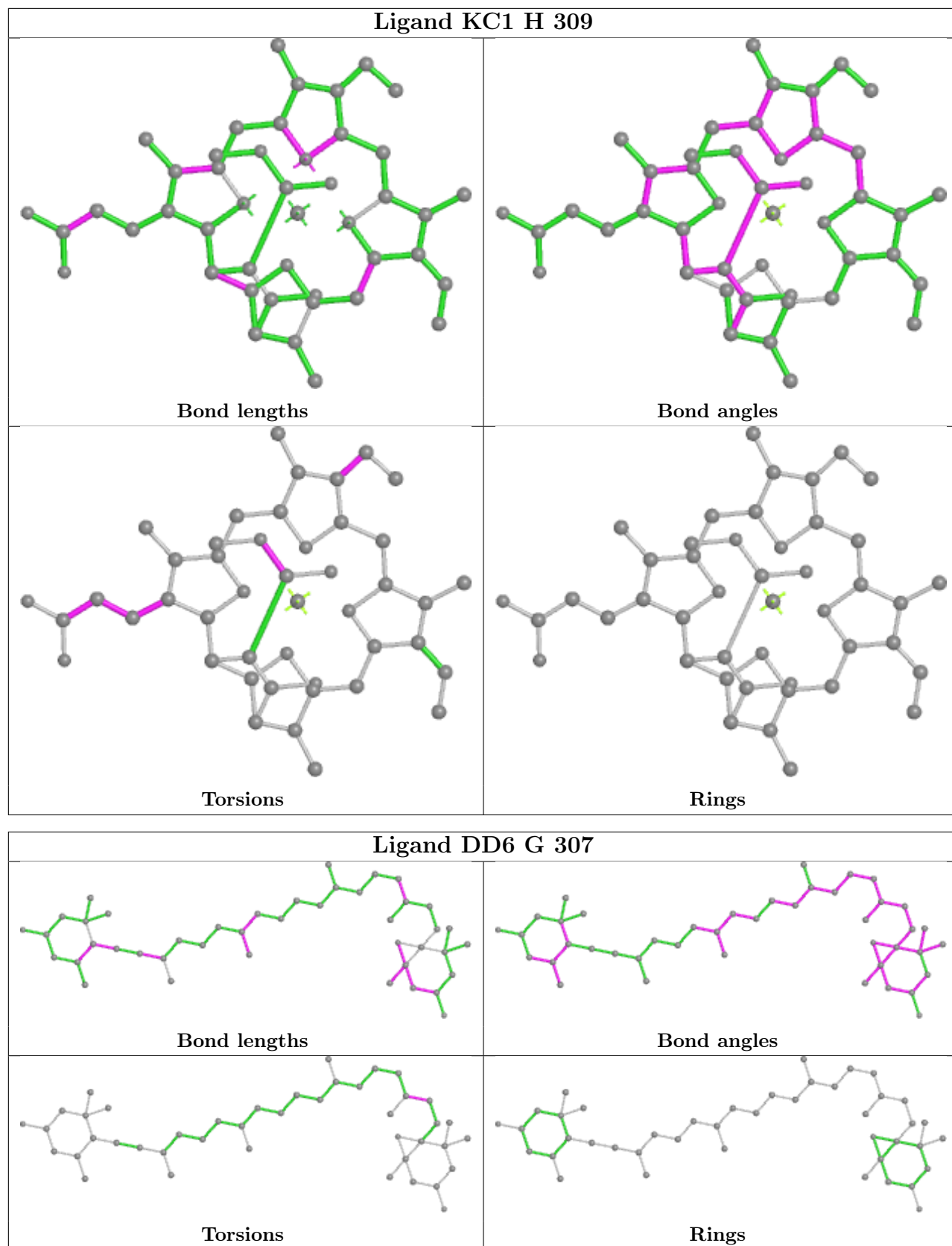


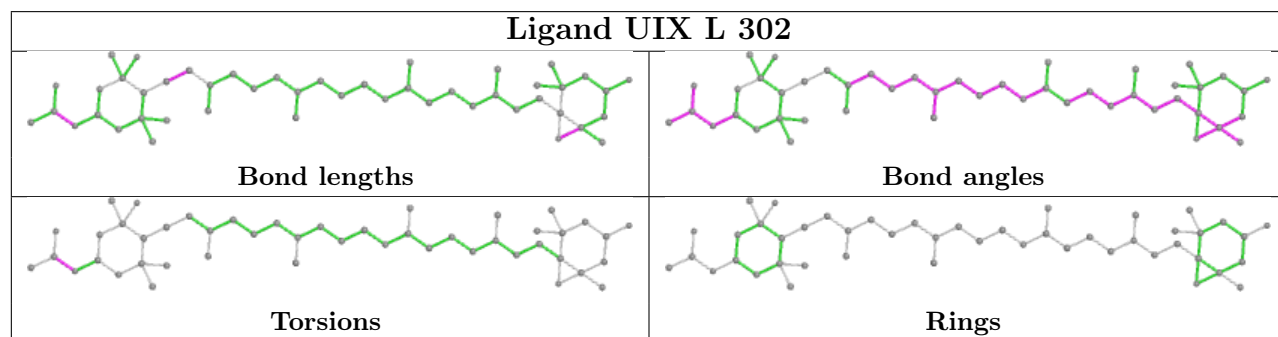
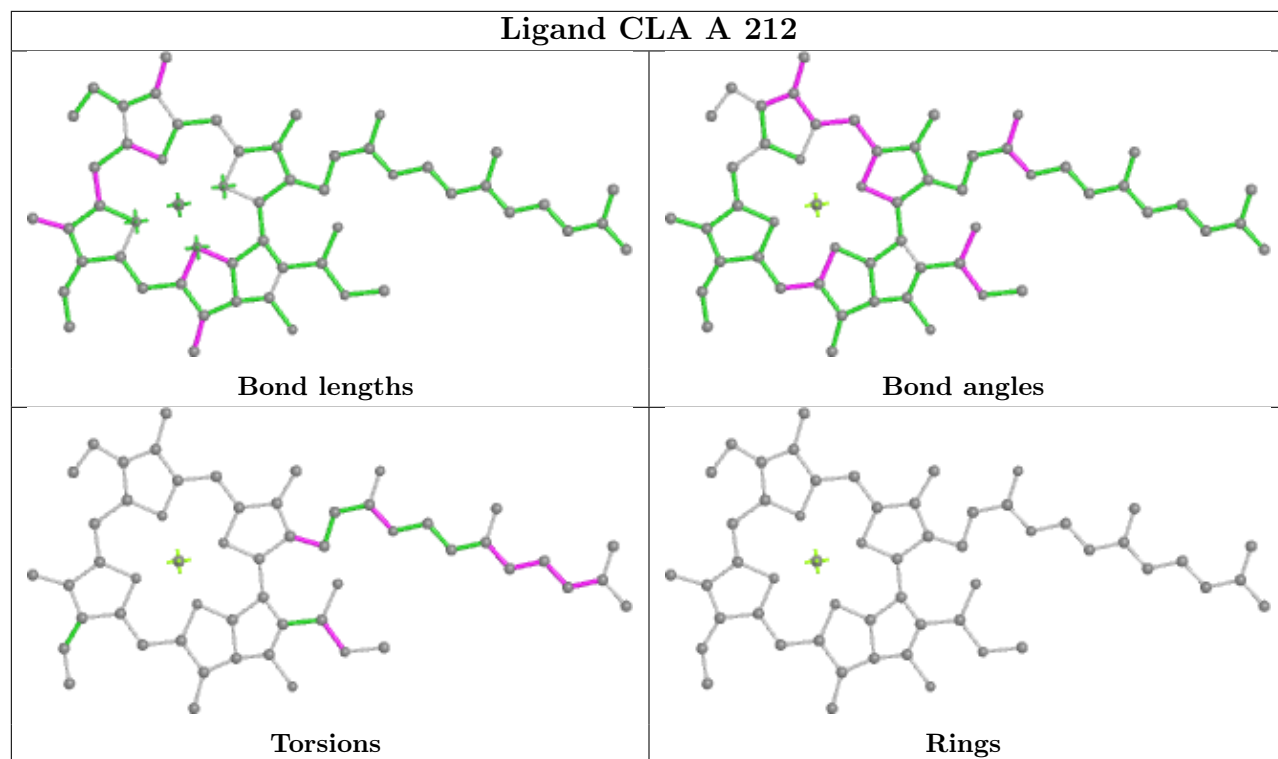


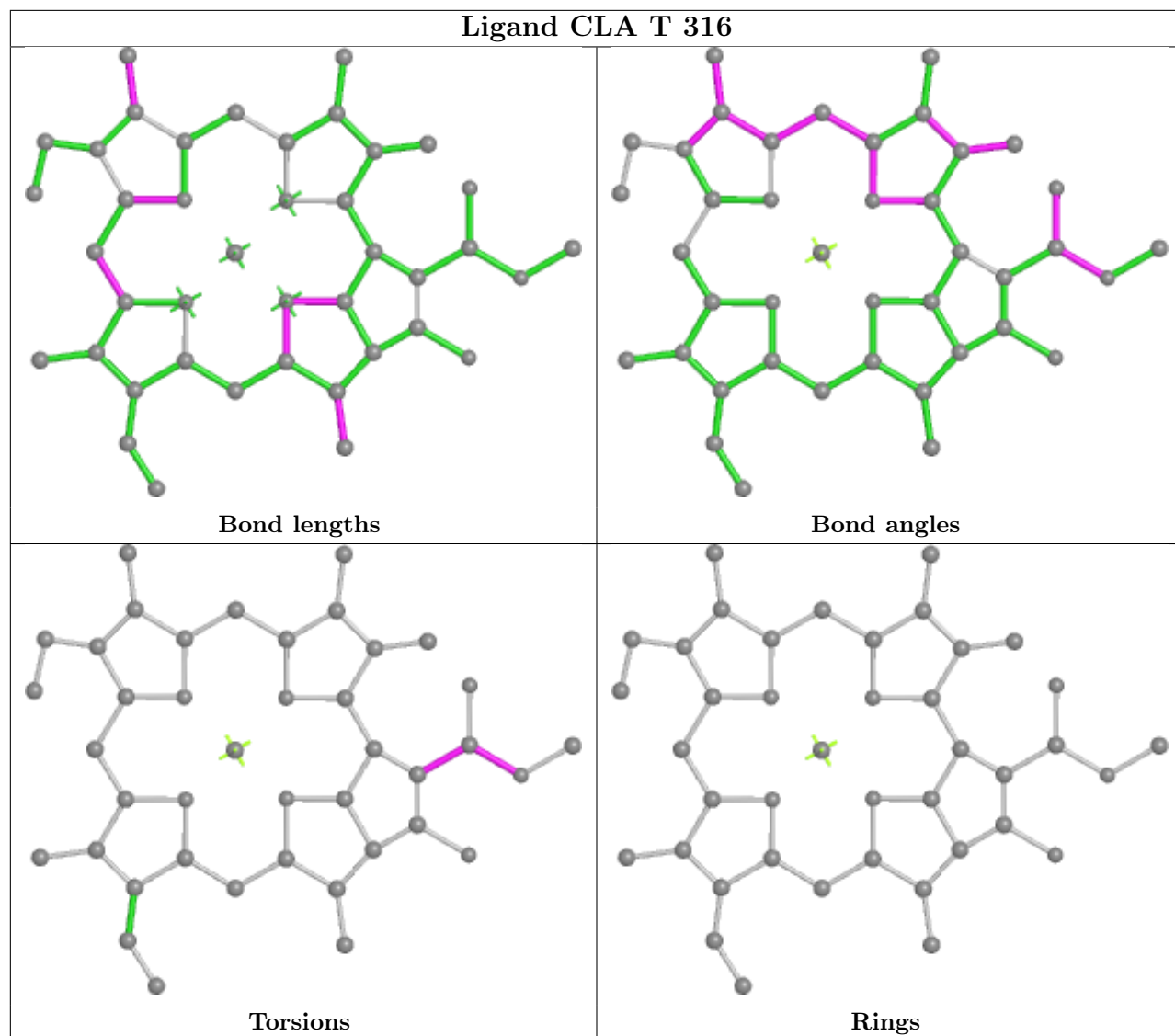


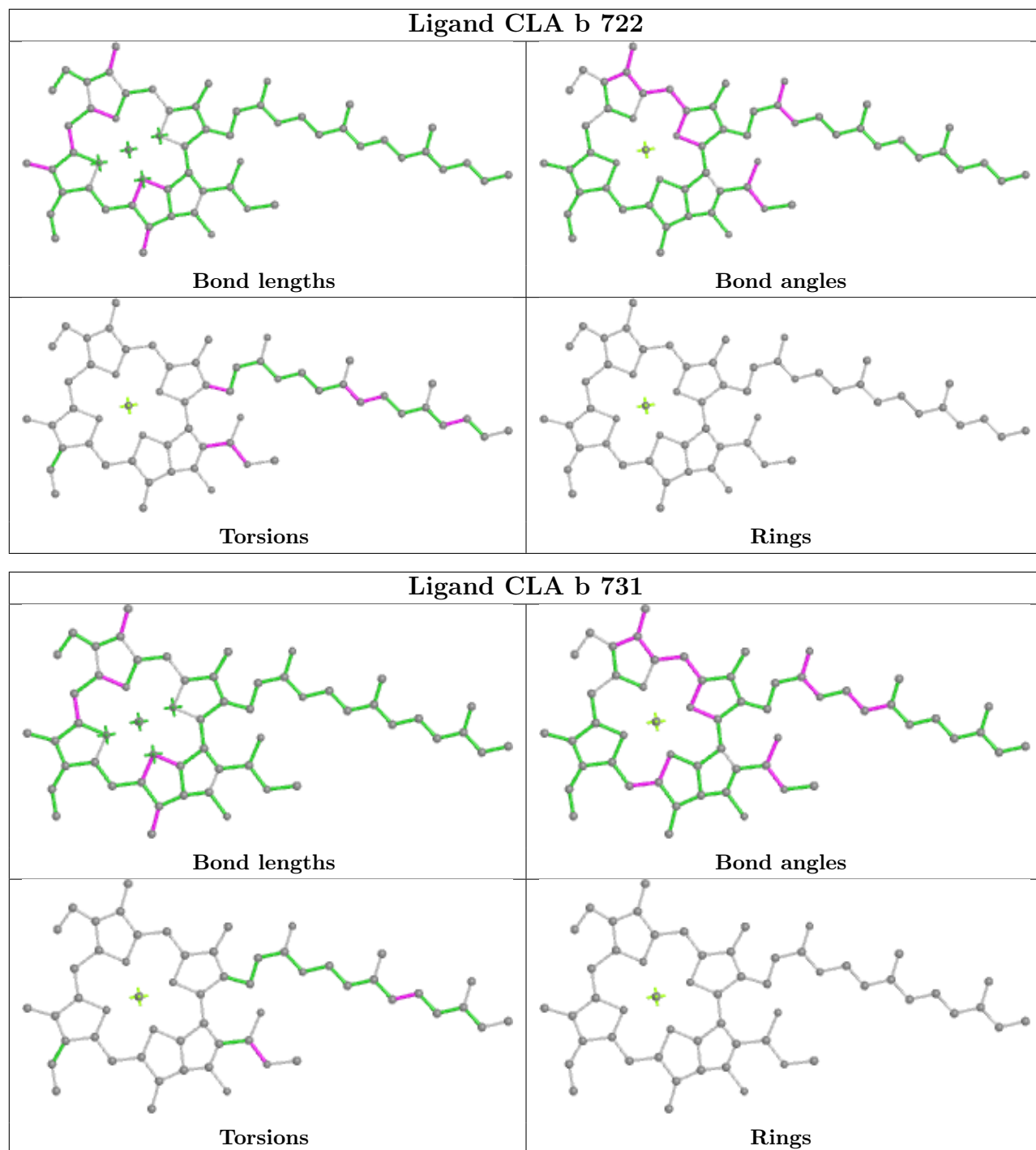




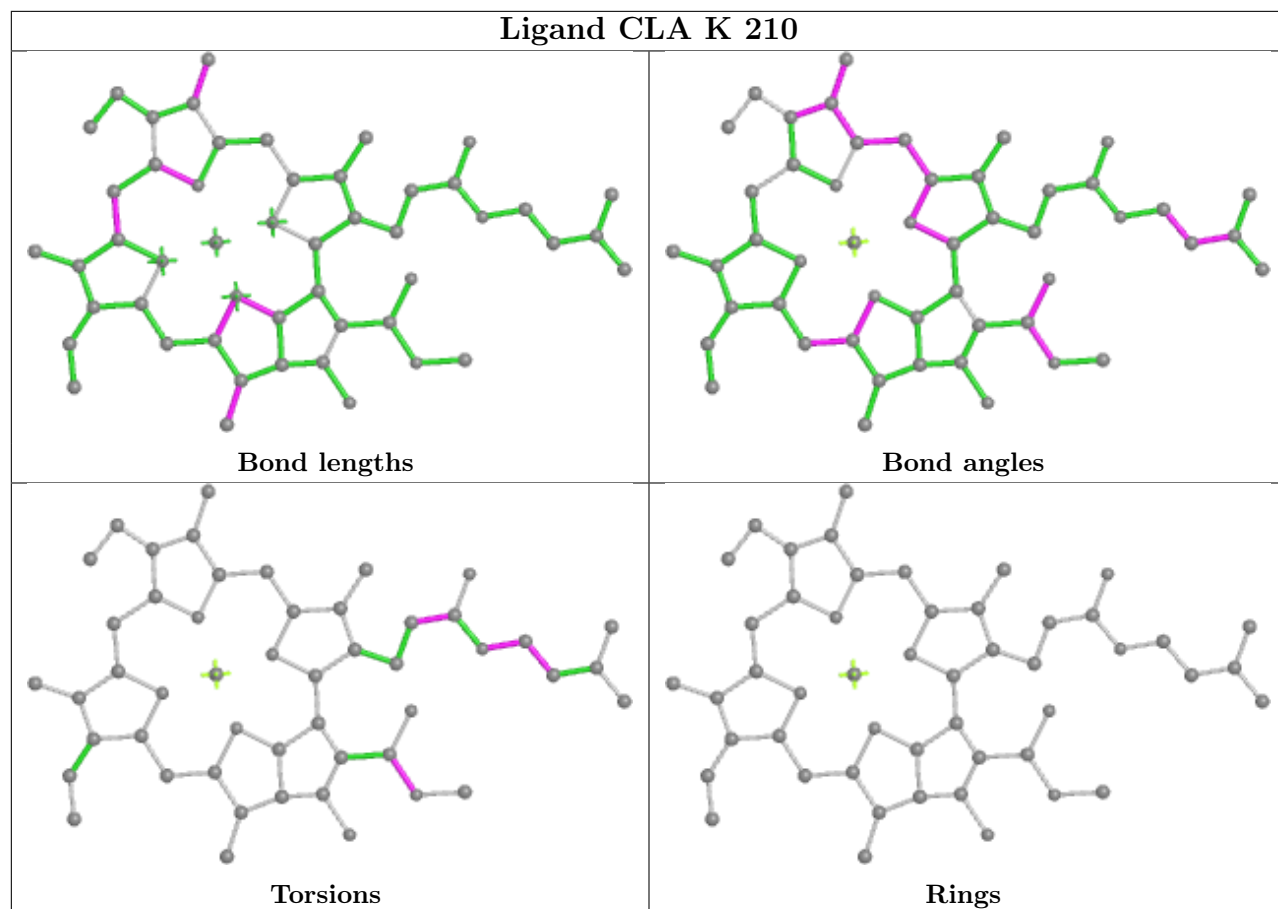


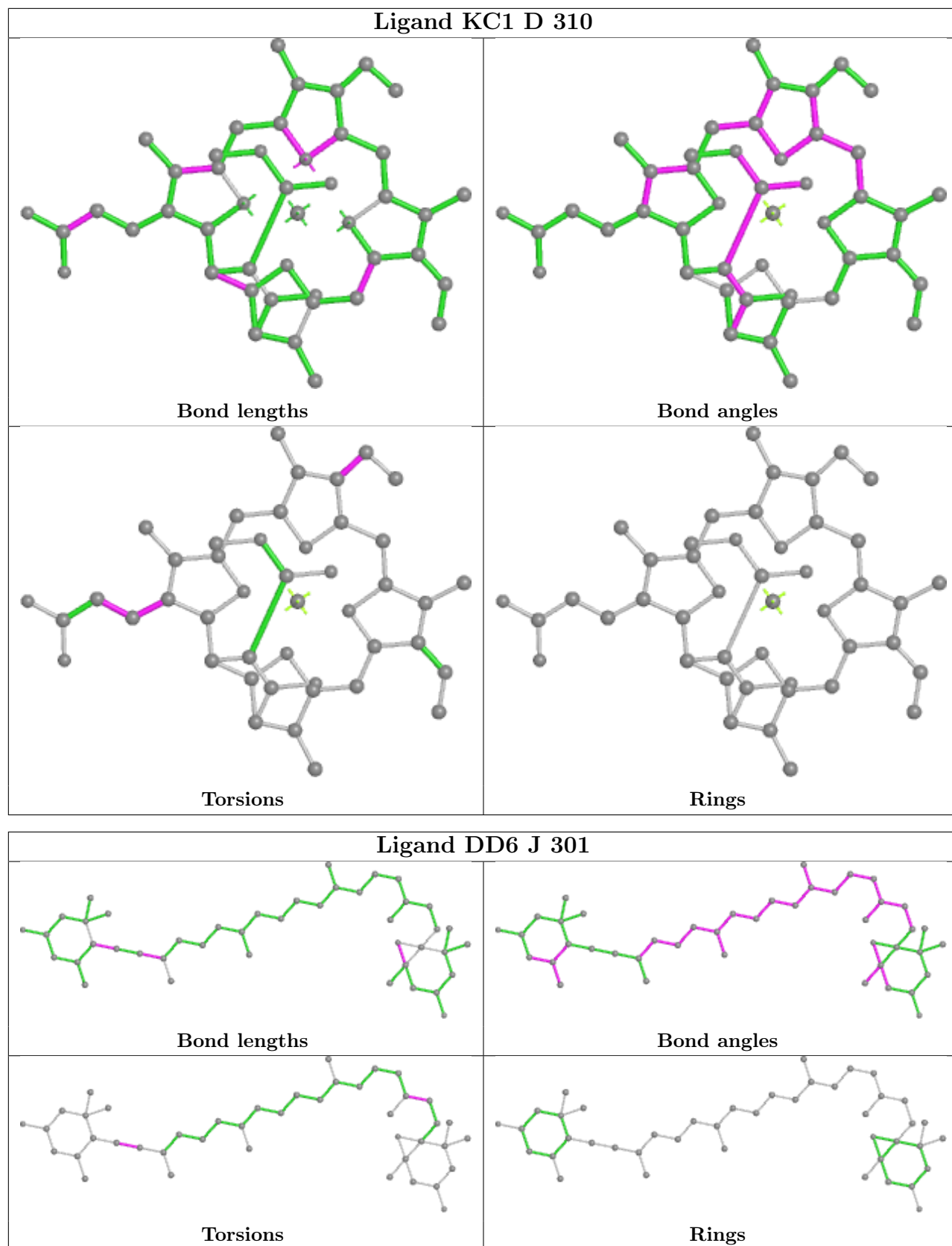


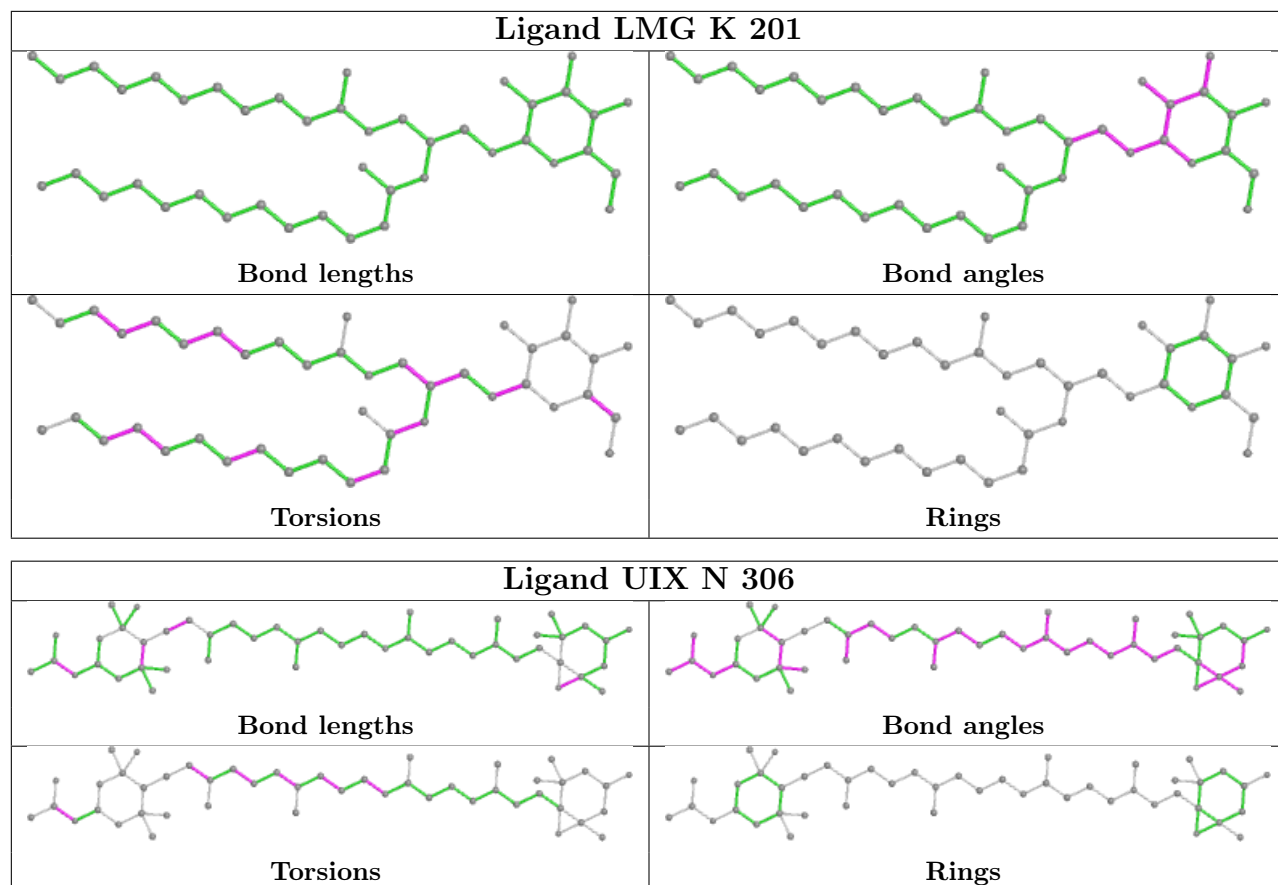


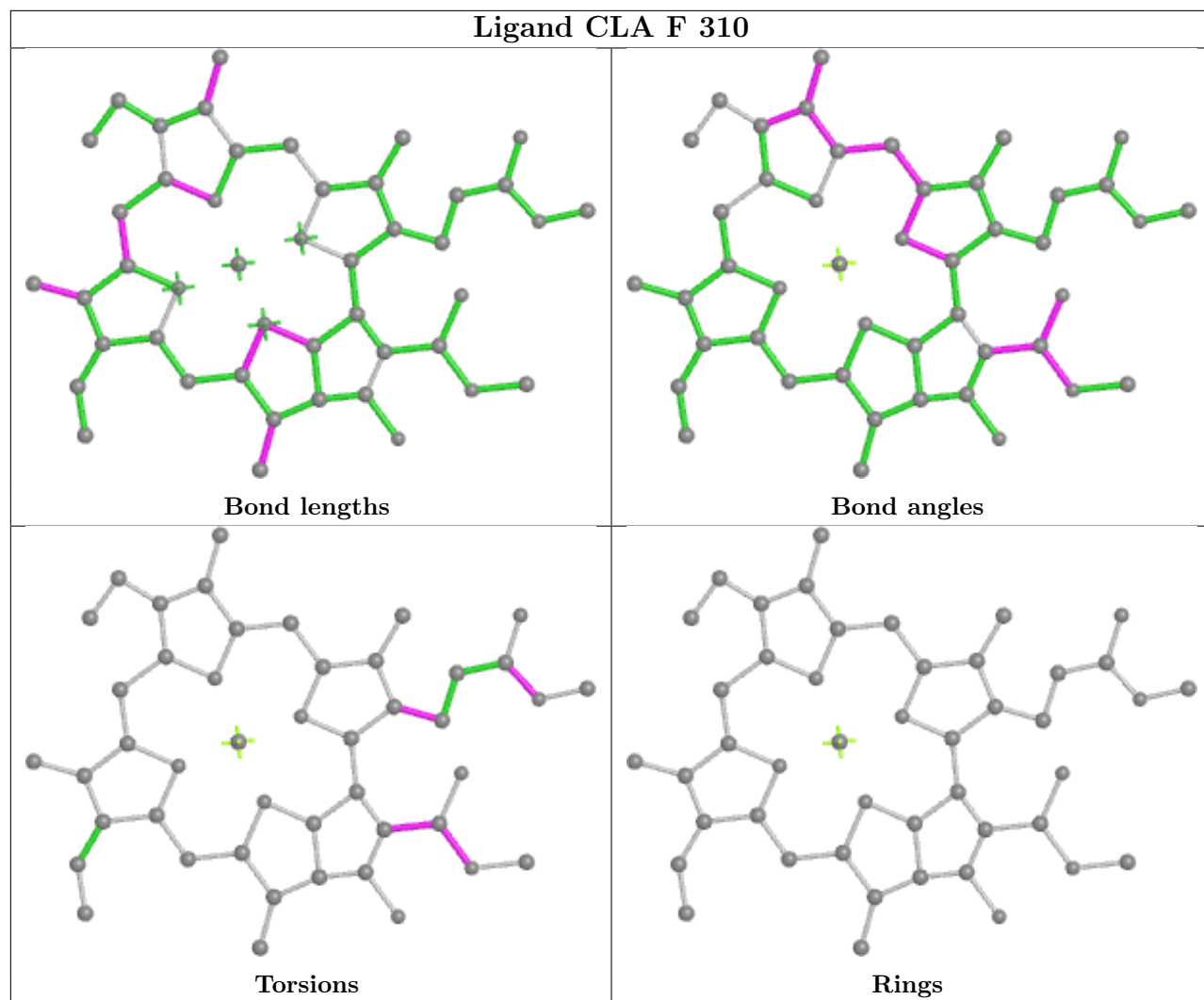


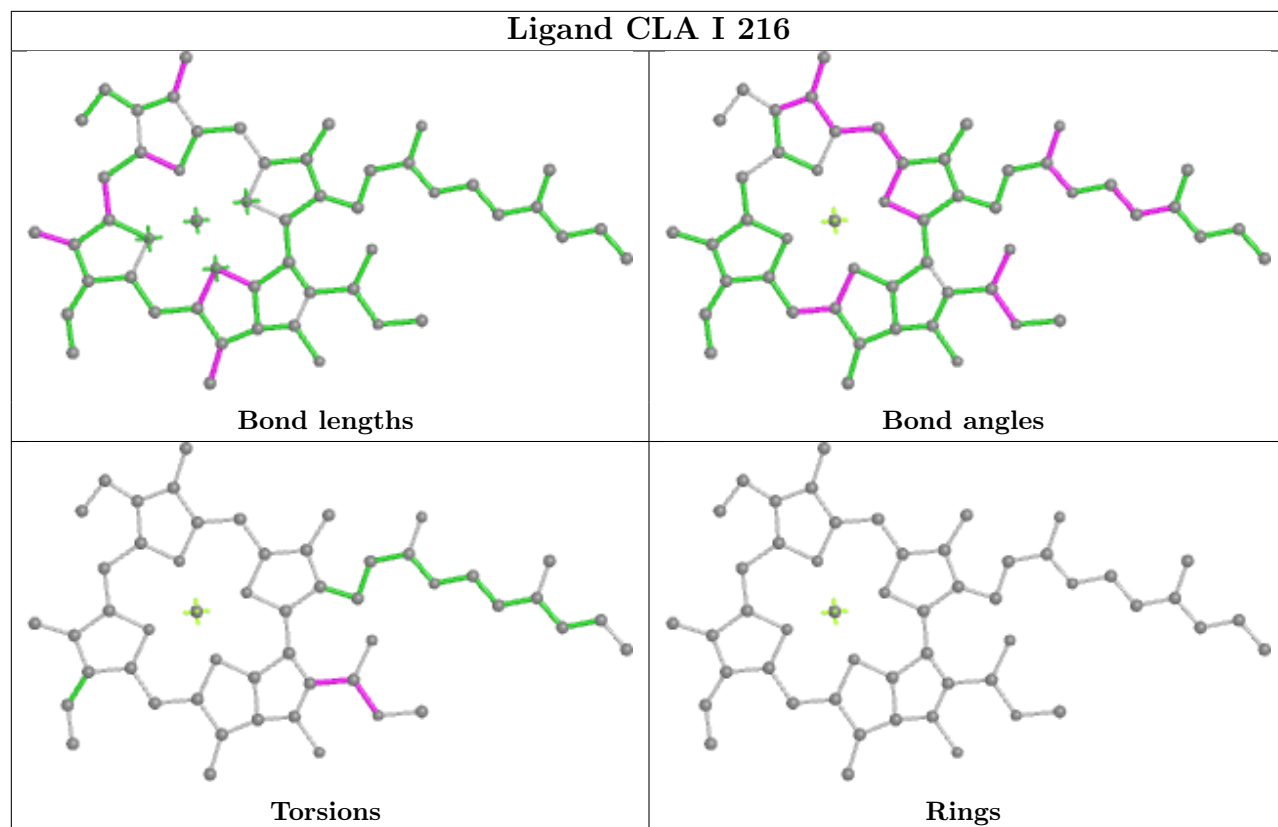


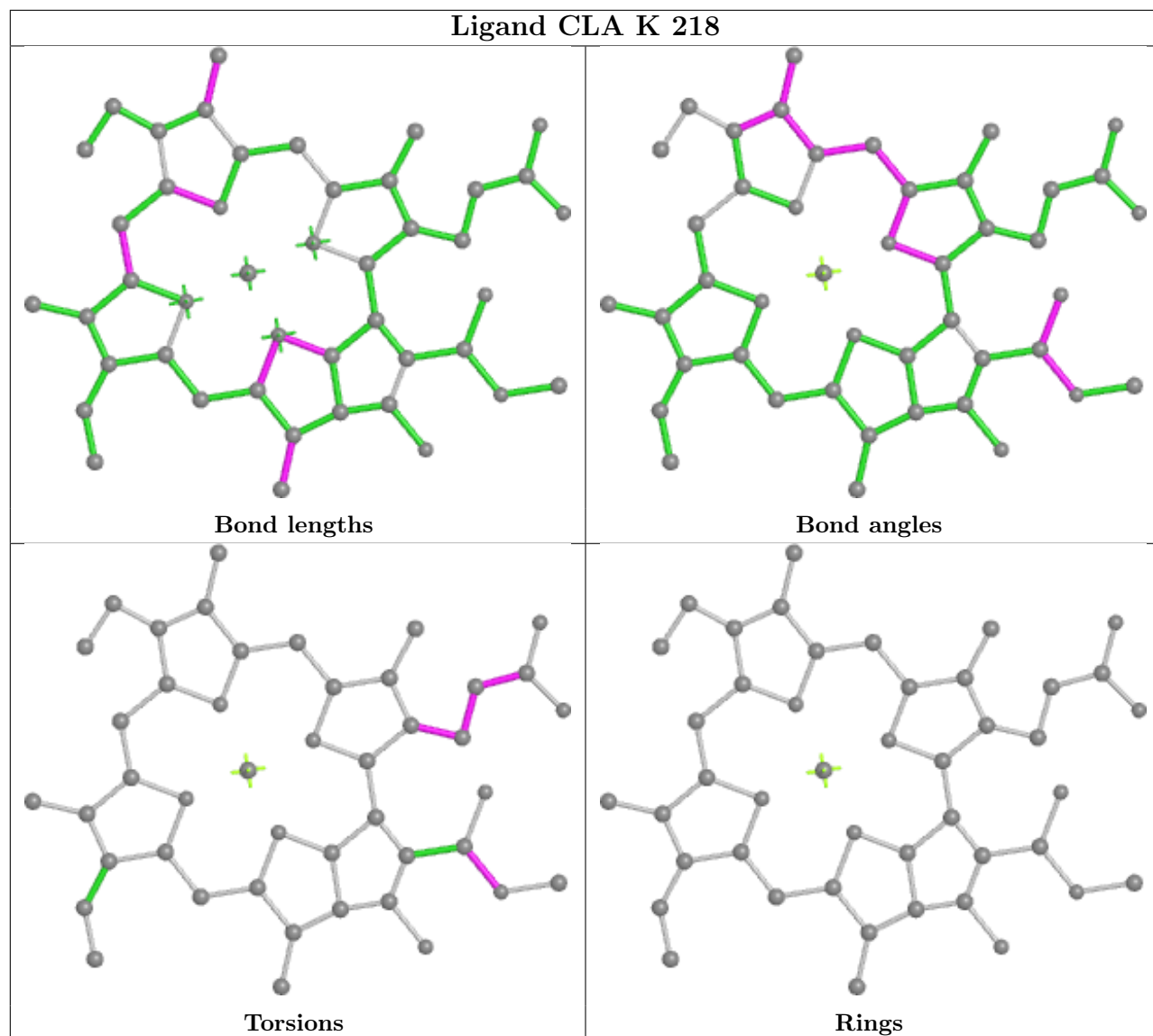


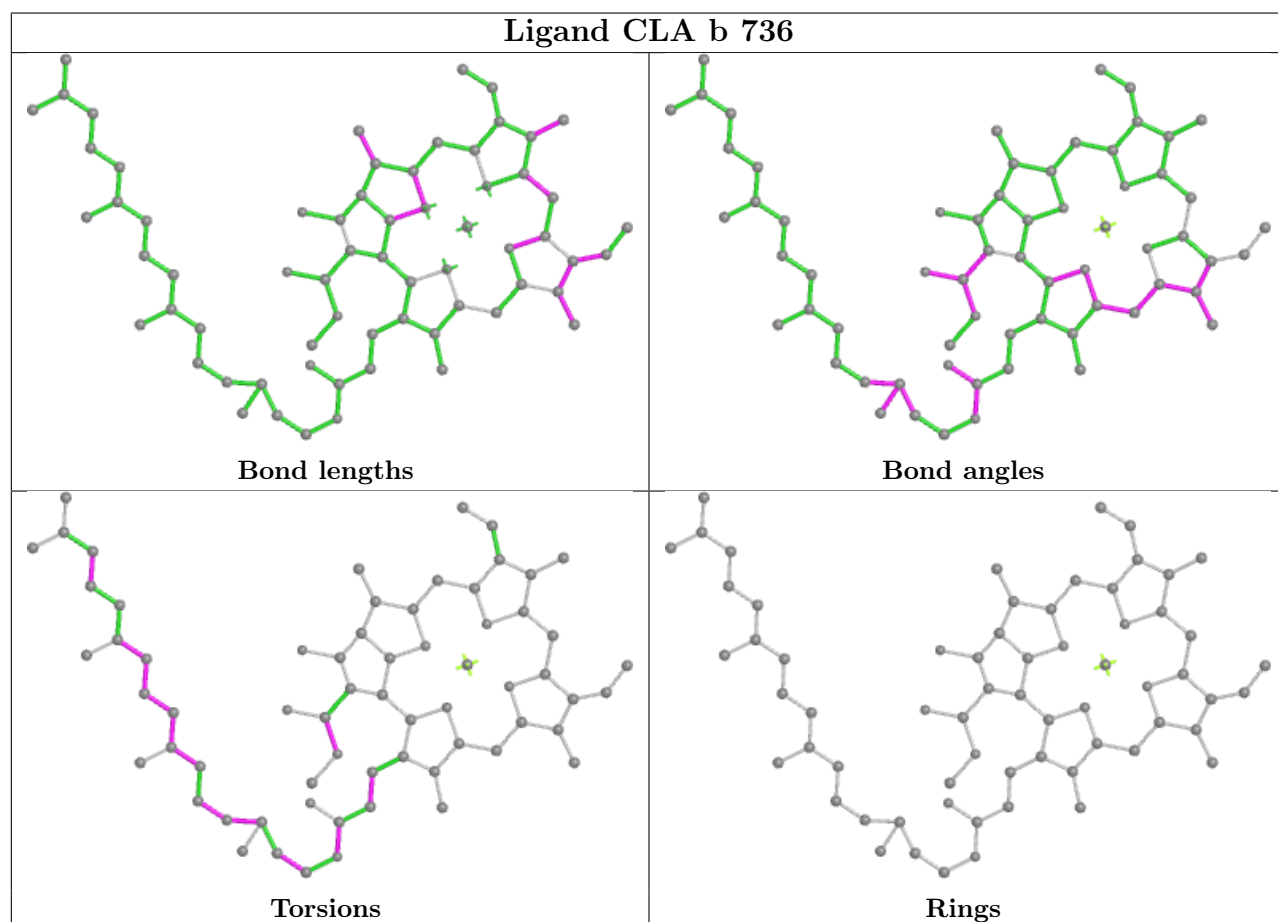
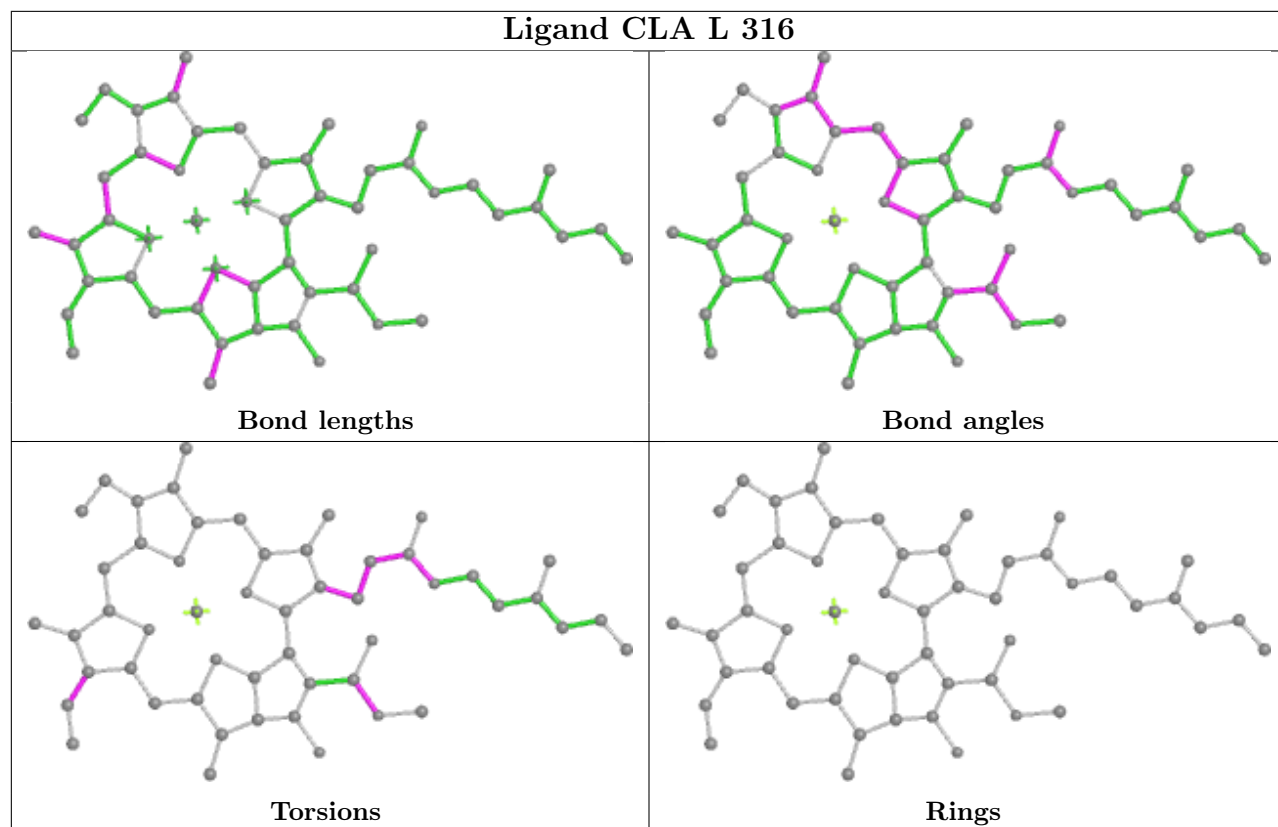


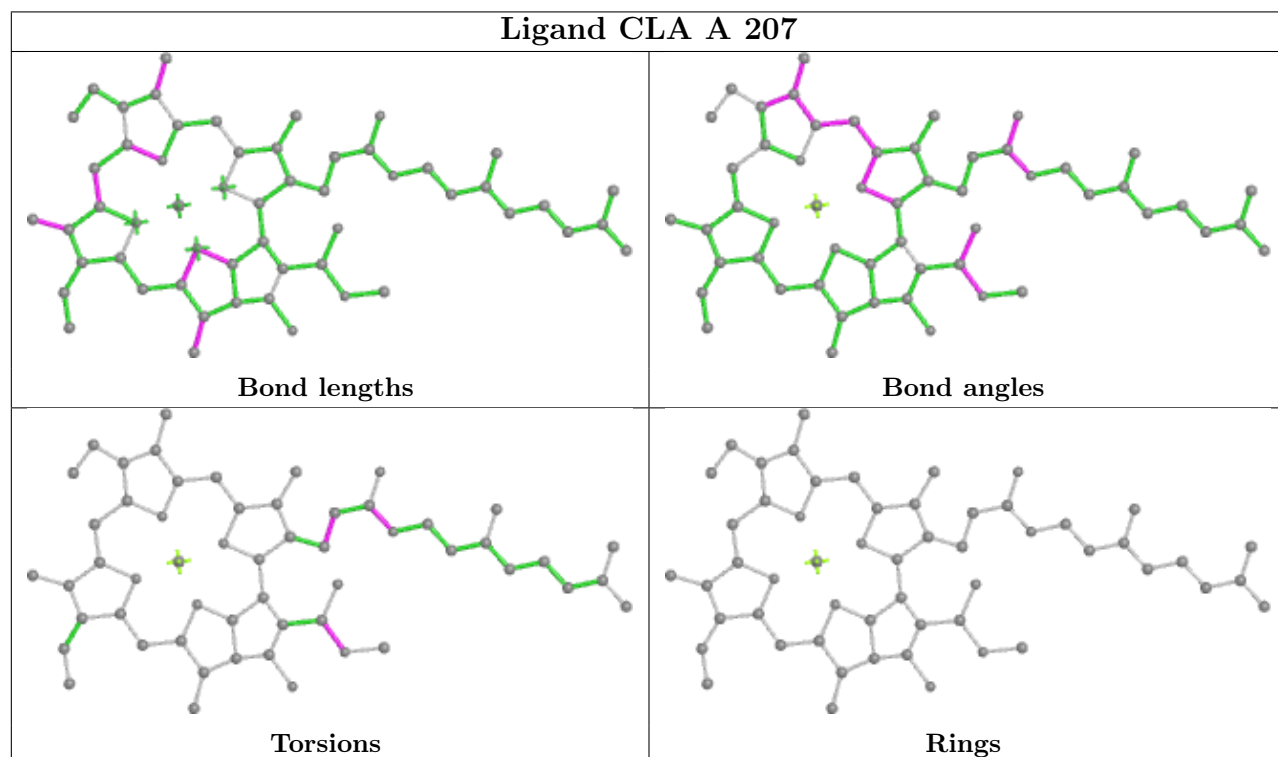
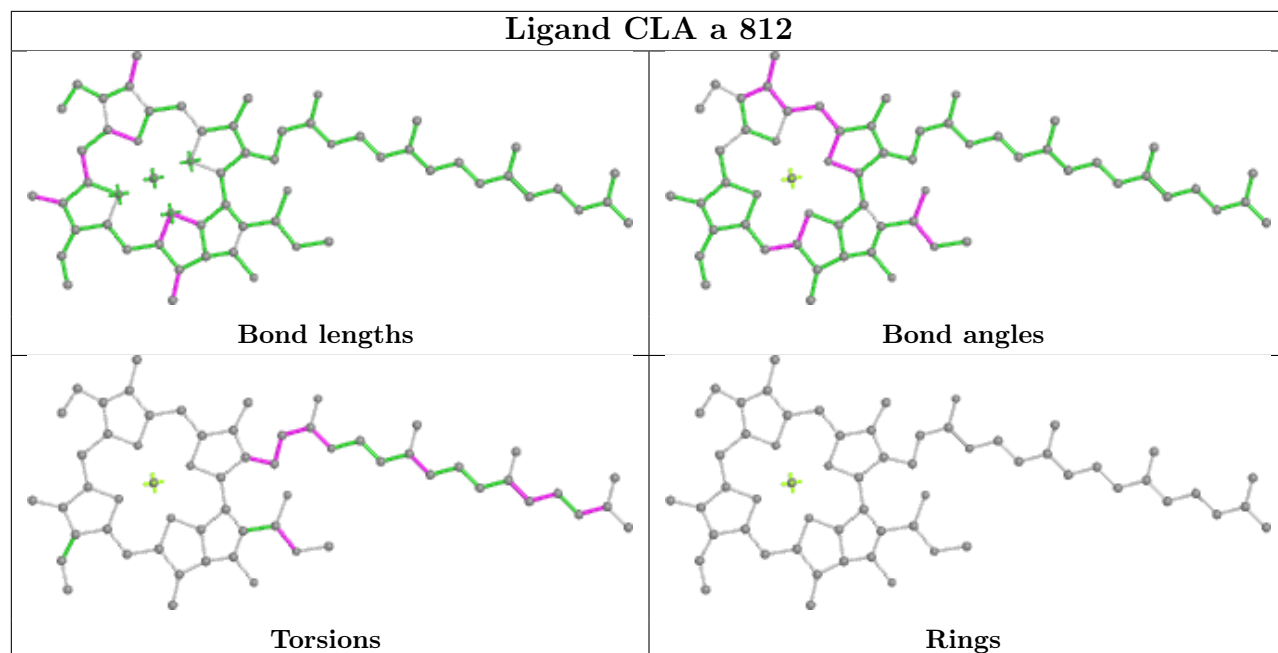




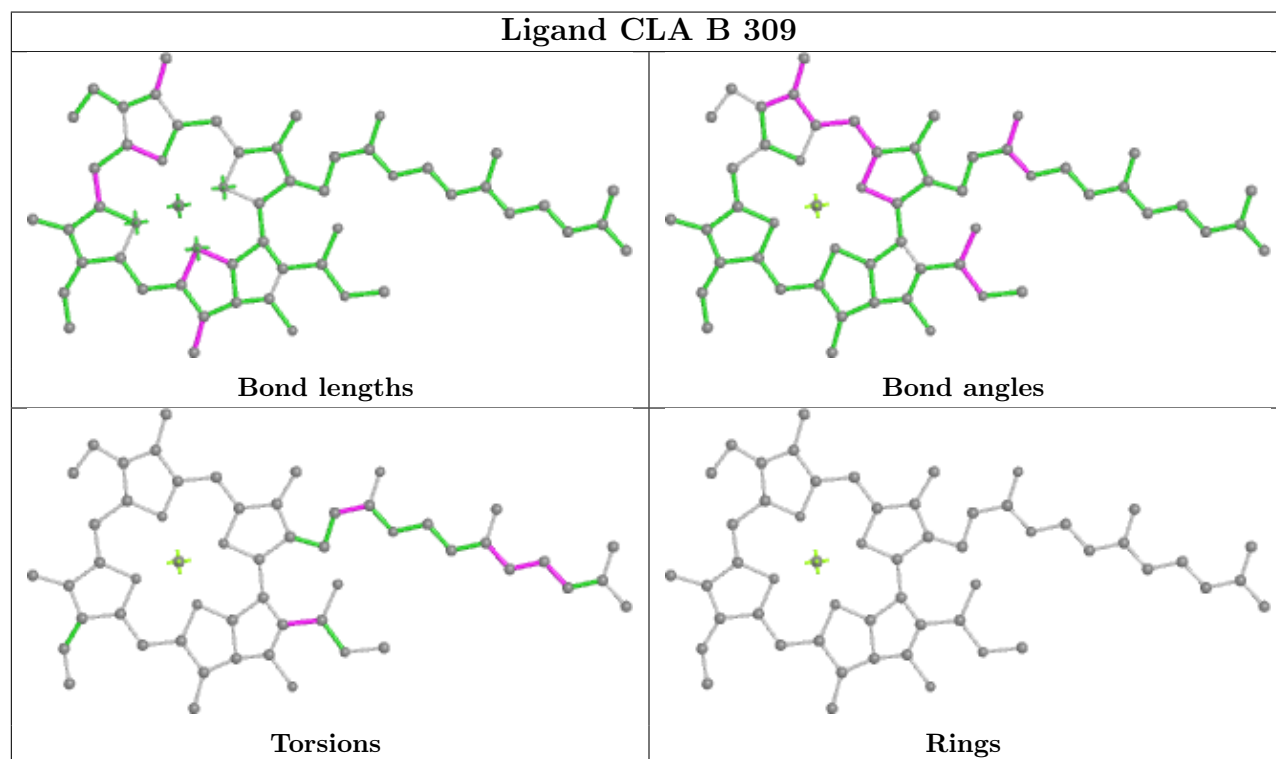
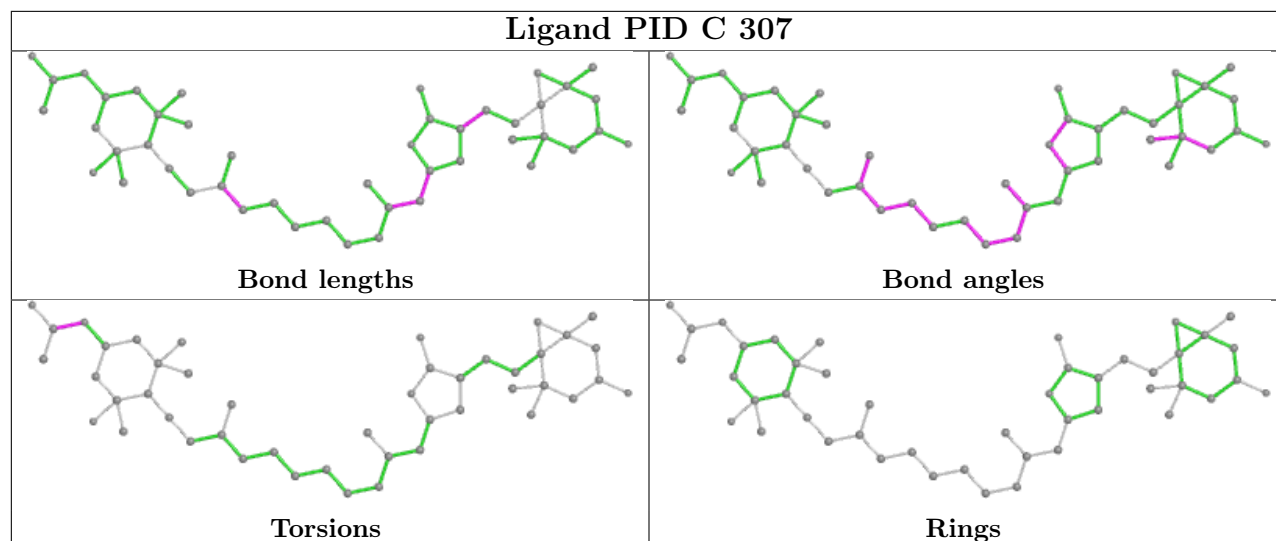


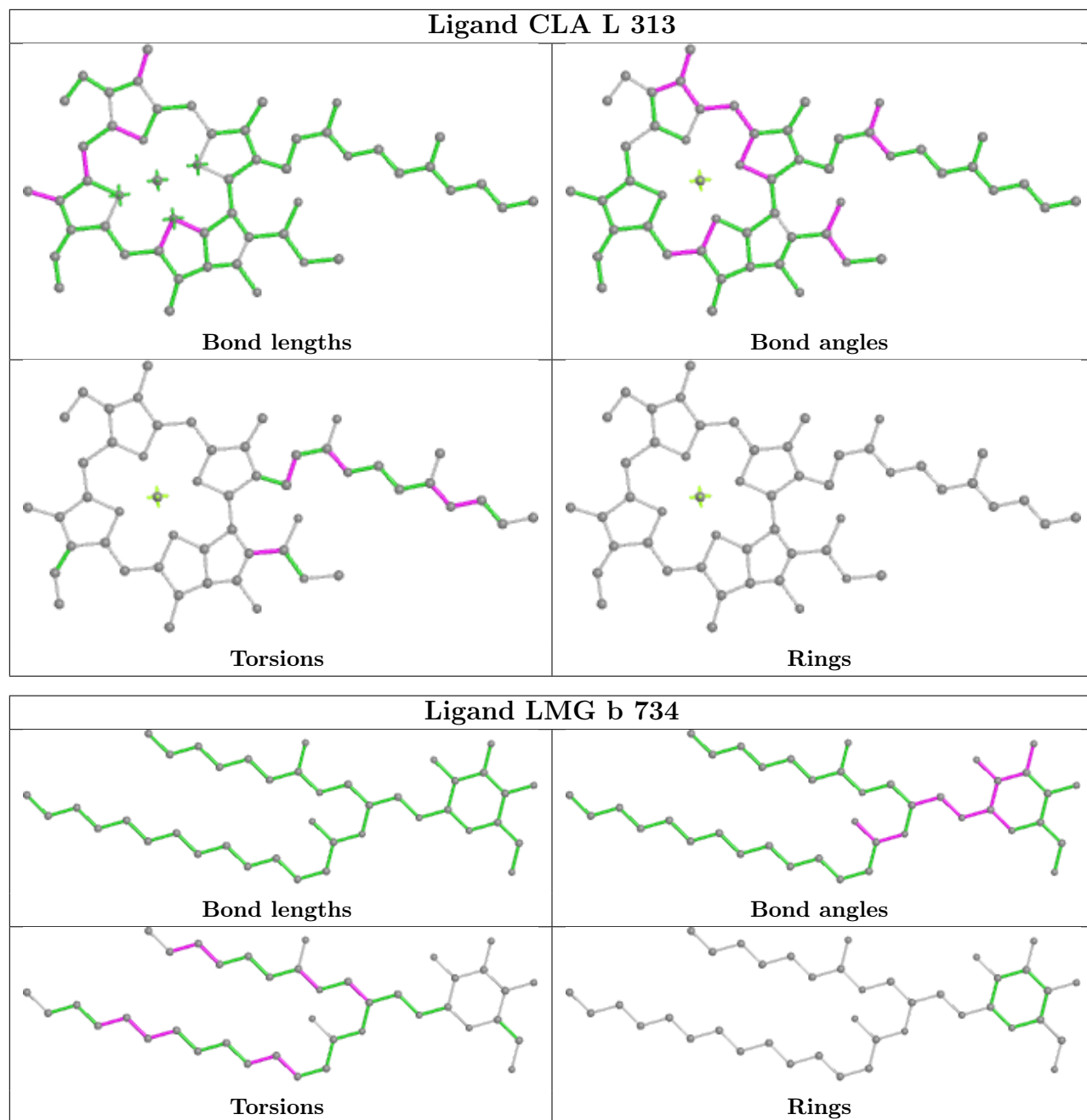


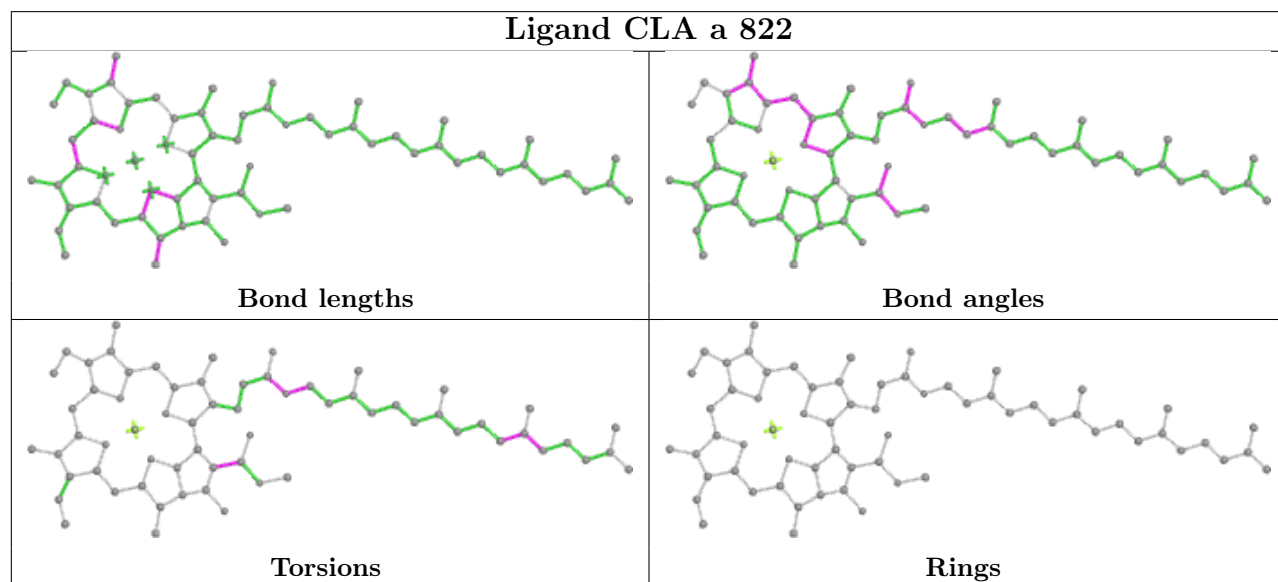
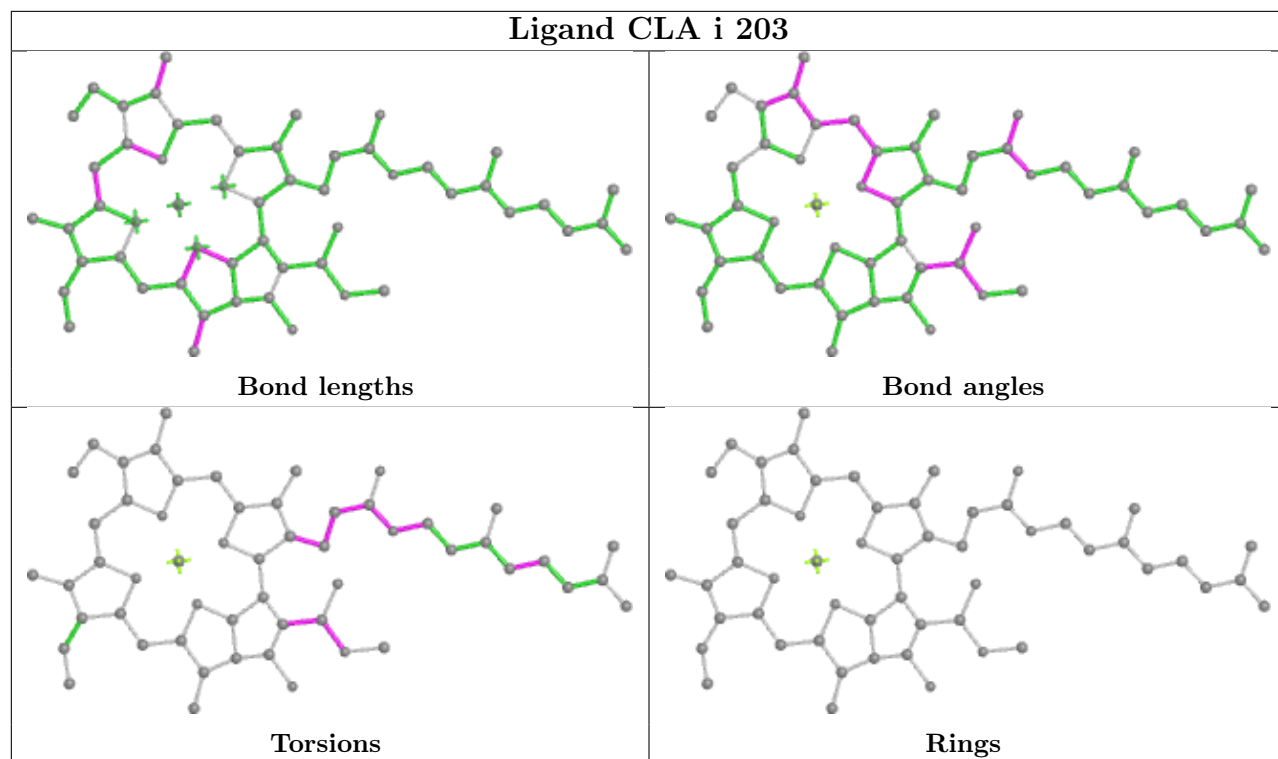


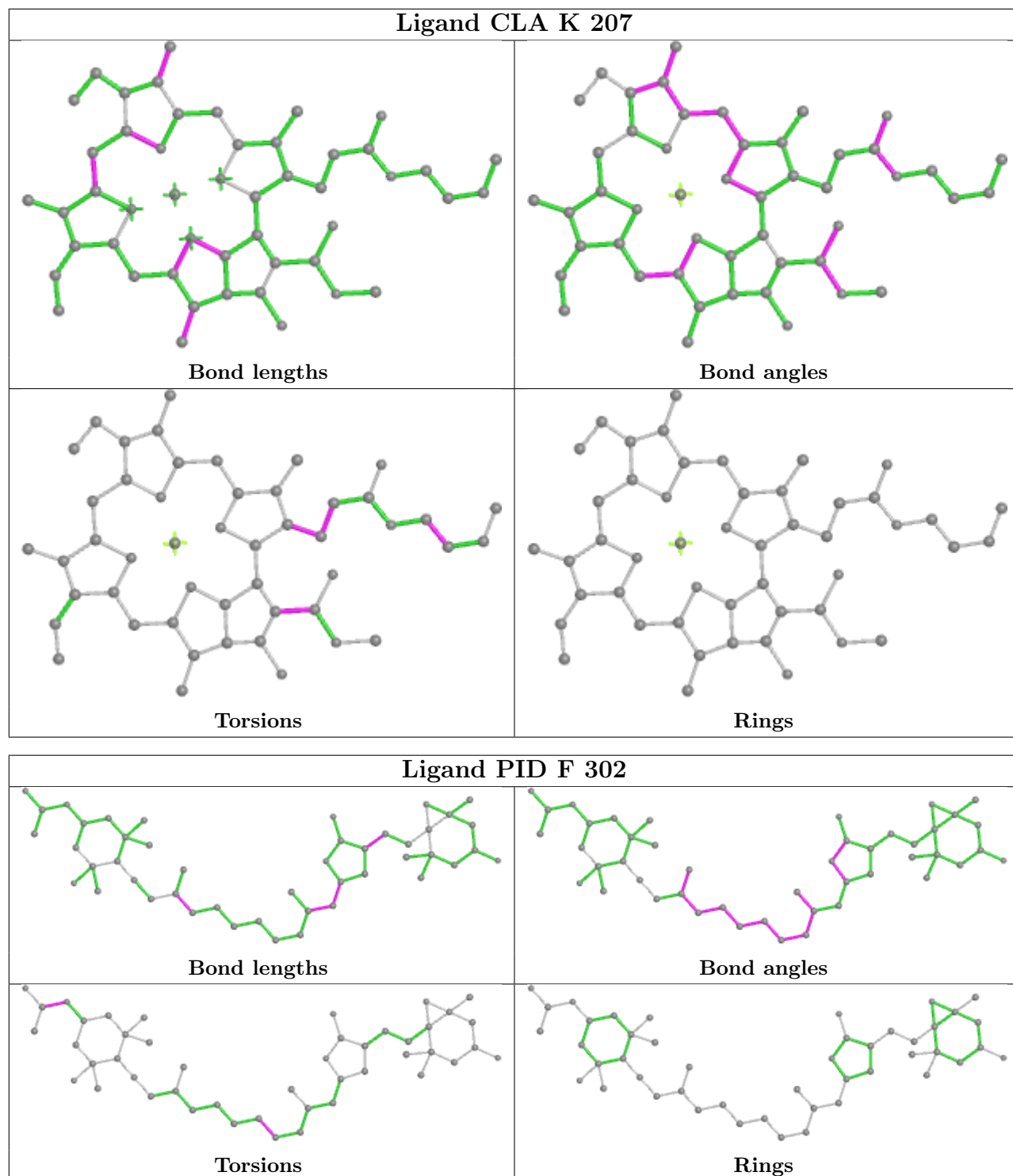


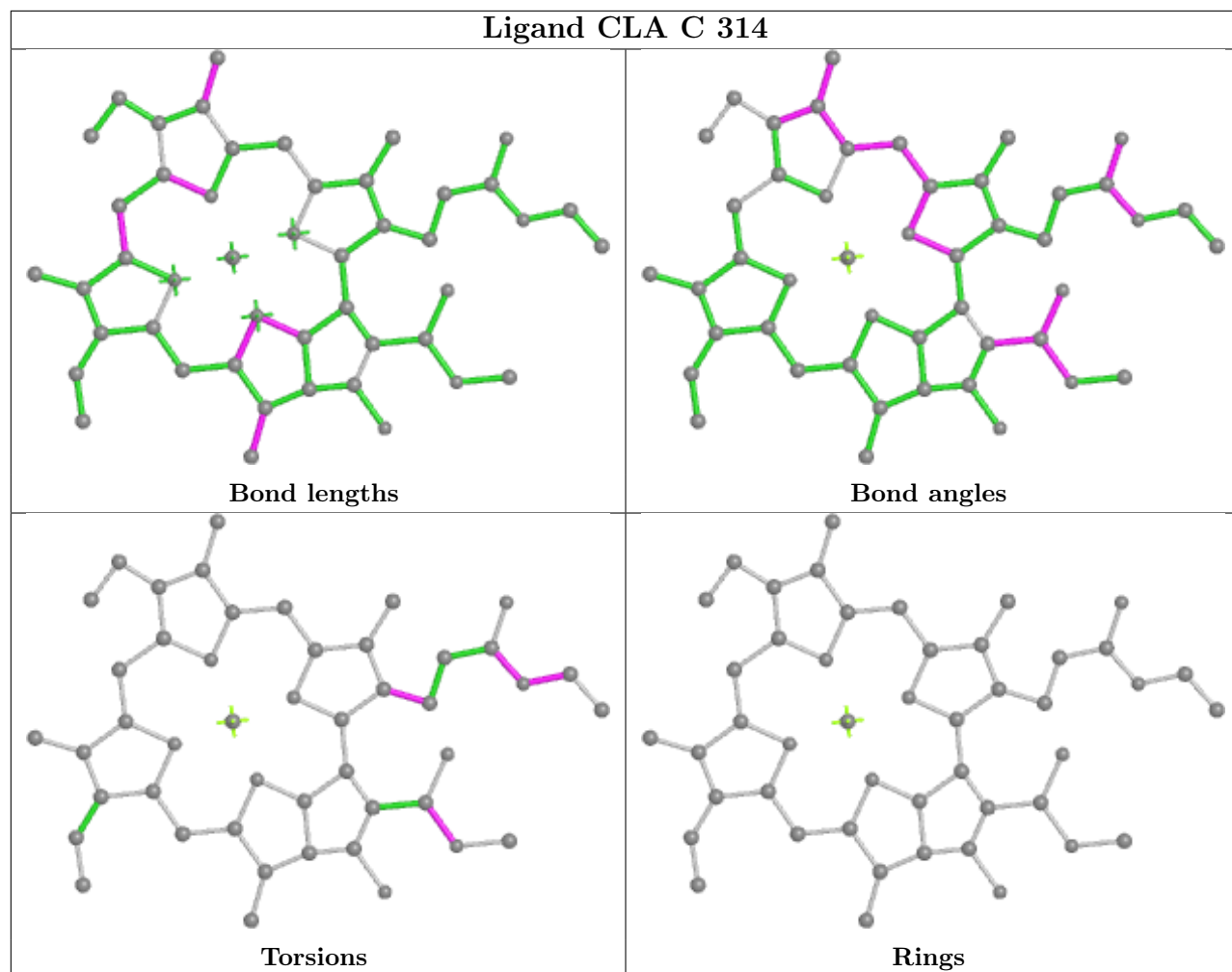


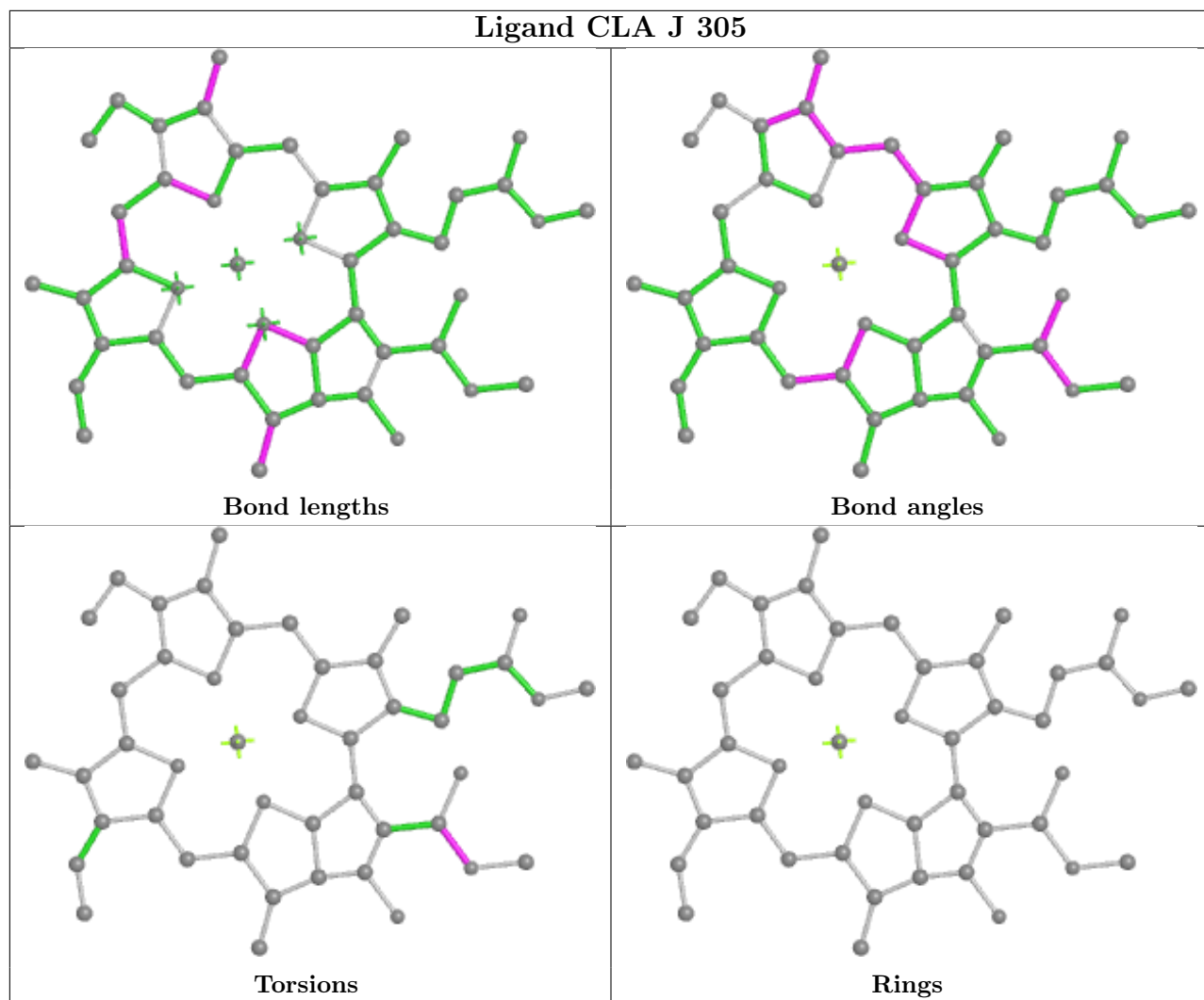


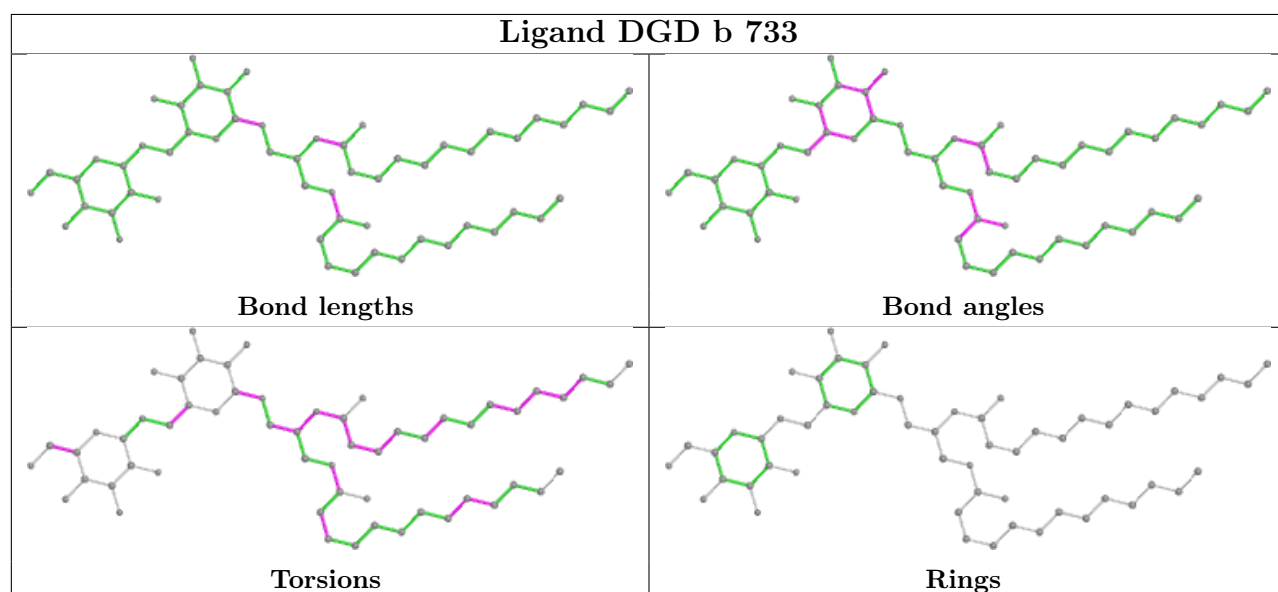
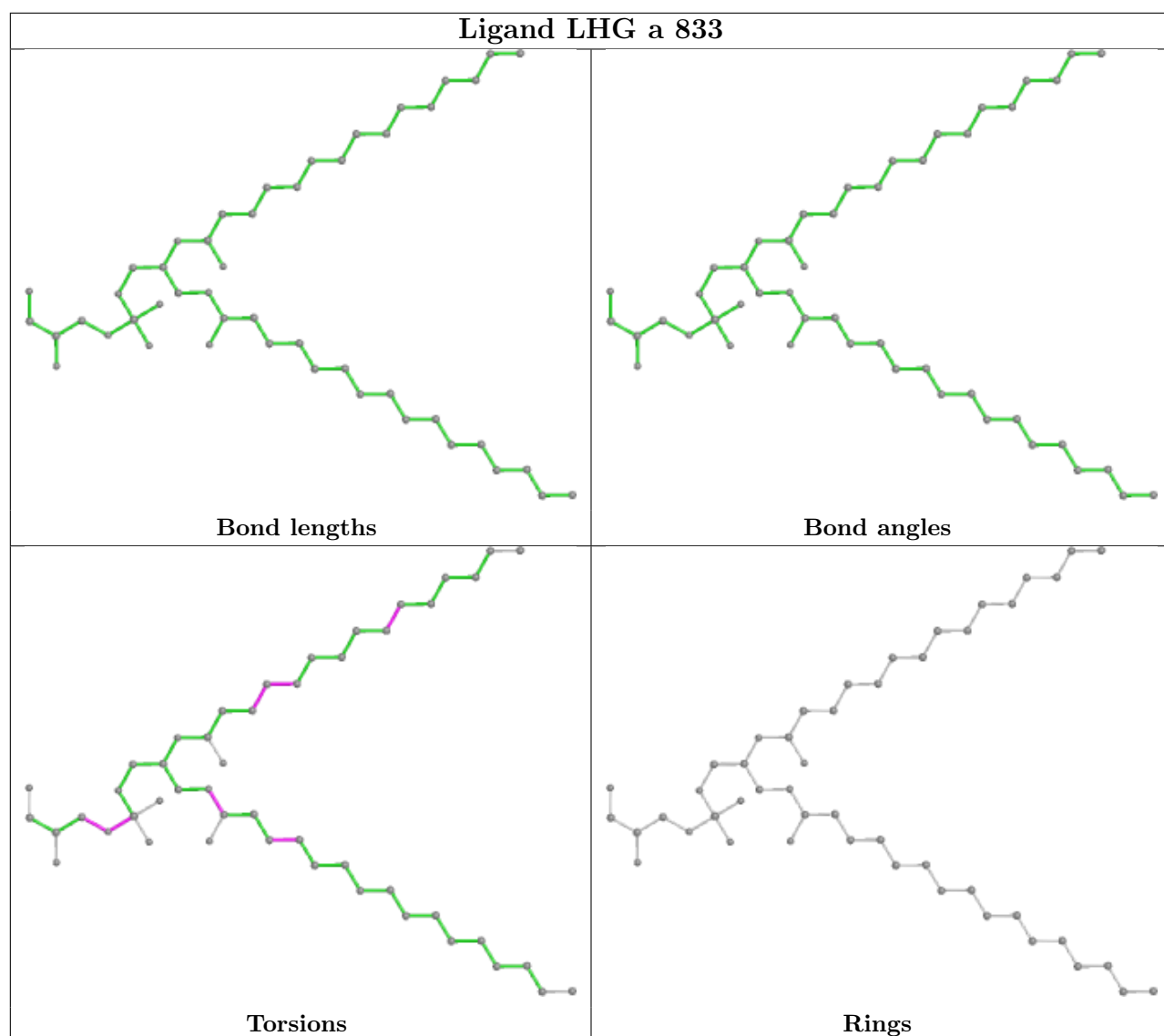


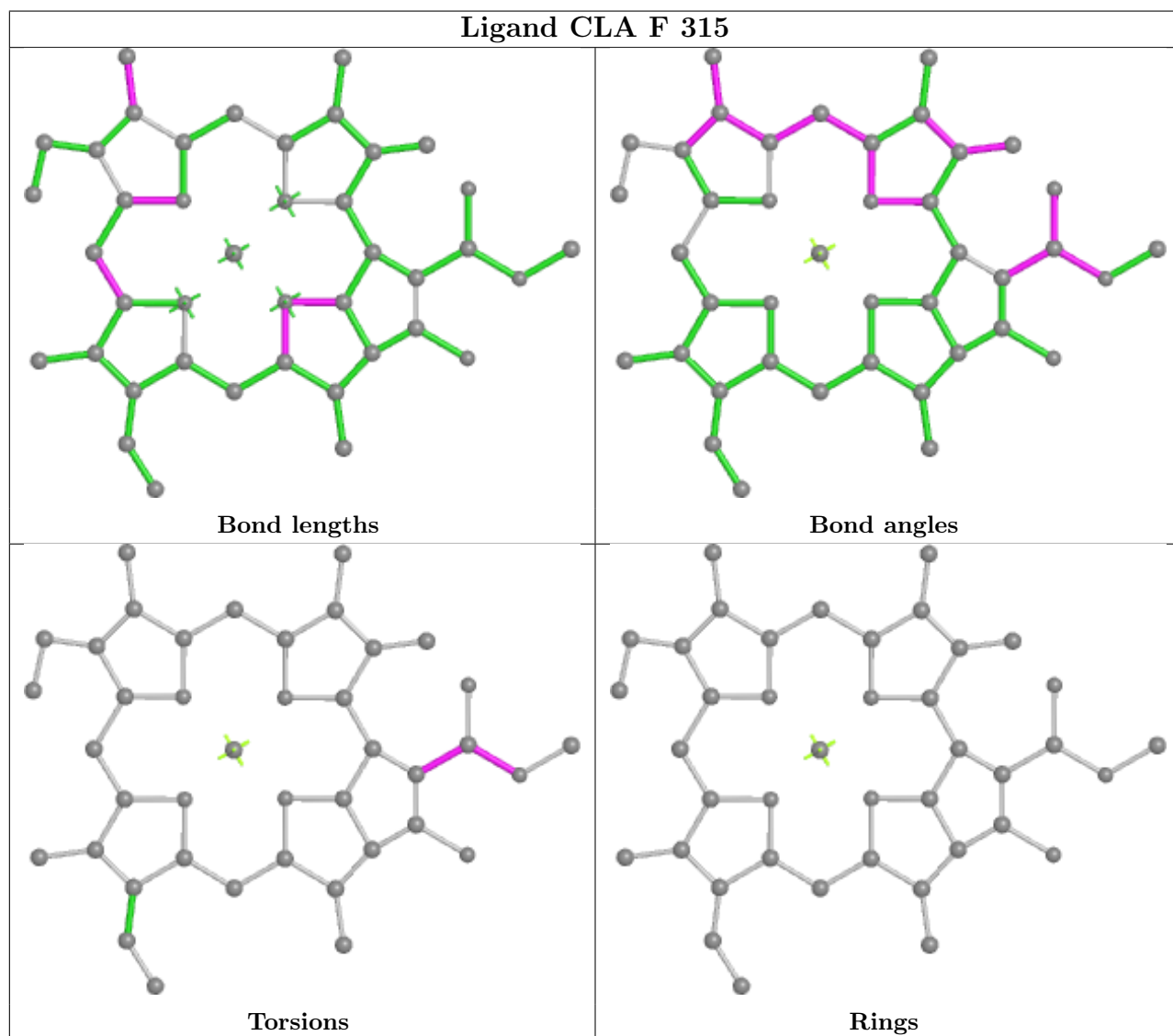
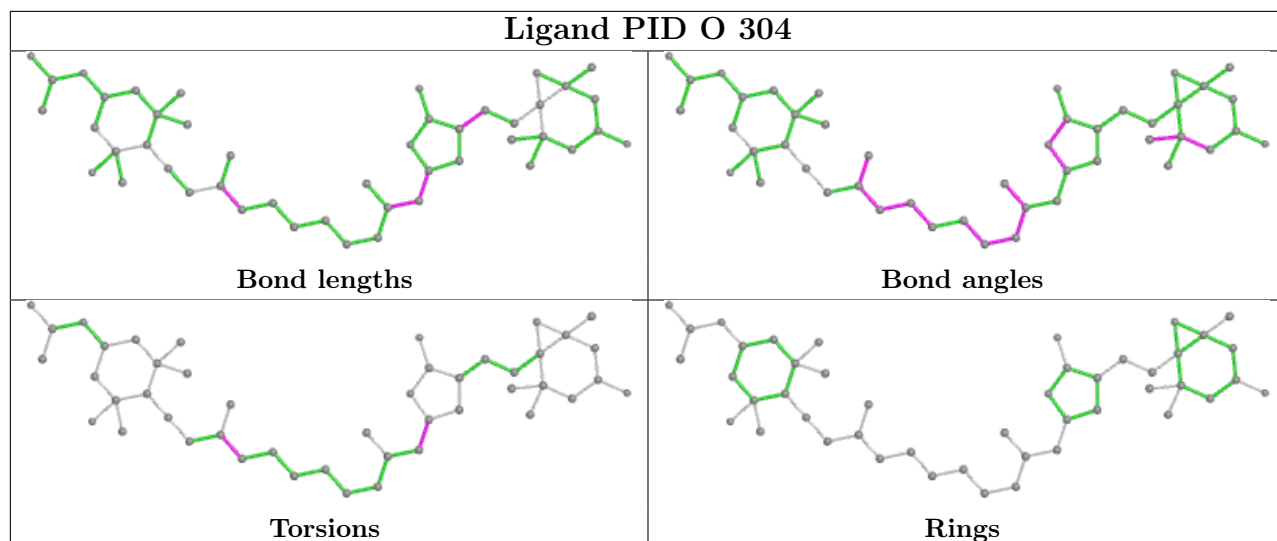




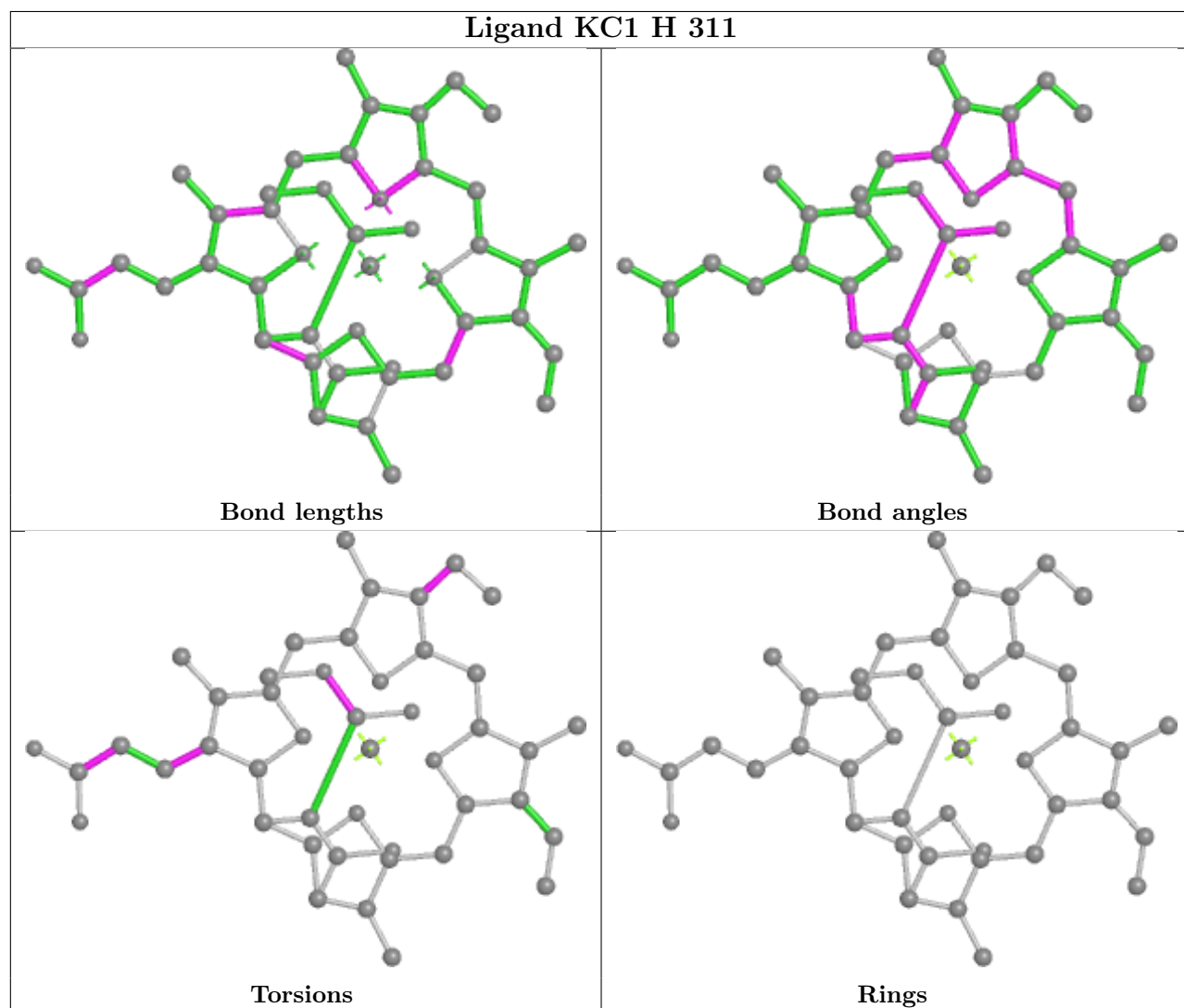
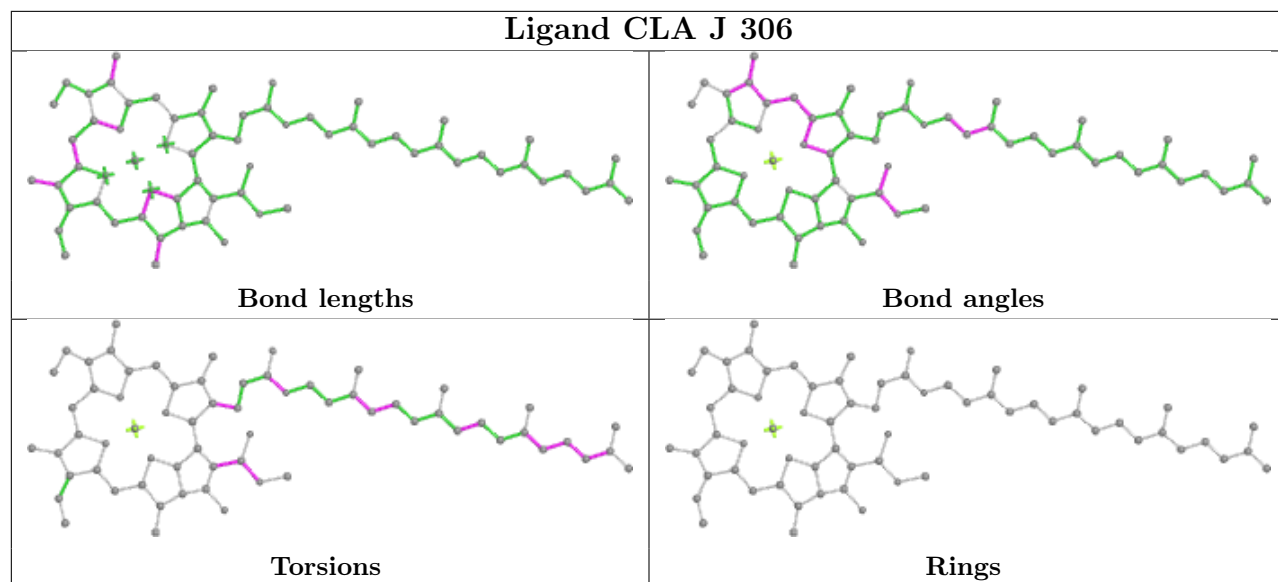


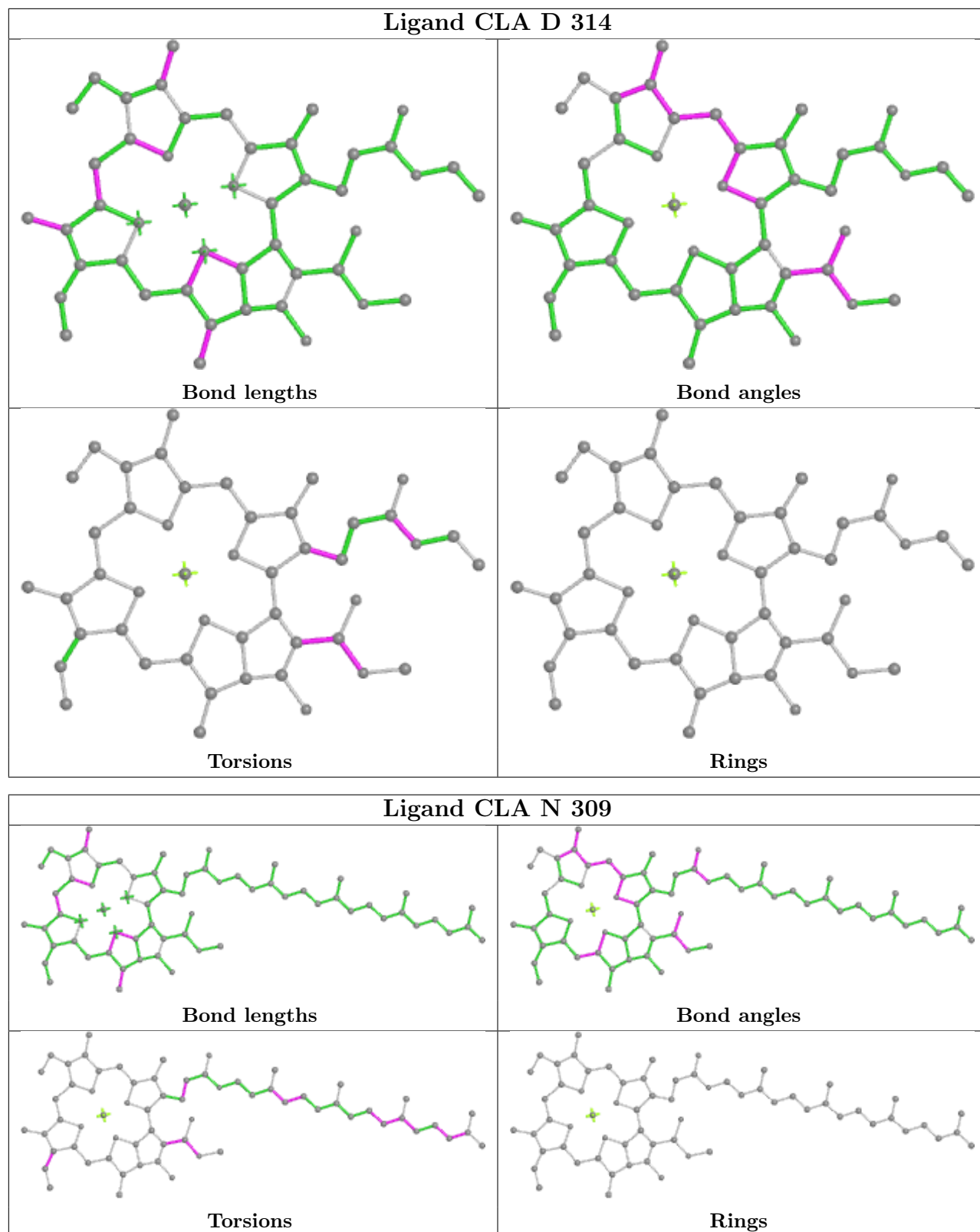


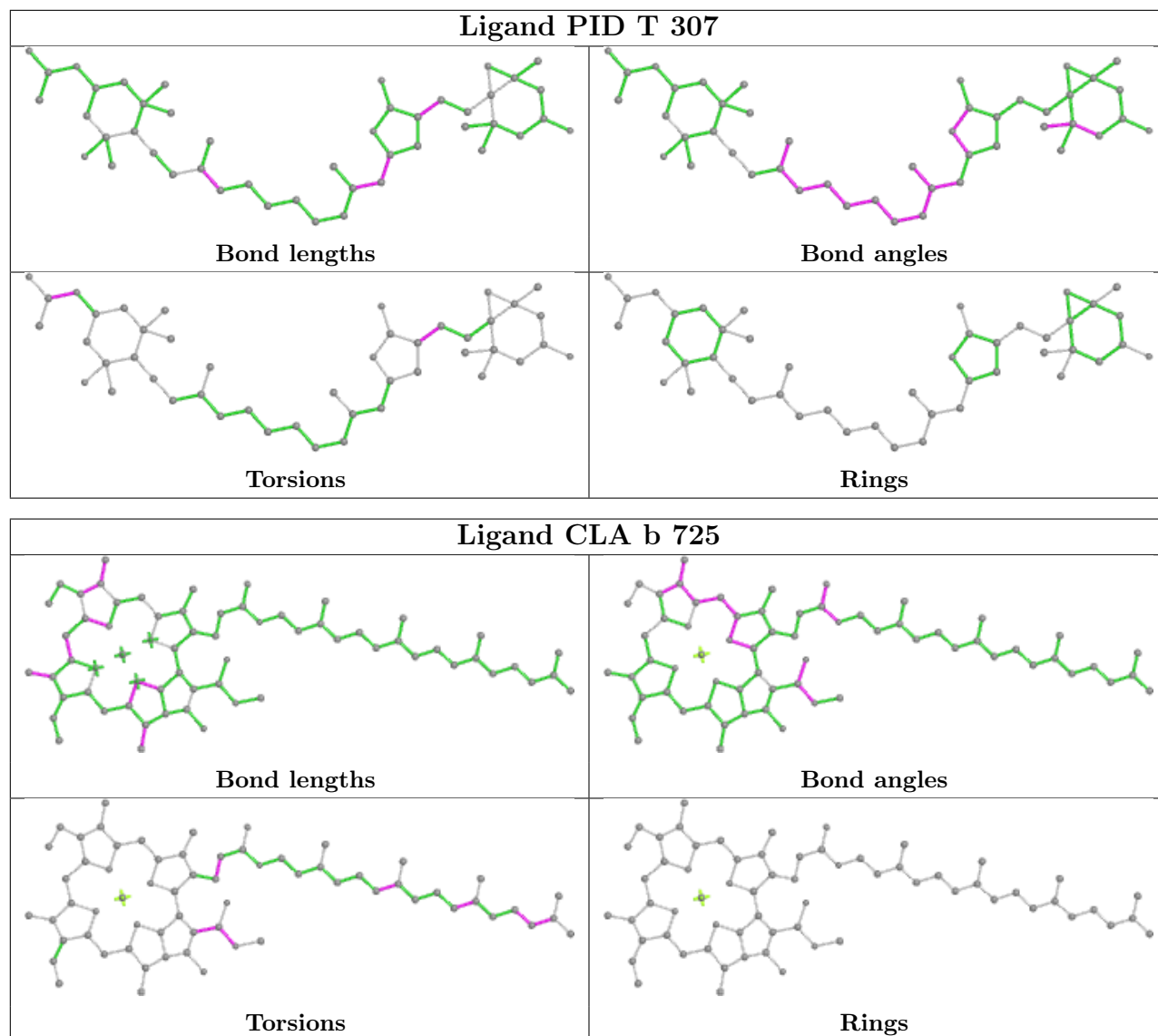


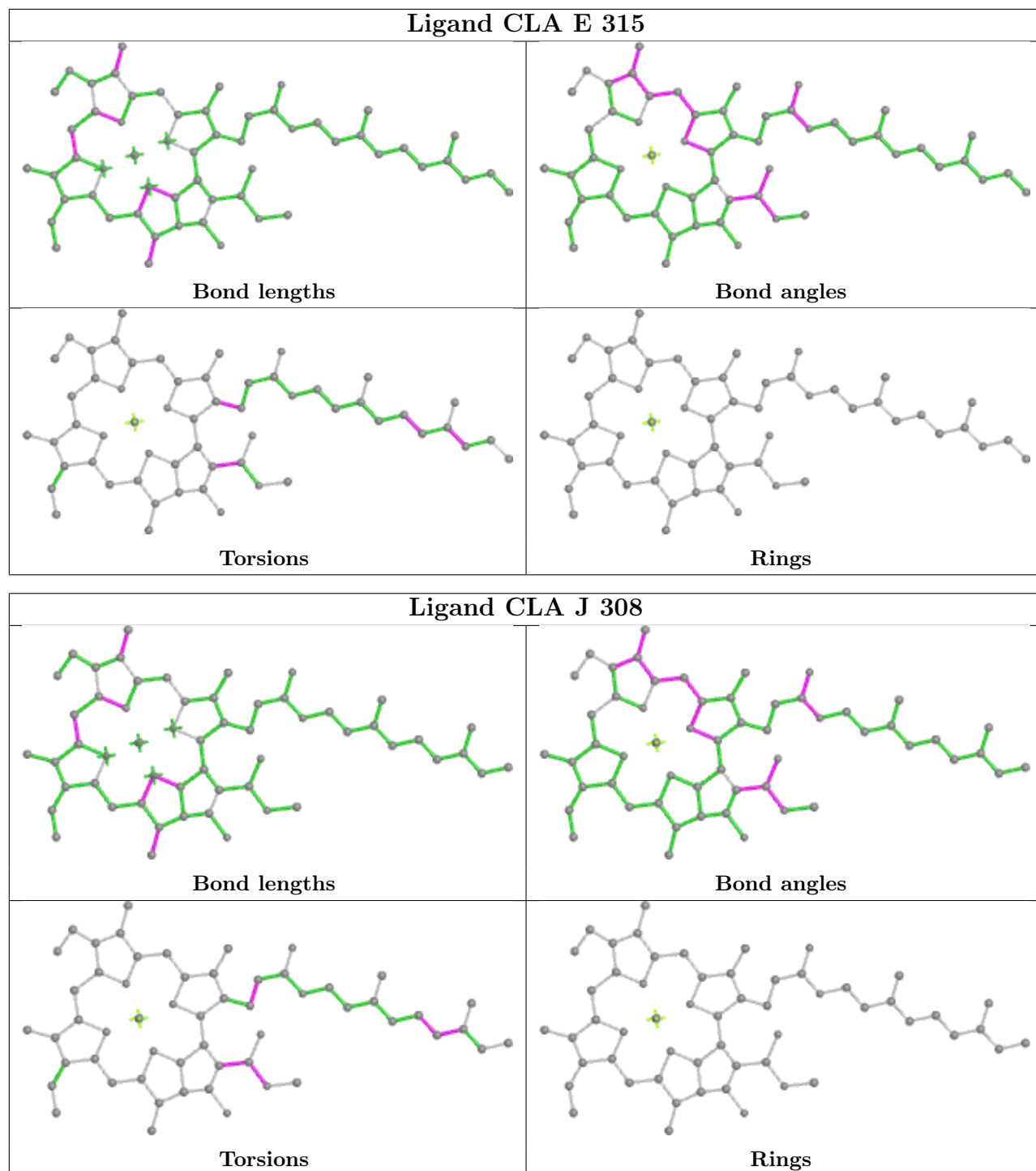


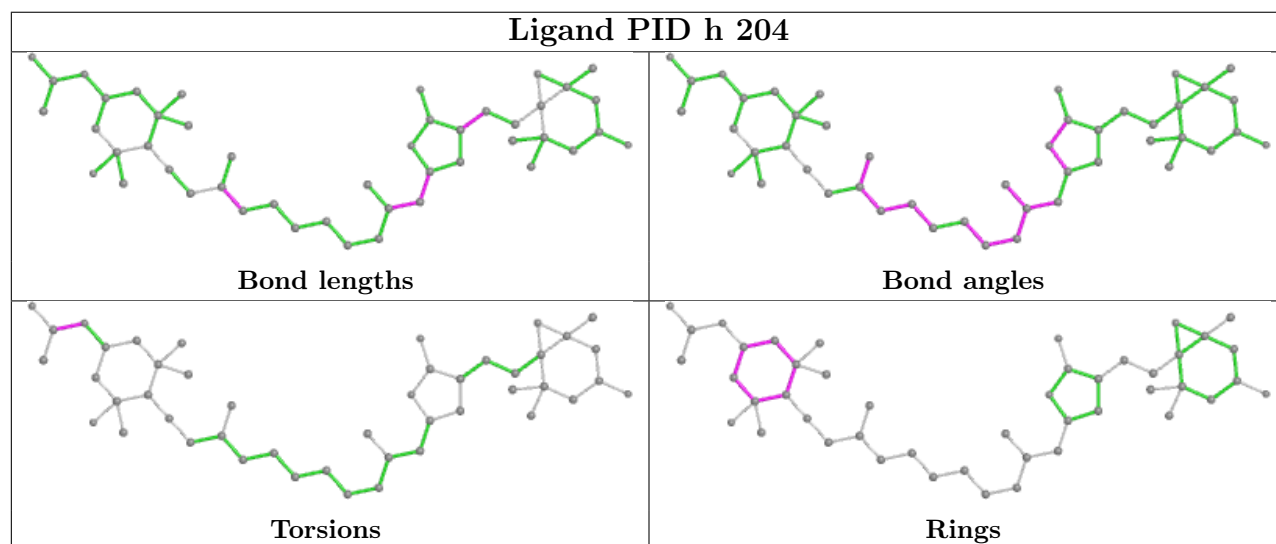
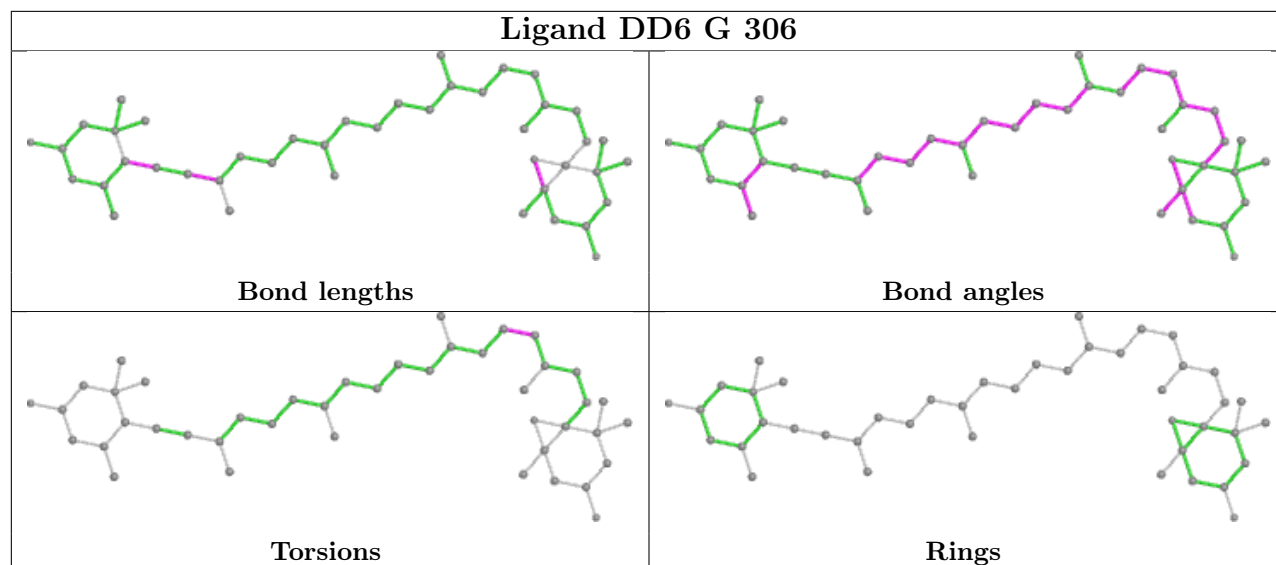


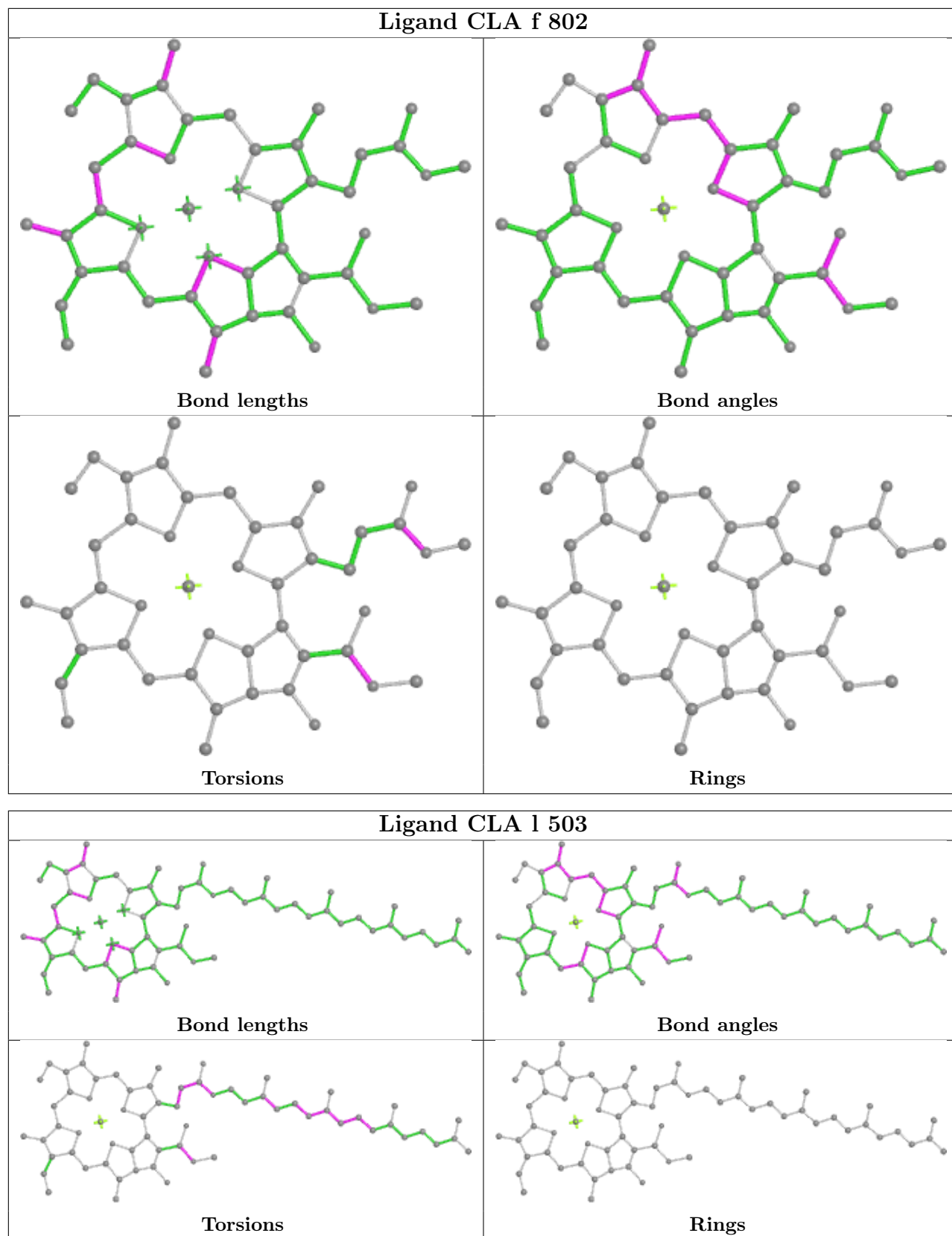


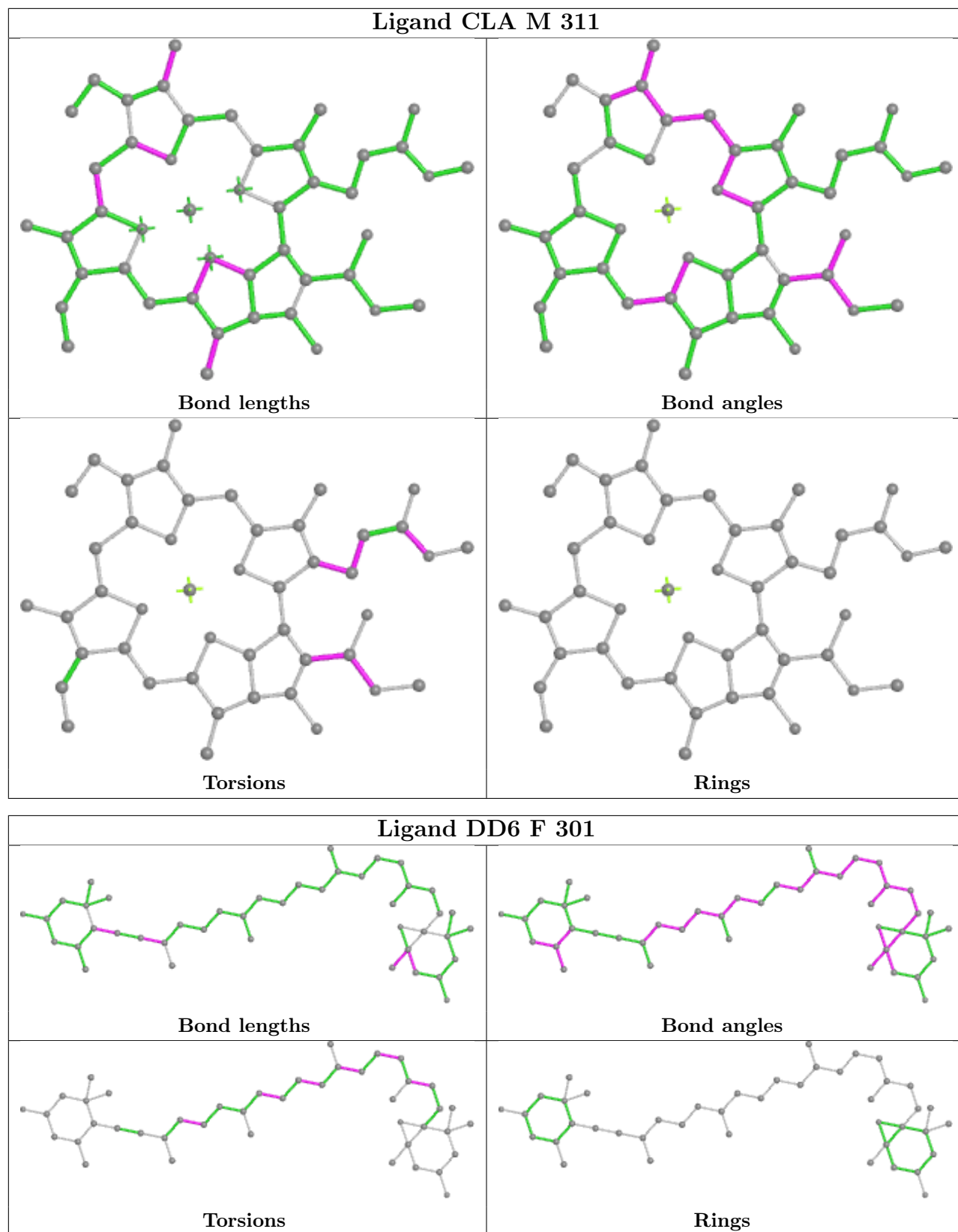


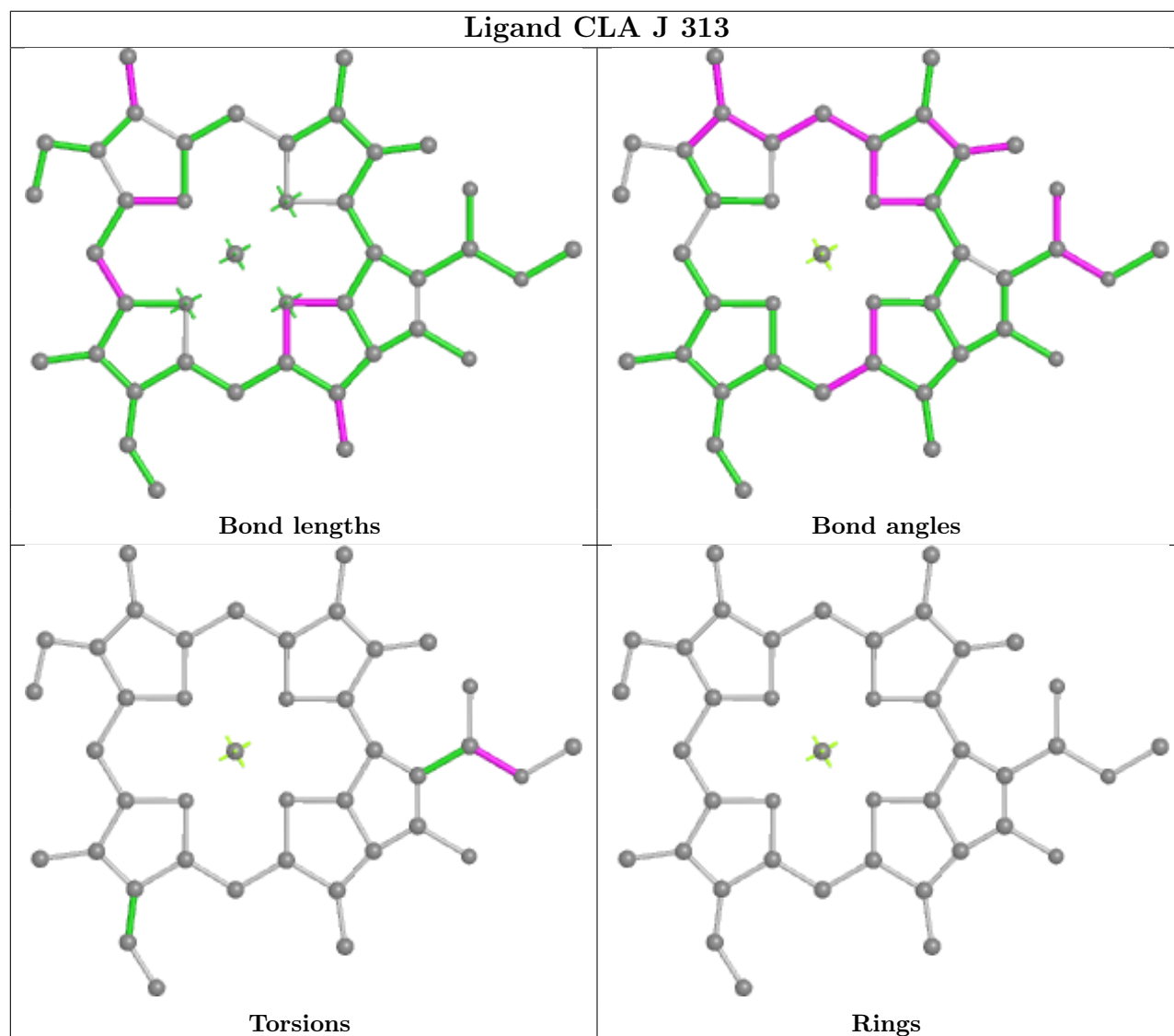
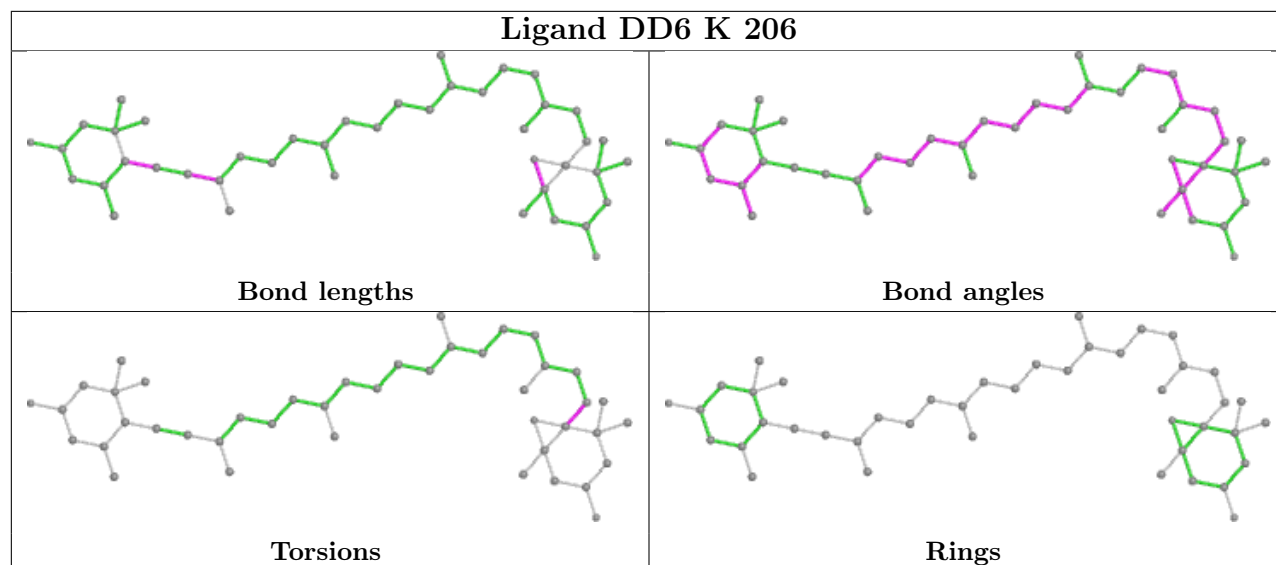




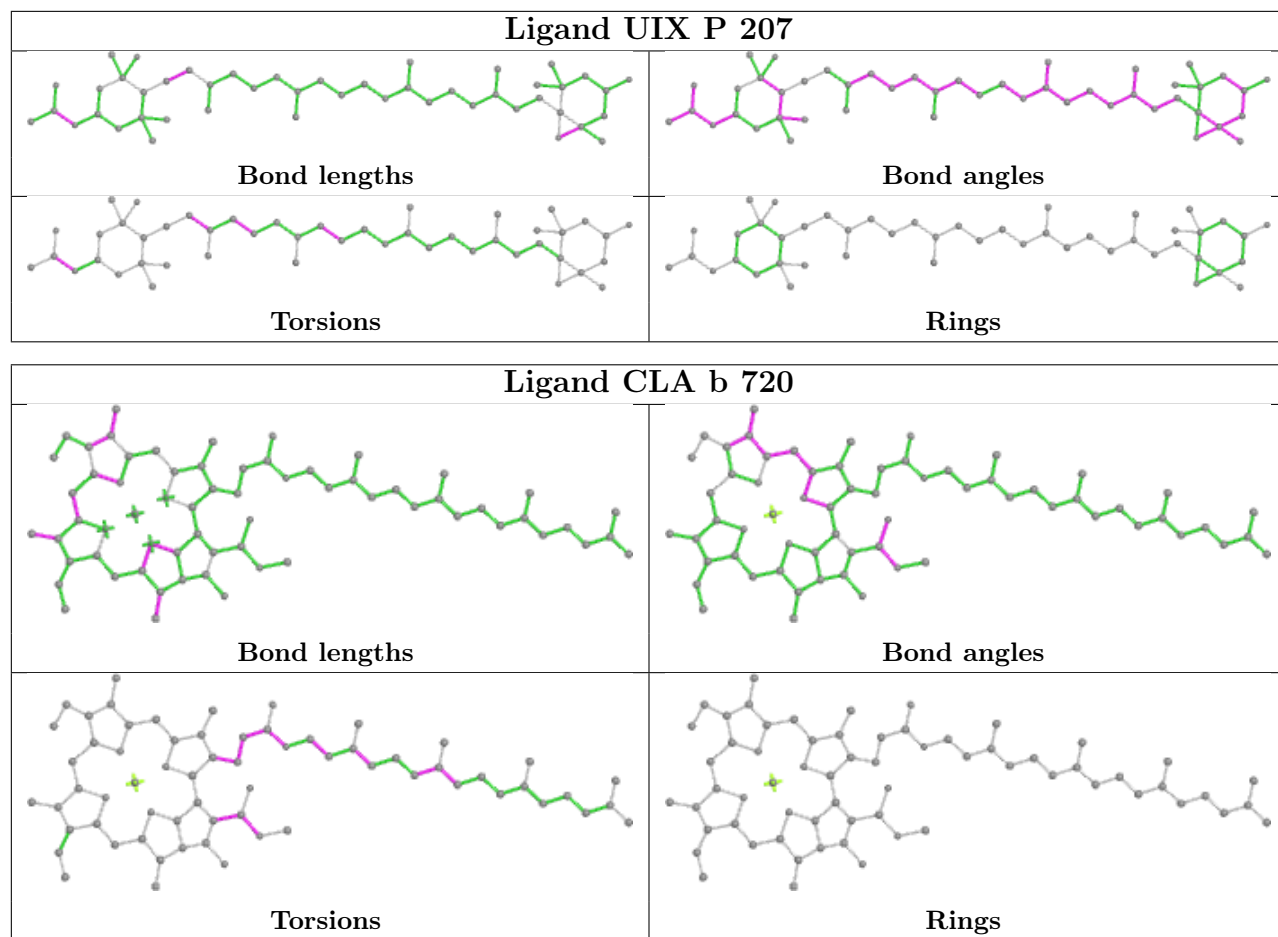


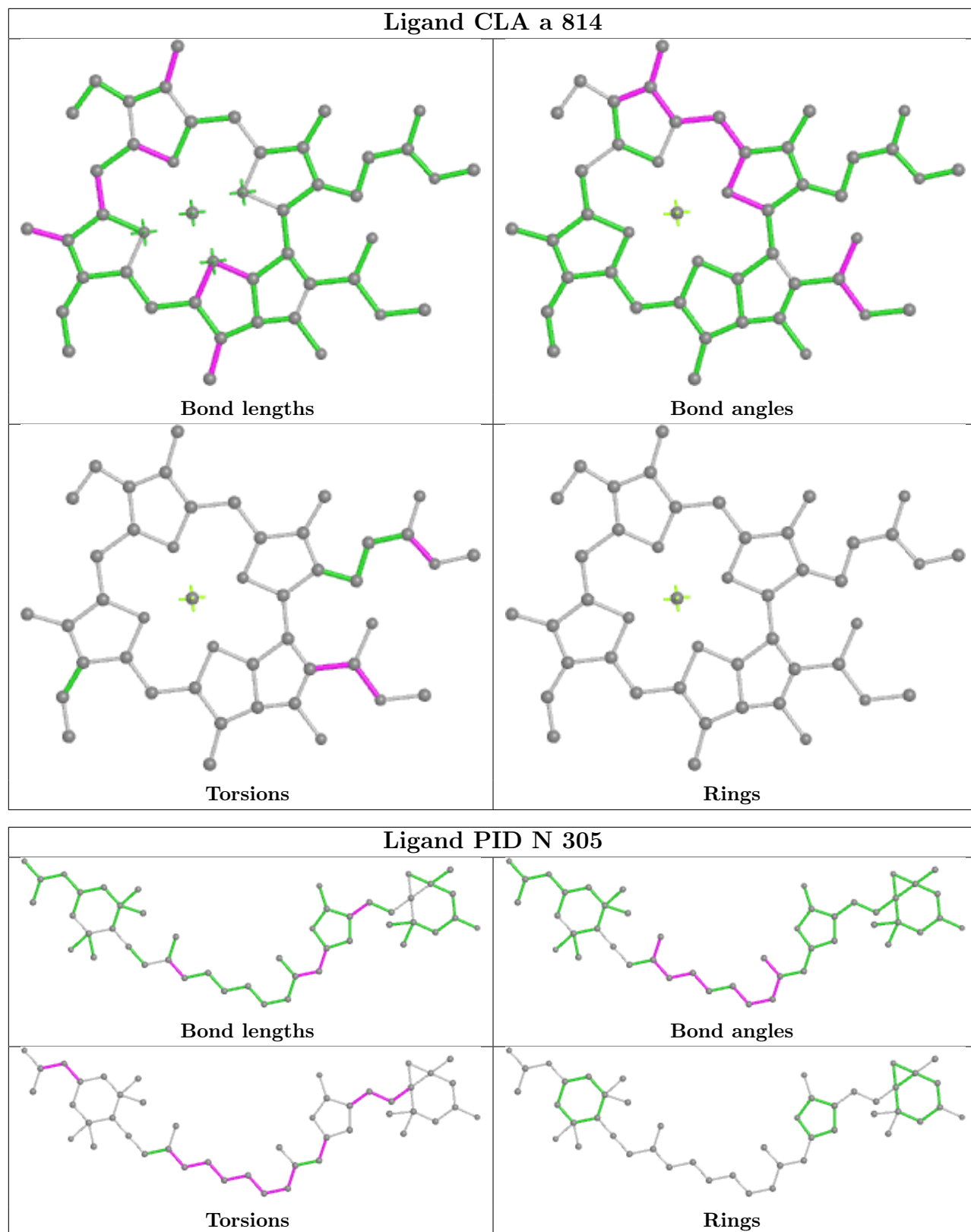


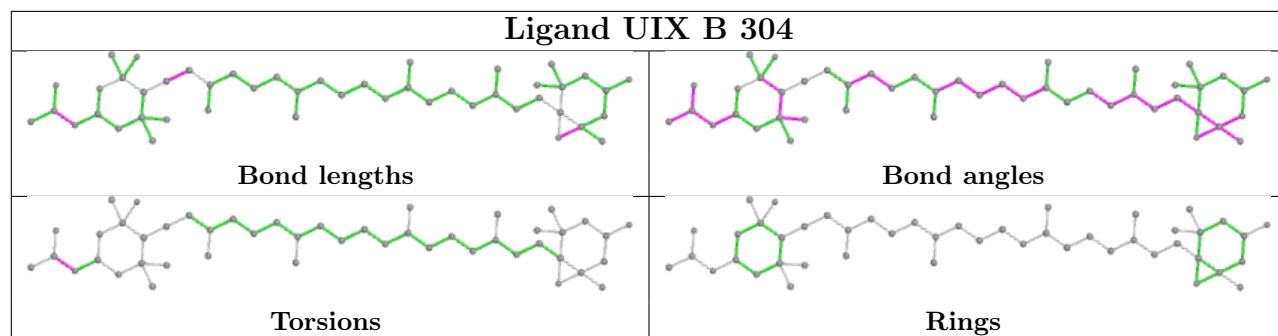
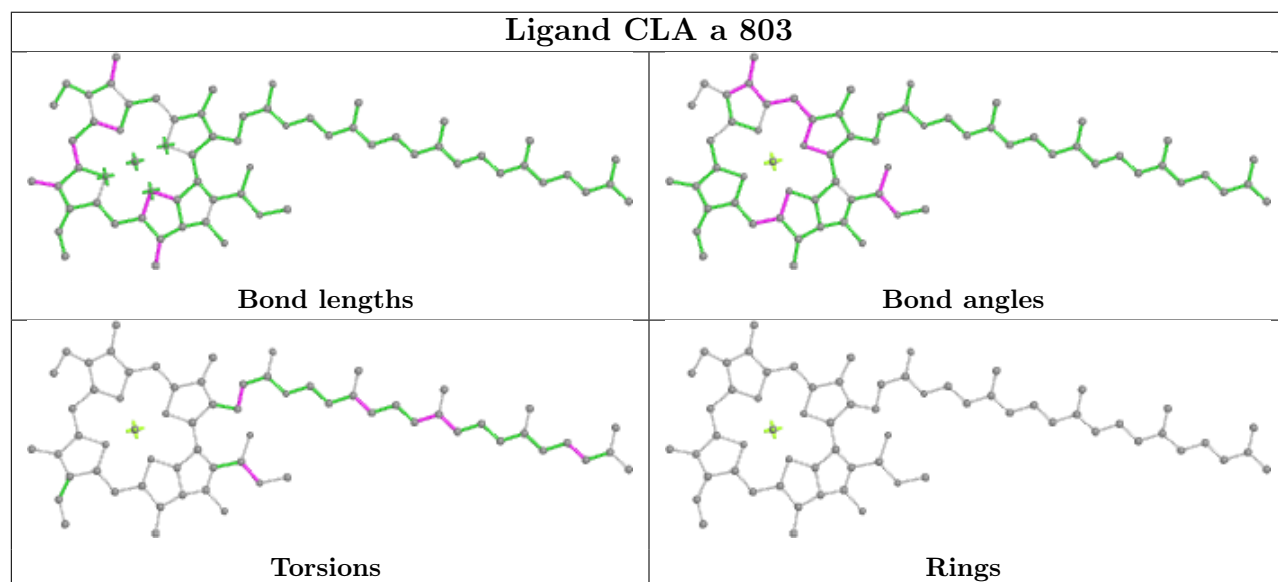
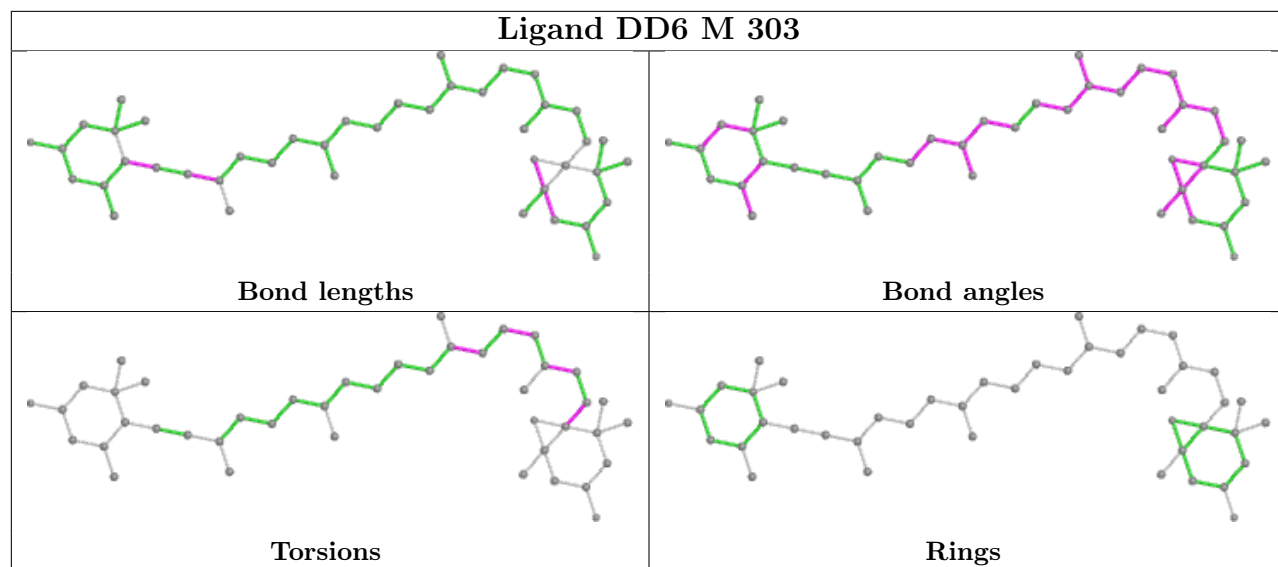


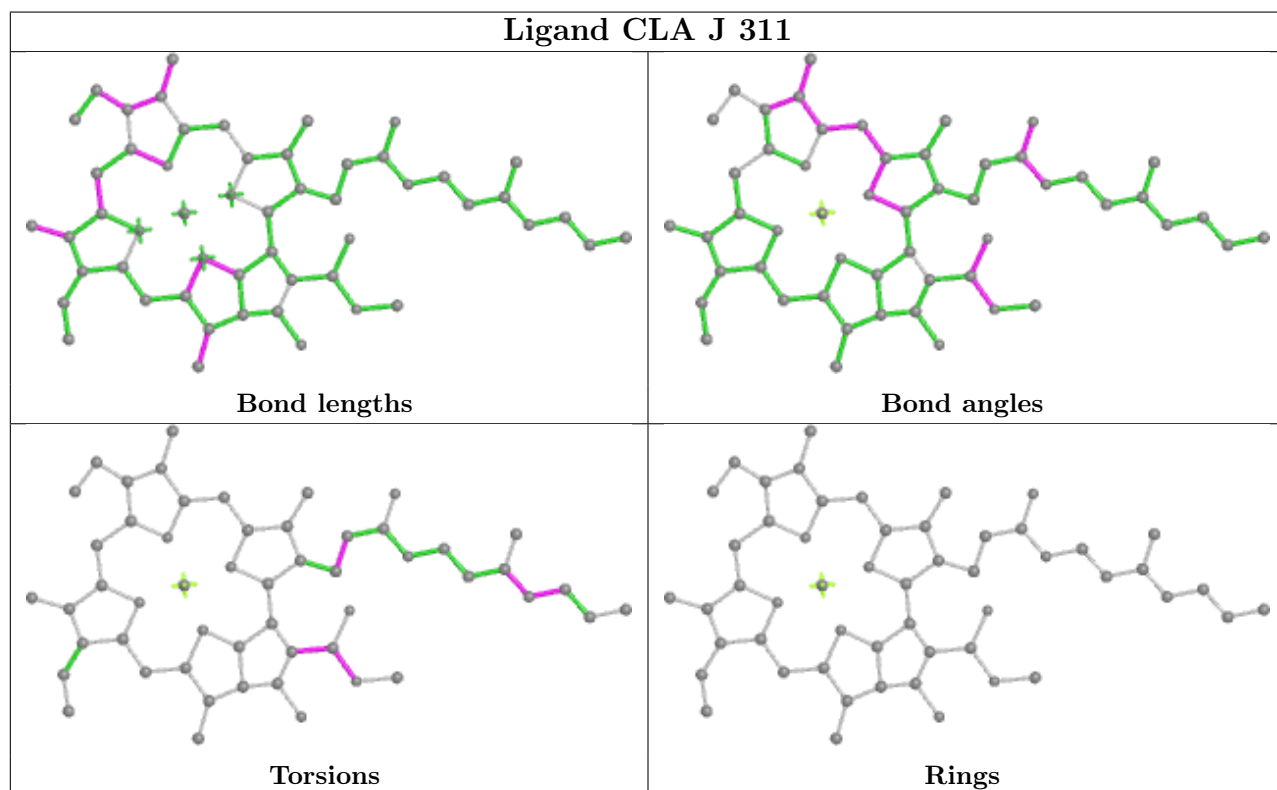
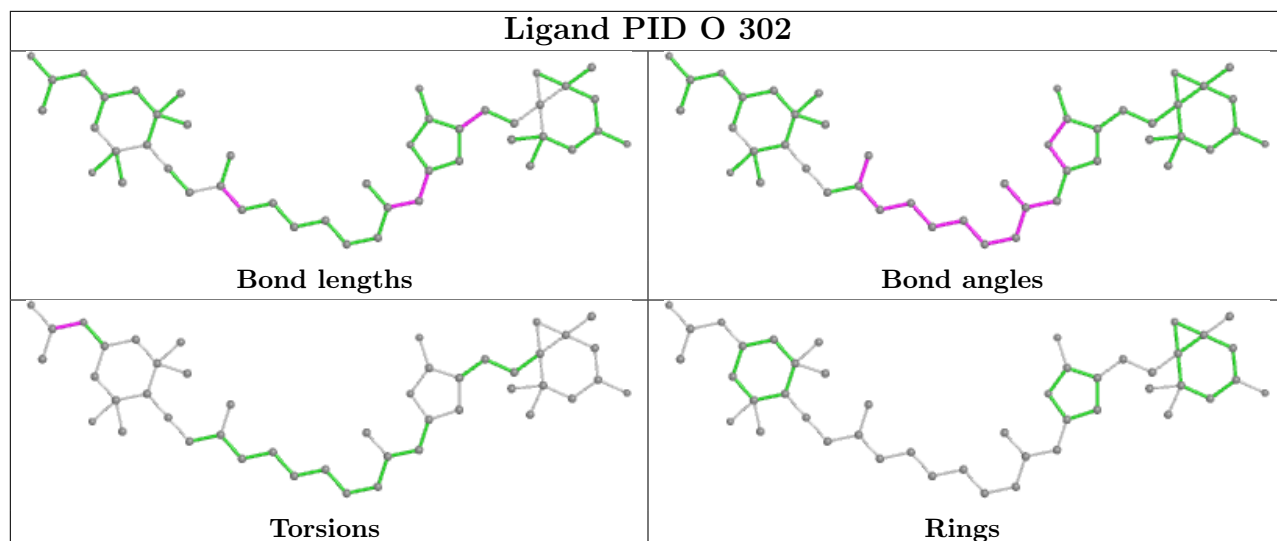


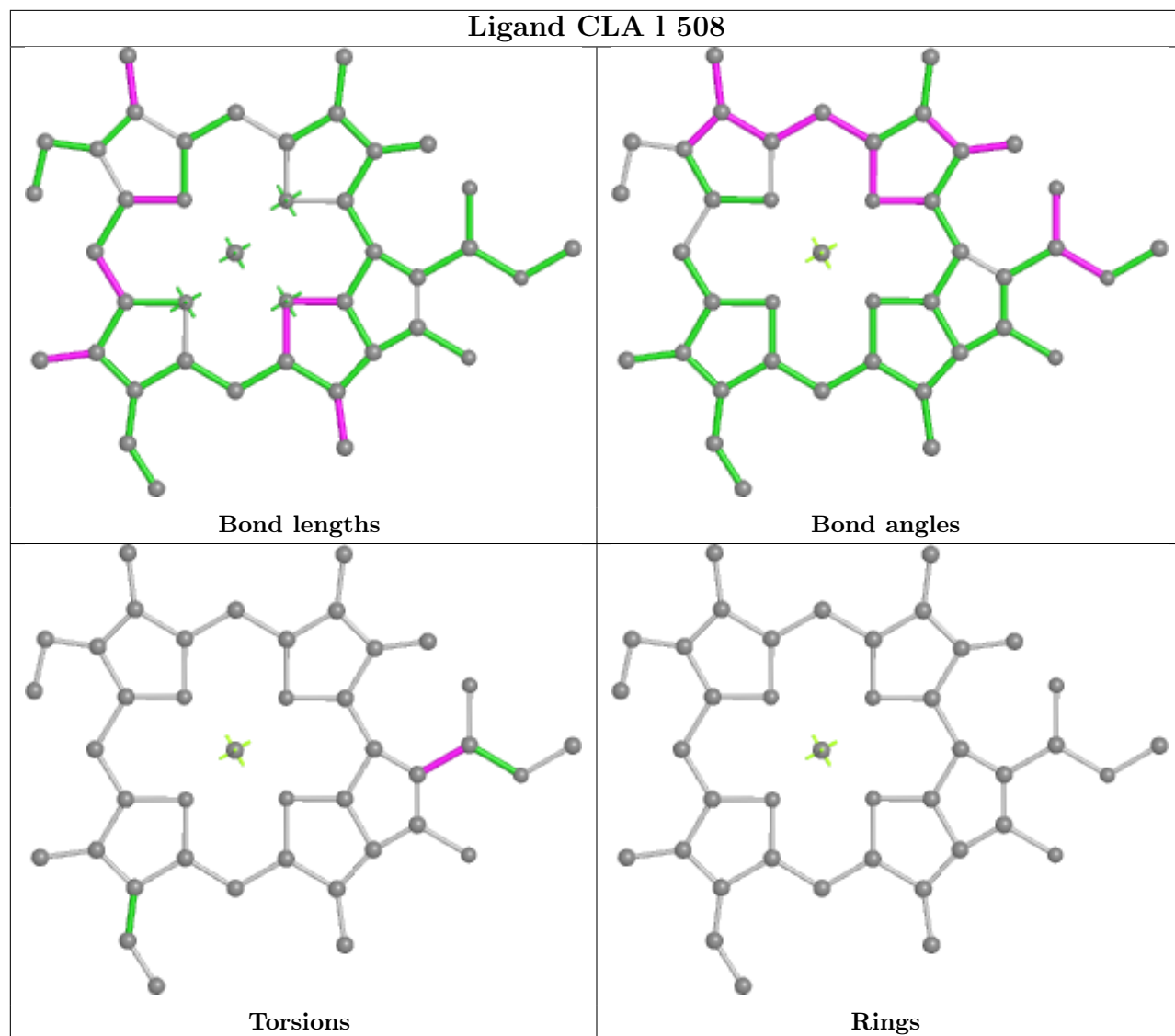


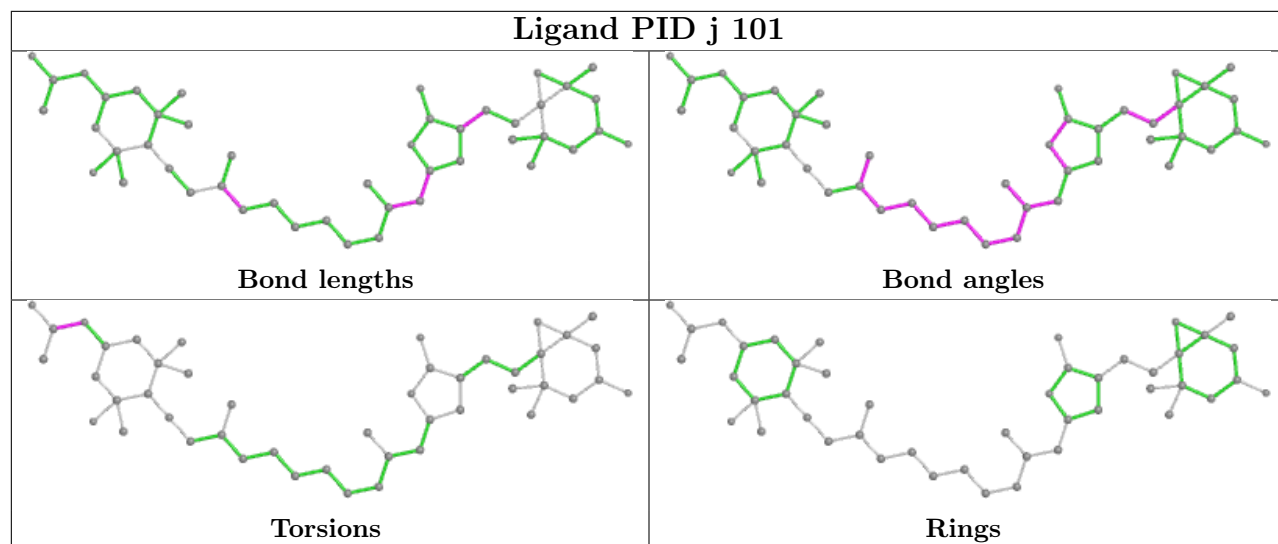
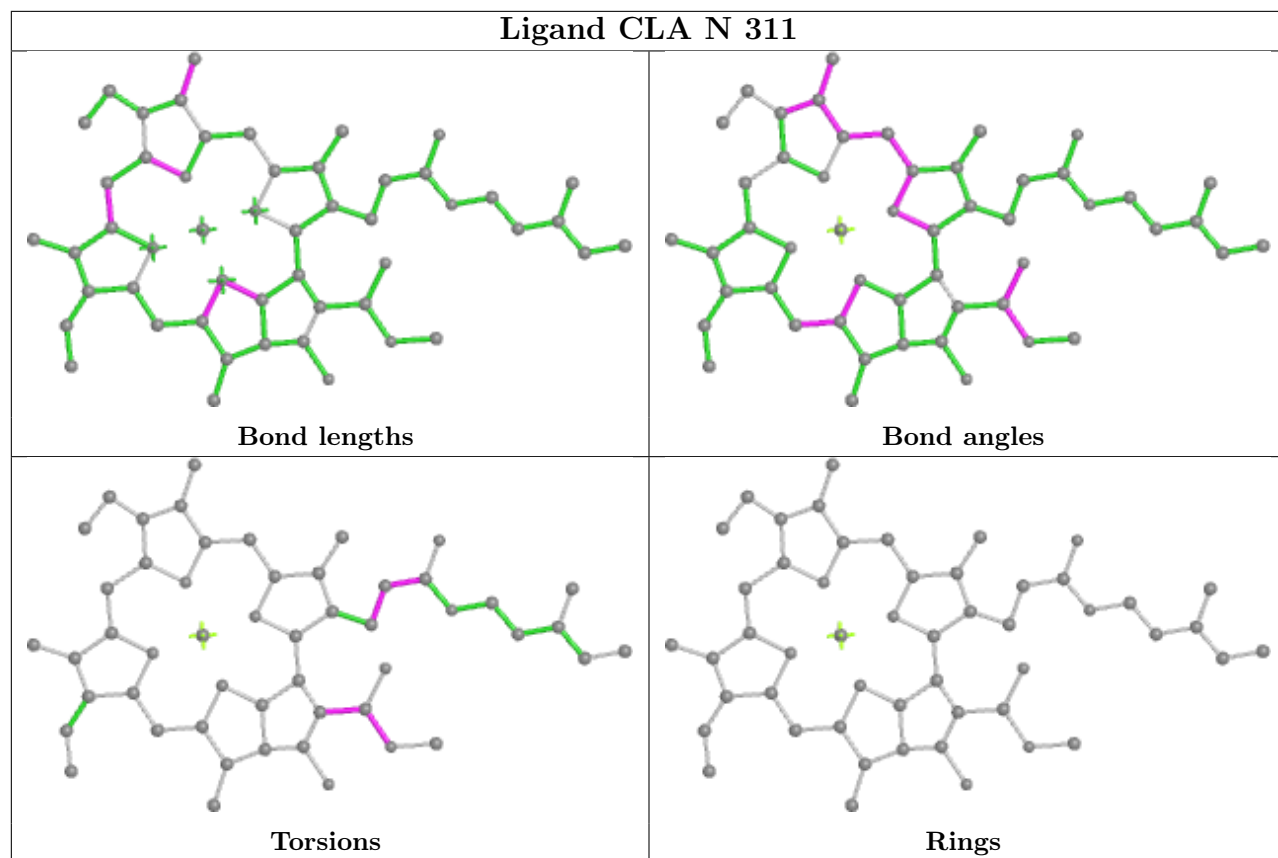


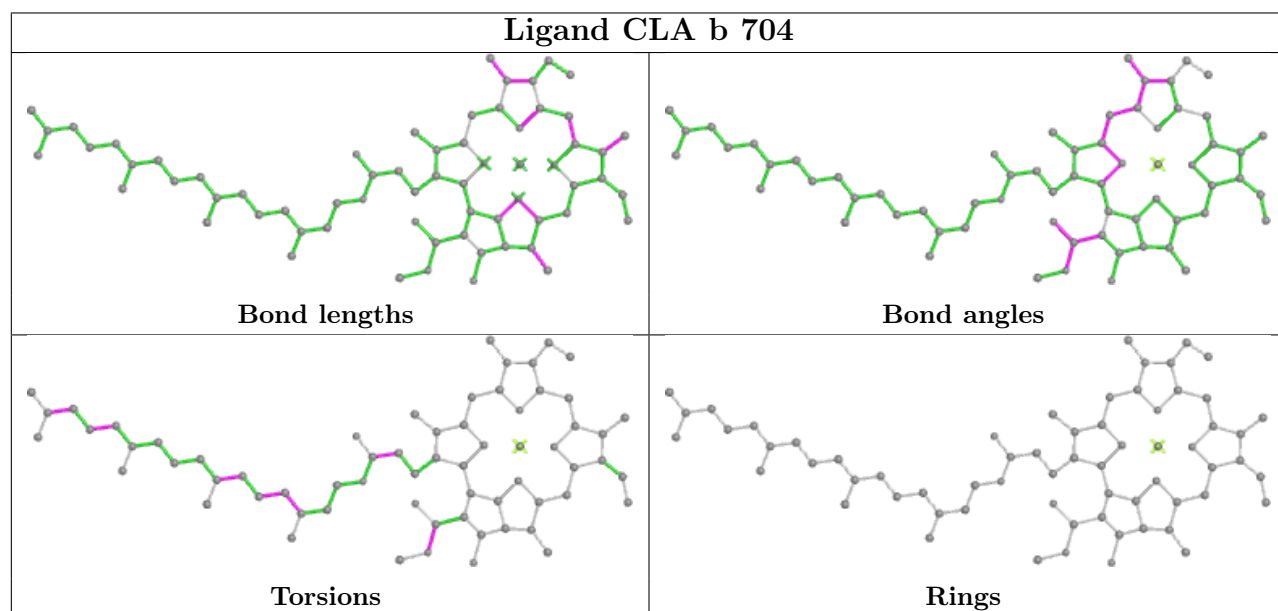
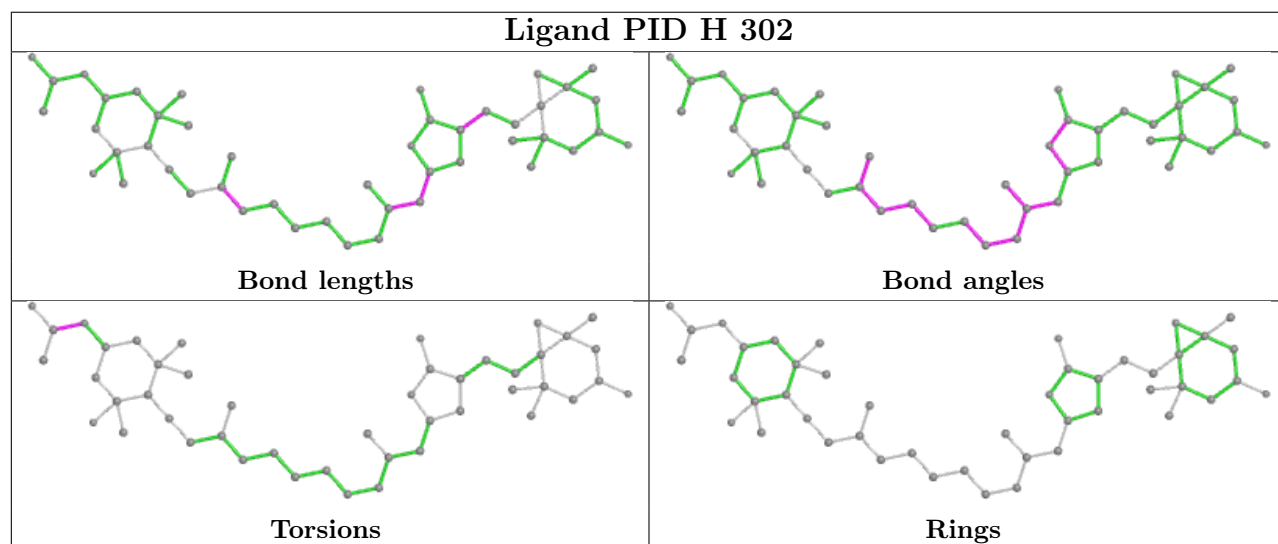
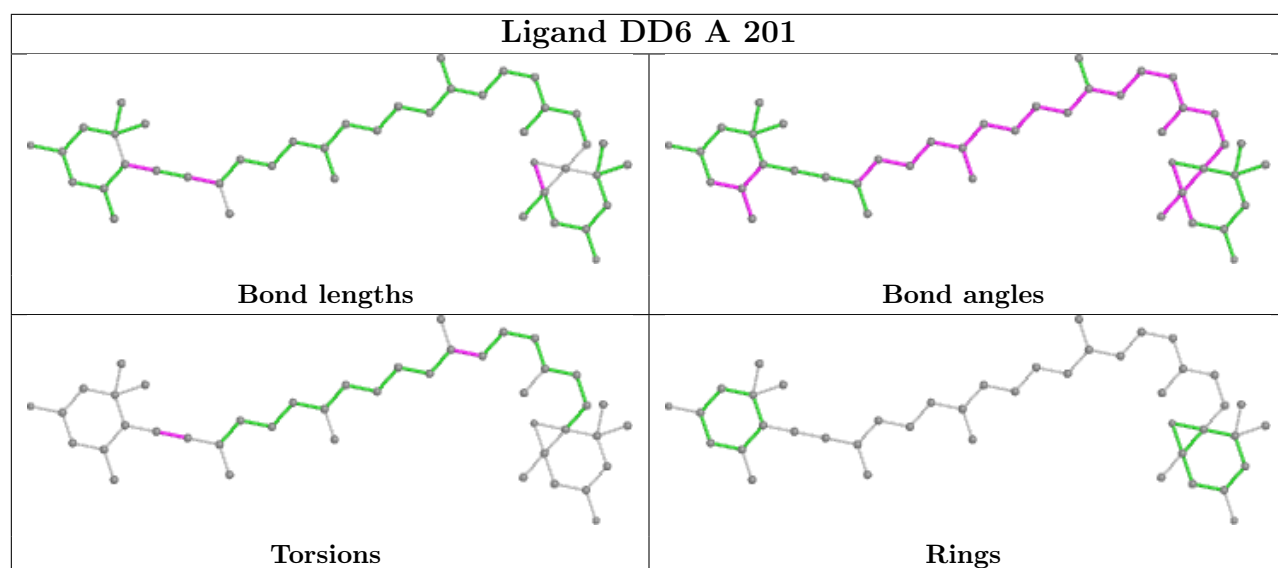


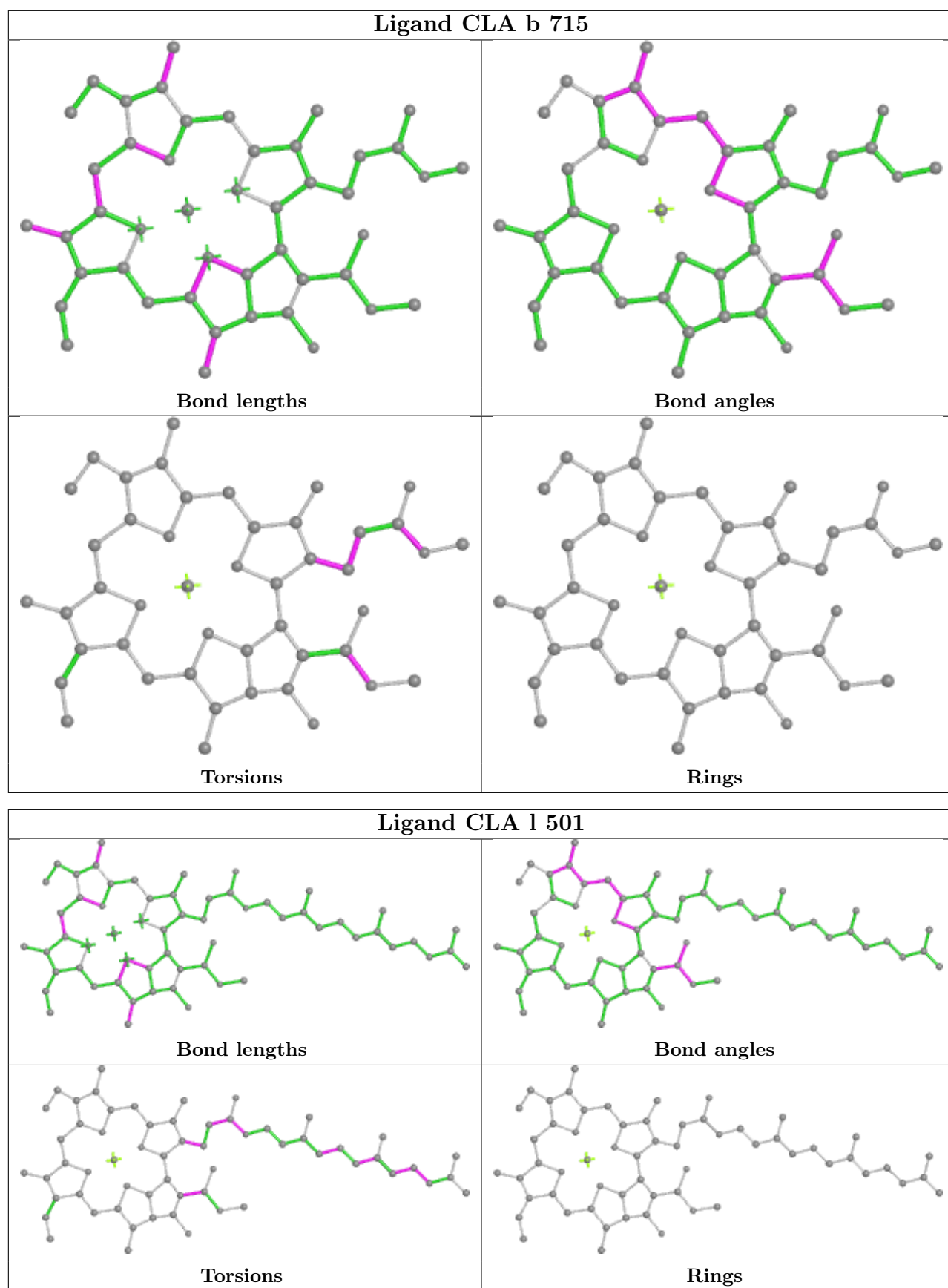




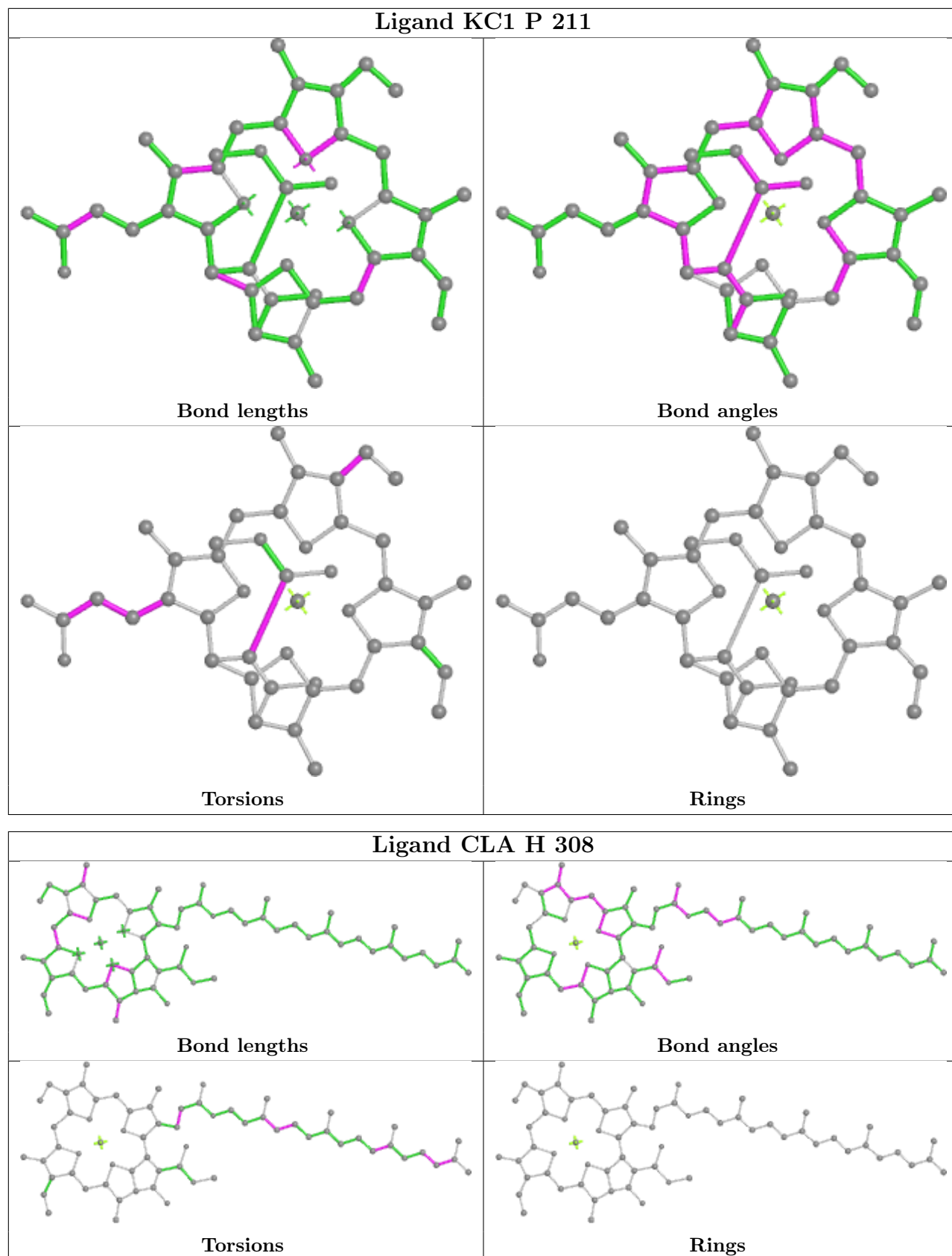


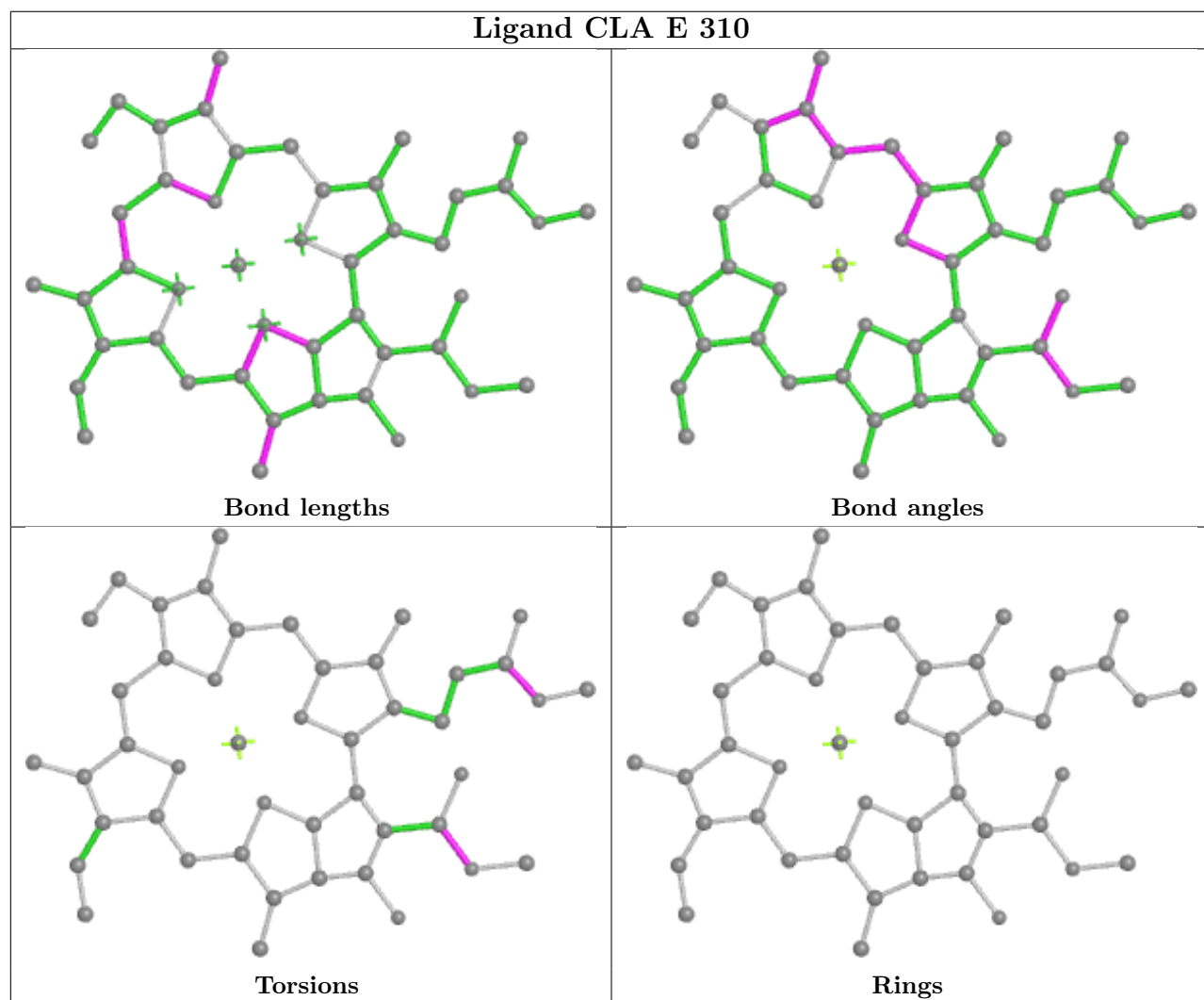
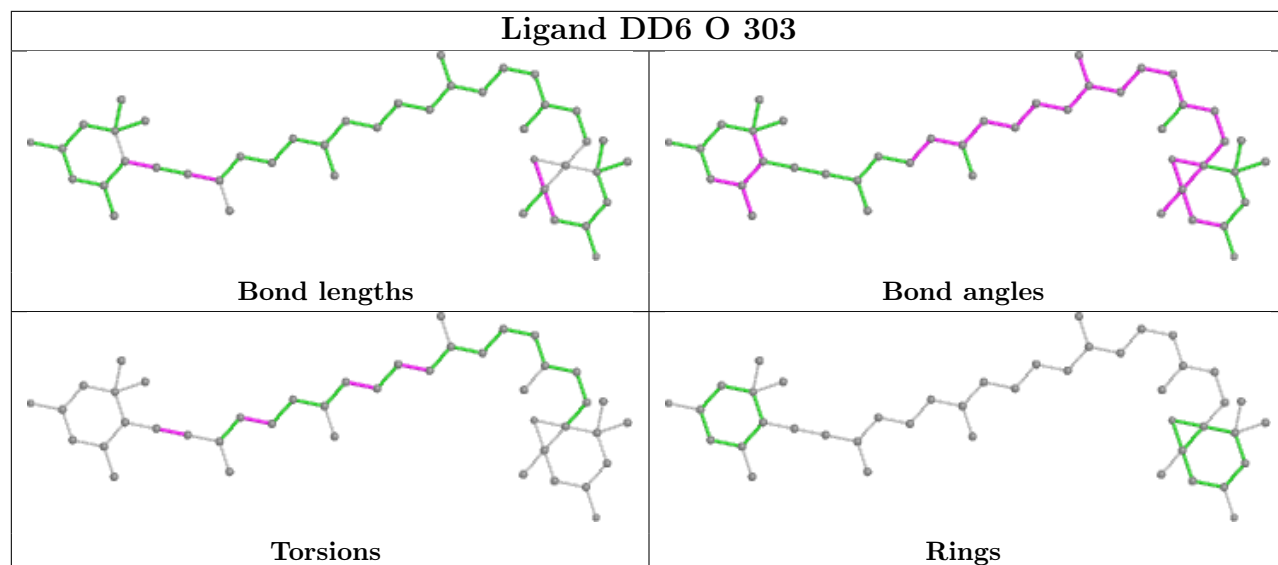


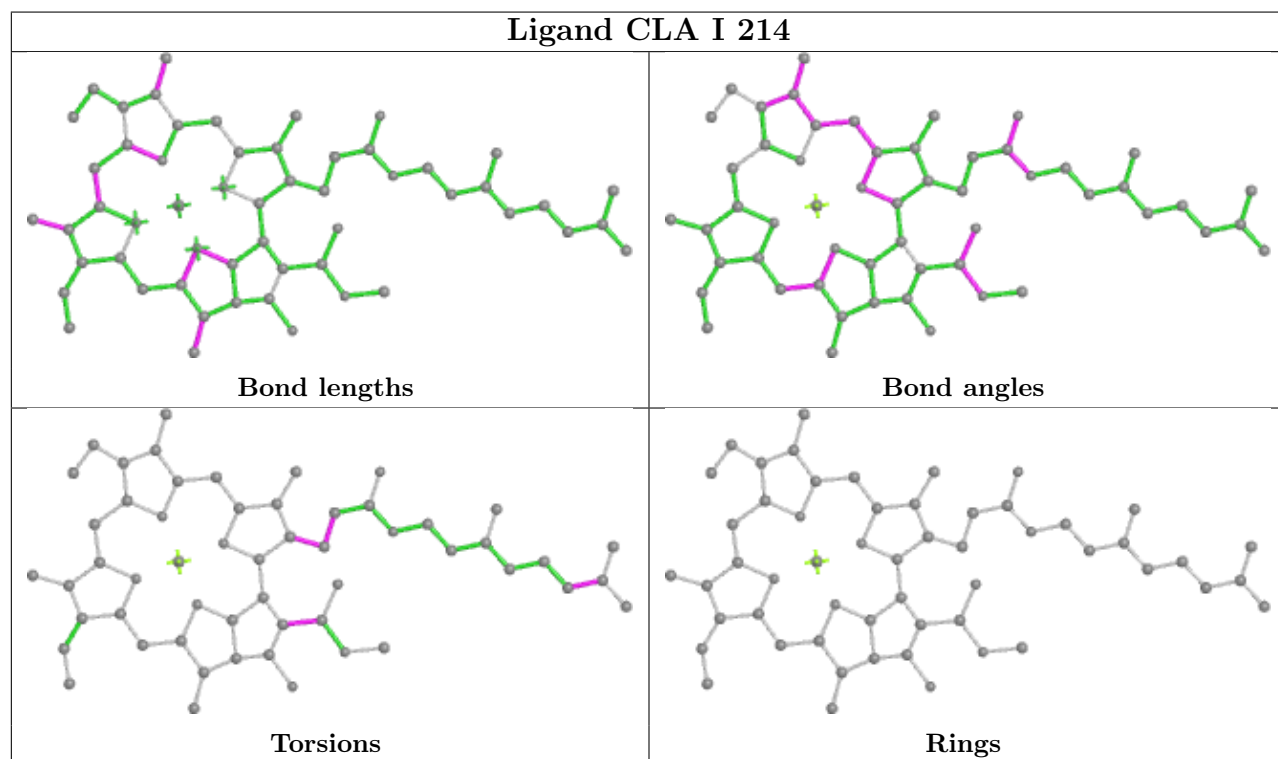
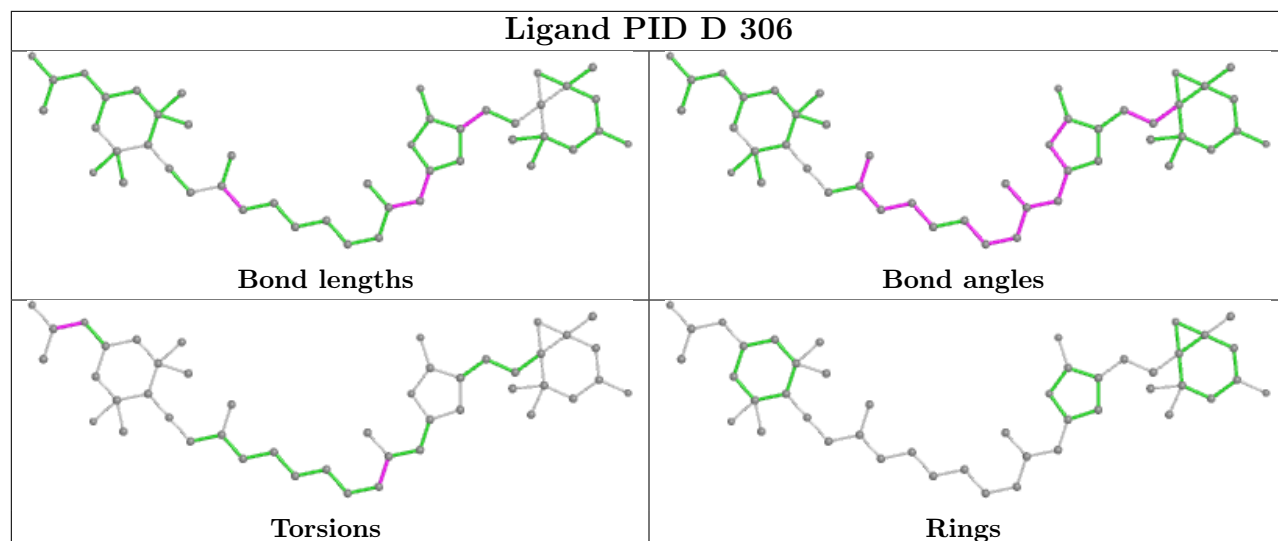


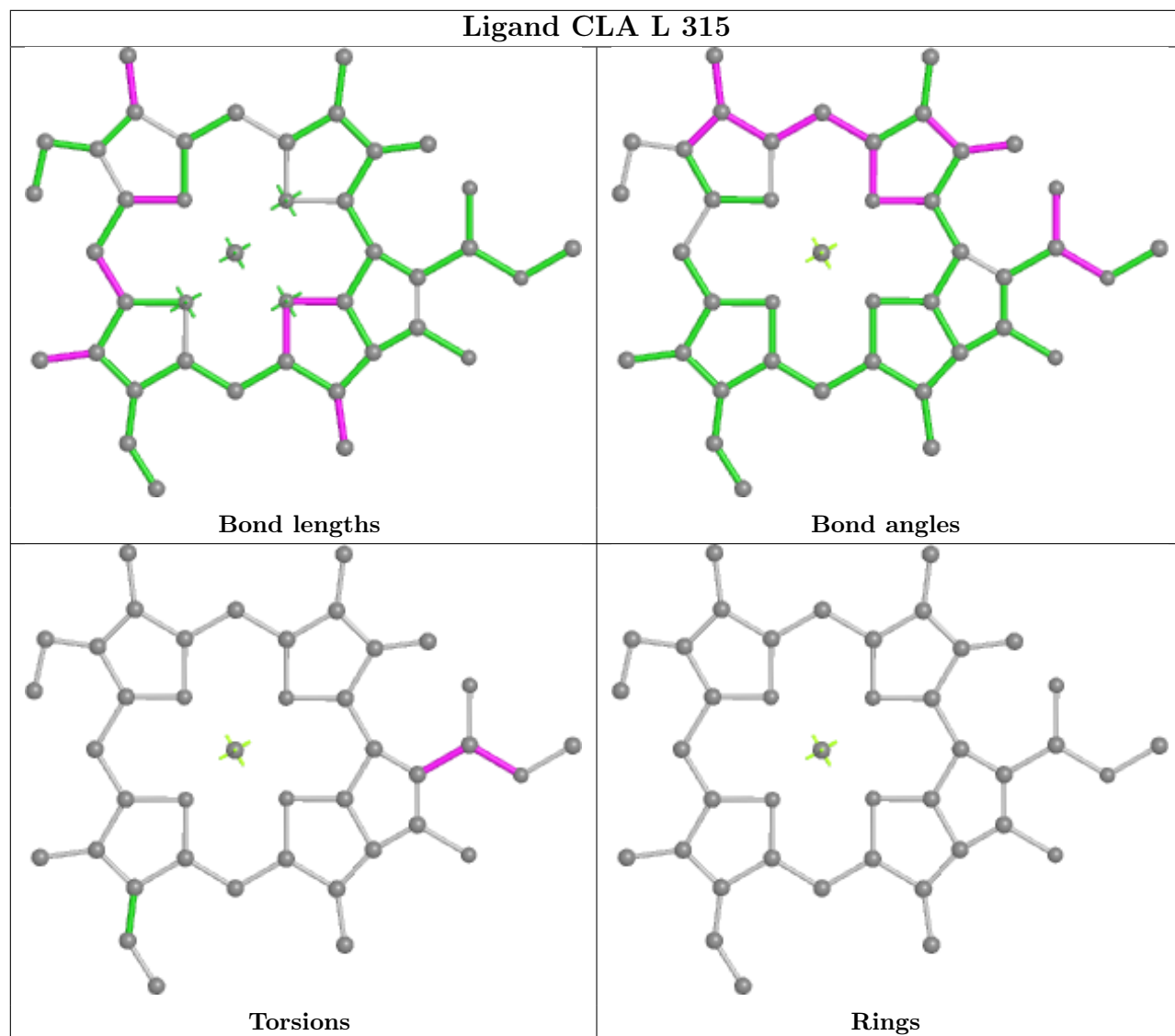


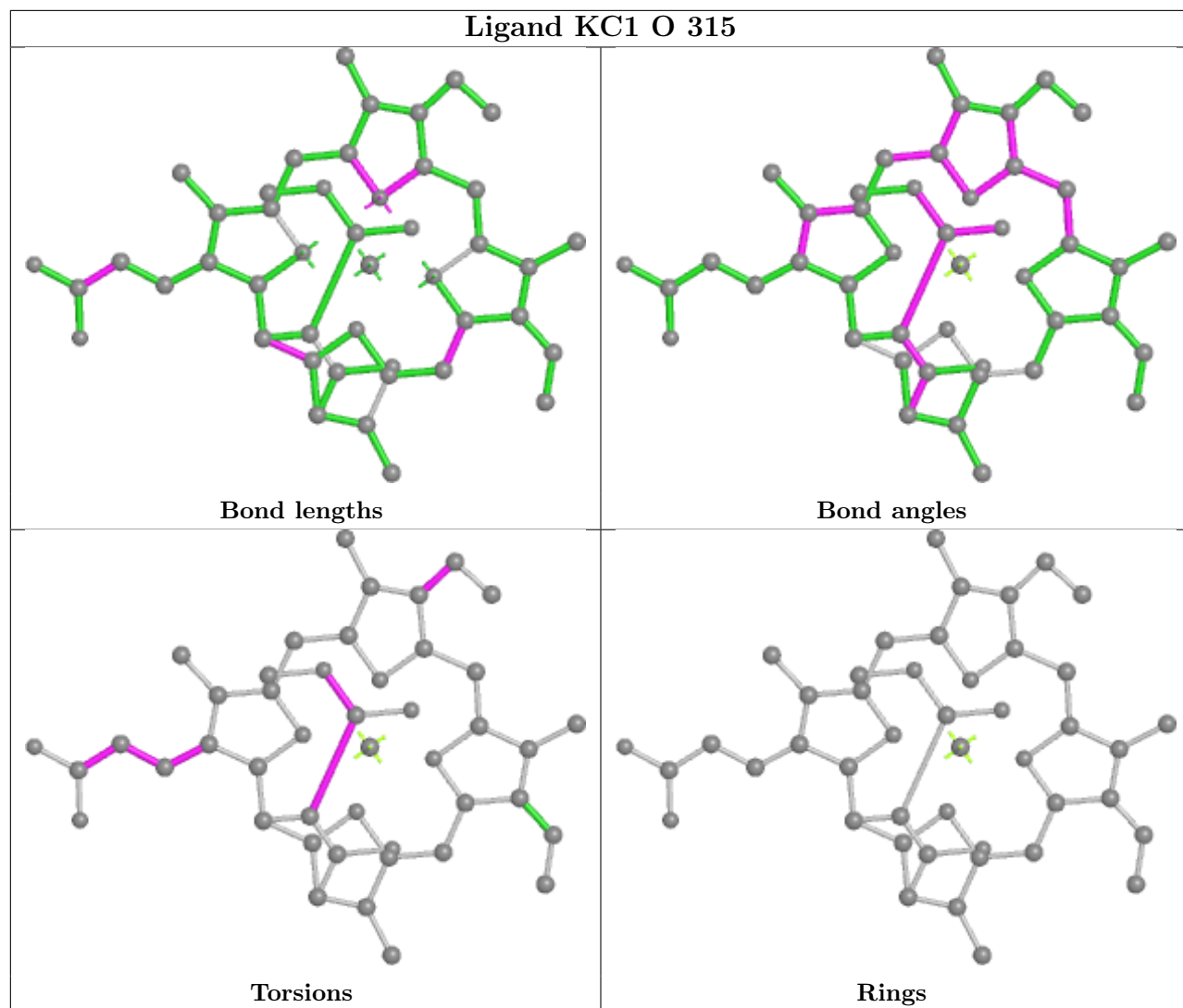


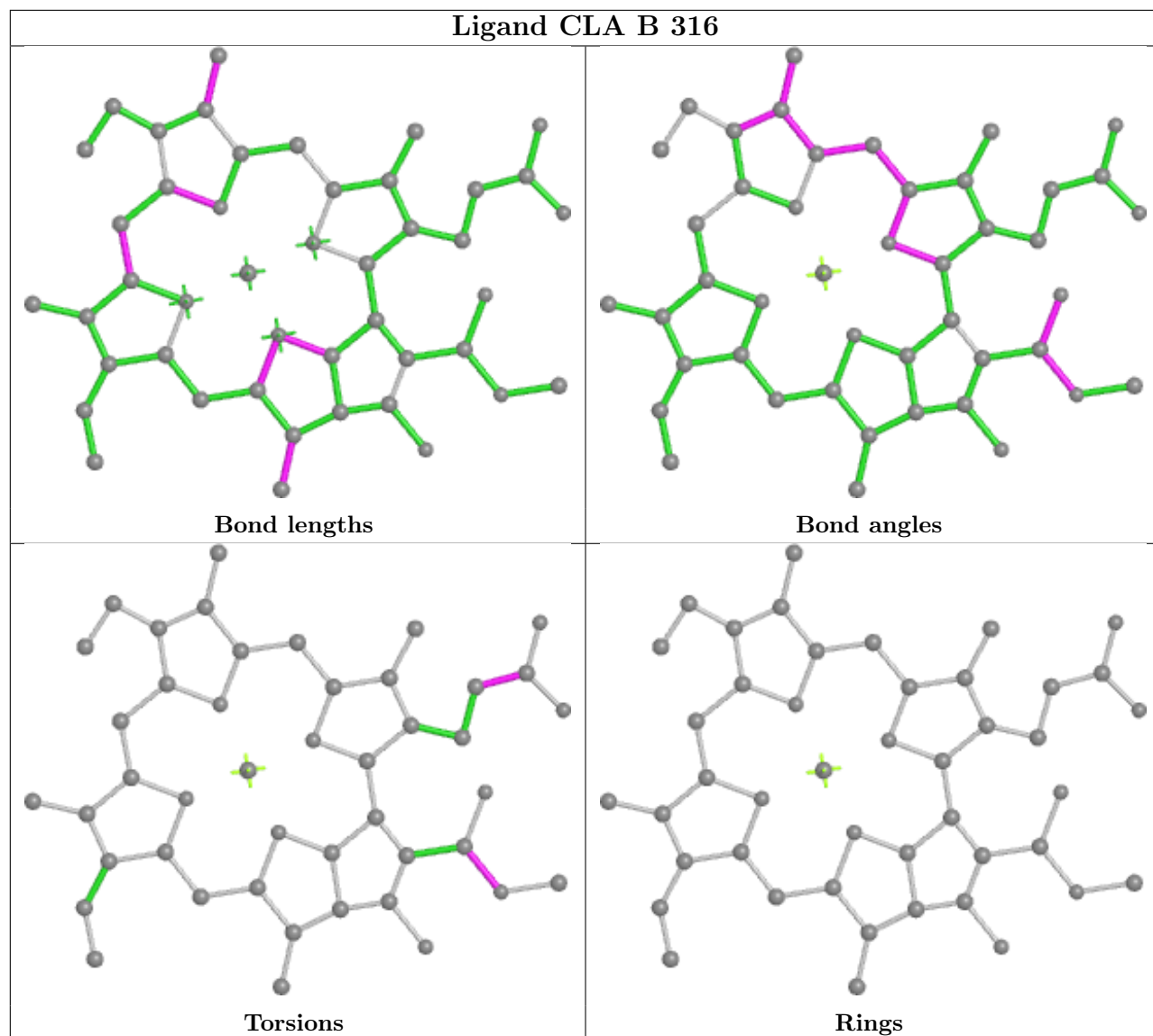


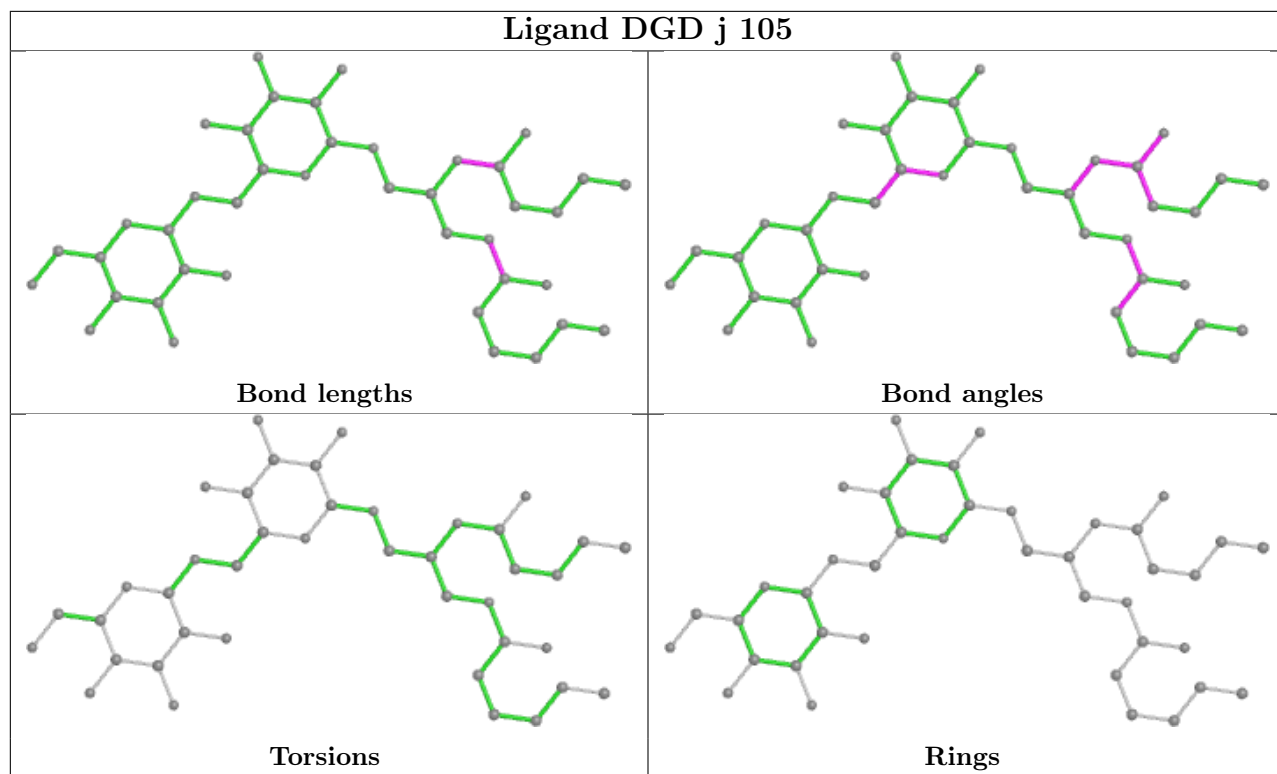


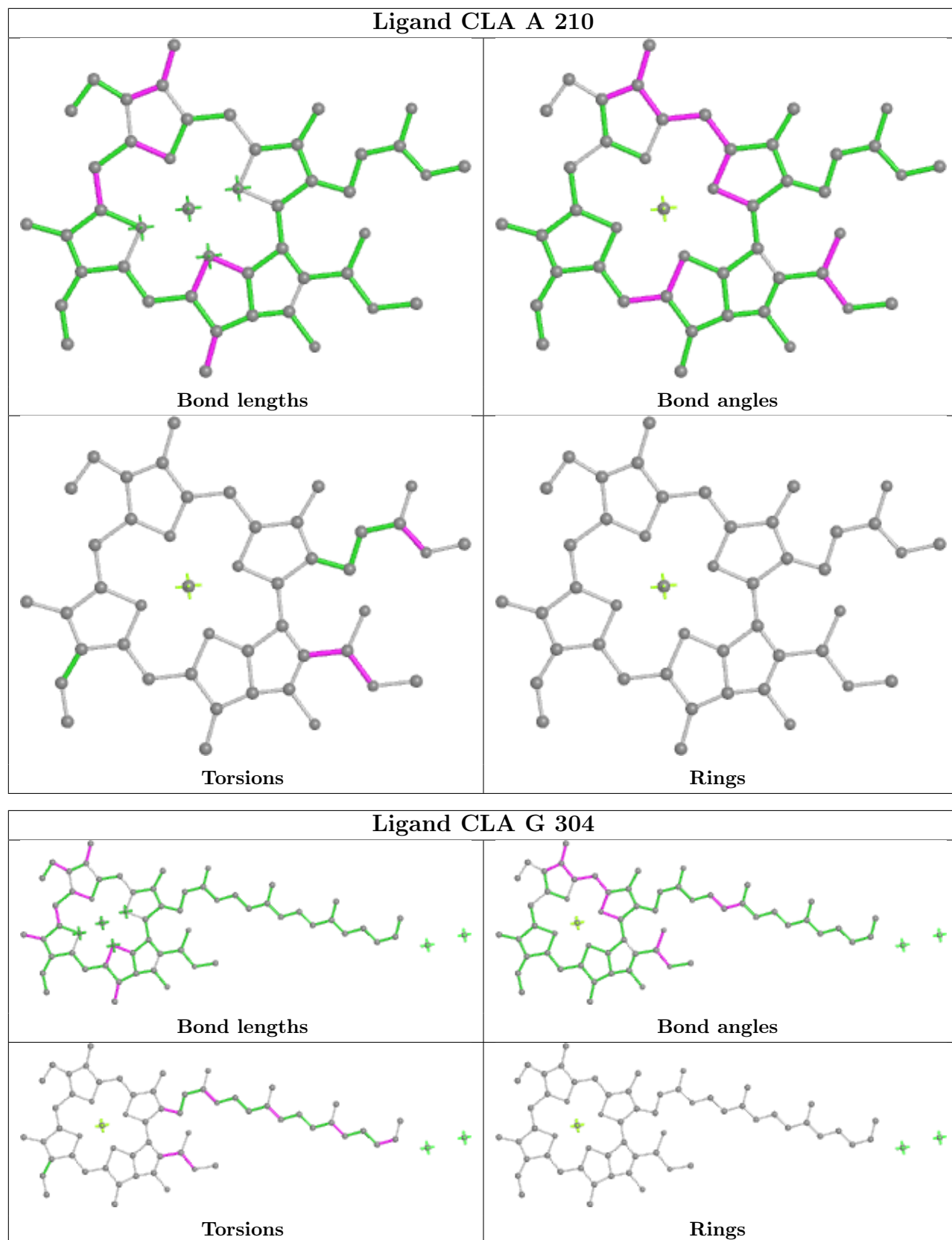




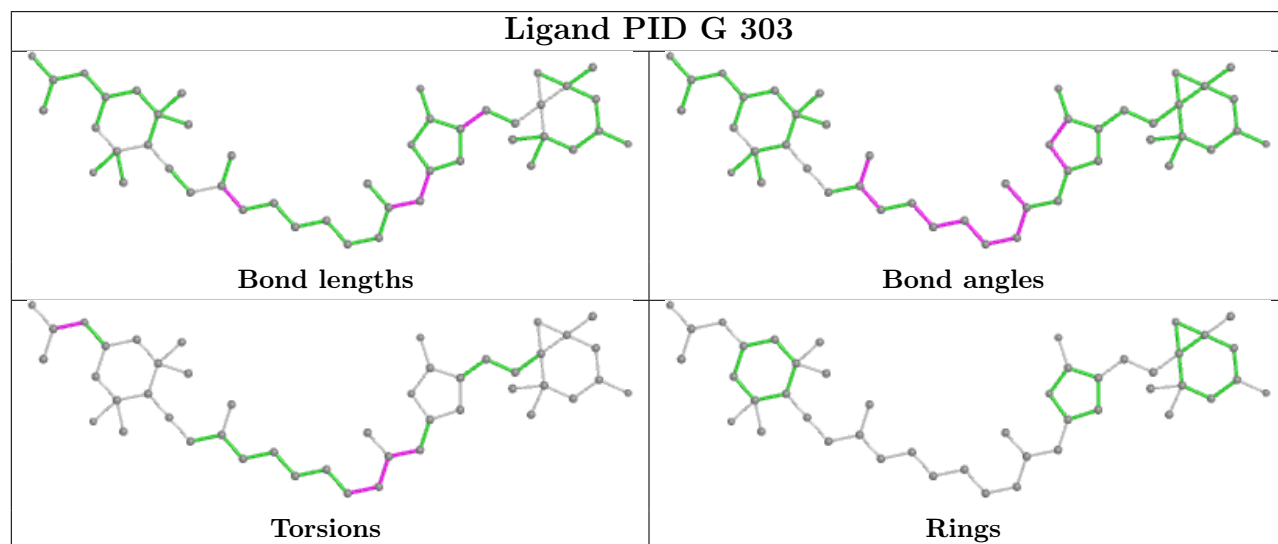
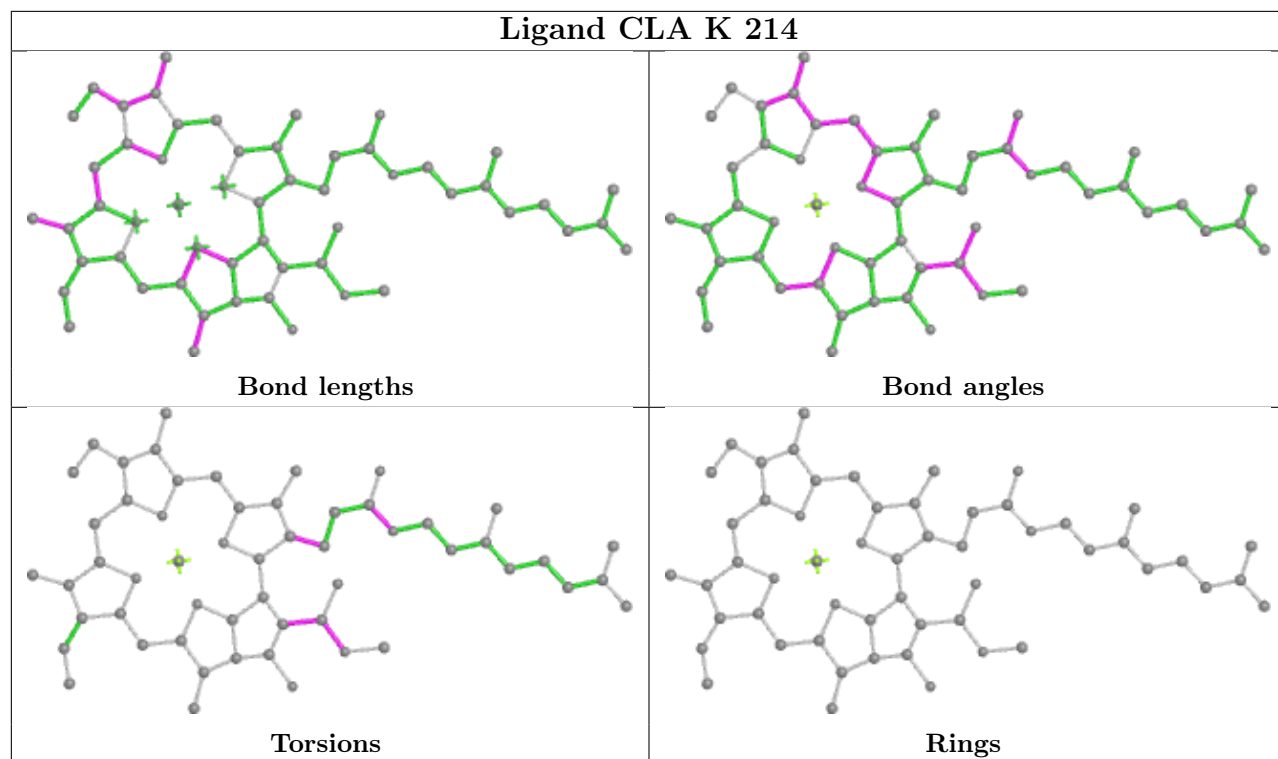


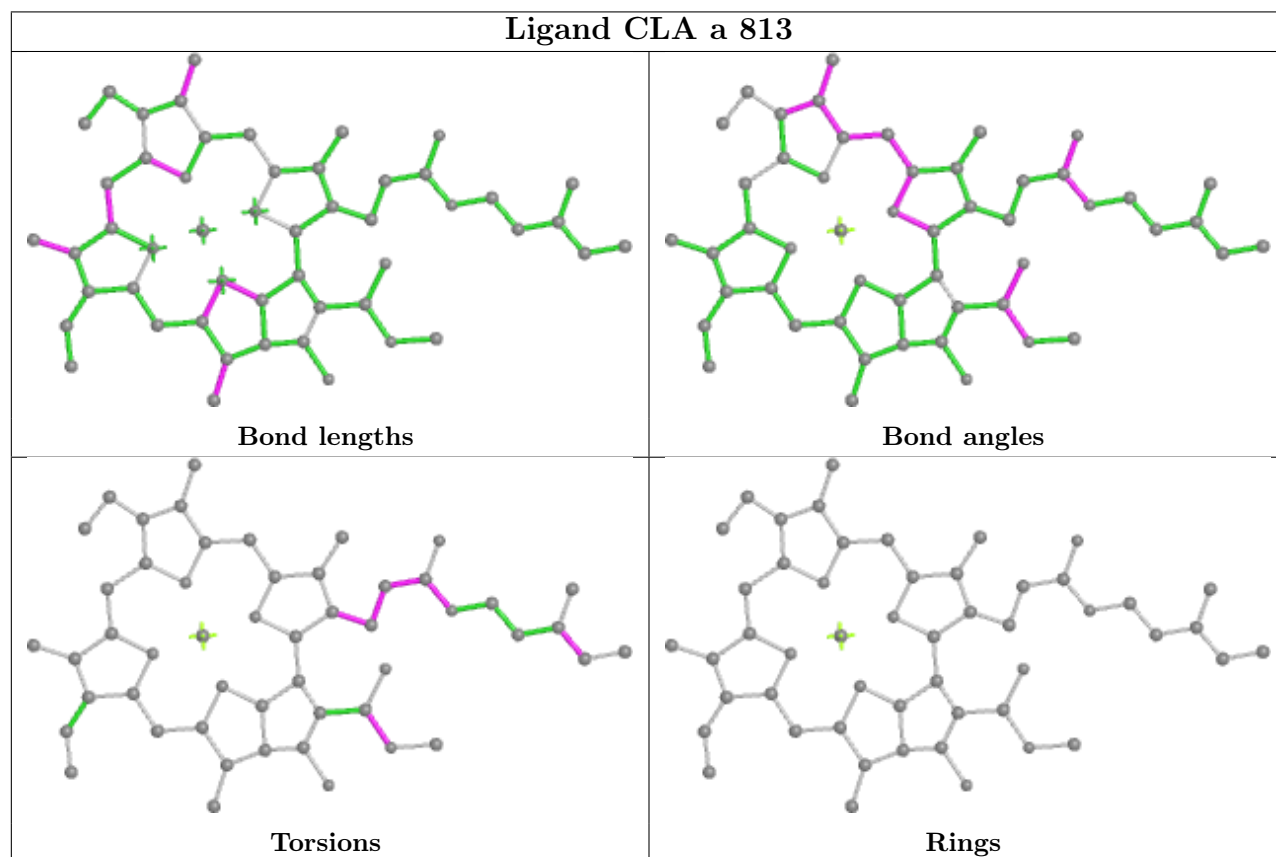
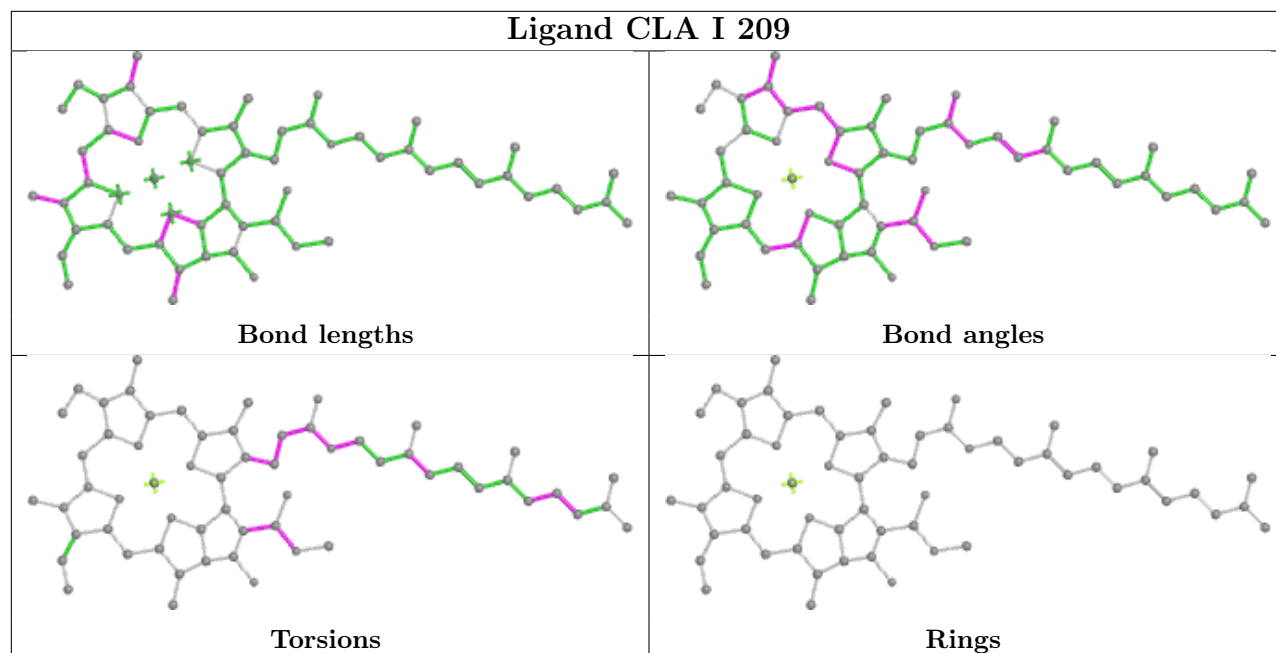


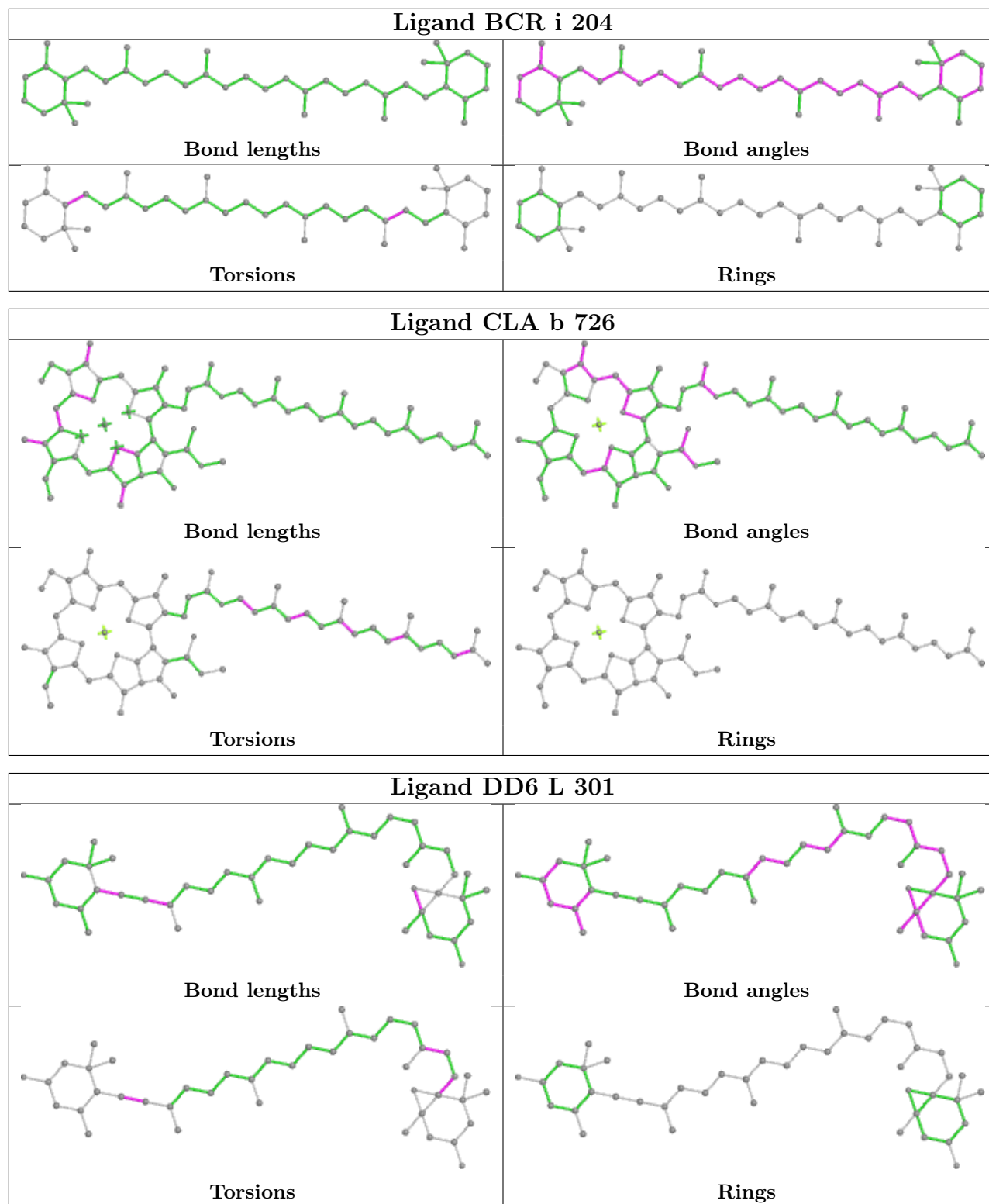


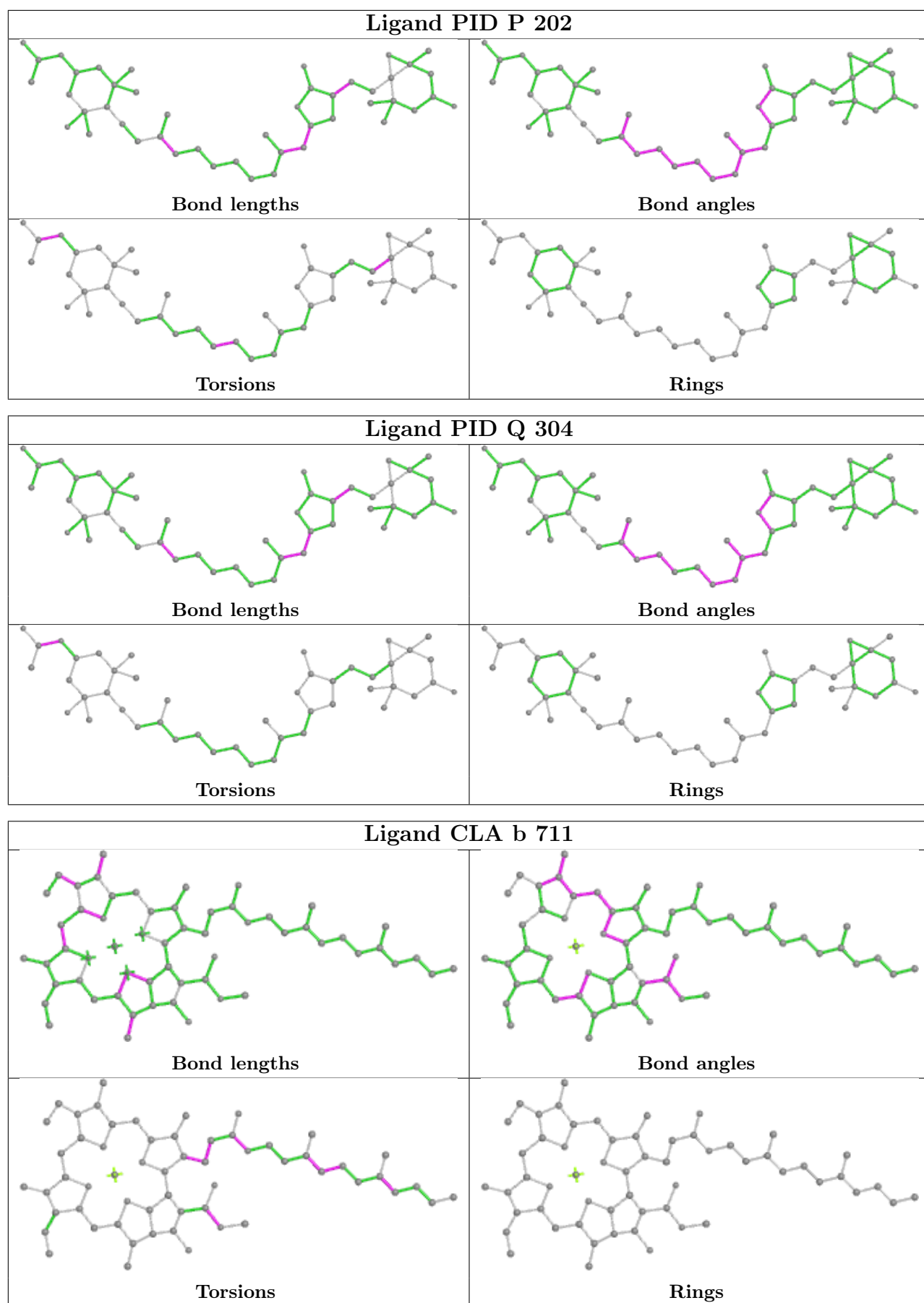


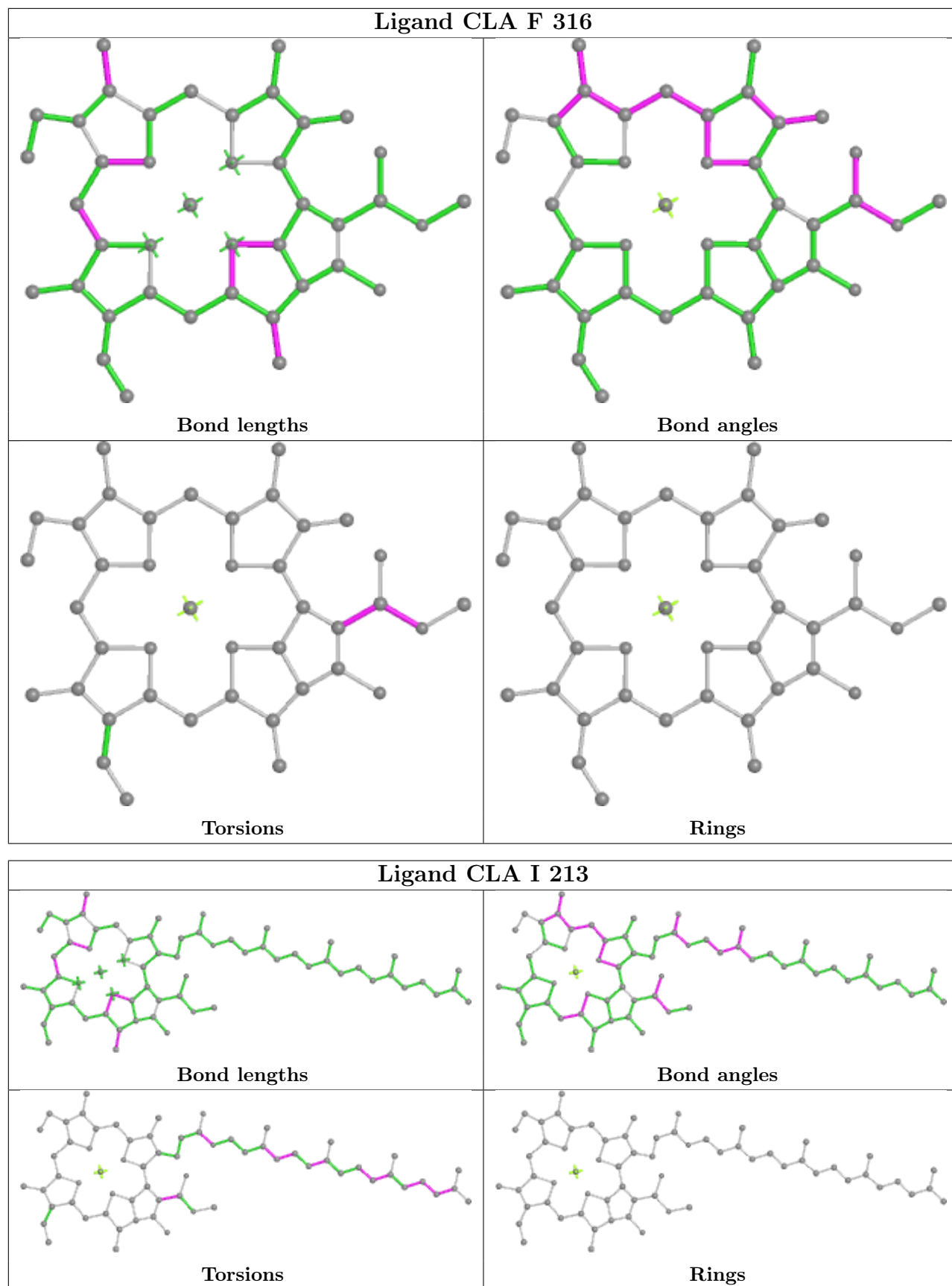


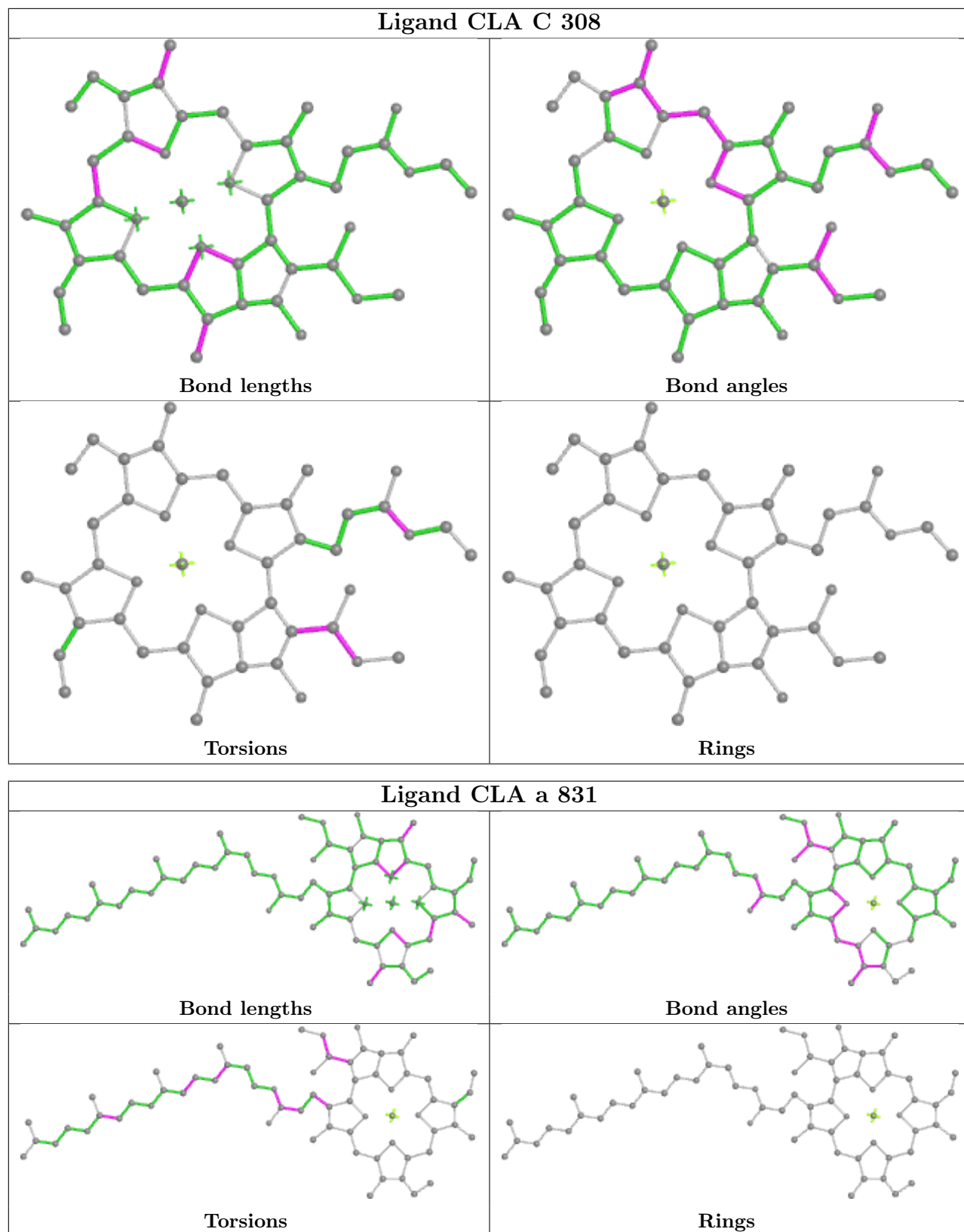


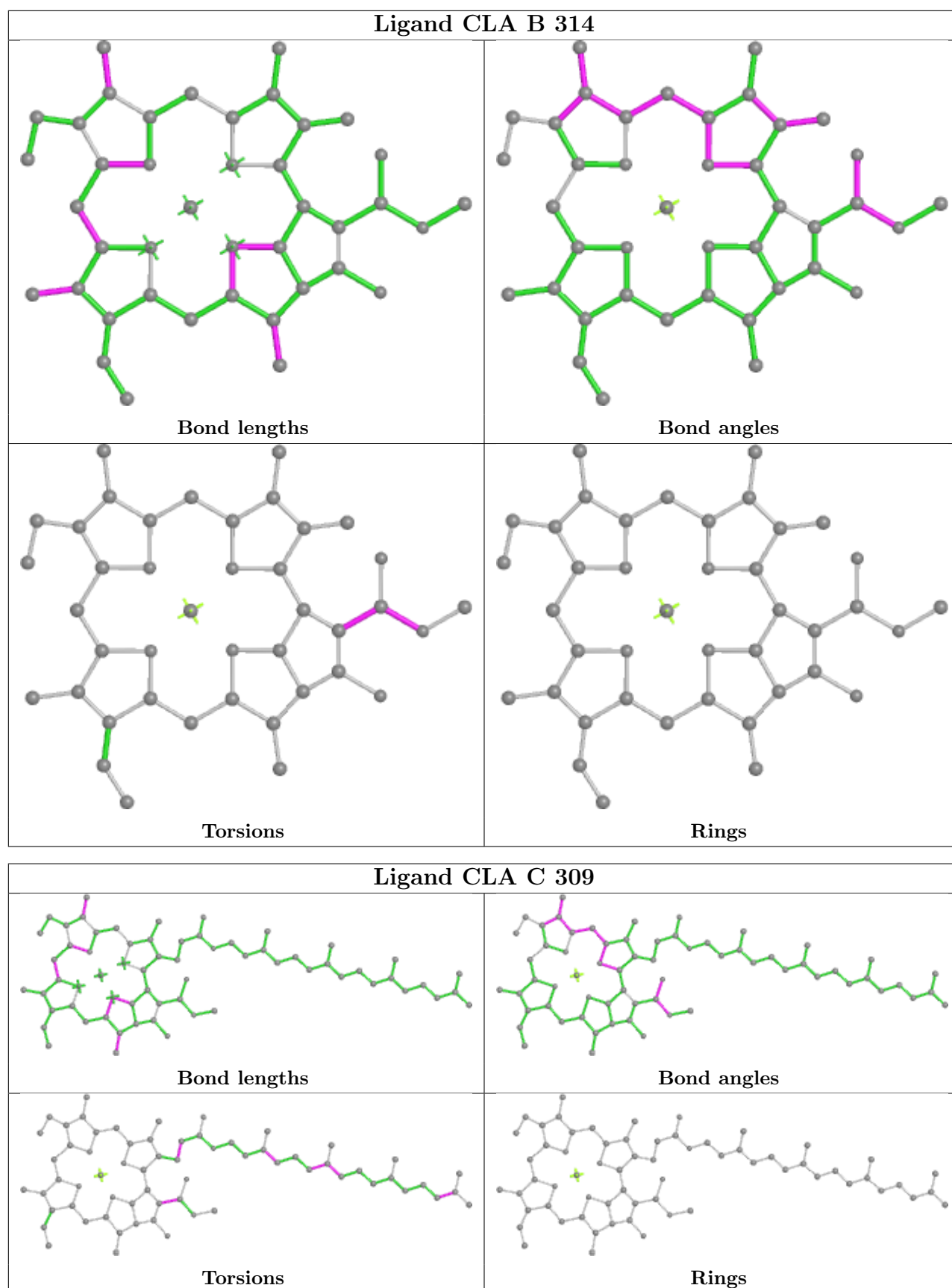


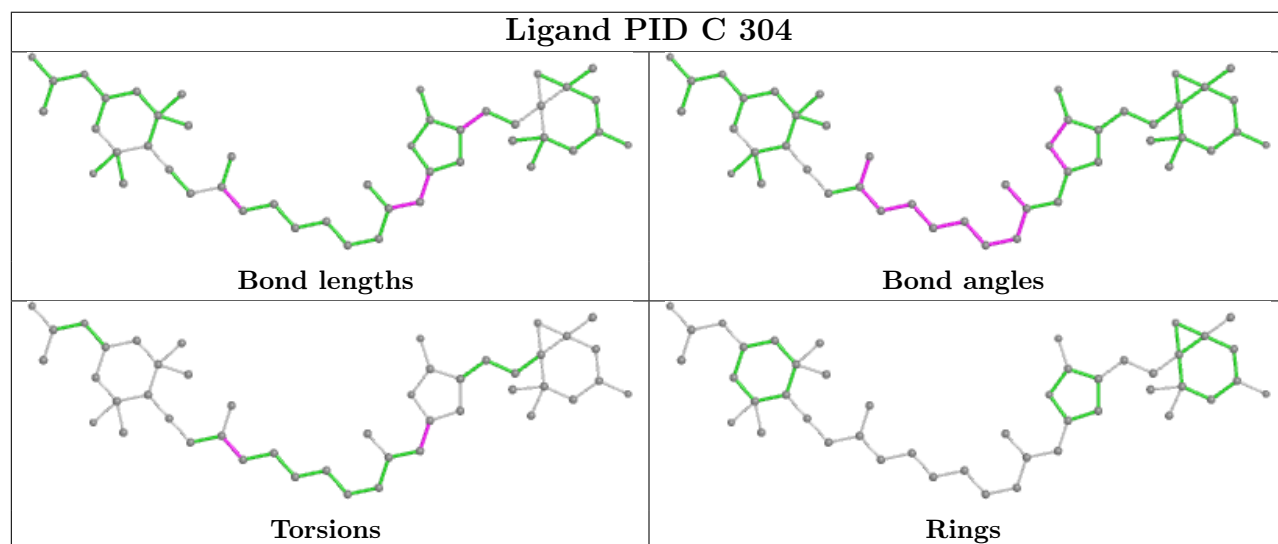
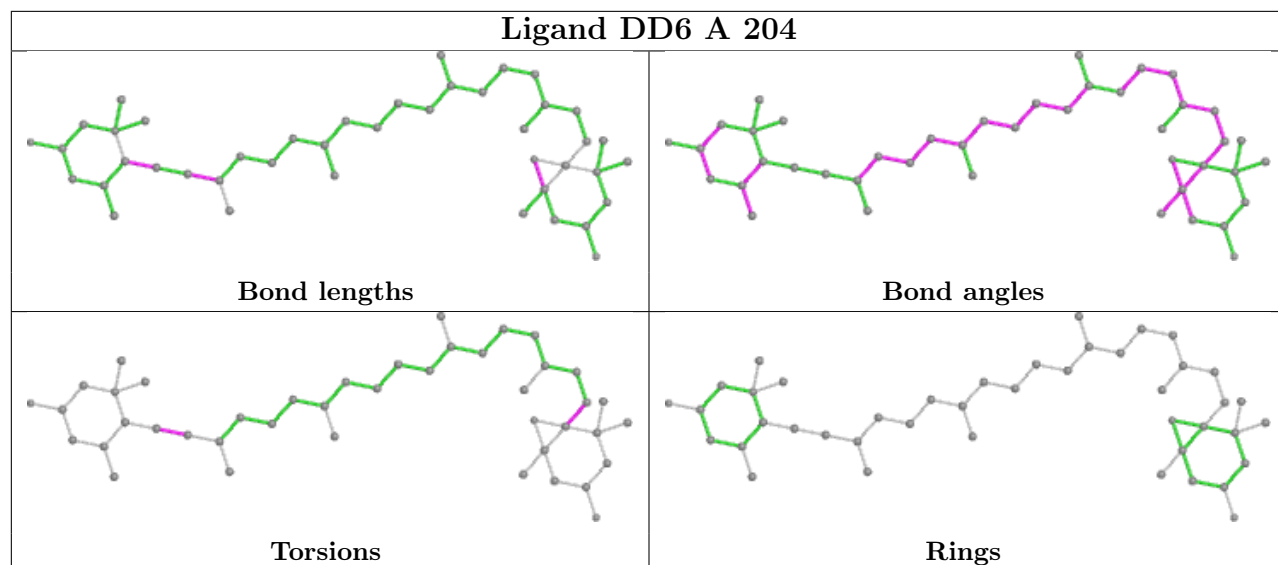




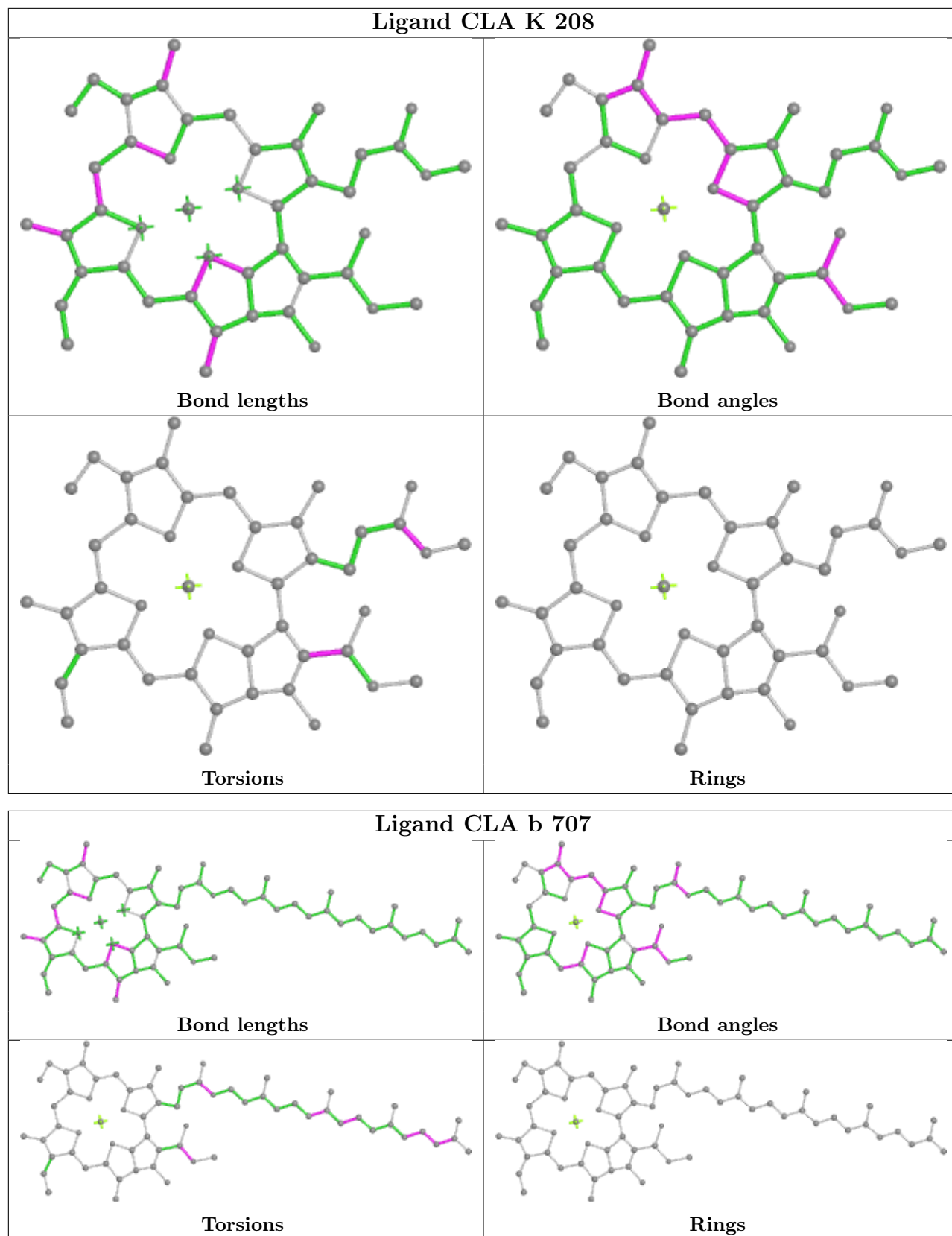


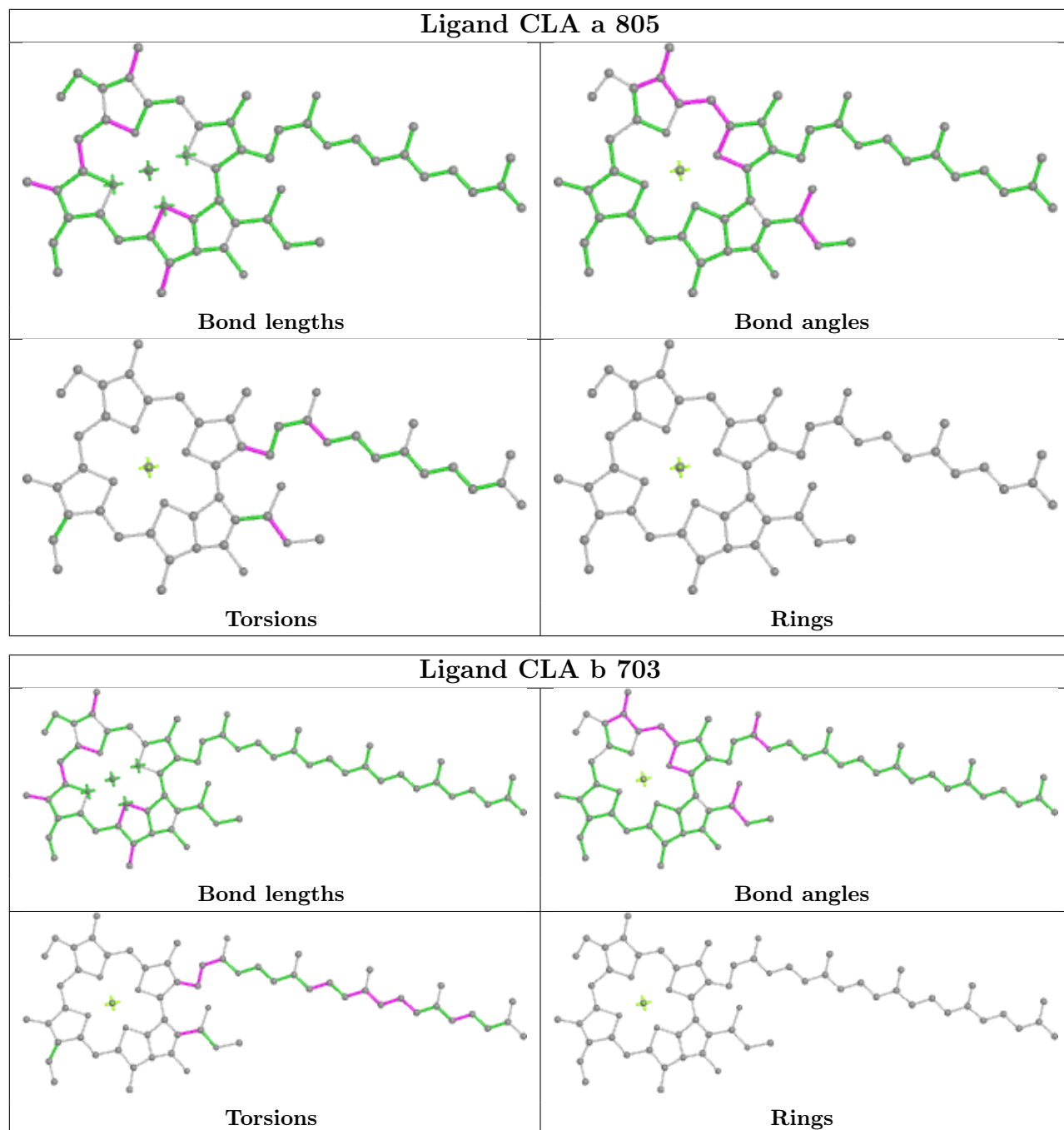


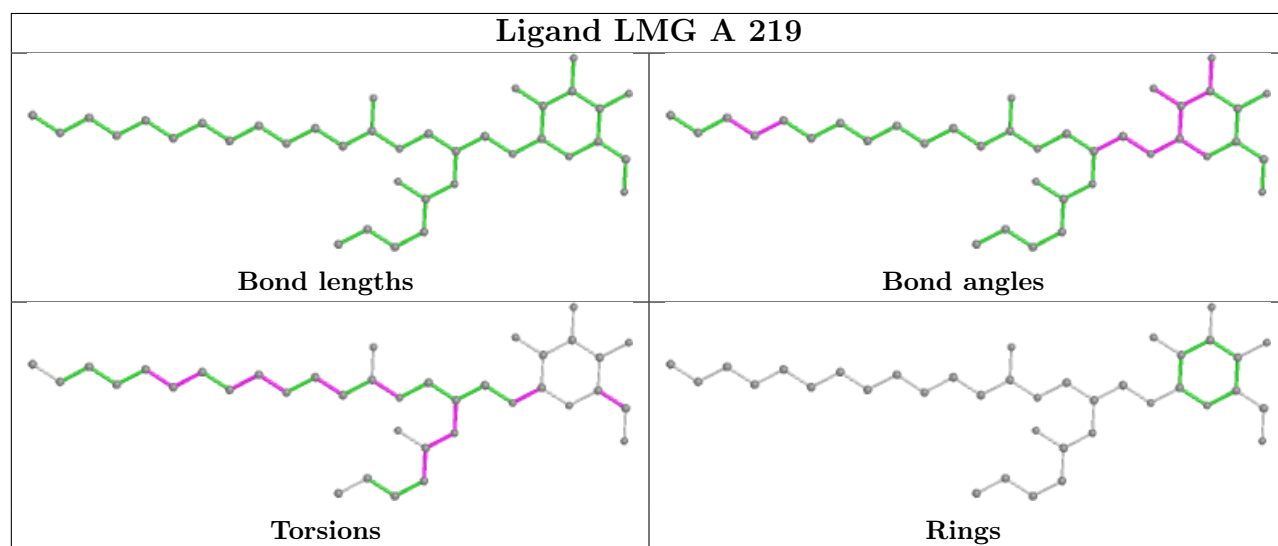
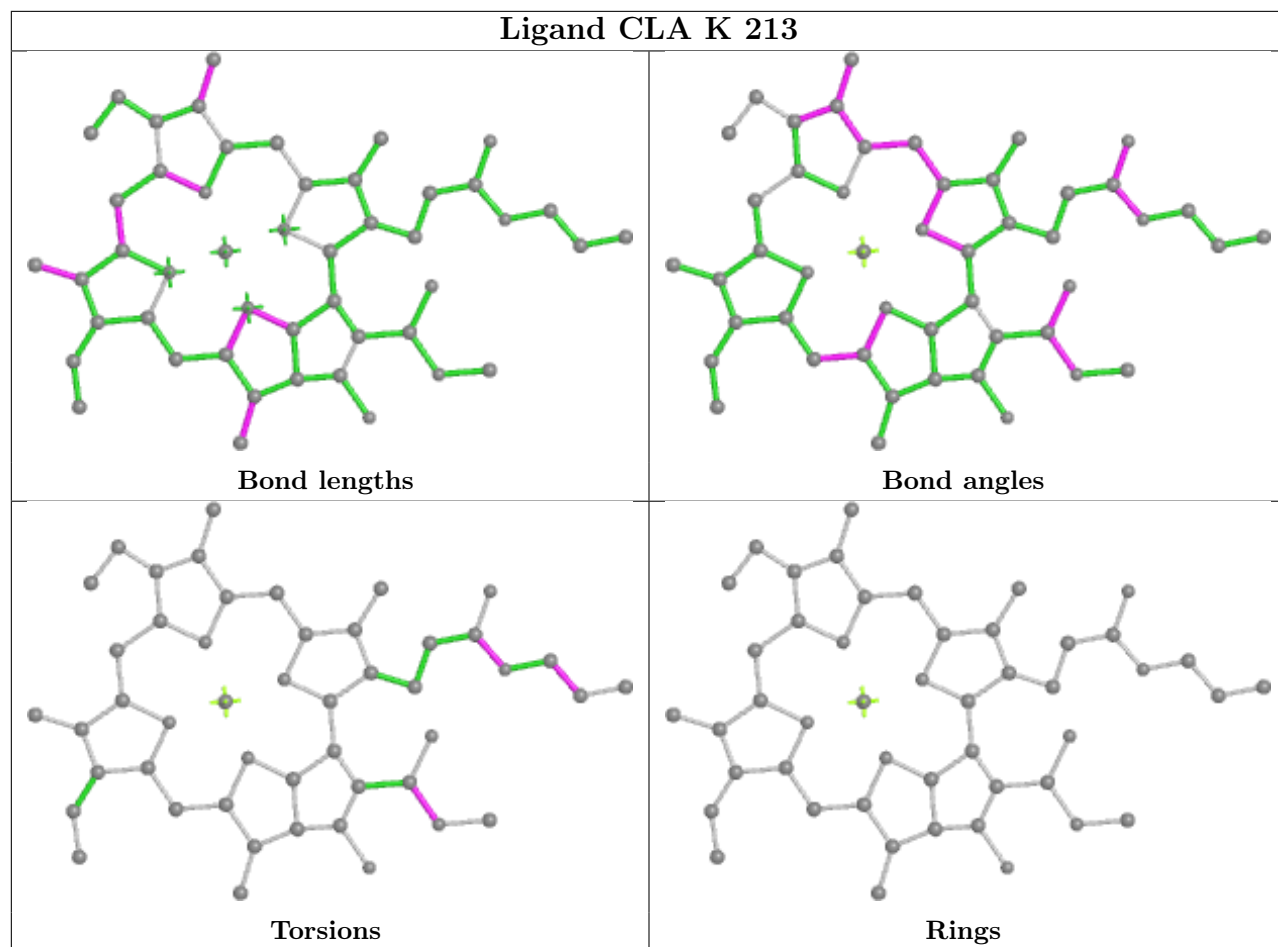


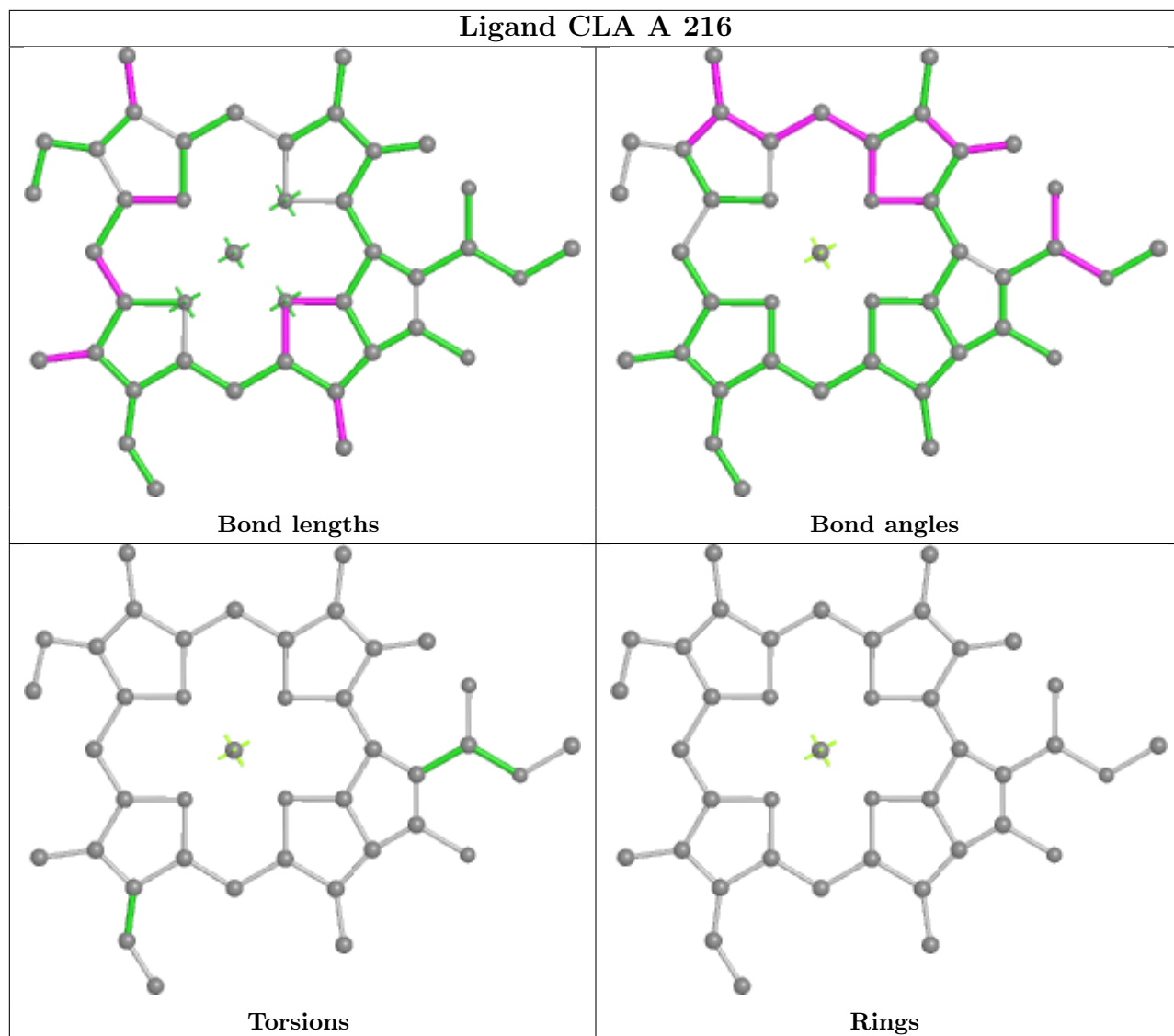


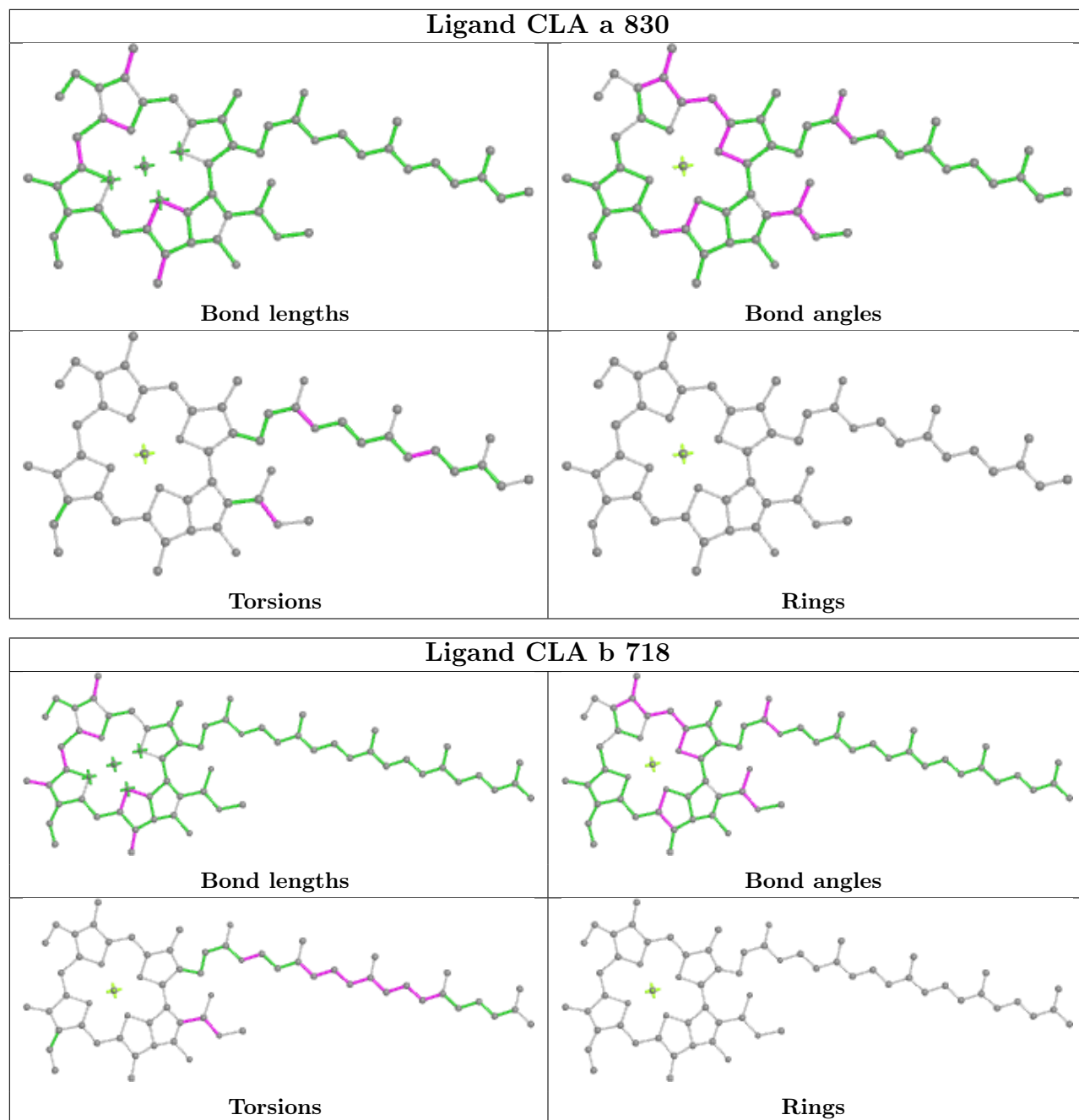


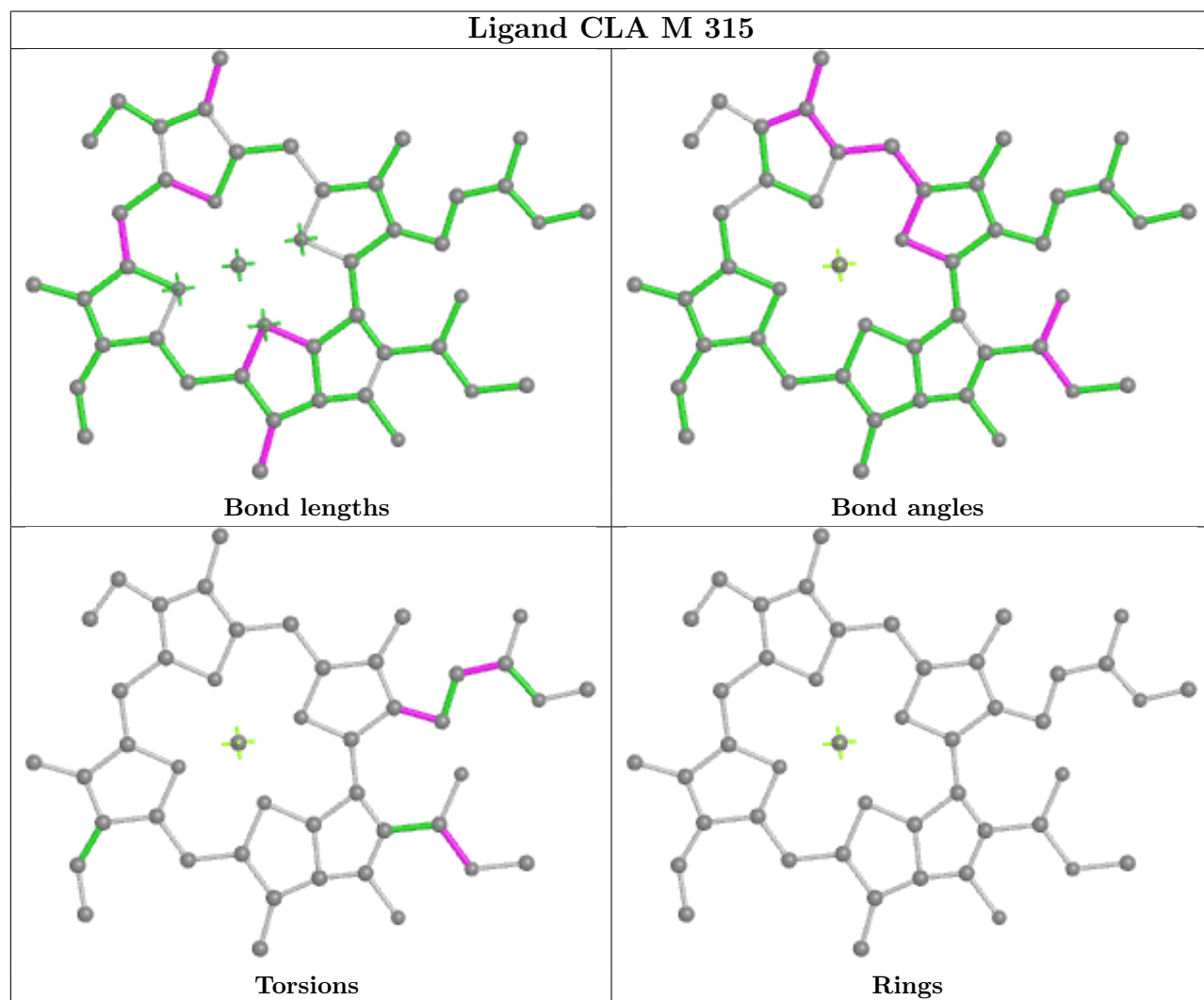
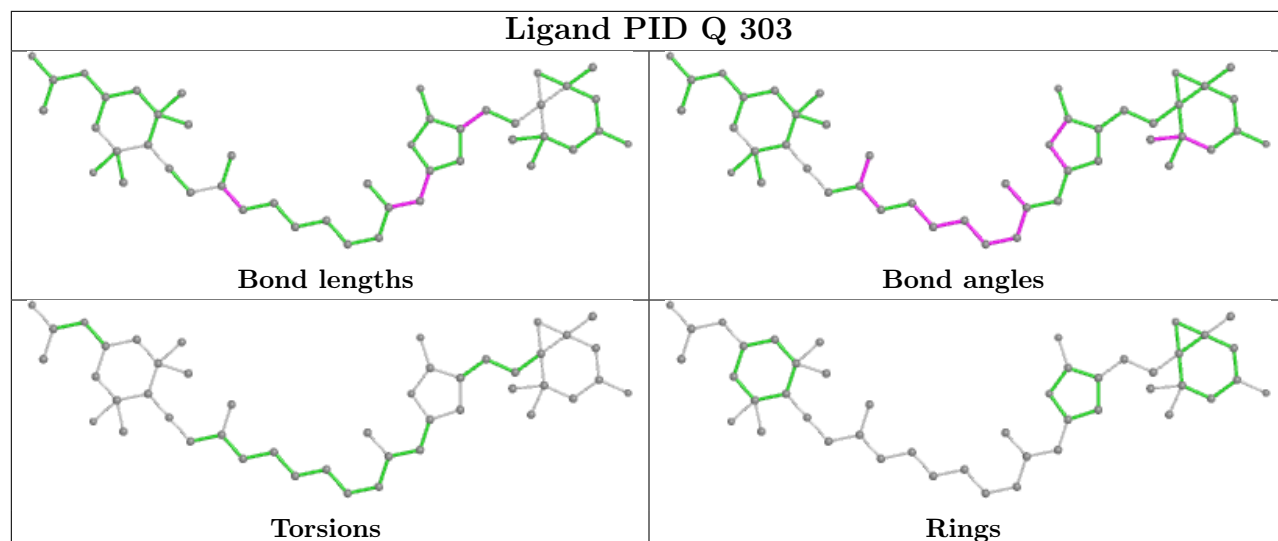


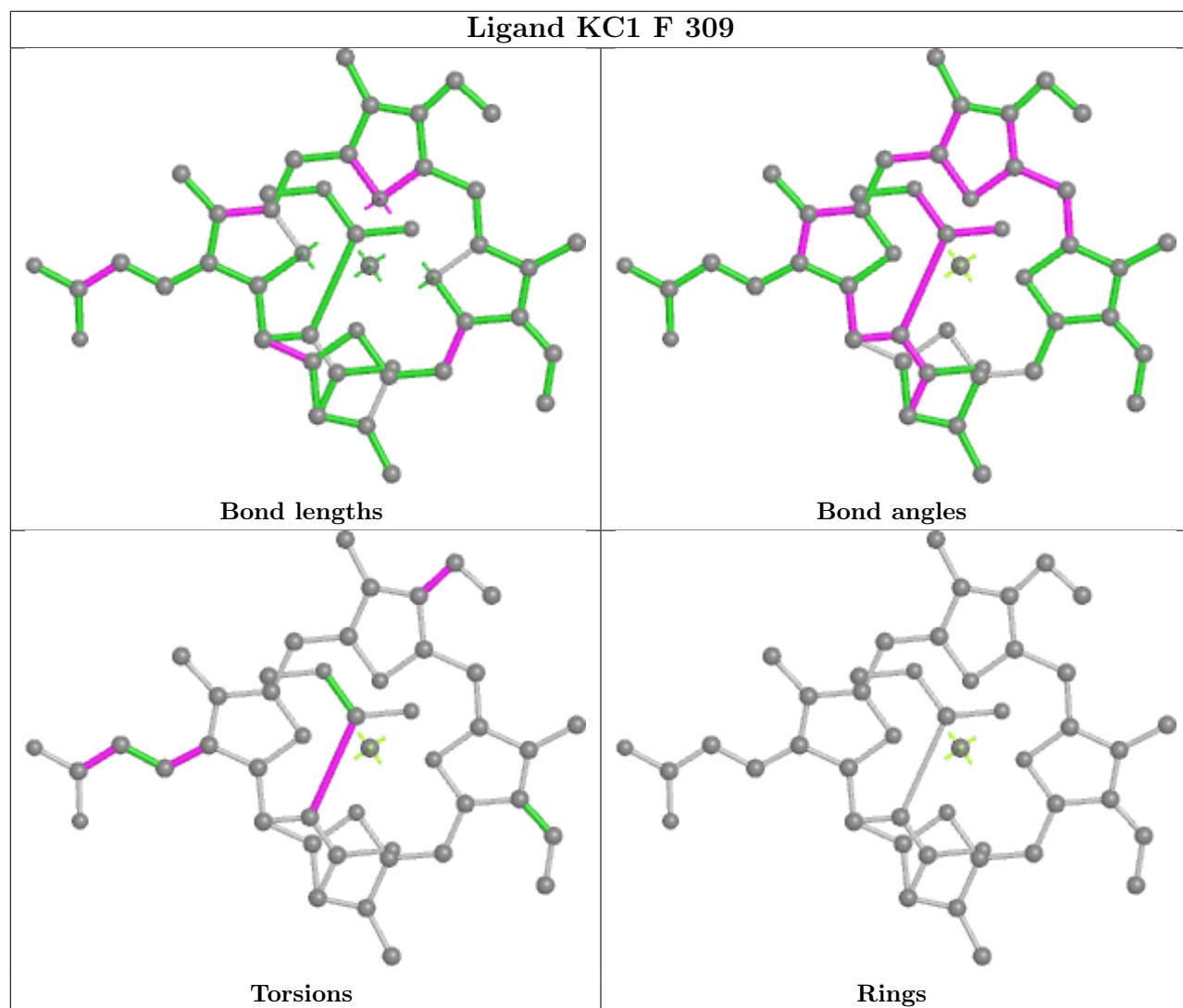
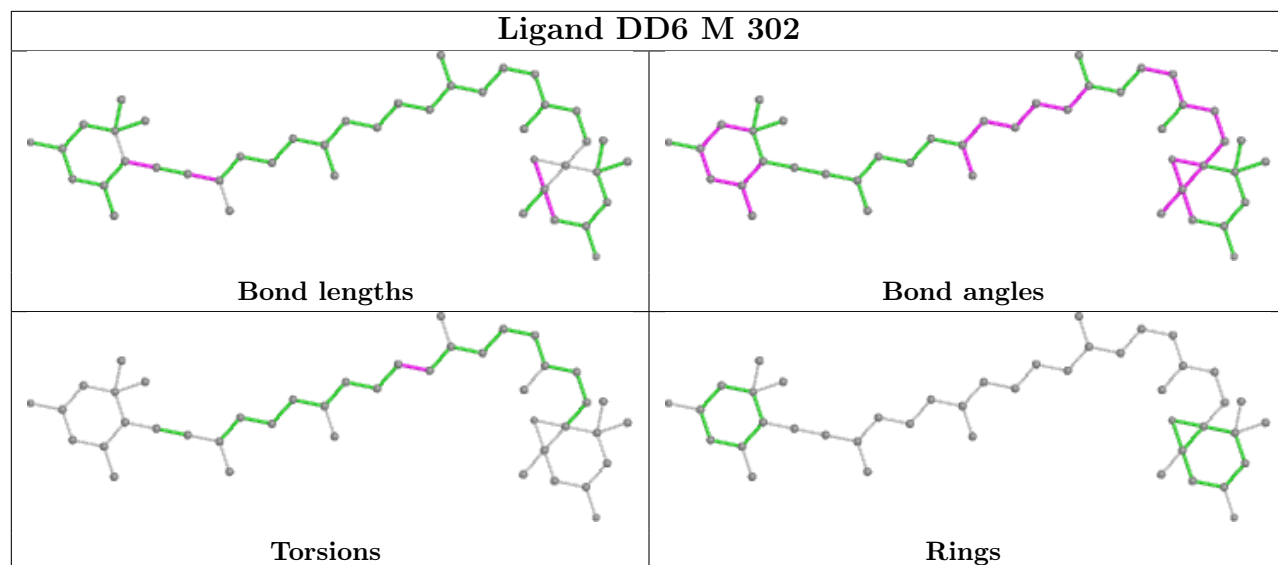


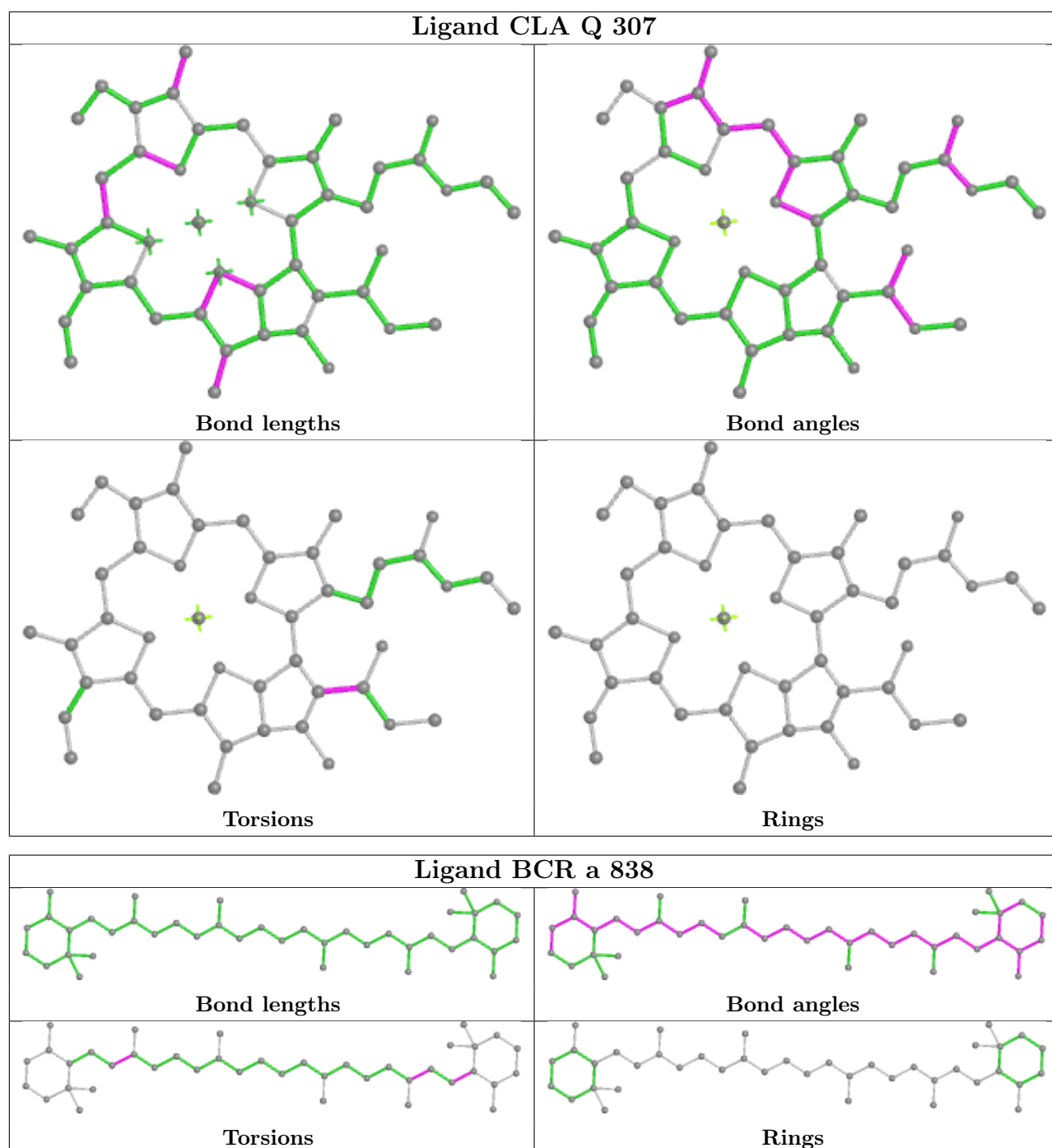




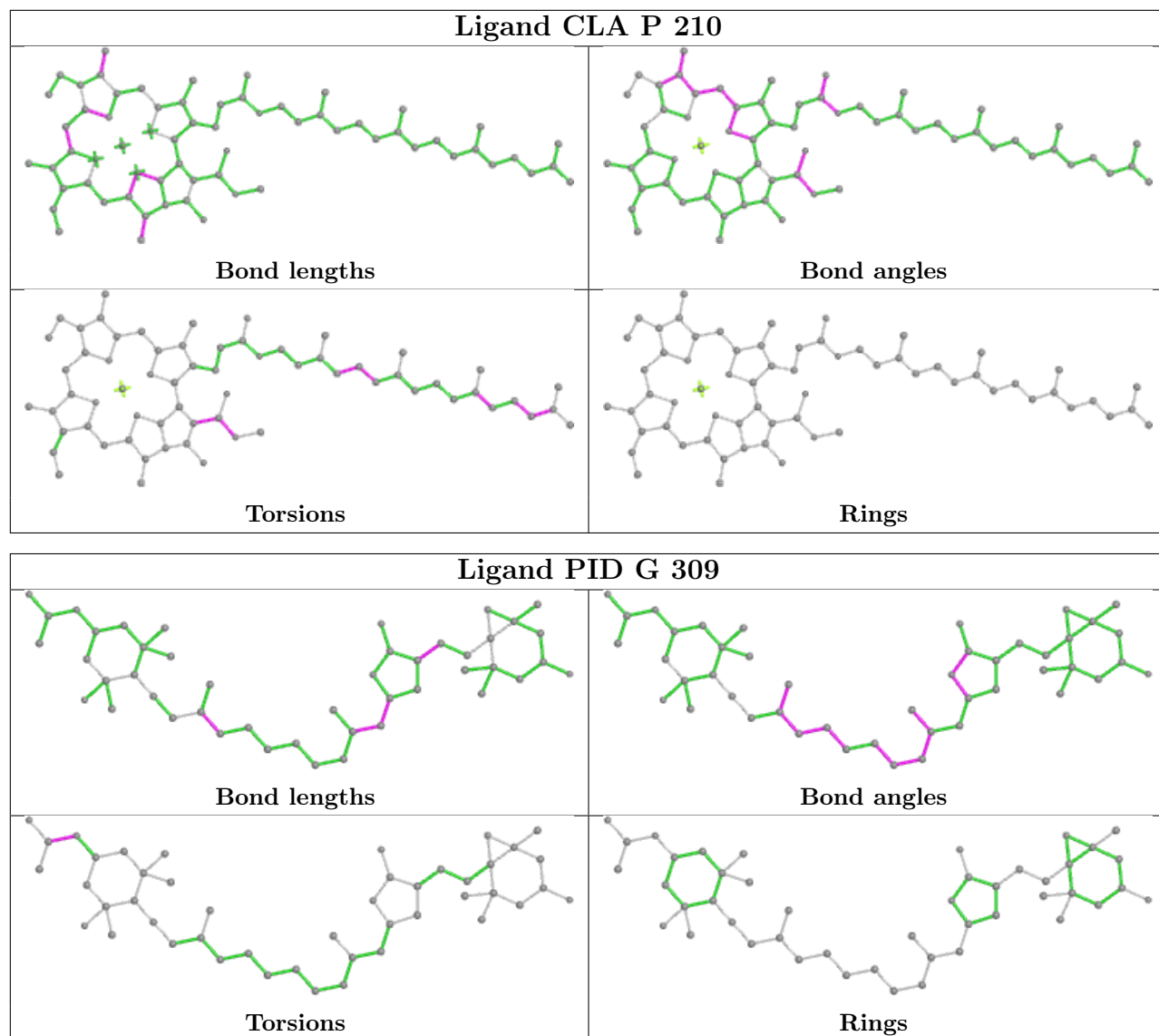


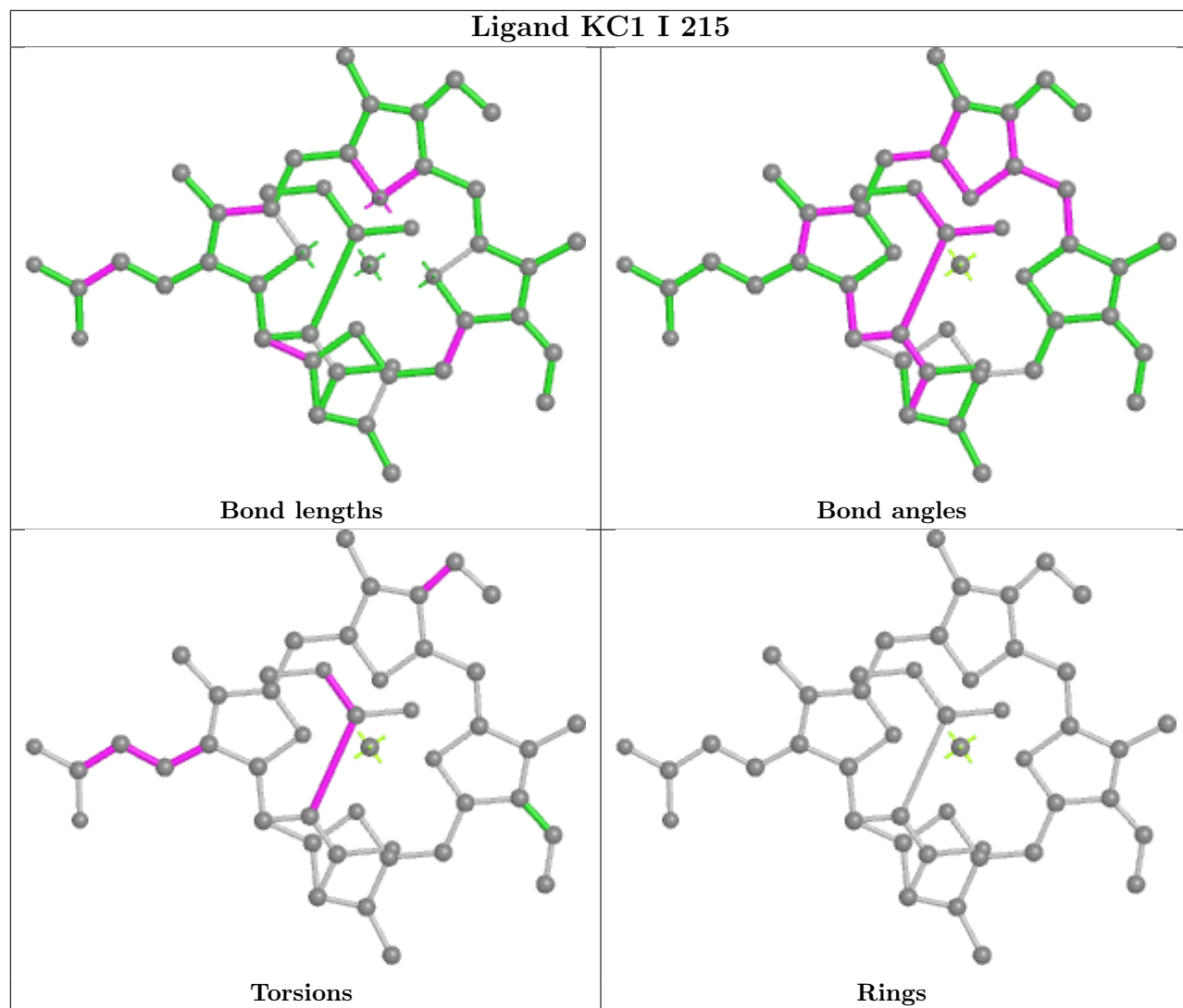


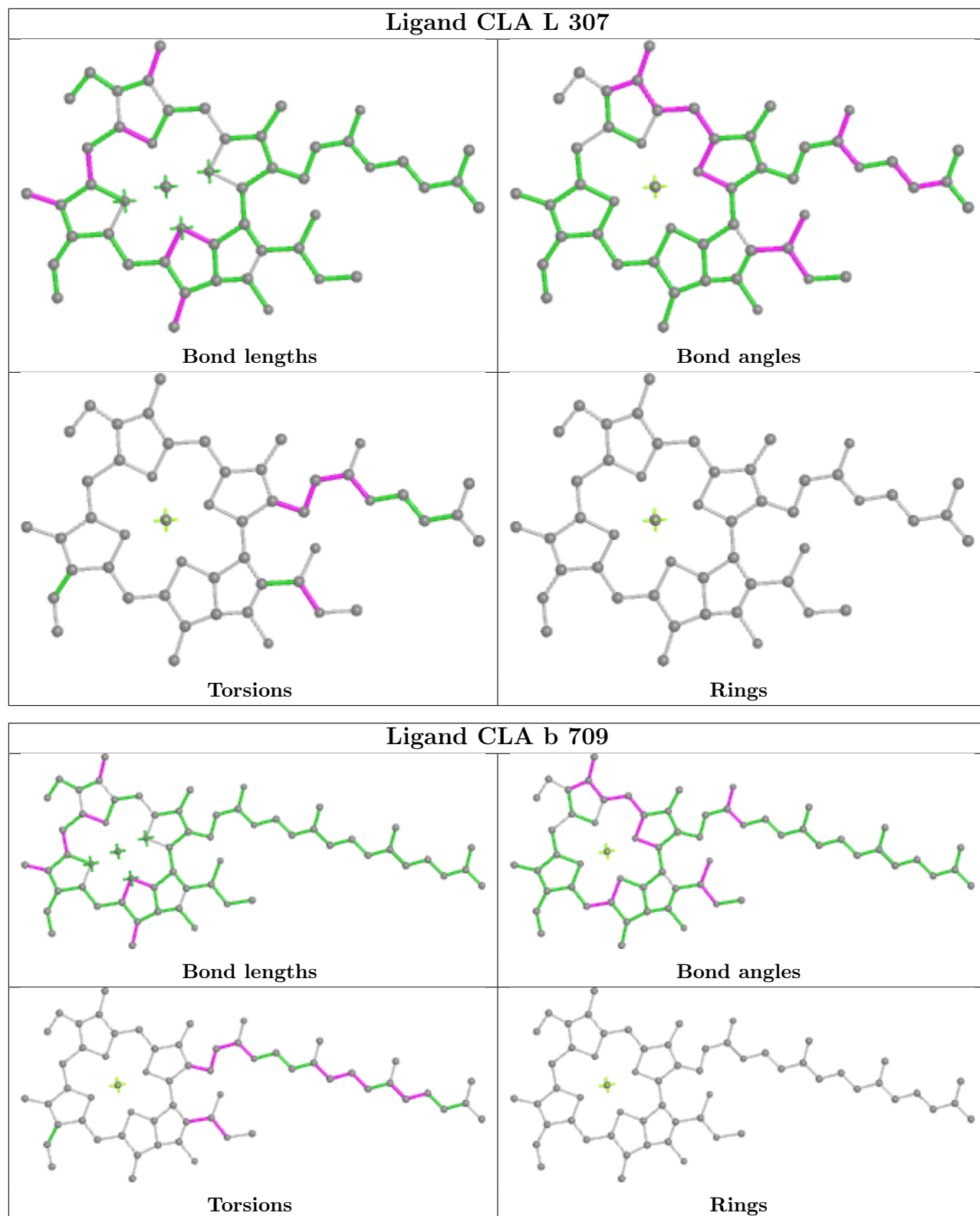


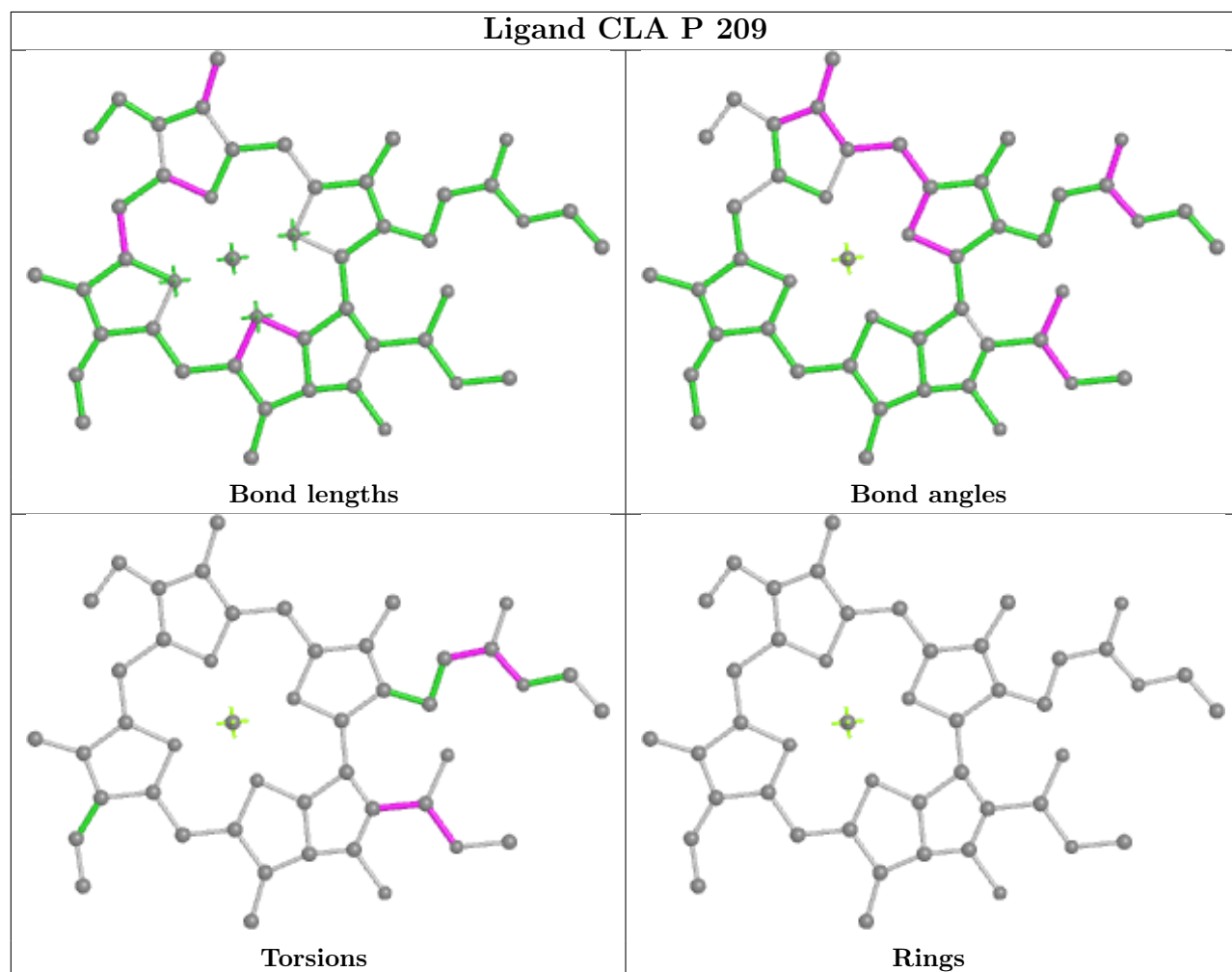
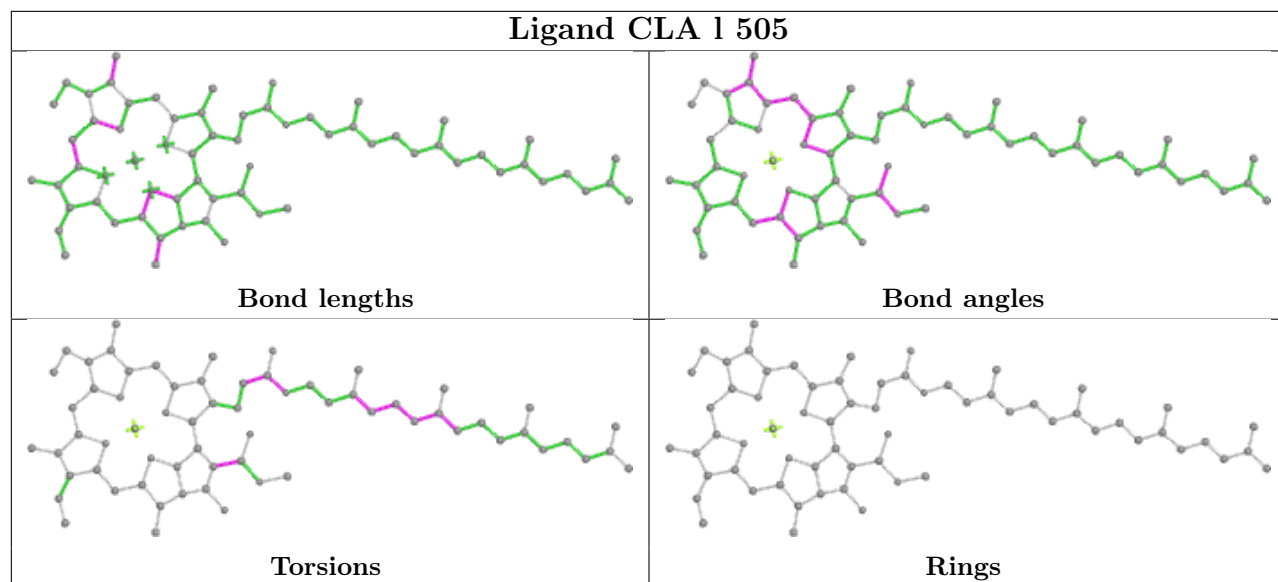


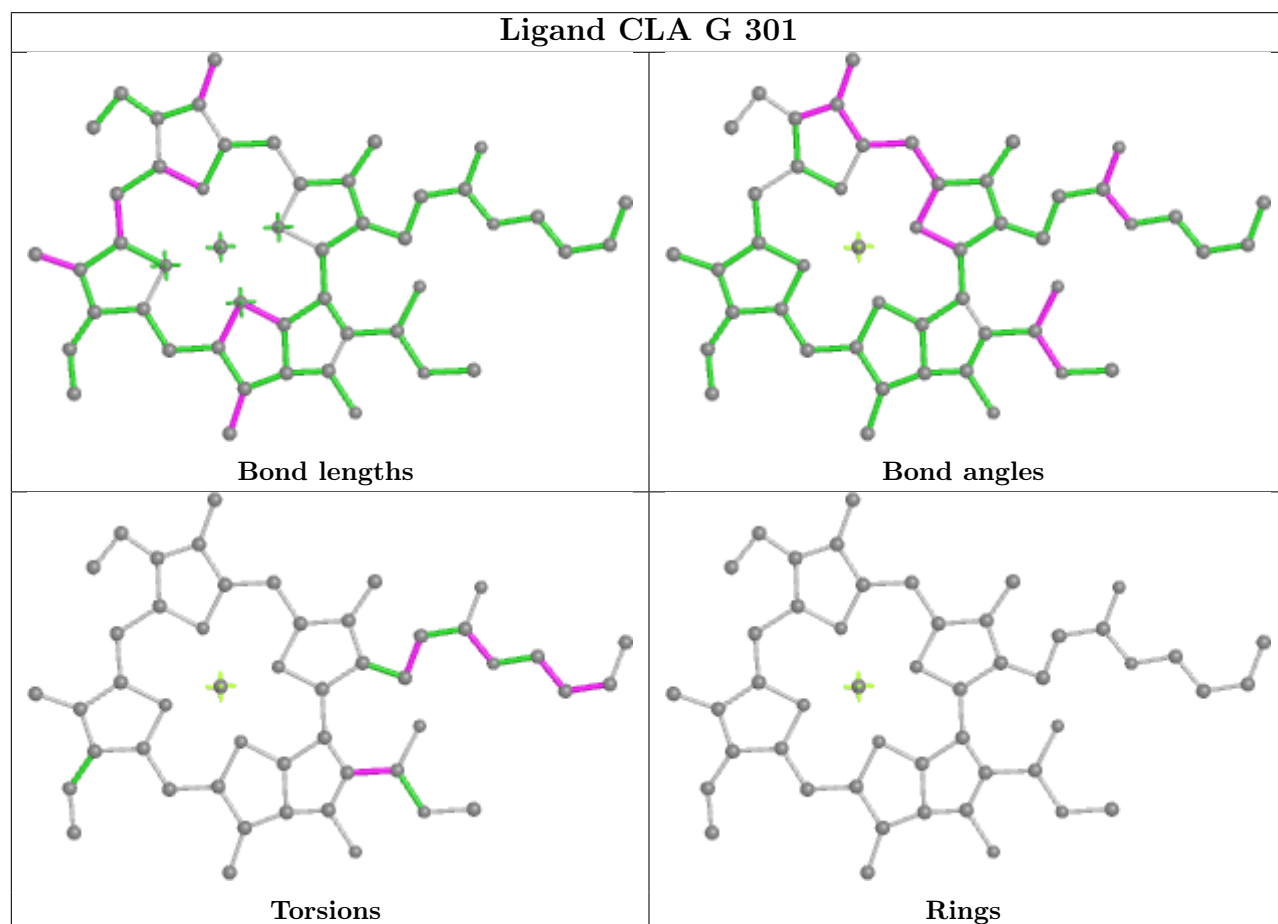
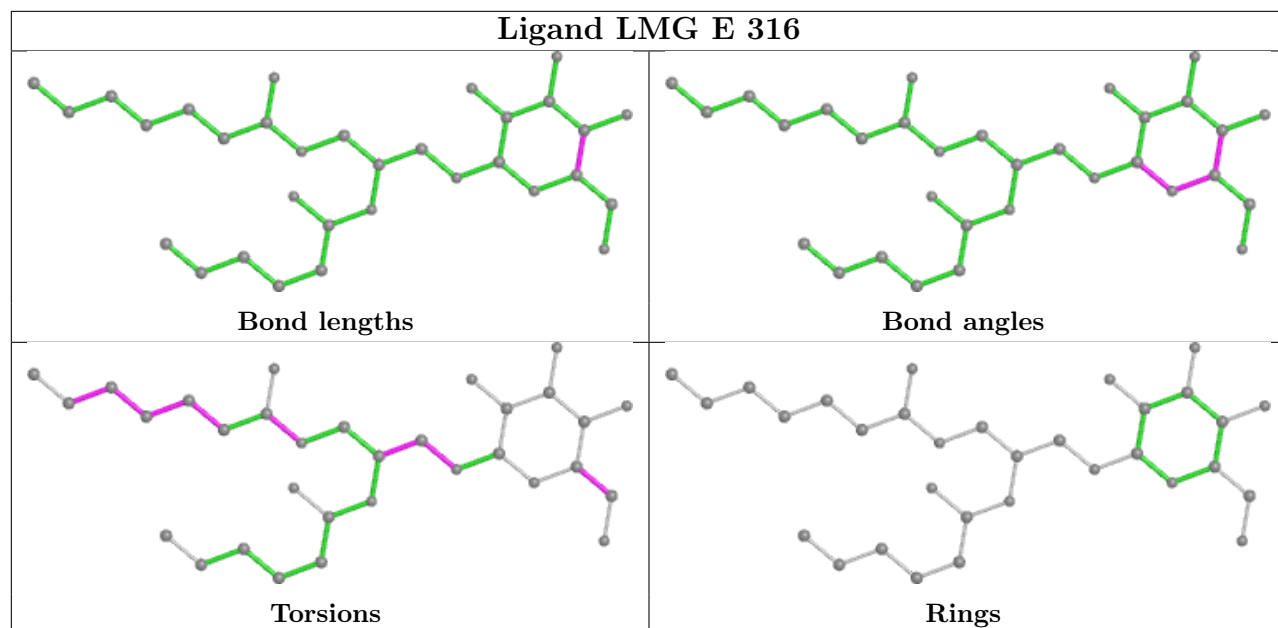


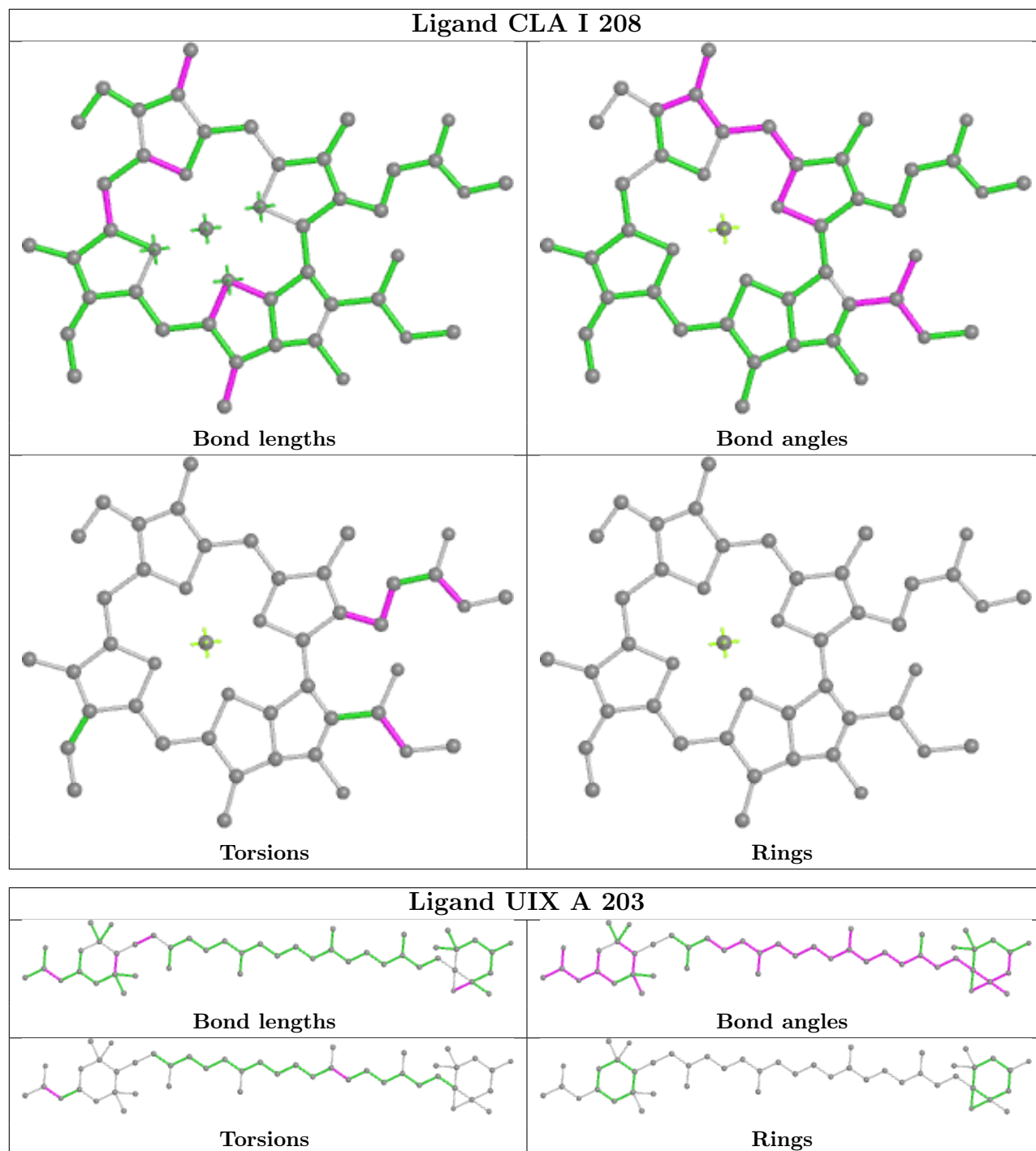


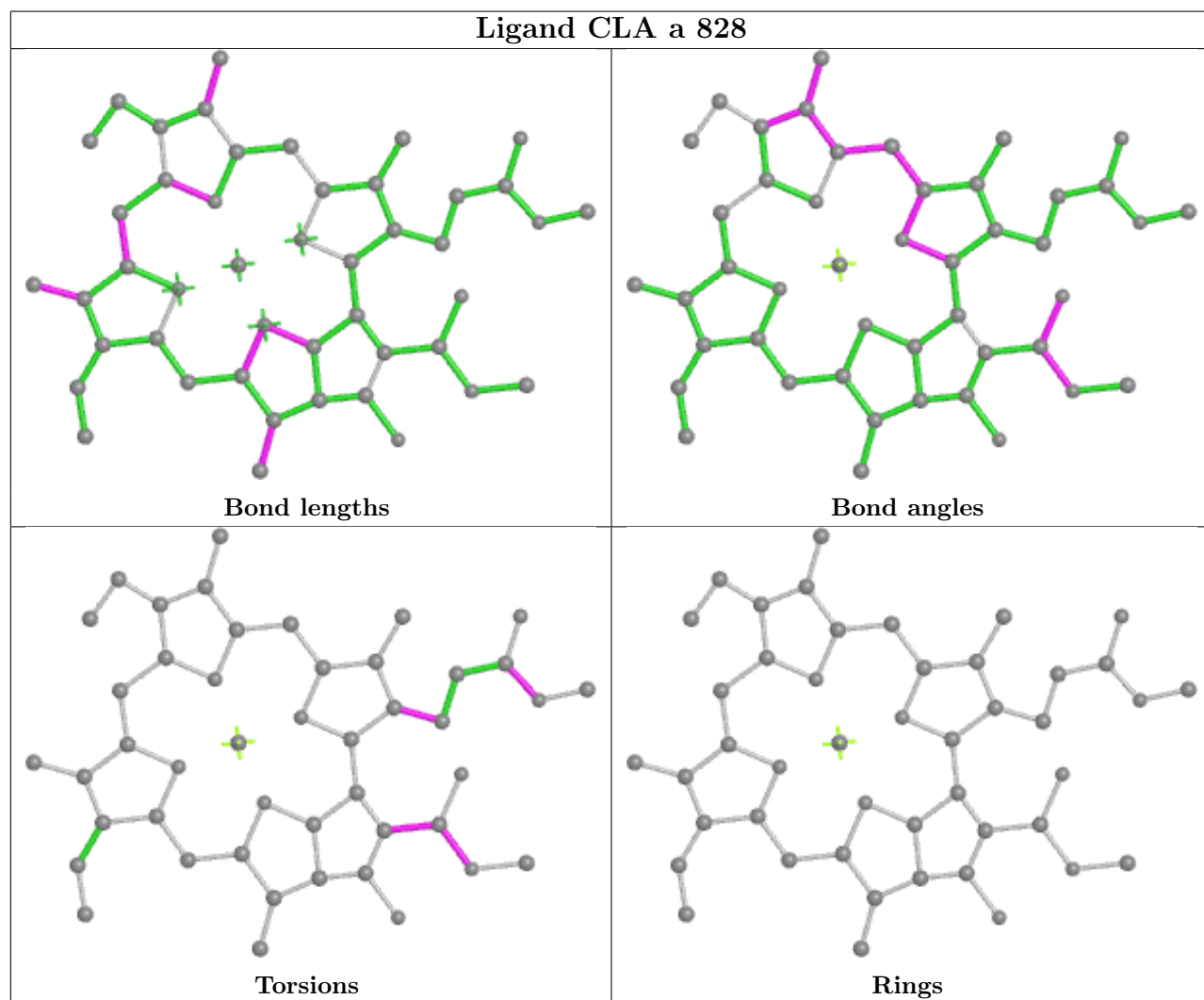
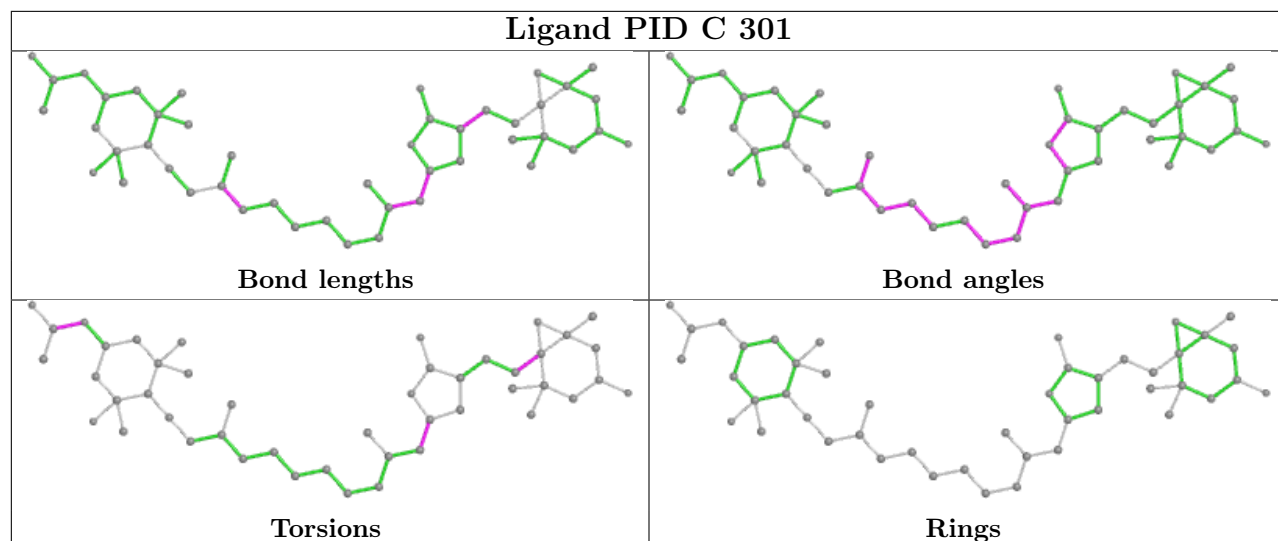


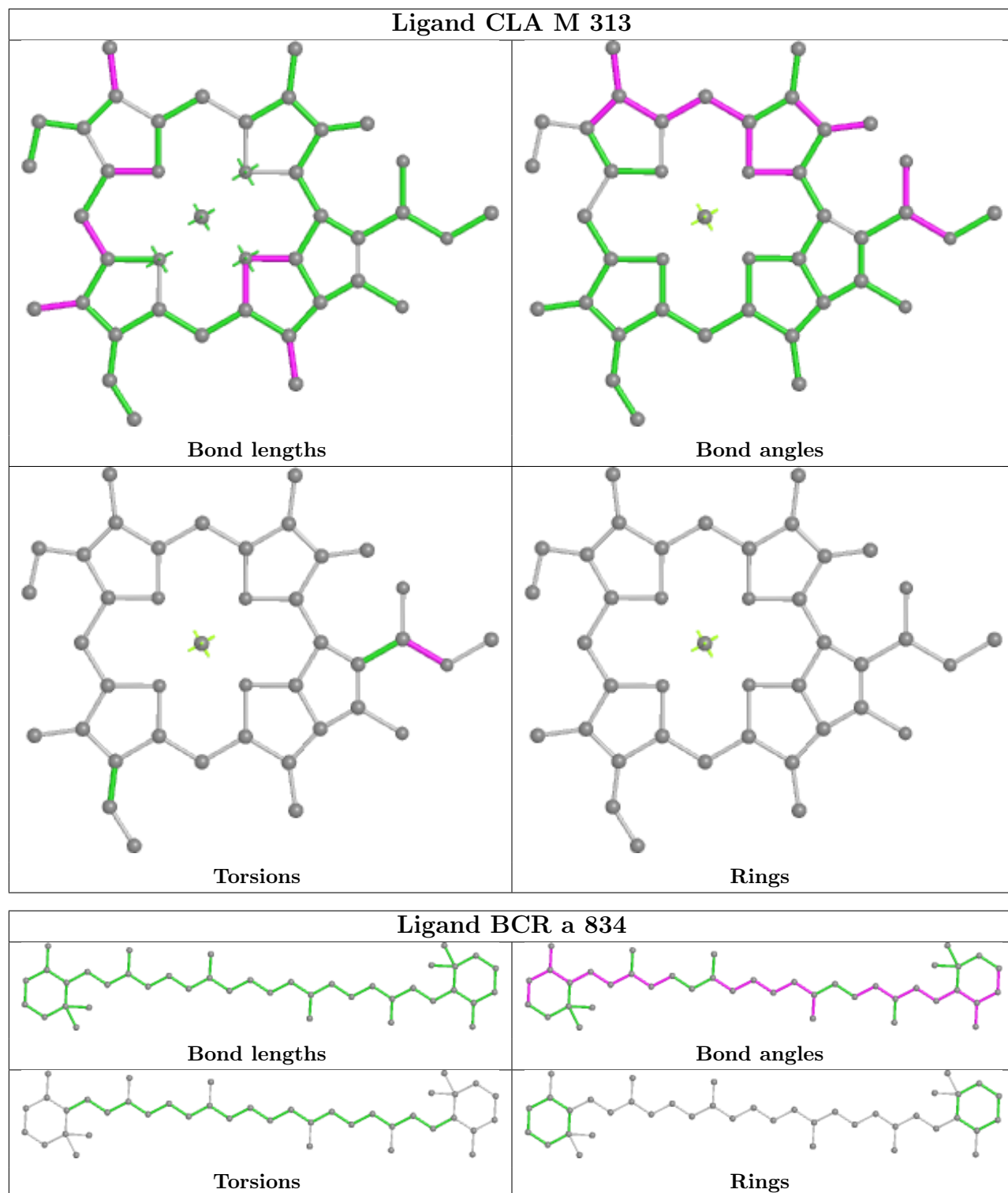




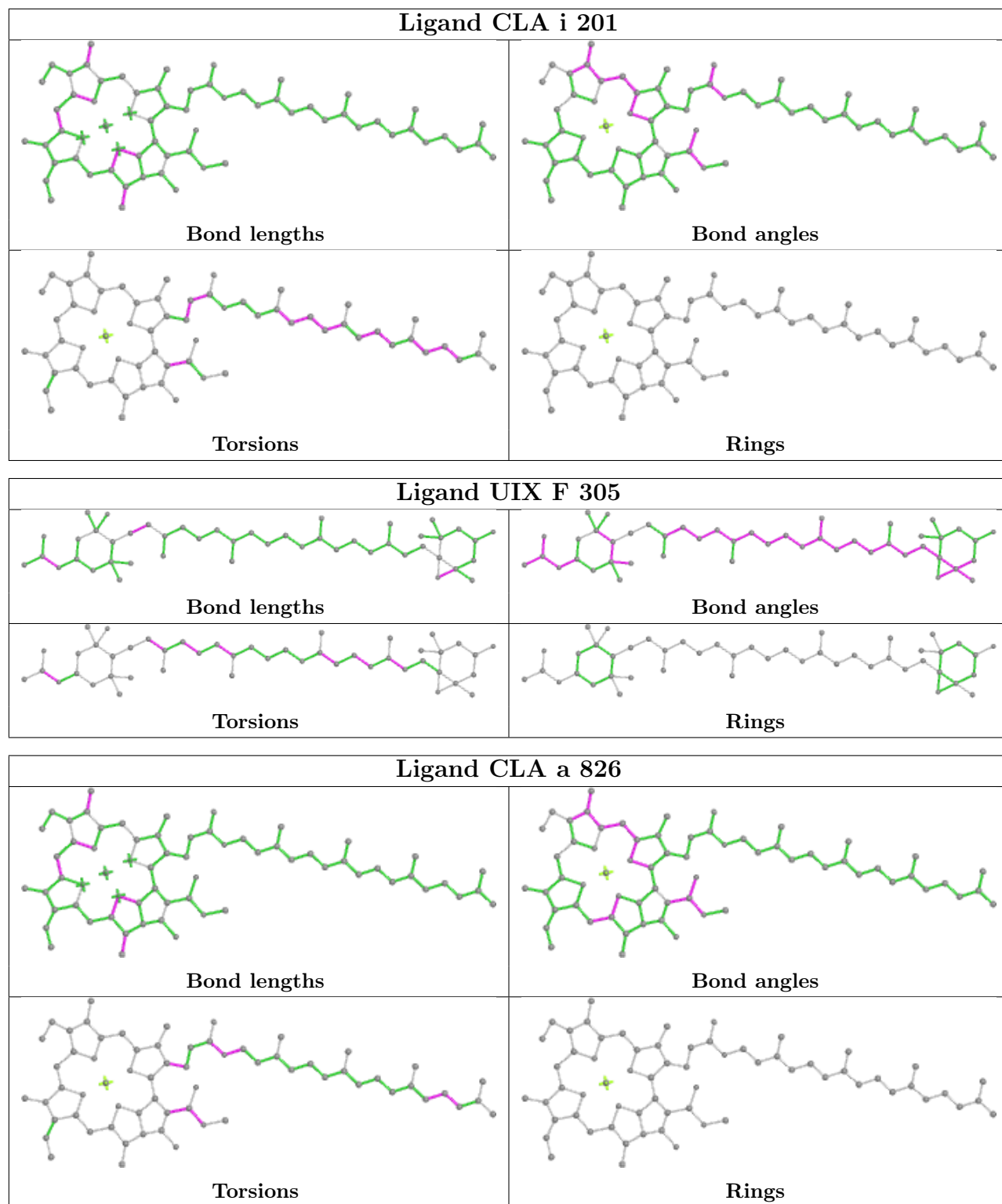


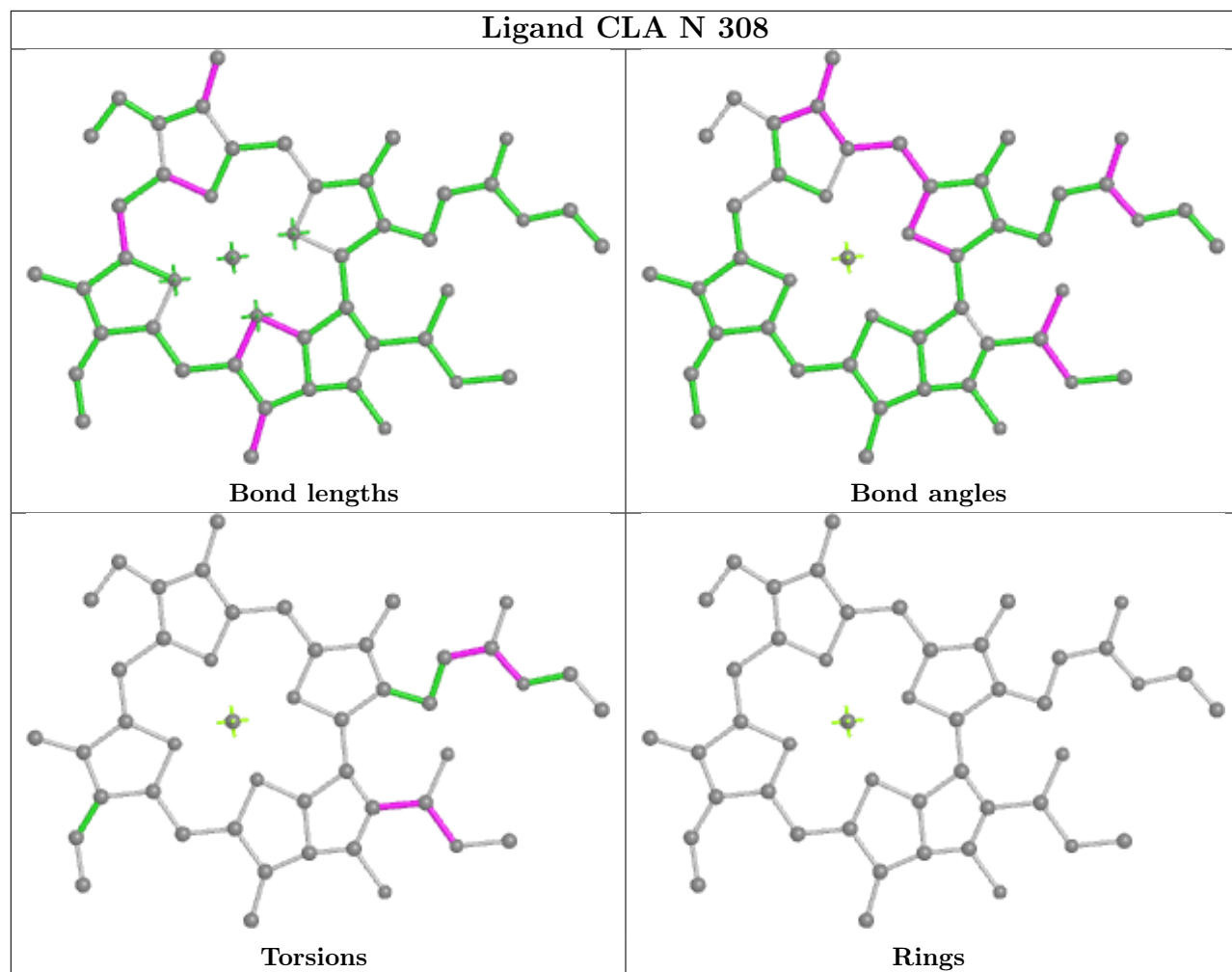


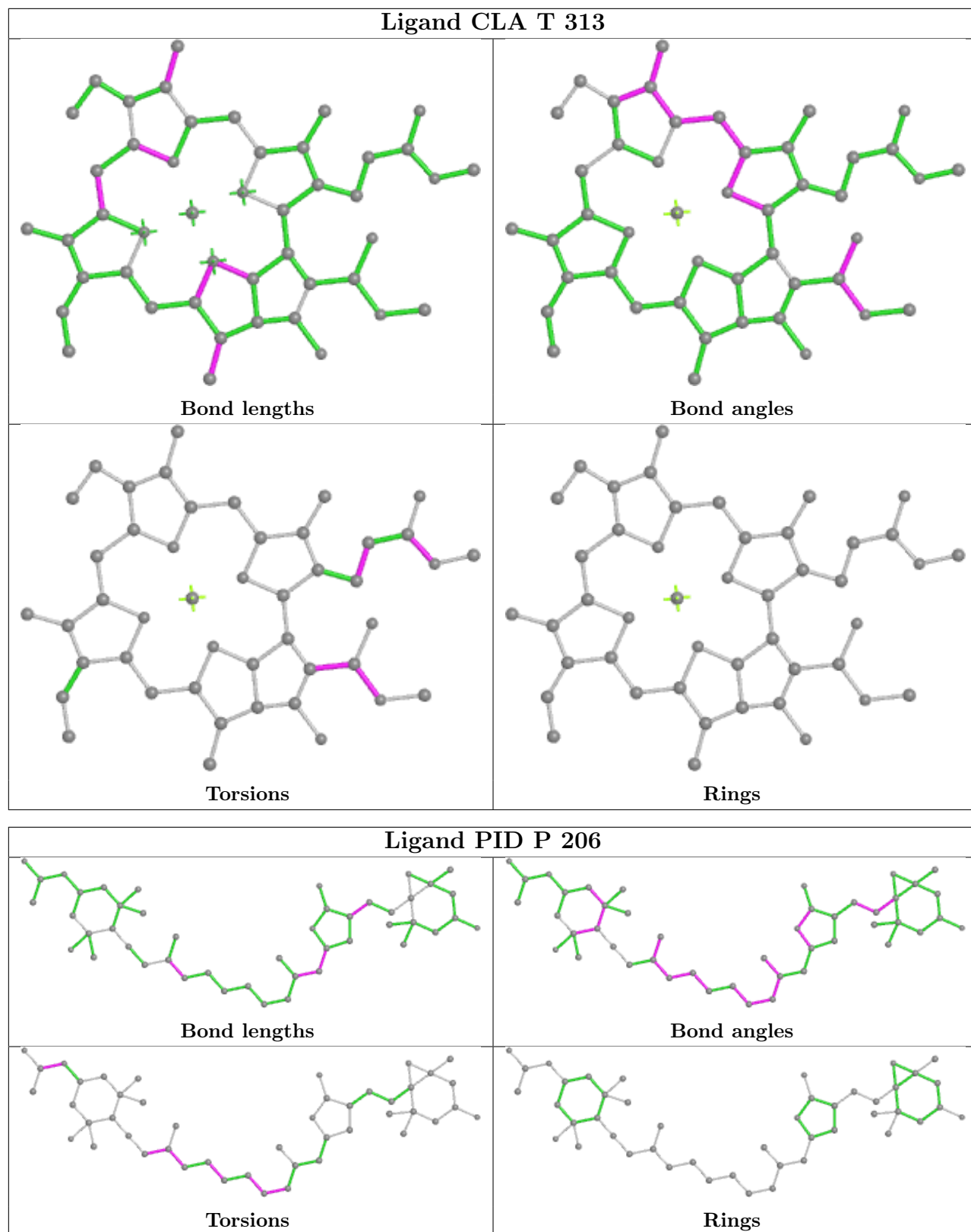


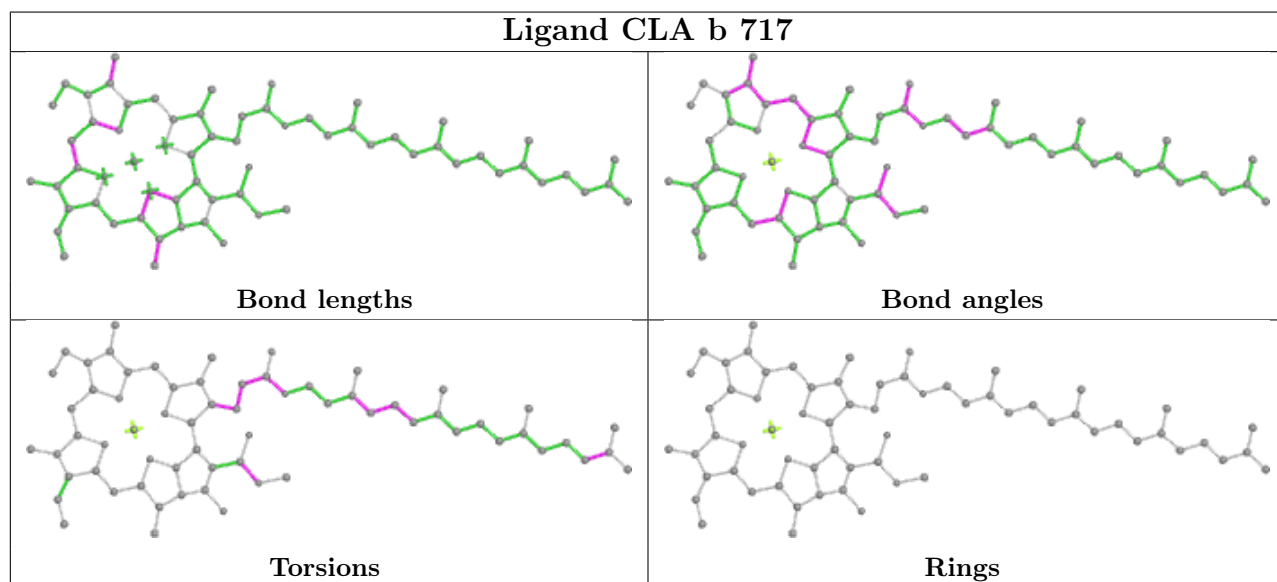
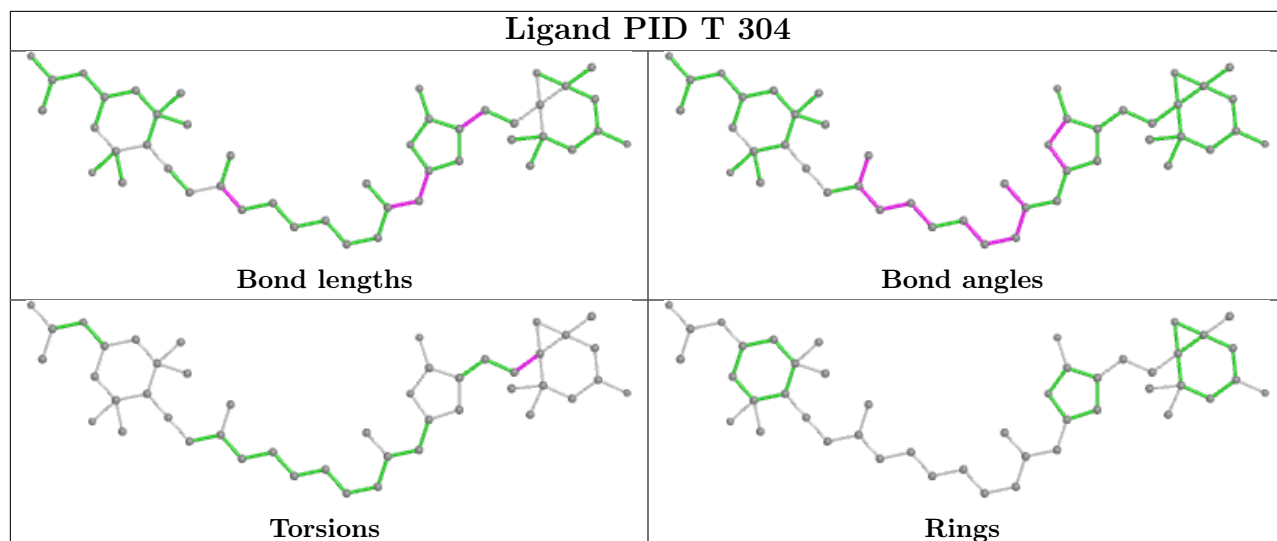


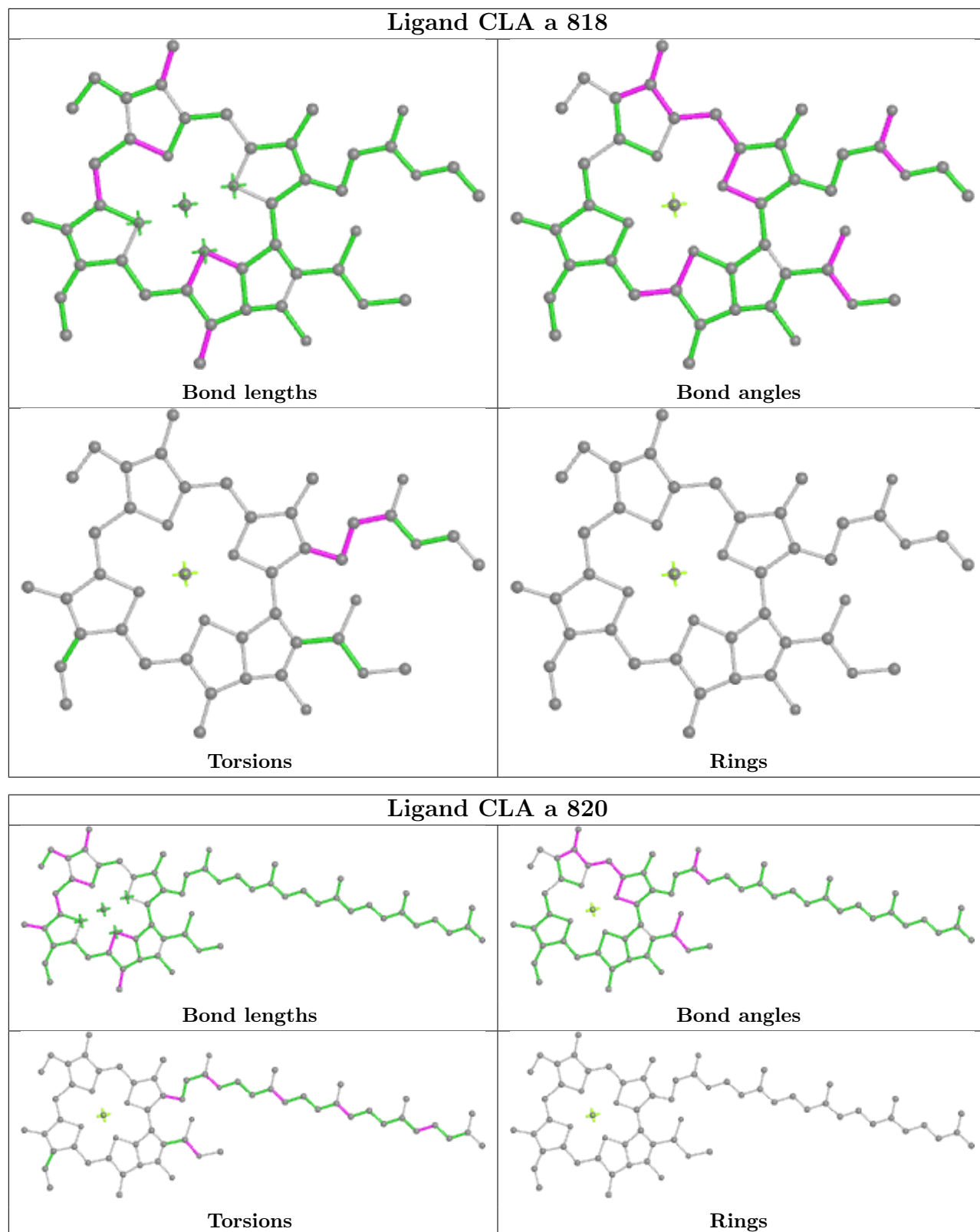


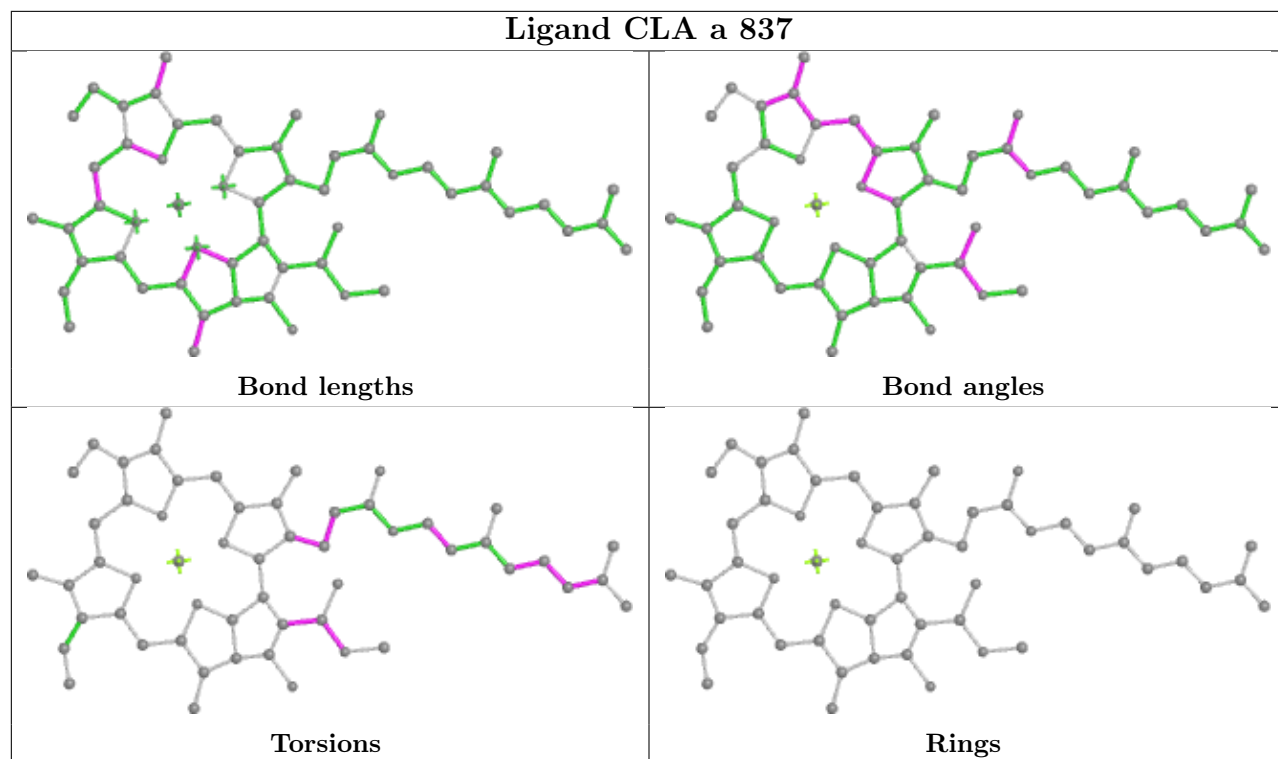


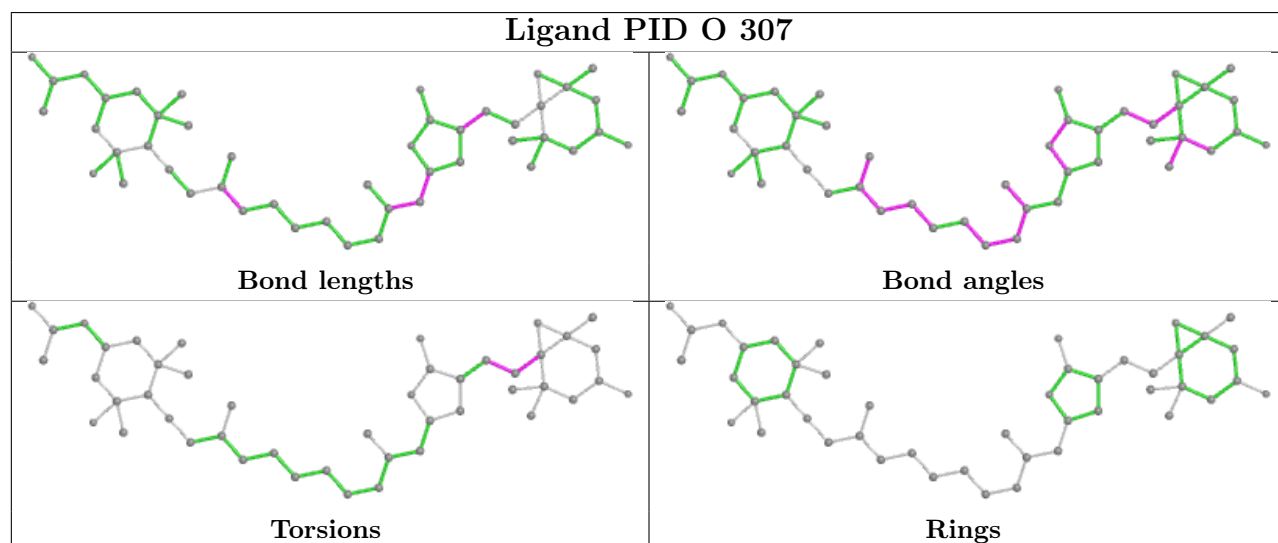
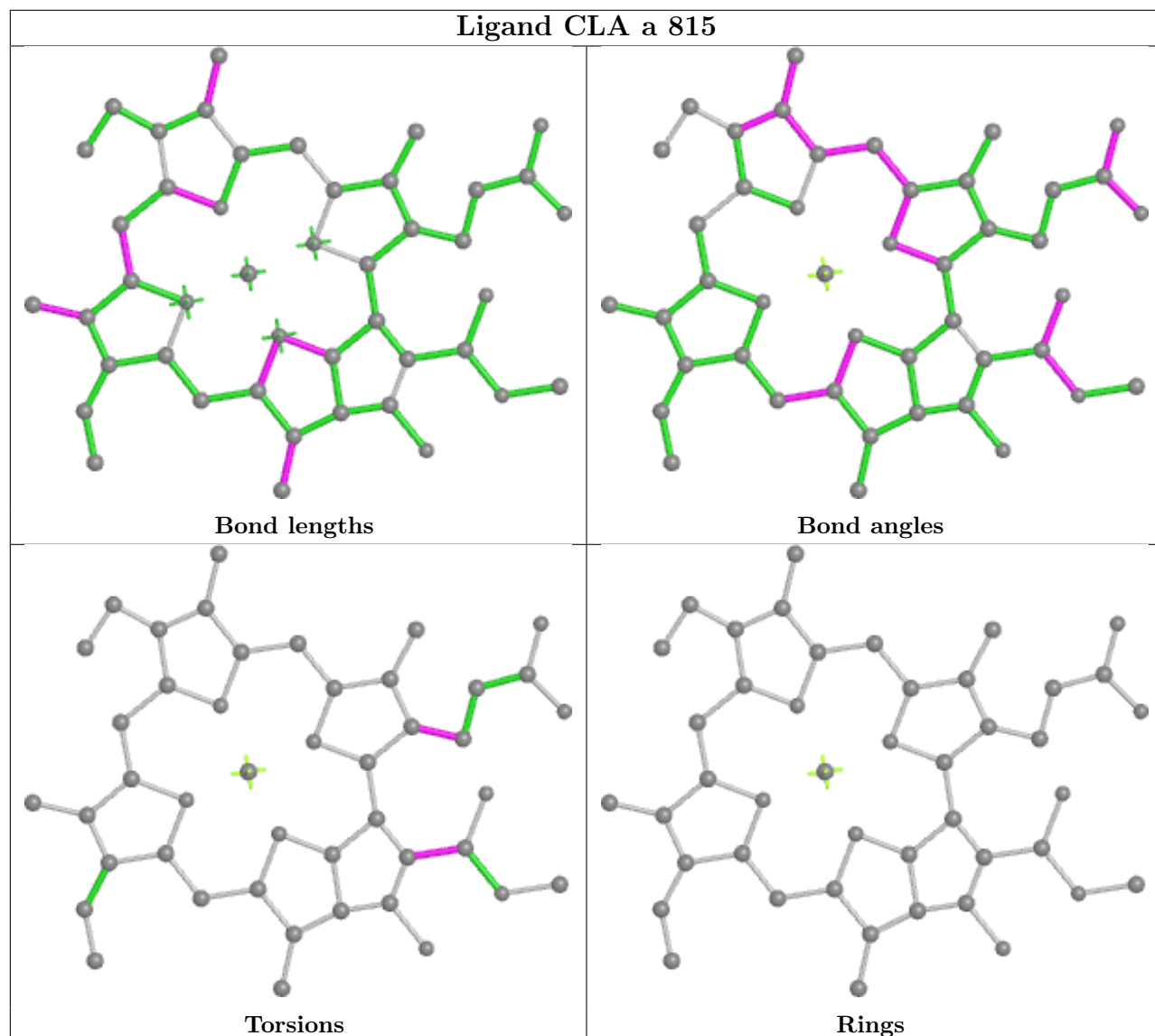


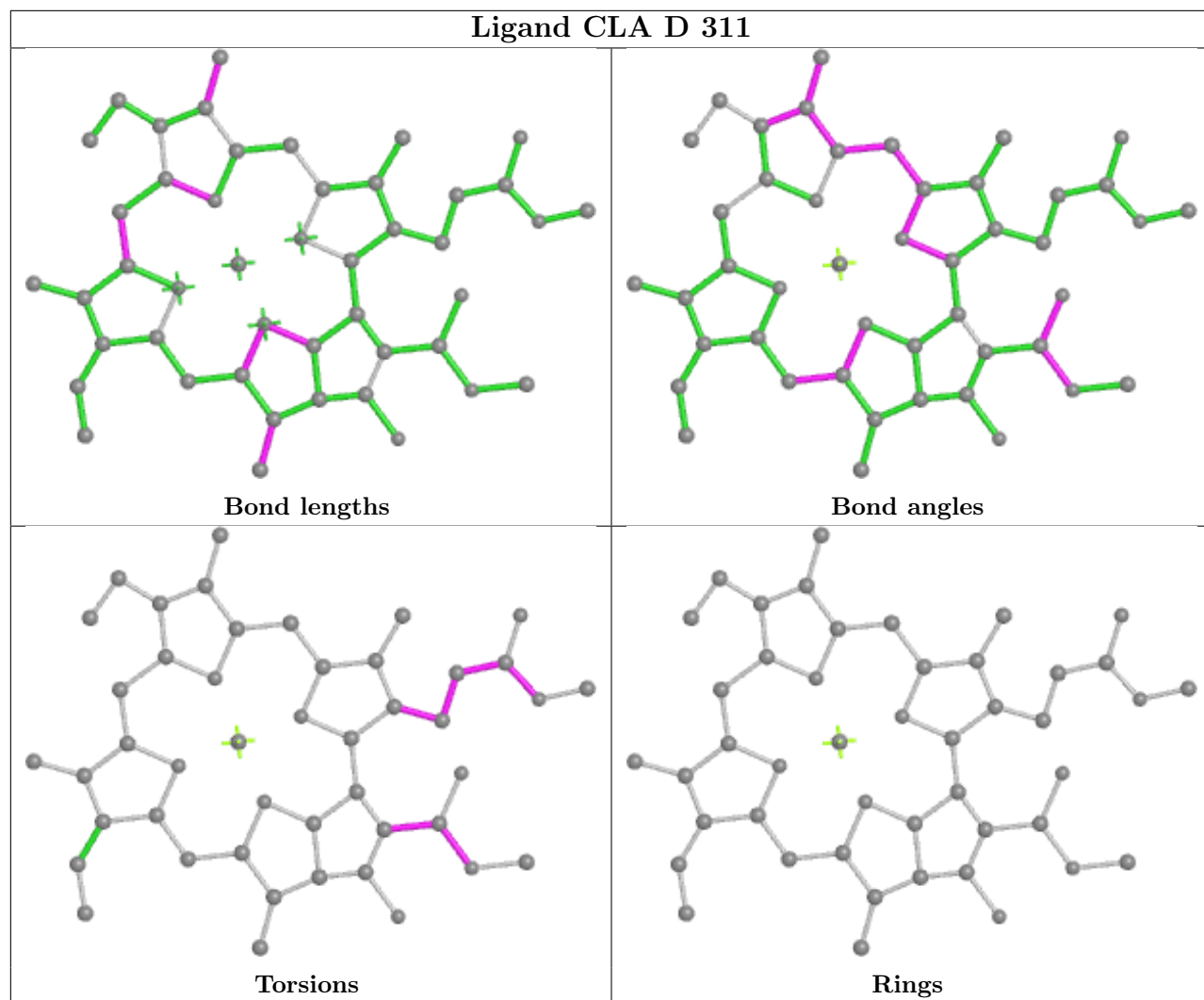




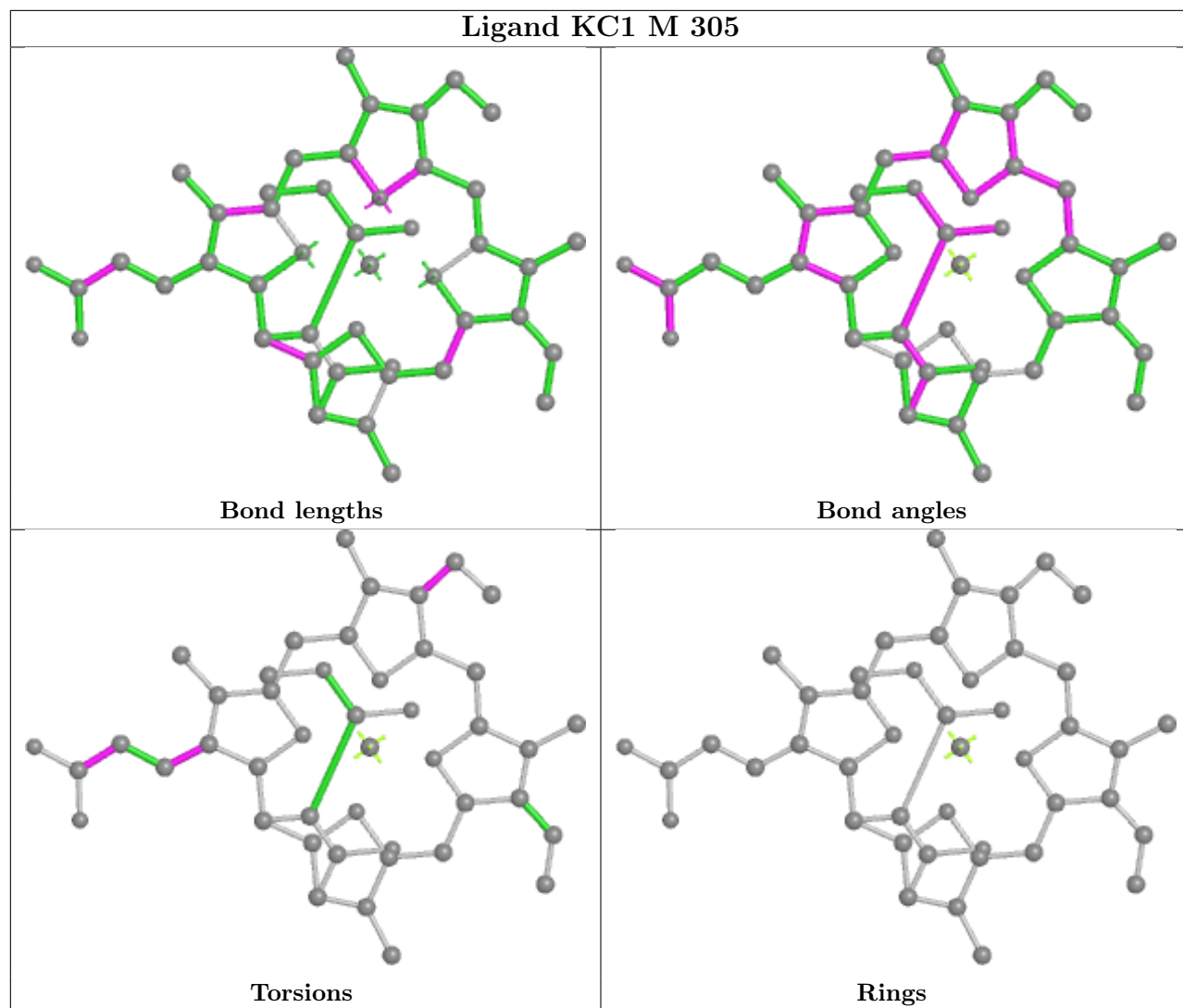


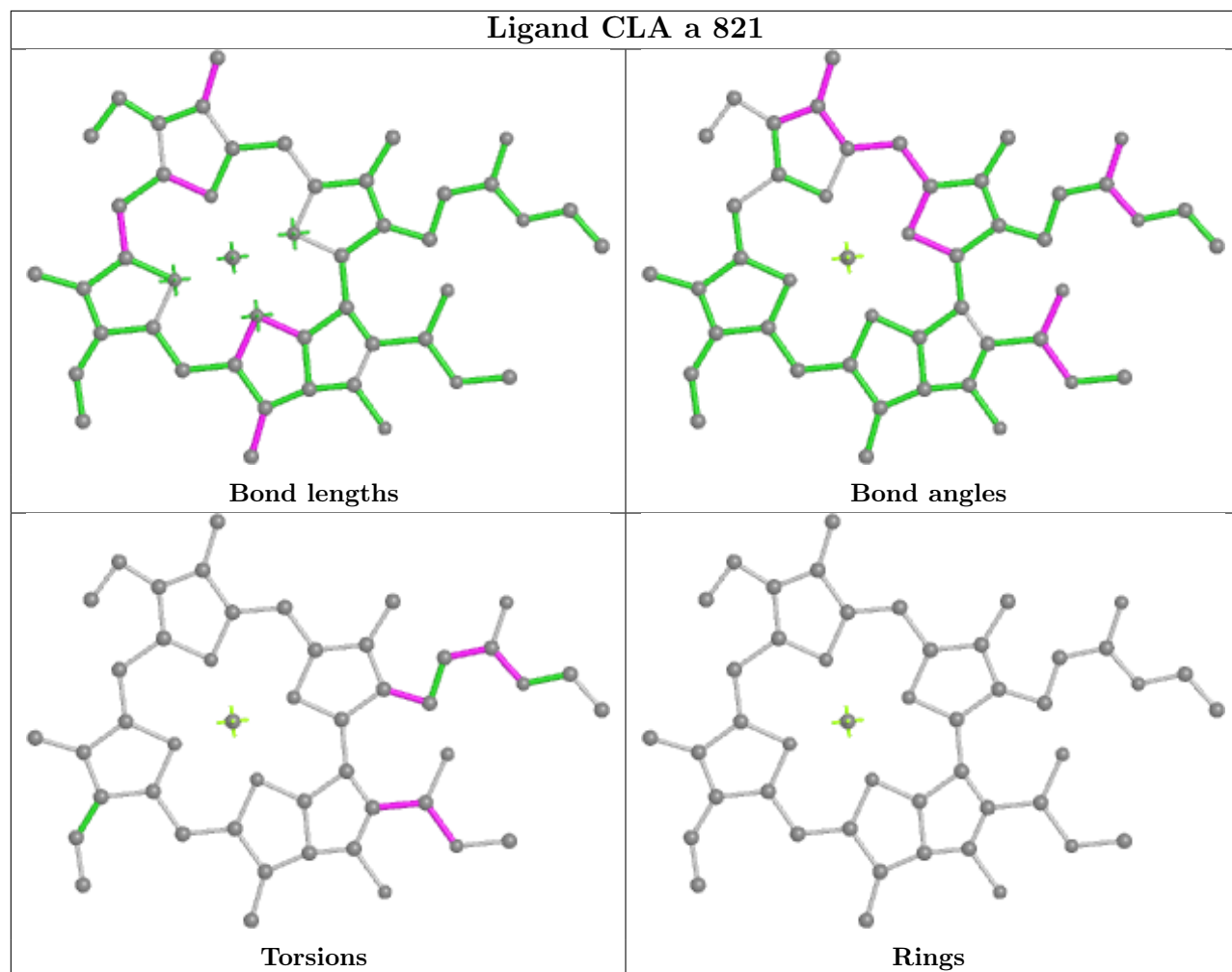


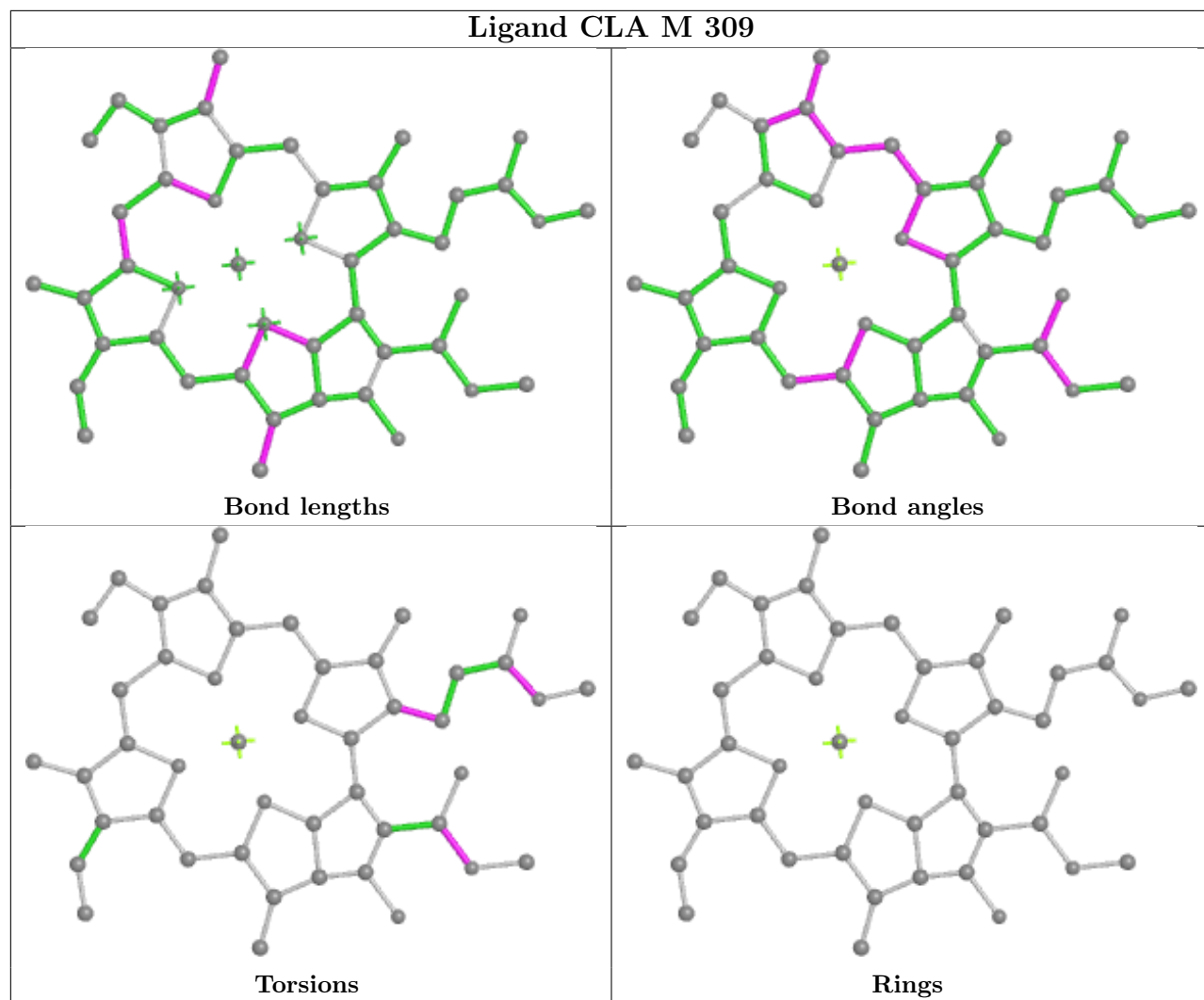


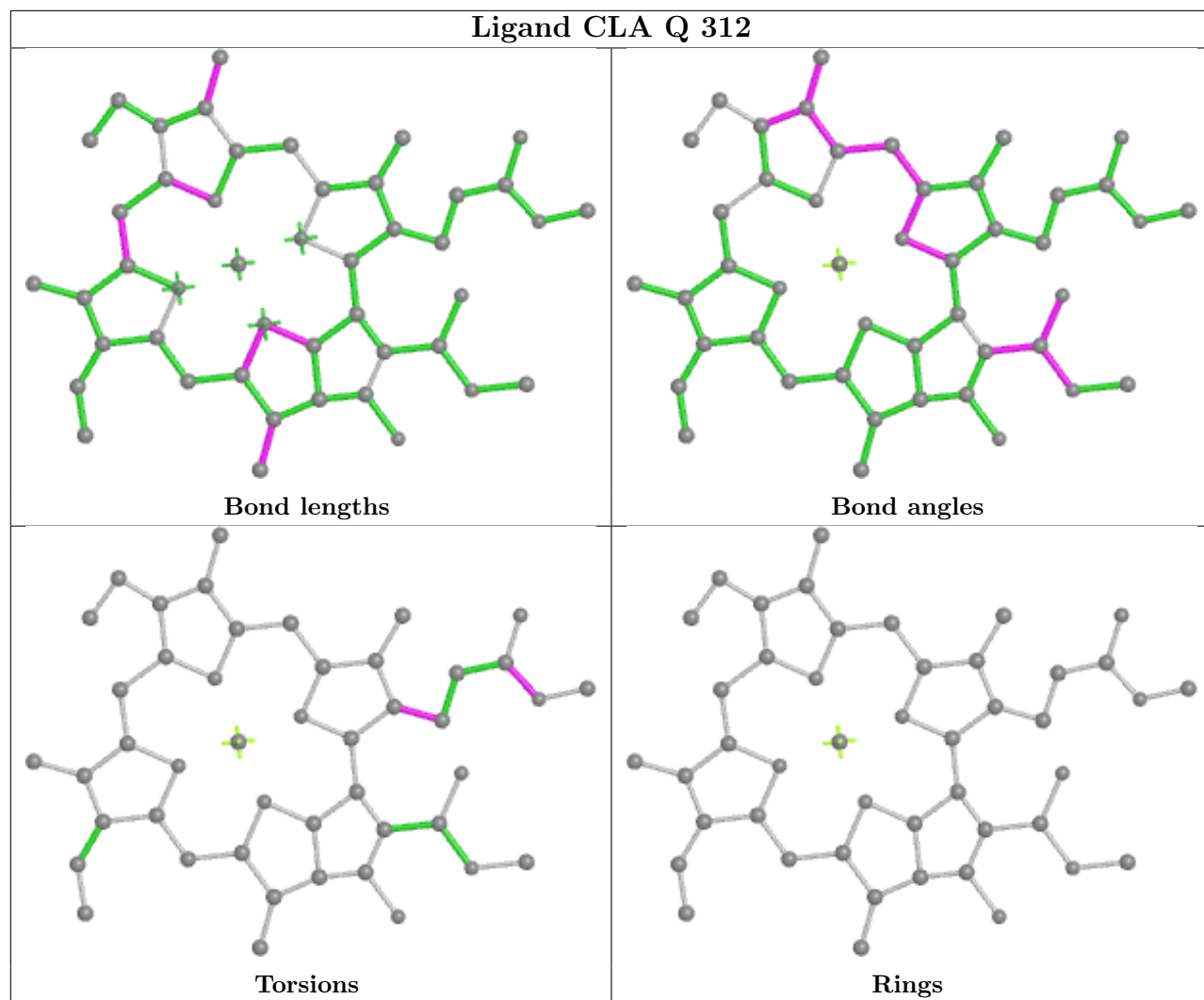


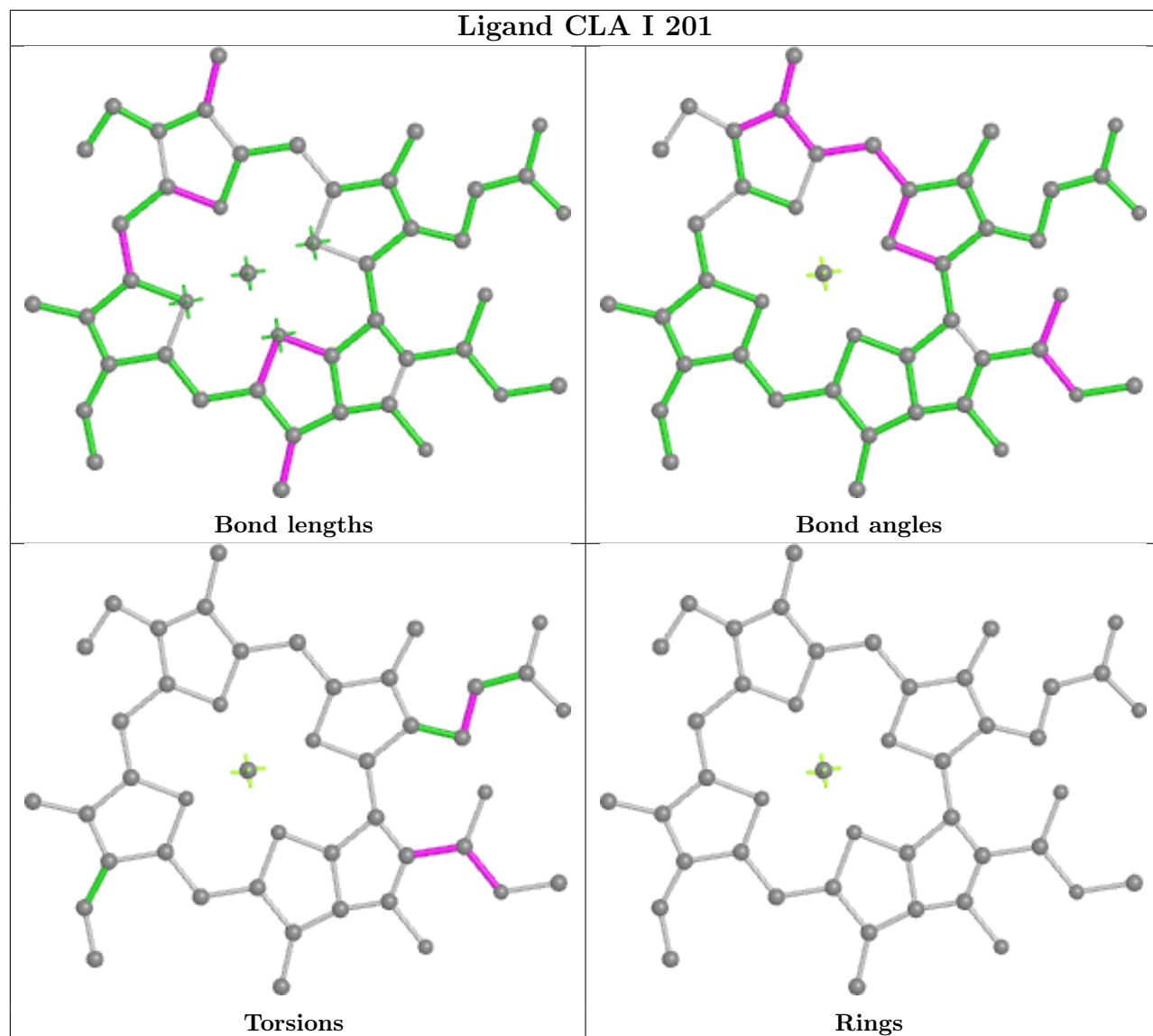


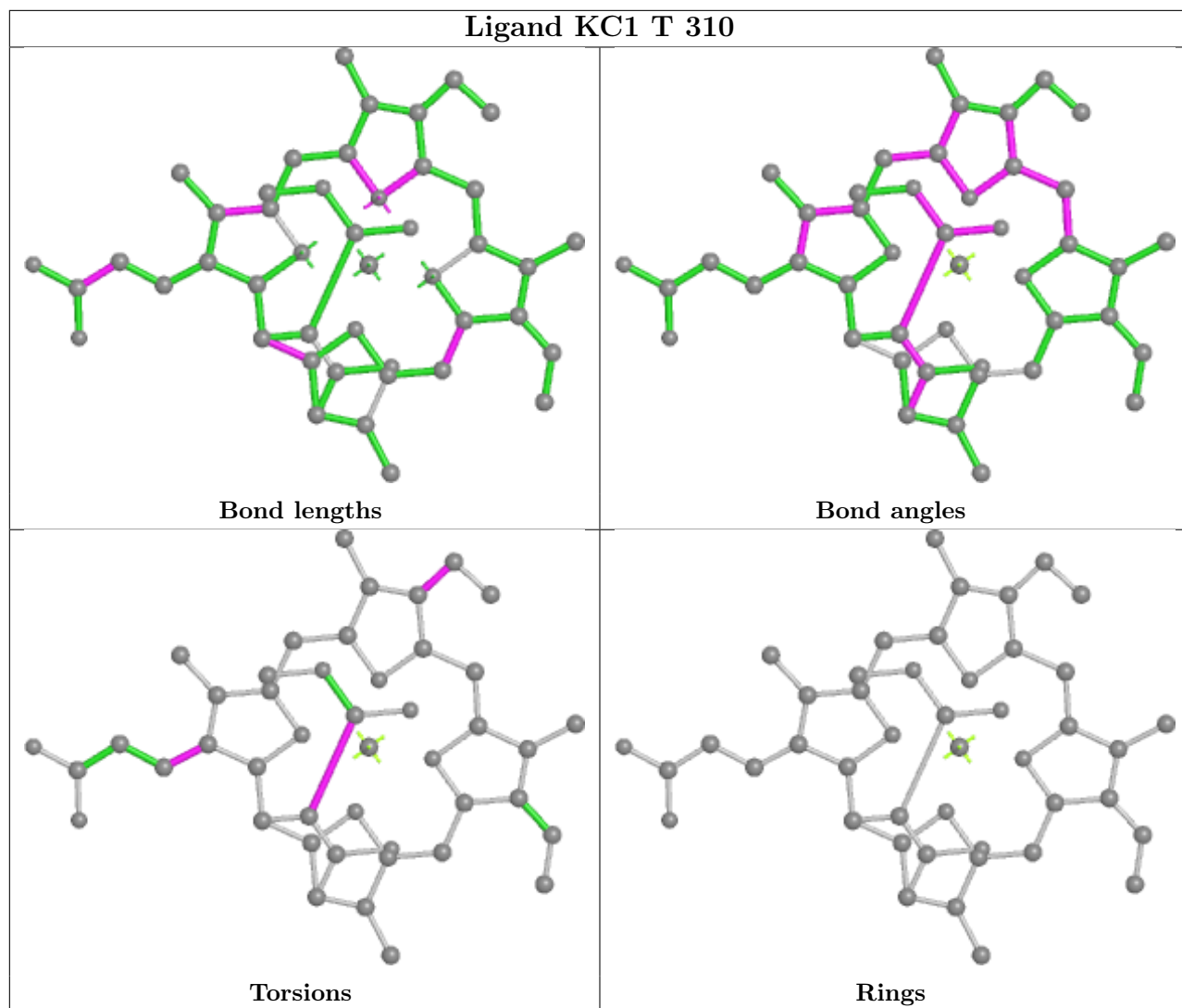


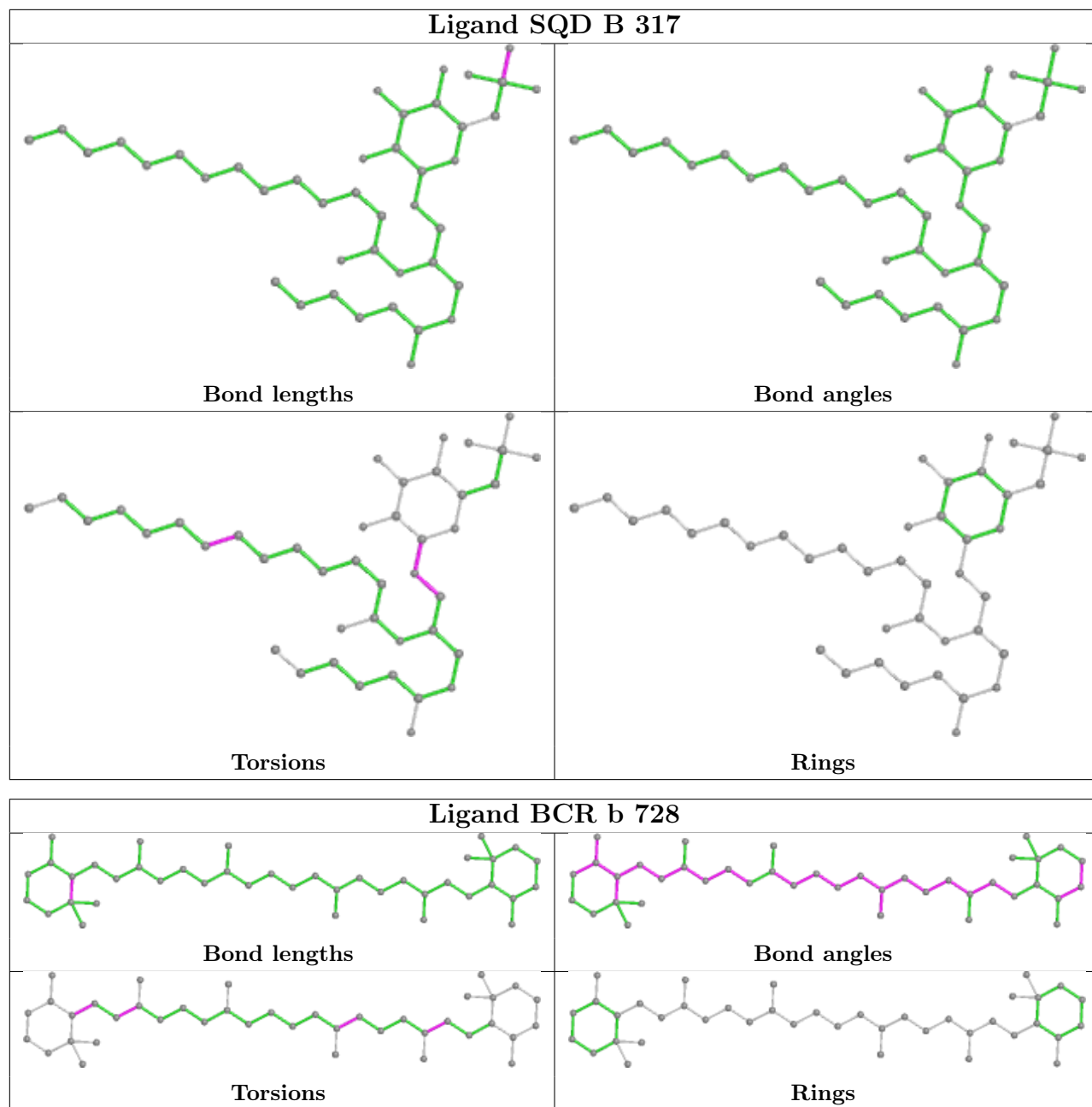


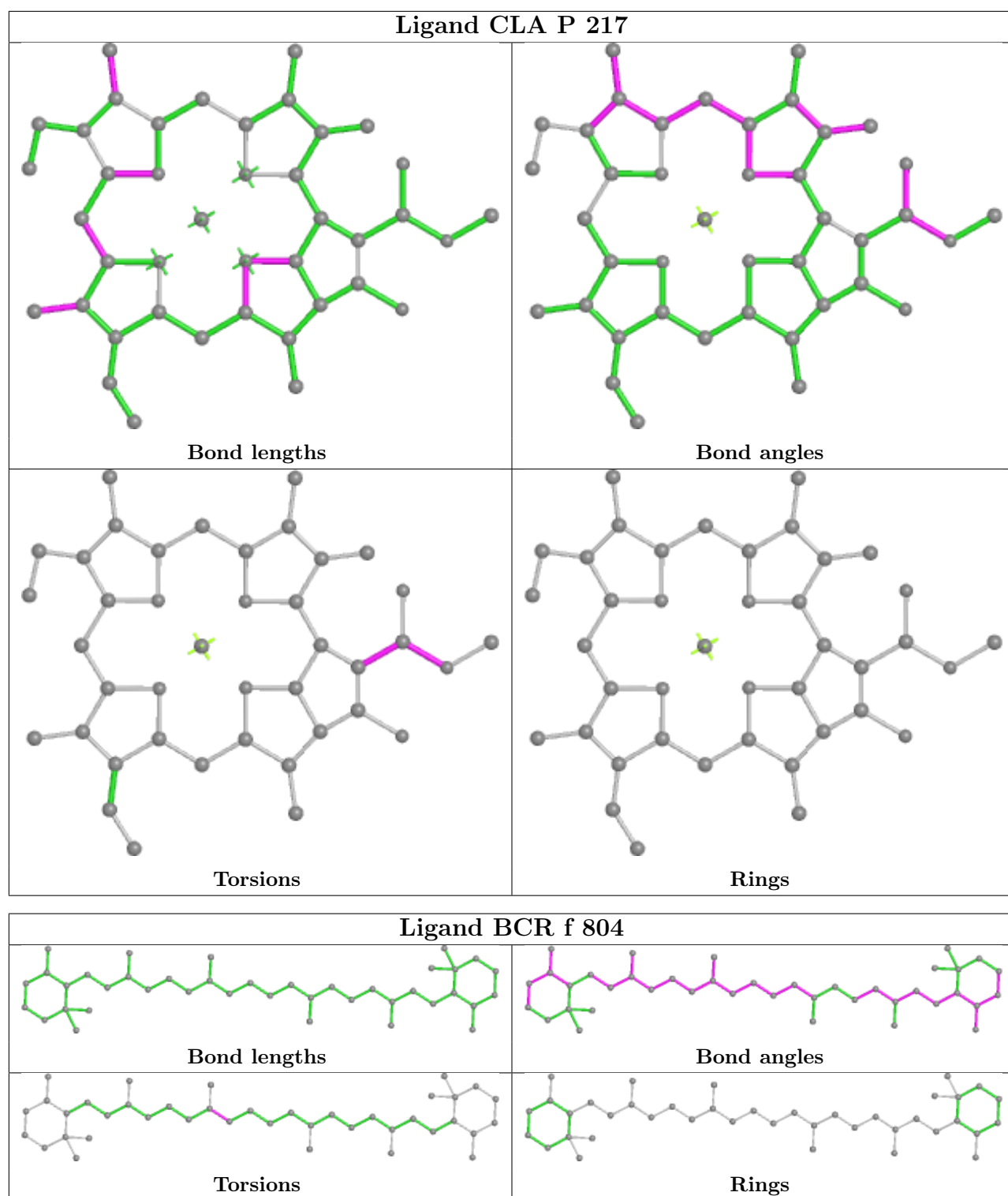




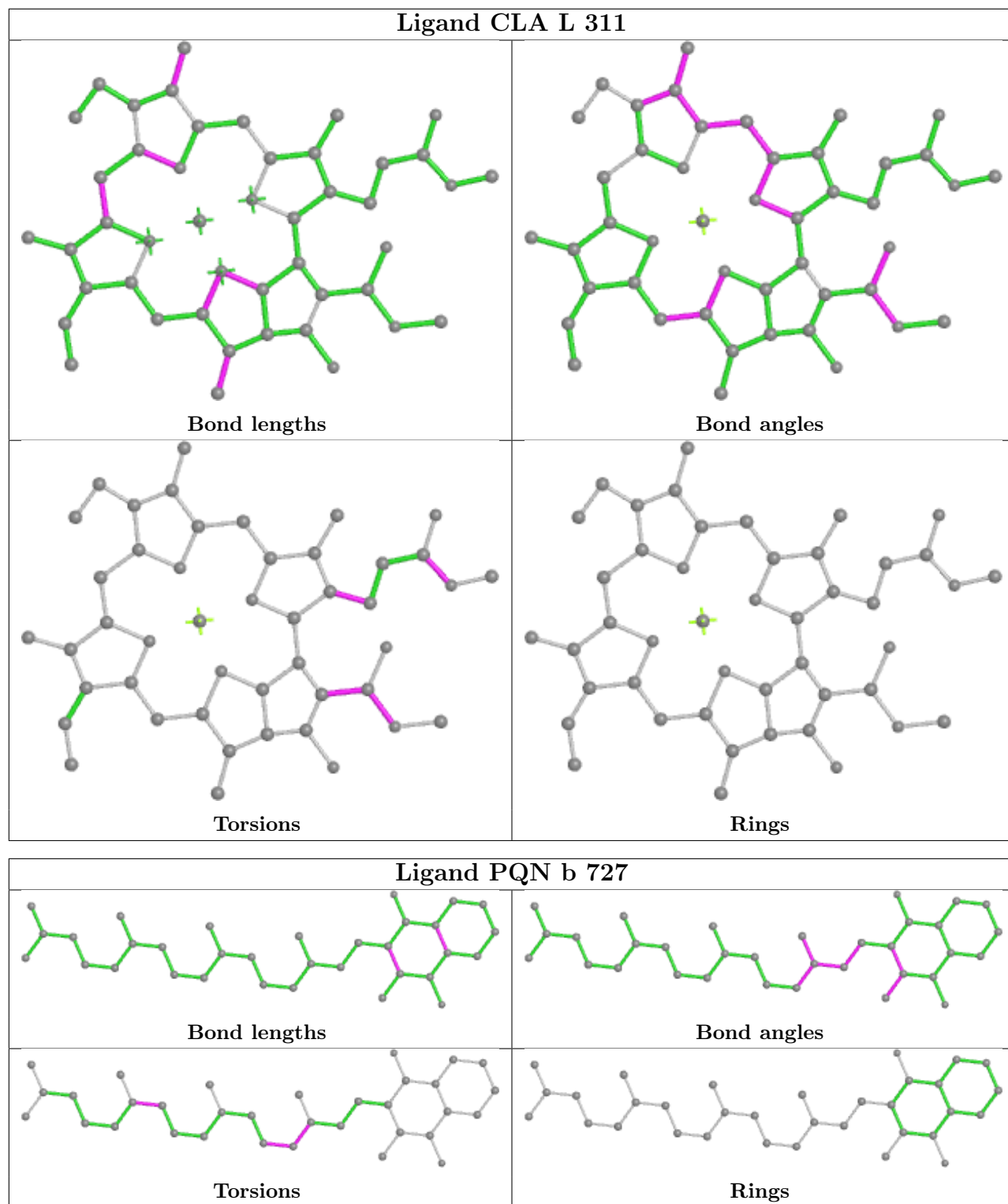


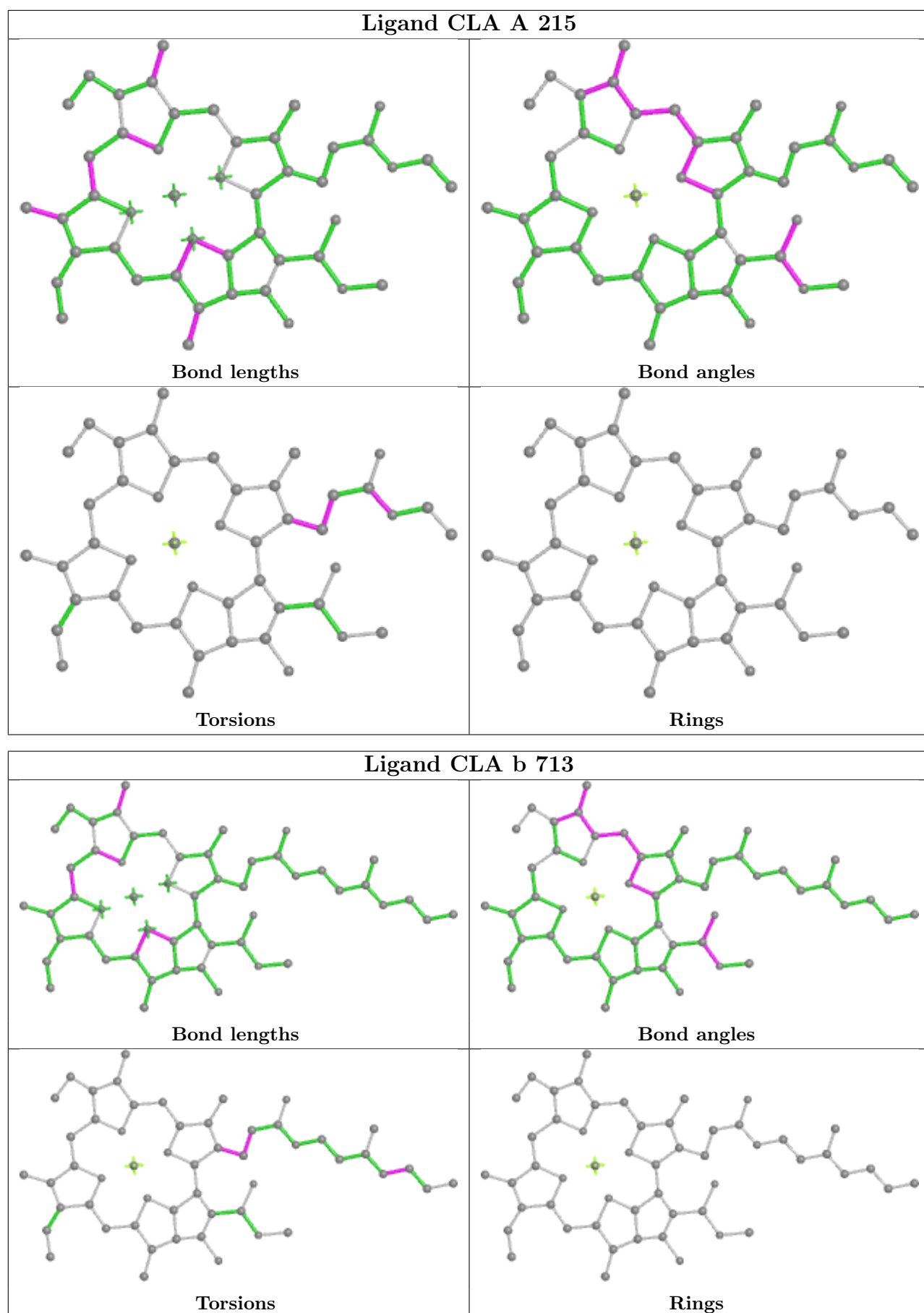


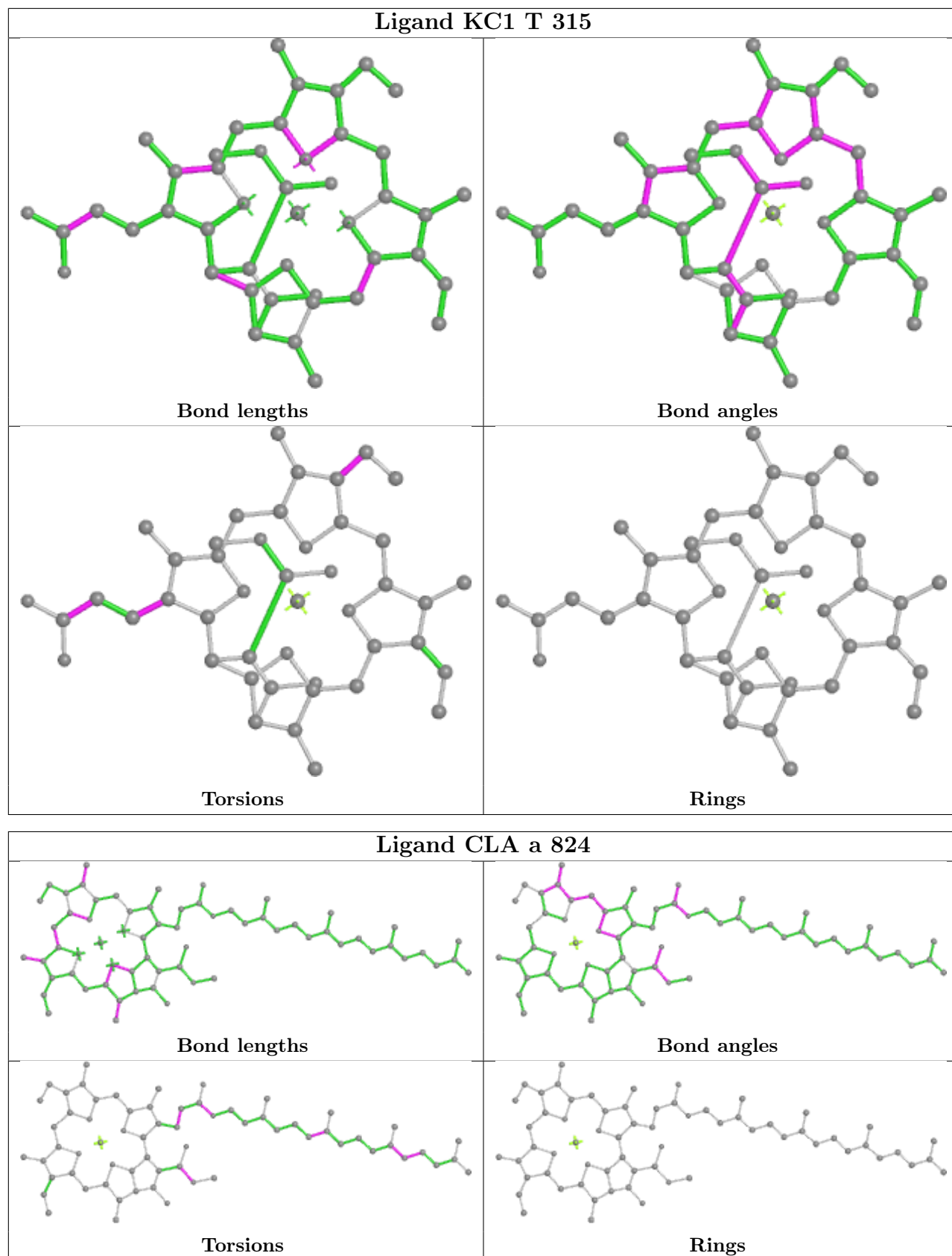


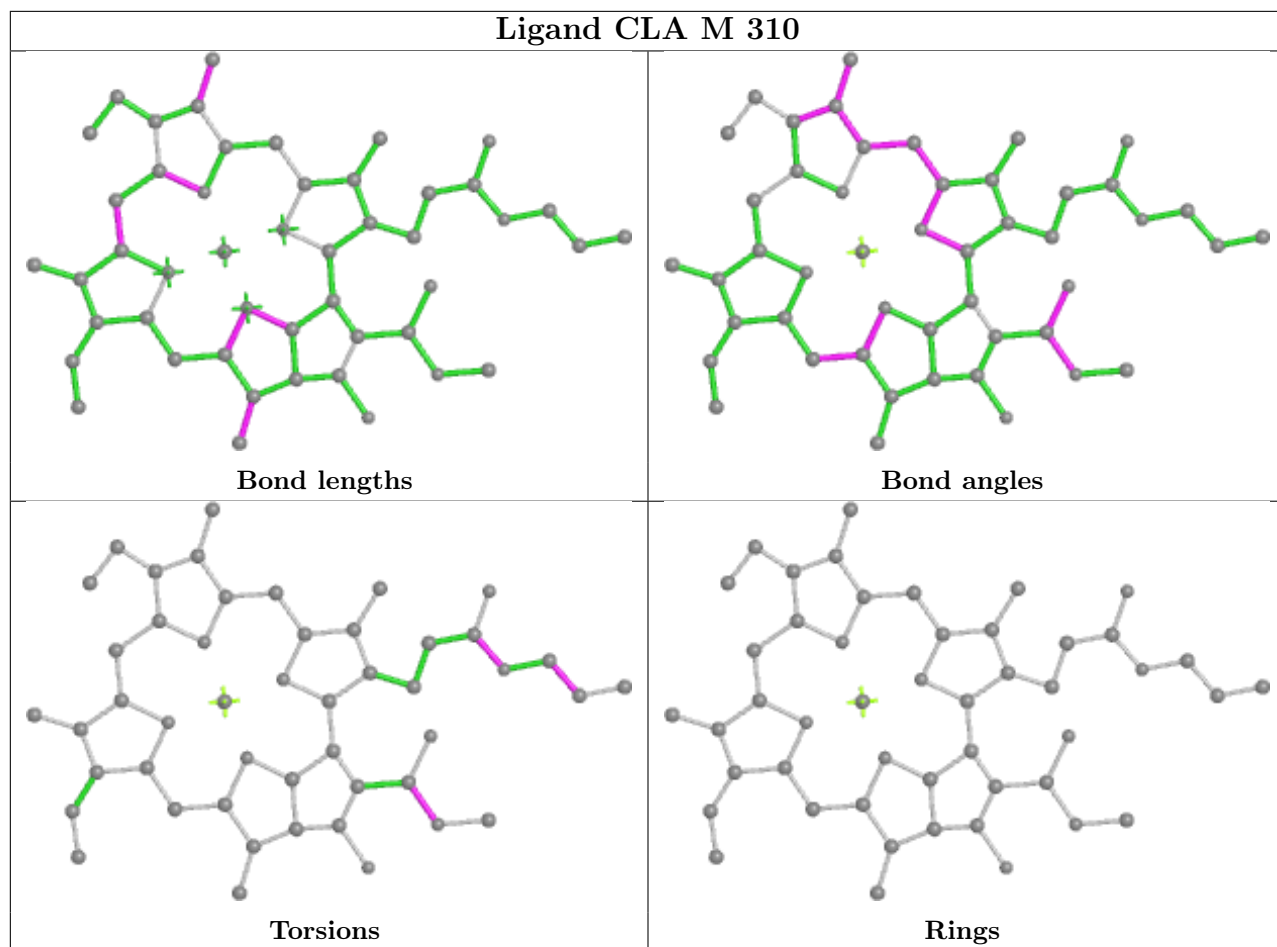


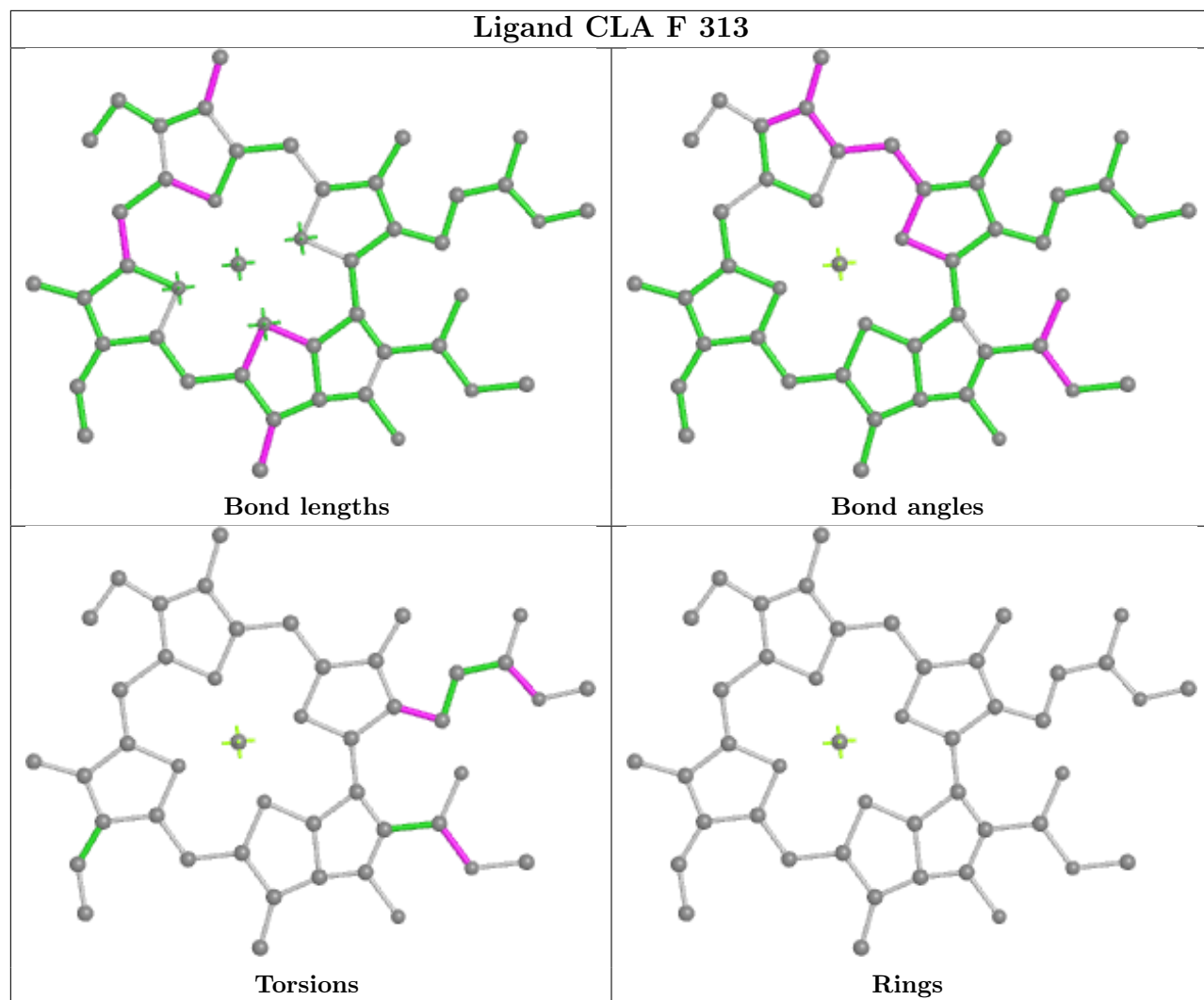


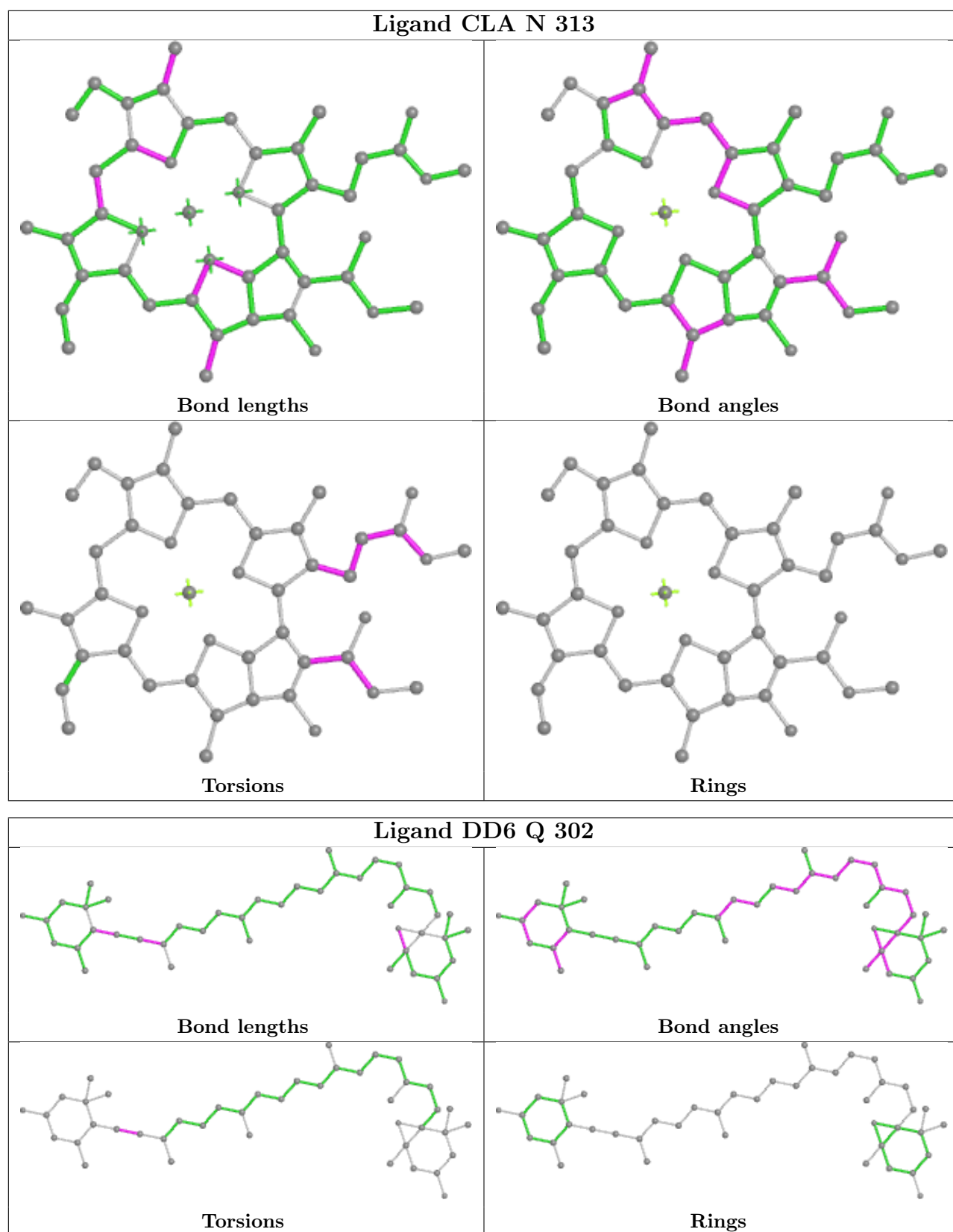


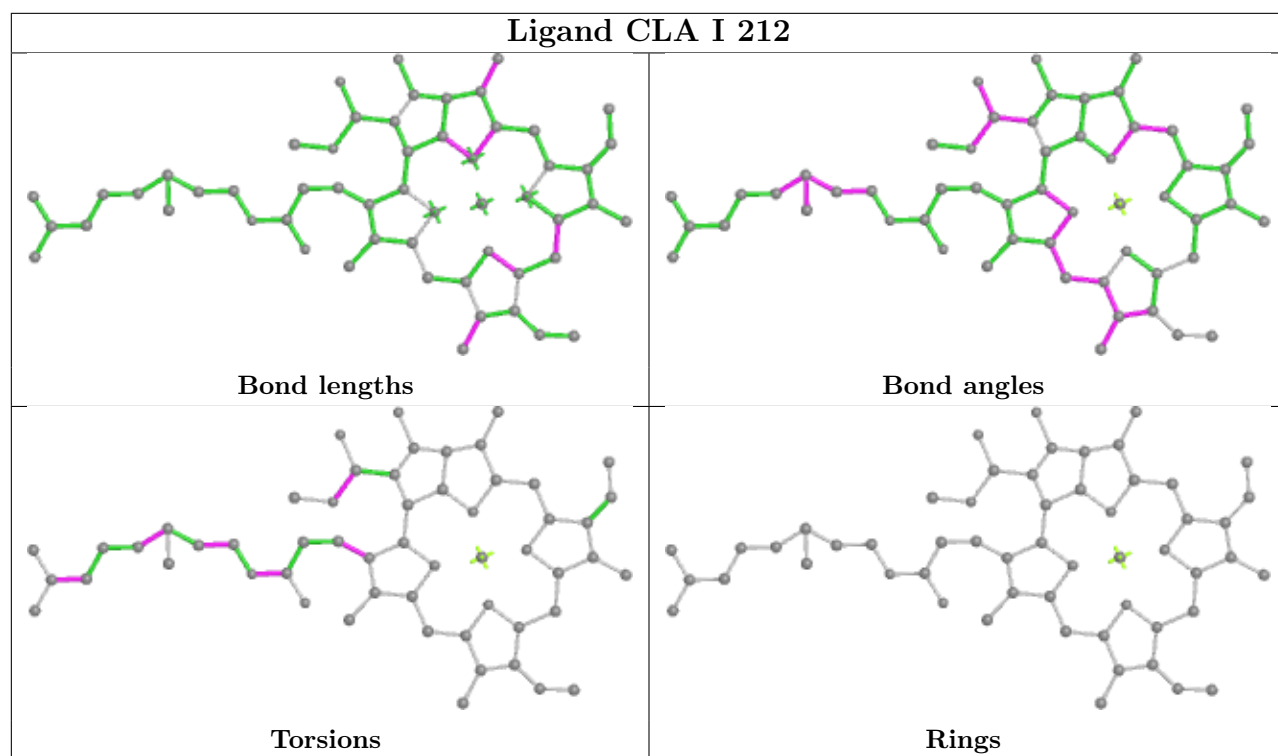
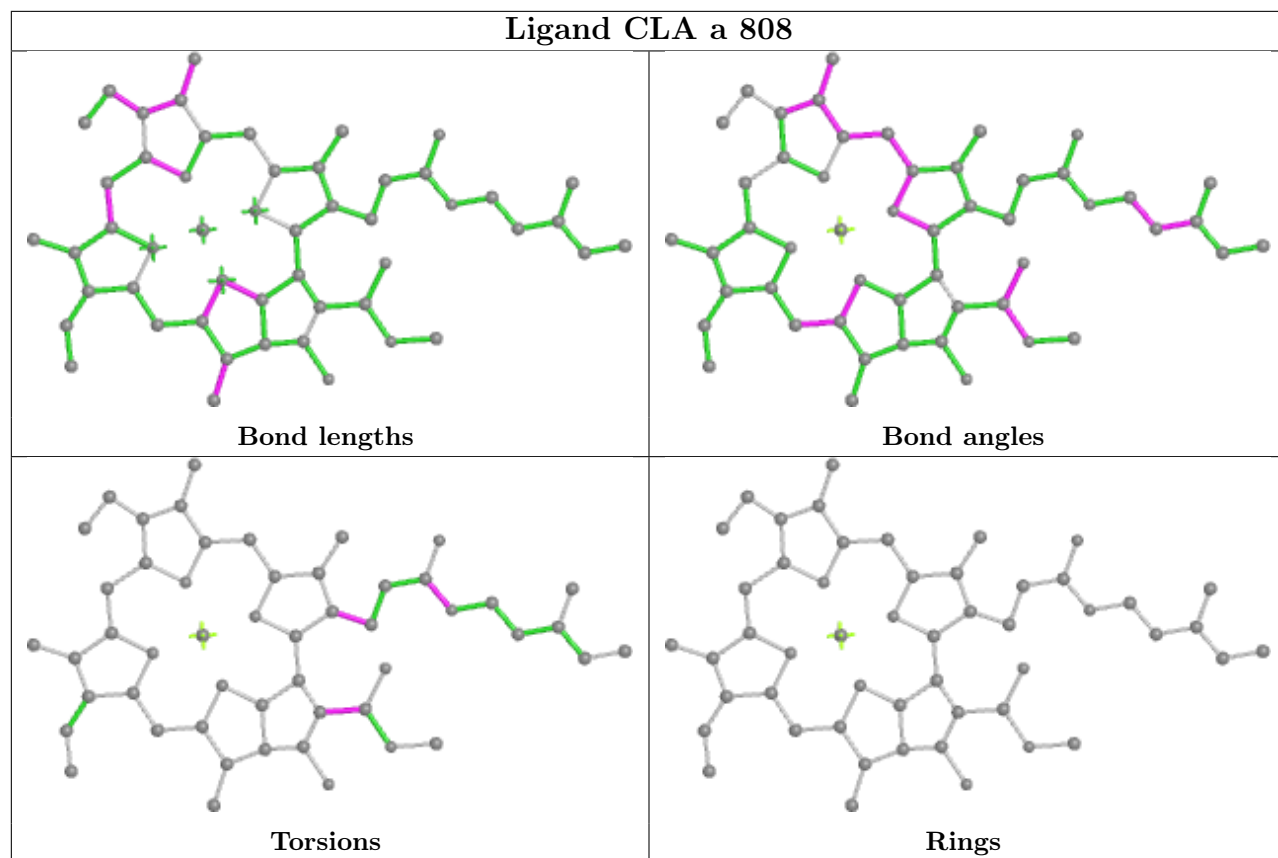


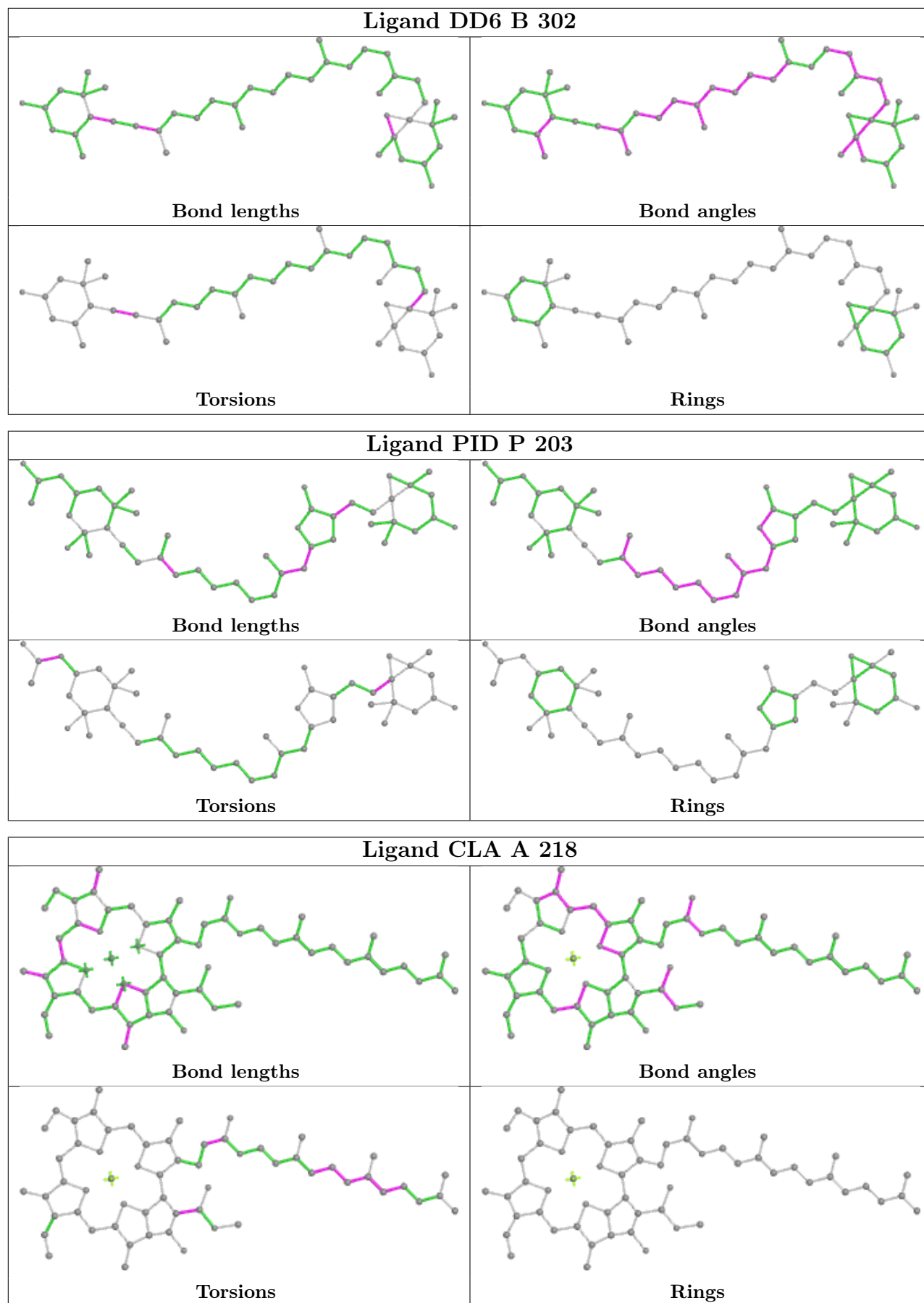




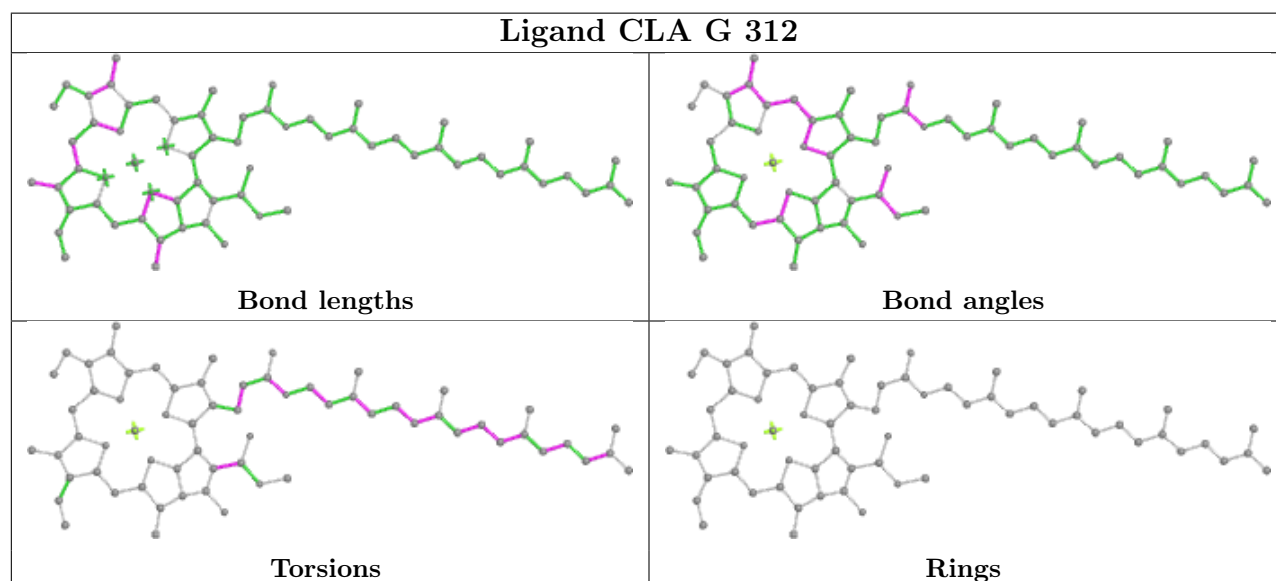
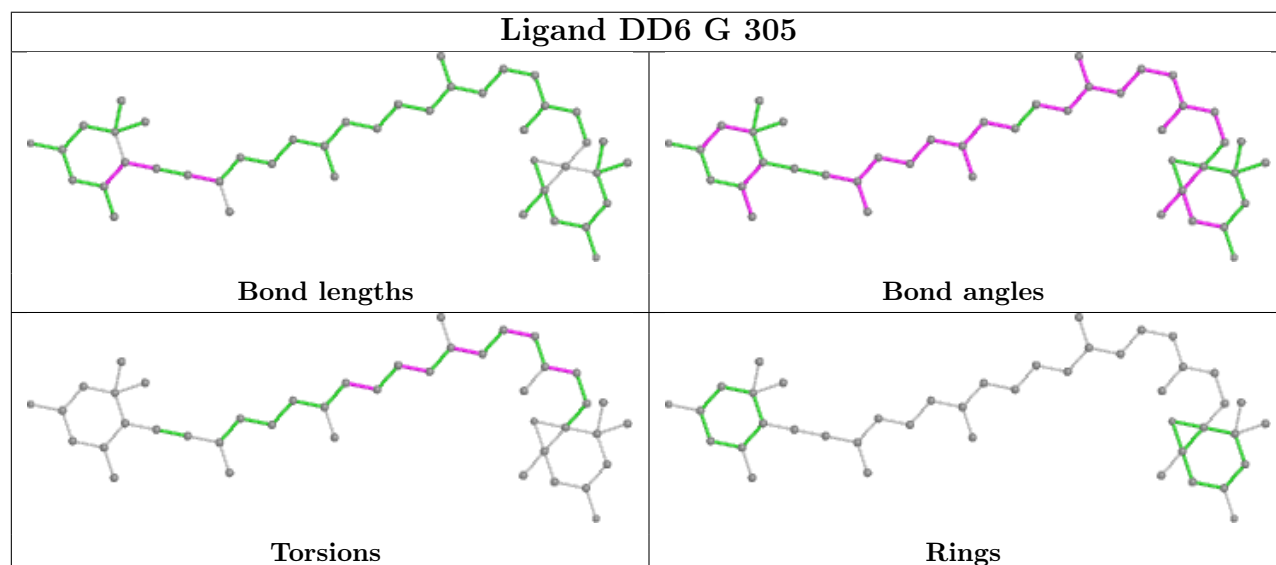
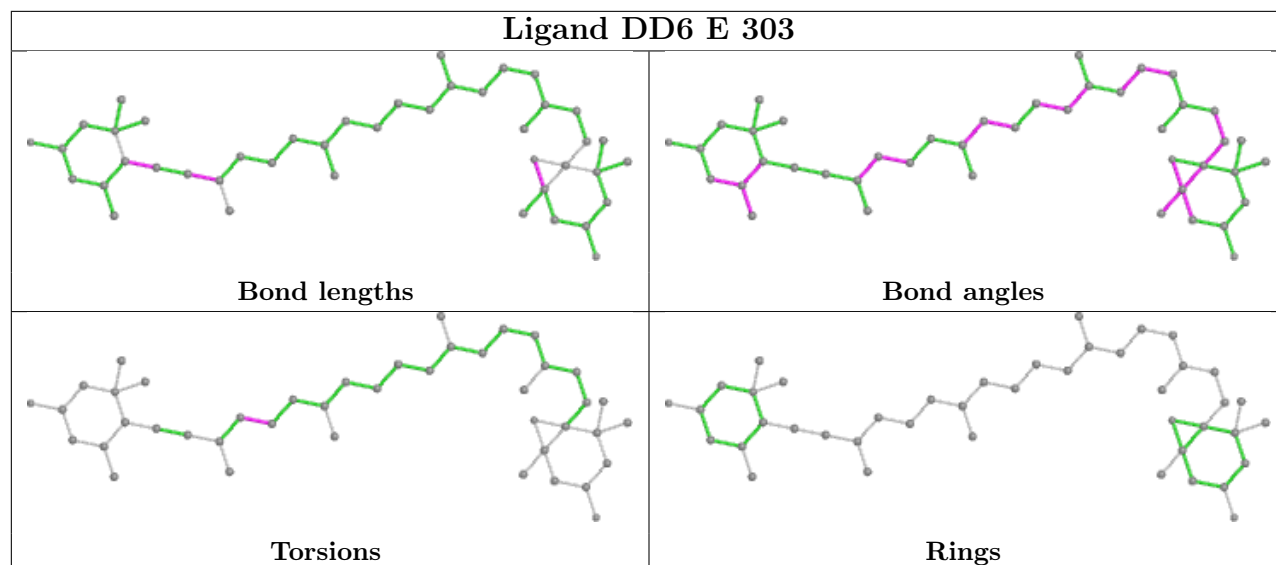


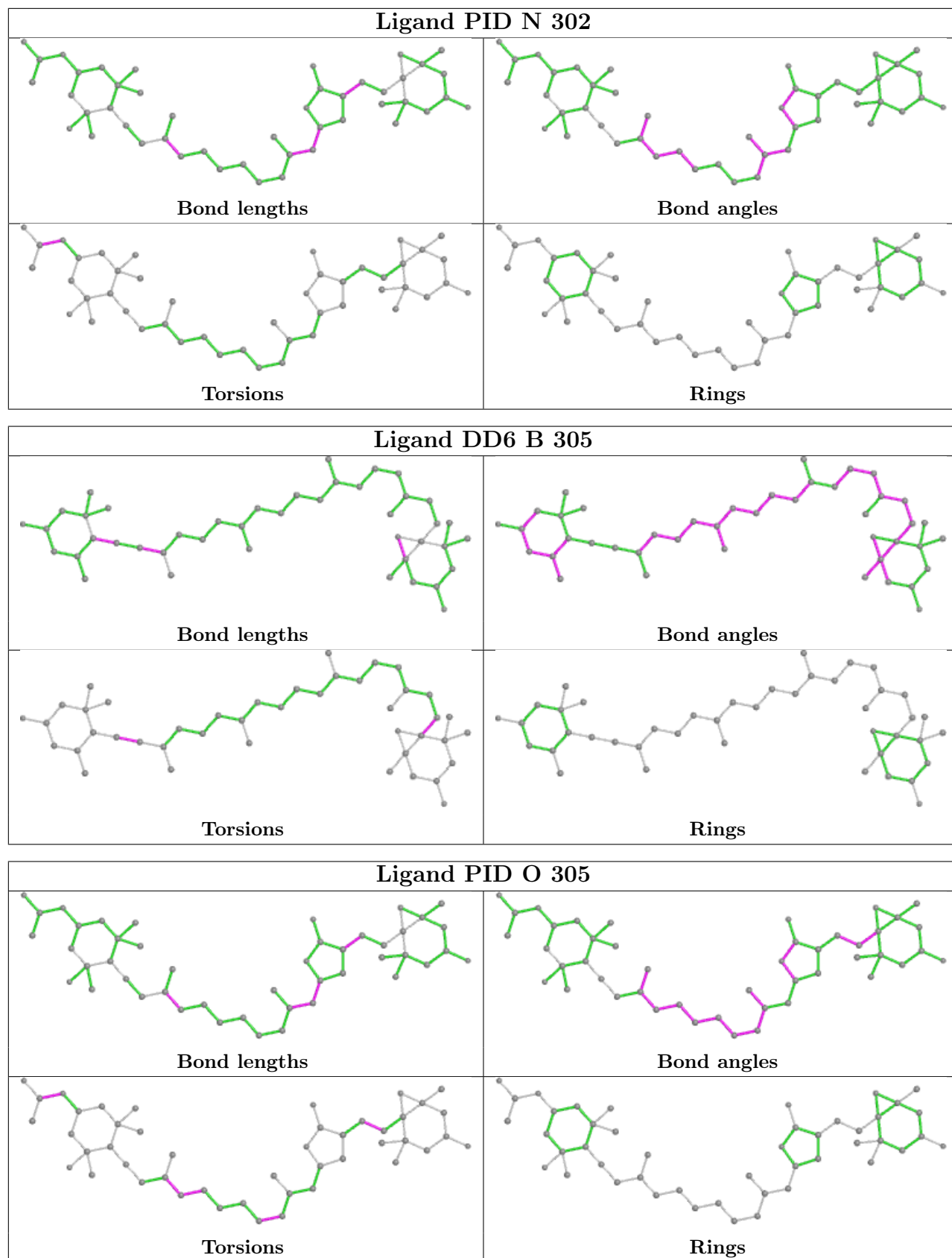


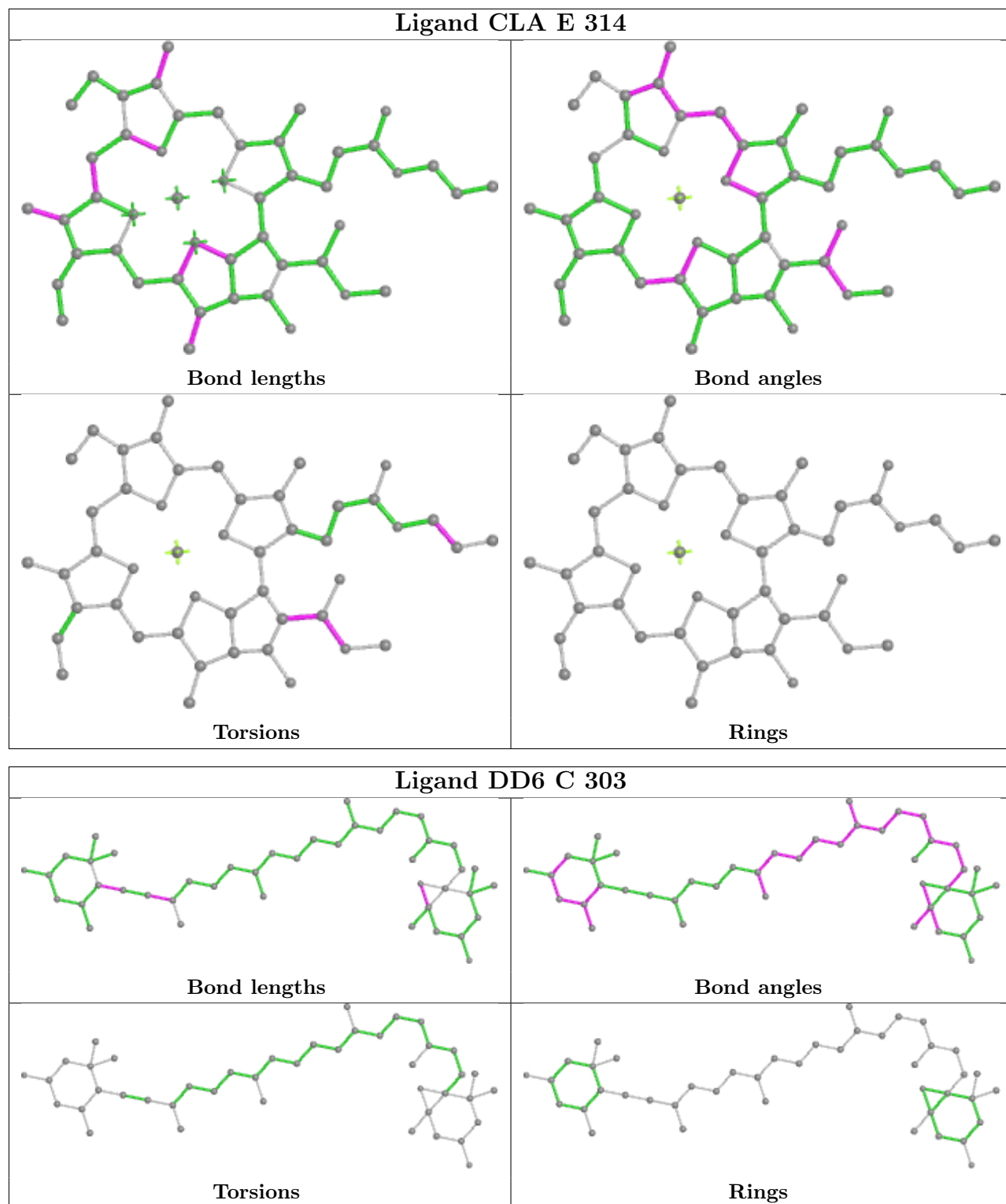


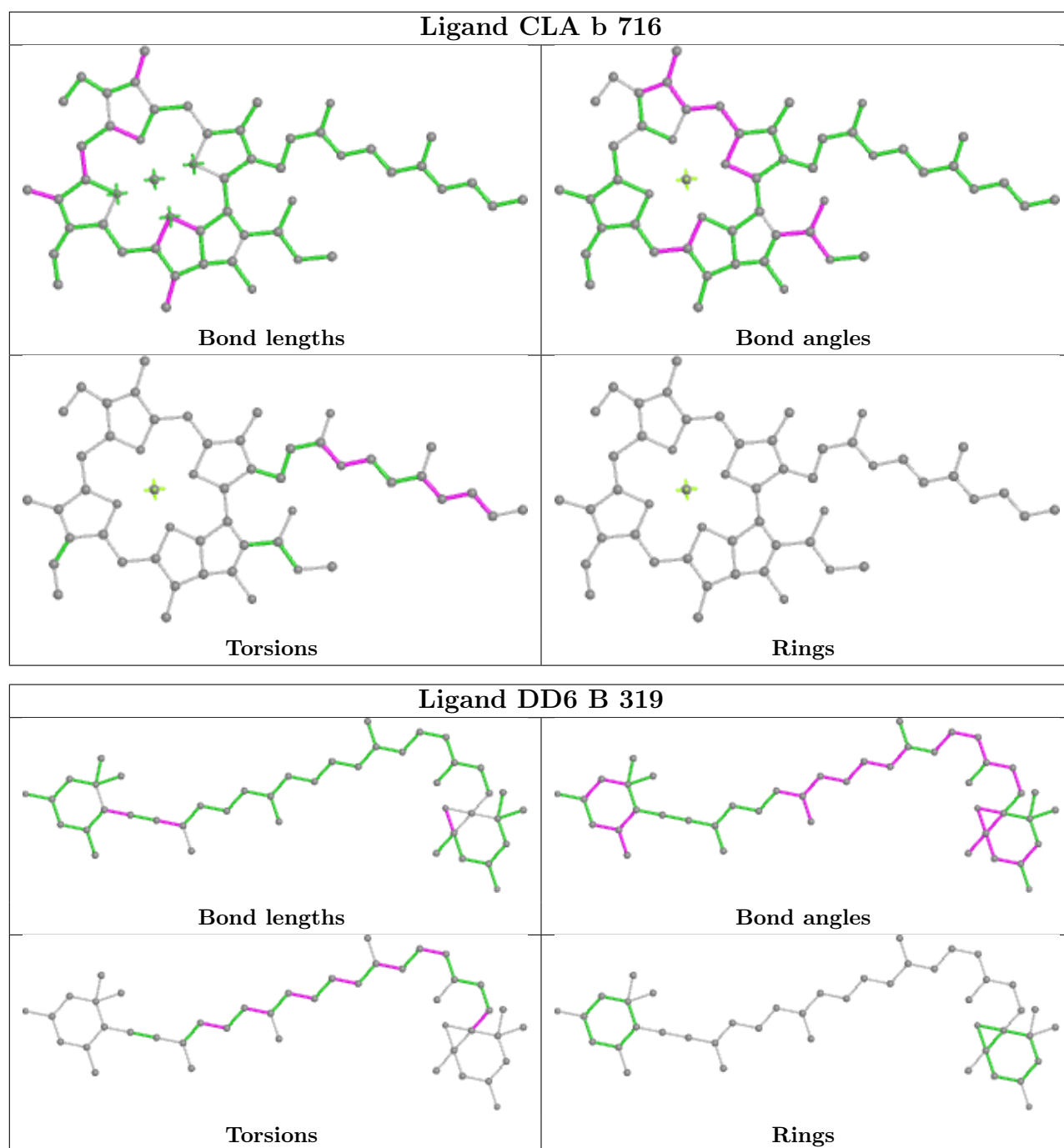


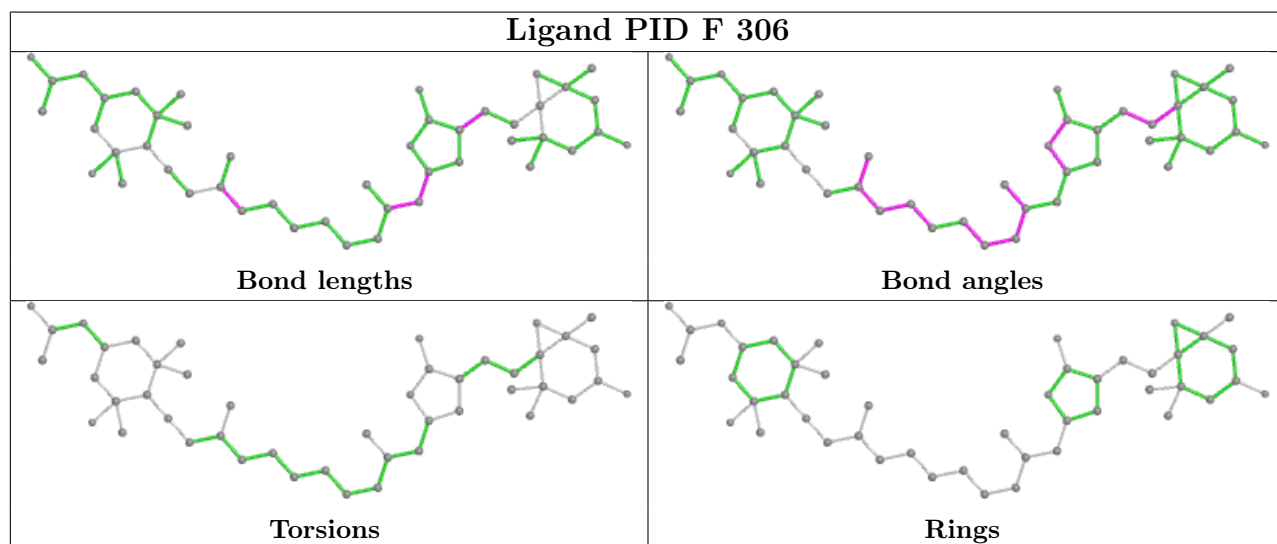
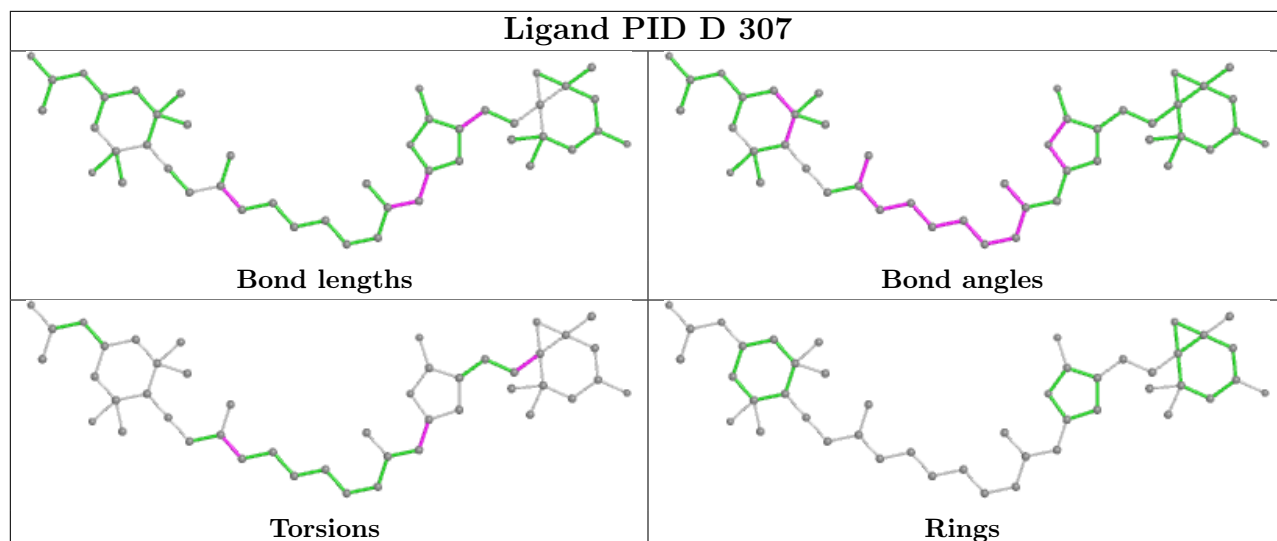


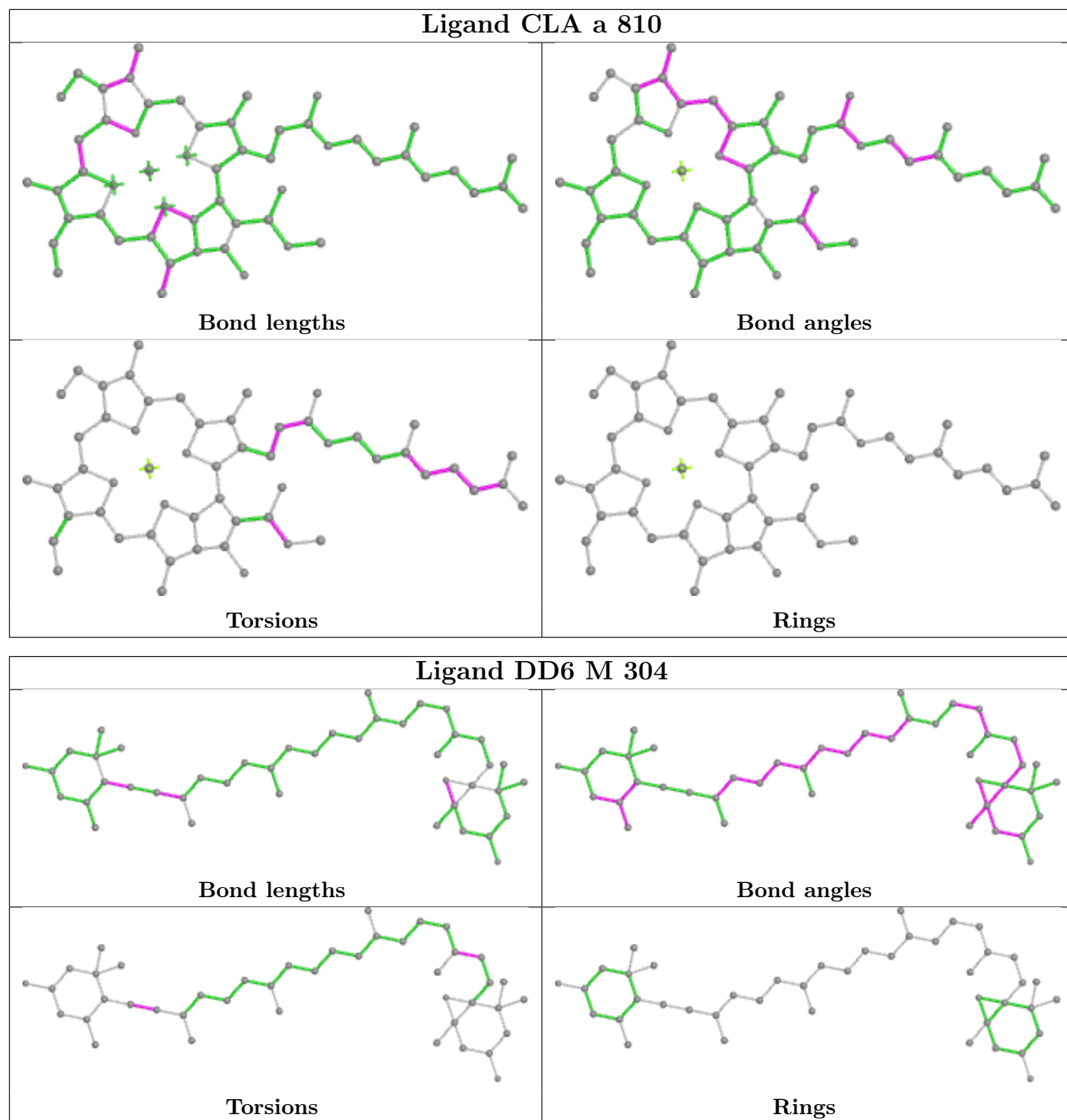


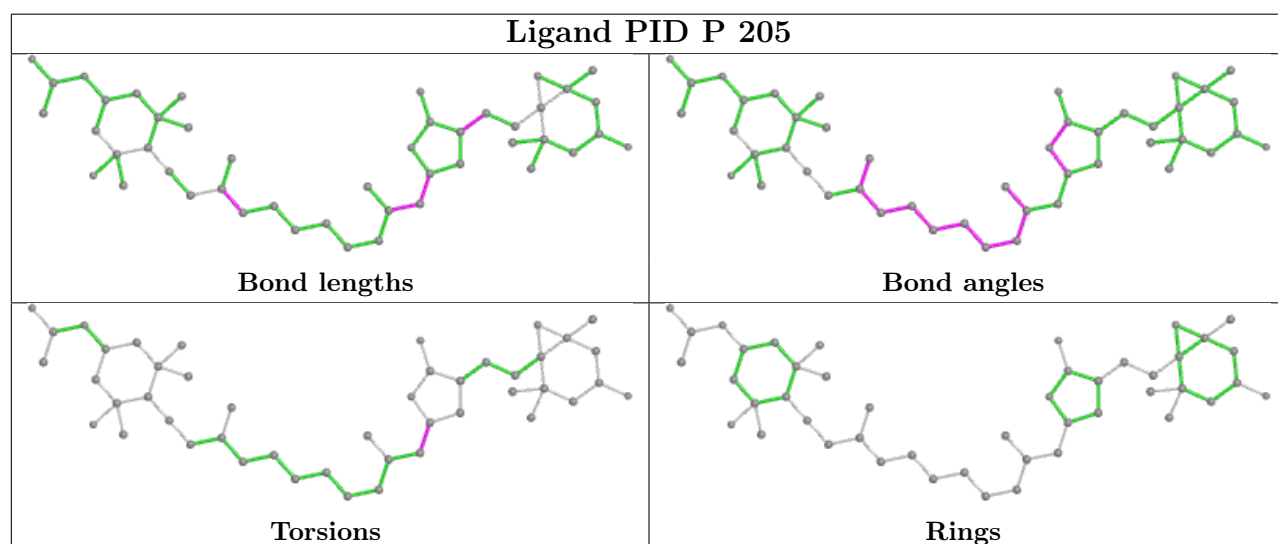
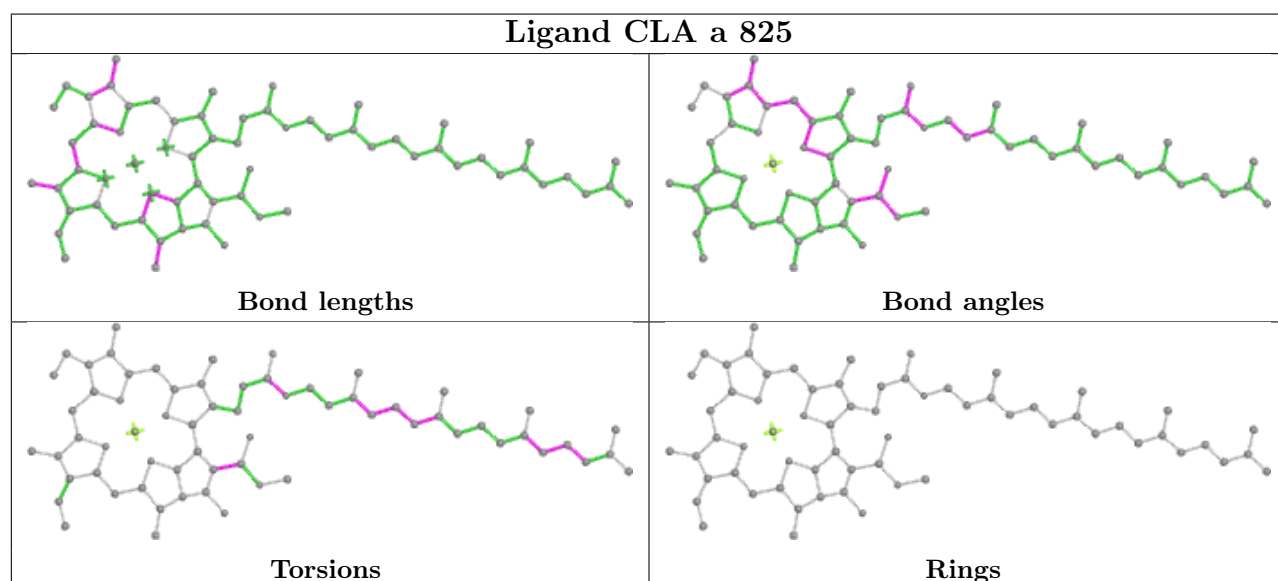
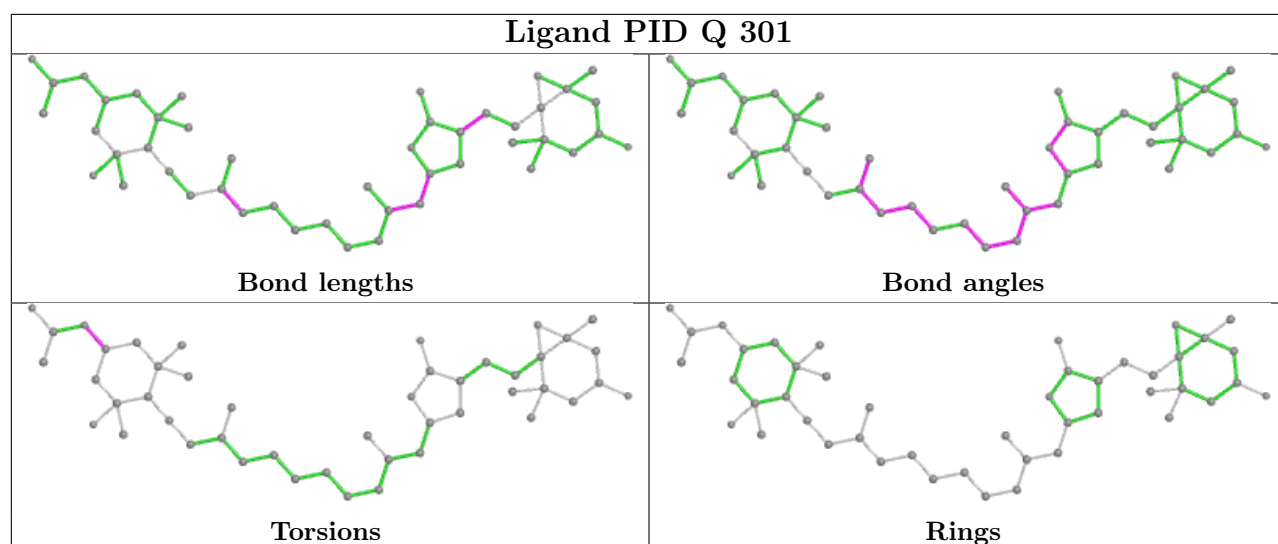


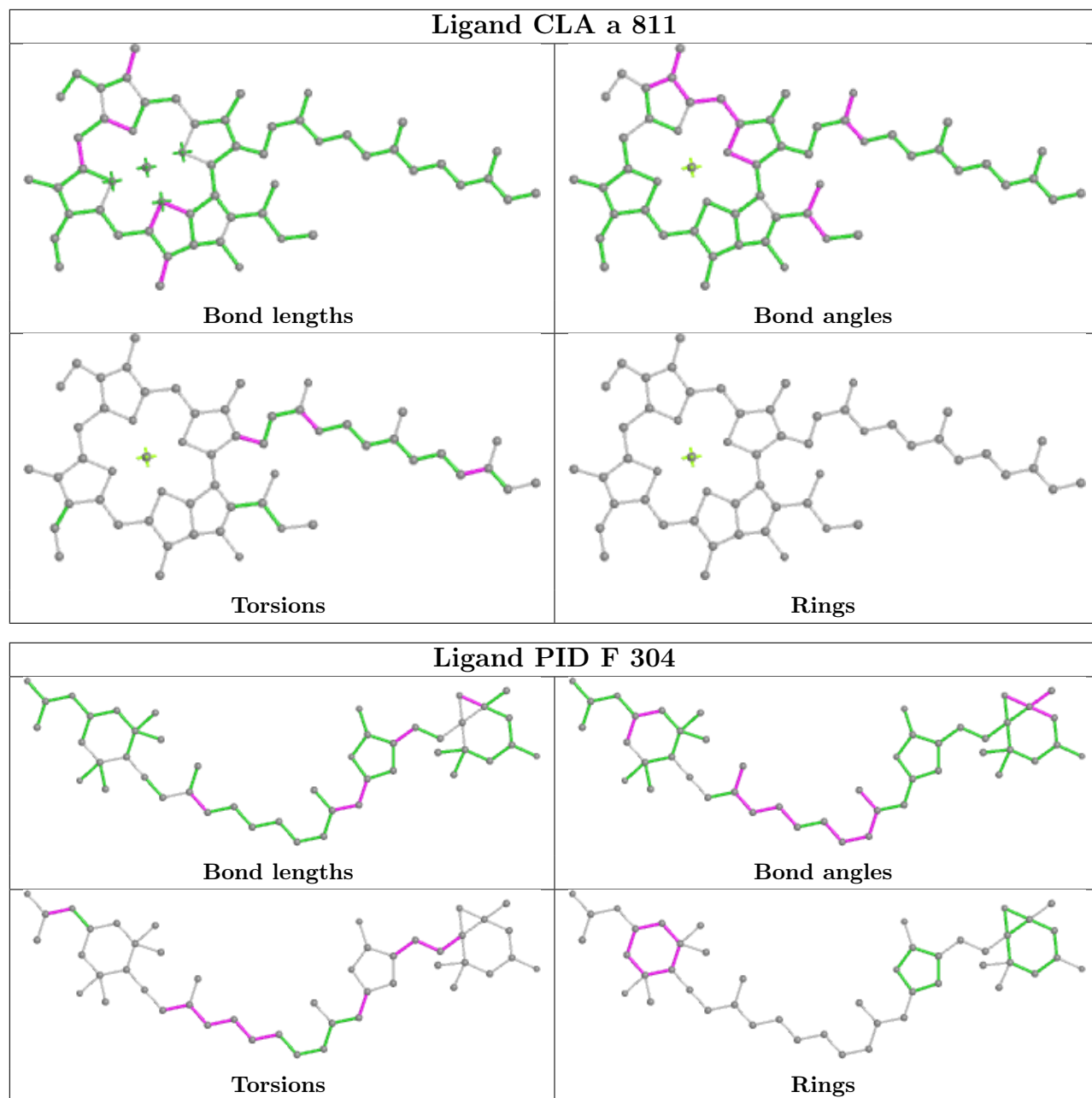




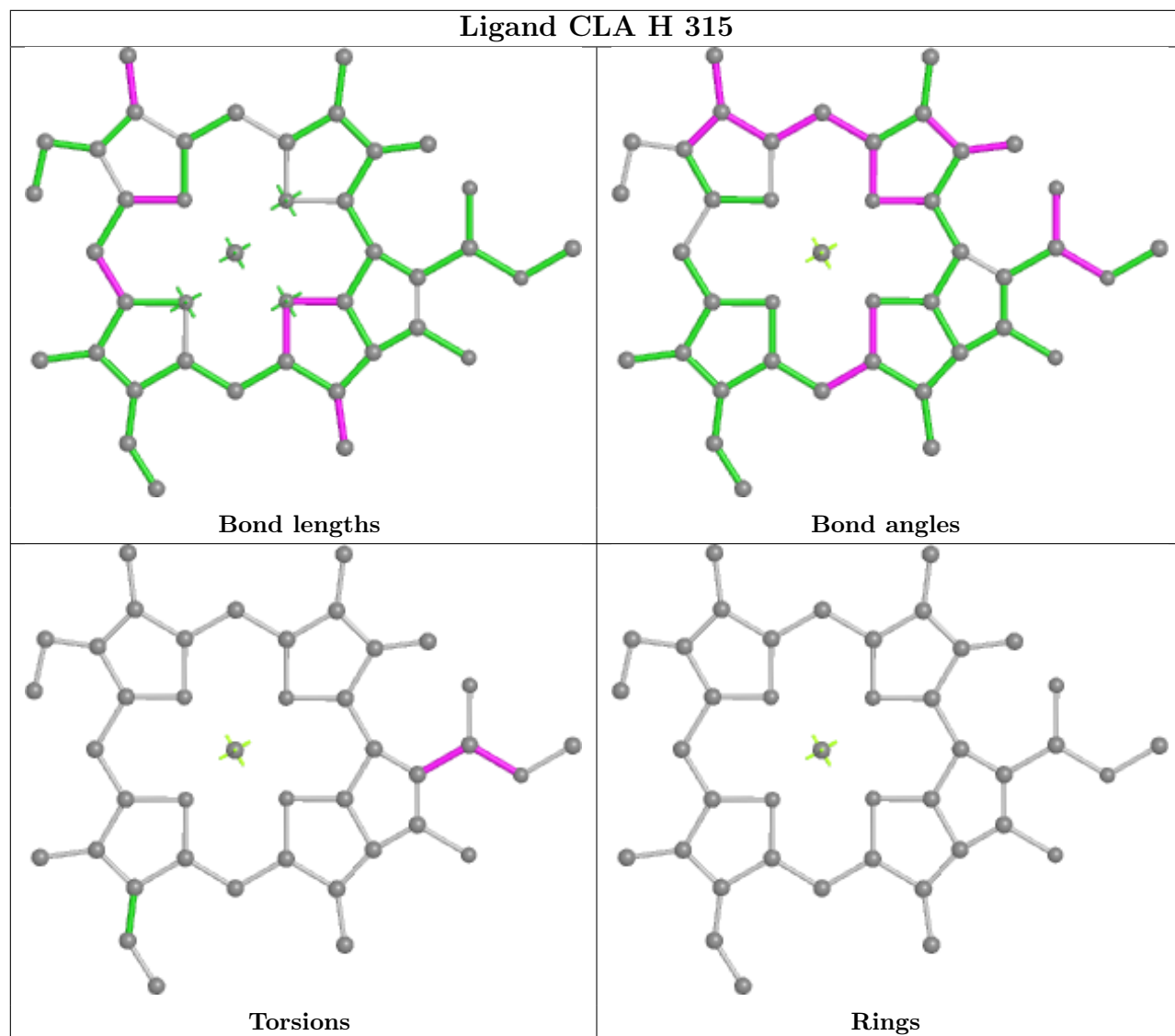


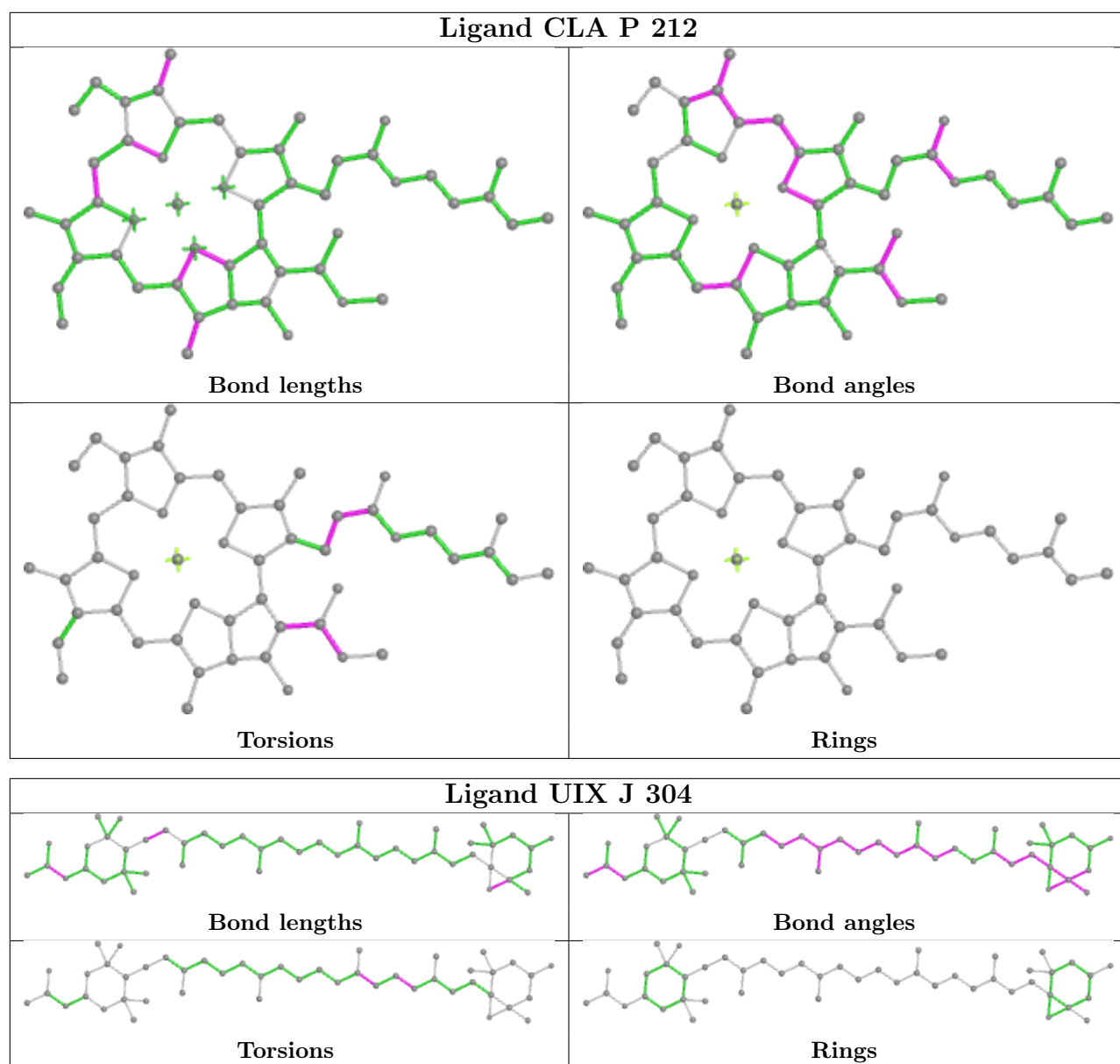


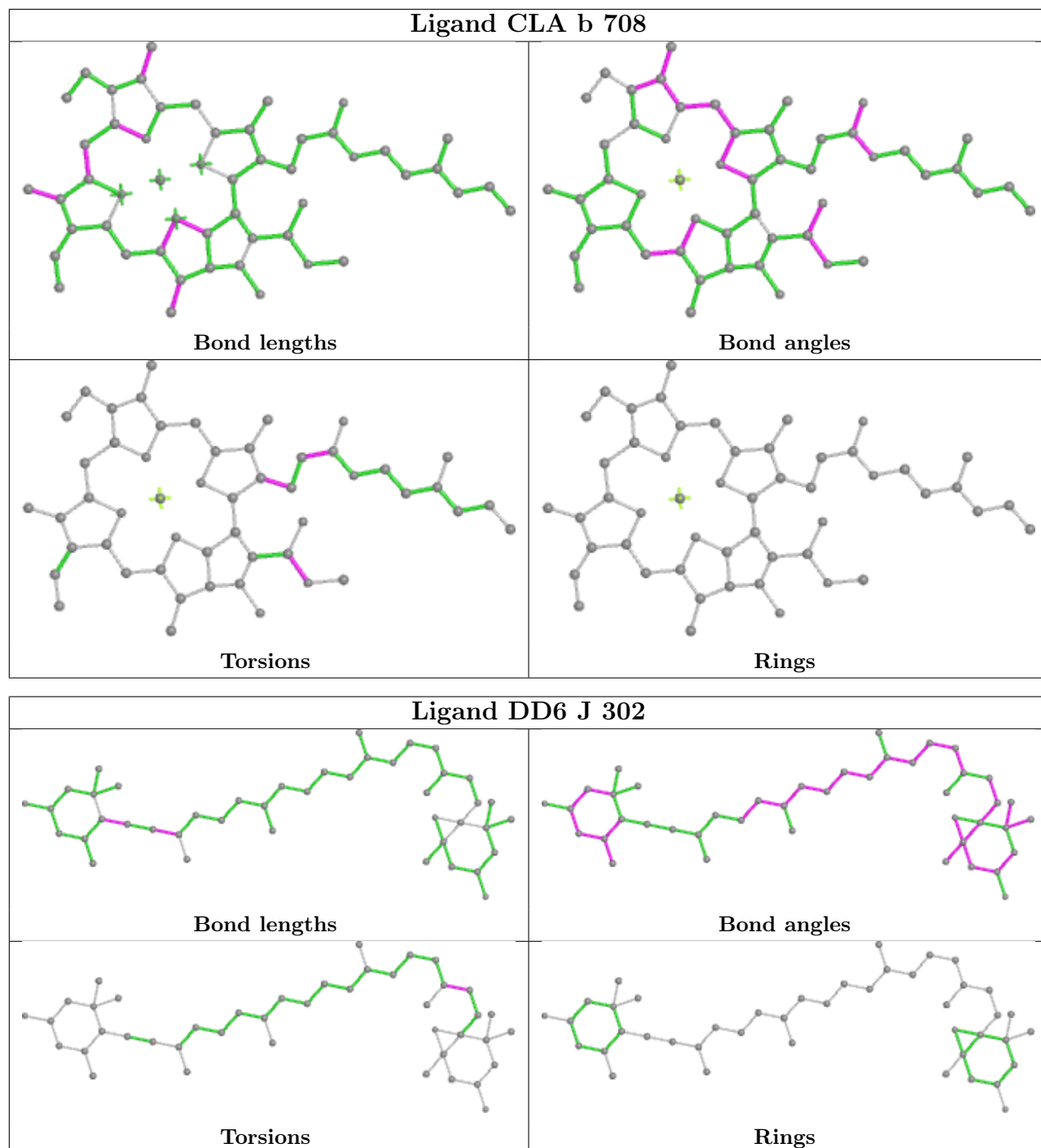


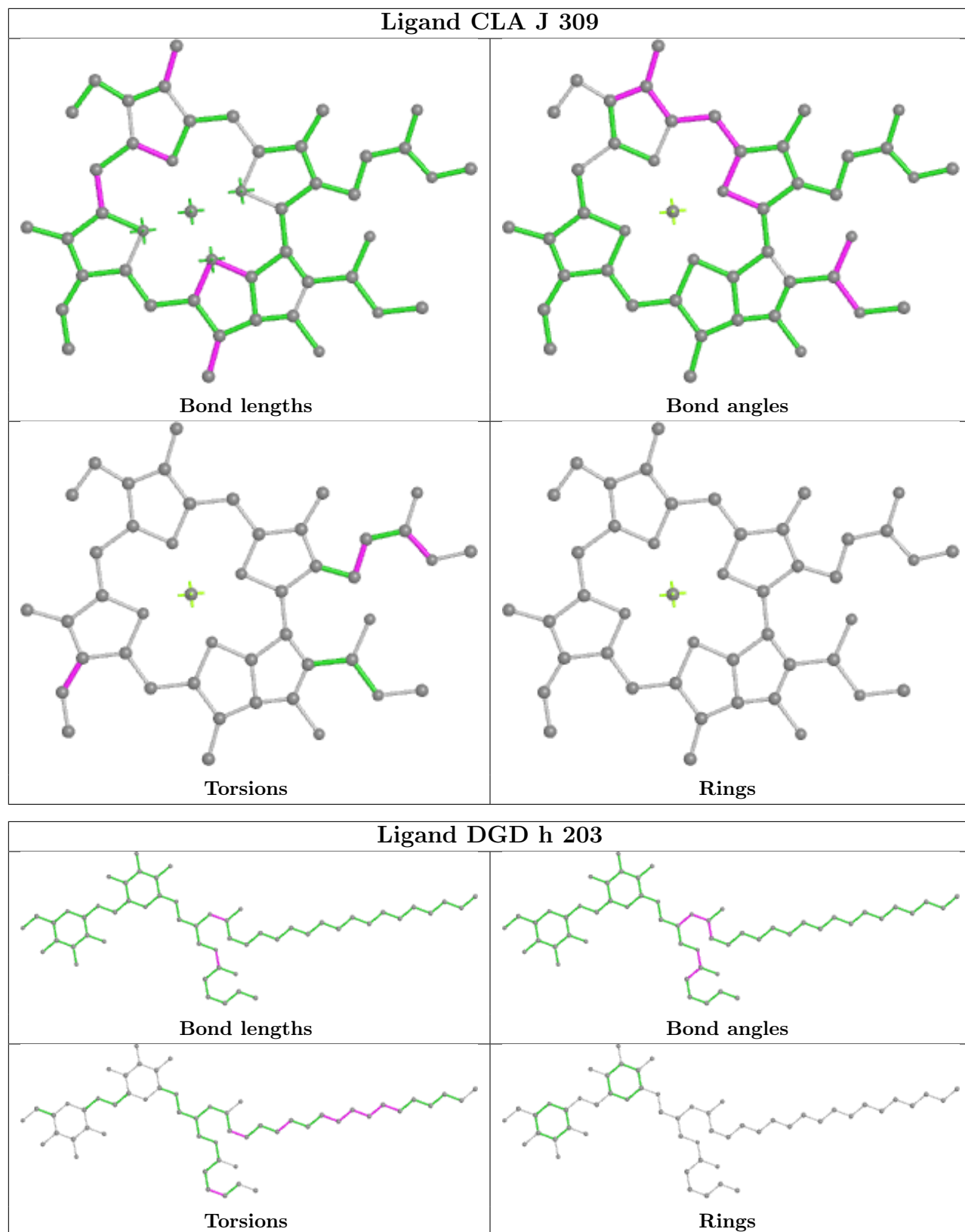


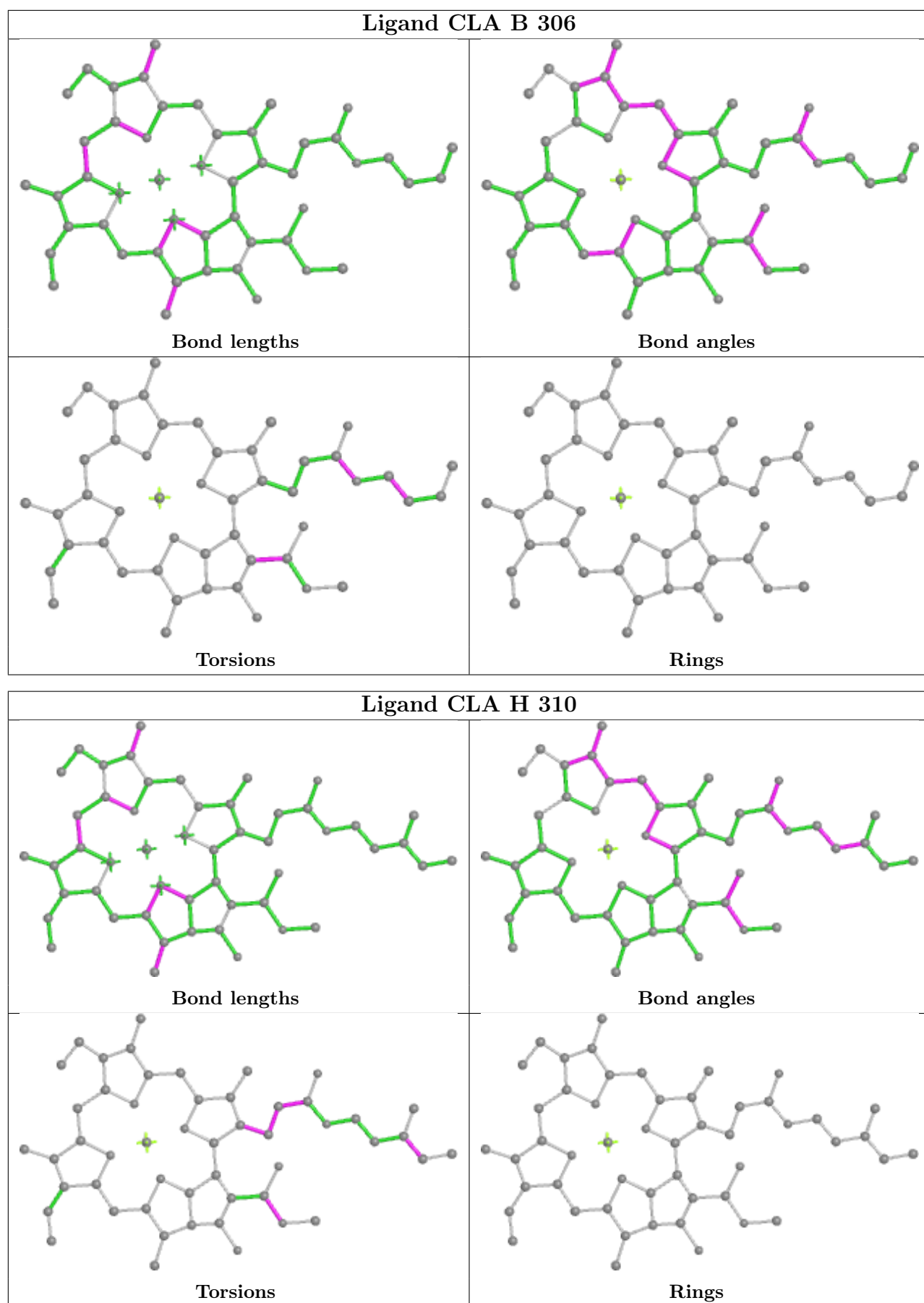


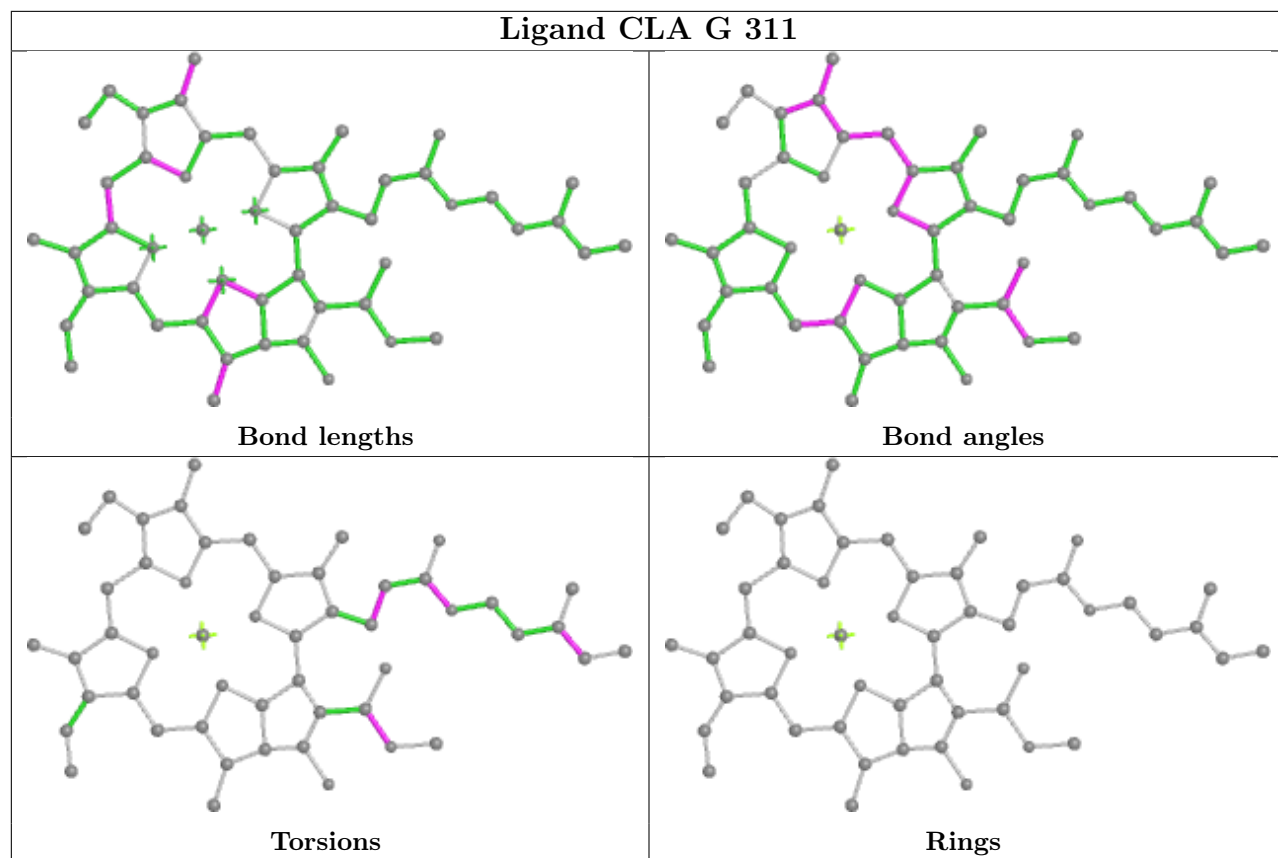


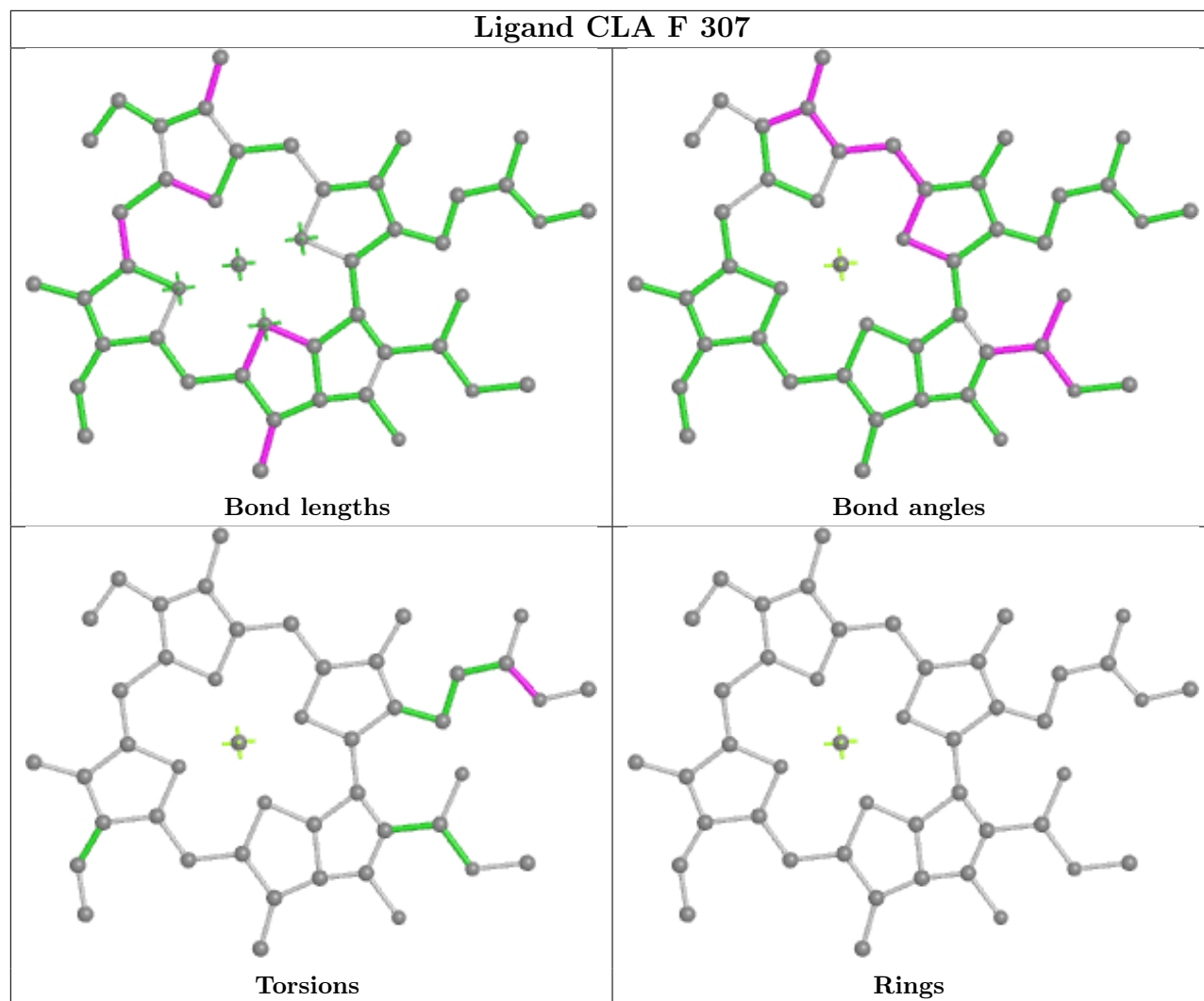


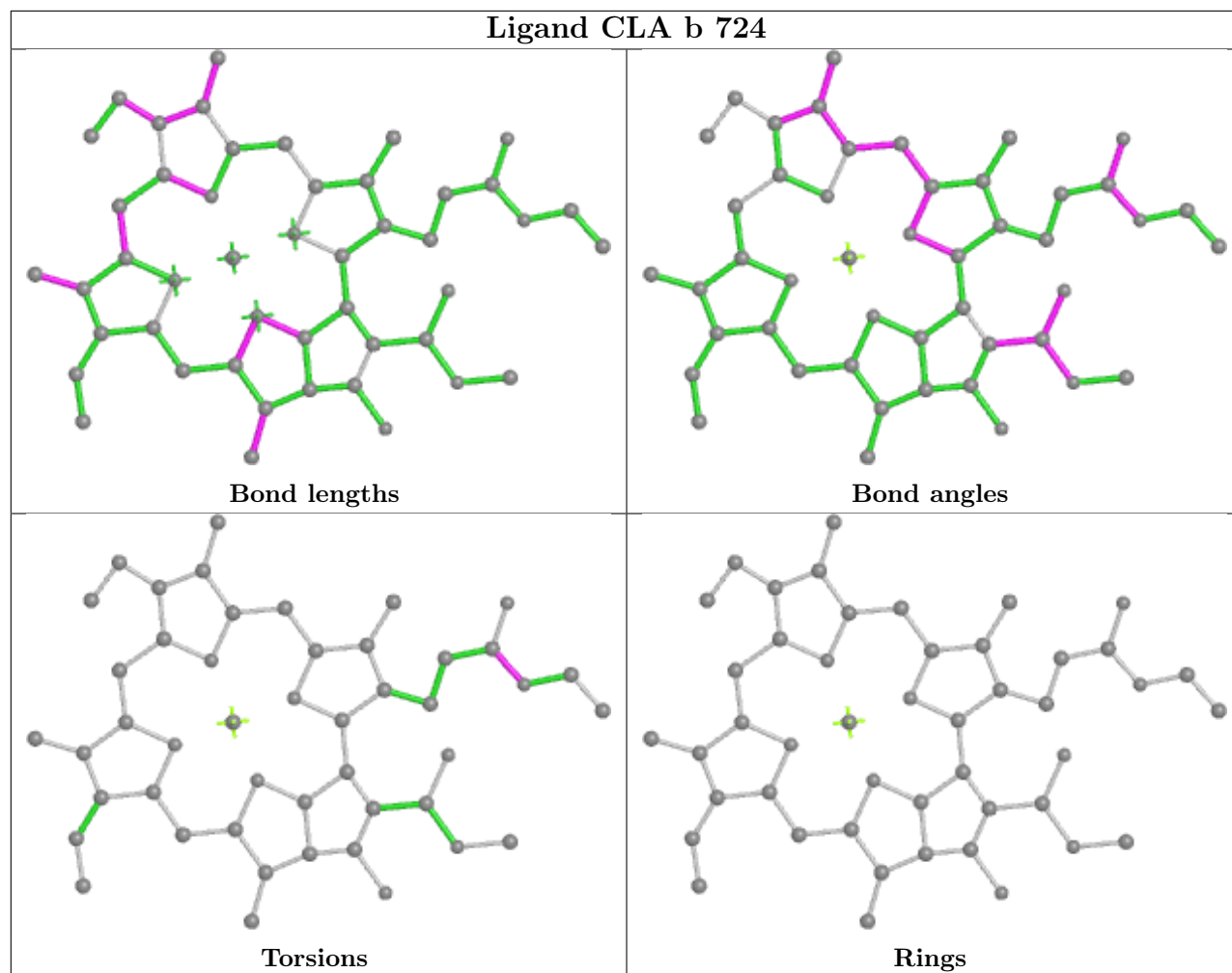




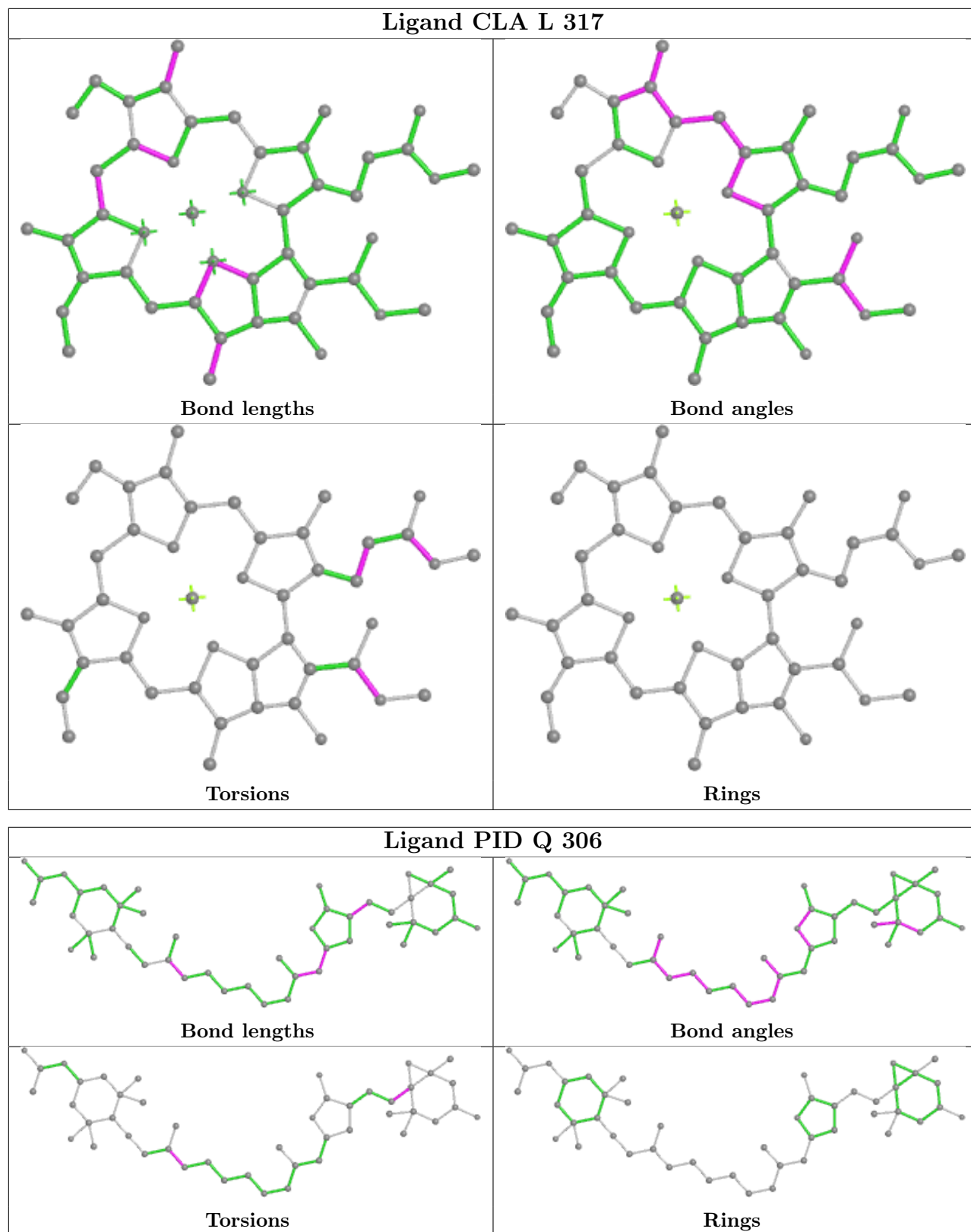


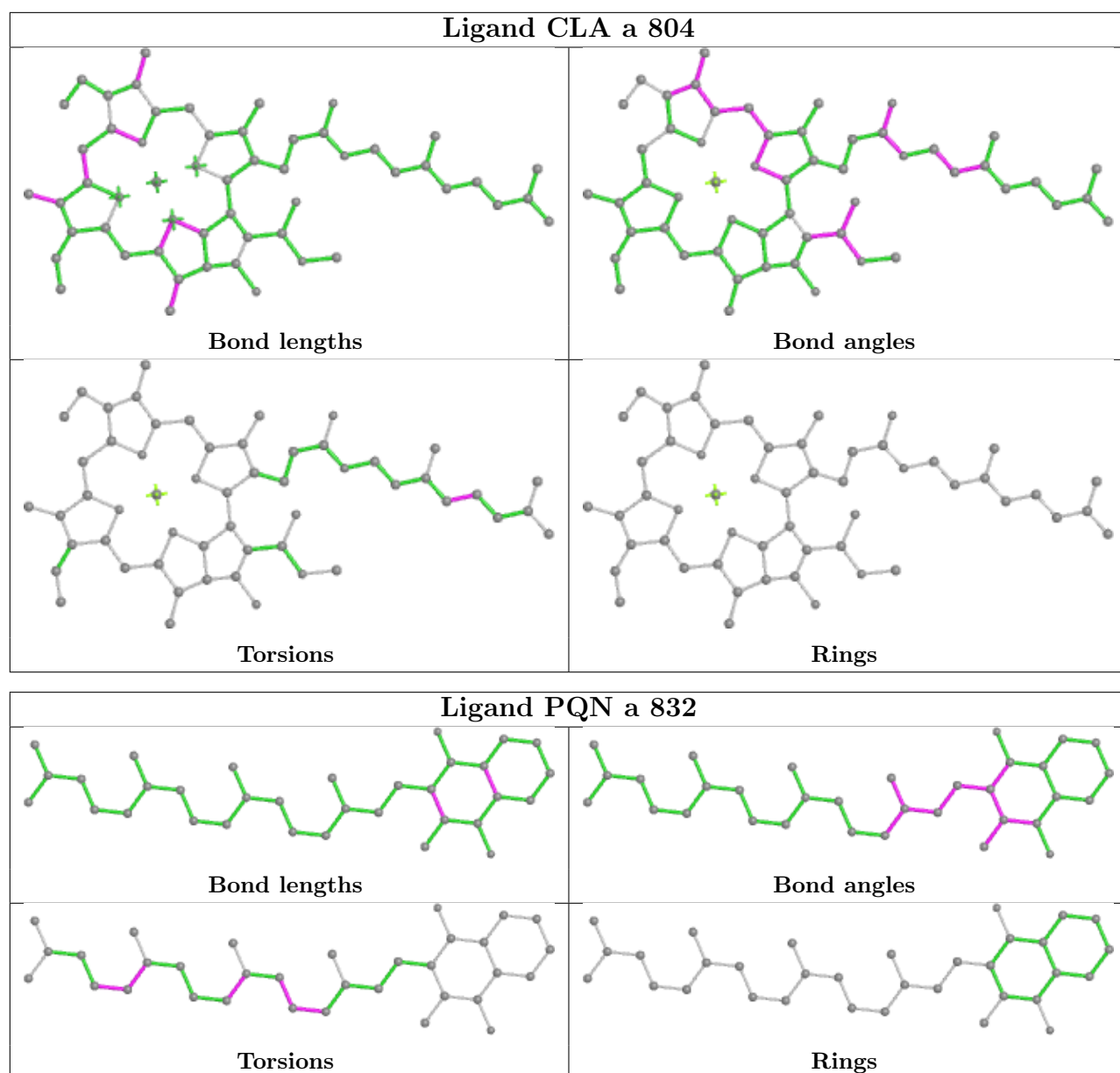


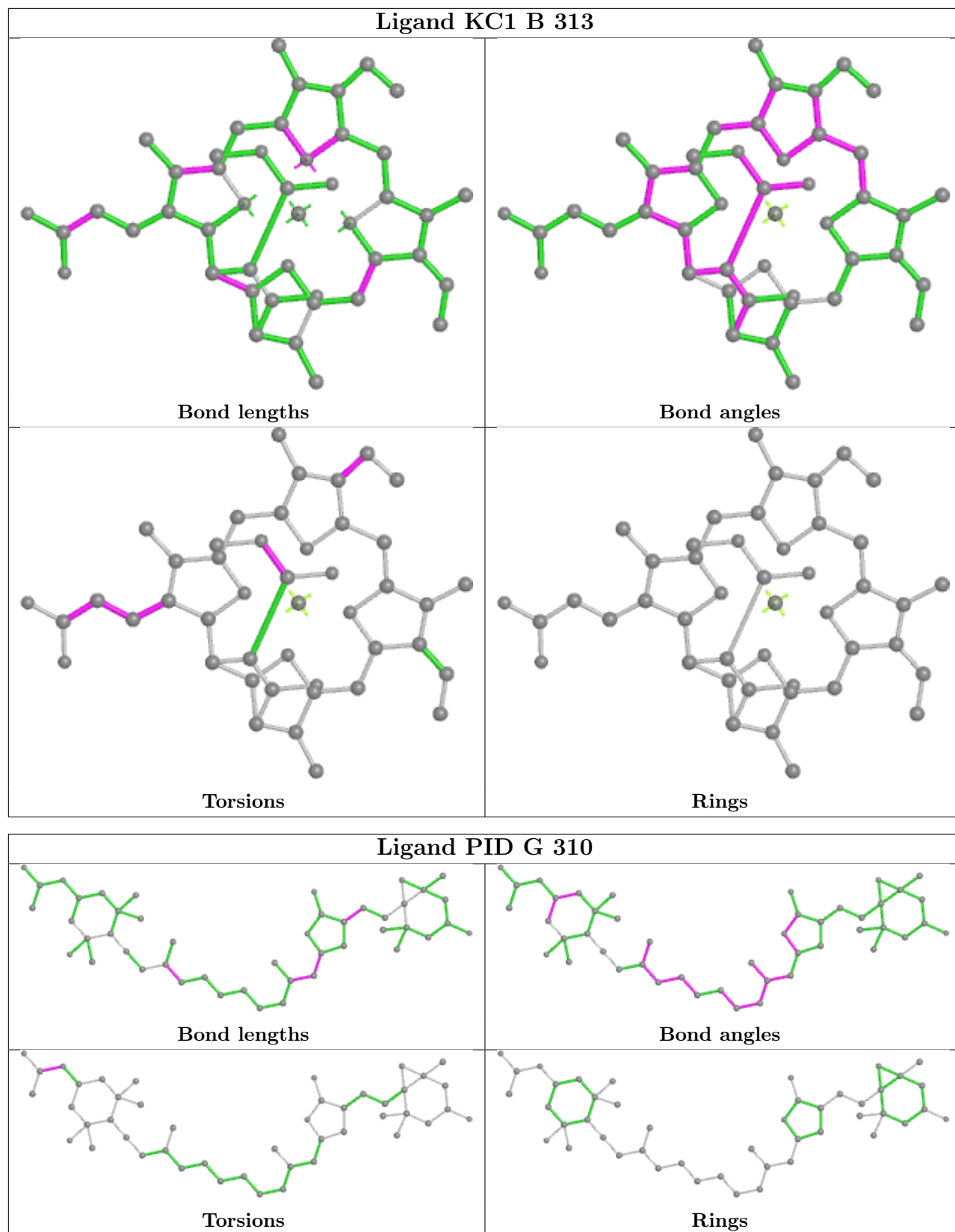


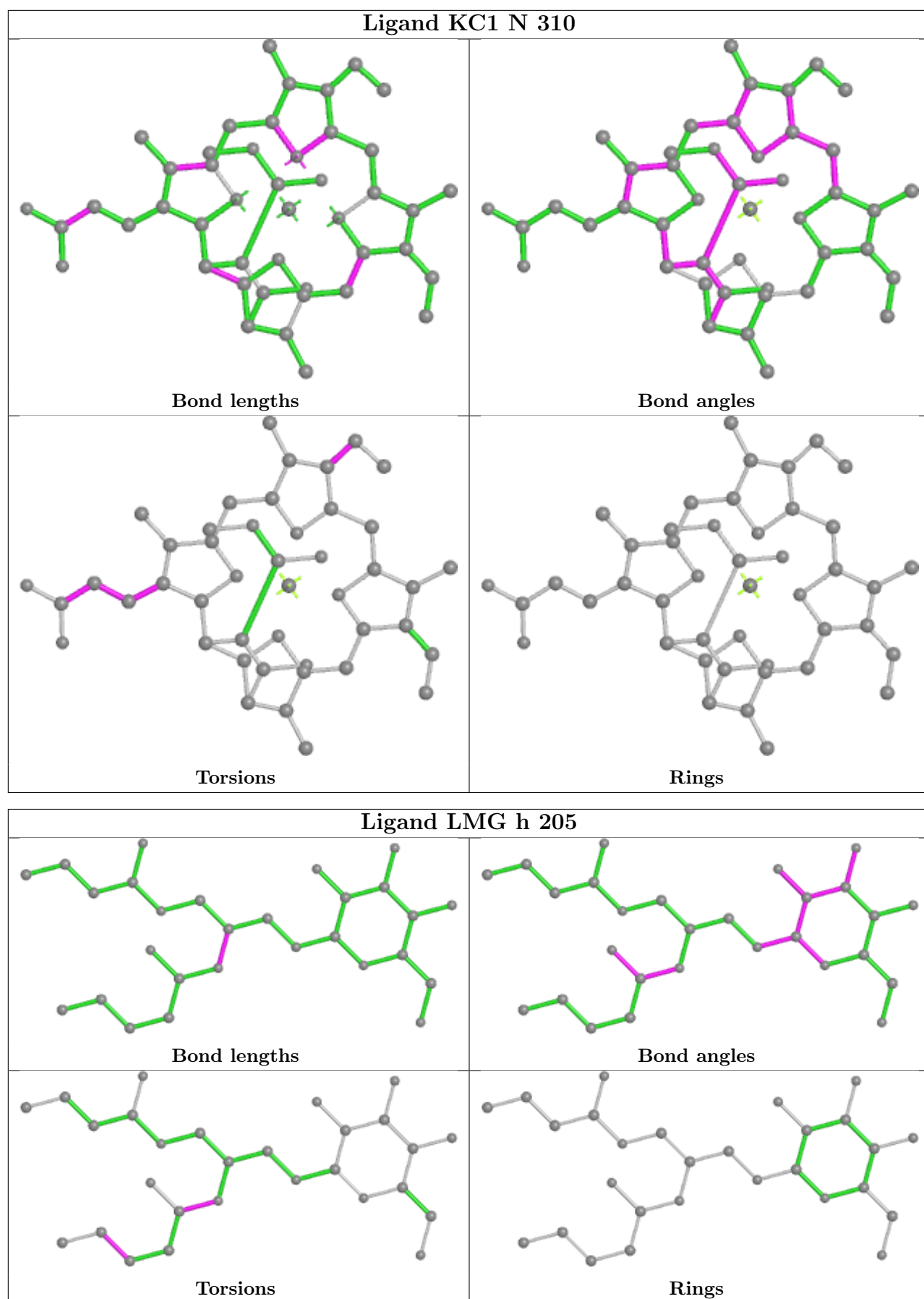


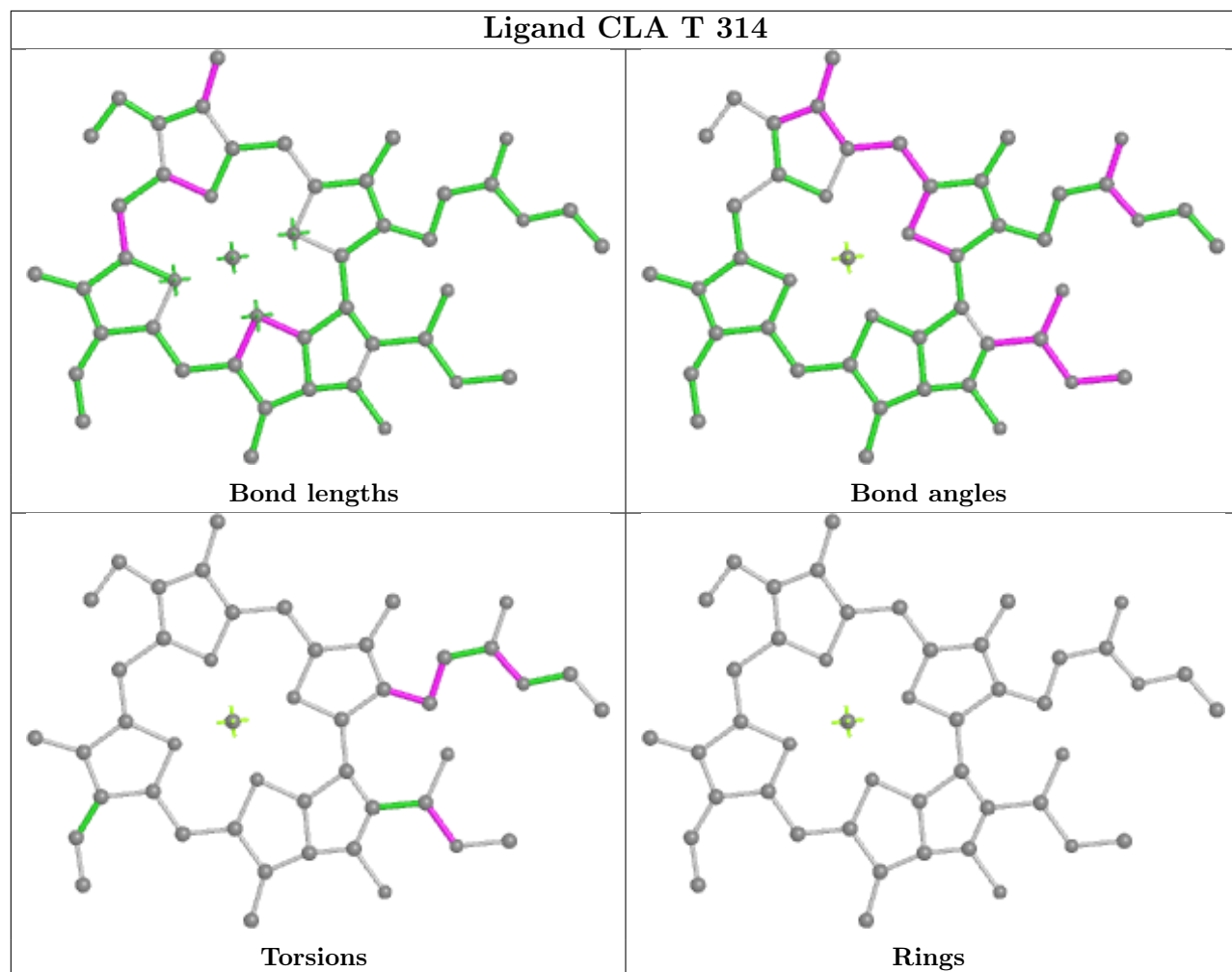


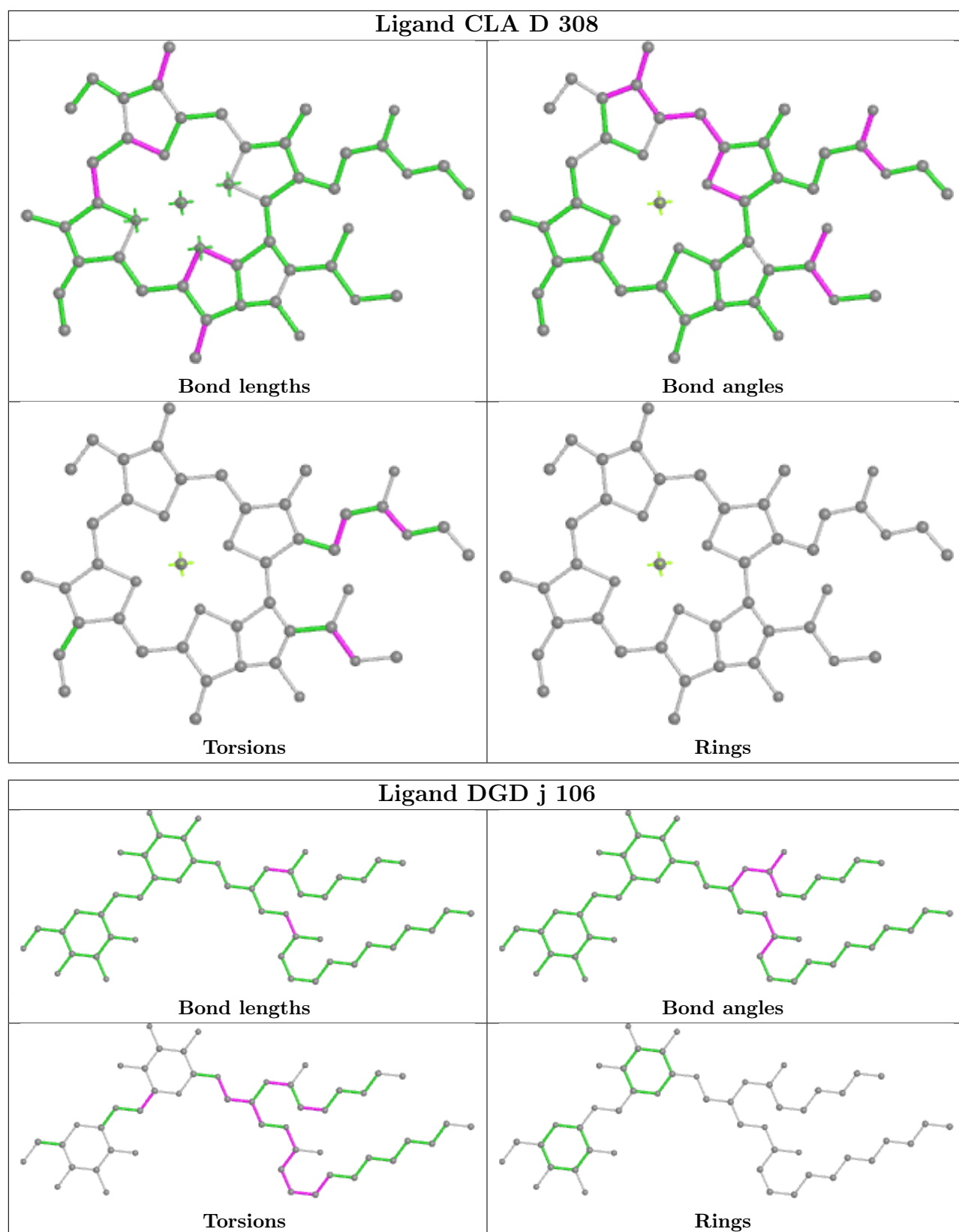


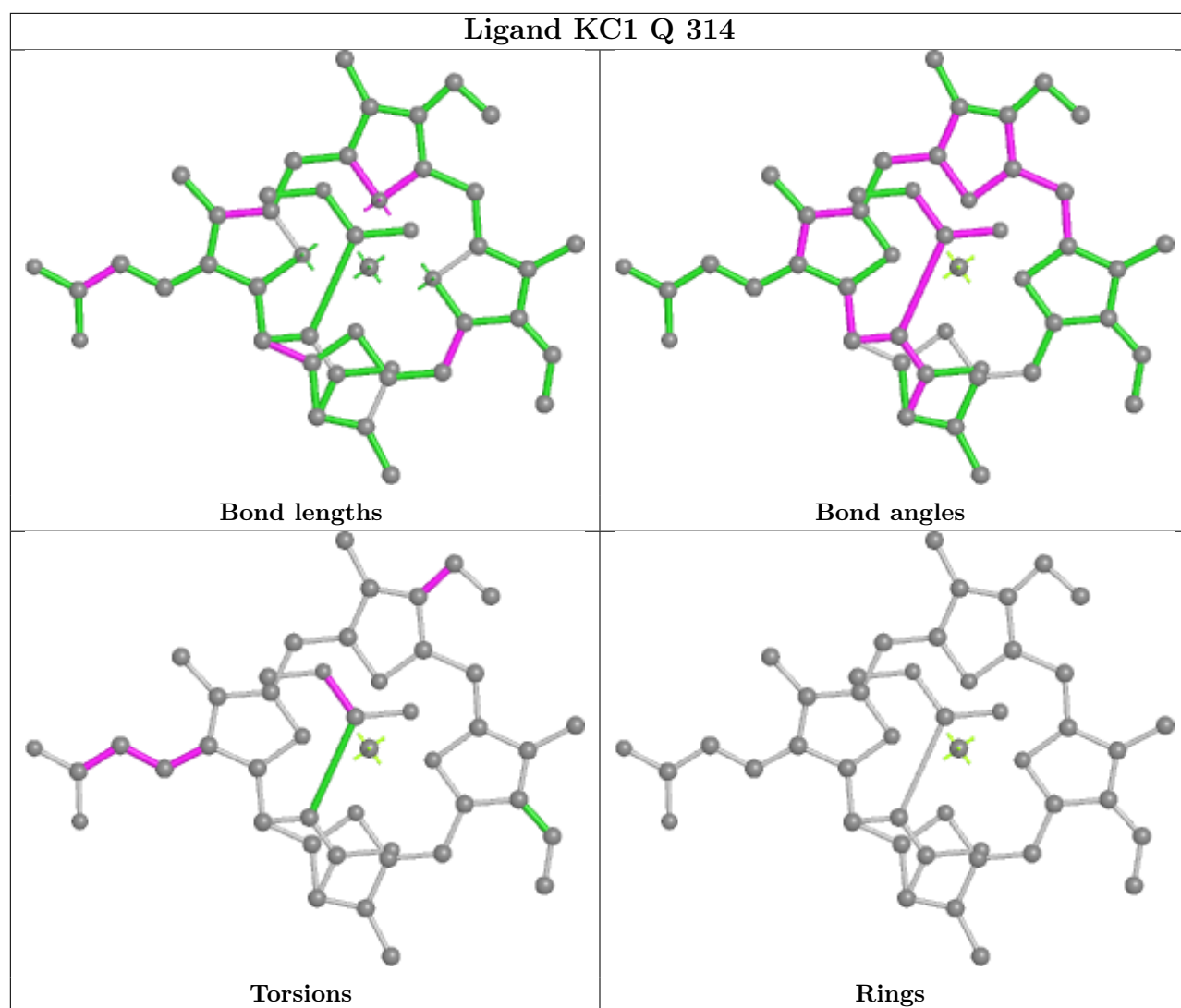
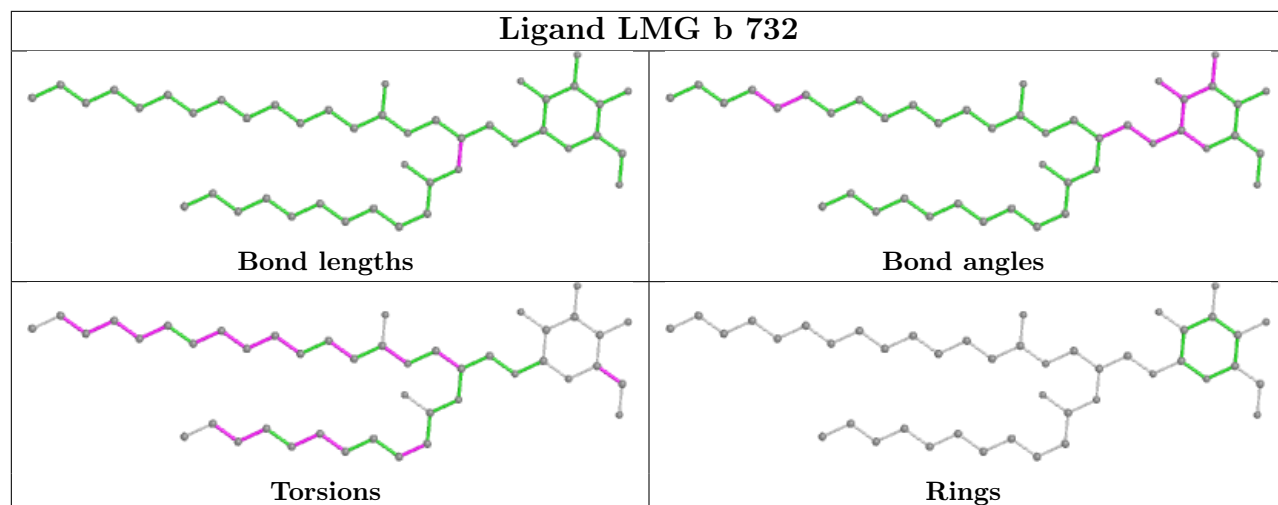


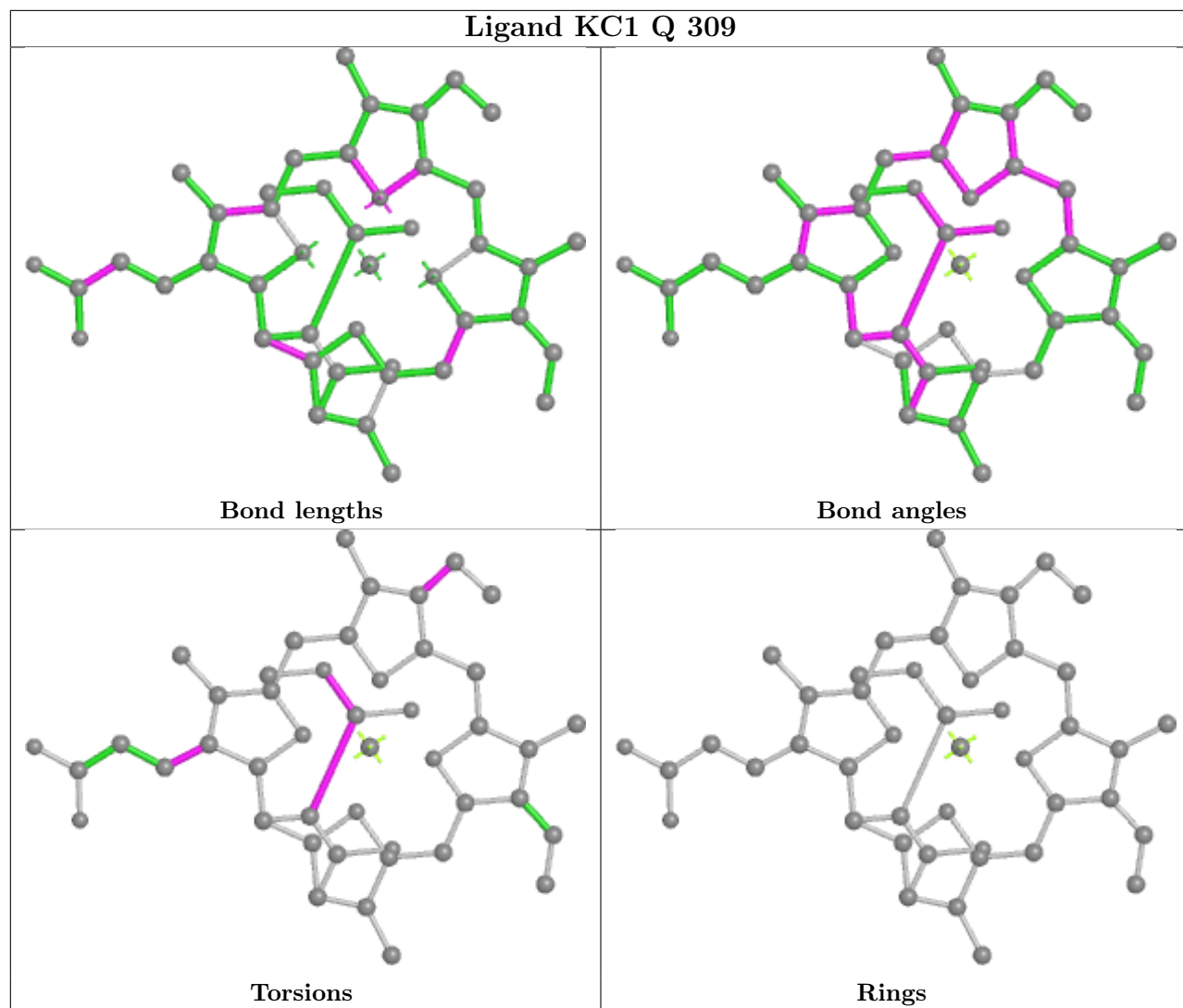




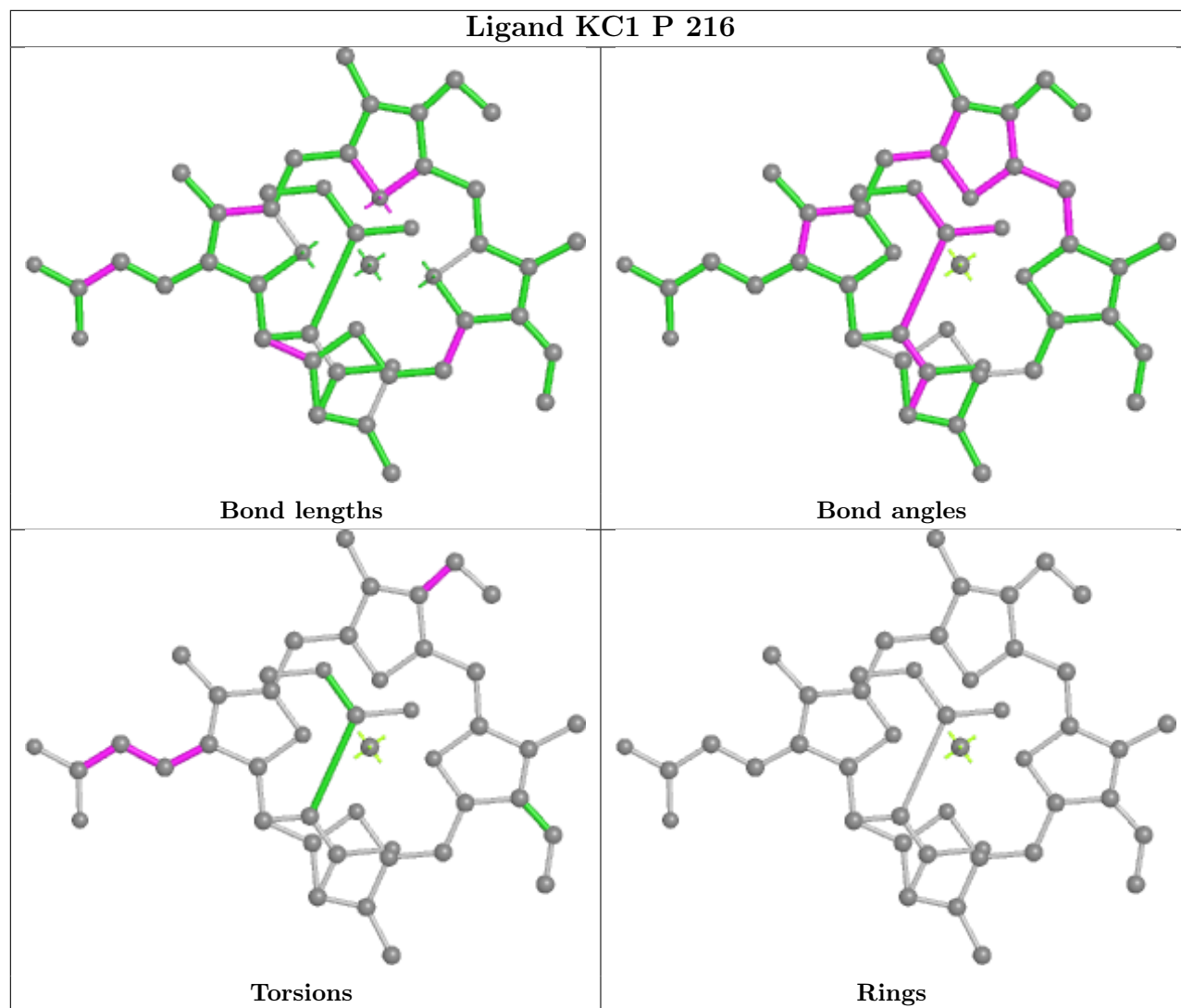


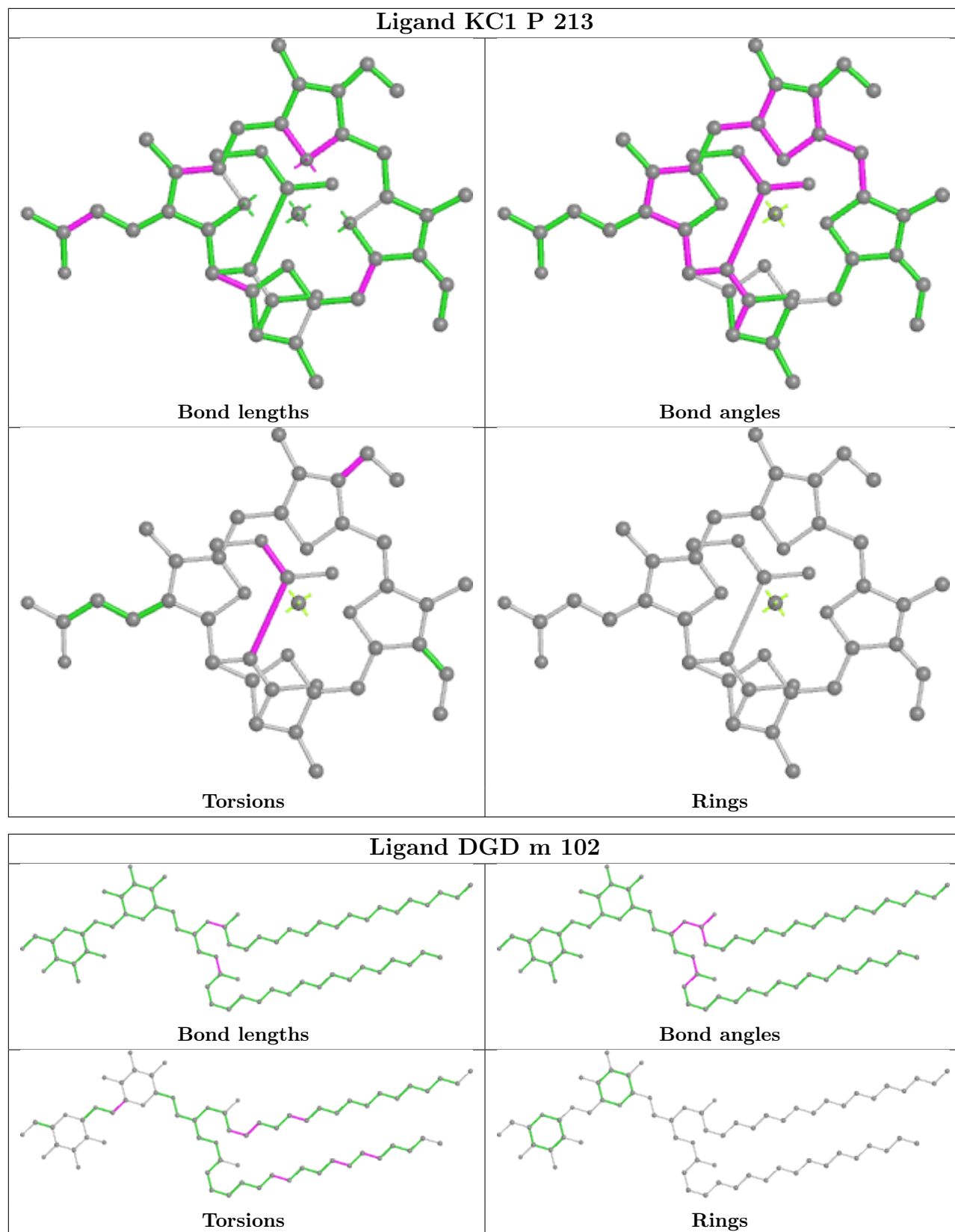


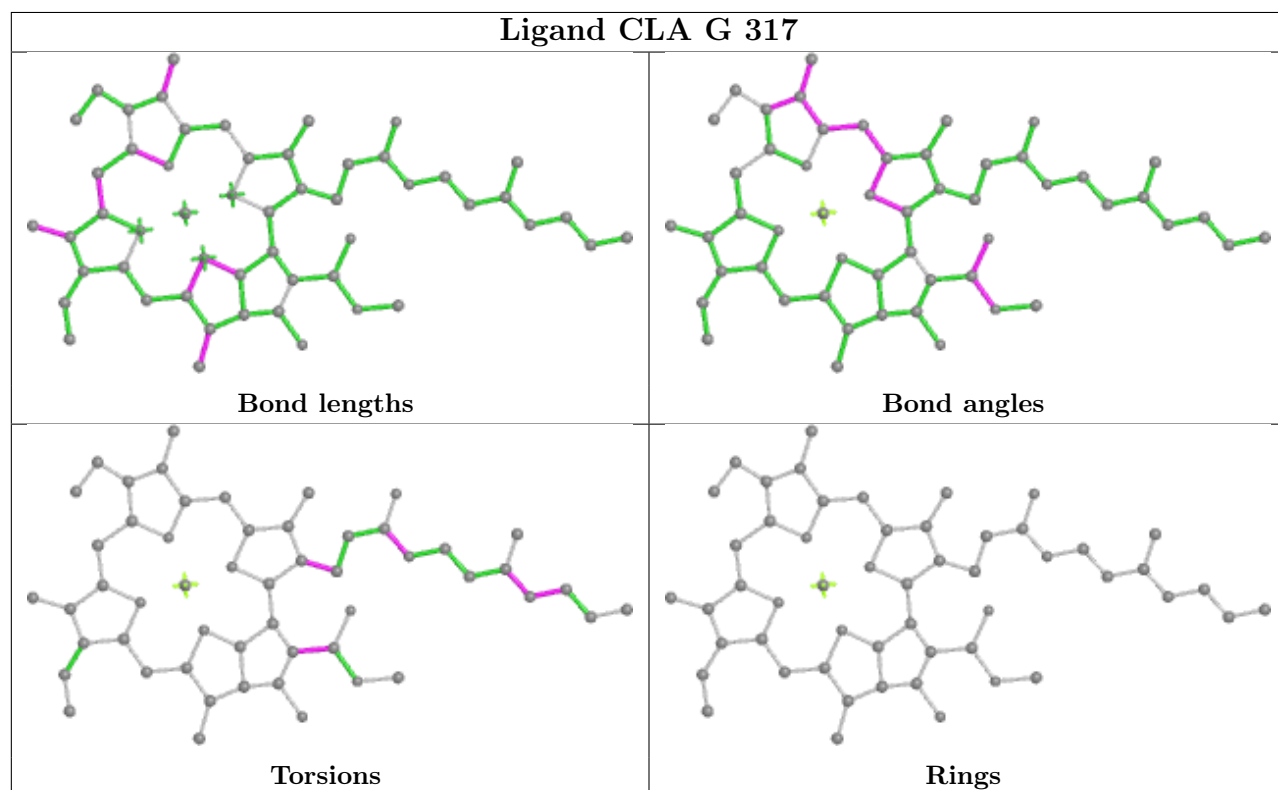
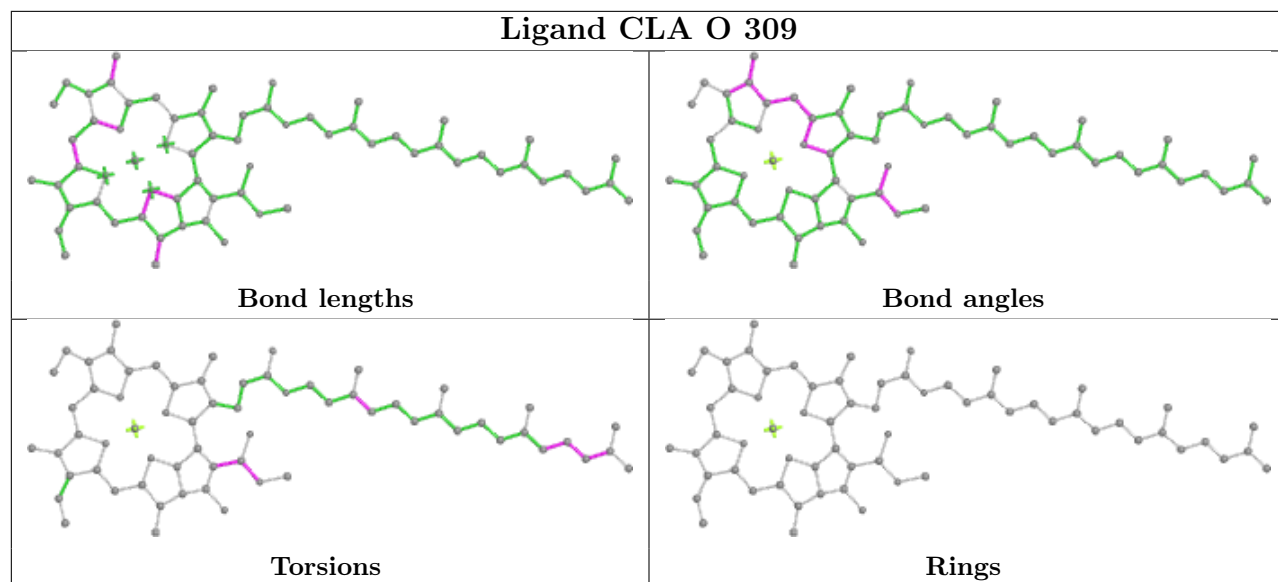


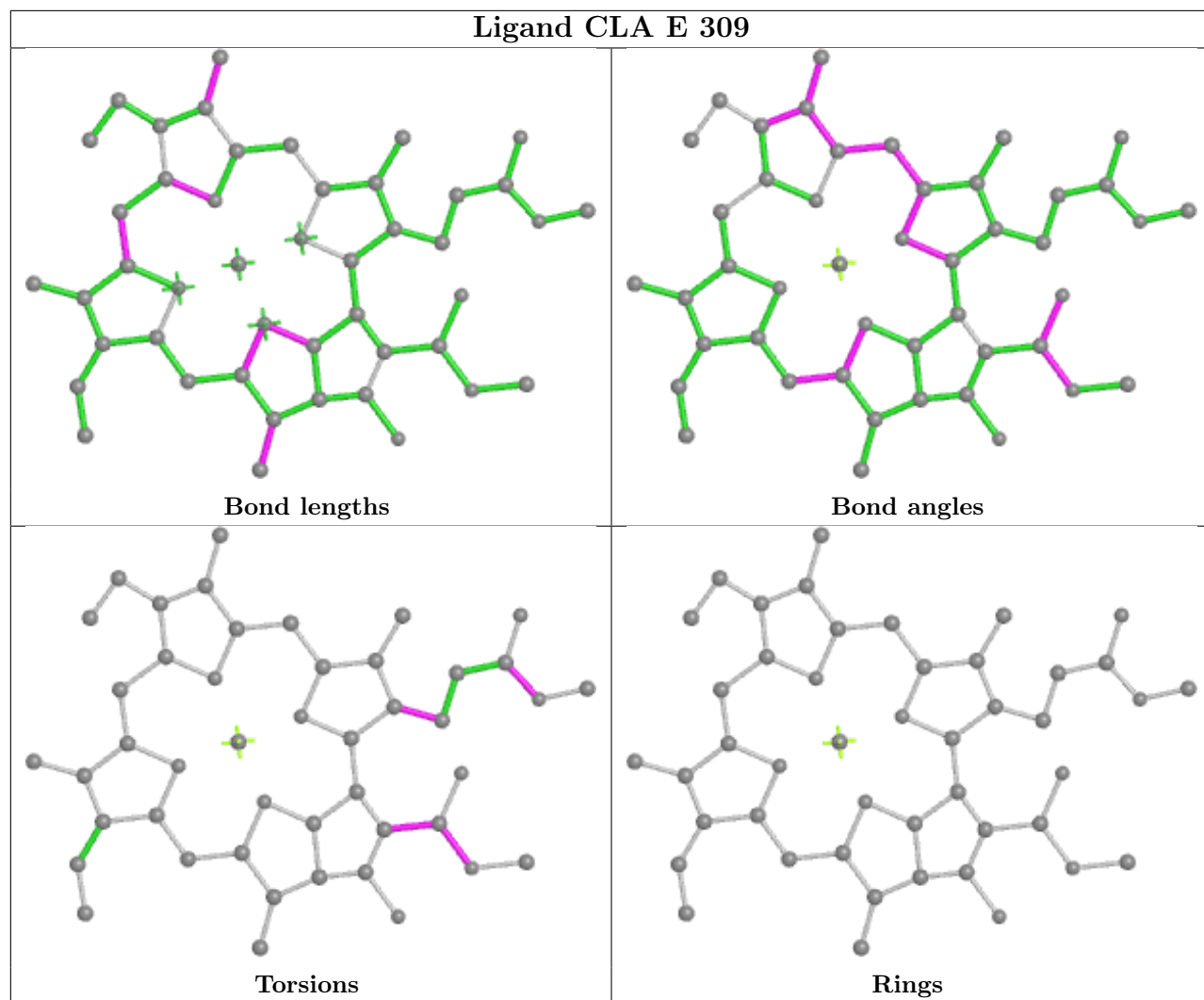


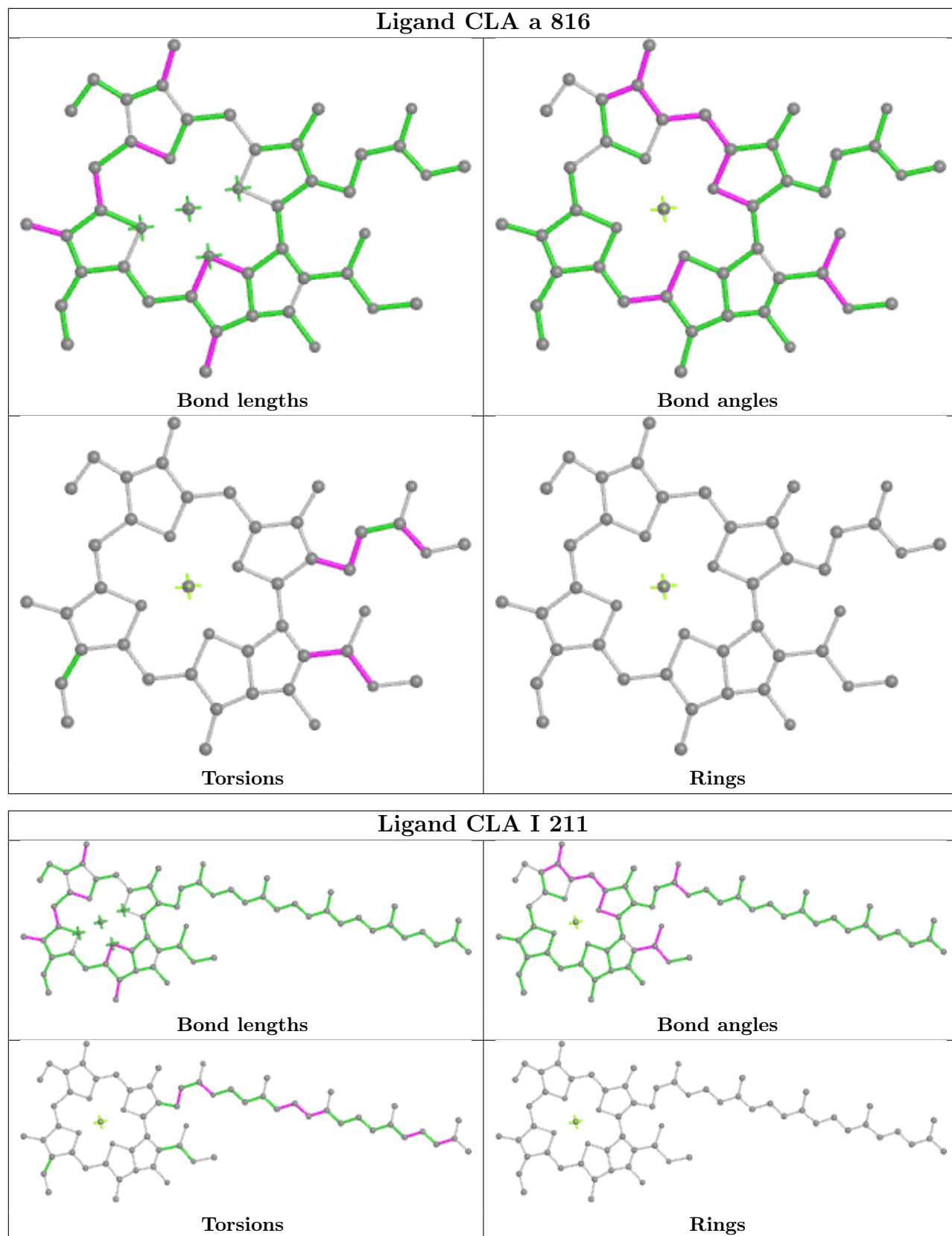


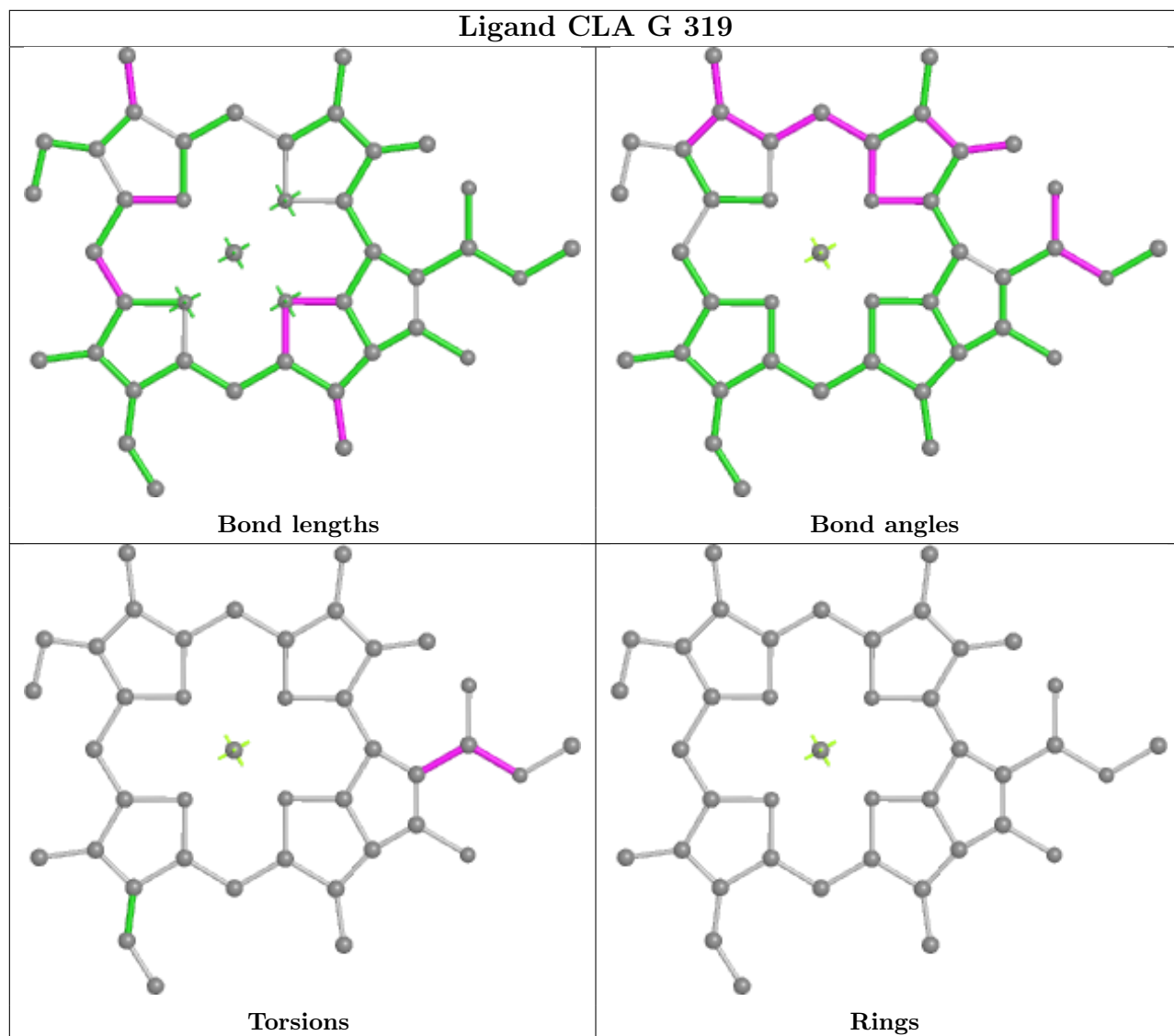


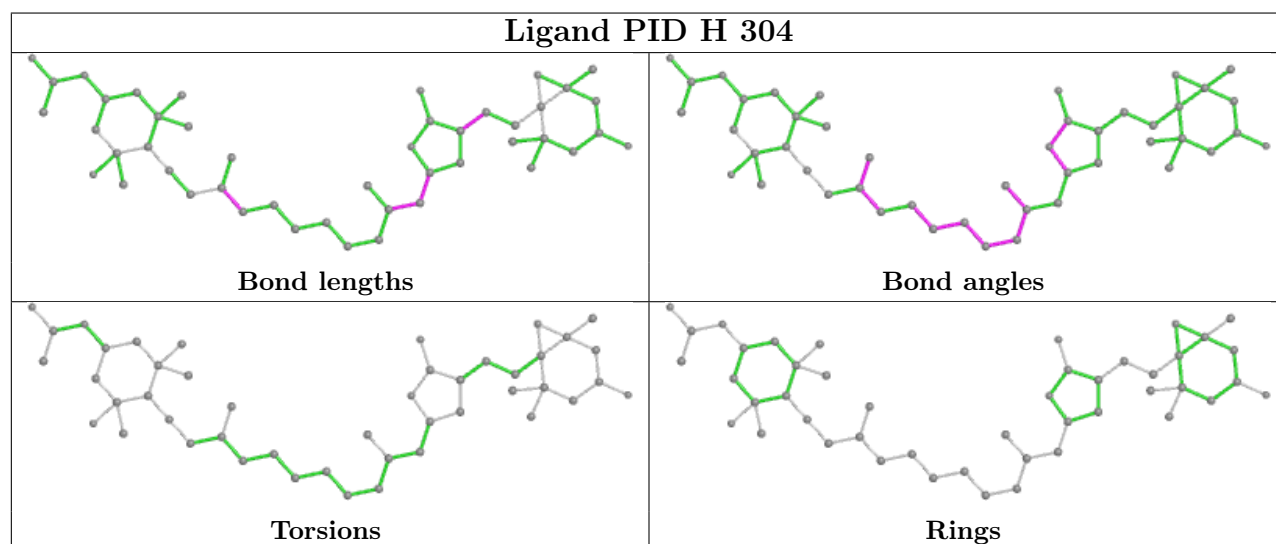
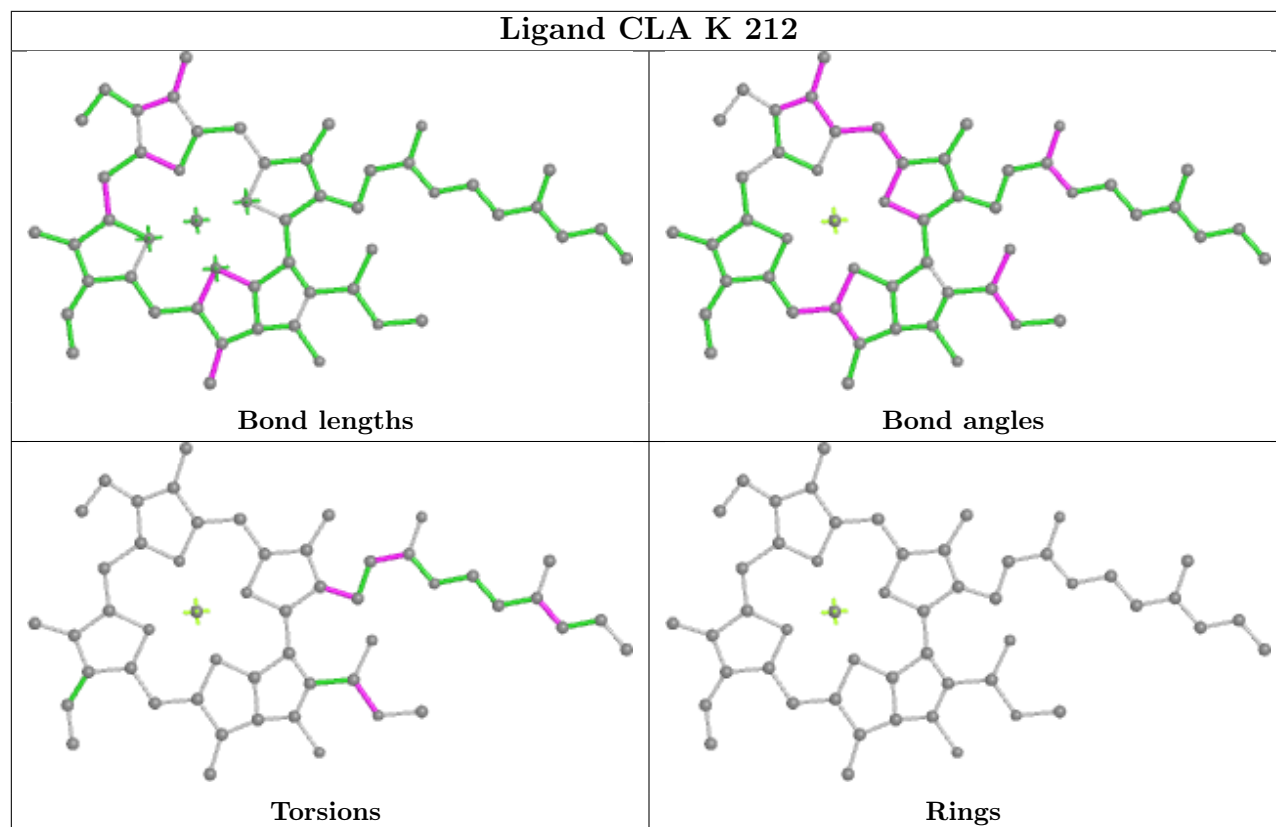


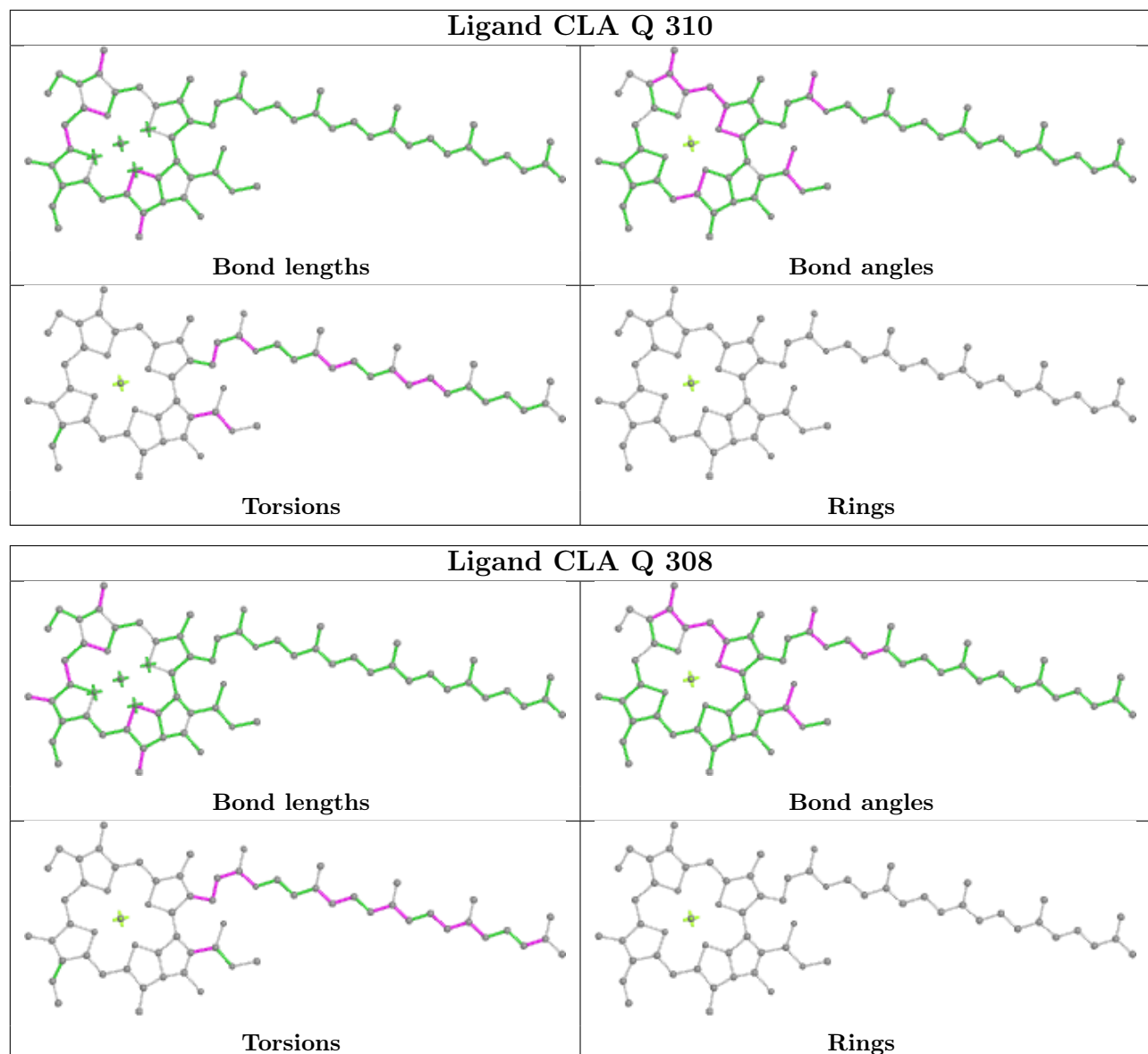




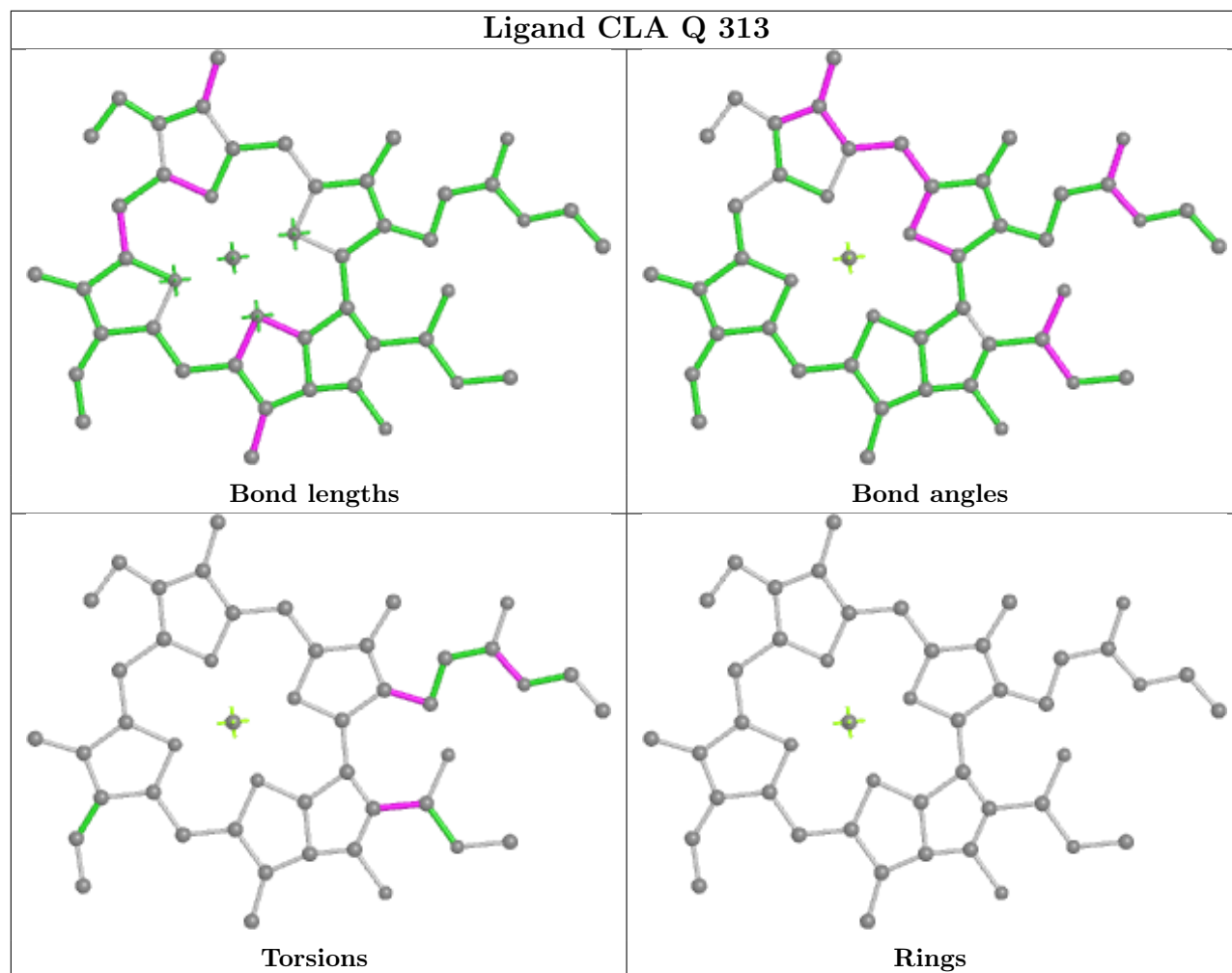


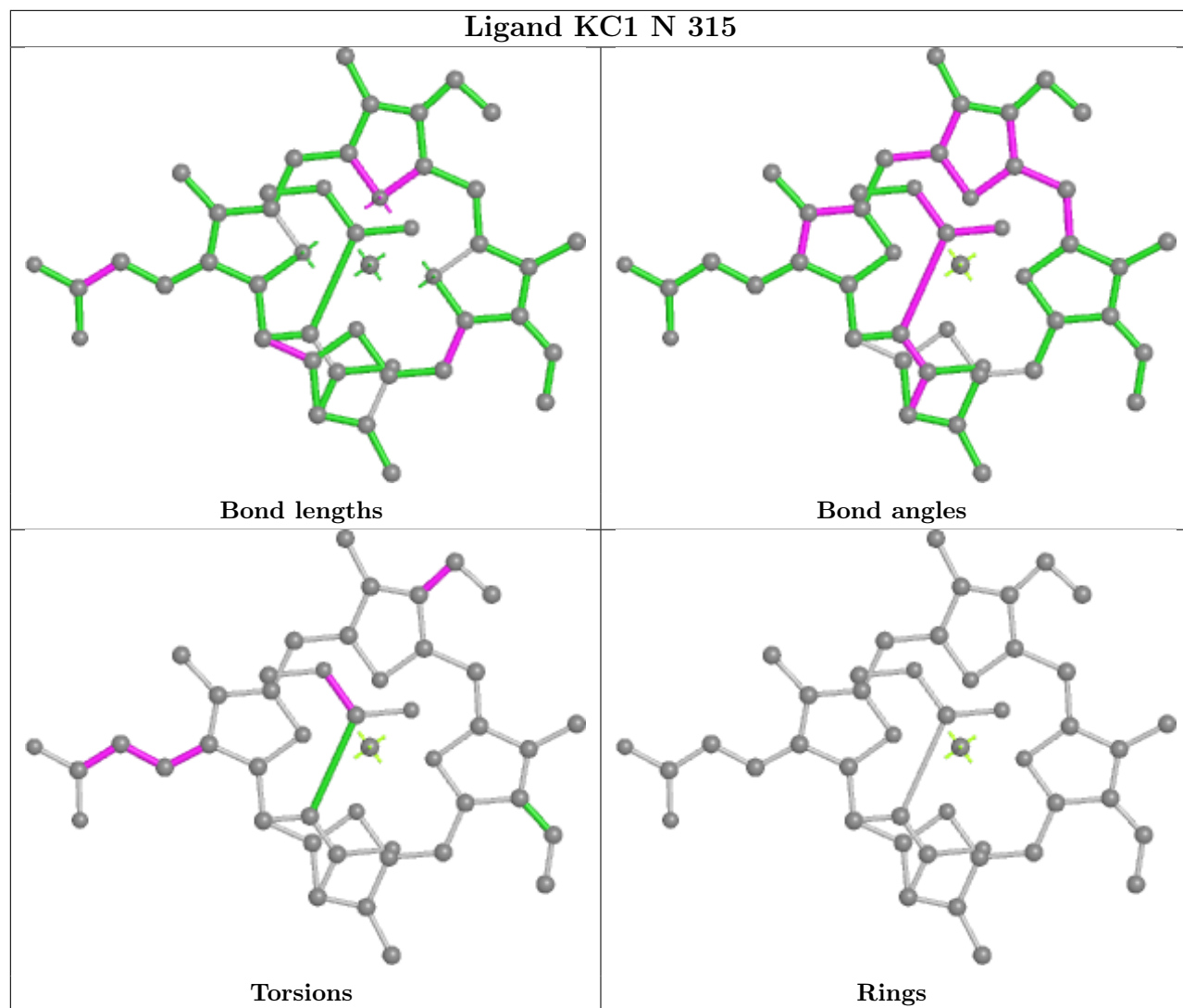


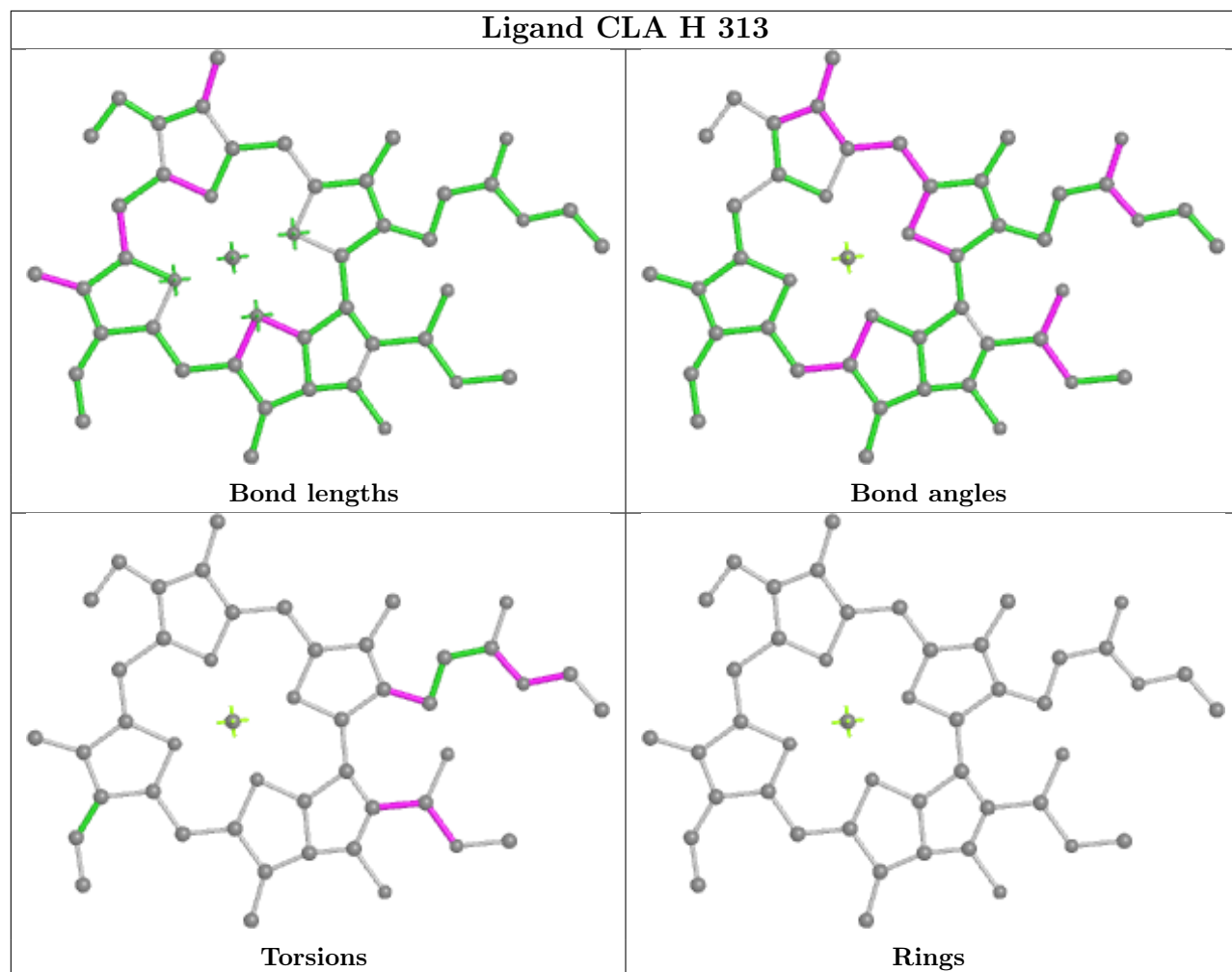


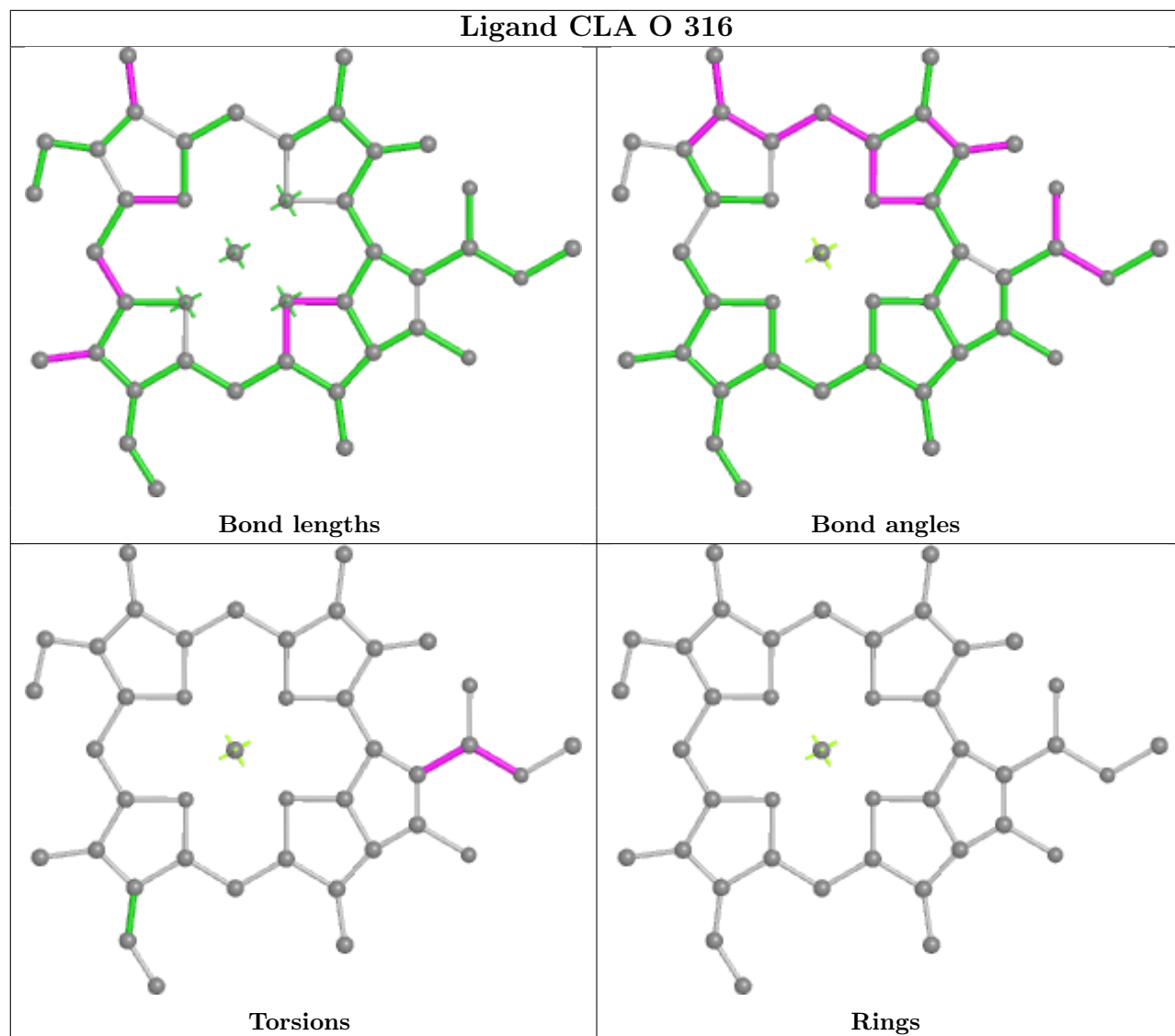


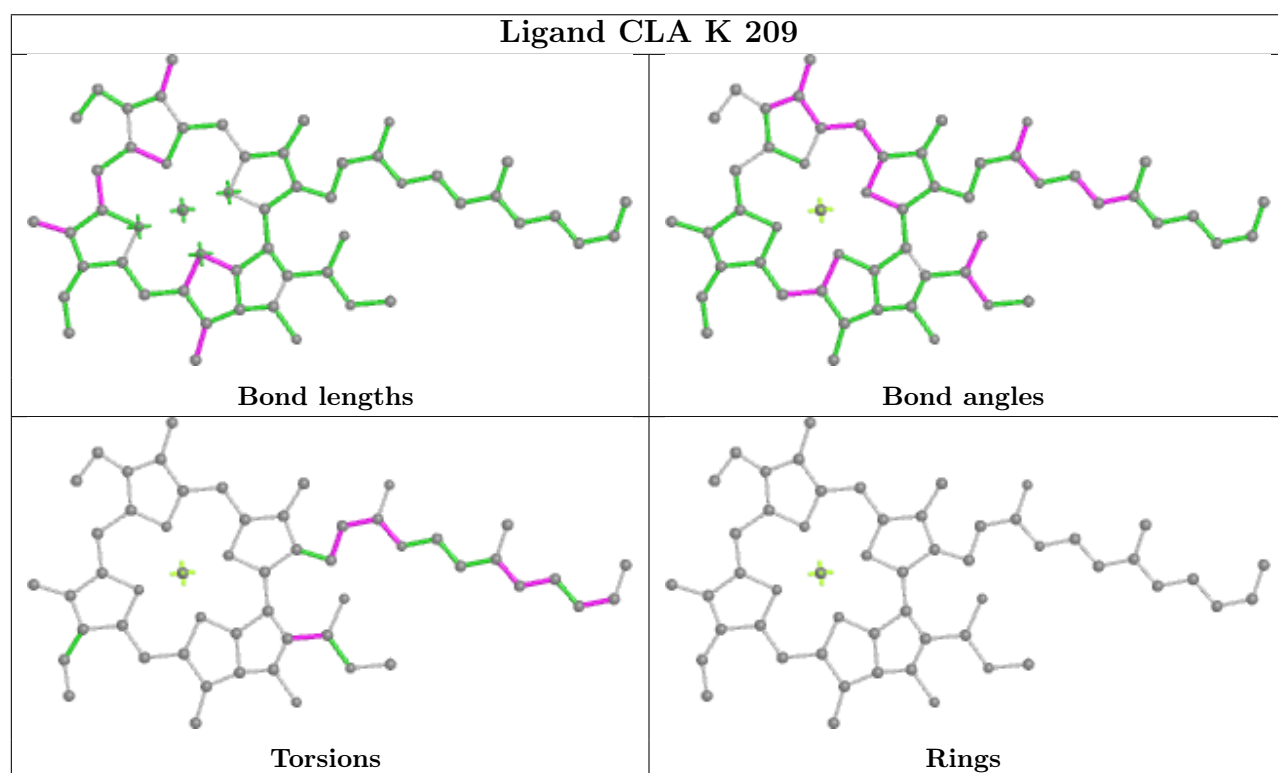
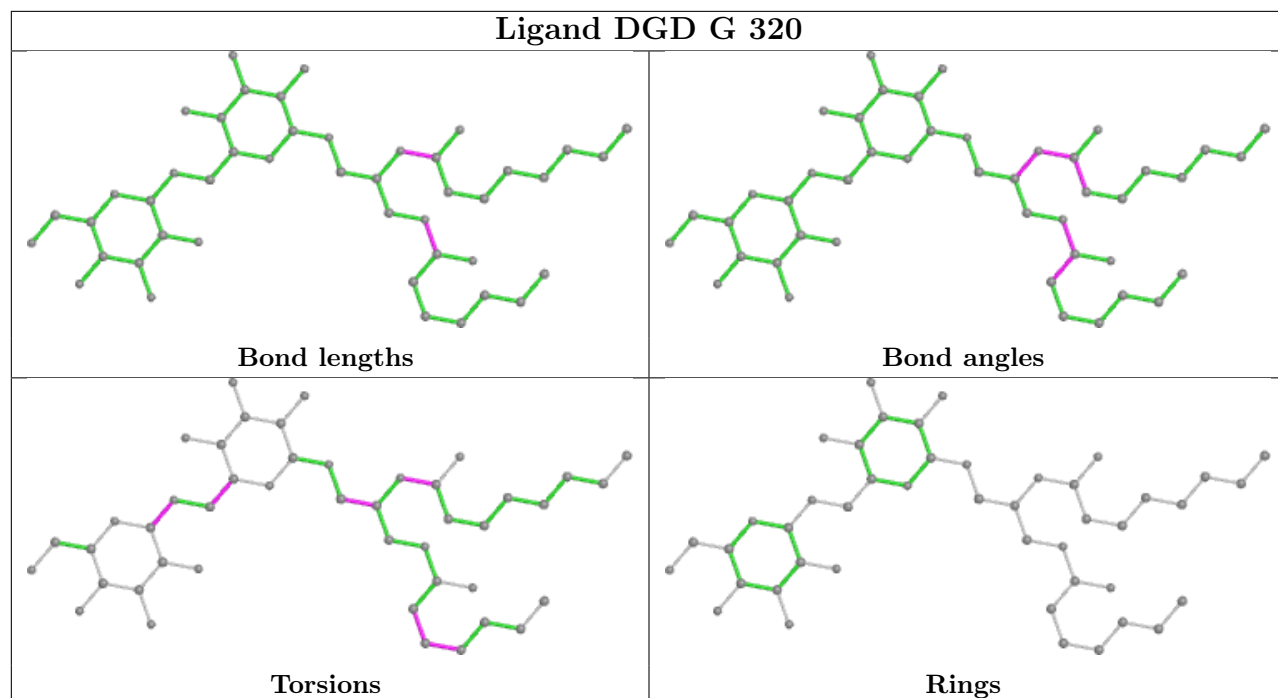


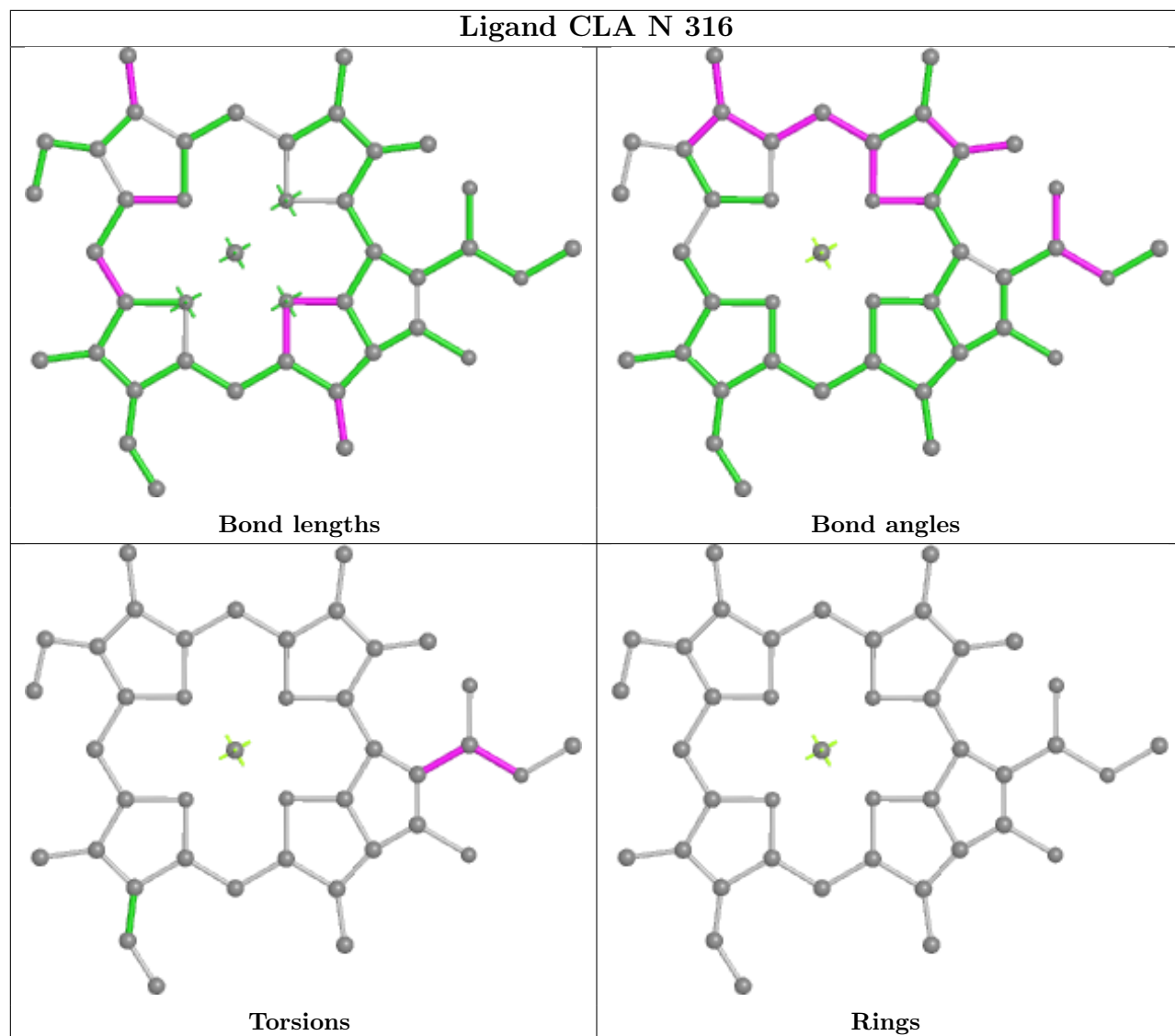


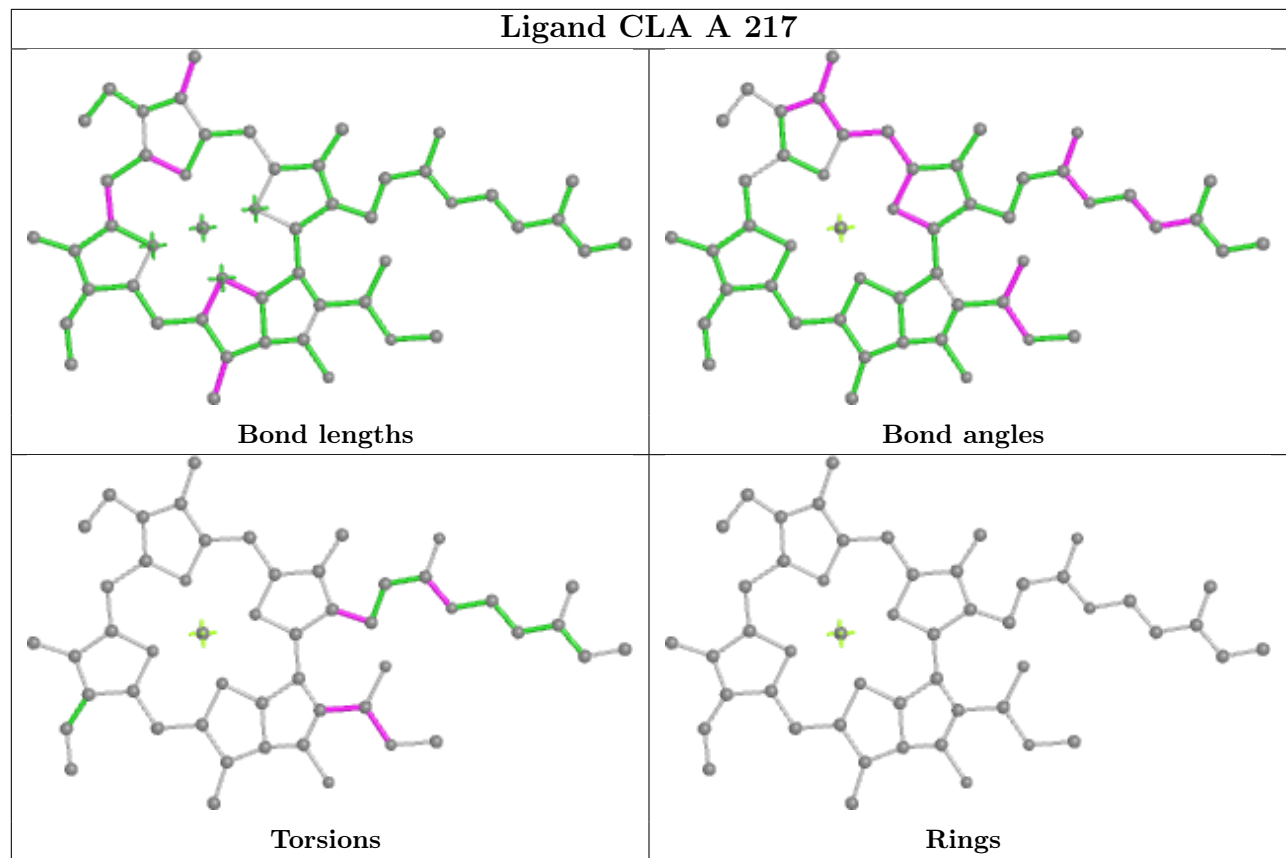


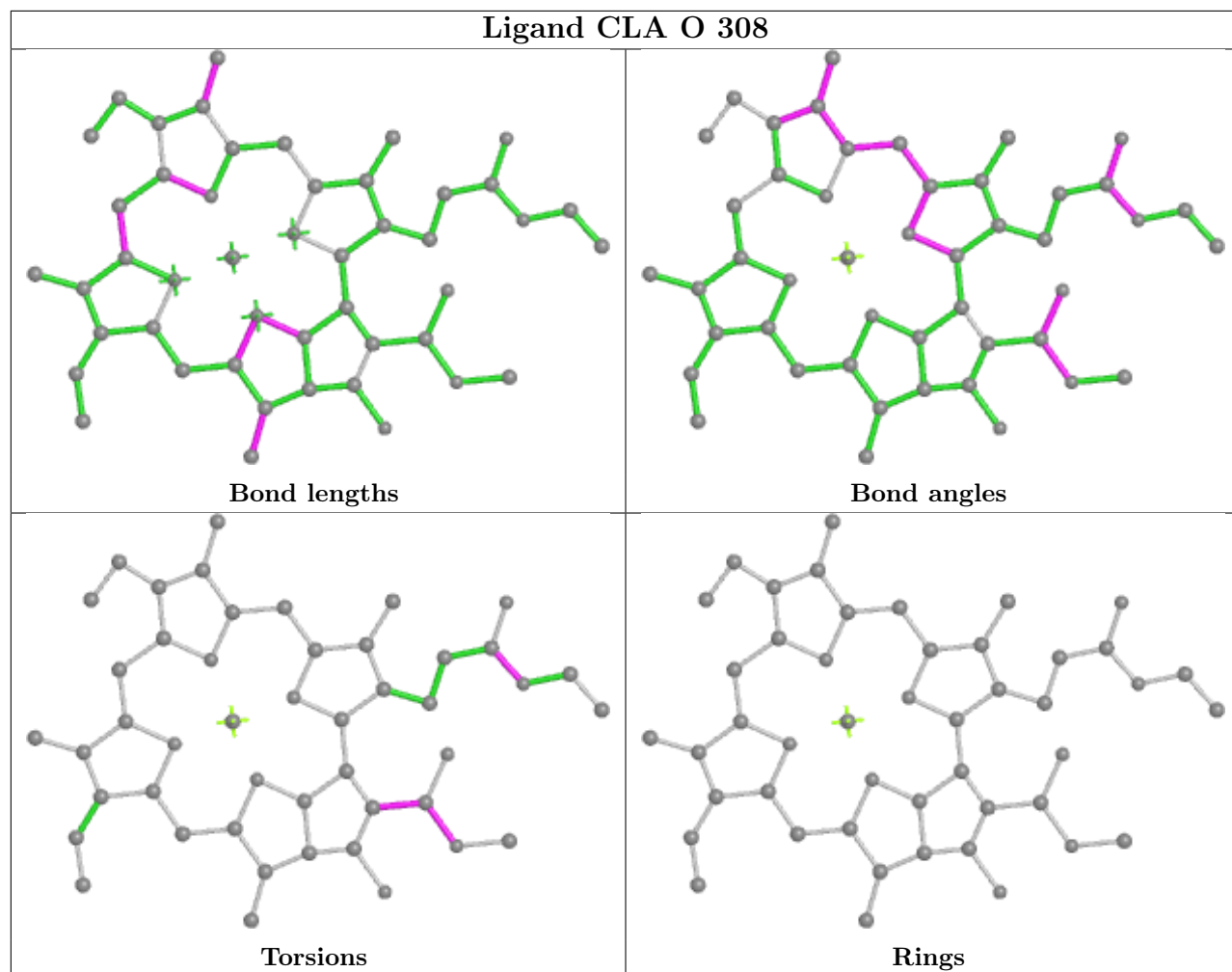




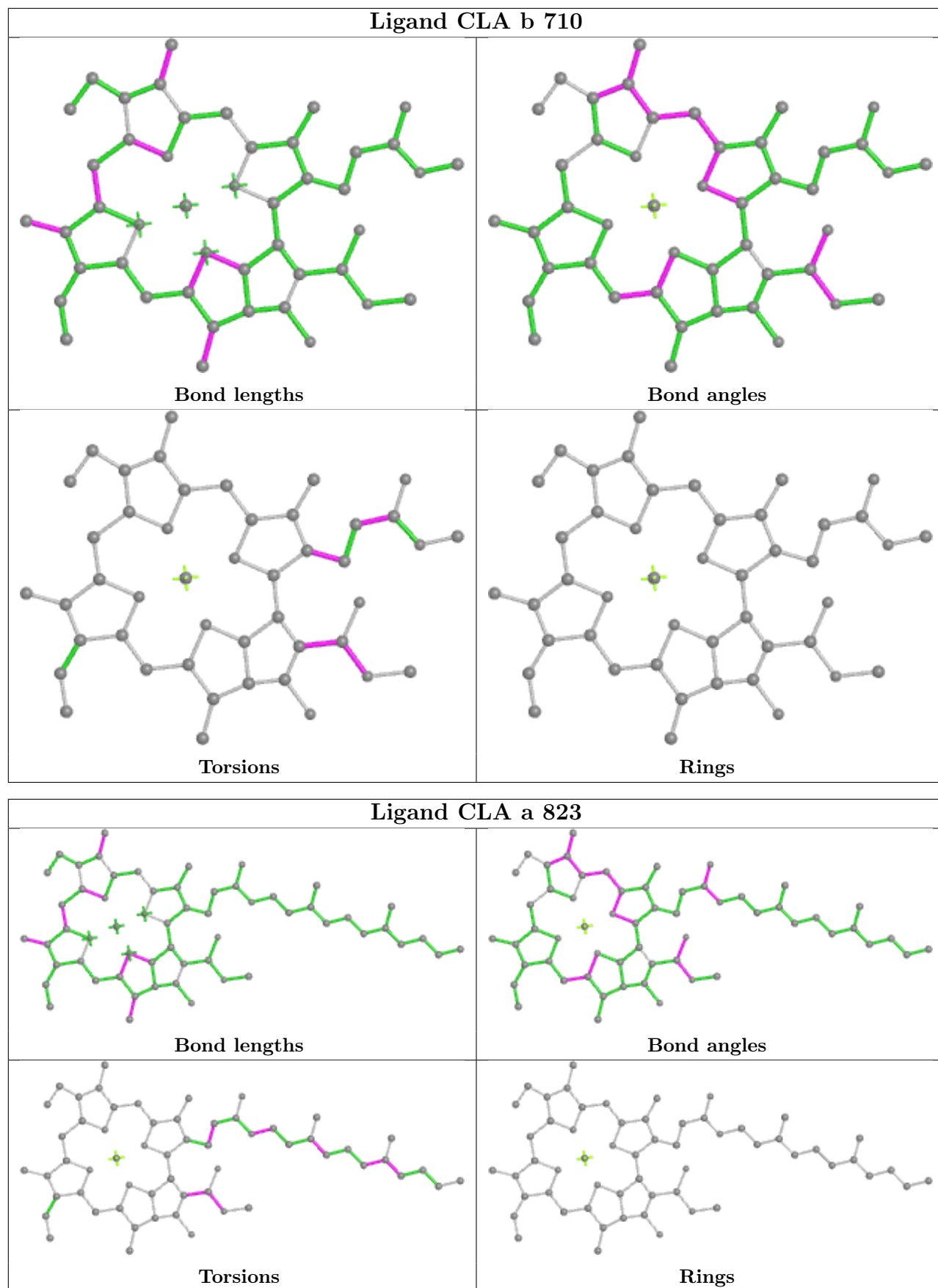


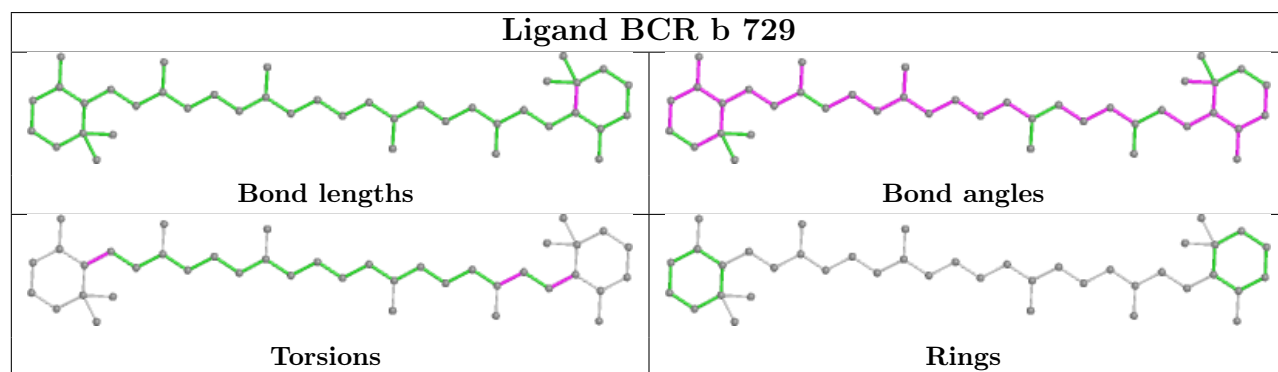
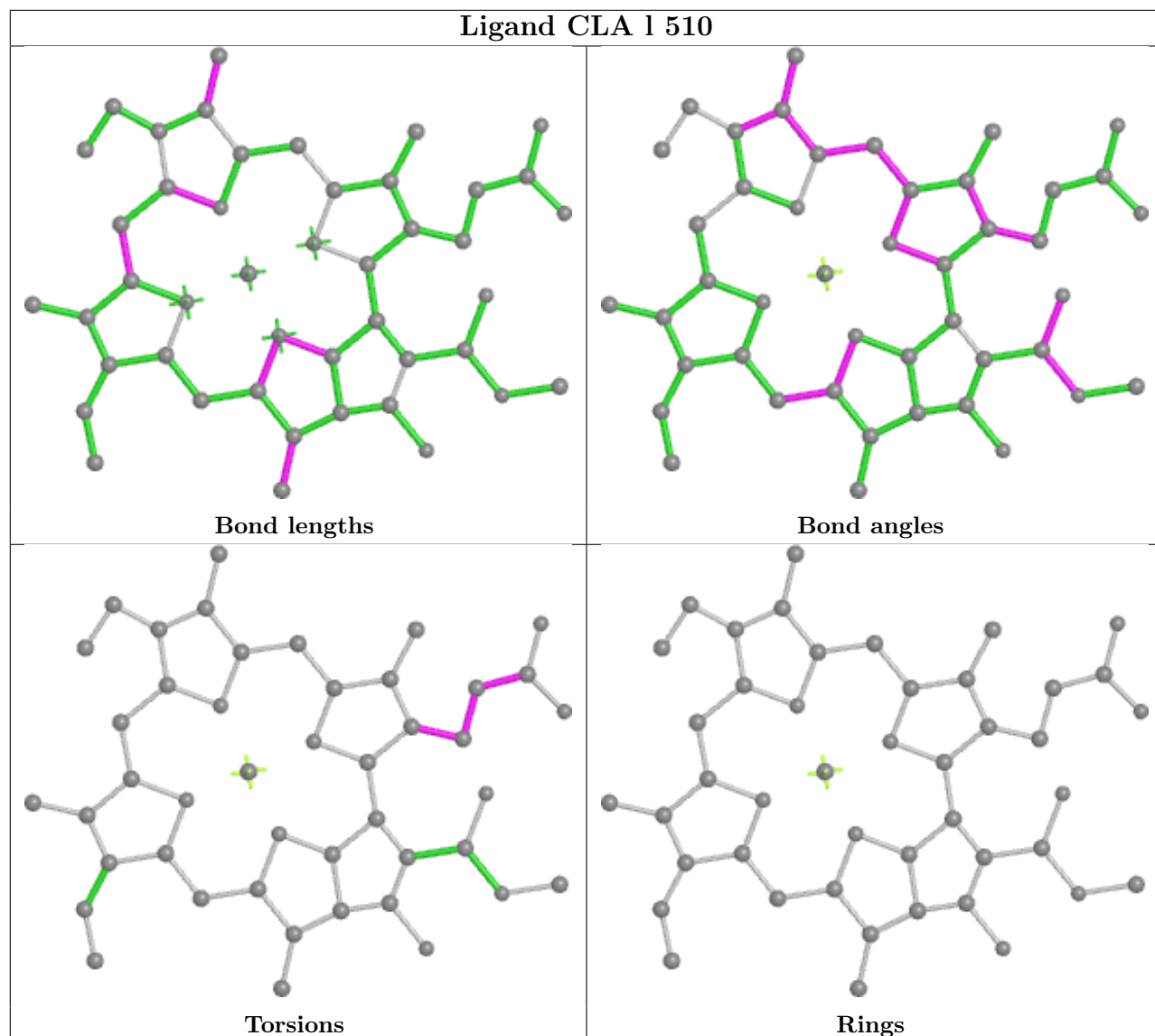


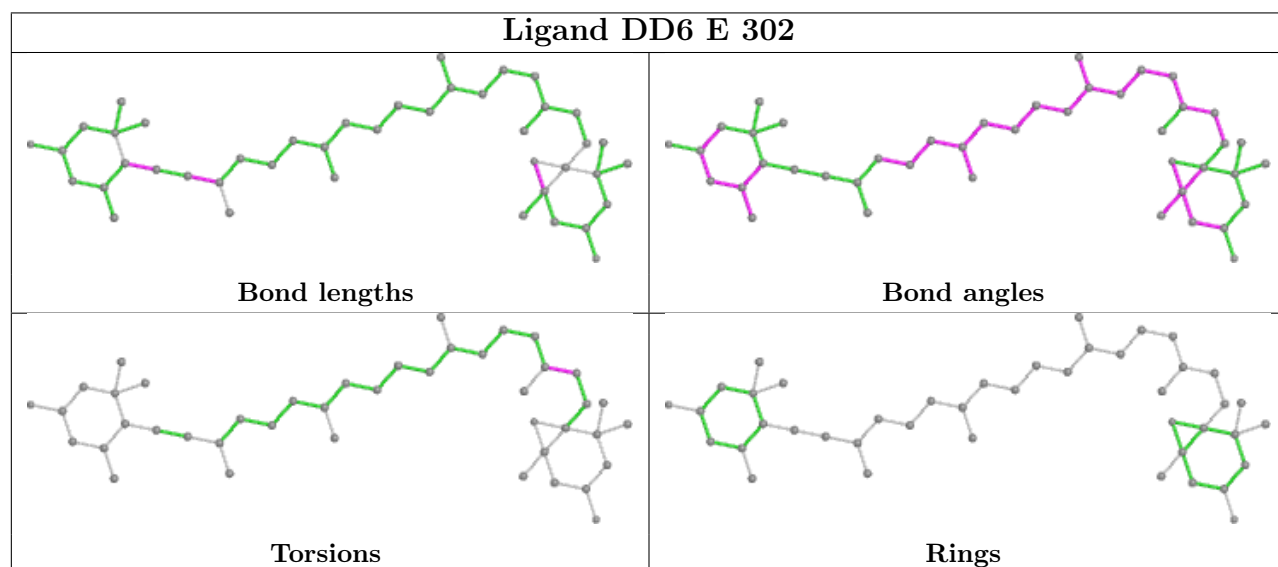
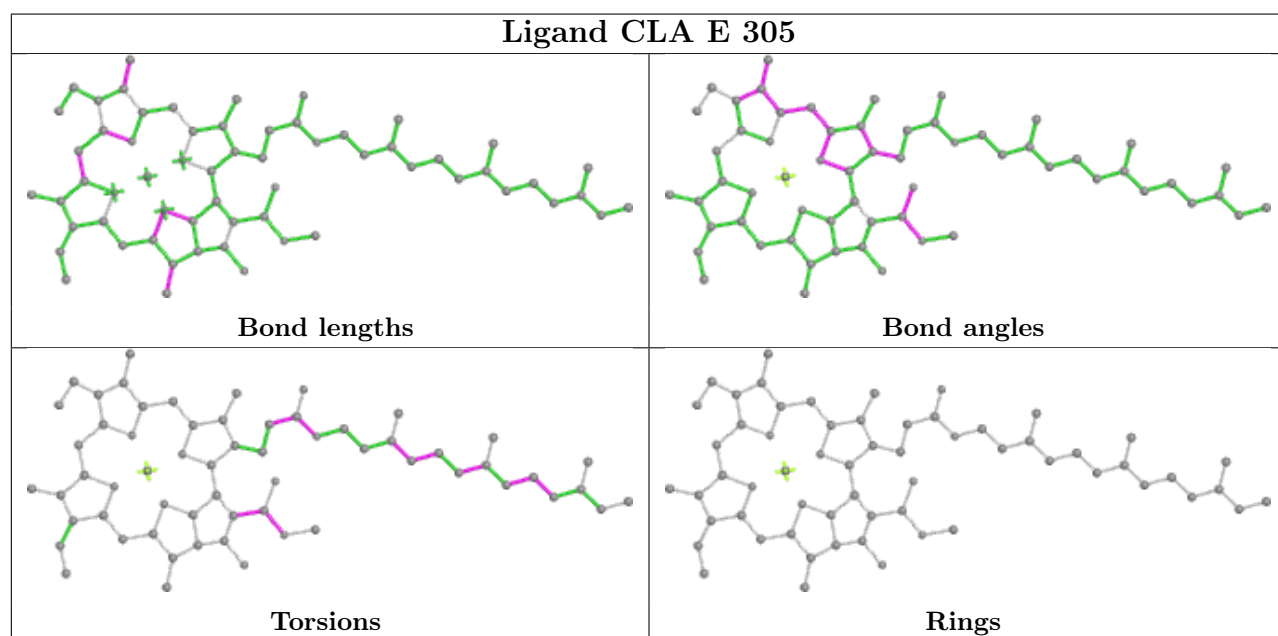
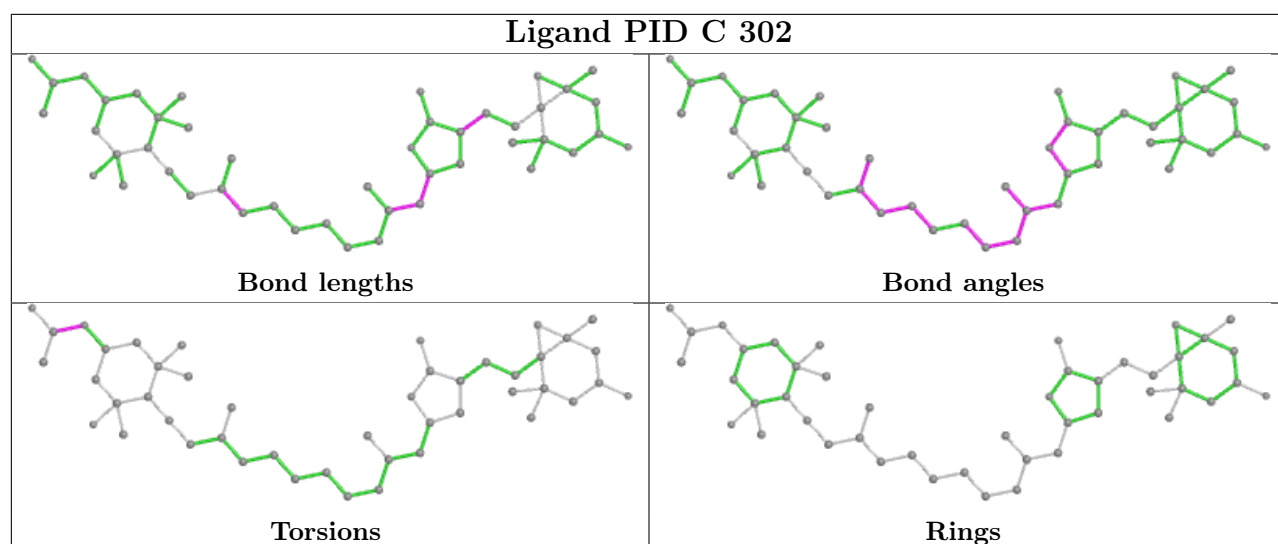


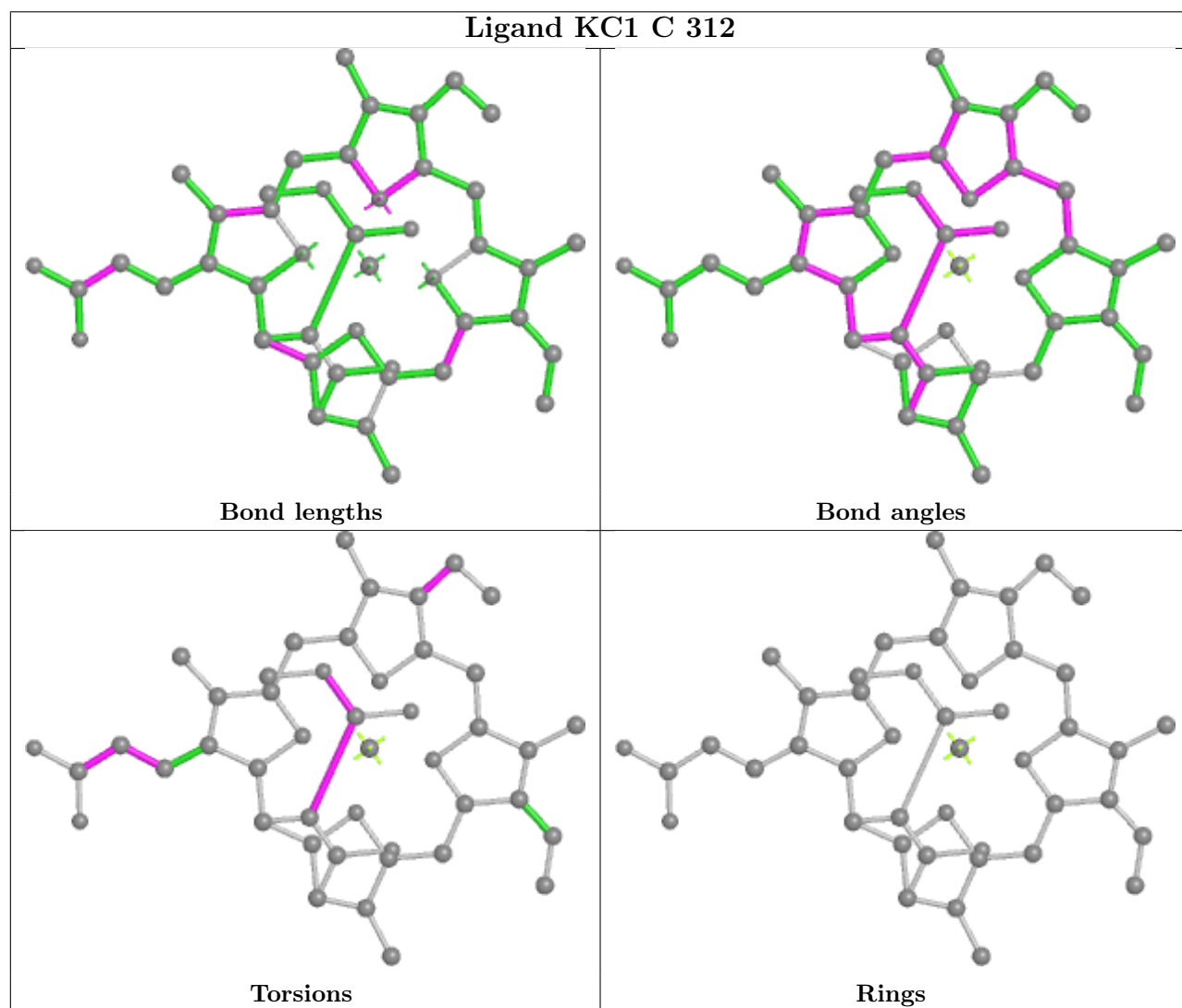
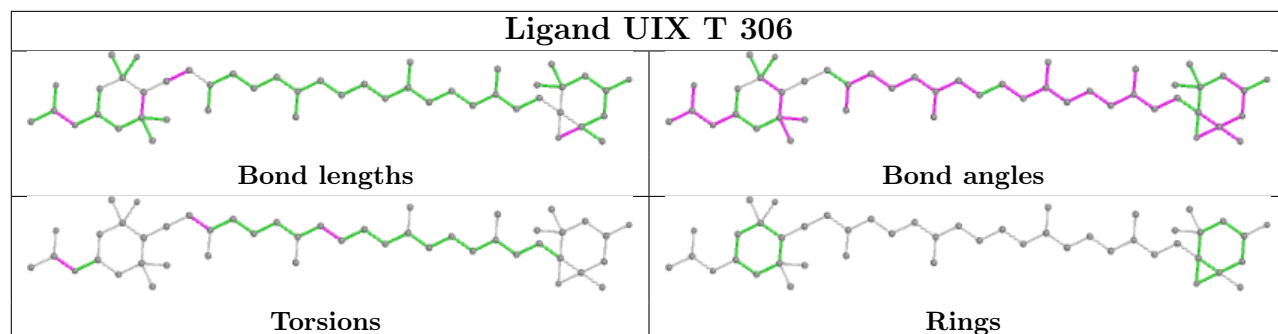


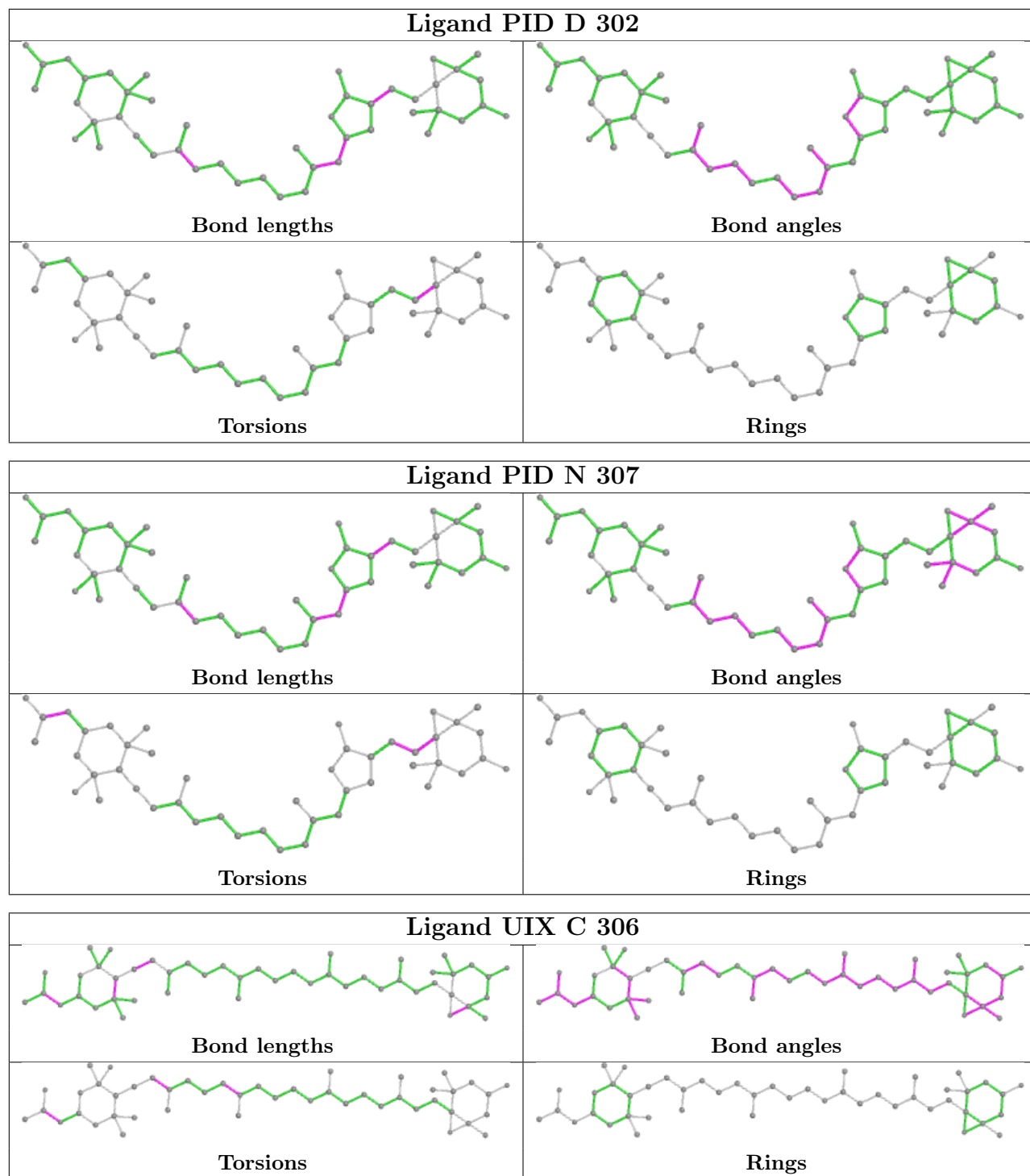


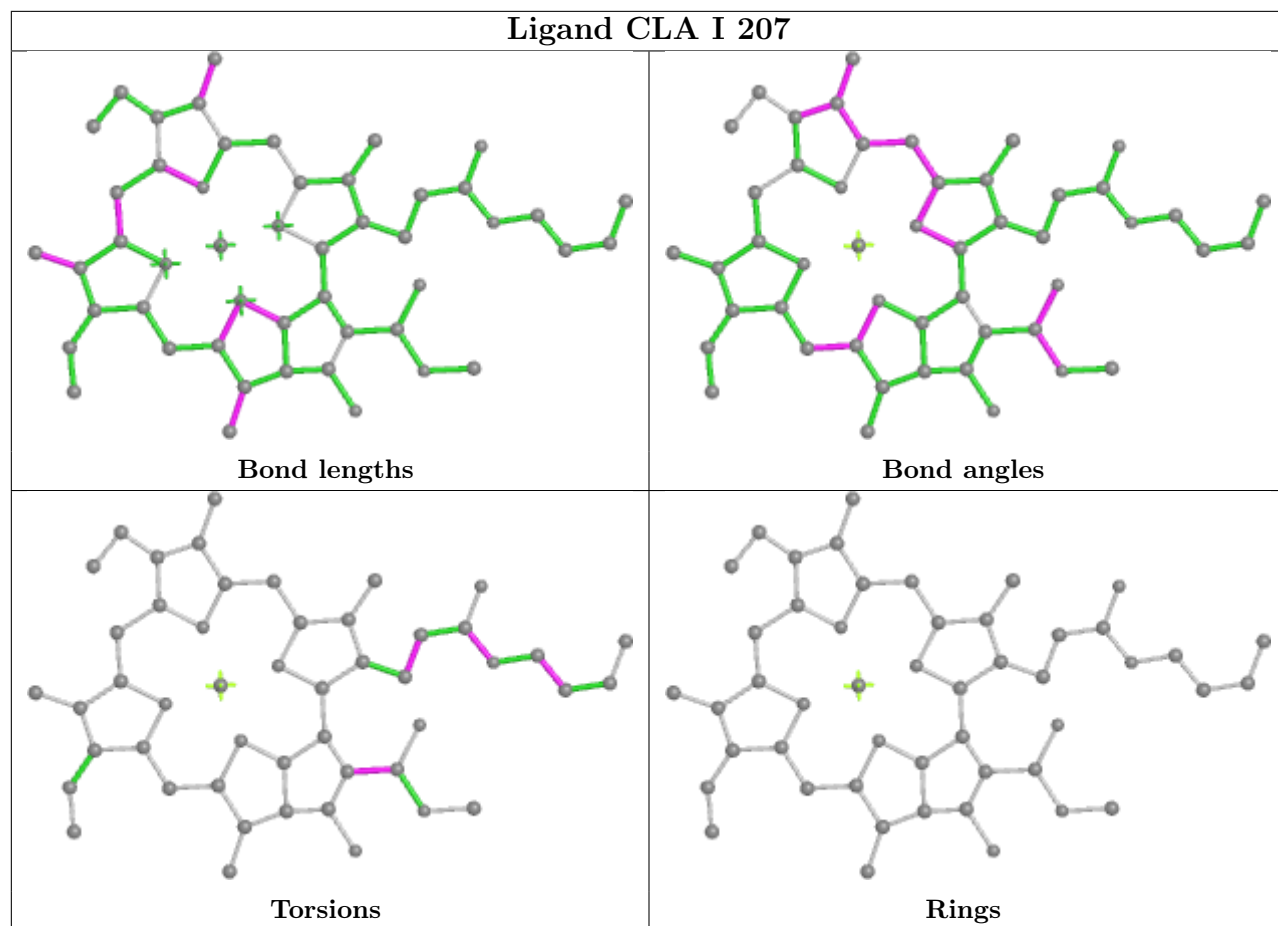


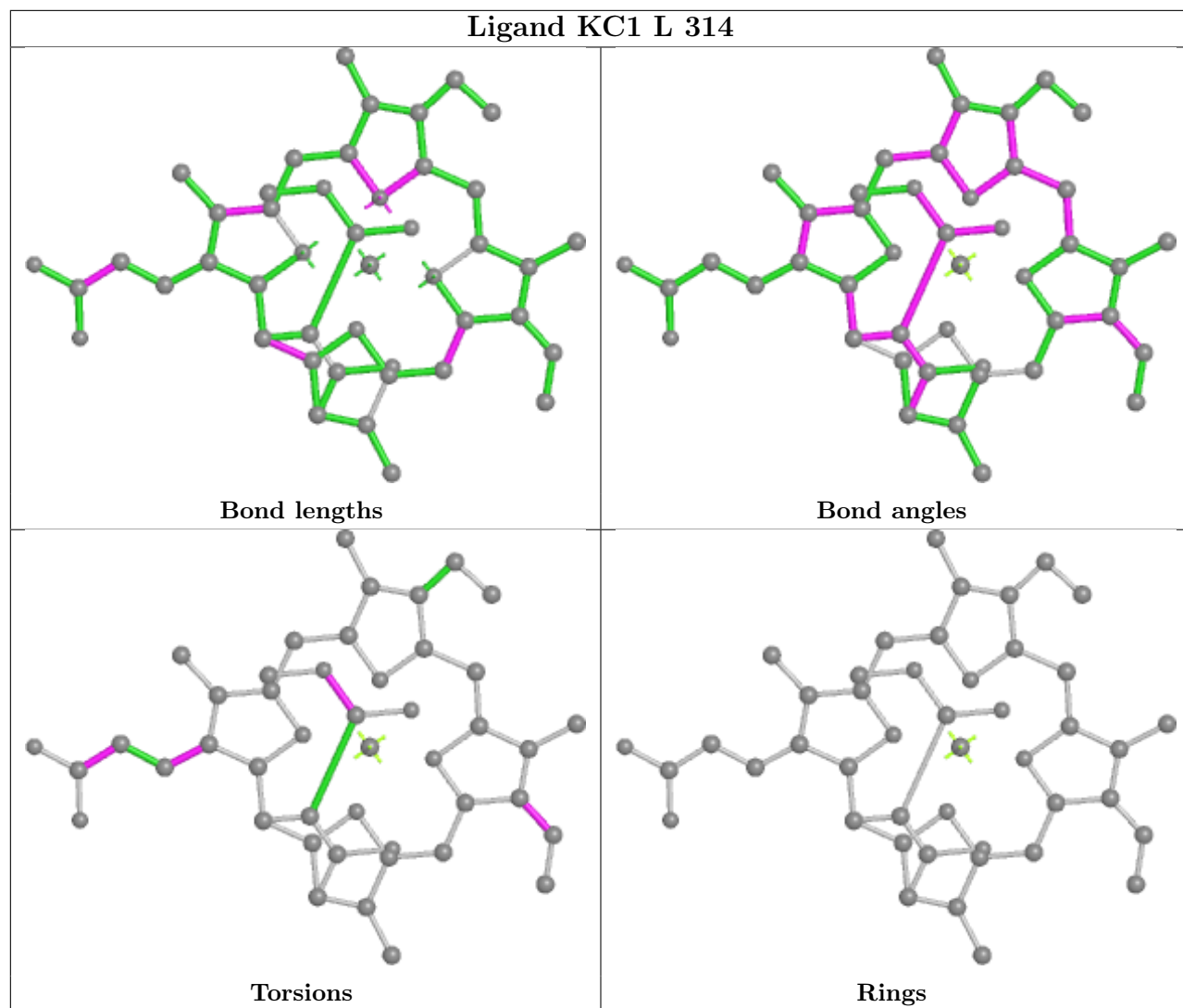


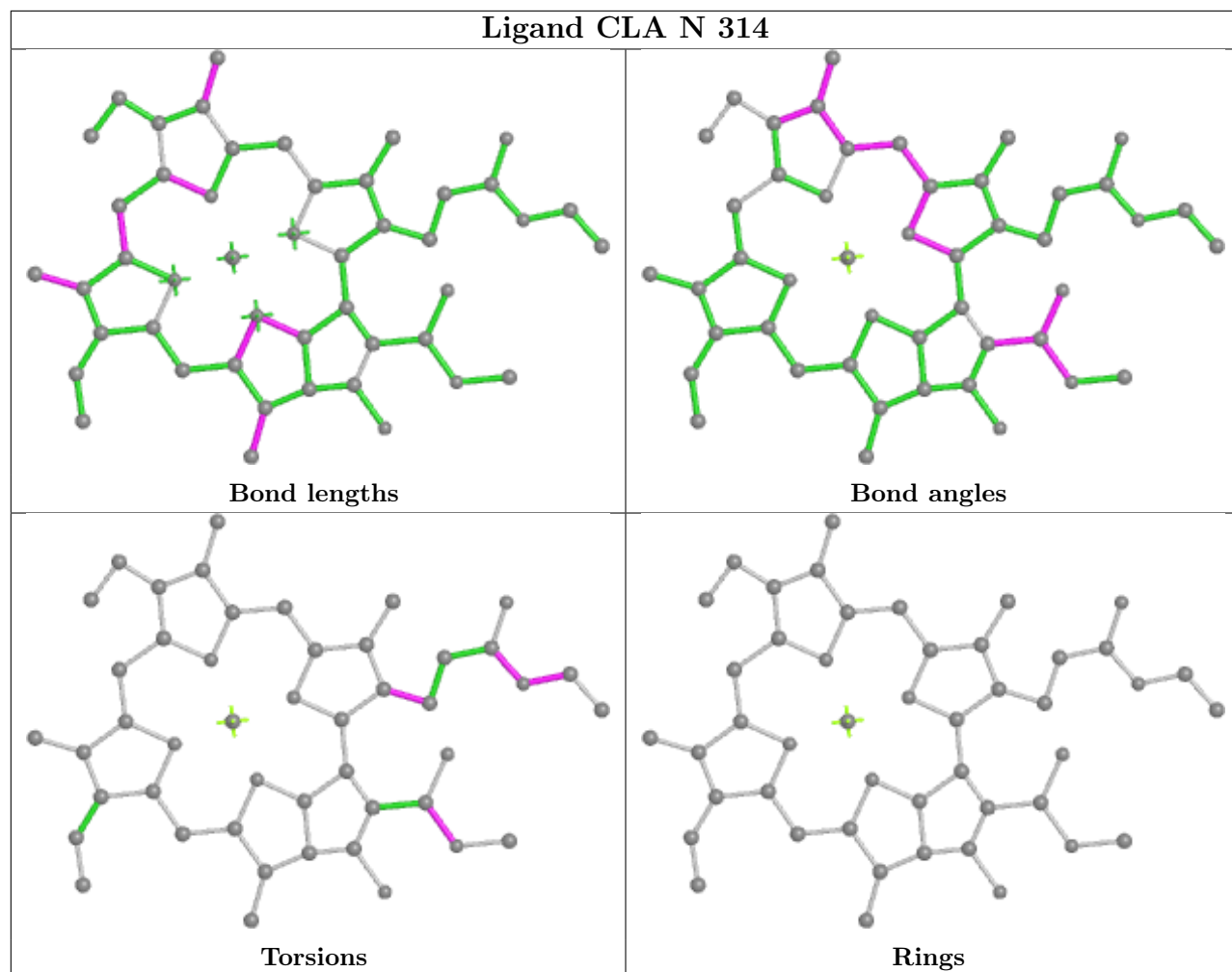




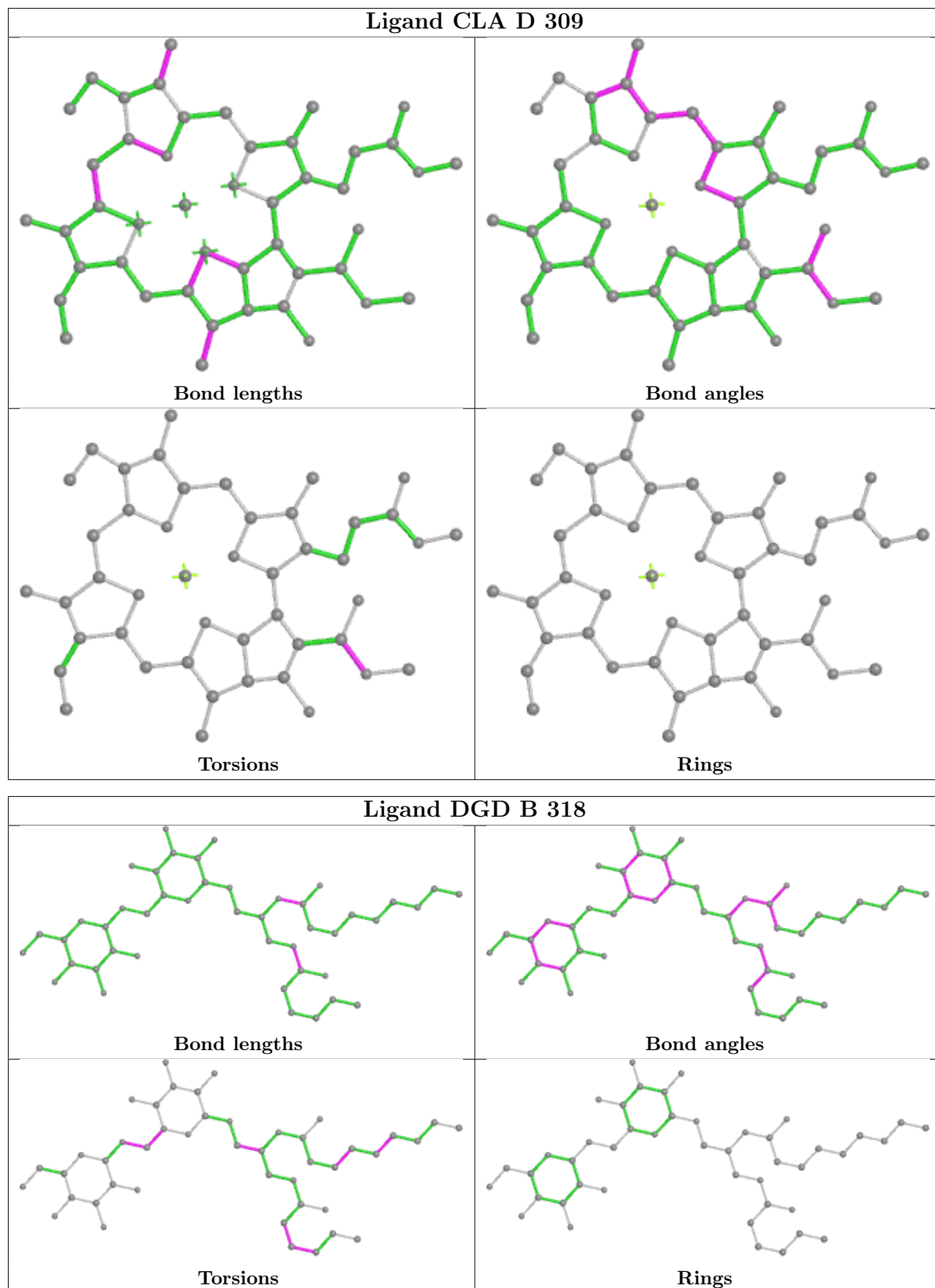


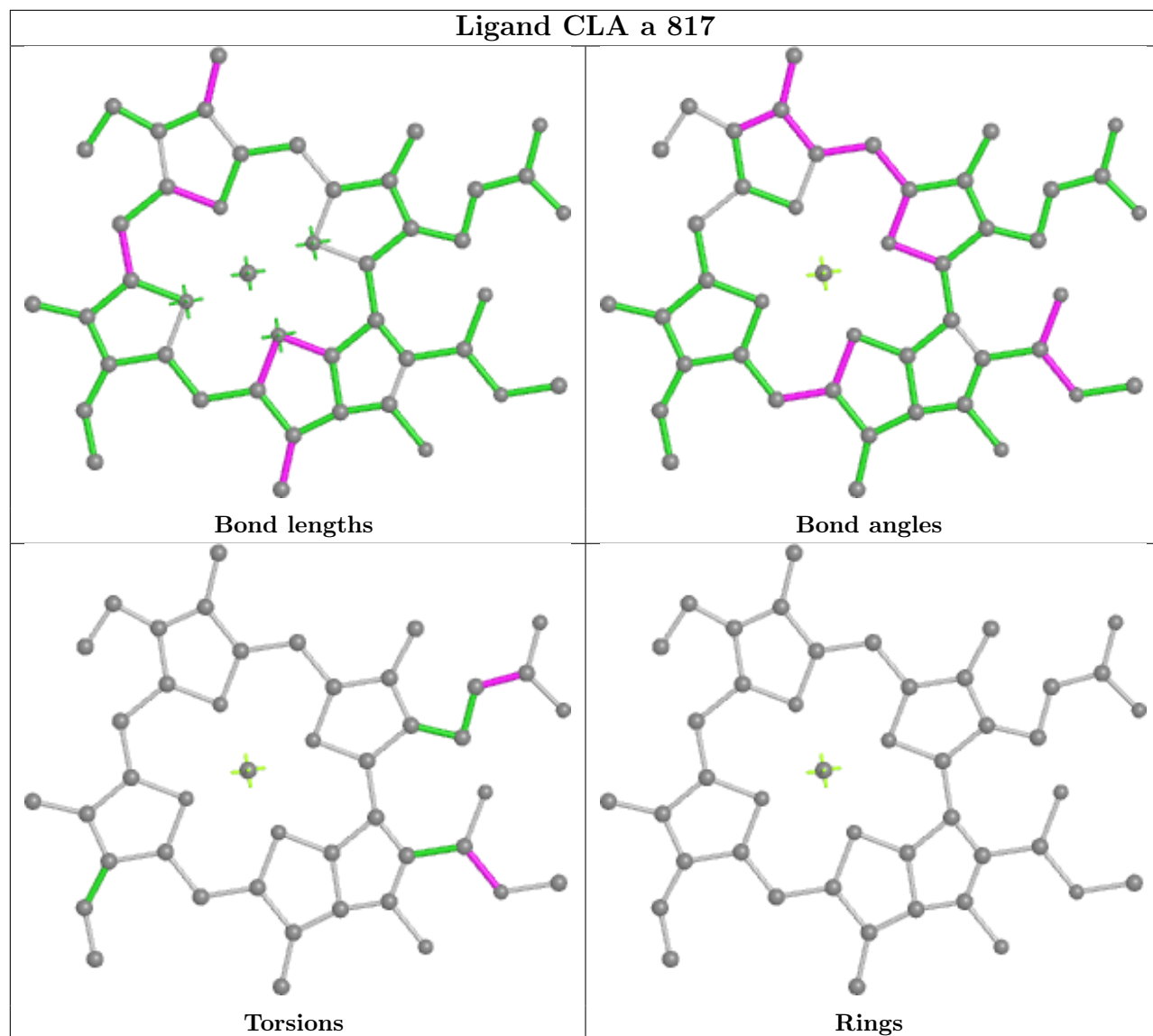


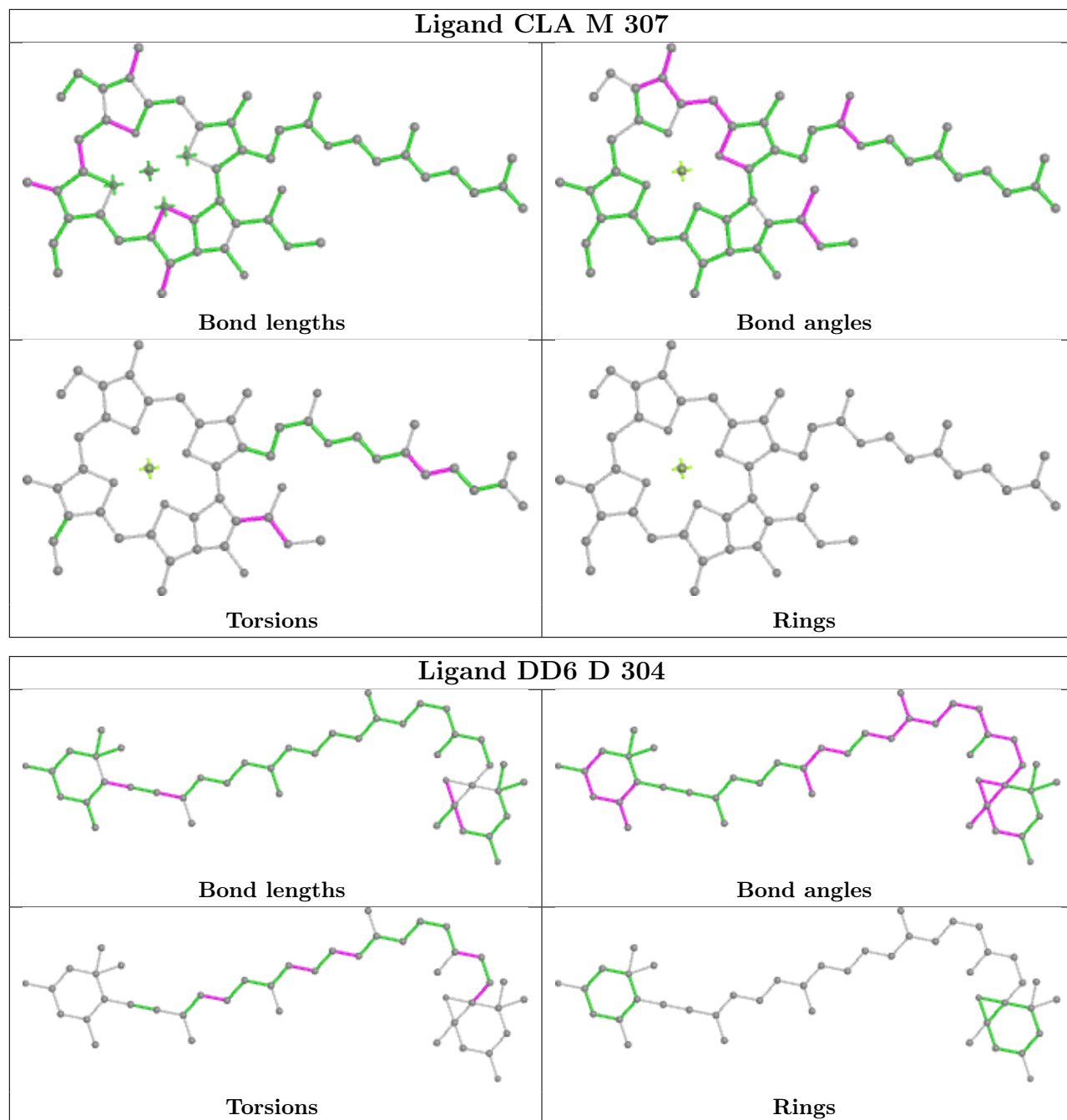


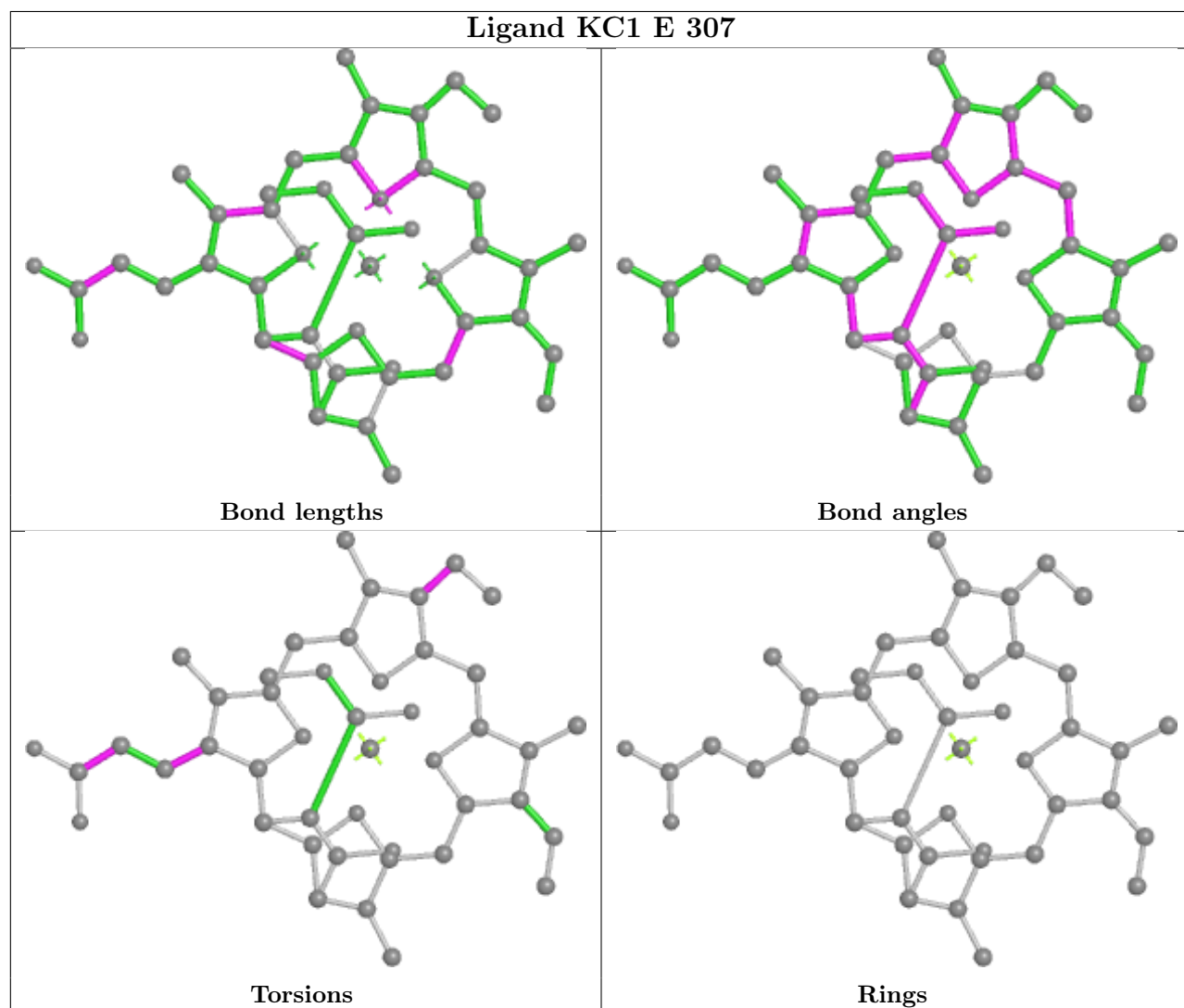
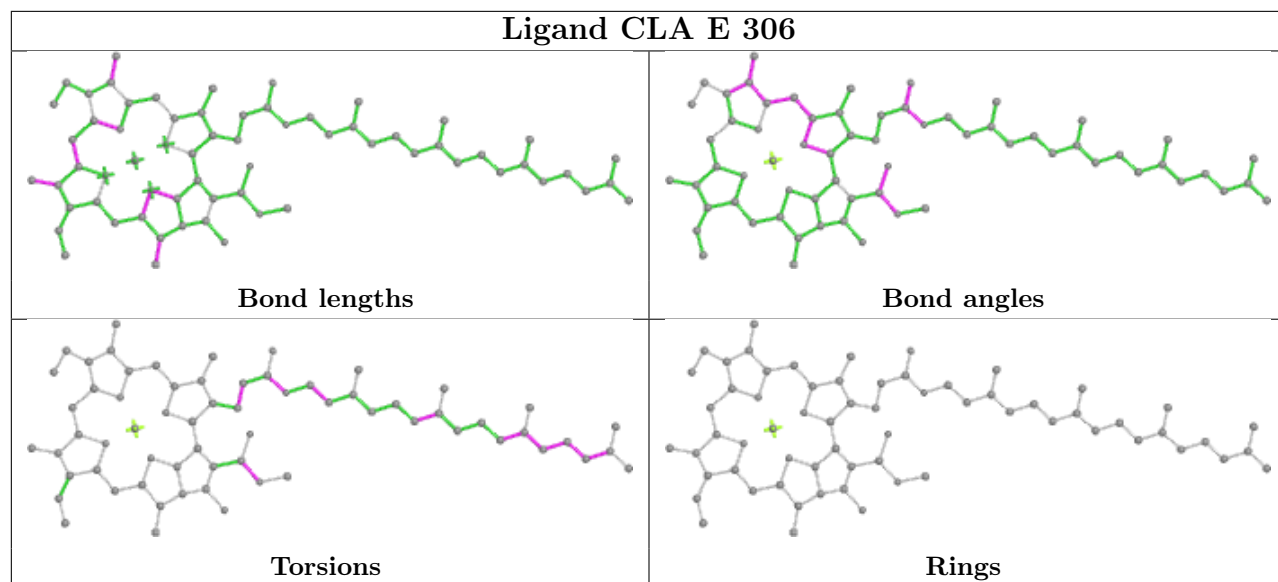


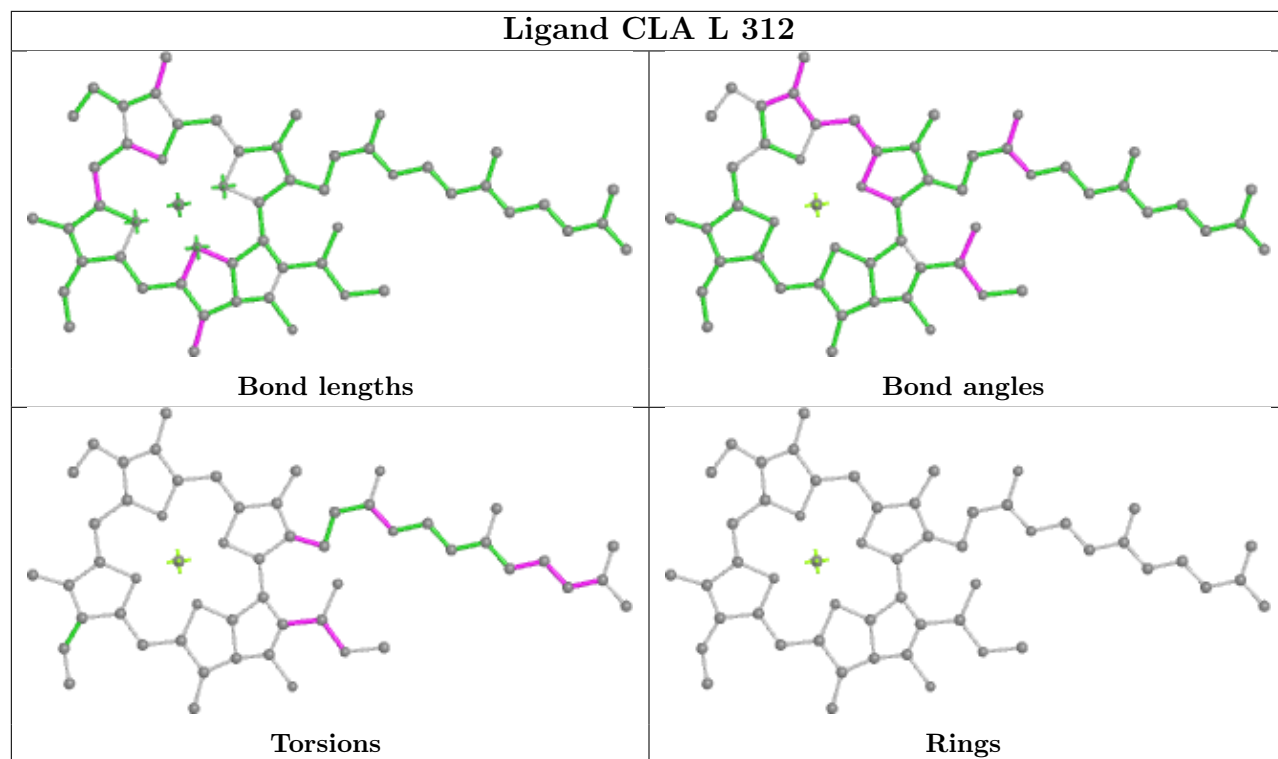


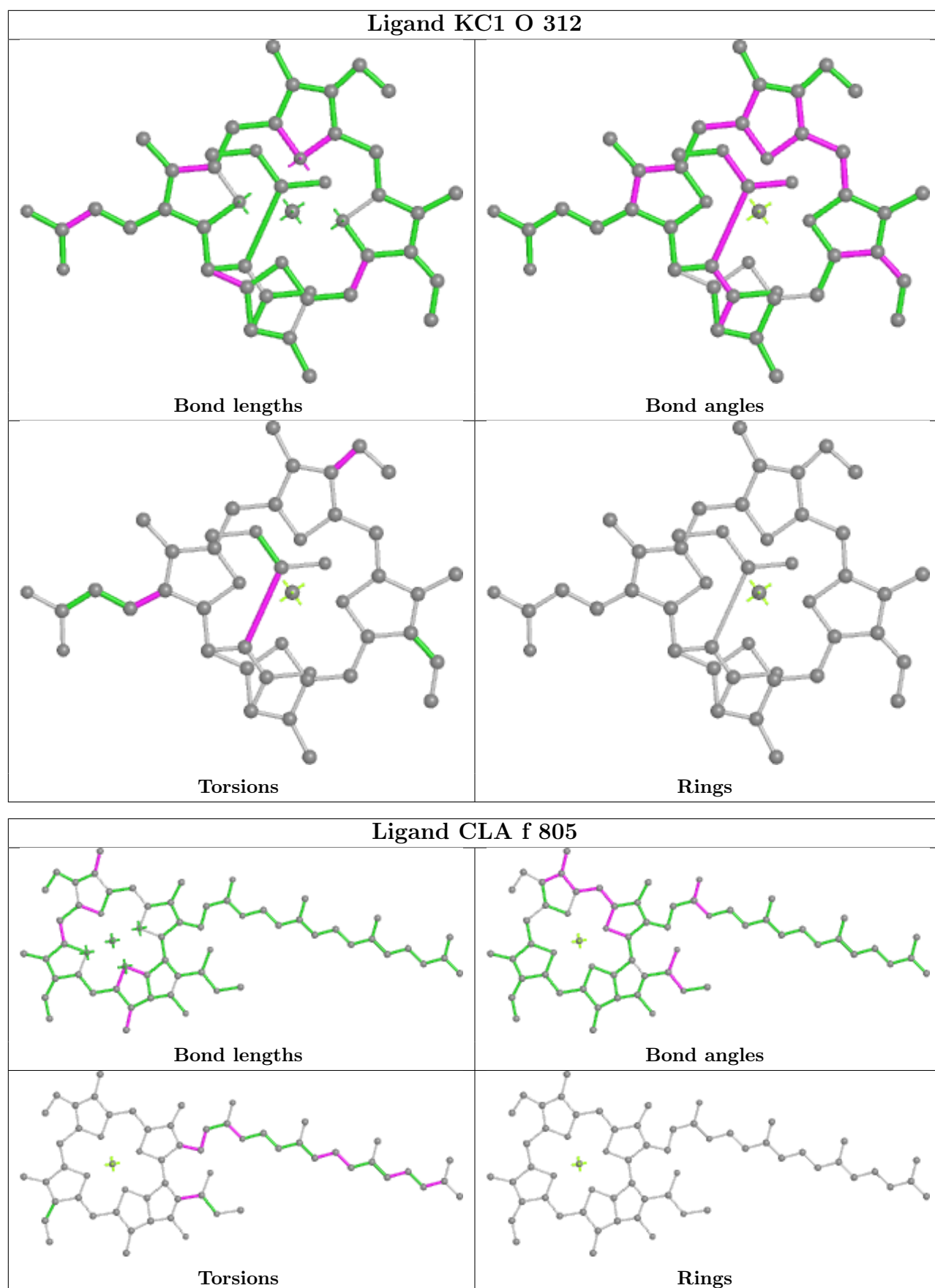


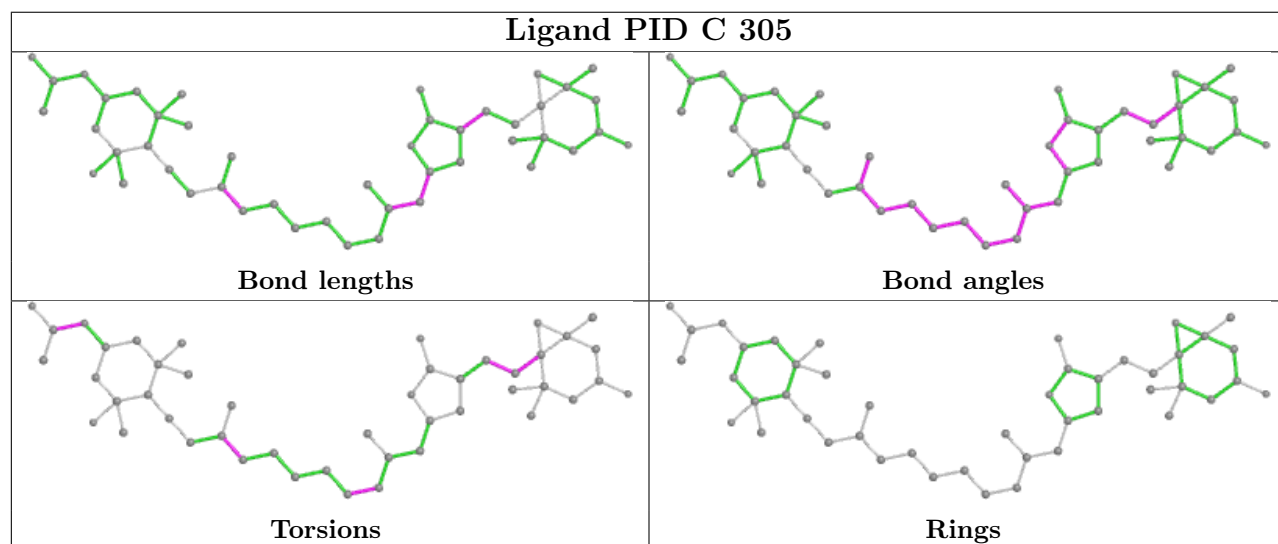
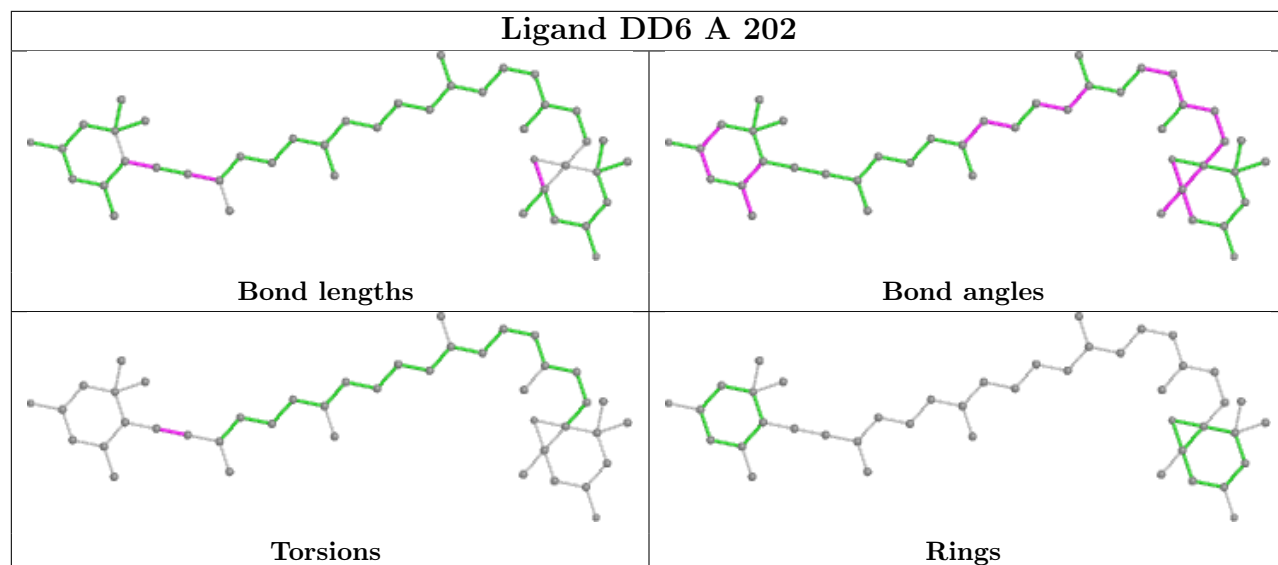


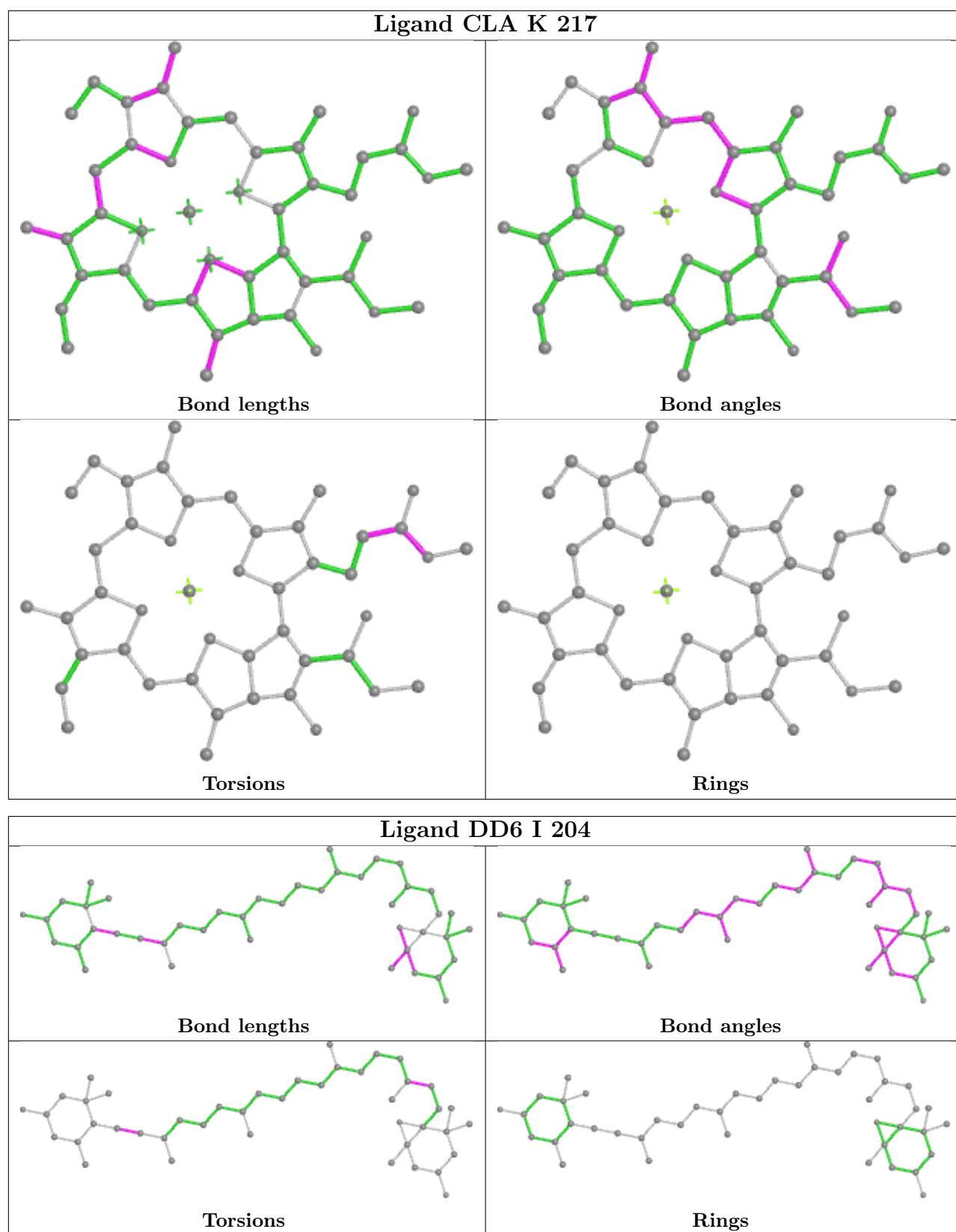




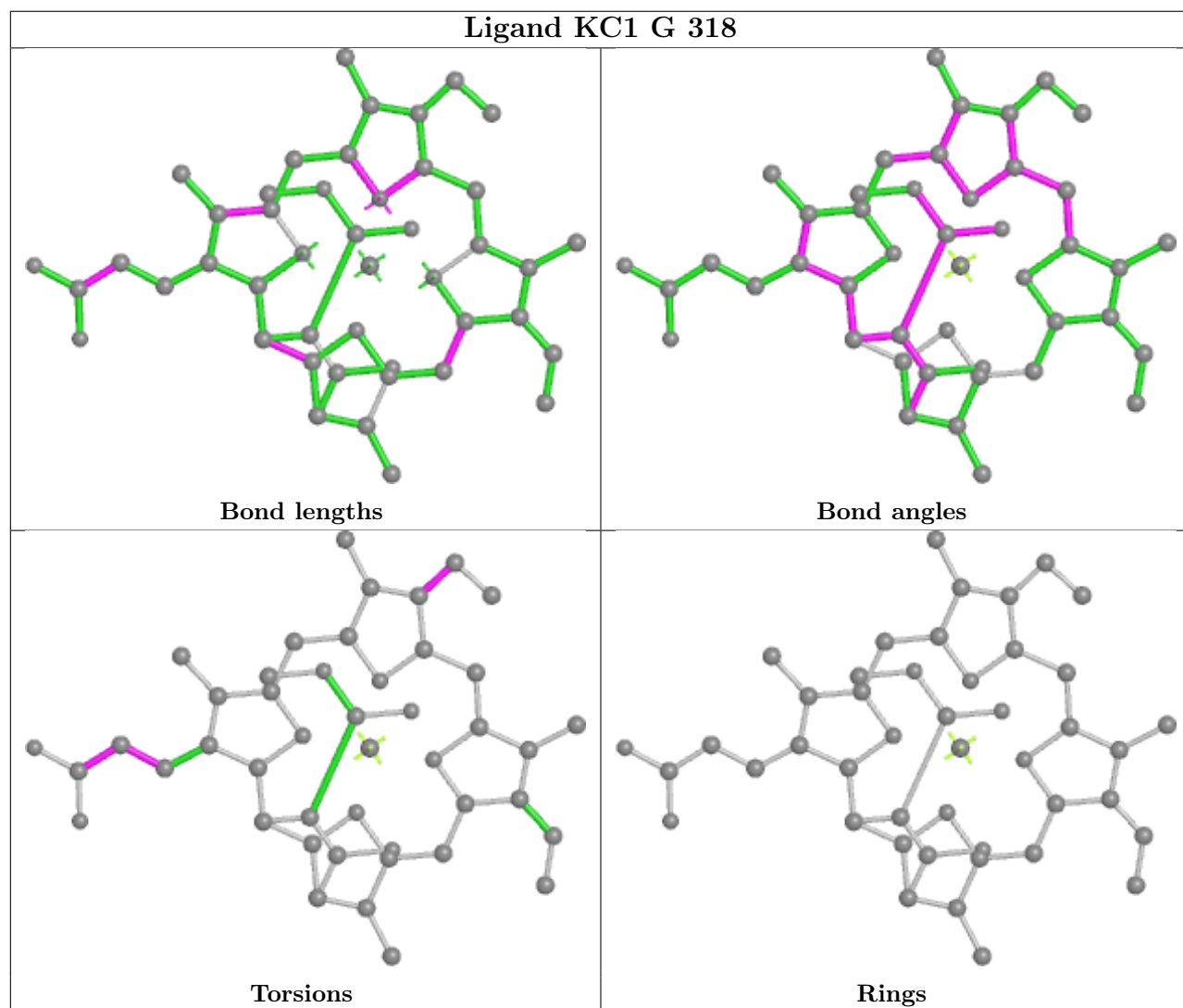
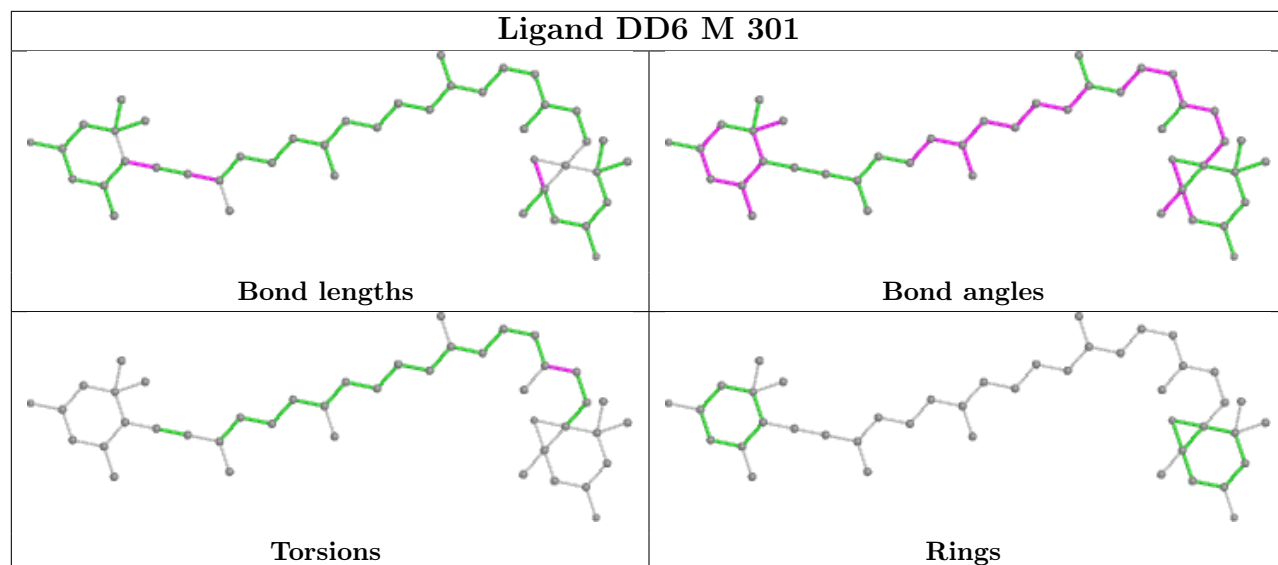


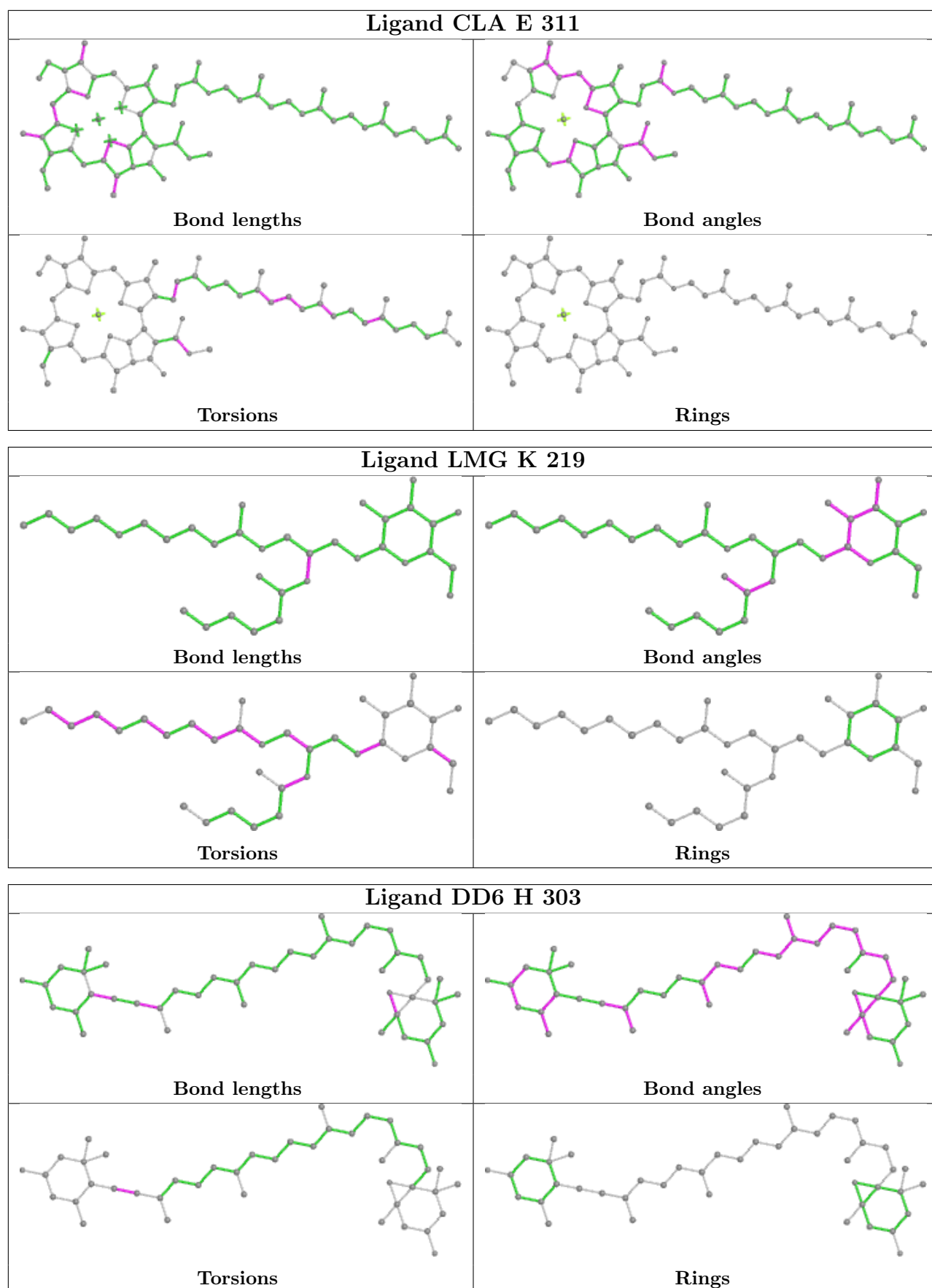


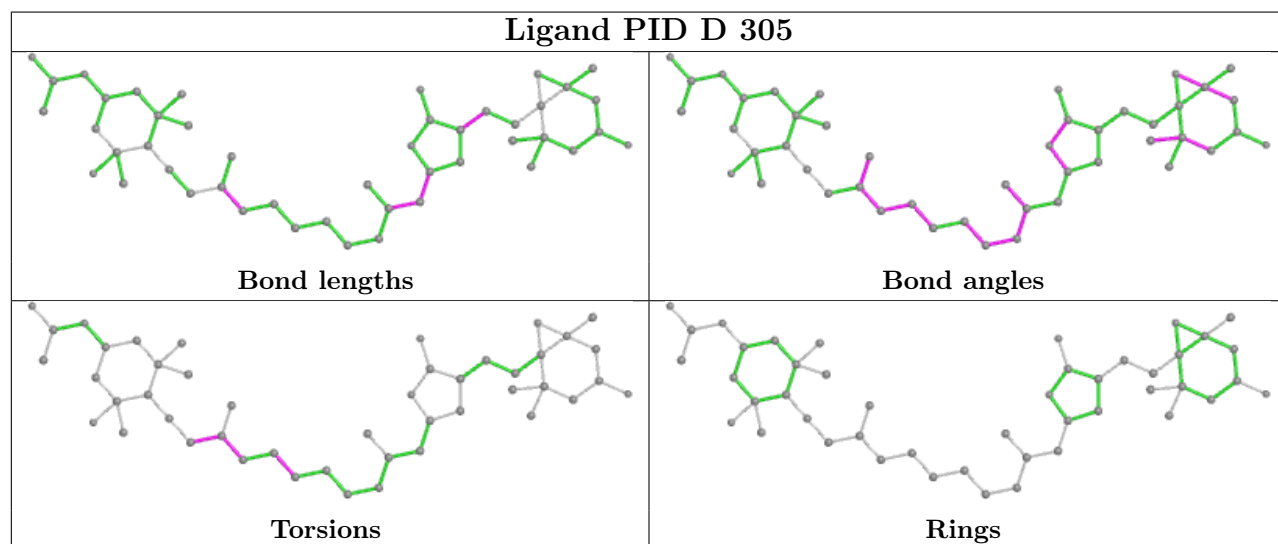
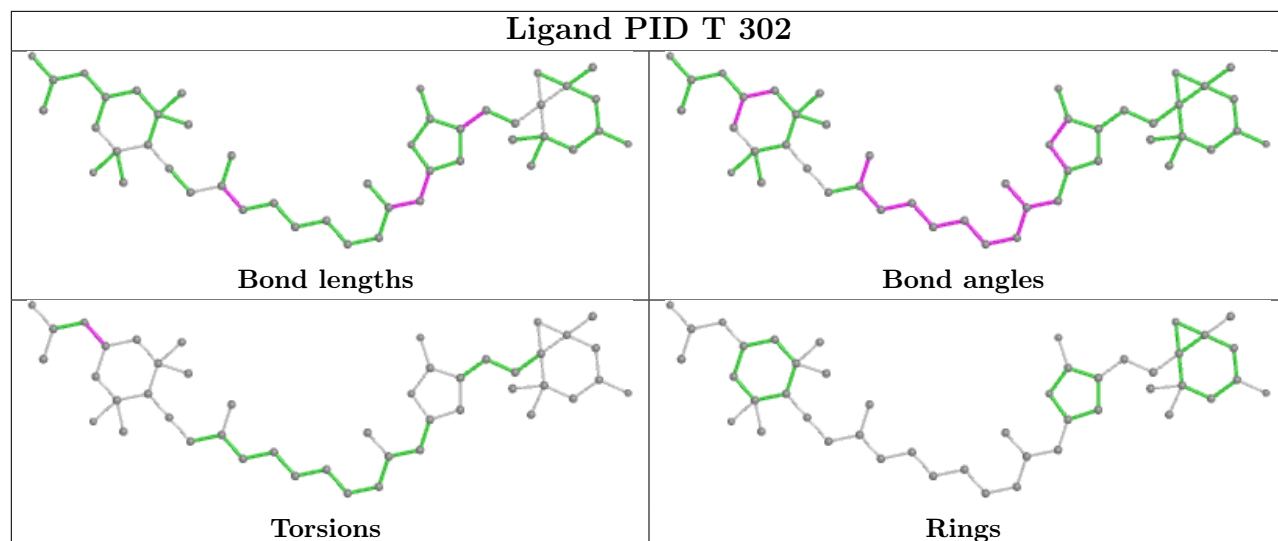


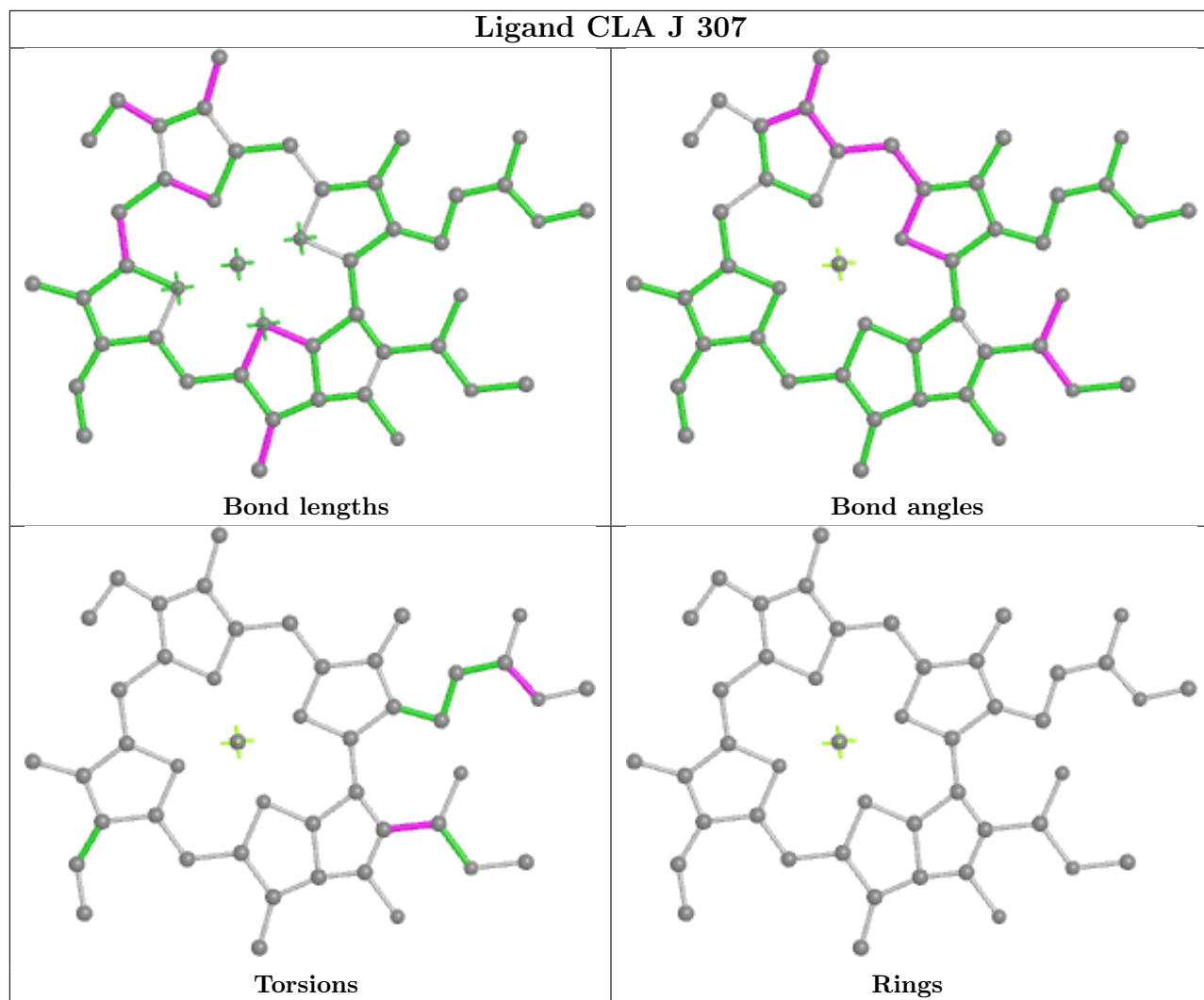


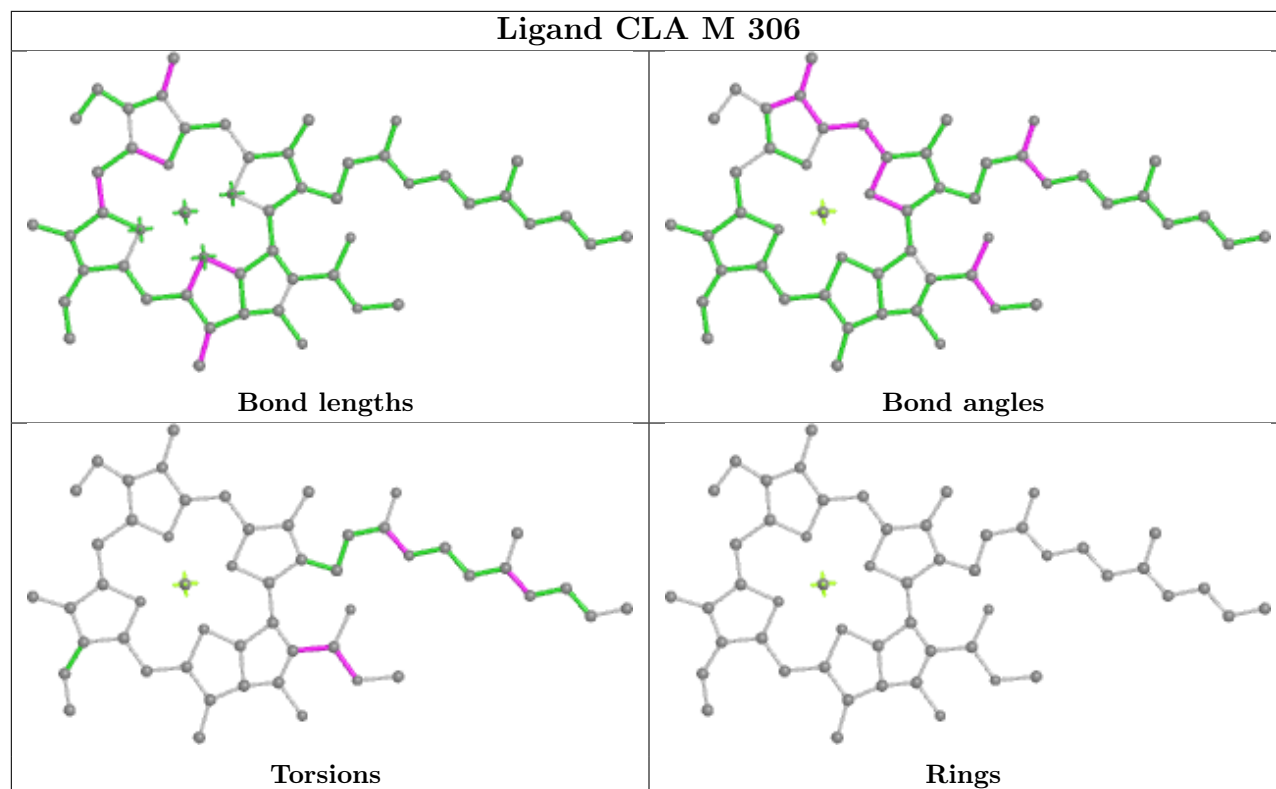


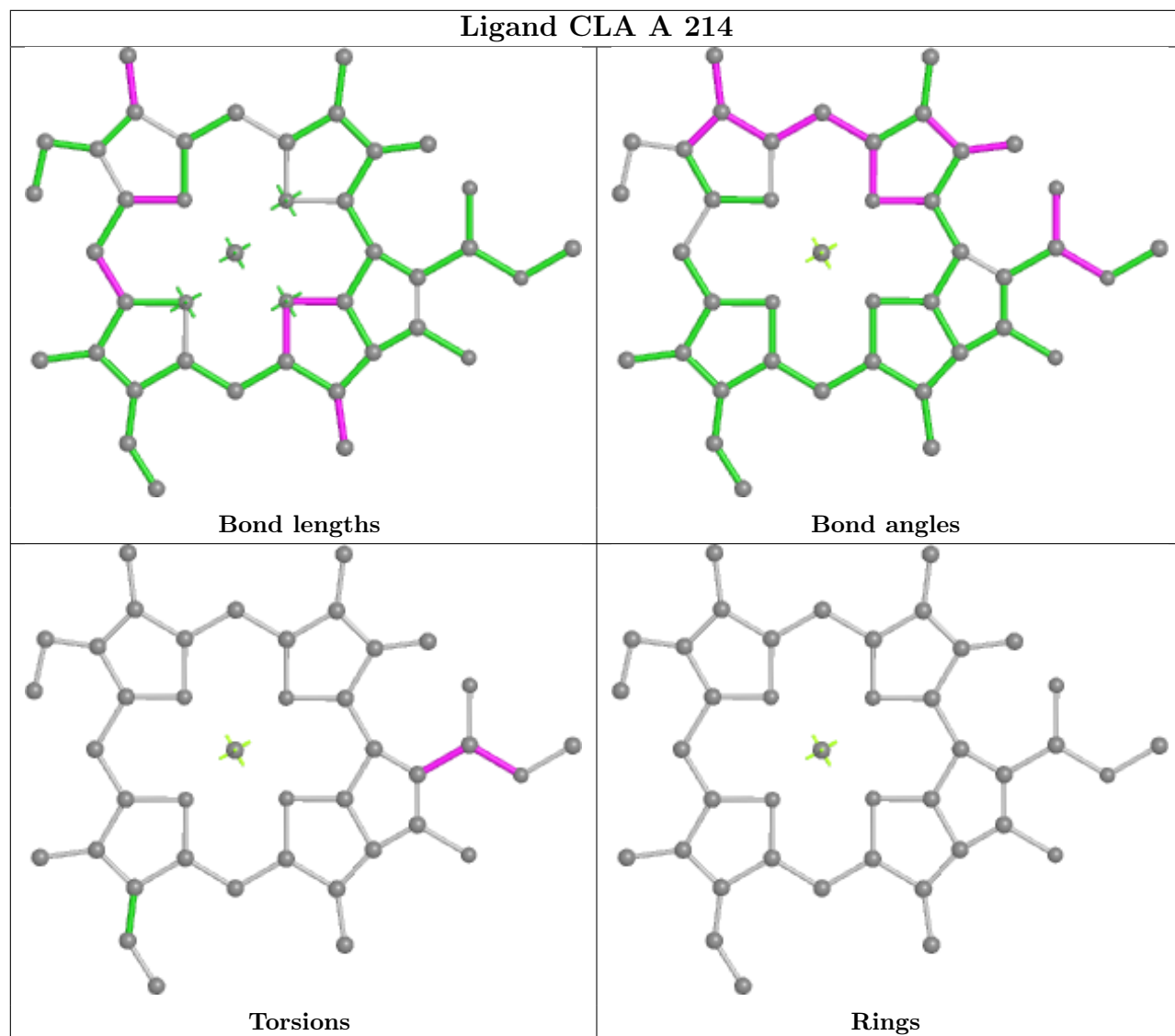


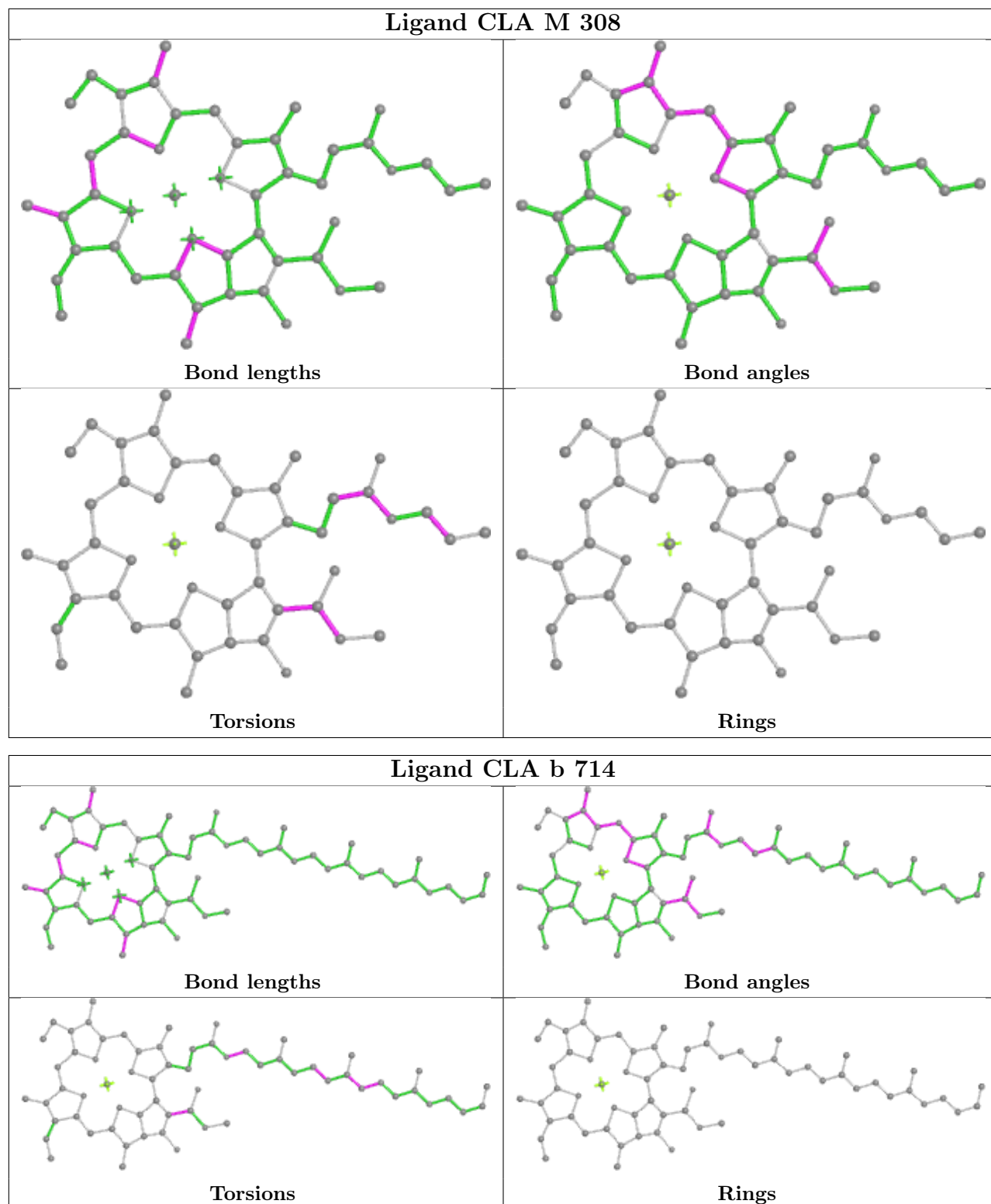


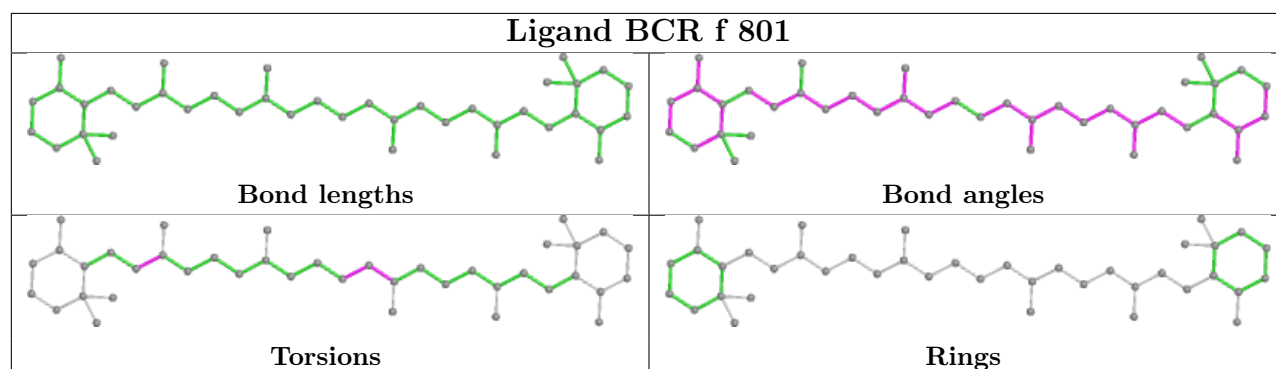
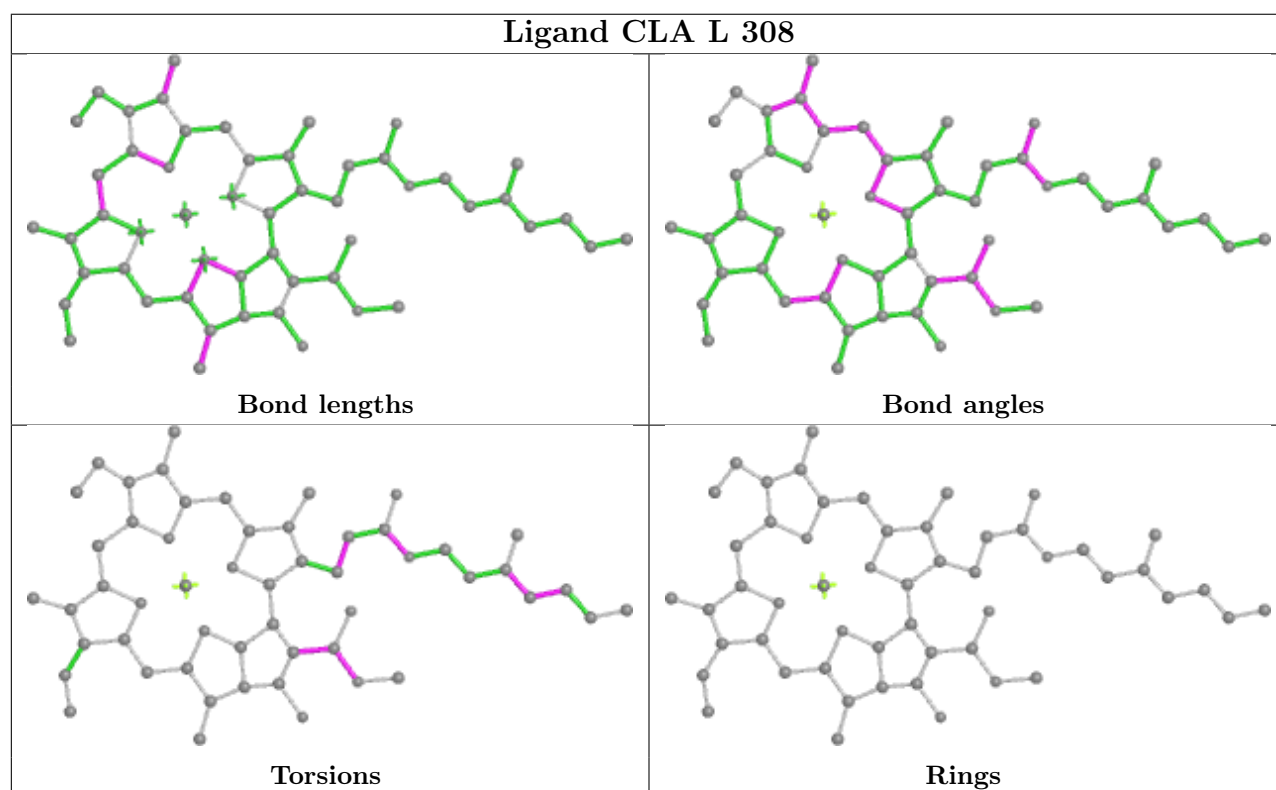
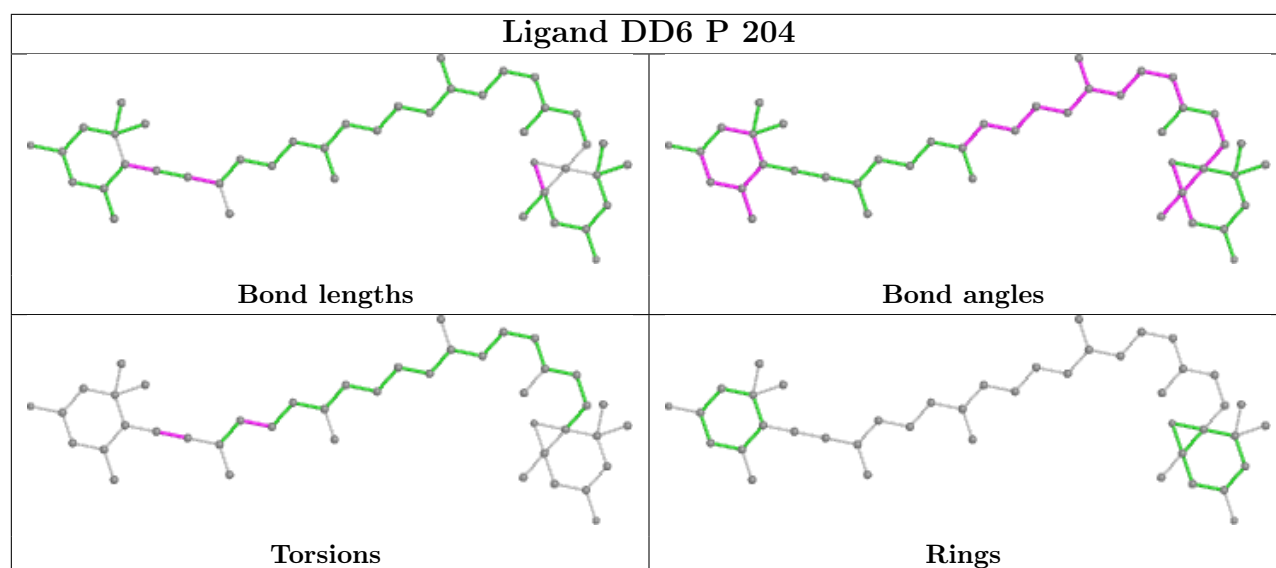




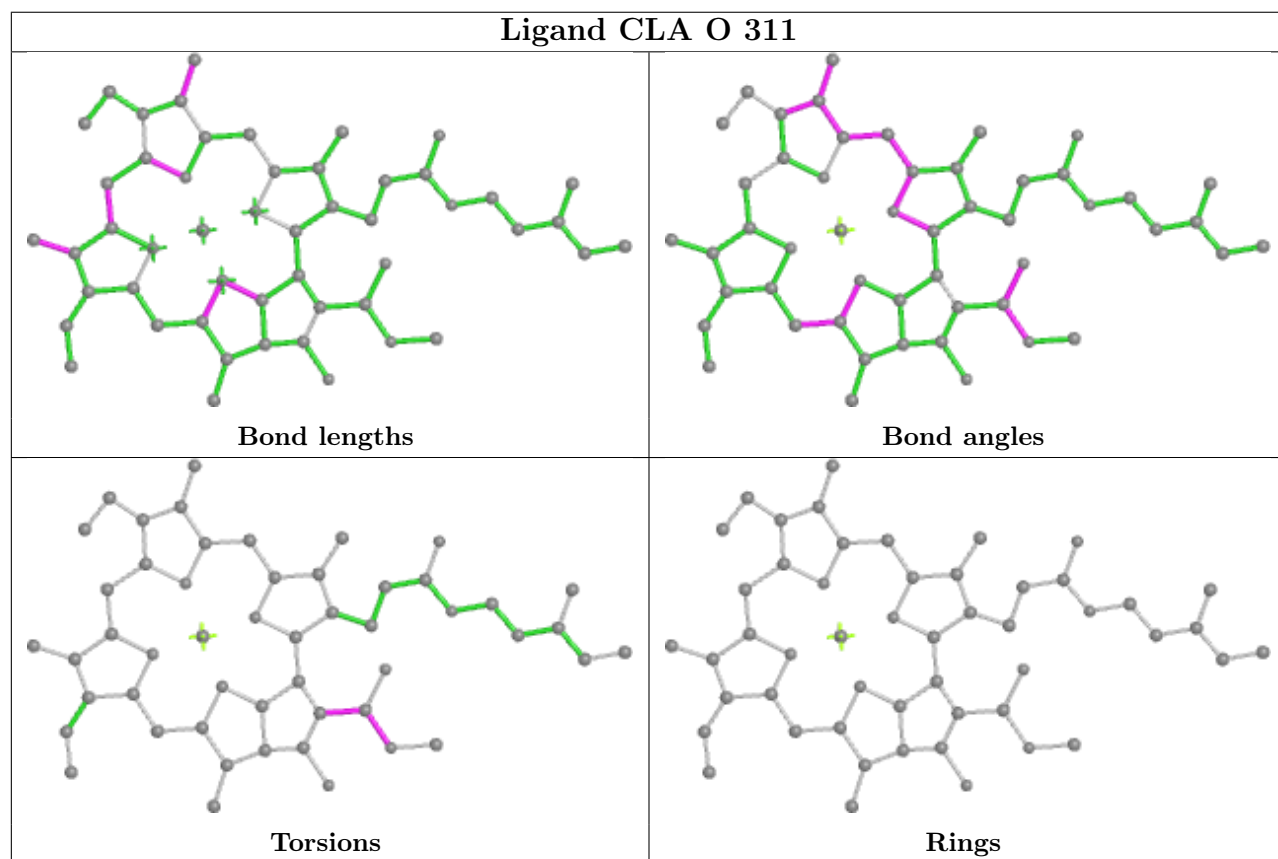
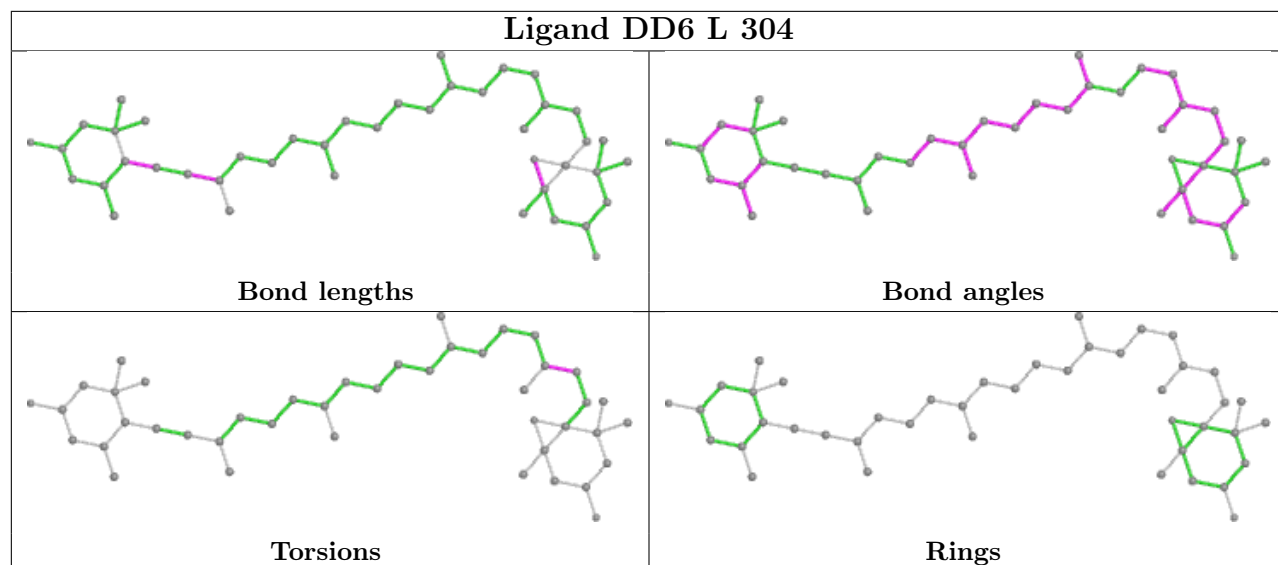


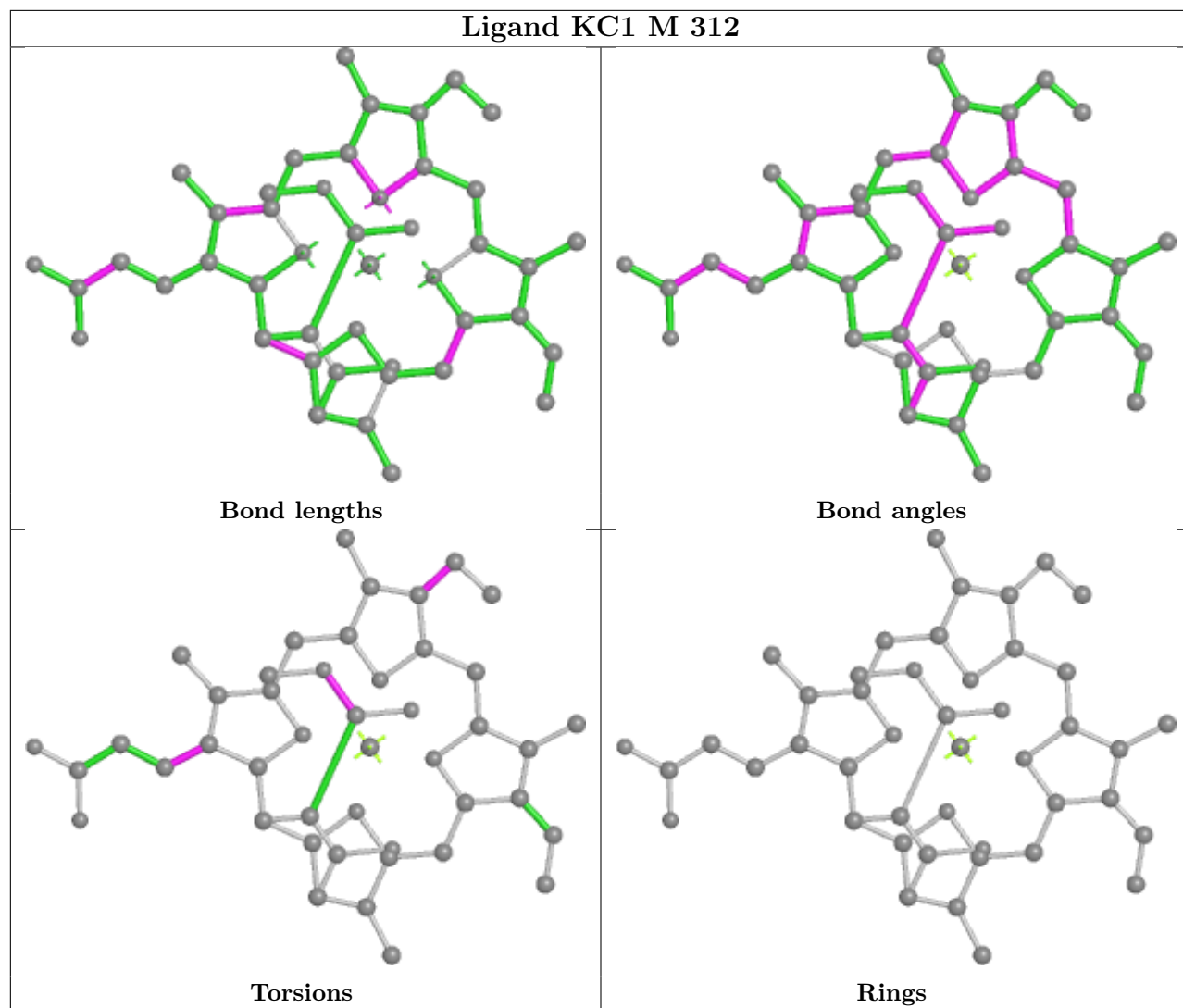


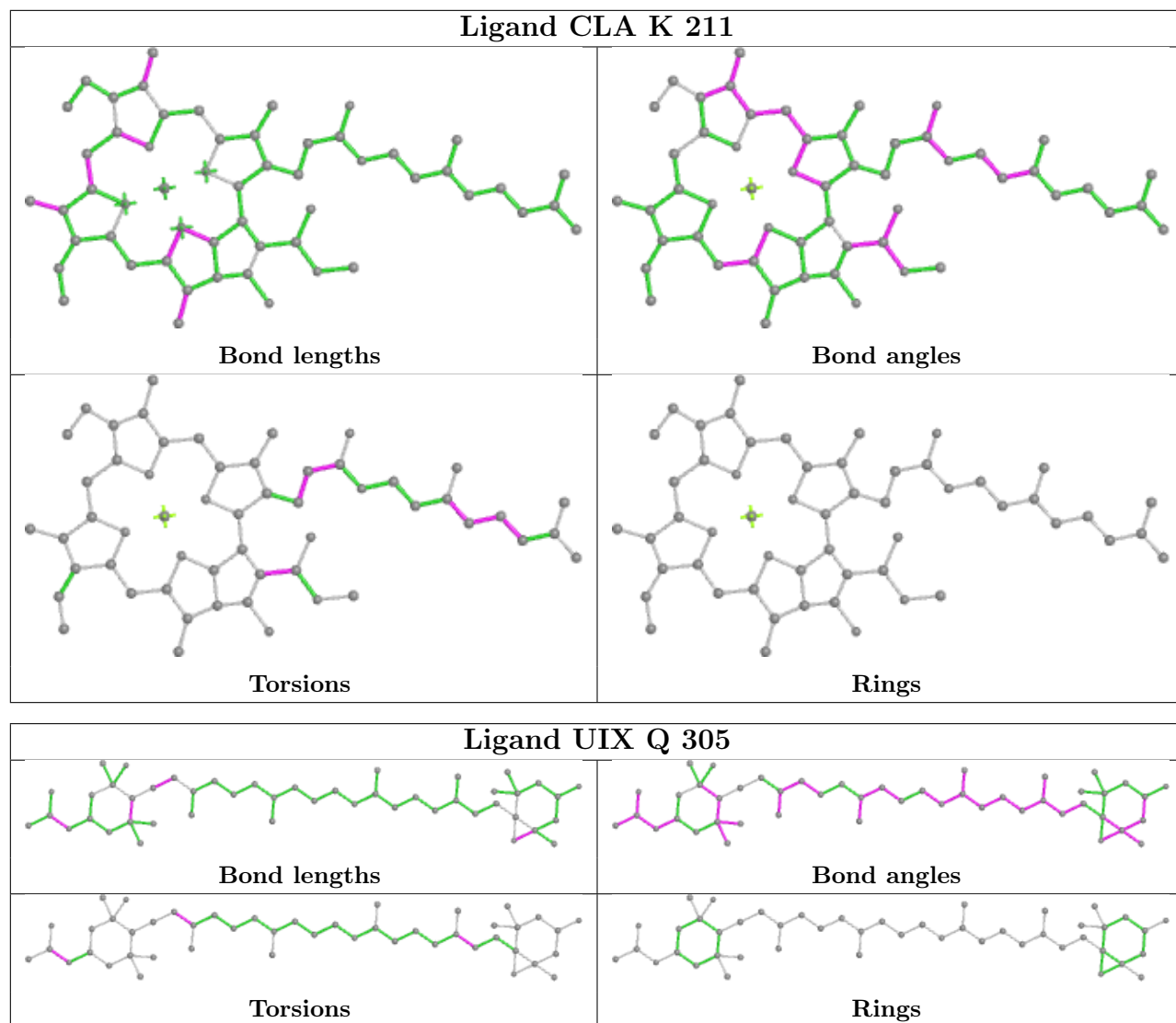


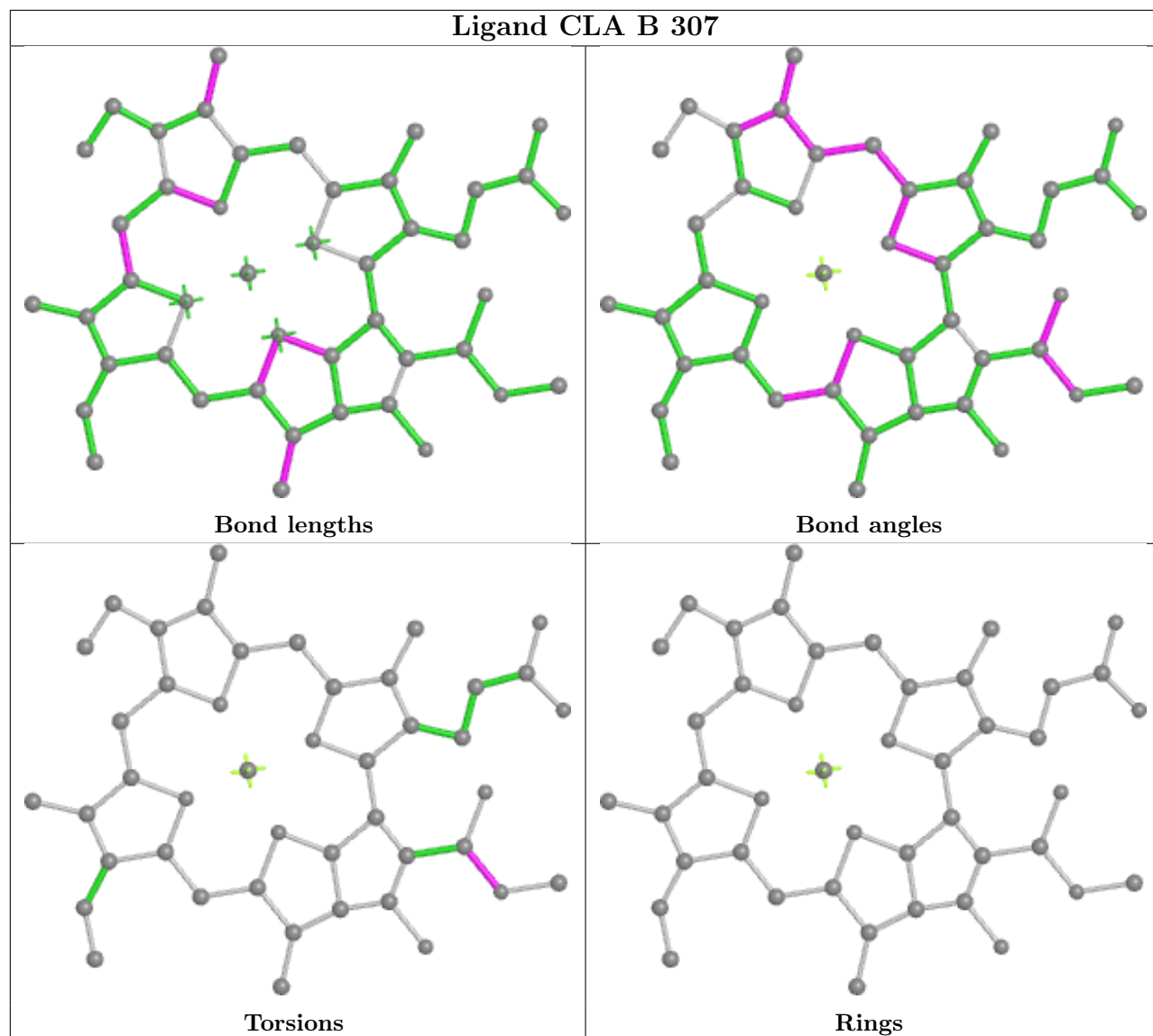


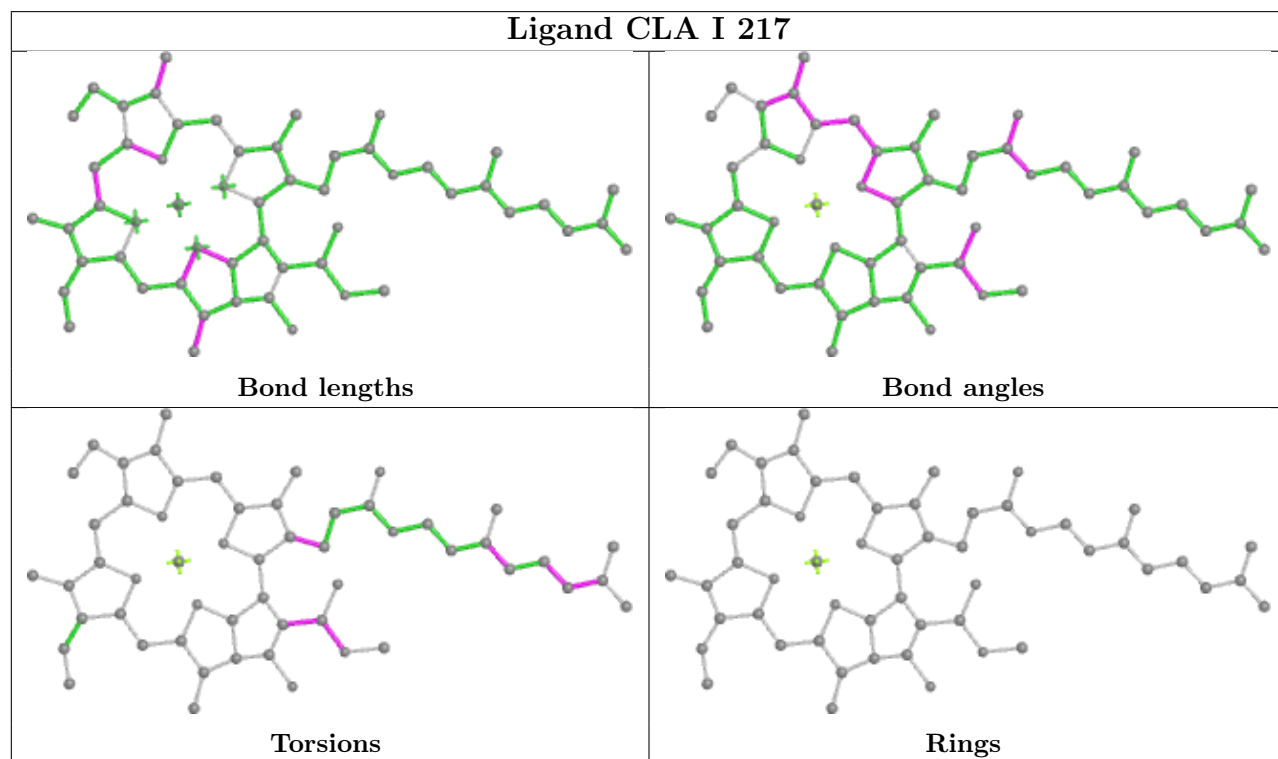
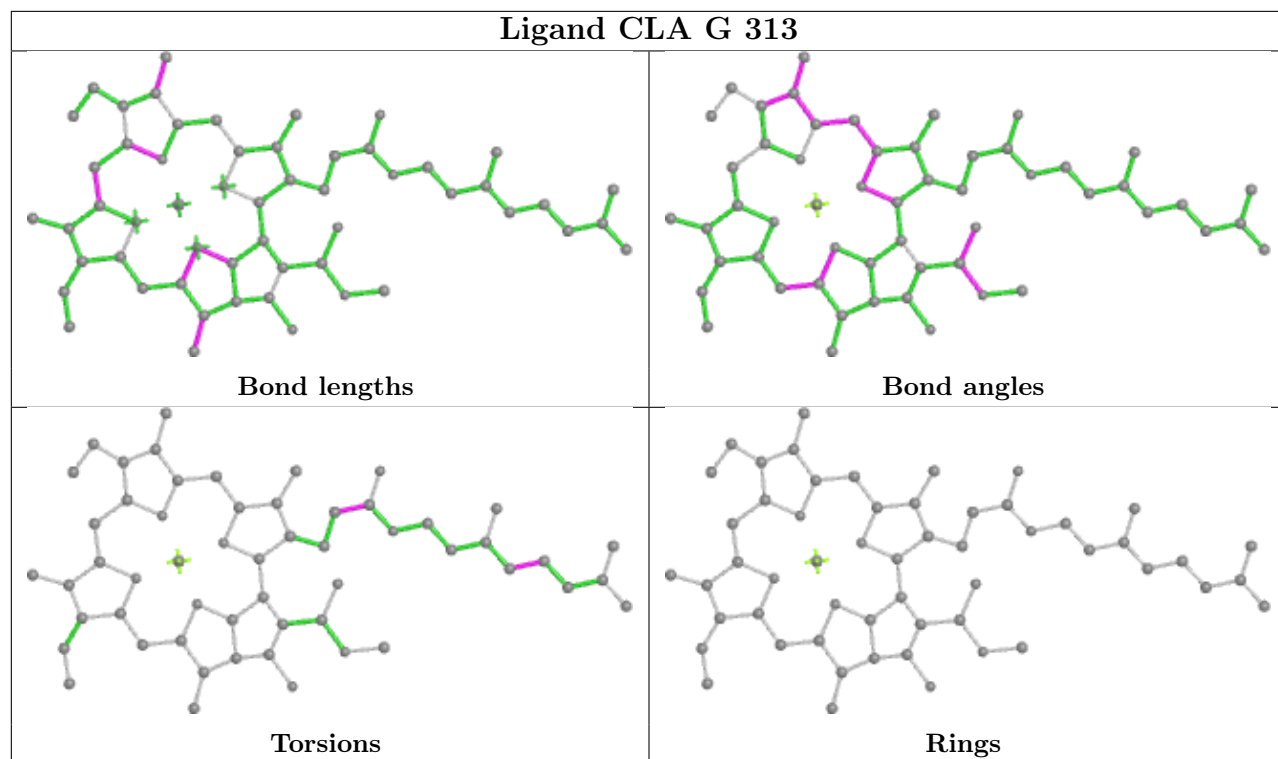


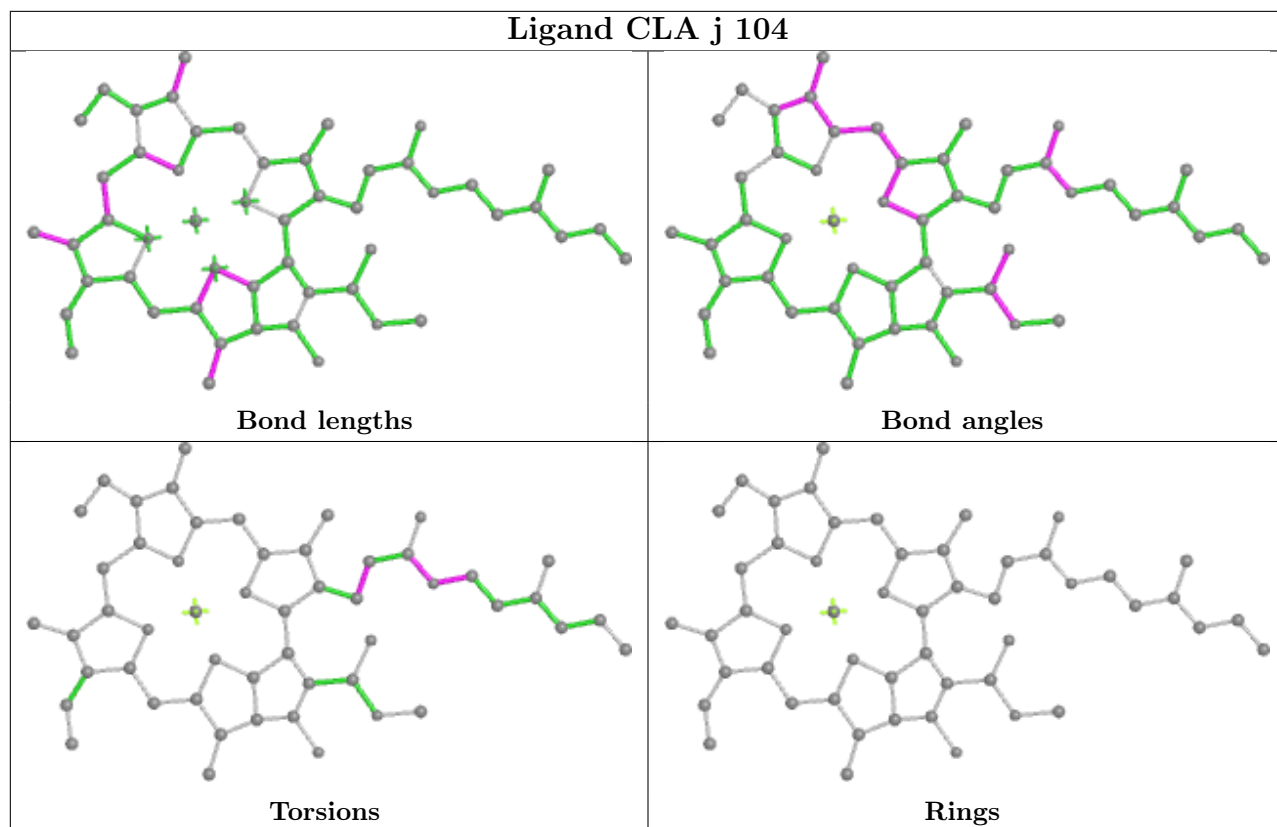


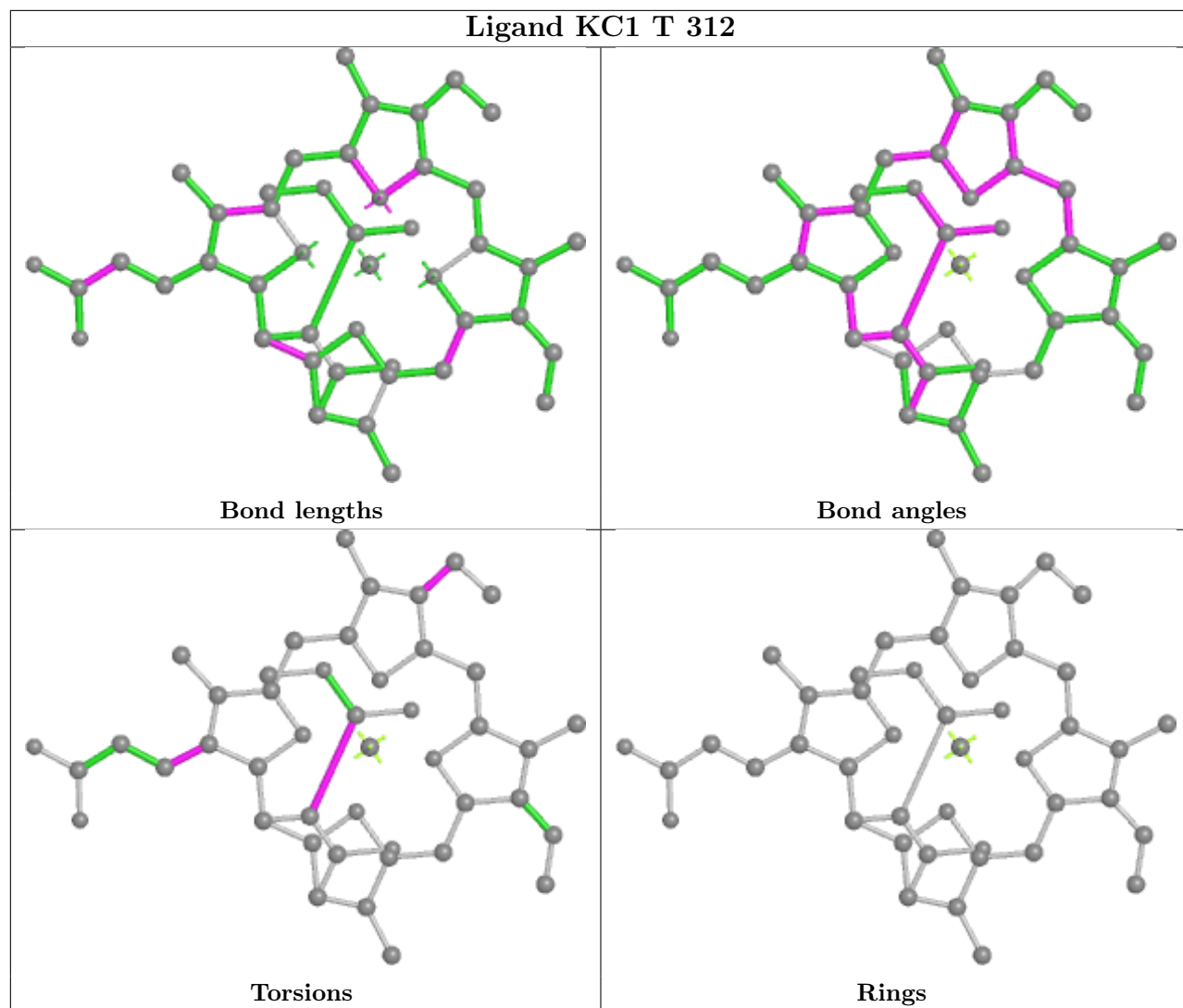


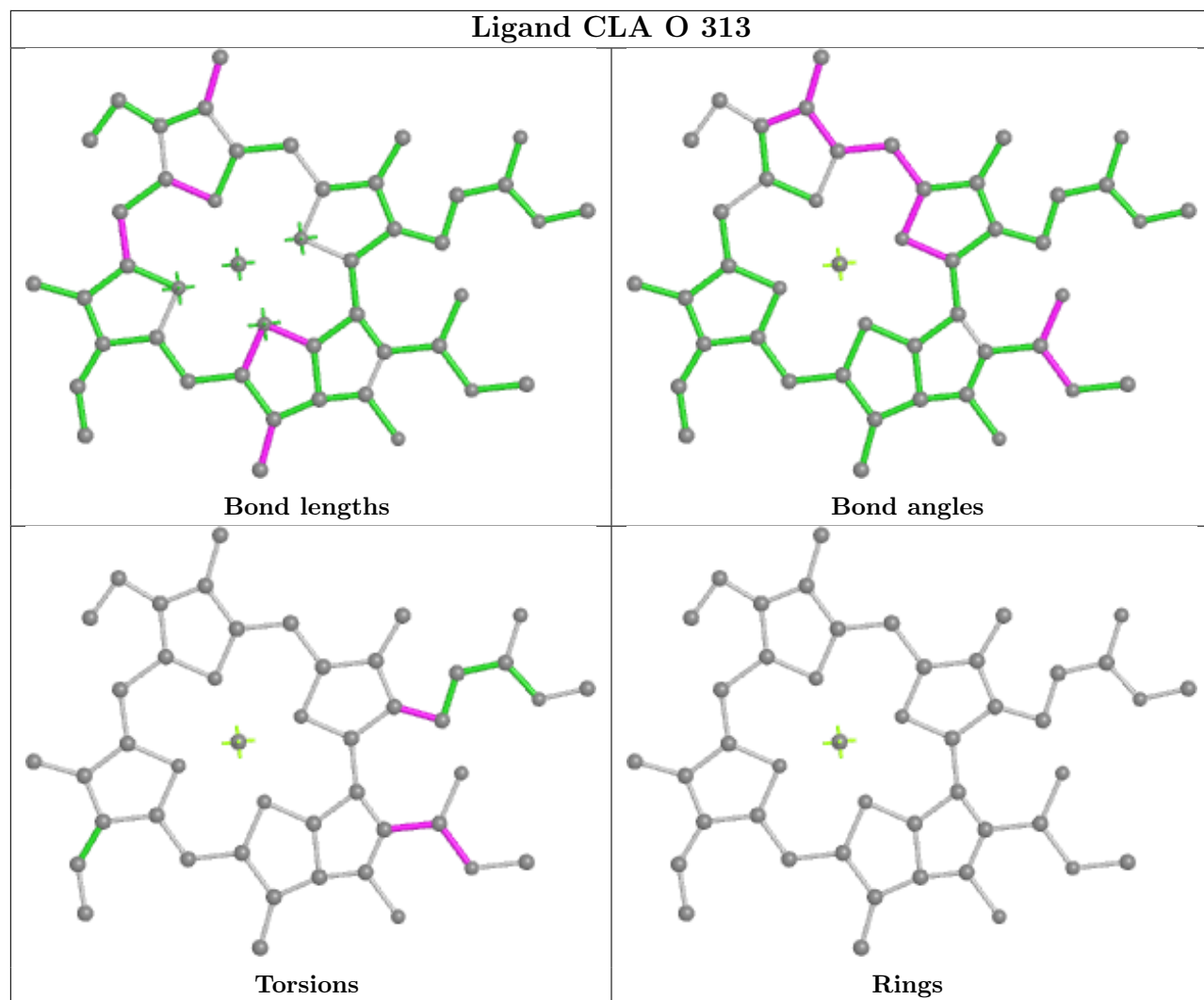




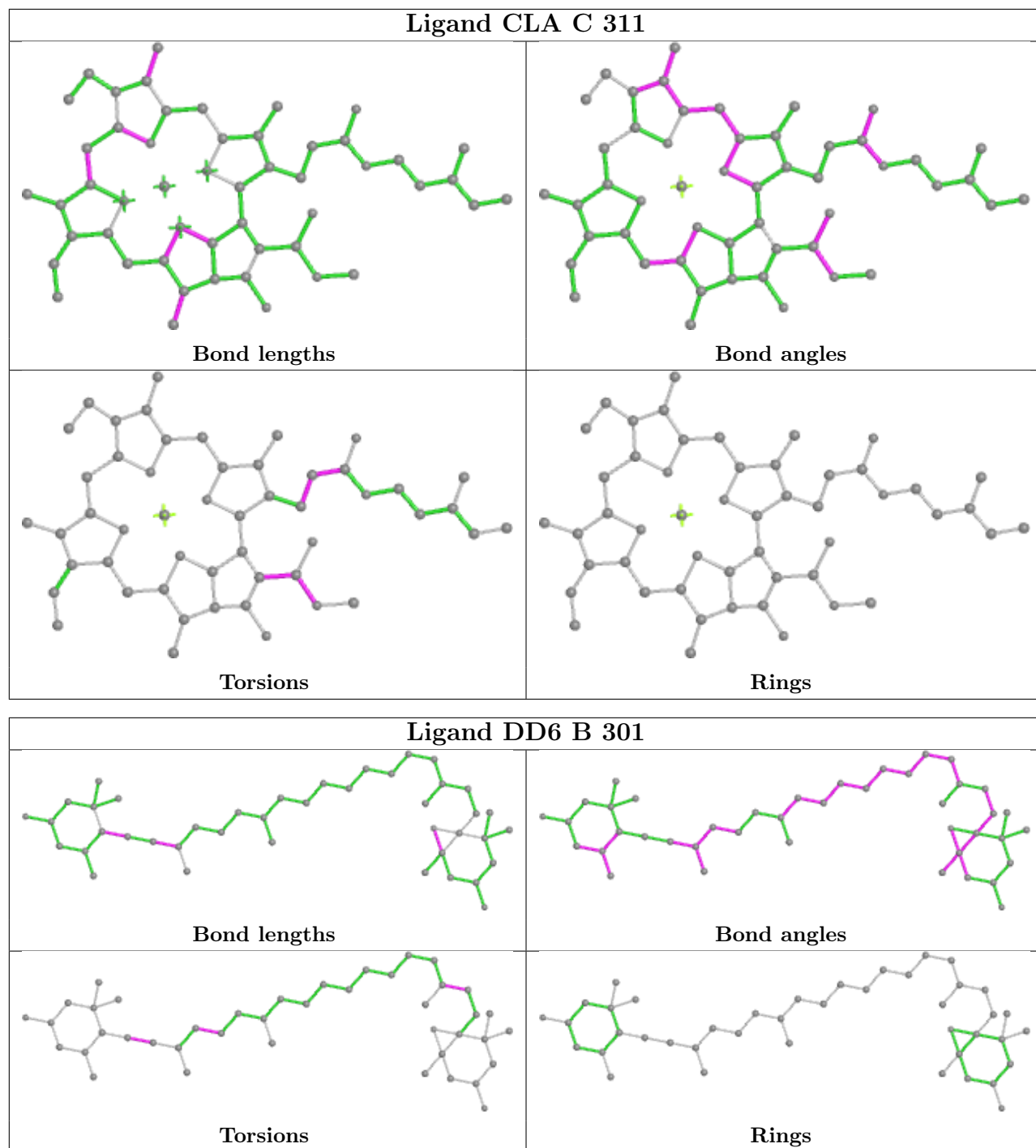


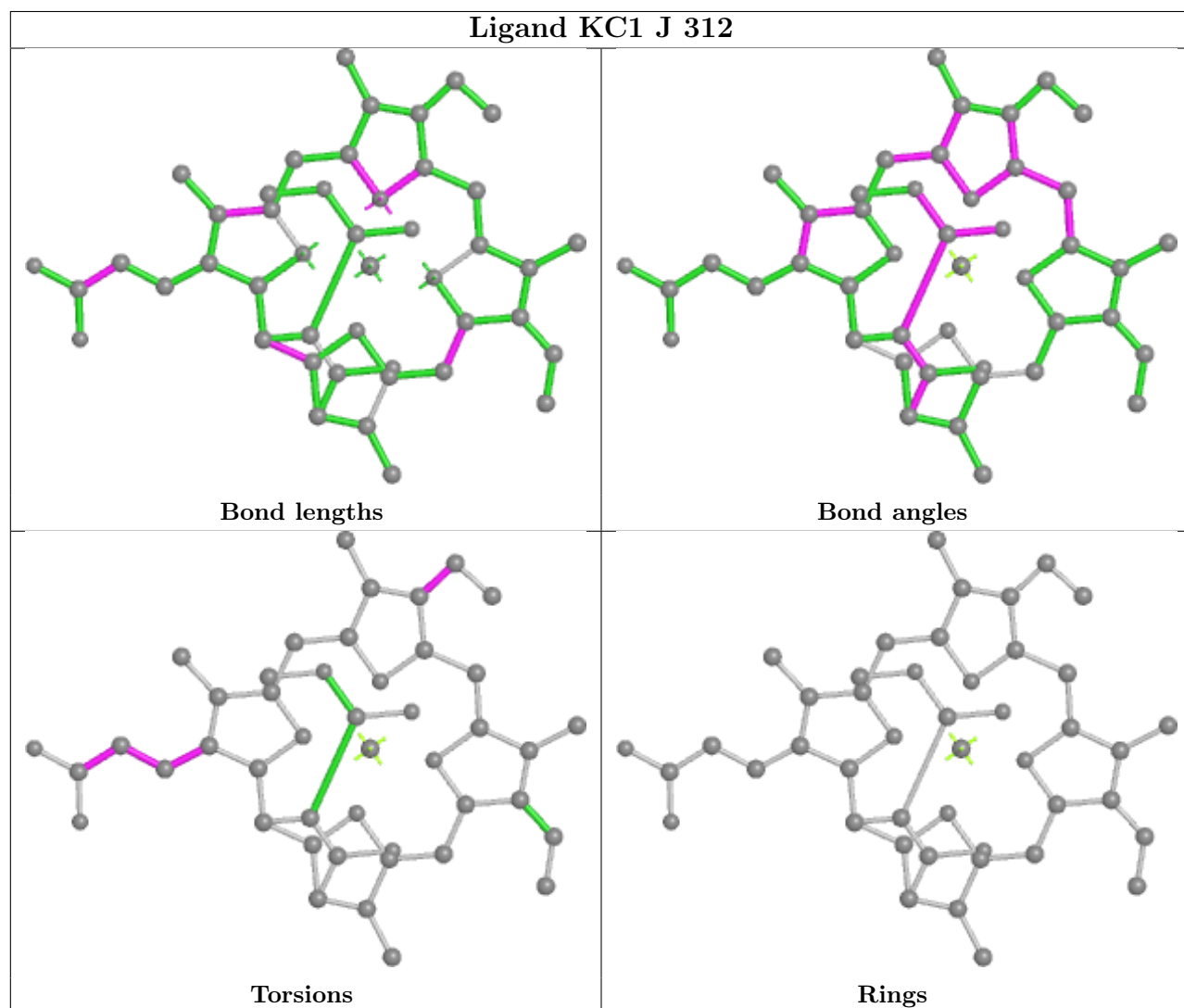
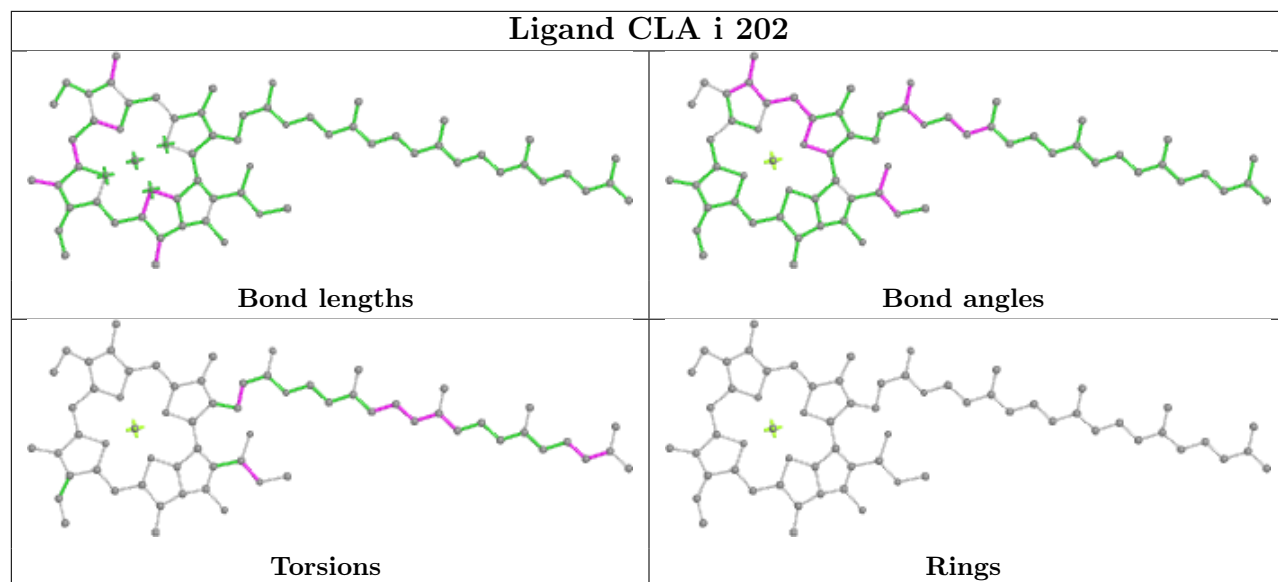


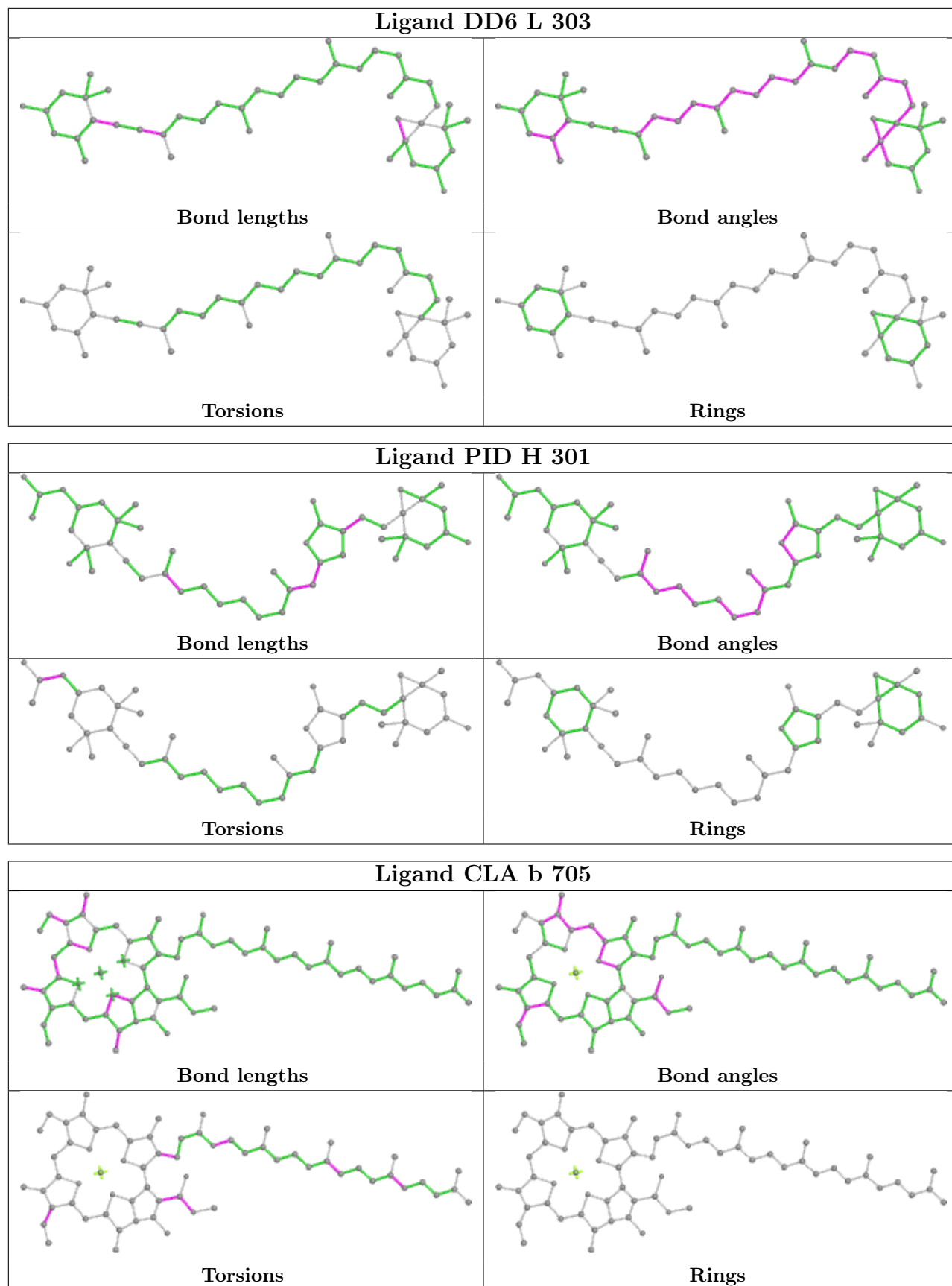


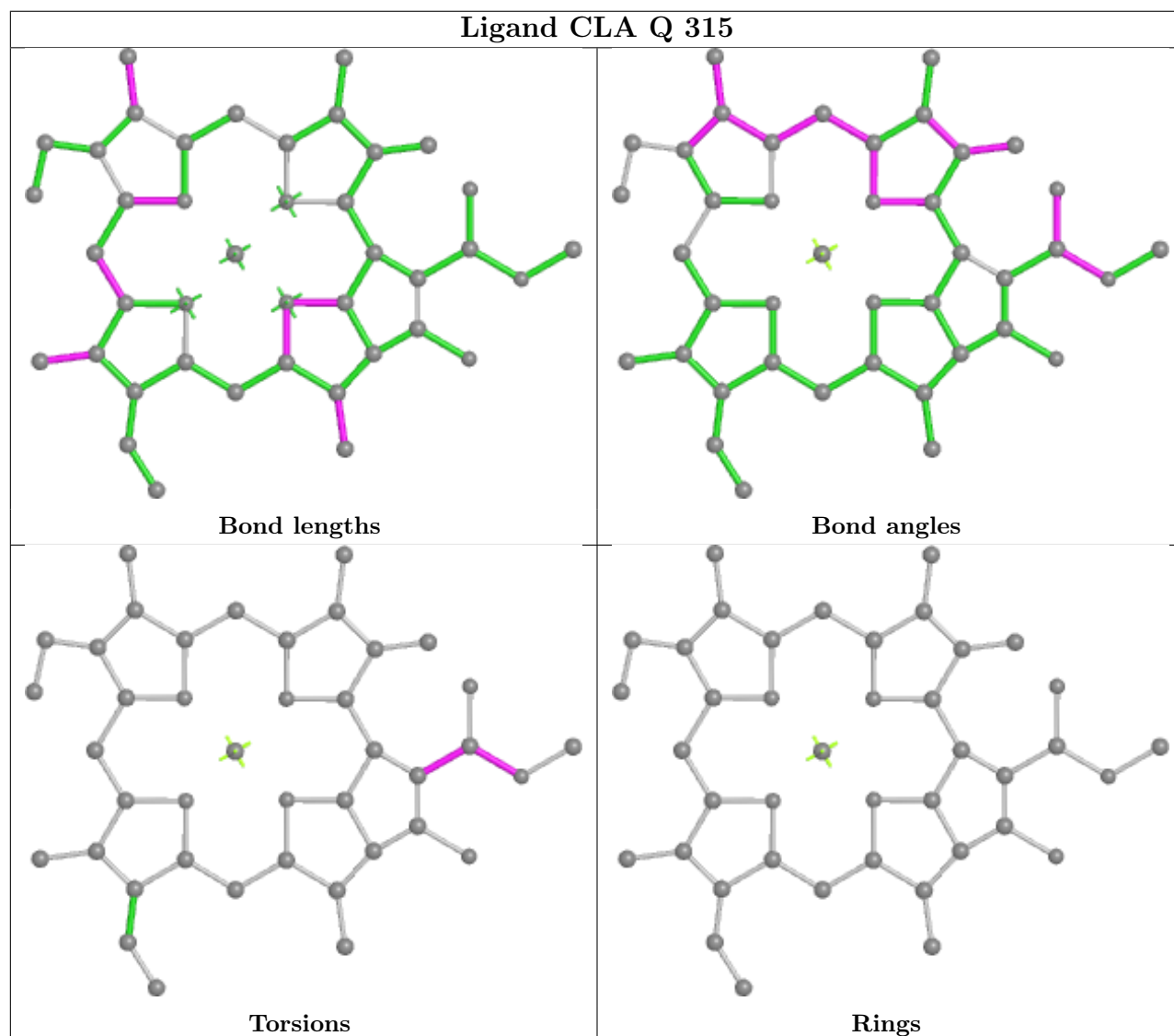
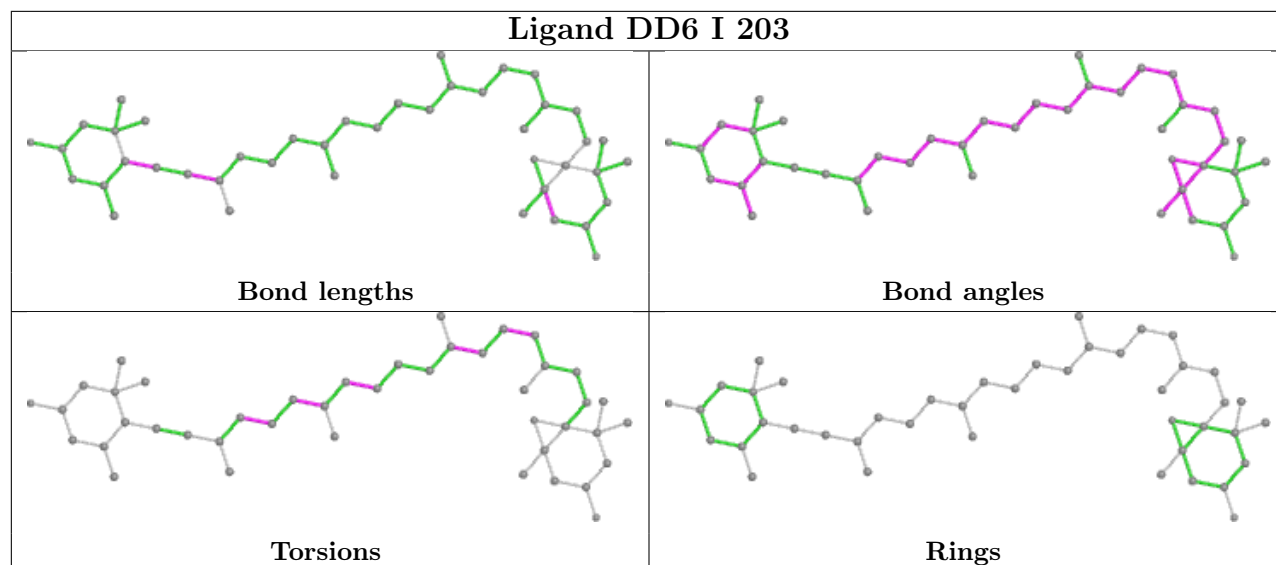


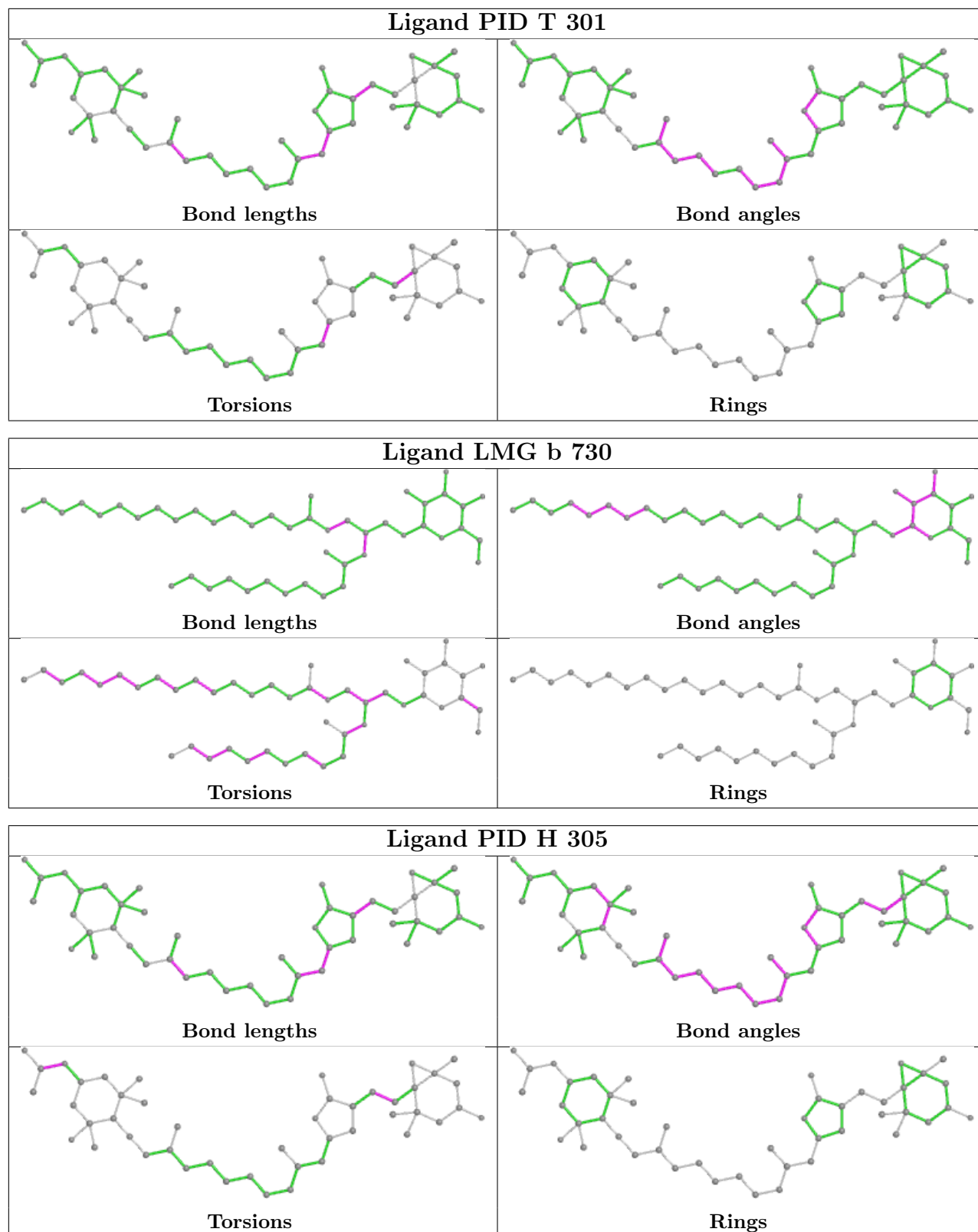


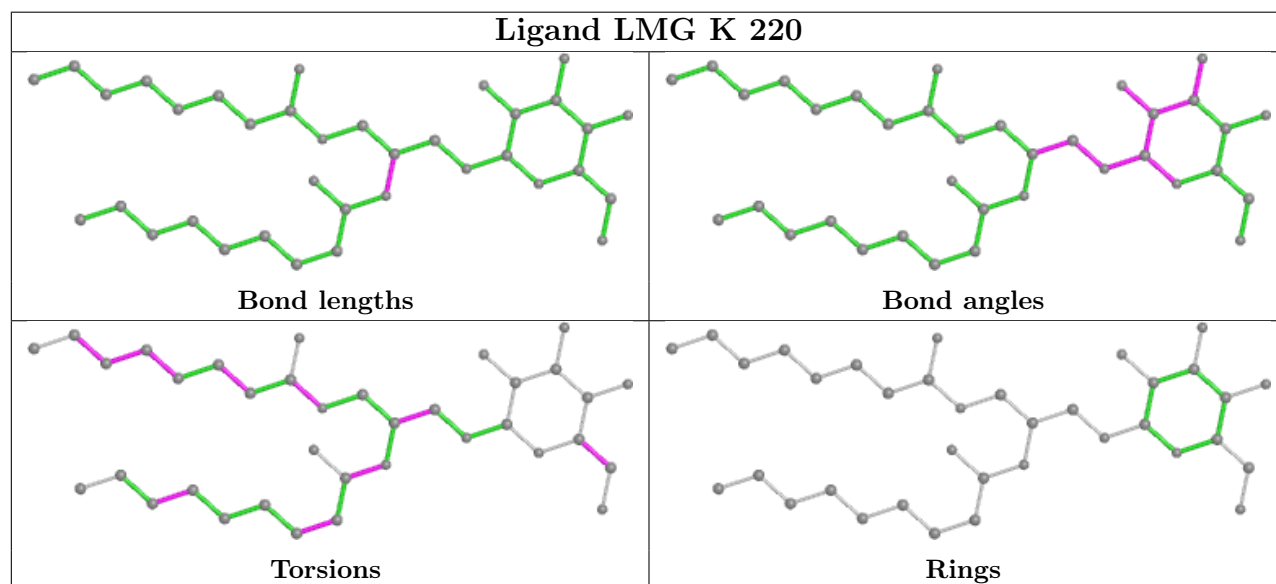
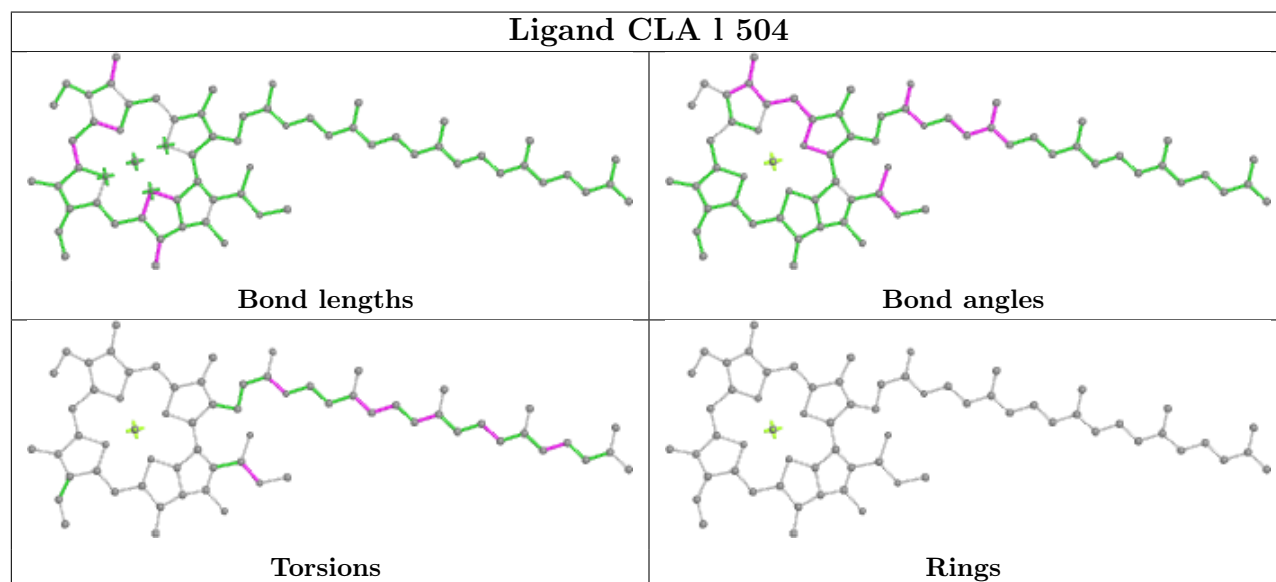
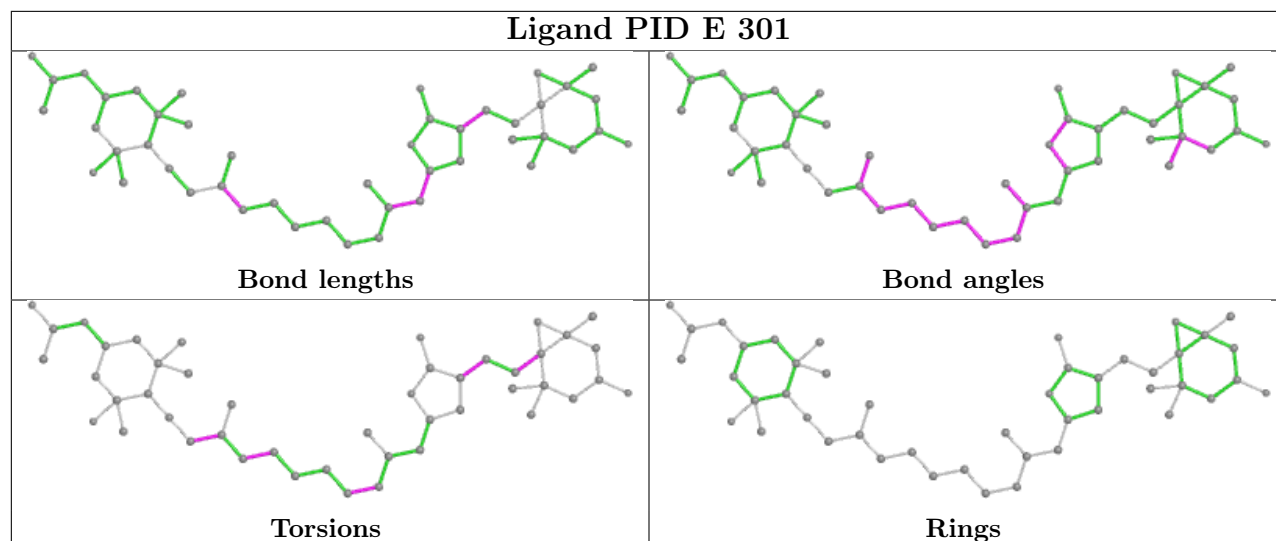


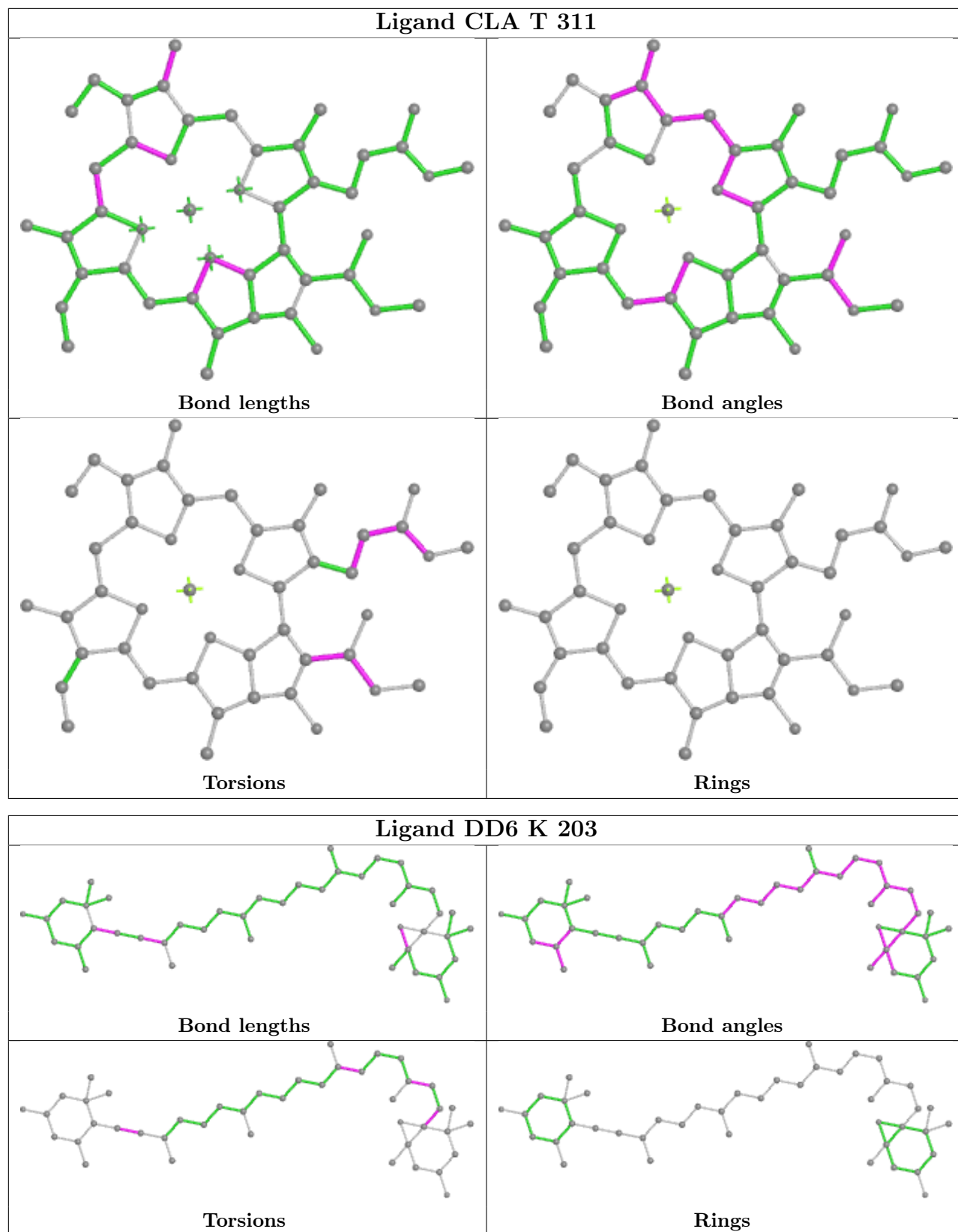


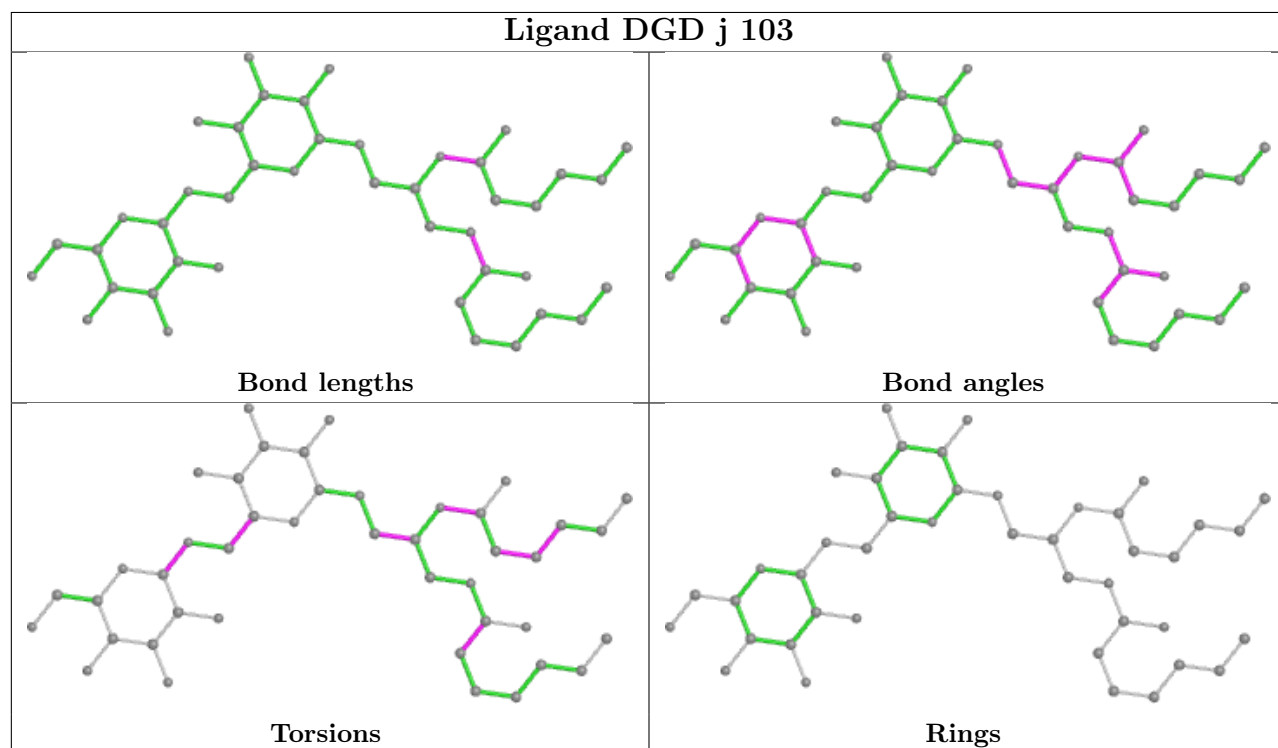
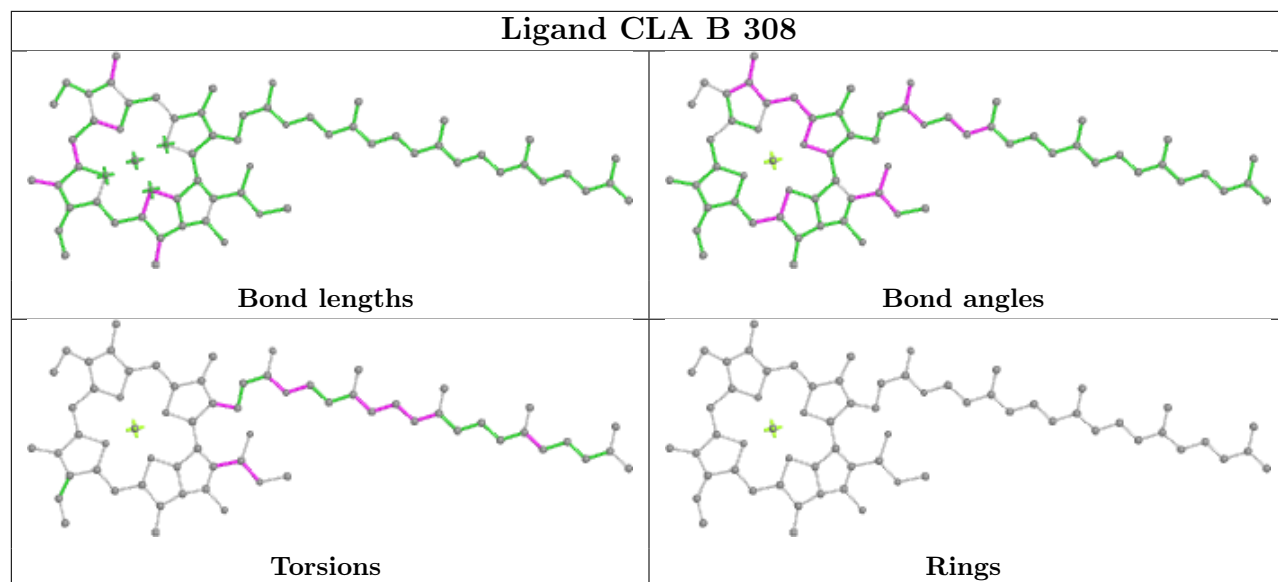




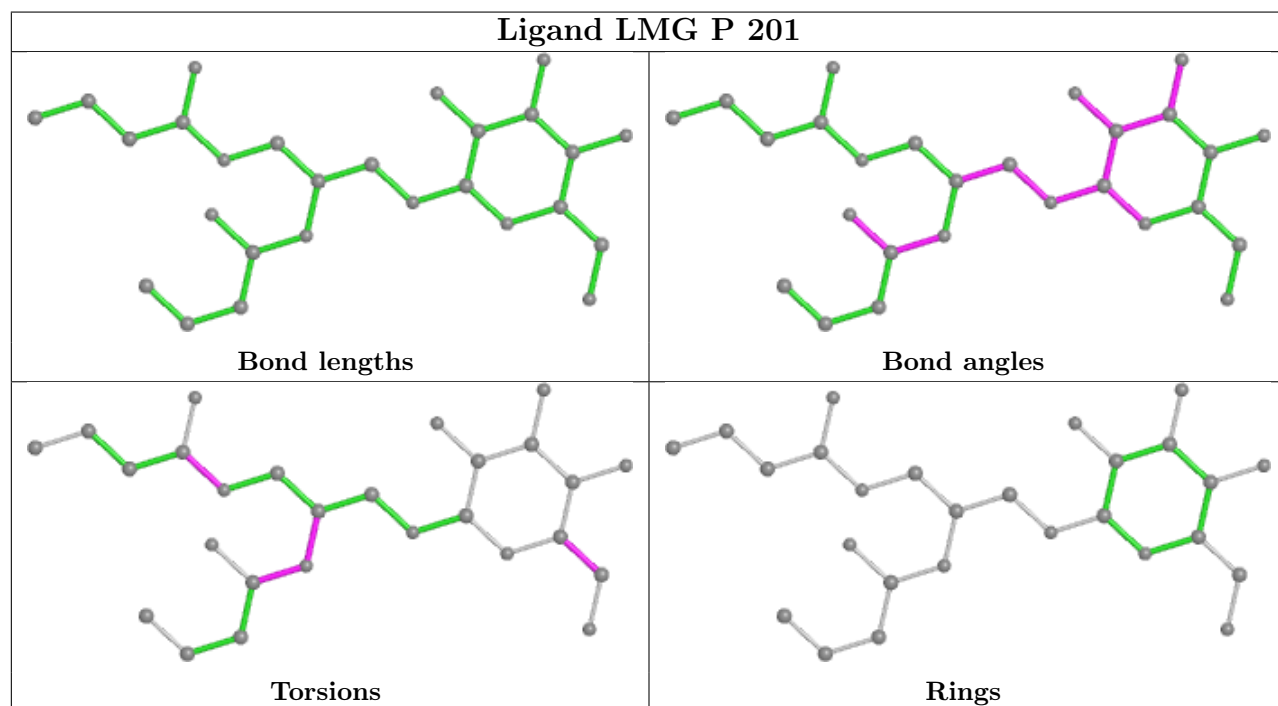
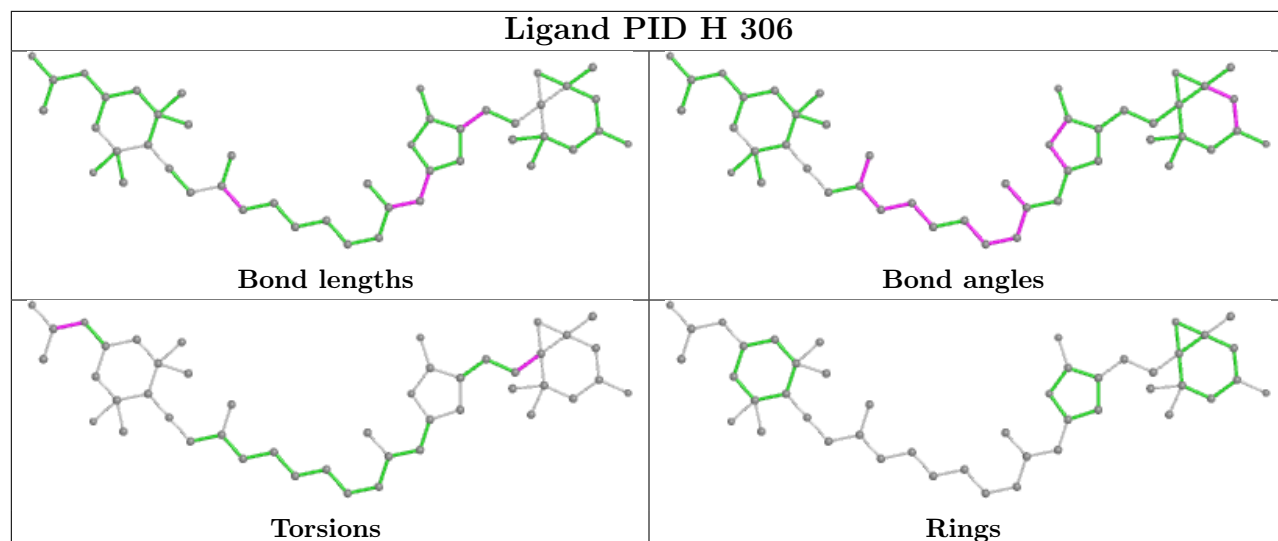


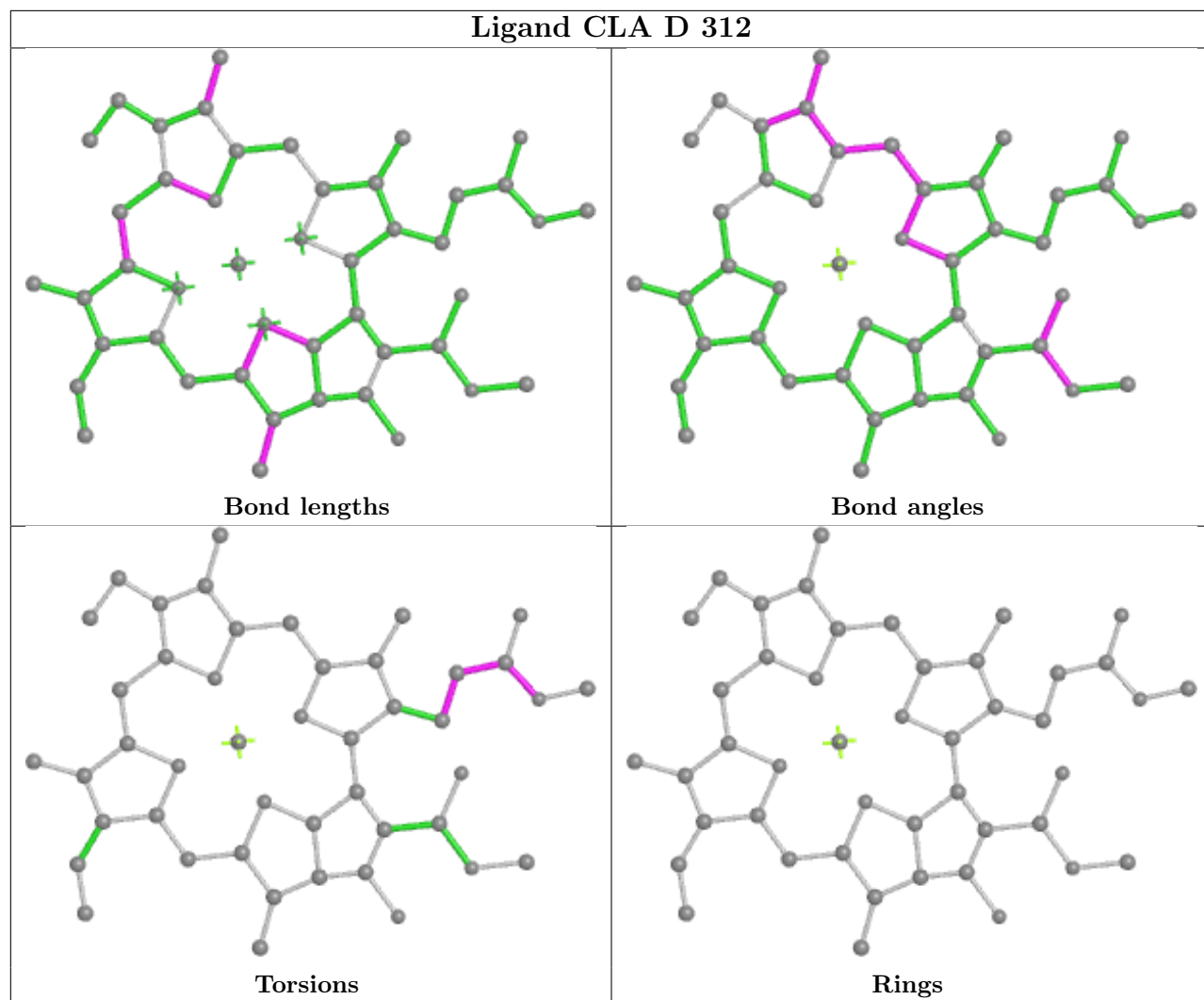


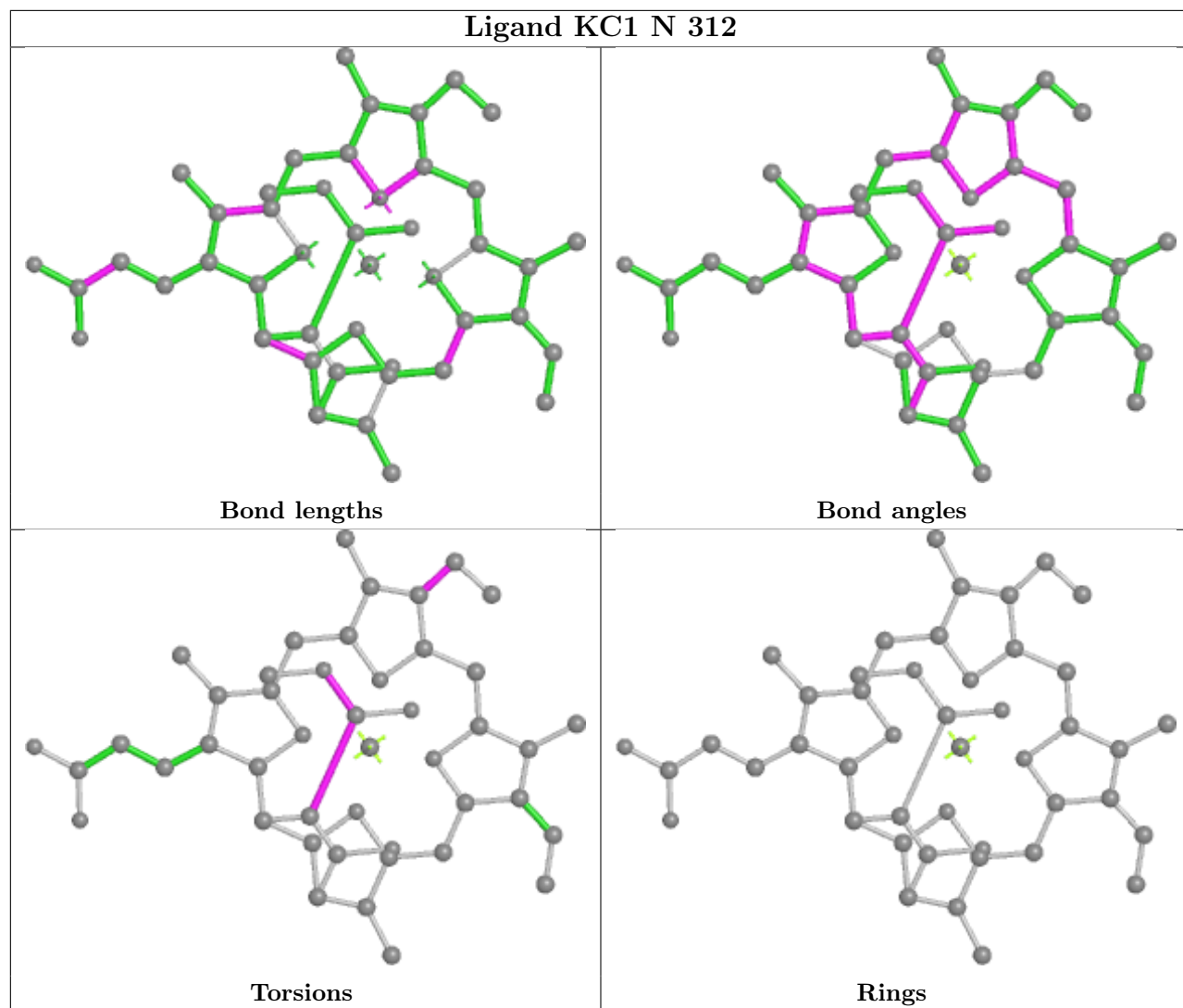


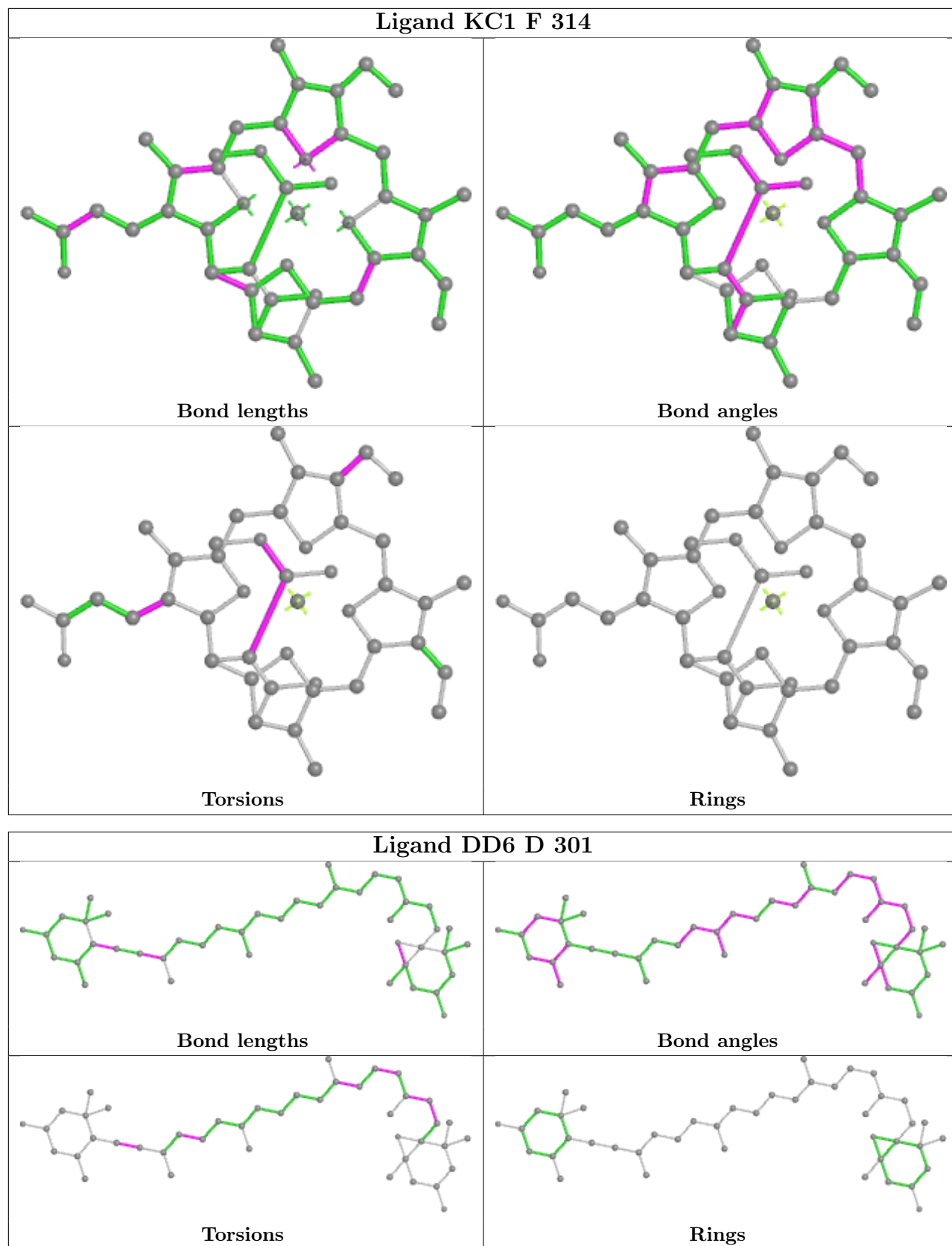


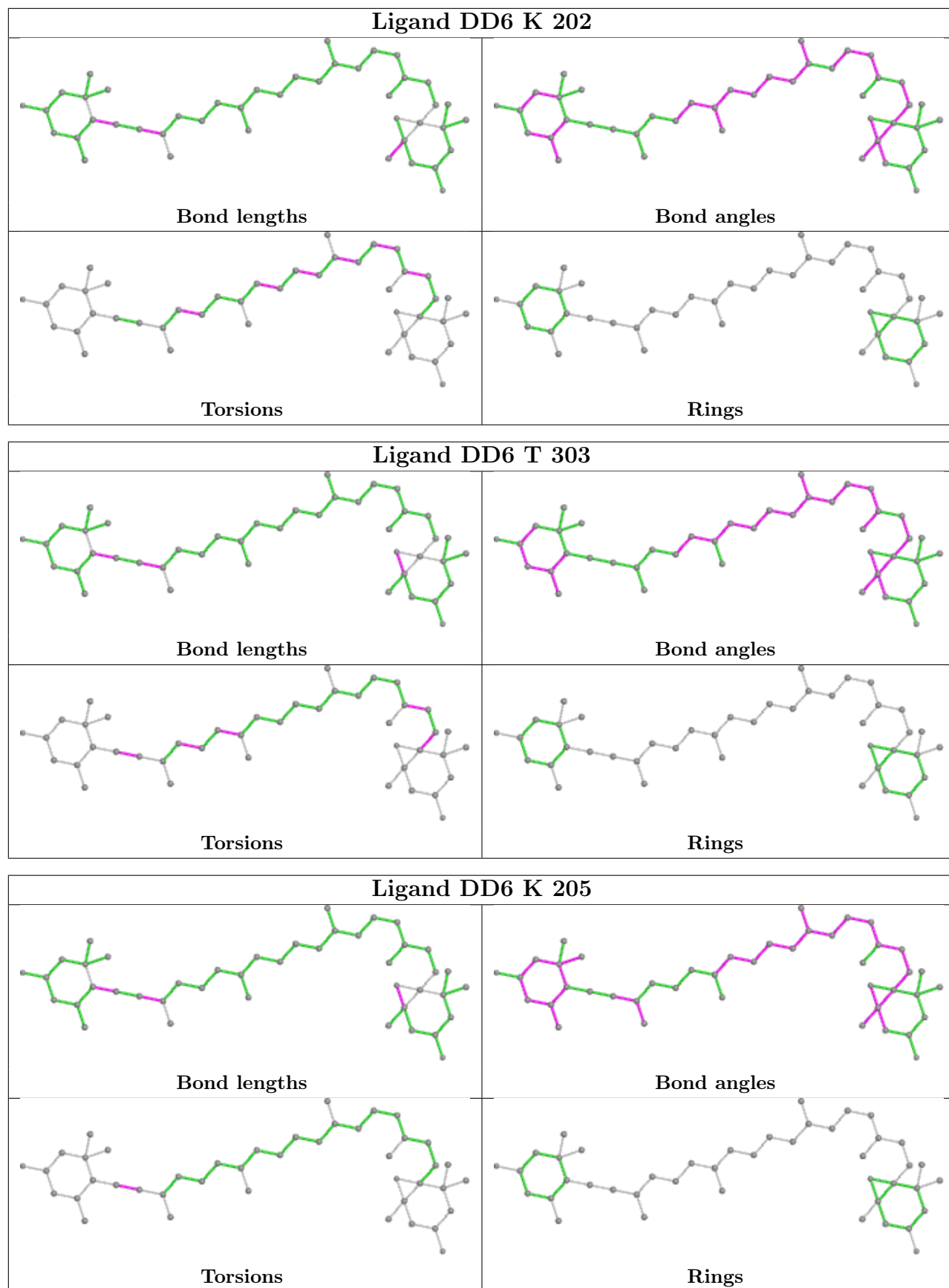


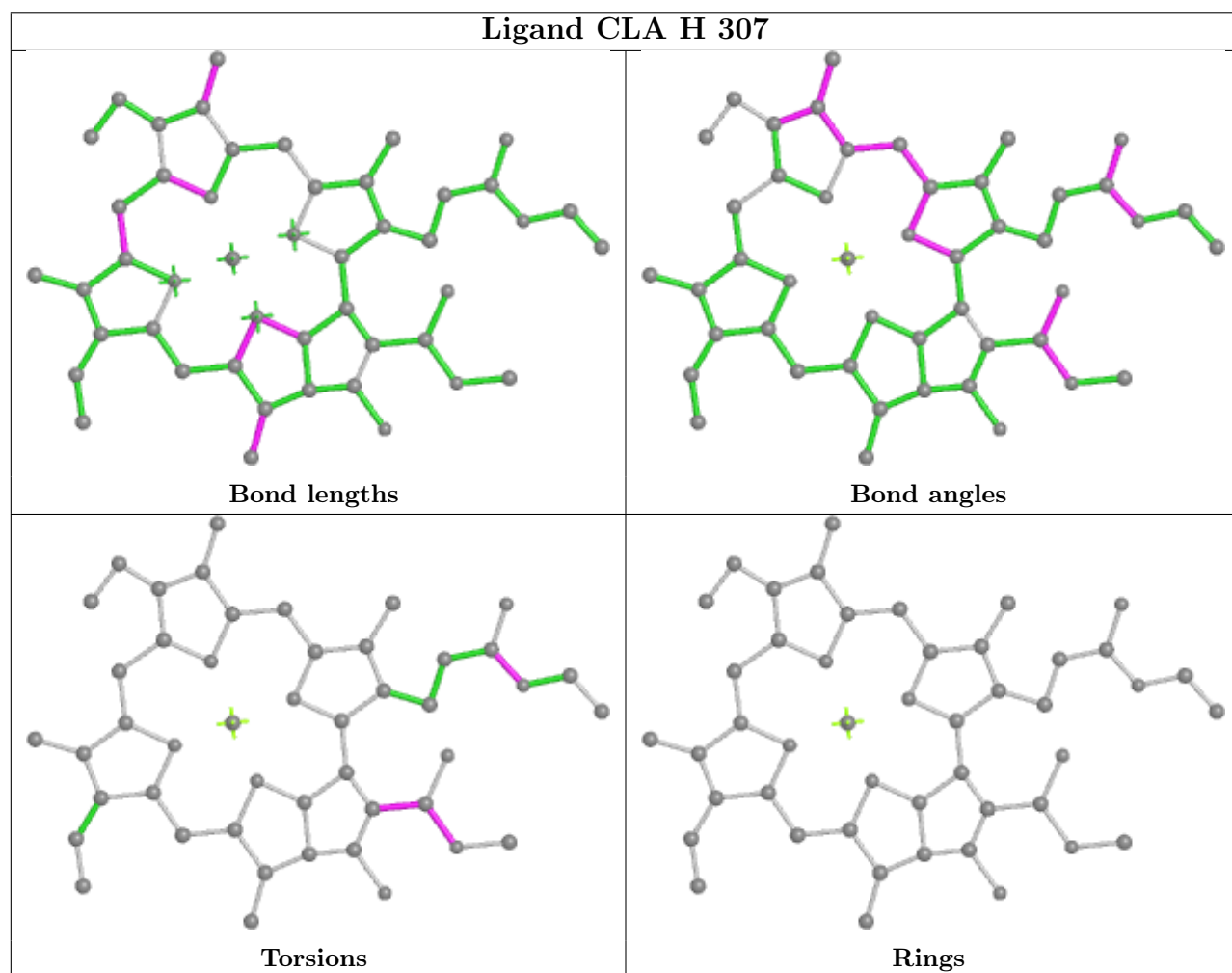
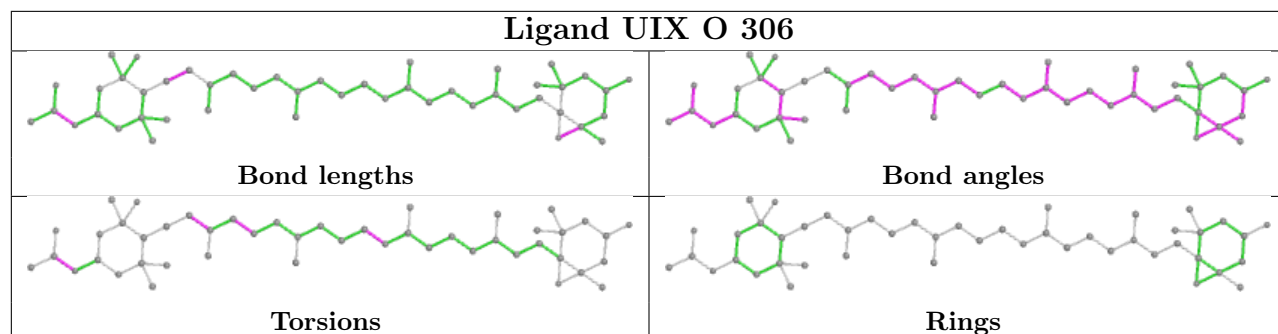


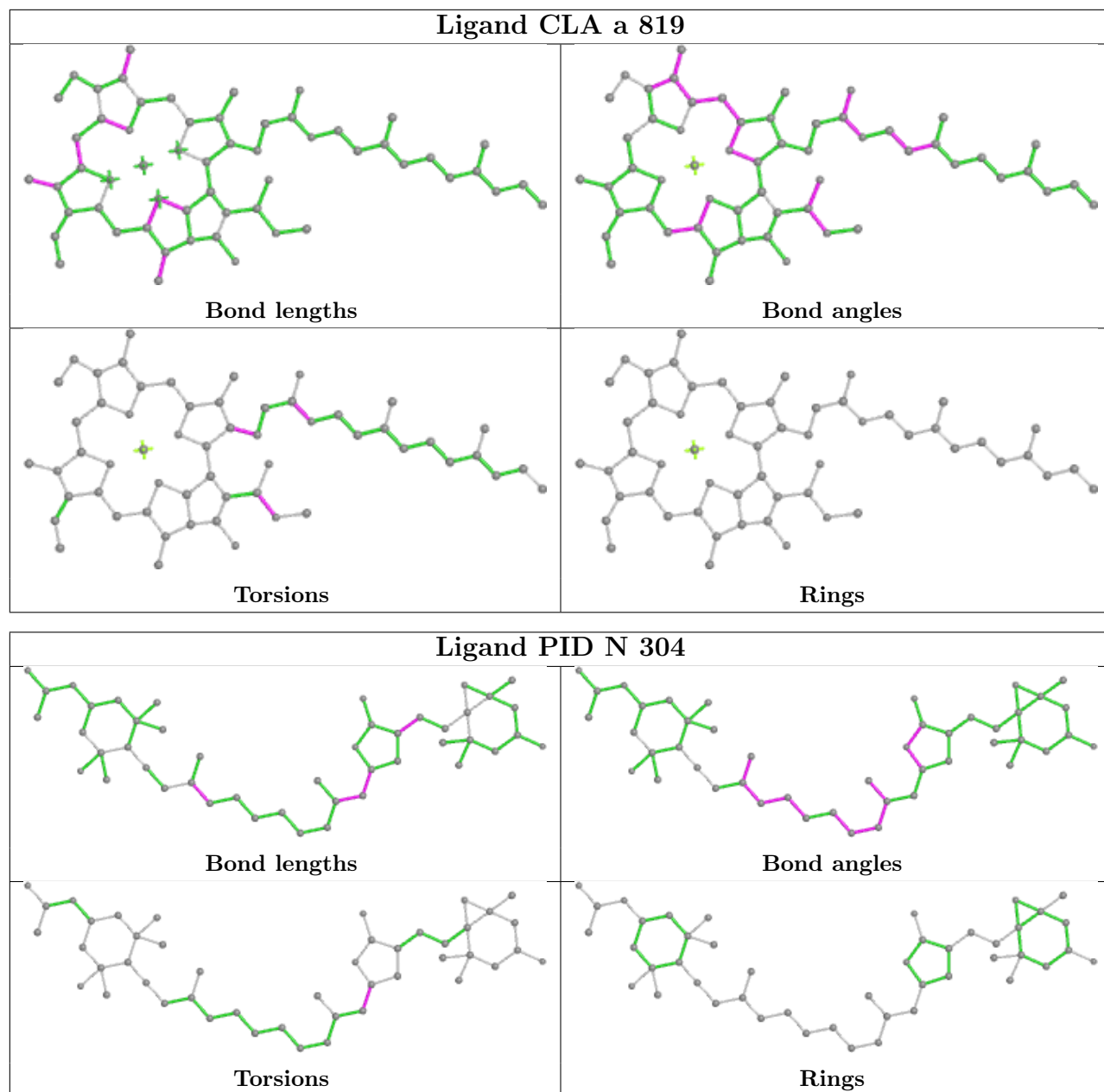


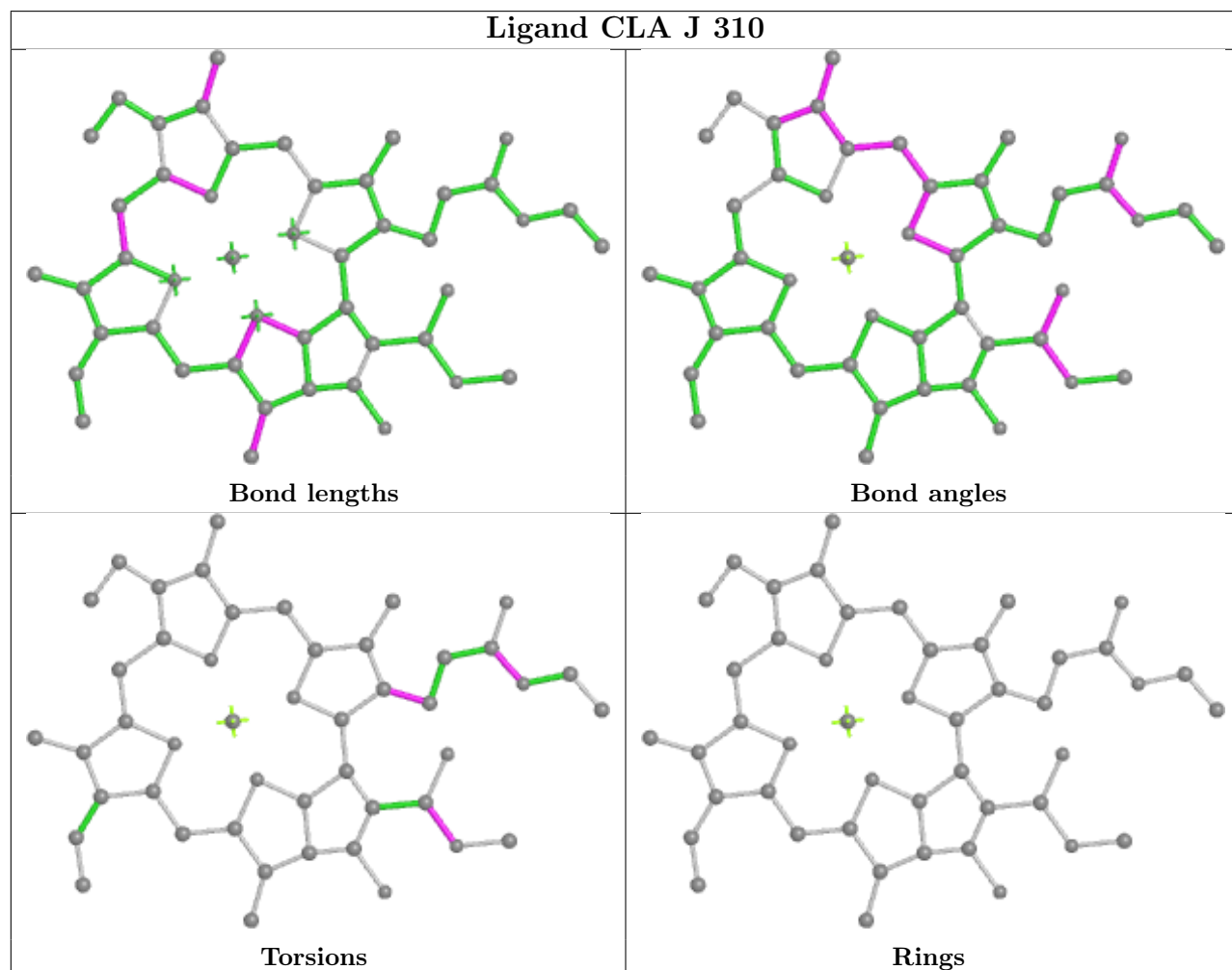
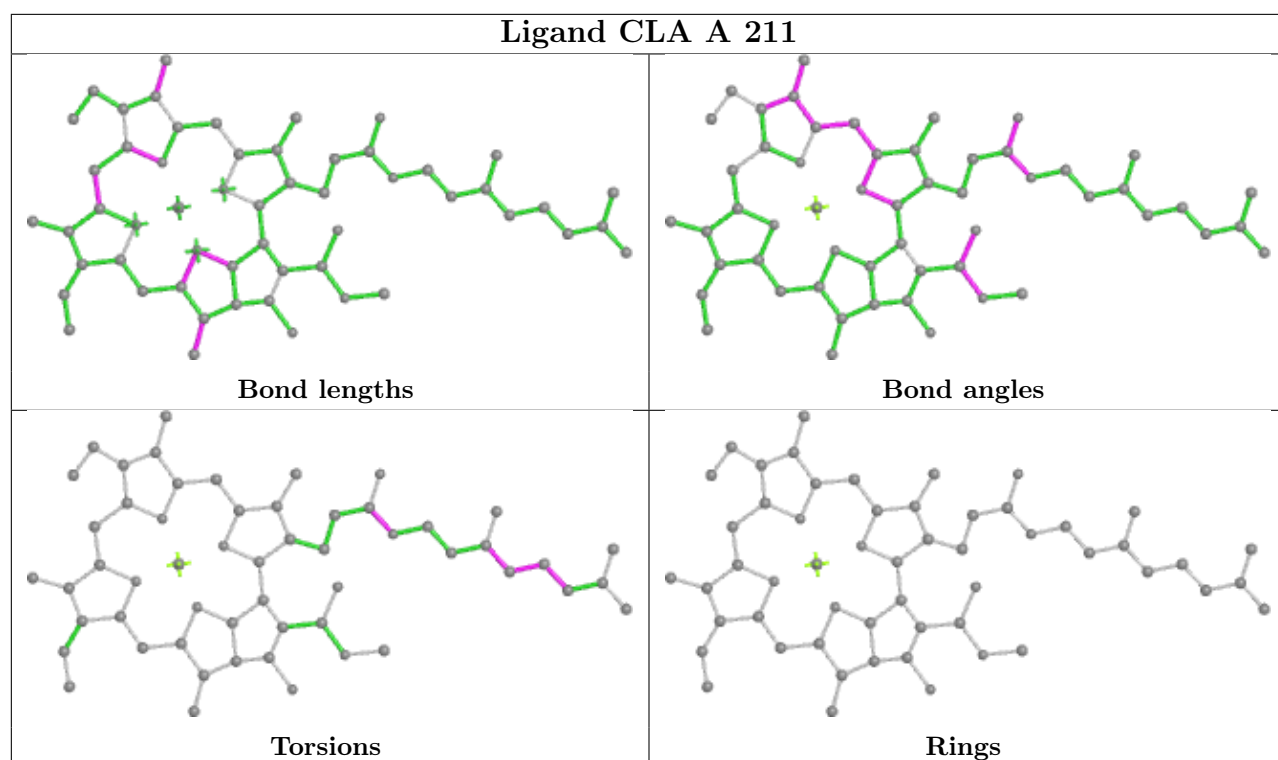




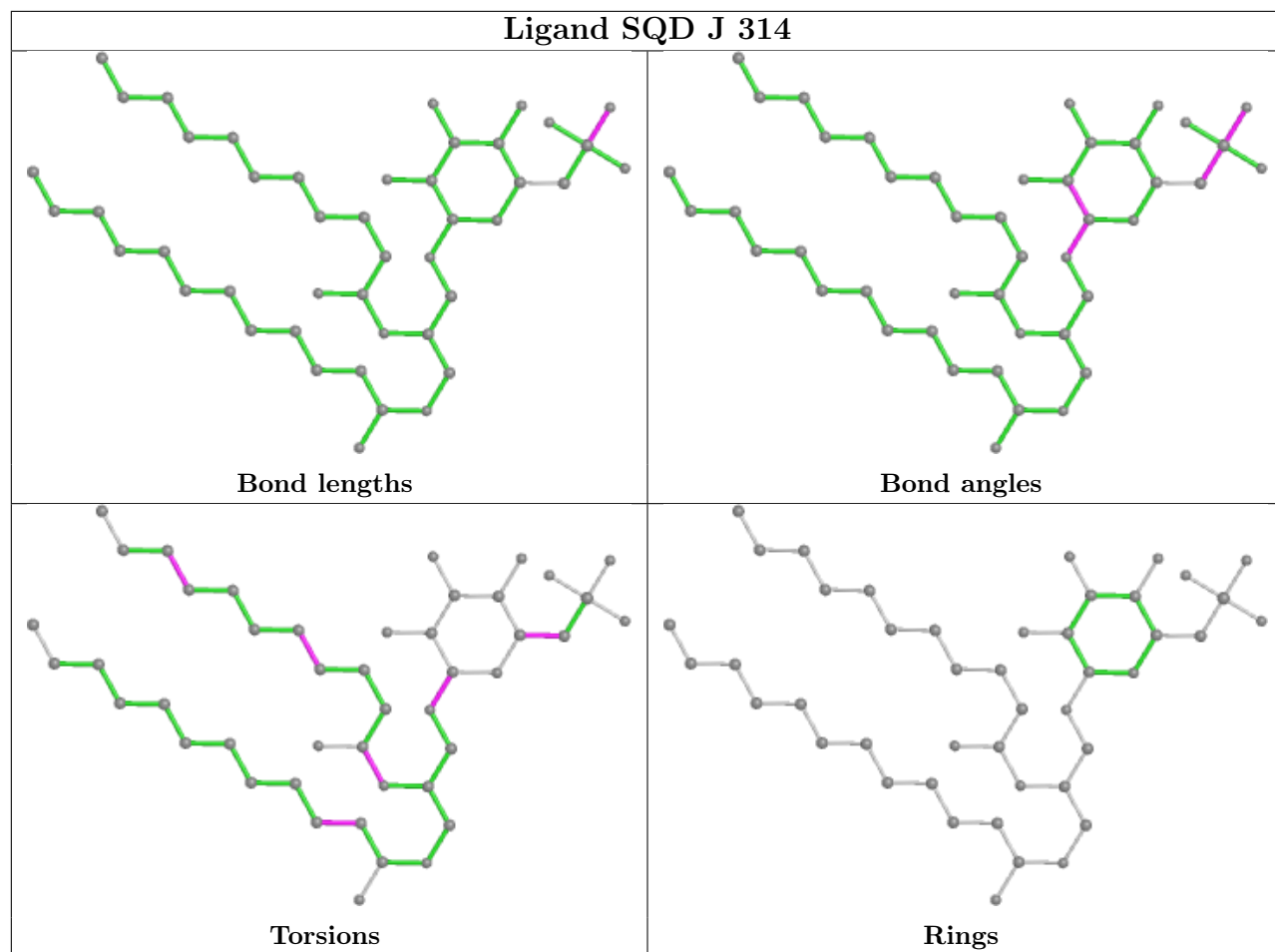


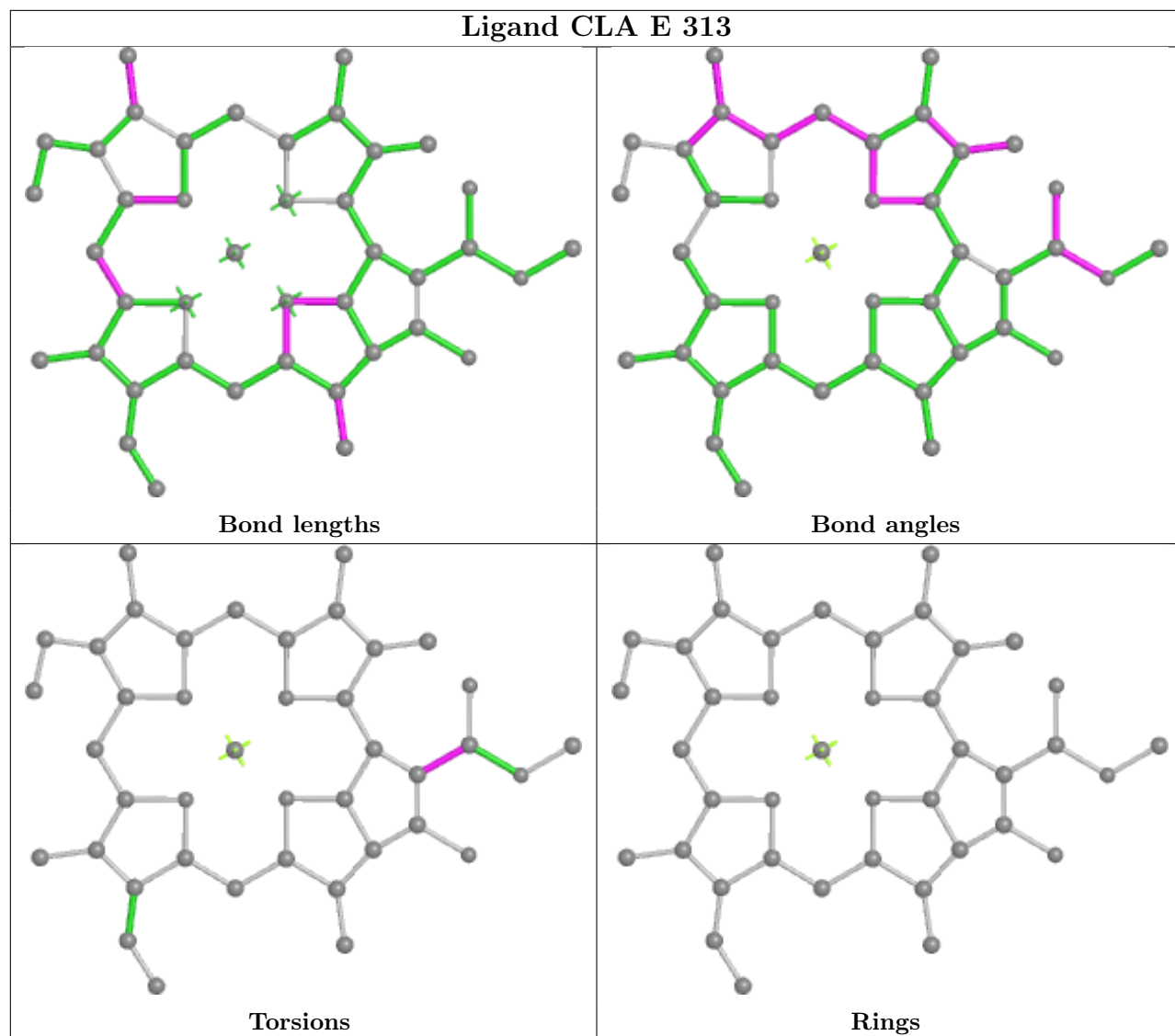


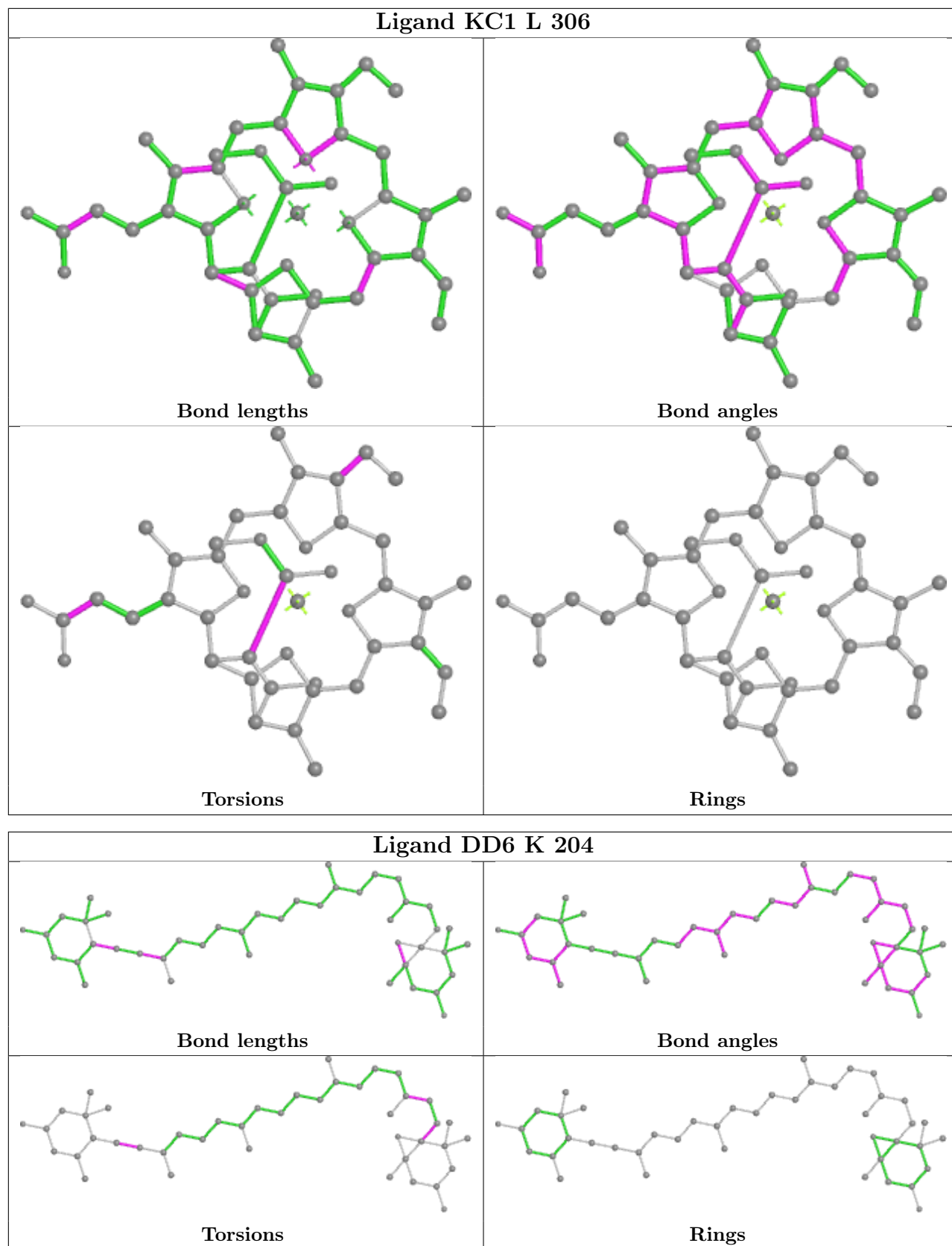


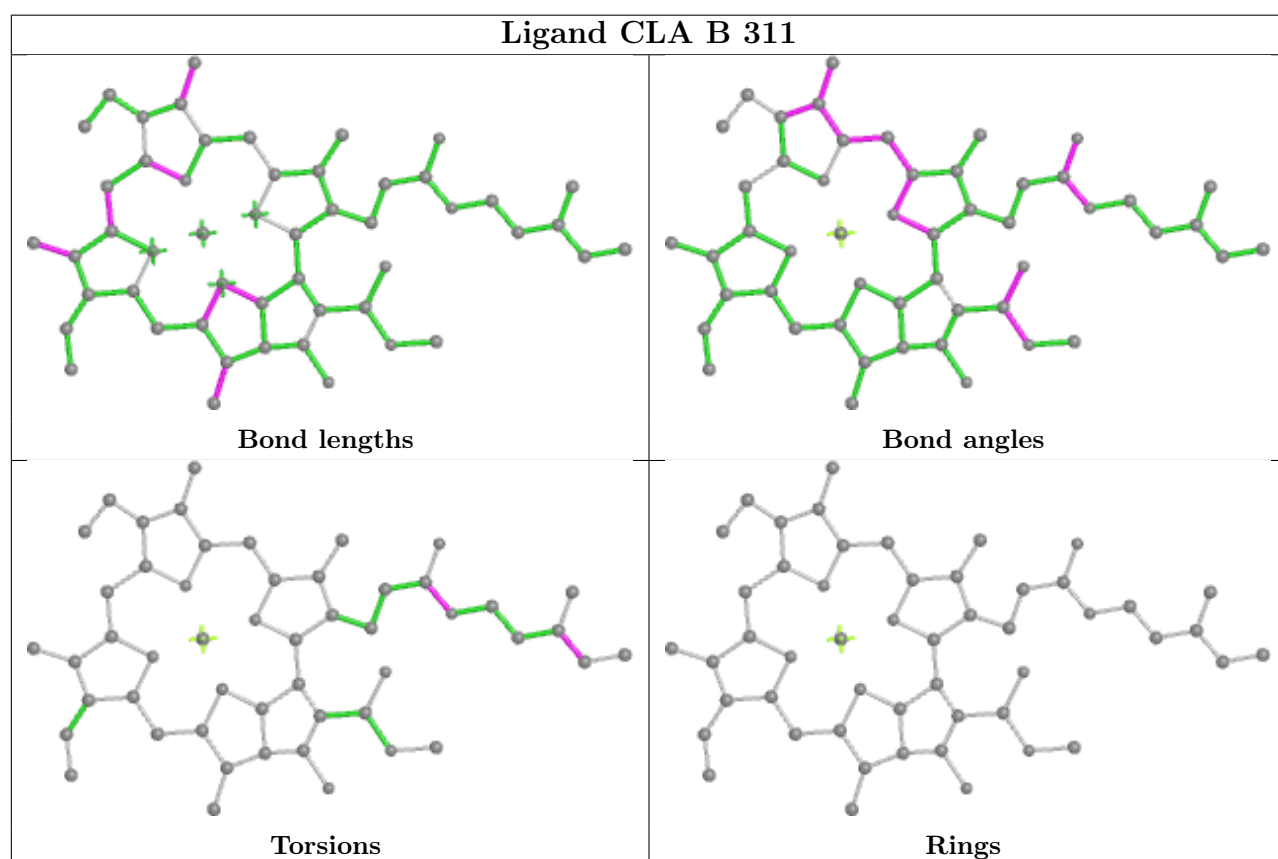
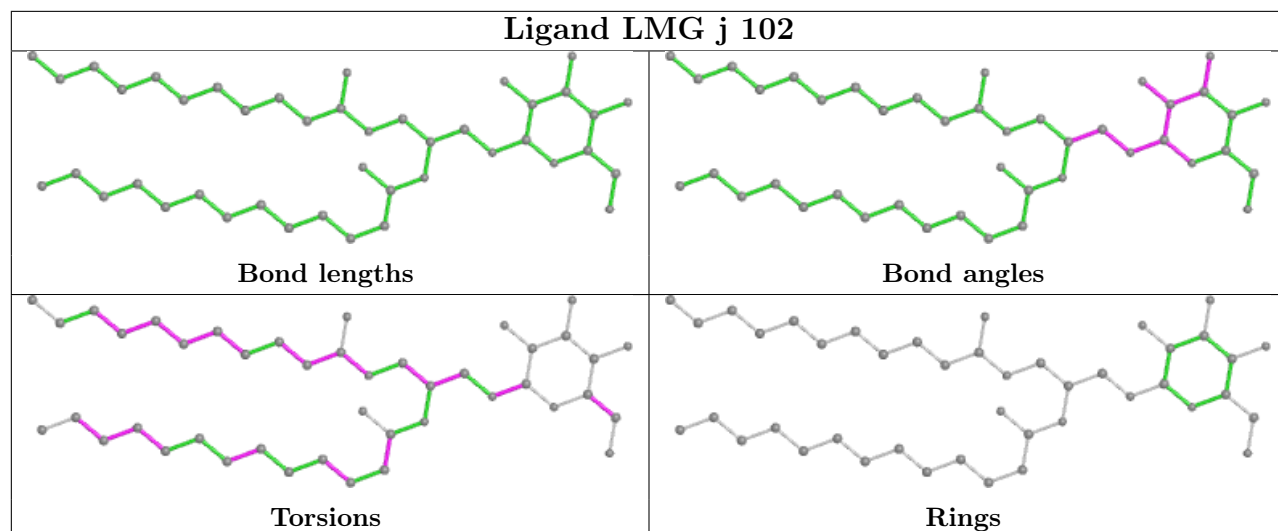


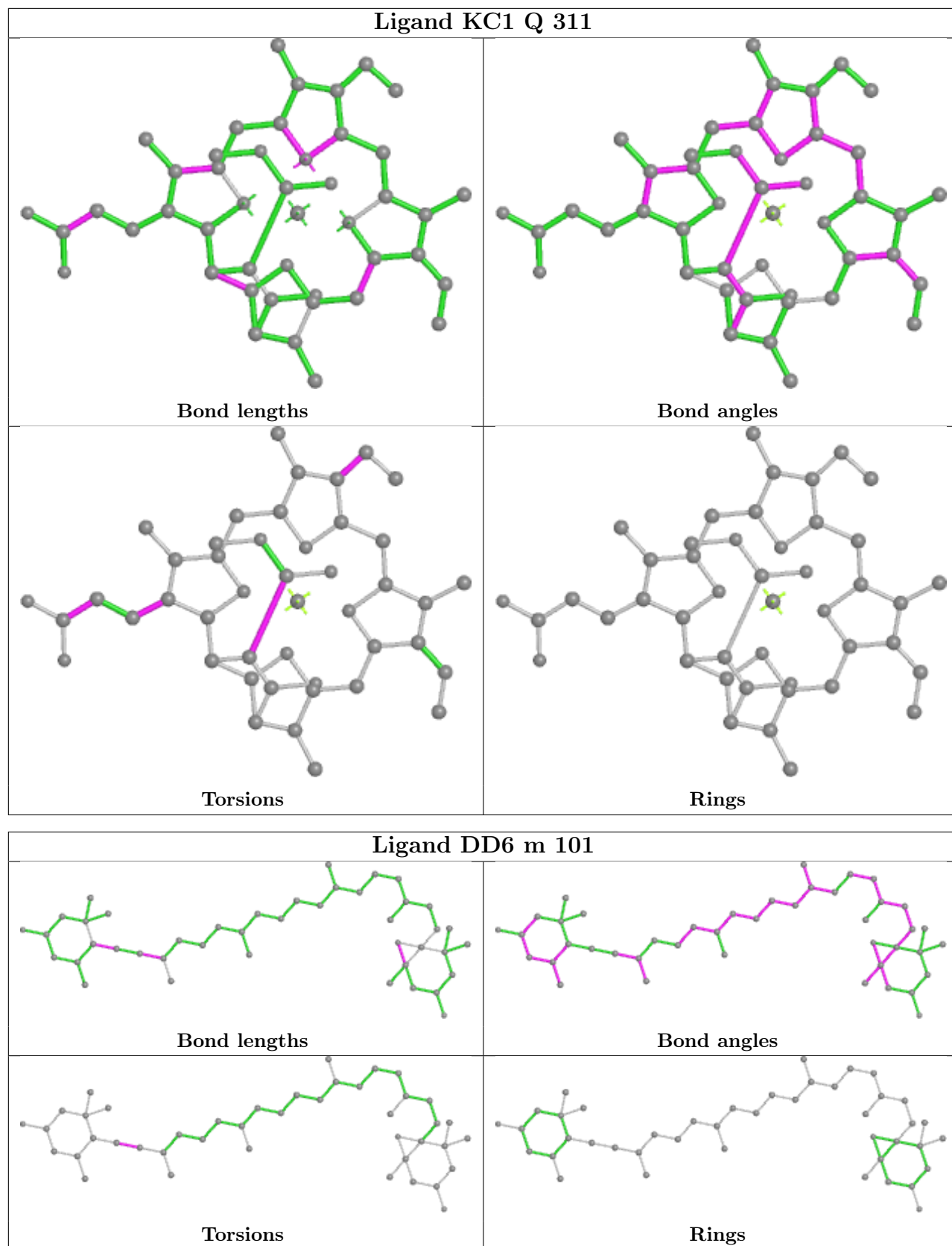


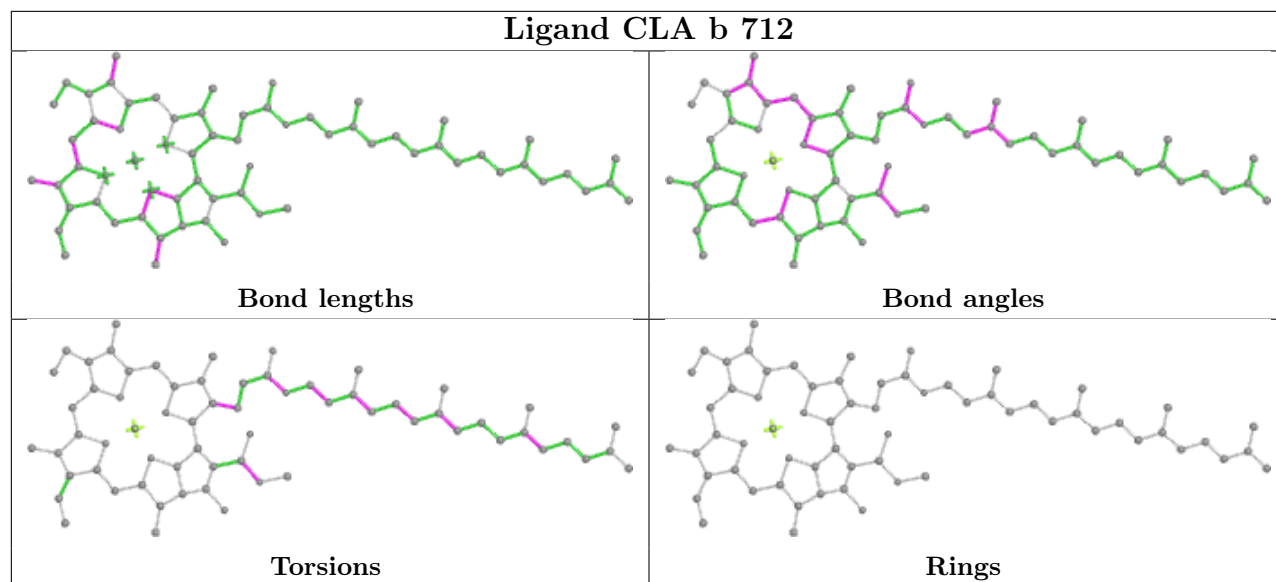












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

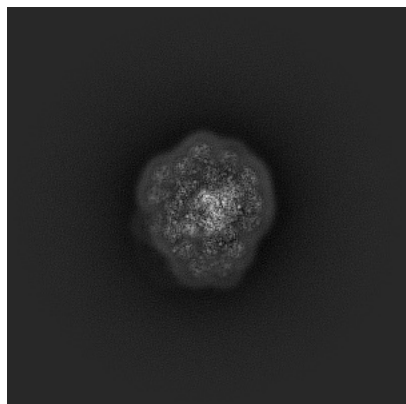
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36678. These allow visual inspection of the internal detail of the map and identification of artifacts.

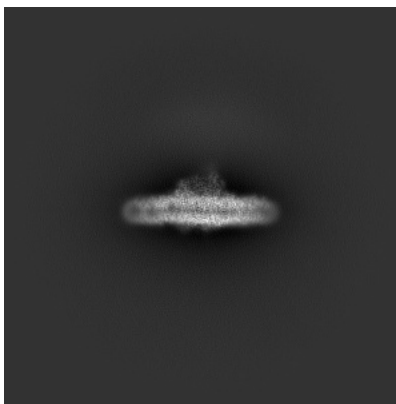
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

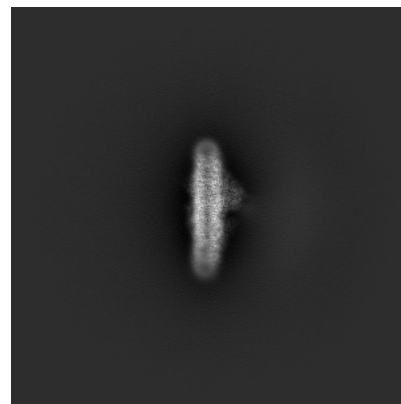
#### 6.1.1 Primary map



X

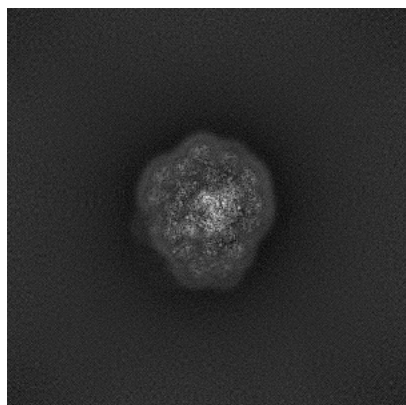


Y

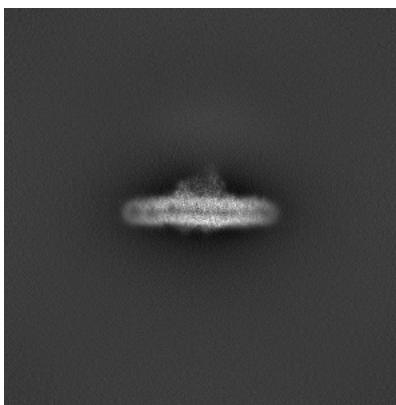


Z

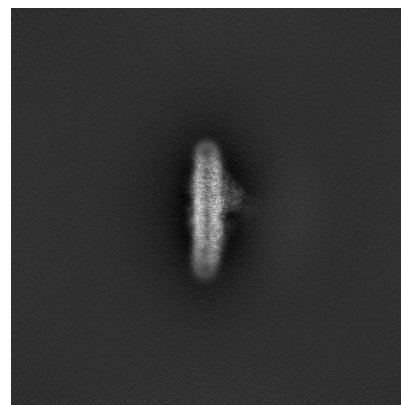
#### 6.1.2 Raw map



X



Y

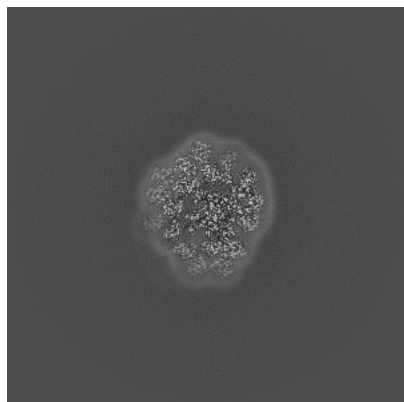


Z

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

## 6.2 Central slices [i](#)

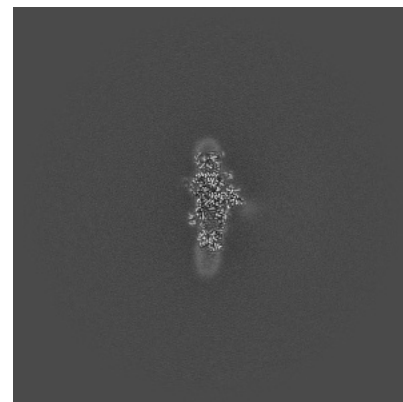
### 6.2.1 Primary map



X Index: 256

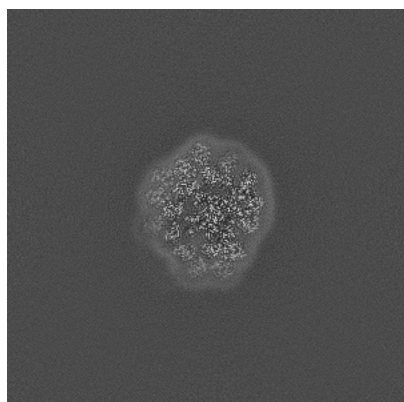


Y Index: 256



Z Index: 256

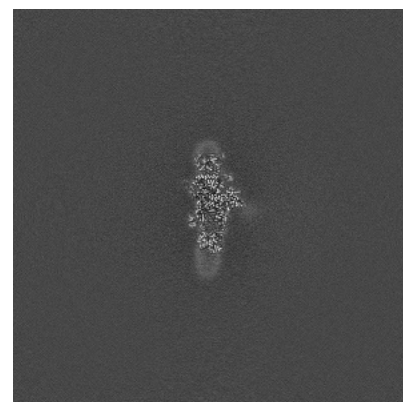
### 6.2.2 Raw map



X Index: 256



Y Index: 256



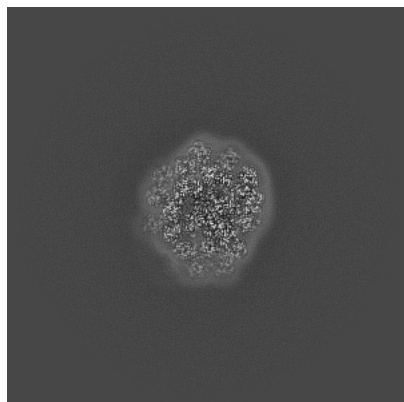
Z Index: 256

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

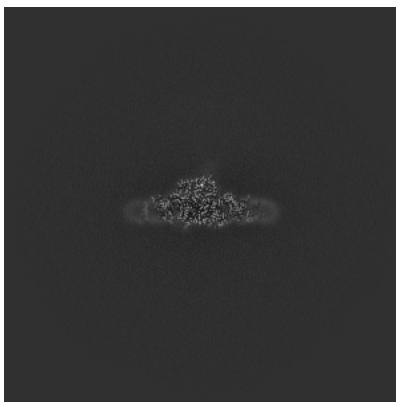


## 6.3 Largest variance slices [i](#)

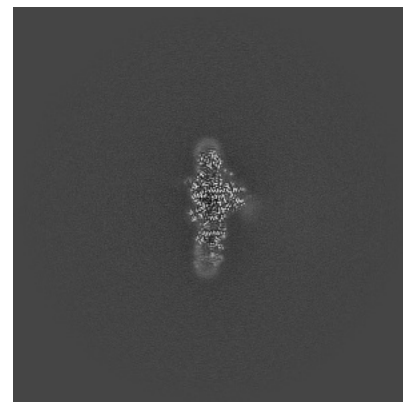
### 6.3.1 Primary map



X Index: 259

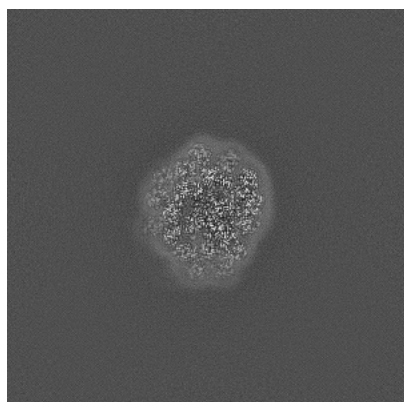


Y Index: 262

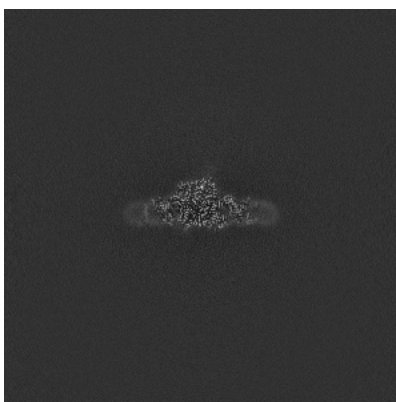


Z Index: 262

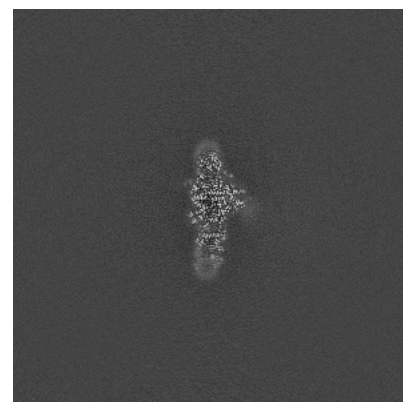
### 6.3.2 Raw map



X Index: 259



Y Index: 262

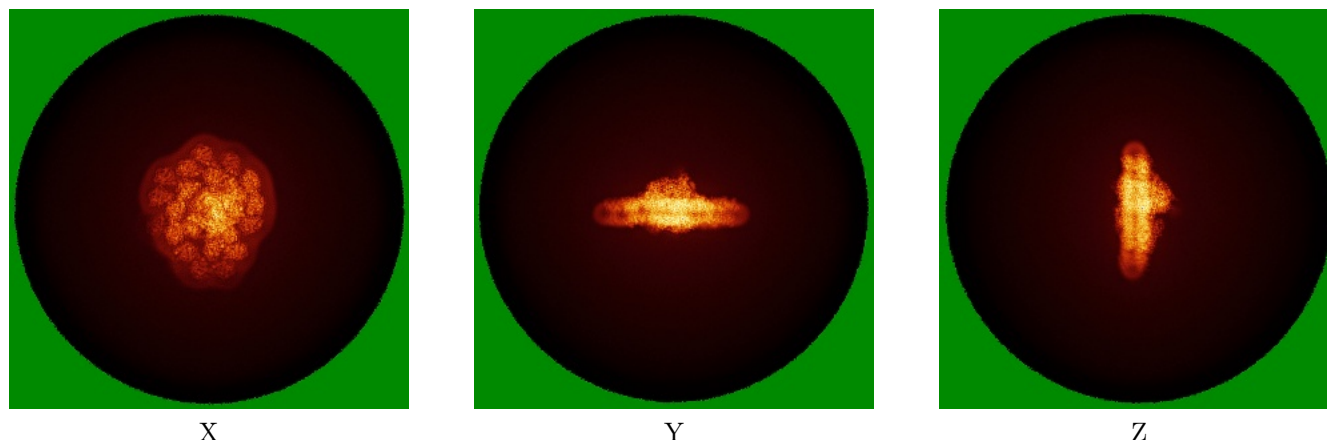


Z Index: 262

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

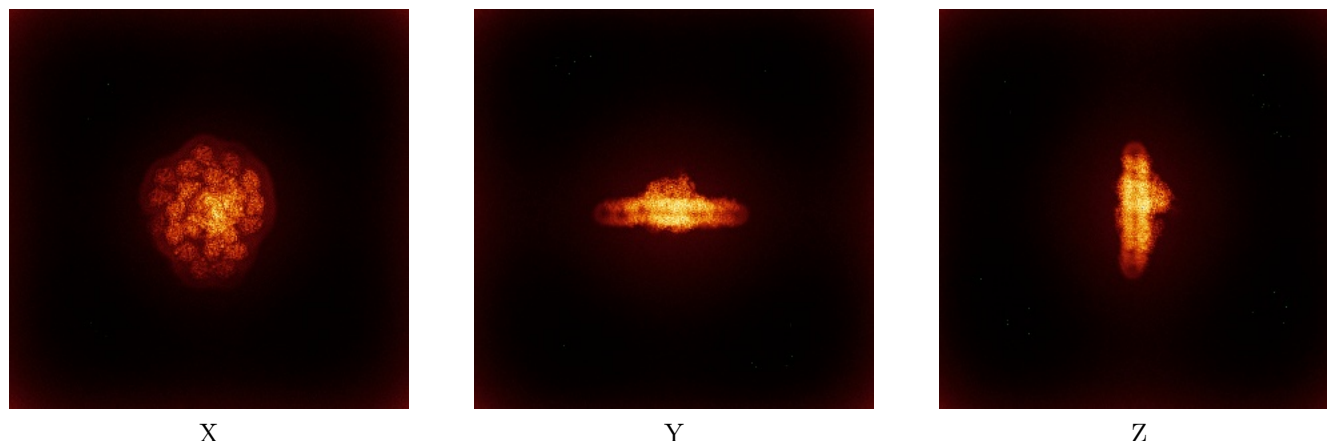


X

Y

Z

### 6.4.2 Raw map



X

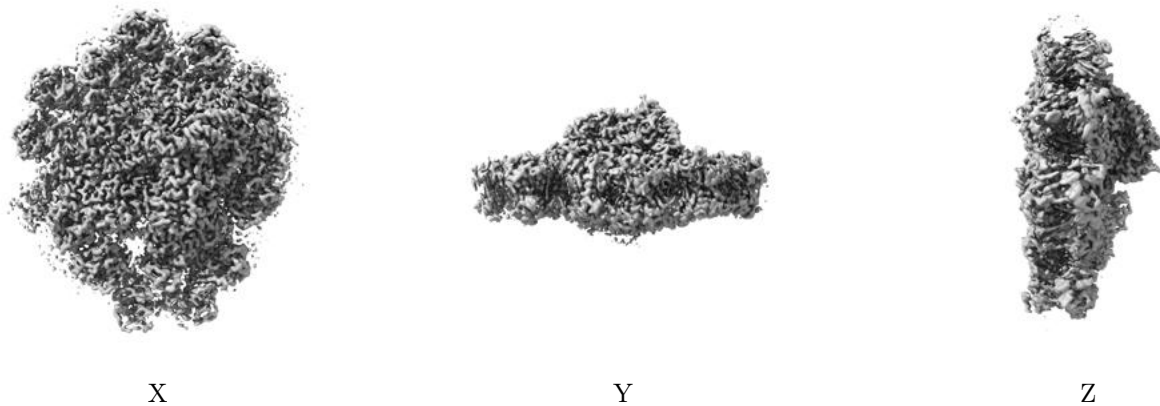
Y

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.

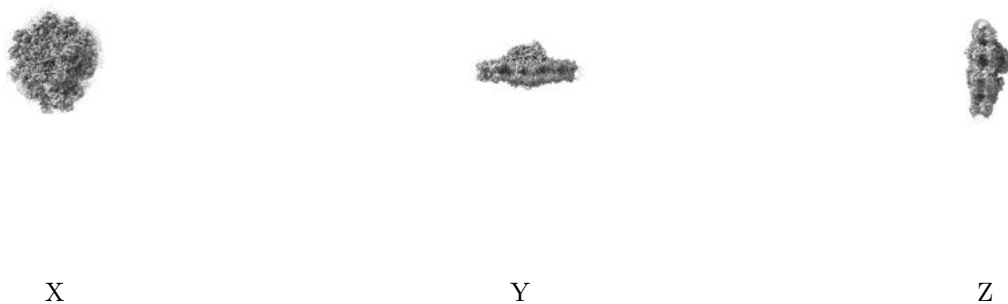
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

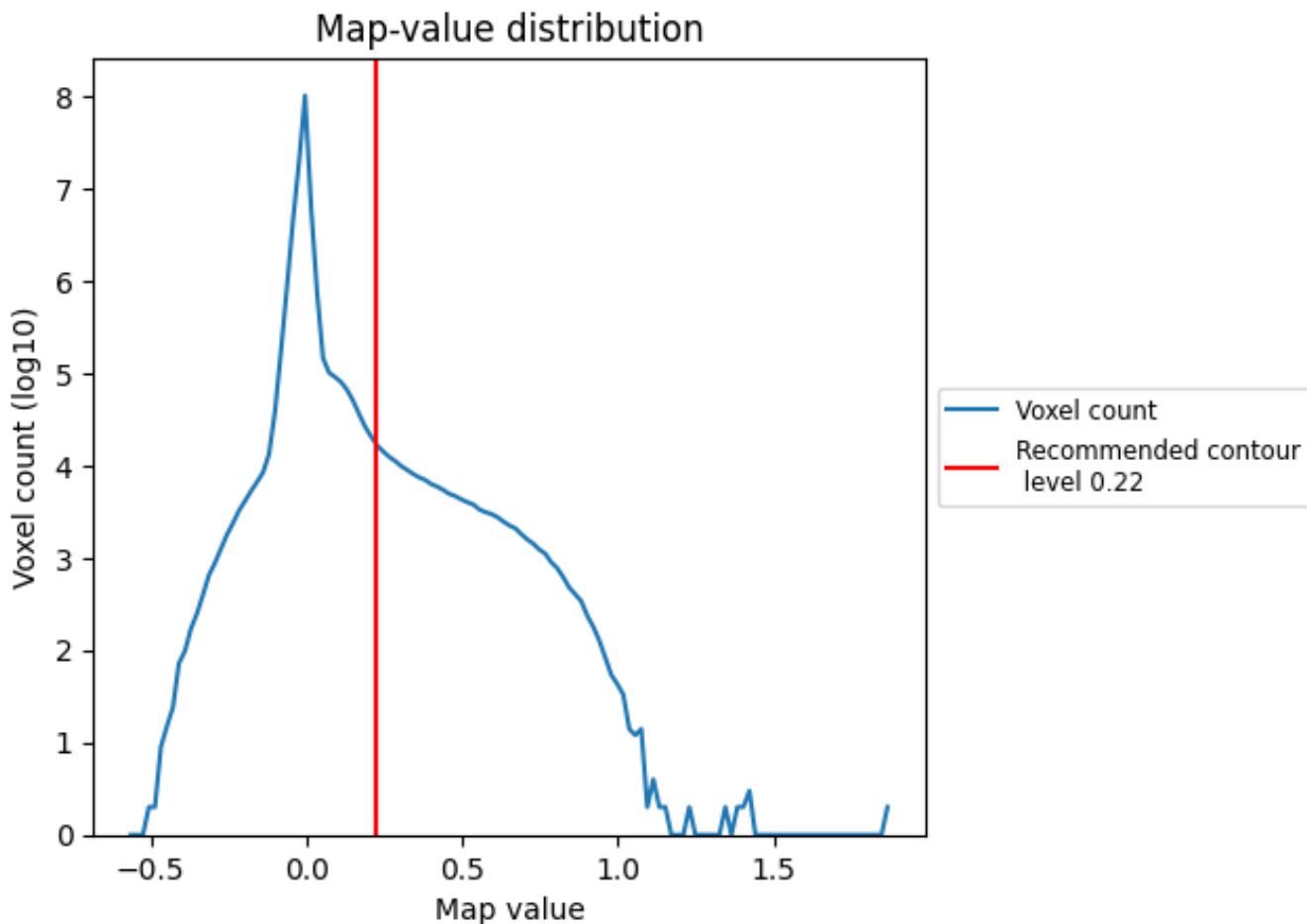
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

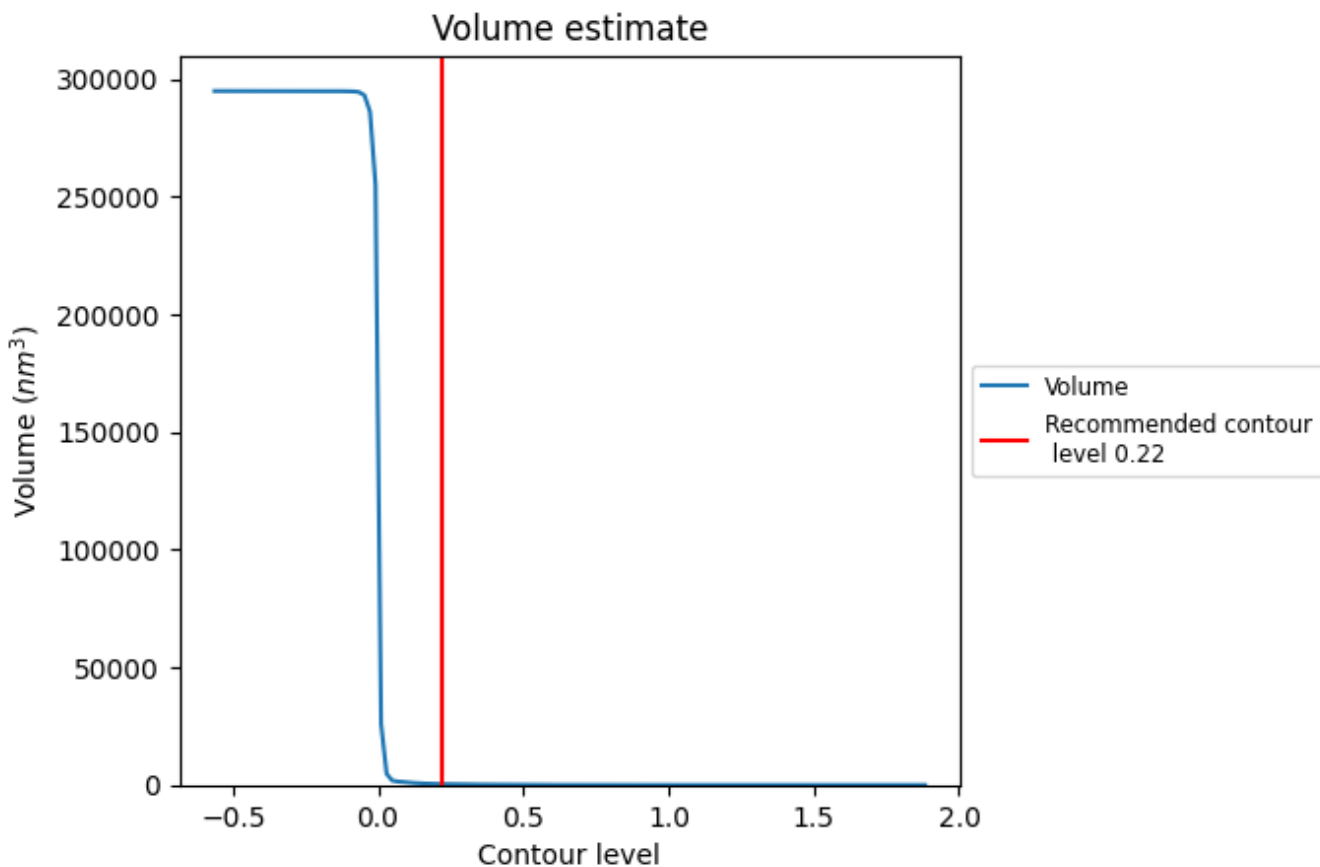
This section contains the results of statistical analysis of the map.

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



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

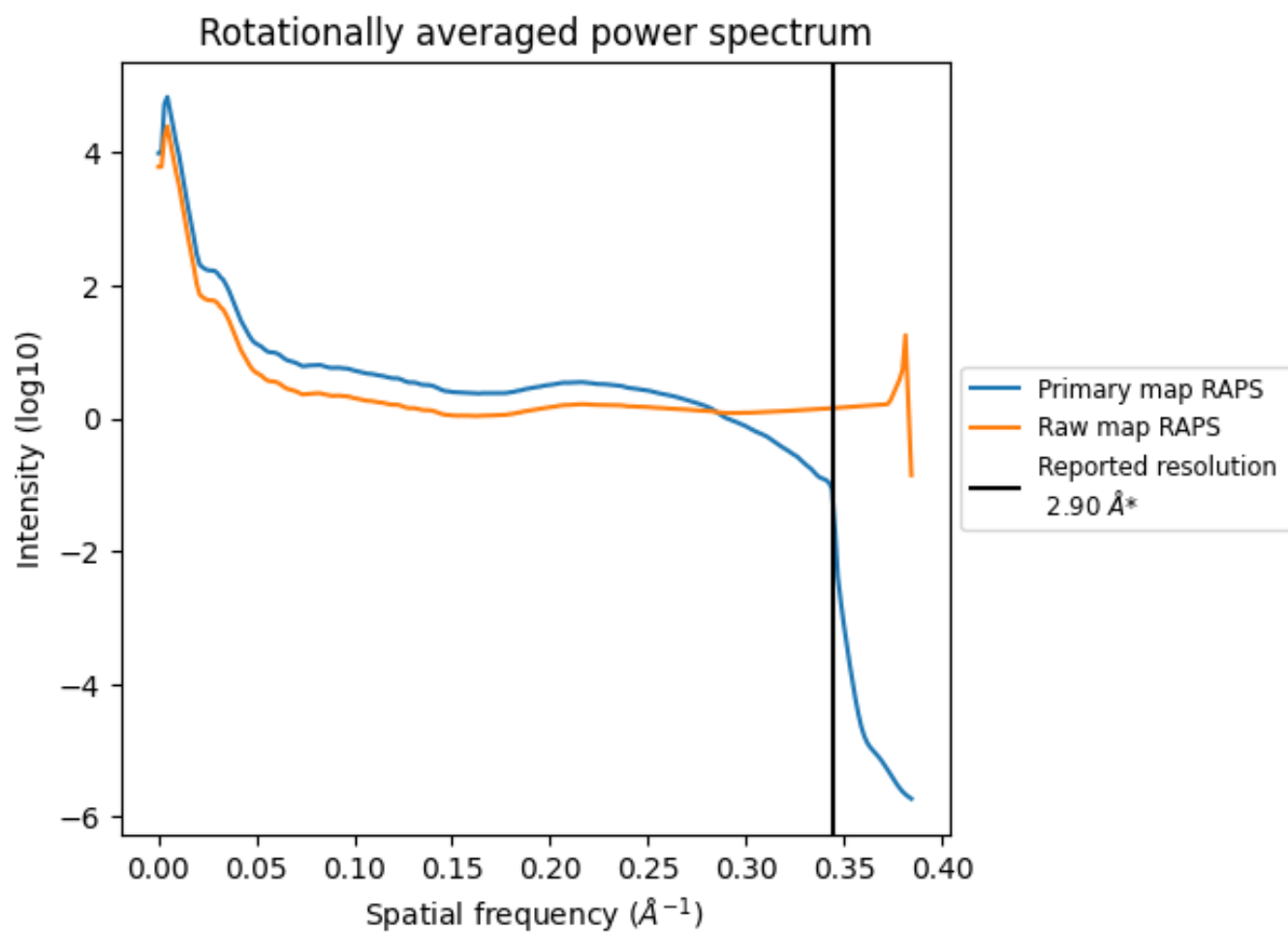
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378  $\text{nm}^3$ ; this corresponds to an approximate mass of 342 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 i

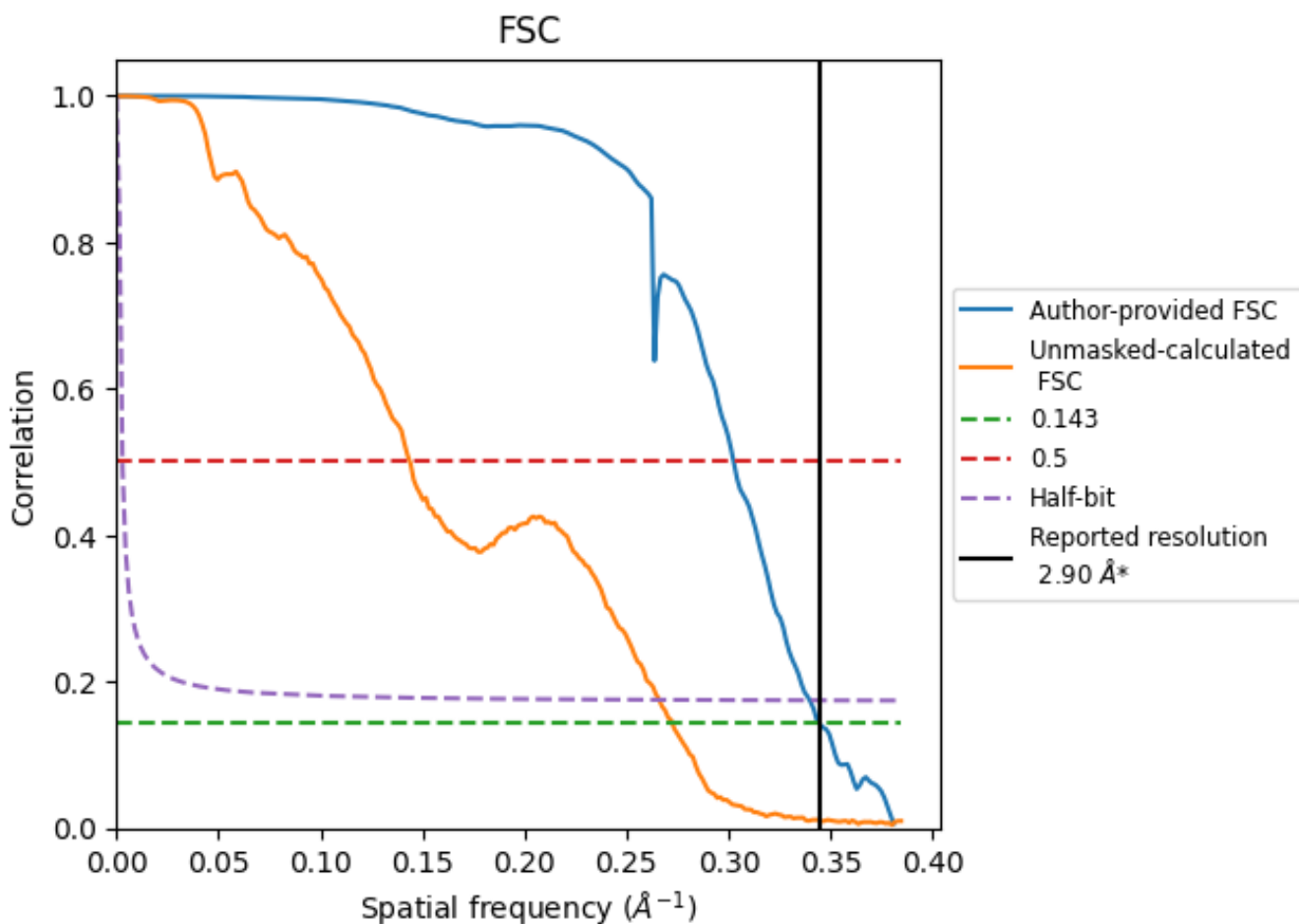


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.31	2.94
Unmasked-calculated*	3.67	6.95	3.76

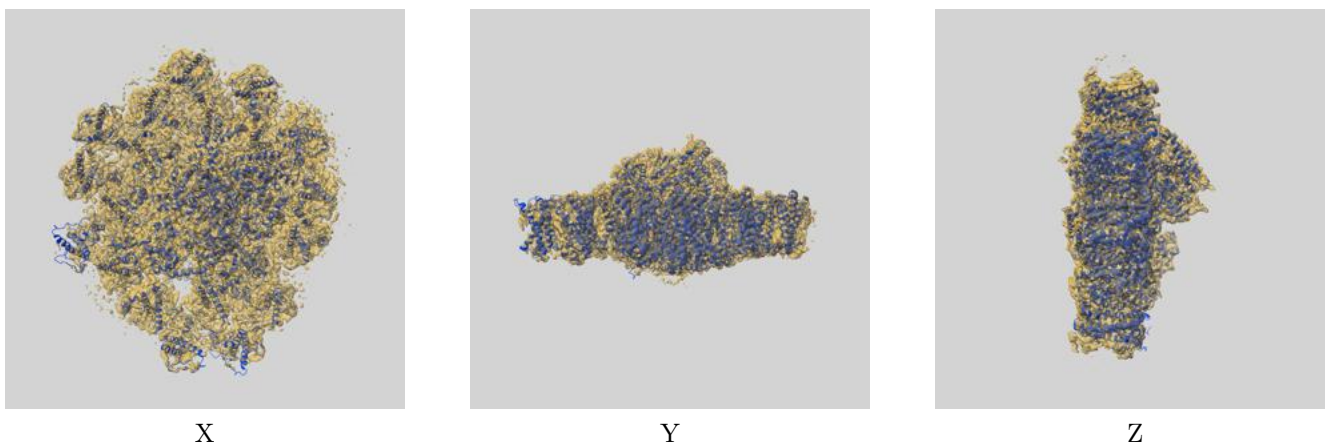
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 2.9 by more than 10 %



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

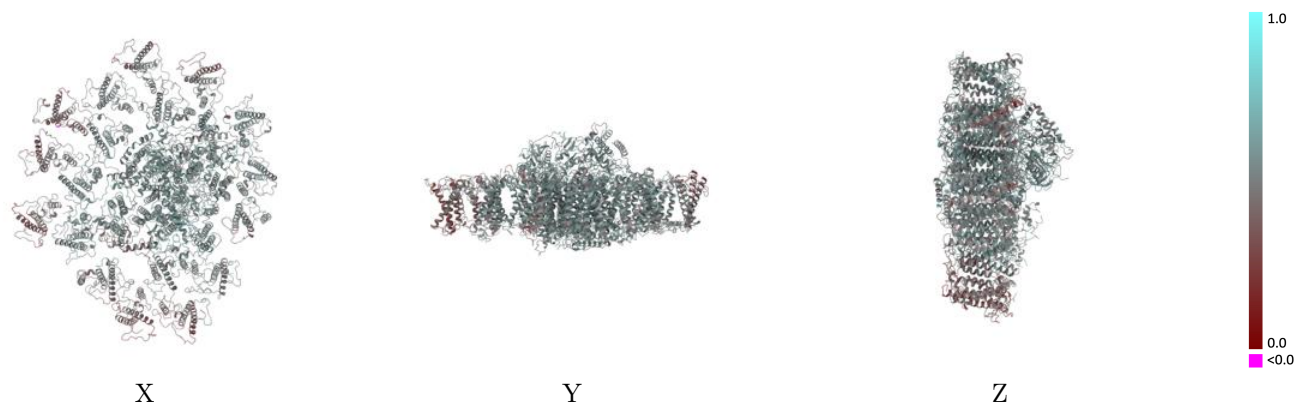
This section contains information regarding the fit between EMDB map EMD-36678 and PDB model 8JW0. Per-residue inclusion information can be found in section 3 on page 40.

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



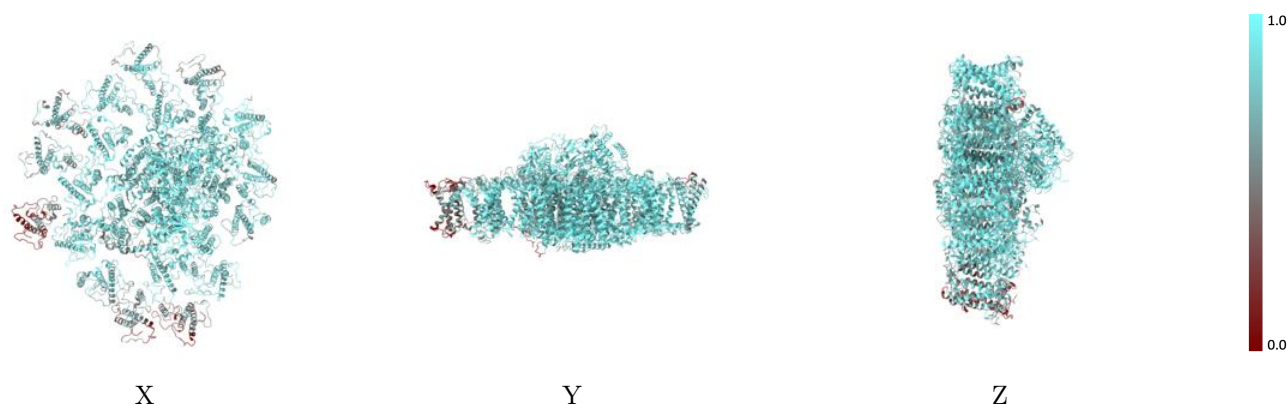
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



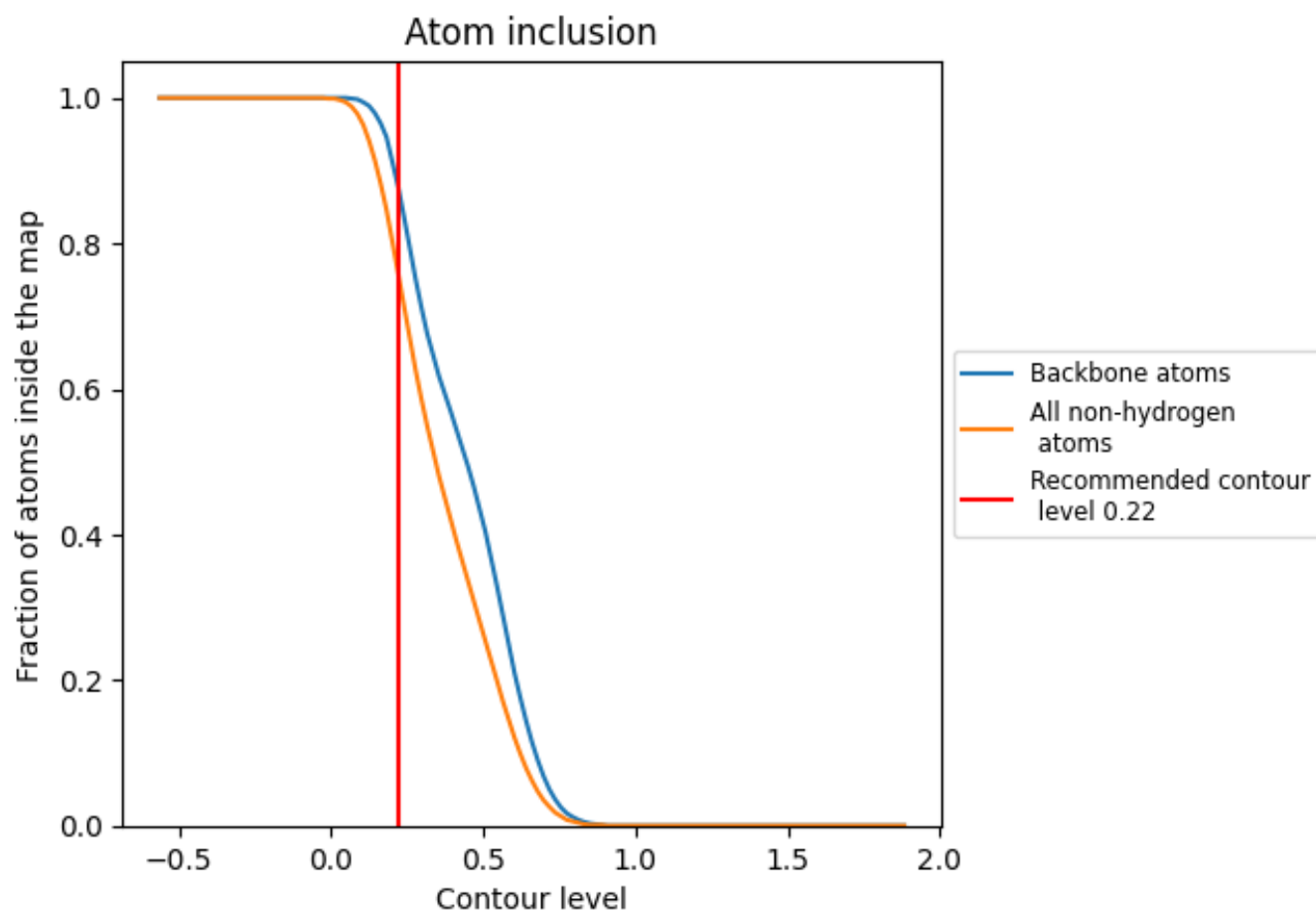
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.22).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 76% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7610	 0.5100
A	 0.8530	 0.5420
B	 0.8250	 0.5400
C	 0.7340	 0.4710
D	 0.6420	 0.4360
E	 0.7510	 0.5040
F	 0.7860	 0.5010
G	 0.8350	 0.5470
H	 0.3850	 0.3860
I	 0.8550	 0.5520
J	 0.8020	 0.5160
K	 0.8480	 0.5520
L	 0.8120	 0.5330
M	 0.7040	 0.4660
N	 0.4320	 0.3830
O	 0.5950	 0.4070
P	 0.2580	 0.3780
Q	 0.8000	 0.5110
T	 0.5580	 0.3790
a	 0.8120	 0.5450
b	 0.8740	 0.5690
c	 0.9430	 0.5590
d	 0.8890	 0.5480
e	 0.9090	 0.5690
f	 0.8360	 0.5440
h	 0.8700	 0.5530
i	 0.8300	 0.5450
j	 0.8020	 0.5450
l	 0.8340	 0.5370
m	 0.7750	 0.5380

