



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 06:36 PM EST

PDB ID : 7UMH  
EMDB ID : EMD-26601  
Title : Energetic robustness to large scale structural dynamics in a photosynthetic supercomplex  
Authors : Harris, D.; Toporik, H.; Schlau-Cohen, G.S.; Mazor, Y.  
Deposited on : 2022-04-07  
Resolution : 2.60 Å(reported)  
Based on initial model : 6NWA

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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39



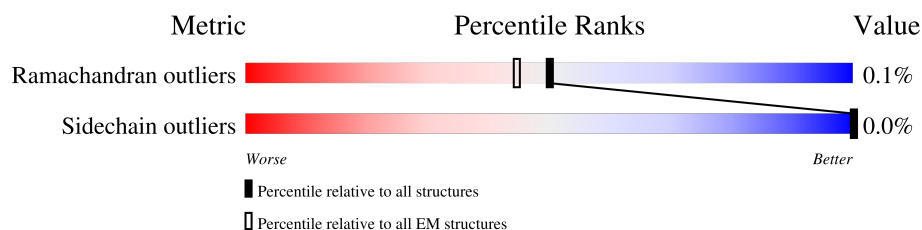
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	751	98% .
1	H	751	98% .
1	a	751	98% .
2	B	731	100%
2	G	731	100%
2	b	731	100%
3	C	81	99% .
3	N	81	99% .
3	c	81	99% .

*Continued on next page...*



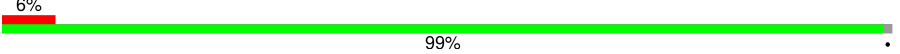
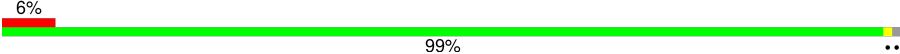

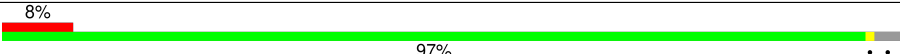
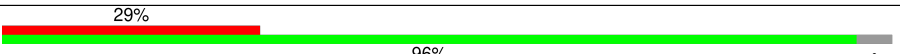
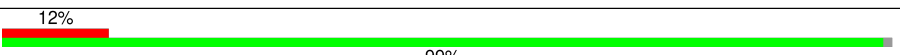
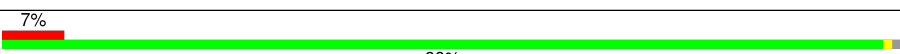
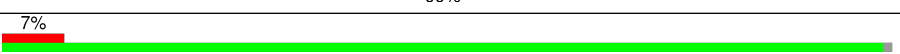
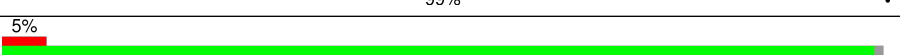
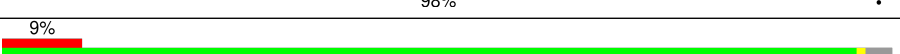
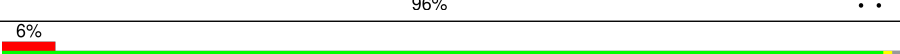
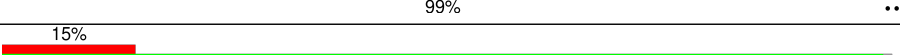
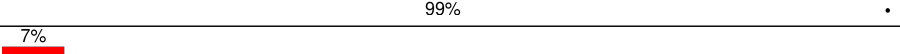
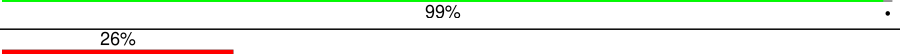
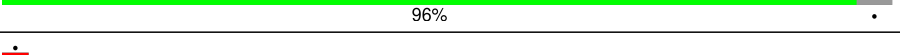
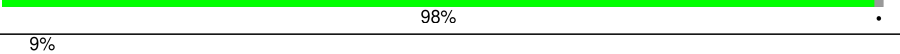
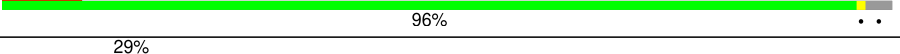
Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	141	
4	P	141	
4	d	141	
5	E	74	
5	O	74	
5	e	74	
6	F	165	
6	Q	165	
6	f	165	
7	I	40	
7	R	40	
7	i	40	
8	J	40	
8	S	40	
8	j	40	
9	K	86	
9	T	86	
9	k	86	
10	L	157	
10	U	157	
10	l	157	
11	M	31	
11	V	31	
11	m	31	
12	W	342	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
12	X	342	
12	Y	342	
12	Z	342	
12	g	342	
12	h	342	
12	n	342	
12	o	342	
12	p	342	
12	q	342	
12	r	342	
12	s	342	
12	t	342	
12	u	342	
12	v	342	
12	w	342	
12	x	342	
12	y	342	

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
15	CL0	A	1011	X	-	-	-
15	CL0	H	1011	X	-	-	-
15	CL0	a	1011	X	-	-	-
16	CLA	A	1013	X	-	-	-
16	CLA	A	1022	X	-	-	-
16	CLA	A	1101	X	-	-	-
16	CLA	A	1102	X	-	-	-
16	CLA	A	1103	X	-	-	-

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	1104	X	-	-	-
16	CLA	A	1105	X	-	-	-
16	CLA	A	1106	X	-	-	-
16	CLA	A	1109	X	-	-	-
16	CLA	A	1110	X	-	-	-
16	CLA	A	1111	X	-	-	-
16	CLA	A	1113	X	-	-	-
16	CLA	A	1114	X	-	-	-
16	CLA	A	1115	X	-	-	-
16	CLA	A	1116	X	-	-	-
16	CLA	A	1117	X	-	-	-
16	CLA	A	1119	X	-	-	-
16	CLA	A	1121	X	-	-	-
16	CLA	A	1122	X	-	-	-
16	CLA	A	1124	X	-	-	-
16	CLA	A	1126	X	-	-	-
16	CLA	A	1127	X	-	-	-
16	CLA	A	1128	X	-	-	-
16	CLA	A	1130	X	-	-	-
16	CLA	A	1132	X	-	-	-
16	CLA	A	1133	X	-	-	-
16	CLA	A	1135	X	-	-	-
16	CLA	A	1136	X	-	-	-
16	CLA	A	1137	X	-	-	-
16	CLA	A	1138	X	-	-	-
16	CLA	A	1139	X	-	-	-
16	CLA	A	1140	X	-	-	-
16	CLA	A	1237	X	-	-	-
16	CLA	A	1801	X	-	-	-
16	CLA	B	1012	X	-	-	-
16	CLA	B	1021	X	-	-	-
16	CLA	B	1201	X	-	-	-
16	CLA	B	1202	X	-	-	-
16	CLA	B	1203	X	-	-	-
16	CLA	B	1204	X	-	-	-
16	CLA	B	1205	X	-	-	-
16	CLA	B	1206	X	-	-	-
16	CLA	B	1208	X	-	-	-
16	CLA	B	1209	X	-	-	-
16	CLA	B	1211	X	-	-	-
16	CLA	B	1212	X	-	-	-
16	CLA	B	1213	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	1214	X	-	-	-
16	CLA	B	1215	X	-	-	-
16	CLA	B	1220	X	-	-	-
16	CLA	B	1223	X	-	-	-
16	CLA	B	1224	X	-	-	-
16	CLA	B	1227	X	-	-	-
16	CLA	B	1229	X	-	-	-
16	CLA	B	1230	X	-	-	-
16	CLA	B	1231	X	-	-	-
16	CLA	B	1232	X	-	-	-
16	CLA	B	1234	X	-	-	-
16	CLA	B	1235	X	-	-	-
16	CLA	B	1236	X	-	-	-
16	CLA	B	1238	X	-	-	-
16	CLA	B	1240	X	-	-	-
16	CLA	F	1301	X	-	-	-
16	CLA	F	1302	X	-	-	-
16	CLA	G	1012	X	-	-	-
16	CLA	G	1021	X	-	-	-
16	CLA	G	1201	X	-	-	-
16	CLA	G	1202	X	-	-	-
16	CLA	G	1203	X	-	-	-
16	CLA	G	1204	X	-	-	-
16	CLA	G	1205	X	-	-	-
16	CLA	G	1206	X	-	-	-
16	CLA	G	1208	X	-	-	-
16	CLA	G	1209	X	-	-	-
16	CLA	G	1212	X	-	-	-
16	CLA	G	1213	X	-	-	-
16	CLA	G	1214	X	-	-	-
16	CLA	G	1215	X	-	-	-
16	CLA	G	1216	X	-	-	-
16	CLA	G	1220	X	-	-	-
16	CLA	G	1221	X	-	-	-
16	CLA	G	1223	X	-	-	-
16	CLA	G	1224	X	-	-	-
16	CLA	G	1225	X	-	-	-
16	CLA	G	1228	X	-	-	-
16	CLA	G	1229	X	-	-	-
16	CLA	G	1230	X	-	-	-
16	CLA	G	1231	X	-	-	-
16	CLA	G	1232	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	G	1234	X	-	-	-
16	CLA	G	1235	X	-	-	-
16	CLA	G	1238	X	-	-	-
16	CLA	G	1239	X	-	-	-
16	CLA	G	1240	X	-	-	-
16	CLA	H	1013	X	-	-	-
16	CLA	H	1022	X	-	-	-
16	CLA	H	1101	X	-	-	-
16	CLA	H	1102	X	-	-	-
16	CLA	H	1103	X	-	-	-
16	CLA	H	1104	X	-	-	-
16	CLA	H	1105	X	-	-	-
16	CLA	H	1106	X	-	-	-
16	CLA	H	1109	X	-	-	-
16	CLA	H	1110	X	-	-	-
16	CLA	H	1111	X	-	-	-
16	CLA	H	1113	X	-	-	-
16	CLA	H	1114	X	-	-	-
16	CLA	H	1116	X	-	-	-
16	CLA	H	1117	X	-	-	-
16	CLA	H	1119	X	-	-	-
16	CLA	H	1121	X	-	-	-
16	CLA	H	1124	X	-	-	-
16	CLA	H	1126	X	-	-	-
16	CLA	H	1127	X	-	-	-
16	CLA	H	1128	X	-	-	-
16	CLA	H	1131	X	-	-	-
16	CLA	H	1132	X	-	-	-
16	CLA	H	1136	X	-	-	-
16	CLA	H	1137	X	-	-	-
16	CLA	H	1138	X	-	-	-
16	CLA	H	1139	X	-	-	-
16	CLA	H	1140	X	-	-	-
16	CLA	H	1237	X	-	-	-
16	CLA	H	1801	X	-	-	-
16	CLA	J	1302	X	-	-	-
16	CLA	K	4002	X	-	-	-
16	CLA	K	4003	X	-	-	-
16	CLA	K	4004	X	-	-	-
16	CLA	L	1503	X	-	-	-
16	CLA	Q	1301	X	-	-	-
16	CLA	Q	1302	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	S	1302	X	-	-	-
16	CLA	T	4002	X	-	-	-
16	CLA	T	4003	X	-	-	-
16	CLA	U	1503	X	-	-	-
16	CLA	W	501	X	-	-	-
16	CLA	W	502	X	-	-	-
16	CLA	W	503	X	-	-	-
16	CLA	W	504	X	-	-	-
16	CLA	W	505	X	-	-	-
16	CLA	W	508	X	-	-	-
16	CLA	W	509	X	-	-	-
16	CLA	W	511	X	-	-	-
16	CLA	W	512	X	-	-	-
16	CLA	W	514	X	-	-	-
16	CLA	W	515	X	-	-	-
16	CLA	W	517	X	-	-	-
16	CLA	X	502	X	-	-	-
16	CLA	X	505	X	-	-	-
16	CLA	X	506	X	-	-	-
16	CLA	X	508	X	-	-	-
16	CLA	X	509	X	-	-	-
16	CLA	X	511	X	-	-	-
16	CLA	X	514	X	-	-	-
16	CLA	X	515	X	-	-	-
16	CLA	Y	501	X	-	-	-
16	CLA	Y	502	X	-	-	-
16	CLA	Y	503	X	-	-	-
16	CLA	Y	504	X	-	-	-
16	CLA	Y	505	X	-	-	-
16	CLA	Y	508	X	-	-	-
16	CLA	Y	509	X	-	-	-
16	CLA	Y	511	X	-	-	-
16	CLA	Y	512	X	-	-	-
16	CLA	Y	514	X	-	-	-
16	CLA	Y	515	X	-	-	-
16	CLA	Z	501	X	-	-	-
16	CLA	Z	502	X	-	-	-
16	CLA	Z	503	X	-	-	-
16	CLA	Z	504	X	-	-	-
16	CLA	Z	505	X	-	-	-
16	CLA	Z	507	X	-	-	-
16	CLA	Z	508	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	Z	509	X	-	-	-
16	CLA	Z	511	X	-	-	-
16	CLA	Z	512	X	-	-	-
16	CLA	Z	514	X	-	-	-
16	CLA	Z	515	X	-	-	-
16	CLA	Z	516	X	-	-	-
16	CLA	Z	517	X	-	-	-
16	CLA	a	1013	X	-	-	-
16	CLA	a	1022	X	-	-	-
16	CLA	a	1101	X	-	-	-
16	CLA	a	1102	X	-	-	-
16	CLA	a	1103	X	-	-	-
16	CLA	a	1104	X	-	-	-
16	CLA	a	1105	X	-	-	-
16	CLA	a	1106	X	-	-	-
16	CLA	a	1109	X	-	-	-
16	CLA	a	1110	X	-	-	-
16	CLA	a	1111	X	-	-	-
16	CLA	a	1113	X	-	-	-
16	CLA	a	1114	X	-	-	-
16	CLA	a	1115	X	-	-	-
16	CLA	a	1116	X	-	-	-
16	CLA	a	1117	X	-	-	-
16	CLA	a	1119	X	-	-	-
16	CLA	a	1121	X	-	-	-
16	CLA	a	1124	X	-	-	-
16	CLA	a	1126	X	-	-	-
16	CLA	a	1127	X	-	-	-
16	CLA	a	1128	X	-	-	-
16	CLA	a	1132	X	-	-	-
16	CLA	a	1135	X	-	-	-
16	CLA	a	1136	X	-	-	-
16	CLA	a	1137	X	-	-	-
16	CLA	a	1138	X	-	-	-
16	CLA	a	1139	X	-	-	-
16	CLA	a	1237	X	-	-	-
16	CLA	a	1801	X	-	-	-
16	CLA	b	1012	X	-	-	-
16	CLA	b	1021	X	-	-	-
16	CLA	b	1201	X	-	-	-
16	CLA	b	1202	X	-	-	-
16	CLA	b	1203	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	b	1204	X	-	-	-
16	CLA	b	1205	X	-	-	-
16	CLA	b	1206	X	-	-	-
16	CLA	b	1208	X	-	-	-
16	CLA	b	1209	X	-	-	-
16	CLA	b	1210	X	-	-	-
16	CLA	b	1211	X	-	-	-
16	CLA	b	1212	X	-	-	-
16	CLA	b	1213	X	-	-	-
16	CLA	b	1214	X	-	-	-
16	CLA	b	1216	X	-	-	-
16	CLA	b	1221	X	-	-	-
16	CLA	b	1223	X	-	-	-
16	CLA	b	1224	X	-	-	-
16	CLA	b	1226	X	-	-	-
16	CLA	b	1227	X	-	-	-
16	CLA	b	1228	X	-	-	-
16	CLA	b	1229	X	-	-	-
16	CLA	b	1231	X	-	-	-
16	CLA	b	1232	X	-	-	-
16	CLA	b	1234	X	-	-	-
16	CLA	b	1235	X	-	-	-
16	CLA	b	1238	X	-	-	-
16	CLA	b	1240	X	-	-	-
16	CLA	f	1301	X	-	-	-
16	CLA	f	1302	X	-	-	-
16	CLA	g	502	X	-	-	-
16	CLA	g	504	X	-	-	-
16	CLA	g	505	X	-	-	-
16	CLA	g	507	X	-	-	-
16	CLA	g	508	X	-	-	-
16	CLA	g	509	X	-	-	-
16	CLA	g	511	X	-	-	-
16	CLA	g	512	X	-	-	-
16	CLA	g	514	X	-	-	-
16	CLA	g	515	X	-	-	-
16	CLA	g	516	X	-	-	-
16	CLA	h	502	X	-	-	-
16	CLA	h	503	X	-	-	-
16	CLA	h	506	X	-	-	-
16	CLA	h	507	X	-	-	-
16	CLA	h	508	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	h	509	X	-	-	-
16	CLA	h	511	X	-	-	-
16	CLA	h	513	X	-	-	-
16	CLA	h	515	X	-	-	-
16	CLA	h	516	X	-	-	-
16	CLA	h	517	X	-	-	-
16	CLA	k	4002	X	-	-	-
16	CLA	k	4003	X	-	-	-
16	CLA	k	4004	X	-	-	-
16	CLA	l	1503	X	-	-	-
16	CLA	n	501	X	-	-	-
16	CLA	n	502	X	-	-	-
16	CLA	n	503	X	-	-	-
16	CLA	n	505	X	-	-	-
16	CLA	n	507	X	-	-	-
16	CLA	n	508	X	-	-	-
16	CLA	n	509	X	-	-	-
16	CLA	n	512	X	-	-	-
16	CLA	n	514	X	-	-	-
16	CLA	n	515	X	-	-	-
16	CLA	n	517	X	-	-	-
16	CLA	o	502	X	-	-	-
16	CLA	o	505	X	-	-	-
16	CLA	o	506	X	-	-	-
16	CLA	o	508	X	-	-	-
16	CLA	o	509	X	-	-	-
16	CLA	o	511	X	-	-	-
16	CLA	o	512	X	-	-	-
16	CLA	o	514	X	-	-	-
16	CLA	o	515	X	-	-	-
16	CLA	p	501	X	-	-	-
16	CLA	p	502	X	-	-	-
16	CLA	p	503	X	-	-	-
16	CLA	p	508	X	-	-	-
16	CLA	p	509	X	-	-	-
16	CLA	p	511	X	-	-	-
16	CLA	p	512	X	-	-	-
16	CLA	p	514	X	-	-	-
16	CLA	p	515	X	-	-	-
16	CLA	p	516	X	-	-	-
16	CLA	q	501	X	-	-	-
16	CLA	q	502	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	q	503	X	-	-	-
16	CLA	q	504	X	-	-	-
16	CLA	q	505	X	-	-	-
16	CLA	q	506	X	-	-	-
16	CLA	q	507	X	-	-	-
16	CLA	q	508	X	-	-	-
16	CLA	q	509	X	-	-	-
16	CLA	q	512	X	-	-	-
16	CLA	q	514	X	-	-	-
16	CLA	q	515	X	-	-	-
16	CLA	q	516	X	-	-	-
16	CLA	r	501	X	-	-	-
16	CLA	r	502	X	-	-	-
16	CLA	r	504	X	-	-	-
16	CLA	r	507	X	-	-	-
16	CLA	r	508	X	-	-	-
16	CLA	r	511	X	-	-	-
16	CLA	r	512	X	-	-	-
16	CLA	r	514	X	-	-	-
16	CLA	r	515	X	-	-	-
16	CLA	r	516	X	-	-	-
16	CLA	s	501	X	-	-	-
16	CLA	s	502	X	-	-	-
16	CLA	s	503	X	-	-	-
16	CLA	s	504	X	-	-	-
16	CLA	s	505	X	-	-	-
16	CLA	s	508	X	-	-	-
16	CLA	s	509	X	-	-	-
16	CLA	s	511	X	-	-	-
16	CLA	s	512	X	-	-	-
16	CLA	s	514	X	-	-	-
16	CLA	s	515	X	-	-	-
16	CLA	t	501	X	-	-	-
16	CLA	t	502	X	-	-	-
16	CLA	t	503	X	-	-	-
16	CLA	t	504	X	-	-	-
16	CLA	t	506	X	-	-	-
16	CLA	t	507	X	-	-	-
16	CLA	t	508	X	-	-	-
16	CLA	t	509	X	-	-	-
16	CLA	t	511	X	-	-	-
16	CLA	t	512	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	t	514	X	-	-	-
16	CLA	t	515	X	-	-	-
16	CLA	t	516	X	-	-	-
16	CLA	t	517	X	-	-	-
16	CLA	u	502	X	-	-	-
16	CLA	u	505	X	-	-	-
16	CLA	u	506	X	-	-	-
16	CLA	u	507	X	-	-	-
16	CLA	u	508	X	-	-	-
16	CLA	u	509	X	-	-	-
16	CLA	u	511	X	-	-	-
16	CLA	u	514	X	-	-	-
16	CLA	u	516	X	-	-	-
16	CLA	v	502	X	-	-	-
16	CLA	v	503	X	-	-	-
16	CLA	v	504	X	-	-	-
16	CLA	v	506	X	-	-	-
16	CLA	v	508	X	-	-	-
16	CLA	v	511	X	-	-	-
16	CLA	v	513	X	-	-	-
16	CLA	v	514	X	-	-	-
16	CLA	v	515	X	-	-	-
16	CLA	v	516	X	-	-	-
16	CLA	v	517	X	-	-	-
16	CLA	w	501	X	-	-	-
16	CLA	w	502	X	-	-	-
16	CLA	w	503	X	-	-	-
16	CLA	w	504	X	-	-	-
16	CLA	w	507	X	-	-	-
16	CLA	w	508	X	-	-	-
16	CLA	w	509	X	-	-	-
16	CLA	w	511	X	-	-	-
16	CLA	w	512	X	-	-	-
16	CLA	w	514	X	-	-	-
16	CLA	w	515	X	-	-	-
16	CLA	w	516	X	-	-	-
16	CLA	w	517	X	-	-	-
16	CLA	x	502	X	-	-	-
16	CLA	x	504	X	-	-	-
16	CLA	x	505	X	-	-	-
16	CLA	x	507	X	-	-	-
16	CLA	x	508	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	x	509	X	-	-	-
16	CLA	x	514	X	-	-	-
16	CLA	x	515	X	-	-	-
16	CLA	x	516	X	-	-	-
16	CLA	y	501	X	-	-	-
16	CLA	y	502	X	-	-	-
16	CLA	y	503	X	-	-	-
16	CLA	y	505	X	-	-	-
16	CLA	y	506	X	-	-	-
16	CLA	y	508	X	-	-	-
16	CLA	y	509	X	-	-	-
16	CLA	y	511	X	-	-	-
16	CLA	y	513	X	-	-	-
16	CLA	y	515	X	-	-	-
16	CLA	y	516	X	-	-	-
16	CLA	y	517	X	-	-	-



## 2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 140516 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 P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	H	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	a	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	G	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	b	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	N	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		
4	d	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	68	Total	C	N	O		0	0
			537	337	95	105			
5	O	68	Total	C	N	O		0	0
			537	337	95	105			
5	e	68	Total	C	N	O		0	0
			537	337	95	105			

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	Q	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	f	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	R	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	i	37	Total	C	N	O	S	0	0
			293	200	41	49	3		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			311	210	46	52	3		
8	S	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	T	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	k	77	Total	C	N	O	S	0	0
			538	353	89	92	4		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	U	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	l	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	V	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is a protein called Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	X	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	Y	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		

*Continued on next page...*

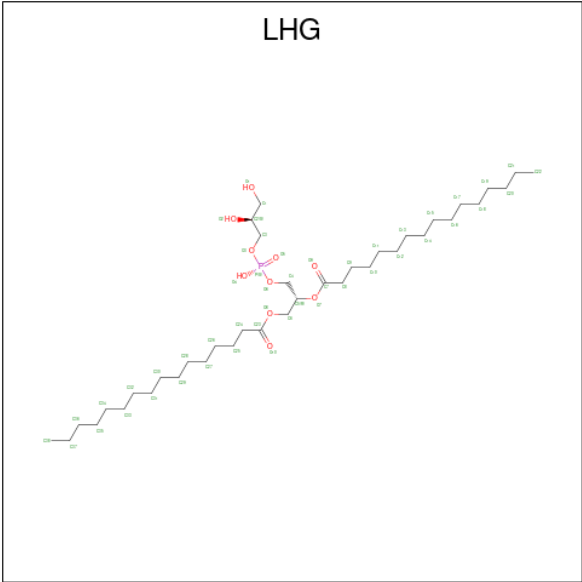


*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	g	333	Total	C	N	O	S	0	0
			2573	1714	420	434	5		
12	h	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	n	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	o	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	p	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		
12	q	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	r	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	s	339	Total	C	N	O	S	0	0
			2617	1741	427	444	5		
12	t	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	u	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	v	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	w	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	x	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	y	330	Total	C	N	O	S	0	0
			2532	1689	409	429	5		

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).





Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			43	32	10	1	
13	A	1	Total	C	O	P	0
			26	15	10	1	
13	B	1	Total	C	O	P	0
			38	27	10	1	
13	G	1	Total	C	O	P	0
			38	27	10	1	
13	H	1	Total	C	O	P	0
			43	32	10	1	
13	H	1	Total	C	O	P	0
			26	15	10	1	
13	I	1	Total	C	O	P	0
			40	29	10	1	
13	R	1	Total	C	O	P	0
			40	29	10	1	
13	X	1	Total	C	O	P	0
			27	16	10	1	
13	Y	1	Total	C	O	P	0
			32	21	10	1	
13	a	1	Total	C	O	P	0
			43	32	10	1	
13	a	1	Total	C	O	P	0
			26	15	10	1	
13	b	1	Total	C	O	P	0
			38	27	10	1	
13	g	1	Total	C	O	P	0
			31	20	10	1	

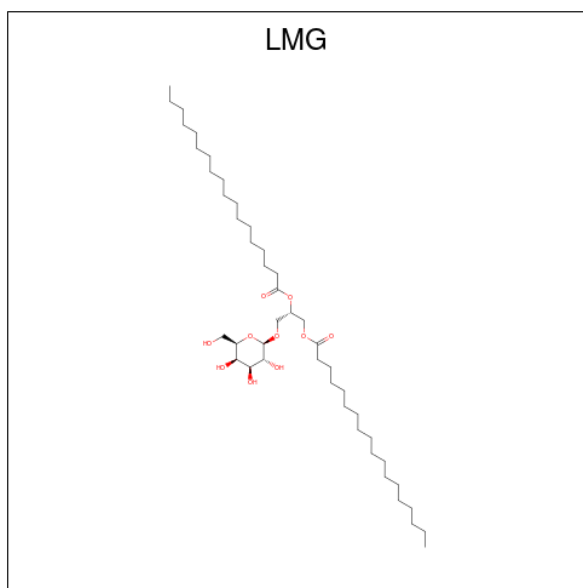
Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
13	i	1	Total	C	O	P	0
			40	29	10	1	
13	o	1	Total	C	O	P	0
			27	16	10	1	
13	p	1	Total	C	O	P	0
			32	21	10	1	
13	r	1	Total	C	O	P	0
			31	20	10	1	
13	s	1	Total	C	O	P	0
			32	21	10	1	
13	u	1	Total	C	O	P	0
			27	16	10	1	
13	x	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O		0
			38	28	10		
14	A	1	Total	C	O		0
			46	36	10		
14	A	1	Total	C	O		0
			32	22	10		
14	B	1	Total	C	O		0
			43	33	10		

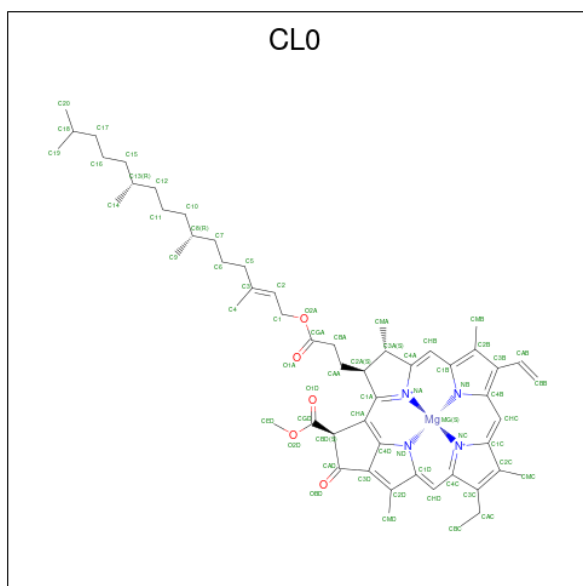
Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
14	F	1	Total	C	O	0
			27	17	10	
14	G	1	Total	C	O	0
			43	33	10	
14	H	1	Total	C	O	0
			38	28	10	
14	H	1	Total	C	O	0
			46	36	10	
14	H	1	Total	C	O	0
			32	22	10	
14	Q	1	Total	C	O	0
			27	17	10	
14	a	1	Total	C	O	0
			38	28	10	
14	a	1	Total	C	O	0
			46	36	10	
14	a	1	Total	C	O	0
			32	22	10	
14	b	1	Total	C	O	0
			43	33	10	
14	f	1	Total	C	O	0
			27	17	10	

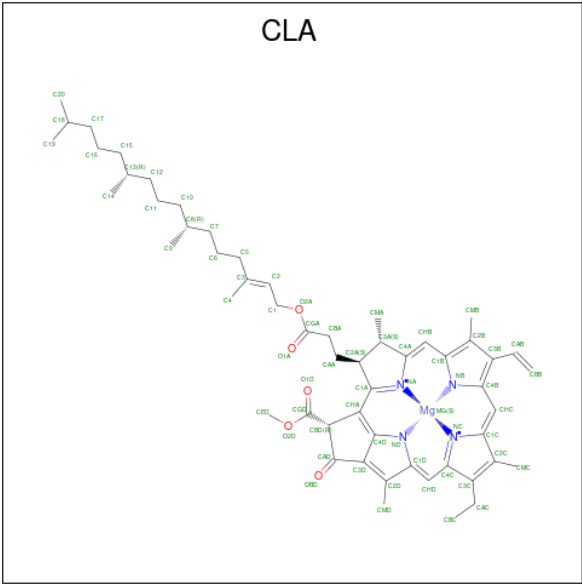
- Molecule 15 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	G	1	Total 62	C 52	Mg 1	N 4	O 5	0
16	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 56	C 46	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	J	1	Total 37	C 31	Mg 1	N 4	O 1	0
16	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	K	1	Total 45	C 35	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	S	1	Total 37	C 31	Mg 1	N 4	O 1	0
16	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	T	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	W	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	W	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	h	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	j	1	Total 37	C 31	Mg 1	N 4	O 1	0
16	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	l	1	Total 60	C 50	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	n	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	n	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	o	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	o	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	o	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	o	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	q	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	t	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	t	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	t	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	u	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	v	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	v	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	v	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	v	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	w	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	w	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	x	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	x	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	x	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	x	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	x	1	Total 46	C 36	Mg 1	N 4	O 5	0
16	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	y	1	Total 46	C 36	Mg 1	N 4	O 5	0

*Continued on next page...*

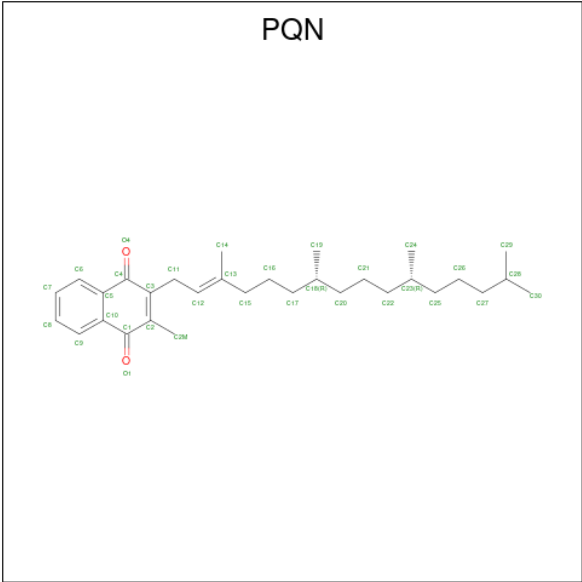


*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
16	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 17 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).

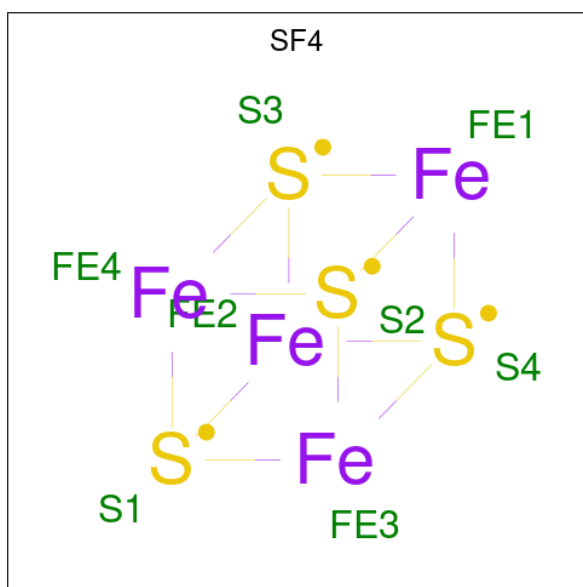




Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			33	31	2	
17	B	1	Total	C	O	0
			33	31	2	
17	G	1	Total	C	O	0
			33	31	2	
17	H	1	Total	C	O	0
			33	31	2	
17	a	1	Total	C	O	0
			33	31	2	
17	b	1	Total	C	O	0
			33	31	2	

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

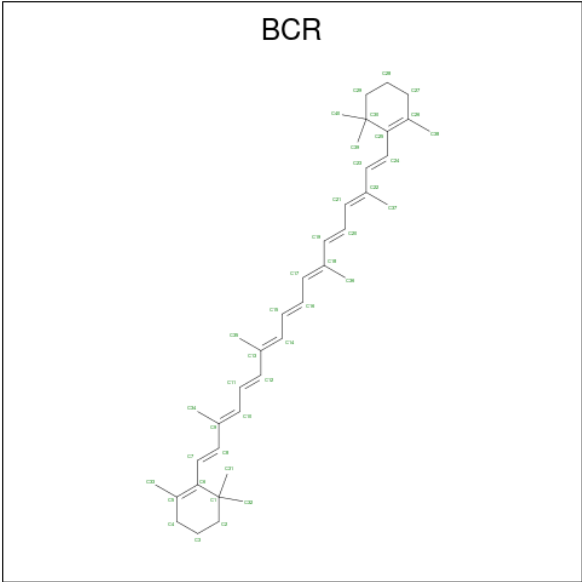




Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	H	1	Total	Fe	S	0
			8	4	4	
18	N	1	Total	Fe	S	0
			8	4	4	
18	N	1	Total	Fe	S	0
			8	4	4	
18	a	1	Total	Fe	S	0
			8	4	4	
18	c	1	Total	Fe	S	0
			8	4	4	
18	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 30 30	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total C 30 30	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	Q	1	Total C 40 40	0
19	R	1	Total C 40 40	0
19	S	1	Total C 40 40	0
19	S	1	Total C 40 40	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
19	S	1	Total C 40 40	0
19	T	1	Total C 40 40	0
19	T	1	Total C 40 40	0
19	U	1	Total C 40 40	0
19	U	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 30 30	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	f	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	i	1	Total C 40 40	0
19	j	1	Total C 40 40	0
19	j	1	Total C 40 40	0
19	j	1	Total C 40 40	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
19	k	1	Total C 40 40	0
19	k	1	Total C 40 40	0
19	l	1	Total C 40 40	0
19	l	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
19	r	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	x	1	Total C 40 40	0
19	x	1	Total C 40 40	0
19	x	1	Total C 40 40	0

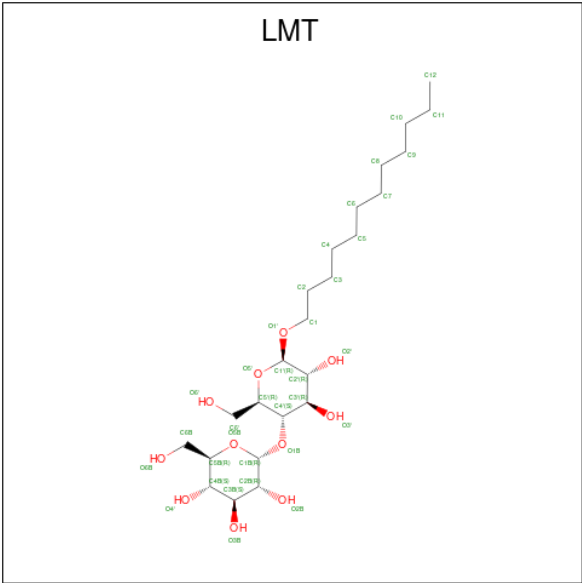
*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
19	x	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0

- Molecule 20 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).

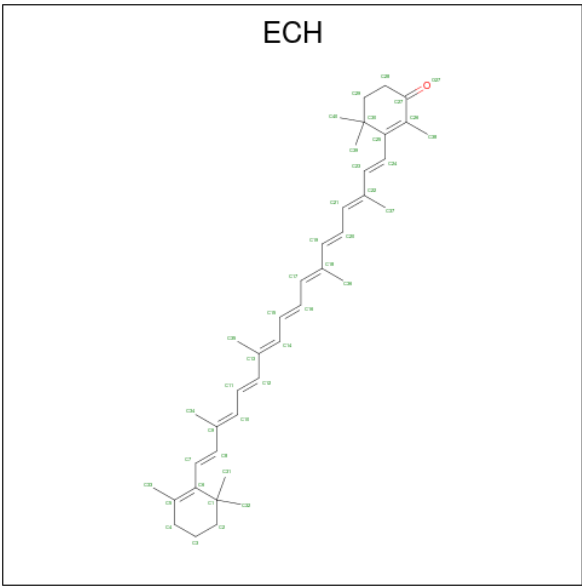


Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total C O 35 24 11	0
20	H	1	Total C O 35 24 11	0
20	L	1	Total C O 35 24 11	0
20	U	1	Total C O 35 24 11	0
20	a	1	Total C O 35 24 11	0
20	l	1	Total C O 35 24 11	0

- Molecule 21 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C<sub>40</sub>H<sub>54</sub>O) (labeled



as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total	C	O	0
			41	40	1	
21	G	1	Total	C	O	0
			41	40	1	
21	I	1	Total	C	O	0
			41	40	1	
21	M	1	Total	C	O	0
			41	40	1	
21	R	1	Total	C	O	0
			41	40	1	
21	V	1	Total	C	O	0
			41	40	1	
21	b	1	Total	C	O	0
			41	40	1	
21	i	1	Total	C	O	0
			41	40	1	
21	m	1	Total	C	O	0
			41	40	1	

- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
22	L	1	Total	Ca	0
			1	1	
22	U	1	Total	Ca	0
			1	1	

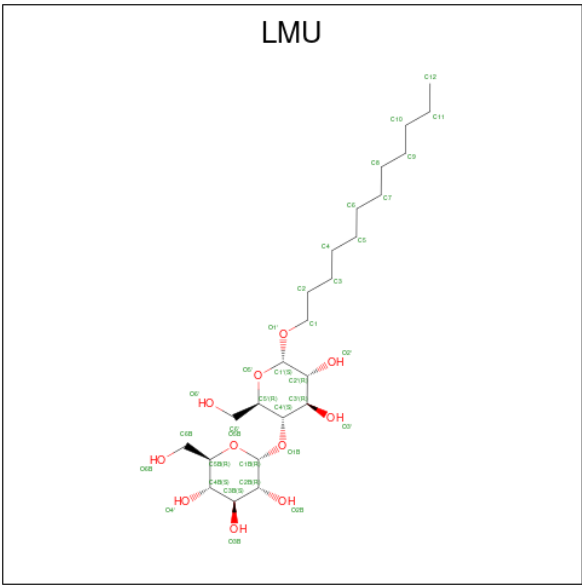
Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
22	1	1	Total	Ca	0
			1	1	

- Molecule 23 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).

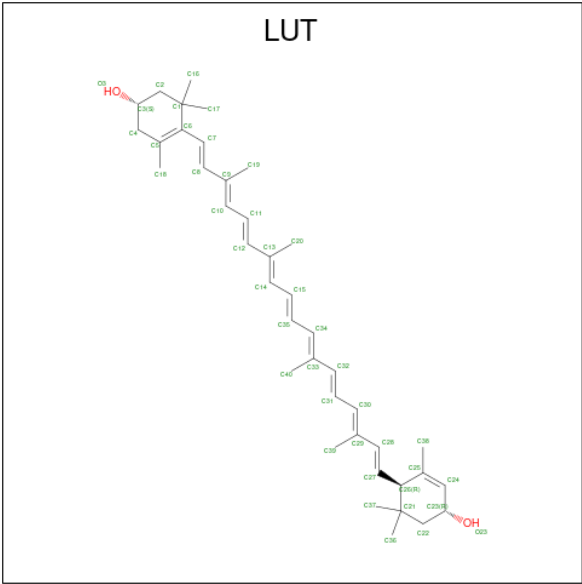


Mol	Chain	Residues	Atoms			AltConf
23	Y	1	Total	C	O	0
			35	24	11	
23	Z	1	Total	C	O	0
			35	24	11	
23	g	1	Total	C	O	0
			35	24	11	
23	p	1	Total	C	O	0
			35	24	11	
23	q	1	Total	C	O	0
			35	24	11	
23	r	1	Total	C	O	0
			35	24	11	
23	s	1	Total	C	O	0
			35	24	11	
23	w	1	Total	C	O	0
			35	24	11	
23	x	1	Total	C	O	0
			35	24	11	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3



,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
24	Z	1	Total	C	O	0
			42	40	2	
24	q	1	Total	C	O	0
			42	40	2	
24	w	1	Total	C	O	0
			42	40	2	

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	A	56	Total	O	0
			56	56	
25	B	52	Total	O	0
			52	52	
25	C	7	Total	O	0
			7	7	
25	D	3	Total	O	0
			3	3	
25	E	4	Total	O	0
			4	4	
25	F	3	Total	O	0
			3	3	
25	G	55	Total	O	0
			55	55	
25	H	52	Total	O	0
			52	52	

Continued on next page...



*Continued from previous page...*

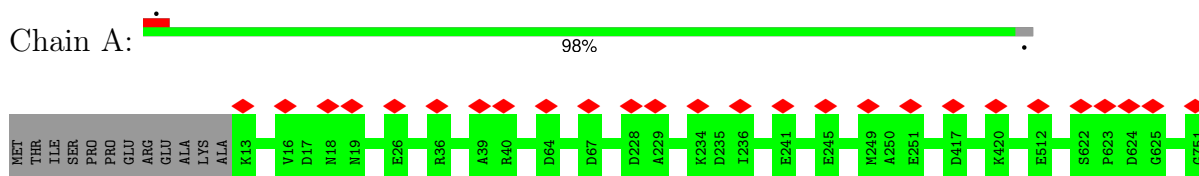
Mol	Chain	Residues	Atoms		AltConf
25	I	1	Total 1	O 1	0
25	J	1	Total 1	O 1	0
25	L	5	Total 5	O 5	0
25	N	13	Total 13	O 13	0
25	O	11	Total 11	O 11	0
25	P	6	Total 6	O 6	0
25	Q	4	Total 4	O 4	0
25	R	1	Total 1	O 1	0
25	S	3	Total 3	O 3	0
25	U	3	Total 3	O 3	0
25	a	57	Total 57	O 57	0
25	b	74	Total 74	O 74	0
25	c	17	Total 17	O 17	0
25	d	7	Total 7	O 7	0
25	e	10	Total 10	O 10	0
25	f	7	Total 7	O 7	0
25	i	1	Total 1	O 1	0
25	j	1	Total 1	O 1	0
25	k	1	Total 1	O 1	0
25	l	6	Total 6	O 6	0



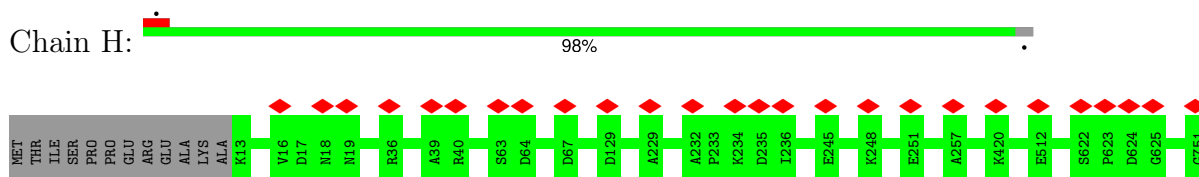
### 3 Residue-property plots

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

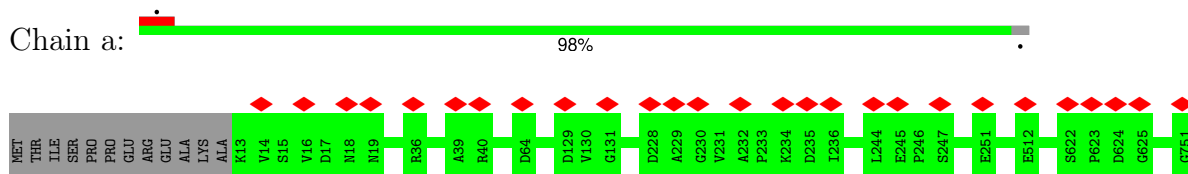
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



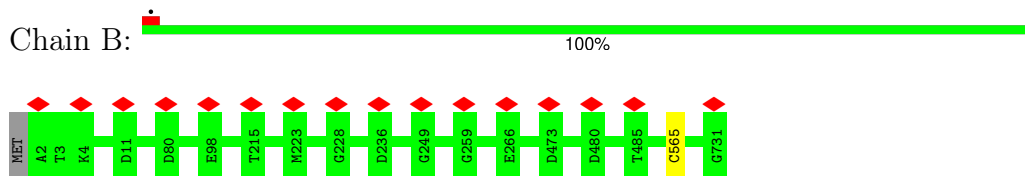
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



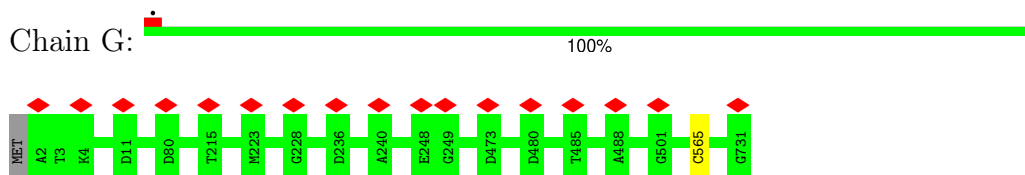
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

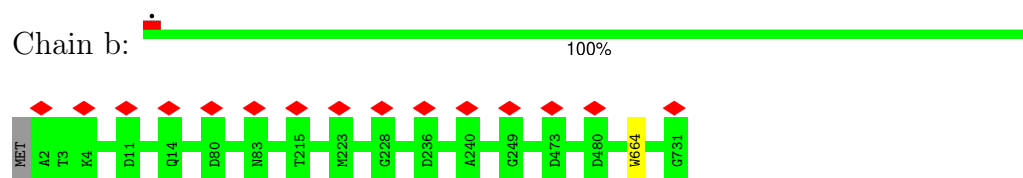


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

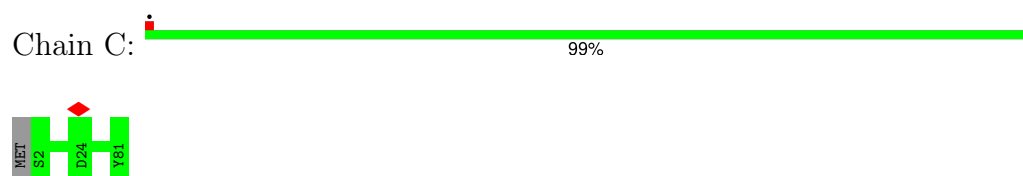




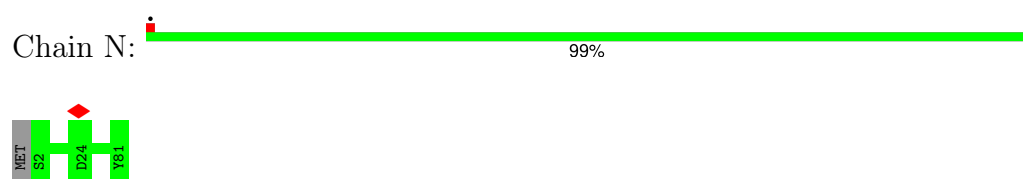
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



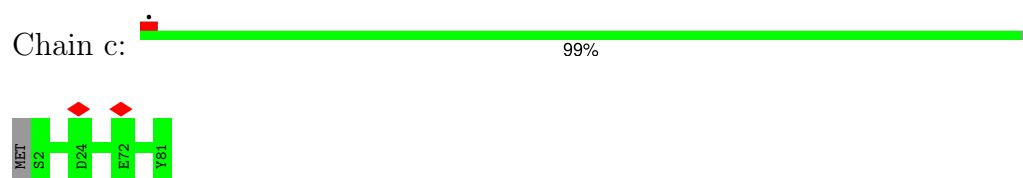
- Molecule 3: Photosystem I iron-sulfur center



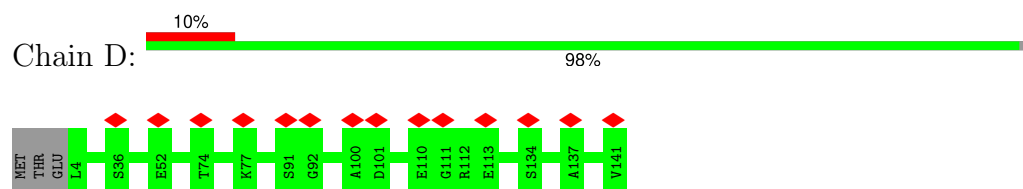
- Molecule 3: Photosystem I iron-sulfur center



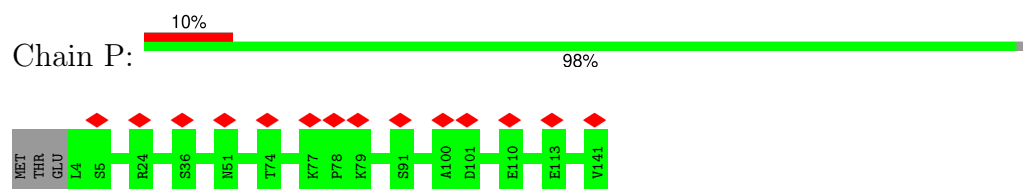
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II



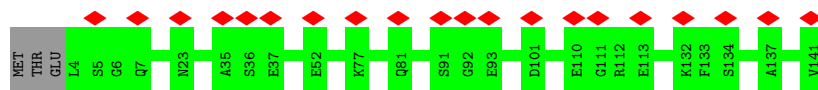
- Molecule 4: Photosystem I reaction center subunit II



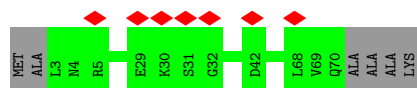
- Molecule 4: Photosystem I reaction center subunit II



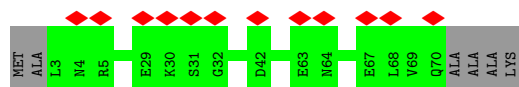
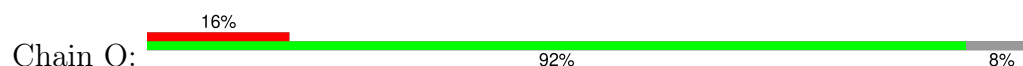




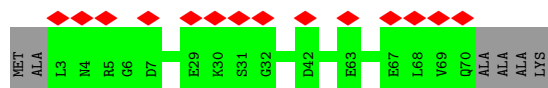
- Molecule 5: Photosystem I reaction center subunit IV



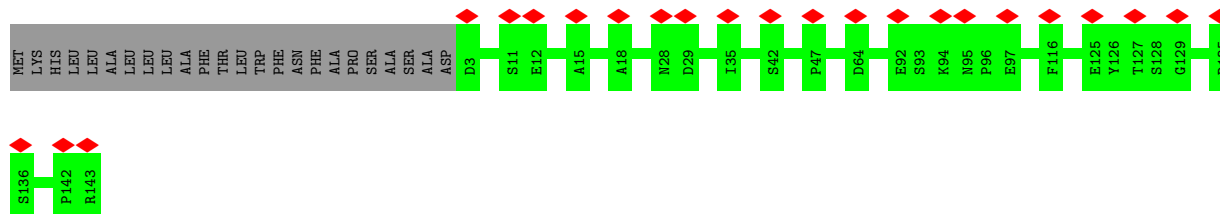
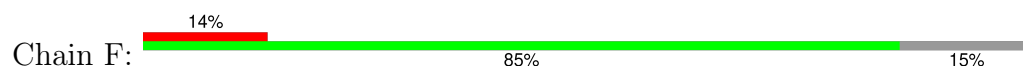
- Molecule 5: Photosystem I reaction center subunit IV



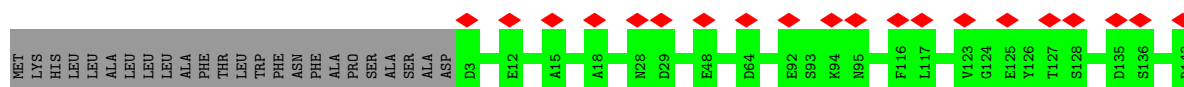
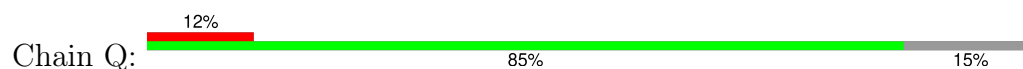
- Molecule 5: Photosystem I reaction center subunit IV



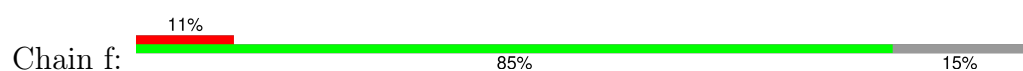
- Molecule 6: Photosystem I reaction center subunit III



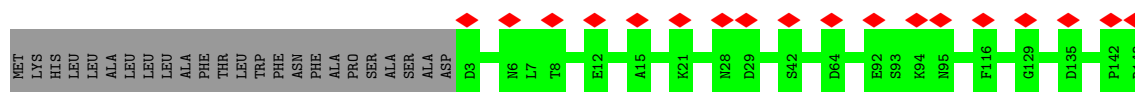
- Molecule 6: Photosystem I reaction center subunit III



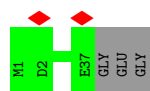
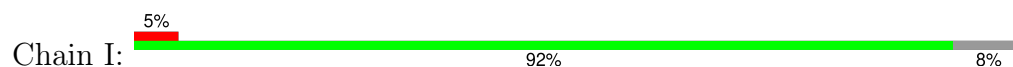
- Molecule 6: Photosystem I reaction center subunit III



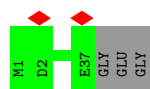
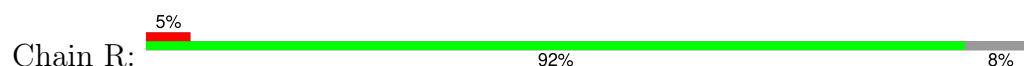




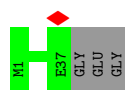
- Molecule 7: Photosystem I reaction center subunit VIII



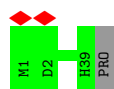
- Molecule 7: Photosystem I reaction center subunit VIII



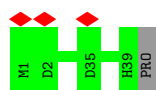
- Molecule 7: Photosystem I reaction center subunit VIII



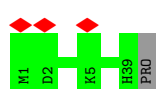
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX

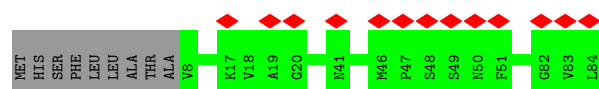
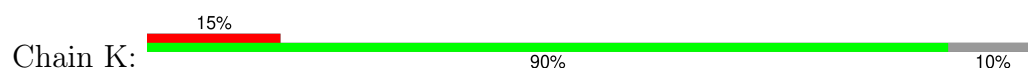


- Molecule 8: Photosystem I reaction center subunit IX

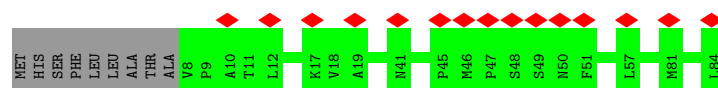
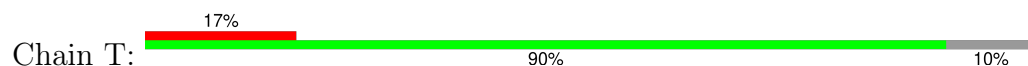


- Molecule 9: Photosystem I reaction center subunit PsaK 1

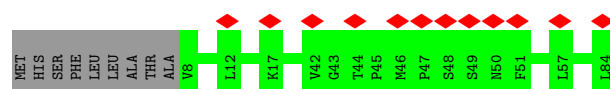
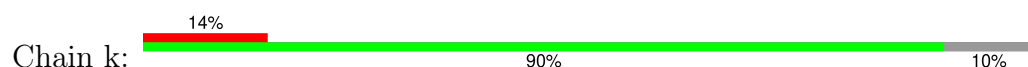




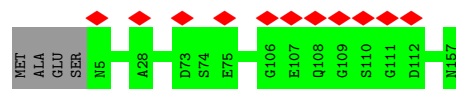
- Molecule 9: Photosystem I reaction center subunit PsaK 1



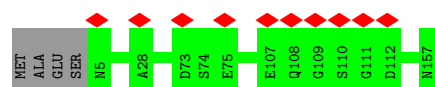
- Molecule 9: Photosystem I reaction center subunit PsaK 1



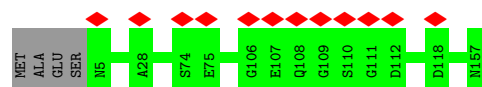
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI

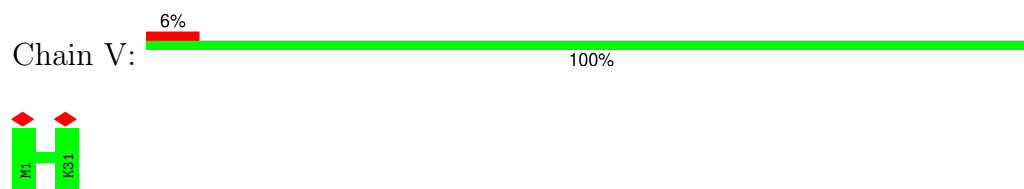


- Molecule 11: Photosystem I reaction center subunit XII

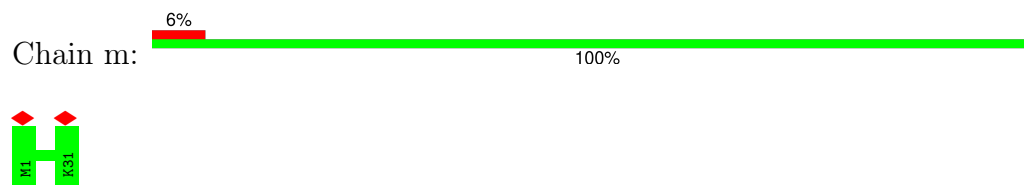




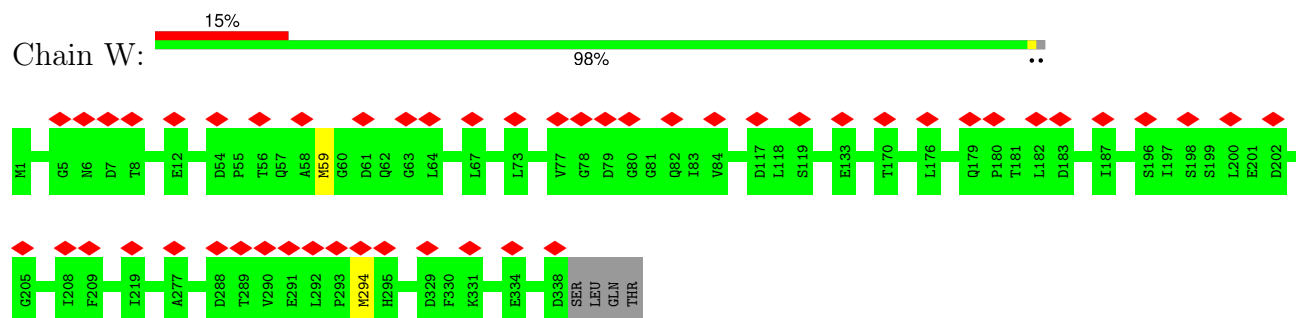
- Molecule 11: Photosystem I reaction center subunit XII



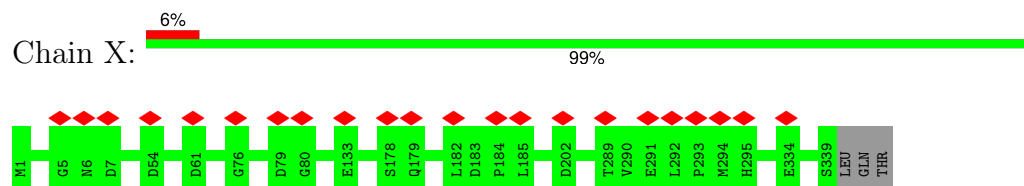
- Molecule 11: Photosystem I reaction center subunit XII



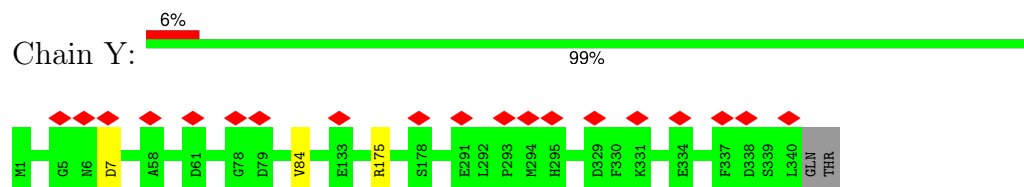
- Molecule 12: Iron stress-induced chlorophyll-binding protein



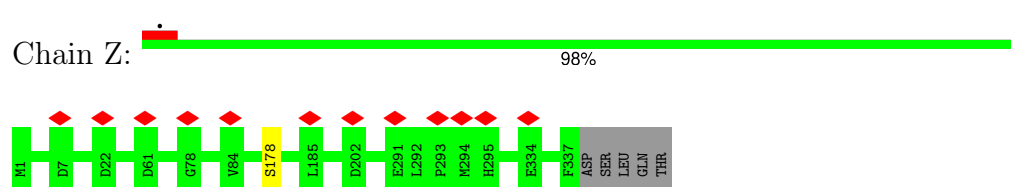
- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein





- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



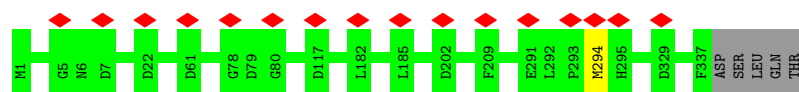
- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein

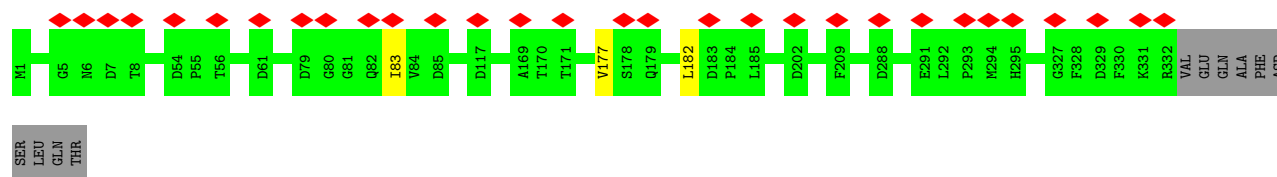






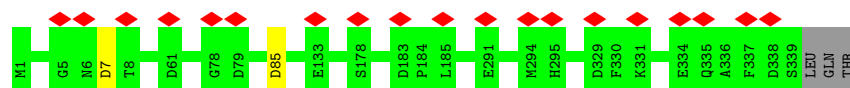
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain r: 96%



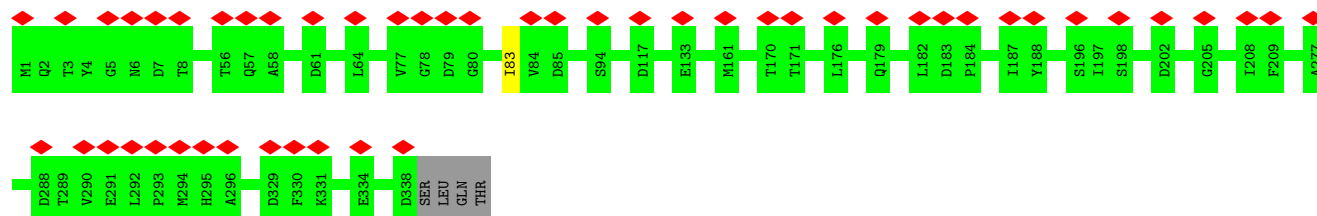
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain s: 99%



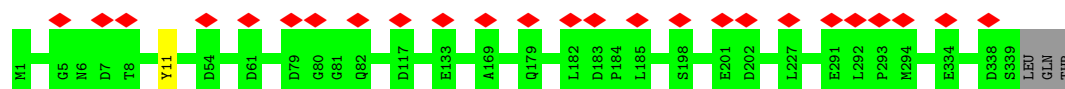
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain t: 99%



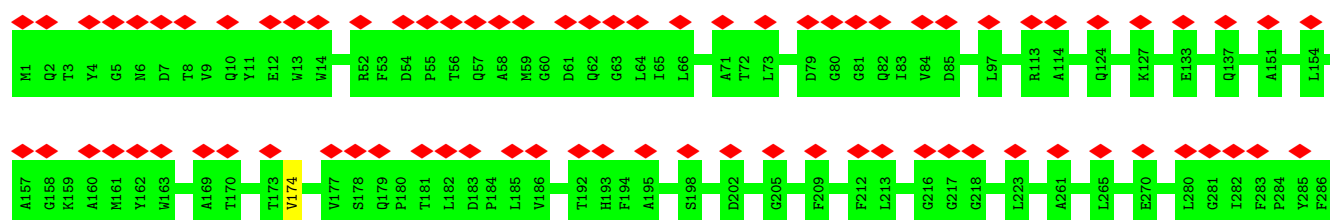
- Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain u: 99%

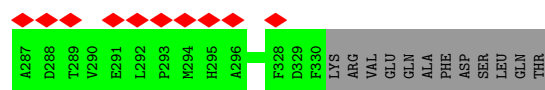


- Molecule 12: Iron stress-induced chlorophyll-binding protein

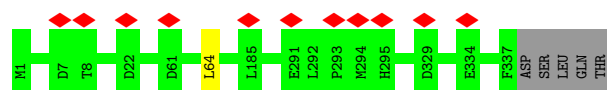
Chain v: 96%



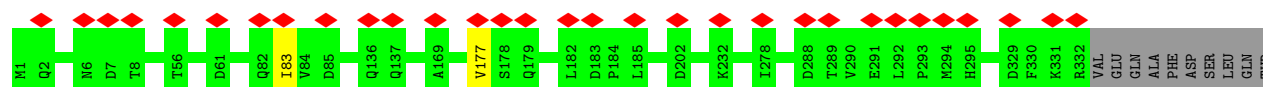




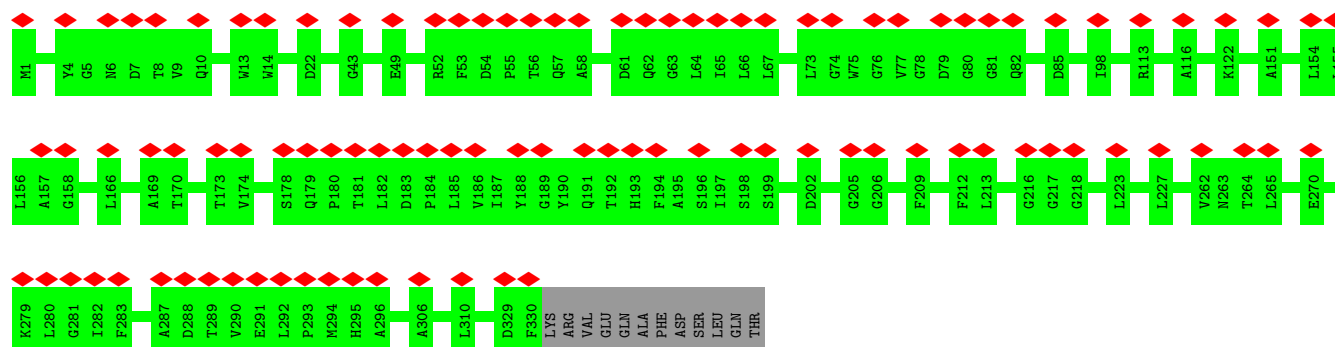
- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein



- Molecule 12: Iron stress-induced chlorophyll-binding protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	70.466	Depositor
Minimum map value	-42.667	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	2.305	Depositor
Recommended contour level	9.2	Depositor
Map size ( $\text{\AA}$ )	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.05, 1.05, 1.05	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CA, LMU, CL0, LMT, PQN, CLA, LHG, LUT, ECH, LMG, BCR

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	0.31	0/5985	0.50	0/8158
1	H	0.31	0/5985	0.51	0/8158
1	a	0.31	0/5985	0.51	0/8158
2	B	0.31	0/5986	0.51	1/8185 (0.0%)
2	G	0.31	1/5986 (0.0%)	0.51	0/8185
2	b	0.31	0/5986	0.51	0/8185
3	C	0.30	0/610	0.58	0/826
3	N	0.31	0/610	0.58	0/826
3	c	0.31	0/610	0.61	0/826
4	D	0.28	0/1102	0.55	0/1485
4	P	0.28	0/1102	0.53	0/1485
4	d	0.29	0/1102	0.53	0/1485
5	E	0.29	0/546	0.54	0/738
5	O	0.28	0/546	0.51	0/738
5	e	0.29	0/546	0.55	0/738
6	F	0.28	0/1130	0.54	0/1535
6	Q	0.28	0/1130	0.54	0/1535
6	f	0.29	0/1130	0.54	0/1535
7	I	0.32	0/304	0.57	0/416
7	R	0.34	0/304	0.59	0/416
7	i	0.31	0/304	0.56	0/416
8	J	0.30	0/319	0.53	0/431
8	S	0.30	0/319	0.54	0/431
8	j	0.32	0/319	0.52	0/431
9	K	0.27	0/549	0.47	0/745
9	T	0.27	0/549	0.51	0/745
9	k	0.27	0/549	0.48	0/745
10	L	0.29	0/1180	0.52	0/1603
10	U	0.30	0/1180	0.53	0/1603
10	l	0.30	0/1180	0.53	0/1603
11	M	0.26	0/241	0.50	0/326
11	V	0.27	0/241	0.58	0/326



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	m	0.29	0/241	0.53	0/326
12	W	0.28	0/2691	0.52	0/3678
12	X	0.28	0/2712	0.51	0/3703
12	Y	0.30	0/2712	0.52	0/3704
12	Z	0.29	0/2693	0.50	0/3678
12	g	0.28	0/2662	0.51	0/3636
12	h	0.28	0/2627	0.51	0/3592
12	n	0.27	0/2691	0.48	0/3678
12	o	0.28	0/2712	0.52	0/3703
12	p	0.29	0/2712	0.51	0/3704
12	q	0.28	0/2693	0.49	0/3678
12	r	0.29	0/2655	0.53	1/3626 (0.0%)
12	s	0.29	0/2707	0.52	0/3697
12	t	0.27	0/2691	0.50	0/3678
12	u	0.28	0/2712	0.50	0/3703
12	v	0.27	0/2627	0.50	0/3592
12	w	0.28	0/2693	0.51	1/3678 (0.0%)
12	x	0.28	0/2655	0.52	0/3626
12	y	0.27	0/2621	0.51	0/3585
All	All	0.29	1/102122 (0.0%)	0.51	3/139283 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
12	Y	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	565	CYS	CB-SG	-5.05	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	565	CYS	CA-CB-SG	6.14	125.06	114.00
12	r	182	LEU	CA-CB-CG	5.39	127.69	115.30
12	w	64	LEU	CA-CB-CG	5.13	127.09	115.30



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	Y	84	VAL	Peptide
2	b	664	TRP	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
1	H	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
1	a	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
2	B	728/731 (100%)	713 (98%)	15 (2%)	0	100	100
2	G	728/731 (100%)	712 (98%)	16 (2%)	0	100	100
2	b	728/731 (100%)	711 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	78 (100%)	0	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	P	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	d	136/141 (96%)	130 (96%)	6 (4%)	0	100	100
5	E	66/74 (89%)	65 (98%)	1 (2%)	0	100	100
5	O	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
5	e	66/74 (89%)	64 (97%)	2 (3%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100	100
6	Q	139/165 (84%)	134 (96%)	5 (4%)	0	100	100
6	f	139/165 (84%)	134 (96%)	5 (4%)	0	100	100
7	I	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	R	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	i	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
8	J	37/40 (92%)	37 (100%)	0	0	100	100
8	S	37/40 (92%)	37 (100%)	0	0	100	100
8	j	37/40 (92%)	37 (100%)	0	0	100	100
9	K	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	T	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	k	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
10	L	151/157 (96%)	150 (99%)	1 (1%)	0	100	100
10	U	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
10	l	151/157 (96%)	147 (97%)	4 (3%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	W	336/342 (98%)	317 (94%)	18 (5%)	1 (0%)	37	59
12	X	337/342 (98%)	318 (94%)	19 (6%)	0	100	100
12	Y	338/342 (99%)	320 (95%)	17 (5%)	1 (0%)	37	59
12	Z	335/342 (98%)	326 (97%)	8 (2%)	1 (0%)	37	59
12	g	331/342 (97%)	304 (92%)	25 (8%)	2 (1%)	22	43
12	h	328/342 (96%)	308 (94%)	20 (6%)	0	100	100
12	n	336/342 (98%)	322 (96%)	14 (4%)	0	100	100
12	o	337/342 (98%)	318 (94%)	17 (5%)	2 (1%)	22	43
12	p	338/342 (99%)	317 (94%)	21 (6%)	0	100	100
12	q	335/342 (98%)	326 (97%)	9 (3%)	0	100	100
12	r	330/342 (96%)	316 (96%)	12 (4%)	2 (1%)	22	43
12	s	337/342 (98%)	321 (95%)	14 (4%)	2 (1%)	22	43
12	t	336/342 (98%)	319 (95%)	16 (5%)	1 (0%)	37	59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	u	337/342 (98%)	322 (96%)	14 (4%)	1 (0%)	37	59
12	v	328/342 (96%)	312 (95%)	15 (5%)	1 (0%)	37	59
12	w	335/342 (98%)	322 (96%)	13 (4%)	0	100	100
12	x	330/342 (96%)	311 (94%)	17 (5%)	2 (1%)	22	43
12	y	328/342 (96%)	307 (94%)	21 (6%)	0	100	100
All	All	12645/13047 (97%)	12150 (96%)	479 (4%)	16 (0%)	50	71

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	W	59	MET
12	v	174	VAL
12	s	85	ASP
12	o	11	TYR
12	s	7	ASP
12	u	11	TYR
12	Y	7	ASP
12	g	83	ILE
12	g	177	VAL
12	o	297	HIS
12	t	83	ILE
12	x	83	ILE
12	x	177	VAL
12	Z	178	SER
12	r	83	ILE
12	r	177	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/603 (98%)	593 (100%)	0	100	100
1	H	593/603 (98%)	593 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	593/603 (98%)	593 (100%)	0	100	100
2	B	582/583 (100%)	582 (100%)	0	100	100
2	G	582/583 (100%)	582 (100%)	0	100	100
2	b	582/583 (100%)	582 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
3	N	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	113/116 (97%)	113 (100%)	0	100	100
4	P	113/116 (97%)	113 (100%)	0	100	100
4	d	113/116 (97%)	113 (100%)	0	100	100
5	E	58/60 (97%)	58 (100%)	0	100	100
5	O	58/60 (97%)	58 (100%)	0	100	100
5	e	58/60 (97%)	58 (100%)	0	100	100
6	F	118/137 (86%)	118 (100%)	0	100	100
6	Q	118/137 (86%)	118 (100%)	0	100	100
6	f	118/137 (86%)	118 (100%)	0	100	100
7	I	31/32 (97%)	31 (100%)	0	100	100
7	R	31/32 (97%)	31 (100%)	0	100	100
7	i	31/32 (97%)	31 (100%)	0	100	100
8	J	34/35 (97%)	34 (100%)	0	100	100
8	S	34/35 (97%)	34 (100%)	0	100	100
8	j	34/35 (97%)	34 (100%)	0	100	100
9	K	55/62 (89%)	55 (100%)	0	100	100
9	T	55/62 (89%)	55 (100%)	0	100	100
9	k	55/62 (89%)	55 (100%)	0	100	100
10	L	115/118 (98%)	115 (100%)	0	100	100
10	U	115/118 (98%)	115 (100%)	0	100	100
10	l	115/118 (98%)	115 (100%)	0	100	100
11	M	25/25 (100%)	25 (100%)	0	100	100
11	V	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	W	252/260 (97%)	251 (100%)	1 (0%)	89	96
12	X	256/260 (98%)	256 (100%)	0	100	100
12	Y	255/260 (98%)	254 (100%)	1 (0%)	89	96
12	Z	253/260 (97%)	253 (100%)	0	100	100
12	g	251/260 (96%)	251 (100%)	0	100	100
12	h	246/260 (95%)	246 (100%)	0	100	100
12	n	252/260 (97%)	252 (100%)	0	100	100
12	o	256/260 (98%)	256 (100%)	0	100	100
12	p	255/260 (98%)	255 (100%)	0	100	100
12	q	253/260 (97%)	252 (100%)	1 (0%)	89	96
12	r	250/260 (96%)	250 (100%)	0	100	100
12	s	255/260 (98%)	255 (100%)	0	100	100
12	t	252/260 (97%)	252 (100%)	0	100	100
12	u	256/260 (98%)	256 (100%)	0	100	100
12	v	246/260 (95%)	246 (100%)	0	100	100
12	w	253/260 (97%)	253 (100%)	0	100	100
12	x	250/260 (96%)	250 (100%)	0	100	100
12	y	245/260 (94%)	245 (100%)	0	100	100
All	All	9912/10200 (97%)	9909 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	W	294	MET
12	Y	175	ARG
12	q	294	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	A	314	ASN
1	A	441	ASN
1	A	538	HIS
1	A	614	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	83	ASN
2	B	366	GLN
2	B	478	ASN
4	D	71	GLN
6	F	22	ASN
2	G	83	ASN
2	G	218	HIS
2	G	264	GLN
2	G	294	ASN
1	H	192	ASN
1	H	216	GLN
1	H	441	ASN
1	H	458	ASN
1	H	538	HIS
1	H	590	HIS
1	H	614	GLN
9	K	26	ASN
4	P	71	GLN
4	P	81	GLN
9	T	26	ASN
10	U	108	GLN
12	W	2	GLN
12	W	31	HIS
12	W	62	GLN
12	W	82	GLN
12	W	191	GLN
12	W	263	ASN
12	X	34	GLN
12	Y	207	HIS
12	Z	207	HIS
1	a	18	ASN
1	a	192	ASN
1	a	590	HIS
1	a	614	GLN
2	b	41	ASN
2	b	76	GLN
2	b	83	ASN
4	d	71	GLN
6	f	99	GLN
12	g	297	HIS
12	g	305	ASN
12	n	2	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
12	n	31	HIS
12	n	191	GLN
12	o	191	GLN
12	p	136	GLN
12	p	191	GLN
12	p	207	HIS
12	q	207	HIS
12	q	263	ASN
12	r	124	GLN
12	r	191	GLN
12	s	136	GLN
12	s	207	HIS
12	t	191	GLN
12	u	179	GLN
12	u	191	GLN
12	u	321	HIS
12	v	124	GLN
12	v	134	ASN
12	v	137	GLN
12	v	316	GLN
12	w	34	GLN
12	w	129	HIS
12	w	335	GLN
12	x	6	ASN
12	x	62	GLN
12	x	263	ASN
12	y	17	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 798 ligands modelled in this entry, 3 are monoatomic - leaving 795 for Mogul analysis.

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$
16	CLA	n	501	-	48,58,73	1.36	3 (6%)	56,95,113	1.16	5 (8%)
19	BCR	a	4008	-	41,41,41	0.91	1 (2%)	56,56,56	1.35	6 (10%)
13	LHG	o	605	-	26,26,48	0.85	0	29,32,54	1.27	2 (6%)
19	BCR	B	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
16	CLA	H	1113	-	43,53,73	1.44	3 (6%)	50,89,113	1.18	3 (6%)
16	CLA	u	511	-	63,73,73	1.15	3 (4%)	74,113,113	1.11	3 (4%)
16	CLA	G	1203	-	63,73,73	1.15	3 (4%)	74,113,113	1.10	4 (5%)
19	BCR	G	4010	-	41,41,41	0.94	0	56,56,56	1.39	9 (16%)
21	ECH	R	4020	-	42,42,42	0.99	3 (7%)	55,58,58	1.93	14 (25%)
16	CLA	s	502	-	48,58,73	1.35	4 (8%)	56,95,113	1.03	2 (3%)
19	BCR	A	4011	-	41,41,41	0.88	0	56,56,56	1.29	4 (7%)
16	CLA	q	507	-	63,73,73	1.19	3 (4%)	74,113,113	1.06	3 (4%)
20	LMT	H	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.91	0
16	CLA	G	1213	-	53,63,73	1.30	3 (5%)	62,101,113	1.05	3 (4%)
16	CLA	X	509	-	58,68,73	1.20	3 (5%)	68,107,113	0.94	4 (5%)
16	CLA	W	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.05	4 (7%)
16	CLA	p	516	-	44,54,73	1.37	3 (6%)	51,90,113	1.00	2 (3%)
16	CLA	a	1137	-	45,55,73	1.35	3 (6%)	52,91,113	1.03	4 (7%)
19	BCR	s	603	-	41,41,41	0.86	0	56,56,56	1.18	6 (10%)
19	BCR	Z	604	-	41,41,41	0.87	0	56,56,56	1.24	6 (10%)
16	CLA	q	504	-	63,73,73	1.18	3 (4%)	74,113,113	1.07	3 (4%)
13	LHG	Y	605	-	31,31,48	0.78	1 (3%)	34,37,54	1.29	4 (11%)
16	CLA	p	504	-	63,73,73	1.17	3 (4%)	74,113,113	0.95	2 (2%)
21	ECH	V	4021	-	42,42,42	0.84	1 (2%)	55,58,58	1.55	7 (12%)
16	CLA	b	1215	-	58,68,73	1.19	3 (5%)	68,107,113	1.14	3 (4%)
16	CLA	a	1114	-	44,54,73	1.41	3 (6%)	51,90,113	1.24	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	b	1202	-	63,73,73	1.17	3 (4%)	74,113,113	0.92	2 (2%)
16	CLA	o	508	12	53,63,73	1.30	3 (5%)	62,101,113	0.90	2 (3%)
16	CLA	v	503	-	44,54,73	1.40	3 (6%)	51,90,113	1.15	3 (5%)
16	CLA	b	1021	-	63,73,73	1.15	3 (4%)	74,113,113	1.05	4 (5%)
16	CLA	g	505	-	63,73,73	1.18	3 (4%)	74,113,113	1.17	5 (6%)
16	CLA	h	505	-	63,73,73	1.21	3 (4%)	74,113,113	1.13	4 (5%)
16	CLA	A	1110	-	52,62,73	1.27	3 (5%)	60,99,113	0.94	2 (3%)
16	CLA	a	1124	25	58,68,73	1.23	3 (5%)	68,107,113	0.99	2 (2%)
16	CLA	a	1106	1	63,73,73	1.15	3 (4%)	74,113,113	1.10	3 (4%)
16	CLA	b	1216	25	45,55,73	1.43	3 (6%)	52,91,113	1.42	5 (9%)
16	CLA	k	4004	-	53,63,73	1.30	3 (5%)	62,101,113	0.94	4 (6%)
16	CLA	H	1013	-	63,73,73	1.14	4 (6%)	74,113,113	1.21	9 (12%)
13	LHG	A	849	-	42,42,48	0.69	1 (2%)	45,48,54	1.23	5 (11%)
16	CLA	o	504	-	58,68,73	1.23	3 (5%)	68,107,113	1.00	3 (4%)
21	ECH	b	4006	-	42,42,42	0.85	2 (4%)	55,58,58	1.52	8 (14%)
16	CLA	H	1138	-	63,73,73	1.16	3 (4%)	74,113,113	0.96	3 (4%)
16	CLA	a	1123	-	63,73,73	1.16	3 (4%)	74,113,113	1.02	4 (5%)
16	CLA	y	508	-	53,63,73	1.31	3 (5%)	62,101,113	1.16	4 (6%)
16	CLA	b	1213	-	53,63,73	1.28	4 (7%)	62,101,113	1.08	5 (8%)
16	CLA	n	513	-	44,54,73	1.41	3 (6%)	51,90,113	0.95	3 (5%)
16	CLA	W	509	-	58,68,73	1.21	3 (5%)	68,107,113	1.03	3 (4%)
16	CLA	n	514	-	48,58,73	1.35	4 (8%)	56,95,113	1.03	4 (7%)
16	CLA	U	1502	-	58,68,73	1.17	3 (5%)	68,107,113	1.08	3 (4%)
16	CLA	Y	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.01	5 (6%)
16	CLA	b	1221	25	63,73,73	1.19	3 (4%)	74,113,113	1.07	3 (4%)
16	CLA	w	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.02	4 (7%)
16	CLA	r	504	-	63,73,73	1.18	3 (4%)	74,113,113	0.93	2 (2%)
19	BCR	G	4017	-	41,41,41	0.87	0	56,56,56	1.18	6 (10%)
13	LHG	I	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.23	4 (9%)
16	CLA	a	1112	-	43,53,73	1.40	3 (6%)	50,89,113	0.95	2 (4%)
16	CLA	h	516	-	44,54,73	1.43	3 (6%)	51,90,113	1.06	3 (5%)
16	CLA	Y	504	-	63,73,73	1.18	3 (4%)	74,113,113	0.95	2 (2%)
16	CLA	B	1218	-	53,63,73	1.29	3 (5%)	62,101,113	1.09	4 (6%)
19	BCR	t	601	-	41,41,41	0.83	0	56,56,56	1.18	6 (10%)
23	LMU	q	605	-	36,36,36	0.83	0	47,47,47	1.13	4 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	1104	-	63,73,73	1.18	3 (4%)	74,113,113	0.92	4 (5%)
14	LMG	B	848	-	43,43,55	0.87	1 (2%)	51,51,63	1.28	6 (11%)
16	CLA	A	1113	-	43,53,73	1.43	3 (6%)	50,89,113	1.05	2 (4%)
16	CLA	x	504	-	63,73,73	1.19	3 (4%)	74,113,113	0.97	4 (5%)
19	BCR	X	603	-	41,41,41	0.85	0	56,56,56	1.15	4 (7%)
19	BCR	U	4022	-	41,41,41	0.88	0	56,56,56	1.32	6 (10%)
16	CLA	G	1235	-	60,70,73	1.16	3 (5%)	70,109,113	1.18	7 (10%)
16	CLA	W	505	-	63,73,73	1.19	3 (4%)	74,113,113	1.12	5 (6%)
13	LHG	a	849	-	42,42,48	0.71	1 (2%)	45,48,54	1.22	4 (8%)
16	CLA	G	1226	-	58,68,73	1.20	4 (6%)	68,107,113	1.07	4 (5%)
16	CLA	Z	512	12	63,73,73	1.18	4 (6%)	74,113,113	1.10	3 (4%)
19	BCR	y	601	-	41,41,41	0.83	0	56,56,56	1.24	6 (10%)
16	CLA	L	1502	-	58,68,73	1.16	3 (5%)	68,107,113	1.08	3 (4%)
16	CLA	H	1126	-	63,73,73	1.17	3 (4%)	74,113,113	1.12	4 (5%)
16	CLA	y	514	-	48,58,73	1.40	4 (8%)	56,95,113	1.05	5 (8%)
19	BCR	G	4005	-	41,41,41	0.85	0	56,56,56	1.14	4 (7%)
16	CLA	G	1210	-	63,73,73	1.17	3 (4%)	74,113,113	1.04	4 (5%)
15	CL0	H	1011	-	63,73,73	1.21	4 (6%)	74,113,113	1.05	6 (8%)
16	CLA	o	502	-	48,58,73	1.33	4 (8%)	56,95,113	0.98	3 (5%)
16	CLA	w	510	-	58,68,73	1.23	3 (5%)	68,107,113	0.95	1 (1%)
16	CLA	g	501	-	48,58,73	1.33	3 (6%)	56,95,113	1.00	3 (5%)
16	CLA	h	501	-	44,54,73	1.44	3 (6%)	51,90,113	1.15	4 (7%)
16	CLA	U	1503	-	63,73,73	1.16	3 (4%)	74,113,113	0.88	3 (4%)
16	CLA	W	510	-	63,73,73	1.20	3 (4%)	74,113,113	0.98	4 (5%)
16	CLA	G	1217	-	43,53,73	1.42	3 (6%)	50,89,113	0.98	2 (4%)
19	BCR	H	4011	-	41,41,41	0.88	0	56,56,56	1.26	6 (10%)
19	BCR	n	603	-	41,41,41	0.83	0	56,56,56	1.20	5 (8%)
19	BCR	w	603	-	41,41,41	0.85	0	56,56,56	1.17	6 (10%)
16	CLA	G	1023	-	63,73,73	1.19	5 (7%)	74,113,113	1.09	6 (8%)
18	SF4	A	3001	-	0,12,12	-	-	-	-	-
16	CLA	s	511	-	63,73,73	1.14	3 (4%)	74,113,113	1.04	5 (6%)
16	CLA	b	1201	-	52,62,73	1.30	3 (5%)	60,99,113	1.13	3 (5%)
16	CLA	B	1209	-	43,53,73	1.43	3 (6%)	50,89,113	1.04	2 (4%)
16	CLA	G	1215	-	58,68,73	1.17	3 (5%)	68,107,113	1.09	2 (2%)
16	CLA	w	511	-	63,73,73	1.16	3 (4%)	74,113,113	1.03	4 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	BCR	j	4012	-	41,41,41	0.88	0	56,56,56	1.29	7 (12%)
16	CLA	A	1129	-	44,54,73	1.35	3 (6%)	51,90,113	1.08	3 (5%)
16	CLA	k	4002	-	43,53,73	1.45	3 (6%)	50,89,113	1.06	3 (6%)
16	CLA	q	512	12	63,73,73	1.18	4 (6%)	74,113,113	1.01	2 (2%)
16	CLA	G	1216	25	45,55,73	1.38	3 (6%)	52,91,113	1.29	3 (5%)
19	BCR	w	602	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)
16	CLA	u	515	-	63,73,73	1.14	3 (4%)	74,113,113	1.04	4 (5%)
17	PQN	A	2001	-	34,34,34	0.37	0	43,45,45	1.08	2 (4%)
16	CLA	Y	512	12	63,73,73	1.19	4 (6%)	74,113,113	1.19	7 (9%)
16	CLA	x	515	-	63,73,73	1.17	3 (4%)	74,113,113	1.12	5 (6%)
16	CLA	X	503	-	44,54,73	1.38	3 (6%)	51,90,113	0.98	1 (1%)
16	CLA	G	1230	-	43,53,73	1.40	3 (6%)	50,89,113	0.96	1 (2%)
21	ECH	I	4020	-	42,42,42	0.88	1 (2%)	55,58,58	1.90	14 (25%)
16	CLA	W	502	-	48,58,73	1.37	4 (8%)	56,95,113	1.10	4 (7%)
16	CLA	a	1022	-	63,73,73	1.17	3 (4%)	74,113,113	1.04	7 (9%)
16	CLA	u	502	-	48,58,73	1.35	4 (8%)	56,95,113	1.04	2 (3%)
16	CLA	Y	506	-	58,68,73	1.24	3 (5%)	68,107,113	1.07	4 (5%)
13	LHG	u	605	-	26,26,48	0.83	0	29,32,54	1.27	2 (6%)
16	CLA	b	1219	-	43,53,73	1.46	3 (6%)	50,89,113	1.08	3 (6%)
16	CLA	s	505	-	63,73,73	1.20	3 (4%)	74,113,113	1.09	5 (6%)
16	CLA	B	1229	-	56,66,73	1.26	3 (5%)	65,104,113	1.02	4 (6%)
13	LHG	x	605	-	30,30,48	0.78	1 (3%)	33,36,54	1.28	3 (9%)
16	CLA	A	1128	-	63,73,73	1.15	4 (6%)	74,113,113	1.12	5 (6%)
19	BCR	Y	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	Z	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.10	4 (7%)
14	LMG	a	4101	-	46,46,55	0.90	2 (4%)	54,54,63	1.22	4 (7%)
20	LMT	A	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.92	0
19	BCR	k	4001	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
16	CLA	F	1302	6	44,54,73	1.44	3 (6%)	51,90,113	0.99	2 (3%)
16	CLA	b	1225	-	63,73,73	1.16	4 (6%)	74,113,113	0.98	4 (5%)
16	CLA	H	1115	-	52,62,73	1.27	3 (5%)	60,99,113	1.17	2 (3%)
16	CLA	B	1219	-	43,53,73	1.44	3 (6%)	50,89,113	1.07	2 (4%)
19	BCR	i	4018	-	41,41,41	0.87	0	56,56,56	1.23	8 (14%)
16	CLA	s	509	-	58,68,73	1.21	3 (5%)	68,107,113	1.00	4 (5%)
16	CLA	b	1208	-	43,53,73	1.40	3 (6%)	50,89,113	1.10	4 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	BCR	p	601	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
16	CLA	b	1222	25	48,58,73	1.36	3 (6%)	56,95,113	1.06	3 (5%)
16	CLA	a	1102	16	54,64,73	1.25	3 (5%)	63,102,113	0.95	2 (3%)
16	CLA	b	1238	25	63,73,73	1.13	3 (4%)	74,113,113	1.00	5 (6%)
16	CLA	W	512	12	58,68,73	1.23	4 (6%)	68,107,113	1.07	4 (5%)
16	CLA	X	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.88	3 (4%)
16	CLA	b	1212	-	43,53,73	1.44	3 (6%)	50,89,113	1.22	3 (6%)
16	CLA	G	1209	-	43,53,73	1.44	3 (6%)	50,89,113	1.09	2 (4%)
19	BCR	l	4022	-	41,41,41	0.89	1 (2%)	56,56,56	1.41	8 (14%)
16	CLA	W	508	12	53,63,73	1.28	3 (5%)	62,101,113	0.89	2 (3%)
19	BCR	o	604	-	41,41,41	0.88	0	56,56,56	1.31	10 (17%)
13	LHG	R	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.24	4 (9%)
16	CLA	B	1203	-	63,73,73	1.16	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	o	514	-	48,58,73	1.40	4 (8%)	56,95,113	1.34	4 (7%)
16	CLA	B	1235	-	60,70,73	1.17	3 (5%)	70,109,113	1.22	8 (11%)
16	CLA	p	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.02	3 (5%)
19	BCR	T	4005	-	41,41,41	0.85	0	56,56,56	1.26	7 (12%)
16	CLA	G	1221	25	63,73,73	1.18	3 (4%)	74,113,113	1.07	3 (4%)
13	LHG	b	4018	16	37,37,48	0.71	0	40,43,54	1.31	5 (12%)
19	BCR	j	4013	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)
16	CLA	a	1107	1	48,58,73	1.35	3 (6%)	56,95,113	1.08	2 (3%)
19	BCR	h	601	-	41,41,41	0.84	0	56,56,56	1.28	7 (12%)
16	CLA	A	1115	-	52,62,73	1.28	4 (7%)	60,99,113	1.20	3 (5%)
16	CLA	H	1139	25	58,68,73	1.23	3 (5%)	68,107,113	0.94	3 (4%)
16	CLA	Z	510	-	58,68,73	1.24	3 (5%)	68,107,113	0.99	2 (2%)
17	PQN	a	2001	-	34,34,34	0.39	0	43,45,45	1.06	2 (4%)
16	CLA	G	1201	-	52,62,73	1.31	3 (5%)	60,99,113	1.02	2 (3%)
16	CLA	G	1218	-	53,63,73	1.30	3 (5%)	62,101,113	1.03	3 (4%)
16	CLA	H	1123	-	63,73,73	1.18	3 (4%)	74,113,113	0.97	4 (5%)
16	CLA	n	511	-	63,73,73	1.19	3 (4%)	74,113,113	1.00	4 (5%)
16	CLA	A	1111	-	53,63,73	1.28	4 (7%)	62,101,113	1.21	4 (6%)
16	CLA	a	1013	-	63,73,73	1.14	4 (6%)	74,113,113	1.16	4 (5%)
14	LMG	G	848	-	43,43,55	0.86	0	51,51,63	1.27	7 (13%)
16	CLA	a	1138	-	63,73,73	1.17	3 (4%)	74,113,113	0.93	3 (4%)
14	LMG	H	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	CLA	u	509	-	58,68,73	1.20	3 (5%)	68,107,113	1.02	4 (5%)
16	CLA	X	512	12	63,73,73	1.13	3 (4%)	74,113,113	1.00	5 (6%)
16	CLA	B	1221	25	63,73,73	1.17	3 (4%)	74,113,113	0.96	1 (1%)
16	CLA	Y	517	12	53,63,73	1.29	3 (5%)	62,101,113	0.95	1 (1%)
16	CLA	W	517	12	53,63,73	1.29	3 (5%)	62,101,113	0.92	2 (3%)
19	BCR	u	602	-	41,41,41	0.88	0	56,56,56	1.36	6 (10%)
16	CLA	x	513	-	44,54,73	1.42	3 (6%)	51,90,113	0.98	1 (1%)
16	CLA	A	1103	-	63,73,73	1.17	3 (4%)	74,113,113	0.96	1 (1%)
13	LHG	X	605	-	26,26,48	0.82	0	29,32,54	1.27	2 (6%)
16	CLA	p	502	-	48,58,73	1.33	3 (6%)	56,95,113	0.99	3 (5%)
16	CLA	A	1106	1	63,73,73	1.15	3 (4%)	74,113,113	1.13	4 (5%)
16	CLA	b	1203	-	63,73,73	1.15	3 (4%)	74,113,113	1.05	5 (6%)
16	CLA	v	506	-	58,68,73	1.24	3 (5%)	68,107,113	1.10	5 (7%)
16	CLA	x	514	-	48,58,73	1.33	3 (6%)	56,95,113	1.05	4 (7%)
16	CLA	A	1133	-	52,62,73	1.26	4 (7%)	60,99,113	1.10	4 (6%)
16	CLA	a	1125	-	63,73,73	1.18	4 (6%)	74,113,113	1.04	3 (4%)
16	CLA	a	1131	-	63,73,73	1.15	3 (4%)	74,113,113	1.04	2 (2%)
16	CLA	Y	509	-	58,68,73	1.20	3 (5%)	68,107,113	1.04	3 (4%)
16	CLA	G	1227	-	47,57,73	1.30	4 (8%)	53,93,113	1.12	4 (7%)
16	CLA	Z	515	-	63,73,73	1.18	3 (4%)	74,113,113	1.11	3 (4%)
16	CLA	o	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.02	3 (4%)
16	CLA	r	516	-	44,54,73	1.40	3 (6%)	51,90,113	1.09	3 (5%)
16	CLA	p	505	-	63,73,73	1.19	3 (4%)	74,113,113	1.04	4 (5%)
16	CLA	A	1132	-	63,73,73	1.12	3 (4%)	74,113,113	1.08	3 (4%)
16	CLA	G	1207	-	63,73,73	1.18	3 (4%)	74,113,113	1.15	5 (6%)
19	BCR	R	4018	-	41,41,41	0.85	0	56,56,56	1.20	7 (12%)
16	CLA	G	1231	25	43,53,73	1.44	3 (6%)	50,89,113	1.09	3 (6%)
16	CLA	A	1123	25	63,73,73	1.18	3 (4%)	74,113,113	1.10	4 (5%)
16	CLA	A	1136	-	63,73,73	1.14	3 (4%)	74,113,113	0.92	2 (2%)
16	CLA	A	1801	13	44,54,73	1.36	3 (6%)	51,90,113	1.23	4 (7%)
16	CLA	A	1105	-	56,66,73	1.24	3 (5%)	65,104,113	0.96	3 (4%)
16	CLA	a	1122	-	57,67,73	1.25	3 (5%)	66,105,113	1.02	2 (3%)
16	CLA	p	510	-	63,73,73	1.19	3 (4%)	74,113,113	0.99	2 (2%)
16	CLA	v	511	-	63,73,73	1.18	3 (4%)	74,113,113	1.06	4 (5%)
16	CLA	g	513	-	44,54,73	1.41	3 (6%)	51,90,113	0.89	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	LMU	r	606	-	36,36,36	0.87	0	47,47,47	1.10	2 (4%)
16	CLA	t	502	-	48,58,73	1.36	4 (8%)	56,95,113	1.01	3 (5%)
16	CLA	t	504	-	58,68,73	1.25	3 (5%)	68,107,113	0.97	3 (4%)
19	BCR	b	4004	-	41,41,41	0.84	0	56,56,56	1.26	6 (10%)
19	BCR	p	604	-	41,41,41	0.87	0	56,56,56	1.23	6 (10%)
16	CLA	T	4003	9	43,53,73	1.44	3 (6%)	50,89,113	0.99	2 (4%)
19	BCR	H	4002	-	41,41,41	0.85	0	56,56,56	1.19	5 (8%)
19	BCR	p	603	-	41,41,41	0.86	0	56,56,56	1.21	5 (8%)
19	BCR	b	4009	-	30,30,41	0.85	0	39,39,56	1.35	6 (15%)
19	BCR	h	603	-	41,41,41	0.83	0	56,56,56	1.19	4 (7%)
16	CLA	b	1220	-	52,62,73	1.34	4 (7%)	60,99,113	1.03	4 (6%)
16	CLA	w	505	-	63,73,73	1.16	3 (4%)	74,113,113	1.04	5 (6%)
16	CLA	k	4003	9	43,53,73	1.45	3 (6%)	50,89,113	1.05	2 (4%)
16	CLA	a	1126	-	63,73,73	1.16	3 (4%)	74,113,113	1.11	3 (4%)
16	CLA	o	510	-	58,68,73	1.24	3 (5%)	68,107,113	0.92	3 (4%)
19	BCR	b	4005	-	41,41,41	0.85	0	56,56,56	1.15	5 (8%)
23	LMU	s	606	-	36,36,36	0.83	0	47,47,47	1.27	4 (8%)
19	BCR	G	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
16	CLA	t	514	-	48,58,73	1.36	3 (6%)	56,95,113	1.06	4 (7%)
15	CL0	a	1011	-	63,73,73	1.21	4 (6%)	74,113,113	0.99	5 (6%)
16	CLA	h	510	-	63,73,73	1.19	3 (4%)	74,113,113	0.95	4 (5%)
16	CLA	o	515	-	63,73,73	1.13	3 (4%)	74,113,113	1.04	4 (5%)
16	CLA	b	1227	-	47,57,73	1.31	4 (8%)	53,93,113	1.09	4 (7%)
19	BCR	t	604	-	41,41,41	0.83	0	56,56,56	1.23	4 (7%)
16	CLA	H	1101	-	63,73,73	1.16	3 (4%)	74,113,113	1.00	2 (2%)
16	CLA	n	509	-	58,68,73	1.21	3 (5%)	68,107,113	0.94	4 (5%)
16	CLA	g	510	-	63,73,73	1.19	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	v	510	-	63,73,73	1.21	3 (4%)	74,113,113	0.98	5 (6%)
19	BCR	Z	603	-	41,41,41	0.85	0	56,56,56	1.17	4 (7%)
16	CLA	G	1222	25	48,58,73	1.36	4 (8%)	56,95,113	1.06	5 (8%)
16	CLA	A	1117	-	63,73,73	1.14	3 (4%)	74,113,113	1.17	4 (5%)
16	CLA	T	4002	-	43,53,73	1.45	3 (6%)	50,89,113	0.95	2 (4%)
16	CLA	q	502	-	48,58,73	1.31	4 (8%)	56,95,113	0.96	1 (1%)
18	SF4	C	102	-	0,12,12	-	-	-	-	-
16	CLA	Y	501	-	48,58,73	1.35	3 (6%)	56,95,113	1.12	4 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	F	1301	25	43,53,73	1.41	3 (6%)	50,89,113	1.13	3 (6%)
16	CLA	G	1208	-	43,53,73	1.39	3 (6%)	50,89,113	1.14	4 (8%)
16	CLA	g	516	-	44,54,73	1.40	3 (6%)	51,90,113	1.16	2 (3%)
16	CLA	v	516	-	44,54,73	1.42	3 (6%)	51,90,113	0.90	2 (3%)
21	ECH	i	4020	-	42,42,42	0.84	1 (2%)	55,58,58	1.84	10 (18%)
16	CLA	B	1210	-	63,73,73	1.17	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	Z	503	-	44,54,73	1.43	4 (9%)	51,90,113	1.00	2 (3%)
20	LMT	L	4101	-	36,36,36	1.17	6 (16%)	47,47,47	1.15	3 (6%)
16	CLA	y	505	-	63,73,73	1.21	3 (4%)	74,113,113	1.21	4 (5%)
16	CLA	a	1134	1	43,53,73	1.41	3 (6%)	50,89,113	1.12	3 (6%)
23	LMU	Z	605	-	36,36,36	0.87	0	47,47,47	1.20	4 (8%)
23	LMU	w	605	-	36,36,36	0.84	0	47,47,47	1.10	4 (8%)
16	CLA	T	4004	-	53,63,73	1.31	3 (5%)	62,101,113	1.10	3 (4%)
14	LMG	F	4017	-	27,27,55	1.10	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	H	1119	25	63,73,73	1.13	3 (4%)	74,113,113	0.94	2 (2%)
19	BCR	x	604	-	41,41,41	0.88	0	56,56,56	1.29	6 (10%)
16	CLA	B	1217	-	43,53,73	1.44	3 (6%)	50,89,113	1.00	1 (2%)
16	CLA	Z	506	-	58,68,73	1.23	3 (5%)	68,107,113	0.98	2 (2%)
16	CLA	H	1130	-	58,68,73	1.17	3 (5%)	68,107,113	0.95	5 (7%)
16	CLA	h	502	-	48,58,73	1.37	3 (6%)	56,95,113	0.96	4 (7%)
16	CLA	B	1204	-	63,73,73	1.16	3 (4%)	74,113,113	0.88	1 (1%)
16	CLA	B	1023	-	63,73,73	1.20	4 (6%)	74,113,113	1.09	4 (5%)
13	LHG	A	851	16	25,25,48	0.87	1 (4%)	28,31,54	1.27	2 (7%)
16	CLA	t	510	-	63,73,73	1.18	3 (4%)	74,113,113	0.96	4 (5%)
16	CLA	q	510	-	58,68,73	1.21	3 (5%)	68,107,113	0.92	3 (4%)
16	CLA	g	502	-	48,58,73	1.31	3 (6%)	56,95,113	0.93	0
19	BCR	B	4014	-	41,41,41	0.88	0	56,56,56	1.25	7 (12%)
13	LHG	r	605	-	30,30,48	0.81	2 (6%)	33,36,54	1.28	3 (9%)
16	CLA	G	1206	2	63,73,73	1.16	3 (4%)	74,113,113	0.91	2 (2%)
16	CLA	Z	511	-	63,73,73	1.15	4 (6%)	74,113,113	1.11	4 (5%)
16	CLA	p	506	-	58,68,73	1.24	3 (5%)	68,107,113	1.08	5 (7%)
16	CLA	g	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.92	4 (5%)
19	BCR	v	601	-	41,41,41	0.83	0	56,56,56	1.30	7 (12%)
16	CLA	t	513	-	44,54,73	1.42	3 (6%)	51,90,113	1.04	4 (7%)
19	BCR	y	604	-	41,41,41	0.87	0	56,56,56	1.29	7 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	B	1227	-	47,57,73	1.32	4 (8%)	53,93,113	1.12	4 (7%)
16	CLA	h	503	-	44,54,73	1.44	3 (6%)	51,90,113	1.17	3 (5%)
16	CLA	n	505	-	63,73,73	1.20	4 (6%)	74,113,113	1.19	4 (5%)
16	CLA	n	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.93	3 (4%)
16	CLA	w	513	-	48,58,73	1.36	3 (6%)	56,95,113	1.07	3 (5%)
16	CLA	w	501	-	48,58,73	1.34	3 (6%)	56,95,113	0.99	3 (5%)
16	CLA	Z	507	-	63,73,73	1.20	3 (4%)	74,113,113	1.01	3 (4%)
16	CLA	B	1207	-	63,73,73	1.19	4 (6%)	74,113,113	1.16	6 (8%)
16	CLA	g	506	-	58,68,73	1.23	3 (5%)	68,107,113	0.98	5 (7%)
16	CLA	p	511	-	63,73,73	1.14	3 (4%)	74,113,113	1.07	5 (6%)
16	CLA	A	1119	25	63,73,73	1.12	3 (4%)	74,113,113	1.00	4 (5%)
16	CLA	t	506	-	58,68,73	1.24	3 (5%)	68,107,113	1.04	4 (5%)
16	CLA	H	1132	-	63,73,73	1.13	3 (4%)	74,113,113	1.04	3 (4%)
13	LHG	i	103	-	39,39,48	0.69	2 (5%)	42,45,54	1.24	5 (11%)
16	CLA	L	1501	10	58,68,73	1.19	3 (5%)	68,107,113	0.97	4 (5%)
16	CLA	Z	504	-	63,73,73	1.17	4 (6%)	74,113,113	1.03	5 (6%)
16	CLA	q	506	-	58,68,73	1.25	3 (5%)	68,107,113	0.97	2 (2%)
16	CLA	o	513	-	44,54,73	1.39	3 (6%)	51,90,113	0.90	0
16	CLA	B	1213	-	53,63,73	1.27	4 (7%)	62,101,113	1.00	3 (4%)
16	CLA	B	1223	-	63,73,73	1.17	3 (4%)	74,113,113	1.01	2 (2%)
16	CLA	A	1118	-	53,63,73	1.28	3 (5%)	62,101,113	0.95	2 (3%)
16	CLA	g	511	-	63,73,73	1.16	3 (4%)	74,113,113	0.96	2 (2%)
16	CLA	u	517	12	53,63,73	1.30	3 (5%)	62,101,113	0.99	3 (4%)
19	BCR	Y	604	-	41,41,41	0.86	0	56,56,56	1.16	6 (10%)
21	ECH	m	4021	-	42,42,42	0.84	0	55,58,58	1.55	9 (16%)
16	CLA	r	515	-	63,73,73	1.18	3 (4%)	74,113,113	1.09	4 (5%)
16	CLA	U	1501	10	58,68,73	1.20	3 (5%)	68,107,113	1.00	3 (4%)
16	CLA	n	506	-	58,68,73	1.23	3 (5%)	68,107,113	1.05	4 (5%)
16	CLA	h	511	-	63,73,73	1.20	4 (6%)	74,113,113	1.00	7 (9%)
16	CLA	r	509	-	63,73,73	1.15	3 (4%)	74,113,113	0.95	3 (4%)
19	BCR	A	4003	-	41,41,41	0.85	0	56,56,56	1.29	7 (12%)
16	CLA	t	516	-	44,54,73	1.41	3 (6%)	51,90,113	1.05	2 (3%)
16	CLA	y	501	-	44,54,73	1.40	3 (6%)	51,90,113	1.19	3 (5%)
20	LMT	U	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
17	PQN	b	2002	-	34,34,34	0.36	0	43,45,45	1.06	2 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	1120	-	47,57,73	1.31	3 (6%)	53,93,113	1.13	5 (9%)
16	CLA	A	1122	-	57,67,73	1.25	3 (5%)	66,105,113	0.97	4 (6%)
16	CLA	A	1127	-	63,73,73	1.17	4 (6%)	74,113,113	1.06	3 (4%)
16	CLA	x	510	-	63,73,73	1.19	3 (4%)	74,113,113	1.01	3 (4%)
16	CLA	g	508	12	53,63,73	1.29	3 (5%)	62,101,113	0.91	2 (3%)
16	CLA	v	508	-	53,63,73	1.32	4 (7%)	62,101,113	1.24	5 (8%)
16	CLA	A	1102	16	54,64,73	1.26	3 (5%)	63,102,113	0.87	1 (1%)
13	LHG	H	849	-	42,42,48	0.68	0	45,48,54	1.21	4 (8%)
16	CLA	u	516	-	44,54,73	1.38	3 (6%)	51,90,113	1.08	3 (5%)
16	CLA	t	507	-	63,73,73	1.22	3 (4%)	74,113,113	0.88	2 (2%)
16	CLA	K	4004	-	53,63,73	1.31	3 (5%)	62,101,113	1.08	4 (6%)
16	CLA	H	1112	-	43,53,73	1.41	3 (6%)	50,89,113	0.97	2 (4%)
16	CLA	h	504	-	58,68,73	1.26	3 (5%)	68,107,113	1.14	5 (7%)
14	LMG	a	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)
19	BCR	U	4019	-	41,41,41	0.86	0	56,56,56	1.49	8 (14%)
19	BCR	o	601	-	41,41,41	0.88	1 (2%)	56,56,56	1.37	8 (14%)
16	CLA	q	515	-	63,73,73	1.18	3 (4%)	74,113,113	1.13	4 (5%)
16	CLA	A	1124	25	58,68,73	1.22	3 (5%)	68,107,113	1.03	3 (4%)
16	CLA	A	1237	25	63,73,73	1.20	4 (6%)	74,113,113	1.10	5 (6%)
16	CLA	n	503	-	44,54,73	1.41	3 (6%)	51,90,113	1.17	4 (7%)
16	CLA	w	515	-	63,73,73	1.17	3 (4%)	74,113,113	1.10	3 (4%)
19	BCR	G	4004	-	41,41,41	0.83	0	56,56,56	1.25	6 (10%)
16	CLA	Y	508	12	53,63,73	1.27	3 (5%)	62,101,113	0.94	3 (4%)
16	CLA	t	503	-	44,54,73	1.42	3 (6%)	51,90,113	1.20	4 (7%)
19	BCR	q	602	-	41,41,41	0.85	0	56,56,56	1.24	6 (10%)
16	CLA	w	503	-	44,54,73	1.43	4 (9%)	51,90,113	1.06	3 (5%)
16	CLA	x	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.97	3 (4%)
16	CLA	A	1130	-	58,68,73	1.20	3 (5%)	68,107,113	0.91	3 (4%)
19	BCR	h	604	-	41,41,41	0.86	0	56,56,56	1.25	6 (10%)
16	CLA	q	517	12	53,63,73	1.29	3 (5%)	62,101,113	1.04	4 (6%)
19	BCR	n	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	g	509	-	63,73,73	1.16	4 (6%)	74,113,113	0.99	2 (2%)
16	CLA	G	1012	25	53,63,73	1.24	3 (5%)	62,101,113	1.22	8 (12%)
16	CLA	b	1228	-	53,63,73	1.28	3 (5%)	62,101,113	1.01	3 (4%)
16	CLA	w	509	-	63,73,73	1.15	3 (4%)	74,113,113	0.94	3 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	B	1212	-	43,53,73	1.43	3 (6%)	50,89,113	1.17	4 (8%)
21	ECH	M	4021	-	42,42,42	0.86	0	55,58,58	1.53	9 (16%)
13	LHG	H	851	16	25,25,48	0.88	1 (4%)	28,31,54	1.27	2 (7%)
19	BCR	r	604	-	41,41,41	0.89	0	56,56,56	1.27	6 (10%)
16	CLA	u	501	-	44,54,73	1.40	3 (6%)	51,90,113	0.93	3 (5%)
19	BCR	L	4019	-	41,41,41	0.90	0	56,56,56	1.41	6 (10%)
16	CLA	y	513	-	44,54,73	1.42	3 (6%)	51,90,113	0.94	2 (3%)
19	BCR	x	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	A	1112	-	43,53,73	1.40	3 (6%)	50,89,113	1.04	3 (6%)
19	BCR	I	4018	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
16	CLA	r	517	12	53,63,73	1.29	3 (5%)	62,101,113	0.95	2 (3%)
16	CLA	a	1109	16	63,73,73	1.17	3 (4%)	74,113,113	1.11	4 (5%)
16	CLA	l	1501	10	58,68,73	1.20	3 (5%)	68,107,113	0.98	3 (4%)
16	CLA	H	1106	1	63,73,73	1.15	3 (4%)	74,113,113	1.09	3 (4%)
16	CLA	A	1114	-	44,54,73	1.39	3 (6%)	51,90,113	1.21	4 (7%)
16	CLA	H	1104	-	63,73,73	1.18	4 (6%)	74,113,113	0.99	4 (5%)
16	CLA	X	515	-	63,73,73	1.15	3 (4%)	74,113,113	1.05	4 (5%)
16	CLA	u	512	12	63,73,73	1.15	4 (6%)	74,113,113	1.03	2 (2%)
16	CLA	x	506	-	58,68,73	1.24	4 (6%)	68,107,113	1.06	4 (5%)
16	CLA	y	503	-	44,54,73	1.45	4 (9%)	51,90,113	1.14	4 (7%)
16	CLA	u	508	12	53,63,73	1.30	3 (5%)	62,101,113	0.93	2 (3%)
13	LHG	g	605	-	30,30,48	0.80	2 (6%)	33,36,54	1.26	3 (9%)
21	ECH	B	4006	-	42,42,42	0.74	0	55,58,58	1.53	11 (20%)
16	CLA	W	501	-	48,58,73	1.34	3 (6%)	56,95,113	1.11	3 (5%)
16	CLA	r	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.92	3 (4%)
19	BCR	k	4005	-	41,41,41	0.85	0	56,56,56	1.26	5 (8%)
19	BCR	T	4001	-	41,41,41	0.86	1 (2%)	56,56,56	1.26	7 (12%)
16	CLA	a	1116	-	52,62,73	1.24	3 (5%)	60,99,113	0.95	3 (5%)
16	CLA	B	1226	-	58,68,73	1.21	4 (6%)	68,107,113	1.02	3 (4%)
16	CLA	x	511	-	63,73,73	1.17	4 (6%)	74,113,113	0.90	2 (2%)
16	CLA	H	1108	-	43,53,73	1.40	3 (6%)	50,89,113	1.19	3 (6%)
16	CLA	a	1135	-	49,59,73	1.34	4 (8%)	56,96,113	1.06	3 (5%)
16	CLA	r	508	12	53,63,73	1.30	3 (5%)	62,101,113	0.93	2 (3%)
16	CLA	s	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.90	3 (4%)
19	BCR	G	4014	-	41,41,41	0.90	1 (2%)	56,56,56	1.29	8 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	LMG	H	4101	-	46,46,55	0.91	1 (2%)	54,54,63	1.23	4 (7%)
14	LMG	b	848	-	43,43,55	0.86	1 (2%)	51,51,63	1.28	6 (11%)
16	CLA	A	1126	-	63,73,73	1.15	3 (4%)	74,113,113	1.15	2 (2%)
16	CLA	H	1107	1	48,58,73	1.35	3 (6%)	56,95,113	1.02	4 (7%)
15	CL0	A	1011	-	63,73,73	1.22	4 (6%)	74,113,113	1.02	5 (6%)
16	CLA	B	1224	-	58,68,73	1.24	4 (6%)	68,107,113	1.10	3 (4%)
16	CLA	B	1231	25	43,53,73	1.43	3 (6%)	50,89,113	1.14	3 (6%)
16	CLA	p	513	-	44,54,73	1.40	3 (6%)	51,90,113	0.91	2 (3%)
16	CLA	G	1219	-	43,53,73	1.44	3 (6%)	50,89,113	1.03	3 (6%)
16	CLA	W	516	-	44,54,73	1.41	3 (6%)	51,90,113	1.04	2 (3%)
16	CLA	b	1226	-	58,68,73	1.21	4 (6%)	68,107,113	1.03	3 (4%)
19	BCR	u	601	-	41,41,41	0.91	1 (2%)	56,56,56	1.38	9 (16%)
19	BCR	t	603	-	41,41,41	0.84	0	56,56,56	1.18	4 (7%)
19	BCR	S	4015	-	41,41,41	0.87	0	56,56,56	1.20	8 (14%)
16	CLA	B	1208	-	43,53,73	1.40	3 (6%)	50,89,113	1.11	4 (8%)
16	CLA	t	517	12	53,63,73	1.28	3 (5%)	62,101,113	0.90	1 (1%)
16	CLA	u	514	-	48,58,73	1.36	3 (6%)	56,95,113	1.16	4 (7%)
19	BCR	r	603	-	41,41,41	0.83	0	56,56,56	1.20	6 (10%)
16	CLA	t	501	-	48,58,73	1.35	3 (6%)	56,95,113	1.12	3 (5%)
14	LMG	f	4017	-	27,27,55	1.09	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	A	1135	-	49,59,73	1.31	4 (8%)	56,96,113	1.13	4 (7%)
16	CLA	q	508	12	53,63,73	1.28	3 (5%)	62,101,113	1.11	4 (6%)
19	BCR	B	4017	-	41,41,41	0.88	0	56,56,56	1.22	6 (10%)
16	CLA	G	1202	-	63,73,73	1.15	3 (4%)	74,113,113	0.91	3 (4%)
16	CLA	A	1121	-	49,59,73	1.34	3 (6%)	56,96,113	1.04	2 (3%)
16	CLA	W	513	-	44,54,73	1.43	3 (6%)	51,90,113	1.00	2 (3%)
19	BCR	A	4002	-	41,41,41	0.84	0	56,56,56	1.15	3 (5%)
16	CLA	o	506	-	58,68,73	1.24	4 (6%)	68,107,113	1.05	4 (5%)
19	BCR	B	4010	-	41,41,41	0.91	0	56,56,56	1.35	8 (14%)
16	CLA	H	1124	-	58,68,73	1.21	3 (5%)	68,107,113	0.89	1 (1%)
16	CLA	H	1237	25	63,73,73	1.18	4 (6%)	74,113,113	1.09	5 (6%)
16	CLA	w	506	-	58,68,73	1.24	4 (6%)	68,107,113	1.06	3 (4%)
16	CLA	Q	1301	25	43,53,73	1.42	3 (6%)	50,89,113	1.12	4 (8%)
19	BCR	J	4012	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
16	CLA	W	503	-	44,54,73	1.39	3 (6%)	51,90,113	1.15	4 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	BCR	X	602	-	41,41,41	0.88	0	56,56,56	1.36	7 (12%)
19	BCR	b	4014	-	41,41,41	0.91	0	56,56,56	1.45	8 (14%)
16	CLA	a	1115	-	52,62,73	1.28	3 (5%)	60,99,113	1.10	2 (3%)
19	BCR	A	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.40	9 (16%)
16	CLA	H	1140	-	63,73,73	1.16	4 (6%)	74,113,113	1.03	2 (2%)
16	CLA	x	509	-	63,73,73	1.14	3 (4%)	74,113,113	0.97	4 (5%)
16	CLA	o	511	-	63,73,73	1.15	3 (4%)	74,113,113	1.04	5 (6%)
16	CLA	s	513	-	44,54,73	1.41	3 (6%)	51,90,113	1.08	3 (5%)
16	CLA	W	507	-	63,73,73	1.22	3 (4%)	74,113,113	0.89	2 (2%)
14	LMG	a	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.24	4 (8%)
24	LUT	w	601	-	42,43,43	0.74	0	51,60,60	1.46	7 (13%)
16	CLA	v	512	12	63,73,73	1.20	3 (4%)	74,113,113	1.04	6 (8%)
16	CLA	W	515	-	63,73,73	1.18	3 (4%)	74,113,113	1.01	4 (5%)
16	CLA	a	1103	-	63,73,73	1.17	3 (4%)	74,113,113	0.97	2 (2%)
16	CLA	r	512	12	63,73,73	1.19	4 (6%)	74,113,113	1.19	4 (5%)
16	CLA	X	508	12	53,63,73	1.30	3 (5%)	62,101,113	0.87	2 (3%)
19	BCR	A	4008	-	41,41,41	0.89	0	56,56,56	1.35	8 (14%)
16	CLA	l	1502	-	58,68,73	1.15	3 (5%)	68,107,113	1.10	3 (4%)
16	CLA	q	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.14	4 (7%)
16	CLA	p	503	-	44,54,73	1.36	4 (9%)	51,90,113	1.08	5 (9%)
20	LMT	a	4202	-	36,36,36	1.17	5 (13%)	47,47,47	0.93	0
16	CLA	X	504	-	58,68,73	1.24	3 (5%)	68,107,113	1.14	3 (4%)
16	CLA	s	512	12	63,73,73	1.20	4 (6%)	74,113,113	1.15	6 (8%)
16	CLA	B	1234	-	48,58,73	1.31	4 (8%)	56,95,113	1.19	5 (8%)
23	LMU	p	606	-	36,36,36	0.83	0	47,47,47	1.33	5 (10%)
16	CLA	H	1131	-	63,73,73	1.16	3 (4%)	74,113,113	1.02	3 (4%)
19	BCR	Y	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	r	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.05	4 (7%)
16	CLA	s	516	-	44,54,73	1.38	3 (6%)	51,90,113	1.02	2 (3%)
16	CLA	B	1012	25	53,63,73	1.25	3 (5%)	62,101,113	1.16	6 (9%)
16	CLA	G	1234	-	48,58,73	1.29	4 (8%)	56,95,113	1.23	5 (8%)
16	CLA	b	1210	-	63,73,73	1.19	3 (4%)	74,113,113	1.04	5 (6%)
16	CLA	b	1229	-	56,66,73	1.26	3 (5%)	65,104,113	0.98	4 (6%)
16	CLA	Y	510	-	63,73,73	1.19	3 (4%)	74,113,113	0.97	3 (4%)
16	CLA	p	509	-	58,68,73	1.20	3 (5%)	68,107,113	0.97	3 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	1107	1	48,58,73	1.35	3 (6%)	56,95,113	1.06	3 (5%)
16	CLA	a	1101	-	63,73,73	1.16	3 (4%)	74,113,113	1.05	4 (5%)
16	CLA	o	517	12	53,63,73	1.28	3 (5%)	62,101,113	0.92	2 (3%)
16	CLA	t	511	-	63,73,73	1.17	3 (4%)	74,113,113	1.02	4 (5%)
19	BCR	g	604	-	41,41,41	0.88	0	56,56,56	1.28	6 (10%)
16	CLA	A	1013	-	63,73,73	1.12	4 (6%)	74,113,113	1.21	8 (10%)
16	CLA	v	509	-	63,73,73	1.17	4 (6%)	74,113,113	0.98	5 (6%)
16	CLA	b	1217	-	43,53,73	1.42	3 (6%)	50,89,113	1.16	4 (8%)
16	CLA	r	505	-	63,73,73	1.18	3 (4%)	74,113,113	1.15	4 (5%)
19	BCR	y	603	-	41,41,41	0.83	0	56,56,56	1.17	5 (8%)
16	CLA	o	509	-	58,68,73	1.20	3 (5%)	68,107,113	0.91	4 (5%)
23	LMU	g	606	-	36,36,36	0.86	0	47,47,47	1.32	5 (10%)
16	CLA	B	1236	-	48,58,73	1.32	4 (8%)	56,95,113	1.05	3 (5%)
16	CLA	Y	515	-	63,73,73	1.14	3 (4%)	74,113,113	1.02	4 (5%)
16	CLA	H	1022	25	63,73,73	1.14	3 (4%)	74,113,113	1.06	6 (8%)
16	CLA	B	1201	-	52,62,73	1.30	3 (5%)	60,99,113	1.01	2 (3%)
16	CLA	A	1131	-	63,73,73	1.16	3 (4%)	74,113,113	1.05	3 (4%)
16	CLA	H	1133	-	52,62,73	1.28	4 (7%)	60,99,113	1.15	3 (5%)
19	BCR	q	603	-	41,41,41	0.84	0	56,56,56	1.16	5 (8%)
23	LMU	Y	606	-	36,36,36	0.84	0	47,47,47	1.36	6 (12%)
16	CLA	H	1135	-	49,59,73	1.33	4 (8%)	56,96,113	1.15	3 (5%)
16	CLA	J	1303	-	35,45,73	1.56	4 (11%)	42,78,113	0.98	2 (4%)
16	CLA	Z	516	-	44,54,73	1.38	3 (6%)	51,90,113	0.98	2 (3%)
16	CLA	A	1101	-	63,73,73	1.17	3 (4%)	74,113,113	0.99	6 (8%)
23	LMU	x	606	-	36,36,36	0.88	0	47,47,47	1.26	6 (12%)
16	CLA	w	507	-	63,73,73	1.20	3 (4%)	74,113,113	0.85	2 (2%)
16	CLA	b	1207	-	63,73,73	1.19	3 (4%)	74,113,113	1.15	4 (5%)
16	CLA	Z	509	-	63,73,73	1.15	3 (4%)	74,113,113	0.96	2 (2%)
16	CLA	s	506	-	58,68,73	1.25	4 (6%)	68,107,113	1.06	6 (8%)
16	CLA	B	1239	-	63,73,73	1.17	3 (4%)	74,113,113	1.09	4 (5%)
16	CLA	y	506	-	58,68,73	1.23	3 (5%)	68,107,113	1.11	5 (7%)
16	CLA	a	1104	-	63,73,73	1.17	4 (6%)	74,113,113	1.00	3 (4%)
16	CLA	a	1113	-	43,53,73	1.44	4 (9%)	50,89,113	1.14	2 (4%)
16	CLA	K	4003	9	43,53,73	1.46	3 (6%)	50,89,113	1.03	2 (4%)
14	LMG	H	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	G	1225	-	63,73,73	1.16	4 (6%)	74,113,113	1.06	3 (4%)
16	CLA	H	1127	-	63,73,73	1.18	4 (6%)	74,113,113	1.11	4 (5%)
13	LHG	a	851	16	25,25,48	0.88	2 (8%)	28,31,54	1.26	2 (7%)
16	CLA	a	1132	-	63,73,73	1.11	3 (4%)	74,113,113	1.15	3 (4%)
19	BCR	B	4004	-	41,41,41	0.83	0	56,56,56	1.26	5 (8%)
16	CLA	G	1224	-	58,68,73	1.24	4 (6%)	68,107,113	1.11	3 (4%)
16	CLA	B	1214	-	53,63,73	1.26	3 (5%)	62,101,113	1.18	3 (4%)
16	CLA	a	1801	13	44,54,73	1.39	3 (6%)	51,90,113	1.22	3 (5%)
16	CLA	H	1111	-	53,63,73	1.28	3 (5%)	62,101,113	1.03	2 (3%)
16	CLA	a	1136	-	63,73,73	1.14	3 (4%)	74,113,113	0.95	2 (2%)
16	CLA	y	511	-	63,73,73	1.19	3 (4%)	74,113,113	1.11	4 (5%)
16	CLA	a	1108	-	43,53,73	1.42	3 (6%)	50,89,113	1.20	3 (6%)
16	CLA	p	517	12	53,63,73	1.29	3 (5%)	62,101,113	0.93	2 (3%)
24	LUT	Z	601	-	42,43,43	0.81	1 (2%)	51,60,60	1.48	6 (11%)
19	BCR	u	604	-	41,41,41	0.89	0	56,56,56	1.35	10 (17%)
16	CLA	t	509	-	58,68,73	1.22	3 (5%)	68,107,113	1.08	4 (5%)
13	LHG	s	605	-	31,31,48	0.79	1 (3%)	34,37,54	1.28	4 (11%)
16	CLA	w	512	12	63,73,73	1.17	4 (6%)	74,113,113	1.10	5 (6%)
16	CLA	A	1109	16	63,73,73	1.18	3 (4%)	74,113,113	1.07	4 (5%)
16	CLA	x	503	-	44,54,73	1.40	3 (6%)	51,90,113	1.04	2 (3%)
16	CLA	y	507	-	63,73,73	1.21	3 (4%)	74,113,113	0.87	2 (2%)
16	CLA	u	513	-	44,54,73	1.40	3 (6%)	51,90,113	0.93	2 (3%)
16	CLA	v	517	-	53,63,73	1.33	3 (5%)	62,101,113	1.00	4 (6%)
16	CLA	X	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.10	5 (6%)
16	CLA	h	506	-	58,68,73	1.26	4 (6%)	68,107,113	1.22	6 (8%)
16	CLA	s	508	12	53,63,73	1.28	3 (5%)	62,101,113	0.95	4 (6%)
16	CLA	y	504	-	58,68,73	1.25	4 (6%)	68,107,113	1.02	5 (7%)
16	CLA	b	1231	25	43,53,73	1.44	3 (6%)	50,89,113	1.17	3 (6%)
16	CLA	A	1134	1	43,53,73	1.42	3 (6%)	50,89,113	0.99	1 (2%)
19	BCR	Z	602	-	41,41,41	0.87	0	56,56,56	1.36	8 (14%)
16	CLA	b	1224	-	58,68,73	1.23	4 (6%)	68,107,113	1.24	4 (5%)
16	CLA	b	1234	-	48,58,73	1.33	3 (6%)	56,95,113	1.19	7 (12%)
18	SF4	H	3001	-	0,12,12	-	-	-	-	-
16	CLA	B	1220	-	51,61,73	1.36	3 (5%)	59,98,113	1.05	5 (8%)
16	CLA	f	1301	25	43,53,73	1.42	3 (6%)	50,89,113	1.04	4 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	Y	516	-	44,54,73	1.38	3 (6%)	51,90,113	1.05	2 (3%)
16	CLA	H	1129	-	44,54,73	1.34	3 (6%)	51,90,113	1.03	3 (5%)
16	CLA	b	1235	-	60,70,73	1.21	4 (6%)	70,109,113	1.13	7 (10%)
19	BCR	r	602	-	41,41,41	0.86	0	56,56,56	1.24	4 (7%)
19	BCR	W	601	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
16	CLA	Z	508	12	53,63,73	1.28	3 (5%)	62,101,113	1.10	4 (6%)
16	CLA	h	507	-	63,73,73	1.18	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	b	1230	-	43,53,73	1.41	3 (6%)	50,89,113	1.10	3 (6%)
16	CLA	a	1140	-	63,73,73	1.15	3 (4%)	74,113,113	1.00	2 (2%)
16	CLA	K	4002	-	43,53,73	1.44	3 (6%)	50,89,113	0.96	2 (4%)
16	CLA	y	512	12	63,73,73	1.20	3 (4%)	74,113,113	0.91	3 (4%)
16	CLA	S	1303	-	35,45,73	1.56	4 (11%)	42,78,113	0.98	2 (4%)
16	CLA	s	517	12	53,63,73	1.32	3 (5%)	62,101,113	0.98	2 (3%)
16	CLA	b	1232	25	43,53,73	1.45	3 (6%)	50,89,113	1.33	3 (6%)
16	CLA	v	513	-	44,54,73	1.44	3 (6%)	51,90,113	0.95	2 (3%)
16	CLA	q	511	-	63,73,73	1.16	3 (4%)	74,113,113	1.09	4 (5%)
16	CLA	o	503	-	44,54,73	1.39	3 (6%)	51,90,113	0.97	2 (3%)
16	CLA	v	501	-	44,54,73	1.43	3 (6%)	51,90,113	1.07	4 (7%)
16	CLA	H	1128	-	63,73,73	1.17	4 (6%)	74,113,113	1.05	5 (6%)
16	CLA	r	513	-	44,54,73	1.42	3 (6%)	51,90,113	0.99	3 (5%)
16	CLA	t	512	12	63,73,73	1.19	4 (6%)	74,113,113	1.11	4 (5%)
14	LMG	Q	4017	-	27,27,55	1.07	1 (3%)	35,35,63	1.18	3 (8%)
16	CLA	G	1223	-	63,73,73	1.17	3 (4%)	74,113,113	1.07	4 (5%)
16	CLA	j	1302	8	43,53,73	1.47	3 (6%)	50,89,113	1.00	3 (6%)
16	CLA	y	510	-	63,73,73	1.19	3 (4%)	74,113,113	0.91	3 (4%)
19	BCR	H	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.30	7 (12%)
16	CLA	r	503	-	44,54,73	1.39	3 (6%)	51,90,113	1.01	2 (3%)
16	CLA	B	1211	-	63,73,73	1.18	4 (6%)	74,113,113	0.97	3 (4%)
19	BCR	x	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	X	506	-	58,68,73	1.23	4 (6%)	68,107,113	1.26	4 (5%)
16	CLA	X	514	-	48,58,73	1.38	4 (8%)	56,95,113	1.29	5 (8%)
16	CLA	j	1303	-	35,45,73	1.56	4 (11%)	42,78,113	1.02	2 (4%)
16	CLA	n	512	12	63,73,73	1.18	4 (6%)	74,113,113	1.06	4 (5%)
16	CLA	t	508	12	53,63,73	1.28	3 (5%)	62,101,113	0.94	2 (3%)
19	BCR	J	4013	-	41,41,41	0.86	0	56,56,56	1.23	8 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	BCR	K	4001	-	41,41,41	0.86	0	56,56,56	1.31	7 (12%)
19	BCR	W	603	-	41,41,41	0.85	0	56,56,56	1.21	3 (5%)
14	LMG	A	4101	-	46,46,55	0.93	2 (4%)	54,54,63	1.23	4 (7%)
16	CLA	n	516	-	44,54,73	1.41	3 (6%)	51,90,113	0.85	1 (1%)
16	CLA	G	1205	-	63,73,73	1.16	4 (6%)	74,113,113	1.09	4 (5%)
16	CLA	H	1122	-	57,67,73	1.23	3 (5%)	66,105,113	0.96	3 (4%)
16	CLA	g	503	-	44,54,73	1.41	3 (6%)	51,90,113	0.99	2 (3%)
16	CLA	X	511	-	63,73,73	1.14	3 (4%)	74,113,113	1.11	6 (8%)
16	CLA	q	505	-	63,73,73	1.16	4 (6%)	74,113,113	1.17	8 (10%)
16	CLA	p	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.94	3 (4%)
19	BCR	o	603	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
16	CLA	a	1111	-	53,63,73	1.28	3 (5%)	62,101,113	1.03	2 (3%)
16	CLA	b	1223	-	63,73,73	1.18	3 (4%)	74,113,113	1.06	1 (1%)
16	CLA	u	503	-	44,54,73	1.39	3 (6%)	51,90,113	0.94	2 (3%)
16	CLA	g	515	-	63,73,73	1.19	3 (4%)	74,113,113	1.12	4 (5%)
16	CLA	a	1110	-	52,62,73	1.25	3 (5%)	60,99,113	0.97	2 (3%)
18	SF4	N	101	-	0,12,12	-	-	-	-	-
16	CLA	x	516	-	44,54,73	1.39	3 (6%)	51,90,113	1.14	3 (5%)
16	CLA	A	1138	-	63,73,73	1.16	3 (4%)	74,113,113	0.90	3 (4%)
19	BCR	b	4017	-	41,41,41	0.87	0	56,56,56	1.16	4 (7%)
16	CLA	g	517	12	53,63,73	1.32	3 (5%)	62,101,113	0.89	1 (1%)
16	CLA	v	514	-	48,58,73	1.38	3 (6%)	56,95,113	0.97	2 (3%)
19	BCR	g	601	-	41,41,41	0.88	0	56,56,56	1.44	9 (16%)
16	CLA	G	1214	-	53,63,73	1.24	4 (7%)	62,101,113	1.09	3 (4%)
16	CLA	a	1133	-	52,62,73	1.30	3 (5%)	60,99,113	0.92	2 (3%)
19	BCR	b	4010	-	41,41,41	0.91	0	56,56,56	1.33	7 (12%)
16	CLA	X	510	-	58,68,73	1.23	3 (5%)	68,107,113	0.91	2 (2%)
16	CLA	b	1205	-	63,73,73	1.16	3 (4%)	74,113,113	1.05	4 (5%)
16	CLA	H	1125	-	63,73,73	1.18	3 (4%)	74,113,113	0.96	2 (2%)
16	CLA	a	1237	25	63,73,73	1.19	4 (6%)	74,113,113	1.12	5 (6%)
19	BCR	q	604	-	41,41,41	0.87	0	56,56,56	1.26	6 (10%)
16	CLA	G	1212	-	43,53,73	1.45	3 (6%)	50,89,113	1.23	4 (8%)
16	CLA	H	1120	-	47,57,73	1.31	3 (6%)	53,93,113	1.19	5 (9%)
13	LHG	p	605	-	31,31,48	0.77	1 (3%)	34,37,54	1.29	4 (11%)
16	CLA	b	1218	-	53,63,73	1.29	3 (5%)	62,101,113	1.00	5 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	Z	505	-	63,73,73	1.19	3 (4%)	74,113,113	0.93	3 (4%)
16	CLA	h	517	-	53,63,73	1.31	3 (5%)	62,101,113	0.96	4 (6%)
16	CLA	H	1110	-	52,62,73	1.27	3 (5%)	60,99,113	0.97	3 (5%)
16	CLA	r	510	-	63,73,73	1.18	3 (4%)	74,113,113	0.96	2 (2%)
20	LMT	l	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
16	CLA	o	512	12	63,73,73	1.17	4 (6%)	74,113,113	1.18	5 (6%)
19	BCR	X	601	-	41,41,41	0.87	1 (2%)	56,56,56	1.33	6 (10%)
16	CLA	W	504	-	58,68,73	1.26	3 (5%)	68,107,113	0.97	3 (4%)
16	CLA	x	501	-	48,58,73	1.36	3 (6%)	56,95,113	1.22	4 (7%)
13	LHG	B	4018	16	37,37,48	0.72	1 (2%)	40,43,54	1.32	5 (12%)
17	PQN	G	2002	-	34,34,34	0.38	0	43,45,45	1.04	2 (4%)
16	CLA	G	1236	-	48,58,73	1.32	3 (6%)	56,95,113	1.05	2 (3%)
16	CLA	X	517	12	53,63,73	1.28	3 (5%)	62,101,113	0.95	4 (6%)
19	BCR	r	601	-	41,41,41	0.86	1 (2%)	56,56,56	1.29	7 (12%)
16	CLA	G	1220	-	52,62,73	1.31	3 (5%)	60,99,113	1.04	3 (5%)
18	SF4	c	101	-	0,12,12	-	-	-	-	-
16	CLA	s	515	-	63,73,73	1.14	3 (4%)	74,113,113	0.98	4 (5%)
16	CLA	q	513	-	48,58,73	1.36	3 (6%)	56,95,113	1.01	3 (5%)
19	BCR	l	4019	-	41,41,41	0.88	0	56,56,56	1.44	8 (14%)
21	ECH	G	4006	-	42,42,42	0.79	0	55,58,58	1.50	8 (14%)
16	CLA	q	501	-	48,58,73	1.35	3 (6%)	56,95,113	0.99	3 (5%)
16	CLA	s	504	-	63,73,73	1.18	3 (4%)	74,113,113	0.90	2 (2%)
19	BCR	g	603	-	41,41,41	0.84	0	56,56,56	1.21	6 (10%)
19	BCR	v	603	-	41,41,41	0.85	0	56,56,56	1.27	8 (14%)
16	CLA	n	508	12	53,63,73	1.29	3 (5%)	62,101,113	0.92	1 (1%)
19	BCR	W	604	-	41,41,41	0.86	0	56,56,56	1.37	9 (16%)
16	CLA	b	1012	25	53,63,73	1.23	3 (5%)	62,101,113	1.24	8 (12%)
14	LMG	A	4201	-	32,32,55	1.00	1 (3%)	40,40,63	1.18	3 (7%)
16	CLA	H	1103	-	63,73,73	1.16	3 (4%)	74,113,113	0.99	3 (4%)
16	CLA	b	1211	-	63,73,73	1.18	3 (4%)	74,113,113	0.94	3 (4%)
19	BCR	Q	4016	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)
16	CLA	t	505	-	63,73,73	1.19	3 (4%)	74,113,113	1.18	5 (6%)
18	SF4	a	3001	-	0,12,12	-	-	-	-	-
16	CLA	Y	502	-	48,58,73	1.34	3 (6%)	56,95,113	0.97	3 (5%)
16	CLA	a	1129	-	44,54,73	1.33	3 (6%)	51,90,113	1.07	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	BCR	f	4016	-	41,41,41	0.87	0	56,56,56	1.29	5 (8%)
16	CLA	X	502	-	48,58,73	1.32	4 (8%)	56,95,113	0.94	2 (3%)
19	BCR	s	604	-	41,41,41	0.87	0	56,56,56	1.22	5 (8%)
19	BCR	L	4022	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
19	BCR	o	602	-	41,41,41	0.88	0	56,56,56	1.37	7 (12%)
16	CLA	n	517	12	53,63,73	1.27	3 (5%)	62,101,113	0.90	1 (1%)
16	CLA	B	1216	25	45,55,73	1.40	4 (8%)	52,91,113	1.09	3 (5%)
16	CLA	q	516	-	44,54,73	1.38	3 (6%)	51,90,113	0.89	1 (1%)
16	CLA	p	512	12	63,73,73	1.21	4 (6%)	74,113,113	1.16	5 (6%)
16	CLA	r	501	-	48,58,73	1.34	3 (6%)	56,95,113	1.15	4 (7%)
16	CLA	Y	514	-	48,58,73	1.35	3 (6%)	56,95,113	1.07	4 (7%)
16	CLA	l	1503	-	63,73,73	1.16	3 (4%)	74,113,113	0.91	3 (4%)
18	SF4	C	101	-	0,12,12	-	-	-	-	-
16	CLA	B	1240	13	44,54,73	1.43	3 (6%)	51,90,113	1.17	3 (5%)
16	CLA	G	1229	-	56,66,73	1.26	3 (5%)	65,104,113	1.03	4 (6%)
16	CLA	G	1232	25	43,53,73	1.44	3 (6%)	50,89,113	1.25	5 (10%)
16	CLA	x	517	12	53,63,73	1.30	3 (5%)	62,101,113	0.90	2 (3%)
16	CLA	h	508	-	53,63,73	1.30	3 (5%)	62,101,113	1.05	4 (6%)
16	CLA	B	1230	-	43,53,73	1.40	3 (6%)	50,89,113	1.05	2 (4%)
16	CLA	g	512	12	63,73,73	1.20	4 (6%)	74,113,113	1.14	4 (5%)
16	CLA	J	1302	8	43,53,73	1.47	3 (6%)	50,89,113	1.09	3 (6%)
16	CLA	s	503	-	44,54,73	1.40	4 (9%)	51,90,113	1.17	4 (7%)
16	CLA	B	1222	25	48,58,73	1.36	3 (6%)	56,95,113	1.02	3 (5%)
19	BCR	H	4008	-	41,41,41	0.90	1 (2%)	56,56,56	1.36	4 (7%)
16	CLA	Q	1302	6	44,54,73	1.42	3 (6%)	51,90,113	0.98	2 (3%)
16	CLA	X	513	-	44,54,73	1.38	3 (6%)	51,90,113	1.02	2 (3%)
18	SF4	c	102	-	0,12,12	-	-	-	-	-
16	CLA	h	512	12	63,73,73	1.21	4 (6%)	74,113,113	0.95	4 (5%)
16	CLA	n	502	-	48,58,73	1.35	4 (8%)	56,95,113	1.06	2 (3%)
19	BCR	j	4015	-	41,41,41	0.88	0	56,56,56	1.22	7 (12%)
16	CLA	a	1121	-	49,59,73	1.35	3 (6%)	56,96,113	1.07	3 (5%)
16	CLA	a	1128	-	63,73,73	1.14	4 (6%)	74,113,113	1.07	5 (6%)
16	CLA	b	1023	-	63,73,73	1.18	4 (6%)	74,113,113	1.09	3 (4%)
14	LMG	A	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)
16	CLA	w	502	-	48,58,73	1.32	4 (8%)	56,95,113	1.10	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	q	503	-	44,54,73	1.42	4 (9%)	51,90,113	1.20	4 (7%)
16	CLA	s	510	-	63,73,73	1.18	3 (4%)	74,113,113	0.92	3 (4%)
16	CLA	H	1137	-	45,55,73	1.35	3 (6%)	52,91,113	1.01	4 (7%)
16	CLA	G	1228	-	53,63,73	1.27	3 (5%)	62,101,113	1.02	3 (4%)
16	CLA	y	517	-	53,63,73	1.33	3 (5%)	62,101,113	1.23	5 (8%)
16	CLA	A	1140	-	63,73,73	1.16	4 (6%)	74,113,113	1.07	3 (4%)
16	CLA	g	514	-	48,58,73	1.34	4 (8%)	56,95,113	1.02	4 (7%)
19	BCR	a	4007	-	41,41,41	0.89	1 (2%)	56,56,56	1.30	5 (8%)
19	BCR	a	4011	-	41,41,41	0.89	0	56,56,56	1.26	5 (8%)
16	CLA	a	1117	-	63,73,73	1.12	3 (4%)	74,113,113	1.17	6 (8%)
16	CLA	b	1240	13	44,54,73	1.42	3 (6%)	51,90,113	1.11	2 (3%)
16	CLA	W	506	-	58,68,73	1.22	3 (5%)	68,107,113	1.05	4 (5%)
16	CLA	B	1215	-	58,68,73	1.16	3 (5%)	68,107,113	1.12	3 (4%)
16	CLA	a	1105	-	56,66,73	1.25	3 (5%)	65,104,113	0.98	4 (6%)
19	BCR	S	4013	-	41,41,41	0.87	0	56,56,56	1.32	7 (12%)
19	BCR	a	4003	-	41,41,41	0.87	0	56,56,56	1.22	4 (7%)
16	CLA	B	1225	-	63,73,73	1.15	4 (6%)	74,113,113	1.05	4 (5%)
16	CLA	f	1302	6	44,54,73	1.43	3 (6%)	51,90,113	1.00	2 (3%)
19	BCR	w	604	-	41,41,41	0.87	0	56,56,56	1.27	6 (10%)
16	CLA	a	1120	-	47,57,73	1.32	3 (6%)	53,93,113	1.23	5 (9%)
16	CLA	h	514	-	48,58,73	1.37	3 (6%)	56,95,113	1.01	4 (7%)
16	CLA	W	511	-	63,73,73	1.18	3 (4%)	74,113,113	1.07	6 (8%)
16	CLA	v	502	-	48,58,73	1.34	3 (6%)	56,95,113	0.96	3 (5%)
19	BCR	Y	603	-	41,41,41	0.85	0	56,56,56	1.16	4 (7%)
16	CLA	H	1116	-	52,62,73	1.23	4 (7%)	60,99,113	1.06	4 (6%)
16	CLA	y	502	-	48,58,73	1.36	3 (6%)	56,95,113	0.97	3 (5%)
16	CLA	B	1206	2	63,73,73	1.15	3 (4%)	74,113,113	0.92	4 (5%)
19	BCR	x	603	-	41,41,41	0.85	0	56,56,56	1.26	6 (10%)
16	CLA	b	1204	-	63,73,73	1.17	3 (4%)	74,113,113	0.92	2 (2%)
16	CLA	q	509	-	63,73,73	1.13	3 (4%)	74,113,113	0.96	4 (5%)
16	CLA	B	1238	25	63,73,73	1.14	3 (4%)	74,113,113	0.98	3 (4%)
16	CLA	H	1102	16	54,64,73	1.24	3 (5%)	63,102,113	0.91	2 (3%)
16	CLA	H	1136	-	63,73,73	1.14	3 (4%)	74,113,113	0.94	2 (2%)
16	CLA	A	1137	-	45,55,73	1.36	3 (6%)	52,91,113	0.98	4 (7%)
16	CLA	H	1801	13	44,54,73	1.36	3 (6%)	51,90,113	1.14	4 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	CLA	u	510	-	58,68,73	1.24	3 (5%)	68,107,113	0.89	3 (4%)
16	CLA	h	509	-	63,73,73	1.19	4 (6%)	74,113,113	1.01	4 (5%)
16	CLA	G	1211	-	63,73,73	1.20	3 (4%)	74,113,113	0.97	2 (2%)
16	CLA	A	1022	25	63,73,73	1.17	3 (4%)	74,113,113	1.00	6 (8%)
16	CLA	p	508	12	53,63,73	1.29	3 (5%)	62,101,113	0.97	4 (6%)
16	CLA	A	1125	-	63,73,73	1.18	3 (4%)	74,113,113	0.96	3 (4%)
16	CLA	n	515	-	63,73,73	1.17	3 (4%)	74,113,113	1.02	3 (4%)
16	CLA	G	1021	-	63,73,73	1.16	3 (4%)	74,113,113	1.11	4 (5%)
16	CLA	a	1130	-	58,68,73	1.18	3 (5%)	68,107,113	0.96	4 (5%)
13	LHG	G	4018	16	37,37,48	0.73	1 (2%)	40,43,54	1.32	5 (12%)
16	CLA	v	515	-	63,73,73	1.21	3 (4%)	74,113,113	1.09	5 (6%)
16	CLA	w	508	12	53,63,73	1.28	3 (5%)	62,101,113	1.00	4 (6%)
19	BCR	X	604	-	41,41,41	0.88	0	56,56,56	1.31	5 (8%)
19	BCR	v	604	-	41,41,41	0.86	0	56,56,56	1.28	8 (14%)
16	CLA	A	1139	25	58,68,73	1.22	3 (5%)	68,107,113	1.03	3 (4%)
16	CLA	b	1206	2	63,73,73	1.14	3 (4%)	74,113,113	0.95	3 (4%)
16	CLA	y	515	-	63,73,73	1.20	3 (4%)	74,113,113	1.06	6 (8%)
16	CLA	B	1205	-	63,73,73	1.18	3 (4%)	74,113,113	1.03	3 (4%)
16	CLA	Z	517	12	53,63,73	1.31	3 (5%)	62,101,113	0.97	2 (3%)
16	CLA	u	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.93	3 (4%)
16	CLA	G	1204	-	63,73,73	1.17	3 (4%)	74,113,113	0.94	2 (2%)
16	CLA	w	504	-	63,73,73	1.17	3 (4%)	74,113,113	0.96	4 (5%)
16	CLA	H	1134	1	43,53,73	1.41	3 (6%)	50,89,113	0.98	1 (2%)
16	CLA	x	512	12	63,73,73	1.19	4 (6%)	74,113,113	1.09	4 (5%)
16	CLA	a	1118	-	53,63,73	1.28	3 (5%)	62,101,113	0.89	1 (1%)
16	CLA	v	505	-	63,73,73	1.23	3 (4%)	74,113,113	1.21	4 (5%)
18	SF4	N	102	-	0,12,12	-	-	-	-	-
19	BCR	H	4003	-	41,41,41	0.86	0	56,56,56	1.22	4 (7%)
16	CLA	s	501	-	48,58,73	1.36	3 (6%)	56,95,113	1.15	4 (7%)
16	CLA	b	1209	-	43,53,73	1.43	3 (6%)	50,89,113	1.06	2 (4%)
16	CLA	t	515	-	63,73,73	1.19	3 (4%)	74,113,113	1.09	3 (4%)
16	CLA	o	501	-	44,54,73	1.38	3 (6%)	51,90,113	1.04	3 (5%)
19	BCR	B	4005	-	41,41,41	0.85	0	56,56,56	1.17	4 (7%)
19	BCR	u	603	-	41,41,41	0.88	0	56,56,56	1.35	8 (14%)
16	CLA	n	504	-	58,68,73	1.25	3 (5%)	68,107,113	1.05	3 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	BCR	p	602	-	41,41,41	0.87	0	56,56,56	1.31	7 (12%)
16	CLA	H	1109	16	63,73,73	1.18	3 (4%)	74,113,113	1.06	4 (5%)
17	PQN	H	2001	-	34,34,34	0.38	0	43,45,45	1.06	2 (4%)
16	CLA	h	515	-	63,73,73	1.20	3 (4%)	74,113,113	1.13	6 (8%)
16	CLA	H	1117	-	63,73,73	1.12	3 (4%)	74,113,113	1.16	6 (8%)
16	CLA	Z	502	-	48,58,73	1.32	4 (8%)	56,95,113	1.03	3 (5%)
16	CLA	a	1139	25	53,63,73	1.28	3 (5%)	62,101,113	0.96	4 (6%)
16	CLA	A	1116	-	52,62,73	1.22	3 (5%)	60,99,113	1.14	6 (10%)
16	CLA	p	515	-	63,73,73	1.14	3 (4%)	74,113,113	1.02	4 (5%)
19	BCR	s	602	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
16	CLA	G	1238	25	63,73,73	1.14	3 (4%)	74,113,113	0.96	3 (4%)
16	CLA	B	1202	-	63,73,73	1.19	3 (4%)	74,113,113	0.92	2 (2%)
19	BCR	n	604	-	41,41,41	0.86	0	56,56,56	1.33	7 (12%)
17	PQN	B	2002	-	34,34,34	0.36	0	43,45,45	1.04	2 (4%)
16	CLA	w	516	-	44,54,73	1.38	3 (6%)	51,90,113	0.96	3 (5%)
19	BCR	S	4012	-	41,41,41	0.88	0	56,56,56	1.28	7 (12%)
16	CLA	X	501	-	44,54,73	1.38	3 (6%)	51,90,113	1.01	3 (5%)
24	LUT	q	601	-	42,43,43	0.77	0	51,60,60	1.51	9 (17%)
16	CLA	G	1240	13	44,54,73	1.43	3 (6%)	51,90,113	1.25	4 (7%)
16	CLA	u	506	-	58,68,73	1.29	4 (6%)	68,107,113	1.63	9 (13%)
19	BCR	K	4005	-	41,41,41	0.86	0	56,56,56	1.28	6 (10%)
16	CLA	Y	513	-	44,54,73	1.41	3 (6%)	51,90,113	0.96	3 (5%)
16	CLA	o	516	-	44,54,73	1.39	3 (6%)	51,90,113	0.95	1 (1%)
16	CLA	w	517	12	53,63,73	1.29	4 (7%)	62,101,113	0.99	1 (1%)
16	CLA	Z	501	-	48,58,73	1.34	3 (6%)	56,95,113	1.00	4 (7%)
16	CLA	Y	503	-	44,54,73	1.36	3 (6%)	51,90,113	1.09	3 (5%)
16	CLA	Y	511	-	63,73,73	1.15	3 (4%)	74,113,113	1.05	5 (6%)
16	CLA	G	1239	-	63,73,73	1.17	3 (4%)	74,113,113	1.12	5 (6%)
16	CLA	Z	513	-	48,58,73	1.34	3 (6%)	56,95,113	0.99	3 (5%)
16	CLA	H	1121	-	49,59,73	1.35	3 (6%)	56,96,113	1.09	2 (3%)
16	CLA	r	506	-	58,68,73	1.22	3 (5%)	68,107,113	1.03	6 (8%)
16	CLA	y	509	-	63,73,73	1.18	3 (4%)	74,113,113	0.87	3 (4%)
16	CLA	o	507	12	63,73,73	1.22	3 (4%)	74,113,113	0.97	2 (2%)
16	CLA	s	514	-	48,58,73	1.34	3 (6%)	56,95,113	1.23	4 (7%)
16	CLA	a	1127	-	63,73,73	1.18	4 (6%)	74,113,113	1.06	3 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	b	1236	-	48,58,73	1.32	3 (6%)	56,95,113	1.13	4 (7%)
19	BCR	s	601	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	L	1503	25	63,73,73	1.16	3 (4%)	74,113,113	0.90	3 (4%)
19	BCR	a	4002	-	41,41,41	0.85	0	56,56,56	1.18	5 (8%)
16	CLA	S	1302	8	43,53,73	1.45	3 (6%)	50,89,113	1.00	3 (6%)
16	CLA	X	516	-	44,54,73	1.38	3 (6%)	51,90,113	1.00	2 (3%)
16	CLA	r	511	-	63,73,73	1.17	3 (4%)	74,113,113	0.90	2 (2%)
16	CLA	n	510	-	63,73,73	1.20	3 (4%)	74,113,113	1.03	3 (4%)
16	CLA	u	504	-	58,68,73	1.24	3 (5%)	68,107,113	0.95	3 (4%)
16	CLA	v	507	12	63,73,73	1.22	3 (4%)	74,113,113	1.01	4 (5%)
16	CLA	A	1108	-	43,53,73	1.42	3 (6%)	50,89,113	0.97	1 (2%)
16	CLA	B	1228	-	53,63,73	1.29	3 (5%)	62,101,113	1.02	3 (4%)
16	CLA	p	501	-	48,58,73	1.35	3 (6%)	56,95,113	1.12	4 (7%)
19	BCR	J	4015	-	41,41,41	0.87	0	56,56,56	1.26	9 (16%)
16	CLA	b	1214	-	53,63,73	1.25	3 (5%)	62,101,113	1.01	3 (4%)
16	CLA	g	504	-	63,73,73	1.19	3 (4%)	74,113,113	0.96	4 (5%)
16	CLA	v	504	-	58,68,73	1.24	3 (5%)	68,107,113	0.98	4 (5%)
16	CLA	x	502	-	48,58,73	1.34	4 (8%)	56,95,113	0.99	2 (3%)
16	CLA	H	1118	-	53,63,73	1.29	3 (5%)	62,101,113	1.00	5 (8%)
16	CLA	b	1239	-	63,73,73	1.16	3 (4%)	74,113,113	1.02	6 (8%)
16	CLA	x	508	12	53,63,73	1.31	3 (5%)	62,101,113	0.91	2 (3%)
16	CLA	H	1105	-	56,66,73	1.23	3 (5%)	65,104,113	1.03	4 (6%)
16	CLA	B	1232	-	43,53,73	1.41	3 (6%)	50,89,113	1.27	4 (8%)
16	CLA	Y	507	12	63,73,73	1.20	3 (4%)	74,113,113	0.93	3 (4%)
16	CLA	h	513	-	44,54,73	1.43	3 (6%)	51,90,113	0.92	2 (3%)
19	BCR	F	4016	-	41,41,41	0.86	0	56,56,56	1.31	8 (14%)
16	CLA	B	1021	-	63,73,73	1.16	3 (4%)	74,113,113	1.08	4 (5%)
16	CLA	r	502	-	48,58,73	1.32	3 (6%)	56,95,113	0.96	1 (1%)
16	CLA	u	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.04	4 (5%)
16	CLA	a	1119	-	63,73,73	1.13	3 (4%)	74,113,113	0.95	4 (5%)
16	CLA	H	1114	-	44,54,73	1.40	3 (6%)	51,90,113	1.21	5 (9%)
16	CLA	x	505	-	63,73,73	1.17	3 (4%)	74,113,113	1.22	5 (6%)
16	CLA	y	516	-	44,54,73	1.44	3 (6%)	51,90,113	1.10	4 (7%)
19	BCR	g	602	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)



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
16	CLA	n	501	-	1/1/12/20	8/19/97/115	-
19	BCR	a	4008	-	-	10/29/63/63	0/2/2/2
13	LHG	o	605	-	-	12/31/31/53	-
19	BCR	B	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	H	1113	-	1/1/11/20	0/13/91/115	-
16	CLA	u	511	-	1/1/15/20	7/37/115/115	-
16	CLA	G	1203	-	1/1/15/20	14/37/115/115	-
19	BCR	G	4010	-	-	17/29/63/63	0/2/2/2
21	ECH	R	4020	-	-	11/29/66/66	0/2/2/2
16	CLA	s	502	-	1/1/12/20	5/19/97/115	-
19	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
16	CLA	q	507	-	1/1/15/20	11/37/115/115	-
20	LMT	H	4202	-	-	8/21/61/61	0/2/2/2
16	CLA	G	1213	-	1/1/13/20	7/25/103/115	-
16	CLA	X	509	-	1/1/14/20	12/31/109/115	-
16	CLA	W	514	-	1/1/12/20	7/19/97/115	-
16	CLA	p	516	-	1/1/11/20	7/15/93/115	-
16	CLA	a	1137	-	1/1/11/20	4/16/94/115	-
19	BCR	s	603	-	-	7/29/63/63	0/2/2/2
19	BCR	Z	604	-	-	19/29/63/63	0/2/2/2
16	CLA	q	504	-	1/1/15/20	13/37/115/115	-
13	LHG	Y	605	-	-	16/36/36/53	-
16	CLA	p	504	-	-	15/37/115/115	-
21	ECH	V	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	b	1215	-	-	5/31/109/115	-
16	CLA	a	1114	-	1/1/11/20	8/15/93/115	-
16	CLA	b	1202	-	1/1/15/20	16/37/115/115	-
16	CLA	o	508	12	1/1/13/20	12/25/103/115	-
16	CLA	v	503	-	1/1/11/20	6/15/93/115	-
16	CLA	b	1021	-	1/1/15/20	16/37/115/115	-
16	CLA	g	505	-	1/1/15/20	9/37/115/115	-
16	CLA	h	505	-	-	5/37/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	1110	-	1/1/12/20	8/24/102/115	-
16	CLA	a	1124	25	1/1/14/20	7/31/109/115	-
16	CLA	a	1106	1	1/1/15/20	16/37/115/115	-
16	CLA	b	1216	25	1/1/11/20	0/16/94/115	-
16	CLA	k	4004	-	1/1/13/20	6/25/103/115	-
16	CLA	H	1013	-	1/1/15/20	13/37/115/115	-
13	LHG	A	849	-	-	19/47/47/53	-
16	CLA	o	504	-	-	9/31/109/115	-
21	ECH	b	4006	-	-	9/29/66/66	0/2/2/2
16	CLA	H	1138	-	1/1/15/20	9/37/115/115	-
16	CLA	a	1123	-	-	13/37/115/115	-
16	CLA	y	508	-	1/1/13/20	9/25/103/115	-
16	CLA	b	1213	-	1/1/13/20	5/25/103/115	-
16	CLA	n	513	-	-	8/15/93/115	-
16	CLA	W	509	-	1/1/14/20	4/31/109/115	-
16	CLA	n	514	-	1/1/12/20	6/19/97/115	-
16	CLA	U	1502	-	-	8/31/109/115	-
16	CLA	Y	505	-	1/1/15/20	13/37/115/115	-
16	CLA	b	1221	25	1/1/15/20	19/37/115/115	-
16	CLA	w	514	-	1/1/12/20	7/19/97/115	-
16	CLA	r	504	-	1/1/15/20	16/37/115/115	-
19	BCR	G	4017	-	-	13/29/63/63	0/2/2/2
13	LHG	I	103	-	-	20/44/44/53	-
16	CLA	h	516	-	1/1/11/20	6/15/93/115	-
16	CLA	a	1112	-	-	5/13/91/115	-
16	CLA	Y	504	-	1/1/15/20	15/37/115/115	-
16	CLA	B	1218	-	-	7/25/103/115	-
19	BCR	t	601	-	-	14/29/63/63	0/2/2/2
23	LMU	q	605	-	-	5/21/61/61	0/2/2/2
16	CLA	A	1104	-	1/1/15/20	18/37/115/115	-
14	LMG	B	848	-	-	18/38/58/70	0/1/1/1
16	CLA	A	1113	-	1/1/11/20	6/13/91/115	-
16	CLA	x	504	-	1/1/15/20	20/37/115/115	-
19	BCR	X	603	-	-	12/29/63/63	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	U	4022	-	-	16/29/63/63	0/2/2/2
16	CLA	G	1235	-	1/1/14/20	9/34/112/115	-
16	CLA	W	505	-	1/1/15/20	18/37/115/115	-
13	LHG	a	849	-	-	17/47/47/53	-
16	CLA	Z	512	12	1/1/15/20	13/37/115/115	-
16	CLA	G	1226	-	-	17/31/109/115	-
19	BCR	y	601	-	-	15/29/63/63	0/2/2/2
16	CLA	L	1502	-	-	8/31/109/115	-
16	CLA	H	1126	-	1/1/15/20	11/37/115/115	-
16	CLA	y	514	-	-	6/19/97/115	-
19	BCR	G	4005	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1210	-	-	15/37/115/115	-
15	CL0	H	1011	-	2/2/20/25	6/37/135/135	-
16	CLA	o	502	-	1/1/12/20	7/19/97/115	-
16	CLA	w	510	-	-	9/31/109/115	-
16	CLA	g	501	-	-	6/19/97/115	-
16	CLA	h	501	-	-	7/15/93/115	-
16	CLA	U	1503	-	1/1/15/20	9/37/115/115	-
16	CLA	W	510	-	-	14/37/115/115	-
16	CLA	G	1217	-	-	7/13/91/115	-
19	BCR	H	4011	-	-	16/29/63/63	0/2/2/2
19	BCR	n	603	-	-	12/29/63/63	0/2/2/2
19	BCR	w	603	-	-	13/29/63/63	0/2/2/2
16	CLA	G	1023	-	-	8/37/115/115	-
18	SF4	A	3001	-	-	-	0/6/5/5
16	CLA	s	511	-	1/1/15/20	13/37/115/115	-
16	CLA	b	1201	-	1/1/12/20	4/24/102/115	-
16	CLA	B	1209	-	1/1/11/20	5/13/91/115	-
16	CLA	G	1215	-	1/1/14/20	6/31/109/115	-
16	CLA	w	511	-	1/1/15/20	8/37/115/115	-
19	BCR	j	4012	-	-	10/29/63/63	0/2/2/2
16	CLA	A	1129	-	-	5/15/93/115	-
16	CLA	k	4002	-	1/1/11/20	5/13/91/115	-
16	CLA	q	512	12	1/1/15/20	14/37/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1216	25	1/1/11/20	3/16/94/115	-
19	BCR	w	602	-	-	11/29/63/63	0/2/2/2
16	CLA	u	515	-	-	16/37/115/115	-
17	PQN	A	2001	-	-	3/23/43/43	0/2/2/2
16	CLA	Y	512	12	1/1/15/20	8/37/115/115	-
16	CLA	x	515	-	1/1/15/20	9/37/115/115	-
16	CLA	X	503	-	-	10/15/93/115	-
16	CLA	G	1230	-	1/1/11/20	6/13/91/115	-
21	ECH	I	4020	-	-	11/29/66/66	0/2/2/2
16	CLA	W	502	-	1/1/12/20	9/19/97/115	-
16	CLA	a	1022	-	1/1/15/20	8/37/115/115	-
16	CLA	u	502	-	1/1/12/20	6/19/97/115	-
16	CLA	Y	506	-	-	12/31/109/115	-
13	LHG	u	605	-	-	12/31/31/53	-
16	CLA	s	505	-	1/1/15/20	11/37/115/115	-
16	CLA	b	1219	-	-	5/13/91/115	-
16	CLA	B	1229	-	1/1/13/20	8/29/107/115	-
13	LHG	x	605	-	-	20/35/35/53	-
16	CLA	A	1128	-	1/1/15/20	19/37/115/115	-
19	BCR	Y	602	-	-	10/29/63/63	0/2/2/2
16	CLA	Z	514	-	1/1/12/20	8/19/97/115	-
14	LMG	a	4101	-	-	21/41/61/70	0/1/1/1
20	LMT	A	4202	-	-	7/21/61/61	0/2/2/2
19	BCR	k	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	F	1302	6	1/1/11/20	7/15/93/115	-
16	CLA	b	1225	-	-	12/37/115/115	-
16	CLA	H	1115	-	-	9/24/102/115	-
16	CLA	B	1219	-	-	4/13/91/115	-
19	BCR	i	4018	-	-	13/29/63/63	0/2/2/2
16	CLA	s	509	-	1/1/14/20	14/31/109/115	-
16	CLA	b	1208	-	1/1/11/20	6/13/91/115	-
19	BCR	p	601	-	-	9/29/63/63	0/2/2/2
16	CLA	b	1222	25	-	7/19/97/115	-
16	CLA	a	1102	16	1/1/13/20	6/27/105/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	b	1238	25	1/1/15/20	16/37/115/115	-
16	CLA	W	512	12	1/1/14/20	16/31/109/115	-
16	CLA	X	507	12	-	8/37/115/115	-
16	CLA	b	1212	-	1/1/11/20	3/13/91/115	-
16	CLA	G	1209	-	1/1/11/20	3/13/91/115	-
19	BCR	l	4022	-	-	18/29/63/63	0/2/2/2
16	CLA	W	508	12	1/1/13/20	7/25/103/115	-
19	BCR	o	604	-	-	18/29/63/63	0/2/2/2
16	CLA	B	1203	-	1/1/15/20	14/37/115/115	-
16	CLA	o	514	-	1/1/12/20	7/19/97/115	-
13	LHG	R	103	-	-	23/44/44/53	-
16	CLA	B	1235	-	1/1/14/20	10/34/112/115	-
16	CLA	p	514	-	1/1/12/20	7/19/97/115	-
19	BCR	T	4005	-	-	9/29/63/63	0/2/2/2
16	CLA	G	1221	25	1/1/15/20	18/37/115/115	-
13	LHG	b	4018	16	-	16/42/42/53	-
19	BCR	j	4013	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1107	1	-	6/19/97/115	-
19	BCR	h	601	-	-	14/29/63/63	0/2/2/2
16	CLA	A	1115	-	1/1/12/20	8/24/102/115	-
16	CLA	H	1139	25	1/1/14/20	11/31/109/115	-
16	CLA	Z	510	-	-	10/31/109/115	-
17	PQN	a	2001	-	-	5/23/43/43	0/2/2/2
16	CLA	G	1201	-	1/1/12/20	4/24/102/115	-
16	CLA	G	1218	-	-	12/25/103/115	-
16	CLA	H	1123	-	-	10/37/115/115	-
16	CLA	n	511	-	-	6/37/115/115	-
16	CLA	A	1111	-	1/1/13/20	6/25/103/115	-
16	CLA	a	1013	-	1/1/15/20	12/37/115/115	-
14	LMG	G	848	-	-	18/38/58/70	0/1/1/1
16	CLA	a	1138	-	1/1/15/20	13/37/115/115	-
14	LMG	H	4201	-	-	10/27/47/70	0/1/1/1
16	CLA	u	509	-	1/1/14/20	6/31/109/115	-
16	CLA	X	512	12	-	10/37/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	1221	25	-	13/37/115/115	-
16	CLA	Y	517	12	-	9/25/103/115	-
16	CLA	W	517	12	1/1/13/20	9/25/103/115	-
19	BCR	u	602	-	-	13/29/63/63	0/2/2/2
16	CLA	x	513	-	-	8/15/93/115	-
16	CLA	A	1103	-	1/1/15/20	9/37/115/115	-
16	CLA	p	502	-	1/1/12/20	3/19/97/115	-
13	LHG	X	605	-	-	12/31/31/53	-
16	CLA	A	1106	1	1/1/15/20	14/37/115/115	-
16	CLA	b	1203	-	1/1/15/20	14/37/115/115	-
16	CLA	v	506	-	1/1/14/20	5/31/109/115	-
16	CLA	x	514	-	1/1/12/20	6/19/97/115	-
16	CLA	A	1133	-	1/1/12/20	9/24/102/115	-
16	CLA	a	1125	-	-	9/37/115/115	-
16	CLA	a	1131	-	-	12/37/115/115	-
16	CLA	Y	509	-	1/1/14/20	15/31/109/115	-
16	CLA	o	505	-	1/1/15/20	14/37/115/115	-
16	CLA	Z	515	-	1/1/15/20	10/37/115/115	-
16	CLA	r	516	-	1/1/11/20	3/15/93/115	-
16	CLA	G	1227	-	-	8/18/96/115	-
16	CLA	p	505	-	-	12/37/115/115	-
16	CLA	A	1132	-	1/1/15/20	15/37/115/115	-
16	CLA	G	1207	-	-	12/37/115/115	-
19	BCR	R	4018	-	-	13/29/63/63	0/2/2/2
16	CLA	G	1231	25	1/1/11/20	3/13/91/115	-
16	CLA	A	1801	13	1/1/11/20	8/15/93/115	-
16	CLA	A	1136	-	1/1/15/20	5/37/115/115	-
16	CLA	A	1123	25	-	8/37/115/115	-
16	CLA	A	1105	-	1/1/13/20	9/29/107/115	-
16	CLA	v	511	-	1/1/15/20	9/37/115/115	-
16	CLA	a	1122	-	-	8/30/108/115	-
16	CLA	p	510	-	-	10/37/115/115	-
16	CLA	g	513	-	-	9/15/93/115	-
23	LMU	r	606	-	-	6/21/61/61	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	t	502	-	1/1/12/20	9/19/97/115	-
16	CLA	t	504	-	1/1/14/20	5/31/109/115	-
19	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
19	BCR	p	604	-	-	15/29/63/63	0/2/2/2
16	CLA	T	4003	9	1/1/11/20	9/13/91/115	-
19	BCR	H	4002	-	-	11/29/63/63	0/2/2/2
19	BCR	p	603	-	-	7/29/63/63	0/2/2/2
19	BCR	b	4009	-	-	7/24/41/63	0/1/1/2
19	BCR	h	603	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1220	-	-	11/24/102/115	-
16	CLA	w	505	-	-	8/37/115/115	-
16	CLA	k	4003	9	1/1/11/20	5/13/91/115	-
16	CLA	a	1126	-	1/1/15/20	11/37/115/115	-
16	CLA	o	510	-	-	5/31/109/115	-
19	BCR	b	4005	-	-	12/29/63/63	0/2/2/2
23	LMU	s	606	-	-	6/21/61/61	0/2/2/2
19	BCR	G	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	t	514	-	1/1/12/20	7/19/97/115	-
15	CL0	a	1011	-	2/2/20/25	7/37/135/135	-
16	CLA	o	515	-	1/1/15/20	15/37/115/115	-
16	CLA	h	510	-	-	7/37/115/115	-
16	CLA	b	1227	-	1/1/11/20	5/18/96/115	-
19	BCR	t	604	-	-	14/29/63/63	0/2/2/2
16	CLA	H	1101	-	1/1/15/20	16/37/115/115	-
16	CLA	n	509	-	1/1/14/20	8/31/109/115	-
16	CLA	g	510	-	-	10/37/115/115	-
16	CLA	v	510	-	-	6/37/115/115	-
19	BCR	Z	603	-	-	8/29/63/63	0/2/2/2
16	CLA	G	1222	25	-	6/19/97/115	-
16	CLA	A	1117	-	1/1/15/20	6/37/115/115	-
16	CLA	T	4002	-	1/1/11/20	5/13/91/115	-
16	CLA	q	502	-	1/1/12/20	6/19/97/115	-
18	SF4	C	102	-	-	-	0/6/5/5
16	CLA	Y	501	-	1/1/12/20	6/19/97/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	F	1301	25	1/1/11/20	2/13/91/115	-
16	CLA	G	1208	-	1/1/11/20	6/13/91/115	-
16	CLA	g	516	-	1/1/11/20	4/15/93/115	-
16	CLA	v	516	-	1/1/11/20	4/15/93/115	-
21	ECH	i	4020	-	-	12/29/66/66	0/2/2/2
16	CLA	Z	503	-	1/1/11/20	8/15/93/115	-
16	CLA	B	1210	-	-	13/37/115/115	-
20	LMT	L	4101	-	-	9/21/61/61	0/2/2/2
16	CLA	y	505	-	1/1/15/20	8/37/115/115	-
16	CLA	a	1134	1	-	4/13/91/115	-
23	LMU	Z	605	-	-	5/21/61/61	0/2/2/2
23	LMU	w	605	-	-	5/21/61/61	0/2/2/2
16	CLA	T	4004	-	-	3/25/103/115	-
14	LMG	F	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	H	1119	25	1/1/15/20	11/37/115/115	-
19	BCR	x	604	-	-	12/29/63/63	0/2/2/2
16	CLA	B	1217	-	-	5/13/91/115	-
16	CLA	Z	506	-	-	7/31/109/115	-
16	CLA	H	1130	-	-	9/31/109/115	-
16	CLA	h	502	-	1/1/12/20	5/19/97/115	-
16	CLA	B	1204	-	1/1/15/20	7/37/115/115	-
16	CLA	B	1023	-	-	8/37/115/115	-
13	LHG	A	851	16	-	7/30/30/53	-
16	CLA	t	510	-	-	9/37/115/115	-
16	CLA	q	510	-	-	8/31/109/115	-
16	CLA	g	502	-	1/1/12/20	4/19/97/115	-
19	BCR	B	4014	-	-	16/29/63/63	0/2/2/2
13	LHG	r	605	-	-	17/35/35/53	-
16	CLA	G	1206	2	1/1/15/20	11/37/115/115	-
16	CLA	Z	511	-	1/1/15/20	3/37/115/115	-
16	CLA	p	506	-	-	13/31/109/115	-
16	CLA	g	507	-	1/1/15/20	7/37/115/115	-
19	BCR	v	601	-	-	11/29/63/63	0/2/2/2
16	CLA	t	513	-	-	6/15/93/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	y	604	-	-	11/29/63/63	0/2/2/2
16	CLA	B	1227	-	1/1/11/20	10/18/96/115	-
16	CLA	h	503	-	1/1/11/20	5/15/93/115	-
16	CLA	n	505	-	1/1/15/20	20/37/115/115	-
16	CLA	n	507	-	1/1/15/20	9/37/115/115	-
16	CLA	w	513	-	-	7/19/97/115	-
16	CLA	w	501	-	1/1/12/20	10/19/97/115	-
16	CLA	Z	507	-	1/1/15/20	14/37/115/115	-
16	CLA	B	1207	-	-	16/37/115/115	-
16	CLA	g	506	-	-	9/31/109/115	-
16	CLA	p	511	-	1/1/15/20	14/37/115/115	-
16	CLA	A	1119	25	1/1/15/20	5/37/115/115	-
16	CLA	t	506	-	1/1/14/20	11/31/109/115	-
16	CLA	H	1132	-	1/1/15/20	15/37/115/115	-
16	CLA	q	506	-	1/1/14/20	10/31/109/115	-
13	LHG	i	103	-	-	22/44/44/53	-
16	CLA	Z	504	-	1/1/15/20	12/37/115/115	-
16	CLA	L	1501	10	-	12/31/109/115	-
16	CLA	o	513	-	-	4/15/93/115	-
16	CLA	B	1213	-	1/1/13/20	7/25/103/115	-
16	CLA	B	1223	-	1/1/15/20	9/37/115/115	-
16	CLA	A	1118	-	-	9/25/103/115	-
16	CLA	g	511	-	1/1/15/20	8/37/115/115	-
16	CLA	u	517	12	-	6/25/103/115	-
19	BCR	Y	604	-	-	14/29/63/63	0/2/2/2
21	ECH	m	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	r	515	-	1/1/15/20	11/37/115/115	-
16	CLA	U	1501	10	-	12/31/109/115	-
16	CLA	n	506	-	-	7/31/109/115	-
16	CLA	h	511	-	1/1/15/20	13/37/115/115	-
16	CLA	r	509	-	-	9/37/115/115	-
19	BCR	A	4003	-	-	9/29/63/63	0/2/2/2
16	CLA	t	516	-	1/1/11/20	7/15/93/115	-
16	CLA	y	501	-	1/1/11/20	6/15/93/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMT	U	4101	-	-	8/21/61/61	0/2/2/2
17	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
16	CLA	A	1122	-	1/1/13/20	7/30/108/115	-
16	CLA	A	1120	-	-	6/18/96/115	-
16	CLA	A	1127	-	1/1/15/20	4/37/115/115	-
16	CLA	x	510	-	-	11/37/115/115	-
16	CLA	g	508	12	1/1/13/20	5/25/103/115	-
16	CLA	v	508	-	1/1/13/20	11/25/103/115	-
16	CLA	A	1102	16	1/1/13/20	6/27/105/115	-
13	LHG	H	849	-	-	17/47/47/53	-
16	CLA	u	516	-	1/1/11/20	7/15/93/115	-
16	CLA	t	507	-	1/1/15/20	9/37/115/115	-
16	CLA	K	4004	-	1/1/13/20	4/25/103/115	-
16	CLA	H	1112	-	-	2/13/91/115	-
16	CLA	h	504	-	-	14/31/109/115	-
14	LMG	a	4201	-	-	11/27/47/70	0/1/1/1
19	BCR	U	4019	-	-	10/29/63/63	0/2/2/2
19	BCR	o	601	-	-	8/29/63/63	0/2/2/2
16	CLA	q	515	-	1/1/15/20	10/37/115/115	-
16	CLA	A	1124	25	1/1/14/20	6/31/109/115	-
16	CLA	A	1237	25	1/1/15/20	10/37/115/115	-
16	CLA	n	503	-	1/1/11/20	7/15/93/115	-
16	CLA	w	515	-	1/1/15/20	12/37/115/115	-
19	BCR	G	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	Y	508	12	1/1/13/20	11/25/103/115	-
16	CLA	t	503	-	1/1/11/20	5/15/93/115	-
19	BCR	q	602	-	-	12/29/63/63	0/2/2/2
16	CLA	w	503	-	1/1/11/20	8/15/93/115	-
16	CLA	x	507	-	1/1/15/20	8/37/115/115	-
16	CLA	A	1130	-	1/1/14/20	9/31/109/115	-
19	BCR	h	604	-	-	13/29/63/63	0/2/2/2
16	CLA	q	517	12	-	9/25/103/115	-
19	BCR	n	601	-	-	12/29/63/63	0/2/2/2
16	CLA	g	509	-	1/1/15/20	8/37/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1012	25	1/1/13/20	7/25/103/115	-
16	CLA	b	1228	-	1/1/13/20	11/25/103/115	-
16	CLA	w	509	-	1/1/15/20	11/37/115/115	-
16	CLA	B	1212	-	1/1/11/20	5/13/91/115	-
21	ECH	M	4021	-	-	15/29/66/66	0/2/2/2
13	LHG	H	851	16	-	7/30/30/53	-
19	BCR	r	604	-	-	15/29/63/63	0/2/2/2
16	CLA	u	501	-	-	5/15/93/115	-
19	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
16	CLA	y	513	-	1/1/11/20	5/15/93/115	-
19	BCR	x	601	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1112	-	-	4/13/91/115	-
19	BCR	I	4018	-	-	11/29/63/63	0/2/2/2
16	CLA	r	517	12	-	10/25/103/115	-
16	CLA	a	1109	16	1/1/15/20	7/37/115/115	-
16	CLA	l	1501	10	-	14/31/109/115	-
16	CLA	H	1106	1	1/1/15/20	15/37/115/115	-
16	CLA	A	1114	-	1/1/11/20	7/15/93/115	-
16	CLA	H	1104	-	1/1/15/20	15/37/115/115	-
16	CLA	X	515	-	1/1/15/20	15/37/115/115	-
16	CLA	y	503	-	1/1/11/20	4/15/93/115	-
16	CLA	u	512	12	-	11/37/115/115	-
16	CLA	x	506	-	-	12/31/109/115	-
16	CLA	u	508	12	1/1/13/20	10/25/103/115	-
13	LHG	g	605	-	-	16/35/35/53	-
21	ECH	B	4006	-	-	10/29/66/66	0/2/2/2
16	CLA	W	501	-	1/1/12/20	8/19/97/115	-
16	CLA	r	507	-	1/1/15/20	11/37/115/115	-
19	BCR	k	4005	-	-	7/29/63/63	0/2/2/2
19	BCR	T	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	a	1116	-	1/1/12/20	8/24/102/115	-
16	CLA	B	1226	-	-	14/31/109/115	-
16	CLA	x	511	-	-	6/37/115/115	-
16	CLA	H	1108	-	-	4/13/91/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	a	1135	-	1/1/12/20	2/21/99/115	-
16	CLA	r	508	12	1/1/13/20	7/25/103/115	-
16	CLA	s	507	12	-	9/37/115/115	-
19	BCR	G	4014	-	-	16/29/63/63	0/2/2/2
14	LMG	H	4101	-	-	23/41/61/70	0/1/1/1
16	CLA	A	1126	-	1/1/15/20	11/37/115/115	-
14	LMG	b	848	-	-	19/38/58/70	0/1/1/1
16	CLA	H	1107	1	-	4/19/97/115	-
15	CL0	A	1011	-	2/2/20/25	8/37/135/135	-
16	CLA	B	1224	-	1/1/14/20	10/31/109/115	-
16	CLA	B	1231	25	1/1/11/20	7/13/91/115	-
16	CLA	p	513	-	-	6/15/93/115	-
16	CLA	G	1219	-	-	6/13/91/115	-
16	CLA	W	516	-	-	5/15/93/115	-
16	CLA	b	1226	-	1/1/14/20	16/31/109/115	-
19	BCR	u	601	-	-	8/29/63/63	0/2/2/2
19	BCR	t	603	-	-	11/29/63/63	0/2/2/2
19	BCR	S	4015	-	-	10/29/63/63	0/2/2/2
16	CLA	B	1208	-	1/1/11/20	4/13/91/115	-
16	CLA	t	517	12	1/1/13/20	6/25/103/115	-
16	CLA	u	514	-	1/1/12/20	4/19/97/115	-
19	BCR	r	603	-	-	11/29/63/63	0/2/2/2
16	CLA	t	501	-	1/1/12/20	7/19/97/115	-
16	CLA	A	1135	-	1/1/12/20	2/21/99/115	-
14	LMG	f	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	q	508	12	1/1/13/20	8/25/103/115	-
19	BCR	B	4017	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1202	-	1/1/15/20	16/37/115/115	-
16	CLA	A	1121	-	1/1/12/20	6/21/99/115	-
16	CLA	W	513	-	-	8/15/93/115	-
19	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
16	CLA	o	506	-	1/1/14/20	15/31/109/115	-
19	BCR	B	4010	-	-	16/29/63/63	0/2/2/2
16	CLA	H	1124	-	1/1/14/20	5/31/109/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1237	25	1/1/15/20	10/37/115/115	-
16	CLA	w	506	-	-	5/31/109/115	-
16	CLA	Q	1301	25	1/1/11/20	0/13/91/115	-
19	BCR	J	4012	-	-	12/29/63/63	0/2/2/2
16	CLA	W	503	-	1/1/11/20	8/15/93/115	-
19	BCR	X	602	-	-	17/29/63/63	0/2/2/2
19	BCR	b	4014	-	-	15/29/63/63	0/2/2/2
16	CLA	a	1115	-	1/1/12/20	8/24/102/115	-
19	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
16	CLA	H	1140	-	1/1/15/20	13/37/115/115	-
16	CLA	x	509	-	1/1/15/20	12/37/115/115	-
16	CLA	o	511	-	1/1/15/20	9/37/115/115	-
16	CLA	s	513	-	-	7/15/93/115	-
16	CLA	W	507	-	-	10/37/115/115	-
14	LMG	a	852	-	-	10/33/53/70	0/1/1/1
24	LUT	w	601	-	-	7/29/67/67	0/2/2/2
16	CLA	v	512	12	-	11/37/115/115	-
16	CLA	W	515	-	1/1/15/20	15/37/115/115	-
16	CLA	a	1103	-	1/1/15/20	12/37/115/115	-
16	CLA	r	512	12	1/1/15/20	9/37/115/115	-
16	CLA	X	508	12	1/1/13/20	13/25/103/115	-
19	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
16	CLA	l	1502	-	-	8/31/109/115	-
16	CLA	q	514	-	1/1/12/20	9/19/97/115	-
16	CLA	p	503	-	1/1/11/20	5/15/93/115	-
20	LMT	a	4202	-	-	8/21/61/61	0/2/2/2
16	CLA	X	504	-	-	15/31/109/115	-
16	CLA	s	512	12	1/1/15/20	7/37/115/115	-
16	CLA	B	1234	-	1/1/12/20	5/19/97/115	-
23	LMU	p	606	-	-	9/21/61/61	0/2/2/2
16	CLA	H	1131	-	1/1/15/20	9/37/115/115	-
19	BCR	Y	601	-	-	12/29/63/63	0/2/2/2
16	CLA	r	514	-	1/1/12/20	9/19/97/115	-
16	CLA	s	516	-	-	9/15/93/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	1012	25	1/1/13/20	11/25/103/115	-
16	CLA	G	1234	-	1/1/12/20	3/19/97/115	-
16	CLA	b	1210	-	1/1/15/20	12/37/115/115	-
16	CLA	b	1229	-	1/1/13/20	8/29/107/115	-
16	CLA	Y	510	-	-	10/37/115/115	-
16	CLA	p	509	-	1/1/14/20	19/31/109/115	-
16	CLA	A	1107	1	-	4/19/97/115	-
16	CLA	a	1101	-	1/1/15/20	18/37/115/115	-
16	CLA	t	511	-	1/1/15/20	8/37/115/115	-
16	CLA	o	517	12	-	9/25/103/115	-
19	BCR	g	604	-	-	16/29/63/63	0/2/2/2
16	CLA	A	1013	-	1/1/15/20	13/37/115/115	-
16	CLA	v	509	-	-	14/37/115/115	-
16	CLA	b	1217	-	-	1/13/91/115	-
16	CLA	r	505	-	-	11/37/115/115	-
19	BCR	y	603	-	-	11/29/63/63	0/2/2/2
16	CLA	o	509	-	1/1/14/20	9/31/109/115	-
23	LMU	g	606	-	-	5/21/61/61	0/2/2/2
16	CLA	B	1236	-	1/1/12/20	9/19/97/115	-
16	CLA	Y	515	-	1/1/15/20	8/37/115/115	-
16	CLA	H	1022	25	1/1/15/20	10/37/115/115	-
16	CLA	B	1201	-	1/1/12/20	4/24/102/115	-
16	CLA	A	1131	-	-	12/37/115/115	-
16	CLA	H	1133	-	-	8/24/102/115	-
19	BCR	q	603	-	-	6/29/63/63	0/2/2/2
23	LMU	Y	606	-	-	6/21/61/61	0/2/2/2
16	CLA	H	1135	-	-	3/21/99/115	-
16	CLA	J	1303	-	-	0/2/76/115	-
16	CLA	Z	516	-	1/1/11/20	9/15/93/115	-
16	CLA	A	1101	-	1/1/15/20	14/37/115/115	-
23	LMU	x	606	-	-	14/21/61/61	0/2/2/2
16	CLA	w	507	-	1/1/15/20	9/37/115/115	-
16	CLA	b	1207	-	-	12/37/115/115	-
16	CLA	Z	509	-	1/1/15/20	15/37/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	s	506	-	-	9/31/109/115	-
16	CLA	y	506	-	1/1/14/20	9/31/109/115	-
16	CLA	B	1239	-	-	13/37/115/115	-
16	CLA	a	1104	-	1/1/15/20	16/37/115/115	-
16	CLA	a	1113	-	1/1/11/20	2/13/91/115	-
16	CLA	K	4003	9	1/1/11/20	8/13/91/115	-
14	LMG	H	852	-	-	6/33/53/70	0/1/1/1
16	CLA	G	1225	-	1/1/15/20	10/37/115/115	-
16	CLA	H	1127	-	1/1/15/20	6/37/115/115	-
13	LHG	a	851	16	-	9/30/30/53	-
16	CLA	a	1132	-	1/1/15/20	14/37/115/115	-
19	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1224	-	1/1/14/20	12/31/109/115	-
16	CLA	B	1214	-	1/1/13/20	8/25/103/115	-
16	CLA	a	1801	13	1/1/11/20	6/15/93/115	-
16	CLA	H	1111	-	1/1/13/20	8/25/103/115	-
16	CLA	a	1136	-	1/1/15/20	9/37/115/115	-
16	CLA	y	511	-	1/1/15/20	11/37/115/115	-
16	CLA	a	1108	-	-	6/13/91/115	-
16	CLA	p	517	12	-	8/25/103/115	-
24	LUT	Z	601	-	-	7/29/67/67	0/2/2/2
19	BCR	u	604	-	-	17/29/63/63	0/2/2/2
16	CLA	t	509	-	1/1/14/20	5/31/109/115	-
16	CLA	w	512	12	1/1/15/20	11/37/115/115	-
13	LHG	s	605	-	-	12/36/36/53	-
16	CLA	A	1109	16	1/1/15/20	7/37/115/115	-
16	CLA	x	503	-	-	7/15/93/115	-
16	CLA	y	507	-	-	11/37/115/115	-
16	CLA	u	513	-	-	6/15/93/115	-
16	CLA	v	517	-	1/1/13/20	14/25/103/115	-
16	CLA	X	505	-	1/1/15/20	10/37/115/115	-
16	CLA	h	506	-	1/1/14/20	9/31/109/115	-
16	CLA	s	508	12	1/1/13/20	8/25/103/115	-
16	CLA	y	504	-	-	12/31/109/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	b	1231	25	1/1/11/20	6/13/91/115	-
16	CLA	A	1134	1	-	4/13/91/115	-
19	BCR	Z	602	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1224	-	1/1/14/20	8/31/109/115	-
16	CLA	b	1234	-	1/1/12/20	3/19/97/115	-
18	SF4	H	3001	-	-	-	0/6/5/5
16	CLA	B	1220	-	1/1/12/20	11/23/101/115	-
16	CLA	f	1301	25	1/1/11/20	2/13/91/115	-
16	CLA	Y	516	-	-	9/15/93/115	-
16	CLA	H	1129	-	-	4/15/93/115	-
16	CLA	b	1235	-	1/1/14/20	12/34/112/115	-
19	BCR	r	602	-	-	16/29/63/63	0/2/2/2
19	BCR	W	601	-	-	16/29/63/63	0/2/2/2
16	CLA	Z	508	12	1/1/13/20	7/25/103/115	-
16	CLA	h	507	-	1/1/15/20	13/37/115/115	-
16	CLA	b	1230	-	-	5/13/91/115	-
16	CLA	a	1140	-	-	11/37/115/115	-
16	CLA	K	4002	-	1/1/11/20	2/13/91/115	-
16	CLA	y	512	12	-	12/37/115/115	-
16	CLA	S	1303	-	-	0/2/76/115	-
16	CLA	s	517	12	-	8/25/103/115	-
16	CLA	b	1232	25	1/1/11/20	6/13/91/115	-
16	CLA	v	513	-	1/1/11/20	2/15/93/115	-
16	CLA	q	511	-	-	4/37/115/115	-
16	CLA	o	503	-	-	3/15/93/115	-
16	CLA	v	501	-	-	6/15/93/115	-
16	CLA	H	1128	-	1/1/15/20	16/37/115/115	-
16	CLA	r	513	-	-	11/15/93/115	-
16	CLA	t	512	12	1/1/15/20	9/37/115/115	-
14	LMG	Q	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	G	1223	-	1/1/15/20	4/37/115/115	-
16	CLA	j	1302	8	-	6/13/91/115	-
16	CLA	y	510	-	-	6/37/115/115	-
19	BCR	H	4007	-	-	8/29/63/63	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	r	503	-	-	8/15/93/115	-
16	CLA	B	1211	-	1/1/15/20	15/37/115/115	-
19	BCR	x	602	-	-	17/29/63/63	0/2/2/2
16	CLA	X	506	-	1/1/14/20	12/31/109/115	-
16	CLA	X	514	-	1/1/12/20	2/19/97/115	-
16	CLA	j	1303	-	-	0/2/76/115	-
16	CLA	n	512	12	1/1/15/20	18/37/115/115	-
16	CLA	t	508	12	1/1/13/20	7/25/103/115	-
19	BCR	J	4013	-	-	9/29/63/63	0/2/2/2
19	BCR	K	4001	-	-	11/29/63/63	0/2/2/2
19	BCR	W	603	-	-	13/29/63/63	0/2/2/2
14	LMG	A	4101	-	-	24/41/61/70	0/1/1/1
16	CLA	n	516	-	-	6/15/93/115	-
16	CLA	G	1205	-	1/1/15/20	8/37/115/115	-
16	CLA	H	1122	-	-	7/30/108/115	-
16	CLA	g	503	-	-	8/15/93/115	-
16	CLA	X	511	-	1/1/15/20	10/37/115/115	-
16	CLA	q	505	-	1/1/15/20	12/37/115/115	-
16	CLA	p	507	12	-	7/37/115/115	-
19	BCR	o	603	-	-	9/29/63/63	0/2/2/2
16	CLA	a	1111	-	1/1/13/20	8/25/103/115	-
16	CLA	b	1223	-	1/1/15/20	9/37/115/115	-
16	CLA	u	503	-	-	7/15/93/115	-
16	CLA	g	515	-	1/1/15/20	8/37/115/115	-
16	CLA	a	1110	-	1/1/12/20	7/24/102/115	-
18	SF4	N	101	-	-	-	0/6/5/5
16	CLA	x	516	-	1/1/11/20	4/15/93/115	-
16	CLA	A	1138	-	1/1/15/20	10/37/115/115	-
19	BCR	b	4017	-	-	12/29/63/63	0/2/2/2
16	CLA	v	514	-	1/1/12/20	6/19/97/115	-
16	CLA	g	517	12	-	9/25/103/115	-
19	BCR	g	601	-	-	17/29/63/63	0/2/2/2
16	CLA	G	1214	-	1/1/13/20	11/25/103/115	-
16	CLA	a	1133	-	-	6/24/102/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	b	4010	-	-	15/29/63/63	0/2/2/2
16	CLA	b	1205	-	1/1/15/20	10/37/115/115	-
16	CLA	X	510	-	-	8/31/109/115	-
16	CLA	H	1125	-	-	10/37/115/115	-
16	CLA	a	1237	25	1/1/15/20	12/37/115/115	-
19	BCR	q	604	-	-	15/29/63/63	0/2/2/2
16	CLA	G	1212	-	1/1/11/20	7/13/91/115	-
16	CLA	H	1120	-	-	7/18/96/115	-
13	LHG	p	605	-	-	13/36/36/53	-
16	CLA	h	517	-	1/1/13/20	9/25/103/115	-
16	CLA	Z	505	-	1/1/15/20	12/37/115/115	-
16	CLA	b	1218	-	-	7/25/103/115	-
16	CLA	H	1110	-	1/1/12/20	7/24/102/115	-
16	CLA	r	510	-	-	11/37/115/115	-
20	LMT	l	4101	-	-	7/21/61/61	0/2/2/2
16	CLA	o	512	12	1/1/15/20	7/37/115/115	-
19	BCR	X	601	-	-	10/29/63/63	0/2/2/2
16	CLA	W	504	-	1/1/14/20	4/31/109/115	-
16	CLA	x	501	-	-	6/19/97/115	-
13	LHG	B	4018	16	-	17/42/42/53	-
17	PQN	G	2002	-	-	10/23/43/43	0/2/2/2
16	CLA	G	1236	-	-	5/19/97/115	-
16	CLA	X	517	12	-	5/25/103/115	-
19	BCR	r	601	-	-	15/29/63/63	0/2/2/2
16	CLA	G	1220	-	1/1/12/20	13/24/102/115	-
18	SF4	c	101	-	-	-	0/6/5/5
16	CLA	s	515	-	1/1/15/20	11/37/115/115	-
16	CLA	q	513	-	-	7/19/97/115	-
19	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
21	ECH	G	4006	-	-	10/29/66/66	0/2/2/2
16	CLA	q	501	-	1/1/12/20	7/19/97/115	-
16	CLA	s	504	-	1/1/15/20	14/37/115/115	-
19	BCR	g	603	-	-	15/29/63/63	0/2/2/2
19	BCR	v	603	-	-	12/29/63/63	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	n	508	12	1/1/13/20	7/25/103/115	-
19	BCR	W	604	-	-	10/29/63/63	0/2/2/2
16	CLA	b	1012	25	1/1/13/20	10/25/103/115	-
14	LMG	A	4201	-	-	13/27/47/70	0/1/1/1
16	CLA	H	1103	-	1/1/15/20	12/37/115/115	-
16	CLA	b	1211	-	1/1/15/20	12/37/115/115	-
19	BCR	Q	4016	-	-	11/29/63/63	0/2/2/2
16	CLA	t	505	-	-	10/37/115/115	-
18	SF4	a	3001	-	-	-	0/6/5/5
16	CLA	Y	502	-	1/1/12/20	4/19/97/115	-
16	CLA	a	1129	-	-	2/15/93/115	-
19	BCR	f	4016	-	-	11/29/63/63	0/2/2/2
16	CLA	X	502	-	1/1/12/20	5/19/97/115	-
19	BCR	s	604	-	-	16/29/63/63	0/2/2/2
19	BCR	L	4022	-	-	14/29/63/63	0/2/2/2
19	BCR	o	602	-	-	14/29/63/63	0/2/2/2
16	CLA	n	517	12	1/1/13/20	9/25/103/115	-
16	CLA	B	1216	25	-	4/16/94/115	-
16	CLA	q	516	-	1/1/11/20	9/15/93/115	-
16	CLA	p	512	12	1/1/15/20	9/37/115/115	-
16	CLA	r	501	-	1/1/12/20	4/19/97/115	-
16	CLA	Y	514	-	1/1/12/20	6/19/97/115	-
16	CLA	l	1503	-	1/1/15/20	12/37/115/115	-
18	SF4	C	101	-	-	-	0/6/5/5
16	CLA	B	1240	13	1/1/11/20	5/15/93/115	-
16	CLA	G	1229	-	1/1/13/20	9/29/107/115	-
16	CLA	G	1232	25	1/1/11/20	5/13/91/115	-
16	CLA	x	517	12	-	7/25/103/115	-
16	CLA	h	508	-	1/1/13/20	10/25/103/115	-
16	CLA	B	1230	-	1/1/11/20	6/13/91/115	-
16	CLA	g	512	12	1/1/15/20	8/37/115/115	-
16	CLA	J	1302	8	1/1/11/20	4/13/91/115	-
16	CLA	s	503	-	1/1/11/20	8/15/93/115	-
16	CLA	B	1222	25	-	6/19/97/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	H	4008	-	-	13/29/63/63	0/2/2/2
16	CLA	Q	1302	6	1/1/11/20	4/15/93/115	-
16	CLA	X	513	-	-	7/15/93/115	-
18	SF4	c	102	-	-	-	0/6/5/5
16	CLA	n	502	-	1/1/12/20	5/19/97/115	-
16	CLA	h	512	12	-	16/37/115/115	-
19	BCR	j	4015	-	-	14/29/63/63	0/2/2/2
16	CLA	a	1121	-	1/1/12/20	5/21/99/115	-
16	CLA	a	1128	-	1/1/15/20	17/37/115/115	-
16	CLA	b	1023	-	-	10/37/115/115	-
16	CLA	w	502	-	1/1/12/20	6/19/97/115	-
14	LMG	A	852	-	-	10/33/53/70	0/1/1/1
16	CLA	q	503	-	1/1/11/20	8/15/93/115	-
16	CLA	s	510	-	-	8/37/115/115	-
16	CLA	H	1137	-	1/1/11/20	4/16/94/115	-
16	CLA	G	1228	-	1/1/13/20	13/25/103/115	-
16	CLA	y	517	-	1/1/13/20	13/25/103/115	-
16	CLA	A	1140	-	1/1/15/20	11/37/115/115	-
16	CLA	g	514	-	1/1/12/20	6/19/97/115	-
19	BCR	a	4007	-	-	7/29/63/63	0/2/2/2
19	BCR	a	4011	-	-	16/29/63/63	0/2/2/2
16	CLA	a	1117	-	1/1/15/20	9/37/115/115	-
16	CLA	b	1240	13	1/1/11/20	4/15/93/115	-
16	CLA	W	506	-	-	9/31/109/115	-
16	CLA	B	1215	-	1/1/14/20	6/31/109/115	-
16	CLA	a	1105	-	1/1/13/20	7/29/107/115	-
19	BCR	S	4013	-	-	10/29/63/63	0/2/2/2
19	BCR	a	4003	-	-	12/29/63/63	0/2/2/2
16	CLA	f	1302	6	1/1/11/20	7/15/93/115	-
16	CLA	B	1225	-	-	11/37/115/115	-
19	BCR	w	604	-	-	17/29/63/63	0/2/2/2
16	CLA	a	1120	-	-	7/18/96/115	-
16	CLA	h	514	-	-	6/19/97/115	-
16	CLA	W	511	-	1/1/15/20	8/37/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	v	502	-	1/1/12/20	5/19/97/115	-
19	BCR	Y	603	-	-	8/29/63/63	0/2/2/2
16	CLA	H	1116	-	1/1/12/20	8/24/102/115	-
16	CLA	y	502	-	1/1/12/20	4/19/97/115	-
16	CLA	B	1206	2	1/1/15/20	17/37/115/115	-
19	BCR	x	603	-	-	14/29/63/63	0/2/2/2
16	CLA	b	1204	-	1/1/15/20	11/37/115/115	-
16	CLA	q	509	-	1/1/15/20	11/37/115/115	-
16	CLA	B	1238	25	1/1/15/20	7/37/115/115	-
16	CLA	H	1102	16	1/1/13/20	5/27/105/115	-
16	CLA	H	1136	-	1/1/15/20	8/37/115/115	-
16	CLA	A	1137	-	1/1/11/20	5/16/94/115	-
16	CLA	H	1801	13	1/1/11/20	4/15/93/115	-
16	CLA	u	510	-	-	8/31/109/115	-
16	CLA	h	509	-	1/1/15/20	16/37/115/115	-
16	CLA	G	1211	-	-	20/37/115/115	-
16	CLA	A	1022	25	1/1/15/20	10/37/115/115	-
16	CLA	p	508	12	1/1/13/20	8/25/103/115	-
16	CLA	A	1125	-	-	10/37/115/115	-
16	CLA	n	515	-	1/1/15/20	14/37/115/115	-
16	CLA	G	1021	-	1/1/15/20	13/37/115/115	-
16	CLA	a	1130	-	-	9/31/109/115	-
16	CLA	v	515	-	1/1/15/20	16/37/115/115	-
16	CLA	w	508	12	1/1/13/20	6/25/103/115	-
13	LHG	G	4018	16	-	12/42/42/53	-
19	BCR	X	604	-	-	19/29/63/63	0/2/2/2
19	BCR	v	604	-	-	12/29/63/63	0/2/2/2
16	CLA	A	1139	25	1/1/14/20	14/31/109/115	-
16	CLA	b	1206	2	1/1/15/20	15/37/115/115	-
16	CLA	y	515	-	1/1/15/20	15/37/115/115	-
16	CLA	B	1205	-	1/1/15/20	8/37/115/115	-
16	CLA	Z	517	12	1/1/13/20	4/25/103/115	-
16	CLA	u	507	12	1/1/15/20	10/37/115/115	-
16	CLA	G	1204	-	1/1/15/20	7/37/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	w	504	-	1/1/15/20	11/37/115/115	-
16	CLA	H	1134	1	-	2/13/91/115	-
16	CLA	x	512	12	-	7/37/115/115	-
16	CLA	a	1118	-	-	9/25/103/115	-
16	CLA	v	505	-	-	11/37/115/115	-
18	SF4	N	102	-	-	-	0/6/5/5
19	BCR	H	4003	-	-	10/29/63/63	0/2/2/2
16	CLA	s	501	-	1/1/12/20	7/19/97/115	-
16	CLA	b	1209	-	1/1/11/20	3/13/91/115	-
16	CLA	t	515	-	1/1/15/20	13/37/115/115	-
16	CLA	o	501	-	-	7/15/93/115	-
19	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
19	BCR	u	603	-	-	9/29/63/63	0/2/2/2
16	CLA	n	504	-	-	4/31/109/115	-
19	BCR	p	602	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1109	16	1/1/15/20	9/37/115/115	-
17	PQN	H	2001	-	-	3/23/43/43	0/2/2/2
16	CLA	h	515	-	1/1/15/20	17/37/115/115	-
16	CLA	H	1117	-	1/1/15/20	8/37/115/115	-
16	CLA	Z	502	-	1/1/12/20	5/19/97/115	-
16	CLA	a	1139	25	1/1/13/20	4/25/103/115	-
16	CLA	A	1116	-	1/1/12/20	10/24/102/115	-
16	CLA	p	515	-	1/1/15/20	13/37/115/115	-
19	BCR	s	602	-	-	11/29/63/63	0/2/2/2
16	CLA	G	1238	25	1/1/15/20	9/37/115/115	-
16	CLA	B	1202	-	1/1/15/20	16/37/115/115	-
19	BCR	n	604	-	-	13/29/63/63	0/2/2/2
17	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
16	CLA	w	516	-	1/1/11/20	8/15/93/115	-
19	BCR	S	4012	-	-	10/29/63/63	0/2/2/2
16	CLA	X	501	-	-	7/15/93/115	-
24	LUT	q	601	-	-	7/29/67/67	0/2/2/2
16	CLA	G	1240	13	1/1/11/20	4/15/93/115	-
16	CLA	u	506	-	1/1/14/20	11/31/109/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	K	4005	-	-	9/29/63/63	0/2/2/2
16	CLA	Y	513	-	-	8/15/93/115	-
16	CLA	o	516	-	-	9/15/93/115	-
16	CLA	w	517	12	1/1/13/20	6/25/103/115	-
16	CLA	Z	501	-	1/1/12/20	7/19/97/115	-
16	CLA	Y	503	-	1/1/11/20	5/15/93/115	-
16	CLA	Y	511	-	1/1/15/20	13/37/115/115	-
16	CLA	G	1239	-	1/1/15/20	14/37/115/115	-
16	CLA	Z	513	-	-	7/19/97/115	-
16	CLA	H	1121	-	1/1/12/20	7/21/99/115	-
16	CLA	r	506	-	-	10/31/109/115	-
16	CLA	y	509	-	1/1/15/20	19/37/115/115	-
16	CLA	o	507	12	-	11/37/115/115	-
16	CLA	s	514	-	1/1/12/20	6/19/97/115	-
16	CLA	a	1127	-	1/1/15/20	3/37/115/115	-
16	CLA	b	1236	-	-	7/19/97/115	-
19	BCR	s	601	-	-	12/29/63/63	0/2/2/2
16	CLA	L	1503	25	1/1/15/20	11/37/115/115	-
19	BCR	a	4002	-	-	12/29/63/63	0/2/2/2
16	CLA	S	1302	8	1/1/11/20	5/13/91/115	-
16	CLA	X	516	-	-	6/15/93/115	-
16	CLA	r	511	-	1/1/15/20	6/37/115/115	-
16	CLA	n	510	-	-	14/37/115/115	-
16	CLA	u	504	-	-	17/31/109/115	-
16	CLA	v	507	12	-	8/37/115/115	-
16	CLA	A	1108	-	-	2/13/91/115	-
16	CLA	B	1228	-	-	13/25/103/115	-
16	CLA	p	501	-	1/1/12/20	5/19/97/115	-
19	BCR	J	4015	-	-	7/29/63/63	0/2/2/2
16	CLA	b	1214	-	1/1/13/20	5/25/103/115	-
16	CLA	g	504	-	1/1/15/20	20/37/115/115	-
16	CLA	v	504	-	1/1/14/20	13/31/109/115	-
16	CLA	x	502	-	1/1/12/20	4/19/97/115	-
16	CLA	H	1118	-	-	11/25/103/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	x	508	12	1/1/13/20	10/25/103/115	-
16	CLA	b	1239	-	-	13/37/115/115	-
16	CLA	H	1105	-	1/1/13/20	8/29/107/115	-
16	CLA	B	1232	-	1/1/11/20	6/13/91/115	-
16	CLA	h	513	-	1/1/11/20	6/15/93/115	-
16	CLA	Y	507	12	-	8/37/115/115	-
19	BCR	F	4016	-	-	9/29/63/63	0/2/2/2
16	CLA	B	1021	-	1/1/15/20	12/37/115/115	-
16	CLA	r	502	-	1/1/12/20	5/19/97/115	-
16	CLA	u	505	-	1/1/15/20	12/37/115/115	-
16	CLA	a	1119	-	1/1/15/20	7/37/115/115	-
16	CLA	H	1114	-	1/1/11/20	7/15/93/115	-
16	CLA	x	505	-	1/1/15/20	8/37/115/115	-
16	CLA	y	516	-	1/1/11/20	6/15/93/115	-
19	BCR	g	602	-	-	14/29/63/63	0/2/2/2

All (1993) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	u	506	CLA	CHB-C4A	6.36	1.39	1.33
16	o	514	CLA	CHB-C4A	6.33	1.38	1.33
16	v	507	CLA	CHB-C4A	6.29	1.38	1.33
15	A	1011	CL0	CHB-C4A	6.25	1.38	1.33
16	b	1216	CLA	CHB-C4A	6.24	1.38	1.33
16	s	506	CLA	CHB-C4A	6.23	1.38	1.33
15	a	1011	CL0	CHB-C4A	6.21	1.38	1.33
16	J	1302	CLA	CHB-C4A	6.20	1.38	1.33
16	B	1220	CLA	CHB-C4A	6.18	1.38	1.33
16	y	503	CLA	CHB-C4A	6.17	1.38	1.33
16	y	514	CLA	CHB-C4A	6.14	1.38	1.33
16	X	514	CLA	CHB-C4A	6.13	1.38	1.33
16	r	507	CLA	CHB-C4A	6.13	1.38	1.33
16	h	503	CLA	CHB-C4A	6.13	1.38	1.33
16	o	507	CLA	CHB-C4A	6.12	1.38	1.33
16	y	516	CLA	CHB-C4A	6.09	1.38	1.33
16	W	507	CLA	CHB-C4A	6.09	1.38	1.33
16	h	504	CLA	CHB-C4A	6.09	1.38	1.33
16	g	507	CLA	CHB-C4A	6.09	1.38	1.33
16	b	1220	CLA	CHB-C4A	6.09	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	1011	CL0	CHB-C4A	6.07	1.38	1.33
16	Y	506	CLA	CHB-C4A	6.07	1.38	1.33
16	w	503	CLA	CHB-C4A	6.07	1.38	1.33
16	p	506	CLA	CHB-C4A	6.06	1.38	1.33
16	t	507	CLA	CHB-C4A	6.06	1.38	1.33
16	h	501	CLA	CHB-C4A	6.06	1.38	1.33
16	Z	503	CLA	CHB-C4A	6.06	1.38	1.33
16	B	1023	CLA	CHB-C4A	6.05	1.38	1.33
16	F	1302	CLA	CHB-C4A	6.05	1.38	1.33
16	j	1302	CLA	CHB-C4A	6.05	1.38	1.33
16	y	507	CLA	CHB-C4A	6.04	1.38	1.33
16	v	505	CLA	CHB-C4A	6.03	1.38	1.33
16	y	517	CLA	CHB-C4A	6.02	1.38	1.33
16	v	513	CLA	CHB-C4A	6.02	1.38	1.33
16	W	513	CLA	CHB-C4A	6.01	1.38	1.33
16	W	502	CLA	CHB-C4A	6.01	1.38	1.33
16	q	503	CLA	CHB-C4A	6.01	1.38	1.33
16	x	506	CLA	CHB-C4A	6.00	1.38	1.33
16	u	507	CLA	CHB-C4A	6.00	1.38	1.33
16	B	1240	CLA	CHB-C4A	6.00	1.38	1.33
16	G	1211	CLA	CHB-C4A	6.00	1.38	1.33
16	h	506	CLA	CHB-C4A	6.00	1.38	1.33
16	h	516	CLA	CHB-C4A	5.99	1.38	1.33
16	x	507	CLA	CHB-C4A	5.99	1.38	1.33
16	f	1302	CLA	CHB-C4A	5.99	1.38	1.33
16	B	1239	CLA	CHB-C4A	5.99	1.38	1.33
16	h	502	CLA	CHB-C4A	5.98	1.38	1.33
16	b	1219	CLA	CHB-C4A	5.98	1.38	1.33
16	s	501	CLA	CHB-C4A	5.98	1.38	1.33
16	t	503	CLA	CHB-C4A	5.98	1.38	1.33
16	v	517	CLA	CHB-C4A	5.98	1.38	1.33
16	y	505	CLA	CHB-C4A	5.98	1.38	1.33
16	a	1237	CLA	CHB-C4A	5.97	1.38	1.33
16	n	507	CLA	CHB-C4A	5.97	1.38	1.33
16	u	508	CLA	CHB-C4A	5.97	1.38	1.33
16	v	508	CLA	CHB-C4A	5.97	1.38	1.33
16	h	513	CLA	CHB-C4A	5.97	1.38	1.33
16	p	501	CLA	CHB-C4A	5.97	1.38	1.33
16	t	513	CLA	CHB-C4A	5.97	1.38	1.33
16	x	508	CLA	CHB-C4A	5.96	1.38	1.33
16	v	501	CLA	CHB-C4A	5.96	1.38	1.33
16	G	1023	CLA	CHB-C4A	5.95	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1240	CLA	CHB-C4A	5.95	1.38	1.33
16	v	514	CLA	CHB-C4A	5.95	1.38	1.33
16	b	1023	CLA	CHB-C4A	5.94	1.38	1.33
16	a	1125	CLA	CHB-C4A	5.94	1.38	1.33
16	H	1114	CLA	CHB-C4A	5.94	1.38	1.33
16	q	506	CLA	CHB-C4A	5.94	1.38	1.33
16	v	516	CLA	CHB-C4A	5.94	1.38	1.33
16	Z	507	CLA	CHB-C4A	5.94	1.38	1.33
16	T	4004	CLA	CHB-C4A	5.94	1.38	1.33
16	s	502	CLA	CHB-C4A	5.94	1.38	1.33
16	T	4002	CLA	CHB-C4A	5.94	1.38	1.33
16	h	512	CLA	CHB-C4A	5.93	1.38	1.33
16	A	1237	CLA	CHB-C4A	5.93	1.38	1.33
16	G	1212	CLA	CHB-C4A	5.93	1.38	1.33
16	S	1302	CLA	CHB-C4A	5.93	1.38	1.33
16	o	508	CLA	CHB-C4A	5.92	1.38	1.33
16	k	4002	CLA	CHB-C4A	5.92	1.38	1.33
16	w	506	CLA	CHB-C4A	5.92	1.38	1.33
16	n	504	CLA	CHB-C4A	5.92	1.38	1.33
16	y	512	CLA	CHB-C4A	5.92	1.38	1.33
16	W	504	CLA	CHB-C4A	5.91	1.38	1.33
16	K	4004	CLA	CHB-C4A	5.91	1.38	1.33
16	Q	1302	CLA	CHB-C4A	5.91	1.38	1.33
16	g	517	CLA	CHB-C4A	5.91	1.38	1.33
16	S	1303	CLA	CHB-C4A	5.90	1.38	1.33
16	H	1121	CLA	CHB-C4A	5.90	1.38	1.33
16	H	1113	CLA	CHB-C4A	5.90	1.38	1.33
16	s	517	CLA	CHB-C4A	5.90	1.38	1.33
16	n	513	CLA	CHB-C4A	5.90	1.38	1.33
16	n	503	CLA	CHB-C4A	5.89	1.38	1.33
16	t	516	CLA	CHB-C4A	5.89	1.38	1.33
16	W	510	CLA	CHB-C4A	5.89	1.38	1.33
16	Y	513	CLA	CHB-C4A	5.89	1.38	1.33
16	Z	517	CLA	CHB-C4A	5.89	1.38	1.33
16	n	501	CLA	CHB-C4A	5.89	1.38	1.33
16	r	508	CLA	CHB-C4A	5.89	1.38	1.33
16	H	1237	CLA	CHB-C4A	5.89	1.38	1.33
16	g	503	CLA	CHB-C4A	5.89	1.38	1.33
16	A	1104	CLA	CHB-C4A	5.88	1.38	1.33
16	x	501	CLA	CHB-C4A	5.88	1.38	1.33
16	G	1239	CLA	CHB-C4A	5.88	1.38	1.33
16	g	508	CLA	CHB-C4A	5.88	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	t	501	CLA	CHB-C4A	5.88	1.38	1.33
16	h	511	CLA	CHB-C4A	5.88	1.38	1.33
16	y	508	CLA	CHB-C4A	5.88	1.38	1.33
16	y	504	CLA	CHB-C4A	5.87	1.38	1.33
16	s	513	CLA	CHB-C4A	5.87	1.38	1.33
16	G	1213	CLA	CHB-C4A	5.87	1.38	1.33
16	r	513	CLA	CHB-C4A	5.87	1.38	1.33
16	A	1125	CLA	CHB-C4A	5.87	1.38	1.33
16	X	508	CLA	CHB-C4A	5.87	1.38	1.33
16	g	506	CLA	CHB-C4A	5.87	1.38	1.33
16	n	514	CLA	CHB-C4A	5.87	1.38	1.33
16	t	502	CLA	CHB-C4A	5.87	1.38	1.33
16	b	1240	CLA	CHB-C4A	5.86	1.38	1.33
16	k	4004	CLA	CHB-C4A	5.86	1.38	1.33
16	Z	506	CLA	CHB-C4A	5.86	1.38	1.33
16	Y	501	CLA	CHB-C4A	5.86	1.38	1.33
16	b	1221	CLA	CHB-C4A	5.86	1.38	1.33
16	K	4002	CLA	CHB-C4A	5.86	1.38	1.33
16	b	1232	CLA	CHB-C4A	5.86	1.38	1.33
16	B	1222	CLA	CHB-C4A	5.86	1.38	1.33
16	H	1125	CLA	CHB-C4A	5.86	1.38	1.33
16	y	502	CLA	CHB-C4A	5.85	1.38	1.33
16	J	1303	CLA	CHB-C4A	5.85	1.38	1.33
16	t	504	CLA	CHB-C4A	5.85	1.38	1.33
16	X	507	CLA	CHB-C4A	5.85	1.38	1.33
16	t	506	CLA	CHB-C4A	5.85	1.38	1.33
16	w	507	CLA	CHB-C4A	5.85	1.38	1.33
16	h	505	CLA	CHB-C4A	5.85	1.38	1.33
16	p	513	CLA	CHB-C4A	5.85	1.38	1.33
16	y	513	CLA	CHB-C4A	5.85	1.38	1.33
16	h	508	CLA	CHB-C4A	5.84	1.38	1.33
16	v	515	CLA	CHB-C4A	5.84	1.38	1.33
16	a	1114	CLA	CHB-C4A	5.84	1.38	1.33
16	a	1122	CLA	CHB-C4A	5.84	1.38	1.33
16	j	1303	CLA	CHB-C4A	5.84	1.38	1.33
16	u	514	CLA	CHB-C4A	5.84	1.38	1.33
16	w	513	CLA	CHB-C4A	5.84	1.38	1.33
16	t	514	CLA	CHB-C4A	5.84	1.38	1.33
16	n	502	CLA	CHB-C4A	5.84	1.38	1.33
16	a	1113	CLA	CHB-C4A	5.83	1.38	1.33
16	x	513	CLA	CHB-C4A	5.83	1.38	1.33
16	a	1121	CLA	CHB-C4A	5.83	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	v	504	CLA	CHB-C4A	5.82	1.38	1.33
16	y	515	CLA	CHB-C4A	5.82	1.38	1.33
16	n	505	CLA	CHB-C4A	5.82	1.38	1.33
16	u	502	CLA	CHB-C4A	5.82	1.38	1.33
16	y	511	CLA	CHB-C4A	5.82	1.38	1.33
16	b	1201	CLA	CHB-C4A	5.81	1.38	1.33
16	u	517	CLA	CHB-C4A	5.81	1.38	1.33
16	B	1211	CLA	CHB-C4A	5.81	1.38	1.33
16	G	1201	CLA	CHB-C4A	5.81	1.38	1.33
16	s	507	CLA	CHB-C4A	5.81	1.38	1.33
16	x	503	CLA	CHB-C4A	5.81	1.38	1.33
16	H	1104	CLA	CHB-C4A	5.81	1.38	1.33
16	H	1107	CLA	CHB-C4A	5.81	1.38	1.33
16	G	1209	CLA	CHB-C4A	5.81	1.38	1.33
16	p	512	CLA	CHB-C4A	5.81	1.38	1.33
16	T	4003	CLA	CHB-C4A	5.80	1.38	1.33
16	a	1107	CLA	CHB-C4A	5.80	1.38	1.33
16	b	1222	CLA	CHB-C4A	5.80	1.38	1.33
16	v	510	CLA	CHB-C4A	5.80	1.38	1.33
16	G	1204	CLA	CHB-C4A	5.80	1.38	1.33
16	r	516	CLA	CHB-C4A	5.80	1.38	1.33
16	B	1202	CLA	CHB-C4A	5.79	1.38	1.33
16	W	505	CLA	CHB-C4A	5.79	1.38	1.33
16	o	506	CLA	CHB-C4A	5.79	1.38	1.33
16	b	1231	CLA	CHB-C4A	5.79	1.38	1.33
16	x	502	CLA	CHB-C4A	5.79	1.38	1.33
16	A	1103	CLA	CHB-C4A	5.79	1.38	1.33
16	G	1220	CLA	CHB-C4A	5.79	1.38	1.33
16	x	510	CLA	CHB-C4A	5.79	1.38	1.33
16	G	1232	CLA	CHB-C4A	5.79	1.38	1.33
16	h	517	CLA	CHB-C4A	5.79	1.38	1.33
16	g	505	CLA	CHB-C4A	5.79	1.38	1.33
16	Y	502	CLA	CHB-C4A	5.79	1.38	1.33
16	r	514	CLA	CHB-C4A	5.79	1.38	1.33
16	n	516	CLA	CHB-C4A	5.78	1.38	1.33
16	p	508	CLA	CHB-C4A	5.78	1.38	1.33
16	G	1224	CLA	CHB-C4A	5.78	1.38	1.33
16	a	1124	CLA	CHB-C4A	5.78	1.38	1.33
16	a	1115	CLA	CHB-C4A	5.78	1.38	1.33
16	o	516	CLA	CHB-C4A	5.78	1.38	1.33
16	A	1109	CLA	CHB-C4A	5.78	1.38	1.33
16	g	512	CLA	CHB-C4A	5.78	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	n	508	CLA	CHB-C4A	5.78	1.38	1.33
16	Y	517	CLA	CHB-C4A	5.78	1.38	1.33
16	a	1103	CLA	CHB-C4A	5.78	1.38	1.33
16	B	1209	CLA	CHB-C4A	5.77	1.38	1.33
16	g	516	CLA	CHB-C4A	5.77	1.38	1.33
16	w	501	CLA	CHB-C4A	5.77	1.38	1.33
16	X	506	CLA	CHB-C4A	5.77	1.38	1.33
16	q	515	CLA	CHB-C4A	5.77	1.38	1.33
16	W	501	CLA	CHB-C4A	5.77	1.38	1.33
16	Y	510	CLA	CHB-C4A	5.77	1.38	1.33
16	g	515	CLA	CHB-C4A	5.77	1.38	1.33
16	u	501	CLA	CHB-C4A	5.77	1.38	1.33
16	A	1121	CLA	CHB-C4A	5.77	1.38	1.33
16	B	1217	CLA	CHB-C4A	5.76	1.38	1.33
16	B	1228	CLA	CHB-C4A	5.76	1.38	1.33
16	q	513	CLA	CHB-C4A	5.76	1.38	1.33
16	v	503	CLA	CHB-C4A	5.76	1.38	1.33
16	x	515	CLA	CHB-C4A	5.76	1.38	1.33
16	B	1219	CLA	CHB-C4A	5.76	1.38	1.33
16	n	511	CLA	CHB-C4A	5.76	1.38	1.33
16	H	1109	CLA	CHB-C4A	5.76	1.38	1.33
16	r	512	CLA	CHB-C4A	5.76	1.38	1.33
16	x	517	CLA	CHB-C4A	5.76	1.38	1.33
16	n	506	CLA	CHB-C4A	5.76	1.38	1.33
16	t	515	CLA	CHB-C4A	5.76	1.38	1.33
16	A	1115	CLA	CHB-C4A	5.76	1.38	1.33
16	A	1114	CLA	CHB-C4A	5.76	1.38	1.33
16	X	504	CLA	CHB-C4A	5.76	1.38	1.33
16	b	1204	CLA	CHB-C4A	5.75	1.38	1.33
16	b	1212	CLA	CHB-C4A	5.75	1.38	1.33
16	r	505	CLA	CHB-C4A	5.75	1.38	1.33
16	n	510	CLA	CHB-C4A	5.75	1.38	1.33
16	u	510	CLA	CHB-C4A	5.75	1.38	1.33
16	u	513	CLA	CHB-C4A	5.75	1.38	1.33
16	h	514	CLA	CHB-C4A	5.75	1.38	1.33
16	p	507	CLA	CHB-C4A	5.75	1.38	1.33
16	o	510	CLA	CHB-C4A	5.74	1.38	1.33
16	v	512	CLA	CHB-C4A	5.74	1.38	1.33
16	Z	515	CLA	CHB-C4A	5.74	1.38	1.33
16	q	501	CLA	CHB-C4A	5.74	1.38	1.33
16	B	1201	CLA	CHB-C4A	5.74	1.38	1.33
16	G	1222	CLA	CHB-C4A	5.74	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	516	CLA	CHB-C4A	5.74	1.38	1.33
16	g	513	CLA	CHB-C4A	5.74	1.38	1.33
16	h	515	CLA	CHB-C4A	5.74	1.38	1.33
16	h	507	CLA	CHB-C4A	5.74	1.38	1.33
16	A	1107	CLA	CHB-C4A	5.74	1.38	1.33
16	B	1224	CLA	CHB-C4A	5.74	1.38	1.33
16	g	510	CLA	CHB-C4A	5.74	1.38	1.33
16	k	4003	CLA	CHB-C4A	5.74	1.38	1.33
16	B	1218	CLA	CHB-C4A	5.73	1.38	1.33
16	G	1218	CLA	CHB-C4A	5.73	1.38	1.33
16	A	1123	CLA	CHB-C4A	5.73	1.38	1.33
16	W	503	CLA	CHB-C4A	5.73	1.38	1.33
16	Y	507	CLA	CHB-C4A	5.73	1.38	1.33
16	W	514	CLA	CHB-C4A	5.73	1.38	1.33
16	r	501	CLA	CHB-C4A	5.73	1.38	1.33
16	r	503	CLA	CHB-C4A	5.73	1.38	1.33
16	B	1216	CLA	CHB-C4A	5.73	1.38	1.33
16	K	4003	CLA	CHB-C4A	5.73	1.38	1.33
16	t	508	CLA	CHB-C4A	5.73	1.38	1.33
16	B	1205	CLA	CHB-C4A	5.73	1.38	1.33
16	v	506	CLA	CHB-C4A	5.73	1.38	1.33
16	A	1113	CLA	CHB-C4A	5.73	1.38	1.33
16	y	501	CLA	CHB-C4A	5.73	1.38	1.33
16	p	517	CLA	CHB-C4A	5.72	1.38	1.33
16	s	508	CLA	CHB-C4A	5.72	1.38	1.33
16	H	1115	CLA	CHB-C4A	5.72	1.38	1.33
16	r	506	CLA	CHB-C4A	5.72	1.38	1.33
16	Y	504	CLA	CHB-C4A	5.72	1.38	1.33
16	b	1211	CLA	CHB-C4A	5.72	1.38	1.33
16	u	516	CLA	CHB-C4A	5.72	1.38	1.33
16	Y	516	CLA	CHB-C4A	5.72	1.38	1.33
16	a	1127	CLA	CHB-C4A	5.72	1.38	1.33
16	G	1219	CLA	CHB-C4A	5.71	1.38	1.33
16	q	507	CLA	CHB-C4A	5.71	1.38	1.33
16	Y	514	CLA	CHB-C4A	5.71	1.38	1.33
16	a	1108	CLA	CHB-C4A	5.71	1.38	1.33
16	h	510	CLA	CHB-C4A	5.71	1.38	1.33
16	q	508	CLA	CHB-C4A	5.71	1.38	1.33
16	G	1231	CLA	CHB-C4A	5.71	1.38	1.33
16	G	1205	CLA	CHB-C4A	5.71	1.38	1.33
16	t	512	CLA	CHB-C4A	5.71	1.38	1.33
16	b	1205	CLA	CHB-C4A	5.70	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1216	CLA	CHB-C4A	5.70	1.38	1.33
16	x	514	CLA	CHB-C4A	5.70	1.38	1.33
16	b	1209	CLA	CHB-C4A	5.70	1.38	1.33
16	g	514	CLA	CHB-C4A	5.70	1.38	1.33
16	B	1207	CLA	CHB-C4A	5.70	1.38	1.33
16	r	510	CLA	CHB-C4A	5.70	1.38	1.33
16	u	504	CLA	CHB-C4A	5.70	1.38	1.33
16	s	512	CLA	CHB-C4A	5.70	1.38	1.33
16	x	516	CLA	CHB-C4A	5.69	1.38	1.33
16	b	1207	CLA	CHB-C4A	5.69	1.38	1.33
16	W	511	CLA	CHB-C4A	5.69	1.38	1.33
16	r	515	CLA	CHB-C4A	5.69	1.38	1.33
16	x	512	CLA	CHB-C4A	5.69	1.38	1.33
16	H	1127	CLA	CHB-C4A	5.69	1.38	1.33
16	w	514	CLA	CHB-C4A	5.68	1.38	1.33
16	B	1213	CLA	CHB-C4A	5.68	1.38	1.33
16	Z	513	CLA	CHB-C4A	5.68	1.38	1.33
16	H	1139	CLA	CHB-C4A	5.68	1.38	1.33
16	b	1202	CLA	CHB-C4A	5.68	1.38	1.33
16	B	1204	CLA	CHB-C4A	5.68	1.38	1.33
16	p	510	CLA	CHB-C4A	5.68	1.38	1.33
16	a	1138	CLA	CHB-C4A	5.68	1.38	1.33
16	b	1213	CLA	CHB-C4A	5.68	1.38	1.33
16	b	1239	CLA	CHB-C4A	5.68	1.38	1.33
16	b	1218	CLA	CHB-C4A	5.68	1.38	1.33
16	x	504	CLA	CHB-C4A	5.68	1.38	1.33
16	W	508	CLA	CHB-C4A	5.68	1.38	1.33
16	p	502	CLA	CHB-C4A	5.68	1.38	1.33
16	W	517	CLA	CHB-C4A	5.67	1.38	1.33
16	b	1225	CLA	CHB-C4A	5.67	1.38	1.33
16	w	515	CLA	CHB-C4A	5.67	1.38	1.33
16	o	502	CLA	CHB-C4A	5.67	1.38	1.33
16	H	1118	CLA	CHB-C4A	5.67	1.38	1.33
16	B	1212	CLA	CHB-C4A	5.67	1.38	1.33
16	A	1122	CLA	CHB-C4A	5.67	1.38	1.33
16	H	1128	CLA	CHB-C4A	5.66	1.38	1.33
16	t	505	CLA	CHB-C4A	5.66	1.38	1.33
16	W	515	CLA	CHB-C4A	5.66	1.38	1.33
16	X	517	CLA	CHB-C4A	5.66	1.38	1.33
16	Z	514	CLA	CHB-C4A	5.66	1.38	1.33
16	y	509	CLA	CHB-C4A	5.66	1.38	1.33
16	A	1108	CLA	CHB-C4A	5.66	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	s	504	CLA	CHB-C4A	5.66	1.38	1.33
16	g	504	CLA	CHB-C4A	5.66	1.38	1.33
16	a	1104	CLA	CHB-C4A	5.66	1.38	1.33
16	h	509	CLA	CHB-C4A	5.66	1.38	1.33
16	s	516	CLA	CHB-C4A	5.66	1.38	1.33
16	Z	505	CLA	CHB-C4A	5.66	1.38	1.33
16	r	504	CLA	CHB-C4A	5.65	1.38	1.33
16	B	1231	CLA	CHB-C4A	5.65	1.38	1.33
16	A	1139	CLA	CHB-C4A	5.65	1.38	1.33
16	X	516	CLA	CHB-C4A	5.65	1.38	1.33
16	s	505	CLA	CHB-C4A	5.65	1.38	1.33
16	w	508	CLA	CHB-C4A	5.65	1.38	1.33
16	A	1124	CLA	CHB-C4A	5.65	1.38	1.33
16	a	1109	CLA	CHB-C4A	5.65	1.38	1.33
16	o	504	CLA	CHB-C4A	5.65	1.38	1.33
16	b	1208	CLA	CHB-C4A	5.64	1.38	1.33
16	o	501	CLA	CHB-C4A	5.64	1.38	1.33
16	x	511	CLA	CHB-C4A	5.64	1.38	1.33
16	G	1225	CLA	CHB-C4A	5.64	1.38	1.33
16	H	1126	CLA	CHB-C4A	5.64	1.38	1.33
16	H	1140	CLA	CHB-C4A	5.64	1.38	1.33
16	W	506	CLA	CHB-C4A	5.64	1.38	1.33
16	v	502	CLA	CHB-C4A	5.64	1.38	1.33
16	Z	501	CLA	CHB-C4A	5.64	1.38	1.33
16	o	517	CLA	CHB-C4A	5.64	1.38	1.33
16	a	1126	CLA	CHB-C4A	5.64	1.38	1.33
16	q	517	CLA	CHB-C4A	5.64	1.38	1.33
16	Z	510	CLA	CHB-C4A	5.63	1.38	1.33
16	r	517	CLA	CHB-C4A	5.63	1.38	1.33
16	G	1229	CLA	CHB-C4A	5.63	1.38	1.33
16	X	501	CLA	CHB-C4A	5.63	1.38	1.33
16	b	1228	CLA	CHB-C4A	5.63	1.38	1.33
16	w	510	CLA	CHB-C4A	5.63	1.38	1.33
16	x	505	CLA	CHB-C4A	5.62	1.38	1.33
16	B	1021	CLA	CHB-C4A	5.62	1.38	1.33
16	a	1134	CLA	CHB-C4A	5.62	1.38	1.33
16	G	1021	CLA	CHB-C4A	5.62	1.38	1.33
16	X	510	CLA	CHB-C4A	5.62	1.38	1.33
16	a	1120	CLA	CHB-C4A	5.61	1.38	1.33
16	A	1127	CLA	CHB-C4A	5.61	1.38	1.33
16	Z	516	CLA	CHB-C4A	5.61	1.38	1.33
16	Y	508	CLA	CHB-C4A	5.61	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	v	511	CLA	CHB-C4A	5.61	1.38	1.33
16	b	1210	CLA	CHB-C4A	5.61	1.38	1.33
16	Z	508	CLA	CHB-C4A	5.61	1.38	1.33
16	a	1105	CLA	CHB-C4A	5.61	1.38	1.33
16	X	503	CLA	CHB-C4A	5.61	1.38	1.33
16	H	1106	CLA	CHB-C4A	5.60	1.38	1.33
16	Y	512	CLA	CHB-C4A	5.60	1.38	1.33
16	b	1217	CLA	CHB-C4A	5.60	1.38	1.33
16	y	506	CLA	CHB-C4A	5.60	1.38	1.33
16	u	503	CLA	CHB-C4A	5.60	1.38	1.33
16	H	1123	CLA	CHB-C4A	5.60	1.38	1.33
16	H	1124	CLA	CHB-C4A	5.60	1.38	1.33
16	y	510	CLA	CHB-C4A	5.60	1.38	1.33
16	a	1133	CLA	CHB-C4A	5.60	1.38	1.33
16	A	1101	CLA	CHB-C4A	5.60	1.38	1.33
16	s	514	CLA	CHB-C4A	5.60	1.38	1.33
16	n	512	CLA	CHB-C4A	5.59	1.38	1.33
16	H	1108	CLA	CHB-C4A	5.59	1.38	1.33
16	H	1138	CLA	CHB-C4A	5.59	1.38	1.33
16	w	516	CLA	CHB-C4A	5.59	1.38	1.33
16	p	514	CLA	CHB-C4A	5.59	1.38	1.33
16	X	513	CLA	CHB-C4A	5.58	1.38	1.33
16	B	1208	CLA	CHB-C4A	5.58	1.38	1.33
16	Z	502	CLA	CHB-C4A	5.58	1.38	1.33
16	q	516	CLA	CHB-C4A	5.58	1.38	1.33
16	r	502	CLA	CHB-C4A	5.58	1.38	1.33
16	a	1801	CLA	CHB-C4A	5.58	1.38	1.33
16	A	1111	CLA	CHB-C4A	5.58	1.38	1.33
16	A	1140	CLA	CHB-C4A	5.58	1.38	1.33
16	G	1202	CLA	CHB-C4A	5.58	1.38	1.33
16	b	1230	CLA	CHB-C4A	5.58	1.38	1.33
16	G	1228	CLA	CHB-C4A	5.57	1.38	1.33
16	p	516	CLA	CHB-C4A	5.57	1.38	1.33
16	H	1110	CLA	CHB-C4A	5.57	1.38	1.33
16	a	1139	CLA	CHB-C4A	5.57	1.38	1.33
16	q	514	CLA	CHB-C4A	5.57	1.38	1.33
16	u	505	CLA	CHB-C4A	5.57	1.38	1.33
16	o	503	CLA	CHB-C4A	5.57	1.38	1.33
16	q	504	CLA	CHB-C4A	5.57	1.38	1.33
16	G	1221	CLA	CHB-C4A	5.57	1.38	1.33
16	w	511	CLA	CHB-C4A	5.57	1.38	1.33
16	t	510	CLA	CHB-C4A	5.56	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	g	501	CLA	CHB-C4A	5.56	1.38	1.33
16	B	1203	CLA	CHB-C4A	5.56	1.38	1.33
16	W	512	CLA	CHB-C4A	5.56	1.38	1.33
16	H	1111	CLA	CHB-C4A	5.56	1.38	1.33
16	s	503	CLA	CHB-C4A	5.56	1.38	1.33
16	B	1229	CLA	CHB-C4A	5.56	1.38	1.33
16	G	1223	CLA	CHB-C4A	5.56	1.38	1.33
16	Z	512	CLA	CHB-C4A	5.55	1.38	1.33
16	H	1134	CLA	CHB-C4A	5.55	1.38	1.33
16	w	517	CLA	CHB-C4A	5.55	1.38	1.33
16	o	513	CLA	CHB-C4A	5.55	1.38	1.33
16	g	511	CLA	CHB-C4A	5.55	1.38	1.33
16	a	1118	CLA	CHB-C4A	5.55	1.38	1.33
16	G	1236	CLA	CHB-C4A	5.55	1.38	1.33
16	Q	1301	CLA	CHB-C4A	5.55	1.38	1.33
16	A	1105	CLA	CHB-C4A	5.54	1.38	1.33
16	w	502	CLA	CHB-C4A	5.54	1.38	1.33
16	f	1301	CLA	CHB-C4A	5.54	1.38	1.33
16	Z	504	CLA	CHB-C4A	5.54	1.38	1.33
16	b	1223	CLA	CHB-C4A	5.54	1.38	1.33
16	n	515	CLA	CHB-C4A	5.54	1.38	1.33
16	A	1134	CLA	CHB-C4A	5.53	1.38	1.33
16	b	1215	CLA	CHB-C4A	5.53	1.38	1.33
16	s	510	CLA	CHB-C4A	5.53	1.38	1.33
16	G	1217	CLA	CHB-C4A	5.53	1.38	1.33
16	t	517	CLA	CHB-C4A	5.53	1.38	1.33
16	t	511	CLA	CHB-C4A	5.53	1.38	1.33
16	A	1102	CLA	CHB-C4A	5.53	1.38	1.33
16	H	1122	CLA	CHB-C4A	5.53	1.38	1.33
16	a	1101	CLA	CHB-C4A	5.53	1.38	1.33
16	a	1135	CLA	CHB-C4A	5.53	1.38	1.33
16	G	1207	CLA	CHB-C4A	5.53	1.38	1.33
16	a	1106	CLA	CHB-C4A	5.53	1.38	1.33
16	p	504	CLA	CHB-C4A	5.52	1.38	1.33
16	p	505	CLA	CHB-C4A	5.52	1.38	1.33
16	B	1225	CLA	CHB-C4A	5.52	1.38	1.33
16	H	1103	CLA	CHB-C4A	5.52	1.38	1.33
16	A	1118	CLA	CHB-C4A	5.51	1.38	1.33
16	b	1224	CLA	CHB-C4A	5.51	1.38	1.33
16	B	1236	CLA	CHB-C4A	5.51	1.38	1.33
16	B	1232	CLA	CHB-C4A	5.51	1.38	1.33
16	b	1229	CLA	CHB-C4A	5.51	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1221	CLA	CHB-C4A	5.51	1.38	1.33
16	b	1236	CLA	CHB-C4A	5.51	1.38	1.33
16	G	1230	CLA	CHB-C4A	5.50	1.38	1.33
16	A	1138	CLA	CHB-C4A	5.50	1.38	1.33
16	X	502	CLA	CHB-C4A	5.50	1.38	1.33
16	a	1013	CLA	CHB-C4A	5.50	1.38	1.33
16	A	1110	CLA	CHB-C4A	5.50	1.38	1.33
16	A	1106	CLA	CHB-C4A	5.49	1.38	1.33
16	H	1133	CLA	CHB-C4A	5.48	1.38	1.33
16	H	1137	CLA	CHB-C4A	5.48	1.38	1.33
16	X	505	CLA	CHB-C4A	5.48	1.38	1.33
16	w	512	CLA	CHB-C4A	5.48	1.38	1.33
16	H	1135	CLA	CHB-C4A	5.48	1.38	1.33
16	H	1105	CLA	CHB-C4A	5.48	1.38	1.33
16	a	1111	CLA	CHB-C4A	5.47	1.38	1.33
16	A	1137	CLA	CHB-C4A	5.47	1.38	1.33
16	H	1120	CLA	CHB-C4A	5.46	1.38	1.33
16	G	1208	CLA	CHB-C4A	5.46	1.38	1.33
16	r	511	CLA	CHB-C4A	5.46	1.38	1.33
16	o	505	CLA	CHB-C4A	5.46	1.38	1.33
16	G	1203	CLA	CHB-C4A	5.46	1.38	1.33
16	A	1128	CLA	CHB-C4A	5.45	1.38	1.33
16	G	1206	CLA	CHB-C4A	5.45	1.38	1.33
16	n	517	CLA	CHB-C4A	5.45	1.38	1.33
16	u	511	CLA	CHB-C4A	5.45	1.38	1.33
16	F	1301	CLA	CHB-C4A	5.44	1.38	1.33
16	B	1223	CLA	CHB-C4A	5.44	1.38	1.33
16	v	509	CLA	CHB-C4A	5.44	1.38	1.33
16	Y	511	CLA	CHB-C4A	5.44	1.38	1.33
16	p	503	CLA	CHB-C4A	5.43	1.38	1.33
16	b	1235	CLA	CHB-C4A	5.43	1.38	1.33
16	A	1126	CLA	CHB-C4A	5.42	1.38	1.33
16	b	1021	CLA	CHB-C4A	5.42	1.38	1.33
16	q	505	CLA	CHB-C4A	5.42	1.38	1.33
16	a	1137	CLA	CHB-C4A	5.42	1.38	1.33
16	q	512	CLA	CHB-C4A	5.42	1.38	1.33
16	H	1112	CLA	CHB-C4A	5.42	1.38	1.33
16	o	511	CLA	CHB-C4A	5.41	1.38	1.33
16	q	502	CLA	CHB-C4A	5.41	1.38	1.33
16	g	502	CLA	CHB-C4A	5.41	1.38	1.33
16	H	1101	CLA	CHB-C4A	5.41	1.38	1.33
16	B	1226	CLA	CHB-C4A	5.41	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1801	CLA	CHB-C4A	5.40	1.38	1.33
16	q	511	CLA	CHB-C4A	5.40	1.38	1.33
16	L	1503	CLA	CHB-C4A	5.40	1.38	1.33
16	B	1230	CLA	CHB-C4A	5.40	1.38	1.33
16	o	512	CLA	CHB-C4A	5.40	1.38	1.33
16	B	1210	CLA	CHB-C4A	5.39	1.38	1.33
16	w	504	CLA	CHB-C4A	5.39	1.38	1.33
16	A	1112	CLA	CHB-C4A	5.39	1.38	1.33
16	a	1140	CLA	CHB-C4A	5.39	1.38	1.33
16	B	1214	CLA	CHB-C4A	5.38	1.38	1.33
16	A	1120	CLA	CHB-C4A	5.37	1.38	1.33
16	a	1102	CLA	CHB-C4A	5.37	1.38	1.33
16	q	510	CLA	CHB-C4A	5.37	1.38	1.33
16	B	1206	CLA	CHB-C4A	5.37	1.38	1.33
16	G	1210	CLA	CHB-C4A	5.37	1.38	1.33
16	a	1110	CLA	CHB-C4A	5.37	1.38	1.33
16	b	1234	CLA	CHB-C4A	5.37	1.38	1.33
16	u	512	CLA	CHB-C4A	5.37	1.38	1.33
16	b	1226	CLA	CHB-C4A	5.37	1.38	1.33
16	b	1227	CLA	CHB-C4A	5.37	1.38	1.33
16	A	1135	CLA	CHB-C4A	5.36	1.38	1.33
16	Y	503	CLA	CHB-C4A	5.36	1.38	1.33
16	H	1131	CLA	CHB-C4A	5.36	1.38	1.33
16	H	1102	CLA	CHB-C4A	5.35	1.38	1.33
16	l	1501	CLA	CHB-C4A	5.35	1.38	1.33
16	Y	505	CLA	CHB-C4A	5.34	1.38	1.33
16	X	515	CLA	CHB-C4A	5.33	1.38	1.33
16	p	511	CLA	CHB-C4A	5.33	1.38	1.33
16	w	505	CLA	CHB-C4A	5.33	1.38	1.33
16	A	1117	CLA	CHB-C4A	5.33	1.38	1.33
16	A	1801	CLA	CHB-C4A	5.33	1.38	1.33
16	Z	511	CLA	CHB-C4A	5.33	1.38	1.33
16	a	1112	CLA	CHB-C4A	5.32	1.38	1.33
16	Y	515	CLA	CHB-C4A	5.31	1.38	1.33
16	a	1123	CLA	CHB-C4A	5.30	1.38	1.33
16	U	1503	CLA	CHB-C4A	5.30	1.38	1.33
16	U	1502	CLA	CHB-C4A	5.29	1.38	1.33
16	n	509	CLA	CHB-C4A	5.29	1.38	1.33
16	t	509	CLA	CHB-C4A	5.29	1.38	1.33
16	U	1501	CLA	CHB-C4A	5.28	1.38	1.33
16	u	515	CLA	CHB-C4A	5.28	1.38	1.33
16	s	511	CLA	CHB-C4A	5.27	1.38	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1136	CLA	CHB-C4A	5.27	1.37	1.33
16	a	1131	CLA	CHB-C4A	5.27	1.37	1.33
16	b	1203	CLA	CHB-C4A	5.26	1.37	1.33
16	B	1227	CLA	CHB-C4A	5.26	1.37	1.33
16	X	511	CLA	CHB-C4A	5.26	1.37	1.33
16	g	509	CLA	CHB-C4A	5.26	1.37	1.33
16	a	1128	CLA	CHB-C4A	5.26	1.37	1.33
16	s	509	CLA	CHB-C4A	5.26	1.37	1.33
16	A	1022	CLA	CHB-C4A	5.25	1.37	1.33
16	A	1129	CLA	CHB-C4A	5.25	1.37	1.33
16	u	509	CLA	CHB-C4A	5.25	1.37	1.33
16	b	1206	CLA	CHB-C4A	5.25	1.37	1.33
16	p	515	CLA	CHB-C4A	5.24	1.37	1.33
16	A	1131	CLA	CHB-C4A	5.24	1.37	1.33
16	A	1130	CLA	CHB-C4A	5.24	1.37	1.33
16	o	509	CLA	CHB-C4A	5.23	1.37	1.33
16	l	1503	CLA	CHB-C4A	5.23	1.37	1.33
16	G	1226	CLA	CHB-C4A	5.23	1.37	1.33
16	s	515	CLA	CHB-C4A	5.23	1.37	1.33
16	W	509	CLA	CHB-C4A	5.23	1.37	1.33
16	X	509	CLA	CHB-C4A	5.23	1.37	1.33
16	A	1136	CLA	CHB-C4A	5.22	1.37	1.33
16	A	1133	CLA	CHB-C4A	5.22	1.37	1.33
16	H	1132	CLA	CHB-C4A	5.22	1.37	1.33
16	G	1215	CLA	CHB-C4A	5.22	1.37	1.33
16	B	1215	CLA	CHB-C4A	5.22	1.37	1.33
16	o	515	CLA	CHB-C4A	5.22	1.37	1.33
16	G	1214	CLA	CHB-C4A	5.21	1.37	1.33
16	H	1129	CLA	CHB-C4A	5.20	1.37	1.33
16	A	1013	CLA	CHB-C4A	5.20	1.37	1.33
16	a	1129	CLA	CHB-C4A	5.19	1.37	1.33
16	L	1502	CLA	CHB-C4A	5.19	1.37	1.33
16	p	509	CLA	CHB-C4A	5.18	1.37	1.33
16	L	1501	CLA	CHB-C4A	5.18	1.37	1.33
16	B	1234	CLA	CHB-C4A	5.18	1.37	1.33
16	w	509	CLA	CHB-C4A	5.18	1.37	1.33
16	H	1013	CLA	CHB-C4A	5.18	1.37	1.33
16	Z	509	CLA	CHB-C4A	5.18	1.37	1.33
16	G	1238	CLA	CHB-C4A	5.17	1.37	1.33
16	H	1022	CLA	CHB-C4A	5.17	1.37	1.33
16	b	1214	CLA	CHB-C4A	5.17	1.37	1.33
16	a	1022	CLA	CHB-C4A	5.16	1.37	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	512	CLA	CHB-C4A	5.16	1.37	1.33
16	G	1227	CLA	CHB-C4A	5.14	1.37	1.33
16	B	1238	CLA	CHB-C4A	5.13	1.37	1.33
16	Y	509	CLA	CHB-C4A	5.12	1.37	1.33
16	a	1117	CLA	CHB-C4A	5.09	1.37	1.33
16	a	1136	CLA	CHB-C4A	5.09	1.37	1.33
16	A	1132	CLA	CHB-C4A	5.08	1.37	1.33
16	b	1238	CLA	CHB-C4A	5.08	1.37	1.33
16	H	1117	CLA	CHB-C4A	5.07	1.37	1.33
16	a	1132	CLA	CHB-C4A	5.07	1.37	1.33
16	r	509	CLA	CHB-C4A	5.05	1.37	1.33
16	G	1234	CLA	CHB-C4A	5.04	1.37	1.33
16	x	509	CLA	CHB-C4A	5.02	1.37	1.33
16	q	509	CLA	CHB-C4A	5.01	1.37	1.33
16	H	1119	CLA	CHB-C4A	5.01	1.37	1.33
16	A	1116	CLA	CHB-C4A	5.00	1.37	1.33
16	l	1502	CLA	CHB-C4A	5.00	1.37	1.33
16	a	1116	CLA	CHB-C4A	4.98	1.37	1.33
16	a	1130	CLA	CHB-C4A	4.96	1.37	1.33
16	B	1235	CLA	CHB-C4A	4.90	1.37	1.33
16	H	1116	CLA	CHB-C4A	4.88	1.37	1.33
16	H	1130	CLA	CHB-C4A	4.87	1.37	1.33
16	a	1119	CLA	CHB-C4A	4.86	1.37	1.33
16	A	1119	CLA	CHB-C4A	4.84	1.37	1.33
16	G	1235	CLA	CHB-C4A	4.81	1.37	1.33
16	B	1012	CLA	CHB-C4A	4.58	1.37	1.33
16	G	1012	CLA	CHB-C4A	4.45	1.37	1.33
16	b	1012	CLA	CHB-C4A	4.33	1.37	1.33
16	b	1012	CLA	CHC-C1C	3.70	1.43	1.34
16	H	1126	CLA	CHC-C1C	3.69	1.43	1.34
16	a	1102	CLA	CHC-C1C	3.68	1.43	1.34
16	B	1012	CLA	CHC-C1C	3.68	1.43	1.34
16	G	1012	CLA	C1D-ND	3.66	1.42	1.37
16	a	1126	CLA	CHC-C1C	3.63	1.43	1.34
16	G	1218	CLA	C1D-ND	3.63	1.42	1.37
16	Z	509	CLA	CHC-C1C	3.63	1.43	1.34
16	q	509	CLA	CHC-C1C	3.63	1.43	1.34
16	X	503	CLA	CHC-C1C	3.62	1.43	1.34
16	n	510	CLA	C1D-ND	3.61	1.42	1.37
16	A	1119	CLA	CHC-C1C	3.60	1.43	1.34
16	H	1013	CLA	CHC-C1C	3.59	1.43	1.34
16	G	1023	CLA	CHC-C1C	3.58	1.43	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	r	509	CLA	CHC-C1C	3.58	1.43	1.34
16	A	1126	CLA	CHC-C1C	3.58	1.43	1.34
16	w	509	CLA	CHC-C1C	3.58	1.43	1.34
16	u	511	CLA	CHC-C1C	3.58	1.43	1.34
16	A	1102	CLA	CHC-C1C	3.58	1.43	1.34
16	B	1210	CLA	CHC-C1C	3.57	1.43	1.34
16	b	1212	CLA	CHC-C1C	3.57	1.43	1.34
16	g	504	CLA	C1D-ND	3.57	1.42	1.37
16	G	1222	CLA	CHC-C1C	3.57	1.43	1.34
16	Y	503	CLA	CHC-C1C	3.57	1.43	1.34
16	H	1102	CLA	CHC-C1C	3.56	1.43	1.34
16	y	510	CLA	C1D-ND	3.56	1.42	1.37
16	A	1106	CLA	CHC-C1C	3.56	1.43	1.34
16	p	510	CLA	C1D-ND	3.56	1.42	1.37
16	y	511	CLA	CHC-C1C	3.56	1.43	1.34
16	B	1218	CLA	C1D-ND	3.56	1.42	1.37
16	h	511	CLA	CHC-C1C	3.56	1.43	1.34
16	B	1202	CLA	CHC-C1C	3.55	1.43	1.34
16	H	1105	CLA	CHC-C1C	3.55	1.43	1.34
16	u	516	CLA	CHC-C1C	3.55	1.43	1.34
16	a	1117	CLA	CHC-C1C	3.55	1.43	1.34
16	G	1212	CLA	CHC-C1C	3.55	1.43	1.34
16	b	1220	CLA	CHC-C1C	3.55	1.43	1.34
16	b	1211	CLA	CHC-C1C	3.55	1.43	1.34
16	x	503	CLA	CHC-C1C	3.55	1.43	1.34
16	A	1134	CLA	CHC-C1C	3.54	1.43	1.34
16	B	1211	CLA	CHC-C1C	3.54	1.43	1.34
16	H	1129	CLA	CHC-C1C	3.54	1.43	1.34
16	W	504	CLA	C1D-ND	3.54	1.42	1.37
16	A	1129	CLA	CHC-C1C	3.54	1.43	1.34
16	h	510	CLA	C1D-ND	3.54	1.42	1.37
16	b	1227	CLA	CHC-C1C	3.54	1.43	1.34
16	t	510	CLA	C1D-ND	3.54	1.42	1.37
16	b	1202	CLA	CHC-C1C	3.54	1.43	1.34
16	B	1216	CLA	CHC-C1C	3.54	1.43	1.34
16	H	1117	CLA	CHC-C1C	3.54	1.43	1.34
16	w	517	CLA	CHC-C1C	3.54	1.43	1.34
16	b	1210	CLA	CHC-C1C	3.54	1.43	1.34
16	b	1221	CLA	CHC-C1C	3.53	1.43	1.34
16	y	513	CLA	C1D-ND	3.53	1.42	1.37
16	B	1212	CLA	CHC-C1C	3.53	1.43	1.34
16	a	1129	CLA	CHC-C1C	3.53	1.43	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	1218	CLA	C1D-ND	3.53	1.42	1.37
16	B	1213	CLA	CHC-C1C	3.53	1.43	1.34
16	x	509	CLA	CHC-C1C	3.53	1.43	1.34
16	o	516	CLA	CHC-C1C	3.53	1.43	1.34
16	W	511	CLA	CHC-C1C	3.53	1.43	1.34
16	h	501	CLA	CHC-C1C	3.53	1.43	1.34
16	g	509	CLA	CHC-C1C	3.53	1.43	1.34
16	G	1202	CLA	CHC-C1C	3.53	1.43	1.34
16	u	503	CLA	CHC-C1C	3.52	1.43	1.34
16	v	515	CLA	C1D-ND	3.52	1.42	1.37
16	v	503	CLA	CHC-C1C	3.52	1.43	1.34
16	b	1222	CLA	CHC-C1C	3.52	1.43	1.34
16	g	517	CLA	C1D-ND	3.52	1.42	1.37
16	H	1139	CLA	CHC-C1C	3.52	1.43	1.34
16	a	1106	CLA	CHC-C1C	3.52	1.43	1.34
16	n	511	CLA	CHC-C1C	3.52	1.43	1.34
16	p	503	CLA	CHC-C1C	3.52	1.43	1.34
16	o	503	CLA	CHC-C1C	3.52	1.43	1.34
16	B	1235	CLA	CHC-C1C	3.51	1.43	1.34
16	B	1023	CLA	CHC-C1C	3.51	1.43	1.34
16	h	505	CLA	CHC-C1C	3.51	1.43	1.34
16	y	516	CLA	CHC-C1C	3.51	1.43	1.34
16	v	505	CLA	CHC-C1C	3.51	1.43	1.34
16	x	505	CLA	CHC-C1C	3.51	1.43	1.34
16	W	510	CLA	C1D-ND	3.51	1.42	1.37
16	y	503	CLA	CHC-C1C	3.51	1.43	1.34
16	y	517	CLA	C1D-ND	3.51	1.42	1.37
16	A	1116	CLA	CHC-C1C	3.51	1.43	1.34
16	h	503	CLA	CHC-C1C	3.51	1.43	1.34
16	t	509	CLA	CHC-C1C	3.51	1.43	1.34
16	a	1013	CLA	CHC-C1C	3.51	1.43	1.34
16	v	508	CLA	CHC-C1C	3.51	1.43	1.34
16	q	508	CLA	CHC-C1C	3.51	1.43	1.34
16	b	1234	CLA	CHC-C1C	3.51	1.43	1.34
16	x	511	CLA	CHC-C1C	3.51	1.43	1.34
16	G	1219	CLA	CHC-C1C	3.50	1.43	1.34
16	o	511	CLA	CHC-C1C	3.50	1.43	1.34
16	v	511	CLA	CHC-C1C	3.50	1.43	1.34
16	G	1210	CLA	CHC-C1C	3.50	1.43	1.34
16	B	1222	CLA	CHC-C1C	3.50	1.43	1.34
16	A	1130	CLA	CHC-C1C	3.50	1.43	1.34
16	Y	507	CLA	C1D-ND	3.50	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1225	CLA	CHC-C1C	3.50	1.43	1.34
16	a	1105	CLA	CHC-C1C	3.50	1.43	1.34
16	G	1203	CLA	CHC-C1C	3.50	1.43	1.34
16	H	1119	CLA	CHC-C1C	3.50	1.43	1.34
16	H	1134	CLA	CHC-C1C	3.50	1.43	1.34
16	X	505	CLA	CHC-C1C	3.50	1.43	1.34
16	Y	515	CLA	CHC-C1C	3.50	1.43	1.34
16	t	503	CLA	CHC-C1C	3.49	1.43	1.34
16	H	1127	CLA	CHC-C1C	3.49	1.43	1.34
16	r	503	CLA	CHC-C1C	3.49	1.43	1.34
16	G	1012	CLA	CHC-C1C	3.49	1.43	1.34
16	s	503	CLA	CHC-C1C	3.49	1.43	1.34
16	t	513	CLA	CHC-C1C	3.49	1.43	1.34
16	y	501	CLA	CHC-C1C	3.49	1.43	1.34
16	A	1117	CLA	CHC-C1C	3.49	1.43	1.34
16	H	1101	CLA	CHC-C1C	3.49	1.43	1.34
16	A	1127	CLA	CHC-C1C	3.49	1.43	1.34
16	G	1235	CLA	CHC-C1C	3.49	1.43	1.34
16	g	511	CLA	CHC-C1C	3.49	1.43	1.34
16	f	1302	CLA	CHC-C1C	3.49	1.43	1.34
16	s	515	CLA	CHC-C1C	3.49	1.43	1.34
16	s	517	CLA	CHC-C1C	3.49	1.43	1.34
16	G	1229	CLA	CHC-C1C	3.49	1.43	1.34
16	W	513	CLA	CHC-C1C	3.49	1.43	1.34
16	n	509	CLA	CHC-C1C	3.49	1.43	1.34
16	y	505	CLA	CHC-C1C	3.49	1.43	1.34
16	v	504	CLA	CHC-C1C	3.48	1.43	1.34
16	L	1501	CLA	CHC-C1C	3.48	1.43	1.34
16	p	514	CLA	CHC-C1C	3.48	1.43	1.34
16	L	1503	CLA	CHC-C1C	3.48	1.43	1.34
16	u	504	CLA	C1D-ND	3.48	1.42	1.37
16	r	511	CLA	CHC-C1C	3.48	1.43	1.34
16	t	511	CLA	CHC-C1C	3.48	1.43	1.34
16	J	1303	CLA	C1D-ND	3.48	1.42	1.37
16	A	1125	CLA	CHC-C1C	3.48	1.43	1.34
16	Y	510	CLA	C1D-ND	3.48	1.42	1.37
16	B	1221	CLA	CHC-C1C	3.48	1.43	1.34
16	p	507	CLA	C1D-ND	3.48	1.42	1.37
16	B	1219	CLA	CHC-C1C	3.48	1.43	1.34
16	g	513	CLA	C1D-ND	3.48	1.42	1.37
16	W	503	CLA	CHC-C1C	3.48	1.43	1.34
16	y	504	CLA	CHC-C1C	3.48	1.43	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1101	CLA	CHC-C1C	3.48	1.43	1.34
16	w	511	CLA	CHC-C1C	3.48	1.43	1.34
16	F	1302	CLA	CHC-C1C	3.48	1.43	1.34
16	G	1227	CLA	CHC-C1C	3.48	1.43	1.34
16	a	1139	CLA	CHC-C1C	3.48	1.43	1.34
16	v	509	CLA	CHC-C1C	3.48	1.43	1.34
16	v	517	CLA	C1D-ND	3.48	1.42	1.37
16	g	503	CLA	CHC-C1C	3.47	1.43	1.34
16	G	1234	CLA	CHC-C1C	3.47	1.43	1.34
16	u	505	CLA	CHC-C1C	3.47	1.43	1.34
16	G	1225	CLA	CHC-C1C	3.47	1.43	1.34
16	X	514	CLA	CHC-C1C	3.47	1.43	1.34
16	b	1235	CLA	CHC-C1C	3.47	1.43	1.34
16	r	517	CLA	C1D-ND	3.47	1.42	1.37
16	Y	511	CLA	CHC-C1C	3.47	1.43	1.34
16	s	510	CLA	C1D-ND	3.47	1.42	1.37
16	Z	516	CLA	CHC-C1C	3.47	1.43	1.34
16	H	1106	CLA	CHC-C1C	3.47	1.43	1.34
16	Z	517	CLA	CHC-C1C	3.47	1.43	1.34
16	u	513	CLA	CHC-C1C	3.47	1.43	1.34
16	B	1205	CLA	C1D-ND	3.47	1.42	1.37
16	s	507	CLA	C1D-ND	3.47	1.42	1.37
16	n	514	CLA	CHC-C1C	3.47	1.43	1.34
16	G	1216	CLA	CHC-C1C	3.47	1.43	1.34
16	b	1203	CLA	CHC-C1C	3.47	1.43	1.34
16	G	1231	CLA	C1D-ND	3.47	1.42	1.37
16	A	1111	CLA	CHC-C1C	3.47	1.43	1.34
16	o	505	CLA	CHC-C1C	3.47	1.43	1.34
16	B	1234	CLA	CHC-C1C	3.47	1.43	1.34
16	s	514	CLA	CHC-C1C	3.47	1.43	1.34
16	q	516	CLA	CHC-C1C	3.47	1.43	1.34
16	h	508	CLA	CHC-C1C	3.46	1.43	1.34
16	J	1303	CLA	CHC-C1C	3.46	1.43	1.34
16	x	516	CLA	CHC-C1C	3.46	1.43	1.34
16	A	1121	CLA	CHC-C1C	3.46	1.43	1.34
16	W	514	CLA	CHC-C1C	3.46	1.43	1.34
16	Z	504	CLA	CHC-C1C	3.46	1.43	1.34
16	n	503	CLA	CHC-C1C	3.46	1.43	1.34
16	J	1302	CLA	CHC-C1C	3.46	1.43	1.34
16	H	1104	CLA	CHC-C1C	3.46	1.43	1.34
16	h	516	CLA	CHC-C1C	3.46	1.43	1.34
16	h	517	CLA	C1D-ND	3.46	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1231	CLA	CHC-C1C	3.46	1.43	1.34
16	q	504	CLA	C1D-ND	3.46	1.42	1.37
16	n	505	CLA	CHC-C1C	3.46	1.43	1.34
16	b	1224	CLA	CHC-C1C	3.46	1.43	1.34
16	g	517	CLA	CHC-C1C	3.46	1.43	1.34
16	W	505	CLA	CHC-C1C	3.46	1.43	1.34
16	X	511	CLA	CHC-C1C	3.46	1.43	1.34
16	n	516	CLA	C1D-ND	3.46	1.42	1.37
16	j	1303	CLA	C1D-ND	3.46	1.42	1.37
16	X	515	CLA	CHC-C1C	3.46	1.43	1.34
16	X	504	CLA	C1D-ND	3.46	1.42	1.37
16	W	517	CLA	CHC-C1C	3.46	1.43	1.34
16	p	511	CLA	CHC-C1C	3.46	1.43	1.34
16	x	501	CLA	CHC-C1C	3.46	1.43	1.34
16	n	517	CLA	CHC-C1C	3.46	1.43	1.34
16	u	517	CLA	CHC-C1C	3.46	1.43	1.34
16	s	511	CLA	CHC-C1C	3.46	1.43	1.34
16	H	1108	CLA	CHC-C1C	3.45	1.43	1.34
16	w	508	CLA	CHC-C1C	3.45	1.43	1.34
16	G	1231	CLA	CHC-C1C	3.45	1.43	1.34
16	h	513	CLA	CHC-C1C	3.45	1.43	1.34
16	W	509	CLA	CHC-C1C	3.45	1.43	1.34
16	q	511	CLA	CHC-C1C	3.45	1.43	1.34
16	j	1303	CLA	CHC-C1C	3.45	1.43	1.34
16	u	514	CLA	CHC-C1C	3.45	1.43	1.34
16	y	513	CLA	CHC-C1C	3.45	1.43	1.34
16	a	1119	CLA	CHC-C1C	3.45	1.43	1.34
16	q	517	CLA	CHC-C1C	3.45	1.43	1.34
16	W	515	CLA	C1D-ND	3.45	1.42	1.37
16	y	517	CLA	CHC-C1C	3.45	1.43	1.34
16	t	505	CLA	CHC-C1C	3.45	1.43	1.34
16	b	1213	CLA	CHC-C1C	3.45	1.43	1.34
16	n	515	CLA	C1D-ND	3.45	1.42	1.37
16	Z	508	CLA	CHC-C1C	3.45	1.43	1.34
16	t	503	CLA	C1D-ND	3.45	1.42	1.37
16	r	504	CLA	CHC-C1C	3.45	1.43	1.34
16	S	1303	CLA	CHC-C1C	3.45	1.43	1.34
16	t	517	CLA	CHC-C1C	3.45	1.43	1.34
16	b	1214	CLA	CHC-C1C	3.45	1.43	1.34
16	t	514	CLA	CHC-C1C	3.45	1.43	1.34
16	A	1108	CLA	CHC-C1C	3.45	1.43	1.34
16	H	1111	CLA	CHC-C1C	3.45	1.43	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	1231	CLA	CHC-C1C	3.45	1.43	1.34
16	U	1501	CLA	CHC-C1C	3.45	1.43	1.34
16	s	505	CLA	CHC-C1C	3.44	1.43	1.34
16	G	1214	CLA	CHC-C1C	3.44	1.43	1.34
16	X	509	CLA	CHC-C1C	3.44	1.43	1.34
16	X	510	CLA	C1D-ND	3.44	1.42	1.37
16	b	1023	CLA	CHC-C1C	3.44	1.43	1.34
16	S	1303	CLA	C1D-ND	3.44	1.42	1.37
16	H	1801	CLA	CHC-C1C	3.44	1.43	1.34
16	a	1130	CLA	CHC-C1C	3.44	1.43	1.34
16	b	1208	CLA	CHC-C1C	3.44	1.43	1.34
16	v	501	CLA	CHC-C1C	3.44	1.43	1.34
16	A	1101	CLA	CHC-C1C	3.44	1.43	1.34
16	a	1127	CLA	CHC-C1C	3.44	1.43	1.34
16	a	1134	CLA	CHC-C1C	3.44	1.43	1.34
16	x	517	CLA	C1D-ND	3.44	1.42	1.37
16	o	513	CLA	C1D-ND	3.44	1.42	1.37
16	Y	514	CLA	CHC-C1C	3.44	1.43	1.34
16	t	504	CLA	CHC-C1C	3.44	1.43	1.34
16	G	1221	CLA	CHC-C1C	3.44	1.43	1.34
16	g	515	CLA	CHC-C1C	3.44	1.43	1.34
16	n	516	CLA	CHC-C1C	3.44	1.43	1.34
16	k	4003	CLA	C1D-ND	3.44	1.42	1.37
16	r	513	CLA	CHC-C1C	3.44	1.43	1.34
16	G	1211	CLA	CHC-C1C	3.44	1.43	1.34
16	a	1104	CLA	CHC-C1C	3.44	1.43	1.34
16	q	505	CLA	CHC-C1C	3.44	1.43	1.34
16	l	1501	CLA	CHC-C1C	3.44	1.43	1.34
16	H	1121	CLA	CHC-C1C	3.44	1.43	1.34
16	j	1302	CLA	CHC-C1C	3.44	1.43	1.34
16	A	1013	CLA	CHC-C1C	3.44	1.43	1.34
16	Y	509	CLA	CHC-C1C	3.44	1.43	1.34
16	h	507	CLA	C1D-ND	3.43	1.42	1.37
16	n	508	CLA	CHC-C1C	3.43	1.43	1.34
16	a	1136	CLA	CHC-C1C	3.43	1.43	1.34
16	H	1130	CLA	CHC-C1C	3.43	1.43	1.34
16	G	1201	CLA	CHC-C1C	3.43	1.43	1.34
16	g	501	CLA	CHC-C1C	3.43	1.43	1.34
16	B	1012	CLA	C1D-ND	3.43	1.42	1.37
16	B	1228	CLA	CHC-C1C	3.43	1.43	1.34
16	p	516	CLA	CHC-C1C	3.43	1.43	1.34
16	w	504	CLA	CHC-C1C	3.43	1.43	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Z	505	CLA	CHC-C1C	3.43	1.43	1.34
16	h	504	CLA	CHC-C1C	3.43	1.43	1.34
16	t	508	CLA	CHC-C1C	3.43	1.43	1.34
16	p	515	CLA	CHC-C1C	3.43	1.43	1.34
16	g	516	CLA	CHC-C1C	3.43	1.43	1.34
16	y	514	CLA	CHC-C1C	3.43	1.43	1.34
16	l	1503	CLA	CHC-C1C	3.43	1.43	1.34
16	G	1228	CLA	CHC-C1C	3.43	1.43	1.34
16	A	1109	CLA	CHC-C1C	3.43	1.43	1.34
16	H	1110	CLA	CHC-C1C	3.43	1.43	1.34
16	o	515	CLA	CHC-C1C	3.43	1.43	1.34
16	o	510	CLA	C1D-ND	3.43	1.42	1.37
16	v	512	CLA	C1D-ND	3.43	1.42	1.37
16	B	1236	CLA	CHC-C1C	3.43	1.43	1.34
16	Z	514	CLA	CHC-C1C	3.43	1.43	1.34
16	y	502	CLA	CHC-C1C	3.43	1.43	1.34
16	A	1139	CLA	CHC-C1C	3.43	1.43	1.34
16	B	1227	CLA	CHC-C1C	3.43	1.43	1.34
16	r	516	CLA	CHC-C1C	3.43	1.43	1.34
16	s	516	CLA	CHC-C1C	3.43	1.43	1.34
16	v	513	CLA	CHC-C1C	3.43	1.43	1.34
16	G	1208	CLA	CHC-C1C	3.43	1.43	1.34
16	h	509	CLA	CHC-C1C	3.43	1.43	1.34
16	W	508	CLA	CHC-C1C	3.43	1.43	1.34
16	u	509	CLA	CHC-C1C	3.43	1.43	1.34
16	y	515	CLA	CHC-C1C	3.43	1.43	1.34
15	A	1011	CL0	CHC-C1C	3.42	1.43	1.34
16	Z	511	CLA	CHC-C1C	3.42	1.43	1.34
16	t	501	CLA	CHC-C1C	3.42	1.43	1.34
16	A	1134	CLA	C1D-ND	3.42	1.42	1.37
16	v	514	CLA	C1D-ND	3.42	1.42	1.37
16	H	1135	CLA	C1D-ND	3.42	1.42	1.37
16	Z	503	CLA	CHC-C1C	3.42	1.43	1.34
16	H	1140	CLA	CHC-C1C	3.42	1.43	1.34
16	a	1140	CLA	CHC-C1C	3.42	1.43	1.34
16	b	1219	CLA	CHC-C1C	3.42	1.43	1.34
16	g	504	CLA	CHC-C1C	3.42	1.43	1.34
16	A	1105	CLA	CHC-C1C	3.42	1.43	1.34
16	S	1302	CLA	CHC-C1C	3.42	1.43	1.34
16	v	517	CLA	CHC-C1C	3.42	1.43	1.34
16	a	1103	CLA	CHC-C1C	3.42	1.43	1.34
16	u	515	CLA	CHC-C1C	3.42	1.43	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	h	515	CLA	CHC-C1C	3.42	1.43	1.34
16	x	517	CLA	CHC-C1C	3.42	1.43	1.34
16	W	516	CLA	C1D-ND	3.42	1.42	1.37
16	u	517	CLA	C1D-ND	3.42	1.42	1.37
16	t	507	CLA	C1D-ND	3.42	1.42	1.37
16	a	1109	CLA	CHC-C1C	3.41	1.43	1.34
16	o	514	CLA	CHC-C1C	3.41	1.43	1.34
16	t	515	CLA	C1D-ND	3.41	1.42	1.37
15	H	1011	CL0	CHC-C1C	3.41	1.43	1.34
16	w	514	CLA	CHC-C1C	3.41	1.43	1.34
16	U	1503	CLA	C1D-ND	3.41	1.42	1.37
16	A	1124	CLA	CHC-C1C	3.41	1.43	1.34
16	v	514	CLA	CHC-C1C	3.41	1.43	1.34
16	v	510	CLA	C1D-ND	3.41	1.42	1.37
16	r	514	CLA	CHC-C1C	3.41	1.43	1.34
16	H	1116	CLA	CHC-C1C	3.41	1.43	1.34
16	n	504	CLA	CHC-C1C	3.41	1.43	1.34
16	X	516	CLA	CHC-C1C	3.41	1.43	1.34
16	b	1236	CLA	CHC-C1C	3.41	1.43	1.34
16	q	504	CLA	CHC-C1C	3.41	1.43	1.34
16	x	504	CLA	CHC-C1C	3.41	1.43	1.34
16	h	514	CLA	CHC-C1C	3.41	1.43	1.34
16	p	509	CLA	CHC-C1C	3.41	1.43	1.34
16	w	515	CLA	CHC-C1C	3.41	1.43	1.34
16	h	515	CLA	C1D-ND	3.41	1.42	1.37
16	w	504	CLA	C1D-ND	3.41	1.42	1.37
16	q	512	CLA	CHC-C1C	3.41	1.43	1.34
16	A	1110	CLA	CHC-C1C	3.41	1.42	1.34
16	B	1229	CLA	CHC-C1C	3.41	1.42	1.34
16	q	514	CLA	CHC-C1C	3.41	1.42	1.34
16	r	517	CLA	CHC-C1C	3.41	1.42	1.34
16	G	1213	CLA	CHC-C1C	3.41	1.42	1.34
16	h	512	CLA	CHC-C1C	3.41	1.42	1.34
16	o	509	CLA	CHC-C1C	3.41	1.42	1.34
16	r	501	CLA	CHC-C1C	3.41	1.42	1.34
16	h	517	CLA	CHC-C1C	3.41	1.42	1.34
16	Y	517	CLA	C1D-ND	3.41	1.42	1.37
16	r	510	CLA	C1D-ND	3.41	1.42	1.37
16	u	510	CLA	C1D-ND	3.41	1.42	1.37
16	h	507	CLA	CHC-C1C	3.40	1.42	1.34
16	v	506	CLA	C1D-ND	3.40	1.42	1.37
16	W	516	CLA	CHC-C1C	3.40	1.42	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	o	517	CLA	CHC-C1C	3.40	1.42	1.34
16	v	502	CLA	CHC-C1C	3.40	1.42	1.34
16	H	1103	CLA	CHC-C1C	3.40	1.42	1.34
16	r	505	CLA	CHC-C1C	3.40	1.42	1.34
16	r	515	CLA	CHC-C1C	3.40	1.42	1.34
16	a	1108	CLA	CHC-C1C	3.40	1.42	1.34
16	s	504	CLA	CHC-C1C	3.40	1.42	1.34
16	H	1136	CLA	CHC-C1C	3.40	1.42	1.34
16	X	512	CLA	CHC-C1C	3.40	1.42	1.34
16	W	501	CLA	CHC-C1C	3.40	1.42	1.34
16	y	507	CLA	CHC-C1C	3.40	1.42	1.34
16	H	1134	CLA	C1D-ND	3.40	1.42	1.37
16	A	1122	CLA	CHC-C1C	3.40	1.42	1.34
16	b	1209	CLA	CHC-C1C	3.40	1.42	1.34
16	p	508	CLA	CHC-C1C	3.40	1.42	1.34
16	B	1230	CLA	CHC-C1C	3.40	1.42	1.34
16	a	1115	CLA	CHC-C1C	3.40	1.42	1.34
16	b	1232	CLA	CHC-C1C	3.40	1.42	1.34
16	h	502	CLA	CHC-C1C	3.40	1.42	1.34
16	Q	1302	CLA	CHC-C1C	3.40	1.42	1.34
16	K	4003	CLA	C1D-ND	3.40	1.42	1.37
16	B	1220	CLA	CHC-C1C	3.40	1.42	1.34
16	F	1301	CLA	C1D-ND	3.40	1.42	1.37
16	u	513	CLA	C1D-ND	3.40	1.42	1.37
16	Y	505	CLA	CHC-C1C	3.40	1.42	1.34
16	h	501	CLA	C1D-ND	3.40	1.42	1.37
16	o	510	CLA	CHC-C1C	3.40	1.42	1.34
16	b	1234	CLA	C1D-ND	3.40	1.42	1.37
16	f	1301	CLA	C1D-ND	3.40	1.42	1.37
16	H	1109	CLA	CHC-C1C	3.40	1.42	1.34
16	B	1231	CLA	C1D-ND	3.40	1.42	1.37
16	q	501	CLA	CHC-C1C	3.40	1.42	1.34
16	x	513	CLA	CHC-C1C	3.40	1.42	1.34
16	b	1225	CLA	CHC-C1C	3.39	1.42	1.34
16	H	1123	CLA	CHC-C1C	3.39	1.42	1.34
16	n	501	CLA	CHC-C1C	3.39	1.42	1.34
16	X	507	CLA	C1D-ND	3.39	1.42	1.37
16	a	1121	CLA	CHC-C1C	3.39	1.42	1.34
16	y	515	CLA	C1D-ND	3.39	1.42	1.37
16	b	1229	CLA	CHC-C1C	3.39	1.42	1.34
16	v	507	CLA	CHC-C1C	3.39	1.42	1.34
16	b	1230	CLA	C1D-ND	3.39	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	t	516	CLA	CHC-C1C	3.39	1.42	1.34
16	g	510	CLA	CHC-C1C	3.39	1.42	1.34
16	g	514	CLA	CHC-C1C	3.39	1.42	1.34
16	q	510	CLA	C1D-ND	3.39	1.42	1.37
16	p	513	CLA	CHC-C1C	3.39	1.42	1.34
16	B	1223	CLA	C1D-ND	3.39	1.42	1.37
16	q	517	CLA	C1D-ND	3.39	1.42	1.37
16	W	504	CLA	CHC-C1C	3.39	1.42	1.34
16	H	1137	CLA	CHC-C1C	3.39	1.42	1.34
16	w	505	CLA	CHC-C1C	3.39	1.42	1.34
16	a	1110	CLA	CHC-C1C	3.39	1.42	1.34
16	b	1206	CLA	CHC-C1C	3.39	1.42	1.34
16	b	1217	CLA	CHC-C1C	3.39	1.42	1.34
16	W	507	CLA	C1D-ND	3.39	1.42	1.37
16	w	516	CLA	C1D-ND	3.39	1.42	1.37
16	s	517	CLA	C1D-ND	3.39	1.42	1.37
16	a	1137	CLA	CHC-C1C	3.39	1.42	1.34
16	v	516	CLA	CHC-C1C	3.39	1.42	1.34
16	Z	501	CLA	CHC-C1C	3.38	1.42	1.34
16	a	1125	CLA	CHC-C1C	3.38	1.42	1.34
16	y	507	CLA	C1D-ND	3.38	1.42	1.37
16	A	1104	CLA	CHC-C1C	3.38	1.42	1.34
16	X	508	CLA	CHC-C1C	3.38	1.42	1.34
16	a	1132	CLA	CHC-C1C	3.38	1.42	1.34
16	A	1131	CLA	CHC-C1C	3.38	1.42	1.34
16	f	1301	CLA	CHC-C1C	3.38	1.42	1.34
16	x	515	CLA	CHC-C1C	3.38	1.42	1.34
16	A	1138	CLA	CHC-C1C	3.38	1.42	1.34
16	n	513	CLA	CHC-C1C	3.38	1.42	1.34
16	u	508	CLA	CHC-C1C	3.38	1.42	1.34
16	w	516	CLA	CHC-C1C	3.38	1.42	1.34
16	B	1208	CLA	CHC-C1C	3.38	1.42	1.34
16	B	1217	CLA	C1D-ND	3.38	1.42	1.37
16	G	1219	CLA	C1D-ND	3.38	1.42	1.37
16	b	1228	CLA	CHC-C1C	3.38	1.42	1.34
16	r	513	CLA	C1D-ND	3.38	1.42	1.37
16	A	1140	CLA	CHC-C1C	3.38	1.42	1.34
16	s	508	CLA	CHC-C1C	3.38	1.42	1.34
16	p	505	CLA	CHC-C1C	3.38	1.42	1.34
16	Y	504	CLA	CHC-C1C	3.38	1.42	1.34
16	n	515	CLA	CHC-C1C	3.38	1.42	1.34
16	v	505	CLA	C1D-ND	3.38	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	y	512	CLA	CHC-C1C	3.38	1.42	1.34
16	g	508	CLA	CHC-C1C	3.38	1.42	1.34
16	x	501	CLA	C1D-ND	3.38	1.42	1.37
16	o	508	CLA	CHC-C1C	3.38	1.42	1.34
16	q	503	CLA	CHC-C1C	3.38	1.42	1.34
16	H	1122	CLA	C1D-ND	3.38	1.42	1.37
16	H	1122	CLA	CHC-C1C	3.38	1.42	1.34
16	a	1116	CLA	CHC-C1C	3.38	1.42	1.34
16	y	508	CLA	CHC-C1C	3.37	1.42	1.34
16	n	507	CLA	C1D-ND	3.37	1.42	1.37
16	o	517	CLA	C1D-ND	3.37	1.42	1.37
16	Z	510	CLA	CHC-C1C	3.37	1.42	1.34
16	s	509	CLA	CHC-C1C	3.37	1.42	1.34
16	x	508	CLA	CHC-C1C	3.37	1.42	1.34
16	Z	510	CLA	C1D-ND	3.37	1.42	1.37
16	a	1122	CLA	CHC-C1C	3.37	1.42	1.34
16	A	1115	CLA	CHC-C1C	3.37	1.42	1.34
16	G	1240	CLA	CHC-C1C	3.37	1.42	1.34
16	v	515	CLA	CHC-C1C	3.37	1.42	1.34
16	H	1125	CLA	CHC-C1C	3.37	1.42	1.34
16	B	1217	CLA	CHC-C1C	3.37	1.42	1.34
16	x	502	CLA	CHC-C1C	3.37	1.42	1.34
16	a	1111	CLA	CHC-C1C	3.37	1.42	1.34
16	t	513	CLA	C1D-ND	3.37	1.42	1.37
16	X	517	CLA	CHC-C1C	3.37	1.42	1.34
16	G	1209	CLA	CHC-C1C	3.37	1.42	1.34
16	Q	1301	CLA	C1D-ND	3.37	1.42	1.37
16	h	514	CLA	C1D-ND	3.37	1.42	1.37
16	v	501	CLA	C1D-ND	3.37	1.42	1.37
16	w	513	CLA	CHC-C1C	3.37	1.42	1.34
16	T	4003	CLA	CHC-C1C	3.37	1.42	1.34
16	G	1240	CLA	C1D-ND	3.37	1.42	1.37
16	A	1103	CLA	CHC-C1C	3.37	1.42	1.34
16	B	1214	CLA	CHC-C1C	3.37	1.42	1.34
16	s	513	CLA	CHC-C1C	3.37	1.42	1.34
16	x	514	CLA	CHC-C1C	3.37	1.42	1.34
16	p	504	CLA	CHC-C1C	3.37	1.42	1.34
16	u	504	CLA	CHC-C1C	3.37	1.42	1.34
16	G	1232	CLA	C1D-ND	3.37	1.42	1.37
16	b	1224	CLA	C1D-ND	3.37	1.42	1.37
16	o	513	CLA	CHC-C1C	3.37	1.42	1.34
16	l	1503	CLA	C1D-ND	3.36	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1220	CLA	CHC-C1C	3.36	1.42	1.34
16	H	1131	CLA	CHC-C1C	3.36	1.42	1.34
16	K	4004	CLA	C1D-ND	3.36	1.42	1.37
16	h	513	CLA	C1D-ND	3.36	1.42	1.37
16	B	1206	CLA	CHC-C1C	3.36	1.42	1.34
16	t	515	CLA	CHC-C1C	3.36	1.42	1.34
16	F	1302	CLA	C1D-ND	3.36	1.42	1.37
16	Z	512	CLA	CHC-C1C	3.36	1.42	1.34
16	Y	508	CLA	CHC-C1C	3.36	1.42	1.34
16	p	517	CLA	CHC-C1C	3.36	1.42	1.34
16	Y	516	CLA	CHC-C1C	3.36	1.42	1.34
16	q	513	CLA	C1D-ND	3.36	1.42	1.37
16	x	513	CLA	C1D-ND	3.36	1.42	1.37
16	H	1113	CLA	CHC-C1C	3.36	1.42	1.34
16	K	4003	CLA	CHC-C1C	3.36	1.42	1.34
16	q	502	CLA	CHC-C1C	3.36	1.42	1.34
16	A	1137	CLA	CHC-C1C	3.36	1.42	1.34
16	b	1231	CLA	C1D-ND	3.36	1.42	1.37
16	w	507	CLA	C1D-ND	3.36	1.42	1.37
16	a	1123	CLA	CHC-C1C	3.36	1.42	1.34
16	u	501	CLA	CHC-C1C	3.36	1.42	1.34
16	s	501	CLA	CHC-C1C	3.36	1.42	1.34
16	B	1209	CLA	C1D-ND	3.36	1.42	1.37
16	B	1204	CLA	CHC-C1C	3.36	1.42	1.34
16	r	508	CLA	CHC-C1C	3.36	1.42	1.34
16	A	1137	CLA	C1D-ND	3.36	1.42	1.37
16	b	1229	CLA	C1D-ND	3.36	1.42	1.37
16	t	516	CLA	C1D-ND	3.36	1.42	1.37
16	w	512	CLA	CHC-C1C	3.36	1.42	1.34
16	B	1201	CLA	CHC-C1C	3.36	1.42	1.34
16	Y	512	CLA	CHC-C1C	3.36	1.42	1.34
16	b	1240	CLA	C1D-ND	3.36	1.42	1.37
16	j	1302	CLA	C1D-ND	3.36	1.42	1.37
16	Y	513	CLA	CHC-C1C	3.36	1.42	1.34
16	t	512	CLA	CHC-C1C	3.36	1.42	1.34
16	A	1123	CLA	CHC-C1C	3.36	1.42	1.34
16	t	511	CLA	C1D-ND	3.36	1.42	1.37
16	o	501	CLA	CHC-C1C	3.35	1.42	1.34
16	W	512	CLA	CHC-C1C	3.35	1.42	1.34
16	g	505	CLA	CHC-C1C	3.35	1.42	1.34
16	Z	502	CLA	CHC-C1C	3.35	1.42	1.34
16	v	512	CLA	CHC-C1C	3.35	1.42	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	y	509	CLA	CHC-C1C	3.35	1.42	1.34
16	Y	517	CLA	CHC-C1C	3.35	1.42	1.34
16	b	1240	CLA	CHC-C1C	3.35	1.42	1.34
16	B	1209	CLA	CHC-C1C	3.35	1.42	1.34
16	H	1114	CLA	CHC-C1C	3.35	1.42	1.34
16	Z	513	CLA	CHC-C1C	3.35	1.42	1.34
16	G	1204	CLA	CHC-C1C	3.35	1.42	1.34
16	H	1132	CLA	CHC-C1C	3.35	1.42	1.34
16	A	1801	CLA	CHC-C1C	3.35	1.42	1.34
16	H	1103	CLA	C1D-ND	3.35	1.42	1.37
16	A	1114	CLA	CHC-C1C	3.35	1.42	1.34
16	p	507	CLA	CHC-C1C	3.35	1.42	1.34
16	G	1217	CLA	C1D-ND	3.35	1.42	1.37
16	W	509	CLA	C1D-ND	3.35	1.42	1.37
16	o	507	CLA	C1D-ND	3.35	1.42	1.37
16	U	1502	CLA	CHC-C1C	3.35	1.42	1.34
16	w	501	CLA	CHC-C1C	3.35	1.42	1.34
16	g	501	CLA	C1D-ND	3.35	1.42	1.37
16	Z	515	CLA	CHC-C1C	3.35	1.42	1.34
16	H	1138	CLA	CHC-C1C	3.35	1.42	1.34
16	g	516	CLA	C1D-ND	3.35	1.42	1.37
16	k	4003	CLA	CHC-C1C	3.35	1.42	1.34
16	b	1205	CLA	C1D-ND	3.35	1.42	1.37
16	a	1133	CLA	CHC-C1C	3.34	1.42	1.34
16	l	1502	CLA	CHC-C1C	3.34	1.42	1.34
16	p	501	CLA	CHC-C1C	3.34	1.42	1.34
16	B	1240	CLA	C1D-ND	3.34	1.42	1.37
16	X	507	CLA	CHC-C1C	3.34	1.42	1.34
16	y	510	CLA	CHC-C1C	3.34	1.42	1.34
16	A	1107	CLA	CHC-C1C	3.34	1.42	1.34
16	u	507	CLA	CHC-C1C	3.34	1.42	1.34
16	L	1503	CLA	C1D-ND	3.34	1.42	1.37
16	o	504	CLA	C1D-ND	3.34	1.42	1.37
16	G	1236	CLA	CHC-C1C	3.34	1.42	1.34
16	b	1012	CLA	C1D-ND	3.34	1.42	1.37
16	h	516	CLA	C1D-ND	3.34	1.42	1.37
16	B	1218	CLA	CHC-C1C	3.34	1.42	1.34
16	H	1112	CLA	CHC-C1C	3.34	1.42	1.34
16	b	1021	CLA	CHC-C1C	3.34	1.42	1.34
16	a	1112	CLA	CHC-C1C	3.34	1.42	1.34
16	u	501	CLA	C1D-ND	3.34	1.42	1.37
16	A	1120	CLA	CHC-C1C	3.34	1.42	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	515	CLA	CHC-C1C	3.34	1.42	1.34
16	x	512	CLA	CHC-C1C	3.34	1.42	1.34
16	L	1502	CLA	CHC-C1C	3.34	1.42	1.34
16	H	1118	CLA	C1D-ND	3.34	1.42	1.37
16	B	1224	CLA	CHC-C1C	3.34	1.42	1.34
16	g	513	CLA	CHC-C1C	3.34	1.42	1.34
16	a	1131	CLA	CHC-C1C	3.34	1.42	1.34
16	q	513	CLA	CHC-C1C	3.34	1.42	1.34
16	a	1138	CLA	CHC-C1C	3.34	1.42	1.34
16	J	1302	CLA	C1D-ND	3.34	1.42	1.37
16	G	1230	CLA	C1D-ND	3.34	1.42	1.37
16	b	1238	CLA	C1D-ND	3.34	1.42	1.37
16	v	513	CLA	C1D-ND	3.34	1.42	1.37
16	v	506	CLA	CHC-C1C	3.34	1.42	1.34
16	K	4004	CLA	CHC-C1C	3.33	1.42	1.34
16	q	515	CLA	CHC-C1C	3.33	1.42	1.34
16	A	1112	CLA	CHC-C1C	3.33	1.42	1.34
16	A	1133	CLA	CHC-C1C	3.33	1.42	1.34
16	F	1301	CLA	CHC-C1C	3.33	1.42	1.34
16	g	502	CLA	CHC-C1C	3.33	1.42	1.34
16	h	505	CLA	C1D-ND	3.33	1.42	1.37
16	A	1122	CLA	C1D-ND	3.33	1.42	1.37
16	W	513	CLA	C1D-ND	3.33	1.42	1.37
16	G	1218	CLA	CHC-C1C	3.33	1.42	1.34
16	H	1115	CLA	CHC-C1C	3.33	1.42	1.34
16	U	1503	CLA	CHC-C1C	3.33	1.42	1.34
16	T	4002	CLA	CHC-C1C	3.33	1.42	1.34
16	T	4003	CLA	C1D-ND	3.33	1.42	1.37
16	H	1124	CLA	CHC-C1C	3.33	1.42	1.34
16	X	513	CLA	C1D-ND	3.33	1.42	1.37
16	Z	506	CLA	C1D-ND	3.33	1.42	1.37
15	a	1011	CL0	CHC-C1C	3.33	1.42	1.34
16	y	505	CLA	C1D-ND	3.33	1.42	1.37
16	B	1224	CLA	C1D-ND	3.33	1.42	1.37
16	x	510	CLA	C1D-ND	3.32	1.42	1.37
16	y	506	CLA	C1D-ND	3.32	1.42	1.37
16	B	1238	CLA	CHC-C1C	3.32	1.42	1.34
16	A	1112	CLA	C1D-ND	3.32	1.42	1.37
16	w	505	CLA	C1D-ND	3.32	1.42	1.37
16	h	506	CLA	CHC-C1C	3.32	1.42	1.34
16	y	506	CLA	CHC-C1C	3.32	1.42	1.34
16	o	512	CLA	CHC-C1C	3.32	1.42	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	1209	CLA	C1D-ND	3.32	1.42	1.37
16	n	507	CLA	CHC-C1C	3.32	1.42	1.34
16	K	4002	CLA	C1D-ND	3.32	1.42	1.37
16	S	1302	CLA	C1D-ND	3.32	1.42	1.37
16	W	503	CLA	C1D-ND	3.32	1.42	1.37
16	A	1132	CLA	CHC-C1C	3.32	1.42	1.34
16	b	1201	CLA	CHC-C1C	3.32	1.42	1.34
16	o	501	CLA	C1D-ND	3.32	1.42	1.37
16	o	505	CLA	C1D-ND	3.32	1.42	1.37
16	w	510	CLA	C1D-ND	3.32	1.42	1.37
16	w	502	CLA	CHC-C1C	3.32	1.42	1.34
16	A	1113	CLA	CHC-C1C	3.32	1.42	1.34
16	B	1202	CLA	C1D-ND	3.32	1.42	1.37
16	G	1209	CLA	C1D-ND	3.32	1.42	1.37
16	k	4002	CLA	C1D-ND	3.31	1.42	1.37
16	t	506	CLA	C1D-ND	3.31	1.42	1.37
16	w	507	CLA	CHC-C1C	3.31	1.42	1.34
16	b	1223	CLA	C1D-ND	3.31	1.42	1.37
16	v	503	CLA	C1D-ND	3.31	1.42	1.37
16	G	1230	CLA	CHC-C1C	3.31	1.42	1.34
16	r	502	CLA	CHC-C1C	3.31	1.42	1.34
16	A	1113	CLA	C1D-ND	3.31	1.42	1.37
16	B	1212	CLA	C1D-ND	3.31	1.42	1.37
16	a	1114	CLA	C1D-ND	3.31	1.42	1.37
16	T	4004	CLA	CHC-C1C	3.31	1.42	1.34
16	Y	507	CLA	CHC-C1C	3.31	1.42	1.34
16	b	1207	CLA	CHC-C1C	3.31	1.42	1.34
16	A	1118	CLA	C1D-ND	3.31	1.42	1.37
16	r	510	CLA	CHC-C1C	3.31	1.42	1.34
16	t	507	CLA	CHC-C1C	3.31	1.42	1.34
16	x	510	CLA	CHC-C1C	3.31	1.42	1.34
16	b	1228	CLA	C1D-ND	3.31	1.42	1.37
16	u	503	CLA	C1D-ND	3.31	1.42	1.37
16	b	1223	CLA	CHC-C1C	3.31	1.42	1.34
16	o	504	CLA	CHC-C1C	3.31	1.42	1.34
16	y	501	CLA	C1D-ND	3.31	1.42	1.37
16	a	1120	CLA	CHC-C1C	3.31	1.42	1.34
16	H	1101	CLA	C1D-ND	3.31	1.42	1.37
16	H	1111	CLA	C1D-ND	3.31	1.42	1.37
16	Y	501	CLA	CHC-C1C	3.31	1.42	1.34
16	X	501	CLA	CHC-C1C	3.31	1.42	1.34
16	Y	501	CLA	C1D-ND	3.31	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1113	CLA	C1D-ND	3.31	1.42	1.37
16	W	507	CLA	CHC-C1C	3.31	1.42	1.34
16	u	510	CLA	CHC-C1C	3.31	1.42	1.34
16	a	1801	CLA	CHC-C1C	3.31	1.42	1.34
16	X	501	CLA	C1D-ND	3.31	1.42	1.37
16	a	1113	CLA	CHC-C1C	3.30	1.42	1.34
16	n	503	CLA	C1D-ND	3.30	1.42	1.37
16	b	1218	CLA	CHC-C1C	3.30	1.42	1.34
16	u	502	CLA	CHC-C1C	3.30	1.42	1.34
16	h	510	CLA	CHC-C1C	3.30	1.42	1.34
16	H	1112	CLA	C1D-ND	3.30	1.42	1.37
16	X	513	CLA	CHC-C1C	3.30	1.42	1.34
16	b	1204	CLA	CHC-C1C	3.30	1.42	1.34
16	r	507	CLA	CHC-C1C	3.30	1.42	1.34
16	a	1111	CLA	C1D-ND	3.30	1.42	1.37
16	K	4002	CLA	CHC-C1C	3.30	1.42	1.34
16	s	512	CLA	CHC-C1C	3.30	1.42	1.34
16	a	1112	CLA	C1D-ND	3.30	1.42	1.37
16	x	506	CLA	CHC-C1C	3.30	1.42	1.34
16	a	1107	CLA	CHC-C1C	3.30	1.42	1.34
16	k	4004	CLA	C1D-ND	3.30	1.42	1.37
16	v	516	CLA	C1D-ND	3.30	1.42	1.37
16	q	507	CLA	CHC-C1C	3.30	1.42	1.34
16	k	4004	CLA	CHC-C1C	3.30	1.42	1.34
16	B	1232	CLA	CHC-C1C	3.30	1.42	1.34
16	H	1120	CLA	CHC-C1C	3.30	1.42	1.34
16	Q	1301	CLA	CHC-C1C	3.30	1.42	1.34
16	r	511	CLA	C1D-ND	3.29	1.42	1.37
16	B	1203	CLA	CHC-C1C	3.29	1.42	1.34
16	H	1133	CLA	CHC-C1C	3.29	1.42	1.34
16	B	1240	CLA	CHC-C1C	3.29	1.42	1.34
16	T	4004	CLA	C1D-ND	3.29	1.42	1.37
16	Z	504	CLA	C1D-ND	3.29	1.42	1.37
16	a	1022	CLA	C1D-ND	3.29	1.42	1.37
16	B	1219	CLA	C1D-ND	3.29	1.42	1.37
16	r	515	CLA	C1D-ND	3.29	1.42	1.37
16	x	504	CLA	C1D-ND	3.29	1.42	1.37
16	r	501	CLA	C1D-ND	3.29	1.42	1.37
16	q	501	CLA	C1D-ND	3.29	1.42	1.37
16	k	4002	CLA	CHC-C1C	3.29	1.42	1.34
16	A	1118	CLA	CHC-C1C	3.29	1.42	1.34
16	r	512	CLA	CHC-C1C	3.29	1.42	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	510	CLA	CHC-C1C	3.29	1.42	1.34
16	q	510	CLA	CHC-C1C	3.29	1.42	1.34
16	B	1228	CLA	C1D-ND	3.29	1.42	1.37
16	A	1136	CLA	CHC-C1C	3.29	1.42	1.34
16	H	1113	CLA	C1D-ND	3.29	1.42	1.37
16	a	1114	CLA	CHC-C1C	3.29	1.42	1.34
16	a	1124	CLA	CHC-C1C	3.29	1.42	1.34
16	v	510	CLA	CHC-C1C	3.28	1.42	1.34
16	G	1223	CLA	CHC-C1C	3.28	1.42	1.34
16	G	1232	CLA	CHC-C1C	3.28	1.42	1.34
16	s	507	CLA	CHC-C1C	3.28	1.42	1.34
16	n	512	CLA	CHC-C1C	3.28	1.42	1.34
16	B	1210	CLA	C1D-ND	3.28	1.42	1.37
16	r	508	CLA	C1D-ND	3.28	1.42	1.37
16	n	502	CLA	CHC-C1C	3.28	1.42	1.34
16	b	1204	CLA	C1D-ND	3.28	1.42	1.37
16	r	516	CLA	C1D-ND	3.28	1.42	1.37
16	r	504	CLA	C1D-ND	3.28	1.42	1.37
16	h	503	CLA	C1D-ND	3.28	1.42	1.37
16	y	508	CLA	C1D-ND	3.28	1.42	1.37
16	G	1238	CLA	CHC-C1C	3.28	1.42	1.34
16	B	1021	CLA	CHC-C1C	3.28	1.42	1.34
16	g	510	CLA	C1D-ND	3.28	1.42	1.37
16	q	507	CLA	C1D-ND	3.28	1.42	1.37
16	U	1501	CLA	C1D-ND	3.28	1.42	1.37
16	n	504	CLA	C1D-ND	3.28	1.42	1.37
16	y	514	CLA	C1D-ND	3.28	1.42	1.37
16	p	512	CLA	CHC-C1C	3.28	1.42	1.34
16	p	517	CLA	C1D-ND	3.28	1.42	1.37
16	x	507	CLA	C1D-ND	3.28	1.42	1.37
16	a	1122	CLA	C1D-ND	3.27	1.42	1.37
16	G	1217	CLA	CHC-C1C	3.27	1.42	1.34
16	t	509	CLA	C1D-ND	3.27	1.42	1.37
16	Z	505	CLA	C1D-ND	3.27	1.42	1.37
16	A	1123	CLA	C1D-ND	3.27	1.42	1.37
16	A	1132	CLA	C1D-ND	3.27	1.42	1.37
16	B	1230	CLA	C1D-ND	3.27	1.42	1.37
16	n	512	CLA	C1D-ND	3.27	1.42	1.37
16	X	504	CLA	CHC-C1C	3.27	1.42	1.34
16	A	1101	CLA	C1D-ND	3.27	1.42	1.37
16	G	1021	CLA	CHC-C1C	3.27	1.42	1.34
16	a	1128	CLA	CHC-C1C	3.27	1.42	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1118	CLA	CHC-C1C	3.27	1.42	1.34
16	B	1207	CLA	CHC-C1C	3.27	1.42	1.34
16	r	512	CLA	C1D-ND	3.27	1.42	1.37
16	H	1022	CLA	CHC-C1C	3.27	1.42	1.34
16	b	1230	CLA	CHC-C1C	3.27	1.42	1.34
16	u	512	CLA	CHC-C1C	3.27	1.42	1.34
16	u	507	CLA	C1D-ND	3.27	1.42	1.37
16	a	1022	CLA	CHC-C1C	3.27	1.42	1.34
16	G	1215	CLA	CHC-C1C	3.27	1.42	1.34
16	r	505	CLA	C1D-ND	3.27	1.42	1.37
16	A	1130	CLA	C1D-ND	3.26	1.42	1.37
16	p	514	CLA	C1D-ND	3.26	1.42	1.37
16	W	502	CLA	CHC-C1C	3.26	1.42	1.34
16	b	1238	CLA	CHC-C1C	3.26	1.42	1.34
16	p	510	CLA	CHC-C1C	3.26	1.42	1.34
16	h	512	CLA	C1D-ND	3.26	1.42	1.37
16	s	512	CLA	C1D-ND	3.26	1.42	1.37
16	t	502	CLA	CHC-C1C	3.26	1.42	1.34
16	B	1201	CLA	C1D-ND	3.26	1.42	1.37
16	b	1201	CLA	C1D-ND	3.26	1.42	1.37
16	B	1215	CLA	CHC-C1C	3.26	1.42	1.34
16	A	1107	CLA	C1D-ND	3.26	1.42	1.37
16	X	505	CLA	C1D-ND	3.26	1.42	1.37
16	g	507	CLA	C1D-ND	3.26	1.42	1.37
16	H	1107	CLA	CHC-C1C	3.26	1.42	1.34
16	G	1238	CLA	C1D-ND	3.26	1.42	1.37
16	W	517	CLA	C1D-ND	3.26	1.42	1.37
16	Z	508	CLA	C1D-ND	3.26	1.42	1.37
16	B	1238	CLA	C1D-ND	3.26	1.42	1.37
16	Z	512	CLA	C1D-ND	3.26	1.42	1.37
16	b	1219	CLA	C1D-ND	3.26	1.42	1.37
16	Y	510	CLA	CHC-C1C	3.26	1.42	1.34
16	G	1201	CLA	C1D-ND	3.26	1.42	1.37
16	G	1224	CLA	C1D-ND	3.26	1.42	1.37
16	a	1130	CLA	C1D-ND	3.26	1.42	1.37
16	b	1217	CLA	C1D-ND	3.26	1.42	1.37
16	Z	507	CLA	C1D-ND	3.25	1.42	1.37
16	Z	515	CLA	C1D-ND	3.25	1.42	1.37
16	Z	513	CLA	C1D-ND	3.25	1.42	1.37
16	n	501	CLA	C1D-ND	3.25	1.42	1.37
16	o	502	CLA	CHC-C1C	3.25	1.42	1.34
16	W	501	CLA	C1D-ND	3.25	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1123	CLA	C1D-ND	3.25	1.42	1.37
16	s	513	CLA	C1D-ND	3.25	1.42	1.37
16	w	503	CLA	CHC-C1C	3.25	1.42	1.34
16	p	505	CLA	C1D-ND	3.25	1.42	1.37
16	b	1216	CLA	C1D-ND	3.25	1.42	1.37
16	W	506	CLA	C1D-ND	3.25	1.42	1.37
16	G	1213	CLA	C1D-ND	3.25	1.42	1.37
16	y	503	CLA	C1D-ND	3.25	1.42	1.37
16	h	508	CLA	C1D-ND	3.25	1.42	1.37
16	A	1135	CLA	CHC-C1C	3.25	1.42	1.34
16	Y	508	CLA	C1D-ND	3.25	1.42	1.37
16	v	507	CLA	C1D-ND	3.25	1.42	1.37
16	G	1226	CLA	CHC-C1C	3.25	1.42	1.34
16	T	4002	CLA	C1D-ND	3.25	1.42	1.37
16	a	1135	CLA	CHC-C1C	3.25	1.42	1.34
16	b	1226	CLA	CHC-C1C	3.25	1.42	1.34
16	p	502	CLA	CHC-C1C	3.25	1.42	1.34
16	B	1232	CLA	C1D-ND	3.25	1.42	1.37
16	L	1501	CLA	C1D-ND	3.25	1.42	1.37
16	u	505	CLA	C1D-ND	3.25	1.42	1.37
16	u	506	CLA	CHC-C1C	3.24	1.42	1.34
16	G	1235	CLA	C1D-ND	3.24	1.42	1.37
16	a	1137	CLA	C1D-ND	3.24	1.42	1.37
16	b	1216	CLA	CHC-C1C	3.24	1.42	1.34
16	X	502	CLA	CHC-C1C	3.24	1.42	1.34
16	G	1228	CLA	C1D-ND	3.24	1.42	1.37
16	G	1207	CLA	CHC-C1C	3.24	1.42	1.34
16	s	503	CLA	C1D-ND	3.24	1.42	1.37
16	x	507	CLA	CHC-C1C	3.24	1.42	1.34
16	o	507	CLA	CHC-C1C	3.24	1.42	1.34
16	a	1118	CLA	C1D-ND	3.24	1.42	1.37
16	p	515	CLA	C1D-ND	3.24	1.42	1.37
16	v	511	CLA	C1D-ND	3.24	1.42	1.37
16	r	506	CLA	C1D-ND	3.24	1.42	1.37
16	s	506	CLA	CHC-C1C	3.24	1.42	1.34
16	b	1210	CLA	C1D-ND	3.24	1.42	1.37
16	b	1235	CLA	C1D-ND	3.24	1.42	1.37
16	n	509	CLA	C1D-ND	3.24	1.42	1.37
16	n	506	CLA	C1D-ND	3.24	1.42	1.37
16	n	517	CLA	C1D-ND	3.24	1.42	1.37
16	H	1118	CLA	CHC-C1C	3.24	1.42	1.34
16	t	501	CLA	C1D-ND	3.24	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	w	514	CLA	C1D-ND	3.24	1.42	1.37
16	B	1223	CLA	CHC-C1C	3.23	1.42	1.34
16	t	506	CLA	CHC-C1C	3.23	1.42	1.34
16	G	1207	CLA	C1D-ND	3.23	1.42	1.37
16	H	1130	CLA	C1D-ND	3.23	1.42	1.37
16	B	1204	CLA	C1D-ND	3.23	1.42	1.37
16	p	513	CLA	C1D-ND	3.23	1.42	1.37
16	W	512	CLA	C1D-ND	3.23	1.42	1.37
16	A	1022	CLA	CHC-C1C	3.23	1.42	1.34
16	p	512	CLA	C1D-ND	3.23	1.42	1.37
16	s	510	CLA	CHC-C1C	3.23	1.42	1.34
16	t	510	CLA	CHC-C1C	3.23	1.42	1.34
16	p	508	CLA	C1D-ND	3.23	1.42	1.37
16	q	516	CLA	C1D-ND	3.23	1.42	1.37
16	A	1138	CLA	C1D-ND	3.23	1.42	1.37
16	a	1132	CLA	C1D-ND	3.23	1.42	1.37
16	a	1801	CLA	C1D-ND	3.23	1.42	1.37
16	r	507	CLA	C1D-ND	3.23	1.42	1.37
16	y	512	CLA	C1D-ND	3.23	1.42	1.37
16	n	505	CLA	C1D-ND	3.23	1.42	1.37
16	t	517	CLA	C1D-ND	3.23	1.42	1.37
16	g	507	CLA	CHC-C1C	3.23	1.42	1.34
16	q	511	CLA	C1D-ND	3.22	1.42	1.37
16	G	1206	CLA	CHC-C1C	3.22	1.42	1.34
16	B	1220	CLA	C1D-ND	3.22	1.42	1.37
16	H	1132	CLA	C1D-ND	3.22	1.42	1.37
16	t	504	CLA	C1D-ND	3.22	1.42	1.37
16	x	508	CLA	C1D-ND	3.22	1.42	1.37
16	Z	517	CLA	C1D-ND	3.22	1.42	1.37
16	p	509	CLA	C1D-ND	3.22	1.42	1.37
16	n	511	CLA	C1D-ND	3.22	1.42	1.37
16	H	1128	CLA	CHC-C1C	3.22	1.42	1.34
16	A	1114	CLA	C1D-ND	3.22	1.42	1.37
16	w	510	CLA	CHC-C1C	3.22	1.42	1.34
16	h	509	CLA	C1D-ND	3.21	1.42	1.37
16	G	1205	CLA	CHC-C1C	3.21	1.42	1.34
16	Z	507	CLA	CHC-C1C	3.21	1.42	1.34
16	G	1208	CLA	C1D-ND	3.21	1.42	1.37
16	s	516	CLA	C1D-ND	3.21	1.42	1.37
16	A	1129	CLA	C1D-ND	3.21	1.42	1.37
16	a	1133	CLA	C1D-ND	3.21	1.42	1.37
16	p	516	CLA	C1D-ND	3.21	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1135	CLA	CHC-C1C	3.21	1.42	1.34
16	W	505	CLA	C1D-ND	3.21	1.42	1.37
16	y	504	CLA	C1D-ND	3.21	1.42	1.37
16	b	1212	CLA	C1D-ND	3.21	1.42	1.37
16	X	517	CLA	C1D-ND	3.21	1.42	1.37
16	l	1501	CLA	C1D-ND	3.21	1.42	1.37
16	b	1215	CLA	CHC-C1C	3.21	1.42	1.34
16	A	1103	CLA	C1D-ND	3.21	1.42	1.37
16	g	515	CLA	C1D-ND	3.21	1.42	1.37
16	X	516	CLA	C1D-ND	3.20	1.42	1.37
16	g	512	CLA	CHC-C1C	3.20	1.42	1.34
16	a	1237	CLA	CHC-C1C	3.20	1.42	1.34
16	Y	516	CLA	C1D-ND	3.20	1.42	1.37
16	b	1207	CLA	C1D-ND	3.20	1.42	1.37
16	u	514	CLA	C1D-ND	3.20	1.42	1.37
16	G	1224	CLA	CHC-C1C	3.20	1.42	1.34
16	q	508	CLA	C1D-ND	3.20	1.42	1.37
16	b	1232	CLA	C1D-ND	3.20	1.42	1.37
16	t	514	CLA	C1D-ND	3.20	1.42	1.37
16	w	517	CLA	C1D-ND	3.20	1.42	1.37
16	A	1120	CLA	C1D-ND	3.20	1.42	1.37
16	y	516	CLA	C1D-ND	3.20	1.42	1.37
16	q	506	CLA	C1D-ND	3.20	1.42	1.37
16	Z	501	CLA	C1D-ND	3.20	1.42	1.37
16	A	1136	CLA	C1D-ND	3.20	1.42	1.37
16	b	1239	CLA	C1D-ND	3.20	1.42	1.37
16	n	506	CLA	CHC-C1C	3.19	1.42	1.34
16	o	516	CLA	C1D-ND	3.19	1.42	1.37
16	o	506	CLA	CHC-C1C	3.19	1.42	1.34
16	q	515	CLA	C1D-ND	3.19	1.42	1.37
16	y	511	CLA	C1D-ND	3.19	1.42	1.37
16	Y	502	CLA	CHC-C1C	3.19	1.42	1.34
16	a	1108	CLA	C1D-ND	3.19	1.42	1.37
16	b	1214	CLA	C1D-ND	3.19	1.42	1.37
16	s	505	CLA	C1D-ND	3.19	1.42	1.37
16	a	1120	CLA	C1D-ND	3.19	1.42	1.37
16	B	1235	CLA	C1D-ND	3.19	1.42	1.37
16	H	1120	CLA	C1D-ND	3.19	1.42	1.37
16	a	1134	CLA	C1D-ND	3.19	1.42	1.37
16	Y	505	CLA	C1D-ND	3.19	1.42	1.37
16	f	1302	CLA	C1D-ND	3.19	1.42	1.37
16	g	506	CLA	C1D-ND	3.18	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	w	503	CLA	C1D-ND	3.18	1.42	1.37
16	B	1239	CLA	C1D-ND	3.18	1.42	1.37
16	b	1205	CLA	CHC-C1C	3.18	1.42	1.34
16	n	513	CLA	C1D-ND	3.18	1.42	1.37
16	o	506	CLA	C1D-ND	3.18	1.42	1.37
16	x	516	CLA	C1D-ND	3.18	1.42	1.37
16	B	1205	CLA	CHC-C1C	3.18	1.42	1.34
16	G	1215	CLA	C1D-ND	3.18	1.42	1.37
16	A	1108	CLA	C1D-ND	3.18	1.42	1.37
16	G	1205	CLA	C1D-ND	3.18	1.42	1.37
16	w	513	CLA	C1D-ND	3.18	1.42	1.37
16	a	1103	CLA	C1D-ND	3.18	1.42	1.37
16	H	1801	CLA	C1D-ND	3.18	1.42	1.37
16	b	1203	CLA	C1D-ND	3.18	1.42	1.37
16	A	1105	CLA	C1D-ND	3.18	1.42	1.37
16	G	1210	CLA	C1D-ND	3.18	1.42	1.37
16	Y	513	CLA	C1D-ND	3.18	1.42	1.37
16	b	1222	CLA	C1D-ND	3.18	1.42	1.37
16	h	502	CLA	C1D-ND	3.18	1.42	1.37
16	s	502	CLA	CHC-C1C	3.17	1.42	1.34
16	G	1204	CLA	C1D-ND	3.17	1.42	1.37
16	A	1801	CLA	C1D-ND	3.17	1.42	1.37
16	Y	509	CLA	C1D-ND	3.17	1.42	1.37
16	h	504	CLA	C1D-ND	3.17	1.42	1.37
16	g	511	CLA	C1D-ND	3.17	1.42	1.37
16	B	1234	CLA	C1D-ND	3.17	1.42	1.37
16	G	1202	CLA	C1D-ND	3.17	1.42	1.37
16	g	506	CLA	CHC-C1C	3.16	1.42	1.34
16	G	1223	CLA	C1D-ND	3.16	1.42	1.37
16	G	1234	CLA	C1D-ND	3.16	1.42	1.37
16	o	503	CLA	C1D-ND	3.16	1.42	1.37
16	o	508	CLA	C1D-ND	3.16	1.42	1.37
16	s	501	CLA	C1D-ND	3.16	1.42	1.37
16	a	1119	CLA	C1D-ND	3.16	1.42	1.37
16	W	511	CLA	C1D-ND	3.16	1.42	1.37
16	a	1107	CLA	C1D-ND	3.16	1.42	1.37
16	t	512	CLA	C1D-ND	3.16	1.42	1.37
16	X	511	CLA	C1D-ND	3.16	1.42	1.37
16	Y	514	CLA	C1D-ND	3.16	1.42	1.37
16	G	1229	CLA	C1D-ND	3.15	1.42	1.37
16	B	1222	CLA	C1D-ND	3.15	1.42	1.37
16	h	506	CLA	C1D-ND	3.15	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1136	CLA	C1D-ND	3.15	1.42	1.37
16	o	509	CLA	C1D-ND	3.15	1.42	1.37
16	t	505	CLA	C1D-ND	3.15	1.42	1.37
16	o	515	CLA	C1D-ND	3.15	1.42	1.37
16	t	508	CLA	C1D-ND	3.15	1.42	1.37
16	X	506	CLA	C1D-ND	3.15	1.42	1.37
16	Z	514	CLA	C1D-ND	3.15	1.42	1.37
16	G	1212	CLA	C1D-ND	3.15	1.42	1.37
16	a	1121	CLA	C1D-ND	3.15	1.42	1.37
16	v	508	CLA	C1D-ND	3.15	1.42	1.37
16	x	514	CLA	C1D-ND	3.15	1.42	1.37
16	G	1220	CLA	C1D-ND	3.15	1.42	1.37
16	Q	1302	CLA	C1D-ND	3.15	1.42	1.37
16	B	1226	CLA	CHC-C1C	3.15	1.42	1.34
16	H	1136	CLA	C1D-ND	3.15	1.42	1.37
16	A	1128	CLA	CHC-C1C	3.15	1.42	1.34
16	W	514	CLA	C1D-ND	3.15	1.42	1.37
16	A	1121	CLA	C1D-ND	3.14	1.42	1.37
16	p	504	CLA	C1D-ND	3.14	1.42	1.37
16	H	1123	CLA	C1D-ND	3.14	1.42	1.37
16	W	506	CLA	CHC-C1C	3.14	1.42	1.34
16	G	1239	CLA	C1D-ND	3.14	1.42	1.37
16	H	1109	CLA	C1D-ND	3.14	1.42	1.37
16	X	515	CLA	C1D-ND	3.14	1.42	1.37
16	H	1137	CLA	C1D-ND	3.14	1.42	1.37
16	H	1133	CLA	C1D-ND	3.14	1.42	1.37
16	b	1202	CLA	C1D-ND	3.14	1.42	1.37
16	s	508	CLA	C1D-ND	3.14	1.42	1.37
16	s	514	CLA	C1D-ND	3.14	1.42	1.37
16	X	508	CLA	C1D-ND	3.14	1.42	1.37
16	r	503	CLA	C1D-ND	3.14	1.42	1.37
16	x	515	CLA	C1D-ND	3.14	1.42	1.37
16	r	506	CLA	CHC-C1C	3.14	1.42	1.34
16	n	510	CLA	CHC-C1C	3.14	1.42	1.34
16	s	504	CLA	C1D-ND	3.14	1.42	1.37
16	w	511	CLA	C1D-ND	3.14	1.42	1.37
16	G	1216	CLA	C1D-ND	3.13	1.42	1.37
16	a	1104	CLA	C1D-ND	3.13	1.42	1.37
16	s	515	CLA	C1D-ND	3.13	1.42	1.37
16	s	509	CLA	C1D-ND	3.13	1.42	1.37
16	p	506	CLA	CHC-C1C	3.13	1.42	1.34
16	y	509	CLA	C1D-ND	3.13	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	509	CLA	C1D-ND	3.13	1.42	1.37
16	q	514	CLA	C1D-ND	3.13	1.42	1.37
16	B	1229	CLA	C1D-ND	3.13	1.42	1.37
16	Y	511	CLA	C1D-ND	3.13	1.42	1.37
16	A	1124	CLA	C1D-ND	3.13	1.42	1.37
16	B	1207	CLA	C1D-ND	3.12	1.42	1.37
16	H	1114	CLA	C1D-ND	3.12	1.42	1.37
16	B	1227	CLA	C1D-ND	3.12	1.42	1.37
16	X	506	CLA	CHC-C1C	3.12	1.42	1.34
16	X	503	CLA	C1D-ND	3.12	1.42	1.37
16	g	508	CLA	C1D-ND	3.12	1.42	1.37
16	Y	506	CLA	CHC-C1C	3.12	1.42	1.34
16	a	1101	CLA	C1D-ND	3.12	1.42	1.37
16	n	514	CLA	C1D-ND	3.12	1.42	1.37
16	G	1222	CLA	C1D-ND	3.12	1.42	1.37
16	H	1138	CLA	C1D-ND	3.12	1.42	1.37
16	Z	503	CLA	C1D-ND	3.12	1.42	1.37
16	a	1135	CLA	C1D-ND	3.12	1.42	1.37
16	B	1203	CLA	C1D-ND	3.12	1.42	1.37
16	Z	516	CLA	C1D-ND	3.12	1.42	1.37
16	w	508	CLA	C1D-ND	3.12	1.42	1.37
16	n	508	CLA	C1D-ND	3.12	1.42	1.37
16	a	1109	CLA	C1D-ND	3.11	1.42	1.37
16	y	502	CLA	C1D-ND	3.11	1.42	1.37
16	H	1102	CLA	C1D-ND	3.11	1.41	1.37
16	H	1107	CLA	C1D-ND	3.11	1.41	1.37
16	A	1237	CLA	CHC-C1C	3.11	1.42	1.34
16	a	1105	CLA	C1D-ND	3.11	1.41	1.37
16	H	1119	CLA	C1D-ND	3.11	1.41	1.37
16	q	512	CLA	C1D-ND	3.11	1.41	1.37
16	A	1133	CLA	C1D-ND	3.11	1.41	1.37
16	u	516	CLA	C1D-ND	3.11	1.41	1.37
16	X	514	CLA	C1D-ND	3.10	1.41	1.37
16	H	1237	CLA	CHC-C1C	3.10	1.42	1.34
16	W	510	CLA	CHC-C1C	3.10	1.42	1.34
16	o	514	CLA	C1D-ND	3.10	1.41	1.37
16	A	1135	CLA	C1D-ND	3.10	1.41	1.37
16	B	1214	CLA	C1D-ND	3.10	1.41	1.37
16	H	1121	CLA	C1D-ND	3.10	1.41	1.37
16	w	506	CLA	CHC-C1C	3.10	1.42	1.34
16	H	1125	CLA	C1D-ND	3.10	1.41	1.37
16	G	1211	CLA	C1D-ND	3.10	1.41	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	v	502	CLA	C1D-ND	3.10	1.41	1.37
16	A	1131	CLA	C1D-ND	3.09	1.41	1.37
16	b	1213	CLA	C1D-ND	3.09	1.41	1.37
16	x	512	CLA	C1D-ND	3.09	1.41	1.37
16	A	1237	CLA	C1D-ND	3.09	1.41	1.37
16	w	501	CLA	C1D-ND	3.09	1.41	1.37
16	Z	506	CLA	CHC-C1C	3.09	1.42	1.34
16	B	1208	CLA	C1D-ND	3.09	1.41	1.37
16	b	1215	CLA	C1D-ND	3.09	1.41	1.37
16	B	1206	CLA	C1D-ND	3.09	1.41	1.37
16	A	1110	CLA	C1D-ND	3.09	1.41	1.37
16	X	512	CLA	C1D-ND	3.09	1.41	1.37
16	p	501	CLA	C1D-ND	3.09	1.41	1.37
16	A	1106	CLA	C1D-ND	3.09	1.41	1.37
16	v	504	CLA	C1D-ND	3.08	1.41	1.37
16	w	506	CLA	C1D-ND	3.08	1.41	1.37
16	H	1108	CLA	C1D-ND	3.08	1.41	1.37
16	u	508	CLA	C1D-ND	3.08	1.41	1.37
16	Y	504	CLA	C1D-ND	3.08	1.41	1.37
16	x	509	CLA	C1D-ND	3.08	1.41	1.37
16	Y	512	CLA	C1D-ND	3.08	1.41	1.37
16	p	511	CLA	C1D-ND	3.08	1.41	1.37
16	g	512	CLA	C1D-ND	3.08	1.41	1.37
16	x	505	CLA	C1D-ND	3.08	1.41	1.37
16	A	1117	CLA	C1D-ND	3.07	1.41	1.37
16	b	1236	CLA	C1D-ND	3.07	1.41	1.37
16	x	503	CLA	C1D-ND	3.07	1.41	1.37
16	q	506	CLA	CHC-C1C	3.07	1.42	1.34
16	b	1208	CLA	C1D-ND	3.07	1.41	1.37
16	A	1104	CLA	C1D-ND	3.07	1.41	1.37
16	H	1131	CLA	C1D-ND	3.07	1.41	1.37
16	a	1124	CLA	C1D-ND	3.07	1.41	1.37
16	g	503	CLA	C1D-ND	3.07	1.41	1.37
16	a	1106	CLA	C1D-ND	3.07	1.41	1.37
16	u	512	CLA	C1D-ND	3.07	1.41	1.37
16	x	506	CLA	C1D-ND	3.07	1.41	1.37
16	H	1129	CLA	C1D-ND	3.06	1.41	1.37
16	H	1106	CLA	C1D-ND	3.06	1.41	1.37
16	v	509	CLA	C1D-ND	3.06	1.41	1.37
16	B	1216	CLA	C1D-ND	3.06	1.41	1.37
16	a	1117	CLA	C1D-ND	3.06	1.41	1.37
16	G	1203	CLA	C1D-ND	3.06	1.41	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1110	CLA	C1D-ND	3.06	1.41	1.37
16	a	1116	CLA	C1D-ND	3.05	1.41	1.37
16	r	502	CLA	C1D-ND	3.05	1.41	1.37
16	W	508	CLA	C1D-ND	3.05	1.41	1.37
16	b	1226	CLA	C1D-ND	3.05	1.41	1.37
16	r	509	CLA	C1D-ND	3.05	1.41	1.37
16	G	1236	CLA	C1D-ND	3.05	1.41	1.37
16	A	1102	CLA	C1D-ND	3.05	1.41	1.37
16	H	1139	CLA	C1D-ND	3.05	1.41	1.37
16	G	1214	CLA	C1D-ND	3.05	1.41	1.37
16	g	505	CLA	C1D-ND	3.04	1.41	1.37
16	u	515	CLA	C1D-ND	3.04	1.41	1.37
16	H	1022	CLA	C1D-ND	3.04	1.41	1.37
16	u	509	CLA	C1D-ND	3.04	1.41	1.37
16	G	1221	CLA	C1D-ND	3.04	1.41	1.37
16	A	1139	CLA	C1D-ND	3.04	1.41	1.37
16	H	1105	CLA	C1D-ND	3.04	1.41	1.37
16	Z	511	CLA	C1D-ND	3.04	1.41	1.37
16	g	509	CLA	C1D-ND	3.04	1.41	1.37
16	s	511	CLA	C1D-ND	3.04	1.41	1.37
16	A	1109	CLA	C1D-ND	3.04	1.41	1.37
16	a	1138	CLA	C1D-ND	3.03	1.41	1.37
16	A	1022	CLA	C1D-ND	3.03	1.41	1.37
16	x	511	CLA	C1D-ND	3.03	1.41	1.37
16	a	1115	CLA	C1D-ND	3.03	1.41	1.37
16	B	1215	CLA	C1D-ND	3.03	1.41	1.37
16	b	1220	CLA	C1D-ND	3.03	1.41	1.37
16	Z	509	CLA	C1D-ND	3.03	1.41	1.37
16	W	502	CLA	C1D-ND	3.03	1.41	1.37
16	h	511	CLA	C1D-ND	3.03	1.41	1.37
16	o	511	CLA	C1D-ND	3.02	1.41	1.37
16	g	502	CLA	C1D-ND	3.02	1.41	1.37
16	r	514	CLA	C1D-ND	3.01	1.41	1.37
16	u	506	CLA	C1D-ND	3.01	1.41	1.37
16	Y	506	CLA	C1D-ND	3.01	1.41	1.37
16	B	1221	CLA	C1D-ND	3.01	1.41	1.37
16	a	1110	CLA	C1D-ND	3.01	1.41	1.37
16	q	509	CLA	C1D-ND	3.01	1.41	1.37
16	A	1111	CLA	C1D-ND	3.01	1.41	1.37
16	b	1221	CLA	C1D-ND	3.01	1.41	1.37
16	o	502	CLA	C1D-ND	3.01	1.41	1.37
16	H	1104	CLA	C1D-ND	3.00	1.41	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	g	514	CLA	C1D-ND	3.00	1.41	1.37
16	w	512	CLA	C1D-ND	3.00	1.41	1.37
16	Y	515	CLA	C1D-ND	3.00	1.41	1.37
16	b	1211	CLA	C1D-ND	3.00	1.41	1.37
16	B	1236	CLA	C1D-ND	3.00	1.41	1.37
16	A	1125	CLA	C1D-ND	3.00	1.41	1.37
16	G	1226	CLA	C1D-ND	2.99	1.41	1.37
16	q	505	CLA	C1D-ND	2.99	1.41	1.37
21	i	4020	ECH	C1-C6	2.99	1.57	1.53
16	a	1129	CLA	C1D-ND	2.99	1.41	1.37
16	A	1119	CLA	C1D-ND	2.99	1.41	1.37
16	G	1206	CLA	C1D-ND	2.99	1.41	1.37
16	w	509	CLA	C1D-ND	2.99	1.41	1.37
16	p	502	CLA	C1D-ND	2.99	1.41	1.37
16	A	1126	CLA	C1D-ND	2.98	1.41	1.37
16	a	1237	CLA	C1D-ND	2.98	1.41	1.37
16	p	506	CLA	C1D-ND	2.98	1.41	1.37
16	Y	503	CLA	C1D-ND	2.98	1.41	1.37
16	a	1102	CLA	C1D-ND	2.98	1.41	1.37
16	b	1206	CLA	C1D-ND	2.97	1.41	1.37
16	G	1227	CLA	C1D-ND	2.97	1.41	1.37
16	b	1227	CLA	C1D-ND	2.97	1.41	1.37
16	G	1239	CLA	CHC-C1C	2.97	1.41	1.34
16	B	1213	CLA	C1D-ND	2.97	1.41	1.37
16	A	1127	CLA	C1D-ND	2.97	1.41	1.37
16	a	1131	CLA	C1D-ND	2.96	1.41	1.37
16	B	1021	CLA	C1D-ND	2.96	1.41	1.37
16	B	1226	CLA	C1D-ND	2.96	1.41	1.37
16	Z	502	CLA	C1D-ND	2.96	1.41	1.37
16	G	1021	CLA	C1D-ND	2.96	1.41	1.37
16	o	512	CLA	C1D-ND	2.95	1.41	1.37
16	X	502	CLA	C1D-ND	2.95	1.41	1.37
16	H	1126	CLA	C1D-ND	2.95	1.41	1.37
16	A	1140	CLA	C1D-ND	2.94	1.41	1.37
16	b	1239	CLA	CHC-C1C	2.94	1.41	1.34
16	a	1140	CLA	C1D-ND	2.94	1.41	1.37
16	a	1139	CLA	C1D-ND	2.94	1.41	1.37
16	w	515	CLA	C1D-ND	2.94	1.41	1.37
16	H	1124	CLA	C1D-ND	2.94	1.41	1.37
16	x	502	CLA	C1D-ND	2.94	1.41	1.37
16	p	503	CLA	C1D-ND	2.93	1.41	1.37
21	R	4020	ECH	C1-C6	2.93	1.57	1.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1126	CLA	C1D-ND	2.93	1.41	1.37
16	t	502	CLA	C1D-ND	2.93	1.41	1.37
16	H	1117	CLA	C1D-ND	2.92	1.41	1.37
16	s	506	CLA	C1D-ND	2.92	1.41	1.37
16	q	502	CLA	C1D-ND	2.92	1.41	1.37
16	u	511	CLA	C1D-ND	2.92	1.41	1.37
16	Y	502	CLA	C1D-ND	2.91	1.41	1.37
16	B	1211	CLA	C1D-ND	2.90	1.41	1.37
16	n	502	CLA	C1D-ND	2.90	1.41	1.37
16	w	502	CLA	C1D-ND	2.90	1.41	1.37
16	b	1021	CLA	C1D-ND	2.90	1.41	1.37
16	l	1502	CLA	C1D-ND	2.90	1.41	1.37
16	a	1125	CLA	C1D-ND	2.90	1.41	1.37
14	A	4101	LMG	C4-C5	2.89	1.59	1.53
16	H	1237	CLA	C1D-ND	2.89	1.41	1.37
16	u	502	CLA	C1D-ND	2.89	1.41	1.37
14	H	4101	LMG	C4-C5	2.88	1.59	1.53
16	a	1127	CLA	C1D-ND	2.88	1.41	1.37
16	H	1116	CLA	C1D-ND	2.88	1.41	1.37
16	B	1239	CLA	CHC-C1C	2.87	1.41	1.34
16	A	1115	CLA	C1D-ND	2.86	1.41	1.37
21	I	4020	ECH	C1-C6	2.85	1.57	1.53
16	H	1127	CLA	C1D-ND	2.84	1.41	1.37
16	U	1502	CLA	C1D-ND	2.84	1.41	1.37
16	A	1116	CLA	C1D-ND	2.82	1.41	1.37
16	H	1128	CLA	C1D-ND	2.81	1.41	1.37
16	H	1115	CLA	C1D-ND	2.81	1.41	1.37
14	a	4101	LMG	C4-C5	2.81	1.59	1.53
16	s	502	CLA	C1D-ND	2.79	1.41	1.37
16	H	1140	CLA	C1D-ND	2.78	1.41	1.37
16	G	1225	CLA	C1D-ND	2.78	1.41	1.37
16	q	503	CLA	C1D-ND	2.78	1.41	1.37
16	b	1225	CLA	C1D-ND	2.77	1.41	1.37
15	A	1011	CL0	C1D-ND	2.77	1.41	1.37
15	H	1011	CL0	C1D-ND	2.77	1.41	1.37
16	L	1502	CLA	C1D-ND	2.76	1.41	1.37
16	A	1128	CLA	C1D-ND	2.74	1.41	1.37
16	a	1128	CLA	C1D-ND	2.73	1.41	1.37
16	B	1225	CLA	C1D-ND	2.71	1.41	1.37
15	a	1011	CL0	C1D-ND	2.70	1.41	1.37
16	B	1023	CLA	C1D-ND	2.70	1.41	1.37
16	b	1023	CLA	C1D-ND	2.67	1.41	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1023	CLA	C1D-ND	2.51	1.41	1.37
20	a	4202	LMT	O3'-C3'	-2.48	1.36	1.43
20	a	4202	LMT	O2'-C2'	-2.45	1.36	1.43
20	A	4202	LMT	O3'-C3'	-2.45	1.36	1.43
20	H	4202	LMT	O3'-C3'	-2.44	1.36	1.43
20	L	4101	LMT	O3'-C3'	-2.44	1.36	1.43
20	U	4101	LMT	O3'-C3'	-2.40	1.37	1.43
21	b	4006	ECH	C2-C1	2.40	1.59	1.54
21	R	4020	ECH	C5-C6	2.40	1.38	1.34
13	a	849	LHG	O7-C5	-2.40	1.41	1.46
20	A	4202	LMT	O2'-C2'	-2.39	1.37	1.43
16	G	1023	CLA	MG-ND	-2.39	2.01	2.05
20	H	4202	LMT	O2'-C2'	-2.39	1.37	1.43
16	u	506	CLA	MG-ND	-2.39	2.01	2.05
16	q	503	CLA	MG-ND	-2.39	2.01	2.05
20	l	4101	LMT	O3'-C3'	-2.38	1.37	1.43
16	b	1023	CLA	MG-ND	-2.35	2.01	2.05
16	A	1013	CLA	MG-ND	-2.34	2.01	2.05
16	A	1111	CLA	MG-ND	-2.34	2.01	2.05
19	A	4007	BCR	C33-C5	-2.33	1.47	1.50
13	g	605	LHG	P-O6	2.33	1.68	1.59
13	A	849	LHG	O7-C5	-2.29	1.41	1.46
19	H	4007	BCR	C33-C5	-2.28	1.47	1.50
16	H	1013	CLA	MG-ND	-2.27	2.01	2.05
16	Y	512	CLA	MG-ND	-2.26	2.01	2.05
20	H	4202	LMT	O2B-C2B	-2.26	1.37	1.43
13	H	851	LHG	O7-C5	-2.26	1.41	1.46
20	A	4202	LMT	O2B-C2B	-2.26	1.37	1.43
20	L	4101	LMT	O2B-C2B	-2.26	1.37	1.43
16	a	1013	CLA	MG-ND	-2.25	2.01	2.05
20	a	4202	LMT	O2B-C2B	-2.25	1.37	1.43
16	j	1303	CLA	CBD-CAD	2.25	1.56	1.51
20	L	4101	LMT	O3B-C3B	-2.25	1.37	1.43
20	L	4101	LMT	O2'-C2'	-2.24	1.37	1.43
16	o	512	CLA	MG-ND	-2.24	2.01	2.05
20	l	4101	LMT	O2B-C2B	-2.24	1.37	1.43
13	x	605	LHG	P-O6	2.23	1.68	1.59
16	J	1303	CLA	CBD-CAD	2.23	1.56	1.51
16	B	1023	CLA	MG-ND	-2.23	2.01	2.05
13	r	605	LHG	P-O6	2.23	1.68	1.59
13	s	605	LHG	O7-C5	-2.23	1.41	1.46
16	B	1216	CLA	MG-ND	-2.22	2.01	2.05

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	U	4101	LMT	O2B-C2B	-2.22	1.37	1.43
20	U	4101	LMT	O3B-C3B	-2.22	1.37	1.43
16	S	1303	CLA	CBD-CAD	2.22	1.56	1.51
19	u	601	BCR	C33-C5	-2.21	1.47	1.50
20	U	4101	LMT	O2'-C2'	-2.21	1.37	1.43
20	l	4101	LMT	O2'-C2'	-2.20	1.37	1.43
14	A	4201	LMG	O7-C8	-2.20	1.41	1.46
16	B	1226	CLA	MG-ND	-2.20	2.01	2.05
16	a	1135	CLA	MG-ND	-2.20	2.01	2.05
14	H	852	LMG	C4-C5	2.20	1.57	1.53
16	a	1128	CLA	MG-ND	-2.19	2.01	2.05
16	p	512	CLA	MG-ND	-2.19	2.01	2.05
16	w	503	CLA	MG-ND	-2.19	2.01	2.05
20	l	4101	LMT	O3B-C3B	-2.19	1.37	1.43
16	b	1226	CLA	MG-ND	-2.19	2.01	2.05
16	H	1127	CLA	MG-ND	-2.18	2.01	2.05
21	R	4020	ECH	C2-C3	-2.18	1.47	1.52
14	f	4017	LMG	C4-C5	2.18	1.57	1.53
13	Y	605	LHG	O7-C5	-2.18	1.41	1.46
16	G	1226	CLA	MG-ND	-2.18	2.01	2.05
13	a	851	LHG	O7-C5	-2.17	1.41	1.46
14	A	852	LMG	C4-C5	2.17	1.57	1.53
13	A	851	LHG	O7-C5	-2.17	1.41	1.46
16	X	514	CLA	MG-ND	-2.17	2.01	2.05
24	Z	601	LUT	C1-C6	-2.17	1.51	1.53
16	w	512	CLA	MG-ND	-2.17	2.01	2.05
20	H	4202	LMT	O3B-C3B	-2.17	1.37	1.43
16	s	512	CLA	MG-ND	-2.17	2.01	2.05
20	a	4202	LMT	O3B-C3B	-2.16	1.37	1.43
16	b	1224	CLA	MG-ND	-2.16	2.01	2.05
16	q	512	CLA	MG-ND	-2.16	2.01	2.05
14	a	852	LMG	C4-C5	2.15	1.57	1.53
16	W	502	CLA	MG-ND	-2.15	2.01	2.05
14	F	4017	LMG	O7-C8	-2.15	1.41	1.46
16	H	1104	CLA	MG-ND	-2.15	2.01	2.05
16	s	506	CLA	MG-ND	-2.14	2.01	2.05
13	p	605	LHG	O7-C5	-2.14	1.41	1.46
20	A	4202	LMT	O3B-C3B	-2.14	1.37	1.43
16	A	1128	CLA	MG-ND	-2.14	2.01	2.05
13	G	4018	LHG	O7-C5	-2.14	1.41	1.46
16	Z	503	CLA	MG-ND	-2.14	2.01	2.05
20	U	4101	LMT	O1'-C1'	-2.13	1.36	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1013	CLA	C1D-ND	2.13	1.40	1.37
13	i	103	LHG	P-O6	2.13	1.67	1.59
16	a	1127	CLA	MG-ND	-2.13	2.01	2.05
14	F	4017	LMG	C4-C5	2.13	1.57	1.53
16	A	1135	CLA	MG-ND	-2.13	2.01	2.05
16	x	512	CLA	MG-ND	-2.13	2.01	2.05
16	Z	512	CLA	MG-ND	-2.13	2.01	2.05
16	h	506	CLA	MG-ND	-2.12	2.01	2.05
19	a	4007	BCR	C33-C5	-2.11	1.47	1.50
16	o	506	CLA	MG-ND	-2.11	2.01	2.05
16	a	1013	CLA	C1D-ND	2.11	1.40	1.37
13	B	4018	LHG	P-O6	2.11	1.67	1.59
16	A	1127	CLA	MG-ND	-2.11	2.01	2.05
13	r	605	LHG	O7-C5	-2.10	1.41	1.46
15	A	1011	CL0	MG-ND	-2.10	2.01	2.05
16	A	1013	CLA	C1D-ND	2.10	1.40	1.37
13	I	103	LHG	P-O6	2.10	1.67	1.59
16	u	502	CLA	MG-ND	-2.10	2.01	2.05
16	v	509	CLA	MG-ND	-2.09	2.01	2.05
16	H	1237	CLA	MG-ND	-2.09	2.01	2.05
16	A	1115	CLA	MG-ND	-2.09	2.01	2.05
16	t	512	CLA	MG-ND	-2.09	2.01	2.05
16	G	1214	CLA	MG-ND	-2.08	2.01	2.05
13	R	103	LHG	O7-C5	-2.08	1.41	1.46
20	L	4101	LMT	O4'-C4B	-2.07	1.37	1.43
16	G	1234	CLA	MG-ND	-2.07	2.01	2.05
16	r	512	CLA	MG-ND	-2.07	2.01	2.05
19	a	4008	BCR	C33-C5	-2.07	1.47	1.50
16	q	505	CLA	MG-ND	-2.07	2.01	2.05
16	B	1225	CLA	MG-ND	-2.07	2.01	2.05
14	a	4201	LMG	O7-C8	-2.07	1.41	1.46
13	g	605	LHG	O7-C5	-2.07	1.41	1.46
16	a	1125	CLA	MG-ND	-2.06	2.01	2.05
20	l	4101	LMT	O1'-C1'	-2.06	1.36	1.40
16	p	503	CLA	MG-ND	-2.06	2.01	2.05
16	A	1237	CLA	MG-ND	-2.06	2.01	2.05
16	s	503	CLA	MG-ND	-2.06	2.01	2.05
16	G	1227	CLA	MG-ND	-2.06	2.01	2.05
16	g	512	CLA	MG-ND	-2.06	2.01	2.05
16	g	514	CLA	MG-ND	-2.06	2.01	2.05
14	A	4101	LMG	C3-C2	2.06	1.57	1.52
19	G	4014	BCR	C38-C26	-2.06	1.47	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1205	CLA	MG-ND	-2.05	2.01	2.05
16	a	1237	CLA	MG-ND	-2.05	2.01	2.05
13	i	103	LHG	O7-C5	-2.05	1.41	1.46
16	h	511	CLA	MG-ND	-2.05	2.01	2.05
20	A	4202	LMT	O1'-C1'	-2.05	1.36	1.40
13	I	103	LHG	O7-C5	-2.05	1.41	1.46
16	G	1225	CLA	MG-ND	-2.05	2.01	2.05
16	s	502	CLA	MG-ND	-2.05	2.01	2.05
13	R	103	LHG	P-O6	2.05	1.67	1.59
16	a	1104	CLA	MG-ND	-2.04	2.01	2.05
20	a	4202	LMT	O4'-C4B	-2.04	1.37	1.43
16	B	1227	CLA	MG-ND	-2.04	2.01	2.05
16	B	1211	CLA	MG-ND	-2.04	2.01	2.05
16	Z	502	CLA	MG-ND	-2.04	2.01	2.05
16	y	504	CLA	MG-ND	-2.04	2.01	2.05
16	w	517	CLA	MG-ND	-2.04	2.01	2.05
16	b	1235	CLA	MG-ND	-2.04	2.01	2.05
14	a	4101	LMG	C1-C2	2.04	1.58	1.52
19	H	4008	BCR	C33-C5	-2.04	1.47	1.50
16	B	1236	CLA	MG-ND	-2.04	2.01	2.05
20	U	4101	LMT	O4'-C4B	-2.04	1.37	1.43
16	y	514	CLA	MG-ND	-2.04	2.01	2.05
16	o	514	CLA	MG-ND	-2.04	2.01	2.05
16	W	512	CLA	MG-ND	-2.04	2.01	2.05
19	T	4001	BCR	C33-C5	-2.04	1.47	1.50
16	b	1213	CLA	MG-ND	-2.04	2.01	2.05
20	L	4101	LMT	O1'-C1'	-2.03	1.36	1.40
16	H	1133	CLA	MG-ND	-2.03	2.01	2.05
16	x	511	CLA	MG-ND	-2.03	2.01	2.05
14	H	4201	LMG	O7-C8	-2.03	1.41	1.46
16	w	506	CLA	MG-ND	-2.03	2.01	2.05
16	H	1140	CLA	MG-ND	-2.03	2.01	2.05
16	B	1234	CLA	MG-ND	-2.03	2.01	2.05
16	A	1133	CLA	MG-ND	-2.03	2.01	2.05
16	H	1116	CLA	MG-ND	-2.03	2.01	2.05
16	G	1222	CLA	MG-ND	-2.03	2.01	2.05
16	H	1135	CLA	MG-ND	-2.03	2.01	2.05
16	t	502	CLA	MG-ND	-2.03	2.01	2.05
19	r	601	BCR	C33-C5	-2.03	1.47	1.50
16	a	1113	CLA	MG-ND	-2.02	2.01	2.05
16	h	512	CLA	MG-ND	-2.02	2.01	2.05
16	H	1128	CLA	MG-ND	-2.02	2.01	2.05

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	4017	LMG	O7-C8	-2.02	1.41	1.46
16	G	1023	CLA	C1D-C2D	-2.02	1.41	1.45
15	H	1011	CL0	MG-ND	-2.02	2.01	2.05
16	b	1227	CLA	MG-ND	-2.02	2.01	2.05
16	g	509	CLA	MG-ND	-2.02	2.01	2.05
16	Z	504	CLA	MG-ND	-2.02	2.01	2.05
16	x	502	CLA	MG-ND	-2.02	2.01	2.05
20	H	4202	LMT	O1'-C1'	-2.02	1.36	1.40
20	l	4101	LMT	O4'-C4B	-2.02	1.38	1.43
16	o	502	CLA	MG-ND	-2.02	2.01	2.05
16	w	502	CLA	MG-ND	-2.02	2.01	2.05
14	B	848	LMG	O7-C8	-2.02	1.41	1.46
16	A	1140	CLA	MG-ND	-2.02	2.01	2.05
16	X	506	CLA	MG-ND	-2.02	2.01	2.05
21	V	4021	ECH	C11-C10	2.02	1.49	1.43
16	h	509	CLA	MG-ND	-2.02	2.01	2.05
16	B	1213	CLA	MG-ND	-2.02	2.01	2.05
16	y	503	CLA	MG-ND	-2.02	2.01	2.05
16	b	1220	CLA	MG-ND	-2.01	2.01	2.05
21	b	4006	ECH	C1-C6	2.01	1.56	1.53
19	o	601	BCR	C33-C5	-2.01	1.47	1.50
16	B	1207	CLA	MG-ND	-2.01	2.01	2.05
16	q	502	CLA	MG-ND	-2.01	2.01	2.05
16	Z	511	CLA	MG-ND	-2.01	2.01	2.05
16	n	505	CLA	MG-ND	-2.01	2.01	2.05
16	v	508	CLA	MG-ND	-2.01	2.01	2.05
13	a	851	LHG	P-O6	2.01	1.67	1.59
14	Q	4017	LMG	O7-C8	-2.01	1.41	1.46
15	a	1011	CL0	MG-ND	-2.01	2.01	2.05
14	b	848	LMG	C3-C2	2.01	1.57	1.52
16	X	502	CLA	MG-ND	-2.01	2.01	2.05
16	x	506	CLA	MG-ND	-2.01	2.01	2.05
19	l	4022	BCR	C27-C26	-2.01	1.47	1.51
16	b	1225	CLA	MG-ND	-2.01	2.01	2.05
16	n	512	CLA	MG-ND	-2.01	2.01	2.05
16	n	502	CLA	MG-ND	-2.00	2.01	2.05
16	n	514	CLA	MG-ND	-2.00	2.01	2.05
16	u	512	CLA	MG-ND	-2.00	2.01	2.05
16	B	1224	CLA	MG-ND	-2.00	2.01	2.05
19	X	601	BCR	C33-C5	-2.00	1.47	1.50
16	G	1224	CLA	MG-ND	-2.00	2.01	2.05

All (3103) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	u	506	CLA	C4A-NA-C1A	8.41	110.52	106.68
21	i	4020	ECH	C8-C9-C10	6.94	129.93	119.01
16	x	505	CLA	C4A-NA-C1A	6.63	109.70	106.68
16	v	505	CLA	C4A-NA-C1A	6.60	109.69	106.68
16	b	1216	CLA	C4A-NA-C1A	6.57	109.68	106.68
16	o	514	CLA	C4A-NA-C1A	6.54	109.66	106.68
16	X	506	CLA	C4A-NA-C1A	6.37	109.58	106.68
16	n	505	CLA	C4A-NA-C1A	6.26	109.53	106.68
16	v	508	CLA	C4A-NA-C1A	6.22	109.52	106.68
16	t	505	CLA	C4A-NA-C1A	6.16	109.49	106.68
16	b	1224	CLA	C4A-NA-C1A	6.14	109.48	106.68
16	g	505	CLA	C4A-NA-C1A	6.09	109.46	106.68
16	q	515	CLA	C4A-NA-C1A	6.04	109.43	106.68
16	A	1106	CLA	C4A-NA-C1A	6.03	109.43	106.68
16	y	517	CLA	C4A-NA-C1A	5.99	109.41	106.68
16	Z	515	CLA	C4A-NA-C1A	5.90	109.37	106.68
16	a	1106	CLA	C4A-NA-C1A	5.85	109.35	106.68
16	y	508	CLA	C4A-NA-C1A	5.83	109.34	106.68
16	b	1212	CLA	C4A-NA-C1A	5.80	109.33	106.68
16	A	1126	CLA	C4A-NA-C1A	5.78	109.32	106.68
16	r	512	CLA	C4A-NA-C1A	5.78	109.32	106.68
16	g	515	CLA	C4A-NA-C1A	5.78	109.32	106.68
16	B	1207	CLA	C4A-NA-C1A	5.77	109.31	106.68
16	h	505	CLA	C4A-NA-C1A	5.77	109.31	106.68
16	x	501	CLA	C4A-NA-C1A	5.71	109.29	106.68
16	b	1232	CLA	C4A-NA-C1A	5.71	109.28	106.68
21	R	4020	ECH	C8-C7-C6	5.67	142.13	127.00
16	t	515	CLA	C4A-NA-C1A	5.64	109.25	106.68
16	b	1215	CLA	C4A-NA-C1A	5.59	109.23	106.68
16	w	515	CLA	C4A-NA-C1A	5.59	109.23	106.68
16	X	504	CLA	C4A-NA-C1A	5.56	109.21	106.68
16	r	505	CLA	C4A-NA-C1A	5.55	109.21	106.68
16	t	512	CLA	C4A-NA-C1A	5.54	109.21	106.68
16	H	1106	CLA	C4A-NA-C1A	5.53	109.20	106.68
16	y	505	CLA	C4A-NA-C1A	5.53	109.20	106.68
16	X	514	CLA	C4A-NA-C1A	5.51	109.19	106.68
16	b	1207	CLA	C4A-NA-C1A	5.50	109.19	106.68
16	a	1114	CLA	C4A-NA-C1A	5.49	109.18	106.68
16	q	508	CLA	C4A-NA-C1A	5.46	109.17	106.68
16	H	1133	CLA	C4A-NA-C1A	5.41	109.15	106.68
16	s	501	CLA	C4A-NA-C1A	5.41	109.15	106.68
16	y	511	CLA	C4A-NA-C1A	5.40	109.14	106.68
16	x	515	CLA	C4A-NA-C1A	5.39	109.14	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	v	515	CLA	C4A-NA-C1A	5.37	109.13	106.68
16	b	1223	CLA	C4A-NA-C1A	5.37	109.13	106.68
21	R	4020	ECH	C7-C8-C9	5.37	134.17	126.23
16	Z	508	CLA	C4A-NA-C1A	5.37	109.13	106.68
16	W	505	CLA	C4A-NA-C1A	5.36	109.12	106.68
16	X	515	CLA	C4A-NA-C1A	5.32	109.11	106.68
21	I	4020	ECH	C7-C8-C9	5.30	134.07	126.23
16	g	510	CLA	C4A-NA-C1A	5.29	109.09	106.68
16	G	1216	CLA	C4A-NA-C1A	5.26	109.08	106.68
16	a	1126	CLA	C4A-NA-C1A	5.26	109.08	106.68
16	G	1212	CLA	C4A-NA-C1A	5.25	109.07	106.68
16	y	501	CLA	C4A-NA-C1A	5.24	109.07	106.68
16	G	1207	CLA	C4A-NA-C1A	5.23	109.07	106.68
16	u	515	CLA	C4A-NA-C1A	5.22	109.06	106.68
16	v	511	CLA	C4A-NA-C1A	5.21	109.06	106.68
16	h	506	CLA	C4A-NA-C1A	5.20	109.05	106.68
16	s	514	CLA	C4A-NA-C1A	5.18	109.04	106.68
16	T	4004	CLA	C4A-NA-C1A	5.18	109.04	106.68
19	U	4019	BCR	C24-C23-C22	-5.15	118.61	126.23
16	G	1232	CLA	C4A-NA-C1A	5.14	109.02	106.68
16	G	1224	CLA	C4A-NA-C1A	5.14	109.02	106.68
16	a	1801	CLA	C4A-NA-C1A	5.12	109.02	106.68
16	r	515	CLA	C4A-NA-C1A	5.12	109.02	106.68
19	l	4019	BCR	C24-C23-C22	-5.10	118.68	126.23
16	G	1205	CLA	C4A-NA-C1A	5.10	109.00	106.68
16	h	507	CLA	C4A-NA-C1A	5.08	109.00	106.68
16	A	1140	CLA	C4A-NA-C1A	5.06	108.99	106.68
16	H	1108	CLA	C4A-NA-C1A	5.06	108.99	106.68
16	Z	512	CLA	C4A-NA-C1A	5.06	108.99	106.68
16	A	1115	CLA	C4A-NA-C1A	5.05	108.98	106.68
16	B	1215	CLA	C4A-NA-C1A	5.04	108.98	106.68
16	u	511	CLA	C4A-NA-C1A	5.03	108.97	106.68
16	B	1212	CLA	C4A-NA-C1A	5.02	108.97	106.68
16	B	1205	CLA	C4A-NA-C1A	5.01	108.97	106.68
21	I	4020	ECH	C8-C7-C6	5.00	140.34	127.00
16	p	512	CLA	C4A-NA-C1A	4.98	108.95	106.68
16	h	504	CLA	C4A-NA-C1A	4.96	108.94	106.68
16	g	516	CLA	C4A-NA-C1A	4.94	108.94	106.68
16	A	1801	CLA	C4A-NA-C1A	4.94	108.93	106.68
16	n	504	CLA	C4A-NA-C1A	4.94	108.93	106.68
16	A	1117	CLA	C4A-NA-C1A	4.93	108.93	106.68
16	B	1232	CLA	C4A-NA-C1A	4.92	108.92	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	q	505	CLA	C4A-NA-C1A	4.91	108.92	106.68
16	A	1131	CLA	C4A-NA-C1A	4.91	108.92	106.68
16	p	501	CLA	C4A-NA-C1A	4.90	108.92	106.68
16	n	515	CLA	C4A-NA-C1A	4.89	108.91	106.68
16	H	1126	CLA	C4A-NA-C1A	4.89	108.91	106.68
16	b	1205	CLA	C4A-NA-C1A	4.89	108.91	106.68
16	n	503	CLA	C4A-NA-C1A	4.88	108.91	106.68
21	i	4020	ECH	C34-C9-C10	-4.87	114.93	122.82
16	G	1215	CLA	C4A-NA-C1A	4.84	108.89	106.68
16	G	1021	CLA	C4A-NA-C1A	4.81	108.88	106.68
16	r	501	CLA	C4A-NA-C1A	4.81	108.88	106.68
16	n	510	CLA	C4A-NA-C1A	4.81	108.87	106.68
16	H	1115	CLA	C4A-NA-C1A	4.81	108.87	106.68
16	A	1111	CLA	C4A-NA-C1A	4.80	108.87	106.68
16	Z	507	CLA	C4A-NA-C1A	4.80	108.87	106.68
16	G	1225	CLA	C4A-NA-C1A	4.79	108.86	106.68
16	a	1108	CLA	C4A-NA-C1A	4.78	108.86	106.68
16	t	509	CLA	C4A-NA-C1A	4.78	108.86	106.68
16	X	511	CLA	C4A-NA-C1A	4.78	108.86	106.68
16	W	515	CLA	C4A-NA-C1A	4.78	108.86	106.68
16	b	1231	CLA	C4A-NA-C1A	4.77	108.86	106.68
16	K	4004	CLA	C4A-NA-C1A	4.77	108.85	106.68
16	H	1127	CLA	C4A-NA-C1A	4.76	108.85	106.68
24	w	601	LUT	C21-C26-C27	4.76	118.30	112.83
16	Z	511	CLA	C4A-NA-C1A	4.76	108.85	106.68
16	h	503	CLA	C4A-NA-C1A	4.75	108.85	106.68
16	A	1114	CLA	C4A-NA-C1A	4.74	108.84	106.68
16	B	1218	CLA	C4A-NA-C1A	4.73	108.84	106.68
16	b	1221	CLA	C4A-NA-C1A	4.73	108.84	106.68
16	a	1117	CLA	C4A-NA-C1A	4.73	108.83	106.68
16	G	1223	CLA	C4A-NA-C1A	4.72	108.83	106.68
16	Y	501	CLA	C4A-NA-C1A	4.72	108.83	106.68
16	A	1109	CLA	C4A-NA-C1A	4.70	108.83	106.68
16	q	507	CLA	C4A-NA-C1A	4.70	108.83	106.68
16	a	1131	CLA	C4A-NA-C1A	4.70	108.82	106.68
16	B	1231	CLA	C4A-NA-C1A	4.69	108.82	106.68
16	h	501	CLA	C4A-NA-C1A	4.67	108.81	106.68
16	s	512	CLA	C4A-NA-C1A	4.66	108.80	106.68
16	b	1023	CLA	C4A-NA-C1A	4.66	108.80	106.68
16	w	512	CLA	C4A-NA-C1A	4.64	108.80	106.68
16	B	1240	CLA	C4A-NA-C1A	4.63	108.79	106.68
16	G	1203	CLA	C4A-NA-C1A	4.62	108.79	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	1120	CLA	C4A-NA-C1A	4.62	108.78	106.68
16	W	511	CLA	C4A-NA-C1A	4.60	108.78	106.68
16	n	512	CLA	C4A-NA-C1A	4.59	108.78	106.68
16	n	501	CLA	C4A-NA-C1A	4.59	108.77	106.68
16	H	1111	CLA	C4A-NA-C1A	4.57	108.76	106.68
16	H	1117	CLA	C4A-NA-C1A	4.57	108.76	106.68
16	H	1140	CLA	C4A-NA-C1A	4.57	108.76	106.68
16	B	1214	CLA	C4A-NA-C1A	4.56	108.76	106.68
24	Z	601	LUT	C21-C26-C27	4.56	118.07	112.83
16	H	1131	CLA	C4A-NA-C1A	4.55	108.76	106.68
16	A	1139	CLA	C4A-NA-C1A	4.55	108.75	106.68
16	b	1217	CLA	C4A-NA-C1A	4.55	108.75	106.68
16	b	1201	CLA	C4A-NA-C1A	4.55	108.75	106.68
16	G	1211	CLA	C4A-NA-C1A	4.54	108.75	106.68
16	u	514	CLA	C4A-NA-C1A	4.54	108.75	106.68
16	v	503	CLA	C4A-NA-C1A	4.54	108.75	106.68
16	G	1208	CLA	C4A-NA-C1A	4.52	108.74	106.68
16	Z	510	CLA	C4A-NA-C1A	4.51	108.74	106.68
16	B	1203	CLA	C4A-NA-C1A	4.50	108.73	106.68
16	B	1208	CLA	C4A-NA-C1A	4.50	108.73	106.68
16	g	512	CLA	C4A-NA-C1A	4.50	108.73	106.68
16	q	511	CLA	C4A-NA-C1A	4.49	108.73	106.68
16	a	1111	CLA	C4A-NA-C1A	4.49	108.73	106.68
16	H	1113	CLA	C4A-NA-C1A	4.49	108.73	106.68
16	B	1227	CLA	C4A-NA-C1A	4.48	108.72	106.68
16	U	1502	CLA	C4A-NA-C1A	4.47	108.72	106.68
16	H	1114	CLA	C4A-NA-C1A	4.46	108.71	106.68
13	X	605	LHG	O4-P-O5	4.46	133.18	112.44
16	B	1225	CLA	C4A-NA-C1A	4.44	108.71	106.68
16	t	506	CLA	C4A-NA-C1A	4.44	108.70	106.68
16	G	1240	CLA	C4A-NA-C1A	4.44	108.70	106.68
16	v	512	CLA	C4A-NA-C1A	4.44	108.70	106.68
16	W	510	CLA	C4A-NA-C1A	4.44	108.70	106.68
16	a	1132	CLA	C4A-NA-C1A	4.44	108.70	106.68
16	B	1228	CLA	C4A-NA-C1A	4.43	108.70	106.68
16	x	510	CLA	C4A-NA-C1A	4.43	108.70	106.68
16	Y	511	CLA	C4A-NA-C1A	4.42	108.69	106.68
16	A	1123	CLA	C4A-NA-C1A	4.41	108.69	106.68
16	a	1237	CLA	C4A-NA-C1A	4.41	108.69	106.68
16	h	515	CLA	C4A-NA-C1A	4.41	108.69	106.68
16	Y	512	CLA	C4A-NA-C1A	4.41	108.69	106.68
16	h	508	CLA	C4A-NA-C1A	4.41	108.69	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	l	1502	CLA	C4A-NA-C1A	4.41	108.69	106.68
13	p	605	LHG	O4-P-O5	4.41	132.94	112.44
16	A	1133	CLA	C4A-NA-C1A	4.41	108.69	106.68
13	R	103	LHG	O4-P-O5	4.41	132.94	112.44
13	u	605	LHG	O4-P-O5	4.40	132.91	112.44
16	o	511	CLA	C4A-NA-C1A	4.39	108.68	106.68
13	A	849	LHG	O4-P-O5	4.39	132.89	112.44
13	I	103	LHG	O4-P-O5	4.39	132.88	112.44
13	a	849	LHG	O4-P-O5	4.39	132.87	112.44
16	X	505	CLA	C4A-NA-C1A	4.38	108.68	106.68
13	H	849	LHG	O4-P-O5	4.38	132.84	112.44
13	o	605	LHG	O4-P-O5	4.38	132.83	112.44
13	i	103	LHG	O4-P-O5	4.38	132.83	112.44
16	b	1240	CLA	C4A-NA-C1A	4.38	108.68	106.68
16	B	1224	CLA	C4A-NA-C1A	4.37	108.67	106.68
13	s	605	LHG	O4-P-O5	4.37	132.75	112.44
13	Y	605	LHG	O4-P-O5	4.36	132.75	112.44
13	G	4018	LHG	O4-P-O5	4.36	132.73	112.44
13	x	605	LHG	O4-P-O5	4.34	132.66	112.44
13	B	4018	LHG	O4-P-O5	4.34	132.64	112.44
16	B	1211	CLA	C4A-NA-C1A	4.34	108.66	106.68
16	B	1021	CLA	C4A-NA-C1A	4.34	108.66	106.68
13	r	605	LHG	O4-P-O5	4.33	132.60	112.44
16	W	503	CLA	C4A-NA-C1A	4.33	108.66	106.68
16	W	509	CLA	C4A-NA-C1A	4.32	108.65	106.68
16	o	512	CLA	C4A-NA-C1A	4.32	108.65	106.68
16	a	1127	CLA	C4A-NA-C1A	4.31	108.65	106.68
21	I	4020	ECH	C33-C5-C6	-4.31	119.78	124.48
16	x	512	CLA	C4A-NA-C1A	4.31	108.64	106.68
16	x	516	CLA	C4A-NA-C1A	4.31	108.64	106.68
16	a	1140	CLA	C4A-NA-C1A	4.30	108.64	106.68
13	g	605	LHG	O4-P-O5	4.30	132.45	112.44
16	b	1228	CLA	C4A-NA-C1A	4.30	108.64	106.68
16	J	1302	CLA	C4A-NA-C1A	4.29	108.64	106.68
13	b	4018	LHG	O4-P-O5	4.29	132.40	112.44
16	t	501	CLA	C4A-NA-C1A	4.28	108.63	106.68
16	A	1237	CLA	C4A-NA-C1A	4.28	108.63	106.68
16	H	1120	CLA	C4A-NA-C1A	4.27	108.63	106.68
16	w	506	CLA	C4A-NA-C1A	4.27	108.63	106.68
16	p	511	CLA	C4A-NA-C1A	4.27	108.62	106.68
16	v	510	CLA	C4A-NA-C1A	4.27	108.62	106.68
16	o	515	CLA	C4A-NA-C1A	4.26	108.62	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	1128	CLA	C4A-NA-C1A	4.26	108.62	106.68
16	y	503	CLA	C4A-NA-C1A	4.25	108.62	106.68
16	t	511	CLA	C4A-NA-C1A	4.25	108.62	106.68
16	H	1128	CLA	C4A-NA-C1A	4.24	108.61	106.68
16	b	1208	CLA	C4A-NA-C1A	4.24	108.61	106.68
16	H	1135	CLA	C4A-NA-C1A	4.24	108.61	106.68
16	q	514	CLA	C4A-NA-C1A	4.23	108.61	106.68
16	a	1113	CLA	C4A-NA-C1A	4.23	108.61	106.68
16	W	512	CLA	C4A-NA-C1A	4.23	108.61	106.68
16	y	515	CLA	C4A-NA-C1A	4.22	108.60	106.68
13	a	851	LHG	O4-P-O5	4.22	132.06	112.44
13	H	851	LHG	O4-P-O5	4.21	132.01	112.44
16	B	1023	CLA	C4A-NA-C1A	4.20	108.60	106.68
13	A	851	LHG	O4-P-O5	4.20	131.98	112.44
21	i	4020	ECH	C11-C10-C9	4.20	133.17	127.28
16	o	507	CLA	C4A-NA-C1A	4.18	108.59	106.68
16	k	4002	CLA	C4A-NA-C1A	4.18	108.59	106.68
16	a	1122	CLA	C4A-NA-C1A	4.18	108.58	106.68
16	A	1128	CLA	C4A-NA-C1A	4.18	108.58	106.68
16	G	1210	CLA	C4A-NA-C1A	4.16	108.58	106.68
16	W	501	CLA	C4A-NA-C1A	4.16	108.58	106.68
16	a	1109	CLA	C4A-NA-C1A	4.16	108.58	106.68
16	n	506	CLA	C4A-NA-C1A	4.15	108.57	106.68
16	w	508	CLA	C4A-NA-C1A	4.15	108.57	106.68
16	s	511	CLA	C4A-NA-C1A	4.13	108.56	106.68
16	w	513	CLA	C4A-NA-C1A	4.12	108.56	106.68
16	r	516	CLA	C4A-NA-C1A	4.11	108.56	106.68
16	Q	1301	CLA	C4A-NA-C1A	4.11	108.55	106.68
16	H	1237	CLA	C4A-NA-C1A	4.10	108.55	106.68
16	G	1209	CLA	C4A-NA-C1A	4.09	108.54	106.68
16	A	1127	CLA	C4A-NA-C1A	4.08	108.54	106.68
16	G	1228	CLA	C4A-NA-C1A	4.08	108.54	106.68
16	B	1239	CLA	C4A-NA-C1A	4.07	108.54	106.68
16	H	1109	CLA	C4A-NA-C1A	4.06	108.53	106.68
16	Y	515	CLA	C4A-NA-C1A	4.06	108.53	106.68
16	H	1013	CLA	CMB-C2B-C1B	-4.05	122.52	128.46
16	W	504	CLA	C4A-NA-C1A	4.05	108.53	106.68
16	Y	506	CLA	C4A-NA-C1A	4.04	108.52	106.68
16	p	510	CLA	C4A-NA-C1A	4.04	108.52	106.68
16	o	505	CLA	C4A-NA-C1A	4.03	108.52	106.68
16	v	509	CLA	C4A-NA-C1A	4.03	108.52	106.68
16	L	1502	CLA	C4A-NA-C1A	4.02	108.51	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	o	501	CLA	C4A-NA-C1A	4.02	108.51	106.68
16	v	506	CLA	C4A-NA-C1A	4.02	108.51	106.68
16	u	516	CLA	C4A-NA-C1A	4.00	108.50	106.68
24	q	601	LUT	C21-C26-C27	4.00	117.42	112.83
16	b	1227	CLA	C4A-NA-C1A	3.99	108.50	106.68
16	G	1227	CLA	C4A-NA-C1A	3.99	108.50	106.68
16	w	502	CLA	C4A-NA-C1A	3.99	108.50	106.68
16	x	507	CLA	C4A-NA-C1A	3.97	108.49	106.68
16	h	512	CLA	C4A-NA-C1A	3.97	108.49	106.68
16	t	510	CLA	C4A-NA-C1A	3.96	108.48	106.68
19	A	4007	BCR	C3-C4-C5	-3.95	107.01	114.06
16	l	1502	CLA	CHD-C1D-ND	-3.93	119.27	124.80
16	F	1301	CLA	C4A-NA-C1A	3.93	108.47	106.68
16	H	1121	CLA	C4A-NA-C1A	3.92	108.47	106.68
21	R	4020	ECH	C1-C6-C5	-3.92	117.28	122.64
16	a	1104	CLA	C4A-NA-C1A	3.91	108.46	106.68
16	G	1239	CLA	CHD-C1D-ND	-3.91	119.31	124.80
19	L	4019	BCR	C24-C23-C22	-3.89	120.48	126.23
16	t	516	CLA	C4A-NA-C1A	3.89	108.45	106.68
16	w	505	CLA	C4A-NA-C1A	3.89	108.45	106.68
16	a	1134	CLA	C4A-NA-C1A	3.88	108.45	106.68
16	a	1125	CLA	C4A-NA-C1A	3.87	108.44	106.68
19	l	4022	BCR	C28-C27-C26	-3.87	107.16	114.06
16	G	1231	CLA	C4A-NA-C1A	3.87	108.44	106.68
23	Z	605	LMU	C1'-O5'-C5'	3.87	121.27	113.72
16	s	505	CLA	C4A-NA-C1A	3.85	108.44	106.68
16	G	1234	CLA	C4A-NA-C1A	3.84	108.43	106.68
16	A	1013	CLA	CMB-C2B-C1B	-3.84	122.84	128.46
16	b	1211	CLA	C4A-NA-C1A	3.83	108.43	106.68
23	g	606	LMU	C1B-O1B-C4'	-3.83	108.90	117.98
21	V	4021	ECH	C33-C5-C6	-3.83	120.31	124.48
16	W	506	CLA	C4A-NA-C1A	3.82	108.42	106.68
21	I	4020	ECH	C1-C6-C5	-3.81	117.43	122.64
16	o	506	CLA	C4A-NA-C1A	3.81	108.42	106.68
21	m	4021	ECH	C33-C5-C6	-3.80	120.34	124.48
16	u	512	CLA	C4A-NA-C1A	3.80	108.41	106.68
24	Z	601	LUT	C7-C8-C9	-3.79	120.62	126.23
16	s	515	CLA	C4A-NA-C1A	3.79	108.41	106.68
19	I	4018	BCR	C2-C1-C6	3.79	115.94	110.44
16	H	1801	CLA	C4A-NA-C1A	3.79	108.41	106.68
16	s	513	CLA	C4A-NA-C1A	3.79	108.41	106.68
16	u	506	CLA	CMC-C2C-C1C	-3.78	119.13	125.03

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	516	CLA	C4A-NA-C1A	3.78	108.40	106.68
24	q	601	LUT	C38-C25-C24	-3.77	114.43	123.36
23	p	606	LMU	C2'-C3'-C4'	3.77	118.24	109.68
16	Y	509	CLA	C4A-NA-C1A	3.77	108.40	106.68
16	t	503	CLA	C4A-NA-C1A	3.75	108.39	106.68
16	B	1239	CLA	CHD-C1D-ND	-3.75	119.53	124.80
16	x	506	CLA	C4A-NA-C1A	3.75	108.39	106.68
16	G	1221	CLA	C4A-NA-C1A	3.74	108.39	106.68
16	b	1225	CLA	C4A-NA-C1A	3.74	108.39	106.68
19	g	601	BCR	C24-C23-C22	-3.74	120.71	126.23
16	h	509	CLA	C4A-NA-C1A	3.73	108.38	106.68
16	q	503	CLA	CHD-C1D-ND	-3.73	119.56	124.80
16	H	1139	CLA	C4A-NA-C1A	3.72	108.38	106.68
21	I	4020	ECH	C34-C9-C10	-3.72	116.79	122.82
16	s	502	CLA	C4A-NA-C1A	3.72	108.37	106.68
16	b	1021	CLA	C4A-NA-C1A	3.71	108.37	106.68
24	Z	601	LUT	C38-C25-C24	-3.71	114.59	123.36
23	x	606	LMU	C4B-C3B-C2B	3.70	117.33	110.83
16	u	505	CLA	C4A-NA-C1A	3.70	108.37	106.68
16	Y	510	CLA	C4A-NA-C1A	3.70	108.37	106.68
21	V	4021	ECH	C1-C6-C5	-3.70	117.59	122.64
19	T	4005	BCR	C2-C1-C6	3.69	115.79	110.44
21	b	4006	ECH	C2-C1-C6	3.68	115.79	110.44
16	H	1125	CLA	C4A-NA-C1A	3.68	108.36	106.68
16	A	1124	CLA	C4A-NA-C1A	3.67	108.35	106.68
16	v	501	CLA	C4A-NA-C1A	3.66	108.35	106.68
16	a	1107	CLA	C4A-NA-C1A	3.66	108.35	106.68
16	q	504	CLA	C4A-NA-C1A	3.66	108.35	106.68
16	H	1104	CLA	C4A-NA-C1A	3.65	108.35	106.68
16	a	1121	CLA	C4A-NA-C1A	3.65	108.35	106.68
16	b	1234	CLA	CMB-C2B-C1B	-3.65	123.11	128.46
16	w	511	CLA	C4A-NA-C1A	3.65	108.34	106.68
23	s	606	LMU	C2'-C3'-C4'	3.65	117.96	109.68
16	h	510	CLA	C4A-NA-C1A	3.65	108.34	106.68
16	X	512	CLA	C4A-NA-C1A	3.64	108.34	106.68
16	s	506	CLA	C4A-NA-C1A	3.64	108.34	106.68
19	K	4005	BCR	C2-C1-C6	3.64	115.72	110.44
19	k	4005	BCR	C2-C1-C6	3.63	115.72	110.44
16	U	1501	CLA	C4A-NA-C1A	3.63	108.33	106.68
16	q	513	CLA	C4A-NA-C1A	3.62	108.33	106.68
16	W	502	CLA	C4A-NA-C1A	3.62	108.33	106.68
16	a	1102	CLA	C4A-NA-C1A	3.61	108.33	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	q	512	CLA	C4A-NA-C1A	3.61	108.33	106.68
16	b	1203	CLA	C4A-NA-C1A	3.61	108.33	106.68
16	A	1111	CLA	OBD-CAD-C3D	-3.61	119.98	128.42
23	Y	606	LMU	C4B-C3B-C2B	3.61	117.16	110.83
24	w	601	LUT	C38-C25-C24	-3.60	114.83	123.36
21	R	4020	ECH	C12-C13-C14	3.60	124.67	119.01
16	v	504	CLA	C4A-NA-C1A	3.59	108.32	106.68
16	B	1209	CLA	C4A-NA-C1A	3.58	108.31	106.68
16	A	1135	CLA	C4A-NA-C1A	3.56	108.30	106.68
16	H	1101	CLA	CHD-C1D-ND	-3.56	119.79	124.80
21	M	4021	ECH	C1-C6-C5	-3.55	117.78	122.64
16	Y	507	CLA	C4A-NA-C1A	3.55	108.30	106.68
16	F	1302	CLA	C4A-NA-C1A	3.55	108.30	106.68
21	B	4006	ECH	C33-C5-C6	-3.55	120.61	124.48
16	n	502	CLA	C4A-NA-C1A	3.54	108.30	106.68
16	b	1213	CLA	C4A-NA-C1A	3.54	108.30	106.68
19	v	601	BCR	C2-C1-C6	3.54	115.58	110.44
16	b	1218	CLA	C4A-NA-C1A	3.54	108.29	106.68
19	a	4007	BCR	C15-C16-C17	-3.53	116.29	123.52
16	b	1210	CLA	C4A-NA-C1A	3.53	108.29	106.68
16	p	515	CLA	C4A-NA-C1A	3.52	108.29	106.68
16	r	510	CLA	C4A-NA-C1A	3.52	108.29	106.68
16	A	1132	CLA	C4A-NA-C1A	3.52	108.28	106.68
16	u	509	CLA	C4A-NA-C1A	3.52	108.28	106.68
16	u	502	CLA	C4A-NA-C1A	3.51	108.28	106.68
19	b	4014	BCR	C15-C16-C17	-3.50	116.35	123.52
16	s	514	CLA	CHD-C1D-ND	-3.50	119.87	124.80
19	g	601	BCR	C15-C16-C17	-3.50	116.35	123.52
16	a	1115	CLA	CHD-C1D-ND	-3.50	119.88	124.80
23	g	606	LMU	C2'-C3'-C4'	3.50	117.62	109.68
16	L	1502	CLA	CHD-C1D-ND	-3.50	119.88	124.80
16	f	1302	CLA	C4A-NA-C1A	3.50	108.27	106.68
21	m	4021	ECH	C8-C9-C10	3.49	124.50	119.01
16	y	504	CLA	C4A-NA-C1A	3.49	108.27	106.68
16	A	1129	CLA	C4A-NA-C1A	3.49	108.27	106.68
16	X	501	CLA	C4A-NA-C1A	3.49	108.27	106.68
16	a	1129	CLA	C4A-NA-C1A	3.48	108.27	106.68
19	Z	602	BCR	C2-C1-C6	3.48	115.49	110.44
16	H	1118	CLA	C4A-NA-C1A	3.47	108.26	106.68
16	B	1210	CLA	C4A-NA-C1A	3.46	108.26	106.68
19	u	601	BCR	C2-C1-C6	3.46	115.46	110.44
21	R	4020	ECH	C11-C10-C9	-3.45	122.44	127.28

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	4006	ECH	C33-C5-C6	-3.45	120.72	124.48
16	Q	1302	CLA	C4A-NA-C1A	3.45	108.25	106.68
16	n	511	CLA	C4A-NA-C1A	3.44	108.25	106.68
19	x	604	BCR	C24-C23-C22	-3.44	121.14	126.23
21	M	4021	ECH	C33-C5-C6	-3.44	120.73	124.48
16	o	502	CLA	C4A-NA-C1A	3.44	108.25	106.68
19	U	4022	BCR	C28-C27-C26	-3.43	107.94	114.06
16	t	514	CLA	CHD-C1D-ND	-3.43	119.98	124.80
16	l	1501	CLA	C4A-NA-C1A	3.43	108.24	106.68
19	o	601	BCR	C2-C1-C6	3.43	115.42	110.44
16	G	1239	CLA	C4A-NA-C1A	3.42	108.24	106.68
16	p	507	CLA	C4A-NA-C1A	3.42	108.24	106.68
23	p	606	LMU	C4B-C3B-C2B	3.41	116.82	110.83
23	Y	606	LMU	C2'-C3'-C4'	3.41	117.42	109.68
21	m	4021	ECH	C1-C6-C5	-3.41	117.98	122.64
16	B	1234	CLA	C4A-NA-C1A	3.41	108.23	106.68
19	H	4008	BCR	C15-C14-C13	-3.41	122.50	127.28
19	H	4007	BCR	C15-C16-C17	-3.40	116.55	123.52
16	G	1235	CLA	C2A-C1A-CHA	3.40	129.78	123.87
16	t	504	CLA	C4A-NA-C1A	3.40	108.23	106.68
16	G	1218	CLA	C4A-NA-C1A	3.40	108.23	106.68
19	p	601	BCR	C2-C1-C6	3.39	115.37	110.44
19	L	4022	BCR	C2-C1-C6	3.39	115.37	110.44
21	G	4006	ECH	C35-C13-C14	-3.39	117.32	122.82
16	n	514	CLA	CHD-C1D-ND	-3.39	120.03	124.80
16	G	1229	CLA	CHD-C1D-ND	-3.39	120.03	124.80
21	B	4006	ECH	C1-C6-C5	-3.39	118.00	122.64
21	R	4020	ECH	C35-C13-C14	-3.39	117.33	122.82
16	g	509	CLA	C4A-NA-C1A	3.39	108.22	106.68
21	V	4021	ECH	C8-C9-C10	3.38	124.33	119.01
16	A	1116	CLA	C4A-NA-C1A	3.38	108.22	106.68
16	H	1126	CLA	CHD-C1D-ND	-3.38	120.05	124.80
21	b	4006	ECH	C35-C13-C14	-3.37	117.35	122.82
19	G	4010	BCR	C15-C16-C17	-3.37	116.62	123.52
16	b	1235	CLA	CAA-C2A-C3A	-3.37	103.89	113.00
19	w	602	BCR	C15-C16-C17	-3.37	116.63	123.52
16	b	1012	CLA	CMB-C2B-C1B	-3.37	123.53	128.46
23	g	606	LMU	O5'-C5'-C4'	3.36	116.67	109.72
19	X	601	BCR	C15-C16-C17	-3.36	116.65	123.52
16	X	513	CLA	C4A-NA-C1A	3.36	108.21	106.68
19	X	604	BCR	C15-C14-C13	-3.35	122.58	127.28
19	g	604	BCR	C24-C23-C22	-3.35	121.28	126.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	y	510	CLA	C4A-NA-C1A	3.34	108.20	106.68
16	g	501	CLA	C4A-NA-C1A	3.34	108.20	106.68
19	X	601	BCR	C24-C23-C22	-3.33	121.31	126.23
23	Y	606	LMU	C1B-O1B-C4'	-3.33	110.09	117.98
19	i	4018	BCR	C2-C1-C6	3.33	115.27	110.44
16	B	1201	CLA	C4A-NA-C1A	3.32	108.19	106.68
19	u	603	BCR	C3-C4-C5	-3.32	108.14	114.06
16	A	1113	CLA	C4A-NA-C1A	3.32	108.19	106.68
16	H	1132	CLA	C4A-NA-C1A	3.32	108.19	106.68
16	a	1013	CLA	CHD-C1D-ND	-3.32	120.14	124.80
16	X	514	CLA	CHD-C1D-ND	-3.31	120.14	124.80
19	q	602	BCR	C15-C16-C17	-3.31	116.75	123.52
16	q	506	CLA	C4A-NA-C1A	3.31	108.19	106.68
16	u	505	CLA	CHD-C1D-ND	-3.31	120.15	124.80
19	r	601	BCR	C15-C16-C17	-3.30	116.76	123.52
21	i	4020	ECH	C33-C5-C6	-3.30	120.88	124.48
21	B	4006	ECH	C35-C13-C14	-3.30	117.47	122.82
19	Z	602	BCR	C15-C16-C17	-3.30	116.77	123.52
21	R	4020	ECH	C24-C23-C22	3.30	131.11	126.23
16	x	514	CLA	C4A-NA-C1A	3.29	108.18	106.68
19	s	601	BCR	C15-C16-C17	-3.29	116.79	123.52
19	h	603	BCR	C24-C23-C22	-3.28	121.38	126.23
21	G	4006	ECH	C1-C6-C5	-3.28	118.15	122.64
19	r	604	BCR	C24-C23-C22	-3.28	121.38	126.23
16	v	507	CLA	C4A-NA-C1A	3.28	108.17	106.68
21	i	4020	ECH	C7-C8-C9	3.28	131.08	126.23
19	o	603	BCR	C2-C1-C6	3.28	115.20	110.44
19	y	604	BCR	C3-C4-C5	-3.27	108.23	114.06
16	A	1111	CLA	CHD-C1D-ND	-3.27	120.21	124.80
21	M	4021	ECH	C8-C9-C10	3.26	124.14	119.01
21	M	4021	ECH	C35-C13-C14	-3.25	117.55	122.82
23	r	606	LMU	C1B-O1B-C4'	-3.25	110.27	117.98
16	B	1023	CLA	CHD-C1D-ND	-3.25	120.23	124.80
16	G	1212	CLA	CHD-C1D-ND	-3.25	120.23	124.80
16	B	1235	CLA	C2A-C1A-CHA	3.24	129.49	123.87
16	G	1234	CLA	CMB-C2B-C1B	-3.24	123.71	128.46
23	x	606	LMU	C1B-O1B-C4'	-3.24	110.30	117.98
16	s	507	CLA	C4A-NA-C1A	3.24	108.16	106.68
16	H	1105	CLA	CHD-C1D-ND	-3.24	120.25	124.80
16	G	1235	CLA	CAA-C2A-C3A	-3.24	104.25	113.00
16	u	514	CLA	CHD-C1D-ND	-3.23	120.25	124.80
21	m	4021	ECH	C34-C9-C10	-3.23	117.58	122.82

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	n	507	CLA	C4A-NA-C1A	3.23	108.15	106.68
19	b	4014	BCR	C11-C10-C9	-3.23	122.75	127.28
16	B	1223	CLA	C4A-NA-C1A	3.22	108.15	106.68
19	B	4004	BCR	C24-C23-C22	-3.22	121.47	126.23
21	V	4021	ECH	C35-C13-C14	-3.22	117.60	122.82
16	y	509	CLA	C4A-NA-C1A	3.22	108.15	106.68
19	A	4008	BCR	C15-C14-C13	-3.22	122.77	127.28
19	o	601	BCR	C15-C16-C17	-3.22	116.94	123.52
21	V	4021	ECH	C34-C9-C10	-3.22	117.61	122.82
16	B	1238	CLA	C4A-NA-C1A	3.21	108.14	106.68
15	H	1011	CL0	C4A-NA-C1A	3.21	108.14	106.68
16	g	514	CLA	CHD-C1D-ND	-3.21	120.29	124.80
19	u	601	BCR	C15-C16-C17	-3.21	116.96	123.52
16	G	1201	CLA	C4A-NA-C1A	3.21	108.14	106.68
16	b	1209	CLA	C4A-NA-C1A	3.21	108.14	106.68
20	L	4101	LMT	C3'-C4'-C5'	-3.21	103.82	110.93
16	g	507	CLA	C4A-NA-C1A	3.20	108.14	106.68
16	A	1107	CLA	C4A-NA-C1A	3.20	108.14	106.68
16	B	1234	CLA	CMB-C2B-C1B	-3.20	123.77	128.46
16	G	1214	CLA	C4A-NA-C1A	3.19	108.14	106.68
19	s	602	BCR	C2-C1-C6	3.19	115.08	110.44
16	A	1120	CLA	C4A-NA-C1A	3.19	108.13	106.68
21	m	4021	ECH	C35-C13-C14	-3.19	117.65	122.82
21	G	4006	ECH	C12-C13-C14	3.19	124.02	119.01
23	p	606	LMU	C1B-O1B-C4'	-3.19	110.43	117.98
19	o	602	BCR	C2-C1-C6	3.18	115.06	110.44
19	o	603	BCR	C3-C4-C5	-3.18	108.38	114.06
16	Z	513	CLA	C4A-NA-C1A	3.18	108.13	106.68
21	B	4006	ECH	C8-C9-C10	3.18	124.02	119.01
16	G	1023	CLA	C4A-NA-C1A	3.18	108.13	106.68
16	g	504	CLA	C4A-NA-C1A	3.18	108.13	106.68
16	a	1132	CLA	CAA-CBA-CGA	-3.17	104.20	113.21
24	w	601	LUT	C22-C23-C24	-3.17	106.48	111.18
21	I	4020	ECH	C24-C23-C22	3.17	130.92	126.23
23	s	606	LMU	C1B-O1B-C4'	-3.16	110.48	117.98
19	u	602	BCR	C2-C1-C6	3.16	115.03	110.44
19	v	601	BCR	C15-C16-C17	-3.16	117.05	123.52
19	b	4004	BCR	C24-C23-C22	-3.16	121.56	126.23
19	H	4008	BCR	C15-C16-C17	-3.16	117.06	123.52
16	A	1136	CLA	C4A-NA-C1A	3.16	108.12	106.68
19	A	4007	BCR	C11-C10-C9	-3.15	122.85	127.28
16	o	514	CLA	CHD-C1D-ND	-3.15	120.36	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	u	603	BCR	C2-C1-C6	3.15	115.02	110.44
16	Z	504	CLA	C4A-NA-C1A	3.15	108.12	106.68
24	q	601	LUT	C31-C32-C33	-3.15	117.73	126.36
19	w	604	BCR	C24-C23-C22	-3.14	121.58	126.23
21	b	4006	ECH	C12-C13-C14	3.14	123.95	119.01
16	W	514	CLA	CHD-C1D-ND	-3.14	120.38	124.80
16	A	1101	CLA	CHD-C1D-ND	-3.14	120.39	124.80
16	y	502	CLA	C4A-NA-C1A	3.14	108.11	106.68
21	G	4006	ECH	C33-C5-C6	-3.14	121.06	124.48
19	h	601	BCR	C27-C26-C25	3.13	126.94	122.70
21	i	4020	ECH	C24-C23-C22	3.13	130.87	126.23
16	G	1023	CLA	CHD-C1D-ND	-3.13	120.40	124.80
19	U	4019	BCR	C15-C16-C17	-3.13	117.12	123.52
16	H	1115	CLA	CHD-C1D-ND	-3.13	120.40	124.80
19	Y	602	BCR	C2-C1-C6	3.12	114.97	110.44
19	y	604	BCR	C2-C1-C6	3.12	114.97	110.44
16	t	513	CLA	C4A-NA-C1A	3.12	108.10	106.68
16	s	503	CLA	C3C-C4C-NC	-3.12	106.44	110.43
16	A	1121	CLA	C4A-NA-C1A	3.11	108.10	106.68
16	x	509	CLA	C4A-NA-C1A	3.11	108.10	106.68
16	p	506	CLA	C4A-NA-C1A	3.11	108.10	106.68
16	G	1238	CLA	C4A-NA-C1A	3.11	108.10	106.68
16	H	1116	CLA	C4A-NA-C1A	3.11	108.10	106.68
16	a	1124	CLA	C4A-NA-C1A	3.11	108.10	106.68
24	w	601	LUT	C7-C8-C9	-3.10	121.65	126.23
21	M	4021	ECH	C34-C9-C10	-3.10	117.80	122.82
13	a	851	LHG	O8-C23-C24	3.10	120.55	111.15
19	y	603	BCR	C24-C23-C22	-3.10	121.66	126.23
16	G	1213	CLA	C4A-NA-C1A	3.09	108.09	106.68
16	B	1229	CLA	CHD-C1D-ND	-3.09	120.45	124.80
19	n	604	BCR	C2-C1-C6	3.09	114.92	110.44
19	B	4004	BCR	C15-C16-C17	-3.09	117.21	123.52
19	b	4014	BCR	C29-C30-C25	3.08	114.92	110.44
16	a	1132	CLA	CHD-C1D-ND	-3.08	120.46	124.80
16	x	516	CLA	CHD-C1D-ND	-3.08	120.46	124.80
19	G	4009	BCR	C15-C16-C17	-3.08	117.22	123.52
16	s	509	CLA	C4A-NA-C1A	3.08	108.08	106.68
19	p	602	BCR	C2-C1-C6	3.07	114.90	110.44
16	Z	516	CLA	CHD-C1D-ND	-3.07	120.49	124.80
21	R	4020	ECH	C2-C1-C6	3.07	114.89	110.44
19	A	4011	BCR	C28-C27-C26	-3.06	108.59	114.06
19	x	601	BCR	C24-C23-C22	-3.06	121.70	126.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	r	514	CLA	CHD-C1D-ND	-3.06	120.49	124.80
19	X	602	BCR	C2-C1-C6	3.06	114.88	110.44
19	W	604	BCR	C2-C1-C6	3.06	114.88	110.44
16	q	504	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
16	A	1132	CLA	CHD-C1D-ND	-3.06	120.50	124.80
16	G	1220	CLA	C4A-NA-C1A	3.05	108.07	106.68
16	x	513	CLA	CHA-C1A-NA	-3.05	119.48	126.39
16	W	503	CLA	CHD-C1D-ND	-3.05	120.51	124.80
19	b	4009	BCR	C15-C16-C17	-3.05	117.28	123.52
16	p	514	CLA	CHD-C1D-ND	-3.05	120.51	124.80
19	v	603	BCR	C39-C30-C25	3.05	115.02	110.24
16	p	508	CLA	C4A-NA-C1A	3.05	108.07	106.68
16	s	506	CLA	CHD-C1D-ND	-3.05	120.52	124.80
19	u	602	BCR	C3-C4-C5	-3.04	108.63	114.06
16	G	1236	CLA	C4A-NA-C1A	3.04	108.07	106.68
16	X	507	CLA	C4A-NA-C1A	3.04	108.07	106.68
16	a	1101	CLA	C4A-NA-C1A	3.04	108.07	106.68
19	W	603	BCR	C15-C16-C17	-3.04	117.30	123.52
19	u	601	BCR	C24-C23-C22	-3.04	121.74	126.23
19	A	4008	BCR	C15-C16-C17	-3.04	117.31	123.52
19	s	602	BCR	C15-C16-C17	-3.03	117.31	123.52
16	b	1206	CLA	CMB-C2B-C1B	-3.03	124.02	128.46
16	H	1103	CLA	CHD-C1D-ND	-3.03	120.54	124.80
16	U	1502	CLA	CHD-C1D-ND	-3.03	120.54	124.80
17	A	2001	PQN	C14-C13-C15	3.03	120.48	115.23
13	A	851	LHG	O8-C23-C24	3.03	120.34	111.15
19	Z	604	BCR	C24-C23-C22	-3.02	121.76	126.23
16	q	503	CLA	C4A-NA-C1A	3.02	108.06	106.68
16	H	1022	CLA	C4A-NA-C1A	3.02	108.06	106.68
16	r	507	CLA	C4A-NA-C1A	3.02	108.06	106.68
16	Y	504	CLA	CHD-C1D-ND	-3.02	120.55	124.80
21	I	4020	ECH	C35-C13-C14	-3.02	117.92	122.82
16	B	1235	CLA	CAA-C2A-C3A	-3.02	104.84	113.00
16	A	1123	CLA	CHD-C1D-ND	-3.02	120.56	124.80
19	A	4007	BCR	C15-C16-C17	-3.02	117.34	123.52
24	w	601	LUT	C31-C32-C33	-3.02	118.09	126.36
19	F	4016	BCR	C11-C10-C9	-3.02	123.05	127.28
19	b	4010	BCR	C24-C23-C22	-3.01	121.78	126.23
16	K	4003	CLA	C4A-NA-C1A	3.01	108.05	106.68
16	A	1103	CLA	CHD-C1D-ND	-3.01	120.56	124.80
19	X	604	BCR	C11-C10-C9	-3.01	123.06	127.28
19	X	604	BCR	C15-C16-C17	-3.01	117.37	123.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	W	604	BCR	C15-C16-C17	-3.01	117.37	123.52
16	o	512	CLA	CAA-CBA-CGA	-3.00	104.68	113.21
16	H	1111	CLA	CHD-C1D-ND	-3.00	120.58	124.80
19	o	602	BCR	C3-C4-C5	-3.00	108.71	114.06
19	x	603	BCR	C11-C10-C9	-3.00	123.07	127.28
16	q	503	CLA	C2D-C1D-ND	-3.00	107.16	110.13
16	p	511	CLA	CHD-C1D-ND	-3.00	120.58	124.80
16	H	1136	CLA	C4A-NA-C1A	2.99	108.04	106.68
16	A	1132	CLA	CAA-CBA-CGA	-2.99	104.72	113.21
16	B	1216	CLA	CMB-C2B-C1B	-2.99	124.08	128.46
16	n	512	CLA	CHA-C1A-NA	-2.99	119.63	126.39
16	b	1202	CLA	CHD-C1D-ND	-2.99	120.60	124.80
16	Y	516	CLA	C4A-NA-C1A	2.99	108.04	106.68
16	G	1207	CLA	CHA-C1A-NA	-2.98	119.63	126.39
16	v	517	CLA	C4A-NA-C1A	2.98	108.04	106.68
19	H	4007	BCR	C11-C10-C9	-2.98	123.10	127.28
16	Z	509	CLA	CHD-C1D-ND	-2.98	120.61	124.80
16	B	1206	CLA	CMB-C2B-C1B	-2.98	124.09	128.46
16	u	504	CLA	C4A-NA-C1A	2.98	108.04	106.68
19	S	4013	BCR	C27-C26-C25	2.98	126.73	122.70
19	p	601	BCR	C27-C26-C25	2.98	126.72	122.70
16	r	512	CLA	CHA-C1A-NA	-2.98	119.65	126.39
19	Y	601	BCR	C27-C26-C25	2.97	126.72	122.70
13	H	851	LHG	O8-C23-C24	2.97	120.16	111.15
16	A	1128	CLA	CHD-C1D-ND	-2.97	120.62	124.80
16	u	506	CLA	C1C-C2C-C3C	-2.96	103.86	106.98
19	q	604	BCR	C24-C23-C22	-2.96	121.85	126.23
16	H	1132	CLA	CAA-CBA-CGA	-2.96	104.79	113.21
16	u	507	CLA	C4A-NA-C1A	2.96	108.03	106.68
16	a	1101	CLA	CHD-C1D-ND	-2.96	120.63	124.80
23	s	606	LMU	C4B-C3B-C2B	2.96	116.03	110.83
16	B	1207	CLA	CHA-C1A-NA	-2.96	119.69	126.39
19	b	4009	BCR	C24-C23-C22	-2.96	121.86	126.23
16	v	508	CLA	CHD-C1D-ND	-2.96	120.64	124.80
16	r	509	CLA	C4A-NA-C1A	2.95	108.03	106.68
19	j	4015	BCR	C11-C10-C9	-2.95	123.14	127.28
19	a	4008	BCR	C15-C14-C13	-2.95	123.14	127.28
16	b	1207	CLA	CHA-C1A-NA	-2.95	119.71	126.39
16	r	513	CLA	C4A-NA-C1A	2.95	108.02	106.68
19	g	604	BCR	C15-C16-C17	-2.95	117.49	123.52
24	q	601	LUT	C22-C23-C24	-2.95	106.81	111.18
16	T	4003	CLA	C4A-NA-C1A	2.95	108.02	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	r	604	BCR	C15-C16-C17	-2.94	117.49	123.52
19	Q	4016	BCR	C11-C10-C9	-2.94	123.15	127.28
16	G	1229	CLA	C4A-NA-C1A	2.94	108.02	106.68
16	H	1129	CLA	C4A-NA-C1A	2.94	108.02	106.68
16	s	508	CLA	C4A-NA-C1A	2.94	108.02	106.68
16	w	503	CLA	CHD-C1D-ND	-2.94	120.67	124.80
14	H	4201	LMG	O6-C1-O1	-2.94	103.10	110.04
16	Z	514	CLA	C4A-NA-C1A	2.94	108.02	106.68
16	a	1137	CLA	C4A-NA-C1A	2.94	108.02	106.68
16	G	1231	CLA	CHA-C1A-NA	-2.94	119.73	126.39
19	n	604	BCR	C3-C4-C5	-2.94	108.81	114.06
16	x	515	CLA	CHD-C1D-ND	-2.94	120.67	124.80
19	a	4008	BCR	C28-C27-C26	-2.94	108.82	114.06
16	A	1125	CLA	C4A-NA-C1A	2.94	108.02	106.68
19	A	4011	BCR	C24-C23-C22	-2.94	121.89	126.23
19	s	602	BCR	C15-C14-C13	-2.94	123.16	127.28
19	s	601	BCR	C24-C23-C22	-2.94	121.89	126.23
16	u	506	CLA	CHA-C1A-NA	-2.93	119.75	126.39
16	A	1128	CLA	CMB-C2B-C1B	-2.93	124.16	128.46
16	h	511	CLA	CHD-C1D-ND	-2.93	120.67	124.80
19	n	603	BCR	C15-C16-C17	-2.93	117.52	123.52
16	o	509	CLA	C4A-NA-C1A	2.93	108.02	106.68
16	a	1136	CLA	C4A-NA-C1A	2.93	108.02	106.68
19	B	4010	BCR	C15-C16-C17	-2.93	117.52	123.52
16	b	1227	CLA	CHD-C1D-ND	-2.93	120.68	124.80
19	y	601	BCR	C15-C16-C17	-2.93	117.53	123.52
19	l	4019	BCR	C15-C16-C17	-2.93	117.53	123.52
14	A	4201	LMG	O6-C1-O1	-2.93	103.13	110.04
16	Z	504	CLA	CHD-C1D-ND	-2.93	120.69	124.80
19	a	4011	BCR	C31-C1-C6	2.93	114.83	110.24
16	v	508	CLA	C2D-C1D-ND	-2.92	107.23	110.13
19	S	4012	BCR	C27-C26-C25	2.92	126.65	122.70
19	h	601	BCR	C15-C16-C17	-2.92	117.54	123.52
19	A	4003	BCR	C30-C25-C26	-2.92	118.65	122.64
24	Z	601	LUT	C22-C23-C24	-2.92	106.85	111.18
16	B	1210	CLA	OBD-CAD-C3D	-2.92	121.60	128.42
16	W	502	CLA	CHD-C1D-ND	-2.91	120.70	124.80
19	p	602	BCR	C15-C16-C17	-2.91	117.56	123.52
16	t	514	CLA	C4A-NA-C1A	2.91	108.01	106.68
16	H	1103	CLA	C4A-NA-C1A	2.91	108.01	106.68
16	Z	502	CLA	C4A-NA-C1A	2.91	108.01	106.68
16	Y	512	CLA	CAA-C2A-C3A	-2.91	105.15	113.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	p	512	CLA	CHA-C1A-NA	-2.90	119.82	126.39
16	G	1227	CLA	CHD-C1D-ND	-2.90	120.72	124.80
20	U	4101	LMT	C3'-C4'-C5'	-2.90	104.50	110.93
19	p	601	BCR	C15-C16-C17	-2.90	117.58	123.52
19	K	4001	BCR	C24-C23-C22	-2.90	121.94	126.23
16	A	1130	CLA	CHD-C1D-ND	-2.90	120.72	124.80
16	Y	514	CLA	CHD-C1D-ND	-2.90	120.72	124.80
16	H	1124	CLA	CHD-C1D-ND	-2.90	120.73	124.80
19	G	4014	BCR	C20-C21-C22	-2.90	123.22	127.28
16	j	1303	CLA	C4A-NA-C1A	2.89	108.00	106.68
19	A	4007	BCR	C2-C1-C6	2.89	114.64	110.44
19	a	4008	BCR	C15-C16-C17	-2.89	117.60	123.52
19	g	601	BCR	C15-C14-C13	-2.89	123.22	127.28
16	B	1021	CLA	CHD-C1D-ND	-2.89	120.73	124.80
16	H	1132	CLA	CHD-C1D-ND	-2.89	120.74	124.80
16	Z	514	CLA	CHD-C1D-ND	-2.89	120.74	124.80
19	b	4004	BCR	C15-C16-C17	-2.89	117.61	123.52
16	p	512	CLA	C1-C2-C3	-2.89	121.47	126.20
19	G	4004	BCR	C24-C23-C22	-2.89	121.96	126.23
16	s	512	CLA	CHA-C1A-NA	-2.89	119.86	126.39
16	q	517	CLA	C4A-NA-C1A	2.88	107.99	106.68
16	G	1225	CLA	CHD-C1D-ND	-2.88	120.75	124.80
16	a	1104	CLA	CHD-C1D-ND	-2.88	120.75	124.80
16	G	1235	CLA	CHD-C1D-ND	-2.88	120.75	124.80
19	G	4010	BCR	C24-C23-C22	-2.88	121.98	126.23
16	u	517	CLA	C2A-C1A-CHA	2.88	128.86	123.87
19	A	4003	BCR	C27-C26-C25	2.87	126.58	122.70
19	b	4009	BCR	C27-C26-C25	2.87	126.58	122.70
23	g	606	LMU	C3'-C4'-C5'	2.87	117.29	110.93
14	a	4201	LMG	O6-C1-O1	-2.87	103.27	110.04
16	B	1222	CLA	C2A-C1A-CHA	2.87	128.84	123.87
16	A	1122	CLA	C4A-NA-C1A	2.87	107.99	106.68
16	a	1125	CLA	CHD-C1D-ND	-2.87	120.77	124.80
17	b	2002	PQN	C11-C12-C13	-2.87	121.89	126.83
13	G	4018	LHG	O8-C23-C24	2.87	120.57	111.83
16	w	511	CLA	CHD-C1D-ND	-2.86	120.77	124.80
19	Z	602	BCR	C27-C26-C25	2.86	126.57	122.70
21	B	4006	ECH	C12-C13-C14	2.86	123.51	119.01
21	I	4020	ECH	C2-C1-C6	2.86	114.59	110.44
16	A	1136	CLA	CHD-C1D-ND	-2.86	120.78	124.80
16	a	1117	CLA	CHD-C1D-ND	-2.86	120.78	124.80
19	l	4019	BCR	C15-C14-C13	-2.86	123.27	127.28

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	601	BCR	C15-C16-C17	-2.85	117.68	123.52
16	x	506	CLA	CHD-C1D-ND	-2.85	120.79	124.80
16	B	1229	CLA	C4A-NA-C1A	2.85	107.98	106.68
16	r	501	CLA	CHD-C1D-ND	-2.85	120.80	124.80
19	o	604	BCR	C15-C14-C13	-2.85	123.29	127.28
19	S	4013	BCR	C15-C16-C17	-2.85	117.69	123.52
19	u	603	BCR	C15-C16-C17	-2.85	117.70	123.52
16	G	1220	CLA	CHD-C1D-ND	-2.84	120.80	124.80
16	B	1235	CLA	CHD-C1D-ND	-2.84	120.80	124.80
16	b	1222	CLA	C2A-C1A-CHA	2.84	128.80	123.87
16	t	512	CLA	CHA-C1A-NA	-2.84	119.96	126.39
19	J	4012	BCR	C15-C16-C17	-2.84	117.71	123.52
16	x	504	CLA	C1-C2-C3	-2.84	121.55	126.20
16	q	505	CLA	C3C-C4C-NC	-2.84	106.80	110.43
16	Y	513	CLA	C4A-NA-C1A	2.83	107.97	106.68
19	G	4009	BCR	C27-C26-C25	2.83	126.53	122.70
16	a	1136	CLA	CHD-C1D-ND	-2.83	120.82	124.80
19	B	4009	BCR	C15-C16-C17	-2.83	117.73	123.52
19	b	4014	BCR	C24-C23-C22	-2.82	122.06	126.23
19	r	602	BCR	C24-C23-C22	-2.82	122.06	126.23
19	L	4019	BCR	C15-C16-C17	-2.82	117.75	123.52
19	x	604	BCR	C15-C16-C17	-2.82	117.75	123.52
16	a	1124	CLA	CHD-C1D-ND	-2.82	120.83	124.80
19	g	602	BCR	C24-C23-C22	-2.82	122.06	126.23
19	a	4007	BCR	C15-C14-C13	-2.82	123.33	127.28
19	r	602	BCR	C15-C16-C17	-2.82	117.75	123.52
19	s	602	BCR	C3-C4-C5	-2.82	109.03	114.06
19	H	4011	BCR	C28-C27-C26	-2.82	109.03	114.06
19	R	4018	BCR	C15-C16-C17	-2.81	117.76	123.52
16	h	507	CLA	CHD-C1D-ND	-2.81	120.84	124.80
16	g	512	CLA	CHA-C1A-NA	-2.81	120.02	126.39
19	X	604	BCR	C24-C23-C22	-2.81	122.07	126.23
16	B	1213	CLA	CHD-C1D-ND	-2.81	120.84	124.80
16	g	511	CLA	C4A-NA-C1A	2.81	107.96	106.68
16	v	507	CLA	CHD-C1D-ND	-2.81	120.84	124.80
16	X	506	CLA	CHA-C1A-NA	-2.81	120.03	126.39
16	W	512	CLA	CHA-C1A-NA	-2.81	120.03	126.39
19	v	603	BCR	C27-C26-C25	2.81	126.50	122.70
16	A	1137	CLA	C4A-NA-C1A	2.81	107.96	106.68
19	B	4009	BCR	C27-C26-C25	2.81	126.50	122.70
19	H	4007	BCR	C15-C14-C13	-2.81	123.34	127.28
19	b	4010	BCR	C15-C16-C17	-2.81	117.77	123.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1118	CLA	CHD-C1D-ND	-2.81	120.85	124.80
16	b	1234	CLA	CHA-C1A-NA	-2.81	120.03	126.39
16	H	1138	CLA	CHD-C1D-ND	-2.81	120.85	124.80
16	X	505	CLA	CHD-C1D-ND	-2.80	120.86	124.80
16	q	515	CLA	CHD-C1D-ND	-2.80	120.86	124.80
19	v	604	BCR	C27-C26-C25	2.80	126.49	122.70
16	a	1135	CLA	C4A-NA-C1A	2.80	107.96	106.68
16	B	1204	CLA	CHD-C1D-ND	-2.80	120.86	124.80
16	B	1210	CLA	CHD-C1D-ND	-2.80	120.86	124.80
16	a	1119	CLA	CHA-C1A-NA	-2.80	120.05	126.39
21	M	4021	ECH	C12-C13-C14	2.80	123.42	119.01
19	p	602	BCR	C15-C14-C13	-2.80	123.35	127.28
13	b	4018	LHG	O8-C23-C24	2.80	120.38	111.83
16	H	1013	CLA	CHD-C1D-ND	-2.80	120.86	124.80
19	j	4012	BCR	C27-C26-C25	2.80	126.49	122.70
16	Y	514	CLA	CHA-C1A-NA	-2.80	120.05	126.39
13	s	605	LHG	O8-C23-C24	2.80	120.37	111.83
19	Z	602	BCR	C24-C23-C22	-2.80	122.09	126.23
14	G	848	LMG	O6-C1-O1	-2.80	103.43	110.04
16	a	1013	CLA	CMB-C2B-C1B	-2.80	124.36	128.46
16	b	1239	CLA	CHD-C1D-ND	-2.79	120.87	124.80
16	o	515	CLA	CHA-C1A-NA	-2.79	120.07	126.39
16	h	506	CLA	C2D-C1D-ND	-2.79	107.36	110.13
16	G	1226	CLA	CMB-C2B-C1B	-2.79	124.37	128.46
19	S	4015	BCR	C15-C14-C13	-2.79	123.36	127.28
16	Y	509	CLA	CHA-C1A-NA	-2.79	120.08	126.39
16	r	517	CLA	C4A-NA-C1A	2.79	107.95	106.68
16	B	1220	CLA	CHD-C1D-ND	-2.79	120.88	124.80
19	L	4019	BCR	C15-C14-C13	-2.78	123.37	127.28
16	L	1501	CLA	C4A-NA-C1A	2.78	107.95	106.68
21	G	4006	ECH	C8-C9-C10	2.78	123.39	119.01
19	W	604	BCR	C15-C14-C13	-2.78	123.38	127.28
19	Z	602	BCR	C3-C4-C5	-2.78	109.10	114.06
16	Z	506	CLA	C4A-NA-C1A	2.78	107.95	106.68
16	H	1114	CLA	CHA-C1A-NA	-2.78	120.10	126.39
19	o	604	BCR	C15-C16-C17	-2.78	117.83	123.52
19	h	604	BCR	C27-C26-C25	2.78	126.46	122.70
19	o	601	BCR	C24-C23-C22	-2.78	122.13	126.23
16	o	505	CLA	CHD-C1D-ND	-2.77	120.90	124.80
16	A	1120	CLA	C3C-C4C-NC	-2.77	106.88	110.43
19	h	601	BCR	C15-C14-C13	-2.77	123.39	127.28
19	w	602	BCR	C15-C14-C13	-2.77	123.39	127.28

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	h	509	CLA	CHD-C1D-ND	-2.77	120.90	124.80
16	y	506	CLA	CMC-C2C-C1C	-2.77	120.71	125.03
16	A	1124	CLA	CHD-C1D-ND	-2.77	120.91	124.80
16	x	514	CLA	CHD-C1D-ND	-2.77	120.91	124.80
19	v	601	BCR	C15-C14-C13	-2.77	123.40	127.28
16	H	1117	CLA	CMB-C2B-C1B	-2.77	124.40	128.46
19	Y	602	BCR	C15-C16-C17	-2.77	117.86	123.52
19	Y	602	BCR	C15-C14-C13	-2.77	123.40	127.28
19	U	4019	BCR	C15-C14-C13	-2.76	123.40	127.28
19	i	4018	BCR	C11-C10-C9	-2.76	123.40	127.28
16	G	1012	CLA	CHD-C1D-ND	-2.76	120.91	124.80
16	b	1023	CLA	CHD-C1D-ND	-2.76	120.92	124.80
16	v	502	CLA	C4A-NA-C1A	2.76	107.94	106.68
16	r	515	CLA	CHD-C1D-ND	-2.76	120.92	124.80
16	u	506	CLA	C2C-C1C-NC	-2.76	107.08	109.98
13	x	605	LHG	O8-C23-C24	2.76	120.25	111.83
19	L	4019	BCR	C29-C30-C25	2.76	114.45	110.44
19	T	4001	BCR	C27-C26-C25	2.76	126.43	122.70
16	q	511	CLA	CHD-C1D-ND	-2.76	120.92	124.80
16	Z	512	CLA	CHA-C1A-NA	-2.76	120.15	126.39
16	h	515	CLA	C2A-C1A-CHA	2.76	128.65	123.87
16	A	1129	CLA	CHD-C1D-ND	-2.76	120.92	124.80
19	o	601	BCR	C15-C14-C13	-2.76	123.41	127.28
21	V	4021	ECH	C12-C13-C14	2.76	123.34	119.01
19	x	604	BCR	C7-C8-C9	-2.76	122.16	126.23
19	y	601	BCR	C15-C14-C13	-2.76	123.41	127.28
15	H	1011	CL0	CMB-C2B-C3B	2.75	130.19	124.68
21	B	4006	ECH	C34-C9-C10	-2.75	118.36	122.82
16	H	1114	CLA	CHD-C1D-ND	-2.75	120.93	124.80
16	a	1129	CLA	CHD-C1D-ND	-2.75	120.93	124.80
19	j	4013	BCR	C15-C16-C17	-2.75	117.89	123.52
16	w	504	CLA	CHD-C1D-ND	-2.75	120.93	124.80
15	a	1011	CL0	C4A-NA-C1A	2.75	107.93	106.68
16	b	1220	CLA	C4A-NA-C1A	2.75	107.93	106.68
16	A	1105	CLA	CHD-C1D-ND	-2.75	120.93	124.80
16	b	1204	CLA	CHD-C1D-ND	-2.75	120.93	124.80
16	Y	504	CLA	C4A-NA-C1A	2.75	107.93	106.68
16	y	506	CLA	C4A-NA-C1A	2.75	107.93	106.68
16	p	514	CLA	CHA-C1A-NA	-2.75	120.17	126.39
19	Z	602	BCR	C15-C14-C13	-2.75	123.42	127.28
16	v	503	CLA	CHD-C1D-ND	-2.75	120.94	124.80
16	t	503	CLA	CHD-C1D-ND	-2.75	120.94	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	s	512	CLA	C1-C2-C3	-2.75	121.70	126.20
16	H	1110	CLA	C4A-NA-C1A	2.75	107.93	106.68
16	X	509	CLA	CHA-C1A-NA	-2.75	120.17	126.39
16	q	514	CLA	CHD-C1D-ND	-2.75	120.94	124.80
16	B	1226	CLA	CMB-C2B-C1B	-2.75	124.43	128.46
19	u	604	BCR	C15-C16-C17	-2.75	117.90	123.52
19	j	4012	BCR	C15-C16-C17	-2.74	117.91	123.52
19	n	603	BCR	C15-C14-C13	-2.74	123.43	127.28
16	B	1202	CLA	CHD-C1D-ND	-2.74	120.94	124.80
16	H	1119	CLA	CHD-C1D-ND	-2.74	120.94	124.80
19	J	4012	BCR	C11-C10-C9	-2.74	123.43	127.28
19	a	4011	BCR	C15-C16-C17	-2.74	117.91	123.52
16	p	509	CLA	CHA-C1A-NA	-2.74	120.19	126.39
16	A	1127	CLA	CHD-C1D-ND	-2.74	120.95	124.80
16	A	1115	CLA	CHD-C1D-ND	-2.74	120.95	124.80
19	B	4009	BCR	C24-C23-C22	-2.74	122.18	126.23
19	j	4015	BCR	C15-C14-C13	-2.74	123.44	127.28
16	B	1215	CLA	CHD-C1D-ND	-2.74	120.95	124.80
19	x	601	BCR	C15-C16-C17	-2.74	117.92	123.52
16	y	505	CLA	CHD-C1D-ND	-2.74	120.95	124.80
19	g	601	BCR	C27-C26-C25	2.74	126.40	122.70
16	b	1203	CLA	CHD-C1D-ND	-2.74	120.95	124.80
16	B	1218	CLA	CHD-C1D-ND	-2.73	120.95	124.80
16	b	1213	CLA	CHD-C1D-ND	-2.73	120.95	124.80
16	b	1230	CLA	CMC-C2C-C1C	-2.73	120.76	125.03
19	l	4019	BCR	C27-C26-C25	2.73	126.40	122.70
19	G	4004	BCR	C15-C16-C17	-2.73	117.93	123.52
19	k	4001	BCR	C15-C16-C17	-2.73	117.93	123.52
19	p	602	BCR	C3-C4-C5	-2.73	109.19	114.06
20	l	4101	LMT	C3'-C4'-C5'	-2.73	104.88	110.93
19	U	4019	BCR	C27-C26-C25	2.73	126.39	122.70
16	G	1216	CLA	CHA-C1A-NA	-2.73	120.21	126.39
23	Z	605	LMU	O5'-C5'-C4'	2.73	115.36	109.72
23	x	606	LMU	C1'-O5'-C5'	2.73	119.05	113.72
16	b	1235	CLA	CHD-C1D-ND	-2.73	120.96	124.80
19	f	4016	BCR	C11-C10-C9	-2.73	123.45	127.28
16	a	1103	CLA	CHD-C1D-ND	-2.73	120.97	124.80
13	p	605	LHG	O8-C23-C24	2.73	120.15	111.83
16	s	517	CLA	CHA-C1A-NA	-2.72	120.22	126.39
19	W	603	BCR	C15-C14-C13	-2.72	123.46	127.28
13	B	4018	LHG	O8-C23-C24	2.72	120.14	111.83
16	s	509	CLA	CHA-C1A-NA	-2.72	120.22	126.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	y	604	BCR	C27-C26-C25	2.72	126.38	122.70
21	m	4021	ECH	C12-C13-C14	2.72	123.29	119.01
16	w	514	CLA	CHD-C1D-ND	-2.72	120.97	124.80
14	B	848	LMG	O6-C1-O1	-2.72	103.61	110.04
16	h	517	CLA	CHD-C1D-ND	-2.72	120.97	124.80
16	n	517	CLA	CHD-C1D-ND	-2.72	120.97	124.80
16	B	1221	CLA	CHD-C1D-ND	-2.72	120.97	124.80
16	A	1101	CLA	C4A-NA-C1A	2.72	107.92	106.68
16	p	505	CLA	C4A-NA-C1A	2.72	107.92	106.68
16	B	1227	CLA	CHD-C1D-ND	-2.72	120.97	124.80
13	r	605	LHG	O8-C23-C24	2.72	120.12	111.83
16	W	517	CLA	CHD-C1D-ND	-2.72	120.98	124.80
19	t	604	BCR	C15-C16-C17	-2.72	117.96	123.52
16	h	514	CLA	CHA-C1A-NA	-2.71	120.25	126.39
16	Y	503	CLA	CHD-C1D-ND	-2.71	120.99	124.80
16	B	1225	CLA	CMB-C2B-C1B	-2.71	124.48	128.46
24	q	601	LUT	C1-C6-C5	-2.71	118.93	122.64
16	b	1012	CLA	C4A-NA-C1A	2.71	107.92	106.68
16	H	1117	CLA	CHD-C1D-ND	-2.71	120.99	124.80
19	y	601	BCR	C27-C26-C25	2.71	126.36	122.70
16	b	1235	CLA	C2A-C1A-CHA	2.71	128.57	123.87
19	a	4007	BCR	C11-C10-C9	-2.71	123.48	127.28
19	h	603	BCR	C27-C26-C25	2.71	126.36	122.70
19	x	603	BCR	C24-C23-C22	-2.71	122.23	126.23
19	s	604	BCR	C24-C23-C22	-2.71	122.23	126.23
19	x	602	BCR	C15-C16-C17	-2.71	117.98	123.52
16	X	506	CLA	CHD-C1D-ND	-2.71	121.00	124.80
19	G	4010	BCR	C15-C14-C13	-2.71	123.48	127.28
19	B	4014	BCR	C20-C21-C22	-2.70	123.48	127.28
16	s	511	CLA	CHD-C1D-ND	-2.70	121.00	124.80
19	Y	602	BCR	C3-C4-C5	-2.70	109.23	114.06
19	W	604	BCR	C3-C4-C5	-2.70	109.23	114.06
19	L	4022	BCR	C27-C26-C25	2.70	126.35	122.70
19	o	603	BCR	C27-C26-C25	2.70	126.35	122.70
16	f	1301	CLA	C4A-NA-C1A	2.70	107.91	106.68
16	x	502	CLA	C4A-NA-C1A	2.70	107.91	106.68
16	q	517	CLA	C2A-C1A-CHA	2.70	128.55	123.87
19	k	4001	BCR	C24-C23-C22	-2.70	122.24	126.23
19	s	604	BCR	C27-C26-C25	2.70	126.35	122.70
16	o	512	CLA	CHA-C1A-NA	-2.70	120.28	126.39
16	r	505	CLA	CHA-C1A-NA	-2.70	120.28	126.39
19	x	604	BCR	C15-C14-C13	-2.70	123.49	127.28

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	606	LMU	O5B-C5B-C4B	2.70	114.56	109.70
13	Y	605	LHG	O8-C23-C24	2.70	120.06	111.83
16	a	1139	CLA	C4A-NA-C1A	2.70	107.91	106.68
16	a	1117	CLA	CMB-C2B-C1B	-2.70	124.50	128.46
19	b	4005	BCR	C15-C16-C17	-2.70	118.00	123.52
16	q	509	CLA	CHD-C1D-ND	-2.70	121.01	124.80
19	W	601	BCR	C28-C27-C26	-2.70	109.25	114.06
17	B	2002	PQN	C14-C13-C15	2.70	119.91	115.23
16	b	1236	CLA	C4A-NA-C1A	2.70	107.91	106.68
16	G	1213	CLA	CHD-C1D-ND	-2.69	121.01	124.80
14	H	4101	LMG	O6-C1-O1	-2.69	103.68	110.04
16	v	511	CLA	CHD-C1D-ND	-2.69	121.01	124.80
19	k	4001	BCR	C15-C14-C13	-2.69	123.50	127.28
16	k	4003	CLA	CHD-C1D-ND	-2.69	121.02	124.80
19	u	601	BCR	C3-C4-C5	-2.69	109.26	114.06
16	q	512	CLA	CHA-C1A-NA	-2.69	120.30	126.39
16	q	504	CLA	CHD-C1D-ND	-2.69	121.02	124.80
21	b	4006	ECH	C8-C9-C10	2.69	123.24	119.01
16	y	514	CLA	CHD-C1D-ND	-2.69	121.02	124.80
19	v	601	BCR	C27-C26-C25	2.69	126.34	122.70
16	G	1235	CLA	C1-C2-C3	-2.69	121.79	126.20
21	i	4020	ECH	C35-C13-C14	-2.69	118.46	122.82
16	o	507	CLA	CHD-C1D-ND	-2.69	121.02	124.80
16	y	501	CLA	CHD-C1D-ND	-2.69	121.02	124.80
19	B	4004	BCR	C15-C14-C13	-2.69	123.51	127.28
19	i	4018	BCR	C15-C16-C17	-2.68	118.03	123.52
19	X	603	BCR	C27-C26-C25	2.68	126.33	122.70
16	n	514	CLA	CHA-C1A-NA	-2.68	120.31	126.39
19	q	602	BCR	C15-C14-C13	-2.68	123.52	127.28
19	B	4014	BCR	C11-C10-C9	-2.68	123.52	127.28
16	v	512	CLA	CHA-C1A-NA	-2.68	120.33	126.39
16	b	1230	CLA	C4A-NA-C1A	2.68	107.90	106.68
16	t	514	CLA	CHA-C1A-NA	-2.68	120.33	126.39
14	a	4101	LMG	O6-C1-O1	-2.68	103.72	110.04
19	q	604	BCR	C11-C10-C9	-2.68	123.53	127.28
21	G	4006	ECH	C34-C9-C10	-2.67	118.48	122.82
19	r	601	BCR	C15-C14-C13	-2.67	123.53	127.28
16	x	504	CLA	CHD-C1D-ND	-2.67	121.04	124.80
16	W	509	CLA	CHA-C1A-NA	-2.67	120.34	126.39
19	p	604	BCR	C27-C26-C25	2.67	126.32	122.70
19	u	604	BCR	C15-C14-C13	-2.67	123.53	127.28
16	A	1117	CLA	CHD-C1D-ND	-2.67	121.05	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	g	601	BCR	C11-C10-C9	-2.67	123.53	127.28
16	H	1102	CLA	CHD-C1D-ND	-2.67	121.05	124.80
16	a	1105	CLA	CHD-C1D-ND	-2.67	121.05	124.80
16	w	504	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
16	y	514	CLA	C4A-NA-C1A	2.67	107.90	106.68
16	x	505	CLA	CHD-C1D-ND	-2.67	121.05	124.80
17	H	2001	PQN	C11-C12-C13	-2.67	122.24	126.83
16	w	512	CLA	CHA-C1A-NA	-2.66	120.36	126.39
16	B	1212	CLA	CHD-C1D-ND	-2.66	121.05	124.80
16	H	1106	CLA	CHD-C1D-ND	-2.66	121.05	124.80
16	a	1110	CLA	CHD-C1D-ND	-2.66	121.05	124.80
16	Q	1301	CLA	CHA-C1A-NA	-2.66	120.36	126.39
16	g	504	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	I	4018	BCR	C11-C10-C9	-2.66	123.54	127.28
19	v	601	BCR	C24-C23-C22	-2.66	122.30	126.23
16	G	1205	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	k	4001	BCR	C27-C26-C25	2.66	126.30	122.70
16	u	501	CLA	C4A-NA-C1A	2.66	107.89	106.68
16	y	511	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	g	603	BCR	C11-C10-C9	-2.66	123.55	127.28
19	w	602	BCR	C27-C26-C25	2.66	126.30	122.70
16	H	1125	CLA	CHD-C1D-ND	-2.66	121.06	124.80
16	H	1121	CLA	CHD-C1D-ND	-2.66	121.06	124.80
16	B	1012	CLA	C4A-NA-C1A	2.66	107.89	106.68
16	B	1208	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	Y	604	BCR	C27-C26-C25	2.66	126.29	122.70
16	w	501	CLA	CHD-C1D-ND	-2.66	121.06	124.80
16	B	1203	CLA	CHD-C1D-ND	-2.66	121.07	124.80
16	b	1229	CLA	CHD-C1D-ND	-2.66	121.07	124.80
16	x	512	CLA	CHA-C1A-NA	-2.65	120.38	126.39
17	G	2002	PQN	C11-C12-C13	-2.65	122.26	126.83
19	b	4010	BCR	C40-C30-C25	2.65	114.41	110.24
19	s	603	BCR	C15-C16-C17	-2.65	118.09	123.52
19	G	4014	BCR	C27-C26-C25	2.65	126.29	122.70
16	A	1114	CLA	CHA-C1A-NA	-2.65	120.38	126.39
19	p	604	BCR	C24-C23-C22	-2.65	122.31	126.23
16	w	506	CLA	CHD-C1D-ND	-2.65	121.07	124.80
19	G	4017	BCR	C27-C26-C25	2.65	126.29	122.70
16	n	508	CLA	CHD-C1D-ND	-2.65	121.07	124.80
16	o	516	CLA	CHD-C1D-ND	-2.65	121.07	124.80
19	U	4019	BCR	C11-C10-C9	-2.65	123.56	127.28
16	Z	503	CLA	CHD-C1D-ND	-2.65	121.07	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	r	603	BCR	C27-C26-C25	2.65	126.28	122.70
16	G	1240	CLA	C2C-C1C-NC	-2.65	107.20	109.98
21	I	4020	ECH	C12-C13-C14	2.65	123.17	119.01
16	h	503	CLA	CHD-C1D-ND	-2.65	121.08	124.80
19	W	601	BCR	C15-C16-C17	-2.65	118.10	123.52
19	S	4013	BCR	C31-C1-C6	2.65	114.39	110.24
23	Z	605	LMU	O5'-C1'-C2'	2.65	115.81	110.37
19	J	4015	BCR	C15-C14-C13	-2.65	123.57	127.28
13	g	605	LHG	O8-C23-C24	2.65	119.90	111.83
19	g	603	BCR	C27-C26-C25	2.65	126.28	122.70
19	G	4004	BCR	C27-C26-C25	2.64	126.28	122.70
16	Y	502	CLA	CHD-C1D-ND	-2.64	121.08	124.80
19	I	4018	BCR	C15-C16-C17	-2.64	118.11	123.52
16	j	1302	CLA	C4A-NA-C1A	2.64	107.88	106.68
16	B	1235	CLA	C1-C2-C3	-2.64	121.87	126.20
16	a	1111	CLA	CHD-C1D-ND	-2.64	121.09	124.80
14	b	848	LMG	O6-C1-O1	-2.64	103.80	110.04
16	b	1221	CLA	CHD-C1D-ND	-2.64	121.09	124.80
16	h	502	CLA	C4A-NA-C1A	2.64	107.88	106.68
16	x	505	CLA	CHA-C1A-NA	-2.64	120.42	126.39
19	B	4010	BCR	C40-C30-C25	2.64	114.38	110.24
19	X	602	BCR	C15-C16-C17	-2.64	118.12	123.52
19	B	4010	BCR	C24-C23-C22	-2.64	122.33	126.23
16	Z	509	CLA	C4A-NA-C1A	2.64	107.88	106.68
19	o	604	BCR	C31-C1-C6	2.64	114.38	110.24
19	b	4004	BCR	C27-C26-C25	2.64	126.27	122.70
19	b	4010	BCR	C27-C26-C25	2.64	126.27	122.70
16	a	1127	CLA	CHD-C1D-ND	-2.64	121.09	124.80
16	w	515	CLA	CHD-C1D-ND	-2.64	121.09	124.80
19	W	603	BCR	C27-C26-C25	2.64	126.27	122.70
16	F	1301	CLA	CHA-C1A-NA	-2.63	120.42	126.39
16	t	504	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	g	511	CLA	CHD-C1D-ND	-2.63	121.10	124.80
19	j	4013	BCR	C24-C23-C22	-2.63	122.34	126.23
19	T	4001	BCR	C24-C23-C22	-2.63	122.34	126.23
16	H	1127	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	A	1116	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	p	506	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	q	506	CLA	CHD-C1D-ND	-2.63	121.10	124.80
19	B	4017	BCR	C27-C26-C25	2.63	126.26	122.70
16	b	1218	CLA	CHD-C1D-ND	-2.63	121.11	124.80
16	w	517	CLA	CHD-C1D-ND	-2.63	121.11	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	4015	BCR	C27-C26-C25	2.62	126.25	122.70
16	g	506	CLA	CHD-C1D-ND	-2.62	121.11	124.80
16	q	514	CLA	CHA-C1A-NA	-2.62	120.45	126.39
19	h	604	BCR	C31-C1-C6	2.62	114.36	110.24
16	a	1123	CLA	C2A-C1A-CHA	2.62	128.42	123.87
16	X	517	CLA	CHD-C1D-ND	-2.62	121.11	124.80
16	A	1135	CLA	CHA-C1A-NA	-2.62	120.46	126.39
19	t	601	BCR	C27-C26-C25	2.62	126.24	122.70
19	B	4004	BCR	C27-C26-C25	2.62	126.24	122.70
16	g	503	CLA	C3C-C4C-NC	-2.62	107.08	110.43
19	X	601	BCR	C15-C14-C13	-2.62	123.61	127.28
19	u	603	BCR	C27-C26-C25	2.62	126.24	122.70
16	x	508	CLA	CHD-C1D-ND	-2.62	121.12	124.80
16	B	1012	CLA	CHD-C1D-ND	-2.62	121.12	124.80
19	p	604	BCR	C15-C16-C17	-2.62	118.17	123.52
16	H	1119	CLA	CHA-C1A-NA	-2.62	120.47	126.39
19	u	603	BCR	C15-C14-C13	-2.61	123.61	127.28
16	q	505	CLA	CHD-C1D-ND	-2.61	121.12	124.80
16	Z	505	CLA	CHD-C1D-ND	-2.61	121.12	124.80
19	s	602	BCR	C27-C26-C25	2.61	126.23	122.70
16	o	510	CLA	C4A-NA-C1A	2.61	107.87	106.68
16	q	508	CLA	CHA-C1A-NA	-2.61	120.47	126.39
19	v	604	BCR	C31-C1-C6	2.61	114.34	110.24
16	h	514	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	w	505	CLA	CHD-C1D-ND	-2.61	121.13	124.80
19	r	601	BCR	C24-C23-C22	-2.61	122.38	126.23
19	J	4015	BCR	C2-C1-C6	2.61	114.23	110.44
16	G	1228	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	H	1136	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	W	514	CLA	CHA-C1A-NA	-2.61	120.49	126.39
19	S	4015	BCR	C27-C26-C25	2.61	126.22	122.70
19	Z	604	BCR	C27-C26-C25	2.61	126.22	122.70
19	o	601	BCR	C3-C4-C5	-2.60	109.41	114.06
16	H	1123	CLA	CHD-C1D-ND	-2.60	121.14	124.80
19	x	601	BCR	C27-C26-C25	2.60	126.22	122.70
16	a	1022	CLA	C3C-C4C-NC	-2.60	107.09	110.43
16	A	1138	CLA	CHD-C1D-ND	-2.60	121.14	124.80
16	A	1101	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
19	p	602	BCR	C27-C26-C25	2.60	126.22	122.70
16	n	509	CLA	CHA-C1A-NA	-2.60	120.50	126.39
16	A	1022	CLA	C4A-NA-C1A	2.60	107.86	106.68
19	u	601	BCR	C15-C14-C13	-2.60	123.63	127.28

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	g	515	CLA	CHD-C1D-ND	-2.60	121.15	124.80
16	u	511	CLA	CHD-C1D-ND	-2.60	121.15	124.80
16	s	516	CLA	C4A-NA-C1A	2.60	107.86	106.68
19	u	604	BCR	C11-C10-C9	-2.60	123.64	127.28
19	y	603	BCR	C27-C26-C25	2.60	126.21	122.70
16	Z	508	CLA	CHA-C1A-NA	-2.59	120.52	126.39
16	H	1129	CLA	CHD-C1D-ND	-2.59	121.15	124.80
16	p	501	CLA	CHD-C1D-ND	-2.59	121.15	124.80
16	x	506	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
13	o	605	LHG	O8-C23-C24	2.59	119.74	111.83
16	Z	507	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
16	w	509	CLA	C4A-NA-C1A	2.59	107.86	106.68
19	q	603	BCR	C11-C10-C9	-2.59	123.64	127.28
16	H	1135	CLA	CHA-C1A-NA	-2.59	120.53	126.39
19	G	4010	BCR	C40-C30-C25	2.59	114.31	110.24
19	x	604	BCR	C27-C26-C25	2.59	126.20	122.70
16	a	1130	CLA	C4A-NA-C1A	2.59	107.86	106.68
16	b	1231	CLA	CHA-C1A-NA	-2.59	120.53	126.39
19	B	4014	BCR	C27-C26-C25	2.59	126.20	122.70
16	t	503	CLA	C3C-C4C-NC	-2.59	107.12	110.43
16	A	1119	CLA	CHD-C1D-ND	-2.59	121.16	124.80
19	X	602	BCR	C3-C4-C5	-2.59	109.44	114.06
16	o	512	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
16	a	1109	CLA	CHD-C1D-ND	-2.59	121.16	124.80
16	u	508	CLA	CHD-C1D-ND	-2.59	121.16	124.80
16	a	1123	CLA	CHA-C1A-NA	-2.59	120.53	126.39
16	w	508	CLA	CHA-C1A-NA	-2.59	120.54	126.39
19	Q	4016	BCR	C27-C26-C25	2.58	126.20	122.70
19	G	4009	BCR	C15-C14-C13	-2.58	123.65	127.28
16	b	1229	CLA	C1D-ND-C4D	-2.58	104.50	106.31
19	p	603	BCR	C15-C16-C17	-2.58	118.23	123.52
19	H	4002	BCR	C27-C26-C25	2.58	126.19	122.70
19	H	4003	BCR	C27-C26-C25	2.58	126.19	122.70
19	Y	602	BCR	C27-C26-C25	2.58	126.19	122.70
16	A	1106	CLA	CHD-C1D-ND	-2.58	121.17	124.80
16	A	1137	CLA	CHD-C1D-ND	-2.58	121.17	124.80
19	n	603	BCR	C27-C26-C25	2.58	126.19	122.70
19	x	603	BCR	C15-C16-C17	-2.58	118.24	123.52
19	t	601	BCR	C24-C23-C22	-2.58	122.42	126.23
16	a	1138	CLA	CHD-C1D-ND	-2.58	121.17	124.80
19	w	604	BCR	C27-C26-C25	2.58	126.19	122.70
13	X	605	LHG	O8-C23-C24	2.58	119.69	111.83

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	g	601	BCR	C31-C1-C6	2.58	114.28	110.24
19	w	604	BCR	C11-C10-C9	-2.58	123.67	127.28
16	B	1236	CLA	C4A-NA-C1A	2.58	107.85	106.68
16	a	1130	CLA	CHD-C1D-ND	-2.58	121.18	124.80
19	q	602	BCR	C27-C26-C25	2.58	126.18	122.70
16	y	505	CLA	CHA-C1A-NA	-2.57	120.56	126.39
19	x	603	BCR	C27-C26-C25	2.57	126.18	122.70
16	A	1122	CLA	CHD-C1D-ND	-2.57	121.18	124.80
16	f	1301	CLA	CHA-C1A-NA	-2.57	120.57	126.39
16	H	1103	CLA	CAA-CBA-CGA	-2.57	105.91	113.21
16	p	512	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
16	B	1230	CLA	CHD-C1D-ND	-2.57	121.19	124.80
19	X	604	BCR	C27-C26-C25	2.57	126.18	122.70
16	p	515	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
16	Y	501	CLA	CHD-C1D-ND	-2.57	121.19	124.80
21	b	4006	ECH	C34-C9-C10	-2.57	118.66	122.82
19	w	603	BCR	C27-C26-C25	2.57	126.17	122.70
13	a	849	LHG	O8-C23-C24	2.57	119.66	111.83
16	B	1238	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	b	1230	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	o	508	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	B	1235	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
16	B	1238	CLA	CHA-C1A-NA	-2.57	120.58	126.39
19	l	4022	BCR	C24-C23-C22	-2.57	122.44	126.23
19	q	603	BCR	C27-C26-C25	2.57	126.17	122.70
19	L	4019	BCR	C11-C10-C9	-2.57	123.68	127.28
19	b	4014	BCR	C15-C14-C13	-2.57	123.68	127.28
19	r	604	BCR	C15-C14-C13	-2.56	123.68	127.28
19	s	604	BCR	C15-C14-C13	-2.56	123.68	127.28
16	s	501	CLA	CHD-C1D-ND	-2.56	121.19	124.80
19	r	602	BCR	C15-C14-C13	-2.56	123.68	127.28
16	g	514	CLA	CHA-C1A-NA	-2.56	120.59	126.39
17	a	2001	PQN	C14-C13-C15	2.56	119.67	115.23
19	B	4010	BCR	C15-C14-C13	-2.56	123.69	127.28
16	X	511	CLA	C2C-C1C-NC	-2.56	107.29	109.98
16	b	1231	CLA	CHD-C1D-ND	-2.56	121.20	124.80
16	s	515	CLA	CHD-C1D-ND	-2.56	121.20	124.80
16	A	1127	CLA	CHA-C1A-NA	-2.56	120.59	126.39
19	a	4002	BCR	C27-C26-C25	2.56	126.16	122.70
16	b	1210	CLA	OBD-CAD-C3D	-2.56	122.44	128.42
16	a	1139	CLA	CHA-C1A-NA	-2.56	120.60	126.39
16	g	512	CLA	O2A-CGA-O1A	-2.56	117.23	123.63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1225	CLA	CHD-C1D-ND	-2.56	121.20	124.80
16	o	502	CLA	CHD-C1D-ND	-2.56	121.20	124.80
19	a	4003	BCR	C27-C26-C25	2.56	126.16	122.70
16	v	514	CLA	CHD-C1D-ND	-2.56	121.20	124.80
19	j	4012	BCR	C11-C10-C9	-2.56	123.69	127.28
16	a	1120	CLA	C3C-C4C-NC	-2.56	107.16	110.43
21	I	4020	ECH	C4-C5-C6	-2.56	119.25	122.70
16	b	1210	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	B	1231	CLA	CHA-C1A-NA	-2.55	120.61	126.39
16	a	1119	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	K	4002	CLA	C4A-NA-C1A	2.55	107.84	106.68
16	X	509	CLA	C4A-NA-C1A	2.55	107.84	106.68
19	t	603	BCR	C27-C26-C25	2.55	126.15	122.70
16	Y	508	CLA	CHA-C1A-NA	-2.55	120.61	126.39
16	h	505	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	B	4014	BCR	C7-C8-C9	-2.55	122.46	126.23
16	G	1216	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	A	4007	BCR	C7-C8-C9	-2.55	122.46	126.23
16	H	1130	CLA	C4A-NA-C1A	2.55	107.84	106.68
16	G	1208	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	r	504	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	r	516	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	R	4018	BCR	C11-C10-C9	-2.55	123.70	127.28
16	B	1012	CLA	CHA-C1A-NA	-2.55	120.61	126.39
19	K	4001	BCR	C15-C16-C17	-2.55	118.30	123.52
19	y	601	BCR	C24-C23-C22	-2.55	122.46	126.23
16	W	511	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	q	508	CLA	CHD-C1D-ND	-2.55	121.21	124.80
14	a	852	LMG	O6-C1-O1	-2.55	104.02	110.04
19	j	4015	BCR	C27-C26-C25	2.55	126.15	122.70
19	p	603	BCR	C11-C10-C9	-2.55	123.70	127.28
19	G	4014	BCR	C7-C8-C9	-2.55	122.47	126.23
16	x	514	CLA	CHA-C1A-NA	-2.55	120.62	126.39
19	T	4005	BCR	C27-C26-C25	2.55	126.15	122.70
19	k	4005	BCR	C27-C26-C25	2.55	126.15	122.70
16	t	508	CLA	CHD-C1D-ND	-2.55	121.22	124.80
19	Z	603	BCR	C27-C26-C25	2.55	126.14	122.70
19	G	4004	BCR	C15-C14-C13	-2.55	123.71	127.28
16	u	512	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
16	u	511	CLA	C2C-C1C-NC	-2.54	107.31	109.98
16	w	508	CLA	CHD-C1D-ND	-2.54	121.22	124.80
16	Y	512	CLA	CHA-C1A-NA	-2.54	120.63	126.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	1225	CLA	CHD-C1D-ND	-2.54	121.22	124.80
16	a	1127	CLA	CHA-C1A-NA	-2.54	120.63	126.39
19	A	4002	BCR	C27-C26-C25	2.54	126.14	122.70
16	G	1235	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
19	p	604	BCR	C15-C14-C13	-2.54	123.71	127.28
16	B	1224	CLA	CHA-C1A-NA	-2.54	120.64	126.39
16	G	1202	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	u	503	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	v	501	CLA	CHD-C1D-ND	-2.54	121.23	124.80
19	g	604	BCR	C27-C26-C25	2.54	126.14	122.70
19	w	602	BCR	C24-C23-C22	-2.54	122.48	126.23
16	g	506	CLA	C1-C2-C3	-2.54	122.04	126.20
19	B	4010	BCR	C27-C26-C25	2.54	126.13	122.70
16	H	1127	CLA	CHA-C1A-NA	-2.54	120.64	126.39
16	b	1226	CLA	CHD-C1D-ND	-2.54	121.23	124.80
19	S	4012	BCR	C15-C16-C17	-2.54	118.33	123.52
16	b	1219	CLA	CHD-C1D-ND	-2.54	121.23	124.80
19	r	603	BCR	C11-C10-C9	-2.54	123.72	127.28
19	K	4005	BCR	C27-C26-C25	2.54	126.13	122.70
16	A	1129	CLA	CHA-C1A-NA	-2.53	120.65	126.39
16	G	1202	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
16	G	1201	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	H	1109	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	t	511	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	y	502	CLA	CHD-C1D-ND	-2.53	121.24	124.80
19	b	4017	BCR	C27-C26-C25	2.53	126.13	122.70
16	f	1302	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	b	1236	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	y	517	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	q	516	CLA	CHD-C1D-ND	-2.53	121.24	124.80
13	i	103	LHG	O8-C23-C24	2.53	119.55	111.83
16	r	514	CLA	C4A-NA-C1A	2.53	107.83	106.68
23	q	605	LMU	O5'-C1'-C2'	2.53	115.57	110.37
16	s	509	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	a	1013	CLA	CMD-C2D-C1D	-2.53	120.28	124.73
19	j	4013	BCR	C27-C26-C25	2.53	126.12	122.70
16	b	1229	CLA	CHA-C1A-NA	-2.53	120.67	126.39
19	G	4010	BCR	C27-C26-C25	2.53	126.12	122.70
16	a	1101	CLA	CMD-C2D-C1D	-2.53	120.28	124.73
16	h	504	CLA	CHD-C1D-ND	-2.53	121.25	124.80
16	H	1122	CLA	C4A-NA-C1A	2.53	107.83	106.68
16	B	1012	CLA	CMB-C2B-C1B	-2.52	124.76	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	u	604	BCR	C2-C1-C6	2.52	114.11	110.44
16	G	1204	CLA	CHD-C1D-ND	-2.52	121.25	124.80
16	q	511	CLA	CMB-C2B-C1B	-2.52	124.76	128.46
19	Z	602	BCR	C11-C10-C9	-2.52	123.74	127.28
16	g	505	CLA	CHD-C1D-ND	-2.52	121.25	124.80
16	g	516	CLA	CHD-C1D-ND	-2.52	121.25	124.80
19	B	4017	BCR	C16-C15-C14	-2.52	118.36	123.52
16	a	1101	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
14	B	848	LMG	O2-C2-C1	-2.52	104.07	110.08
13	u	605	LHG	O8-C23-C24	2.52	119.52	111.83
16	r	506	CLA	C1-C2-C3	-2.52	122.07	126.20
15	A	1011	CL0	C4A-NA-C1A	2.52	107.83	106.68
19	K	4001	BCR	C15-C14-C13	-2.52	123.75	127.28
14	b	848	LMG	O2-C2-C1	-2.52	104.08	110.08
16	v	502	CLA	CHD-C1D-ND	-2.52	121.26	124.80
16	b	1224	CLA	CHA-C1A-NA	-2.52	120.69	126.39
16	h	505	CLA	CHA-C1A-NA	-2.52	120.69	126.39
16	Y	515	CLA	CHD-C1D-ND	-2.52	121.26	124.80
19	G	4014	BCR	C11-C10-C9	-2.51	123.75	127.28
16	b	1236	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
19	j	4013	BCR	C31-C1-C6	2.51	114.18	110.24
19	F	4016	BCR	C27-C26-C25	2.51	126.10	122.70
19	p	603	BCR	C27-C26-C25	2.51	126.10	122.70
14	Q	4017	LMG	O6-C1-O1	-2.51	104.11	110.04
16	p	502	CLA	C4A-NA-C1A	2.51	107.82	106.68
19	I	4018	BCR	C27-C26-C25	2.51	126.09	122.70
19	H	4011	BCR	C15-C16-C17	-2.51	118.39	123.52
16	Q	1302	CLA	CHD-C1D-ND	-2.51	121.27	124.80
19	g	604	BCR	C15-C14-C13	-2.51	123.76	127.28
16	A	1110	CLA	CHD-C1D-ND	-2.51	121.27	124.80
16	g	506	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
16	H	1138	CLA	C1-C2-C3	-2.51	122.09	126.20
16	A	1013	CLA	CHD-C1D-ND	-2.51	121.27	124.80
16	A	1134	CLA	CHD-C1D-ND	-2.51	121.27	124.80
19	B	4017	BCR	C10-C11-C12	-2.51	115.94	123.20
16	y	504	CLA	CHA-C1A-NA	-2.51	120.72	126.39
16	t	517	CLA	CHD-C1D-ND	-2.51	121.28	124.80
16	a	1106	CLA	CHD-C1D-ND	-2.50	121.28	124.80
19	g	602	BCR	C15-C16-C17	-2.50	118.40	123.52
16	a	1135	CLA	CHA-C1A-NA	-2.50	120.72	126.39
19	o	603	BCR	C15-C16-C17	-2.50	118.40	123.52
16	X	516	CLA	C4A-NA-C1A	2.50	107.82	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	1220	CLA	CHD-C1D-ND	-2.50	121.28	124.80
19	W	604	BCR	C27-C26-C25	2.50	126.08	122.70
19	R	4018	BCR	C15-C14-C13	-2.50	123.77	127.28
13	G	4018	LHG	C11-C10-C9	-2.50	101.73	114.37
16	a	1115	CLA	C2A-C1A-CHA	2.50	128.20	123.87
16	o	514	CLA	CHA-C1A-NA	-2.50	120.73	126.39
23	x	606	LMU	O5B-C5B-C4B	2.50	114.20	109.70
16	b	1212	CLA	CHD-C1D-ND	-2.50	121.29	124.80
16	v	516	CLA	CHD-C1D-ND	-2.50	121.29	124.80
16	G	1215	CLA	CHD-C1D-ND	-2.50	121.29	124.80
19	u	603	BCR	C11-C10-C9	-2.50	123.78	127.28
21	R	4020	ECH	C34-C9-C10	-2.50	118.77	122.82
16	b	1205	CLA	CHD-C1D-ND	-2.50	121.29	124.80
19	I	4018	BCR	C3-C4-C5	-2.50	109.61	114.06
16	n	515	CLA	CHD-C1D-ND	-2.50	121.29	124.80
16	B	1234	CLA	CHA-C1A-NA	-2.50	120.74	126.39
13	H	849	LHG	O8-C23-C24	2.49	119.44	111.83
19	U	4022	BCR	C2-C1-C6	2.49	114.06	110.44
19	J	4015	BCR	C15-C16-C17	-2.49	118.42	123.52
16	b	1211	CLA	CHD-C1D-ND	-2.49	121.30	124.80
19	G	4004	BCR	C11-C10-C9	-2.49	123.78	127.28
16	b	1202	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
16	p	515	CLA	CHD-C1D-ND	-2.49	121.30	124.80
19	l	4019	BCR	C11-C10-C9	-2.49	123.78	127.28
16	A	1121	CLA	CHD-C1D-ND	-2.49	121.30	124.80
16	b	1228	CLA	CHD-C1D-ND	-2.49	121.30	124.80
16	B	1214	CLA	C3C-C4C-NC	-2.49	107.24	110.43
19	t	604	BCR	C15-C14-C13	-2.49	123.79	127.28
19	w	604	BCR	C15-C16-C17	-2.49	118.42	123.52
16	v	517	CLA	CHD-C1D-ND	-2.49	121.30	124.80
19	r	604	BCR	C27-C26-C25	2.49	126.07	122.70
16	s	514	CLA	CHA-C1A-NA	-2.49	120.76	126.39
16	y	517	CLA	CHA-C1A-NA	-2.49	120.76	126.39
16	b	1234	CLA	CHD-C1D-ND	-2.49	121.30	124.80
16	h	501	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
19	B	4014	BCR	C15-C16-C17	-2.49	118.43	123.52
16	Y	505	CLA	C4A-NA-C1A	2.49	107.81	106.68
16	y	507	CLA	CHD-C1D-ND	-2.49	121.31	124.80
19	o	604	BCR	C27-C26-C25	2.48	126.06	122.70
21	I	4020	ECH	C8-C9-C10	2.48	122.91	119.01
16	u	510	CLA	C4A-NA-C1A	2.48	107.81	106.68
16	G	1221	CLA	CHD-C1D-ND	-2.48	121.31	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Z	515	CLA	CHD-C1D-ND	-2.48	121.31	124.80
16	H	1022	CLA	C3C-C4C-NC	-2.48	107.25	110.43
23	q	605	LMU	C1B-O1B-C4'	-2.48	112.10	117.98
16	a	1129	CLA	CHA-C1A-NA	-2.48	120.78	126.39
19	u	602	BCR	C15-C16-C17	-2.48	118.45	123.52
16	T	4002	CLA	CHD-C1D-ND	-2.48	121.31	124.80
16	A	1123	CLA	CHA-C1A-NA	-2.48	120.78	126.39
16	X	514	CLA	CHA-C1A-NA	-2.48	120.78	126.39
19	A	4008	BCR	C28-C27-C26	-2.48	109.64	114.06
16	h	514	CLA	C4A-NA-C1A	2.48	107.81	106.68
19	b	4014	BCR	C7-C8-C9	-2.48	122.57	126.23
16	G	1232	CLA	CHA-C1A-NA	-2.48	120.78	126.39
16	n	501	CLA	CHD-C1D-ND	-2.48	121.32	124.80
19	A	4011	BCR	C15-C16-C17	-2.48	118.45	123.52
16	Y	506	CLA	CHD-C1D-ND	-2.48	121.32	124.80
16	G	1240	CLA	CMC-C2C-C1C	-2.48	121.17	125.03
19	k	4005	BCR	C24-C23-C22	-2.47	122.57	126.23
16	y	514	CLA	CHA-C1A-NA	-2.47	120.79	126.39
16	a	1122	CLA	CHD-C1D-ND	-2.47	121.32	124.80
19	g	604	BCR	C11-C10-C9	-2.47	123.81	127.28
13	R	103	LHG	O8-C23-C24	2.47	119.38	111.83
16	b	1201	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
16	A	1114	CLA	CHD-C1D-ND	-2.47	121.32	124.80
16	G	1238	CLA	CHD-C1D-ND	-2.47	121.32	124.80
19	A	4007	BCR	C15-C14-C13	-2.47	123.81	127.28
19	A	4003	BCR	C15-C16-C17	-2.47	118.46	123.52
14	H	852	LMG	O6-C1-O1	-2.47	104.20	110.04
16	s	508	CLA	CHA-C1A-NA	-2.47	120.80	126.39
16	g	509	CLA	CHD-C1D-ND	-2.47	121.33	124.80
16	k	4002	CLA	CHD-C1D-ND	-2.47	121.33	124.80
19	J	4013	BCR	C27-C26-C25	2.47	126.04	122.70
16	A	1125	CLA	CHD-C1D-ND	-2.47	121.33	124.80
16	t	503	CLA	CHA-C1A-NA	-2.47	120.80	126.39
13	s	605	LHG	C11-C10-C9	-2.47	101.89	114.37
16	b	1232	CLA	CHD-C1D-ND	-2.47	121.33	124.80
16	r	507	CLA	CHD-C1D-ND	-2.47	121.33	124.80
16	G	1227	CLA	CHA-C1A-NA	-2.47	120.80	126.39
16	h	517	CLA	C4A-NA-C1A	2.47	107.81	106.68
16	t	502	CLA	C4A-NA-C1A	2.47	107.81	106.68
17	G	2002	PQN	C14-C13-C15	2.47	119.51	115.23
16	A	1102	CLA	CHD-C1D-ND	-2.47	121.33	124.80
14	G	848	LMG	O2-C2-C1	-2.47	104.20	110.08

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	v	506	CLA	CHA-C1A-NA	-2.47	120.81	126.39
16	g	505	CLA	CHA-C1A-NA	-2.46	120.81	126.39
16	a	1114	CLA	CHA-C1A-NA	-2.46	120.81	126.39
13	b	4018	LHG	C11-C10-C9	-2.46	101.92	114.37
16	a	1105	CLA	CMB-C2B-C1B	-2.46	124.85	128.46
16	H	1110	CLA	CHD-C1D-ND	-2.46	121.34	124.80
16	H	1139	CLA	CHA-C1A-NA	-2.46	120.81	126.39
16	t	509	CLA	CHA-C1A-NA	-2.46	120.81	126.39
19	u	604	BCR	C24-C23-C22	-2.46	122.59	126.23
13	x	605	LHG	C11-C10-C9	-2.46	101.92	114.37
16	h	511	CLA	C2C-C1C-NC	-2.46	107.40	109.98
16	b	1216	CLA	CMB-C2B-C3B	-2.46	119.77	124.68
16	y	508	CLA	CHA-C1A-NA	-2.46	120.82	126.39
16	h	516	CLA	CHD-C1D-ND	-2.46	121.34	124.80
16	h	512	CLA	CHA-C1A-NA	-2.46	120.82	126.39
16	s	505	CLA	CHD-C1D-ND	-2.46	121.34	124.80
13	B	4018	LHG	C11-C10-C9	-2.46	101.95	114.37
16	u	516	CLA	CHD-C1D-ND	-2.46	121.34	124.80
16	G	1218	CLA	CHA-C1A-NA	-2.46	120.83	126.39
16	a	1102	CLA	CHD-C1D-ND	-2.46	121.35	124.80
16	H	1129	CLA	CHA-C1A-NA	-2.46	120.83	126.39
19	n	601	BCR	C7-C8-C9	-2.46	122.60	126.23
14	A	852	LMG	O6-C1-O1	-2.46	104.24	110.04
19	v	604	BCR	C2-C1-C6	2.46	114.01	110.44
16	p	506	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
16	Z	514	CLA	CHA-C1A-NA	-2.45	120.83	126.39
16	y	515	CLA	CHD-C1D-ND	-2.45	121.35	124.80
19	S	4013	BCR	C24-C23-C22	-2.45	122.60	126.23
16	r	512	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
16	H	1104	CLA	CHD-C1D-ND	-2.45	121.35	124.80
19	r	604	BCR	C11-C10-C9	-2.45	123.84	127.28
16	H	1105	CLA	C4A-NA-C1A	2.45	107.80	106.68
16	X	501	CLA	CHD-C1D-ND	-2.45	121.35	124.80
19	q	604	BCR	C27-C26-C25	2.45	126.02	122.70
16	G	1226	CLA	C3C-C4C-NC	-2.45	107.29	110.43
16	S	1302	CLA	C4A-NA-C1A	2.45	107.80	106.68
16	w	516	CLA	C4A-NA-C1A	2.45	107.80	106.68
16	o	515	CLA	CHD-C1D-ND	-2.45	121.36	124.80
19	t	601	BCR	C15-C16-C17	-2.45	118.51	123.52
24	q	601	LUT	C1-C6-C7	2.45	122.29	115.65
16	q	515	CLA	C2D-C1D-ND	-2.45	107.70	110.13
13	A	849	LHG	O8-C23-C24	2.45	119.30	111.83

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	W	601	BCR	C11-C10-C9	-2.45	123.84	127.28
19	s	601	BCR	C15-C14-C13	-2.45	123.84	127.28
24	Z	601	LUT	C1-C6-C5	-2.45	119.29	122.64
17	a	2001	PQN	C11-C12-C13	-2.45	122.61	126.83
16	v	505	CLA	CHA-C1A-NA	-2.45	120.85	126.39
19	b	4004	BCR	C15-C14-C13	-2.45	123.85	127.28
16	v	504	CLA	CHD-C1D-ND	-2.45	121.36	124.80
16	v	511	CLA	CHA-C1A-NA	-2.45	120.85	126.39
16	y	503	CLA	CHD-C1D-ND	-2.45	121.36	124.80
19	x	602	BCR	C15-C14-C13	-2.45	123.85	127.28
15	A	1011	CL0	CHD-C1D-ND	-2.44	121.36	124.80
16	S	1303	CLA	CHD-C1D-ND	-2.44	121.36	124.80
16	u	507	CLA	CHD-C1D-ND	-2.44	121.36	124.80
15	A	1011	CL0	O2A-CGA-O1A	-2.44	117.52	123.63
16	B	1216	CLA	CHD-C1D-ND	-2.44	121.36	124.80
16	G	1214	CLA	C3C-C4C-NC	-2.44	107.30	110.43
16	G	1218	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	S	1302	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	r	508	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	A	4007	BCR	C28-C27-C26	-2.44	109.70	114.06
16	X	516	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	b	4017	BCR	C16-C15-C14	-2.44	118.53	123.52
13	g	605	LHG	C11-C10-C9	-2.44	102.04	114.37
16	B	1219	CLA	CHD-C1D-ND	-2.44	121.37	124.80
13	r	605	LHG	C11-C10-C9	-2.44	102.04	114.37
16	A	1117	CLA	CMB-C2B-C1B	-2.44	124.88	128.46
19	B	4009	BCR	C15-C14-C13	-2.44	123.86	127.28
19	K	4001	BCR	C40-C30-C25	2.44	114.07	110.24
19	J	4013	BCR	C2-C1-C6	2.44	113.98	110.44
16	s	503	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	t	507	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	a	1128	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	b	1021	CLA	CHD-C1D-ND	-2.44	121.38	124.80
16	n	509	CLA	CHD-C1D-ND	-2.44	121.38	124.80
19	t	604	BCR	C24-C23-C22	-2.44	122.63	126.23
19	u	604	BCR	C31-C1-C6	2.43	114.06	110.24
23	w	605	LMU	O5'-C1'-C2'	2.43	115.37	110.37
19	a	4011	BCR	C1-C6-C5	-2.43	119.31	122.64
21	i	4020	ECH	C1-C6-C5	-2.43	119.31	122.64
16	a	1137	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	b	1012	CLA	CHD-C1D-ND	-2.43	121.38	124.80
19	t	603	BCR	C15-C16-C17	-2.43	118.54	123.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1109	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	p	507	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	k	4003	CLA	C4A-NA-C1A	2.43	107.79	106.68
19	n	601	BCR	C11-C10-C9	-2.43	123.87	127.28
14	H	852	LMG	C1-C2-C3	-2.43	104.89	110.01
19	s	604	BCR	C15-C16-C17	-2.43	118.54	123.52
15	H	1011	CL0	O2A-CGA-O1A	-2.43	117.54	123.63
16	B	1202	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
16	a	1123	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	w	516	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	x	509	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	B	1023	CLA	C2A-C1A-CHA	2.43	128.09	123.87
16	q	515	CLA	CHA-C1A-NA	-2.43	120.89	126.39
19	p	604	BCR	C33-C5-C6	-2.43	121.83	124.48
16	G	1226	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	H	1022	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	X	510	CLA	C4A-NA-C1A	2.43	107.79	106.68
14	a	852	LMG	C38-C37-C36	-2.43	102.08	114.37
16	G	1238	CLA	CHA-C1A-NA	-2.43	120.89	126.39
19	G	4014	BCR	C24-C23-C22	-2.43	122.64	126.23
16	b	1208	CLA	CHD-C1D-ND	-2.43	121.38	124.80
17	H	2001	PQN	C14-C13-C15	2.43	119.44	115.23
19	s	603	BCR	C27-C26-C25	2.43	125.99	122.70
16	k	4004	CLA	C4A-NA-C1A	2.43	107.79	106.68
19	J	4013	BCR	C15-C16-C17	-2.43	118.55	123.52
16	y	510	CLA	CHA-C1A-NA	-2.43	120.89	126.39
16	W	512	CLA	CHD-C1D-ND	-2.43	121.39	124.80
16	X	509	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
16	B	1232	CLA	CHA-C1A-NA	-2.43	120.90	126.39
16	A	1126	CLA	CHD-C1D-ND	-2.43	121.39	124.80
16	A	1109	CLA	CHA-C1A-NA	-2.42	120.90	126.39
16	H	1133	CLA	CHA-C1A-NA	-2.42	120.90	126.39
16	J	1303	CLA	CHD-C1D-ND	-2.42	121.39	124.80
16	t	505	CLA	CHA-C1A-NA	-2.42	120.90	126.39
19	o	602	BCR	C15-C16-C17	-2.42	118.56	123.52
16	U	1503	CLA	CHA-C1A-NA	-2.42	120.91	126.39
16	B	1213	CLA	C4A-NA-C1A	2.42	107.78	106.68
16	a	1121	CLA	CHD-C1D-ND	-2.42	121.39	124.80
16	b	1238	CLA	CHA-C1A-NA	-2.42	120.91	126.39
16	A	1119	CLA	CHA-C1A-NA	-2.42	120.91	126.39
15	H	1011	CL0	CHD-C1D-ND	-2.42	121.39	124.80
19	a	4007	BCR	C28-C27-C26	-2.42	109.74	114.06

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	852	LMG	C38-C37-C36	-2.42	102.13	114.37
19	Y	603	BCR	C27-C26-C25	2.42	125.97	122.70
16	s	513	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
16	Y	516	CLA	CHD-C1D-ND	-2.42	121.40	124.80
16	w	509	CLA	CHD-C1D-ND	-2.42	121.40	124.80
13	p	605	LHG	C11-C10-C9	-2.42	102.14	114.37
16	G	1023	CLA	C4D-C3D-CAD	-2.42	105.48	108.11
16	a	1114	CLA	CHD-C1D-ND	-2.42	121.40	124.80
16	H	1013	CLA	CAA-C2A-C1A	-2.42	104.05	111.97
16	b	1012	CLA	CMB-C2B-C3B	2.42	129.51	124.68
16	y	506	CLA	CHA-C1A-NA	-2.42	120.92	126.39
21	R	4020	ECH	C10-C11-C12	2.42	130.20	123.20
16	B	1220	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
19	H	4008	BCR	C7-C8-C9	-2.41	122.66	126.23
16	k	4004	CLA	CHA-C1A-NA	-2.41	120.93	126.39
19	I	4018	BCR	C15-C14-C13	-2.41	123.89	127.28
16	o	511	CLA	CHD-C1D-ND	-2.41	121.41	124.80
19	S	4015	BCR	C11-C10-C9	-2.41	123.89	127.28
16	Z	515	CLA	CHA-C1A-NA	-2.41	120.93	126.39
16	H	1128	CLA	CMD-C2D-C1D	-2.41	120.48	124.73
16	A	1123	CLA	C2A-C1A-CHA	2.41	128.05	123.87
16	r	505	CLA	CHD-C1D-ND	-2.41	121.41	124.80
16	s	506	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
16	u	506	CLA	CHD-C1D-ND	-2.41	121.41	124.80
13	I	103	LHG	O8-C23-C24	2.41	119.18	111.83
16	Z	503	CLA	CHA-C1A-NA	-2.41	120.93	126.39
16	u	509	CLA	CHA-C1A-NA	-2.41	120.93	126.39
19	W	601	BCR	C7-C8-C9	-2.41	122.67	126.23
19	l	4022	BCR	C2-C1-C6	2.41	113.94	110.44
19	r	603	BCR	C15-C16-C17	-2.41	118.59	123.52
16	b	1214	CLA	C3C-C4C-NC	-2.41	107.34	110.43
16	y	507	CLA	C4A-NA-C1A	2.41	107.78	106.68
16	W	504	CLA	CHD-C1D-ND	-2.41	121.41	124.80
16	b	1215	CLA	CHD-C1D-ND	-2.41	121.41	124.80
13	Y	605	LHG	C11-C10-C9	-2.41	102.19	114.37
16	H	1109	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
19	H	4011	BCR	C24-C23-C22	-2.41	122.67	126.23
16	r	512	CLA	CHD-C1D-ND	-2.41	121.42	124.80
15	A	1011	CL0	CMB-C2B-C3B	2.41	129.49	124.68
19	h	604	BCR	C2-C1-C6	2.41	113.94	110.44
16	A	1135	CLA	C2D-C1D-ND	-2.40	107.75	110.13
16	r	514	CLA	CHA-C1A-NA	-2.40	120.95	126.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	1011	CL0	CMB-C2B-C3B	2.40	129.48	124.68
16	s	510	CLA	C4A-NA-C1A	2.40	107.78	106.68
14	A	852	LMG	C1-C2-C3	-2.40	104.96	110.01
19	G	4010	BCR	C7-C8-C9	-2.40	122.68	126.23
19	G	4017	BCR	C30-C25-C26	-2.40	119.35	122.64
16	n	512	CLA	CHD-C1D-ND	-2.40	121.42	124.80
16	W	513	CLA	C4A-NA-C1A	2.40	107.77	106.68
16	J	1302	CLA	CHD-C1D-ND	-2.40	121.42	124.80
16	b	1209	CLA	CHD-C1D-ND	-2.40	121.42	124.80
16	w	515	CLA	CHA-C1A-NA	-2.40	120.96	126.39
19	J	4013	BCR	C24-C23-C22	-2.40	122.69	126.23
16	n	505	CLA	CHA-C1A-NA	-2.40	120.96	126.39
16	W	509	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	w	603	BCR	C2-C1-C6	2.40	113.92	110.44
19	R	4018	BCR	C27-C26-C25	2.40	125.94	122.70
16	A	1237	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	a	4011	BCR	C27-C26-C25	2.40	125.94	122.70
16	v	509	CLA	CHA-C1A-NA	-2.40	120.96	126.39
19	s	604	BCR	C33-C5-C6	-2.40	121.87	124.48
16	x	503	CLA	CHD-C1D-ND	-2.40	121.43	124.80
16	o	511	CLA	CMB-C2B-C1B	-2.40	124.94	128.46
16	H	1137	CLA	CHD-C1D-ND	-2.40	121.43	124.80
16	k	4004	CLA	CHD-C1D-ND	-2.40	121.43	124.80
16	x	517	CLA	CHD-C1D-ND	-2.40	121.43	124.80
17	B	2002	PQN	C11-C12-C13	-2.40	122.70	126.83
16	B	1210	CLA	CHA-C1A-NA	-2.40	120.97	126.39
16	r	515	CLA	CHA-C1A-NA	-2.40	120.97	126.39
19	a	4008	BCR	C30-C25-C26	-2.40	119.36	122.64
16	g	517	CLA	CHD-C1D-ND	-2.40	121.43	124.80
14	A	4101	LMG	C38-C37-C36	-2.39	102.26	114.37
19	p	601	BCR	C15-C14-C13	-2.39	123.92	127.28
14	a	852	LMG	C1-C2-C3	-2.39	104.97	110.01
16	B	1201	CLA	CHD-C1D-ND	-2.39	121.43	124.80
16	a	1125	CLA	C4D-C3D-CAD	-2.39	105.51	108.11
16	r	511	CLA	CMB-C2B-C1B	-2.39	124.95	128.46
16	A	1133	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	G	1240	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	X	507	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	s	509	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
16	b	1239	CLA	CHA-C1A-NA	-2.39	120.97	126.39
19	F	4016	BCR	C40-C30-C25	2.39	114.00	110.24
16	s	501	CLA	CHA-C1A-NA	-2.39	120.97	126.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	1210	CLA	CHD-C1D-ND	-2.39	121.44	124.80
19	j	4012	BCR	C15-C14-C13	-2.39	123.93	127.28
16	b	1206	CLA	CHA-C1A-NA	-2.39	120.98	126.39
16	x	512	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
16	W	505	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	Y	512	CLA	C1-C2-C3	-2.39	122.28	126.20
16	G	1234	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
14	A	852	LMG	C38-C37-C36	-2.39	102.30	114.37
16	g	515	CLA	CHA-C1A-NA	-2.39	120.98	126.39
16	W	502	CLA	CMD-C2D-C1D	-2.39	120.53	124.73
16	j	1303	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	K	4004	CLA	CHA-C1A-NA	-2.39	120.99	126.39
16	h	510	CLA	CHA-C1A-NA	-2.39	120.99	126.39
16	K	4004	CLA	CHD-C1D-ND	-2.39	121.45	124.80
16	Y	511	CLA	CHD-C1D-ND	-2.39	121.45	124.80
16	a	1134	CLA	CHD-C1D-ND	-2.39	121.45	124.80
16	t	506	CLA	CHD-C1D-ND	-2.39	121.45	124.80
16	y	515	CLA	C2A-C1A-CHA	2.38	128.01	123.87
16	B	1239	CLA	C1C-C2C-C3C	-2.38	104.47	106.98
19	Z	604	BCR	C11-C10-C9	-2.38	123.93	127.28
16	p	508	CLA	CHD-C1D-ND	-2.38	121.45	124.80
19	b	4009	BCR	C15-C14-C13	-2.38	123.94	127.28
19	b	4010	BCR	C15-C14-C13	-2.38	123.94	127.28
19	o	601	BCR	C11-C10-C9	-2.38	123.94	127.28
15	a	1011	CL0	O2A-CGA-O1A	-2.38	117.67	123.63
16	J	1303	CLA	C4A-NA-C1A	2.38	107.77	106.68
23	p	606	LMU	O5B-C5B-C4B	2.38	113.99	109.70
19	v	603	BCR	C30-C25-C26	-2.38	119.38	122.64
16	G	1222	CLA	C3C-C4C-NC	-2.38	107.38	110.43
13	b	4018	LHG	C20-C19-C18	-2.38	102.34	114.37
19	T	4001	BCR	C15-C14-C13	-2.38	123.94	127.28
19	S	4012	BCR	C11-C10-C9	-2.38	123.94	127.28
19	j	4012	BCR	C33-C5-C6	-2.38	121.89	124.48
19	S	4012	BCR	C7-C8-C9	-2.38	122.72	126.23
19	h	601	BCR	C11-C10-C9	-2.38	123.94	127.28
16	p	509	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
16	H	1118	CLA	CHD-C1D-ND	-2.38	121.46	124.80
16	X	511	CLA	CHD-C1D-ND	-2.38	121.46	124.80
14	f	4017	LMG	O6-C1-O1	-2.38	104.43	110.04
16	H	1123	CLA	CHA-C1A-NA	-2.38	121.01	126.39
16	x	515	CLA	CHA-C1A-NA	-2.38	121.01	126.39
16	Y	508	CLA	O2A-CGA-O1A	-2.38	117.69	123.63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	n	515	CLA	CHA-C1A-NA	-2.38	121.01	126.39
19	J	4012	BCR	C15-C14-C13	-2.38	123.95	127.28
16	G	1217	CLA	C1D-ND-C4D	-2.37	104.65	106.31
16	b	1216	CLA	CHA-C1A-NA	-2.37	121.02	126.39
19	i	4018	BCR	C27-C26-C25	2.37	125.91	122.70
16	Y	503	CLA	C3C-C4C-NC	-2.37	107.39	110.43
19	J	4015	BCR	C11-C10-C9	-2.37	123.95	127.28
16	h	508	CLA	CHD-C1D-ND	-2.37	121.46	124.80
16	B	1228	CLA	CHD-C1D-ND	-2.37	121.47	124.80
16	H	1120	CLA	C3C-C4C-NC	-2.37	107.39	110.43
16	p	508	CLA	CHA-C1A-NA	-2.37	121.03	126.39
16	p	511	CLA	CHA-C1A-NA	-2.37	121.03	126.39
16	L	1503	CLA	CHD-C1D-ND	-2.37	121.47	124.80
16	X	504	CLA	CHA-C1A-NA	-2.37	121.03	126.39
16	v	517	CLA	CHA-C1A-NA	-2.37	121.03	126.39
16	A	1117	CLA	C1-C2-C3	-2.37	122.32	126.20
16	b	1203	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
19	B	4014	BCR	C24-C23-C22	-2.37	122.73	126.23
16	s	512	CLA	CHD-C1D-ND	-2.37	121.47	124.80
16	g	510	CLA	CHA-C1A-NA	-2.37	121.03	126.39
16	Y	507	CLA	CHD-C1D-ND	-2.37	121.47	124.80
19	X	602	BCR	C15-C14-C13	-2.37	123.96	127.28
16	A	1118	CLA	C4A-NA-C1A	2.37	107.76	106.68
19	A	4003	BCR	C40-C30-C25	2.36	113.95	110.24
16	A	1119	CLA	CMB-C2B-C1B	-2.36	124.99	128.46
19	K	4001	BCR	C27-C26-C25	2.36	125.90	122.70
16	n	505	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	s	512	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
13	B	4018	LHG	C20-C19-C18	-2.36	102.44	114.37
16	W	510	CLA	CHA-C1A-NA	-2.36	121.05	126.39
16	G	1222	CLA	C2A-C1A-CHA	2.36	127.96	123.87
16	G	1234	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	a	1116	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	r	517	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	W	501	CLA	CHD-C1D-ND	-2.36	121.48	124.80
14	b	848	LMG	C38-C37-C36	-2.36	102.45	114.37
16	H	1116	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	n	511	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	G	1228	CLA	CHA-C1A-NA	-2.36	121.05	126.39
19	f	4016	BCR	C27-C26-C25	2.36	125.89	122.70
19	j	4013	BCR	C1-C6-C5	-2.36	119.42	122.64
16	F	1302	CLA	CHD-C1D-ND	-2.36	121.49	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	517	CLA	C4A-NA-C1A	2.36	107.75	106.68
19	K	4001	BCR	C11-C10-C9	-2.36	123.97	127.28
16	B	1211	CLA	CHA-C1A-NA	-2.35	121.06	126.39
19	n	604	BCR	C15-C16-C17	-2.35	118.70	123.52
23	w	605	LMU	C1B-O1B-C4'	-2.35	112.40	117.98
16	a	1109	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
16	B	1218	CLA	CHA-C1A-NA	-2.35	121.06	126.39
16	a	1237	CLA	CHD-C1D-ND	-2.35	121.49	124.80
19	J	4013	BCR	C31-C1-C6	2.35	113.93	110.24
16	p	503	CLA	C3C-C4C-NC	-2.35	107.42	110.43
16	H	1120	CLA	CHD-C1D-ND	-2.35	121.49	124.80
16	Z	504	CLA	CHA-C1A-NA	-2.35	121.06	126.39
16	Y	517	CLA	C4A-NA-C1A	2.35	107.75	106.68
19	Z	603	BCR	C11-C10-C9	-2.35	123.98	127.28
19	Z	603	BCR	C15-C16-C17	-2.35	118.71	123.52
16	r	511	CLA	CHD-C1D-ND	-2.35	121.49	124.80
16	g	508	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	w	505	CLA	C1-C2-C3	-2.35	122.35	126.20
16	v	510	CLA	CHA-C1A-NA	-2.35	121.07	126.39
16	b	1222	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	n	513	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	G	1229	CLA	CHA-C1A-NA	-2.35	121.07	126.39
16	h	506	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	G	1230	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	g	503	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	B	4017	BCR	C30-C25-C26	-2.35	119.43	122.64
19	X	601	BCR	C11-C10-C9	-2.35	123.98	127.28
16	s	511	CLA	CHA-C1A-NA	-2.35	121.07	126.39
19	H	4002	BCR	C24-C23-C22	-2.35	122.76	126.23
16	r	506	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
13	H	849	LHG	C11-C10-C9	-2.35	102.50	114.37
16	x	505	CLA	C3C-C4C-NC	-2.35	107.42	110.43
19	h	601	BCR	C33-C5-C6	-2.35	121.92	124.48
16	n	510	CLA	CHA-C1A-NA	-2.35	121.08	126.39
19	s	602	BCR	C11-C10-C9	-2.35	123.99	127.28
19	T	4001	BCR	C11-C10-C9	-2.35	123.99	127.28
19	l	4022	BCR	C31-C1-C6	2.35	113.92	110.24
16	q	509	CLA	C4A-NA-C1A	2.35	107.75	106.68
16	r	509	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	R	4018	BCR	C33-C5-C6	-2.35	121.92	124.48
19	p	602	BCR	C11-C10-C9	-2.34	123.99	127.28
16	A	1133	CLA	CHA-C1A-NA	-2.34	121.08	126.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	1108	CLA	CHA-C1A-NA	-2.34	121.08	126.39
19	q	604	BCR	C15-C16-C17	-2.34	118.72	123.52
16	b	1234	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
16	o	517	CLA	CHD-C1D-ND	-2.34	121.50	124.80
16	t	515	CLA	CHD-C1D-ND	-2.34	121.50	124.80
16	v	513	CLA	CHD-C1D-ND	-2.34	121.50	124.80
16	p	508	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
16	Y	509	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
16	Y	501	CLA	CHA-C1A-NA	-2.34	121.09	126.39
16	a	1119	CLA	CMB-C2B-C1B	-2.34	125.03	128.46
16	o	501	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	p	503	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	y	504	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	b	1238	CLA	C1-C2-C3	-2.34	122.36	126.20
16	B	1229	CLA	CHA-C1A-NA	-2.34	121.09	126.39
16	h	503	CLA	CHA-C1A-NA	-2.34	121.09	126.39
14	B	848	LMG	O3-C3-C2	-2.34	104.86	110.38
23	Z	605	LMU	C1B-O1B-C4'	-2.34	112.44	117.98
19	K	4005	BCR	C24-C23-C22	-2.34	122.78	126.23
19	v	601	BCR	C3-C4-C5	-2.34	109.89	114.06
16	H	1113	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	U	1501	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	Z	517	CLA	CHD-C1D-ND	-2.34	121.51	124.80
19	Y	602	BCR	C11-C10-C9	-2.34	124.00	127.28
16	G	1211	CLA	CHA-C1A-NA	-2.34	121.10	126.39
16	W	515	CLA	CHA-C1A-NA	-2.34	121.10	126.39
19	y	601	BCR	C33-C5-C6	-2.34	121.94	124.48
16	n	503	CLA	CHD-C1D-ND	-2.34	121.52	124.80
16	b	1235	CLA	CHA-C1A-NA	-2.34	121.10	126.39
16	b	1220	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
16	G	1012	CLA	CHA-C1A-NA	-2.33	121.10	126.39
16	H	1109	CLA	CHA-C1A-NA	-2.33	121.10	126.39
16	t	510	CLA	CHA-C1A-NA	-2.33	121.10	126.39
16	A	1013	CLA	C2A-C3A-C4A	-2.33	98.10	101.87
16	a	1123	CLA	CMB-C2B-C1B	-2.33	125.04	128.46
19	s	601	BCR	C27-C26-C25	2.33	125.86	122.70
16	p	516	CLA	CHD-C1D-ND	-2.33	121.52	124.80
16	L	1503	CLA	C2A-C1A-CHA	2.33	127.92	123.87
19	b	4004	BCR	C11-C10-C9	-2.33	124.01	127.28
21	I	4020	ECH	O27-C27-C26	2.33	123.07	120.98
16	B	1235	CLA	CMB-C2B-C1B	-2.33	125.04	128.46
16	b	1239	CLA	C4A-NA-C1A	2.33	107.74	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	1239	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
16	T	4004	CLA	CHD-C1D-ND	-2.33	121.52	124.80
16	Z	511	CLA	CHD-C1D-ND	-2.33	121.52	124.80
16	q	507	CLA	CHD-C1D-ND	-2.33	121.52	124.80
19	o	602	BCR	C15-C14-C13	-2.33	124.01	127.28
16	y	516	CLA	CHA-C1A-NA	-2.33	121.11	126.39
13	G	4018	LHG	C20-C19-C18	-2.33	102.59	114.37
19	L	4022	BCR	C24-C23-C22	-2.33	122.79	126.23
14	A	4101	LMG	O6-C1-O1	-2.33	104.54	110.04
16	a	1138	CLA	C1-C2-C3	-2.33	122.38	126.20
19	g	602	BCR	C15-C14-C13	-2.33	124.01	127.28
16	Z	508	CLA	CHD-C1D-ND	-2.33	121.53	124.80
14	H	4101	LMG	C38-C37-C36	-2.33	102.60	114.37
19	G	4014	BCR	C30-C25-C26	-2.33	119.45	122.64
16	G	1232	CLA	CHD-C1D-ND	-2.33	121.53	124.80
16	A	1112	CLA	C2A-C1A-CHA	2.33	127.91	123.87
16	b	1220	CLA	CHA-C1A-NA	-2.33	121.12	126.39
16	a	1138	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
16	o	504	CLA	CHD-C1D-ND	-2.33	121.53	124.80
19	Y	601	BCR	C15-C14-C13	-2.33	124.02	127.28
16	B	1206	CLA	CHA-C1A-NA	-2.33	121.12	126.39
19	o	604	BCR	C1-C6-C5	-2.33	119.46	122.64
16	b	1216	CLA	CHD-C1D-ND	-2.33	121.53	124.80
16	n	507	CLA	CHD-C1D-ND	-2.33	121.53	124.80
16	p	502	CLA	CHD-C1D-ND	-2.33	121.53	124.80
16	q	517	CLA	CHD-C1D-ND	-2.33	121.53	124.80
16	h	508	CLA	CHA-C1A-NA	-2.33	121.13	126.39
16	h	515	CLA	C1-C2-C3	-2.32	122.39	126.20
19	j	4015	BCR	C1-C6-C5	-2.32	119.46	122.64
19	t	603	BCR	C15-C14-C13	-2.32	124.02	127.28
16	h	504	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
16	a	1134	CLA	CHA-C1A-NA	-2.32	121.13	126.39
16	h	513	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	B	1235	CLA	CHA-C1A-NA	-2.32	121.14	126.39
16	b	1224	CLA	CMC-C2C-C1C	-2.32	121.41	125.03
19	L	4022	BCR	C3-C4-C5	-2.32	109.92	114.06
16	u	506	CLA	C3C-C4C-NC	-2.32	107.46	110.43
16	X	512	CLA	CMB-C2B-C1B	-2.32	125.06	128.46
19	G	4005	BCR	C15-C16-C17	-2.32	118.77	123.52
16	b	1023	CLA	C2A-C1A-CHA	2.32	127.89	123.87
21	G	4006	ECH	C24-C23-C22	2.32	129.66	126.23
19	g	601	BCR	C2-C1-C6	2.32	113.81	110.44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	x	601	BCR	C7-C8-C9	-2.32	122.81	126.23
16	G	1023	CLA	C2A-C1A-CHA	2.32	127.89	123.87
19	T	4005	BCR	C3-C4-C5	-2.32	109.92	114.06
16	A	1104	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	p	512	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	B	1234	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	h	501	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	u	509	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
16	H	1801	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	r	513	CLA	C1C-C2C-C3C	-2.32	104.55	106.98
19	B	4005	BCR	C15-C16-C17	-2.32	118.78	123.52
16	G	1204	CLA	C4A-NA-C1A	2.31	107.73	106.68
16	n	509	CLA	C4A-NA-C1A	2.31	107.73	106.68
19	W	601	BCR	C15-C14-C13	-2.31	124.03	127.28
16	A	1113	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	y	504	CLA	C2D-C1D-ND	-2.31	107.84	110.13
16	t	515	CLA	CHA-C1A-NA	-2.31	121.15	126.39
16	H	1122	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	r	502	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	y	513	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	t	507	CLA	C4A-NA-C1A	2.31	107.73	106.68
14	G	848	LMG	O1-C7-C8	-2.31	105.19	110.82
16	G	1220	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
19	k	4001	BCR	C11-C10-C9	-2.31	124.04	127.28
16	W	503	CLA	CHA-C1A-NA	-2.31	121.16	126.39
15	H	1011	CL0	CMB-C2B-C1B	-2.31	125.07	128.46
16	h	517	CLA	CHA-C1A-NA	-2.31	121.16	126.39
19	a	4011	BCR	C24-C23-C22	-2.31	122.82	126.23
16	G	1231	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	Z	507	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	B	1220	CLA	C2C-C1C-NC	-2.31	107.56	109.98
16	T	4004	CLA	CHA-C1A-NA	-2.31	121.17	126.39
16	y	512	CLA	CHA-C1A-NA	-2.31	121.17	126.39
16	w	504	CLA	C1-C2-C3	-2.31	122.42	126.20
19	h	601	BCR	C24-C23-C22	-2.31	122.82	126.23
19	n	601	BCR	C24-C23-C22	-2.31	122.82	126.23
19	w	604	BCR	C16-C15-C14	-2.31	118.80	123.52
19	H	4003	BCR	C11-C10-C9	-2.31	124.04	127.28
16	B	1207	CLA	CHD-C1D-ND	-2.31	121.56	124.80
16	q	509	CLA	CHA-C1A-NA	-2.31	121.17	126.39
19	n	604	BCR	C15-C14-C13	-2.31	124.04	127.28
16	p	516	CLA	C4A-NA-C1A	2.31	107.73	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	g	507	CLA	CHD-C1D-ND	-2.31	121.56	124.80
16	v	507	CLA	CHA-C1A-NA	-2.30	121.17	126.39
16	Z	505	CLA	C1-C2-C3	-2.30	122.42	126.20
16	L	1501	CLA	CHD-C1D-ND	-2.30	121.56	124.80
16	s	504	CLA	CHD-C1D-ND	-2.30	121.56	124.80
16	B	1227	CLA	CHA-C1A-NA	-2.30	121.17	126.39
16	H	1105	CLA	CHA-C1A-NA	-2.30	121.17	126.39
19	Z	603	BCR	C15-C14-C13	-2.30	124.05	127.28
16	B	1021	CLA	C2A-C1A-CHA	2.30	127.86	123.87
16	b	1232	CLA	CHA-C1A-NA	-2.30	121.17	126.39
16	G	1023	CLA	C2C-C1C-NC	-2.30	107.56	109.98
19	a	4003	BCR	C33-C5-C6	-2.30	121.97	124.48
16	A	1112	CLA	CHD-C1D-ND	-2.30	121.56	124.80
19	A	4003	BCR	C33-C5-C6	-2.30	121.97	124.48
16	H	1013	CLA	C2A-C3A-C4A	-2.30	98.15	101.87
16	y	513	CLA	C4A-NA-C1A	2.30	107.73	106.68
19	g	602	BCR	C7-C8-C9	-2.30	122.83	126.23
14	a	4101	LMG	C38-C37-C36	-2.30	102.75	114.37
16	Y	513	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
16	h	515	CLA	CHA-C1A-NA	-2.30	121.19	126.39
16	s	504	CLA	C1-C2-C3	-2.30	122.43	126.20
14	F	4017	LMG	O6-C1-O1	-2.30	104.61	110.04
19	q	604	BCR	C16-C15-C14	-2.30	118.82	123.52
16	q	507	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
16	b	1239	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
16	q	505	CLA	CMB-C2B-C1B	-2.30	125.09	128.46
16	G	1224	CLA	CHA-C1A-NA	-2.30	121.19	126.39
16	B	1224	CLA	CHD-C1D-ND	-2.30	121.57	124.80
19	p	603	BCR	C7-C8-C9	-2.30	122.84	126.23
19	B	4005	BCR	C30-C25-C26	-2.30	119.50	122.64
16	H	1127	CLA	C1-C2-C3	-2.30	122.44	126.20
16	a	1120	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
16	G	1012	CLA	CMB-C2B-C1B	-2.30	125.09	128.46
16	b	1204	CLA	C4A-NA-C1A	2.29	107.73	106.68
14	G	848	LMG	O3-C3-C2	-2.29	104.97	110.38
14	B	848	LMG	O1-C7-C8	-2.29	105.24	110.82
16	G	1235	CLA	CHA-C1A-NA	-2.29	121.20	126.39
16	s	508	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
16	n	511	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
16	a	1237	CLA	C1C-C2C-C3C	-2.29	104.57	106.98
16	H	1013	CLA	C3A-C2A-C1A	-2.29	97.90	101.34
16	Q	1301	CLA	CHD-C1D-ND	-2.29	121.58	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	t	516	CLA	CHD-C1D-ND	-2.29	121.58	124.80
16	a	1130	CLA	C1-C2-C3	-2.29	122.44	126.20
17	A	2001	PQN	C11-C12-C13	-2.29	122.88	126.83
16	G	1217	CLA	CHD-C1D-ND	-2.29	121.58	124.80
16	u	513	CLA	C2A-C1A-CHA	2.29	127.84	123.87
19	W	604	BCR	C24-C23-C22	-2.29	122.85	126.23
19	p	601	BCR	C3-C4-C5	-2.29	109.97	114.06
16	G	1225	CLA	CHA-C1A-NA	-2.29	121.20	126.39
16	t	504	CLA	CHA-C1A-NA	-2.29	121.20	126.39
16	y	511	CLA	CHA-C1A-NA	-2.29	121.20	126.39
19	A	4003	BCR	C15-C14-C13	-2.29	124.07	127.28
19	o	603	BCR	C15-C14-C13	-2.29	124.07	127.28
16	Y	505	CLA	CHD-C1D-ND	-2.29	121.58	124.80
16	Z	501	CLA	CHA-C1A-NA	-2.29	121.21	126.39
16	x	509	CLA	CHA-C1A-NA	-2.29	121.21	126.39
19	x	601	BCR	C15-C14-C13	-2.29	124.07	127.28
16	s	503	CLA	C4A-NA-C1A	2.29	107.72	106.68
16	h	507	CLA	CHA-C1A-NA	-2.29	121.22	126.39
16	h	516	CLA	C1C-C2C-C3C	-2.29	104.58	106.98
19	b	4005	BCR	C15-C14-C13	-2.29	124.07	127.28
19	y	601	BCR	C11-C10-C9	-2.29	124.07	127.28
16	K	4002	CLA	CHD-C1D-ND	-2.28	121.59	124.80
24	Z	601	LUT	C31-C32-C33	-2.28	120.10	126.36
19	G	4017	BCR	C10-C11-C12	-2.28	116.58	123.20
16	S	1303	CLA	C4A-NA-C1A	2.28	107.72	106.68
19	G	4005	BCR	C27-C26-C25	2.28	125.79	122.70
19	J	4015	BCR	C1-C6-C5	-2.28	119.52	122.64
16	B	1239	CLA	C3C-C4C-NC	-2.28	107.50	110.43
19	s	603	BCR	C15-C14-C13	-2.28	124.08	127.28
16	n	511	CLA	CHA-C1A-NA	-2.28	121.22	126.39
16	Y	505	CLA	C2A-C1A-CHA	2.28	127.83	123.87
16	W	513	CLA	CHA-C1A-NA	-2.28	121.22	126.39
16	t	502	CLA	CHA-C1A-NA	-2.28	121.22	126.39
16	b	1226	CLA	C3C-C4C-NC	-2.28	107.51	110.43
16	n	502	CLA	CHD-C1D-ND	-2.28	121.59	124.80
19	S	4012	BCR	C24-C23-C22	-2.28	122.86	126.23
16	H	1122	CLA	CHA-C1A-NA	-2.28	121.22	126.39
16	v	501	CLA	CHA-C1A-NA	-2.28	121.23	126.39
19	G	4017	BCR	C15-C16-C17	-2.28	118.85	123.52
16	v	503	CLA	CHA-C1A-NA	-2.28	121.23	126.39
16	G	1012	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
24	w	601	LUT	C3-C4-C5	-2.28	106.50	112.18

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	511	CLA	CHA-C1A-NA	-2.28	121.23	126.39
16	r	513	CLA	CHA-C1A-NA	-2.28	121.23	126.39
14	H	4101	LMG	O2-C2-C1	-2.28	104.64	110.08
13	i	103	LHG	C11-C10-C9	-2.28	102.85	114.37
16	y	505	CLA	C4D-C3D-CAD	-2.28	105.63	108.11
16	t	509	CLA	CHD-C1D-ND	-2.28	121.60	124.80
16	B	1230	CLA	C4A-NA-C1A	2.28	107.72	106.68
16	Z	517	CLA	C4A-NA-C1A	2.28	107.72	106.68
16	Z	504	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
16	G	1236	CLA	CHA-C1A-NA	-2.28	121.23	126.39
16	u	504	CLA	CHA-C1A-NA	-2.28	121.23	126.39
16	p	505	CLA	CHD-C1D-ND	-2.28	121.60	124.80
16	w	514	CLA	CHA-C1A-NA	-2.28	121.24	126.39
19	G	4010	BCR	C10-C11-C12	-2.28	116.61	123.20
19	F	4016	BCR	C15-C16-C17	-2.28	118.86	123.52
19	S	4013	BCR	C1-C6-C5	-2.27	119.53	122.64
16	H	1801	CLA	C3C-C4C-NC	-2.27	107.52	110.43
19	o	602	BCR	C20-C21-C22	-2.27	124.09	127.28
16	B	1214	CLA	CHD-C1D-ND	-2.27	121.60	124.80
16	X	510	CLA	CHD-C1D-ND	-2.27	121.60	124.80
16	t	512	CLA	CHD-C1D-ND	-2.27	121.60	124.80
19	n	604	BCR	C27-C26-C25	2.27	125.78	122.70
14	b	848	LMG	O3-C3-C2	-2.27	105.02	110.38
16	a	1108	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	o	509	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
19	J	4012	BCR	C33-C5-C6	-2.27	122.00	124.48
16	o	506	CLA	CHA-C1A-NA	-2.27	121.25	126.39
16	s	513	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	v	603	BCR	C11-C10-C9	-2.27	124.09	127.28
16	G	1203	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	p	505	CLA	C2D-C1D-ND	-2.27	107.88	110.13
24	q	601	LUT	C15-C35-C34	-2.27	118.87	123.52
19	g	603	BCR	C33-C5-C6	-2.27	122.01	124.48
16	h	509	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
16	x	510	CLA	CHA-C1A-NA	-2.27	121.25	126.39
19	J	4015	BCR	C7-C8-C9	-2.27	122.88	126.23
19	g	604	BCR	C7-C8-C9	-2.27	122.88	126.23
16	b	1236	CLA	CHA-C1A-NA	-2.27	121.25	126.39
16	B	1231	CLA	CHD-C1D-ND	-2.27	121.61	124.80
13	Y	605	LHG	C27-C26-C25	-2.27	102.91	114.37
19	B	4005	BCR	C15-C14-C13	-2.27	124.10	127.28
19	q	602	BCR	C7-C8-C9	-2.27	122.88	126.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	1221	CLA	CHA-C1A-NA	-2.27	121.26	126.39
19	x	603	BCR	C33-C5-C6	-2.27	122.01	124.48
19	l	4022	BCR	C15-C16-C17	-2.27	118.88	123.52
16	x	511	CLA	CHD-C1D-ND	-2.26	121.61	124.80
16	b	1228	CLA	CHA-C1A-NA	-2.26	121.26	126.39
13	R	103	LHG	C11-C10-C9	-2.26	102.92	114.37
19	B	4010	BCR	C7-C8-C9	-2.26	122.89	126.23
19	j	4012	BCR	C7-C8-C9	-2.26	122.89	126.23
16	Z	511	CLA	CHA-C1A-NA	-2.26	121.27	126.39
16	v	501	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
16	t	511	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
19	W	601	BCR	C29-C30-C25	2.26	113.72	110.44
16	b	1217	CLA	CHA-C1A-NA	-2.26	121.27	126.39
16	K	4003	CLA	CHD-C1D-ND	-2.26	121.62	124.80
13	A	849	LHG	C11-C10-C9	-2.26	102.94	114.37
19	r	601	BCR	C11-C10-C9	-2.26	124.11	127.28
16	A	1107	CLA	C1-C2-C3	-2.26	123.10	126.76
16	o	501	CLA	CHA-C1A-NA	-2.26	121.27	126.39
19	R	4018	BCR	C7-C8-C9	-2.26	122.89	126.23
19	T	4001	BCR	C15-C16-C17	-2.26	118.89	123.52
16	B	1235	CLA	CHD-C1D-C2D	2.26	130.19	125.49
16	B	1212	CLA	CHA-C1A-NA	-2.26	121.27	126.39
16	X	505	CLA	CHA-C1A-NA	-2.26	121.27	126.39
16	G	1203	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
16	A	1116	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
16	A	1116	CLA	C2D-C1D-ND	-2.26	107.89	110.13
19	b	4010	BCR	C30-C25-C26	-2.26	119.55	122.64
16	B	1216	CLA	CHA-C1A-NA	-2.26	121.28	126.39
16	r	503	CLA	C3C-C4C-NC	-2.26	107.54	110.43
16	A	1106	CLA	CHA-C1A-NA	-2.26	121.28	126.39
16	y	515	CLA	CHA-C1A-NA	-2.26	121.28	126.39
23	Y	606	LMU	C1'-C2'-C3'	2.26	114.76	110.01
19	K	4005	BCR	C3-C4-C5	-2.26	110.03	114.06
19	H	4008	BCR	C33-C5-C6	-2.26	122.02	124.48
16	b	1208	CLA	CHA-C1A-NA	-2.26	121.28	126.39
16	H	1130	CLA	C1-C2-C3	-2.26	122.50	126.20
16	r	503	CLA	CHD-C1D-ND	-2.26	121.63	124.80
16	A	1109	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
16	H	1137	CLA	C4A-NA-C1A	2.26	107.71	106.68
16	Y	515	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
16	H	1130	CLA	CHD-C1D-ND	-2.26	121.63	124.80
16	o	510	CLA	CHD-C1D-ND	-2.26	121.63	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	511	CLA	CMB-C2B-C1B	-2.25	125.15	128.46
16	n	503	CLA	C3C-C4C-NC	-2.25	107.54	110.43
17	b	2002	PQN	C14-C13-C15	2.25	119.14	115.23
16	b	1238	CLA	CHD-C1D-ND	-2.25	121.63	124.80
16	x	503	CLA	C3C-C4C-NC	-2.25	107.54	110.43
16	a	1107	CLA	C1-C2-C3	-2.25	123.12	126.76
16	b	1239	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
16	h	511	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
19	J	4012	BCR	C7-C8-C9	-2.25	122.90	126.23
19	U	4022	BCR	C31-C1-C6	2.25	113.78	110.24
16	x	507	CLA	CHD-C1D-ND	-2.25	121.63	124.80
23	x	606	LMU	C1B-C2B-C3B	2.25	114.75	110.01
19	t	603	BCR	C33-C5-C6	-2.25	122.03	124.48
13	I	103	LHG	C11-C10-C9	-2.25	102.99	114.37
16	A	1135	CLA	CHD-C1D-ND	-2.25	121.63	124.80
16	B	1223	CLA	CHD-C1D-ND	-2.25	121.63	124.80
16	H	1107	CLA	CHD-C1D-ND	-2.25	121.63	124.80
24	w	601	LUT	C15-C35-C34	-2.25	118.91	123.52
16	A	1131	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	t	601	BCR	C15-C14-C13	-2.25	124.12	127.28
19	p	602	BCR	C24-C23-C22	-2.25	122.91	126.23
16	Z	501	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	b	4014	BCR	C30-C25-C26	-2.25	119.56	122.64
19	q	602	BCR	C24-C23-C22	-2.25	122.91	126.23
19	A	4008	BCR	C33-C5-C6	-2.25	122.03	124.48
19	p	604	BCR	C11-C10-C9	-2.25	124.12	127.28
16	y	516	CLA	C4A-NA-C1A	2.25	107.70	106.68
16	W	507	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	t	505	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	i	4018	BCR	C15-C14-C13	-2.25	124.12	127.28
16	t	511	CLA	CHA-C1A-NA	-2.25	121.30	126.39
16	y	506	CLA	C3C-C4C-NC	-2.25	107.55	110.43
16	y	517	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
16	A	1022	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	x	601	BCR	C11-C10-C9	-2.25	124.13	127.28
16	B	1209	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	b	1217	CLA	C1D-ND-C4D	-2.25	104.74	106.31
16	A	1116	CLA	CHA-C1A-NA	-2.25	121.31	126.39
16	A	1013	CLA	CAA-CBA-CGA	-2.25	106.83	113.21
16	B	1234	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
19	x	603	BCR	C15-C14-C13	-2.25	124.13	127.28
16	W	505	CLA	CHA-C1A-NA	-2.25	121.31	126.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	s	603	BCR	C7-C8-C9	-2.24	122.92	126.23
16	H	1116	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	a	1116	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
19	h	603	BCR	C11-C10-C9	-2.24	124.13	127.28
16	h	515	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	r	505	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	G	1207	CLA	C1-O2A-CGA	2.24	122.08	116.65
16	b	1235	CLA	C1-C2-C3	-2.24	122.53	126.20
16	H	1123	CLA	C2A-C1A-CHA	2.24	127.76	123.87
19	s	602	BCR	C24-C23-C22	-2.24	122.92	126.23
16	u	510	CLA	CHD-C1D-ND	-2.24	121.65	124.80
16	G	1222	CLA	CHD-C1D-ND	-2.24	121.65	124.80
16	r	501	CLA	CHA-C1A-NA	-2.24	121.32	126.39
19	J	4013	BCR	C1-C6-C5	-2.24	119.58	122.64
19	a	4008	BCR	C33-C5-C6	-2.24	122.04	124.48
19	l	4022	BCR	C20-C21-C22	-2.24	124.14	127.28
16	Y	511	CLA	CMB-C2B-C1B	-2.24	125.18	128.46
16	n	513	CLA	C1C-C2C-C3C	-2.24	104.63	106.98
16	s	516	CLA	CHD-C1D-ND	-2.24	121.65	124.80
16	g	513	CLA	C4A-NA-C1A	2.24	107.70	106.68
19	q	603	BCR	C15-C16-C17	-2.24	118.94	123.52
16	b	1213	CLA	CHA-C1A-NA	-2.24	121.32	126.39
19	u	602	BCR	C20-C21-C22	-2.24	124.14	127.28
16	A	1801	CLA	CHD-C1D-ND	-2.24	121.66	124.80
14	H	4201	LMG	O3-C3-C2	-2.24	105.10	110.38
19	t	601	BCR	C11-C10-C9	-2.24	124.14	127.28
16	a	1022	CLA	CMB-C2B-C1B	-2.24	125.18	128.46
16	p	503	CLA	C2D-C1D-ND	-2.24	107.91	110.13
21	M	4021	ECH	C2-C1-C6	2.24	113.69	110.44
15	a	1011	CL0	CHD-C1D-ND	-2.24	121.66	124.80
16	A	1107	CLA	CHD-C1D-ND	-2.24	121.66	124.80
16	Y	514	CLA	C4A-NA-C1A	2.24	107.70	106.68
16	b	1238	CLA	C4A-NA-C1A	2.24	107.70	106.68
19	b	4017	BCR	C10-C11-C12	-2.24	116.72	123.20
19	H	4007	BCR	C28-C27-C26	-2.24	110.07	114.06
16	G	1234	CLA	CHA-C1A-NA	-2.23	121.33	126.39
16	A	1138	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
19	S	4015	BCR	C24-C23-C22	-2.23	122.93	126.23
23	Y	606	LMU	C1B-C2B-C3B	2.23	114.71	110.01
16	u	504	CLA	CHD-C1D-ND	-2.23	121.66	124.80
16	v	509	CLA	C2D-C1D-ND	-2.23	107.92	110.13
19	K	4005	BCR	C15-C16-C17	-2.23	118.95	123.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	1214	CLA	CHD-C1D-ND	-2.23	121.66	124.80
16	b	1211	CLA	CHA-C1A-NA	-2.23	121.33	126.39
16	w	503	CLA	C2C-C1C-NC	-2.23	107.64	109.98
16	q	510	CLA	C4A-NA-C1A	2.23	107.70	106.68
19	G	4014	BCR	C15-C16-C17	-2.23	118.95	123.52
19	Q	4016	BCR	C15-C16-C17	-2.23	118.95	123.52
19	F	4016	BCR	C7-C8-C9	-2.23	122.93	126.23
19	n	604	BCR	C24-C23-C22	-2.23	122.93	126.23
16	A	1022	CLA	C4D-C3D-CAD	-2.23	105.68	108.11
13	R	103	LHG	C27-C26-C25	-2.23	103.08	114.37
16	a	1117	CLA	CHD-C1D-C2D	2.23	130.13	125.49
14	a	4201	LMG	O3-C3-C2	-2.23	105.11	110.38
16	X	508	CLA	CHD-C1D-ND	-2.23	121.66	124.80
16	G	1012	CLA	CMB-C2B-C3B	2.23	129.14	124.68
14	b	848	LMG	O1-C7-C8	-2.23	105.39	110.82
19	b	4005	BCR	C27-C26-C25	2.23	125.72	122.70
19	B	4004	BCR	C11-C10-C9	-2.23	124.15	127.28
19	v	603	BCR	C15-C14-C13	-2.23	124.15	127.28
16	W	510	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
16	U	1503	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
13	b	4018	LHG	C18-C17-C16	-2.23	103.10	114.37
16	r	506	CLA	C4A-NA-C1A	2.23	107.70	106.68
13	a	849	LHG	C11-C10-C9	-2.23	103.10	114.37
16	o	506	CLA	CHD-C1D-ND	-2.23	121.67	124.80
13	G	4018	LHG	C18-C17-C16	-2.23	103.11	114.37
16	t	513	CLA	CHD-C1D-ND	-2.23	121.67	124.80
16	W	501	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
16	A	1108	CLA	CHD-C1D-ND	-2.23	121.67	124.80
23	w	605	LMU	C1'-O5'-C5'	2.23	118.07	113.72
16	F	1301	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	Z	602	BCR	C1-C6-C5	-2.23	119.59	122.64
16	X	502	CLA	CHA-C1A-NA	-2.22	121.35	126.39
16	h	508	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
21	B	4006	ECH	C15-C16-C17	2.22	128.07	123.52
14	A	4201	LMG	O3-C3-C2	-2.22	105.13	110.38
16	r	506	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	p	515	CLA	CHA-C1A-NA	-2.22	121.35	126.39
16	a	1128	CLA	CHA-C1A-NA	-2.22	121.36	126.39
16	h	515	CLA	CHD-C1D-ND	-2.22	121.67	124.80
19	q	603	BCR	C15-C14-C13	-2.22	124.16	127.28
16	q	511	CLA	CHA-C1A-NA	-2.22	121.36	126.39
16	t	514	CLA	O2A-CGA-O1A	-2.22	118.07	123.63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	h	516	CLA	CHA-C1A-NA	-2.22	121.36	126.39
16	a	1126	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	H	1120	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
16	y	516	CLA	CHD-C1D-ND	-2.22	121.68	124.80
16	G	1232	CLA	C2A-C1A-CHA	2.22	127.72	123.87
16	T	4003	CLA	CHD-C1D-ND	-2.22	121.68	124.80
16	v	509	CLA	CHD-C1D-ND	-2.22	121.68	124.80
16	B	1203	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
23	p	606	LMU	C1'-C2'-C3'	2.22	114.68	110.01
16	W	511	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
21	R	4020	ECH	C2-C3-C4	-2.22	106.40	111.28
19	S	4013	BCR	C2-C1-C6	2.22	113.66	110.44
16	b	1212	CLA	CHA-C1A-NA	-2.22	121.37	126.39
19	X	603	BCR	C30-C25-C26	-2.22	119.61	122.64
16	H	1138	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
16	X	505	CLA	C2A-C1A-CHA	2.22	127.72	123.87
16	Y	501	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
19	G	4017	BCR	C16-C15-C14	-2.22	118.98	123.52
19	p	603	BCR	C15-C14-C13	-2.22	124.17	127.28
16	n	501	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
16	u	509	CLA	CHD-C1D-ND	-2.22	121.68	124.80
15	H	1011	CL0	C1B-CHB-C4A	-2.22	125.81	130.04
16	H	1104	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
19	w	603	BCR	C16-C15-C14	-2.22	118.98	123.52
16	W	506	CLA	CHD-C1D-ND	-2.22	121.69	124.80
16	v	516	CLA	CHA-C1A-NA	-2.22	121.38	126.39
19	S	4012	BCR	C33-C5-C6	-2.22	122.07	124.48
19	G	4014	BCR	C16-C15-C14	-2.21	118.99	123.52
16	w	507	CLA	CHA-C1A-NA	-2.21	121.38	126.39
16	A	1013	CLA	CAA-C2A-C1A	-2.21	104.72	111.97
16	a	1131	CLA	CHD-C1D-ND	-2.21	121.69	124.80
16	q	501	CLA	CHD-C1D-ND	-2.21	121.69	124.80
16	s	515	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
16	X	515	CLA	CHA-C1A-NA	-2.21	121.38	126.39
16	h	502	CLA	CHD-C1D-ND	-2.21	121.69	124.80
16	p	511	CLA	CMB-C2B-C1B	-2.21	125.22	128.46
21	b	4006	ECH	C24-C23-C22	2.21	129.50	126.23
14	A	4101	LMG	O2-C2-C1	-2.21	104.81	110.08
16	x	516	CLA	CHA-C1A-NA	-2.21	121.39	126.39
16	H	1120	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
19	u	601	BCR	C11-C10-C9	-2.21	124.18	127.28
16	g	506	CLA	C4A-NA-C1A	2.21	107.69	106.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	4007	BCR	C1-C6-C5	-2.21	119.62	122.64
19	r	603	BCR	C15-C14-C13	-2.21	124.18	127.28
16	G	1206	CLA	CHA-C1A-NA	-2.21	121.39	126.39
16	A	1237	CLA	CHA-C1A-NA	-2.21	121.39	126.39
14	G	848	LMG	C38-C37-C36	-2.21	103.20	114.37
19	Y	603	BCR	C15-C16-C17	-2.21	119.00	123.52
16	b	1201	CLA	CHD-C1D-ND	-2.21	121.70	124.80
16	A	1013	CLA	C4A-NA-C1A	2.21	107.69	106.68
16	W	504	CLA	CHA-C1A-NA	-2.21	121.39	126.39
16	v	514	CLA	CHA-C1A-NA	-2.21	121.39	126.39
16	v	512	CLA	CAA-CBA-CGA	-2.21	106.94	113.21
16	n	506	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
19	f	4016	BCR	C16-C15-C14	-2.21	119.01	123.52
19	r	603	BCR	C33-C5-C6	-2.20	122.08	124.48
13	B	4018	LHG	C18-C17-C16	-2.20	103.23	114.37
19	W	604	BCR	C40-C30-C25	2.20	113.70	110.24
16	p	501	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	A	1139	CLA	CHA-C1A-NA	-2.20	121.40	126.39
19	s	601	BCR	C33-C5-C6	-2.20	122.08	124.48
19	b	4004	BCR	C7-C8-C9	-2.20	122.98	126.23
16	s	505	CLA	C2A-C1A-CHA	2.20	127.69	123.87
16	b	1235	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	Y	505	CLA	CHA-C1A-NA	-2.20	121.40	126.39
16	a	1108	CLA	CHA-C1A-NA	-2.20	121.40	126.39
16	X	503	CLA	CHD-C1D-ND	-2.20	121.70	124.80
16	w	507	CLA	CHD-C1D-ND	-2.20	121.70	124.80
19	A	4007	BCR	C29-C30-C25	2.20	113.64	110.44
14	B	848	LMG	C38-C37-C36	-2.20	103.24	114.37
16	X	509	CLA	CHD-C1D-ND	-2.20	121.70	124.80
19	o	603	BCR	C30-C25-C26	-2.20	119.63	122.64
19	x	602	BCR	C24-C23-C22	-2.20	122.98	126.23
16	h	507	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	b	1207	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	t	505	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	H	1108	CLA	CHD-C1D-ND	-2.20	121.70	124.80
16	W	515	CLA	CHD-C1D-ND	-2.20	121.70	124.80
16	B	1220	CLA	C4A-NA-C1A	2.20	107.68	106.68
16	a	1119	CLA	C1B-CHB-C4A	-2.20	125.84	130.04
16	H	1801	CLA	C1C-C2C-C3C	-2.20	104.67	106.98
16	B	1232	CLA	CHD-C1D-ND	-2.20	121.71	124.80
16	B	1236	CLA	CHA-C1A-NA	-2.20	121.41	126.39
19	J	4012	BCR	C27-C26-C25	2.20	125.67	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	s	505	CLA	C2D-C1D-ND	-2.20	107.95	110.13
16	b	1214	CLA	CHD-C1D-ND	-2.20	121.71	124.80
16	p	517	CLA	CHD-C1D-ND	-2.20	121.71	124.80
16	A	1120	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
19	w	602	BCR	C7-C8-C9	-2.20	122.98	126.23
19	v	603	BCR	C15-C16-C17	-2.20	119.02	123.52
16	Y	506	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
16	Z	513	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	Y	601	BCR	C33-C5-C6	-2.20	122.09	124.48
14	A	852	LMG	O2-C2-C1	-2.20	104.84	110.08
16	B	1229	CLA	C1D-ND-C4D	-2.20	104.77	106.31
16	H	1134	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	a	4007	BCR	C29-C30-C25	2.20	113.63	110.44
16	H	1117	CLA	C1-C2-C3	-2.20	122.60	126.20
16	L	1502	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
16	k	4004	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
19	t	601	BCR	C7-C8-C9	-2.20	122.99	126.23
16	n	516	CLA	CHD-C1D-ND	-2.20	121.71	124.80
16	v	510	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
16	q	503	CLA	CMD-C2D-C1D	-2.19	120.86	124.73
16	b	1240	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	B	4014	BCR	C30-C25-C26	-2.19	119.64	122.64
16	o	503	CLA	CHA-C1A-NA	-2.19	121.42	126.39
16	A	1013	CLA	CMD-C2D-C1D	-2.19	120.87	124.73
16	n	510	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
19	p	601	BCR	C24-C23-C22	-2.19	122.99	126.23
19	l	4022	BCR	C1-C6-C5	-2.19	119.64	122.64
16	b	1225	CLA	CHA-C1A-NA	-2.19	121.43	126.39
16	o	504	CLA	CHA-C1A-NA	-2.19	121.43	126.39
19	Q	4016	BCR	C15-C14-C13	-2.19	124.21	127.28
16	G	1208	CLA	CHA-C1A-NA	-2.19	121.43	126.39
16	B	1012	CLA	CMB-C2B-C3B	2.19	129.06	124.68
16	H	1139	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
19	h	604	BCR	C30-C25-C26	-2.19	119.64	122.64
19	Z	604	BCR	C15-C14-C13	-2.19	124.21	127.28
16	H	1237	CLA	C1C-C2C-C3C	-2.19	104.68	106.98
16	s	508	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	x	501	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	o	511	CLA	CHA-C1A-NA	-2.19	121.44	126.39
16	Z	512	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	S	4015	BCR	C15-C16-C17	-2.19	119.04	123.52
16	B	1218	CLA	O2A-CGA-O1A	-2.19	118.16	123.63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	1801	CLA	CHA-C1A-NA	-2.19	121.44	126.39
16	G	1229	CLA	C1D-ND-C4D	-2.19	104.78	106.31
16	v	515	CLA	C2A-C1A-CHA	2.19	127.66	123.87
16	A	1140	CLA	CHD-C1D-ND	-2.19	121.73	124.80
16	j	1302	CLA	CHD-C1D-ND	-2.19	121.73	124.80
16	n	506	CLA	CHD-C1D-ND	-2.19	121.73	124.80
16	r	508	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	Y	511	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	q	508	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	B	1205	CLA	CHD-C1D-ND	-2.19	121.73	124.80
19	v	604	BCR	C30-C25-C26	-2.18	119.65	122.64
19	o	601	BCR	C27-C26-C25	2.18	125.66	122.70
16	Z	508	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
19	j	4012	BCR	C24-C23-C22	-2.18	123.00	126.23
16	Z	514	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
19	s	601	BCR	C7-C8-C9	-2.18	123.01	126.23
16	v	505	CLA	CHD-C1D-ND	-2.18	121.73	124.80
19	X	601	BCR	C7-C8-C9	-2.18	123.01	126.23
16	n	514	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	n	501	CLA	CHA-C1A-NA	-2.18	121.45	126.39
14	a	4101	LMG	O2-C2-C1	-2.18	104.88	110.08
16	W	506	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	v	509	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
19	A	4008	BCR	C7-C8-C9	-2.18	123.01	126.23
16	s	510	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	B	1228	CLA	CHA-C1A-NA	-2.18	121.45	126.39
19	Y	601	BCR	C24-C23-C22	-2.18	123.01	126.23
23	r	606	LMU	C4B-C3B-C2B	2.18	114.66	110.83
16	G	1224	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	x	512	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	p	511	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	a	1022	CLA	C2C-C1C-NC	-2.18	107.69	109.98
16	w	514	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
16	b	1224	CLA	CHD-C1D-ND	-2.18	121.74	124.80
14	G	848	LMG	O7-C10-O9	-2.18	118.61	123.70
16	X	512	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
16	o	514	CLA	CHD-C1D-C2D	2.18	130.02	125.49
19	S	4013	BCR	C15-C14-C13	-2.18	124.22	127.28
23	q	605	LMU	C1'-O5'-C5'	2.18	117.97	113.72
16	W	511	CLA	CHA-C1A-NA	-2.18	121.46	126.39
19	u	602	BCR	C15-C14-C13	-2.18	124.22	127.28
16	g	507	CLA	C1-C2-C3	-2.18	122.63	126.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	y	506	CLA	CHD-C1D-ND	-2.18	121.74	124.80
16	h	504	CLA	CHA-C1A-NA	-2.17	121.47	126.39
13	I	103	LHG	C27-C26-C25	-2.17	103.38	114.37
19	l	4019	BCR	C37-C22-C21	-2.17	119.29	122.82
16	p	502	CLA	C1-C2-C3	-2.17	123.24	126.76
16	b	1219	CLA	C2D-C1D-ND	-2.17	107.97	110.13
16	W	507	CLA	C4A-NA-C1A	2.17	107.67	106.68
19	G	4005	BCR	C15-C14-C13	-2.17	124.23	127.28
19	w	602	BCR	C11-C10-C9	-2.17	124.23	127.28
16	v	515	CLA	CHD-C1D-ND	-2.17	121.74	124.80
16	t	513	CLA	CHA-C1A-NA	-2.17	121.47	126.39
19	Z	604	BCR	C15-C16-C17	-2.17	119.07	123.52
16	B	1203	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
19	a	4003	BCR	C29-C30-C25	2.17	113.60	110.44
14	A	4201	LMG	O2-C2-C1	-2.17	104.90	110.08
16	H	1101	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
16	p	506	CLA	C1D-ND-C4D	-2.17	104.79	106.31
13	A	849	LHG	C27-C26-C25	-2.17	103.39	114.37
16	u	515	CLA	CHA-C1A-NA	-2.17	121.47	126.39
16	A	1128	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	p	514	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
19	b	4017	BCR	C30-C25-C26	-2.17	119.67	122.64
16	r	509	CLA	CHA-C1A-NA	-2.17	121.48	126.39
16	w	501	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
19	o	603	BCR	C7-C8-C9	-2.17	123.03	126.23
16	q	501	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
19	A	4011	BCR	C10-C11-C12	-2.17	116.91	123.20
16	G	1205	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	b	1218	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	h	506	CLA	CHA-C1A-NA	-2.17	121.48	126.39
16	X	511	CLA	CMB-C2B-C1B	-2.17	125.28	128.46
16	b	1207	CLA	CHD-C1D-ND	-2.17	121.75	124.80
19	W	604	BCR	C11-C10-C9	-2.17	124.24	127.28
16	B	1021	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
14	F	4017	LMG	O2-C2-C1	-2.17	104.91	110.08
16	X	511	CLA	CHA-C1A-NA	-2.17	121.49	126.39
16	a	1022	CLA	C4A-NA-C1A	2.17	107.67	106.68
19	f	4016	BCR	C40-C30-C25	2.17	113.64	110.24
16	x	507	CLA	C1-C2-C3	-2.17	122.65	126.20
16	a	1140	CLA	CHD-C1D-ND	-2.17	121.75	124.80
16	s	511	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
19	A	4008	BCR	C24-C23-C22	-2.17	123.03	126.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	516	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	v	510	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	s	514	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
16	o	505	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
16	w	516	CLA	CHA-C1A-NA	-2.16	121.49	126.39
16	s	506	CLA	C2D-C1D-ND	-2.16	107.98	110.13
19	o	603	BCR	C11-C10-C9	-2.16	124.24	127.28
16	G	1226	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	G	1012	CLA	C1-C2-C3	-2.16	122.65	126.20
19	y	604	BCR	C16-C15-C14	-2.16	119.09	123.52
16	h	511	CLA	CHA-C1A-NA	-2.16	121.49	126.39
16	b	1205	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	y	516	CLA	CHD-C1D-C2D	2.16	129.99	125.49
14	Q	4017	LMG	O2-C2-C1	-2.16	104.92	110.08
19	Z	604	BCR	C33-C5-C6	-2.16	122.12	124.48
16	a	1120	CLA	C1C-C2C-C3C	-2.16	104.71	106.98
19	j	4013	BCR	C2-C1-C6	2.16	113.58	110.44
16	b	1012	CLA	C1-C2-C3	-2.16	122.66	126.20
19	X	602	BCR	C20-C21-C22	-2.16	124.25	127.28
21	m	4021	ECH	C19-C18-C17	2.16	122.41	119.01
16	a	1104	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	B	1226	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	Z	501	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	x	515	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	H	1107	CLA	C1-C2-C3	-2.16	123.27	126.76
16	h	517	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	l	1501	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	o	503	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	A	1115	CLA	C2A-C1A-CHA	2.16	127.61	123.87
21	I	4020	ECH	C2-C3-C4	-2.16	106.53	111.28
16	X	515	CLA	CHD-C1D-ND	-2.16	121.76	124.80
19	H	4003	BCR	C15-C16-C17	-2.16	119.10	123.52
16	h	509	CLA	CHA-C1A-NA	-2.16	121.50	126.39
16	Y	510	CLA	CHD-C1D-ND	-2.16	121.77	124.80
19	x	604	BCR	C11-C10-C9	-2.16	124.25	127.28
19	w	604	BCR	C33-C5-C6	-2.16	122.13	124.48
14	Q	4017	LMG	O3-C3-C2	-2.16	105.29	110.38
16	Z	502	CLA	CHD-C1D-ND	-2.16	121.77	124.80
19	W	604	BCR	C30-C25-C26	-2.16	119.69	122.64
16	H	1022	CLA	CMB-C2B-C1B	-2.16	125.30	128.46
16	y	503	CLA	CHA-C1A-NA	-2.16	121.51	126.39
16	a	1128	CLA	O2A-CGA-O1A	-2.16	118.23	123.63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	t	510	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
16	a	1109	CLA	CHA-C1A-NA	-2.16	121.51	126.39
19	b	4014	BCR	C16-C15-C14	-2.16	119.11	123.52
16	h	505	CLA	C2A-C1A-CHA	2.16	127.61	123.87
16	s	506	CLA	CHA-C1A-NA	-2.16	121.51	126.39
16	y	501	CLA	CHA-C1A-NA	-2.16	121.51	126.39
13	i	103	LHG	C27-C26-C25	-2.16	103.47	114.37
16	g	505	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
16	u	502	CLA	CHD-C1D-ND	-2.16	121.77	124.80
16	y	509	CLA	CHD-C1D-ND	-2.16	121.77	124.80
16	G	1239	CLA	CHA-C1A-NA	-2.16	121.51	126.39
16	H	1107	CLA	C4A-NA-C1A	2.15	107.66	106.68
16	b	1214	CLA	CHA-C1A-NA	-2.15	121.51	126.39
19	G	4005	BCR	C30-C25-C26	-2.15	119.69	122.64
19	f	4016	BCR	C15-C16-C17	-2.15	119.11	123.52
16	t	506	CLA	CHA-C1A-NA	-2.15	121.51	126.39
16	s	501	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
19	u	604	BCR	C27-C26-C25	2.15	125.61	122.70
16	p	513	CLA	CHD-C1D-ND	-2.15	121.77	124.80
16	H	1237	CLA	CHA-C1A-NA	-2.15	121.52	126.39
16	l	1502	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
16	B	1225	CLA	CHA-C1A-NA	-2.15	121.52	126.39
16	g	514	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
19	A	4002	BCR	C15-C16-C17	-2.15	119.11	123.52
19	T	4005	BCR	C24-C23-C22	-2.15	123.05	126.23
19	o	604	BCR	C2-C1-C6	2.15	113.56	110.44
16	s	512	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
19	j	4015	BCR	C7-C8-C9	-2.15	123.05	126.23
16	W	505	CLA	C3C-C4C-NC	-2.15	107.67	110.43
16	X	504	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	a	1013	CLA	C3A-C2A-C1A	-2.15	98.12	101.34
19	F	4016	BCR	C15-C14-C13	-2.15	124.26	127.28
19	v	604	BCR	C15-C16-C17	-2.15	119.12	123.52
19	o	604	BCR	C40-C30-C25	2.15	113.62	110.24
16	a	1113	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	a	1110	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
16	B	1207	CLA	C1-O2A-CGA	2.15	121.86	116.65
16	g	501	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	n	505	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
16	a	1237	CLA	CHA-C1A-NA	-2.15	121.53	126.39
16	h	510	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
21	i	4020	ECH	C2-C1-C6	2.15	113.56	110.44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	512	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	h	511	CLA	C4A-NA-C1A	2.15	107.66	106.68
16	a	1133	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
16	B	1240	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	Z	502	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	G	1219	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	b	1206	CLA	CHD-C1D-ND	-2.15	121.78	124.80
19	h	604	BCR	C1-C6-C5	-2.15	119.70	122.64
16	l	1503	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	o	506	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	h	514	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	G	1223	CLA	C7-C6-C5	-2.15	107.54	113.26
16	B	1208	CLA	CHA-C1A-NA	-2.15	121.53	126.39
16	s	511	CLA	CMB-C2B-C1B	-2.14	125.31	128.46
16	X	502	CLA	CHD-C1D-ND	-2.14	121.78	124.80
16	Y	512	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	q	514	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	B	1023	CLA	C4D-C3D-CAD	-2.14	105.78	108.11
16	U	1502	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	b	1021	CLA	C2A-C1A-CHA	2.14	127.59	123.87
16	y	508	CLA	CHD-C1D-ND	-2.14	121.79	124.80
16	y	512	CLA	CHD-C1D-ND	-2.14	121.79	124.80
20	L	4101	LMT	C3B-C4B-C5B	-2.14	106.35	110.23
19	a	4002	BCR	C15-C16-C17	-2.14	119.14	123.52
16	v	504	CLA	C2D-C1D-ND	-2.14	108.01	110.13
16	K	4004	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	b	1012	CLA	C2A-C1A-CHA	2.14	127.58	123.87
16	G	1207	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
21	b	4006	ECH	C1-C6-C5	-2.14	119.71	122.64
16	u	506	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
16	t	512	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	b	1234	CLA	C4A-NA-C1A	2.14	107.66	106.68
16	A	1112	CLA	O2A-CGA-O1A	-2.14	117.83	123.33
16	b	1215	CLA	CHA-C1A-NA	-2.14	121.55	126.39
16	Y	514	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	Y	515	CLA	CMB-C2B-C1B	-2.14	125.32	128.46
19	u	601	BCR	C1-C6-C5	-2.14	119.72	122.64
16	H	1128	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
19	q	604	BCR	C33-C5-C6	-2.14	122.15	124.48
16	Y	503	CLA	C4D-C3D-CAD	-2.14	105.78	108.11
16	A	1013	CLA	CHA-C1A-NA	-2.14	121.55	126.39
16	B	1222	CLA	CHD-C1D-ND	-2.14	121.80	124.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	u	515	CLA	CHD-C1D-ND	-2.14	121.80	124.80
16	v	506	CLA	CHD-C1D-ND	-2.14	121.80	124.80
19	n	603	BCR	C11-C10-C9	-2.14	124.28	127.28
14	a	4101	LMG	O3-C3-C2	-2.14	105.34	110.38
16	X	512	CLA	C2A-C1A-CHA	2.14	127.57	123.87
19	x	602	BCR	C7-C8-C9	-2.14	123.08	126.23
19	u	601	BCR	C28-C27-C26	-2.14	110.25	114.06
16	x	504	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
16	p	513	CLA	C1C-C2C-C3C	-2.13	104.73	106.98
19	u	604	BCR	C1-C6-C5	-2.13	119.72	122.64
16	l	1503	CLA	CHD-C1D-ND	-2.13	121.80	124.80
16	G	1012	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
19	H	4002	BCR	C16-C15-C14	-2.13	119.15	123.52
19	s	603	BCR	C11-C10-C9	-2.13	124.29	127.28
16	n	501	CLA	C1C-C2C-C3C	-2.13	104.74	106.98
16	A	1105	CLA	CHA-C1A-NA	-2.13	121.56	126.39
16	t	501	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
13	H	849	LHG	C27-C26-C25	-2.13	103.59	114.37
16	y	512	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	H	1137	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
19	u	602	BCR	C28-C27-C26	-2.13	110.26	114.06
16	b	1229	CLA	C4A-NA-C1A	2.13	107.65	106.68
16	v	513	CLA	C4A-NA-C1A	2.13	107.65	106.68
16	p	501	CLA	CHA-C1A-NA	-2.13	121.57	126.39
21	B	4006	ECH	O27-C27-C26	2.13	122.89	120.98
16	u	510	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	G	1209	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	t	501	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	a	1105	CLA	CHA-C1A-NA	-2.13	121.57	126.39
16	g	504	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	a	1118	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	X	506	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	Y	508	CLA	C4A-NA-C1A	2.13	107.65	106.68
19	n	601	BCR	C15-C16-C17	-2.13	119.17	123.52
16	G	1202	CLA	CHA-C1A-NA	-2.13	121.57	126.39
16	n	514	CLA	CHD-C1D-C2D	2.13	129.91	125.49
16	g	515	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
16	o	515	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
16	B	1206	CLA	CHD-C1D-ND	-2.13	121.81	124.80
19	U	4022	BCR	C20-C21-C22	-2.13	124.30	127.28
24	q	601	LUT	C7-C8-C9	-2.13	123.09	126.23
16	B	1232	CLA	C2A-C1A-CHA	2.13	127.56	123.87

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	1105	CLA	CHD-C1D-C2D	2.13	129.91	125.49
16	a	1022	CLA	CAA-CBA-CGA	-2.13	107.17	113.21
16	q	505	CLA	CHA-C1A-NA	-2.13	121.58	126.39
16	v	508	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
19	w	603	BCR	C10-C11-C12	-2.12	117.04	123.20
16	h	512	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
19	T	4005	BCR	C16-C15-C14	-2.12	119.17	123.52
16	w	513	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
16	n	504	CLA	CHD-C1D-ND	-2.12	121.81	124.80
16	v	506	CLA	CMB-C2B-C1B	-2.12	125.34	128.46
16	A	1104	CLA	C4A-NA-C1A	2.12	107.65	106.68
19	Y	601	BCR	C7-C8-C9	-2.12	123.09	126.23
16	b	1021	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
19	Y	603	BCR	C16-C15-C14	-2.12	119.17	123.52
16	v	515	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
16	H	1112	CLA	O2A-CGA-O1A	-2.12	117.87	123.33
16	A	1120	CLA	CHD-C1D-ND	-2.12	121.81	124.80
16	H	1128	CLA	CHA-C1A-NA	-2.12	121.58	126.39
16	x	501	CLA	CHA-C1A-NA	-2.12	121.58	126.39
16	y	504	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
14	F	4017	LMG	O3-C3-C2	-2.12	105.37	110.38
19	J	4012	BCR	C24-C23-C22	-2.12	123.10	126.23
14	f	4017	LMG	O2-C2-C1	-2.12	105.02	110.08
16	o	509	CLA	CHD-C1D-ND	-2.12	121.82	124.80
23	s	606	LMU	C1'-C2'-C3'	2.12	114.47	110.01
19	K	4001	BCR	C30-C25-C26	-2.12	119.74	122.64
16	A	1124	CLA	C1C-C2C-C3C	-2.12	104.75	106.98
16	A	1139	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
19	Y	604	BCR	C24-C23-C22	-2.12	123.10	126.23
19	r	604	BCR	C7-C8-C9	-2.12	123.10	126.23
16	a	1116	CLA	CHA-C1A-NA	-2.12	121.59	126.39
16	v	508	CLA	CHA-C1A-NA	-2.12	121.59	126.39
19	Q	4016	BCR	C16-C15-C14	-2.12	119.18	123.52
16	a	1022	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	f	1301	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	w	510	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	Z	513	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	r	603	BCR	C30-C25-C26	-2.12	119.74	122.64
16	H	1013	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
19	F	4016	BCR	C16-C15-C14	-2.12	119.18	123.52
16	b	1239	CLA	C3C-C4C-NC	-2.12	107.72	110.43
19	X	603	BCR	C15-C16-C17	-2.12	119.19	123.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Z	506	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	x	502	CLA	CHD-C1D-ND	-2.12	121.82	124.80
19	k	4005	BCR	C16-C15-C14	-2.12	119.19	123.52
16	X	517	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
16	v	515	CLA	CHA-C1A-NA	-2.12	121.60	126.39
16	q	505	CLA	C1-C2-C3	-2.12	122.73	126.20
14	A	4101	LMG	O3-C3-C2	-2.12	105.39	110.38
16	p	504	CLA	CHD-C1D-ND	-2.12	121.83	124.80
16	s	505	CLA	CHA-C1A-NA	-2.12	121.60	126.39
19	k	4005	BCR	C3-C4-C5	-2.11	110.28	114.06
16	Y	506	CLA	CHA-C1A-NA	-2.11	121.60	126.39
16	B	1217	CLA	CHD-C1D-ND	-2.11	121.83	124.80
16	H	1131	CLA	CHD-C1D-ND	-2.11	121.83	124.80
19	X	602	BCR	C27-C26-C25	2.11	125.56	122.70
19	W	601	BCR	C24-C23-C22	-2.11	123.11	126.23
16	x	508	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
16	A	1138	CLA	C1-C2-C3	-2.11	122.73	126.20
16	Y	507	CLA	C1-C2-C3	-2.11	122.73	126.20
19	S	4015	BCR	C1-C6-C5	-2.11	119.75	122.64
19	U	4022	BCR	C1-C6-C5	-2.11	119.75	122.64
19	J	4015	BCR	C24-C23-C22	-2.11	123.11	126.23
19	H	4002	BCR	C16-C17-C18	-2.11	124.32	127.28
19	A	4003	BCR	C38-C26-C27	-2.11	109.09	113.60
16	X	501	CLA	CHA-C1A-NA	-2.11	121.61	126.39
16	g	513	CLA	CHA-C1A-NA	-2.11	121.61	126.39
16	H	1128	CLA	CHD-C1D-ND	-2.11	121.83	124.80
16	B	1206	CLA	C4A-NA-C1A	2.11	107.64	106.68
16	H	1116	CLA	CHA-C1A-NA	-2.11	121.61	126.39
19	v	604	BCR	C1-C6-C5	-2.11	119.75	122.64
19	u	604	BCR	C40-C30-C25	2.11	113.55	110.24
16	h	506	CLA	C3C-C4C-NC	-2.11	107.73	110.43
16	b	1227	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
16	Y	505	CLA	C1-C2-C3	-2.11	122.74	126.20
16	x	514	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	t	509	CLA	C7-C6-C5	-2.11	107.64	113.26
21	R	4020	ECH	C32-C1-C6	-2.11	106.94	110.24
16	a	1120	CLA	CHD-C1D-ND	-2.11	121.84	124.80
19	H	4011	BCR	C29-C30-C25	2.11	113.50	110.44
16	a	1105	CLA	CHD-C1D-C2D	2.11	129.87	125.49
16	b	1234	CLA	C1-C2-C3	-2.11	123.35	126.76
16	o	508	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	A	1114	CLA	C4D-CHA-C1A	-2.11	118.73	121.24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1215	CLA	CHA-C1A-NA	-2.11	121.62	126.39
14	H	4101	LMG	O3-C3-C2	-2.11	105.41	110.38
13	a	849	LHG	C27-C26-C25	-2.11	103.72	114.37
16	v	505	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	H	1117	CLA	CHD-C1D-C2D	2.10	129.87	125.49
16	A	1104	CLA	C11-C12-C13	-2.10	108.97	115.97
16	p	504	CLA	C1-C2-C3	-2.10	122.75	126.20
16	u	517	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
19	n	601	BCR	C28-C27-C26	-2.10	110.30	114.06
16	h	513	CLA	CHA-C1A-NA	-2.10	121.63	126.39
16	A	1110	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
16	W	506	CLA	CHA-C1A-NA	-2.10	121.63	126.39
16	r	515	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	v	517	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	B	1236	CLA	CHD-C1D-ND	-2.10	121.84	124.80
19	g	603	BCR	C16-C15-C14	-2.10	119.22	123.52
16	A	1137	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
23	w	605	LMU	C4B-C3B-C2B	2.10	114.52	110.83
16	g	506	CLA	CHA-C1A-NA	-2.10	121.63	126.39
16	X	508	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	A	1104	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	s	507	CLA	CHD-C1D-ND	-2.10	121.84	124.80
16	H	1102	CLA	CMB-C2B-C1B	-2.10	125.38	128.46
19	u	603	BCR	C7-C8-C9	-2.10	123.13	126.23
16	X	505	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	a	1137	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	y	503	CLA	C3C-C4C-NC	-2.10	107.74	110.43
19	j	4015	BCR	C30-C25-C26	-2.10	119.77	122.64
16	H	1133	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	W	508	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	a	1139	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	t	510	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	b	1222	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	x	506	CLA	CHA-C1A-NA	-2.10	121.64	126.39
16	G	1021	CLA	C2A-C1A-CHA	2.10	127.51	123.87
16	H	1126	CLA	CHA-C1A-NA	-2.10	121.64	126.39
16	w	502	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	W	505	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	G	1208	CLA	O2A-CGA-O1A	-2.10	117.94	123.33
19	T	4005	BCR	C15-C16-C17	-2.10	119.23	123.52
16	r	510	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	u	506	CLA	CHC-C1C-C2C	-2.10	121.00	126.94

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1022	CLA	CAA-CBA-CGA	-2.10	107.26	113.21
16	b	1226	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
19	Y	604	BCR	C33-C5-C6	-2.10	122.20	124.48
19	x	602	BCR	C33-C5-C6	-2.10	122.20	124.48
16	H	1013	CLA	CHA-C1A-NA	-2.10	121.64	126.39
16	g	510	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
16	l	1503	CLA	C4A-NA-C1A	2.10	107.64	106.68
13	s	605	LHG	C27-C26-C25	-2.10	103.78	114.37
16	a	1126	CLA	CHA-C1A-NA	-2.09	121.65	126.39
19	b	4009	BCR	C30-C25-C26	-2.09	119.77	122.64
16	y	508	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
16	b	1012	CLA	CAA-C2A-C3A	-2.09	107.34	113.00
16	X	513	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	w	504	CLA	CHA-C1A-NA	-2.09	121.65	126.39
19	x	602	BCR	C11-C10-C9	-2.09	124.34	127.28
16	G	1213	CLA	CHA-C1A-NA	-2.09	121.65	126.39
16	b	1012	CLA	CHA-C1A-NA	-2.09	121.65	126.39
19	S	4015	BCR	C7-C8-C9	-2.09	123.14	126.23
19	r	601	BCR	C7-C8-C9	-2.09	123.14	126.23
19	b	4005	BCR	C30-C25-C26	-2.09	119.78	122.64
16	A	1137	CLA	CHA-C1A-NA	-2.09	121.66	126.39
16	B	1227	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
16	q	505	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
21	G	4006	ECH	C2-C1-C6	2.09	113.48	110.44
19	K	4005	BCR	C11-C10-C9	-2.09	124.35	127.28
16	G	1212	CLA	CHA-C1A-NA	-2.09	121.66	126.39
16	r	516	CLA	CHA-C1A-NA	-2.09	121.66	126.39
19	w	602	BCR	C30-C25-C26	-2.09	119.78	122.64
16	a	1117	CLA	C1-C2-C3	-2.09	122.77	126.20
16	H	1237	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	g	510	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	v	512	CLA	CHD-C1D-ND	-2.09	121.86	124.80
24	q	601	LUT	C11-C10-C9	2.09	130.21	127.28
16	B	1213	CLA	CHD-C1D-C2D	2.09	129.83	125.49
16	B	1205	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
16	t	506	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
16	u	505	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
13	i	103	LHG	C5-O7-C7	-2.09	112.80	117.80
19	J	4012	BCR	C30-C25-C26	-2.09	119.78	122.64
16	Y	513	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	W	512	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
15	A	1011	CL0	CMB-C2B-C1B	-2.09	125.40	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	g	606	LMU	C4B-C3B-C2B	2.09	114.50	110.83
19	i	4018	BCR	C30-C25-C26	-2.09	119.78	122.64
19	j	4015	BCR	C2-C1-C6	2.09	113.47	110.44
16	H	1106	CLA	CHA-C1A-NA	-2.09	121.67	126.39
16	w	505	CLA	CHA-C1A-NA	-2.09	121.67	126.39
16	x	511	CLA	CMB-C2B-C1B	-2.09	125.40	128.46
16	G	1021	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	y	514	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	n	513	CLA	C4A-NA-C1A	2.08	107.63	106.68
19	g	601	BCR	C1-C6-C5	-2.08	119.79	122.64
16	B	1220	CLA	CHA-C1A-NA	-2.08	121.67	126.39
16	H	1140	CLA	CHD-C1D-ND	-2.08	121.87	124.80
16	Y	502	CLA	CHA-C1A-NA	-2.08	121.68	126.39
16	a	1130	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	o	502	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	A	1101	CLA	C11-C10-C8	-2.08	109.05	115.97
16	A	1122	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	G	4004	BCR	C7-C8-C9	-2.08	123.16	126.23
16	H	1114	CLA	CHD-C1D-C2D	2.08	129.81	125.49
16	r	506	CLA	C1C-C2C-C3C	-2.08	104.79	106.98
16	Z	501	CLA	C4A-NA-C1A	2.08	107.63	106.68
16	w	511	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	A	4008	BCR	C29-C30-C25	2.08	113.46	110.44
16	G	1239	CLA	C3C-C4C-NC	-2.08	107.77	110.43
19	h	603	BCR	C1-C6-C5	-2.08	119.79	122.64
16	G	1223	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	v	507	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	Y	510	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	H	1131	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	o	604	BCR	C11-C10-C9	-2.08	124.36	127.28
16	X	515	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	w	514	CLA	C4A-NA-C1A	2.08	107.63	106.68
16	n	506	CLA	CHA-C1A-NA	-2.08	121.69	126.39
16	H	1110	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	y	603	BCR	C16-C15-C14	-2.08	119.27	123.52
16	r	507	CLA	C1-C2-C3	-2.08	122.79	126.20
16	Y	512	CLA	CHA-C4D-ND	2.08	136.83	132.55
16	p	510	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	Y	602	BCR	C24-C23-C22	-2.08	123.16	126.23
19	S	4012	BCR	C15-C14-C13	-2.08	124.37	127.28
19	o	602	BCR	C11-C10-C9	-2.08	124.37	127.28
16	W	514	CLA	O2A-CGA-O1A	-2.08	118.44	123.63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	g	601	BCR	C7-C8-C9	-2.08	123.16	126.23
14	a	852	LMG	O2-C2-C1	-2.08	105.13	110.08
16	B	1219	CLA	O2A-CGA-O1A	-2.08	117.99	123.33
16	L	1503	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
19	I	4018	BCR	C30-C25-C26	-2.08	119.80	122.64
16	B	1222	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
16	H	1022	CLA	CAA-CBA-CGA	-2.07	107.32	113.21
21	B	4006	ECH	C37-C22-C21	-2.07	119.45	122.82
16	G	1219	CLA	O2A-CGA-O1A	-2.07	118.00	123.33
19	x	602	BCR	C27-C26-C25	2.07	125.51	122.70
19	o	602	BCR	C28-C27-C26	-2.07	110.36	114.06
19	o	604	BCR	C30-C25-C26	-2.07	119.80	122.64
19	y	604	BCR	C24-C23-C22	-2.07	123.17	126.23
16	a	1121	CLA	CHA-C1A-NA	-2.07	121.70	126.39
16	b	1210	CLA	CHA-C1A-NA	-2.07	121.70	126.39
16	b	1219	CLA	O2A-CGA-O1A	-2.07	118.00	123.33
16	x	510	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
16	h	501	CLA	CHA-C1A-NA	-2.07	121.70	126.39
16	w	509	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
19	g	602	BCR	C33-C5-C6	-2.07	122.22	124.48
16	G	1021	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	Y	604	BCR	C15-C16-C17	-2.07	119.28	123.52
16	w	506	CLA	CHA-C1A-NA	-2.07	121.70	126.39
19	G	4010	BCR	C8-C7-C6	-2.07	121.47	127.00
16	p	507	CLA	C1-C2-C3	-2.07	122.81	126.20
14	B	848	LMG	O7-C10-O9	-2.07	118.86	123.70
16	b	1238	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
16	v	504	CLA	CHA-C1A-NA	-2.07	121.70	126.39
16	H	1013	CLA	CMB-C2B-C3B	2.07	128.82	124.68
16	g	513	CLA	CHD-C1D-ND	-2.07	121.89	124.80
16	A	1131	CLA	CHA-C1A-NA	-2.07	121.71	126.39
16	H	1104	CLA	CHA-C4D-ND	2.07	136.82	132.55
16	v	506	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	f	4017	LMG	O3-C3-C2	-2.07	105.50	110.38
16	b	1203	CLA	C4-C3-C5	2.07	118.82	115.23
20	L	4101	LMT	O5B-C1B-C2B	2.07	114.62	110.37
16	A	1116	CLA	C4D-C3D-CAD	-2.07	105.86	108.11
16	s	506	CLA	CMD-C2D-C1D	-2.07	121.09	124.73
16	w	505	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
16	G	1235	CLA	CHD-C1D-C2D	2.07	129.78	125.49
21	B	4006	ECH	C24-C23-C22	2.07	129.29	126.23
19	B	4017	BCR	C16-C17-C18	-2.07	124.38	127.28

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	X	603	BCR	C15-C14-C13	-2.07	124.38	127.28
16	p	517	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
16	A	1130	CLA	C1-C2-C3	-2.07	122.81	126.20
16	B	1208	CLA	O2A-CGA-O1A	-2.07	118.02	123.33
23	q	605	LMU	C4B-C3B-C2B	2.06	114.45	110.83
19	u	601	BCR	C27-C26-C25	2.06	125.49	122.70
19	G	4009	BCR	C21-C20-C19	-2.06	117.22	123.20
16	X	511	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
16	X	507	CLA	C1-C2-C3	-2.06	122.81	126.20
16	g	505	CLA	C1-C2-C3	-2.06	122.81	126.20
16	A	1801	CLA	C1C-C2C-C3C	-2.06	104.81	106.98
16	u	501	CLA	CHD-C1D-ND	-2.06	121.90	124.80
16	J	1302	CLA	O2A-CGA-O1A	-2.06	118.02	123.33
16	A	1140	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
19	n	601	BCR	C29-C30-C25	2.06	113.44	110.44
16	X	517	CLA	CHA-C1A-NA	-2.06	121.72	126.39
16	H	1107	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	T	4002	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
19	y	604	BCR	C30-C25-C26	-2.06	119.82	122.64
16	u	514	CLA	CHA-C1A-NA	-2.06	121.72	126.39
19	Q	4016	BCR	C24-C23-C22	-2.06	123.19	126.23
16	A	1237	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	G	1227	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
19	T	4001	BCR	C33-C5-C6	-2.06	122.23	124.48
19	U	4019	BCR	C37-C22-C21	-2.06	119.48	122.82
16	v	502	CLA	C1-C2-C3	-2.06	123.43	126.76
16	h	511	CLA	C3C-C4C-NC	-2.06	107.79	110.43
19	v	604	BCR	C3-C4-C5	-2.06	110.38	114.06
19	y	604	BCR	C1-C6-C5	-2.06	119.82	122.64
16	G	1206	CLA	C4A-NA-C1A	2.06	107.62	106.68
16	G	1222	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	b	1205	CLA	C1C-C2C-C3C	-2.06	104.81	106.98
19	G	4010	BCR	C30-C25-C26	-2.06	119.82	122.64
16	p	509	CLA	CHD-C1D-ND	-2.06	121.91	124.80
19	r	601	BCR	C27-C26-C25	2.06	125.49	122.70
16	A	1237	CLA	C1-C2-C3	-2.06	122.82	126.20
19	p	601	BCR	C20-C21-C22	-2.06	124.39	127.28
16	r	501	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
16	A	1120	CLA	C1C-C2C-C3C	-2.06	104.81	106.98
19	r	601	BCR	C33-C5-C6	-2.06	122.24	124.48
19	U	4022	BCR	C15-C16-C17	-2.06	119.31	123.52
16	b	1227	CLA	CHA-C1A-NA	-2.06	121.73	126.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	4018	BCR	C1-C6-C5	-2.06	119.82	122.64
19	g	603	BCR	C30-C25-C26	-2.06	119.82	122.64
16	n	503	CLA	CHA-C1A-NA	-2.06	121.73	126.39
19	A	4008	BCR	C35-C13-C14	-2.06	119.48	122.82
16	y	515	CLA	CMB-C2B-C1B	-2.06	125.44	128.46
16	w	508	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
16	q	513	CLA	CHD-C1D-ND	-2.06	121.91	124.80
16	u	517	CLA	CHD-C1D-ND	-2.06	121.91	124.80
21	V	4021	ECH	C19-C18-C17	2.06	122.24	119.01
16	q	517	CLA	CHA-C1A-NA	-2.06	121.73	126.39
21	I	4020	ECH	C38-C26-C25	-2.06	120.80	124.11
19	H	4007	BCR	C29-C30-C25	2.06	113.43	110.44
16	H	1135	CLA	CHD-C1D-ND	-2.06	121.91	124.80
16	a	1112	CLA	CHD-C1D-ND	-2.06	121.91	124.80
16	a	1137	CLA	CHA-C1A-NA	-2.06	121.73	126.39
16	k	4002	CLA	CHA-C1A-NA	-2.06	121.73	126.39
16	H	1237	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
16	t	513	CLA	C2A-C1A-CHA	2.06	127.44	123.87
16	G	1012	CLA	O2D-CGD-CBD	2.06	114.82	111.23
19	t	604	BCR	C27-C26-C25	2.06	125.48	122.70
16	b	1218	CLA	C1C-C2C-C3C	-2.06	104.82	106.98
16	b	1213	CLA	CHD-C1D-C2D	2.06	129.76	125.49
16	B	1012	CLA	C1-C2-C3	-2.06	122.83	126.20
16	t	508	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
16	w	512	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
16	a	1106	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	G	1207	CLA	C2A-C1A-CHA	2.05	127.43	123.87
16	H	1112	CLA	CHD-C1D-ND	-2.05	121.91	124.80
16	H	1137	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	b	1218	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	u	503	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	b	1221	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
19	U	4019	BCR	C20-C21-C22	-2.05	124.40	127.28
16	b	1217	CLA	O2A-CGA-O1A	-2.05	118.05	123.33
16	r	514	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
16	g	504	CLA	C1-C2-C3	-2.05	122.83	126.20
19	R	4018	BCR	C30-C25-C26	-2.05	119.83	122.64
16	A	1111	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	s	517	CLA	CHD-C1D-ND	-2.05	121.91	124.80
19	F	4016	BCR	C30-C25-C26	-2.05	119.83	122.64
19	H	4011	BCR	C7-C8-C9	-2.05	123.20	126.23
19	Y	604	BCR	C15-C14-C13	-2.05	124.40	127.28

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	515	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
19	q	603	BCR	C30-C25-C26	-2.05	119.83	122.64
19	s	602	BCR	C30-C25-C26	-2.05	119.83	122.64
16	n	512	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
13	p	605	LHG	C27-C26-C25	-2.05	104.00	114.37
16	a	1103	CLA	CAA-CBA-CGA	-2.05	107.39	113.21
16	b	1213	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
16	o	517	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
16	h	512	CLA	CHD-C1D-ND	-2.05	121.92	124.80
16	G	1232	CLA	O2A-CGA-O1A	-2.05	118.06	123.33
16	a	1112	CLA	O2A-CGA-O1A	-2.05	118.06	123.33
16	H	1113	CLA	O2A-CGA-O1A	-2.05	118.06	123.33
16	a	1133	CLA	CHD-C1D-ND	-2.05	121.92	124.80
19	k	4001	BCR	C40-C30-C25	2.05	113.45	110.24
16	o	510	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
19	g	603	BCR	C15-C16-C17	-2.05	119.33	123.52
16	b	1208	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
19	W	601	BCR	C30-C25-C26	-2.05	119.84	122.64
16	u	516	CLA	CHA-C1A-NA	-2.05	121.76	126.39
16	S	1302	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
21	R	4020	ECH	C34-C9-C8	2.05	121.21	118.09
16	W	510	CLA	CHD-C1D-ND	-2.04	121.92	124.80
19	J	4015	BCR	C30-C25-C26	-2.04	119.84	122.64
16	r	506	CLA	CHA-C1A-NA	-2.04	121.76	126.39
16	u	513	CLA	CHA-C1A-NA	-2.04	121.76	126.39
19	X	601	BCR	C27-C26-C25	2.04	125.47	122.70
14	a	4201	LMG	O2-C2-C1	-2.04	105.20	110.08
16	b	1210	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	w	512	CLA	CMB-C2B-C1B	-2.04	125.46	128.46
16	t	502	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	G	1205	CLA	CHA-C1A-NA	-2.04	121.77	126.39
19	L	4019	BCR	C27-C26-C25	2.04	125.46	122.70
16	L	1501	CLA	CHA-C1A-NA	-2.04	121.77	126.39
16	H	1117	CLA	C3C-C4C-NC	-2.04	107.81	110.43
16	x	515	CLA	C2D-C1D-ND	-2.04	108.11	110.13
19	b	4009	BCR	C11-C10-C9	-2.04	124.36	127.48
16	n	509	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	A	1022	CLA	C1-C2-C3	-2.04	122.85	126.20
16	A	1101	CLA	C1-C2-C3	-2.04	122.85	126.20
16	A	1105	CLA	CMB-C2B-C1B	-2.04	125.47	128.46
16	H	1130	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	h	506	CLA	O2A-CGA-O1A	-2.04	118.52	123.63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	u	515	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	v	604	BCR	C16-C15-C14	-2.04	119.34	123.52
16	u	507	CLA	C1-C2-C3	-2.04	122.85	126.20
16	s	502	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	v	511	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
19	v	603	BCR	C24-C23-C22	-2.04	123.22	126.23
16	H	1126	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	W	502	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
19	L	4022	BCR	C15-C16-C17	-2.04	119.35	123.52
16	g	501	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	q	509	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	A	1128	CLA	CHA-C1A-NA	-2.04	121.77	126.39
19	B	4009	BCR	C11-C10-C9	-2.04	124.36	127.48
16	p	503	CLA	C4D-C3D-CAD	-2.04	105.89	108.11
16	A	1119	CLA	CHD-C1D-C2D	2.04	129.72	125.49
16	s	515	CLA	CHA-C1A-NA	-2.04	121.78	126.39
19	l	4019	BCR	C20-C21-C22	-2.04	124.42	127.28
19	a	4008	BCR	C29-C30-C25	2.04	113.40	110.44
16	q	510	CLA	CHD-C1D-ND	-2.04	121.94	124.80
19	A	4002	BCR	C24-C23-C22	-2.04	123.22	126.23
16	B	1226	CLA	C3C-C4C-NC	-2.04	107.82	110.43
16	H	1118	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	a	1139	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	r	504	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	B	1207	CLA	C2A-C1A-CHA	2.04	127.40	123.87
19	j	4013	BCR	C30-C25-C26	-2.04	119.85	122.64
19	o	601	BCR	C1-C6-C5	-2.04	119.85	122.64
19	Q	4016	BCR	C7-C8-C9	-2.04	123.22	126.23
19	u	604	BCR	C3-C4-C5	-2.04	110.43	114.06
16	Y	502	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
16	v	512	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
16	H	1022	CLA	C2D-C1D-ND	-2.03	108.11	110.13
16	s	507	CLA	C1-C2-C3	-2.03	122.86	126.20
16	o	511	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	B	1211	CLA	CHD-C1D-ND	-2.03	121.94	124.80
16	t	505	CLA	C3C-C4C-NC	-2.03	107.82	110.43
19	u	603	BCR	C30-C25-C26	-2.03	119.86	122.64
16	w	511	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	o	509	CLA	CHA-C1A-NA	-2.03	121.78	126.39
16	y	502	CLA	C1-C2-C3	-2.03	123.47	126.76
16	a	1117	CLA	C3C-C4C-NC	-2.03	107.83	110.43
19	H	4002	BCR	C30-C25-C26	-2.03	119.86	122.64

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	1022	CLA	CHA-C1A-NA	-2.03	121.79	126.39
15	a	1011	CL0	CMB-C2B-C1B	-2.03	125.48	128.46
16	a	1801	CLA	CHD-C1D-ND	-2.03	121.94	124.80
16	n	504	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	H	1013	CLA	C1-O2A-CGA	2.03	121.57	116.65
16	y	511	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	y	515	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	b	1235	CLA	C3A-C2A-C1A	-2.03	98.30	101.34
19	o	604	BCR	C24-C23-C22	-2.03	123.23	126.23
14	b	848	LMG	O7-C10-O9	-2.03	118.96	123.70
19	Y	603	BCR	C30-C25-C26	-2.03	119.86	122.64
19	v	601	BCR	C1-C6-C5	-2.03	119.86	122.64
16	x	517	CLA	C4A-NA-C1A	2.03	107.61	106.68
21	i	4020	ECH	O27-C27-C28	-2.03	117.54	120.87
16	H	1118	CLA	C1D-ND-C4D	-2.03	104.89	106.31
16	x	504	CLA	C2A-C1A-CHA	2.03	127.39	123.87
16	G	1223	CLA	CHA-C1A-NA	-2.03	121.80	126.39
19	h	601	BCR	C38-C26-C25	-2.03	122.27	124.48
19	J	4013	BCR	C30-C25-C26	-2.03	119.86	122.64
16	Z	504	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	a	1128	CLA	C1-C2-C3	-2.03	122.87	126.20
16	j	1302	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
16	b	1234	CLA	C4D-C3D-CAD	-2.03	105.90	108.11
16	X	517	CLA	C2A-C1A-CHA	2.03	127.39	123.87
16	s	503	CLA	CHA-C1A-NA	-2.03	121.80	126.39
16	W	503	CLA	C3C-C4C-NC	-2.03	107.83	110.43
19	T	4005	BCR	C11-C10-C9	-2.03	124.43	127.28
19	S	4015	BCR	C30-C25-C26	-2.03	119.86	122.64
19	w	603	BCR	C30-C25-C26	-2.03	119.86	122.64
14	H	852	LMG	O2-C2-C1	-2.03	105.24	110.08
16	y	517	CLA	C1C-C2C-C3C	-2.03	104.85	106.98
19	r	602	BCR	C27-C26-C25	2.03	125.44	122.70
19	a	4002	BCR	C30-C25-C26	-2.03	119.87	122.64
21	M	4021	ECH	C19-C18-C17	2.03	122.20	119.01
16	A	1101	CLA	CHA-C1A-NA	-2.03	121.80	126.39
16	h	502	CLA	C1-C2-C3	-2.03	123.48	126.76
16	x	501	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
19	s	603	BCR	C21-C20-C19	-2.03	117.33	123.20
21	B	4006	ECH	C23-C22-C21	2.03	122.19	119.01
21	m	4021	ECH	C15-C16-C17	2.03	127.66	123.52
16	a	1237	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
19	n	604	BCR	C7-C8-C9	-2.03	123.24	126.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	y	509	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
16	q	505	CLA	CHD-C1D-C2D	2.02	129.70	125.49
19	B	4010	BCR	C30-C25-C26	-2.02	119.87	122.64
16	G	1210	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	X	514	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	g	508	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	g	514	CLA	C1-C2-C3	-2.02	123.49	126.76
19	g	602	BCR	C28-C27-C26	-2.02	110.45	114.06
19	i	4018	BCR	C1-C6-C5	-2.02	119.87	122.64
16	x	505	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	X	512	CLA	CHD-C1D-ND	-2.02	121.96	124.80
16	W	511	CLA	C2D-C1D-ND	-2.02	108.12	110.13
16	Z	510	CLA	CHA-C1A-NA	-2.02	121.81	126.39
19	G	4009	BCR	C11-C10-C9	-2.02	124.39	127.48
19	B	4010	BCR	C10-C11-C12	-2.02	117.34	123.20
16	G	1023	CLA	CMD-C2D-C1D	-2.02	121.17	124.73
16	A	1106	CLA	C1-C2-C3	-2.02	122.89	126.20
16	y	514	CLA	C1C-C2C-C3C	-2.02	104.86	106.98
19	a	4003	BCR	C15-C14-C13	-2.02	124.44	127.28
16	G	1212	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
16	U	1501	CLA	CHA-C1A-NA	-2.02	121.82	126.39
16	A	1022	CLA	CHA-C1A-NA	-2.02	121.82	126.39
16	w	513	CLA	CHD-C1D-ND	-2.02	121.96	124.80
16	q	510	CLA	CHA-C1A-NA	-2.02	121.82	126.39
19	J	4013	BCR	C16-C15-C14	-2.02	119.39	123.52
19	Y	604	BCR	C11-C10-C9	-2.02	124.45	127.28
19	a	4002	BCR	C15-C14-C13	-2.02	124.45	127.28
16	H	1118	CLA	C3C-C4C-NC	-2.02	107.84	110.43
16	b	1216	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
19	g	602	BCR	C27-C26-C25	2.02	125.43	122.70
16	B	1240	CLA	CHA-C1A-NA	-2.02	121.82	126.39
16	h	510	CLA	CHD-C1D-ND	-2.02	121.96	124.80
19	h	604	BCR	C15-C16-C17	-2.02	119.39	123.52
16	G	1222	CLA	CHD-C1D-C2D	2.02	129.68	125.49
16	h	502	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
16	G	1203	CLA	C4-C3-C5	2.02	118.73	115.23
16	s	510	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
16	n	507	CLA	C1-C2-C3	-2.02	122.89	126.20
16	A	1133	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
16	f	1301	CLA	O2A-CGA-O1A	-2.02	118.15	123.33
19	p	601	BCR	C1-C6-C5	-2.02	119.88	122.64
16	u	505	CLA	CHA-C1A-NA	-2.02	121.83	126.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	X	514	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
16	h	504	CLA	CHD-C1D-C2D	2.01	129.68	125.49
16	Q	1301	CLA	O2A-CGA-O1A	-2.01	118.15	123.33
16	A	1130	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
19	H	4011	BCR	C10-C11-C12	-2.01	117.36	123.20
19	l	4022	BCR	C16-C15-C14	-2.01	119.40	123.52
19	n	603	BCR	C7-C8-C9	-2.01	123.26	126.23
16	u	508	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	x	509	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	h	511	CLA	CHD-C1D-C2D	2.01	129.68	125.49
16	w	503	CLA	CHA-C1A-NA	-2.01	121.83	126.39
19	G	4017	BCR	C15-C14-C13	-2.01	124.45	127.28
19	s	601	BCR	C30-C25-C26	-2.01	119.89	122.64
16	w	501	CLA	C1-C2-C3	-2.01	123.51	126.76
16	B	1207	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	w	502	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	G	1210	CLA	CHA-C1A-NA	-2.01	121.83	126.39
16	Z	516	CLA	C4A-NA-C1A	2.01	107.60	106.68
16	b	1203	CLA	C2D-C1D-ND	-2.01	108.14	110.13
19	y	603	BCR	C11-C10-C9	-2.01	124.46	127.28
19	X	602	BCR	C1-C6-C5	-2.01	119.89	122.64
19	v	603	BCR	C1-C6-C5	-2.01	119.89	122.64
16	q	501	CLA	C1-C2-C3	-2.01	123.51	126.76
16	H	1114	CLA	C2A-C1A-CHA	2.01	127.36	123.87
14	H	4201	LMG	O2-C2-C1	-2.01	105.28	110.08
19	l	4019	BCR	C31-C1-C6	2.01	113.40	110.24
16	Z	511	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
16	B	1212	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
16	Z	505	CLA	CHA-C1A-NA	-2.01	121.84	126.39
16	A	1801	CLA	CHA-C1A-NA	-2.01	121.84	126.39
16	g	512	CLA	CHD-C1D-ND	-2.01	121.97	124.80
16	A	1125	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
14	G	848	LMG	O1-C1-C2	-2.01	105.22	108.27
21	M	4021	ECH	C10-C11-C12	2.01	129.02	123.20
16	p	505	CLA	CHA-C1A-NA	-2.01	121.84	126.39
16	G	1219	CLA	CMB-C2B-C1B	-2.01	125.51	128.46
16	H	1123	CLA	CMB-C2B-C1B	-2.01	125.51	128.46
16	v	512	CLA	C2A-C1A-CHA	2.01	127.35	123.87
19	H	4007	BCR	C7-C8-C9	-2.01	123.26	126.23
19	B	4017	BCR	C15-C14-C13	-2.01	124.46	127.28
19	H	4003	BCR	C15-C14-C13	-2.01	124.46	127.28
16	A	1122	CLA	O2A-CGA-O1A	-2.01	118.61	123.63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	y	510	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
21	R	4020	ECH	O27-C27-C28	-2.01	117.58	120.87
16	l	1501	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
19	b	4010	BCR	C10-C11-C12	-2.01	117.38	123.20
19	b	4005	BCR	C24-C23-C22	-2.01	123.27	126.23
16	a	1135	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	L	1501	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	p	503	CLA	CHD-C1D-C2D	2.01	129.66	125.49
16	p	506	CLA	CHA-C1A-NA	-2.01	121.85	126.39
16	U	1503	CLA	CHD-C1D-ND	-2.01	121.98	124.80
16	o	504	CLA	C2D-C1D-ND	-2.01	108.14	110.13
16	q	502	CLA	C4A-NA-C1A	2.01	107.59	106.68
19	H	4007	BCR	C1-C6-C5	-2.01	119.89	122.64
16	W	508	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
16	q	513	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
19	B	4005	BCR	C28-C27-C26	-2.00	110.48	114.06
19	L	4022	BCR	C20-C21-C22	-2.00	124.47	127.28
23	x	606	LMU	O5'-C1'-C2'	2.00	114.49	110.37
16	v	510	CLA	C1C-C2C-C3C	-2.00	104.87	106.98
16	b	1225	CLA	C2D-C1D-ND	-2.00	108.14	110.13
19	w	603	BCR	C31-C1-C6	2.00	113.39	110.24
16	w	512	CLA	CHD-C1D-ND	-2.00	121.98	124.80
21	m	4021	ECH	O27-C27-C26	2.00	122.78	120.98
19	y	603	BCR	C1-C6-C5	-2.00	119.90	122.64
16	H	1130	CLA	CHA-C1A-NA	-2.00	121.86	126.39
19	T	4001	BCR	C1-C6-C5	-2.00	119.90	122.64
19	q	602	BCR	C33-C5-C6	-2.00	122.30	124.48
16	u	501	CLA	CHA-C1A-NA	-2.00	121.86	126.39
13	A	849	LHG	O8-C23-O10	-2.00	118.62	123.63
19	i	4018	BCR	C3-C4-C5	-2.00	110.49	114.06
16	g	507	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
19	U	4019	BCR	C7-C8-C9	-2.00	123.27	126.23
16	W	514	CLA	CHD-C1D-C2D	2.00	129.65	125.49
16	u	514	CLA	CHD-C1D-C2D	2.00	129.65	125.49
19	a	4002	BCR	C24-C23-C22	-2.00	123.28	126.23
16	o	512	CLA	C2A-C1A-CHA	2.00	127.34	123.87

All (405) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	1011	CL0	NC
15	A	1011	CL0	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
15	H	1011	CL0	NC
15	H	1011	CL0	ND
15	a	1011	CL0	NC
15	a	1011	CL0	ND
16	A	1013	CLA	ND
16	A	1022	CLA	ND
16	A	1101	CLA	ND
16	A	1102	CLA	ND
16	A	1103	CLA	ND
16	A	1104	CLA	ND
16	A	1105	CLA	ND
16	A	1106	CLA	ND
16	A	1109	CLA	ND
16	A	1110	CLA	ND
16	A	1111	CLA	ND
16	A	1113	CLA	ND
16	A	1114	CLA	ND
16	A	1115	CLA	ND
16	A	1116	CLA	ND
16	A	1117	CLA	ND
16	A	1119	CLA	ND
16	A	1121	CLA	ND
16	A	1122	CLA	ND
16	A	1124	CLA	ND
16	A	1126	CLA	ND
16	A	1127	CLA	ND
16	A	1128	CLA	ND
16	A	1130	CLA	ND
16	A	1132	CLA	ND
16	A	1133	CLA	ND
16	A	1135	CLA	ND
16	A	1136	CLA	ND
16	A	1137	CLA	ND
16	A	1138	CLA	ND
16	A	1139	CLA	ND
16	A	1140	CLA	ND
16	A	1237	CLA	ND
16	A	1801	CLA	ND
16	B	1012	CLA	ND
16	B	1021	CLA	ND
16	B	1201	CLA	ND
16	B	1202	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	B	1203	CLA	ND
16	B	1204	CLA	ND
16	B	1205	CLA	ND
16	B	1206	CLA	ND
16	B	1208	CLA	ND
16	B	1209	CLA	ND
16	B	1211	CLA	ND
16	B	1212	CLA	ND
16	B	1213	CLA	ND
16	B	1214	CLA	ND
16	B	1215	CLA	ND
16	B	1220	CLA	ND
16	B	1223	CLA	ND
16	B	1224	CLA	ND
16	B	1227	CLA	ND
16	B	1229	CLA	ND
16	B	1230	CLA	ND
16	B	1231	CLA	ND
16	B	1232	CLA	ND
16	B	1234	CLA	ND
16	B	1235	CLA	ND
16	B	1236	CLA	ND
16	B	1238	CLA	ND
16	B	1240	CLA	ND
16	F	1301	CLA	ND
16	F	1302	CLA	ND
16	G	1012	CLA	ND
16	G	1021	CLA	ND
16	G	1201	CLA	ND
16	G	1202	CLA	ND
16	G	1203	CLA	ND
16	G	1204	CLA	ND
16	G	1205	CLA	ND
16	G	1206	CLA	ND
16	G	1208	CLA	ND
16	G	1209	CLA	ND
16	G	1212	CLA	ND
16	G	1213	CLA	ND
16	G	1214	CLA	ND
16	G	1215	CLA	ND
16	G	1216	CLA	ND
16	G	1220	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	G	1221	CLA	ND
16	G	1223	CLA	ND
16	G	1224	CLA	ND
16	G	1225	CLA	ND
16	G	1228	CLA	ND
16	G	1229	CLA	ND
16	G	1230	CLA	ND
16	G	1231	CLA	ND
16	G	1232	CLA	ND
16	G	1234	CLA	ND
16	G	1235	CLA	ND
16	G	1238	CLA	ND
16	G	1239	CLA	ND
16	G	1240	CLA	ND
16	H	1013	CLA	ND
16	H	1022	CLA	ND
16	H	1101	CLA	ND
16	H	1102	CLA	ND
16	H	1103	CLA	ND
16	H	1104	CLA	ND
16	H	1105	CLA	ND
16	H	1106	CLA	ND
16	H	1109	CLA	ND
16	H	1110	CLA	ND
16	H	1111	CLA	ND
16	H	1113	CLA	ND
16	H	1114	CLA	ND
16	H	1116	CLA	ND
16	H	1117	CLA	ND
16	H	1119	CLA	ND
16	H	1121	CLA	ND
16	H	1124	CLA	ND
16	H	1126	CLA	ND
16	H	1127	CLA	ND
16	H	1128	CLA	ND
16	H	1131	CLA	ND
16	H	1132	CLA	ND
16	H	1136	CLA	ND
16	H	1137	CLA	ND
16	H	1138	CLA	ND
16	H	1139	CLA	ND
16	H	1140	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	H	1237	CLA	ND
16	H	1801	CLA	ND
16	J	1302	CLA	ND
16	K	4002	CLA	ND
16	K	4003	CLA	ND
16	K	4004	CLA	ND
16	L	1503	CLA	ND
16	Q	1301	CLA	ND
16	Q	1302	CLA	ND
16	S	1302	CLA	ND
16	T	4002	CLA	ND
16	T	4003	CLA	ND
16	U	1503	CLA	ND
16	W	501	CLA	ND
16	W	502	CLA	ND
16	W	503	CLA	ND
16	W	504	CLA	ND
16	W	505	CLA	ND
16	W	508	CLA	ND
16	W	509	CLA	ND
16	W	511	CLA	ND
16	W	512	CLA	ND
16	W	514	CLA	ND
16	W	515	CLA	ND
16	W	517	CLA	ND
16	X	502	CLA	ND
16	X	505	CLA	ND
16	X	506	CLA	ND
16	X	508	CLA	ND
16	X	509	CLA	ND
16	X	511	CLA	ND
16	X	514	CLA	ND
16	X	515	CLA	ND
16	Y	501	CLA	ND
16	Y	502	CLA	ND
16	Y	503	CLA	ND
16	Y	504	CLA	ND
16	Y	505	CLA	ND
16	Y	508	CLA	ND
16	Y	509	CLA	ND
16	Y	511	CLA	ND
16	Y	512	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	Y	514	CLA	ND
16	Y	515	CLA	ND
16	Z	501	CLA	ND
16	Z	502	CLA	ND
16	Z	503	CLA	ND
16	Z	504	CLA	ND
16	Z	505	CLA	ND
16	Z	507	CLA	ND
16	Z	508	CLA	ND
16	Z	509	CLA	ND
16	Z	511	CLA	ND
16	Z	512	CLA	ND
16	Z	514	CLA	ND
16	Z	515	CLA	ND
16	Z	516	CLA	ND
16	Z	517	CLA	ND
16	a	1013	CLA	ND
16	a	1022	CLA	ND
16	a	1101	CLA	ND
16	a	1102	CLA	ND
16	a	1103	CLA	ND
16	a	1104	CLA	ND
16	a	1105	CLA	ND
16	a	1106	CLA	ND
16	a	1109	CLA	ND
16	a	1110	CLA	ND
16	a	1111	CLA	ND
16	a	1113	CLA	ND
16	a	1114	CLA	ND
16	a	1115	CLA	ND
16	a	1116	CLA	ND
16	a	1117	CLA	ND
16	a	1119	CLA	ND
16	a	1121	CLA	ND
16	a	1124	CLA	ND
16	a	1126	CLA	ND
16	a	1127	CLA	ND
16	a	1128	CLA	ND
16	a	1132	CLA	ND
16	a	1135	CLA	ND
16	a	1136	CLA	ND
16	a	1137	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	a	1138	CLA	ND
16	a	1139	CLA	ND
16	a	1237	CLA	ND
16	a	1801	CLA	ND
16	b	1012	CLA	ND
16	b	1021	CLA	ND
16	b	1201	CLA	ND
16	b	1202	CLA	ND
16	b	1203	CLA	ND
16	b	1204	CLA	ND
16	b	1205	CLA	ND
16	b	1206	CLA	ND
16	b	1208	CLA	ND
16	b	1209	CLA	ND
16	b	1210	CLA	ND
16	b	1211	CLA	ND
16	b	1212	CLA	ND
16	b	1213	CLA	ND
16	b	1214	CLA	ND
16	b	1216	CLA	ND
16	b	1221	CLA	ND
16	b	1223	CLA	ND
16	b	1224	CLA	ND
16	b	1226	CLA	ND
16	b	1227	CLA	ND
16	b	1228	CLA	ND
16	b	1229	CLA	ND
16	b	1231	CLA	ND
16	b	1232	CLA	ND
16	b	1234	CLA	ND
16	b	1235	CLA	ND
16	b	1238	CLA	ND
16	b	1240	CLA	ND
16	f	1301	CLA	ND
16	f	1302	CLA	ND
16	g	502	CLA	ND
16	g	504	CLA	ND
16	g	505	CLA	ND
16	g	507	CLA	ND
16	g	508	CLA	ND
16	g	509	CLA	ND
16	g	511	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	g	512	CLA	ND
16	g	514	CLA	ND
16	g	515	CLA	ND
16	g	516	CLA	ND
16	h	502	CLA	ND
16	h	503	CLA	ND
16	h	506	CLA	ND
16	h	507	CLA	ND
16	h	508	CLA	ND
16	h	509	CLA	ND
16	h	511	CLA	ND
16	h	513	CLA	ND
16	h	515	CLA	ND
16	h	516	CLA	ND
16	h	517	CLA	ND
16	k	4002	CLA	ND
16	k	4003	CLA	ND
16	k	4004	CLA	ND
16	l	1503	CLA	ND
16	n	501	CLA	ND
16	n	502	CLA	ND
16	n	503	CLA	ND
16	n	505	CLA	ND
16	n	507	CLA	ND
16	n	508	CLA	ND
16	n	509	CLA	ND
16	n	512	CLA	ND
16	n	514	CLA	ND
16	n	515	CLA	ND
16	n	517	CLA	ND
16	o	502	CLA	ND
16	o	505	CLA	ND
16	o	506	CLA	ND
16	o	508	CLA	ND
16	o	509	CLA	ND
16	o	511	CLA	ND
16	o	512	CLA	ND
16	o	514	CLA	ND
16	o	515	CLA	ND
16	p	501	CLA	ND
16	p	502	CLA	ND
16	p	503	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	p	508	CLA	ND
16	p	509	CLA	ND
16	p	511	CLA	ND
16	p	512	CLA	ND
16	p	514	CLA	ND
16	p	515	CLA	ND
16	p	516	CLA	ND
16	q	501	CLA	ND
16	q	502	CLA	ND
16	q	503	CLA	ND
16	q	504	CLA	ND
16	q	505	CLA	ND
16	q	506	CLA	ND
16	q	507	CLA	ND
16	q	508	CLA	ND
16	q	509	CLA	ND
16	q	512	CLA	ND
16	q	514	CLA	ND
16	q	515	CLA	ND
16	q	516	CLA	ND
16	r	501	CLA	ND
16	r	502	CLA	ND
16	r	504	CLA	ND
16	r	507	CLA	ND
16	r	508	CLA	ND
16	r	511	CLA	ND
16	r	512	CLA	ND
16	r	514	CLA	ND
16	r	515	CLA	ND
16	r	516	CLA	ND
16	s	501	CLA	ND
16	s	502	CLA	ND
16	s	503	CLA	ND
16	s	504	CLA	ND
16	s	505	CLA	ND
16	s	508	CLA	ND
16	s	509	CLA	ND
16	s	511	CLA	ND
16	s	512	CLA	ND
16	s	514	CLA	ND
16	s	515	CLA	ND
16	t	501	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	t	502	CLA	ND
16	t	503	CLA	ND
16	t	504	CLA	ND
16	t	506	CLA	ND
16	t	507	CLA	ND
16	t	508	CLA	ND
16	t	509	CLA	ND
16	t	511	CLA	ND
16	t	512	CLA	ND
16	t	514	CLA	ND
16	t	515	CLA	ND
16	t	516	CLA	ND
16	t	517	CLA	ND
16	u	502	CLA	ND
16	u	505	CLA	ND
16	u	506	CLA	ND
16	u	507	CLA	ND
16	u	508	CLA	ND
16	u	509	CLA	ND
16	u	511	CLA	ND
16	u	514	CLA	ND
16	u	516	CLA	ND
16	v	502	CLA	ND
16	v	503	CLA	ND
16	v	504	CLA	ND
16	v	506	CLA	ND
16	v	508	CLA	ND
16	v	511	CLA	ND
16	v	513	CLA	ND
16	v	514	CLA	ND
16	v	515	CLA	ND
16	v	516	CLA	ND
16	v	517	CLA	ND
16	w	501	CLA	ND
16	w	502	CLA	ND
16	w	503	CLA	ND
16	w	504	CLA	ND
16	w	507	CLA	ND
16	w	508	CLA	ND
16	w	509	CLA	ND
16	w	511	CLA	ND
16	w	512	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	w	514	CLA	ND
16	w	515	CLA	ND
16	w	516	CLA	ND
16	w	517	CLA	ND
16	x	502	CLA	ND
16	x	504	CLA	ND
16	x	505	CLA	ND
16	x	507	CLA	ND
16	x	508	CLA	ND
16	x	509	CLA	ND
16	x	514	CLA	ND
16	x	515	CLA	ND
16	x	516	CLA	ND
16	y	501	CLA	ND
16	y	502	CLA	ND
16	y	503	CLA	ND
16	y	505	CLA	ND
16	y	506	CLA	ND
16	y	508	CLA	ND
16	y	509	CLA	ND
16	y	511	CLA	ND
16	y	513	CLA	ND
16	y	515	CLA	ND
16	y	516	CLA	ND
16	y	517	CLA	ND

All (7417) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	849	LHG	O1-C1-C2-O2
13	A	849	LHG	O1-C1-C2-C3
13	A	849	LHG	C3-O3-P-O5
13	A	851	LHG	C3-O3-P-O5
13	B	4018	LHG	O1-C1-C2-O2
13	B	4018	LHG	O1-C1-C2-C3
13	B	4018	LHG	C3-O3-P-O5
13	G	4018	LHG	O1-C1-C2-C3
13	G	4018	LHG	C3-O3-P-O5
13	H	851	LHG	C3-O3-P-O5
13	I	103	LHG	C3-O3-P-O5
13	I	103	LHG	C4-O6-P-O3
13	I	103	LHG	C4-O6-P-O4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	R	103	LHG	C3-O3-P-O6
13	R	103	LHG	C4-O6-P-O4
13	X	605	LHG	C3-O3-P-O5
13	Y	605	LHG	C3-O3-P-O4
13	Y	605	LHG	C3-O3-P-O6
13	Y	605	LHG	C4-O6-P-O3
13	a	849	LHG	O1-C1-C2-C3
13	a	851	LHG	C3-O3-P-O5
13	a	851	LHG	O9-C7-O7-C5
13	a	851	LHG	C8-C7-O7-C5
13	b	4018	LHG	O1-C1-C2-C3
13	b	4018	LHG	C3-O3-P-O5
13	g	605	LHG	C1-C2-C3-O3
13	g	605	LHG	C4-O6-P-O3
13	g	605	LHG	C4-O6-P-O5
13	i	103	LHG	C3-O3-P-O6
13	i	103	LHG	C4-O6-P-O4
13	o	605	LHG	O1-C1-C2-C3
13	p	605	LHG	C4-O6-P-O3
13	p	605	LHG	O7-C5-C6-O8
13	r	605	LHG	C1-C2-C3-O3
13	r	605	LHG	C3-O3-P-O4
13	r	605	LHG	C3-O3-P-O5
13	r	605	LHG	C4-O6-P-O3
13	r	605	LHG	C4-O6-P-O4
13	r	605	LHG	C5-C4-O6-P
13	s	605	LHG	C3-O3-P-O4
13	s	605	LHG	C3-O3-P-O5
13	s	605	LHG	C3-O3-P-O6
13	s	605	LHG	C4-O6-P-O3
13	s	605	LHG	O7-C5-C6-O8
13	u	605	LHG	O1-C1-C2-O2
13	u	605	LHG	O1-C1-C2-C3
13	u	605	LHG	C3-O3-P-O4
13	x	605	LHG	C3-O3-P-O5
13	x	605	LHG	C4-O6-P-O3
13	x	605	LHG	C4-O6-P-O4
13	x	605	LHG	C5-C4-O6-P
14	A	852	LMG	O7-C8-C9-O8
14	A	4101	LMG	O6-C1-O1-C7
14	A	4101	LMG	O1-C7-C8-O7
14	A	4101	LMG	O9-C10-O7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	A	4101	LMG	C11-C10-O7-C8
14	H	4101	LMG	O6-C1-O1-C7
14	H	4101	LMG	O1-C7-C8-O7
14	H	4101	LMG	O9-C10-O7-C8
14	H	4201	LMG	O7-C8-C9-O8
14	a	852	LMG	O7-C8-C9-O8
14	a	4101	LMG	O6-C1-O1-C7
14	a	4101	LMG	O1-C7-C8-O7
14	a	4101	LMG	O9-C10-O7-C8
16	A	1022	CLA	C1A-C2A-CAA-CBA
16	A	1101	CLA	C1A-C2A-CAA-CBA
16	A	1103	CLA	CAD-CBD-CGD-O1D
16	A	1103	CLA	CAD-CBD-CGD-O2D
16	A	1104	CLA	CBD-CGD-O2D-CED
16	A	1106	CLA	CHA-CBD-CGD-O1D
16	A	1106	CLA	CHA-CBD-CGD-O2D
16	A	1107	CLA	C1A-C2A-CAA-CBA
16	A	1111	CLA	C1A-C2A-CAA-CBA
16	A	1111	CLA	C3A-C2A-CAA-CBA
16	A	1112	CLA	C1A-C2A-CAA-CBA
16	A	1112	CLA	CBD-CGD-O2D-CED
16	A	1113	CLA	CBD-CGD-O2D-CED
16	A	1114	CLA	C1A-C2A-CAA-CBA
16	A	1114	CLA	CHA-CBD-CGD-O1D
16	A	1114	CLA	CHA-CBD-CGD-O2D
16	A	1115	CLA	C1A-C2A-CAA-CBA
16	A	1116	CLA	C3A-C2A-CAA-CBA
16	A	1116	CLA	CBD-CGD-O2D-CED
16	A	1117	CLA	CBD-CGD-O2D-CED
16	A	1118	CLA	C1A-C2A-CAA-CBA
16	A	1120	CLA	CBD-CGD-O2D-CED
16	A	1121	CLA	C1A-C2A-CAA-CBA
16	A	1128	CLA	CHA-CBD-CGD-O1D
16	A	1128	CLA	CHA-CBD-CGD-O2D
16	A	1130	CLA	C1A-C2A-CAA-CBA
16	A	1131	CLA	CBD-CGD-O2D-CED
16	A	1132	CLA	CHA-CBD-CGD-O1D
16	A	1132	CLA	CHA-CBD-CGD-O2D
16	A	1135	CLA	C1A-C2A-CAA-CBA
16	A	1135	CLA	C3A-C2A-CAA-CBA
16	A	1137	CLA	C1A-C2A-CAA-CBA
16	A	1137	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	1138	CLA	C1A-C2A-CAA-CBA
16	A	1140	CLA	C1A-C2A-CAA-CBA
16	B	1012	CLA	C1A-C2A-CAA-CBA
16	B	1012	CLA	C3A-C2A-CAA-CBA
16	B	1202	CLA	C1A-C2A-CAA-CBA
16	B	1202	CLA	C3A-C2A-CAA-CBA
16	B	1203	CLA	C1A-C2A-CAA-CBA
16	B	1203	CLA	C3A-C2A-CAA-CBA
16	B	1203	CLA	CBD-CGD-O2D-CED
16	B	1205	CLA	CHA-CBD-CGD-O1D
16	B	1205	CLA	CHA-CBD-CGD-O2D
16	B	1206	CLA	C1A-C2A-CAA-CBA
16	B	1206	CLA	C3A-C2A-CAA-CBA
16	B	1207	CLA	CHA-CBD-CGD-O1D
16	B	1207	CLA	CHA-CBD-CGD-O2D
16	B	1207	CLA	CBD-CGD-O2D-CED
16	B	1209	CLA	C1A-C2A-CAA-CBA
16	B	1210	CLA	C1A-C2A-CAA-CBA
16	B	1211	CLA	C1A-C2A-CAA-CBA
16	B	1211	CLA	CBD-CGD-O2D-CED
16	B	1214	CLA	C1A-C2A-CAA-CBA
16	B	1214	CLA	C3A-C2A-CAA-CBA
16	B	1215	CLA	CBD-CGD-O2D-CED
16	B	1217	CLA	C1A-C2A-CAA-CBA
16	B	1219	CLA	CBD-CGD-O2D-CED
16	B	1220	CLA	C1A-C2A-CAA-CBA
16	B	1221	CLA	C1A-C2A-CAA-CBA
16	B	1221	CLA	C3A-C2A-CAA-CBA
16	B	1221	CLA	C14-C13-C15-C16
16	B	1222	CLA	CHA-CBD-CGD-O1D
16	B	1222	CLA	CHA-CBD-CGD-O2D
16	B	1227	CLA	CHA-CBD-CGD-O2D
16	B	1228	CLA	C1A-C2A-CAA-CBA
16	B	1230	CLA	C1A-C2A-CAA-CBA
16	B	1230	CLA	C3A-C2A-CAA-CBA
16	B	1231	CLA	C1A-C2A-CAA-CBA
16	B	1231	CLA	C3A-C2A-CAA-CBA
16	B	1232	CLA	CAD-CBD-CGD-O1D
16	B	1232	CLA	CAD-CBD-CGD-O2D
16	B	1234	CLA	C1A-C2A-CAA-CBA
16	B	1235	CLA	CBD-CGD-O2D-CED
16	B	1235	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1236	CLA	C1A-C2A-CAA-CBA
16	B	1239	CLA	C1A-C2A-CAA-CBA
16	B	1239	CLA	C3A-C2A-CAA-CBA
16	F	1301	CLA	CBD-CGD-O2D-CED
16	F	1302	CLA	CBD-CGD-O2D-CED
16	G	1012	CLA	C1A-C2A-CAA-CBA
16	G	1012	CLA	C3A-C2A-CAA-CBA
16	G	1021	CLA	CBD-CGD-O2D-CED
16	G	1202	CLA	C1A-C2A-CAA-CBA
16	G	1202	CLA	C3A-C2A-CAA-CBA
16	G	1207	CLA	CBD-CGD-O2D-CED
16	G	1209	CLA	C1A-C2A-CAA-CBA
16	G	1210	CLA	C1A-C2A-CAA-CBA
16	G	1211	CLA	C1A-C2A-CAA-CBA
16	G	1211	CLA	CBD-CGD-O2D-CED
16	G	1212	CLA	CHA-CBD-CGD-O1D
16	G	1212	CLA	CHA-CBD-CGD-O2D
16	G	1213	CLA	C1A-C2A-CAA-CBA
16	G	1214	CLA	C3A-C2A-CAA-CBA
16	G	1217	CLA	C1A-C2A-CAA-CBA
16	G	1218	CLA	C1A-C2A-CAA-CBA
16	G	1218	CLA	O1A-CGA-O2A-C1
16	G	1220	CLA	C1A-C2A-CAA-CBA
16	G	1221	CLA	C1A-C2A-CAA-CBA
16	G	1221	CLA	C3A-C2A-CAA-CBA
16	G	1222	CLA	CHA-CBD-CGD-O1D
16	G	1222	CLA	CHA-CBD-CGD-O2D
16	G	1230	CLA	C1A-C2A-CAA-CBA
16	G	1231	CLA	C1A-C2A-CAA-CBA
16	G	1232	CLA	CBD-CGD-O2D-CED
16	G	1235	CLA	CBD-CGD-O2D-CED
16	G	1235	CLA	O1D-CGD-O2D-CED
16	G	1236	CLA	C1A-C2A-CAA-CBA
16	G	1239	CLA	C1A-C2A-CAA-CBA
16	G	1239	CLA	C3A-C2A-CAA-CBA
16	G	1240	CLA	CBD-CGD-O2D-CED
16	H	1013	CLA	CBD-CGD-O2D-CED
16	H	1022	CLA	C1A-C2A-CAA-CBA
16	H	1101	CLA	C1A-C2A-CAA-CBA
16	H	1104	CLA	CHA-CBD-CGD-O2D
16	H	1106	CLA	CHA-CBD-CGD-O1D
16	H	1106	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	H	1106	CLA	C11-C12-C13-C14
16	H	1107	CLA	C1A-C2A-CAA-CBA
16	H	1108	CLA	C1A-C2A-CAA-CBA
16	H	1111	CLA	C1A-C2A-CAA-CBA
16	H	1111	CLA	C3A-C2A-CAA-CBA
16	H	1112	CLA	C1A-C2A-CAA-CBA
16	H	1114	CLA	C1A-C2A-CAA-CBA
16	H	1114	CLA	C3A-C2A-CAA-CBA
16	H	1115	CLA	C1A-C2A-CAA-CBA
16	H	1116	CLA	C3A-C2A-CAA-CBA
16	H	1118	CLA	C1A-C2A-CAA-CBA
16	H	1121	CLA	C1A-C2A-CAA-CBA
16	H	1128	CLA	C1A-C2A-CAA-CBA
16	H	1128	CLA	CHA-CBD-CGD-O1D
16	H	1128	CLA	CHA-CBD-CGD-O2D
16	H	1130	CLA	C1A-C2A-CAA-CBA
16	H	1131	CLA	CBD-CGD-O2D-CED
16	H	1132	CLA	CHA-CBD-CGD-O1D
16	H	1132	CLA	CHA-CBD-CGD-O2D
16	H	1135	CLA	C1A-C2A-CAA-CBA
16	H	1135	CLA	C3A-C2A-CAA-CBA
16	H	1137	CLA	C1A-C2A-CAA-CBA
16	H	1137	CLA	CBD-CGD-O2D-CED
16	H	1140	CLA	C1A-C2A-CAA-CBA
16	H	1237	CLA	C11-C10-C8-C9
16	H	1801	CLA	CBA-CGA-O2A-C1
16	H	1801	CLA	CAD-CBD-CGD-O1D
16	H	1801	CLA	CAD-CBD-CGD-O2D
16	K	4003	CLA	C1A-C2A-CAA-CBA
16	K	4003	CLA	C3A-C2A-CAA-CBA
16	S	1302	CLA	CBD-CGD-O2D-CED
16	T	4003	CLA	C1A-C2A-CAA-CBA
16	T	4003	CLA	C3A-C2A-CAA-CBA
16	W	501	CLA	C3A-C2A-CAA-CBA
16	W	501	CLA	CAD-CBD-CGD-O1D
16	W	501	CLA	CAD-CBD-CGD-O2D
16	W	502	CLA	CHA-CBD-CGD-O1D
16	W	502	CLA	CHA-CBD-CGD-O2D
16	W	503	CLA	C1A-C2A-CAA-CBA
16	W	505	CLA	CHA-CBD-CGD-O2D
16	W	506	CLA	CHA-CBD-CGD-O1D
16	W	506	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	W	508	CLA	C1A-C2A-CAA-CBA
16	W	508	CLA	C3A-C2A-CAA-CBA
16	W	508	CLA	CBD-CGD-O2D-CED
16	W	511	CLA	C1A-C2A-CAA-CBA
16	W	512	CLA	CBD-CGD-O2D-CED
16	W	513	CLA	CAD-CBD-CGD-O1D
16	W	513	CLA	CAD-CBD-CGD-O2D
16	W	513	CLA	CBD-CGD-O2D-CED
16	W	514	CLA	CBD-CGD-O2D-CED
16	X	502	CLA	CHA-CBD-CGD-O1D
16	X	502	CLA	CHA-CBD-CGD-O2D
16	X	503	CLA	C1A-C2A-CAA-CBA
16	X	504	CLA	C1A-C2A-CAA-CBA
16	X	504	CLA	C3A-C2A-CAA-CBA
16	X	504	CLA	CBD-CGD-O2D-CED
16	X	506	CLA	C1A-C2A-CAA-CBA
16	X	506	CLA	C3A-C2A-CAA-CBA
16	X	506	CLA	CBD-CGD-O2D-CED
16	X	506	CLA	O1D-CGD-O2D-CED
16	X	508	CLA	CBD-CGD-O2D-CED
16	X	513	CLA	C1A-C2A-CAA-CBA
16	X	513	CLA	C3A-C2A-CAA-CBA
16	X	513	CLA	CBD-CGD-O2D-CED
16	X	514	CLA	CBD-CGD-O2D-CED
16	X	514	CLA	O1D-CGD-O2D-CED
16	X	516	CLA	C1A-C2A-CAA-CBA
16	Y	501	CLA	CAD-CBD-CGD-O1D
16	Y	501	CLA	CAD-CBD-CGD-O2D
16	Y	502	CLA	CHA-CBD-CGD-O1D
16	Y	502	CLA	CHA-CBD-CGD-O2D
16	Y	503	CLA	C1A-C2A-CAA-CBA
16	Y	504	CLA	CHA-CBD-CGD-O1D
16	Y	504	CLA	CHA-CBD-CGD-O2D
16	Y	506	CLA	CBD-CGD-O2D-CED
16	Y	507	CLA	CBD-CGD-O2D-CED
16	Y	508	CLA	C1A-C2A-CAA-CBA
16	Y	508	CLA	CHA-CBD-CGD-O1D
16	Y	508	CLA	CHA-CBD-CGD-O2D
16	Y	511	CLA	CBD-CGD-O2D-CED
16	Y	512	CLA	O1A-CGA-O2A-C1
16	Y	513	CLA	C1A-C2A-CAA-CBA
16	Y	513	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	Y	513	CLA	CBA-CGA-O2A-C1
16	Y	513	CLA	O1A-CGA-O2A-C1
16	Y	514	CLA	CBD-CGD-O2D-CED
16	Y	515	CLA	O1A-CGA-O2A-C1
16	Y	515	CLA	CAD-CBD-CGD-O2D
16	Y	516	CLA	C1A-C2A-CAA-CBA
16	Y	516	CLA	C3A-C2A-CAA-CBA
16	Y	517	CLA	C3A-C2A-CAA-CBA
16	Z	501	CLA	CAD-CBD-CGD-O1D
16	Z	501	CLA	CAD-CBD-CGD-O2D
16	Z	503	CLA	C1A-C2A-CAA-CBA
16	Z	503	CLA	CBA-CGA-O2A-C1
16	Z	504	CLA	C3A-C2A-CAA-CBA
16	Z	504	CLA	CBD-CGD-O2D-CED
16	Z	504	CLA	O1D-CGD-O2D-CED
16	Z	504	CLA	C11-C10-C8-C7
16	Z	507	CLA	CBA-CGA-O2A-C1
16	Z	507	CLA	CBD-CGD-O2D-CED
16	Z	509	CLA	C1A-C2A-CAA-CBA
16	Z	509	CLA	C3A-C2A-CAA-CBA
16	Z	513	CLA	CHA-CBD-CGD-O1D
16	Z	513	CLA	CHA-CBD-CGD-O2D
16	Z	516	CLA	C1A-C2A-CAA-CBA
16	Z	516	CLA	CAD-CBD-CGD-O1D
16	Z	516	CLA	CAD-CBD-CGD-O2D
16	a	1101	CLA	C1A-C2A-CAA-CBA
16	a	1102	CLA	C3A-C2A-CAA-CBA
16	a	1104	CLA	CBD-CGD-O2D-CED
16	a	1106	CLA	CHA-CBD-CGD-O1D
16	a	1106	CLA	CHA-CBD-CGD-O2D
16	a	1107	CLA	C1A-C2A-CAA-CBA
16	a	1108	CLA	C1A-C2A-CAA-CBA
16	a	1108	CLA	CBD-CGD-O2D-CED
16	a	1111	CLA	C1A-C2A-CAA-CBA
16	a	1112	CLA	C1A-C2A-CAA-CBA
16	a	1114	CLA	C1A-C2A-CAA-CBA
16	a	1114	CLA	CBD-CGD-O2D-CED
16	a	1115	CLA	C4-C3-C5-C6
16	a	1116	CLA	C3A-C2A-CAA-CBA
16	a	1118	CLA	C1A-C2A-CAA-CBA
16	a	1121	CLA	C1A-C2A-CAA-CBA
16	a	1121	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1128	CLA	CHA-CBD-CGD-O1D
16	a	1128	CLA	CHA-CBD-CGD-O2D
16	a	1130	CLA	C1A-C2A-CAA-CBA
16	a	1132	CLA	CHA-CBD-CGD-O1D
16	a	1132	CLA	CHA-CBD-CGD-O2D
16	a	1135	CLA	C1A-C2A-CAA-CBA
16	a	1135	CLA	C3A-C2A-CAA-CBA
16	a	1137	CLA	C1A-C2A-CAA-CBA
16	a	1137	CLA	CBD-CGD-O2D-CED
16	a	1138	CLA	C1A-C2A-CAA-CBA
16	a	1140	CLA	C1A-C2A-CAA-CBA
16	a	1237	CLA	C1A-C2A-CAA-CBA
16	b	1021	CLA	CBD-CGD-O2D-CED
16	b	1202	CLA	C1A-C2A-CAA-CBA
16	b	1202	CLA	C3A-C2A-CAA-CBA
16	b	1203	CLA	CBD-CGD-O2D-CED
16	b	1205	CLA	CHA-CBD-CGD-O1D
16	b	1205	CLA	CHA-CBD-CGD-O2D
16	b	1206	CLA	C1A-C2A-CAA-CBA
16	b	1206	CLA	C3A-C2A-CAA-CBA
16	b	1206	CLA	CBD-CGD-O2D-CED
16	b	1207	CLA	CHA-CBD-CGD-O2D
16	b	1207	CLA	CBD-CGD-O2D-CED
16	b	1208	CLA	C1A-C2A-CAA-CBA
16	b	1209	CLA	C1A-C2A-CAA-CBA
16	b	1210	CLA	C1A-C2A-CAA-CBA
16	b	1210	CLA	C3A-C2A-CAA-CBA
16	b	1211	CLA	C1A-C2A-CAA-CBA
16	b	1213	CLA	C1A-C2A-CAA-CBA
16	b	1214	CLA	C1A-C2A-CAA-CBA
16	b	1219	CLA	CBD-CGD-O2D-CED
16	b	1222	CLA	CHA-CBD-CGD-O1D
16	b	1222	CLA	CHA-CBD-CGD-O2D
16	b	1230	CLA	C1A-C2A-CAA-CBA
16	b	1230	CLA	C3A-C2A-CAA-CBA
16	b	1231	CLA	C1A-C2A-CAA-CBA
16	b	1232	CLA	CAD-CBD-CGD-O1D
16	b	1232	CLA	CAD-CBD-CGD-O2D
16	b	1235	CLA	C1A-C2A-CAA-CBA
16	b	1236	CLA	C1A-C2A-CAA-CBA
16	b	1239	CLA	C1A-C2A-CAA-CBA
16	b	1239	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	f	1301	CLA	CBD-CGD-O2D-CED
16	g	501	CLA	C1A-C2A-CAA-CBA
16	g	501	CLA	CHA-CBD-CGD-O2D
16	g	503	CLA	C1A-C2A-CAA-CBA
16	g	504	CLA	CBD-CGD-O2D-CED
16	g	508	CLA	C1A-C2A-CAA-CBA
16	g	508	CLA	C3A-C2A-CAA-CBA
16	g	511	CLA	CBD-CGD-O2D-CED
16	g	512	CLA	C4-C3-C5-C6
16	g	513	CLA	CAD-CBD-CGD-O2D
16	g	513	CLA	CBD-CGD-O2D-CED
16	g	517	CLA	C1A-C2A-CAA-CBA
16	g	517	CLA	CBD-CGD-O2D-CED
16	h	501	CLA	CAD-CBD-CGD-O1D
16	h	501	CLA	CAD-CBD-CGD-O2D
16	h	503	CLA	CBA-CGA-O2A-C1
16	h	503	CLA	O1A-CGA-O2A-C1
16	h	503	CLA	CAD-CBD-CGD-O2D
16	h	504	CLA	C1A-C2A-CAA-CBA
16	h	504	CLA	CHA-CBD-CGD-O1D
16	h	504	CLA	CHA-CBD-CGD-O2D
16	h	505	CLA	CBD-CGD-O2D-CED
16	h	505	CLA	O1D-CGD-O2D-CED
16	h	507	CLA	CAD-CBD-CGD-O1D
16	h	507	CLA	CAD-CBD-CGD-O2D
16	h	507	CLA	C6-C7-C8-C9
16	h	508	CLA	C1A-C2A-CAA-CBA
16	h	508	CLA	C3A-C2A-CAA-CBA
16	h	509	CLA	C1A-C2A-CAA-CBA
16	h	509	CLA	C3A-C2A-CAA-CBA
16	h	509	CLA	CHA-CBD-CGD-O2D
16	h	510	CLA	CBD-CGD-O2D-CED
16	h	513	CLA	CBA-CGA-O2A-C1
16	h	513	CLA	O1A-CGA-O2A-C1
16	h	514	CLA	CBD-CGD-O2D-CED
16	h	515	CLA	CHA-CBD-CGD-O1D
16	h	515	CLA	CHA-CBD-CGD-O2D
16	h	515	CLA	C4-C3-C5-C6
16	h	516	CLA	C1A-C2A-CAA-CBA
16	h	516	CLA	CAD-CBD-CGD-O1D
16	h	516	CLA	CAD-CBD-CGD-O2D
16	j	1302	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	k	4002	CLA	C3A-C2A-CAA-CBA
16	k	4003	CLA	C1A-C2A-CAA-CBA
16	k	4003	CLA	C3A-C2A-CAA-CBA
16	l	1503	CLA	C2-C1-O2A-CGA
16	n	501	CLA	C3A-C2A-CAA-CBA
16	n	503	CLA	CBA-CGA-O2A-C1
16	n	503	CLA	CAD-CBD-CGD-O1D
16	n	503	CLA	CAD-CBD-CGD-O2D
16	n	505	CLA	CHA-CBD-CGD-O1D
16	n	505	CLA	CHA-CBD-CGD-O2D
16	n	506	CLA	CHA-CBD-CGD-O1D
16	n	506	CLA	CHA-CBD-CGD-O2D
16	n	507	CLA	CHA-CBD-CGD-O1D
16	n	507	CLA	CHA-CBD-CGD-O2D
16	n	508	CLA	C3A-C2A-CAA-CBA
16	n	508	CLA	CBD-CGD-O2D-CED
16	n	511	CLA	CBD-CGD-O2D-CED
16	n	512	CLA	CBD-CGD-O2D-CED
16	n	513	CLA	C1A-C2A-CAA-CBA
16	n	513	CLA	C3A-C2A-CAA-CBA
16	n	513	CLA	CBA-CGA-O2A-C1
16	n	513	CLA	O1A-CGA-O2A-C1
16	n	513	CLA	CAD-CBD-CGD-O1D
16	n	513	CLA	CAD-CBD-CGD-O2D
16	n	513	CLA	CBD-CGD-O2D-CED
16	n	514	CLA	CBD-CGD-O2D-CED
16	n	516	CLA	C1A-C2A-CAA-CBA
16	o	501	CLA	C1A-C2A-CAA-CBA
16	o	501	CLA	CBA-CGA-O2A-C1
16	o	501	CLA	O1A-CGA-O2A-C1
16	o	502	CLA	CHA-CBD-CGD-O1D
16	o	502	CLA	CHA-CBD-CGD-O2D
16	o	503	CLA	CBD-CGD-O2D-CED
16	o	504	CLA	C1A-C2A-CAA-CBA
16	o	504	CLA	CBD-CGD-O2D-CED
16	o	505	CLA	CBD-CGD-O2D-CED
16	o	506	CLA	CBD-CGD-O2D-CED
16	o	507	CLA	CBD-CGD-O2D-CED
16	o	508	CLA	CBD-CGD-O2D-CED
16	o	511	CLA	C1A-C2A-CAA-CBA
16	o	514	CLA	CBD-CGD-O2D-CED
16	o	517	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	p	501	CLA	CAD-CBD-CGD-O1D
16	p	501	CLA	CAD-CBD-CGD-O2D
16	p	504	CLA	C3A-C2A-CAA-CBA
16	p	504	CLA	CHA-CBD-CGD-O1D
16	p	504	CLA	CHA-CBD-CGD-O2D
16	p	506	CLA	CHA-CBD-CGD-O2D
16	p	506	CLA	CBD-CGD-O2D-CED
16	p	507	CLA	CBD-CGD-O2D-CED
16	p	508	CLA	C1A-C2A-CAA-CBA
16	p	509	CLA	C2-C3-C5-C6
16	p	509	CLA	C4-C3-C5-C6
16	p	513	CLA	C1A-C2A-CAA-CBA
16	p	513	CLA	C3A-C2A-CAA-CBA
16	p	513	CLA	CBA-CGA-O2A-C1
16	p	513	CLA	O1A-CGA-O2A-C1
16	p	514	CLA	CBD-CGD-O2D-CED
16	p	515	CLA	CBA-CGA-O2A-C1
16	p	515	CLA	CAD-CBD-CGD-O1D
16	p	515	CLA	CAD-CBD-CGD-O2D
16	p	517	CLA	C3A-C2A-CAA-CBA
16	q	501	CLA	C1A-C2A-CAA-CBA
16	q	501	CLA	C3A-C2A-CAA-CBA
16	q	501	CLA	CAD-CBD-CGD-O1D
16	q	501	CLA	CAD-CBD-CGD-O2D
16	q	503	CLA	C1A-C2A-CAA-CBA
16	q	503	CLA	CBA-CGA-O2A-C1
16	q	503	CLA	O1A-CGA-O2A-C1
16	q	504	CLA	C1A-C2A-CAA-CBA
16	q	504	CLA	CBD-CGD-O2D-CED
16	q	504	CLA	O1D-CGD-O2D-CED
16	q	510	CLA	C1A-C2A-CAA-CBA
16	q	510	CLA	C3A-C2A-CAA-CBA
16	q	513	CLA	C1A-C2A-CAA-CBA
16	q	513	CLA	C3A-C2A-CAA-CBA
16	q	513	CLA	CHA-CBD-CGD-O1D
16	q	513	CLA	CHA-CBD-CGD-O2D
16	q	516	CLA	C1A-C2A-CAA-CBA
16	q	516	CLA	C3A-C2A-CAA-CBA
16	q	516	CLA	CAD-CBD-CGD-O1D
16	q	516	CLA	CAD-CBD-CGD-O2D
16	q	517	CLA	CHA-CBD-CGD-O1D
16	q	517	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	r	501	CLA	C1A-C2A-CAA-CBA
16	r	503	CLA	C1A-C2A-CAA-CBA
16	r	504	CLA	CBD-CGD-O2D-CED
16	r	512	CLA	C2-C3-C5-C6
16	r	512	CLA	C4-C3-C5-C6
16	r	513	CLA	C1A-C2A-CAA-CBA
16	r	513	CLA	C3A-C2A-CAA-CBA
16	r	513	CLA	CAD-CBD-CGD-O1D
16	r	513	CLA	CAD-CBD-CGD-O2D
16	r	513	CLA	CBD-CGD-O2D-CED
16	r	515	CLA	O1A-CGA-O2A-C1
16	r	515	CLA	CHA-CBD-CGD-O1D
16	r	515	CLA	CHA-CBD-CGD-O2D
16	r	517	CLA	C1A-C2A-CAA-CBA
16	r	517	CLA	CHA-CBD-CGD-O1D
16	r	517	CLA	CHA-CBD-CGD-O2D
16	s	501	CLA	CAD-CBD-CGD-O1D
16	s	501	CLA	CAD-CBD-CGD-O2D
16	s	503	CLA	C1A-C2A-CAA-CBA
16	s	504	CLA	CHA-CBD-CGD-O1D
16	s	504	CLA	CHA-CBD-CGD-O2D
16	s	508	CLA	C1A-C2A-CAA-CBA
16	s	508	CLA	CHA-CBD-CGD-O1D
16	s	508	CLA	CHA-CBD-CGD-O2D
16	s	511	CLA	CBD-CGD-O2D-CED
16	s	513	CLA	C1A-C2A-CAA-CBA
16	s	513	CLA	CBA-CGA-O2A-C1
16	s	513	CLA	O1A-CGA-O2A-C1
16	s	513	CLA	CAD-CBD-CGD-O2D
16	s	514	CLA	CBD-CGD-O2D-CED
16	s	515	CLA	CAD-CBD-CGD-O1D
16	s	515	CLA	CAD-CBD-CGD-O2D
16	s	516	CLA	CAD-CBD-CGD-O1D
16	s	516	CLA	CAD-CBD-CGD-O2D
16	t	501	CLA	C1A-C2A-CAA-CBA
16	t	501	CLA	C3A-C2A-CAA-CBA
16	t	501	CLA	CAD-CBD-CGD-O1D
16	t	501	CLA	CAD-CBD-CGD-O2D
16	t	502	CLA	CHA-CBD-CGD-O1D
16	t	502	CLA	CHA-CBD-CGD-O2D
16	t	503	CLA	CAD-CBD-CGD-O1D
16	t	503	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	t	506	CLA	CHA-CBD-CGD-O1D
16	t	506	CLA	CHA-CBD-CGD-O2D
16	t	507	CLA	CBD-CGD-O2D-CED
16	t	508	CLA	C1A-C2A-CAA-CBA
16	t	508	CLA	C3A-C2A-CAA-CBA
16	t	508	CLA	CBD-CGD-O2D-CED
16	t	508	CLA	O1D-CGD-O2D-CED
16	t	511	CLA	CBD-CGD-O2D-CED
16	t	512	CLA	CBD-CGD-O2D-CED
16	t	513	CLA	CAD-CBD-CGD-O1D
16	t	513	CLA	CAD-CBD-CGD-O2D
16	t	513	CLA	CBD-CGD-O2D-CED
16	t	514	CLA	CBD-CGD-O2D-CED
16	t	515	CLA	CHA-CBD-CGD-O1D
16	t	515	CLA	CHA-CBD-CGD-O2D
16	t	516	CLA	CAD-CBD-CGD-O2D
16	u	501	CLA	C1A-C2A-CAA-CBA
16	u	501	CLA	CBA-CGA-O2A-C1
16	u	501	CLA	O1A-CGA-O2A-C1
16	u	502	CLA	CHA-CBD-CGD-O1D
16	u	502	CLA	CHA-CBD-CGD-O2D
16	u	504	CLA	C1A-C2A-CAA-CBA
16	u	504	CLA	CBD-CGD-O2D-CED
16	u	504	CLA	C11-C10-C8-C9
16	u	505	CLA	CBD-CGD-O2D-CED
16	u	506	CLA	C1A-C2A-CAA-CBA
16	u	506	CLA	CBD-CGD-O2D-CED
16	u	508	CLA	CBD-CGD-O2D-CED
16	u	508	CLA	C2-C3-C5-C6
16	u	508	CLA	C4-C3-C5-C6
16	u	511	CLA	C1A-C2A-CAA-CBA
16	u	513	CLA	C1A-C2A-CAA-CBA
16	u	513	CLA	CBD-CGD-O2D-CED
16	u	514	CLA	CBD-CGD-O2D-CED
16	u	515	CLA	CBD-CGD-O2D-CED
16	u	516	CLA	CHA-CBD-CGD-O1D
16	u	516	CLA	CHA-CBD-CGD-O2D
16	u	516	CLA	CBD-CGD-O2D-CED
16	v	501	CLA	CAD-CBD-CGD-O1D
16	v	501	CLA	CAD-CBD-CGD-O2D
16	v	503	CLA	CAD-CBD-CGD-O1D
16	v	503	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	v	504	CLA	C1A-C2A-CAA-CBA
16	v	504	CLA	C3A-C2A-CAA-CBA
16	v	504	CLA	CHA-CBD-CGD-O1D
16	v	504	CLA	CHA-CBD-CGD-O2D
16	v	505	CLA	CBD-CGD-O2D-CED
16	v	505	CLA	O1D-CGD-O2D-CED
16	v	506	CLA	CBD-CGD-O2D-CED
16	v	508	CLA	C1A-C2A-CAA-CBA
16	v	508	CLA	C3A-C2A-CAA-CBA
16	v	509	CLA	C1A-C2A-CAA-CBA
16	v	509	CLA	C3A-C2A-CAA-CBA
16	v	509	CLA	CHA-CBD-CGD-O1D
16	v	509	CLA	CHA-CBD-CGD-O2D
16	v	511	CLA	CBD-CGD-O2D-CED
16	v	513	CLA	C1A-C2A-CAA-CBA
16	v	513	CLA	C3A-C2A-CAA-CBA
16	v	514	CLA	C1A-C2A-CAA-CBA
16	v	515	CLA	CHA-CBD-CGD-O1D
16	v	515	CLA	CHA-CBD-CGD-O2D
16	v	516	CLA	C1A-C2A-CAA-CBA
16	v	517	CLA	CBD-CGD-O2D-CED
16	w	501	CLA	C1A-C2A-CAA-CBA
16	w	501	CLA	CAD-CBD-CGD-O1D
16	w	501	CLA	CAD-CBD-CGD-O2D
16	w	503	CLA	C1A-C2A-CAA-CBA
16	w	503	CLA	CBA-CGA-O2A-C1
16	w	504	CLA	C1A-C2A-CAA-CBA
16	w	504	CLA	CBD-CGD-O2D-CED
16	w	504	CLA	O1D-CGD-O2D-CED
16	w	507	CLA	CBD-CGD-O2D-CED
16	w	509	CLA	C1A-C2A-CAA-CBA
16	w	509	CLA	C3A-C2A-CAA-CBA
16	w	510	CLA	C1A-C2A-CAA-CBA
16	w	510	CLA	C3A-C2A-CAA-CBA
16	w	511	CLA	CBD-CGD-O2D-CED
16	w	513	CLA	C1A-C2A-CAA-CBA
16	w	513	CLA	CHA-CBD-CGD-O1D
16	w	513	CLA	CHA-CBD-CGD-O2D
16	w	516	CLA	CBA-CGA-O2A-C1
16	w	516	CLA	CAD-CBD-CGD-O1D
16	w	516	CLA	CAD-CBD-CGD-O2D
16	x	501	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	x	501	CLA	CAD-CBD-CGD-O1D
16	x	501	CLA	CAD-CBD-CGD-O2D
16	x	504	CLA	C1A-C2A-CAA-CBA
16	x	504	CLA	CBD-CGD-O2D-CED
16	x	505	CLA	CBD-CGD-O2D-CED
16	x	508	CLA	CAD-CBD-CGD-O1D
16	x	508	CLA	CAD-CBD-CGD-O2D
16	x	509	CLA	C1A-C2A-CAA-CBA
16	x	509	CLA	C3A-C2A-CAA-CBA
16	x	513	CLA	CBA-CGA-O2A-C1
16	x	513	CLA	O1A-CGA-O2A-C1
16	x	513	CLA	CAD-CBD-CGD-O1D
16	x	513	CLA	CAD-CBD-CGD-O2D
16	x	515	CLA	CHA-CBD-CGD-O1D
16	x	515	CLA	CHA-CBD-CGD-O2D
16	x	516	CLA	CHA-CBD-CGD-O1D
16	x	516	CLA	CHA-CBD-CGD-O2D
16	x	517	CLA	CAD-CBD-CGD-O2D
16	y	501	CLA	CAD-CBD-CGD-O1D
16	y	501	CLA	CAD-CBD-CGD-O2D
16	y	502	CLA	CBD-CGD-O2D-CED
16	y	503	CLA	CBA-CGA-O2A-C1
16	y	503	CLA	O1A-CGA-O2A-C1
16	y	504	CLA	CHA-CBD-CGD-O1D
16	y	504	CLA	CHA-CBD-CGD-O2D
16	y	505	CLA	CBD-CGD-O2D-CED
16	y	506	CLA	CBD-CGD-O2D-CED
16	y	508	CLA	C1A-C2A-CAA-CBA
16	y	508	CLA	C3A-C2A-CAA-CBA
16	y	508	CLA	CAD-CBD-CGD-O1D
16	y	508	CLA	CAD-CBD-CGD-O2D
16	y	509	CLA	C1A-C2A-CAA-CBA
16	y	509	CLA	C3A-C2A-CAA-CBA
16	y	509	CLA	CHA-CBD-CGD-O1D
16	y	509	CLA	CHA-CBD-CGD-O2D
16	y	510	CLA	CBD-CGD-O2D-CED
16	y	511	CLA	CBD-CGD-O2D-CED
16	y	512	CLA	CBD-CGD-O2D-CED
16	y	513	CLA	CBA-CGA-O2A-C1
16	y	513	CLA	O1A-CGA-O2A-C1
16	y	514	CLA	C1A-C2A-CAA-CBA
16	y	515	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	y	515	CLA	CHA-CBD-CGD-O2D
16	y	516	CLA	C1A-C2A-CAA-CBA
16	y	516	CLA	CAD-CBD-CGD-O1D
16	y	516	CLA	CAD-CBD-CGD-O2D
16	y	517	CLA	C2-C1-O2A-CGA
16	y	517	CLA	CAD-CBD-CGD-O1D
16	y	517	CLA	CAD-CBD-CGD-O2D
19	A	4002	BCR	C7-C8-C9-C34
19	A	4002	BCR	C21-C22-C23-C24
19	A	4003	BCR	C6-C7-C8-C9
19	A	4003	BCR	C18-C19-C20-C21
19	A	4003	BCR	C20-C21-C22-C23
19	A	4003	BCR	C20-C21-C22-C37
19	A	4003	BCR	C22-C23-C24-C25
19	A	4007	BCR	C21-C22-C23-C24
19	A	4008	BCR	C7-C8-C9-C10
19	A	4008	BCR	C20-C21-C22-C37
19	A	4011	BCR	C11-C10-C9-C8
19	A	4011	BCR	C11-C10-C9-C34
19	A	4011	BCR	C18-C19-C20-C21
19	A	4011	BCR	C19-C20-C21-C22
19	A	4011	BCR	C21-C22-C23-C24
19	B	4004	BCR	C7-C8-C9-C10
19	B	4004	BCR	C18-C19-C20-C21
19	B	4004	BCR	C37-C22-C23-C24
19	B	4004	BCR	C22-C23-C24-C25
19	B	4005	BCR	C7-C8-C9-C34
19	B	4005	BCR	C21-C22-C23-C24
19	B	4005	BCR	C37-C22-C23-C24
19	B	4009	BCR	C18-C19-C20-C21
19	B	4009	BCR	C20-C21-C22-C23
19	B	4009	BCR	C20-C21-C22-C37
19	B	4010	BCR	C10-C11-C12-C13
19	B	4010	BCR	C17-C18-C19-C20
19	B	4010	BCR	C18-C19-C20-C21
19	B	4010	BCR	C20-C21-C22-C23
19	B	4010	BCR	C21-C22-C23-C24
19	B	4010	BCR	C22-C23-C24-C25
19	B	4014	BCR	C7-C8-C9-C10
19	B	4014	BCR	C7-C8-C9-C34
19	B	4014	BCR	C12-C13-C14-C15
19	B	4014	BCR	C35-C13-C14-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	B	4014	BCR	C17-C18-C19-C20
19	B	4014	BCR	C18-C19-C20-C21
19	B	4014	BCR	C20-C21-C22-C37
19	B	4017	BCR	C11-C10-C9-C34
19	B	4017	BCR	C20-C21-C22-C23
19	B	4017	BCR	C20-C21-C22-C37
19	B	4017	BCR	C21-C22-C23-C24
19	G	4004	BCR	C18-C19-C20-C21
19	G	4005	BCR	C21-C22-C23-C24
19	G	4005	BCR	C37-C22-C23-C24
19	G	4010	BCR	C6-C7-C8-C9
19	G	4010	BCR	C15-C16-C17-C18
19	G	4010	BCR	C17-C18-C19-C20
19	G	4010	BCR	C18-C19-C20-C21
19	G	4010	BCR	C21-C22-C23-C24
19	G	4010	BCR	C22-C23-C24-C25
19	G	4014	BCR	C7-C8-C9-C10
19	G	4014	BCR	C7-C8-C9-C34
19	G	4014	BCR	C12-C13-C14-C15
19	G	4014	BCR	C35-C13-C14-C15
19	G	4014	BCR	C20-C21-C22-C37
19	G	4014	BCR	C37-C22-C23-C24
19	G	4017	BCR	C10-C11-C12-C13
19	G	4017	BCR	C20-C21-C22-C37
19	G	4017	BCR	C21-C22-C23-C24
19	H	4002	BCR	C6-C7-C8-C9
19	H	4002	BCR	C21-C22-C23-C24
19	H	4003	BCR	C7-C8-C9-C10
19	H	4003	BCR	C7-C8-C9-C34
19	H	4003	BCR	C21-C22-C23-C24
19	H	4007	BCR	C21-C22-C23-C24
19	H	4008	BCR	C7-C8-C9-C34
19	H	4008	BCR	C18-C19-C20-C21
19	H	4011	BCR	C11-C10-C9-C8
19	H	4011	BCR	C11-C10-C9-C34
19	H	4011	BCR	C10-C11-C12-C13
19	H	4011	BCR	C21-C22-C23-C24
19	I	4018	BCR	C20-C21-C22-C23
19	I	4018	BCR	C21-C22-C23-C24
19	I	4018	BCR	C37-C22-C23-C24
19	J	4012	BCR	C6-C7-C8-C9
19	J	4012	BCR	C7-C8-C9-C10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	J	4012	BCR	C7-C8-C9-C34
19	J	4012	BCR	C21-C22-C23-C24
19	J	4012	BCR	C37-C22-C23-C24
19	J	4013	BCR	C18-C19-C20-C21
19	J	4013	BCR	C21-C22-C23-C24
19	J	4015	BCR	C7-C8-C9-C10
19	J	4015	BCR	C22-C23-C24-C25
19	K	4001	BCR	C21-C22-C23-C24
19	K	4005	BCR	C37-C22-C23-C24
19	L	4019	BCR	C7-C8-C9-C10
19	L	4022	BCR	C7-C8-C9-C10
19	L	4022	BCR	C20-C21-C22-C37
19	Q	4016	BCR	C11-C10-C9-C8
19	R	4018	BCR	C21-C22-C23-C24
19	S	4012	BCR	C6-C7-C8-C9
19	S	4012	BCR	C7-C8-C9-C10
19	S	4012	BCR	C7-C8-C9-C34
19	S	4012	BCR	C21-C22-C23-C24
19	S	4012	BCR	C37-C22-C23-C24
19	S	4013	BCR	C18-C19-C20-C21
19	S	4013	BCR	C37-C22-C23-C24
19	S	4015	BCR	C7-C8-C9-C10
19	S	4015	BCR	C7-C8-C9-C34
19	S	4015	BCR	C22-C23-C24-C25
19	T	4001	BCR	C21-C22-C23-C24
19	T	4001	BCR	C37-C22-C23-C24
19	T	4005	BCR	C6-C7-C8-C9
19	T	4005	BCR	C37-C22-C23-C24
19	U	4019	BCR	C7-C8-C9-C10
19	U	4019	BCR	C37-C22-C23-C24
19	U	4019	BCR	C23-C24-C25-C26
19	U	4019	BCR	C23-C24-C25-C30
19	U	4022	BCR	C6-C7-C8-C9
19	U	4022	BCR	C7-C8-C9-C10
19	W	601	BCR	C7-C8-C9-C10
19	W	601	BCR	C10-C11-C12-C13
19	W	601	BCR	C17-C18-C19-C20
19	W	601	BCR	C36-C18-C19-C20
19	W	601	BCR	C20-C21-C22-C23
19	W	601	BCR	C20-C21-C22-C37
19	W	601	BCR	C37-C22-C23-C24
19	W	601	BCR	C22-C23-C24-C25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	W	603	BCR	C6-C7-C8-C9
19	W	603	BCR	C7-C8-C9-C10
19	W	603	BCR	C7-C8-C9-C34
19	W	603	BCR	C10-C11-C12-C13
19	W	604	BCR	C10-C11-C12-C13
19	W	604	BCR	C22-C23-C24-C25
19	X	601	BCR	C21-C22-C23-C24
19	X	602	BCR	C6-C7-C8-C9
19	X	602	BCR	C7-C8-C9-C10
19	X	602	BCR	C7-C8-C9-C34
19	X	602	BCR	C10-C11-C12-C13
19	X	602	BCR	C14-C15-C16-C17
19	X	602	BCR	C20-C21-C22-C23
19	X	602	BCR	C20-C21-C22-C37
19	X	603	BCR	C6-C7-C8-C9
19	X	603	BCR	C20-C21-C22-C37
19	X	603	BCR	C22-C23-C24-C25
19	X	604	BCR	C7-C8-C9-C10
19	X	604	BCR	C7-C8-C9-C34
19	X	604	BCR	C16-C17-C18-C19
19	X	604	BCR	C16-C17-C18-C36
19	X	604	BCR	C18-C19-C20-C21
19	X	604	BCR	C20-C21-C22-C23
19	X	604	BCR	C20-C21-C22-C37
19	Y	601	BCR	C7-C8-C9-C10
19	Y	601	BCR	C7-C8-C9-C34
19	Y	601	BCR	C20-C21-C22-C37
19	Y	602	BCR	C21-C22-C23-C24
19	Y	603	BCR	C20-C21-C22-C37
19	Y	603	BCR	C22-C23-C24-C25
19	Y	604	BCR	C6-C7-C8-C9
19	Y	604	BCR	C7-C8-C9-C34
19	Y	604	BCR	C11-C10-C9-C8
19	Y	604	BCR	C11-C12-C13-C14
19	Y	604	BCR	C11-C12-C13-C35
19	Y	604	BCR	C21-C22-C23-C24
19	Y	604	BCR	C37-C22-C23-C24
19	Z	602	BCR	C20-C21-C22-C37
19	Z	602	BCR	C21-C22-C23-C24
19	Z	603	BCR	C20-C21-C22-C37
19	Z	604	BCR	C7-C8-C9-C10
19	Z	604	BCR	C7-C8-C9-C34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	Z	604	BCR	C11-C10-C9-C8
19	Z	604	BCR	C11-C10-C9-C34
19	Z	604	BCR	C10-C11-C12-C13
19	Z	604	BCR	C11-C12-C13-C14
19	Z	604	BCR	C11-C12-C13-C35
19	Z	604	BCR	C14-C15-C16-C17
19	a	4002	BCR	C11-C12-C13-C35
19	a	4002	BCR	C20-C21-C22-C37
19	a	4002	BCR	C21-C22-C23-C24
19	a	4003	BCR	C6-C7-C8-C9
19	a	4003	BCR	C21-C22-C23-C24
19	a	4008	BCR	C7-C8-C9-C10
19	a	4008	BCR	C7-C8-C9-C34
19	a	4008	BCR	C37-C22-C23-C24
19	a	4008	BCR	C22-C23-C24-C25
19	a	4008	BCR	C23-C24-C25-C26
19	a	4008	BCR	C23-C24-C25-C30
19	a	4011	BCR	C11-C10-C9-C8
19	a	4011	BCR	C11-C10-C9-C34
19	a	4011	BCR	C20-C21-C22-C37
19	a	4011	BCR	C21-C22-C23-C24
19	a	4011	BCR	C37-C22-C23-C24
19	b	4004	BCR	C37-C22-C23-C24
19	b	4005	BCR	C6-C7-C8-C9
19	b	4005	BCR	C7-C8-C9-C34
19	b	4005	BCR	C21-C22-C23-C24
19	b	4005	BCR	C37-C22-C23-C24
19	b	4009	BCR	C18-C19-C20-C21
19	b	4009	BCR	C20-C21-C22-C23
19	b	4009	BCR	C20-C21-C22-C37
19	b	4010	BCR	C10-C11-C12-C13
19	b	4010	BCR	C17-C18-C19-C20
19	b	4010	BCR	C18-C19-C20-C21
19	b	4010	BCR	C21-C22-C23-C24
19	b	4010	BCR	C22-C23-C24-C25
19	b	4014	BCR	C7-C8-C9-C10
19	b	4014	BCR	C35-C13-C14-C15
19	b	4017	BCR	C20-C21-C22-C23
19	b	4017	BCR	C20-C21-C22-C37
19	b	4017	BCR	C21-C22-C23-C24
19	f	4016	BCR	C37-C22-C23-C24
19	g	601	BCR	C7-C8-C9-C10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	g	601	BCR	C7-C8-C9-C34
19	g	601	BCR	C16-C17-C18-C36
19	g	601	BCR	C37-C22-C23-C24
19	g	602	BCR	C10-C11-C12-C13
19	g	602	BCR	C20-C21-C22-C37
19	g	602	BCR	C37-C22-C23-C24
19	g	603	BCR	C6-C7-C8-C9
19	g	603	BCR	C9-C10-C11-C12
19	g	603	BCR	C10-C11-C12-C13
19	g	603	BCR	C18-C19-C20-C21
19	g	603	BCR	C20-C21-C22-C23
19	g	603	BCR	C20-C21-C22-C37
19	g	604	BCR	C6-C7-C8-C9
19	g	604	BCR	C7-C8-C9-C10
19	g	604	BCR	C18-C19-C20-C21
19	g	604	BCR	C21-C22-C23-C24
19	h	601	BCR	C20-C21-C22-C37
19	h	601	BCR	C37-C22-C23-C24
19	h	603	BCR	C6-C7-C8-C9
19	h	603	BCR	C7-C8-C9-C10
19	h	603	BCR	C22-C23-C24-C25
19	h	604	BCR	C7-C8-C9-C34
19	h	604	BCR	C21-C22-C23-C24
19	h	604	BCR	C22-C23-C24-C25
19	i	4018	BCR	C21-C22-C23-C24
19	i	4018	BCR	C37-C22-C23-C24
19	j	4012	BCR	C7-C8-C9-C10
19	j	4012	BCR	C7-C8-C9-C34
19	j	4012	BCR	C21-C22-C23-C24
19	j	4012	BCR	C37-C22-C23-C24
19	j	4013	BCR	C16-C17-C18-C36
19	j	4013	BCR	C18-C19-C20-C21
19	j	4013	BCR	C20-C21-C22-C23
19	j	4013	BCR	C21-C22-C23-C24
19	j	4015	BCR	C7-C8-C9-C34
19	j	4015	BCR	C16-C17-C18-C36
19	j	4015	BCR	C22-C23-C24-C25
19	k	4001	BCR	C21-C22-C23-C24
19	k	4005	BCR	C37-C22-C23-C24
19	l	4019	BCR	C37-C22-C23-C24
19	l	4022	BCR	C6-C7-C8-C9
19	l	4022	BCR	C7-C8-C9-C10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	l	4022	BCR	C17-C18-C19-C20
19	l	4022	BCR	C19-C20-C21-C22
19	l	4022	BCR	C20-C21-C22-C37
19	n	601	BCR	C7-C8-C9-C10
19	n	601	BCR	C19-C20-C21-C22
19	n	601	BCR	C20-C21-C22-C37
19	n	601	BCR	C37-C22-C23-C24
19	n	603	BCR	C6-C7-C8-C9
19	n	603	BCR	C10-C11-C12-C13
19	n	604	BCR	C15-C16-C17-C18
19	n	604	BCR	C22-C23-C24-C25
19	o	601	BCR	C21-C22-C23-C24
19	o	601	BCR	C37-C22-C23-C24
19	o	602	BCR	C6-C7-C8-C9
19	o	602	BCR	C18-C19-C20-C21
19	o	602	BCR	C20-C21-C22-C23
19	o	602	BCR	C20-C21-C22-C37
19	o	603	BCR	C6-C7-C8-C9
19	o	603	BCR	C7-C8-C9-C10
19	o	603	BCR	C7-C8-C9-C34
19	o	604	BCR	C21-C22-C23-C24
19	p	601	BCR	C20-C21-C22-C37
19	p	601	BCR	C21-C22-C23-C24
19	p	602	BCR	C21-C22-C23-C24
19	p	603	BCR	C20-C21-C22-C37
19	p	604	BCR	C6-C7-C8-C9
19	p	604	BCR	C7-C8-C9-C34
19	p	604	BCR	C21-C22-C23-C24
19	p	604	BCR	C37-C22-C23-C24
19	q	602	BCR	C21-C22-C23-C24
19	q	604	BCR	C11-C12-C13-C14
19	q	604	BCR	C11-C12-C13-C35
19	q	604	BCR	C21-C22-C23-C24
19	r	601	BCR	C7-C8-C9-C10
19	r	601	BCR	C7-C8-C9-C34
19	r	601	BCR	C10-C11-C12-C13
19	r	601	BCR	C20-C21-C22-C37
19	r	601	BCR	C21-C22-C23-C24
19	r	601	BCR	C37-C22-C23-C24
19	r	602	BCR	C7-C8-C9-C34
19	r	602	BCR	C11-C10-C9-C8
19	r	602	BCR	C10-C11-C12-C13

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	r	602	BCR	C37-C22-C23-C24
19	r	603	BCR	C20-C21-C22-C23
19	r	603	BCR	C20-C21-C22-C37
19	r	604	BCR	C6-C7-C8-C9
19	r	604	BCR	C11-C10-C9-C34
19	r	604	BCR	C18-C19-C20-C21
19	r	604	BCR	C21-C22-C23-C24
19	s	601	BCR	C7-C8-C9-C10
19	s	601	BCR	C21-C22-C23-C24
19	s	601	BCR	C37-C22-C23-C24
19	s	604	BCR	C6-C7-C8-C9
19	s	604	BCR	C7-C8-C9-C34
19	s	604	BCR	C11-C12-C13-C14
19	s	604	BCR	C11-C12-C13-C35
19	s	604	BCR	C21-C22-C23-C24
19	t	601	BCR	C7-C8-C9-C10
19	t	601	BCR	C10-C11-C12-C13
19	t	601	BCR	C11-C12-C13-C14
19	t	601	BCR	C11-C12-C13-C35
19	t	601	BCR	C18-C19-C20-C21
19	t	601	BCR	C19-C20-C21-C22
19	t	603	BCR	C7-C8-C9-C10
19	t	603	BCR	C7-C8-C9-C34
19	t	603	BCR	C11-C10-C9-C8
19	t	603	BCR	C20-C21-C22-C37
19	t	604	BCR	C7-C8-C9-C10
19	t	604	BCR	C7-C8-C9-C34
19	t	604	BCR	C11-C10-C9-C8
19	t	604	BCR	C11-C10-C9-C34
19	t	604	BCR	C10-C11-C12-C13
19	t	604	BCR	C22-C23-C24-C25
19	u	601	BCR	C7-C8-C9-C10
19	u	601	BCR	C7-C8-C9-C34
19	u	601	BCR	C37-C22-C23-C24
19	u	602	BCR	C7-C8-C9-C34
19	u	603	BCR	C6-C7-C8-C9
19	u	603	BCR	C7-C8-C9-C10
19	u	603	BCR	C7-C8-C9-C34
19	u	604	BCR	C20-C21-C22-C23
19	u	604	BCR	C20-C21-C22-C37
19	u	604	BCR	C21-C22-C23-C24
19	u	604	BCR	C22-C23-C24-C25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	v	601	BCR	C21-C22-C23-C24
19	v	601	BCR	C37-C22-C23-C24
19	v	601	BCR	C22-C23-C24-C25
19	v	603	BCR	C6-C7-C8-C9
19	v	603	BCR	C7-C8-C9-C10
19	v	603	BCR	C21-C22-C23-C24
19	v	603	BCR	C22-C23-C24-C25
19	v	604	BCR	C7-C8-C9-C34
19	v	604	BCR	C21-C22-C23-C24
19	v	604	BCR	C22-C23-C24-C25
19	v	604	BCR	C23-C24-C25-C26
19	w	603	BCR	C6-C7-C8-C9
19	w	603	BCR	C7-C8-C9-C10
19	w	603	BCR	C10-C11-C12-C13
19	w	603	BCR	C20-C21-C22-C37
19	w	604	BCR	C11-C10-C9-C34
19	w	604	BCR	C11-C12-C13-C14
19	w	604	BCR	C11-C12-C13-C35
19	w	604	BCR	C21-C22-C23-C24
19	x	601	BCR	C7-C8-C9-C10
19	x	601	BCR	C20-C21-C22-C37
19	x	602	BCR	C6-C7-C8-C9
19	x	602	BCR	C11-C10-C9-C8
19	x	602	BCR	C11-C10-C9-C34
19	x	602	BCR	C10-C11-C12-C13
19	x	602	BCR	C11-C12-C13-C35
19	x	602	BCR	C14-C15-C16-C17
19	x	602	BCR	C21-C22-C23-C24
19	x	602	BCR	C37-C22-C23-C24
19	x	603	BCR	C6-C7-C8-C9
19	x	603	BCR	C18-C19-C20-C21
19	x	604	BCR	C6-C7-C8-C9
19	x	604	BCR	C18-C19-C20-C21
19	x	604	BCR	C21-C22-C23-C24
19	y	601	BCR	C21-C22-C23-C24
19	y	601	BCR	C22-C23-C24-C25
19	y	603	BCR	C6-C7-C8-C9
19	y	603	BCR	C7-C8-C9-C10
19	y	603	BCR	C22-C23-C24-C25
19	y	604	BCR	C7-C8-C9-C34
19	y	604	BCR	C21-C22-C23-C24
19	y	604	BCR	C22-C23-C24-C25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	B	4006	ECH	C7-C8-C9-C10
21	B	4006	ECH	C7-C8-C9-C34
21	B	4006	ECH	C21-C22-C23-C24
21	B	4006	ECH	C37-C22-C23-C24
21	G	4006	ECH	C7-C8-C9-C10
21	G	4006	ECH	C7-C8-C9-C34
21	G	4006	ECH	C21-C22-C23-C24
21	I	4020	ECH	C1-C6-C7-C8
21	I	4020	ECH	C7-C8-C9-C10
21	I	4020	ECH	C7-C8-C9-C34
21	I	4020	ECH	C9-C10-C11-C12
21	I	4020	ECH	C11-C12-C13-C14
21	I	4020	ECH	C11-C12-C13-C35
21	I	4020	ECH	C21-C22-C23-C24
21	I	4020	ECH	C37-C22-C23-C24
21	M	4021	ECH	C9-C10-C11-C12
21	M	4021	ECH	C21-C22-C23-C24
21	M	4021	ECH	C37-C22-C23-C24
21	M	4021	ECH	C23-C24-C25-C26
21	R	4020	ECH	C11-C12-C13-C14
21	R	4020	ECH	C11-C12-C13-C35
21	V	4021	ECH	C11-C12-C13-C35
21	V	4021	ECH	C21-C22-C23-C24
21	V	4021	ECH	C37-C22-C23-C24
21	V	4021	ECH	C23-C24-C25-C26
21	b	4006	ECH	C21-C22-C23-C24
21	i	4020	ECH	C11-C12-C13-C14
21	i	4020	ECH	C21-C22-C23-C24
21	i	4020	ECH	C37-C22-C23-C24
21	m	4021	ECH	C7-C8-C9-C10
21	m	4021	ECH	C7-C8-C9-C34
21	m	4021	ECH	C11-C12-C13-C35
21	m	4021	ECH	C23-C24-C25-C26
23	Y	606	LMU	C2'-C1'-O1'-C1
23	Y	606	LMU	O5'-C1'-O1'-C1
23	p	606	LMU	C2'-C1'-O1'-C1
23	p	606	LMU	O5'-C1'-O1'-C1
23	q	605	LMU	C2'-C1'-O1'-C1
23	s	606	LMU	C2'-C1'-O1'-C1
23	s	606	LMU	O5'-C1'-O1'-C1
23	x	606	LMU	C2'-C1'-O1'-C1
24	Z	601	LUT	C7-C8-C9-C10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	Z	601	LUT	C7-C8-C9-C19
24	Z	601	LUT	C27-C28-C29-C30
24	Z	601	LUT	C27-C28-C29-C39
24	Z	601	LUT	C31-C32-C33-C34
24	q	601	LUT	C27-C28-C29-C30
24	q	601	LUT	C27-C28-C29-C39
24	q	601	LUT	C31-C32-C33-C34
24	q	601	LUT	C31-C32-C33-C40
24	w	601	LUT	C27-C28-C29-C30
24	w	601	LUT	C27-C28-C29-C39
24	w	601	LUT	C31-C32-C33-C34
24	w	601	LUT	C31-C32-C33-C40
16	A	1108	CLA	O1D-CGD-O2D-CED
16	B	1021	CLA	O1D-CGD-O2D-CED
16	B	1240	CLA	O1D-CGD-O2D-CED
16	H	1104	CLA	O1D-CGD-O2D-CED
16	H	1108	CLA	O1D-CGD-O2D-CED
16	W	508	CLA	O1D-CGD-O2D-CED
16	W	511	CLA	O1D-CGD-O2D-CED
16	W	514	CLA	O1D-CGD-O2D-CED
16	X	513	CLA	O1D-CGD-O2D-CED
16	X	515	CLA	O1D-CGD-O2D-CED
16	Y	514	CLA	O1D-CGD-O2D-CED
16	a	1108	CLA	O1D-CGD-O2D-CED
16	b	1021	CLA	O1D-CGD-O2D-CED
16	b	1229	CLA	O1D-CGD-O2D-CED
16	h	512	CLA	O1D-CGD-O2D-CED
16	h	514	CLA	O1D-CGD-O2D-CED
16	n	512	CLA	O1D-CGD-O2D-CED
16	o	505	CLA	O1D-CGD-O2D-CED
16	o	506	CLA	O1D-CGD-O2D-CED
16	o	514	CLA	O1D-CGD-O2D-CED
16	p	511	CLA	O1D-CGD-O2D-CED
16	p	514	CLA	O1D-CGD-O2D-CED
16	q	503	CLA	O1D-CGD-O2D-CED
16	r	511	CLA	O1D-CGD-O2D-CED
16	s	511	CLA	O1D-CGD-O2D-CED
16	s	514	CLA	O1D-CGD-O2D-CED
16	t	511	CLA	O1D-CGD-O2D-CED
16	t	514	CLA	O1D-CGD-O2D-CED
16	u	506	CLA	O1D-CGD-O2D-CED
16	u	514	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	u	515	CLA	O1D-CGD-O2D-CED
16	v	504	CLA	O1D-CGD-O2D-CED
16	w	503	CLA	O1D-CGD-O2D-CED
16	w	511	CLA	O1D-CGD-O2D-CED
16	y	504	CLA	O1D-CGD-O2D-CED
16	y	505	CLA	O1D-CGD-O2D-CED
16	y	512	CLA	O1D-CGD-O2D-CED
16	A	1112	CLA	O1D-CGD-O2D-CED
16	B	1229	CLA	O1D-CGD-O2D-CED
16	G	1021	CLA	O1D-CGD-O2D-CED
16	H	1131	CLA	O1D-CGD-O2D-CED
16	W	507	CLA	O1D-CGD-O2D-CED
16	Y	504	CLA	O1D-CGD-O2D-CED
16	Y	511	CLA	O1D-CGD-O2D-CED
16	Z	503	CLA	O1D-CGD-O2D-CED
16	Z	514	CLA	O1D-CGD-O2D-CED
16	b	1240	CLA	O1D-CGD-O2D-CED
16	f	1301	CLA	O1D-CGD-O2D-CED
16	h	506	CLA	O1D-CGD-O2D-CED
16	h	510	CLA	O1D-CGD-O2D-CED
16	n	508	CLA	O1D-CGD-O2D-CED
16	u	505	CLA	O1D-CGD-O2D-CED
16	u	513	CLA	O1D-CGD-O2D-CED
16	A	1108	CLA	CBD-CGD-O2D-CED
16	A	1111	CLA	CBD-CGD-O2D-CED
16	A	1121	CLA	CBD-CGD-O2D-CED
16	A	1122	CLA	CBD-CGD-O2D-CED
16	A	1132	CLA	CBD-CGD-O2D-CED
16	A	1801	CLA	CBD-CGD-O2D-CED
16	B	1021	CLA	CBD-CGD-O2D-CED
16	B	1224	CLA	CBD-CGD-O2D-CED
16	B	1229	CLA	CBD-CGD-O2D-CED
16	B	1239	CLA	CBD-CGD-O2D-CED
16	B	1240	CLA	CBD-CGD-O2D-CED
16	G	1208	CLA	CBD-CGD-O2D-CED
16	G	1219	CLA	CBD-CGD-O2D-CED
16	G	1220	CLA	CBD-CGD-O2D-CED
16	G	1229	CLA	CBD-CGD-O2D-CED
16	G	1239	CLA	CBD-CGD-O2D-CED
16	H	1104	CLA	CBD-CGD-O2D-CED
16	H	1108	CLA	CBD-CGD-O2D-CED
16	H	1116	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	H	1121	CLA	CBD-CGD-O2D-CED
16	K	4002	CLA	CBD-CGD-O2D-CED
16	W	502	CLA	CBD-CGD-O2D-CED
16	W	503	CLA	CBD-CGD-O2D-CED
16	W	507	CLA	CBD-CGD-O2D-CED
16	W	511	CLA	CBD-CGD-O2D-CED
16	X	503	CLA	CBD-CGD-O2D-CED
16	X	507	CLA	CBD-CGD-O2D-CED
16	X	511	CLA	CBD-CGD-O2D-CED
16	X	515	CLA	CBD-CGD-O2D-CED
16	Y	504	CLA	CBD-CGD-O2D-CED
16	Z	503	CLA	CBD-CGD-O2D-CED
16	Z	506	CLA	CBD-CGD-O2D-CED
16	Z	510	CLA	CBD-CGD-O2D-CED
16	Z	511	CLA	CBD-CGD-O2D-CED
16	Z	514	CLA	CBD-CGD-O2D-CED
16	a	1013	CLA	CBD-CGD-O2D-CED
16	a	1120	CLA	CBD-CGD-O2D-CED
16	a	1121	CLA	CBD-CGD-O2D-CED
16	a	1122	CLA	CBD-CGD-O2D-CED
16	a	1131	CLA	CBD-CGD-O2D-CED
16	a	1801	CLA	CBD-CGD-O2D-CED
16	b	1023	CLA	CBD-CGD-O2D-CED
16	b	1215	CLA	CBD-CGD-O2D-CED
16	b	1220	CLA	CBD-CGD-O2D-CED
16	b	1224	CLA	CBD-CGD-O2D-CED
16	b	1229	CLA	CBD-CGD-O2D-CED
16	b	1230	CLA	CBD-CGD-O2D-CED
16	b	1232	CLA	CBD-CGD-O2D-CED
16	b	1240	CLA	CBD-CGD-O2D-CED
16	g	507	CLA	CBD-CGD-O2D-CED
16	g	514	CLA	CBD-CGD-O2D-CED
16	g	516	CLA	CBD-CGD-O2D-CED
16	h	504	CLA	CBD-CGD-O2D-CED
16	h	506	CLA	CBD-CGD-O2D-CED
16	h	512	CLA	CBD-CGD-O2D-CED
16	h	513	CLA	CBD-CGD-O2D-CED
16	k	4002	CLA	CBD-CGD-O2D-CED
16	n	502	CLA	CBD-CGD-O2D-CED
16	n	507	CLA	CBD-CGD-O2D-CED
16	o	511	CLA	CBD-CGD-O2D-CED
16	p	504	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	p	511	CLA	CBD-CGD-O2D-CED
16	q	502	CLA	CBD-CGD-O2D-CED
16	q	503	CLA	CBD-CGD-O2D-CED
16	q	506	CLA	CBD-CGD-O2D-CED
16	q	511	CLA	CBD-CGD-O2D-CED
16	q	514	CLA	CBD-CGD-O2D-CED
16	r	505	CLA	CBD-CGD-O2D-CED
16	r	507	CLA	CBD-CGD-O2D-CED
16	r	510	CLA	CBD-CGD-O2D-CED
16	r	511	CLA	CBD-CGD-O2D-CED
16	s	504	CLA	CBD-CGD-O2D-CED
16	s	507	CLA	CBD-CGD-O2D-CED
16	u	503	CLA	CBD-CGD-O2D-CED
16	u	507	CLA	CBD-CGD-O2D-CED
16	v	504	CLA	CBD-CGD-O2D-CED
16	v	508	CLA	CBD-CGD-O2D-CED
16	v	510	CLA	CBD-CGD-O2D-CED
16	v	512	CLA	CBD-CGD-O2D-CED
16	w	503	CLA	CBD-CGD-O2D-CED
16	w	510	CLA	CBD-CGD-O2D-CED
16	w	514	CLA	CBD-CGD-O2D-CED
16	x	507	CLA	CBD-CGD-O2D-CED
16	x	510	CLA	CBD-CGD-O2D-CED
16	x	511	CLA	CBD-CGD-O2D-CED
16	x	513	CLA	CBD-CGD-O2D-CED
16	x	517	CLA	CBD-CGD-O2D-CED
16	y	504	CLA	CBD-CGD-O2D-CED
16	y	507	CLA	CBD-CGD-O2D-CED
16	y	513	CLA	CBD-CGD-O2D-CED
16	A	1130	CLA	O1A-CGA-O2A-C1
16	B	1203	CLA	O1A-CGA-O2A-C1
16	B	1220	CLA	O1A-CGA-O2A-C1
16	G	1203	CLA	O1A-CGA-O2A-C1
16	G	1226	CLA	O1A-CGA-O2A-C1
16	H	1130	CLA	O1A-CGA-O2A-C1
16	L	1503	CLA	O1A-CGA-O2A-C1
16	W	502	CLA	O1A-CGA-O2A-C1
16	Y	509	CLA	O1A-CGA-O2A-C1
16	Y	517	CLA	O1A-CGA-O2A-C1
16	Z	501	CLA	O1A-CGA-O2A-C1
16	Z	507	CLA	O1A-CGA-O2A-C1
16	Z	513	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	b	1203	CLA	O1A-CGA-O2A-C1
16	b	1226	CLA	O1A-CGA-O2A-C1
16	b	1227	CLA	O1A-CGA-O2A-C1
16	g	512	CLA	O1A-CGA-O2A-C1
16	h	515	CLA	O1A-CGA-O2A-C1
16	h	517	CLA	O1A-CGA-O2A-C1
16	l	1503	CLA	O1A-CGA-O2A-C1
16	o	505	CLA	O1A-CGA-O2A-C1
16	o	515	CLA	O1A-CGA-O2A-C1
16	p	509	CLA	O1A-CGA-O2A-C1
16	p	512	CLA	O1A-CGA-O2A-C1
16	p	515	CLA	O1A-CGA-O2A-C1
16	p	517	CLA	O1A-CGA-O2A-C1
16	q	507	CLA	O1A-CGA-O2A-C1
16	r	510	CLA	O1A-CGA-O2A-C1
16	s	509	CLA	O1A-CGA-O2A-C1
16	s	512	CLA	O1A-CGA-O2A-C1
16	s	517	CLA	O1A-CGA-O2A-C1
16	u	508	CLA	O1A-CGA-O2A-C1
16	v	515	CLA	O1A-CGA-O2A-C1
16	X	513	CLA	O1A-CGA-O2A-C1
16	Z	503	CLA	O1A-CGA-O2A-C1
16	n	503	CLA	O1A-CGA-O2A-C1
16	w	503	CLA	O1A-CGA-O2A-C1
16	w	516	CLA	O1A-CGA-O2A-C1
16	g	511	CLA	O1D-CGD-O2D-CED
16	n	514	CLA	O1D-CGD-O2D-CED
16	s	504	CLA	O1D-CGD-O2D-CED
16	W	503	CLA	CBA-CGA-O2A-C1
16	X	503	CLA	CBA-CGA-O2A-C1
16	X	513	CLA	CBA-CGA-O2A-C1
16	h	516	CLA	CBA-CGA-O2A-C1
16	y	501	CLA	CBA-CGA-O2A-C1
16	G	1208	CLA	O1D-CGD-O2D-CED
16	G	1229	CLA	O1D-CGD-O2D-CED
16	a	1131	CLA	O1D-CGD-O2D-CED
16	g	507	CLA	O1D-CGD-O2D-CED
16	n	507	CLA	O1D-CGD-O2D-CED
16	o	511	CLA	O1D-CGD-O2D-CED
16	p	504	CLA	O1D-CGD-O2D-CED
16	q	511	CLA	O1D-CGD-O2D-CED
16	q	514	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	r	507	CLA	O1D-CGD-O2D-CED
16	v	510	CLA	O1D-CGD-O2D-CED
16	v	512	CLA	O1D-CGD-O2D-CED
16	w	514	CLA	O1D-CGD-O2D-CED
16	x	507	CLA	O1D-CGD-O2D-CED
16	x	511	CLA	O1D-CGD-O2D-CED
14	a	852	LMG	C29-C28-O8-C9
16	B	1211	CLA	CBA-CGA-O2A-C1
16	G	1211	CLA	CBA-CGA-O2A-C1
16	Y	509	CLA	CBA-CGA-O2A-C1
16	Y	517	CLA	CBA-CGA-O2A-C1
16	a	1130	CLA	CBA-CGA-O2A-C1
16	g	512	CLA	CBA-CGA-O2A-C1
16	h	515	CLA	CBA-CGA-O2A-C1
16	h	517	CLA	CBA-CGA-O2A-C1
16	p	509	CLA	CBA-CGA-O2A-C1
16	p	512	CLA	CBA-CGA-O2A-C1
16	p	517	CLA	CBA-CGA-O2A-C1
16	q	507	CLA	CBA-CGA-O2A-C1
16	s	509	CLA	CBA-CGA-O2A-C1
16	s	512	CLA	CBA-CGA-O2A-C1
16	t	501	CLA	CBA-CGA-O2A-C1
16	v	507	CLA	CBA-CGA-O2A-C1
16	v	515	CLA	CBA-CGA-O2A-C1
16	x	510	CLA	CBA-CGA-O2A-C1
16	B	1232	CLA	CBD-CGD-O2D-CED
16	G	1215	CLA	CBD-CGD-O2D-CED
16	J	1302	CLA	CBD-CGD-O2D-CED
16	L	1501	CLA	CBD-CGD-O2D-CED
16	a	1113	CLA	CBD-CGD-O2D-CED
16	b	1201	CLA	CBD-CGD-O2D-CED
16	h	508	CLA	CBD-CGD-O2D-CED
16	q	510	CLA	CBD-CGD-O2D-CED
14	A	852	LMG	O10-C28-O8-C9
14	H	4201	LMG	O10-C28-O8-C9
14	a	852	LMG	O10-C28-O8-C9
14	a	4201	LMG	O10-C28-O8-C9
16	A	1118	CLA	O1A-CGA-O2A-C1
16	A	1120	CLA	O1A-CGA-O2A-C1
16	A	1132	CLA	O1A-CGA-O2A-C1
16	A	1133	CLA	O1A-CGA-O2A-C1
16	A	1237	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1211	CLA	O1A-CGA-O2A-C1
16	B	1218	CLA	O1A-CGA-O2A-C1
16	B	1226	CLA	O1A-CGA-O2A-C1
16	B	1236	CLA	O1A-CGA-O2A-C1
16	G	1211	CLA	O1A-CGA-O2A-C1
16	G	1227	CLA	O1A-CGA-O2A-C1
16	G	1236	CLA	O1A-CGA-O2A-C1
16	H	1118	CLA	O1A-CGA-O2A-C1
16	H	1120	CLA	O1A-CGA-O2A-C1
16	H	1132	CLA	O1A-CGA-O2A-C1
16	H	1133	CLA	O1A-CGA-O2A-C1
16	H	1237	CLA	O1A-CGA-O2A-C1
16	W	505	CLA	O1A-CGA-O2A-C1
16	W	508	CLA	O1A-CGA-O2A-C1
16	W	515	CLA	O1A-CGA-O2A-C1
16	X	506	CLA	O1A-CGA-O2A-C1
16	Z	502	CLA	O1A-CGA-O2A-C1
16	a	1118	CLA	O1A-CGA-O2A-C1
16	a	1120	CLA	O1A-CGA-O2A-C1
16	a	1130	CLA	O1A-CGA-O2A-C1
16	a	1132	CLA	O1A-CGA-O2A-C1
16	a	1237	CLA	O1A-CGA-O2A-C1
16	b	1211	CLA	O1A-CGA-O2A-C1
16	b	1218	CLA	O1A-CGA-O2A-C1
16	b	1236	CLA	O1A-CGA-O2A-C1
16	g	501	CLA	O1A-CGA-O2A-C1
16	g	505	CLA	O1A-CGA-O2A-C1
16	g	508	CLA	O1A-CGA-O2A-C1
16	g	515	CLA	O1A-CGA-O2A-C1
16	g	517	CLA	O1A-CGA-O2A-C1
16	h	502	CLA	O1A-CGA-O2A-C1
16	h	508	CLA	O1A-CGA-O2A-C1
16	h	510	CLA	O1A-CGA-O2A-C1
16	n	505	CLA	O1A-CGA-O2A-C1
16	n	508	CLA	O1A-CGA-O2A-C1
16	n	515	CLA	O1A-CGA-O2A-C1
16	o	508	CLA	O1A-CGA-O2A-C1
16	q	501	CLA	O1A-CGA-O2A-C1
16	r	505	CLA	O1A-CGA-O2A-C1
16	r	508	CLA	O1A-CGA-O2A-C1
16	r	512	CLA	O1A-CGA-O2A-C1
16	s	515	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	t	501	CLA	O1A-CGA-O2A-C1
16	t	505	CLA	O1A-CGA-O2A-C1
16	t	508	CLA	O1A-CGA-O2A-C1
16	t	515	CLA	O1A-CGA-O2A-C1
16	v	502	CLA	O1A-CGA-O2A-C1
16	v	507	CLA	O1A-CGA-O2A-C1
16	v	510	CLA	O1A-CGA-O2A-C1
16	w	501	CLA	O1A-CGA-O2A-C1
16	w	507	CLA	O1A-CGA-O2A-C1
16	x	505	CLA	O1A-CGA-O2A-C1
16	x	508	CLA	O1A-CGA-O2A-C1
16	x	510	CLA	O1A-CGA-O2A-C1
16	x	512	CLA	O1A-CGA-O2A-C1
16	x	515	CLA	O1A-CGA-O2A-C1
16	y	508	CLA	O1A-CGA-O2A-C1
16	y	510	CLA	O1A-CGA-O2A-C1
16	y	515	CLA	O1A-CGA-O2A-C1
16	y	517	CLA	O1A-CGA-O2A-C1
16	H	1801	CLA	O1A-CGA-O2A-C1
16	y	501	CLA	O1A-CGA-O2A-C1
16	A	1104	CLA	O1D-CGD-O2D-CED
16	A	1120	CLA	O1D-CGD-O2D-CED
16	A	1137	CLA	O1D-CGD-O2D-CED
16	G	1211	CLA	O1D-CGD-O2D-CED
16	G	1220	CLA	O1D-CGD-O2D-CED
16	G	1232	CLA	O1D-CGD-O2D-CED
16	G	1240	CLA	O1D-CGD-O2D-CED
16	S	1302	CLA	O1D-CGD-O2D-CED
16	Y	507	CLA	O1D-CGD-O2D-CED
16	a	1013	CLA	O1D-CGD-O2D-CED
16	b	1206	CLA	O1D-CGD-O2D-CED
16	b	1239	CLA	O1D-CGD-O2D-CED
16	g	504	CLA	O1D-CGD-O2D-CED
16	n	511	CLA	O1D-CGD-O2D-CED
16	o	503	CLA	O1D-CGD-O2D-CED
16	o	507	CLA	O1D-CGD-O2D-CED
16	p	506	CLA	O1D-CGD-O2D-CED
16	s	507	CLA	O1D-CGD-O2D-CED
16	u	507	CLA	O1D-CGD-O2D-CED
16	w	507	CLA	O1D-CGD-O2D-CED
16	x	505	CLA	O1D-CGD-O2D-CED
16	A	1113	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	1116	CLA	O1D-CGD-O2D-CED
16	B	1203	CLA	O1D-CGD-O2D-CED
16	B	1207	CLA	O1D-CGD-O2D-CED
16	B	1211	CLA	O1D-CGD-O2D-CED
16	F	1302	CLA	O1D-CGD-O2D-CED
16	H	1013	CLA	O1D-CGD-O2D-CED
16	H	1137	CLA	O1D-CGD-O2D-CED
16	X	508	CLA	O1D-CGD-O2D-CED
16	Z	507	CLA	O1D-CGD-O2D-CED
16	a	1104	CLA	O1D-CGD-O2D-CED
16	a	1137	CLA	O1D-CGD-O2D-CED
16	b	1207	CLA	O1D-CGD-O2D-CED
16	g	517	CLA	O1D-CGD-O2D-CED
16	n	513	CLA	O1D-CGD-O2D-CED
16	o	504	CLA	O1D-CGD-O2D-CED
16	o	508	CLA	O1D-CGD-O2D-CED
16	p	507	CLA	O1D-CGD-O2D-CED
16	r	504	CLA	O1D-CGD-O2D-CED
16	r	513	CLA	O1D-CGD-O2D-CED
16	t	507	CLA	O1D-CGD-O2D-CED
16	t	512	CLA	O1D-CGD-O2D-CED
16	u	504	CLA	O1D-CGD-O2D-CED
16	u	508	CLA	O1D-CGD-O2D-CED
16	u	516	CLA	O1D-CGD-O2D-CED
16	v	506	CLA	O1D-CGD-O2D-CED
16	v	511	CLA	O1D-CGD-O2D-CED
16	x	504	CLA	O1D-CGD-O2D-CED
16	y	502	CLA	O1D-CGD-O2D-CED
16	y	506	CLA	O1D-CGD-O2D-CED
16	y	510	CLA	O1D-CGD-O2D-CED
16	y	511	CLA	O1D-CGD-O2D-CED
16	H	1132	CLA	CBD-CGD-O2D-CED
16	r	517	CLA	CBD-CGD-O2D-CED
16	u	506	CLA	O1A-CGA-O2A-C1
16	v	508	CLA	O1A-CGA-O2A-C1
16	A	1131	CLA	O1D-CGD-O2D-CED
16	t	513	CLA	O1D-CGD-O2D-CED
16	X	501	CLA	CBA-CGA-O2A-C1
16	t	516	CLA	O1A-CGA-O2A-C1
16	A	1013	CLA	C3-C5-C6-C7
16	A	1109	CLA	C3-C5-C6-C7
16	A	1115	CLA	C3-C5-C6-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1204	CLA	C3-C5-C6-C7
16	B	1205	CLA	C3-C5-C6-C7
16	B	1218	CLA	C3-C5-C6-C7
16	B	1225	CLA	C3-C5-C6-C7
16	B	1226	CLA	C3-C5-C6-C7
16	G	1205	CLA	C3-C5-C6-C7
16	G	1225	CLA	C3-C5-C6-C7
16	H	1013	CLA	C3-C5-C6-C7
16	H	1104	CLA	C3-C5-C6-C7
16	H	1119	CLA	C3-C5-C6-C7
16	H	1124	CLA	C3-C5-C6-C7
16	H	1128	CLA	C3-C5-C6-C7
16	H	1131	CLA	C3-C5-C6-C7
16	H	1133	CLA	C3-C5-C6-C7
16	W	512	CLA	C3-C5-C6-C7
16	X	504	CLA	C3-C5-C6-C7
16	X	517	CLA	C3-C5-C6-C7
16	Y	509	CLA	C3-C5-C6-C7
16	Y	512	CLA	C3-C5-C6-C7
16	Y	515	CLA	C3-C5-C6-C7
16	Z	505	CLA	C3-C5-C6-C7
16	Z	510	CLA	C3-C5-C6-C7
16	a	1119	CLA	C3-C5-C6-C7
16	a	1124	CLA	C3-C5-C6-C7
16	b	1012	CLA	C3-C5-C6-C7
16	b	1205	CLA	C3-C5-C6-C7
16	b	1211	CLA	C3-C5-C6-C7
16	b	1223	CLA	C3-C5-C6-C7
16	b	1225	CLA	C3-C5-C6-C7
16	b	1226	CLA	C3-C5-C6-C7
16	b	1235	CLA	C3-C5-C6-C7
16	g	515	CLA	C3-C5-C6-C7
16	h	504	CLA	C3-C5-C6-C7
16	h	512	CLA	C3-C5-C6-C7
16	o	505	CLA	C3-C5-C6-C7
16	o	509	CLA	C3-C5-C6-C7
16	o	517	CLA	C3-C5-C6-C7
16	p	509	CLA	C3-C5-C6-C7
16	p	512	CLA	C3-C5-C6-C7
16	p	515	CLA	C3-C5-C6-C7
16	q	517	CLA	C3-C5-C6-C7
16	r	505	CLA	C3-C5-C6-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	r	508	CLA	C3-C5-C6-C7
16	r	512	CLA	C3-C5-C6-C7
16	r	515	CLA	C3-C5-C6-C7
16	s	509	CLA	C3-C5-C6-C7
16	s	512	CLA	C3-C5-C6-C7
16	s	515	CLA	C3-C5-C6-C7
16	t	510	CLA	C3-C5-C6-C7
16	u	517	CLA	C3-C5-C6-C7
16	v	504	CLA	C3-C5-C6-C7
16	v	506	CLA	C3-C5-C6-C7
16	v	511	CLA	C3-C5-C6-C7
16	v	512	CLA	C3-C5-C6-C7
16	w	508	CLA	C3-C5-C6-C7
16	w	517	CLA	C3-C5-C6-C7
16	x	515	CLA	C3-C5-C6-C7
16	y	512	CLA	C3-C5-C6-C7
16	b	1219	CLA	O1D-CGD-O2D-CED
14	A	852	LMG	C29-C28-O8-C9
14	H	4201	LMG	C29-C28-O8-C9
16	A	1105	CLA	CBA-CGA-O2A-C1
16	A	1118	CLA	CBA-CGA-O2A-C1
16	A	1120	CLA	CBA-CGA-O2A-C1
16	A	1130	CLA	CBA-CGA-O2A-C1
16	A	1132	CLA	CBA-CGA-O2A-C1
16	A	1237	CLA	CBA-CGA-O2A-C1
16	B	1203	CLA	CBA-CGA-O2A-C1
16	B	1218	CLA	CBA-CGA-O2A-C1
16	B	1220	CLA	CBA-CGA-O2A-C1
16	B	1236	CLA	CBA-CGA-O2A-C1
16	G	1203	CLA	CBA-CGA-O2A-C1
16	G	1218	CLA	CBA-CGA-O2A-C1
16	G	1226	CLA	CBA-CGA-O2A-C1
16	G	1227	CLA	CBA-CGA-O2A-C1
16	G	1236	CLA	CBA-CGA-O2A-C1
16	H	1118	CLA	CBA-CGA-O2A-C1
16	H	1120	CLA	CBA-CGA-O2A-C1
16	H	1130	CLA	CBA-CGA-O2A-C1
16	H	1132	CLA	CBA-CGA-O2A-C1
16	H	1237	CLA	CBA-CGA-O2A-C1
16	L	1503	CLA	CBA-CGA-O2A-C1
16	W	502	CLA	CBA-CGA-O2A-C1
16	W	505	CLA	CBA-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	W	515	CLA	CBA-CGA-O2A-C1
16	X	506	CLA	CBA-CGA-O2A-C1
16	Y	512	CLA	CBA-CGA-O2A-C1
16	Y	515	CLA	CBA-CGA-O2A-C1
16	Z	501	CLA	CBA-CGA-O2A-C1
16	Z	502	CLA	CBA-CGA-O2A-C1
16	Z	513	CLA	CBA-CGA-O2A-C1
16	a	1105	CLA	CBA-CGA-O2A-C1
16	a	1118	CLA	CBA-CGA-O2A-C1
16	a	1120	CLA	CBA-CGA-O2A-C1
16	a	1132	CLA	CBA-CGA-O2A-C1
16	a	1237	CLA	CBA-CGA-O2A-C1
16	b	1021	CLA	CBA-CGA-O2A-C1
16	b	1203	CLA	CBA-CGA-O2A-C1
16	b	1211	CLA	CBA-CGA-O2A-C1
16	b	1218	CLA	CBA-CGA-O2A-C1
16	b	1226	CLA	CBA-CGA-O2A-C1
16	b	1227	CLA	CBA-CGA-O2A-C1
16	b	1236	CLA	CBA-CGA-O2A-C1
16	g	515	CLA	CBA-CGA-O2A-C1
16	h	502	CLA	CBA-CGA-O2A-C1
16	h	508	CLA	CBA-CGA-O2A-C1
16	l	1503	CLA	CBA-CGA-O2A-C1
16	n	505	CLA	CBA-CGA-O2A-C1
16	n	508	CLA	CBA-CGA-O2A-C1
16	n	510	CLA	CBA-CGA-O2A-C1
16	n	515	CLA	CBA-CGA-O2A-C1
16	o	505	CLA	CBA-CGA-O2A-C1
16	o	515	CLA	CBA-CGA-O2A-C1
16	q	501	CLA	CBA-CGA-O2A-C1
16	q	513	CLA	CBA-CGA-O2A-C1
16	q	515	CLA	CBA-CGA-O2A-C1
16	r	501	CLA	CBA-CGA-O2A-C1
16	r	508	CLA	CBA-CGA-O2A-C1
16	r	510	CLA	CBA-CGA-O2A-C1
16	r	515	CLA	CBA-CGA-O2A-C1
16	s	501	CLA	CBA-CGA-O2A-C1
16	s	517	CLA	CBA-CGA-O2A-C1
16	t	505	CLA	CBA-CGA-O2A-C1
16	t	508	CLA	CBA-CGA-O2A-C1
16	t	515	CLA	CBA-CGA-O2A-C1
16	u	508	CLA	CBA-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	w	501	CLA	CBA-CGA-O2A-C1
16	w	507	CLA	CBA-CGA-O2A-C1
16	x	505	CLA	CBA-CGA-O2A-C1
16	x	508	CLA	CBA-CGA-O2A-C1
16	x	515	CLA	CBA-CGA-O2A-C1
16	y	515	CLA	CBA-CGA-O2A-C1
16	y	517	CLA	CBA-CGA-O2A-C1
16	B	1201	CLA	CBD-CGD-O2D-CED
16	B	1206	CLA	CBD-CGD-O2D-CED
16	B	1216	CLA	CBD-CGD-O2D-CED
16	B	1231	CLA	CBD-CGD-O2D-CED
16	H	1117	CLA	CBD-CGD-O2D-CED
16	H	1126	CLA	CBD-CGD-O2D-CED
16	T	4002	CLA	CBD-CGD-O2D-CED
16	U	1501	CLA	CBD-CGD-O2D-CED
16	W	505	CLA	CBD-CGD-O2D-CED
16	Y	505	CLA	CBD-CGD-O2D-CED
16	Y	517	CLA	CBD-CGD-O2D-CED
16	Z	512	CLA	CBD-CGD-O2D-CED
16	a	1116	CLA	CBD-CGD-O2D-CED
16	a	1117	CLA	CBD-CGD-O2D-CED
16	a	1126	CLA	CBD-CGD-O2D-CED
16	a	1132	CLA	CBD-CGD-O2D-CED
16	b	1208	CLA	CBD-CGD-O2D-CED
16	b	1228	CLA	CBD-CGD-O2D-CED
16	b	1231	CLA	CBD-CGD-O2D-CED
16	b	1235	CLA	CBD-CGD-O2D-CED
16	f	1302	CLA	CBD-CGD-O2D-CED
16	g	505	CLA	CBD-CGD-O2D-CED
16	g	510	CLA	CBD-CGD-O2D-CED
16	h	511	CLA	CBD-CGD-O2D-CED
16	l	1501	CLA	CBD-CGD-O2D-CED
16	n	517	CLA	CBD-CGD-O2D-CED
16	p	505	CLA	CBD-CGD-O2D-CED
16	p	516	CLA	CBD-CGD-O2D-CED
16	q	512	CLA	CBD-CGD-O2D-CED
16	r	509	CLA	CBD-CGD-O2D-CED
16	r	512	CLA	CBD-CGD-O2D-CED
16	s	502	CLA	CBD-CGD-O2D-CED
16	s	516	CLA	CBD-CGD-O2D-CED
16	t	516	CLA	CBD-CGD-O2D-CED
16	v	509	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	w	512	CLA	CBD-CGD-O2D-CED
16	w	516	CLA	CBD-CGD-O2D-CED
16	y	509	CLA	CBD-CGD-O2D-CED
14	H	4101	LMG	C11-C10-O7-C8
14	a	4101	LMG	C11-C10-O7-C8
16	A	1117	CLA	O1D-CGD-O2D-CED
16	B	1215	CLA	O1D-CGD-O2D-CED
16	B	1219	CLA	O1D-CGD-O2D-CED
16	F	1301	CLA	O1D-CGD-O2D-CED
16	G	1219	CLA	O1D-CGD-O2D-CED
16	W	512	CLA	O1D-CGD-O2D-CED
16	W	513	CLA	O1D-CGD-O2D-CED
16	X	504	CLA	O1D-CGD-O2D-CED
16	Y	506	CLA	O1D-CGD-O2D-CED
16	Z	510	CLA	O1D-CGD-O2D-CED
16	b	1203	CLA	O1D-CGD-O2D-CED
16	b	1215	CLA	O1D-CGD-O2D-CED
16	g	513	CLA	O1D-CGD-O2D-CED
16	u	503	CLA	O1D-CGD-O2D-CED
16	v	517	CLA	O1D-CGD-O2D-CED
16	x	513	CLA	O1D-CGD-O2D-CED
16	y	507	CLA	O1D-CGD-O2D-CED
16	B	1239	CLA	O1A-CGA-O2A-C1
16	t	502	CLA	O1A-CGA-O2A-C1
16	u	505	CLA	O1A-CGA-O2A-C1
16	A	1801	CLA	O1A-CGA-O2A-C1
16	W	516	CLA	O1A-CGA-O2A-C1
16	X	501	CLA	O1A-CGA-O2A-C1
16	X	503	CLA	O1A-CGA-O2A-C1
16	f	1302	CLA	O1A-CGA-O2A-C1
16	o	513	CLA	O1A-CGA-O2A-C1
16	u	513	CLA	O1A-CGA-O2A-C1
23	p	606	LMU	C4'-C5'-C6'-O6'
16	G	1207	CLA	O1D-CGD-O2D-CED
16	X	511	CLA	O1D-CGD-O2D-CED
16	a	1114	CLA	O1D-CGD-O2D-CED
16	B	1218	CLA	C4-C3-C5-C6
16	G	1203	CLA	C4-C3-C5-C6
16	h	504	CLA	C4-C3-C5-C6
16	p	504	CLA	C4-C3-C5-C6
16	s	504	CLA	C4-C3-C5-C6
16	a	1115	CLA	C2-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	g	512	CLA	C2-C3-C5-C6
16	h	515	CLA	C2-C3-C5-C6
16	A	1801	CLA	CBA-CGA-O2A-C1
16	W	516	CLA	CBA-CGA-O2A-C1
16	f	1302	CLA	CBA-CGA-O2A-C1
16	o	513	CLA	CBA-CGA-O2A-C1
16	t	516	CLA	CBA-CGA-O2A-C1
16	u	513	CLA	CBA-CGA-O2A-C1
16	G	1216	CLA	CBD-CGD-O2D-CED
16	W	517	CLA	CBD-CGD-O2D-CED
16	a	1138	CLA	CBD-CGD-O2D-CED
16	A	1801	CLA	O1D-CGD-O2D-CED
16	G	1239	CLA	O1D-CGD-O2D-CED
16	W	503	CLA	O1D-CGD-O2D-CED
16	X	503	CLA	O1D-CGD-O2D-CED
16	Z	511	CLA	O1D-CGD-O2D-CED
16	g	516	CLA	O1D-CGD-O2D-CED
16	h	513	CLA	O1D-CGD-O2D-CED
16	q	506	CLA	O1D-CGD-O2D-CED
16	x	510	CLA	O1D-CGD-O2D-CED
16	B	1227	CLA	C2A-CAA-CBA-CGA
16	a	1127	CLA	C2A-CAA-CBA-CGA
16	r	508	CLA	C2A-CAA-CBA-CGA
16	t	510	CLA	O1A-CGA-O2A-C1
16	t	517	CLA	O1A-CGA-O2A-C1
16	w	515	CLA	O1A-CGA-O2A-C1
16	w	517	CLA	O1A-CGA-O2A-C1
16	A	1128	CLA	C3-C5-C6-C7
16	A	1133	CLA	C3-C5-C6-C7
16	B	1220	CLA	C3-C5-C6-C7
16	B	1223	CLA	C3-C5-C6-C7
16	G	1226	CLA	C3-C5-C6-C7
16	Z	517	CLA	C3-C5-C6-C7
16	a	1104	CLA	C3-C5-C6-C7
16	a	1115	CLA	C3-C5-C6-C7
16	a	1128	CLA	C3-C5-C6-C7
16	g	512	CLA	C3-C5-C6-C7
16	o	504	CLA	C3-C5-C6-C7
16	r	517	CLA	C3-C5-C6-C7
16	u	504	CLA	C3-C5-C6-C7
16	u	506	CLA	C3-C5-C6-C7
16	u	508	CLA	C3-C5-C6-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	v	515	CLA	C3-C5-C6-C7
16	w	510	CLA	C3-C5-C6-C7
16	x	508	CLA	C3-C5-C6-C7
16	y	506	CLA	C3-C5-C6-C7
13	A	849	LHG	C24-C23-O8-C6
14	A	4101	LMG	C29-C28-O8-C9
14	a	4201	LMG	C29-C28-O8-C9
16	A	1124	CLA	CBA-CGA-O2A-C1
16	A	1131	CLA	CBA-CGA-O2A-C1
16	A	1133	CLA	CBA-CGA-O2A-C1
16	B	1021	CLA	CBA-CGA-O2A-C1
16	B	1226	CLA	CBA-CGA-O2A-C1
16	B	1227	CLA	CBA-CGA-O2A-C1
16	G	1021	CLA	CBA-CGA-O2A-C1
16	G	1223	CLA	CBA-CGA-O2A-C1
16	G	1229	CLA	CBA-CGA-O2A-C1
16	H	1128	CLA	CBA-CGA-O2A-C1
16	H	1133	CLA	CBA-CGA-O2A-C1
16	U	1502	CLA	CBA-CGA-O2A-C1
16	W	508	CLA	CBA-CGA-O2A-C1
16	X	504	CLA	CBA-CGA-O2A-C1
16	Y	501	CLA	CBA-CGA-O2A-C1
16	Z	515	CLA	CBA-CGA-O2A-C1
16	Z	517	CLA	CBA-CGA-O2A-C1
16	b	1229	CLA	CBA-CGA-O2A-C1
16	g	501	CLA	CBA-CGA-O2A-C1
16	g	505	CLA	CBA-CGA-O2A-C1
16	g	508	CLA	CBA-CGA-O2A-C1
16	g	517	CLA	CBA-CGA-O2A-C1
16	h	510	CLA	CBA-CGA-O2A-C1
16	o	508	CLA	CBA-CGA-O2A-C1
16	o	509	CLA	CBA-CGA-O2A-C1
16	q	505	CLA	CBA-CGA-O2A-C1
16	r	505	CLA	CBA-CGA-O2A-C1
16	r	512	CLA	CBA-CGA-O2A-C1
16	s	515	CLA	CBA-CGA-O2A-C1
16	t	506	CLA	CBA-CGA-O2A-C1
16	t	510	CLA	CBA-CGA-O2A-C1
16	t	517	CLA	CBA-CGA-O2A-C1
16	u	504	CLA	CBA-CGA-O2A-C1
16	u	515	CLA	CBA-CGA-O2A-C1
16	v	502	CLA	CBA-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	v	508	CLA	CBA-CGA-O2A-C1
16	v	510	CLA	CBA-CGA-O2A-C1
16	x	512	CLA	CBA-CGA-O2A-C1
16	x	517	CLA	CBA-CGA-O2A-C1
16	y	502	CLA	CBA-CGA-O2A-C1
16	y	504	CLA	CBA-CGA-O2A-C1
16	y	508	CLA	CBA-CGA-O2A-C1
16	y	510	CLA	CBA-CGA-O2A-C1
16	y	512	CLA	CBA-CGA-O2A-C1
16	W	503	CLA	O1A-CGA-O2A-C1
14	B	848	LMG	O6-C5-C6-O5
16	Z	509	CLA	CBD-CGD-O2D-CED
20	l	4101	LMT	O5B-C5B-C6B-O6B
19	Z	604	BCR	C9-C10-C11-C12
19	b	4014	BCR	C13-C14-C15-C16
19	g	602	BCR	C9-C10-C11-C12
19	g	602	BCR	C19-C20-C21-C22
19	o	604	BCR	C9-C10-C11-C12
19	r	604	BCR	C13-C14-C15-C16
19	t	604	BCR	C9-C10-C11-C12
19	x	601	BCR	C19-C20-C21-C22
21	R	4020	ECH	C9-C10-C11-C12
24	q	601	LUT	C29-C30-C31-C32
24	w	601	LUT	C29-C30-C31-C32
16	B	1227	CLA	O1A-CGA-O2A-C1
16	G	1021	CLA	O1A-CGA-O2A-C1
16	H	1105	CLA	O1A-CGA-O2A-C1
16	W	517	CLA	O1A-CGA-O2A-C1
16	X	505	CLA	O1A-CGA-O2A-C1
16	X	508	CLA	O1A-CGA-O2A-C1
16	X	515	CLA	O1A-CGA-O2A-C1
16	Z	515	CLA	O1A-CGA-O2A-C1
16	Z	517	CLA	O1A-CGA-O2A-C1
16	b	1021	CLA	O1A-CGA-O2A-C1
16	g	510	CLA	O1A-CGA-O2A-C1
16	n	510	CLA	O1A-CGA-O2A-C1
16	n	517	CLA	O1A-CGA-O2A-C1
16	q	513	CLA	O1A-CGA-O2A-C1
16	q	517	CLA	O1A-CGA-O2A-C1
16	r	501	CLA	O1A-CGA-O2A-C1
16	s	501	CLA	O1A-CGA-O2A-C1
16	u	510	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	x	501	CLA	O1A-CGA-O2A-C1
16	x	517	CLA	O1A-CGA-O2A-C1
16	b	1023	CLA	O1D-CGD-O2D-CED
16	h	516	CLA	O1A-CGA-O2A-C1
20	H	4202	LMT	O5'-C5'-C6'-O6'
16	A	1121	CLA	O1D-CGD-O2D-CED
16	H	1116	CLA	O1D-CGD-O2D-CED
16	K	4002	CLA	O1D-CGD-O2D-CED
16	g	514	CLA	O1D-CGD-O2D-CED
16	k	4002	CLA	O1D-CGD-O2D-CED
16	r	505	CLA	O1D-CGD-O2D-CED
16	y	513	CLA	O1D-CGD-O2D-CED
16	A	1104	CLA	C3-C5-C6-C7
16	B	1012	CLA	C3-C5-C6-C7
16	G	1218	CLA	C3-C5-C6-C7
16	H	1106	CLA	C3-C5-C6-C7
16	H	1140	CLA	C3-C5-C6-C7
16	X	505	CLA	C3-C5-C6-C7
16	X	509	CLA	C3-C5-C6-C7
16	X	510	CLA	C3-C5-C6-C7
16	a	1109	CLA	C3-C5-C6-C7
16	b	1204	CLA	C3-C5-C6-C7
16	g	509	CLA	C3-C5-C6-C7
16	o	506	CLA	C3-C5-C6-C7
16	t	512	CLA	C3-C5-C6-C7
16	A	1107	CLA	CBD-CGD-O2D-CED
16	G	1203	CLA	CBD-CGD-O2D-CED
16	T	4004	CLA	CBD-CGD-O2D-CED
16	X	501	CLA	CBD-CGD-O2D-CED
16	q	517	CLA	CBD-CGD-O2D-CED
16	r	503	CLA	CBD-CGD-O2D-CED
16	x	503	CLA	CBD-CGD-O2D-CED
16	y	517	CLA	CBD-CGD-O2D-CED
23	p	606	LMU	C2B-C1B-O1B-C4'
13	g	605	LHG	O2-C2-C3-O3
13	r	605	LHG	O2-C2-C3-O3
16	B	1224	CLA	O1D-CGD-O2D-CED
16	H	1121	CLA	O1D-CGD-O2D-CED
16	W	502	CLA	O1D-CGD-O2D-CED
16	a	1121	CLA	O1D-CGD-O2D-CED
16	n	502	CLA	O1D-CGD-O2D-CED
16	v	508	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	x	517	CLA	O1D-CGD-O2D-CED
16	A	1115	CLA	CBA-CGA-O2A-C1
16	A	1128	CLA	CBA-CGA-O2A-C1
16	B	1239	CLA	CBA-CGA-O2A-C1
16	H	1105	CLA	CBA-CGA-O2A-C1
16	H	1115	CLA	CBA-CGA-O2A-C1
16	H	1122	CLA	CBA-CGA-O2A-C1
16	H	1131	CLA	CBA-CGA-O2A-C1
16	L	1501	CLA	CBA-CGA-O2A-C1
16	L	1502	CLA	CBA-CGA-O2A-C1
16	U	1501	CLA	CBA-CGA-O2A-C1
16	W	510	CLA	CBA-CGA-O2A-C1
16	W	511	CLA	CBA-CGA-O2A-C1
16	W	517	CLA	CBA-CGA-O2A-C1
16	Y	502	CLA	CBA-CGA-O2A-C1
16	a	1122	CLA	CBA-CGA-O2A-C1
16	a	1128	CLA	CBA-CGA-O2A-C1
16	a	1131	CLA	CBA-CGA-O2A-C1
16	b	1239	CLA	CBA-CGA-O2A-C1
16	g	510	CLA	CBA-CGA-O2A-C1
16	l	1502	CLA	CBA-CGA-O2A-C1
16	n	517	CLA	CBA-CGA-O2A-C1
16	o	504	CLA	CBA-CGA-O2A-C1
16	o	506	CLA	CBA-CGA-O2A-C1
16	r	517	CLA	CBA-CGA-O2A-C1
16	t	502	CLA	CBA-CGA-O2A-C1
16	u	505	CLA	CBA-CGA-O2A-C1
16	u	506	CLA	CBA-CGA-O2A-C1
16	u	510	CLA	CBA-CGA-O2A-C1
16	w	512	CLA	CBA-CGA-O2A-C1
16	w	517	CLA	CBA-CGA-O2A-C1
16	x	501	CLA	CBA-CGA-O2A-C1
16	x	506	CLA	CBA-CGA-O2A-C1
20	A	4202	LMT	O5'-C5'-C6'-O6'
20	a	4202	LMT	O5B-C5B-C6B-O6B
20	a	4202	LMT	O5'-C5'-C6'-O6'
23	q	605	LMU	O5'-C5'-C6'-O6'
16	A	1105	CLA	O1A-CGA-O2A-C1
16	B	1021	CLA	O1A-CGA-O2A-C1
16	G	1229	CLA	O1A-CGA-O2A-C1
16	H	1128	CLA	O1A-CGA-O2A-C1
16	a	1105	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	b	1229	CLA	O1A-CGA-O2A-C1
16	q	515	CLA	O1A-CGA-O2A-C1
16	y	502	CLA	O1A-CGA-O2A-C1
16	B	1239	CLA	O1D-CGD-O2D-CED
16	X	507	CLA	O1D-CGD-O2D-CED
16	Z	506	CLA	O1D-CGD-O2D-CED
16	b	1220	CLA	O1D-CGD-O2D-CED
16	r	510	CLA	O1D-CGD-O2D-CED
23	Y	606	LMU	O5'-C5'-C6'-O6'
16	Y	513	CLA	CBD-CGD-O2D-CED
16	h	502	CLA	CBD-CGD-O2D-CED
16	s	505	CLA	CBD-CGD-O2D-CED
16	H	1114	CLA	CBA-CGA-O2A-C1
16	A	1132	CLA	O1D-CGD-O2D-CED
23	x	606	LMU	C2B-C1B-O1B-C4'
14	A	4101	LMG	O10-C28-O8-C9
16	L	1502	CLA	O1A-CGA-O2A-C1
16	a	1122	CLA	O1A-CGA-O2A-C1
16	l	1502	CLA	O1A-CGA-O2A-C1
16	u	504	CLA	O1A-CGA-O2A-C1
16	w	512	CLA	O1A-CGA-O2A-C1
16	y	504	CLA	O1A-CGA-O2A-C1
16	y	512	CLA	O1A-CGA-O2A-C1
16	A	1111	CLA	O1D-CGD-O2D-CED
16	a	1120	CLA	O1D-CGD-O2D-CED
16	a	1122	CLA	O1D-CGD-O2D-CED
16	a	1140	CLA	C3-C5-C6-C7
16	u	509	CLA	C3-C5-C6-C7
16	A	1138	CLA	CBD-CGD-O2D-CED
16	H	1136	CLA	CBD-CGD-O2D-CED
16	j	1302	CLA	CBD-CGD-O2D-CED
16	o	501	CLA	CBD-CGD-O2D-CED
16	u	512	CLA	CBD-CGD-O2D-CED
16	x	509	CLA	CBD-CGD-O2D-CED
20	L	4101	LMT	O5B-C5B-C6B-O6B
16	q	502	CLA	O1D-CGD-O2D-CED
16	X	505	CLA	CBA-CGA-O2A-C1
16	X	508	CLA	CBA-CGA-O2A-C1
16	X	515	CLA	CBA-CGA-O2A-C1
16	q	517	CLA	CBA-CGA-O2A-C1
16	w	513	CLA	CBA-CGA-O2A-C1
16	w	515	CLA	CBA-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	H	1133	CLA	C4-C3-C5-C6
16	Y	509	CLA	C4-C3-C5-C6
16	Z	507	CLA	C4-C3-C5-C6
16	a	1110	CLA	C4-C3-C5-C6
16	G	1203	CLA	C2-C3-C5-C6
16	h	504	CLA	C2-C3-C5-C6
16	s	504	CLA	C2-C3-C5-C6
16	A	1115	CLA	O1A-CGA-O2A-C1
16	A	1124	CLA	O1A-CGA-O2A-C1
16	A	1128	CLA	O1A-CGA-O2A-C1
16	A	1131	CLA	O1A-CGA-O2A-C1
16	H	1115	CLA	O1A-CGA-O2A-C1
16	H	1122	CLA	O1A-CGA-O2A-C1
16	L	1501	CLA	O1A-CGA-O2A-C1
16	U	1502	CLA	O1A-CGA-O2A-C1
16	Y	501	CLA	O1A-CGA-O2A-C1
16	b	1239	CLA	O1A-CGA-O2A-C1
16	o	504	CLA	O1A-CGA-O2A-C1
16	o	509	CLA	O1A-CGA-O2A-C1
16	q	505	CLA	O1A-CGA-O2A-C1
16	r	517	CLA	O1A-CGA-O2A-C1
16	u	515	CLA	O1A-CGA-O2A-C1
16	A	1122	CLA	O1D-CGD-O2D-CED
16	w	510	CLA	O1D-CGD-O2D-CED
14	B	848	LMG	C4-C5-C6-O5
20	l	4101	LMT	C4B-C5B-C6B-O6B
16	A	1105	CLA	CBD-CGD-O2D-CED
16	A	1126	CLA	CBD-CGD-O2D-CED
16	A	1136	CLA	CBD-CGD-O2D-CED
16	B	1226	CLA	CBD-CGD-O2D-CED
16	G	1205	CLA	CBD-CGD-O2D-CED
16	G	1221	CLA	CBD-CGD-O2D-CED
16	G	1230	CLA	CBD-CGD-O2D-CED
16	H	1119	CLA	CBD-CGD-O2D-CED
16	b	1221	CLA	CBD-CGD-O2D-CED
16	w	508	CLA	CBD-CGD-O2D-CED
16	a	1801	CLA	O1D-CGD-O2D-CED
16	b	1232	CLA	O1D-CGD-O2D-CED
16	y	509	CLA	C5-C6-C7-C8
13	g	605	LHG	C5-C4-O6-P
23	s	606	LMU	O5'-C5'-C6'-O6'
20	L	4101	LMT	C4'-C5'-C6'-O6'

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1218	CLA	C2A-CAA-CBA-CGA
16	H	1127	CLA	C2A-CAA-CBA-CGA
16	X	516	CLA	C2A-CAA-CBA-CGA
16	Y	509	CLA	C2A-CAA-CBA-CGA
16	o	515	CLA	C2A-CAA-CBA-CGA
16	p	509	CLA	C2A-CAA-CBA-CGA
23	Y	606	LMU	O5B-C1B-O1B-C4'
23	p	606	LMU	O5B-C1B-O1B-C4'
23	x	606	LMU	O5B-C1B-O1B-C4'
16	G	1215	CLA	O1D-CGD-O2D-CED
16	a	1113	CLA	O1D-CGD-O2D-CED
16	b	1224	CLA	O1D-CGD-O2D-CED
16	h	504	CLA	O1D-CGD-O2D-CED
16	q	510	CLA	O1D-CGD-O2D-CED
16	G	1223	CLA	O1A-CGA-O2A-C1
16	H	1131	CLA	O1A-CGA-O2A-C1
16	W	511	CLA	O1A-CGA-O2A-C1
16	X	504	CLA	O1A-CGA-O2A-C1
16	a	1128	CLA	O1A-CGA-O2A-C1
16	a	1131	CLA	O1A-CGA-O2A-C1
16	o	506	CLA	O1A-CGA-O2A-C1
16	t	506	CLA	O1A-CGA-O2A-C1
16	x	506	CLA	O1A-CGA-O2A-C1
16	B	1211	CLA	C3-C5-C6-C7
14	A	4201	LMG	O6-C1-O1-C7
14	H	4201	LMG	O6-C1-O1-C7
14	a	4201	LMG	O6-C1-O1-C7
23	p	606	LMU	O5'-C5'-C6'-O6'
23	Z	605	LMU	C4'-C5'-C6'-O6'
23	Y	606	LMU	C2B-C1B-O1B-C4'
16	h	508	CLA	O1D-CGD-O2D-CED
16	B	1229	CLA	CBA-CGA-O2A-C1
16	G	1239	CLA	CBA-CGA-O2A-C1
16	U	1503	CLA	CBA-CGA-O2A-C1
16	W	512	CLA	CBA-CGA-O2A-C1
16	l	1501	CLA	CBA-CGA-O2A-C1
16	o	512	CLA	CBA-CGA-O2A-C1
16	p	501	CLA	CBA-CGA-O2A-C1
16	r	507	CLA	CBA-CGA-O2A-C1
16	u	509	CLA	CBA-CGA-O2A-C1
16	A	1139	CLA	CBD-CGD-O2D-CED
16	B	1210	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1220	CLA	CBD-CGD-O2D-CED
16	B	1227	CLA	CBD-CGD-O2D-CED
16	B	1230	CLA	CBD-CGD-O2D-CED
16	B	1238	CLA	CBD-CGD-O2D-CED
16	G	1214	CLA	CBD-CGD-O2D-CED
16	G	1218	CLA	CBD-CGD-O2D-CED
16	G	1224	CLA	CBD-CGD-O2D-CED
16	G	1228	CLA	CBD-CGD-O2D-CED
16	H	1107	CLA	CBD-CGD-O2D-CED
16	H	1111	CLA	CBD-CGD-O2D-CED
16	H	1122	CLA	CBD-CGD-O2D-CED
16	a	1107	CLA	CBD-CGD-O2D-CED
16	a	1128	CLA	CBD-CGD-O2D-CED
16	g	512	CLA	CBD-CGD-O2D-CED
16	n	503	CLA	CBD-CGD-O2D-CED
16	p	508	CLA	CBD-CGD-O2D-CED
16	u	502	CLA	CBD-CGD-O2D-CED
16	w	517	CLA	CBD-CGD-O2D-CED
16	x	502	CLA	CBD-CGD-O2D-CED
16	x	514	CLA	CBD-CGD-O2D-CED
16	y	514	CLA	CBD-CGD-O2D-CED
20	U	4101	LMT	O5B-C5B-C6B-O6B
23	g	606	LMU	O5'-C5'-C6'-O6'
16	o	516	CLA	CBA-CGA-O2A-C1
16	v	503	CLA	CBA-CGA-O2A-C1
16	B	1229	CLA	O1A-CGA-O2A-C1
16	U	1501	CLA	O1A-CGA-O2A-C1
16	W	510	CLA	O1A-CGA-O2A-C1
16	Y	502	CLA	O1A-CGA-O2A-C1
16	l	1501	CLA	O1A-CGA-O2A-C1
16	w	513	CLA	O1A-CGA-O2A-C1
16	b	1230	CLA	O1D-CGD-O2D-CED
23	q	605	LMU	C4'-C5'-C6'-O6'
16	A	1022	CLA	CBD-CGD-O2D-CED
16	G	1226	CLA	CBD-CGD-O2D-CED
16	H	1115	CLA	CBD-CGD-O2D-CED
16	H	1139	CLA	CBD-CGD-O2D-CED
16	Y	509	CLA	CBD-CGD-O2D-CED
16	o	515	CLA	CBD-CGD-O2D-CED
16	q	516	CLA	CBD-CGD-O2D-CED
16	r	502	CLA	CBD-CGD-O2D-CED
16	x	512	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	1106	CLA	C3-C5-C6-C7
16	n	506	CLA	C3-C5-C6-C7
16	b	1201	CLA	O1D-CGD-O2D-CED
20	U	4101	LMT	C4B-C5B-C6B-O6B
20	a	4202	LMT	C4'-C5'-C6'-O6'
23	p	606	LMU	C4B-C5B-C6B-O6B
19	Z	602	BCR	C19-C20-C21-C22
19	q	604	BCR	C9-C10-C11-C12
19	r	602	BCR	C9-C10-C11-C12
19	w	604	BCR	C9-C10-C11-C12
16	G	1239	CLA	O1A-CGA-O2A-C1
16	W	512	CLA	O1A-CGA-O2A-C1
16	p	501	CLA	O1A-CGA-O2A-C1
16	u	509	CLA	O1A-CGA-O2A-C1
13	R	103	LHG	O9-C7-O7-C5
13	B	4018	LHG	C1-C2-C3-O3
16	H	1132	CLA	O1D-CGD-O2D-CED
16	J	1302	CLA	O1D-CGD-O2D-CED
16	r	517	CLA	O1D-CGD-O2D-CED
14	A	4201	LMG	C29-C28-O8-C9
15	H	1011	CL0	CBA-CGA-O2A-C1
16	A	1122	CLA	CBA-CGA-O2A-C1
16	B	1202	CLA	CBA-CGA-O2A-C1
16	B	1224	CLA	CBA-CGA-O2A-C1
16	B	1225	CLA	CBA-CGA-O2A-C1
16	G	1202	CLA	CBA-CGA-O2A-C1
16	G	1222	CLA	CBA-CGA-O2A-C1
16	G	1224	CLA	CBA-CGA-O2A-C1
16	H	1106	CLA	CBA-CGA-O2A-C1
16	X	507	CLA	CBA-CGA-O2A-C1
16	X	509	CLA	CBA-CGA-O2A-C1
16	Y	507	CLA	CBA-CGA-O2A-C1
16	Y	510	CLA	CBA-CGA-O2A-C1
16	Y	514	CLA	CBA-CGA-O2A-C1
16	Z	509	CLA	CBA-CGA-O2A-C1
16	Z	514	CLA	CBA-CGA-O2A-C1
16	a	1124	CLA	CBA-CGA-O2A-C1
16	b	1202	CLA	CBA-CGA-O2A-C1
16	b	1221	CLA	CBA-CGA-O2A-C1
16	b	1224	CLA	CBA-CGA-O2A-C1
16	b	1235	CLA	CBA-CGA-O2A-C1
16	b	1238	CLA	CBA-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	g	504	CLA	CBA-CGA-O2A-C1
16	g	509	CLA	CBA-CGA-O2A-C1
16	h	507	CLA	CBA-CGA-O2A-C1
16	h	511	CLA	CBA-CGA-O2A-C1
16	n	506	CLA	CBA-CGA-O2A-C1
16	o	507	CLA	CBA-CGA-O2A-C1
16	p	510	CLA	CBA-CGA-O2A-C1
16	q	514	CLA	CBA-CGA-O2A-C1
16	s	510	CLA	CBA-CGA-O2A-C1
16	t	512	CLA	CBA-CGA-O2A-C1
16	v	505	CLA	CBA-CGA-O2A-C1
16	v	517	CLA	CBA-CGA-O2A-C1
16	w	509	CLA	CBA-CGA-O2A-C1
16	w	514	CLA	CBA-CGA-O2A-C1
16	x	509	CLA	CBA-CGA-O2A-C1
16	g	503	CLA	CBA-CGA-O2A-C1
16	Z	508	CLA	CBD-CGD-O2D-CED
16	p	515	CLA	CBD-CGD-O2D-CED
23	g	606	LMU	C4'-C5'-C6'-O6'
23	x	606	LMU	C4'-C5'-C6'-O6'
16	B	1232	CLA	O1D-CGD-O2D-CED
16	L	1501	CLA	O1D-CGD-O2D-CED
16	a	1132	CLA	O1D-CGD-O2D-CED
20	l	4101	LMT	C4'-C5'-C6'-O6'
16	B	1203	CLA	C4-C3-C5-C6
16	b	1203	CLA	C4-C3-C5-C6
16	B	1203	CLA	C2-C3-C5-C6
16	B	1218	CLA	C2-C3-C5-C6
16	H	1133	CLA	C2-C3-C5-C6
16	Y	509	CLA	C2-C3-C5-C6
16	Z	507	CLA	C2-C3-C5-C6
16	b	1203	CLA	C2-C3-C5-C6
16	p	504	CLA	C2-C3-C5-C6
16	H	1103	CLA	C3-C5-C6-C7
16	b	1229	CLA	C3-C5-C6-C7
16	q	507	CLA	C3-C5-C6-C7
16	x	510	CLA	C3-C5-C6-C7
16	B	1228	CLA	CBD-CGD-O2D-CED
16	G	1201	CLA	CBD-CGD-O2D-CED
16	H	1128	CLA	CBD-CGD-O2D-CED
16	q	508	CLA	CBD-CGD-O2D-CED
16	A	1106	CLA	C11-C12-C13-C14

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	1237	CLA	C11-C10-C8-C9
16	G	1211	CLA	C11-C12-C13-C14
16	G	1221	CLA	C14-C13-C15-C16
16	H	1101	CLA	C14-C13-C15-C16
16	H	1140	CLA	C6-C7-C8-C9
16	X	504	CLA	C11-C10-C8-C9
16	Y	511	CLA	C14-C13-C15-C16
16	a	1106	CLA	C11-C12-C13-C14
16	a	1237	CLA	C11-C10-C8-C9
16	b	1023	CLA	C11-C12-C13-C14
16	g	504	CLA	C11-C10-C8-C9
16	g	506	CLA	C6-C7-C8-C9
16	h	512	CLA	C11-C12-C13-C14
16	h	515	CLA	C11-C10-C8-C9
16	p	511	CLA	C14-C13-C15-C16
16	r	504	CLA	C11-C10-C8-C9
16	r	506	CLA	C6-C7-C8-C9
16	s	511	CLA	C14-C13-C15-C16
16	v	515	CLA	C11-C10-C8-C9
16	v	515	CLA	C11-C12-C13-C14
16	x	504	CLA	C11-C10-C8-C9
16	x	506	CLA	C6-C7-C8-C9
16	y	510	CLA	C6-C7-C8-C9
20	A	4202	LMT	C4'-C5'-C6'-O6'
20	H	4202	LMT	C4'-C5'-C6'-O6'
16	g	510	CLA	O1D-CGD-O2D-CED
16	p	516	CLA	O1D-CGD-O2D-CED
16	q	512	CLA	O1D-CGD-O2D-CED
16	t	516	CLA	O1D-CGD-O2D-CED
14	A	4201	LMG	C2-C1-O1-C7
14	H	4201	LMG	C2-C1-O1-C7
14	a	4201	LMG	C2-C1-O1-C7
23	Z	605	LMU	C2'-C1'-O1'-C1
23	w	605	LMU	C2'-C1'-O1'-C1
16	p	503	CLA	CBA-CGA-O2A-C1
16	t	513	CLA	CBA-CGA-O2A-C1
13	X	605	LHG	O2-C2-C3-O3
13	u	605	LHG	O2-C2-C3-O3
16	B	1231	CLA	O1D-CGD-O2D-CED
16	Z	512	CLA	O1D-CGD-O2D-CED
16	a	1126	CLA	O1D-CGD-O2D-CED
16	g	505	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	h	511	CLA	O1D-CGD-O2D-CED
16	n	517	CLA	O1D-CGD-O2D-CED
16	w	502	CLA	CBA-CGA-O2A-C1
16	G	1222	CLA	O1A-CGA-O2A-C1
16	Z	514	CLA	O1A-CGA-O2A-C1
16	o	507	CLA	O1A-CGA-O2A-C1
16	o	512	CLA	O1A-CGA-O2A-C1
16	q	514	CLA	O1A-CGA-O2A-C1
16	v	505	CLA	O1A-CGA-O2A-C1
16	A	1128	CLA	CBD-CGD-O2D-CED
16	H	1120	CLA	CBD-CGD-O2D-CED
16	b	1208	CLA	O1D-CGD-O2D-CED
16	b	1235	CLA	O1D-CGD-O2D-CED
16	v	509	CLA	O1D-CGD-O2D-CED
19	A	4002	BCR	C11-C12-C13-C35
19	A	4008	BCR	C7-C8-C9-C34
19	A	4008	BCR	C37-C22-C23-C24
19	A	4011	BCR	C7-C8-C9-C34
19	B	4004	BCR	C7-C8-C9-C34
19	B	4009	BCR	C36-C18-C19-C20
19	B	4010	BCR	C11-C12-C13-C35
19	B	4014	BCR	C36-C18-C19-C20
19	F	4016	BCR	C7-C8-C9-C34
19	F	4016	BCR	C37-C22-C23-C24
19	G	4004	BCR	C7-C8-C9-C34
19	G	4004	BCR	C37-C22-C23-C24
19	G	4005	BCR	C7-C8-C9-C34
19	G	4010	BCR	C37-C22-C23-C24
19	H	4002	BCR	C11-C12-C13-C35
19	H	4002	BCR	C37-C22-C23-C24
19	H	4003	BCR	C37-C22-C23-C24
19	H	4007	BCR	C37-C22-C23-C24
19	H	4008	BCR	C37-C22-C23-C24
19	H	4011	BCR	C7-C8-C9-C34
19	J	4013	BCR	C37-C22-C23-C24
19	J	4015	BCR	C7-C8-C9-C34
19	K	4001	BCR	C7-C8-C9-C34
19	L	4019	BCR	C7-C8-C9-C34
19	L	4019	BCR	C37-C22-C23-C24
19	L	4022	BCR	C7-C8-C9-C34
19	Q	4016	BCR	C7-C8-C9-C34
19	Q	4016	BCR	C37-C22-C23-C24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	R	4018	BCR	C37-C22-C23-C24
19	U	4019	BCR	C7-C8-C9-C34
19	W	601	BCR	C7-C8-C9-C34
19	W	604	BCR	C7-C8-C9-C34
19	X	601	BCR	C7-C8-C9-C34
19	X	601	BCR	C37-C22-C23-C24
19	X	603	BCR	C7-C8-C9-C34
19	X	604	BCR	C37-C22-C23-C24
19	Y	601	BCR	C37-C22-C23-C24
19	Y	602	BCR	C7-C8-C9-C34
19	a	4002	BCR	C7-C8-C9-C34
19	a	4003	BCR	C37-C22-C23-C24
19	b	4004	BCR	C7-C8-C9-C34
19	b	4009	BCR	C36-C18-C19-C20
19	b	4010	BCR	C37-C22-C23-C24
19	b	4014	BCR	C7-C8-C9-C34
19	b	4014	BCR	C37-C22-C23-C24
19	g	602	BCR	C11-C12-C13-C35
19	g	603	BCR	C7-C8-C9-C34
19	g	603	BCR	C11-C12-C13-C35
19	g	604	BCR	C11-C12-C13-C35
19	h	603	BCR	C37-C22-C23-C24
19	k	4001	BCR	C37-C22-C23-C24
19	n	601	BCR	C7-C8-C9-C34
19	n	603	BCR	C7-C8-C9-C34
19	o	602	BCR	C7-C8-C9-C34
19	o	604	BCR	C7-C8-C9-C34
19	o	604	BCR	C37-C22-C23-C24
19	p	601	BCR	C7-C8-C9-C34
19	p	604	BCR	C11-C12-C13-C35
19	q	602	BCR	C7-C8-C9-C34
19	q	602	BCR	C37-C22-C23-C24
19	q	604	BCR	C7-C8-C9-C34
19	r	603	BCR	C11-C12-C13-C35
19	r	604	BCR	C11-C12-C13-C35
19	s	601	BCR	C7-C8-C9-C34
19	s	602	BCR	C37-C22-C23-C24
19	s	604	BCR	C37-C22-C23-C24
19	t	601	BCR	C7-C8-C9-C34
19	u	604	BCR	C7-C8-C9-C34
19	u	604	BCR	C37-C22-C23-C24
19	v	603	BCR	C37-C22-C23-C24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	v	604	BCR	C37-C22-C23-C24
19	w	602	BCR	C7-C8-C9-C34
19	w	602	BCR	C37-C22-C23-C24
19	w	603	BCR	C7-C8-C9-C34
19	w	604	BCR	C7-C8-C9-C34
19	x	601	BCR	C7-C8-C9-C34
19	x	601	BCR	C37-C22-C23-C24
19	x	602	BCR	C7-C8-C9-C34
19	x	604	BCR	C7-C8-C9-C34
19	x	604	BCR	C11-C12-C13-C35
19	y	601	BCR	C37-C22-C23-C24
19	y	603	BCR	C37-C22-C23-C24
19	y	604	BCR	C37-C22-C23-C24
21	G	4006	ECH	C37-C22-C23-C24
21	M	4021	ECH	C7-C8-C9-C34
21	R	4020	ECH	C7-C8-C9-C34
21	b	4006	ECH	C37-C22-C23-C24
21	i	4020	ECH	C7-C8-C9-C34
21	i	4020	ECH	C11-C12-C13-C35
21	m	4021	ECH	C37-C22-C23-C24
24	Z	601	LUT	C31-C32-C33-C40
20	L	4101	LMT	O5'-C5'-C6'-O6'
19	B	4009	BCR	C17-C18-C19-C20
19	G	4004	BCR	C7-C8-C9-C10
19	G	4004	BCR	C21-C22-C23-C24
19	H	4008	BCR	C7-C8-C9-C10
19	H	4008	BCR	C21-C22-C23-C24
19	K	4001	BCR	C7-C8-C9-C10
19	L	4019	BCR	C21-C22-C23-C24
19	S	4013	BCR	C21-C22-C23-C24
19	T	4001	BCR	C7-C8-C9-C10
19	X	601	BCR	C7-C8-C9-C10
19	Y	601	BCR	C21-C22-C23-C24
19	Y	604	BCR	C7-C8-C9-C10
19	Z	602	BCR	C7-C8-C9-C10
19	b	4004	BCR	C7-C8-C9-C10
19	b	4009	BCR	C17-C18-C19-C20
19	g	602	BCR	C11-C12-C13-C14
19	g	602	BCR	C21-C22-C23-C24
19	h	601	BCR	C21-C22-C23-C24
19	h	604	BCR	C7-C8-C9-C10
19	i	4018	BCR	C7-C8-C9-C10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	j	4015	BCR	C7-C8-C9-C10
19	k	4001	BCR	C7-C8-C9-C10
19	l	4019	BCR	C7-C8-C9-C10
19	l	4019	BCR	C21-C22-C23-C24
19	n	603	BCR	C7-C8-C9-C10
19	n	604	BCR	C7-C8-C9-C10
19	o	601	BCR	C7-C8-C9-C10
19	o	604	BCR	C7-C8-C9-C10
19	p	602	BCR	C7-C8-C9-C10
19	q	602	BCR	C7-C8-C9-C10
19	r	602	BCR	C7-C8-C9-C10
19	s	602	BCR	C7-C8-C9-C10
19	s	603	BCR	C7-C8-C9-C10
19	u	601	BCR	C21-C22-C23-C24
19	v	604	BCR	C7-C8-C9-C10
19	w	602	BCR	C21-C22-C23-C24
19	x	601	BCR	C21-C22-C23-C24
19	y	604	BCR	C7-C8-C9-C10
21	M	4021	ECH	C7-C8-C9-C10
21	R	4020	ECH	C7-C8-C9-C10
21	V	4021	ECH	C11-C12-C13-C14
21	m	4021	ECH	C11-C12-C13-C14
16	A	1132	CLA	C2A-CAA-CBA-CGA
16	B	1217	CLA	C2A-CAA-CBA-CGA
16	B	1228	CLA	C2A-CAA-CBA-CGA
16	H	1106	CLA	C2A-CAA-CBA-CGA
16	H	1132	CLA	C2A-CAA-CBA-CGA
16	L	1501	CLA	C2A-CAA-CBA-CGA
16	a	1118	CLA	C2A-CAA-CBA-CGA
16	a	1129	CLA	C2A-CAA-CBA-CGA
16	b	1218	CLA	C2A-CAA-CBA-CGA
16	b	1228	CLA	C2A-CAA-CBA-CGA
16	g	505	CLA	C2A-CAA-CBA-CGA
16	h	503	CLA	C2A-CAA-CBA-CGA
16	q	517	CLA	C2A-CAA-CBA-CGA
16	x	508	CLA	C2A-CAA-CBA-CGA
13	R	103	LHG	C7-C8-C9-C10
16	T	4002	CLA	O1D-CGD-O2D-CED
16	A	1122	CLA	O1A-CGA-O2A-C1
16	X	507	CLA	O1A-CGA-O2A-C1
16	a	1124	CLA	O1A-CGA-O2A-C1
16	b	1235	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	p	510	CLA	O1A-CGA-O2A-C1
16	w	514	CLA	O1A-CGA-O2A-C1
16	G	1225	CLA	C13-C15-C16-C17
16	A	1134	CLA	CBD-CGD-O2D-CED
14	F	4017	LMG	C11-C10-O7-C8
14	Q	4017	LMG	C11-C10-O7-C8
16	A	1129	CLA	CBA-CGA-O2A-C1
23	x	606	LMU	C4B-C5B-C6B-O6B
13	g	605	LHG	C24-C23-O8-C6
16	B	1228	CLA	CBA-CGA-O2A-C1
16	H	1124	CLA	CBA-CGA-O2A-C1
16	H	1140	CLA	CBA-CGA-O2A-C1
16	W	506	CLA	CBA-CGA-O2A-C1
16	a	1140	CLA	CBA-CGA-O2A-C1
16	r	509	CLA	CBA-CGA-O2A-C1
16	s	502	CLA	CBA-CGA-O2A-C1
16	x	502	CLA	CBA-CGA-O2A-C1
16	x	507	CLA	CBA-CGA-O2A-C1
16	G	1214	CLA	C5-C6-C7-C8
16	a	1237	CLA	C13-C15-C16-C17
13	I	103	LHG	C23-C24-C25-C26
16	B	1220	CLA	C2-C1-O2A-CGA
16	B	1228	CLA	C2-C1-O2A-CGA
16	G	1228	CLA	C2-C1-O2A-CGA
16	L	1503	CLA	C2-C1-O2A-CGA
16	t	501	CLA	C2-C1-O2A-CGA
16	h	511	CLA	O1A-CGA-O2A-C1
16	w	509	CLA	O1A-CGA-O2A-C1
16	B	1201	CLA	O1D-CGD-O2D-CED
16	B	1216	CLA	O1D-CGD-O2D-CED
16	H	1117	CLA	O1D-CGD-O2D-CED
16	H	1126	CLA	O1D-CGD-O2D-CED
16	Y	517	CLA	O1D-CGD-O2D-CED
16	a	1117	CLA	O1D-CGD-O2D-CED
16	s	516	CLA	O1D-CGD-O2D-CED
16	w	516	CLA	O1D-CGD-O2D-CED
20	U	4101	LMT	C4'-C5'-C6'-O6'
16	p	510	CLA	CBD-CGD-O2D-CED
16	A	1022	CLA	C8-C10-C11-C12
16	A	1125	CLA	C8-C10-C11-C12
16	B	1221	CLA	C8-C10-C11-C12
16	G	1202	CLA	C5-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	Y	509	CLA	C10-C11-C12-C13
16	a	1101	CLA	C15-C16-C17-C18
16	a	1106	CLA	C5-C6-C7-C8
16	b	1202	CLA	C5-C6-C7-C8
13	G	4018	LHG	O1-C1-C2-O2
16	q	510	CLA	C3-C5-C6-C7
16	x	512	CLA	C3-C5-C6-C7
16	Y	505	CLA	O1D-CGD-O2D-CED
16	s	510	CLA	O1A-CGA-O2A-C1
16	x	509	CLA	O1A-CGA-O2A-C1
16	A	1101	CLA	C15-C16-C17-C18
16	s	509	CLA	C5-C6-C7-C8
17	B	2002	PQN	C18-C20-C21-C22
16	T	4003	CLA	CBD-CGD-O2D-CED
16	X	509	CLA	CBD-CGD-O2D-CED
16	b	1222	CLA	CBD-CGD-O2D-CED
16	g	502	CLA	CBD-CGD-O2D-CED
23	x	606	LMU	O5'-C5'-C6'-O6'
14	b	848	LMG	C4-C5-C6-O5
16	A	1104	CLA	C11-C10-C8-C7
16	A	1139	CLA	C11-C10-C8-C7
16	H	1136	CLA	C11-C10-C8-C7
16	H	1139	CLA	C11-C10-C8-C7
16	Z	507	CLA	C6-C7-C8-C10
16	a	1104	CLA	C11-C10-C8-C7
16	b	1210	CLA	C11-C10-C8-C7
16	v	505	CLA	C11-C12-C13-C15
16	B	1206	CLA	O1D-CGD-O2D-CED
16	A	1140	CLA	CBA-CGA-O2A-C1
16	H	1123	CLA	CBA-CGA-O2A-C1
16	h	512	CLA	CBA-CGA-O2A-C1
16	p	507	CLA	CBA-CGA-O2A-C1
16	q	509	CLA	CBA-CGA-O2A-C1
16	x	514	CLA	CBA-CGA-O2A-C1
16	r	504	CLA	C15-C16-C17-C18
16	t	517	CLA	C5-C6-C7-C8
16	f	1302	CLA	O1D-CGD-O2D-CED
16	l	1501	CLA	O1D-CGD-O2D-CED
13	R	103	LHG	C23-C24-C25-C26
14	G	848	LMG	C28-C29-C30-C31
19	G	4005	BCR	C19-C20-C21-C22
19	H	4011	BCR	C19-C20-C21-C22

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	W	603	BCR	C9-C10-C11-C12
19	X	604	BCR	C15-C16-C17-C18
19	g	604	BCR	C9-C10-C11-C12
19	n	603	BCR	C9-C10-C11-C12
19	r	604	BCR	C9-C10-C11-C12
19	u	604	BCR	C9-C10-C11-C12
19	u	604	BCR	C15-C16-C17-C18
19	v	603	BCR	C9-C10-C11-C12
19	x	603	BCR	C15-C16-C17-C18
19	x	604	BCR	C9-C10-C11-C12
16	G	1224	CLA	O1A-CGA-O2A-C1
16	a	1116	CLA	O1D-CGD-O2D-CED
16	r	512	CLA	O1D-CGD-O2D-CED
16	s	502	CLA	O1D-CGD-O2D-CED
16	B	1235	CLA	C3-C5-C6-C7
16	G	1235	CLA	C3-C5-C6-C7
16	Z	506	CLA	C3-C5-C6-C7
16	x	509	CLA	C3-C5-C6-C7
16	Y	512	CLA	C10-C11-C12-C13
16	h	508	CLA	C5-C6-C7-C8
16	q	509	CLA	C10-C11-C12-C13
16	v	504	CLA	C10-C11-C12-C13
17	G	2002	PQN	C18-C20-C21-C22
16	A	1114	CLA	CBA-CGA-O2A-C1
16	b	1231	CLA	O1D-CGD-O2D-CED
23	Z	605	LMU	O5'-C5'-C6'-O6'
13	B	4018	LHG	C7-C8-C9-C10
13	b	4018	LHG	C7-C8-C9-C10
13	x	605	LHG	C23-C24-C25-C26
13	A	849	LHG	O10-C23-O8-C6
16	U	1503	CLA	O1A-CGA-O2A-C1
16	X	509	CLA	O1A-CGA-O2A-C1
16	Y	507	CLA	O1A-CGA-O2A-C1
16	Y	510	CLA	O1A-CGA-O2A-C1
16	Y	514	CLA	O1A-CGA-O2A-C1
16	b	1224	CLA	O1A-CGA-O2A-C1
16	b	1238	CLA	O1A-CGA-O2A-C1
16	g	504	CLA	O1A-CGA-O2A-C1
16	t	512	CLA	O1A-CGA-O2A-C1
16	v	517	CLA	O1A-CGA-O2A-C1
16	U	1501	CLA	O1D-CGD-O2D-CED
16	b	1228	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	r	509	CLA	O1D-CGD-O2D-CED
16	y	509	CLA	O1D-CGD-O2D-CED
16	A	1103	CLA	C15-C16-C17-C18
16	A	1104	CLA	C10-C11-C12-C13
16	A	1139	CLA	C10-C11-C12-C13
16	B	1023	CLA	C13-C15-C16-C17
16	B	1235	CLA	C8-C10-C11-C12
16	G	1229	CLA	C5-C6-C7-C8
16	H	1101	CLA	C13-C15-C16-C17
16	H	1103	CLA	C13-C15-C16-C17
16	H	1106	CLA	C5-C6-C7-C8
16	H	1128	CLA	C8-C10-C11-C12
16	L	1501	CLA	C10-C11-C12-C13
16	Y	509	CLA	C5-C6-C7-C8
16	Z	506	CLA	C5-C6-C7-C8
16	g	515	CLA	C8-C10-C11-C12
16	o	504	CLA	C5-C6-C7-C8
16	w	504	CLA	C13-C15-C16-C17
23	x	606	LMU	O5B-C5B-C6B-O6B
16	A	1105	CLA	C2A-CAA-CBA-CGA
16	A	1106	CLA	C2A-CAA-CBA-CGA
16	A	1118	CLA	C2A-CAA-CBA-CGA
16	A	1127	CLA	C2A-CAA-CBA-CGA
16	B	1229	CLA	C2A-CAA-CBA-CGA
16	G	1217	CLA	C2A-CAA-CBA-CGA
16	G	1238	CLA	C2A-CAA-CBA-CGA
16	H	1105	CLA	C2A-CAA-CBA-CGA
16	U	1501	CLA	C2A-CAA-CBA-CGA
16	W	501	CLA	C2A-CAA-CBA-CGA
16	W	504	CLA	C2A-CAA-CBA-CGA
16	W	505	CLA	C2A-CAA-CBA-CGA
16	W	517	CLA	C2A-CAA-CBA-CGA
16	X	515	CLA	C2A-CAA-CBA-CGA
16	Z	503	CLA	C2A-CAA-CBA-CGA
16	Z	517	CLA	C2A-CAA-CBA-CGA
16	a	1105	CLA	C2A-CAA-CBA-CGA
16	a	1106	CLA	C2A-CAA-CBA-CGA
16	a	1132	CLA	C2A-CAA-CBA-CGA
16	b	1211	CLA	C2A-CAA-CBA-CGA
16	b	1223	CLA	C2A-CAA-CBA-CGA
16	b	1238	CLA	C2A-CAA-CBA-CGA
16	n	505	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	n	515	CLA	C2A-CAA-CBA-CGA
16	n	517	CLA	C2A-CAA-CBA-CGA
16	o	505	CLA	C2A-CAA-CBA-CGA
16	o	506	CLA	C2A-CAA-CBA-CGA
16	q	503	CLA	C2A-CAA-CBA-CGA
16	r	504	CLA	C2A-CAA-CBA-CGA
16	r	505	CLA	C2A-CAA-CBA-CGA
16	r	517	CLA	C2A-CAA-CBA-CGA
16	s	501	CLA	C2A-CAA-CBA-CGA
16	s	509	CLA	C2A-CAA-CBA-CGA
16	t	504	CLA	C2A-CAA-CBA-CGA
16	t	505	CLA	C2A-CAA-CBA-CGA
16	t	506	CLA	C2A-CAA-CBA-CGA
16	t	515	CLA	C2A-CAA-CBA-CGA
16	t	517	CLA	C2A-CAA-CBA-CGA
16	u	515	CLA	C2A-CAA-CBA-CGA
16	v	504	CLA	C2A-CAA-CBA-CGA
16	w	515	CLA	C2A-CAA-CBA-CGA
16	x	504	CLA	C2A-CAA-CBA-CGA
16	x	517	CLA	C2A-CAA-CBA-CGA
16	y	503	CLA	C2A-CAA-CBA-CGA
19	A	4008	BCR	C18-C19-C20-C21
19	A	4011	BCR	C10-C11-C12-C13
19	G	4014	BCR	C18-C19-C20-C21
19	H	4011	BCR	C18-C19-C20-C21
19	K	4001	BCR	C10-C11-C12-C13
19	T	4001	BCR	C10-C11-C12-C13
19	X	602	BCR	C18-C19-C20-C21
19	a	4011	BCR	C10-C11-C12-C13
19	a	4011	BCR	C18-C19-C20-C21
19	b	4004	BCR	C18-C19-C20-C21
19	b	4005	BCR	C18-C19-C20-C21
19	k	4001	BCR	C10-C11-C12-C13
19	l	4022	BCR	C10-C11-C12-C13
19	o	604	BCR	C10-C11-C12-C13
19	r	603	BCR	C18-C19-C20-C21
19	t	603	BCR	C10-C11-C12-C13
19	u	603	BCR	C18-C19-C20-C21
16	A	1130	CLA	C8-C10-C11-C12
16	H	1101	CLA	C8-C10-C11-C12
16	H	1109	CLA	C13-C15-C16-C17
16	H	1126	CLA	C15-C16-C17-C18

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	L	1503	CLA	C15-C16-C17-C18
16	W	515	CLA	C10-C11-C12-C13
16	X	506	CLA	C8-C10-C11-C12
16	X	508	CLA	C5-C6-C7-C8
16	Z	504	CLA	C13-C15-C16-C17
16	a	1101	CLA	C13-C15-C16-C17
16	b	1021	CLA	C5-C6-C7-C8
16	b	1221	CLA	C10-C11-C12-C13
16	h	507	CLA	C15-C16-C17-C18
16	n	515	CLA	C10-C11-C12-C13
16	o	517	CLA	C5-C6-C7-C8
16	p	511	CLA	C8-C10-C11-C12
16	r	512	CLA	C5-C6-C7-C8
16	s	504	CLA	C15-C16-C17-C18
16	s	511	CLA	C8-C10-C11-C12
16	s	512	CLA	C10-C11-C12-C13
16	v	508	CLA	C5-C6-C7-C8
16	v	515	CLA	C5-C6-C7-C8
16	y	512	CLA	C5-C6-C7-C8
20	a	4202	LMT	C4B-C5B-C6B-O6B
23	x	606	LMU	O1'-C1-C2-C3
13	A	849	LHG	C23-C24-C25-C26
13	g	605	LHG	C23-C24-C25-C26
13	i	103	LHG	C23-C24-C25-C26
13	r	605	LHG	C23-C24-C25-C26
13	s	605	LHG	C23-C24-C25-C26
14	B	848	LMG	C28-C29-C30-C31
16	W	505	CLA	O1D-CGD-O2D-CED
16	b	1240	CLA	CBA-CGA-O2A-C1
16	s	503	CLA	CBA-CGA-O2A-C1
16	B	1202	CLA	O1A-CGA-O2A-C1
16	B	1225	CLA	O1A-CGA-O2A-C1
16	G	1202	CLA	O1A-CGA-O2A-C1
16	Z	509	CLA	O1A-CGA-O2A-C1
16	g	509	CLA	O1A-CGA-O2A-C1
16	h	507	CLA	O1A-CGA-O2A-C1
16	n	506	CLA	O1A-CGA-O2A-C1
16	A	1139	CLA	C3-C5-C6-C7
14	G	848	LMG	O6-C1-O1-C7
14	b	848	LMG	O6-C1-O1-C7
19	A	4002	BCR	C6-C7-C8-C9
19	B	4005	BCR	C6-C7-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	h	604	BCR	C6-C7-C8-C9
19	j	4012	BCR	C6-C7-C8-C9
19	t	603	BCR	C6-C7-C8-C9
19	v	604	BCR	C6-C7-C8-C9
19	w	604	BCR	C22-C23-C24-C25
19	y	604	BCR	C6-C7-C8-C9
23	Z	605	LMU	O5'-C1'-O1'-C1
23	w	605	LMU	O5'-C1'-O1'-C1
23	x	606	LMU	O5'-C1'-O1'-C1
23	p	606	LMU	O5B-C5B-C6B-O6B
16	A	1101	CLA	C13-C15-C16-C17
16	A	1106	CLA	C5-C6-C7-C8
16	A	1131	CLA	C5-C6-C7-C8
16	B	1206	CLA	C10-C11-C12-C13
16	H	1013	CLA	C13-C15-C16-C17
16	H	1125	CLA	C5-C6-C7-C8
16	H	1128	CLA	C10-C11-C12-C13
16	H	1139	CLA	C10-C11-C12-C13
16	X	504	CLA	C8-C10-C11-C12
16	Y	504	CLA	C15-C16-C17-C18
16	Y	511	CLA	C5-C6-C7-C8
16	Z	504	CLA	C5-C6-C7-C8
16	Z	505	CLA	C8-C10-C11-C12
16	Z	509	CLA	C10-C11-C12-C13
16	a	1125	CLA	C5-C6-C7-C8
16	a	1125	CLA	C8-C10-C11-C12
16	a	1140	CLA	C5-C6-C7-C8
16	b	1229	CLA	C5-C6-C7-C8
16	b	1235	CLA	C8-C10-C11-C12
16	b	1238	CLA	C8-C10-C11-C12
16	h	506	CLA	C5-C6-C7-C8
16	h	512	CLA	C5-C6-C7-C8
16	o	506	CLA	C8-C10-C11-C12
16	o	508	CLA	C5-C6-C7-C8
16	p	509	CLA	C5-C6-C7-C8
16	q	506	CLA	C5-C6-C7-C8
16	t	515	CLA	C10-C11-C12-C13
16	u	508	CLA	C5-C6-C7-C8
16	y	511	CLA	C10-C11-C12-C13
13	B	4018	LHG	O2-C2-C3-O3
13	I	103	LHG	O2-C2-C3-O3
13	b	4018	LHG	O2-C2-C3-O3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	x	605	LHG	O2-C2-C3-O3
13	H	849	LHG	C24-C23-O8-C6
16	G	1228	CLA	CBA-CGA-O2A-C1
16	B	1224	CLA	O1A-CGA-O2A-C1
16	H	1106	CLA	O1A-CGA-O2A-C1
16	b	1202	CLA	O1A-CGA-O2A-C1
16	b	1221	CLA	O1A-CGA-O2A-C1
16	r	507	CLA	O1A-CGA-O2A-C1
16	w	502	CLA	O1A-CGA-O2A-C1
16	H	1140	CLA	C5-C6-C7-C8
16	W	506	CLA	C8-C10-C11-C12
16	a	1103	CLA	C15-C16-C17-C18
16	b	1023	CLA	C13-C15-C16-C17
16	b	1205	CLA	C13-C15-C16-C17
16	n	512	CLA	C10-C11-C12-C13
16	n	517	CLA	C5-C6-C7-C8
16	p	504	CLA	C15-C16-C17-C18
16	q	504	CLA	C8-C10-C11-C12
16	q	504	CLA	C13-C15-C16-C17
16	r	505	CLA	C5-C6-C7-C8
23	g	606	LMU	O1'-C1-C2-C3
16	G	1216	CLA	O1D-CGD-O2D-CED
16	T	4004	CLA	O1D-CGD-O2D-CED
16	p	516	CLA	CBA-CGA-O2A-C1
16	t	503	CLA	CBA-CGA-O2A-C1
16	H	1139	CLA	C3-C5-C6-C7
16	W	517	CLA	C3-C5-C6-C7
16	b	1207	CLA	C3-C5-C6-C7
16	A	1107	CLA	O1D-CGD-O2D-CED
16	W	517	CLA	O1D-CGD-O2D-CED
16	Z	509	CLA	O1D-CGD-O2D-CED
16	a	1138	CLA	O1D-CGD-O2D-CED
16	p	505	CLA	O1D-CGD-O2D-CED
16	A	1105	CLA	C5-C6-C7-C8
16	A	1127	CLA	C8-C10-C11-C12
16	A	1128	CLA	C10-C11-C12-C13
16	G	1023	CLA	C15-C16-C17-C18
16	H	1022	CLA	C15-C16-C17-C18
16	H	1103	CLA	C15-C16-C17-C18
16	H	1105	CLA	C5-C6-C7-C8
16	U	1501	CLA	C10-C11-C12-C13
16	Y	511	CLA	C8-C10-C11-C12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1105	CLA	C5-C6-C7-C8
16	a	1109	CLA	C15-C16-C17-C18
16	q	512	CLA	C10-C11-C12-C13
16	t	505	CLA	C15-C16-C17-C18
16	u	505	CLA	C5-C6-C7-C8
16	u	506	CLA	C8-C10-C11-C12
16	y	515	CLA	C5-C6-C7-C8
20	l	4101	LMT	O5'-C5'-C6'-O6'
15	H	1011	CL0	O1A-CGA-O2A-C1
16	W	506	CLA	O1A-CGA-O2A-C1
16	s	502	CLA	O1A-CGA-O2A-C1
16	a	1110	CLA	C2-C3-C5-C6
13	G	4018	LHG	C23-C24-C25-C26
13	a	851	LHG	C7-C8-C9-C10
16	G	1203	CLA	O1D-CGD-O2D-CED
16	X	501	CLA	O1D-CGD-O2D-CED
16	r	503	CLA	O1D-CGD-O2D-CED
16	w	512	CLA	O1D-CGD-O2D-CED
16	y	517	CLA	O1D-CGD-O2D-CED
16	H	1114	CLA	O1A-CGA-O2A-C1
16	A	1109	CLA	C15-C16-C17-C18
16	A	1140	CLA	C15-C16-C17-C18
16	B	1021	CLA	C5-C6-C7-C8
16	B	1202	CLA	C5-C6-C7-C8
16	G	1238	CLA	C13-C15-C16-C17
16	H	1127	CLA	C15-C16-C17-C18
16	Y	504	CLA	C8-C10-C11-C12
16	Y	510	CLA	C15-C16-C17-C18
16	Y	512	CLA	C15-C16-C17-C18
16	Z	505	CLA	C15-C16-C17-C18
16	h	507	CLA	C8-C10-C11-C12
16	p	510	CLA	C15-C16-C17-C18
16	q	517	CLA	C5-C6-C7-C8
16	w	509	CLA	C10-C11-C12-C13
16	w	515	CLA	C15-C16-C17-C18
16	y	509	CLA	C10-C11-C12-C13
16	G	1220	CLA	CBA-CGA-O2A-C1
16	b	1220	CLA	CBA-CGA-O2A-C1
16	g	502	CLA	CBA-CGA-O2A-C1
16	g	507	CLA	CBA-CGA-O2A-C1
16	h	504	CLA	CBA-CGA-O2A-C1
16	k	4004	CLA	CBA-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	n	507	CLA	CBA-CGA-O2A-C1
16	p	506	CLA	CBA-CGA-O2A-C1
16	Y	508	CLA	CBD-CGD-O2D-CED
16	a	1136	CLA	CBD-CGD-O2D-CED
16	n	505	CLA	CBD-CGD-O2D-CED
16	o	509	CLA	CBD-CGD-O2D-CED
16	u	511	CLA	CBD-CGD-O2D-CED
16	w	502	CLA	CBD-CGD-O2D-CED
16	x	508	CLA	CBD-CGD-O2D-CED
16	H	1124	CLA	O1A-CGA-O2A-C1
16	a	1140	CLA	O1A-CGA-O2A-C1
16	p	507	CLA	O1A-CGA-O2A-C1
16	r	509	CLA	O1A-CGA-O2A-C1
16	q	517	CLA	O1D-CGD-O2D-CED
16	G	1240	CLA	CBA-CGA-O2A-C1
16	Z	516	CLA	CBA-CGA-O2A-C1
16	r	516	CLA	CBA-CGA-O2A-C1
16	u	503	CLA	CBA-CGA-O2A-C1
16	x	503	CLA	CBA-CGA-O2A-C1
23	r	606	LMU	C4'-C5'-C6'-O6'
16	A	1128	CLA	C8-C10-C11-C12
16	a	1022	CLA	C15-C16-C17-C18
16	x	512	CLA	C5-C6-C7-C8
16	B	1203	CLA	C3-C5-C6-C7
16	a	1106	CLA	C3-C5-C6-C7
16	a	1132	CLA	C3-C5-C6-C7
16	q	508	CLA	C3-C5-C6-C7
16	x	506	CLA	C3-C5-C6-C7
16	a	1111	CLA	CBD-CGD-O2D-CED
19	W	601	BCR	C19-C20-C21-C22
19	h	603	BCR	C9-C10-C11-C12
19	o	602	BCR	C19-C20-C21-C22
19	r	602	BCR	C19-C20-C21-C22
19	s	603	BCR	C9-C10-C11-C12
19	x	602	BCR	C13-C14-C15-C16
19	x	604	BCR	C13-C14-C15-C16
16	G	1021	CLA	C13-C15-C16-C17
16	H	1125	CLA	C8-C10-C11-C12
16	H	1237	CLA	C8-C10-C11-C12
16	a	1128	CLA	C10-C11-C12-C13
16	B	1228	CLA	O1A-CGA-O2A-C1
16	h	512	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	q	509	CLA	O1A-CGA-O2A-C1
14	b	848	LMG	O6-C5-C6-O5
14	A	4101	LMG	C28-C29-C30-C31
13	b	4018	LHG	C1-C2-C3-O3
13	x	605	LHG	C1-C2-C3-O3
16	B	1235	CLA	C2A-CAA-CBA-CGA
16	B	1238	CLA	C2A-CAA-CBA-CGA
16	G	1228	CLA	C2A-CAA-CBA-CGA
16	H	1118	CLA	C2A-CAA-CBA-CGA
16	L	1503	CLA	C2A-CAA-CBA-CGA
16	W	515	CLA	C2A-CAA-CBA-CGA
16	X	508	CLA	C2A-CAA-CBA-CGA
16	Z	515	CLA	C2A-CAA-CBA-CGA
16	l	1501	CLA	C2A-CAA-CBA-CGA
16	o	516	CLA	C2A-CAA-CBA-CGA
16	w	517	CLA	C2A-CAA-CBA-CGA
16	x	503	CLA	O1D-CGD-O2D-CED
13	r	605	LHG	C24-C23-O8-C6
15	a	1011	CL0	CBA-CGA-O2A-C1
16	Z	512	CLA	CBA-CGA-O2A-C1
16	a	1123	CLA	CBA-CGA-O2A-C1
16	b	1222	CLA	CBA-CGA-O2A-C1
16	q	502	CLA	CBA-CGA-O2A-C1
16	r	514	CLA	CBA-CGA-O2A-C1
16	u	507	CLA	CBA-CGA-O2A-C1
16	A	1013	CLA	C8-C10-C11-C12
16	A	1126	CLA	C15-C16-C17-C18
16	B	1203	CLA	C10-C11-C12-C13
16	B	1205	CLA	C13-C15-C16-C17
16	G	1021	CLA	C5-C6-C7-C8
16	H	1013	CLA	C8-C10-C11-C12
16	H	1022	CLA	C8-C10-C11-C12
16	H	1101	CLA	C15-C16-C17-C18
16	H	1118	CLA	C5-C6-C7-C8
16	H	1139	CLA	C5-C6-C7-C8
16	H	1237	CLA	C10-C11-C12-C13
16	W	510	CLA	C13-C15-C16-C17
16	X	517	CLA	C5-C6-C7-C8
16	b	1204	CLA	C13-C15-C16-C17
16	g	504	CLA	C13-C15-C16-C17
16	g	512	CLA	C5-C6-C7-C8
16	h	511	CLA	C5-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	l	1501	CLA	C10-C11-C12-C13
16	o	504	CLA	C8-C10-C11-C12
16	p	504	CLA	C5-C6-C7-C8
16	p	512	CLA	C10-C11-C12-C13
16	s	509	CLA	C10-C11-C12-C13
16	u	515	CLA	C15-C16-C17-C18
16	v	512	CLA	C5-C6-C7-C8
16	w	504	CLA	C5-C6-C7-C8
16	w	510	CLA	C5-C6-C7-C8
16	x	511	CLA	C5-C6-C7-C8
17	B	2002	PQN	C23-C25-C26-C27
17	G	2002	PQN	C23-C25-C26-C27
16	K	4003	CLA	CBD-CGD-O2D-CED
16	Z	516	CLA	CBD-CGD-O2D-CED
16	n	510	CLA	CBD-CGD-O2D-CED
16	u	510	CLA	CBD-CGD-O2D-CED
16	A	1109	CLA	C10-C11-C12-C13
16	G	1221	CLA	C13-C15-C16-C17
16	G	1225	CLA	C15-C16-C17-C18
16	a	1126	CLA	C15-C16-C17-C18
16	a	1237	CLA	C10-C11-C12-C13
16	b	1221	CLA	C13-C15-C16-C17
16	n	510	CLA	C13-C15-C16-C17
16	p	511	CLA	C5-C6-C7-C8
16	p	515	CLA	C8-C10-C11-C12
16	u	504	CLA	C8-C10-C11-C12
23	w	605	LMU	C4'-C5'-C6'-O6'
23	r	606	LMU	O5'-C5'-C6'-O6'
16	A	1125	CLA	C5-C6-C7-C8
16	A	1128	CLA	C15-C16-C17-C18
16	B	1221	CLA	C13-C15-C16-C17
16	B	1229	CLA	C5-C6-C7-C8
16	W	517	CLA	C5-C6-C7-C8
16	a	1237	CLA	C8-C10-C11-C12
16	b	1021	CLA	C13-C15-C16-C17
16	b	1203	CLA	C10-C11-C12-C13
16	b	1211	CLA	C13-C15-C16-C17
16	b	1238	CLA	C5-C6-C7-C8
16	o	505	CLA	C5-C6-C7-C8
16	q	511	CLA	C5-C6-C7-C8
16	s	510	CLA	C5-C6-C7-C8
16	s	511	CLA	C5-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	v	511	CLA	C5-C6-C7-C8
16	w	504	CLA	C8-C10-C11-C12
16	B	1235	CLA	CBA-CGA-O2A-C1
16	W	501	CLA	CBA-CGA-O2A-C1
16	a	1104	CLA	CBA-CGA-O2A-C1
16	n	511	CLA	CBA-CGA-O2A-C1
16	p	508	CLA	CBA-CGA-O2A-C1
16	r	506	CLA	CBA-CGA-O2A-C1
16	s	507	CLA	CBA-CGA-O2A-C1
16	L	1502	CLA	C4-C3-C5-C6
16	r	505	CLA	C4-C3-C5-C6
16	Y	513	CLA	O1D-CGD-O2D-CED
16	x	509	CLA	O1D-CGD-O2D-CED
16	A	1139	CLA	C5-C6-C7-C8
16	G	1203	CLA	C10-C11-C12-C13
16	G	1224	CLA	C5-C6-C7-C8
16	H	1131	CLA	C5-C6-C7-C8
16	a	1130	CLA	C8-C10-C11-C12
16	b	1238	CLA	C10-C11-C12-C13
16	g	504	CLA	C15-C16-C17-C18
16	h	515	CLA	C10-C11-C12-C13
16	u	517	CLA	C5-C6-C7-C8
16	x	504	CLA	C13-C15-C16-C17
16	X	508	CLA	C3-C5-C6-C7
16	Z	508	CLA	C3-C5-C6-C7
16	a	1133	CLA	C3-C5-C6-C7
16	b	1203	CLA	C3-C5-C6-C7
16	a	1106	CLA	CBD-CGD-O2D-CED
16	W	510	CLA	C11-C10-C8-C9
16	h	502	CLA	O1D-CGD-O2D-CED
16	x	507	CLA	O1A-CGA-O2A-C1
13	A	851	LHG	O9-C7-O7-C5
14	G	848	LMG	C2-C1-O1-C7
14	b	848	LMG	C2-C1-O1-C7
16	a	1104	CLA	C10-C11-C12-C13
16	a	1128	CLA	C13-C15-C16-C17
16	r	504	CLA	C13-C15-C16-C17
16	x	504	CLA	C15-C16-C17-C18
13	p	605	LHG	C23-C24-C25-C26
16	j	1302	CLA	O1D-CGD-O2D-CED
16	s	505	CLA	O1D-CGD-O2D-CED
13	R	103	LHG	O2-C2-C3-O3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	K	4004	CLA	CBA-CGA-O2A-C1
16	G	1226	CLA	C11-C12-C13-C14
16	b	1012	CLA	C6-C7-C8-C9
16	W	515	CLA	C5-C6-C7-C8
16	s	515	CLA	C5-C6-C7-C8
16	H	1140	CLA	O1A-CGA-O2A-C1
16	x	502	CLA	O1A-CGA-O2A-C1
19	A	4002	BCR	C20-C21-C22-C37
19	A	4011	BCR	C20-C21-C22-C37
19	B	4010	BCR	C20-C21-C22-C37
19	B	4017	BCR	C35-C13-C14-C15
19	G	4005	BCR	C20-C21-C22-C37
19	H	4002	BCR	C20-C21-C22-C37
19	H	4003	BCR	C20-C21-C22-C37
19	H	4008	BCR	C20-C21-C22-C37
19	H	4011	BCR	C20-C21-C22-C37
19	I	4018	BCR	C35-C13-C14-C15
19	J	4013	BCR	C16-C17-C18-C36
19	J	4015	BCR	C16-C17-C18-C36
19	L	4022	BCR	C16-C17-C18-C36
19	R	4018	BCR	C35-C13-C14-C15
19	S	4015	BCR	C16-C17-C18-C36
19	T	4005	BCR	C16-C17-C18-C36
19	a	4003	BCR	C20-C21-C22-C37
19	b	4005	BCR	C20-C21-C22-C37
19	b	4010	BCR	C11-C10-C9-C34
19	b	4014	BCR	C20-C21-C22-C37
19	f	4016	BCR	C35-C13-C14-C15
19	g	602	BCR	C11-C10-C9-C34
19	g	604	BCR	C11-C10-C9-C34
19	g	604	BCR	C16-C17-C18-C36
19	h	604	BCR	C20-C21-C22-C37
19	l	4022	BCR	C16-C17-C18-C36
19	n	604	BCR	C16-C17-C18-C36
19	o	601	BCR	C20-C21-C22-C37
19	o	604	BCR	C20-C21-C22-C37
19	q	603	BCR	C20-C21-C22-C37
19	q	604	BCR	C11-C10-C9-C34
19	r	601	BCR	C16-C17-C18-C36
19	r	602	BCR	C11-C10-C9-C34
19	r	602	BCR	C16-C17-C18-C36
19	r	602	BCR	C20-C21-C22-C37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	r	604	BCR	C16-C17-C18-C36
19	s	601	BCR	C16-C17-C18-C36
19	s	601	BCR	C20-C21-C22-C37
19	t	601	BCR	C20-C21-C22-C37
19	u	602	BCR	C20-C21-C22-C37
19	u	603	BCR	C20-C21-C22-C37
19	v	601	BCR	C20-C21-C22-C37
19	v	603	BCR	C20-C21-C22-C37
19	v	604	BCR	C20-C21-C22-C37
19	w	604	BCR	C35-C13-C14-C15
19	w	604	BCR	C16-C17-C18-C36
19	x	602	BCR	C20-C21-C22-C37
19	y	601	BCR	C20-C21-C22-C37
15	a	1011	CL0	C3-C5-C6-C7
20	U	4101	LMT	O5'-C5'-C6'-O6'
16	A	1013	CLA	C13-C15-C16-C17
16	A	1237	CLA	C13-C15-C16-C17
16	p	515	CLA	C15-C16-C17-C18
19	A	4007	BCR	C37-C22-C23-C24
19	A	4011	BCR	C37-C22-C23-C24
19	G	4017	BCR	C37-C22-C23-C24
19	H	4002	BCR	C7-C8-C9-C34
19	H	4011	BCR	C37-C22-C23-C24
19	I	4018	BCR	C7-C8-C9-C34
19	K	4001	BCR	C37-C22-C23-C24
19	R	4018	BCR	C7-C8-C9-C34
19	T	4001	BCR	C7-C8-C9-C34
19	U	4022	BCR	C7-C8-C9-C34
19	U	4022	BCR	C11-C12-C13-C35
19	W	601	BCR	C11-C12-C13-C35
19	Y	602	BCR	C37-C22-C23-C24
19	Z	602	BCR	C7-C8-C9-C34
19	f	4016	BCR	C7-C8-C9-C34
19	g	601	BCR	C11-C12-C13-C35
19	g	604	BCR	C7-C8-C9-C34
19	h	604	BCR	C37-C22-C23-C24
19	i	4018	BCR	C7-C8-C9-C34
19	k	4001	BCR	C7-C8-C9-C34
19	l	4019	BCR	C7-C8-C9-C34
19	l	4022	BCR	C7-C8-C9-C34
19	o	601	BCR	C7-C8-C9-C34
19	p	601	BCR	C37-C22-C23-C24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	p	602	BCR	C7-C8-C9-C34
19	p	602	BCR	C37-C22-C23-C24
19	s	602	BCR	C7-C8-C9-C34
19	s	603	BCR	C7-C8-C9-C34
21	M	4021	ECH	C11-C12-C13-C35
21	R	4020	ECH	C37-C22-C23-C24
21	i	4020	ECH	C36-C18-C19-C20
19	A	4008	BCR	C21-C22-C23-C24
19	B	4004	BCR	C21-C22-C23-C24
19	G	4014	BCR	C17-C18-C19-C20
19	H	4008	BCR	C17-C18-C19-C20
19	I	4018	BCR	C7-C8-C9-C10
19	R	4018	BCR	C7-C8-C9-C10
19	U	4019	BCR	C21-C22-C23-C24
19	W	601	BCR	C21-C22-C23-C24
19	W	604	BCR	C7-C8-C9-C10
19	X	603	BCR	C7-C8-C9-C10
19	Y	602	BCR	C7-C8-C9-C10
19	Y	603	BCR	C21-C22-C23-C24
19	b	4004	BCR	C21-C22-C23-C24
19	g	601	BCR	C21-C22-C23-C24
19	g	603	BCR	C7-C8-C9-C10
19	h	603	BCR	C21-C22-C23-C24
19	k	4005	BCR	C21-C22-C23-C24
19	o	602	BCR	C21-C22-C23-C24
19	p	604	BCR	C7-C8-C9-C10
19	r	602	BCR	C21-C22-C23-C24
19	s	604	BCR	C7-C8-C9-C10
19	u	604	BCR	C7-C8-C9-C10
19	w	602	BCR	C7-C8-C9-C10
19	x	603	BCR	C7-C8-C9-C10
19	y	603	BCR	C21-C22-C23-C24
21	M	4021	ECH	C11-C12-C13-C14
21	i	4020	ECH	C7-C8-C9-C10
21	m	4021	ECH	C21-C22-C23-C24
16	A	1140	CLA	O1A-CGA-O2A-C1
16	H	1123	CLA	O1A-CGA-O2A-C1
16	a	1123	CLA	O1A-CGA-O2A-C1
16	k	4004	CLA	O1A-CGA-O2A-C1
16	x	514	CLA	O1A-CGA-O2A-C1
16	A	1116	CLA	C2A-CAA-CBA-CGA
16	B	1218	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1220	CLA	C2A-CAA-CBA-CGA
16	G	1229	CLA	C2A-CAA-CBA-CGA
16	G	1235	CLA	C2A-CAA-CBA-CGA
16	H	1126	CLA	C2A-CAA-CBA-CGA
16	H	1138	CLA	C2A-CAA-CBA-CGA
16	Y	516	CLA	C2A-CAA-CBA-CGA
16	a	1110	CLA	C2A-CAA-CBA-CGA
16	b	1201	CLA	C2A-CAA-CBA-CGA
16	g	508	CLA	C2A-CAA-CBA-CGA
16	g	511	CLA	C2A-CAA-CBA-CGA
16	g	515	CLA	C2A-CAA-CBA-CGA
16	n	501	CLA	C2A-CAA-CBA-CGA
16	o	502	CLA	C2A-CAA-CBA-CGA
16	p	502	CLA	C2A-CAA-CBA-CGA
16	q	515	CLA	C2A-CAA-CBA-CGA
16	r	513	CLA	C2A-CAA-CBA-CGA
16	r	515	CLA	C2A-CAA-CBA-CGA
16	s	515	CLA	C2A-CAA-CBA-CGA
16	s	516	CLA	C2A-CAA-CBA-CGA
16	s	517	CLA	C2A-CAA-CBA-CGA
16	u	508	CLA	C2A-CAA-CBA-CGA
16	u	516	CLA	C2A-CAA-CBA-CGA
16	v	505	CLA	C2A-CAA-CBA-CGA
16	w	503	CLA	C2A-CAA-CBA-CGA
16	x	505	CLA	C2A-CAA-CBA-CGA
16	x	515	CLA	C2A-CAA-CBA-CGA
16	y	517	CLA	C2A-CAA-CBA-CGA
17	b	2002	PQN	C15-C16-C17-C18
13	I	103	LHG	O1-C1-C2-C3
13	X	605	LHG	O1-C1-C2-C3
16	G	1222	CLA	CBD-CGD-O2D-CED
16	H	1136	CLA	O1D-CGD-O2D-CED
23	Y	606	LMU	C4'-C5'-C6'-O6'
16	A	1140	CLA	C16-C17-C18-C20
16	G	1206	CLA	C16-C17-C18-C20
16	G	1215	CLA	C11-C12-C13-C14
16	H	1140	CLA	C16-C17-C18-C20
16	X	505	CLA	C16-C17-C18-C19
16	Z	510	CLA	C11-C12-C13-C15
16	b	1021	CLA	C16-C17-C18-C19
16	b	1206	CLA	C16-C17-C18-C19
16	h	510	CLA	C16-C17-C18-C19

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	h	510	CLA	C16-C17-C18-C20
16	k	4004	CLA	C6-C7-C8-C9
16	o	505	CLA	C16-C17-C18-C19
16	A	1138	CLA	O1D-CGD-O2D-CED
16	o	501	CLA	O1D-CGD-O2D-CED
16	u	512	CLA	O1D-CGD-O2D-CED
16	G	1220	CLA	O1A-CGA-O2A-C1
16	G	1228	CLA	O1A-CGA-O2A-C1
16	n	507	CLA	O1A-CGA-O2A-C1
16	p	506	CLA	O1A-CGA-O2A-C1
15	A	1011	CL0	C3-C5-C6-C7
16	B	1229	CLA	C3-C5-C6-C7
16	H	1115	CLA	C3-C5-C6-C7
16	s	505	CLA	C3-C5-C6-C7
16	G	1226	CLA	C10-C11-C12-C13
16	q	512	CLA	C13-C15-C16-C17
19	A	4008	BCR	C20-C21-C22-C23
19	B	4010	BCR	C16-C17-C18-C19
19	B	4014	BCR	C20-C21-C22-C23
19	F	4016	BCR	C11-C10-C9-C8
19	G	4009	BCR	C16-C17-C18-C19
19	G	4010	BCR	C11-C10-C9-C8
19	G	4010	BCR	C16-C17-C18-C19
19	G	4014	BCR	C20-C21-C22-C23
19	G	4017	BCR	C20-C21-C22-C23
19	K	4005	BCR	C16-C17-C18-C19
19	R	4018	BCR	C12-C13-C14-C15
19	R	4018	BCR	C20-C21-C22-C23
19	S	4013	BCR	C20-C21-C22-C23
19	T	4005	BCR	C16-C17-C18-C19
19	U	4022	BCR	C11-C10-C9-C8
19	W	603	BCR	C11-C10-C9-C8
19	X	603	BCR	C20-C21-C22-C23
19	X	604	BCR	C11-C10-C9-C8
19	Y	601	BCR	C20-C21-C22-C23
19	Y	603	BCR	C20-C21-C22-C23
19	Z	603	BCR	C20-C21-C22-C23
19	Z	604	BCR	C12-C13-C14-C15
19	a	4002	BCR	C20-C21-C22-C23
19	a	4003	BCR	C11-C10-C9-C8
19	a	4003	BCR	C16-C17-C18-C19
19	a	4008	BCR	C20-C21-C22-C23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	a	4011	BCR	C20-C21-C22-C23
19	b	4010	BCR	C16-C17-C18-C19
19	b	4014	BCR	C11-C10-C9-C8
19	b	4014	BCR	C12-C13-C14-C15
19	b	4014	BCR	C16-C17-C18-C19
19	g	601	BCR	C16-C17-C18-C19
19	g	601	BCR	C20-C21-C22-C23
19	g	602	BCR	C11-C10-C9-C8
19	g	604	BCR	C11-C10-C9-C8
19	h	601	BCR	C20-C21-C22-C23
19	h	604	BCR	C11-C10-C9-C8
19	i	4018	BCR	C11-C10-C9-C8
19	i	4018	BCR	C16-C17-C18-C19
19	i	4018	BCR	C20-C21-C22-C23
19	j	4013	BCR	C16-C17-C18-C19
19	l	4022	BCR	C11-C10-C9-C8
19	n	601	BCR	C20-C21-C22-C23
19	n	603	BCR	C11-C10-C9-C8
19	n	604	BCR	C16-C17-C18-C19
19	o	604	BCR	C20-C21-C22-C23
19	p	601	BCR	C20-C21-C22-C23
19	p	603	BCR	C20-C21-C22-C23
19	p	604	BCR	C11-C10-C9-C8
19	q	604	BCR	C11-C10-C9-C8
19	r	601	BCR	C20-C21-C22-C23
19	r	604	BCR	C11-C10-C9-C8
19	r	604	BCR	C20-C21-C22-C23
19	s	604	BCR	C11-C10-C9-C8
19	s	604	BCR	C12-C13-C14-C15
19	u	602	BCR	C20-C21-C22-C23
19	v	601	BCR	C12-C13-C14-C15
19	v	604	BCR	C11-C10-C9-C8
19	w	603	BCR	C20-C21-C22-C23
19	w	604	BCR	C11-C10-C9-C8
19	x	603	BCR	C16-C17-C18-C19
19	x	603	BCR	C20-C21-C22-C23
20	A	4202	LMT	O5'-C1'-O1'-C1
20	H	4202	LMT	O5'-C1'-O1'-C1
20	a	4202	LMT	O5'-C1'-O1'-C1
23	q	605	LMU	O5'-C1'-O1'-C1
16	A	1136	CLA	O1D-CGD-O2D-CED
13	H	851	LHG	C8-C7-O7-C5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	R	103	LHG	C8-C7-O7-C5
16	b	1239	CLA	C15-C16-C17-C18
16	s	504	CLA	C5-C6-C7-C8
16	A	1105	CLA	O1D-CGD-O2D-CED
16	B	1210	CLA	O1D-CGD-O2D-CED
16	G	1205	CLA	O1D-CGD-O2D-CED
16	B	1220	CLA	O1D-CGD-O2D-CED
16	B	1226	CLA	O1D-CGD-O2D-CED
16	G	1221	CLA	O1D-CGD-O2D-CED
16	b	1221	CLA	O1D-CGD-O2D-CED
16	w	508	CLA	O1D-CGD-O2D-CED
13	a	849	LHG	C24-C23-O8-C6
16	b	1213	CLA	CBA-CGA-O2A-C1
16	s	508	CLA	CBA-CGA-O2A-C1
16	u	512	CLA	CBA-CGA-O2A-C1
16	X	505	CLA	C5-C6-C7-C8
16	b	1238	CLA	CBD-CGD-O2D-CED
16	H	1119	CLA	O1D-CGD-O2D-CED
16	H	1123	CLA	C2-C1-O2A-CGA
16	Z	509	CLA	C2-C1-O2A-CGA
16	a	1123	CLA	C2-C1-O2A-CGA
16	b	1228	CLA	C2-C1-O2A-CGA
16	o	516	CLA	O1A-CGA-O2A-C1
16	p	517	CLA	C2-C1-O2A-CGA
16	q	509	CLA	C2-C1-O2A-CGA
16	w	509	CLA	C2-C1-O2A-CGA
16	B	1226	CLA	C11-C12-C13-C15
16	B	1228	CLA	C6-C7-C8-C9
16	G	1021	CLA	C16-C17-C18-C19
16	G	1206	CLA	C16-C17-C18-C19
16	H	1140	CLA	C16-C17-C18-C19
16	W	512	CLA	C11-C12-C13-C14
16	X	515	CLA	C16-C17-C18-C20
16	a	1124	CLA	C11-C12-C13-C14
16	a	1140	CLA	C16-C17-C18-C19
16	b	1204	CLA	C16-C17-C18-C20
16	o	515	CLA	C16-C17-C18-C20
17	b	2002	PQN	C26-C27-C28-C29
16	b	1220	CLA	O1A-CGA-O2A-C1
16	g	502	CLA	O1A-CGA-O2A-C1
16	g	507	CLA	O1A-CGA-O2A-C1
16	h	504	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	1127	CLA	C15-C16-C17-C18
16	G	1211	CLA	C10-C11-C12-C13
16	H	1127	CLA	C5-C6-C7-C8
16	h	504	CLA	C8-C10-C11-C12
16	y	505	CLA	C15-C16-C17-C18
14	a	852	LMG	O6-C5-C6-O5
13	G	4018	LHG	C11-C12-C13-C14
16	g	516	CLA	CBA-CGA-O2A-C1
19	G	4009	BCR	C14-C15-C16-C17
19	b	4017	BCR	C14-C15-C16-C17
19	o	604	BCR	C14-C15-C16-C17
19	x	603	BCR	C14-C15-C16-C17
14	A	852	LMG	C30-C31-C32-C33
16	G	1230	CLA	O1D-CGD-O2D-CED
16	x	502	CLA	O1D-CGD-O2D-CED
23	w	605	LMU	O5'-C5'-C6'-O6'
16	A	1022	CLA	C15-C16-C17-C18
16	G	1206	CLA	C8-C10-C11-C12
16	X	506	CLA	C10-C11-C12-C13
16	p	517	CLA	C5-C6-C7-C8
13	R	103	LHG	C11-C10-C9-C8
16	n	503	CLA	O1D-CGD-O2D-CED
16	g	514	CLA	CBA-CGA-O2A-C1
13	I	103	LHG	O1-C1-C2-O2
13	X	605	LHG	O1-C1-C2-O2
13	b	4018	LHG	O1-C1-C2-O2
13	o	605	LHG	O1-C1-C2-O2
20	A	4202	LMT	C2-C1-O1'-C1'
20	H	4202	LMT	C2-C1-O1'-C1'
20	a	4202	LMT	C2-C1-O1'-C1'
23	x	606	LMU	C2-C1-O1'-C1'
16	u	505	CLA	C3-C5-C6-C7
16	G	1218	CLA	O1D-CGD-O2D-CED
16	G	1228	CLA	O1D-CGD-O2D-CED
16	a	1107	CLA	O1D-CGD-O2D-CED
16	p	508	CLA	O1D-CGD-O2D-CED
16	y	514	CLA	O1D-CGD-O2D-CED
16	W	513	CLA	CBA-CGA-O2A-C1
16	u	516	CLA	CBA-CGA-O2A-C1
16	B	1206	CLA	C16-C17-C18-C19
16	B	1206	CLA	C16-C17-C18-C20
16	G	1215	CLA	C11-C12-C13-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1228	CLA	C6-C7-C8-C9
16	G	1228	CLA	C6-C7-C8-C10
16	X	505	CLA	C16-C17-C18-C20
16	Z	510	CLA	C11-C12-C13-C14
16	a	1124	CLA	C11-C12-C13-C15
16	a	1140	CLA	C16-C17-C18-C20
16	b	1021	CLA	C16-C17-C18-C20
16	b	1206	CLA	C16-C17-C18-C20
16	b	1228	CLA	C6-C7-C8-C9
16	h	515	CLA	C16-C17-C18-C20
16	k	4004	CLA	C6-C7-C8-C10
16	v	517	CLA	C6-C7-C8-C9
16	w	509	CLA	C16-C17-C18-C19
16	x	509	CLA	C16-C17-C18-C19
16	x	509	CLA	C16-C17-C18-C20
16	A	1126	CLA	O1D-CGD-O2D-CED
16	G	1224	CLA	O1D-CGD-O2D-CED
16	x	514	CLA	O1D-CGD-O2D-CED
16	v	503	CLA	O1A-CGA-O2A-C1
16	b	1222	CLA	O1A-CGA-O2A-C1
16	A	1110	CLA	C2A-CAA-CBA-CGA
16	A	1126	CLA	C2A-CAA-CBA-CGA
16	B	1201	CLA	C2A-CAA-CBA-CGA
16	H	1110	CLA	C2A-CAA-CBA-CGA
16	a	1138	CLA	C2A-CAA-CBA-CGA
16	y	515	CLA	C2A-CAA-CBA-CGA
14	a	852	LMG	C34-C35-C36-C37
16	A	1133	CLA	C5-C6-C7-C8
16	H	1125	CLA	C15-C16-C17-C18
16	Y	512	CLA	C8-C10-C11-C12
16	a	1125	CLA	C15-C16-C17-C18
16	a	1128	CLA	C8-C10-C11-C12
16	b	1225	CLA	C15-C16-C17-C18
16	w	511	CLA	C5-C6-C7-C8
13	A	851	LHG	C8-C7-O7-C5
14	f	4017	LMG	C11-C10-O7-C8
16	A	1139	CLA	O1D-CGD-O2D-CED
16	w	517	CLA	O1D-CGD-O2D-CED
16	G	1210	CLA	C11-C10-C8-C7
16	H	1128	CLA	C11-C12-C13-C15
16	a	1125	CLA	C11-C10-C8-C7
16	v	512	CLA	C6-C7-C8-C10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	B	2002	PQN	C21-C22-C23-C25
17	G	2002	PQN	C21-C22-C23-C25
13	B	4018	LHG	C11-C12-C13-C14
13	H	849	LHG	C28-C29-C30-C31
16	B	1207	CLA	C5-C6-C7-C8
16	B	1221	CLA	C10-C11-C12-C13
16	Z	515	CLA	C8-C10-C11-C12
16	a	1131	CLA	C5-C6-C7-C8
16	n	504	CLA	C5-C6-C7-C8
16	r	509	CLA	C13-C15-C16-C17
16	v	509	CLA	C13-C15-C16-C17
13	I	103	LHG	C28-C29-C30-C31
14	a	852	LMG	C30-C31-C32-C33
16	g	503	CLA	O1A-CGA-O2A-C1
15	a	1011	CL0	O1A-CGA-O2A-C1
16	Z	512	CLA	O1A-CGA-O2A-C1
16	q	502	CLA	O1A-CGA-O2A-C1
16	s	507	CLA	O1A-CGA-O2A-C1
16	u	507	CLA	O1A-CGA-O2A-C1
16	a	1103	CLA	C3-C5-C6-C7
16	A	1022	CLA	C3A-C2A-CAA-CBA
16	A	1115	CLA	C3A-C2A-CAA-CBA
16	A	1118	CLA	C3A-C2A-CAA-CBA
16	A	1121	CLA	C3A-C2A-CAA-CBA
16	A	1130	CLA	C3A-C2A-CAA-CBA
16	A	1137	CLA	C3A-C2A-CAA-CBA
16	B	1023	CLA	C3A-C2A-CAA-CBA
16	B	1210	CLA	C3A-C2A-CAA-CBA
16	B	1211	CLA	C3A-C2A-CAA-CBA
16	B	1213	CLA	C3A-C2A-CAA-CBA
16	B	1216	CLA	C3A-C2A-CAA-CBA
16	B	1217	CLA	C3A-C2A-CAA-CBA
16	B	1223	CLA	C3A-C2A-CAA-CBA
16	B	1234	CLA	C3A-C2A-CAA-CBA
16	B	1236	CLA	C3A-C2A-CAA-CBA
16	F	1302	CLA	C3A-C2A-CAA-CBA
16	G	1023	CLA	C3A-C2A-CAA-CBA
16	G	1203	CLA	C3A-C2A-CAA-CBA
16	G	1206	CLA	C3A-C2A-CAA-CBA
16	G	1209	CLA	C3A-C2A-CAA-CBA
16	G	1210	CLA	C3A-C2A-CAA-CBA
16	G	1211	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1213	CLA	C3A-C2A-CAA-CBA
16	G	1218	CLA	C3A-C2A-CAA-CBA
16	G	1230	CLA	C3A-C2A-CAA-CBA
16	G	1231	CLA	C3A-C2A-CAA-CBA
16	G	1236	CLA	C3A-C2A-CAA-CBA
16	H	1022	CLA	C3A-C2A-CAA-CBA
16	H	1115	CLA	C3A-C2A-CAA-CBA
16	H	1118	CLA	C3A-C2A-CAA-CBA
16	H	1121	CLA	C3A-C2A-CAA-CBA
16	H	1123	CLA	C3A-C2A-CAA-CBA
16	H	1130	CLA	C3A-C2A-CAA-CBA
16	H	1140	CLA	C3A-C2A-CAA-CBA
16	Q	1302	CLA	C3A-C2A-CAA-CBA
16	T	4002	CLA	C3A-C2A-CAA-CBA
16	W	511	CLA	C3A-C2A-CAA-CBA
16	X	503	CLA	C3A-C2A-CAA-CBA
16	X	517	CLA	C3A-C2A-CAA-CBA
16	Y	504	CLA	C3A-C2A-CAA-CBA
16	Y	508	CLA	C3A-C2A-CAA-CBA
16	Y	509	CLA	C3A-C2A-CAA-CBA
16	Z	501	CLA	C3A-C2A-CAA-CBA
16	Z	510	CLA	C3A-C2A-CAA-CBA
16	a	1022	CLA	C3A-C2A-CAA-CBA
16	a	1111	CLA	C3A-C2A-CAA-CBA
16	a	1115	CLA	C3A-C2A-CAA-CBA
16	a	1118	CLA	C3A-C2A-CAA-CBA
16	a	1123	CLA	C3A-C2A-CAA-CBA
16	a	1130	CLA	C3A-C2A-CAA-CBA
16	a	1140	CLA	C3A-C2A-CAA-CBA
16	b	1012	CLA	C3A-C2A-CAA-CBA
16	b	1023	CLA	C3A-C2A-CAA-CBA
16	b	1203	CLA	C3A-C2A-CAA-CBA
16	b	1209	CLA	C3A-C2A-CAA-CBA
16	b	1211	CLA	C3A-C2A-CAA-CBA
16	b	1213	CLA	C3A-C2A-CAA-CBA
16	b	1221	CLA	C3A-C2A-CAA-CBA
16	b	1223	CLA	C3A-C2A-CAA-CBA
16	b	1231	CLA	C3A-C2A-CAA-CBA
16	b	1236	CLA	C3A-C2A-CAA-CBA
16	b	1239	CLA	C3A-C2A-CAA-CBA
16	f	1302	CLA	C3A-C2A-CAA-CBA
16	g	501	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	g	509	CLA	C3A-C2A-CAA-CBA
16	g	513	CLA	C3A-C2A-CAA-CBA
16	g	517	CLA	C3A-C2A-CAA-CBA
16	h	507	CLA	C3A-C2A-CAA-CBA
16	n	516	CLA	C3A-C2A-CAA-CBA
16	o	504	CLA	C3A-C2A-CAA-CBA
16	o	517	CLA	C3A-C2A-CAA-CBA
16	p	508	CLA	C3A-C2A-CAA-CBA
16	p	509	CLA	C3A-C2A-CAA-CBA
16	q	503	CLA	C3A-C2A-CAA-CBA
16	q	504	CLA	C3A-C2A-CAA-CBA
16	q	509	CLA	C3A-C2A-CAA-CBA
16	r	504	CLA	C3A-C2A-CAA-CBA
16	r	509	CLA	C3A-C2A-CAA-CBA
16	r	517	CLA	C3A-C2A-CAA-CBA
16	s	503	CLA	C3A-C2A-CAA-CBA
16	s	504	CLA	C3A-C2A-CAA-CBA
16	s	508	CLA	C3A-C2A-CAA-CBA
16	s	509	CLA	C3A-C2A-CAA-CBA
16	s	513	CLA	C3A-C2A-CAA-CBA
16	u	501	CLA	C3A-C2A-CAA-CBA
16	u	504	CLA	C3A-C2A-CAA-CBA
16	u	506	CLA	C3A-C2A-CAA-CBA
16	u	517	CLA	C3A-C2A-CAA-CBA
16	w	501	CLA	C3A-C2A-CAA-CBA
16	w	504	CLA	C3A-C2A-CAA-CBA
16	x	501	CLA	C3A-C2A-CAA-CBA
16	x	504	CLA	C3A-C2A-CAA-CBA
16	x	513	CLA	C3A-C2A-CAA-CBA
16	B	1227	CLA	O1D-CGD-O2D-CED
16	B	1230	CLA	O1D-CGD-O2D-CED
16	g	512	CLA	O1D-CGD-O2D-CED
13	R	103	LHG	C31-C32-C33-C34
16	B	1214	CLA	C4C-C3C-CAC-CBC
16	A	1130	CLA	C10-C11-C12-C13
16	A	1237	CLA	C8-C10-C11-C12
16	B	1202	CLA	C13-C15-C16-C17
16	Y	511	CLA	C13-C15-C16-C17
16	a	1109	CLA	C10-C11-C12-C13
16	q	504	CLA	C5-C6-C7-C8
16	s	510	CLA	C15-C16-C17-C18
16	w	505	CLA	C15-C16-C17-C18

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	B	2002	PQN	C20-C21-C22-C23
17	G	2002	PQN	C25-C26-C27-C28
14	F	4017	LMG	C28-C29-C30-C31
14	Q	4017	LMG	C28-C29-C30-C31
16	H	1111	CLA	O1D-CGD-O2D-CED
13	A	851	LHG	C7-C8-C9-C10
13	G	4018	LHG	C7-C8-C9-C10
13	a	849	LHG	C23-C24-C25-C26
19	B	4014	BCR	C19-C20-C21-C22
19	L	4022	BCR	C19-C20-C21-C22
19	X	602	BCR	C9-C10-C11-C12
19	t	604	BCR	C13-C14-C15-C16
21	V	4021	ECH	C9-C10-C11-C12
16	A	1140	CLA	C16-C17-C18-C19
16	B	1228	CLA	C6-C7-C8-C10
16	G	1238	CLA	C16-C17-C18-C19
16	G	1238	CLA	C16-C17-C18-C20
16	b	1228	CLA	C6-C7-C8-C10
16	o	505	CLA	C16-C17-C18-C20
16	v	517	CLA	C6-C7-C8-C10
23	w	605	LMU	O5B-C5B-C6B-O6B
16	W	501	CLA	O1A-CGA-O2A-C1
16	p	508	CLA	O1A-CGA-O2A-C1
20	L	4101	LMT	O5B-C1B-O1B-C4'
16	H	1106	CLA	CBD-CGD-O2D-CED
16	W	506	CLA	CBD-CGD-O2D-CED
16	X	502	CLA	CBD-CGD-O2D-CED
16	s	509	CLA	CBD-CGD-O2D-CED
16	a	1128	CLA	O1D-CGD-O2D-CED
16	u	502	CLA	O1D-CGD-O2D-CED
16	H	1104	CLA	CBA-CGA-O2A-C1
16	a	1110	CLA	CBA-CGA-O2A-C1
16	a	1115	CLA	CBA-CGA-O2A-C1
16	b	1228	CLA	CBA-CGA-O2A-C1
16	h	514	CLA	CBA-CGA-O2A-C1
16	n	501	CLA	CBA-CGA-O2A-C1
16	o	502	CLA	CBA-CGA-O2A-C1
13	x	605	LHG	C11-C10-C9-C8
16	A	1132	CLA	C3-C5-C6-C7
16	B	1238	CLA	C3-C5-C6-C7
16	G	1203	CLA	C3-C5-C6-C7
16	Y	505	CLA	C3-C5-C6-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1110	CLA	C3-C5-C6-C7
13	H	849	LHG	C23-C24-C25-C26
16	n	512	CLA	C8-C10-C11-C12
16	x	504	CLA	C8-C10-C11-C12
23	s	606	LMU	C2B-C1B-O1B-C4'
13	H	849	LHG	C30-C31-C32-C33
13	R	103	LHG	C25-C26-C27-C28
13	i	103	LHG	C27-C28-C29-C30
23	x	606	LMU	C2-C3-C4-C5
16	K	4004	CLA	O1A-CGA-O2A-C1
16	a	1104	CLA	O1A-CGA-O2A-C1
16	b	1213	CLA	O1A-CGA-O2A-C1
16	n	511	CLA	O1A-CGA-O2A-C1
16	r	514	CLA	O1A-CGA-O2A-C1
16	u	512	CLA	O1A-CGA-O2A-C1
20	L	4101	LMT	C4B-C5B-C6B-O6B
13	b	4018	LHG	C14-C15-C16-C17
13	b	4018	LHG	C16-C17-C18-C19
16	A	1022	CLA	O1D-CGD-O2D-CED
16	H	1107	CLA	O1D-CGD-O2D-CED
16	B	1012	CLA	C5-C6-C7-C8
16	K	4003	CLA	C4C-C3C-CAC-CBC
16	H	1122	CLA	O1D-CGD-O2D-CED
16	B	1226	CLA	C11-C12-C13-C14
16	G	1021	CLA	C16-C17-C18-C20
16	X	515	CLA	C16-C17-C18-C19
16	o	515	CLA	C16-C17-C18-C19
16	B	1235	CLA	O1A-CGA-O2A-C1
16	r	506	CLA	O1A-CGA-O2A-C1
19	A	4003	BCR	C1-C6-C7-C8
19	A	4003	BCR	C5-C6-C7-C8
19	A	4008	BCR	C1-C6-C7-C8
19	A	4008	BCR	C23-C24-C25-C30
19	A	4011	BCR	C1-C6-C7-C8
19	A	4011	BCR	C23-C24-C25-C26
19	A	4011	BCR	C23-C24-C25-C30
19	B	4009	BCR	C23-C24-C25-C30
19	G	4004	BCR	C23-C24-C25-C30
19	G	4010	BCR	C1-C6-C7-C8
19	G	4010	BCR	C5-C6-C7-C8
19	H	4002	BCR	C1-C6-C7-C8
19	H	4011	BCR	C1-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	H	4011	BCR	C23-C24-C25-C26
19	H	4011	BCR	C23-C24-C25-C30
19	J	4012	BCR	C1-C6-C7-C8
19	J	4012	BCR	C5-C6-C7-C8
19	L	4022	BCR	C23-C24-C25-C26
19	L	4022	BCR	C23-C24-C25-C30
19	R	4018	BCR	C1-C6-C7-C8
19	R	4018	BCR	C5-C6-C7-C8
19	S	4012	BCR	C5-C6-C7-C8
19	S	4013	BCR	C23-C24-C25-C26
19	S	4013	BCR	C23-C24-C25-C30
19	T	4001	BCR	C1-C6-C7-C8
19	W	601	BCR	C1-C6-C7-C8
19	W	601	BCR	C23-C24-C25-C26
19	W	601	BCR	C23-C24-C25-C30
19	W	603	BCR	C1-C6-C7-C8
19	X	601	BCR	C1-C6-C7-C8
19	Y	601	BCR	C23-C24-C25-C26
19	Y	601	BCR	C23-C24-C25-C30
19	Y	604	BCR	C1-C6-C7-C8
19	Y	604	BCR	C5-C6-C7-C8
19	Y	604	BCR	C23-C24-C25-C26
19	Y	604	BCR	C23-C24-C25-C30
19	Z	602	BCR	C23-C24-C25-C26
19	Z	602	BCR	C23-C24-C25-C30
19	a	4002	BCR	C1-C6-C7-C8
19	a	4003	BCR	C1-C6-C7-C8
19	a	4003	BCR	C5-C6-C7-C8
19	a	4011	BCR	C23-C24-C25-C26
19	a	4011	BCR	C23-C24-C25-C30
19	g	603	BCR	C1-C6-C7-C8
19	g	603	BCR	C5-C6-C7-C8
19	g	604	BCR	C23-C24-C25-C30
19	h	601	BCR	C1-C6-C7-C8
19	h	601	BCR	C5-C6-C7-C8
19	h	601	BCR	C23-C24-C25-C26
19	h	601	BCR	C23-C24-C25-C30
19	h	603	BCR	C23-C24-C25-C30
19	h	604	BCR	C23-C24-C25-C26
19	h	604	BCR	C23-C24-C25-C30
19	j	4012	BCR	C1-C6-C7-C8
19	j	4012	BCR	C5-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	p	601	BCR	C1-C6-C7-C8
19	p	601	BCR	C23-C24-C25-C26
19	p	601	BCR	C23-C24-C25-C30
19	p	604	BCR	C1-C6-C7-C8
19	p	604	BCR	C5-C6-C7-C8
19	p	604	BCR	C23-C24-C25-C26
19	p	604	BCR	C23-C24-C25-C30
19	q	604	BCR	C1-C6-C7-C8
19	q	604	BCR	C5-C6-C7-C8
19	r	603	BCR	C1-C6-C7-C8
19	r	603	BCR	C5-C6-C7-C8
19	s	604	BCR	C1-C6-C7-C8
19	s	604	BCR	C5-C6-C7-C8
19	s	604	BCR	C23-C24-C25-C26
19	s	604	BCR	C23-C24-C25-C30
19	t	603	BCR	C1-C6-C7-C8
19	t	603	BCR	C5-C6-C7-C8
19	v	601	BCR	C23-C24-C25-C26
19	v	601	BCR	C23-C24-C25-C30
19	v	604	BCR	C23-C24-C25-C30
19	w	604	BCR	C1-C6-C7-C8
19	w	604	BCR	C5-C6-C7-C8
19	x	603	BCR	C1-C6-C7-C8
19	x	603	BCR	C5-C6-C7-C8
19	x	604	BCR	C1-C6-C7-C8
19	y	601	BCR	C1-C6-C7-C8
19	y	601	BCR	C5-C6-C7-C8
19	y	601	BCR	C23-C24-C25-C26
19	y	601	BCR	C23-C24-C25-C30
19	y	604	BCR	C23-C24-C25-C26
19	y	604	BCR	C23-C24-C25-C30
21	I	4020	ECH	C5-C6-C7-C8
21	M	4021	ECH	C5-C6-C7-C8
21	i	4020	ECH	C1-C6-C7-C8
21	i	4020	ECH	C5-C6-C7-C8
21	m	4021	ECH	C5-C6-C7-C8
24	q	601	LUT	C1-C6-C7-C8
24	q	601	LUT	C5-C6-C7-C8
16	B	1214	CLA	CBD-CGD-O2D-CED
16	t	513	CLA	O1A-CGA-O2A-C1
16	k	4003	CLA	C4C-C3C-CAC-CBC
16	G	1214	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1235	CLA	CBA-CGA-O2A-C1
16	w	505	CLA	CBA-CGA-O2A-C1
16	A	1237	CLA	C10-C11-C12-C13
16	B	1211	CLA	C13-C15-C16-C17
16	X	512	CLA	C3-C5-C6-C7
16	r	509	CLA	C3-C5-C6-C7
16	v	501	CLA	CBA-CGA-O2A-C1
14	G	848	LMG	C34-C35-C36-C37
16	A	1138	CLA	C2A-CAA-CBA-CGA
16	G	1201	CLA	C2A-CAA-CBA-CGA
16	W	508	CLA	C2A-CAA-CBA-CGA
16	X	505	CLA	C2A-CAA-CBA-CGA
16	Y	501	CLA	C2A-CAA-CBA-CGA
16	a	1116	CLA	C2A-CAA-CBA-CGA
16	a	1126	CLA	C2A-CAA-CBA-CGA
16	b	1229	CLA	C2A-CAA-CBA-CGA
16	g	504	CLA	C2A-CAA-CBA-CGA
16	g	513	CLA	C2A-CAA-CBA-CGA
16	k	4002	CLA	C2A-CAA-CBA-CGA
16	o	508	CLA	C2A-CAA-CBA-CGA
16	p	501	CLA	C2A-CAA-CBA-CGA
16	q	505	CLA	C2A-CAA-CBA-CGA
16	u	505	CLA	C2A-CAA-CBA-CGA
16	x	503	CLA	C2A-CAA-CBA-CGA
16	y	504	CLA	C2A-CAA-CBA-CGA
16	y	505	CLA	C2A-CAA-CBA-CGA
16	h	515	CLA	C8-C10-C11-C12
16	n	509	CLA	C10-C11-C12-C13
13	Y	605	LHG	C24-C25-C26-C27
14	A	4201	LMG	O10-C28-O8-C9
16	a	1115	CLA	O1A-CGA-O2A-C1
16	g	514	CLA	O1A-CGA-O2A-C1
16	n	501	CLA	O1A-CGA-O2A-C1
16	s	508	CLA	O1A-CGA-O2A-C1
16	p	503	CLA	O1A-CGA-O2A-C1
13	I	103	LHG	C27-C28-C29-C30
13	H	851	LHG	O9-C7-O7-C5
13	a	849	LHG	O9-C7-O7-C5
16	A	1022	CLA	C4C-C3C-CAC-CBC
16	Y	504	CLA	C4-C3-C5-C6
16	a	1136	CLA	C4-C3-C5-C6
16	b	1228	CLA	C4-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1238	CLA	O1D-CGD-O2D-CED
16	r	502	CLA	O1D-CGD-O2D-CED
19	A	4003	BCR	C10-C11-C12-C13
19	G	4005	BCR	C18-C19-C20-C21
19	J	4012	BCR	C10-C11-C12-C13
19	K	4001	BCR	C18-C19-C20-C21
19	L	4019	BCR	C10-C11-C12-C13
19	T	4001	BCR	C18-C19-C20-C21
19	Y	604	BCR	C10-C11-C12-C13
19	a	4008	BCR	C10-C11-C12-C13
19	b	4014	BCR	C10-C11-C12-C13
19	f	4016	BCR	C18-C19-C20-C21
19	g	601	BCR	C18-C19-C20-C21
19	g	604	BCR	C10-C11-C12-C13
19	j	4015	BCR	C18-C19-C20-C21
19	l	4019	BCR	C10-C11-C12-C13
19	o	604	BCR	C18-C19-C20-C21
19	q	604	BCR	C10-C11-C12-C13
19	u	602	BCR	C18-C19-C20-C21
19	u	604	BCR	C10-C11-C12-C13
19	v	603	BCR	C18-C19-C20-C21
19	w	604	BCR	C10-C11-C12-C13
19	y	601	BCR	C10-C11-C12-C13
16	G	1221	CLA	C10-C11-C12-C13
16	X	512	CLA	C15-C16-C17-C18
16	L	1502	CLA	C2-C3-C5-C6
16	r	505	CLA	C2-C3-C5-C6
16	b	1204	CLA	C16-C17-C18-C19
20	H	4202	LMT	O1'-C1-C2-C3
14	H	4101	LMG	C28-C29-C30-C31
13	x	605	LHG	C24-C23-O8-C6
16	G	1213	CLA	CBA-CGA-O2A-C1
16	g	506	CLA	CBA-CGA-O2A-C1
16	p	502	CLA	CBA-CGA-O2A-C1
16	t	514	CLA	CBA-CGA-O2A-C1
16	g	505	CLA	C3-C5-C6-C7
16	a	1106	CLA	C11-C10-C8-C9
16	v	515	CLA	C6-C7-C8-C9
14	a	4101	LMG	C30-C31-C32-C33
16	b	1207	CLA	C5-C6-C7-C8
16	A	1122	CLA	C4C-C3C-CAC-CBC
16	Y	509	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	A	4008	BCR	C6-C7-C8-C9
19	B	4010	BCR	C6-C7-C8-C9
19	B	4017	BCR	C22-C23-C24-C25
19	a	4002	BCR	C6-C7-C8-C9
19	g	601	BCR	C6-C7-C8-C9
19	v	601	BCR	C6-C7-C8-C9
14	B	848	LMG	C13-C14-C15-C16
16	a	1112	CLA	CBD-CGD-O2D-CED
16	X	511	CLA	C8-C10-C11-C12
16	a	1101	CLA	C5-C6-C7-C8
16	g	509	CLA	C13-C15-C16-C17
16	q	515	CLA	C15-C16-C17-C18
16	v	505	CLA	C10-C11-C12-C13
14	A	4101	LMG	C30-C31-C32-C33
14	b	848	LMG	C34-C35-C36-C37
20	l	4101	LMT	C4-C5-C6-C7
16	A	1114	CLA	O1A-CGA-O2A-C1
14	H	4101	LMG	C30-C31-C32-C33
20	a	4202	LMT	O1'-C1-C2-C3
16	H	1109	CLA	C10-C11-C12-C13
16	v	517	CLA	C3-C5-C6-C7
16	G	1210	CLA	CBA-CGA-O2A-C1
16	v	511	CLA	CBA-CGA-O2A-C1
19	G	4010	BCR	C13-C14-C15-C16
19	G	4014	BCR	C13-C14-C15-C16
19	U	4019	BCR	C9-C10-C11-C12
19	X	602	BCR	C19-C20-C21-C22
19	Z	604	BCR	C13-C14-C15-C16
19	p	604	BCR	C13-C14-C15-C16
19	u	604	BCR	C19-C20-C21-C22
15	A	1011	CL0	C16-C17-C18-C19
16	W	512	CLA	C11-C12-C13-C15
16	p	509	CLA	C11-C12-C13-C15
16	u	515	CLA	C16-C17-C18-C20
13	A	849	LHG	C8-C7-O7-C5
13	H	849	LHG	C8-C7-O7-C5
13	a	849	LHG	C8-C7-O7-C5
14	a	4201	LMG	C11-C10-O7-C8
16	H	1104	CLA	O1A-CGA-O2A-C1
14	b	848	LMG	C35-C36-C37-C38
16	B	1021	CLA	C13-C15-C16-C17
16	Z	512	CLA	C8-C10-C11-C12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1127	CLA	C15-C16-C17-C18
16	n	515	CLA	C13-C15-C16-C17
14	Q	4017	LMG	O9-C10-O7-C8
16	A	1129	CLA	O1A-CGA-O2A-C1
14	B	848	LMG	C34-C35-C36-C37
16	a	1133	CLA	C5-C6-C7-C8
16	q	503	CLA	C2C-C3C-CAC-CBC
16	a	1110	CLA	O1A-CGA-O2A-C1
16	G	1223	CLA	C13-C15-C16-C17
19	A	4002	BCR	C37-C22-C23-C24
19	a	4007	BCR	C37-C22-C23-C24
19	h	603	BCR	C7-C8-C9-C34
19	n	604	BCR	C7-C8-C9-C34
19	r	603	BCR	C7-C8-C9-C34
19	r	604	BCR	C7-C8-C9-C34
19	u	602	BCR	C37-C22-C23-C24
19	v	603	BCR	C7-C8-C9-C34
19	y	603	BCR	C7-C8-C9-C34
24	w	601	LUT	C7-C8-C9-C19
16	H	1129	CLA	CBA-CGA-O2A-C1
14	b	848	LMG	C28-C29-C30-C31
15	H	1011	CL0	C3-C5-C6-C7
16	H	1102	CLA	C3-C5-C6-C7
16	W	515	CLA	C3-C5-C6-C7
19	B	4014	BCR	C21-C22-C23-C24
19	K	4005	BCR	C21-C22-C23-C24
19	L	4022	BCR	C21-C22-C23-C24
19	l	4022	BCR	C21-C22-C23-C24
19	u	602	BCR	C21-C22-C23-C24
19	x	602	BCR	C11-C12-C13-C14
13	a	849	LHG	C30-C31-C32-C33
16	l	1503	CLA	C2A-CAA-CBA-CGA
16	o	501	CLA	C2A-CAA-CBA-CGA
16	A	1117	CLA	C16-C17-C18-C20
16	b	1012	CLA	C6-C7-C8-C10
16	b	1215	CLA	C11-C12-C13-C15
16	p	509	CLA	C11-C12-C13-C14
17	b	2002	PQN	C26-C27-C28-C30
16	Y	510	CLA	CBD-CGD-O2D-CED
16	a	1119	CLA	CBD-CGD-O2D-CED
16	G	1205	CLA	C4-C3-C5-C6
16	G	1213	CLA	C4-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	W	512	CLA	C4-C3-C5-C6
16	X	508	CLA	C4-C3-C5-C6
16	a	1136	CLA	C2-C3-C5-C6
13	Y	605	LHG	C23-C24-C25-C26
16	G	1023	CLA	C10-C11-C12-C13
16	H	1130	CLA	C8-C10-C11-C12
16	Y	505	CLA	C8-C10-C11-C12
16	a	1022	CLA	C13-C15-C16-C17
16	g	505	CLA	C8-C10-C11-C12
16	o	506	CLA	C10-C11-C12-C13
13	A	849	LHG	C30-C31-C32-C33
16	w	503	CLA	C2C-C3C-CAC-CBC
16	G	1226	CLA	O1D-CGD-O2D-CED
16	H	1139	CLA	O1D-CGD-O2D-CED
16	b	1228	CLA	O1A-CGA-O2A-C1
16	h	514	CLA	O1A-CGA-O2A-C1
16	o	502	CLA	O1A-CGA-O2A-C1
16	b	1218	CLA	C3-C5-C6-C7
16	H	1109	CLA	C15-C16-C17-C18
16	w	506	CLA	C5-C6-C7-C8
15	A	1011	CL0	CBA-CGA-O2A-C1
16	v	512	CLA	CBA-CGA-O2A-C1
13	i	103	LHG	C7-C8-C9-C10
13	I	103	LHG	C30-C31-C32-C33
14	F	4017	LMG	O9-C10-O7-C8
14	A	852	LMG	O6-C5-C6-O5
16	B	1225	CLA	C15-C16-C17-C18
16	X	504	CLA	C5-C6-C7-C8
16	Y	504	CLA	C5-C6-C7-C8
16	q	505	CLA	C15-C16-C17-C18
16	u	515	CLA	C10-C11-C12-C13
16	G	1226	CLA	C11-C12-C13-C15
16	W	505	CLA	C16-C17-C18-C20
20	A	4202	LMT	O1'-C1-C2-C3
13	H	851	LHG	C7-C8-C9-C10
13	b	4018	LHG	C23-C24-C25-C26
16	A	1125	CLA	C15-C16-C17-C18
16	A	1126	CLA	C8-C10-C11-C12
16	H	1127	CLA	C8-C10-C11-C12
16	Y	510	CLA	C5-C6-C7-C8
16	b	1207	CLA	C13-C15-C16-C17
16	q	512	CLA	C8-C10-C11-C12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	w	509	CLA	C15-C16-C17-C18
16	x	515	CLA	C8-C10-C11-C12
16	y	505	CLA	C8-C10-C11-C12
16	H	1115	CLA	O1D-CGD-O2D-CED
16	o	515	CLA	O1D-CGD-O2D-CED
16	x	512	CLA	O1D-CGD-O2D-CED
14	A	4101	LMG	O6-C5-C6-O5
14	H	4101	LMG	O6-C5-C6-O5
16	b	1240	CLA	O1A-CGA-O2A-C1
16	s	517	CLA	C3-C5-C6-C7
13	o	605	LHG	O7-C5-C6-O8
13	u	605	LHG	O7-C5-C6-O8
14	B	848	LMG	O7-C8-C9-O8
14	G	848	LMG	O7-C8-C9-O8
14	a	4201	LMG	O7-C8-C9-O8
16	q	516	CLA	O1D-CGD-O2D-CED
16	a	1101	CLA	CBA-CGA-O2A-C1
16	n	514	CLA	CBA-CGA-O2A-C1
16	u	505	CLA	C15-C16-C17-C18
16	v	505	CLA	C5-C6-C7-C8
16	y	508	CLA	C5-C6-C7-C8
23	Z	605	LMU	O5B-C5B-C6B-O6B
23	s	606	LMU	C4'-C5'-C6'-O6'
16	G	1220	CLA	C2-C1-O2A-CGA
16	B	1012	CLA	C6-C7-C8-C9
16	W	505	CLA	C16-C17-C18-C19
16	H	1140	CLA	C15-C16-C17-C18
16	p	504	CLA	C8-C10-C11-C12
17	G	2002	PQN	C20-C21-C22-C23
16	H	1132	CLA	C4-C3-C5-C6
16	a	1013	CLA	C4-C3-C5-C6
16	b	1205	CLA	C4-C3-C5-C6
16	h	507	CLA	C4-C3-C5-C6
16	n	512	CLA	C4-C3-C5-C6
16	q	512	CLA	C4-C3-C5-C6
16	G	1229	CLA	C3-C5-C6-C7
16	H	1132	CLA	C3-C5-C6-C7
16	h	506	CLA	C3-C5-C6-C7
16	W	512	CLA	C2-C3-C5-C6
16	t	509	CLA	C10-C11-C12-C13
16	A	1122	CLA	C2A-CAA-CBA-CGA
16	A	1237	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1219	CLA	C2A-CAA-CBA-CGA
16	B	1223	CLA	C2A-CAA-CBA-CGA
16	B	1224	CLA	C2A-CAA-CBA-CGA
16	G	1219	CLA	C2A-CAA-CBA-CGA
16	H	1116	CLA	C2A-CAA-CBA-CGA
16	H	1122	CLA	C2A-CAA-CBA-CGA
16	H	1237	CLA	C2A-CAA-CBA-CGA
16	Y	515	CLA	C2A-CAA-CBA-CGA
16	a	1022	CLA	C2A-CAA-CBA-CGA
16	a	1237	CLA	C2A-CAA-CBA-CGA
16	b	1224	CLA	C2A-CAA-CBA-CGA
16	h	501	CLA	C2A-CAA-CBA-CGA
16	h	505	CLA	C2A-CAA-CBA-CGA
16	h	515	CLA	C2A-CAA-CBA-CGA
16	n	509	CLA	C2A-CAA-CBA-CGA
16	o	513	CLA	C2A-CAA-CBA-CGA
16	p	508	CLA	C2A-CAA-CBA-CGA
16	p	515	CLA	C2A-CAA-CBA-CGA
16	q	507	CLA	C2A-CAA-CBA-CGA
16	t	508	CLA	C2A-CAA-CBA-CGA
16	w	505	CLA	C2A-CAA-CBA-CGA
16	w	513	CLA	C2A-CAA-CBA-CGA
16	h	517	CLA	CBD-CGD-O2D-CED
16	B	1228	CLA	O1D-CGD-O2D-CED
16	A	1101	CLA	CBA-CGA-O2A-C1
16	W	507	CLA	CBA-CGA-O2A-C1
16	t	511	CLA	CBA-CGA-O2A-C1
16	p	516	CLA	O1A-CGA-O2A-C1
16	t	503	CLA	O1A-CGA-O2A-C1
16	x	503	CLA	O1A-CGA-O2A-C1
16	H	1128	CLA	O1D-CGD-O2D-CED
16	Z	508	CLA	O1D-CGD-O2D-CED
16	a	1140	CLA	C15-C16-C17-C18
16	q	505	CLA	C10-C11-C12-C13
16	t	515	CLA	C13-C15-C16-C17
14	H	4201	LMG	C10-C11-C12-C13
16	u	515	CLA	C16-C17-C18-C19
13	a	849	LHG	O1-C1-C2-O2
16	G	1213	CLA	O1A-CGA-O2A-C1
16	t	514	CLA	O1A-CGA-O2A-C1
16	w	505	CLA	O1A-CGA-O2A-C1
16	G	1211	CLA	C3-C5-C6-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	Y	517	CLA	C3-C5-C6-C7
13	a	849	LHG	C24-C25-C26-C27
16	A	1109	CLA	C1A-C2A-CAA-CBA
16	A	1116	CLA	C1A-C2A-CAA-CBA
16	A	1119	CLA	C1A-C2A-CAA-CBA
16	A	1122	CLA	C1A-C2A-CAA-CBA
16	A	1126	CLA	C1A-C2A-CAA-CBA
16	A	1128	CLA	C1A-C2A-CAA-CBA
16	A	1133	CLA	C1A-C2A-CAA-CBA
16	A	1237	CLA	C1A-C2A-CAA-CBA
16	B	1208	CLA	C1A-C2A-CAA-CBA
16	B	1212	CLA	C1A-C2A-CAA-CBA
16	B	1213	CLA	C1A-C2A-CAA-CBA
16	B	1216	CLA	C1A-C2A-CAA-CBA
16	B	1218	CLA	C1A-C2A-CAA-CBA
16	B	1223	CLA	C1A-C2A-CAA-CBA
16	B	1224	CLA	C1A-C2A-CAA-CBA
16	B	1225	CLA	C1A-C2A-CAA-CBA
16	B	1226	CLA	C1A-C2A-CAA-CBA
16	F	1302	CLA	C1A-C2A-CAA-CBA
16	G	1203	CLA	C1A-C2A-CAA-CBA
16	G	1206	CLA	C1A-C2A-CAA-CBA
16	G	1208	CLA	C1A-C2A-CAA-CBA
16	G	1212	CLA	C1A-C2A-CAA-CBA
16	G	1214	CLA	C1A-C2A-CAA-CBA
16	G	1216	CLA	C1A-C2A-CAA-CBA
16	G	1224	CLA	C1A-C2A-CAA-CBA
16	G	1225	CLA	C1A-C2A-CAA-CBA
16	G	1226	CLA	C1A-C2A-CAA-CBA
16	G	1228	CLA	C1A-C2A-CAA-CBA
16	H	1109	CLA	C1A-C2A-CAA-CBA
16	H	1116	CLA	C1A-C2A-CAA-CBA
16	H	1119	CLA	C1A-C2A-CAA-CBA
16	H	1126	CLA	C1A-C2A-CAA-CBA
16	H	1129	CLA	C1A-C2A-CAA-CBA
16	H	1138	CLA	C1A-C2A-CAA-CBA
16	H	1237	CLA	C1A-C2A-CAA-CBA
16	Q	1302	CLA	C1A-C2A-CAA-CBA
16	T	4002	CLA	C1A-C2A-CAA-CBA
16	W	501	CLA	C1A-C2A-CAA-CBA
16	W	512	CLA	C1A-C2A-CAA-CBA
16	W	515	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	X	501	CLA	C1A-C2A-CAA-CBA
16	X	511	CLA	C1A-C2A-CAA-CBA
16	X	517	CLA	C1A-C2A-CAA-CBA
16	Y	501	CLA	C1A-C2A-CAA-CBA
16	Y	504	CLA	C1A-C2A-CAA-CBA
16	Y	506	CLA	C1A-C2A-CAA-CBA
16	Y	509	CLA	C1A-C2A-CAA-CBA
16	Y	511	CLA	C1A-C2A-CAA-CBA
16	Y	514	CLA	C1A-C2A-CAA-CBA
16	Y	515	CLA	C1A-C2A-CAA-CBA
16	Y	517	CLA	C1A-C2A-CAA-CBA
16	Z	501	CLA	C1A-C2A-CAA-CBA
16	Z	504	CLA	C1A-C2A-CAA-CBA
16	Z	505	CLA	C1A-C2A-CAA-CBA
16	Z	506	CLA	C1A-C2A-CAA-CBA
16	Z	510	CLA	C1A-C2A-CAA-CBA
16	a	1022	CLA	C1A-C2A-CAA-CBA
16	a	1102	CLA	C1A-C2A-CAA-CBA
16	a	1109	CLA	C1A-C2A-CAA-CBA
16	a	1115	CLA	C1A-C2A-CAA-CBA
16	a	1116	CLA	C1A-C2A-CAA-CBA
16	a	1119	CLA	C1A-C2A-CAA-CBA
16	a	1126	CLA	C1A-C2A-CAA-CBA
16	a	1128	CLA	C1A-C2A-CAA-CBA
16	a	1129	CLA	C1A-C2A-CAA-CBA
16	a	1134	CLA	C1A-C2A-CAA-CBA
16	b	1012	CLA	C1A-C2A-CAA-CBA
16	b	1023	CLA	C1A-C2A-CAA-CBA
16	b	1203	CLA	C1A-C2A-CAA-CBA
16	b	1212	CLA	C1A-C2A-CAA-CBA
16	b	1217	CLA	C1A-C2A-CAA-CBA
16	b	1218	CLA	C1A-C2A-CAA-CBA
16	b	1219	CLA	C1A-C2A-CAA-CBA
16	b	1221	CLA	C1A-C2A-CAA-CBA
16	b	1223	CLA	C1A-C2A-CAA-CBA
16	b	1224	CLA	C1A-C2A-CAA-CBA
16	b	1225	CLA	C1A-C2A-CAA-CBA
16	b	1228	CLA	C1A-C2A-CAA-CBA
16	f	1302	CLA	C1A-C2A-CAA-CBA
16	g	509	CLA	C1A-C2A-CAA-CBA
16	g	513	CLA	C1A-C2A-CAA-CBA
16	g	514	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	h	512	CLA	C1A-C2A-CAA-CBA
16	h	514	CLA	C1A-C2A-CAA-CBA
16	h	517	CLA	C1A-C2A-CAA-CBA
16	k	4002	CLA	C1A-C2A-CAA-CBA
16	n	501	CLA	C1A-C2A-CAA-CBA
16	n	503	CLA	C1A-C2A-CAA-CBA
16	n	504	CLA	C1A-C2A-CAA-CBA
16	n	508	CLA	C1A-C2A-CAA-CBA
16	n	511	CLA	C1A-C2A-CAA-CBA
16	n	512	CLA	C1A-C2A-CAA-CBA
16	n	514	CLA	C1A-C2A-CAA-CBA
16	n	515	CLA	C1A-C2A-CAA-CBA
16	o	514	CLA	C1A-C2A-CAA-CBA
16	o	515	CLA	C1A-C2A-CAA-CBA
16	o	516	CLA	C1A-C2A-CAA-CBA
16	p	504	CLA	C1A-C2A-CAA-CBA
16	p	505	CLA	C1A-C2A-CAA-CBA
16	p	506	CLA	C1A-C2A-CAA-CBA
16	p	509	CLA	C1A-C2A-CAA-CBA
16	p	511	CLA	C1A-C2A-CAA-CBA
16	p	514	CLA	C1A-C2A-CAA-CBA
16	p	515	CLA	C1A-C2A-CAA-CBA
16	p	516	CLA	C1A-C2A-CAA-CBA
16	p	517	CLA	C1A-C2A-CAA-CBA
16	q	506	CLA	C1A-C2A-CAA-CBA
16	q	509	CLA	C1A-C2A-CAA-CBA
16	q	512	CLA	C1A-C2A-CAA-CBA
16	q	514	CLA	C1A-C2A-CAA-CBA
16	r	504	CLA	C1A-C2A-CAA-CBA
16	r	509	CLA	C1A-C2A-CAA-CBA
16	s	504	CLA	C1A-C2A-CAA-CBA
16	s	506	CLA	C1A-C2A-CAA-CBA
16	s	509	CLA	C1A-C2A-CAA-CBA
16	s	511	CLA	C1A-C2A-CAA-CBA
16	s	514	CLA	C1A-C2A-CAA-CBA
16	t	503	CLA	C1A-C2A-CAA-CBA
16	t	512	CLA	C1A-C2A-CAA-CBA
16	t	514	CLA	C1A-C2A-CAA-CBA
16	u	517	CLA	C1A-C2A-CAA-CBA
16	v	501	CLA	C1A-C2A-CAA-CBA
16	v	503	CLA	C1A-C2A-CAA-CBA
16	v	511	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	v	517	CLA	C1A-C2A-CAA-CBA
16	w	506	CLA	C1A-C2A-CAA-CBA
16	w	512	CLA	C1A-C2A-CAA-CBA
16	w	516	CLA	C1A-C2A-CAA-CBA
16	x	506	CLA	C1A-C2A-CAA-CBA
16	x	513	CLA	C1A-C2A-CAA-CBA
16	x	514	CLA	C1A-C2A-CAA-CBA
16	x	515	CLA	C1A-C2A-CAA-CBA
16	y	501	CLA	C1A-C2A-CAA-CBA
16	y	504	CLA	C1A-C2A-CAA-CBA
16	y	506	CLA	C1A-C2A-CAA-CBA
16	y	512	CLA	C1A-C2A-CAA-CBA
16	A	1134	CLA	O1D-CGD-O2D-CED
13	Y	605	LHG	C24-C23-O8-C6
16	a	1105	CLA	CBD-CGD-O2D-CED
16	b	1012	CLA	C5-C6-C7-C8
13	B	4018	LHG	C12-C13-C14-C15
16	G	1235	CLA	O1A-CGA-O2A-C1
14	a	852	LMG	C32-C33-C34-C35
16	G	1218	CLA	C5-C6-C7-C8
16	G	1201	CLA	O1D-CGD-O2D-CED
13	X	605	LHG	O6-C4-C5-C6
13	H	849	LHG	O9-C7-O7-C5
13	i	103	LHG	O9-C7-O7-C5
13	H	849	LHG	C24-C25-C26-C27
16	A	1013	CLA	C11-C12-C13-C15
16	A	1022	CLA	C12-C13-C15-C16
16	A	1101	CLA	C11-C10-C8-C7
16	A	1119	CLA	C6-C7-C8-C10
16	A	1125	CLA	C11-C10-C8-C7
16	B	1202	CLA	C6-C7-C8-C10
16	B	1204	CLA	C6-C7-C8-C10
16	B	1206	CLA	C11-C10-C8-C7
16	B	1207	CLA	C12-C13-C15-C16
16	B	1210	CLA	C11-C10-C8-C7
16	B	1211	CLA	C6-C7-C8-C10
16	B	1221	CLA	C12-C13-C15-C16
16	B	1225	CLA	C6-C7-C8-C10
16	B	1225	CLA	C12-C13-C15-C16
16	B	1235	CLA	C6-C7-C8-C10
16	G	1023	CLA	C12-C13-C15-C16
16	G	1202	CLA	C6-C7-C8-C10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1211	CLA	C6-C7-C8-C10
16	G	1211	CLA	C11-C12-C13-C15
16	G	1225	CLA	C6-C7-C8-C10
16	G	1235	CLA	C6-C7-C8-C10
16	H	1022	CLA	C12-C13-C15-C16
16	H	1101	CLA	C6-C7-C8-C10
16	H	1117	CLA	C11-C12-C13-C15
16	W	510	CLA	C6-C7-C8-C10
16	W	512	CLA	C6-C7-C8-C10
16	W	515	CLA	C12-C13-C15-C16
16	X	506	CLA	C6-C7-C8-C10
16	X	511	CLA	C11-C12-C13-C15
16	Y	505	CLA	C11-C10-C8-C7
16	Y	506	CLA	C11-C10-C8-C7
16	Y	511	CLA	C6-C7-C8-C10
16	Z	505	CLA	C11-C12-C13-C15
16	Z	507	CLA	C11-C10-C8-C7
16	Z	512	CLA	C11-C12-C13-C15
16	a	1013	CLA	C11-C10-C8-C7
16	a	1022	CLA	C12-C13-C15-C16
16	a	1119	CLA	C12-C13-C15-C16
16	a	1123	CLA	C11-C12-C13-C15
16	a	1131	CLA	C6-C7-C8-C10
16	b	1202	CLA	C6-C7-C8-C10
16	b	1204	CLA	C6-C7-C8-C10
16	b	1206	CLA	C12-C13-C15-C16
16	b	1207	CLA	C12-C13-C15-C16
16	b	1210	CLA	C6-C7-C8-C10
16	b	1221	CLA	C11-C10-C8-C7
16	b	1225	CLA	C6-C7-C8-C10
16	b	1225	CLA	C12-C13-C15-C16
16	g	506	CLA	C11-C10-C8-C7
16	g	510	CLA	C6-C7-C8-C10
16	h	506	CLA	C11-C10-C8-C7
16	h	511	CLA	C12-C13-C15-C16
16	h	512	CLA	C11-C12-C13-C15
16	h	515	CLA	C6-C7-C8-C10
16	n	510	CLA	C6-C7-C8-C10
16	n	512	CLA	C6-C7-C8-C10
16	n	512	CLA	C11-C12-C13-C15
16	n	515	CLA	C6-C7-C8-C10
16	o	511	CLA	C11-C12-C13-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	q	512	CLA	C12-C13-C15-C16
16	r	515	CLA	C11-C12-C13-C15
16	s	511	CLA	C11-C12-C13-C15
16	t	506	CLA	C11-C10-C8-C7
16	t	512	CLA	C11-C12-C13-C15
16	u	511	CLA	C11-C12-C13-C15
16	u	512	CLA	C6-C7-C8-C10
16	v	507	CLA	C11-C10-C8-C7
16	y	507	CLA	C11-C10-C8-C7
16	y	511	CLA	C12-C13-C15-C16
16	y	515	CLA	C11-C10-C8-C7
16	G	1207	CLA	C13-C15-C16-C17
16	t	505	CLA	C8-C10-C11-C12
16	r	516	CLA	O1A-CGA-O2A-C1
16	G	1210	CLA	O1A-CGA-O2A-C1
16	p	502	CLA	O1A-CGA-O2A-C1
14	f	4017	LMG	O6-C5-C6-O5
16	H	1120	CLA	O1D-CGD-O2D-CED
16	p	515	CLA	O1D-CGD-O2D-CED
16	y	514	CLA	CBA-CGA-O2A-C1
14	G	848	LMG	C4-C5-C6-O5
16	n	515	CLA	CBD-CGD-O2D-CED
16	a	1103	CLA	C13-C15-C16-C17
23	s	606	LMU	O5B-C1B-O1B-C4'
16	A	1132	CLA	C4-C3-C5-C6
16	B	1204	CLA	C4-C3-C5-C6
16	b	1204	CLA	C4-C3-C5-C6
16	A	1132	CLA	C2-C3-C5-C6
16	G	1205	CLA	C2-C3-C5-C6
16	a	1132	CLA	C2-C3-C5-C6
16	b	1204	CLA	C2-C3-C5-C6
16	o	509	CLA	C2-C3-C5-C6
16	h	509	CLA	C4C-C3C-CAC-CBC
16	v	511	CLA	O1A-CGA-O2A-C1
13	r	605	LHG	C11-C10-C9-C8
16	H	1122	CLA	C4C-C3C-CAC-CBC
16	p	506	CLA	C4C-C3C-CAC-CBC
16	B	1210	CLA	C10-C11-C12-C13
16	H	1125	CLA	C13-C15-C16-C17
16	h	509	CLA	C15-C16-C17-C18
14	f	4017	LMG	C28-C29-C30-C31
16	A	1022	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1012	CLA	C2A-CAA-CBA-CGA
16	H	1022	CLA	C2A-CAA-CBA-CGA
16	H	1129	CLA	C2A-CAA-CBA-CGA
16	X	513	CLA	C2A-CAA-CBA-CGA
16	s	505	CLA	C2A-CAA-CBA-CGA
16	s	508	CLA	C2A-CAA-CBA-CGA
16	u	501	CLA	C2A-CAA-CBA-CGA
16	v	515	CLA	C2A-CAA-CBA-CGA
16	y	501	CLA	C2A-CAA-CBA-CGA
16	A	1125	CLA	C11-C10-C8-C9
16	A	1128	CLA	C11-C12-C13-C14
16	A	1131	CLA	C11-C10-C8-C9
16	B	1202	CLA	C6-C7-C8-C9
16	B	1203	CLA	C14-C13-C15-C16
16	B	1204	CLA	C6-C7-C8-C9
16	B	1211	CLA	C6-C7-C8-C9
16	B	1221	CLA	C11-C10-C8-C9
16	G	1221	CLA	C6-C7-C8-C9
16	G	1221	CLA	C11-C10-C8-C9
16	G	1224	CLA	C11-C10-C8-C9
16	G	1225	CLA	C6-C7-C8-C9
16	H	1022	CLA	C14-C13-C15-C16
16	H	1131	CLA	C11-C10-C8-C9
16	W	505	CLA	C11-C12-C13-C14
16	W	512	CLA	C6-C7-C8-C9
16	W	515	CLA	C6-C7-C8-C9
16	X	515	CLA	C6-C7-C8-C9
16	Y	506	CLA	C11-C10-C8-C9
16	Z	512	CLA	C11-C12-C13-C14
16	a	1104	CLA	C11-C10-C8-C9
16	a	1128	CLA	C11-C12-C13-C14
16	b	1210	CLA	C6-C7-C8-C9
16	b	1211	CLA	C6-C7-C8-C9
16	b	1225	CLA	C14-C13-C15-C16
16	b	1226	CLA	C6-C7-C8-C9
16	g	511	CLA	C11-C10-C8-C9
16	h	506	CLA	C11-C10-C8-C9
16	n	506	CLA	C11-C10-C8-C9
16	n	510	CLA	C6-C7-C8-C9
16	n	512	CLA	C11-C10-C8-C9
16	o	515	CLA	C6-C7-C8-C9
16	p	505	CLA	C11-C10-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	q	506	CLA	C6-C7-C8-C9
16	q	506	CLA	C11-C10-C8-C9
16	r	511	CLA	C11-C10-C8-C9
16	r	515	CLA	C11-C12-C13-C14
16	u	504	CLA	C6-C7-C8-C9
16	u	506	CLA	C6-C7-C8-C9
16	x	506	CLA	C11-C10-C8-C9
16	x	511	CLA	C14-C13-C15-C16
16	y	507	CLA	C11-C10-C8-C9
16	y	511	CLA	C6-C7-C8-C9
16	y	511	CLA	C14-C13-C15-C16
17	b	2002	PQN	C24-C23-C25-C26
20	U	4101	LMT	C4-C5-C6-C7
14	a	4101	LMG	C28-C29-C30-C31
19	y	603	BCR	C9-C10-C11-C12
16	A	1128	CLA	O1D-CGD-O2D-CED
13	R	103	LHG	C24-C23-O8-C6
14	H	852	LMG	C29-C28-O8-C9
16	A	1123	CLA	CBA-CGA-O2A-C1
16	W	514	CLA	CBA-CGA-O2A-C1
16	X	512	CLA	CBA-CGA-O2A-C1
16	h	509	CLA	CBA-CGA-O2A-C1
16	x	504	CLA	CBA-CGA-O2A-C1
16	a	1130	CLA	C10-C11-C12-C13
16	Z	516	CLA	O1A-CGA-O2A-C1
14	A	4101	LMG	C17-C18-C19-C20
14	F	4017	LMG	O6-C5-C6-O5
16	B	1222	CLA	CBD-CGD-O2D-CED
16	H	1138	CLA	CBD-CGD-O2D-CED
16	Y	516	CLA	CBD-CGD-O2D-CED
13	A	849	LHG	C29-C30-C31-C32
16	X	505	CLA	C10-C11-C12-C13
16	a	1101	CLA	C8-C10-C11-C12
16	a	1138	CLA	C10-C11-C12-C13
14	A	4201	LMG	C28-C29-C30-C31
16	q	508	CLA	O1D-CGD-O2D-CED
13	X	605	LHG	C4-C5-C6-O8
13	p	605	LHG	C4-C5-C6-O8
13	u	605	LHG	C4-C5-C6-O8
14	A	852	LMG	C7-C8-C9-O8
14	H	4201	LMG	C7-C8-C9-O8
14	a	852	LMG	C7-C8-C9-O8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	a	4201	LMG	C7-C8-C9-O8
23	q	605	LMU	O5B-C5B-C6B-O6B
13	b	4018	LHG	C17-C18-C19-C20
16	G	1207	CLA	C5-C6-C7-C8
16	Y	505	CLA	C13-C15-C16-C17
16	g	502	CLA	O1D-CGD-O2D-CED
16	H	1127	CLA	CBA-CGA-O2A-C1
16	Y	508	CLA	CBA-CGA-O2A-C1
16	a	1136	CLA	CBA-CGA-O2A-C1
16	b	1210	CLA	CBA-CGA-O2A-C1
16	p	514	CLA	CBA-CGA-O2A-C1
16	s	506	CLA	CBA-CGA-O2A-C1
16	s	511	CLA	CBA-CGA-O2A-C1
14	H	852	LMG	O6-C5-C6-O5
14	Q	4017	LMG	O6-C5-C6-O5
16	B	1012	CLA	C6-C7-C8-C10
16	G	1202	CLA	C16-C17-C18-C20
16	Z	509	CLA	C16-C17-C18-C19
16	b	1215	CLA	C11-C12-C13-C14
16	n	505	CLA	C16-C17-C18-C20
14	A	852	LMG	C34-C35-C36-C37
20	a	4202	LMT	C1-C2-C3-C4
15	A	1011	CL0	O1A-CGA-O2A-C1
16	g	506	CLA	O1A-CGA-O2A-C1
16	T	4003	CLA	O1D-CGD-O2D-CED
19	I	4018	BCR	C20-C21-C22-C37
19	X	602	BCR	C11-C10-C9-C34
19	a	4007	BCR	C16-C17-C18-C36
19	b	4017	BCR	C16-C17-C18-C36
19	j	4015	BCR	C11-C10-C9-C34
19	l	4019	BCR	C20-C21-C22-C37
19	o	603	BCR	C20-C21-C22-C37
19	s	602	BCR	C16-C17-C18-C36
19	y	604	BCR	C20-C21-C22-C37
16	A	1127	CLA	C5-C6-C7-C8
16	a	1127	CLA	C8-C10-C11-C12
16	p	505	CLA	C13-C15-C16-C17
16	W	507	CLA	O1A-CGA-O2A-C1
16	n	514	CLA	O1A-CGA-O2A-C1
16	v	512	CLA	O1A-CGA-O2A-C1
14	A	4101	LMG	C14-C15-C16-C17
16	o	509	CLA	C4-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	v	504	CLA	C4-C3-C5-C6
16	A	1101	CLA	C2-C3-C5-C6
16	A	1123	CLA	C2-C3-C5-C6
16	B	1204	CLA	C2-C3-C5-C6
16	H	1132	CLA	C2-C3-C5-C6
16	Y	504	CLA	C2-C3-C5-C6
16	b	1205	CLA	C2-C3-C5-C6
16	n	512	CLA	C2-C3-C5-C6
16	q	512	CLA	C2-C3-C5-C6
16	G	1240	CLA	O1A-CGA-O2A-C1
16	B	1205	CLA	C10-C11-C12-C13
16	H	1131	CLA	C15-C16-C17-C18
16	a	1101	CLA	C10-C11-C12-C13
16	a	1131	CLA	C13-C15-C16-C17
16	q	509	CLA	C8-C10-C11-C12
16	u	504	CLA	C5-C6-C7-C8
19	B	4014	BCR	C37-C22-C23-C24
19	L	4022	BCR	C37-C22-C23-C24
19	S	4013	BCR	C7-C8-C9-C34
19	U	4022	BCR	C37-C22-C23-C24
19	X	602	BCR	C37-C22-C23-C24
19	l	4022	BCR	C37-C22-C23-C24
19	r	601	BCR	C11-C12-C13-C35
19	x	603	BCR	C7-C8-C9-C34
19	y	601	BCR	C7-C8-C9-C34
20	l	4101	LMT	O5B-C1B-O1B-C4'
16	A	1117	CLA	C16-C17-C18-C19
16	n	505	CLA	C16-C17-C18-C19
13	i	103	LHG	C29-C30-C31-C32
14	a	4101	LMG	O6-C5-C6-O5
19	G	4014	BCR	C21-C22-C23-C24
19	U	4022	BCR	C21-C22-C23-C24
19	X	602	BCR	C21-C22-C23-C24
19	h	601	BCR	C7-C8-C9-C10
19	n	601	BCR	C21-C22-C23-C24
19	q	604	BCR	C7-C8-C9-C10
16	t	511	CLA	O1A-CGA-O2A-C1
16	Z	510	CLA	C5-C6-C7-C8
16	p	511	CLA	C13-C15-C16-C17
13	I	103	LHG	C29-C30-C31-C32
16	Y	508	CLA	C2A-CAA-CBA-CGA
16	t	516	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	v	507	CLA	C2A-CAA-CBA-CGA
16	x	511	CLA	C2A-CAA-CBA-CGA
16	r	503	CLA	CBA-CGA-O2A-C1
16	y	516	CLA	CBA-CGA-O2A-C1
16	g	504	CLA	C8-C10-C11-C12
16	a	1101	CLA	O1A-CGA-O2A-C1
16	b	1222	CLA	O1D-CGD-O2D-CED
16	A	1110	CLA	CBA-CGA-O2A-C1
16	B	1222	CLA	CBA-CGA-O2A-C1
13	a	849	LHG	C10-C11-C12-C13
14	G	848	LMG	C13-C14-C15-C16
16	u	503	CLA	O1A-CGA-O2A-C1
19	S	4012	BCR	C10-C11-C12-C13
19	a	4003	BCR	C10-C11-C12-C13
19	k	4001	BCR	C18-C19-C20-C21
16	A	1125	CLA	C13-C15-C16-C17
16	G	1224	CLA	C8-C10-C11-C12
19	S	4015	BCR	C9-C10-C11-C12
19	b	4005	BCR	C19-C20-C21-C22
19	w	604	BCR	C15-C16-C17-C18
15	A	1011	CL0	C16-C17-C18-C20
16	H	1101	CLA	C16-C17-C18-C20
13	B	4018	LHG	C16-C17-C18-C19
16	q	516	CLA	CBA-CGA-O2A-C1
13	g	605	LHG	O10-C23-O8-C6
16	y	514	CLA	O1A-CGA-O2A-C1
14	a	4101	LMG	C31-C32-C33-C34
16	s	503	CLA	O1A-CGA-O2A-C1
19	A	4003	BCR	C16-C17-C18-C19
19	G	4004	BCR	C20-C21-C22-C23
19	R	4018	BCR	C16-C17-C18-C19
19	X	601	BCR	C16-C17-C18-C19
19	g	603	BCR	C11-C10-C9-C8
19	i	4018	BCR	C12-C13-C14-C15
19	n	604	BCR	C20-C21-C22-C23
19	t	603	BCR	C20-C21-C22-C23
14	a	4101	LMG	C14-C15-C16-C17
13	p	605	LHG	O6-C4-C5-O7
19	K	4001	BCR	C6-C7-C8-C9
19	Z	604	BCR	C22-C23-C24-C25
19	b	4017	BCR	C22-C23-C24-C25
19	o	603	BCR	C22-C23-C24-C25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1225	CLA	C13-C15-C16-C17
16	X	509	CLA	O1D-CGD-O2D-CED
13	I	103	LHG	C24-C23-O8-C6
16	A	1116	CLA	CBA-CGA-O2A-C1
16	p	511	CLA	CBA-CGA-O2A-C1
16	r	502	CLA	CBA-CGA-O2A-C1
16	s	514	CLA	CBA-CGA-O2A-C1
16	g	503	CLA	CBD-CGD-O2D-CED
16	X	512	CLA	O1A-CGA-O2A-C1
16	Y	508	CLA	O1A-CGA-O2A-C1
13	H	849	LHG	C27-C28-C29-C30
16	A	1101	CLA	C4-C3-C5-C6
16	A	1110	CLA	C4-C3-C5-C6
16	B	1228	CLA	C4-C3-C5-C6
16	G	1220	CLA	C4-C3-C5-C6
16	G	1228	CLA	C4-C3-C5-C6
16	U	1502	CLA	C4-C3-C5-C6
16	a	1132	CLA	C4-C3-C5-C6
16	B	1205	CLA	C2-C3-C5-C6
16	b	1228	CLA	C2-C3-C5-C6
16	l	1501	CLA	C2-C3-C5-C6
16	A	1110	CLA	C3-C5-C6-C7
16	o	506	CLA	C11-C12-C13-C15
13	H	849	LHG	C25-C26-C27-C28
14	H	852	LMG	C30-C31-C32-C33
13	p	605	LHG	C27-C28-C29-C30
14	H	4201	LMG	C14-C15-C16-C17
16	x	506	CLA	C5-C6-C7-C8
13	R	103	LHG	O7-C5-C6-O8
13	Y	605	LHG	O7-C5-C6-O8
13	x	605	LHG	O7-C5-C6-O8
14	b	848	LMG	O7-C8-C9-O8
14	H	4101	LMG	C13-C14-C15-C16
16	p	510	CLA	O1D-CGD-O2D-CED
15	A	1011	CL0	CAA-CBA-CGA-O2A
16	X	509	CLA	CAA-CBA-CGA-O2A
16	T	4003	CLA	C4C-C3C-CAC-CBC
16	s	503	CLA	C4C-C3C-CAC-CBC
16	G	1211	CLA	C2A-CAA-CBA-CGA
16	G	1224	CLA	C2A-CAA-CBA-CGA
16	H	1120	CLA	C2A-CAA-CBA-CGA
16	A	1140	CLA	C3-C5-C6-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1224	CLA	C3-C5-C6-C7
16	G	1238	CLA	C3-C5-C6-C7
16	b	1224	CLA	C3-C5-C6-C7
16	n	517	CLA	C3-C5-C6-C7
16	G	1221	CLA	C8-C10-C11-C12
16	Y	517	CLA	C2-C1-O2A-CGA
13	X	605	LHG	C11-C10-C9-C8
16	A	1101	CLA	O1A-CGA-O2A-C1
14	H	4101	LMG	C31-C32-C33-C34
14	b	848	LMG	C29-C28-O8-C9
16	Y	511	CLA	CBA-CGA-O2A-C1
16	a	1106	CLA	CBA-CGA-O2A-C1
16	n	504	CLA	CBA-CGA-O2A-C1
16	g	515	CLA	CBD-CGD-O2D-CED
16	t	502	CLA	CBD-CGD-O2D-CED
16	a	1122	CLA	C4C-C3C-CAC-CBC
16	A	1013	CLA	C10-C11-C12-C13
16	b	1023	CLA	C10-C11-C12-C13
16	w	515	CLA	C13-C15-C16-C17
16	A	1123	CLA	O1A-CGA-O2A-C1
16	s	506	CLA	O1A-CGA-O2A-C1
16	y	517	CLA	C3-C5-C6-C7
14	a	852	LMG	C33-C34-C35-C36
16	Y	508	CLA	O1D-CGD-O2D-CED
16	a	1136	CLA	O1D-CGD-O2D-CED
16	u	511	CLA	O1D-CGD-O2D-CED
16	w	502	CLA	O1D-CGD-O2D-CED
16	b	1220	CLA	C6-C7-C8-C9
16	A	1132	CLA	C13-C15-C16-C17
16	Y	506	CLA	C8-C10-C11-C12
16	r	504	CLA	C8-C10-C11-C12
16	s	504	CLA	C8-C10-C11-C12
16	u	506	CLA	C5-C6-C7-C8
16	u	509	CLA	C10-C11-C12-C13
20	A	4202	LMT	C1-C2-C3-C4
16	H	1102	CLA	C11-C10-C8-C9
16	a	1117	CLA	C16-C17-C18-C20
16	A	1123	CLA	C4-C3-C5-C6
16	B	1223	CLA	C4-C3-C5-C6
16	G	1214	CLA	C4-C3-C5-C6
16	L	1501	CLA	C4-C3-C5-C6
16	b	1223	CLA	C4-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	h	509	CLA	C4-C3-C5-C6
16	l	1501	CLA	C4-C3-C5-C6
16	l	1502	CLA	C4-C3-C5-C6
16	v	512	CLA	C4-C3-C5-C6
16	X	509	CLA	C2-C3-C5-C6
13	R	103	LHG	C27-C28-C29-C30
16	H	1133	CLA	C5-C6-C7-C8
16	H	1110	CLA	CBA-CGA-O2A-C1
16	Z	505	CLA	CBA-CGA-O2A-C1
16	u	517	CLA	CBA-CGA-O2A-C1
16	A	1109	CLA	C5-C6-C7-C8
16	B	1203	CLA	C15-C16-C17-C18
16	G	1205	CLA	C13-C15-C16-C17
16	H	1136	CLA	C8-C10-C11-C12
16	b	1205	CLA	C10-C11-C12-C13
16	h	515	CLA	C5-C6-C7-C8
16	a	1133	CLA	C6-C7-C8-C9
13	A	849	LHG	C10-C11-C12-C13
13	r	605	LHG	O1-C1-C2-O2
16	A	1013	CLA	C11-C12-C13-C14
16	A	1022	CLA	C14-C13-C15-C16
16	A	1101	CLA	C11-C10-C8-C9
16	A	1117	CLA	C11-C12-C13-C14
16	A	1119	CLA	C6-C7-C8-C9
16	A	1131	CLA	C6-C7-C8-C9
16	B	1206	CLA	C11-C10-C8-C9
16	B	1206	CLA	C11-C12-C13-C14
16	B	1207	CLA	C14-C13-C15-C16
16	B	1223	CLA	C14-C13-C15-C16
16	B	1225	CLA	C6-C7-C8-C9
16	B	1225	CLA	C14-C13-C15-C16
16	B	1226	CLA	C6-C7-C8-C9
16	G	1207	CLA	C14-C13-C15-C16
16	G	1211	CLA	C6-C7-C8-C9
16	G	1211	CLA	C14-C13-C15-C16
16	H	1013	CLA	C11-C12-C13-C14
16	H	1117	CLA	C11-C12-C13-C14
16	H	1119	CLA	C14-C13-C15-C16
16	H	1125	CLA	C11-C10-C8-C9
16	H	1125	CLA	C14-C13-C15-C16
16	H	1128	CLA	C11-C12-C13-C14
16	L	1502	CLA	C11-C10-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	W	510	CLA	C6-C7-C8-C9
16	X	504	CLA	C6-C7-C8-C9
16	X	506	CLA	C6-C7-C8-C9
16	X	511	CLA	C11-C12-C13-C14
16	Y	505	CLA	C11-C10-C8-C9
16	Y	511	CLA	C6-C7-C8-C9
16	Z	505	CLA	C11-C12-C13-C14
16	Z	507	CLA	C11-C10-C8-C9
16	a	1022	CLA	C14-C13-C15-C16
16	a	1117	CLA	C11-C12-C13-C14
16	a	1119	CLA	C14-C13-C15-C16
16	a	1123	CLA	C11-C12-C13-C14
16	a	1125	CLA	C11-C10-C8-C9
16	a	1131	CLA	C6-C7-C8-C9
16	b	1202	CLA	C6-C7-C8-C9
16	b	1204	CLA	C6-C7-C8-C9
16	b	1206	CLA	C6-C7-C8-C9
16	b	1207	CLA	C14-C13-C15-C16
16	b	1210	CLA	C11-C10-C8-C9
16	b	1221	CLA	C6-C7-C8-C9
16	b	1221	CLA	C11-C10-C8-C9
16	b	1221	CLA	C11-C12-C13-C14
16	b	1225	CLA	C6-C7-C8-C9
16	g	506	CLA	C11-C10-C8-C9
16	g	510	CLA	C6-C7-C8-C9
16	h	511	CLA	C14-C13-C15-C16
16	h	515	CLA	C6-C7-C8-C9
16	n	510	CLA	C11-C10-C8-C9
16	n	512	CLA	C6-C7-C8-C9
16	n	512	CLA	C11-C12-C13-C14
16	n	515	CLA	C6-C7-C8-C9
16	o	506	CLA	C6-C7-C8-C9
16	o	511	CLA	C11-C12-C13-C14
16	p	506	CLA	C11-C10-C8-C9
16	q	504	CLA	C11-C12-C13-C14
16	q	512	CLA	C14-C13-C15-C16
16	s	505	CLA	C11-C10-C8-C9
16	s	506	CLA	C11-C10-C8-C9
16	s	511	CLA	C11-C12-C13-C14
16	t	506	CLA	C11-C10-C8-C9
16	t	512	CLA	C11-C12-C13-C14
16	t	515	CLA	C6-C7-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	u	511	CLA	C11-C12-C13-C14
16	u	515	CLA	C14-C13-C15-C16
16	v	507	CLA	C11-C10-C8-C9
16	w	506	CLA	C6-C7-C8-C9
16	y	515	CLA	C11-C10-C8-C9
16	x	508	CLA	O1D-CGD-O2D-CED
16	H	1237	CLA	C13-C15-C16-C17
16	l	1503	CLA	C13-C15-C16-C17
16	t	512	CLA	C5-C6-C7-C8
16	y	507	CLA	C5-C6-C7-C8
20	U	4101	LMT	O5B-C1B-O1B-C4'
16	a	1111	CLA	O1D-CGD-O2D-CED
16	o	509	CLA	O1D-CGD-O2D-CED
16	A	1138	CLA	C10-C11-C12-C13
16	G	1210	CLA	C10-C11-C12-C13
16	p	510	CLA	C5-C6-C7-C8
16	H	1127	CLA	O1A-CGA-O2A-C1
16	B	1209	CLA	C2A-CAA-CBA-CGA
16	H	1130	CLA	C2A-CAA-CBA-CGA
16	n	508	CLA	C2A-CAA-CBA-CGA
14	a	4101	LMG	C2-C1-O1-C7
16	A	1106	CLA	C10-C11-C12-C13
16	H	1132	CLA	C13-C15-C16-C17
16	y	509	CLA	C8-C10-C11-C12
13	R	103	LHG	C29-C30-C31-C32
13	b	4018	LHG	C18-C19-C20-C21
16	X	506	CLA	C3-C5-C6-C7
16	a	1125	CLA	C3-C5-C6-C7
16	q	505	CLA	C3-C5-C6-C7
17	G	2002	PQN	C13-C15-C16-C17
13	R	103	LHG	C32-C33-C34-C35
13	o	605	LHG	C11-C10-C9-C8
13	G	4018	LHG	O6-C4-C5-C6
13	b	4018	LHG	O6-C4-C5-C6
13	o	605	LHG	O6-C4-C5-C6
13	p	605	LHG	O6-C4-C5-C6
13	x	605	LHG	O6-C4-C5-C6
13	A	849	LHG	C28-C29-C30-C31
14	H	4101	LMG	C34-C35-C36-C37
16	a	1111	CLA	C4C-C3C-CAC-CBC
13	H	849	LHG	C32-C33-C34-C35
14	A	4201	LMG	C14-C15-C16-C17

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	h	509	CLA	CAA-CBA-CGA-O2A
16	A	1117	CLA	C11-C12-C13-C15
16	A	1119	CLA	C12-C13-C15-C16
16	A	1128	CLA	C11-C12-C13-C15
16	A	1131	CLA	C6-C7-C8-C10
16	A	1131	CLA	C11-C10-C8-C7
16	B	1202	CLA	C11-C12-C13-C15
16	B	1203	CLA	C12-C13-C15-C16
16	B	1221	CLA	C11-C10-C8-C7
16	B	1226	CLA	C6-C7-C8-C10
16	G	1204	CLA	C12-C13-C15-C16
16	G	1207	CLA	C12-C13-C15-C16
16	G	1211	CLA	C12-C13-C15-C16
16	G	1221	CLA	C6-C7-C8-C10
16	G	1221	CLA	C11-C10-C8-C7
16	G	1224	CLA	C11-C10-C8-C7
16	H	1013	CLA	C11-C12-C13-C15
16	H	1106	CLA	C6-C7-C8-C10
16	H	1109	CLA	C6-C7-C8-C10
16	H	1109	CLA	C11-C12-C13-C15
16	H	1119	CLA	C12-C13-C15-C16
16	H	1125	CLA	C11-C10-C8-C7
16	H	1125	CLA	C12-C13-C15-C16
16	H	1130	CLA	C11-C10-C8-C7
16	H	1131	CLA	C11-C10-C8-C7
16	L	1501	CLA	C11-C10-C8-C7
16	W	505	CLA	C11-C12-C13-C15
16	W	515	CLA	C6-C7-C8-C10
16	X	515	CLA	C6-C7-C8-C10
16	Y	510	CLA	C11-C12-C13-C15
16	Y	511	CLA	C12-C13-C15-C16
16	Z	510	CLA	C6-C7-C8-C10
16	a	1117	CLA	C11-C12-C13-C15
16	a	1128	CLA	C11-C12-C13-C15
16	a	1130	CLA	C11-C10-C8-C7
16	a	1131	CLA	C11-C10-C8-C7
16	b	1203	CLA	C12-C13-C15-C16
16	b	1211	CLA	C6-C7-C8-C10
16	b	1221	CLA	C6-C7-C8-C10
16	b	1226	CLA	C6-C7-C8-C10
16	g	504	CLA	C12-C13-C15-C16
16	g	510	CLA	C11-C12-C13-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	g	511	CLA	C11-C10-C8-C7
16	l	1503	CLA	C11-C10-C8-C7
16	n	505	CLA	C11-C12-C13-C15
16	n	506	CLA	C11-C10-C8-C7
16	n	512	CLA	C11-C10-C8-C7
16	n	512	CLA	C12-C13-C15-C16
16	o	505	CLA	C6-C7-C8-C10
16	o	506	CLA	C6-C7-C8-C10
16	o	515	CLA	C6-C7-C8-C10
16	p	505	CLA	C11-C10-C8-C7
16	p	506	CLA	C11-C10-C8-C7
16	q	504	CLA	C11-C12-C13-C15
16	q	510	CLA	C6-C7-C8-C10
16	r	511	CLA	C11-C10-C8-C7
16	s	505	CLA	C11-C10-C8-C7
16	s	506	CLA	C11-C10-C8-C7
16	s	509	CLA	C6-C7-C8-C10
16	s	510	CLA	C11-C12-C13-C15
16	t	515	CLA	C6-C7-C8-C10
16	u	504	CLA	C11-C10-C8-C7
16	u	506	CLA	C6-C7-C8-C10
16	u	507	CLA	C11-C10-C8-C7
16	u	515	CLA	C12-C13-C15-C16
16	v	509	CLA	C6-C7-C8-C10
16	w	506	CLA	C6-C7-C8-C10
16	x	504	CLA	C11-C12-C13-C15
16	x	511	CLA	C12-C13-C15-C16
16	y	504	CLA	C11-C10-C8-C7
16	y	509	CLA	C6-C7-C8-C10
16	y	511	CLA	C6-C7-C8-C10
17	b	2002	PQN	C22-C23-C25-C26
16	H	1013	CLA	C10-C11-C12-C13
16	s	505	CLA	C13-C15-C16-C17
16	u	515	CLA	C8-C10-C11-C12
16	h	509	CLA	O1A-CGA-O2A-C1
16	x	504	CLA	O1A-CGA-O2A-C1
13	i	103	LHG	O2-C2-C3-O3
13	u	605	LHG	C11-C10-C9-C8
16	K	4003	CLA	O1D-CGD-O2D-CED
16	p	514	CLA	O1A-CGA-O2A-C1
16	s	511	CLA	O1A-CGA-O2A-C1
16	A	1138	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	1139	CLA	C3A-C2A-CAA-CBA
16	B	1205	CLA	C4-C3-C5-C6
16	B	1210	CLA	C4-C3-C5-C6
16	B	1220	CLA	C3A-C2A-CAA-CBA
16	B	1226	CLA	C3A-C2A-CAA-CBA
16	G	1204	CLA	C4-C3-C5-C6
16	G	1226	CLA	C3A-C2A-CAA-CBA
16	H	1107	CLA	C3A-C2A-CAA-CBA
16	H	1118	CLA	C4-C3-C5-C6
16	H	1138	CLA	C3A-C2A-CAA-CBA
16	H	1139	CLA	C3A-C2A-CAA-CBA
16	X	516	CLA	C3A-C2A-CAA-CBA
16	Z	516	CLA	C3A-C2A-CAA-CBA
16	a	1101	CLA	C4-C3-C5-C6
16	a	1137	CLA	C3A-C2A-CAA-CBA
16	a	1138	CLA	C3A-C2A-CAA-CBA
16	b	1210	CLA	C4-C3-C5-C6
16	b	1214	CLA	C3A-C2A-CAA-CBA
16	g	503	CLA	C3A-C2A-CAA-CBA
16	o	516	CLA	C3A-C2A-CAA-CBA
16	p	516	CLA	C3A-C2A-CAA-CBA
16	r	501	CLA	C3A-C2A-CAA-CBA
16	s	516	CLA	C3A-C2A-CAA-CBA
16	u	513	CLA	C3A-C2A-CAA-CBA
16	v	516	CLA	C3A-C2A-CAA-CBA
16	w	513	CLA	C3A-C2A-CAA-CBA
16	x	504	CLA	C4-C3-C5-C6
16	y	512	CLA	C4-C3-C5-C6
16	y	514	CLA	C3A-C2A-CAA-CBA
16	y	517	CLA	C4-C3-C5-C6
16	o	512	CLA	C5-C6-C7-C8
16	G	1222	CLA	O1D-CGD-O2D-CED
16	p	514	CLA	CAA-CBA-CGA-O2A
16	H	1118	CLA	C2-C3-C5-C6
16	h	509	CLA	C2-C3-C5-C6
16	u	510	CLA	O1D-CGD-O2D-CED
16	A	1110	CLA	O1A-CGA-O2A-C1
16	W	514	CLA	O1A-CGA-O2A-C1
16	b	1210	CLA	O1A-CGA-O2A-C1
16	u	512	CLA	C13-C15-C16-C17
16	v	509	CLA	CBA-CGA-O2A-C1
19	B	4005	BCR	C19-C20-C21-C22

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	B	4010	BCR	C15-C16-C17-C18
19	G	4014	BCR	C19-C20-C21-C22
19	H	4011	BCR	C9-C10-C11-C12
19	S	4013	BCR	C19-C20-C21-C22
19	T	4001	BCR	C9-C10-C11-C12
19	U	4022	BCR	C19-C20-C21-C22
19	a	4011	BCR	C9-C10-C11-C12
19	n	604	BCR	C13-C14-C15-C16
19	o	604	BCR	C15-C16-C17-C18
19	o	604	BCR	C19-C20-C21-C22
19	p	604	BCR	C9-C10-C11-C12
19	s	604	BCR	C9-C10-C11-C12
19	s	604	BCR	C13-C14-C15-C16
19	u	602	BCR	C19-C20-C21-C22
19	w	602	BCR	C19-C20-C21-C22
19	y	601	BCR	C9-C10-C11-C12
21	m	4021	ECH	C9-C10-C11-C12
16	o	506	CLA	C11-C12-C13-C14
16	o	505	CLA	C15-C16-C17-C18
19	h	601	BCR	C7-C8-C9-C34
16	a	1136	CLA	O1A-CGA-O2A-C1
16	n	505	CLA	O1D-CGD-O2D-CED
16	n	510	CLA	O1D-CGD-O2D-CED
14	a	4101	LMG	C33-C34-C35-C36
16	a	1126	CLA	C13-C15-C16-C17
16	o	511	CLA	C8-C10-C11-C12
19	Z	603	BCR	C21-C22-C23-C24
19	f	4016	BCR	C21-C22-C23-C24
19	s	602	BCR	C21-C22-C23-C24
13	A	851	LHG	C4-C5-C6-O8
13	H	851	LHG	C4-C5-C6-O8
13	R	103	LHG	C4-C5-C6-O8
13	o	605	LHG	C4-C5-C6-O8
14	A	4101	LMG	O1-C7-C8-C9
14	B	848	LMG	C7-C8-C9-O8
14	H	4101	LMG	O1-C7-C8-C9
14	H	4101	LMG	C7-C8-C9-O8
14	a	4101	LMG	C7-C8-C9-O8
13	A	849	LHG	C24-C25-C26-C27
16	t	506	CLA	CBD-CGD-O2D-CED
16	w	509	CLA	C16-C17-C18-C20
16	A	1103	CLA	C13-C15-C16-C17

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1211	CLA	C8-C10-C11-C12
16	a	1106	CLA	C10-C11-C12-C13
16	x	509	CLA	C13-C15-C16-C17
14	a	4201	LMG	C14-C15-C16-C17
16	g	505	CLA	C5-C6-C7-C8
16	H	1123	CLA	C4-C3-C5-C6
16	X	509	CLA	C4-C3-C5-C6
16	a	1103	CLA	C4-C3-C5-C6
16	h	512	CLA	C4-C3-C5-C6
16	u	512	CLA	C4-C3-C5-C6
16	v	509	CLA	C4-C3-C5-C6
16	w	512	CLA	C4-C3-C5-C6
16	t	514	CLA	CAA-CBA-CGA-O2A
16	B	1210	CLA	C2-C3-C5-C6
16	L	1501	CLA	C2-C3-C5-C6
16	b	1210	CLA	C2-C3-C5-C6
16	h	512	CLA	C2-C3-C5-C6
16	u	512	CLA	C2-C3-C5-C6
16	v	512	CLA	C2-C3-C5-C6
16	y	512	CLA	C2-C3-C5-C6
20	H	4202	LMT	C1-C2-C3-C4
16	A	1126	CLA	C3-C5-C6-C7
16	o	510	CLA	C3-C5-C6-C7
16	t	506	CLA	C3-C5-C6-C7
17	B	2002	PQN	C13-C15-C16-C17
16	a	1106	CLA	O1D-CGD-O2D-CED
16	W	510	CLA	CBD-CGD-O2D-CED
16	H	1114	CLA	C4C-C3C-CAC-CBC
16	Z	516	CLA	O1D-CGD-O2D-CED
16	B	1238	CLA	C16-C17-C18-C19
16	L	1503	CLA	C16-C17-C18-C19
13	I	103	LHG	O9-C7-O7-C5
13	G	4018	LHG	O6-C4-C5-O7
13	a	849	LHG	O6-C4-C5-O7
13	b	4018	LHG	O6-C4-C5-O7
13	g	605	LHG	O6-C4-C5-O7
13	u	605	LHG	O6-C4-C5-O7
16	r	502	CLA	O1A-CGA-O2A-C1
16	Z	503	CLA	C2C-C3C-CAC-CBC
13	a	849	LHG	C32-C33-C34-C35
19	A	4002	BCR	C1-C6-C7-C8
19	A	4002	BCR	C23-C24-C25-C30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	A	4007	BCR	C1-C6-C7-C8
19	A	4007	BCR	C23-C24-C25-C30
19	B	4004	BCR	C1-C6-C7-C8
19	B	4004	BCR	C23-C24-C25-C30
19	B	4005	BCR	C1-C6-C7-C8
19	B	4010	BCR	C1-C6-C7-C8
19	B	4014	BCR	C23-C24-C25-C30
19	B	4017	BCR	C1-C6-C7-C8
19	B	4017	BCR	C23-C24-C25-C30
19	F	4016	BCR	C1-C6-C7-C8
19	G	4004	BCR	C1-C6-C7-C8
19	G	4005	BCR	C1-C6-C7-C8
19	G	4009	BCR	C23-C24-C25-C30
19	G	4014	BCR	C1-C6-C7-C8
19	G	4014	BCR	C23-C24-C25-C30
19	G	4017	BCR	C1-C6-C7-C8
19	G	4017	BCR	C23-C24-C25-C30
19	H	4002	BCR	C23-C24-C25-C30
19	H	4003	BCR	C1-C6-C7-C8
19	H	4007	BCR	C1-C6-C7-C8
19	H	4007	BCR	C23-C24-C25-C30
19	H	4008	BCR	C1-C6-C7-C8
19	H	4008	BCR	C23-C24-C25-C30
19	I	4018	BCR	C1-C6-C7-C8
19	J	4015	BCR	C23-C24-C25-C30
19	K	4001	BCR	C1-C6-C7-C8
19	K	4005	BCR	C23-C24-C25-C30
19	L	4019	BCR	C1-C6-C7-C8
19	L	4022	BCR	C1-C6-C7-C8
19	Q	4016	BCR	C1-C6-C7-C8
19	Q	4016	BCR	C23-C24-C25-C30
19	S	4012	BCR	C1-C6-C7-C8
19	S	4012	BCR	C23-C24-C25-C30
19	S	4015	BCR	C1-C6-C7-C8
19	S	4015	BCR	C23-C24-C25-C30
19	T	4001	BCR	C23-C24-C25-C30
19	T	4005	BCR	C1-C6-C7-C8
19	T	4005	BCR	C23-C24-C25-C30
19	U	4019	BCR	C1-C6-C7-C8
19	U	4022	BCR	C23-C24-C25-C30
19	W	603	BCR	C23-C24-C25-C30
19	W	604	BCR	C1-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	X	602	BCR	C1-C6-C7-C8
19	X	603	BCR	C1-C6-C7-C8
19	X	603	BCR	C5-C6-C7-C8
19	X	603	BCR	C23-C24-C25-C30
19	X	604	BCR	C1-C6-C7-C8
19	X	604	BCR	C23-C24-C25-C30
19	Y	601	BCR	C1-C6-C7-C8
19	Y	602	BCR	C23-C24-C25-C30
19	Y	603	BCR	C1-C6-C7-C8
19	Z	602	BCR	C1-C6-C7-C8
19	Z	603	BCR	C1-C6-C7-C8
19	Z	603	BCR	C23-C24-C25-C30
19	Z	604	BCR	C1-C6-C7-C8
19	Z	604	BCR	C23-C24-C25-C30
19	a	4007	BCR	C1-C6-C7-C8
19	a	4007	BCR	C23-C24-C25-C30
19	a	4008	BCR	C1-C6-C7-C8
19	b	4004	BCR	C1-C6-C7-C8
19	b	4004	BCR	C23-C24-C25-C30
19	b	4005	BCR	C1-C6-C7-C8
19	b	4009	BCR	C23-C24-C25-C30
19	b	4010	BCR	C1-C6-C7-C8
19	b	4017	BCR	C1-C6-C7-C8
19	f	4016	BCR	C1-C6-C7-C8
19	g	601	BCR	C23-C24-C25-C30
19	g	602	BCR	C1-C6-C7-C8
19	g	603	BCR	C23-C24-C25-C30
19	g	604	BCR	C1-C6-C7-C8
19	g	604	BCR	C23-C24-C25-C26
19	h	603	BCR	C1-C6-C7-C8
19	h	604	BCR	C1-C6-C7-C8
19	j	4013	BCR	C23-C24-C25-C30
19	j	4015	BCR	C1-C6-C7-C8
19	j	4015	BCR	C23-C24-C25-C30
19	k	4001	BCR	C1-C6-C7-C8
19	k	4001	BCR	C23-C24-C25-C30
19	k	4005	BCR	C23-C24-C25-C30
19	l	4019	BCR	C1-C6-C7-C8
19	l	4019	BCR	C23-C24-C25-C26
19	l	4019	BCR	C23-C24-C25-C30
19	l	4022	BCR	C23-C24-C25-C30
19	n	601	BCR	C1-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	n	601	BCR	C23-C24-C25-C30
19	n	603	BCR	C1-C6-C7-C8
19	n	603	BCR	C23-C24-C25-C30
19	n	604	BCR	C1-C6-C7-C8
19	o	601	BCR	C1-C6-C7-C8
19	o	602	BCR	C1-C6-C7-C8
19	o	602	BCR	C23-C24-C25-C30
19	o	603	BCR	C1-C6-C7-C8
19	o	603	BCR	C23-C24-C25-C30
19	p	602	BCR	C23-C24-C25-C30
19	p	603	BCR	C1-C6-C7-C8
19	p	603	BCR	C23-C24-C25-C30
19	q	602	BCR	C1-C6-C7-C8
19	q	603	BCR	C1-C6-C7-C8
19	q	603	BCR	C23-C24-C25-C30
19	q	604	BCR	C23-C24-C25-C30
19	r	601	BCR	C1-C6-C7-C8
19	r	602	BCR	C1-C6-C7-C8
19	r	603	BCR	C23-C24-C25-C30
19	r	604	BCR	C1-C6-C7-C8
19	r	604	BCR	C23-C24-C25-C30
19	s	601	BCR	C1-C6-C7-C8
19	s	601	BCR	C5-C6-C7-C8
19	s	602	BCR	C1-C6-C7-C8
19	s	602	BCR	C23-C24-C25-C30
19	s	603	BCR	C1-C6-C7-C8
19	s	603	BCR	C23-C24-C25-C30
19	t	601	BCR	C1-C6-C7-C8
19	t	601	BCR	C23-C24-C25-C30
19	t	603	BCR	C23-C24-C25-C30
19	t	604	BCR	C1-C6-C7-C8
19	u	601	BCR	C1-C6-C7-C8
19	u	602	BCR	C1-C6-C7-C8
19	u	602	BCR	C23-C24-C25-C30
19	u	603	BCR	C1-C6-C7-C8
19	u	603	BCR	C23-C24-C25-C30
19	v	601	BCR	C1-C6-C7-C8
19	v	603	BCR	C1-C6-C7-C8
19	v	604	BCR	C1-C6-C7-C8
19	w	602	BCR	C1-C6-C7-C8
19	w	603	BCR	C23-C24-C25-C30
19	w	604	BCR	C23-C24-C25-C30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	x	601	BCR	C1-C6-C7-C8
19	x	601	BCR	C23-C24-C25-C30
19	x	602	BCR	C1-C6-C7-C8
19	x	603	BCR	C23-C24-C25-C30
19	x	604	BCR	C23-C24-C25-C30
19	y	603	BCR	C23-C24-C25-C30
19	y	604	BCR	C1-C6-C7-C8
21	B	4006	ECH	C23-C24-C25-C30
21	M	4021	ECH	C1-C6-C7-C8
21	b	4006	ECH	C23-C24-C25-C30
21	m	4021	ECH	C1-C6-C7-C8
23	g	606	LMU	C6-C7-C8-C9
16	H	1106	CLA	O1D-CGD-O2D-CED
13	p	605	LHG	C5-C4-O6-P
14	H	4101	LMG	C33-C34-C35-C36
16	Y	516	CLA	CBA-CGA-O2A-C1
16	B	1222	CLA	O1A-CGA-O2A-C1
16	k	4004	CLA	C5-C6-C7-C8
16	u	512	CLA	C8-C10-C11-C12
16	v	510	CLA	C15-C16-C17-C18
16	b	1238	CLA	O1D-CGD-O2D-CED
23	g	606	LMU	C4-C5-C6-C7
16	g	516	CLA	O1A-CGA-O2A-C1
16	W	509	CLA	C2A-CAA-CBA-CGA
16	b	1219	CLA	C2A-CAA-CBA-CGA
16	p	516	CLA	C2A-CAA-CBA-CGA
16	A	1132	CLA	C15-C16-C17-C18
16	H	1104	CLA	C10-C11-C12-C13
16	H	1106	CLA	C10-C11-C12-C13
16	Z	512	CLA	C10-C11-C12-C13
16	a	1103	CLA	C10-C11-C12-C13
16	a	1136	CLA	C8-C10-C11-C12
16	s	506	CLA	C8-C10-C11-C12
17	A	2001	PQN	C25-C26-C27-C28
13	A	851	LHG	O7-C5-C6-O8
13	X	605	LHG	O7-C5-C6-O8
13	g	605	LHG	O7-C5-C6-O8
13	s	605	LHG	C27-C28-C29-C30
16	o	515	CLA	C3-C5-C6-C7
16	W	506	CLA	O1D-CGD-O2D-CED
19	G	4004	BCR	C10-C11-C12-C13
19	G	4010	BCR	C10-C11-C12-C13

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	L	4022	BCR	C10-C11-C12-C13
19	Z	603	BCR	C18-C19-C20-C21
19	p	602	BCR	C10-C11-C12-C13
16	a	1132	CLA	C13-C15-C16-C17
16	b	1206	CLA	C15-C16-C17-C18
16	G	1214	CLA	C2-C3-C5-C6
16	a	1101	CLA	C2-C3-C5-C6
16	b	1223	CLA	C2-C3-C5-C6
16	w	512	CLA	C2-C3-C5-C6
14	A	4101	LMG	C18-C19-C20-C21
16	W	517	CLA	C6-C7-C8-C9
16	X	508	CLA	C6-C7-C8-C9
16	a	1117	CLA	C16-C17-C18-C19
16	h	515	CLA	C16-C17-C18-C19
13	B	4018	LHG	C9-C10-C11-C12
14	a	4101	LMG	C34-C35-C36-C37
16	W	512	CLA	C10-C11-C12-C13
16	A	1119	CLA	C14-C13-C15-C16
16	B	1210	CLA	C6-C7-C8-C9
16	G	1202	CLA	C6-C7-C8-C9
16	G	1204	CLA	C14-C13-C15-C16
16	H	1101	CLA	C6-C7-C8-C9
16	H	1106	CLA	C6-C7-C8-C9
16	H	1109	CLA	C11-C12-C13-C14
16	H	1126	CLA	C6-C7-C8-C9
16	H	1130	CLA	C11-C10-C8-C9
16	Y	510	CLA	C11-C12-C13-C14
16	Z	504	CLA	C11-C10-C8-C9
16	a	1130	CLA	C11-C10-C8-C9
16	b	1203	CLA	C14-C13-C15-C16
16	g	504	CLA	C11-C12-C13-C14
16	l	1503	CLA	C11-C10-C8-C9
16	q	510	CLA	C6-C7-C8-C9
16	s	510	CLA	C11-C12-C13-C14
16	v	505	CLA	C11-C12-C13-C14
16	v	506	CLA	C11-C10-C8-C9
16	v	509	CLA	C6-C7-C8-C9
14	B	848	LMG	O6-C1-O1-C7
19	G	4017	BCR	C22-C23-C24-C25
19	H	4008	BCR	C6-C7-C8-C9
19	L	4019	BCR	C6-C7-C8-C9
19	L	4022	BCR	C6-C7-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	T	4001	BCR	C6-C7-C8-C9
19	b	4004	BCR	C22-C23-C24-C25
19	h	601	BCR	C6-C7-C8-C9
19	n	604	BCR	C6-C7-C8-C9
19	t	604	BCR	C6-C7-C8-C9
19	u	602	BCR	C6-C7-C8-C9
19	x	602	BCR	C22-C23-C24-C25
16	G	1227	CLA	CBD-CGD-O2D-CED
16	s	514	CLA	O1A-CGA-O2A-C1
16	G	1210	CLA	C4C-C3C-CAC-CBC
16	B	1214	CLA	O1D-CGD-O2D-CED
16	q	512	CLA	C15-C16-C17-C18
19	j	4015	BCR	C14-C15-C16-C17
19	r	602	BCR	C14-C15-C16-C17
19	u	604	BCR	C14-C15-C16-C17
16	L	1503	CLA	C16-C17-C18-C20
16	b	1226	CLA	C11-C12-C13-C15
16	B	1239	CLA	C3-C5-C6-C7
16	n	515	CLA	C3-C5-C6-C7
16	q	515	CLA	C3-C5-C6-C7
16	u	515	CLA	C3-C5-C6-C7
16	A	1104	CLA	CBA-CGA-O2A-C1
13	p	605	LHG	C11-C10-C9-C8
14	A	4101	LMG	C2-C1-O1-C7
14	H	4101	LMG	C2-C1-O1-C7
16	G	1227	CLA	O2A-C1-C2-C3
16	b	1227	CLA	O2A-C1-C2-C3
16	a	1123	CLA	CBD-CGD-O2D-CED
13	a	851	LHG	C11-C10-C9-C8
16	a	1022	CLA	C4C-C3C-CAC-CBC
16	h	511	CLA	C2C-C3C-CAC-CBC
16	q	510	CLA	C5-C6-C7-C8
16	s	509	CLA	O1D-CGD-O2D-CED
16	p	511	CLA	O1A-CGA-O2A-C1
16	x	507	CLA	C5-C6-C7-C8
13	x	605	LHG	O1-C1-C2-O2
14	B	848	LMG	C29-C28-O8-C9
16	H	1103	CLA	CBA-CGA-O2A-C1
19	X	604	BCR	C13-C14-C15-C16
19	a	4007	BCR	C19-C20-C21-C22
19	h	601	BCR	C9-C10-C11-C12
15	a	1011	CL0	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	r	503	CLA	CAA-CBA-CGA-O2A
13	Y	605	LHG	C27-C28-C29-C30
16	B	1223	CLA	C2-C3-C5-C6
16	G	1204	CLA	C2-C3-C5-C6
16	H	1123	CLA	C2-C3-C5-C6
16	a	1103	CLA	C2-C3-C5-C6
16	v	509	CLA	C2-C3-C5-C6
16	y	517	CLA	C2-C3-C5-C6
14	G	848	LMG	O6-C5-C6-O5
16	H	1138	CLA	C8-C10-C11-C12
16	Z	511	CLA	C4C-C3C-CAC-CBC
16	G	1220	CLA	C2C-C3C-CAC-CBC
16	X	502	CLA	O1D-CGD-O2D-CED
16	H	1138	CLA	C10-C11-C12-C13
16	u	516	CLA	O1A-CGA-O2A-C1
13	I	103	LHG	C1-C2-C3-O3
19	G	4009	BCR	C16-C17-C18-C36
19	H	4007	BCR	C16-C17-C18-C36
19	J	4012	BCR	C16-C17-C18-C36
19	K	4005	BCR	C16-C17-C18-C36
19	L	4019	BCR	C20-C21-C22-C37
19	Q	4016	BCR	C11-C10-C9-C34
19	U	4022	BCR	C16-C17-C18-C36
19	a	4011	BCR	C16-C17-C18-C36
19	g	601	BCR	C11-C10-C9-C34
19	j	4013	BCR	C35-C13-C14-C15
19	j	4013	BCR	C20-C21-C22-C37
19	q	604	BCR	C16-C17-C18-C36
19	s	604	BCR	C16-C17-C18-C36
19	t	601	BCR	C16-C17-C18-C36
16	H	1109	CLA	C3-C5-C6-C7
16	y	515	CLA	C3-C5-C6-C7
16	a	1140	CLA	C8-C10-C11-C12
16	b	1211	CLA	C8-C10-C11-C12
14	a	4101	LMG	C13-C14-C15-C16
13	g	605	LHG	O6-C4-C5-C6
13	u	605	LHG	O6-C4-C5-C6
16	v	504	CLA	C8-C10-C11-C12
19	G	4017	BCR	C7-C8-C9-C34
19	S	4015	BCR	C11-C12-C13-C35
19	n	601	BCR	C11-C12-C13-C35
19	o	602	BCR	C37-C22-C23-C24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	Y	605	LHG	C11-C10-C9-C8
16	a	1114	CLA	CBA-CGA-O2A-C1
16	A	1106	CLA	C6-C7-C8-C10
16	A	1125	CLA	C12-C13-C15-C16
16	A	1128	CLA	C12-C13-C15-C16
16	A	1130	CLA	C11-C10-C8-C7
16	A	1131	CLA	C12-C13-C15-C16
16	B	1021	CLA	C11-C12-C13-C15
16	B	1021	CLA	C12-C13-C15-C16
16	B	1210	CLA	C6-C7-C8-C10
16	B	1211	CLA	C12-C13-C15-C16
16	G	1021	CLA	C11-C12-C13-C15
16	G	1021	CLA	C12-C13-C15-C16
16	G	1203	CLA	C12-C13-C15-C16
16	G	1206	CLA	C11-C10-C8-C7
16	G	1210	CLA	C6-C7-C8-C10
16	H	1103	CLA	C11-C10-C8-C7
16	H	1104	CLA	C11-C10-C8-C7
16	H	1126	CLA	C6-C7-C8-C10
16	H	1128	CLA	C12-C13-C15-C16
16	H	1140	CLA	C6-C7-C8-C10
16	U	1501	CLA	C11-C10-C8-C7
16	U	1502	CLA	C6-C7-C8-C10
16	U	1503	CLA	C12-C13-C15-C16
16	Y	507	CLA	C11-C10-C8-C7
16	Y	512	CLA	C11-C12-C13-C15
16	a	1101	CLA	C11-C10-C8-C7
16	a	1106	CLA	C6-C7-C8-C10
16	a	1109	CLA	C11-C12-C13-C15
16	b	1021	CLA	C11-C12-C13-C15
16	b	1021	CLA	C12-C13-C15-C16
16	b	1206	CLA	C6-C7-C8-C10
16	g	504	CLA	C11-C12-C13-C15
16	h	505	CLA	C11-C12-C13-C15
16	h	507	CLA	C6-C7-C8-C10
16	l	1502	CLA	C6-C7-C8-C10
16	o	510	CLA	C11-C10-C8-C7
16	p	509	CLA	C11-C10-C8-C7
16	p	510	CLA	C11-C12-C13-C15
16	q	515	CLA	C11-C12-C13-C15
16	r	504	CLA	C11-C12-C13-C15
16	w	504	CLA	C11-C10-C8-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	w	510	CLA	C6-C7-C8-C10
16	w	511	CLA	C6-C7-C8-C10
14	a	4101	LMG	C17-C18-C19-C20
16	w	501	CLA	CBD-CGD-O2D-CED
16	X	515	CLA	C13-C15-C16-C17
16	b	1223	CLA	C8-C10-C11-C12
16	s	511	CLA	C13-C15-C16-C17
19	T	4005	BCR	C21-C22-C23-C24
19	W	603	BCR	C11-C12-C13-C14
19	g	603	BCR	C11-C12-C13-C14
19	o	602	BCR	C17-C18-C19-C20
19	p	604	BCR	C11-C12-C13-C14
19	r	603	BCR	C7-C8-C9-C10
19	r	603	BCR	C11-C12-C13-C14
19	u	602	BCR	C7-C8-C9-C10
19	w	603	BCR	C11-C12-C13-C14
19	w	604	BCR	C7-C8-C9-C10
19	y	601	BCR	C7-C8-C9-C10
21	R	4020	ECH	C21-C22-C23-C24
21	i	4020	ECH	C17-C18-C19-C20
16	G	1221	CLA	CBA-CGA-O2A-C1
16	n	502	CLA	CBA-CGA-O2A-C1
16	t	507	CLA	CBA-CGA-O2A-C1
16	W	513	CLA	O1A-CGA-O2A-C1
16	Z	505	CLA	O1A-CGA-O2A-C1
16	u	517	CLA	O1A-CGA-O2A-C1
16	W	506	CLA	C4C-C3C-CAC-CBC
16	r	505	CLA	C8-C10-C11-C12
17	B	2002	PQN	C25-C26-C27-C28
16	A	1120	CLA	C2A-CAA-CBA-CGA
16	W	516	CLA	C2A-CAA-CBA-CGA
16	Y	505	CLA	C2A-CAA-CBA-CGA
16	Z	513	CLA	C2A-CAA-CBA-CGA
16	a	1122	CLA	C2A-CAA-CBA-CGA
16	A	1124	CLA	C11-C12-C13-C14
16	X	508	CLA	C6-C7-C8-C10
16	x	504	CLA	C16-C17-C18-C20
16	a	1112	CLA	O1D-CGD-O2D-CED
14	f	4017	LMG	O9-C10-O7-C8
13	s	605	LHG	C11-C10-C9-C8
16	A	1115	CLA	C4-C3-C5-C6
16	G	1210	CLA	C4-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	H	1101	CLA	C4-C3-C5-C6
16	U	1501	CLA	C4-C3-C5-C6
16	X	515	CLA	C4-C3-C5-C6
16	a	1104	CLA	C4-C3-C5-C6
16	A	1104	CLA	O1A-CGA-O2A-C1
16	A	1116	CLA	O1A-CGA-O2A-C1
16	a	1106	CLA	O1A-CGA-O2A-C1
16	n	504	CLA	O1A-CGA-O2A-C1
16	x	504	CLA	C2-C3-C5-C6
16	X	509	CLA	C10-C11-C12-C13
16	n	505	CLA	C8-C10-C11-C12
14	H	4201	LMG	C28-C29-C30-C31
16	p	505	CLA	C3-C5-C6-C7
13	i	103	LHG	C10-C11-C12-C13
16	G	1217	CLA	CBD-CGD-O2D-CED
13	r	605	LHG	O10-C23-O8-C6
16	H	1110	CLA	O1A-CGA-O2A-C1
16	w	507	CLA	C5-C6-C7-C8
19	h	604	BCR	C19-C20-C21-C22
19	j	4015	BCR	C9-C10-C11-C12
19	w	602	BCR	C15-C16-C17-C18
19	a	4003	BCR	C14-C15-C16-C17
19	w	602	BCR	C14-C15-C16-C17
13	I	103	LHG	C10-C11-C12-C13
13	a	849	LHG	C28-C29-C30-C31
14	A	4101	LMG	C34-C35-C36-C37
16	H	1101	CLA	C16-C17-C18-C19
16	W	517	CLA	C6-C7-C8-C10
16	H	1013	CLA	O1A-CGA-O2A-C1
16	Y	511	CLA	O1A-CGA-O2A-C1
16	v	509	CLA	O1A-CGA-O2A-C1
16	B	1207	CLA	C13-C15-C16-C17
16	G	1239	CLA	C8-C10-C11-C12
16	a	1102	CLA	C5-C6-C7-C8
16	p	512	CLA	C8-C10-C11-C12
16	t	505	CLA	C10-C11-C12-C13
13	i	103	LHG	C25-C26-C27-C28
19	X	601	BCR	C20-C21-C22-C23
19	l	4022	BCR	C20-C21-C22-C23
19	s	601	BCR	C16-C17-C18-C19
16	a	1117	CLA	C8-C10-C11-C12
16	q	505	CLA	C5-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	849	LHG	O6-C4-C5-O7
16	B	1227	CLA	O2A-C1-C2-C3
13	s	605	LHG	C4-C5-C6-O8
14	a	4101	LMG	O1-C7-C8-C9
14	b	848	LMG	O1-C7-C8-C9
16	H	1103	CLA	C10-C11-C12-C13
16	r	507	CLA	C5-C6-C7-C8
16	G	1202	CLA	C16-C17-C18-C19
16	a	1139	CLA	C6-C7-C8-C10
16	H	1125	CLA	C3-C5-C6-C7
16	w	515	CLA	C3-C5-C6-C7
16	A	1013	CLA	O1A-CGA-O2A-C1
16	A	1102	CLA	C5-C6-C7-C8
16	H	1110	CLA	C4-C3-C5-C6
16	o	512	CLA	C4-C3-C5-C6
16	A	1129	CLA	C2A-CAA-CBA-CGA
16	B	1213	CLA	C2A-CAA-CBA-CGA
16	F	1302	CLA	C2A-CAA-CBA-CGA
16	S	1302	CLA	C2A-CAA-CBA-CGA
16	X	509	CLA	C2A-CAA-CBA-CGA
16	a	1107	CLA	C2A-CAA-CBA-CGA
16	p	505	CLA	C2A-CAA-CBA-CGA
16	X	508	CLA	C2-C3-C5-C6
16	h	507	CLA	C2-C3-C5-C6
13	G	4018	LHG	C16-C17-C18-C19
13	H	849	LHG	C10-C11-C12-C13
16	B	1222	CLA	O1D-CGD-O2D-CED
16	G	1206	CLA	C5-C6-C7-C8
16	W	505	CLA	C8-C10-C11-C12
16	W	509	CLA	C10-C11-C12-C13
16	a	1132	CLA	C15-C16-C17-C18
16	p	505	CLA	C8-C10-C11-C12
16	v	512	CLA	C8-C10-C11-C12
13	i	103	LHG	O7-C5-C6-O8
13	r	605	LHG	O7-C5-C6-O8
14	H	4101	LMG	O7-C8-C9-O8
14	a	4101	LMG	O7-C8-C9-O8
14	b	848	LMG	O1-C7-C8-O7
16	B	1226	CLA	C8-C10-C11-C12
16	H	1132	CLA	C8-C10-C11-C12
16	A	1125	CLA	C14-C13-C15-C16
16	G	1021	CLA	C11-C12-C13-C14

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1021	CLA	C14-C13-C15-C16
16	G	1206	CLA	C11-C10-C8-C9
16	G	1210	CLA	C6-C7-C8-C9
16	Z	507	CLA	C6-C7-C8-C9
16	a	1013	CLA	C11-C10-C8-C9
16	a	1109	CLA	C11-C12-C13-C14
16	n	505	CLA	C14-C13-C15-C16
16	o	510	CLA	C11-C10-C8-C9
16	p	509	CLA	C11-C10-C8-C9
16	p	510	CLA	C11-C12-C13-C14
16	r	504	CLA	C11-C12-C13-C14
16	w	510	CLA	C6-C7-C8-C9
16	w	511	CLA	C6-C7-C8-C9
16	y	506	CLA	C11-C10-C8-C9
16	y	509	CLA	C6-C7-C8-C9
16	Z	509	CLA	C16-C17-C18-C20
16	Z	512	CLA	C16-C17-C18-C19
16	W	514	CLA	CAA-CBA-CGA-O2A
16	q	508	CLA	CAA-CBA-CGA-O2A
16	H	1117	CLA	C15-C16-C17-C18
16	b	1221	CLA	C8-C10-C11-C12
16	v	516	CLA	CBD-CGD-O2D-CED
14	A	4101	LMG	C33-C34-C35-C36
16	G	1211	CLA	C13-C15-C16-C17
16	a	1126	CLA	C8-C10-C11-C12
16	b	1226	CLA	C8-C10-C11-C12
16	u	511	CLA	C8-C10-C11-C12
16	t	507	CLA	O1A-CGA-O2A-C1
16	b	1238	CLA	C3-C5-C6-C7
14	b	848	LMG	C31-C32-C33-C34
16	a	1119	CLA	O1D-CGD-O2D-CED
16	b	1220	CLA	C2-C1-O2A-CGA
19	Y	602	BCR	C13-C14-C15-C16
19	p	602	BCR	C13-C14-C15-C16
23	r	606	LMU	C2'-C1'-O1'-C1
16	H	1116	CLA	CBA-CGA-O2A-C1
15	H	1011	CL0	C16-C17-C18-C19
16	a	1237	CLA	C16-C17-C18-C20
16	b	1221	CLA	C16-C17-C18-C20
16	A	1136	CLA	C8-C10-C11-C12
16	q	509	CLA	C13-C15-C16-C17
16	t	511	CLA	C10-C11-C12-C13

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1105	CLA	O1D-CGD-O2D-CED
16	y	509	CLA	C4C-C3C-CAC-CBC
16	A	1118	CLA	C4-C3-C5-C6
16	G	1224	CLA	C4-C3-C5-C6
16	v	508	CLA	C4-C3-C5-C6
16	y	508	CLA	C4-C3-C5-C6
16	B	1229	CLA	C2C-C3C-CAC-CBC
16	t	515	CLA	C3-C5-C6-C7
16	G	1210	CLA	C2-C3-C5-C6
16	G	1213	CLA	C2-C3-C5-C6
13	R	103	LHG	C1-C2-C3-O3
16	H	1130	CLA	C10-C11-C12-C13
16	Z	509	CLA	C15-C16-C17-C18
16	q	509	CLA	C15-C16-C17-C18
16	x	505	CLA	C8-C10-C11-C12
13	i	103	LHG	C31-C32-C33-C34
16	Q	1302	CLA	C2A-CAA-CBA-CGA
16	y	513	CLA	C2A-CAA-CBA-CGA
16	Y	510	CLA	O1D-CGD-O2D-CED
13	H	849	LHG	O10-C23-O8-C6
16	G	1221	CLA	O1A-CGA-O2A-C1
16	H	1103	CLA	O1A-CGA-O2A-C1
16	n	502	CLA	O1A-CGA-O2A-C1
13	b	4018	LHG	C11-C12-C13-C14
16	A	1123	CLA	C5-C6-C7-C8
16	b	1225	CLA	C13-C15-C16-C17
16	B	1214	CLA	C3-C5-C6-C7
16	W	506	CLA	C3-C5-C6-C7
16	w	512	CLA	C8-C10-C11-C12
13	A	849	LHG	C32-C33-C34-C35
16	h	517	CLA	O1D-CGD-O2D-CED
16	B	1224	CLA	C11-C12-C13-C15
16	G	1221	CLA	C16-C17-C18-C20
16	g	504	CLA	C16-C17-C18-C20
16	t	517	CLA	C6-C7-C8-C9
14	A	4201	LMG	C4-C5-C6-O5
19	Z	602	BCR	C36-C18-C19-C20
16	A	1139	CLA	C1A-C2A-CAA-CBA
16	A	1801	CLA	C1A-C2A-CAA-CBA
16	B	1023	CLA	C1A-C2A-CAA-CBA
16	B	1227	CLA	C1A-C2A-CAA-CBA
16	G	1023	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1234	CLA	C1A-C2A-CAA-CBA
16	H	1123	CLA	C1A-C2A-CAA-CBA
16	H	1129	CLA	O1A-CGA-O2A-C1
16	H	1139	CLA	C1A-C2A-CAA-CBA
16	K	4004	CLA	C1A-C2A-CAA-CBA
16	W	505	CLA	C1A-C2A-CAA-CBA
16	W	514	CLA	C1A-C2A-CAA-CBA
16	Y	505	CLA	C1A-C2A-CAA-CBA
16	Z	514	CLA	C1A-C2A-CAA-CBA
16	a	1120	CLA	C1A-C2A-CAA-CBA
16	a	1122	CLA	C1A-C2A-CAA-CBA
16	a	1123	CLA	C1A-C2A-CAA-CBA
16	b	1234	CLA	C1A-C2A-CAA-CBA
16	g	506	CLA	C1A-C2A-CAA-CBA
16	g	515	CLA	C1A-C2A-CAA-CBA
16	h	507	CLA	C1A-C2A-CAA-CBA
16	p	503	CLA	C1A-C2A-CAA-CBA
16	r	516	CLA	C1A-C2A-CAA-CBA
16	s	505	CLA	C1A-C2A-CAA-CBA
16	t	511	CLA	C1A-C2A-CAA-CBA
16	v	501	CLA	O1A-CGA-O2A-C1
16	y	503	CLA	C1A-C2A-CAA-CBA
16	y	507	CLA	C1A-C2A-CAA-CBA
16	Y	516	CLA	O1D-CGD-O2D-CED
16	g	503	CLA	O1D-CGD-O2D-CED
16	n	515	CLA	O1D-CGD-O2D-CED
16	t	502	CLA	O1D-CGD-O2D-CED
13	B	4018	LHG	C18-C19-C20-C21
13	A	851	LHG	C9-C10-C11-C12
19	K	4005	BCR	C6-C7-C8-C9
19	k	4001	BCR	C6-C7-C8-C9
19	l	4019	BCR	C6-C7-C8-C9
16	n	514	CLA	CAA-CBA-CGA-O2A
16	U	1501	CLA	C2-C3-C5-C6
16	a	1013	CLA	C2-C3-C5-C6
16	o	512	CLA	C2-C3-C5-C6
19	U	4019	BCR	C11-C12-C13-C14
19	x	604	BCR	C7-C8-C9-C10
16	B	1238	CLA	C16-C17-C18-C20
16	l	1501	CLA	C11-C12-C13-C14
16	H	1118	CLA	C3-C5-C6-C7
16	h	512	CLA	C15-C16-C17-C18

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	b	1213	CLA	C2A-CAA-CBA-CGA
16	g	503	CLA	C2A-CAA-CBA-CGA
16	v	503	CLA	C2A-CAA-CBA-CGA
16	u	504	CLA	C10-C11-C12-C13
13	H	849	LHG	O6-C4-C5-C6
13	a	849	LHG	O6-C4-C5-C6
16	G	1210	CLA	CBD-CGD-O2D-CED
16	x	516	CLA	CBA-CGA-O2A-C1
13	i	103	LHG	C32-C33-C34-C35
16	B	1207	CLA	C3-C5-C6-C7
16	A	1103	CLA	C11-C10-C8-C7
16	A	1109	CLA	C11-C12-C13-C15
16	A	1126	CLA	C6-C7-C8-C10
16	B	1206	CLA	C6-C7-C8-C10
16	B	1239	CLA	C12-C13-C15-C16
16	G	1239	CLA	C6-C7-C8-C10
16	H	1104	CLA	C11-C12-C13-C15
16	L	1502	CLA	C6-C7-C8-C10
16	W	504	CLA	C6-C7-C8-C10
16	W	507	CLA	C11-C10-C8-C7
16	X	507	CLA	C11-C10-C8-C7
16	X	510	CLA	C11-C10-C8-C7
16	Z	515	CLA	C11-C12-C13-C15
16	a	1103	CLA	C11-C10-C8-C7
16	a	1126	CLA	C6-C7-C8-C10
16	a	1128	CLA	C12-C13-C15-C16
16	a	1131	CLA	C12-C13-C15-C16
16	a	1138	CLA	C11-C10-C8-C7
16	a	1237	CLA	C11-C10-C8-C7
16	b	1204	CLA	C12-C13-C15-C16
16	b	1211	CLA	C12-C13-C15-C16
16	b	1239	CLA	C6-C7-C8-C10
16	g	507	CLA	C11-C10-C8-C7
16	h	504	CLA	C11-C10-C8-C7
16	h	511	CLA	C6-C7-C8-C10
16	l	1501	CLA	C11-C10-C8-C7
16	l	1503	CLA	C12-C13-C15-C16
16	n	507	CLA	C11-C10-C8-C7
16	n	510	CLA	C12-C13-C15-C16
16	o	505	CLA	C11-C10-C8-C7
16	o	507	CLA	C11-C10-C8-C7
16	p	507	CLA	C11-C10-C8-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	p	511	CLA	C12-C13-C15-C16
16	p	512	CLA	C11-C12-C13-C15
16	q	504	CLA	C6-C7-C8-C10
16	q	507	CLA	C11-C10-C8-C7
16	q	512	CLA	C6-C7-C8-C10
16	r	504	CLA	C12-C13-C15-C16
16	r	507	CLA	C11-C10-C8-C7
16	r	510	CLA	C11-C12-C13-C15
16	s	507	CLA	C11-C10-C8-C7
16	s	512	CLA	C11-C12-C13-C15
16	s	515	CLA	C6-C7-C8-C10
16	t	504	CLA	C6-C7-C8-C10
16	t	507	CLA	C11-C10-C8-C7
16	t	511	CLA	C6-C7-C8-C10
16	v	506	CLA	C11-C10-C8-C7
16	w	504	CLA	C6-C7-C8-C10
16	w	507	CLA	C11-C10-C8-C7
16	w	515	CLA	C11-C12-C13-C15
16	x	504	CLA	C12-C13-C15-C16
16	x	506	CLA	C11-C10-C8-C7
16	x	510	CLA	C6-C7-C8-C10
16	y	509	CLA	C11-C12-C13-C15
17	a	2001	PQN	C16-C17-C18-C20
17	a	2001	PQN	C21-C22-C23-C25
16	b	1221	CLA	C16-C17-C18-C19
16	b	1226	CLA	C11-C12-C13-C14
16	q	507	CLA	C5-C6-C7-C8
16	A	1103	CLA	CBA-CGA-O2A-C1
16	A	1106	CLA	CBA-CGA-O2A-C1
16	H	1013	CLA	CBA-CGA-O2A-C1
16	X	511	CLA	CBA-CGA-O2A-C1
16	a	1103	CLA	CBA-CGA-O2A-C1
13	R	103	LHG	C10-C11-C12-C13
16	b	1205	CLA	CBD-CGD-O2D-CED
13	Y	605	LHG	C5-C4-O6-P
13	r	605	LHG	C2-C3-O3-P
16	G	1220	CLA	C3A-C2A-CAA-CBA
16	a	1118	CLA	C4-C3-C5-C6
16	p	503	CLA	C3A-C2A-CAA-CBA
16	w	503	CLA	C3A-C2A-CAA-CBA
16	y	504	CLA	C3A-C2A-CAA-CBA
16	H	1117	CLA	C16-C17-C18-C20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	Z	512	CLA	C16-C17-C18-C20
16	o	508	CLA	C6-C7-C8-C9
16	r	506	CLA	C11-C12-C13-C14
16	H	1138	CLA	O1D-CGD-O2D-CED
13	I	103	LHG	C11-C10-C9-C8
13	H	849	LHG	O6-C4-C5-O7
13	X	605	LHG	O6-C4-C5-O7
13	o	605	LHG	O6-C4-C5-O7
13	x	605	LHG	O6-C4-C5-O7
13	i	103	LHG	C8-C7-O7-C5
16	b	1235	CLA	C2A-CAA-CBA-CGA
16	q	508	CLA	C2A-CAA-CBA-CGA
16	A	1104	CLA	C11-C10-C8-C9
16	A	1130	CLA	C11-C10-C8-C9
16	A	1131	CLA	C14-C13-C15-C16
16	B	1021	CLA	C11-C12-C13-C14
16	B	1021	CLA	C14-C13-C15-C16
16	B	1202	CLA	C11-C12-C13-C14
16	B	1211	CLA	C14-C13-C15-C16
16	B	1223	CLA	C11-C10-C8-C9
16	G	1023	CLA	C14-C13-C15-C16
16	G	1203	CLA	C14-C13-C15-C16
16	H	1103	CLA	C11-C10-C8-C9
16	H	1109	CLA	C6-C7-C8-C9
16	U	1501	CLA	C11-C10-C8-C9
16	U	1503	CLA	C11-C10-C8-C9
16	U	1503	CLA	C14-C13-C15-C16
16	a	1101	CLA	C11-C10-C8-C9
16	a	1131	CLA	C11-C10-C8-C9
16	b	1021	CLA	C11-C12-C13-C14
16	b	1021	CLA	C14-C13-C15-C16
16	g	504	CLA	C14-C13-C15-C16
16	g	510	CLA	C11-C12-C13-C14
16	h	505	CLA	C11-C12-C13-C14
16	l	1502	CLA	C6-C7-C8-C9
16	l	1503	CLA	C6-C7-C8-C9
16	n	512	CLA	C14-C13-C15-C16
16	q	515	CLA	C11-C12-C13-C14
16	r	506	CLA	C11-C10-C8-C9
16	s	515	CLA	C6-C7-C8-C9
16	w	504	CLA	C6-C7-C8-C9
19	A	4011	BCR	C9-C10-C11-C12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	U	4022	BCR	C13-C14-C15-C16
19	W	604	BCR	C15-C16-C17-C18
19	g	601	BCR	C13-C14-C15-C16
19	h	601	BCR	C19-C20-C21-C22
19	q	602	BCR	C19-C20-C21-C22
19	r	601	BCR	C9-C10-C11-C12
19	s	602	BCR	C13-C14-C15-C16
19	t	601	BCR	C15-C16-C17-C18
21	M	4021	ECH	C13-C14-C15-C16
16	r	513	CLA	CBA-CGA-O2A-C1
16	g	506	CLA	C5-C6-C7-C8
16	s	512	CLA	C15-C16-C17-C18
16	A	1120	CLA	C1-C2-C3-C4
16	B	1227	CLA	C1-C2-C3-C4
16	G	1227	CLA	C1-C2-C3-C4
16	H	1120	CLA	C1-C2-C3-C4
16	a	1120	CLA	C1-C2-C3-C4
16	b	1227	CLA	C1-C2-C3-C4
16	t	506	CLA	O1D-CGD-O2D-CED
16	A	1138	CLA	C8-C10-C11-C12
13	H	851	LHG	O7-C5-C6-O8
14	G	848	LMG	O1-C7-C8-O7
16	G	1227	CLA	O1D-CGD-O2D-CED
14	b	848	LMG	C16-C17-C18-C19
15	A	1011	CL0	C2C-C3C-CAC-CBC
16	a	1801	CLA	CBA-CGA-O2A-C1
16	h	501	CLA	CBA-CGA-O2A-C1
16	n	515	CLA	C5-C6-C7-C8
14	H	4101	LMG	C18-C19-C20-C21
13	Y	605	LHG	C4-C5-C6-O8
13	i	103	LHG	C4-C5-C6-O8
14	G	848	LMG	C7-C8-C9-O8
16	v	509	CLA	CAA-CBA-CGA-O2A
16	G	1224	CLA	C2-C3-C5-C6
16	v	504	CLA	C2-C3-C5-C6
14	A	4201	LMG	O6-C5-C6-O5
16	G	1212	CLA	CBD-CGD-O2D-CED
16	A	1801	CLA	CAD-CBD-CGD-O2D
16	B	1012	CLA	CAD-CBD-CGD-O2D
16	B	1202	CLA	CAD-CBD-CGD-O2D
16	B	1210	CLA	CAD-CBD-CGD-O2D
16	B	1234	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1012	CLA	CAD-CBD-CGD-O2D
16	H	1103	CLA	CAD-CBD-CGD-O2D
16	H	1111	CLA	CAD-CBD-CGD-O2D
16	W	503	CLA	CAD-CBD-CGD-O2D
16	W	510	CLA	CAD-CBD-CGD-O2D
16	W	516	CLA	CAD-CBD-CGD-O2D
16	X	503	CLA	CAD-CBD-CGD-O2D
16	X	510	CLA	CAD-CBD-CGD-O2D
16	Y	513	CLA	CAD-CBD-CGD-O2D
16	Y	516	CLA	CAD-CBD-CGD-O2D
16	Z	514	CLA	CAD-CBD-CGD-O2D
16	a	1103	CLA	CAD-CBD-CGD-O2D
16	a	1111	CLA	CAD-CBD-CGD-O2D
16	b	1012	CLA	CAD-CBD-CGD-O2D
16	b	1202	CLA	CAD-CBD-CGD-O2D
16	h	506	CLA	CAD-CBD-CGD-O2D
16	h	517	CLA	CAD-CBD-CGD-O2D
16	n	501	CLA	CAD-CBD-CGD-O2D
16	n	510	CLA	CAD-CBD-CGD-O2D
16	n	516	CLA	CAD-CBD-CGD-O2D
16	n	517	CLA	CAD-CBD-CGD-O2D
16	o	507	CLA	CAD-CBD-CGD-O2D
16	p	513	CLA	CAD-CBD-CGD-O2D
16	q	514	CLA	CAD-CBD-CGD-O2D
16	r	514	CLA	CAD-CBD-CGD-O2D
16	s	503	CLA	CAD-CBD-CGD-O2D
16	t	510	CLA	CAD-CBD-CGD-O2D
16	u	503	CLA	CAD-CBD-CGD-O2D
16	v	508	CLA	CAD-CBD-CGD-O2D
16	v	517	CLA	CAD-CBD-CGD-O2D
16	y	506	CLA	CAD-CBD-CGD-O2D
16	y	507	CLA	CAD-CBD-CGD-O2D
13	x	605	LHG	O10-C23-O8-C6
16	A	1103	CLA	O1A-CGA-O2A-C1
16	W	510	CLA	O1D-CGD-O2D-CED
14	G	848	LMG	C29-C28-O8-C9
16	H	1136	CLA	CBA-CGA-O2A-C1
16	t	504	CLA	CBA-CGA-O2A-C1
16	b	1238	CLA	C16-C17-C18-C19
16	B	1211	CLA	C2A-CAA-CBA-CGA
16	B	1231	CLA	C2A-CAA-CBA-CGA
16	h	512	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	h	513	CLA	C2A-CAA-CBA-CGA
16	t	509	CLA	C2A-CAA-CBA-CGA
16	w	508	CLA	C2A-CAA-CBA-CGA
16	G	1226	CLA	C5-C6-C7-C8
16	X	515	CLA	C15-C16-C17-C18
16	A	1106	CLA	O1A-CGA-O2A-C1
16	H	1116	CLA	O1A-CGA-O2A-C1
13	B	4018	LHG	C3-O3-P-O6
13	B	4018	LHG	C4-O6-P-O5
13	H	849	LHG	C3-O3-P-O5
13	R	103	LHG	C3-O3-P-O5
13	R	103	LHG	C4-O6-P-O3
13	Y	605	LHG	C3-O3-P-O5
13	Y	605	LHG	C4-O6-P-O5
13	a	849	LHG	C3-O3-P-O5
13	g	605	LHG	C3-O3-P-O5
13	g	605	LHG	C4-O6-P-O4
13	i	103	LHG	C3-O3-P-O5
13	o	605	LHG	C3-O3-P-O5
13	o	605	LHG	C4-O6-P-O3
13	o	605	LHG	C4-O6-P-O5
13	p	605	LHG	C4-O6-P-O5
13	r	605	LHG	C3-O3-P-O6
13	s	605	LHG	C4-O6-P-O5
13	x	605	LHG	C3-O3-P-O4
13	x	605	LHG	C3-O3-P-O6
16	A	1104	CLA	CHA-CBD-CGD-O1D
16	A	1104	CLA	CHA-CBD-CGD-O2D
16	A	1801	CLA	CAD-CBD-CGD-O1D
16	B	1012	CLA	CAD-CBD-CGD-O1D
16	B	1202	CLA	CAD-CBD-CGD-O1D
16	B	1210	CLA	CAD-CBD-CGD-O1D
16	B	1212	CLA	CHA-CBD-CGD-O1D
16	B	1212	CLA	CHA-CBD-CGD-O2D
16	B	1227	CLA	CHA-CBD-CGD-O1D
16	B	1234	CLA	CAD-CBD-CGD-O1D
16	G	1012	CLA	CAD-CBD-CGD-O1D
16	G	1207	CLA	CHA-CBD-CGD-O1D
16	G	1207	CLA	CHA-CBD-CGD-O2D
16	G	1210	CLA	CAD-CBD-CGD-O1D
16	G	1218	CLA	CHA-CBD-CGD-O1D
16	G	1218	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1227	CLA	CHA-CBD-CGD-O1D
16	G	1227	CLA	CHA-CBD-CGD-O2D
16	G	1234	CLA	CAD-CBD-CGD-O1D
16	H	1103	CLA	CAD-CBD-CGD-O1D
16	H	1104	CLA	CHA-CBD-CGD-O1D
16	H	1111	CLA	CAD-CBD-CGD-O1D
16	H	1135	CLA	CAD-CBD-CGD-O1D
16	T	4003	CLA	CHA-CBD-CGD-O1D
16	T	4003	CLA	CHA-CBD-CGD-O2D
16	W	503	CLA	CAD-CBD-CGD-O1D
16	W	505	CLA	CHA-CBD-CGD-O1D
16	W	507	CLA	CHA-CBD-CGD-O1D
16	W	507	CLA	CHA-CBD-CGD-O2D
16	W	510	CLA	CAD-CBD-CGD-O1D
16	W	515	CLA	CHA-CBD-CGD-O1D
16	W	515	CLA	CHA-CBD-CGD-O2D
16	W	516	CLA	CAD-CBD-CGD-O1D
16	X	503	CLA	CAD-CBD-CGD-O1D
16	X	510	CLA	CAD-CBD-CGD-O1D
16	Y	506	CLA	CHA-CBD-CGD-O1D
16	Y	506	CLA	CHA-CBD-CGD-O2D
16	Y	513	CLA	CAD-CBD-CGD-O1D
16	Y	515	CLA	CAD-CBD-CGD-O1D
16	Y	516	CLA	CAD-CBD-CGD-O1D
16	Z	514	CLA	CAD-CBD-CGD-O1D
16	a	1103	CLA	CAD-CBD-CGD-O1D
16	a	1104	CLA	CHA-CBD-CGD-O1D
16	a	1104	CLA	CHA-CBD-CGD-O2D
16	a	1111	CLA	CAD-CBD-CGD-O1D
16	a	1114	CLA	CHA-CBD-CGD-O1D
16	a	1114	CLA	CHA-CBD-CGD-O2D
16	b	1012	CLA	CAD-CBD-CGD-O1D
16	b	1202	CLA	CAD-CBD-CGD-O1D
16	b	1207	CLA	CHA-CBD-CGD-O1D
16	b	1226	CLA	CAD-CBD-CGD-O1D
16	f	1302	CLA	CAD-CBD-CGD-O1D
16	g	501	CLA	CHA-CBD-CGD-O1D
16	g	513	CLA	CAD-CBD-CGD-O1D
16	h	503	CLA	CAD-CBD-CGD-O1D
16	h	506	CLA	CAD-CBD-CGD-O1D
16	h	509	CLA	CHA-CBD-CGD-O1D
16	h	517	CLA	CAD-CBD-CGD-O1D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	j	1302	CLA	CAD-CBD-CGD-O1D
16	n	501	CLA	CAD-CBD-CGD-O1D
16	n	510	CLA	CAD-CBD-CGD-O1D
16	n	516	CLA	CAD-CBD-CGD-O1D
16	n	517	CLA	CAD-CBD-CGD-O1D
16	o	507	CLA	CAD-CBD-CGD-O1D
16	o	516	CLA	CHA-CBD-CGD-O1D
16	o	516	CLA	CHA-CBD-CGD-O2D
16	p	506	CLA	CHA-CBD-CGD-O1D
16	p	513	CLA	CAD-CBD-CGD-O1D
16	q	512	CLA	CHA-CBD-CGD-O1D
16	q	514	CLA	CAD-CBD-CGD-O1D
16	r	508	CLA	CHA-CBD-CGD-O1D
16	r	508	CLA	CHA-CBD-CGD-O2D
16	r	514	CLA	CAD-CBD-CGD-O1D
16	s	503	CLA	CAD-CBD-CGD-O1D
16	s	513	CLA	CAD-CBD-CGD-O1D
16	t	510	CLA	CAD-CBD-CGD-O1D
16	t	516	CLA	CAD-CBD-CGD-O1D
16	u	503	CLA	CAD-CBD-CGD-O1D
16	v	508	CLA	CAD-CBD-CGD-O1D
16	v	514	CLA	CAD-CBD-CGD-O1D
16	v	517	CLA	CAD-CBD-CGD-O1D
16	w	515	CLA	CHA-CBD-CGD-O1D
16	w	515	CLA	CHA-CBD-CGD-O2D
16	x	517	CLA	CAD-CBD-CGD-O1D
16	y	506	CLA	CAD-CBD-CGD-O1D
16	y	507	CLA	CAD-CBD-CGD-O1D
16	y	511	CLA	CAD-CBD-CGD-O1D
19	L	4019	BCR	C9-C10-C11-C12
19	Q	4016	BCR	C35-C13-C14-C15
19	X	604	BCR	C19-C20-C21-C22
19	b	4017	BCR	C13-C14-C15-C16
19	y	601	BCR	C35-C13-C14-C15
21	R	4020	ECH	C13-C14-C15-C16
21	V	4021	ECH	C13-C14-C15-C16
16	G	1202	CLA	C4-C3-C5-C6
16	h	508	CLA	C4-C3-C5-C6
19	A	4008	BCR	C23-C24-C25-C26
19	G	4004	BCR	C23-C24-C25-C26
19	H	4003	BCR	C23-C24-C25-C30
19	Y	601	BCR	C5-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	Y	602	BCR	C1-C6-C7-C8
19	Y	603	BCR	C23-C24-C25-C30
19	Z	604	BCR	C5-C6-C7-C8
19	j	4012	BCR	C23-C24-C25-C30
19	k	4005	BCR	C1-C6-C7-C8
19	p	602	BCR	C1-C6-C7-C8
19	t	604	BCR	C23-C24-C25-C30
19	w	603	BCR	C1-C6-C7-C8
19	y	604	BCR	C5-C6-C7-C8
16	Z	514	CLA	CAA-CBA-CGA-O2A
16	A	1110	CLA	C2-C3-C5-C6
16	A	1118	CLA	C2-C3-C5-C6
16	G	1220	CLA	C2-C3-C5-C6
16	H	1101	CLA	C2-C3-C5-C6
16	U	1502	CLA	C2-C3-C5-C6
16	a	1104	CLA	C2-C3-C5-C6
16	y	508	CLA	C2-C3-C5-C6
16	K	4004	CLA	C5-C6-C7-C8
13	Y	605	LHG	C2-C3-O3-P
13	g	605	LHG	C2-C3-O3-P
13	s	605	LHG	C2-C3-O3-P
13	x	605	LHG	C2-C3-O3-P
16	F	1302	CLA	CBA-CGA-O2A-C1
16	B	1211	CLA	C10-C11-C12-C13
16	a	1140	CLA	C10-C11-C12-C13
13	b	4018	LHG	C15-C16-C17-C18
16	A	1124	CLA	C11-C12-C13-C15
16	B	1202	CLA	C16-C17-C18-C19
16	G	1221	CLA	C16-C17-C18-C19
16	x	504	CLA	C16-C17-C18-C19
16	g	515	CLA	O1D-CGD-O2D-CED
16	B	1235	CLA	CAA-CBA-CGA-O2A
24	w	601	LUT	C7-C8-C9-C10
16	X	511	CLA	O1A-CGA-O2A-C1
16	t	504	CLA	O1A-CGA-O2A-C1
16	H	1128	CLA	C13-C15-C16-C17
16	q	514	CLA	CAA-CBA-CGA-O2A
16	w	512	CLA	C16-C17-C18-C19
17	G	2002	PQN	C26-C27-C28-C29
16	H	1132	CLA	C5-C6-C7-C8
16	a	1132	CLA	C5-C6-C7-C8
16	q	511	CLA	C13-C15-C16-C17

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	r	506	CLA	C5-C6-C7-C8
16	v	507	CLA	C5-C6-C7-C8
16	A	1102	CLA	C11-C10-C8-C7
13	x	605	LHG	C24-C25-C26-C27
16	r	503	CLA	O1A-CGA-O2A-C1
16	y	516	CLA	O1A-CGA-O2A-C1
19	Z	602	BCR	C10-C11-C12-C13
19	l	4022	BCR	C18-C19-C20-C21
16	w	508	CLA	CAA-CBA-CGA-O2A
23	p	606	LMU	C1-C2-C3-C4
16	G	1228	CLA	C2-C3-C5-C6
19	h	601	BCR	C15-C16-C17-C18
16	g	504	CLA	C16-C17-C18-C19
16	A	1126	CLA	C13-C15-C16-C17
16	B	1023	CLA	C10-C11-C12-C13
16	s	507	CLA	C8-C10-C11-C12
17	b	2002	PQN	C20-C21-C22-C23
13	A	849	LHG	O6-C4-C5-C6
14	B	848	LMG	C29-C30-C31-C32
14	G	848	LMG	C29-C30-C31-C32
16	a	1116	CLA	CBA-CGA-O2A-C1
16	X	516	CLA	CBA-CGA-O2A-C1
16	a	1103	CLA	O1A-CGA-O2A-C1
16	x	505	CLA	C3-C5-C6-C7
16	Z	515	CLA	C10-C11-C12-C13
16	Y	503	CLA	CAA-CBA-CGA-O2A
16	Y	508	CLA	CAA-CBA-CGA-O2A
16	A	1106	CLA	C6-C7-C8-C9
16	B	1206	CLA	C6-C7-C8-C9
16	B	1221	CLA	C6-C7-C8-C9
16	G	1211	CLA	C11-C10-C8-C9
16	G	1223	CLA	C14-C13-C15-C16
16	G	1239	CLA	C6-C7-C8-C9
16	H	1104	CLA	C11-C12-C13-C14
16	H	1128	CLA	C14-C13-C15-C16
16	L	1501	CLA	C11-C10-C8-C9
16	U	1502	CLA	C6-C7-C8-C9
16	W	505	CLA	C14-C13-C15-C16
16	X	510	CLA	C11-C10-C8-C9
16	Z	505	CLA	C6-C7-C8-C9
16	Z	510	CLA	C6-C7-C8-C9
16	a	1101	CLA	C6-C7-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1103	CLA	C11-C10-C8-C9
16	a	1106	CLA	C6-C7-C8-C9
16	b	1021	CLA	C11-C10-C8-C9
16	b	1202	CLA	C14-C13-C15-C16
16	b	1239	CLA	C6-C7-C8-C9
16	h	504	CLA	C11-C10-C8-C9
16	n	515	CLA	C11-C12-C13-C14
16	o	505	CLA	C6-C7-C8-C9
16	o	505	CLA	C11-C10-C8-C9
16	o	507	CLA	C11-C10-C8-C9
16	q	504	CLA	C6-C7-C8-C9
16	q	507	CLA	C11-C10-C8-C9
16	s	509	CLA	C6-C7-C8-C9
16	s	512	CLA	C11-C12-C13-C14
16	t	505	CLA	C11-C10-C8-C9
16	t	515	CLA	C11-C12-C13-C14
16	u	507	CLA	C11-C10-C8-C9
16	w	507	CLA	C11-C10-C8-C9
16	x	504	CLA	C11-C12-C13-C14
16	y	504	CLA	C11-C10-C8-C9
16	y	509	CLA	C11-C10-C8-C9
16	A	1136	CLA	C11-C10-C8-C7
16	B	1221	CLA	C6-C7-C8-C10
16	X	504	CLA	C11-C10-C8-C7
16	X	512	CLA	C6-C7-C8-C10
16	a	1101	CLA	C6-C7-C8-C10
16	a	1128	CLA	C11-C10-C8-C7
16	q	506	CLA	C6-C7-C8-C10
16	t	505	CLA	C11-C10-C8-C7
16	u	510	CLA	C6-C7-C8-C10
16	y	506	CLA	C11-C10-C8-C7
19	A	4011	BCR	C16-C17-C18-C19
19	B	4010	BCR	C11-C10-C9-C8
19	G	4005	BCR	C11-C10-C9-C8
19	G	4017	BCR	C11-C10-C9-C8
19	L	4022	BCR	C11-C10-C9-C8
19	U	4022	BCR	C20-C21-C22-C23
19	b	4010	BCR	C20-C21-C22-C23
19	p	603	BCR	C11-C10-C9-C8
19	v	601	BCR	C20-C21-C22-C23
19	y	601	BCR	C12-C13-C14-C15
19	y	601	BCR	C20-C21-C22-C23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	H	4101	LMG	C10-C11-C12-C13
19	A	4011	BCR	C22-C23-C24-C25
15	H	1011	CL0	C16-C17-C18-C20
16	b	1202	CLA	C16-C17-C18-C20
16	o	508	CLA	C6-C7-C8-C10
14	H	4101	LMG	C14-C15-C16-C17
15	H	1011	CL0	CAA-CBA-CGA-O2A
16	Y	504	CLA	CAA-CBA-CGA-O2A
16	w	514	CLA	CAA-CBA-CGA-O2A
16	n	505	CLA	C10-C11-C12-C13
16	b	1201	CLA	C6-C7-C8-C9
16	o	510	CLA	CBD-CGD-O2D-CED
16	H	1126	CLA	C13-C15-C16-C17
16	s	505	CLA	C8-C10-C11-C12
14	A	4201	LMG	O7-C10-C11-C12
16	w	504	CLA	CAA-CBA-CGA-O2A
16	B	1228	CLA	C2-C3-C5-C6
16	l	1502	CLA	C2-C3-C5-C6
16	u	512	CLA	C3-C5-C6-C7
16	G	1210	CLA	O1D-CGD-O2D-CED
16	o	511	CLA	CBA-CGA-O2A-C1
16	a	1237	CLA	C16-C17-C18-C19
16	q	506	CLA	C11-C12-C13-C14
16	q	506	CLA	C11-C12-C13-C15
16	t	517	CLA	C6-C7-C8-C10
14	H	4101	LMG	C29-C30-C31-C32
16	H	1136	CLA	O1A-CGA-O2A-C1
16	w	501	CLA	O1D-CGD-O2D-CED
16	G	1235	CLA	CAA-CBA-CGA-O2A
16	a	1801	CLA	CAA-CBA-CGA-O2A
13	o	605	LHG	C24-C25-C26-C27
16	v	516	CLA	O1D-CGD-O2D-CED
16	n	512	CLA	C13-C15-C16-C17
16	G	1207	CLA	C3-C5-C6-C7
16	A	1013	CLA	CBA-CGA-O2A-C1
19	b	4004	BCR	C13-C14-C15-C16
19	i	4018	BCR	C9-C10-C11-C12
13	p	605	LHG	C26-C27-C28-C29
14	b	848	LMG	C11-C10-O7-C8
16	s	516	CLA	CBA-CGA-O2A-C1
16	Z	508	CLA	CAA-CBA-CGA-O2A
16	s	508	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1203	CLA	C2A-CAA-CBA-CGA
16	b	1209	CLA	C2A-CAA-CBA-CGA
16	n	509	CLA	C3-C5-C6-C7
16	a	1013	CLA	O1A-CGA-O2A-C1
16	o	511	CLA	O1A-CGA-O2A-C1
16	G	1239	CLA	C15-C16-C17-C18
16	w	501	CLA	C2-C1-O2A-CGA
16	v	507	CLA	C16-C17-C18-C19
16	x	506	CLA	C11-C12-C13-C14
14	a	4201	LMG	O7-C10-C11-C12
16	g	513	CLA	CAA-CBA-CGA-O2A
16	g	514	CLA	CAA-CBA-CGA-O2A
16	p	508	CLA	CAA-CBA-CGA-O2A
14	A	4101	LMG	C11-C12-C13-C14
14	G	848	LMG	O1-C7-C8-C9
16	b	1205	CLA	O1D-CGD-O2D-CED
16	a	1119	CLA	C5-C6-C7-C8
16	B	1012	CLA	C2C-C3C-CAC-CBC
19	W	603	BCR	C11-C12-C13-C35
19	a	4002	BCR	C37-C22-C23-C24
16	q	516	CLA	O1A-CGA-O2A-C1
16	b	1202	CLA	C16-C17-C18-C19
16	B	1206	CLA	C3-C5-C6-C7
16	b	1012	CLA	C2C-C3C-CAC-CBC
16	G	1229	CLA	C2C-C3C-CAC-CBC
14	F	4017	LMG	C8-C7-O1-C1
16	G	1217	CLA	O1D-CGD-O2D-CED
16	a	1116	CLA	O1A-CGA-O2A-C1
16	Z	512	CLA	C5-C6-C7-C8
16	B	1203	CLA	C2A-CAA-CBA-CGA
16	G	1012	CLA	C2A-CAA-CBA-CGA
16	Z	516	CLA	C2A-CAA-CBA-CGA
16	a	1130	CLA	C2A-CAA-CBA-CGA
16	a	1136	CLA	C2A-CAA-CBA-CGA
16	b	1227	CLA	C2A-CAA-CBA-CGA
16	b	1231	CLA	C2A-CAA-CBA-CGA
16	u	514	CLA	C2A-CAA-CBA-CGA
16	v	502	CLA	C2A-CAA-CBA-CGA
16	G	1212	CLA	O1D-CGD-O2D-CED
19	g	604	BCR	C13-C14-C15-C16
19	l	4019	BCR	C9-C10-C11-C12
16	A	1102	CLA	C11-C10-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	h	511	CLA	C16-C17-C18-C19
16	l	1501	CLA	C11-C12-C13-C15
16	L	1502	CLA	C3-C5-C6-C7
23	x	606	LMU	C11-C10-C9-C8
16	b	1220	CLA	C4-C3-C5-C6
17	b	2002	PQN	C14-C13-C15-C16
16	G	1202	CLA	C15-C16-C17-C18
16	s	504	CLA	CAA-CBA-CGA-O2A
16	h	508	CLA	C2-C3-C5-C6
16	v	508	CLA	C2-C3-C5-C6
16	n	512	CLA	CBA-CGA-O2A-C1
16	q	515	CLA	C13-C15-C16-C17
16	a	1123	CLA	O1D-CGD-O2D-CED
16	G	1218	CLA	C4C-C3C-CAC-CBC
16	G	1239	CLA	C4C-C3C-CAC-CBC
16	y	517	CLA	C6-C7-C8-C10
16	b	1214	CLA	C4C-C3C-CAC-CBC
14	a	852	LMG	C28-C29-C30-C31
16	A	1126	CLA	C6-C7-C8-C9
16	A	1128	CLA	C14-C13-C15-C16
16	X	507	CLA	C11-C10-C8-C9
16	X	511	CLA	C11-C10-C8-C9
16	Z	504	CLA	C6-C7-C8-C9
16	a	1128	CLA	C11-C10-C8-C9
16	a	1131	CLA	C14-C13-C15-C16
16	h	511	CLA	C6-C7-C8-C9
16	n	505	CLA	C11-C12-C13-C14
16	n	507	CLA	C11-C10-C8-C9
16	q	512	CLA	C6-C7-C8-C9
16	t	504	CLA	C6-C7-C8-C9
16	u	510	CLA	C6-C7-C8-C9
16	w	515	CLA	C11-C12-C13-C14
16	x	510	CLA	C6-C7-C8-C9
16	y	505	CLA	C11-C10-C8-C9
17	B	2002	PQN	C21-C22-C23-C24
17	G	2002	PQN	C21-C22-C23-C24
17	a	2001	PQN	C16-C17-C18-C19
16	b	1206	CLA	C13-C15-C16-C17
16	B	1236	CLA	O1D-CGD-O2D-CED
16	A	1133	CLA	C6-C7-C8-C9
16	A	1132	CLA	C5-C6-C7-C8
16	w	512	CLA	C16-C17-C18-C20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	i	103	LHG	C28-C29-C30-C31
13	X	605	LHG	C24-C23-O8-C6
16	A	1124	CLA	C5-C6-C7-C8
16	b	1238	CLA	C13-C15-C16-C17
16	n	505	CLA	C15-C16-C17-C18
16	n	512	CLA	O1A-CGA-O2A-C1
13	r	605	LHG	C11-C12-C13-C14
16	Z	508	CLA	C2A-CAA-CBA-CGA
16	n	502	CLA	C2A-CAA-CBA-CGA
14	A	852	LMG	C29-C30-C31-C32
14	H	4201	LMG	O7-C10-C11-C12
16	X	515	CLA	C2-C3-C5-C6
16	t	506	CLA	C8-C10-C11-C12
13	s	605	LHG	C24-C25-C26-C27
13	G	4018	LHG	C12-C13-C14-C15
19	J	4013	BCR	C19-C20-C21-C22
19	q	602	BCR	C15-C16-C17-C18
16	B	1207	CLA	C15-C16-C17-C18
15	a	1011	CL0	C16-C17-C18-C19
16	B	1224	CLA	C11-C12-C13-C14
16	q	509	CLA	C16-C17-C18-C19
14	a	4101	LMG	C29-C30-C31-C32
20	L	4101	LMT	C2B-C1B-O1B-C4'
14	b	848	LMG	C17-C18-C19-C20
16	G	1221	CLA	C12-C13-C15-C16
16	H	1106	CLA	C11-C12-C13-C15
16	U	1503	CLA	C11-C10-C8-C7
16	a	1106	CLA	C11-C12-C13-C15
16	a	1138	CLA	C11-C12-C13-C15
16	g	505	CLA	C6-C7-C8-C10
16	h	515	CLA	C11-C10-C8-C7
16	n	505	CLA	C11-C10-C8-C7
16	p	511	CLA	C6-C7-C8-C10
16	r	506	CLA	C11-C10-C8-C7
16	v	515	CLA	C11-C12-C13-C15
16	b	1225	CLA	C5-C6-C7-C8
16	A	1111	CLA	CBA-CGA-O2A-C1
16	H	1117	CLA	C16-C17-C18-C19
16	b	1238	CLA	C16-C17-C18-C20
16	r	506	CLA	C11-C12-C13-C15
16	v	507	CLA	C16-C17-C18-C20
14	b	848	LMG	C33-C34-C35-C36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	Z	509	CLA	C13-C15-C16-C17
16	A	1111	CLA	O1A-CGA-O2A-C1
13	a	851	LHG	O7-C5-C6-O8
16	A	1105	CLA	C3A-C2A-CAA-CBA
16	A	1107	CLA	C3A-C2A-CAA-CBA
16	A	1112	CLA	C3A-C2A-CAA-CBA
16	B	1209	CLA	C3A-C2A-CAA-CBA
16	G	1217	CLA	C3A-C2A-CAA-CBA
16	G	1232	CLA	C3A-C2A-CAA-CBA
16	G	1234	CLA	C3A-C2A-CAA-CBA
16	H	1105	CLA	C3A-C2A-CAA-CBA
16	H	1128	CLA	C3A-C2A-CAA-CBA
16	H	1137	CLA	C3A-C2A-CAA-CBA
16	W	513	CLA	C3A-C2A-CAA-CBA
16	Y	503	CLA	C3A-C2A-CAA-CBA
16	Z	503	CLA	C3A-C2A-CAA-CBA
16	Z	513	CLA	C3A-C2A-CAA-CBA
16	a	1105	CLA	C3A-C2A-CAA-CBA
16	a	1107	CLA	C3A-C2A-CAA-CBA
16	a	1108	CLA	C3A-C2A-CAA-CBA
16	a	1114	CLA	C3A-C2A-CAA-CBA
16	h	516	CLA	C3A-C2A-CAA-CBA
16	o	503	CLA	C3A-C2A-CAA-CBA
16	o	506	CLA	C3A-C2A-CAA-CBA
16	o	511	CLA	C3A-C2A-CAA-CBA
16	r	503	CLA	C3A-C2A-CAA-CBA
16	s	517	CLA	C3A-C2A-CAA-CBA
16	u	503	CLA	C3A-C2A-CAA-CBA
16	y	507	CLA	C3A-C2A-CAA-CBA
16	y	516	CLA	C3A-C2A-CAA-CBA
16	W	501	CLA	CAA-CBA-CGA-O2A
16	a	1116	CLA	CAA-CBA-CGA-O2A
17	b	2002	PQN	C12-C13-C15-C16
16	u	502	CLA	C2A-CAA-CBA-CGA
16	H	1125	CLA	C10-C11-C12-C13
16	W	511	CLA	C10-C11-C12-C13
16	B	1240	CLA	CBA-CGA-O2A-C1
19	A	4011	BCR	C16-C17-C18-C36
19	F	4016	BCR	C35-C13-C14-C15
19	G	4009	BCR	C20-C21-C22-C37
19	H	4007	BCR	C20-C21-C22-C37
19	H	4011	BCR	C16-C17-C18-C36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	U	4022	BCR	C20-C21-C22-C37
19	X	604	BCR	C35-C13-C14-C15
19	Z	604	BCR	C35-C13-C14-C15
19	a	4002	BCR	C11-C10-C9-C34
19	b	4014	BCR	C16-C17-C18-C36
19	b	4017	BCR	C35-C13-C14-C15
19	n	603	BCR	C11-C10-C9-C34
19	w	603	BCR	C35-C13-C14-C15
21	B	4006	ECH	C11-C10-C9-C34
21	B	4006	ECH	C20-C21-C22-C37
21	G	4006	ECH	C11-C10-C9-C34
21	G	4006	ECH	C20-C21-C22-C37
21	I	4020	ECH	C11-C10-C9-C34
21	M	4021	ECH	C11-C10-C9-C34
21	R	4020	ECH	C11-C10-C9-C34
21	V	4021	ECH	C11-C10-C9-C34
21	b	4006	ECH	C11-C10-C9-C34
21	b	4006	ECH	C20-C21-C22-C37
21	i	4020	ECH	C11-C10-C9-C34
21	m	4021	ECH	C11-C10-C9-C34
16	b	1206	CLA	C3-C5-C6-C7
16	W	505	CLA	C15-C16-C17-C18
16	o	509	CLA	C10-C11-C12-C13
14	A	4101	LMG	C29-C30-C31-C32
16	G	1214	CLA	C4C-C3C-CAC-CBC
16	b	1203	CLA	C15-C16-C17-C18
14	H	4101	LMG	C17-C18-C19-C20
14	b	848	LMG	C13-C14-C15-C16
16	B	1236	CLA	CBD-CGD-O2D-CED
16	G	1012	CLA	C2C-C3C-CAC-CBC
15	A	1011	CL0	CAA-CBA-CGA-O1A
16	A	1123	CLA	C2-C1-O2A-CGA
16	W	507	CLA	C2-C1-O2A-CGA
16	X	512	CLA	C2-C1-O2A-CGA
19	H	4008	BCR	C19-C20-C21-C22
19	k	4005	BCR	C13-C14-C15-C16
19	l	4022	BCR	C13-C14-C15-C16
21	M	4021	ECH	C15-C16-C17-C18
23	r	606	LMU	C1-C2-C3-C4
16	B	1023	CLA	C15-C16-C17-C18
16	b	1206	CLA	C8-C10-C11-C12
19	G	4010	BCR	C7-C8-C9-C34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	J	4012	BCR	C11-C12-C13-C35
19	J	4013	BCR	C11-C12-C13-C35
16	G	1235	CLA	C5-C6-C7-C8
16	t	515	CLA	C5-C6-C7-C8
16	X	504	CLA	C10-C11-C12-C13
16	h	510	CLA	C13-C15-C16-C17
19	B	4005	BCR	C7-C8-C9-C10
19	b	4005	BCR	C7-C8-C9-C10
13	i	103	LHG	C11-C10-C9-C8
14	B	848	LMG	C17-C18-C19-C20
16	H	1124	CLA	C4-C3-C5-C6
16	H	1123	CLA	C4C-C3C-CAC-CBC
13	H	849	LHG	C7-C8-C9-C10
16	a	1118	CLA	C2-C3-C5-C6
17	G	2002	PQN	C26-C27-C28-C30
16	G	1023	CLA	C13-C15-C16-C17
16	H	1101	CLA	C10-C11-C12-C13
16	H	1123	CLA	C8-C10-C11-C12
16	A	1136	CLA	C2A-CAA-CBA-CGA
16	G	1220	CLA	C2A-CAA-CBA-CGA
16	a	1120	CLA	C2A-CAA-CBA-CGA
16	q	514	CLA	C2A-CAA-CBA-CGA
16	q	516	CLA	C2A-CAA-CBA-CGA
16	A	1134	CLA	CAA-CBA-CGA-O1A
19	A	4007	BCR	C14-C15-C16-C17
19	q	602	BCR	C14-C15-C16-C17
16	X	515	CLA	C3-C5-C6-C7
16	y	509	CLA	C3-C5-C6-C7
16	t	510	CLA	C5-C6-C7-C8
16	b	1220	CLA	C2C-C3C-CAC-CBC
16	A	1113	CLA	CAA-CBA-CGA-O1A
16	A	1106	CLA	C11-C10-C8-C9
16	A	1139	CLA	C6-C7-C8-C9
16	B	1202	CLA	C14-C13-C15-C16
16	G	1226	CLA	C6-C7-C8-C9
16	H	1106	CLA	C11-C10-C8-C9
16	H	1132	CLA	C6-C7-C8-C9
16	H	1139	CLA	C6-C7-C8-C9
16	L	1503	CLA	C6-C7-C8-C9
16	U	1502	CLA	C11-C10-C8-C9
16	U	1503	CLA	C6-C7-C8-C9
16	W	504	CLA	C6-C7-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	W	507	CLA	C11-C10-C8-C9
16	b	1221	CLA	C14-C13-C15-C16
16	b	1223	CLA	C14-C13-C15-C16
16	b	1238	CLA	C6-C7-C8-C9
16	l	1501	CLA	C11-C10-C8-C9
16	l	1502	CLA	C11-C10-C8-C9
16	n	505	CLA	C11-C10-C8-C9
16	p	507	CLA	C11-C10-C8-C9
16	p	511	CLA	C6-C7-C8-C9
16	p	511	CLA	C11-C12-C13-C14
16	t	507	CLA	C11-C10-C8-C9
16	t	511	CLA	C6-C7-C8-C9
16	v	511	CLA	C6-C7-C8-C9
16	x	504	CLA	C14-C13-C15-C16
16	B	1228	CLA	C5-C6-C7-C8
16	G	1203	CLA	C15-C16-C17-C18
16	H	1132	CLA	C15-C16-C17-C18
16	b	1206	CLA	C10-C11-C12-C13
16	r	515	CLA	C8-C10-C11-C12
14	H	852	LMG	C37-C38-C39-C40
16	A	1116	CLA	CAA-CBA-CGA-O2A
14	A	4101	LMG	C9-C8-O7-C10
14	a	4101	LMG	C7-C8-O7-C10
16	n	516	CLA	CBD-CGD-O2D-CED
19	W	604	BCR	C13-C14-C15-C16
19	Y	604	BCR	C13-C14-C15-C16
19	b	4010	BCR	C15-C16-C17-C18
24	Z	601	LUT	C29-C30-C31-C32
16	H	1104	CLA	C4-C3-C5-C6
16	H	1115	CLA	C4-C3-C5-C6
16	q	509	CLA	C16-C17-C18-C20
16	v	517	CLA	C4C-C3C-CAC-CBC
16	H	1123	CLA	C2C-C3C-CAC-CBC
16	B	1213	CLA	CBD-CGD-O2D-CED
16	p	509	CLA	CBD-CGD-O2D-CED
16	G	1202	CLA	CAA-CBA-CGA-O2A
16	u	509	CLA	CAA-CBA-CGA-O2A
16	H	1124	CLA	C2-C3-C5-C6
16	A	1013	CLA	C2A-CAA-CBA-CGA
16	A	1130	CLA	C2A-CAA-CBA-CGA
16	G	1215	CLA	C2A-CAA-CBA-CGA
16	G	1231	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	Z	505	CLA	C2A-CAA-CBA-CGA
16	u	509	CLA	C2A-CAA-CBA-CGA
16	B	1213	CLA	O1D-CGD-O2D-CED
16	X	509	CLA	CAA-CBA-CGA-O1A
16	A	1129	CLA	C1A-C2A-CAA-CBA
16	G	1207	CLA	C1A-C2A-CAA-CBA
16	G	1215	CLA	C1A-C2A-CAA-CBA
16	G	1232	CLA	C1A-C2A-CAA-CBA
16	H	1103	CLA	C1A-C2A-CAA-CBA
16	H	1120	CLA	C1A-C2A-CAA-CBA
16	W	504	CLA	C1A-C2A-CAA-CBA
16	Z	513	CLA	C1A-C2A-CAA-CBA
16	a	1139	CLA	C1A-C2A-CAA-CBA
16	b	1220	CLA	C1A-C2A-CAA-CBA
16	p	512	CLA	C1A-C2A-CAA-CBA
16	q	508	CLA	C1A-C2A-CAA-CBA
16	r	512	CLA	C1A-C2A-CAA-CBA
16	s	515	CLA	C1A-C2A-CAA-CBA
16	s	516	CLA	C1A-C2A-CAA-CBA
16	t	515	CLA	C1A-C2A-CAA-CBA
16	w	508	CLA	C1A-C2A-CAA-CBA
16	w	511	CLA	C1A-C2A-CAA-CBA
16	w	514	CLA	C1A-C2A-CAA-CBA
19	F	4016	BCR	C12-C13-C14-C15
19	H	4003	BCR	C16-C17-C18-C19
19	H	4011	BCR	C16-C17-C18-C19
19	Q	4016	BCR	C12-C13-C14-C15
19	X	604	BCR	C12-C13-C14-C15
19	Y	601	BCR	C12-C13-C14-C15
19	a	4011	BCR	C16-C17-C18-C19
19	f	4016	BCR	C12-C13-C14-C15
19	j	4015	BCR	C16-C17-C18-C19
21	B	4006	ECH	C11-C10-C9-C8
21	B	4006	ECH	C20-C21-C22-C23
21	G	4006	ECH	C11-C10-C9-C8
21	G	4006	ECH	C20-C21-C22-C23
21	I	4020	ECH	C11-C10-C9-C8
21	M	4021	ECH	C11-C10-C9-C8
21	R	4020	ECH	C11-C10-C9-C8
21	V	4021	ECH	C11-C10-C9-C8
21	b	4006	ECH	C11-C10-C9-C8
21	b	4006	ECH	C20-C21-C22-C23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	i	4020	ECH	C11-C10-C9-C8
21	m	4021	ECH	C11-C10-C9-C8
16	X	504	CLA	C11-C12-C13-C14
16	S	1302	CLA	CAA-CBA-CGA-O1A
13	I	103	LHG	C7-C8-C9-C10
16	X	506	CLA	C5-C6-C7-C8
16	b	1229	CLA	C2C-C3C-CAC-CBC
16	Z	507	CLA	C3-C5-C6-C7
19	A	4002	BCR	C5-C6-C7-C8
19	A	4002	BCR	C23-C24-C25-C26
19	A	4007	BCR	C5-C6-C7-C8
19	A	4007	BCR	C23-C24-C25-C26
19	A	4008	BCR	C5-C6-C7-C8
19	A	4011	BCR	C5-C6-C7-C8
19	B	4004	BCR	C5-C6-C7-C8
19	B	4004	BCR	C23-C24-C25-C26
19	B	4005	BCR	C5-C6-C7-C8
19	B	4009	BCR	C23-C24-C25-C26
19	B	4010	BCR	C5-C6-C7-C8
19	B	4010	BCR	C23-C24-C25-C26
19	B	4010	BCR	C23-C24-C25-C30
19	B	4014	BCR	C1-C6-C7-C8
19	B	4014	BCR	C5-C6-C7-C8
19	B	4014	BCR	C23-C24-C25-C26
19	B	4017	BCR	C5-C6-C7-C8
19	B	4017	BCR	C23-C24-C25-C26
19	F	4016	BCR	C5-C6-C7-C8
19	F	4016	BCR	C23-C24-C25-C30
19	G	4004	BCR	C5-C6-C7-C8
19	G	4005	BCR	C5-C6-C7-C8
19	G	4009	BCR	C23-C24-C25-C26
19	G	4010	BCR	C23-C24-C25-C30
19	G	4014	BCR	C5-C6-C7-C8
19	G	4014	BCR	C23-C24-C25-C26
19	G	4017	BCR	C5-C6-C7-C8
19	G	4017	BCR	C23-C24-C25-C26
19	H	4002	BCR	C5-C6-C7-C8
19	H	4002	BCR	C23-C24-C25-C26
19	H	4003	BCR	C5-C6-C7-C8
19	H	4003	BCR	C23-C24-C25-C26
19	H	4007	BCR	C5-C6-C7-C8
19	H	4007	BCR	C23-C24-C25-C26

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	H	4008	BCR	C5-C6-C7-C8
19	H	4008	BCR	C23-C24-C25-C26
19	H	4011	BCR	C5-C6-C7-C8
19	I	4018	BCR	C5-C6-C7-C8
19	J	4012	BCR	C23-C24-C25-C30
19	J	4013	BCR	C1-C6-C7-C8
19	J	4013	BCR	C23-C24-C25-C30
19	J	4015	BCR	C23-C24-C25-C26
19	K	4001	BCR	C5-C6-C7-C8
19	K	4005	BCR	C1-C6-C7-C8
19	K	4005	BCR	C5-C6-C7-C8
19	K	4005	BCR	C23-C24-C25-C26
19	L	4019	BCR	C5-C6-C7-C8
19	L	4019	BCR	C23-C24-C25-C26
19	L	4019	BCR	C23-C24-C25-C30
19	L	4022	BCR	C5-C6-C7-C8
19	Q	4016	BCR	C5-C6-C7-C8
19	Q	4016	BCR	C23-C24-C25-C26
19	S	4012	BCR	C23-C24-C25-C26
19	S	4013	BCR	C1-C6-C7-C8
19	S	4015	BCR	C5-C6-C7-C8
19	S	4015	BCR	C23-C24-C25-C26
19	T	4001	BCR	C5-C6-C7-C8
19	T	4001	BCR	C23-C24-C25-C26
19	T	4005	BCR	C5-C6-C7-C8
19	T	4005	BCR	C23-C24-C25-C26
19	U	4019	BCR	C5-C6-C7-C8
19	U	4022	BCR	C23-C24-C25-C26
19	W	601	BCR	C5-C6-C7-C8
19	W	603	BCR	C5-C6-C7-C8
19	W	603	BCR	C23-C24-C25-C26
19	W	604	BCR	C5-C6-C7-C8
19	W	604	BCR	C23-C24-C25-C30
19	X	601	BCR	C5-C6-C7-C8
19	X	601	BCR	C23-C24-C25-C26
19	X	601	BCR	C23-C24-C25-C30
19	X	602	BCR	C5-C6-C7-C8
19	X	602	BCR	C23-C24-C25-C26
19	X	602	BCR	C23-C24-C25-C30
19	X	603	BCR	C23-C24-C25-C26
19	X	604	BCR	C5-C6-C7-C8
19	X	604	BCR	C23-C24-C25-C26

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	Y	602	BCR	C5-C6-C7-C8
19	Y	602	BCR	C23-C24-C25-C26
19	Y	603	BCR	C5-C6-C7-C8
19	Z	602	BCR	C5-C6-C7-C8
19	Z	603	BCR	C5-C6-C7-C8
19	Z	603	BCR	C23-C24-C25-C26
19	Z	604	BCR	C23-C24-C25-C26
19	a	4002	BCR	C5-C6-C7-C8
19	a	4002	BCR	C23-C24-C25-C30
19	a	4003	BCR	C23-C24-C25-C30
19	a	4007	BCR	C5-C6-C7-C8
19	a	4007	BCR	C23-C24-C25-C26
19	a	4008	BCR	C5-C6-C7-C8
19	b	4004	BCR	C5-C6-C7-C8
19	b	4004	BCR	C23-C24-C25-C26
19	b	4005	BCR	C5-C6-C7-C8
19	b	4005	BCR	C23-C24-C25-C30
19	b	4009	BCR	C23-C24-C25-C26
19	b	4010	BCR	C5-C6-C7-C8
19	b	4010	BCR	C23-C24-C25-C30
19	b	4014	BCR	C1-C6-C7-C8
19	b	4014	BCR	C5-C6-C7-C8
19	b	4017	BCR	C5-C6-C7-C8
19	b	4017	BCR	C23-C24-C25-C30
19	f	4016	BCR	C5-C6-C7-C8
19	f	4016	BCR	C23-C24-C25-C26
19	f	4016	BCR	C23-C24-C25-C30
19	g	601	BCR	C1-C6-C7-C8
19	g	601	BCR	C5-C6-C7-C8
19	g	601	BCR	C23-C24-C25-C26
19	g	602	BCR	C5-C6-C7-C8
19	g	602	BCR	C23-C24-C25-C26
19	g	602	BCR	C23-C24-C25-C30
19	g	603	BCR	C23-C24-C25-C26
19	g	604	BCR	C5-C6-C7-C8
19	h	603	BCR	C5-C6-C7-C8
19	h	603	BCR	C23-C24-C25-C26
19	h	604	BCR	C5-C6-C7-C8
19	i	4018	BCR	C1-C6-C7-C8
19	j	4012	BCR	C23-C24-C25-C26
19	j	4013	BCR	C23-C24-C25-C26
19	j	4015	BCR	C5-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	j	4015	BCR	C23-C24-C25-C26
19	k	4001	BCR	C5-C6-C7-C8
19	k	4001	BCR	C23-C24-C25-C26
19	k	4005	BCR	C5-C6-C7-C8
19	k	4005	BCR	C23-C24-C25-C26
19	l	4019	BCR	C5-C6-C7-C8
19	l	4022	BCR	C23-C24-C25-C26
19	n	601	BCR	C5-C6-C7-C8
19	n	601	BCR	C23-C24-C25-C26
19	n	603	BCR	C5-C6-C7-C8
19	n	603	BCR	C23-C24-C25-C26
19	n	604	BCR	C5-C6-C7-C8
19	n	604	BCR	C23-C24-C25-C30
19	o	601	BCR	C5-C6-C7-C8
19	o	601	BCR	C23-C24-C25-C30
19	o	602	BCR	C5-C6-C7-C8
19	o	602	BCR	C23-C24-C25-C26
19	o	603	BCR	C5-C6-C7-C8
19	o	603	BCR	C23-C24-C25-C26
19	p	601	BCR	C5-C6-C7-C8
19	p	602	BCR	C5-C6-C7-C8
19	p	602	BCR	C23-C24-C25-C26
19	p	603	BCR	C5-C6-C7-C8
19	p	603	BCR	C23-C24-C25-C26
19	q	602	BCR	C5-C6-C7-C8
19	q	602	BCR	C23-C24-C25-C30
19	q	603	BCR	C5-C6-C7-C8
19	q	603	BCR	C23-C24-C25-C26
19	q	604	BCR	C23-C24-C25-C26
19	r	601	BCR	C5-C6-C7-C8
19	r	601	BCR	C23-C24-C25-C30
19	r	602	BCR	C5-C6-C7-C8
19	r	602	BCR	C23-C24-C25-C30
19	r	603	BCR	C23-C24-C25-C26
19	r	604	BCR	C5-C6-C7-C8
19	r	604	BCR	C23-C24-C25-C26
19	s	602	BCR	C5-C6-C7-C8
19	s	602	BCR	C23-C24-C25-C26
19	s	603	BCR	C5-C6-C7-C8
19	s	603	BCR	C23-C24-C25-C26
19	t	601	BCR	C5-C6-C7-C8
19	t	601	BCR	C23-C24-C25-C26

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	t	603	BCR	C23-C24-C25-C26
19	t	604	BCR	C5-C6-C7-C8
19	t	604	BCR	C23-C24-C25-C26
19	u	601	BCR	C5-C6-C7-C8
19	u	601	BCR	C23-C24-C25-C30
19	u	602	BCR	C5-C6-C7-C8
19	u	602	BCR	C23-C24-C25-C26
19	u	603	BCR	C5-C6-C7-C8
19	u	603	BCR	C23-C24-C25-C26
19	u	604	BCR	C1-C6-C7-C8
19	v	601	BCR	C5-C6-C7-C8
19	v	603	BCR	C5-C6-C7-C8
19	v	603	BCR	C23-C24-C25-C30
19	v	604	BCR	C5-C6-C7-C8
19	w	602	BCR	C5-C6-C7-C8
19	w	602	BCR	C23-C24-C25-C30
19	w	603	BCR	C5-C6-C7-C8
19	w	603	BCR	C23-C24-C25-C26
19	w	604	BCR	C23-C24-C25-C26
19	x	601	BCR	C5-C6-C7-C8
19	x	601	BCR	C23-C24-C25-C26
19	x	602	BCR	C5-C6-C7-C8
19	x	602	BCR	C23-C24-C25-C30
19	x	603	BCR	C23-C24-C25-C26
19	x	604	BCR	C5-C6-C7-C8
19	x	604	BCR	C23-C24-C25-C26
19	y	603	BCR	C1-C6-C7-C8
19	y	603	BCR	C5-C6-C7-C8
19	y	603	BCR	C23-C24-C25-C26
21	G	4006	ECH	C23-C24-C25-C30
21	V	4021	ECH	C5-C6-C7-C8
21	V	4021	ECH	C23-C24-C25-C30
21	b	4006	ECH	C1-C6-C7-C8
21	m	4021	ECH	C23-C24-C25-C30
16	p	503	CLA	C4C-C3C-CAC-CBC
16	j	1302	CLA	CAA-CBA-CGA-O2A
16	w	509	CLA	C13-C15-C16-C17
13	G	4018	LHG	C2-C3-O3-P
13	u	605	LHG	C2-C3-O3-P
16	h	511	CLA	C16-C17-C18-C20
16	G	1228	CLA	C5-C6-C7-C8
16	A	1134	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	U	1503	CLA	C4-C3-C5-C6
16	a	1124	CLA	C4-C3-C5-C6
16	a	1138	CLA	C4-C3-C5-C6
16	b	1238	CLA	C4-C3-C5-C6
16	g	517	CLA	C4-C3-C5-C6
16	o	508	CLA	C4-C3-C5-C6
16	r	514	CLA	O1D-CGD-O2D-CED
14	A	4101	LMG	C31-C32-C33-C34
16	S	1302	CLA	CAA-CBA-CGA-O2A
16	j	1302	CLA	CAA-CBA-CGA-O1A
16	Y	516	CLA	O1A-CGA-O2A-C1
19	k	4001	BCR	C9-C10-C11-C12
16	A	1104	CLA	C12-C13-C15-C16
16	A	1138	CLA	C11-C10-C8-C7
16	A	1237	CLA	C11-C10-C8-C7
16	B	1023	CLA	C11-C10-C8-C7
16	G	1202	CLA	C11-C12-C13-C15
16	G	1225	CLA	C12-C13-C15-C16
16	G	1226	CLA	C6-C7-C8-C10
16	X	511	CLA	C11-C10-C8-C7
16	Y	509	CLA	C6-C7-C8-C10
16	Z	504	CLA	C6-C7-C8-C10
16	Z	506	CLA	C6-C7-C8-C10
16	b	1235	CLA	C12-C13-C15-C16
16	b	1238	CLA	C6-C7-C8-C10
16	g	504	CLA	C11-C10-C8-C7
16	g	506	CLA	C6-C7-C8-C10
16	g	511	CLA	C12-C13-C15-C16
16	h	509	CLA	C6-C7-C8-C10
16	r	506	CLA	C6-C7-C8-C10
16	s	504	CLA	C12-C13-C15-C16
16	w	511	CLA	C12-C13-C15-C16
16	x	506	CLA	C6-C7-C8-C10
16	x	507	CLA	C11-C10-C8-C7
16	y	505	CLA	C11-C10-C8-C7
16	H	1136	CLA	C2A-CAA-CBA-CGA
16	b	1203	CLA	C2A-CAA-CBA-CGA
16	b	1221	CLA	C2A-CAA-CBA-CGA
16	r	510	CLA	C2A-CAA-CBA-CGA
16	x	510	CLA	C2A-CAA-CBA-CGA
16	p	509	CLA	O1D-CGD-O2D-CED
13	B	4018	LHG	C23-C24-C25-C26

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	G	1205	CLA	C15-C16-C17-C18
16	L	1503	CLA	C10-C11-C12-C13
13	H	849	LHG	O7-C5-C6-O8
13	I	103	LHG	O7-C5-C6-O8
13	a	849	LHG	O7-C5-C6-O8
16	A	1113	CLA	CAA-CBA-CGA-O2A
16	o	513	CLA	C4C-C3C-CAC-CBC
16	A	1115	CLA	C5-C6-C7-C8
16	n	501	CLA	CAA-CBA-CGA-O2A
16	a	1114	CLA	O1A-CGA-O2A-C1
16	b	1239	CLA	C5-C6-C7-C8
16	x	506	CLA	C11-C12-C13-C15
16	y	517	CLA	C6-C7-C8-C9
16	H	1102	CLA	C11-C10-C8-C7
16	H	1101	CLA	C5-C6-C7-C8
19	j	4015	BCR	C11-C12-C13-C35
16	a	1133	CLA	O1A-CGA-O2A-C1
16	b	1218	CLA	C4-C3-C5-C6
16	u	505	CLA	C4-C3-C5-C6
16	v	517	CLA	C4-C3-C5-C6
16	A	1101	CLA	CBD-CGD-O2D-CED
16	n	509	CLA	CBA-CGA-O2A-C1
16	H	1116	CLA	CAA-CBA-CGA-O2A
16	y	509	CLA	CAA-CBA-CGA-O2A
16	B	1211	CLA	C15-C16-C17-C18
16	A	1115	CLA	C2-C3-C5-C6
16	H	1104	CLA	C2-C3-C5-C6
16	H	1110	CLA	C2-C3-C5-C6
16	a	1124	CLA	C2-C3-C5-C6
16	a	1138	CLA	C2-C3-C5-C6
16	n	516	CLA	O1D-CGD-O2D-CED
16	Y	507	CLA	C2-C1-O2A-CGA
16	X	512	CLA	CBD-CGD-O2D-CED
16	r	514	CLA	CBD-CGD-O2D-CED
16	a	1139	CLA	C6-C7-C8-C9
16	o	510	CLA	O1D-CGD-O2D-CED
16	b	1223	CLA	C10-C11-C12-C13
16	a	1133	CLA	CBA-CGA-O2A-C1
13	i	103	LHG	C9-C10-C11-C12
16	g	510	CLA	C2A-CAA-CBA-CGA
16	r	502	CLA	C2A-CAA-CBA-CGA
16	J	1302	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	1013	CLA	C11-C10-C8-C9
16	B	1023	CLA	C11-C10-C8-C9
16	G	1226	CLA	C11-C10-C8-C9
16	a	1104	CLA	C11-C12-C13-C14
16	h	512	CLA	C6-C7-C8-C9
16	q	507	CLA	C14-C13-C15-C16
16	H	1117	CLA	C8-C10-C11-C12
16	A	1123	CLA	C4C-C3C-CAC-CBC
19	Q	4016	BCR	C9-C10-C11-C12
19	o	604	BCR	C13-C14-C15-C16
19	q	604	BCR	C15-C16-C17-C18
21	m	4021	ECH	C13-C14-C15-C16
16	A	1139	CLA	C8-C10-C11-C12
16	Z	515	CLA	C15-C16-C17-C18
14	G	848	LMG	C17-C18-C19-C20
16	A	1104	CLA	C4-C3-C5-C6
16	B	1206	CLA	C4-C3-C5-C6
16	B	1224	CLA	C4-C3-C5-C6
16	Y	505	CLA	C4-C3-C5-C6
16	b	1225	CLA	C4-C3-C5-C6
16	b	1235	CLA	C4-C3-C5-C6
16	g	504	CLA	C4-C3-C5-C6
16	s	509	CLA	C4-C3-C5-C6
17	H	2001	PQN	C14-C13-C15-C16
16	A	1128	CLA	C13-C15-C16-C17
16	G	1225	CLA	C5-C6-C7-C8
16	H	1104	CLA	C15-C16-C17-C18
16	Z	509	CLA	C8-C10-C11-C12
16	b	1232	CLA	CAA-CBA-CGA-O2A
16	A	1104	CLA	C2-C3-C5-C6
16	G	1202	CLA	C2-C3-C5-C6
16	v	517	CLA	C2-C3-C5-C6
16	H	1022	CLA	O1D-CGD-O2D-CED
16	n	509	CLA	O1A-CGA-O2A-C1
16	A	1103	CLA	C3-C5-C6-C7
16	b	1214	CLA	O1D-CGD-O2D-CED
16	G	1205	CLA	C10-C11-C12-C13
16	a	1136	CLA	C5-C6-C7-C8
13	R	103	LHG	C9-C10-C11-C12
16	q	504	CLA	CAA-CBA-CGA-O2A
13	a	851	LHG	C4-C5-C6-O8
16	B	1208	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1108	CLA	CAA-CBA-CGA-O2A
16	B	1220	CLA	C2C-C3C-CAC-CBC
14	H	852	LMG	O10-C28-O8-C9
16	H	1013	CLA	C2A-CAA-CBA-CGA
16	X	502	CLA	C2A-CAA-CBA-CGA
16	Y	517	CLA	C2A-CAA-CBA-CGA
16	a	1115	CLA	C2A-CAA-CBA-CGA
16	r	511	CLA	C2A-CAA-CBA-CGA
16	s	504	CLA	C2A-CAA-CBA-CGA
16	H	1119	CLA	C16-C17-C18-C20
16	Z	508	CLA	C6-C7-C8-C10
16	A	1801	CLA	CAA-CBA-CGA-O2A
16	B	1202	CLA	CAA-CBA-CGA-O2A
16	b	1210	CLA	CBD-CGD-O2D-CED
13	a	849	LHG	O10-C23-O8-C6
16	A	1133	CLA	C4-C3-C5-C6
16	A	1138	CLA	C4-C3-C5-C6
16	g	506	CLA	C4-C3-C5-C6
16	o	515	CLA	C4-C3-C5-C6
16	x	506	CLA	C4-C3-C5-C6
16	h	509	CLA	CAA-CBA-CGA-O1A
16	H	1138	CLA	CAA-CBA-CGA-O2A
16	Z	504	CLA	CAA-CBA-CGA-O2A
16	b	1202	CLA	CAA-CBA-CGA-O2A
16	g	503	CLA	CAA-CBA-CGA-O2A
16	A	1104	CLA	C15-C16-C17-C18
16	B	1235	CLA	C5-C6-C7-C8
16	A	1125	CLA	O1A-CGA-O2A-C1
16	A	1139	CLA	O1A-CGA-O2A-C1
16	r	504	CLA	O1A-CGA-O2A-C1
16	p	504	CLA	CAA-CBA-CGA-O2A
16	s	514	CLA	CAA-CBA-CGA-O2A
16	r	509	CLA	C4C-C3C-CAC-CBC
16	B	1213	CLA	O1A-CGA-O2A-C1
16	B	1231	CLA	CAA-CBA-CGA-O2A
16	B	1215	CLA	C11-C12-C13-C14
16	h	509	CLA	C16-C17-C18-C19
16	y	515	CLA	C16-C17-C18-C19
14	A	4201	LMG	O9-C10-O7-C8
16	r	513	CLA	O1A-CGA-O2A-C1
16	x	516	CLA	O1A-CGA-O2A-C1
13	X	605	LHG	C1-C2-C3-O3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	H	4002	BCR	C11-C10-C9-C34
19	Z	604	BCR	C16-C17-C18-C36
19	x	603	BCR	C20-C21-C22-C37
16	B	1206	CLA	C8-C10-C11-C12
16	B	1223	CLA	C10-C11-C12-C13
16	x	510	CLA	C13-C15-C16-C17
20	L	4101	LMT	O1'-C1-C2-C3
16	H	1134	CLA	CAA-CBA-CGA-O1A
13	B	4018	LHG	O6-C4-C5-C6
13	Y	605	LHG	O6-C4-C5-C6
16	A	1128	CLA	C16-C17-C18-C19
16	q	505	CLA	C16-C17-C18-C19
16	H	1139	CLA	C4-C3-C5-C6
16	b	1224	CLA	C4-C3-C5-C6
13	g	605	LHG	C11-C10-C9-C8
16	w	515	CLA	C10-C11-C12-C13
16	H	1134	CLA	CAA-CBA-CGA-O2A
16	k	4003	CLA	CAA-CBA-CGA-O2A
14	B	848	LMG	C11-C10-O7-C8
13	o	605	LHG	C2-C3-O3-P
16	A	1106	CLA	C11-C12-C13-C15
16	G	1226	CLA	C11-C10-C8-C7
16	H	1237	CLA	C11-C10-C8-C7
16	W	511	CLA	C6-C7-C8-C10
16	h	512	CLA	C6-C7-C8-C10
16	r	510	CLA	C6-C7-C8-C10
16	v	511	CLA	C6-C7-C8-C10
16	a	1134	CLA	O1D-CGD-O2D-CED
16	b	1210	CLA	O1D-CGD-O2D-CED
16	a	1112	CLA	CAA-CBA-CGA-O2A
16	a	1801	CLA	O1A-CGA-O2A-C1
19	t	604	BCR	C15-C16-C17-C18
19	x	603	BCR	C9-C10-C11-C12
21	V	4021	ECH	C15-C16-C17-C18
16	U	1503	CLA	C13-C15-C16-C17
16	B	1210	CLA	C4C-C3C-CAC-CBC
14	A	4201	LMG	C10-C11-C12-C13
16	J	1302	CLA	CAA-CBA-CGA-O1A
16	p	514	CLA	CAA-CBA-CGA-O1A
16	t	514	CLA	CAA-CBA-CGA-O1A
16	A	1104	CLA	C11-C12-C13-C14
16	B	1021	CLA	C11-C10-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	1204	CLA	C14-C13-C15-C16
16	B	1207	CLA	C11-C12-C13-C14
16	G	1221	CLA	C11-C12-C13-C14
16	L	1503	CLA	C11-C10-C8-C9
16	Y	504	CLA	C6-C7-C8-C9
16	Y	511	CLA	C11-C12-C13-C14
16	Z	515	CLA	C11-C12-C13-C14
16	b	1204	CLA	C14-C13-C15-C16
16	g	507	CLA	C11-C10-C8-C9
16	p	512	CLA	C11-C12-C13-C14
16	r	507	CLA	C11-C10-C8-C9
16	r	507	CLA	C14-C13-C15-C16
16	r	510	CLA	C6-C7-C8-C9
16	s	507	CLA	C11-C10-C8-C9
16	s	511	CLA	C6-C7-C8-C9
16	u	507	CLA	C6-C7-C8-C9
16	u	512	CLA	C6-C7-C8-C9
16	v	505	CLA	C11-C10-C8-C9
16	y	505	CLA	C11-C12-C13-C14
16	y	515	CLA	C11-C12-C13-C14
17	B	2002	PQN	C24-C23-C25-C26
17	G	2002	PQN	C24-C23-C25-C26
14	H	852	LMG	C33-C34-C35-C36
14	G	848	LMG	O10-C28-O8-C9
14	Q	4017	LMG	C8-C7-O1-C1
14	f	4017	LMG	C8-C7-O1-C1
16	a	1134	CLA	CBD-CGD-O2D-CED
16	x	514	CLA	CAA-CBA-CGA-O2A
16	G	1217	CLA	CAA-CBA-CGA-O2A
16	a	1108	CLA	CAA-CBA-CGA-O1A
16	A	1124	CLA	C2A-CAA-CBA-CGA
16	a	1013	CLA	C2A-CAA-CBA-CGA
16	o	514	CLA	C2A-CAA-CBA-CGA
16	v	517	CLA	C2A-CAA-CBA-CGA
16	B	1012	CLA	C2-C1-O2A-CGA
16	B	1206	CLA	C2-C1-O2A-CGA
16	G	1214	CLA	C2-C1-O2A-CGA
16	W	505	CLA	C2-C1-O2A-CGA
16	Y	506	CLA	C2-C1-O2A-CGA
16	a	1104	CLA	C2-C1-O2A-CGA
16	b	1239	CLA	C2-C1-O2A-CGA
16	p	515	CLA	C2-C1-O2A-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	r	514	CLA	C2-C1-O2A-CGA
16	s	506	CLA	C2-C1-O2A-CGA
16	s	507	CLA	C2-C1-O2A-CGA
16	s	517	CLA	C2-C1-O2A-CGA
16	u	515	CLA	C2-C1-O2A-CGA
16	v	502	CLA	C2-C1-O2A-CGA
16	h	509	CLA	C16-C17-C18-C20
16	y	515	CLA	C16-C17-C18-C20
16	p	517	CLA	CBD-CGD-O2D-CED
16	G	1207	CLA	C15-C16-C17-C18
16	H	1140	CLA	C10-C11-C12-C13
16	Z	507	CLA	C5-C6-C7-C8
16	A	1125	CLA	CBA-CGA-O2A-C1
16	A	1113	CLA	C3A-C2A-CAA-CBA
16	A	1114	CLA	C3A-C2A-CAA-CBA
16	A	1140	CLA	C3A-C2A-CAA-CBA
16	B	1228	CLA	C3A-C2A-CAA-CBA
16	H	1103	CLA	C3A-C2A-CAA-CBA
16	W	503	CLA	C3A-C2A-CAA-CBA
16	a	1139	CLA	C3A-C2A-CAA-CBA
16	a	1237	CLA	C3A-C2A-CAA-CBA
16	b	1208	CLA	C3A-C2A-CAA-CBA
16	b	1234	CLA	C3A-C2A-CAA-CBA
16	g	504	CLA	C3A-C2A-CAA-CBA
16	h	504	CLA	C3A-C2A-CAA-CBA
16	o	501	CLA	C3A-C2A-CAA-CBA
16	p	512	CLA	C3A-C2A-CAA-CBA
16	u	511	CLA	C3A-C2A-CAA-CBA
16	B	1208	CLA	CAA-CBA-CGA-O1A
16	B	1209	CLA	CAA-CBA-CGA-O2A
16	Y	503	CLA	C4C-C3C-CAC-CBC
16	h	511	CLA	C3-C5-C6-C7
16	B	1217	CLA	CAA-CBA-CGA-O2A
16	T	4003	CLA	CAA-CBA-CGA-O2A
16	B	1213	CLA	CBA-CGA-O2A-C1
16	B	1021	CLA	CAA-CBA-CGA-O2A
16	a	1133	CLA	CAA-CBA-CGA-O2A
16	a	1138	CLA	CAA-CBA-CGA-O2A
16	r	514	CLA	CAA-CBA-CGA-O2A
14	A	4101	LMG	C7-C8-O7-C10
14	H	4101	LMG	C9-C8-O7-C10
14	a	4101	LMG	C9-C8-O7-C10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	A	4002	BCR	C10-C11-C12-C13
19	R	4018	BCR	C10-C11-C12-C13
19	W	603	BCR	C18-C19-C20-C21
19	i	4018	BCR	C10-C11-C12-C13
19	r	601	BCR	C18-C19-C20-C21
16	b	1234	CLA	CBD-CGD-O2D-CED
16	B	1230	CLA	CAA-CBA-CGA-O2A
16	A	1138	CLA	CAA-CBA-CGA-O2A
16	B	1225	CLA	C5-C6-C7-C8
16	Y	506	CLA	O1A-CGA-O2A-C1
16	q	505	CLA	C16-C17-C18-C20
16	K	4003	CLA	CAA-CBA-CGA-O2A
16	b	1232	CLA	CAA-CBA-CGA-O1A
16	b	1220	CLA	C5-C6-C7-C8
16	u	504	CLA	C4C-C3C-CAC-CBC
14	A	852	LMG	C36-C37-C38-C39
16	B	1217	CLA	CAA-CBA-CGA-O1A
16	B	1231	CLA	CAA-CBA-CGA-O1A
20	L	4101	LMT	C2-C3-C4-C5
16	A	1139	CLA	CBA-CGA-O2A-C1
16	r	504	CLA	CBA-CGA-O2A-C1
13	A	849	LHG	C26-C27-C28-C29
16	y	511	CLA	C8-C10-C11-C12
13	Y	605	LHG	O10-C23-O8-C6
15	a	1011	CL0	C16-C17-C18-C20
16	H	1126	CLA	C16-C17-C18-C20
19	X	603	BCR	C11-C10-C9-C8
16	X	509	CLA	C4C-C3C-CAC-CBC
16	H	1140	CLA	C8-C10-C11-C12
16	y	511	CLA	C5-C6-C7-C8
17	H	2001	PQN	C20-C21-C22-C23
13	X	605	LHG	C2-C3-O3-P
13	u	605	LHG	C1-C2-C3-O3
16	a	1102	CLA	CBD-CGD-O2D-CED
16	A	1140	CLA	O1D-CGD-O2D-CED
19	A	4002	BCR	C22-C23-C24-C25
19	X	604	BCR	C22-C23-C24-C25
19	q	603	BCR	C22-C23-C24-C25
16	Z	504	CLA	C10-C11-C12-C13
16	b	1205	CLA	C15-C16-C17-C18
16	n	515	CLA	C15-C16-C17-C18
16	p	509	CLA	C8-C10-C11-C12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	K	4003	CLA	CAA-CBA-CGA-O1A
13	I	103	LHG	C4-C5-C6-O8
13	g	605	LHG	C4-C5-C6-O8
13	x	605	LHG	C4-C5-C6-O8
14	A	4101	LMG	C7-C8-C9-O8
14	A	4201	LMG	C7-C8-C9-O8
14	B	848	LMG	O1-C7-C8-C9
16	o	517	CLA	O1A-CGA-O2A-C1
16	w	509	CLA	C8-C10-C11-C12
16	o	509	CLA	CAA-CBA-CGA-O2A
16	h	501	CLA	O1A-CGA-O2A-C1
16	G	1217	CLA	CAA-CBA-CGA-O1A
16	w	501	CLA	C4C-C3C-CAC-CBC
16	W	515	CLA	O1D-CGD-O2D-CED
16	G	1225	CLA	C4-C3-C5-C6
16	l	1503	CLA	C4-C3-C5-C6
16	p	505	CLA	C4-C3-C5-C6
16	x	515	CLA	C4-C3-C5-C6
19	w	603	BCR	C9-C10-C11-C12
16	a	1126	CLA	C3-C5-C6-C7
16	B	1240	CLA	C4C-C3C-CAC-CBC
16	B	1221	CLA	C16-C17-C18-C19
16	a	1117	CLA	C13-C15-C16-C17
16	B	1209	CLA	CAA-CBA-CGA-O1A
16	a	1112	CLA	CAA-CBA-CGA-O1A
16	B	1206	CLA	CAA-CBA-CGA-O2A
14	B	848	LMG	C35-C36-C37-C38
16	U	1502	CLA	C3-C5-C6-C7
16	w	506	CLA	C3-C5-C6-C7
16	A	1116	CLA	C5-C6-C7-C8
14	A	852	LMG	O1-C7-C8-O7
14	A	4101	LMG	O7-C8-C9-O8
16	B	1230	CLA	CAA-CBA-CGA-O1A
16	T	4003	CLA	CAA-CBA-CGA-O1A
16	q	504	CLA	C10-C11-C12-C13
19	G	4010	BCR	C14-C15-C16-C17
16	A	1103	CLA	C11-C10-C8-C9
16	A	1109	CLA	C11-C12-C13-C14
16	A	1132	CLA	C6-C7-C8-C9
16	L	1502	CLA	C6-C7-C8-C9
16	W	515	CLA	C14-C13-C15-C16
16	Y	507	CLA	C11-C10-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1126	CLA	C6-C7-C8-C9
16	a	1128	CLA	C14-C13-C15-C16
16	a	1132	CLA	C6-C7-C8-C9
16	a	1138	CLA	C11-C10-C8-C9
16	r	504	CLA	C14-C13-C15-C16
16	v	512	CLA	C6-C7-C8-C9
17	a	2001	PQN	C21-C22-C23-C24
16	H	1110	CLA	CAA-CBA-CGA-O2A
16	n	509	CLA	CAA-CBA-CGA-O2A
16	y	507	CLA	CAA-CBA-CGA-O2A
16	r	503	CLA	CAA-CBA-CGA-O1A
16	B	1212	CLA	CAA-CBA-CGA-O2A
16	b	1208	CLA	CAA-CBA-CGA-O2A
16	k	4003	CLA	CAA-CBA-CGA-O1A
19	n	603	BCR	C11-C12-C13-C14
19	o	602	BCR	C7-C8-C9-C10
16	l	1503	CLA	C3-C5-C6-C7
16	u	515	CLA	C13-C15-C16-C17
16	A	1139	CLA	C4-C3-C5-C6
16	b	1226	CLA	CAA-CBA-CGA-O2A
16	u	514	CLA	CAA-CBA-CGA-O2A
16	b	1225	CLA	CBA-CGA-O2A-C1
16	A	1121	CLA	C2A-CAA-CBA-CGA
16	Y	503	CLA	C2A-CAA-CBA-CGA
16	q	513	CLA	C2A-CAA-CBA-CGA
16	A	1013	CLA	C6-C7-C8-C10
16	A	1013	CLA	C11-C10-C8-C7
16	A	1104	CLA	C11-C12-C13-C15
16	B	1239	CLA	C11-C10-C8-C7
16	H	1101	CLA	C12-C13-C15-C16
16	L	1503	CLA	C11-C10-C8-C7
16	W	510	CLA	C11-C10-C8-C7
16	X	504	CLA	C6-C7-C8-C10
16	X	505	CLA	C12-C13-C15-C16
16	Y	504	CLA	C6-C7-C8-C10
16	Z	512	CLA	C6-C7-C8-C10
16	a	1013	CLA	C12-C13-C15-C16
16	a	1104	CLA	C11-C12-C13-C15
16	b	1221	CLA	C11-C12-C13-C15
16	o	512	CLA	C6-C7-C8-C10
16	p	504	CLA	C12-C13-C15-C16
16	p	511	CLA	C11-C12-C13-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	q	507	CLA	C12-C13-C15-C16
16	r	504	CLA	C11-C10-C8-C7
16	r	507	CLA	C12-C13-C15-C16
16	s	511	CLA	C6-C7-C8-C10
16	u	504	CLA	C6-C7-C8-C10
16	v	505	CLA	C11-C10-C8-C7
16	x	504	CLA	C11-C10-C8-C7
16	x	509	CLA	C11-C10-C8-C7
16	y	510	CLA	C6-C7-C8-C10
16	y	515	CLA	C11-C12-C13-C15
17	A	2001	PQN	C16-C17-C18-C20
17	H	2001	PQN	C16-C17-C18-C20
16	Z	515	CLA	C3-C5-C6-C7
15	a	1011	CL0	CAA-CBA-CGA-O1A
19	F	4016	BCR	C23-C24-C25-C26
19	G	4005	BCR	C23-C24-C25-C26
19	G	4005	BCR	C23-C24-C25-C30
19	G	4010	BCR	C23-C24-C25-C26
19	I	4018	BCR	C23-C24-C25-C26
19	I	4018	BCR	C23-C24-C25-C30
19	J	4012	BCR	C23-C24-C25-C26
19	J	4013	BCR	C23-C24-C25-C26
19	J	4015	BCR	C5-C6-C7-C8
19	K	4001	BCR	C23-C24-C25-C26
19	K	4001	BCR	C23-C24-C25-C30
19	R	4018	BCR	C23-C24-C25-C26
19	R	4018	BCR	C23-C24-C25-C30
19	S	4013	BCR	C5-C6-C7-C8
19	U	4022	BCR	C1-C6-C7-C8
19	U	4022	BCR	C5-C6-C7-C8
19	W	604	BCR	C23-C24-C25-C26
19	Y	603	BCR	C23-C24-C25-C26
19	a	4002	BCR	C23-C24-C25-C26
19	a	4003	BCR	C23-C24-C25-C26
19	a	4011	BCR	C1-C6-C7-C8
19	a	4011	BCR	C5-C6-C7-C8
19	b	4005	BCR	C23-C24-C25-C26
19	b	4010	BCR	C23-C24-C25-C26
19	b	4014	BCR	C23-C24-C25-C26
19	b	4014	BCR	C23-C24-C25-C30
19	b	4017	BCR	C23-C24-C25-C26
19	i	4018	BCR	C5-C6-C7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	i	4018	BCR	C23-C24-C25-C30
19	j	4013	BCR	C1-C6-C7-C8
19	j	4013	BCR	C5-C6-C7-C8
19	l	4022	BCR	C1-C6-C7-C8
19	l	4022	BCR	C5-C6-C7-C8
19	n	604	BCR	C23-C24-C25-C26
19	o	604	BCR	C1-C6-C7-C8
19	o	604	BCR	C5-C6-C7-C8
19	o	604	BCR	C23-C24-C25-C26
19	o	604	BCR	C23-C24-C25-C30
19	q	602	BCR	C23-C24-C25-C26
19	r	601	BCR	C23-C24-C25-C26
19	r	602	BCR	C23-C24-C25-C26
19	s	601	BCR	C23-C24-C25-C26
19	s	601	BCR	C23-C24-C25-C30
19	u	601	BCR	C23-C24-C25-C26
19	u	604	BCR	C5-C6-C7-C8
19	u	604	BCR	C23-C24-C25-C26
19	u	604	BCR	C23-C24-C25-C30
19	w	602	BCR	C23-C24-C25-C26
19	x	602	BCR	C23-C24-C25-C26
21	B	4006	ECH	C23-C24-C25-C26
21	G	4006	ECH	C23-C24-C25-C26
21	M	4021	ECH	C23-C24-C25-C30
21	R	4020	ECH	C1-C6-C7-C8
21	V	4021	ECH	C1-C6-C7-C8
21	b	4006	ECH	C5-C6-C7-C8
16	Y	514	CLA	CAA-CBA-CGA-O2A
16	v	501	CLA	CAA-CBA-CGA-O2A
16	x	503	CLA	CAA-CBA-CGA-O2A
13	A	849	LHG	O9-C7-O7-C5
16	A	1104	CLA	C2-C1-O2A-CGA
16	G	1239	CLA	C2-C1-O2A-CGA
16	W	502	CLA	C2-C1-O2A-CGA
16	X	507	CLA	C2-C1-O2A-CGA
16	Z	515	CLA	C2-C1-O2A-CGA
16	g	507	CLA	C2-C1-O2A-CGA
16	h	508	CLA	C2-C1-O2A-CGA
16	p	506	CLA	C2-C1-O2A-CGA
16	p	507	CLA	C2-C1-O2A-CGA
16	q	515	CLA	C2-C1-O2A-CGA
16	r	511	CLA	C2-C1-O2A-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	x	507	CLA	C2-C1-O2A-CGA
16	X	510	CLA	C11-C12-C13-C15
16	a	1013	CLA	C8-C10-C11-C12
16	h	515	CLA	C13-C15-C16-C17
13	u	605	LHG	C24-C25-C26-C27
16	G	1023	CLA	C8-C10-C11-C12
20	L	4101	LMT	C4-C5-C6-C7
16	A	1110	CLA	CAA-CBA-CGA-O2A
16	G	1220	CLA	CAA-CBA-CGA-O2A
16	Q	1302	CLA	CAA-CBA-CGA-O2A
20	l	4101	LMT	C2B-C1B-O1B-C4'
13	B	4018	LHG	C15-C16-C17-C18
16	Y	506	CLA	CBA-CGA-O2A-C1
16	a	1013	CLA	CBA-CGA-O2A-C1
16	B	1221	CLA	C16-C17-C18-C20
16	v	515	CLA	C16-C17-C18-C20
16	G	1211	CLA	C4-C3-C5-C6
16	H	1119	CLA	C4-C3-C5-C6
13	I	103	LHG	O8-C23-C24-C25
13	R	103	LHG	O8-C23-C24-C25
14	a	4101	LMG	O8-C28-C29-C30
16	A	1101	CLA	CAA-CBA-CGA-O2A
16	A	1133	CLA	CAA-CBA-CGA-O2A
16	L	1501	CLA	CAA-CBA-CGA-O2A
16	n	505	CLA	CAA-CBA-CGA-O2A
16	o	517	CLA	CAA-CBA-CGA-O2A
16	q	507	CLA	CAA-CBA-CGA-O2A
16	A	1139	CLA	C2-C3-C5-C6
16	G	1211	CLA	C2-C3-C5-C6
16	H	1119	CLA	C2-C3-C5-C6
16	H	1139	CLA	C2-C3-C5-C6
16	a	1123	CLA	C2-C3-C5-C6
16	p	517	CLA	O1D-CGD-O2D-CED
16	a	1125	CLA	O1A-CGA-O2A-C1
16	b	1225	CLA	O1A-CGA-O2A-C1
16	A	1114	CLA	C4C-C3C-CAC-CBC
16	A	1101	CLA	C2A-CAA-CBA-CGA
16	B	1215	CLA	C2A-CAA-CBA-CGA
16	a	1117	CLA	C2A-CAA-CBA-CGA
16	w	514	CLA	C2A-CAA-CBA-CGA
16	B	1238	CLA	C13-C15-C16-C17
16	W	505	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1118	CLA	CAA-CBA-CGA-O2A
16	b	1236	CLA	CAA-CBA-CGA-O2A
16	o	514	CLA	CAA-CBA-CGA-O2A
16	r	513	CLA	CAA-CBA-CGA-O2A
16	s	517	CLA	CAA-CBA-CGA-O2A
16	v	514	CLA	CAA-CBA-CGA-O2A
16	y	512	CLA	CAA-CBA-CGA-O2A
16	F	1302	CLA	O1A-CGA-O2A-C1
16	X	516	CLA	O1A-CGA-O2A-C1
13	G	4018	LHG	C15-C16-C17-C18
16	A	1128	CLA	C16-C17-C18-C20
16	A	1123	CLA	C8-C10-C11-C12
13	R	103	LHG	C30-C31-C32-C33
16	b	1226	CLA	O1D-CGD-O2D-CED
16	b	1207	CLA	C15-C16-C17-C18
16	n	509	CLA	C5-C6-C7-C8
16	p	515	CLA	C10-C11-C12-C13
13	A	849	LHG	C25-C26-C27-C28
16	Z	502	CLA	O1D-CGD-O2D-CED
16	H	1102	CLA	CAA-CBA-CGA-O2A
16	p	505	CLA	CAA-CBA-CGA-O2A
16	u	505	CLA	CAA-CBA-CGA-O2A
14	a	4201	LMG	O9-C10-C11-C12
19	B	4004	BCR	C15-C16-C17-C18
20	H	4202	LMT	C4B-C5B-C6B-O6B
16	Z	508	CLA	C6-C7-C8-C9
16	t	509	CLA	C4C-C3C-CAC-CBC
16	H	1022	CLA	C4-C3-C5-C6
19	Y	602	BCR	C10-C11-C12-C13
13	a	851	LHG	O7-C7-C8-C9
16	X	508	CLA	CAA-CBA-CGA-O2A
16	o	502	CLA	CAA-CBA-CGA-O2A
16	t	502	CLA	CAA-CBA-CGA-O2A
16	u	507	CLA	CAA-CBA-CGA-O2A
16	H	1115	CLA	C2-C3-C5-C6
16	b	1220	CLA	C2-C3-C5-C6
16	g	517	CLA	C2-C3-C5-C6
16	H	1114	CLA	CBD-CGD-O2D-CED
16	G	1230	CLA	CAA-CBA-CGA-O2A
16	H	1111	CLA	C4C-C3C-CAC-CBC
16	T	4002	CLA	C2A-CAA-CBA-CGA
20	U	4101	LMT	C2B-C1B-O1B-C4'

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	Z	502	CLA	CAA-CBA-CGA-O2A
16	p	510	CLA	CAA-CBA-CGA-O2A
16	x	508	CLA	CAA-CBA-CGA-O2A
13	p	605	LHG	C24-C23-O8-C6
16	o	517	CLA	CBA-CGA-O2A-C1
16	a	1102	CLA	O1A-CGA-O2A-C1
16	G	1202	CLA	C11-C12-C13-C14
16	Y	509	CLA	C6-C7-C8-C9
16	Y	512	CLA	C11-C12-C13-C14
16	h	509	CLA	C6-C7-C8-C9
16	l	1503	CLA	C14-C13-C15-C16
16	r	510	CLA	C11-C12-C13-C14
16	v	504	CLA	C11-C10-C8-C9
16	a	1104	CLA	C15-C16-C17-C18
16	H	1105	CLA	CAA-CBA-CGA-O2A
16	H	1133	CLA	CAA-CBA-CGA-O2A
16	U	1501	CLA	CAA-CBA-CGA-O2A
16	Y	505	CLA	CAA-CBA-CGA-O2A
16	o	508	CLA	CAA-CBA-CGA-O2A
16	s	510	CLA	CAA-CBA-CGA-O2A
16	t	505	CLA	CAA-CBA-CGA-O2A
14	b	848	LMG	C7-C8-C9-O8
16	y	504	CLA	C8-C10-C11-C12
16	A	1102	CLA	C1A-C2A-CAA-CBA
16	A	1113	CLA	C1A-C2A-CAA-CBA
16	B	1207	CLA	C1A-C2A-CAA-CBA
16	B	1215	CLA	C1A-C2A-CAA-CBA
16	G	1204	CLA	C1A-C2A-CAA-CBA
16	H	1122	CLA	C1A-C2A-CAA-CBA
16	T	4004	CLA	C1A-C2A-CAA-CBA
16	a	1801	CLA	C1A-C2A-CAA-CBA
16	b	1207	CLA	C1A-C2A-CAA-CBA
16	g	504	CLA	C1A-C2A-CAA-CBA
16	r	514	CLA	C1A-C2A-CAA-CBA
16	r	515	CLA	C1A-C2A-CAA-CBA
16	s	501	CLA	C1A-C2A-CAA-CBA
16	w	505	CLA	C1A-C2A-CAA-CBA
16	W	515	CLA	CBD-CGD-O2D-CED
16	a	1106	CLA	C4-C3-C5-C6
16	a	1123	CLA	C4-C3-C5-C6
16	x	512	CLA	C4-C3-C5-C6
19	p	604	BCR	C22-C23-C24-C25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	r	606	LMU	O5'-C1'-O1'-C1
13	r	605	LHG	O8-C23-C24-C25
16	A	1118	CLA	CAA-CBA-CGA-O2A
16	W	502	CLA	CAA-CBA-CGA-O2A
16	Y	510	CLA	CAA-CBA-CGA-O2A
16	a	1101	CLA	CAA-CBA-CGA-O2A
16	q	502	CLA	CAA-CBA-CGA-O2A
16	s	505	CLA	CAA-CBA-CGA-O2A
16	w	502	CLA	CAA-CBA-CGA-O2A
16	w	505	CLA	CAA-CBA-CGA-O2A
16	x	510	CLA	CAA-CBA-CGA-O2A
16	b	1238	CLA	C2-C3-C5-C6
13	A	849	LHG	O7-C5-C6-O8
14	A	4201	LMG	O7-C8-C9-O8
19	X	603	BCR	C21-C22-C23-C24
19	g	601	BCR	C11-C12-C13-C14
21	V	4021	ECH	C7-C8-C9-C10
19	B	4017	BCR	C13-C14-C15-C16
19	G	4017	BCR	C9-C10-C11-C12
19	f	4016	BCR	C19-C20-C21-C22
16	W	510	CLA	C15-C16-C17-C18
16	A	1140	CLA	CBD-CGD-O2D-CED
16	b	1214	CLA	CBD-CGD-O2D-CED
23	x	606	LMU	C6-C7-C8-C9
13	a	851	LHG	C24-C23-O8-C6
16	a	1125	CLA	CBA-CGA-O2A-C1
13	p	605	LHG	C24-C25-C26-C27
16	G	1208	CLA	CAA-CBA-CGA-O2A
16	G	1219	CLA	CAA-CBA-CGA-O2A
14	A	4101	LMG	O8-C28-C29-C30
16	A	1013	CLA	CAA-CBA-CGA-O2A
16	A	1102	CLA	CAA-CBA-CGA-O2A
16	B	1214	CLA	CAA-CBA-CGA-O2A
16	B	1226	CLA	CAA-CBA-CGA-O2A
16	B	1236	CLA	CAA-CBA-CGA-O2A
16	G	1226	CLA	CAA-CBA-CGA-O2A
16	H	1013	CLA	CAA-CBA-CGA-O2A
16	W	509	CLA	CAA-CBA-CGA-O2A
16	Z	505	CLA	CAA-CBA-CGA-O2A
16	Z	507	CLA	CAA-CBA-CGA-O2A
16	Z	509	CLA	CAA-CBA-CGA-O2A
16	a	1013	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	h	501	CLA	CAA-CBA-CGA-O2A
16	l	1501	CLA	CAA-CBA-CGA-O2A
16	o	516	CLA	CAA-CBA-CGA-O2A
16	q	505	CLA	CAA-CBA-CGA-O2A
16	a	1125	CLA	C4C-C3C-CAC-CBC
16	B	1204	CLA	C2A-CAA-CBA-CGA
16	G	1204	CLA	C2A-CAA-CBA-CGA
16	G	1209	CLA	C2A-CAA-CBA-CGA
16	b	1215	CLA	C2A-CAA-CBA-CGA
16	b	1236	CLA	C2A-CAA-CBA-CGA
14	G	848	LMG	C14-C15-C16-C17
16	a	1121	CLA	C4C-C3C-CAC-CBC
16	v	515	CLA	C4C-C3C-CAC-CBC
16	H	1119	CLA	C5-C6-C7-C8
16	b	1021	CLA	C8-C10-C11-C12
16	p	506	CLA	C8-C10-C11-C12
16	q	506	CLA	C8-C10-C11-C12
16	x	505	CLA	C10-C11-C12-C13
16	G	1212	CLA	CAA-CBA-CGA-O2A
16	G	1238	CLA	O1A-CGA-O2A-C1
14	B	848	LMG	C14-C15-C16-C17
16	H	1118	CLA	CAA-CBA-CGA-O2A
16	t	509	CLA	CAA-CBA-CGA-O2A
17	a	2001	PQN	C25-C26-C27-C28
14	b	848	LMG	C14-C15-C16-C17
16	B	1212	CLA	CAA-CBA-CGA-O1A
16	A	1121	CLA	C2-C3-C5-C6
16	H	1121	CLA	C2-C3-C5-C6
16	G	1238	CLA	O1D-CGD-O2D-CED
16	a	1102	CLA	O1D-CGD-O2D-CED
16	q	505	CLA	C4-C3-C5-C6
16	B	1202	CLA	C2-C1-O2A-CGA
16	G	1012	CLA	C2-C1-O2A-CGA
16	G	1206	CLA	C2-C1-O2A-CGA
16	H	1101	CLA	C2-C1-O2A-CGA
16	H	1119	CLA	C2-C1-O2A-CGA
16	a	1107	CLA	C2-C1-O2A-CGA
16	b	1202	CLA	C2-C1-O2A-CGA
16	b	1206	CLA	C2-C1-O2A-CGA
16	g	511	CLA	C2-C1-O2A-CGA
16	h	502	CLA	C2-C1-O2A-CGA
16	h	517	CLA	C2-C1-O2A-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	n	505	CLA	C2-C1-O2A-CGA
16	o	506	CLA	C2-C1-O2A-CGA
16	o	514	CLA	C2-C1-O2A-CGA
16	r	507	CLA	C2-C1-O2A-CGA
16	w	515	CLA	C2-C1-O2A-CGA
16	B	1207	CLA	CAA-CBA-CGA-O2A
16	B	1207	CLA	C11-C12-C13-C15
16	H	1104	CLA	C12-C13-C15-C16
16	H	1126	CLA	C11-C12-C13-C15
16	H	1138	CLA	C11-C10-C8-C7
16	X	512	CLA	C11-C10-C8-C7
16	Y	504	CLA	C12-C13-C15-C16
16	a	1109	CLA	C6-C7-C8-C10
16	b	1023	CLA	C11-C12-C13-C15
16	b	1202	CLA	C11-C12-C13-C15
16	h	507	CLA	C11-C10-C8-C7
16	o	506	CLA	C11-C10-C8-C7
16	o	515	CLA	C11-C10-C8-C7
16	p	504	CLA	C6-C7-C8-C10
16	p	509	CLA	C6-C7-C8-C10
16	u	507	CLA	C6-C7-C8-C10
16	v	510	CLA	C12-C13-C15-C16
17	B	2002	PQN	C22-C23-C25-C26
16	B	1239	CLA	C8-C10-C11-C12
16	a	1138	CLA	C8-C10-C11-C12
16	u	504	CLA	C11-C12-C13-C14
23	x	606	LMU	C7-C8-C9-C10
14	H	4101	LMG	C7-C8-O7-C10
16	A	1126	CLA	C5-C6-C7-C8
13	b	4018	LHG	C10-C11-C12-C13
20	H	4202	LMT	C11-C10-C9-C8
16	b	1212	CLA	CAA-CBA-CGA-O2A
16	Y	515	CLA	C8-C10-C11-C12
16	u	515	CLA	C5-C6-C7-C8
14	G	848	LMG	C33-C34-C35-C36
16	X	501	CLA	C2A-CAA-CBA-CGA
16	a	1101	CLA	C2A-CAA-CBA-CGA
16	b	1012	CLA	C2A-CAA-CBA-CGA
16	b	1204	CLA	C2A-CAA-CBA-CGA
16	g	517	CLA	C2A-CAA-CBA-CGA
16	o	507	CLA	C5-C6-C7-C8
16	B	1215	CLA	C11-C12-C13-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	848	LMG	C33-C34-C35-C36
13	H	851	LHG	O8-C23-C24-C25
16	G	1239	CLA	C5-C6-C7-C8
16	w	512	CLA	C10-C11-C12-C13
16	y	506	CLA	C5-C6-C7-C8
13	x	605	LHG	O7-C7-C8-C9
16	X	503	CLA	CAA-CBA-CGA-O2A
16	g	509	CLA	CAA-CBA-CGA-O2A
16	r	505	CLA	CAA-CBA-CGA-O2A
16	B	1234	CLA	O1A-CGA-O2A-C1
16	n	511	CLA	C10-C11-C12-C13
16	B	1232	CLA	CAA-CBA-CGA-O1A
16	b	1208	CLA	CAA-CBA-CGA-O1A
16	A	1106	CLA	C4-C3-C5-C6
16	A	1128	CLA	C3A-C2A-CAA-CBA
16	A	1237	CLA	C3A-C2A-CAA-CBA
16	B	1208	CLA	C3A-C2A-CAA-CBA
16	B	1219	CLA	C3A-C2A-CAA-CBA
16	G	1208	CLA	C3A-C2A-CAA-CBA
16	G	1219	CLA	C3A-C2A-CAA-CBA
16	G	1228	CLA	C3A-C2A-CAA-CBA
16	G	1229	CLA	C4-C3-C5-C6
16	H	1101	CLA	C3A-C2A-CAA-CBA
16	H	1108	CLA	C3A-C2A-CAA-CBA
16	H	1112	CLA	C3A-C2A-CAA-CBA
16	W	512	CLA	C3A-C2A-CAA-CBA
16	X	501	CLA	C3A-C2A-CAA-CBA
16	Y	506	CLA	C3A-C2A-CAA-CBA
16	a	1101	CLA	C3A-C2A-CAA-CBA
16	b	1021	CLA	C3A-C2A-CAA-CBA
16	b	1202	CLA	C4-C3-C5-C6
16	b	1226	CLA	C3A-C2A-CAA-CBA
16	b	1235	CLA	C3A-C2A-CAA-CBA
16	p	506	CLA	C3A-C2A-CAA-CBA
16	s	506	CLA	C3A-C2A-CAA-CBA
16	v	514	CLA	C3A-C2A-CAA-CBA
16	y	512	CLA	C3A-C2A-CAA-CBA
16	o	517	CLA	CAA-CBA-CGA-O1A
16	X	515	CLA	C5-C6-C7-C8
16	h	512	CLA	C13-C15-C16-C17
16	q	515	CLA	C8-C10-C11-C12
20	U	4101	LMT	C3-C4-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	b	1021	CLA	CAA-CBA-CGA-O2A
16	b	1218	CLA	C2-C3-C5-C6
16	u	505	CLA	C2-C3-C5-C6
19	b	4010	BCR	C11-C10-C9-C8
19	q	602	BCR	C16-C17-C18-C19
19	s	601	BCR	C20-C21-C22-C23
16	G	1220	CLA	CAA-CBA-CGA-O1A
16	q	508	CLA	CAA-CBA-CGA-O1A
16	r	513	CLA	CAA-CBA-CGA-O1A
16	v	514	CLA	CAA-CBA-CGA-O1A
16	y	509	CLA	O1A-CGA-O2A-C1
13	B	4018	LHG	O6-C4-C5-O7
16	B	1205	CLA	C15-C16-C17-C18
16	A	1104	CLA	CAA-CBA-CGA-O2A
16	u	508	CLA	CAA-CBA-CGA-O2A
16	s	501	CLA	C4C-C3C-CAC-CBC
16	A	1133	CLA	CAA-CBA-CGA-O1A
16	L	1501	CLA	CAA-CBA-CGA-O1A
16	b	1226	CLA	CAA-CBA-CGA-O1A
16	p	505	CLA	CAA-CBA-CGA-O1A
16	u	505	CLA	CAA-CBA-CGA-O1A
16	b	1226	CLA	CBD-CGD-O2D-CED
16	A	1131	CLA	C2A-CAA-CBA-CGA
16	h	517	CLA	C2A-CAA-CBA-CGA
16	b	1231	CLA	CAA-CBA-CGA-O2A
16	B	1239	CLA	C11-C10-C8-C9
16	B	1239	CLA	C14-C13-C15-C16
16	G	1204	CLA	C6-C7-C8-C9
16	H	1136	CLA	C11-C10-C8-C9
16	W	512	CLA	C11-C10-C8-C9
16	X	512	CLA	C6-C7-C8-C9
16	Z	506	CLA	C6-C7-C8-C9
16	b	1211	CLA	C14-C13-C15-C16
16	b	1235	CLA	C14-C13-C15-C16
16	g	511	CLA	C14-C13-C15-C16
16	n	510	CLA	C14-C13-C15-C16
16	o	515	CLA	C11-C10-C8-C9
16	p	504	CLA	C6-C7-C8-C9
16	p	509	CLA	C6-C7-C8-C9
16	s	507	CLA	C14-C13-C15-C16
16	s	515	CLA	C11-C10-C8-C9
16	w	507	CLA	C14-C13-C15-C16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	w	511	CLA	C14-C13-C15-C16
16	x	507	CLA	C11-C10-C8-C9
16	x	509	CLA	C11-C10-C8-C9
16	y	509	CLA	C11-C12-C13-C14
17	A	2001	PQN	C16-C17-C18-C19
16	B	1220	CLA	CAA-CBA-CGA-O2A
16	G	1021	CLA	CAA-CBA-CGA-O2A
16	A	1118	CLA	CAA-CBA-CGA-O1A
16	B	1236	CLA	CAA-CBA-CGA-O1A
16	W	514	CLA	CAA-CBA-CGA-O1A
16	X	508	CLA	CAA-CBA-CGA-O1A
16	a	1101	CLA	CAA-CBA-CGA-O1A
16	a	1118	CLA	CAA-CBA-CGA-O1A
16	n	509	CLA	CAA-CBA-CGA-O1A
13	a	849	LHG	C13-C14-C15-C16
16	y	515	CLA	C13-C15-C16-C17
16	H	1114	CLA	O1D-CGD-O2D-CED
20	A	4202	LMT	C11-C10-C9-C8
16	a	1123	CLA	C4C-C3C-CAC-CBC
16	A	1140	CLA	C5-C6-C7-C8
16	G	1225	CLA	C10-C11-C12-C13
16	g	510	CLA	C13-C15-C16-C17
16	t	507	CLA	C5-C6-C7-C8
16	g	513	CLA	C4C-C3C-CAC-CBC
16	X	510	CLA	C4-C3-C5-C6
16	q	508	CLA	C4-C3-C5-C6
16	w	510	CLA	C4-C3-C5-C6
16	A	1101	CLA	CAA-CBA-CGA-O1A
16	H	1105	CLA	CAA-CBA-CGA-O1A
16	b	1236	CLA	CAA-CBA-CGA-O1A
16	s	517	CLA	CAA-CBA-CGA-O1A
16	w	505	CLA	CAA-CBA-CGA-O1A
16	y	512	CLA	CAA-CBA-CGA-O1A
16	s	516	CLA	O1A-CGA-O2A-C1
16	s	506	CLA	O1D-CGD-O2D-CED
16	h	514	CLA	CAA-CBA-CGA-O2A
16	o	508	CLA	C2-C3-C5-C6
16	s	509	CLA	C2-C3-C5-C6
14	B	848	LMG	O10-C28-O8-C9
16	A	1116	CLA	C6-C7-C8-C9
16	B	1240	CLA	O1A-CGA-O2A-C1
16	H	1118	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	W	505	CLA	CAA-CBA-CGA-O1A
16	o	508	CLA	CAA-CBA-CGA-O1A
16	G	1206	CLA	C15-C16-C17-C18
16	b	1226	CLA	C5-C6-C7-C8
16	o	515	CLA	C5-C6-C7-C8
16	a	1122	CLA	C11-C12-C13-C14
16	Z	501	CLA	C4C-C3C-CAC-CBC
16	Y	509	CLA	CAA-CBA-CGA-O2A
16	o	507	CLA	CAA-CBA-CGA-O2A
16	G	1219	CLA	CAA-CBA-CGA-O1A
16	b	1230	CLA	CAA-CBA-CGA-O2A
16	Y	507	CLA	C8-C10-C11-C12
16	G	1238	CLA	CBD-CGD-O2D-CED
19	G	4009	BCR	C17-C18-C19-C20
19	L	4019	BCR	C11-C12-C13-C14
19	Z	604	BCR	C21-C22-C23-C24
19	a	4011	BCR	C17-C18-C19-C20
19	u	604	BCR	C11-C12-C13-C14
16	G	1238	CLA	CBA-CGA-O2A-C1
16	b	1239	CLA	C4C-C3C-CAC-CBC
16	A	1110	CLA	CAA-CBA-CGA-O1A
16	H	1110	CLA	CAA-CBA-CGA-O1A
16	U	1501	CLA	CAA-CBA-CGA-O1A
16	W	502	CLA	CAA-CBA-CGA-O1A
16	Y	505	CLA	CAA-CBA-CGA-O1A
16	Z	502	CLA	CAA-CBA-CGA-O1A
16	p	510	CLA	CAA-CBA-CGA-O1A
16	t	505	CLA	CAA-CBA-CGA-O1A
16	w	502	CLA	CAA-CBA-CGA-O1A
16	x	503	CLA	CAA-CBA-CGA-O1A
16	x	508	CLA	CAA-CBA-CGA-O1A
16	y	507	CLA	CAA-CBA-CGA-O1A
16	B	1239	CLA	C4C-C3C-CAC-CBC
14	a	4201	LMG	C28-C29-C30-C31
19	j	4012	BCR	C10-C11-C12-C13
16	t	510	CLA	C8-C10-C11-C12
16	G	1212	CLA	CAA-CBA-CGA-O1A
16	G	1232	CLA	CAA-CBA-CGA-O2A
14	B	848	LMG	C2-C1-O1-C7
16	H	1102	CLA	CAA-CBA-CGA-O1A
16	Y	510	CLA	CAA-CBA-CGA-O1A
16	Z	507	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	Z	509	CLA	CAA-CBA-CGA-O1A
16	o	502	CLA	CAA-CBA-CGA-O1A
16	o	514	CLA	CAA-CBA-CGA-O1A
16	o	516	CLA	CAA-CBA-CGA-O1A
16	q	505	CLA	CAA-CBA-CGA-O1A
16	s	510	CLA	CAA-CBA-CGA-O1A
16	u	507	CLA	CAA-CBA-CGA-O1A
16	G	1214	CLA	CAA-CBA-CGA-O2A
16	W	510	CLA	CAA-CBA-CGA-O2A
16	a	1110	CLA	CAA-CBA-CGA-O2A
16	b	1023	CLA	CAA-CBA-CGA-O2A
16	n	510	CLA	CAA-CBA-CGA-O2A
16	r	510	CLA	CAA-CBA-CGA-O2A
16	u	510	CLA	CAA-CBA-CGA-O2A
16	B	1207	CLA	C2A-CAA-CBA-CGA
16	B	1236	CLA	C2A-CAA-CBA-CGA
16	H	1111	CLA	C2A-CAA-CBA-CGA
16	H	1121	CLA	C2A-CAA-CBA-CGA
16	u	504	CLA	C2A-CAA-CBA-CGA
16	v	515	CLA	C16-C17-C18-C19
16	G	1208	CLA	CAA-CBA-CGA-O1A
16	G	1230	CLA	CAA-CBA-CGA-O1A
16	W	513	CLA	C4C-C3C-CAC-CBC
16	q	501	CLA	C4C-C3C-CAC-CBC
16	G	1213	CLA	O1D-CGD-O2D-CED
16	X	510	CLA	O1D-CGD-O2D-CED
16	B	1214	CLA	CAA-CBA-CGA-O1A
16	H	1133	CLA	CAA-CBA-CGA-O1A
16	W	509	CLA	CAA-CBA-CGA-O1A
16	Z	505	CLA	CAA-CBA-CGA-O1A
16	q	507	CLA	CAA-CBA-CGA-O1A
16	G	1239	CLA	C4-C3-C5-C6
16	r	506	CLA	C4-C3-C5-C6
16	W	507	CLA	C5-C6-C7-C8
16	G	1236	CLA	CAA-CBA-CGA-O2A
16	X	516	CLA	CAA-CBA-CGA-O2A
16	b	1207	CLA	CAA-CBA-CGA-O2A
16	g	504	CLA	CAA-CBA-CGA-O2A
16	t	510	CLA	CAA-CBA-CGA-O2A
16	w	516	CLA	CAA-CBA-CGA-O2A
16	Y	505	CLA	C2-C3-C5-C6
16	l	1502	CLA	C3-C5-C6-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	X	512	CLA	O1D-CGD-O2D-CED
16	b	1212	CLA	CAA-CBA-CGA-O1A
19	p	602	BCR	C9-C10-C11-C12
19	s	602	BCR	C15-C16-C17-C18
13	i	103	LHG	O10-C23-C24-C25
16	n	505	CLA	CAA-CBA-CGA-O1A
16	h	506	CLA	O1A-CGA-O2A-C1
16	Y	508	CLA	C6-C7-C8-C10
16	A	1101	CLA	CAD-CBD-CGD-O2D
16	A	1105	CLA	CAD-CBD-CGD-O2D
16	A	1129	CLA	CAD-CBD-CGD-O2D
16	G	1210	CLA	CAD-CBD-CGD-O2D
16	H	1105	CLA	CAD-CBD-CGD-O2D
16	H	1121	CLA	CAD-CBD-CGD-O2D
16	K	4003	CLA	CAD-CBD-CGD-O2D
16	X	507	CLA	CAD-CBD-CGD-O2D
16	a	1123	CLA	CAD-CBD-CGD-O2D
16	b	1219	CLA	CAD-CBD-CGD-O2D
16	b	1226	CLA	CAD-CBD-CGD-O2D
16	h	513	CLA	CAD-CBD-CGD-O2D
16	o	517	CLA	CAD-CBD-CGD-O2D
16	r	507	CLA	CAD-CBD-CGD-O2D
16	s	502	CLA	CAD-CBD-CGD-O2D
16	u	510	CLA	CAD-CBD-CGD-O2D
16	v	514	CLA	CAD-CBD-CGD-O2D
16	w	507	CLA	CAD-CBD-CGD-O2D
16	y	511	CLA	CAD-CBD-CGD-O2D
16	A	1105	CLA	CAA-CBA-CGA-O2A
16	B	1201	CLA	CAA-CBA-CGA-O2A
16	G	1206	CLA	CAA-CBA-CGA-O2A
16	p	509	CLA	CAA-CBA-CGA-O2A
16	r	515	CLA	CAA-CBA-CGA-O2A
16	A	1102	CLA	CAA-CBA-CGA-O1A
16	h	501	CLA	CAA-CBA-CGA-O1A
16	l	1501	CLA	CAA-CBA-CGA-O1A
16	a	1111	CLA	O1A-CGA-O2A-C1
16	y	509	CLA	CBA-CGA-O2A-C1
19	Y	601	BCR	C6-C7-C8-C9
19	o	604	BCR	C22-C23-C24-C25
19	x	601	BCR	C6-C7-C8-C9
16	G	1202	CLA	C2-C1-O2A-CGA
16	Z	512	CLA	C2-C1-O2A-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	a	1126	CLA	C2-C1-O2A-CGA
16	b	1222	CLA	C2-C1-O2A-CGA
16	k	4004	CLA	C2-C1-O2A-CGA
16	n	507	CLA	C2-C1-O2A-CGA
16	t	502	CLA	C2-C1-O2A-CGA
16	t	507	CLA	C2-C1-O2A-CGA
16	B	1207	CLA	CAA-CBA-CGA-O1A
16	b	1023	CLA	CAA-CBA-CGA-O1A
16	t	502	CLA	CAA-CBA-CGA-O1A
16	v	502	CLA	O1D-CGD-O2D-CED
14	G	848	LMG	O7-C10-C11-C12
16	X	517	CLA	CAA-CBA-CGA-O2A
16	r	508	CLA	CAA-CBA-CGA-O2A
16	v	515	CLA	CAA-CBA-CGA-O2A
16	H	1022	CLA	CBD-CGD-O2D-CED
16	G	1214	CLA	C6-C7-C8-C10
16	A	1132	CLA	C8-C10-C11-C12
16	v	515	CLA	C8-C10-C11-C12
16	G	1207	CLA	C2A-CAA-CBA-CGA
16	B	1232	CLA	CAA-CBA-CGA-O2A
16	g	509	CLA	CAA-CBA-CGA-O1A
16	n	510	CLA	CAA-CBA-CGA-O1A
16	t	509	CLA	CAA-CBA-CGA-O1A
16	w	505	CLA	C13-C15-C16-C17
13	i	103	LHG	O8-C23-C24-C25
14	H	4101	LMG	O8-C28-C29-C30
16	A	1137	CLA	CAA-CBA-CGA-O2A
16	G	1201	CLA	CAA-CBA-CGA-O2A
16	H	1237	CLA	CAA-CBA-CGA-O2A
16	X	505	CLA	CAA-CBA-CGA-O2A
16	o	512	CLA	CAA-CBA-CGA-O2A
16	s	503	CLA	CAA-CBA-CGA-O2A
16	t	507	CLA	CAA-CBA-CGA-O2A
16	y	515	CLA	CAA-CBA-CGA-O2A
16	a	1134	CLA	CAA-CBA-CGA-O2A
16	H	1126	CLA	C16-C17-C18-C19
16	H	1013	CLA	CAA-CBA-CGA-O1A
16	r	510	CLA	CAA-CBA-CGA-O1A
13	i	103	LHG	C30-C31-C32-C33
16	B	1023	CLA	CAA-CBA-CGA-O2A
16	W	512	CLA	CAA-CBA-CGA-O2A
16	b	1239	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

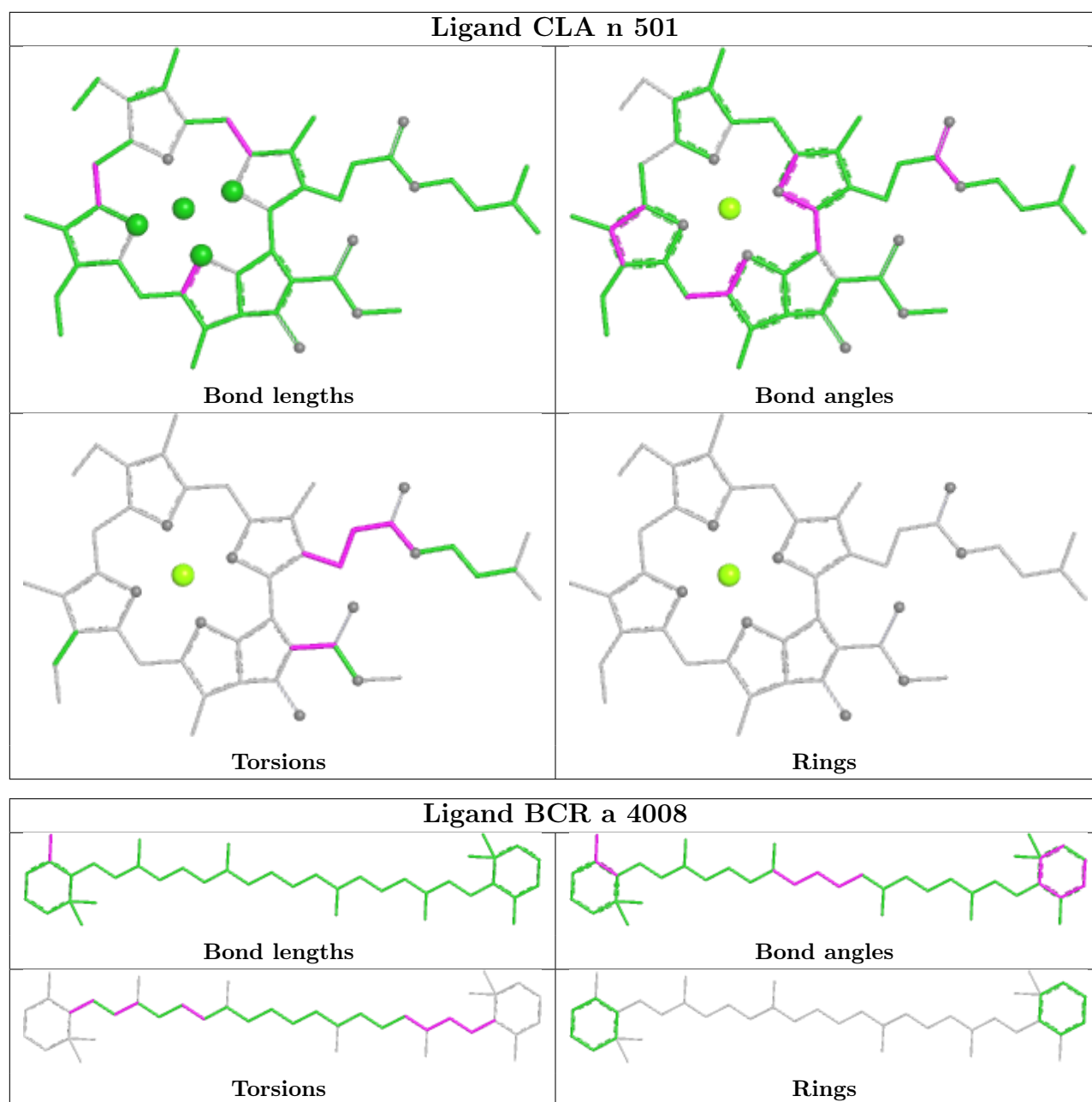
Mol	Chain	Res	Type	Atoms
16	s	513	CLA	CAA-CBA-CGA-O2A
16	u	502	CLA	CAA-CBA-CGA-O2A
16	B	1226	CLA	CAA-CBA-CGA-O1A
16	G	1226	CLA	CAA-CBA-CGA-O1A
16	W	510	CLA	CAA-CBA-CGA-O1A
16	X	503	CLA	CAA-CBA-CGA-O1A
16	o	507	CLA	CAA-CBA-CGA-O1A
16	q	502	CLA	CAA-CBA-CGA-O1A
16	s	505	CLA	CAA-CBA-CGA-O1A
16	t	510	CLA	CAA-CBA-CGA-O1A
16	x	510	CLA	CAA-CBA-CGA-O1A
23	r	606	LMU	C7-C8-C9-C10

There are no ring outliers.

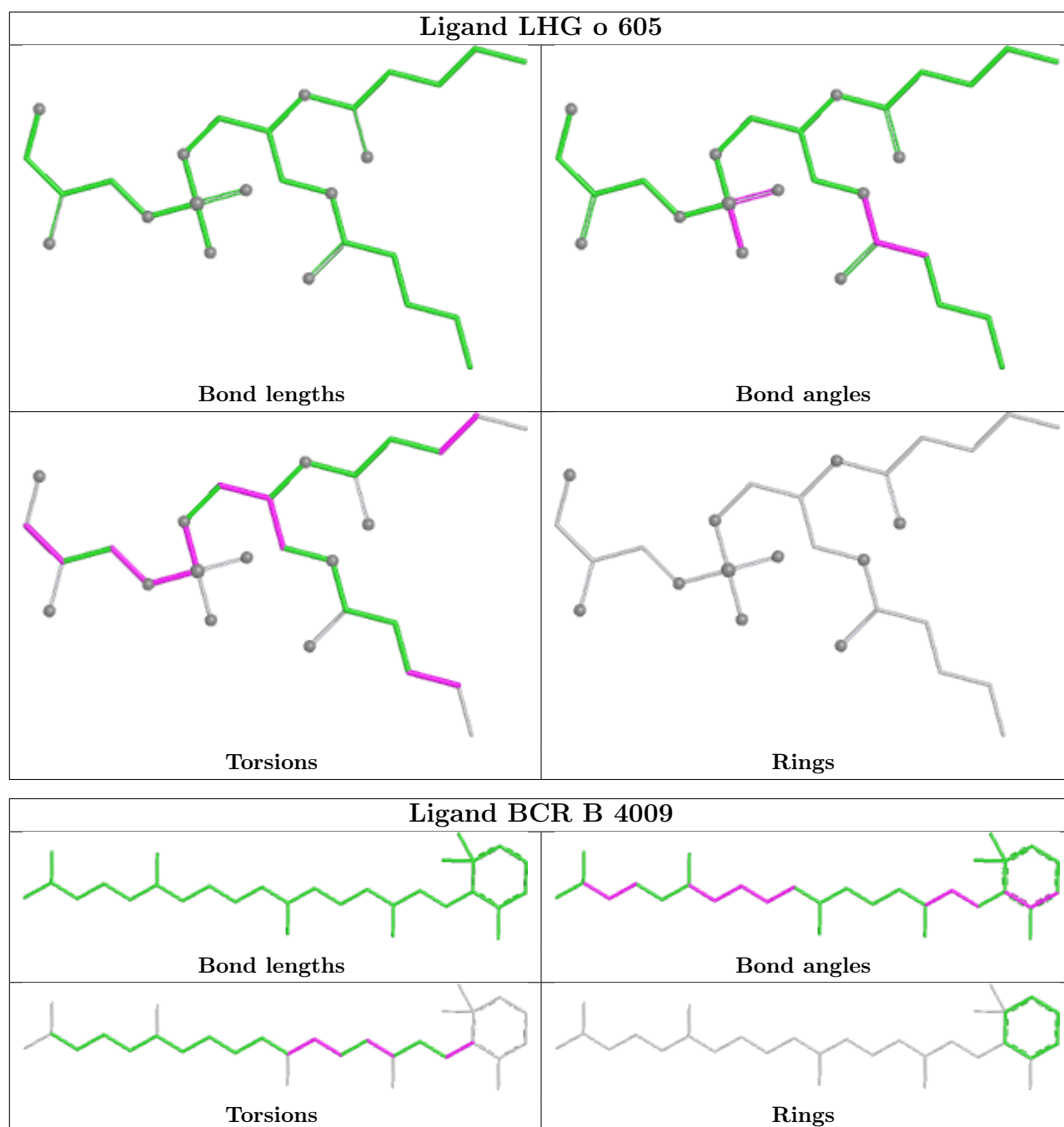
No monomer is involved in short contacts.

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.



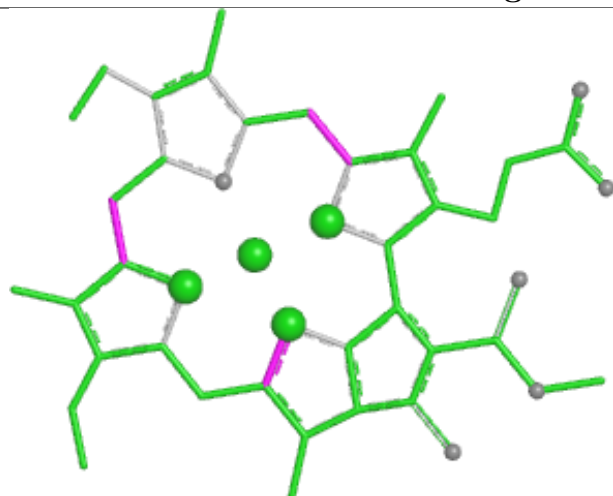




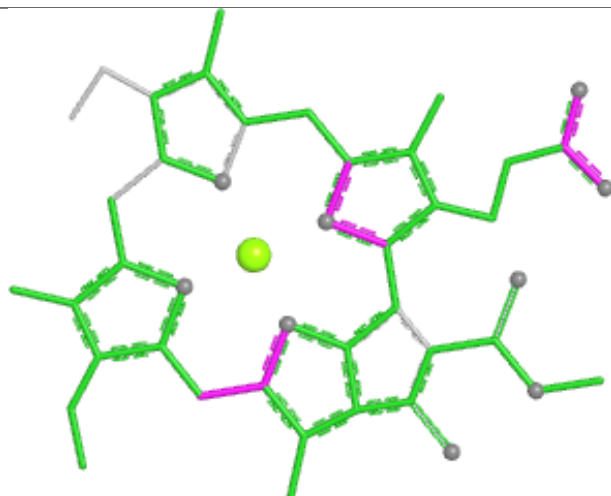




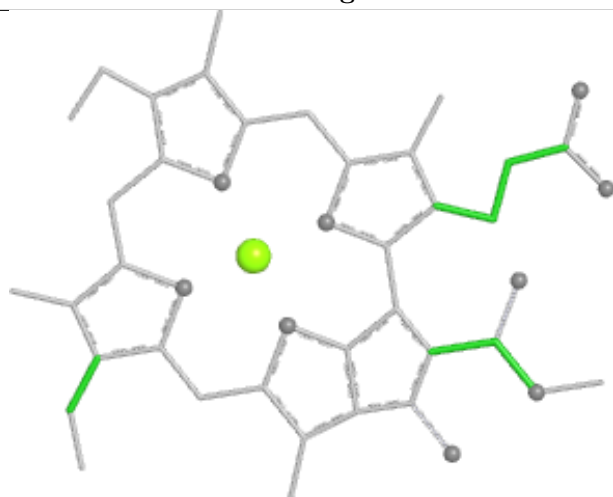
## Ligand CLA H 1113



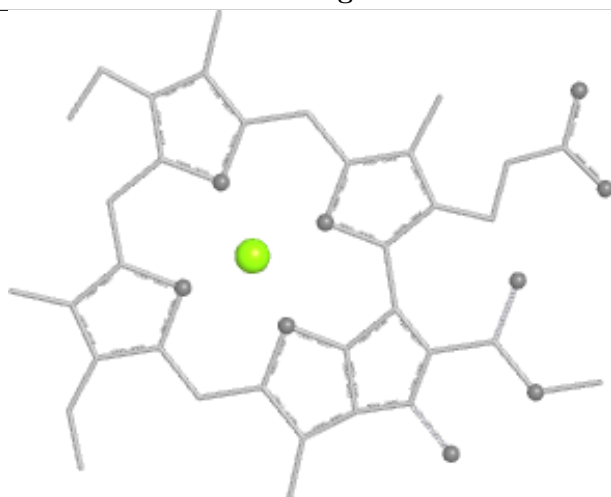
Bond lengths



Bond angles

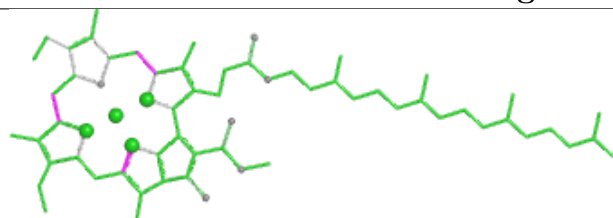


Torsions

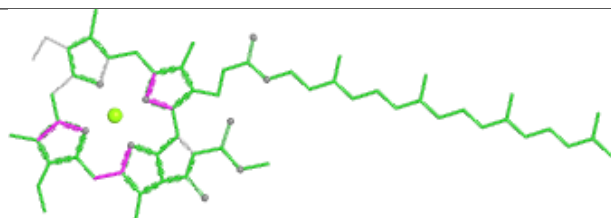


Rings

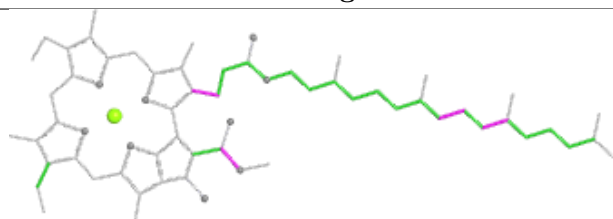
## Ligand CLA u 511



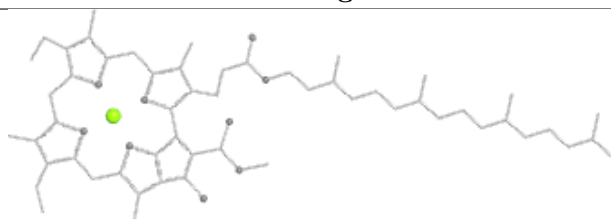
Bond lengths



Bond angles

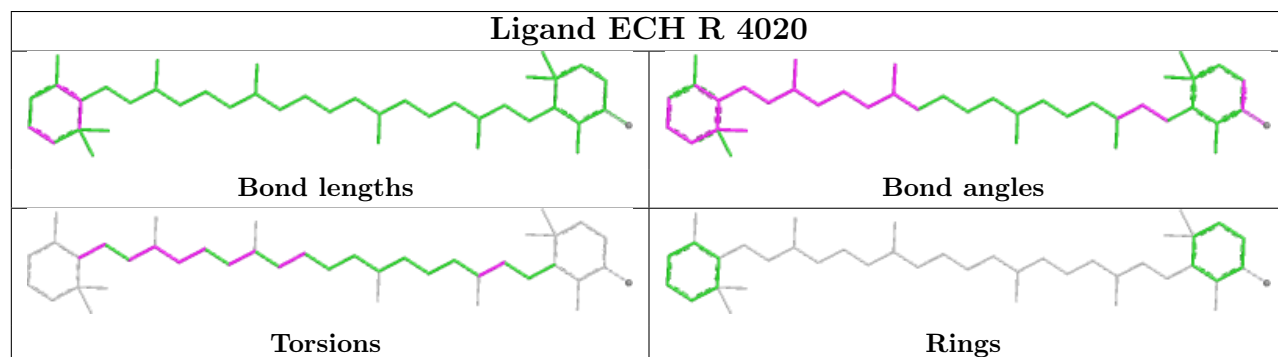
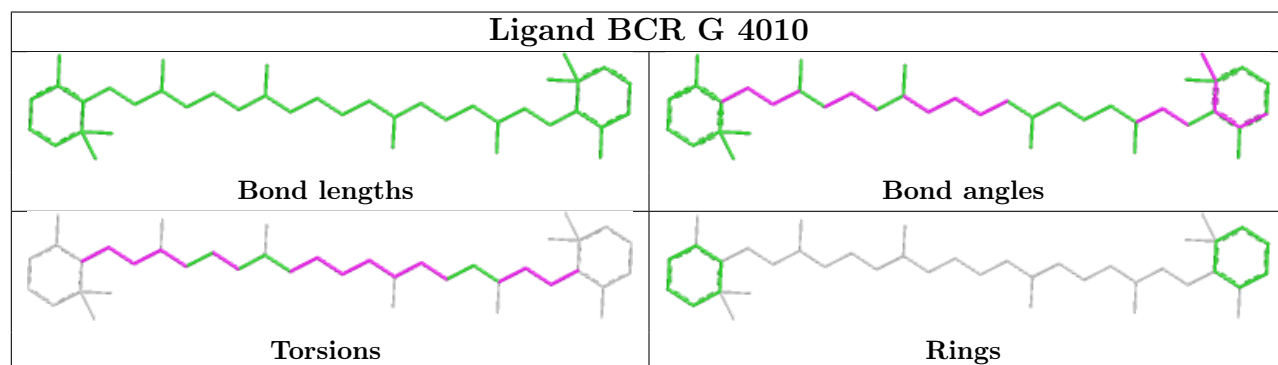
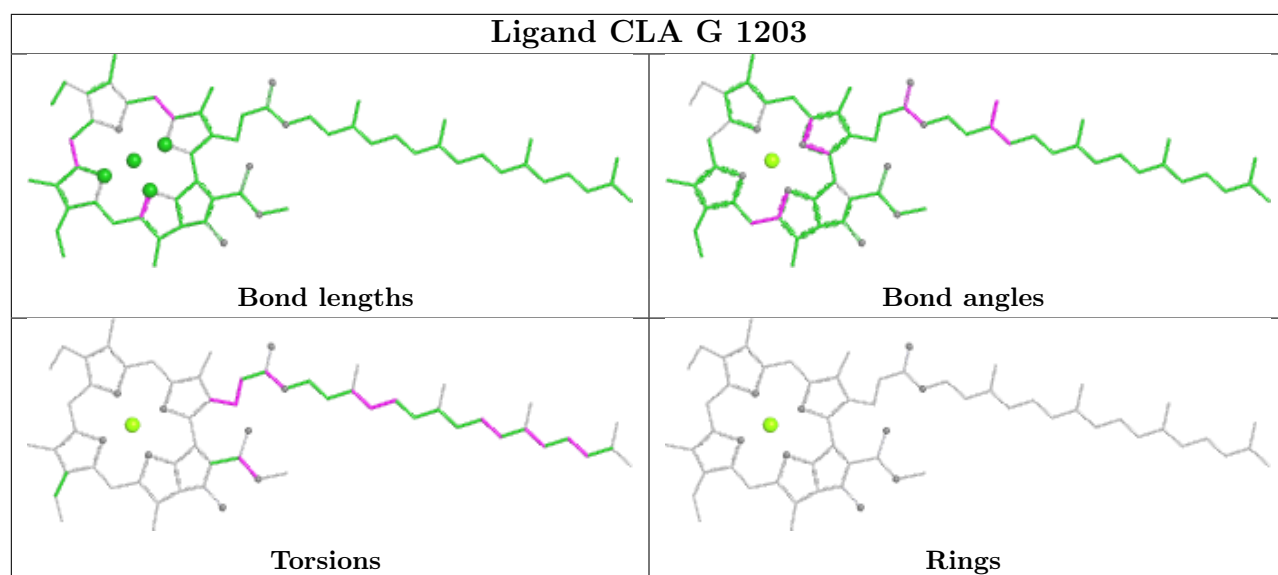


Torsions

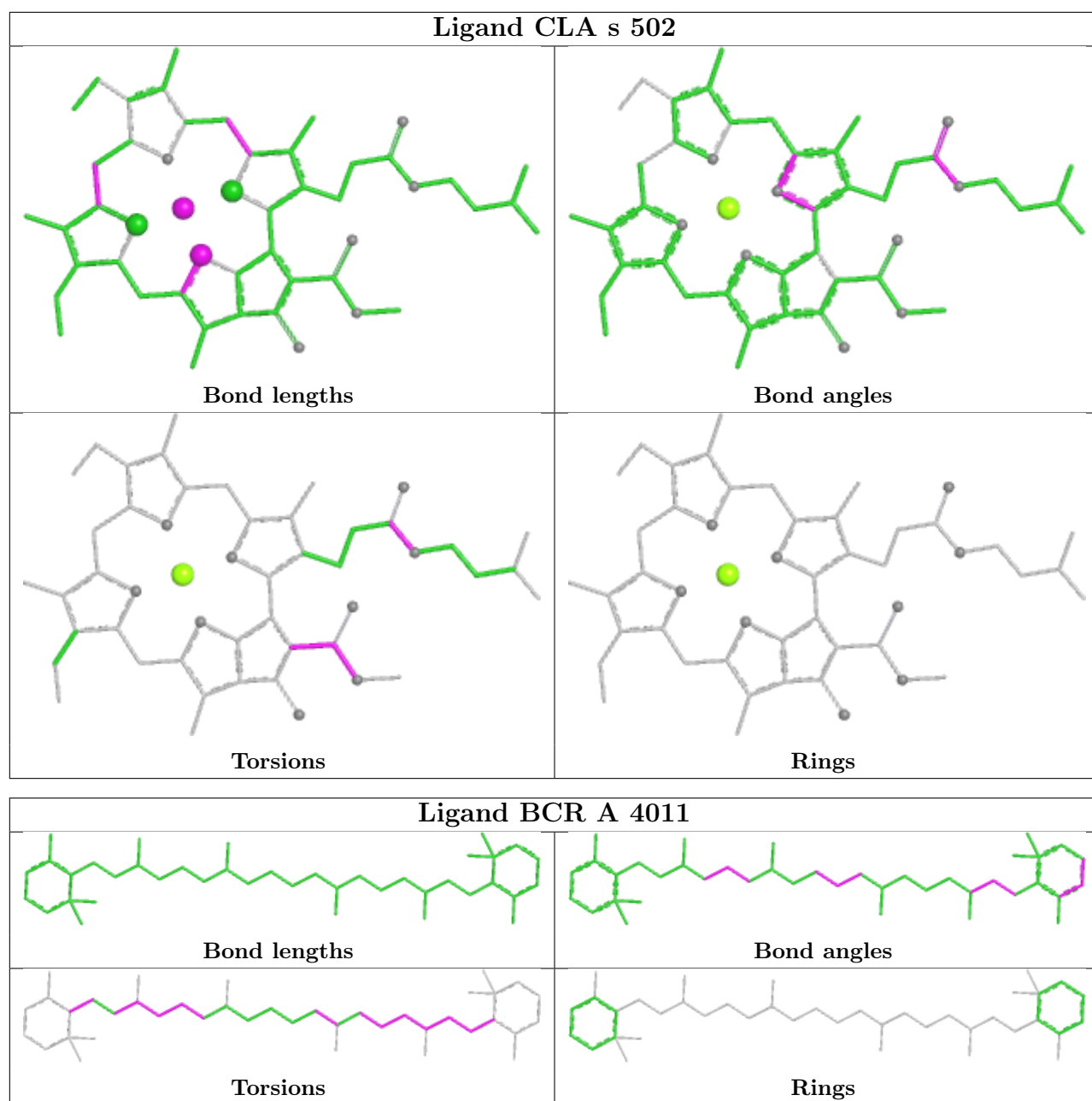


Rings

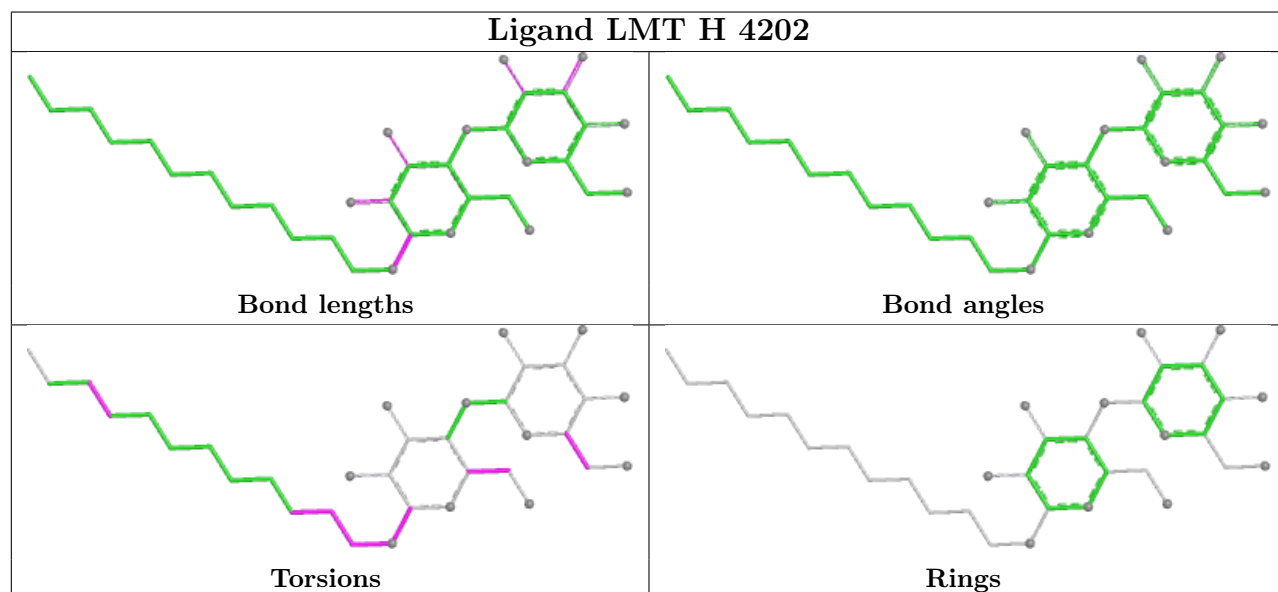
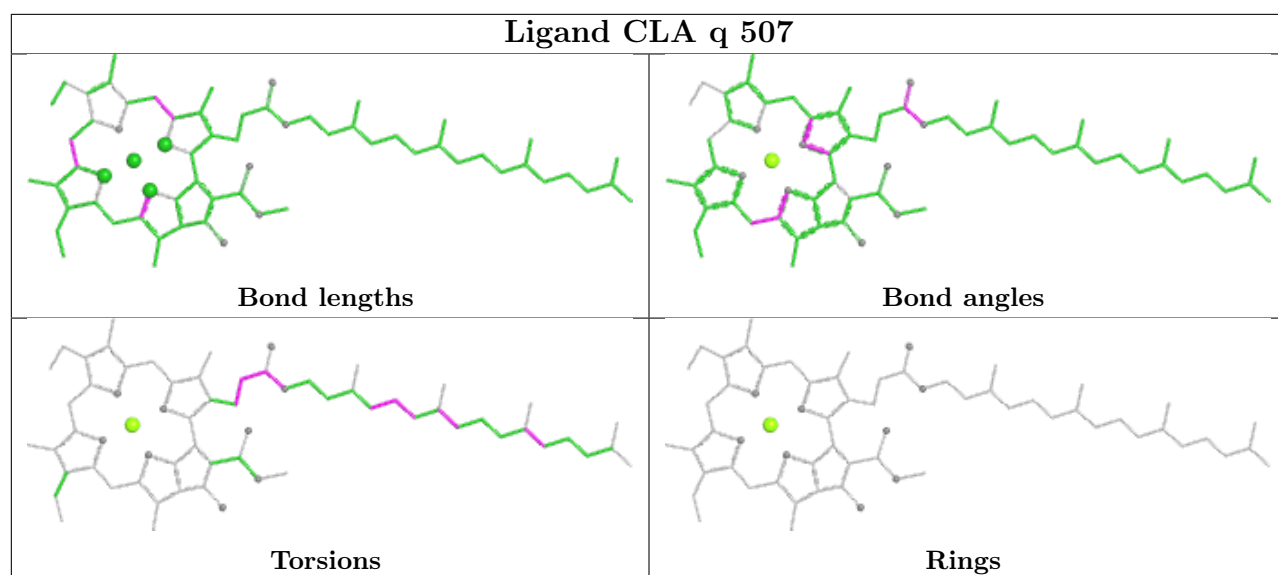






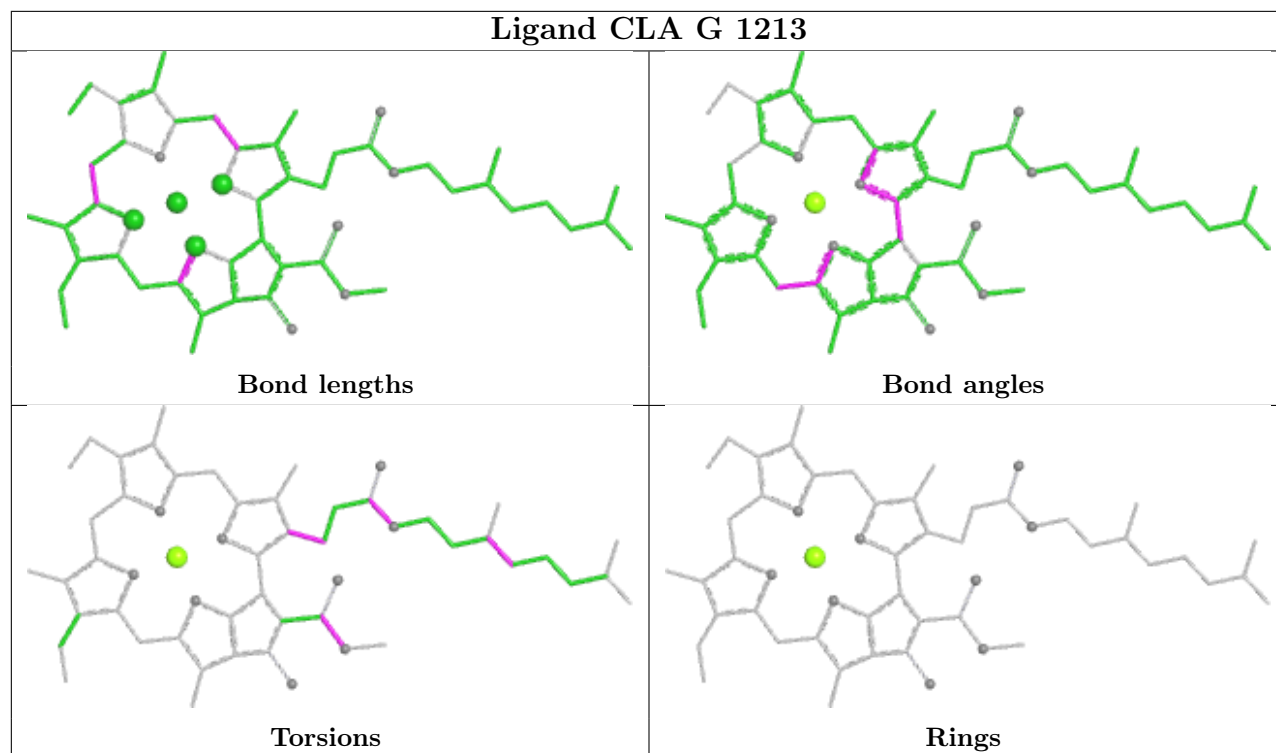




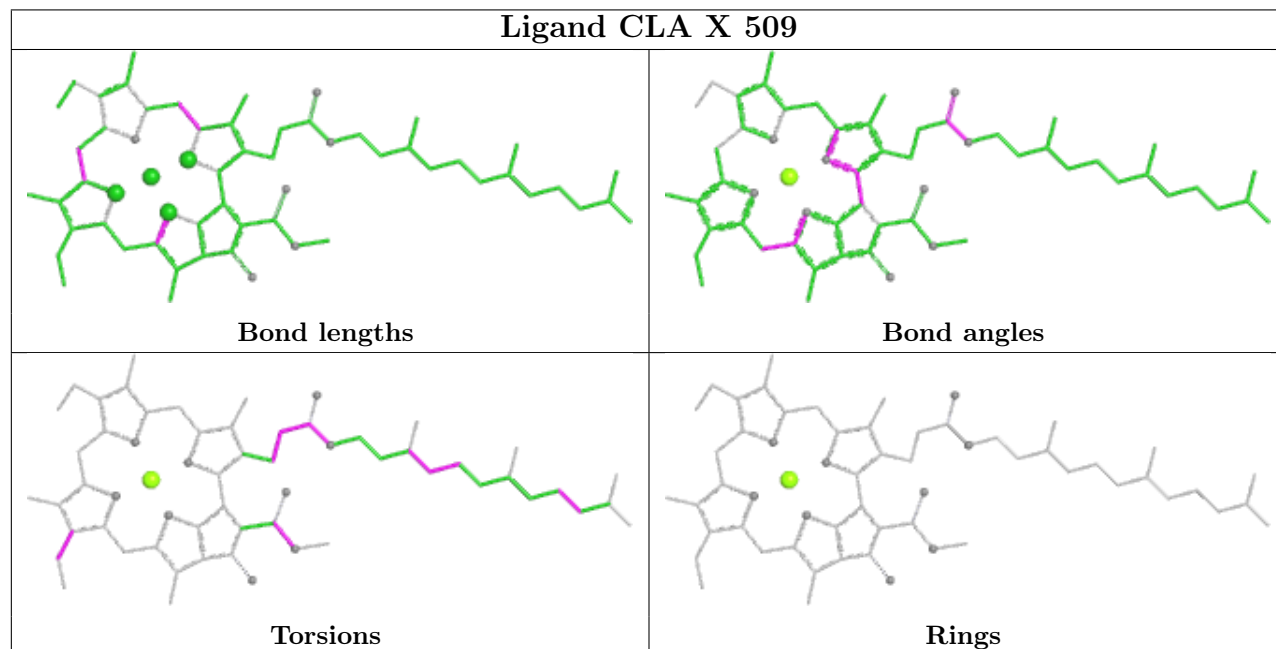




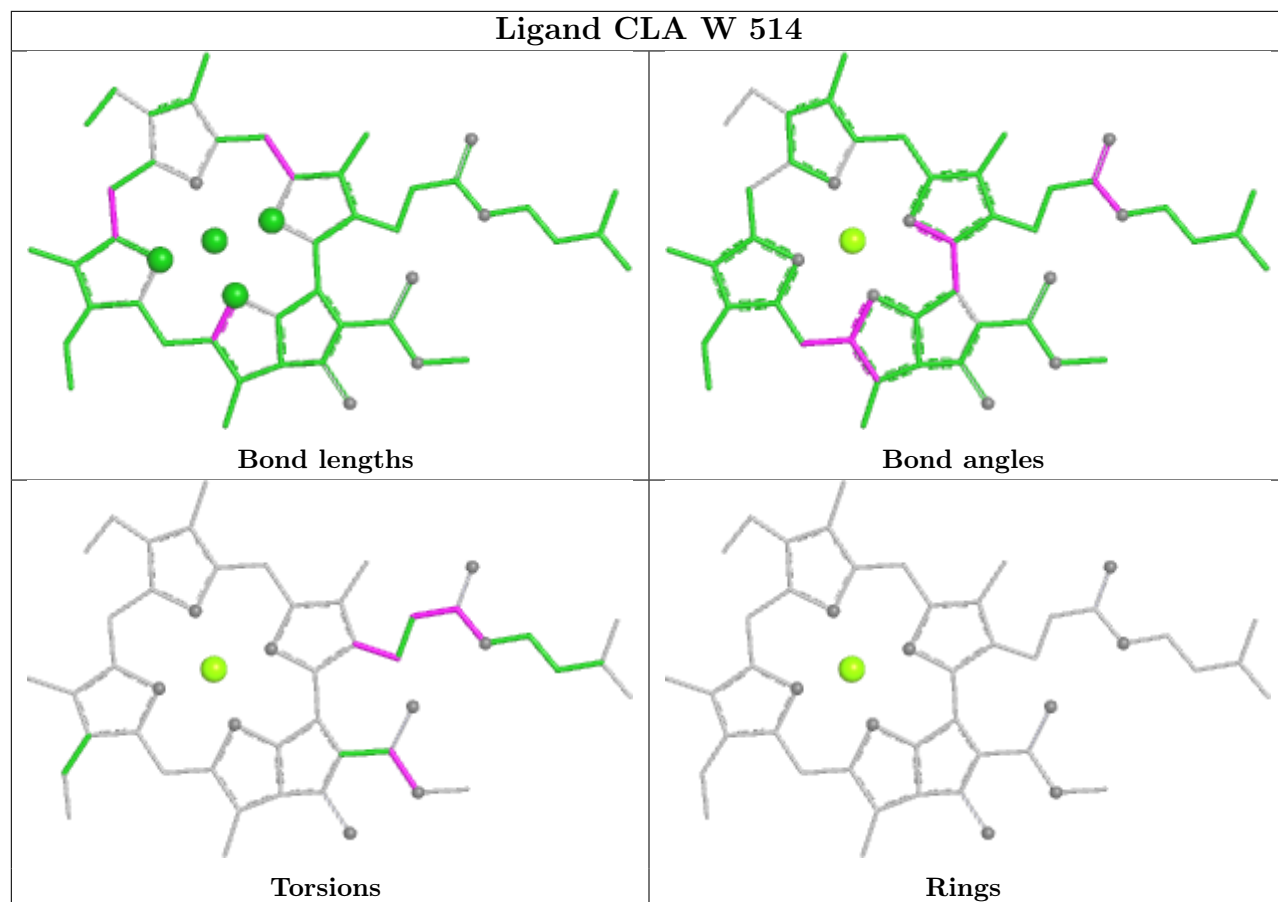
## Ligand CLA G 1213



## Ligand CLA X 509

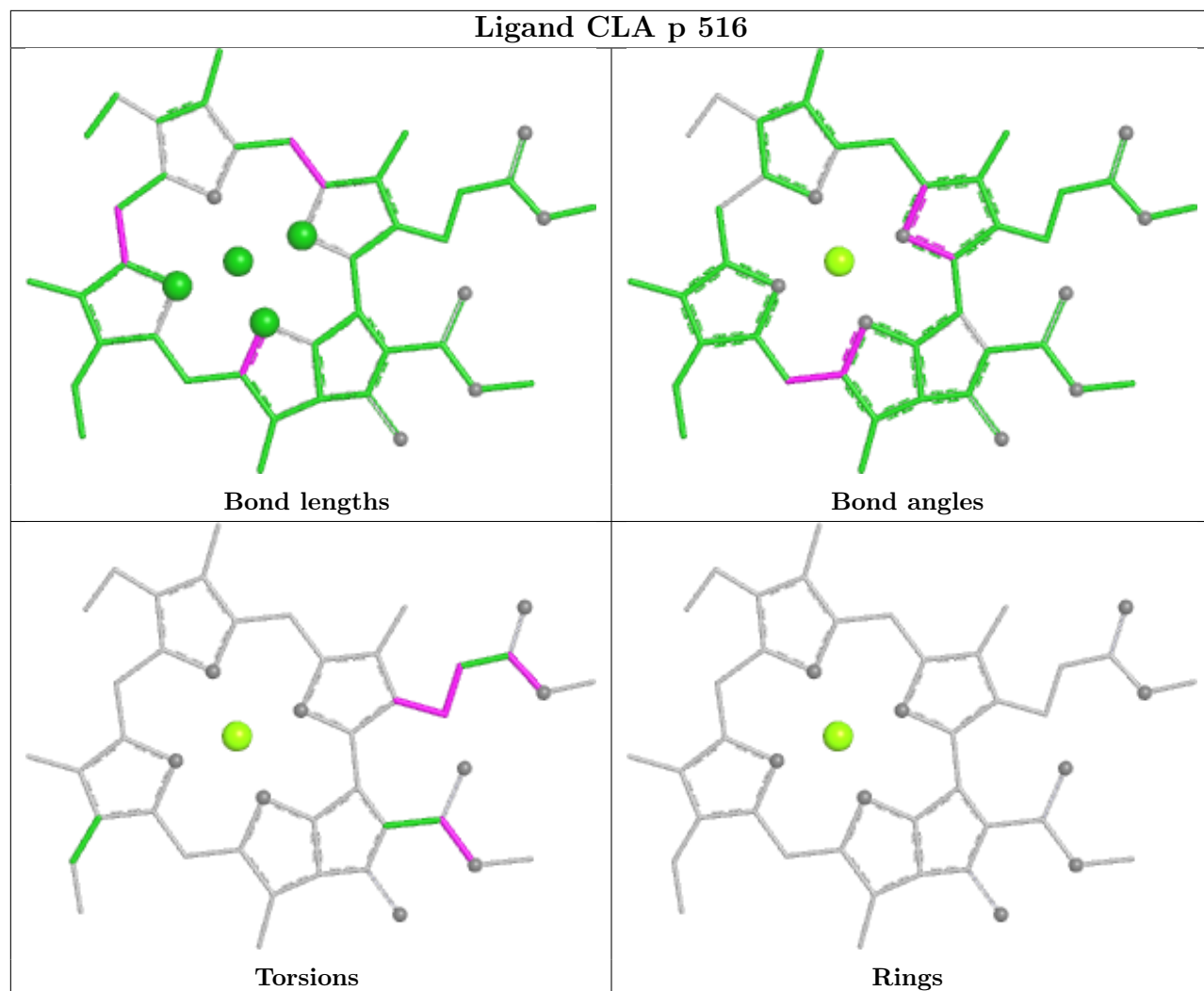




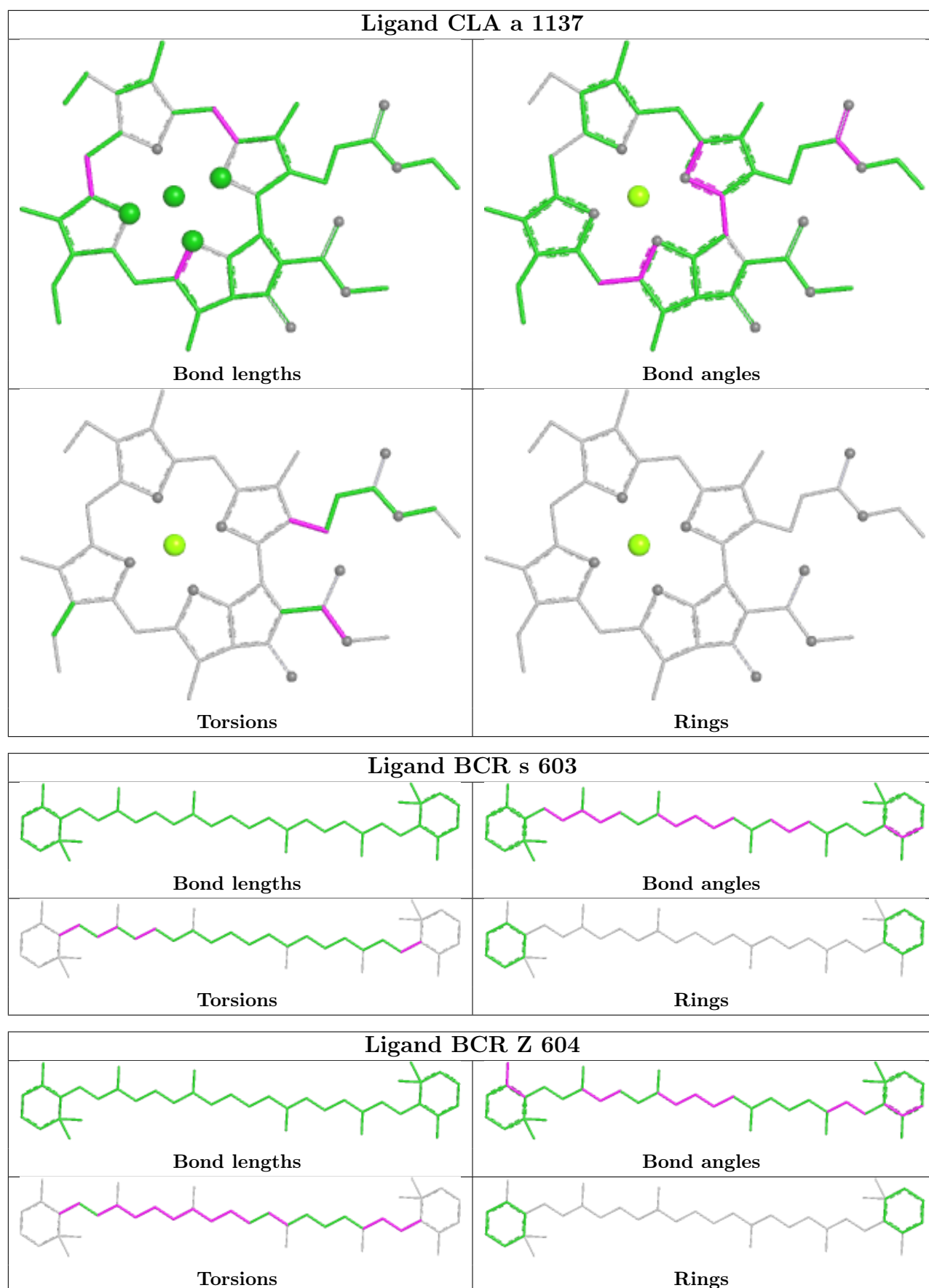




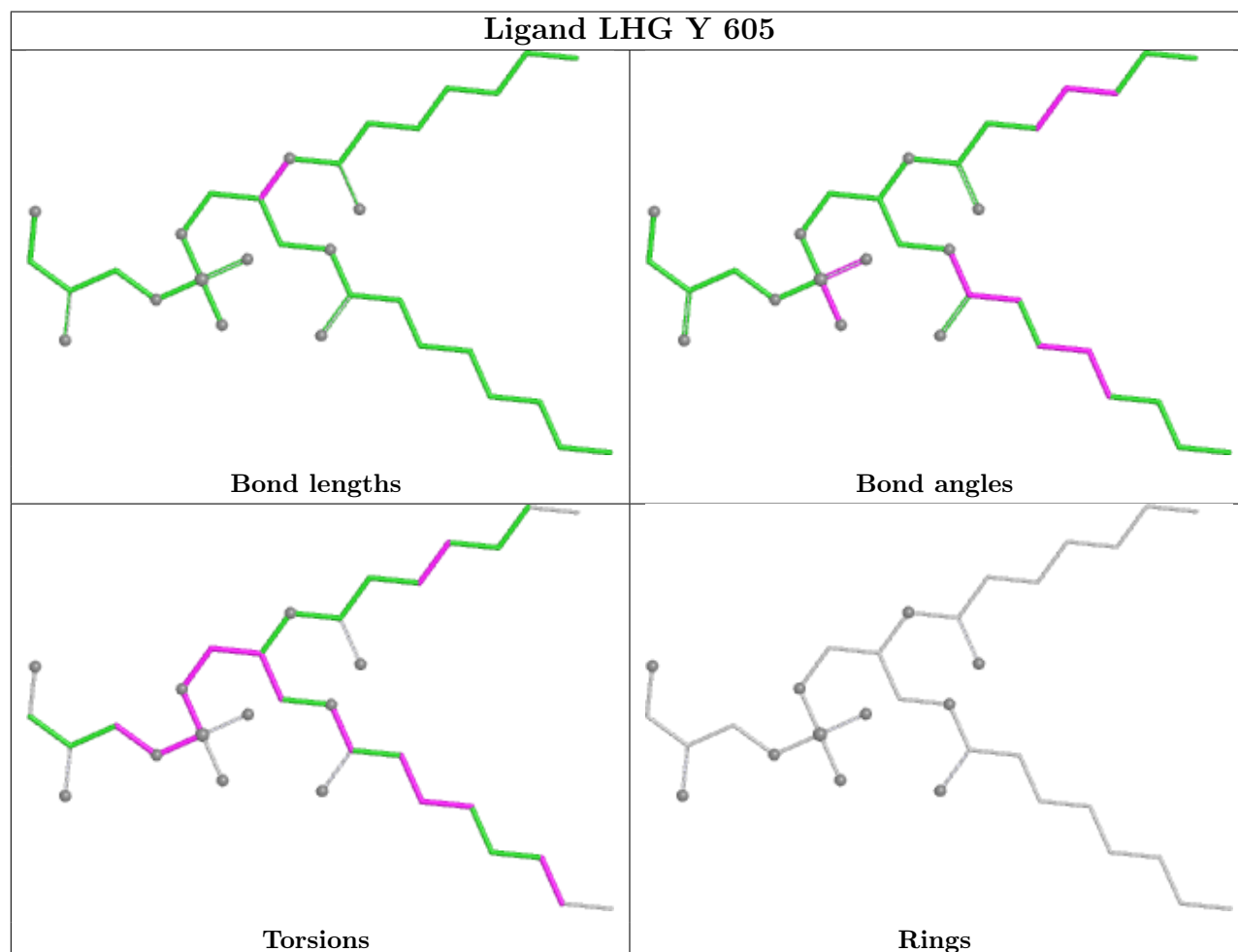
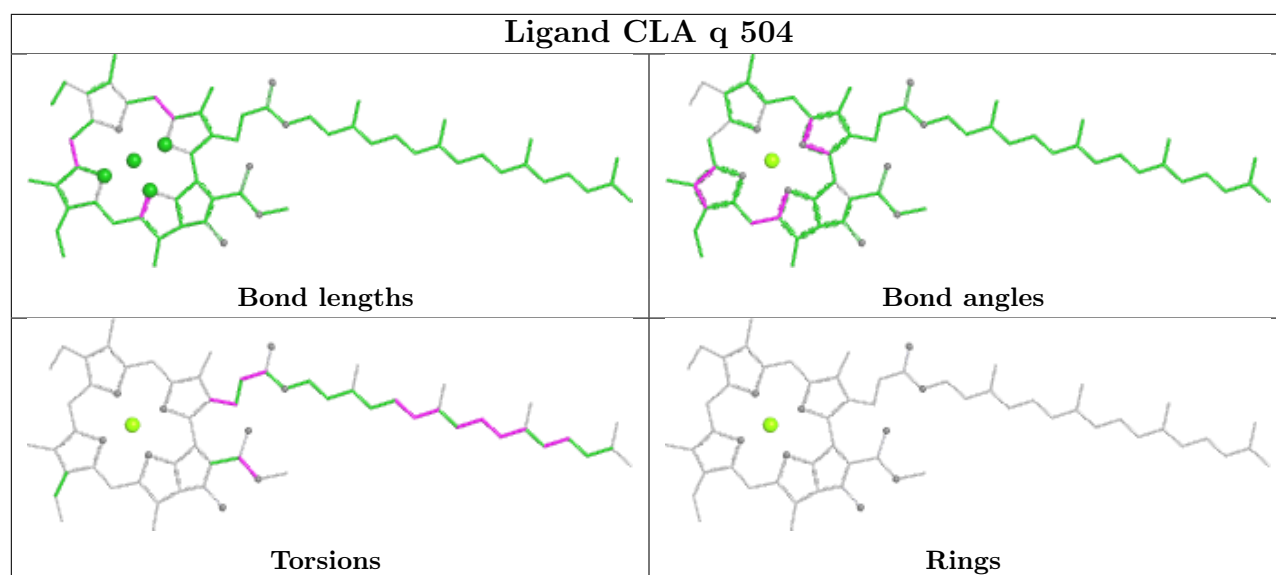
## Ligand CLA p 516



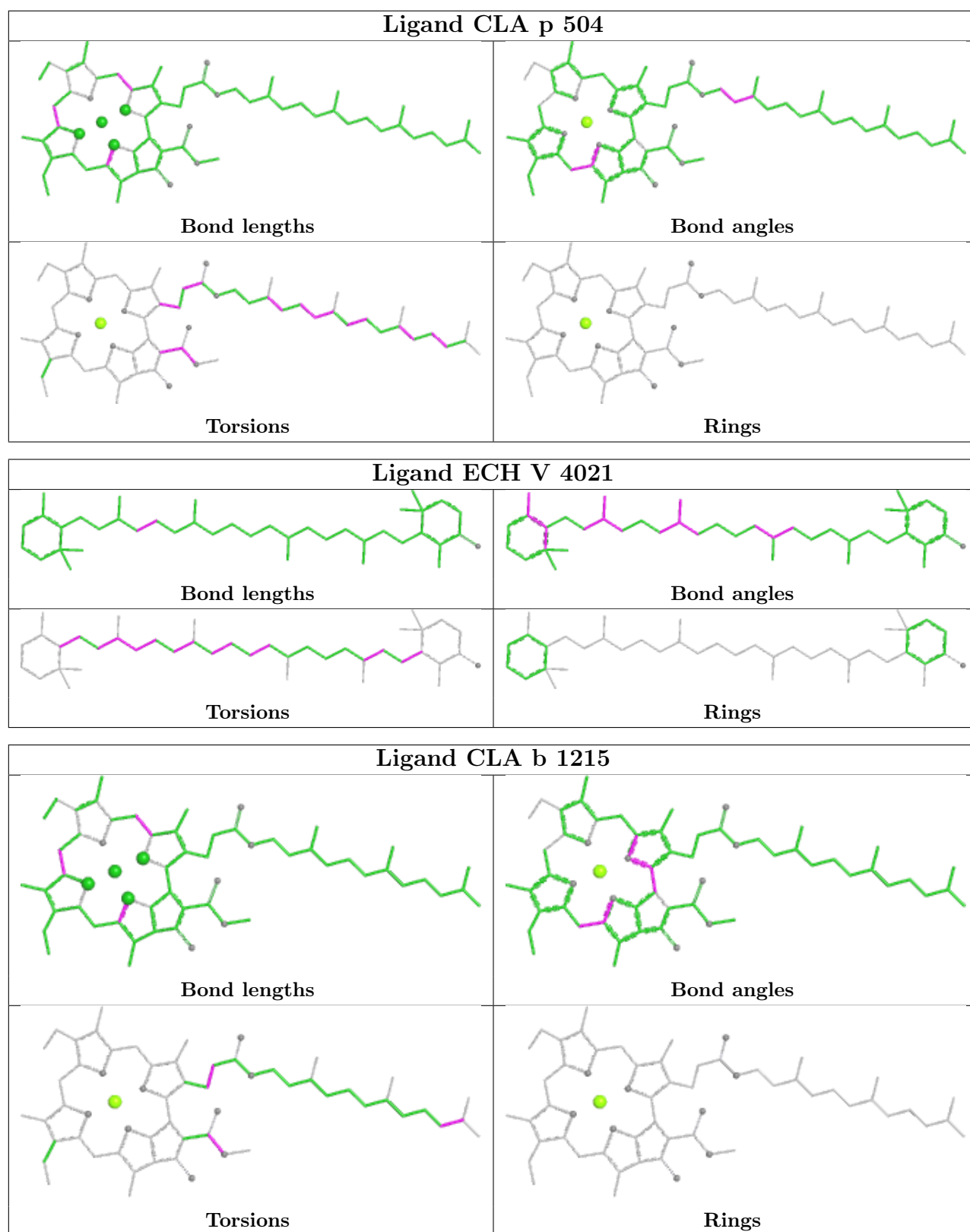




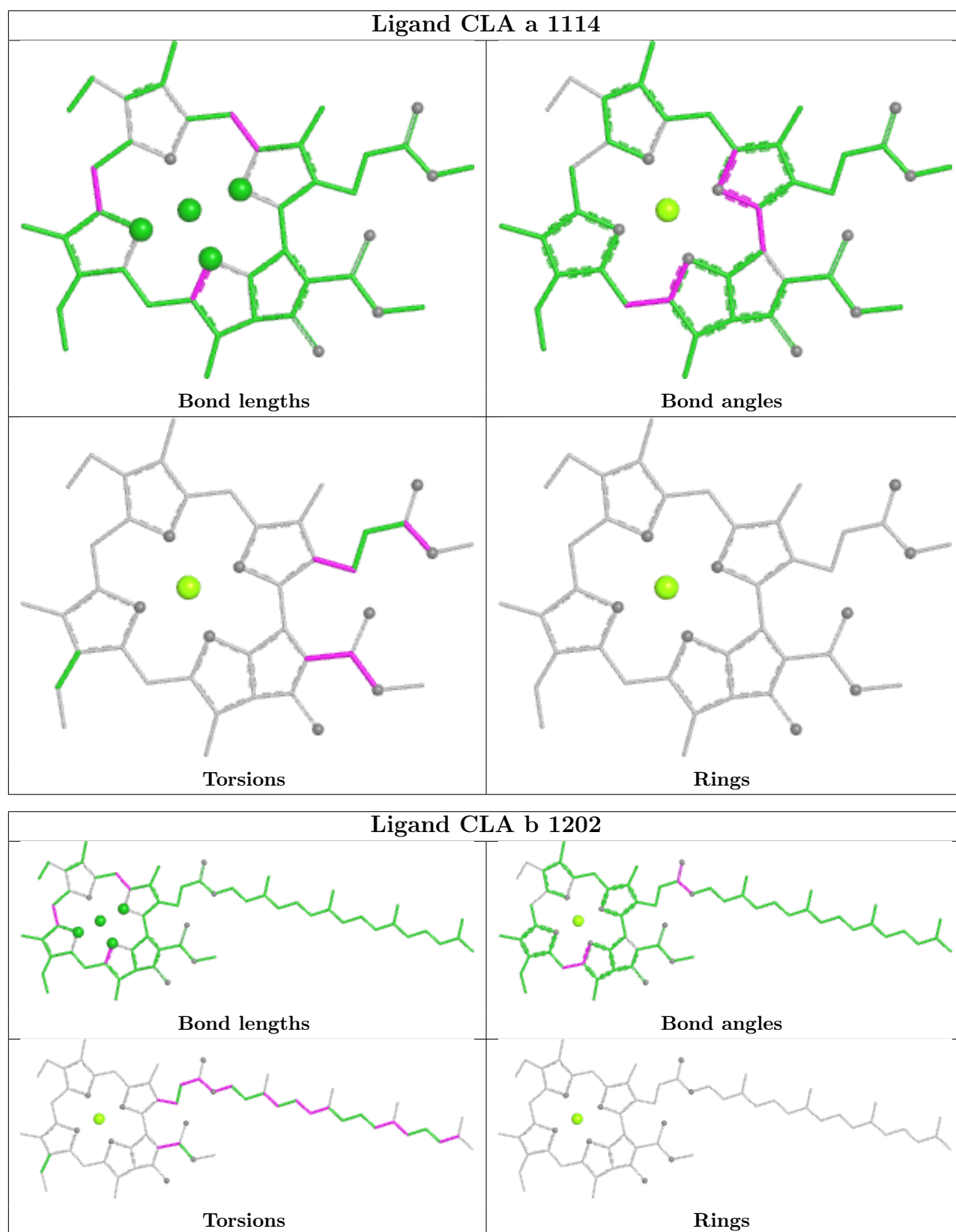




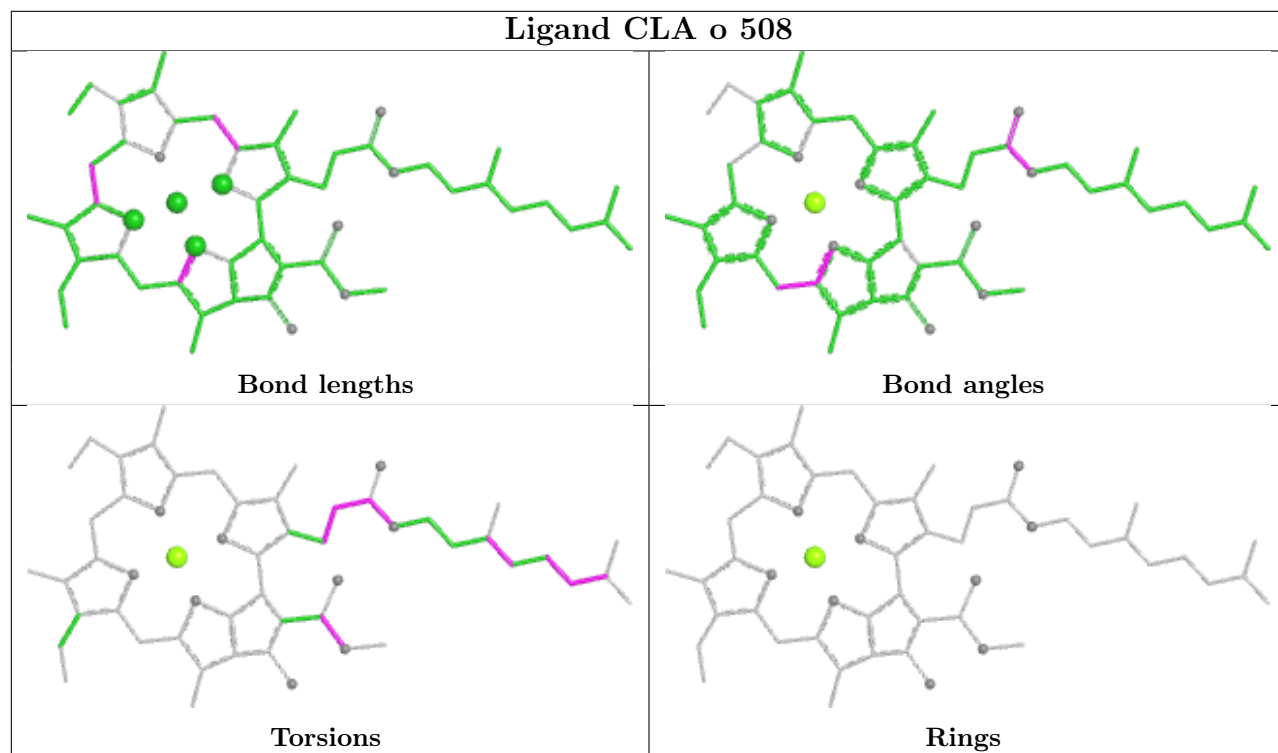






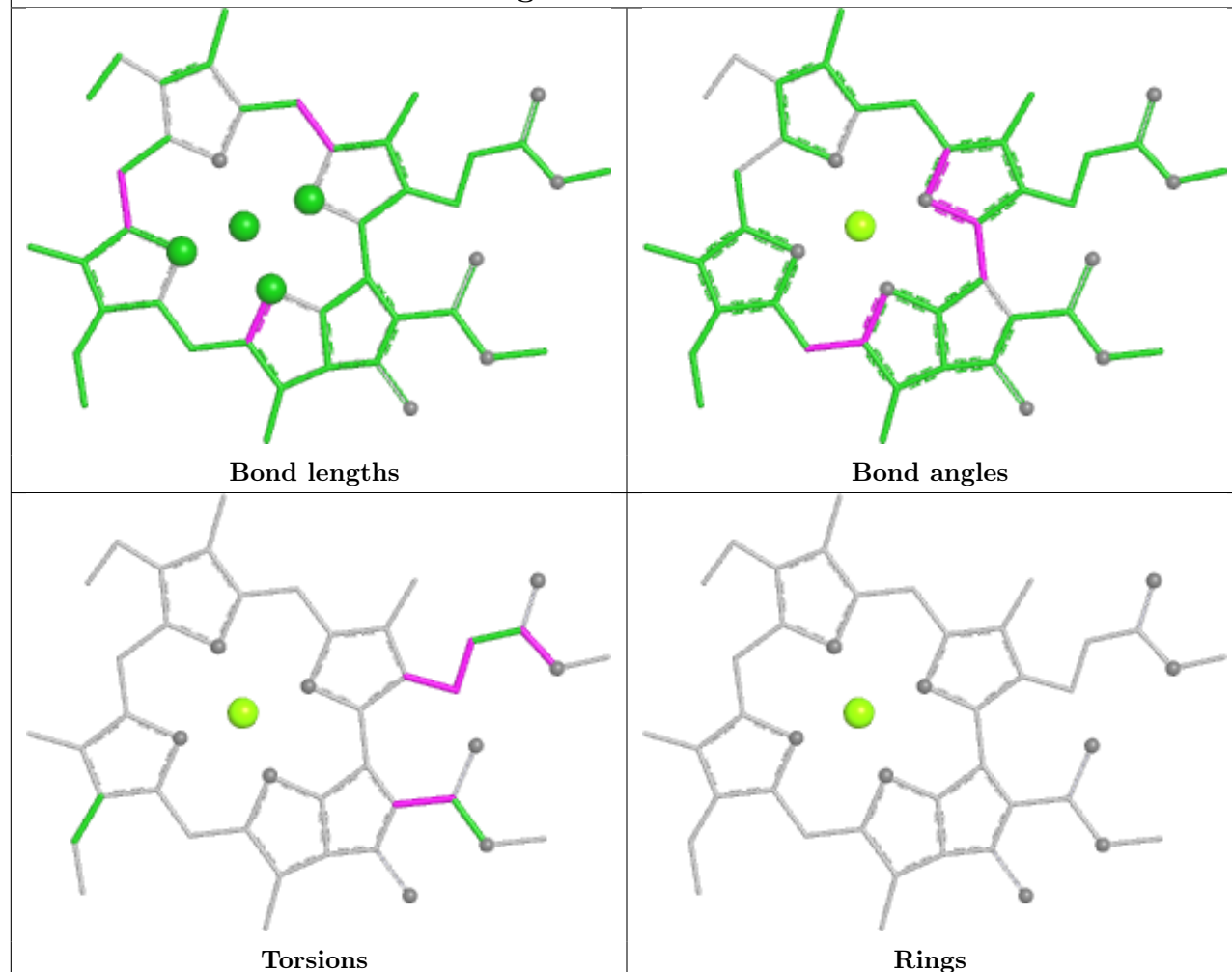




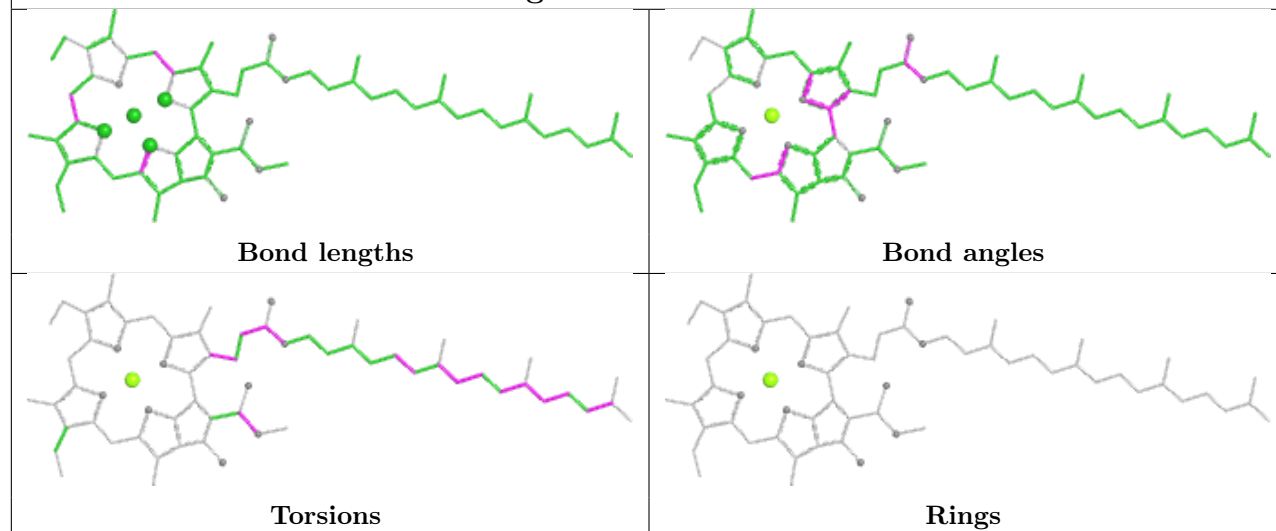




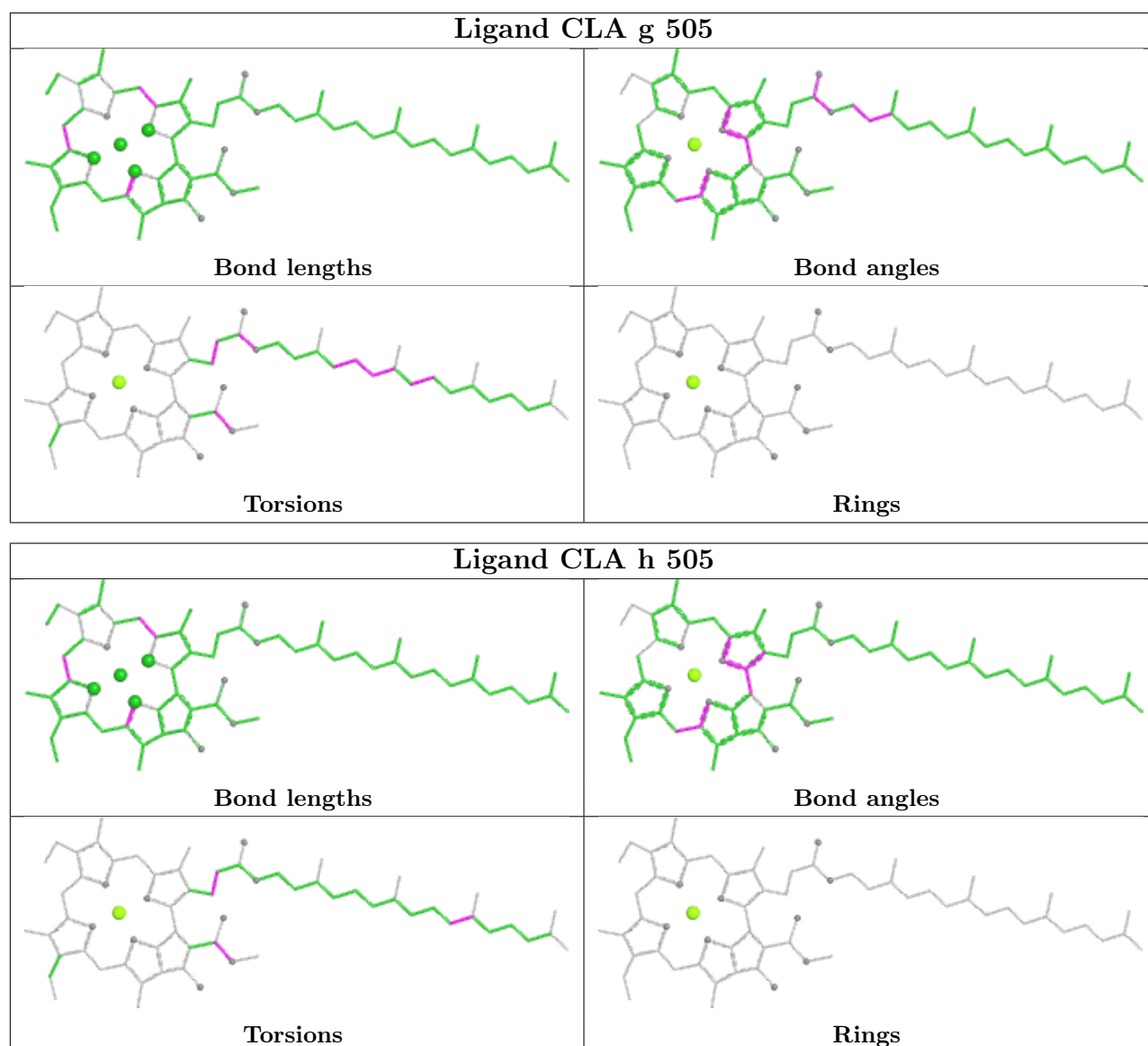
## Ligand CLA v 503



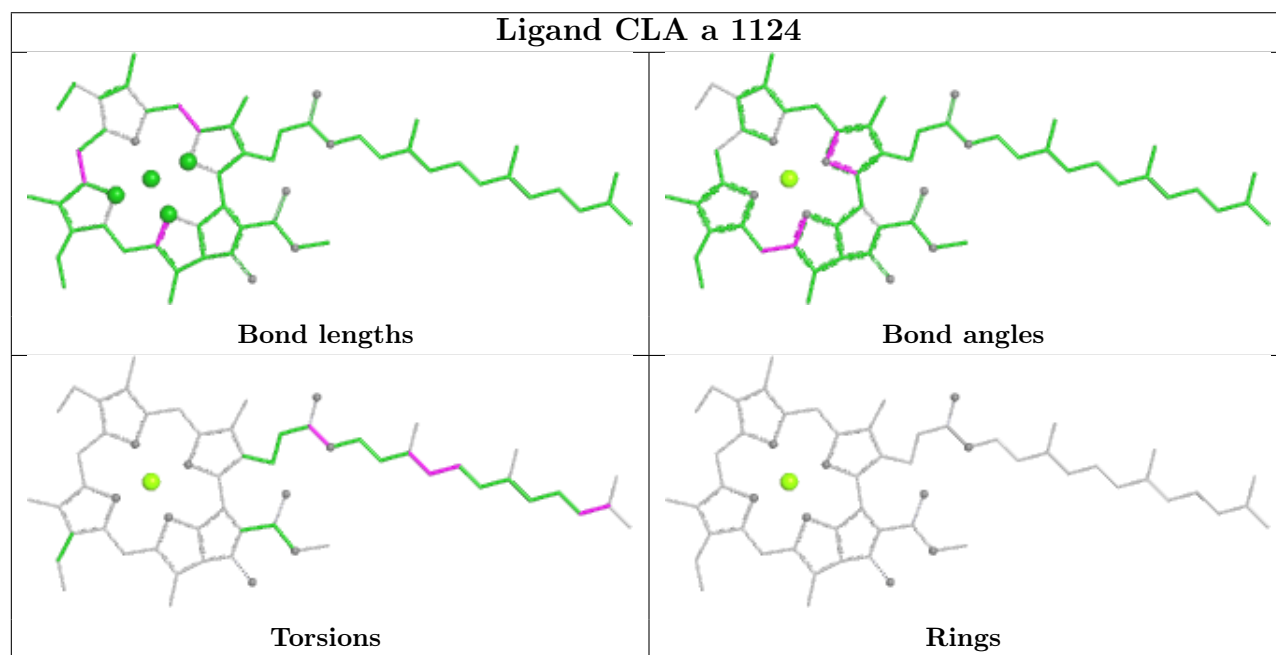
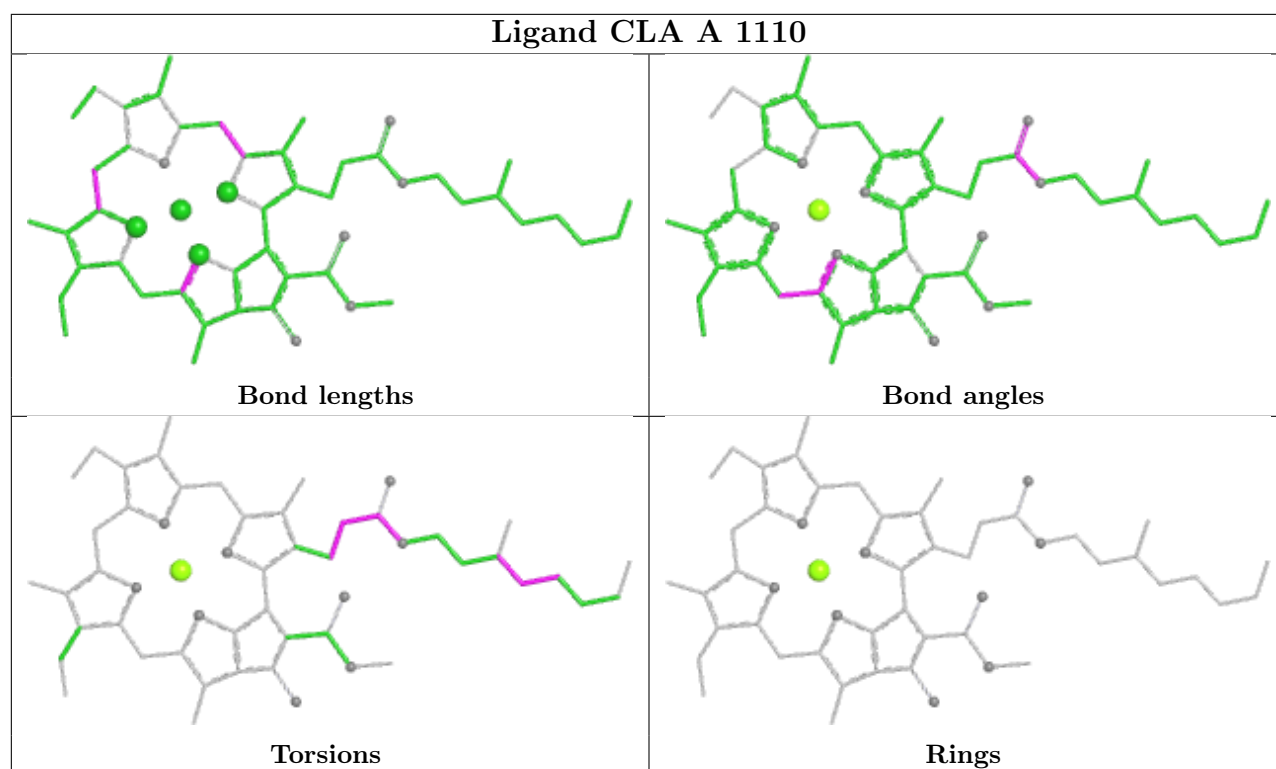
## Ligand CLA b 1021



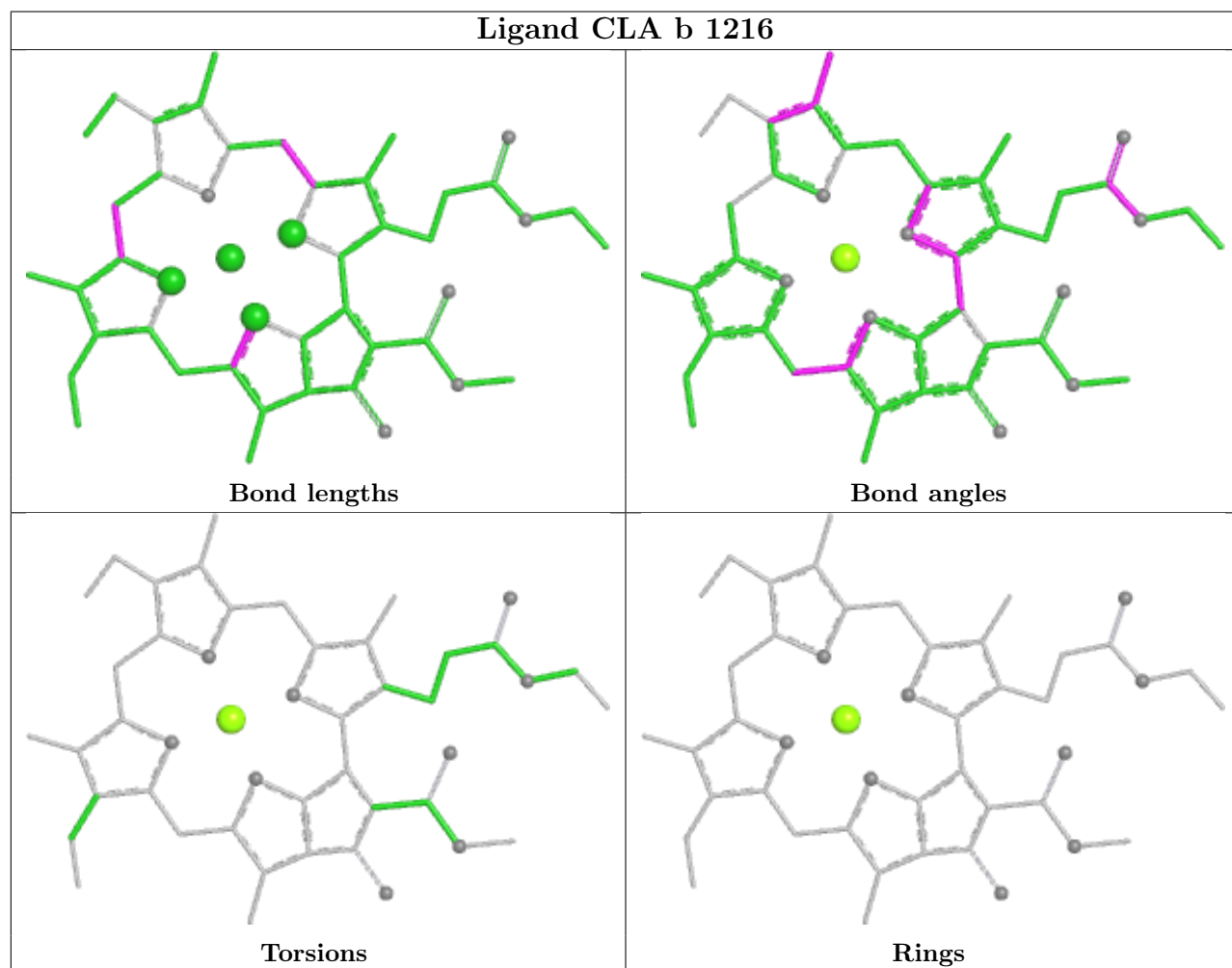
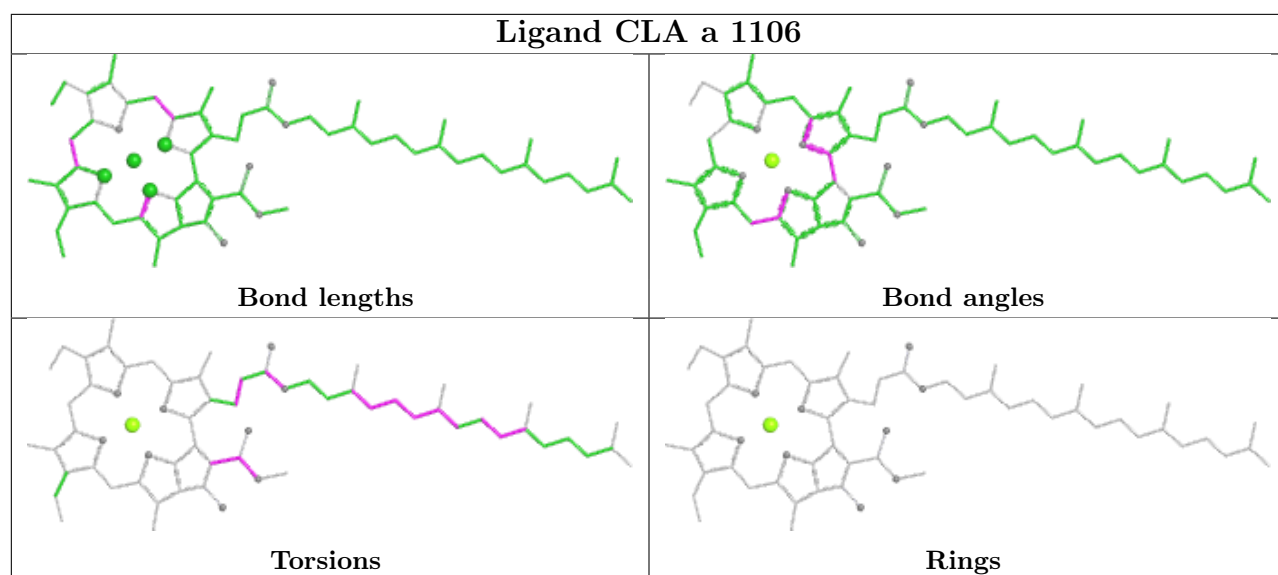




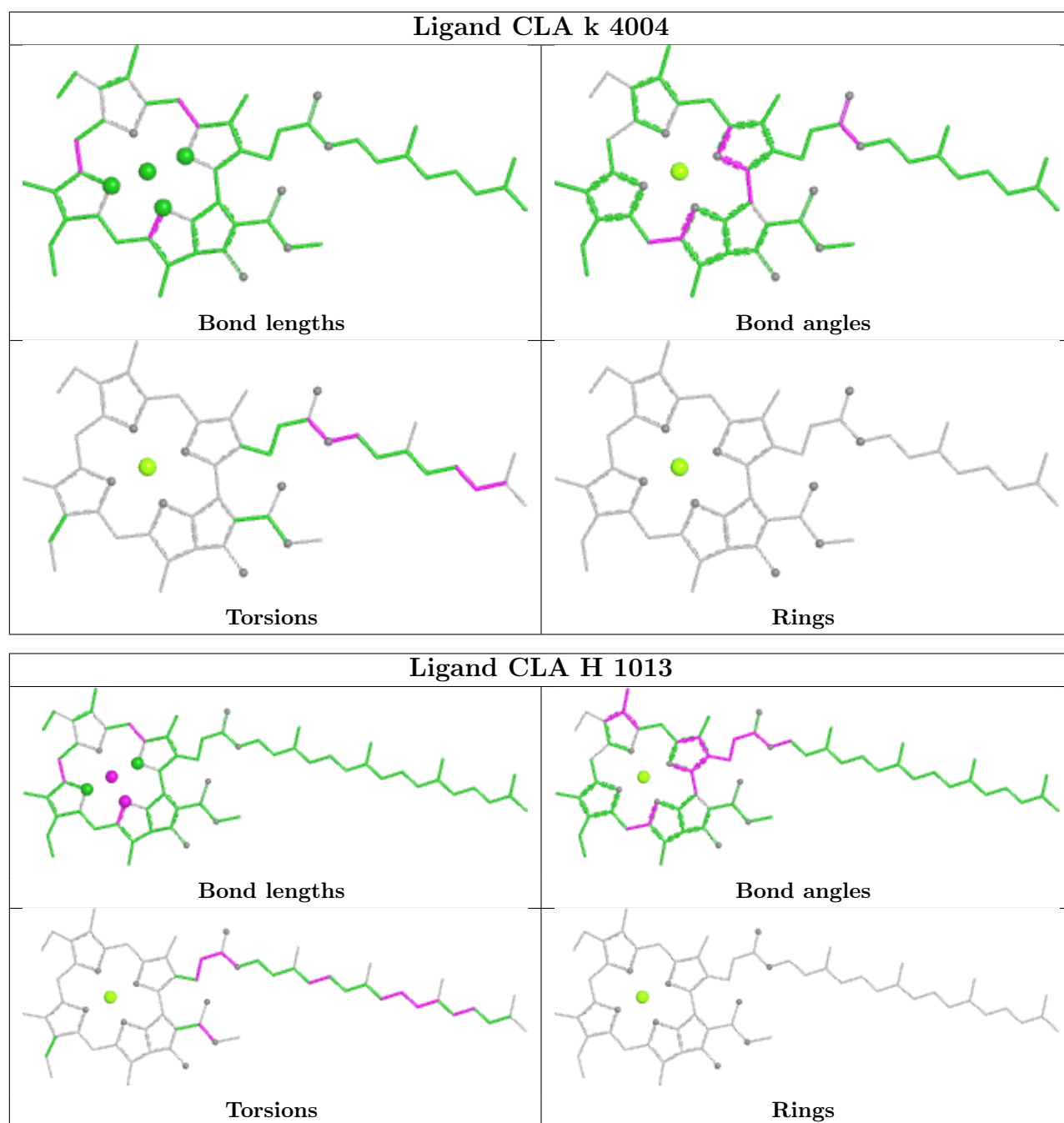




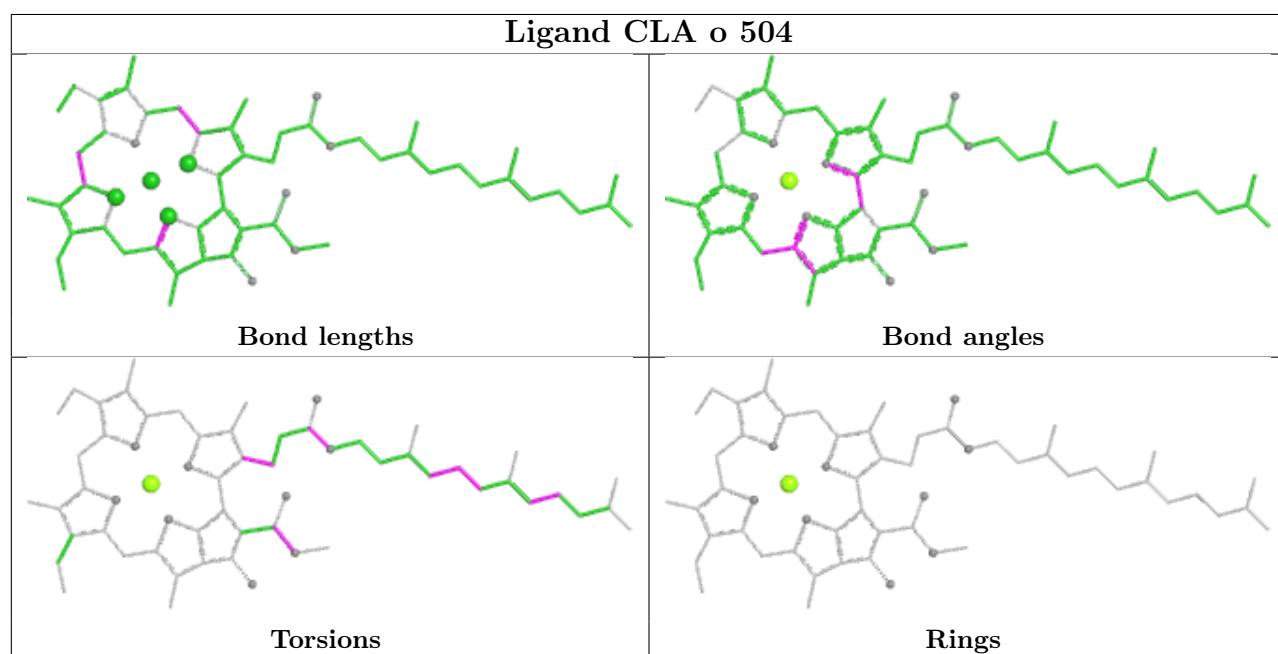
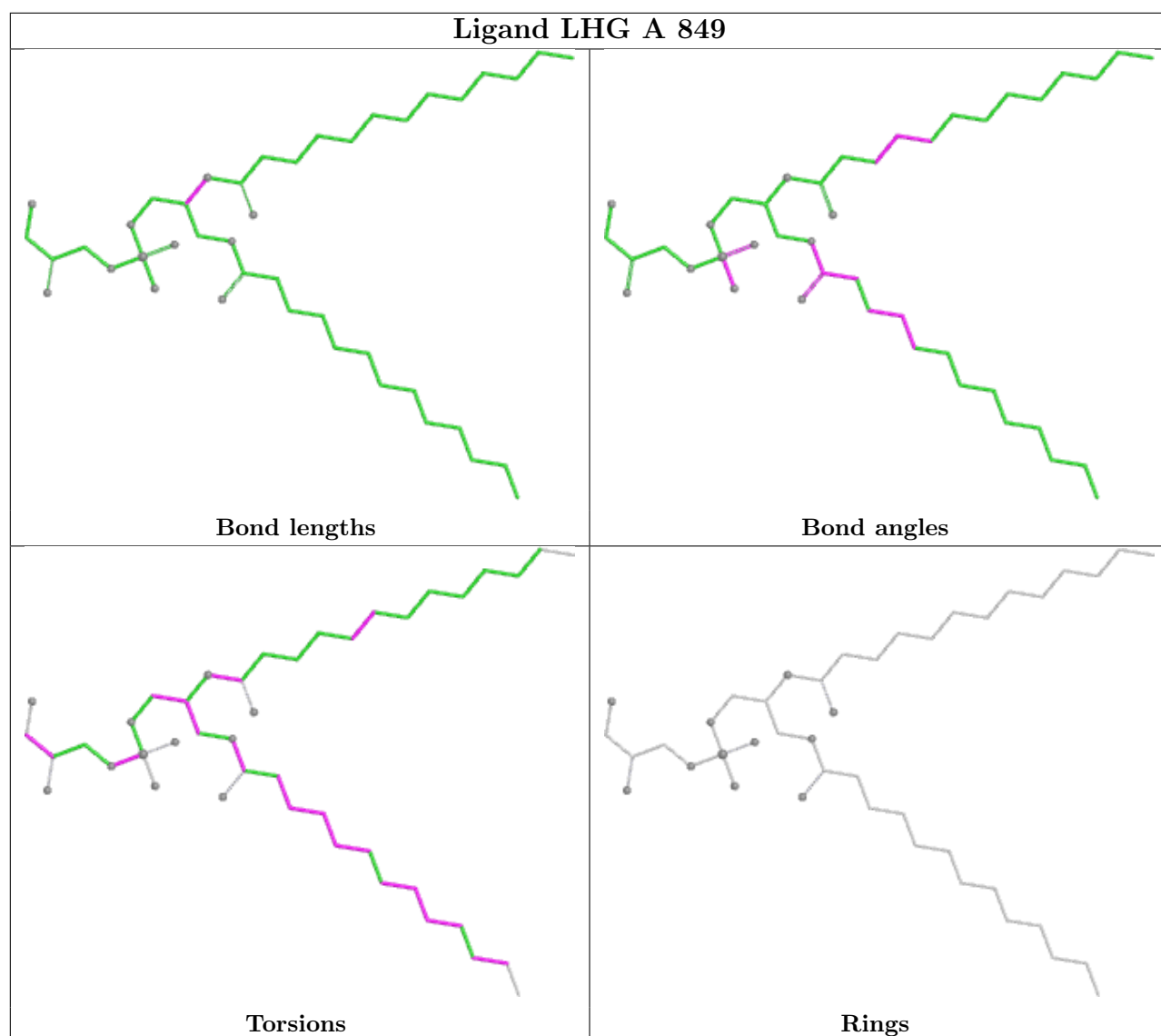




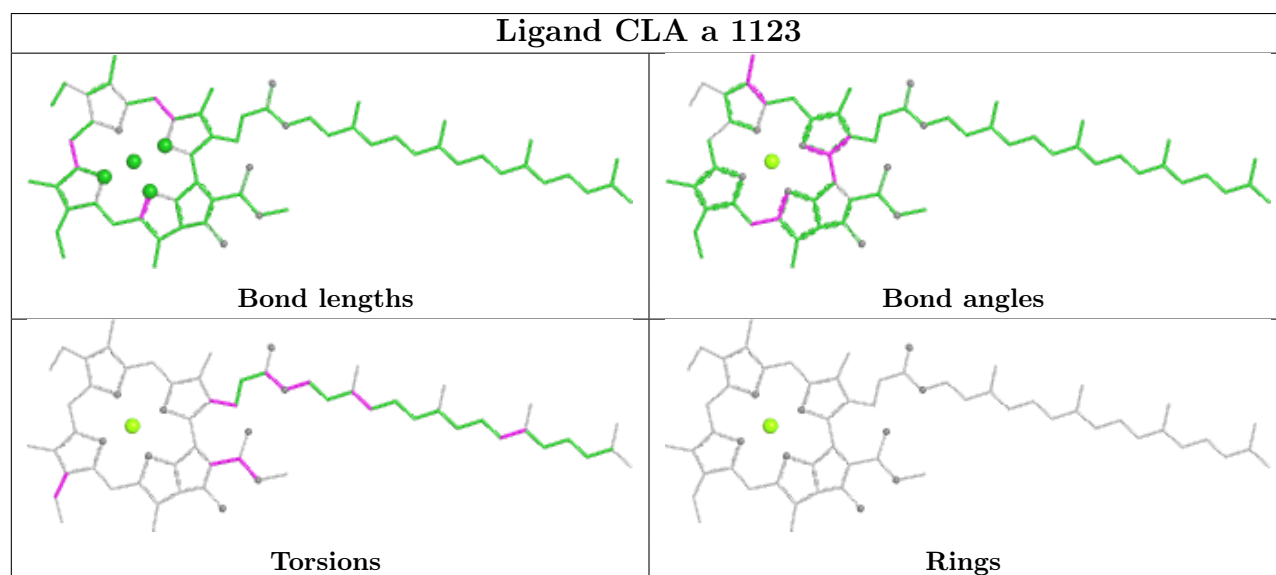
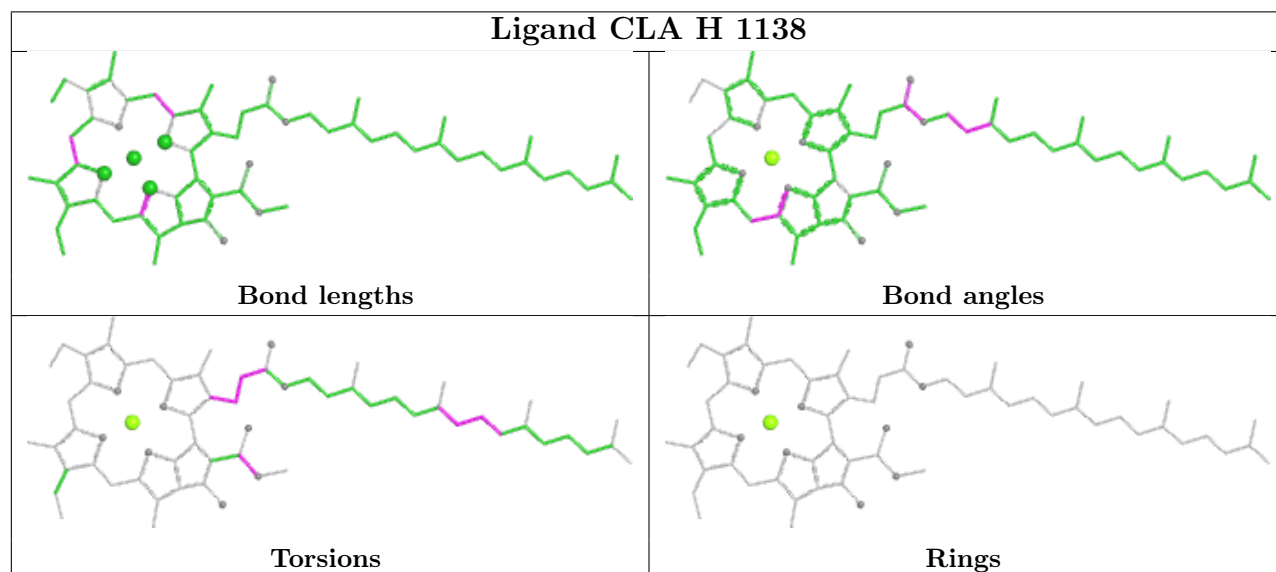
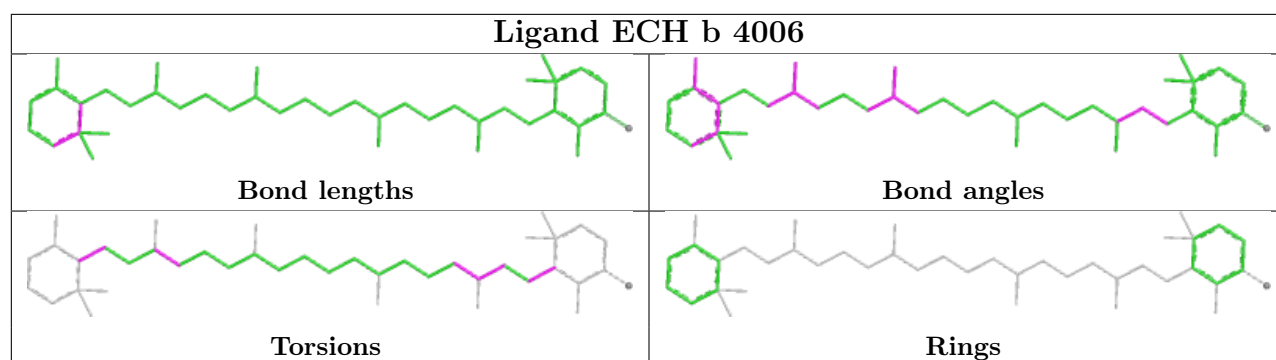






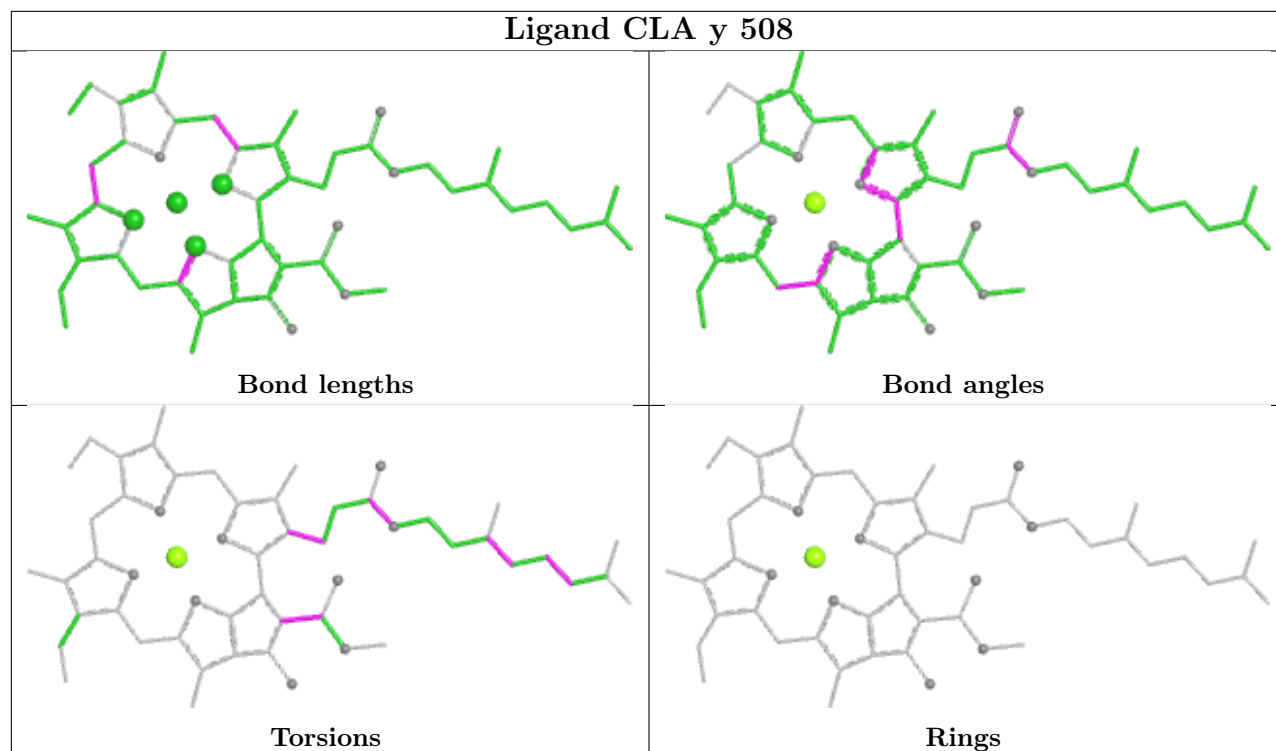




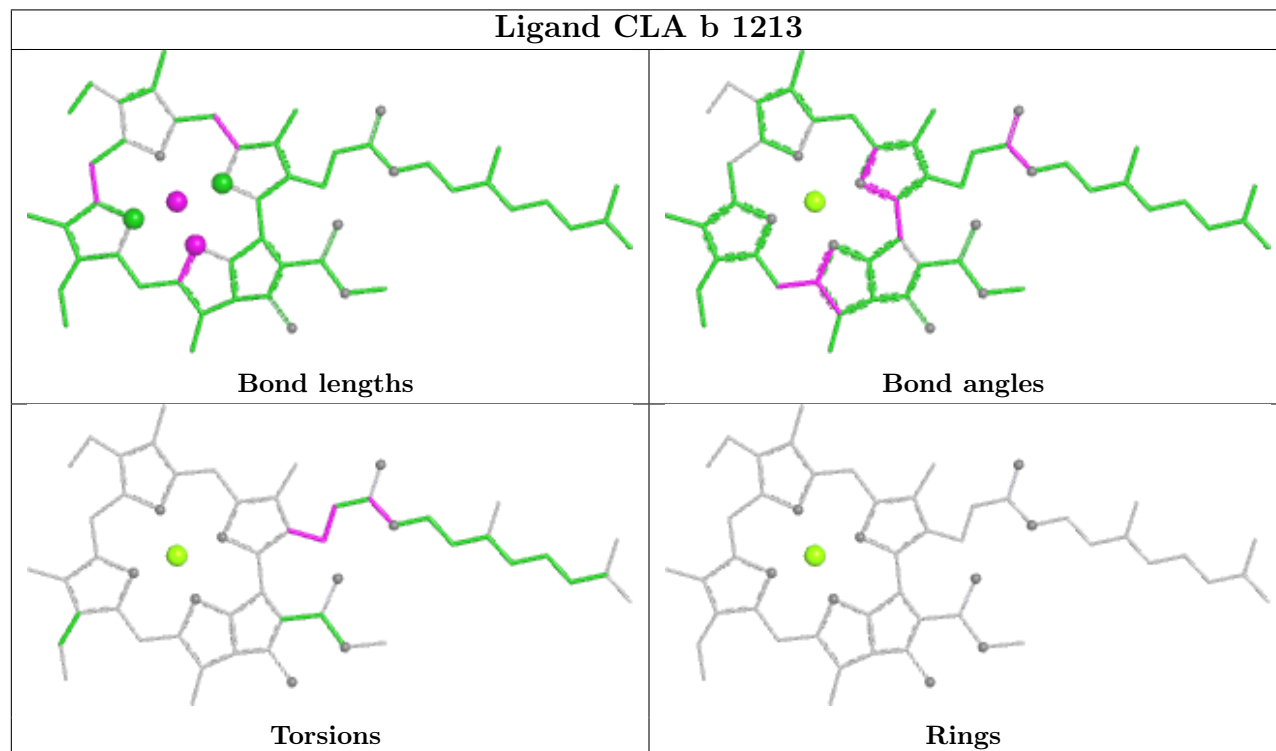




## Ligand CLA y 508

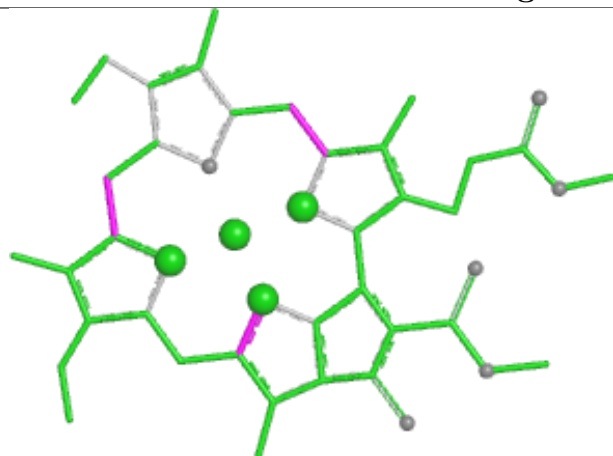


## Ligand CLA b 1213

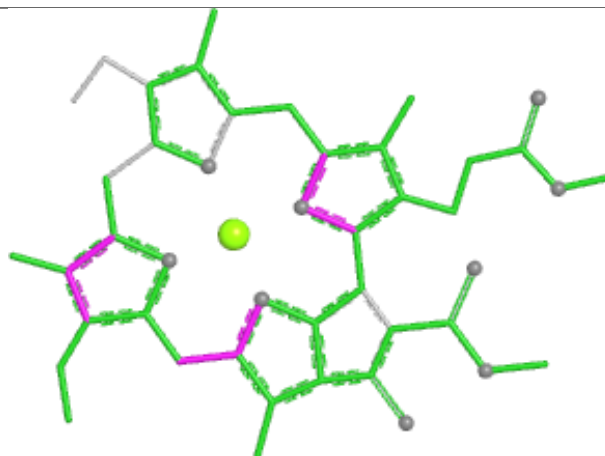




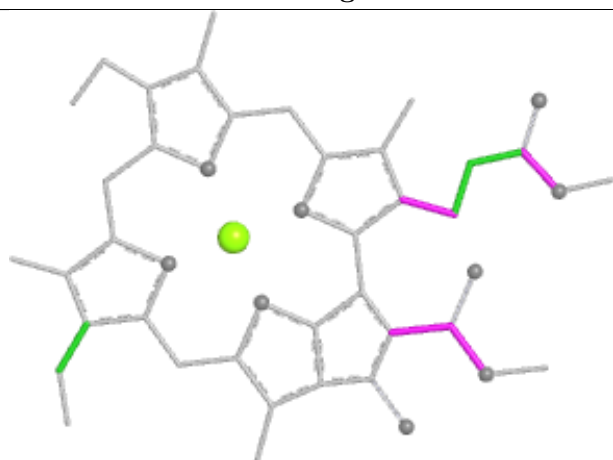
## Ligand CLA n 513



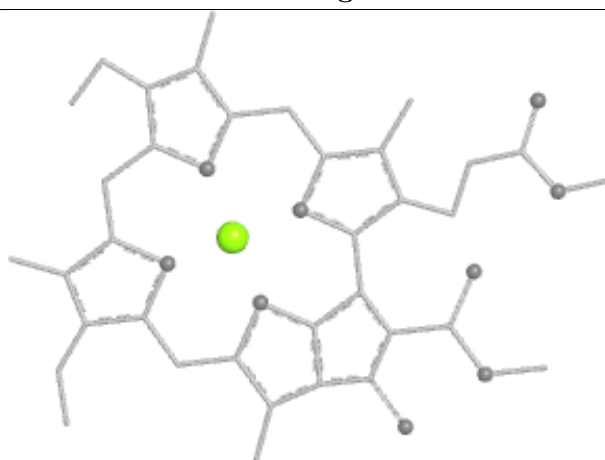
Bond lengths



Bond angles

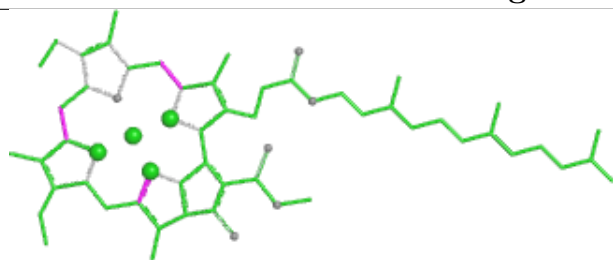


Torsions

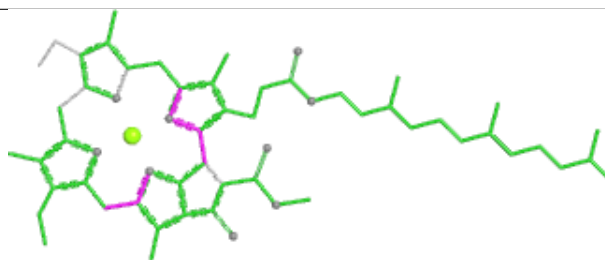


Rings

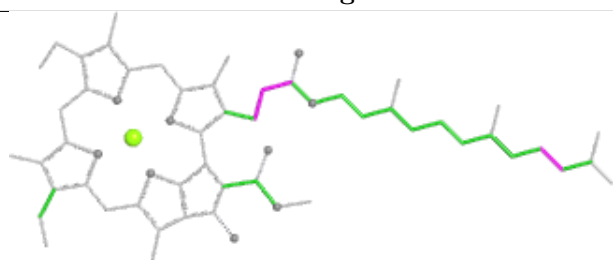
## Ligand CLA W 509



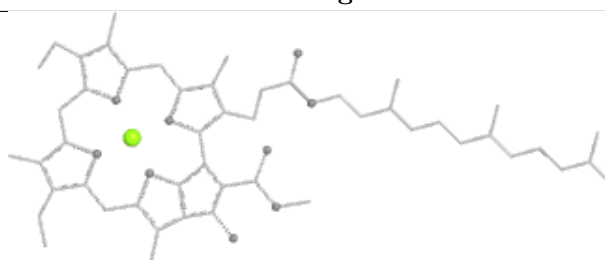
Bond lengths



Bond angles



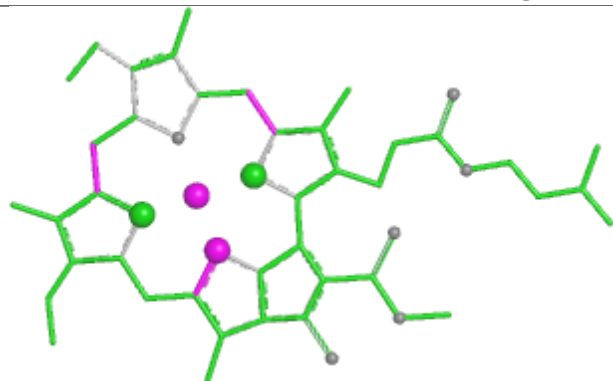
Torsions



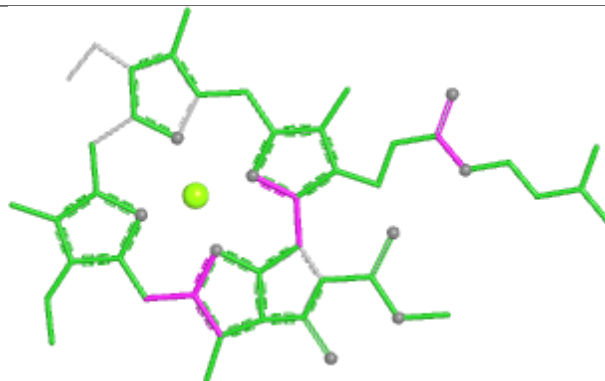
Rings



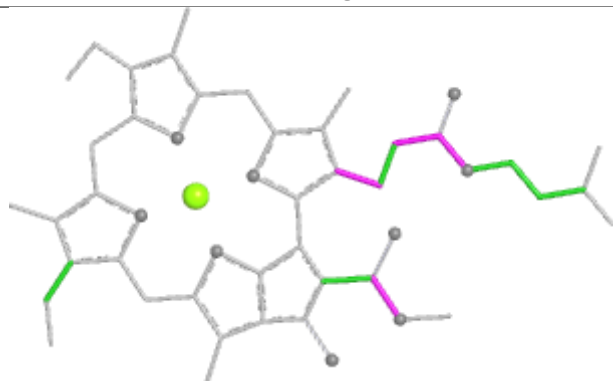
## Ligand CLA n 514



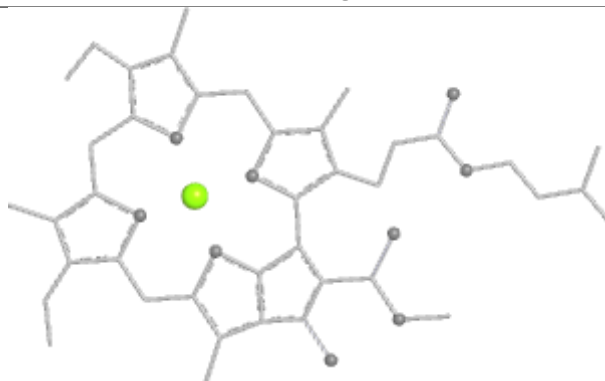
Bond lengths



Bond angles

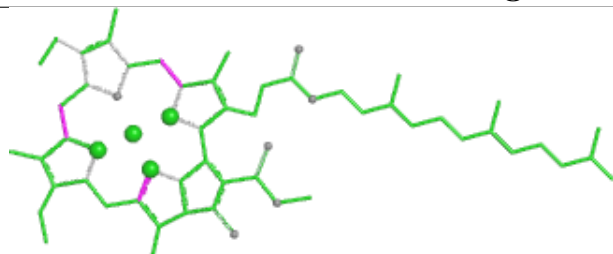


Torsions

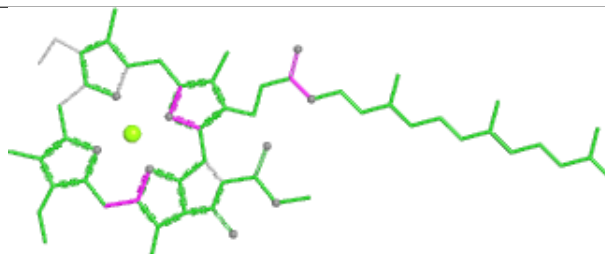


Rings

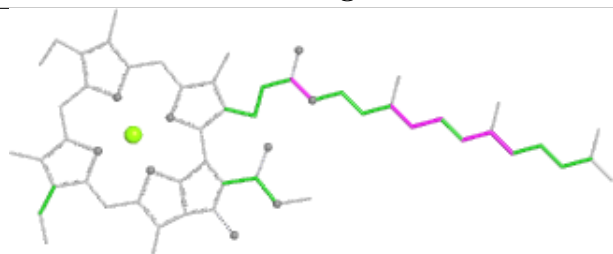
## Ligand CLA U 1502



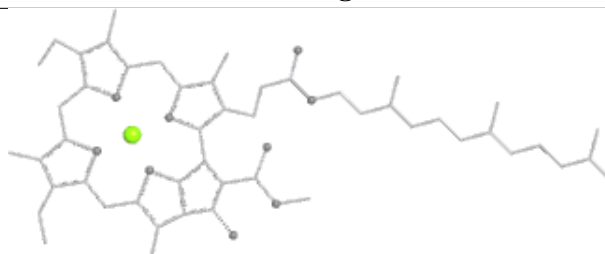
Bond lengths



Bond angles

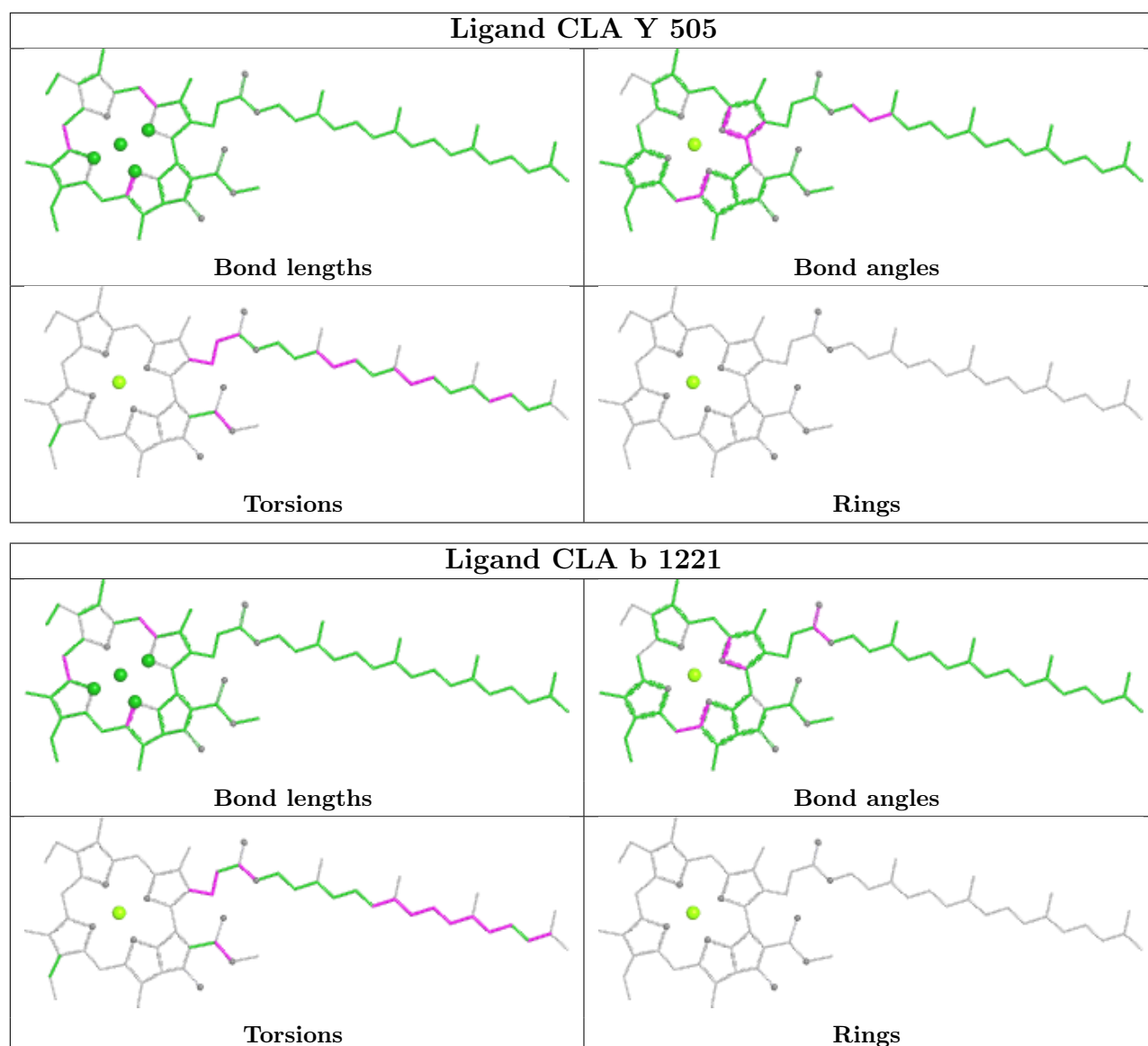


Torsions

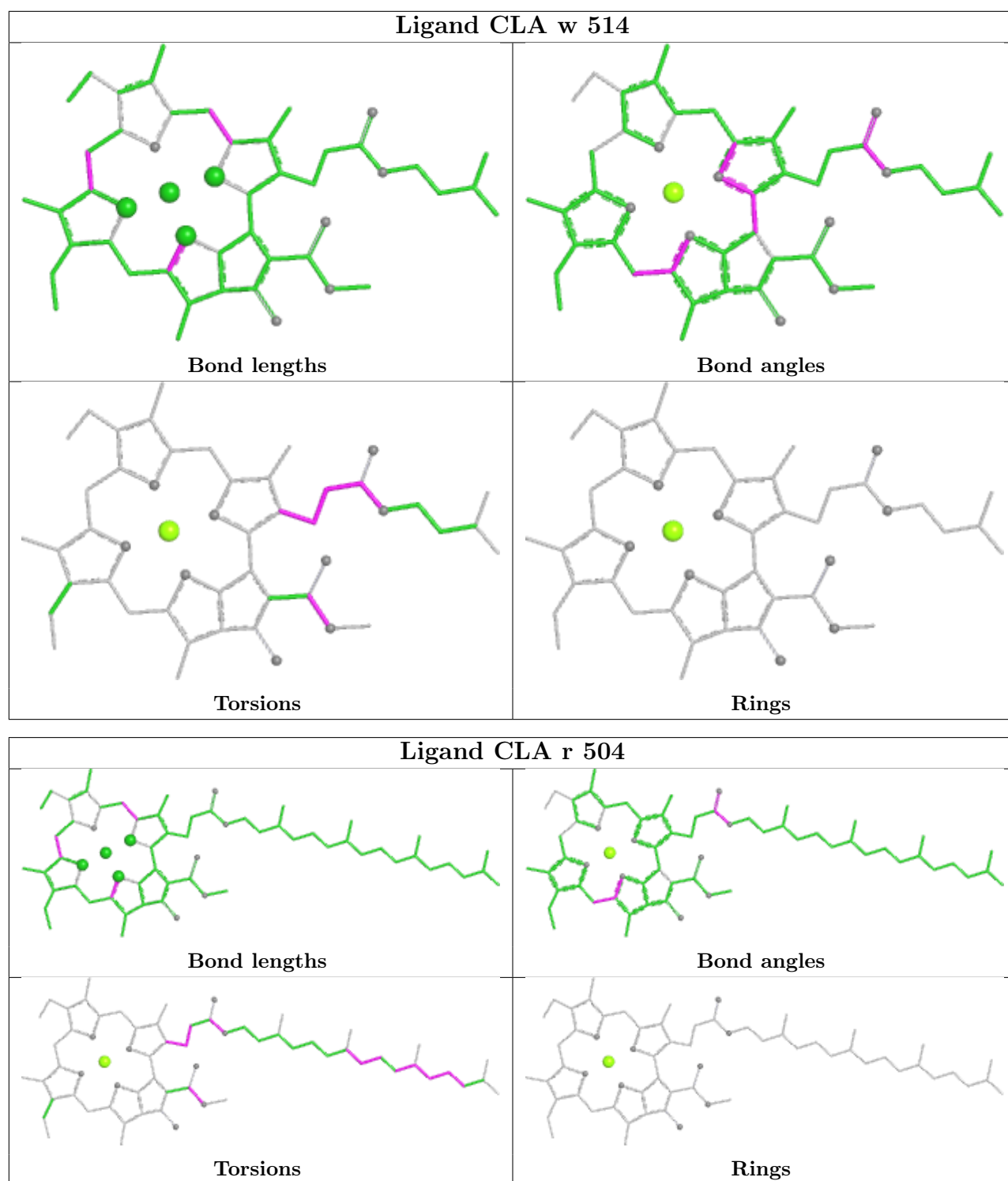


Rings

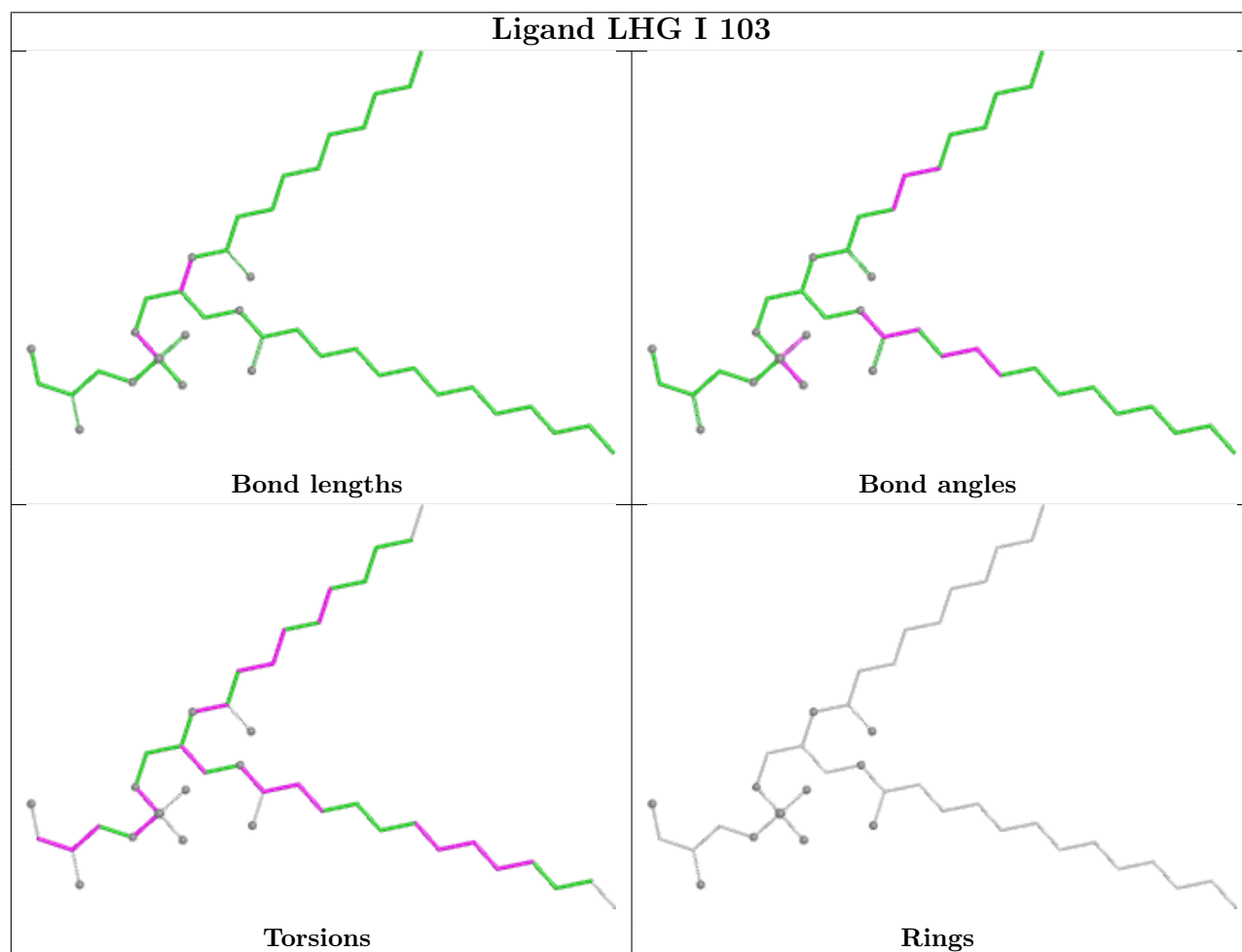
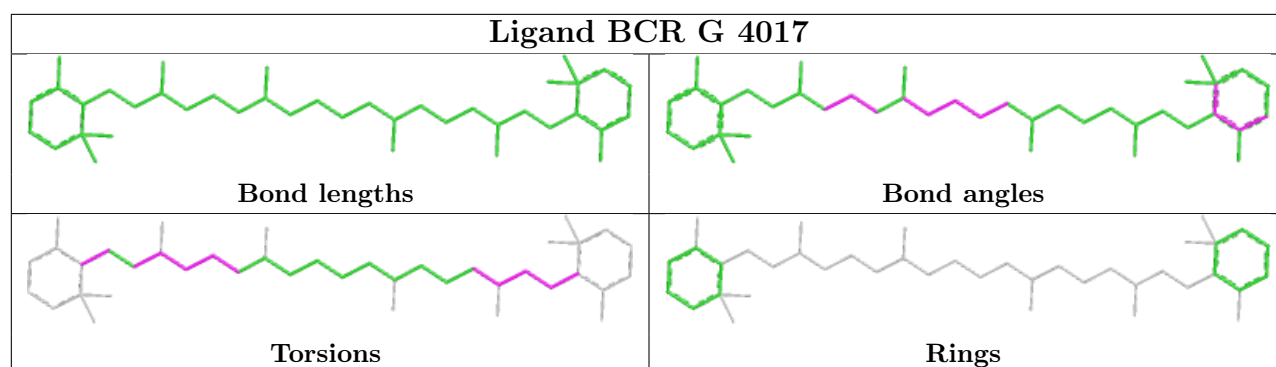




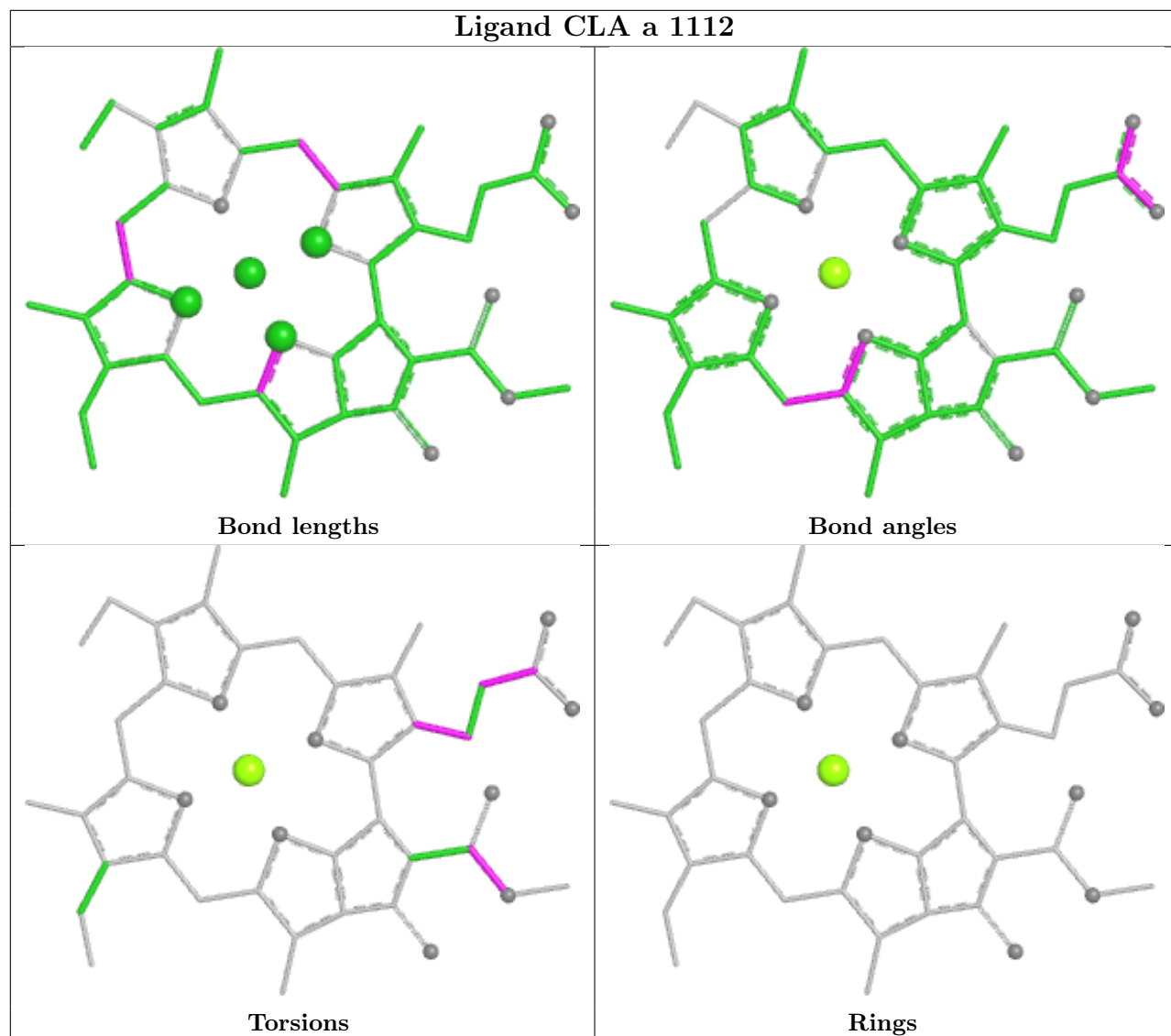






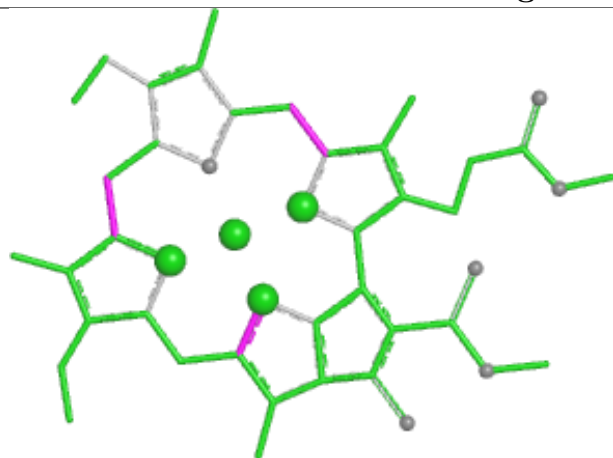




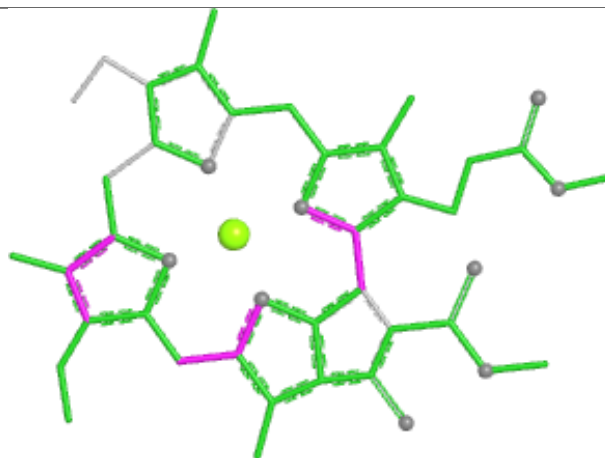




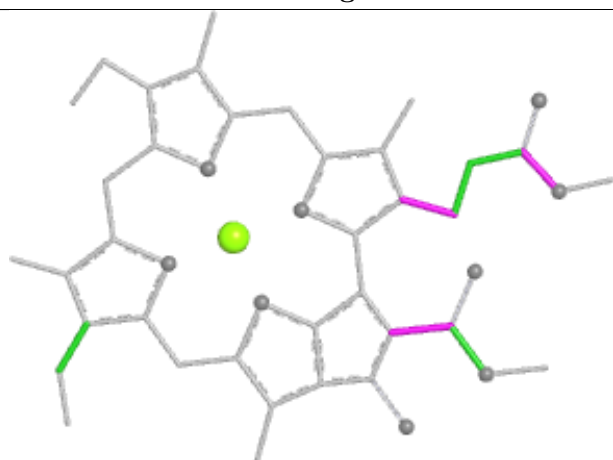
## Ligand CLA h 516



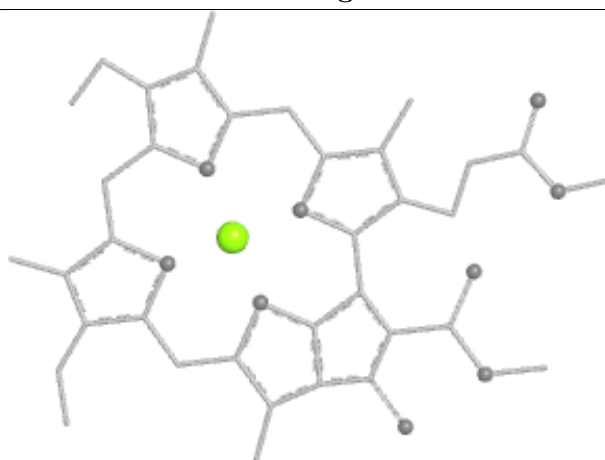
Bond lengths



Bond angles

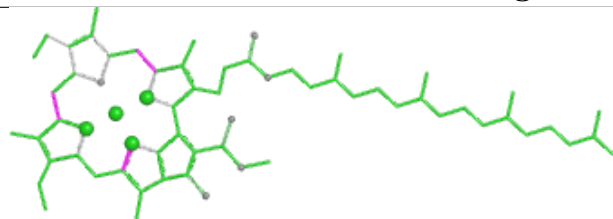


Torsions

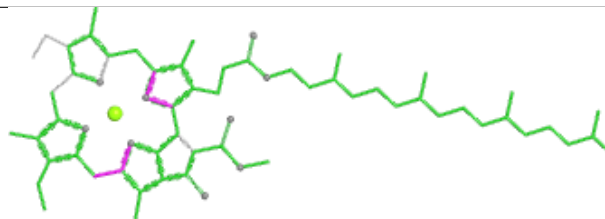


Rings

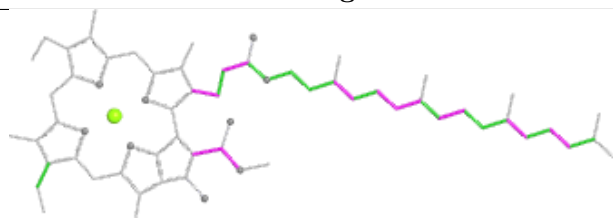
## Ligand CLA Y 504



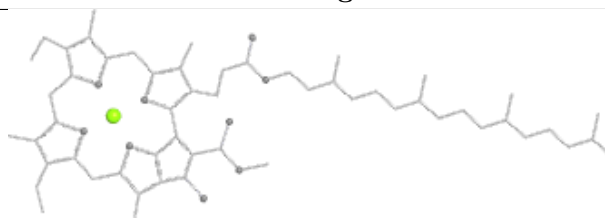
Bond lengths



Bond angles

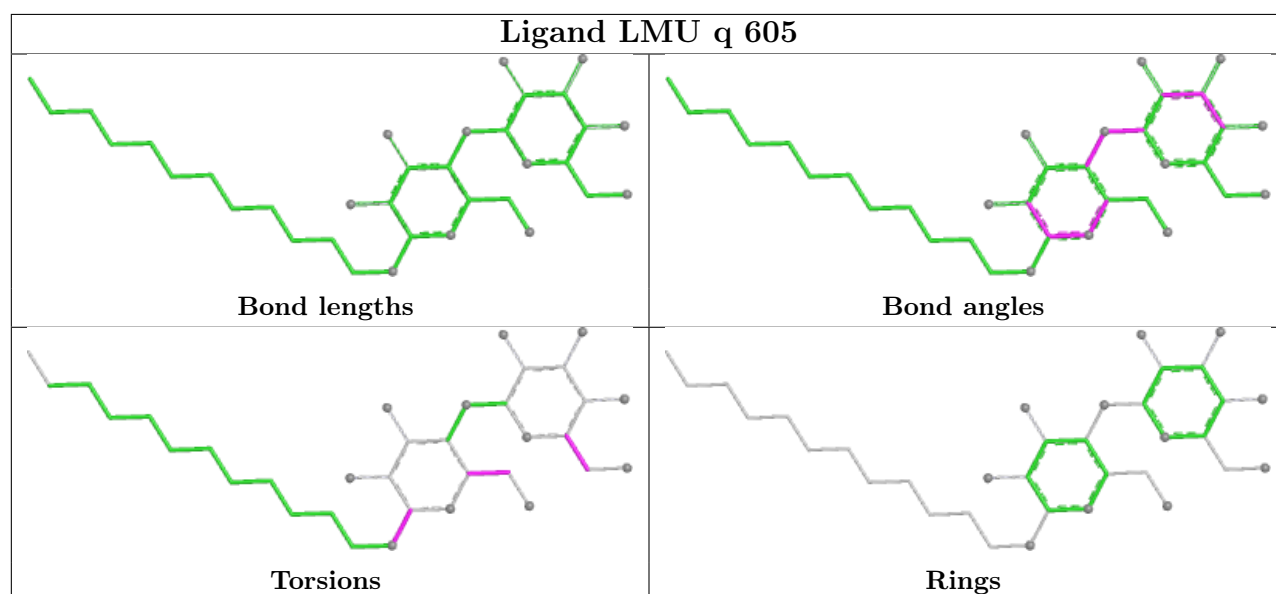
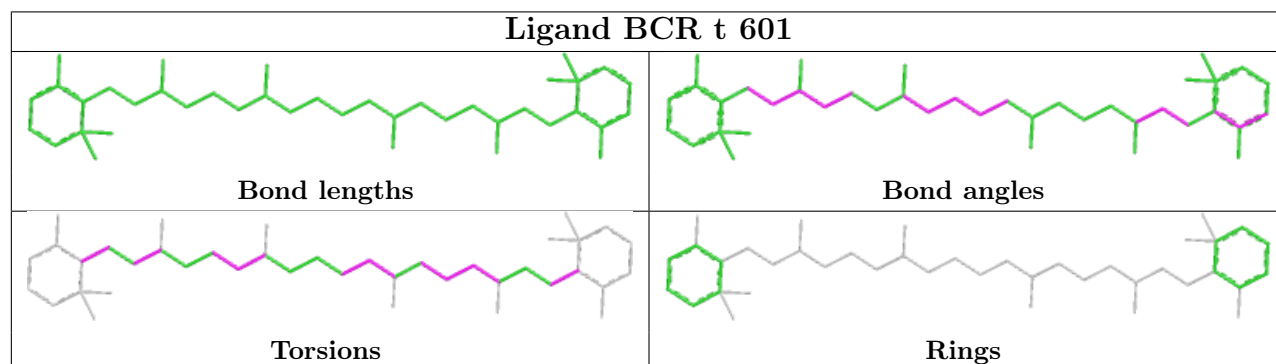
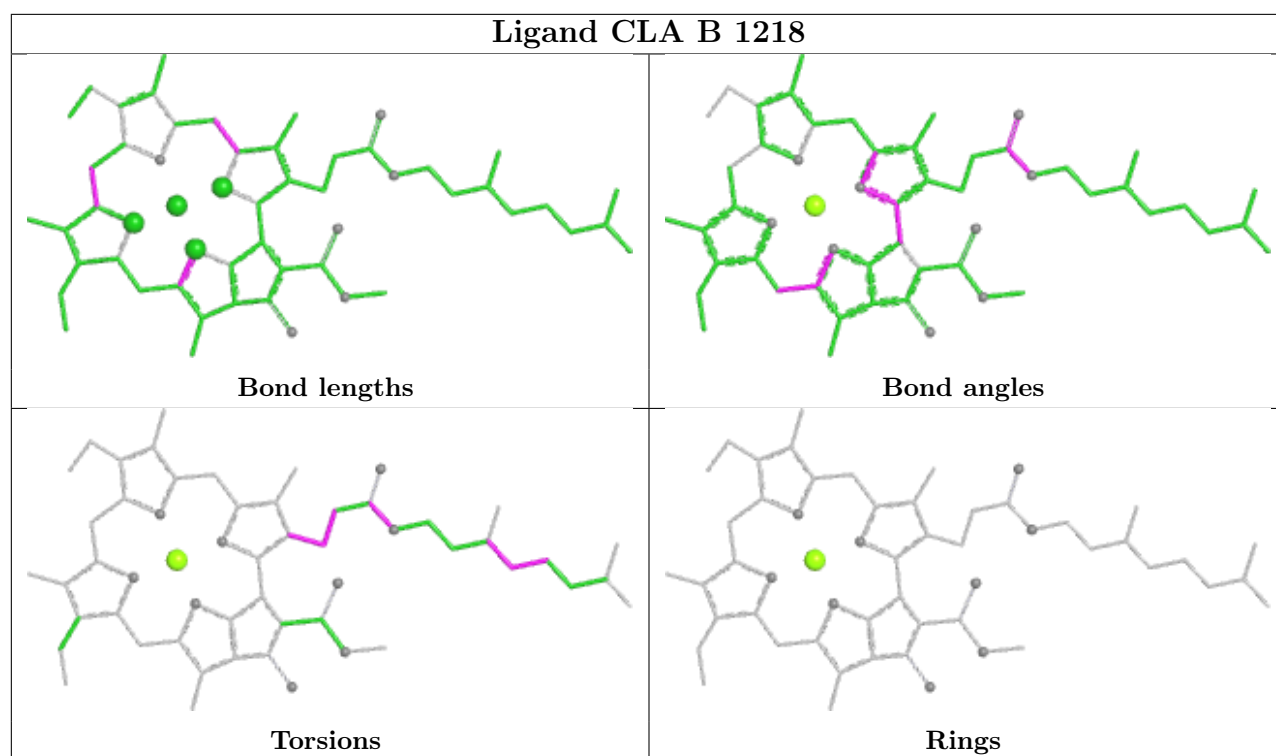


Torsions

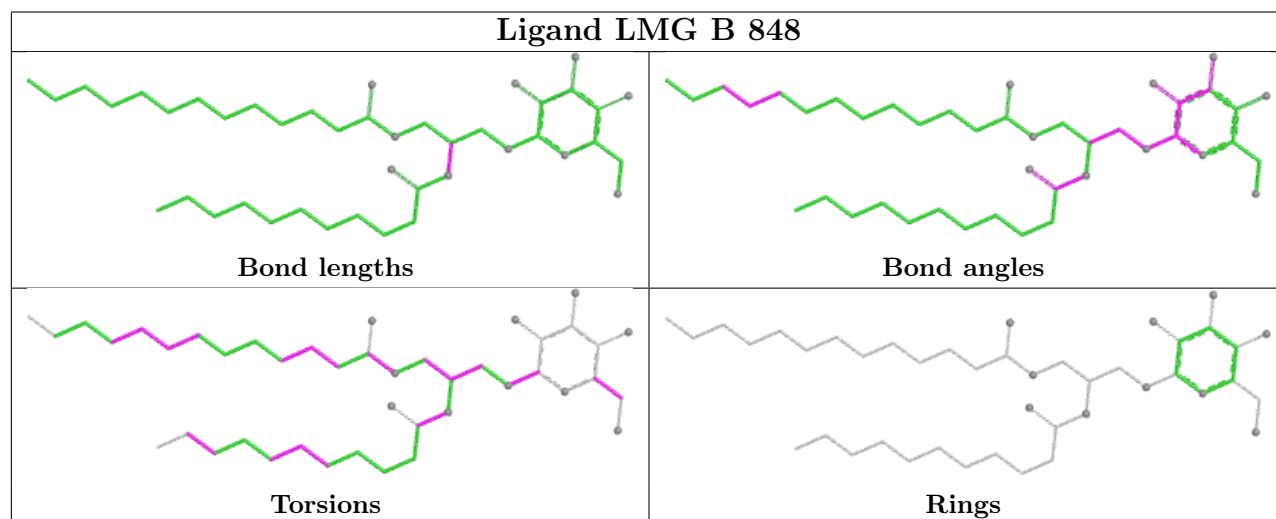
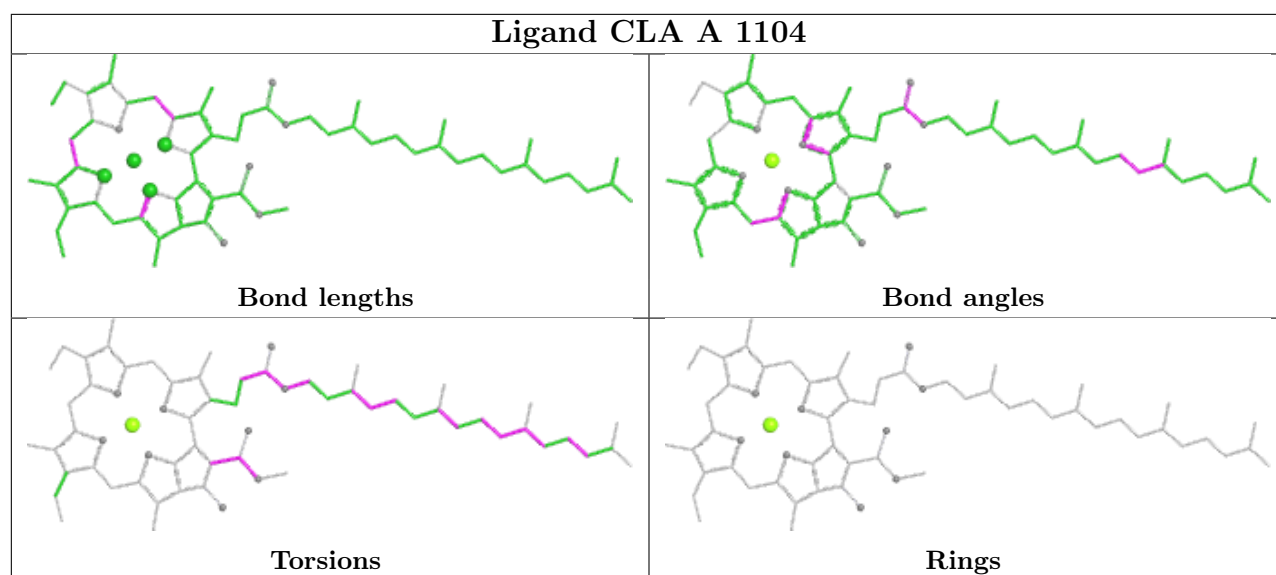


Rings

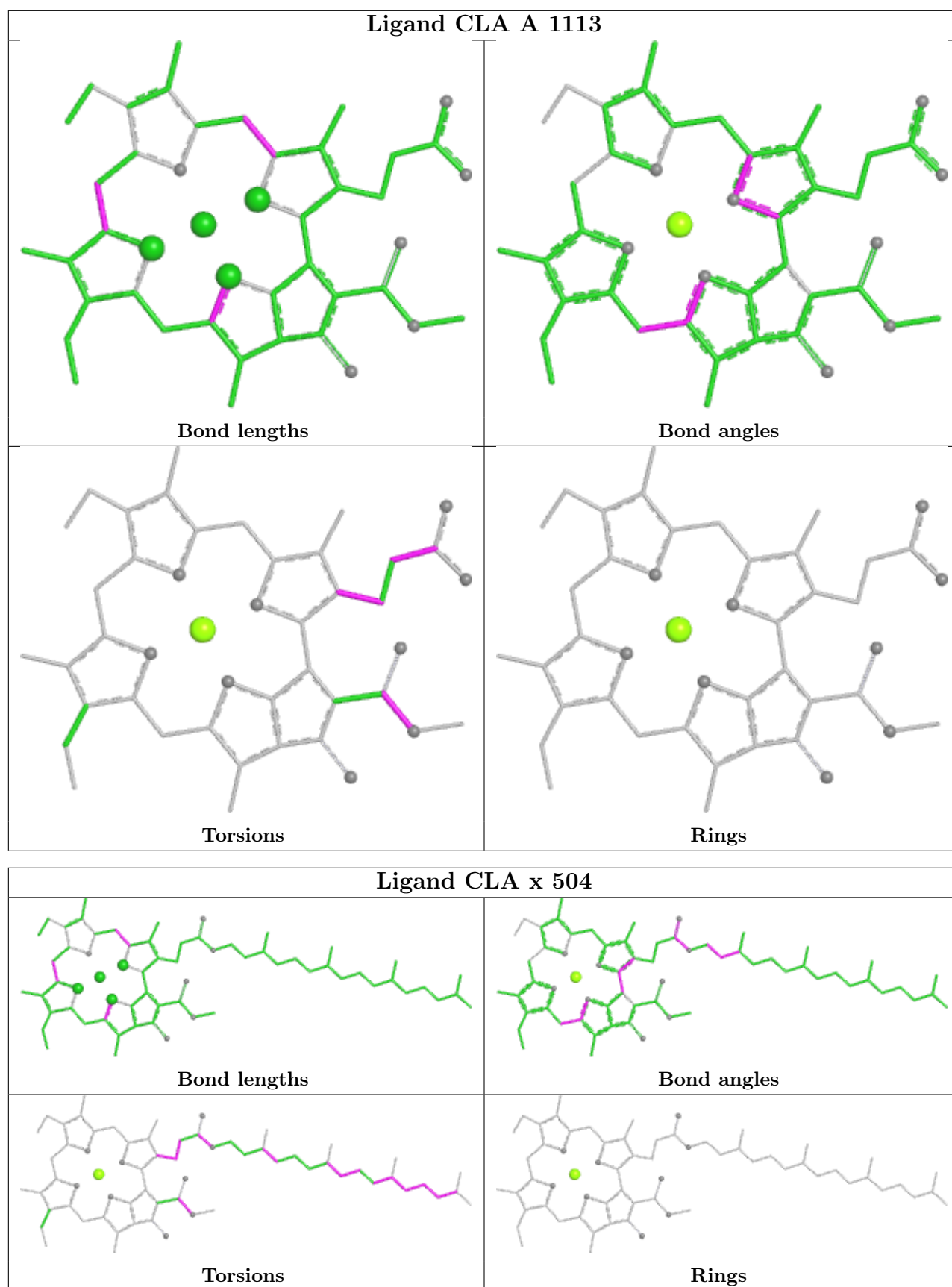




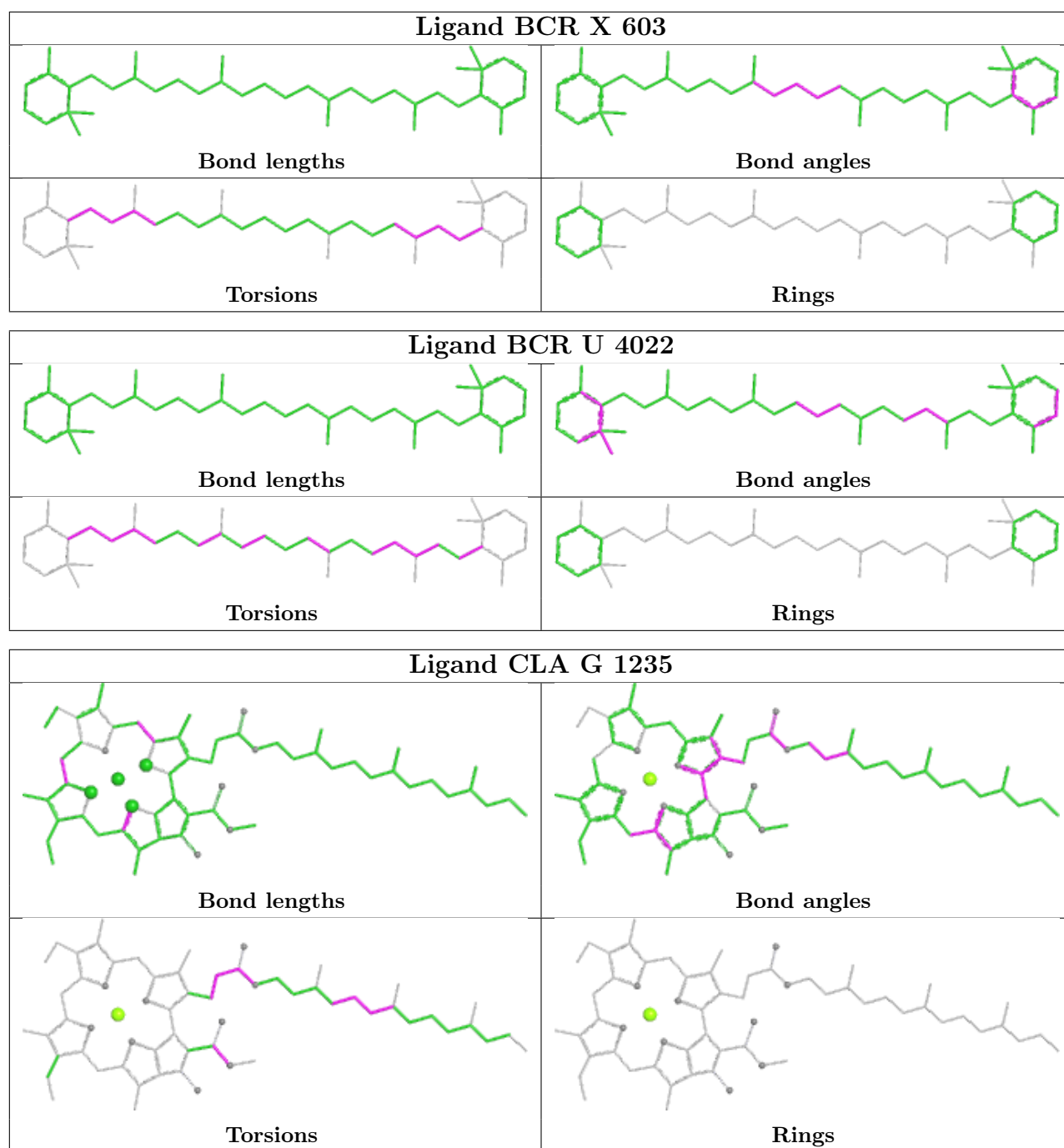




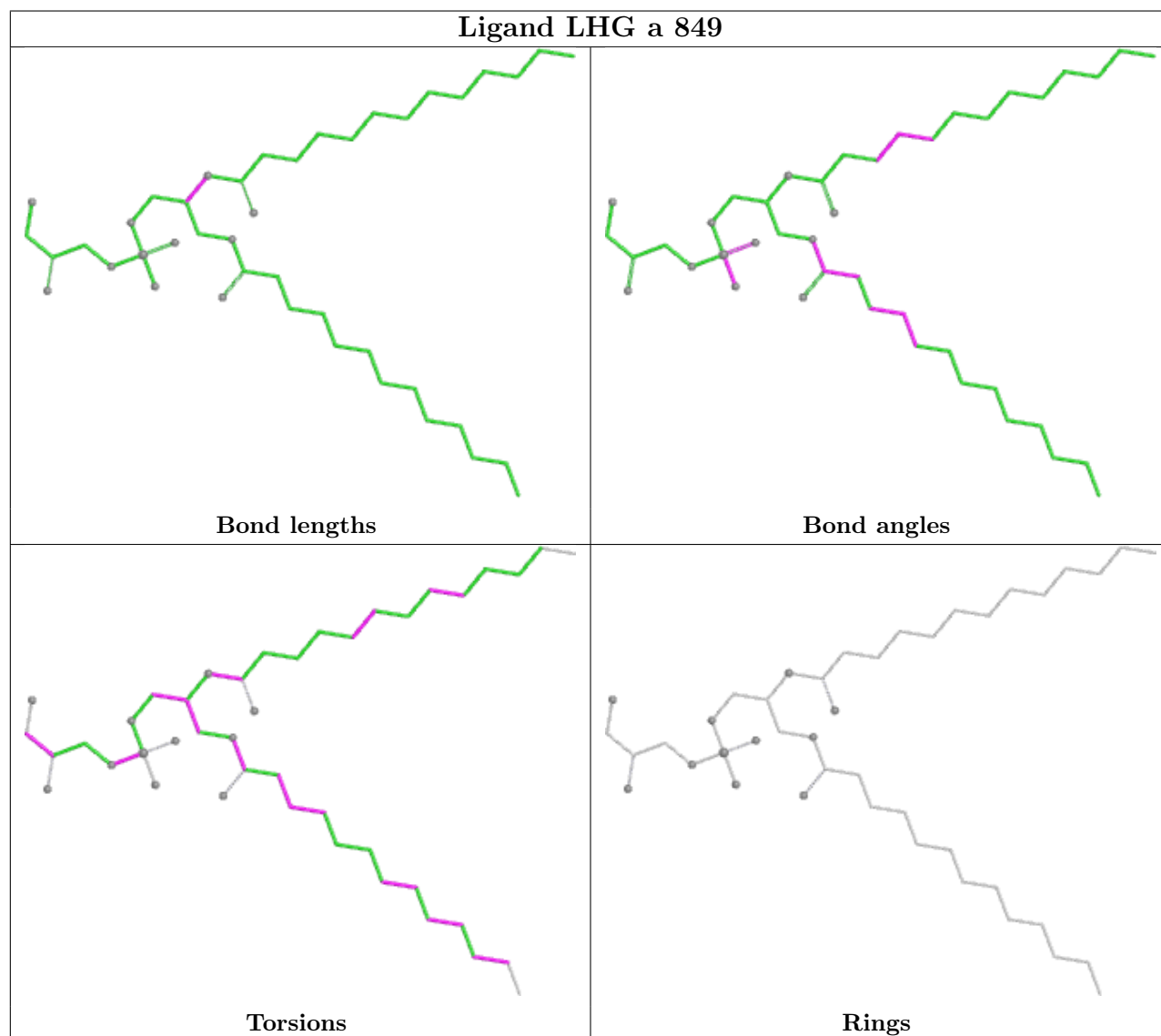
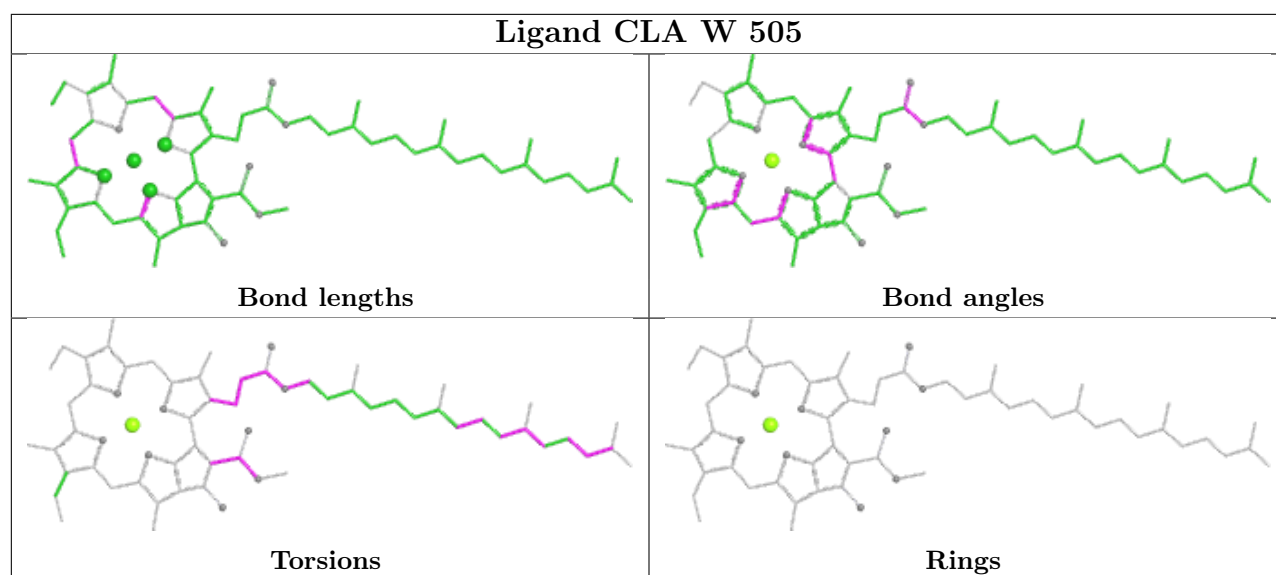




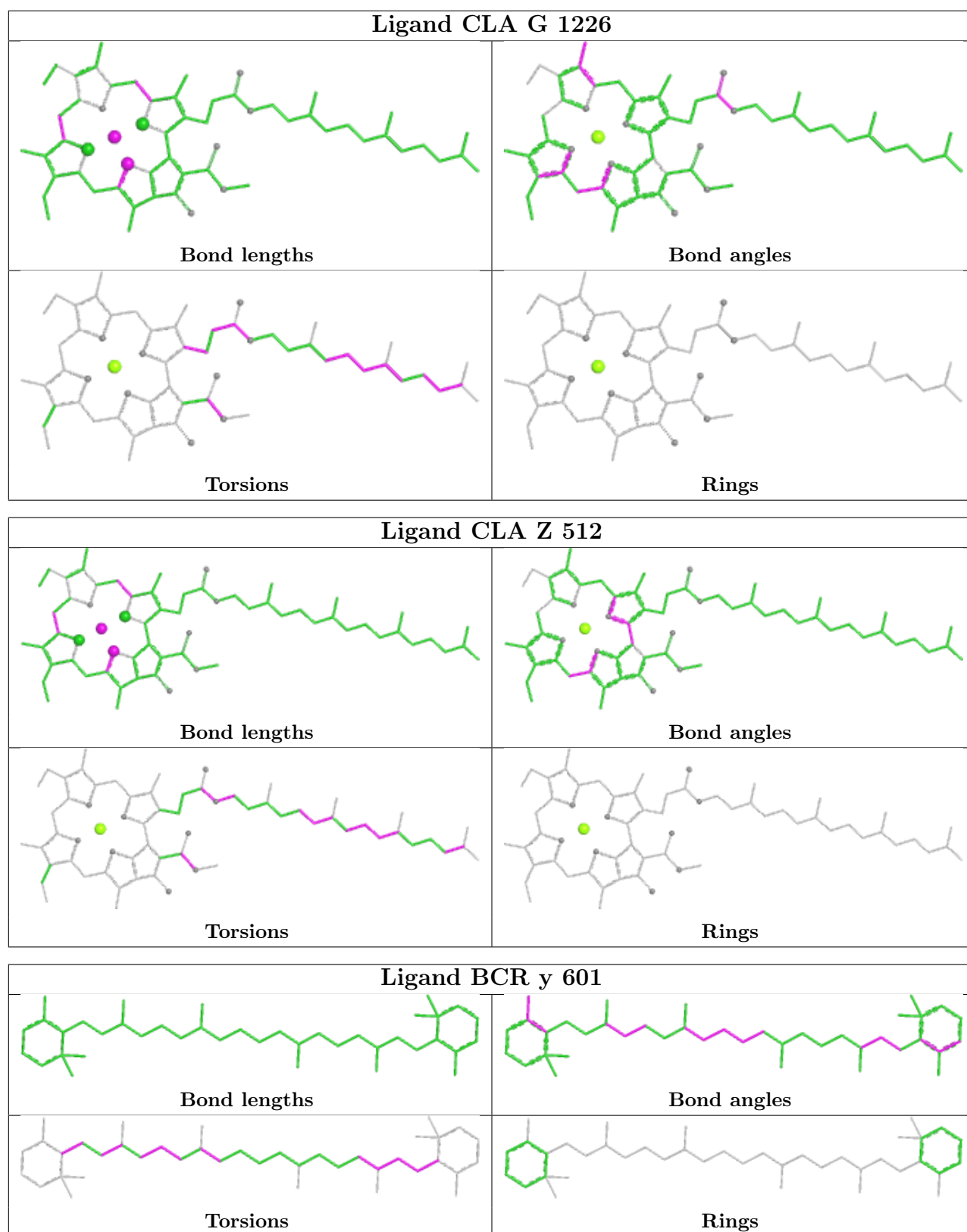




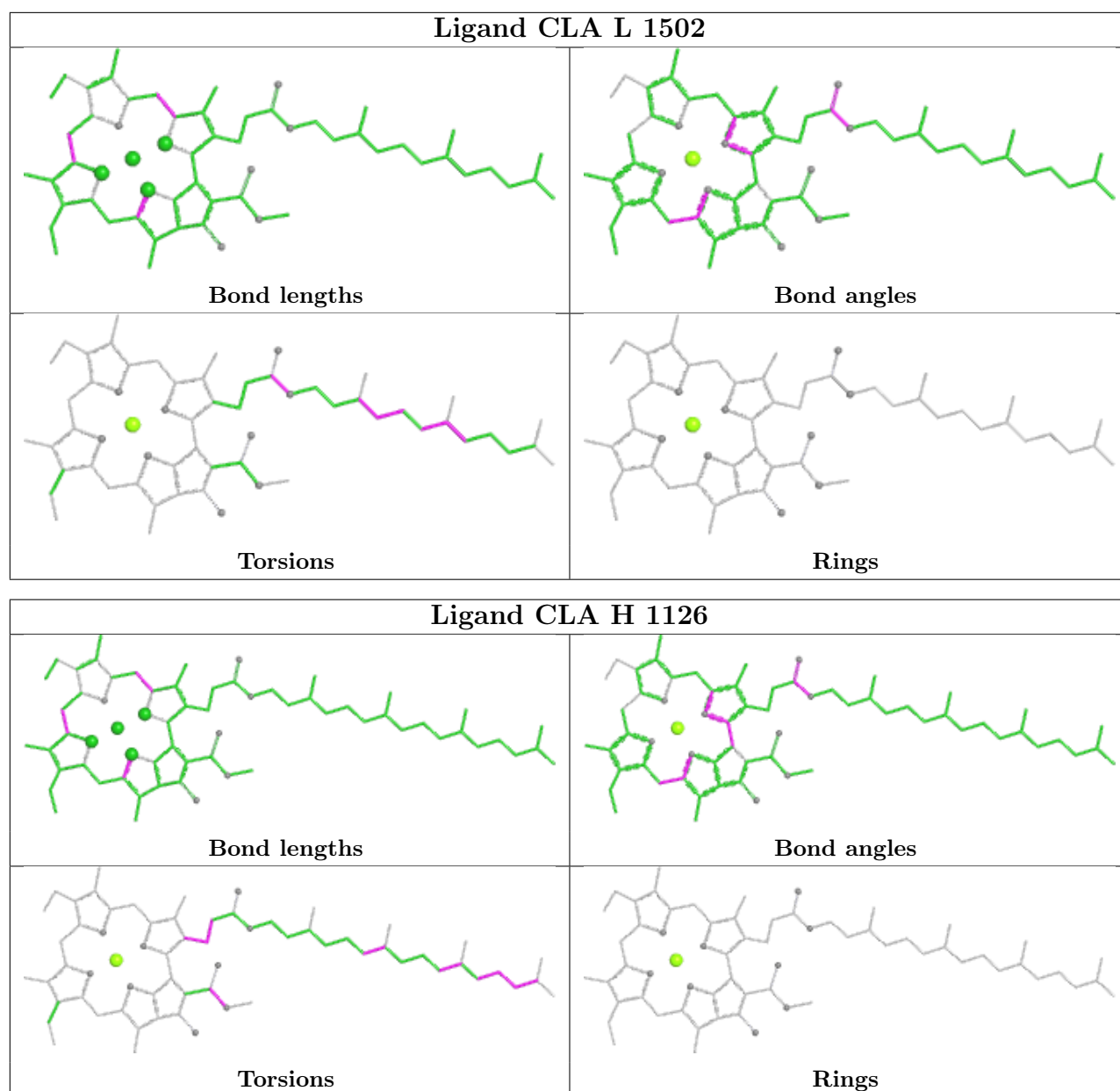




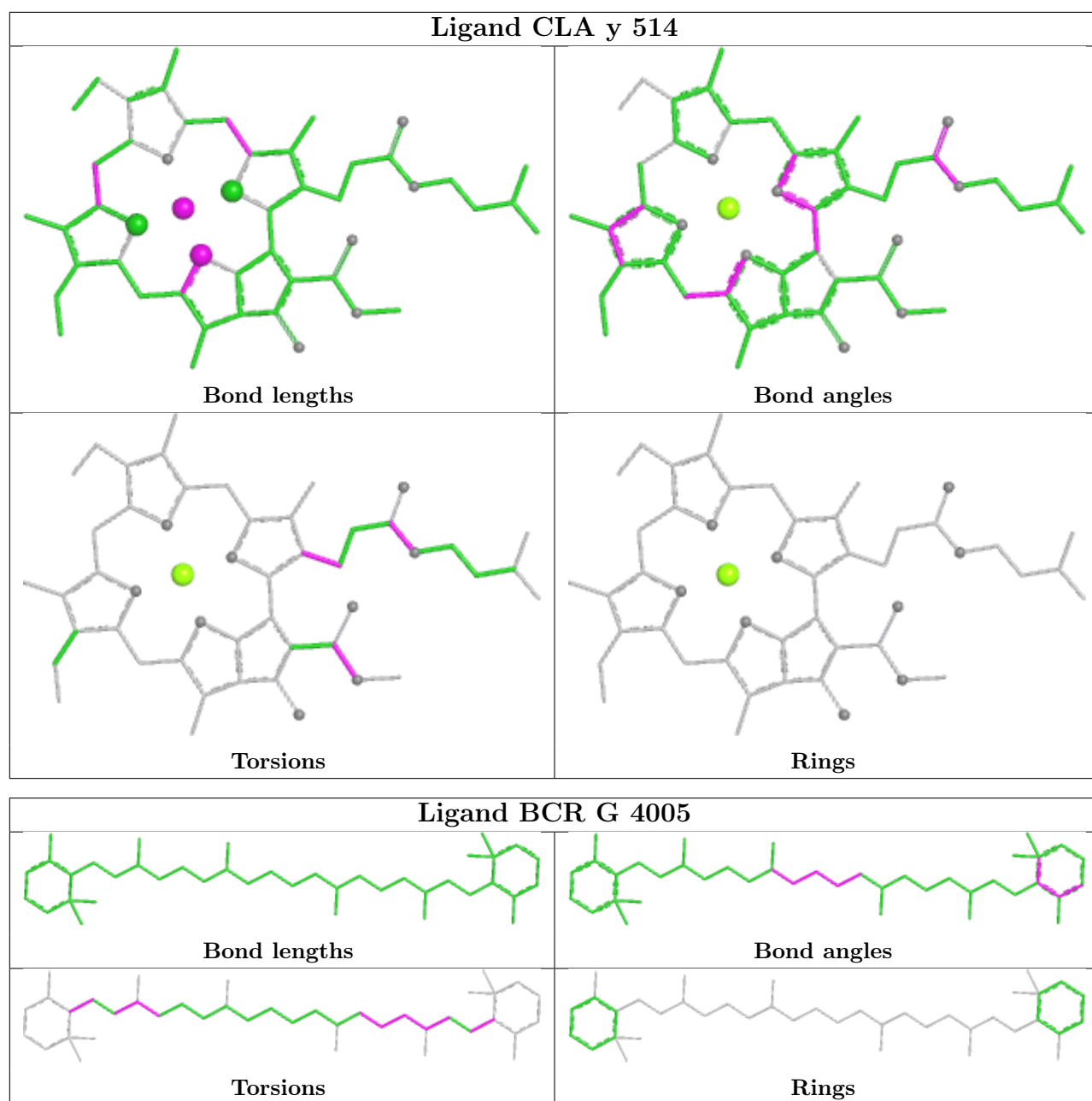




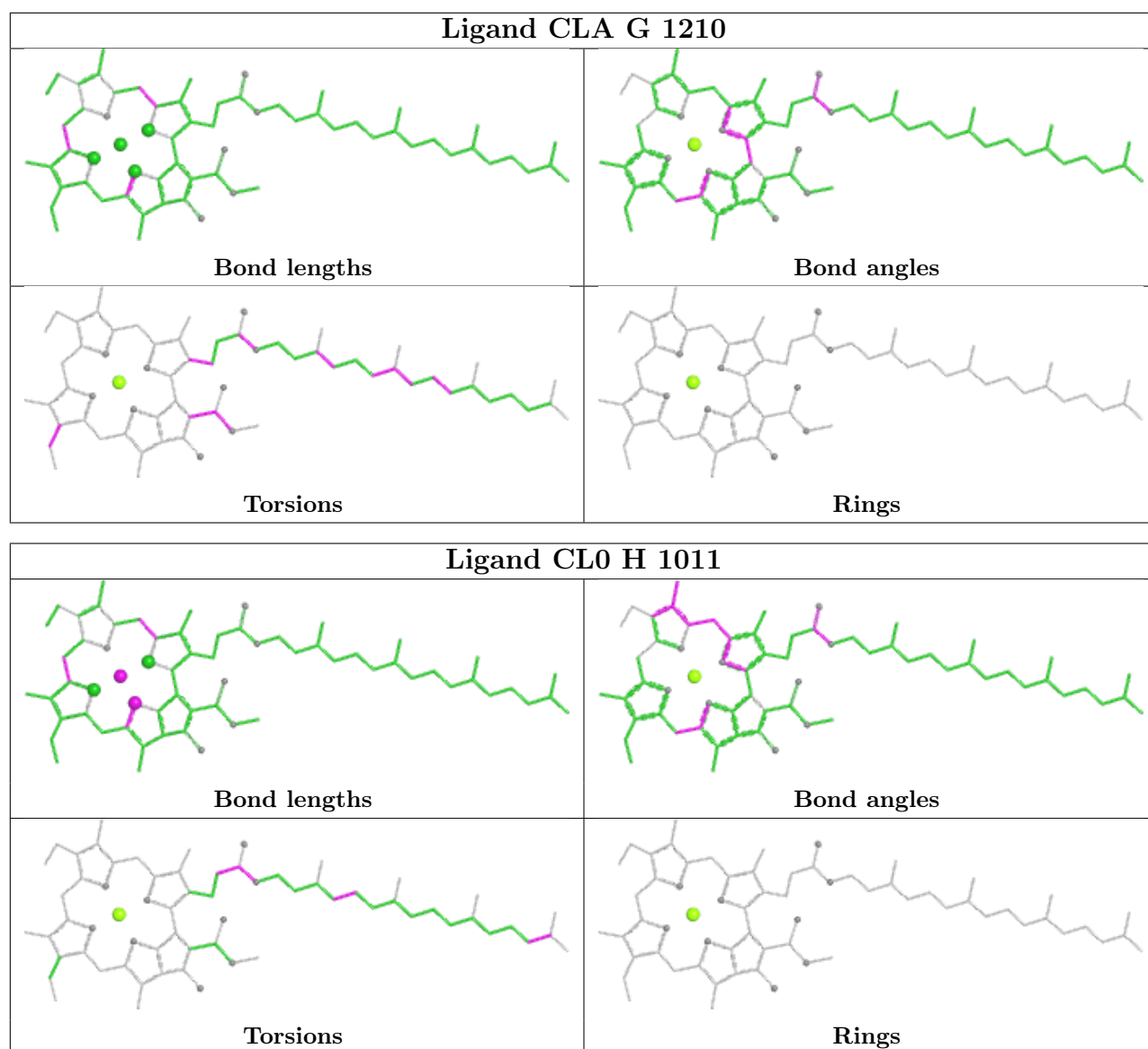






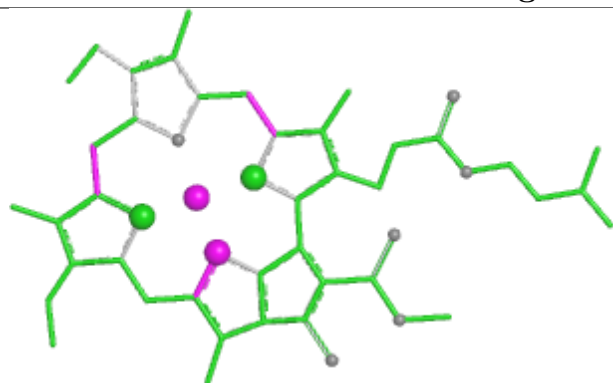




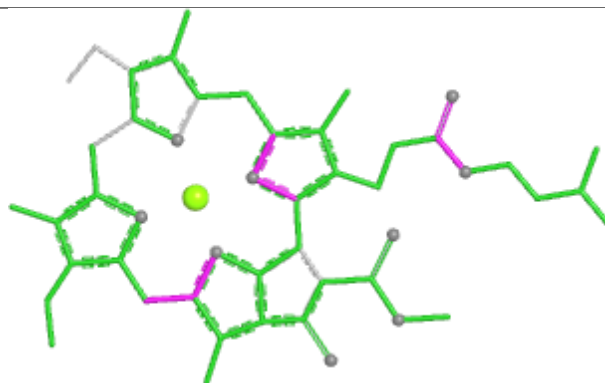




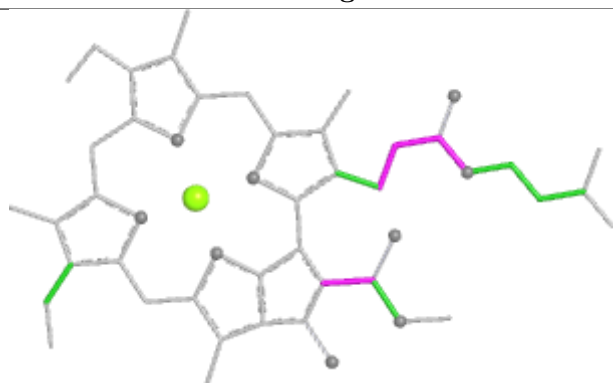
## Ligand CLA o 502



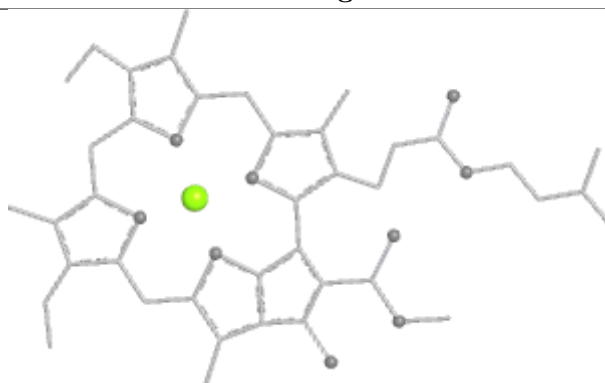
Bond lengths



Bond angles

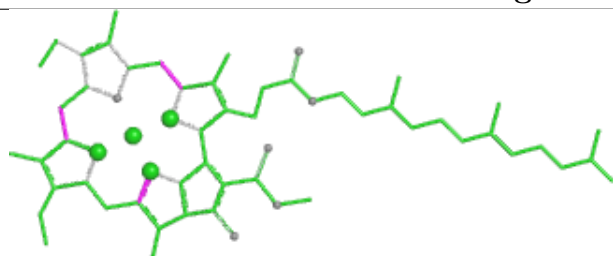


Torsions

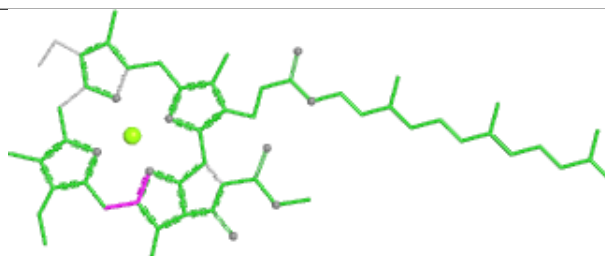


Rings

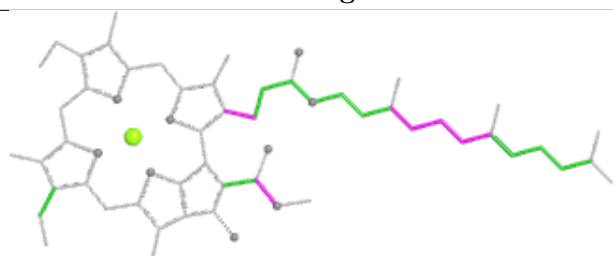
## Ligand CLA w 510



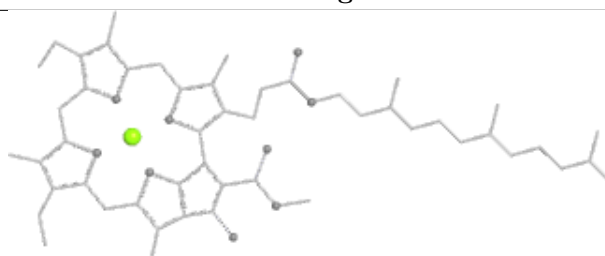
Bond lengths



Bond angles

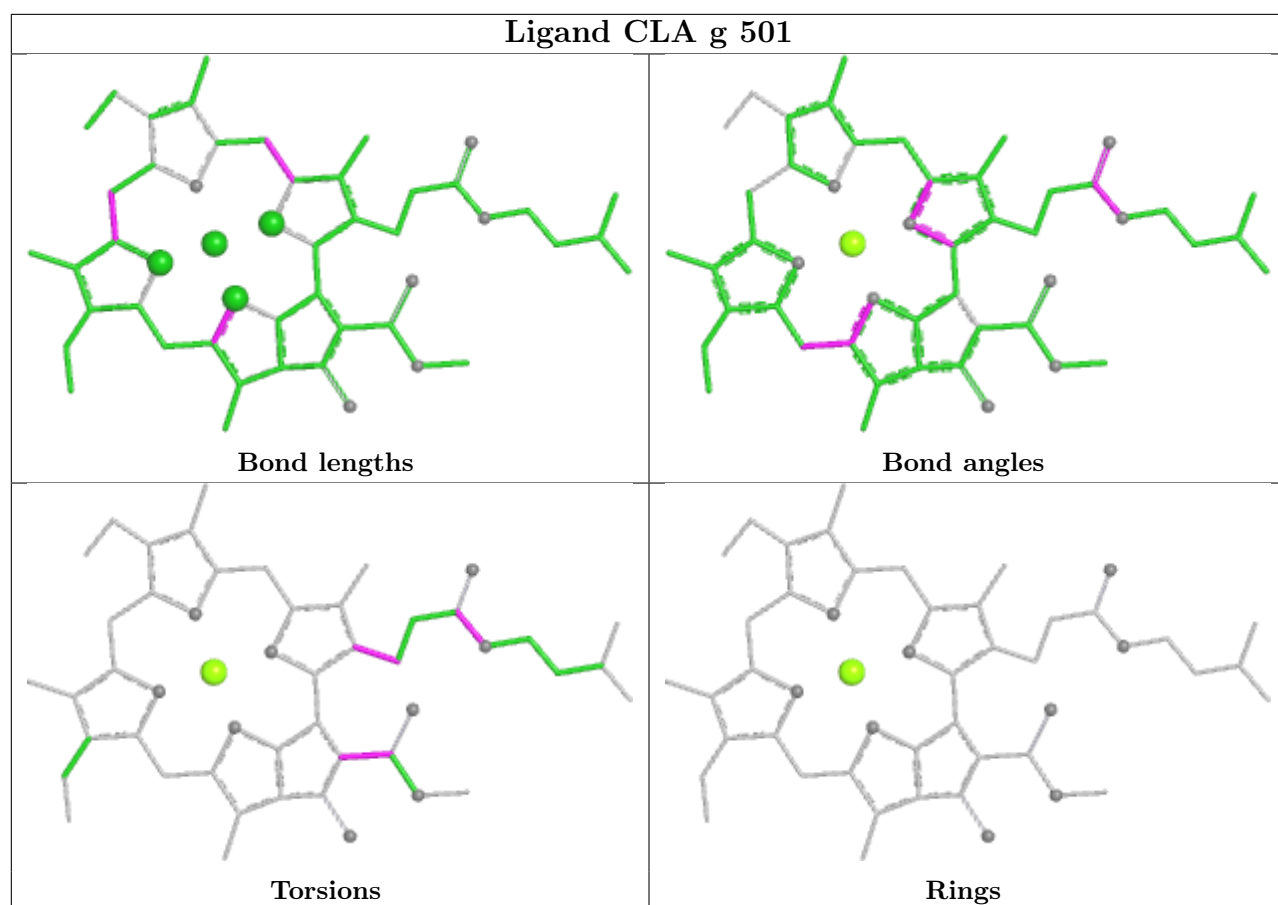


Torsions



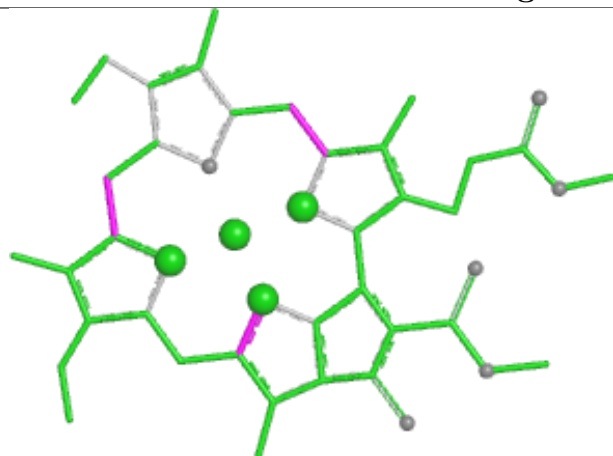
Rings



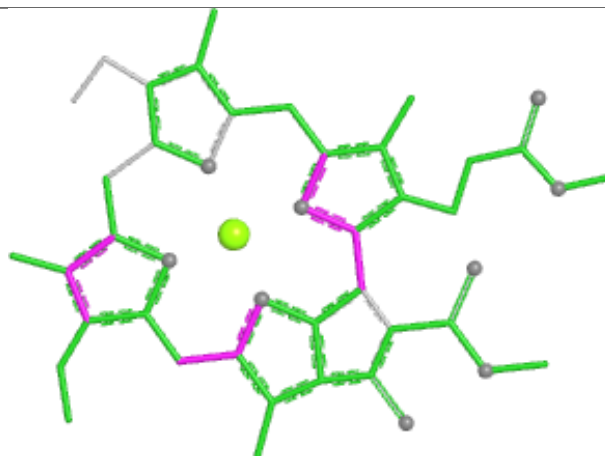




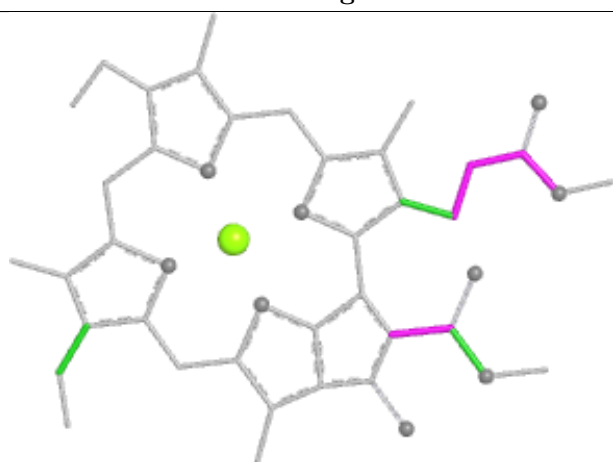
## Ligand CLA h 501



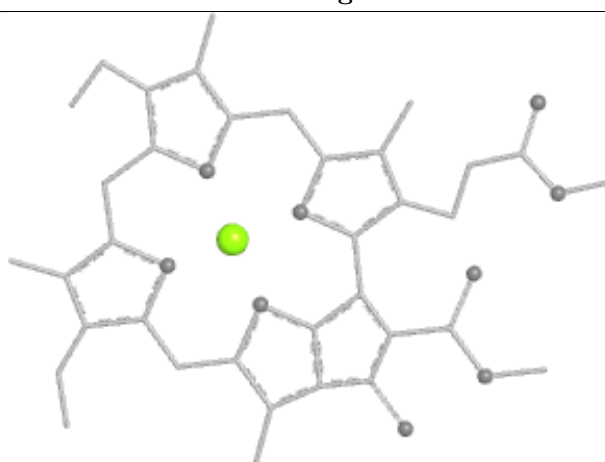
Bond lengths



Bond angles

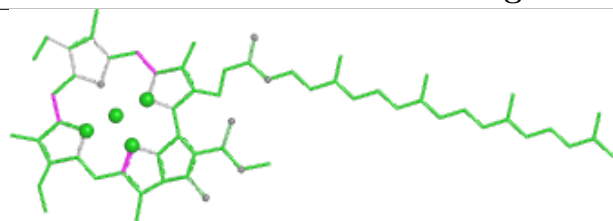


Torsions

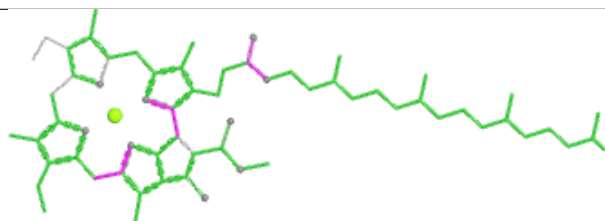


Rings

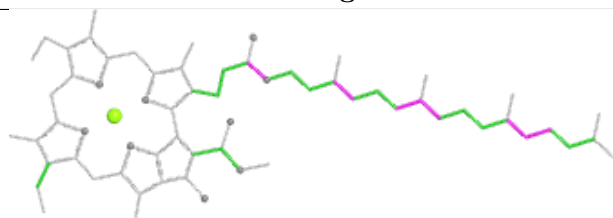
## Ligand CLA U 1503



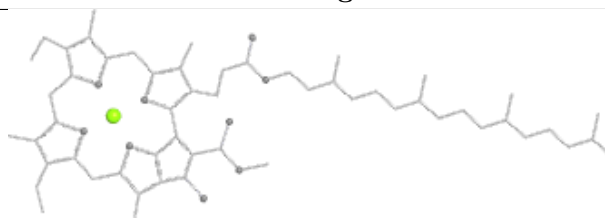
Bond lengths



Bond angles

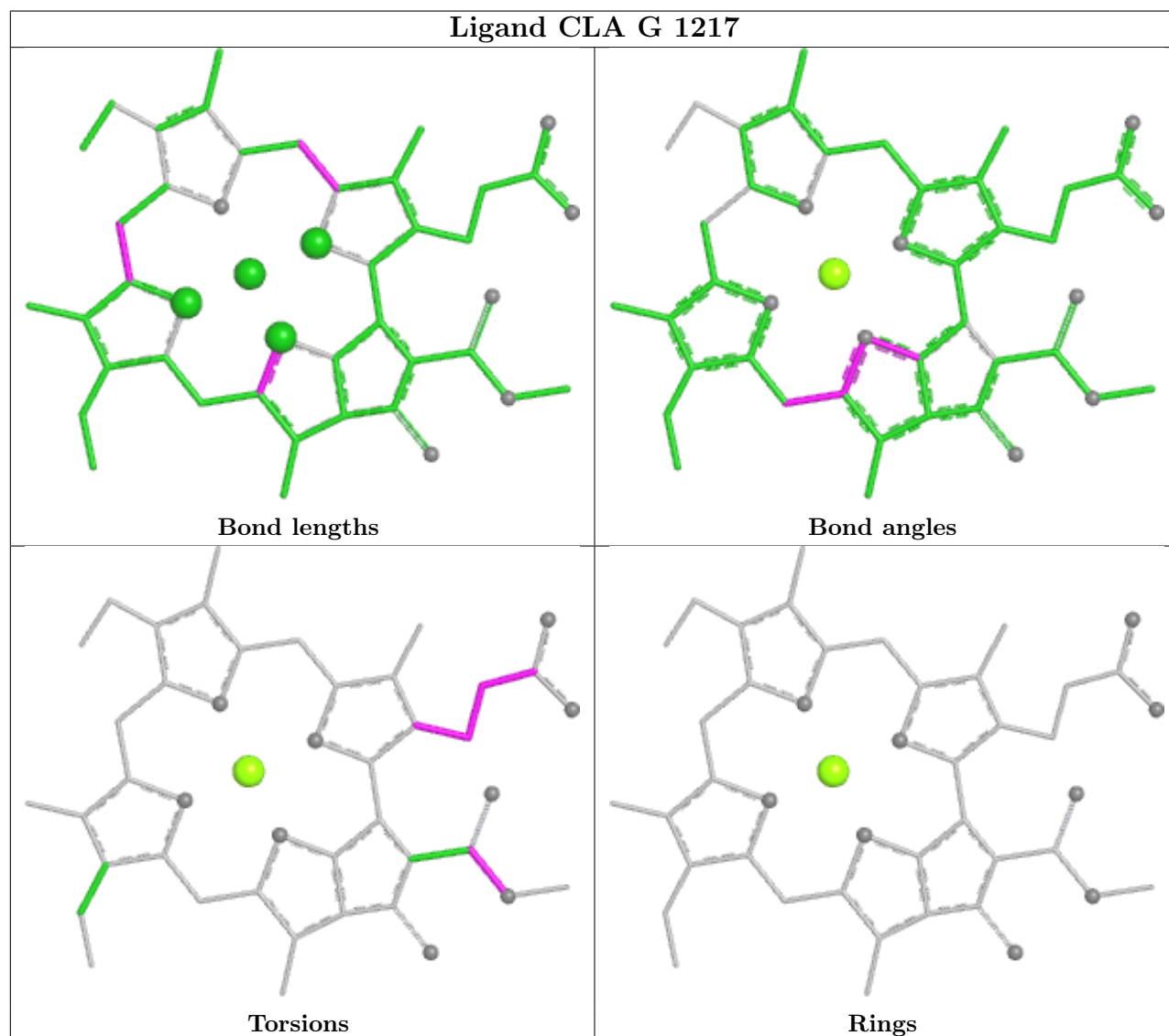
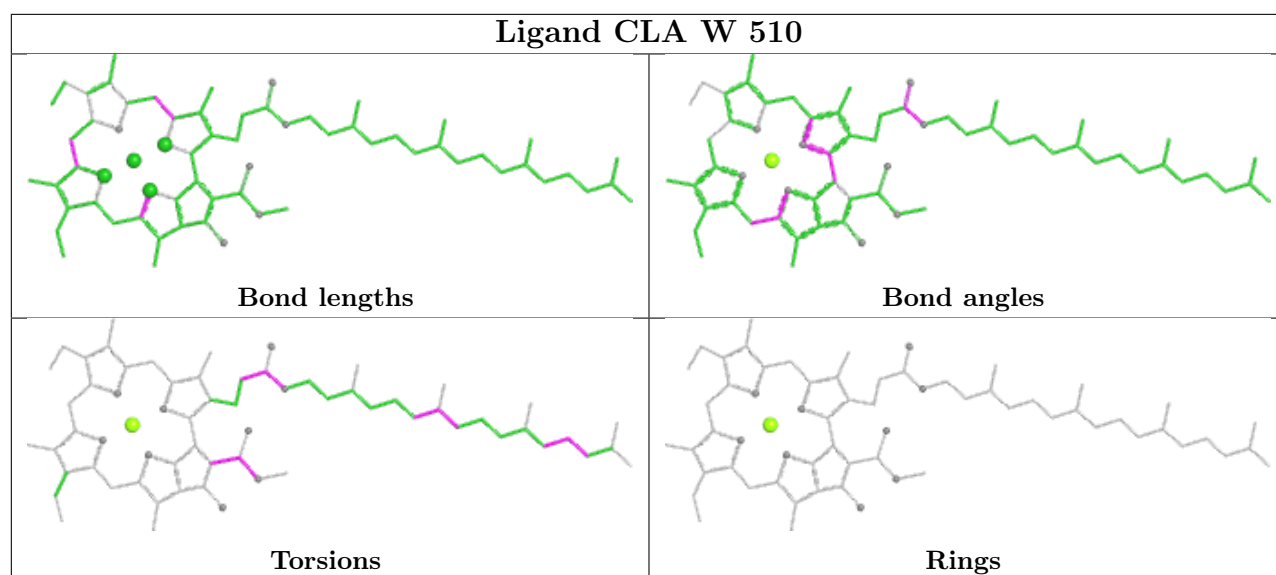


Torsions

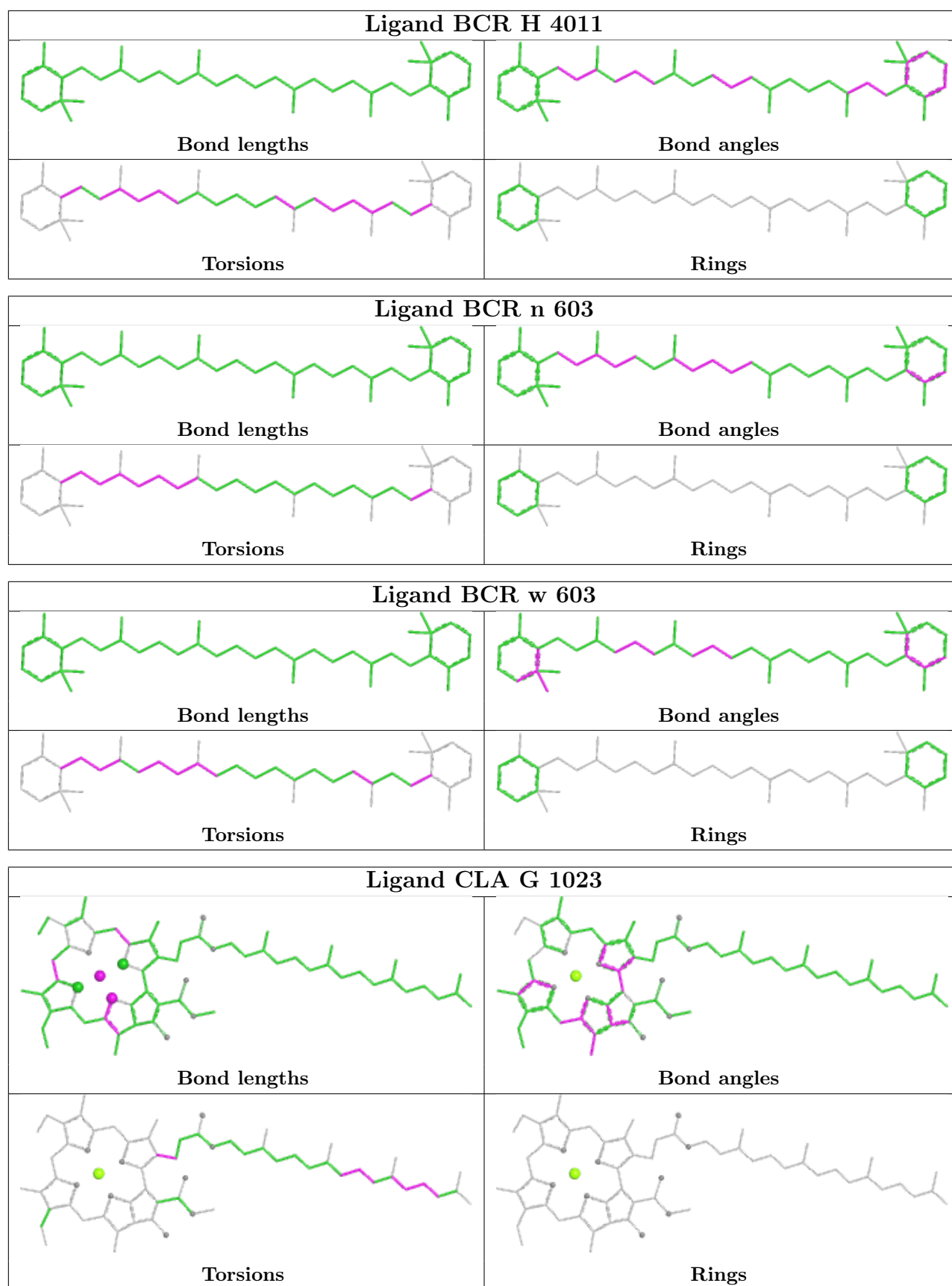


Rings

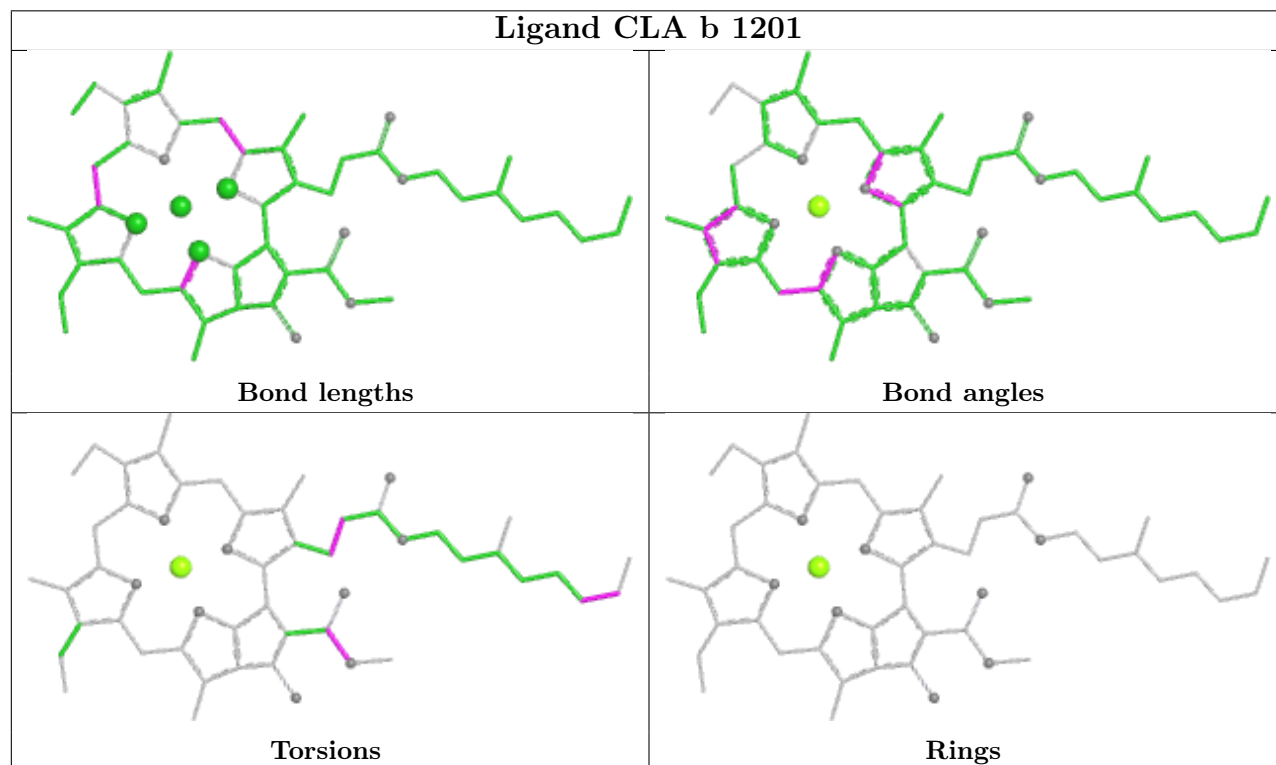
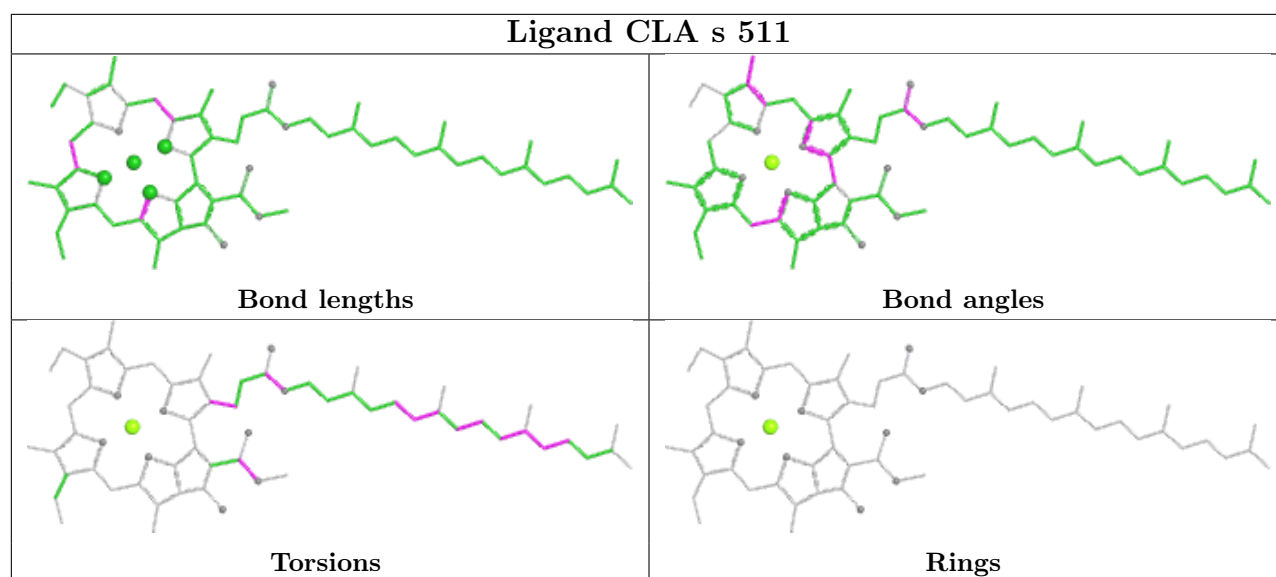






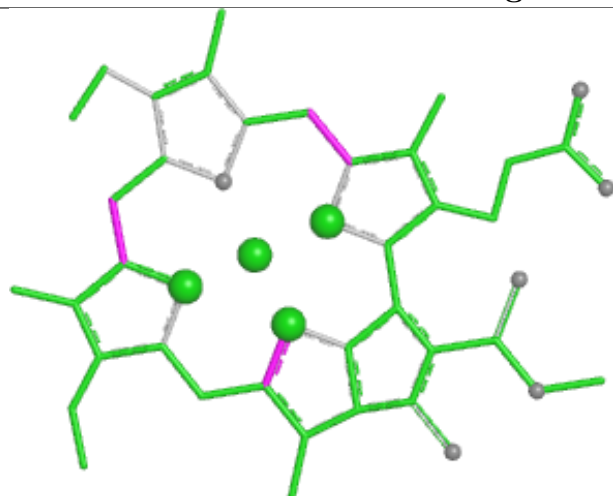




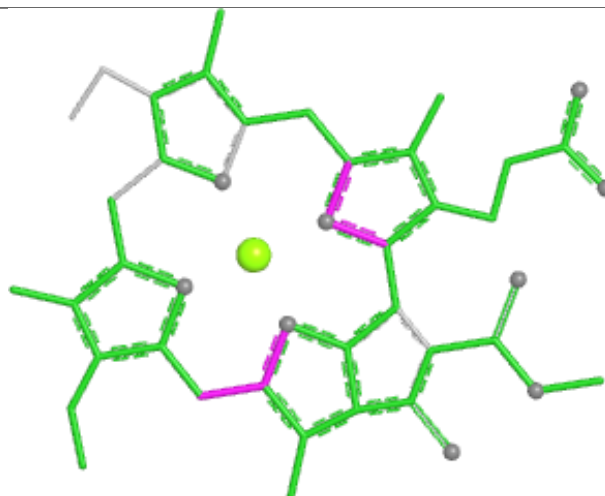




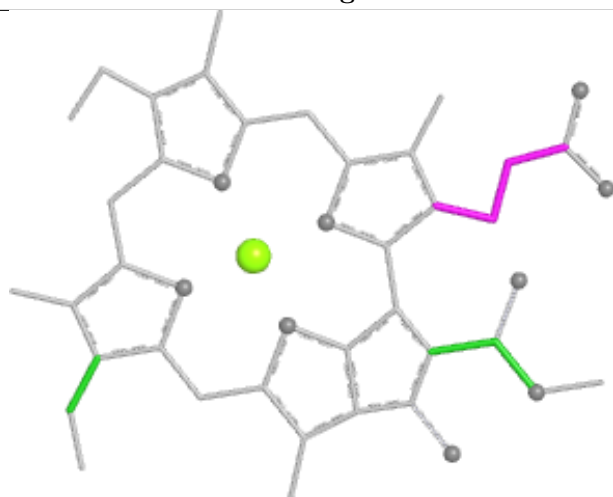
## Ligand CLA B 1209



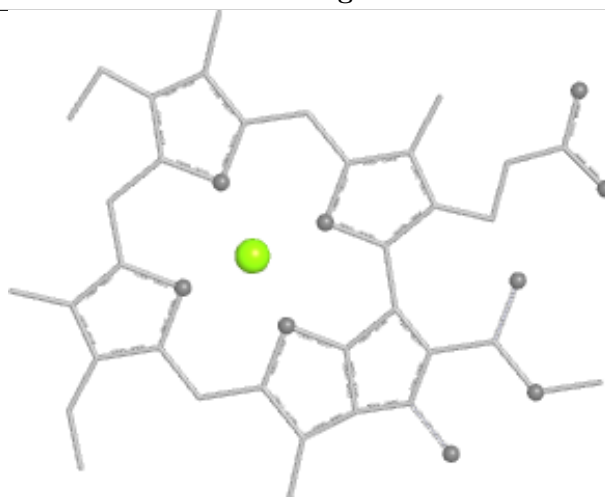
Bond lengths



Bond angles

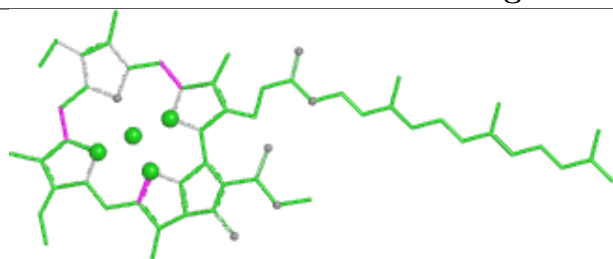


Torsions

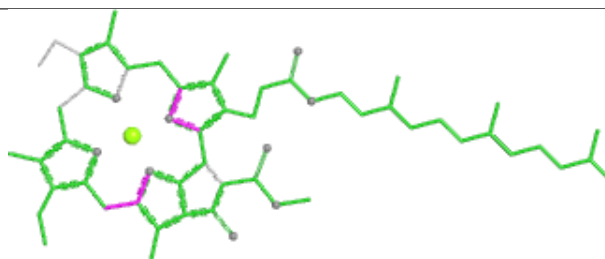


Rings

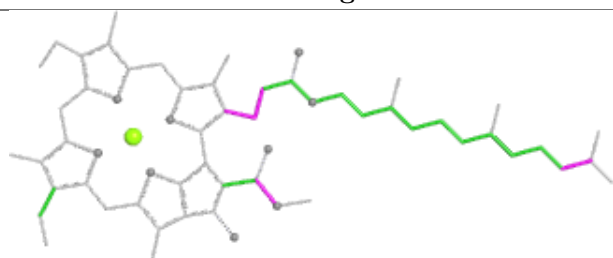
## Ligand CLA G 1215



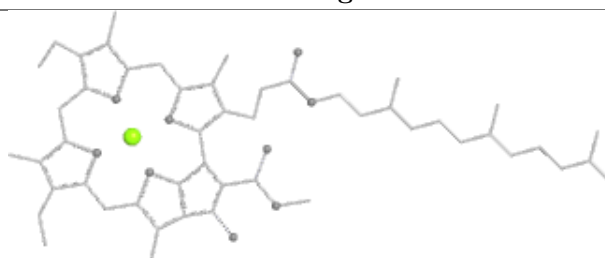
Bond lengths



Bond angles

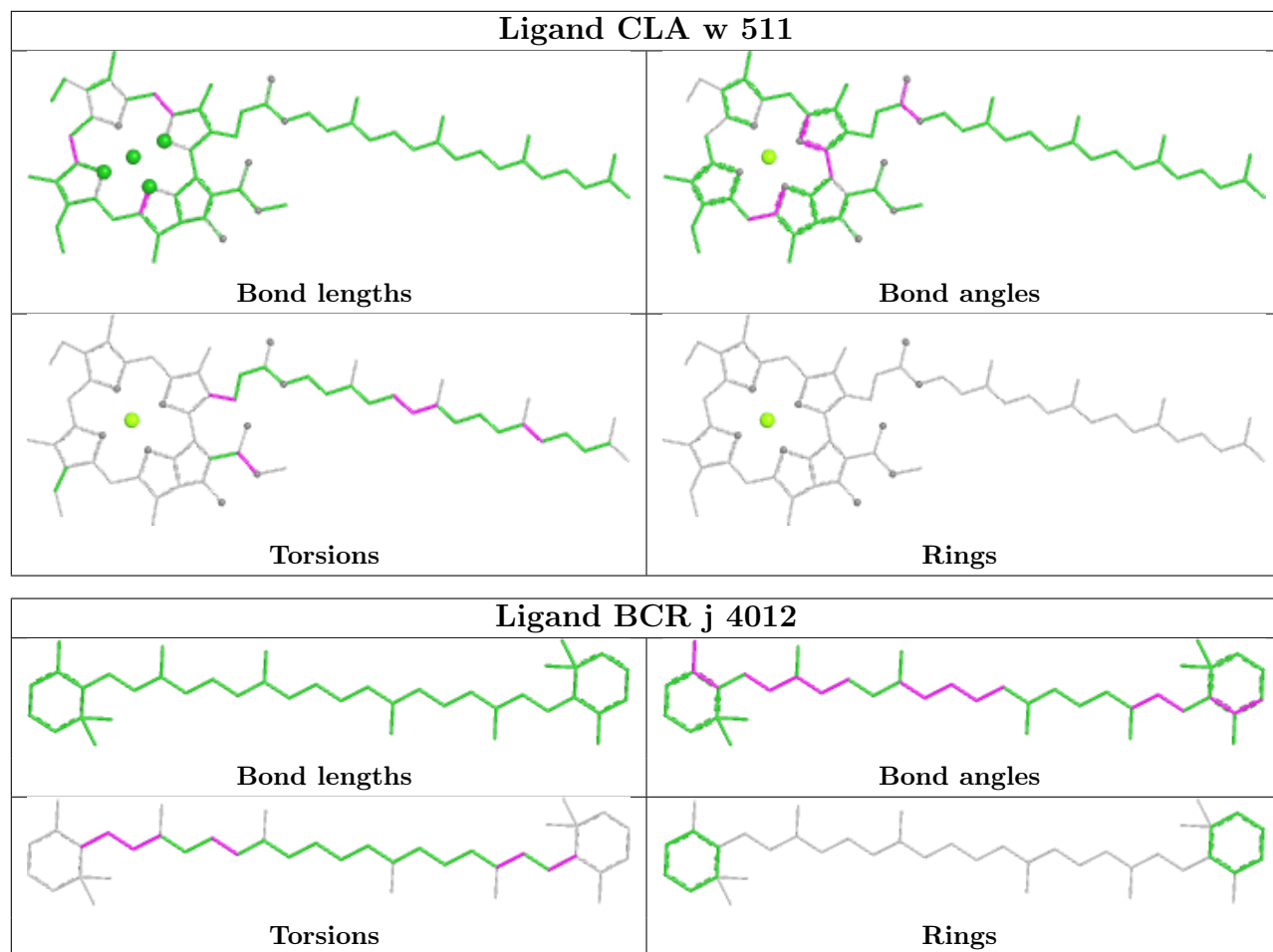


Torsions

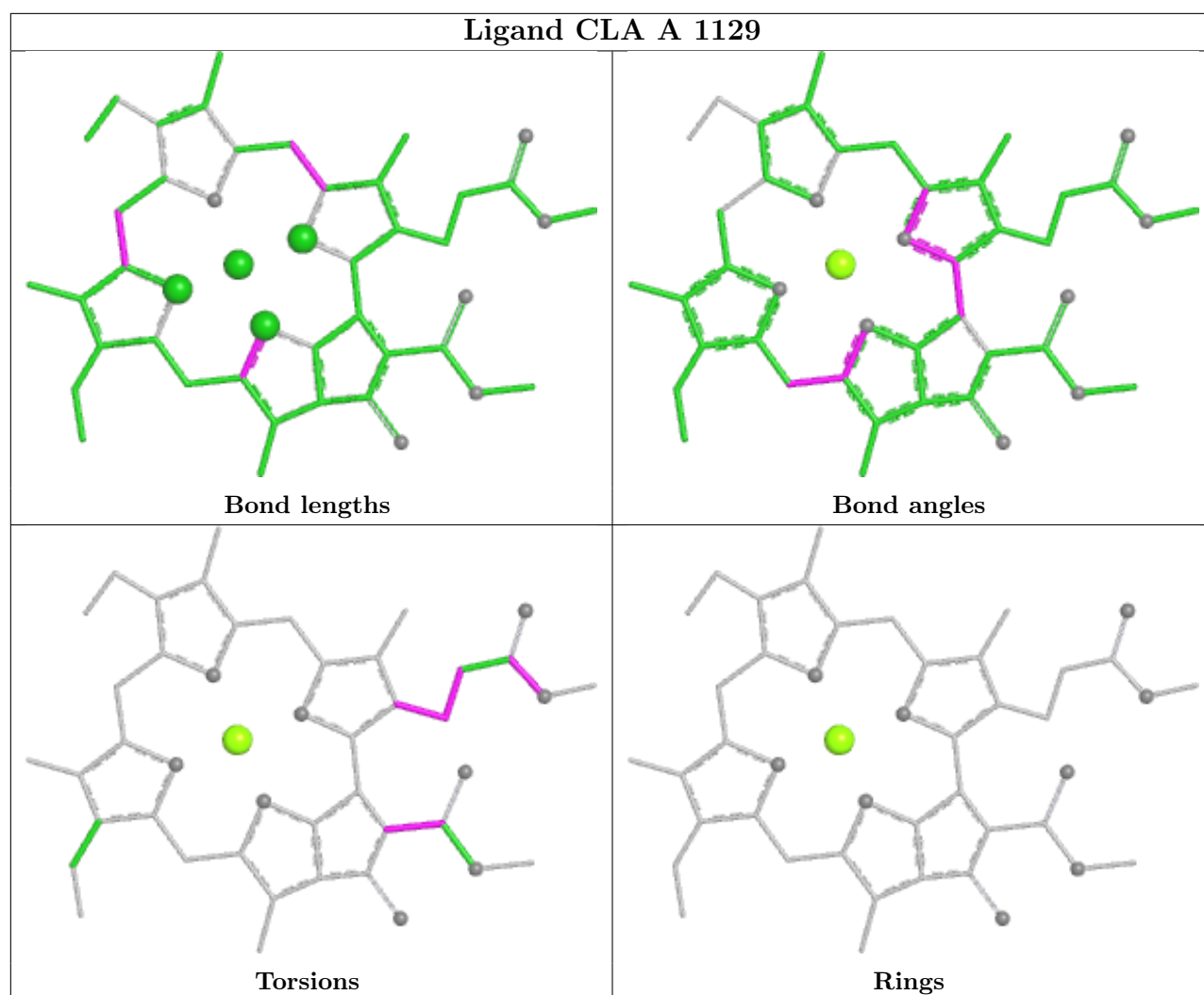


Rings

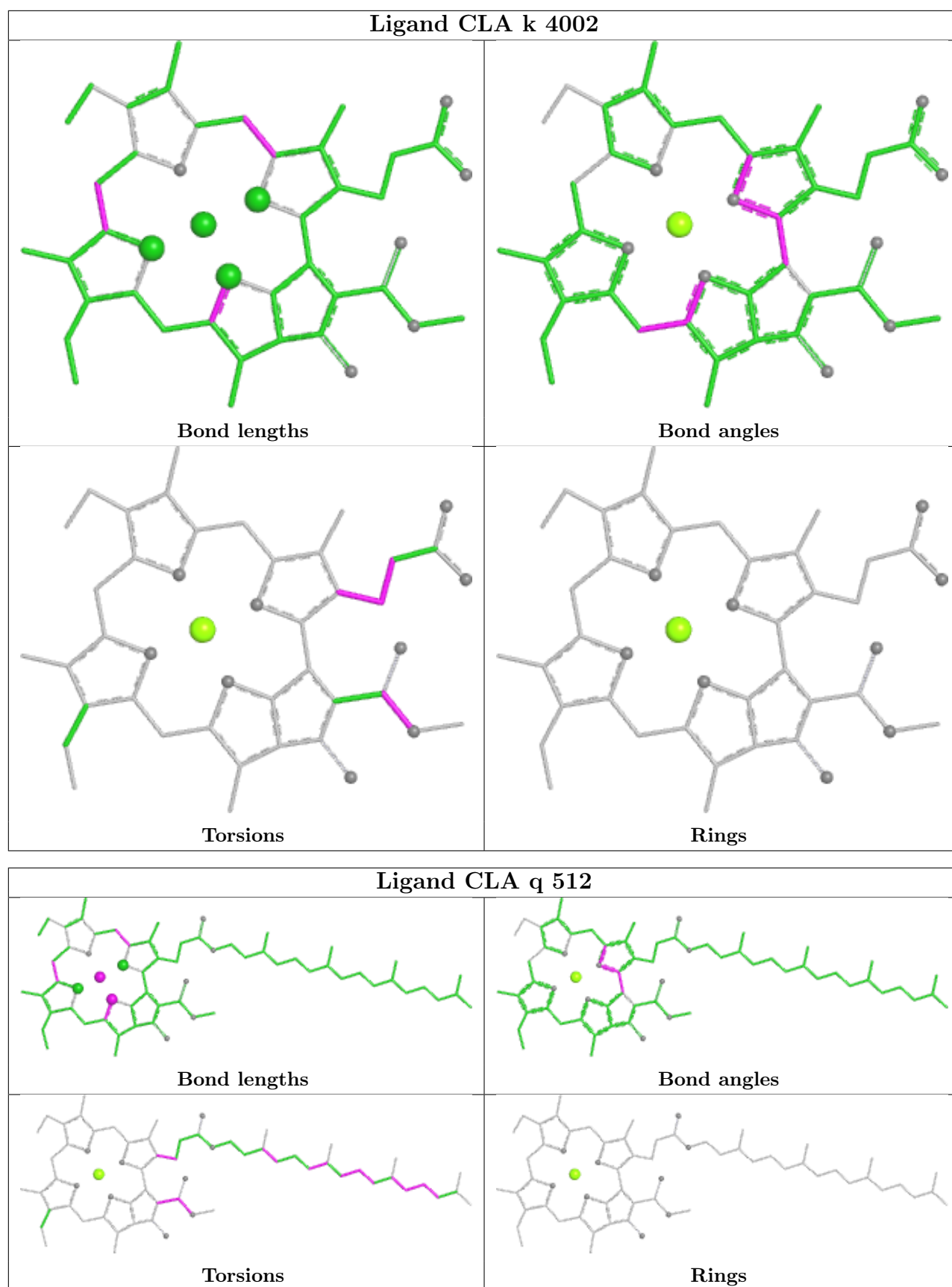






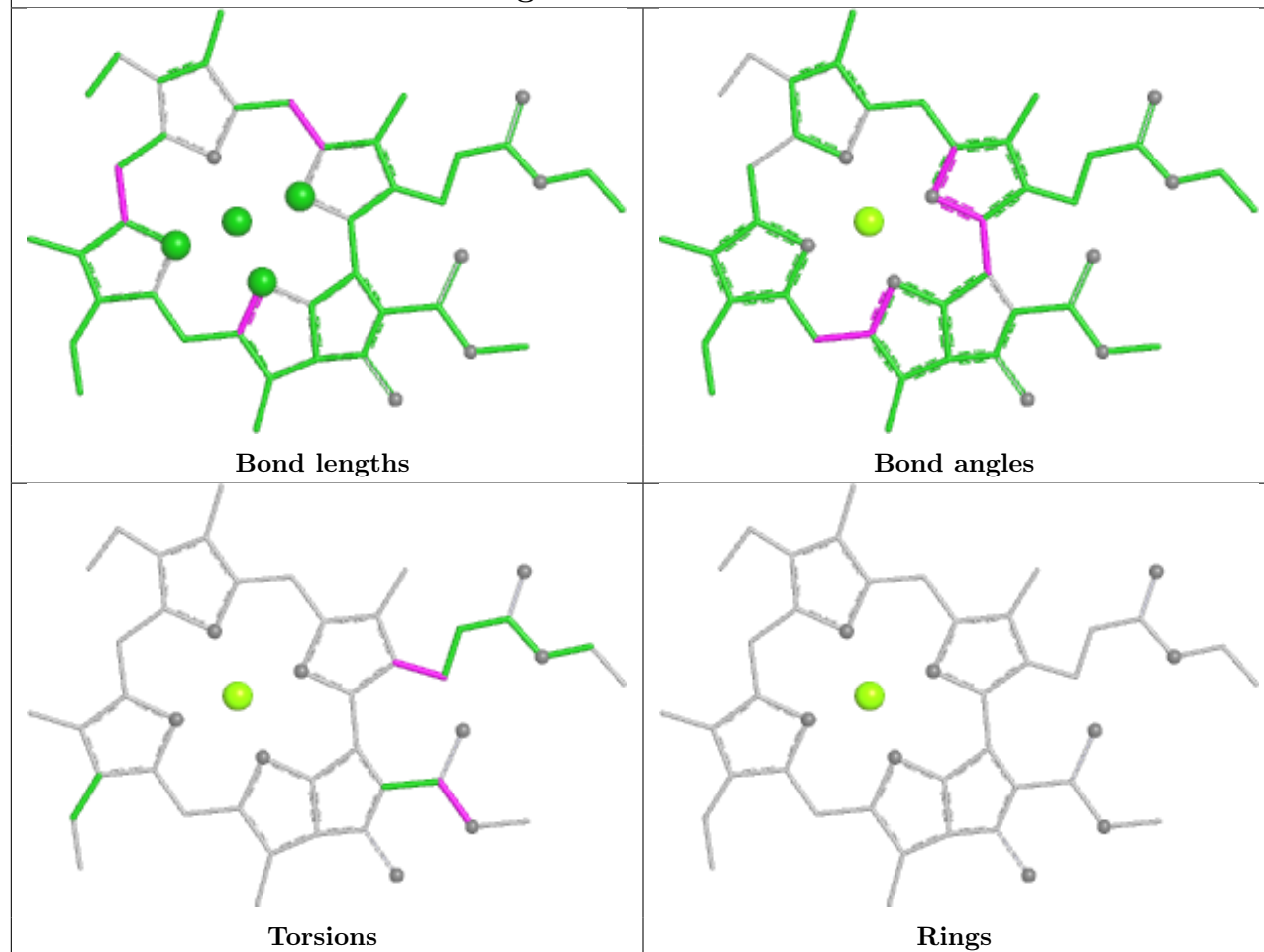




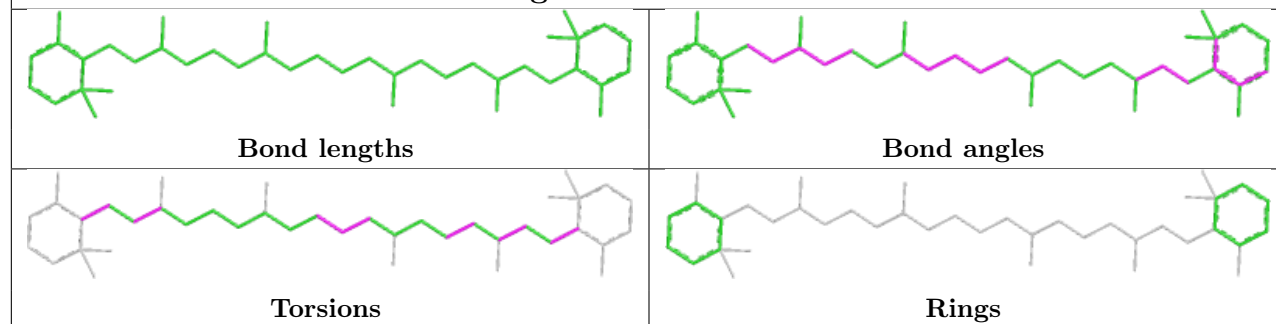




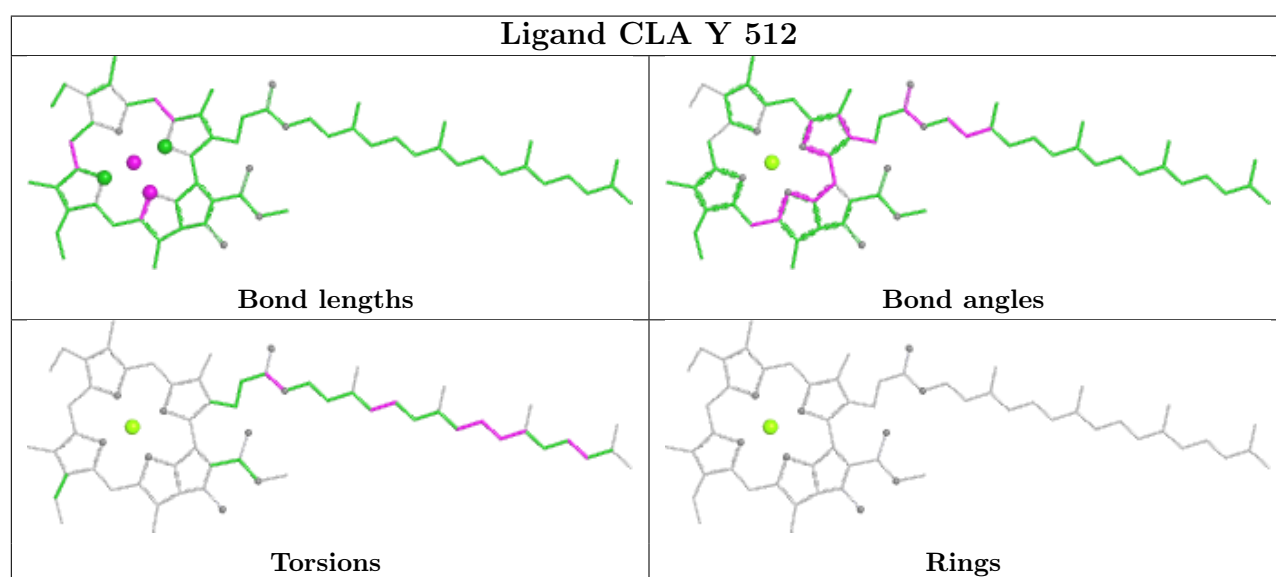
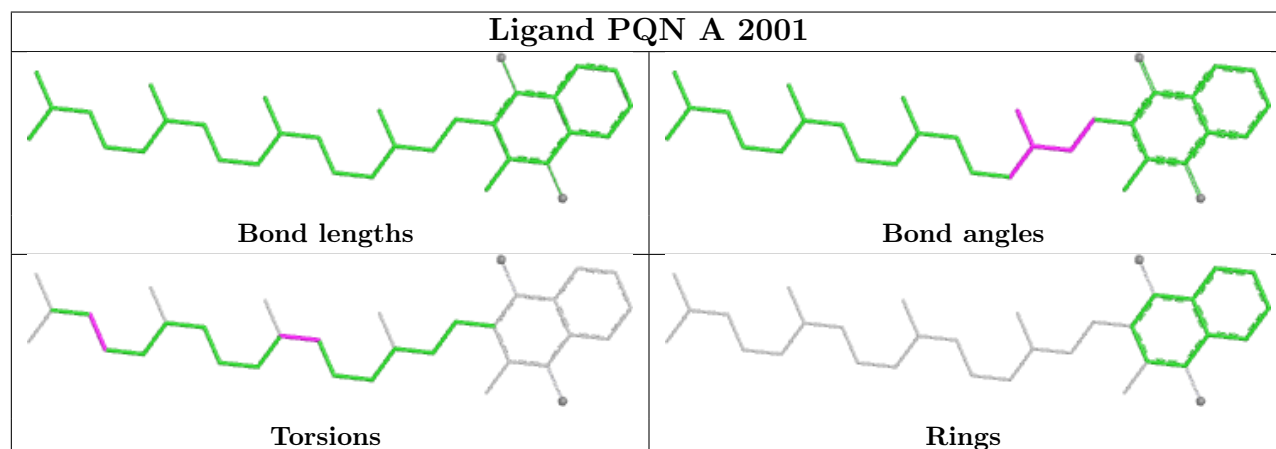
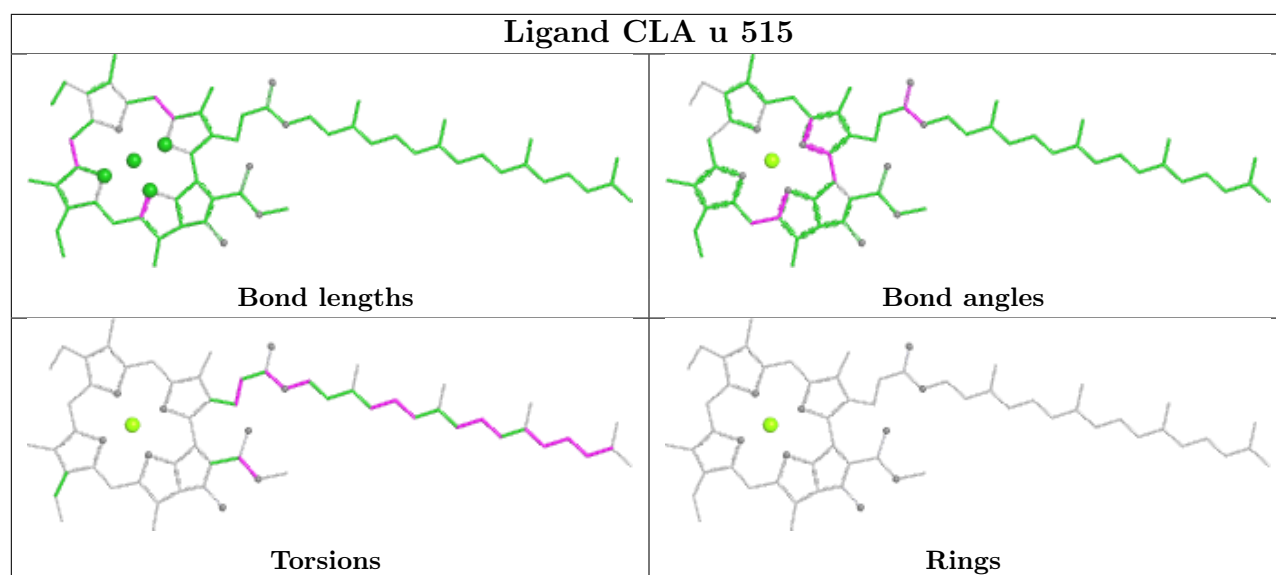
## Ligand CLA G 1216



## Ligand BCR w 602

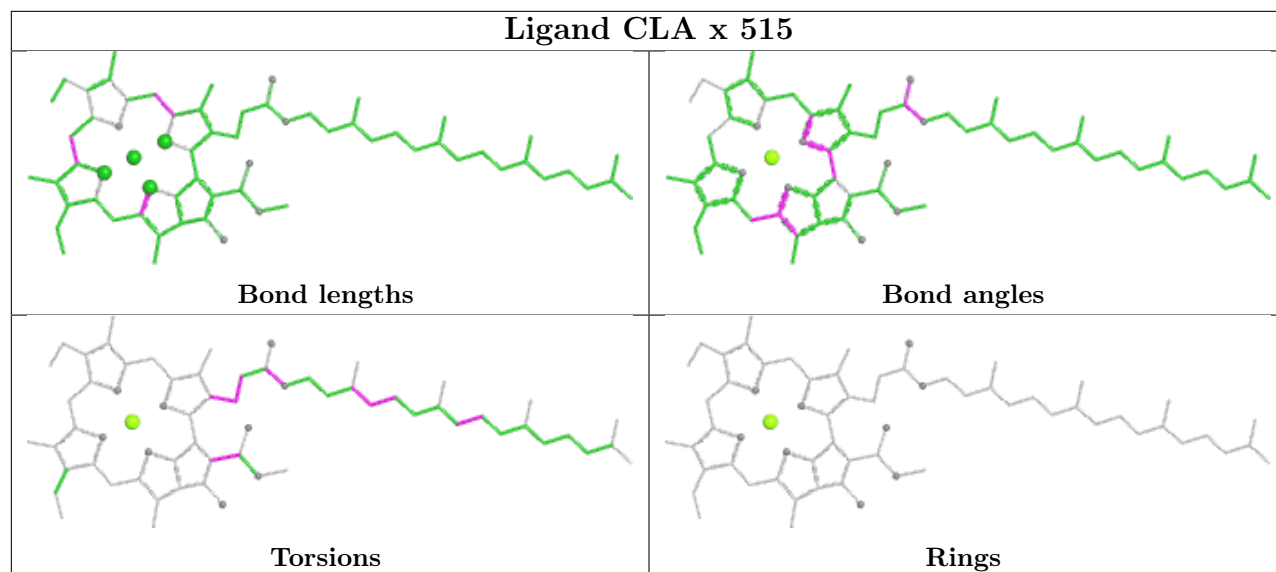




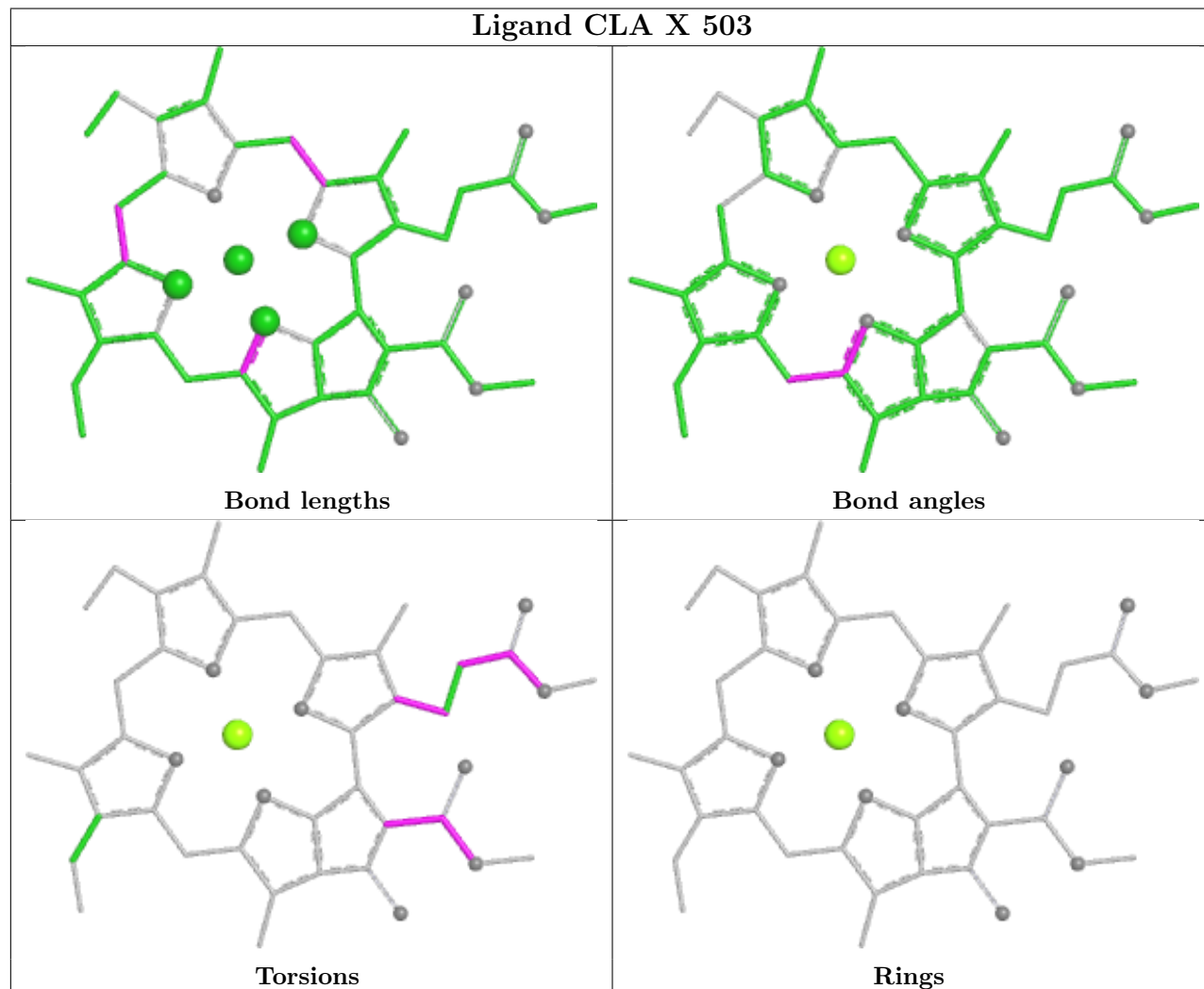




## Ligand CLA x 515

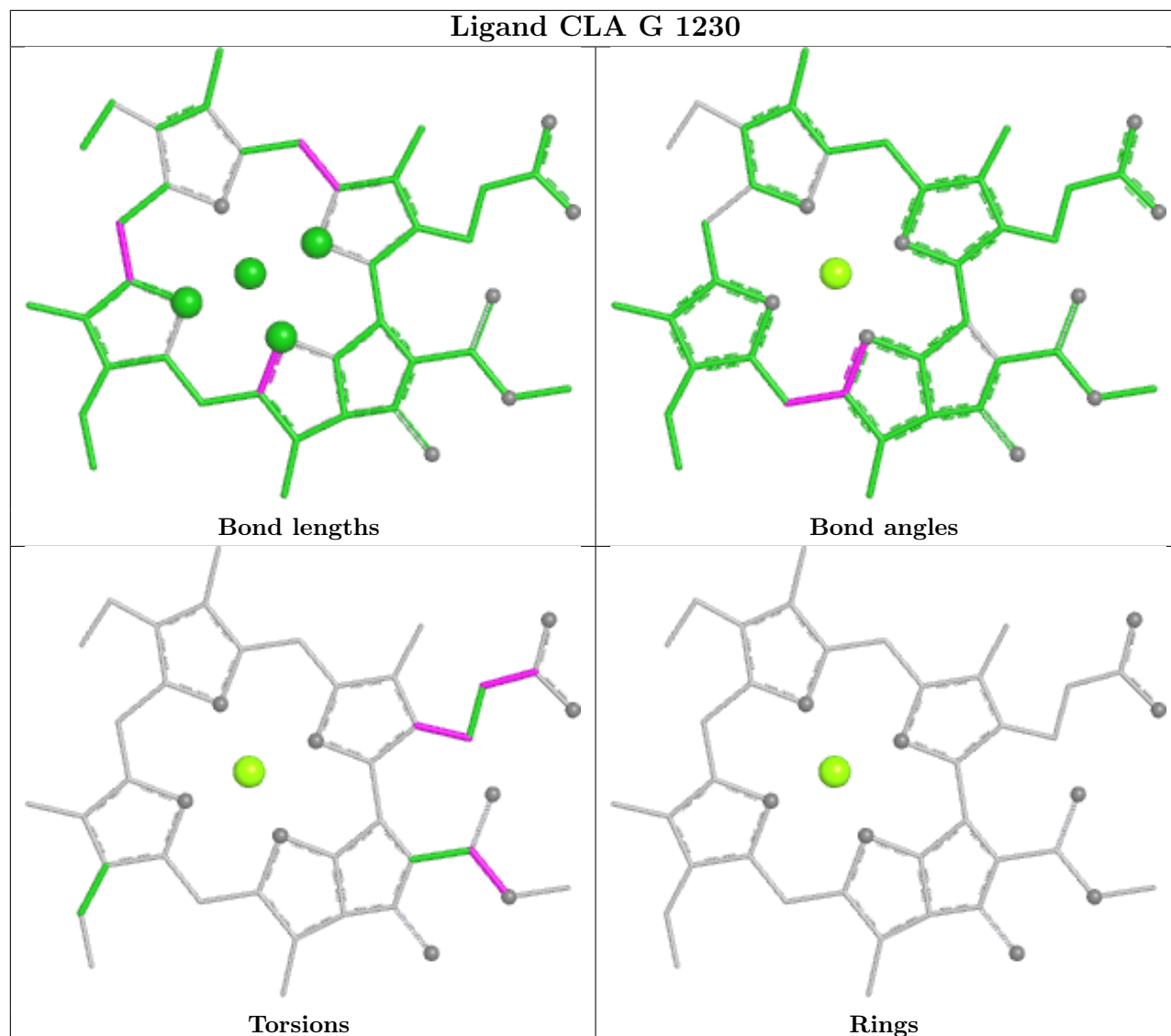


## Ligand CLA X 503

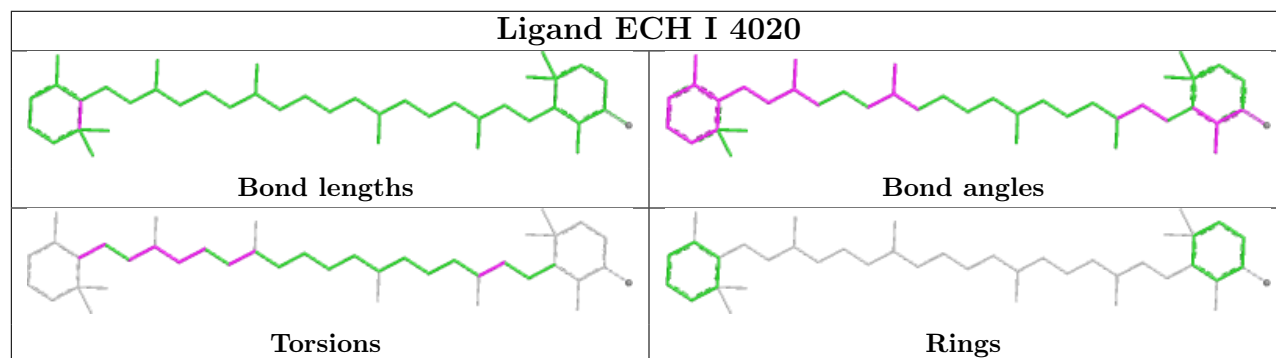




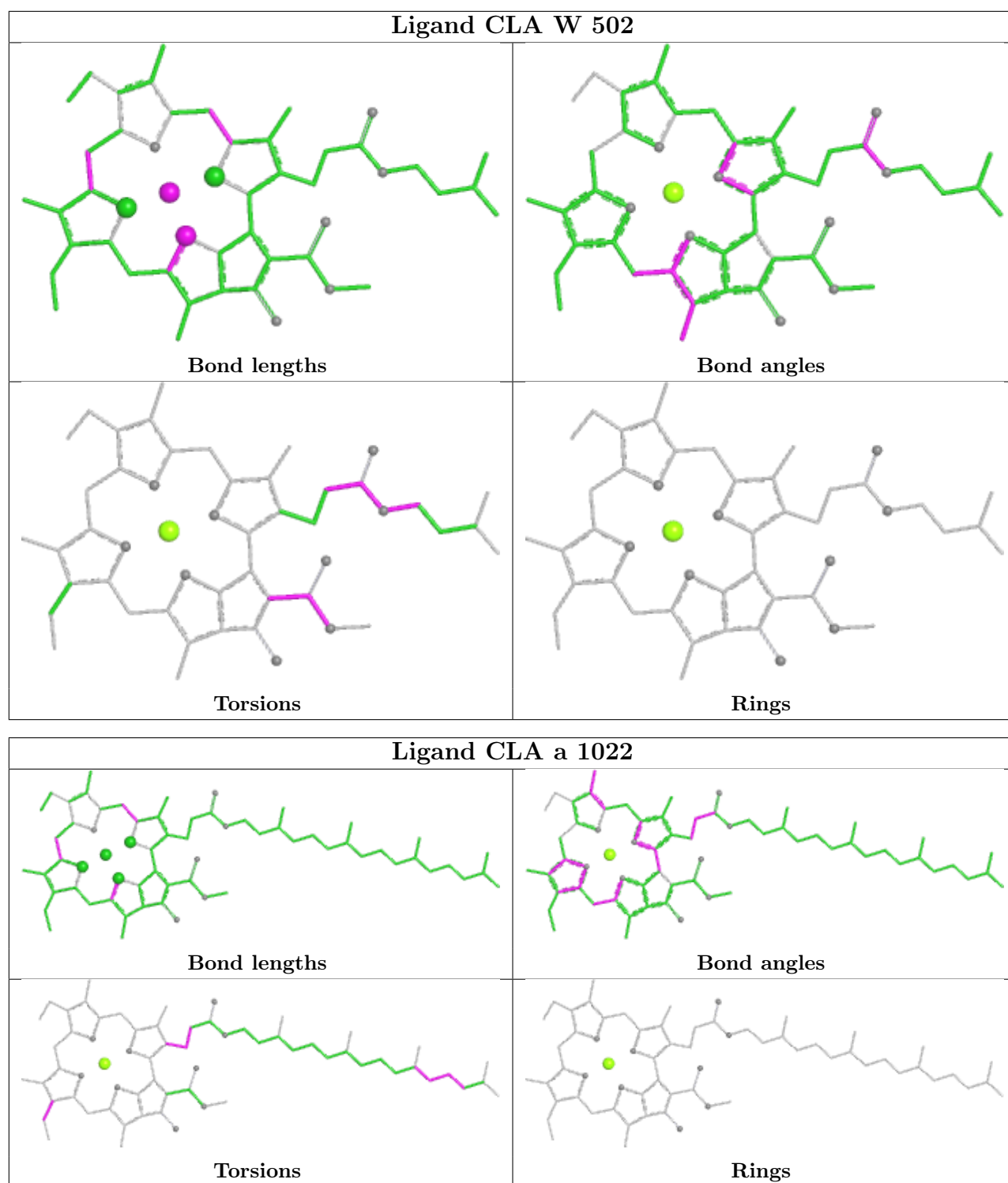
## Ligand CLA G 1230



## Ligand ECH I 4020

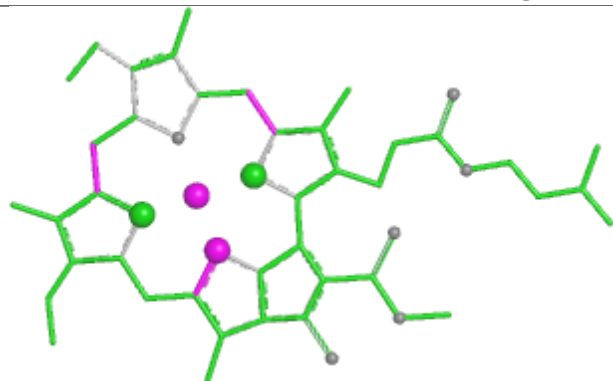




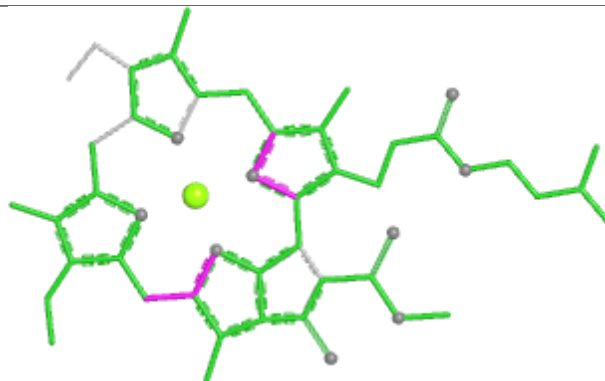




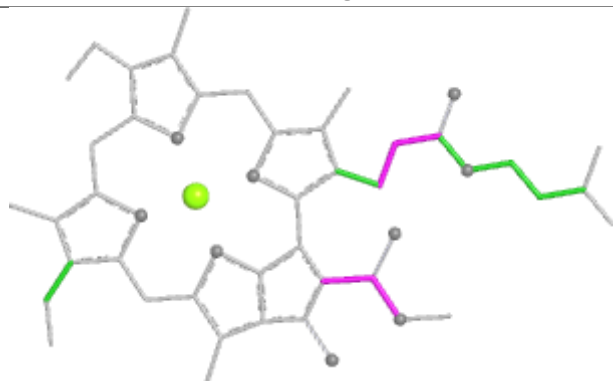
## Ligand CLA u 502



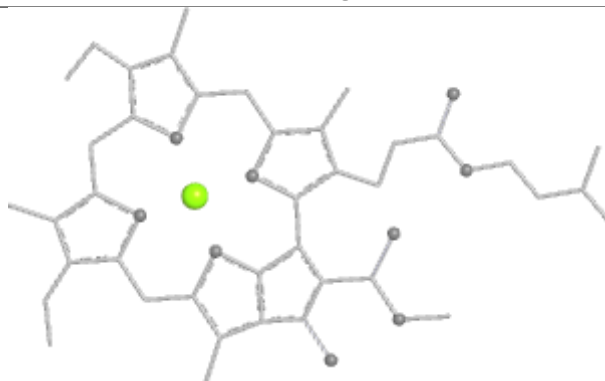
Bond lengths



Bond angles

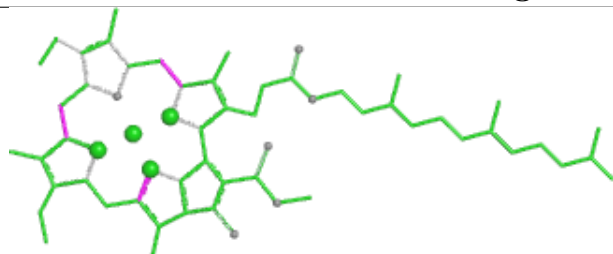


Torsions

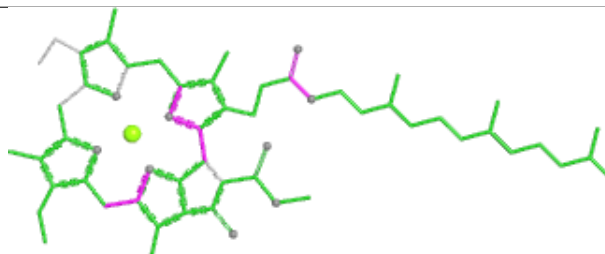


Rings

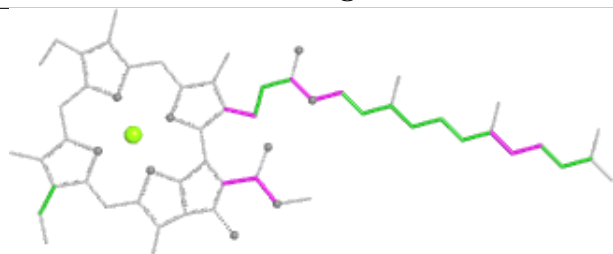
## Ligand CLA Y 506



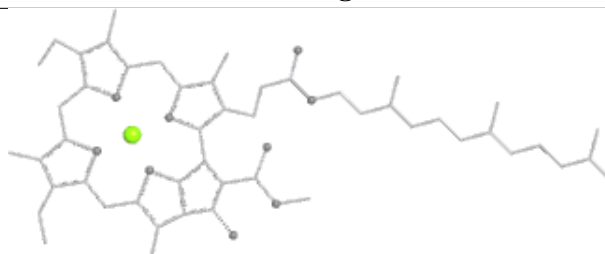
Bond lengths



Bond angles

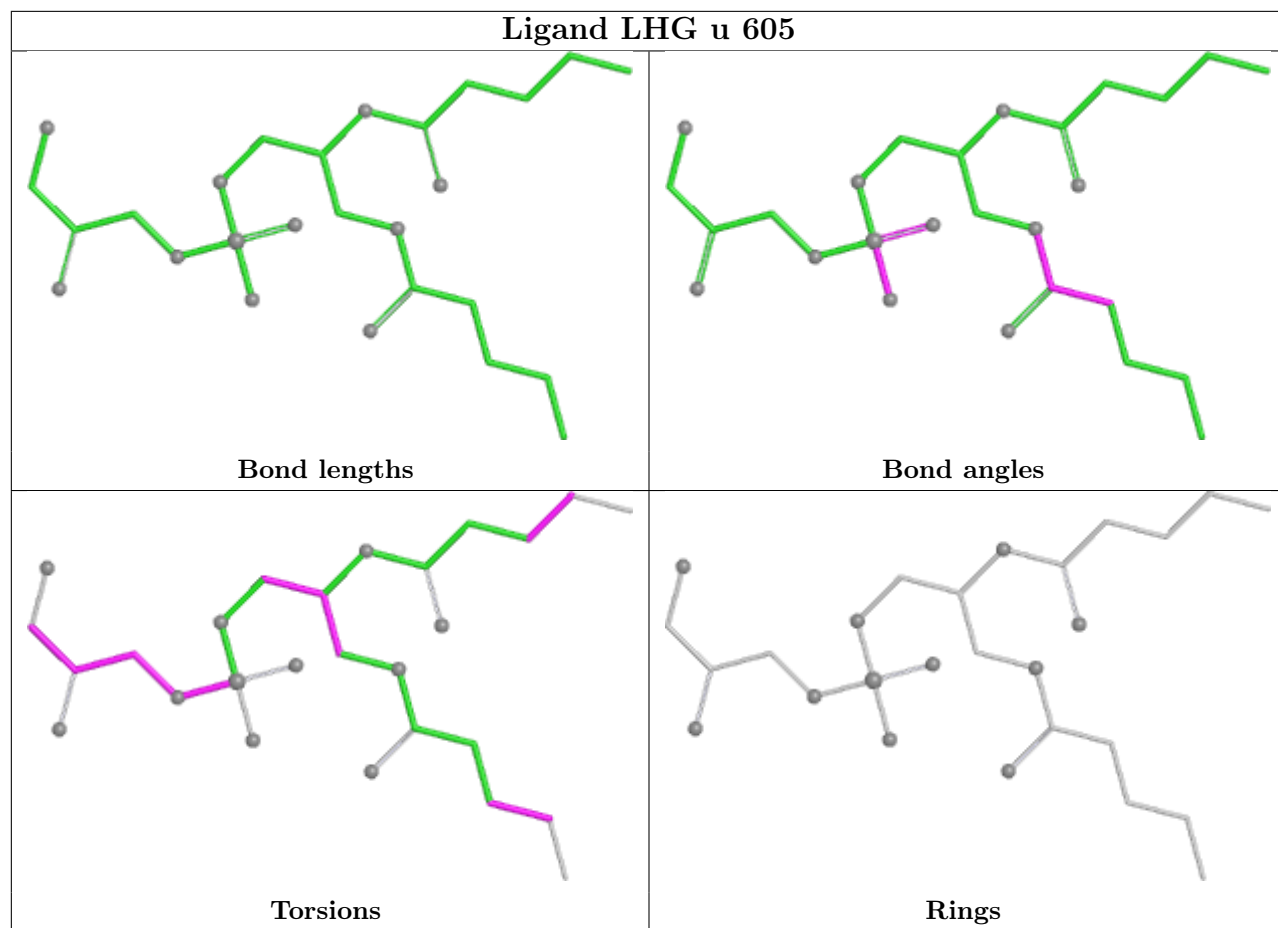


Torsions

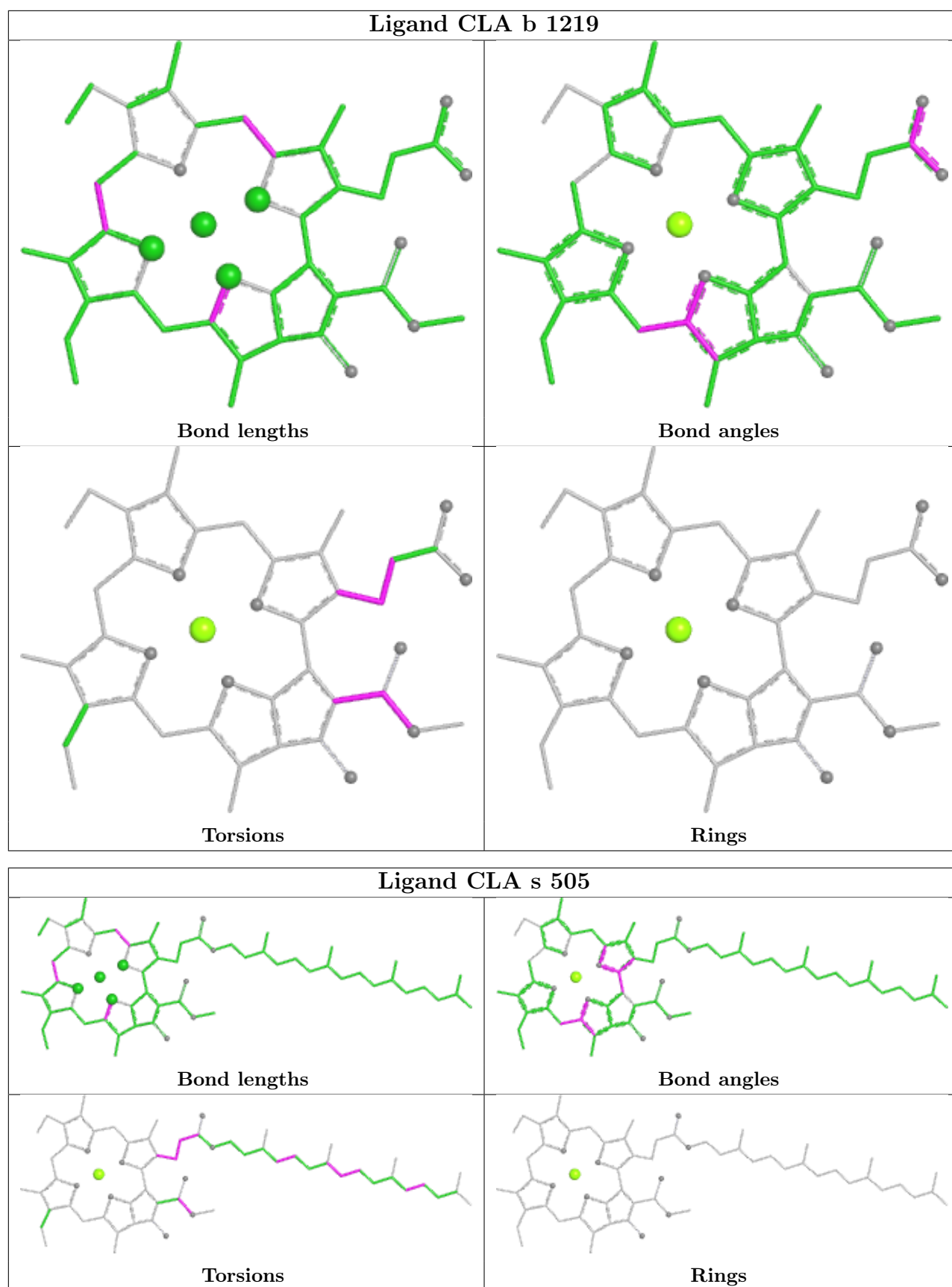


Rings

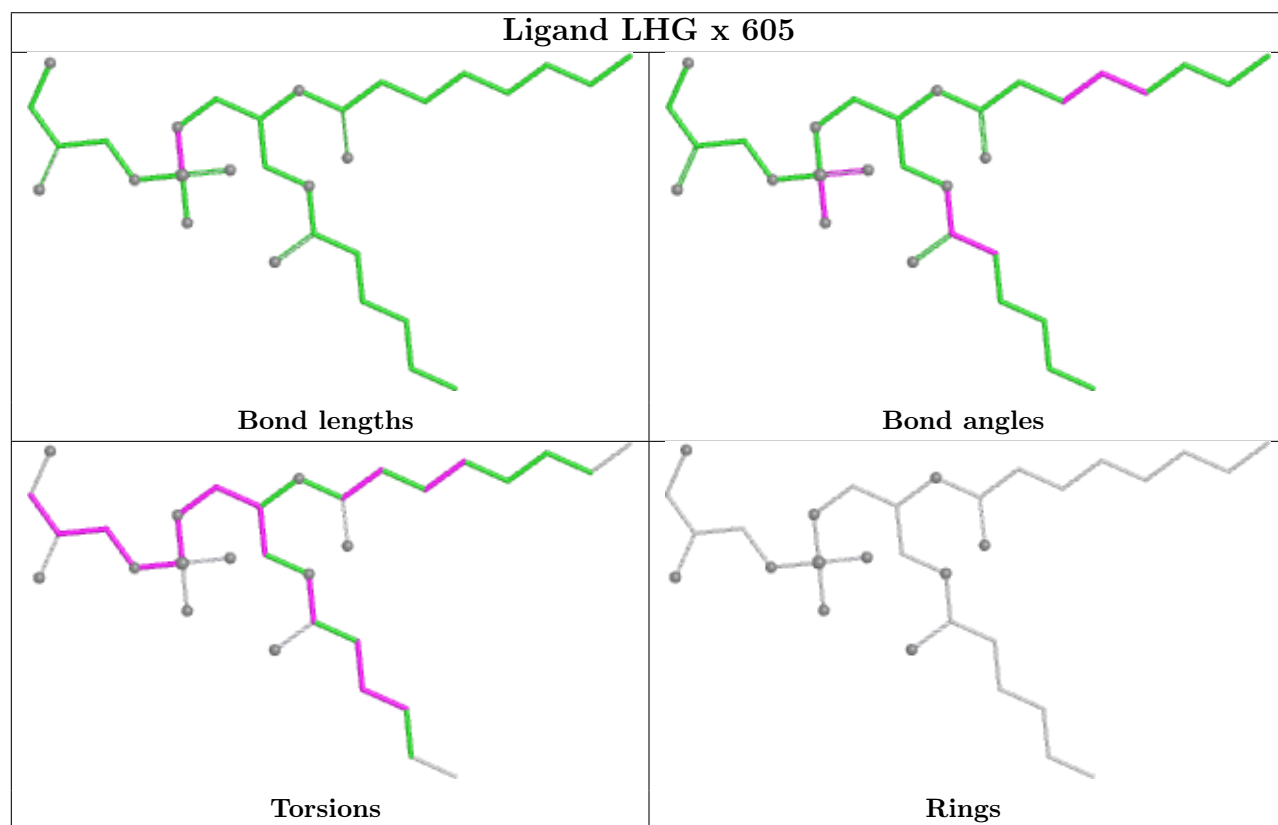
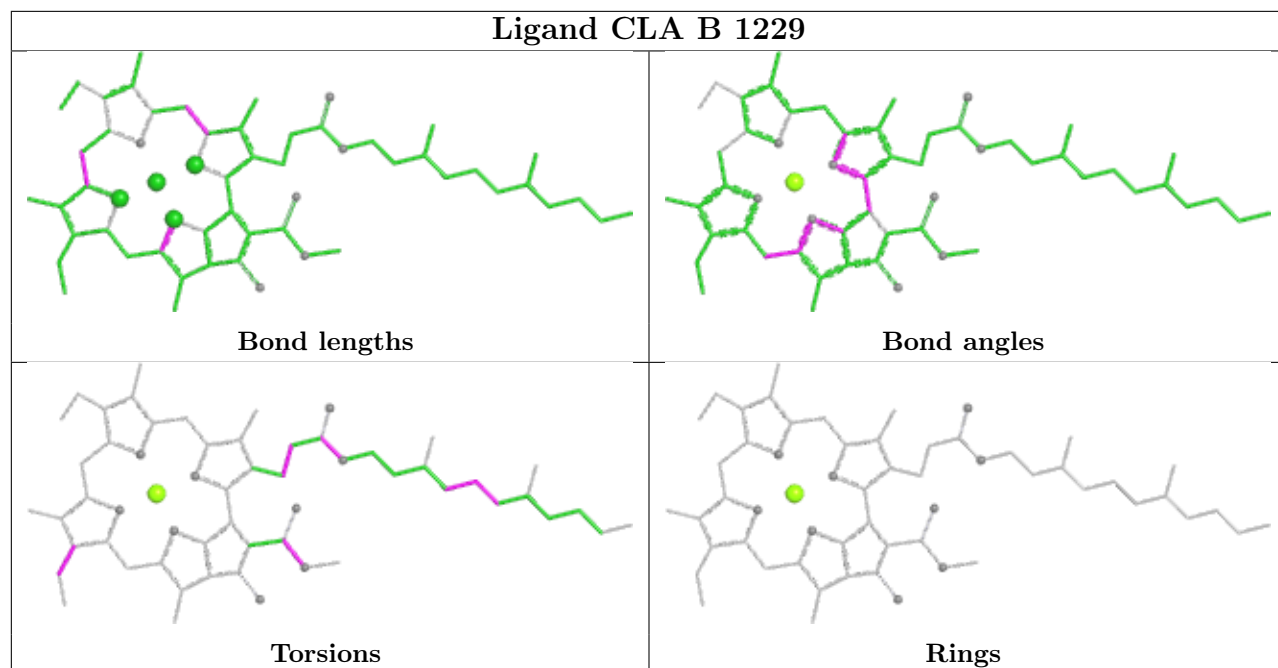




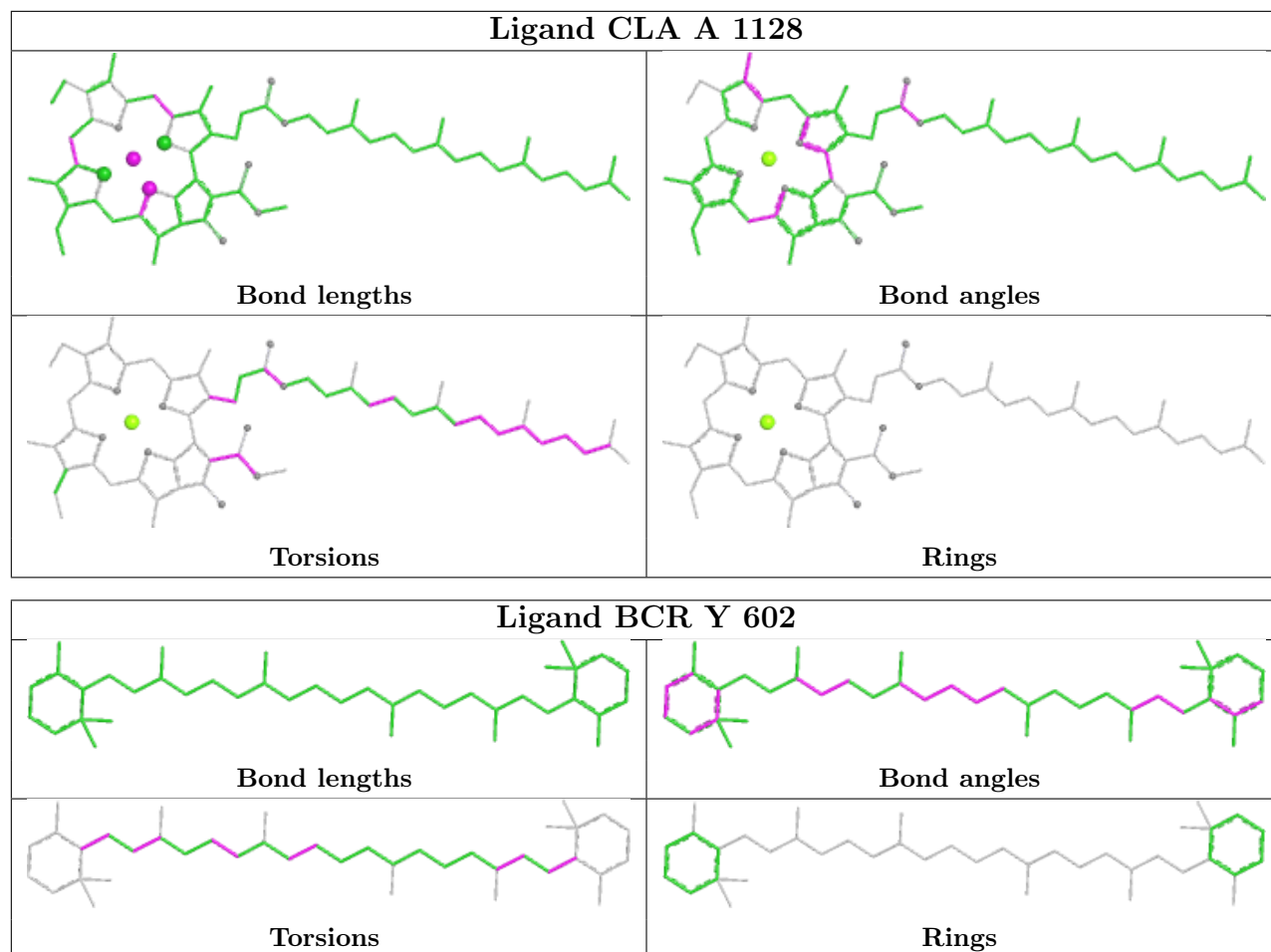




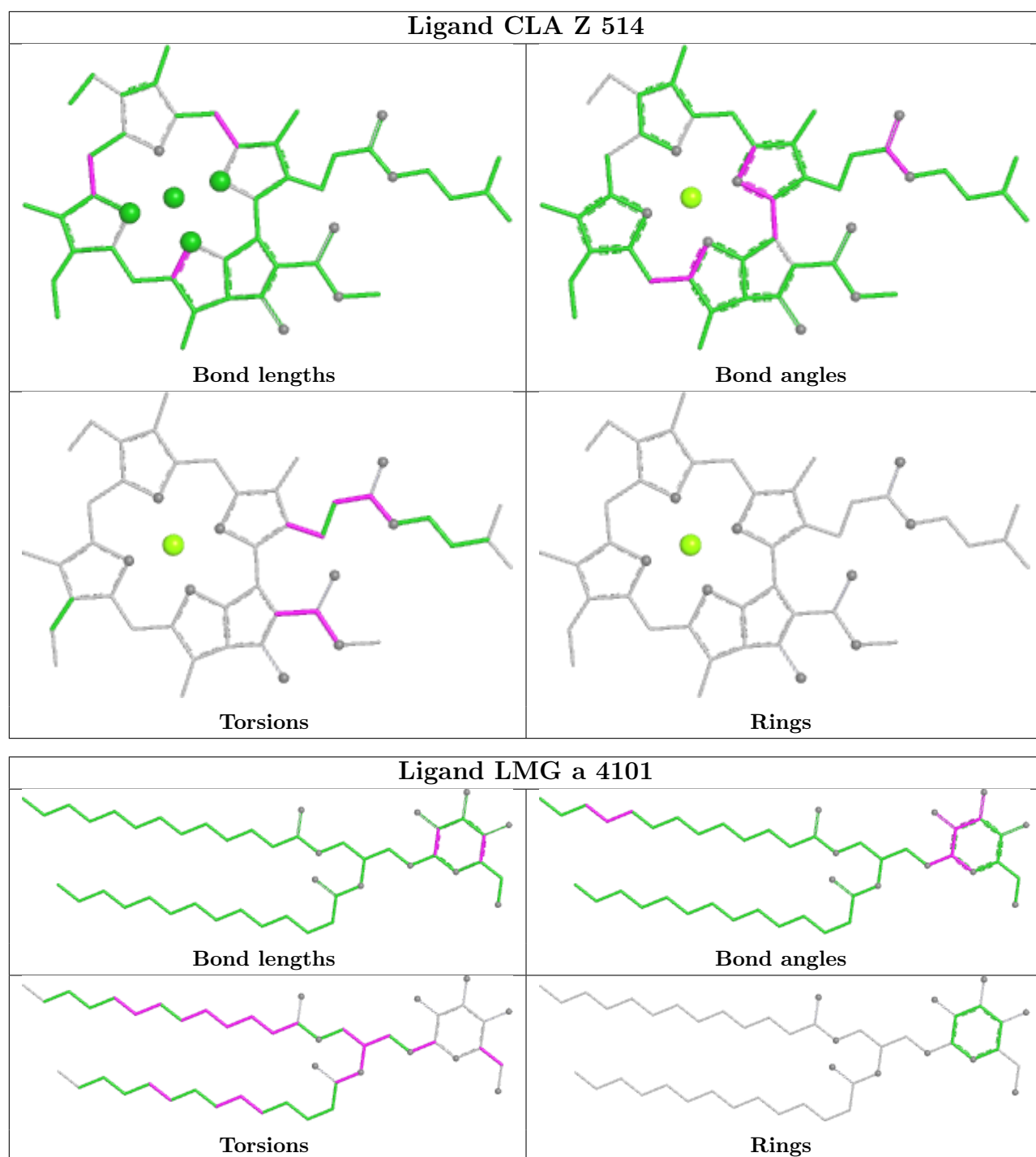




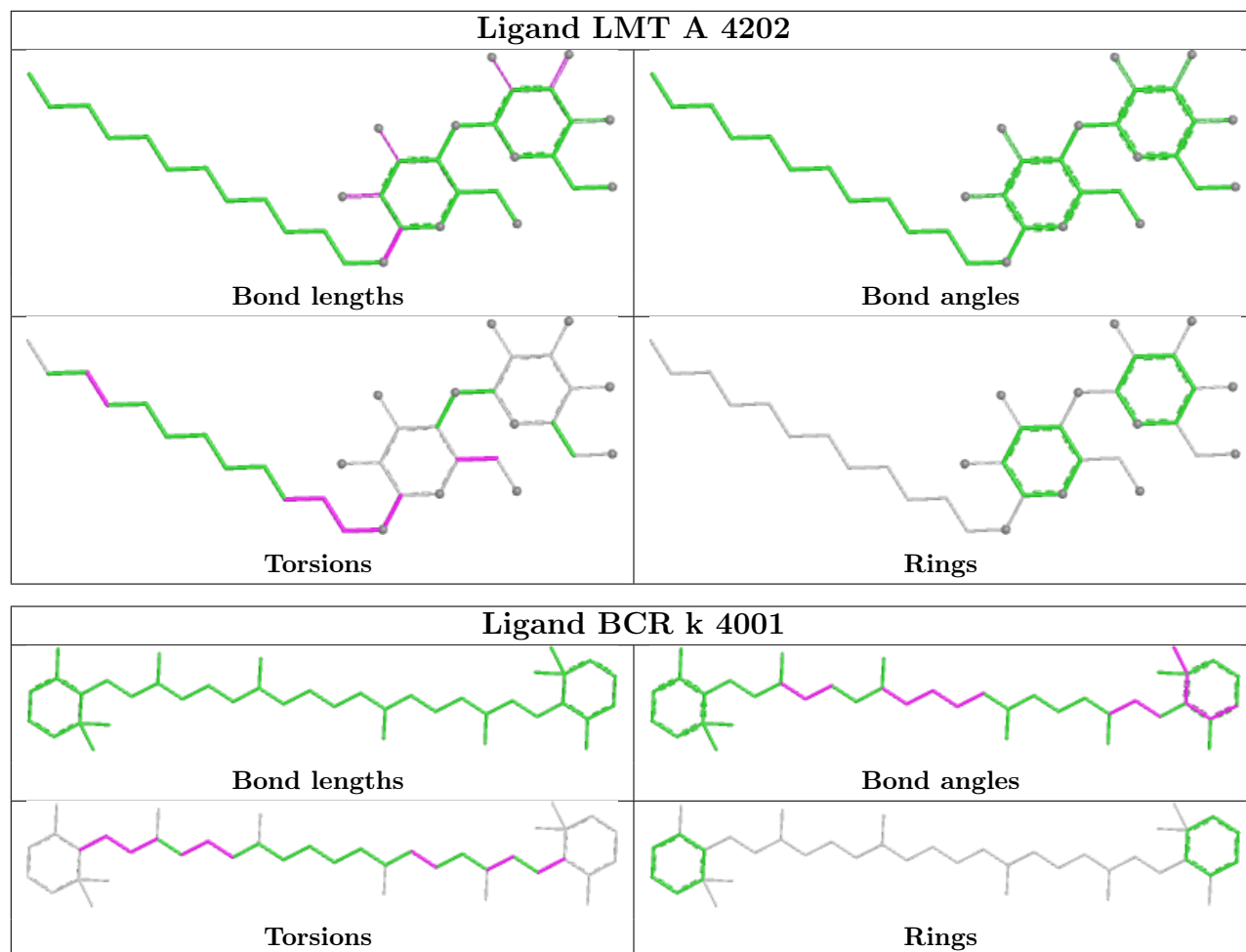




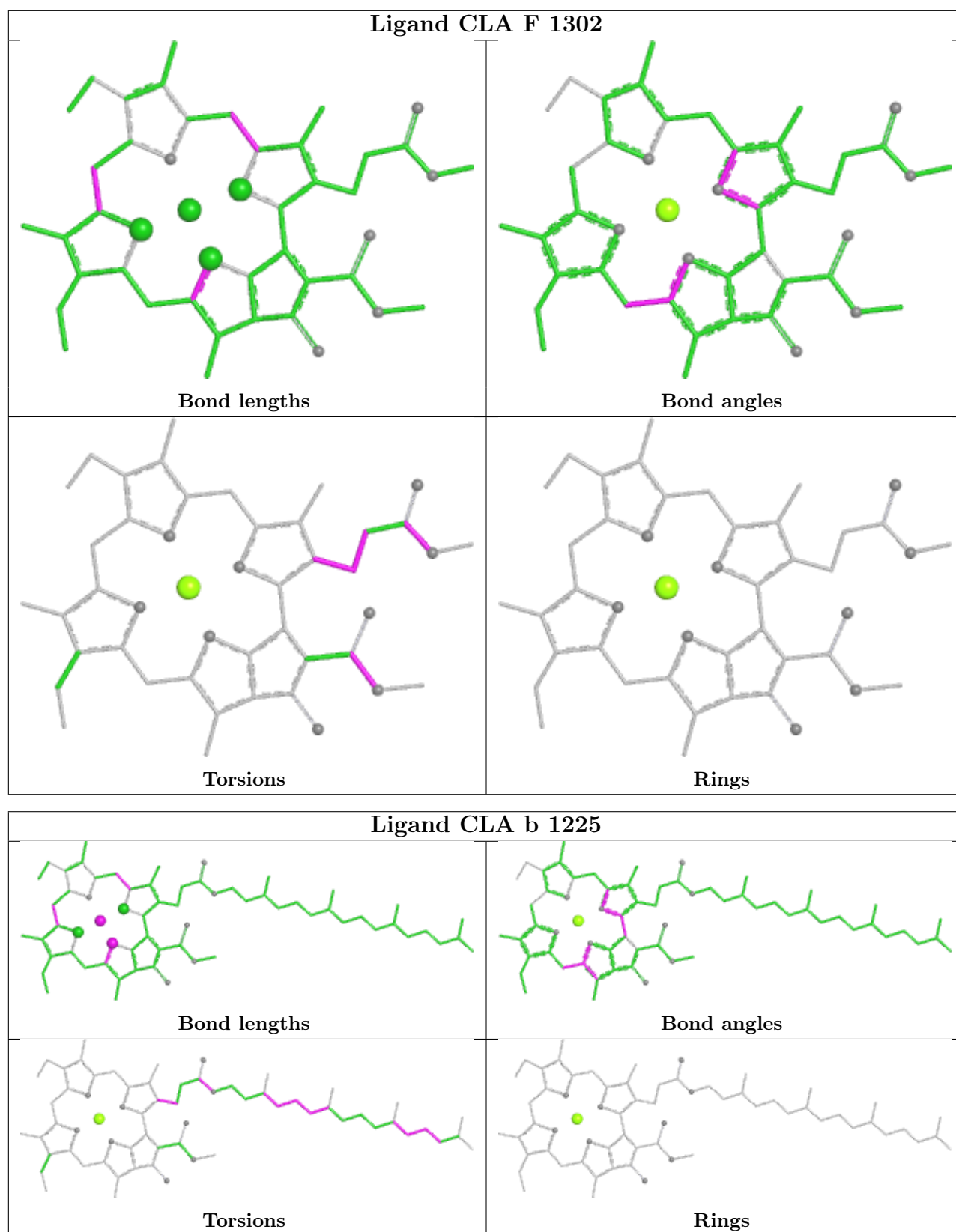




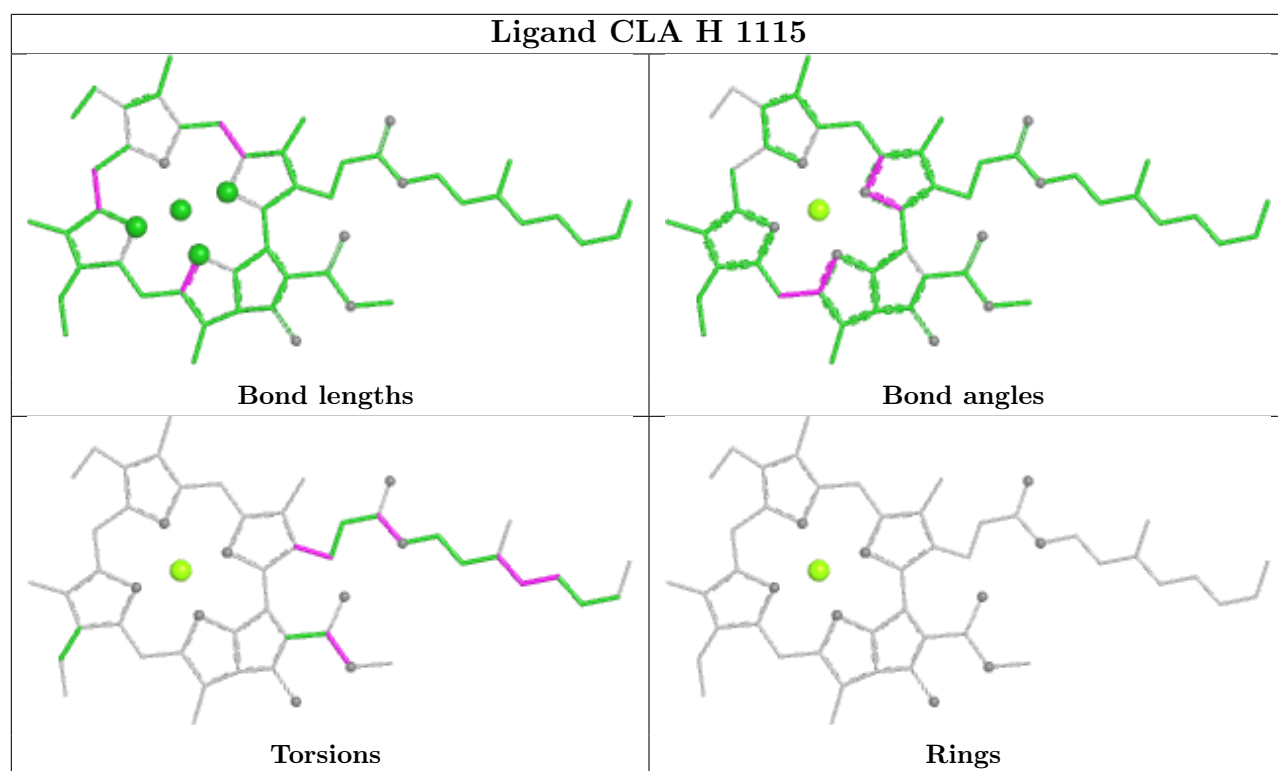




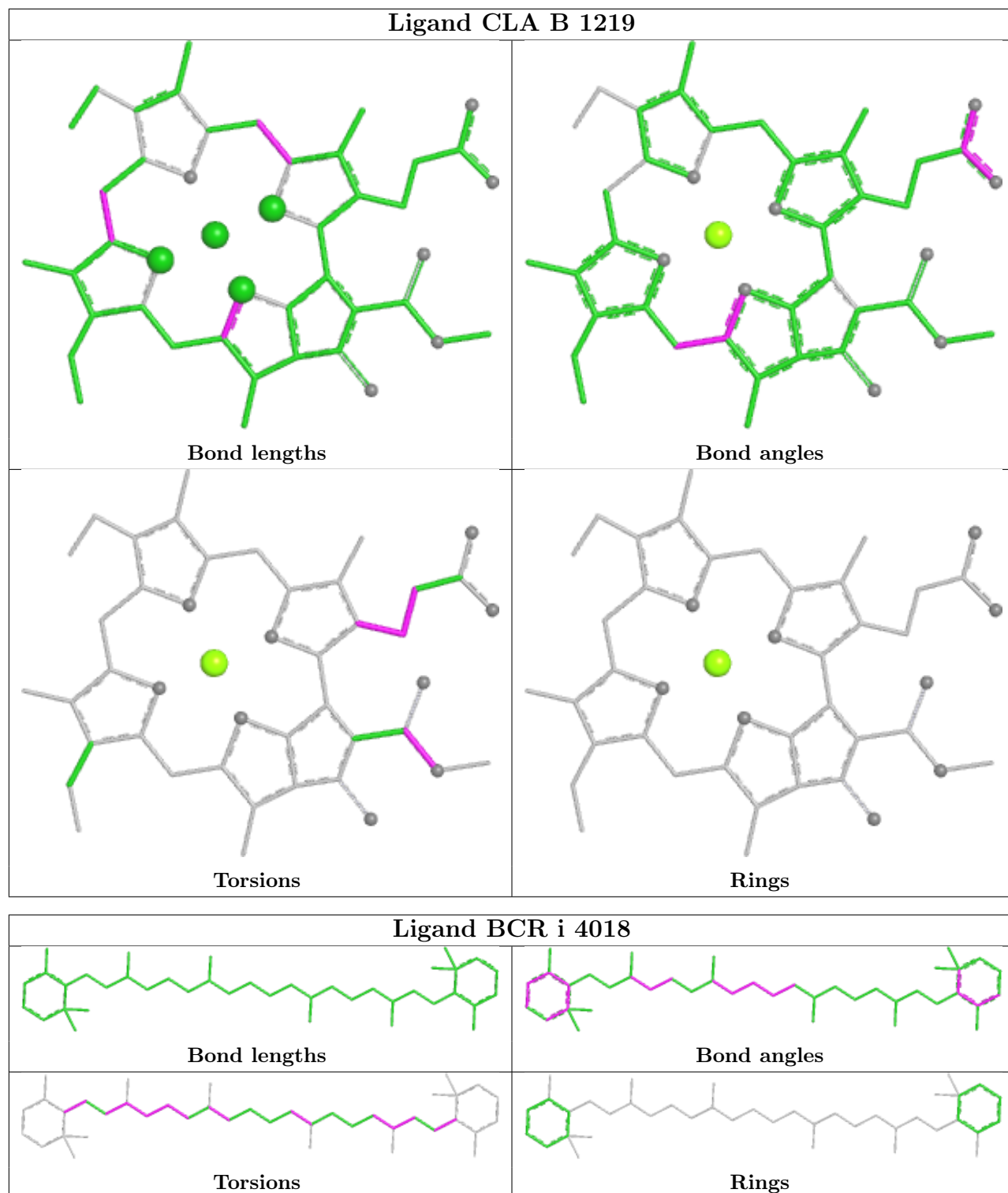






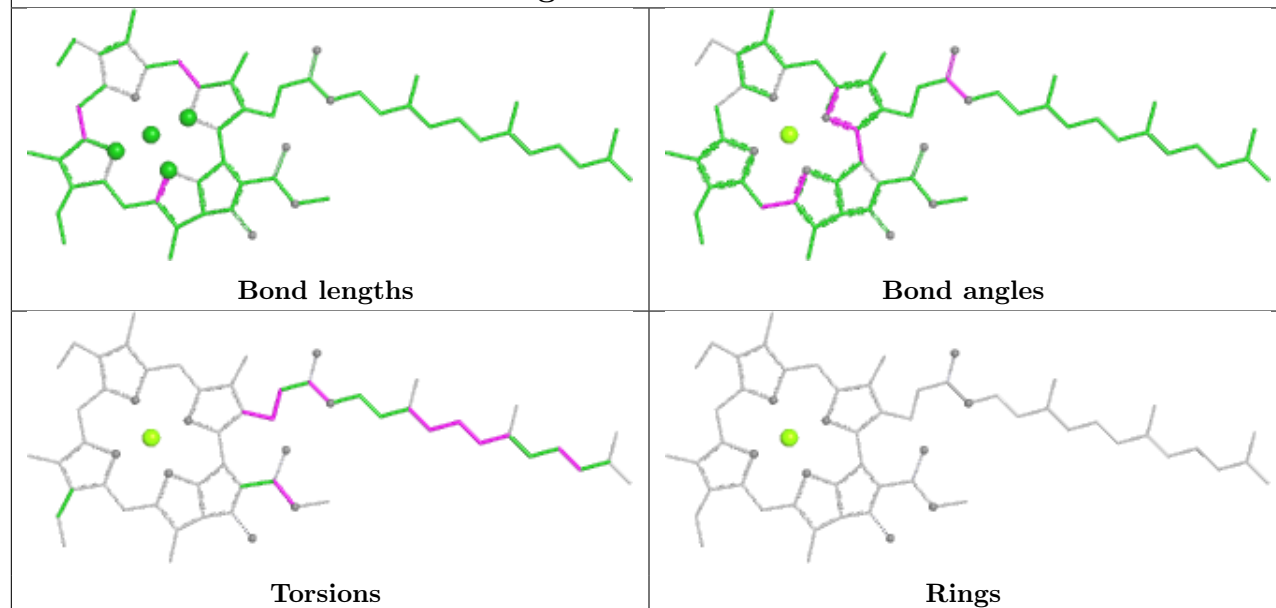




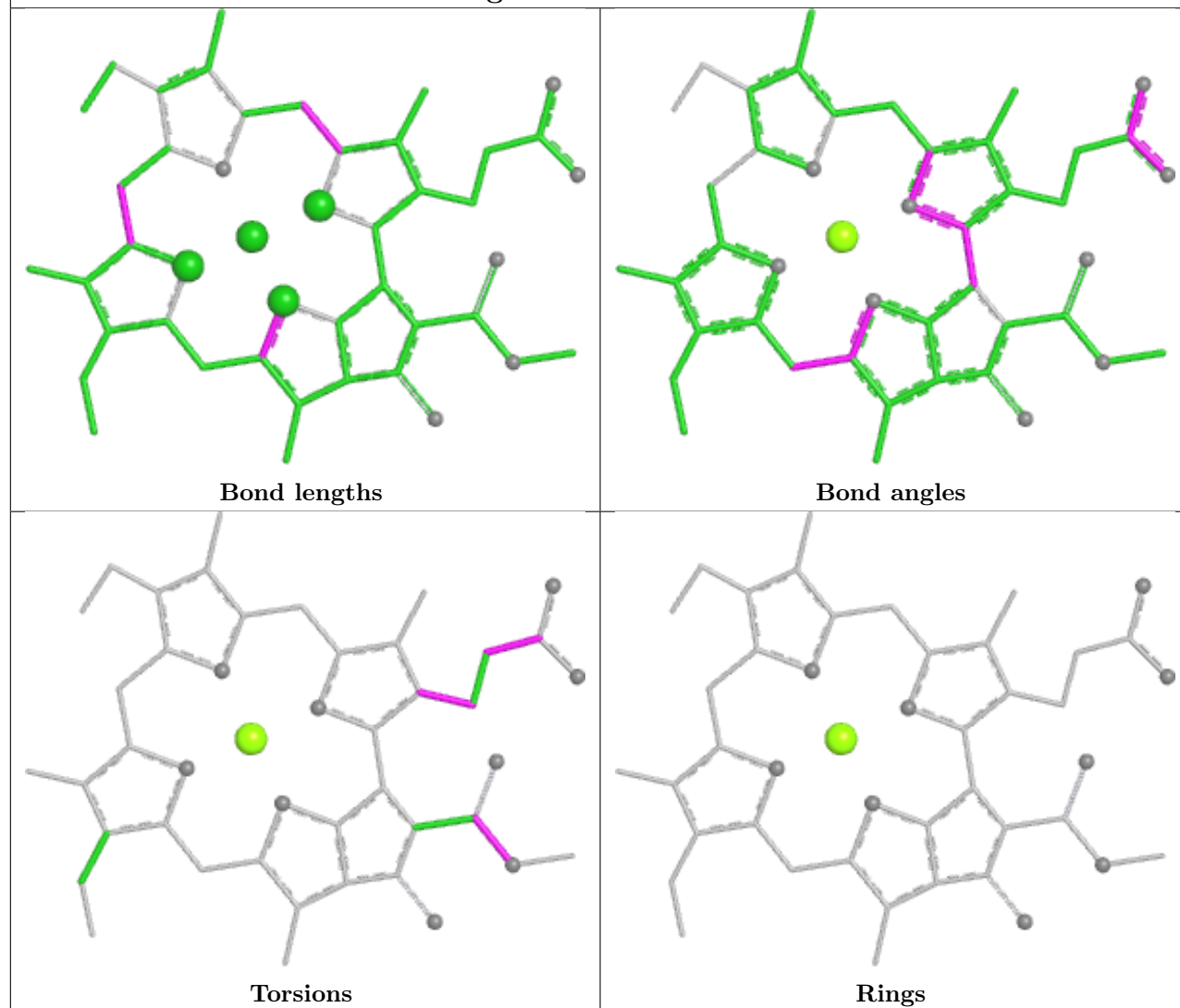




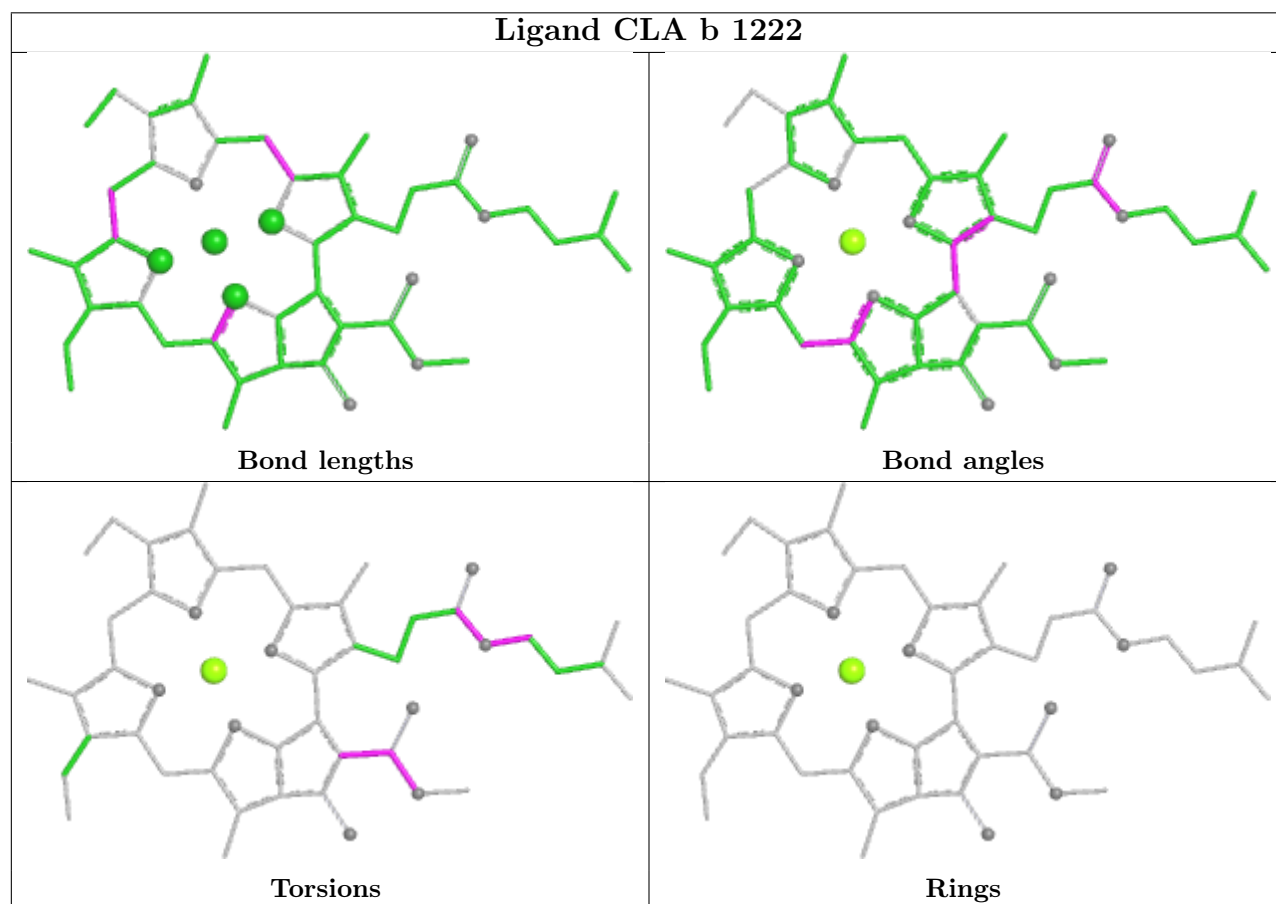
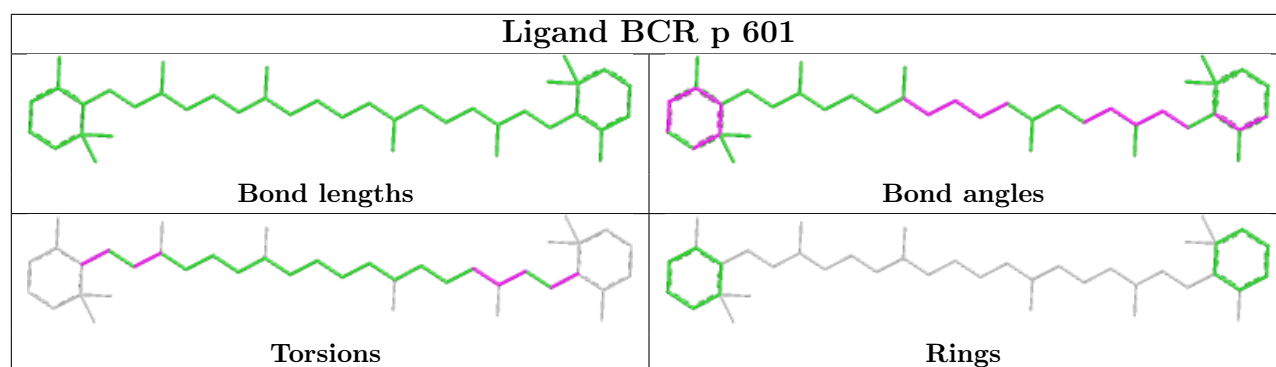
## Ligand CLA s 509



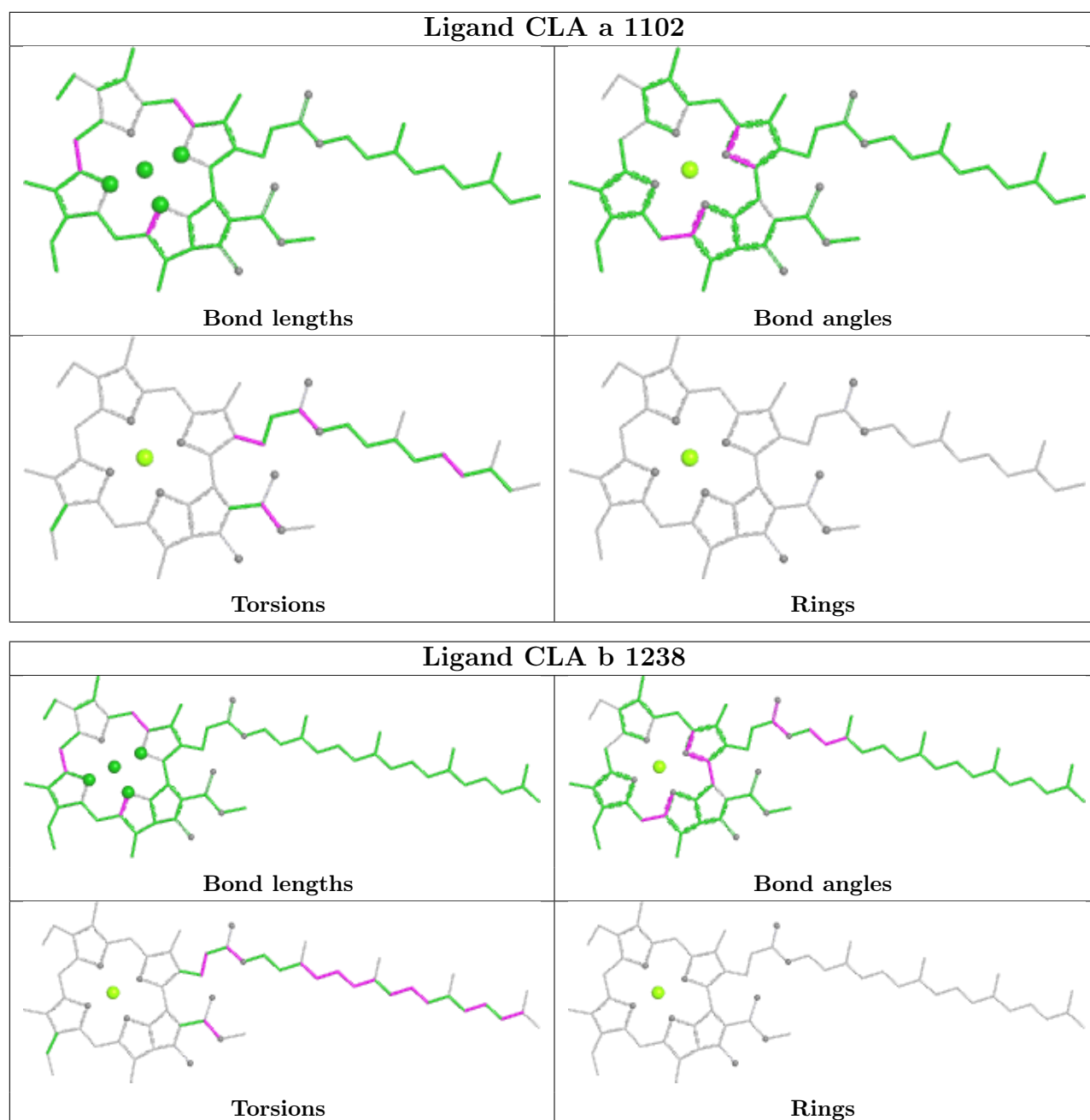
## Ligand CLA b 1208



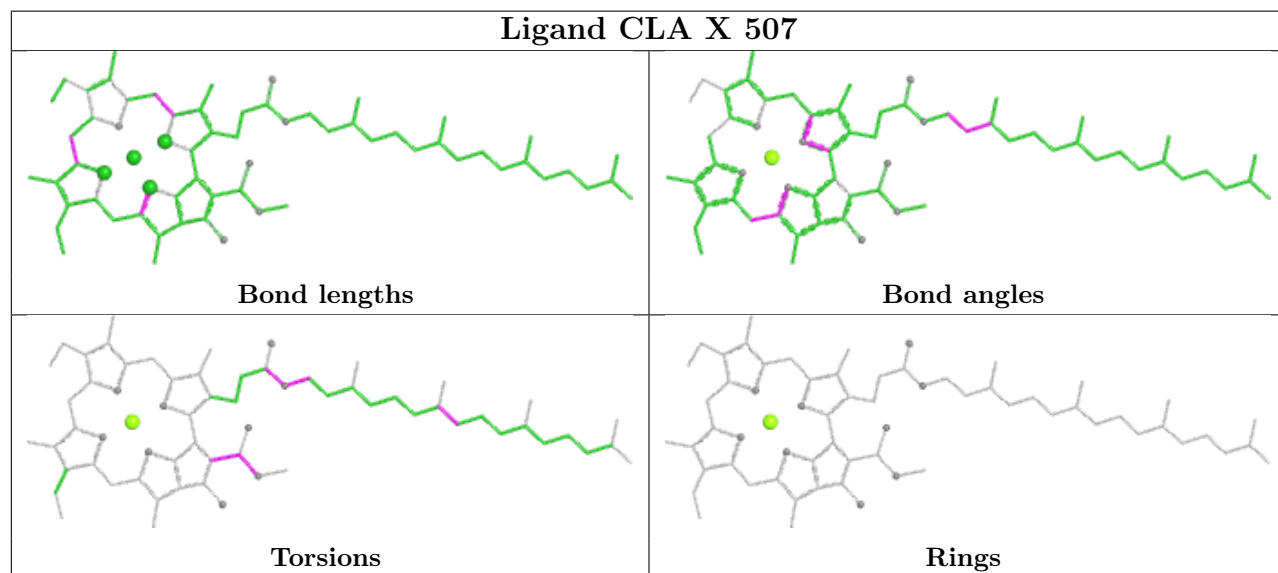
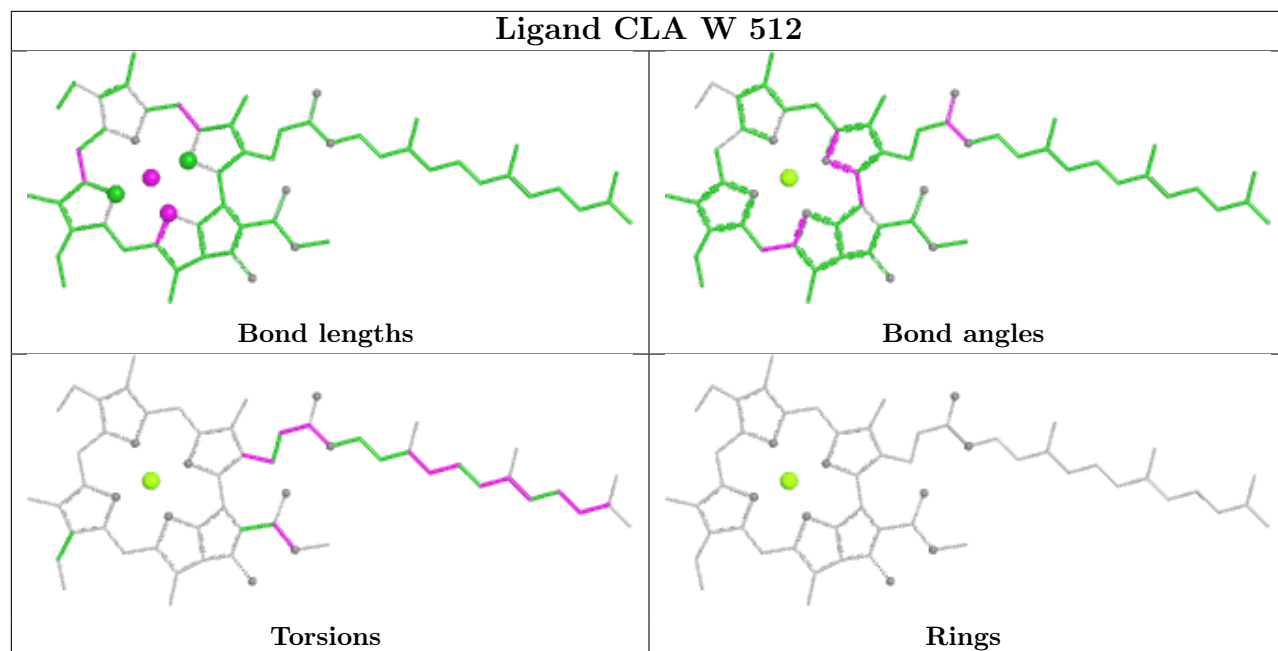




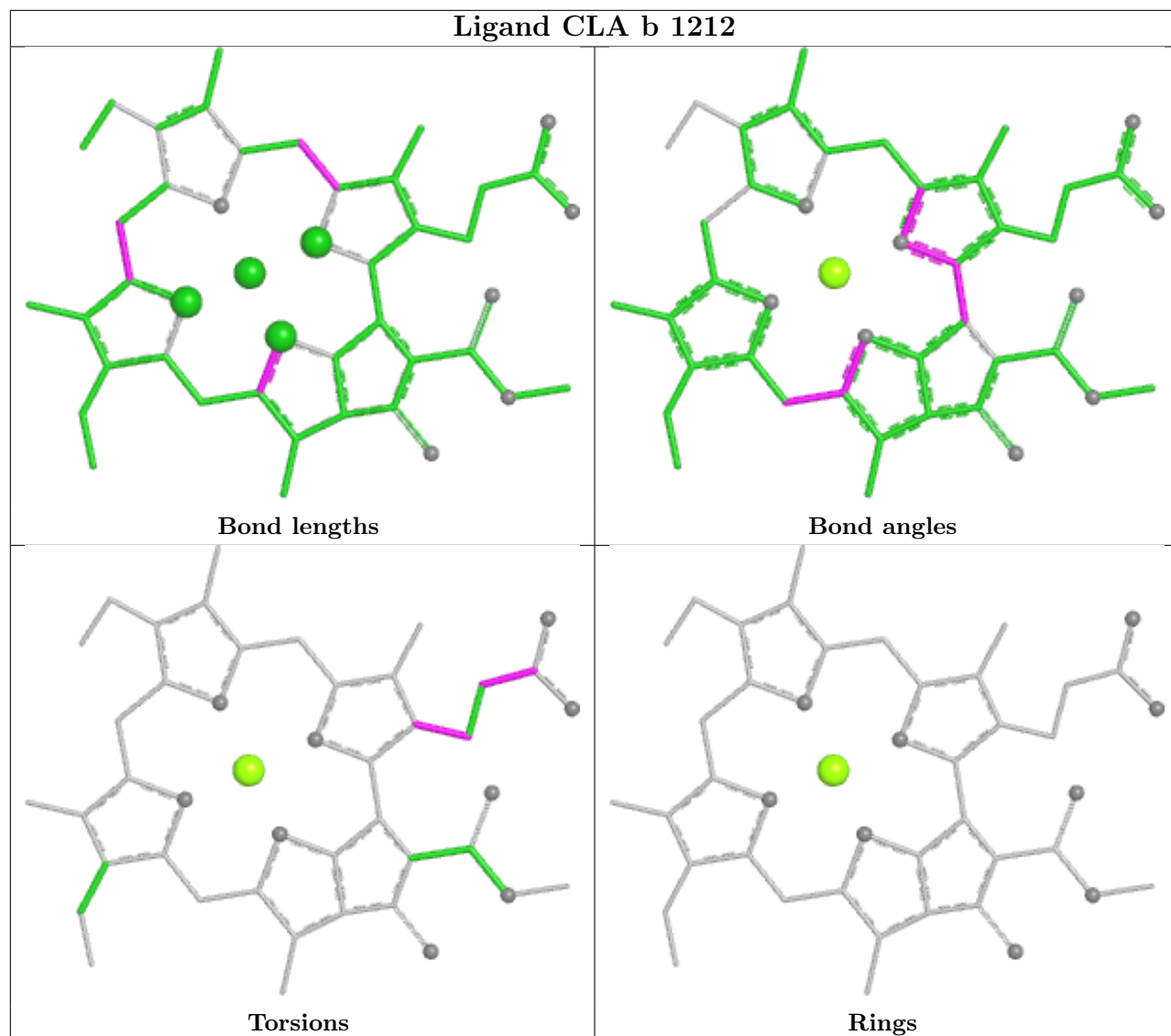






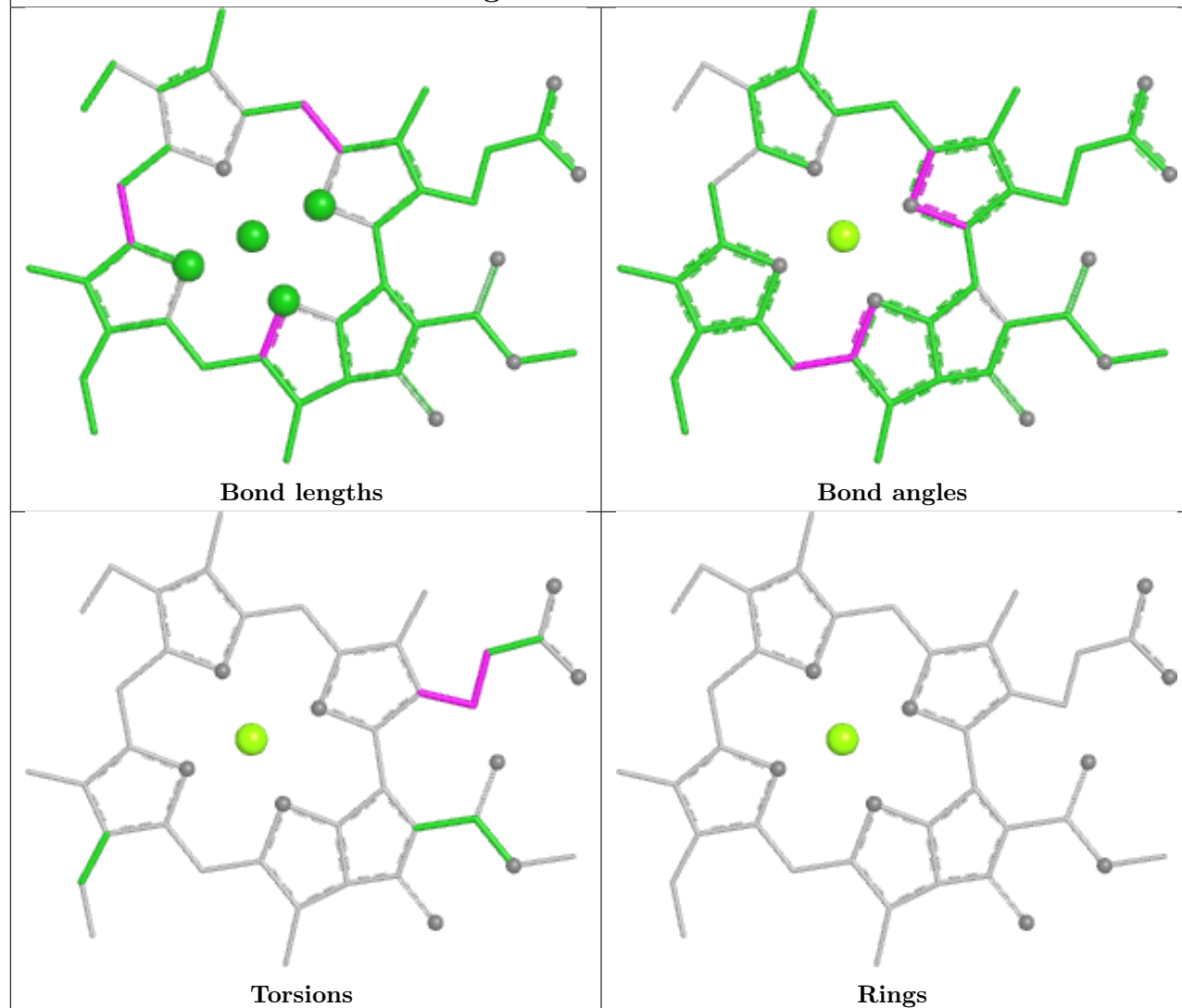




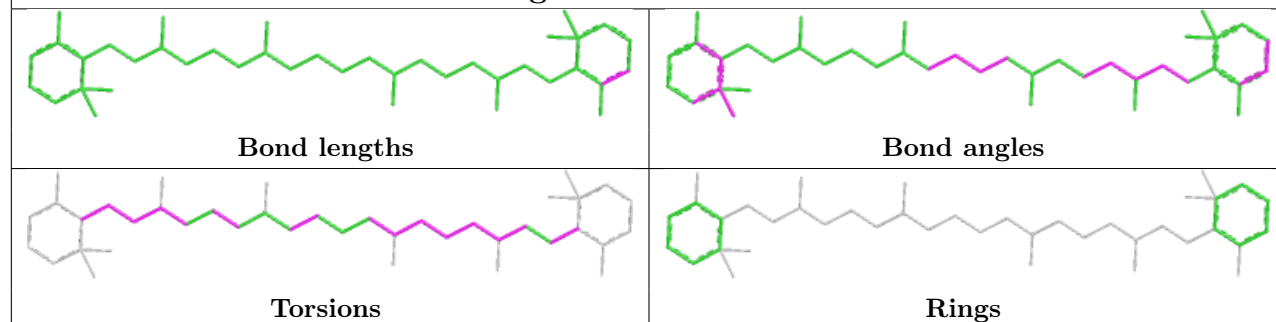




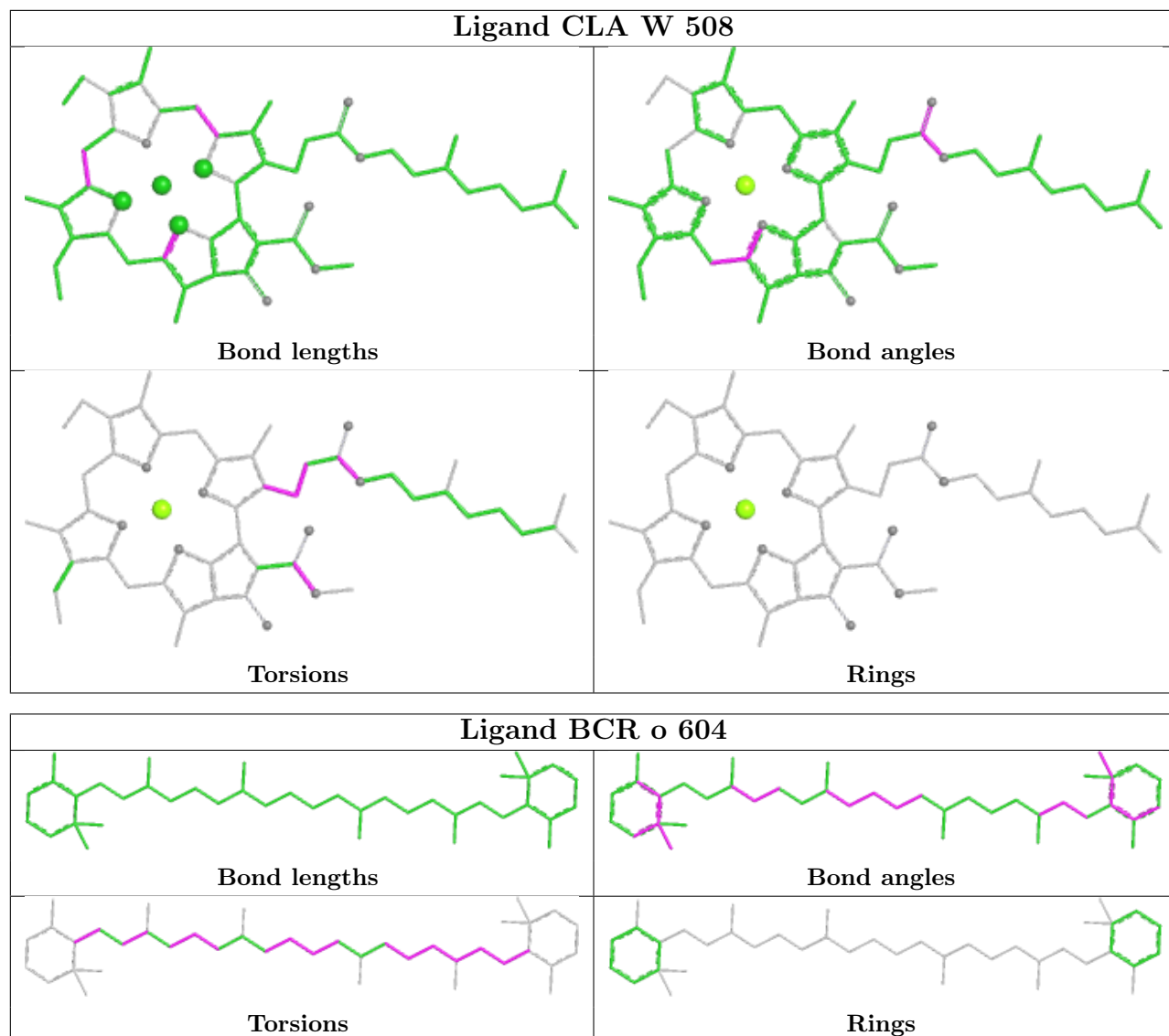
## Ligand CLA G 1209



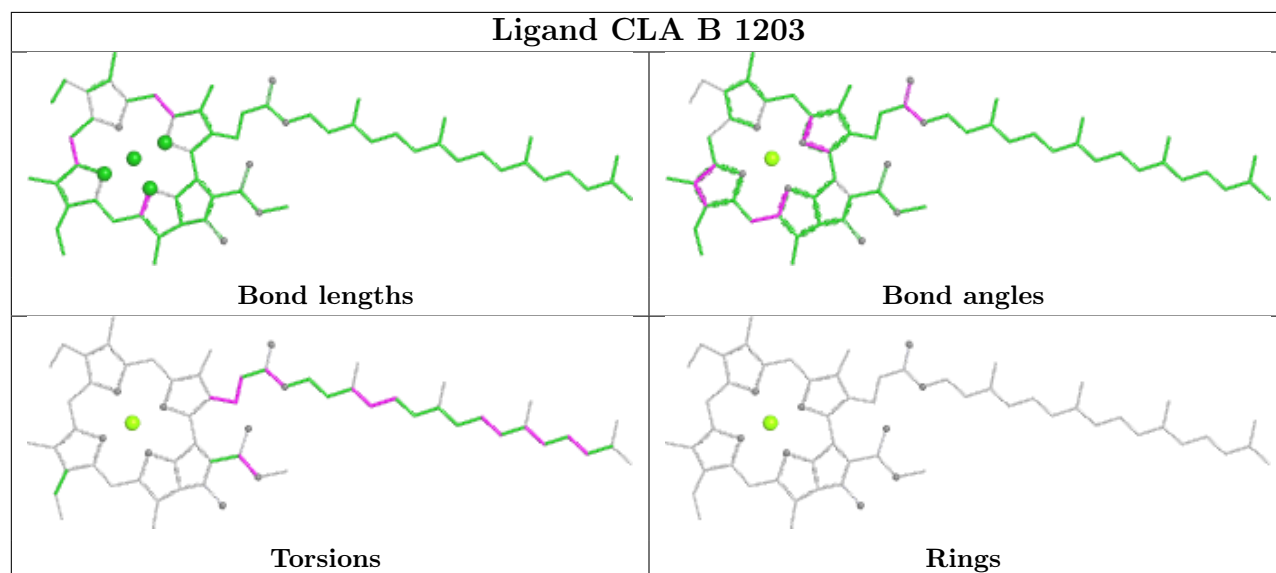
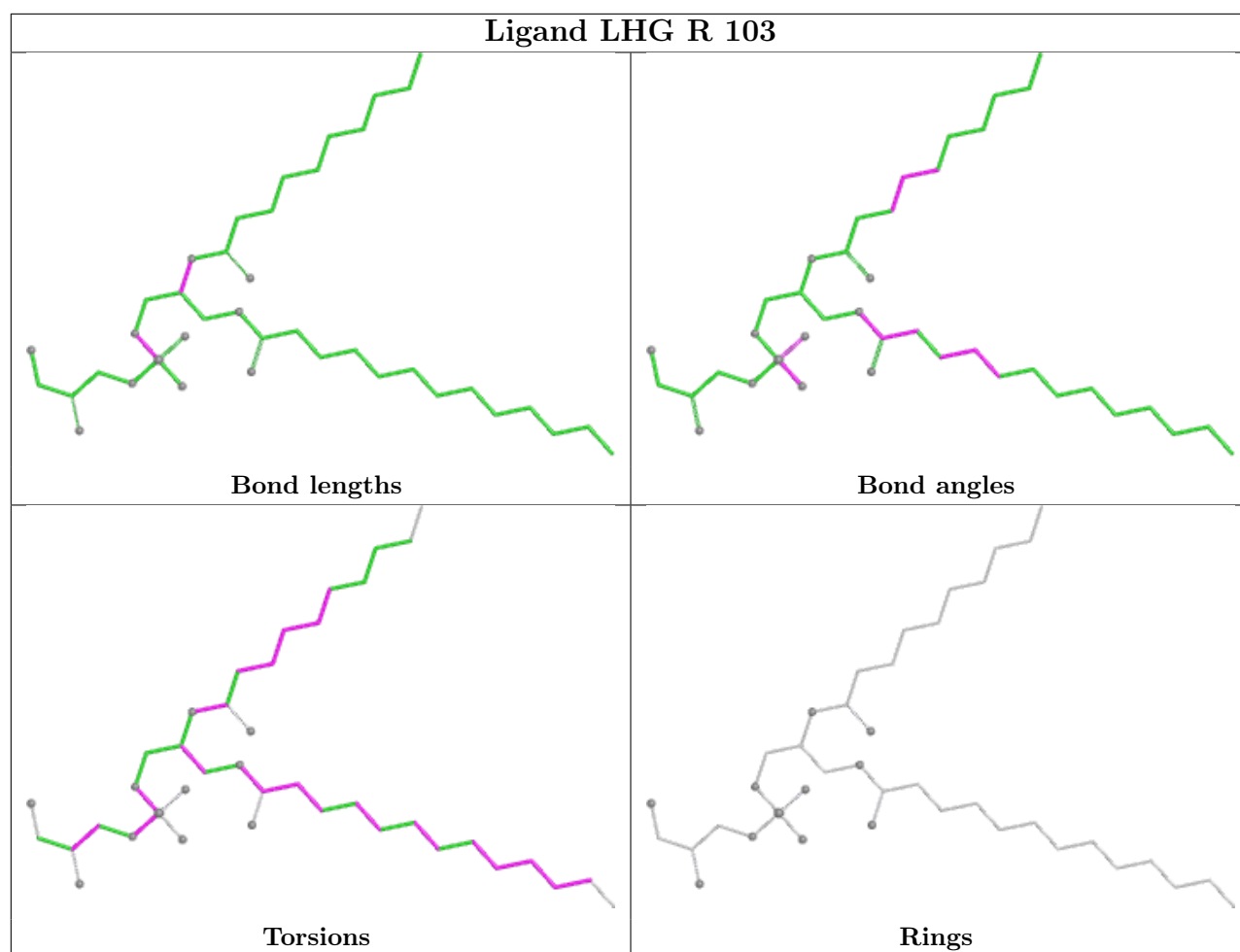
## Ligand BCR 1 4022





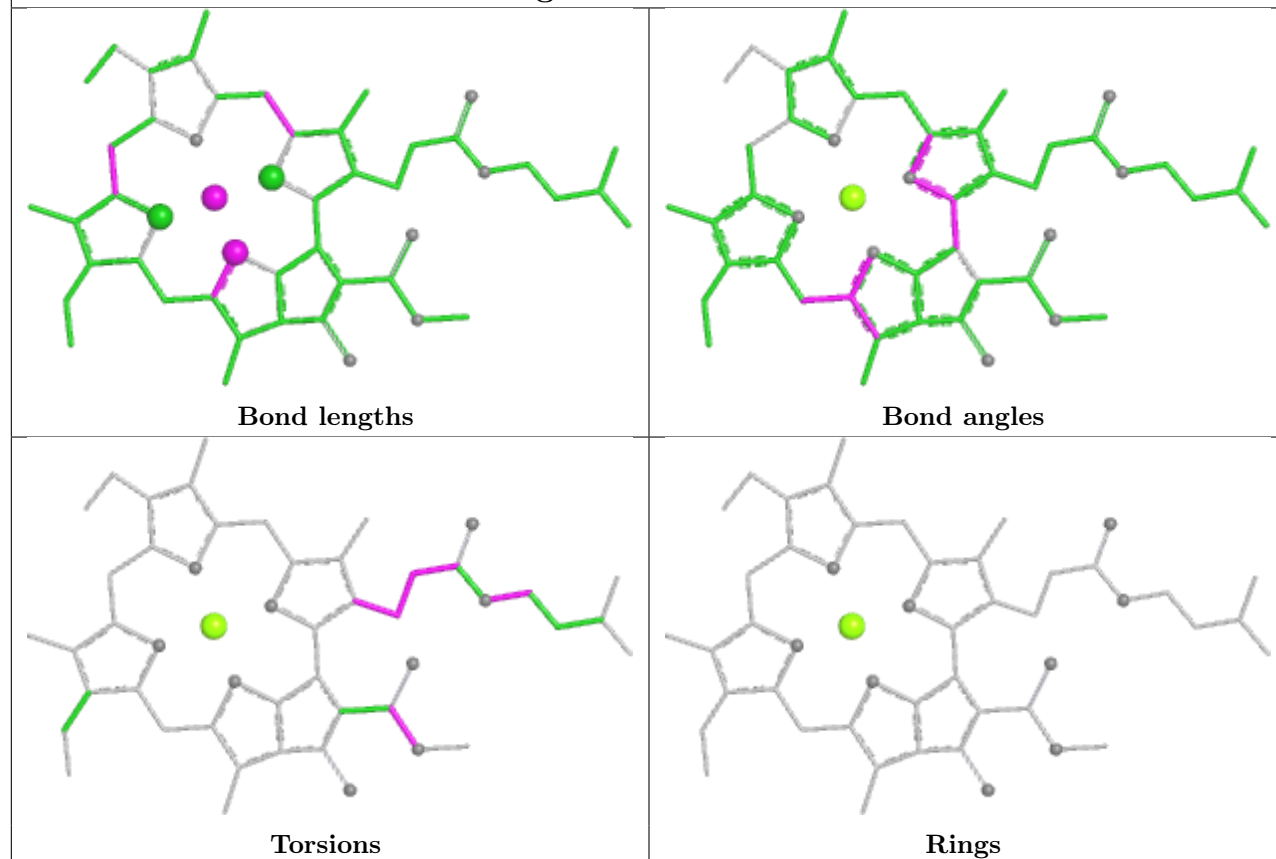




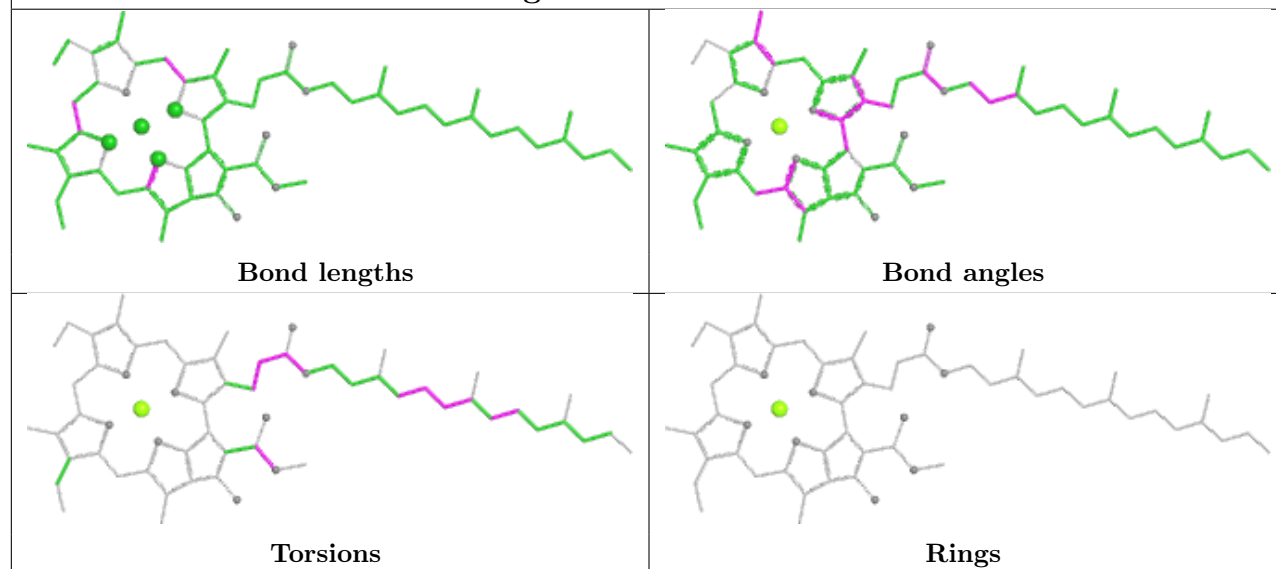




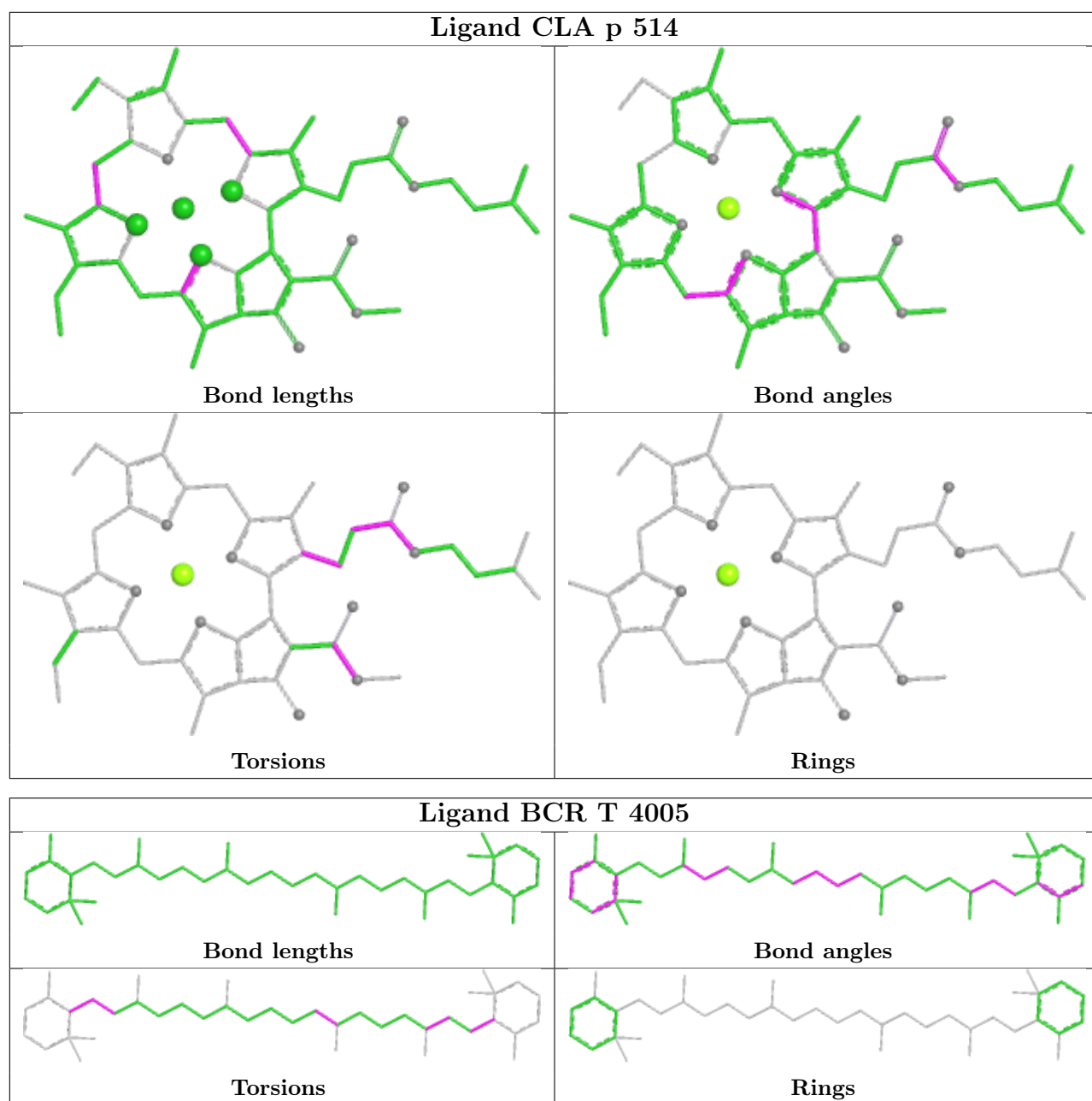
## Ligand CLA o 514



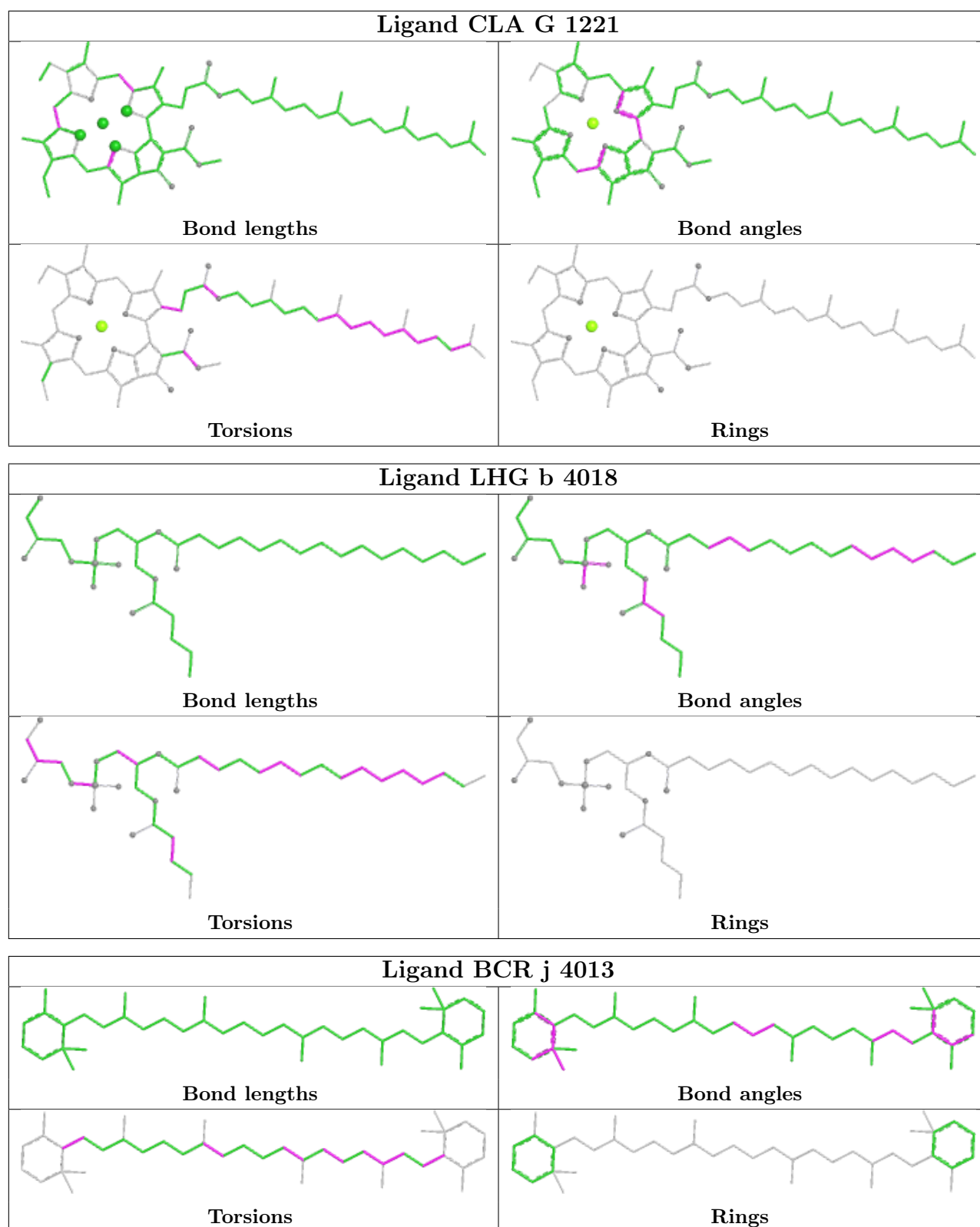
## Ligand CLA B 1235



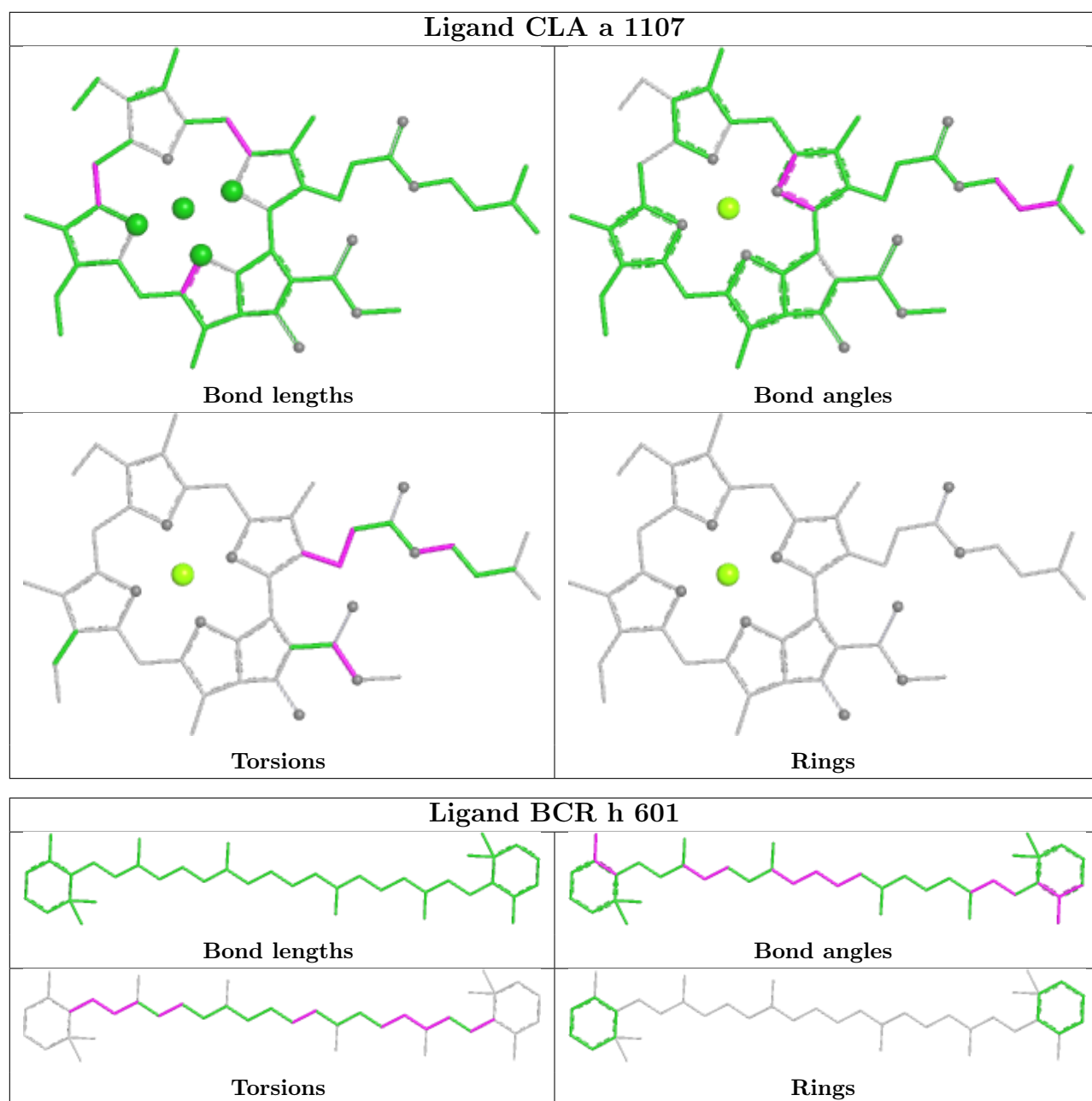




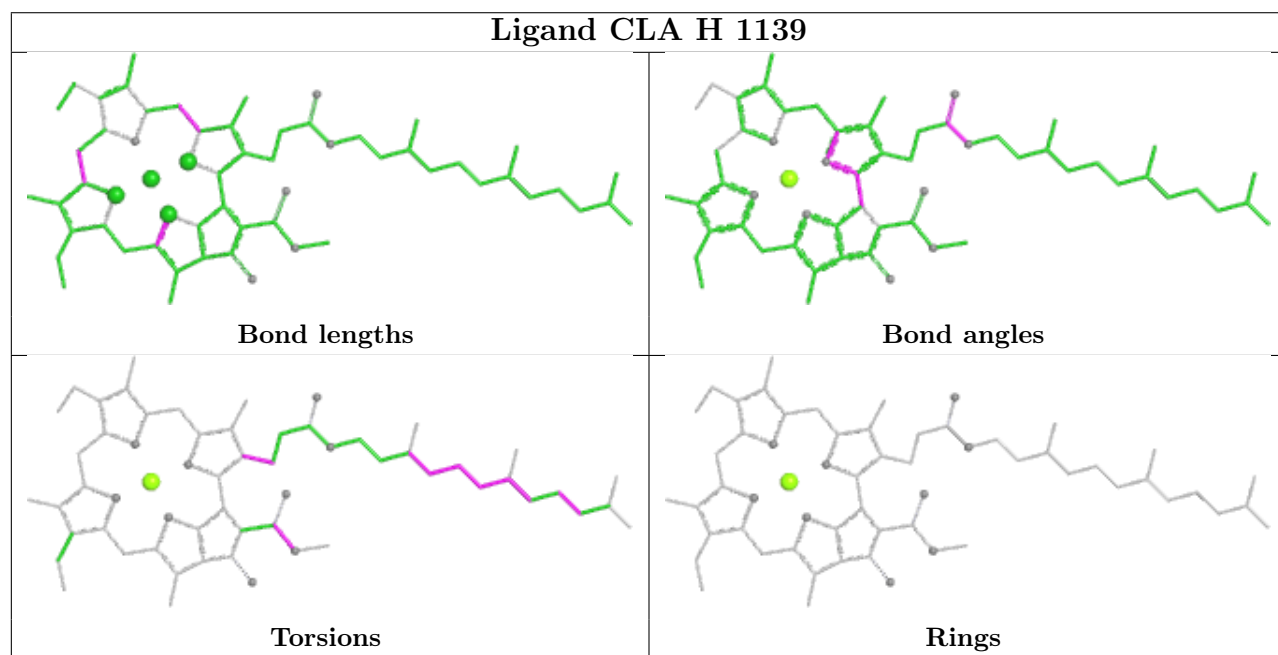
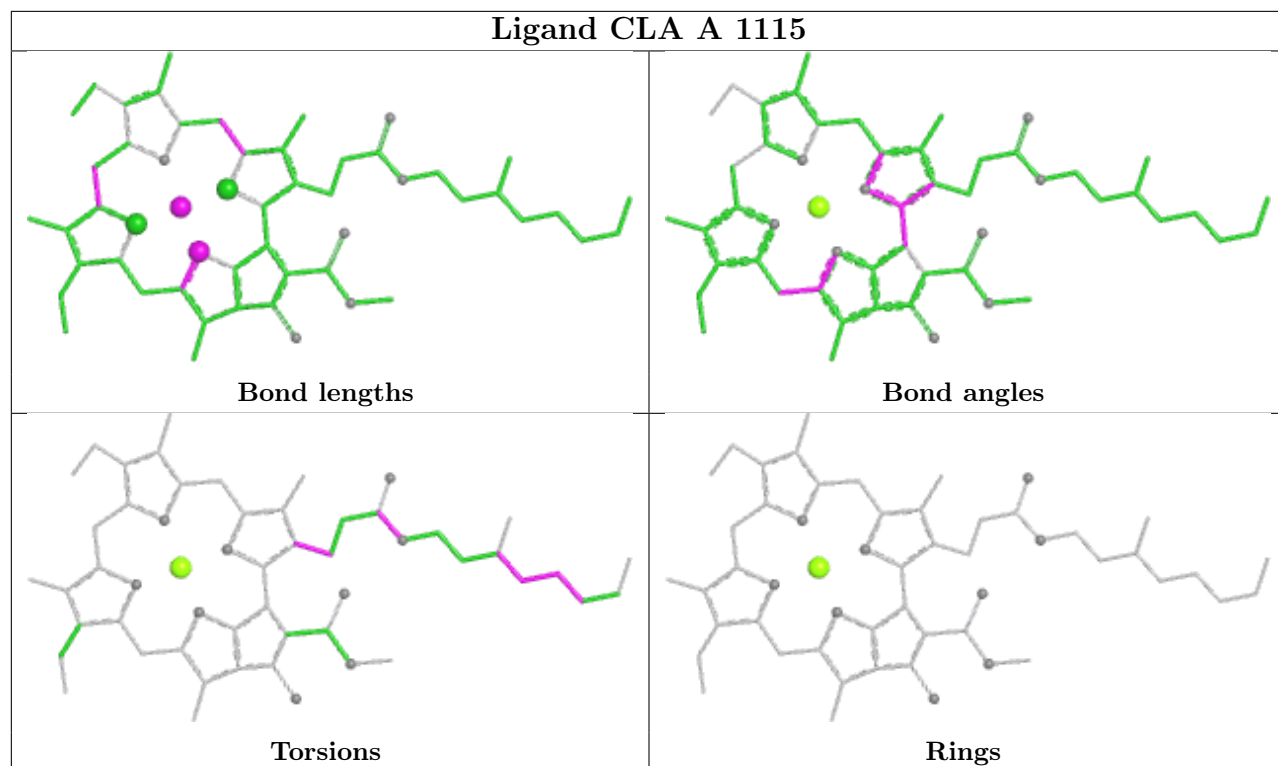




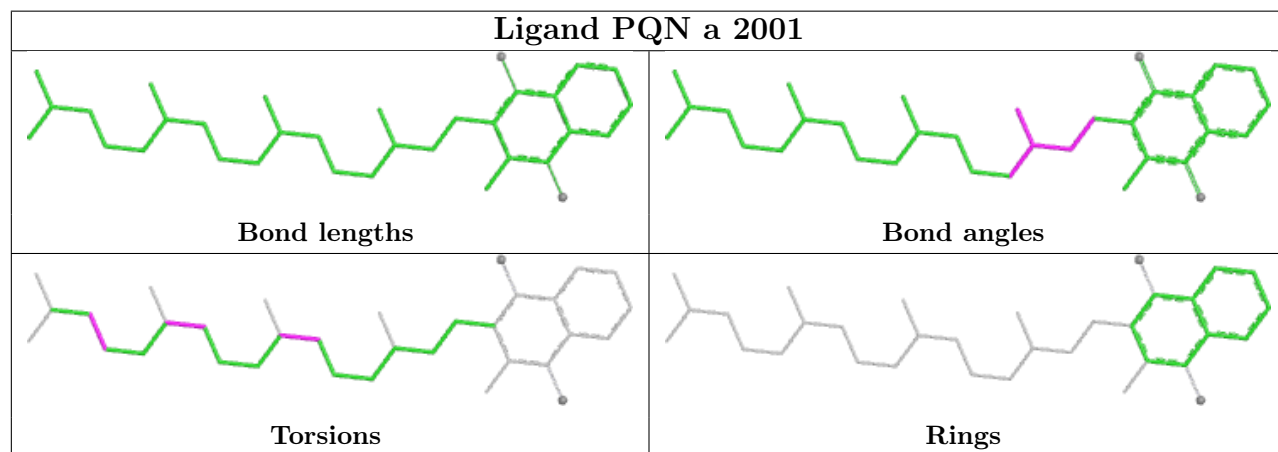
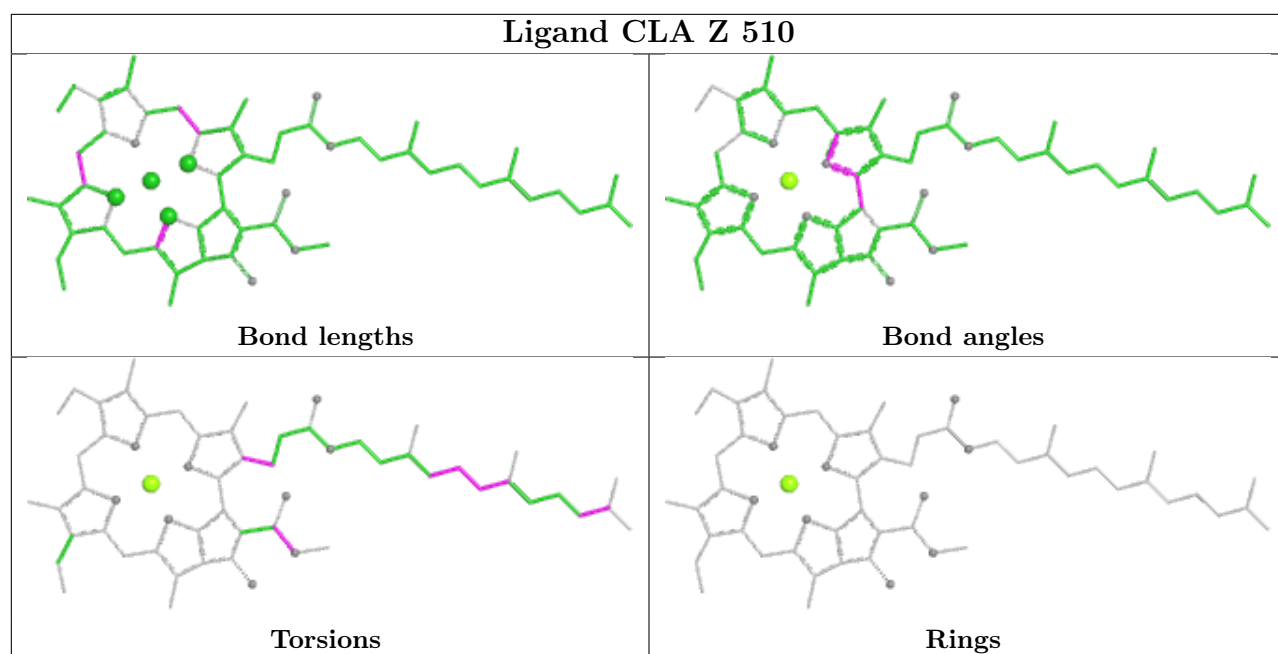




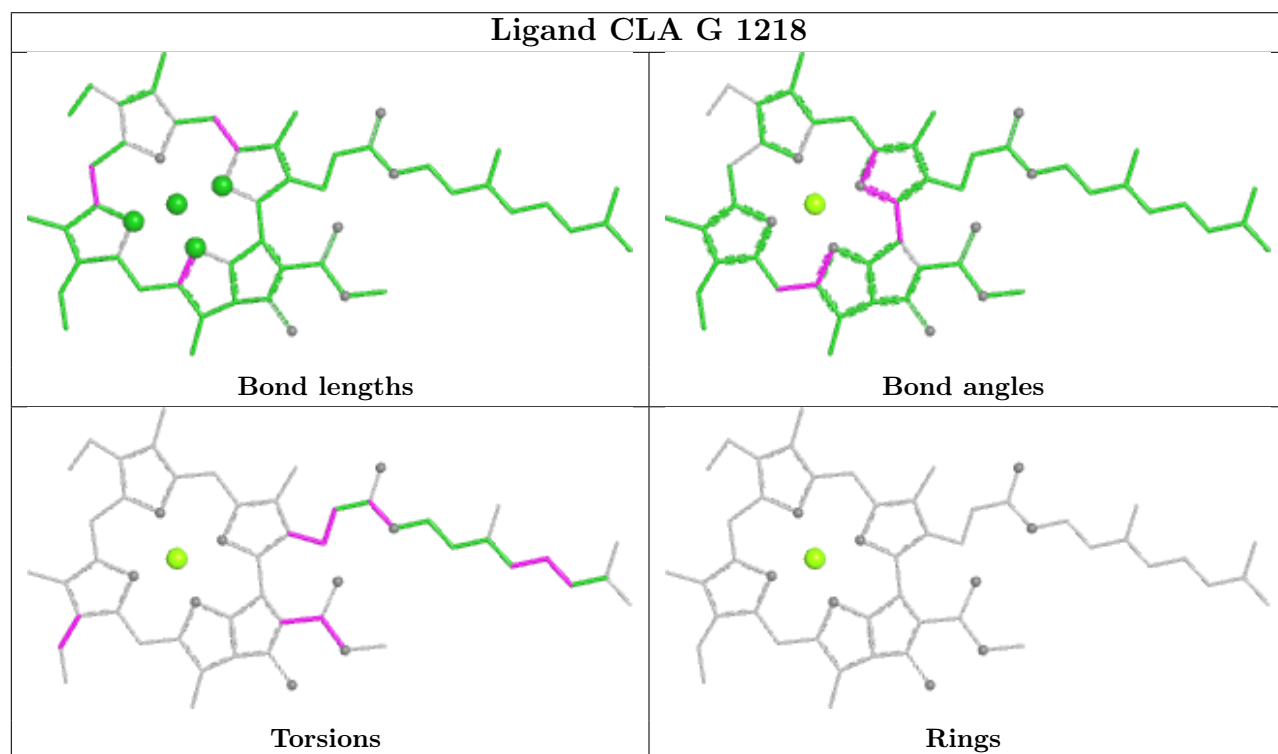
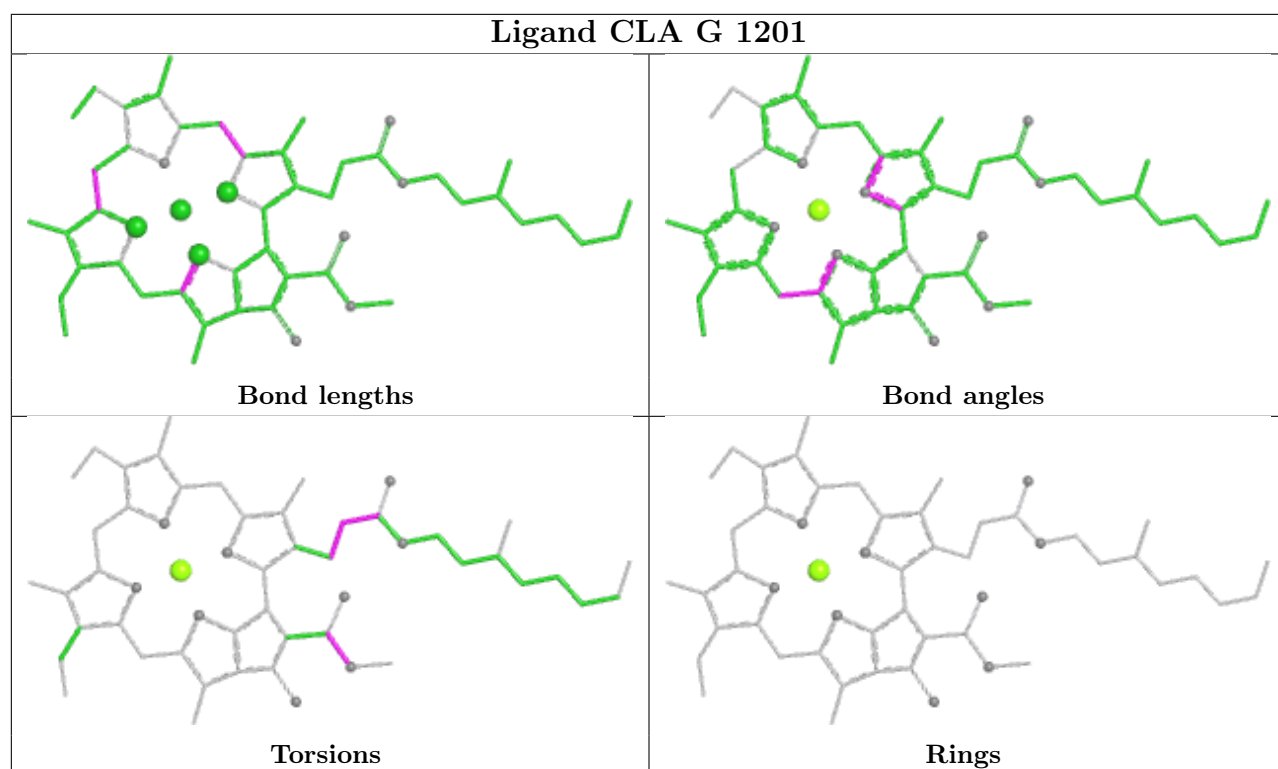




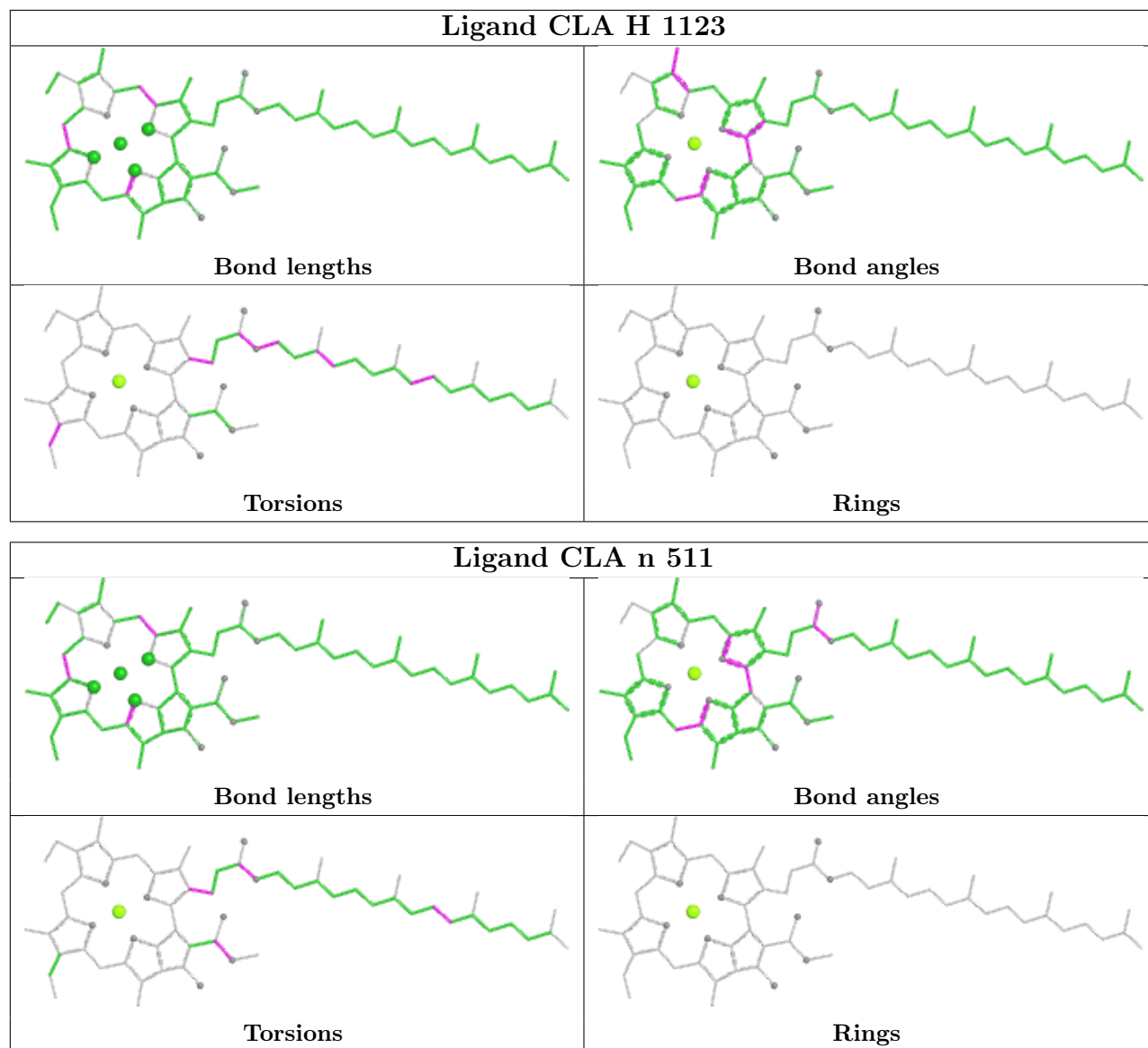




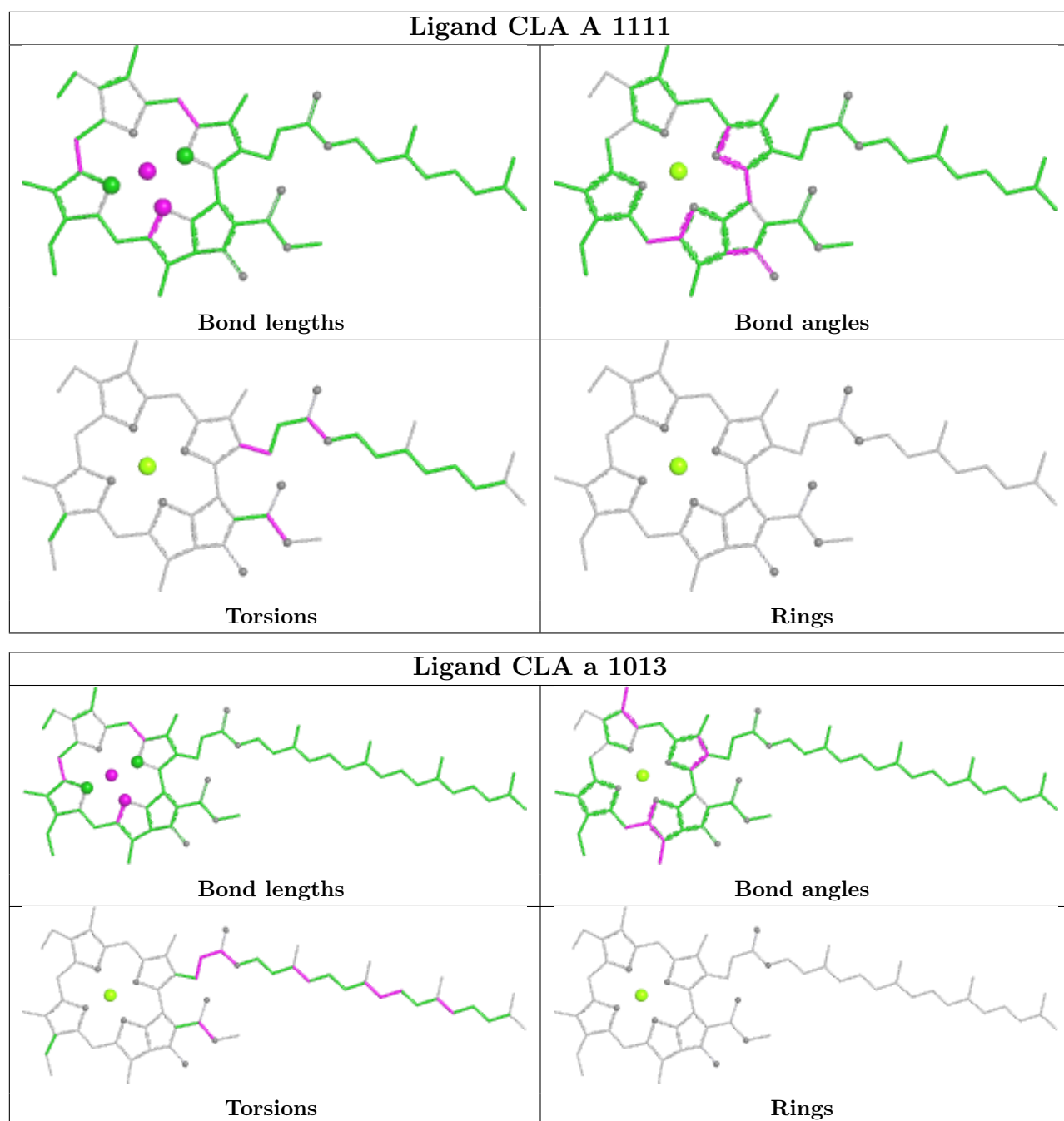




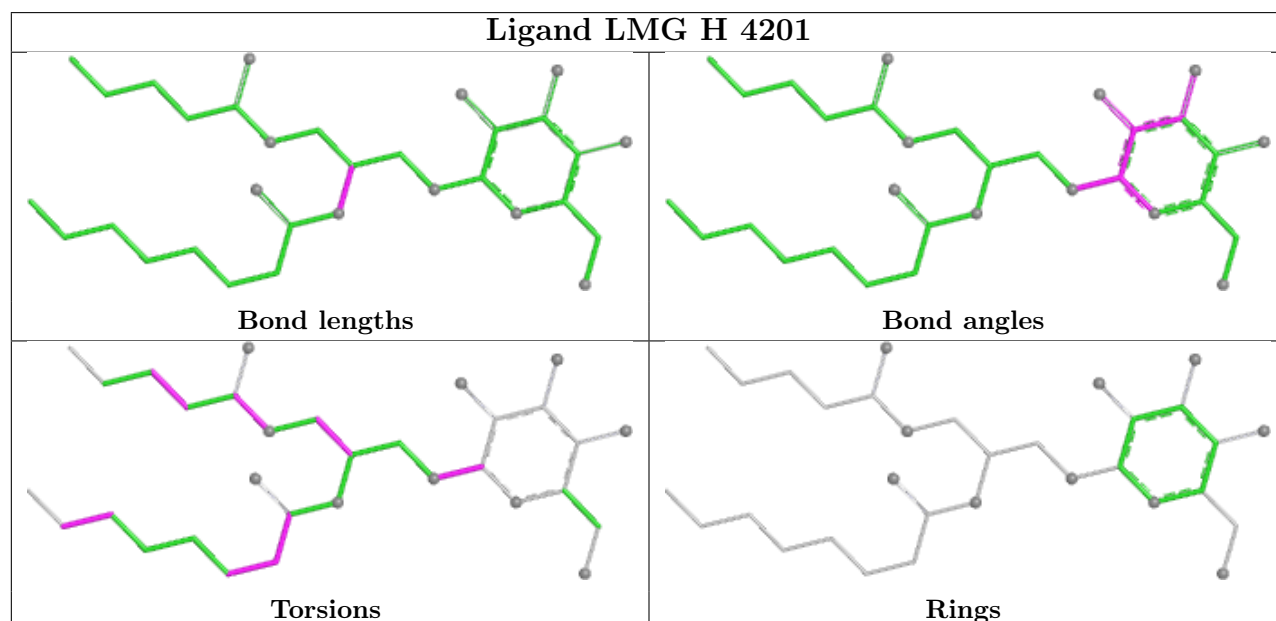
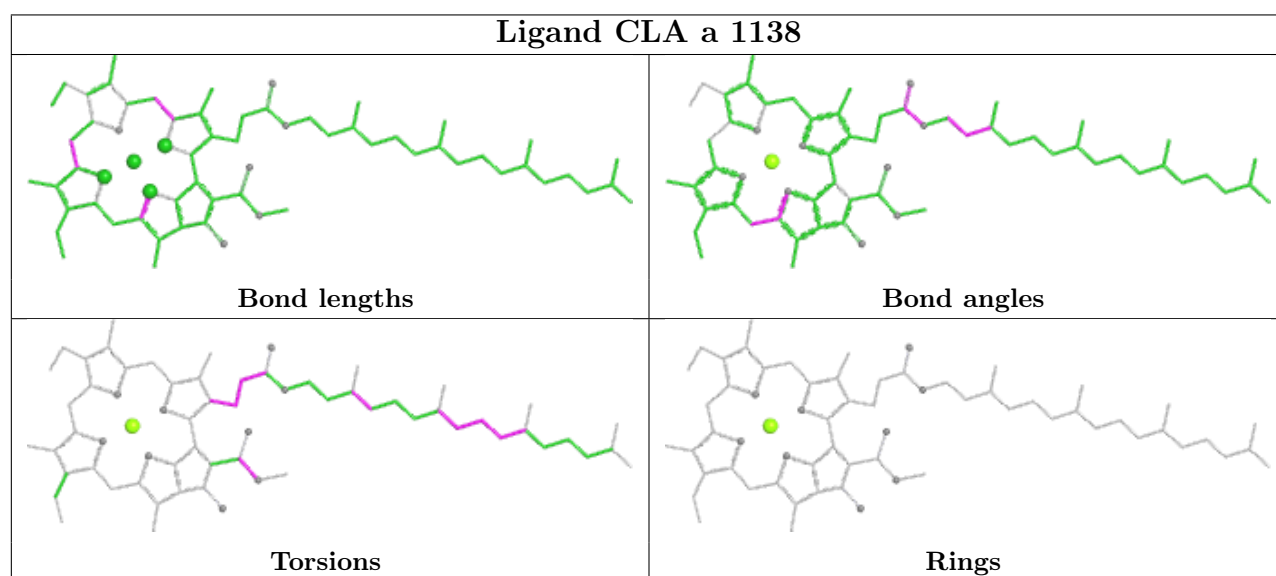
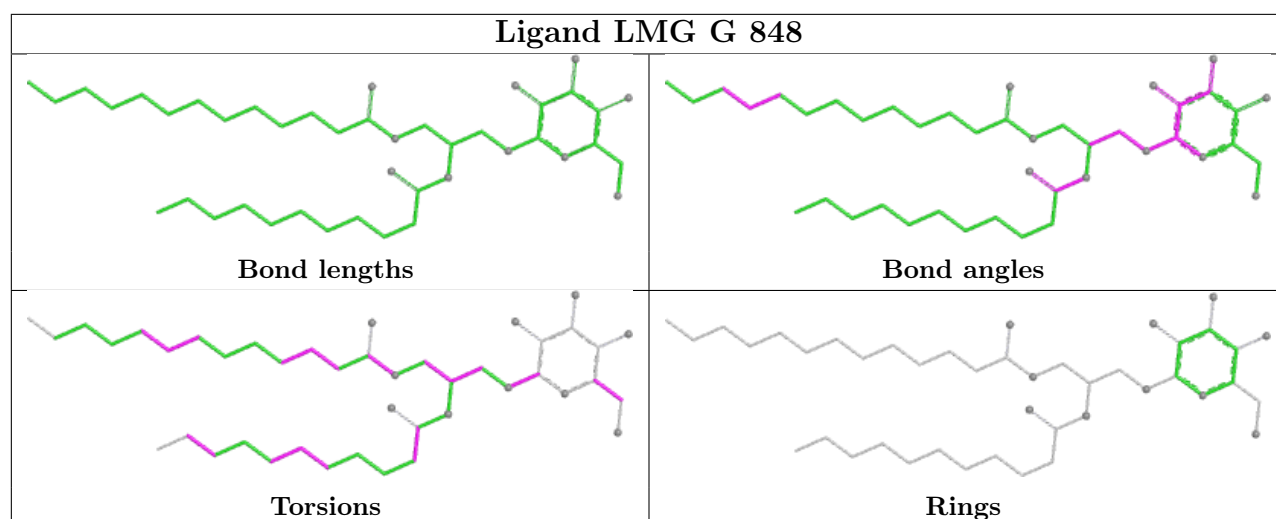






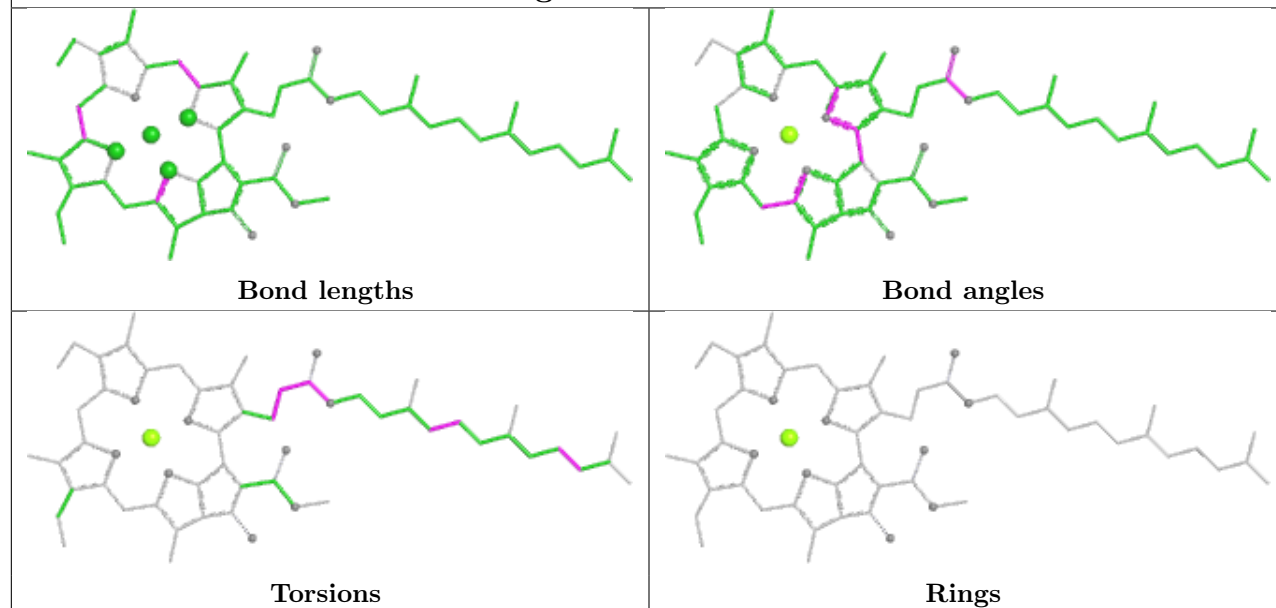




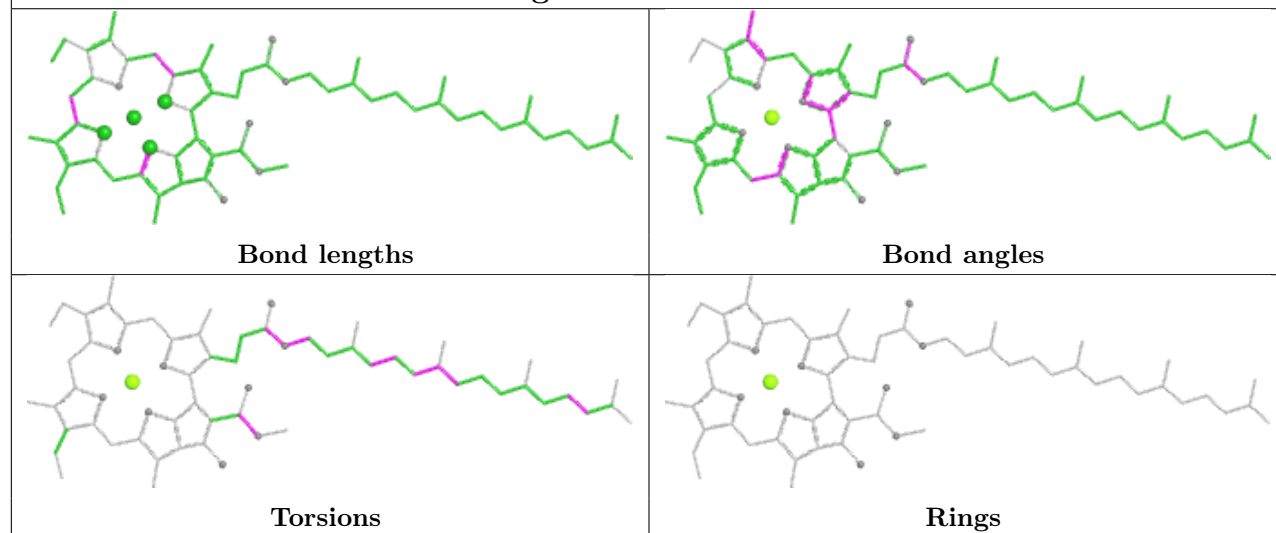




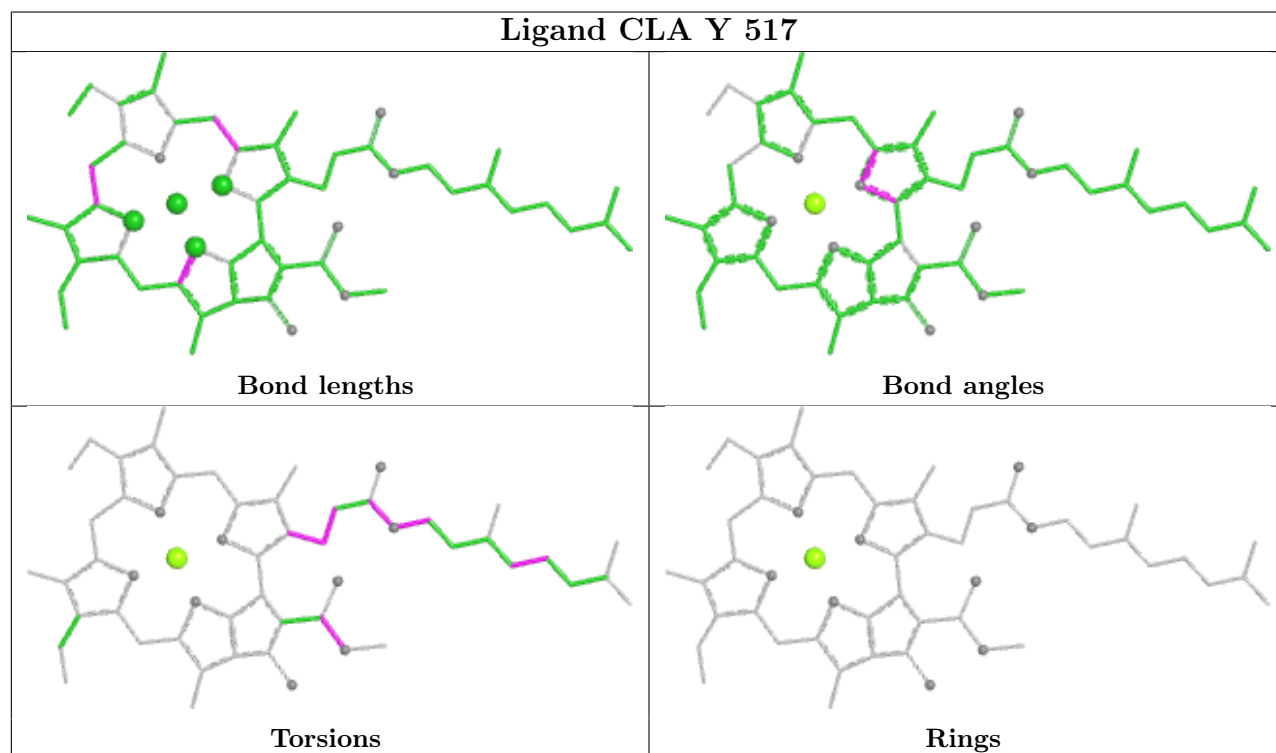
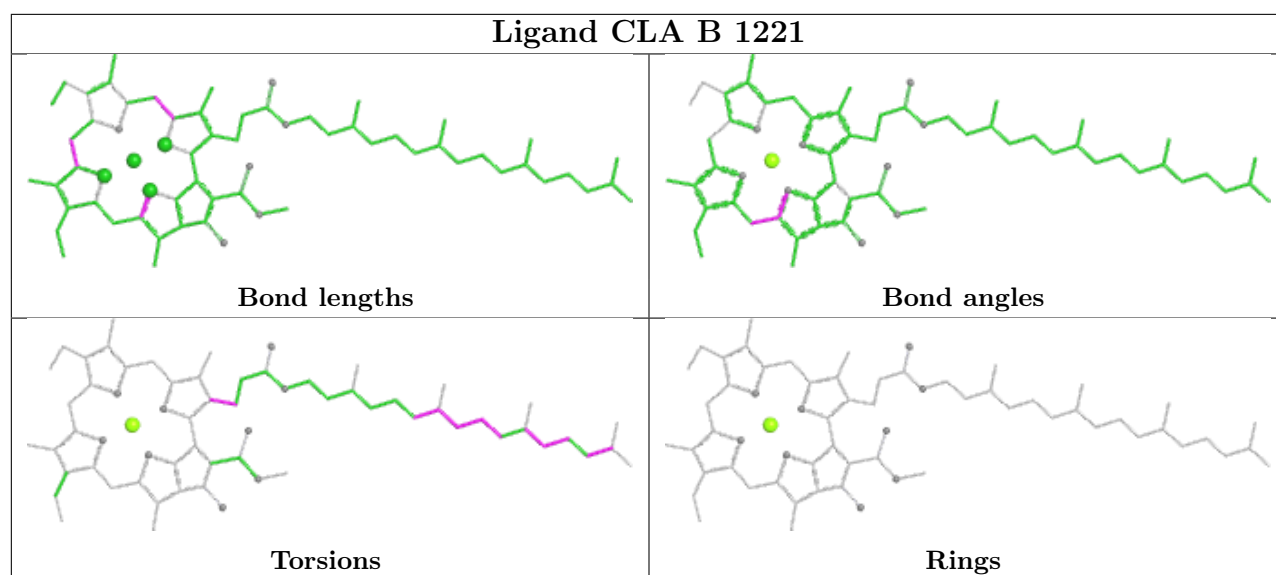
## Ligand CLA u 509



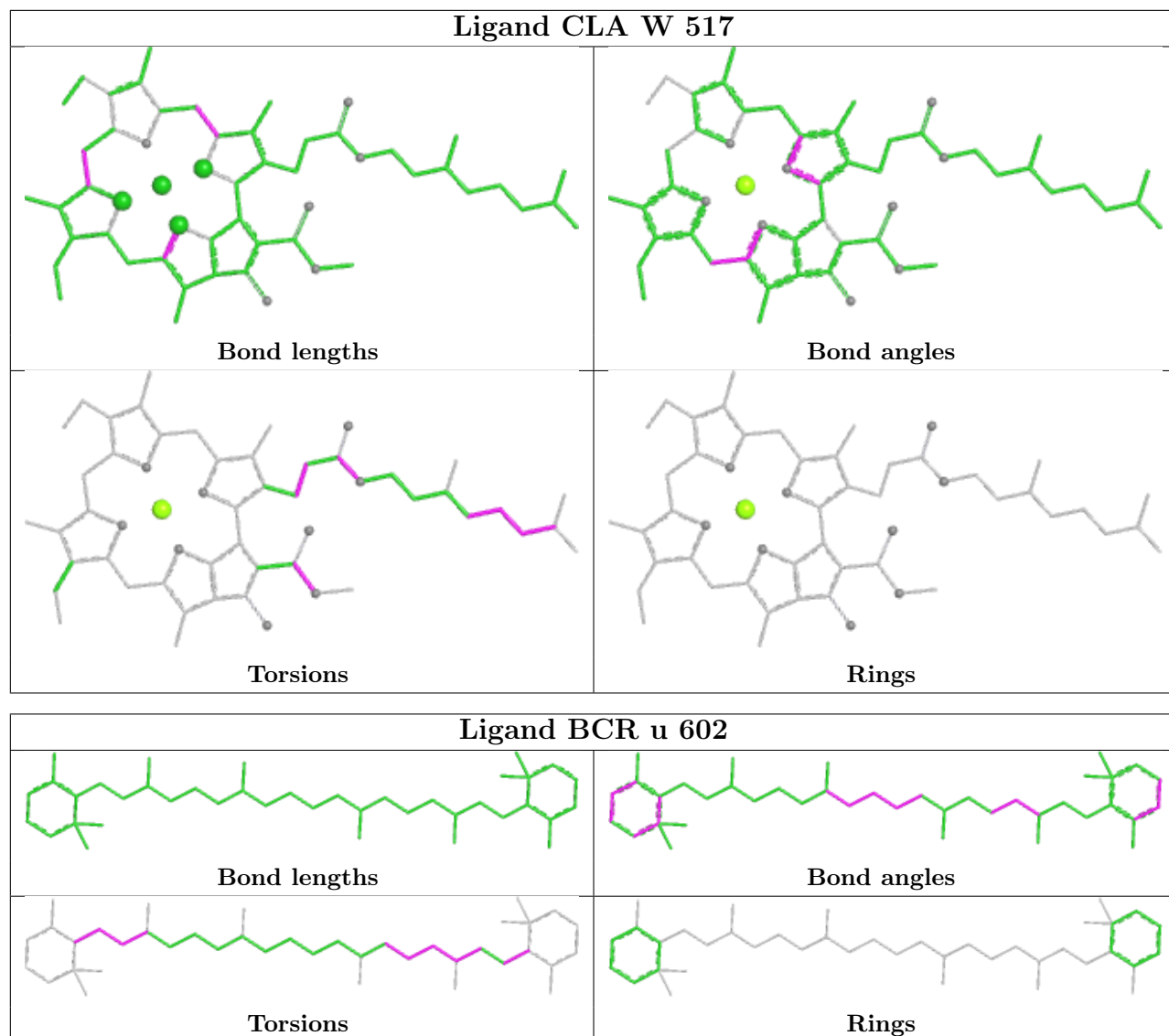
## Ligand CLA X 512





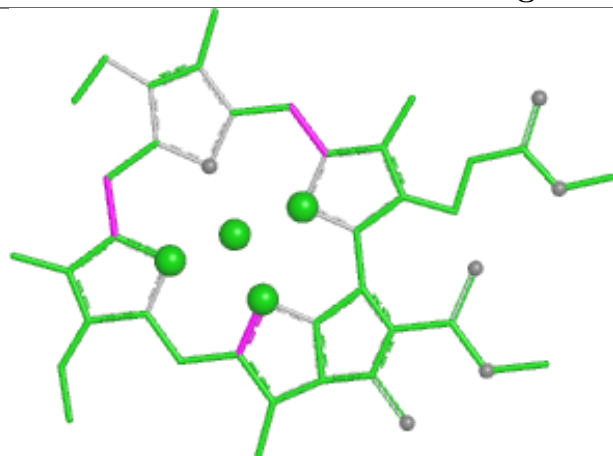




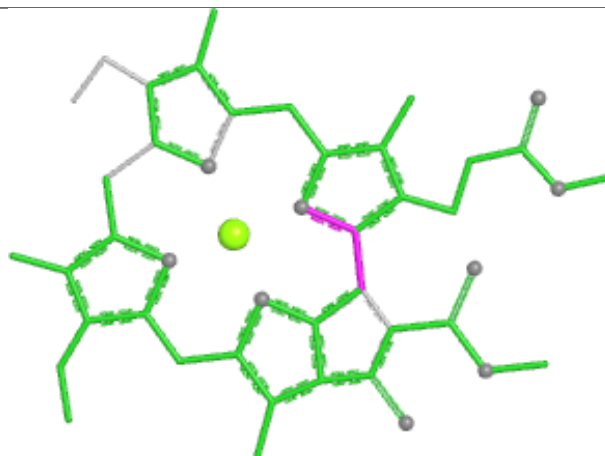




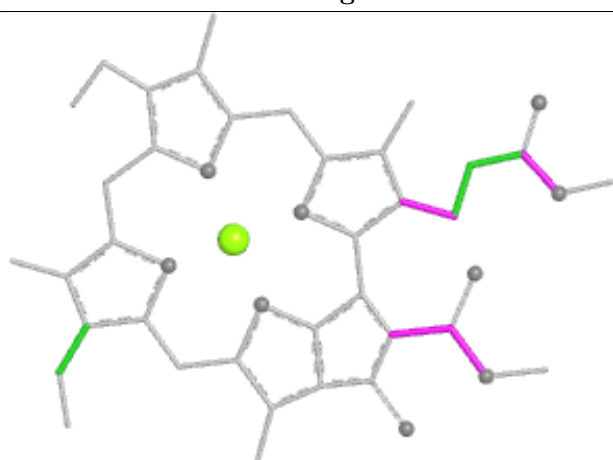
## Ligand CLA x 513



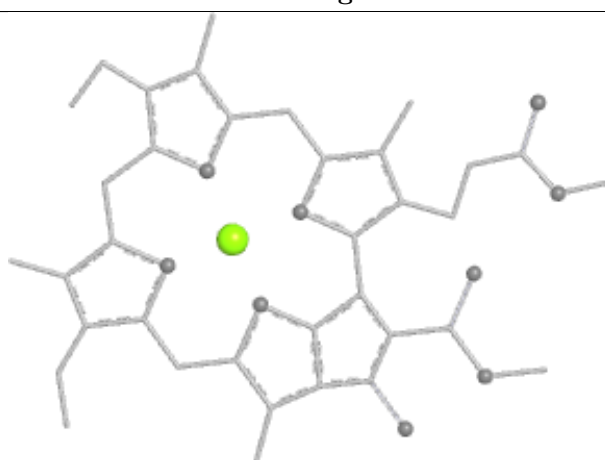
Bond lengths



Bond angles

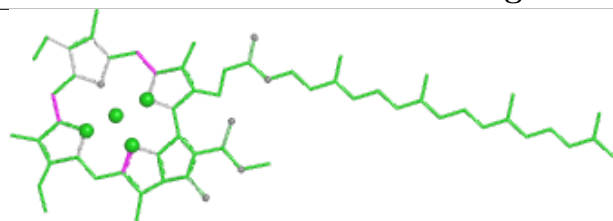


Torsions

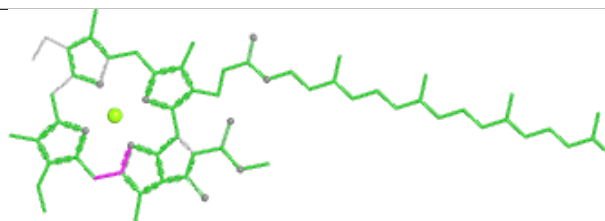


Rings

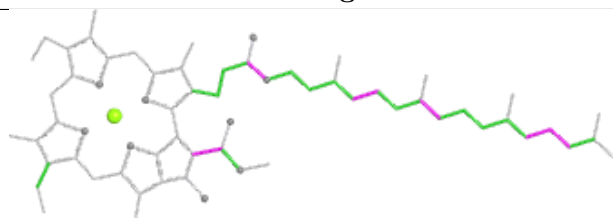
## Ligand CLA A 1103



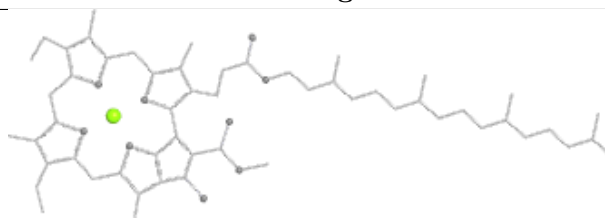
Bond lengths



Bond angles

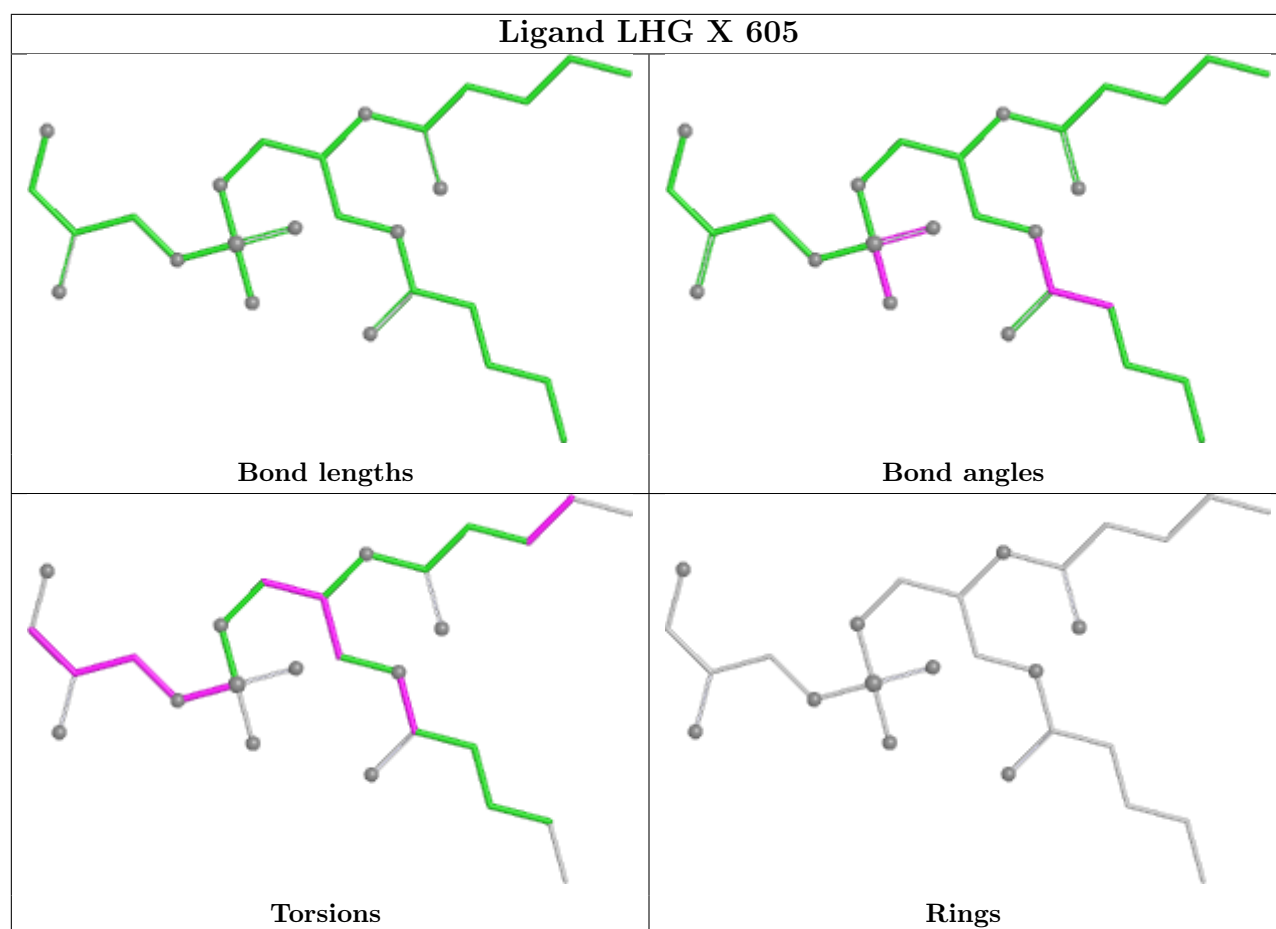


Torsions



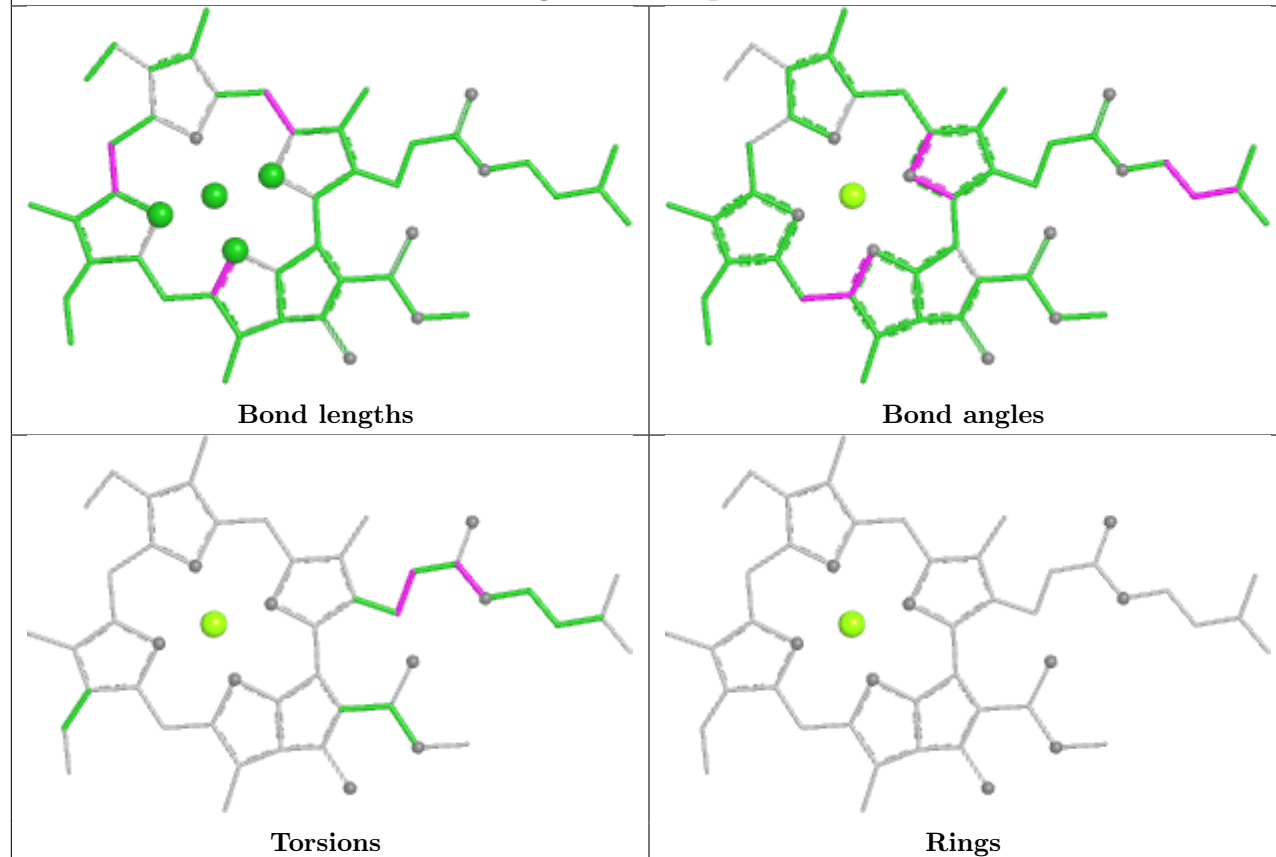
Rings



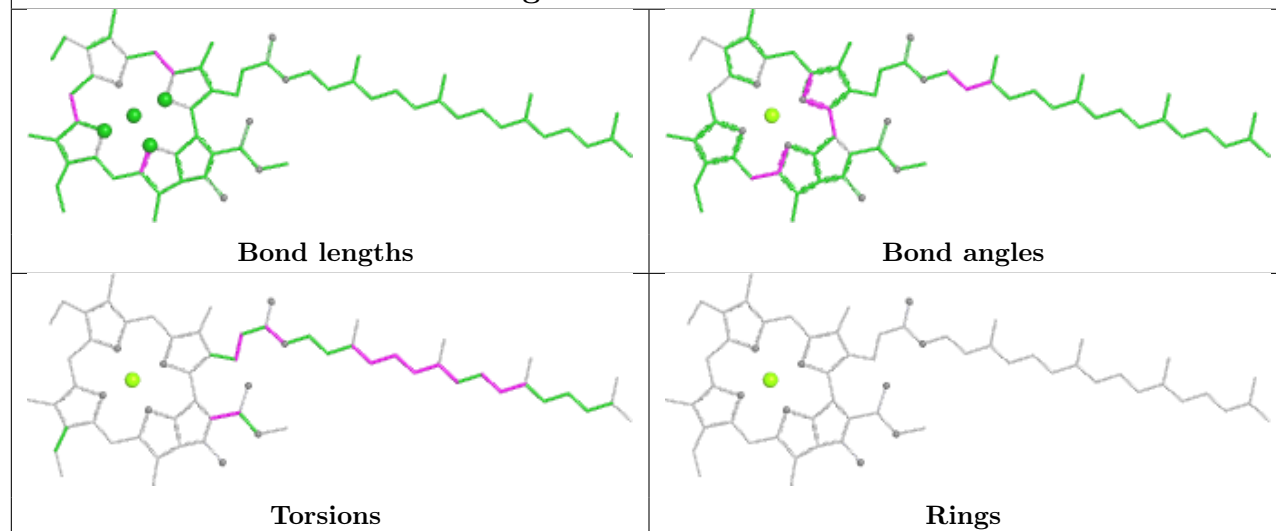




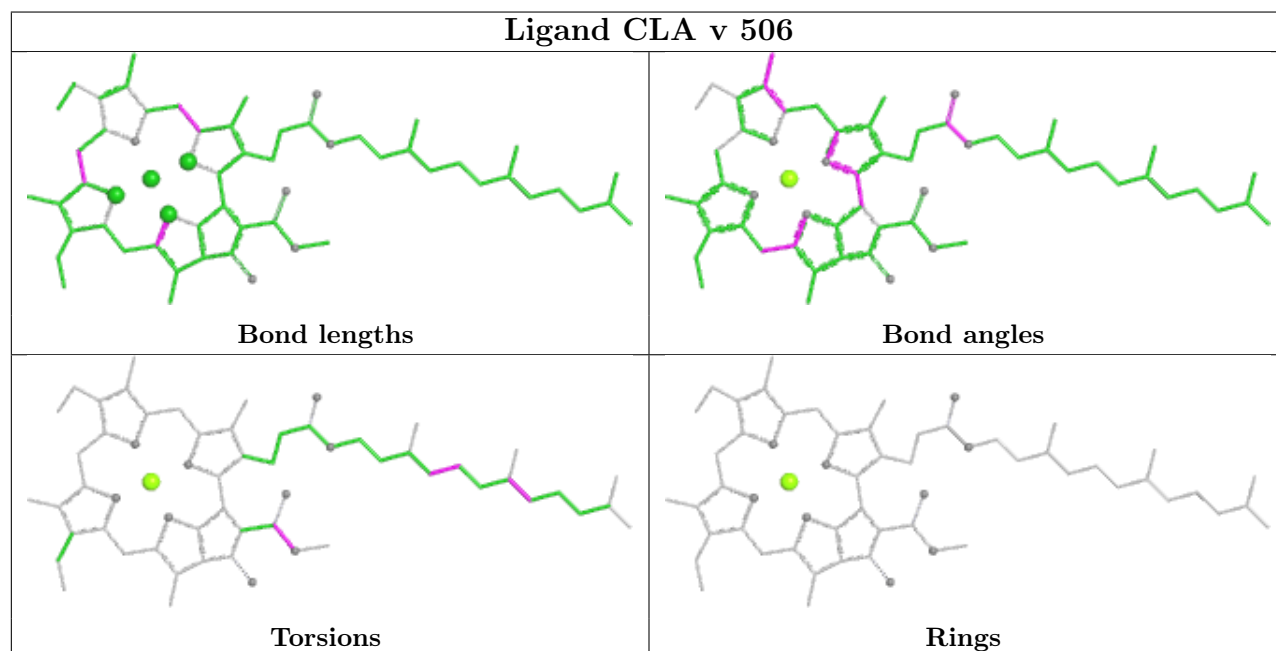
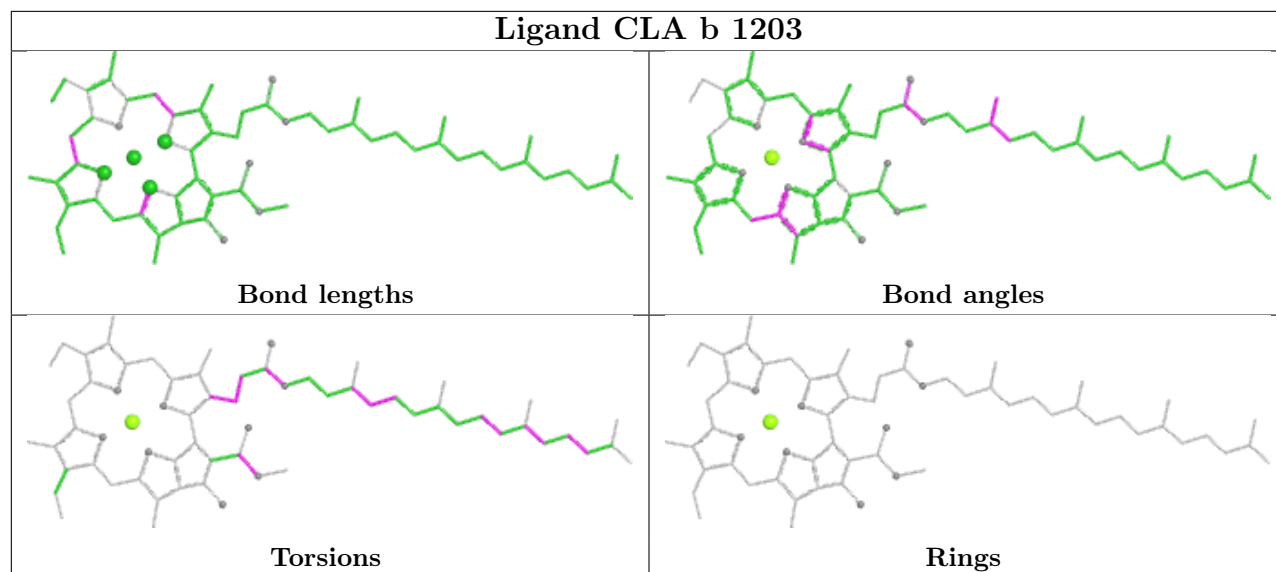
## Ligand CLA p 502



## Ligand CLA A 1106

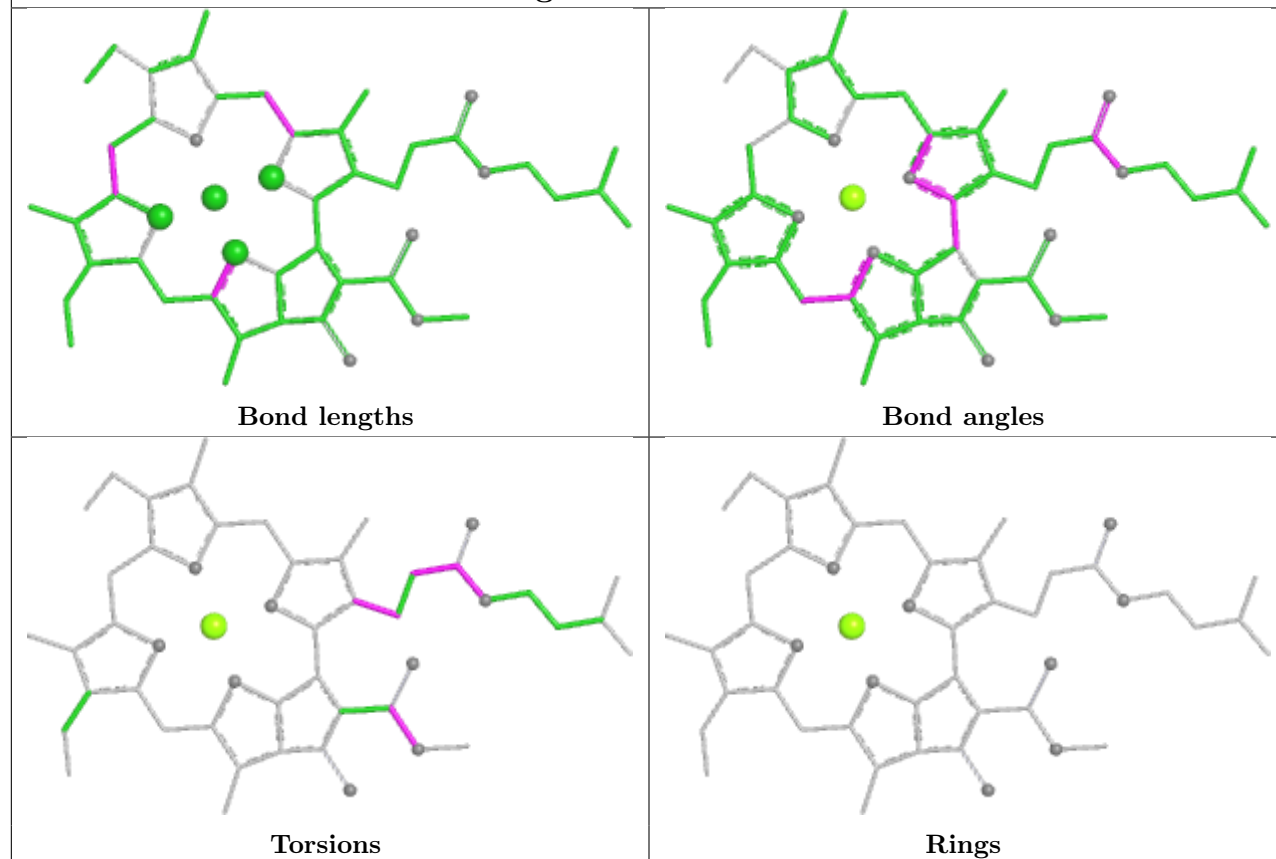




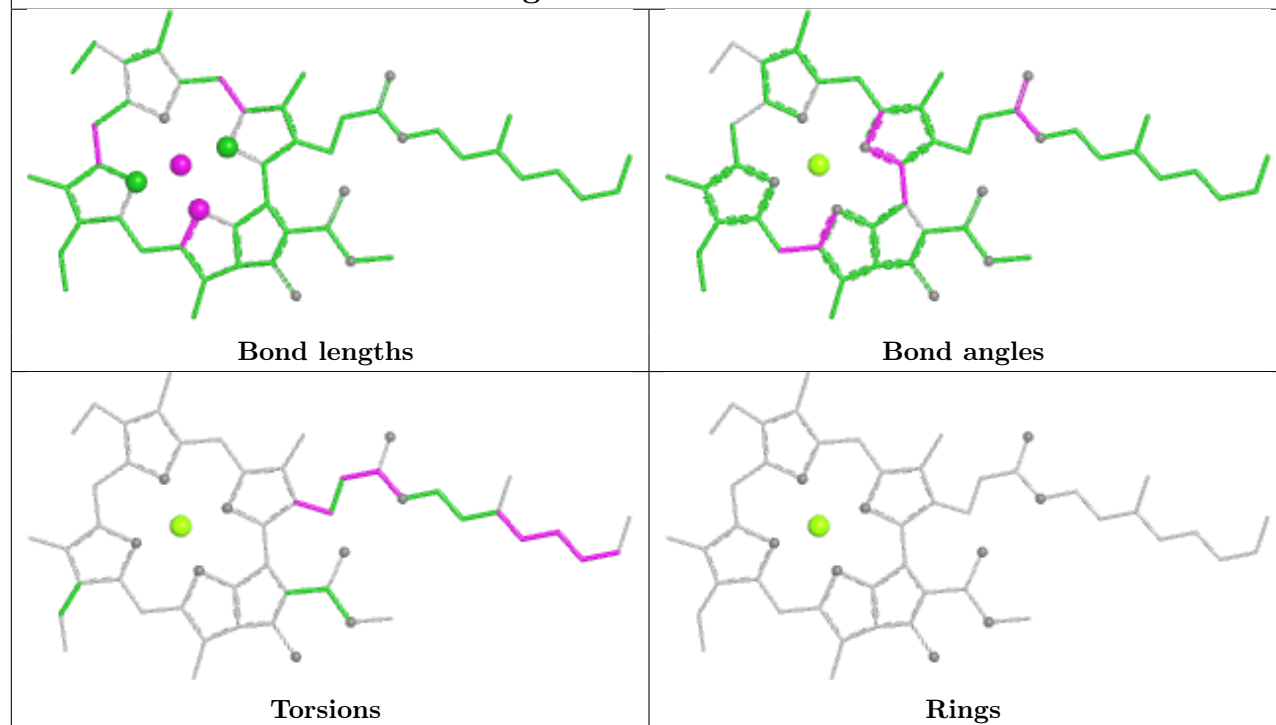




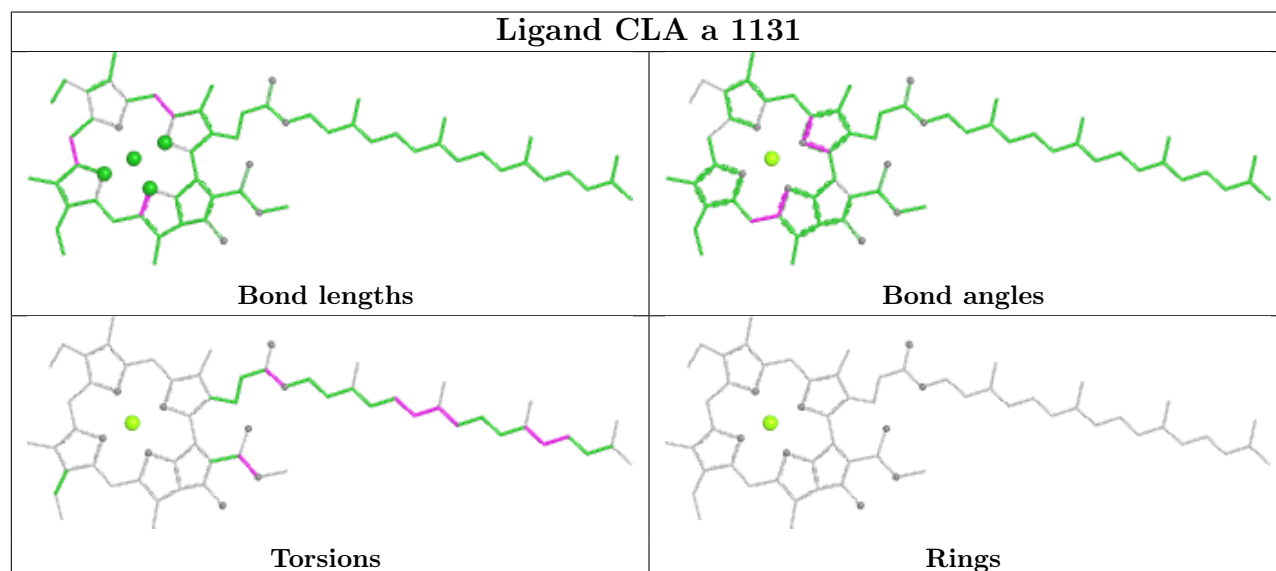
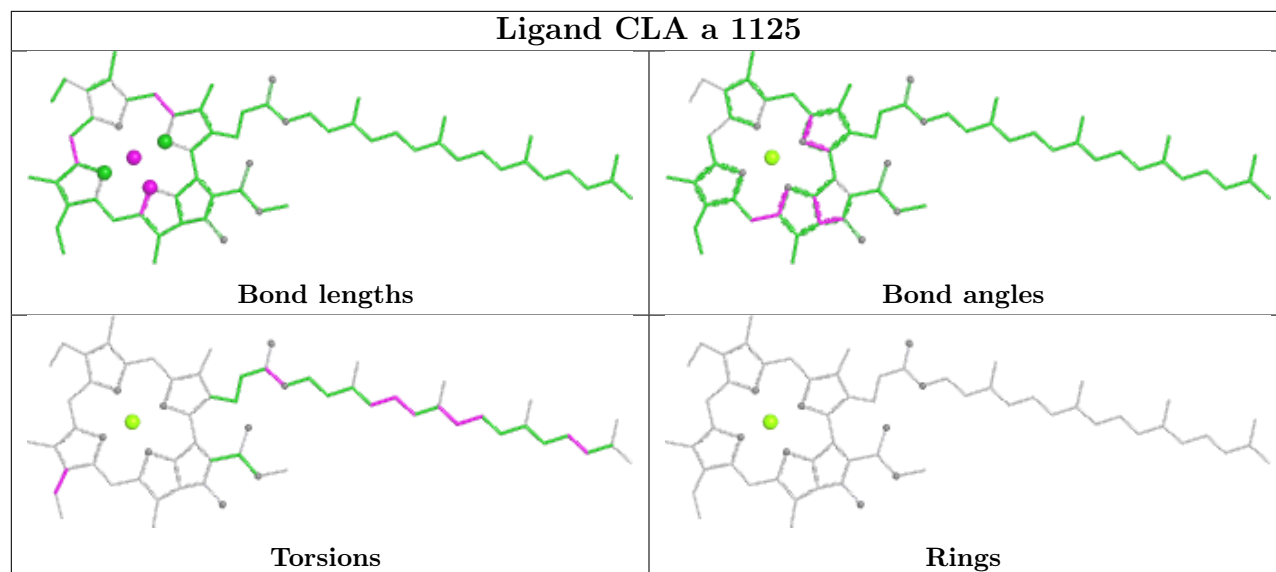
## Ligand CLA x 514



## Ligand CLA A 1133

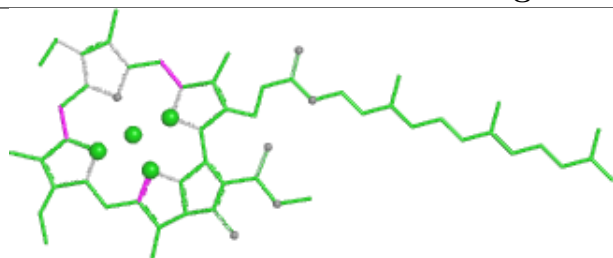




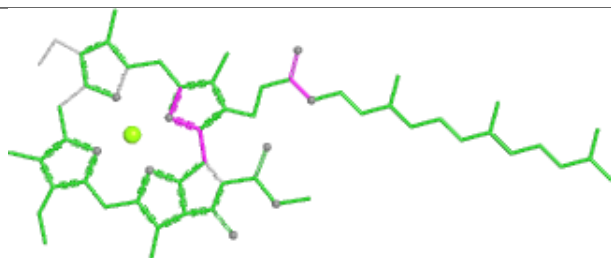




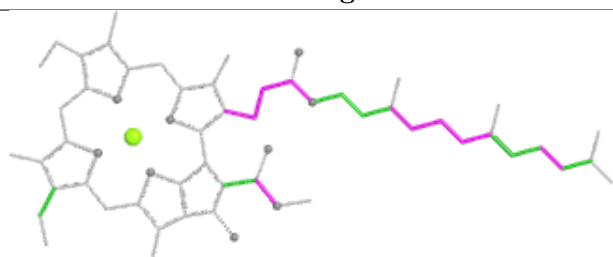
## Ligand CLA Y 509



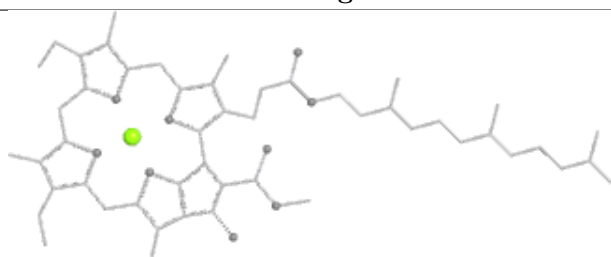
Bond lengths



Bond angles

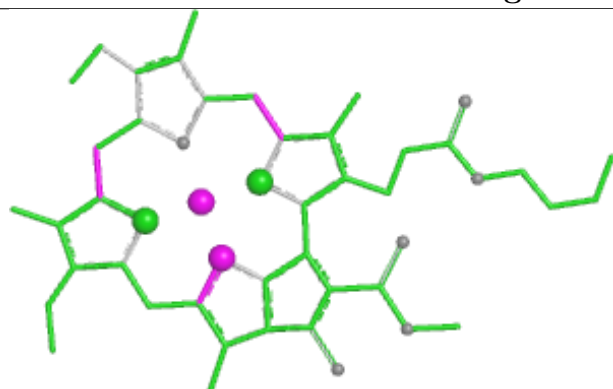


Torsions

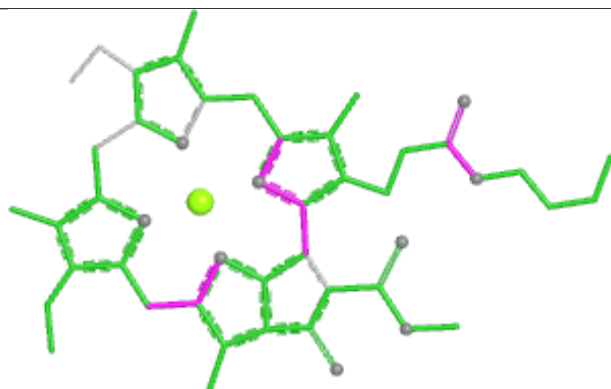


Rings

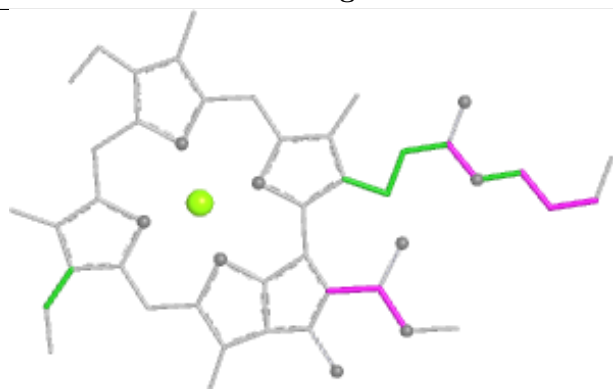
## Ligand CLA G 1227



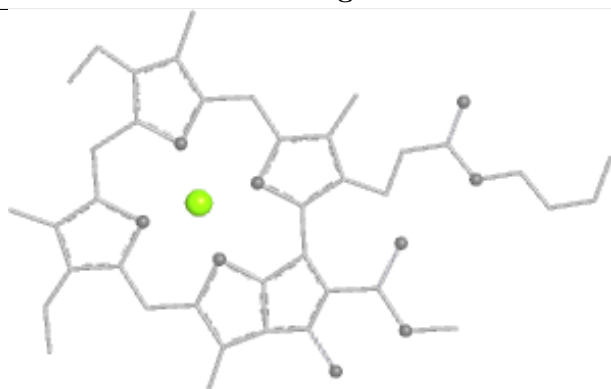
Bond lengths



Bond angles

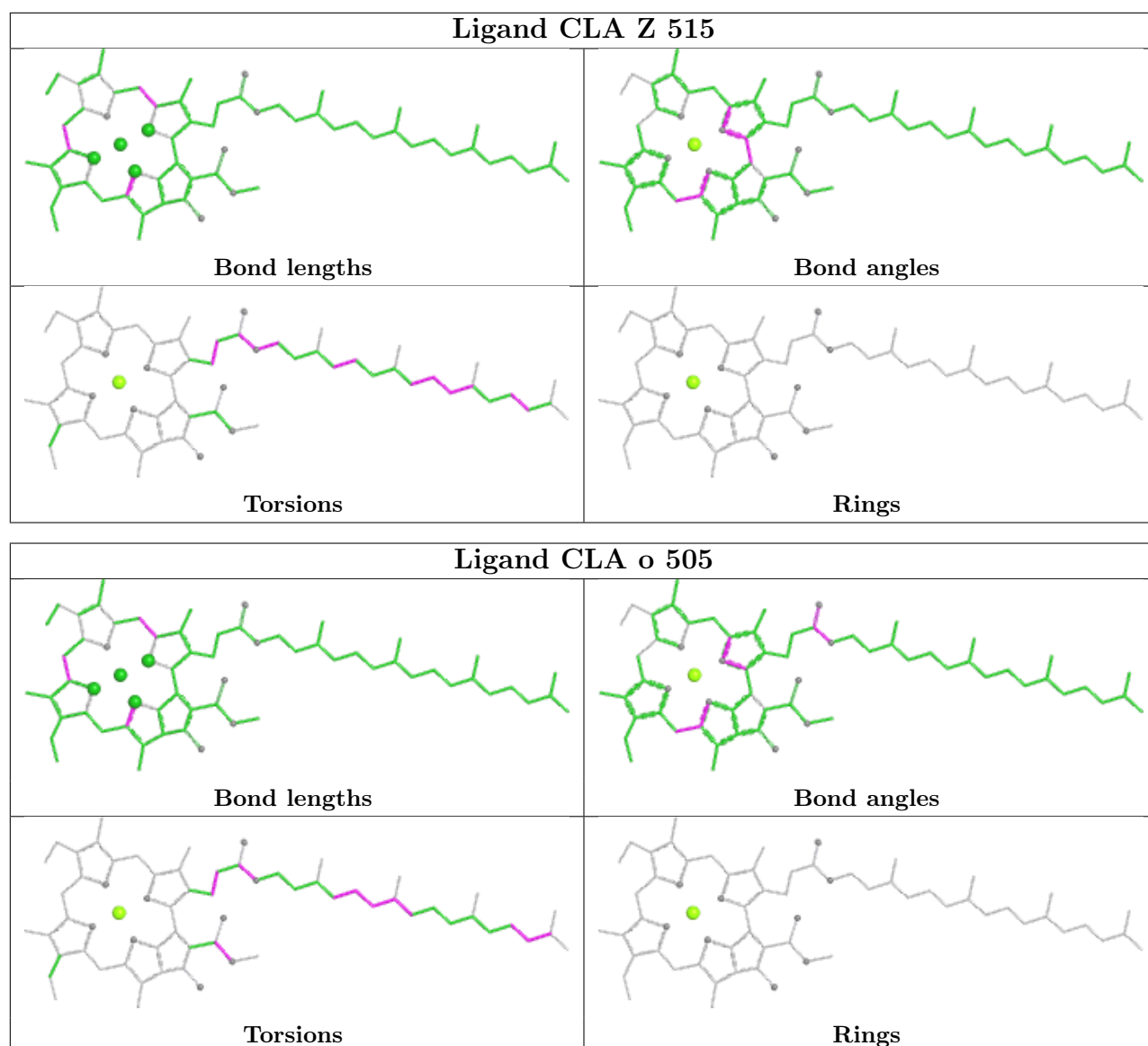


Torsions



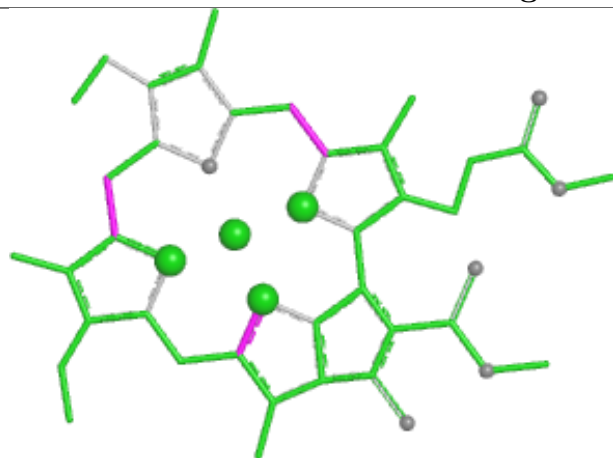
Rings



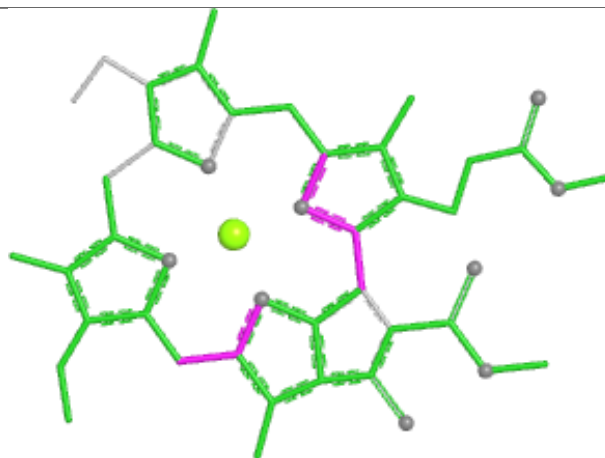




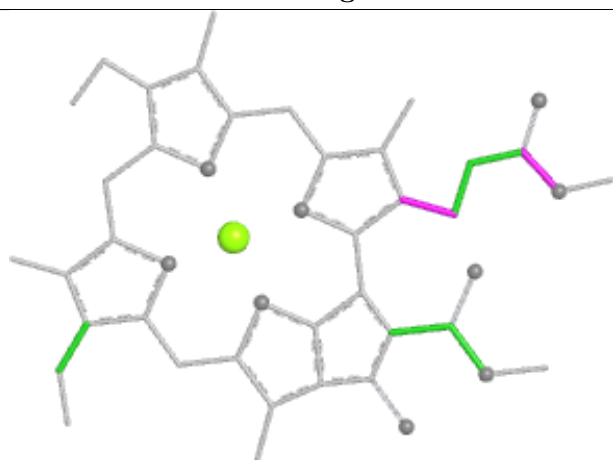
## Ligand CLA r 516



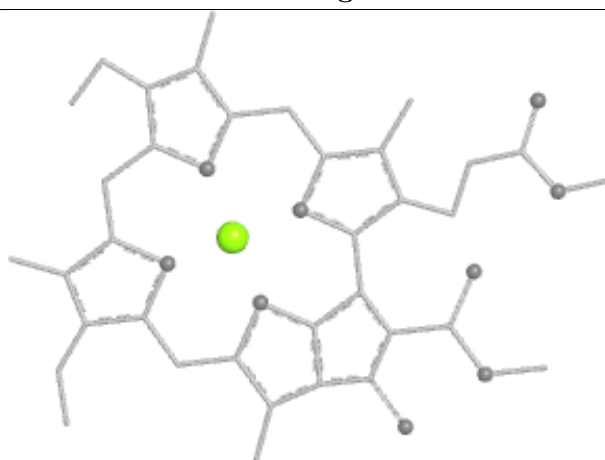
Bond lengths



Bond angles

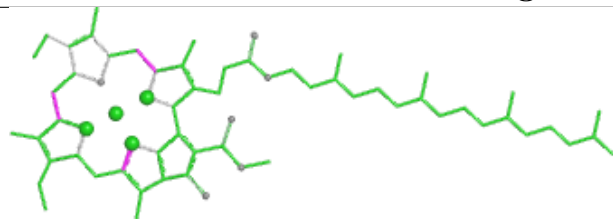


Torsions

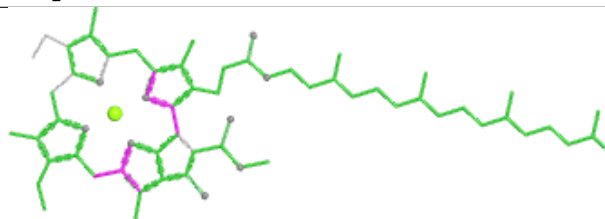


Rings

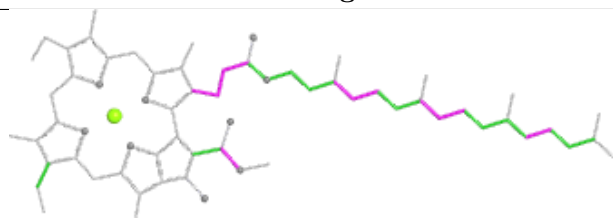
## Ligand CLA p 505



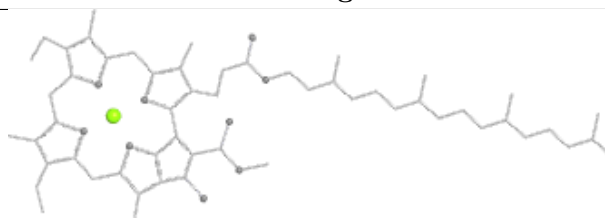
Bond lengths



Bond angles

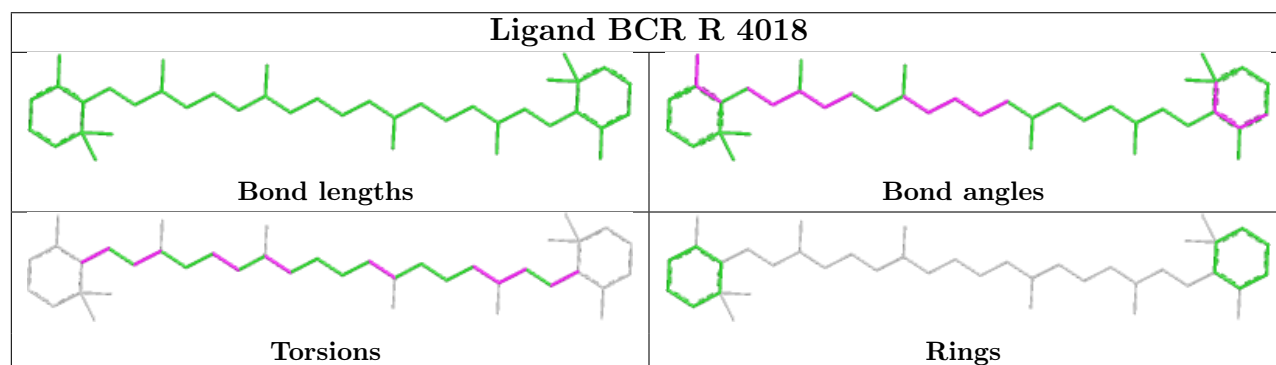
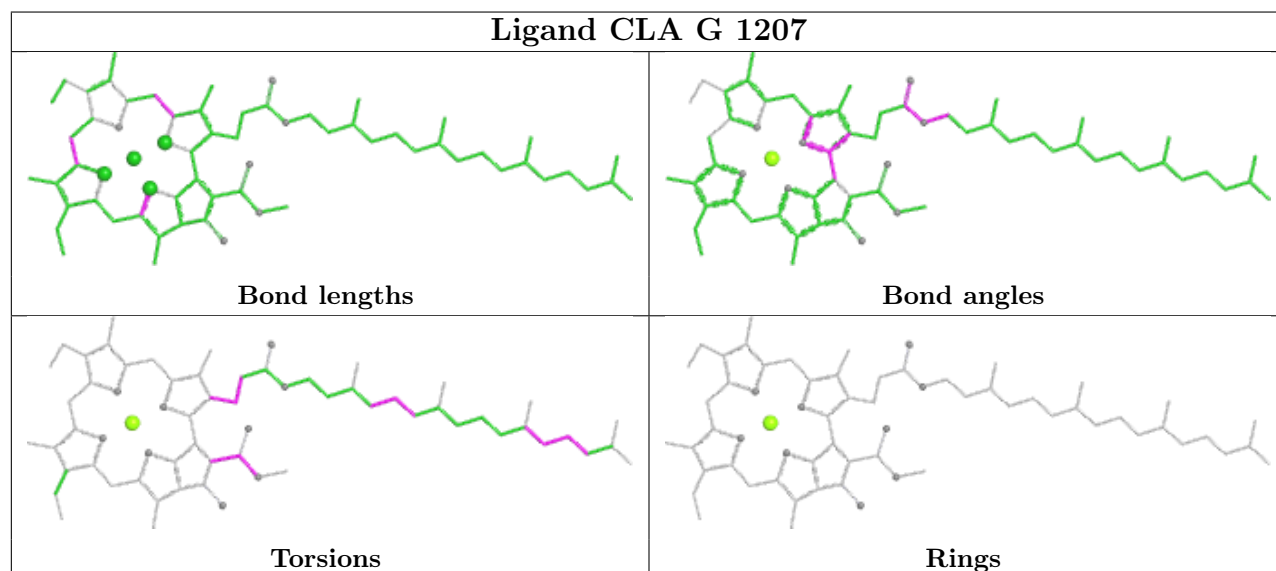
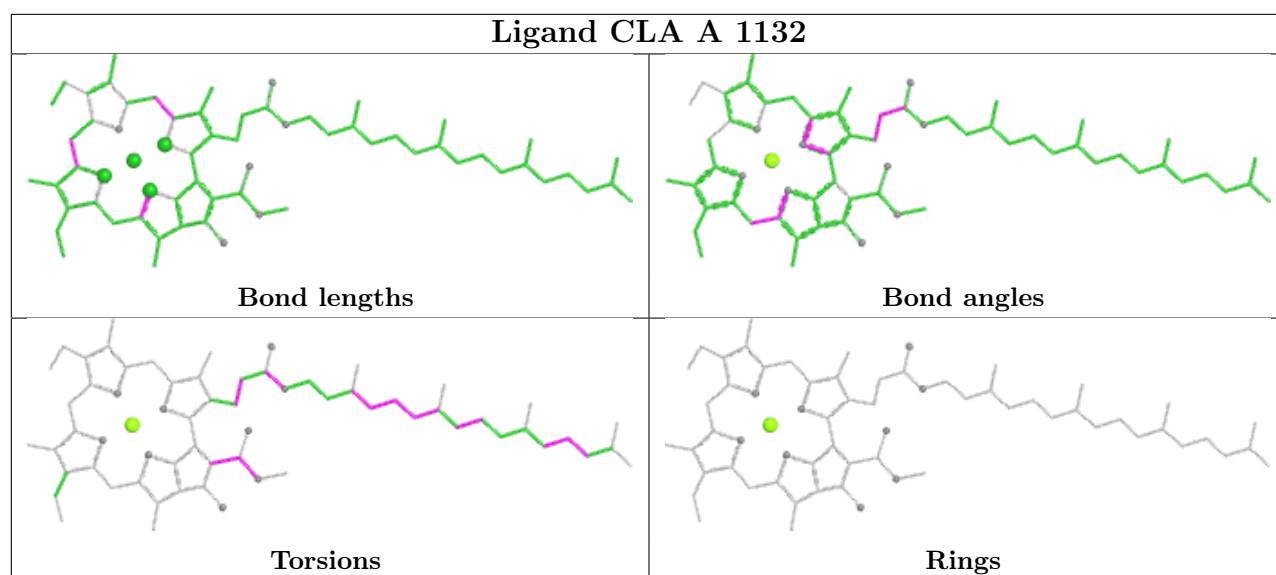


Torsions



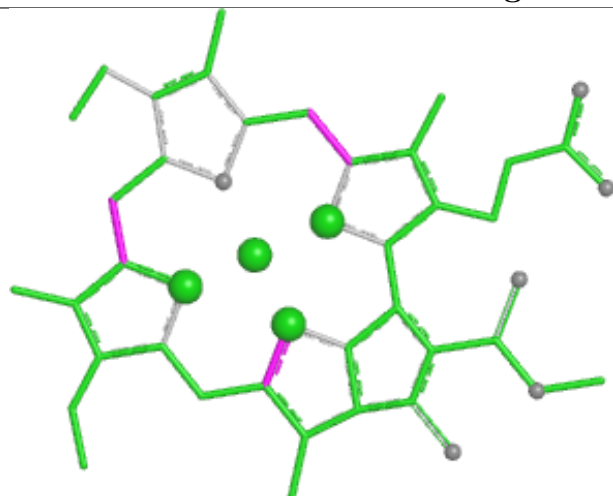
Rings



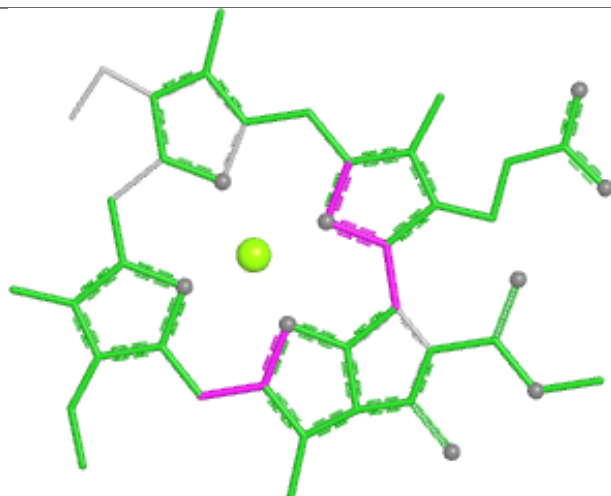




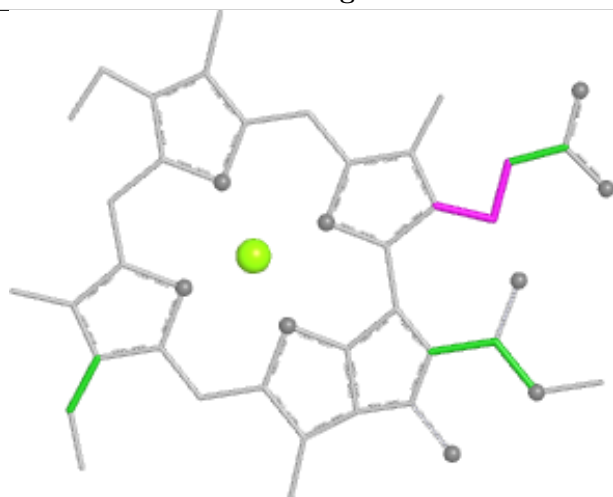
## Ligand CLA G 1231



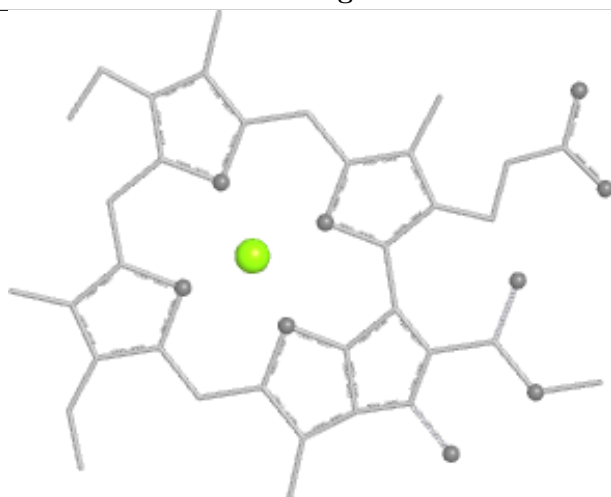
Bond lengths



Bond angles

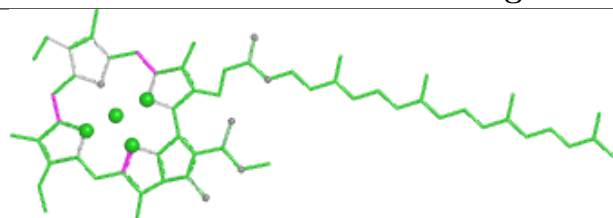


Torsions

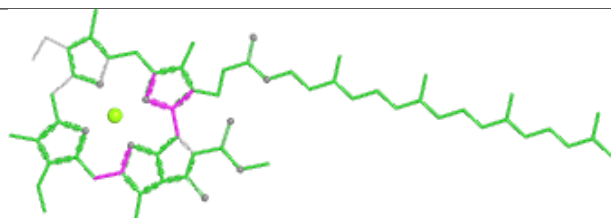


Rings

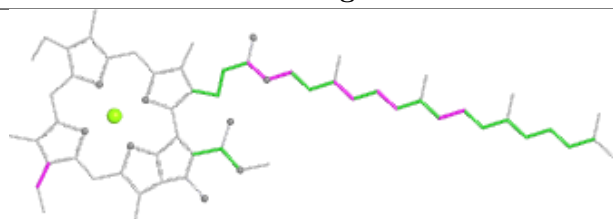
## Ligand CLA A 1123



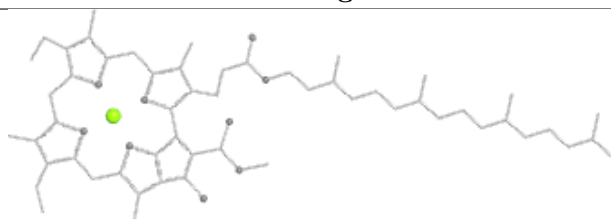
Bond lengths



Bond angles



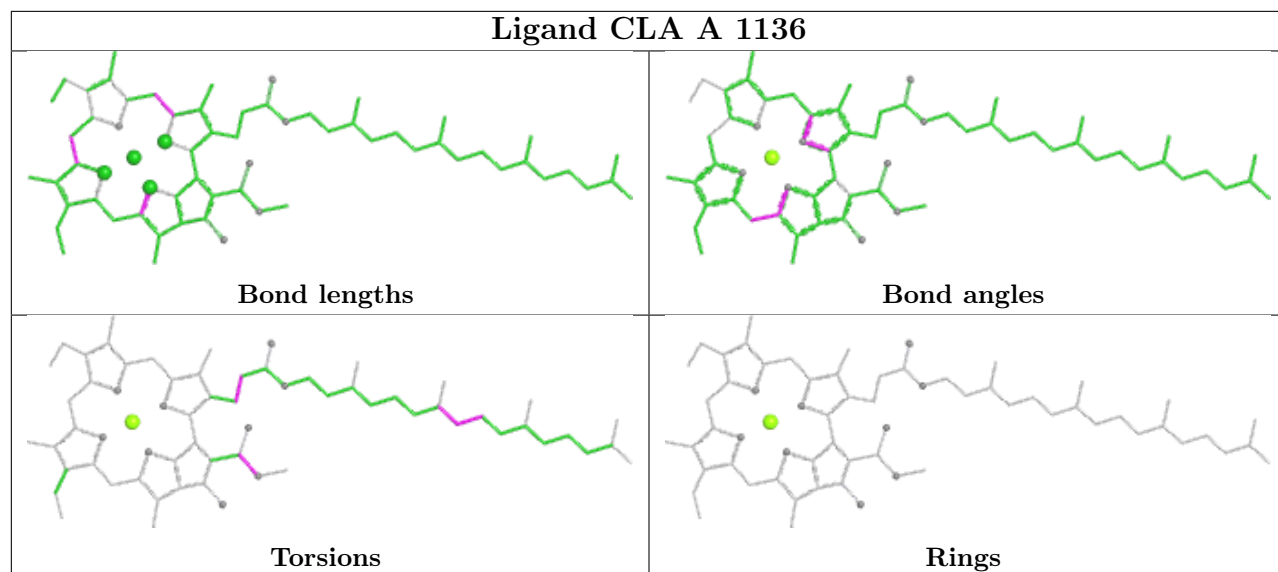
Torsions



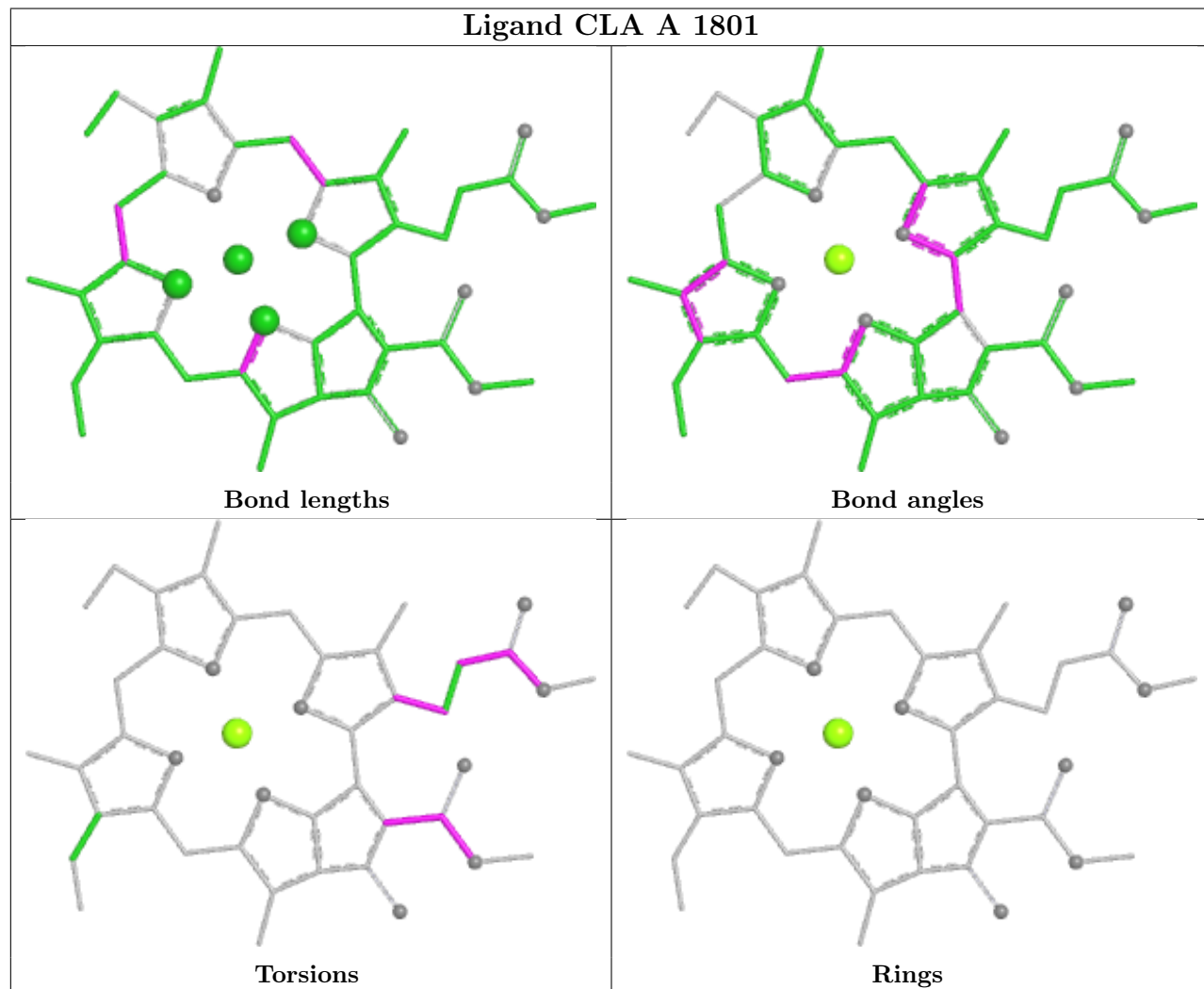
Rings



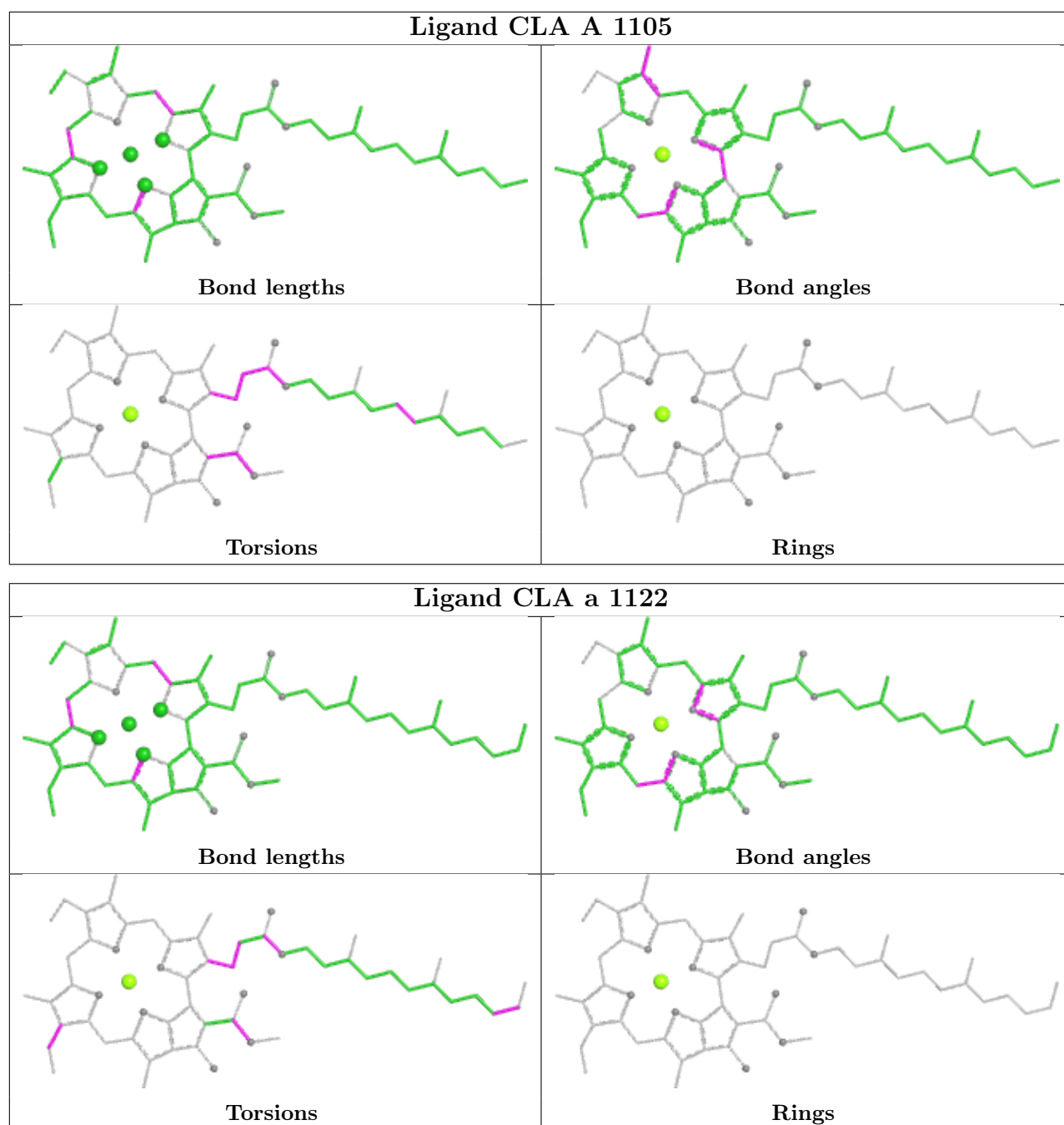
## Ligand CLA A 1136



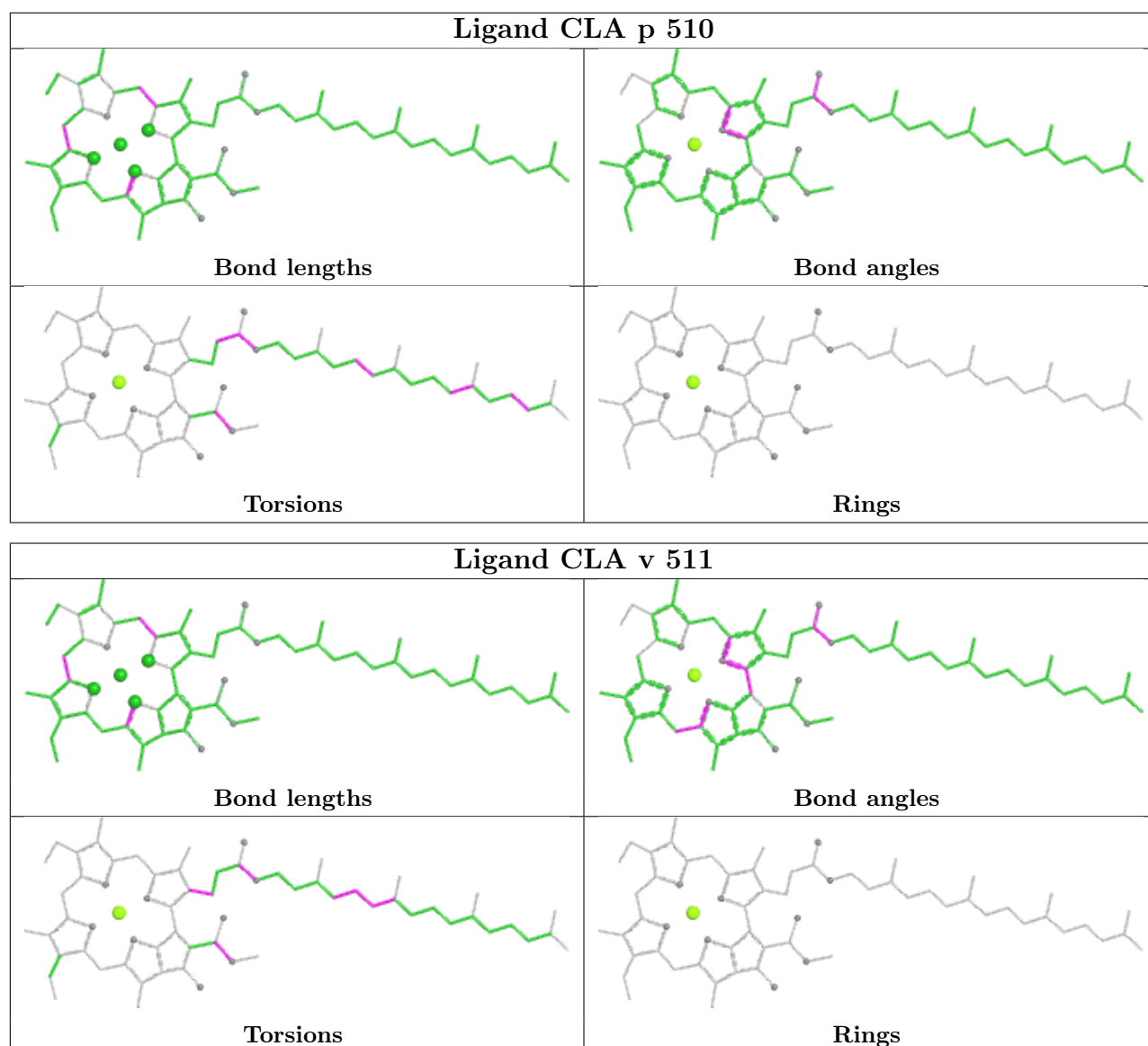
## Ligand CLA A 1801





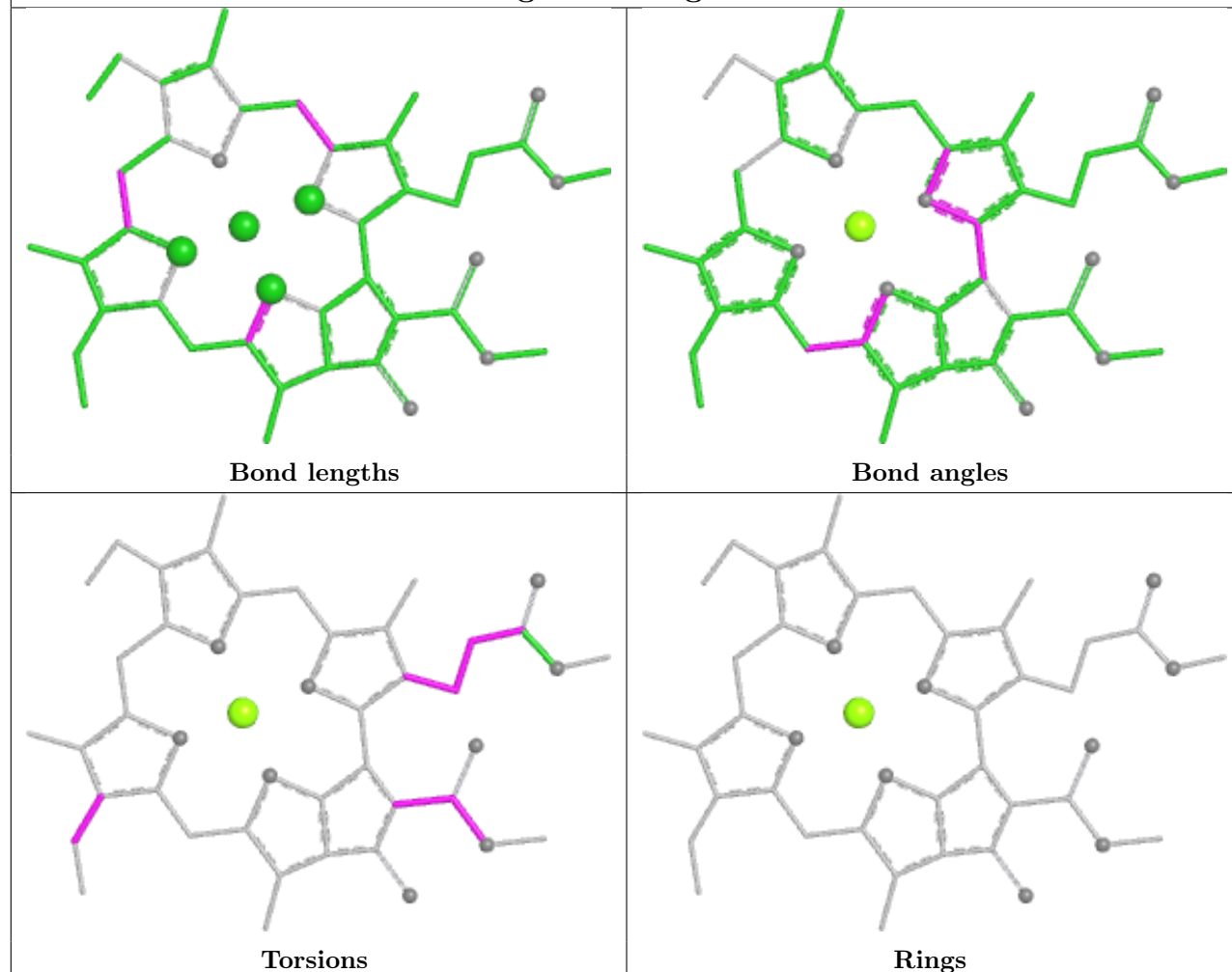




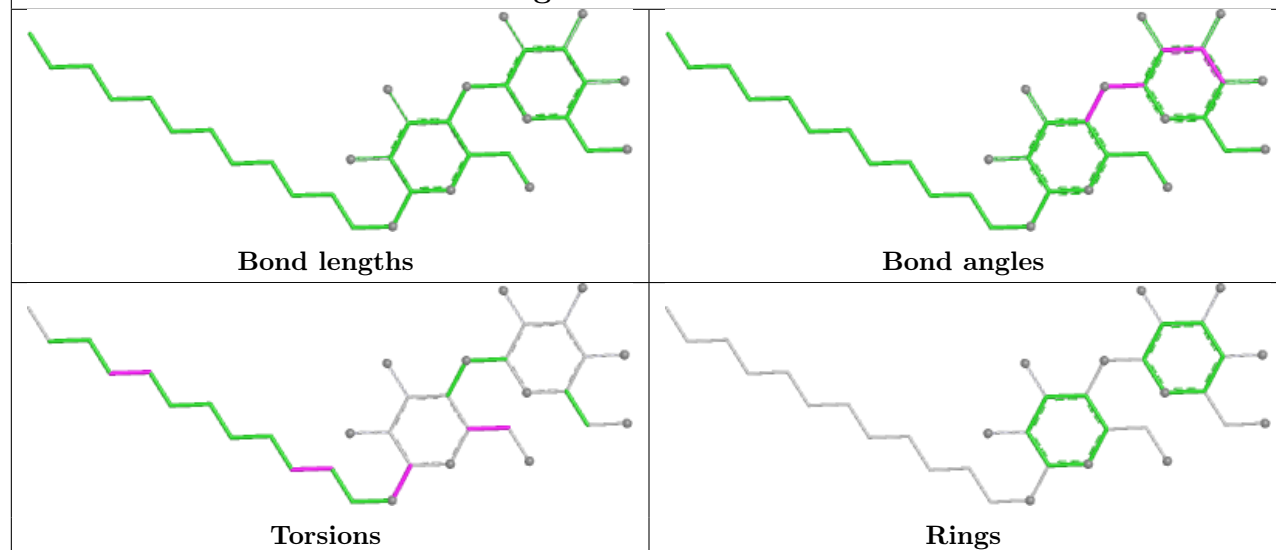




## Ligand CLA g 513

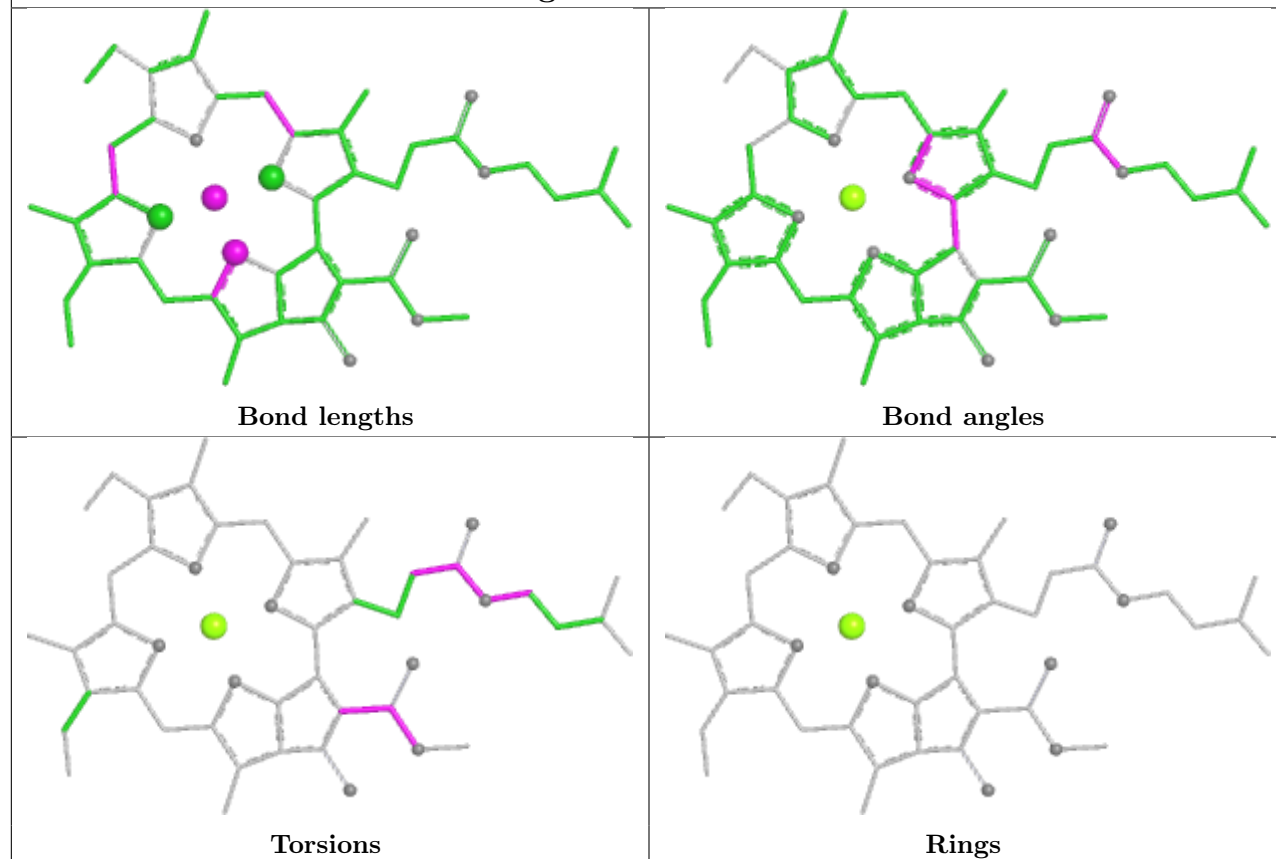


## Ligand LMU r 606

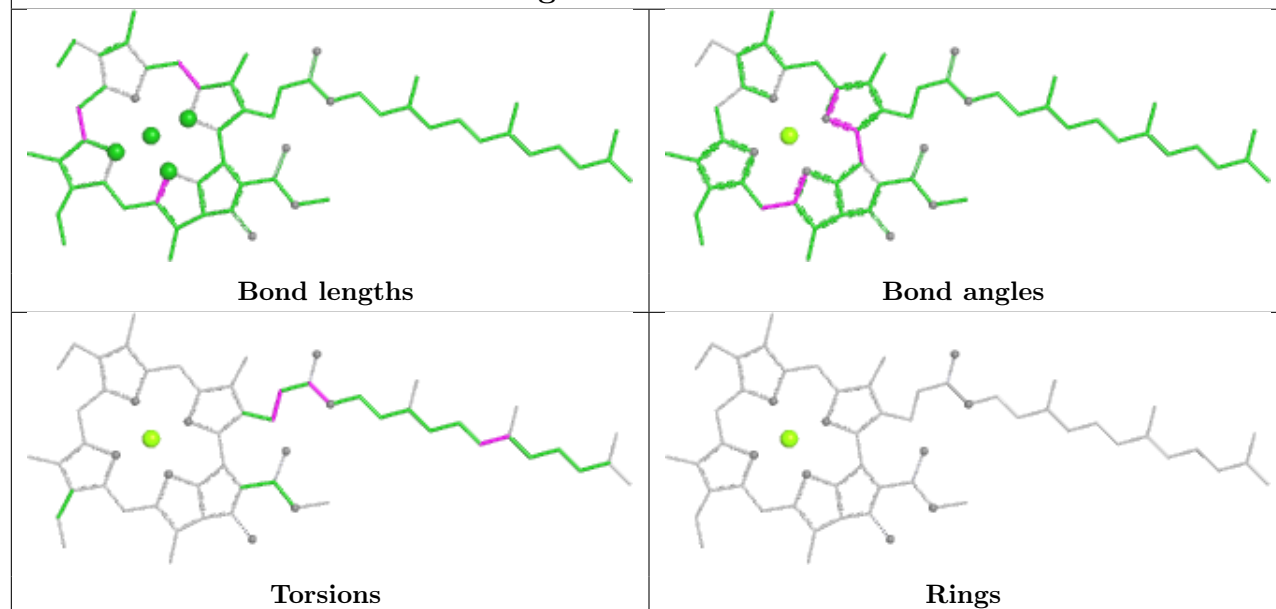




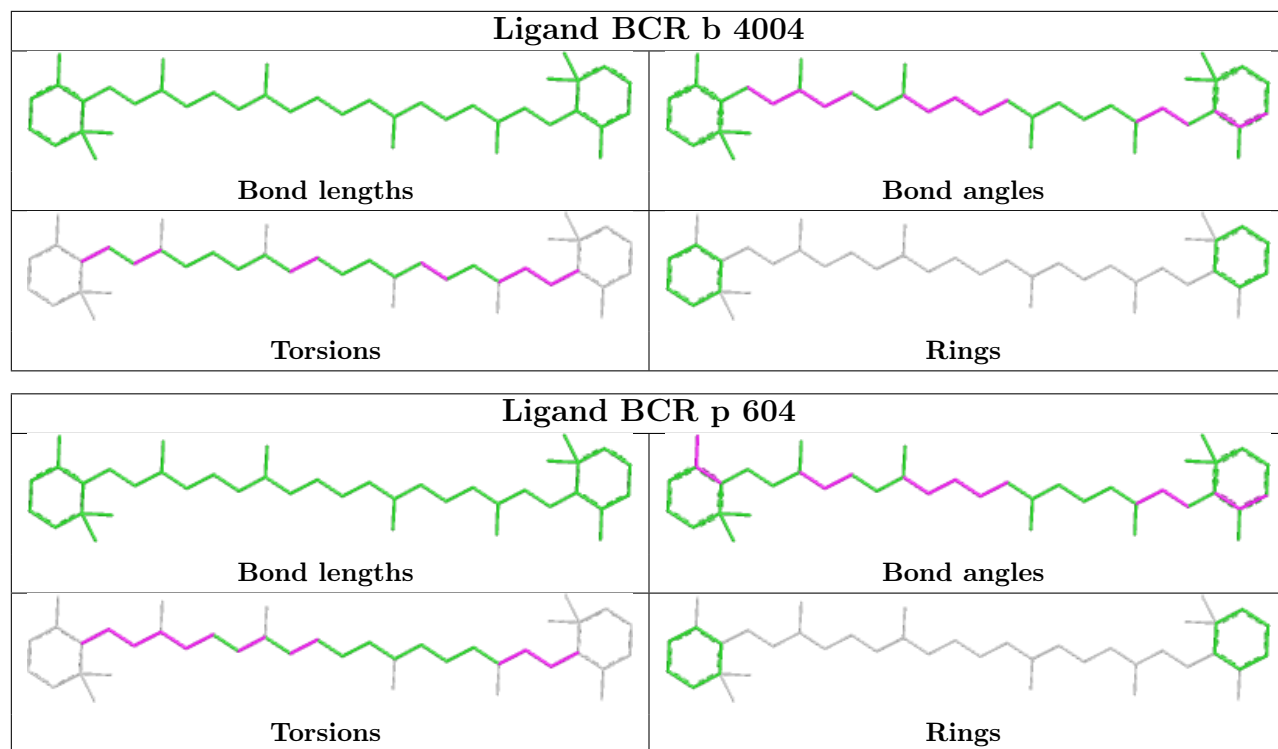
## Ligand CLA t 502



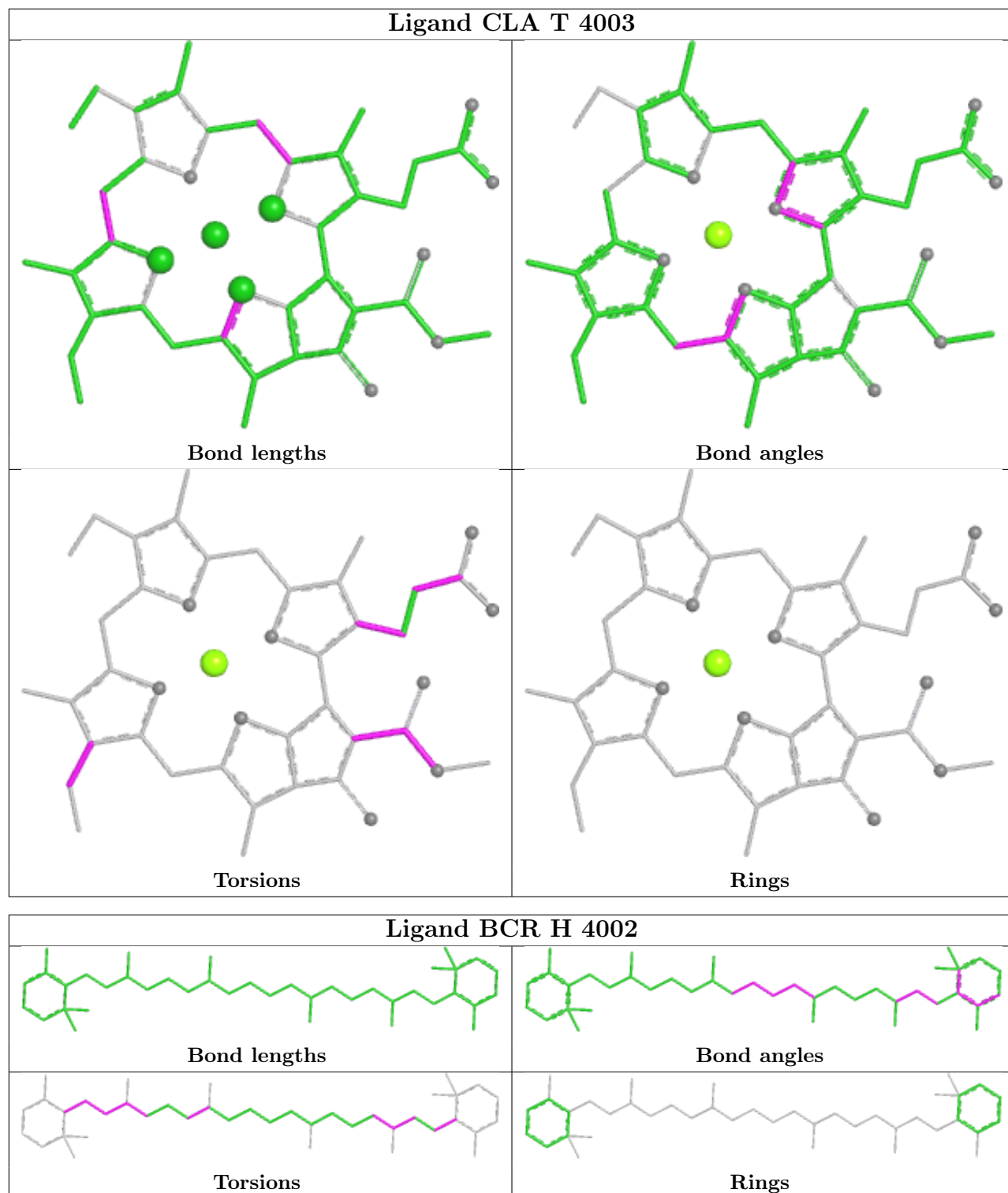
## Ligand CLA t 504



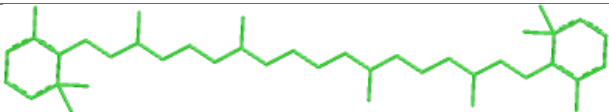
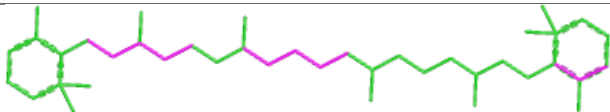
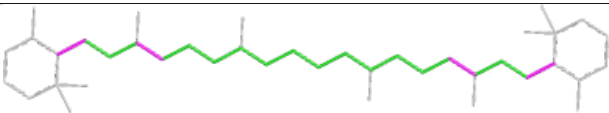
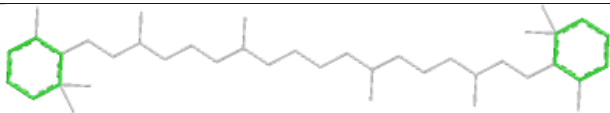


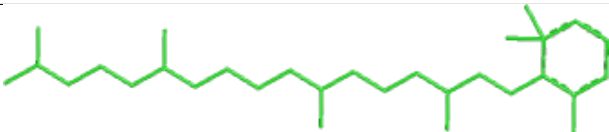
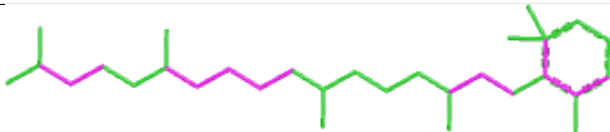
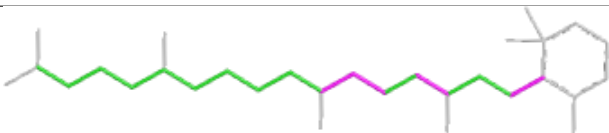
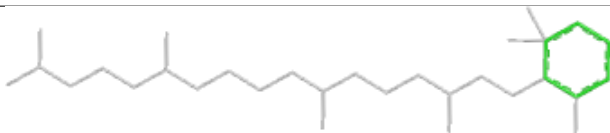


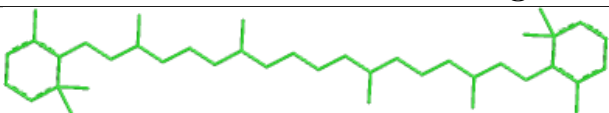
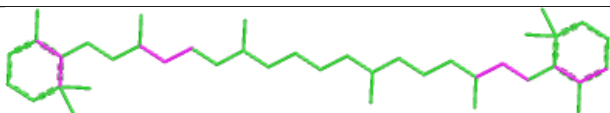

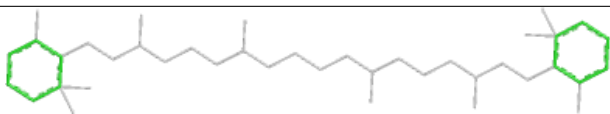




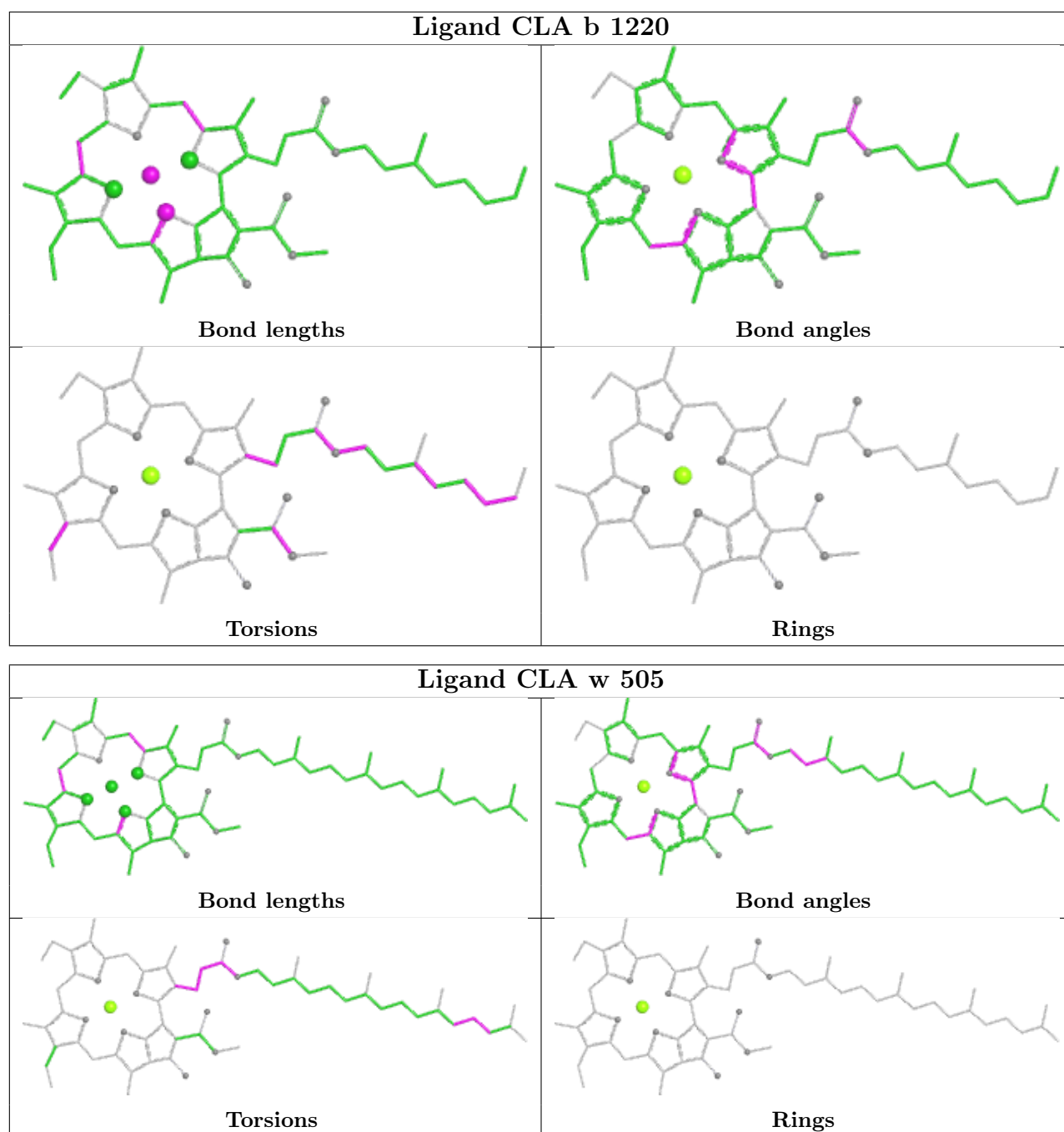


Ligand BCR p 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

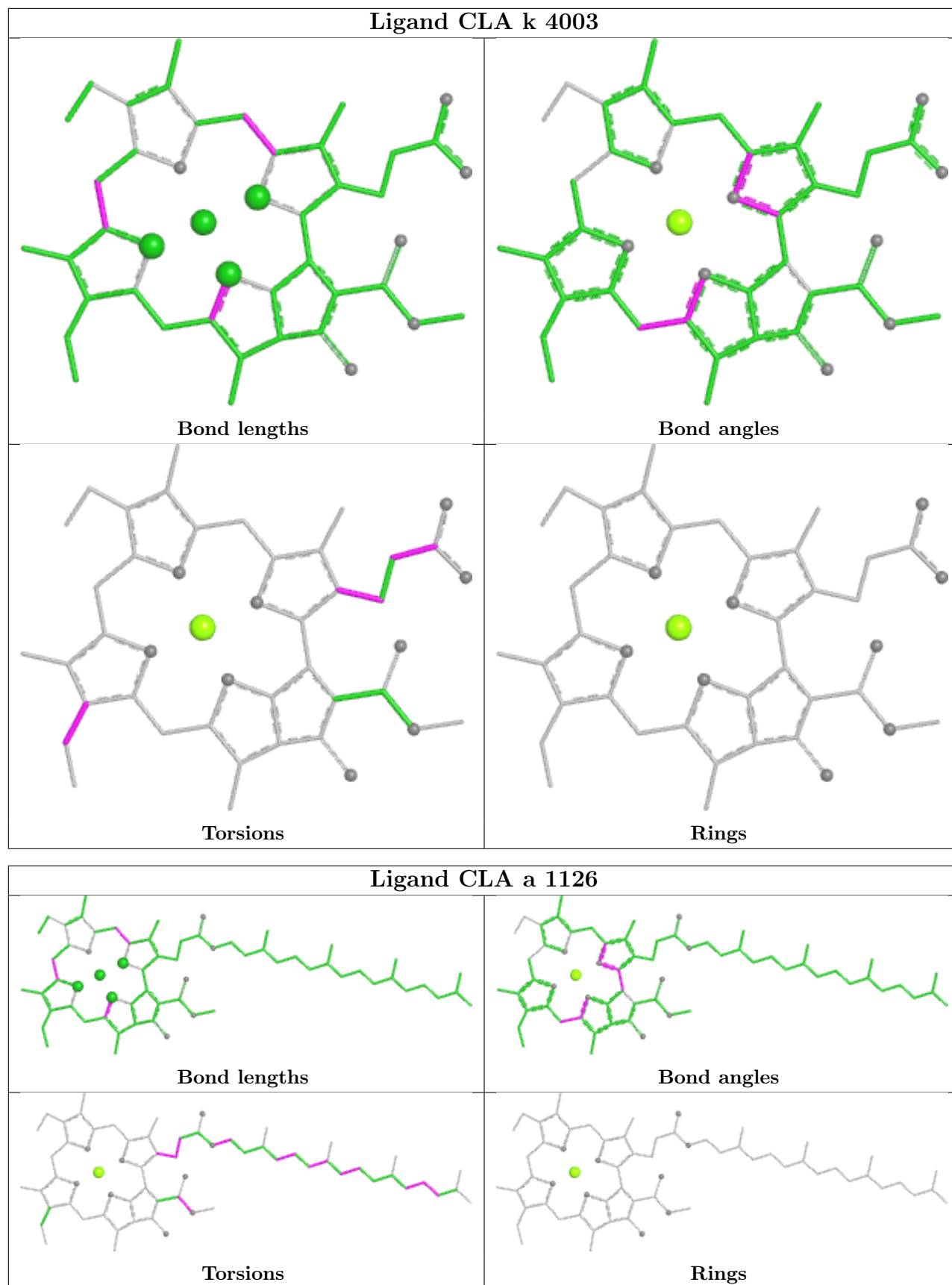
Ligand BCR b 4009	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR h 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

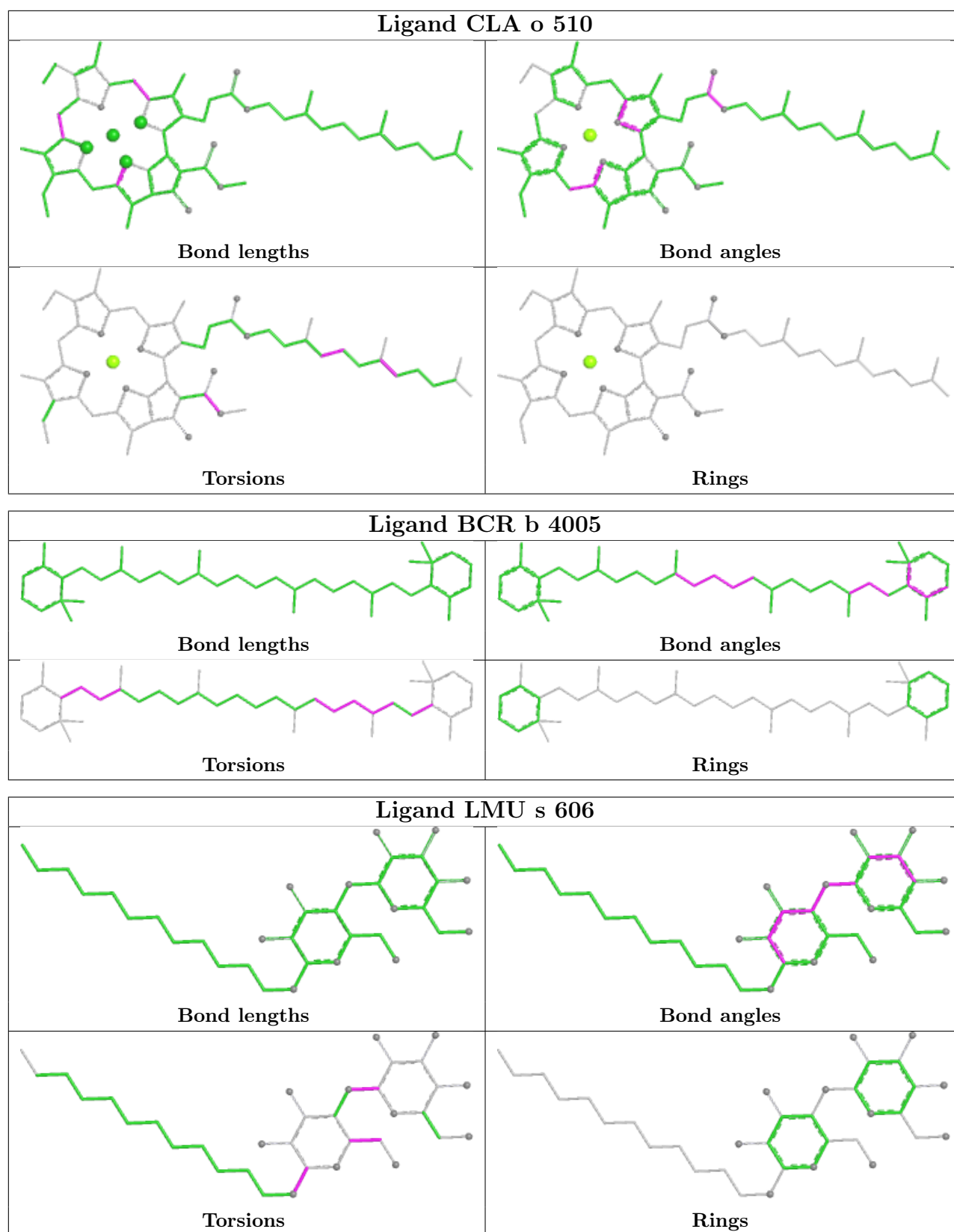




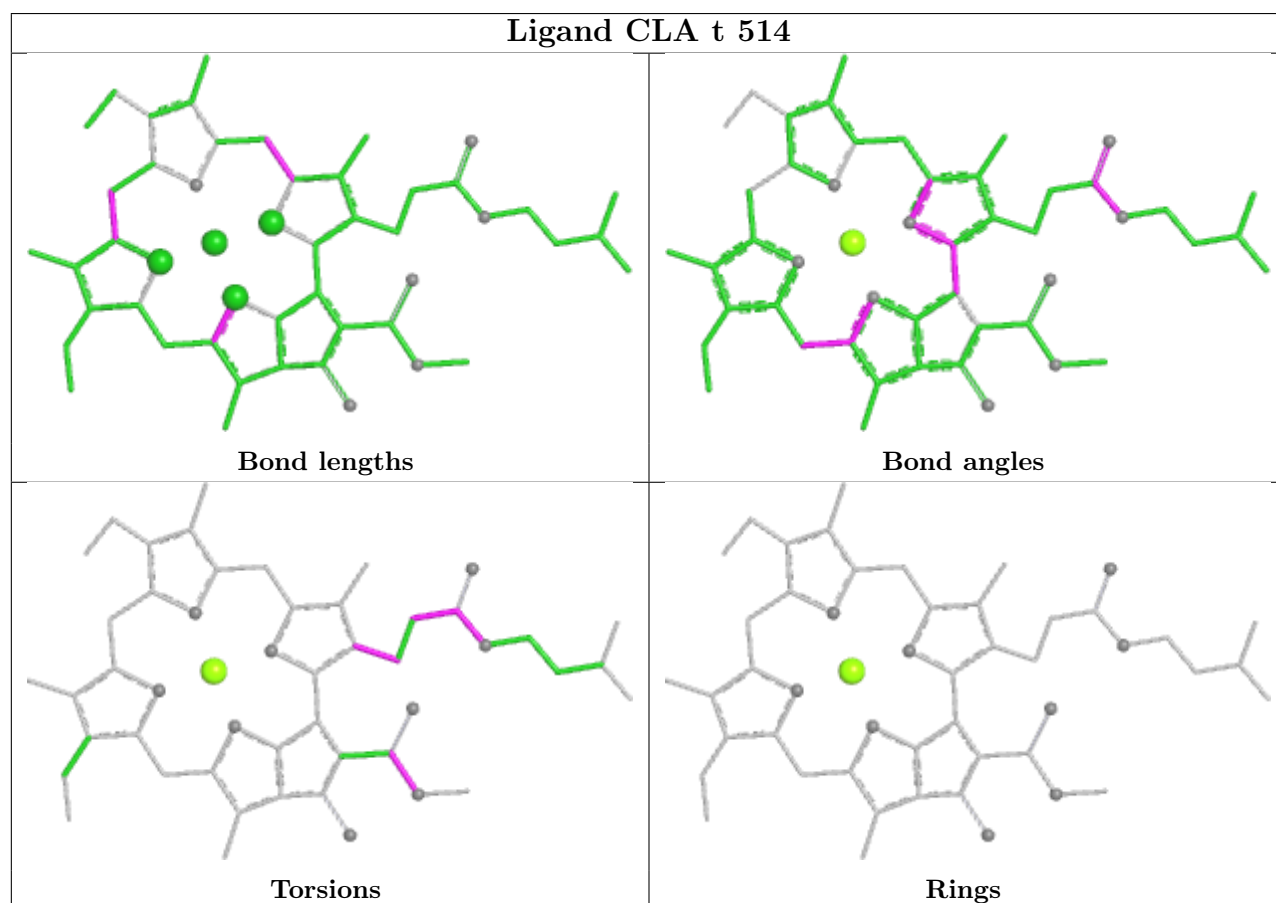
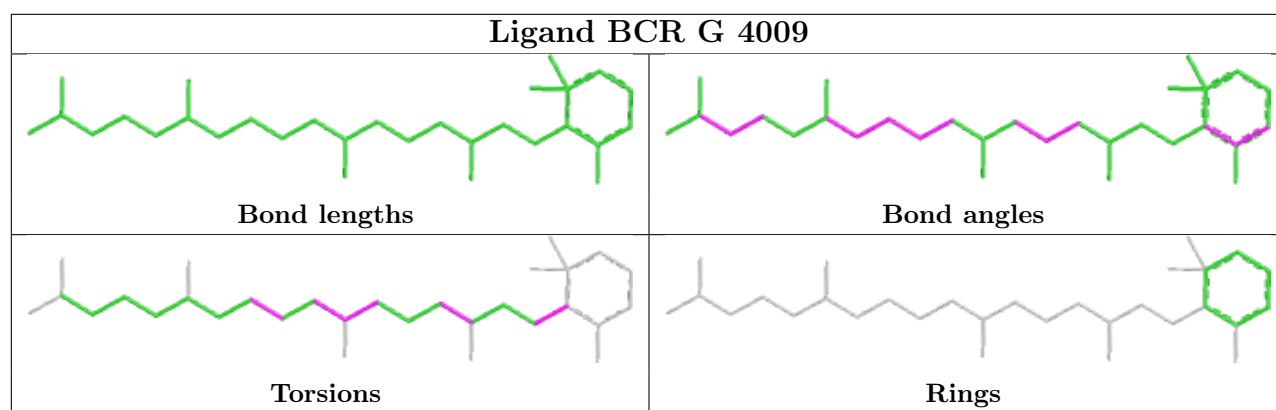




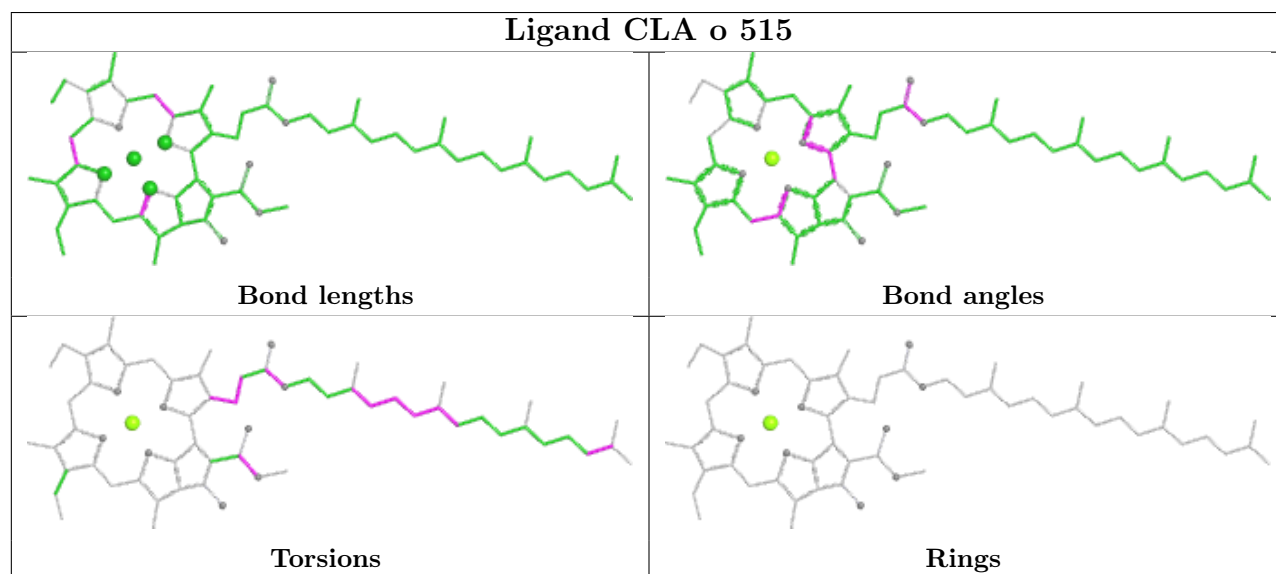
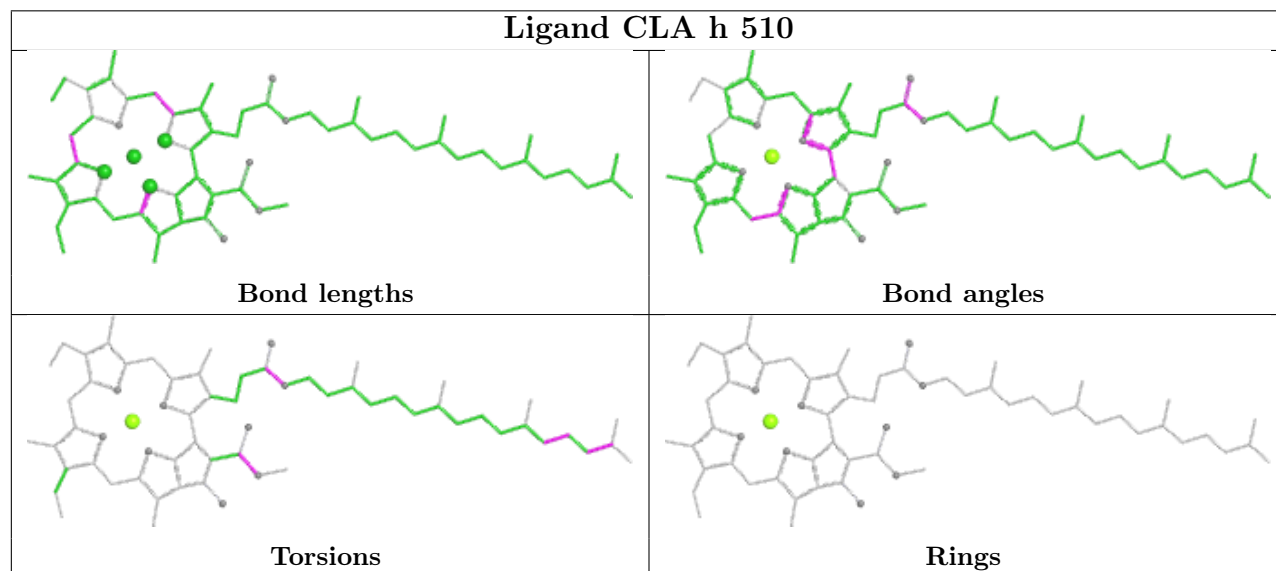
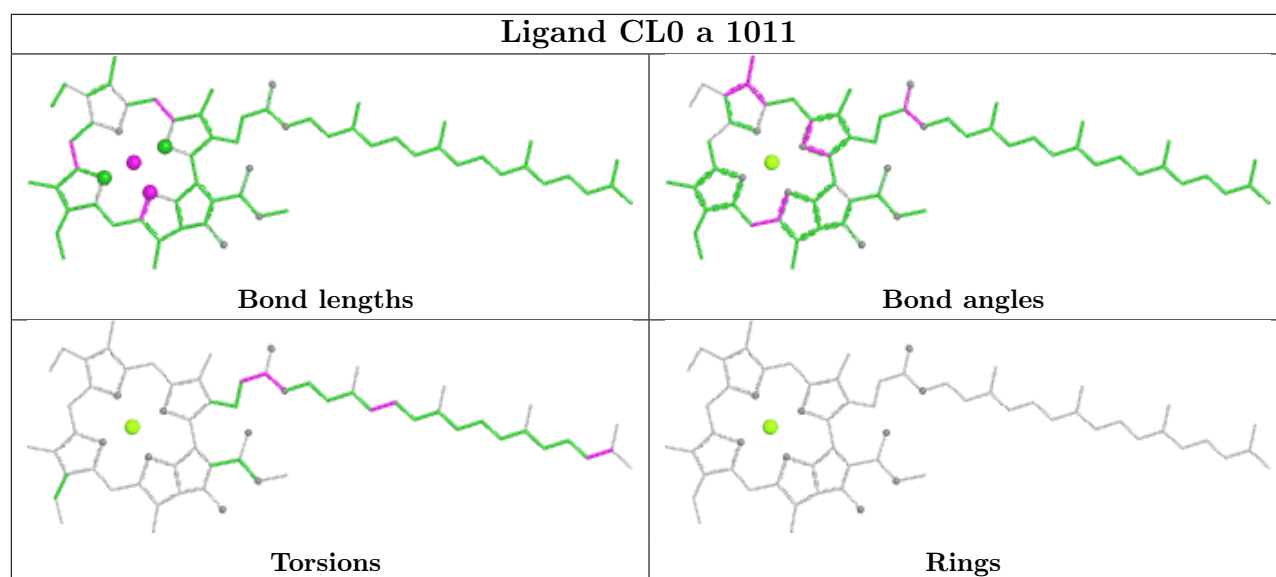




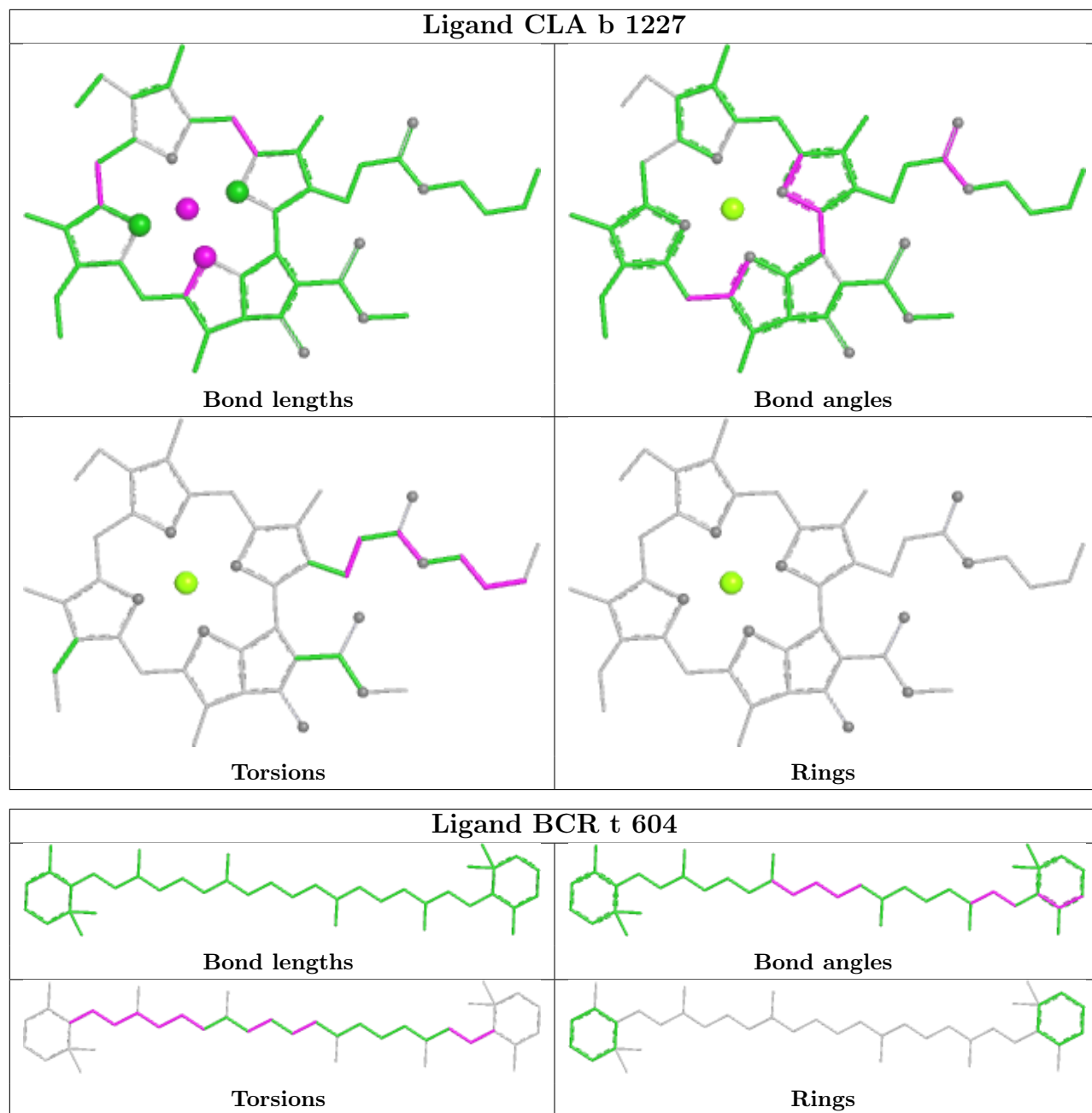




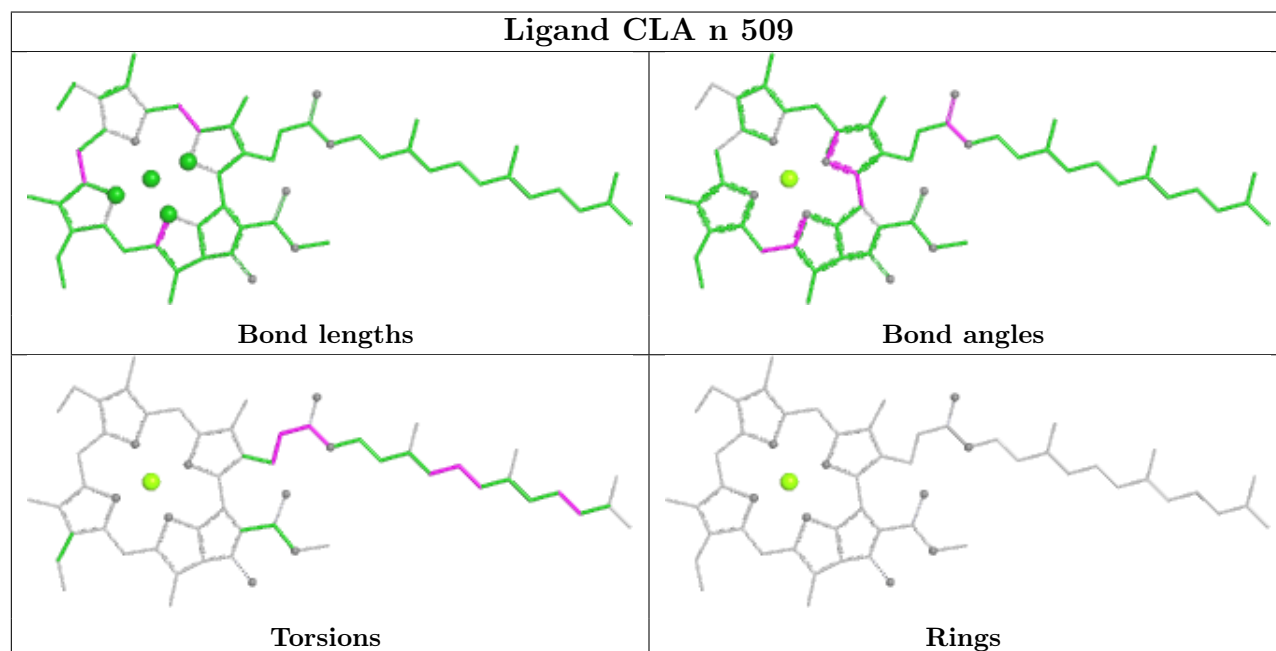
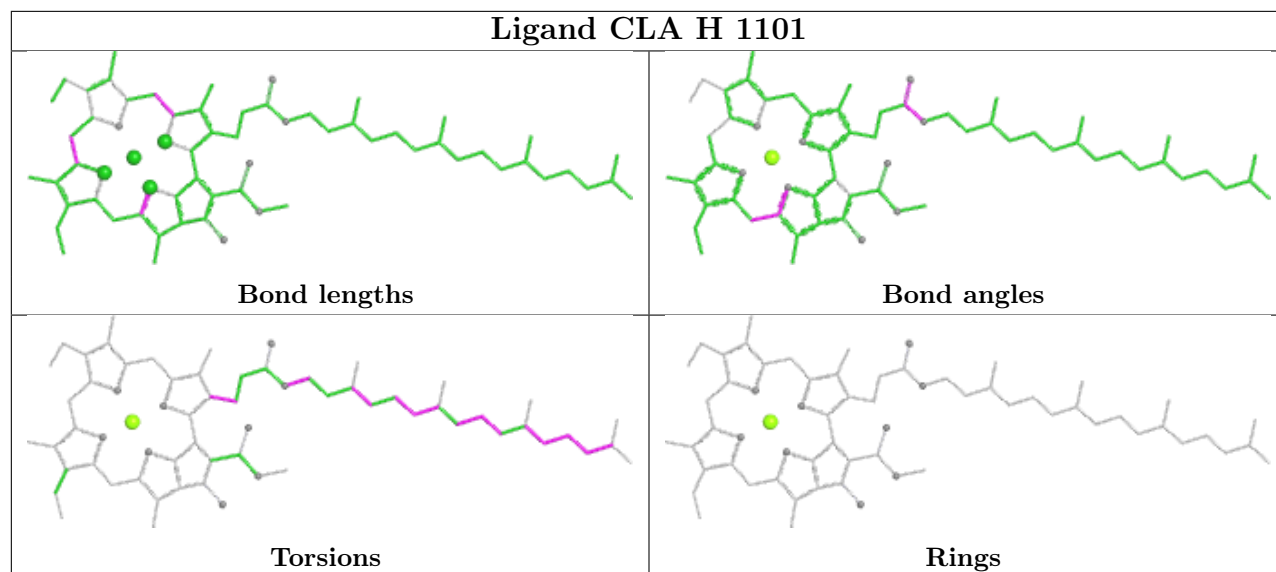




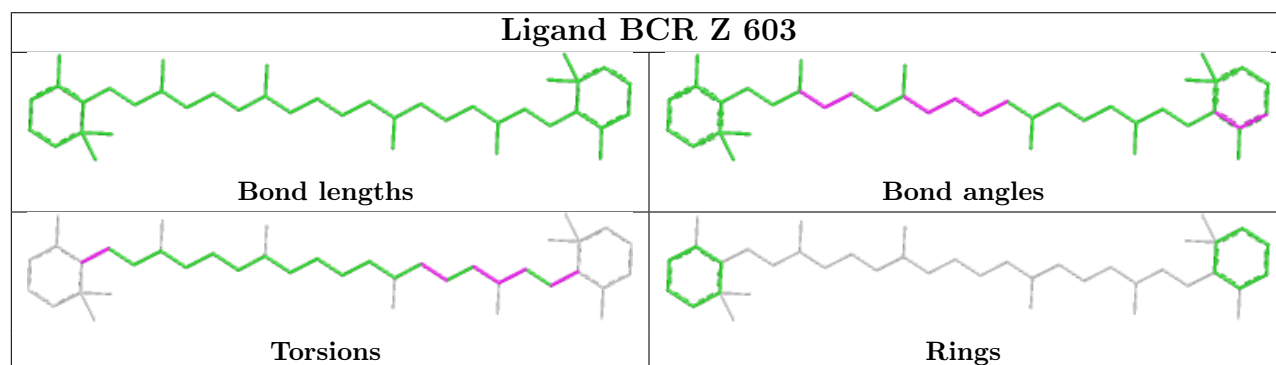
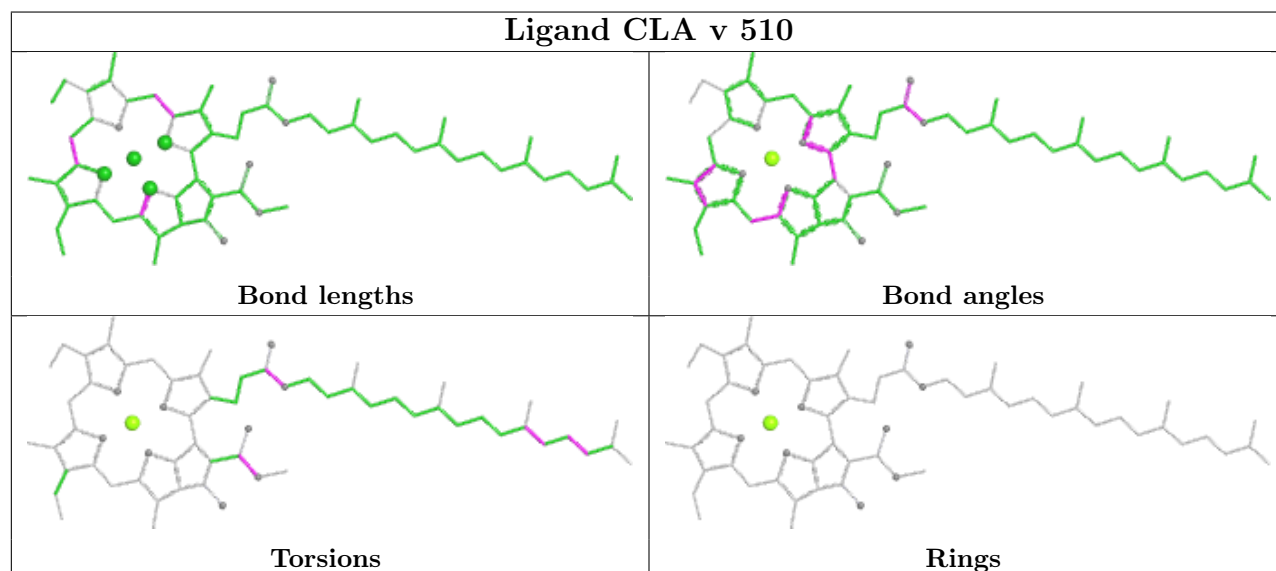
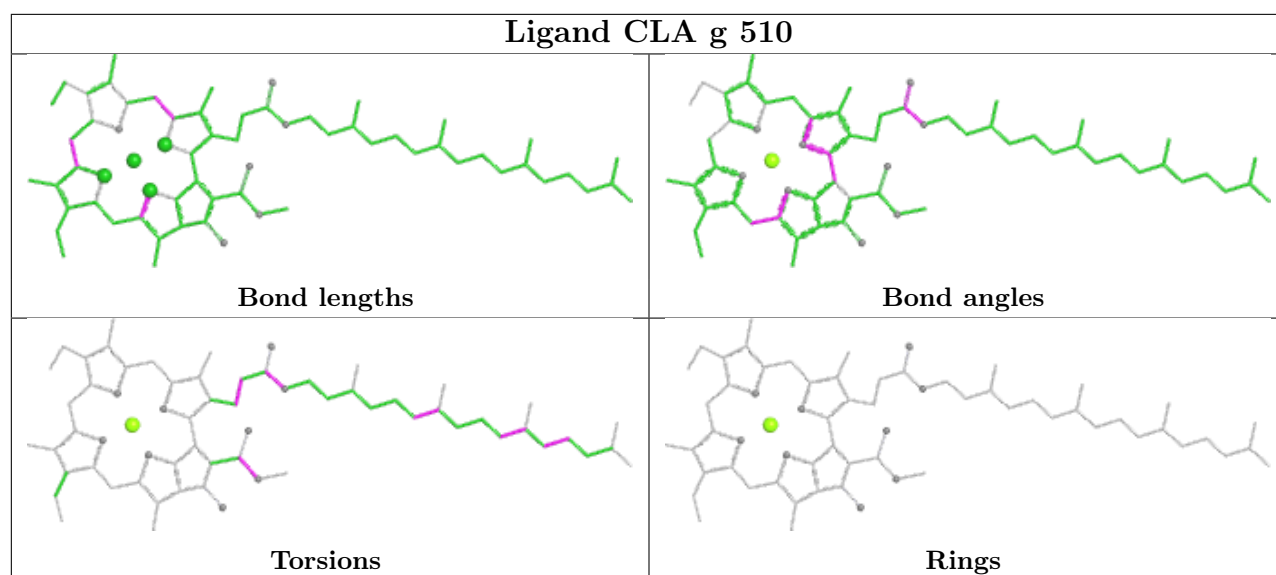






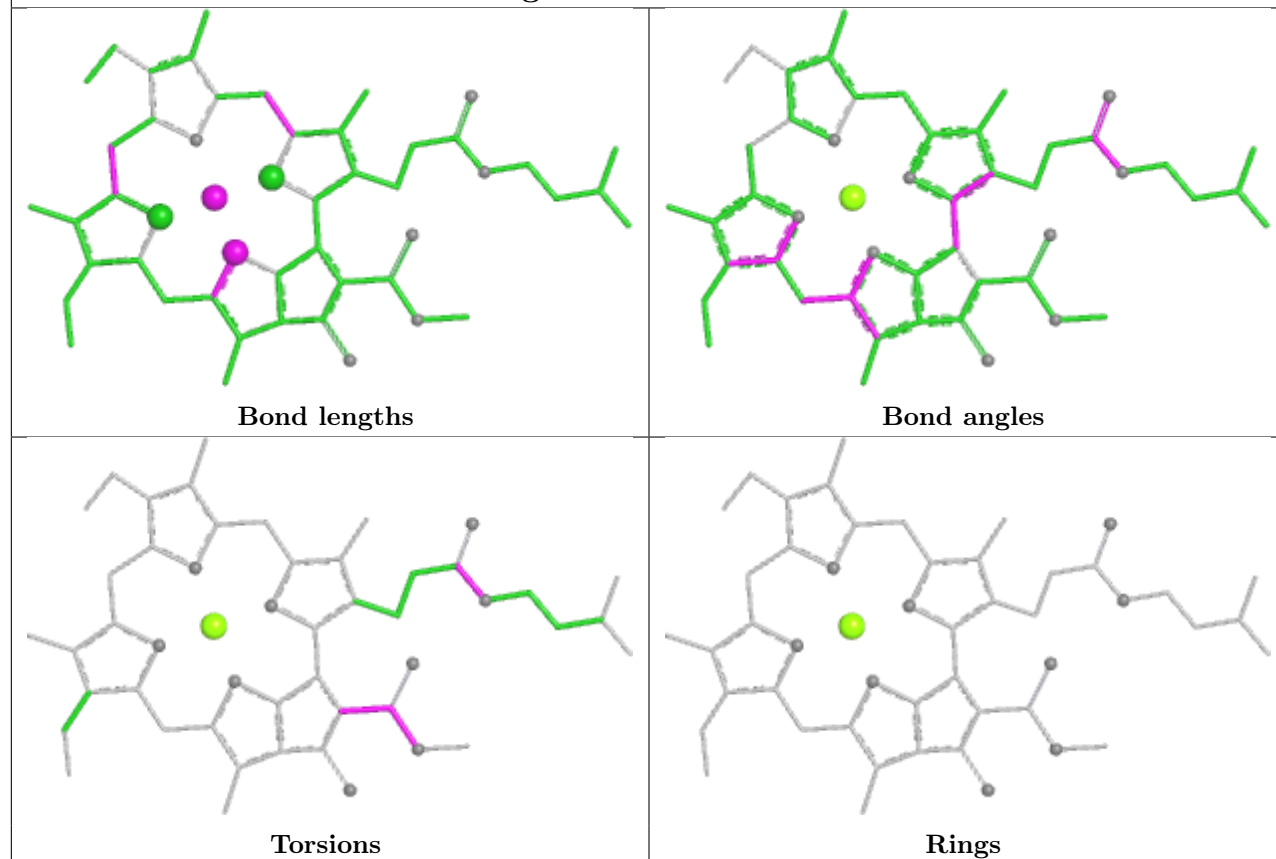




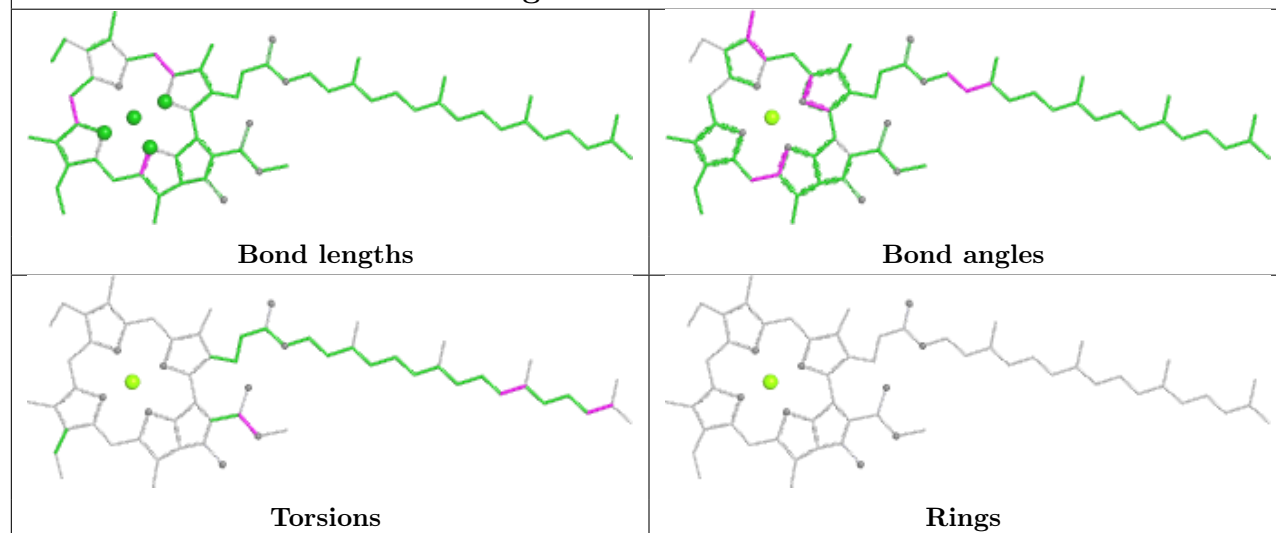




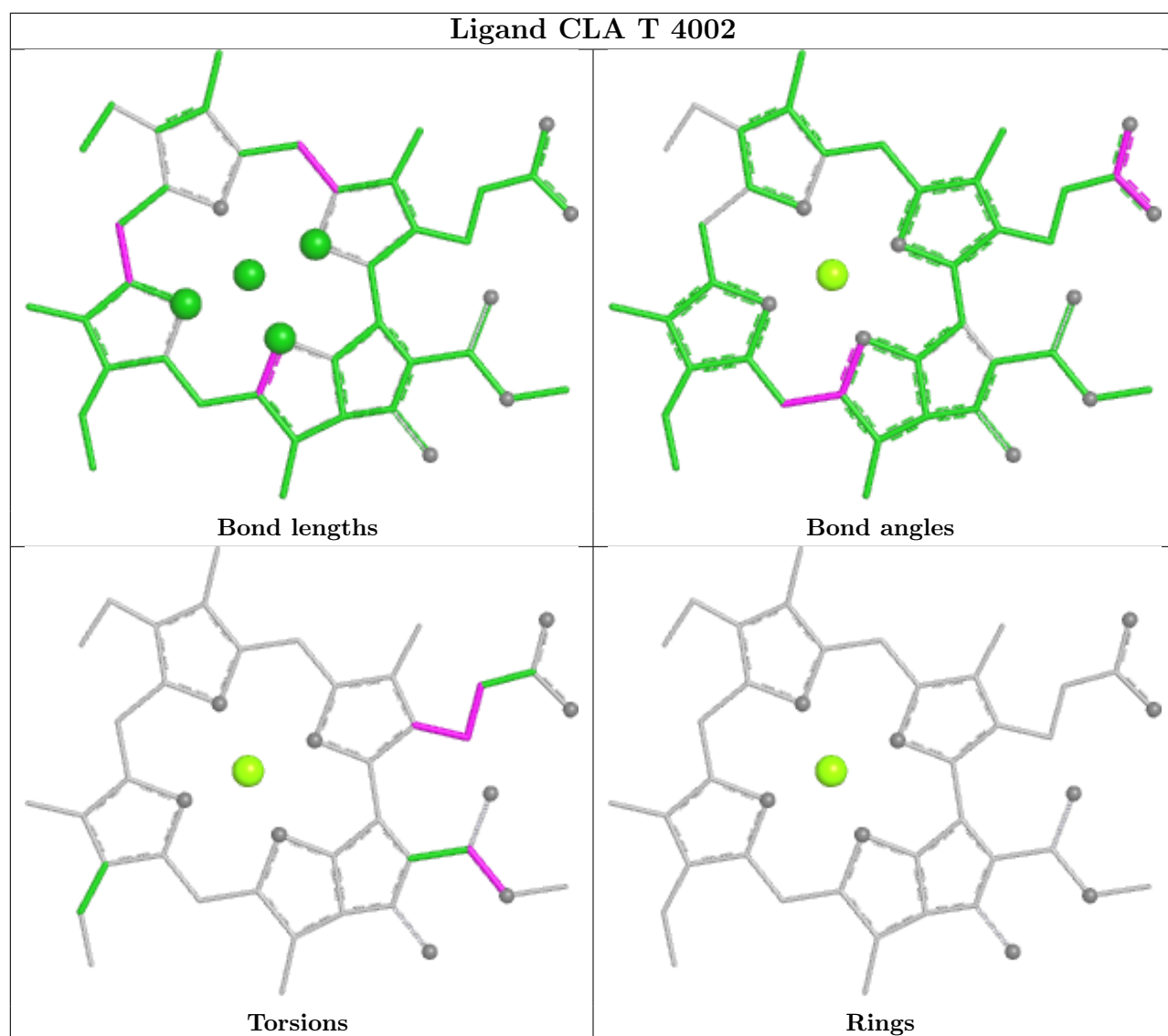
## Ligand CLA G 1222



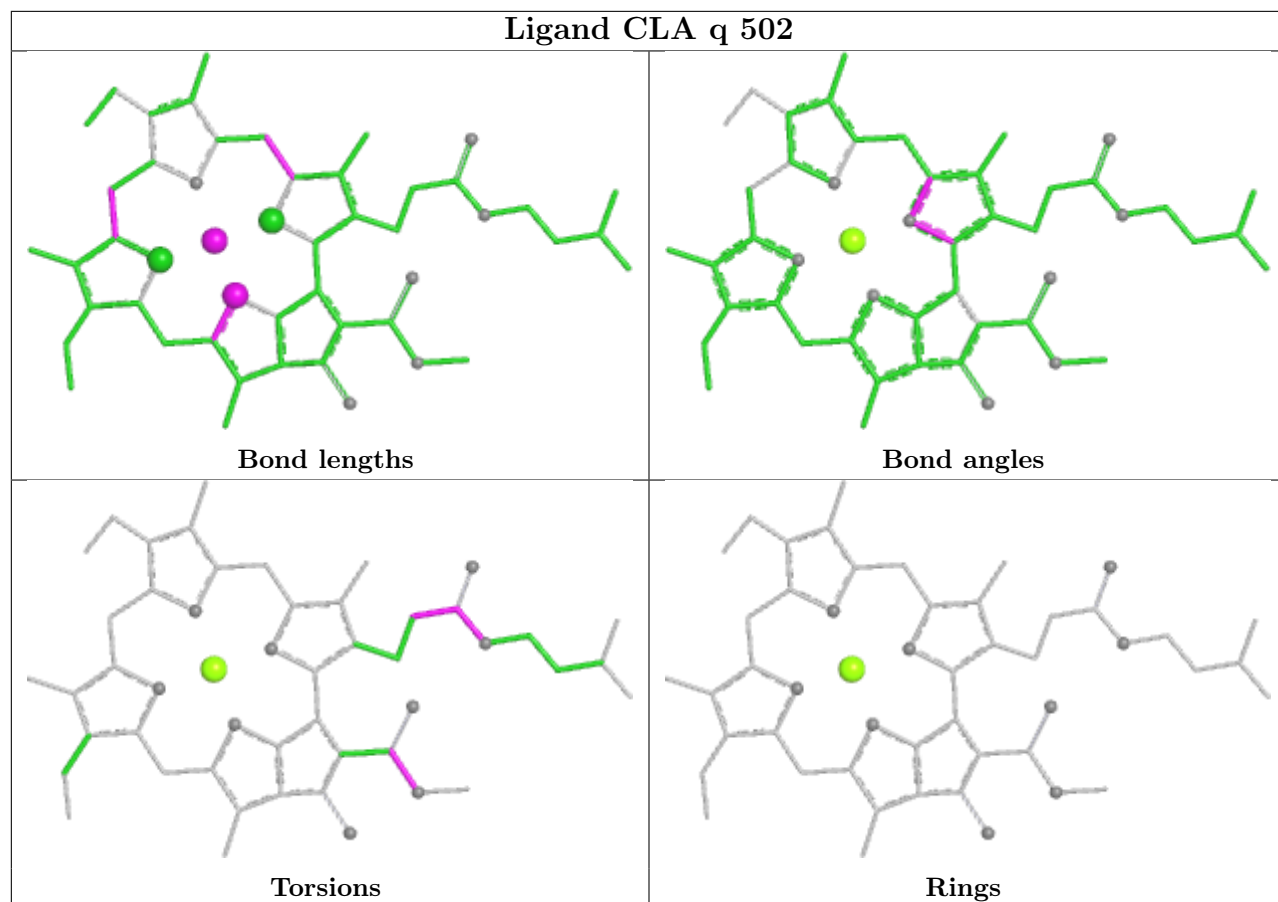
## Ligand CLA A 1117



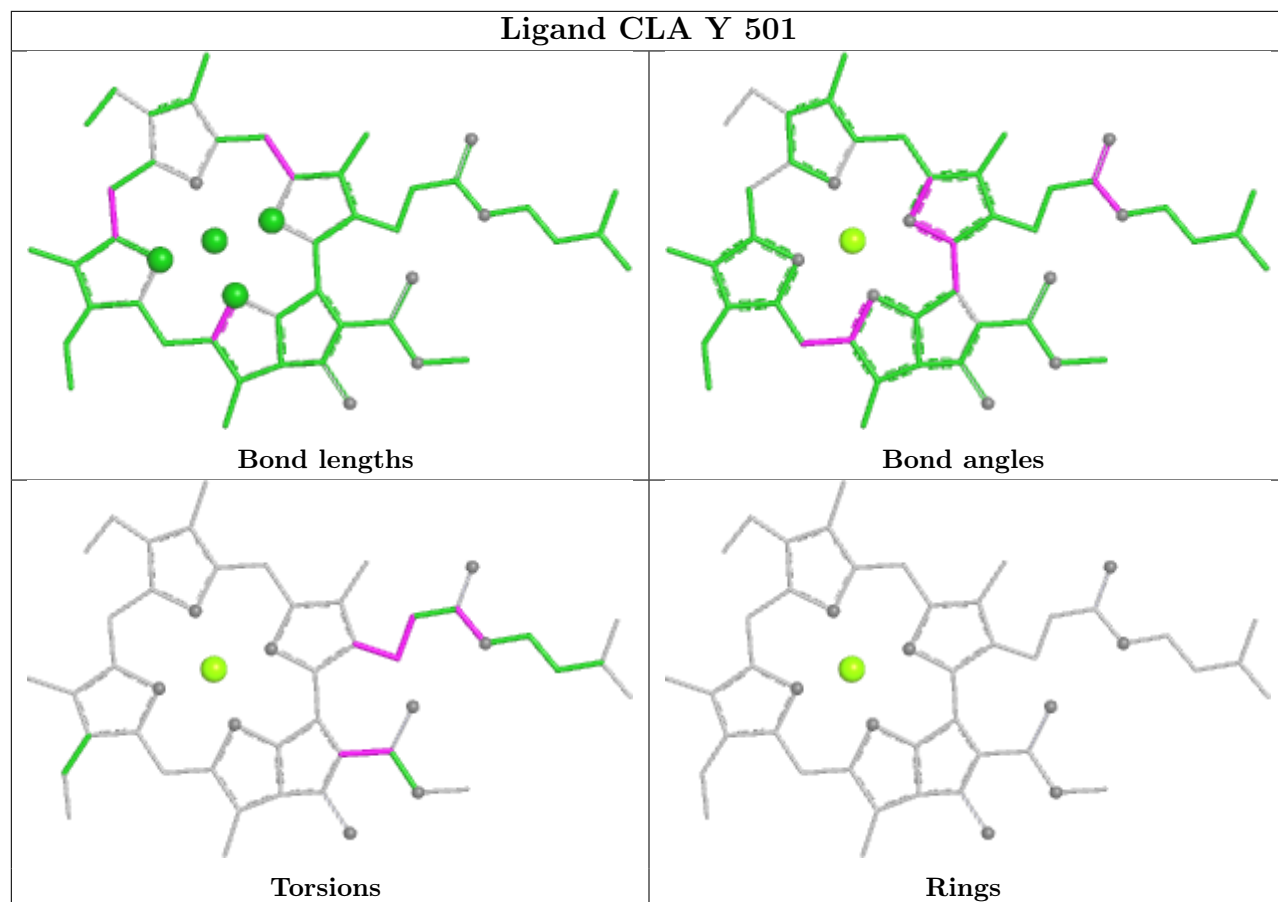




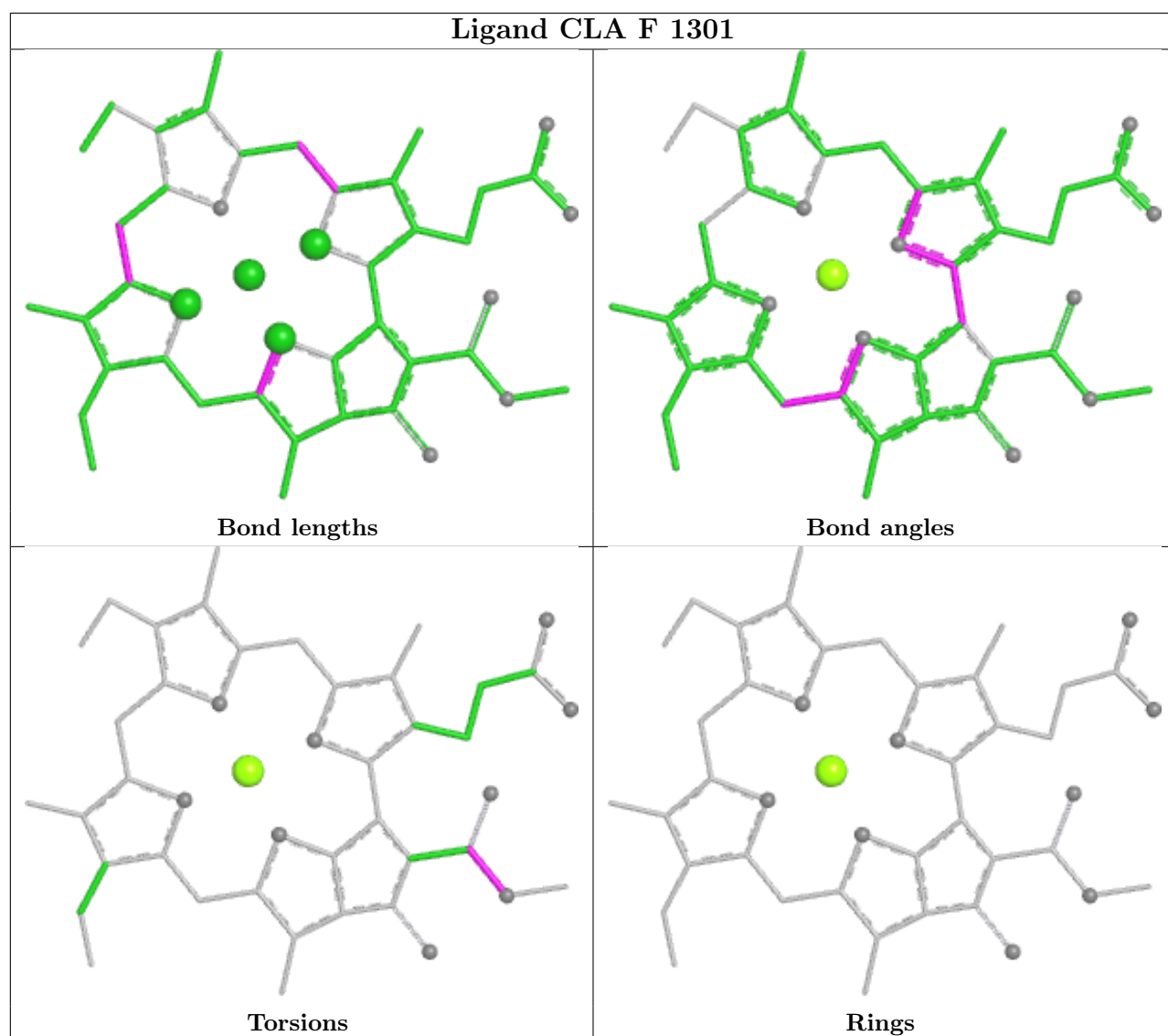




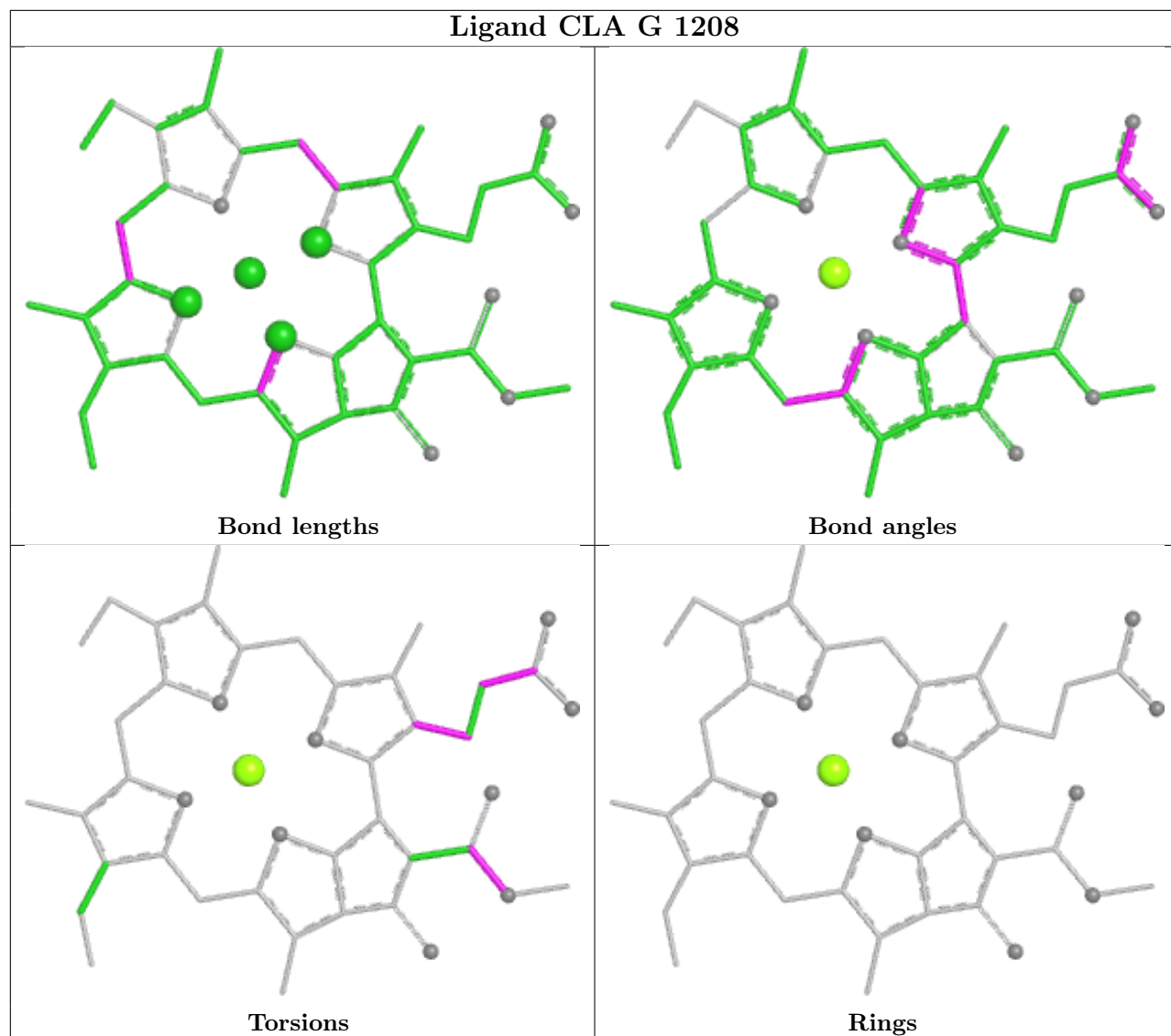






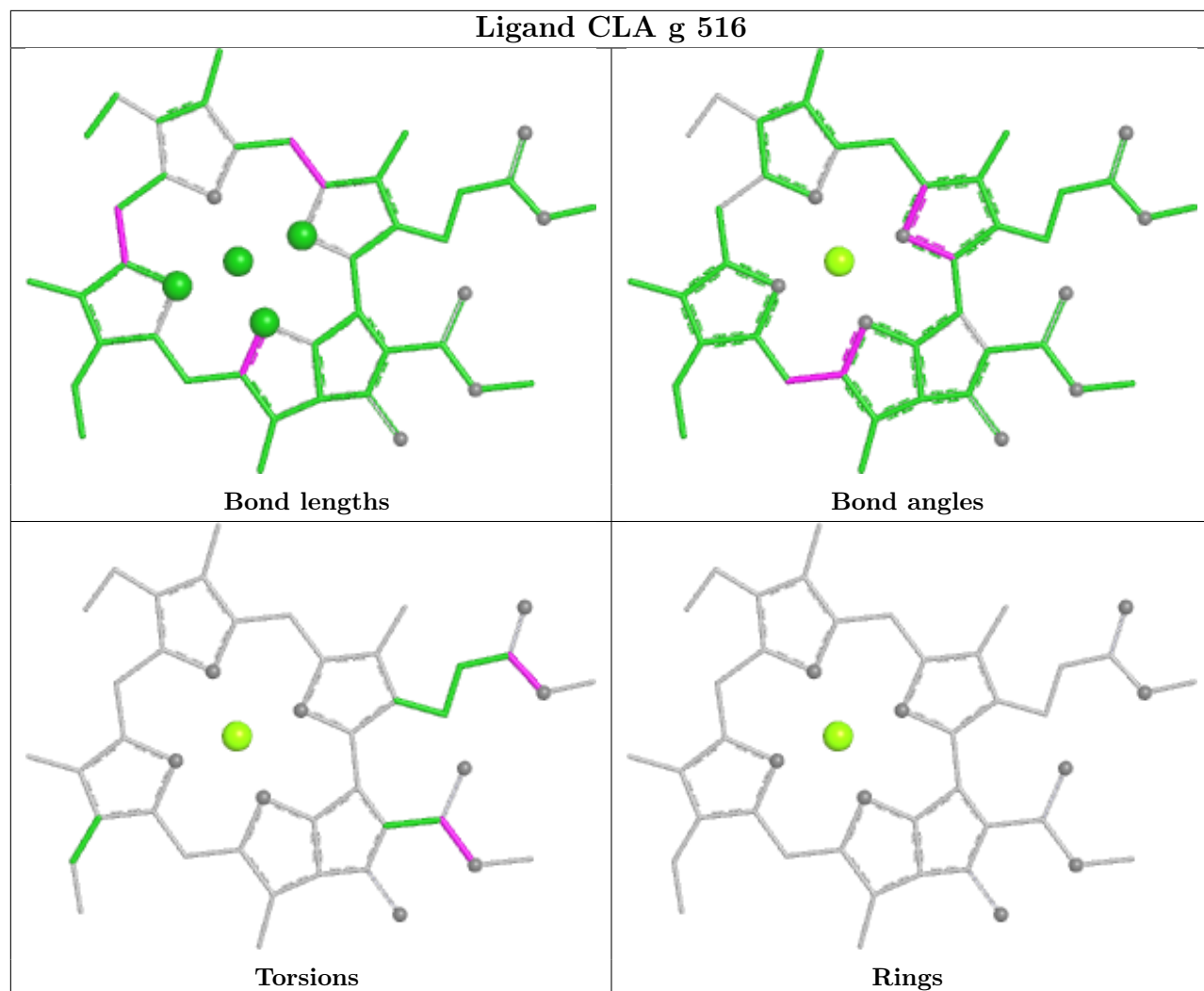






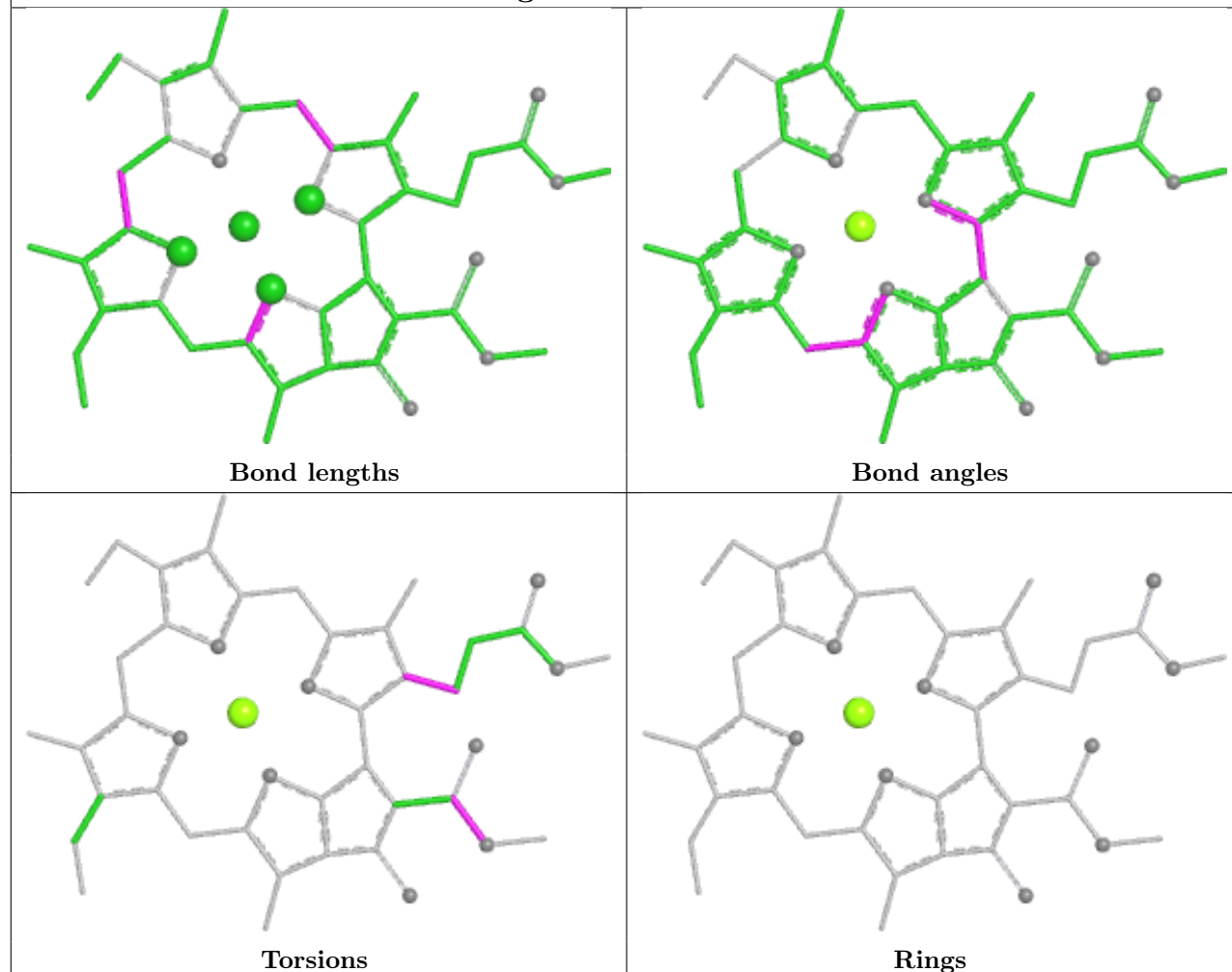


## Ligand CLA g 516

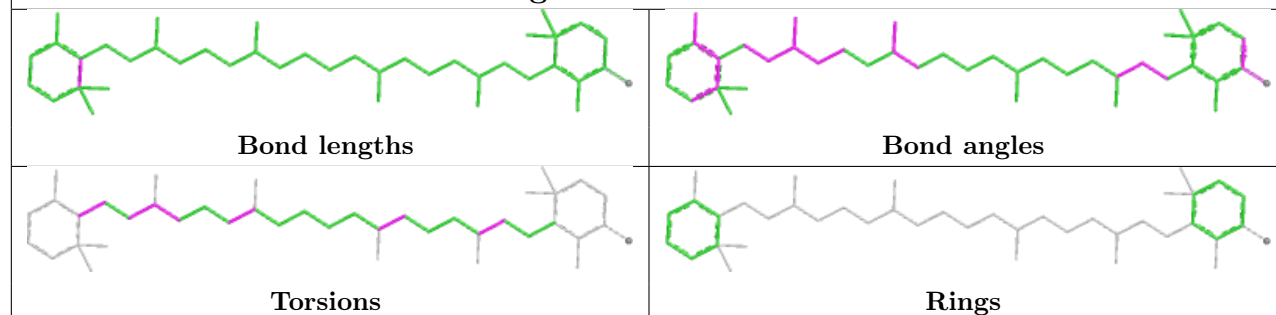




## Ligand CLA v 516

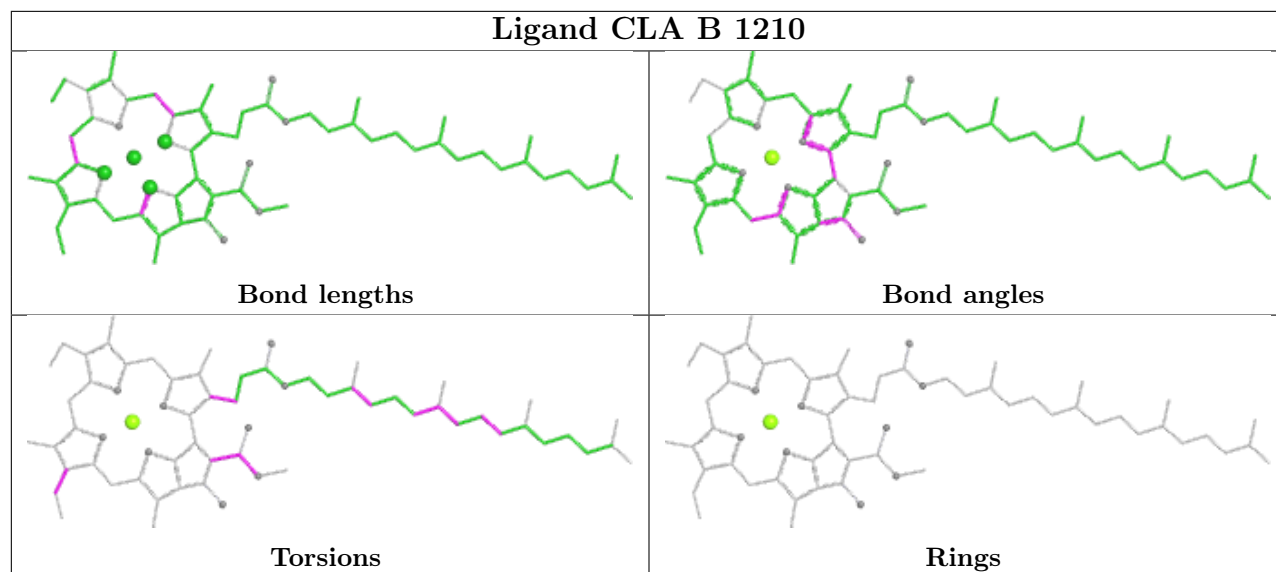


## Ligand ECH i 4020

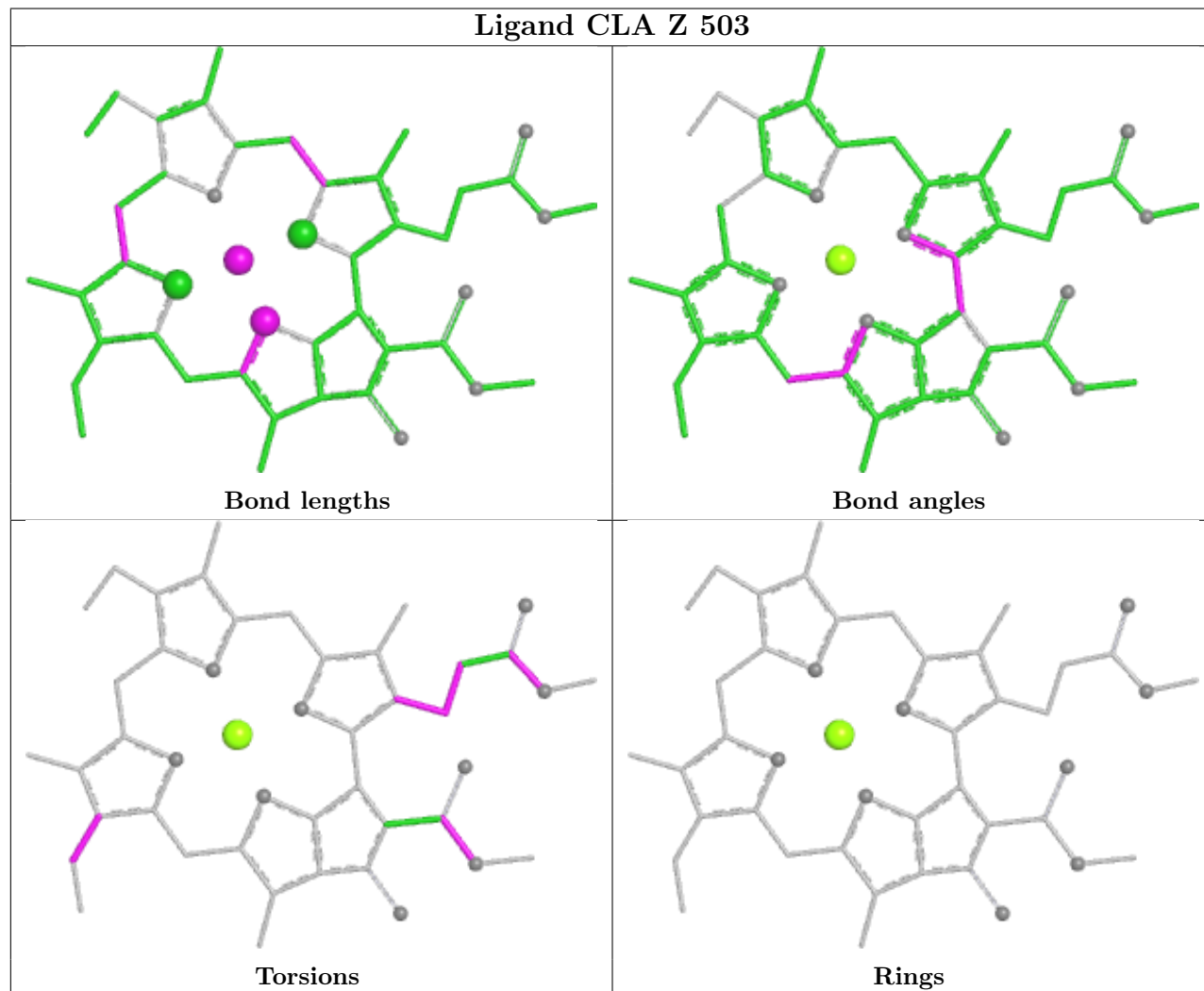




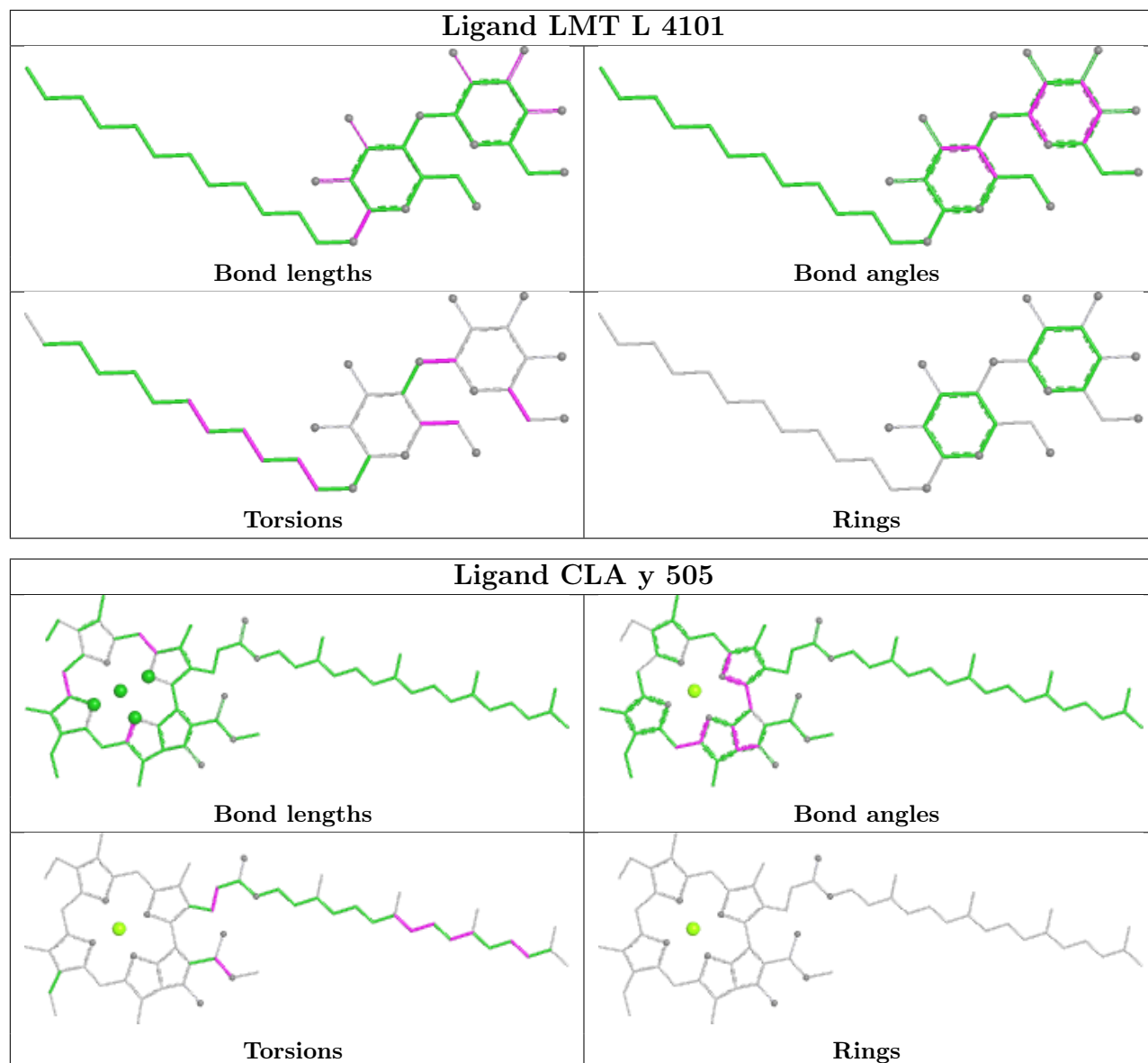
## Ligand CLA B 1210



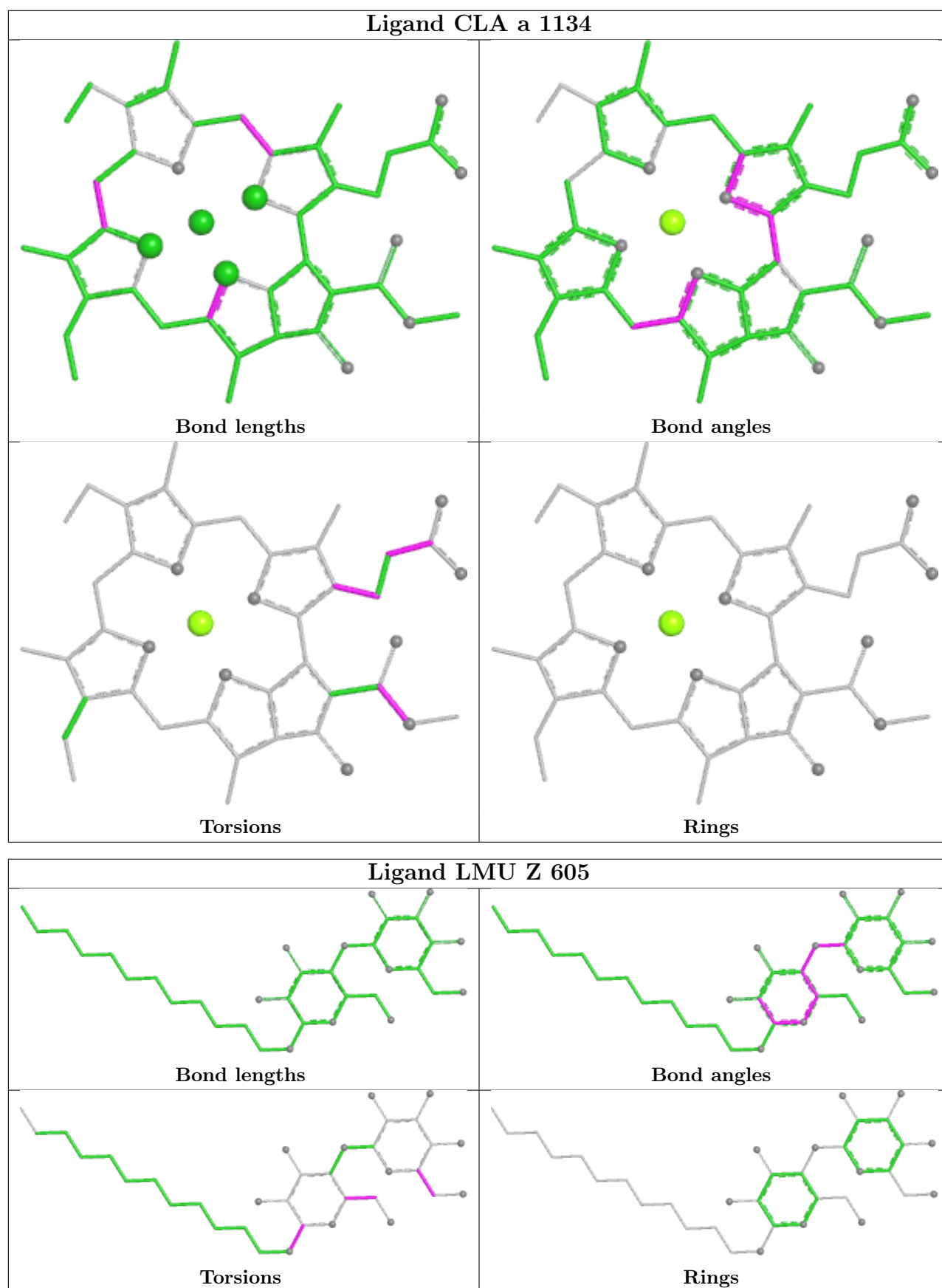
## Ligand CLA Z 503



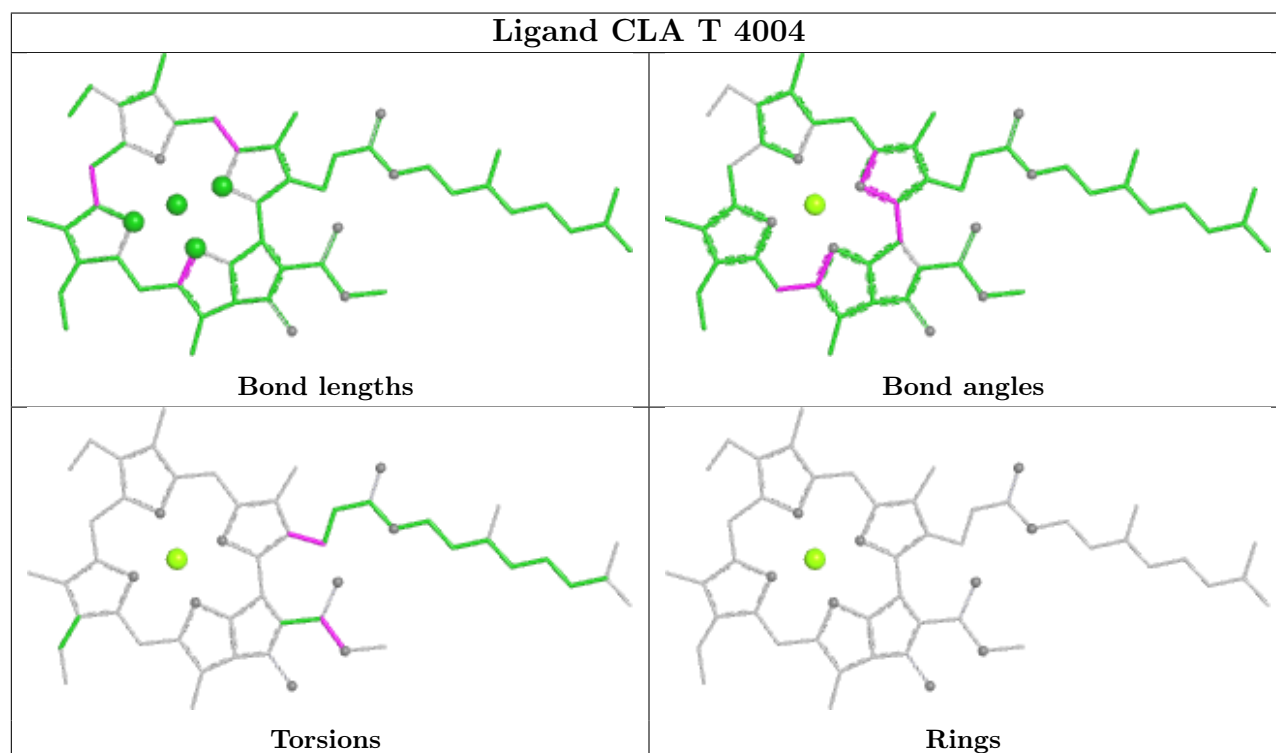
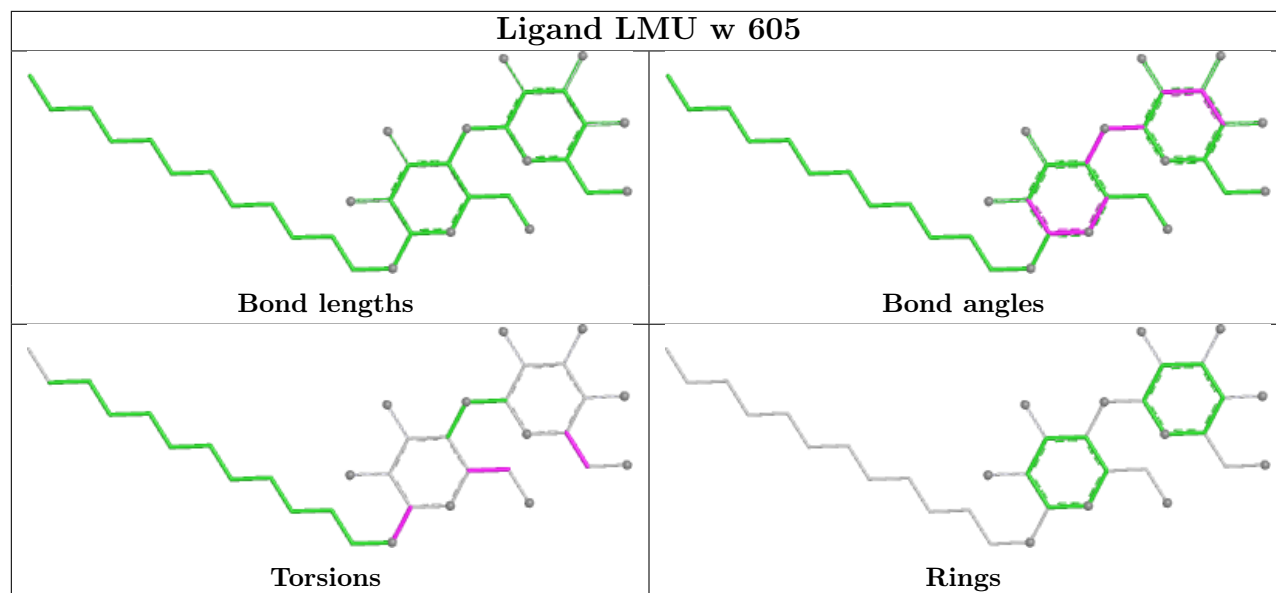




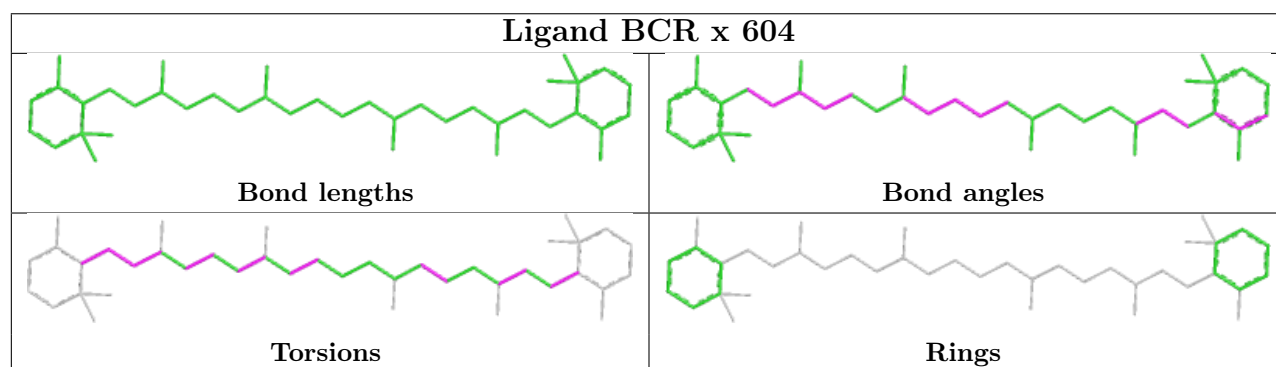
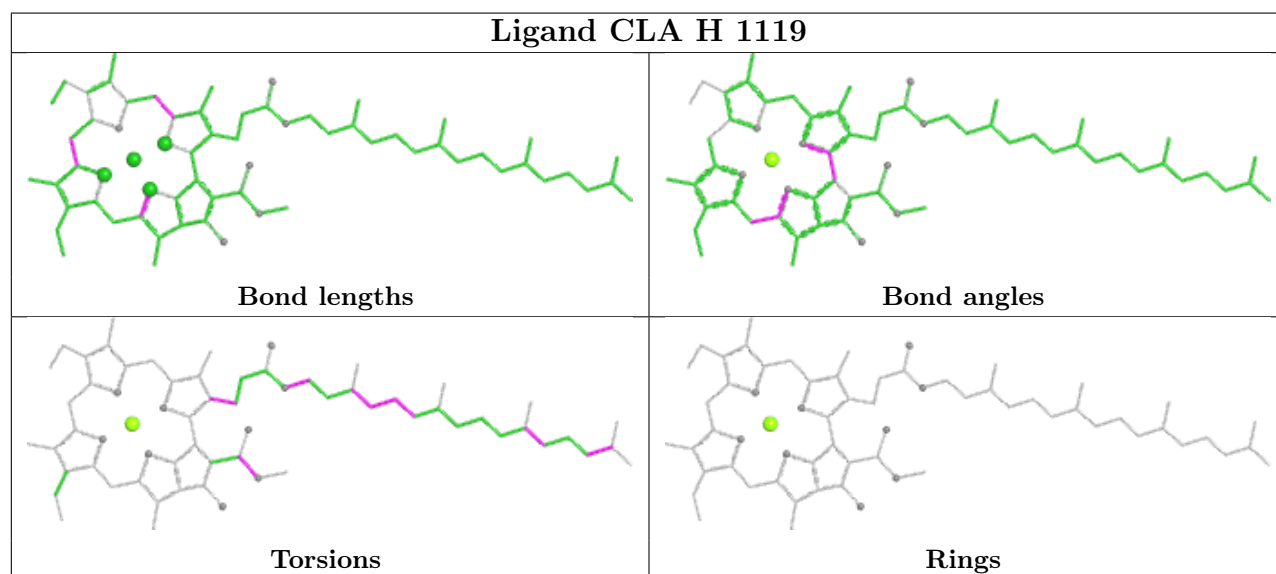
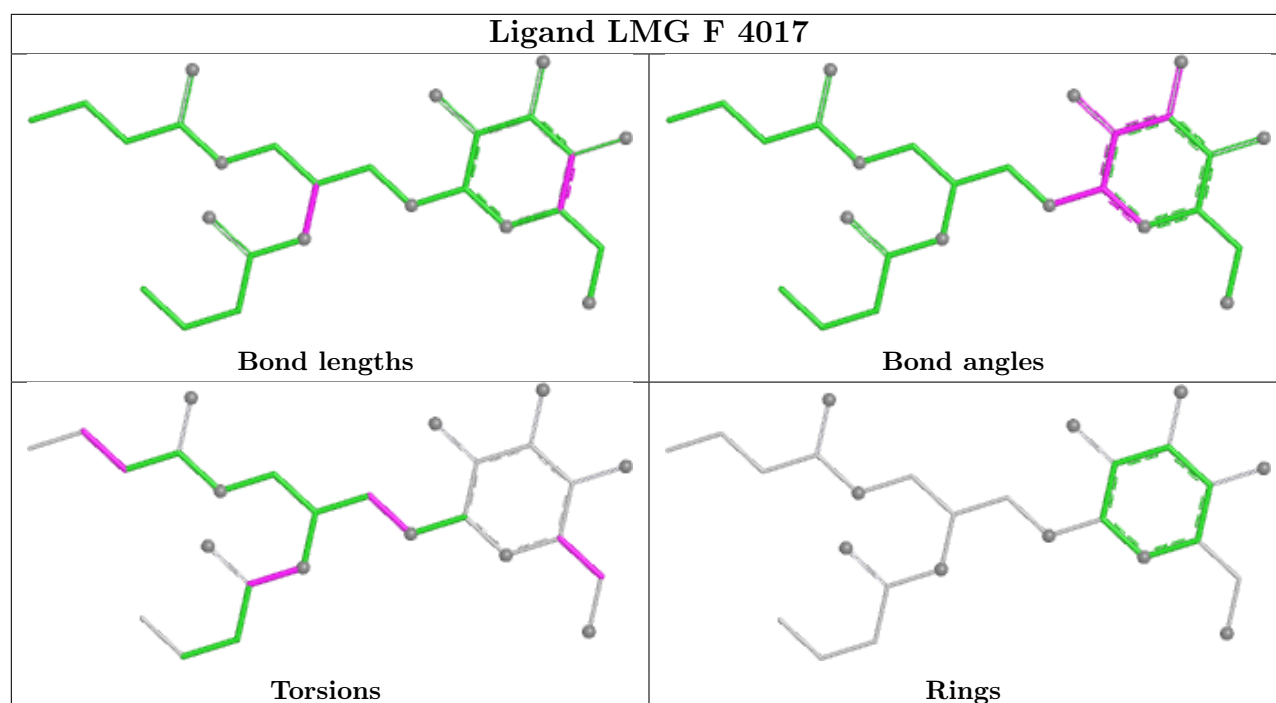






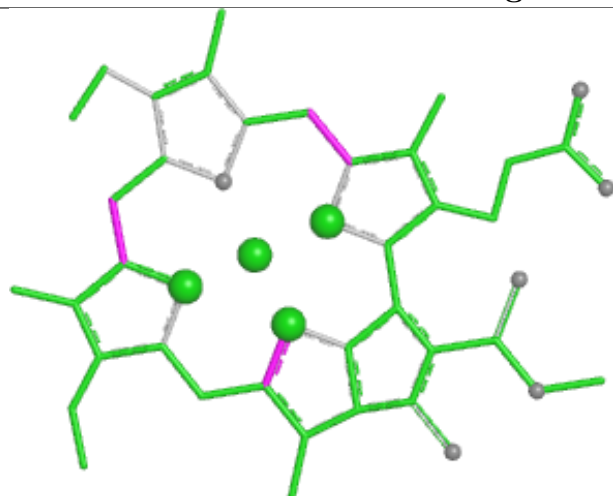




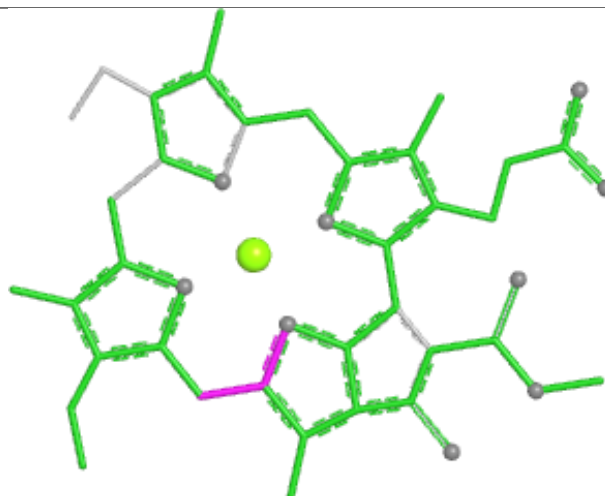




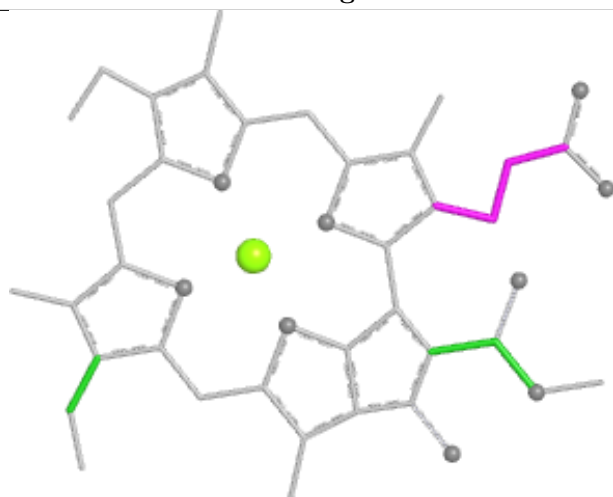
## Ligand CLA B 1217



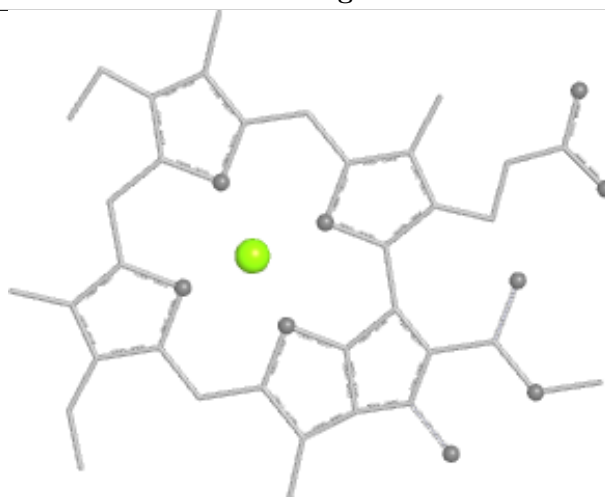
Bond lengths



Bond angles

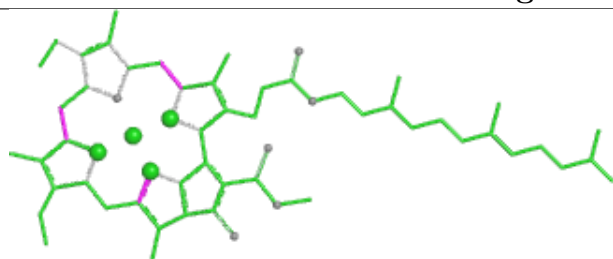


Torsions

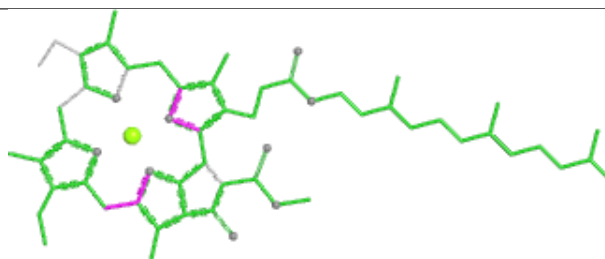


Rings

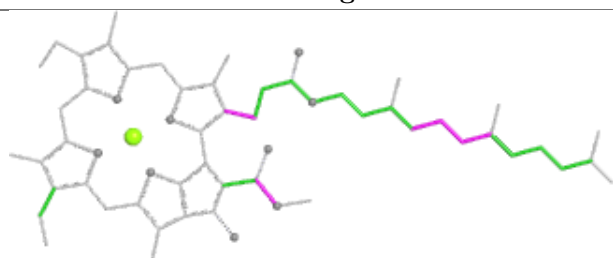
## Ligand CLA Z 506



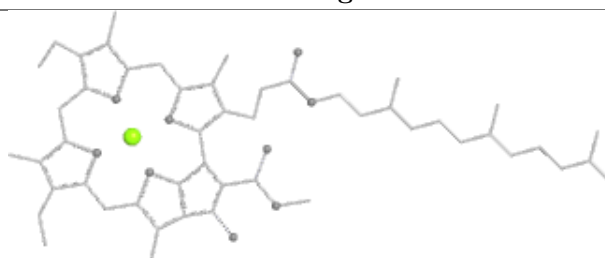
Bond lengths



Bond angles



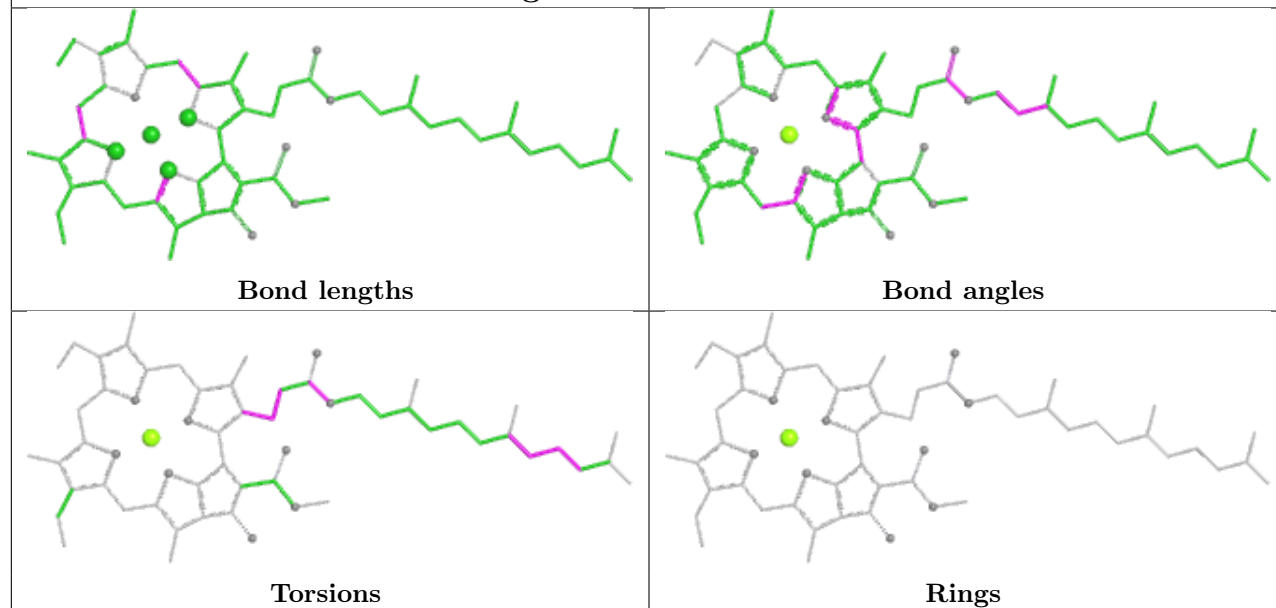
Torsions



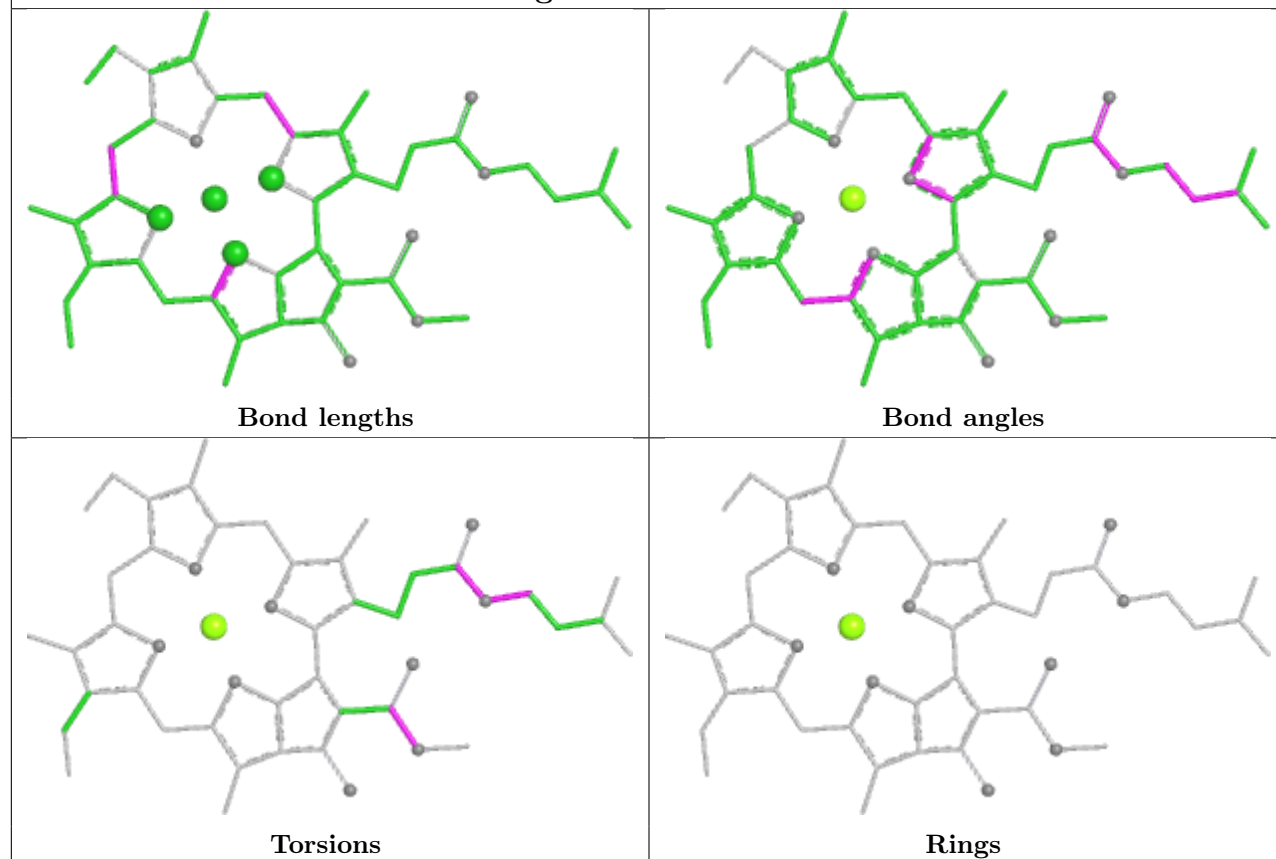
Rings



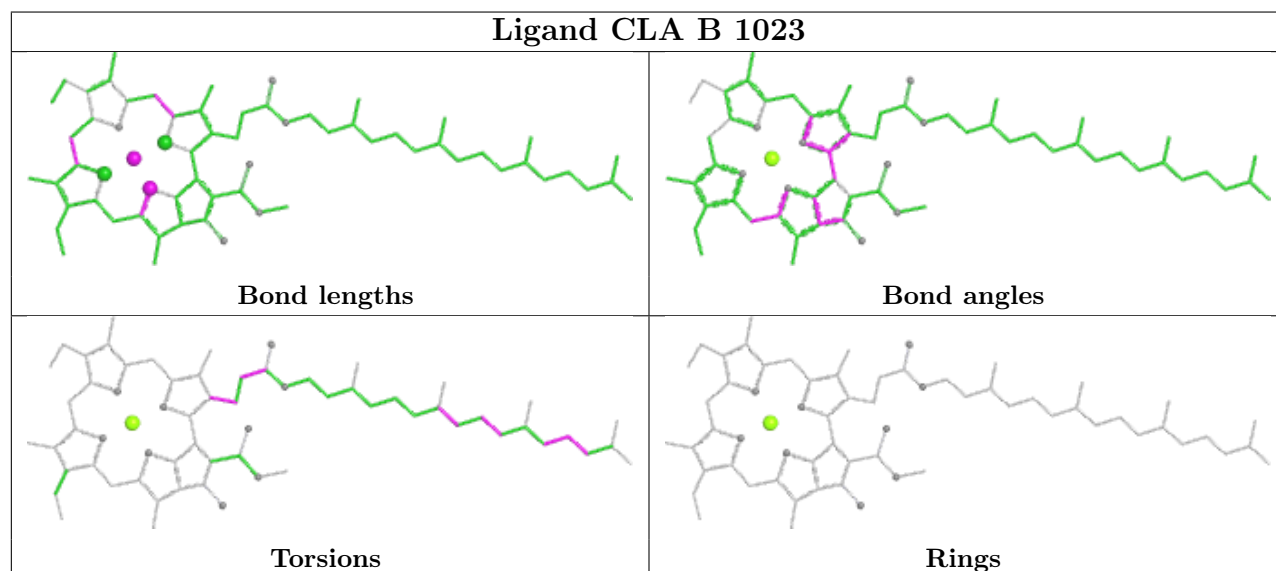
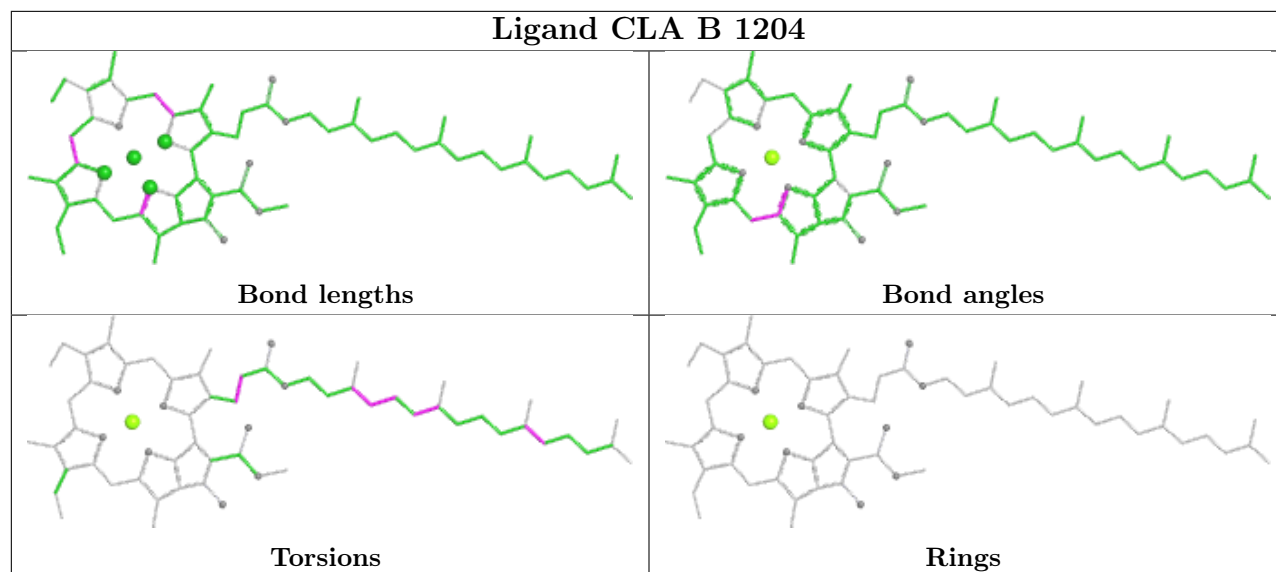
## Ligand CLA H 1130



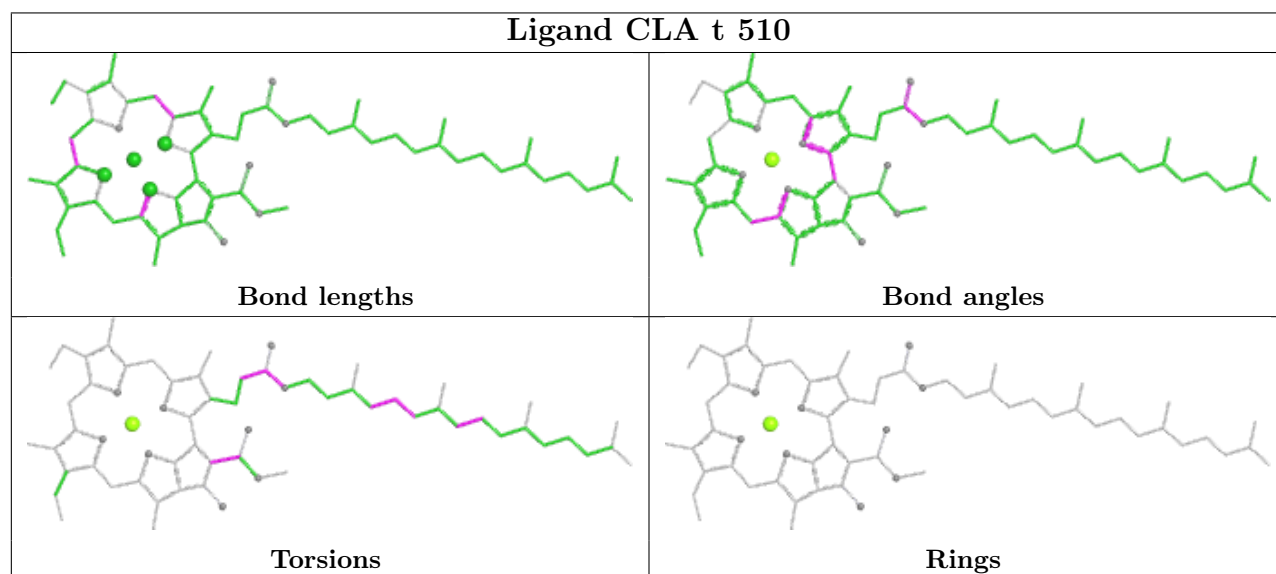
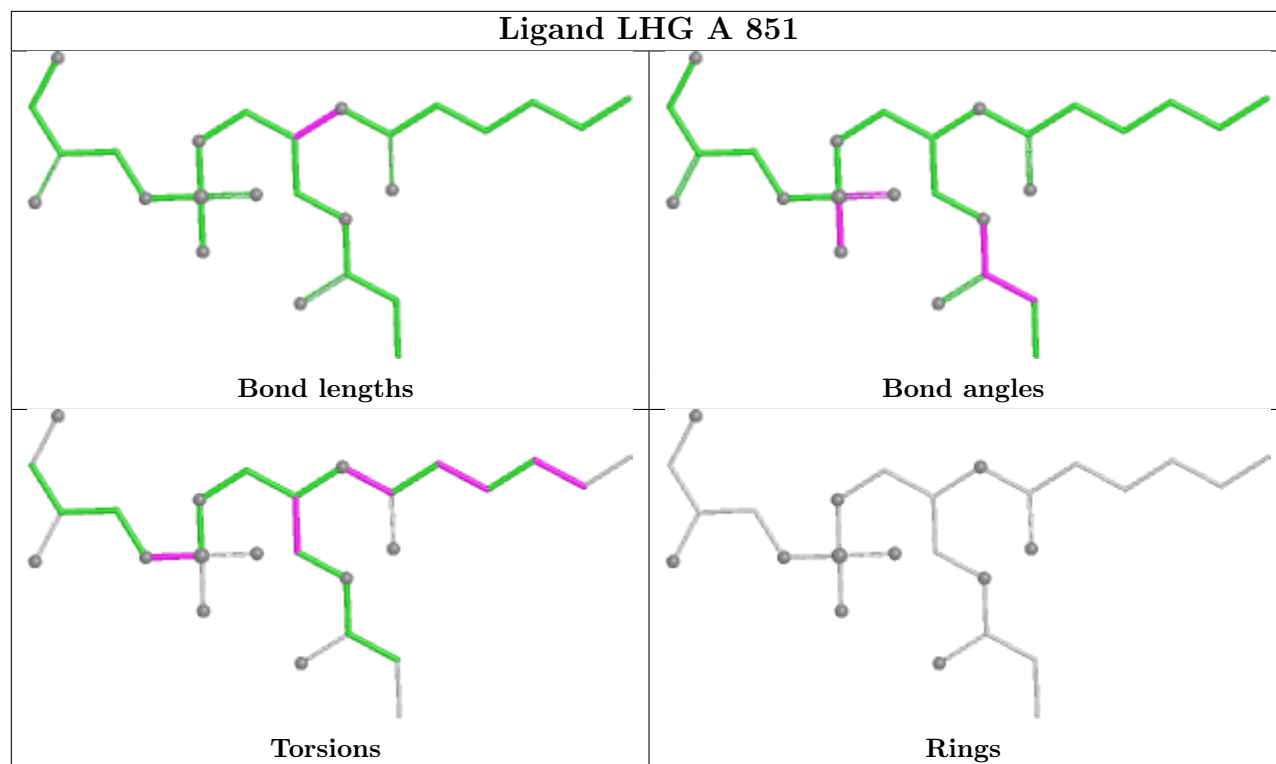
## Ligand CLA h 502





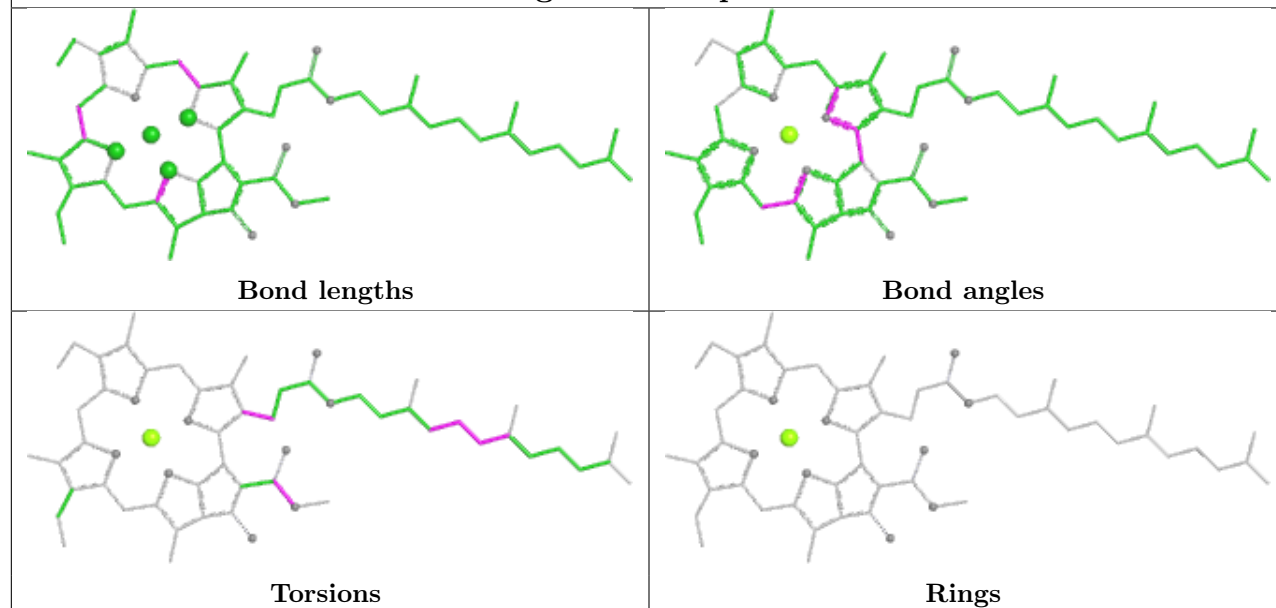




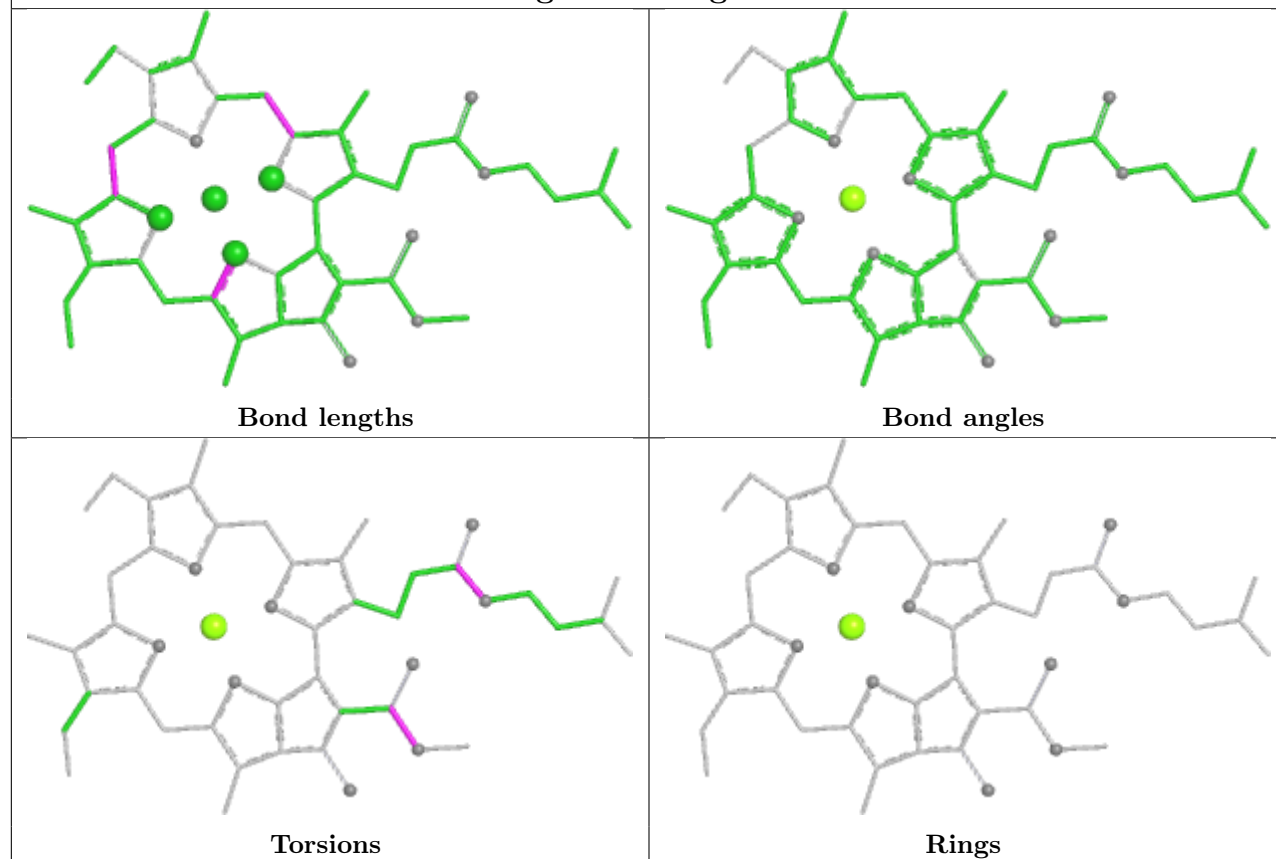




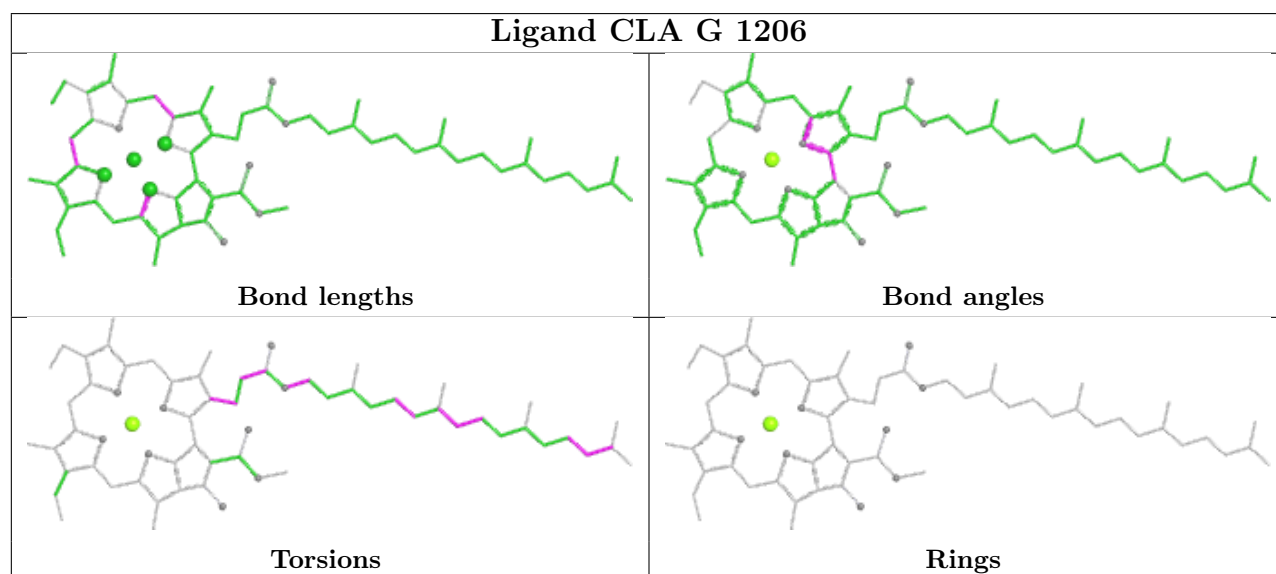
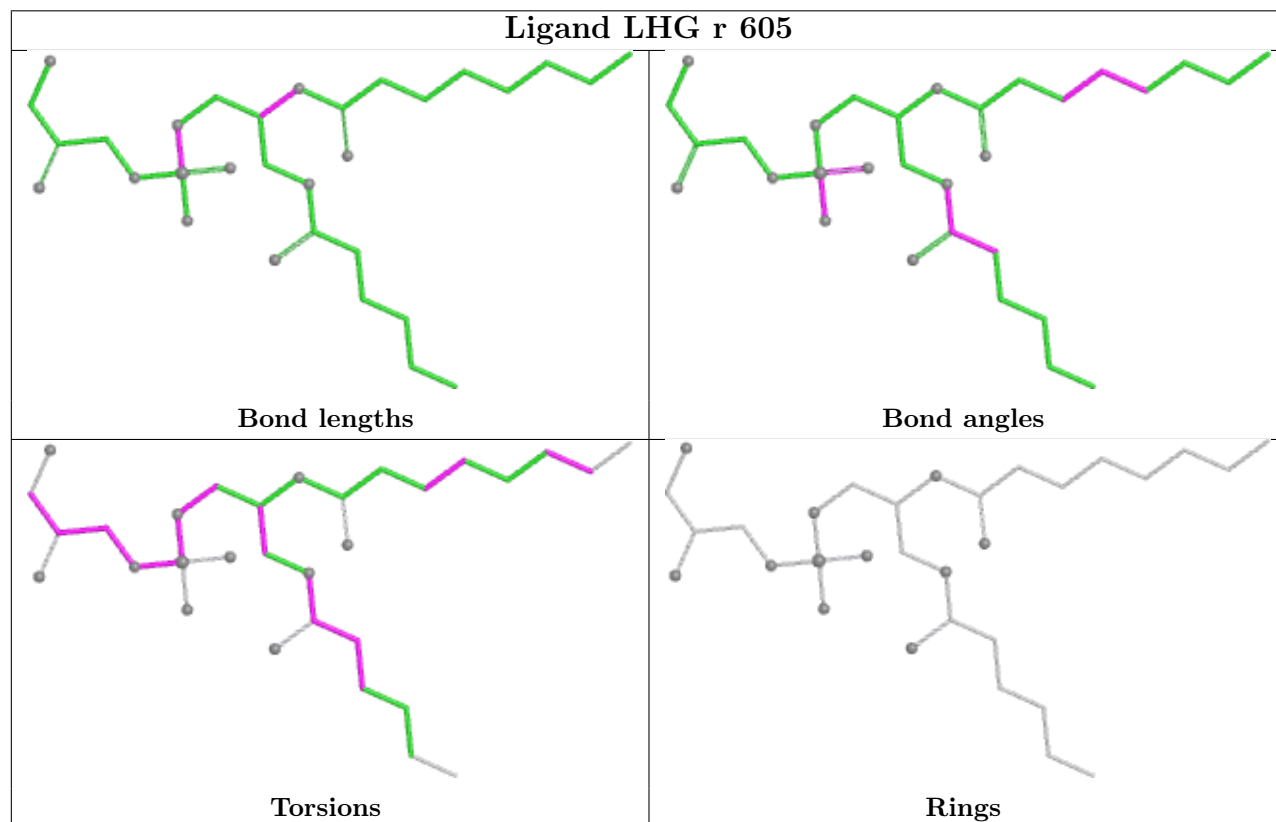
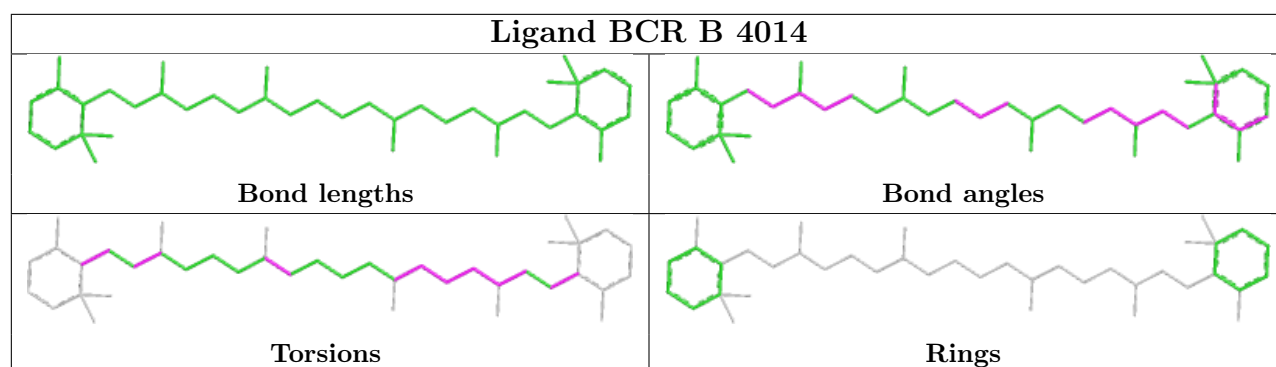
## Ligand CLA q 510



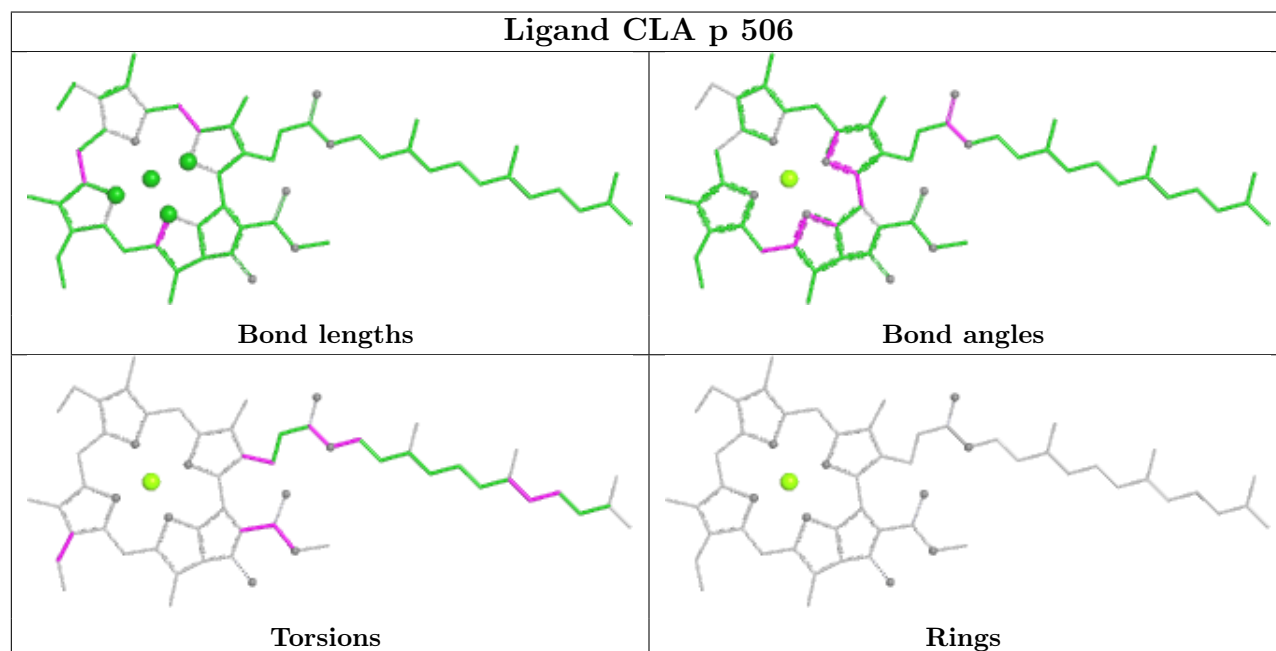
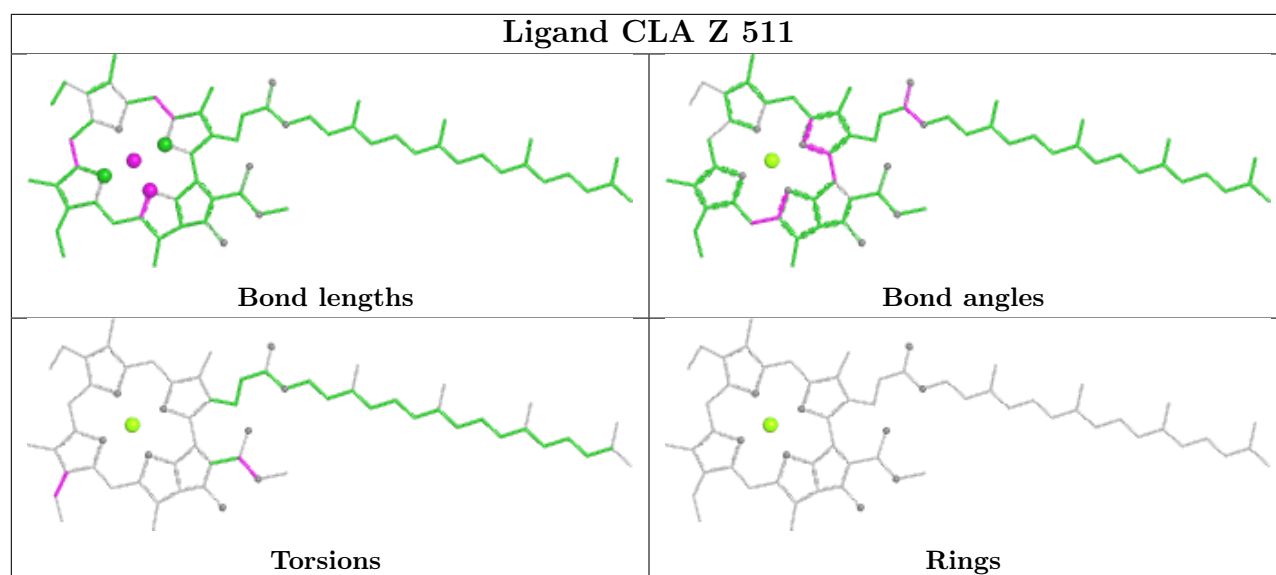
## Ligand CLA g 502



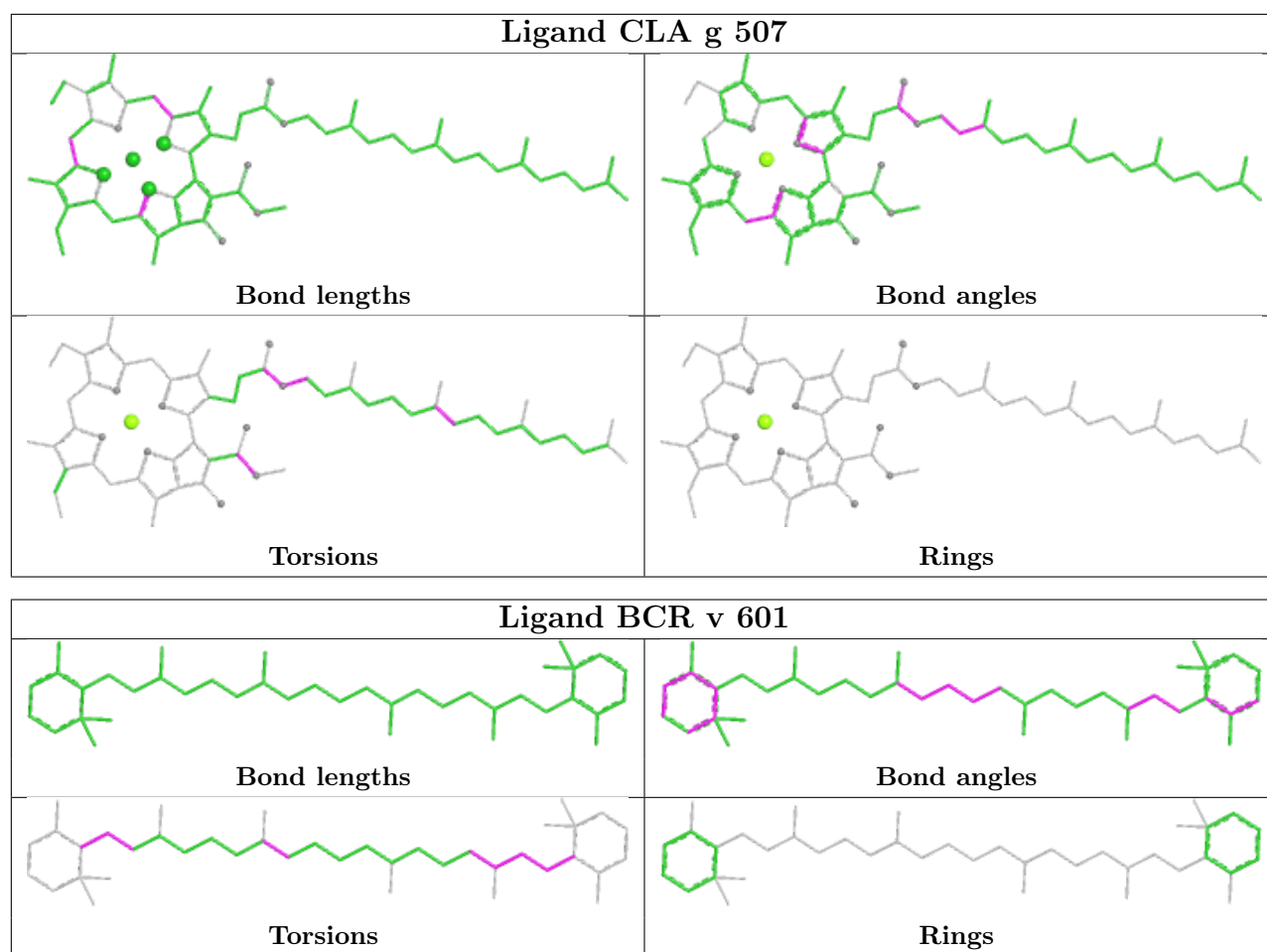






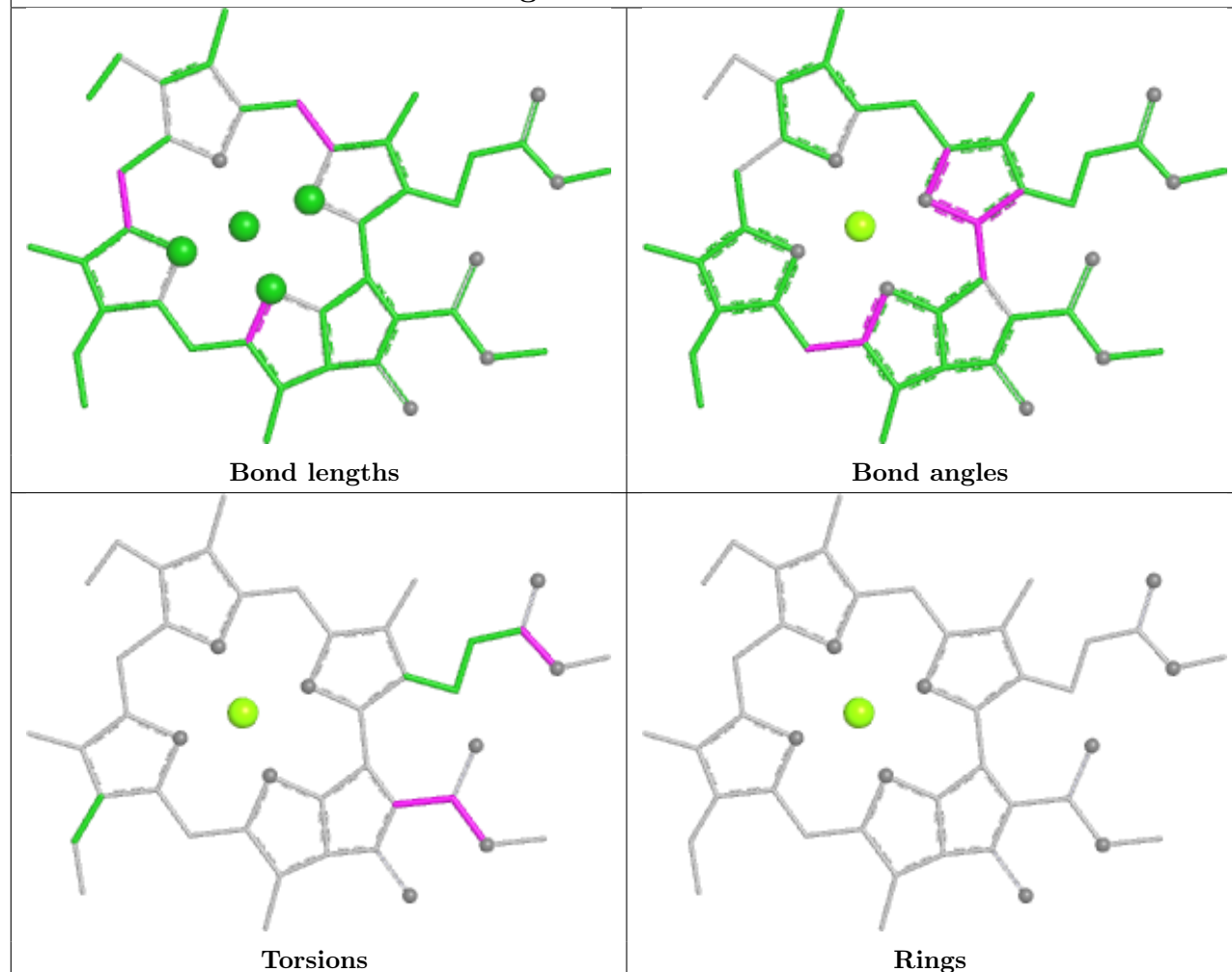




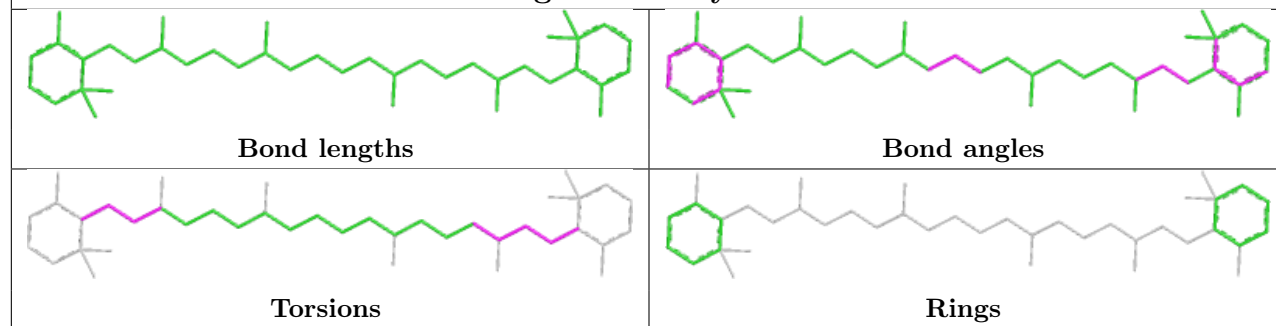




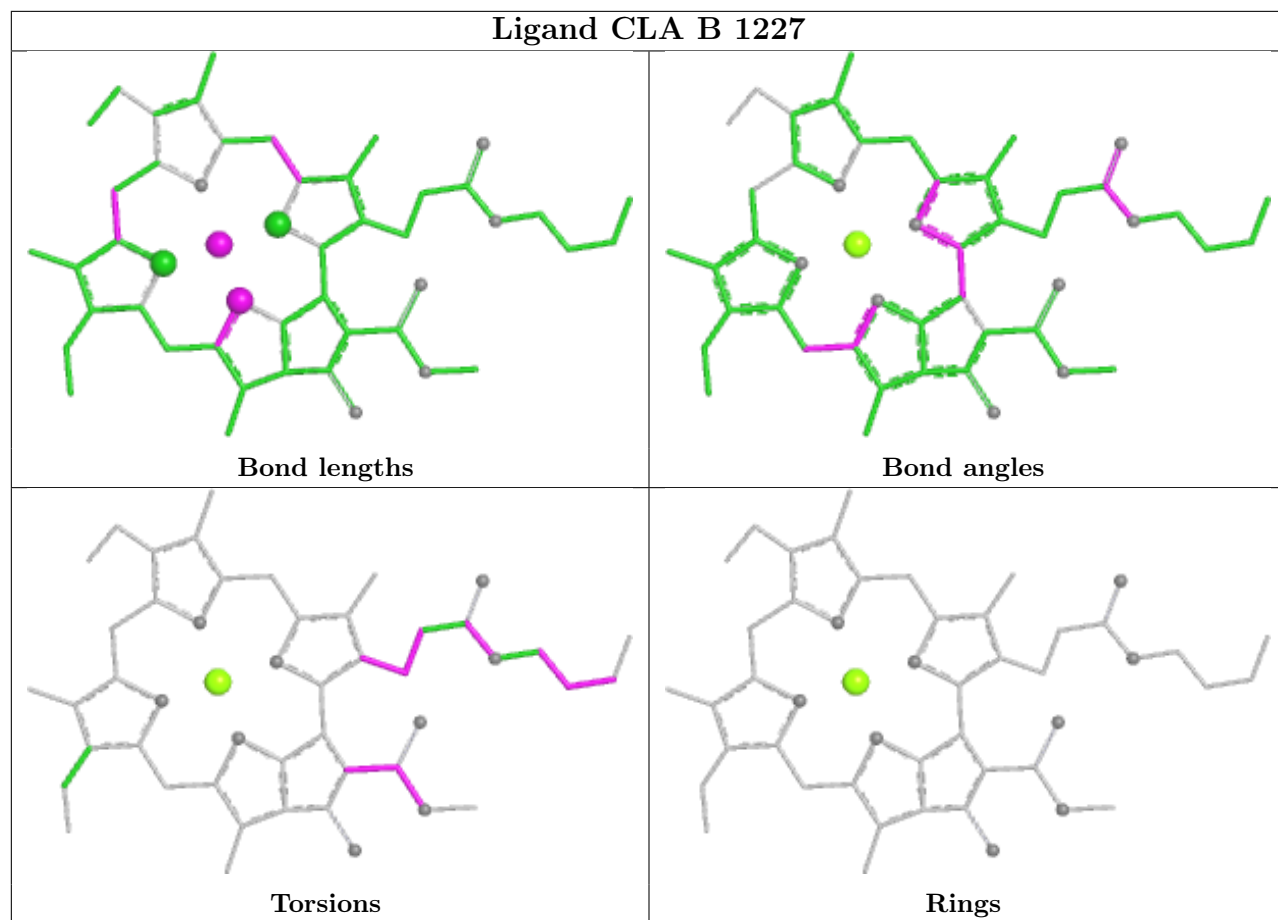
## Ligand CLA t 513



## Ligand BCR y 604

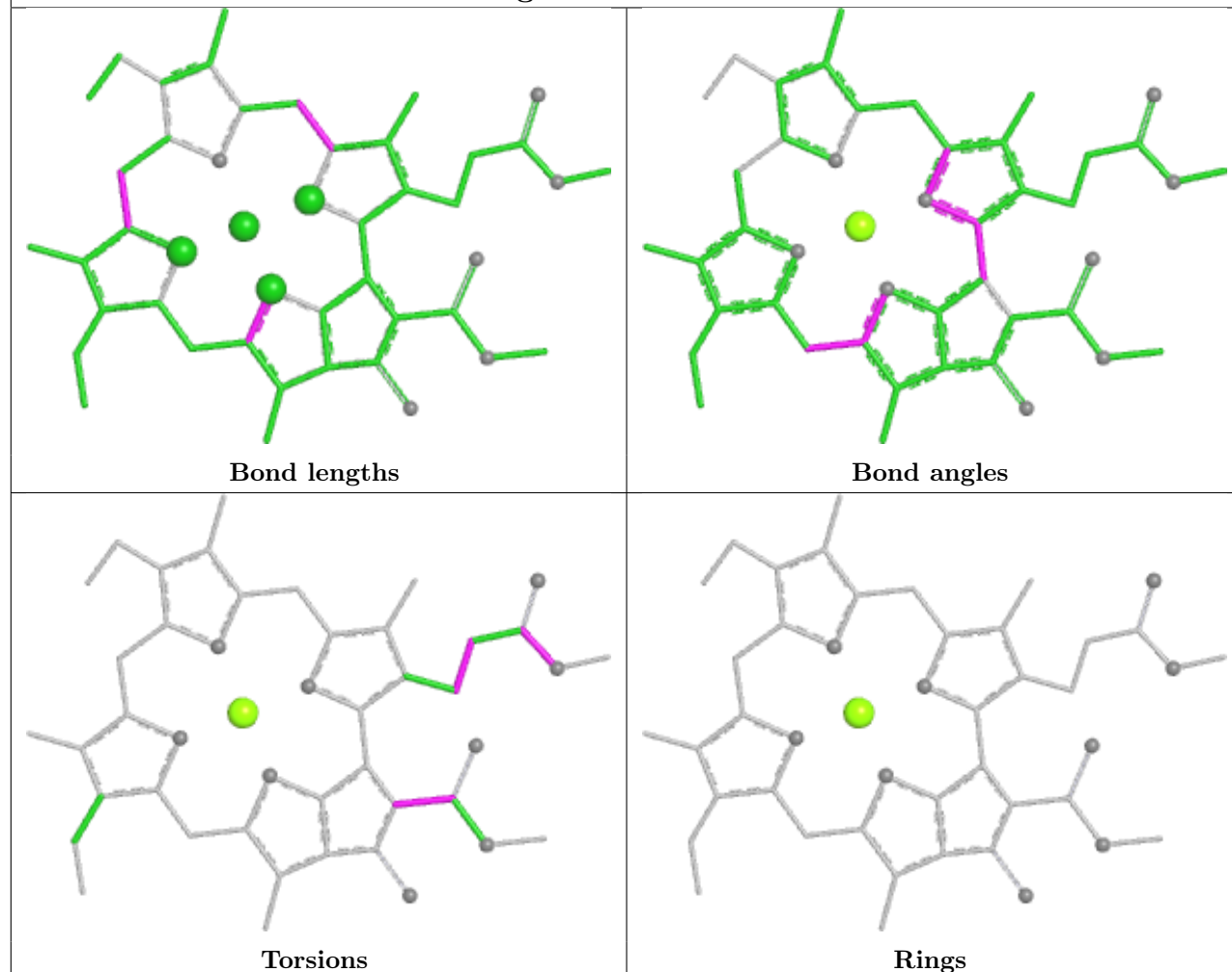




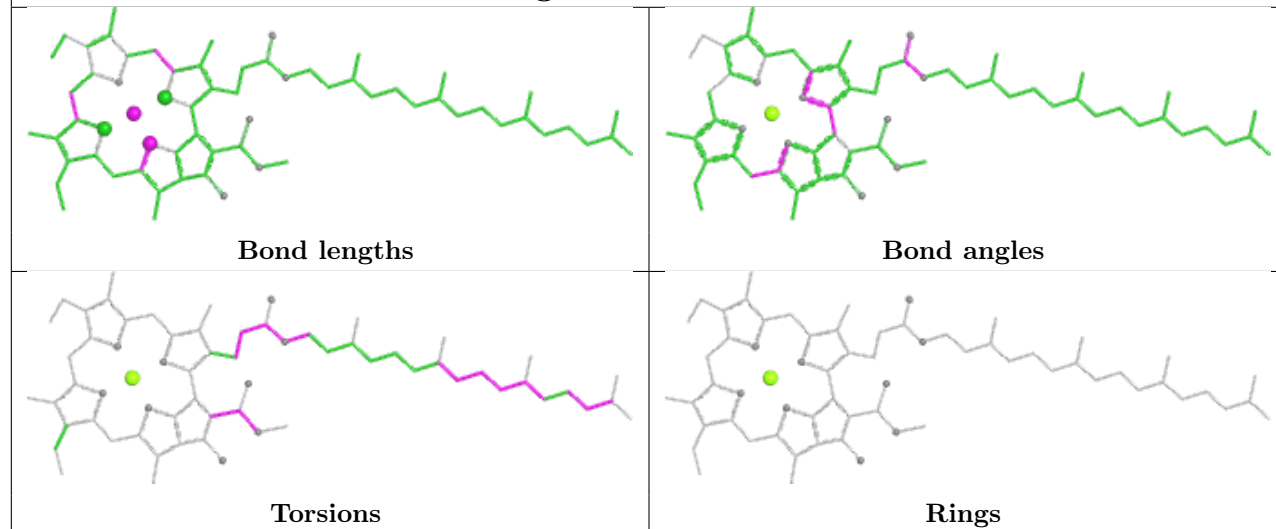




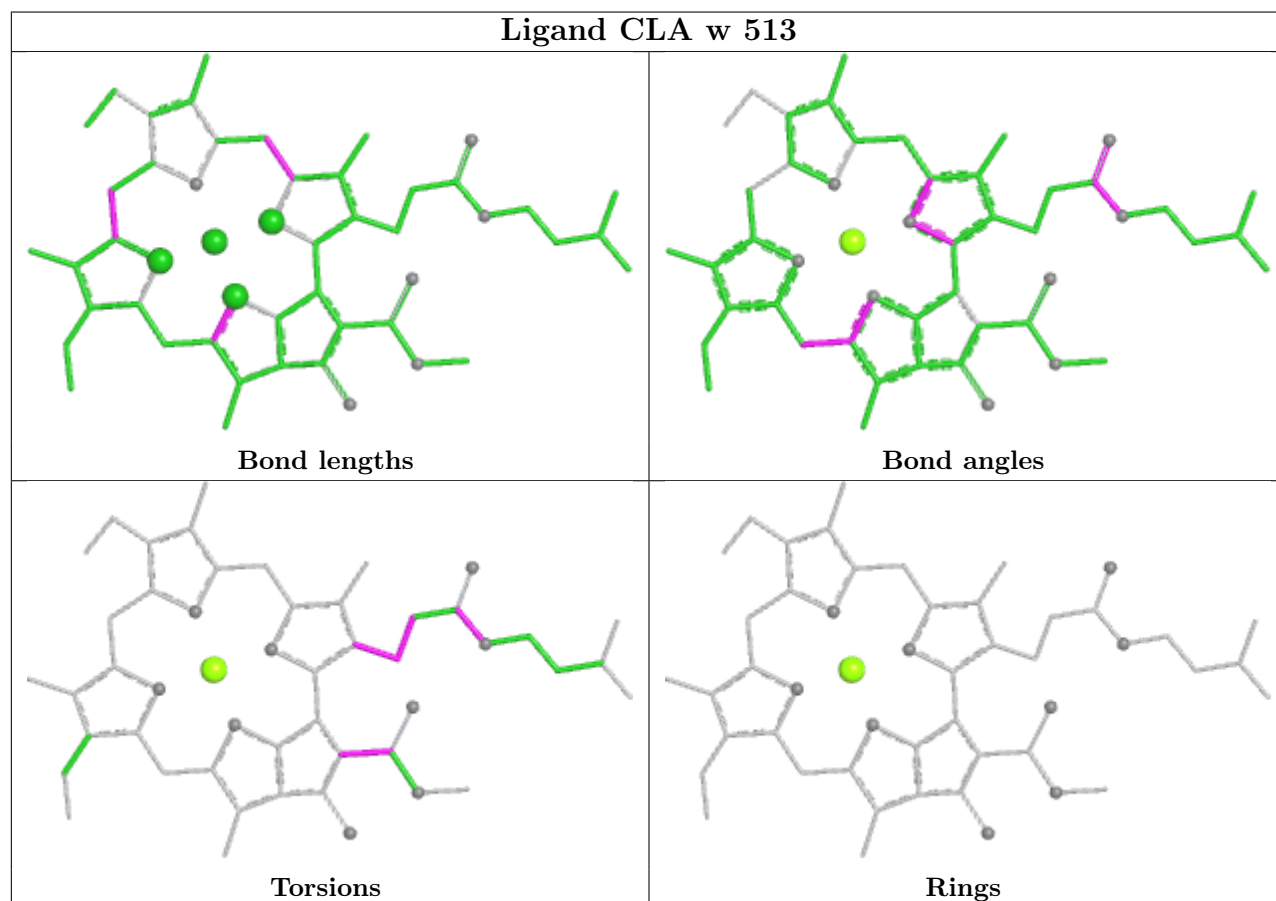
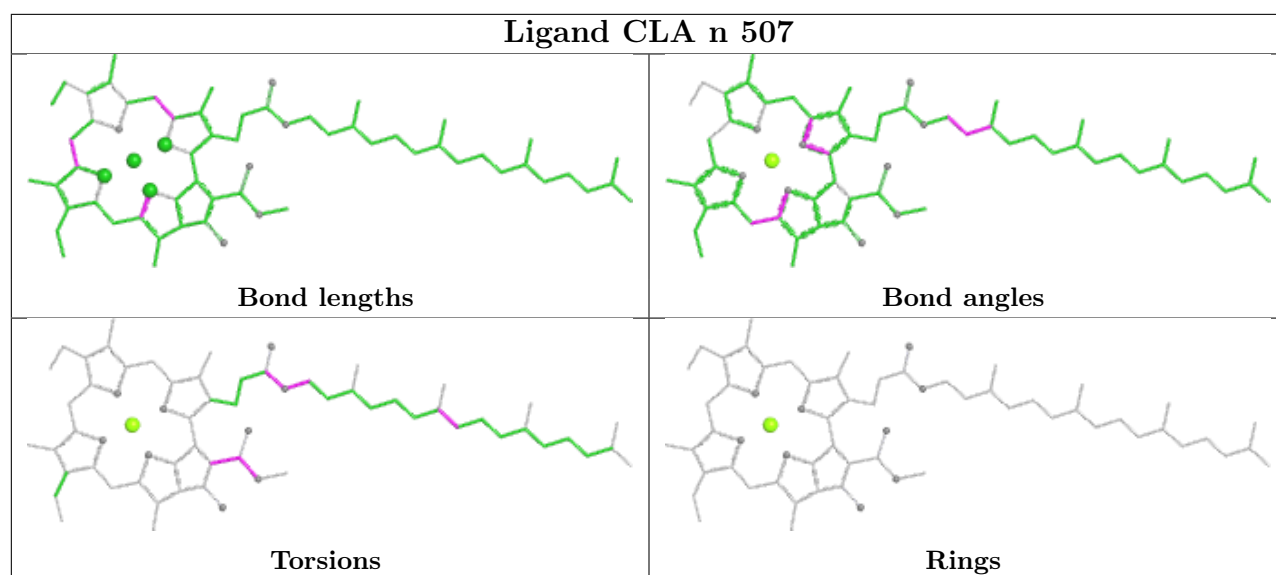
## Ligand CLA h 503



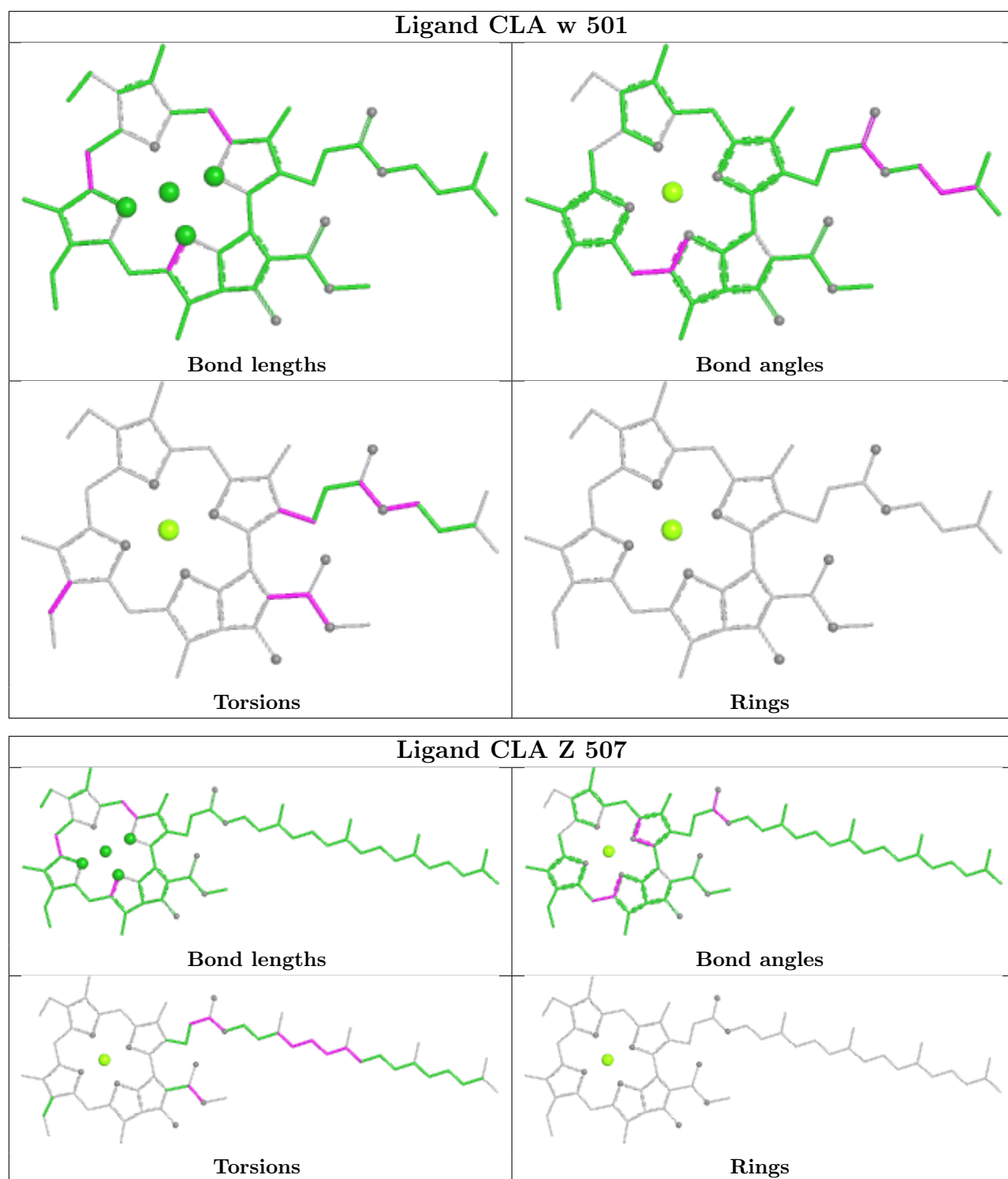
## Ligand CLA n 505



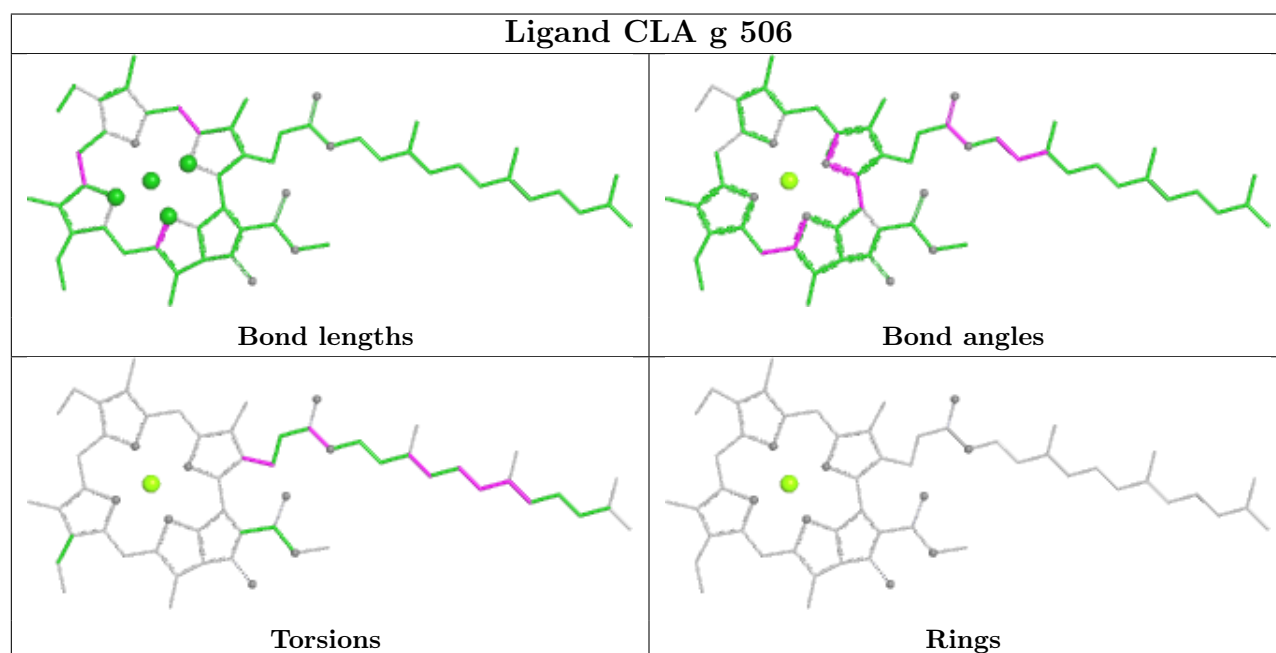
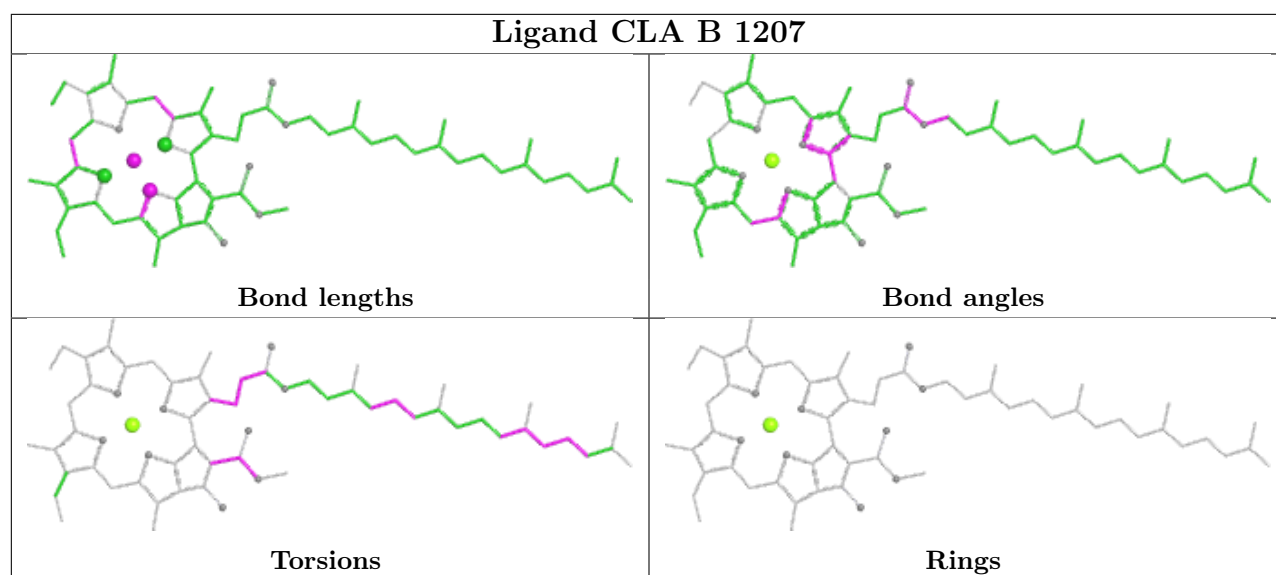




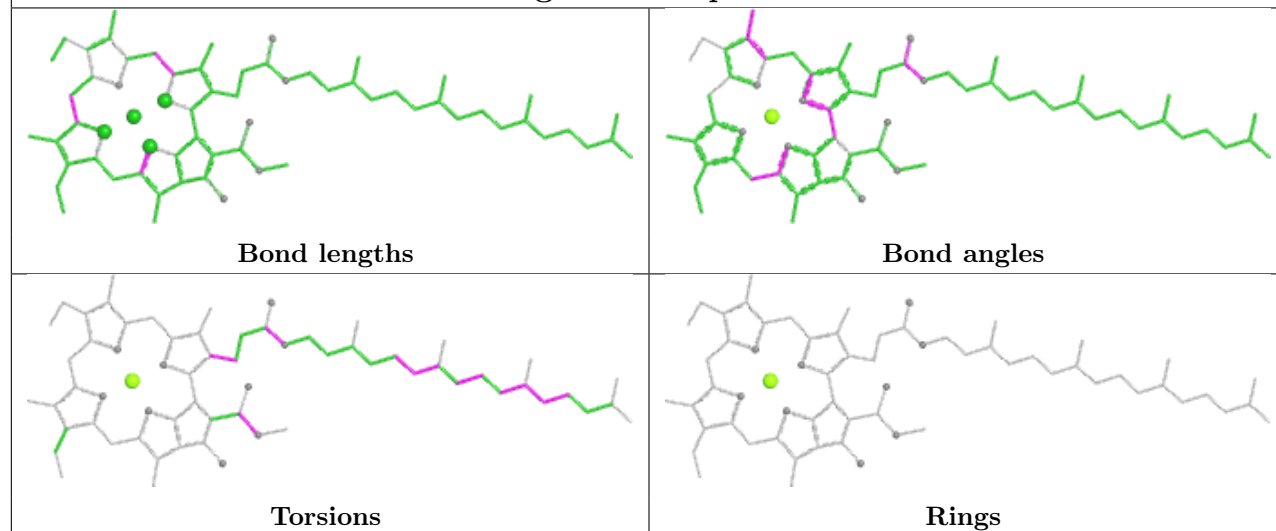
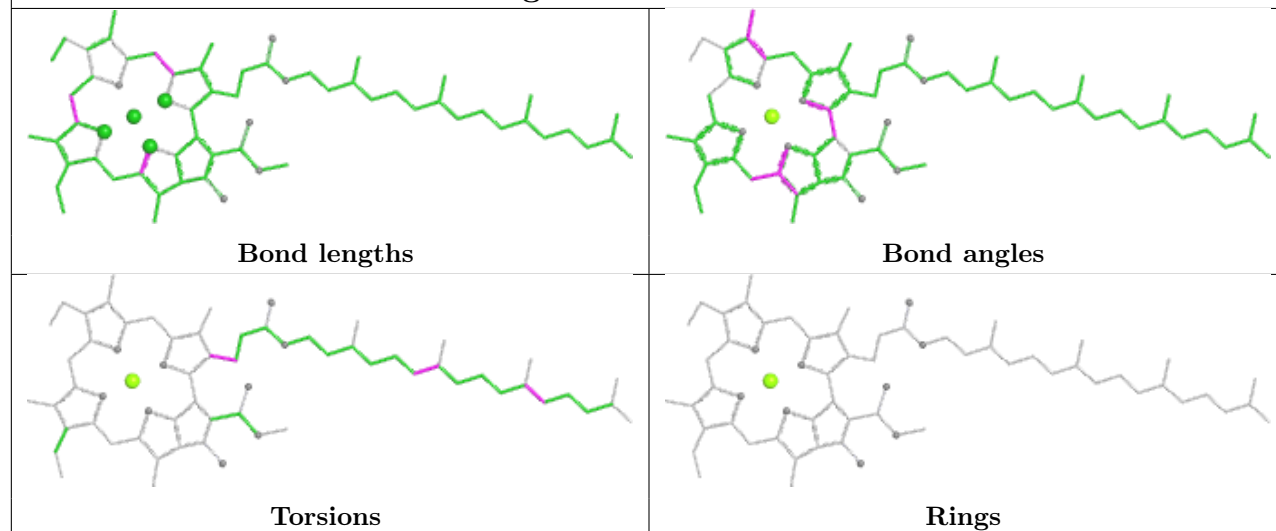






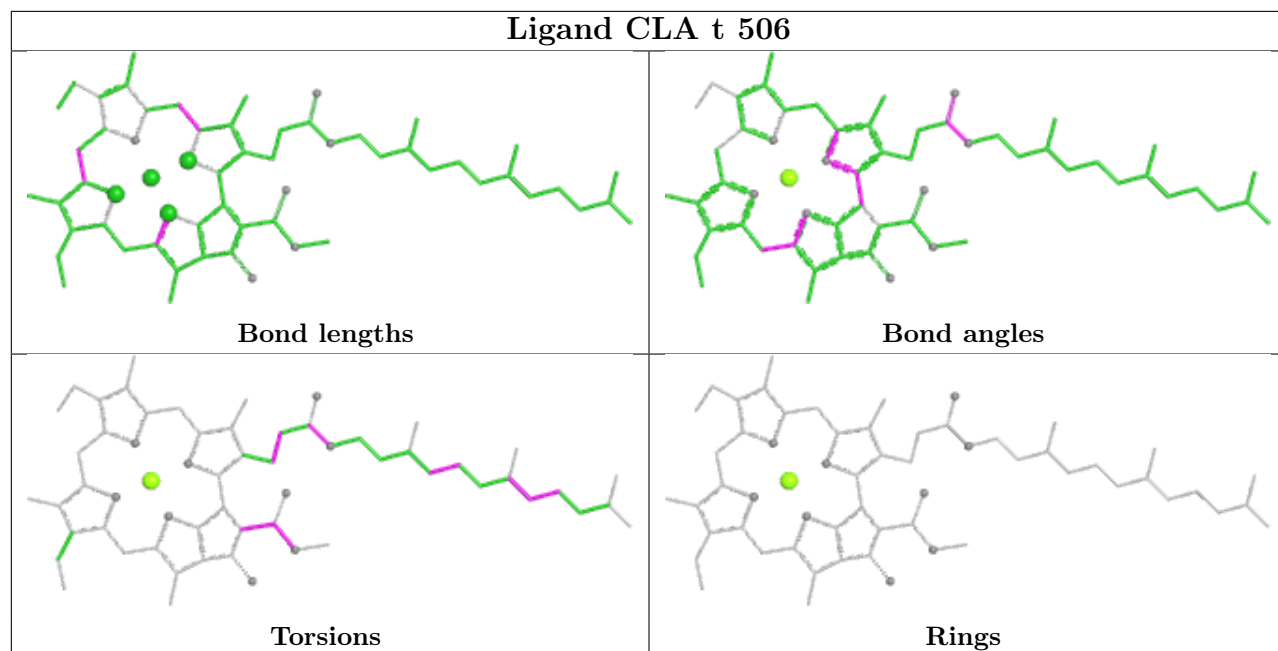




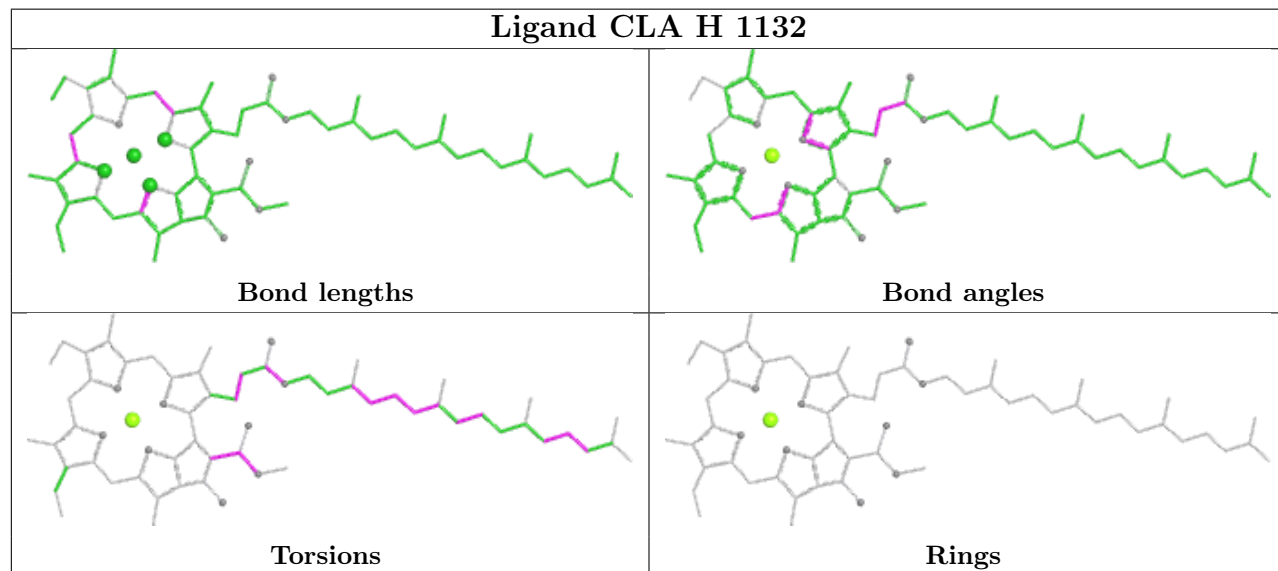
**Ligand CLA p 511****Ligand CLA A 1119**



## Ligand CLA t 506

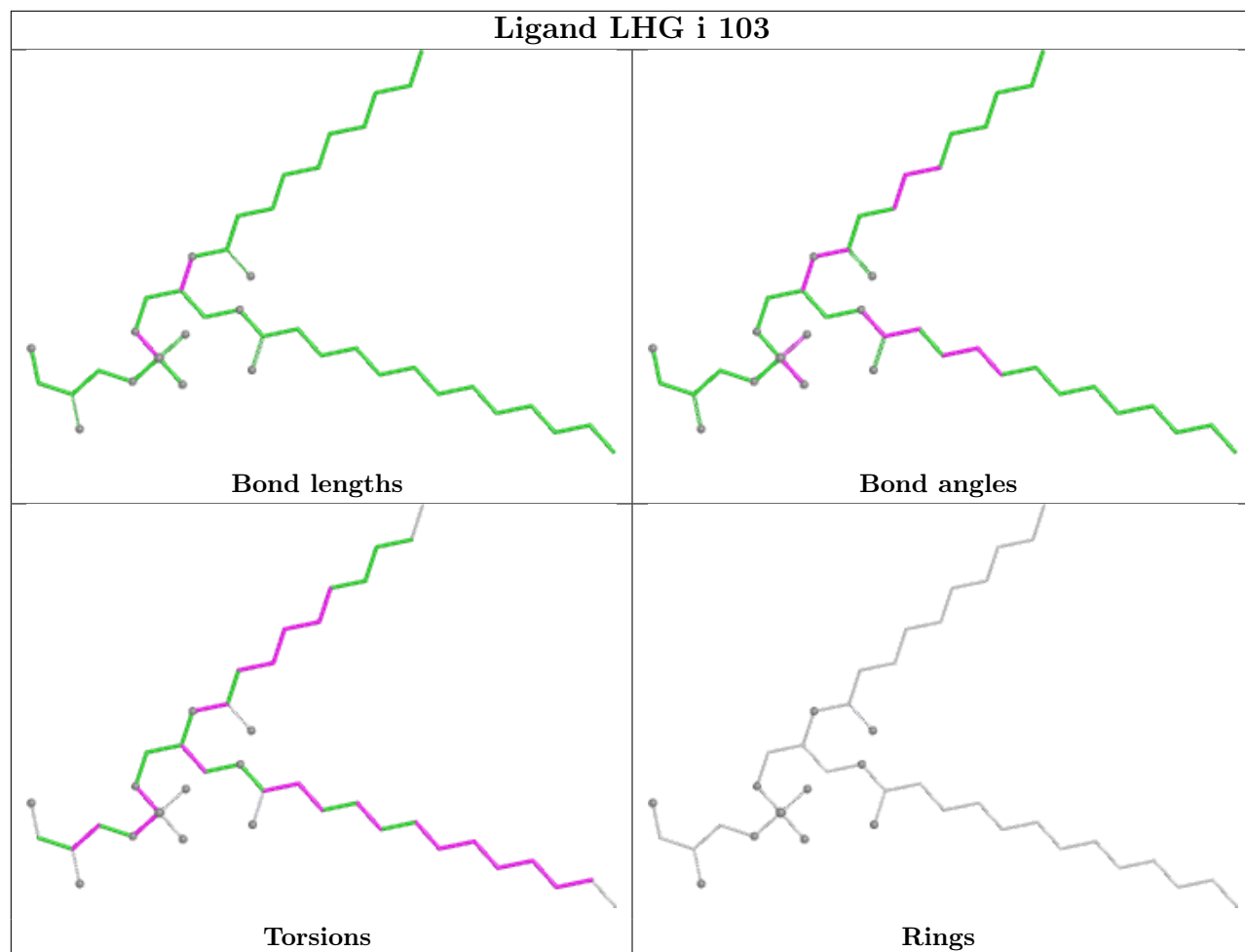


## Ligand CLA H 1132

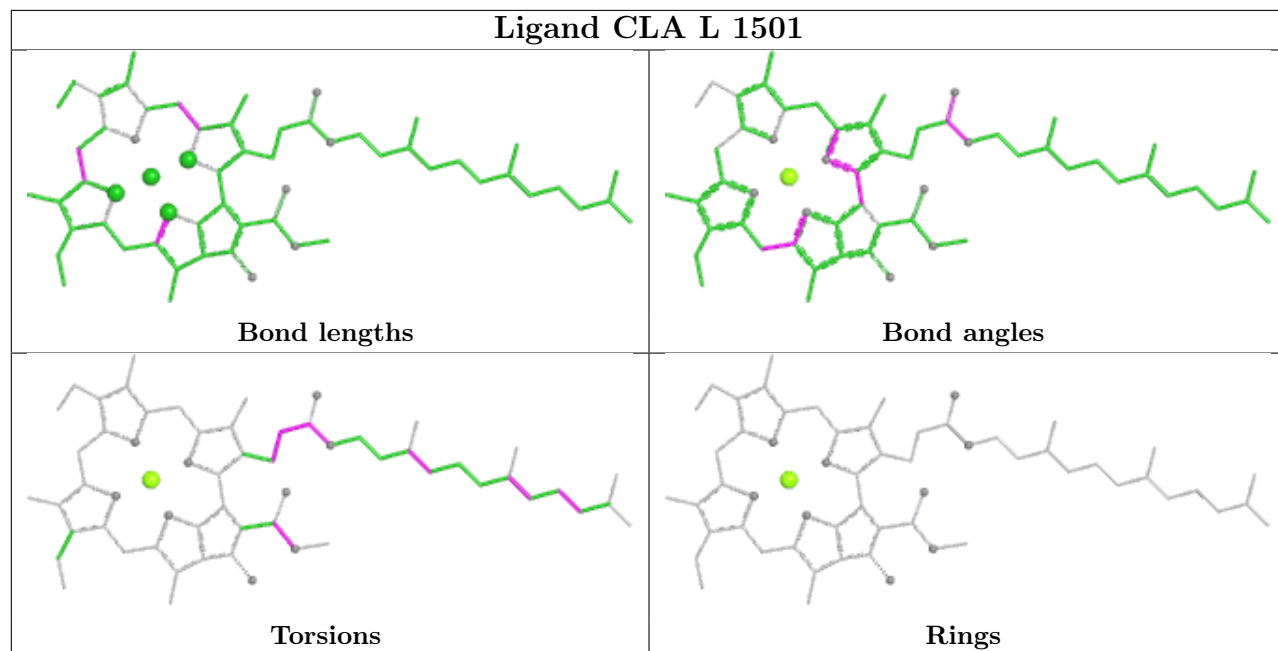




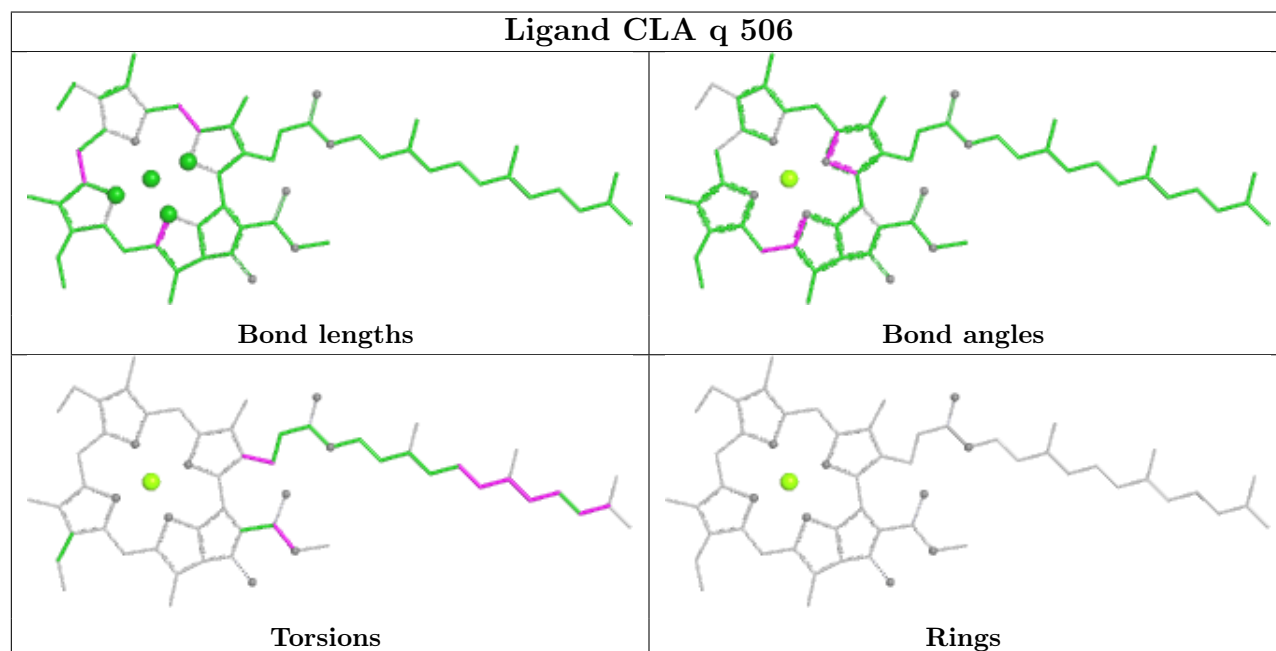
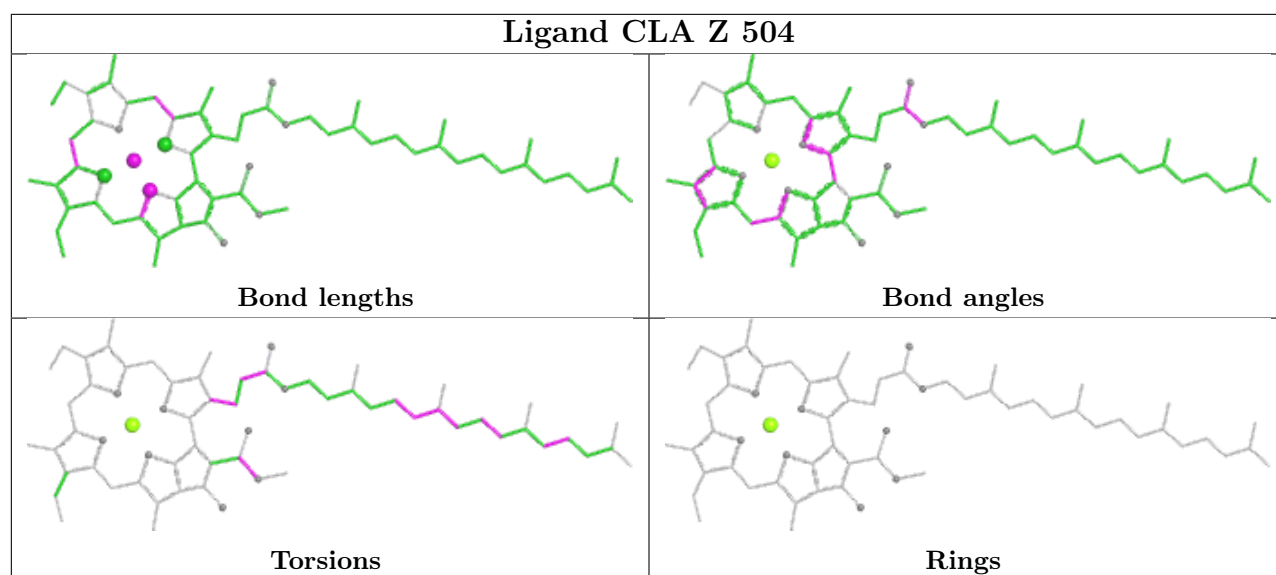
## Ligand LHG i 103



## Ligand CLA L 1501

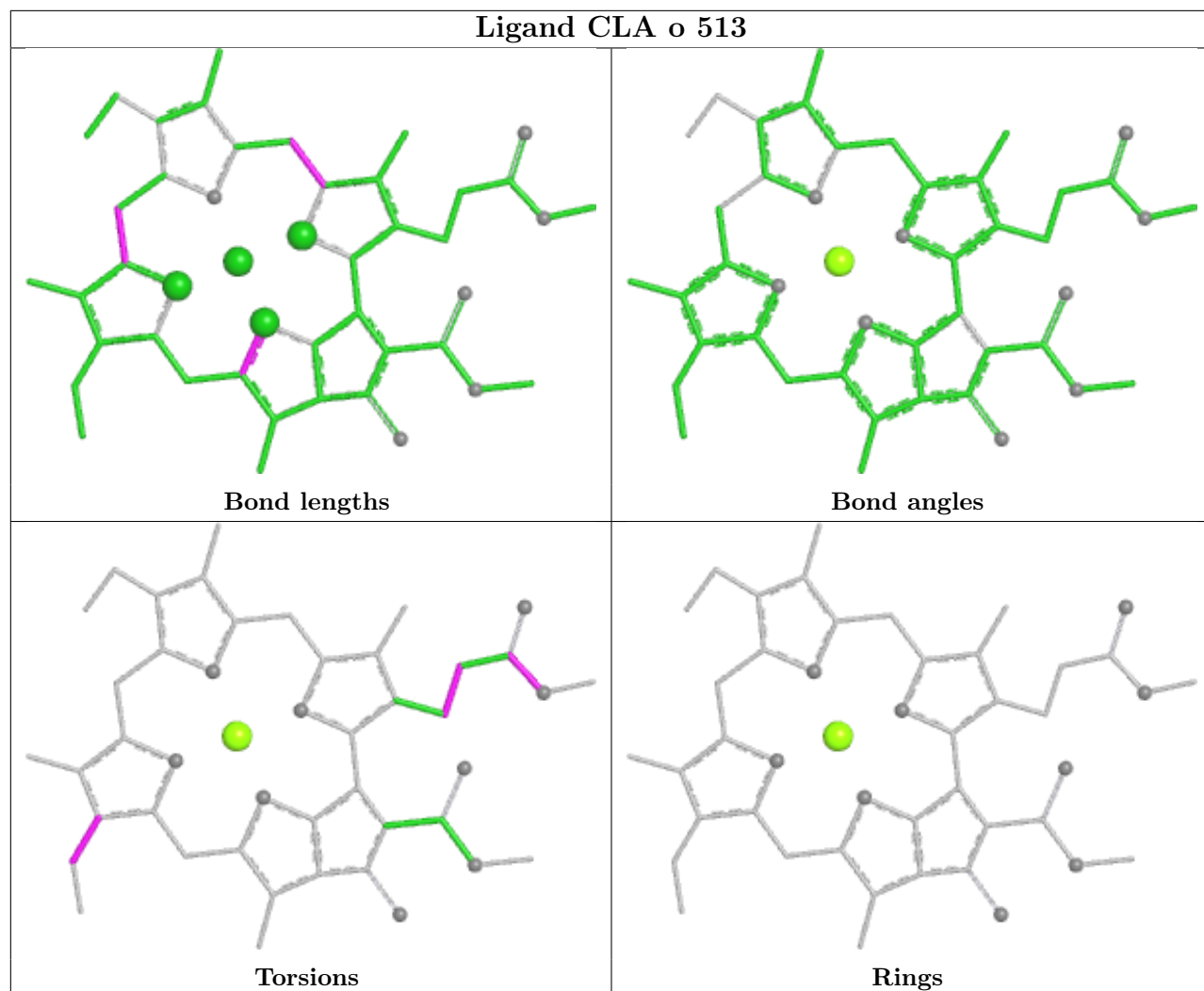




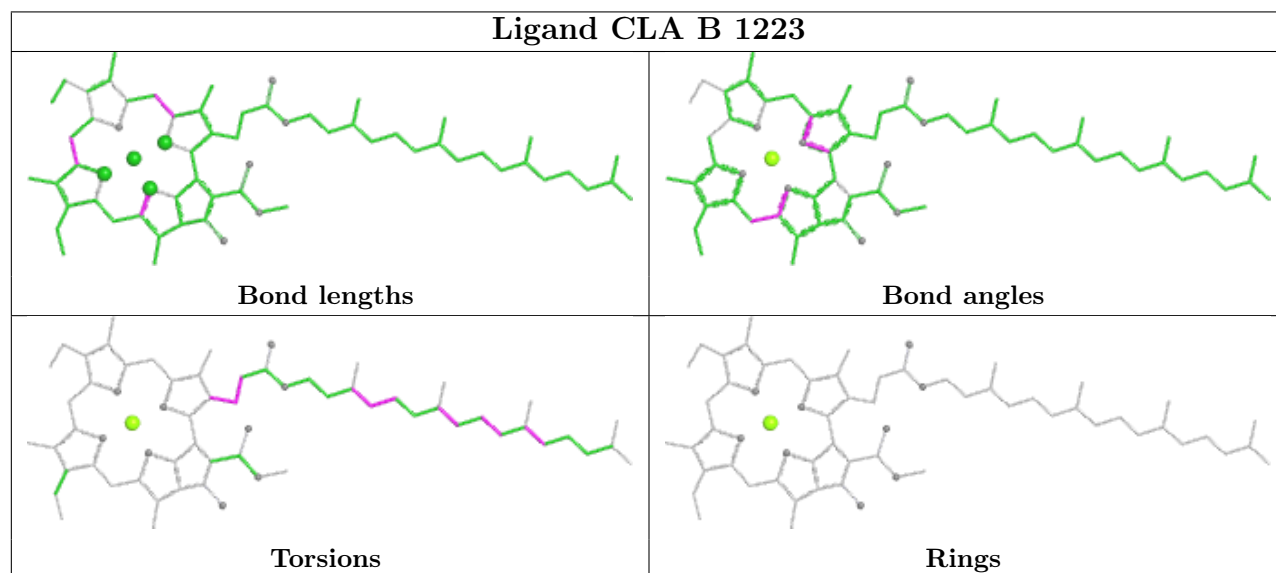
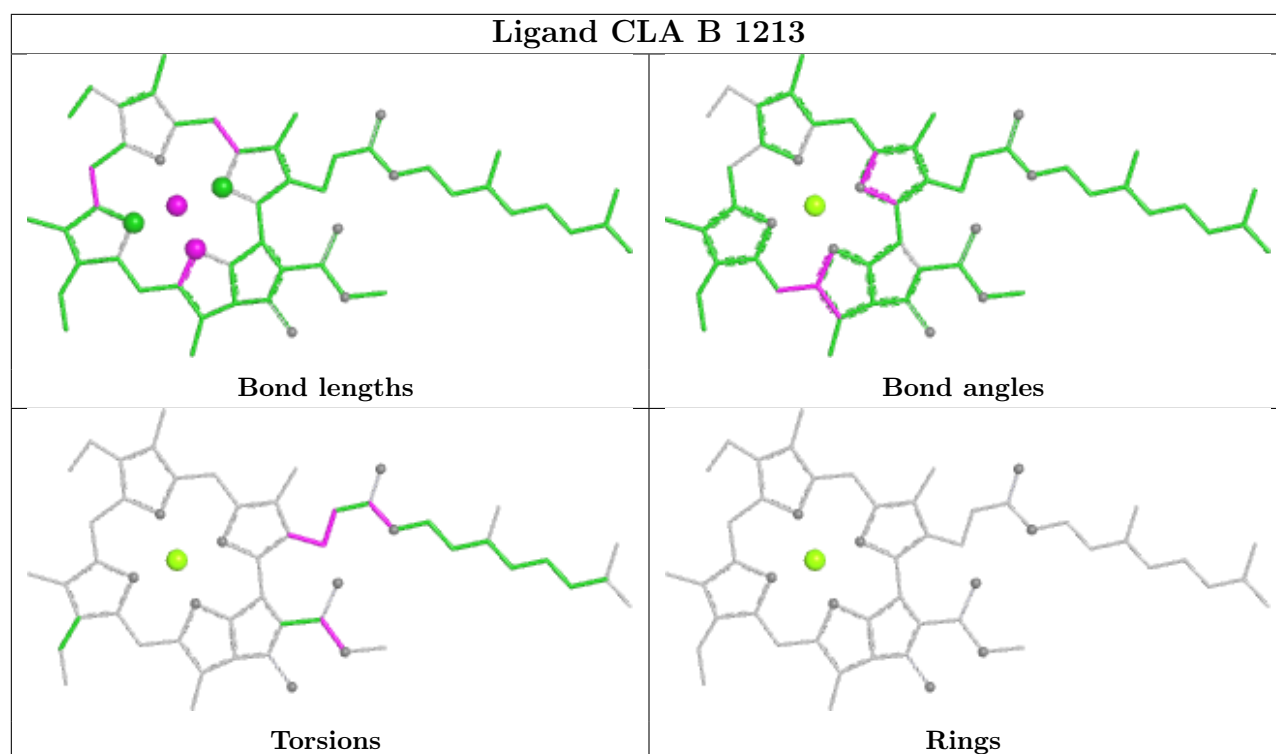




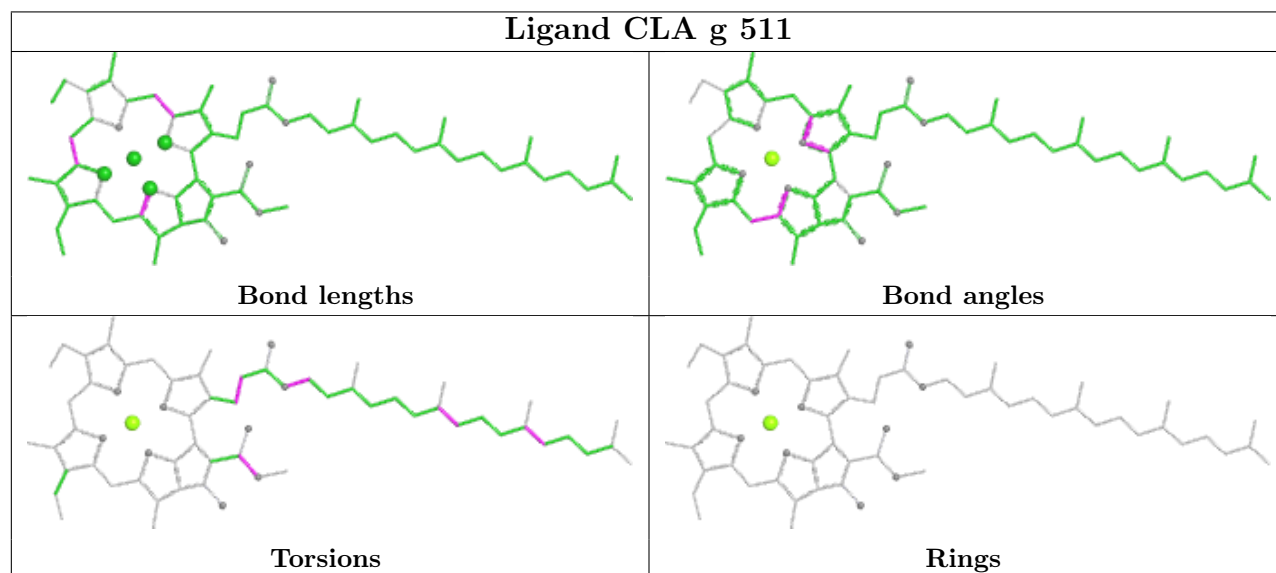
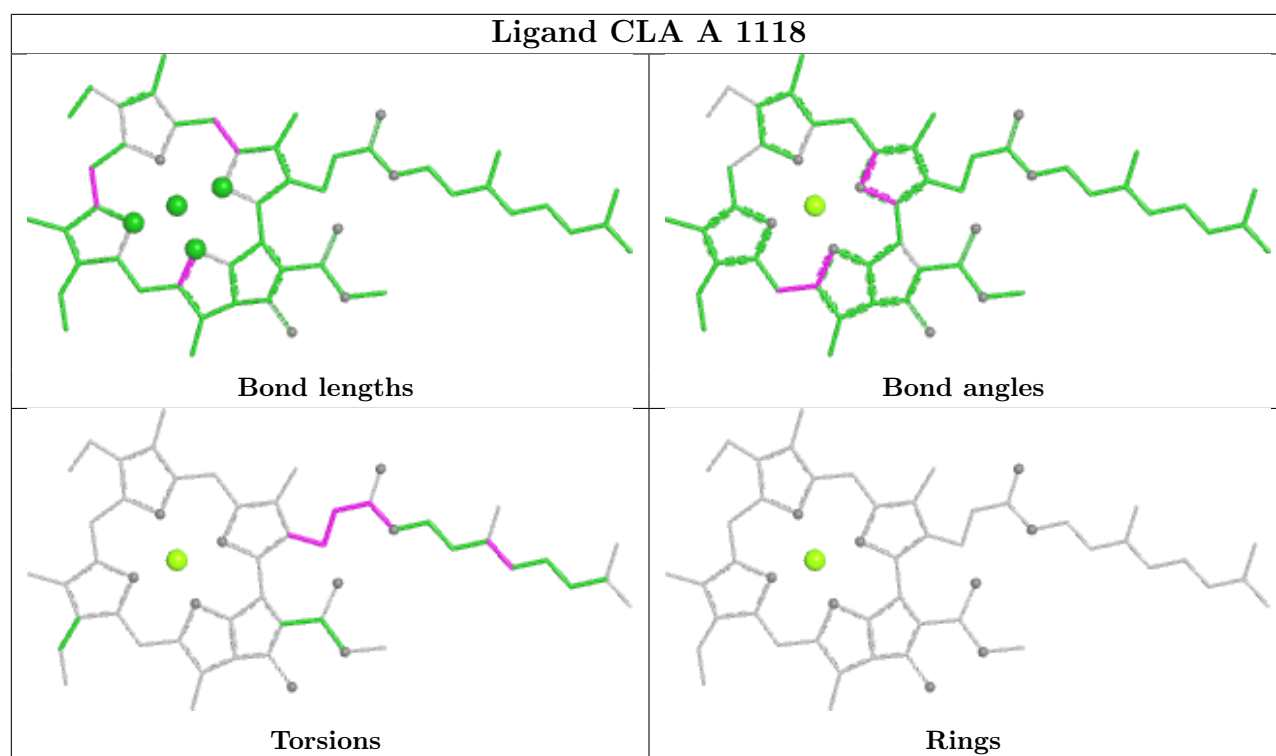
## Ligand CLA o 513



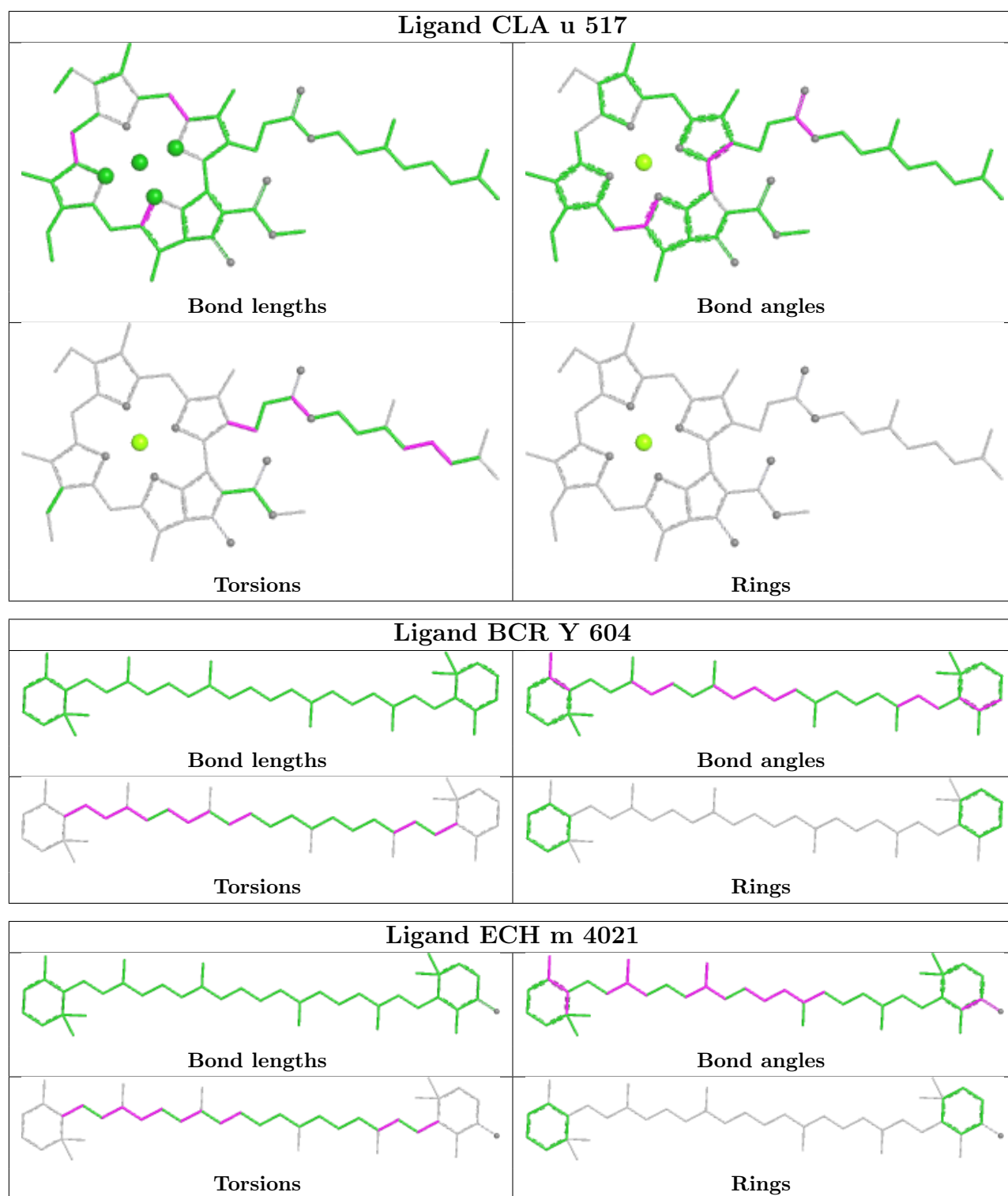




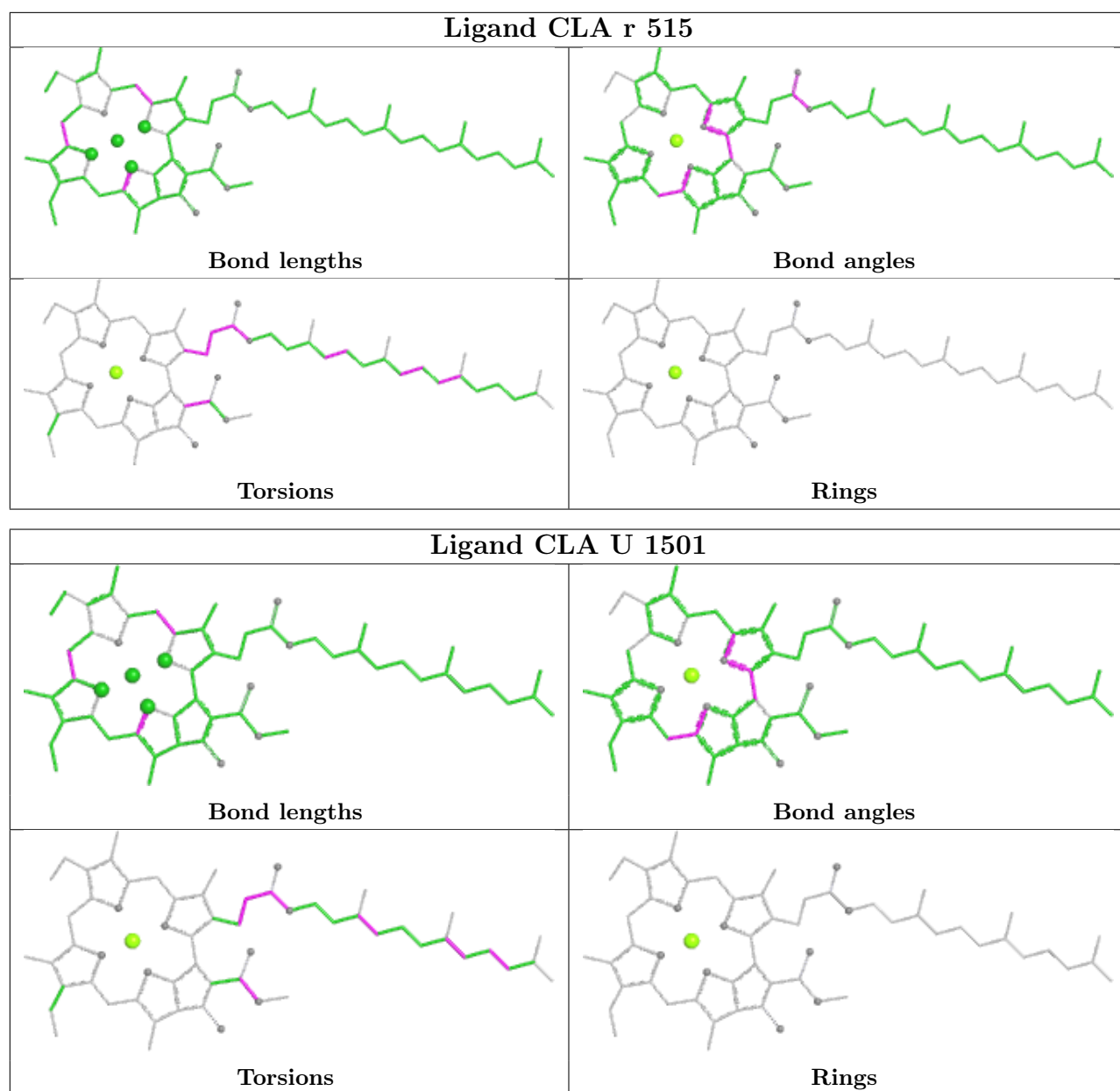






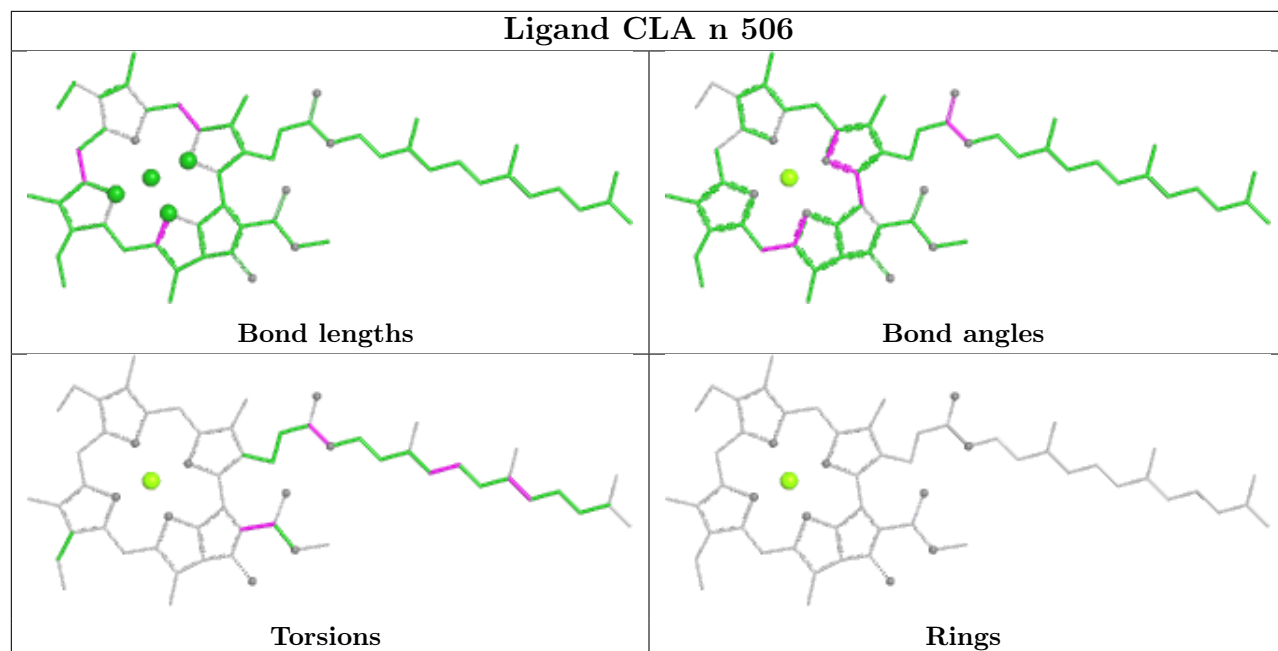




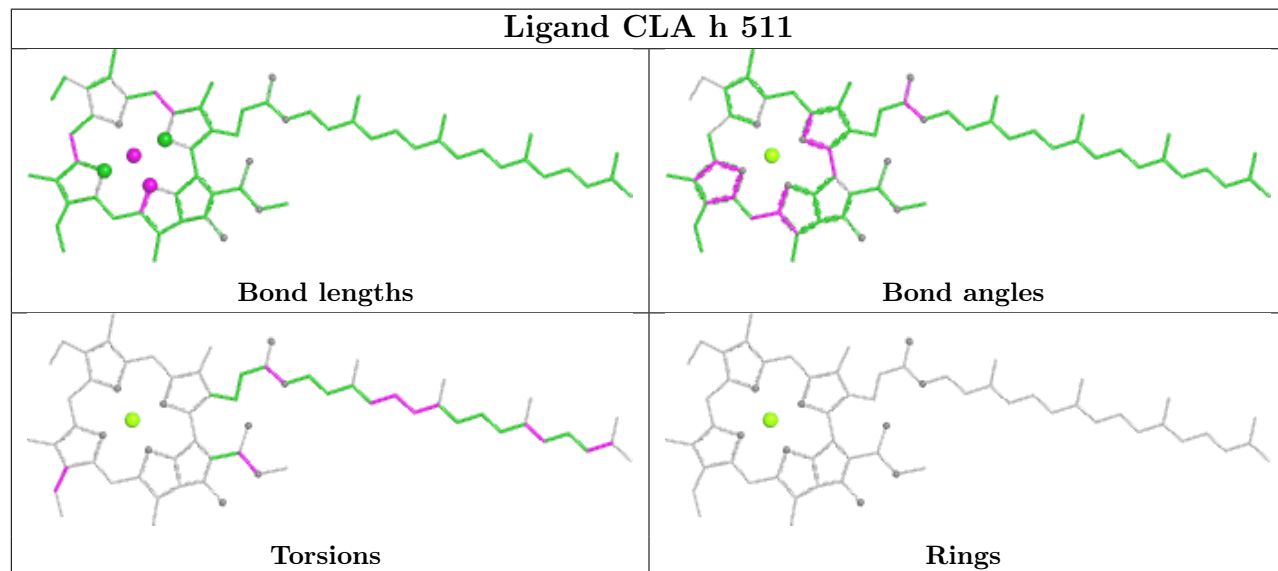




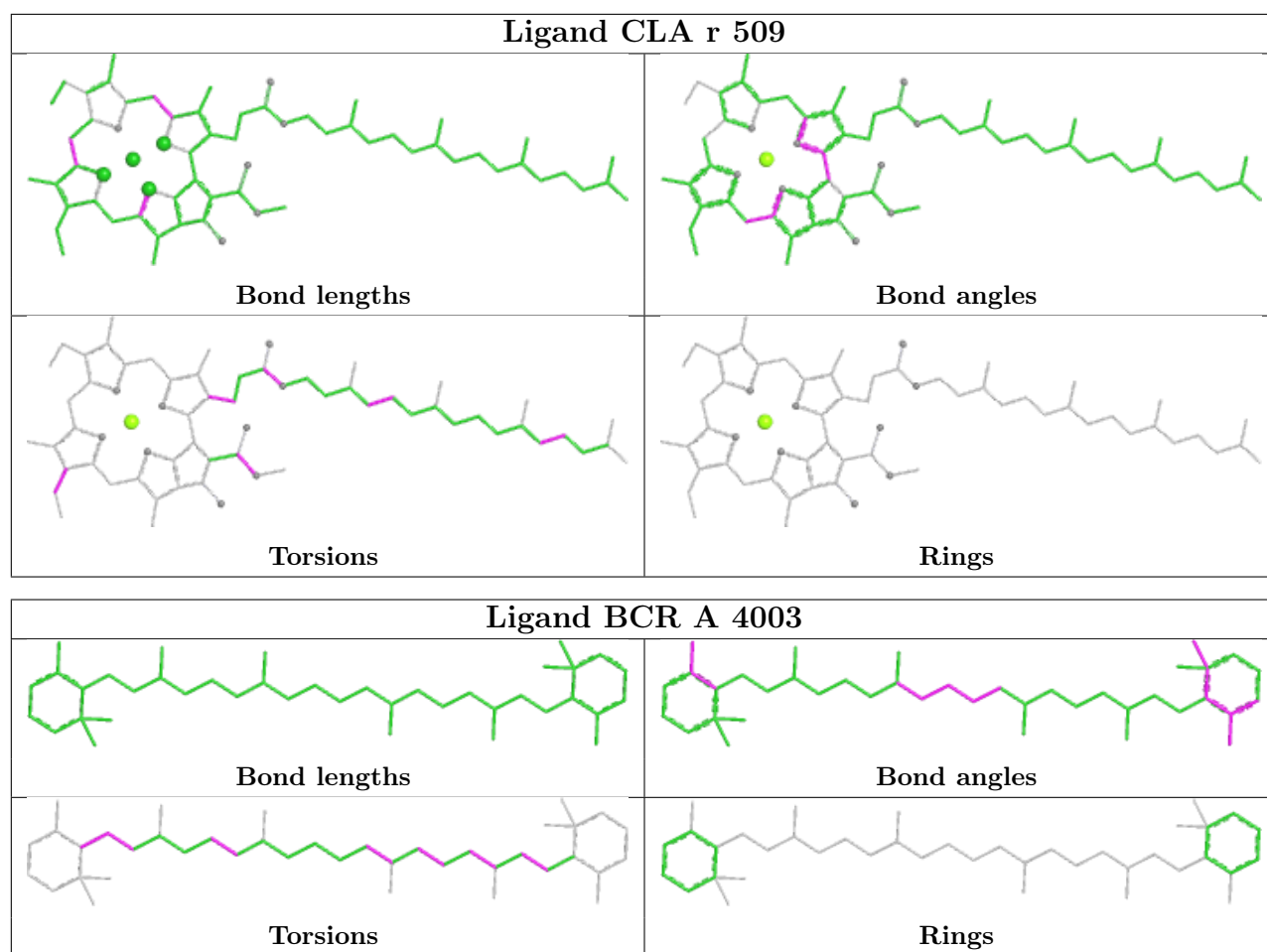
## Ligand CLA n 506



## Ligand CLA h 511

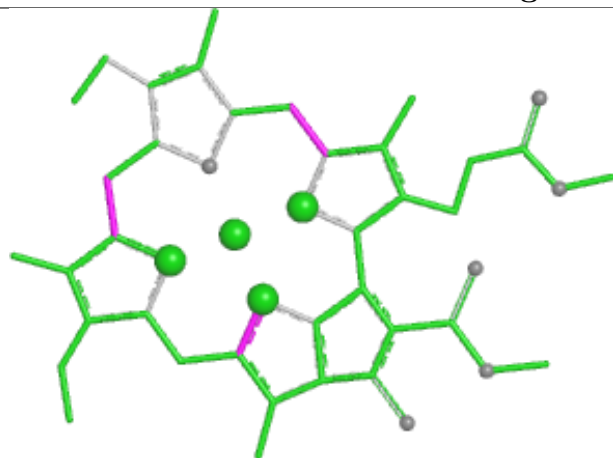




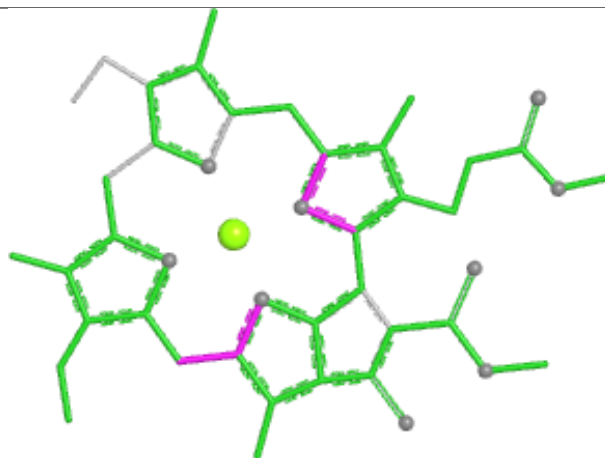




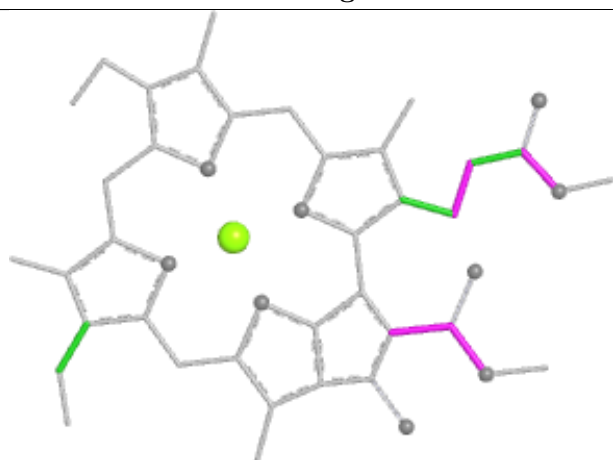
## Ligand CLA t 516



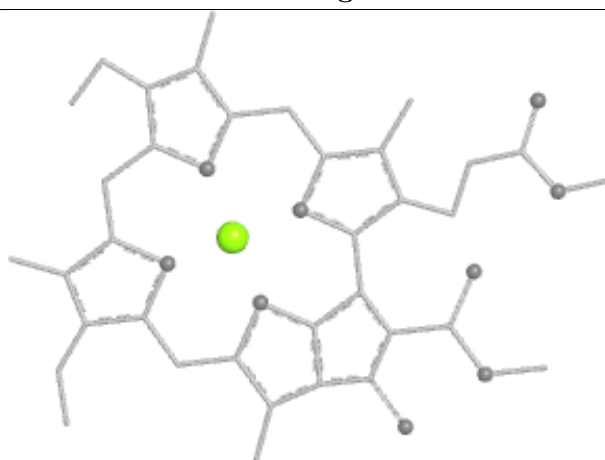
Bond lengths



Bond angles



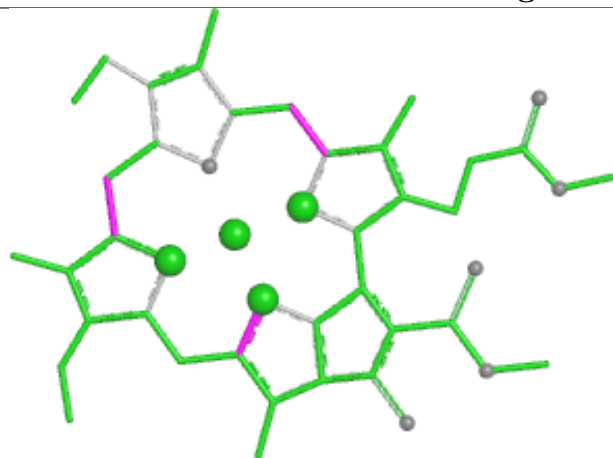
Torsions



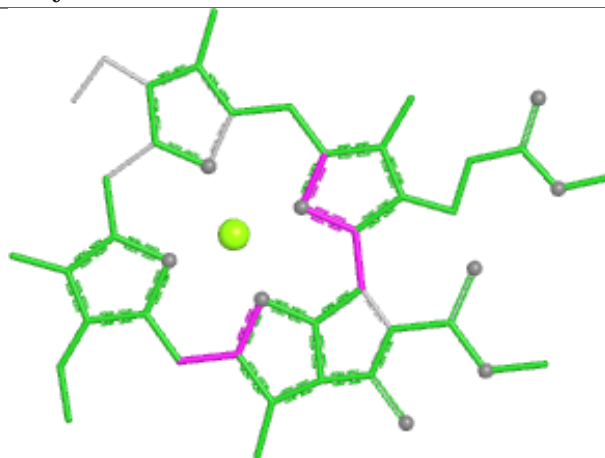
Rings



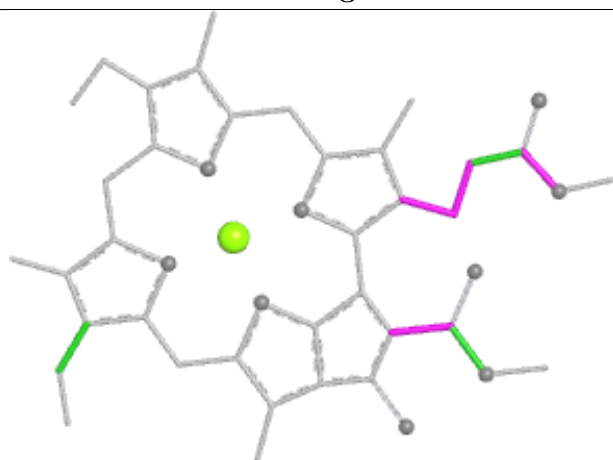
## Ligand CLA y 501



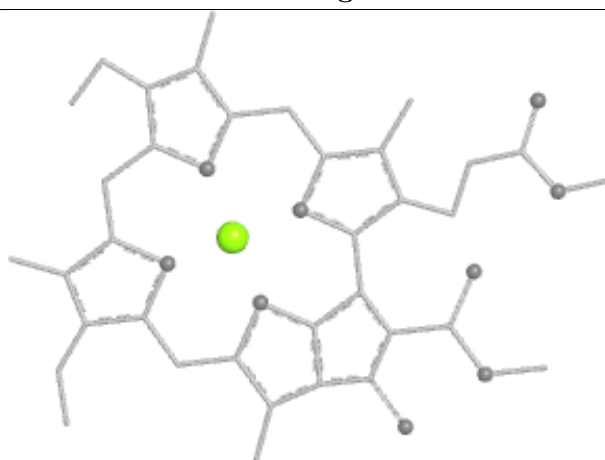
Bond lengths



Bond angles

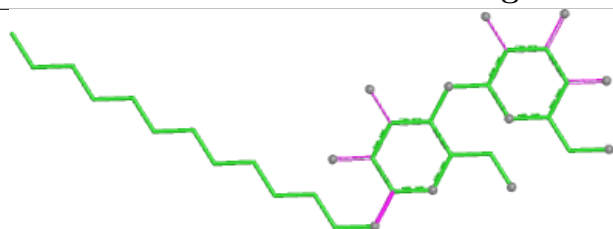


Torsions

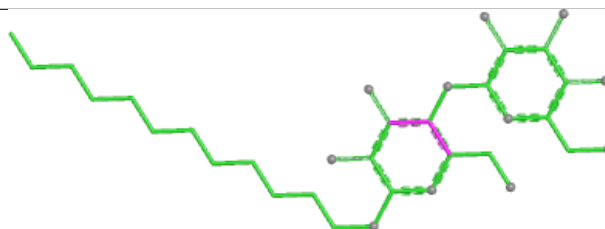


Rings

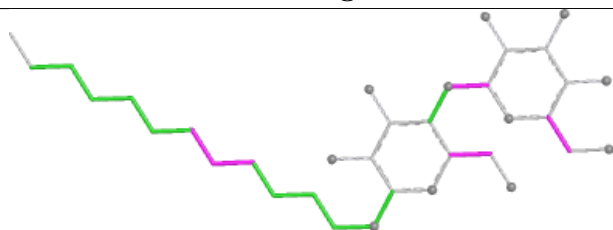
## Ligand LMT U 4101



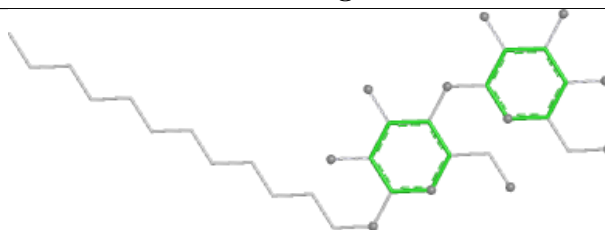
Bond lengths



Bond angles

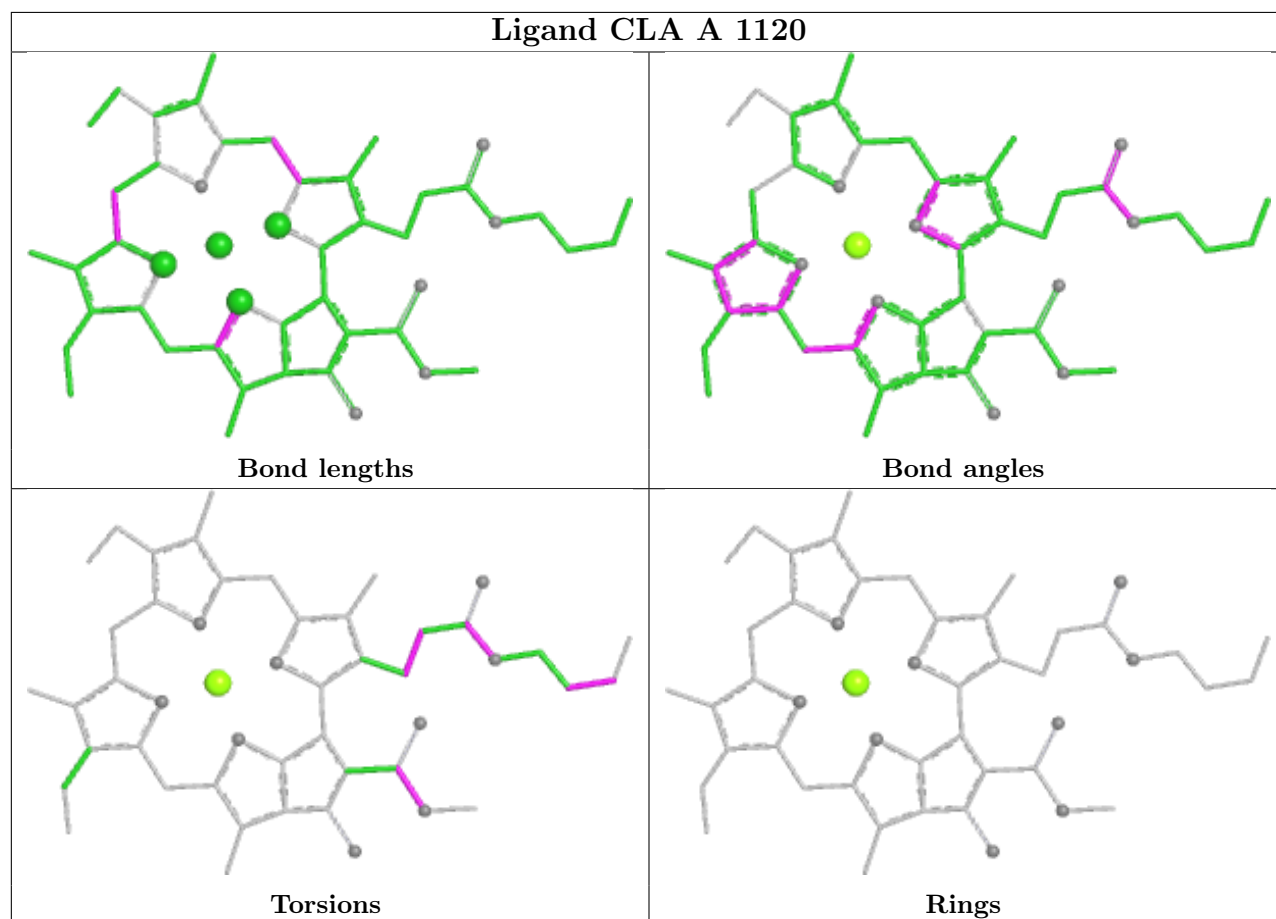
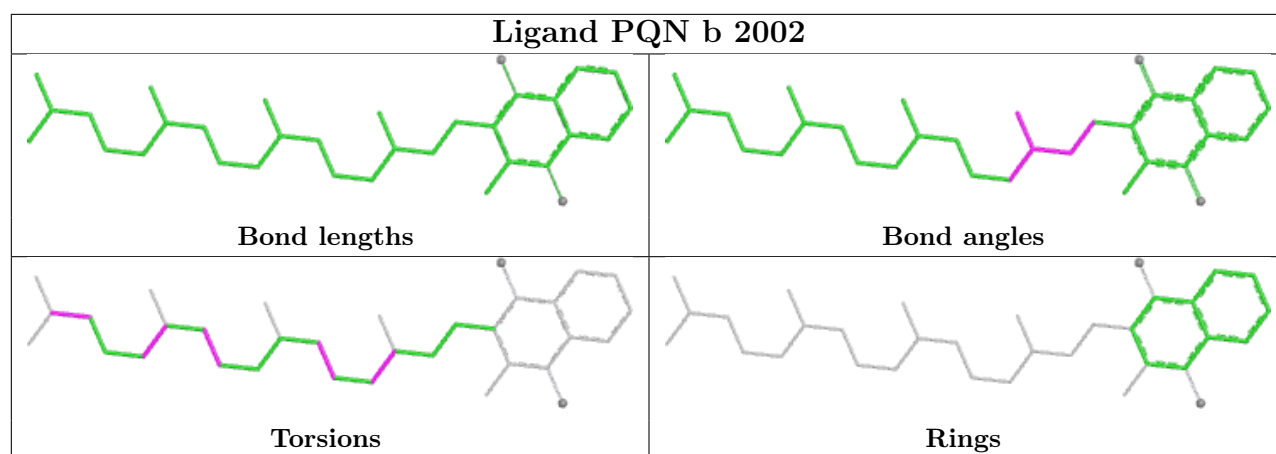


Torsions



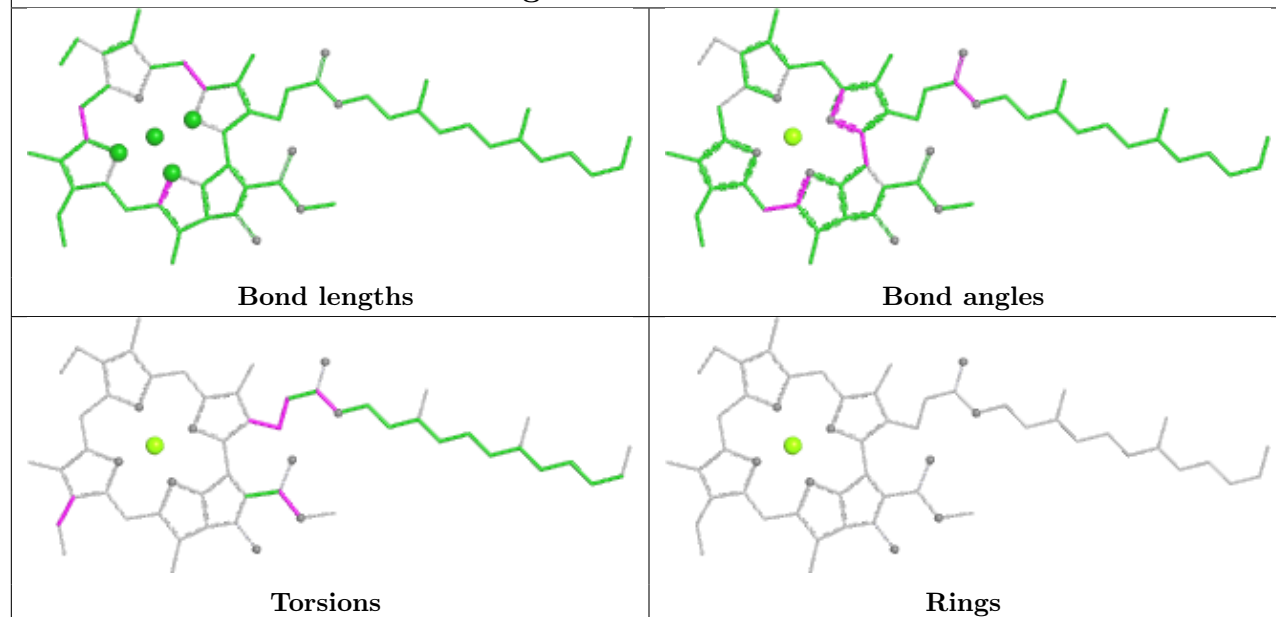
Rings



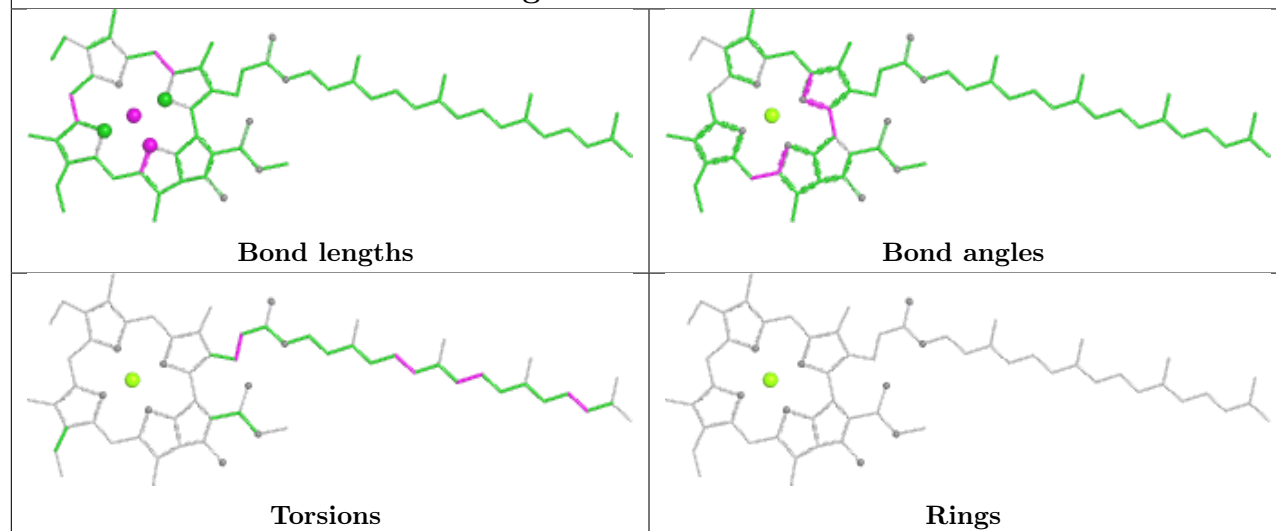




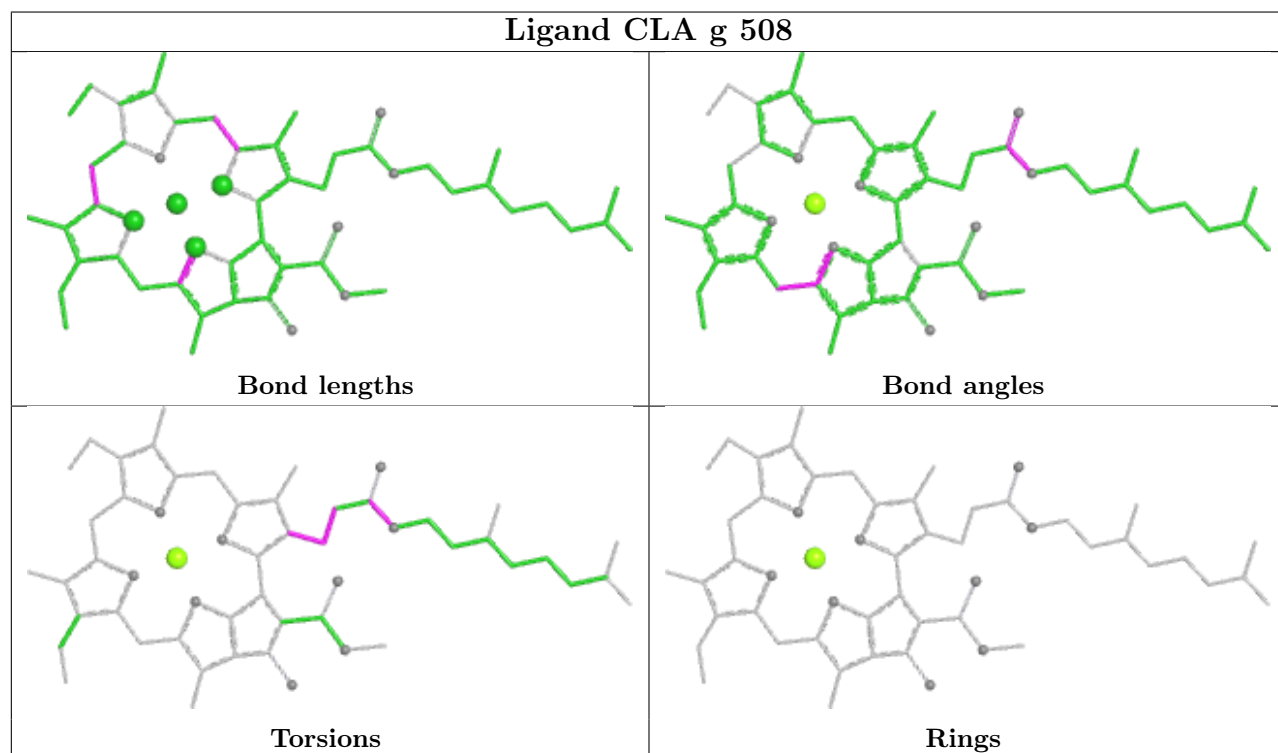
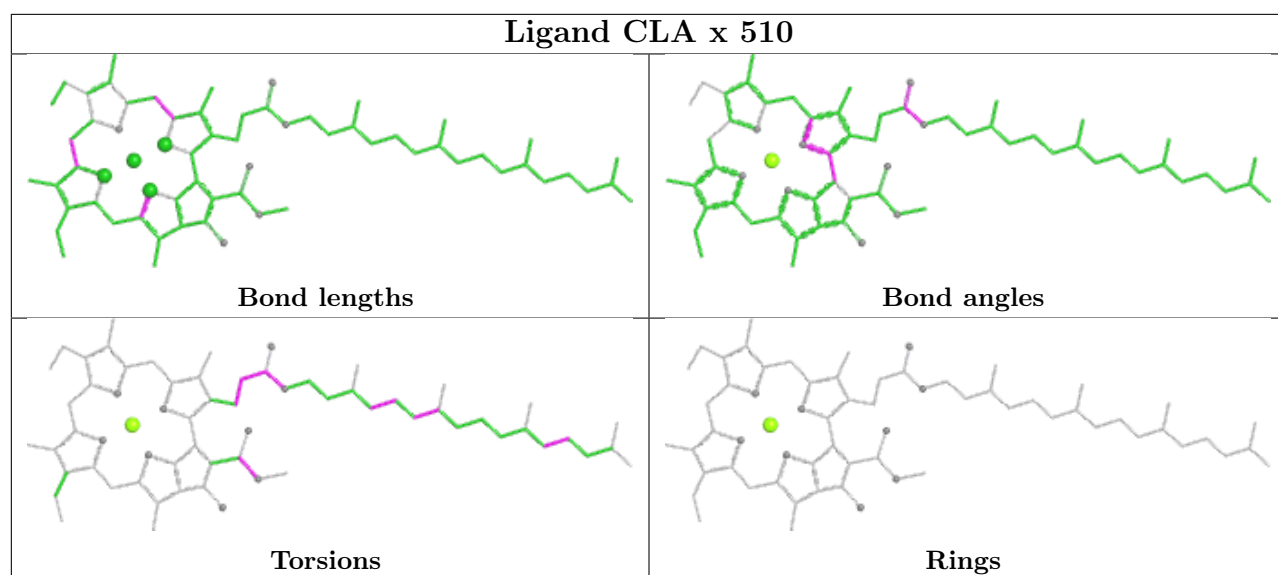
## Ligand CLA A 1122



## Ligand CLA A 1127

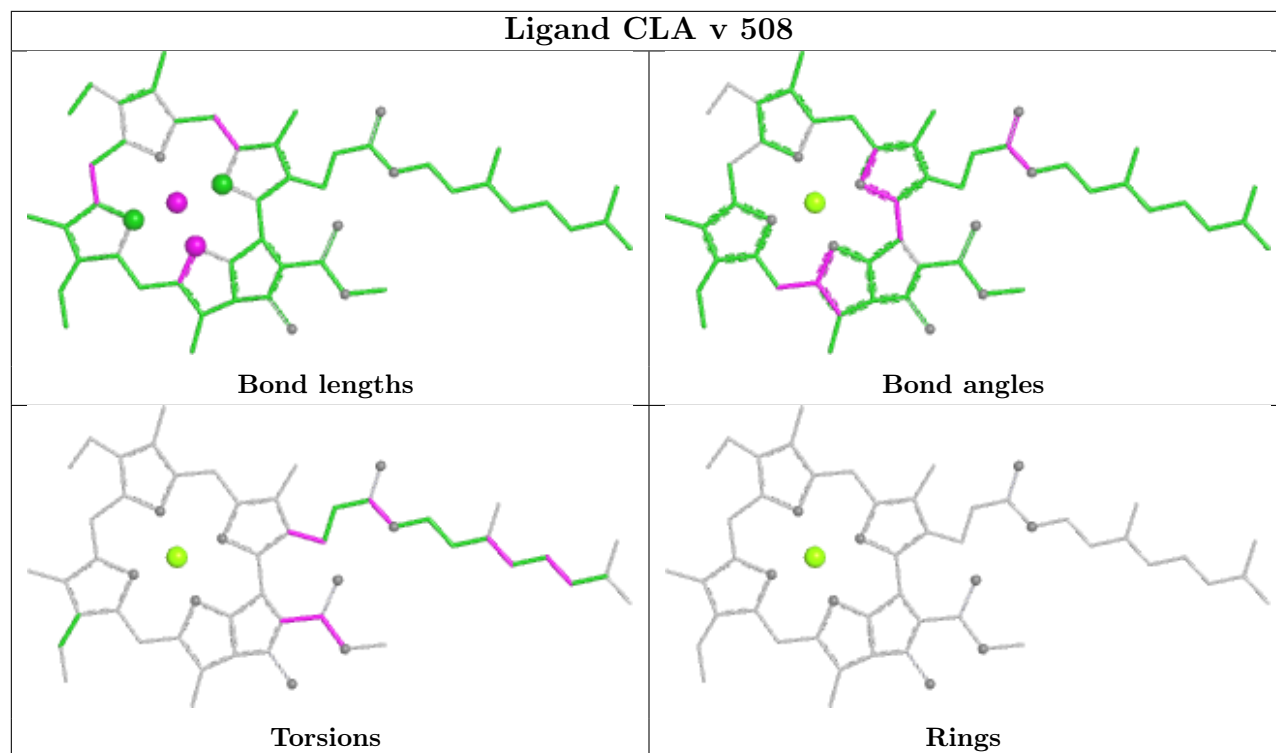




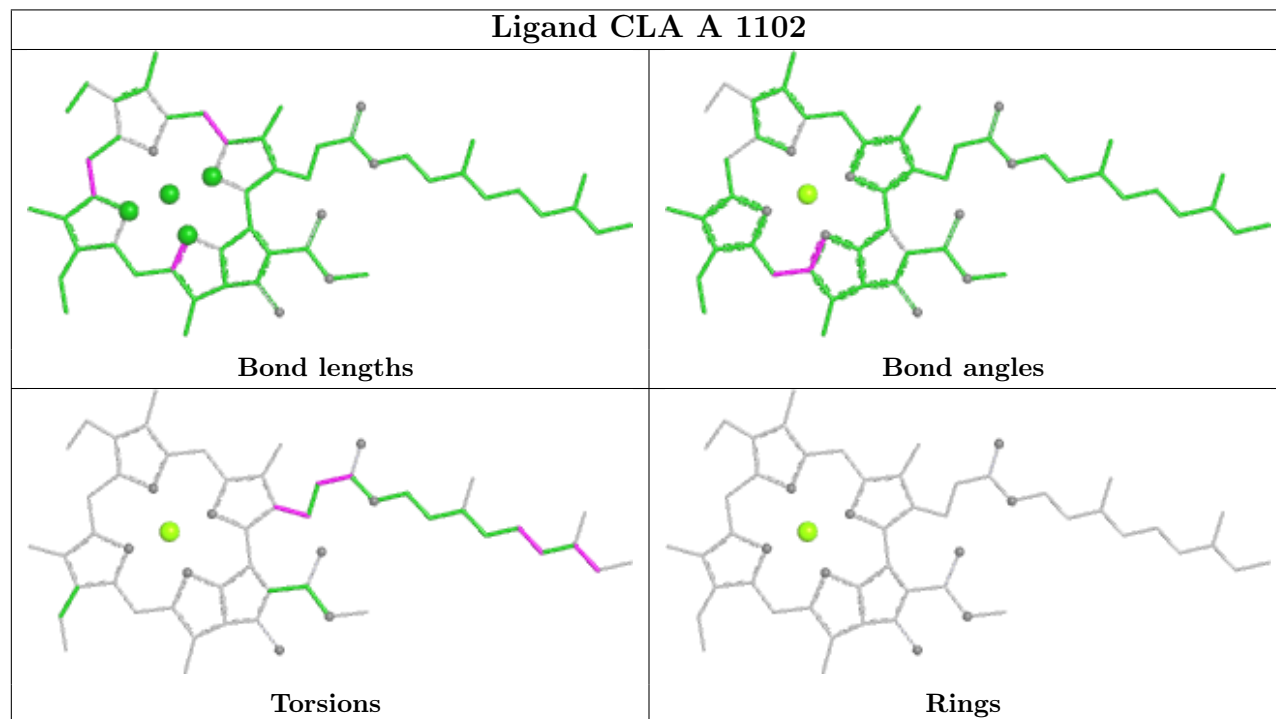




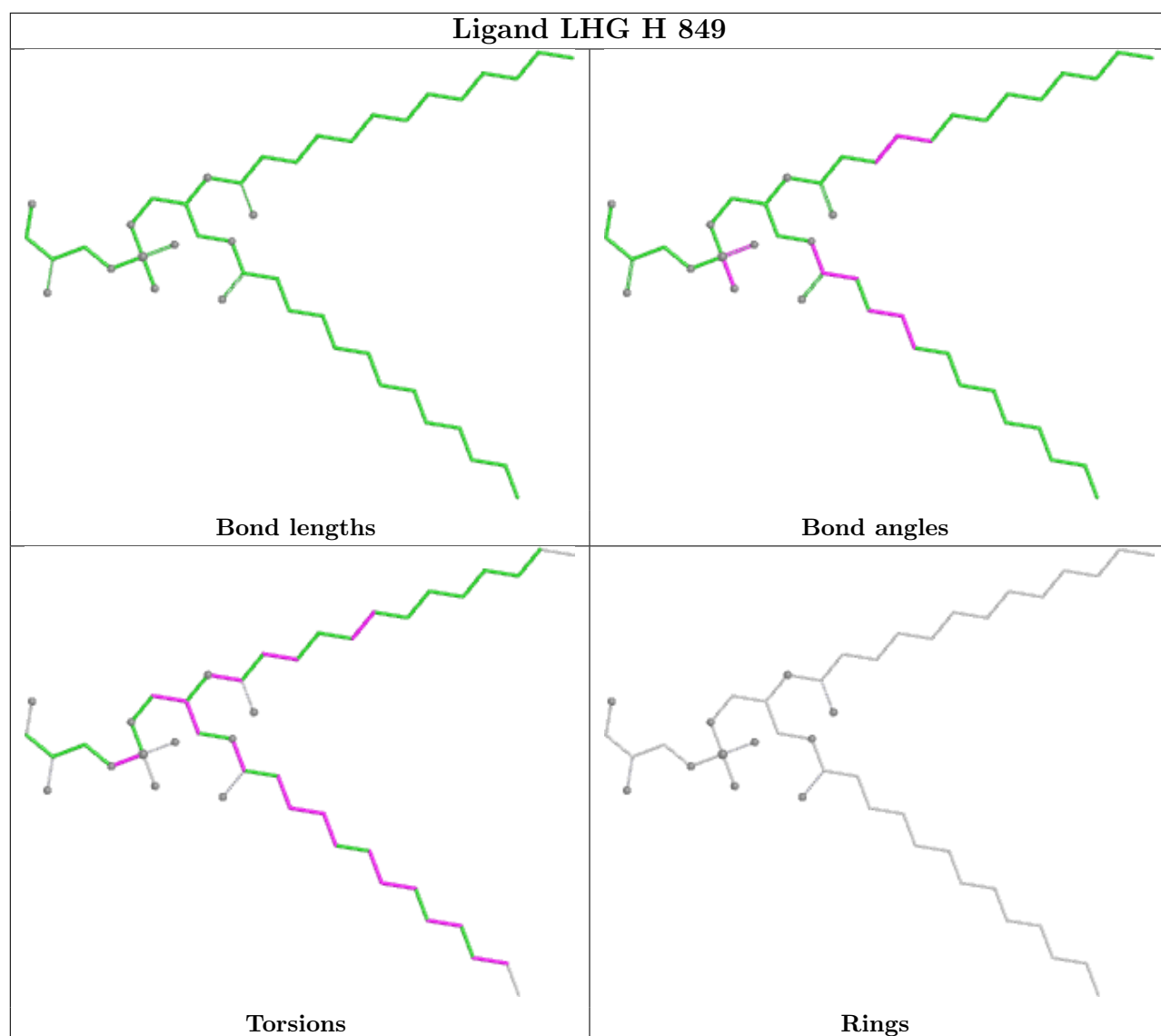
## Ligand CLA v 508



## Ligand CLA A 1102

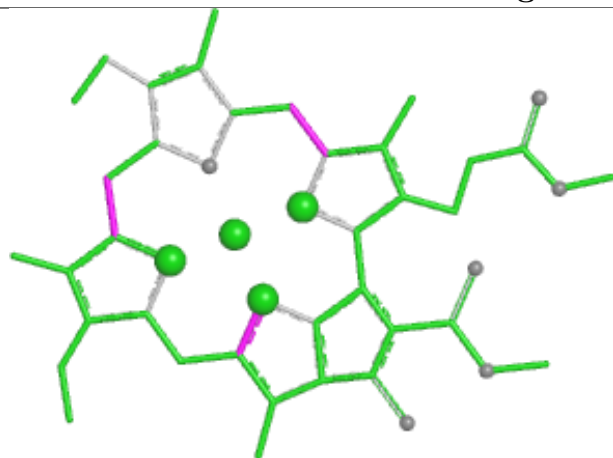




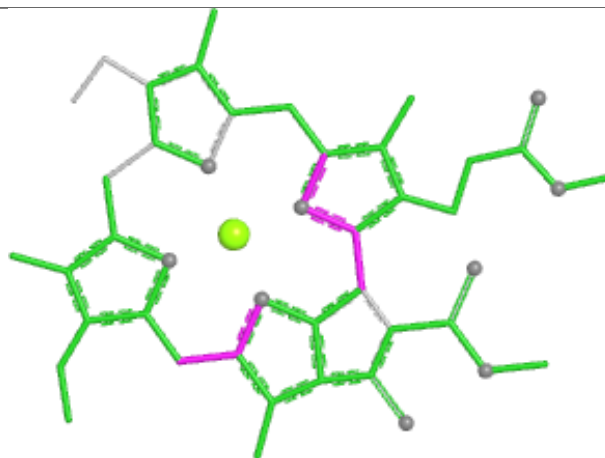




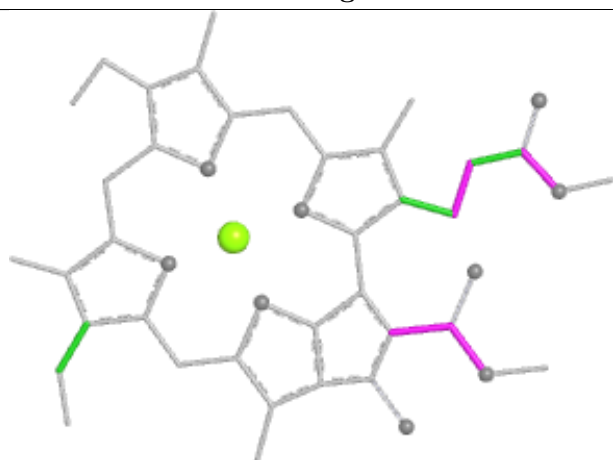
## Ligand CLA u 516



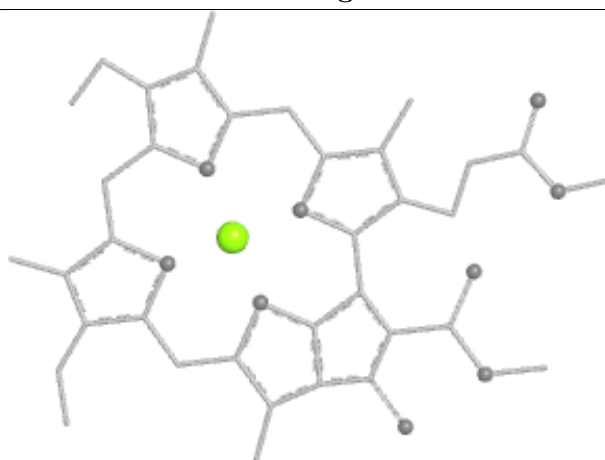
Bond lengths



Bond angles

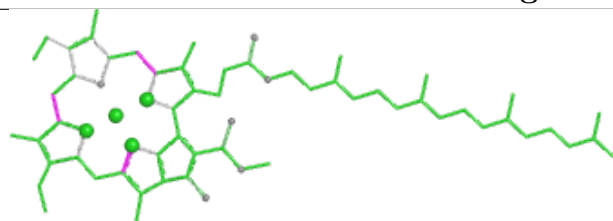


Torsions

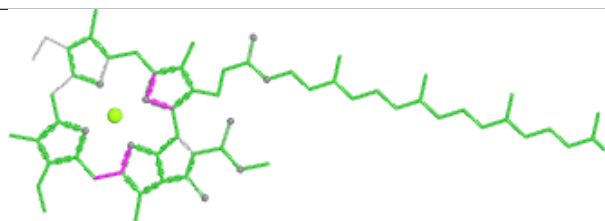


Rings

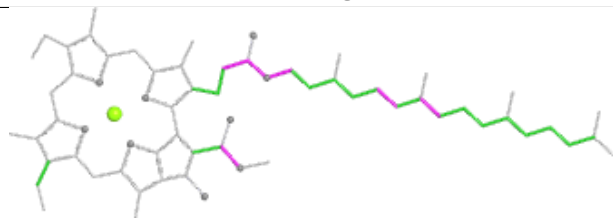
## Ligand CLA t 507



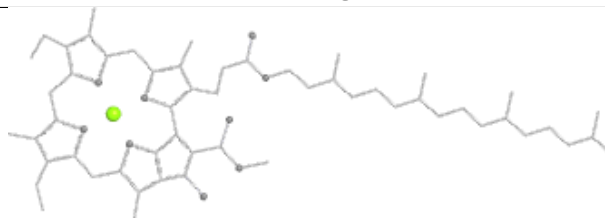
Bond lengths



Bond angles

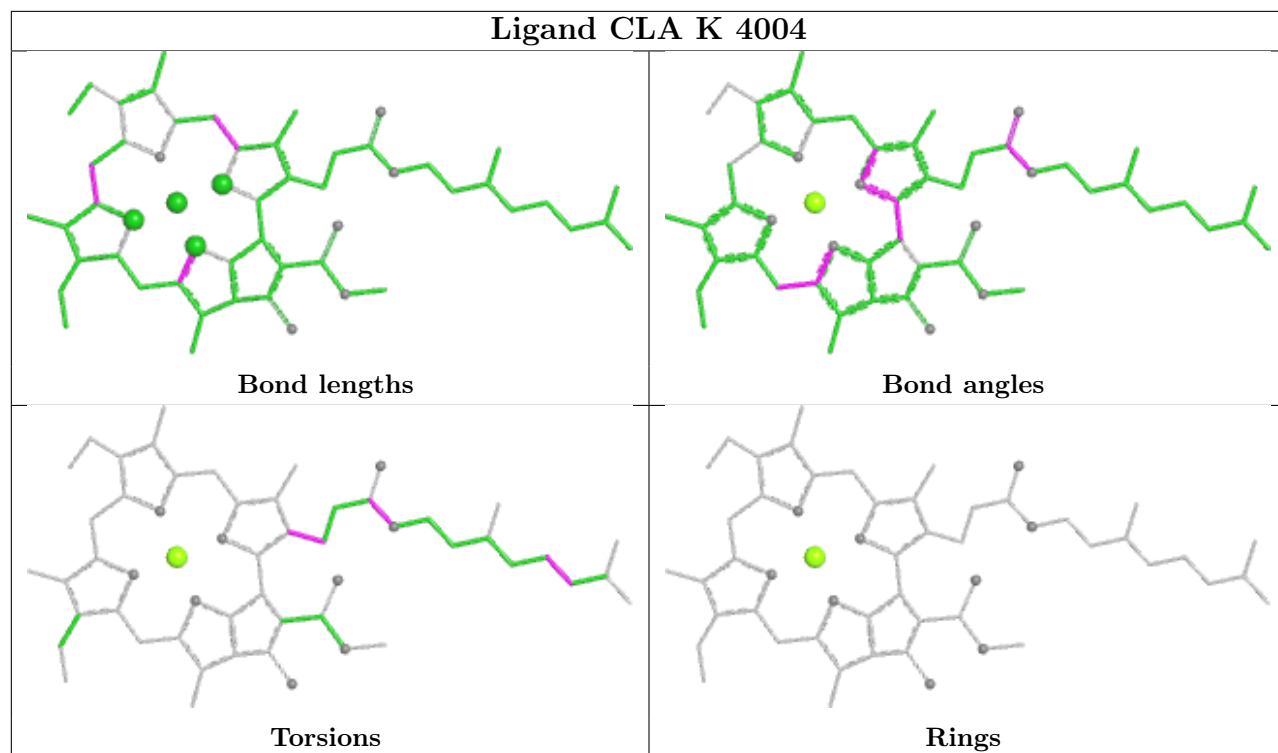


Torsions



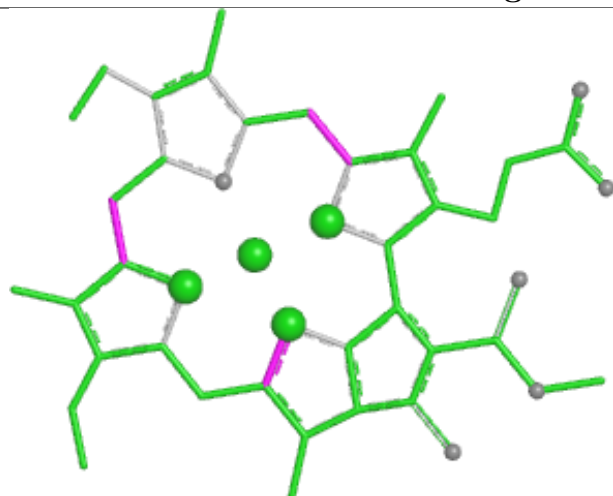
Rings



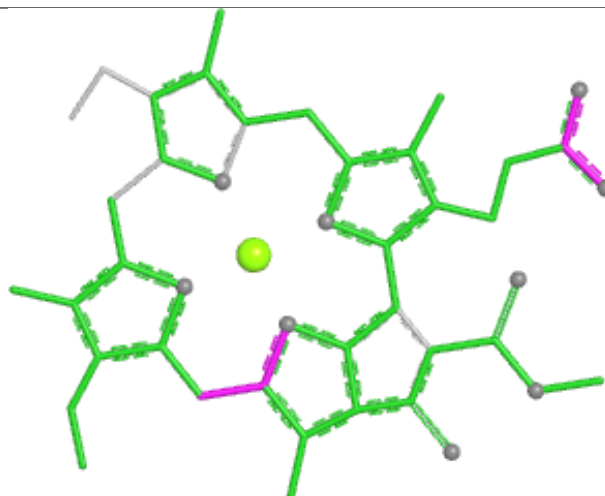




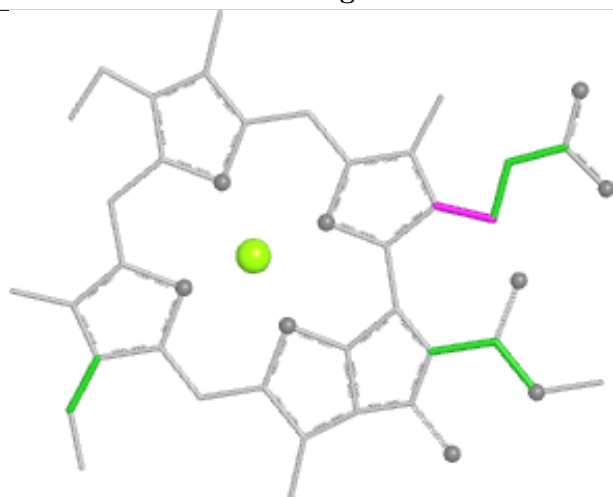
## Ligand CLA H 1112



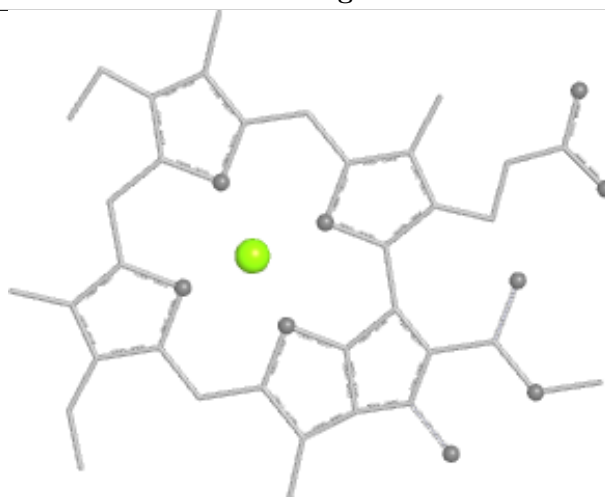
Bond lengths



Bond angles

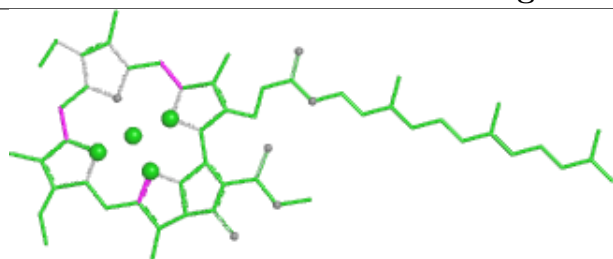


Torsions

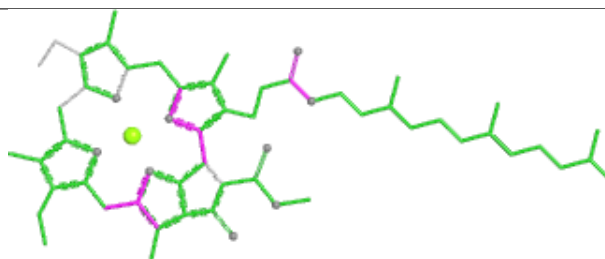


Rings

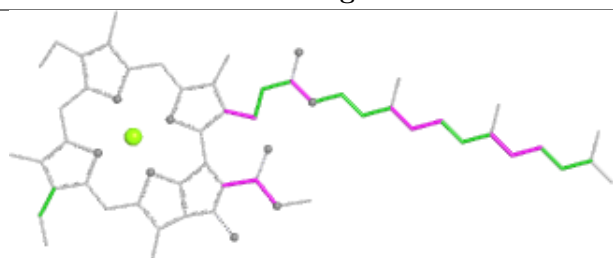
## Ligand CLA h 504



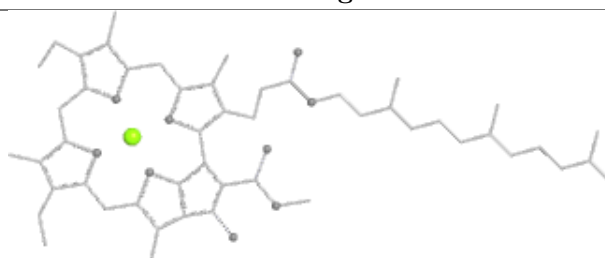
Bond lengths



Bond angles

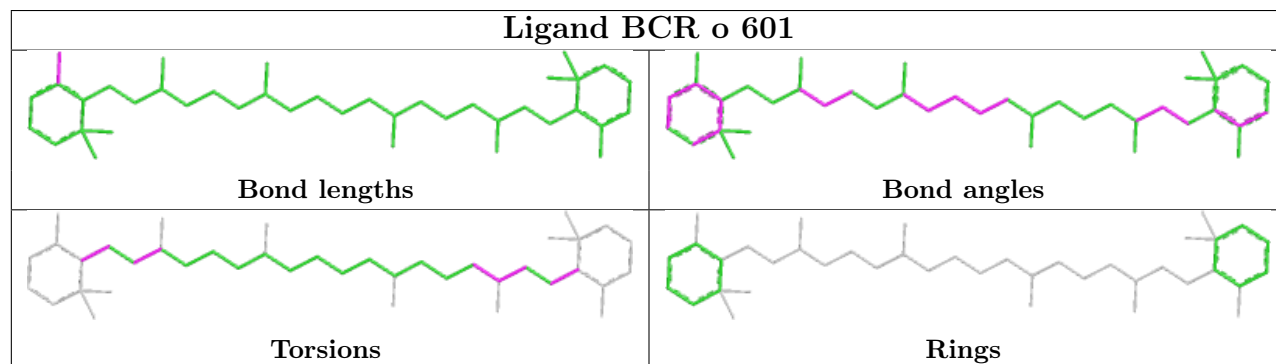
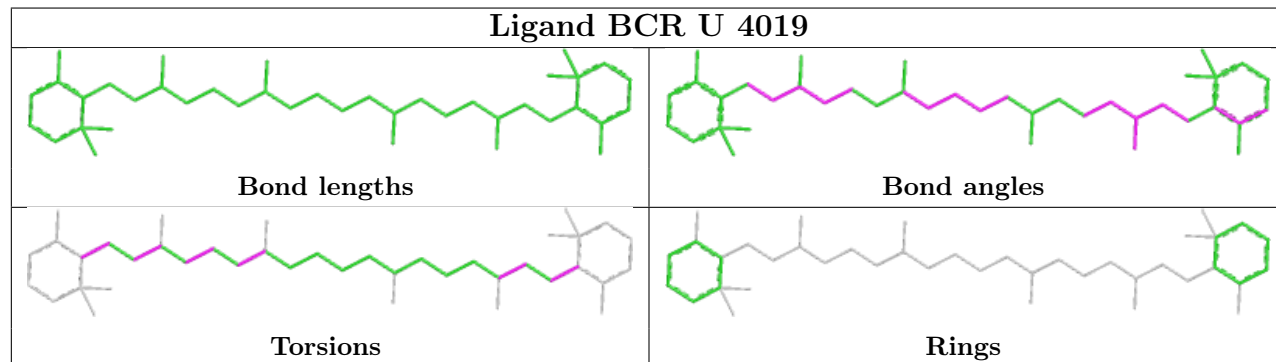
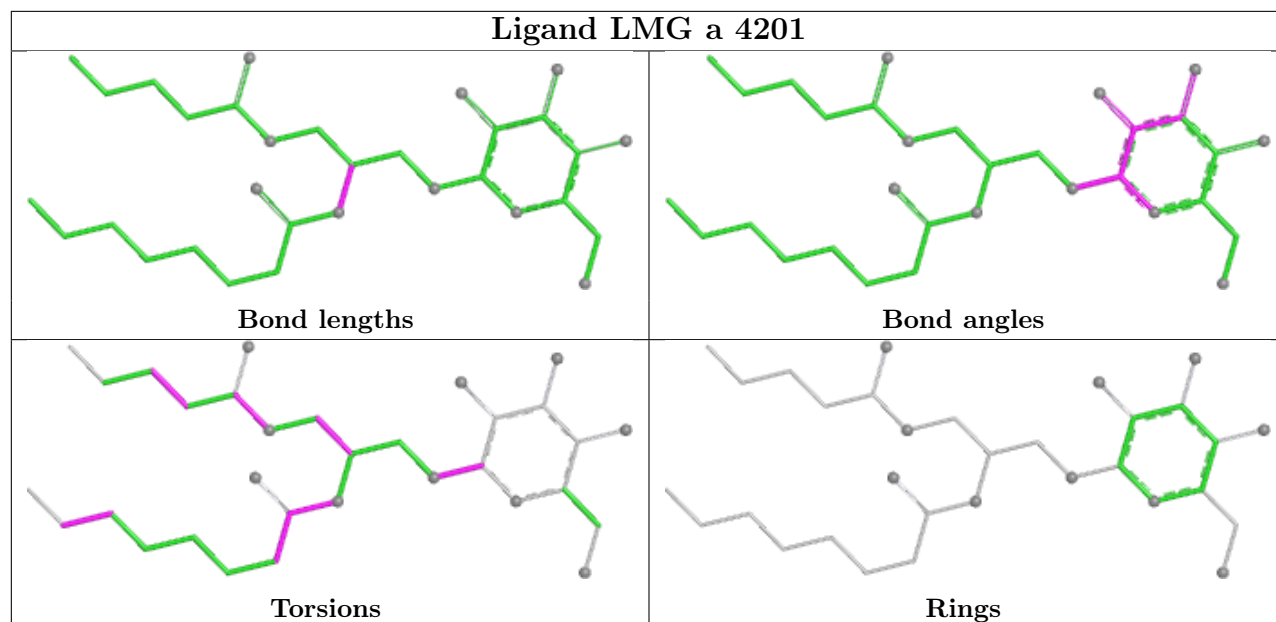


Torsions

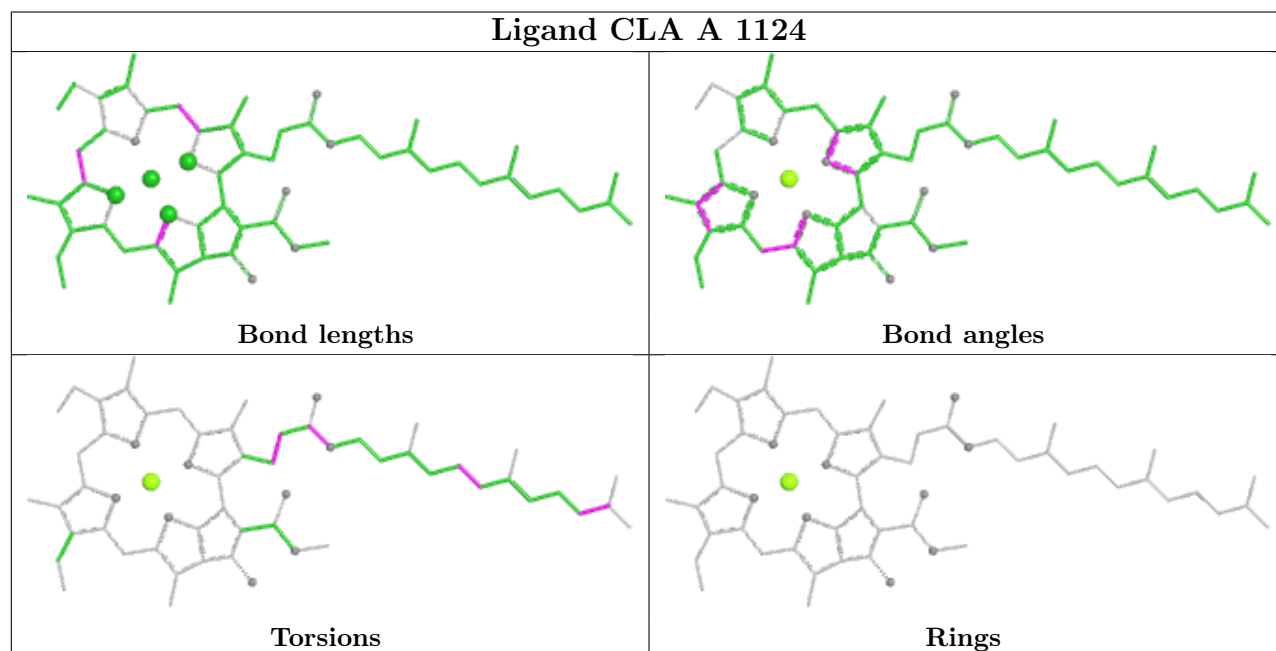
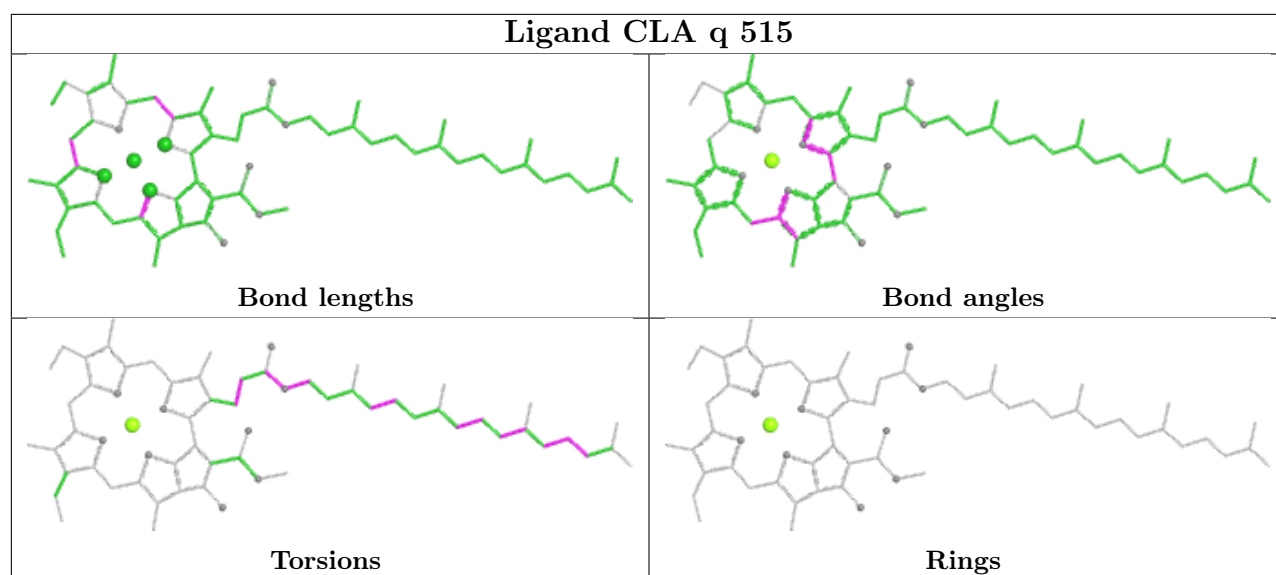


Rings



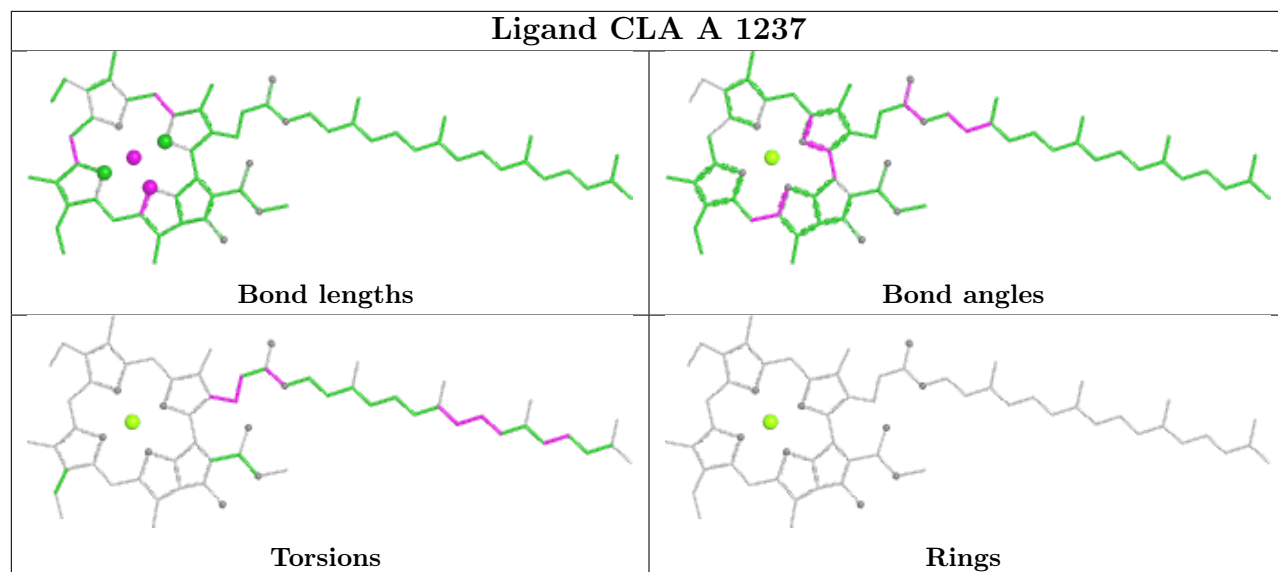




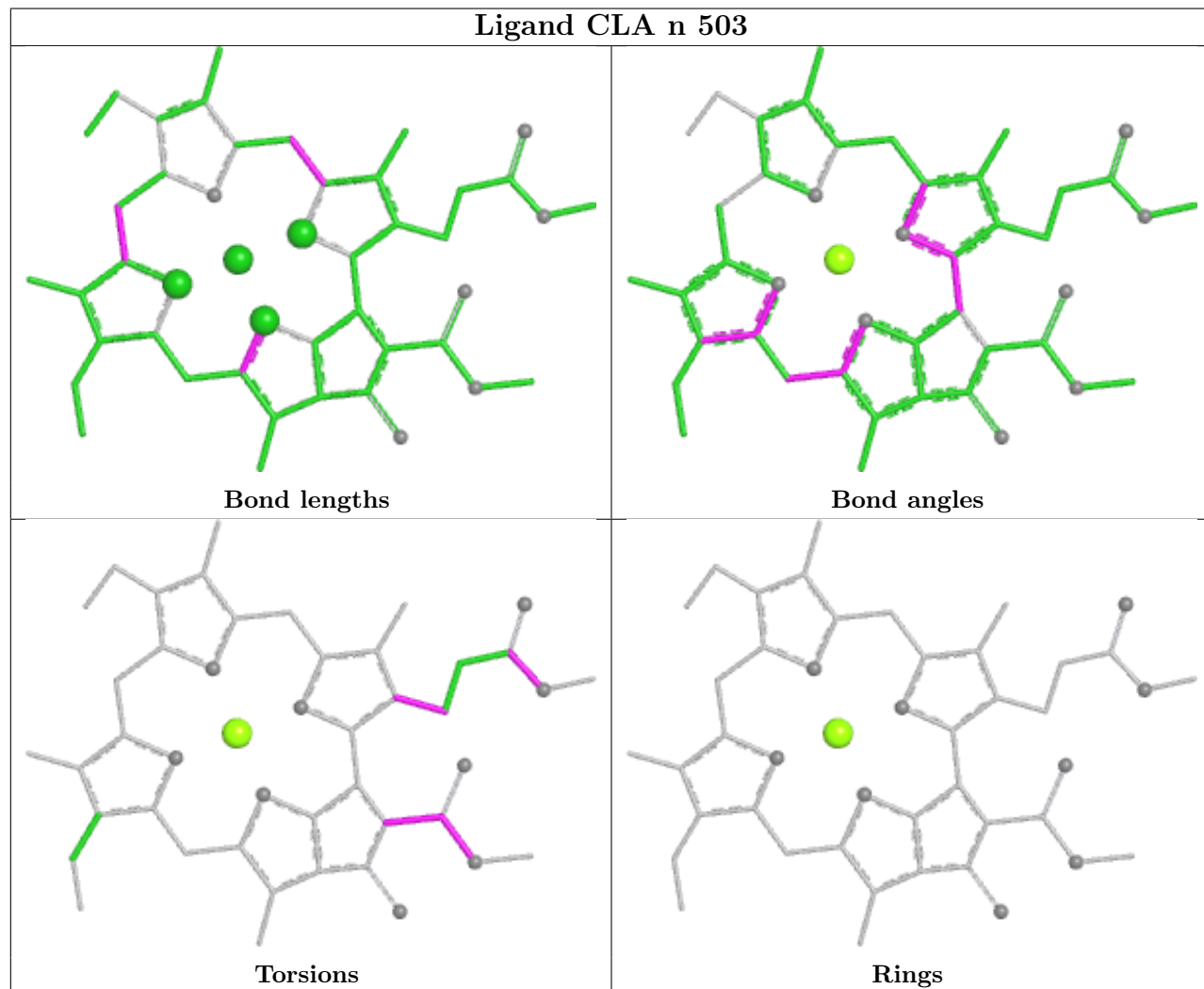




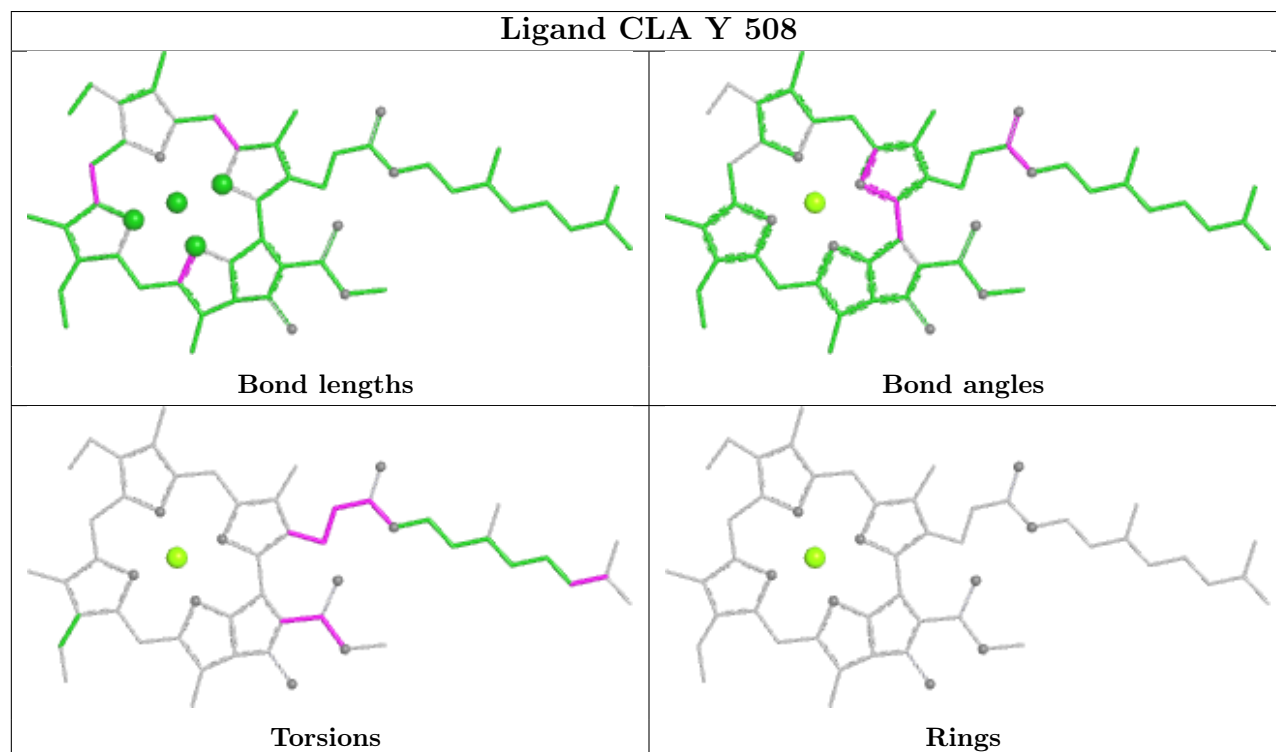
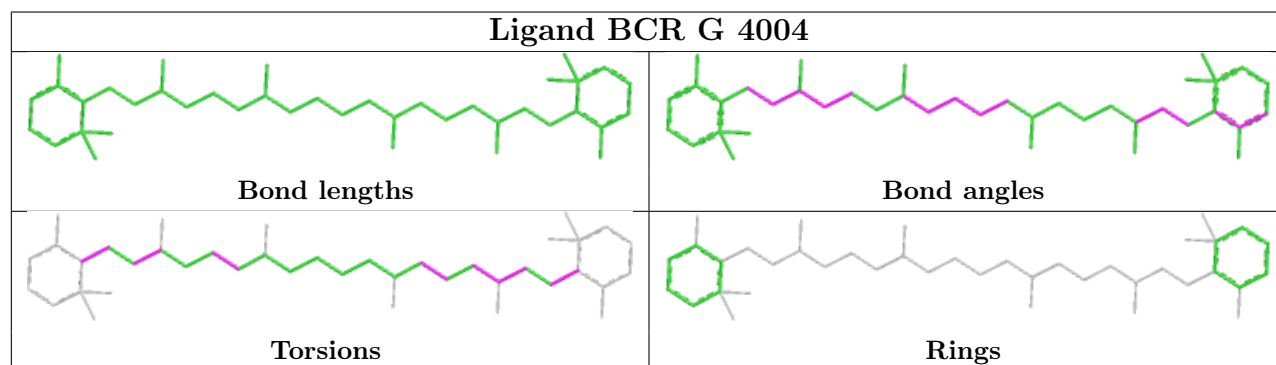
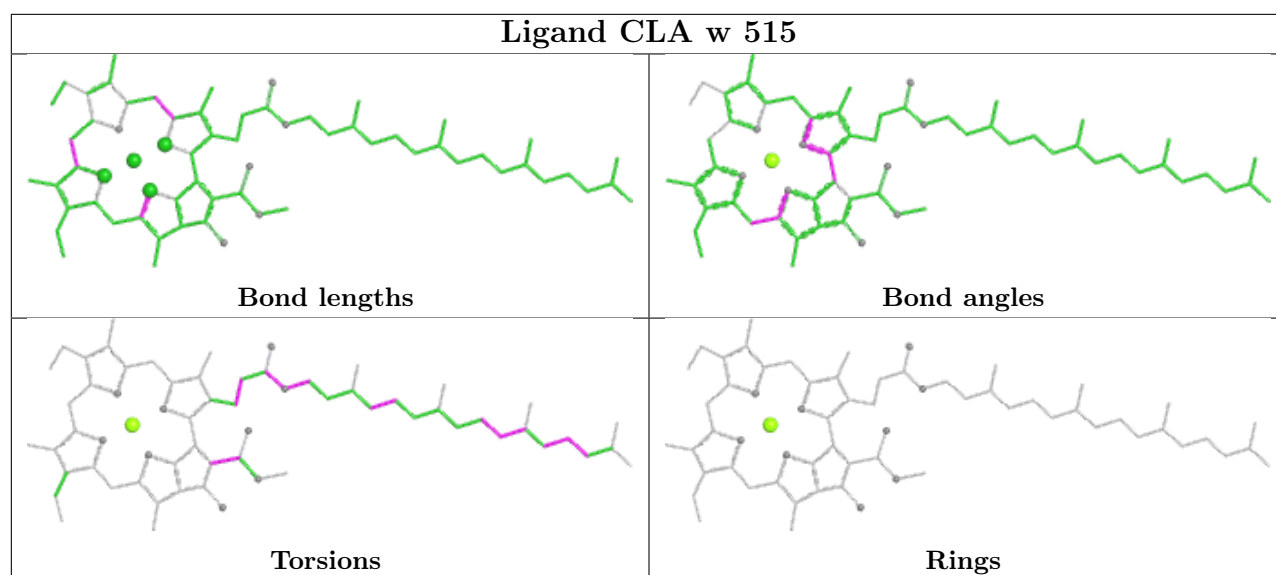
## Ligand CLA A 1237



## Ligand CLA n 503

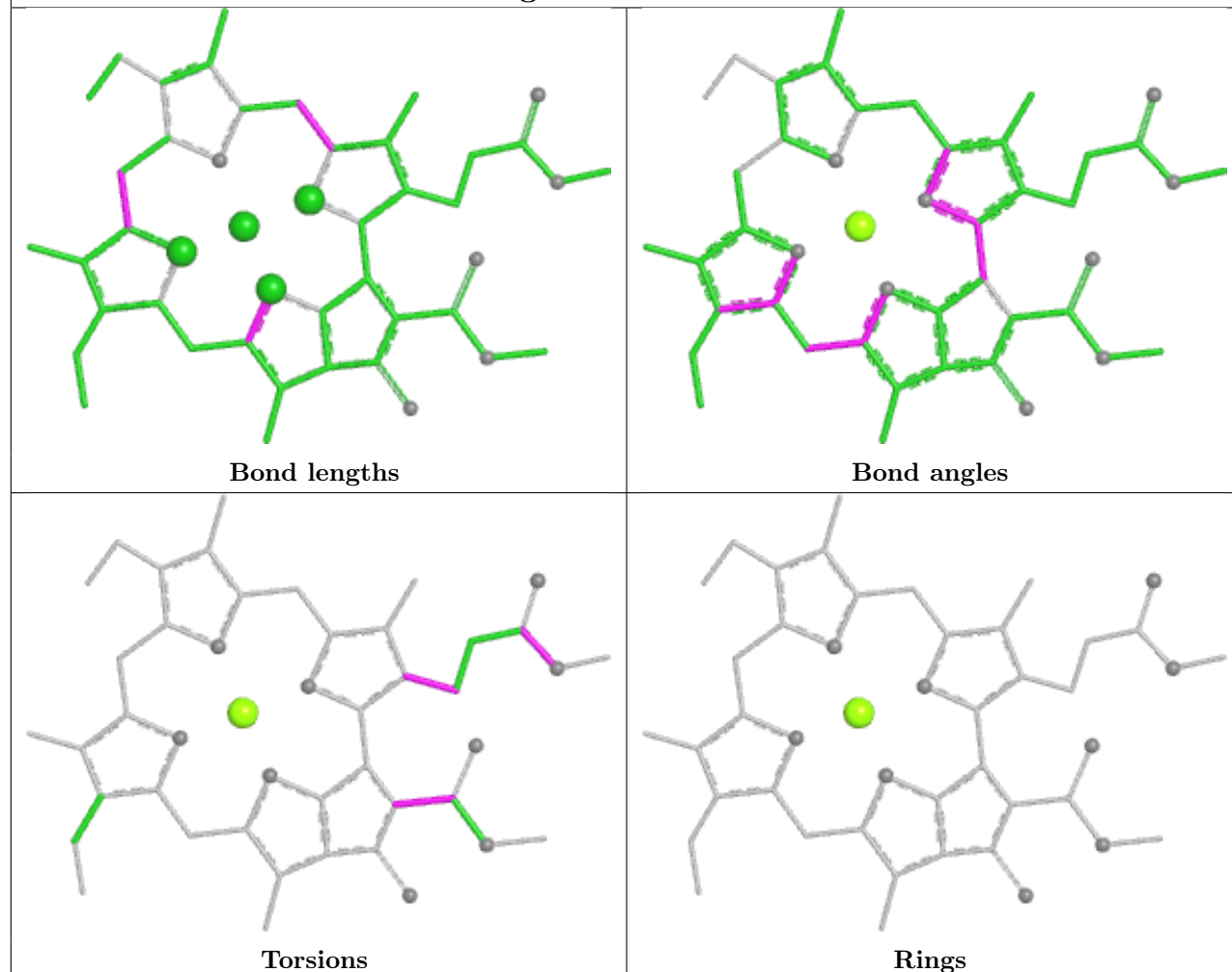




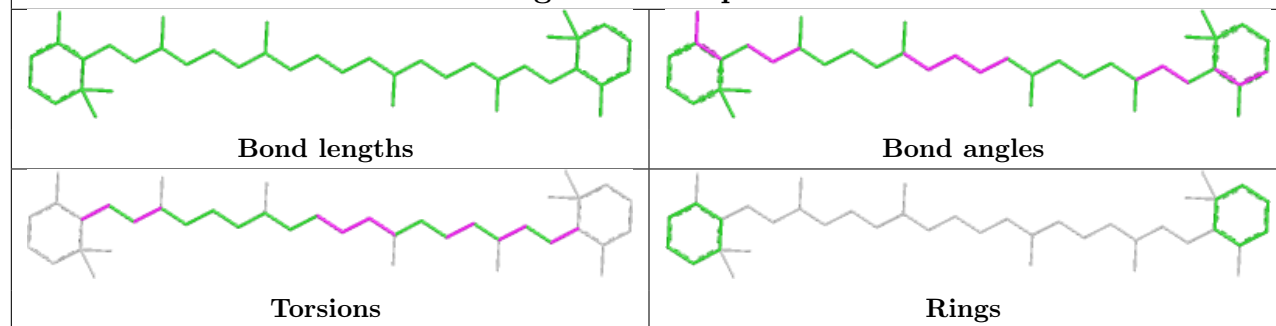




## Ligand CLA t 503

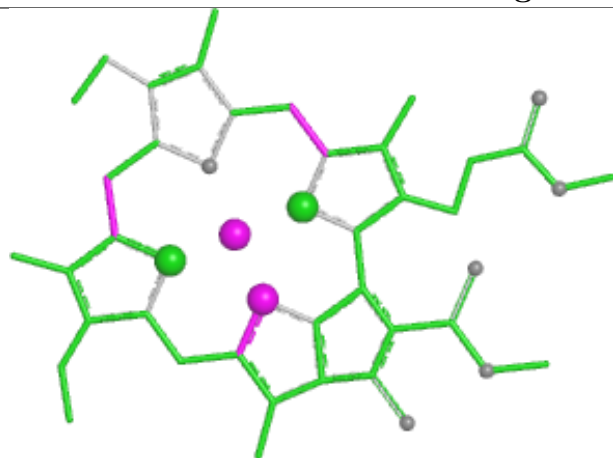


## Ligand BCR q 602

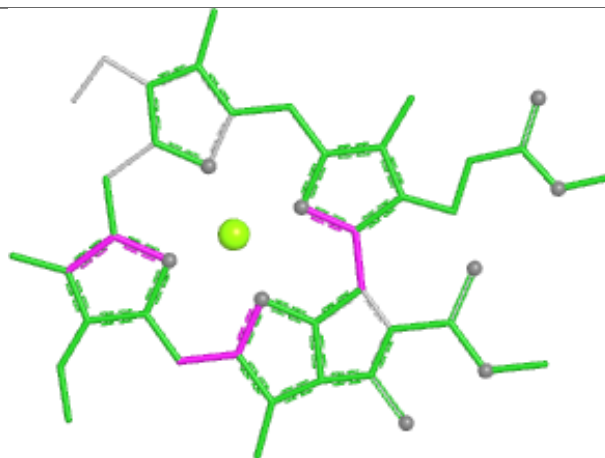




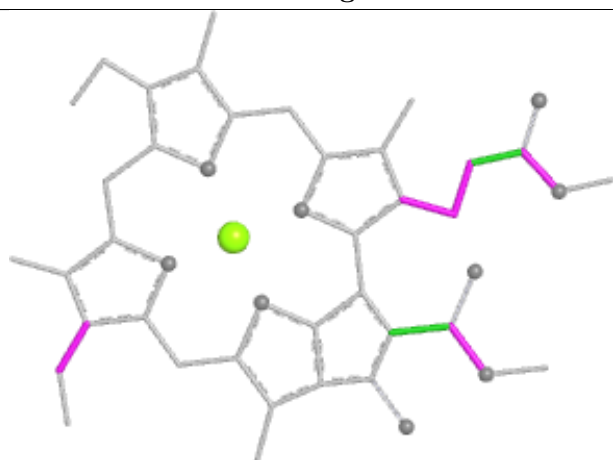
## Ligand CLA w 503



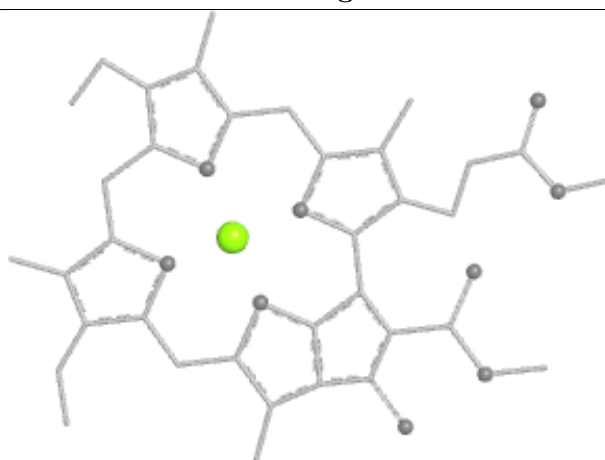
Bond lengths



Bond angles

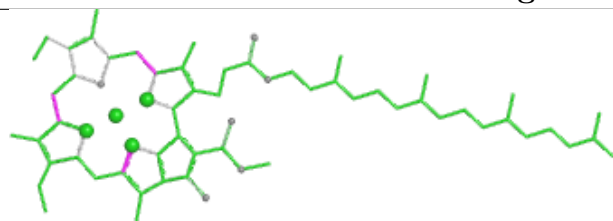


Torsions

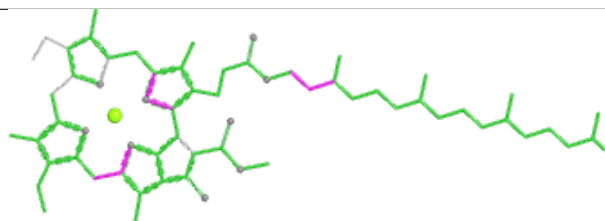


Rings

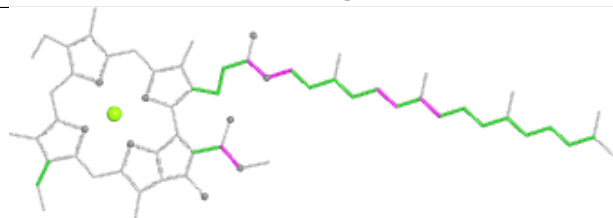
## Ligand CLA x 507



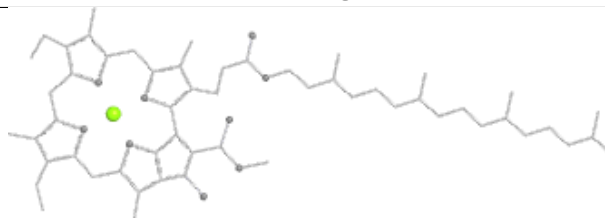
Bond lengths



Bond angles

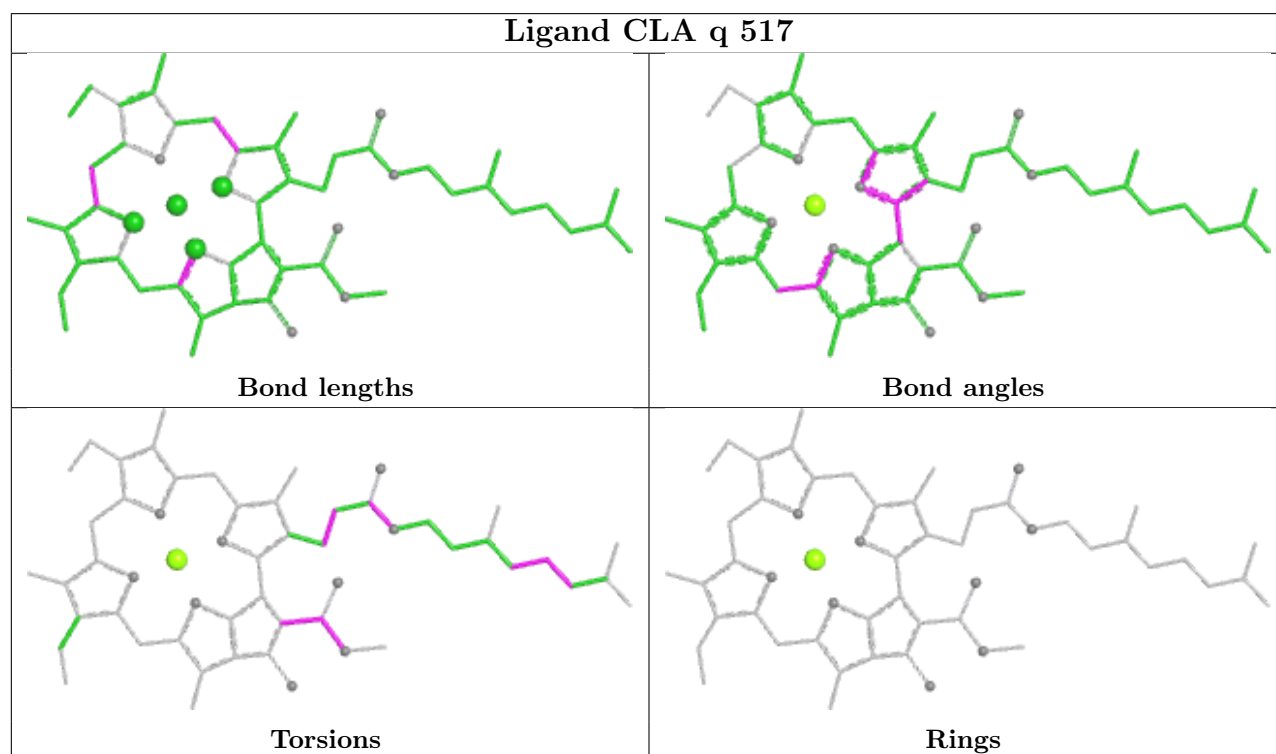
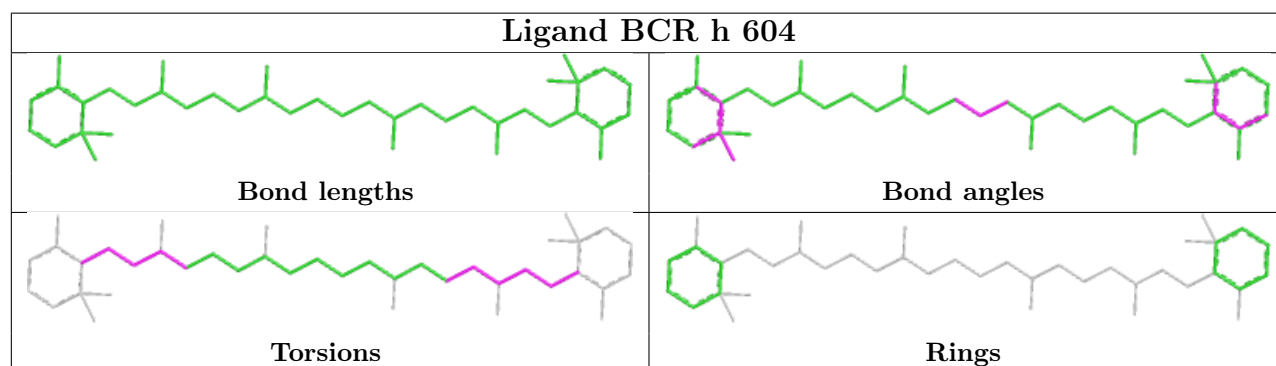
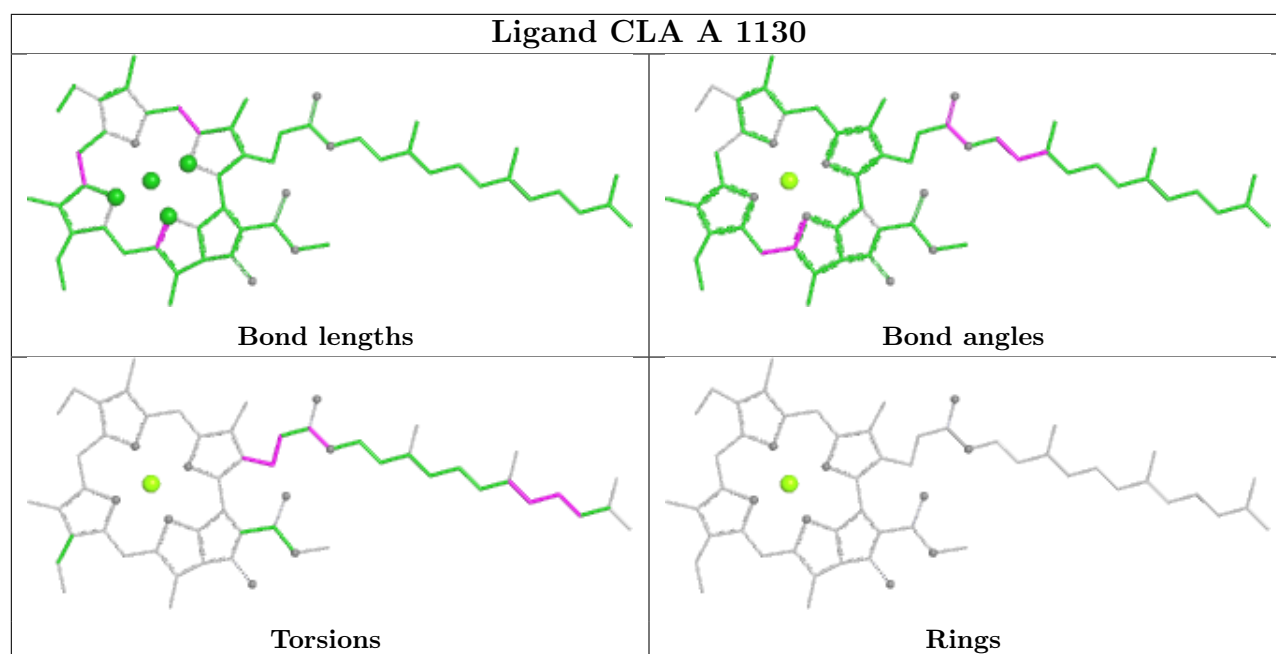


Torsions

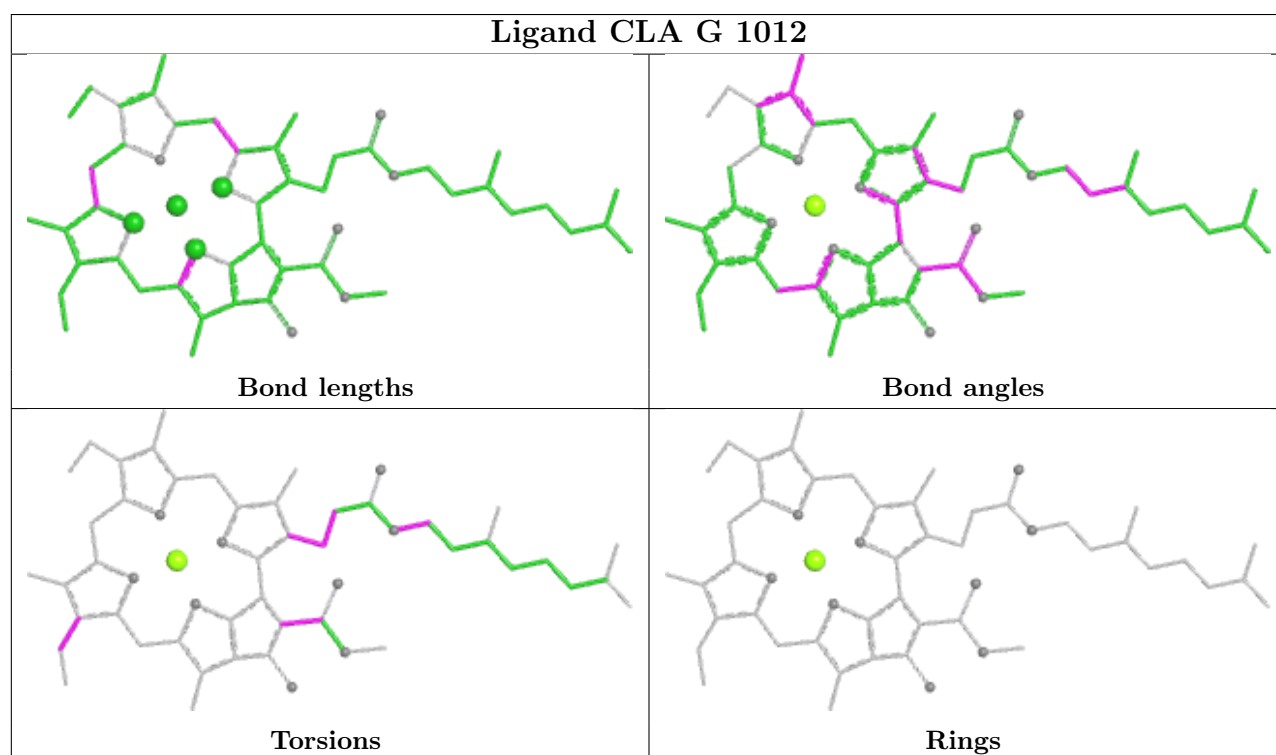
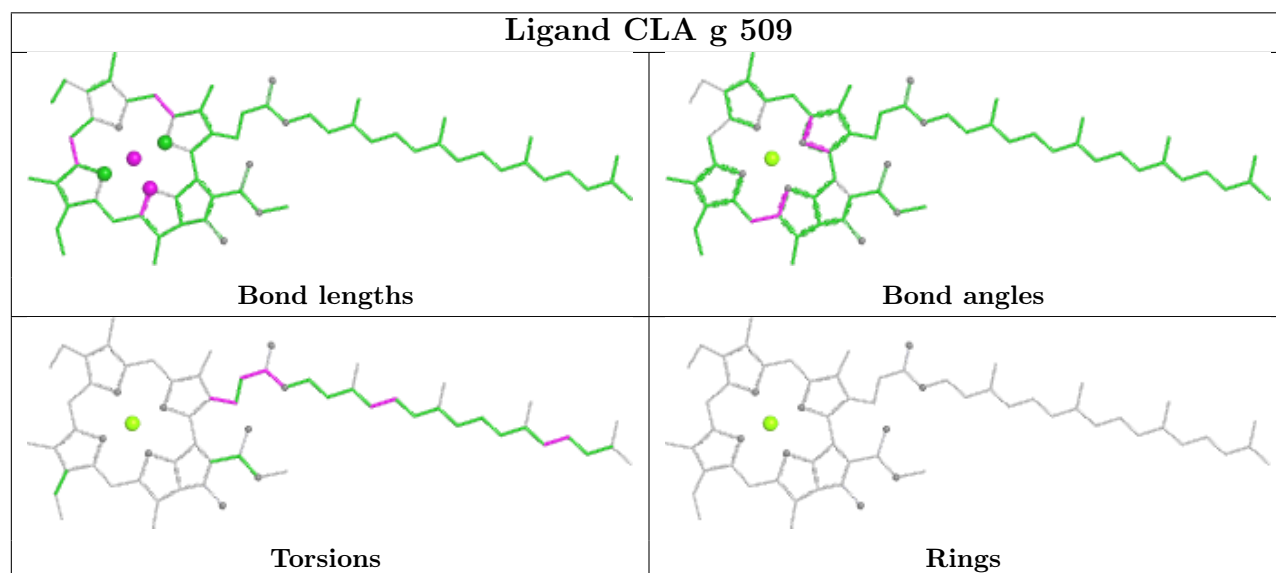
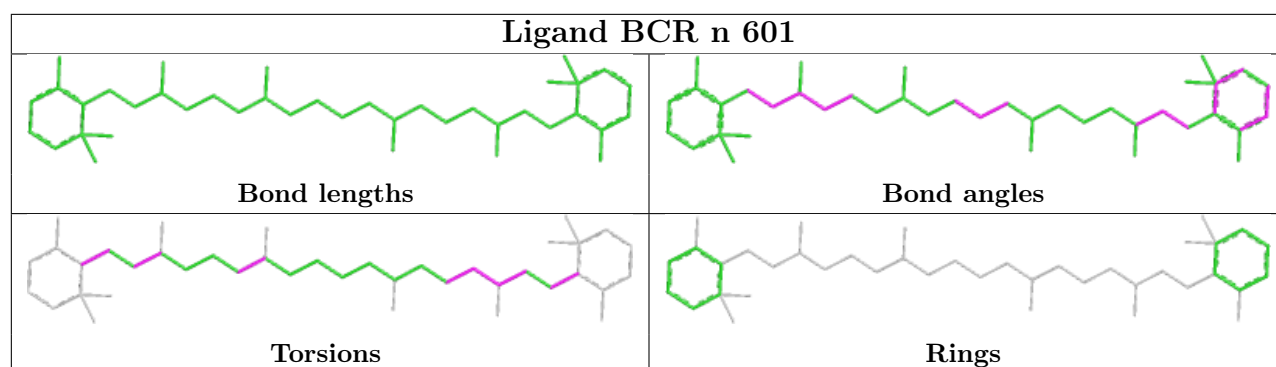


Rings

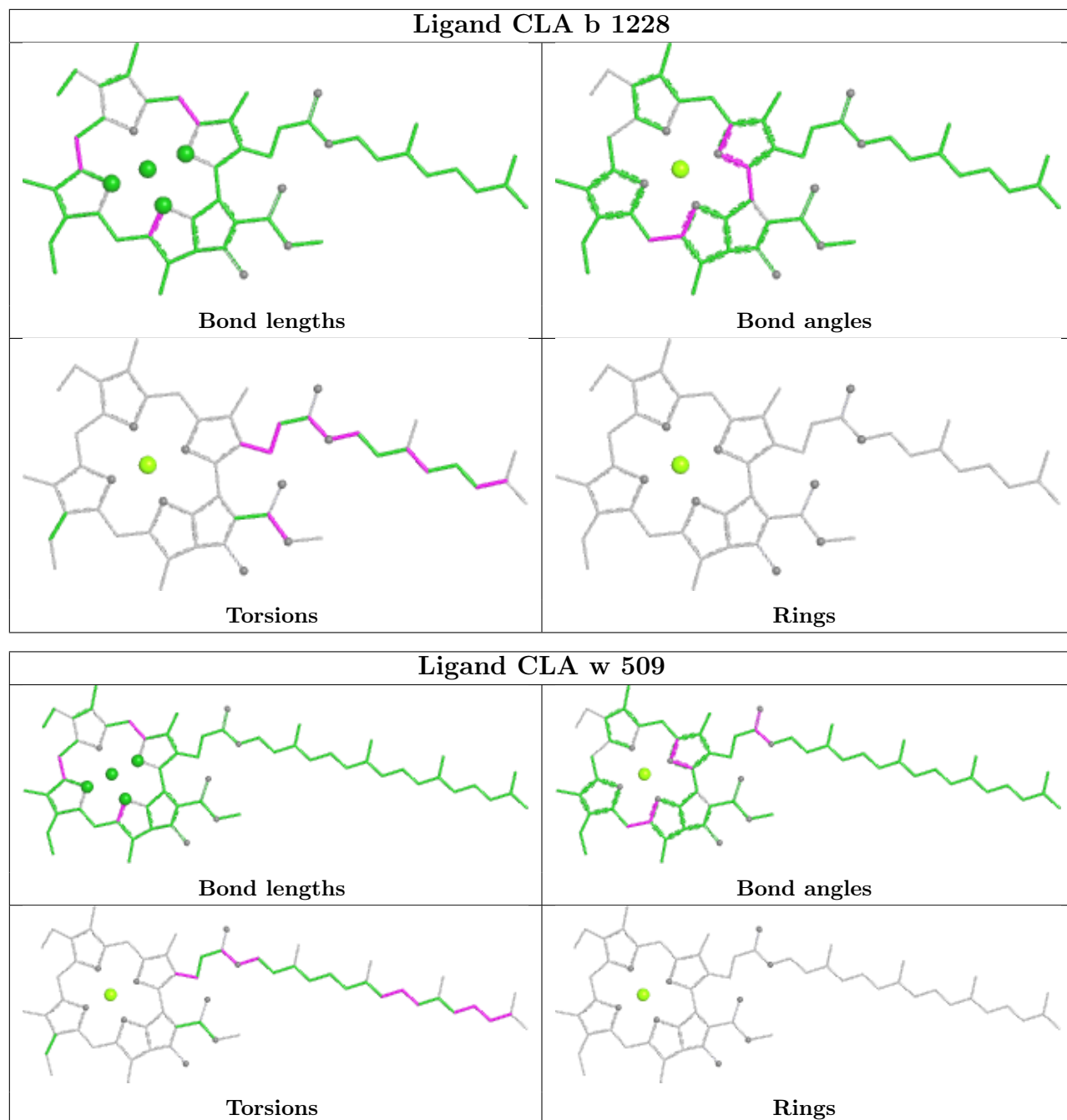






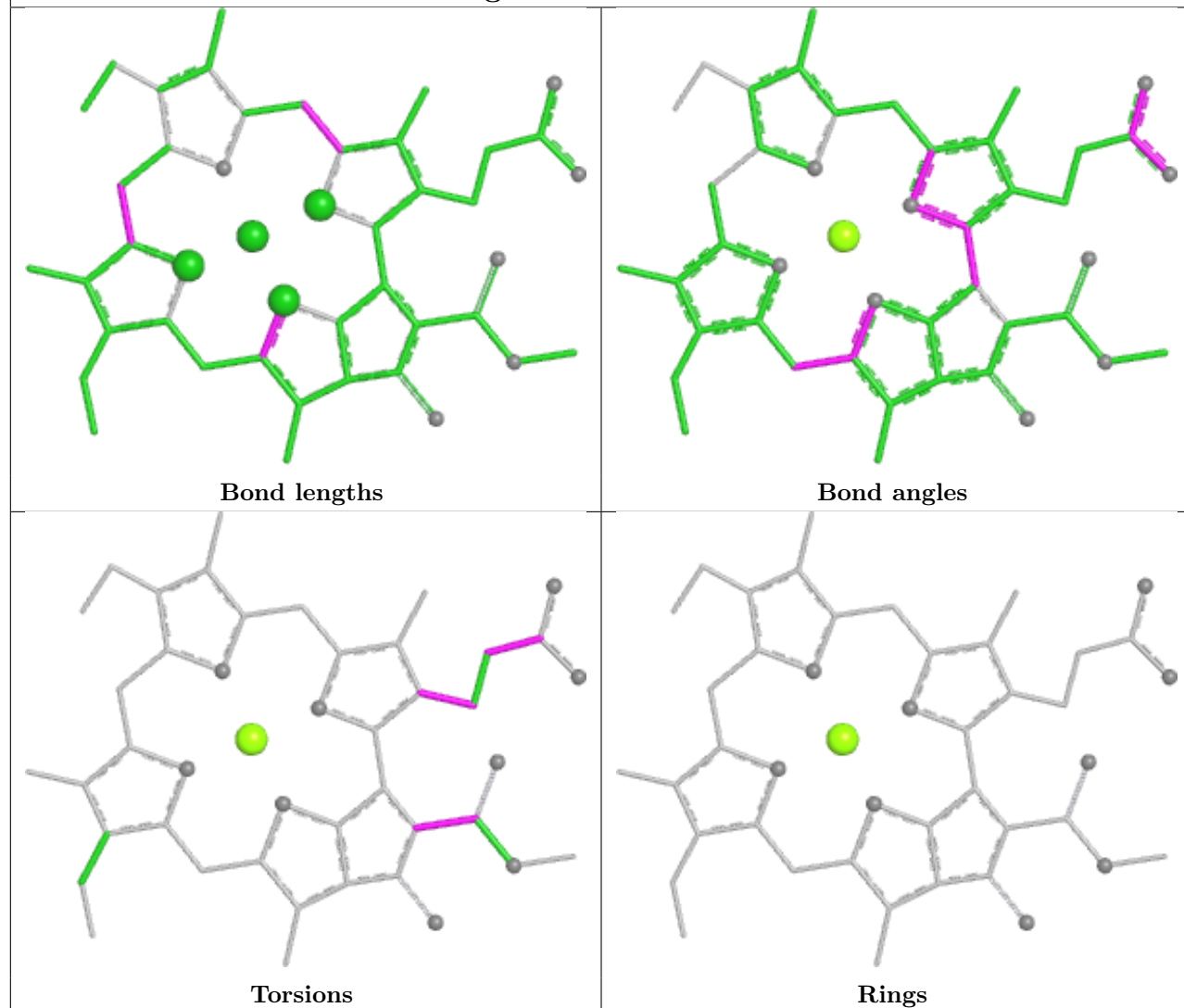




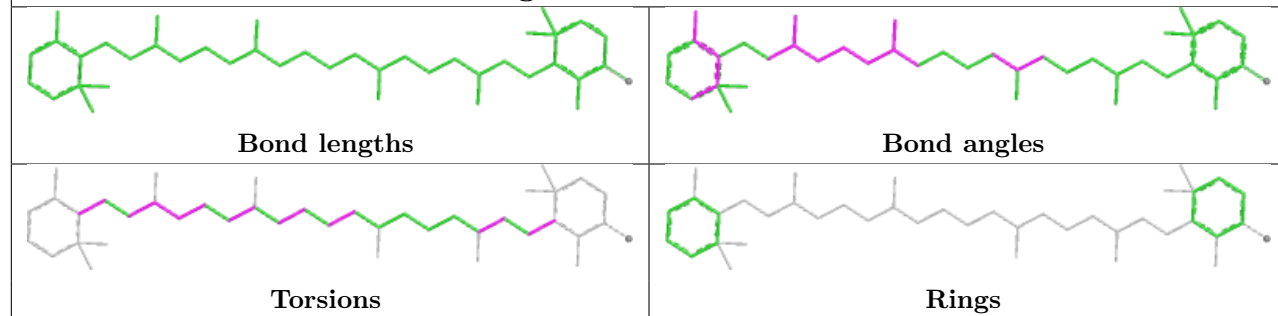




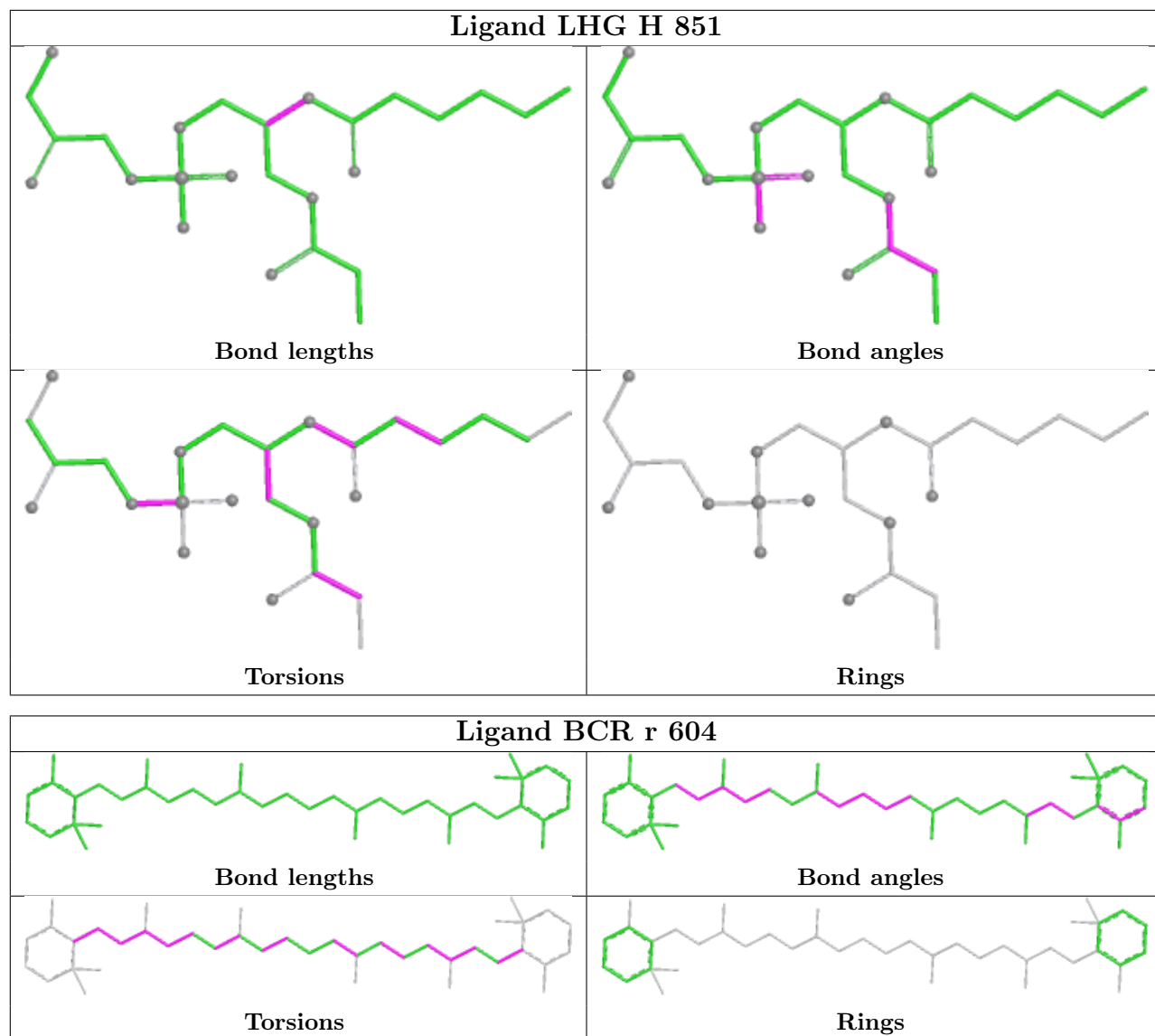
## Ligand CLA B 1212



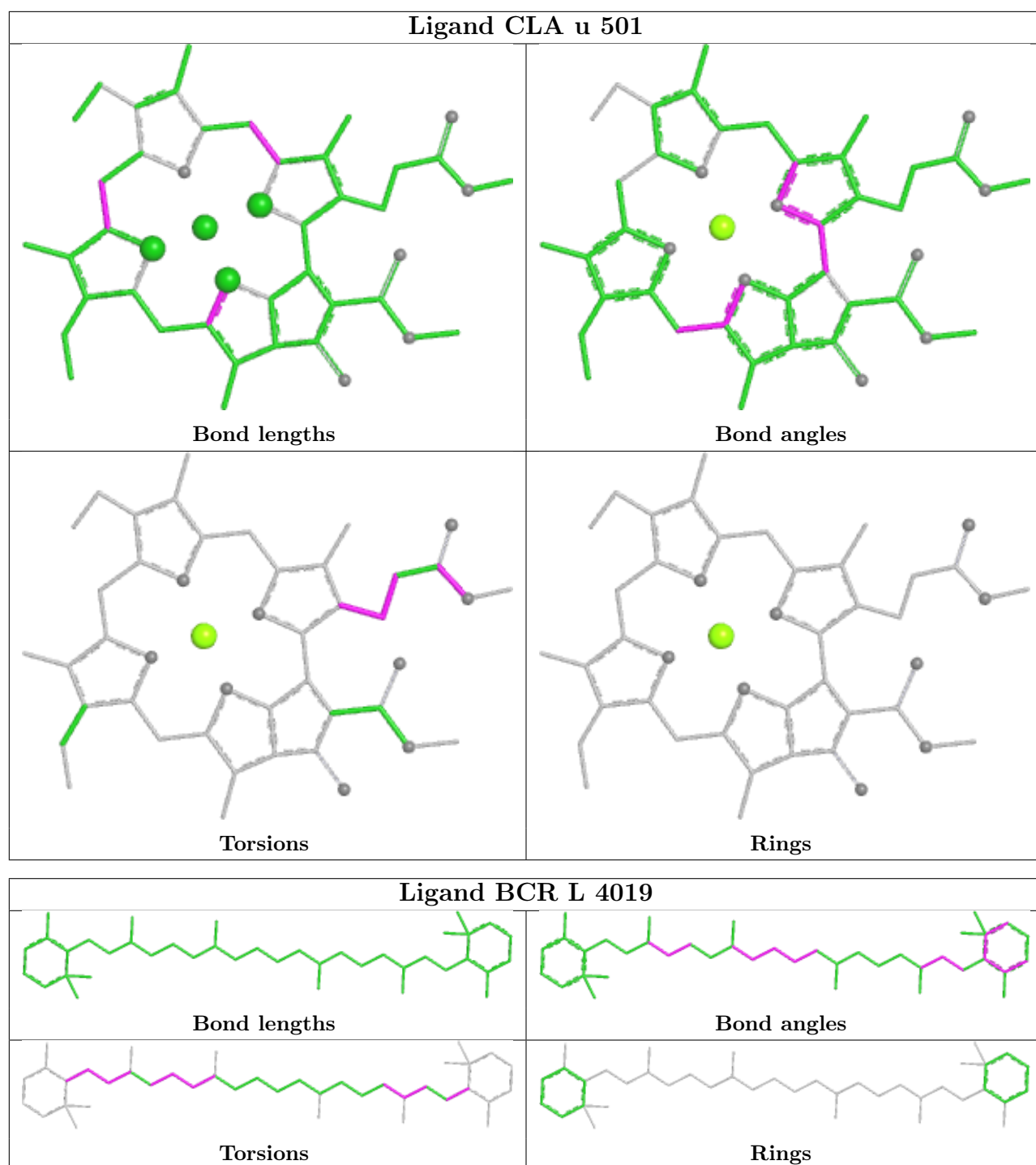
## Ligand ECH M 4021





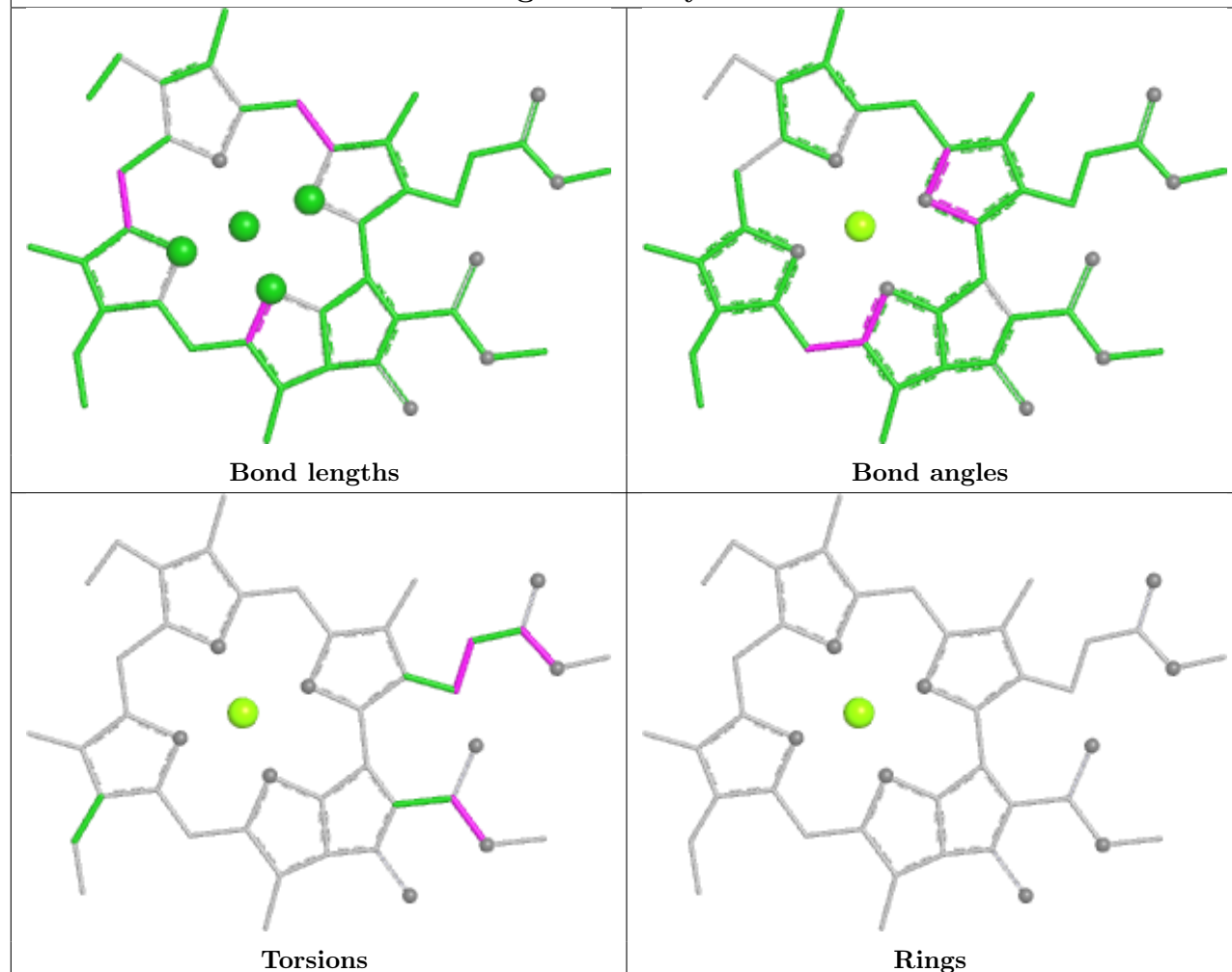




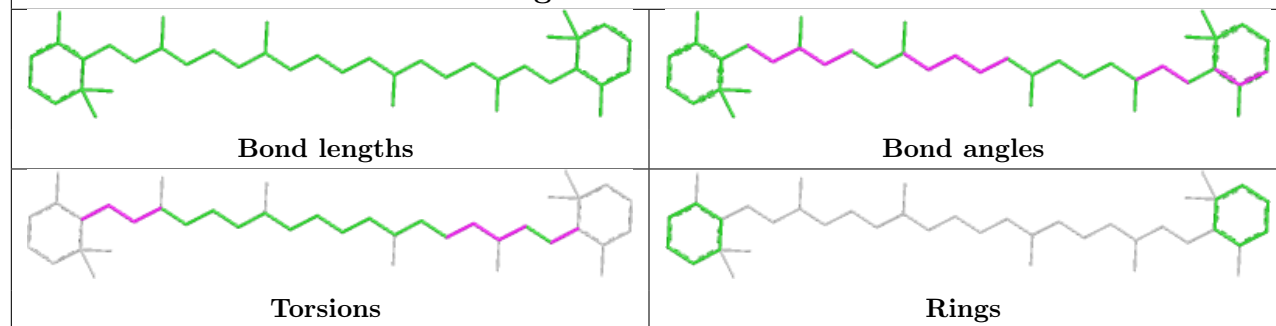




## Ligand CLA y 513

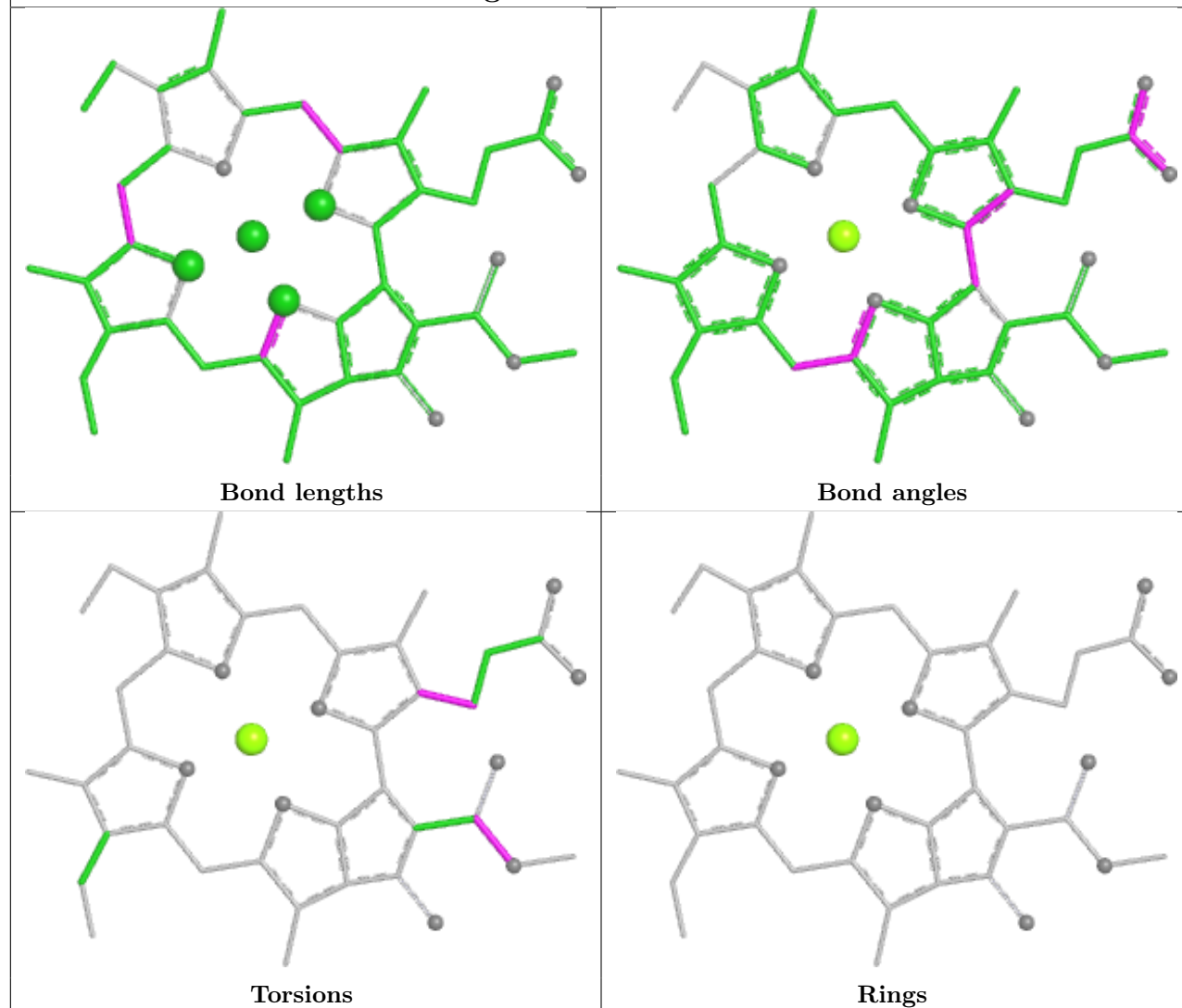


## Ligand BCR x 601

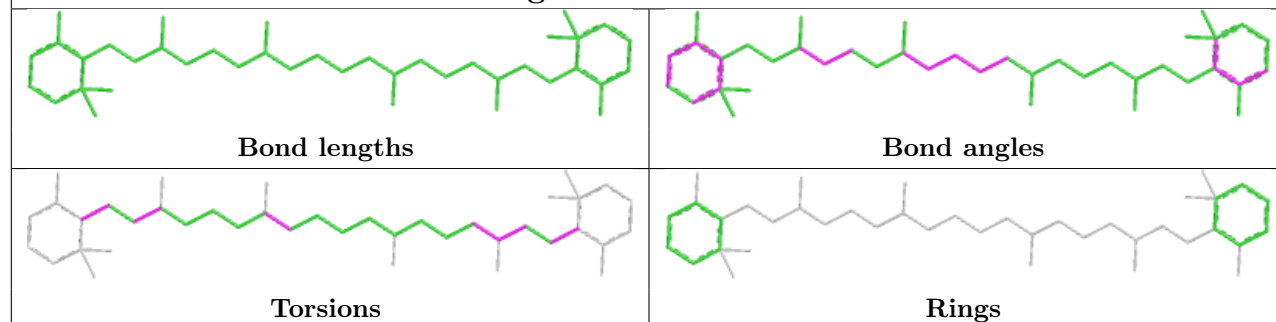




## Ligand CLA A 1112

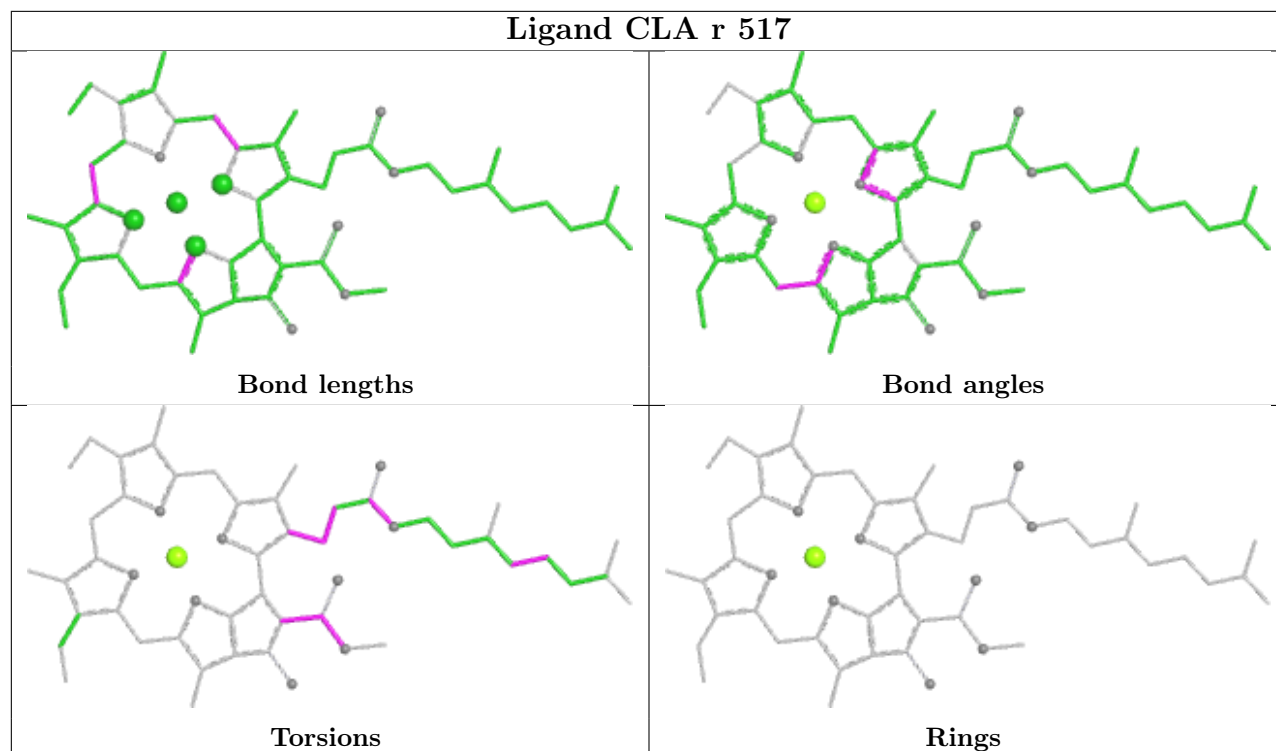


## Ligand BCR I 4018

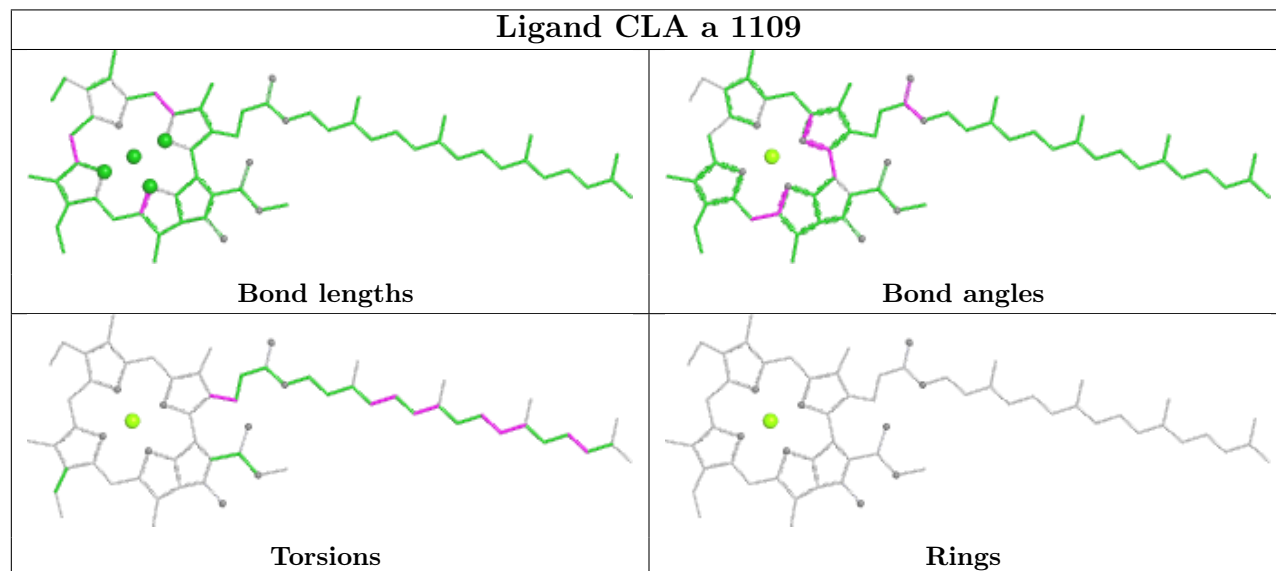




## Ligand CLA r 517

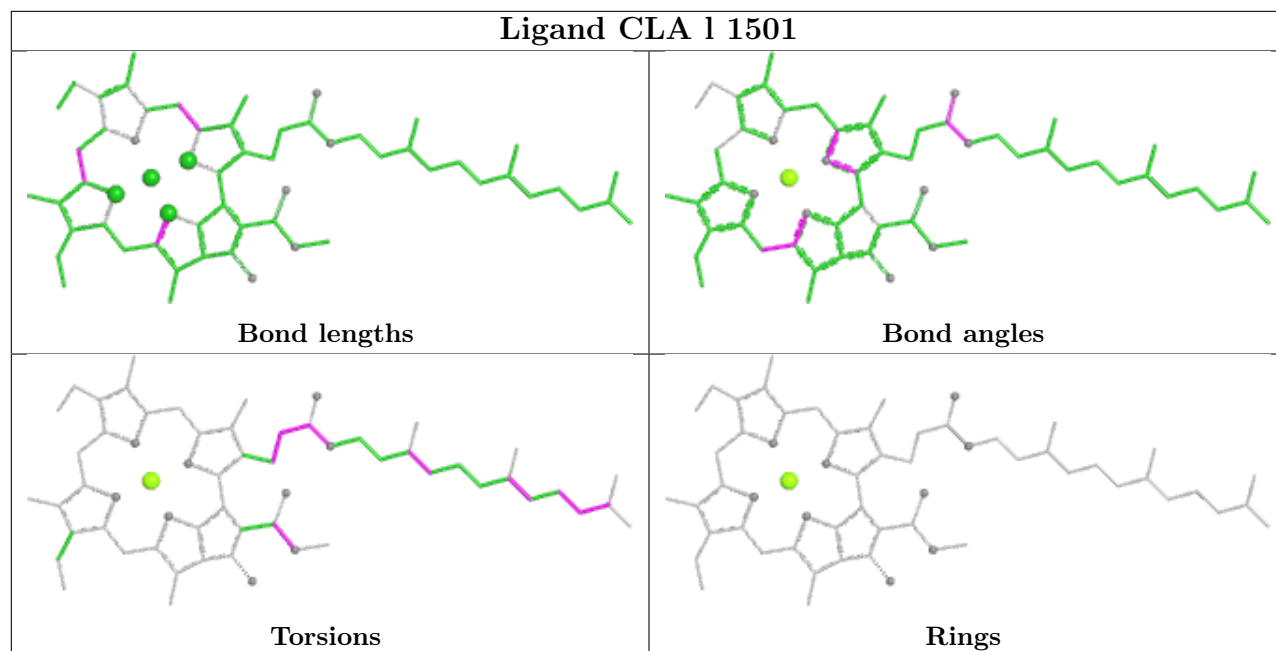


## Ligand CLA a 1109

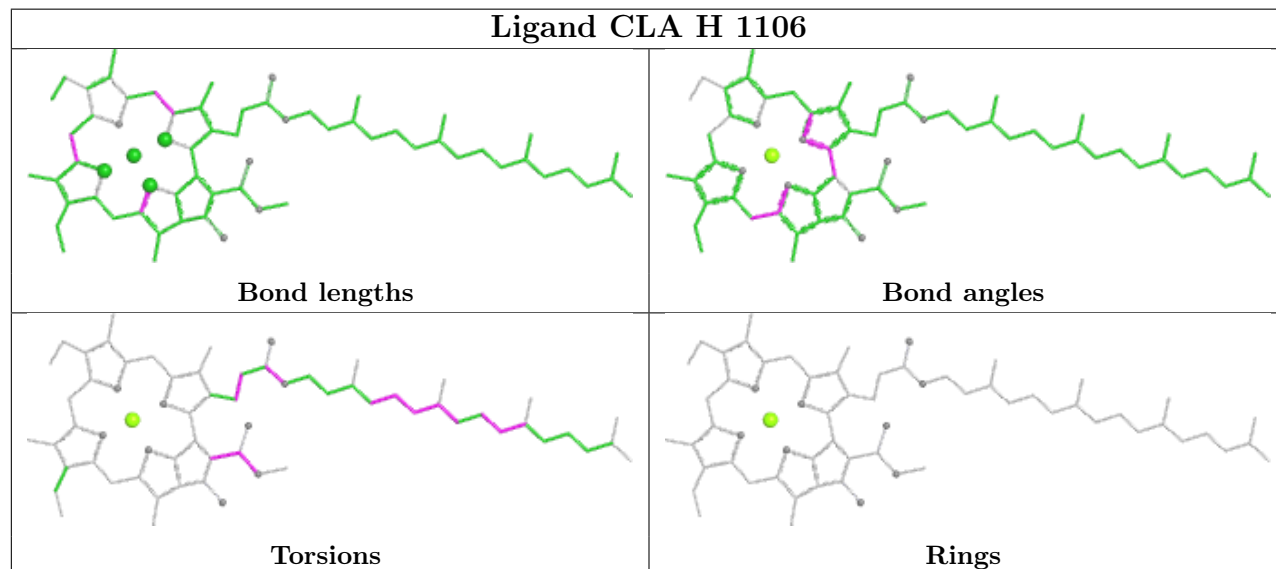




## Ligand CLA 1 1501

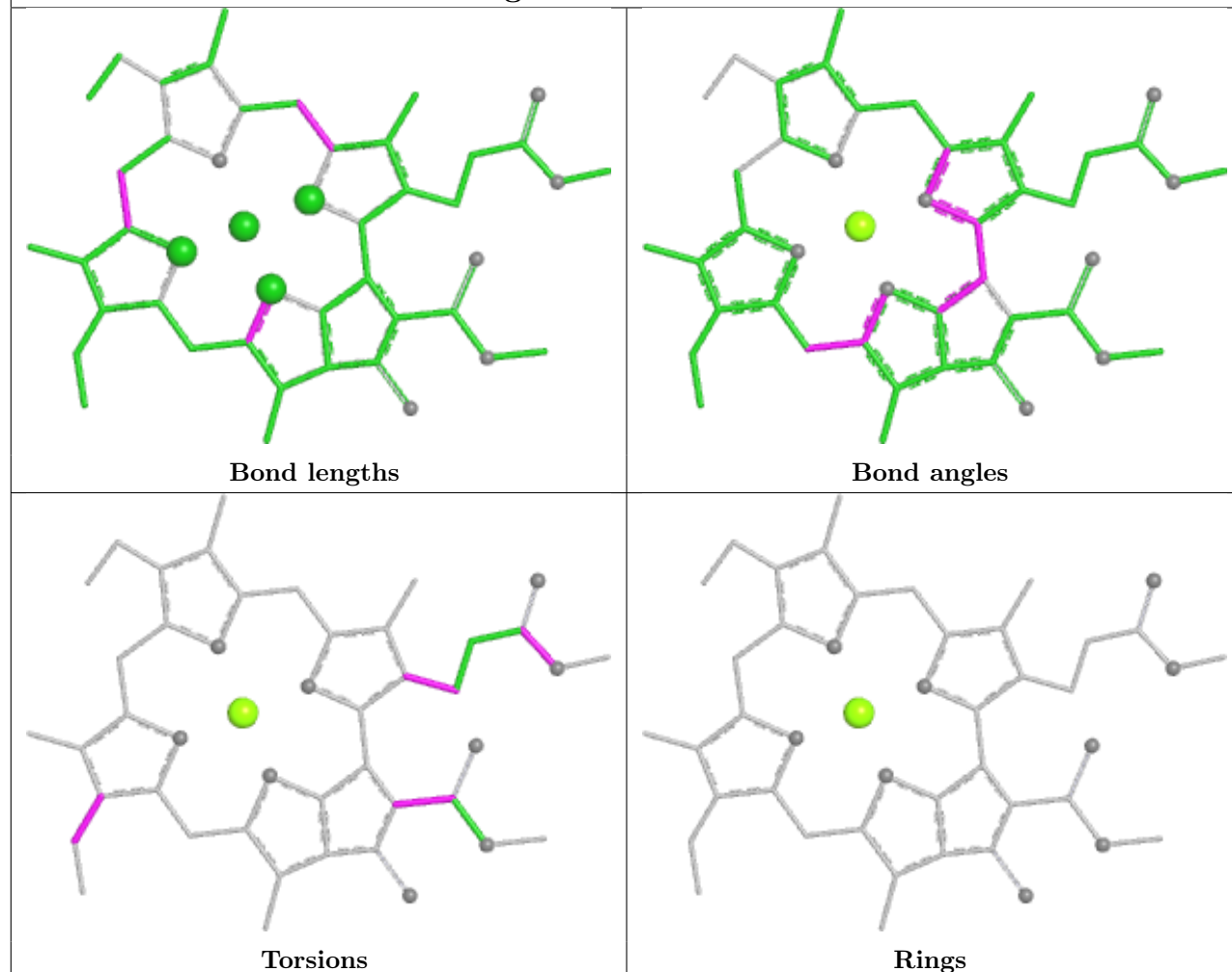


## Ligand CLA H 1106

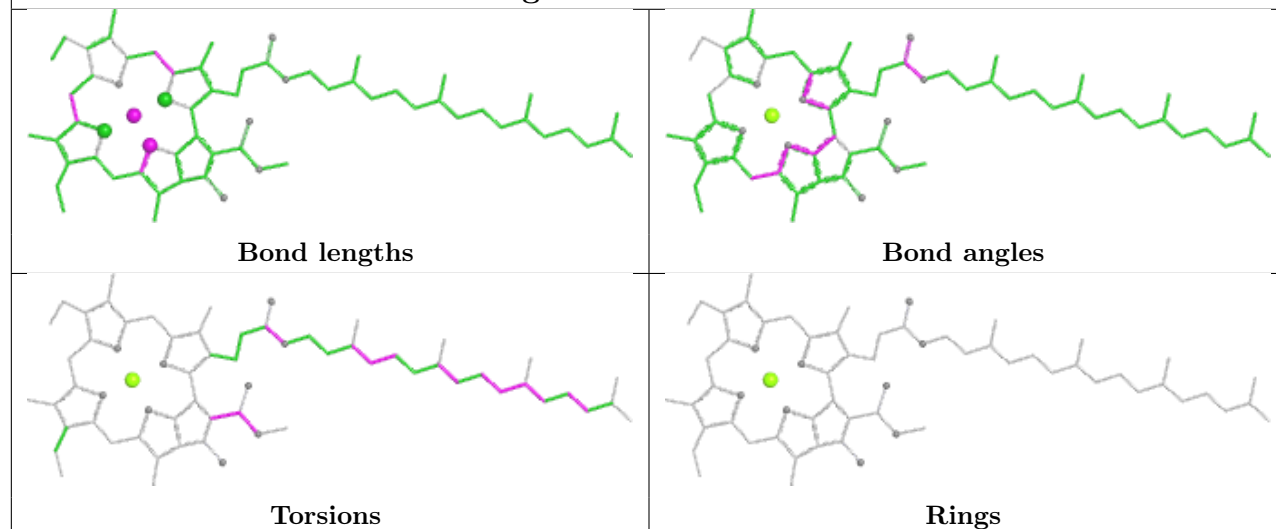




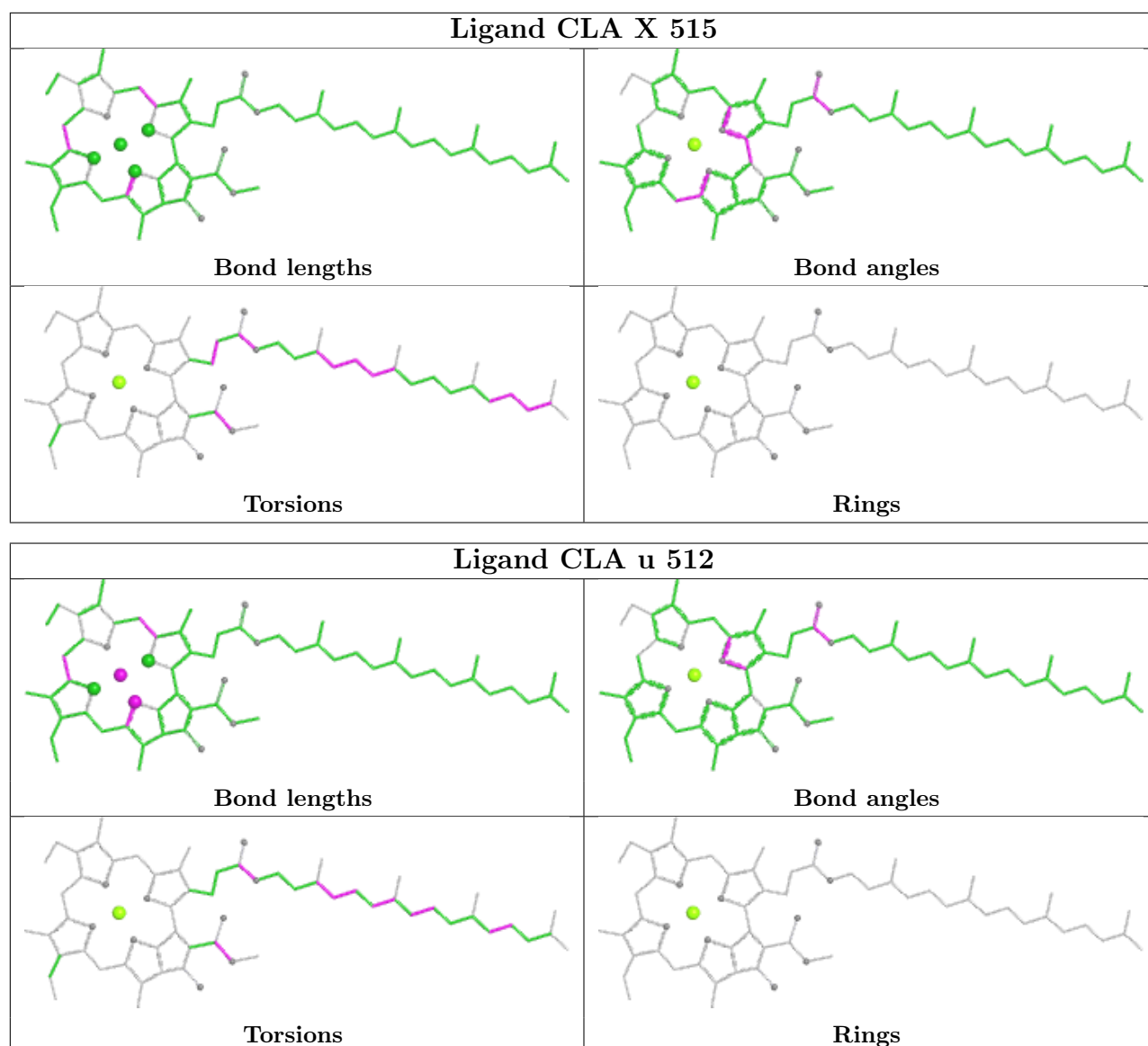
## Ligand CLA A 1114



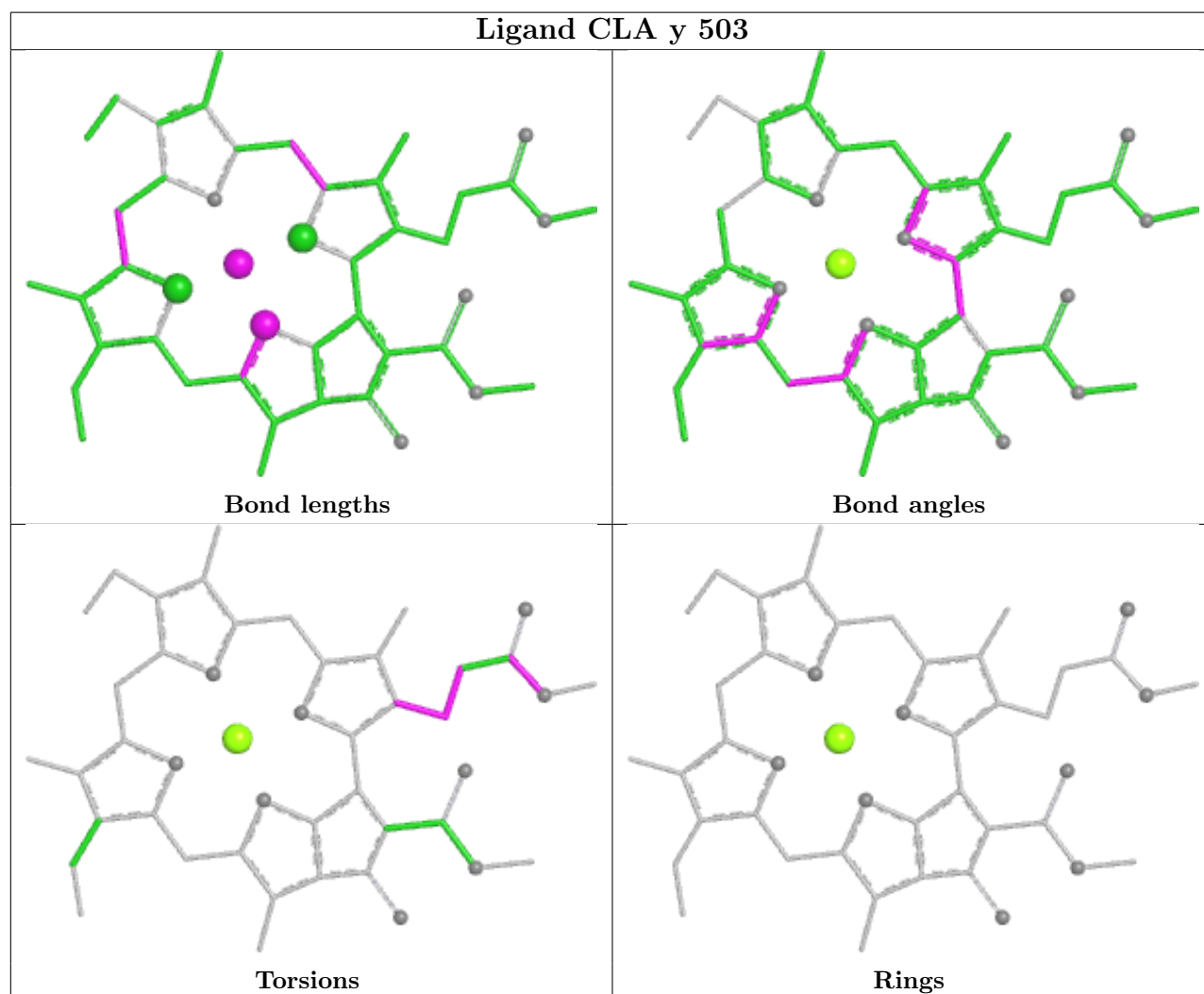
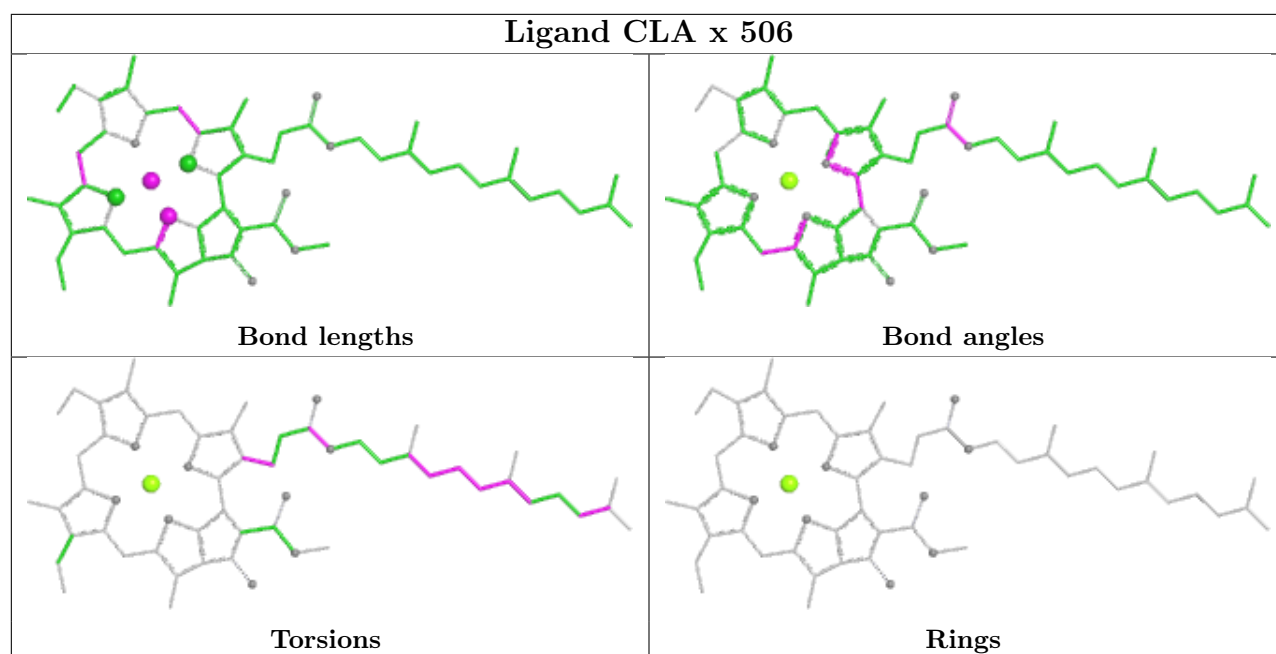
## Ligand CLA H 1104



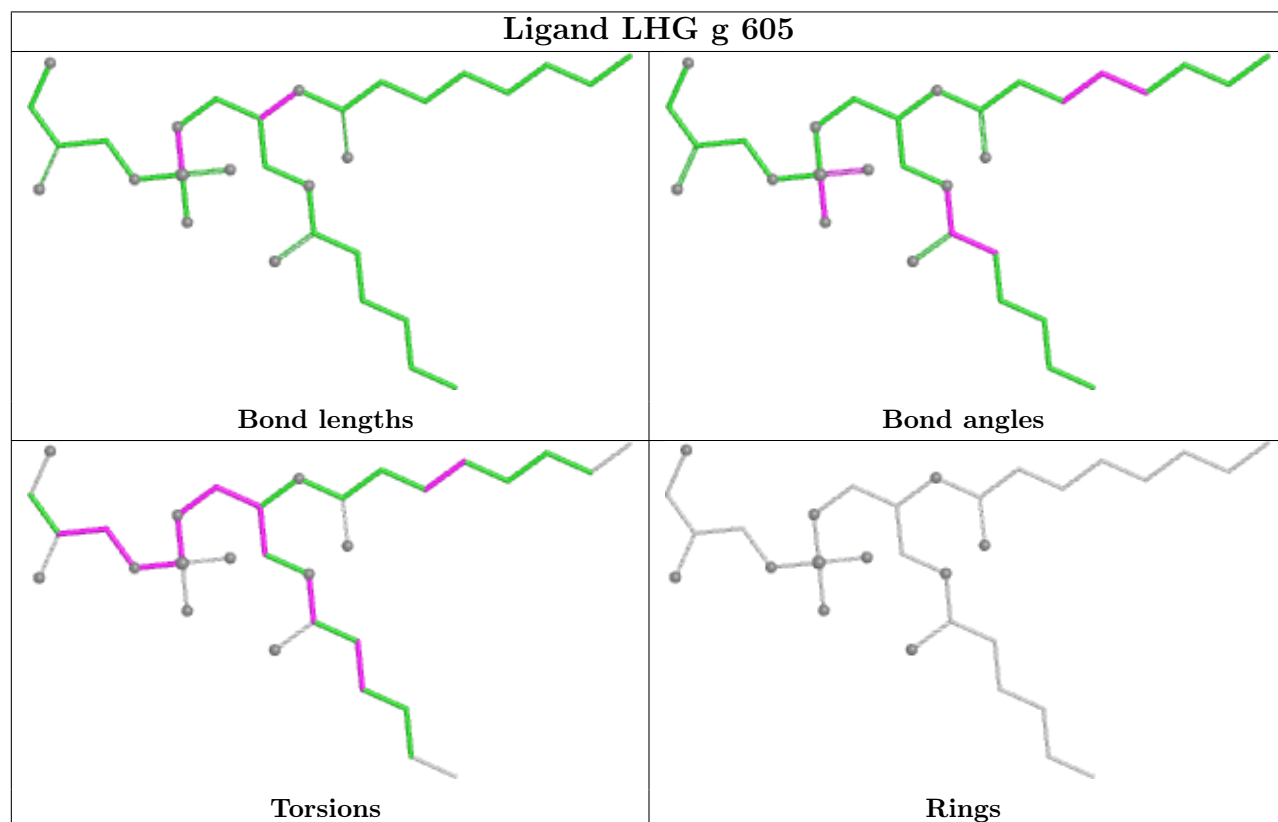
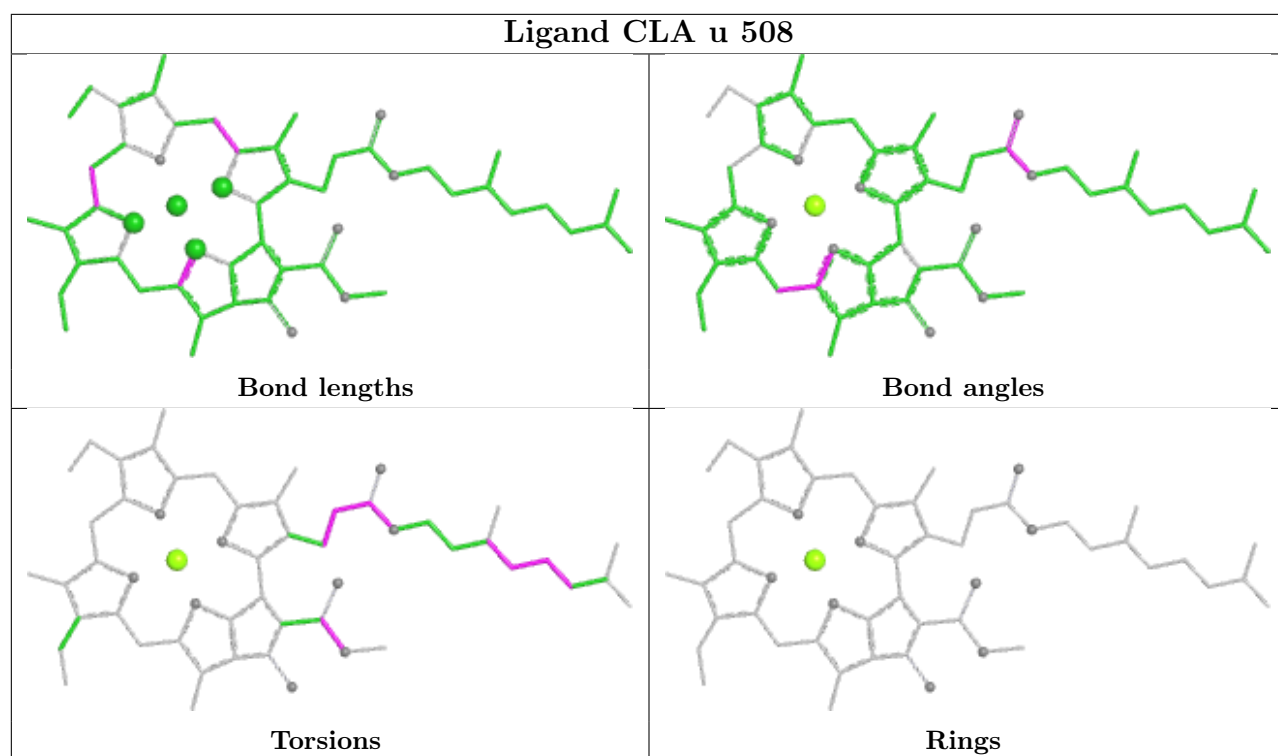




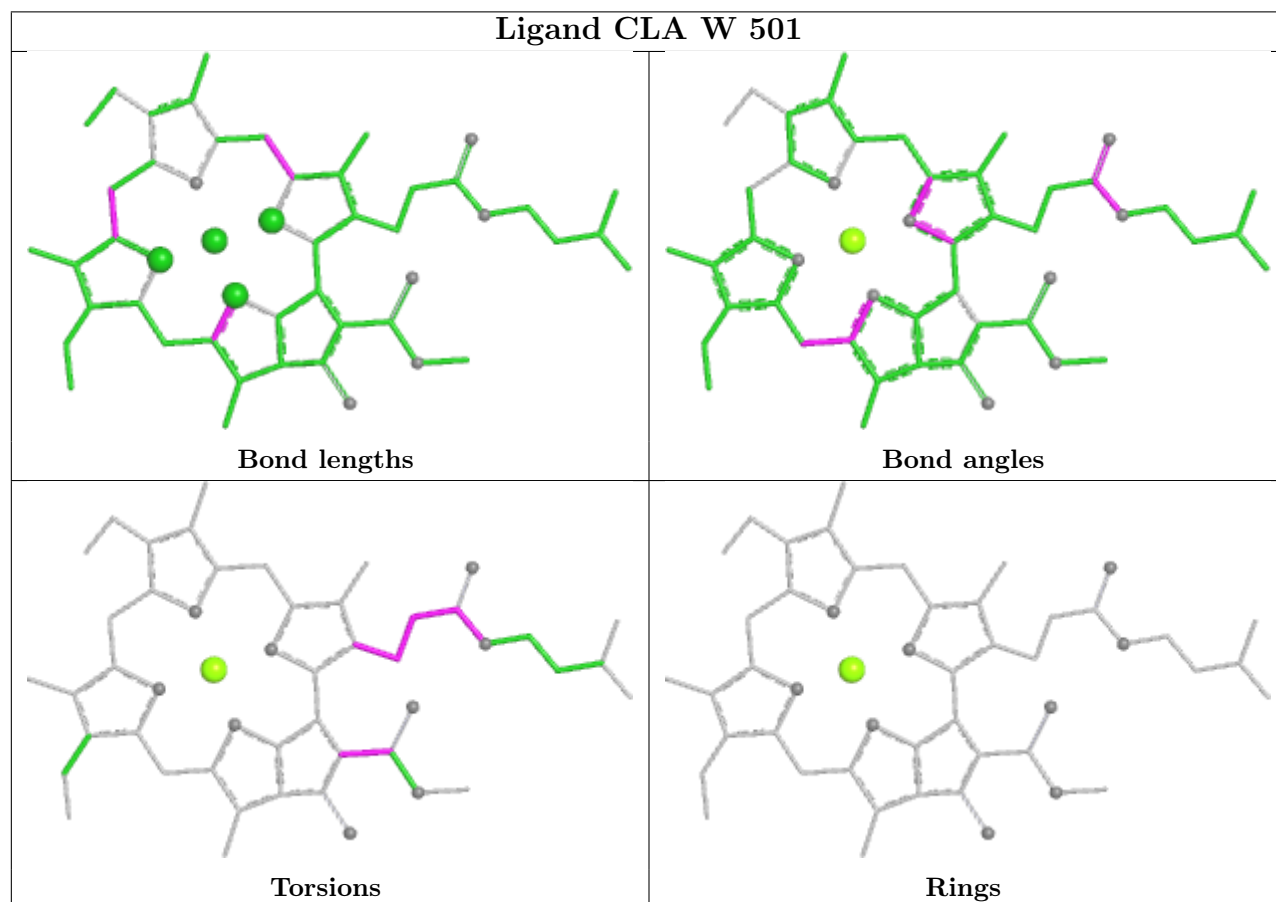
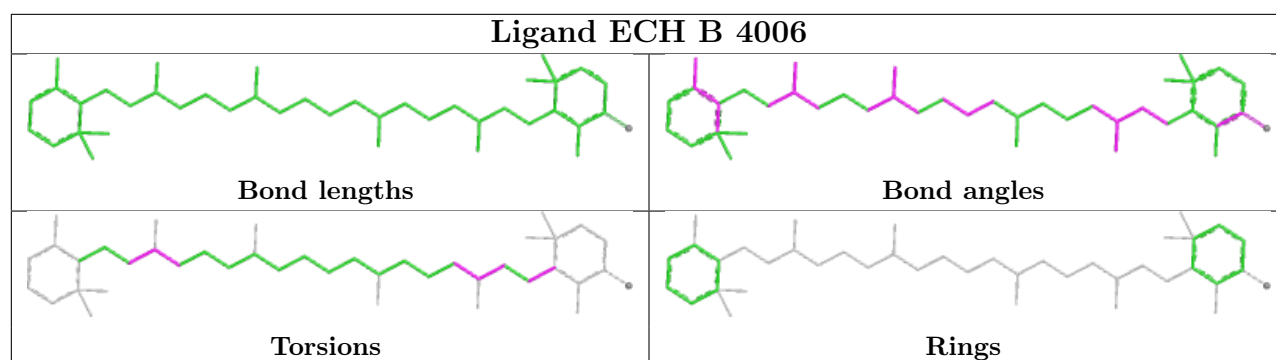




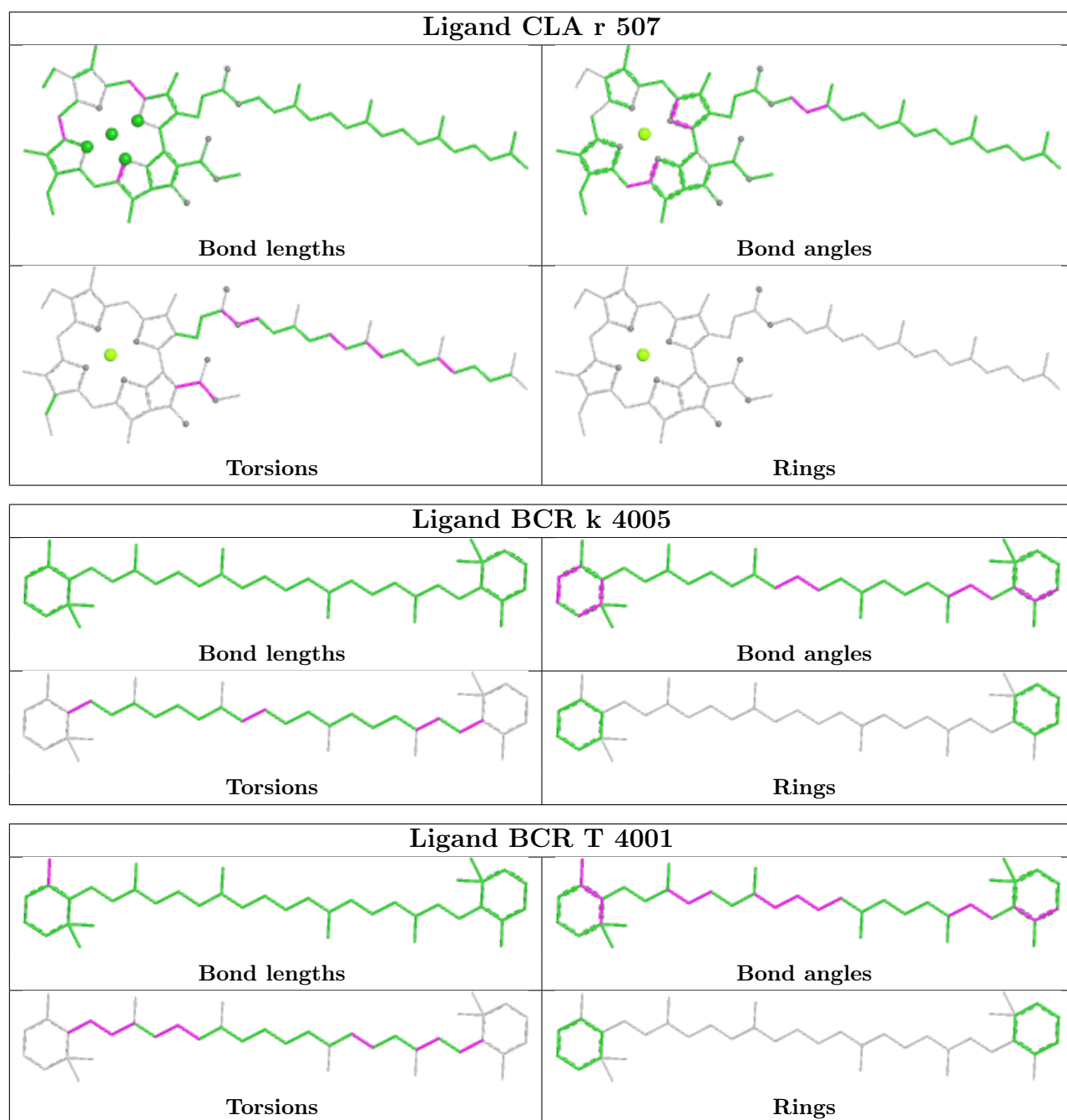




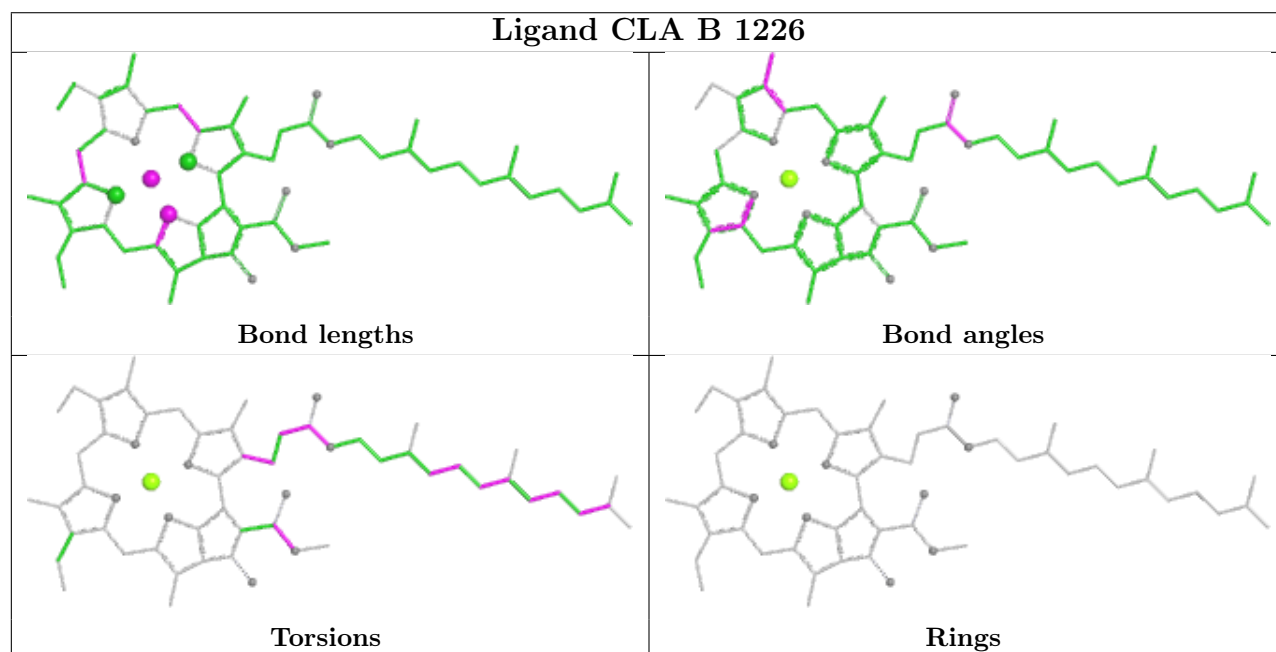
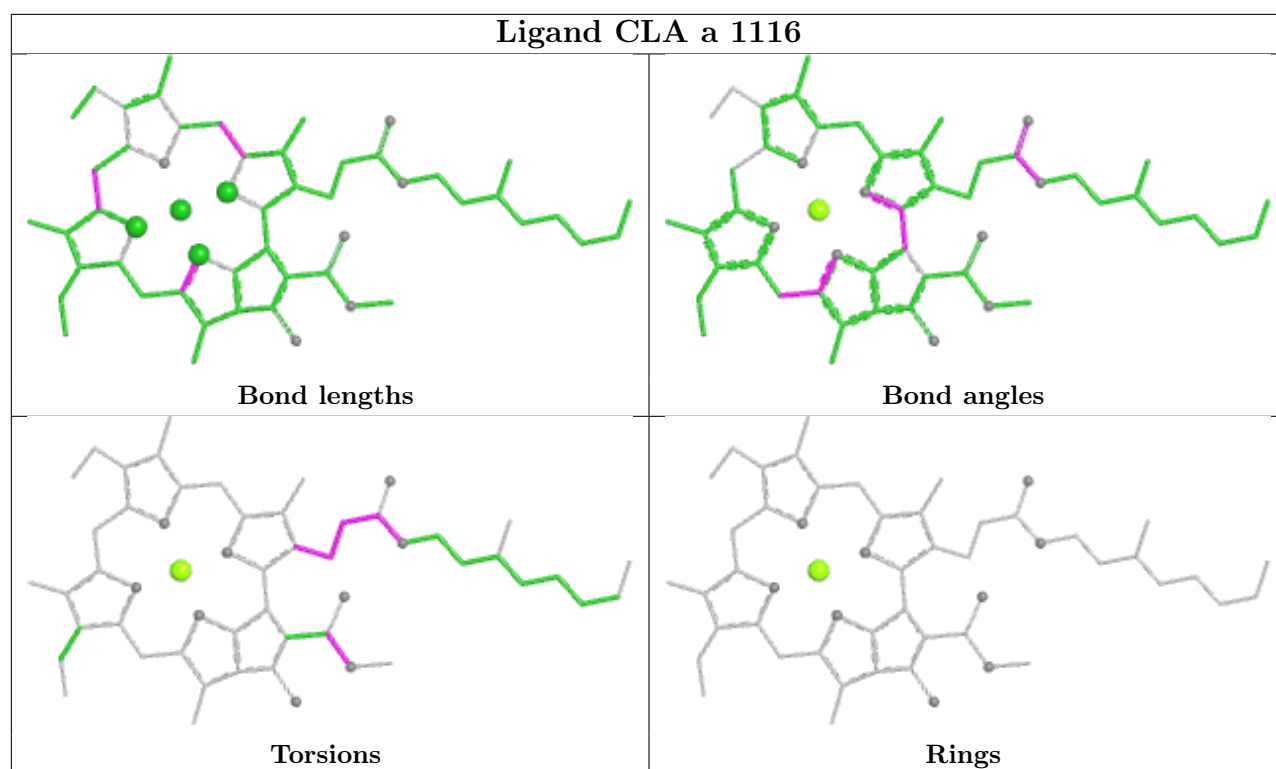




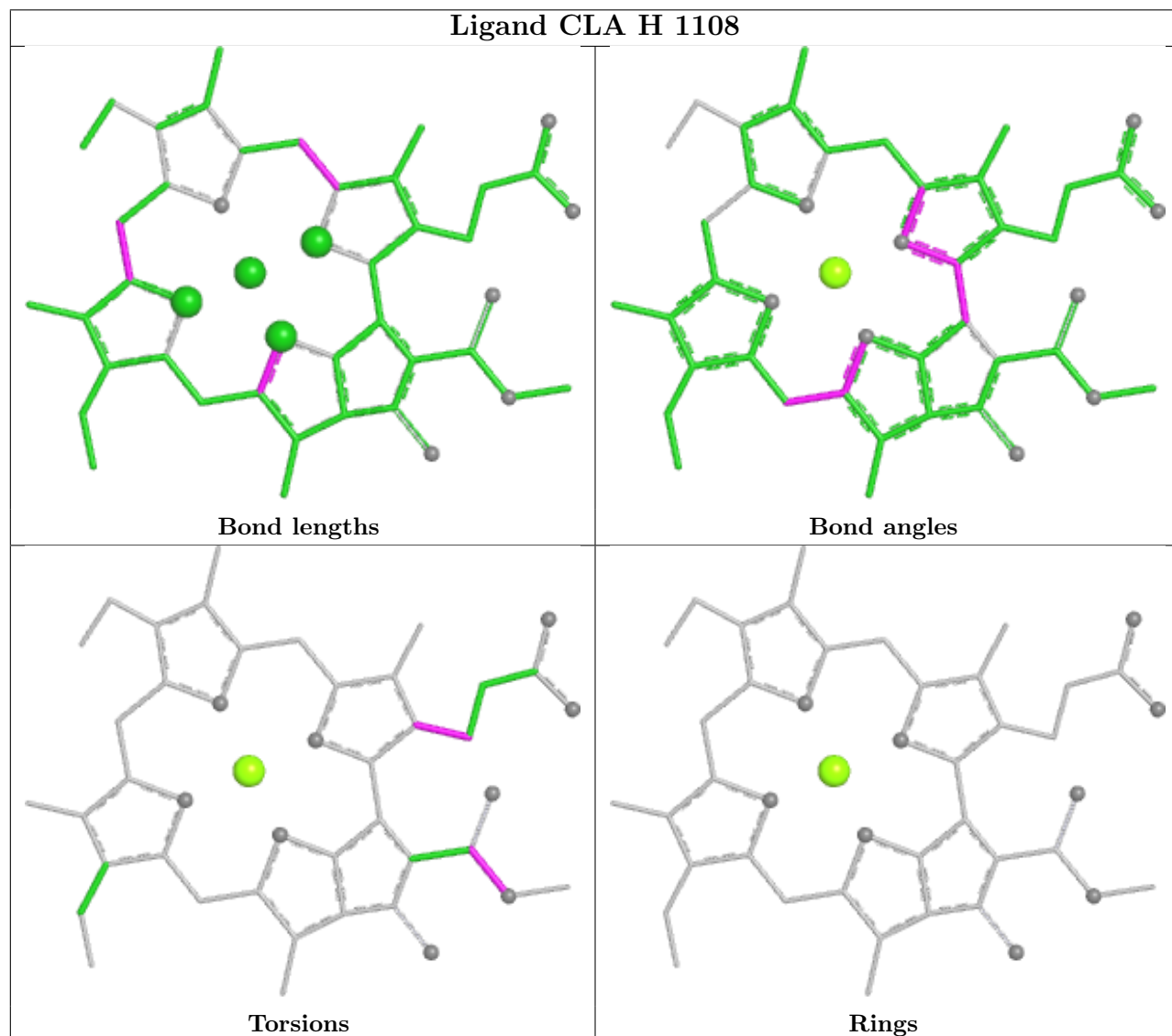
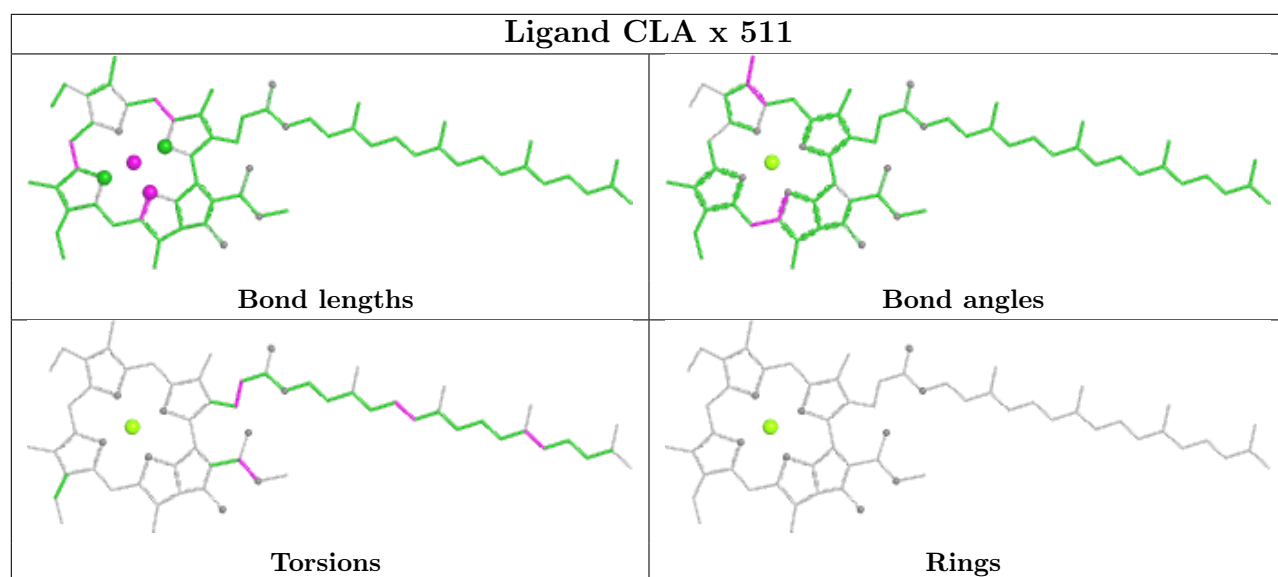




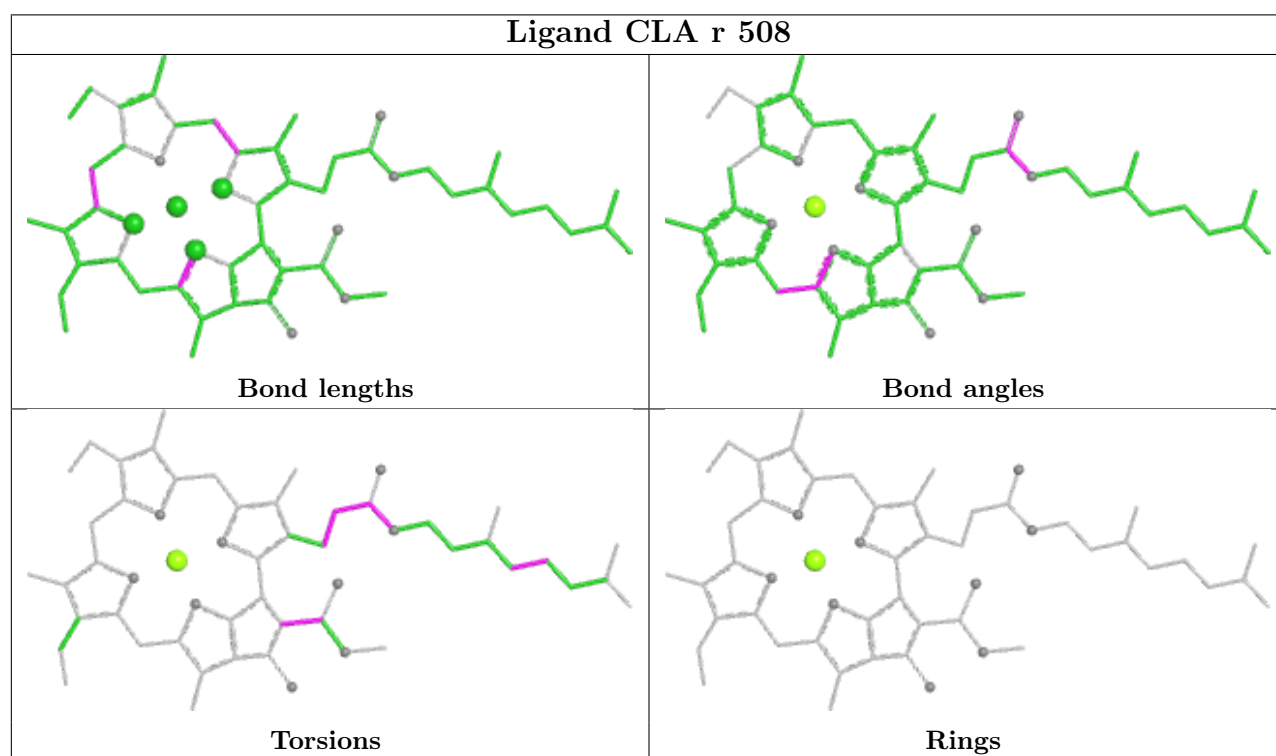
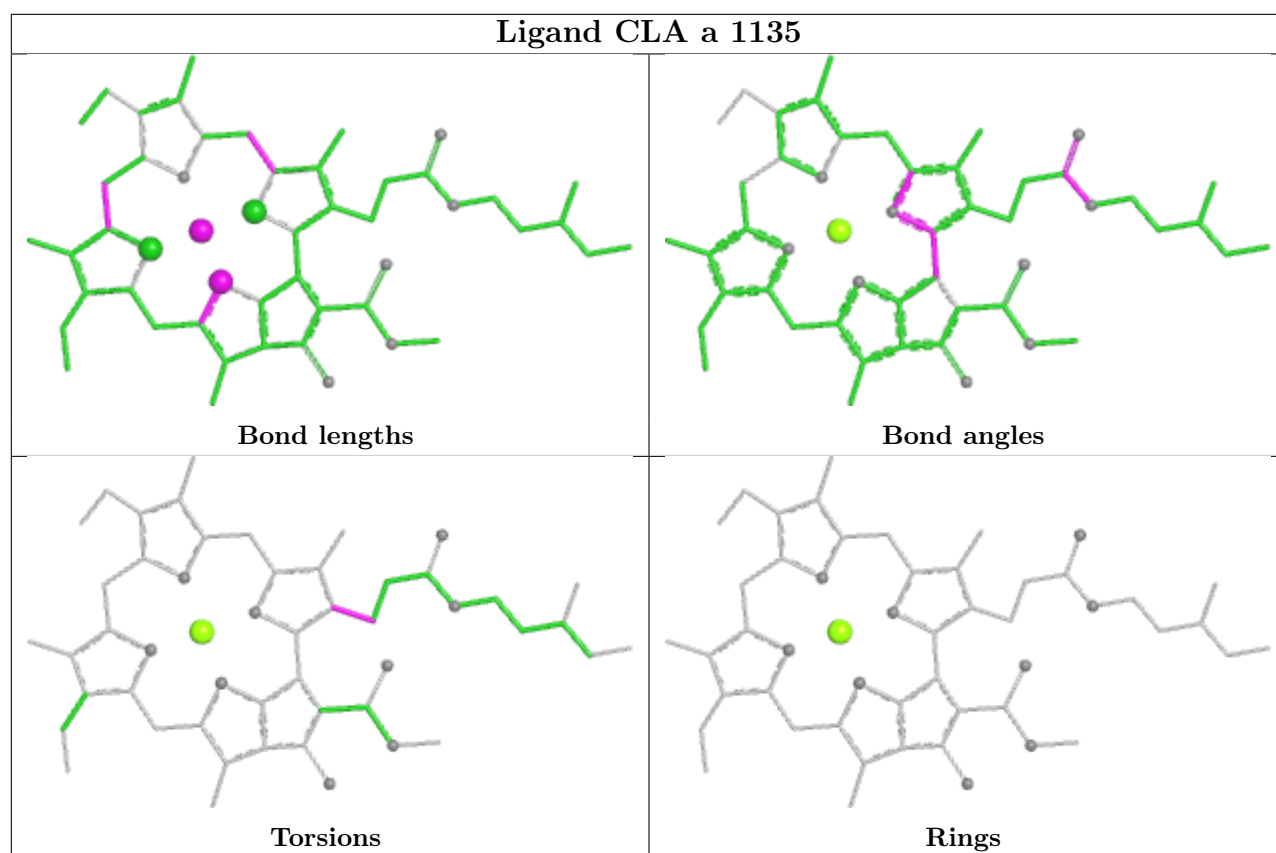




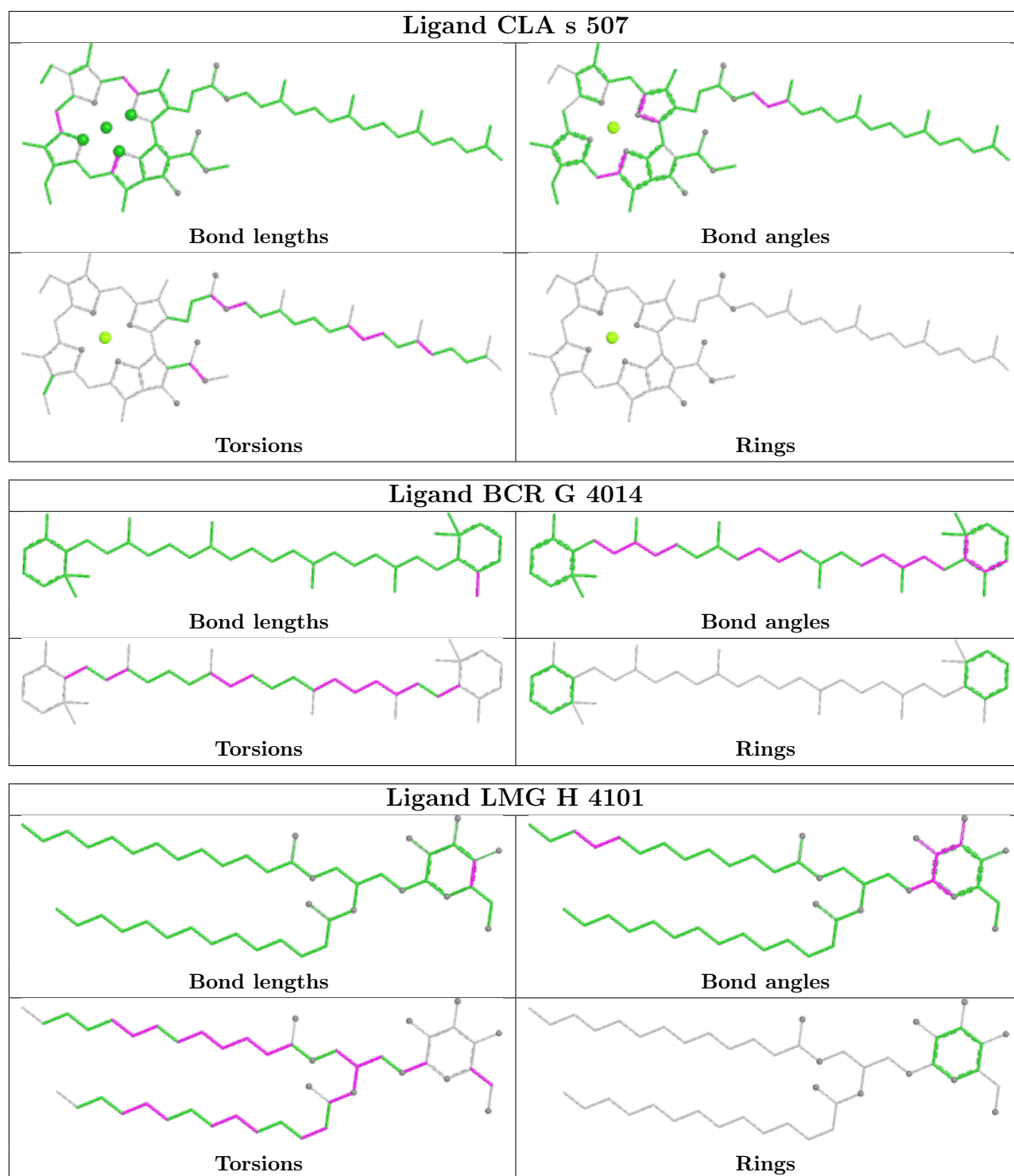




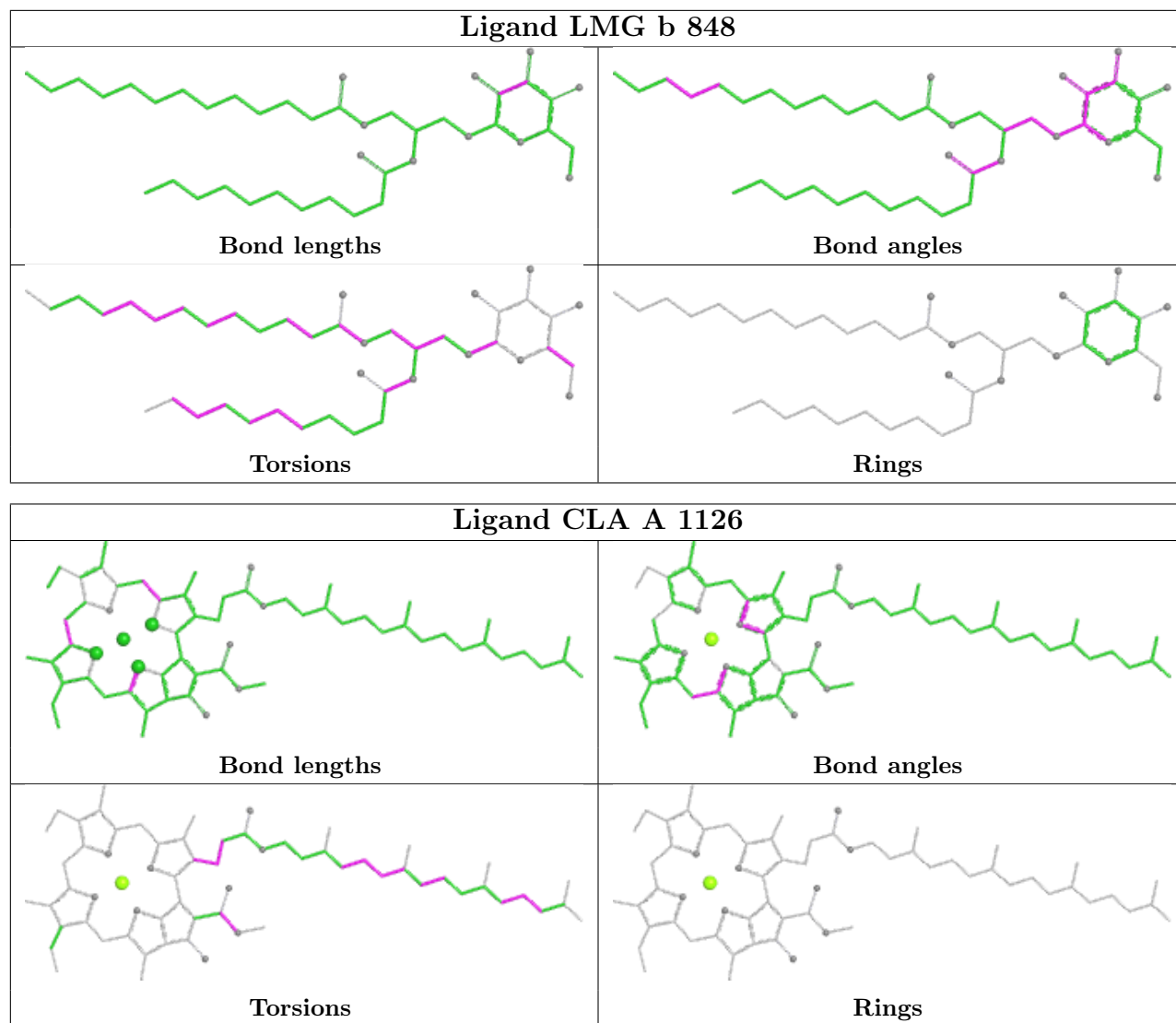






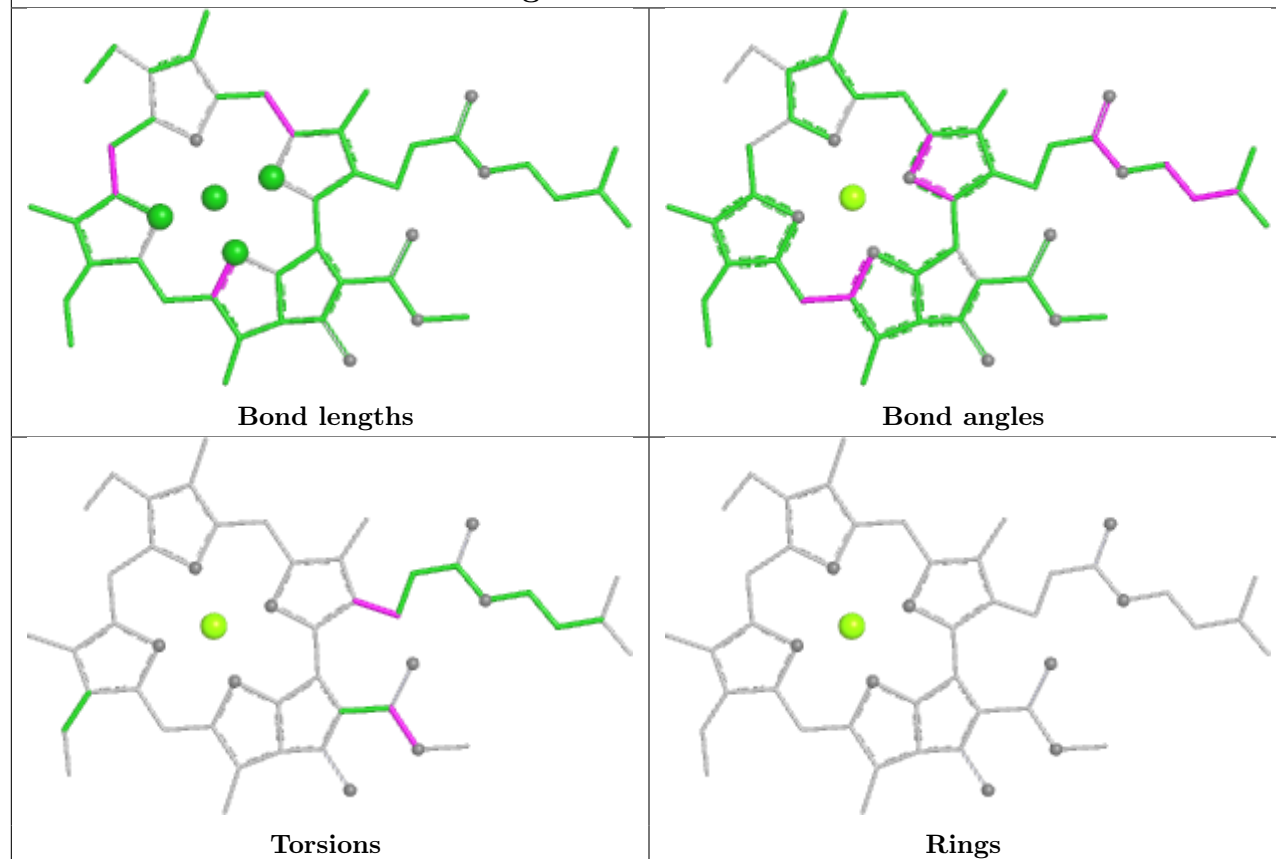




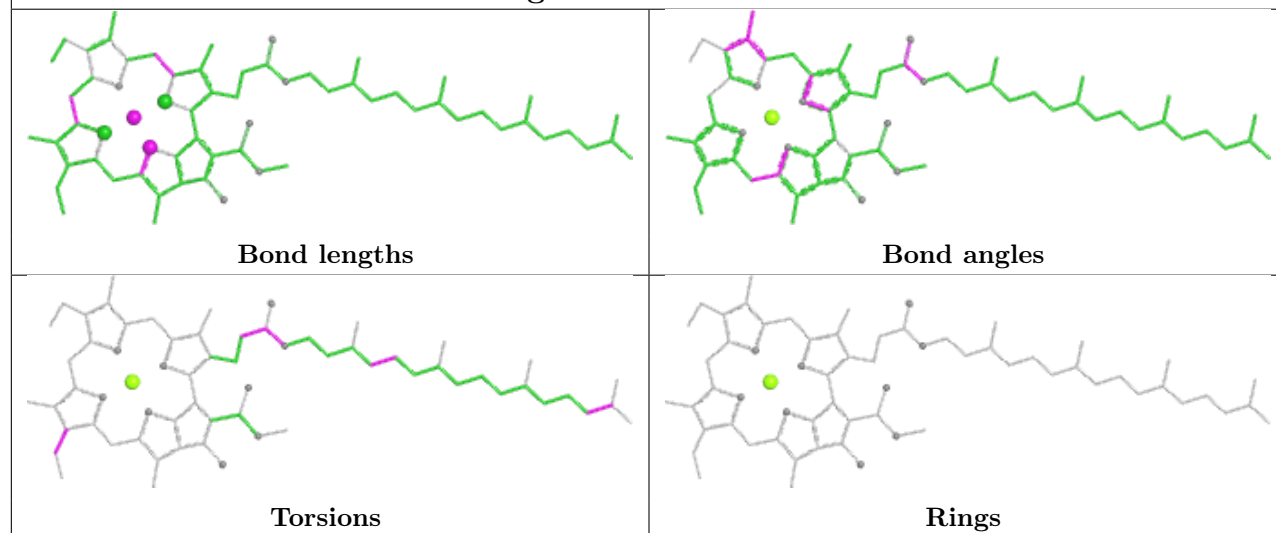




## Ligand CLA H 1107

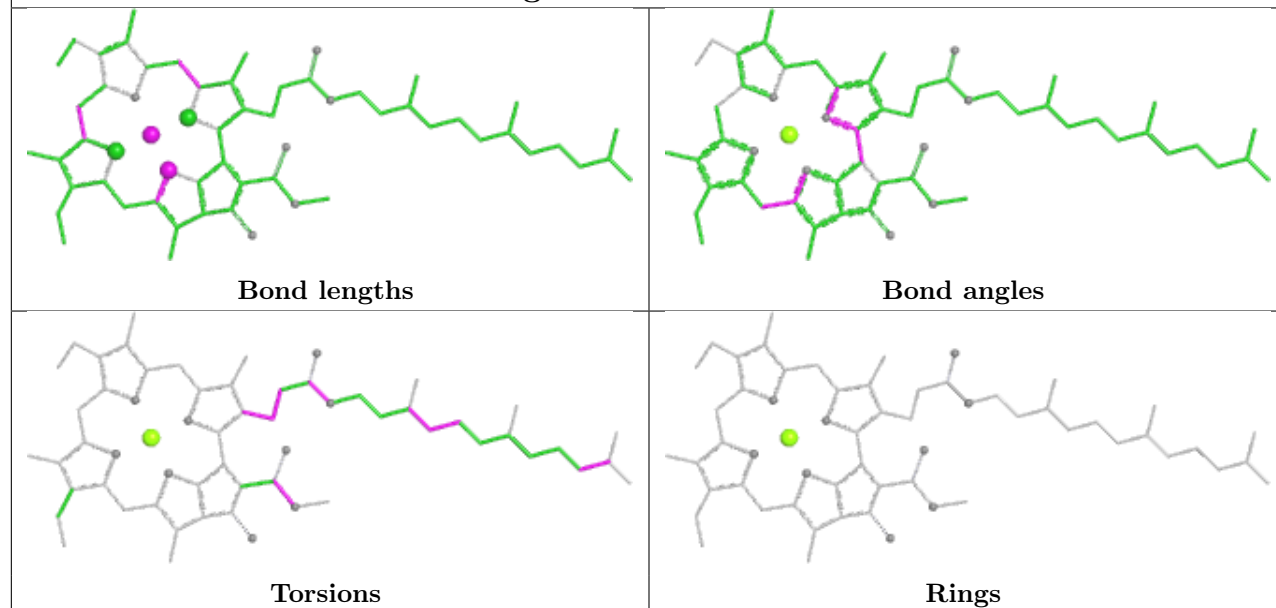


## Ligand CL0 A 1011

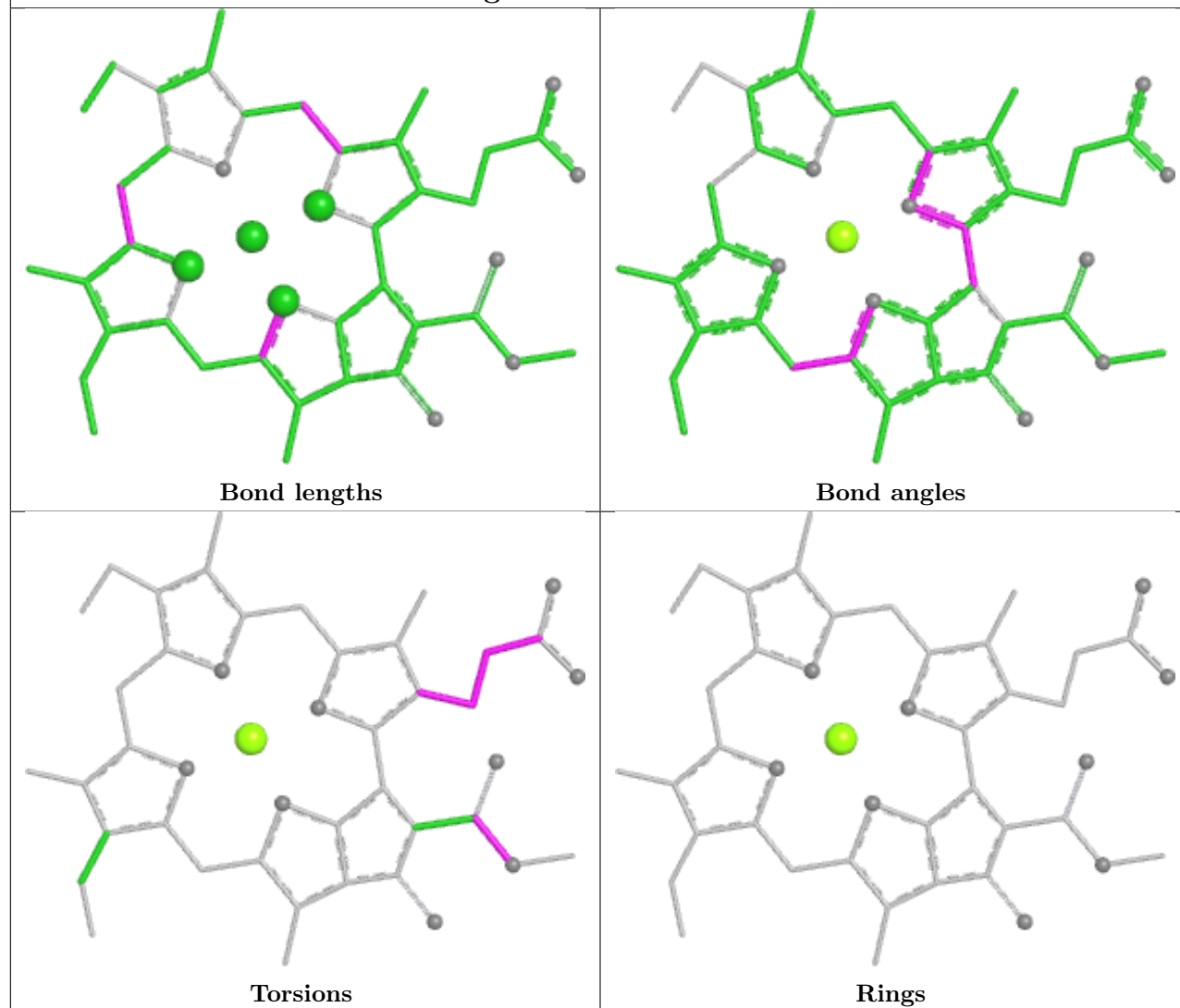




## Ligand CLA B 1224

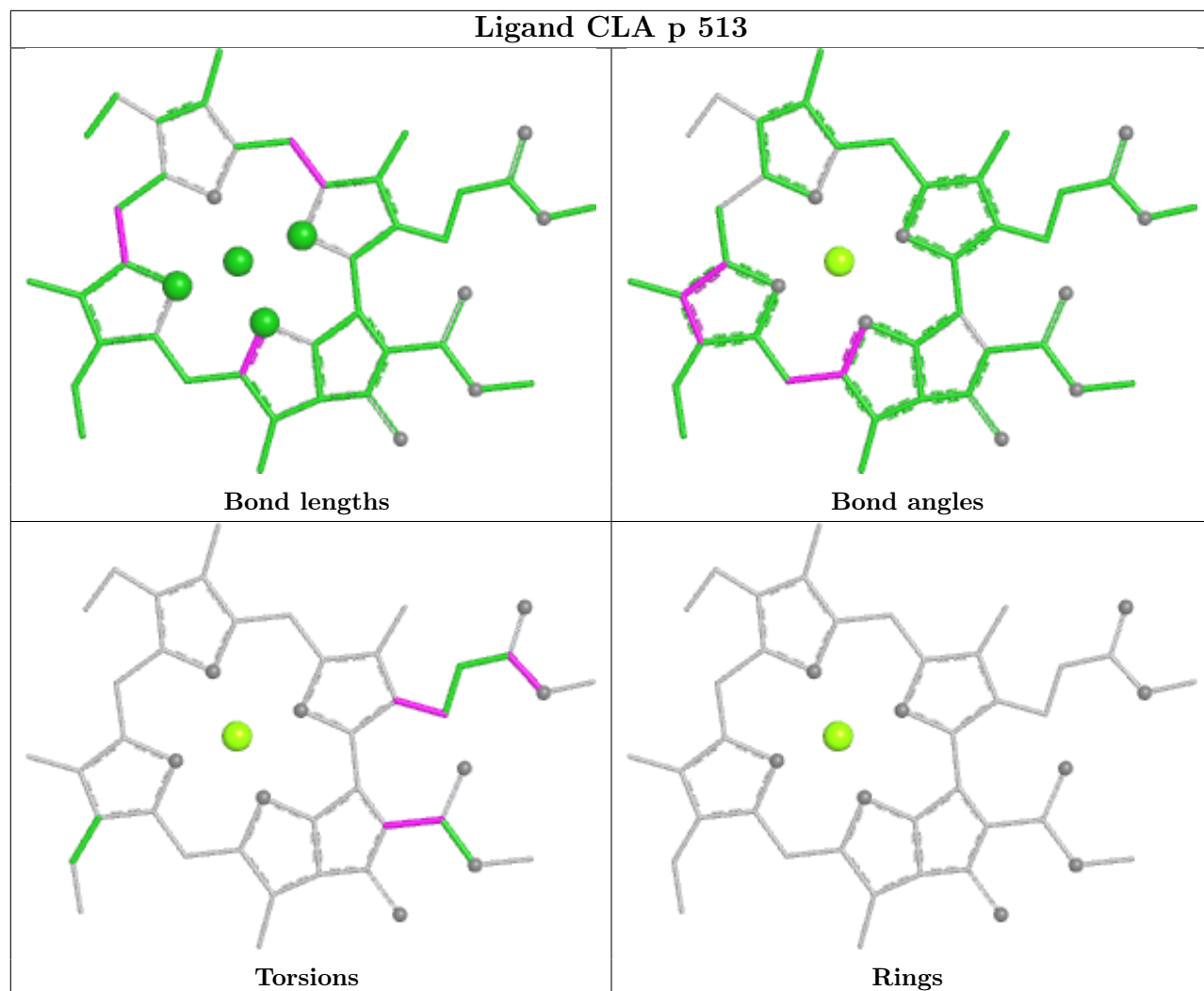


## Ligand CLA B 1231



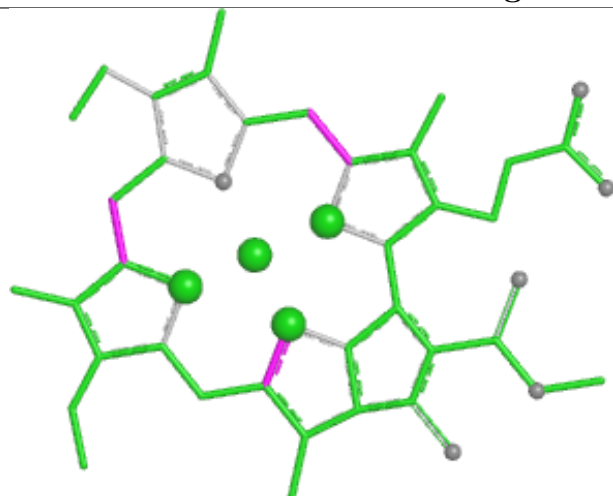


## Ligand CLA p 513

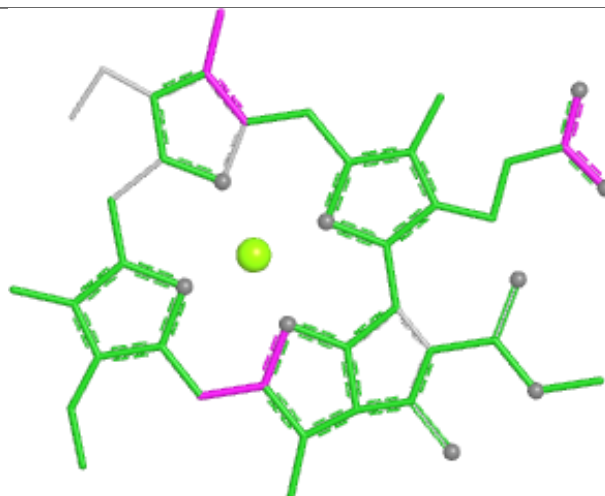




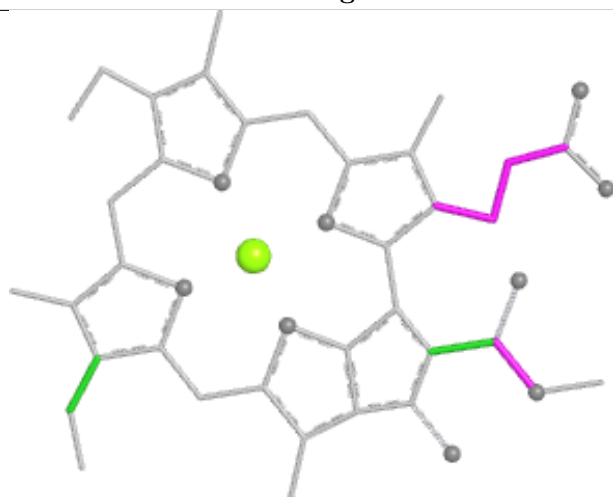
## Ligand CLA G 1219



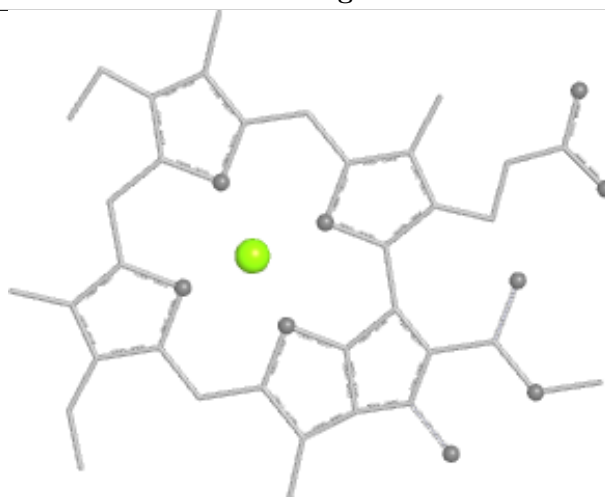
Bond lengths



Bond angles

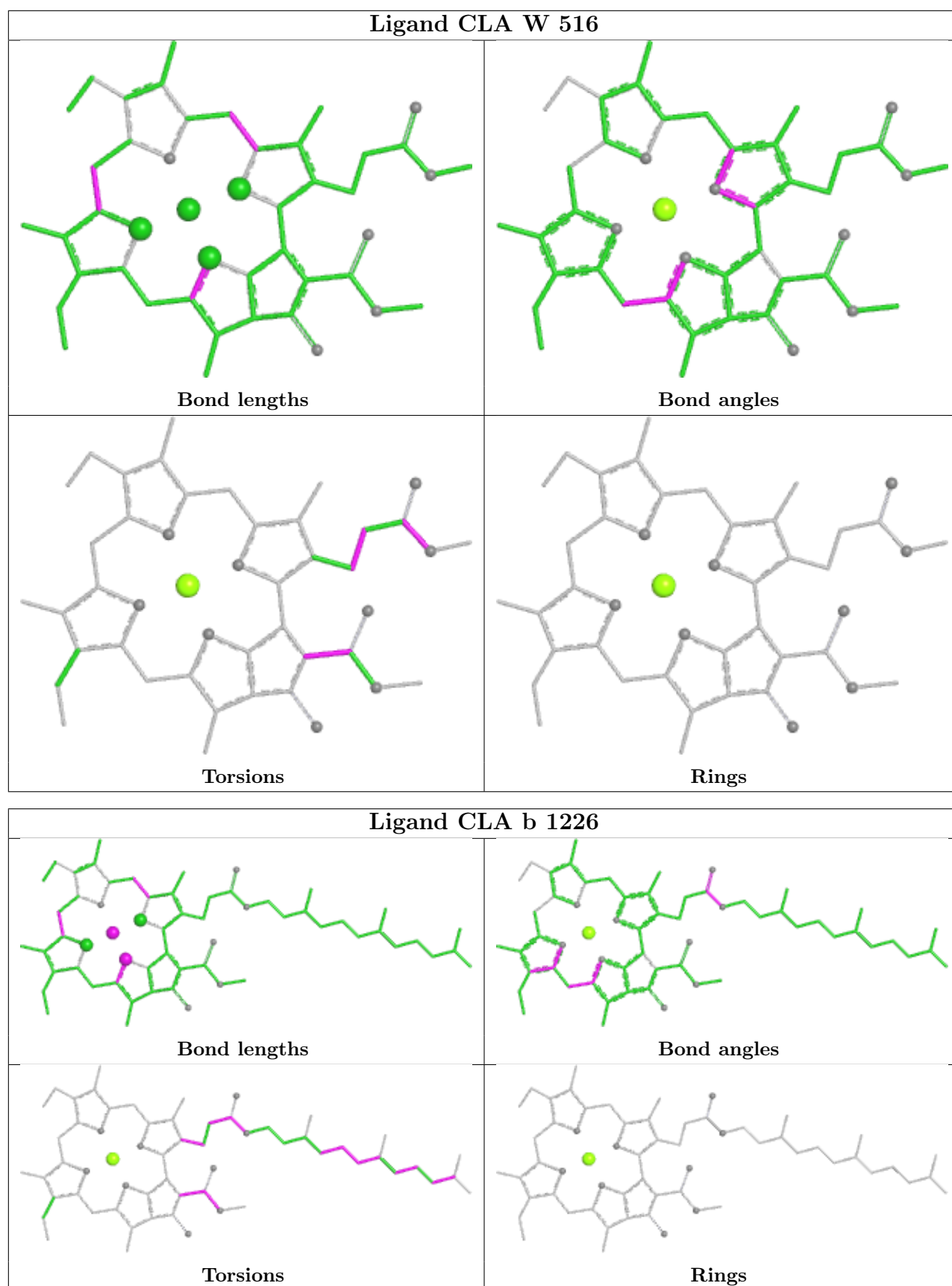


Torsions

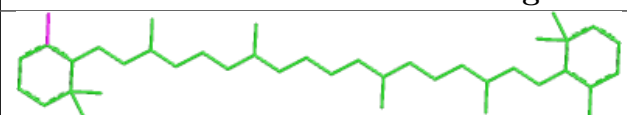
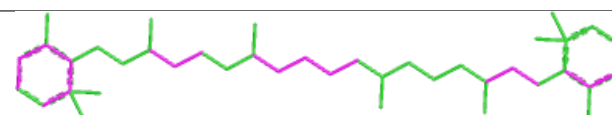
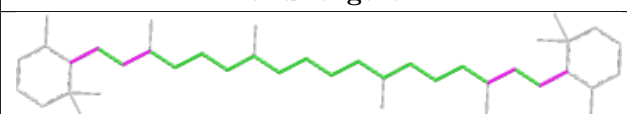
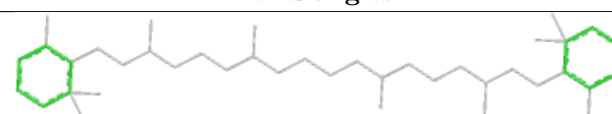



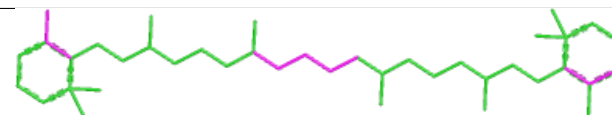
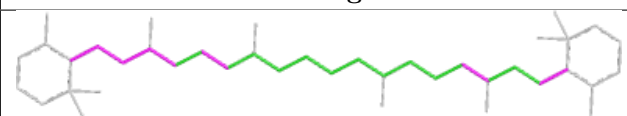
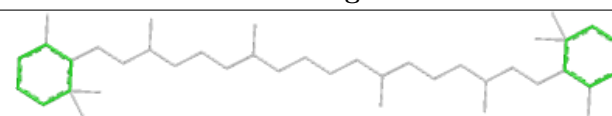
Rings

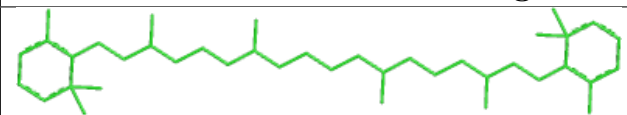
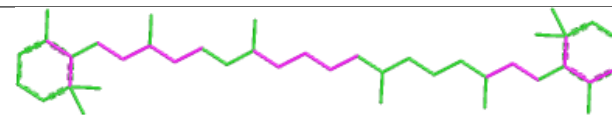
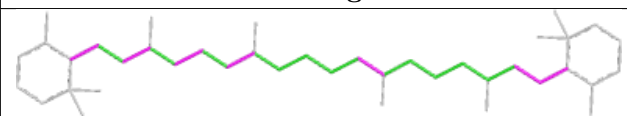
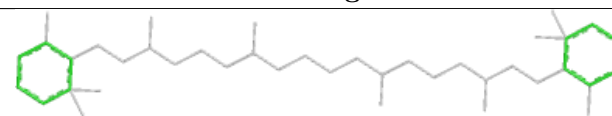




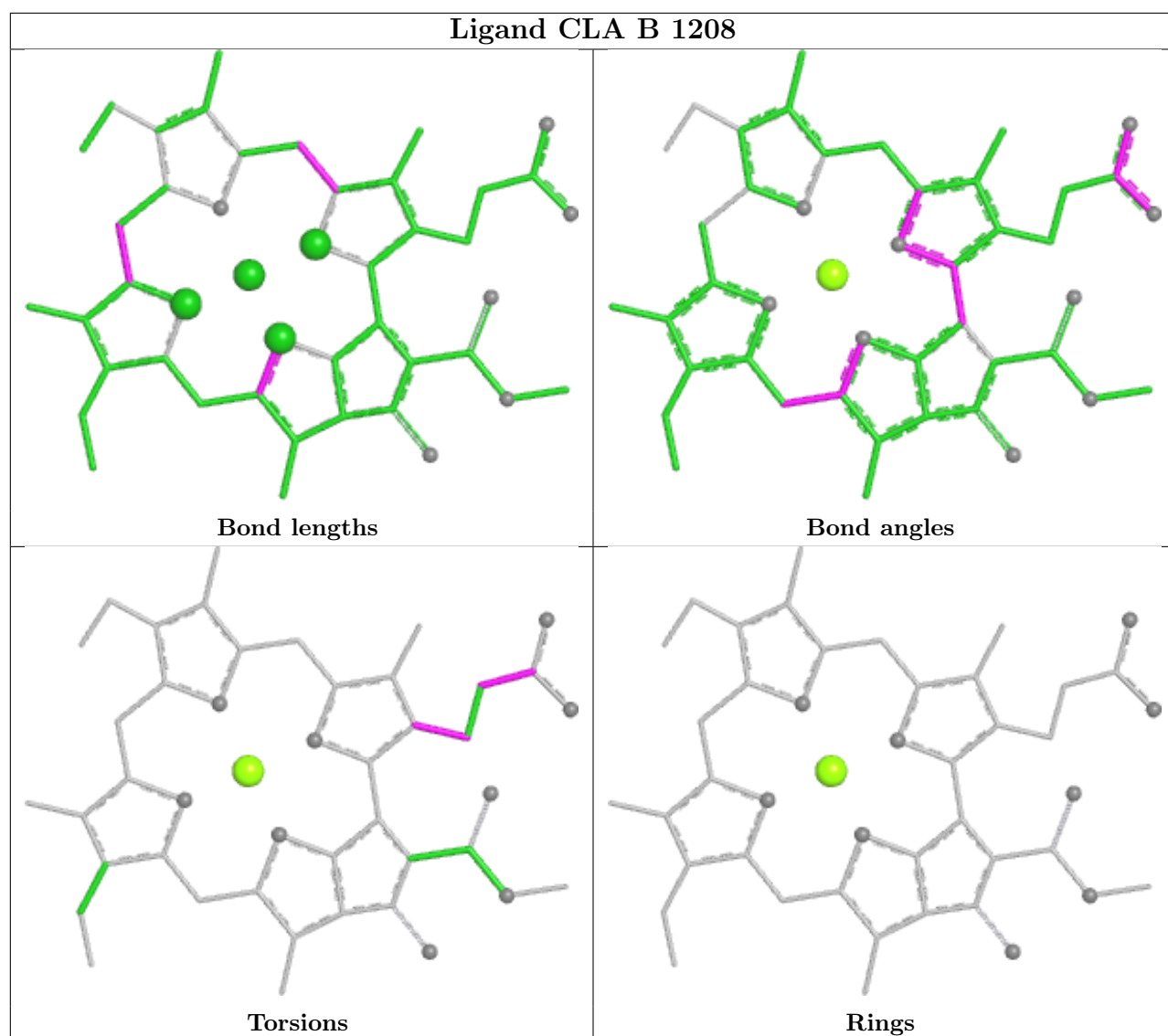


Ligand BCR u 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR t 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

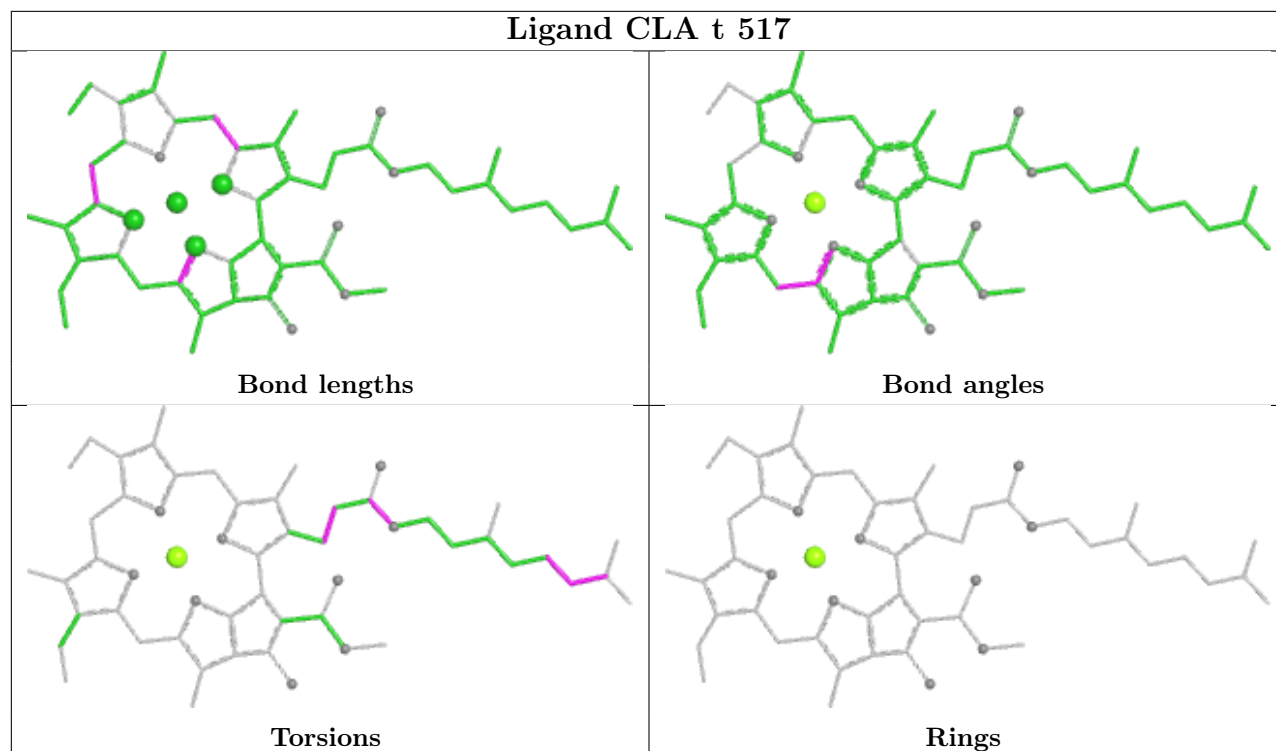
Ligand BCR S 4015	
	
Bond lengths	Bond angles
	
Torsions	Rings



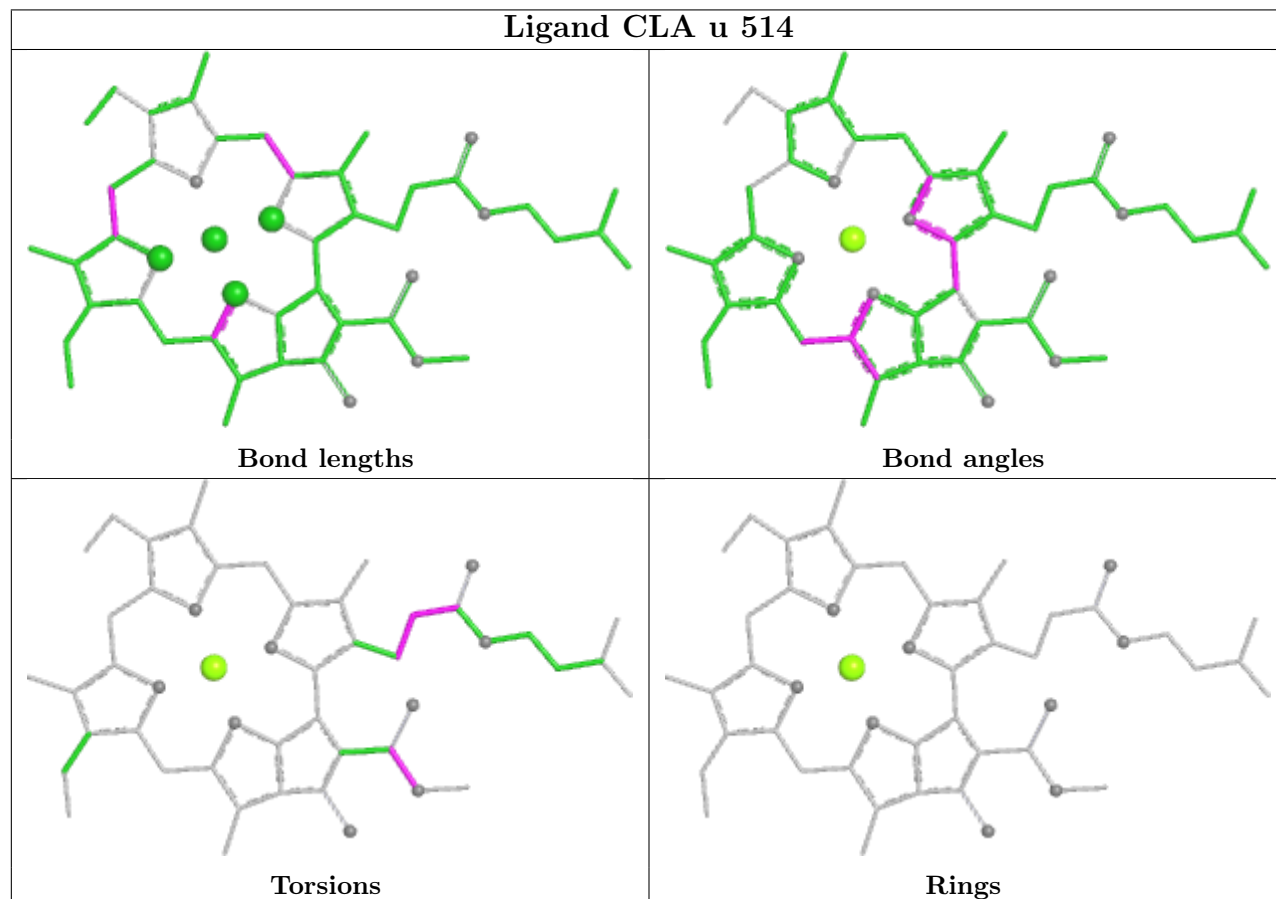




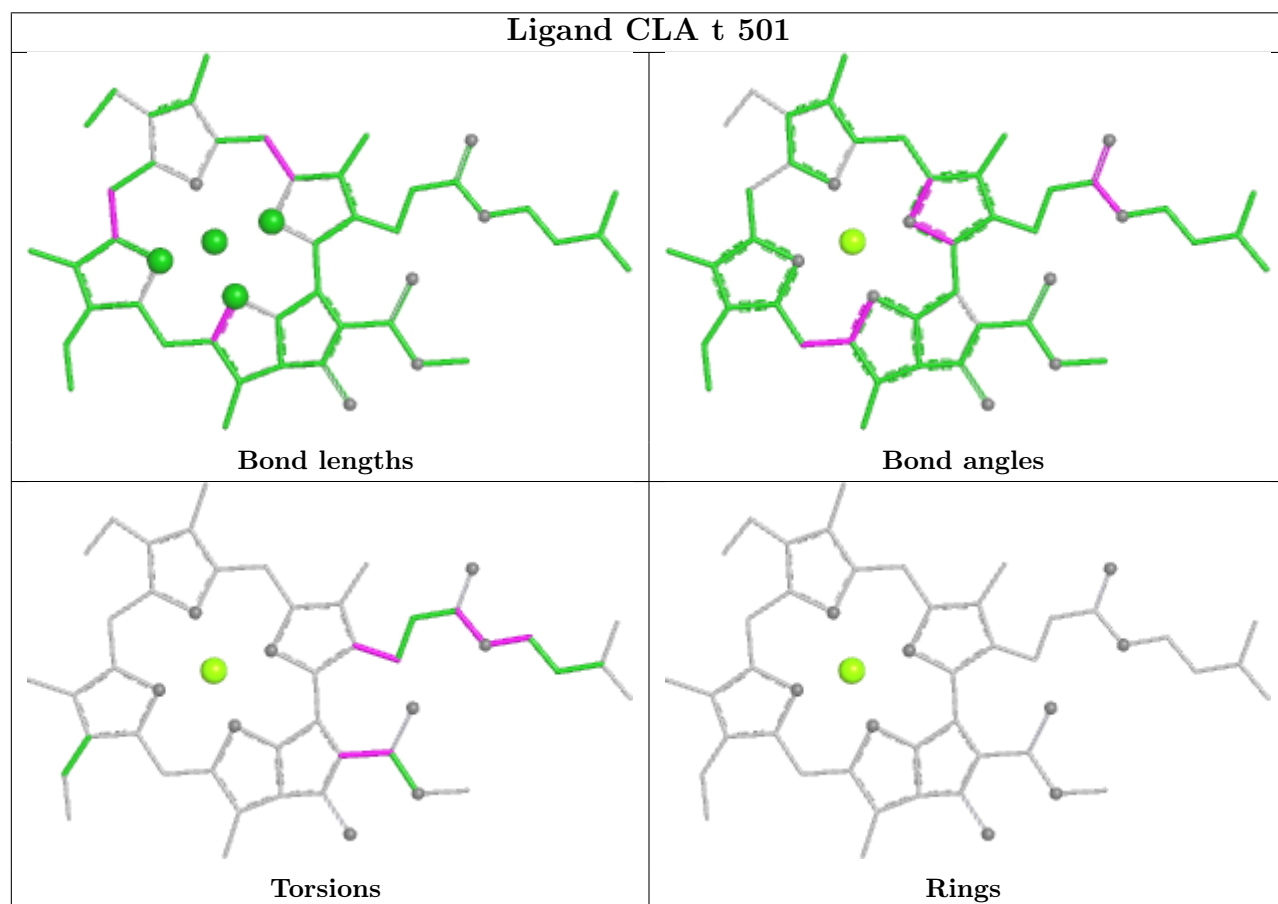
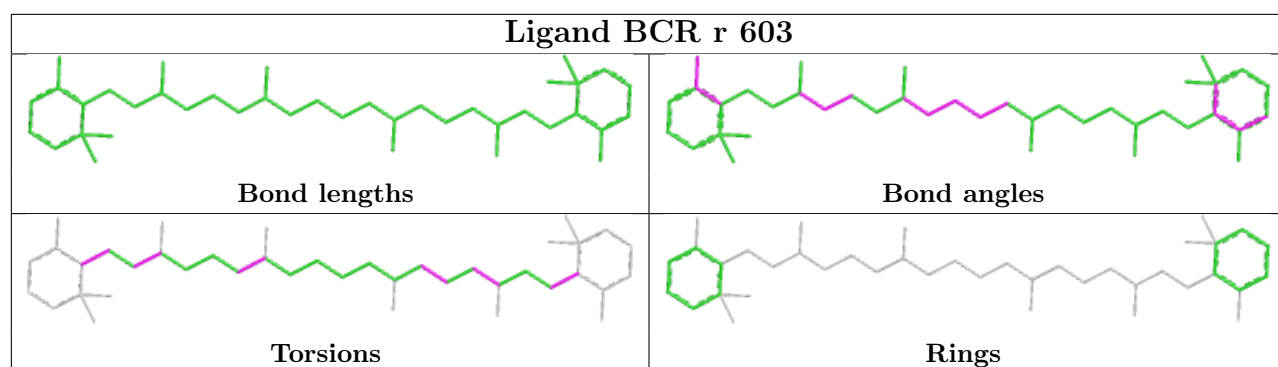
## Ligand CLA t 517



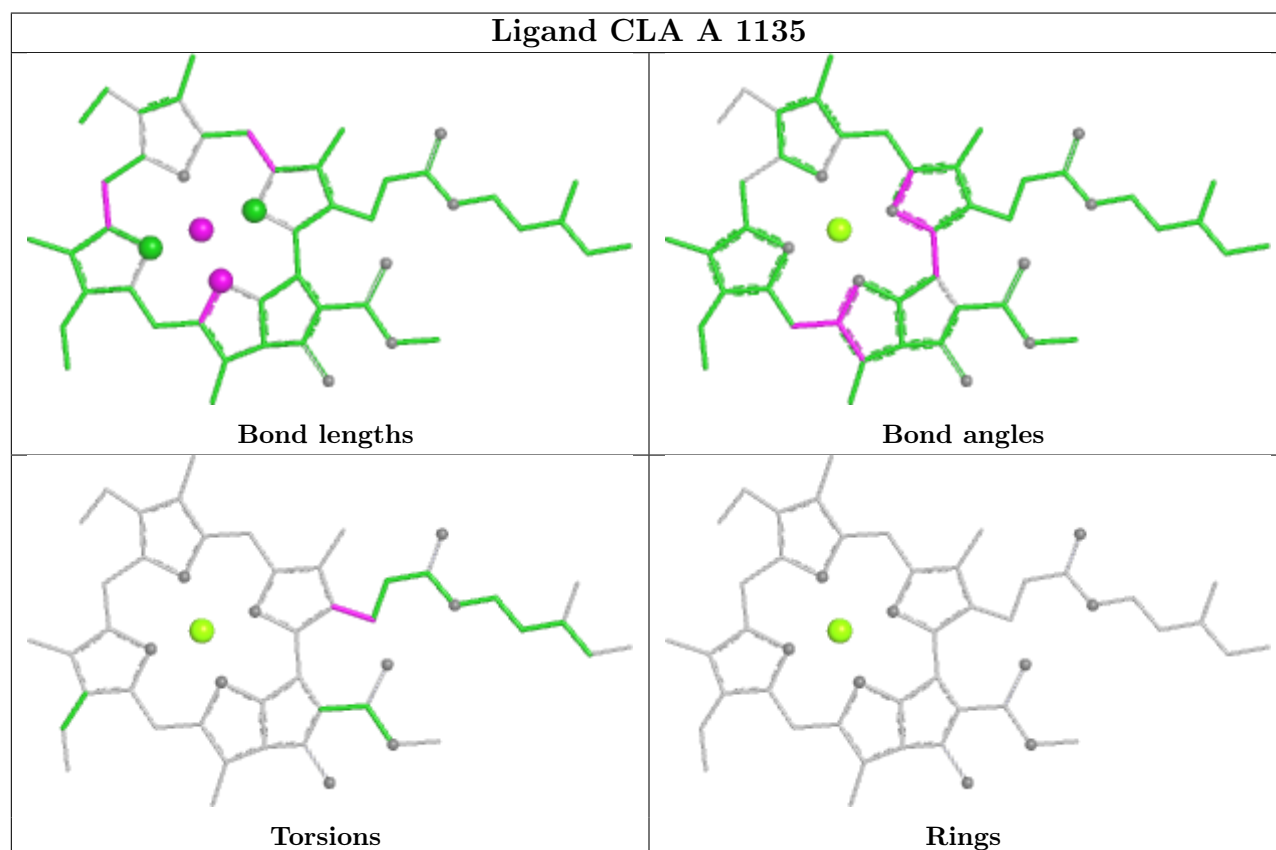
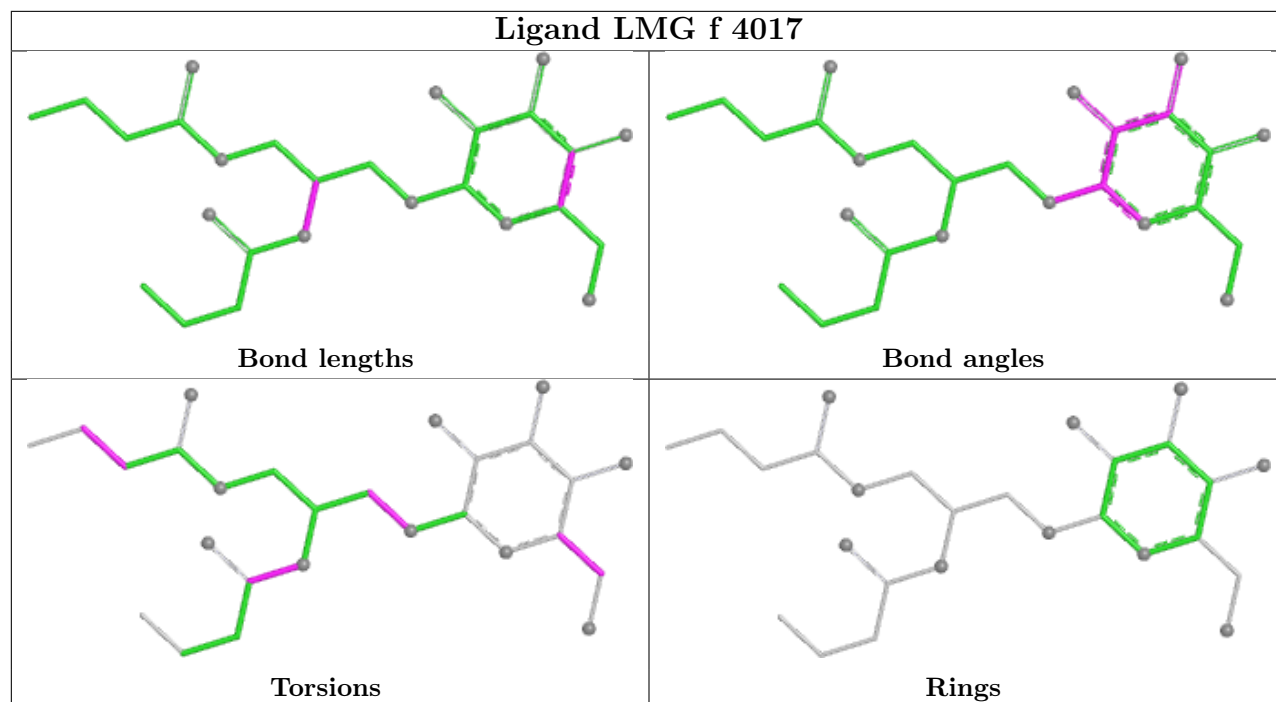
## Ligand CLA u 514



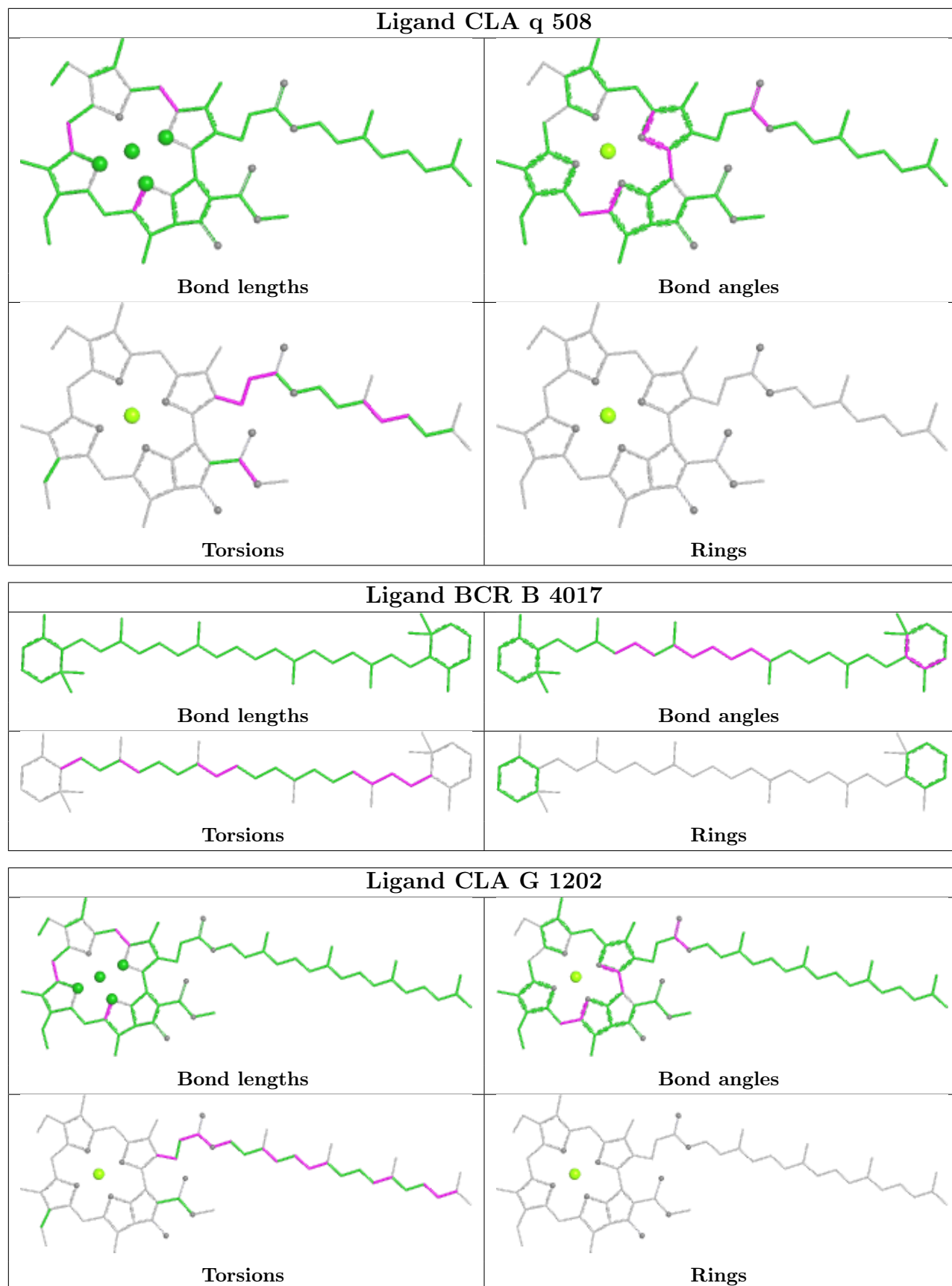




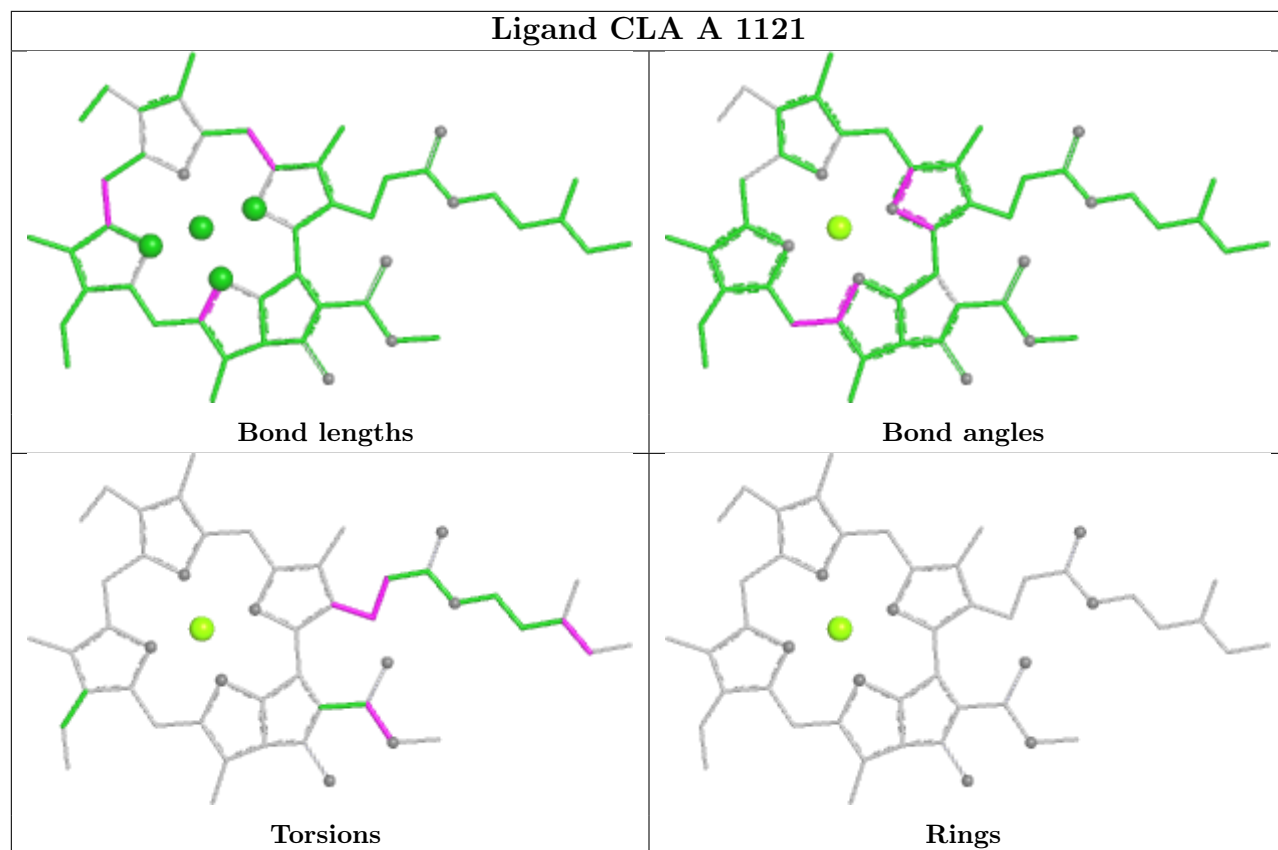




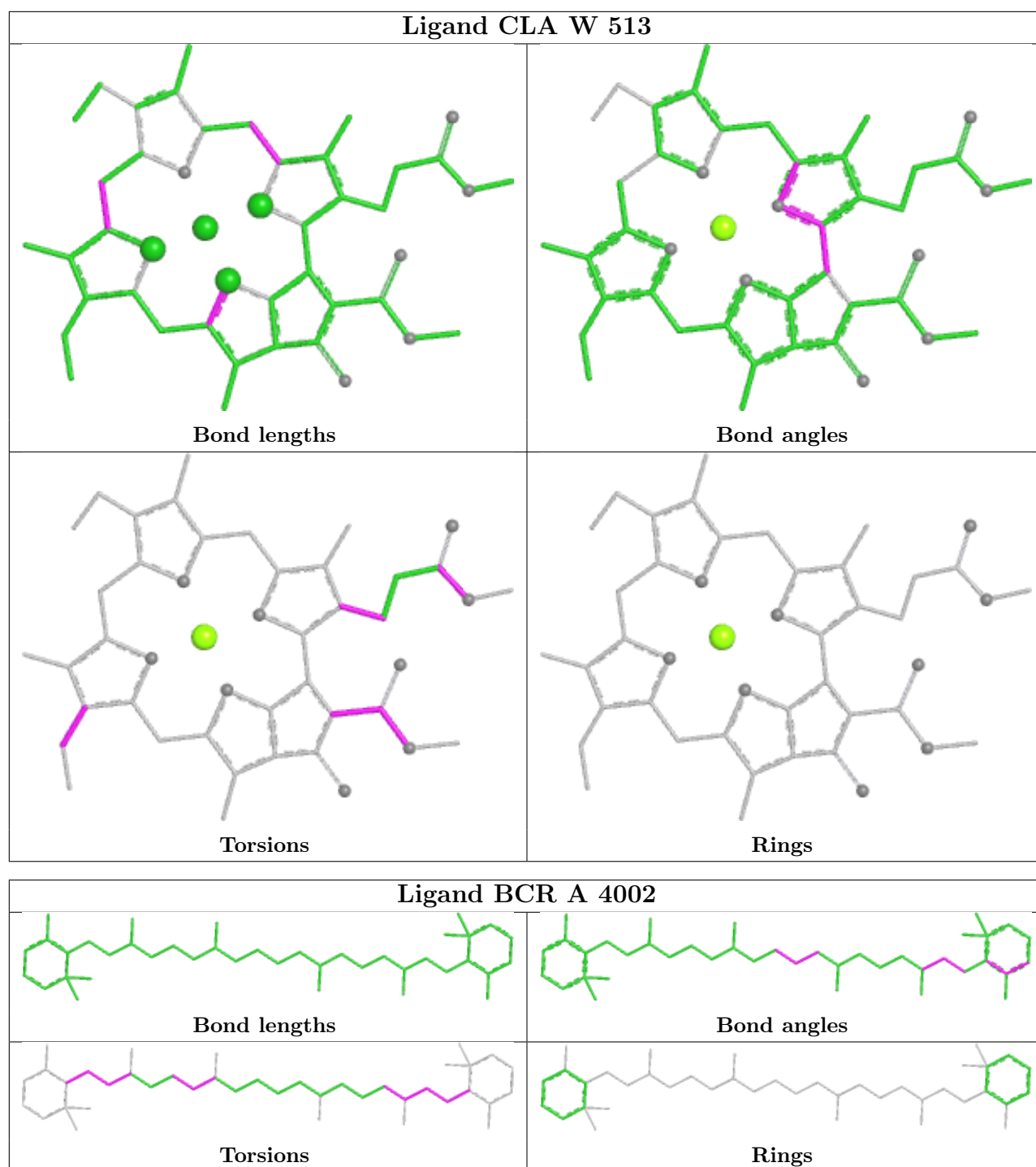






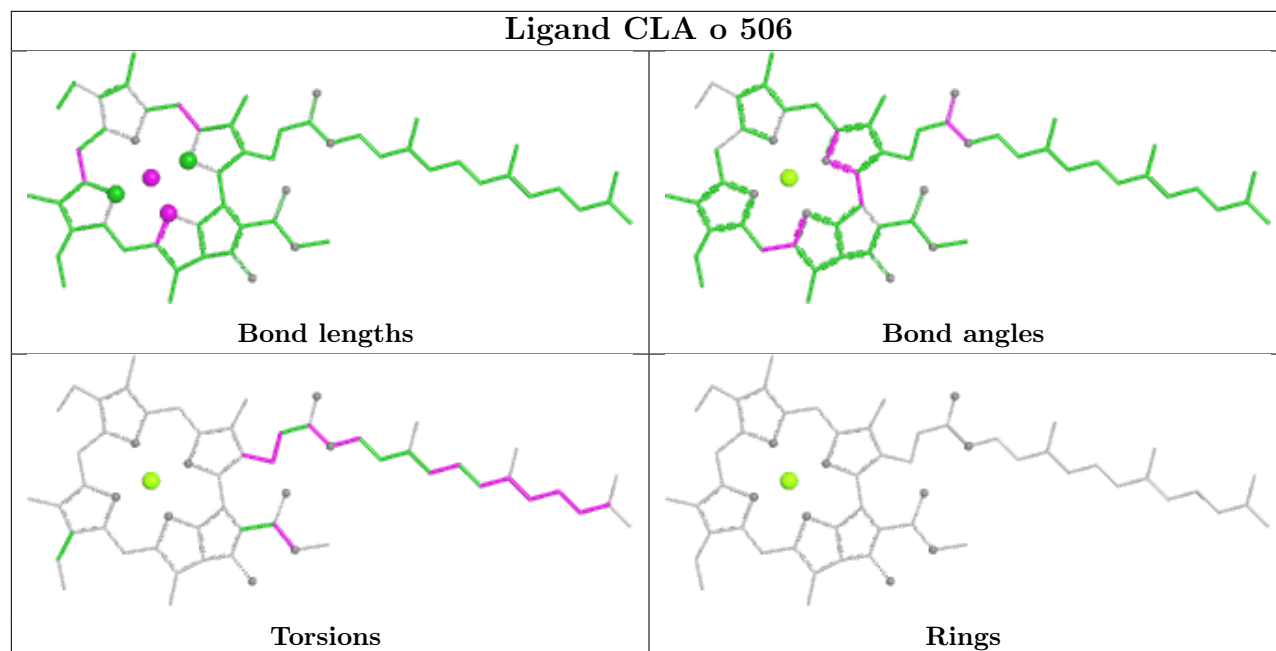




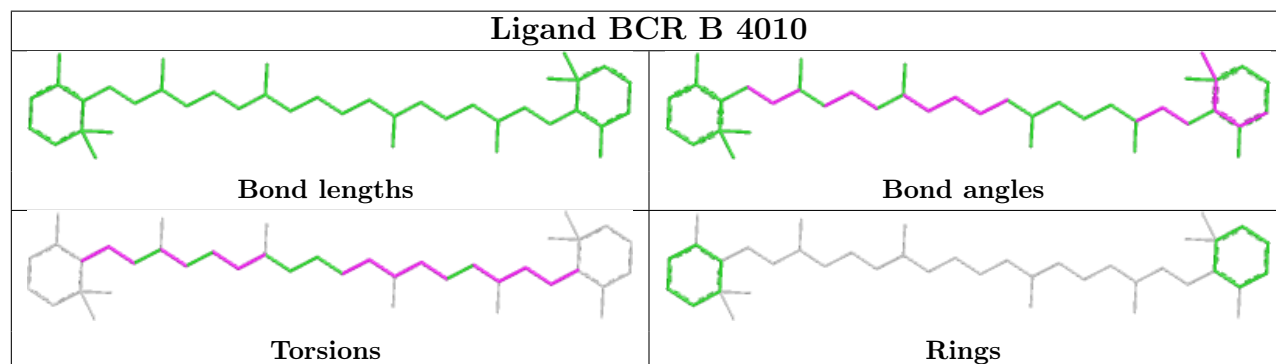




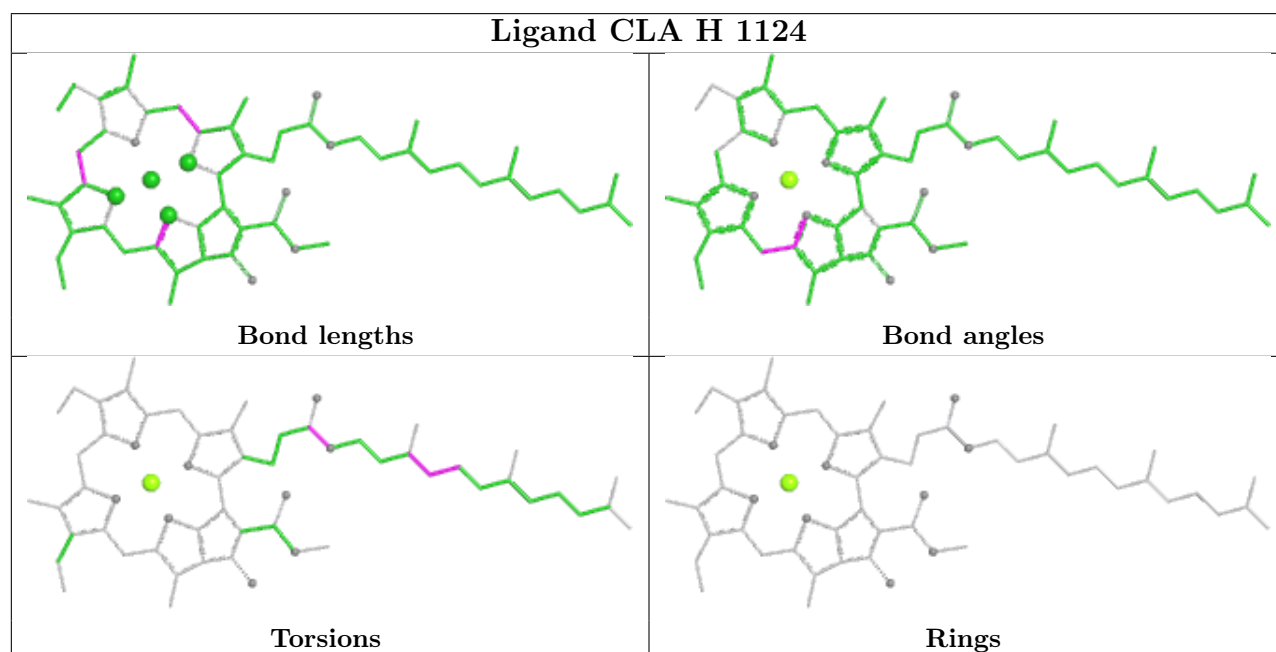
## Ligand CLA o 506



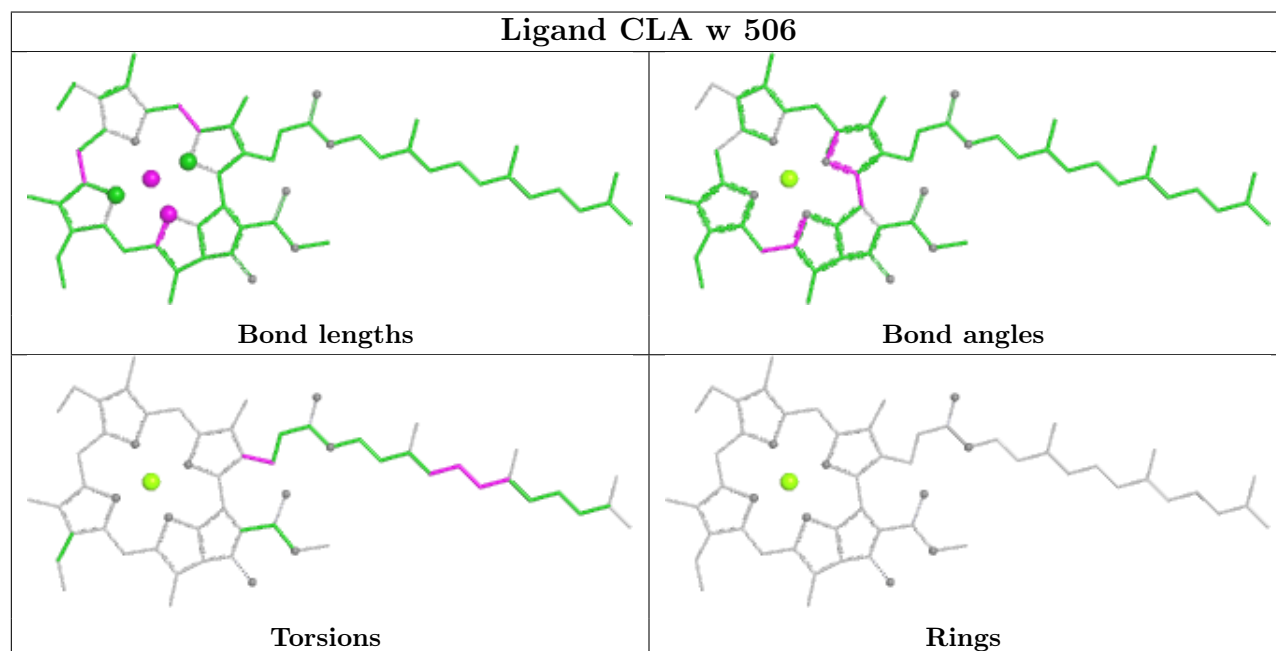
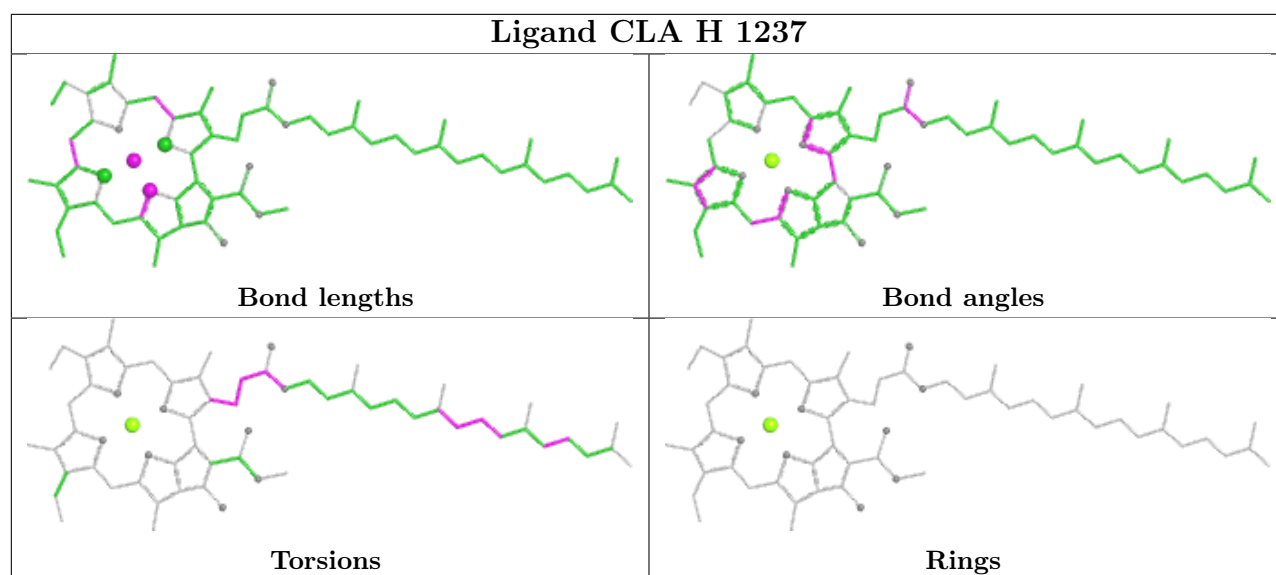
## Ligand BCR B 4010



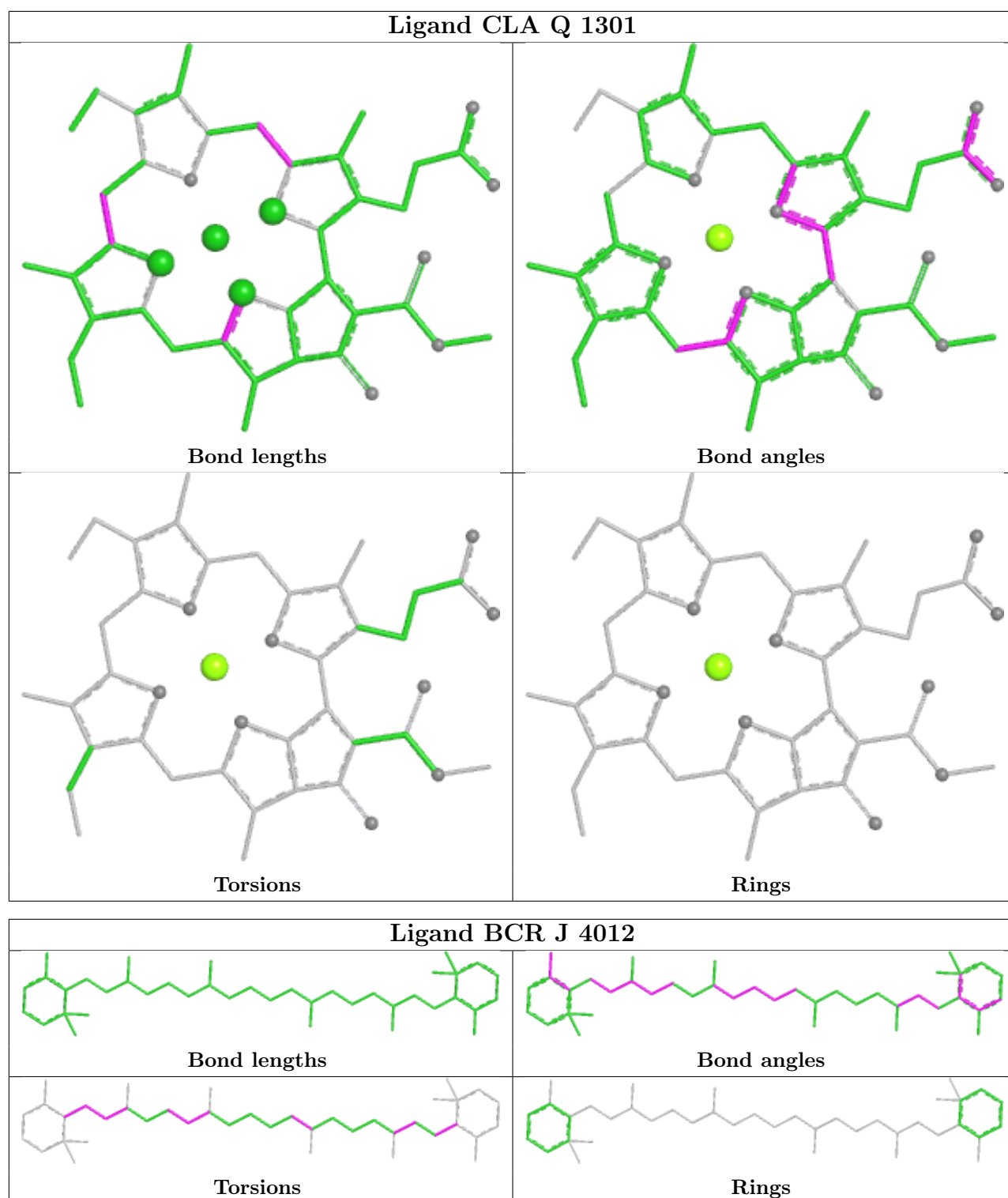
## Ligand CLA H 1124



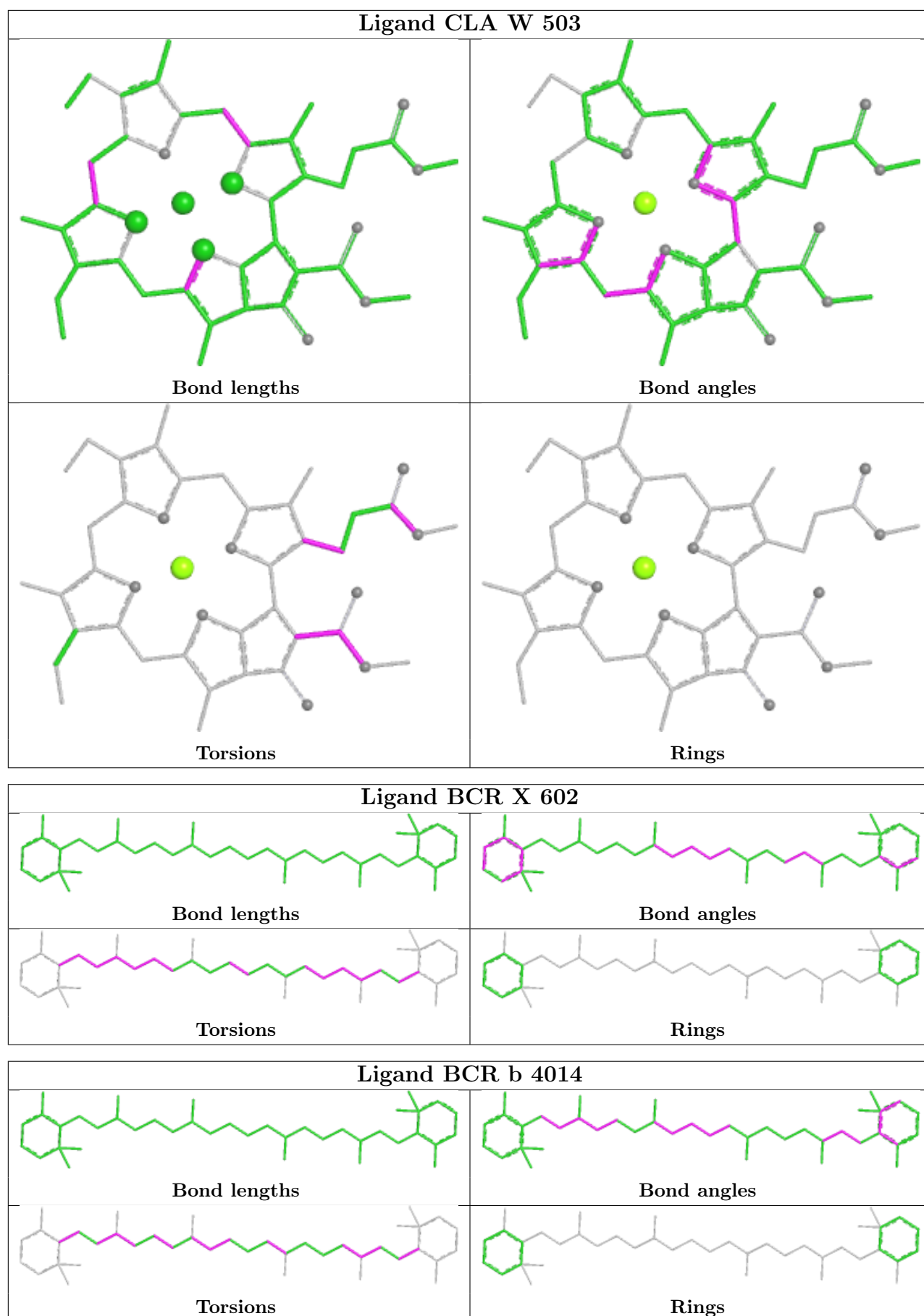




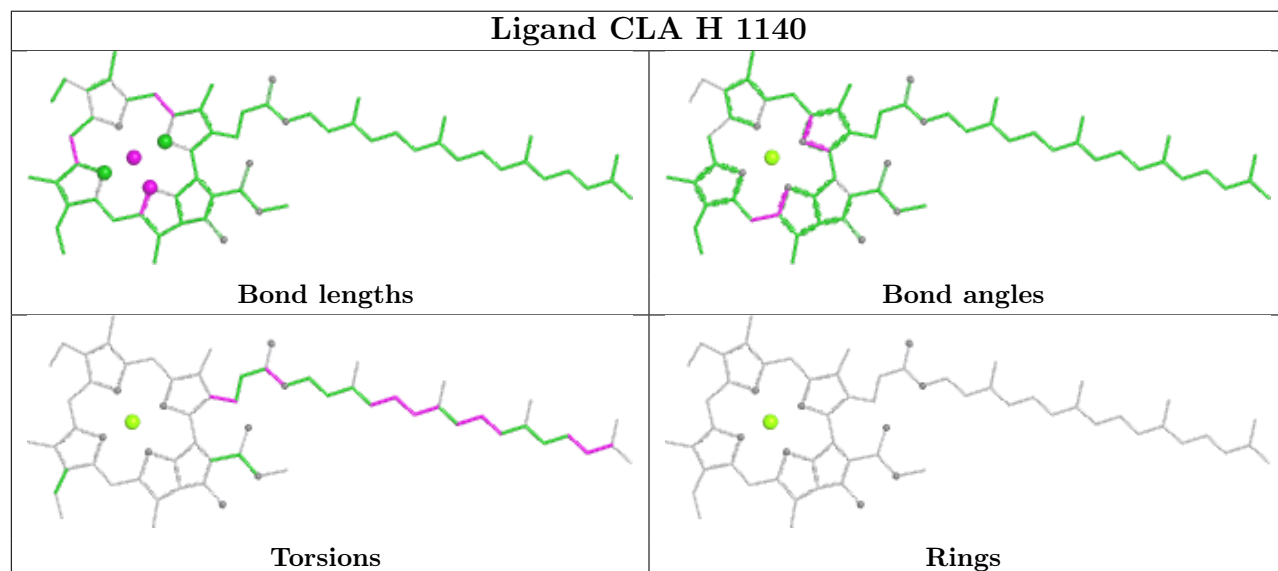
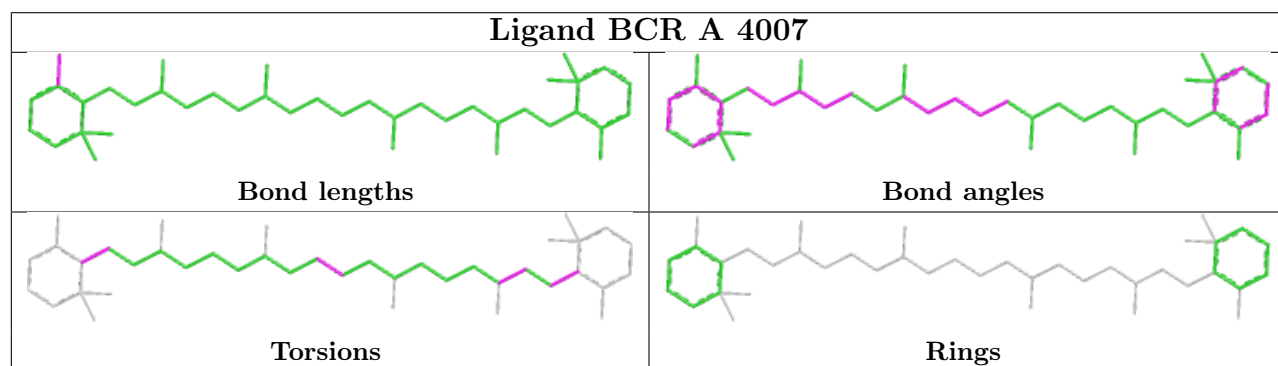
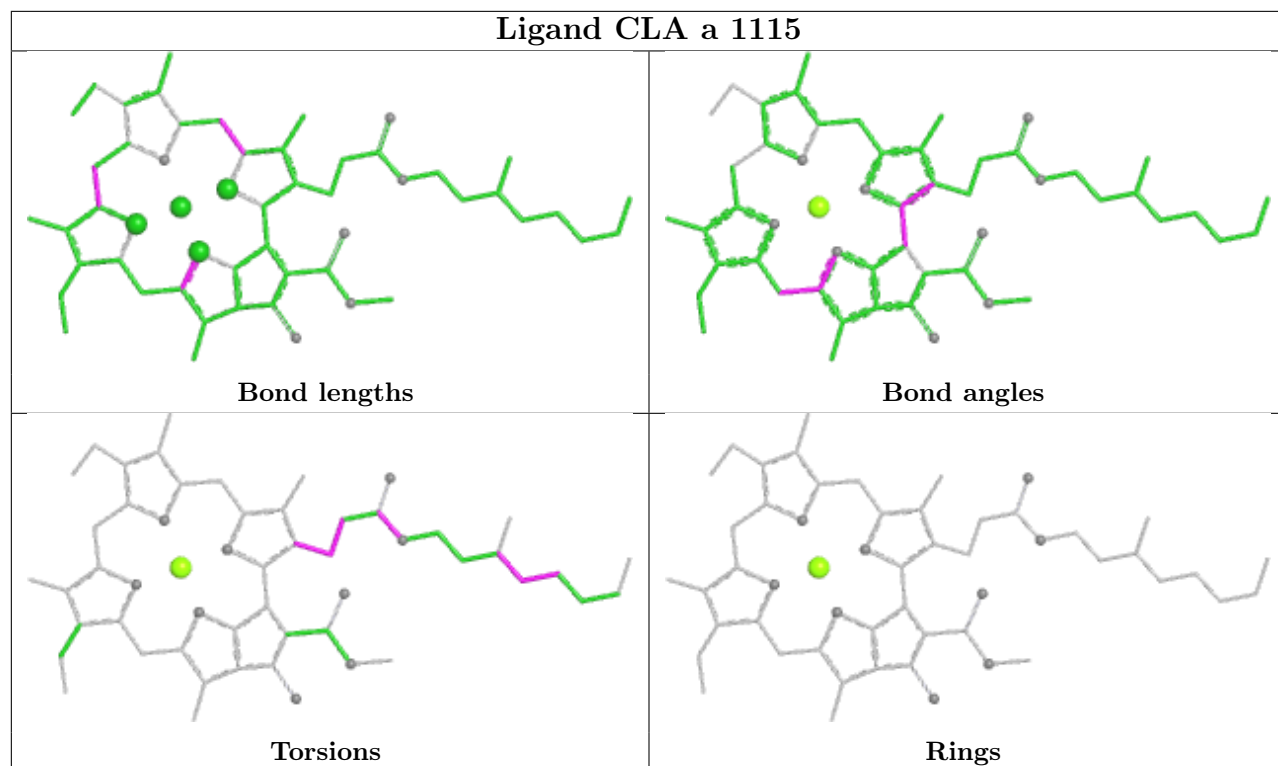




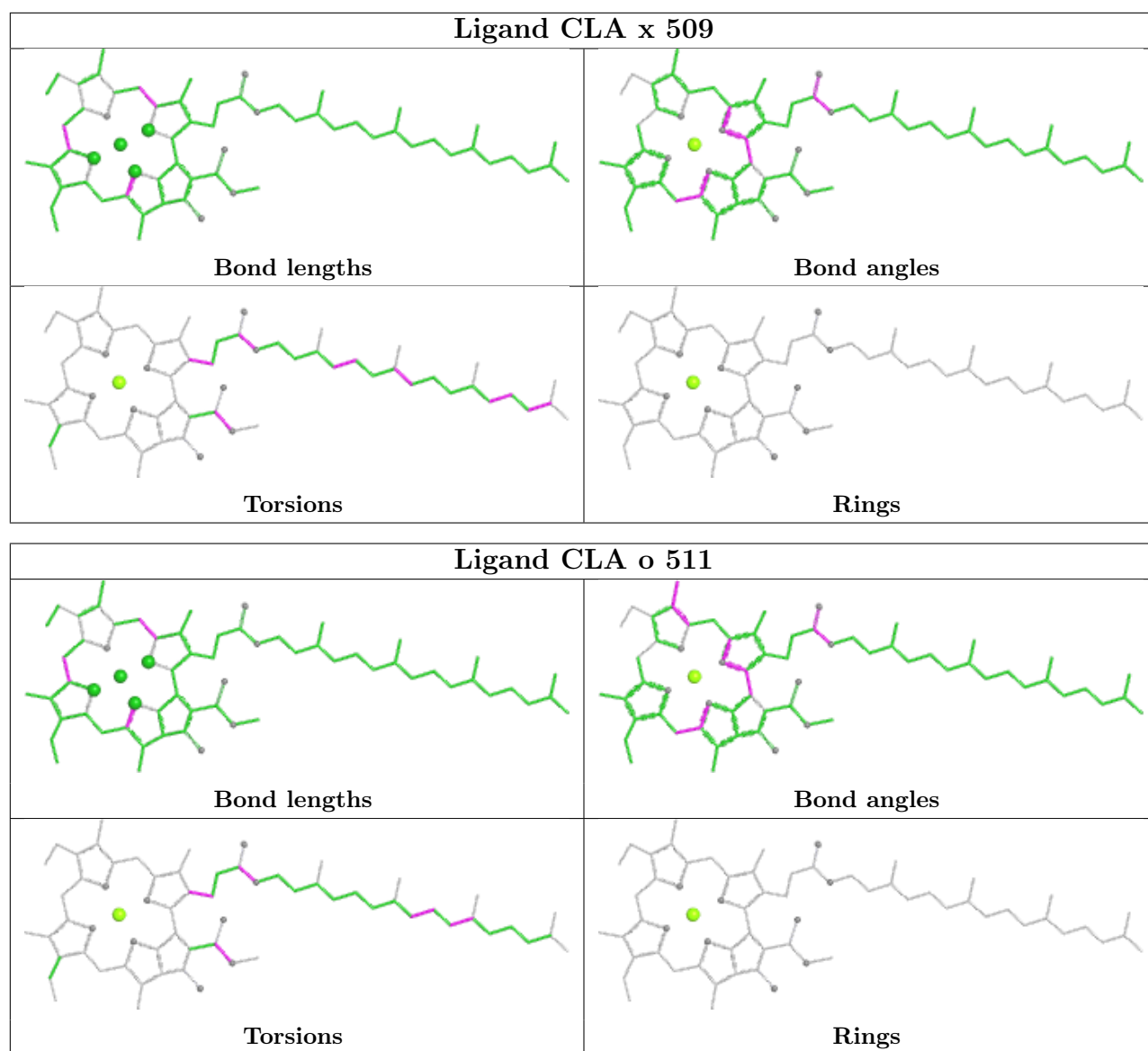






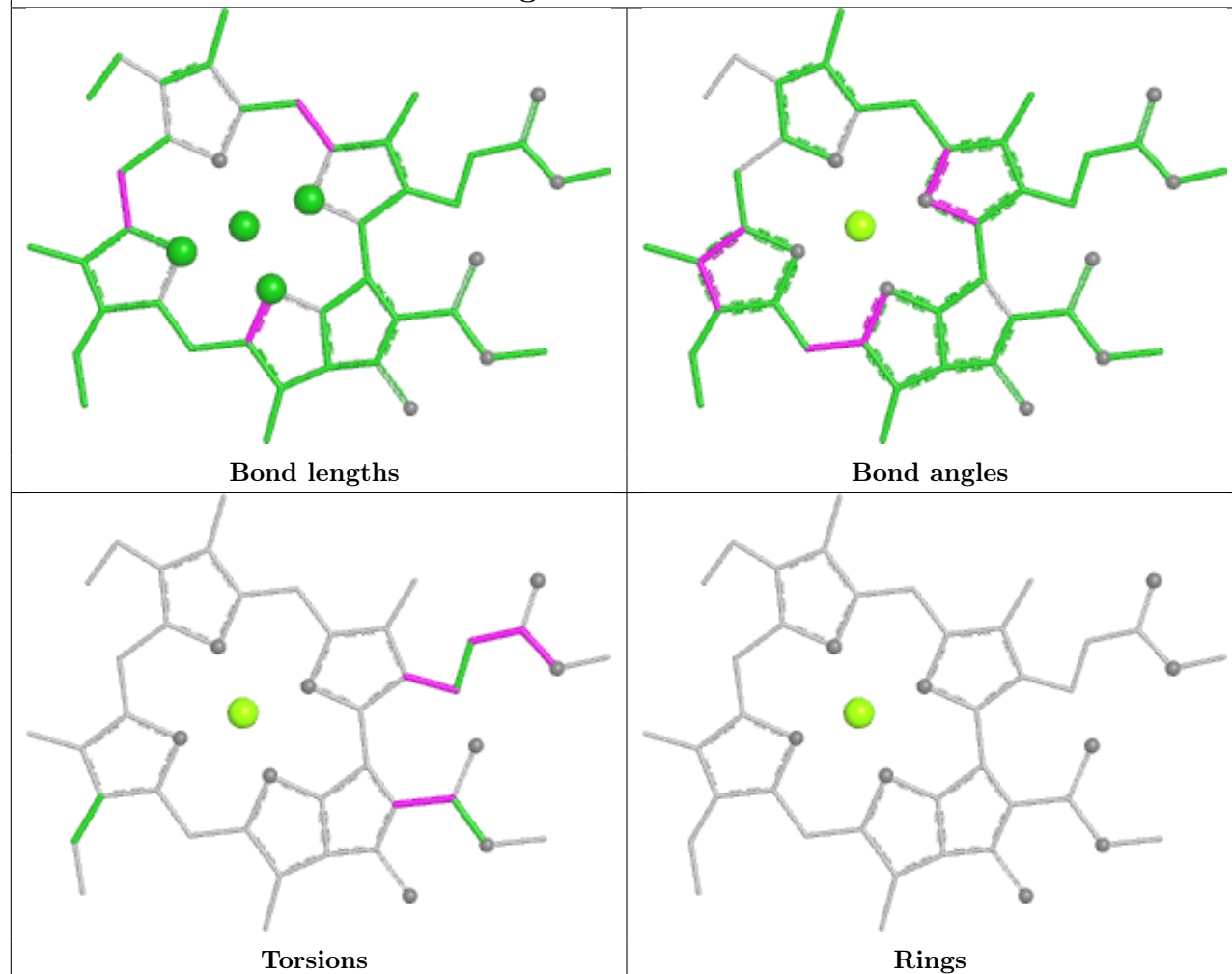




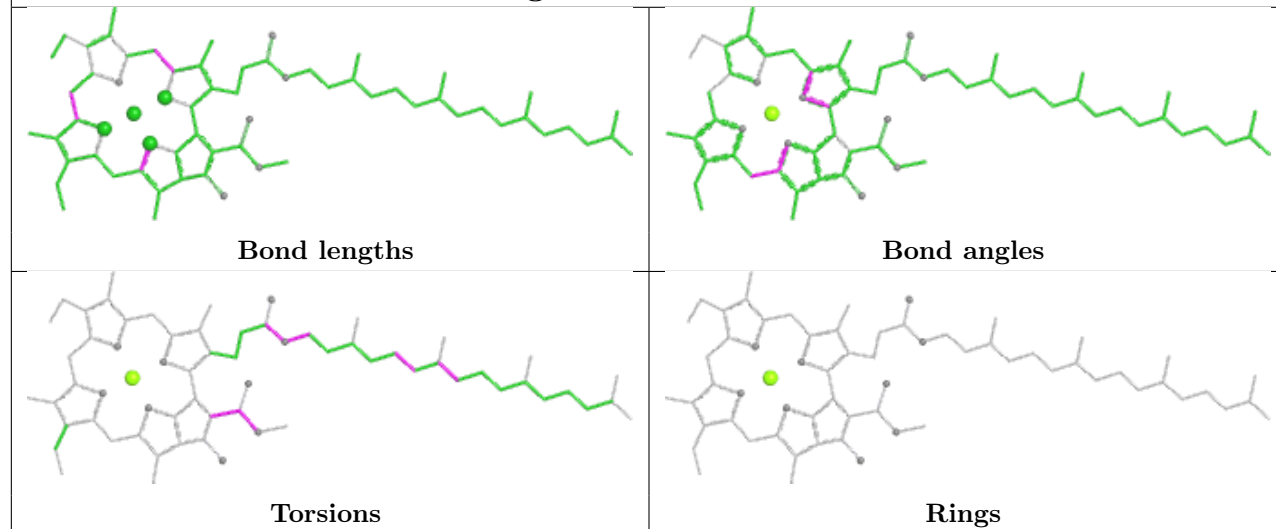




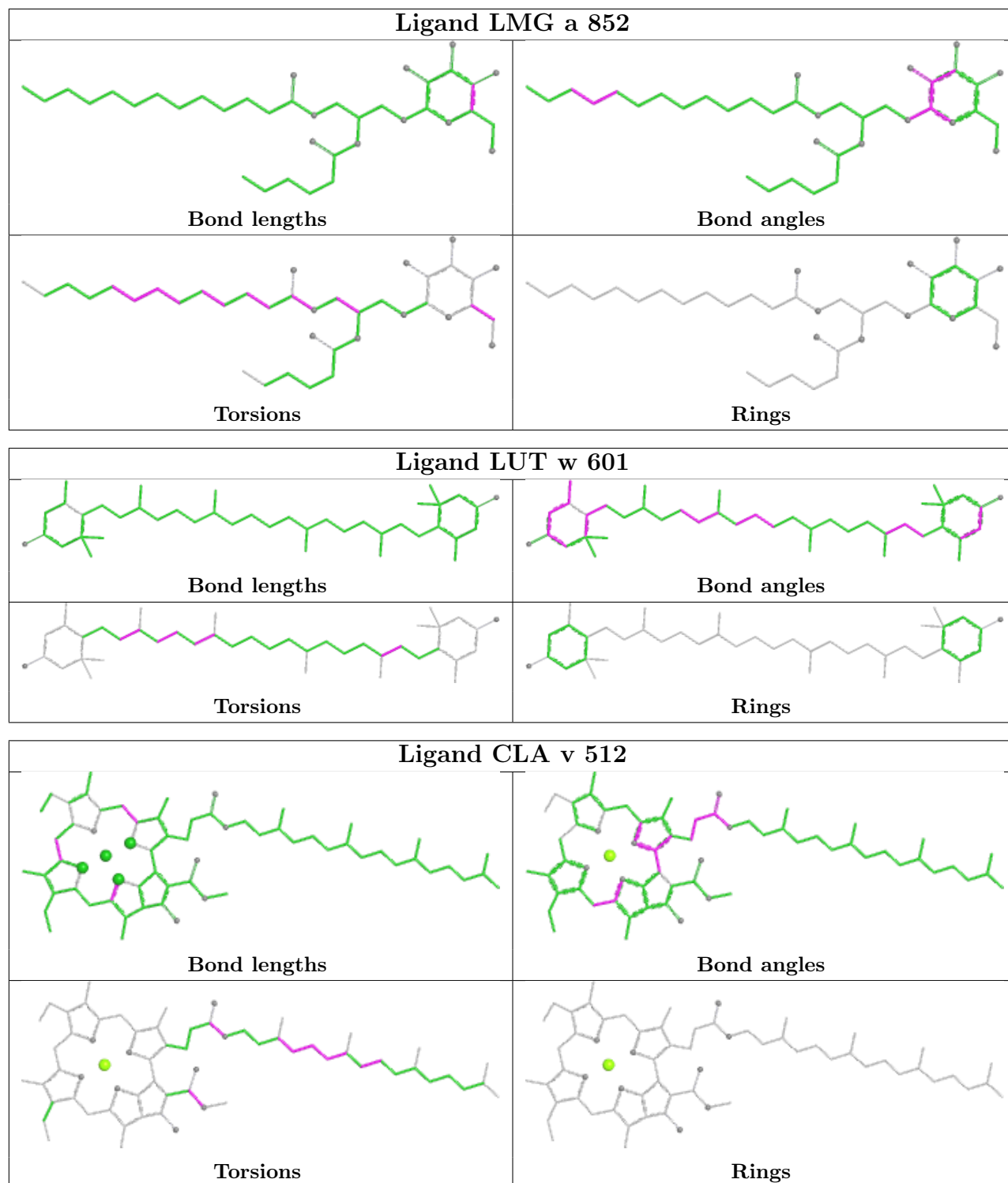
## Ligand CLA s 513



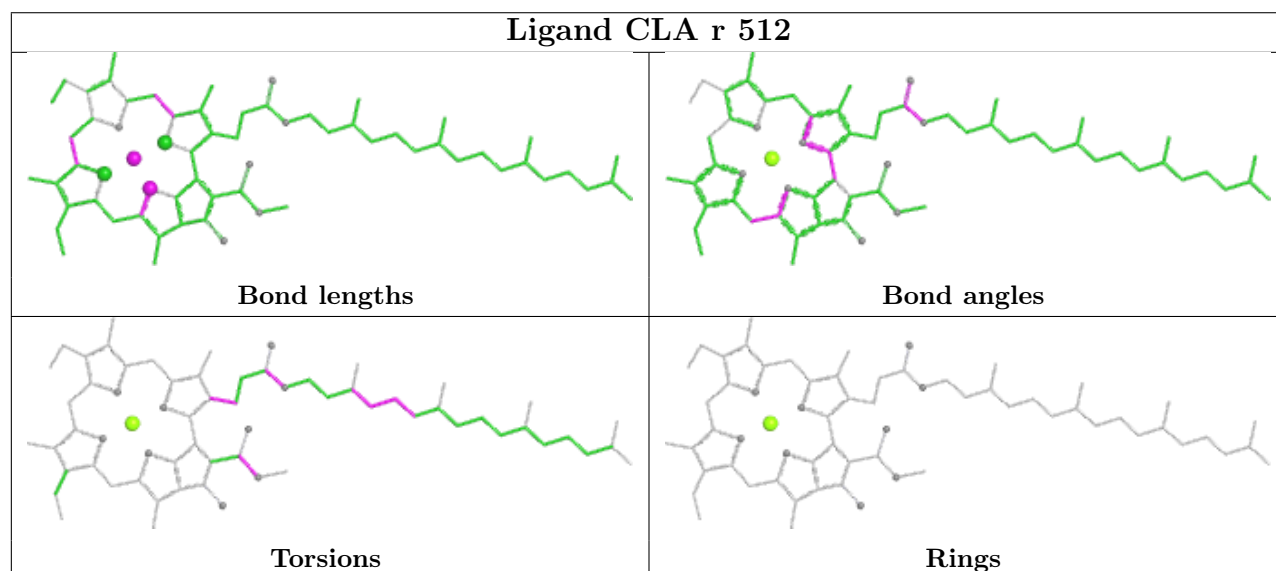
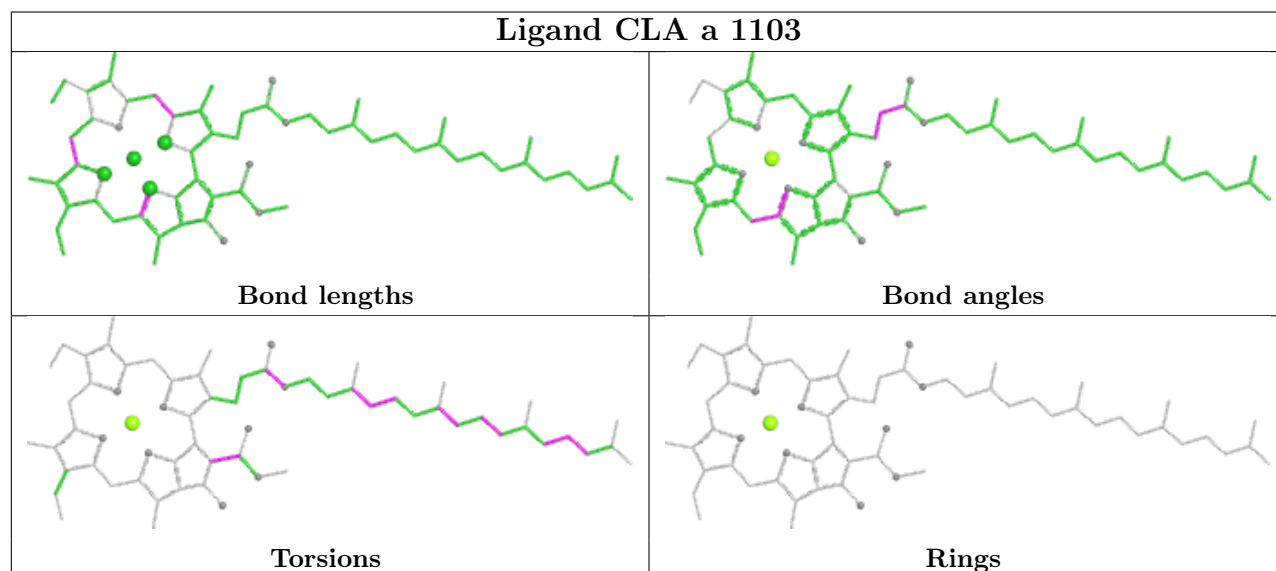
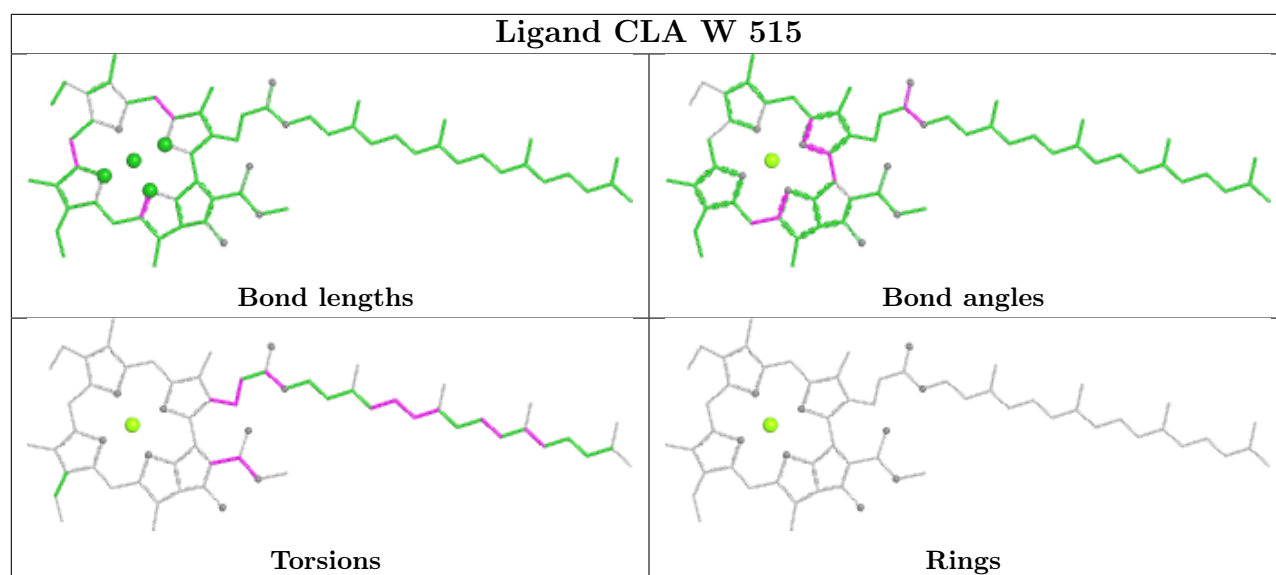
## Ligand CLA W 507



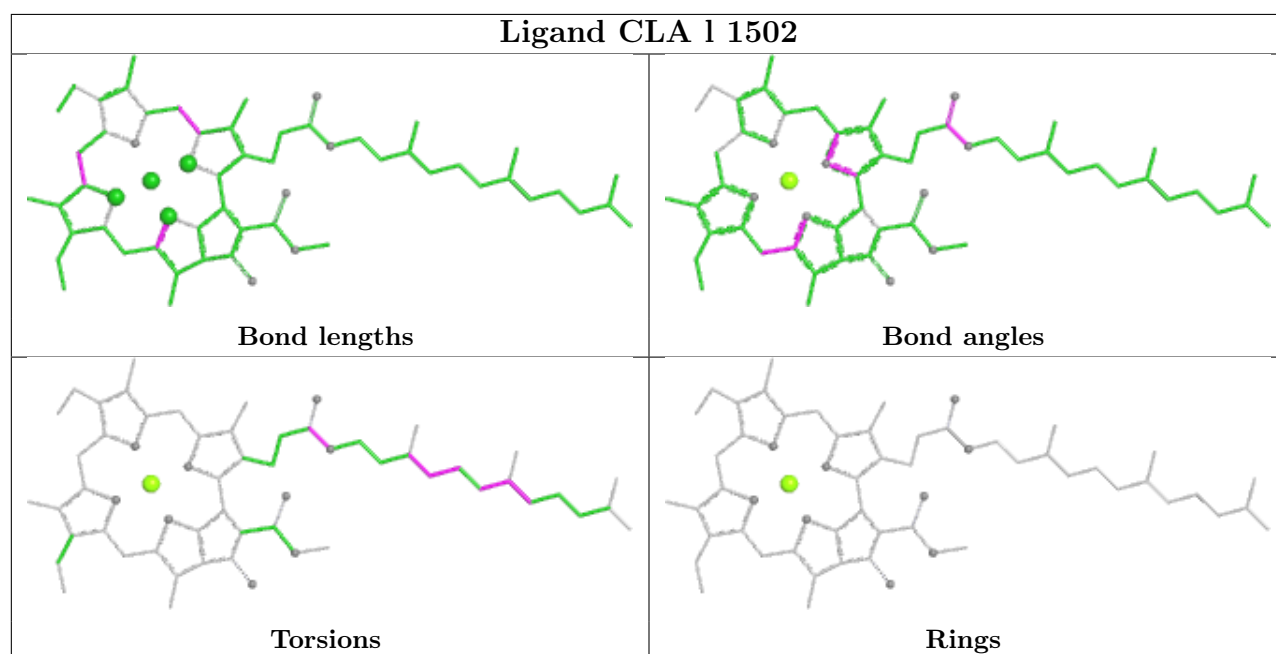
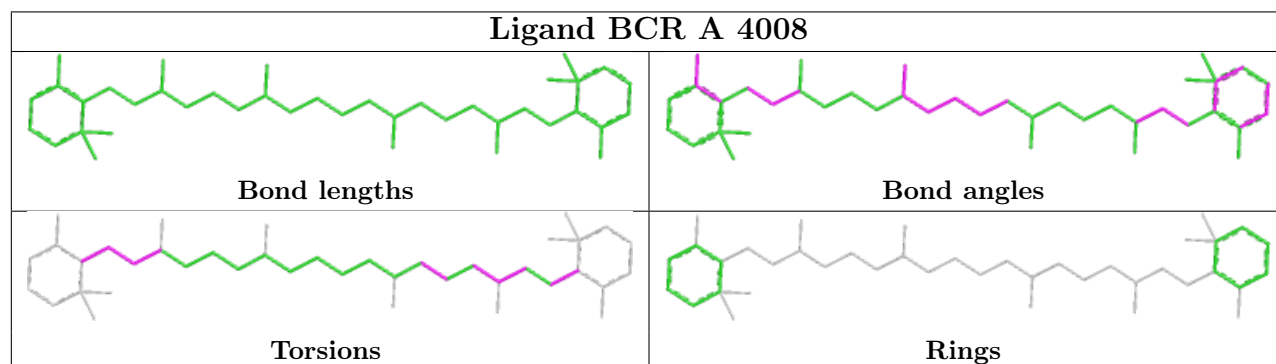
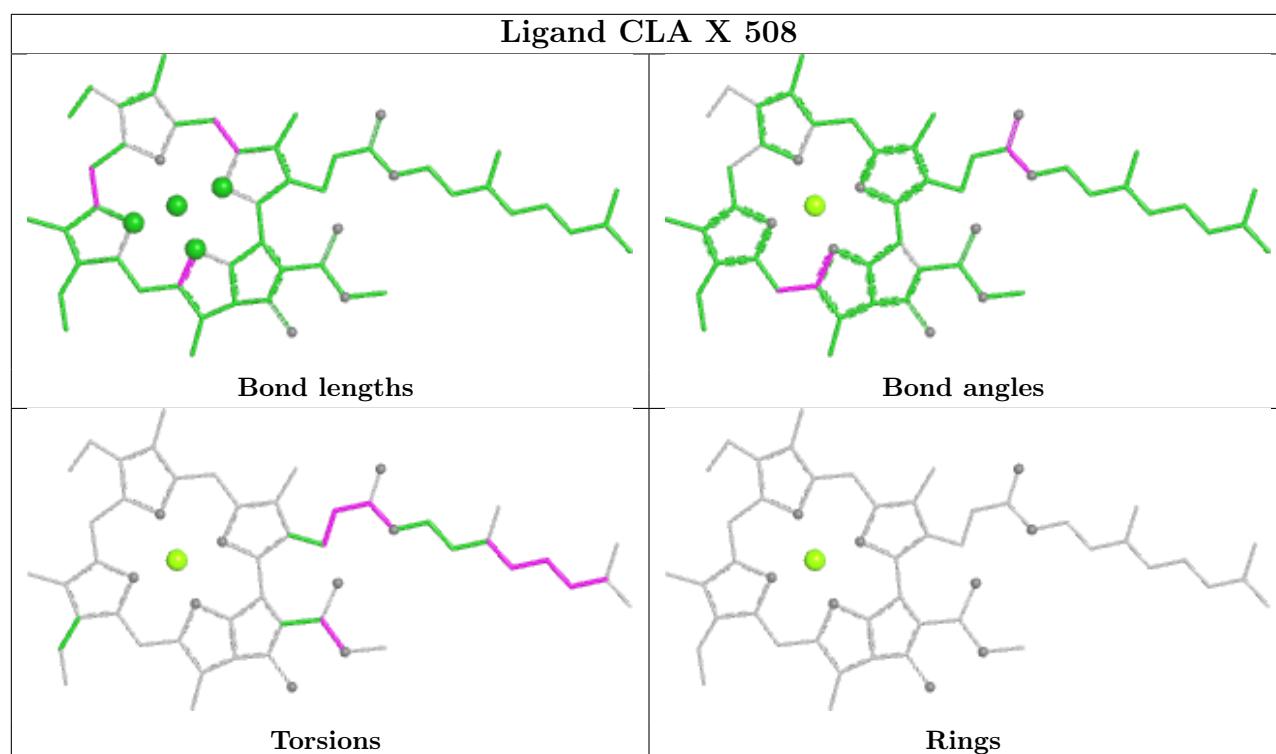




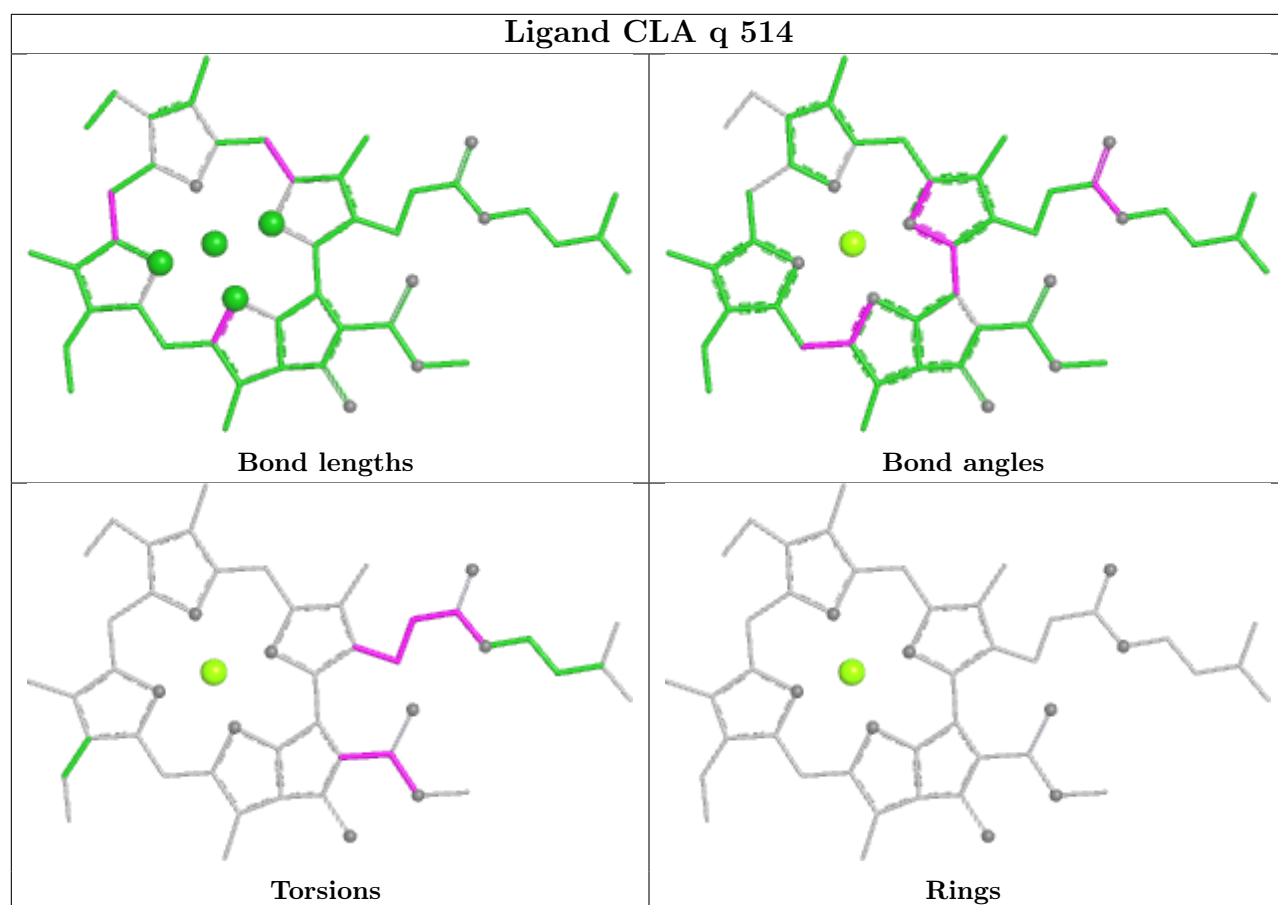






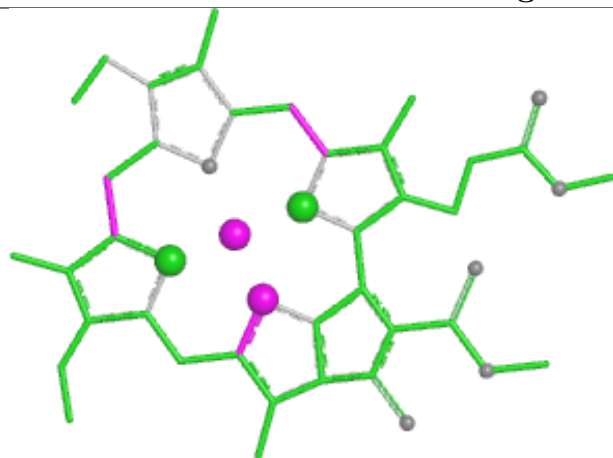




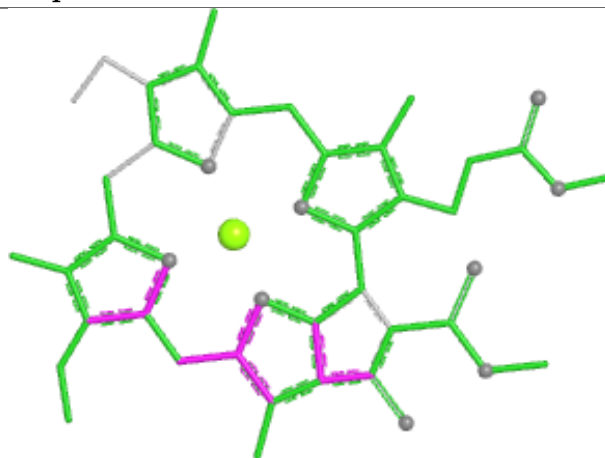




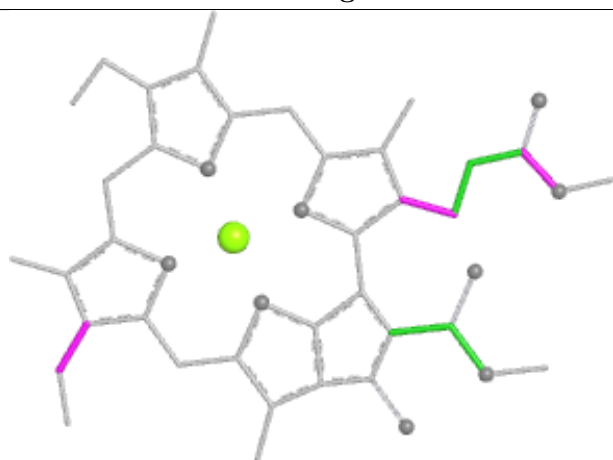
## Ligand CLA p 503



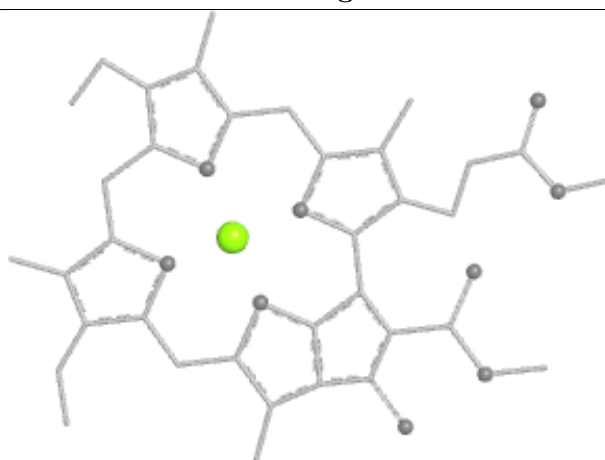
Bond lengths



Bond angles

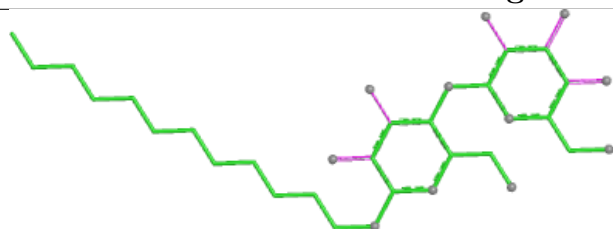


Torsions

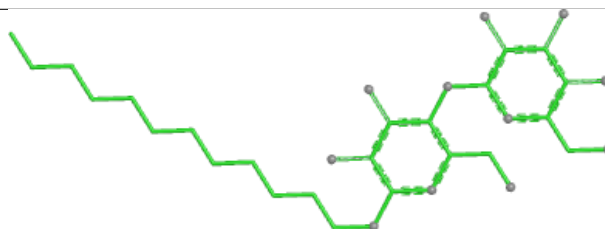


Rings

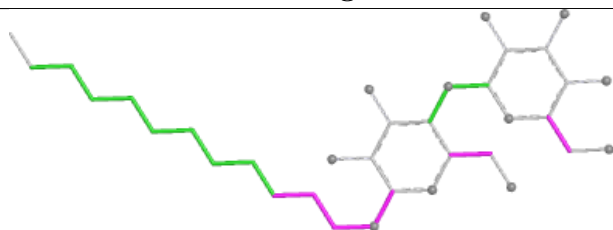
## Ligand LMT a 4202



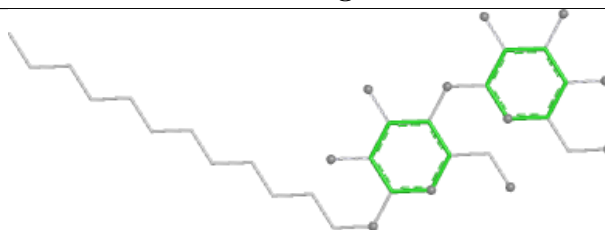
Bond lengths



Bond angles

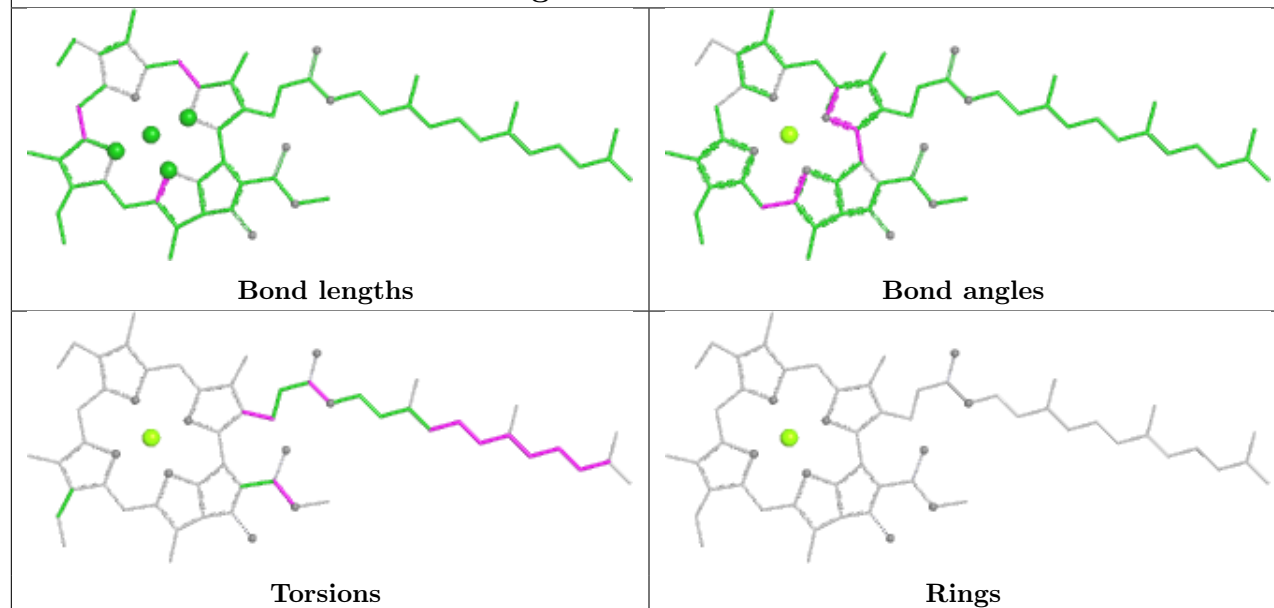
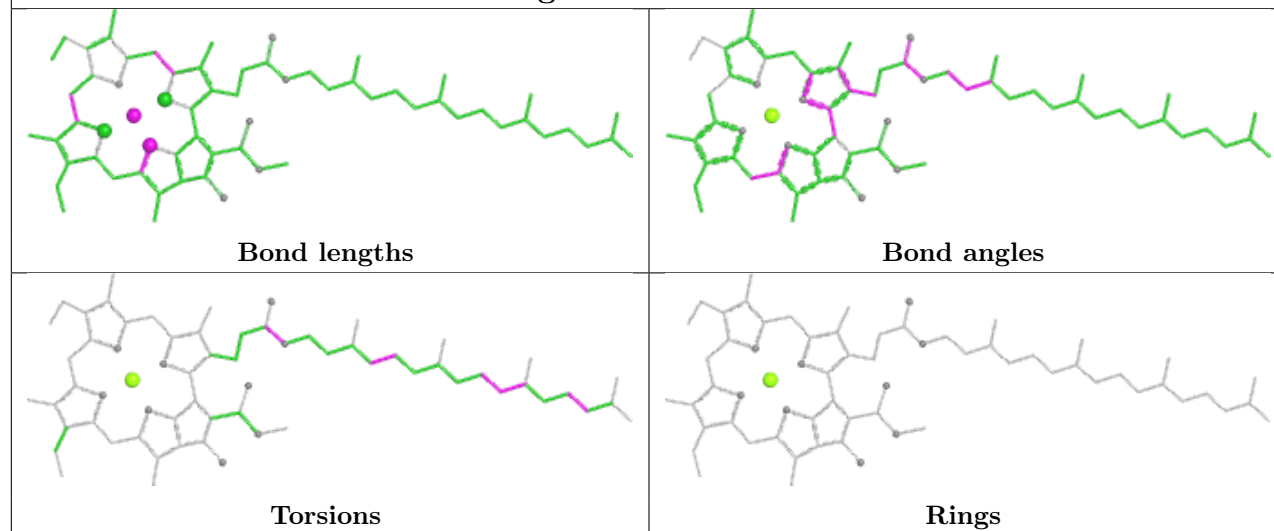


Torsions

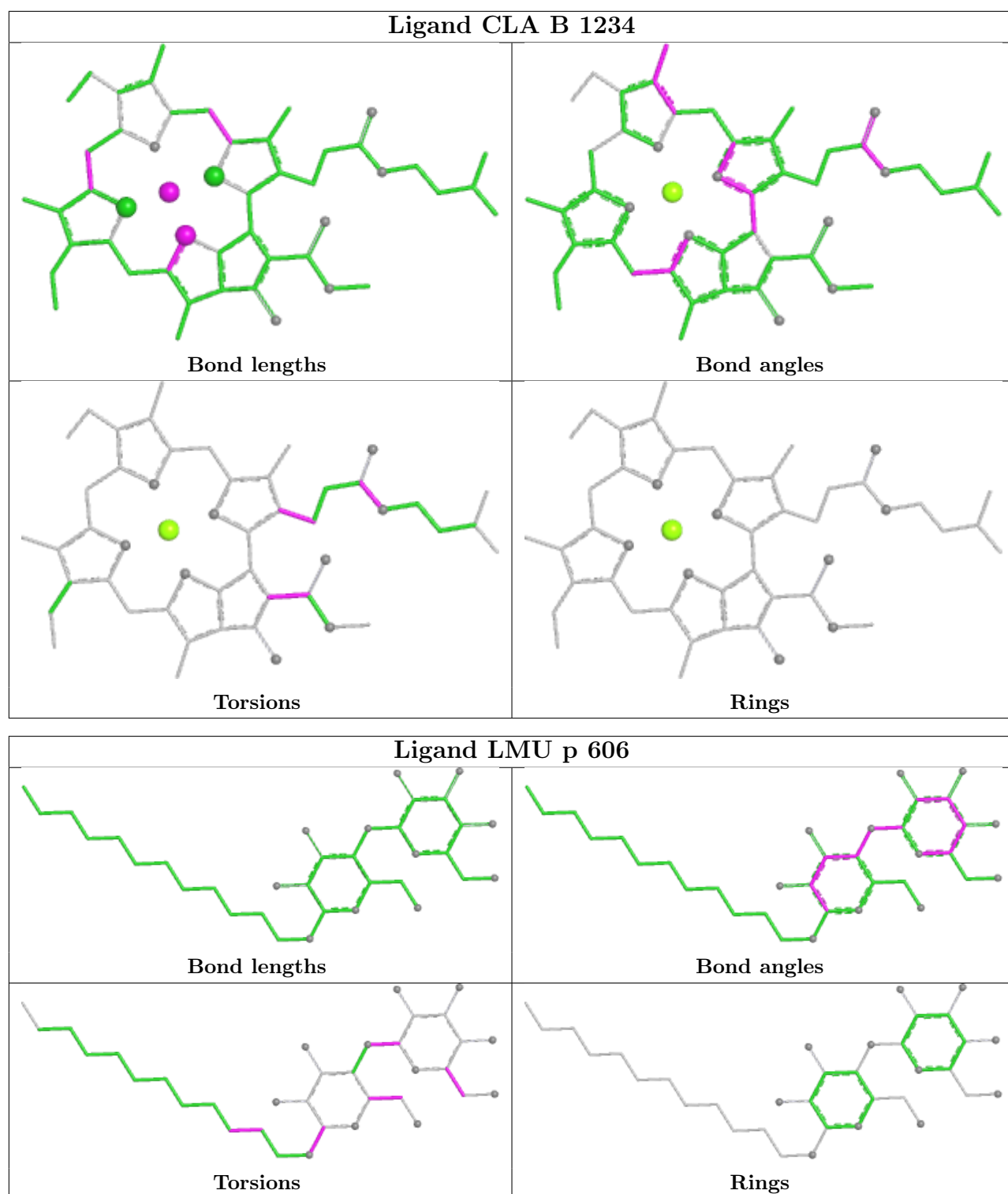


Rings

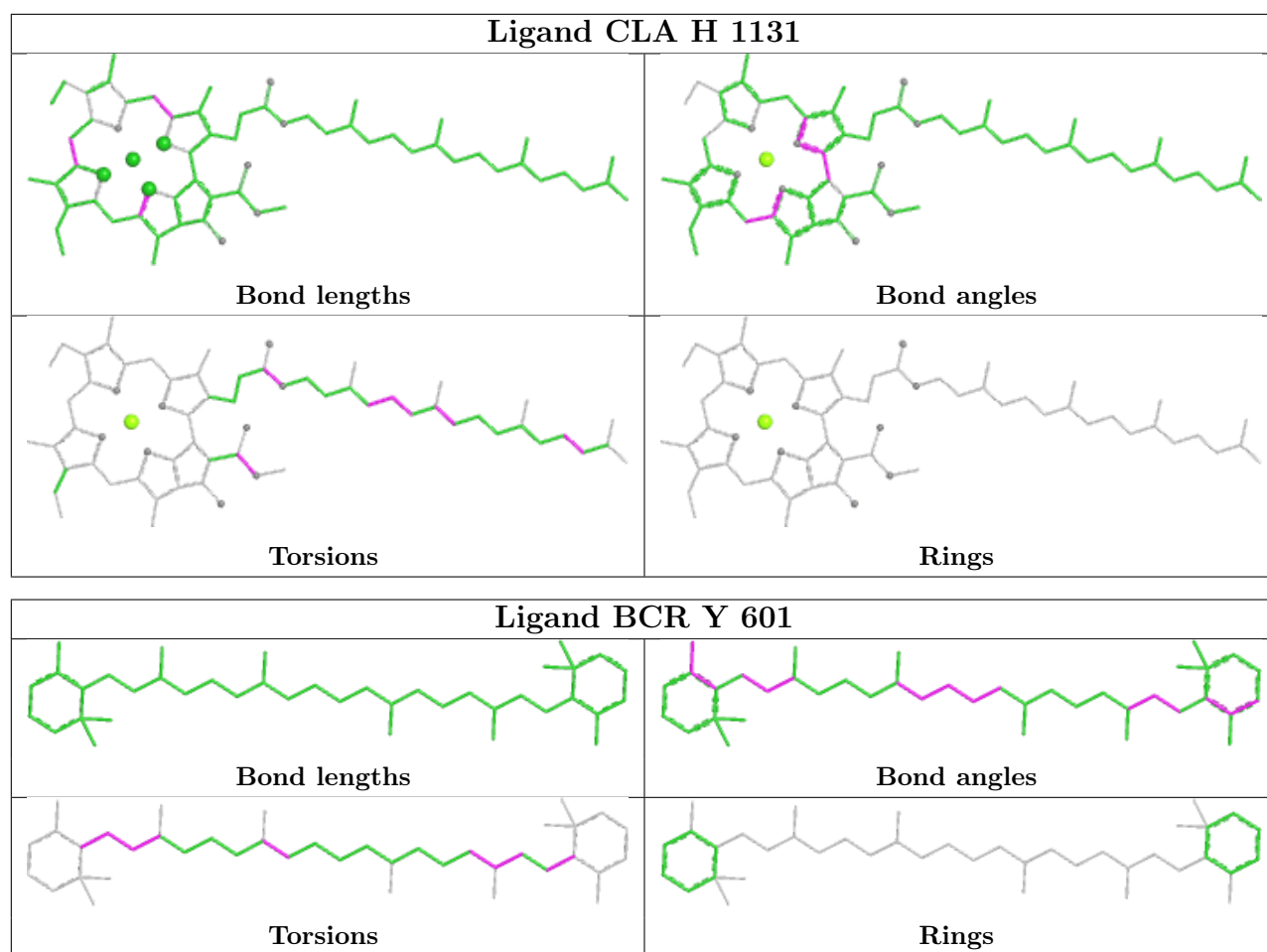


**Ligand CLA X 504****Ligand CLA s 512**

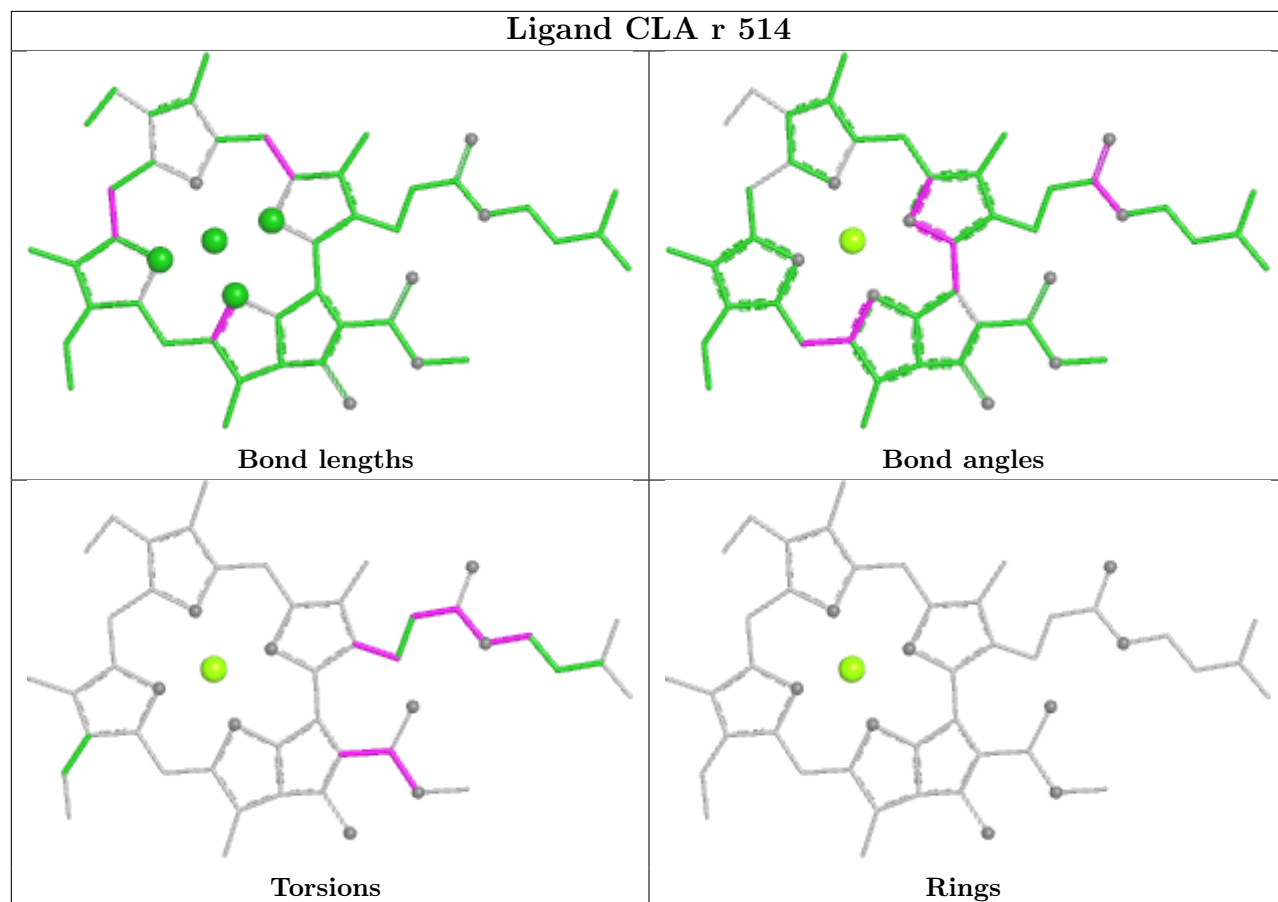






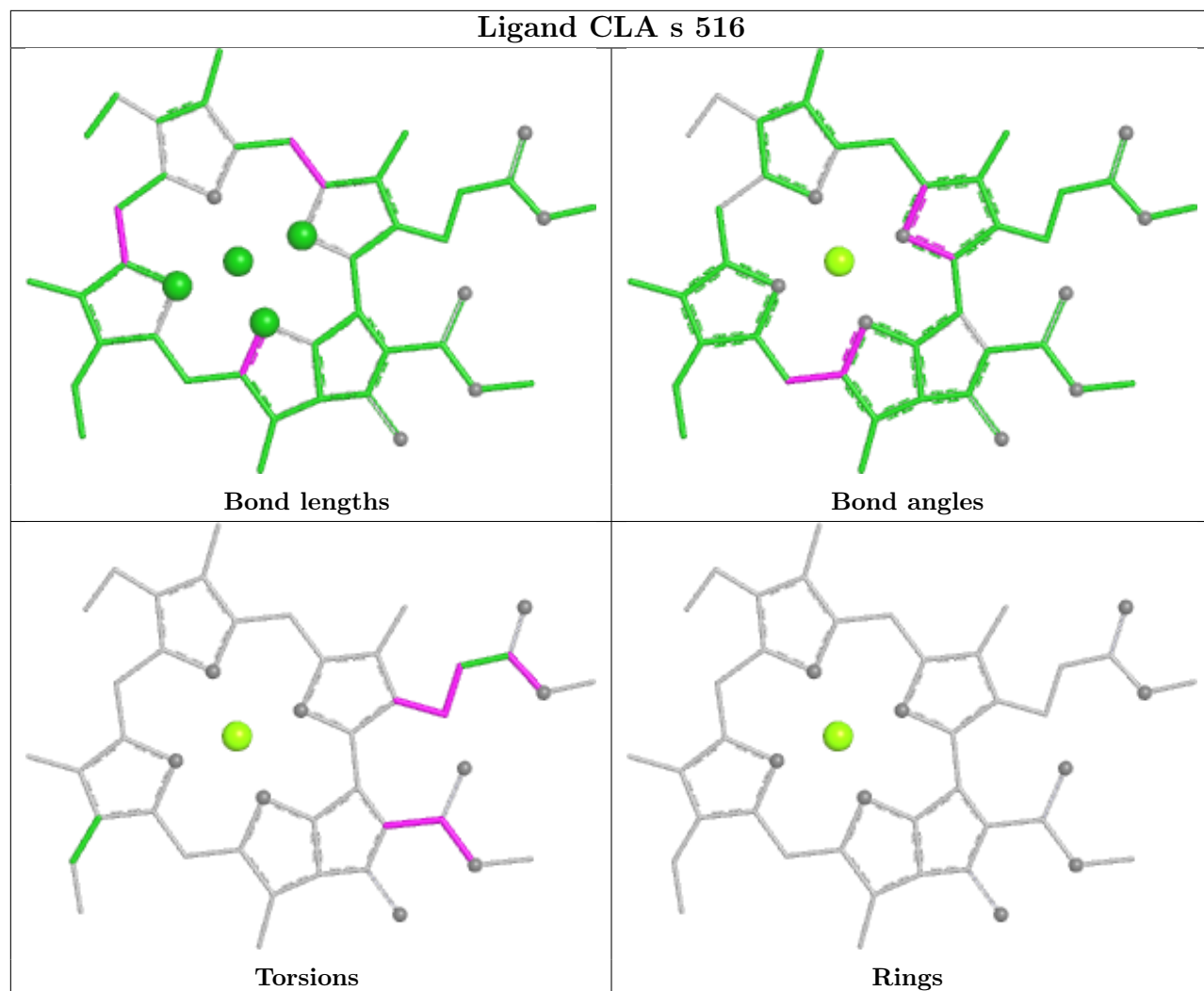






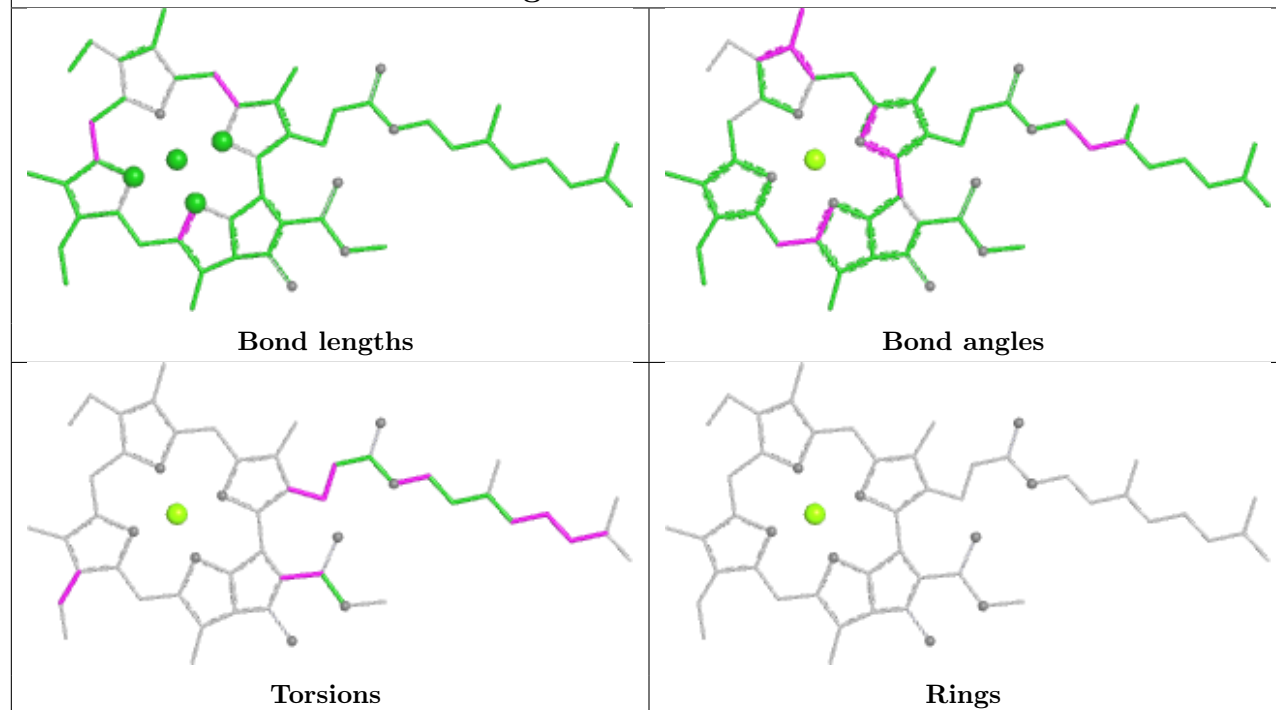


## Ligand CLA s 516

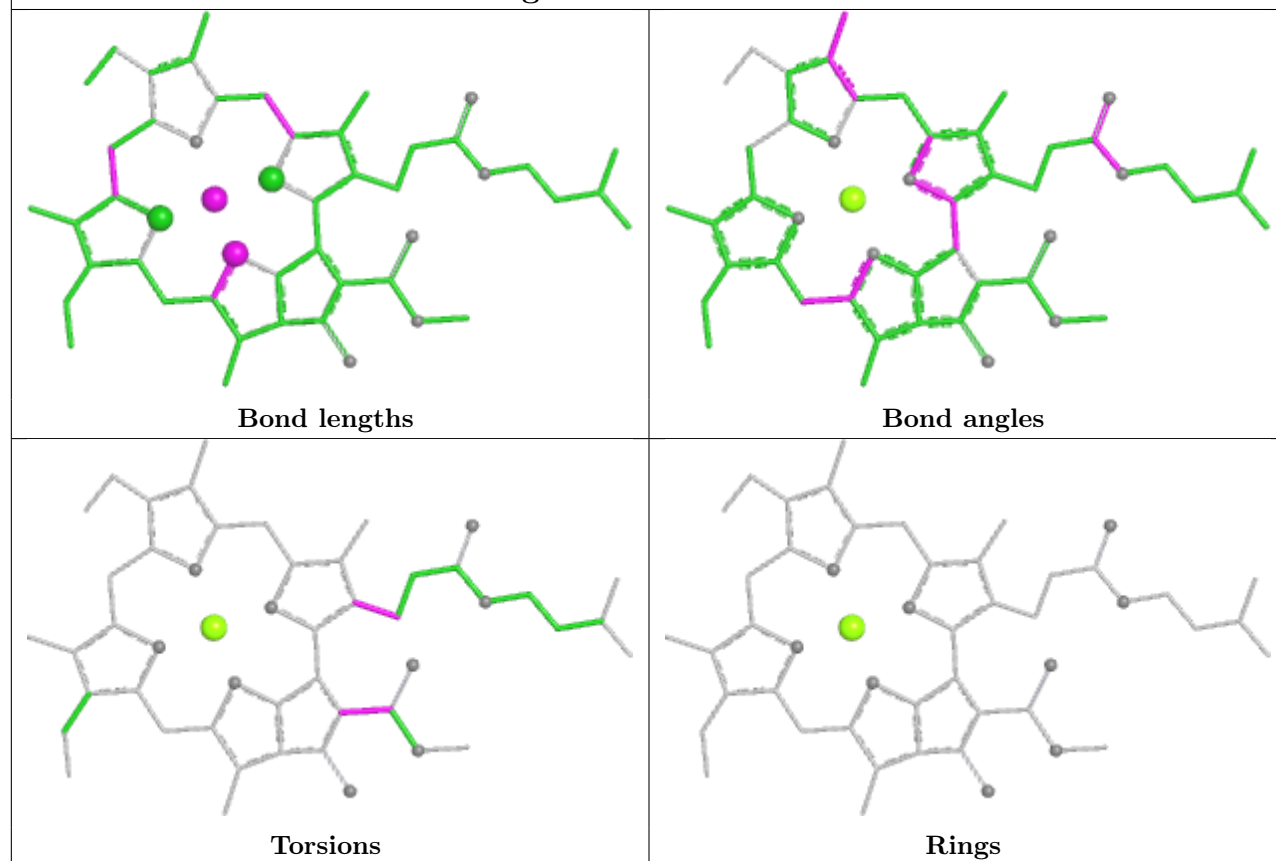




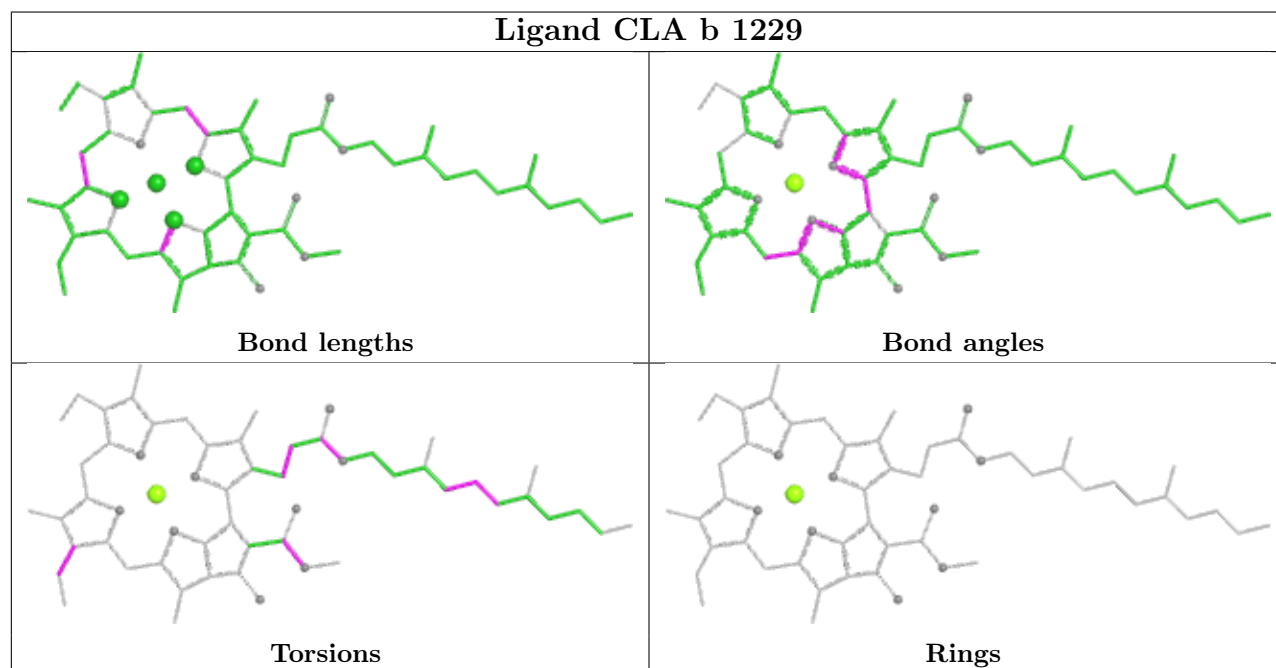
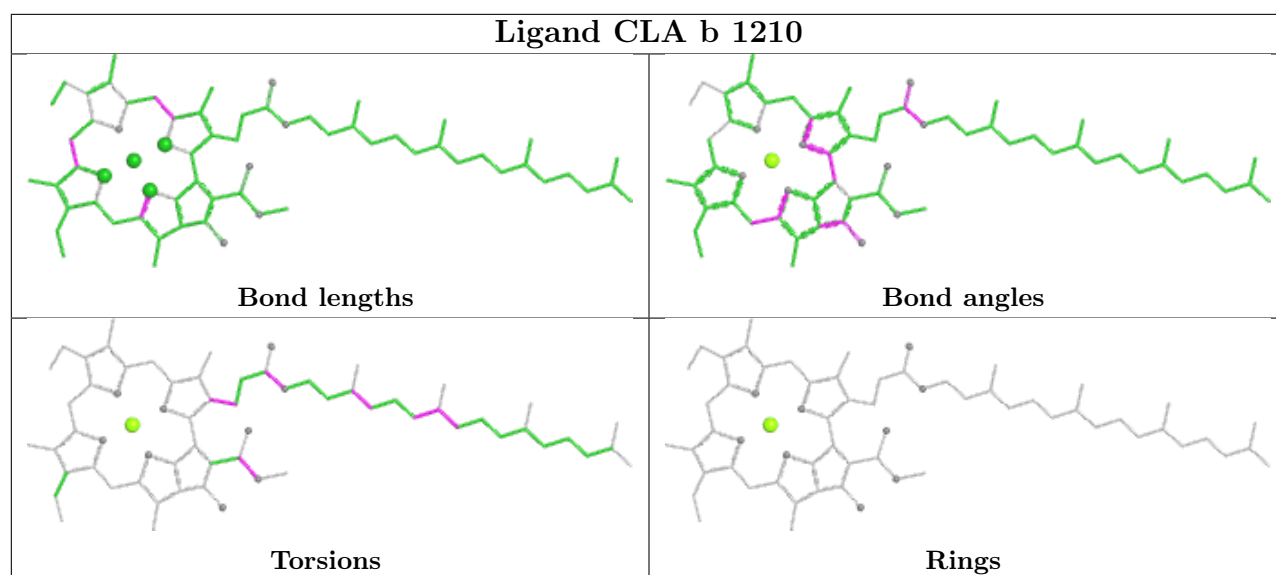
## Ligand CLA B 1012



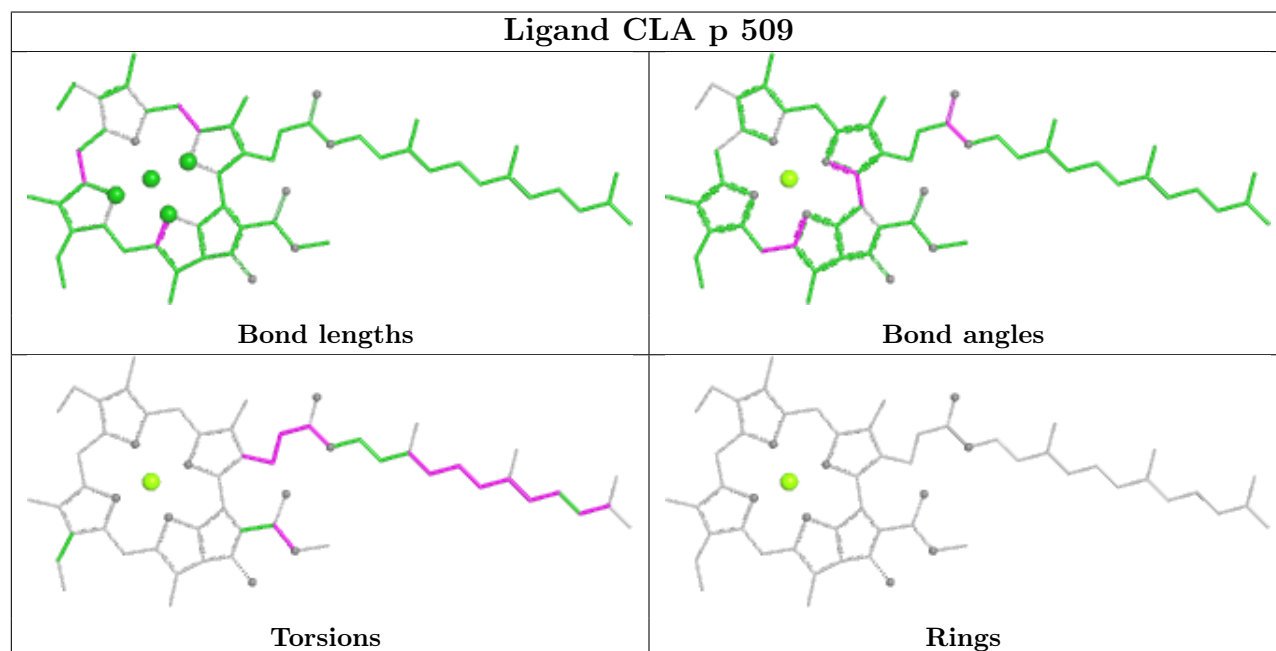
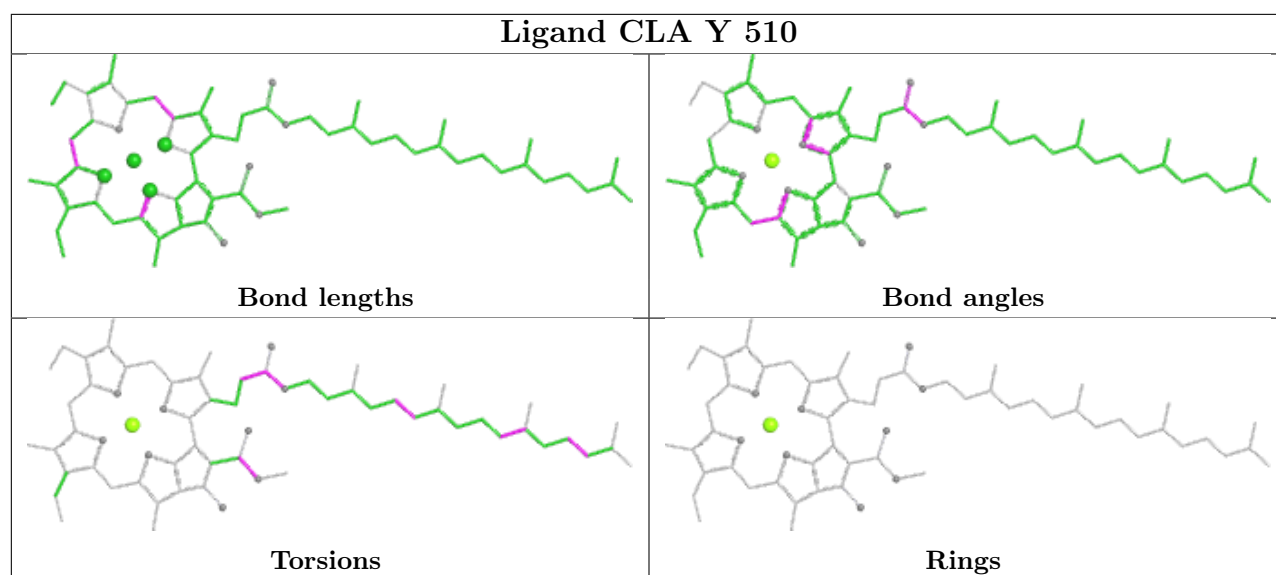
## Ligand CLA G 1234





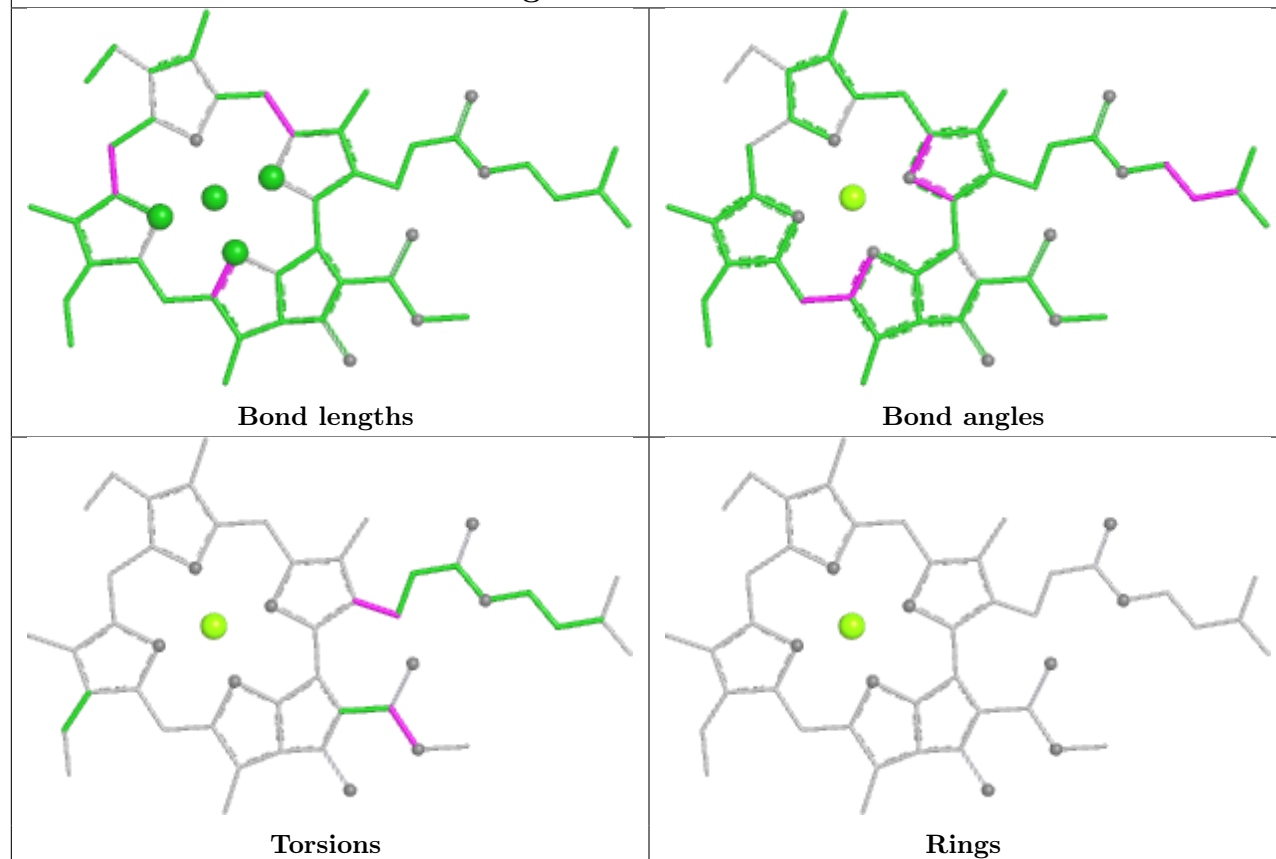




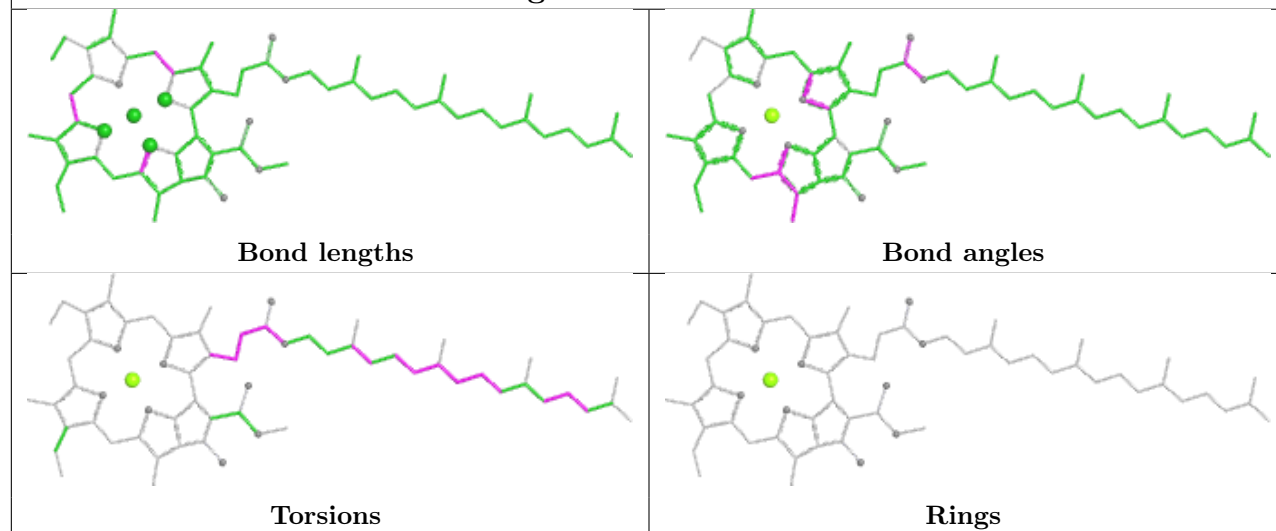




## Ligand CLA A 1107

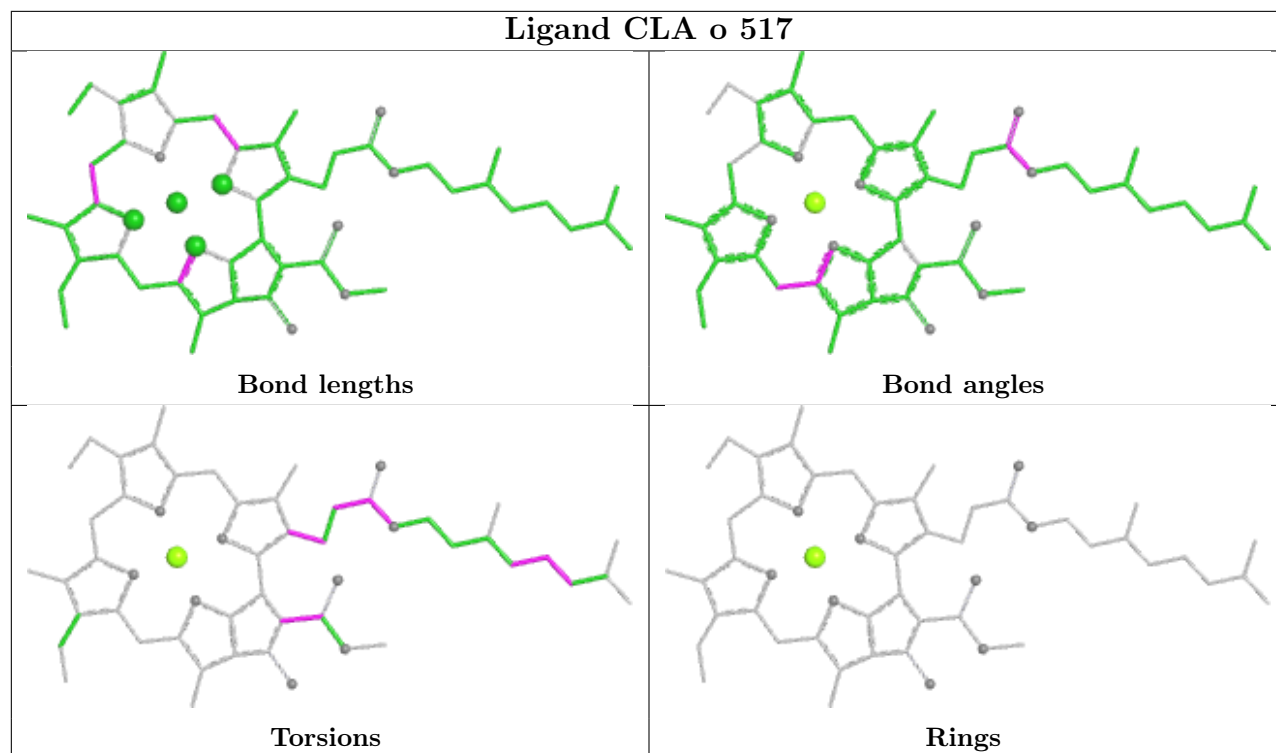


## Ligand CLA a 1101

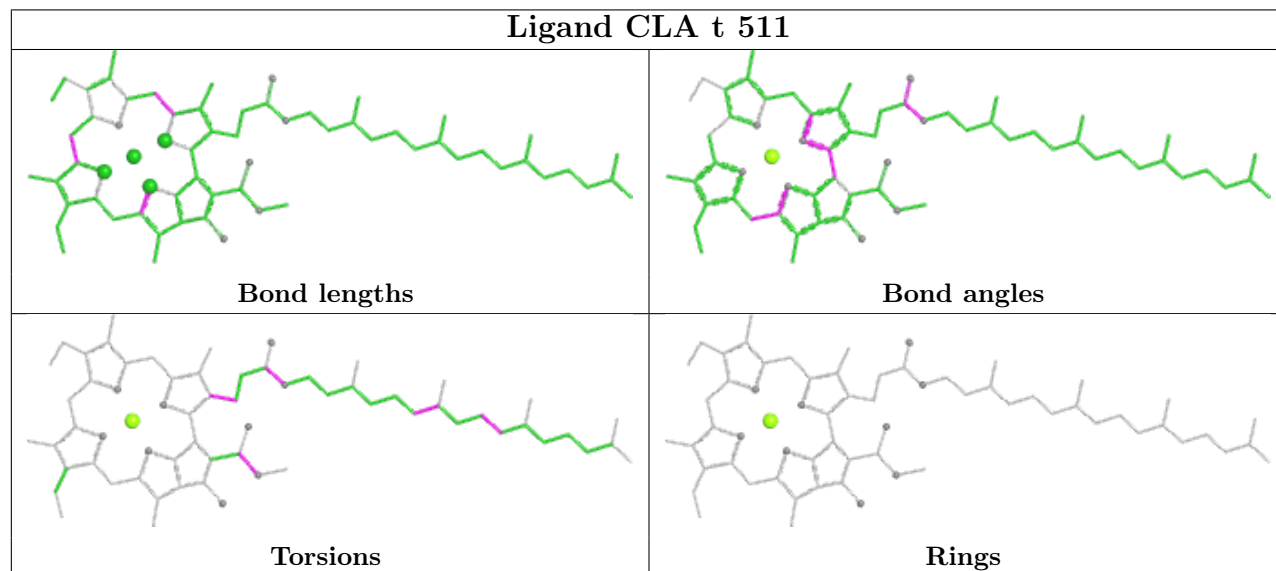




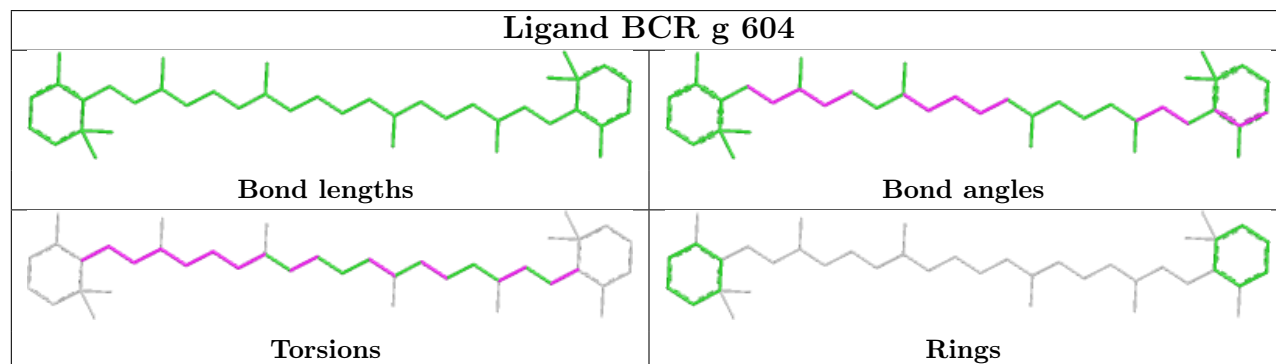
## Ligand CLA o 517



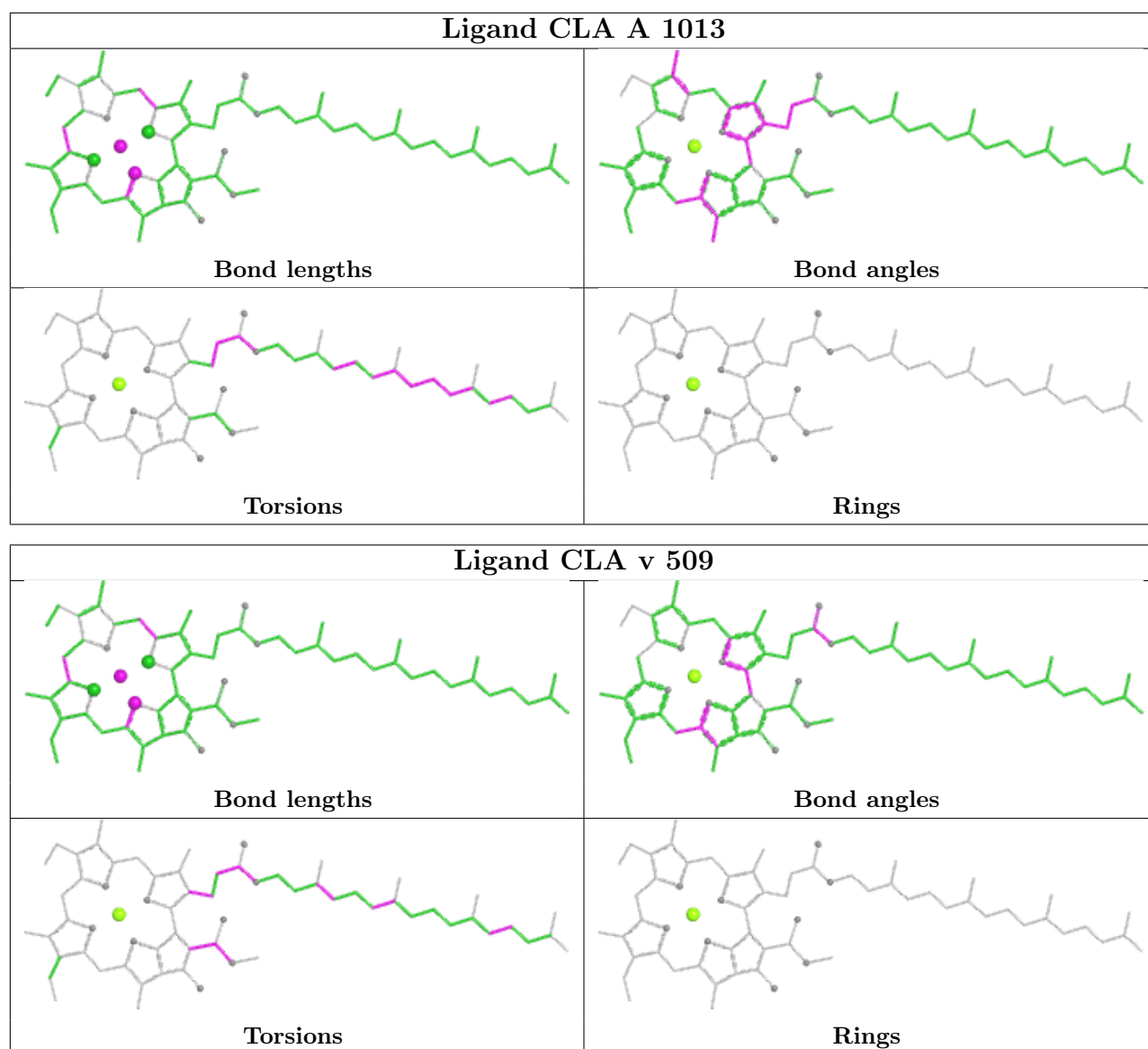
## Ligand CLA t 511



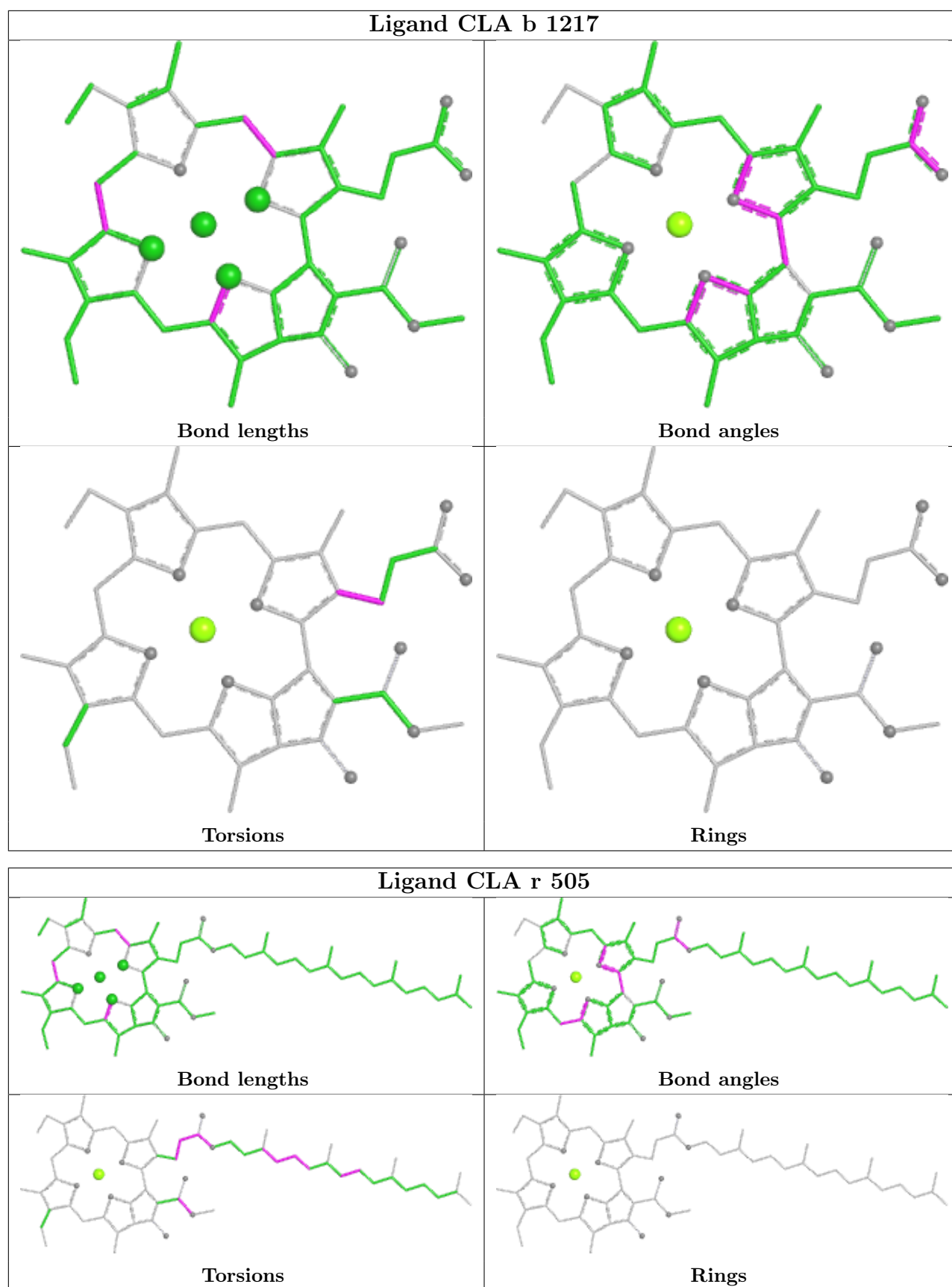
## Ligand BCR g 604



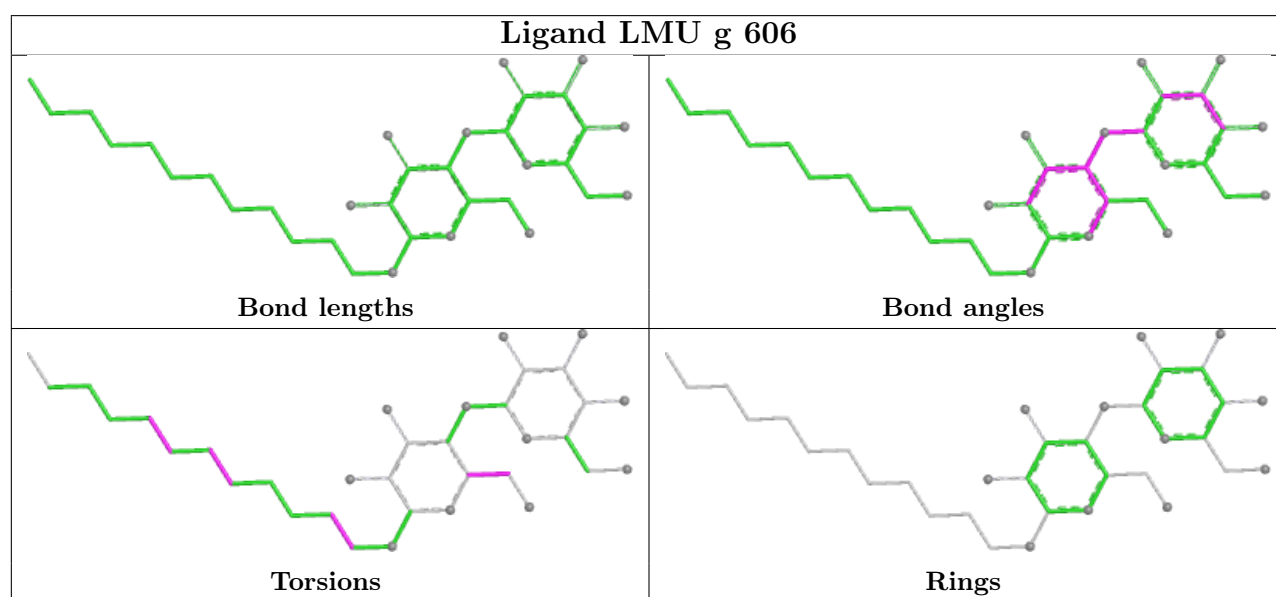
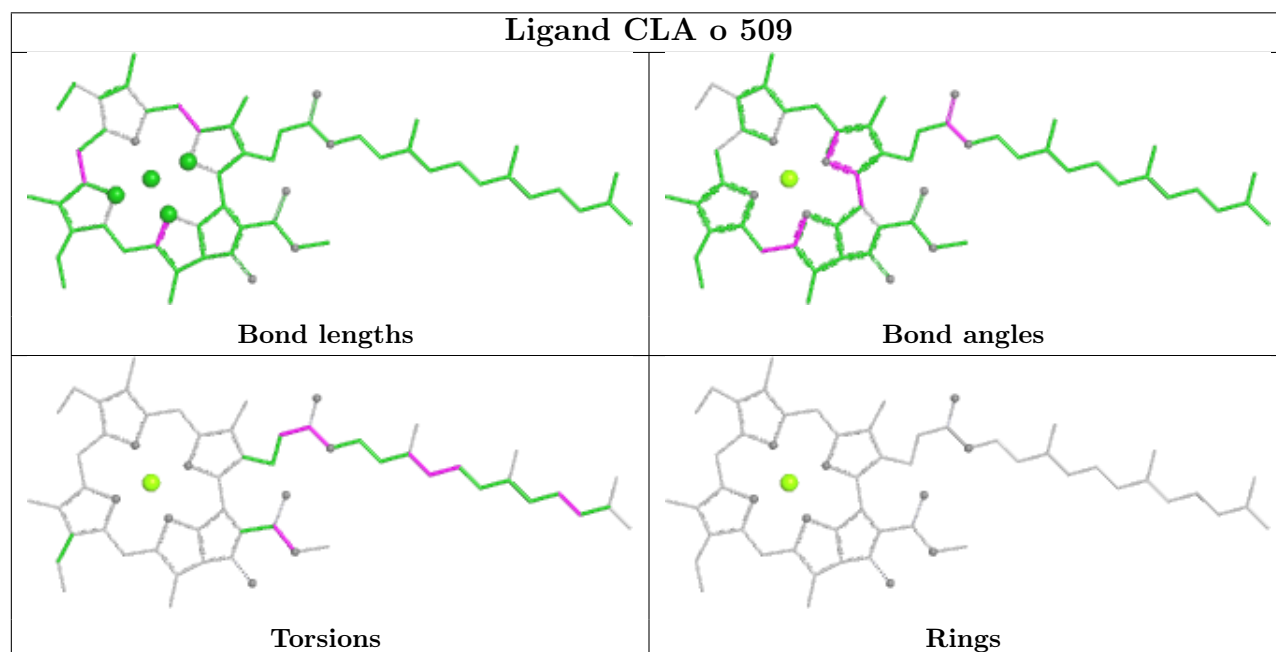
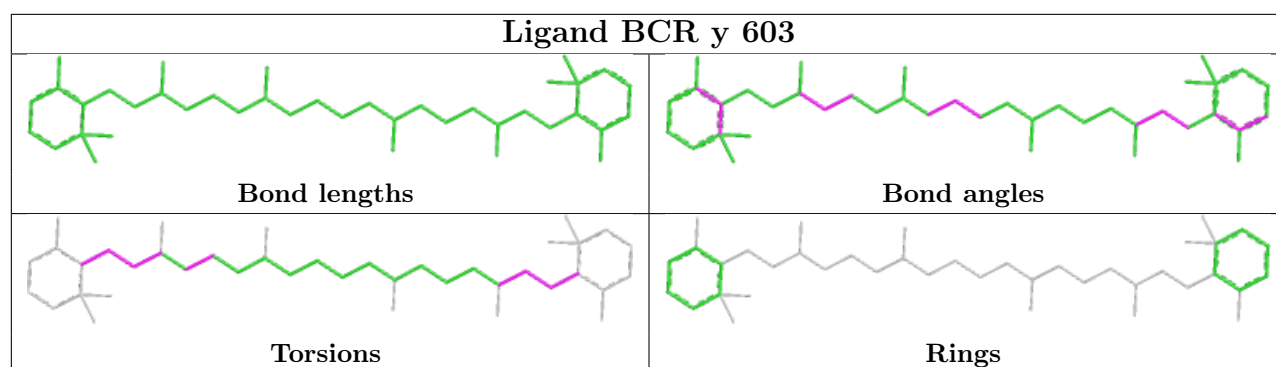






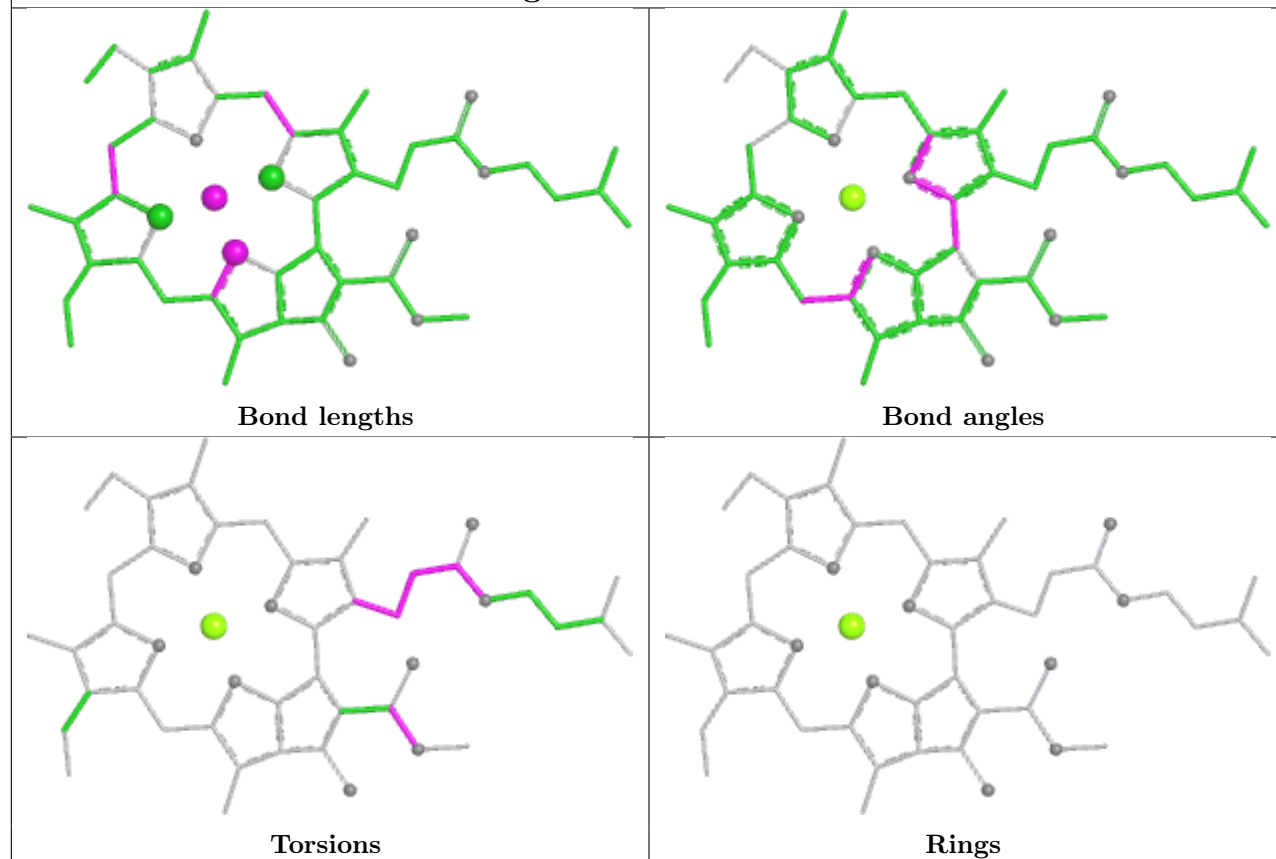




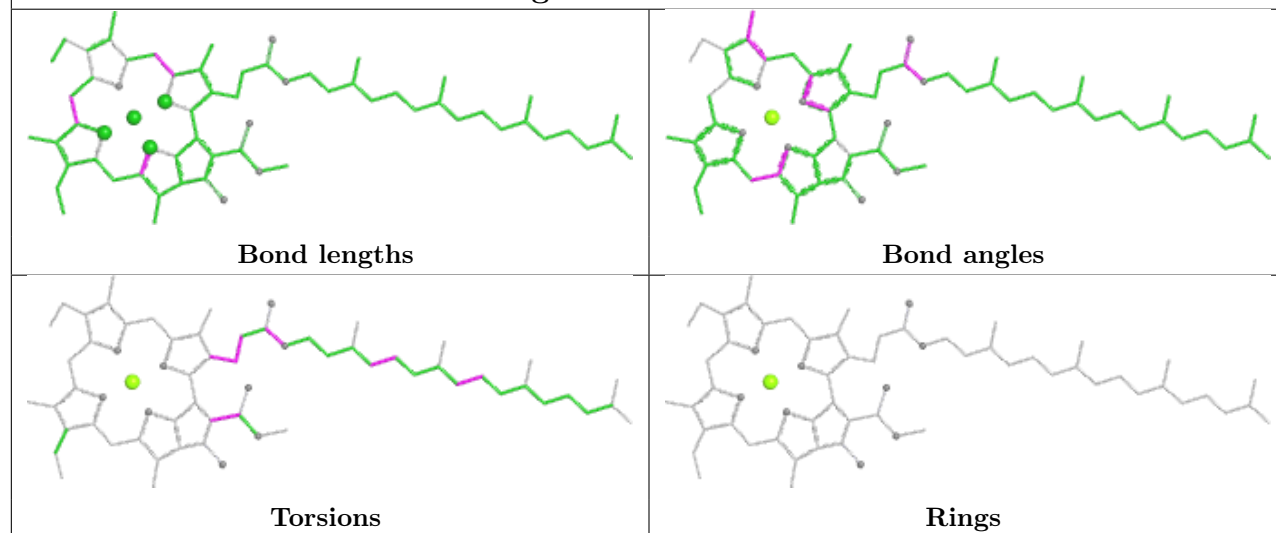




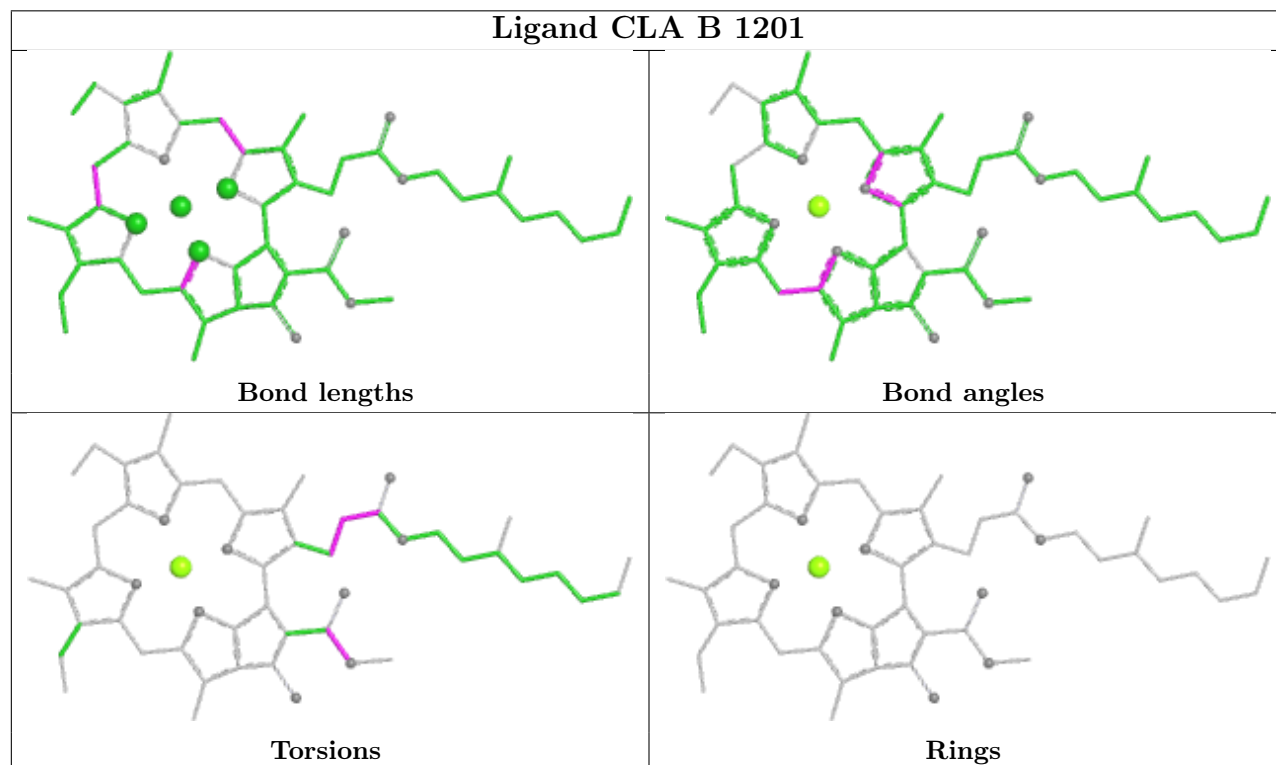
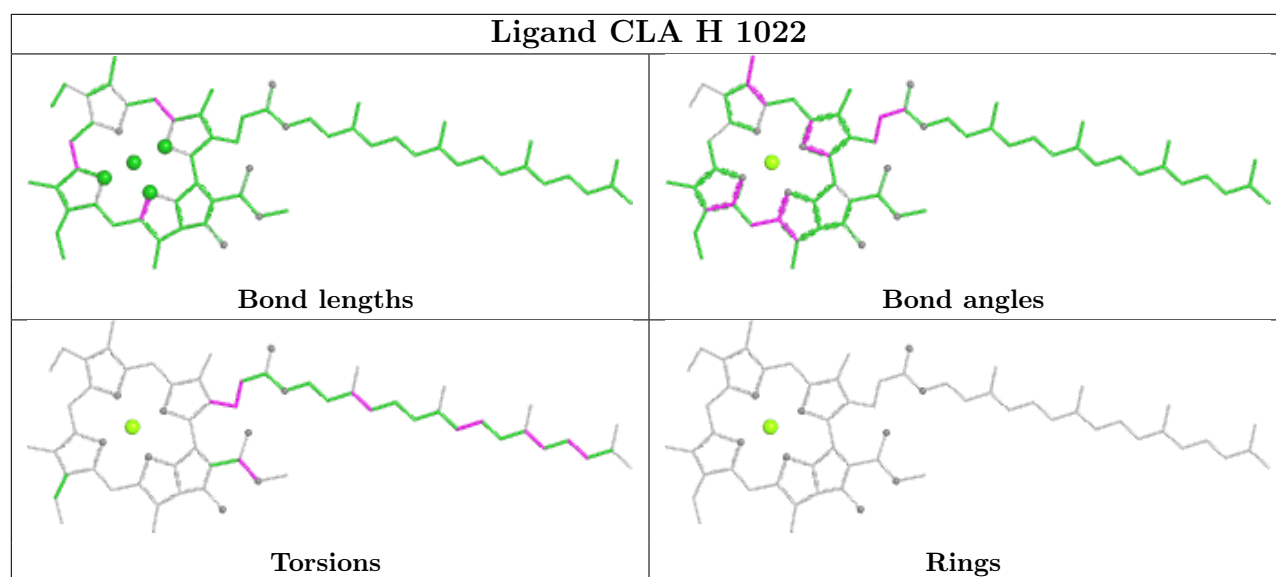
## Ligand CLA B 1236



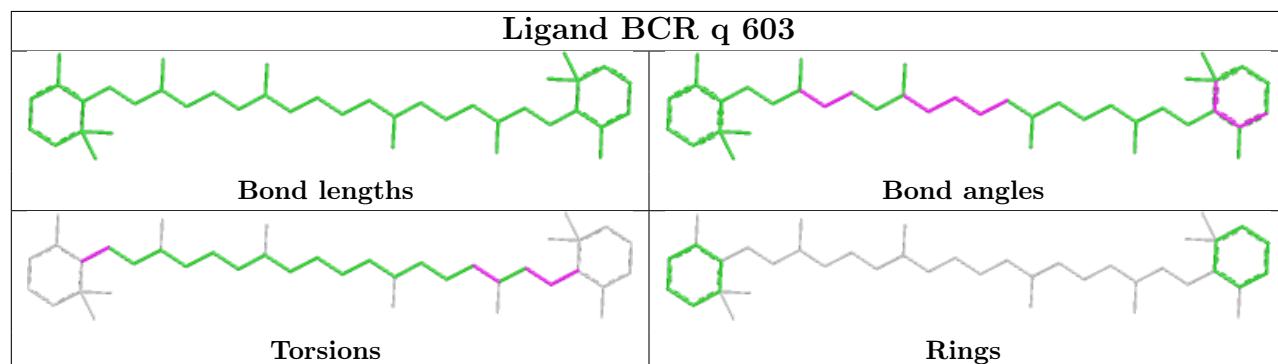
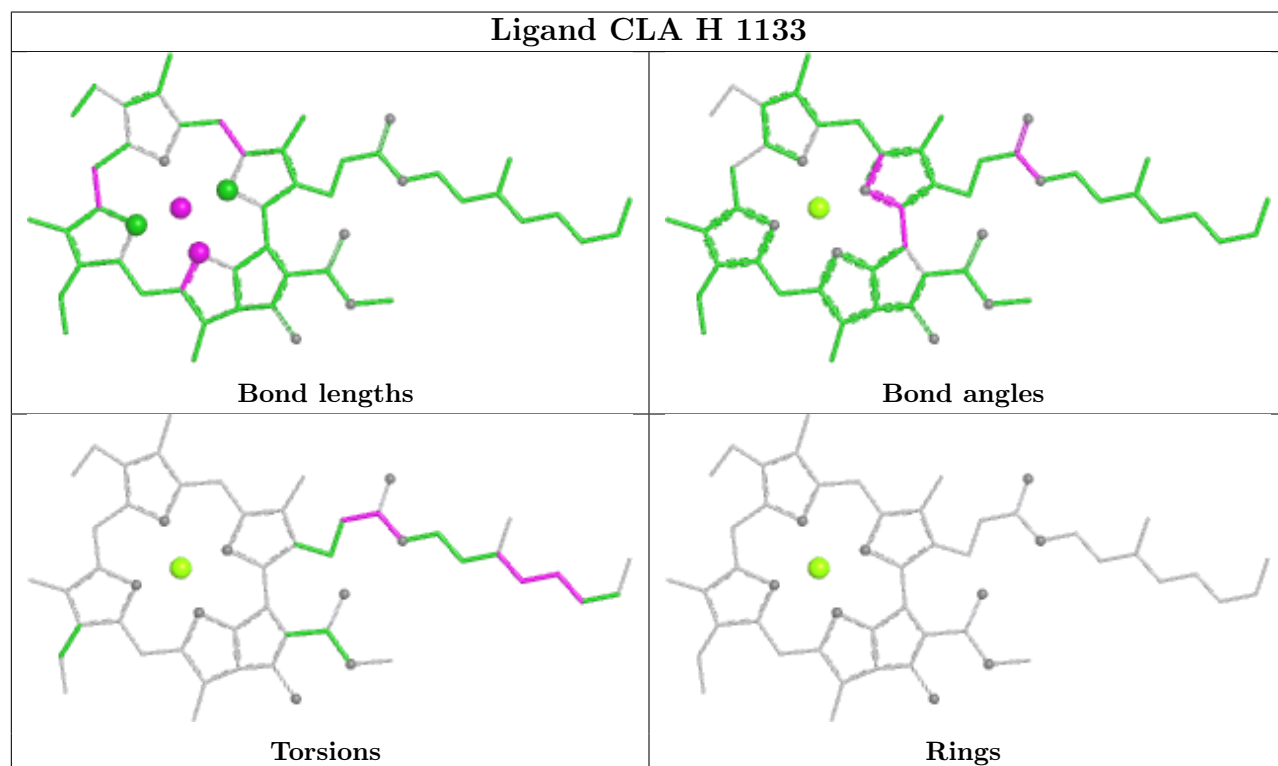
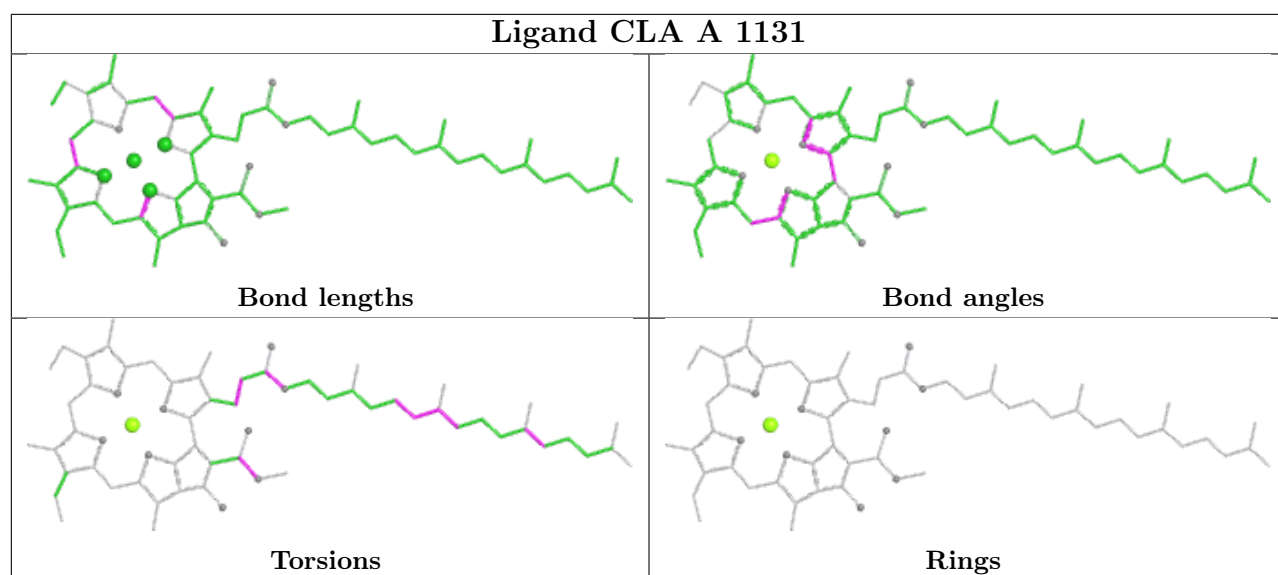
## Ligand CLA Y 515



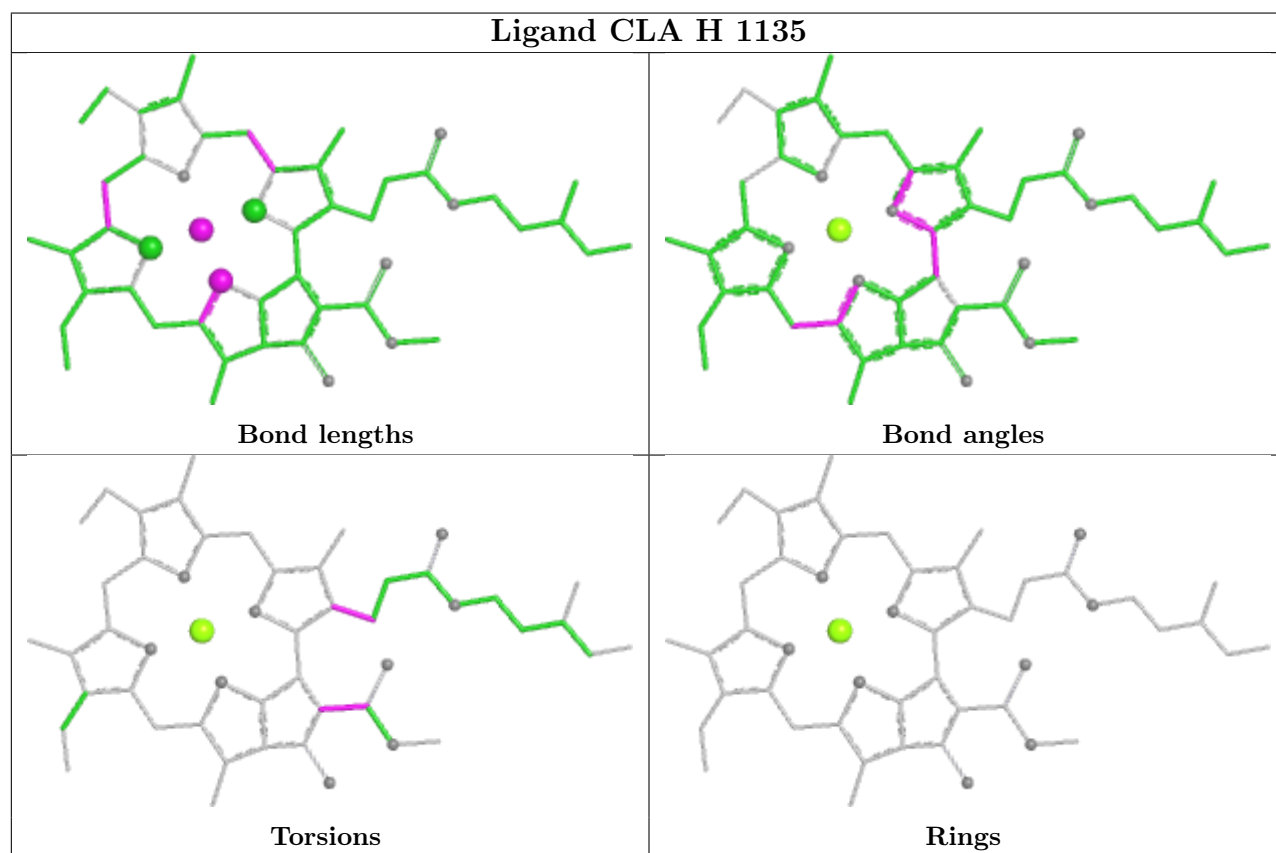
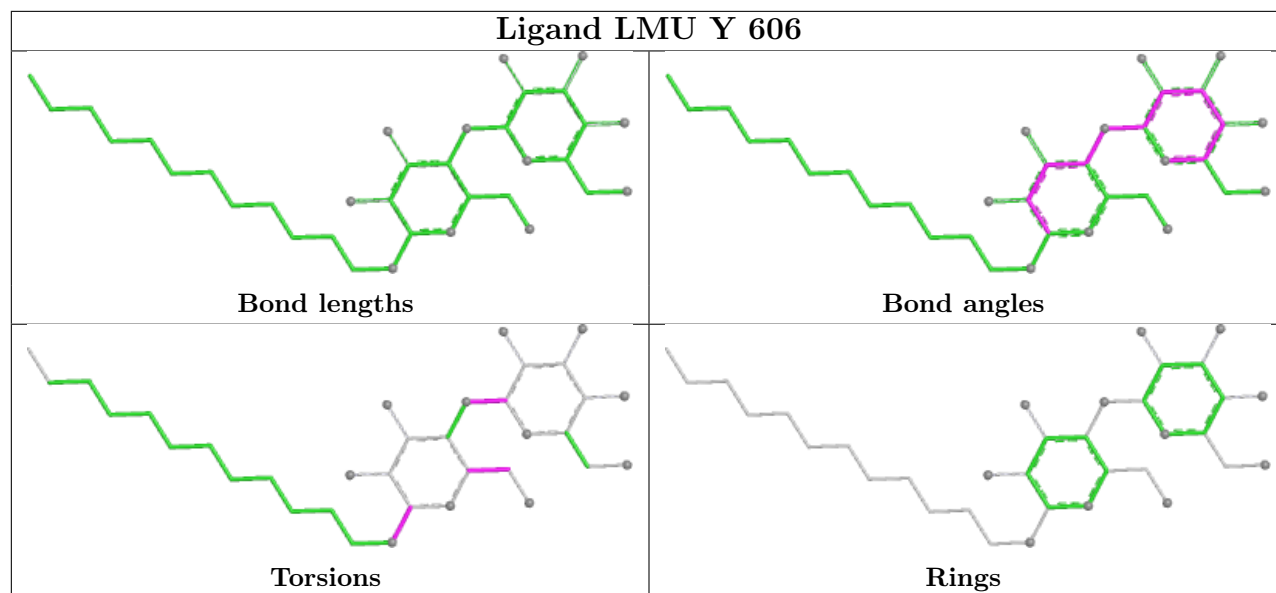




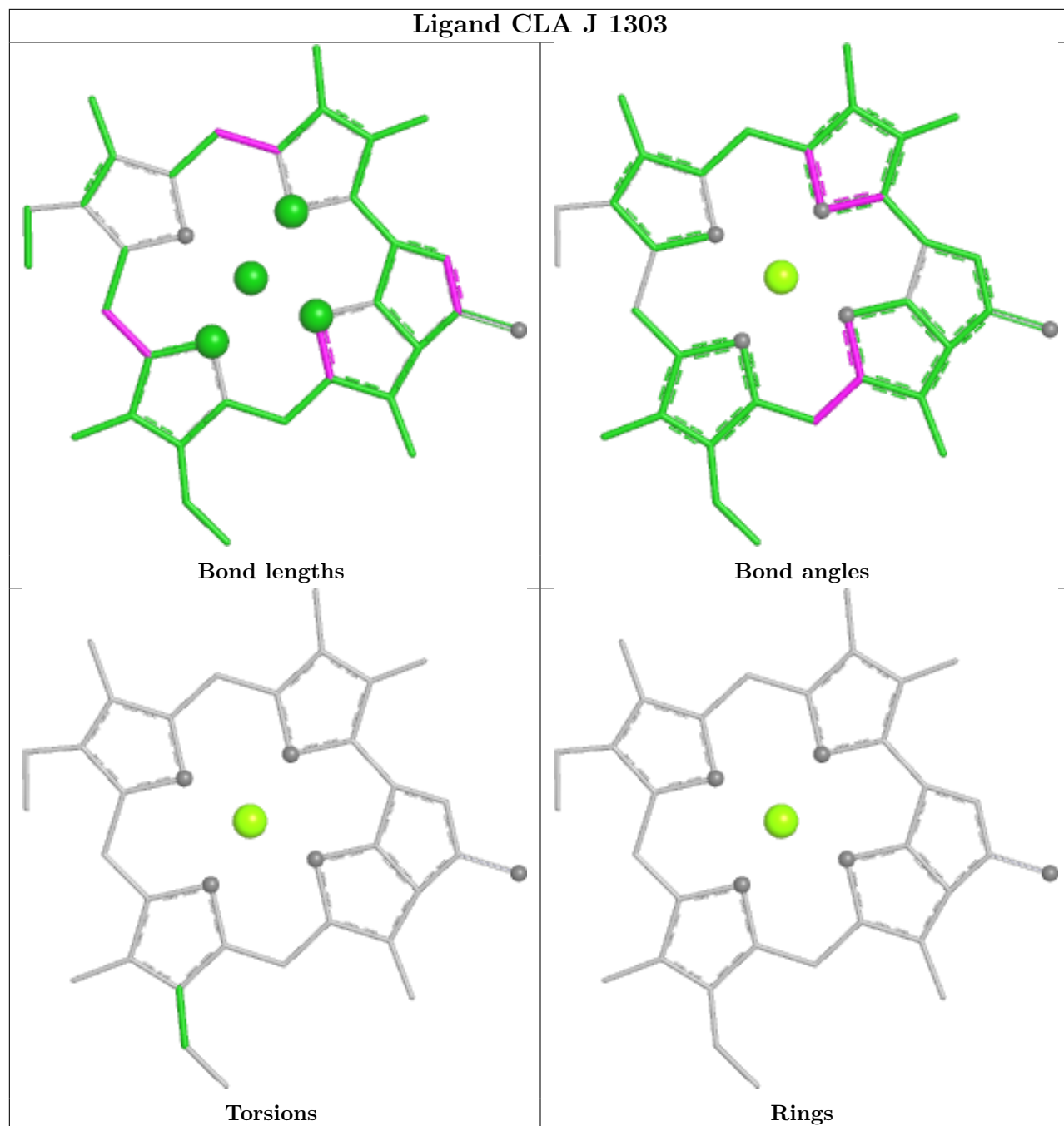






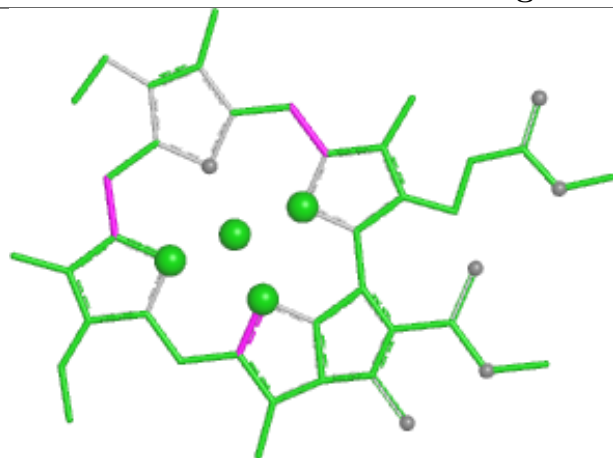




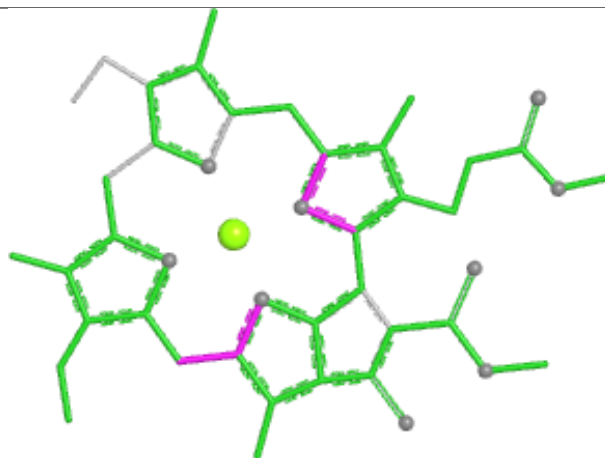




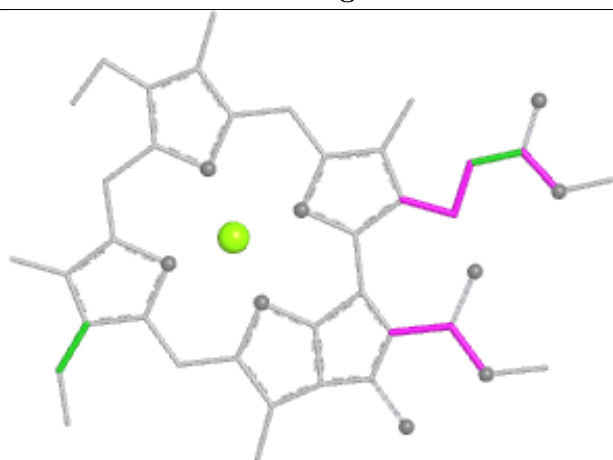
## Ligand CLA Z 516



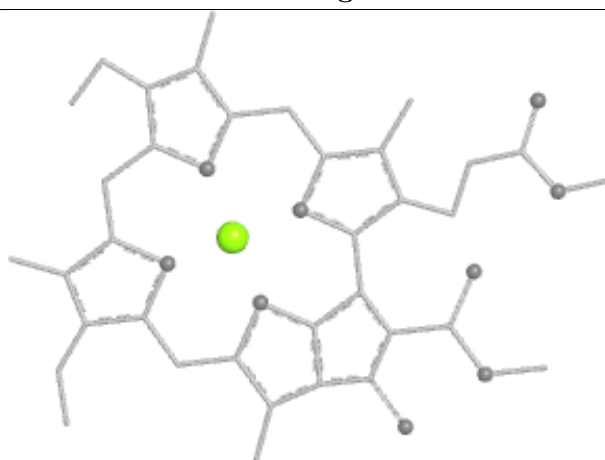
Bond lengths



Bond angles

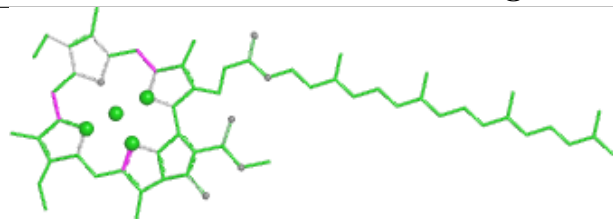


Torsions

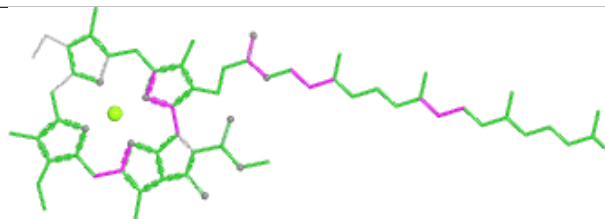


Rings

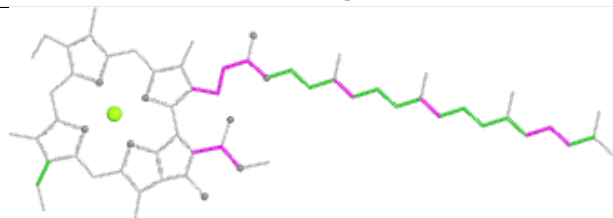
## Ligand CLA A 1101



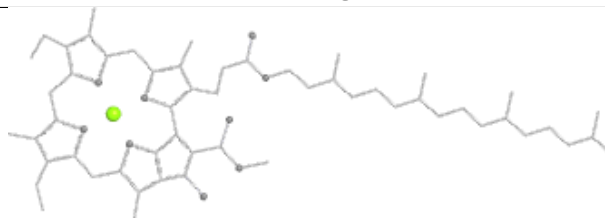
Bond lengths



Bond angles

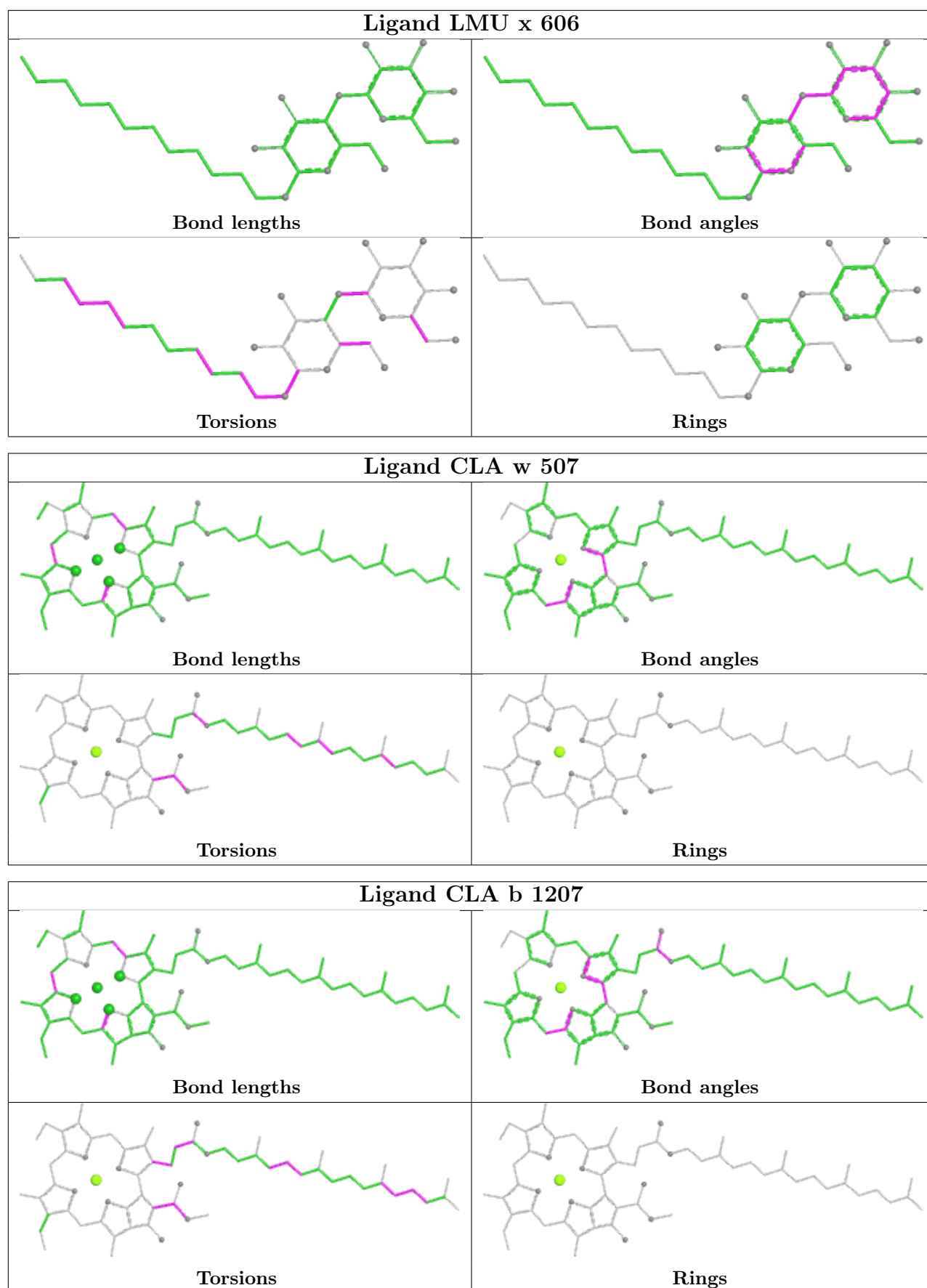


Torsions

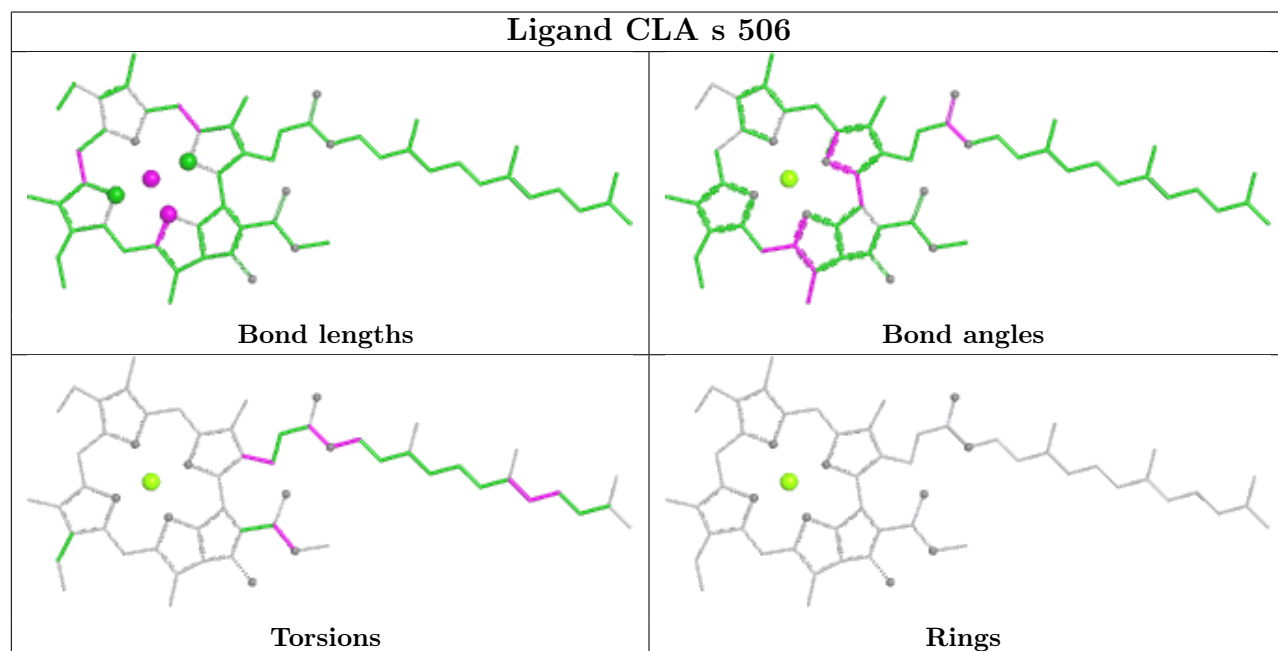
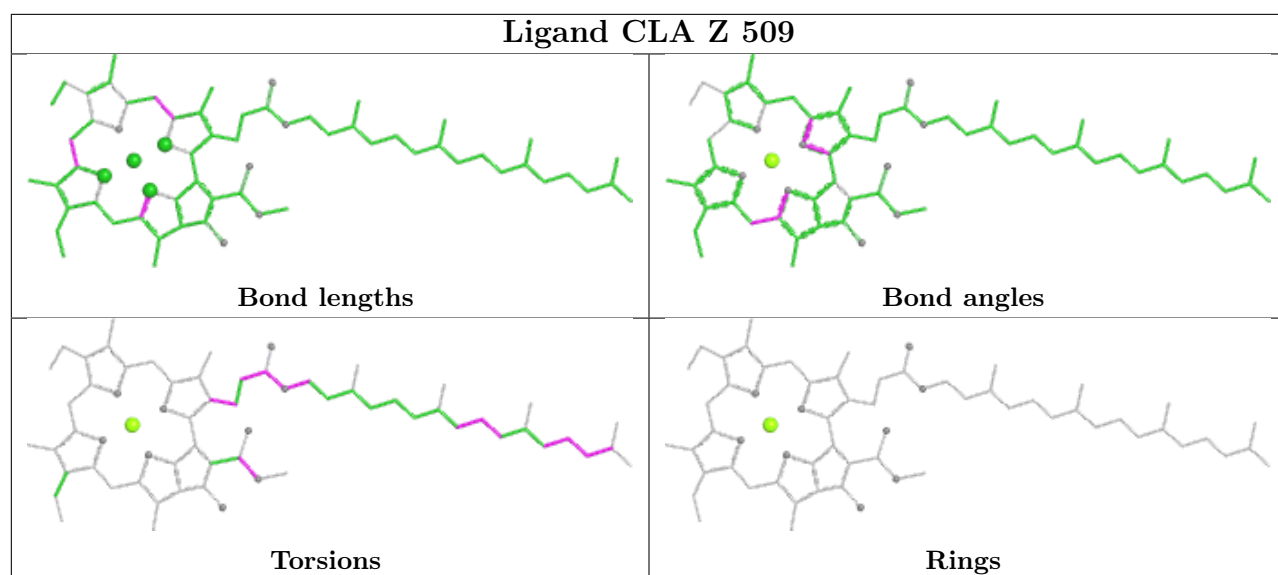


Rings

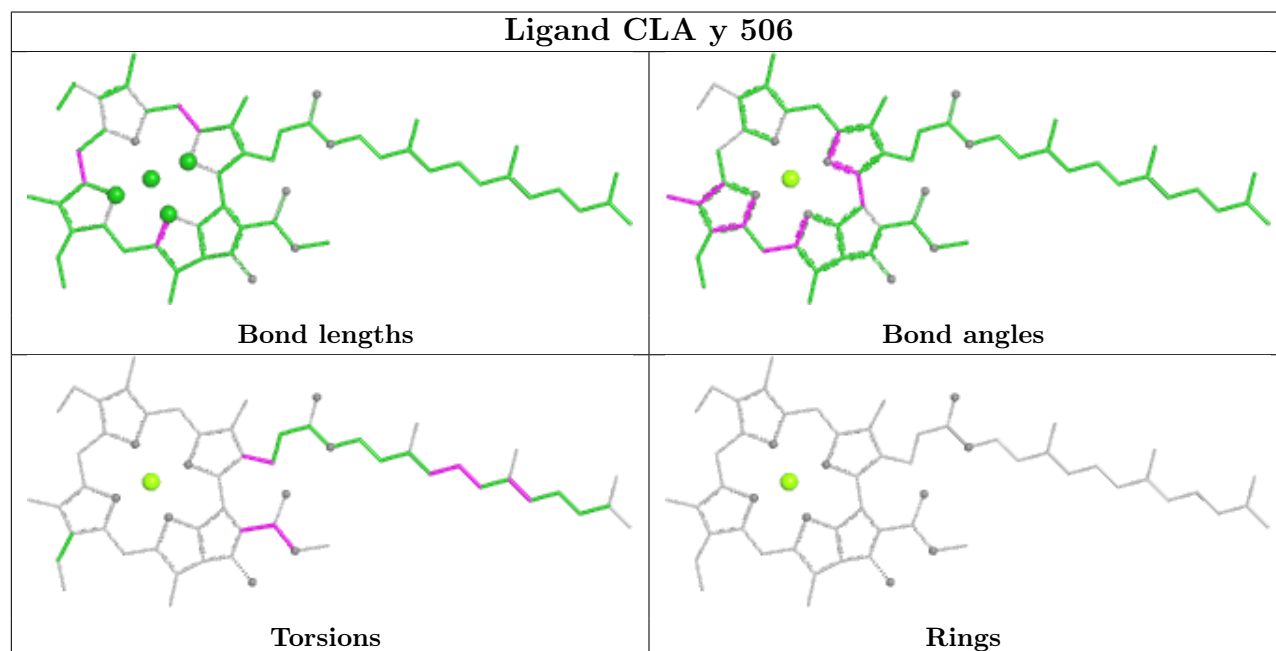
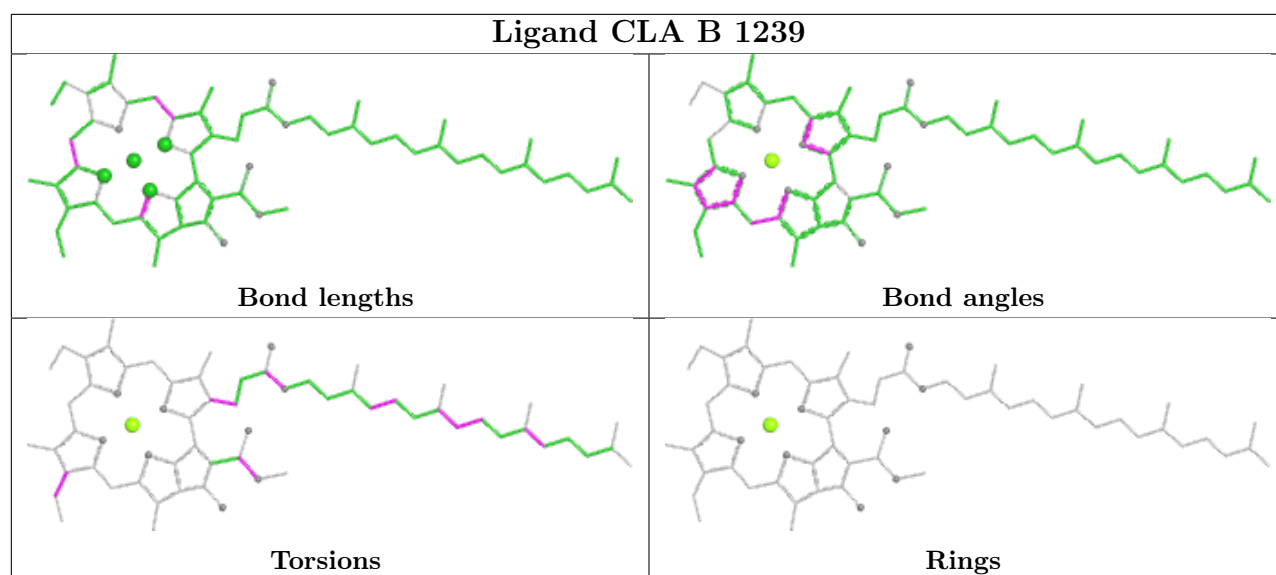




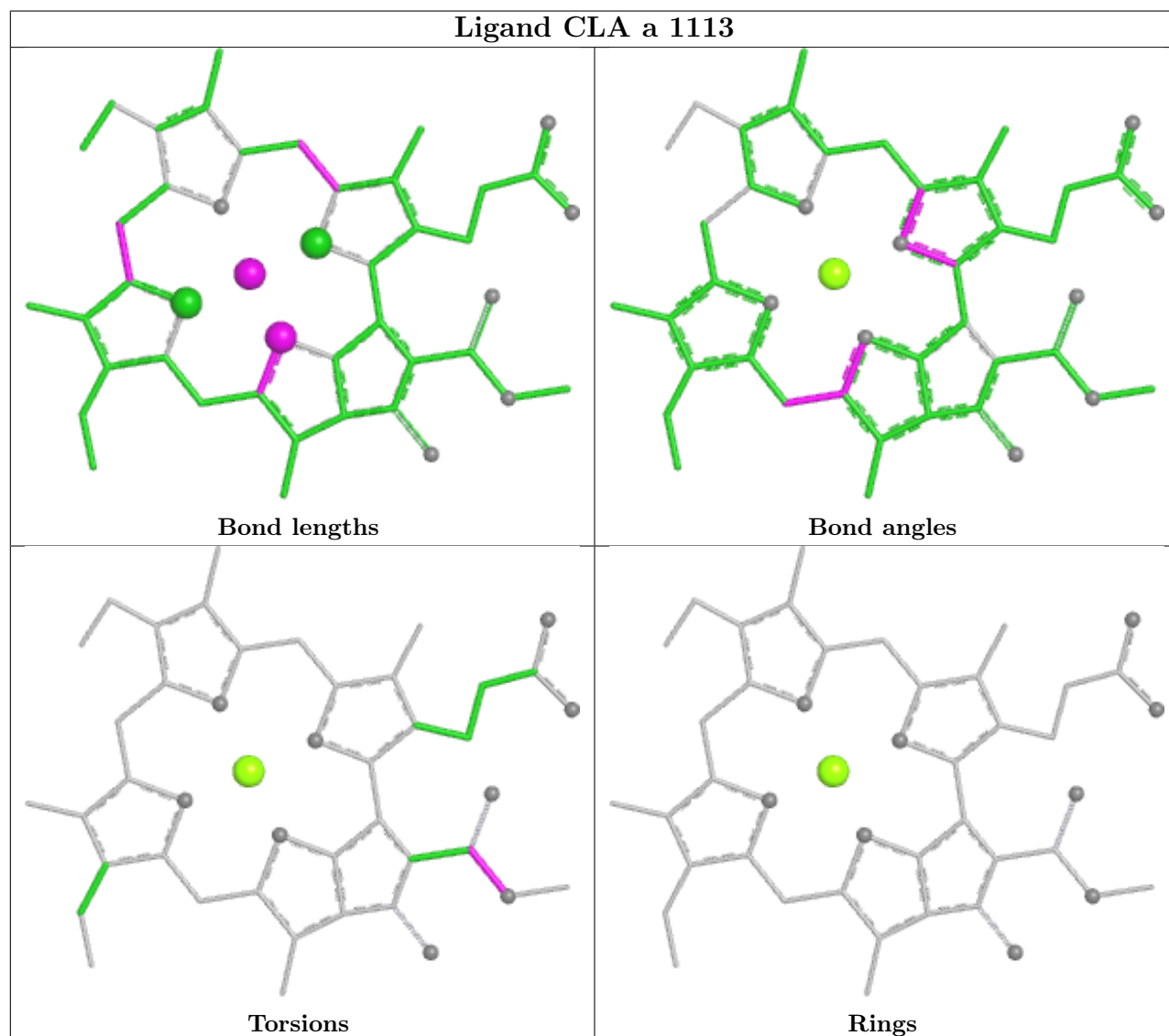
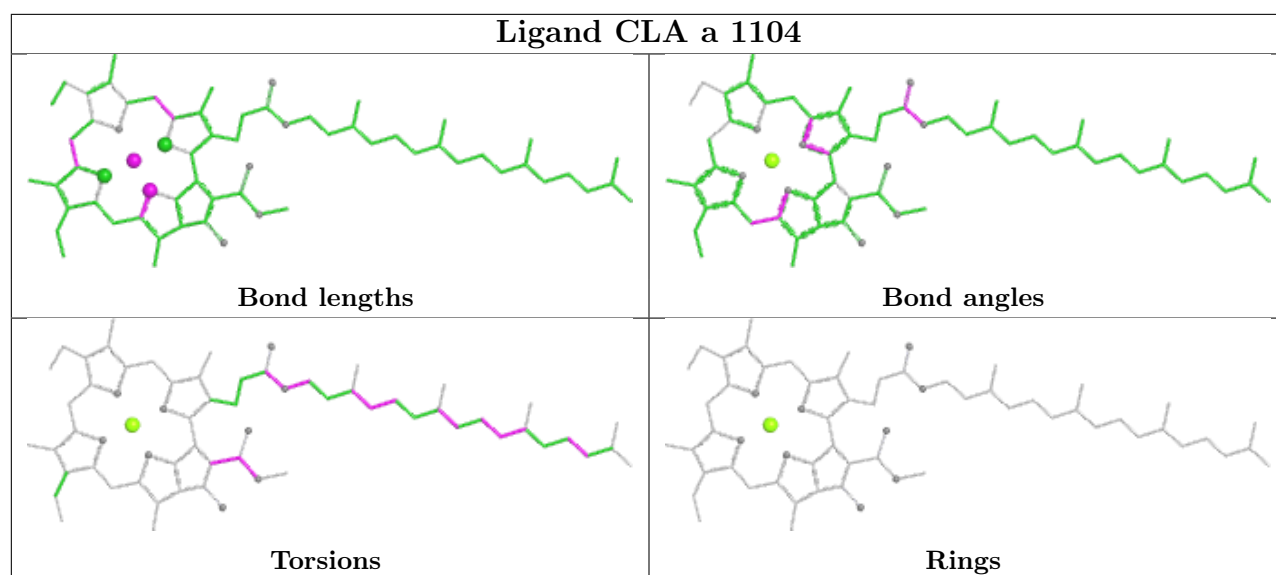






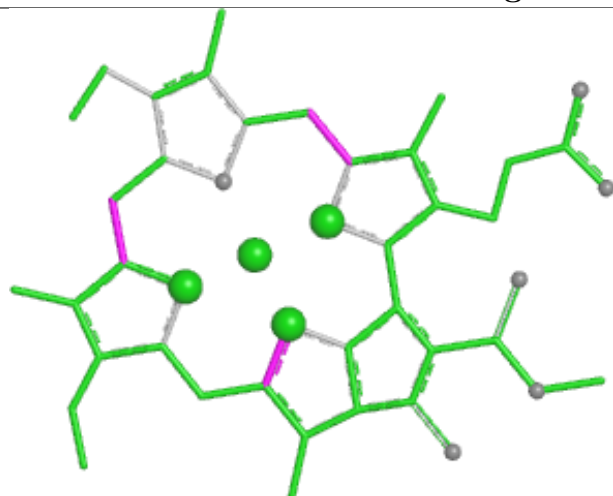




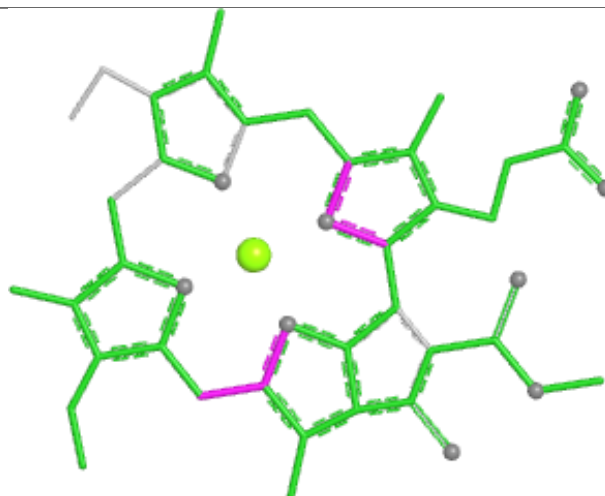




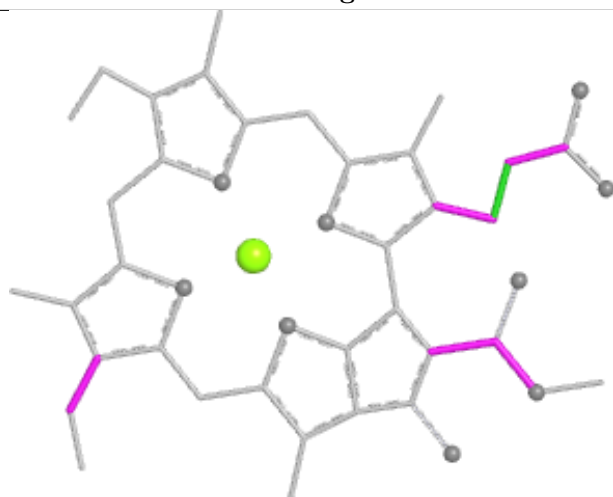
## Ligand CLA K 4003



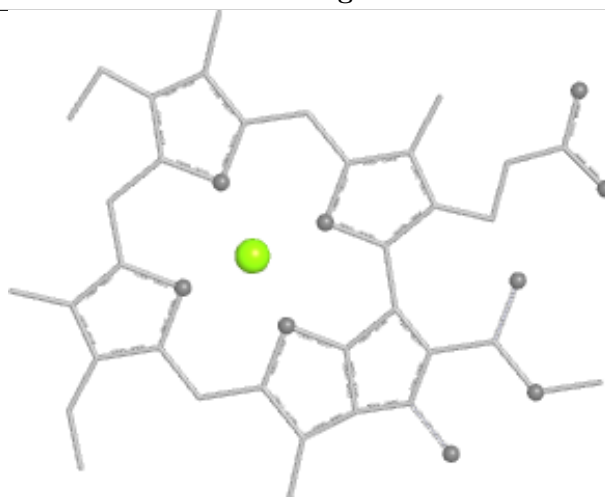
Bond lengths



Bond angles

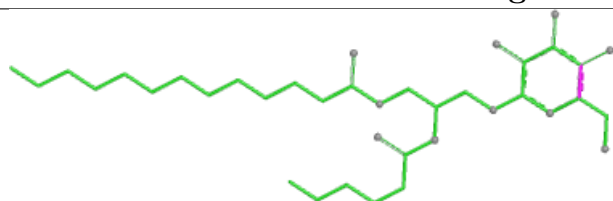


Torsions

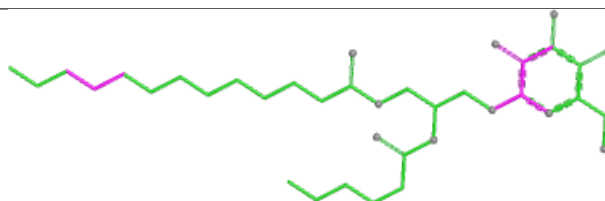


Rings

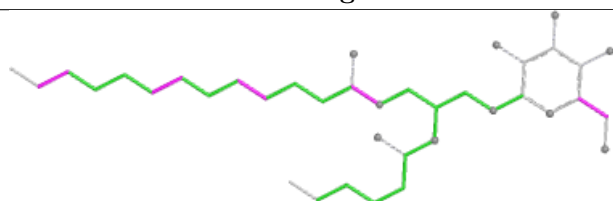
## Ligand LMG H 852



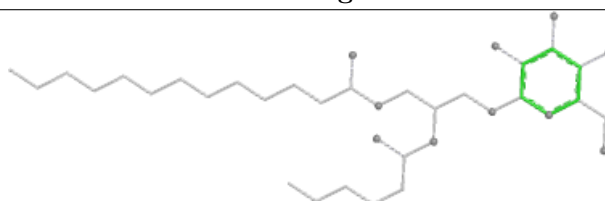
Bond lengths



Bond angles

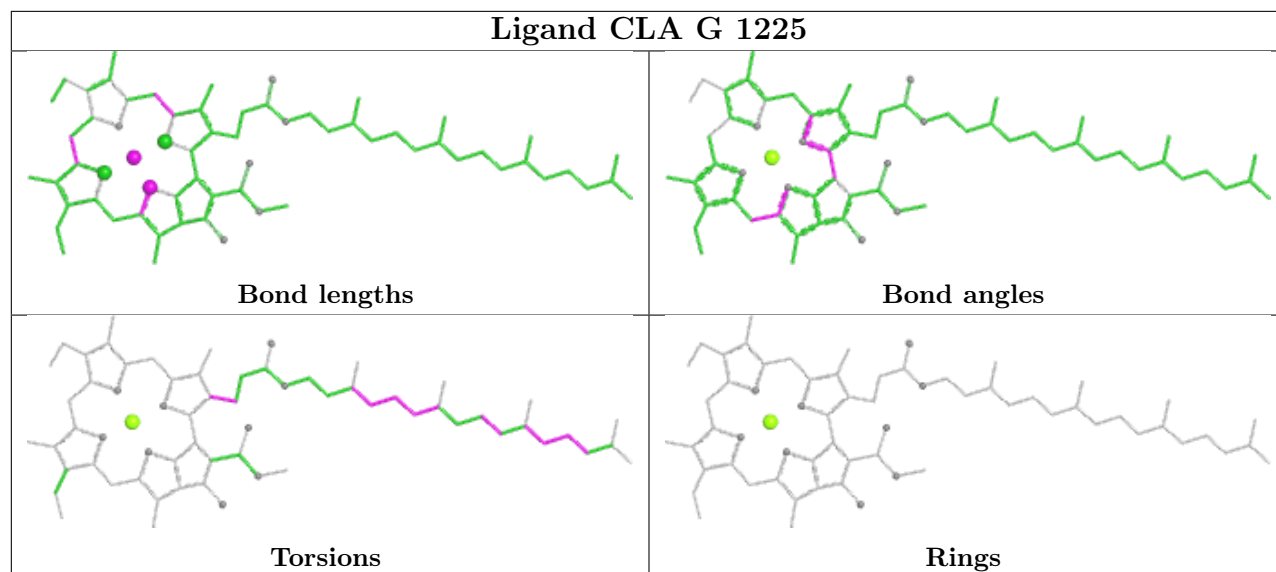
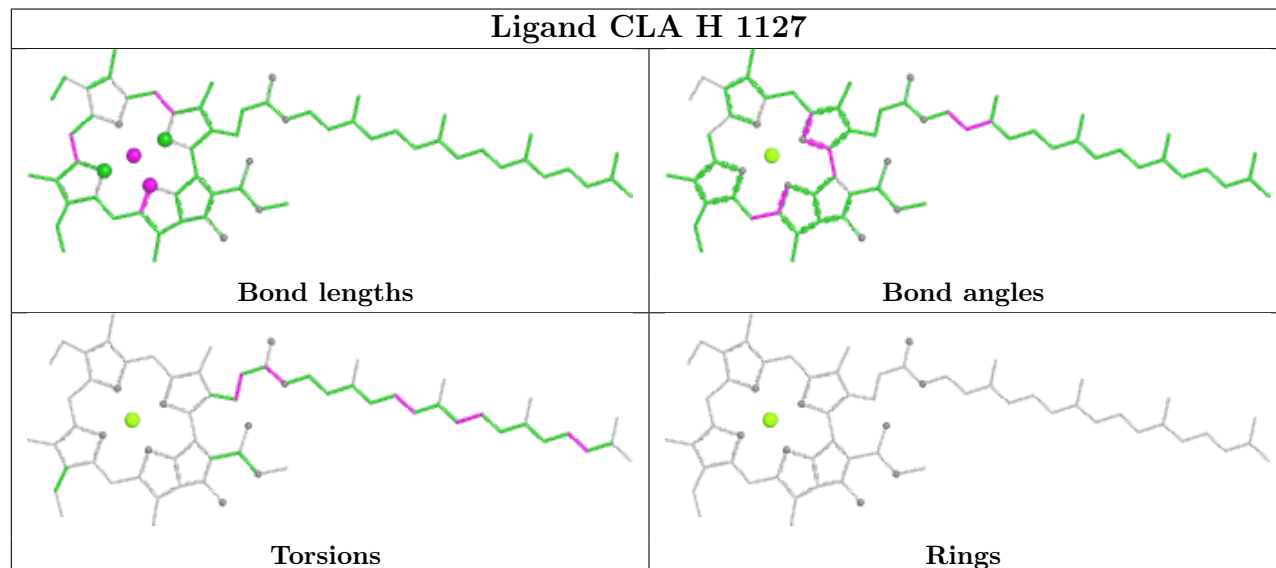


Torsions

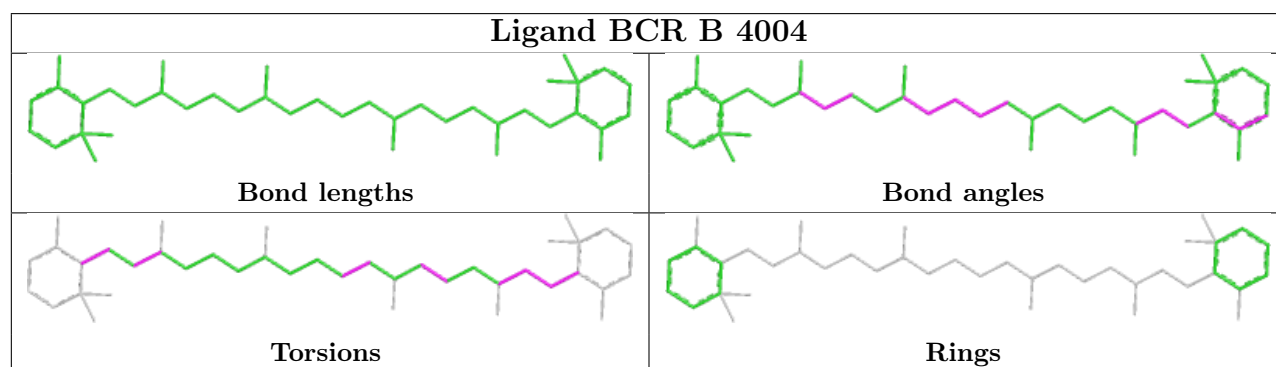
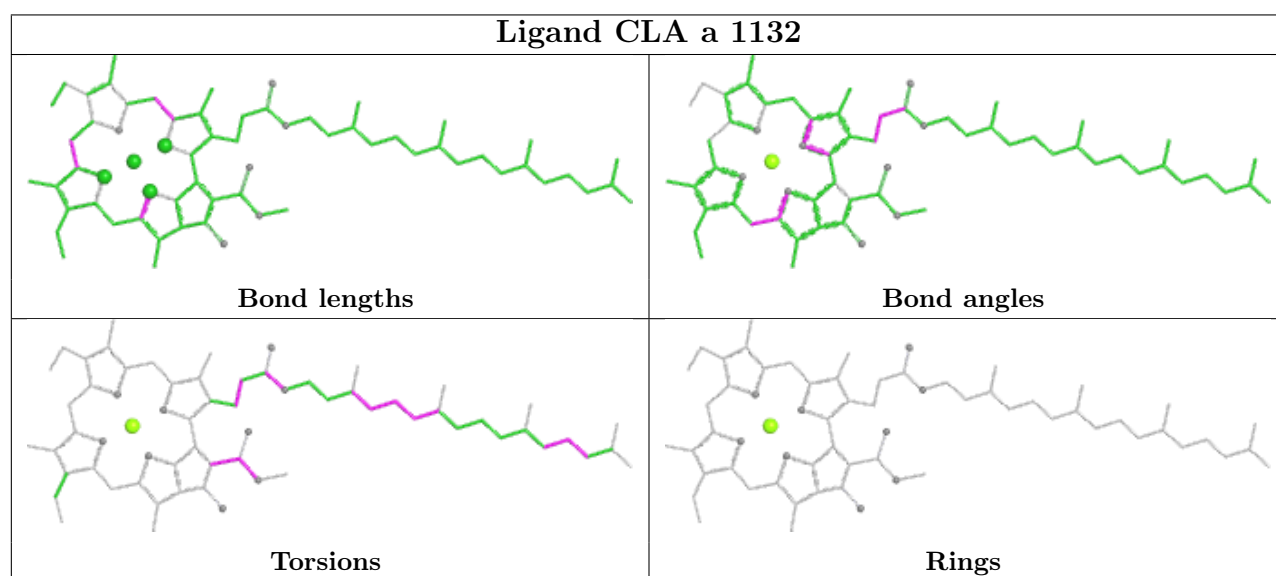
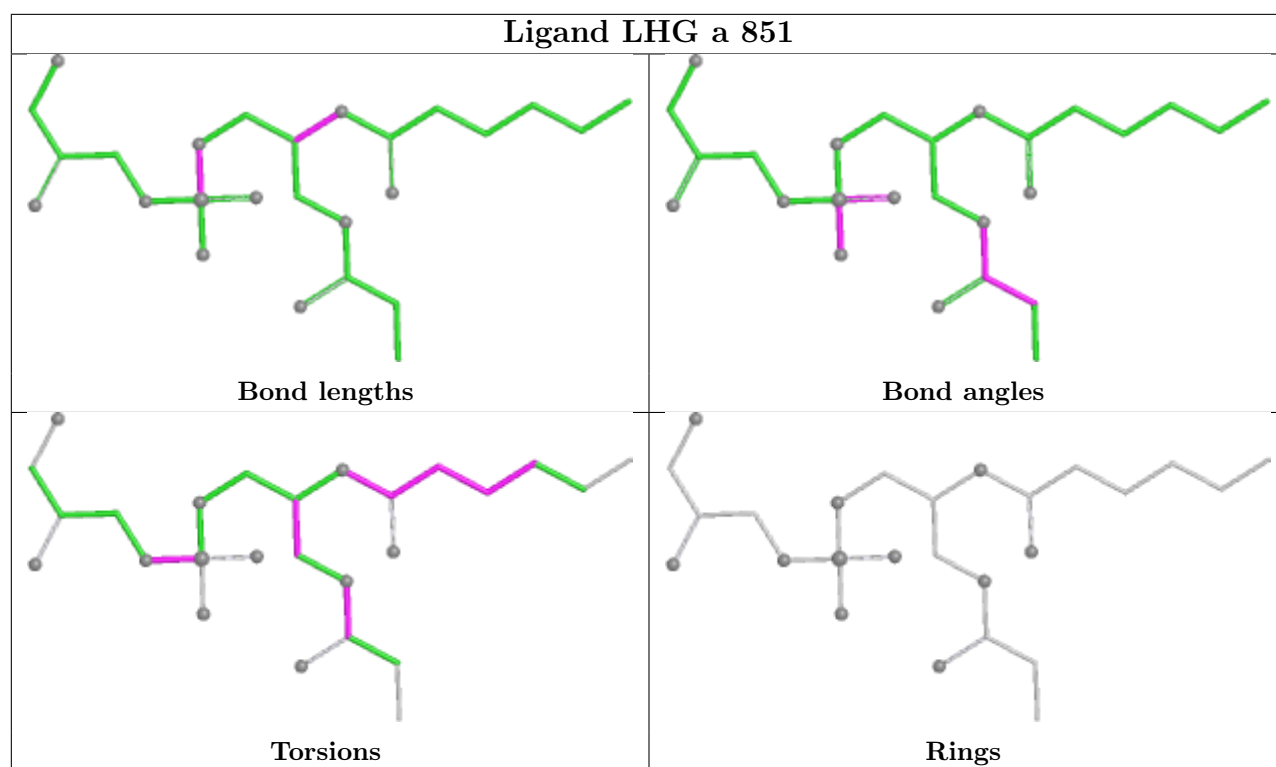


Rings



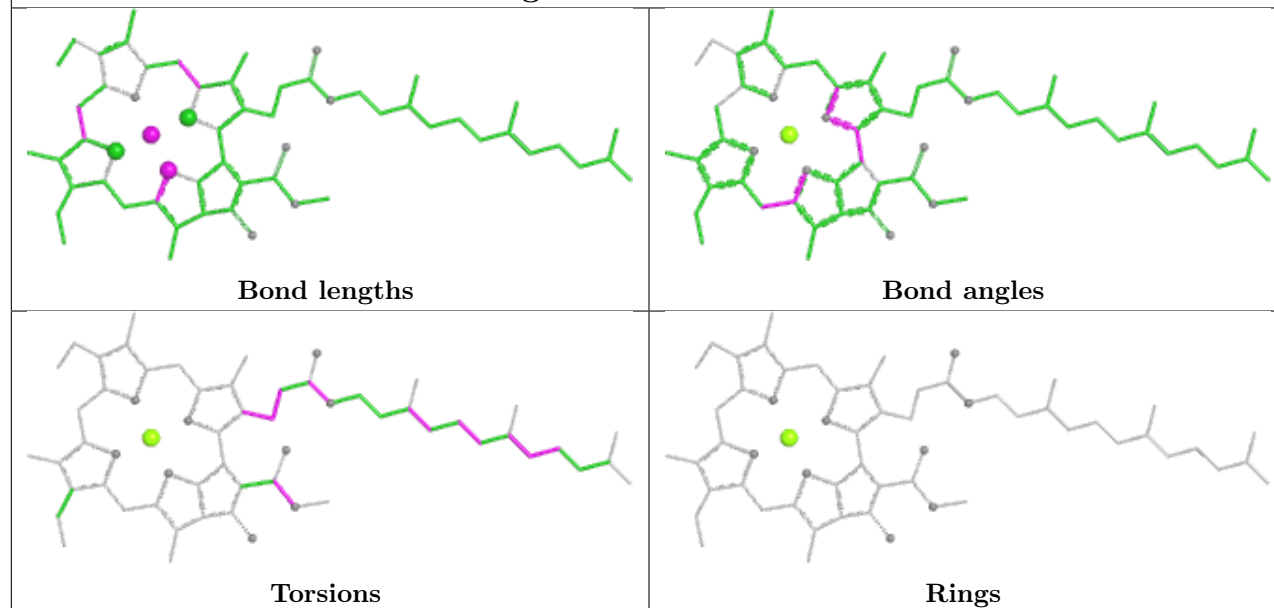
**Ligand CLA G 1225****Ligand CLA H 1127**



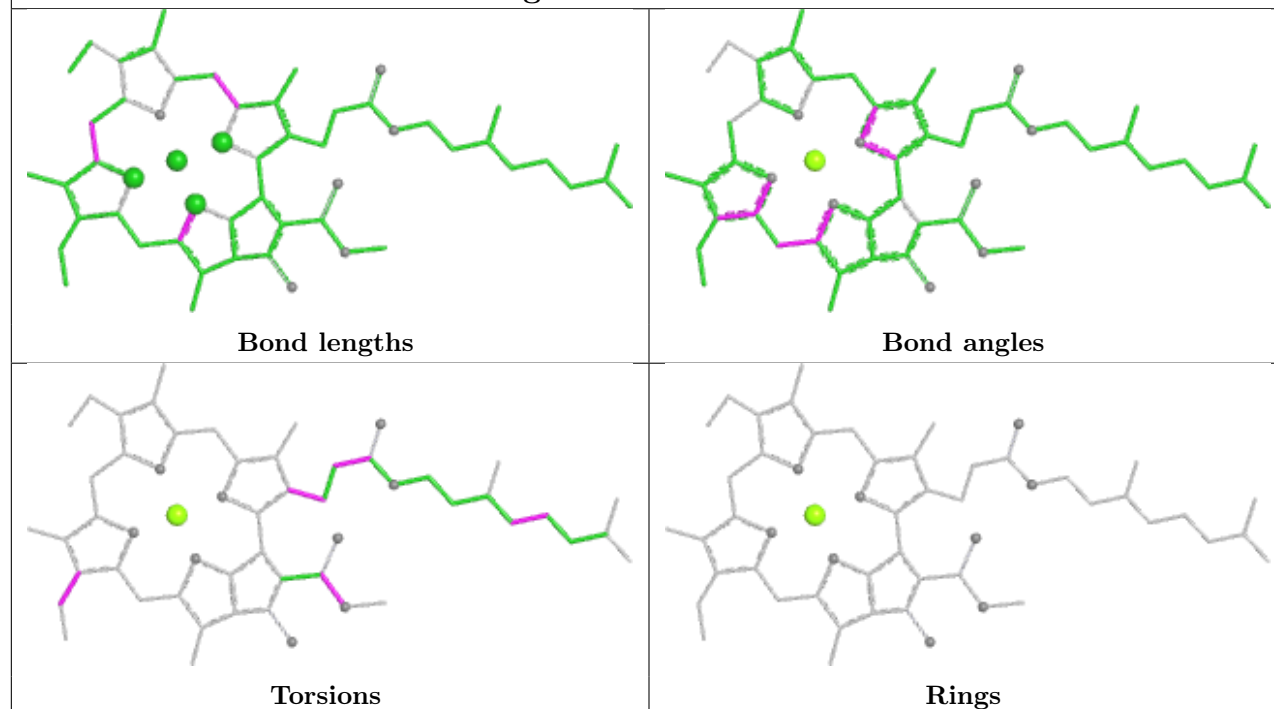




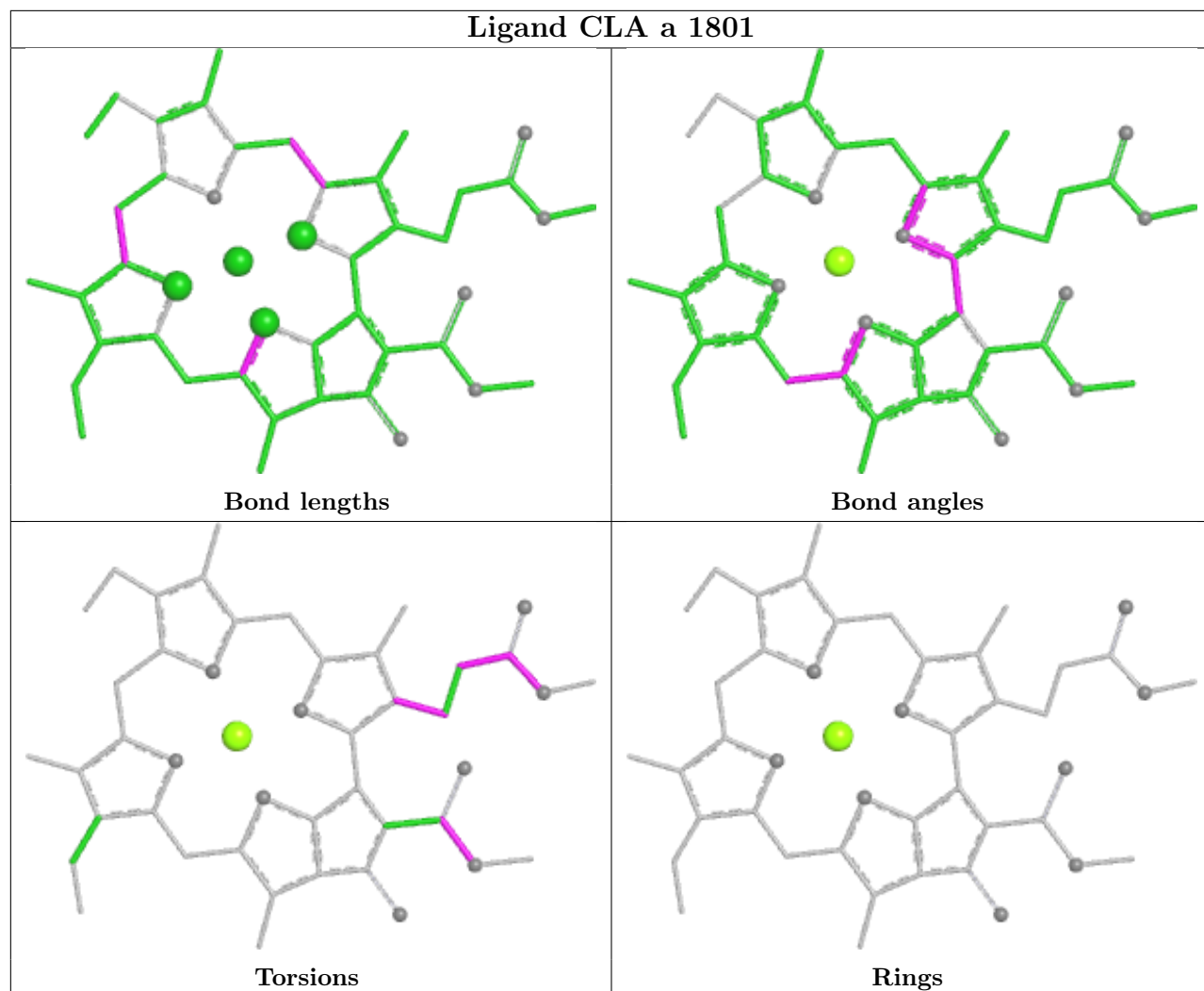
## Ligand CLA G 1224



## Ligand CLA B 1214

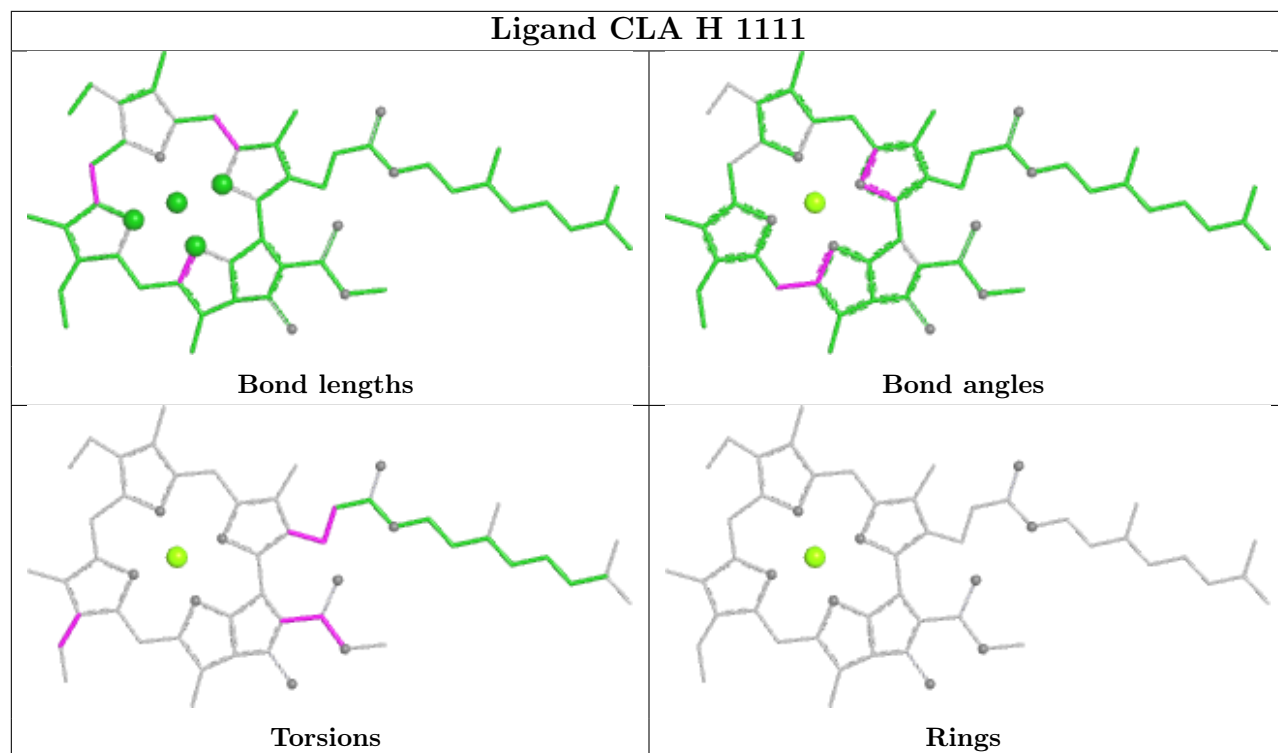




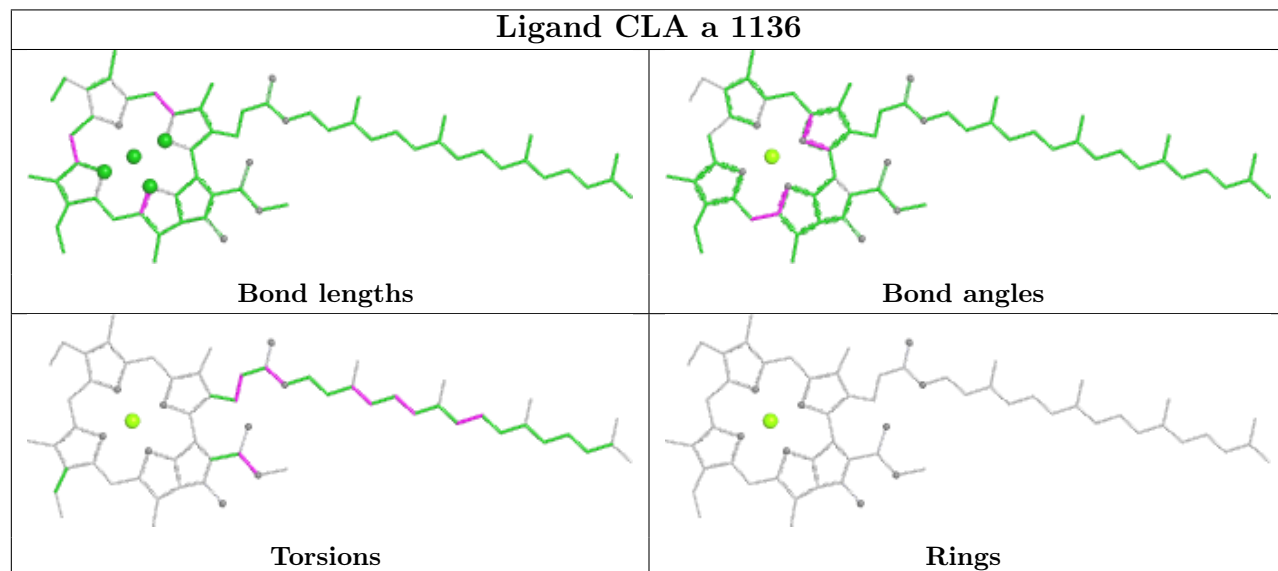




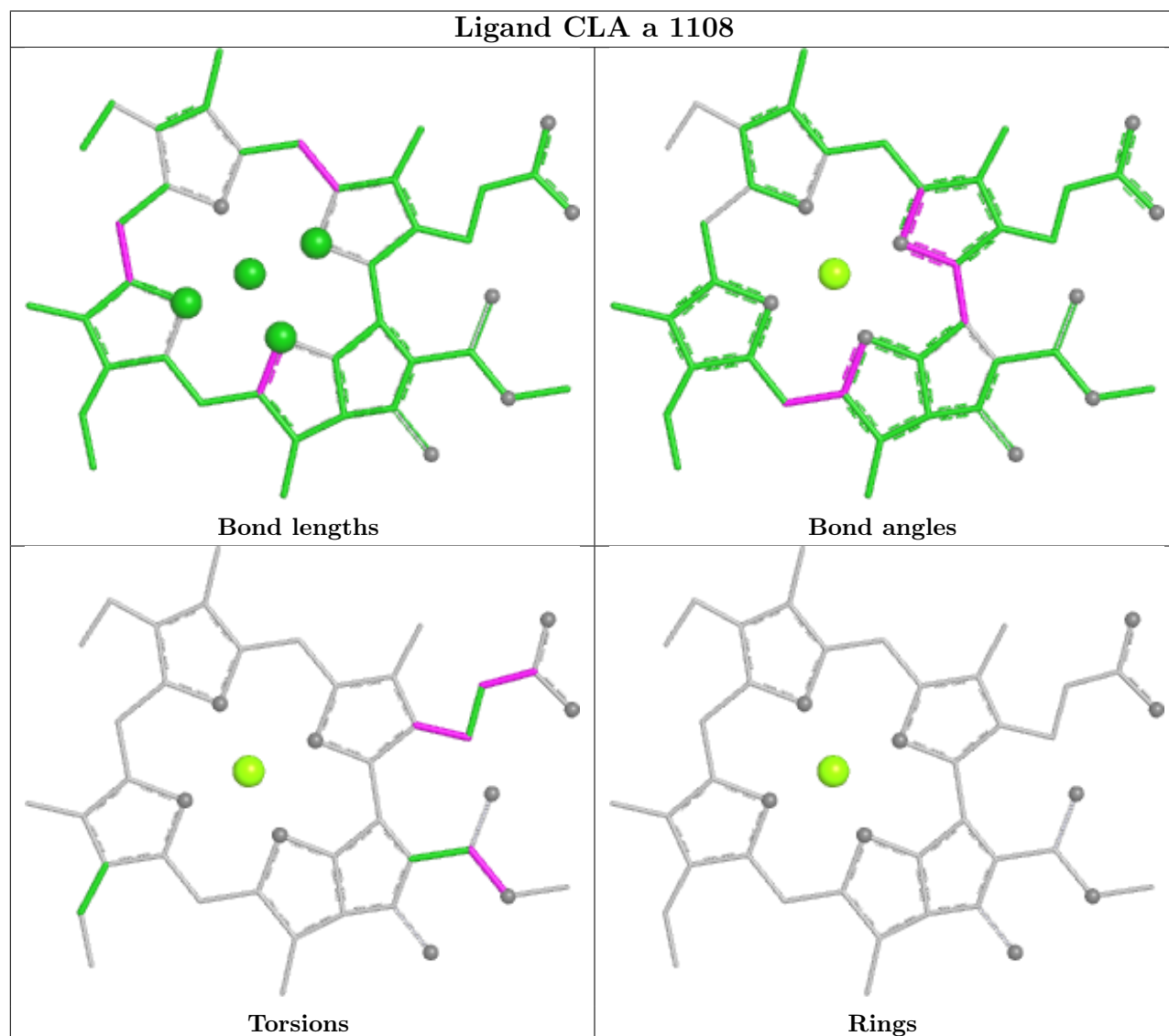
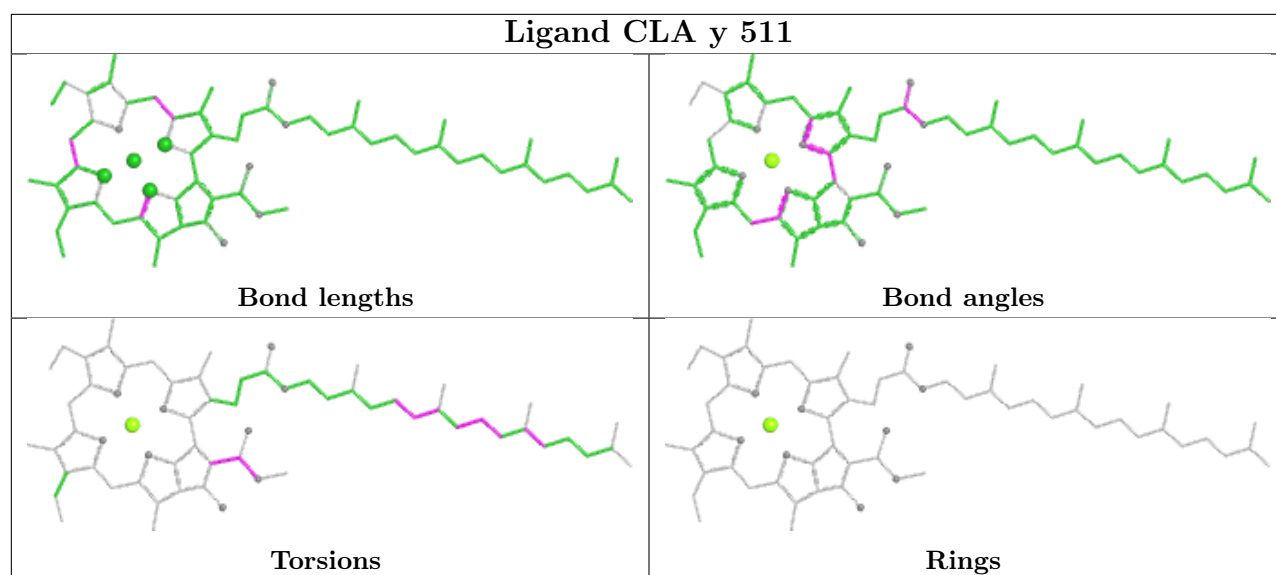
## Ligand CLA H 1111



## Ligand CLA a 1136

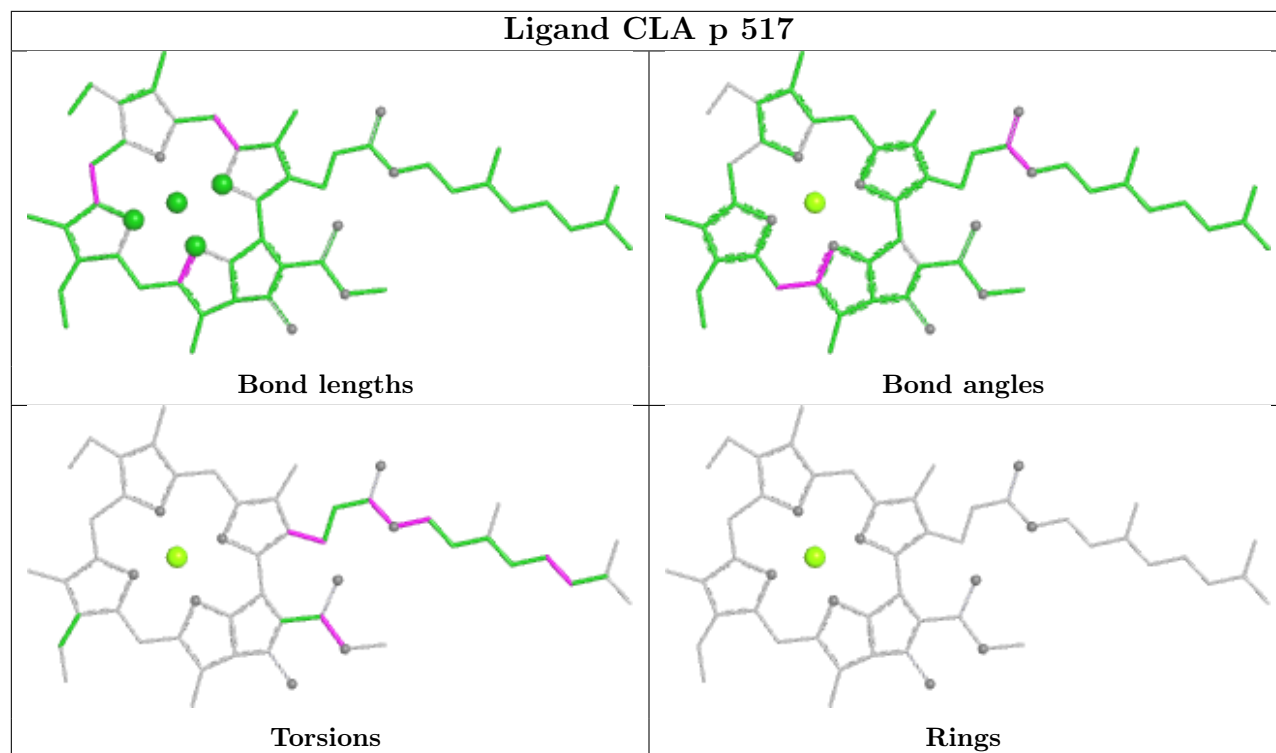




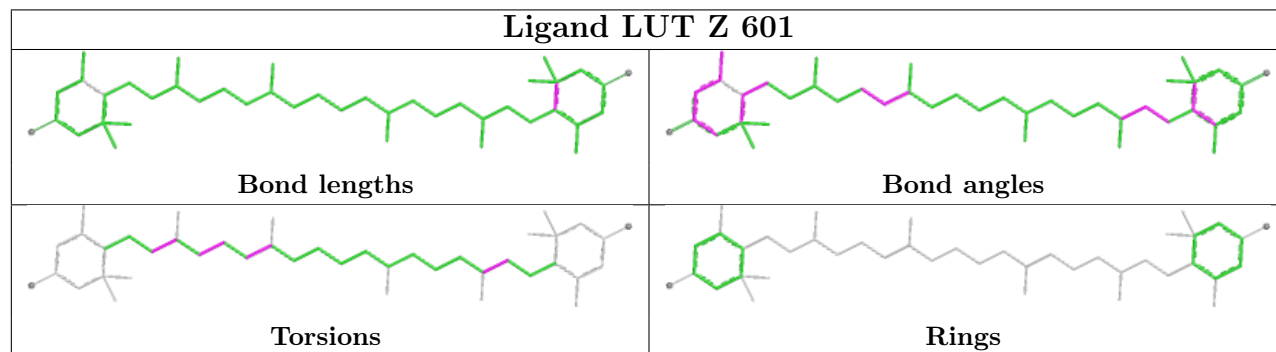




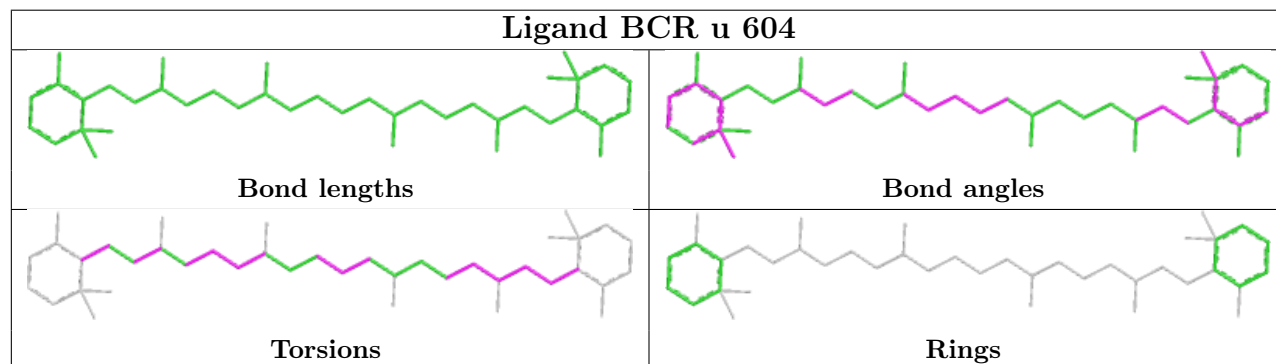
## Ligand CLA p 517



## Ligand LUT Z 601

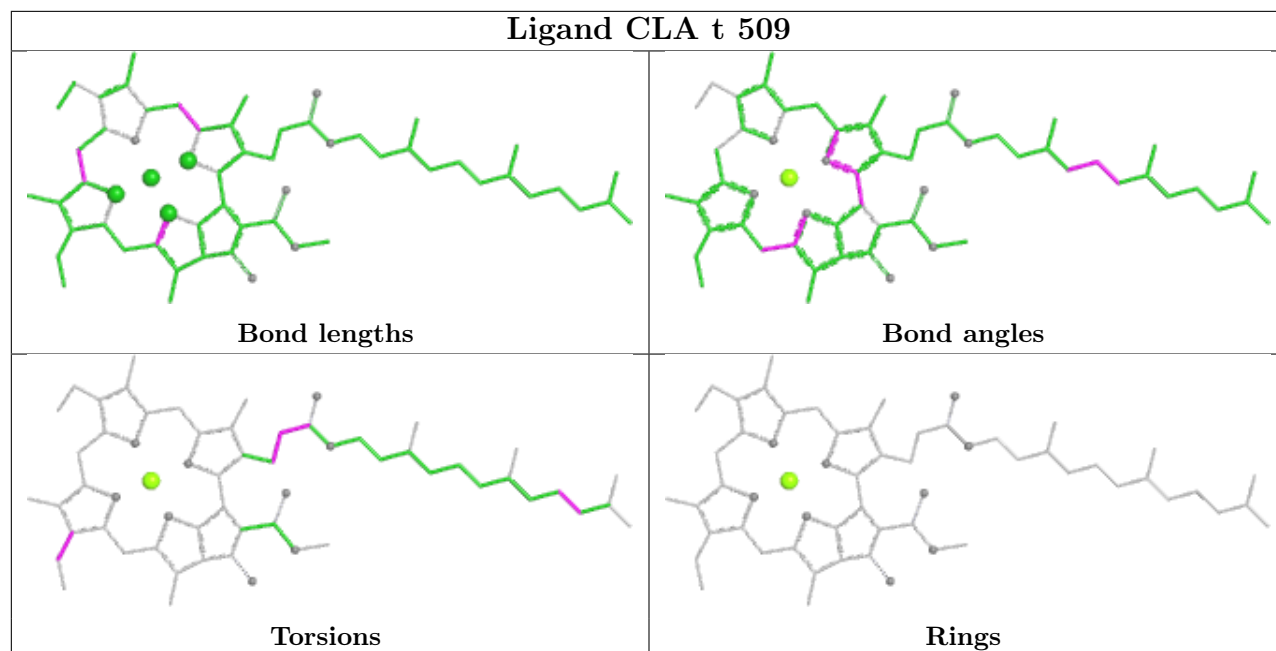


## Ligand BCR u 604

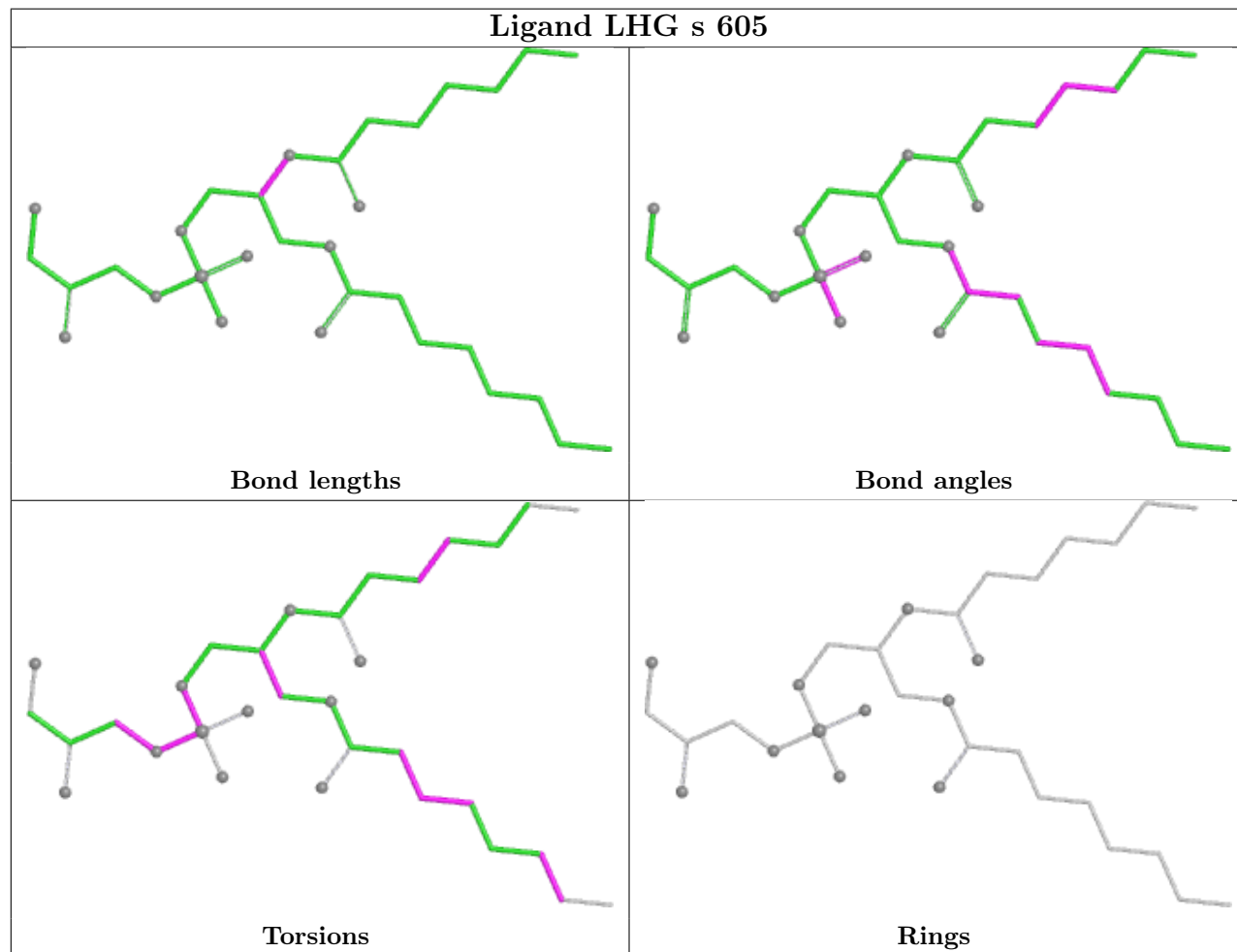




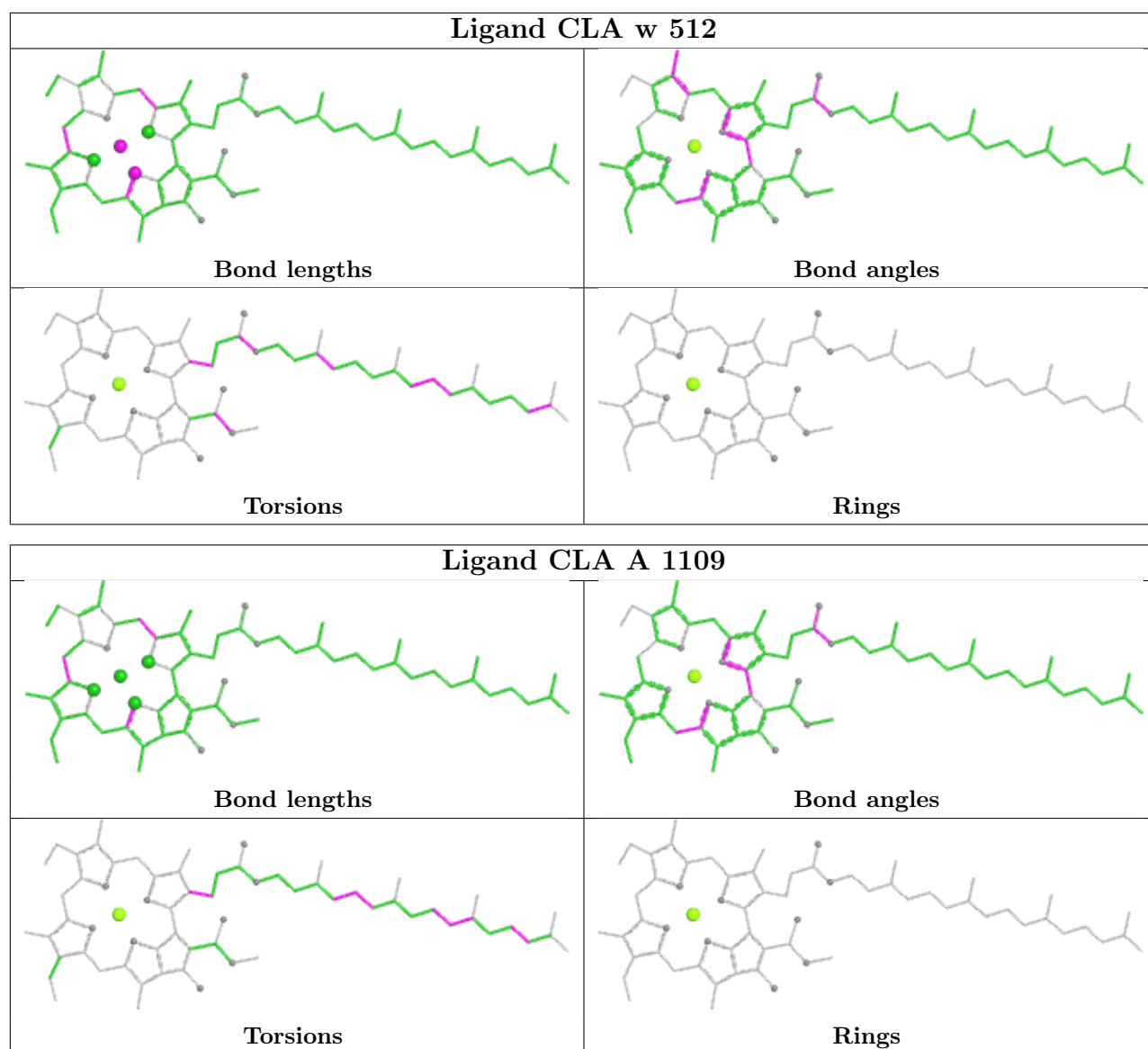
## Ligand CLA t 509



## Ligand LHG s 605

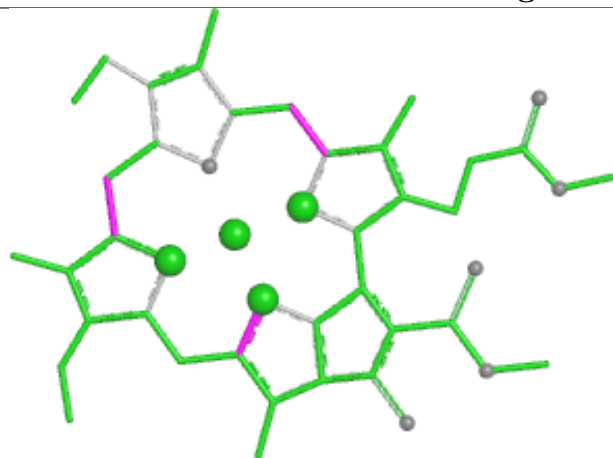




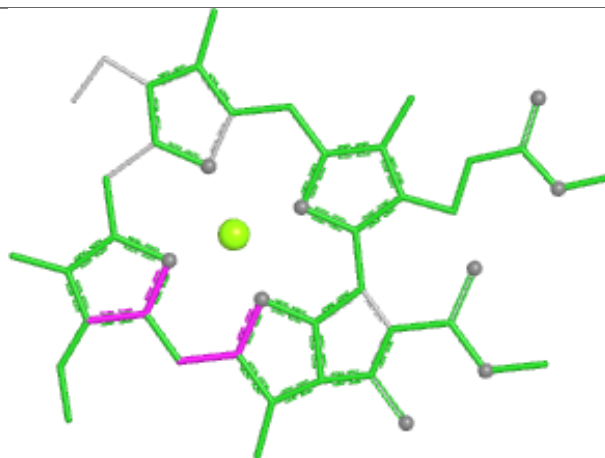




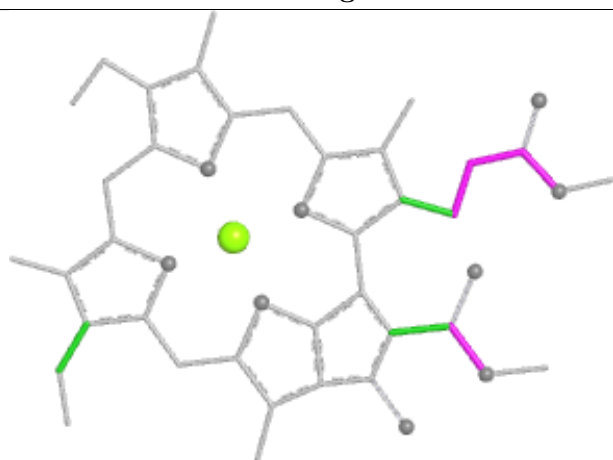
## Ligand CLA x 503



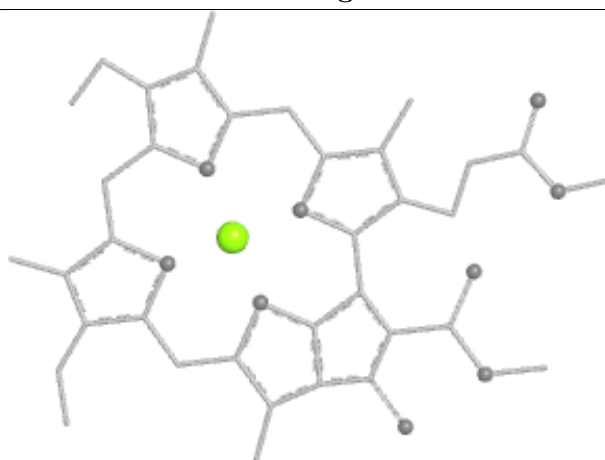
Bond lengths



Bond angles

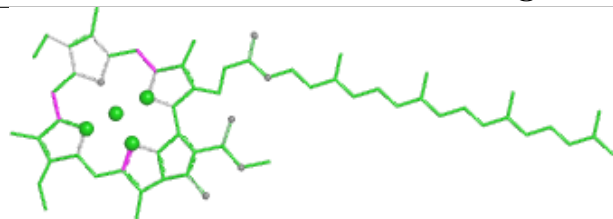


Torsions

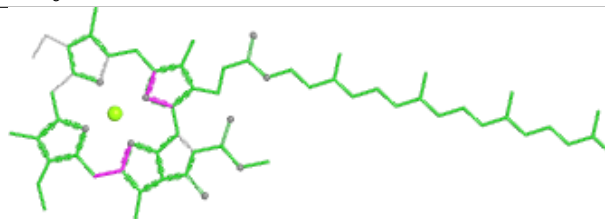


Rings

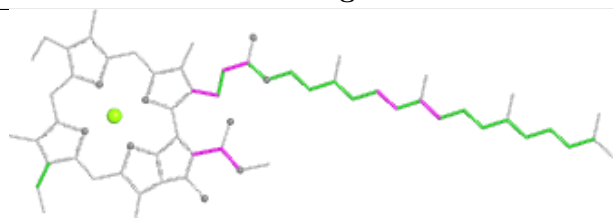
## Ligand CLA y 507



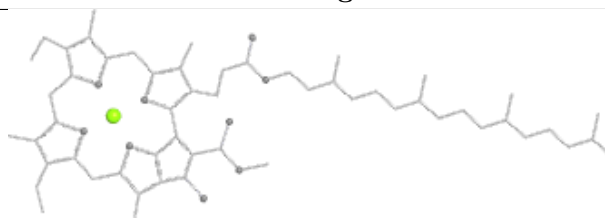
Bond lengths



Bond angles



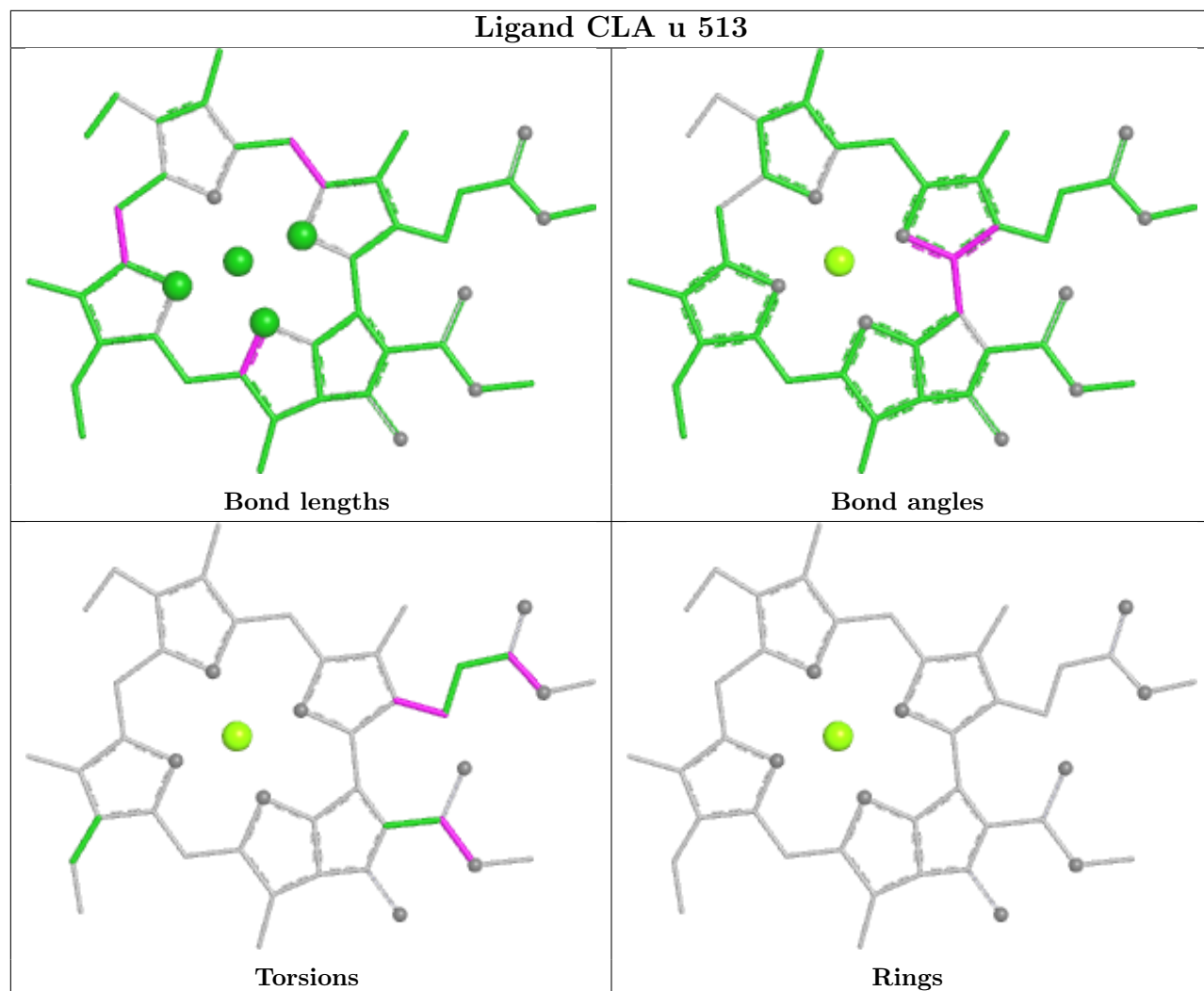
Torsions



Rings

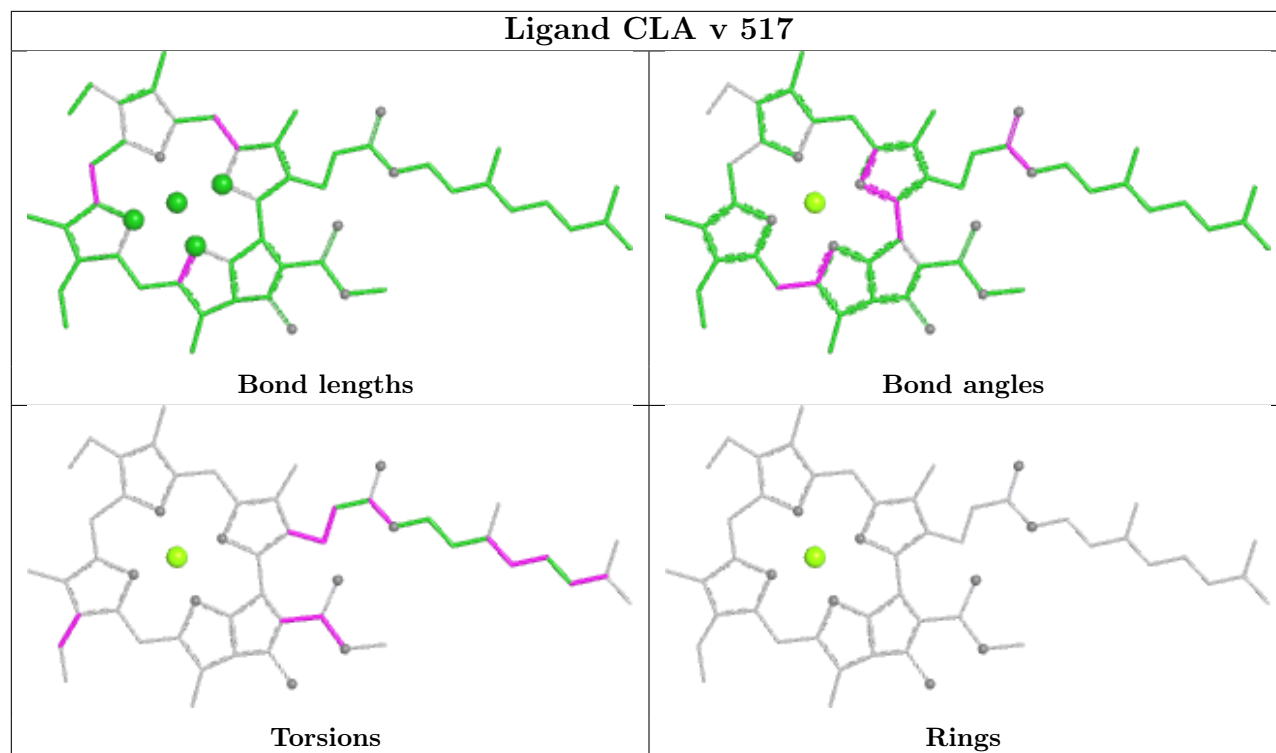


## Ligand CLA u 513

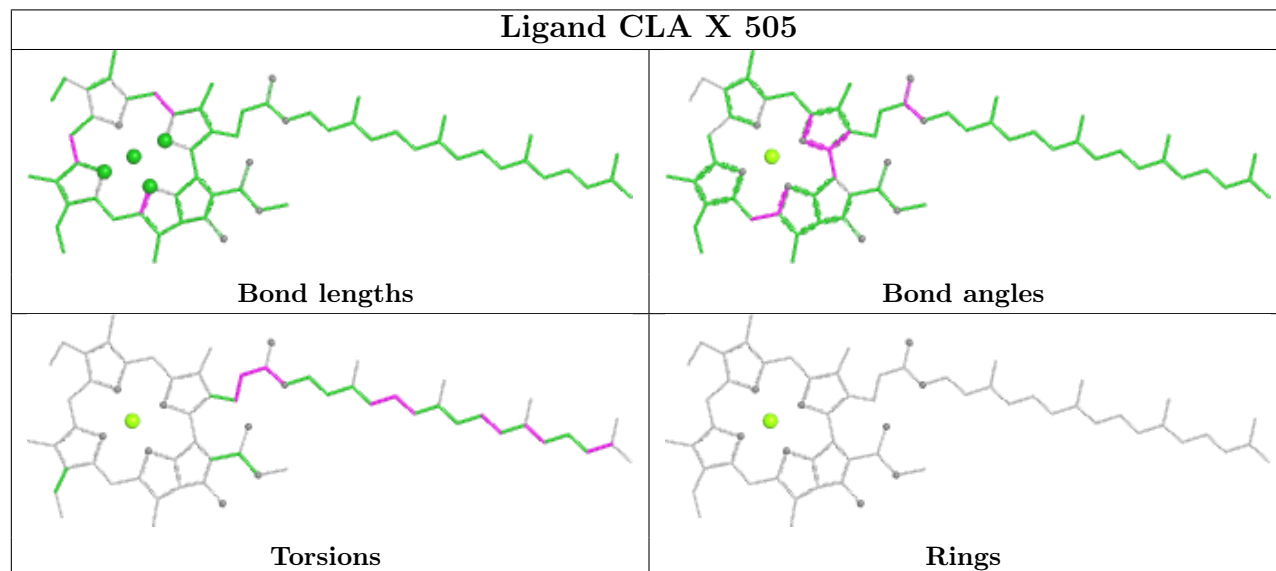




## Ligand CLA v 517

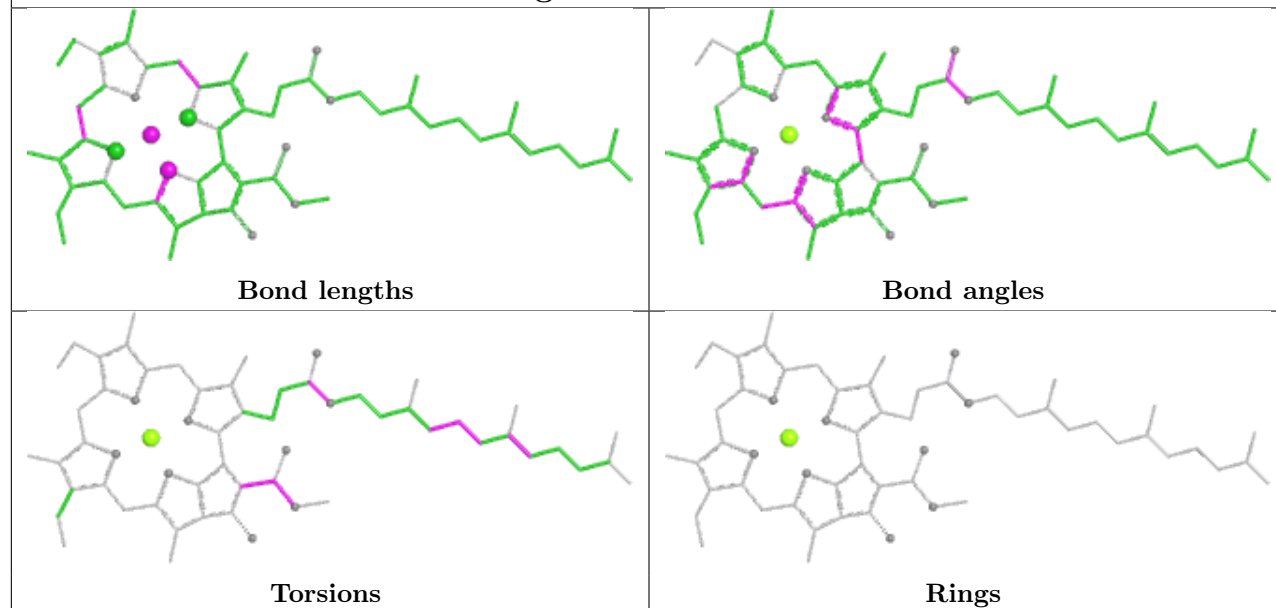


## Ligand CLA X 505

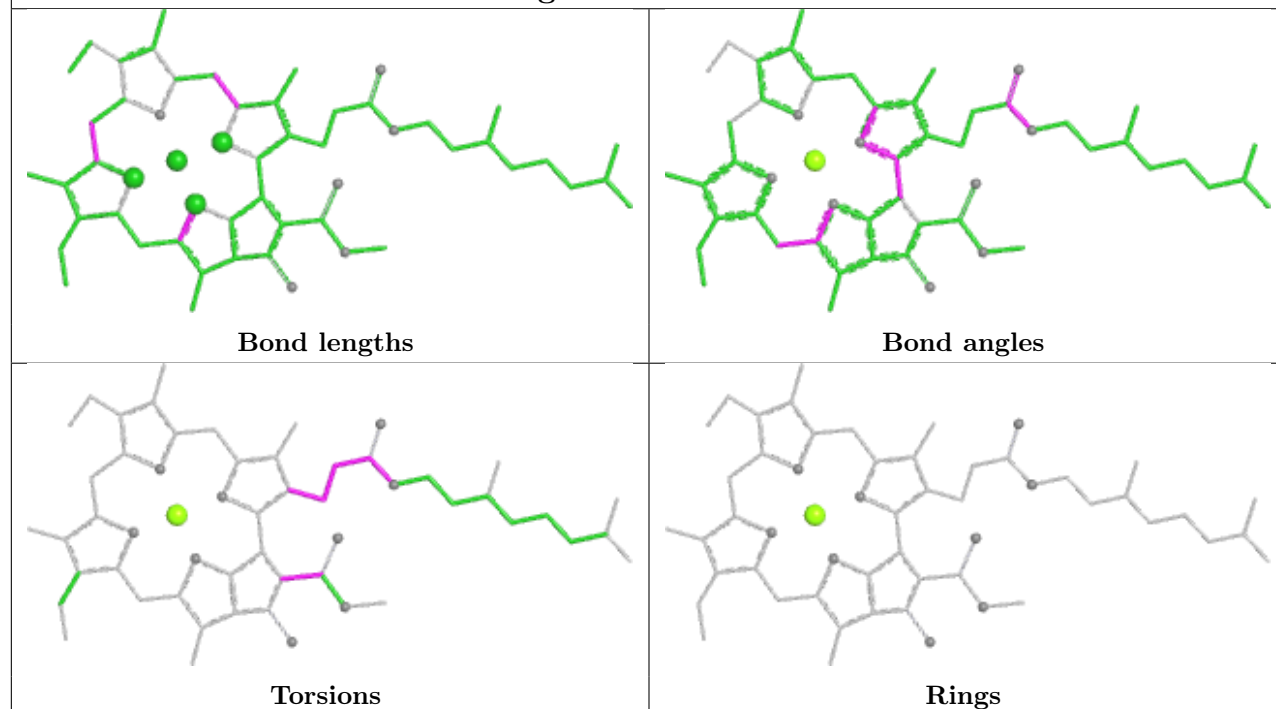




## Ligand CLA h 506

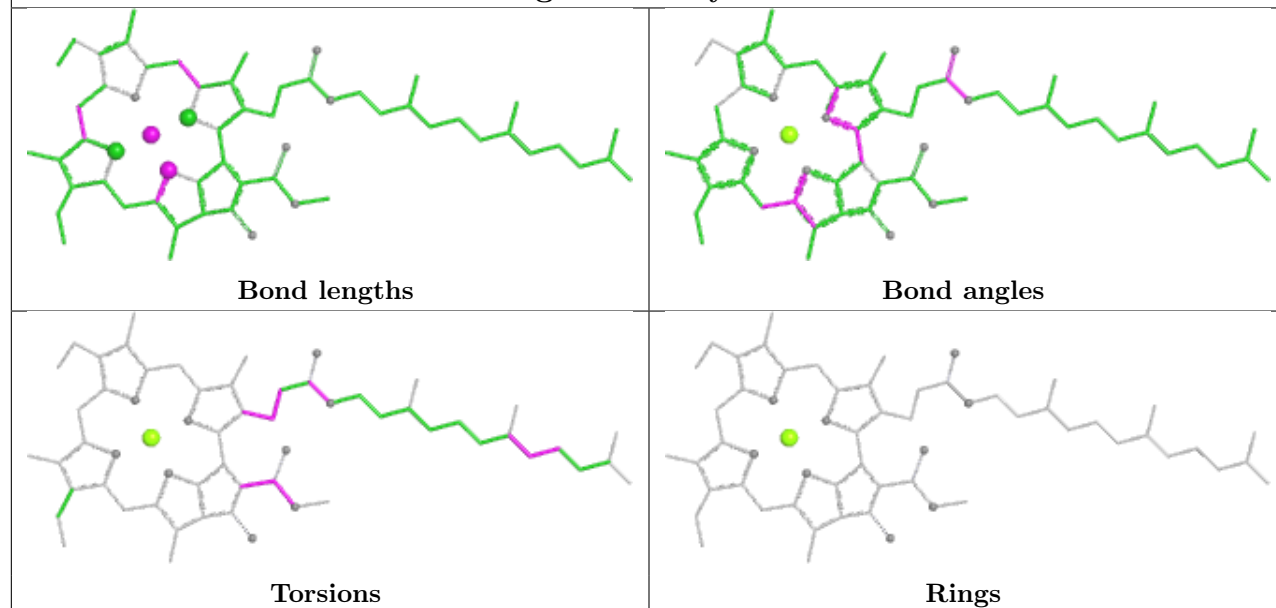


## Ligand CLA s 508

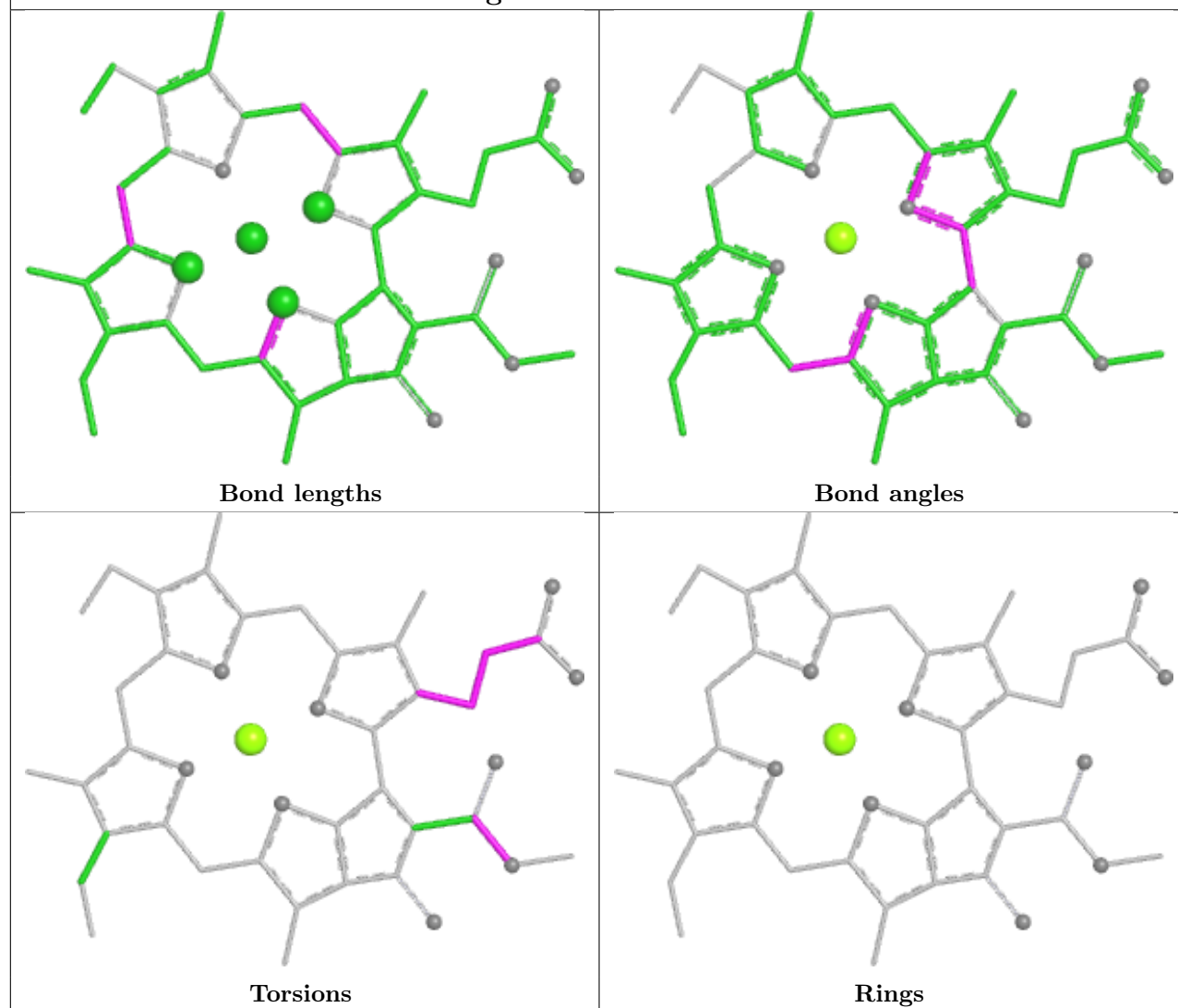




## Ligand CLA y 504

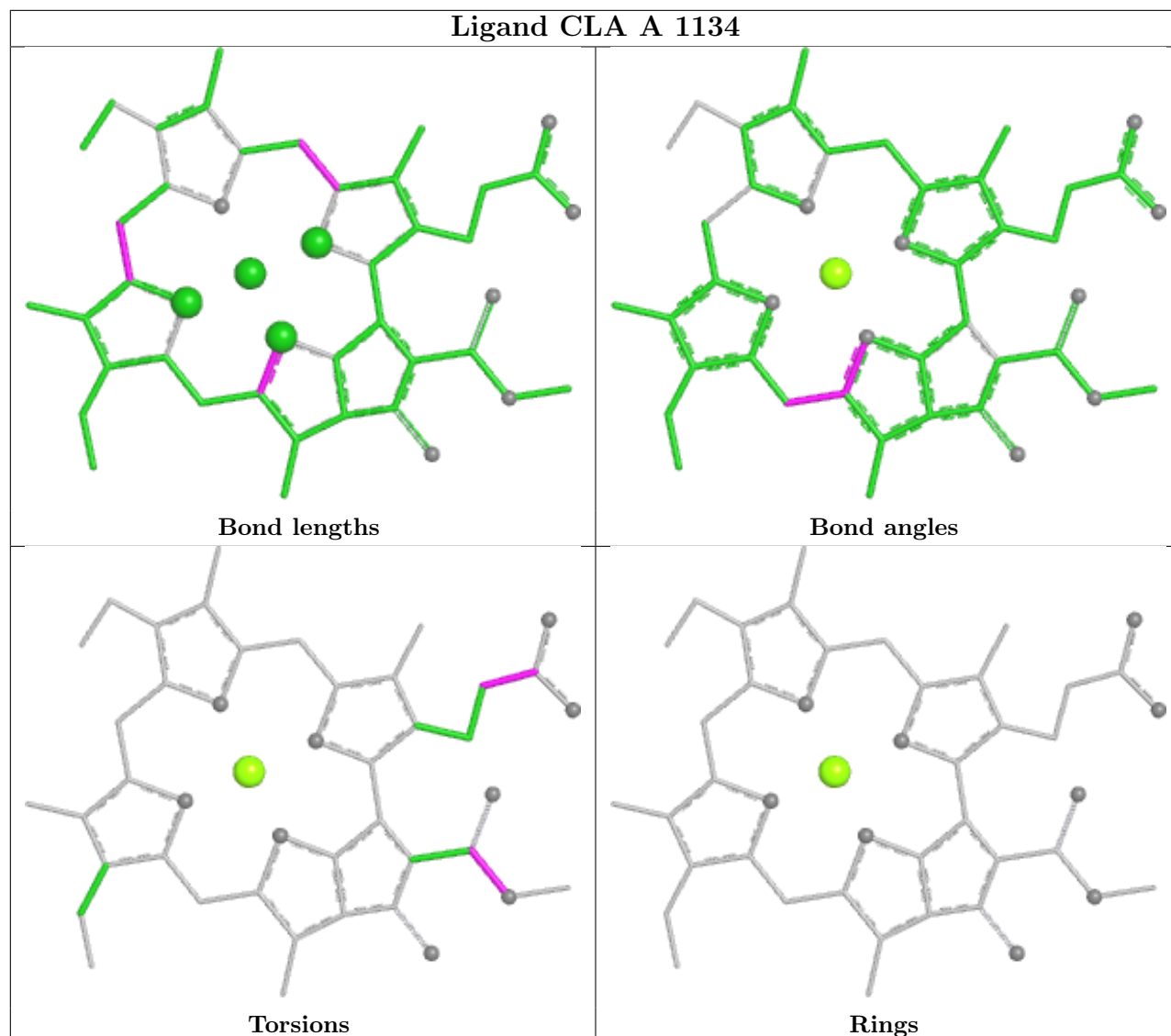


## Ligand CLA b 1231

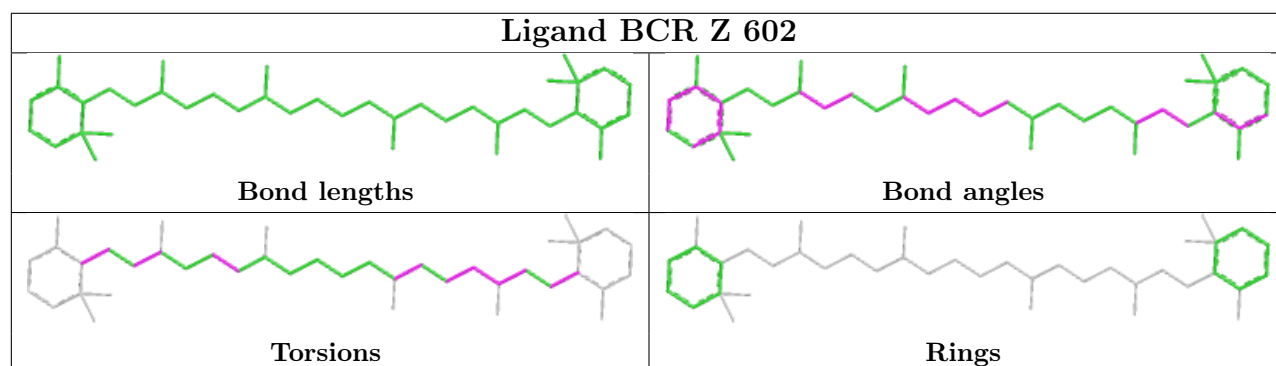




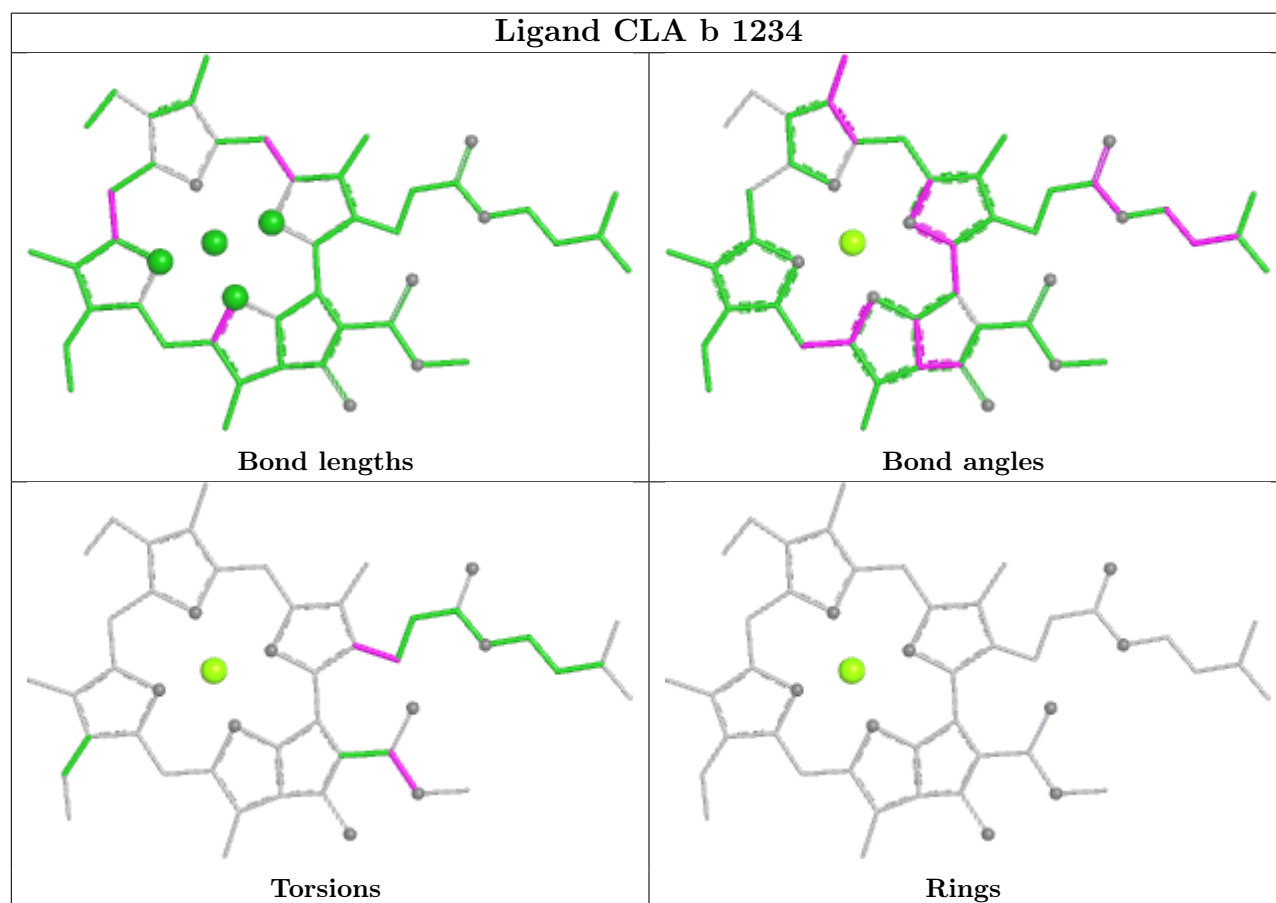
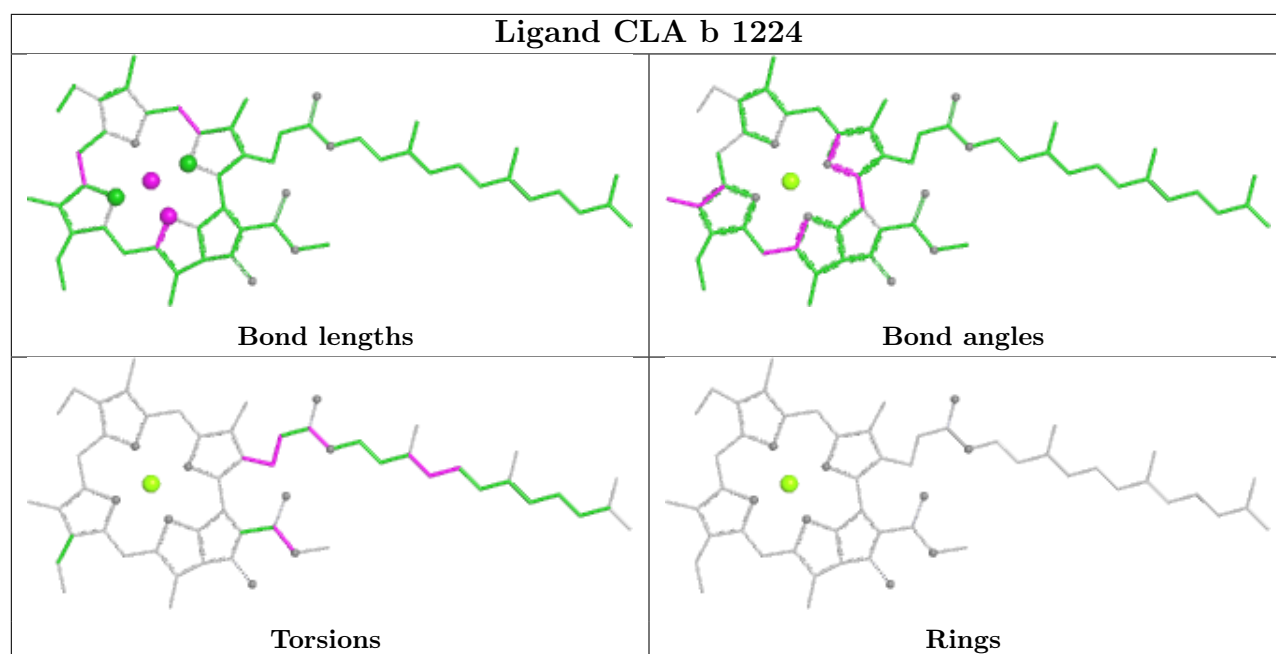
## Ligand CLA A 1134



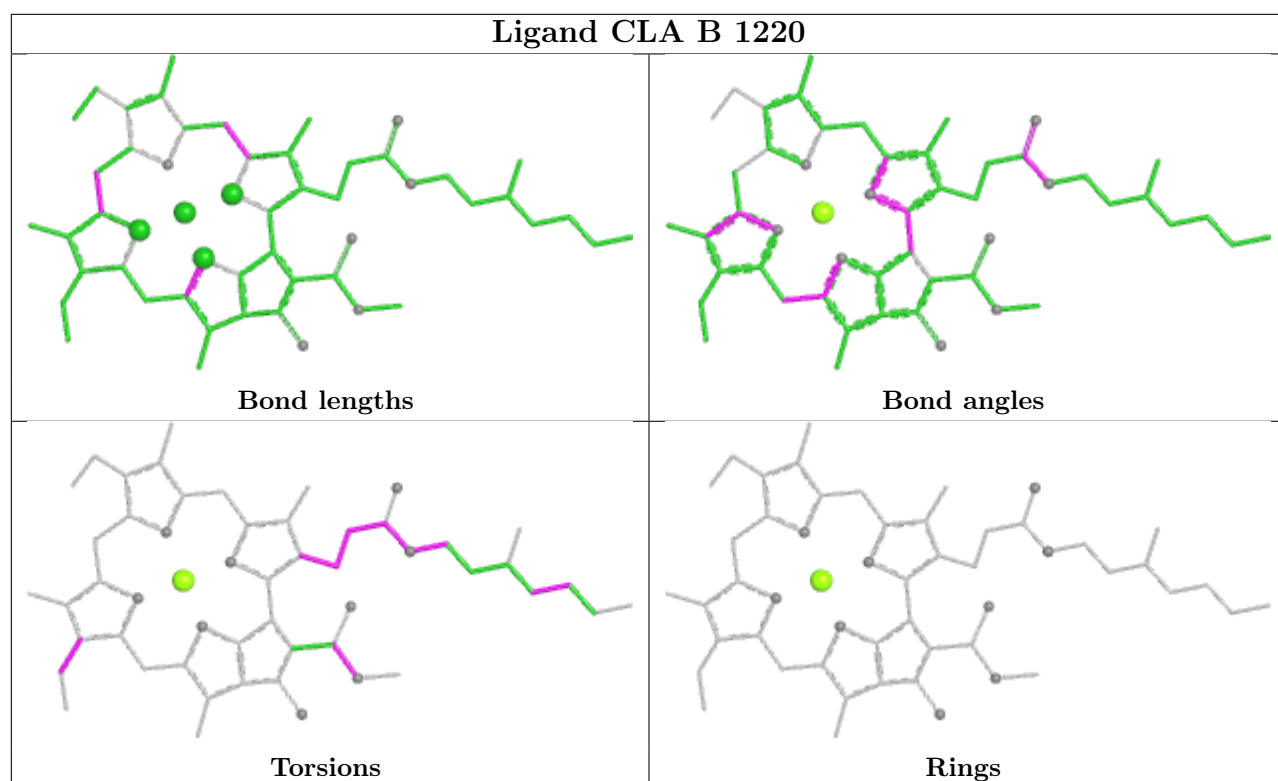
## Ligand BCR Z 602



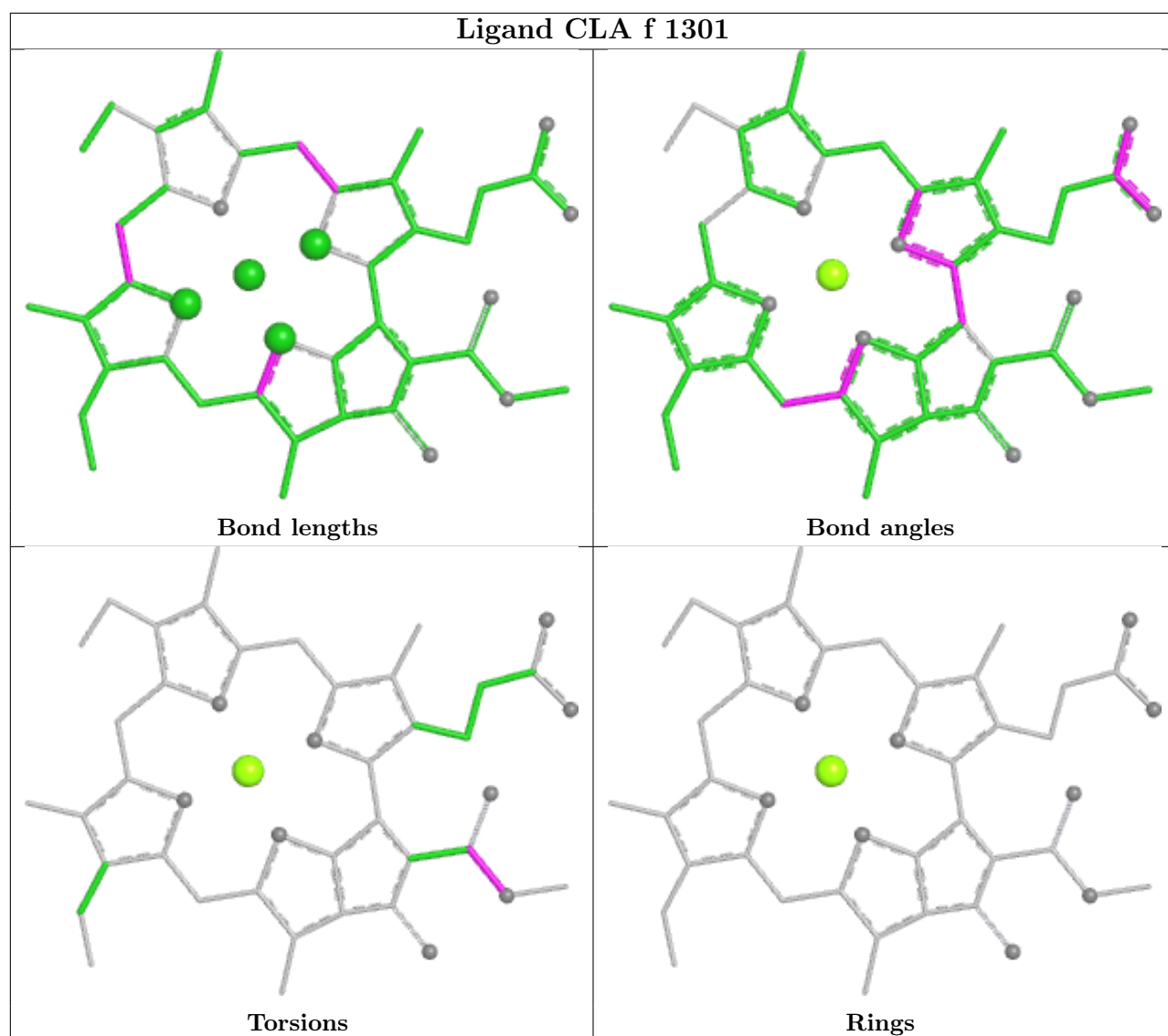






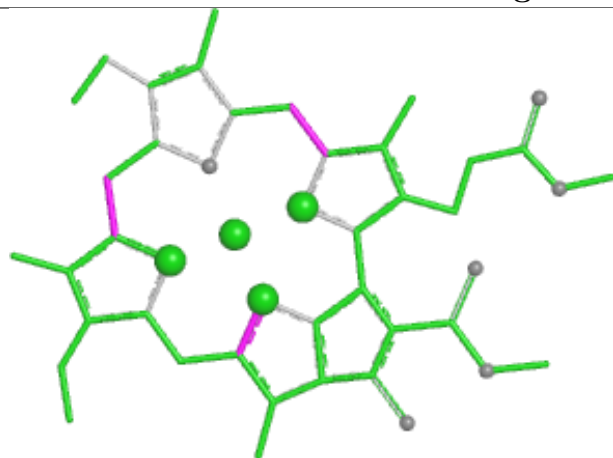




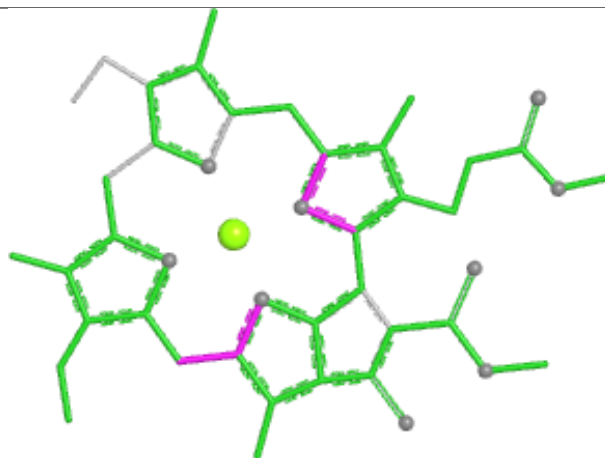




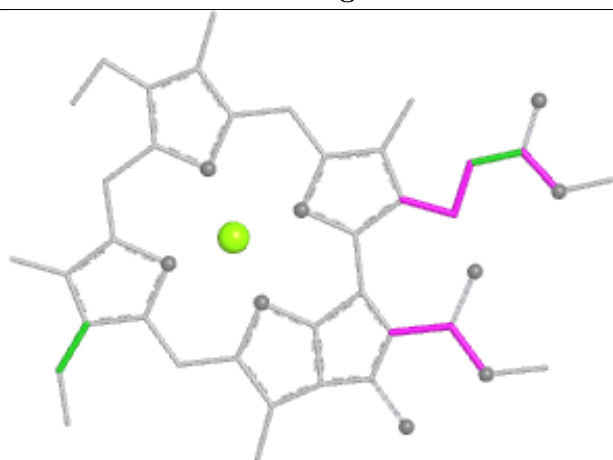
## Ligand CLA Y 516



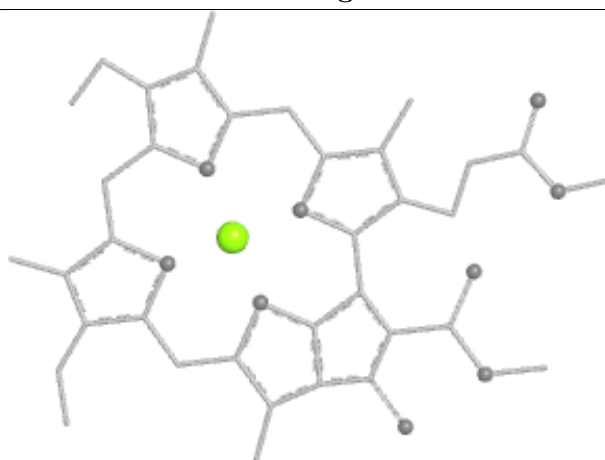
Bond lengths



Bond angles



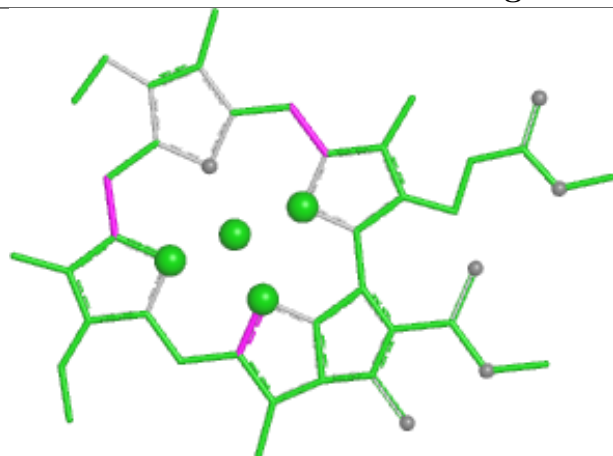
Torsions



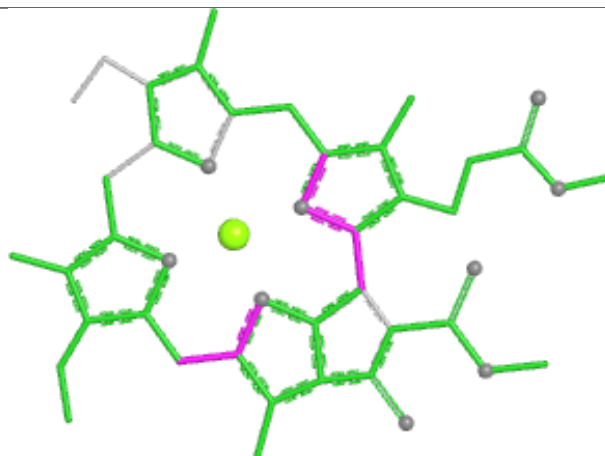
Rings



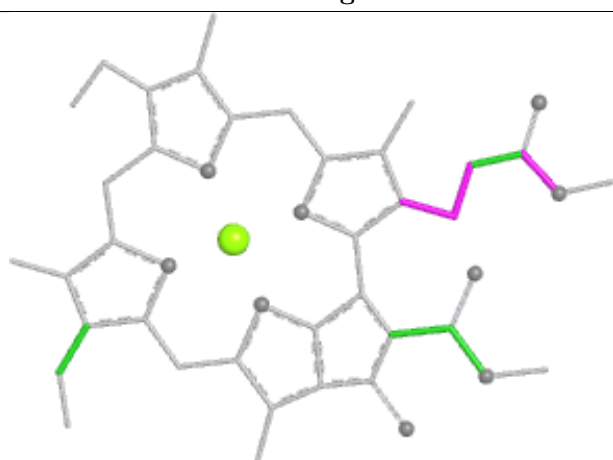
## Ligand CLA H 1129



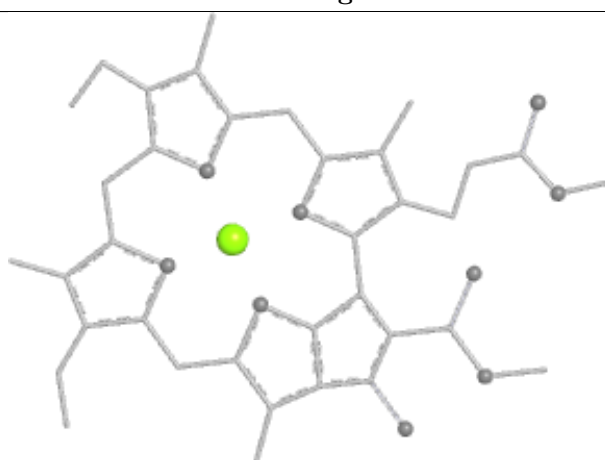
Bond lengths



Bond angles

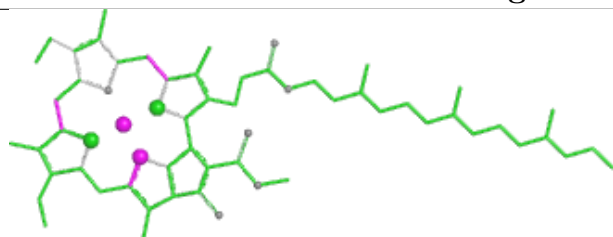


Torsions

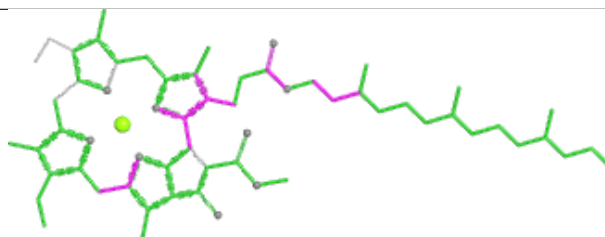


Rings

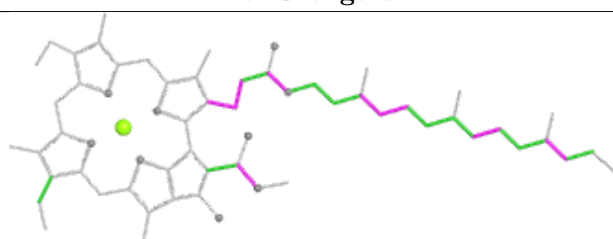
## Ligand CLA b 1235



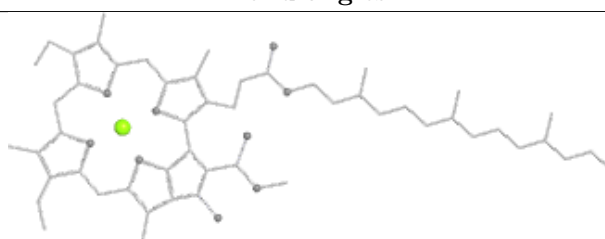
Bond lengths



Bond angles

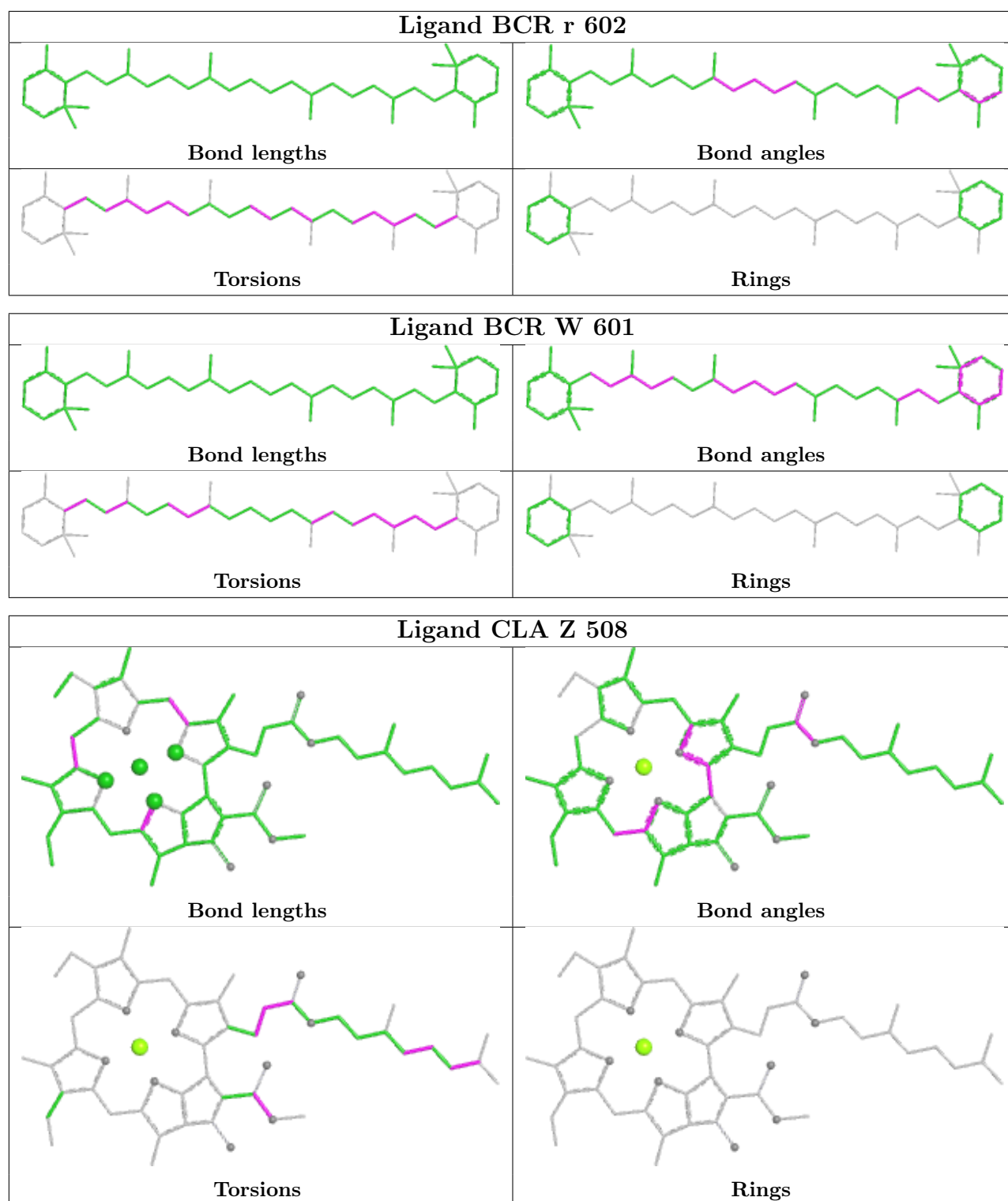


Torsions

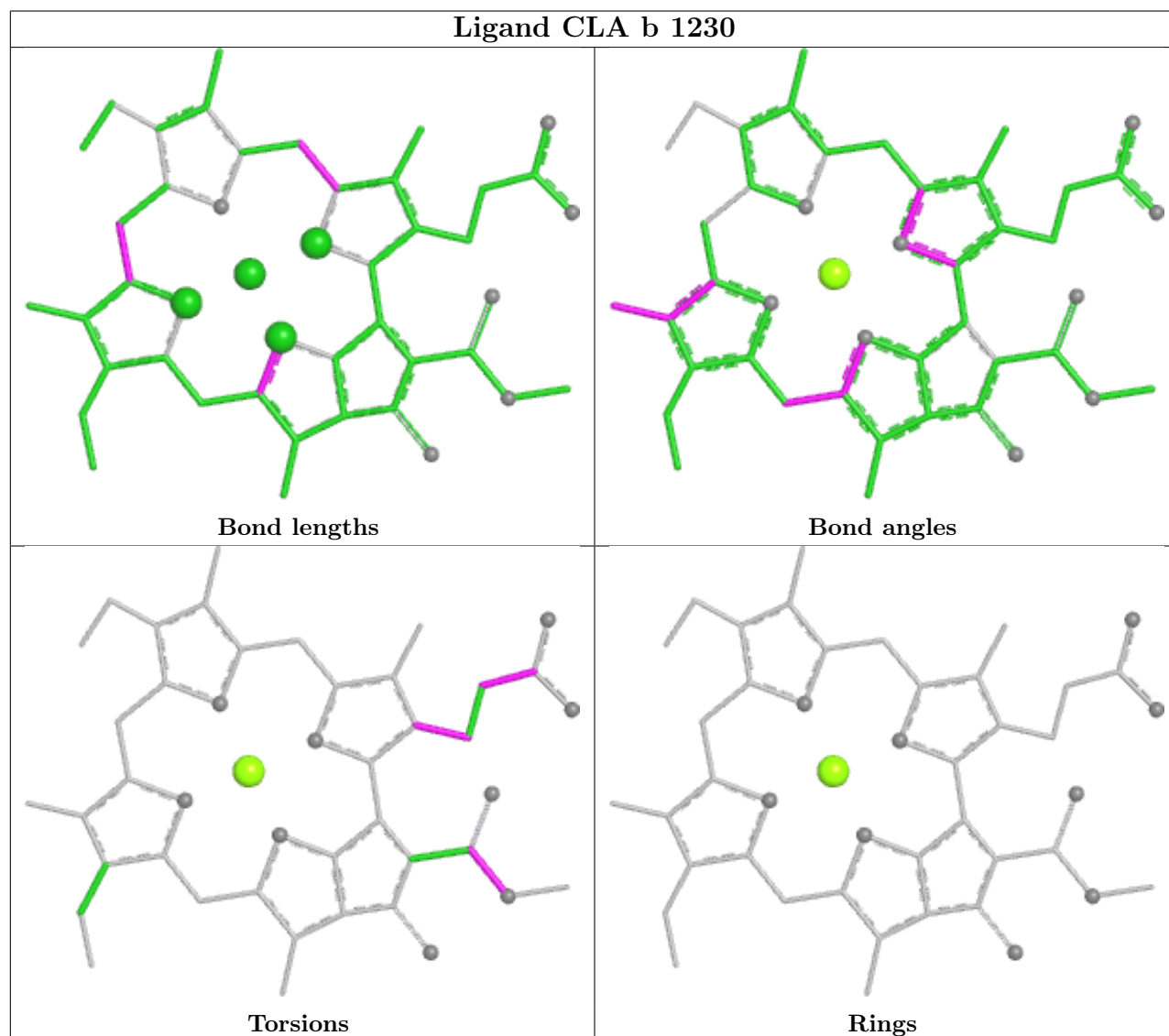
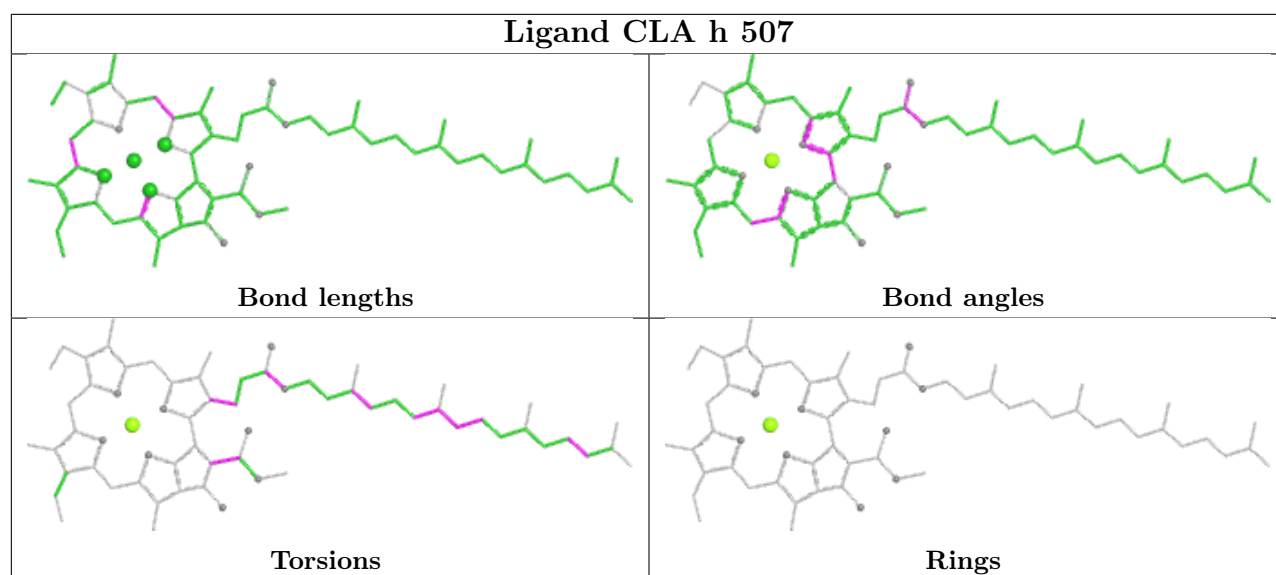


Rings

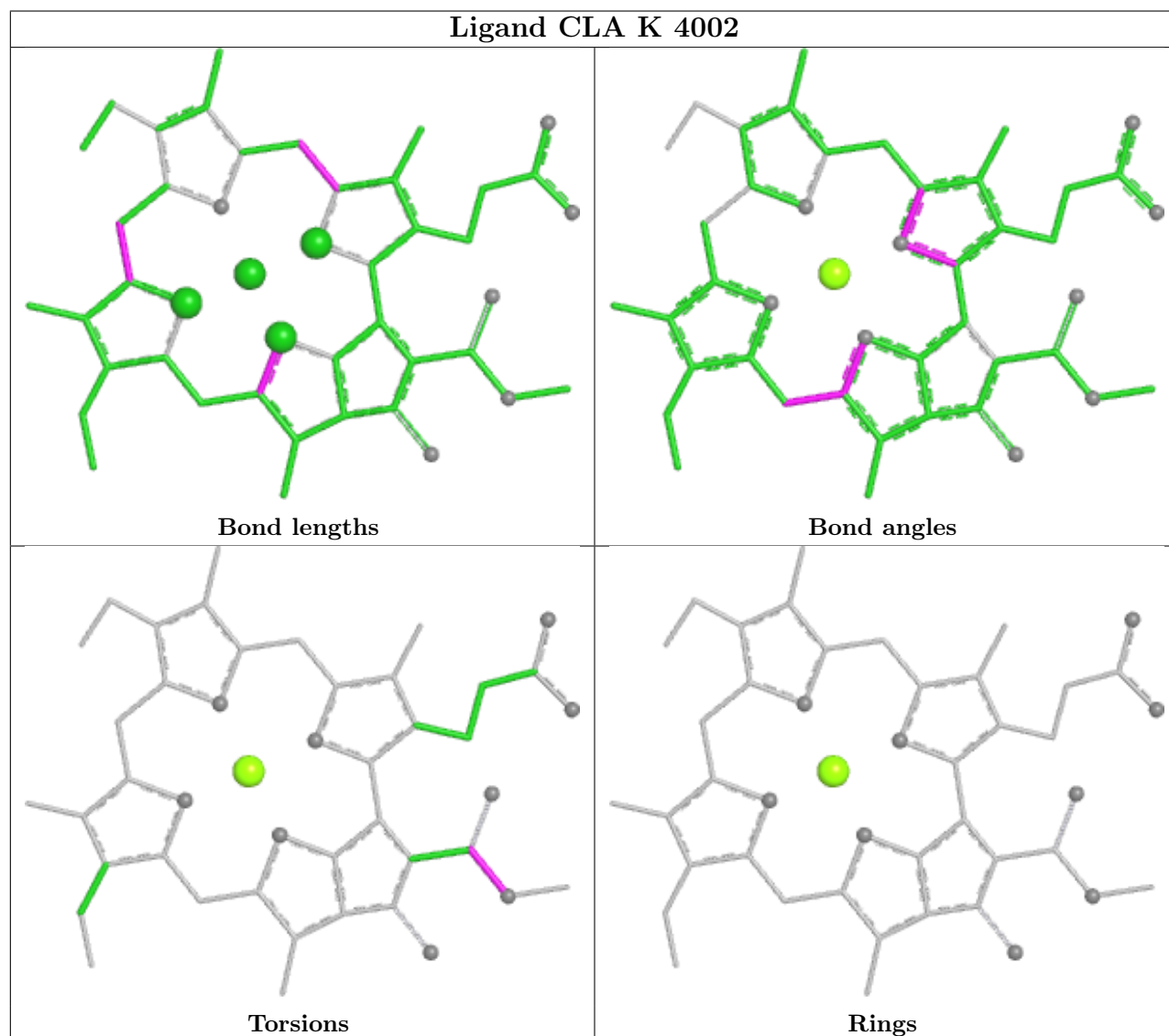
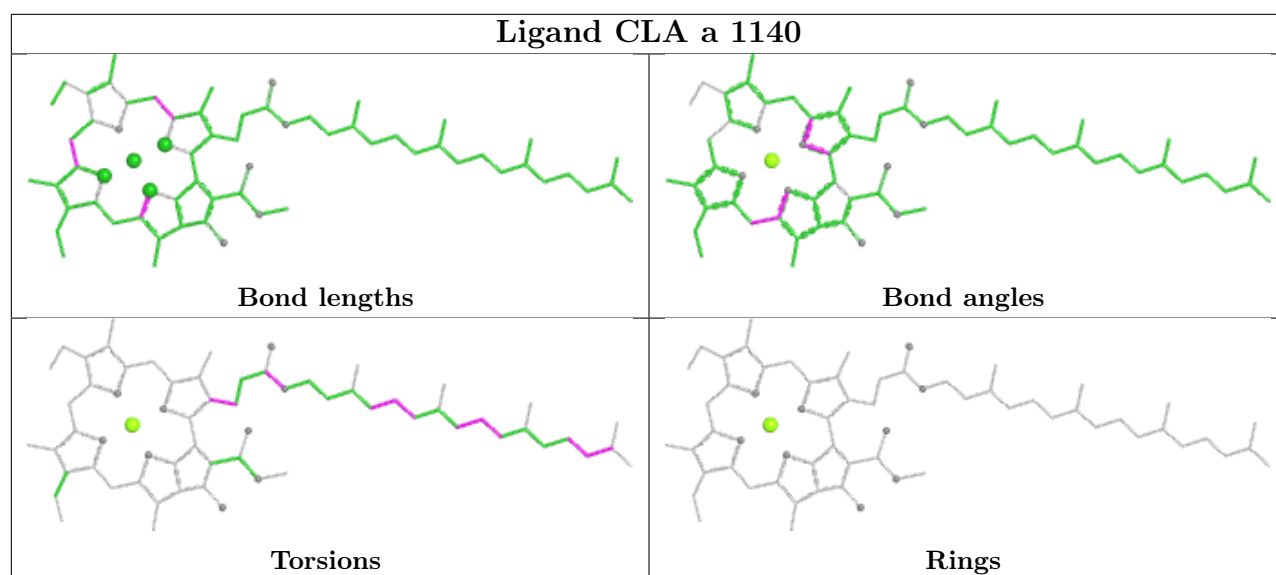




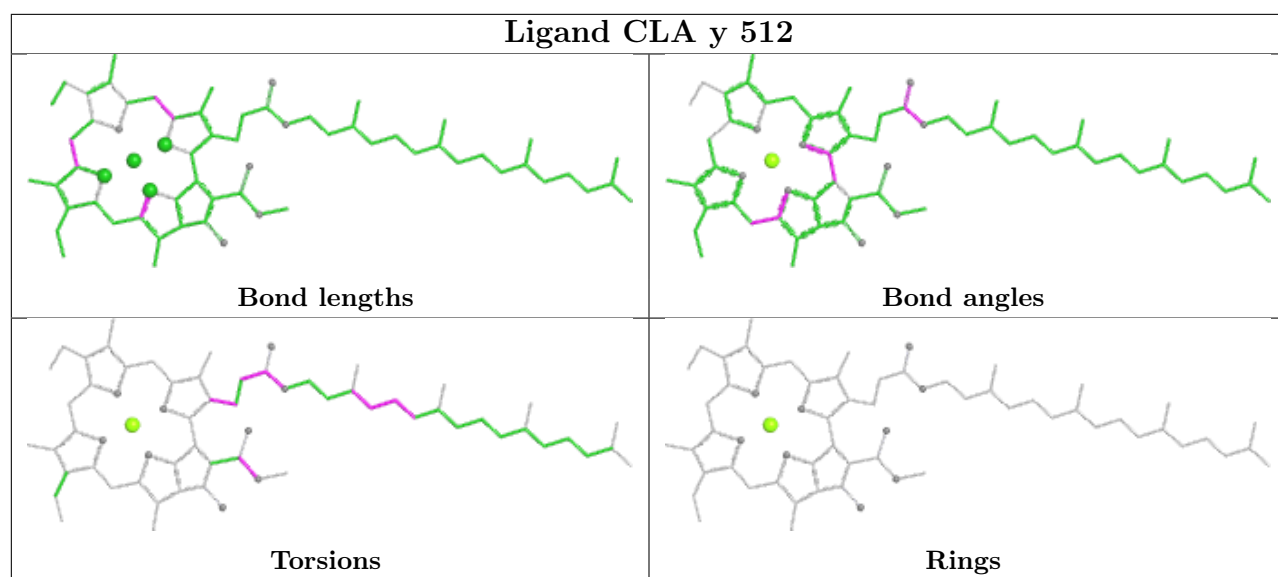




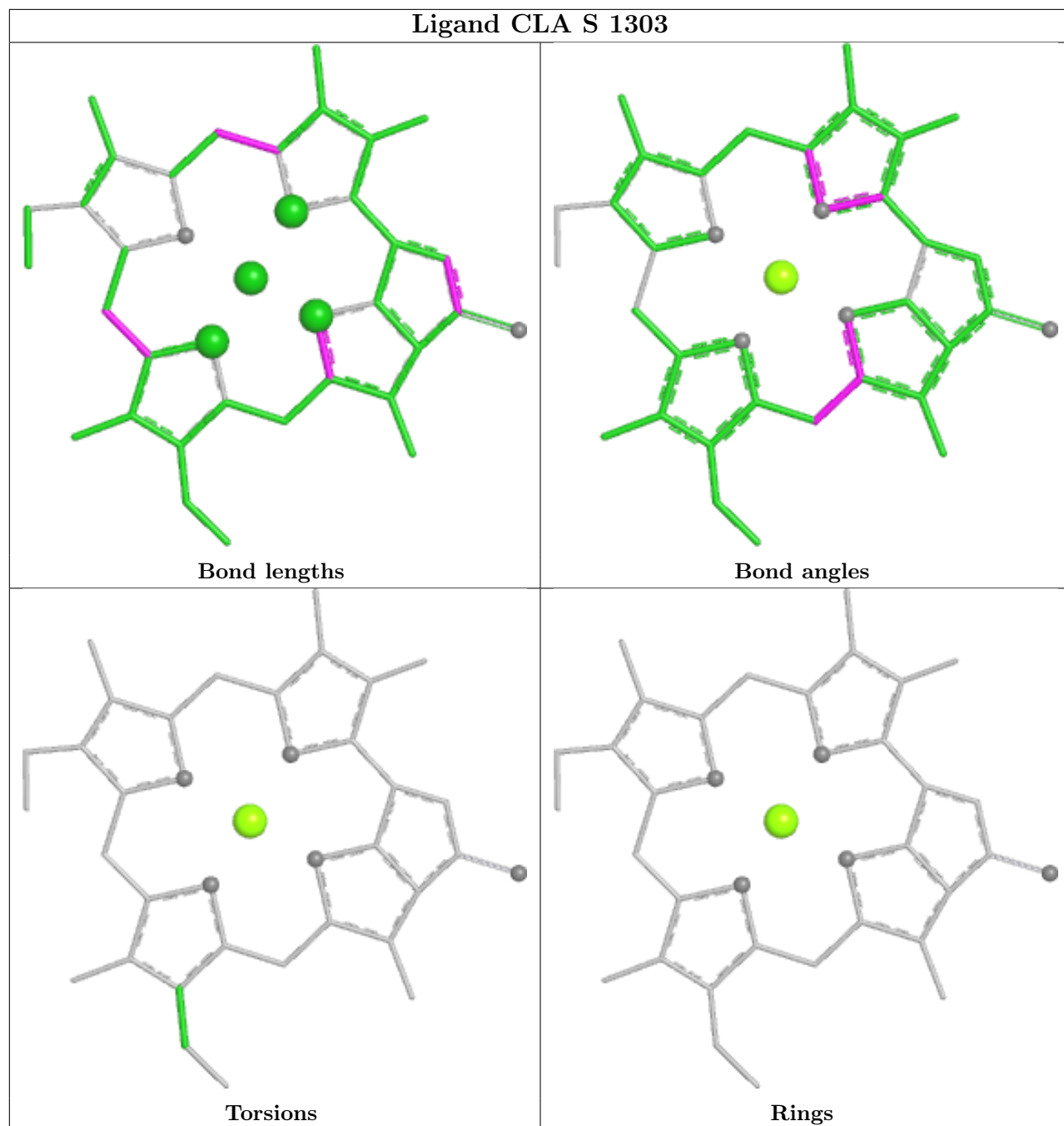




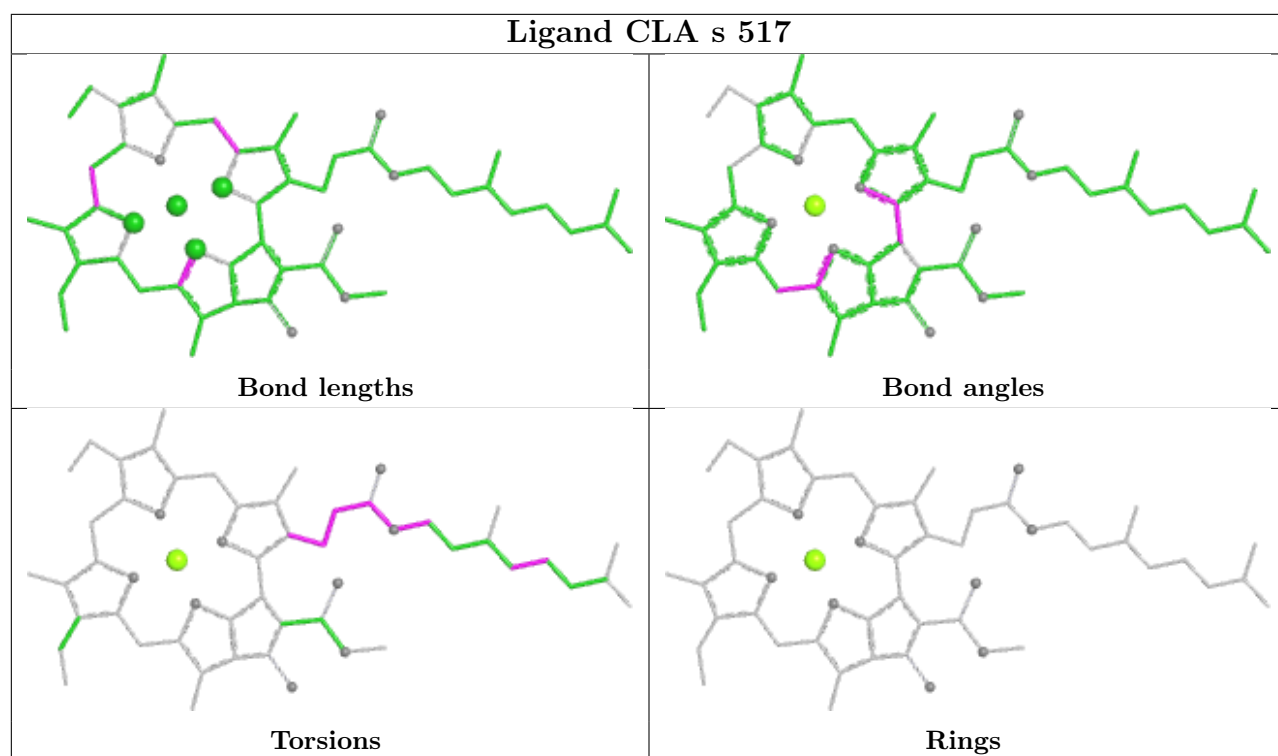




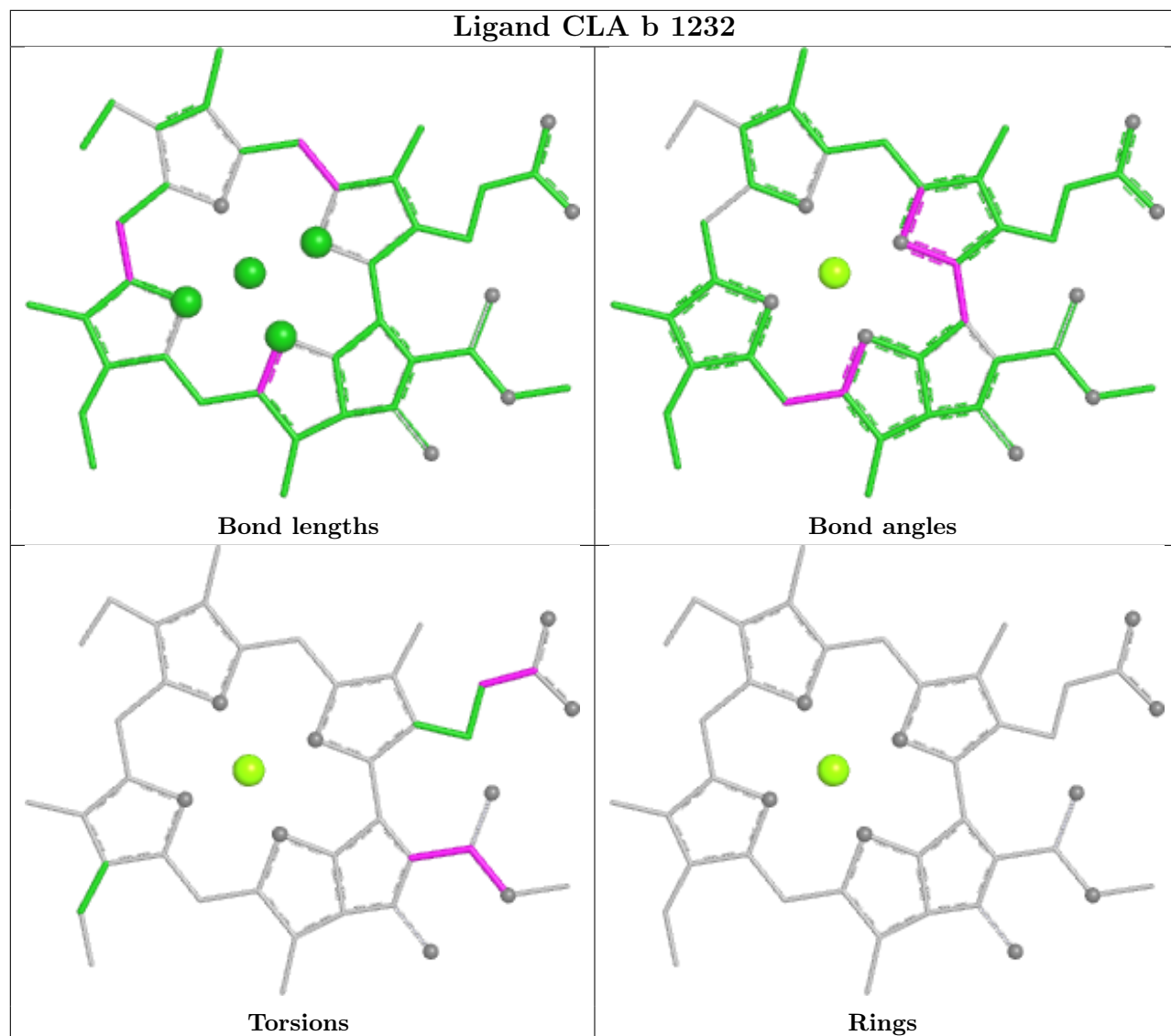






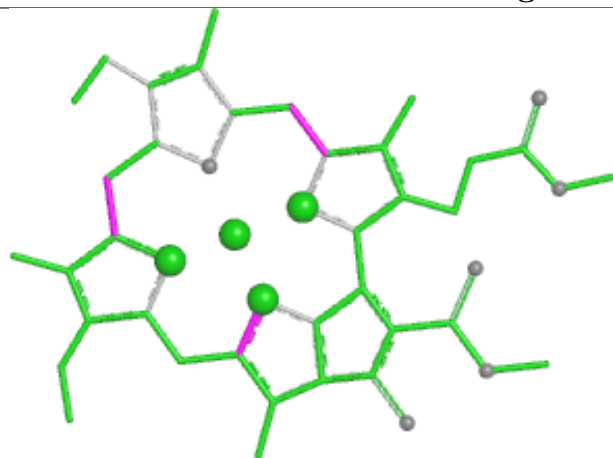




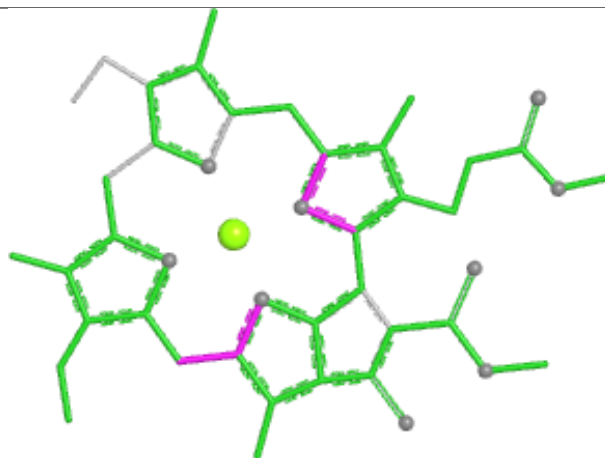




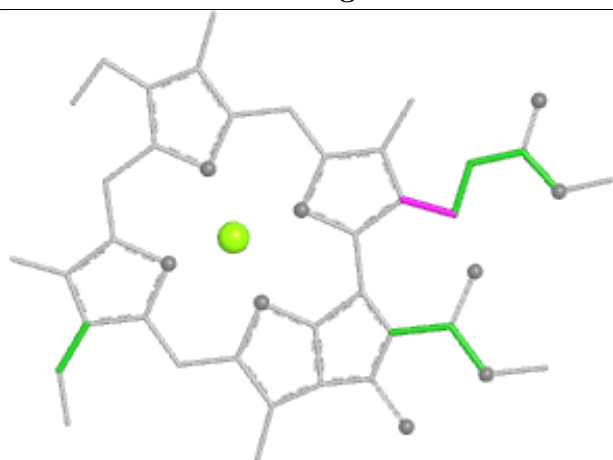
## Ligand CLA v 513



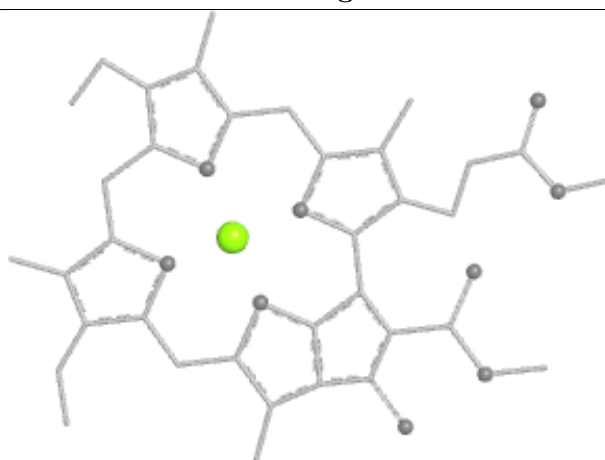
Bond lengths



Bond angles

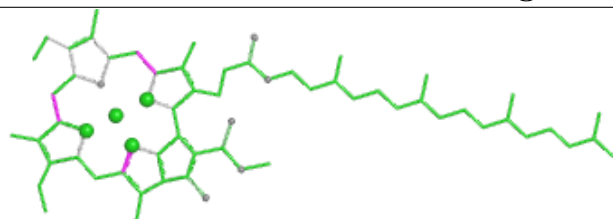


Torsions

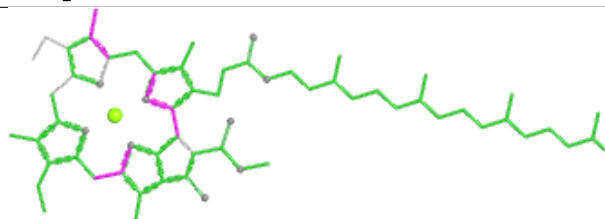


Rings

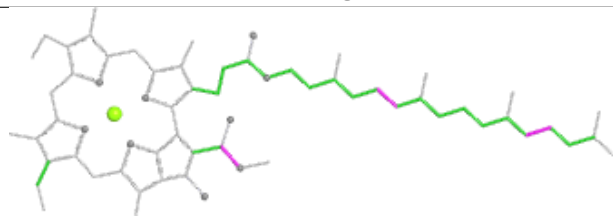
## Ligand CLA q 511



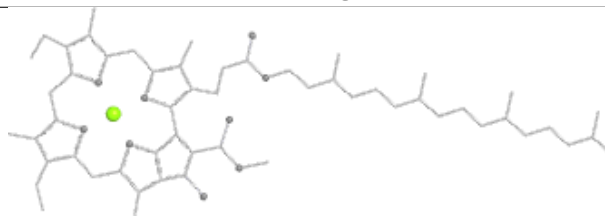
Bond lengths



Bond angles



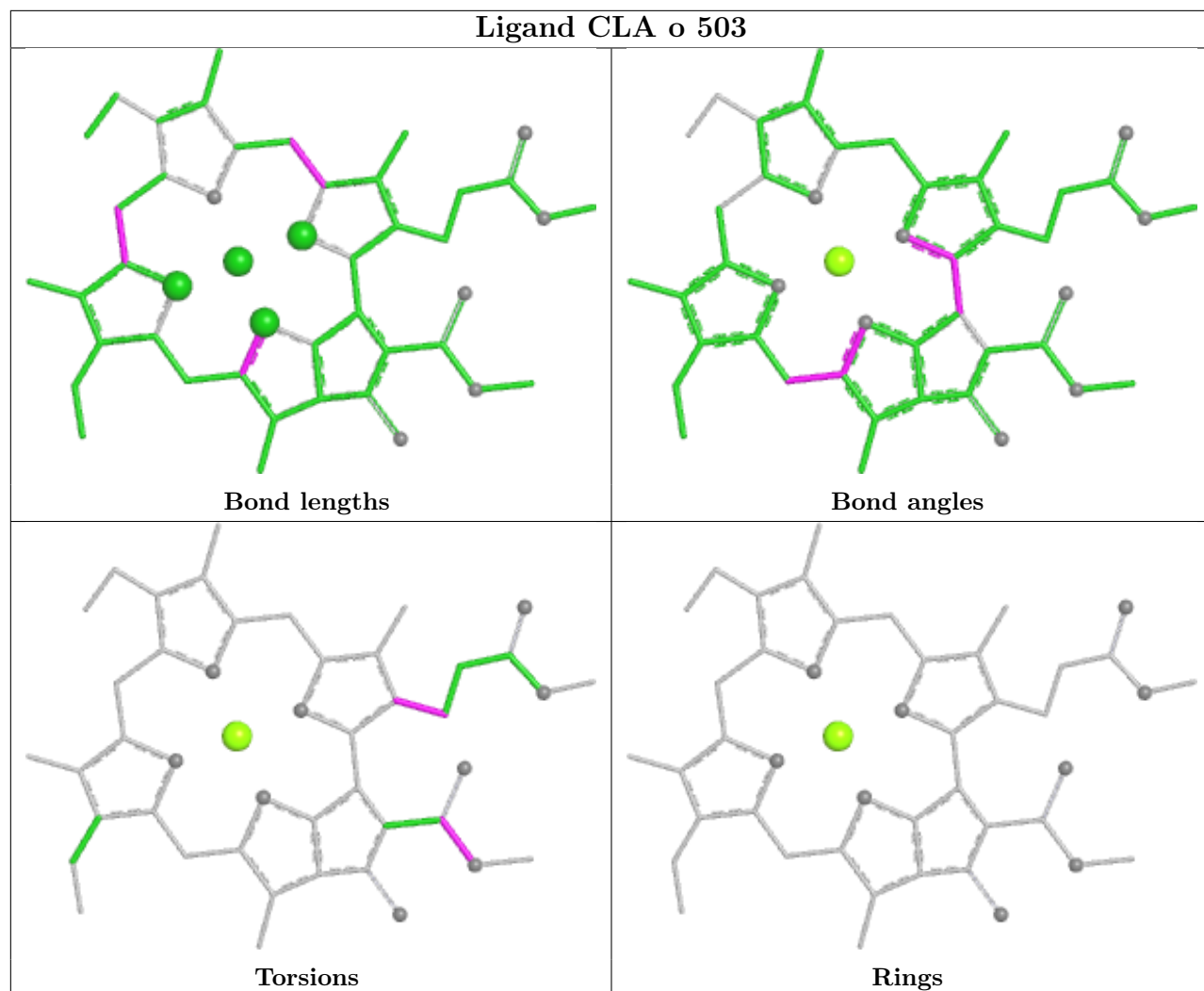
Torsions



Rings

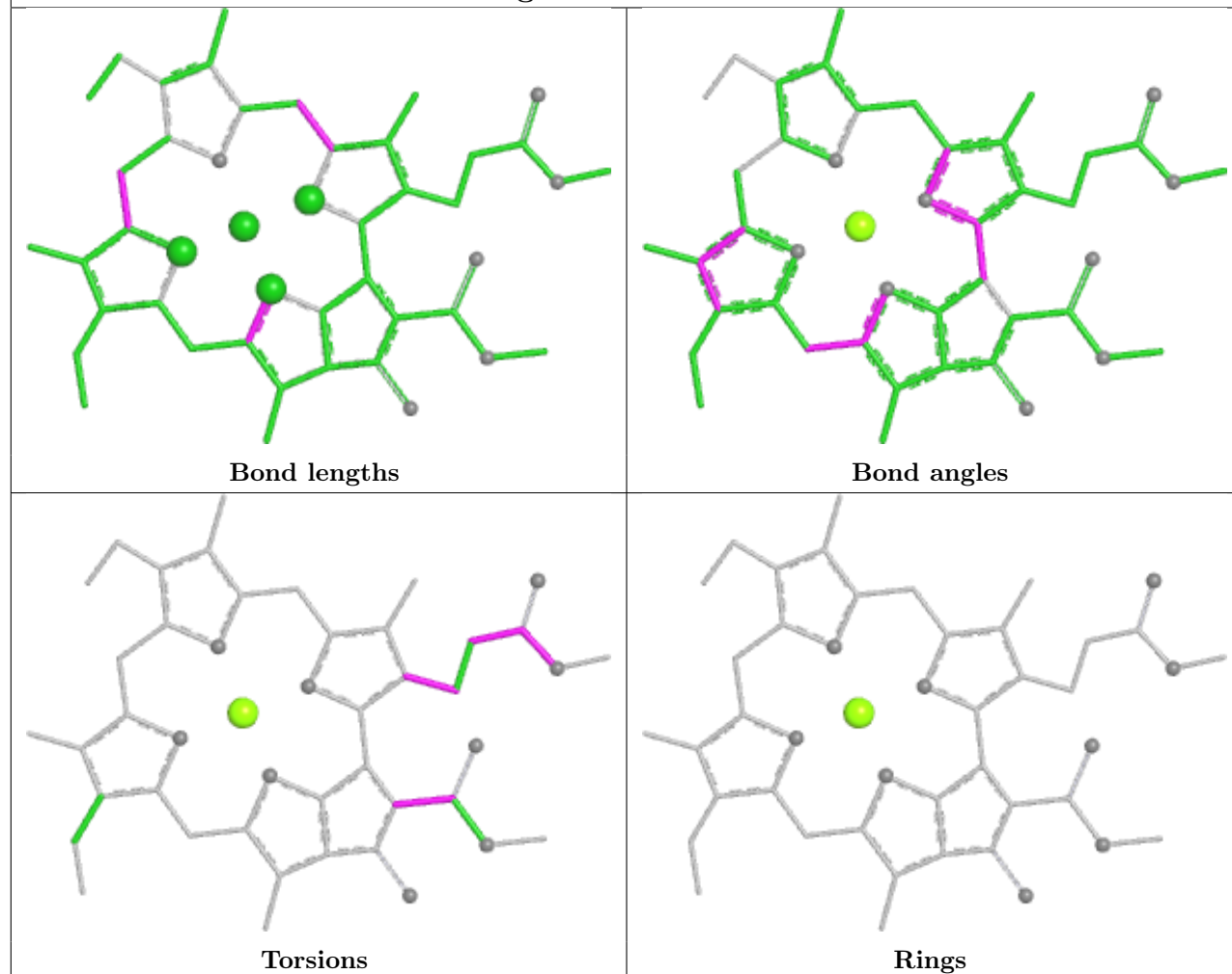


## Ligand CLA o 503

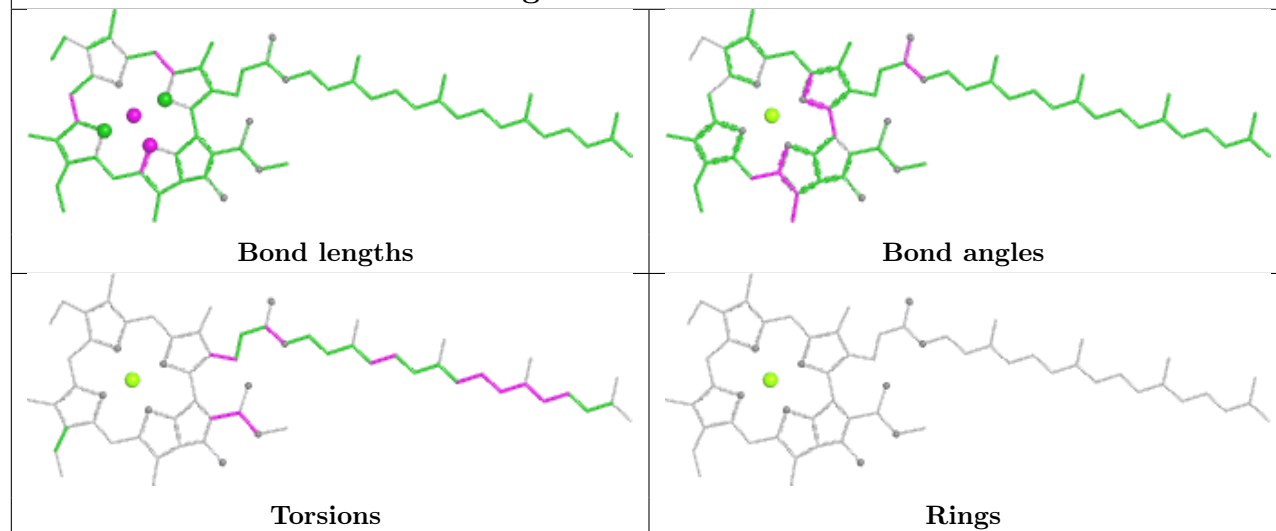




## Ligand CLA v 501

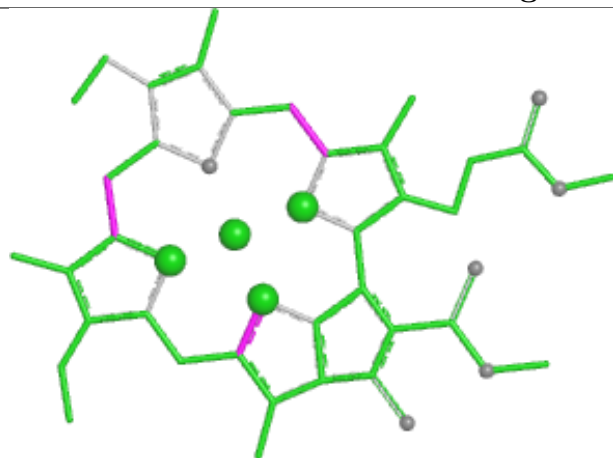


## Ligand CLA H 1128

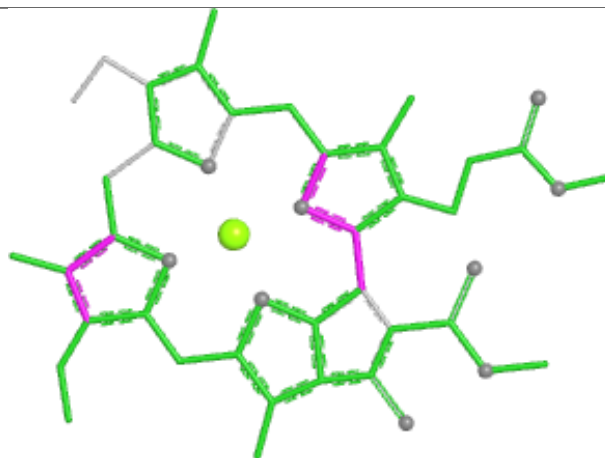




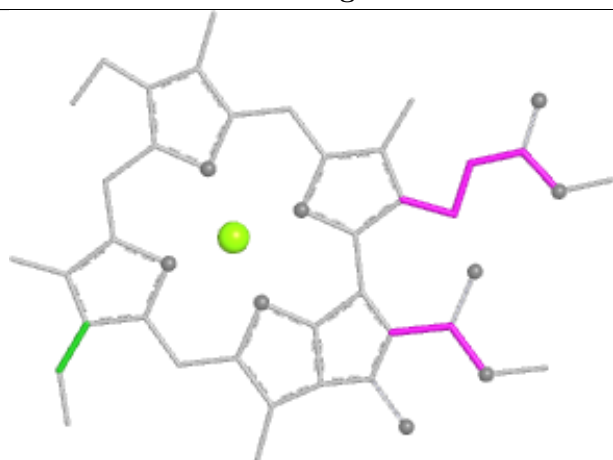
## Ligand CLA r 513



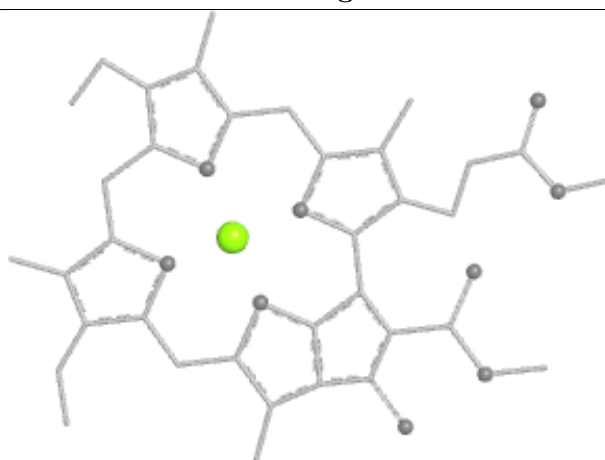
Bond lengths



Bond angles

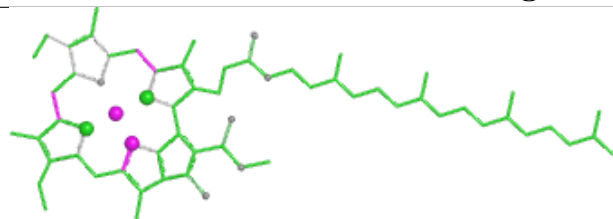


Torsions

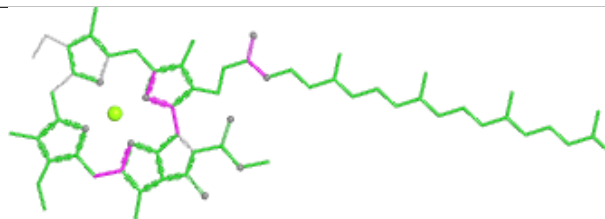


Rings

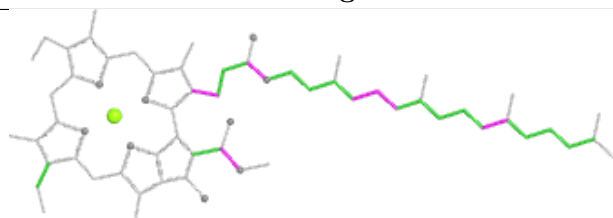
## Ligand CLA t 512



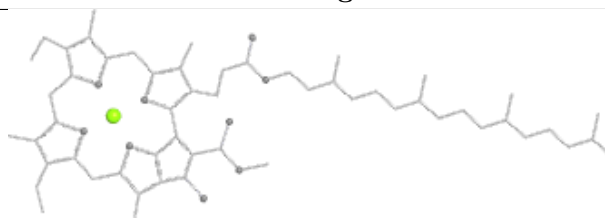
Bond lengths



Bond angles

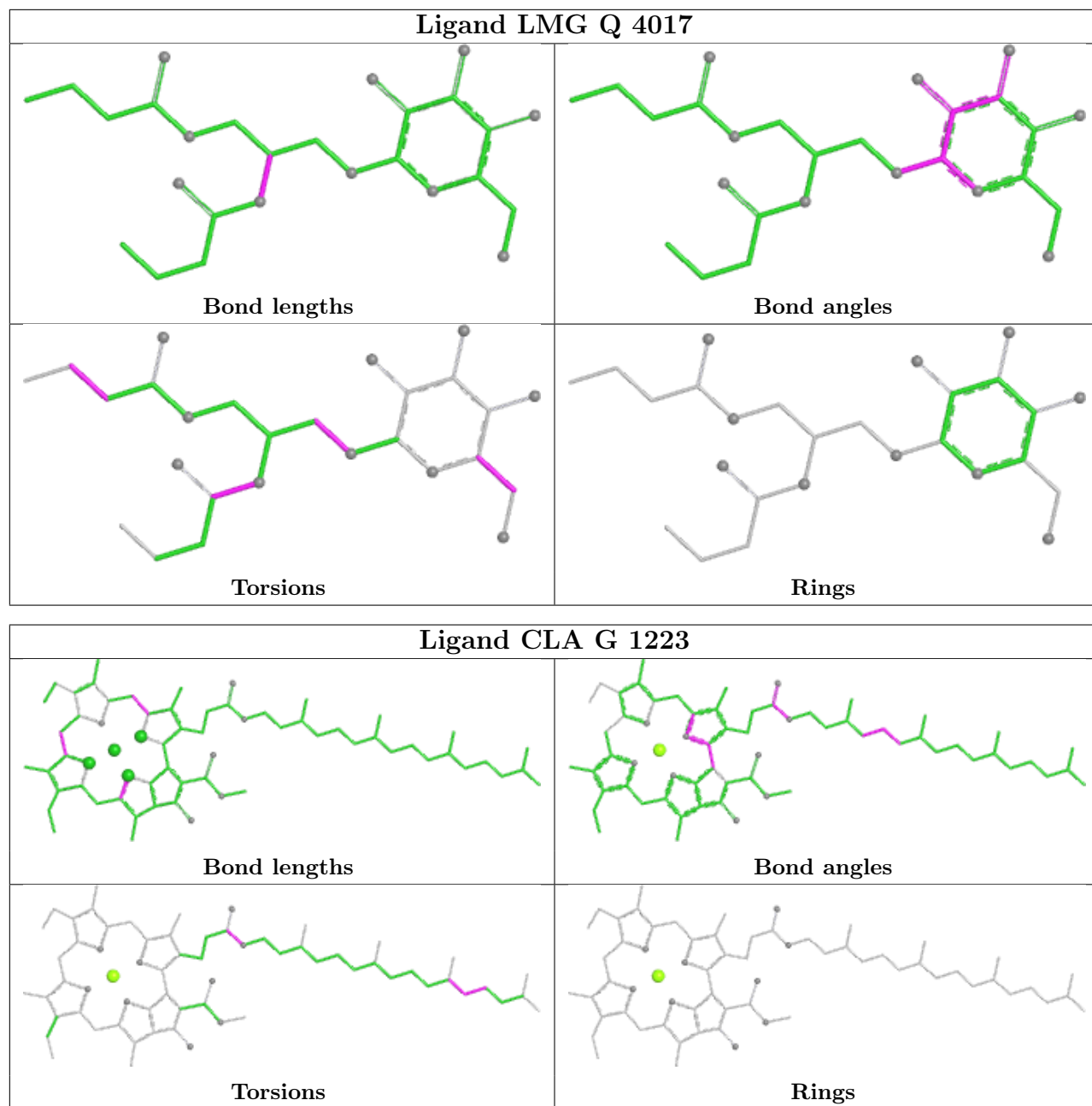


Torsions

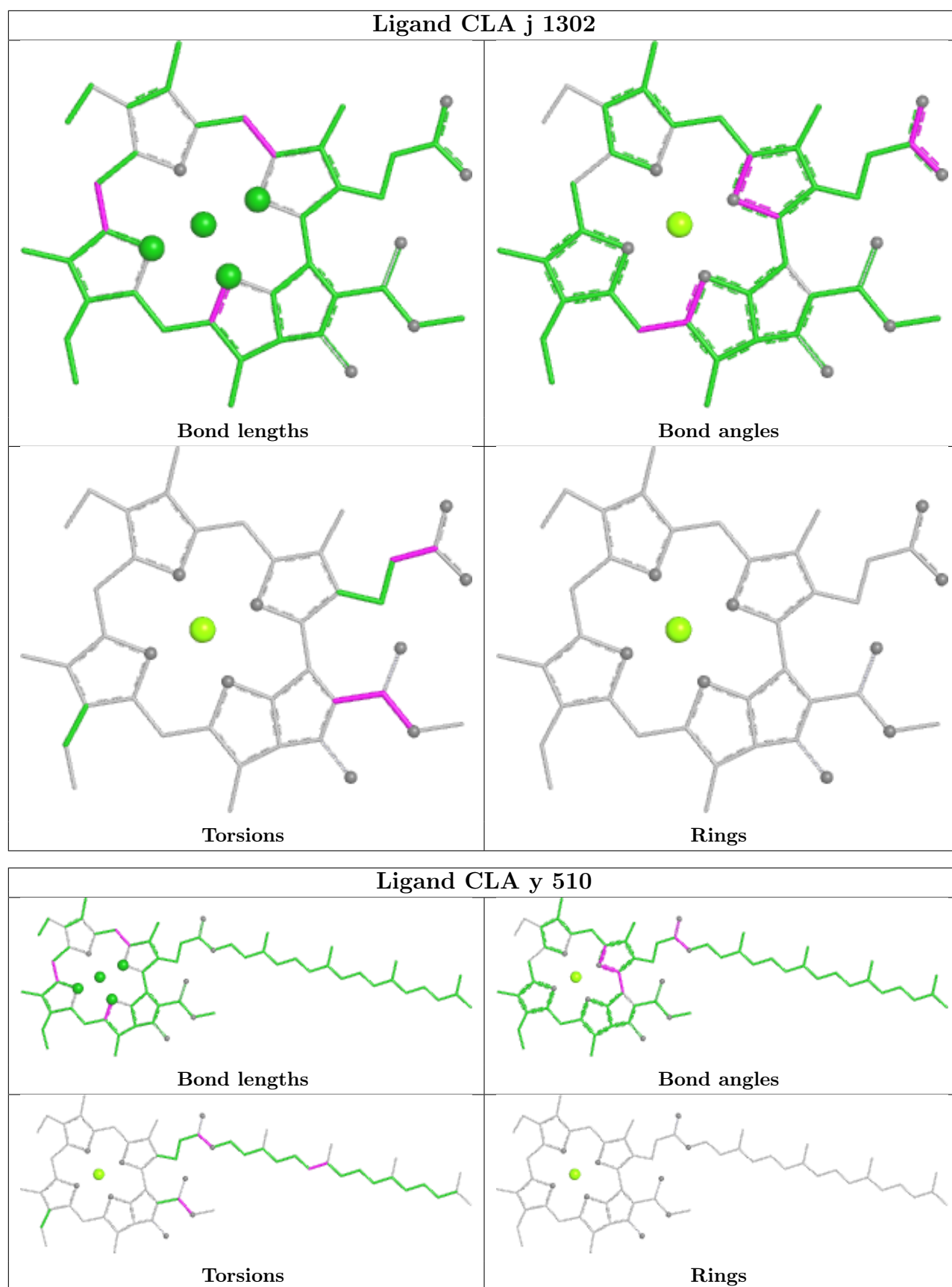


Rings

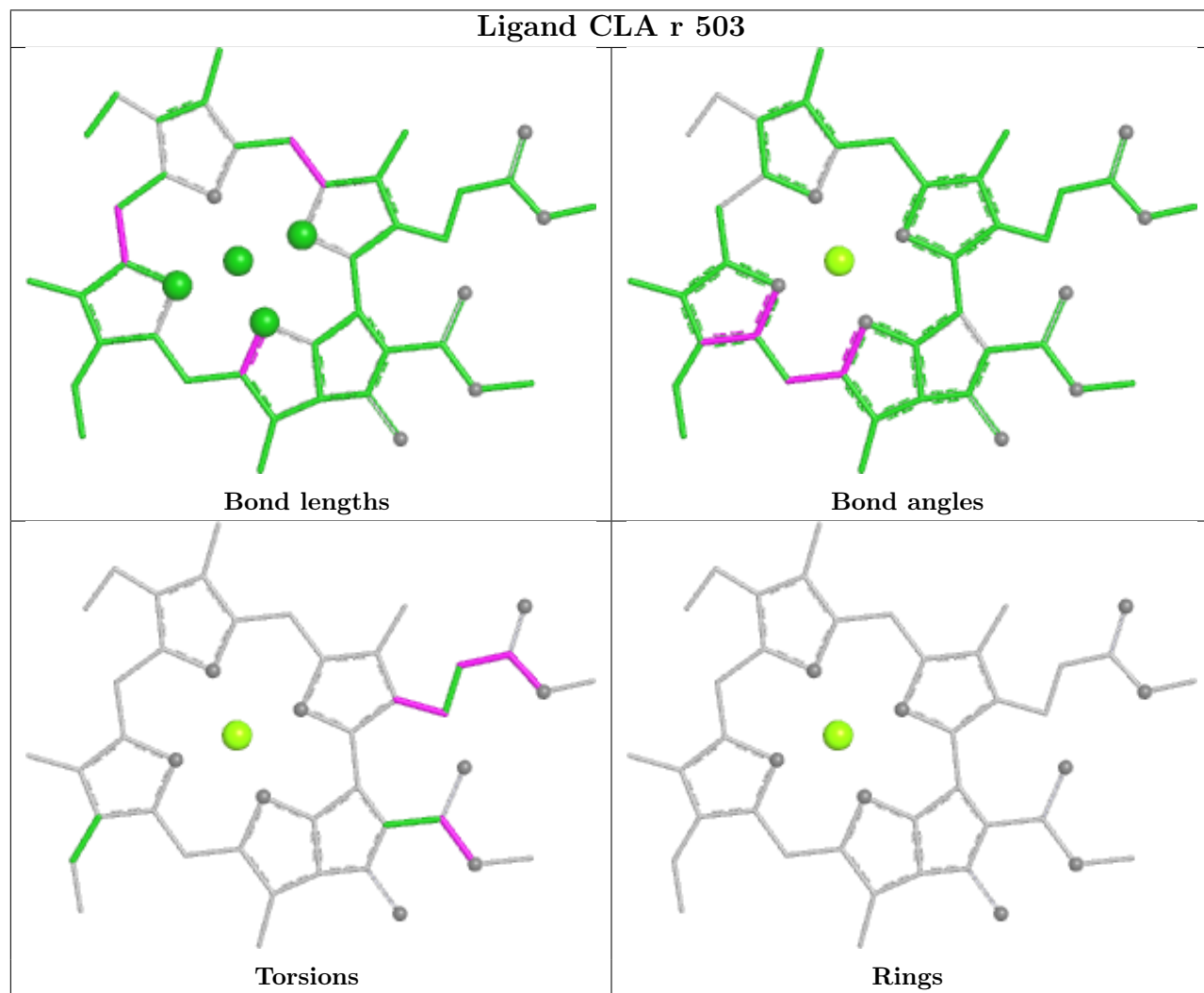
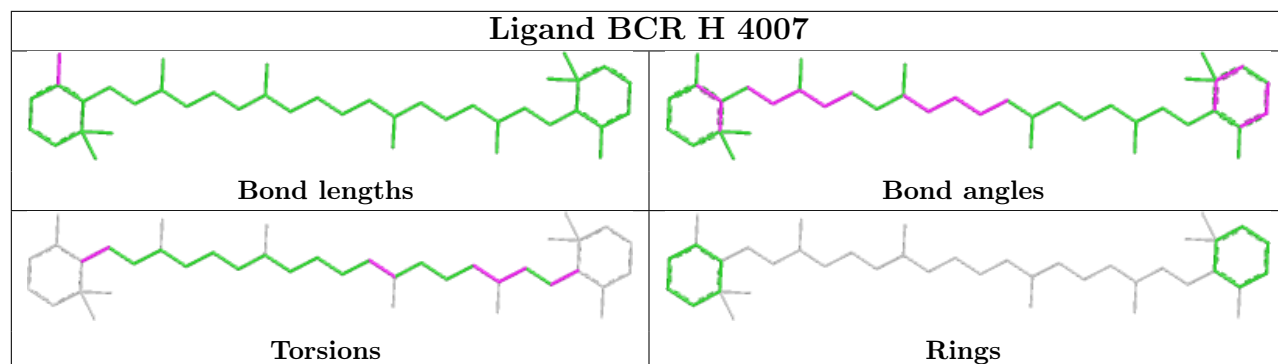




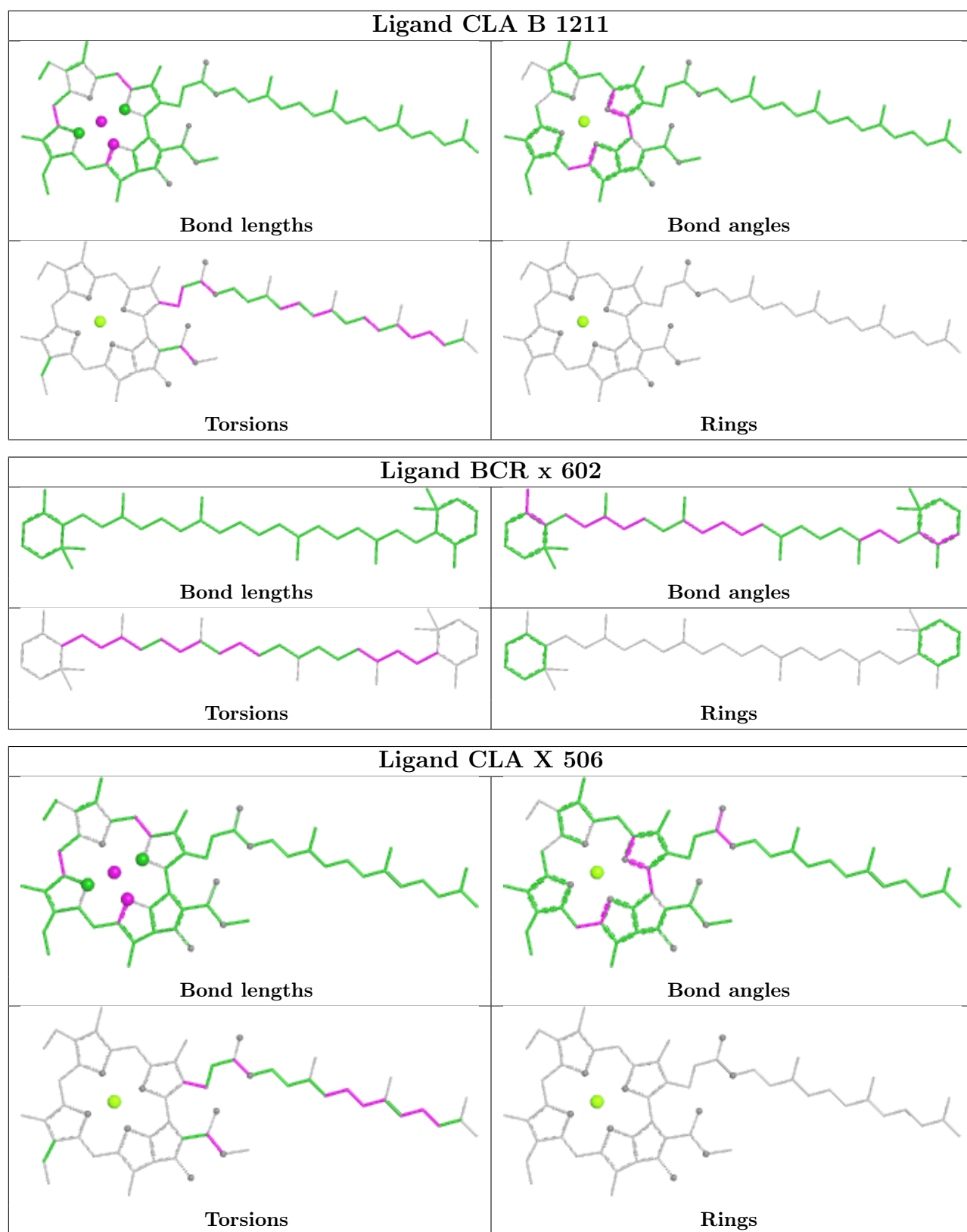




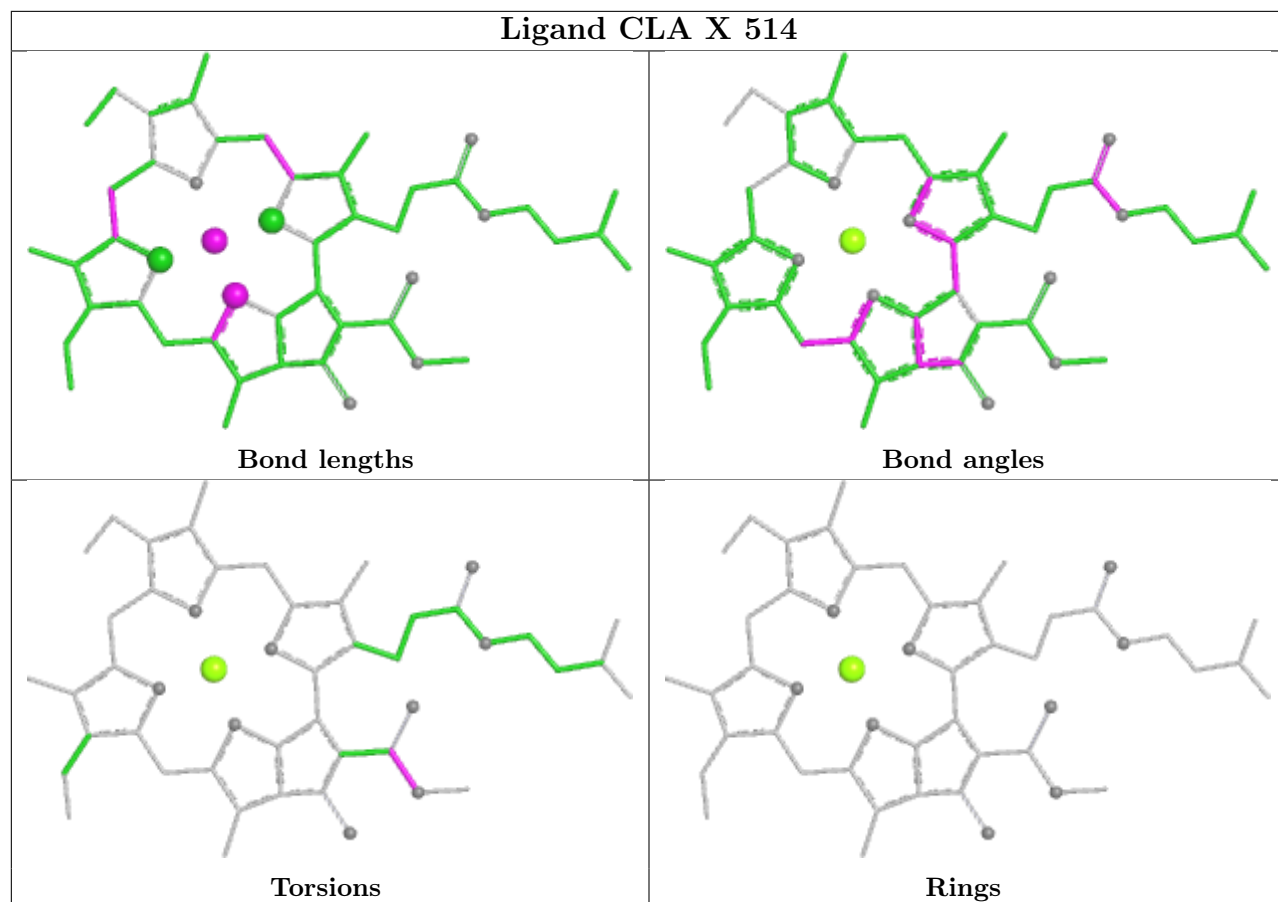






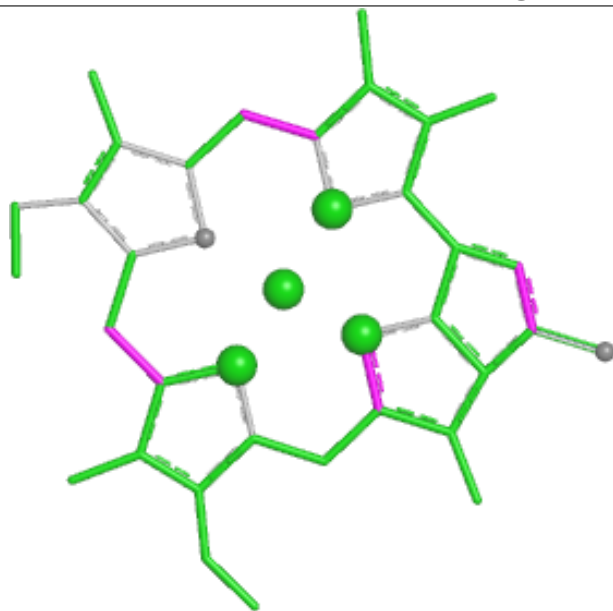




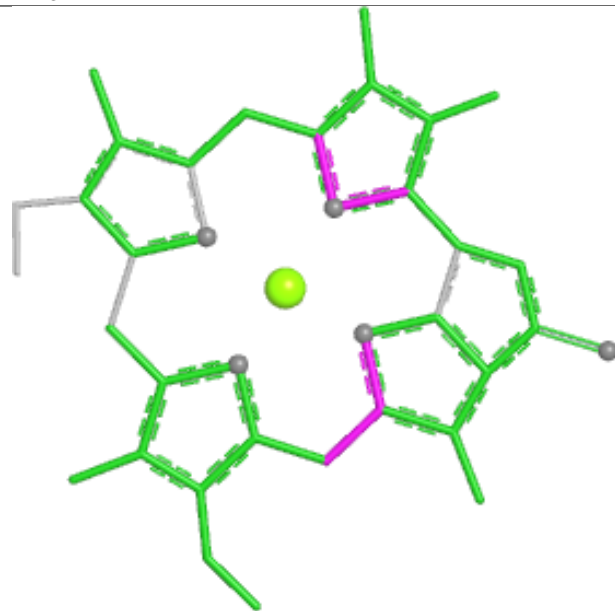




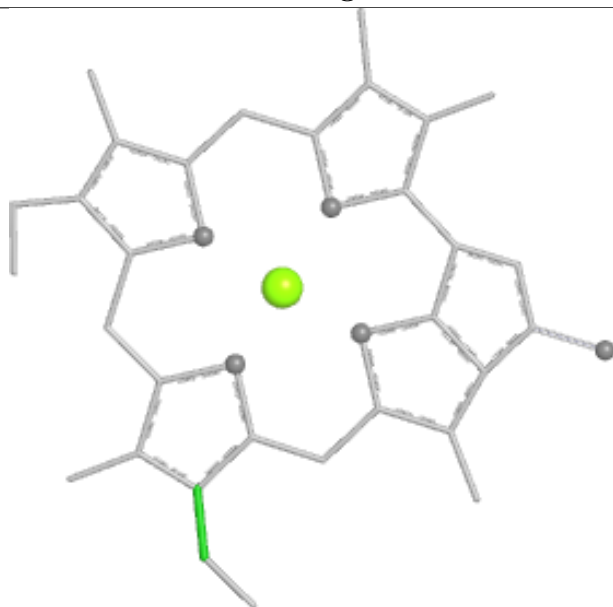
## Ligand CLA j 1303



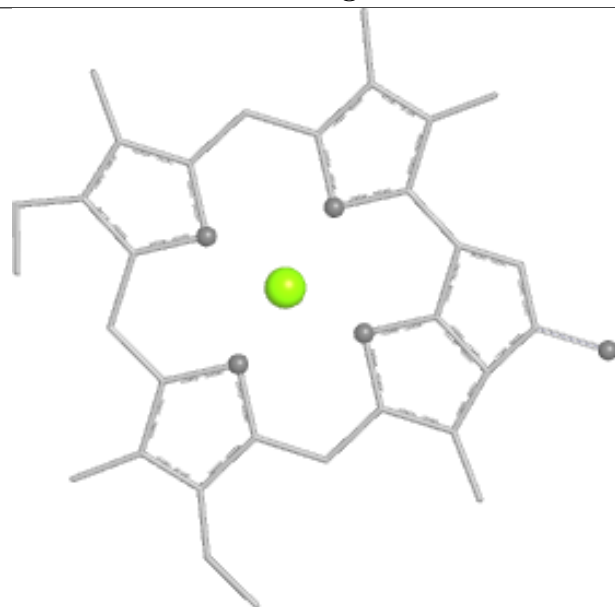
Bond lengths



Bond angles

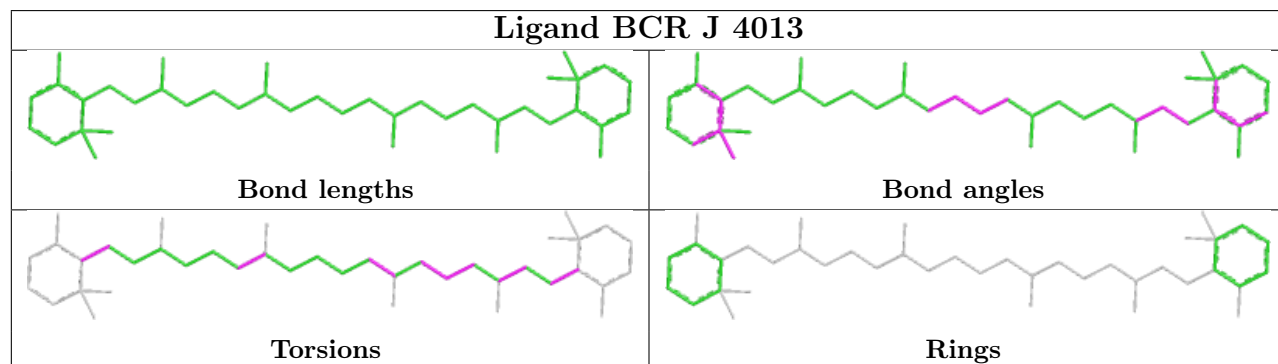
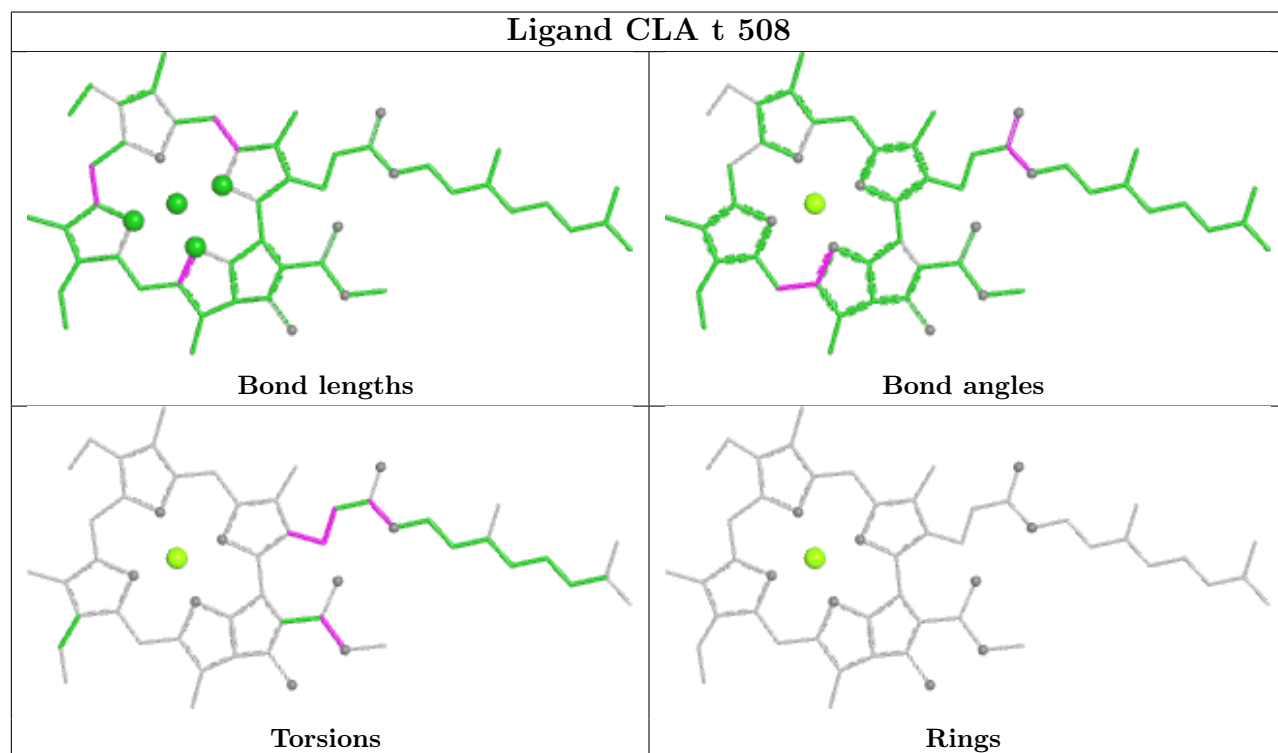
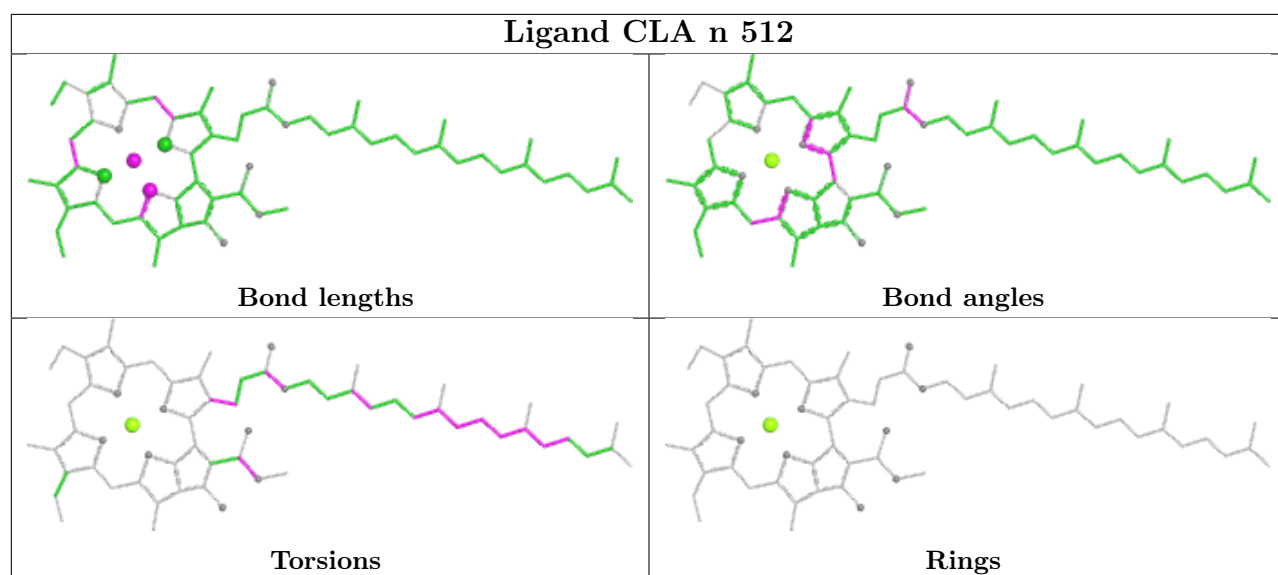


Torsions

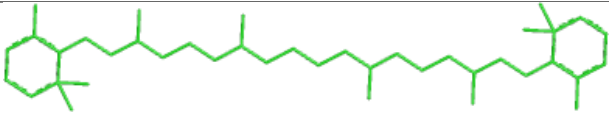
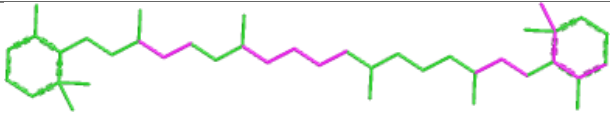
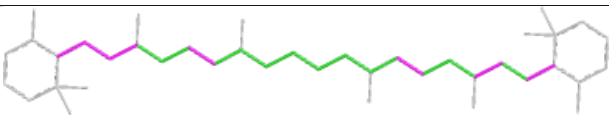
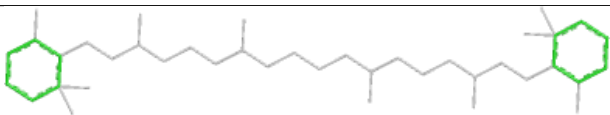

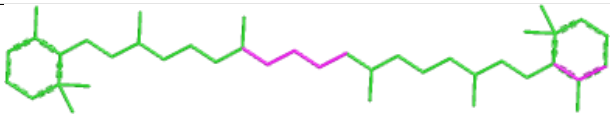
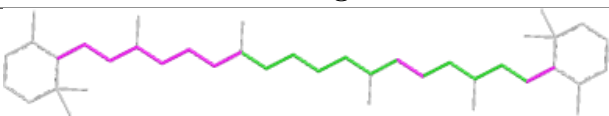
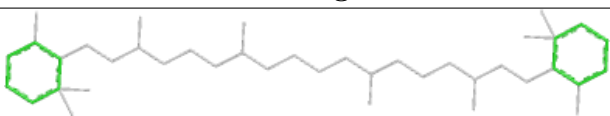
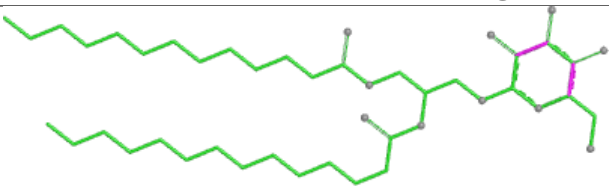
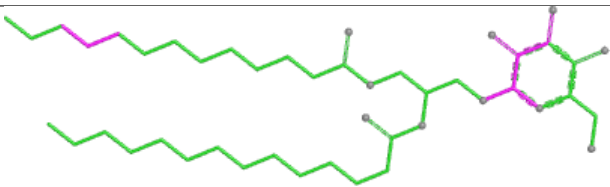
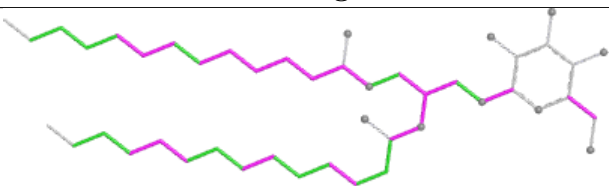
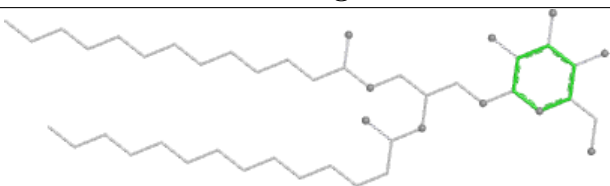


Rings



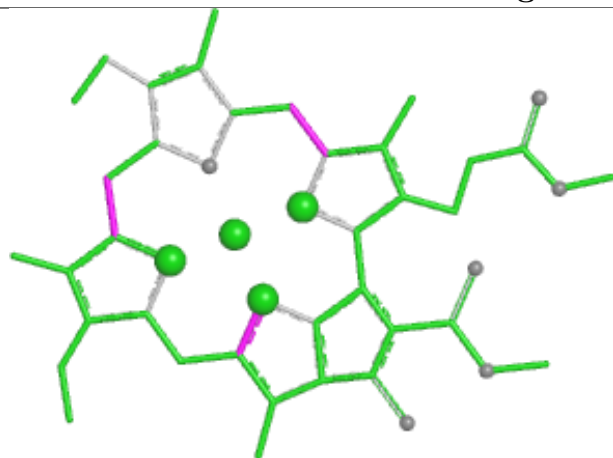




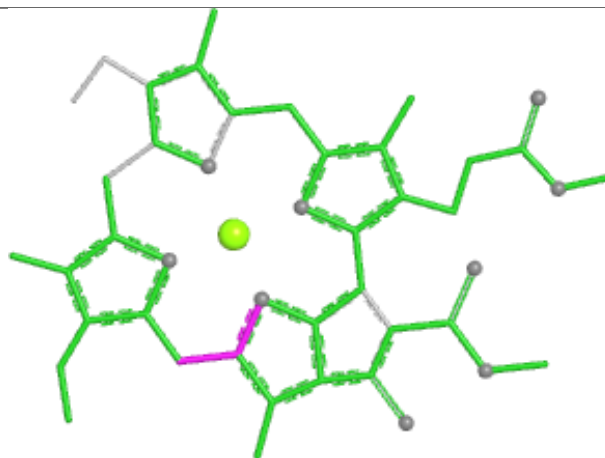
Ligand BCR K 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR W 603	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 4101	
 Bond lengths	 Bond angles
 Torsions	 Rings



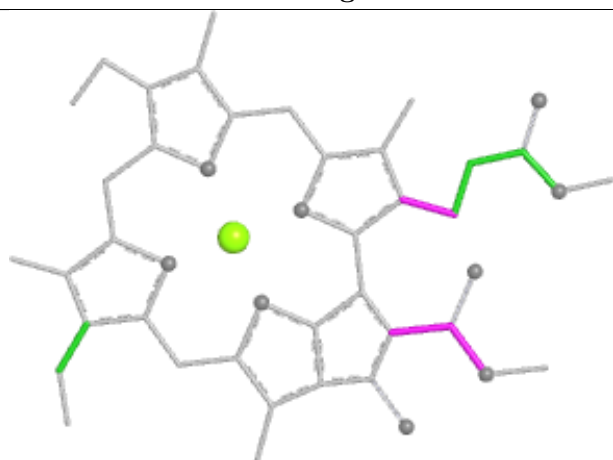
## Ligand CLA n 516



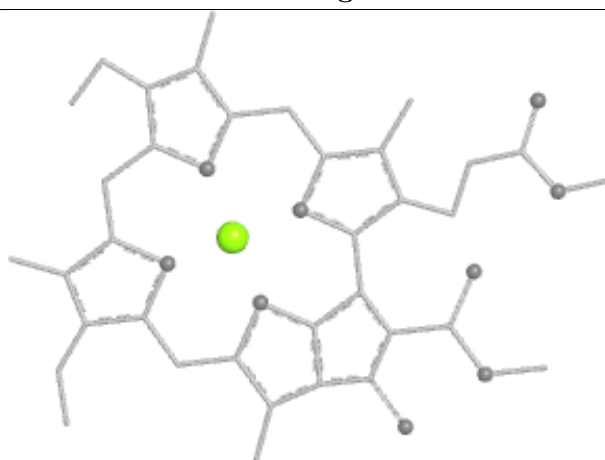
Bond lengths



Bond angles

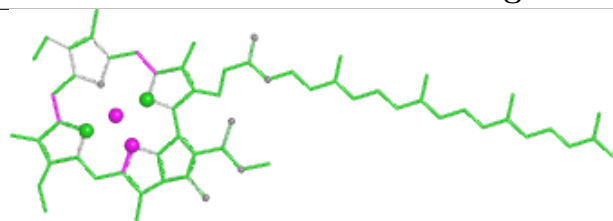


Torsions

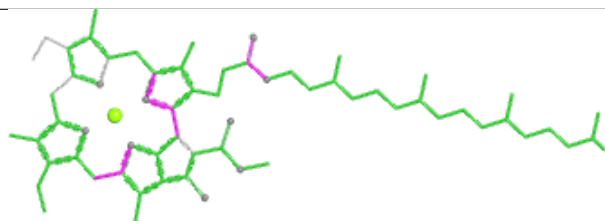


Rings

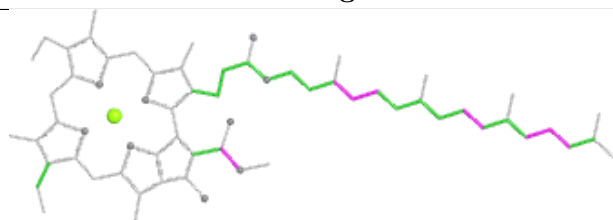
## Ligand CLA G 1205



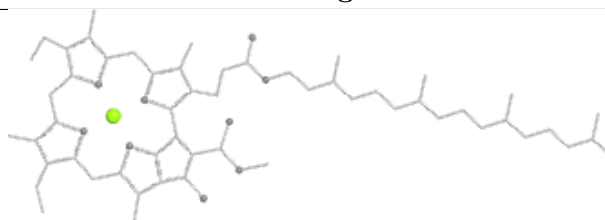
Bond lengths



Bond angles



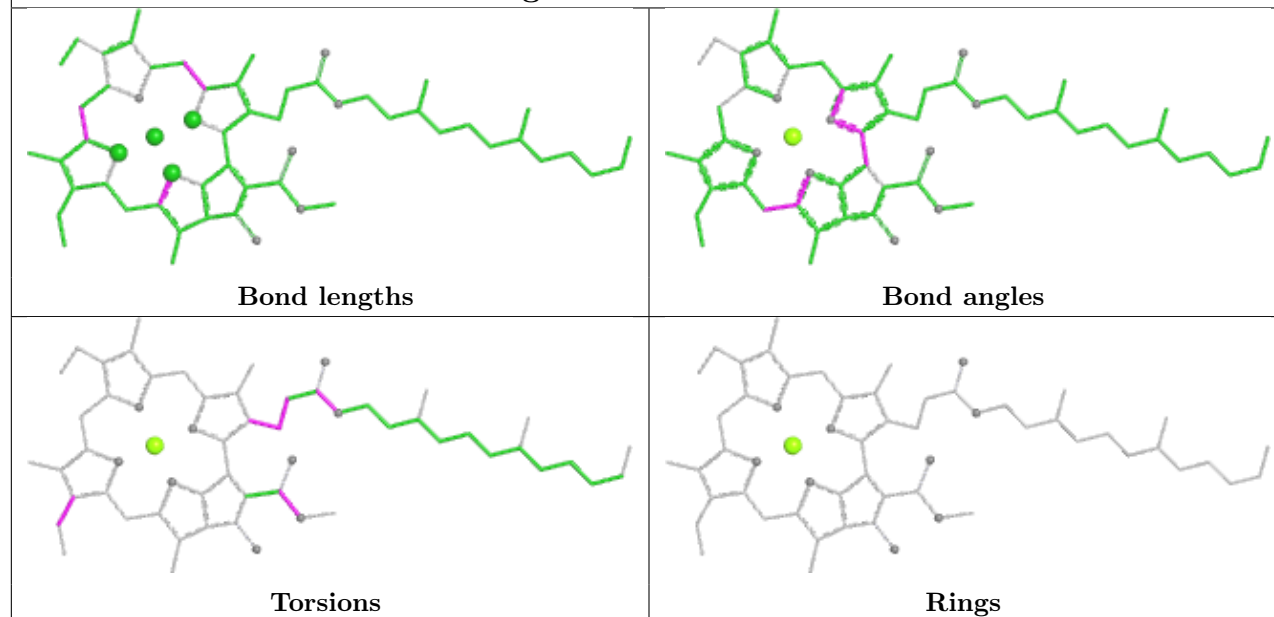
Torsions



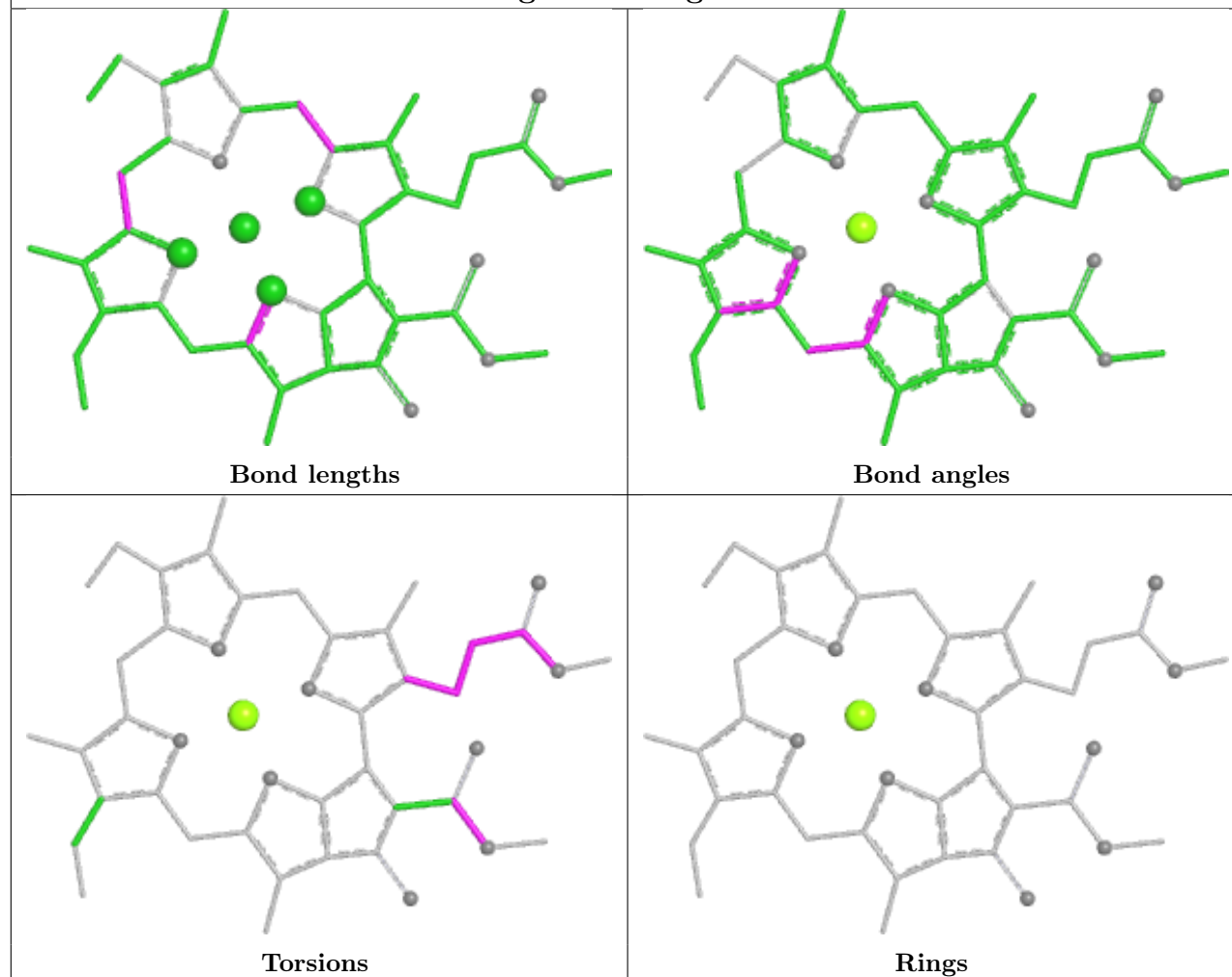
Rings



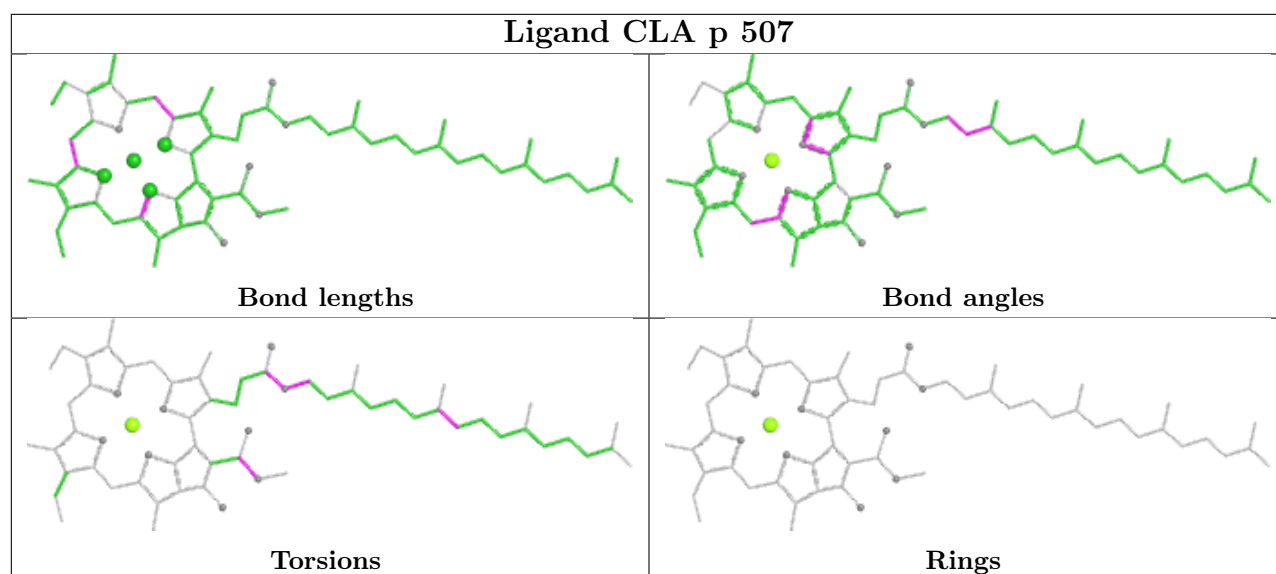
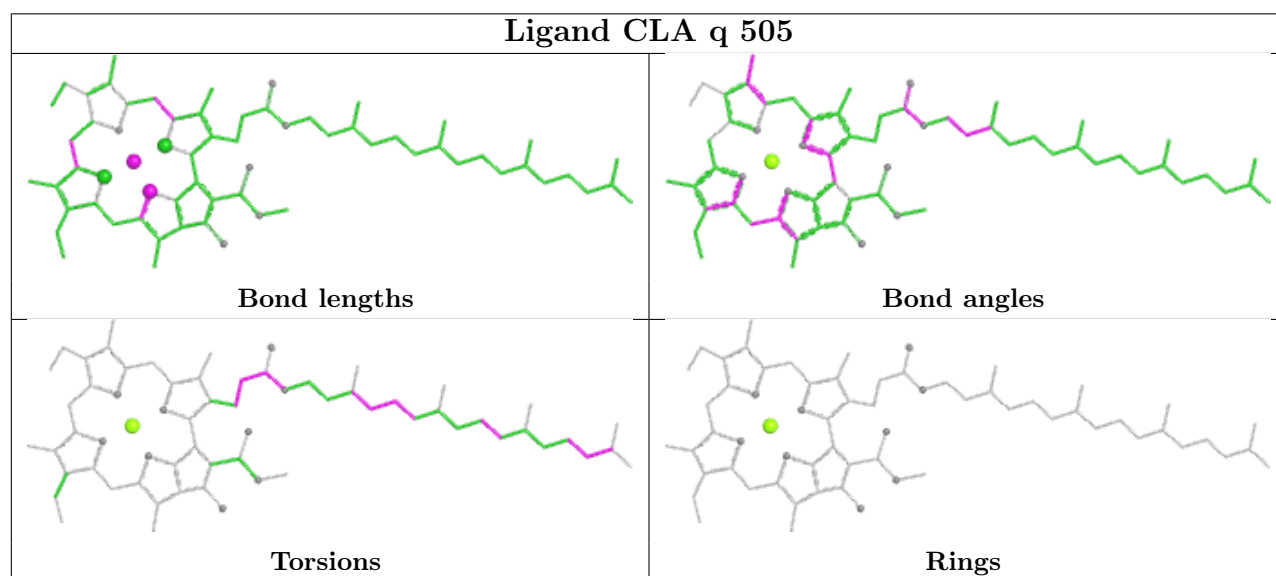
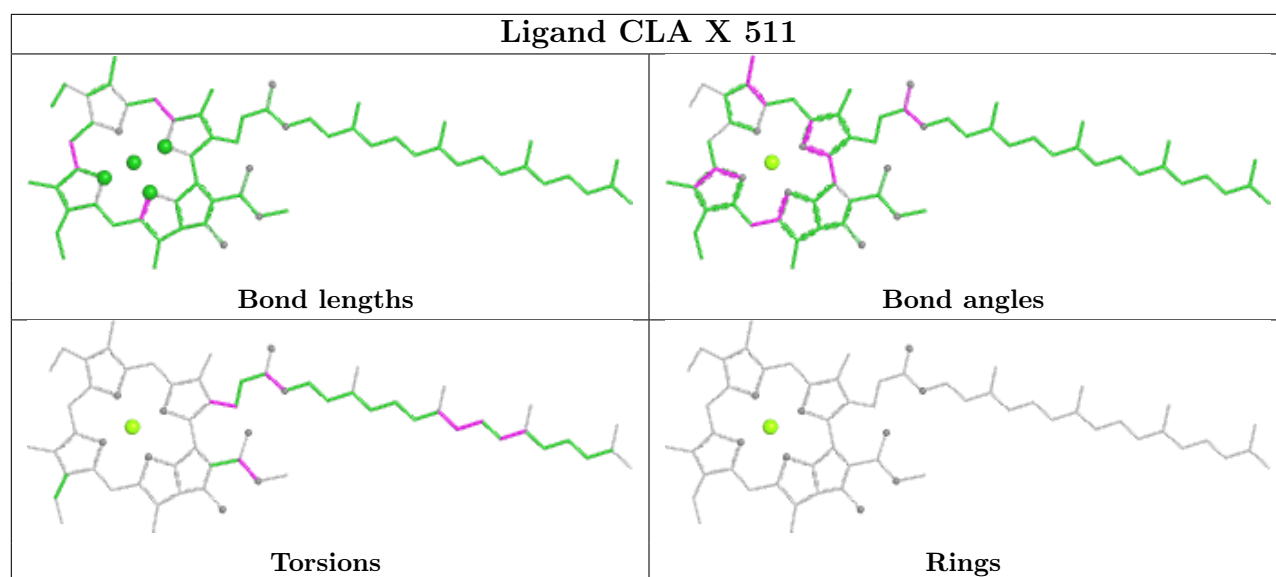
## Ligand CLA H 1122



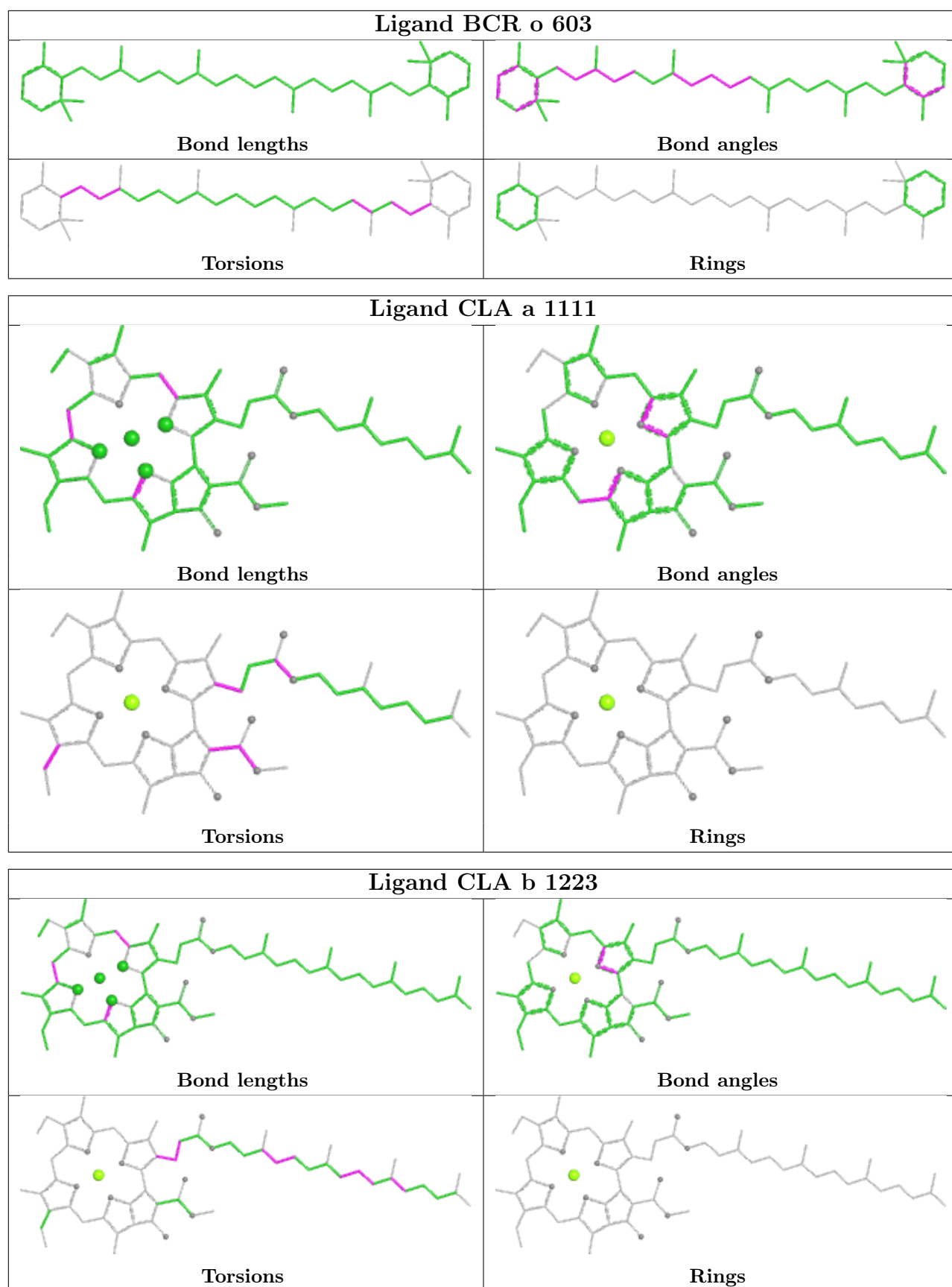
## Ligand CLA g 503





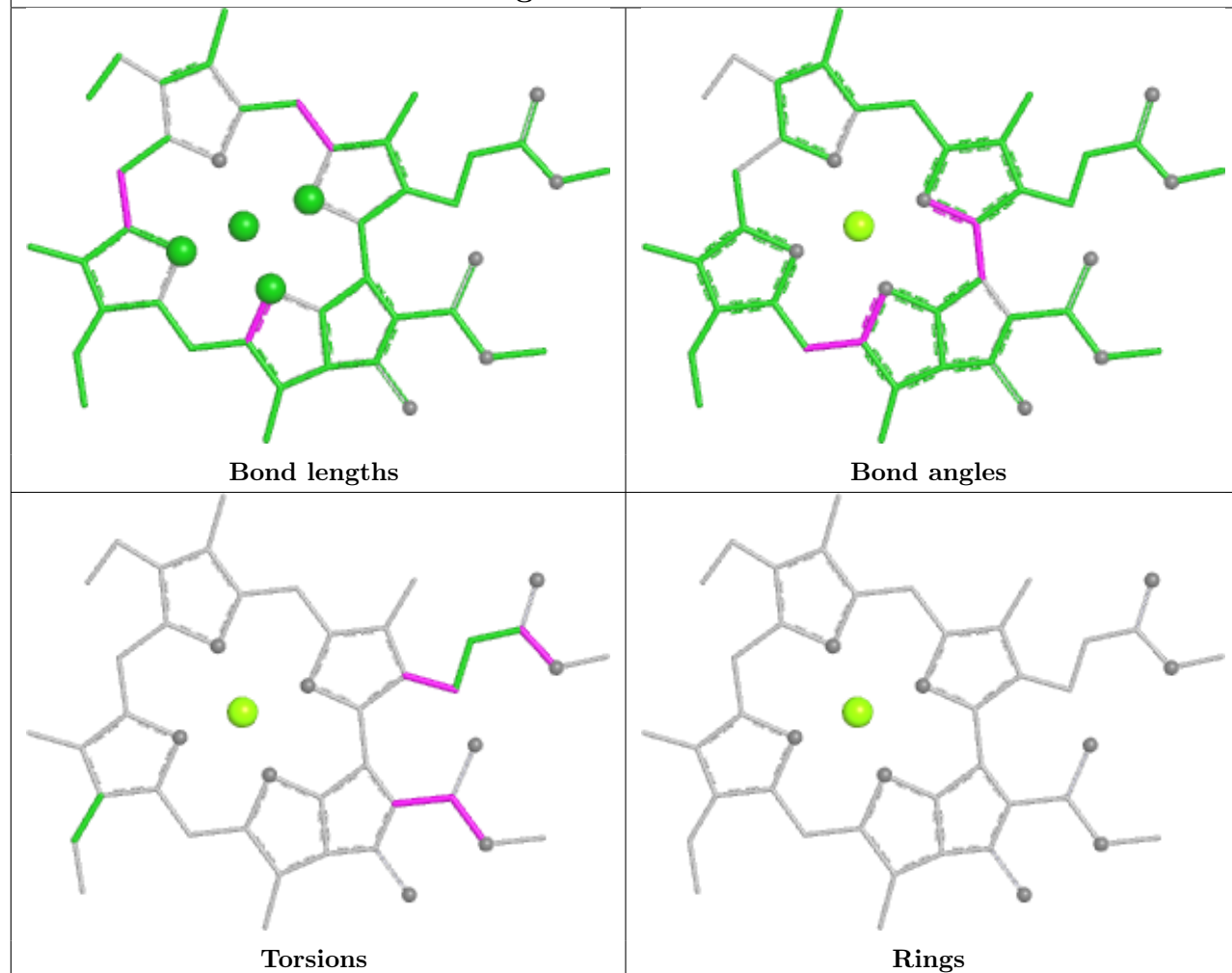




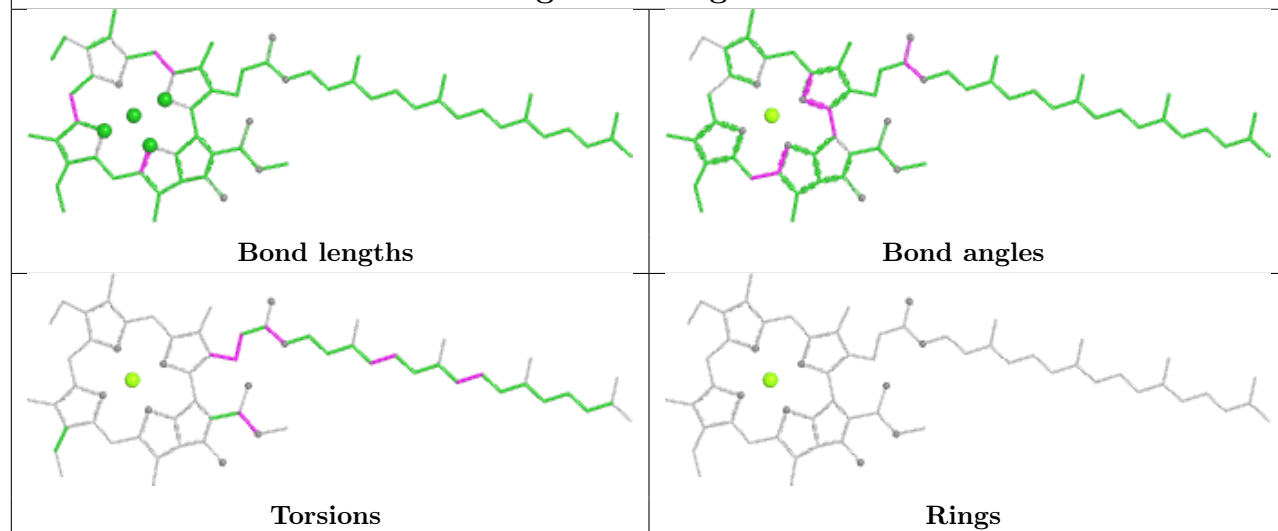




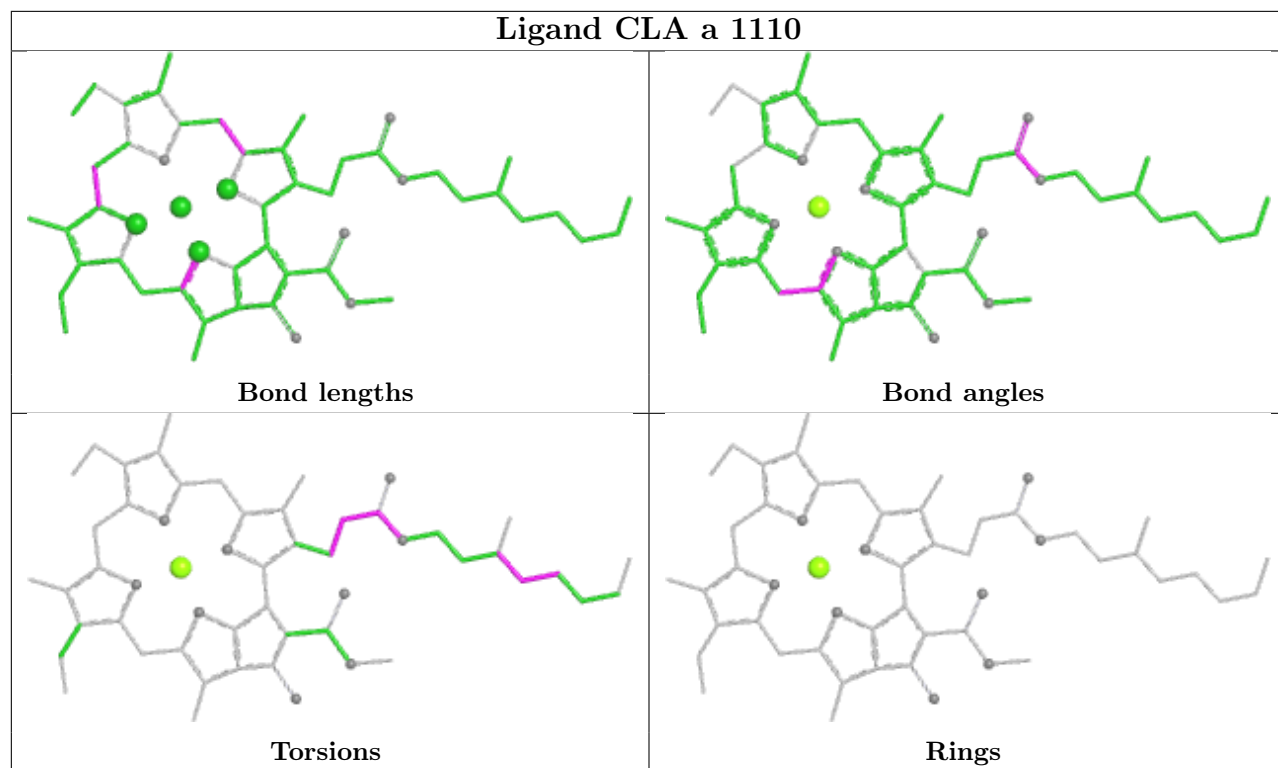
## Ligand CLA u 503



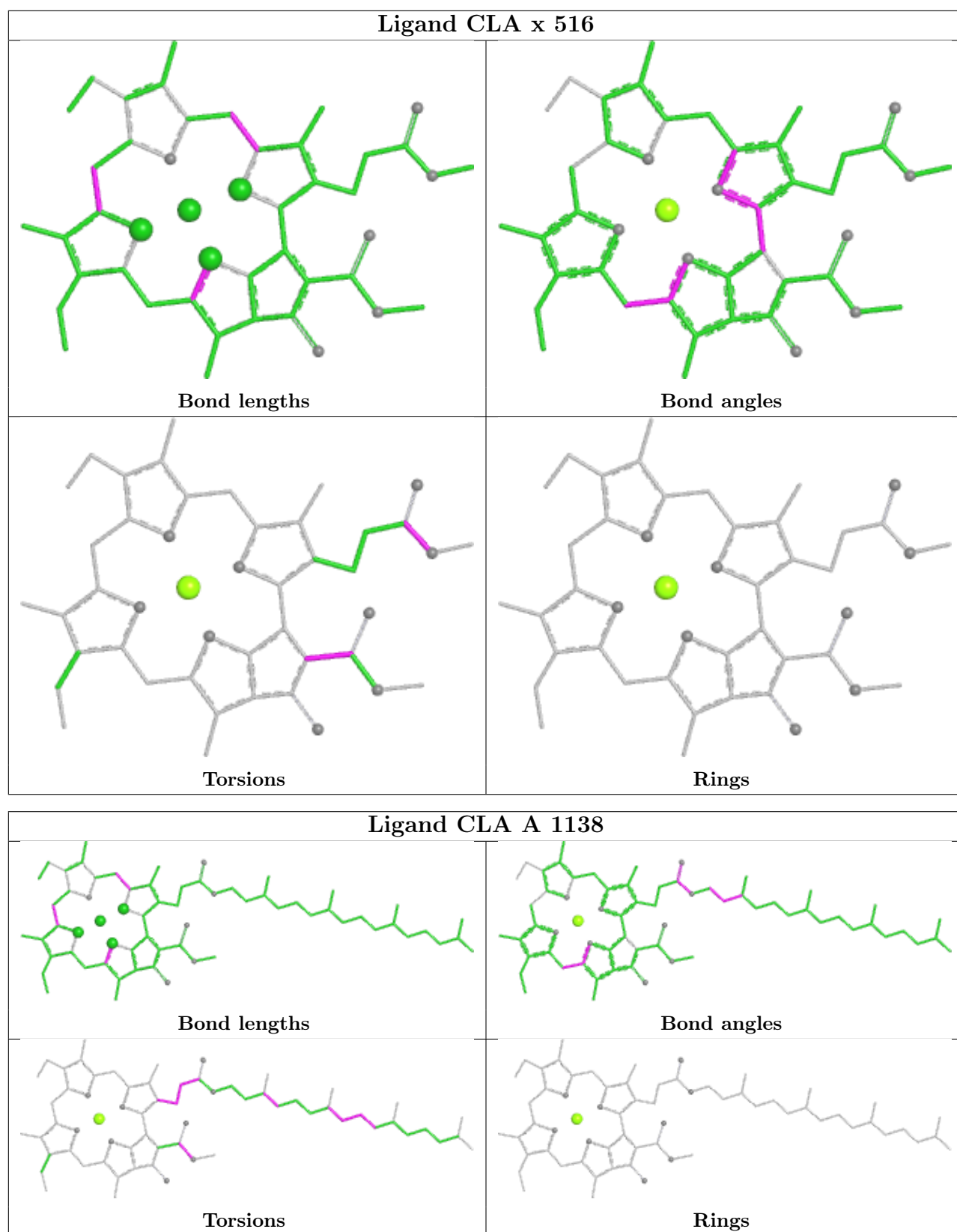
## Ligand CLA g 515



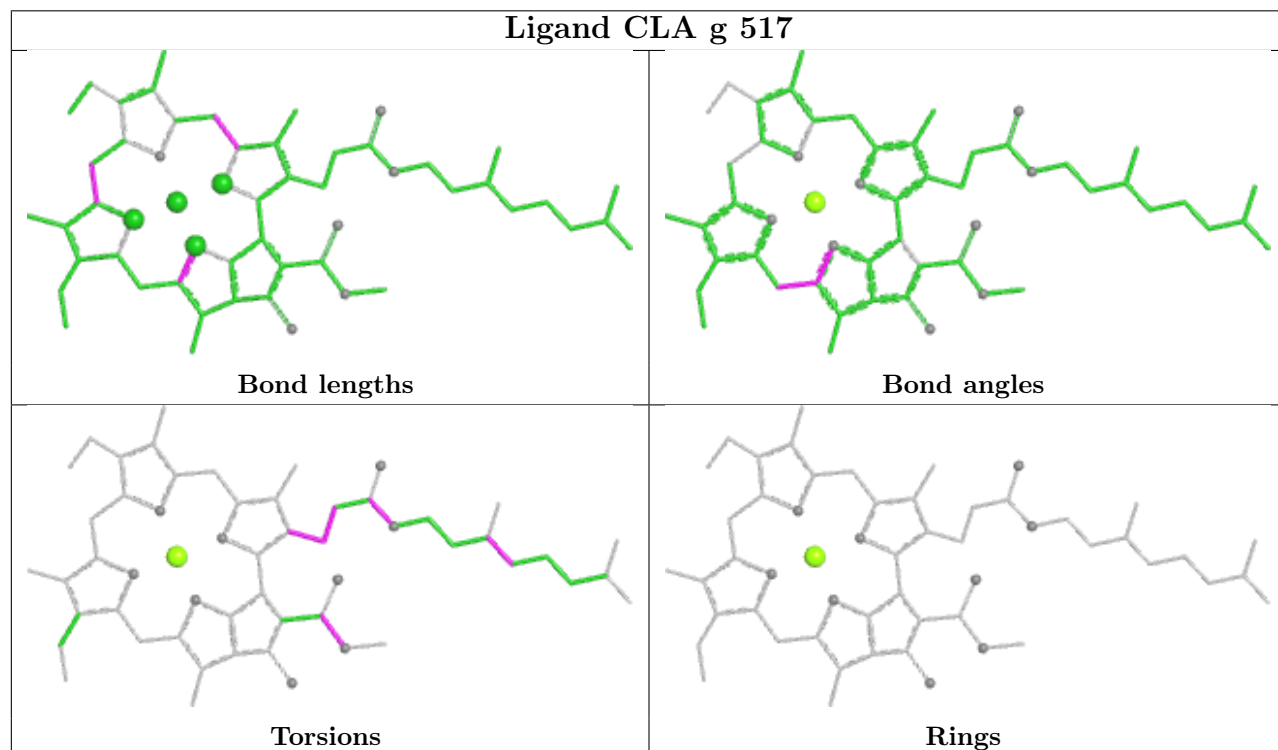
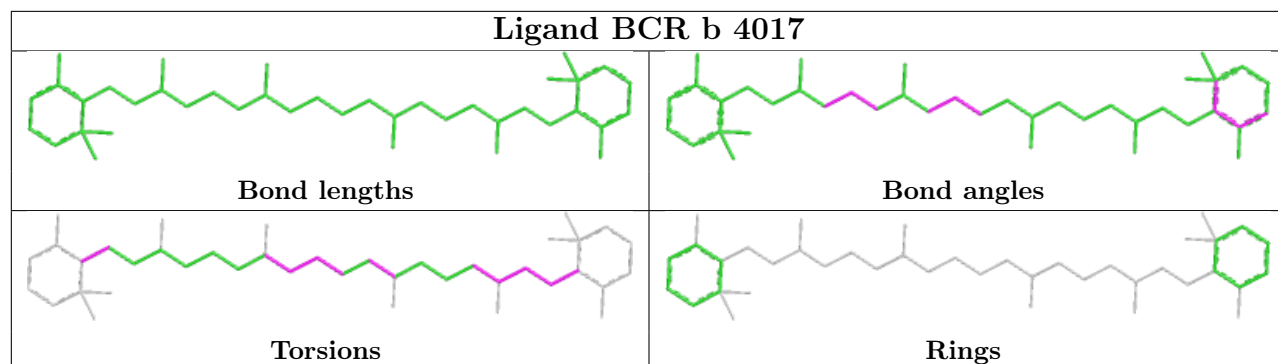




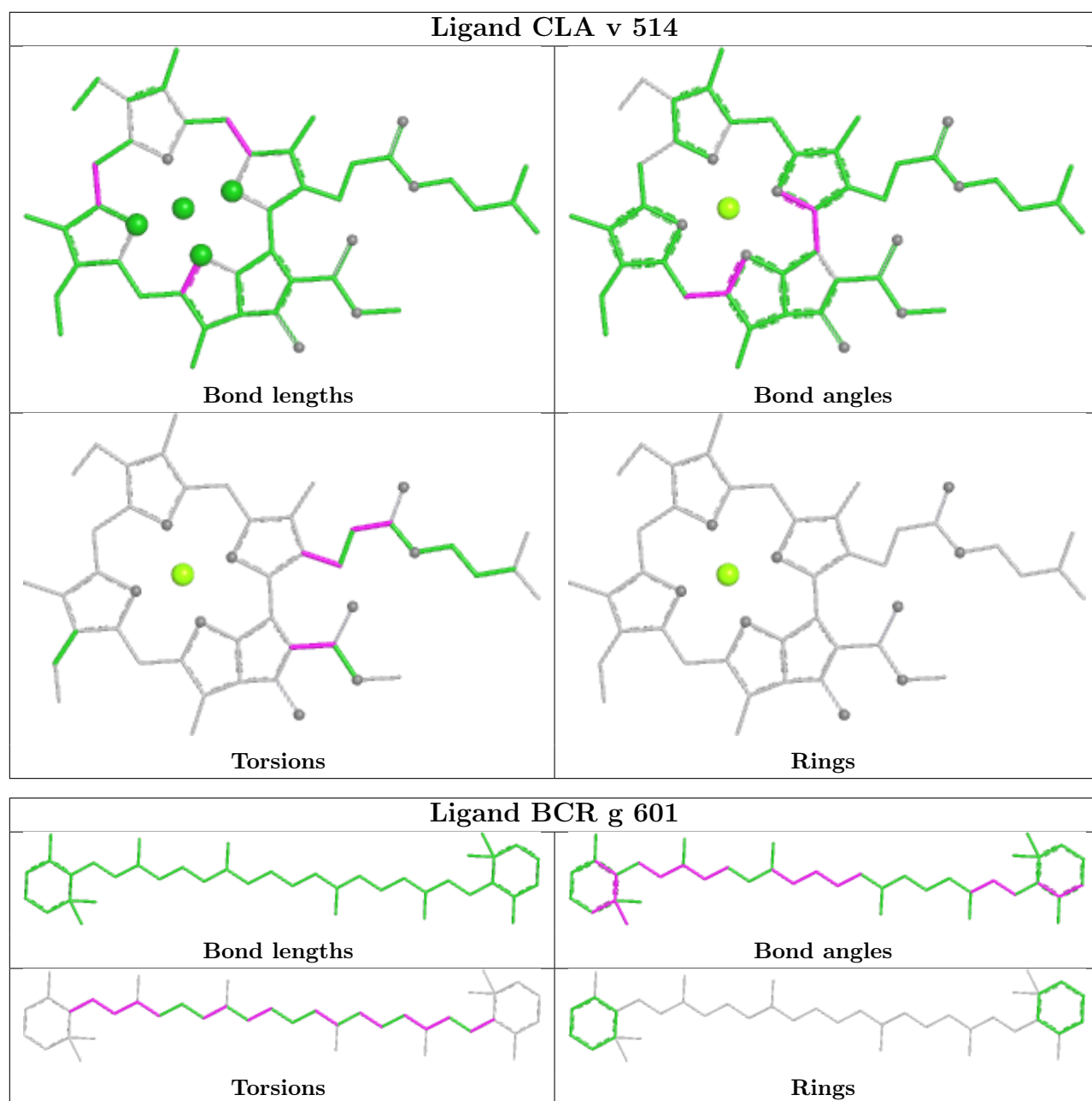






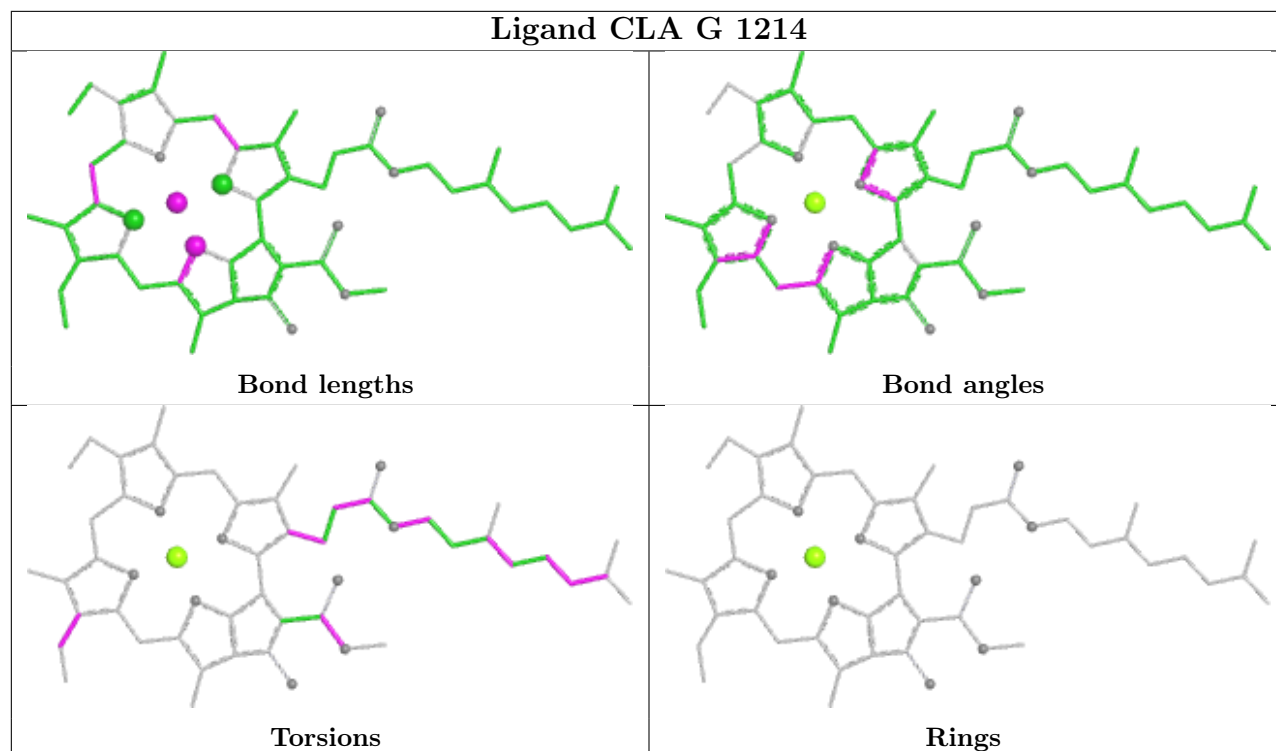




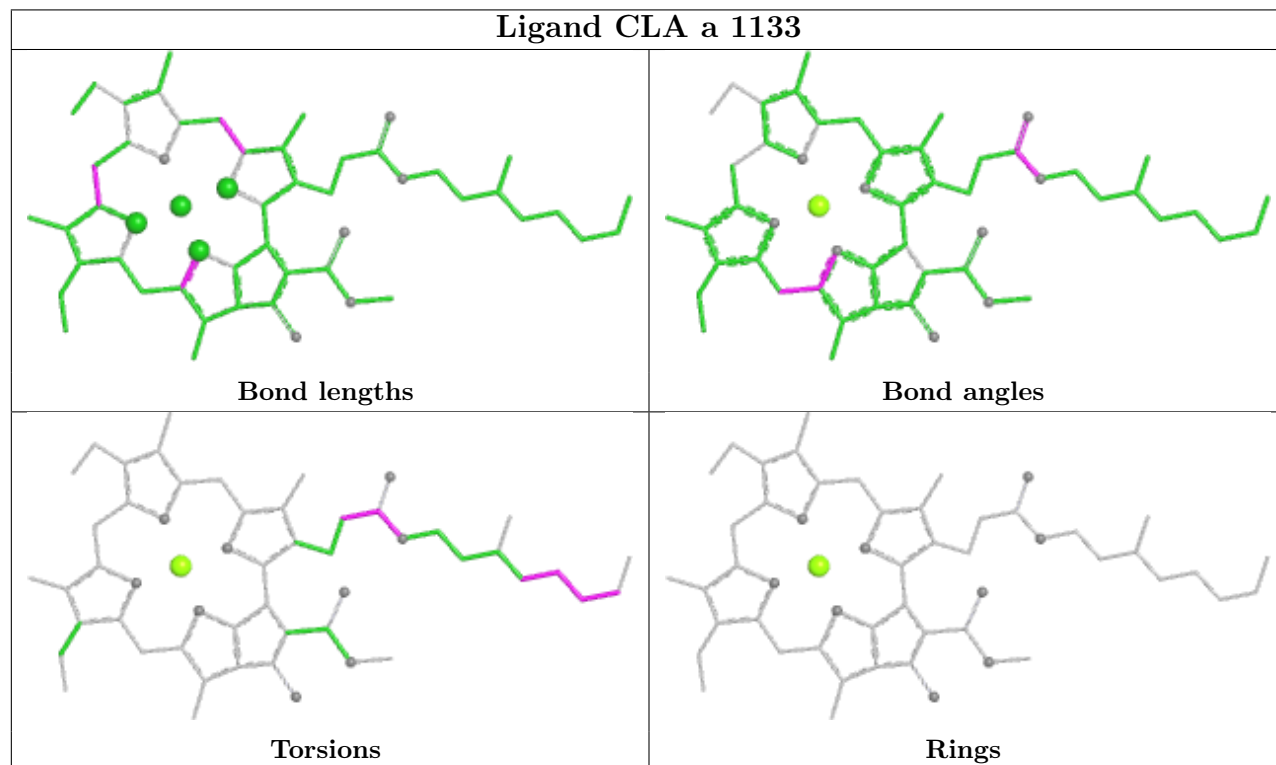




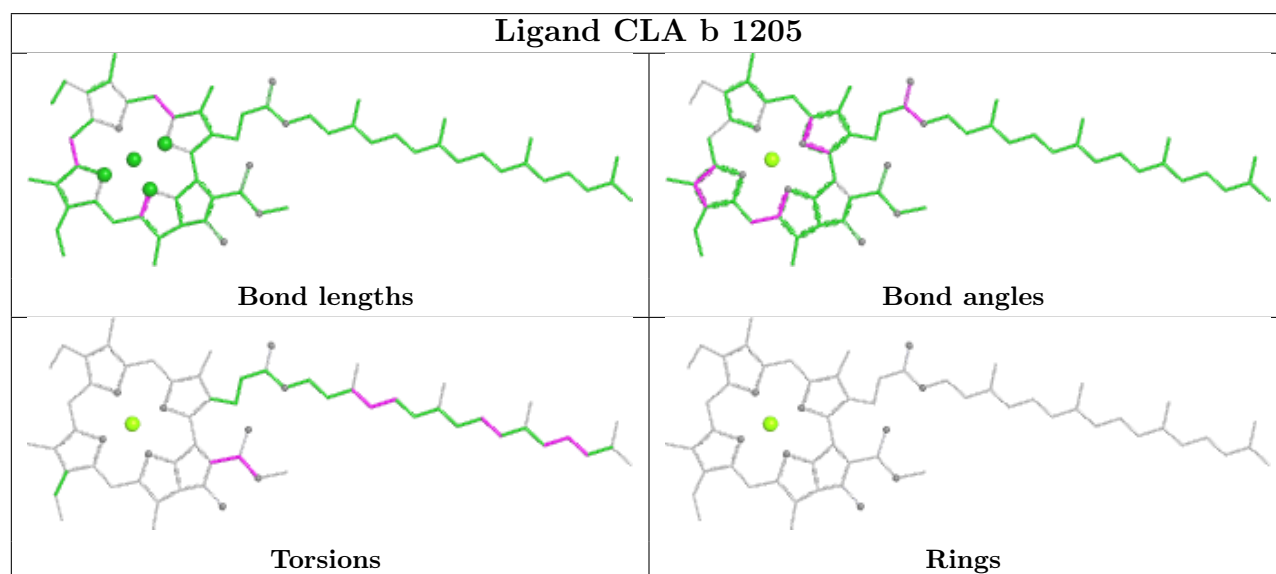
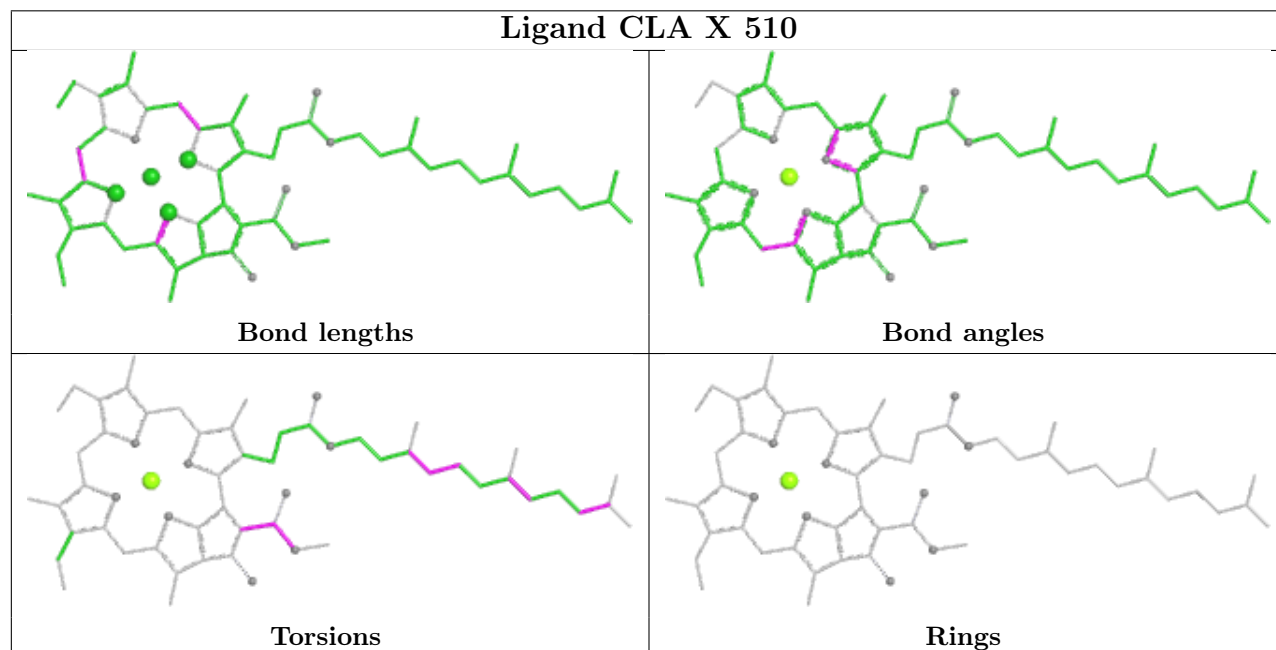
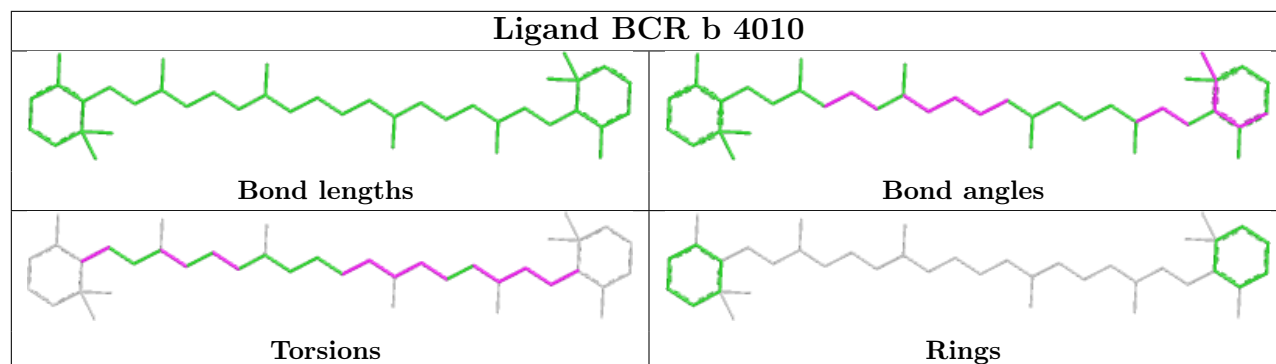
## Ligand CLA G 1214



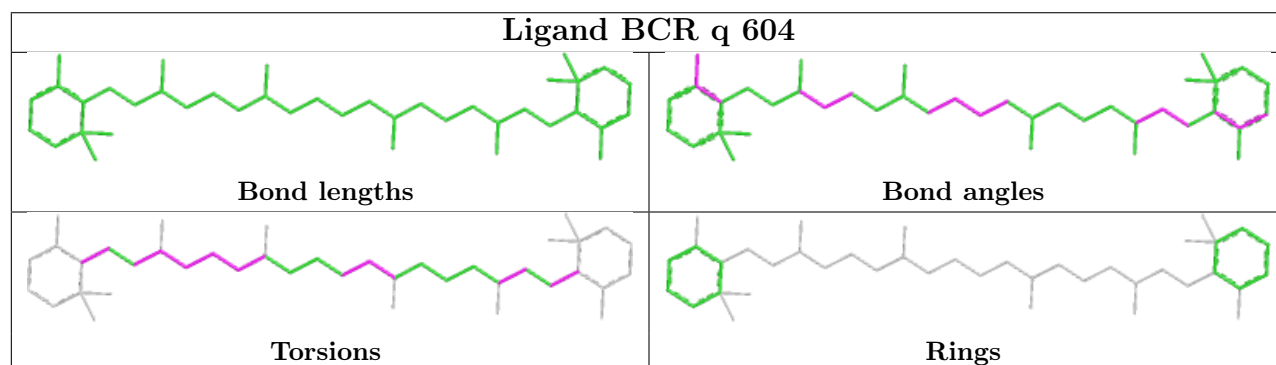
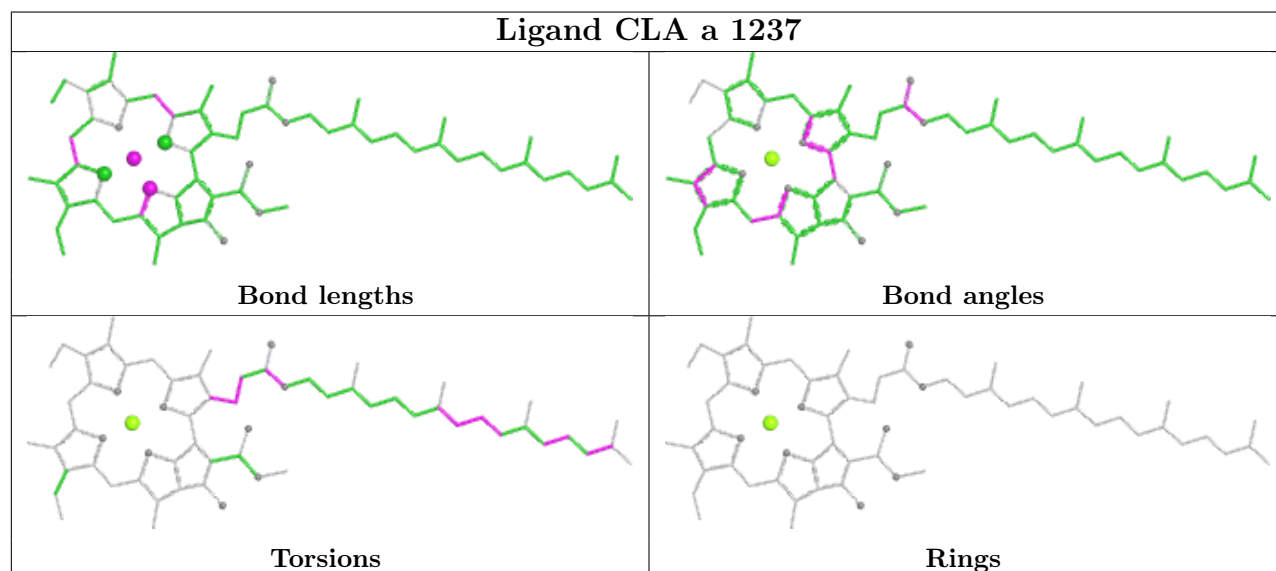
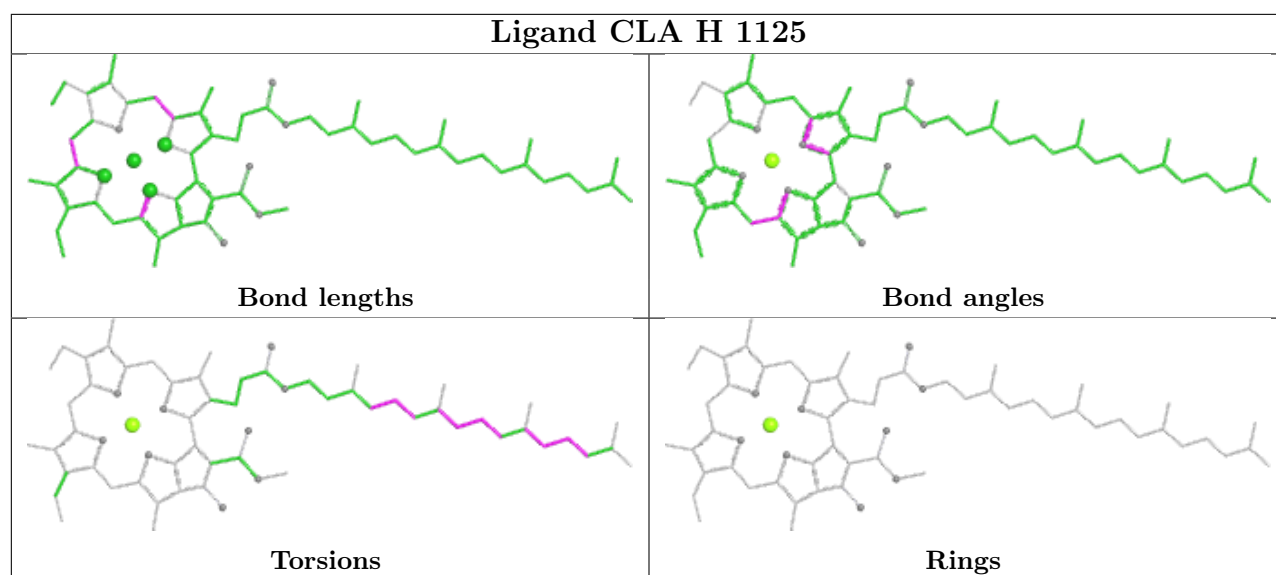
## Ligand CLA a 1133



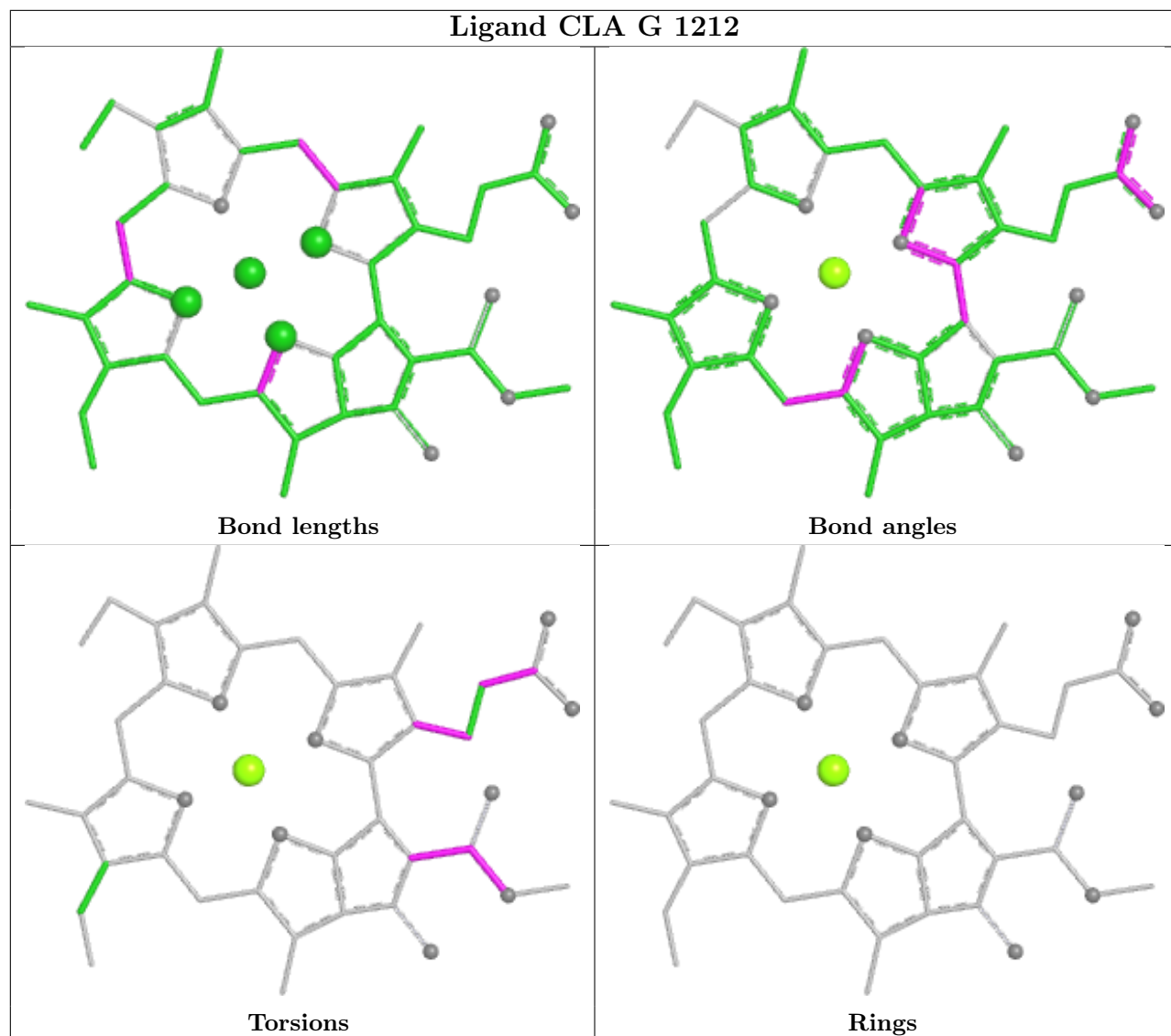




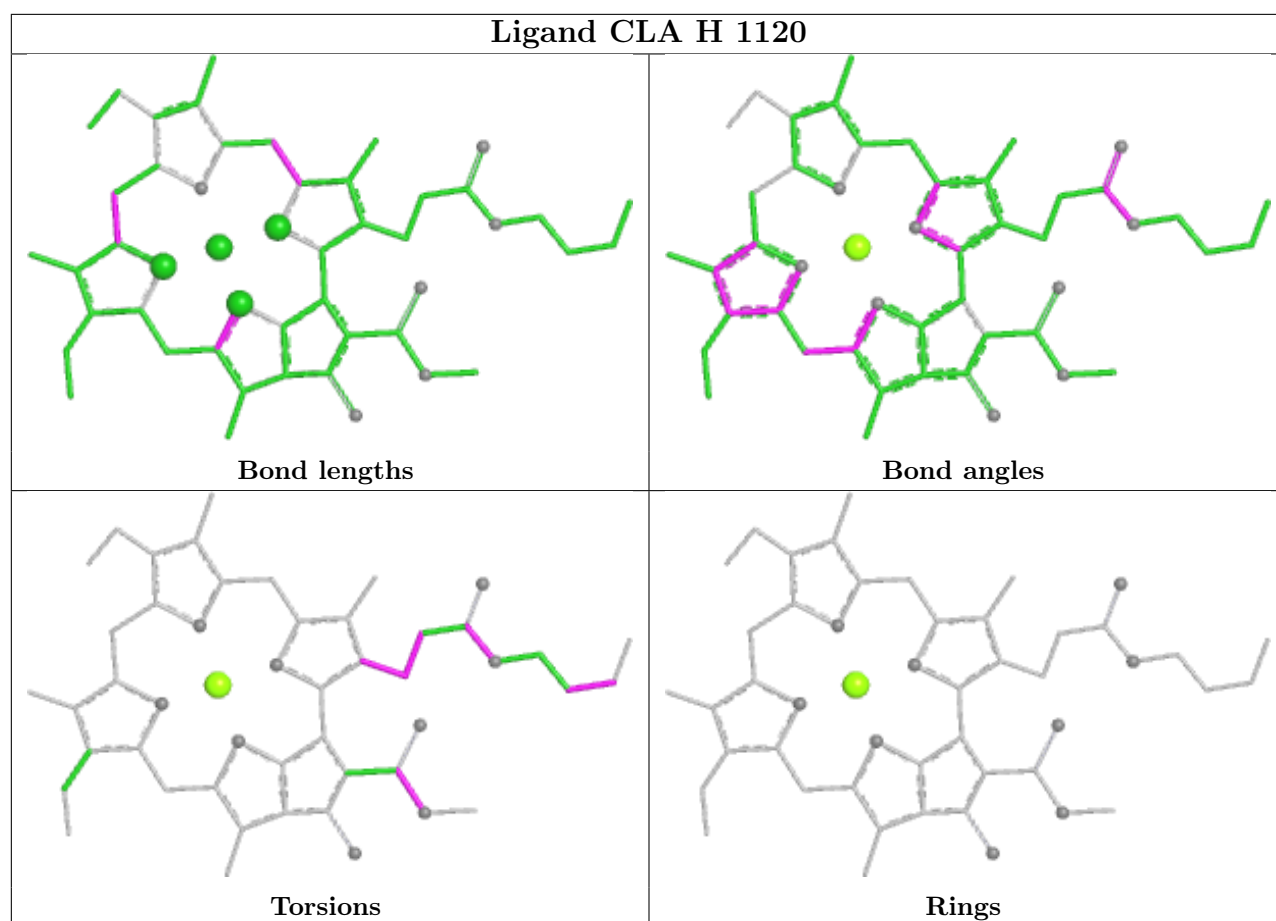




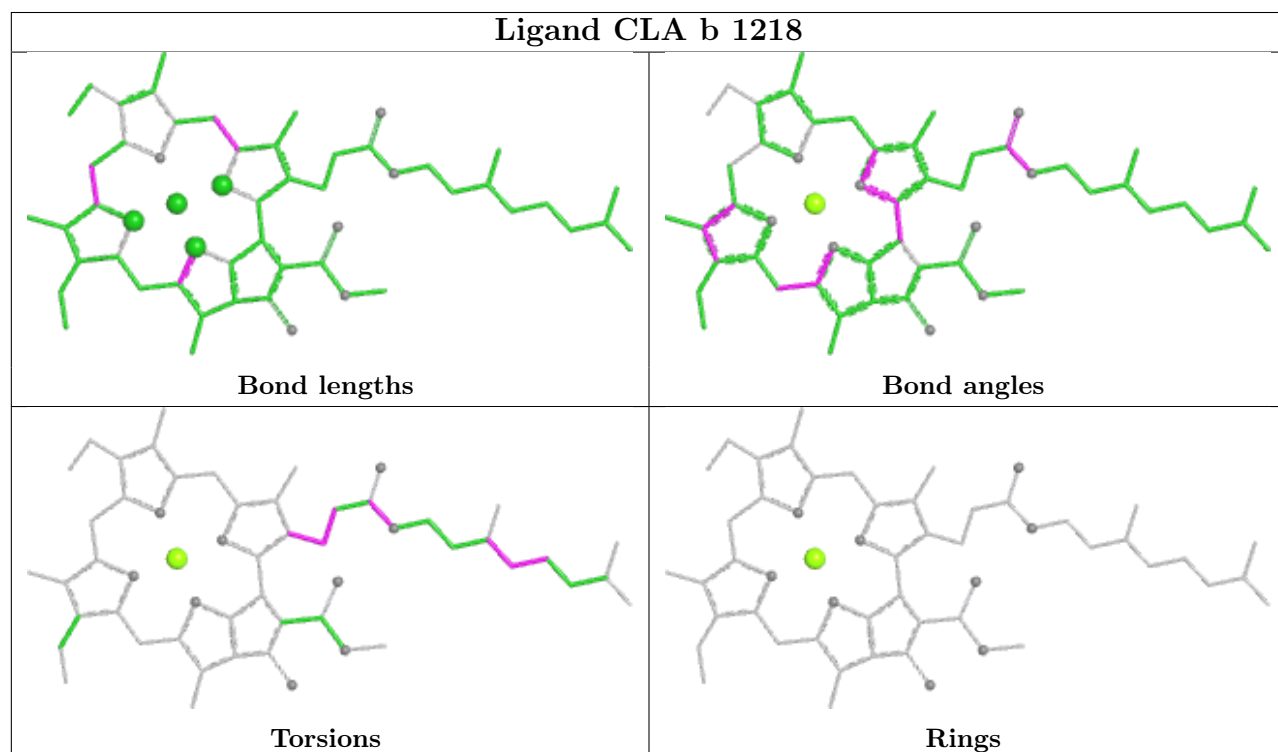
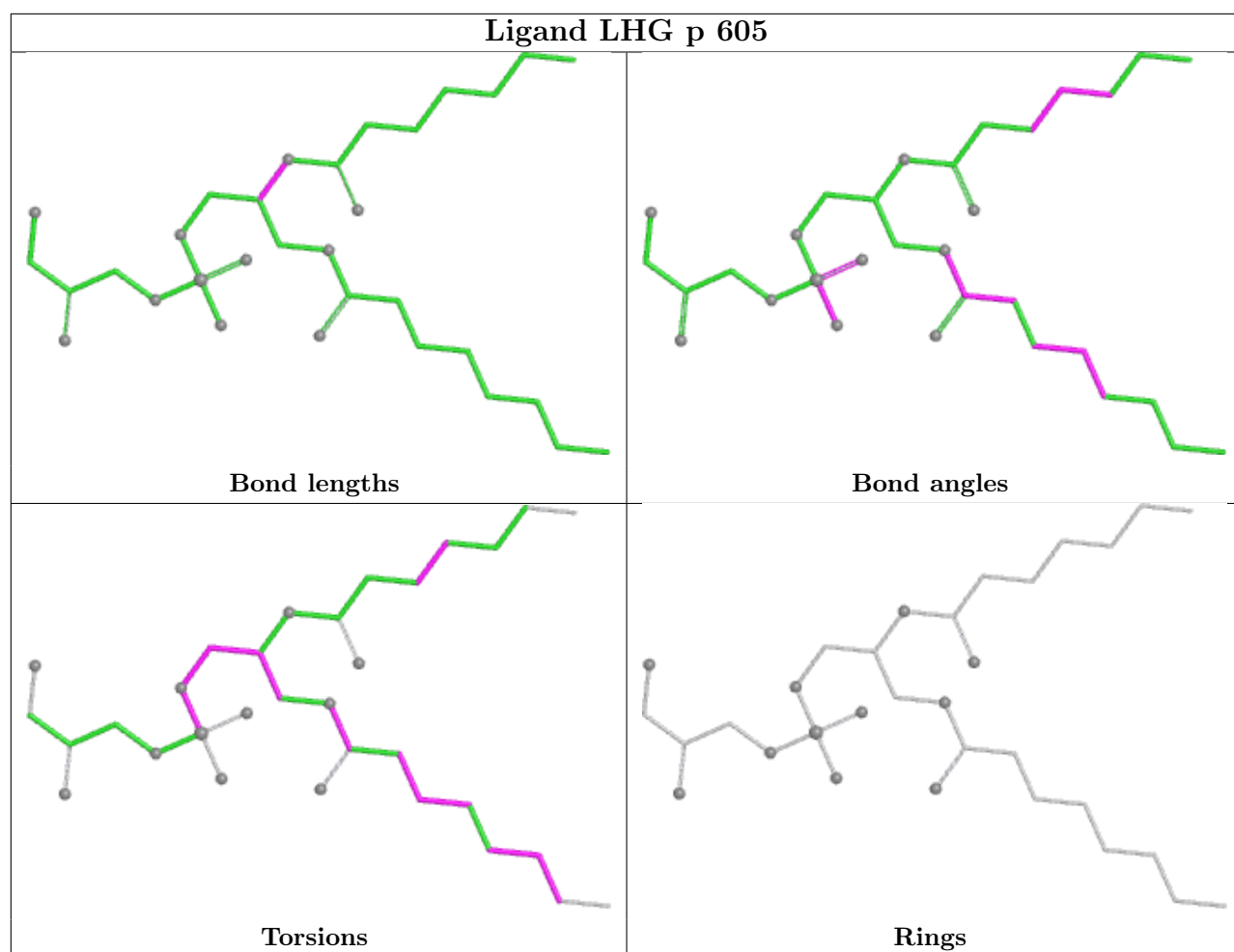




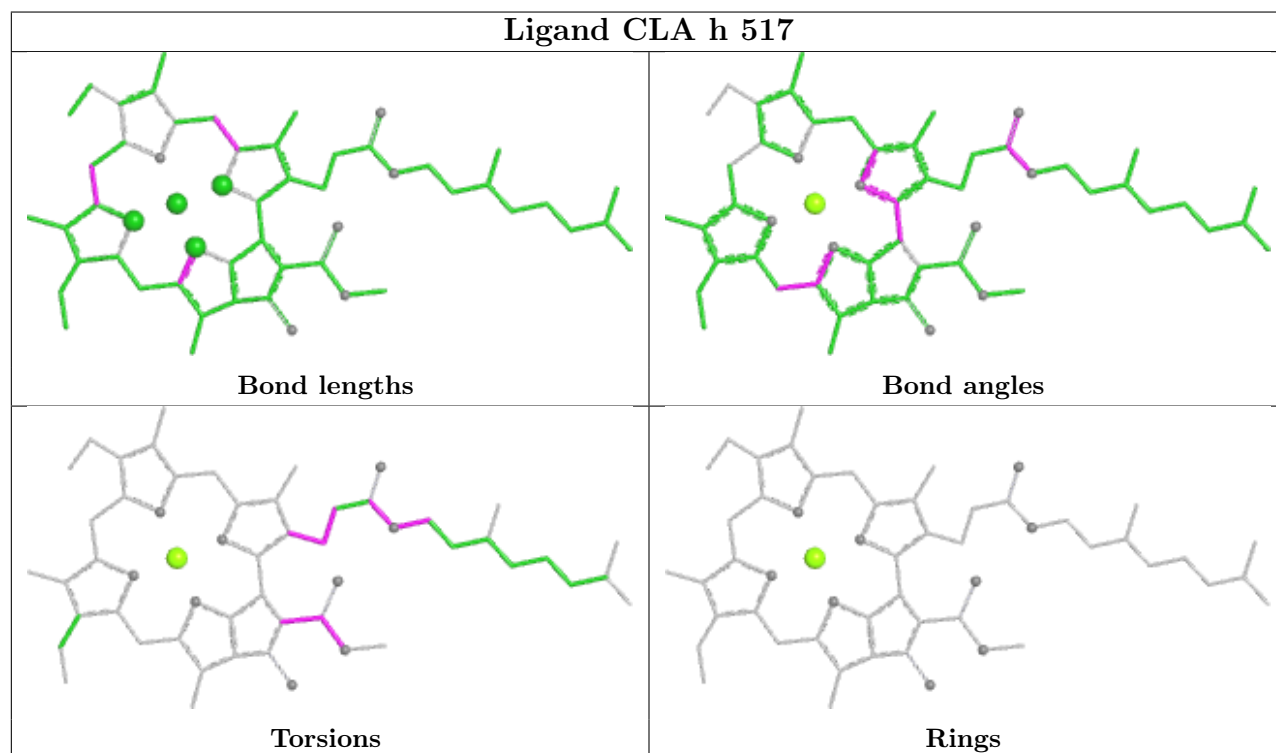
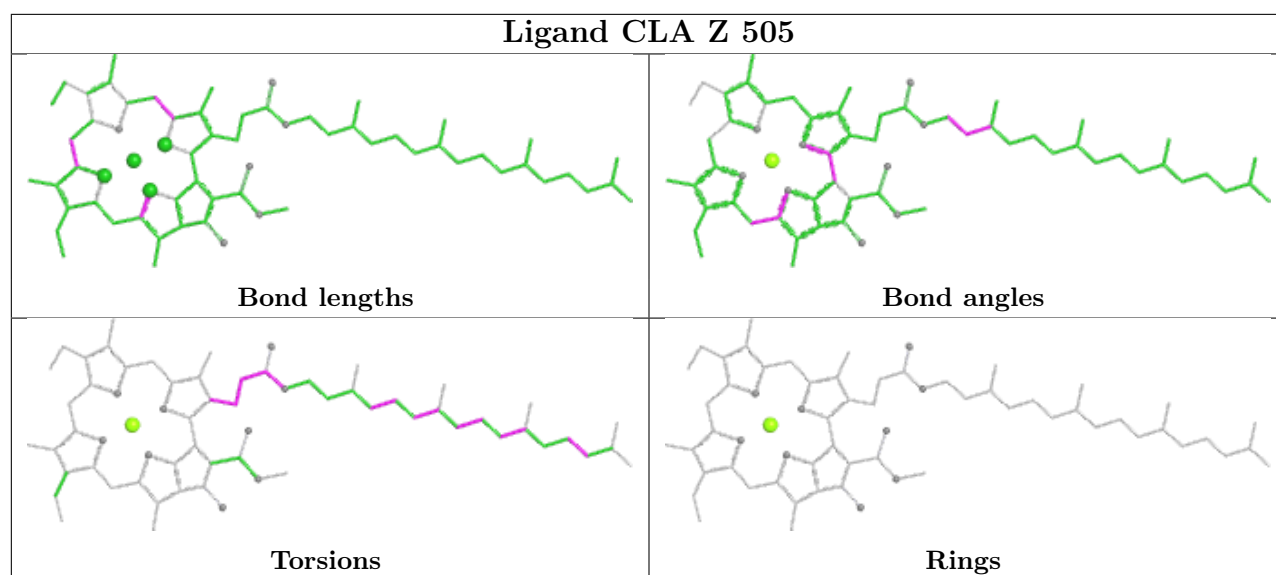




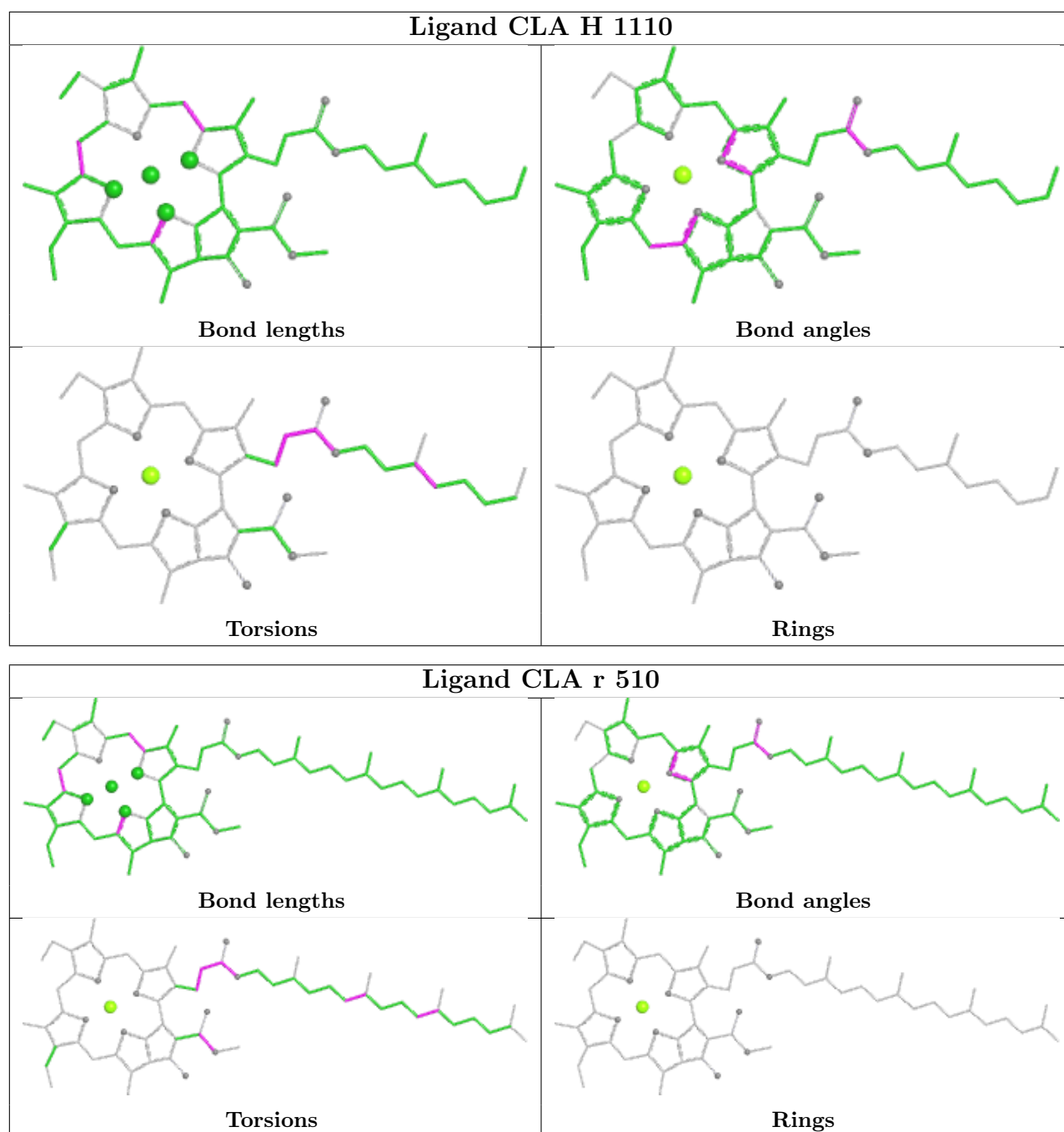




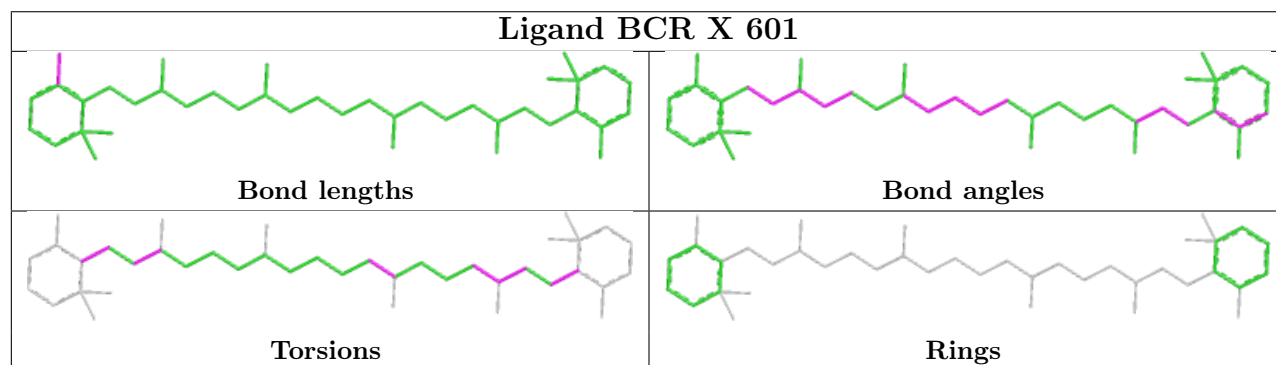
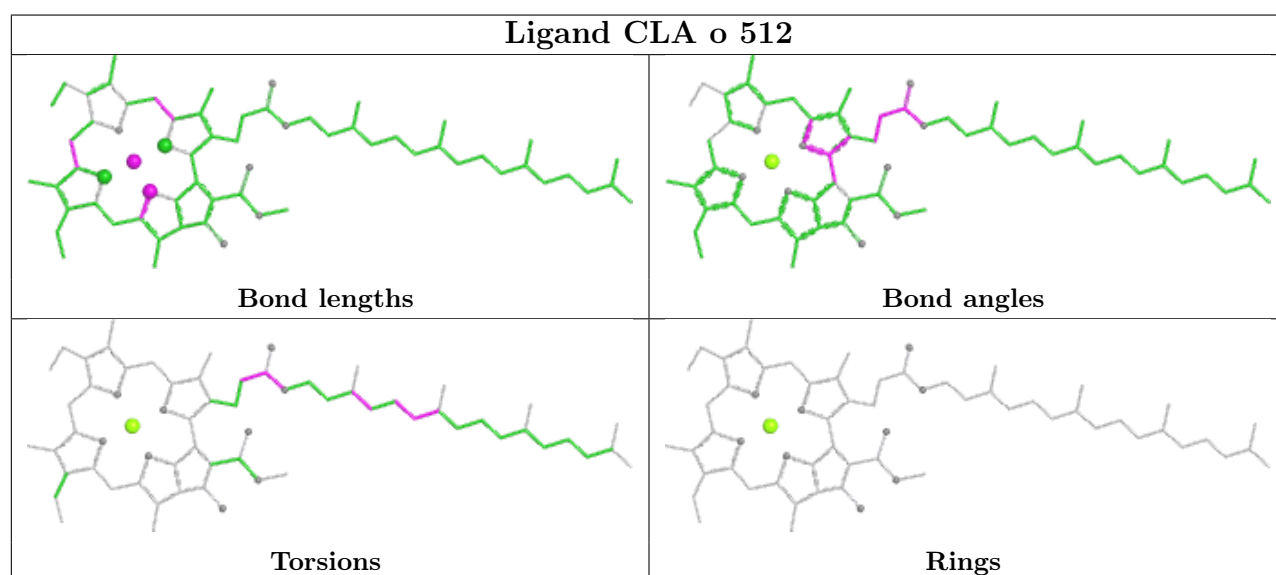
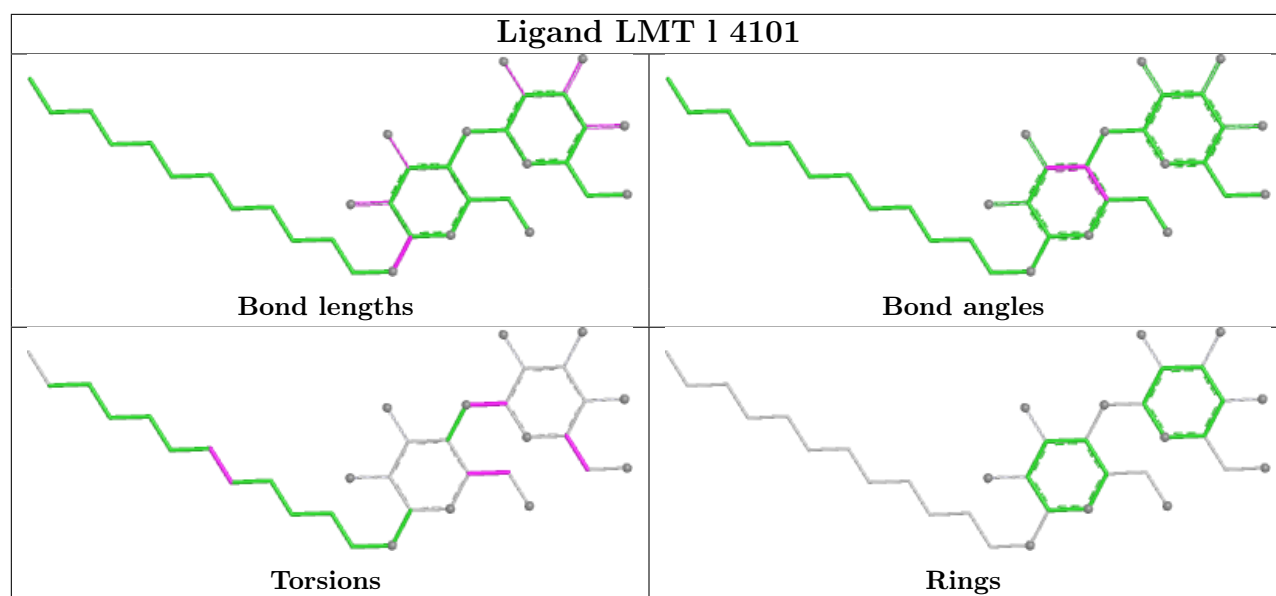




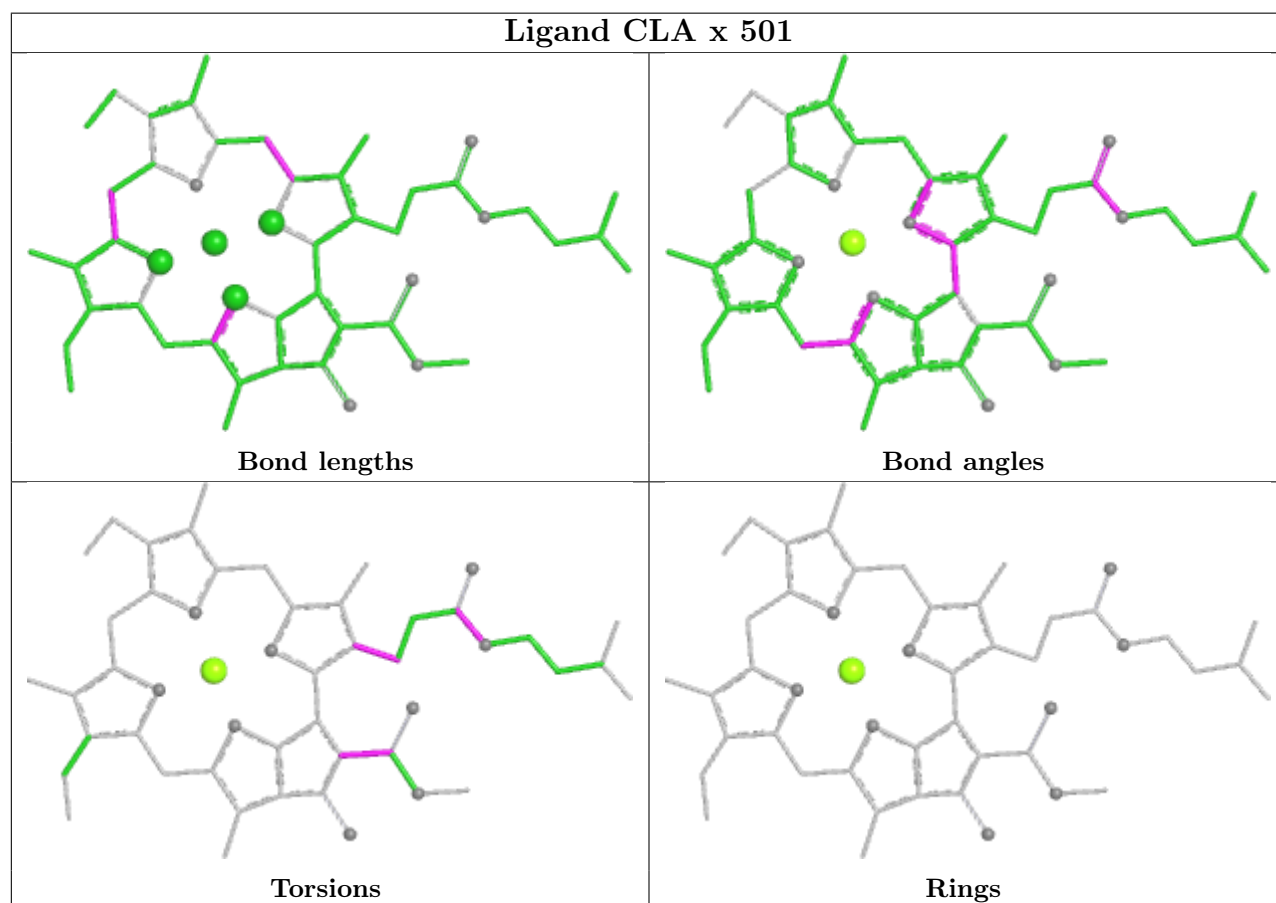
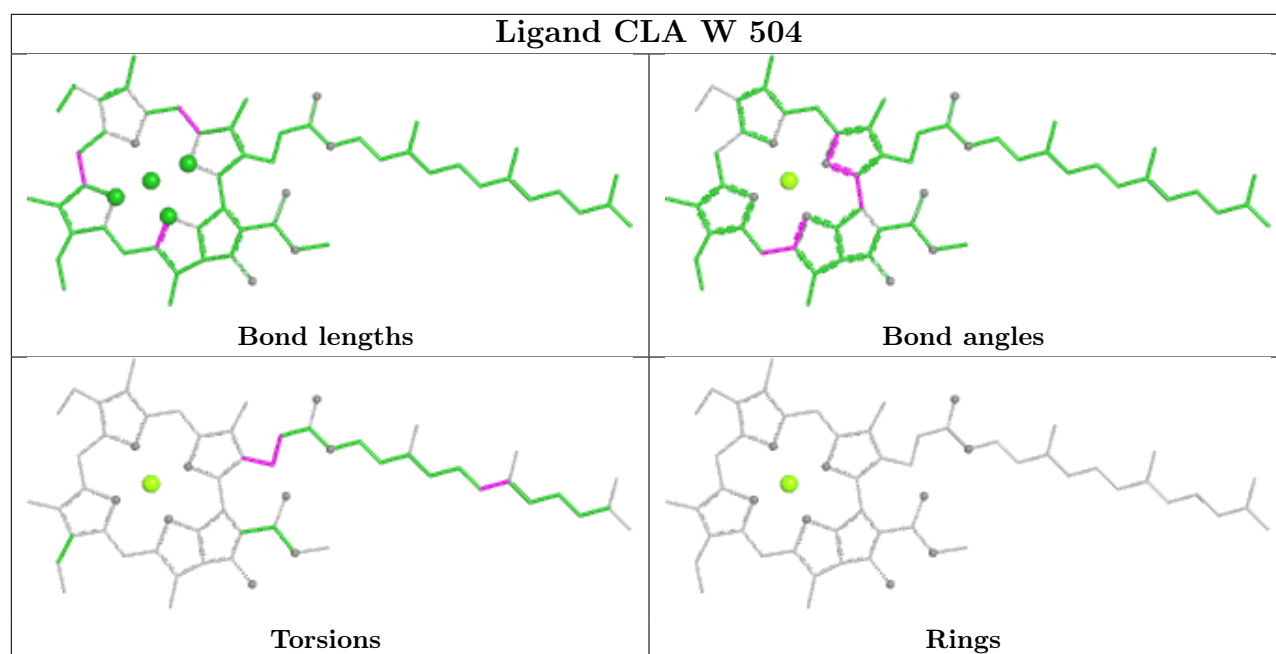




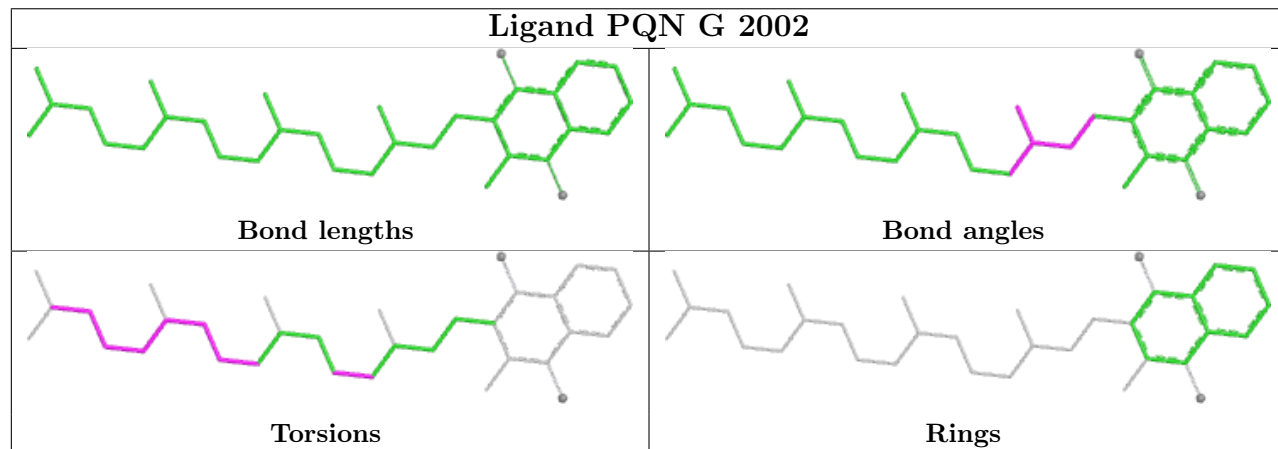
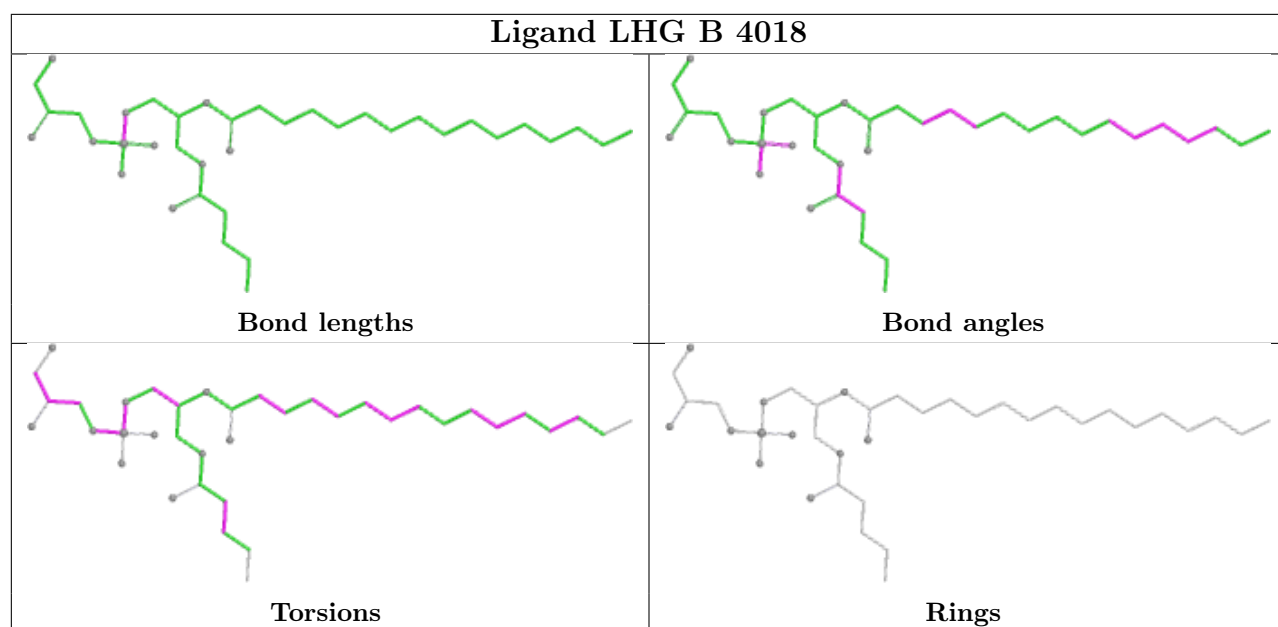






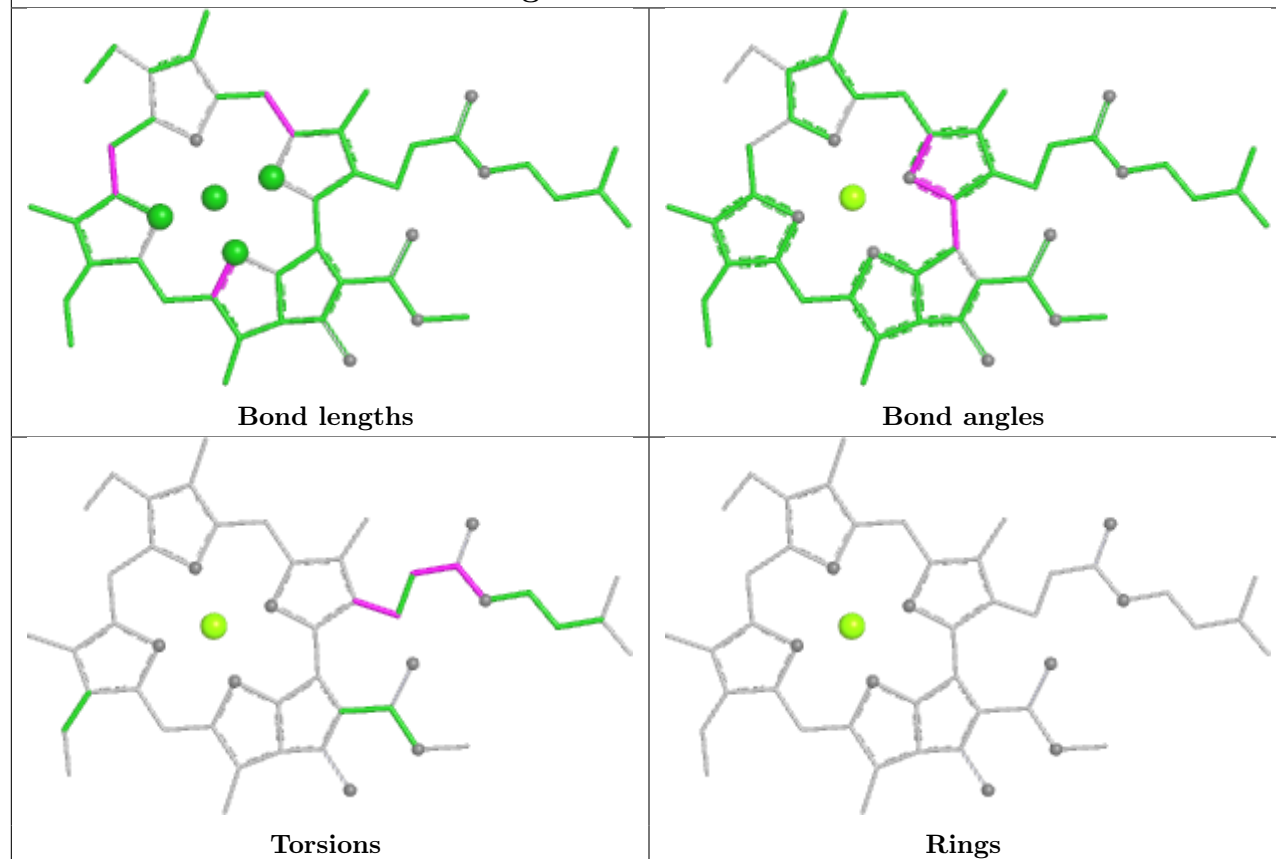




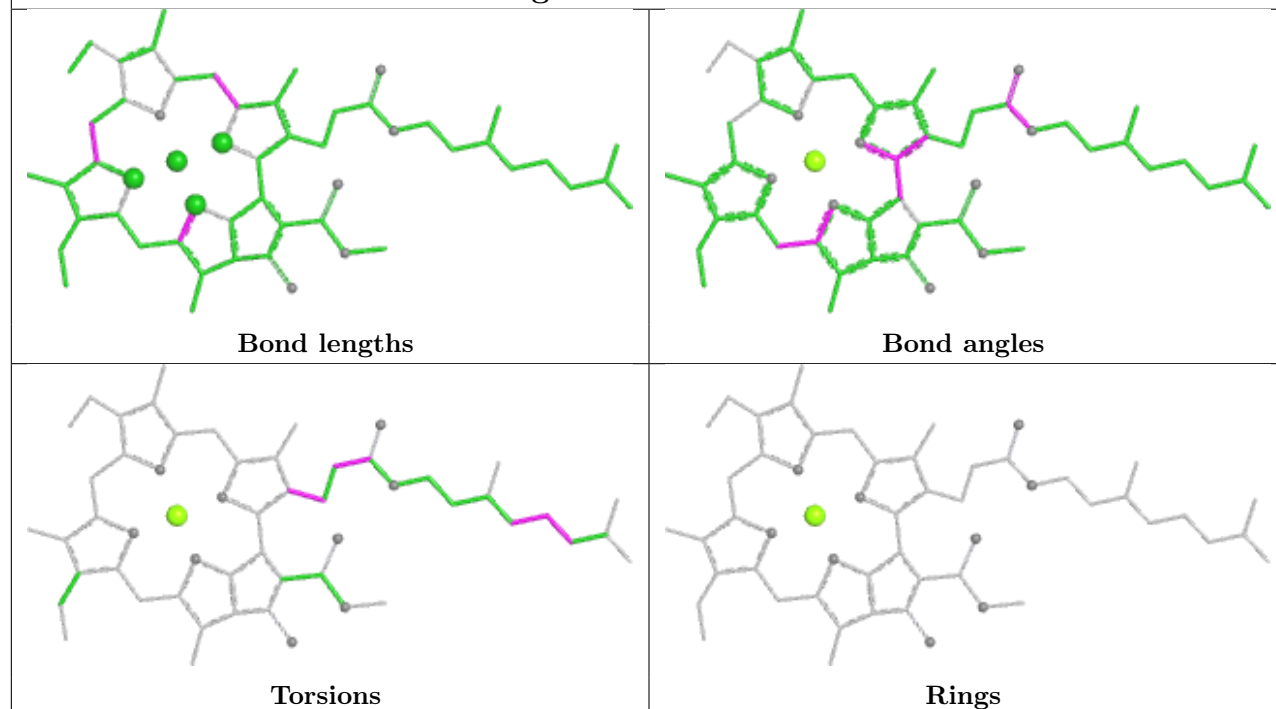




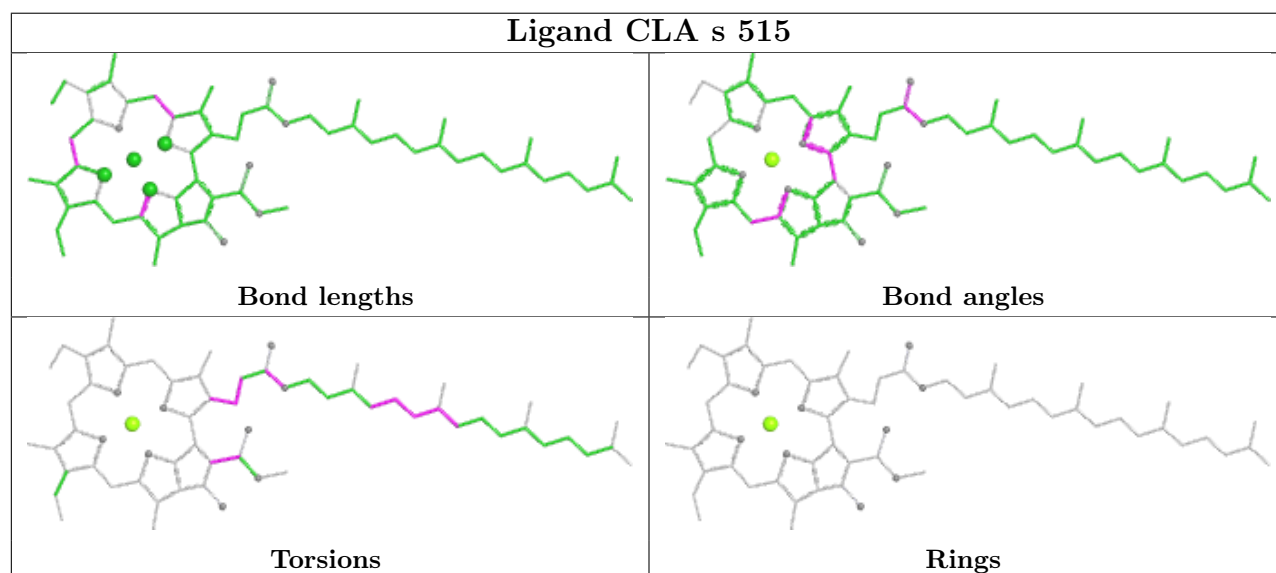
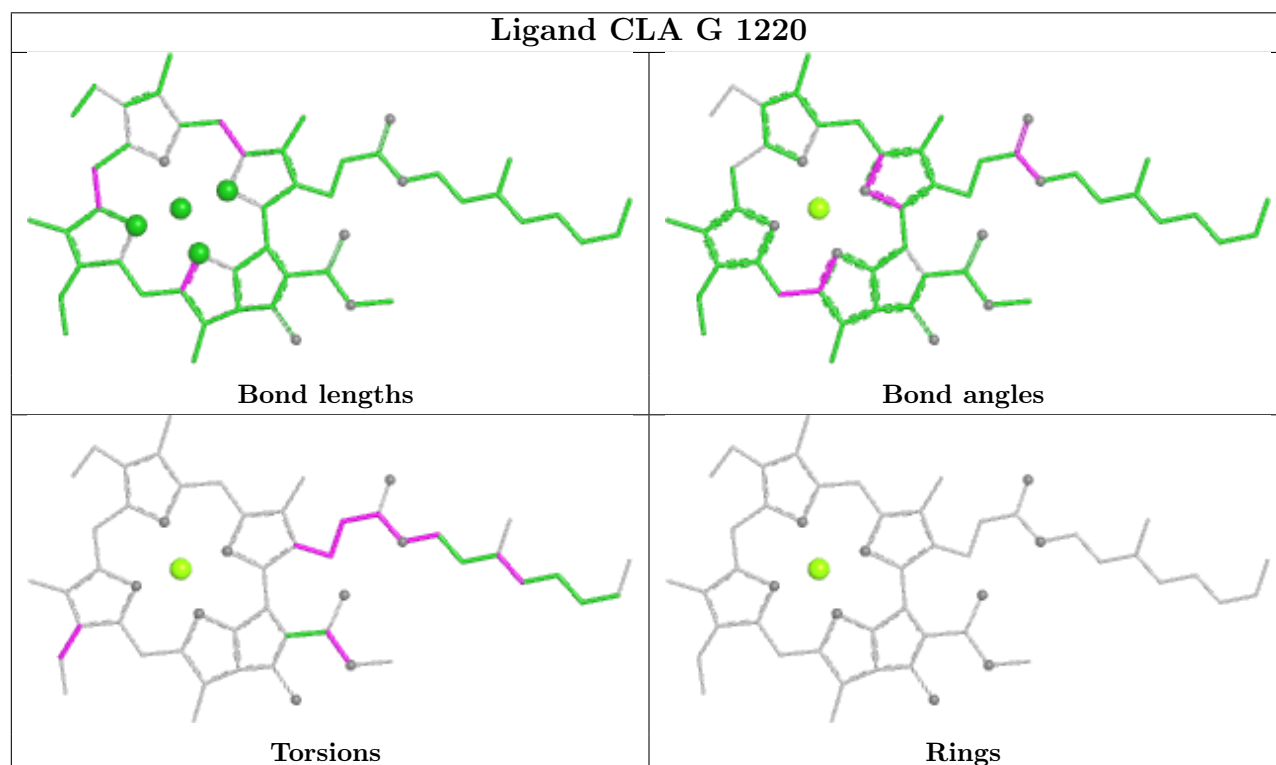
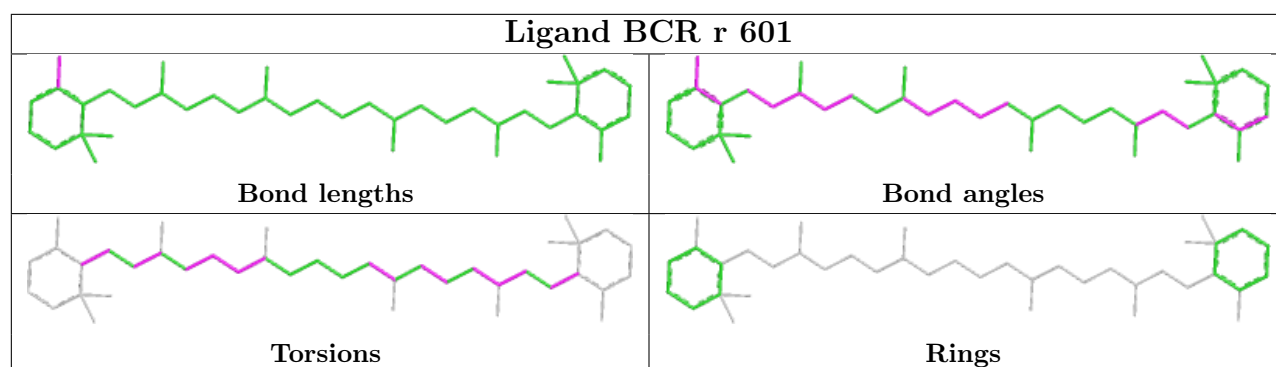
## Ligand CLA G 1236



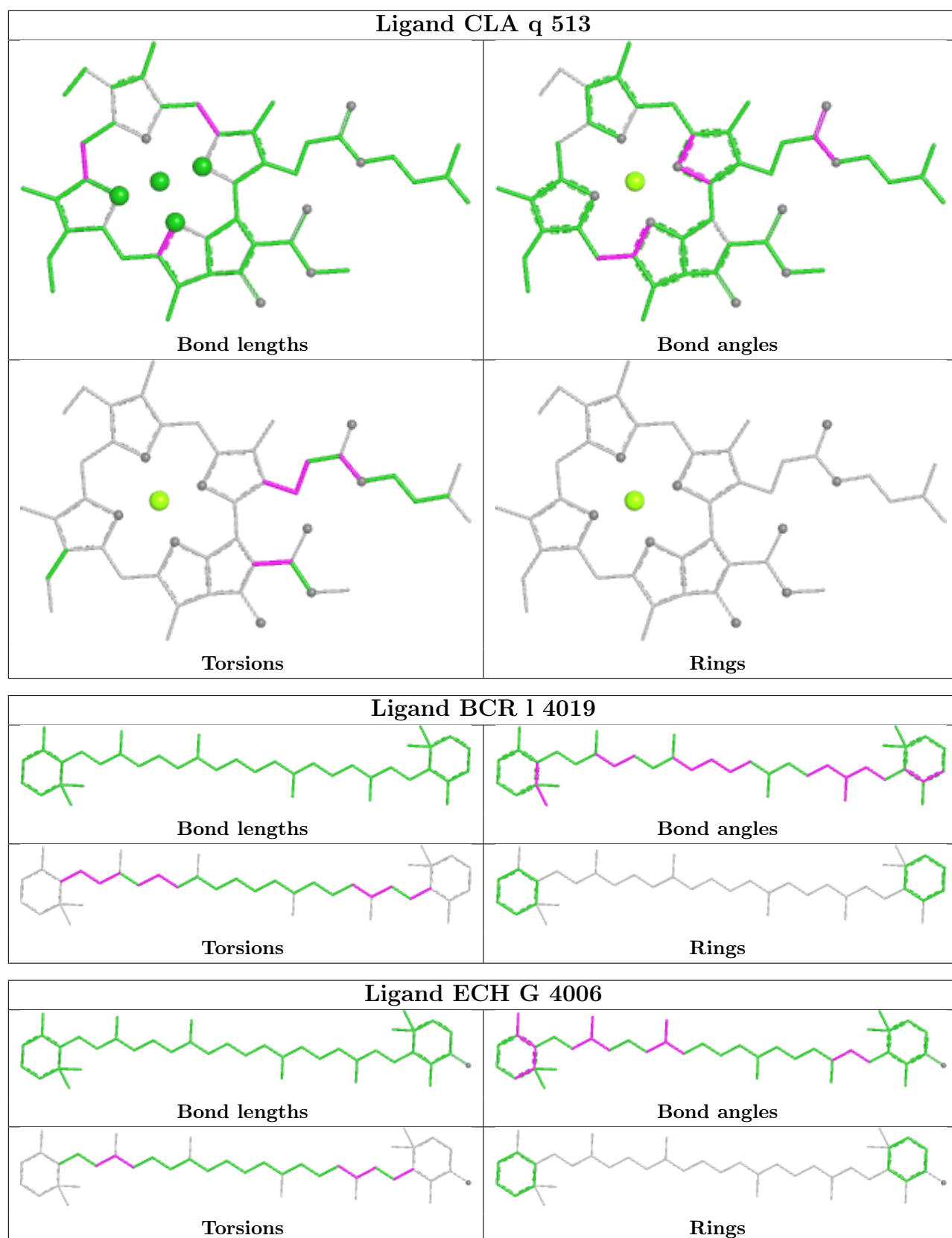
## Ligand CLA X 517





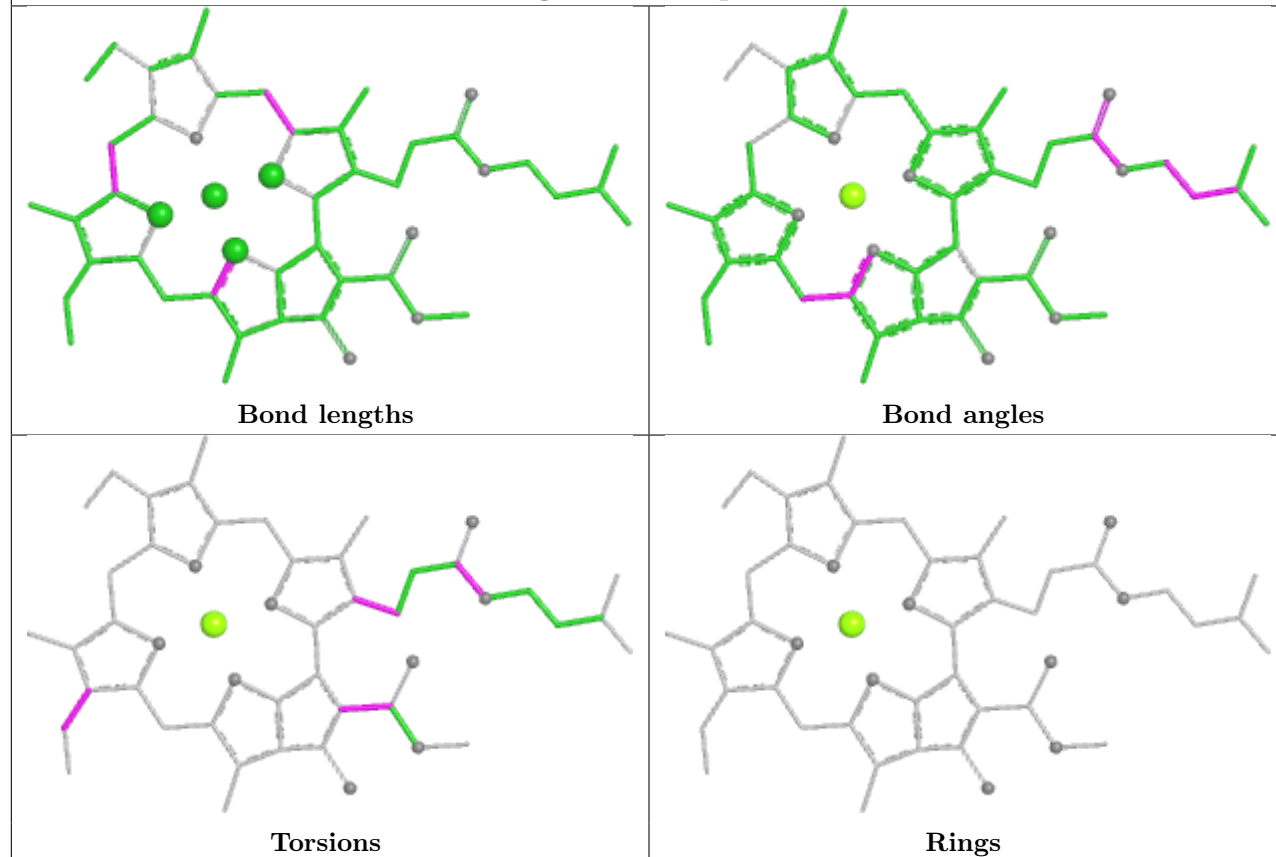




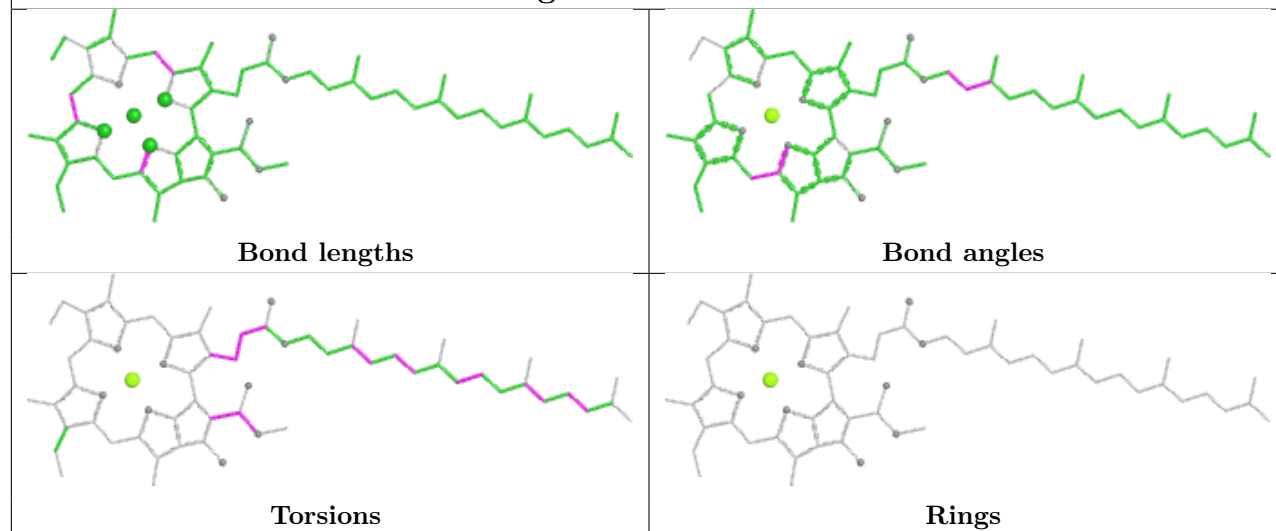




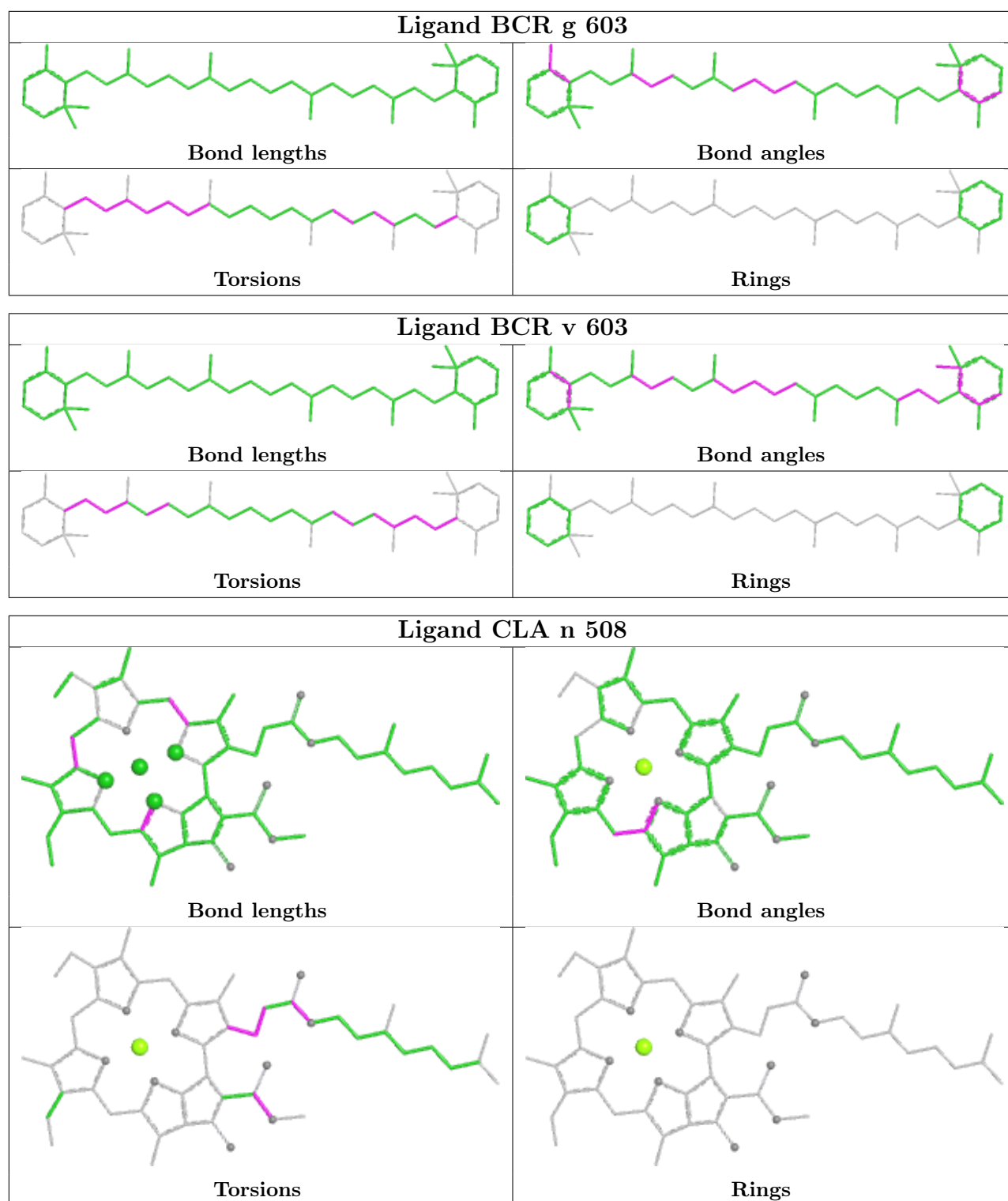
## Ligand CLA q 501



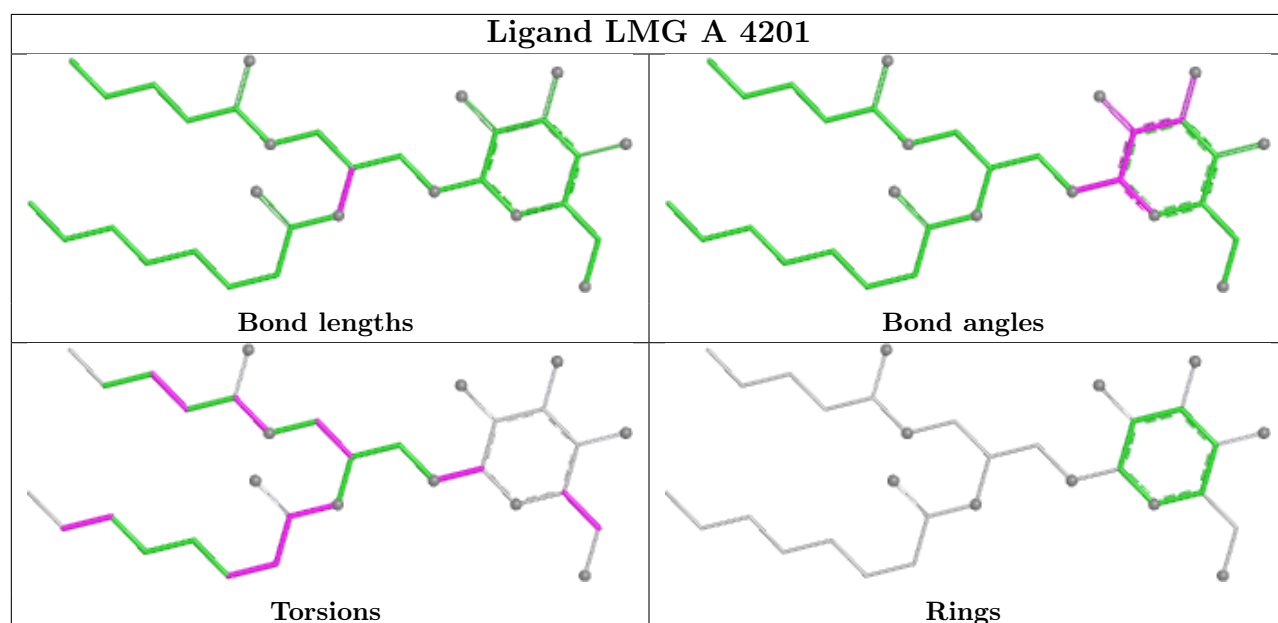
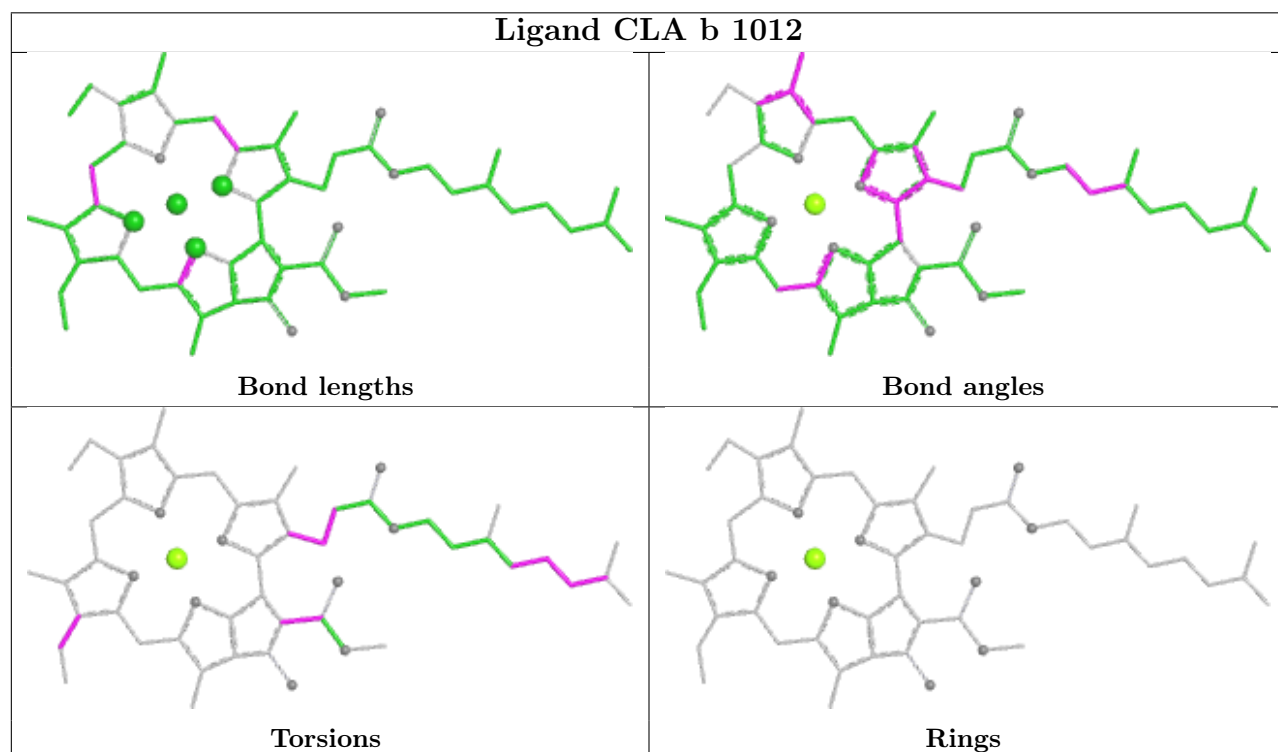
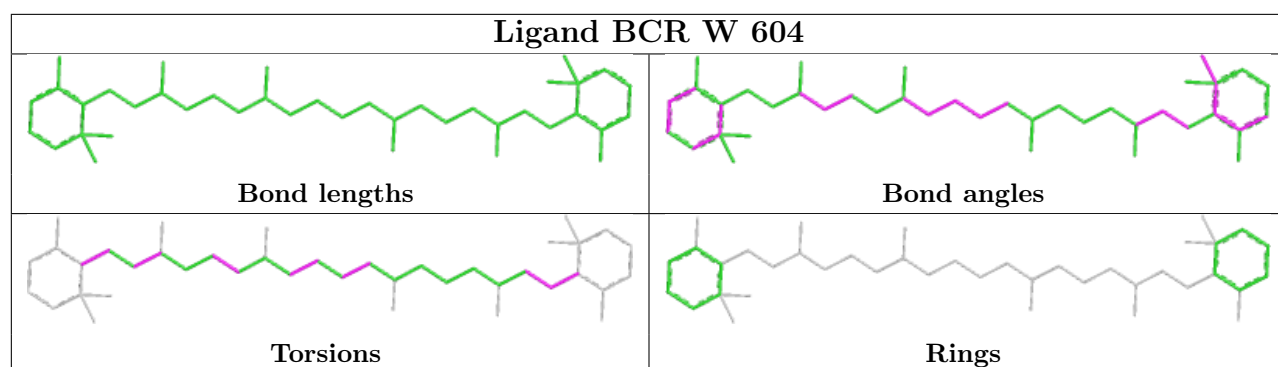
## Ligand CLA s 504



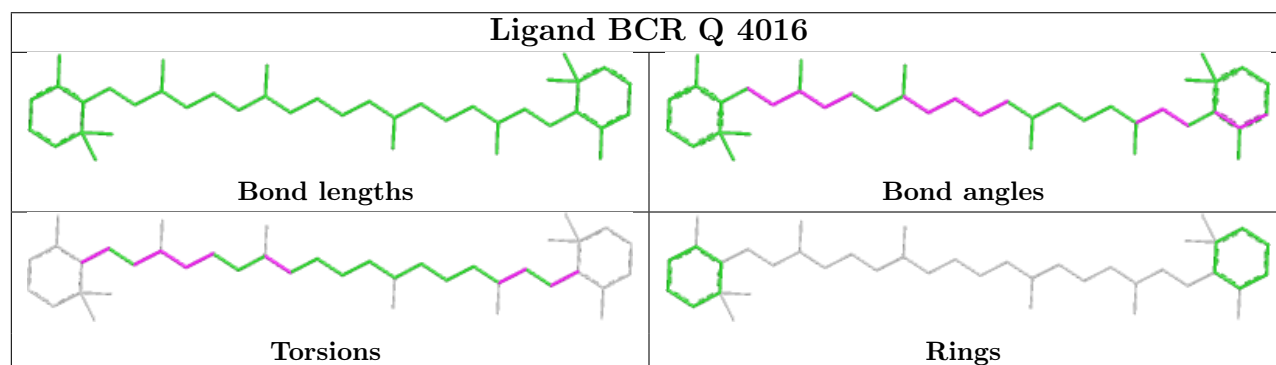
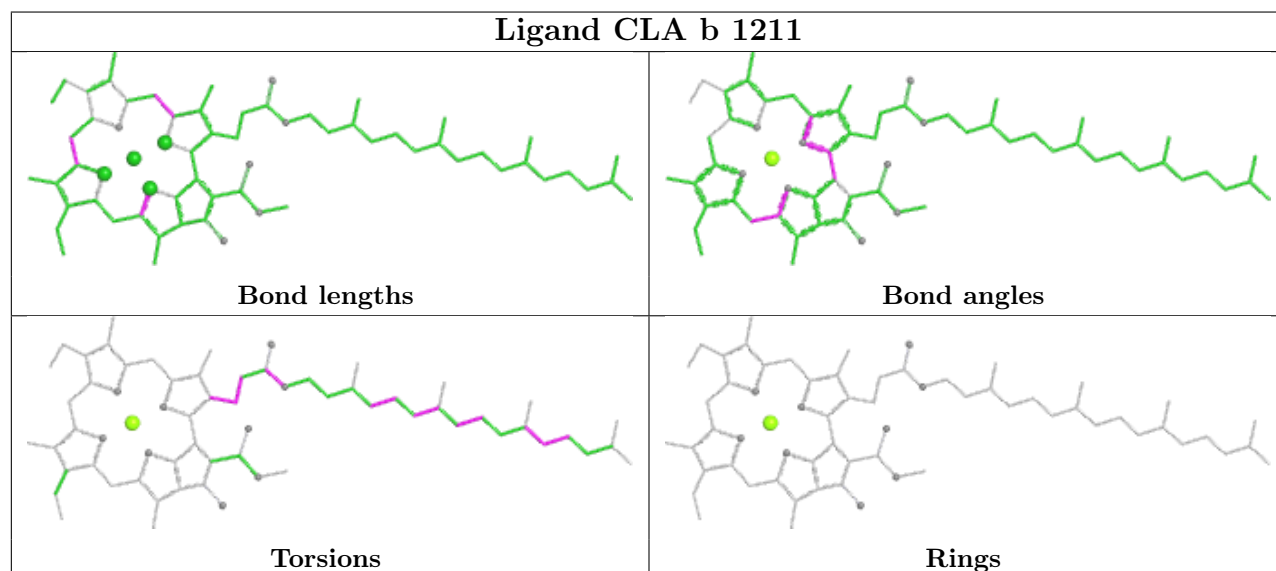
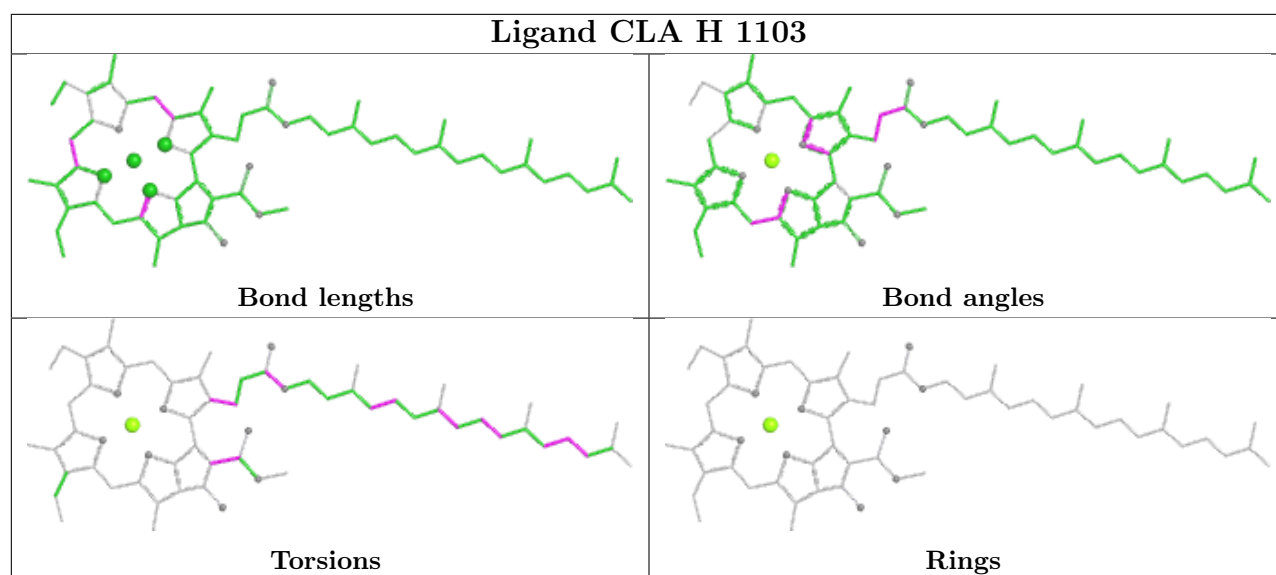




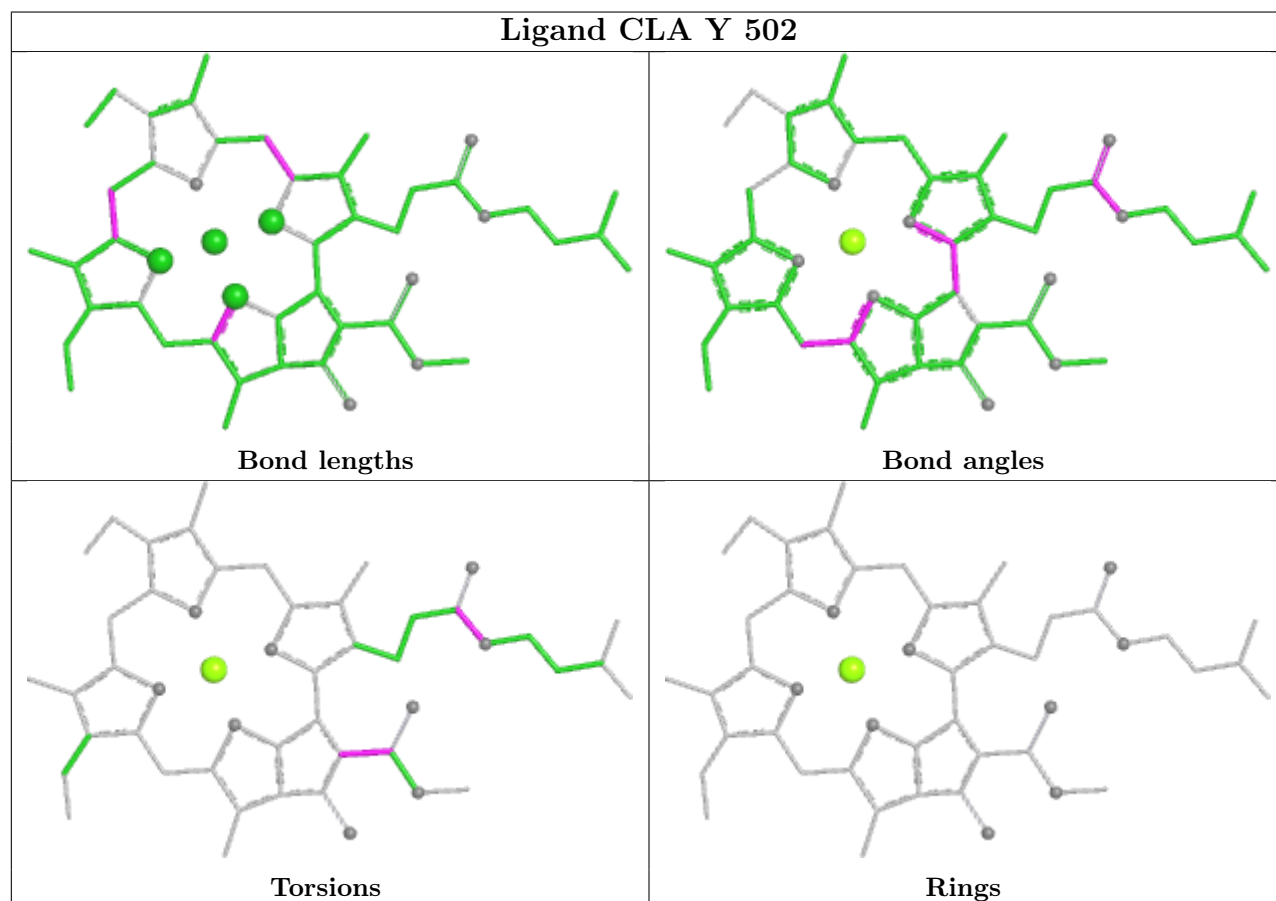
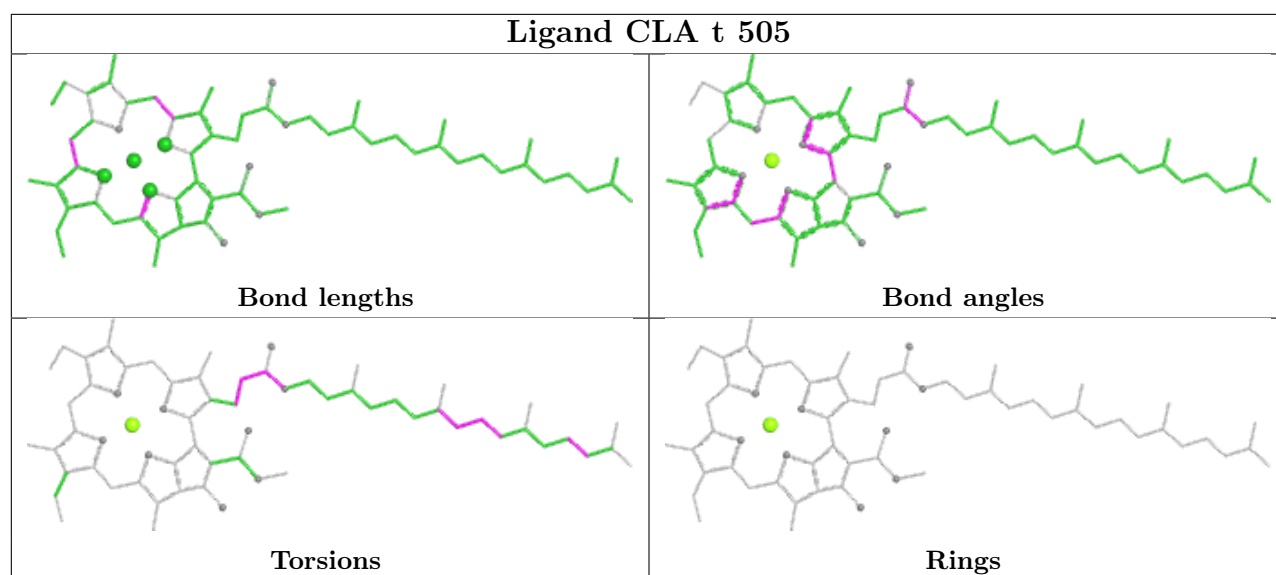




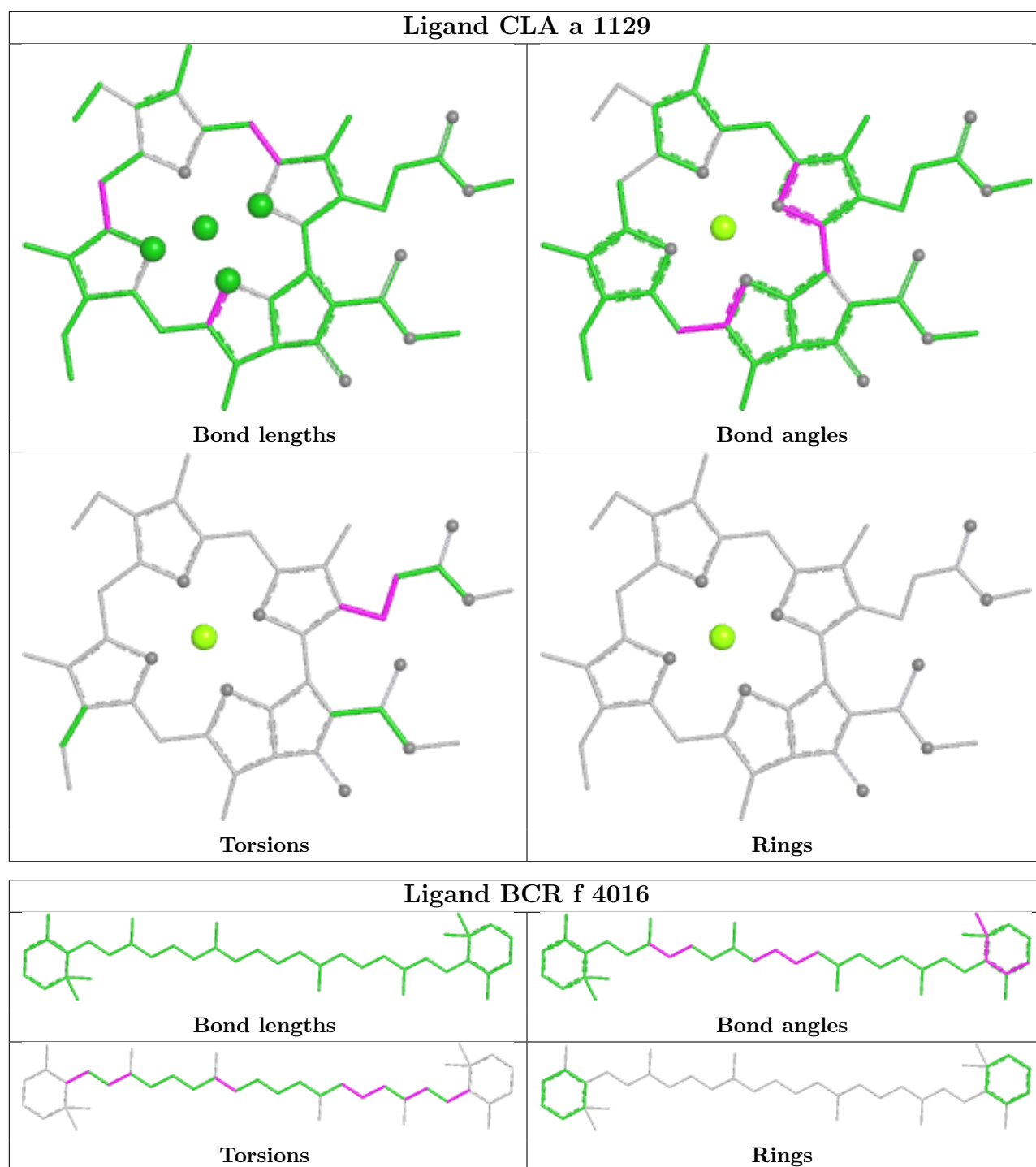




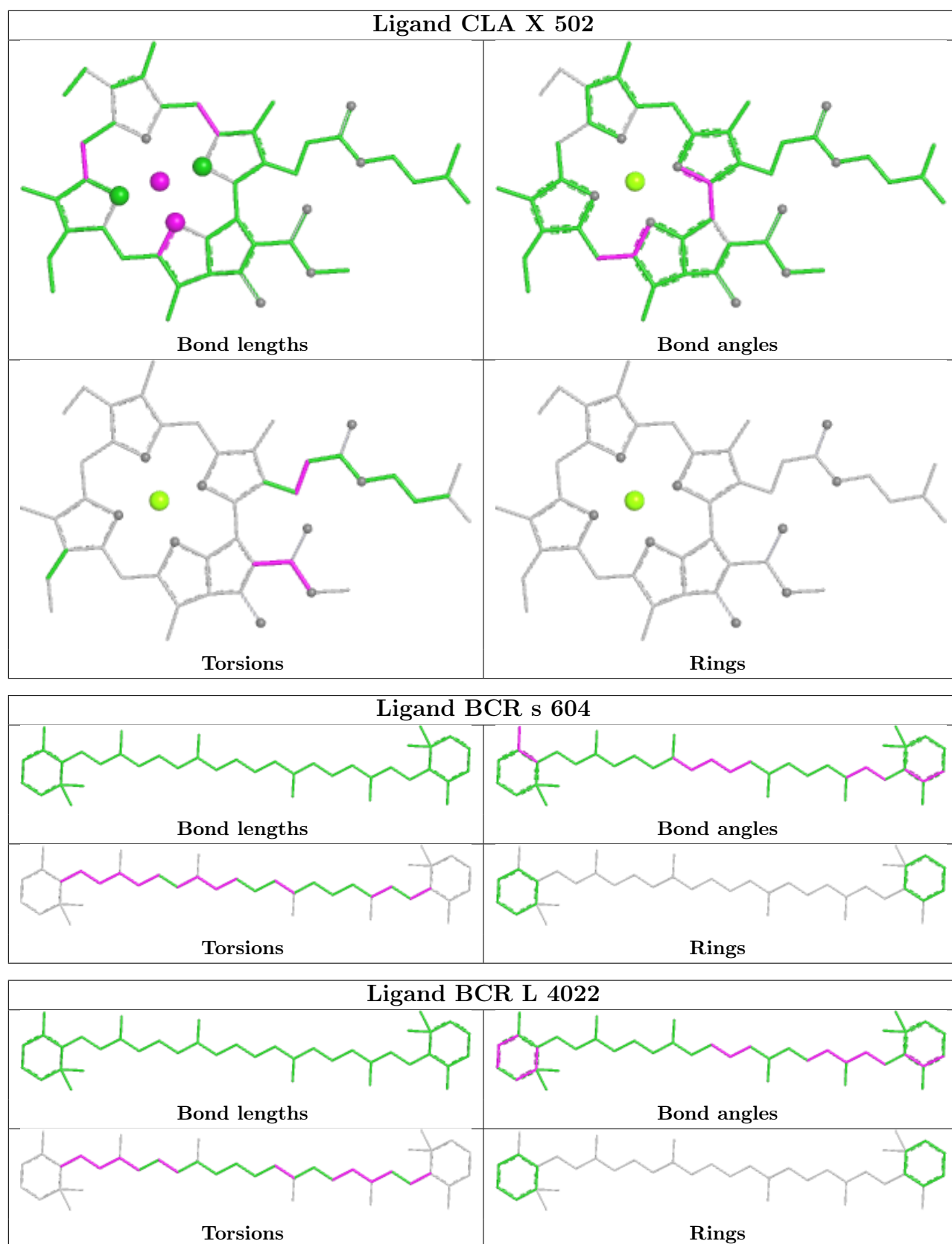




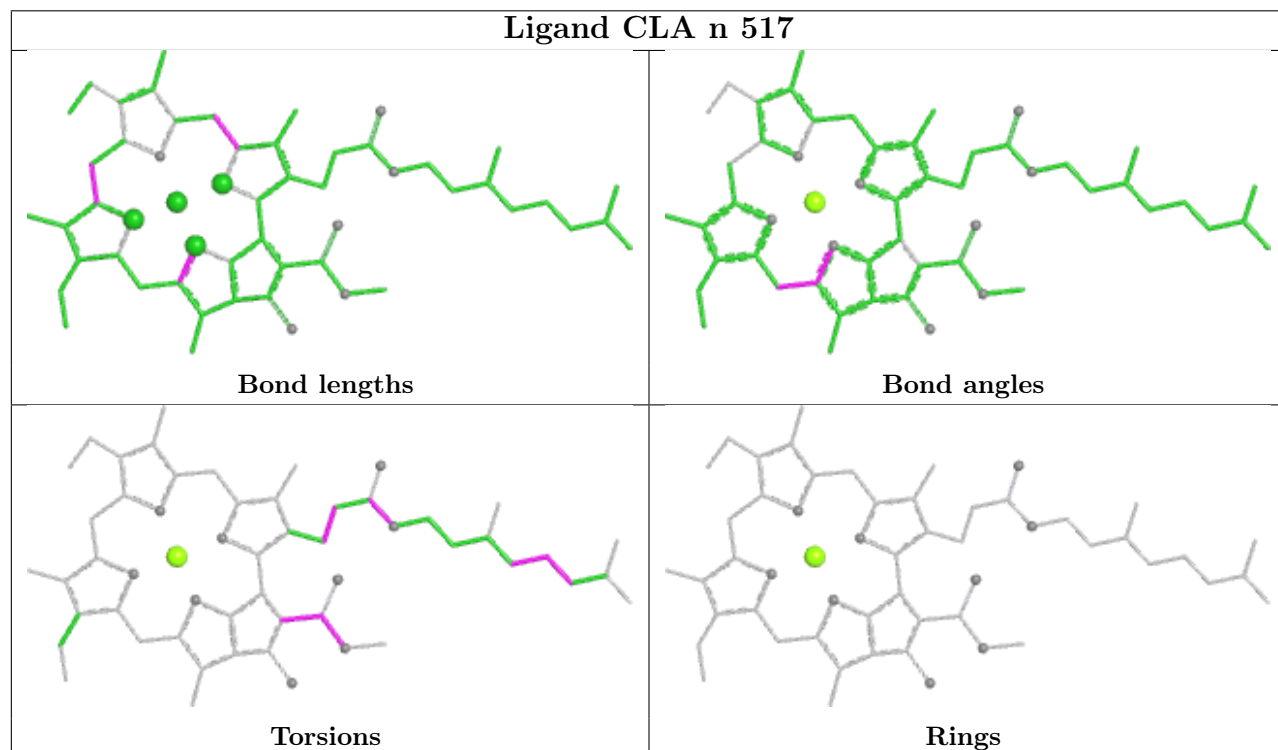
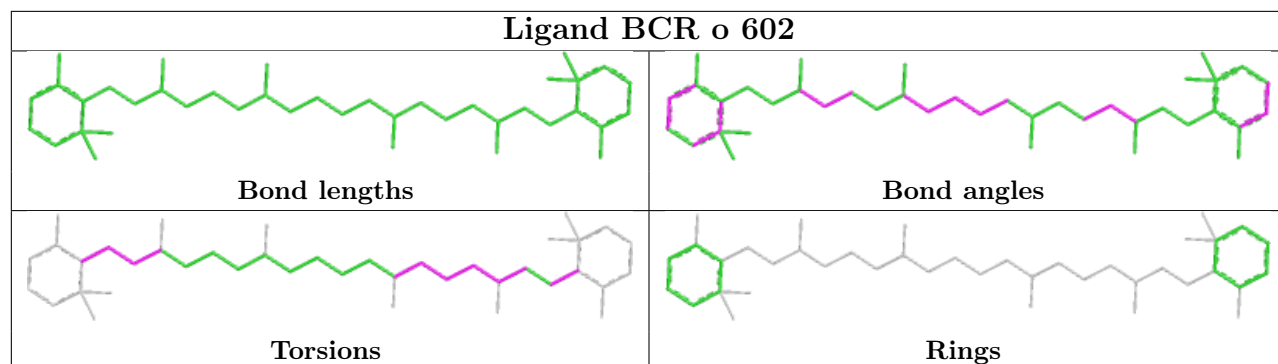




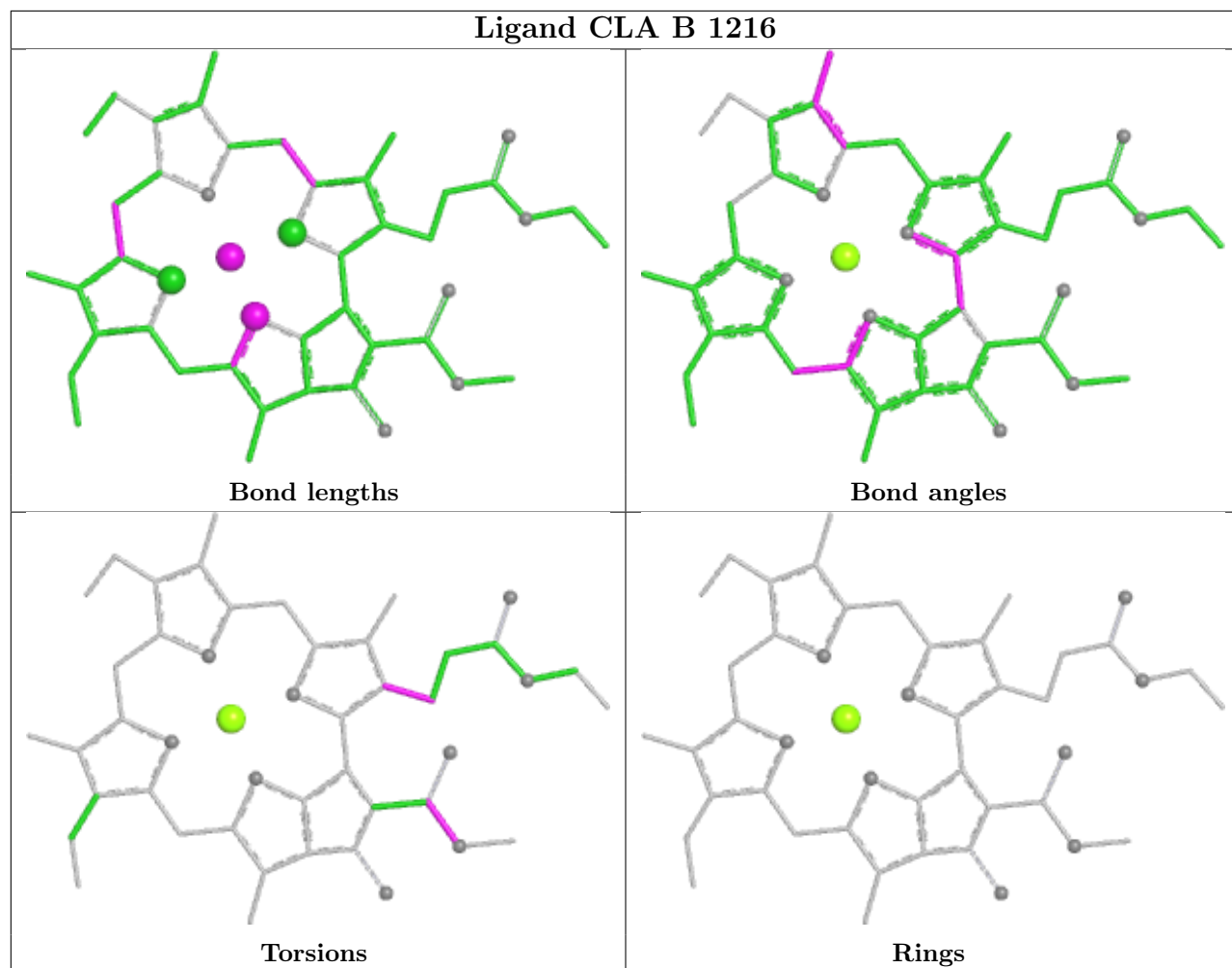






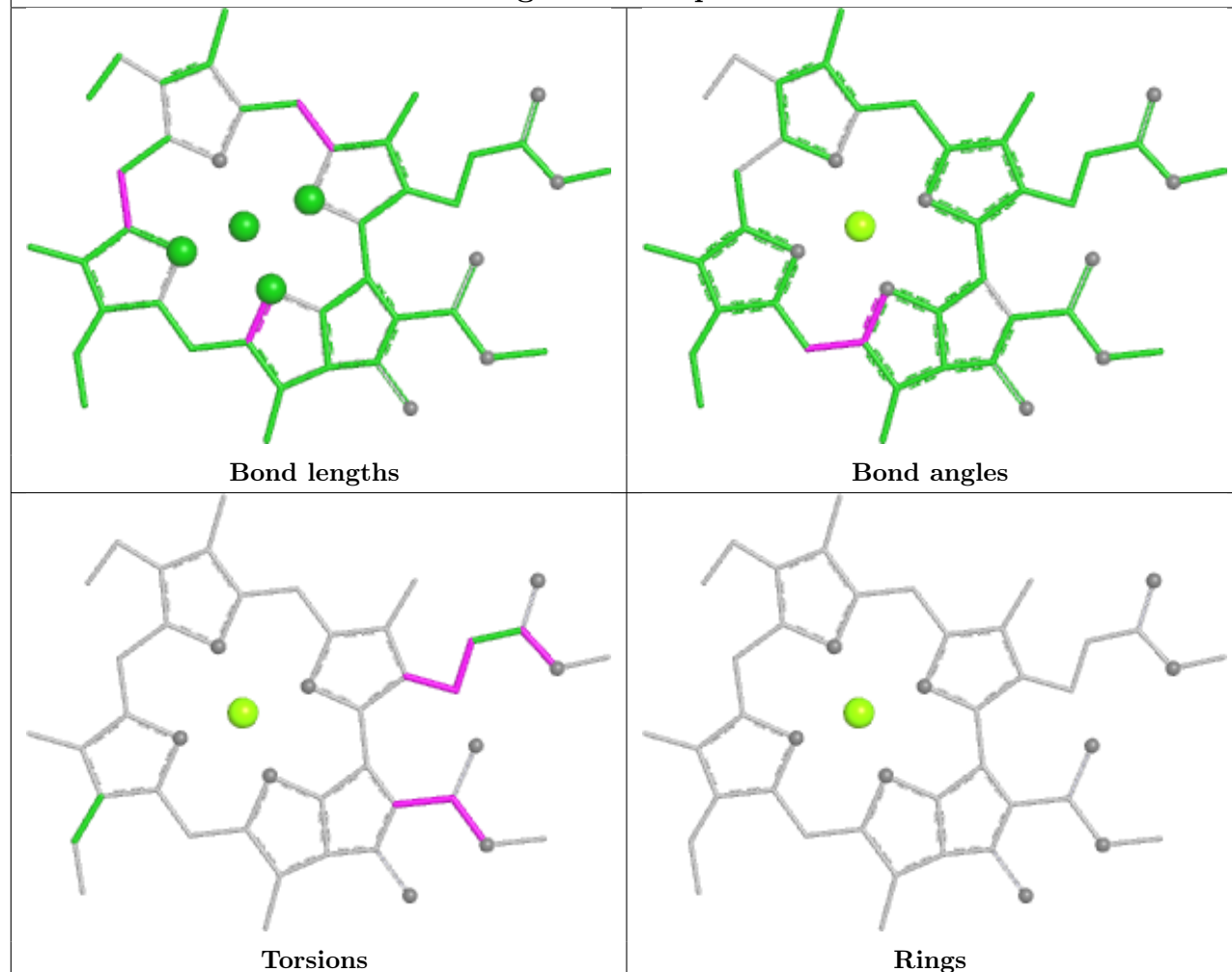




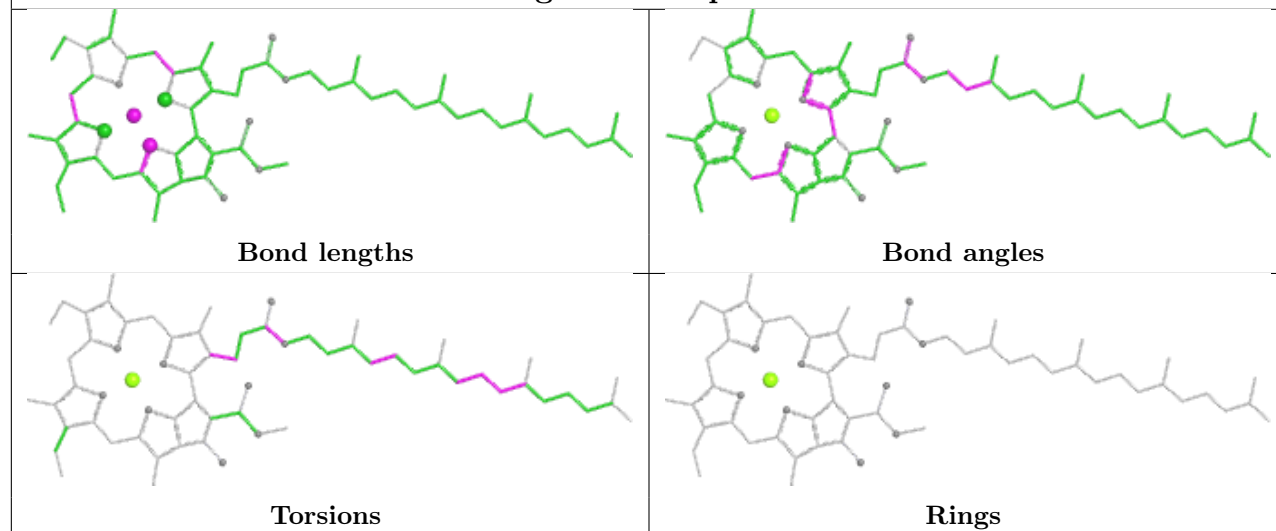




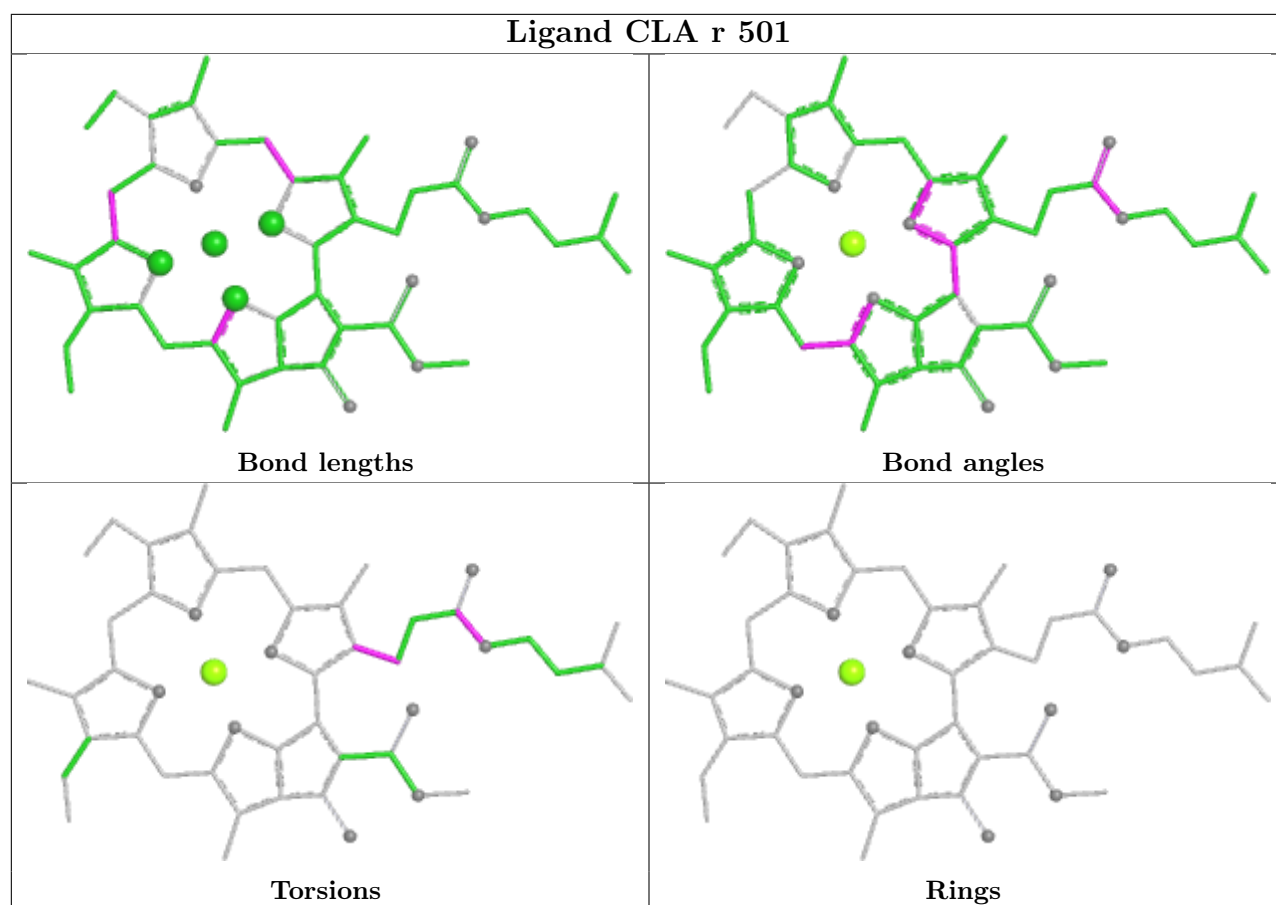
## Ligand CLA q 516



## Ligand CLA p 512

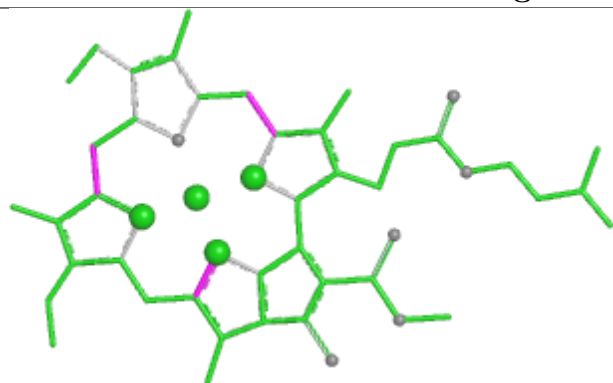




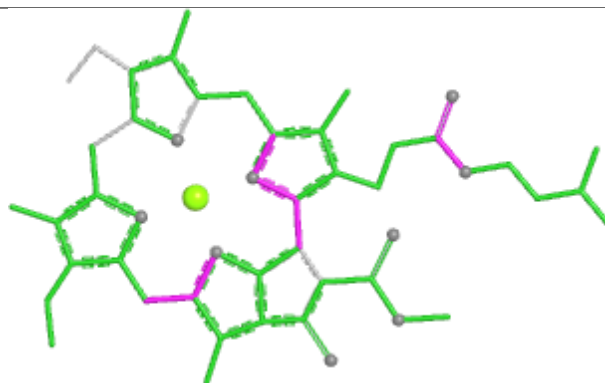




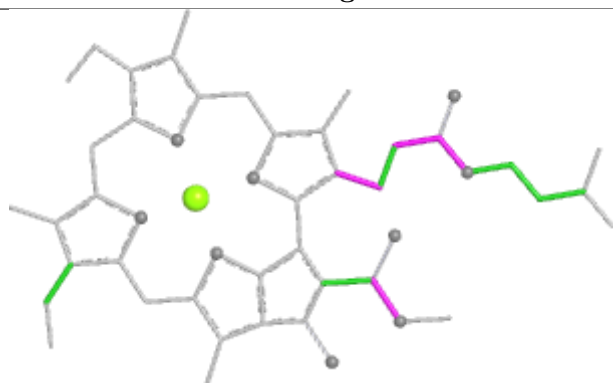
## Ligand CLA Y 514



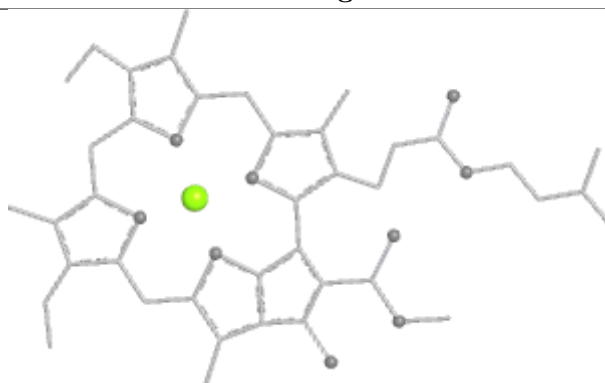
Bond lengths



Bond angles

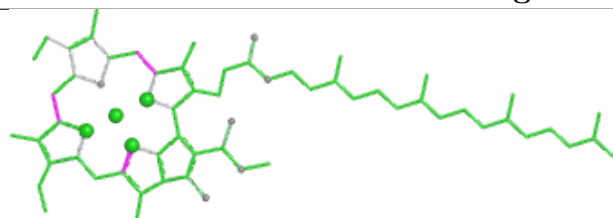


Torsions

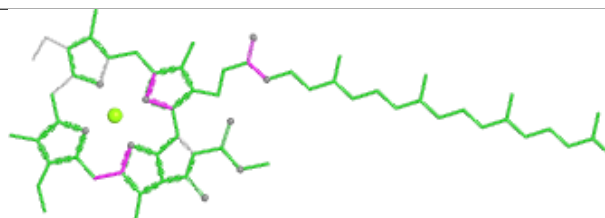


Rings

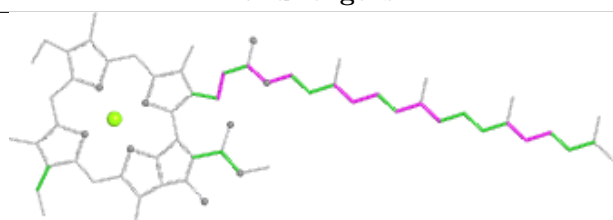
## Ligand CLA I 1503



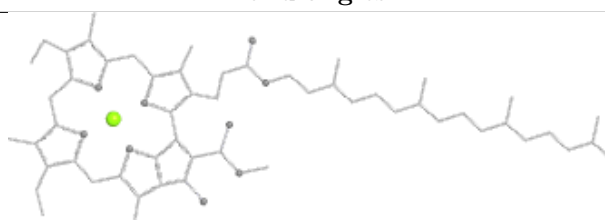
Bond lengths



Bond angles



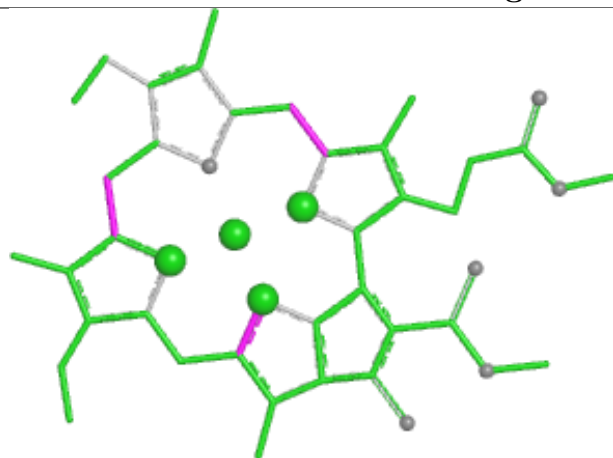
Torsions



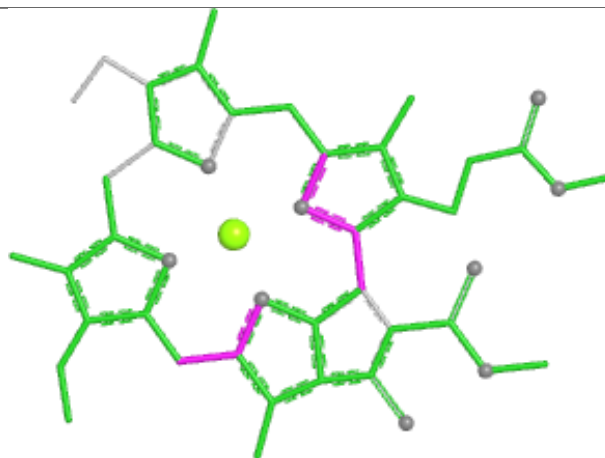
Rings



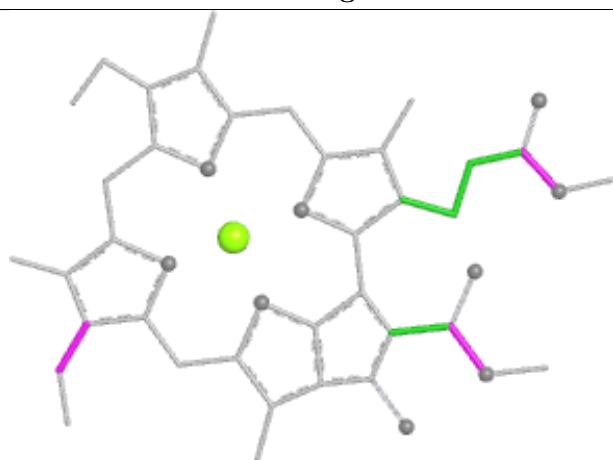
## Ligand CLA B 1240



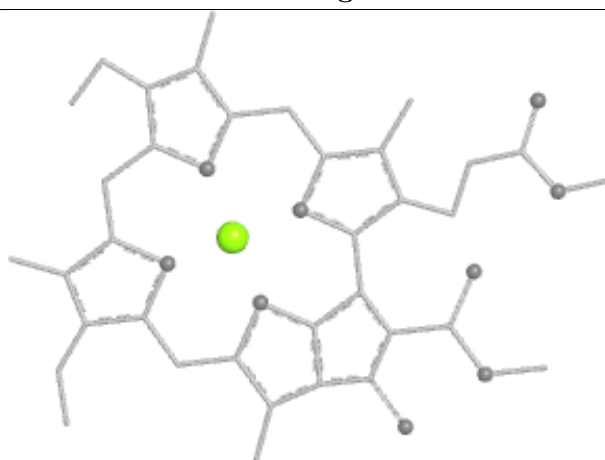
Bond lengths



Bond angles

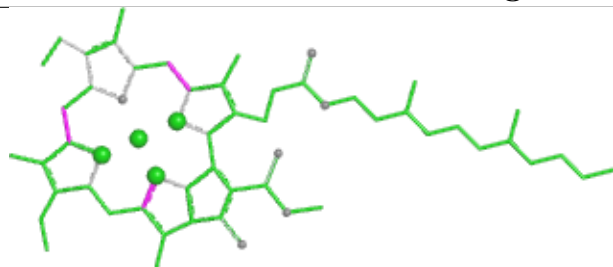


Torsions

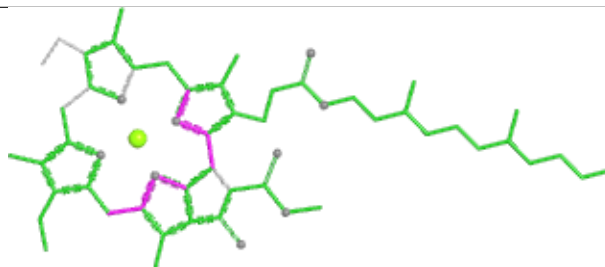


Rings

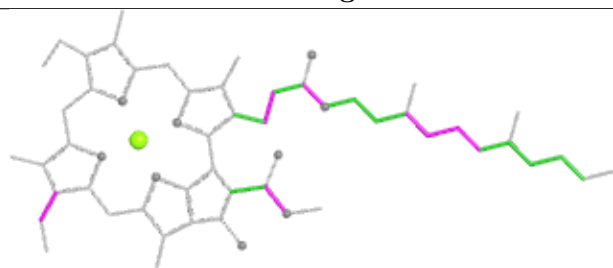
## Ligand CLA G 1229



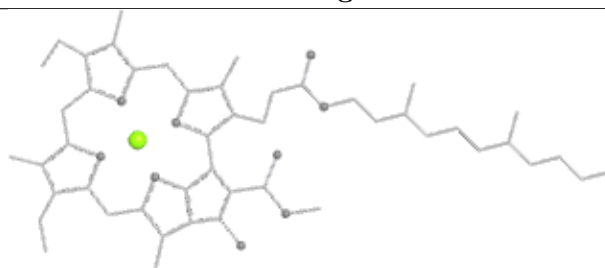
Bond lengths



Bond angles



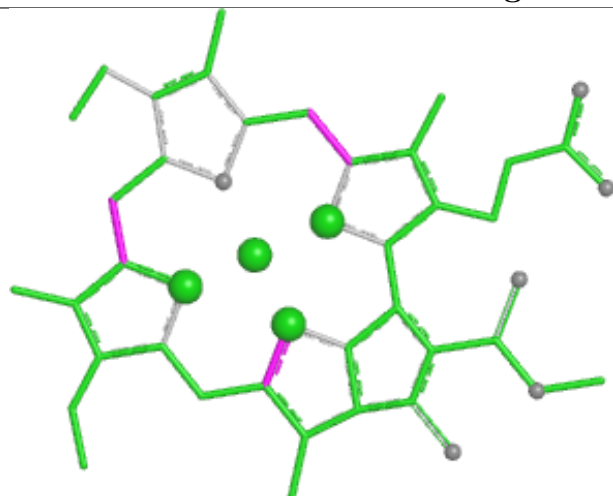
Torsions



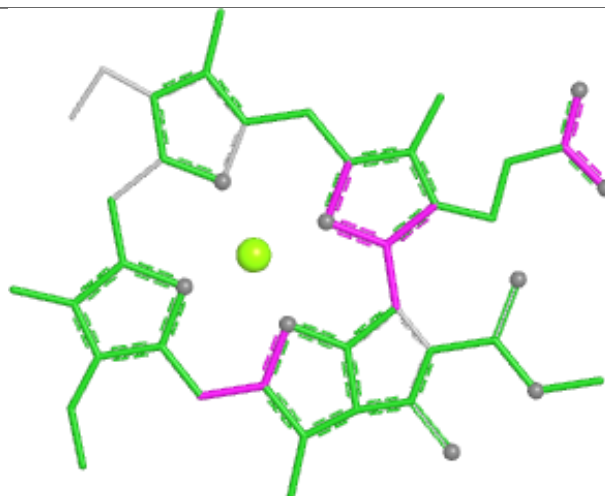
Rings



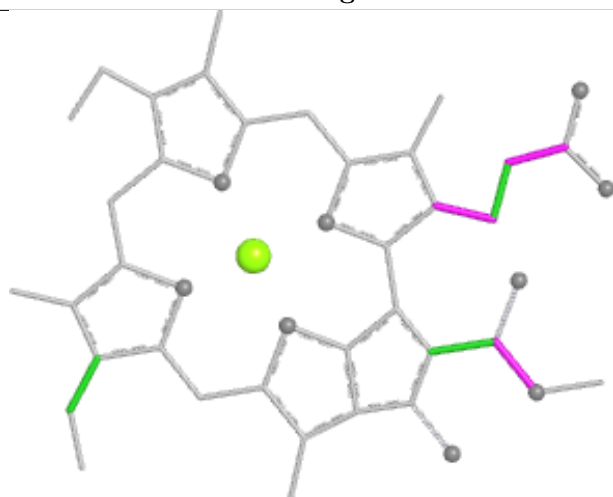
## Ligand CLA G 1232



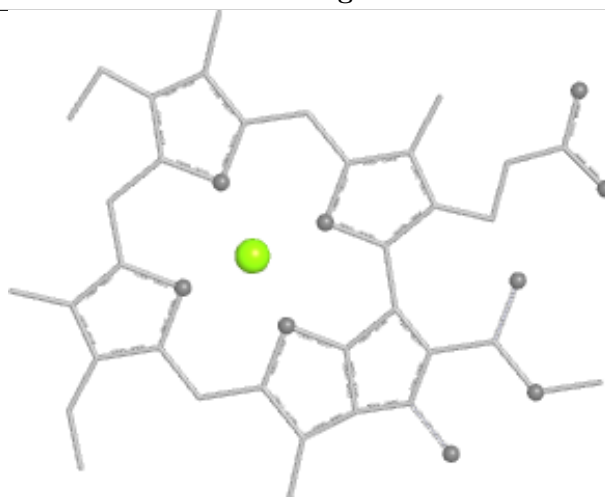
Bond lengths



Bond angles



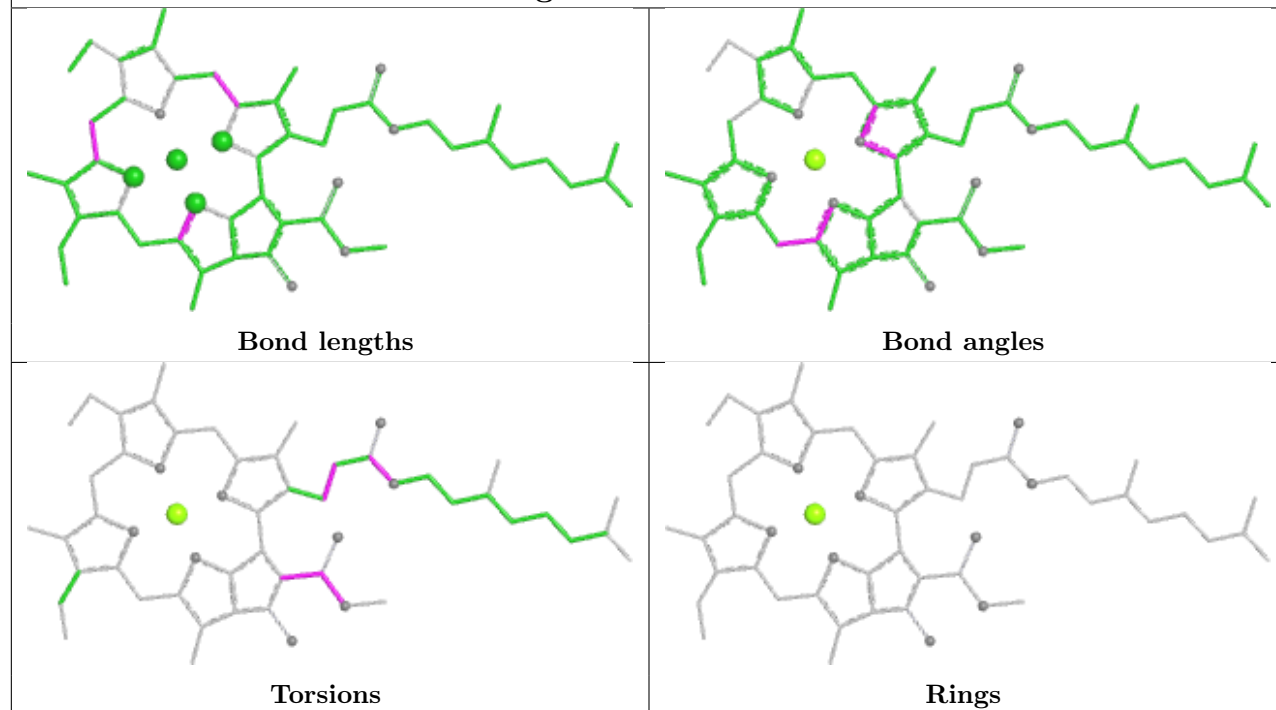
Torsions



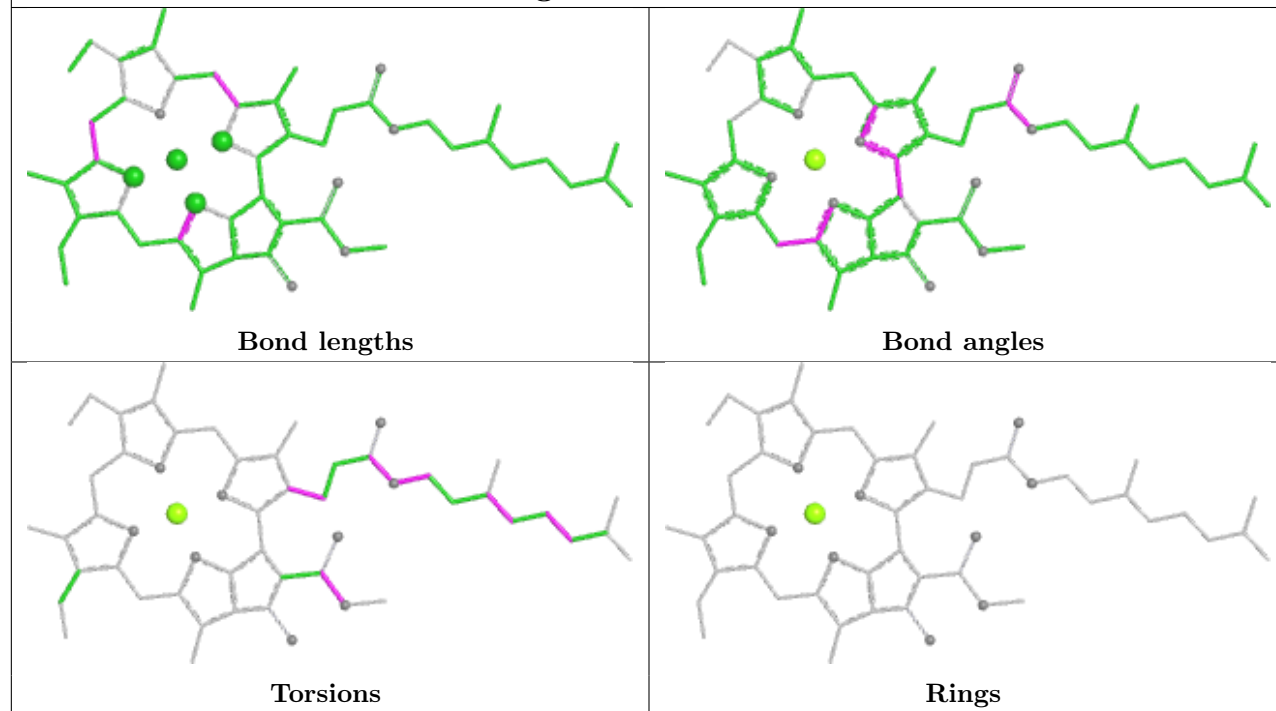
Rings



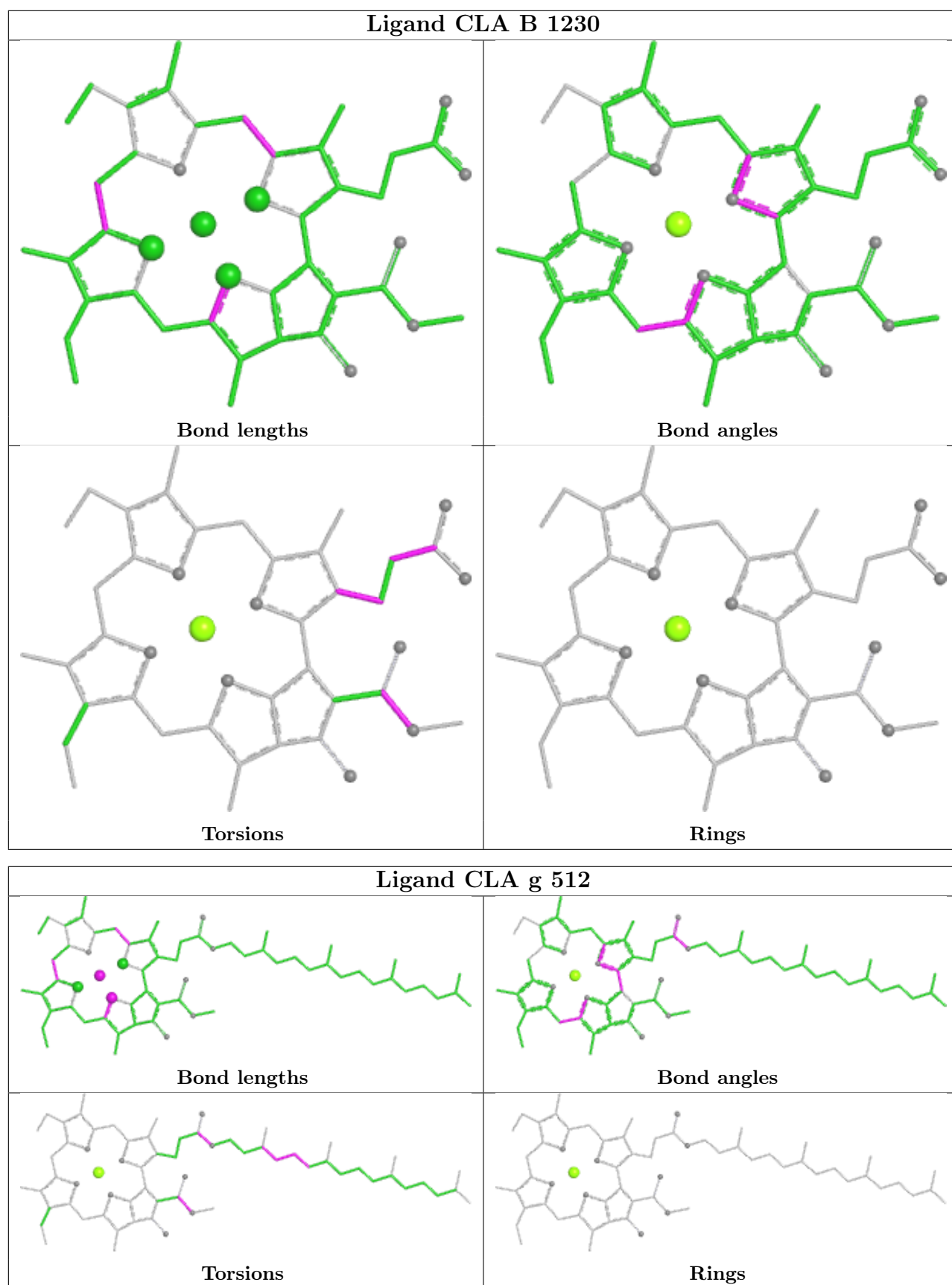
## Ligand CLA x 517



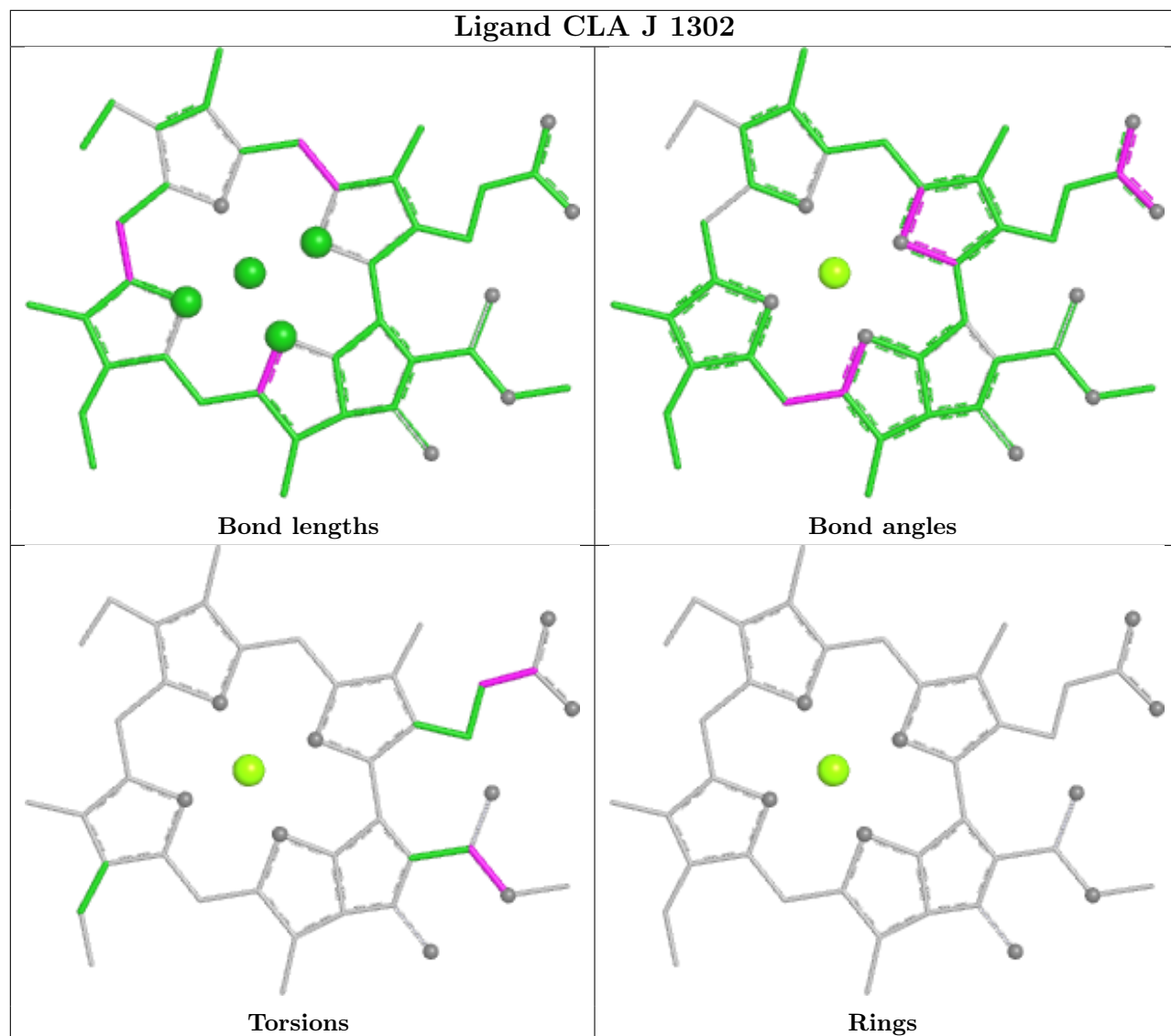
## Ligand CLA h 508





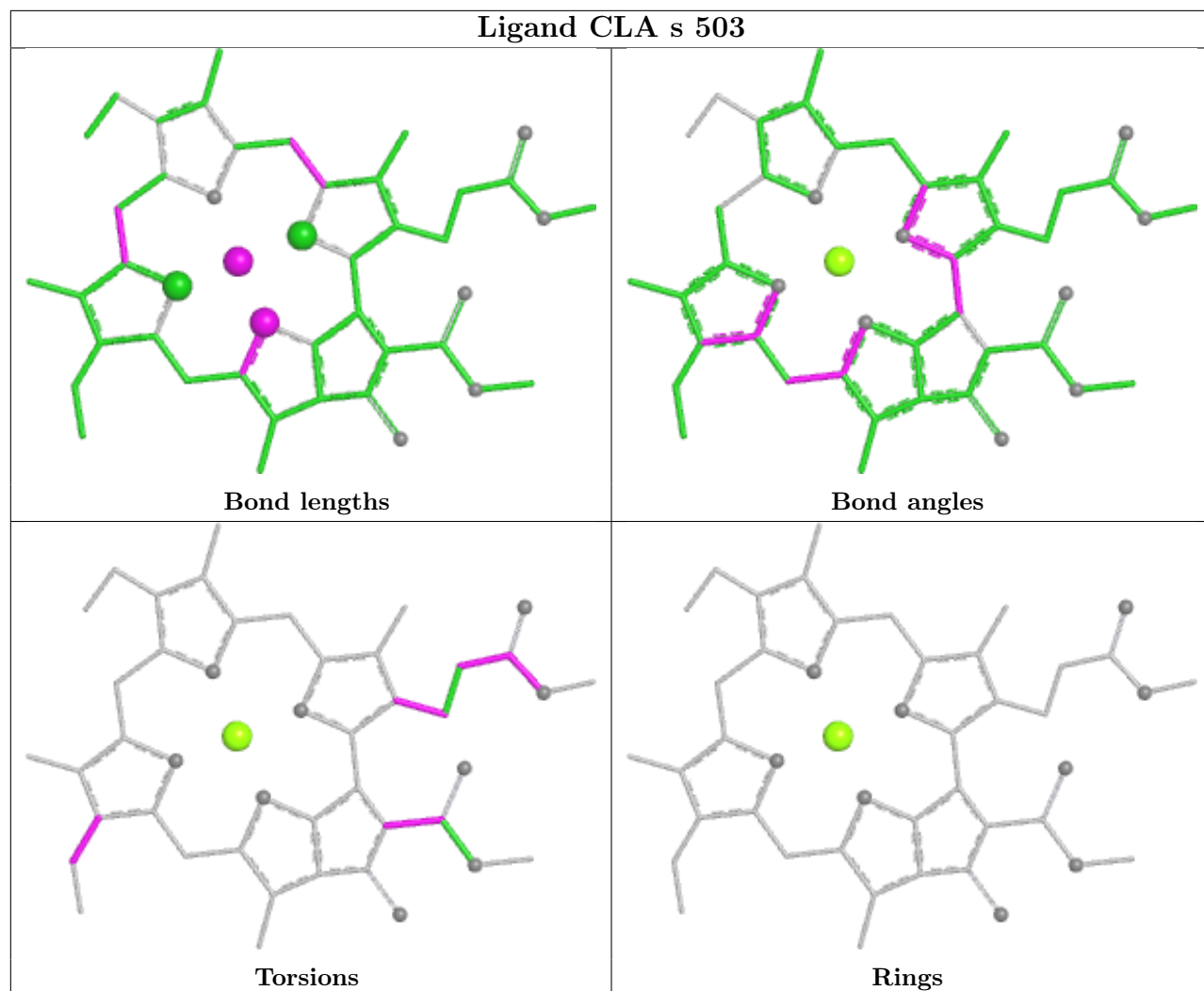




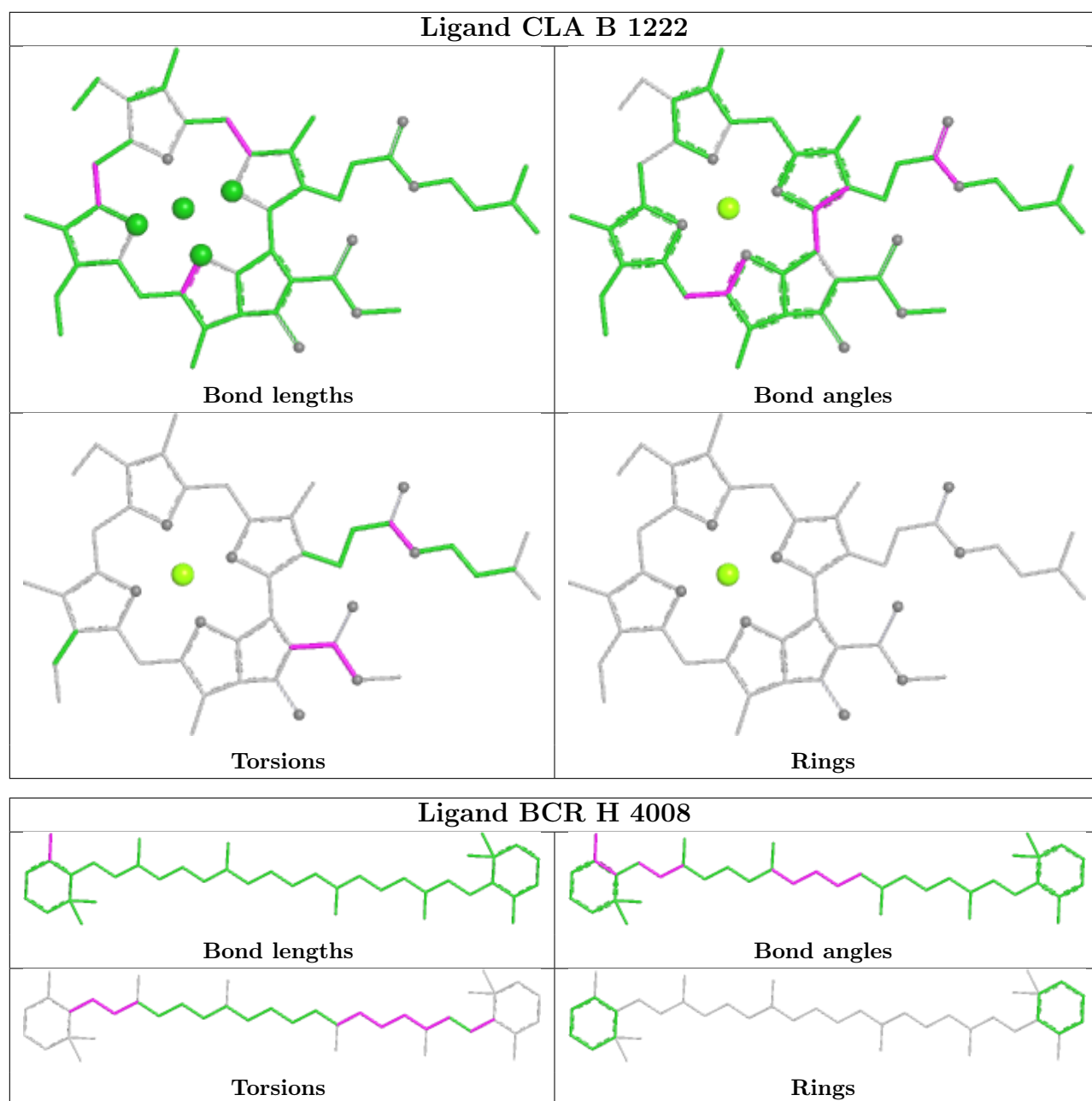




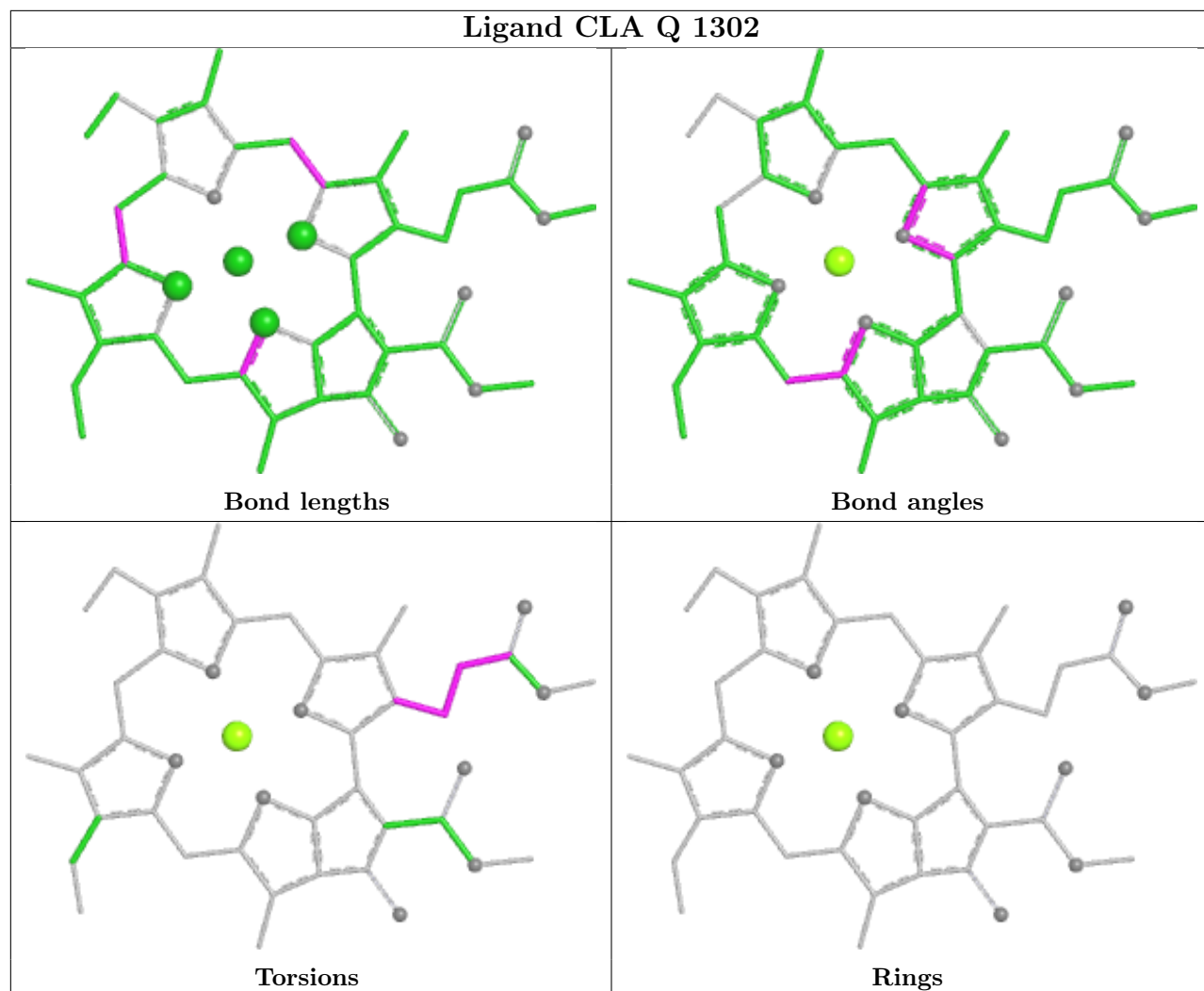
## Ligand CLA s 503





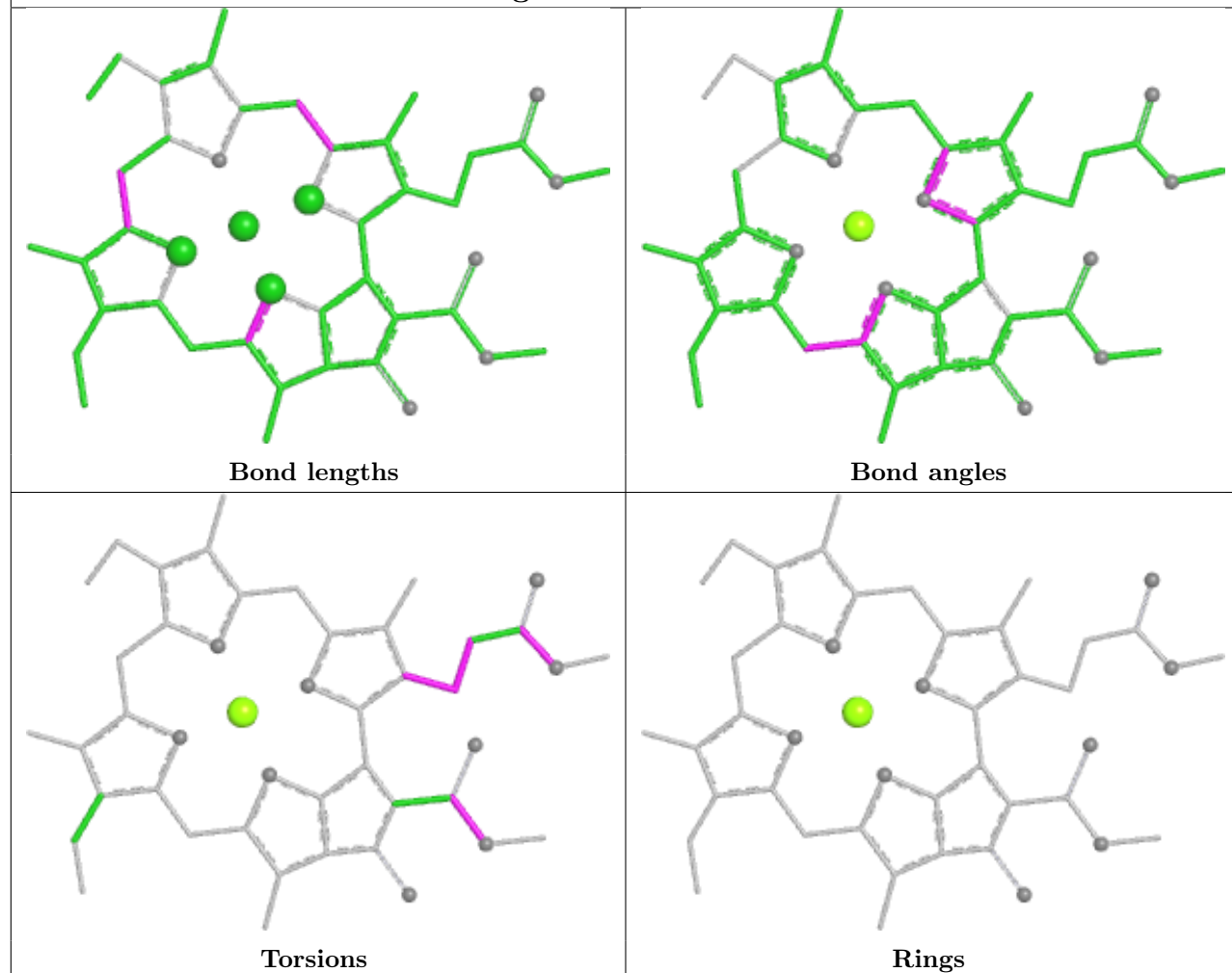




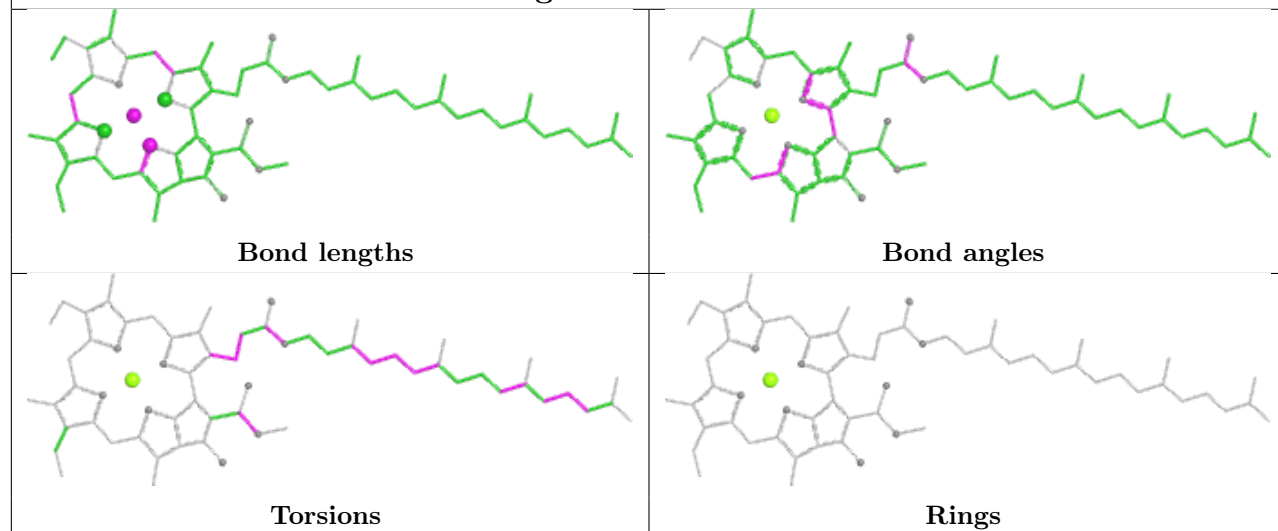




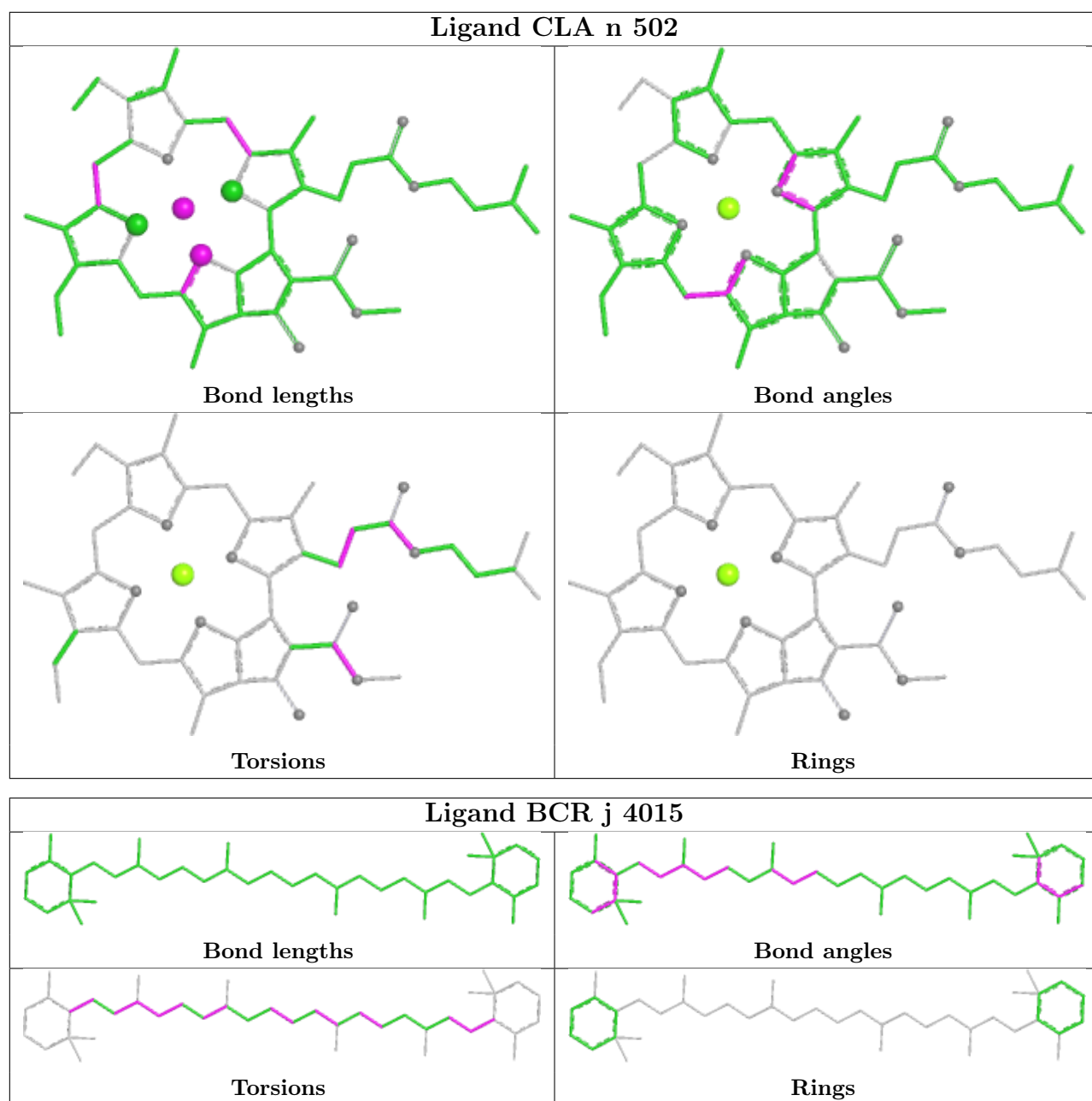
## Ligand CLA X 513



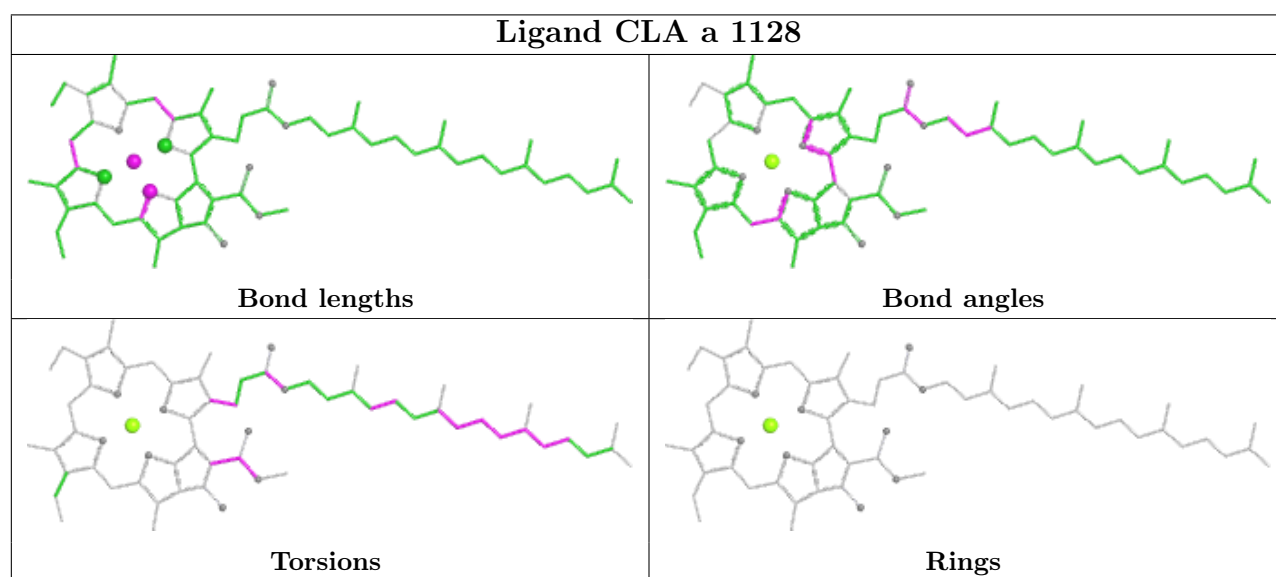
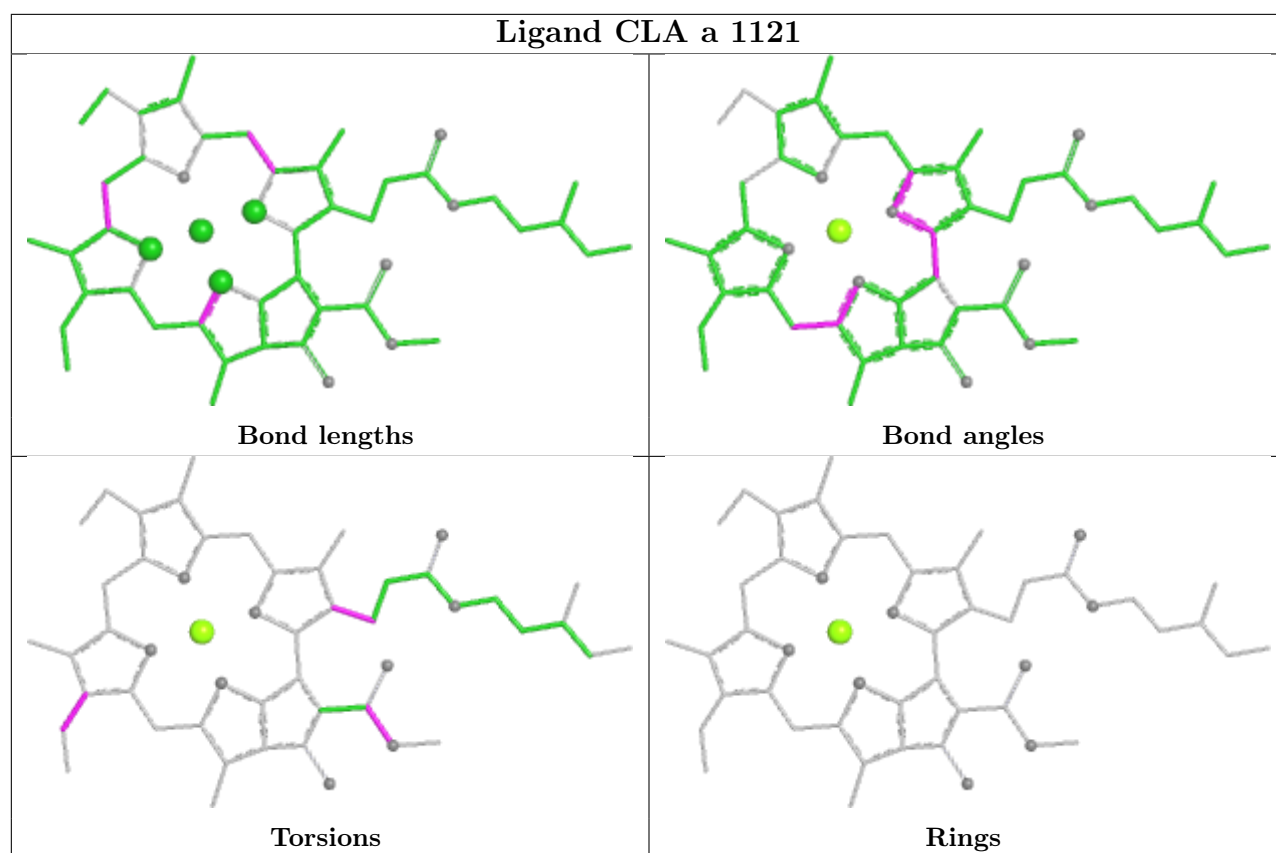
## Ligand CLA h 512



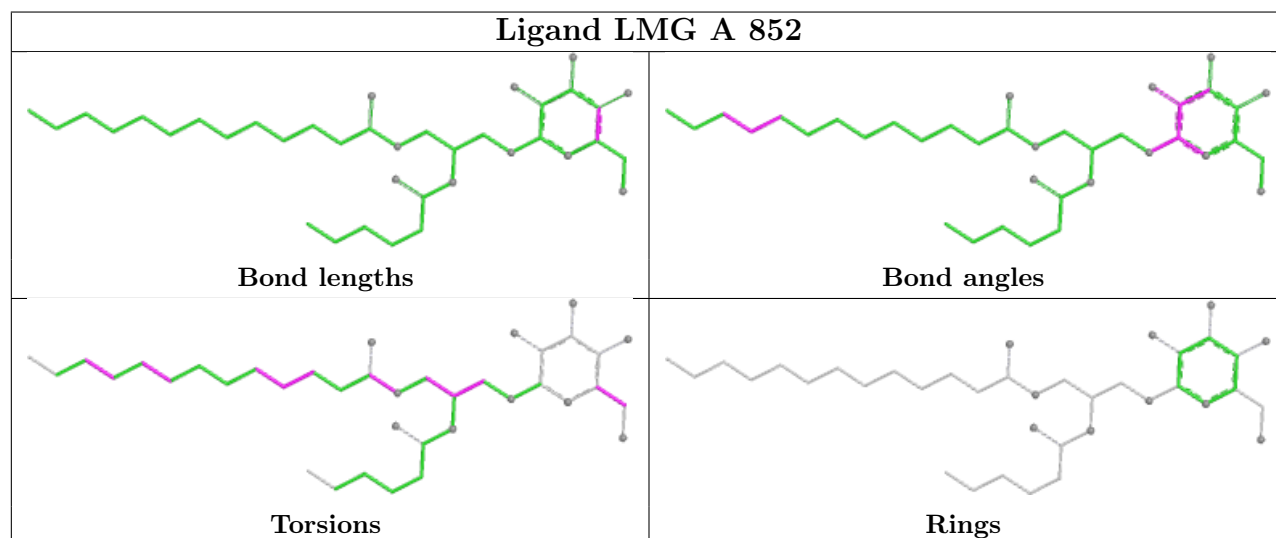
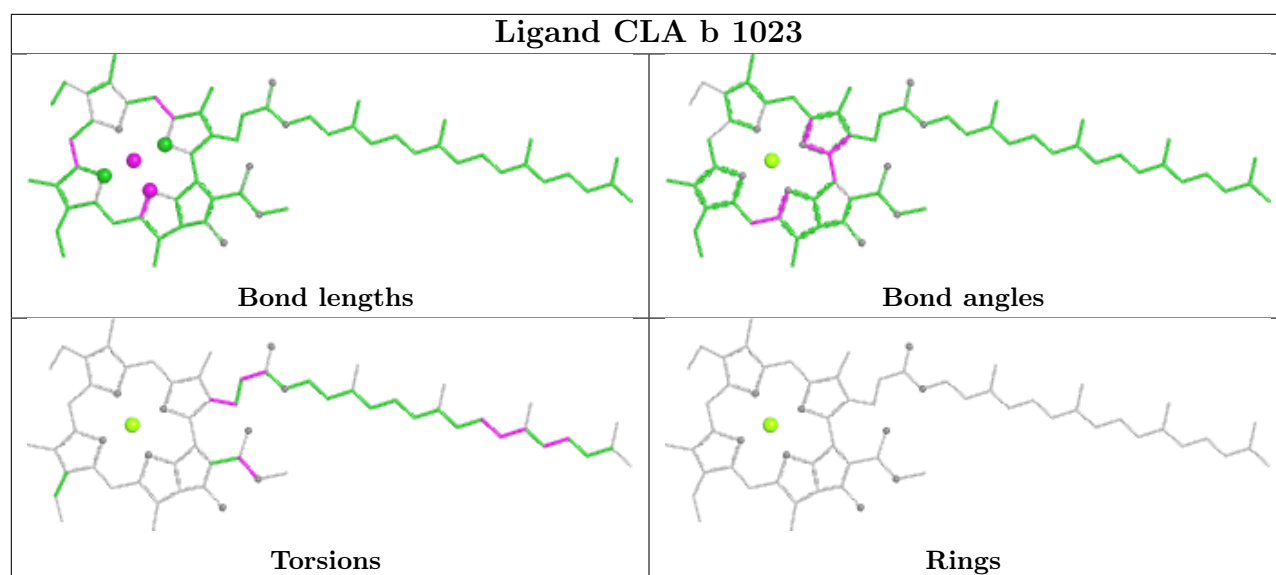




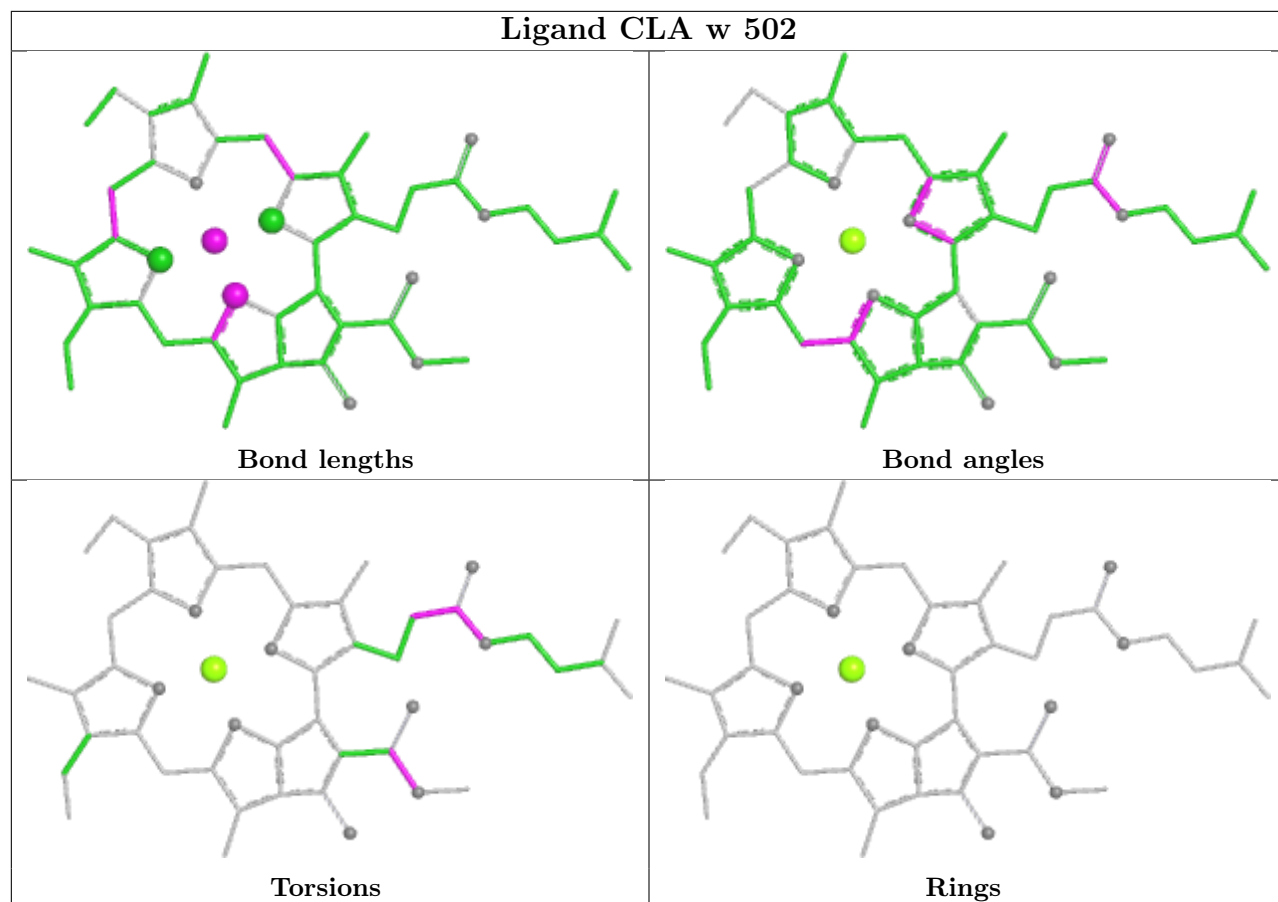






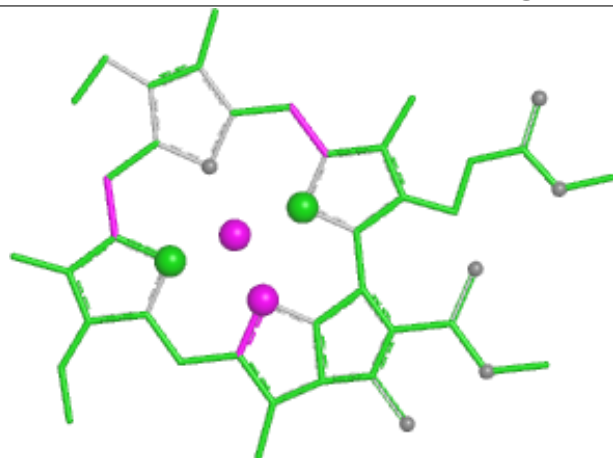




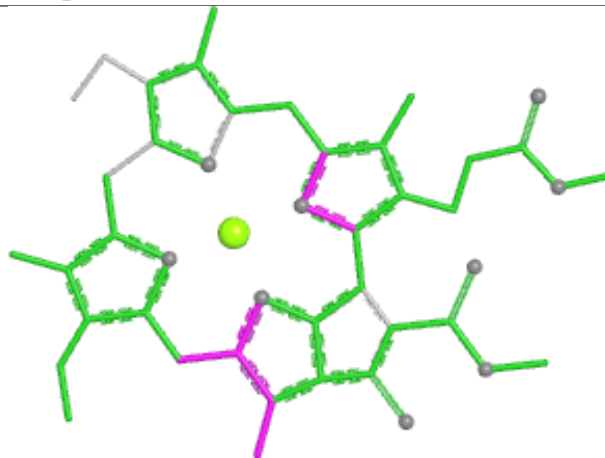




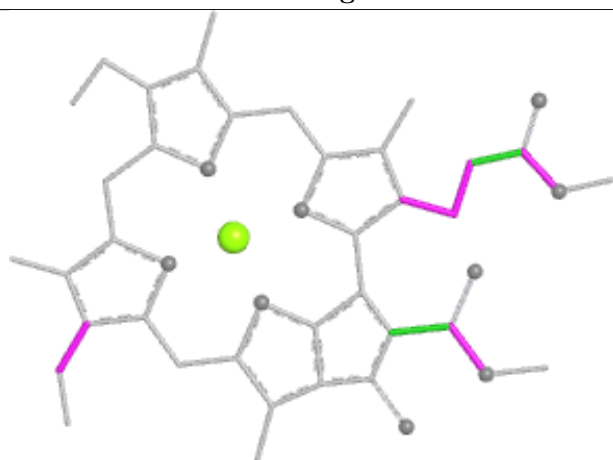
## Ligand CLA q 503



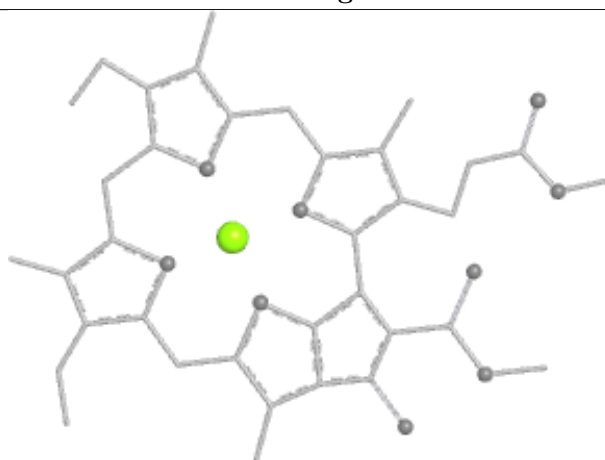
Bond lengths



Bond angles

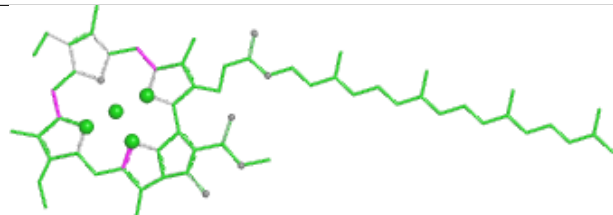


Torsions

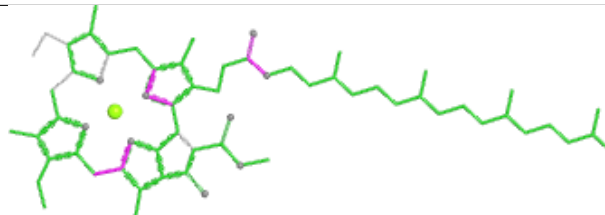


Rings

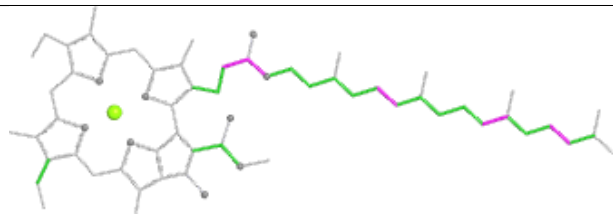
## Ligand CLA s 510



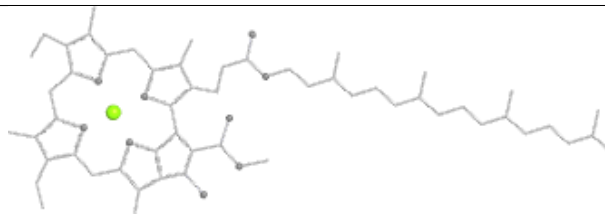
Bond lengths



Bond angles



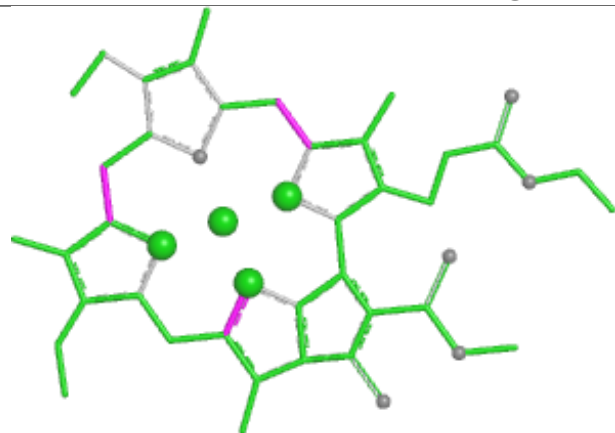
Torsions



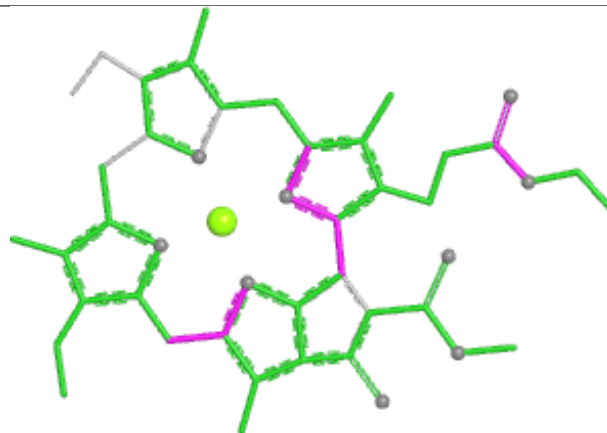
Rings



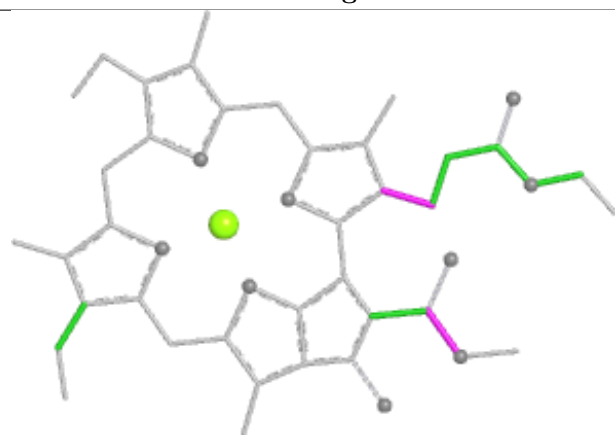
## Ligand CLA H 1137



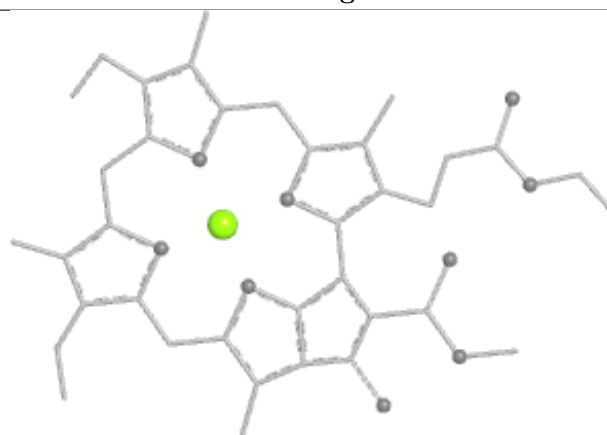
Bond lengths



Bond angles

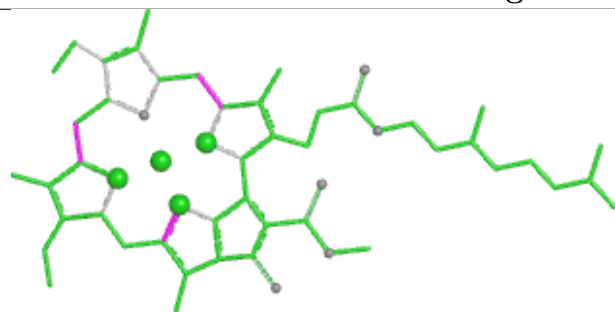


Torsions

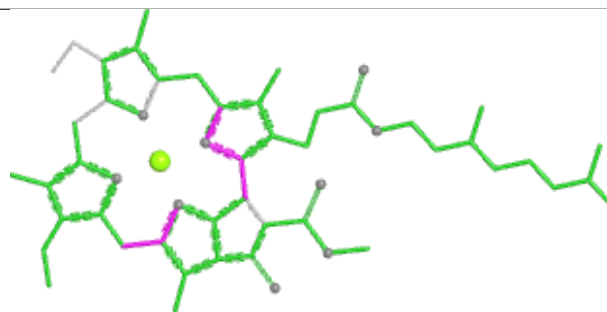


Rings

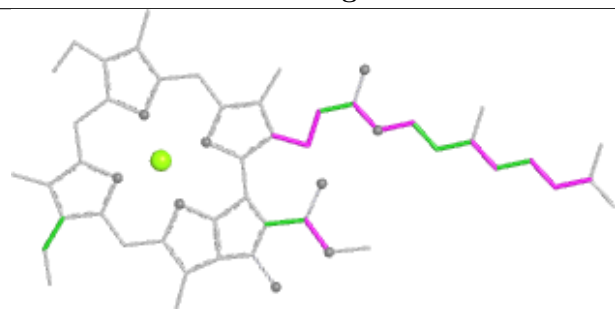
## Ligand CLA G 1228



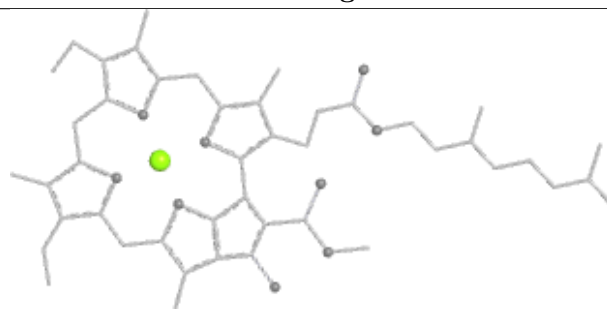
Bond lengths



Bond angles



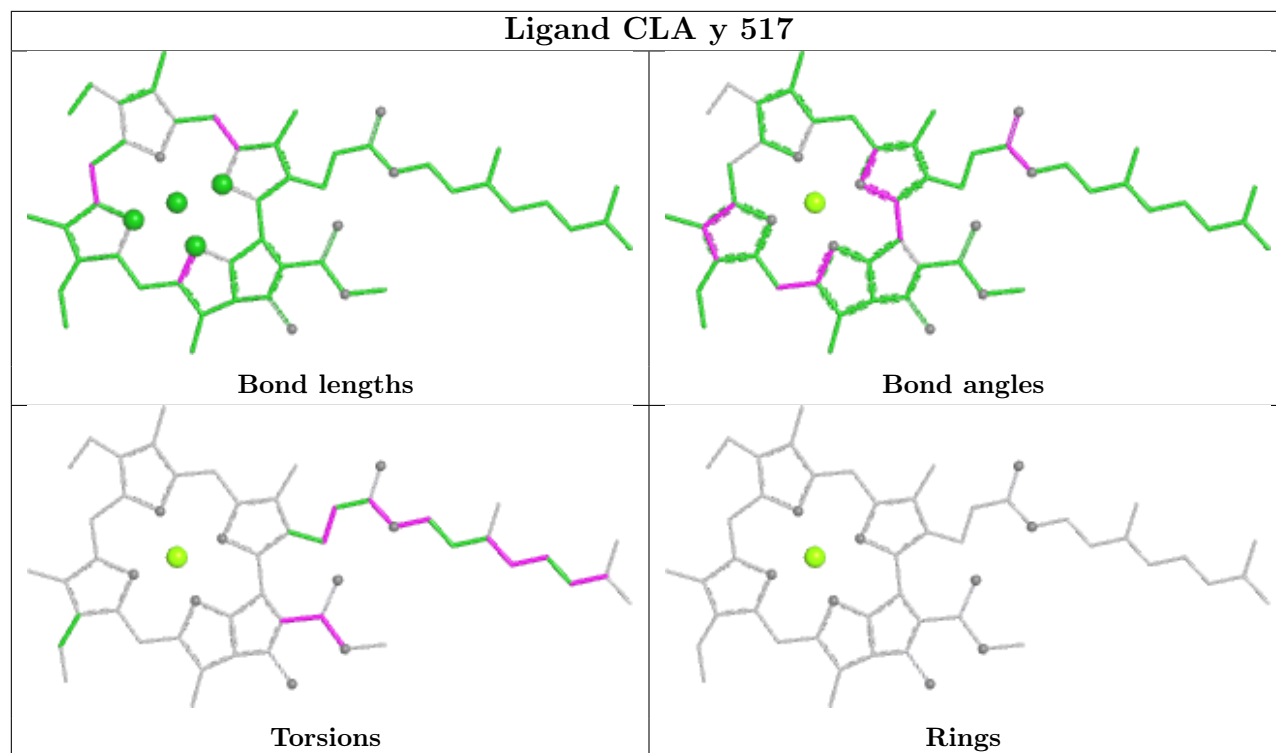
Torsions



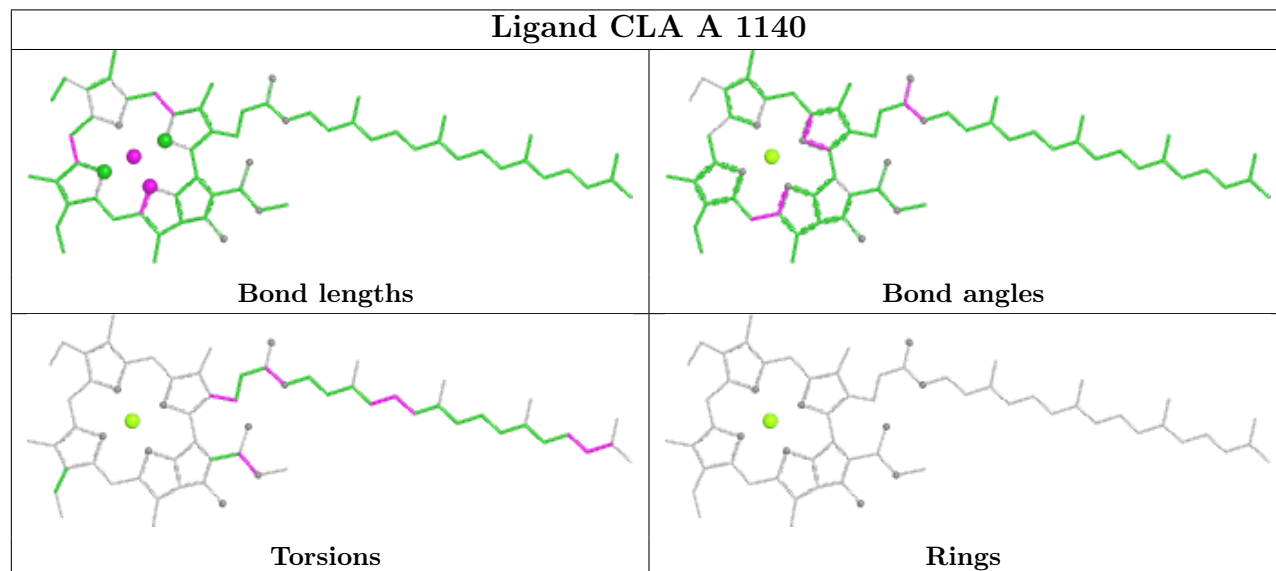
Rings



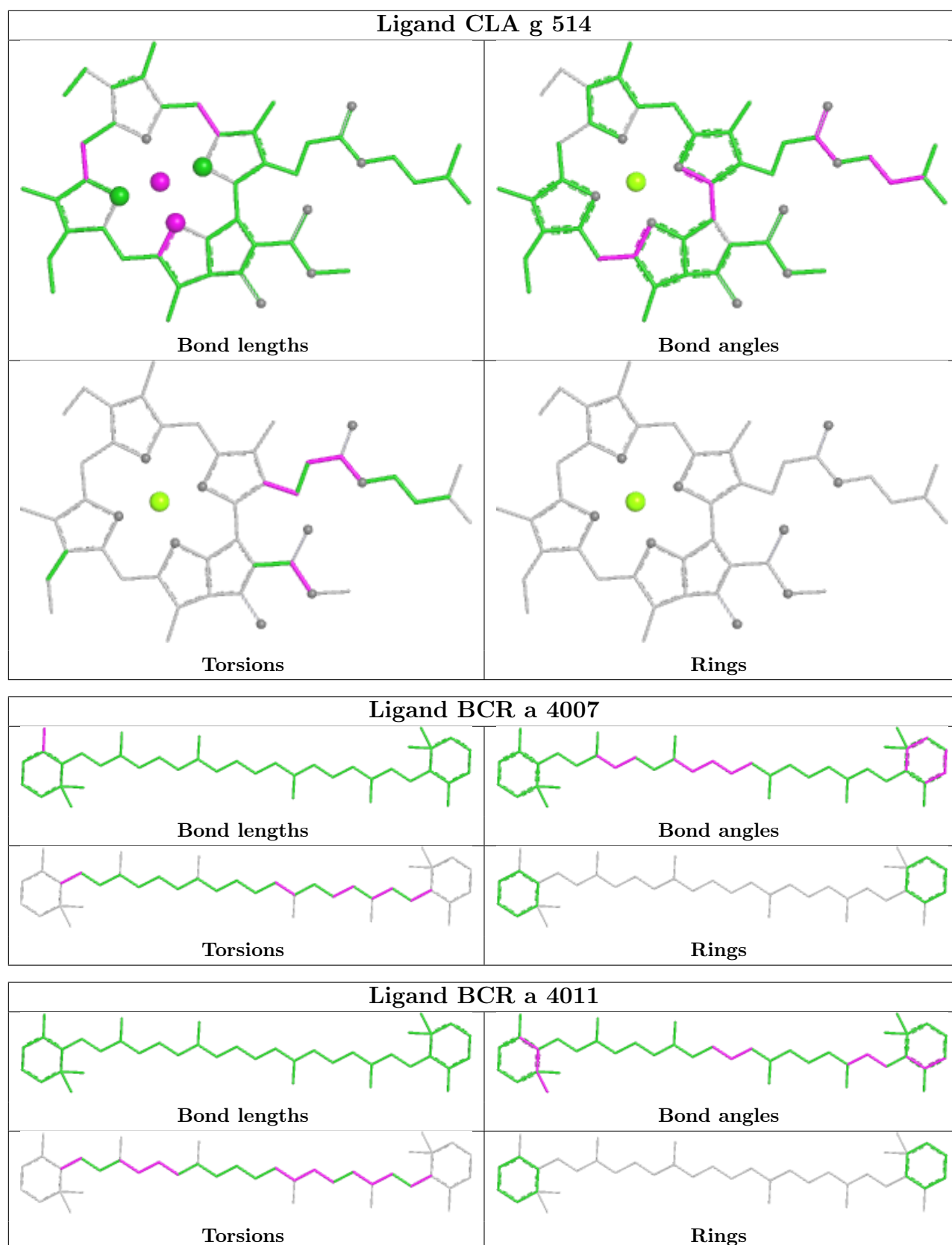
## Ligand CLA y 517



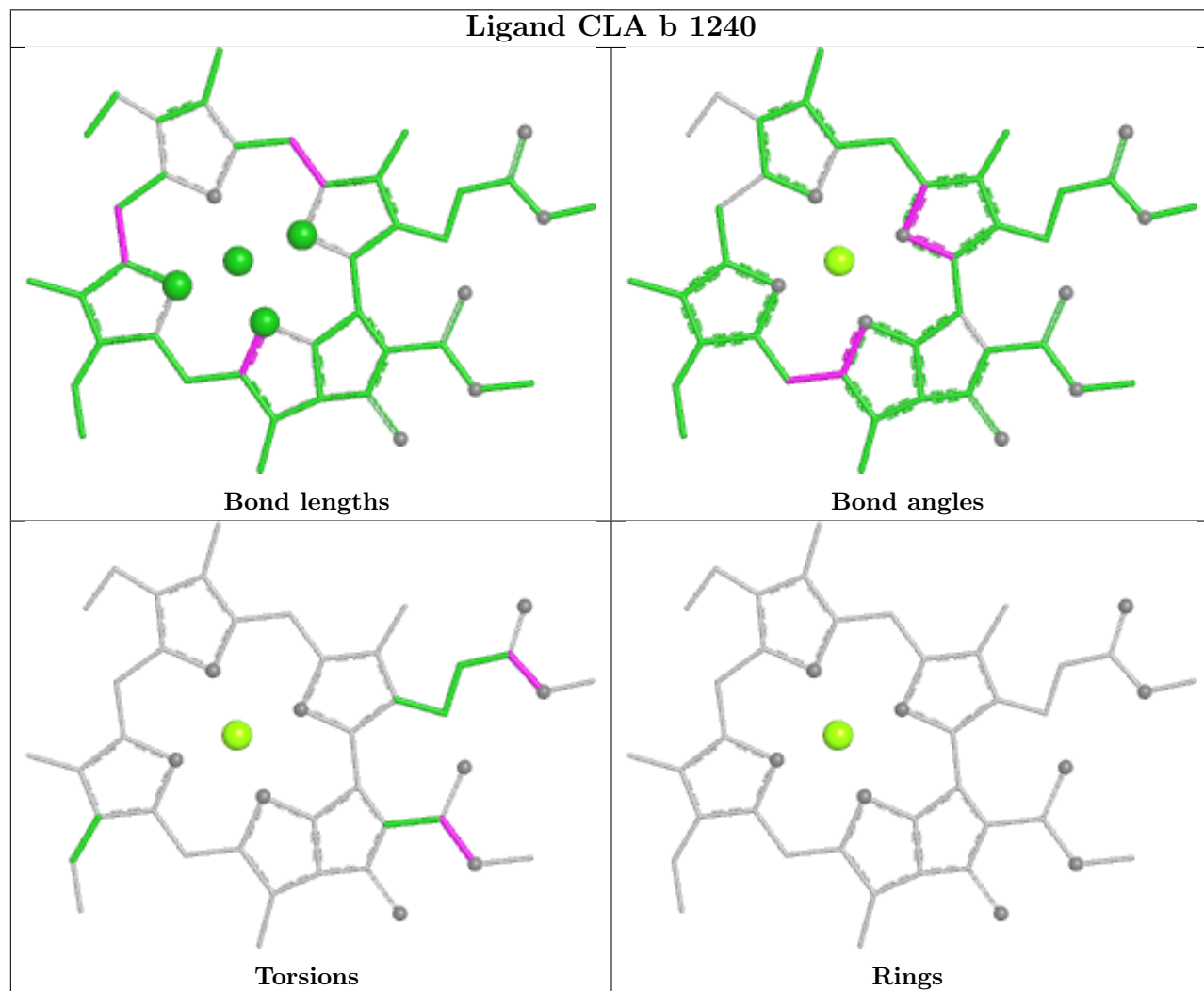
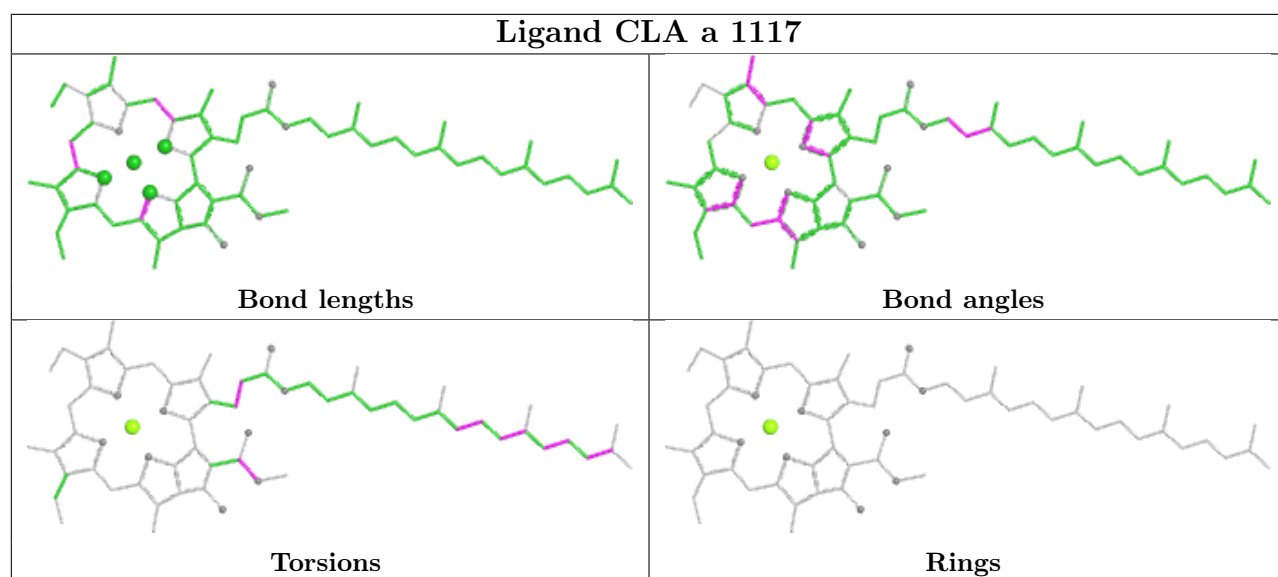
## Ligand CLA A 1140



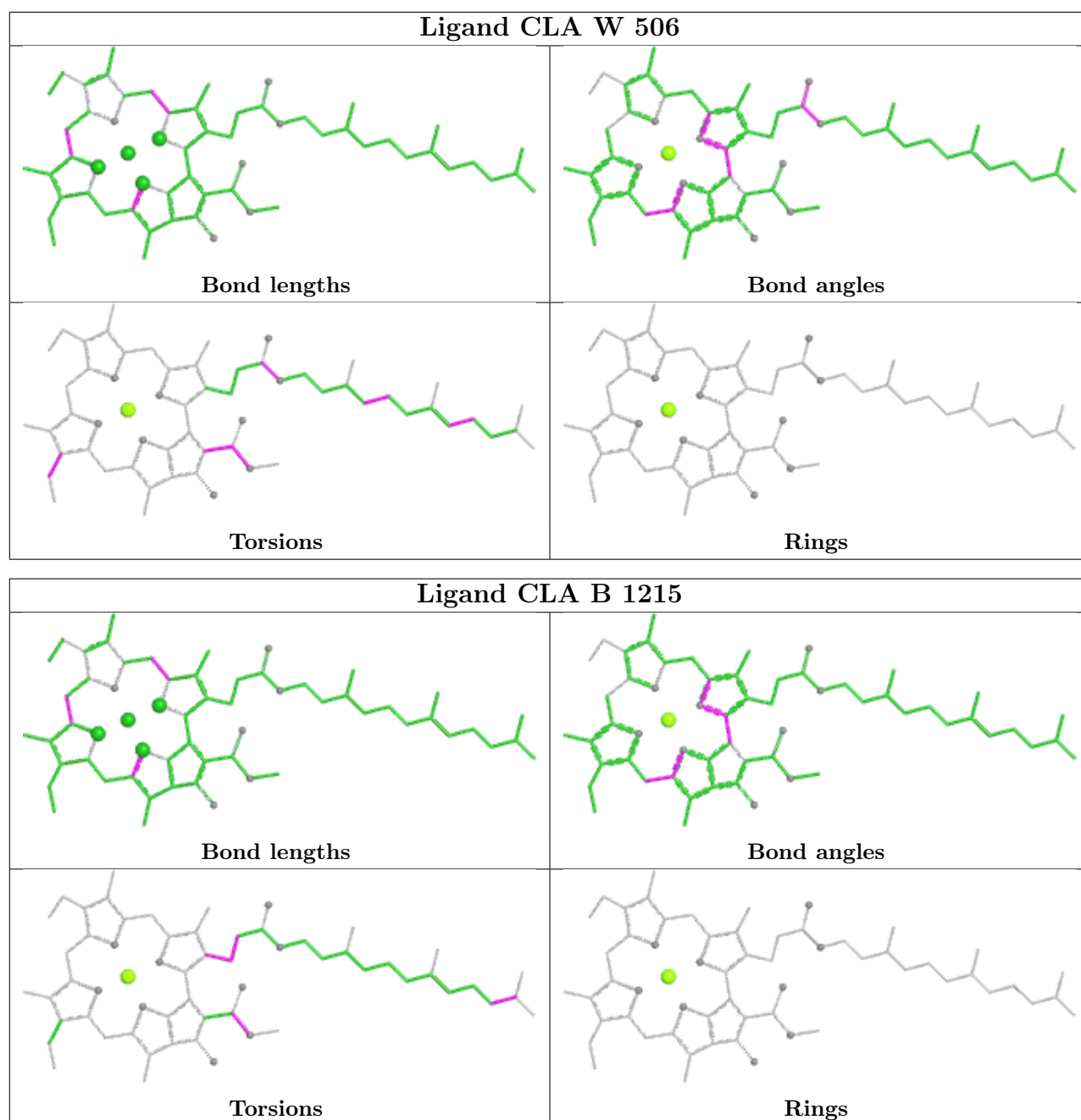




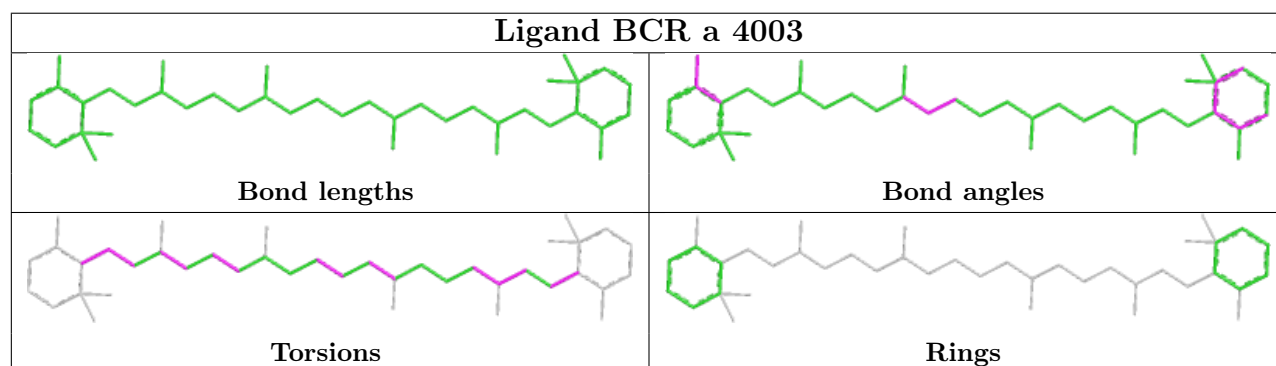
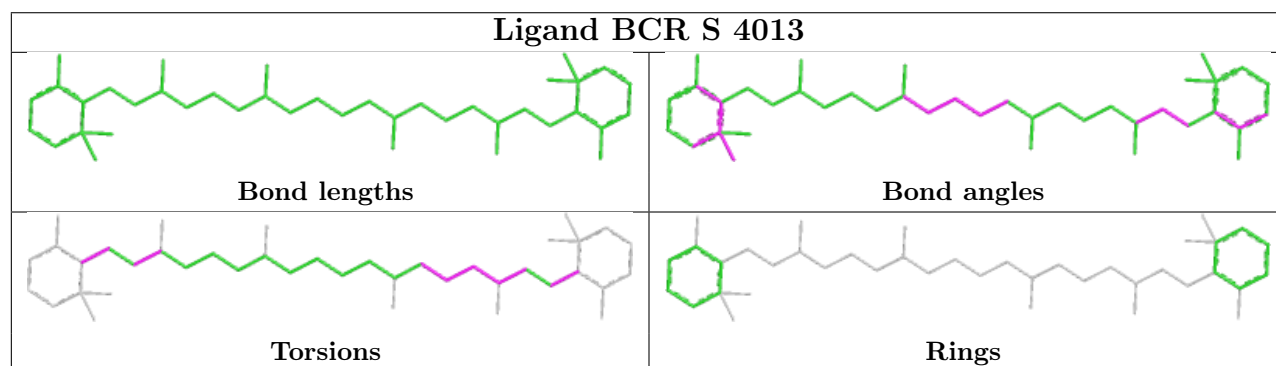
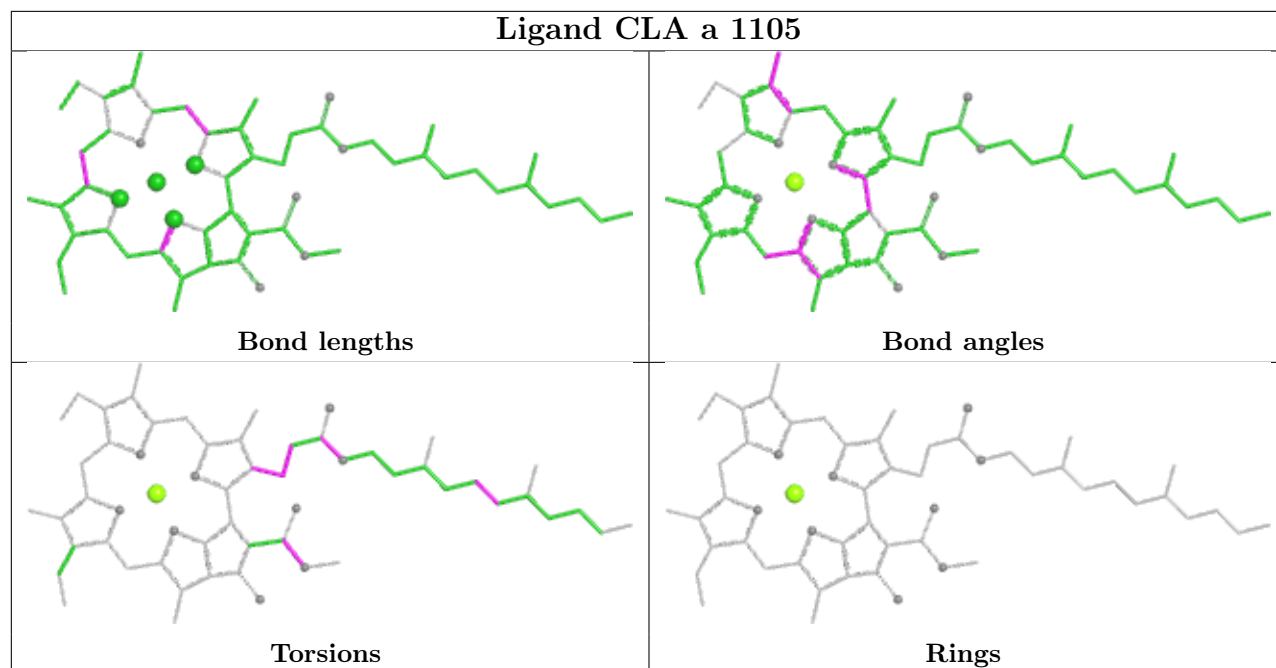






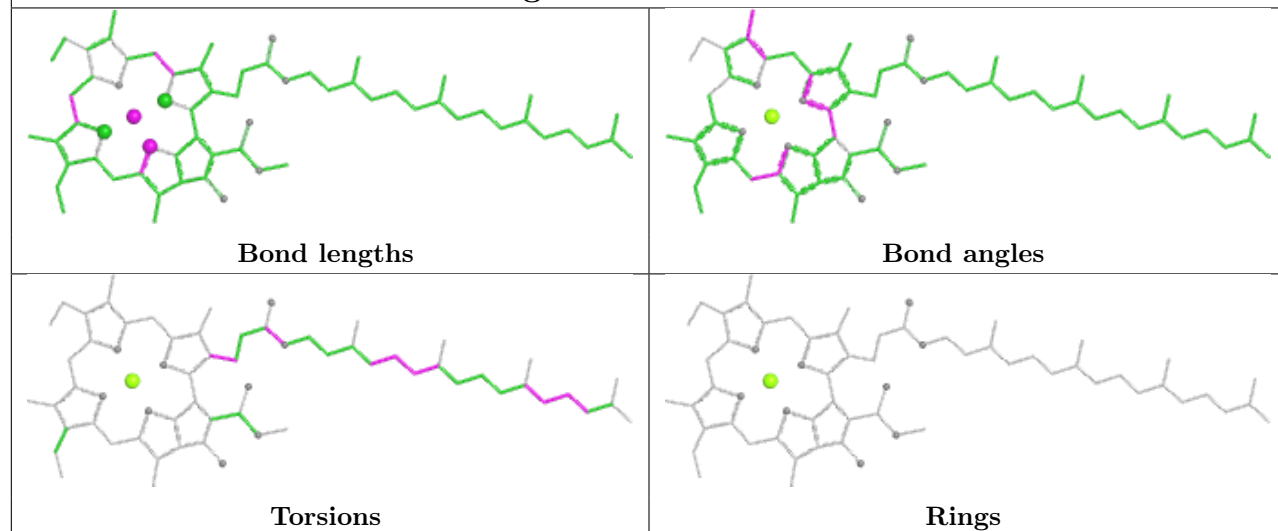




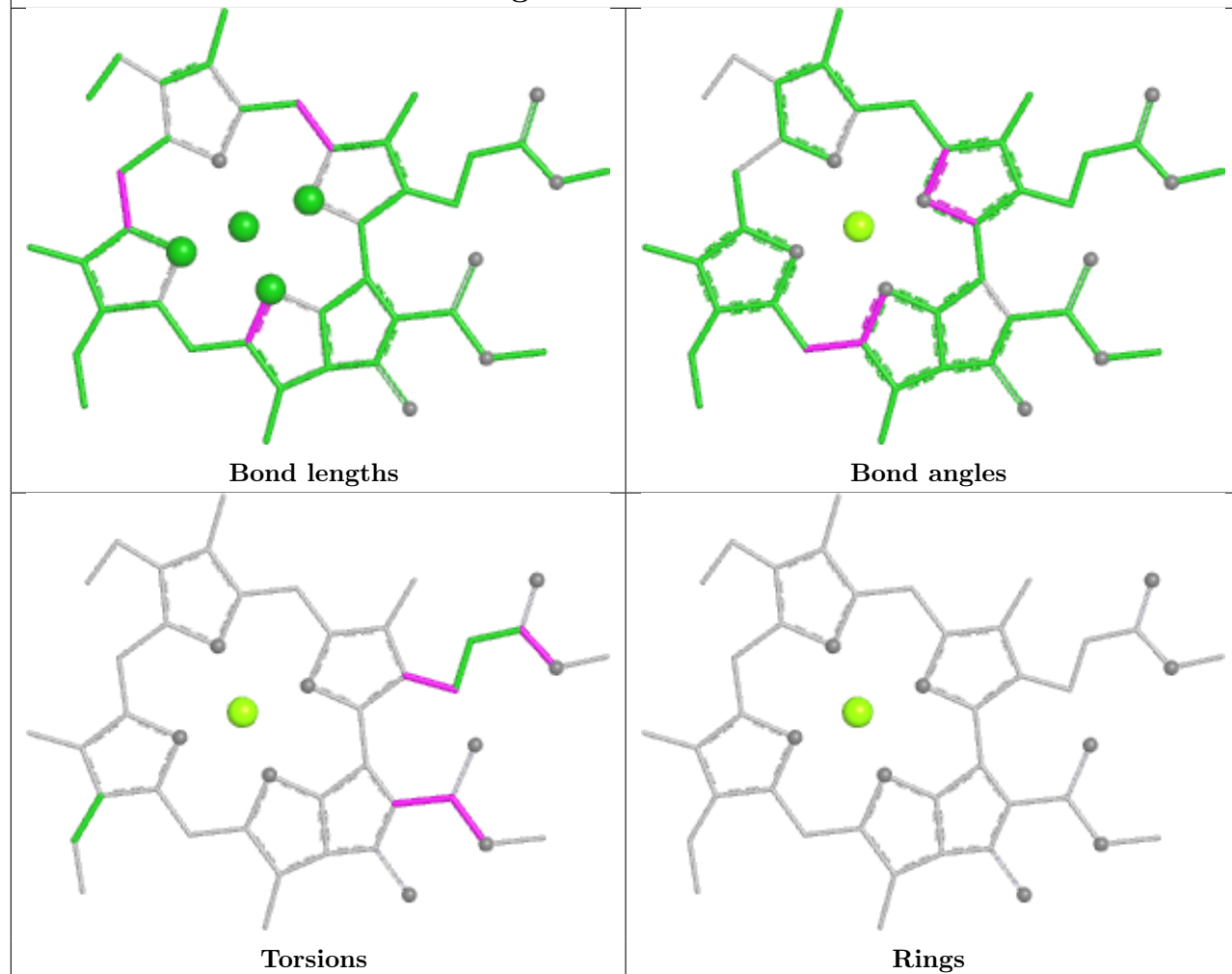




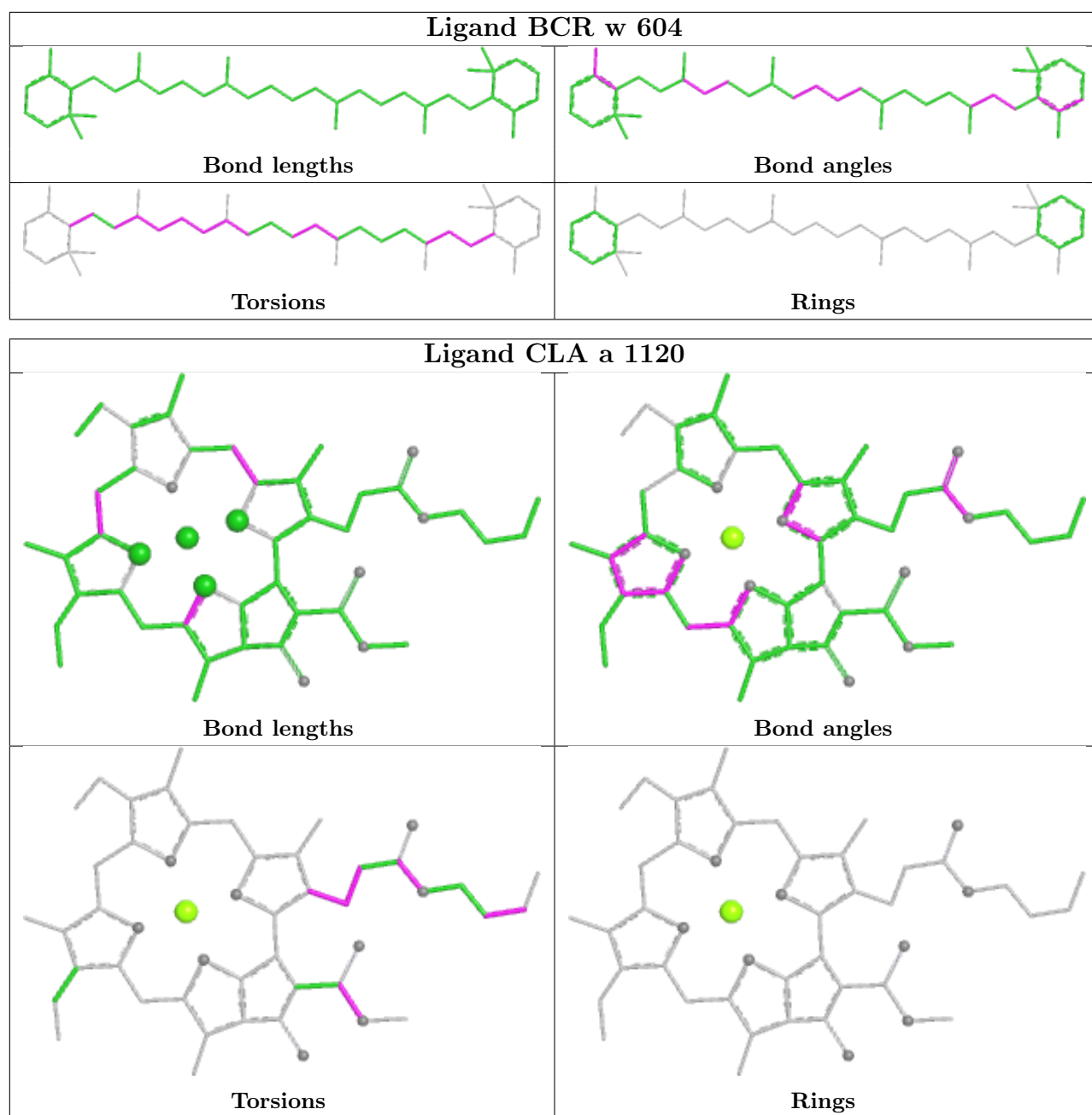
## Ligand CLA B 1225



## Ligand CLA f 1302

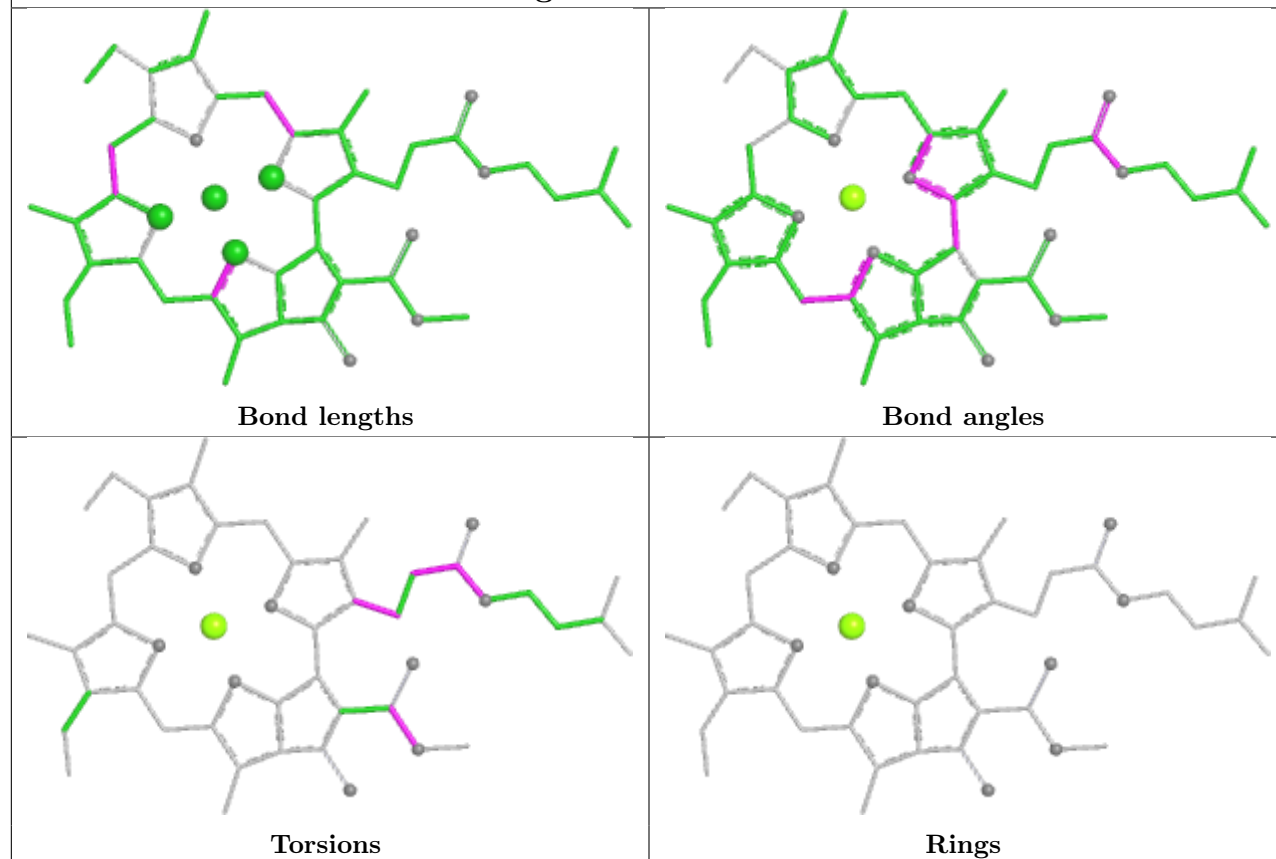




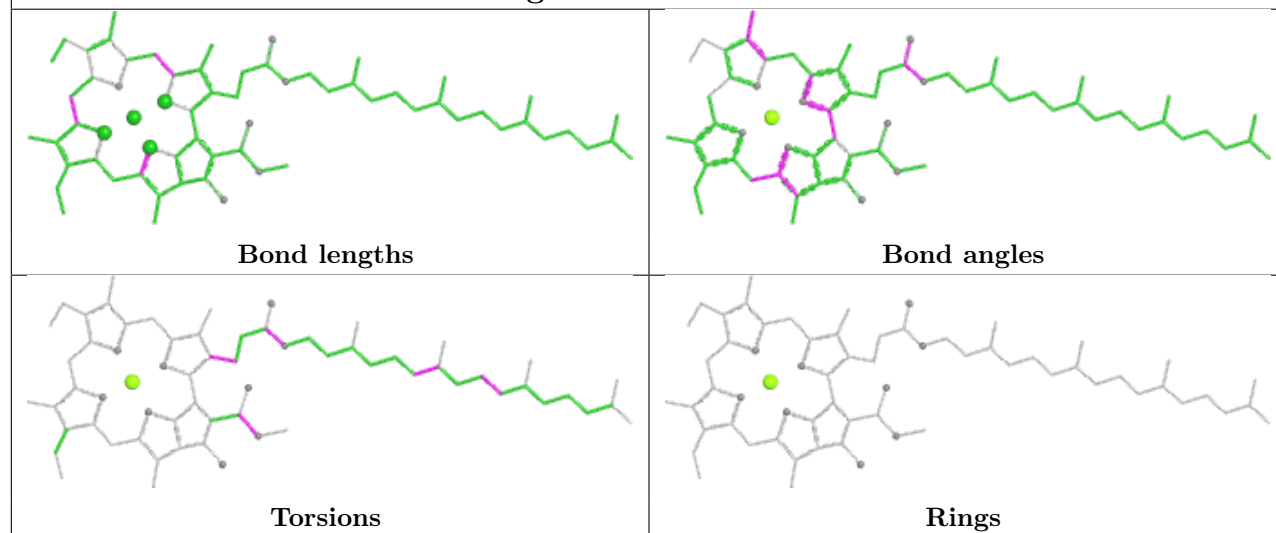




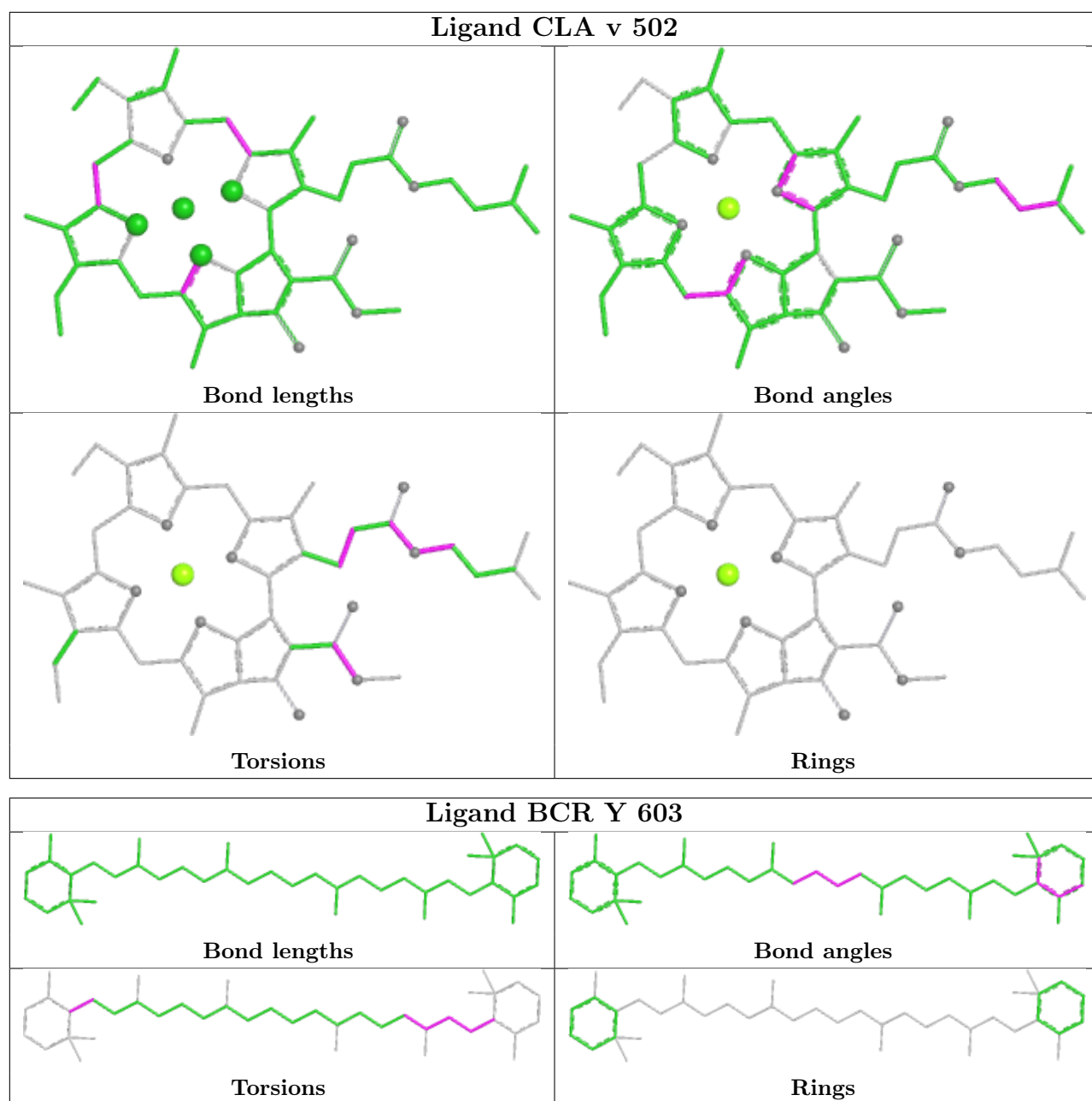
## Ligand CLA h 514



## Ligand CLA W 511

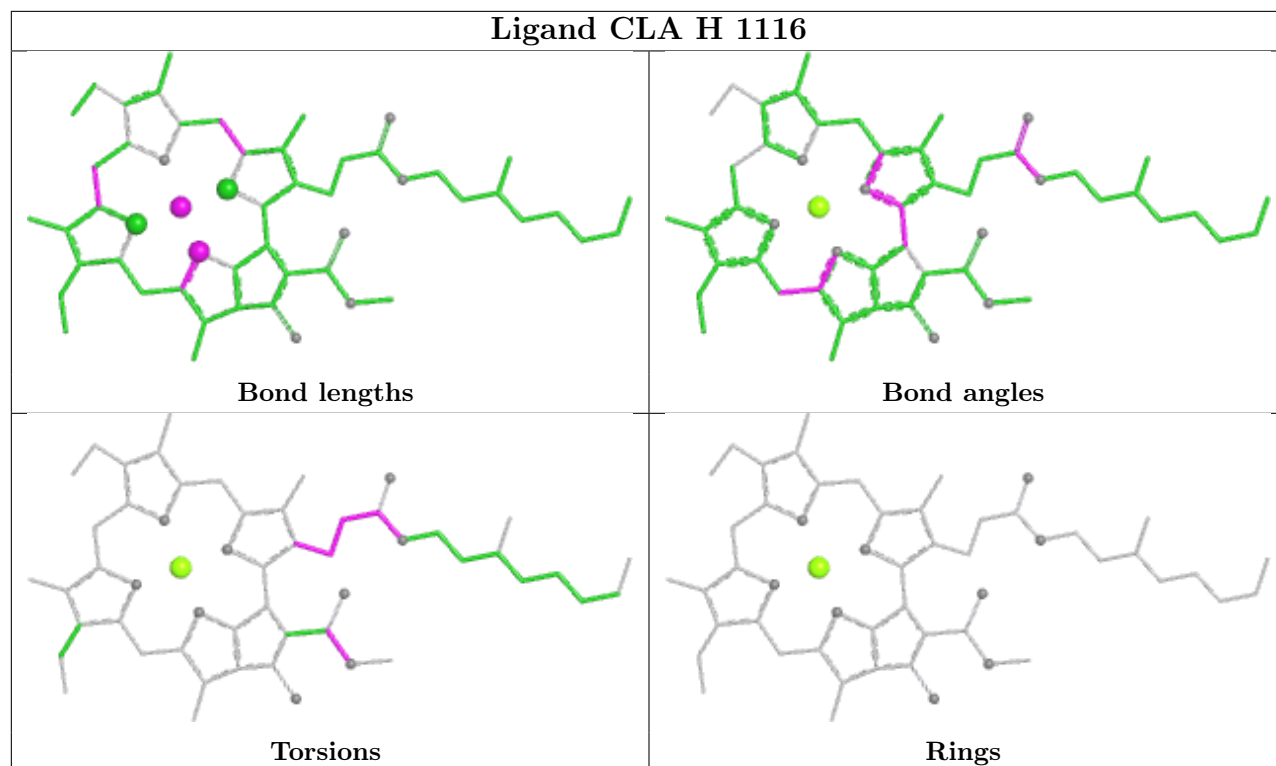




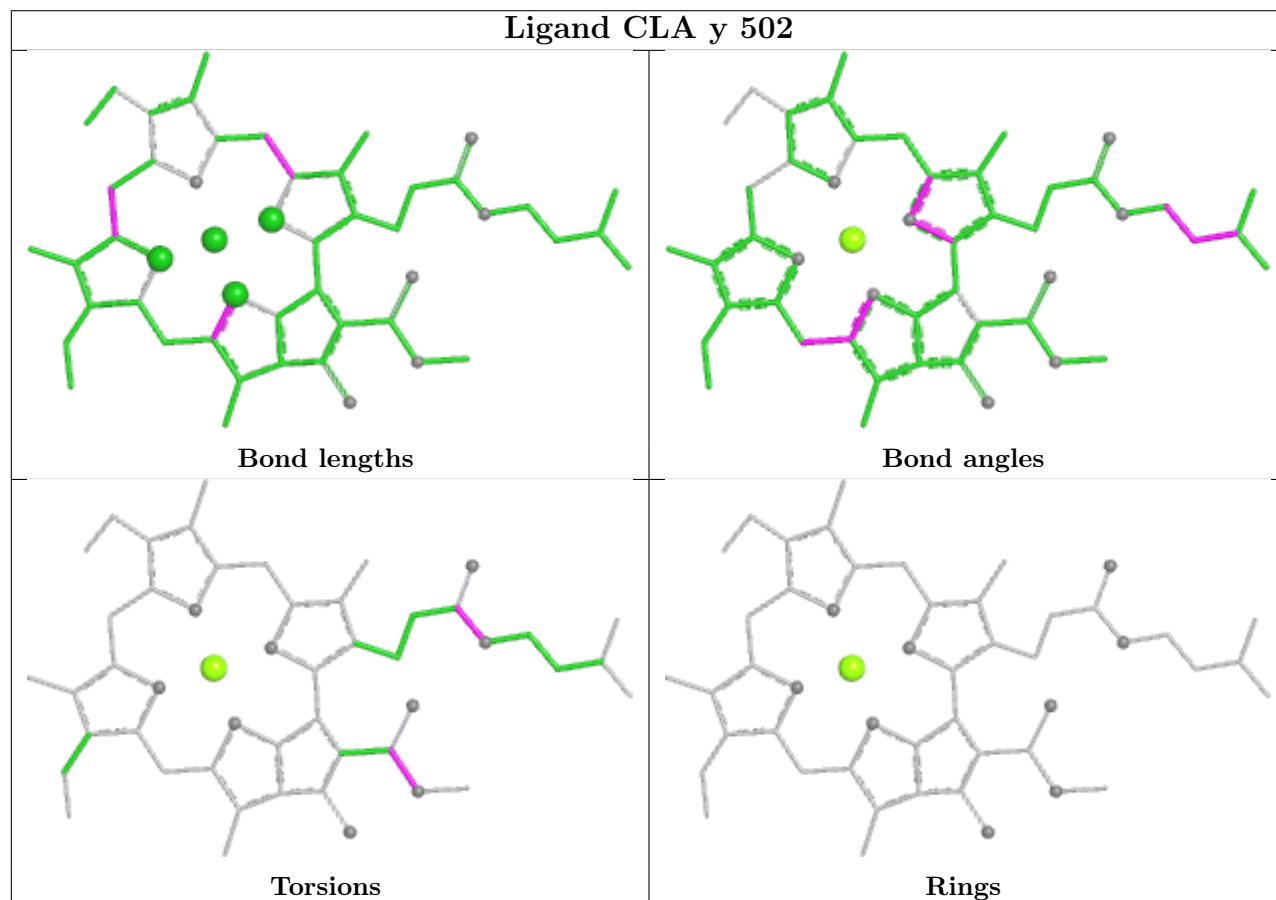




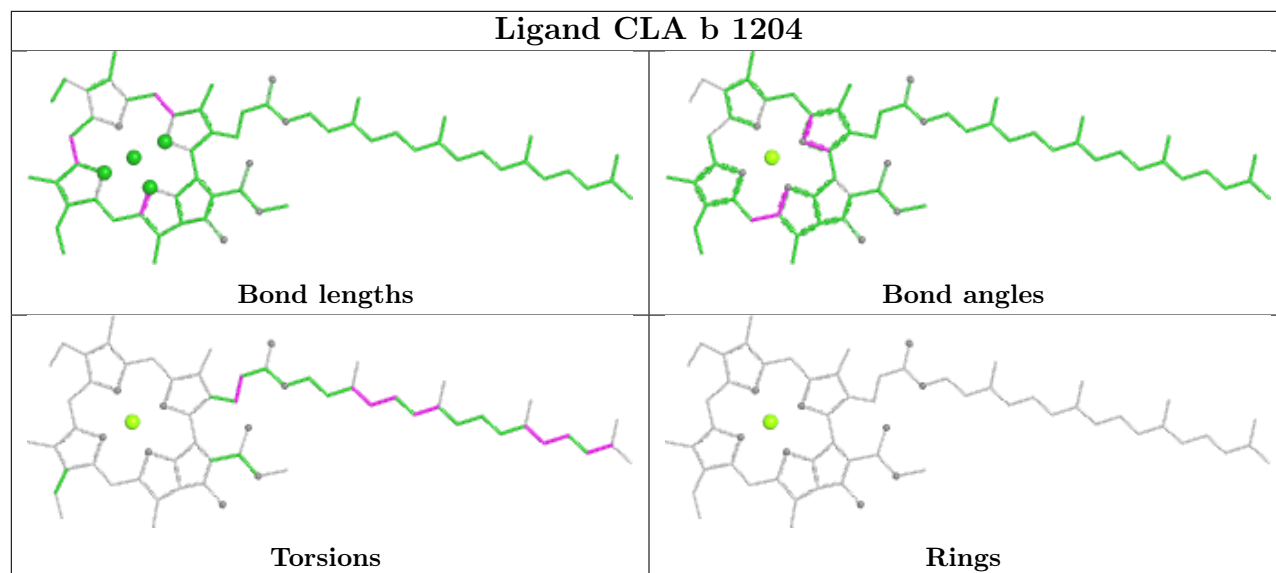
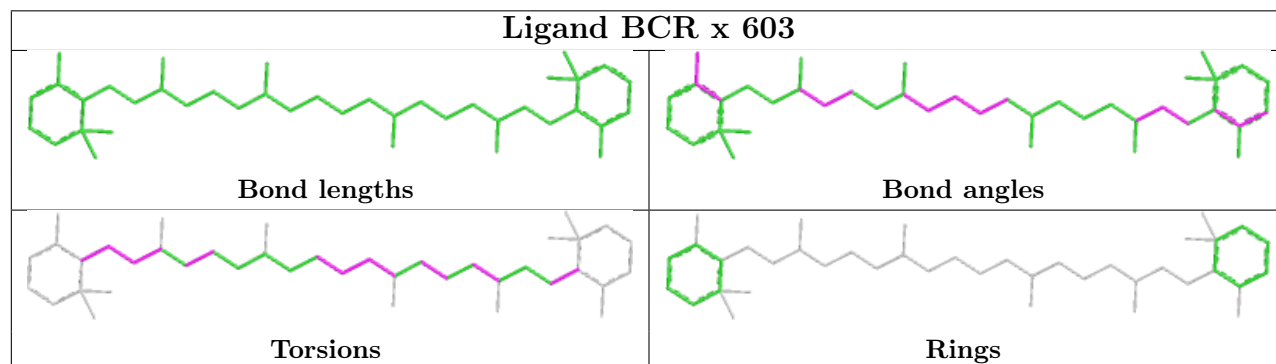
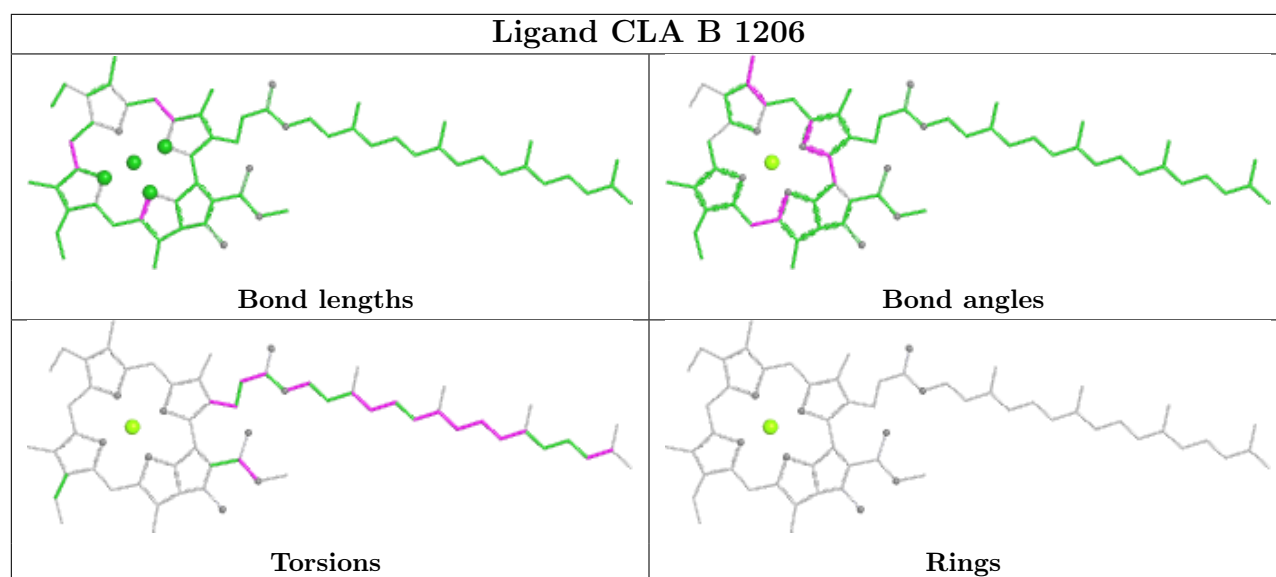
## Ligand CLA H 1116



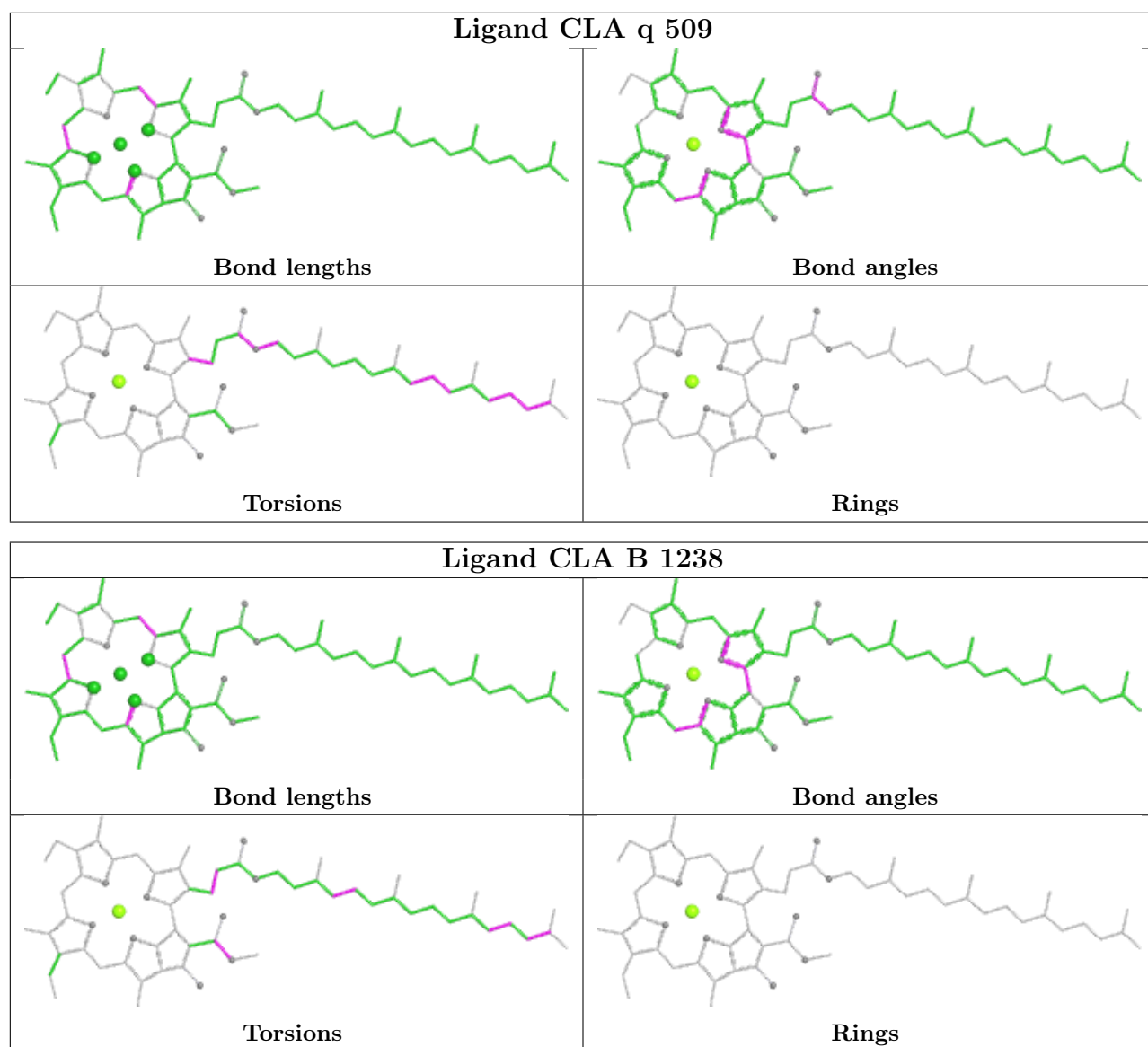
## Ligand CLA y 502



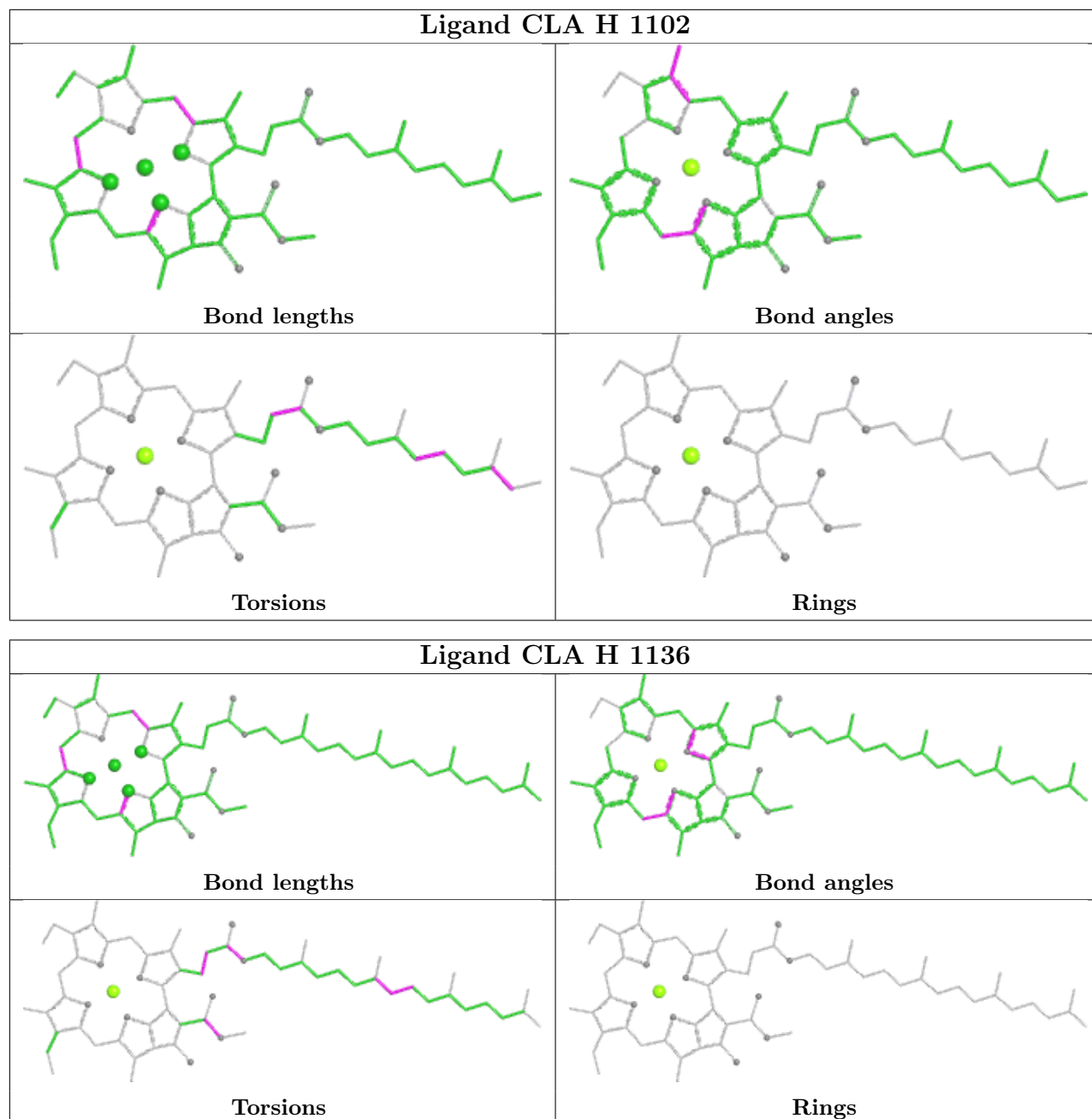






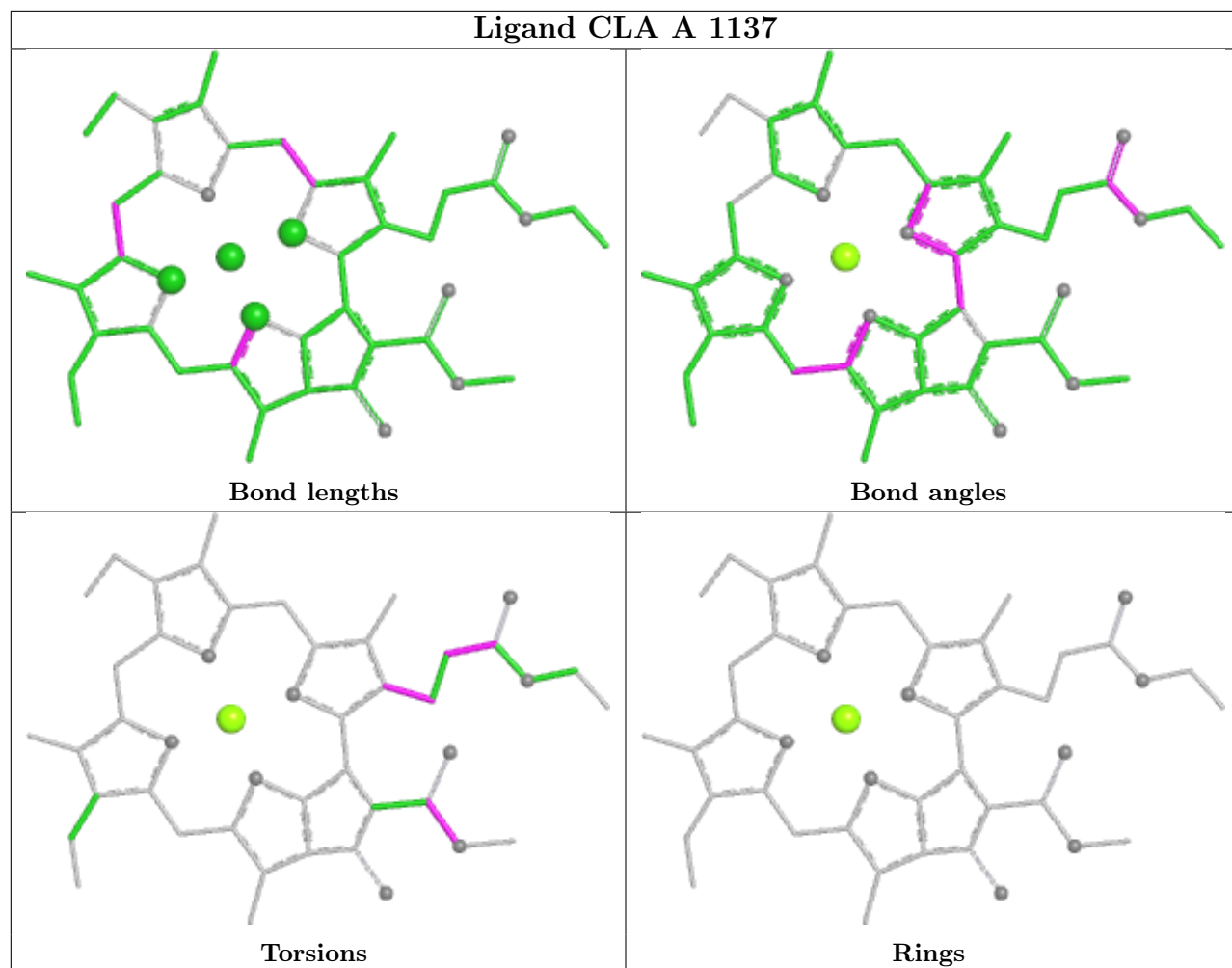






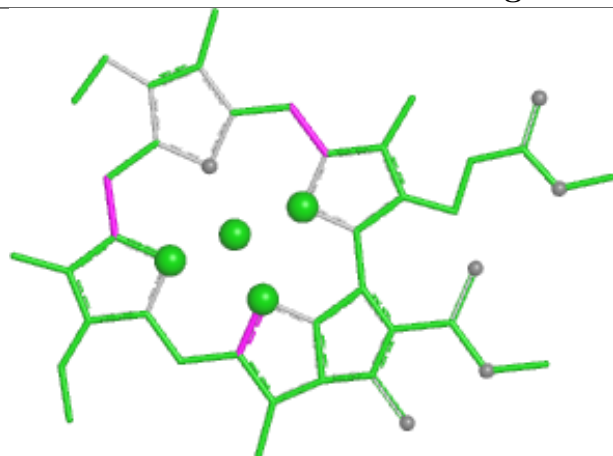


## Ligand CLA A 1137

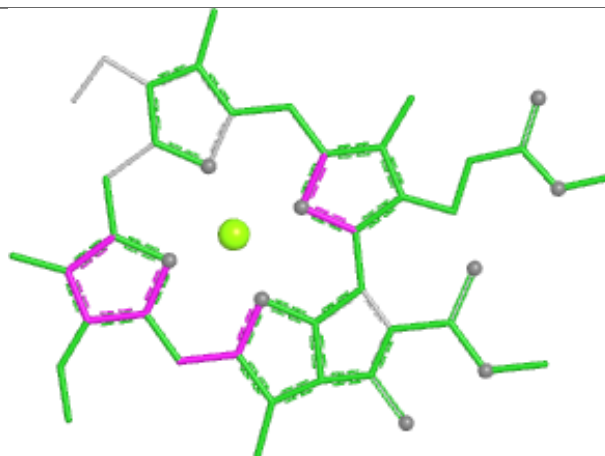




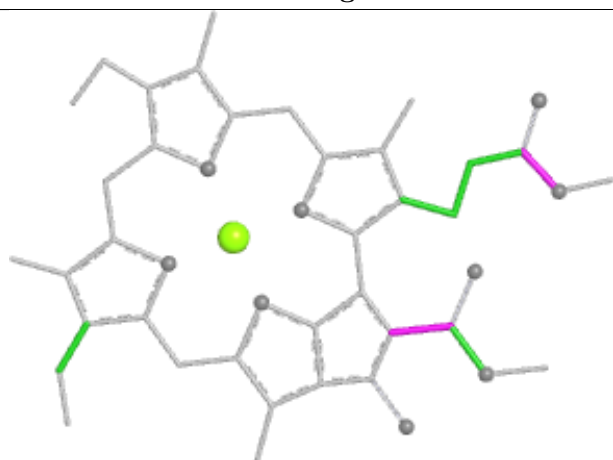
## Ligand CLA H 1801



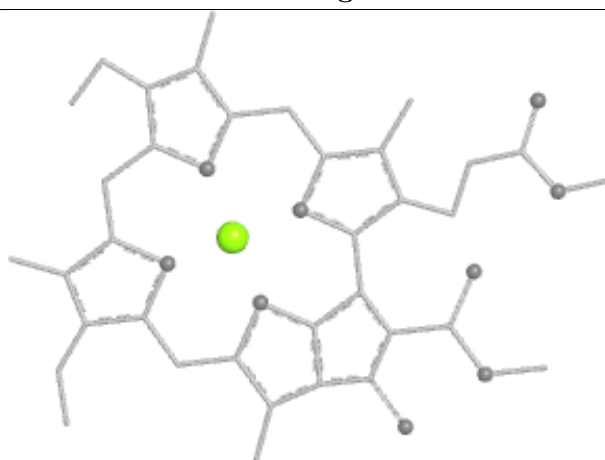
Bond lengths



Bond angles

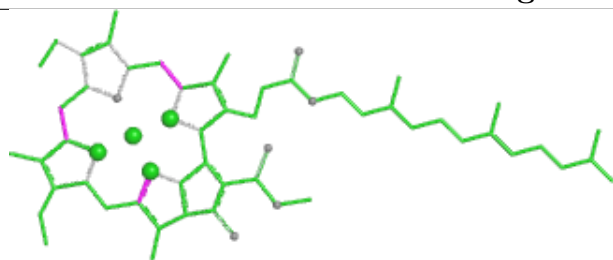


Torsions

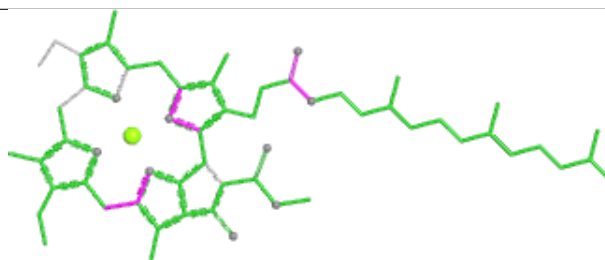


Rings

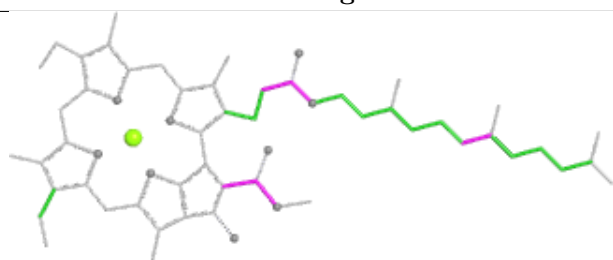
## Ligand CLA u 510



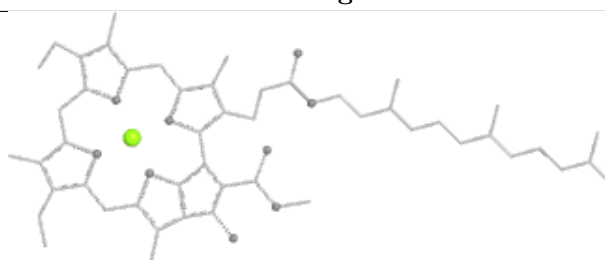
Bond lengths



Bond angles



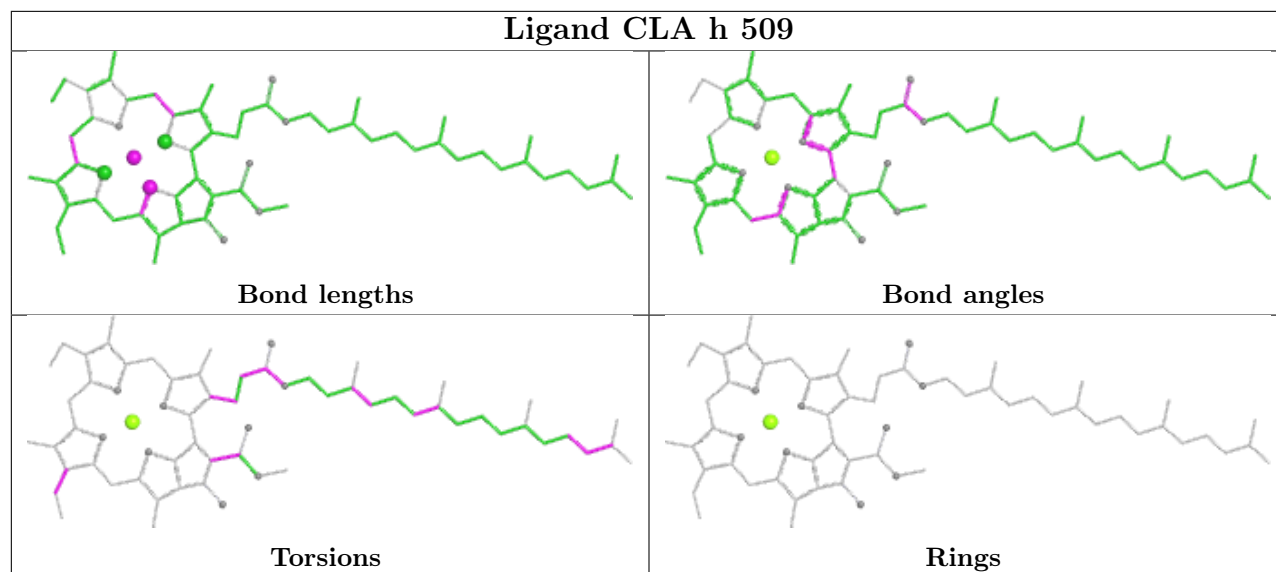
Torsions



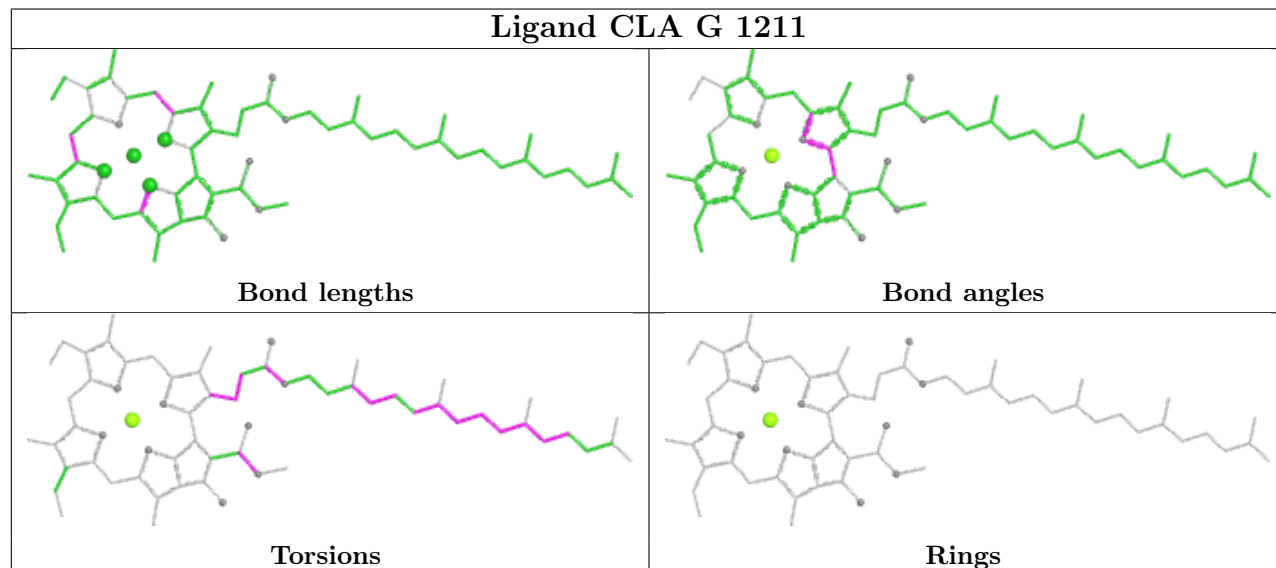
Rings



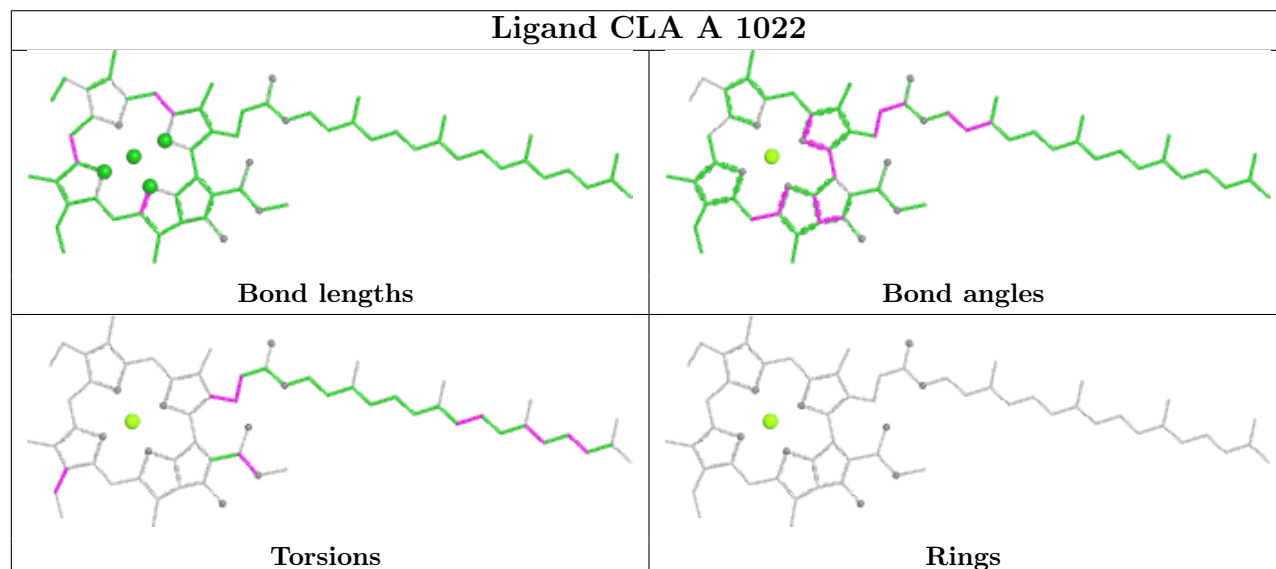
## Ligand CLA h 509



## Ligand CLA G 1211

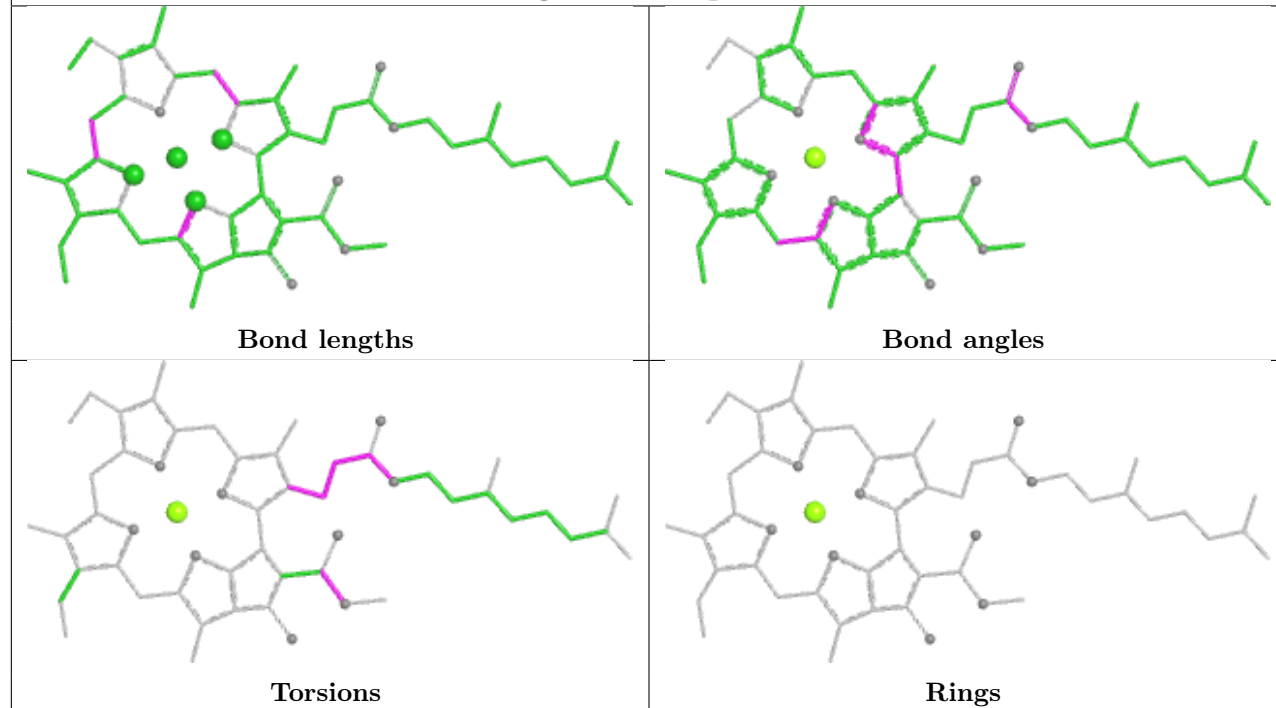


## Ligand CLA A 1022

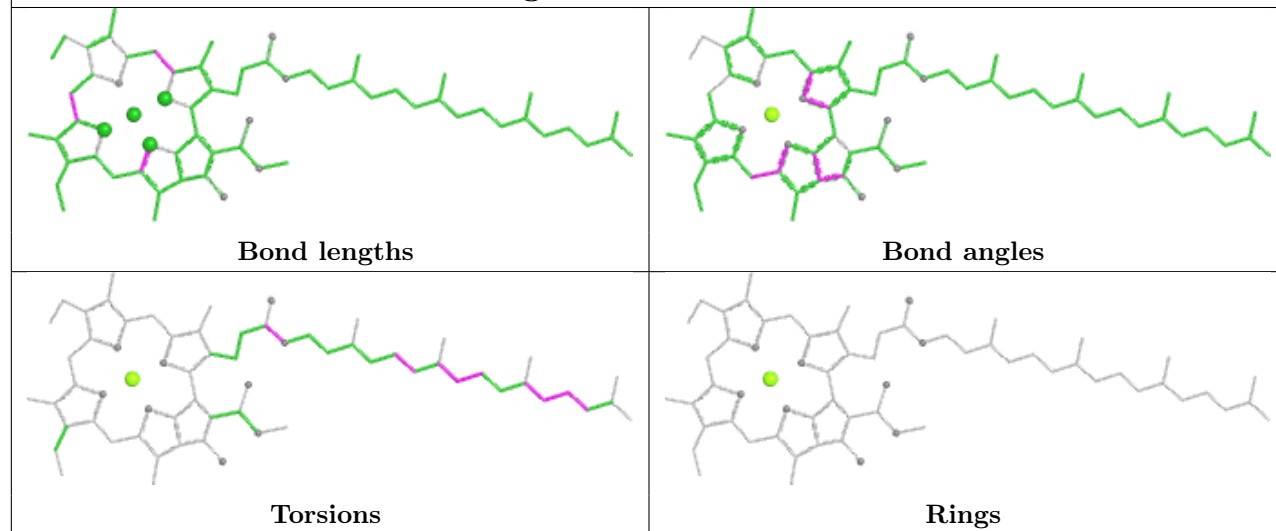




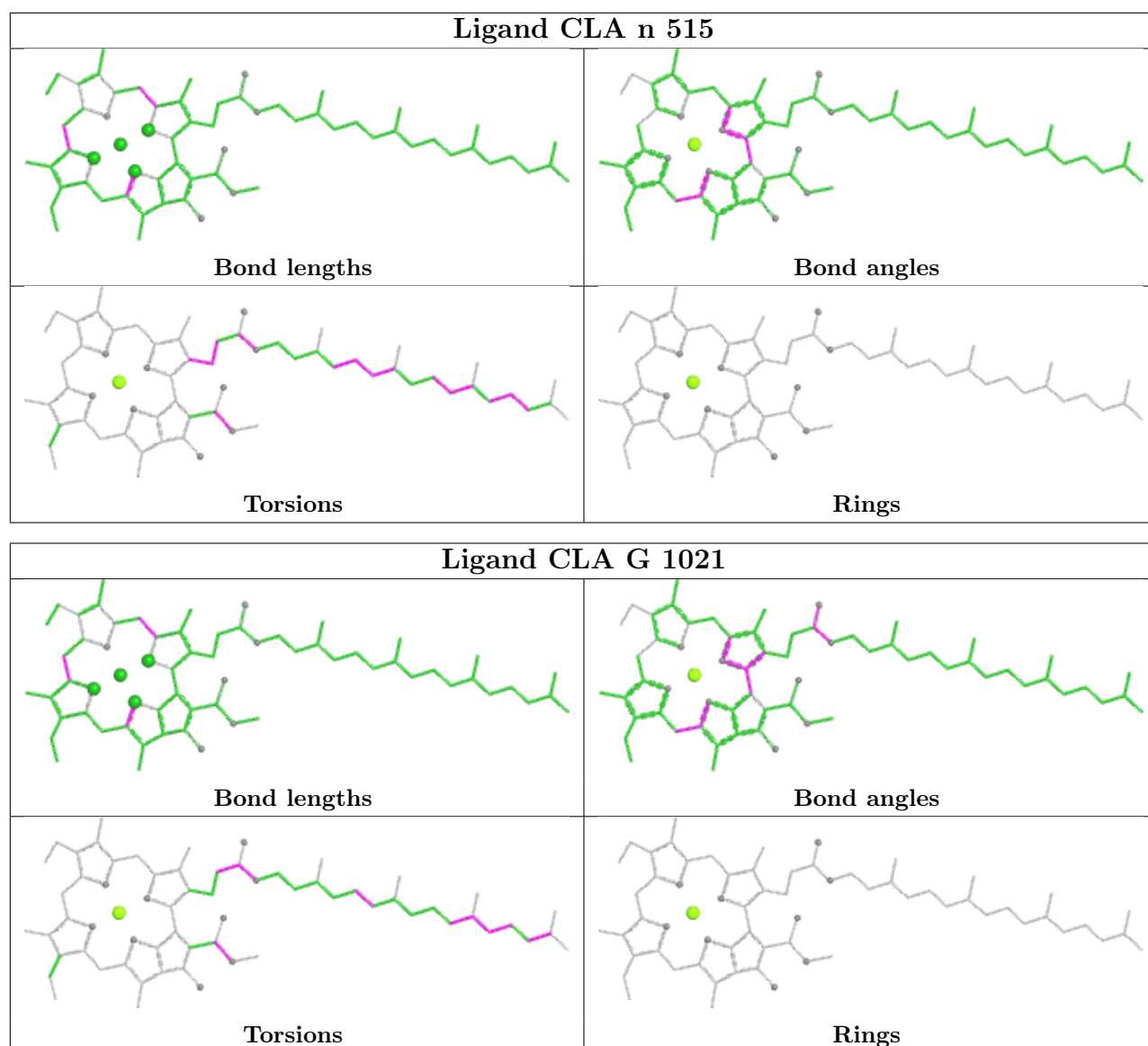
## Ligand CLA p 508



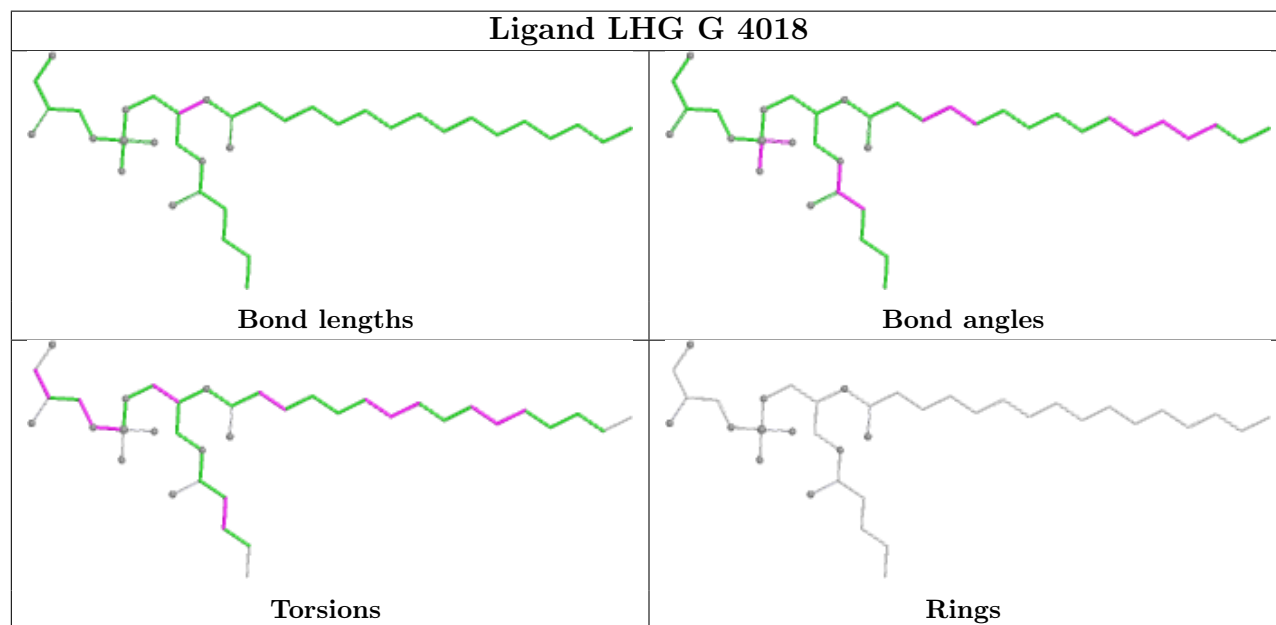
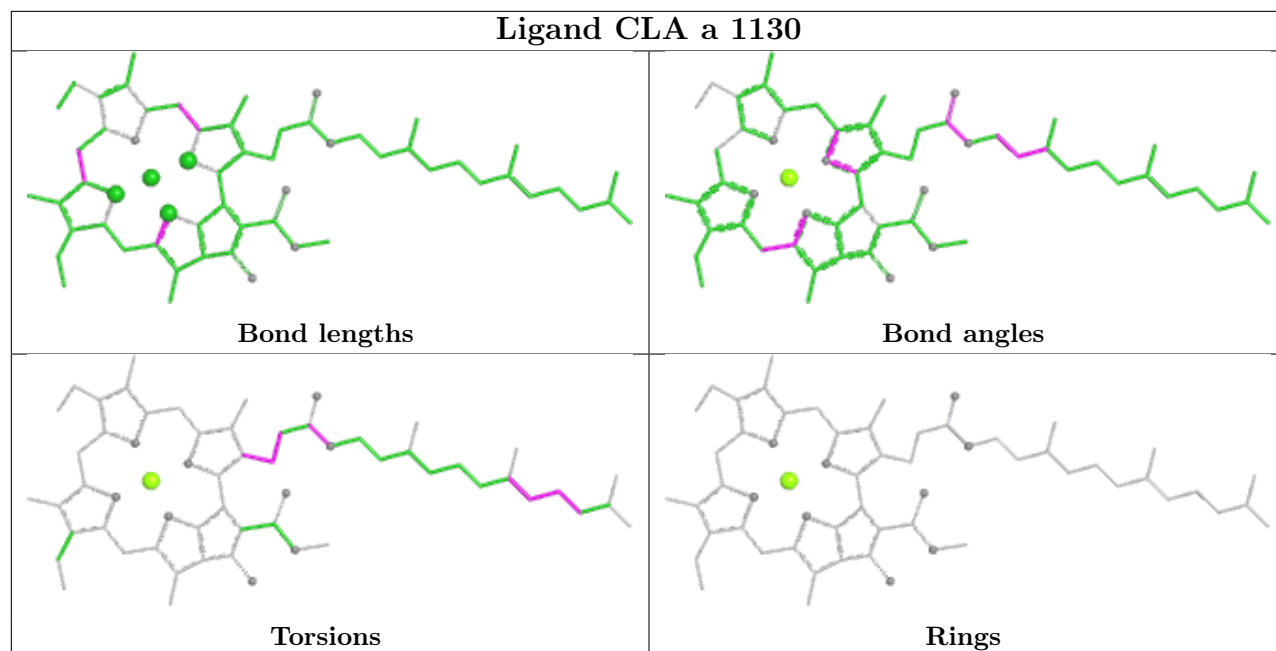
## Ligand CLA A 1125



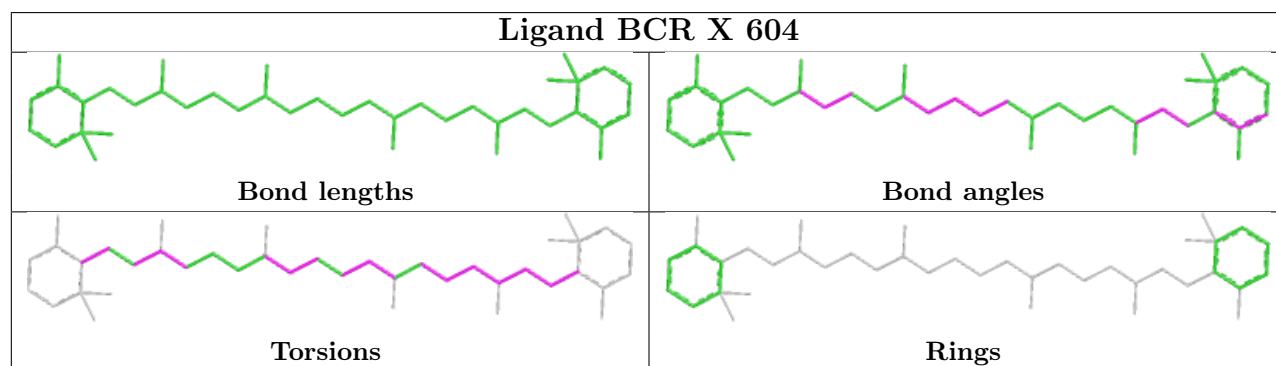
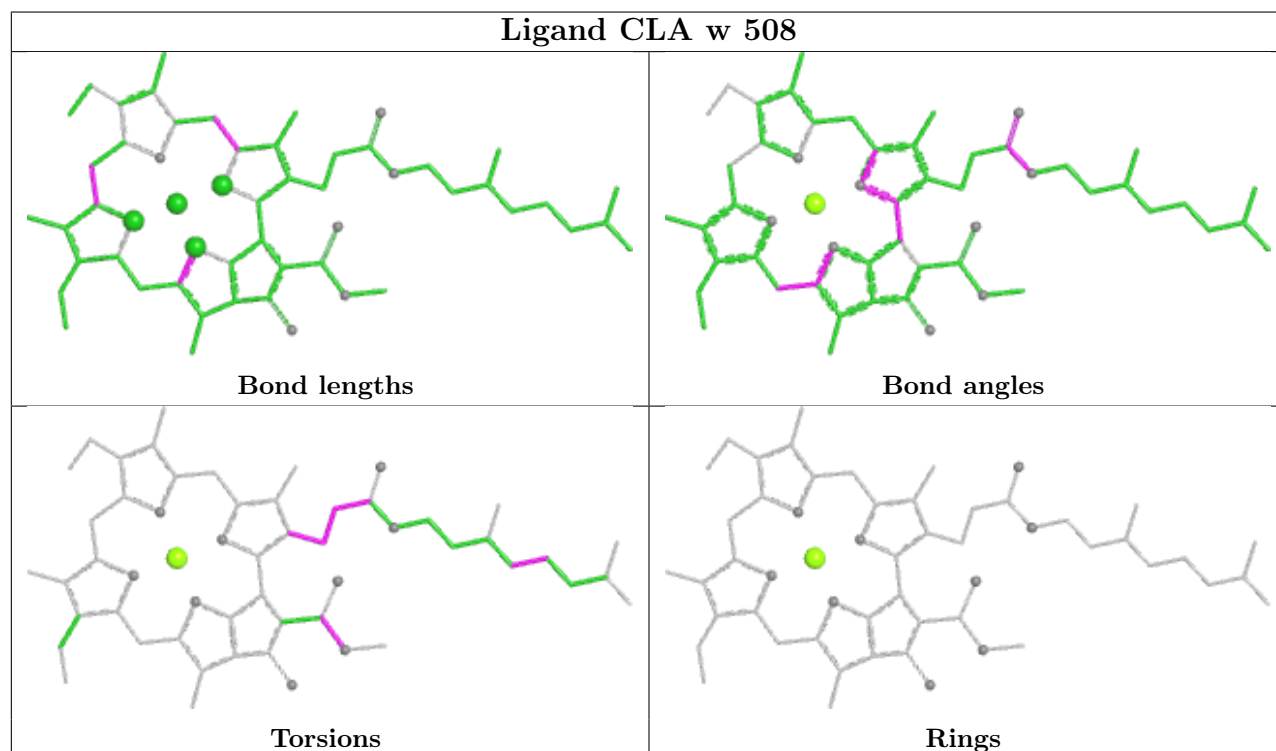
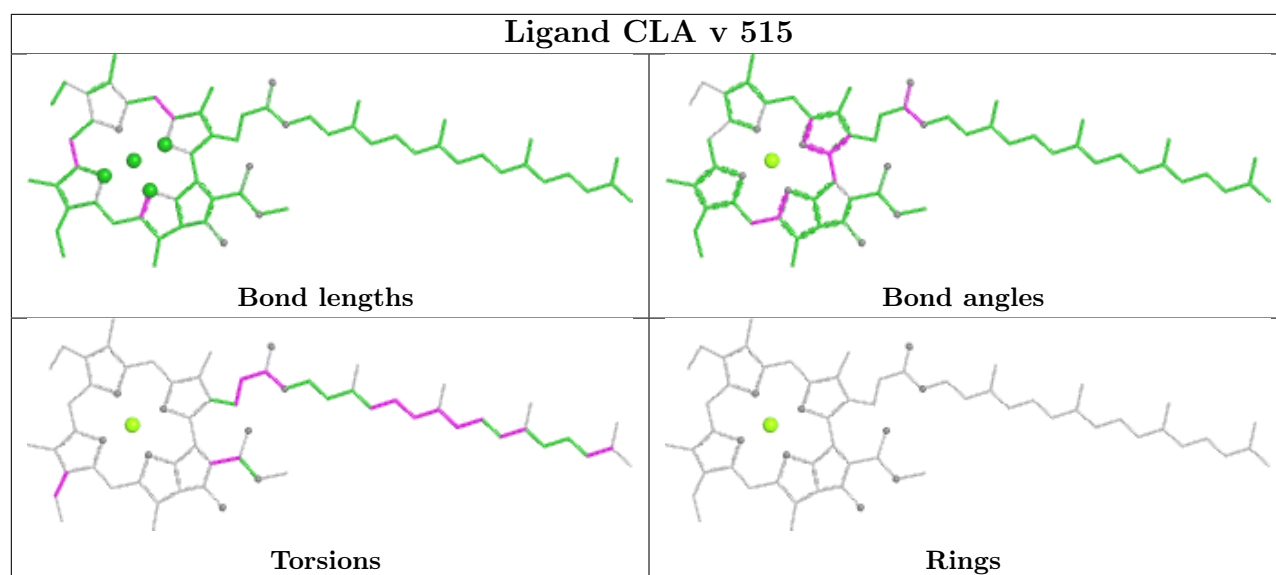




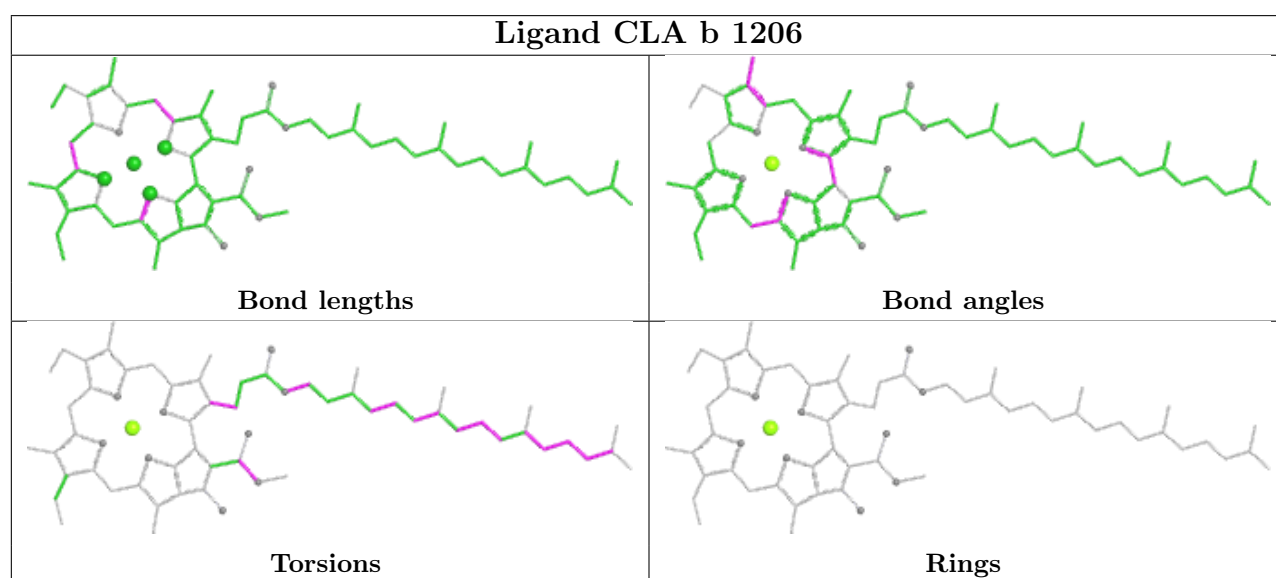
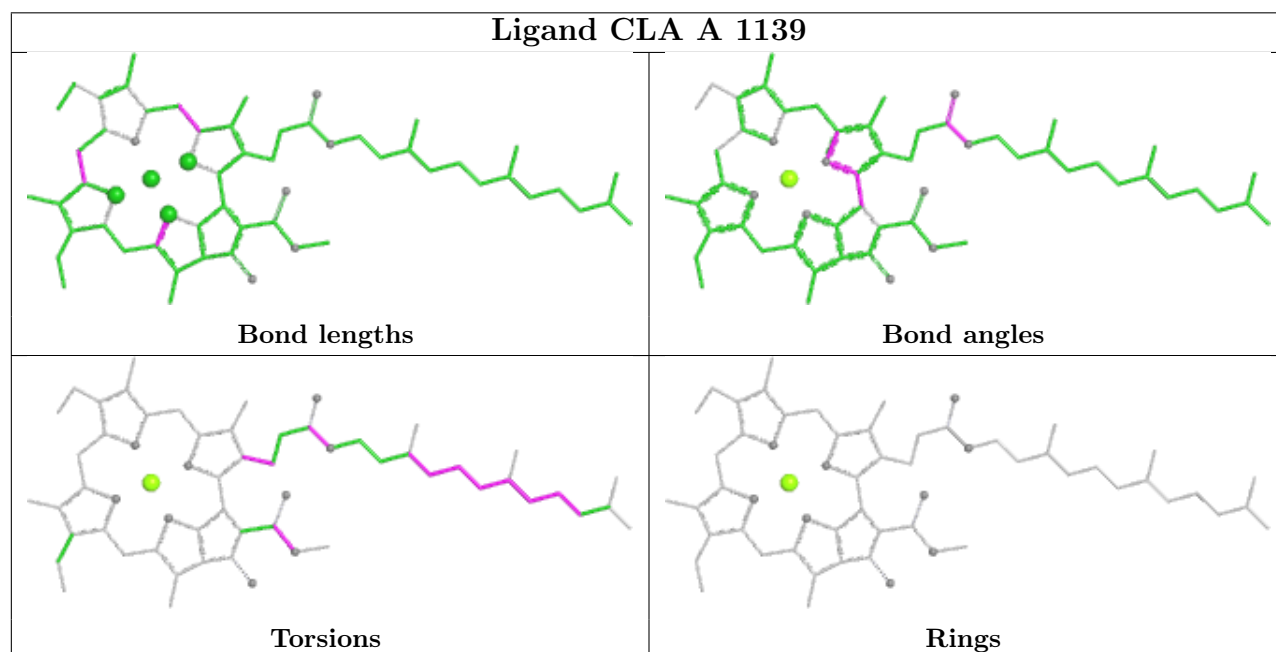
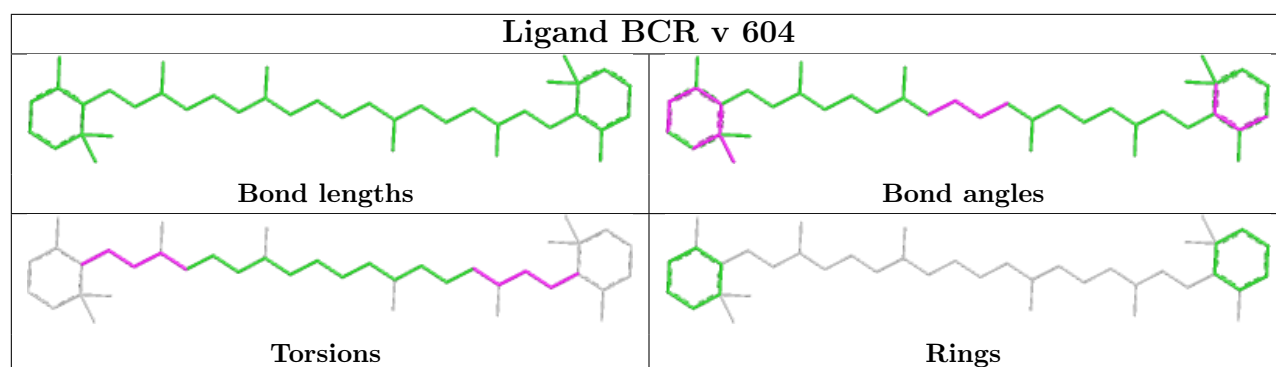




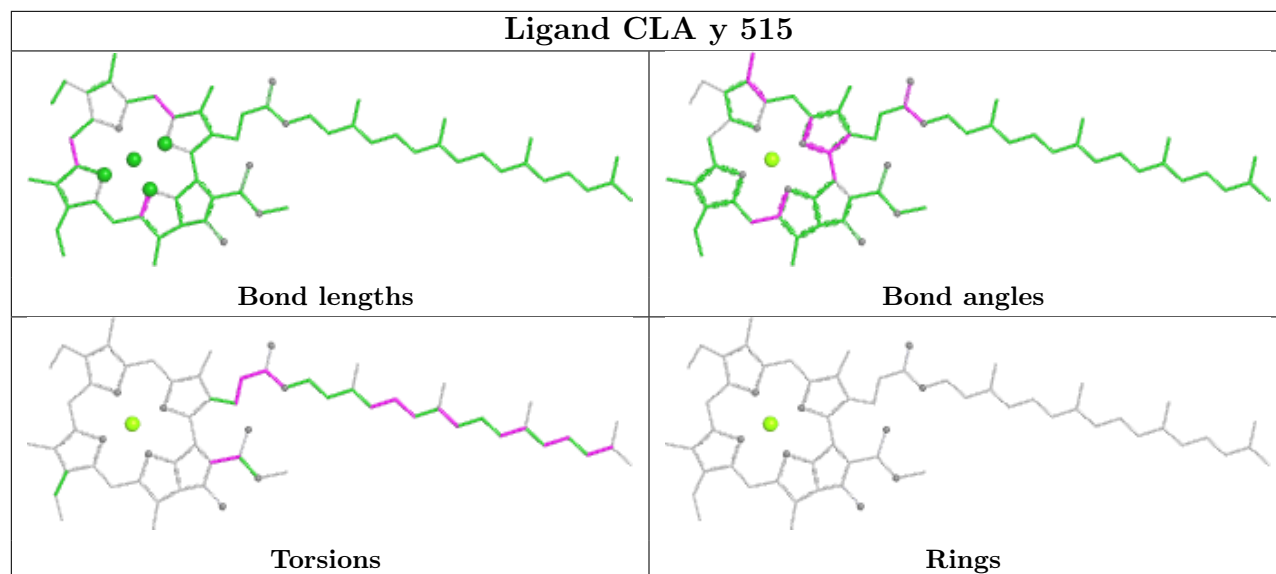
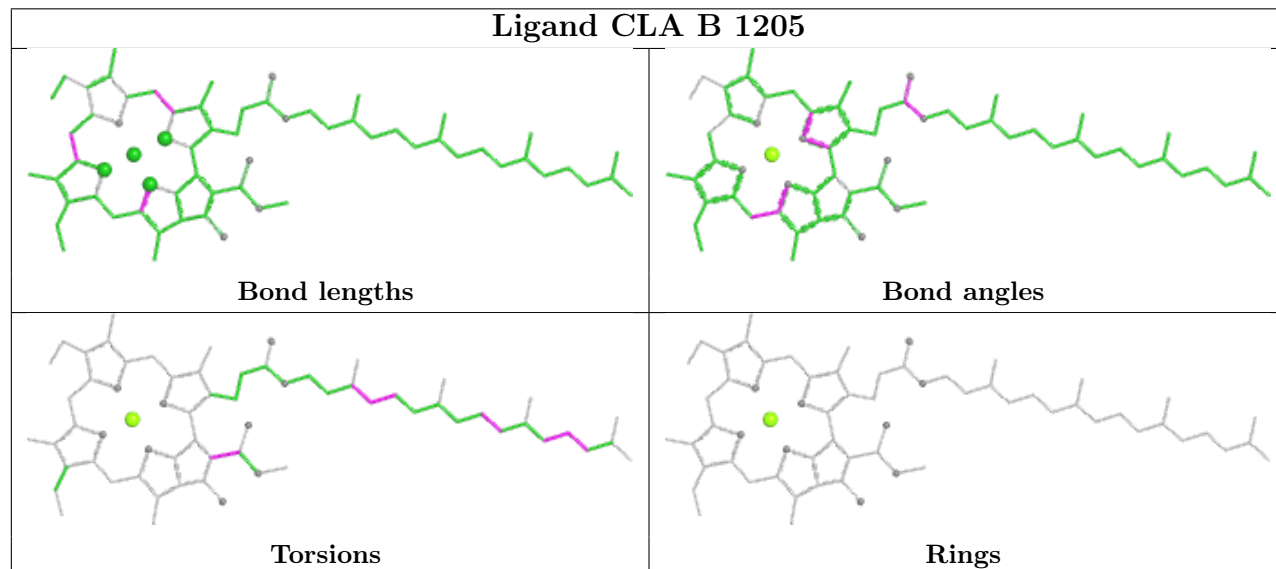






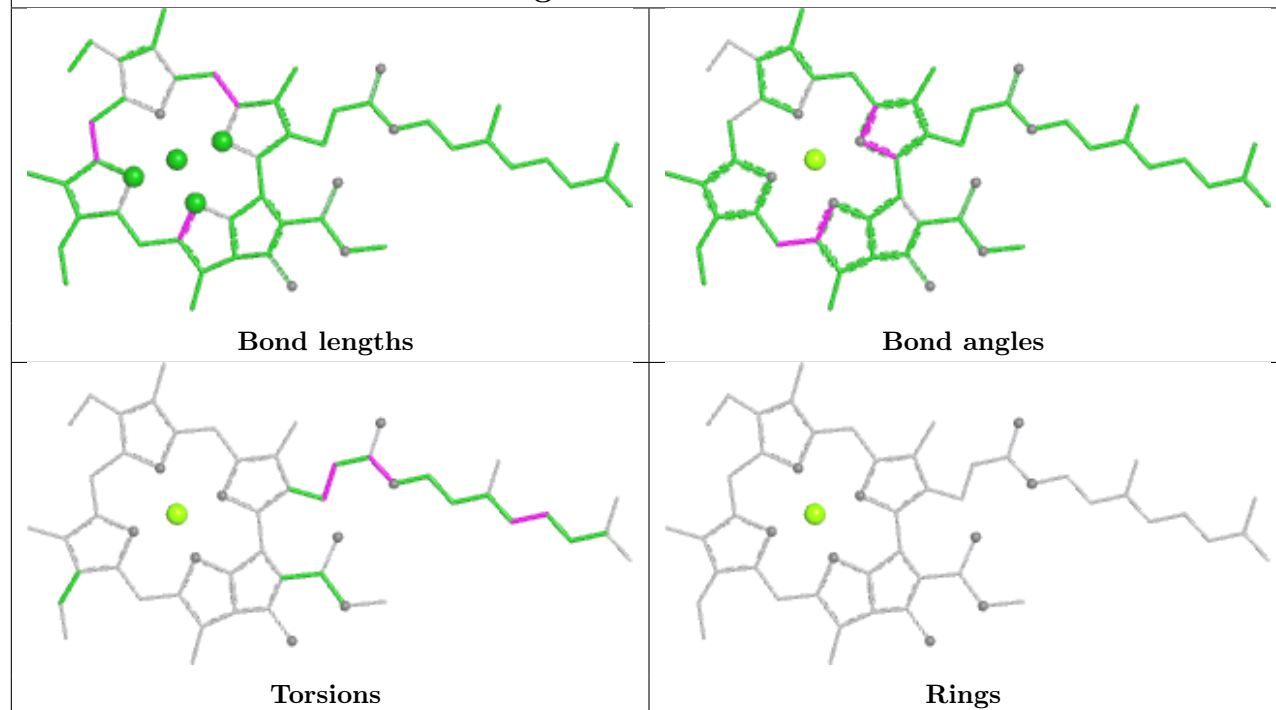




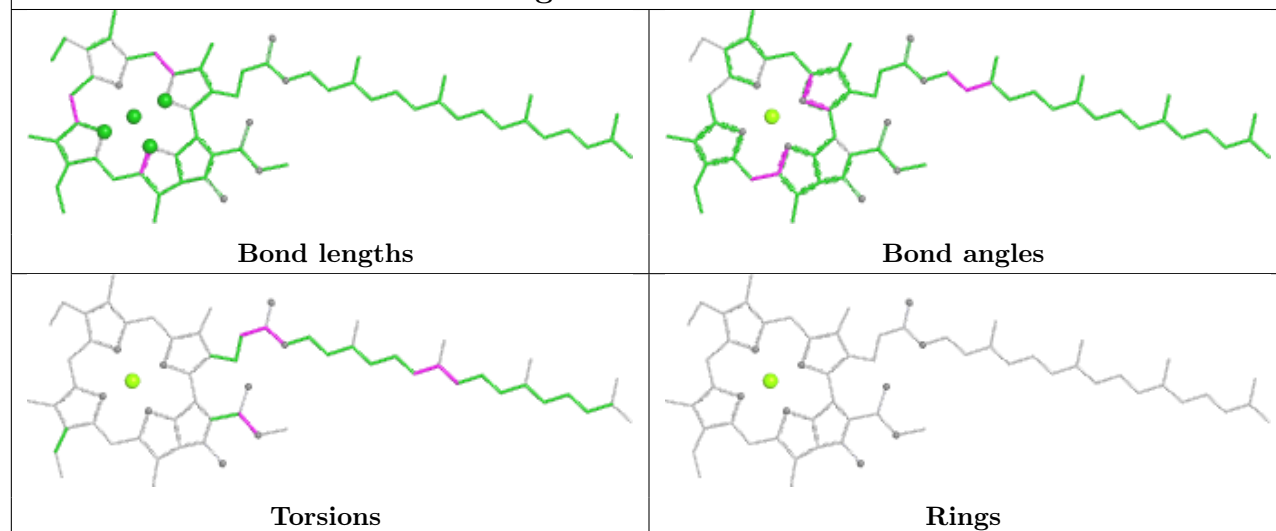
**Ligand CLA y 515****Ligand CLA B 1205**



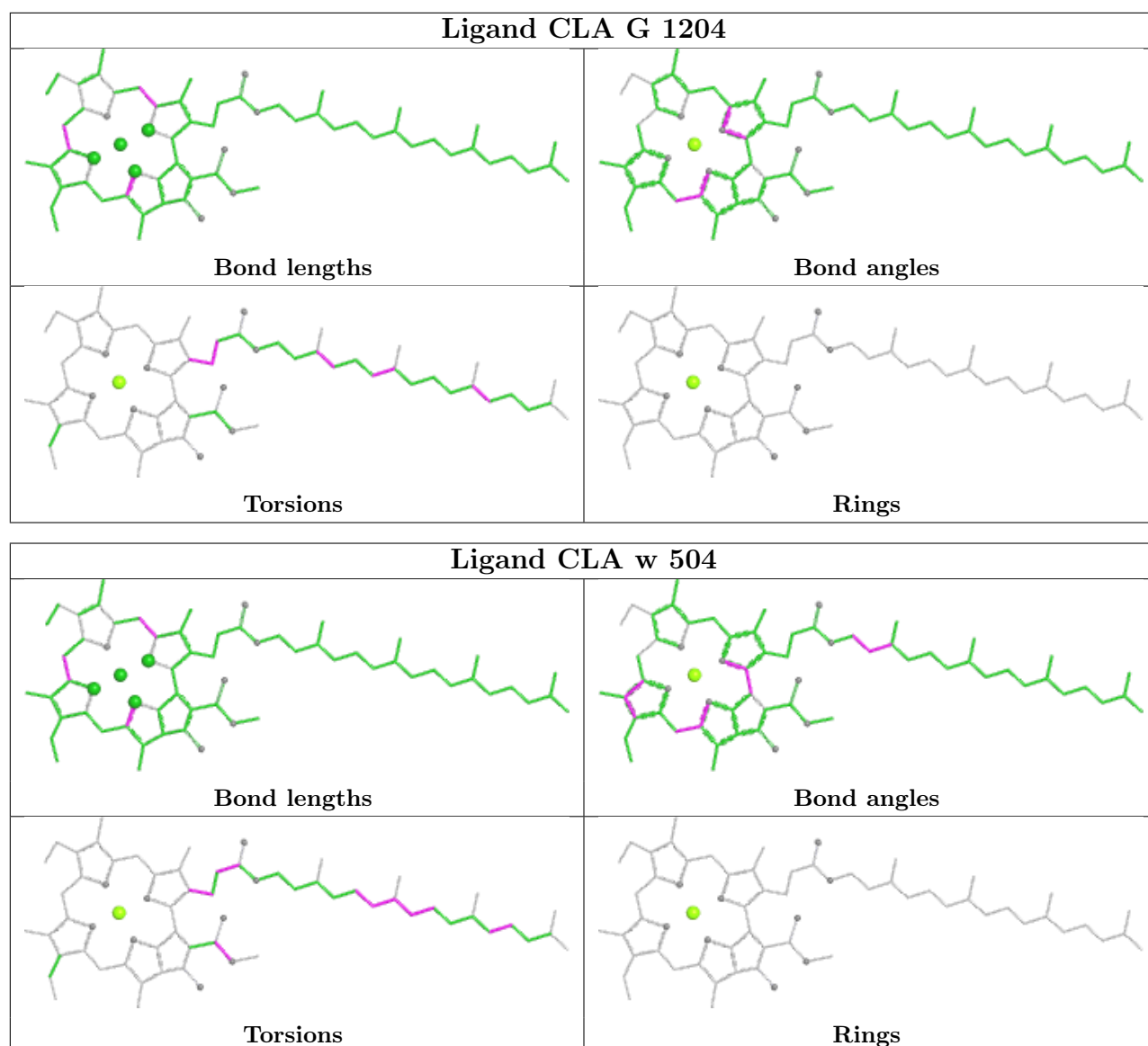
## Ligand CLA Z 517



## Ligand CLA u 507

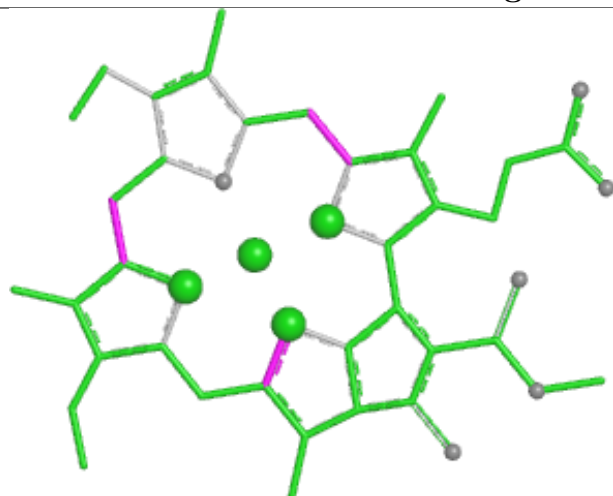




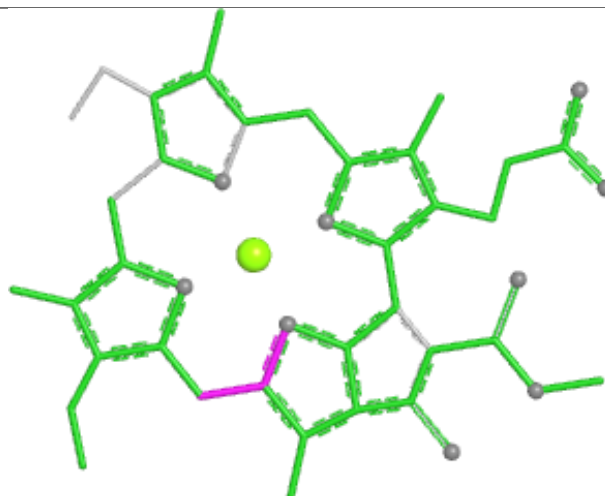




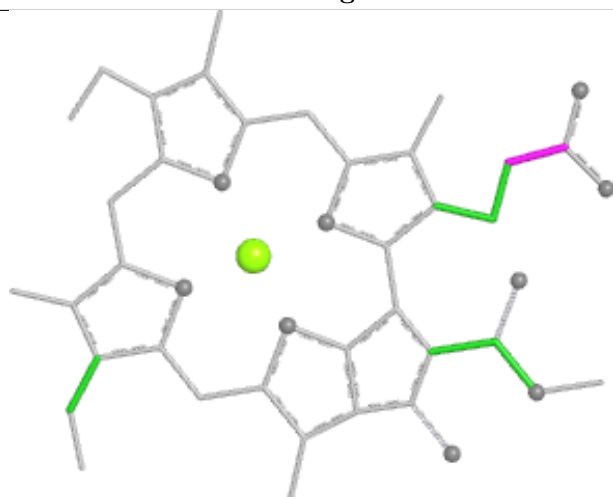
## Ligand CLA H 1134



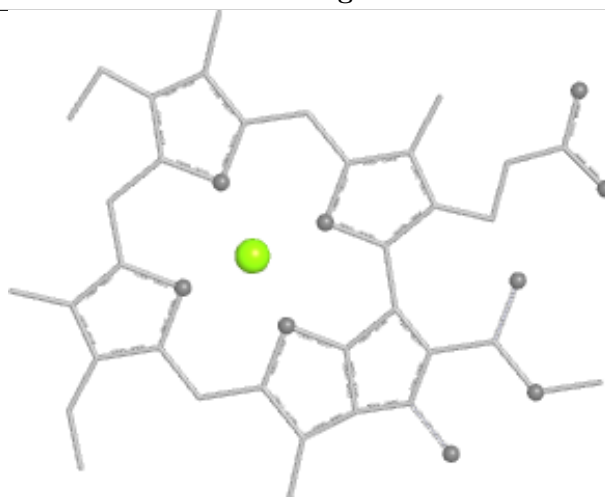
Bond lengths



Bond angles

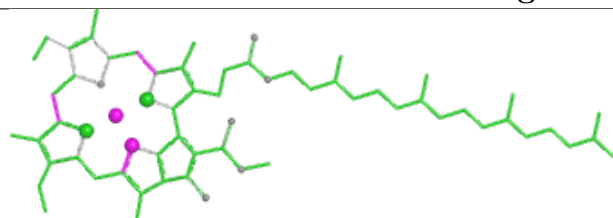


Torsions

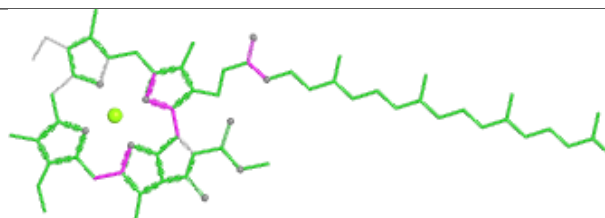


Rings

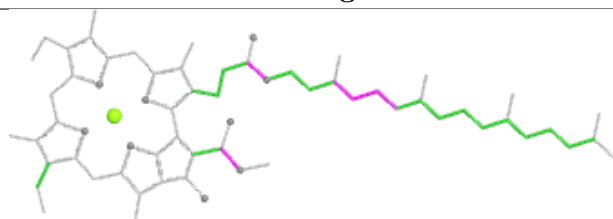
## Ligand CLA x 512



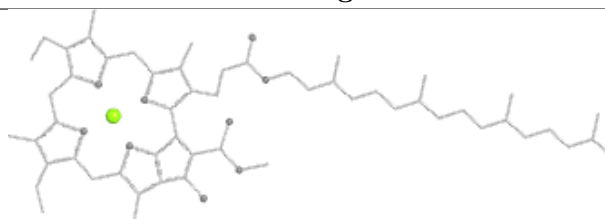
Bond lengths



Bond angles

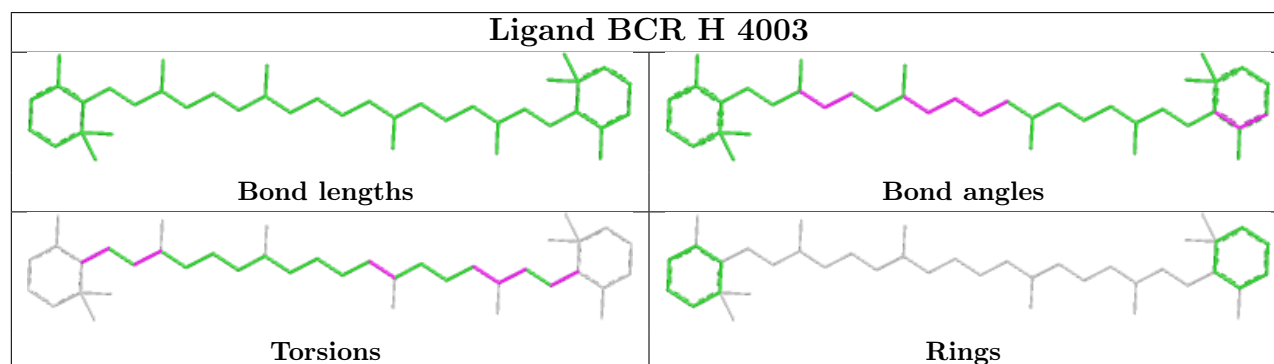
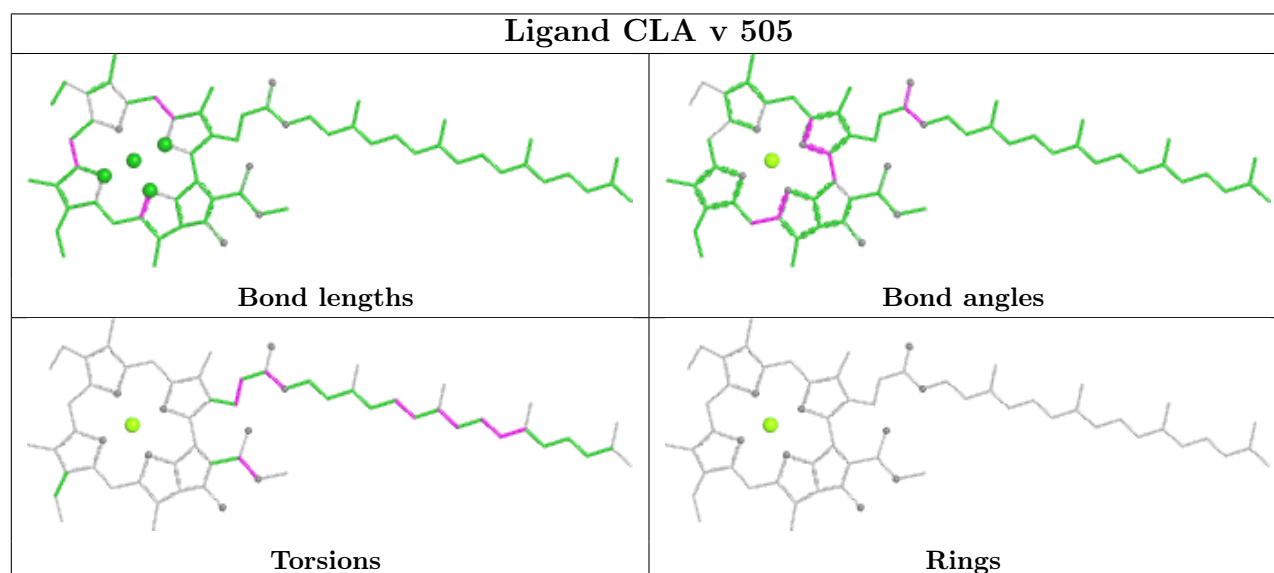
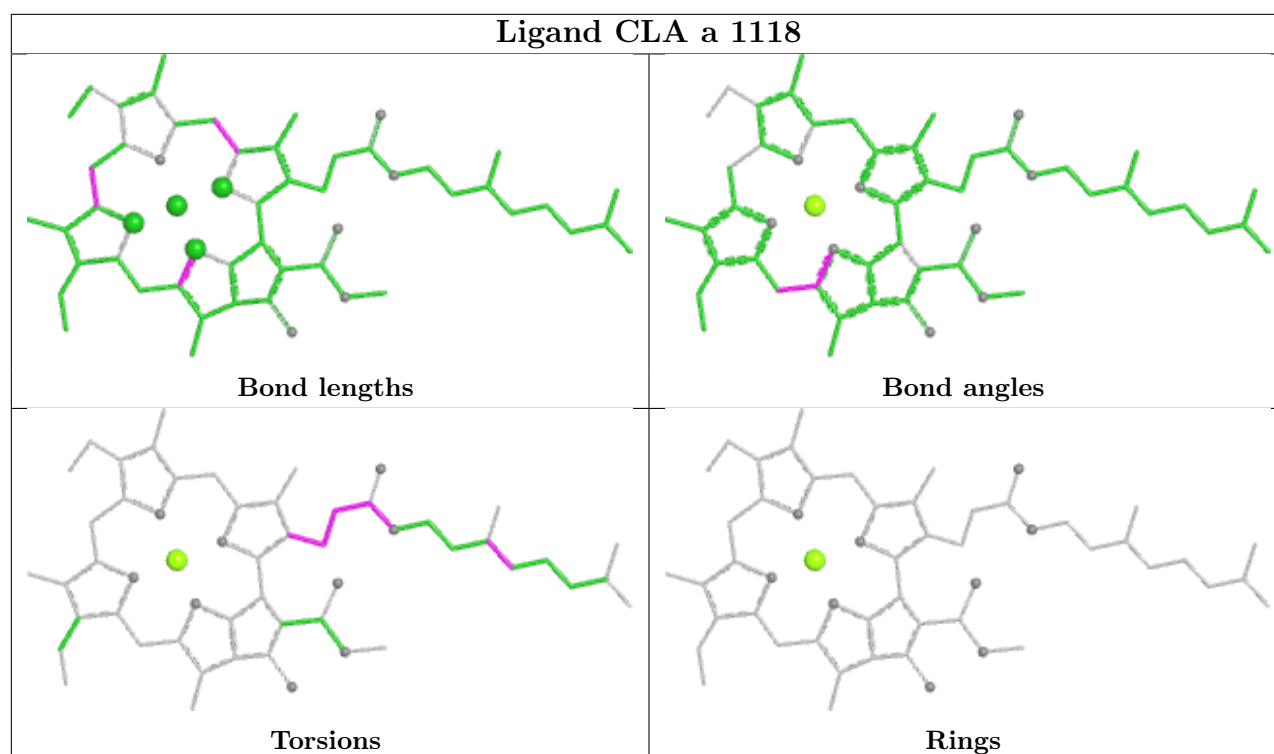


Torsions

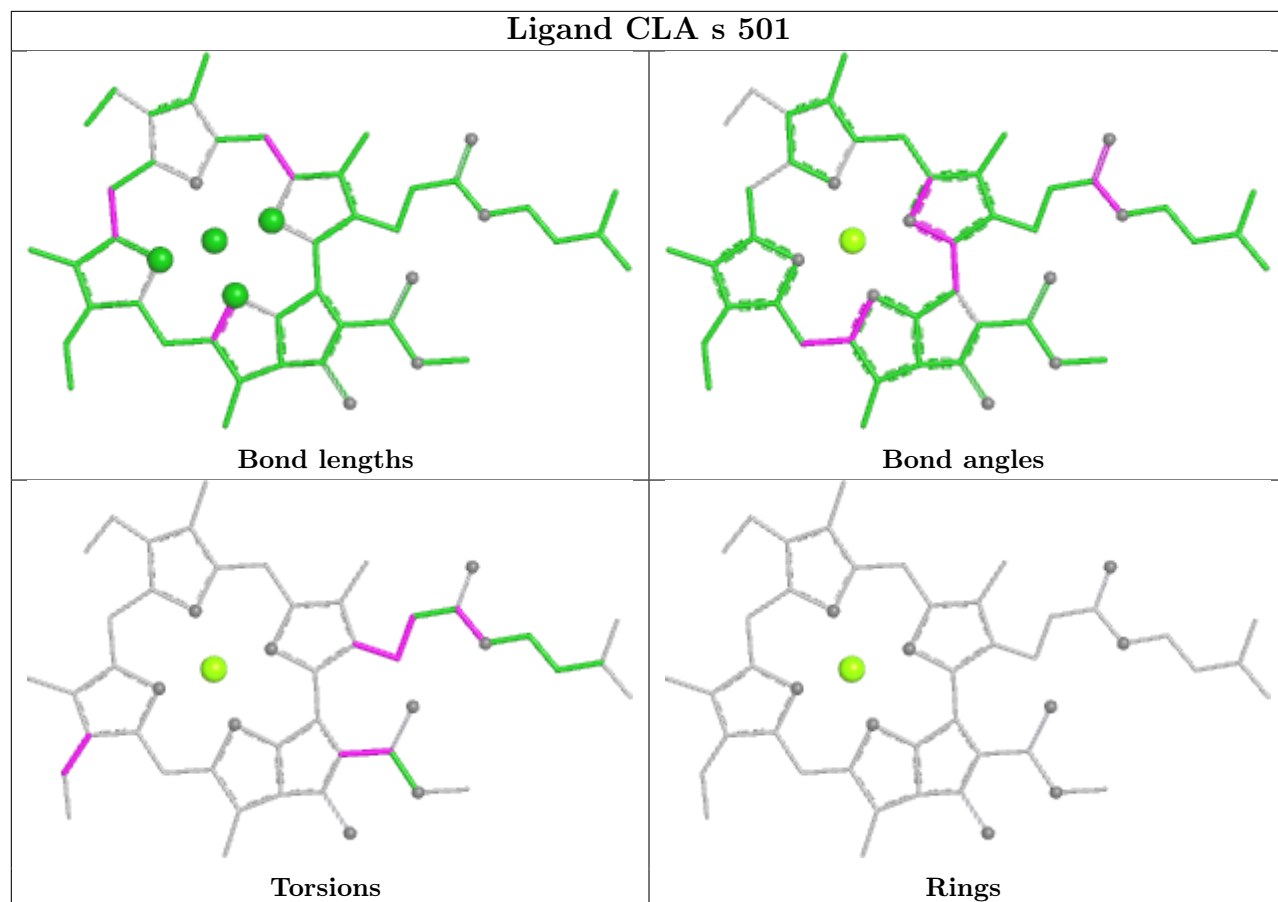


Rings

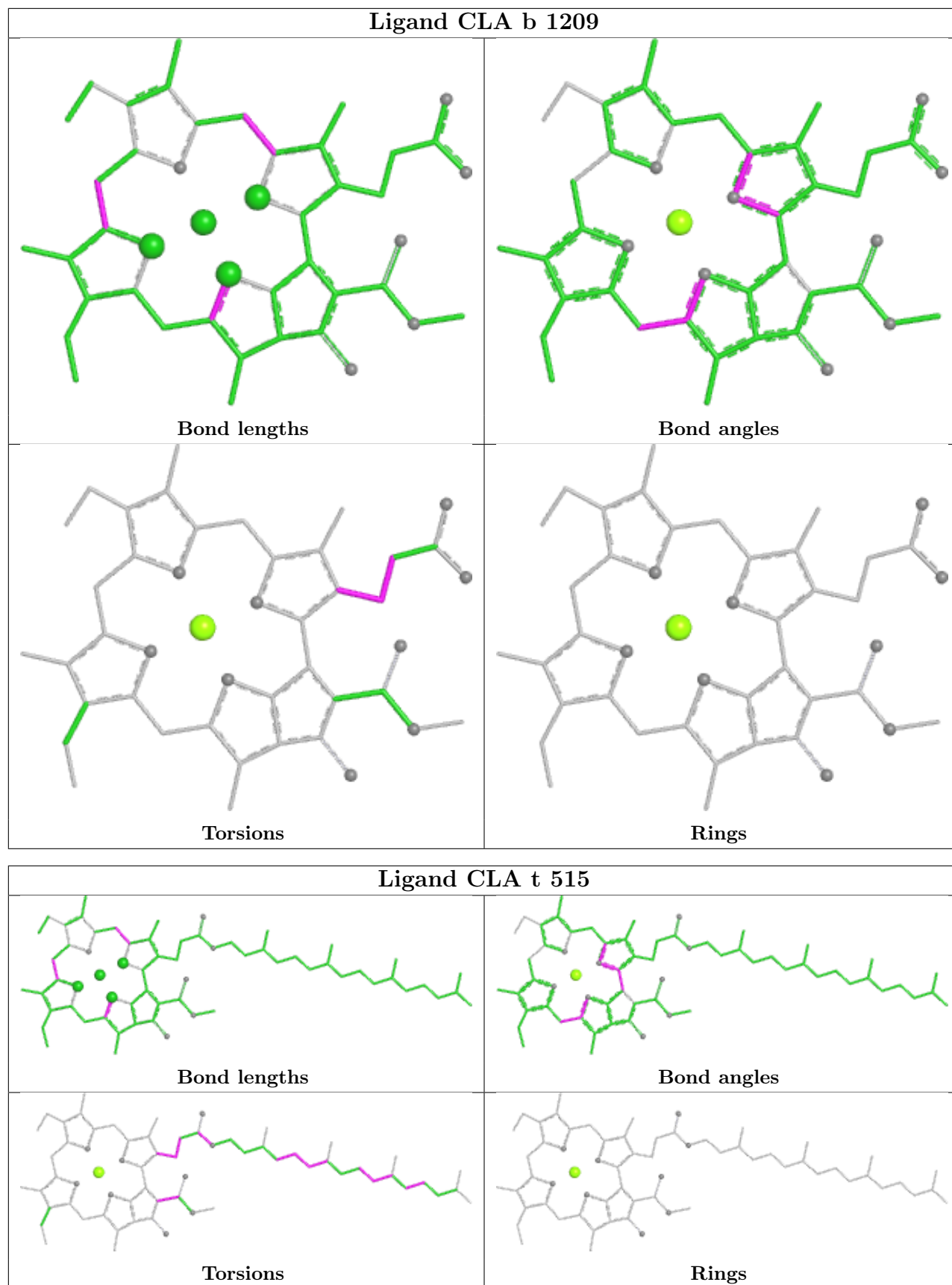




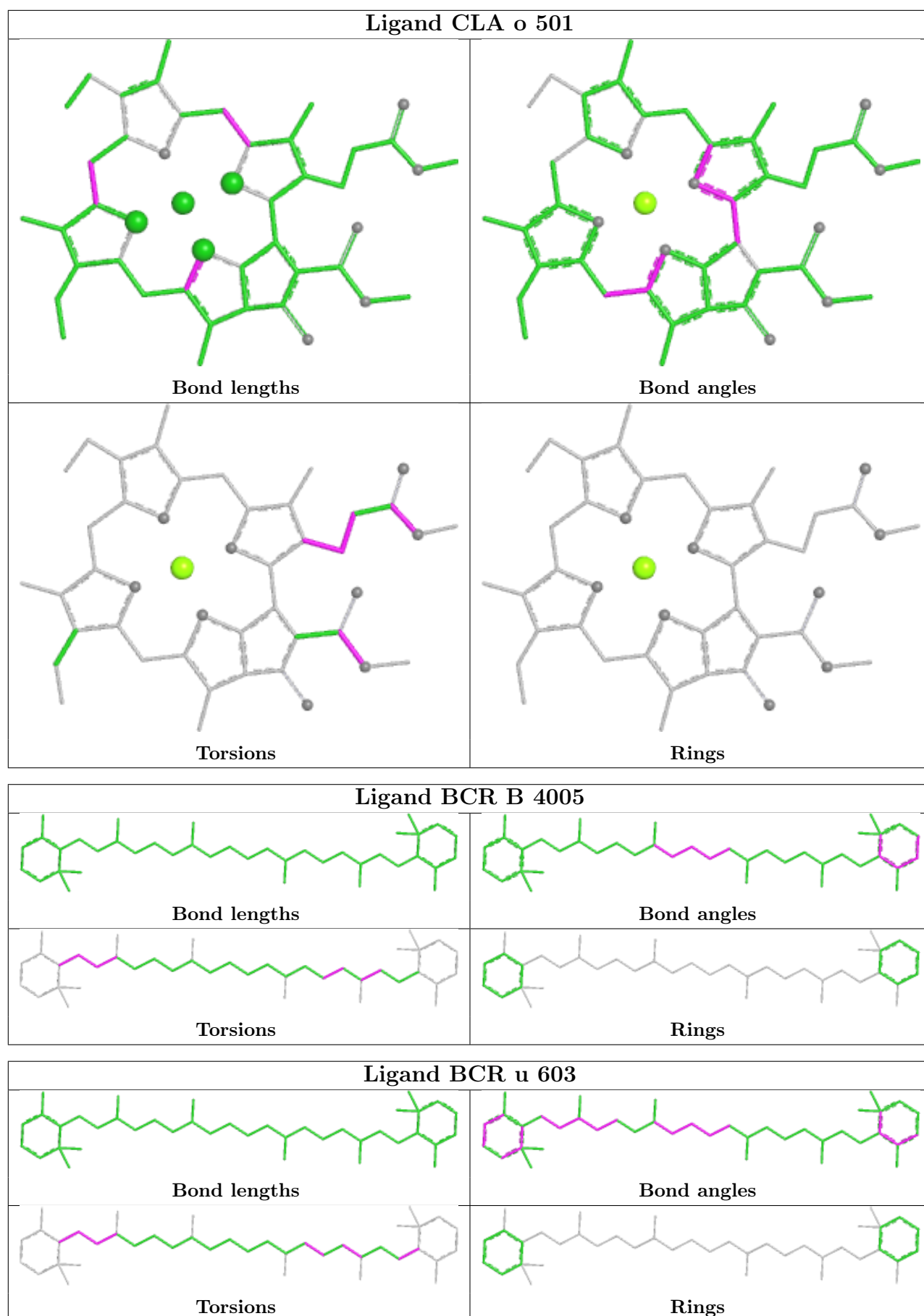




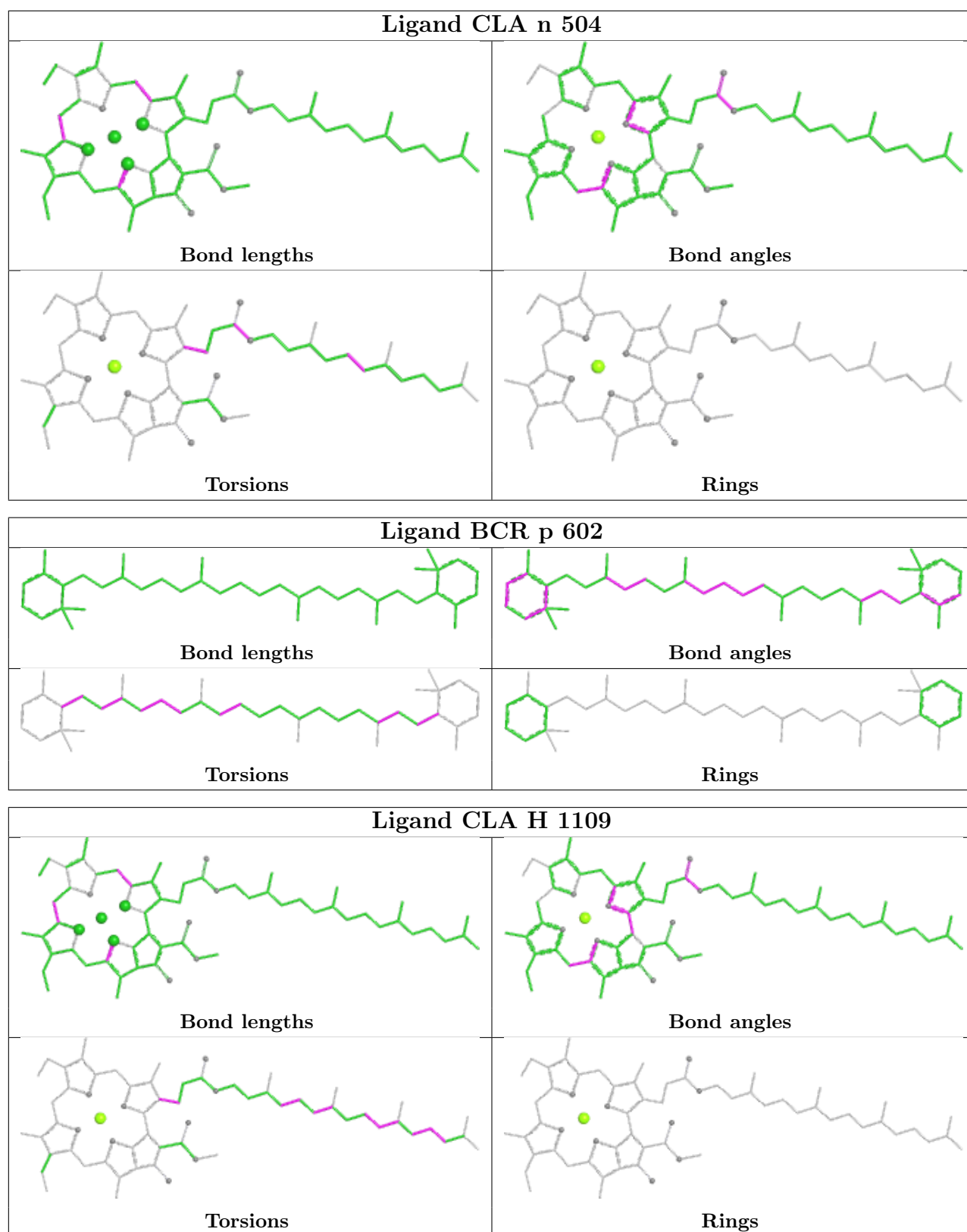




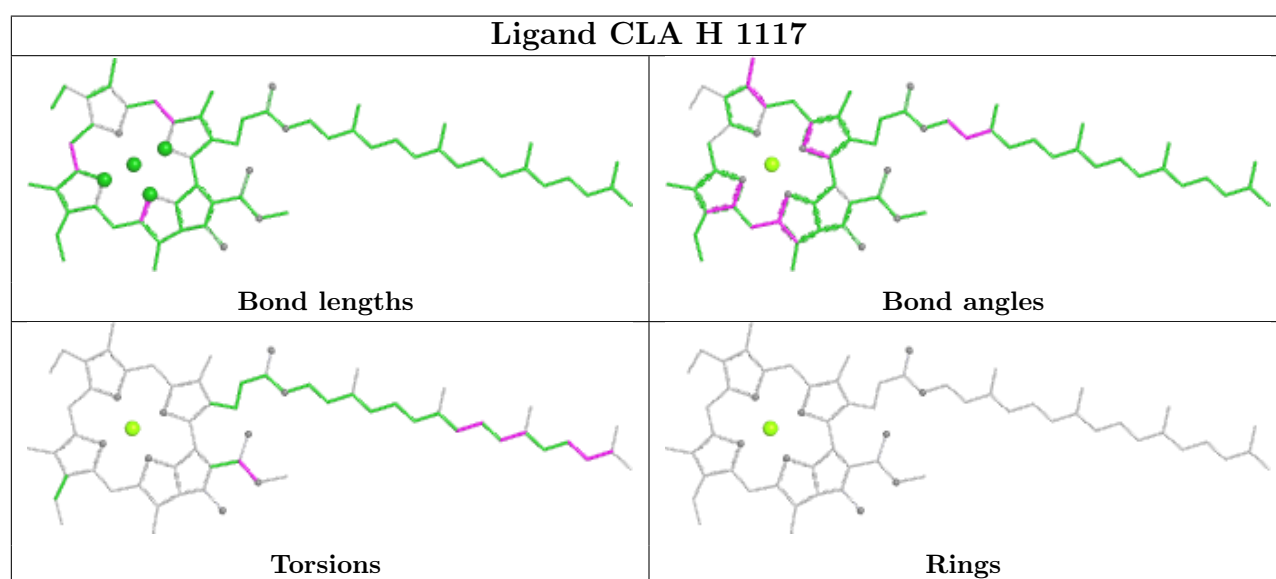
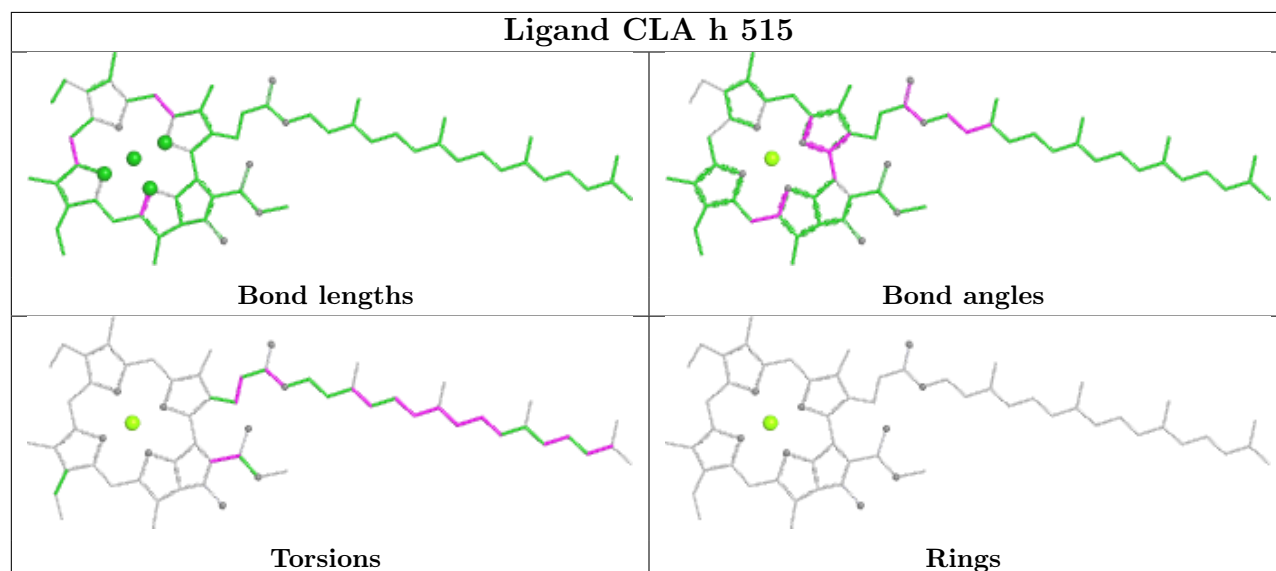
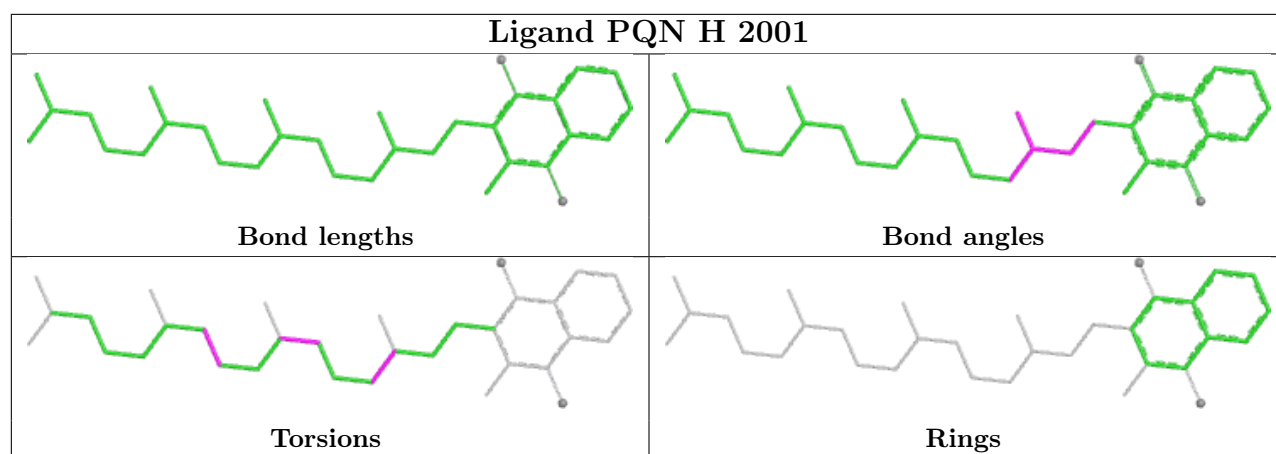






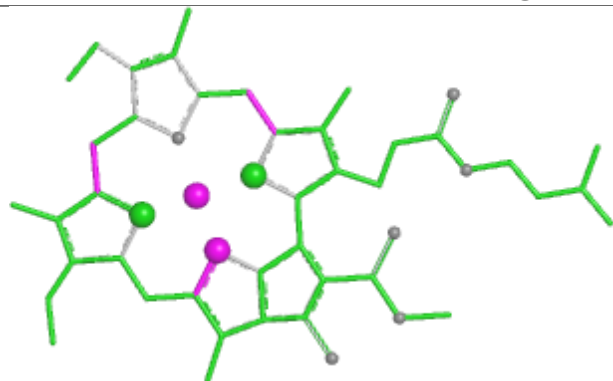




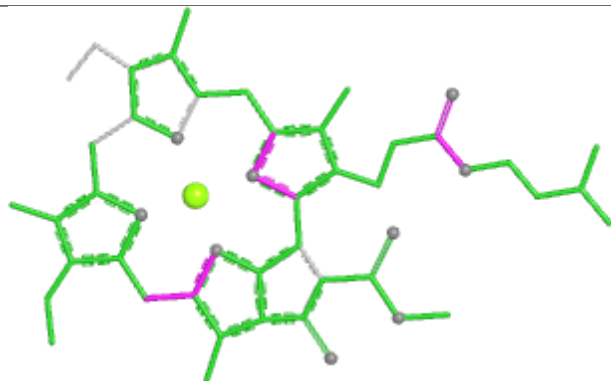




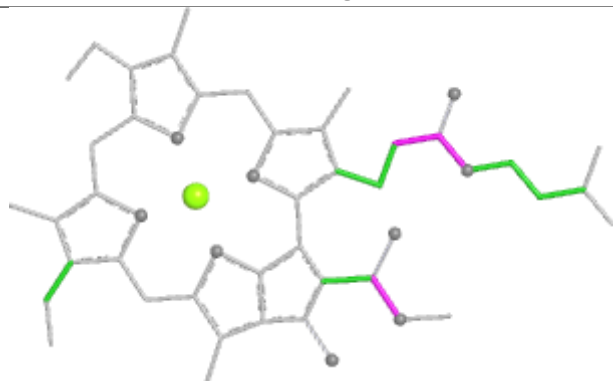
## Ligand CLA Z 502



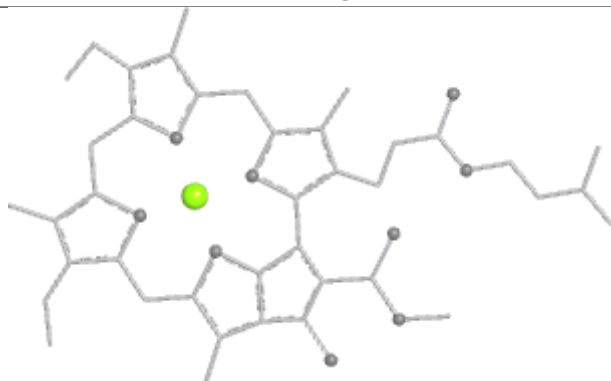
Bond lengths



Bond angles

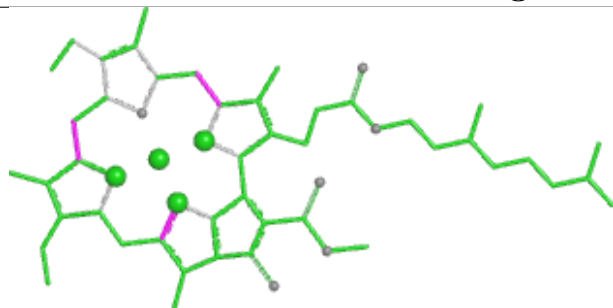


Torsions

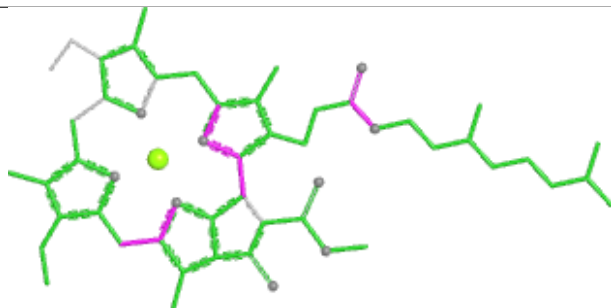


Rings

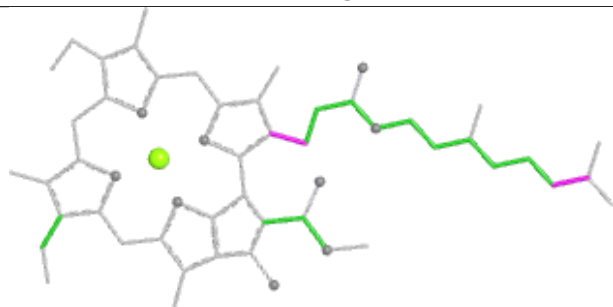
## Ligand CLA a 1139



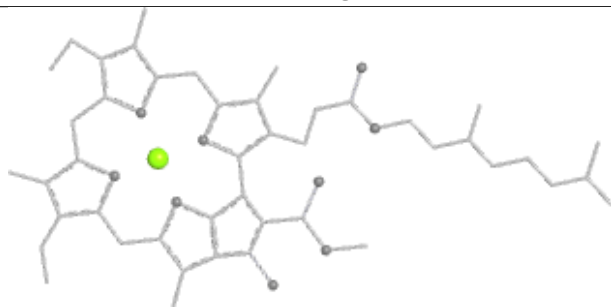
Bond lengths



Bond angles

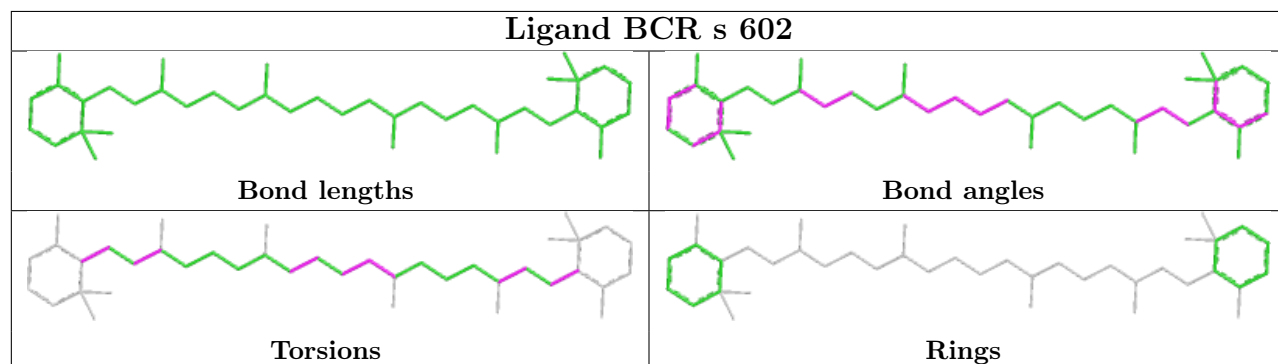
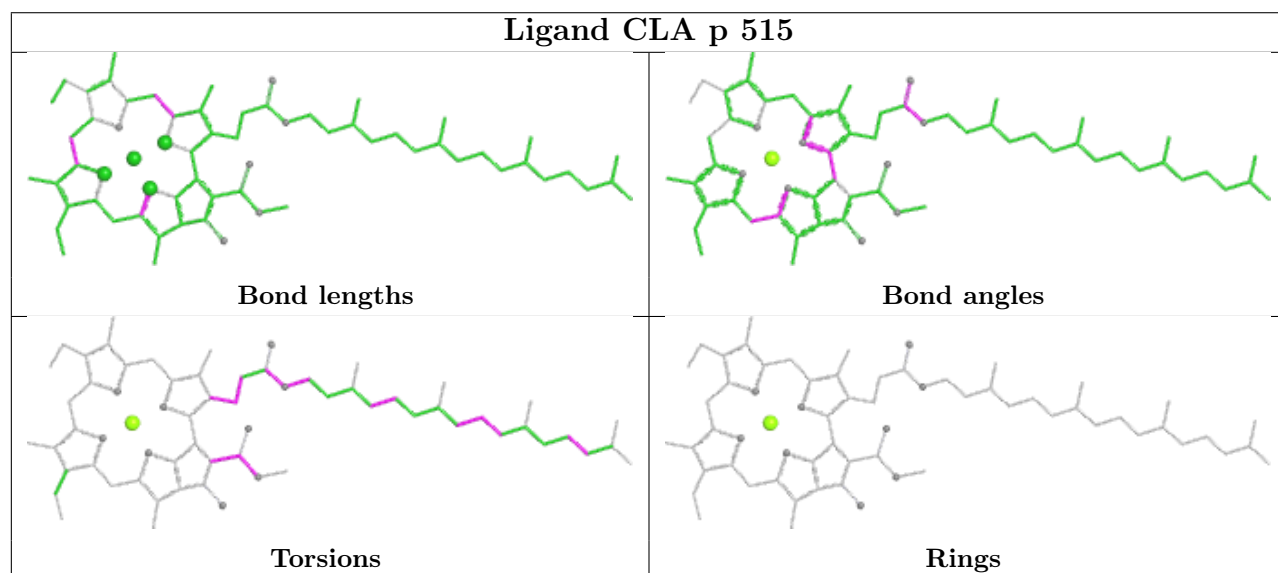
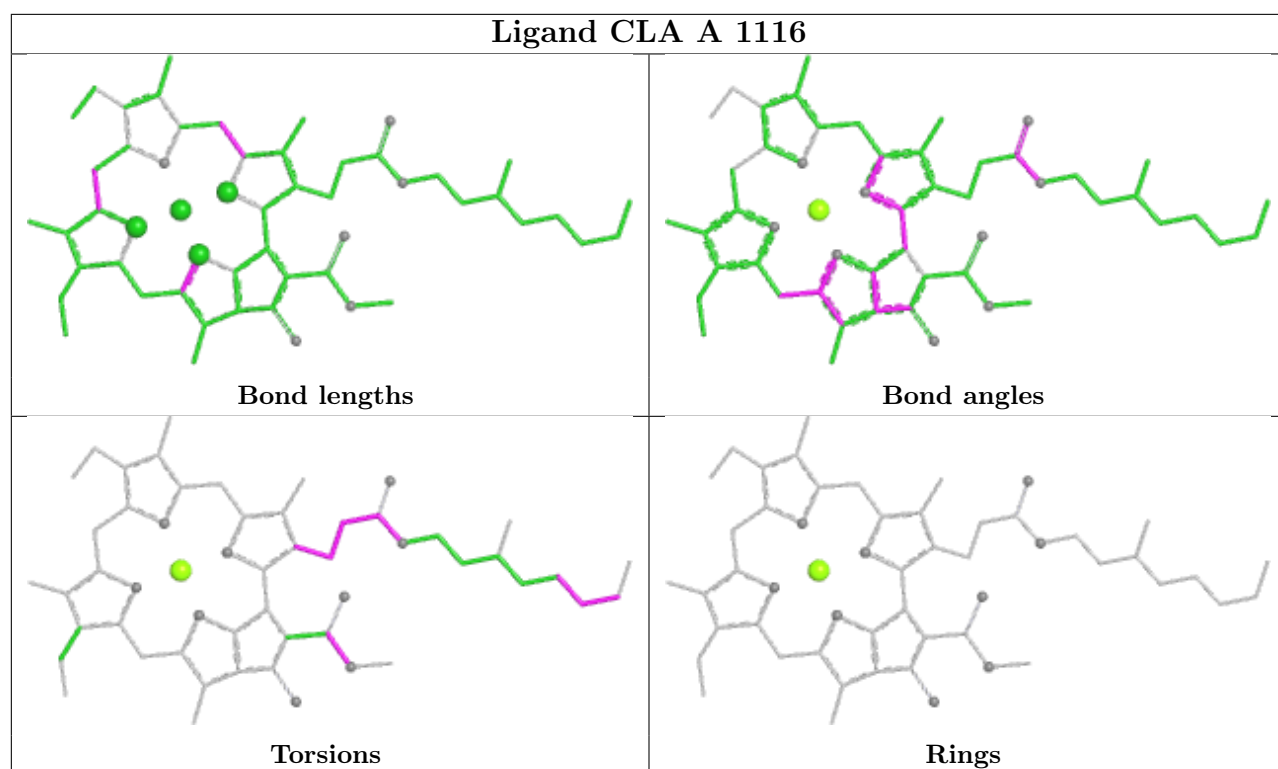


Torsions

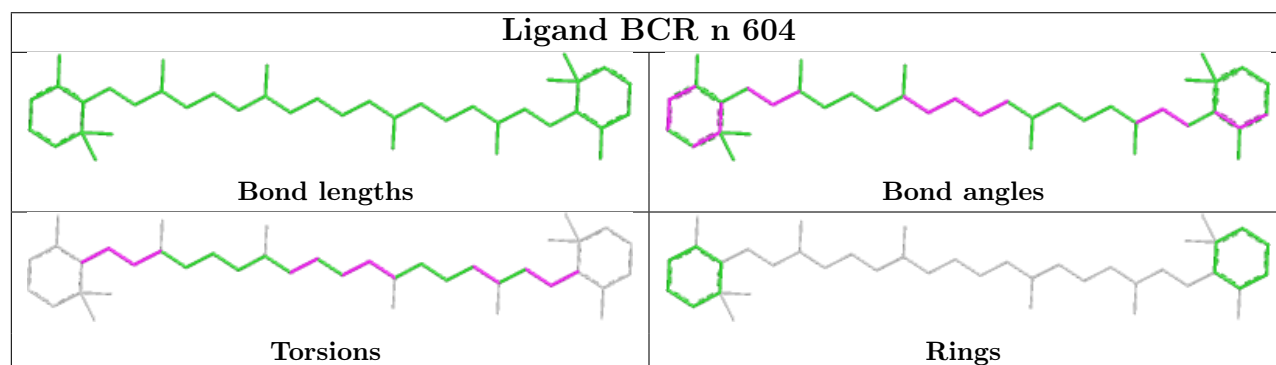
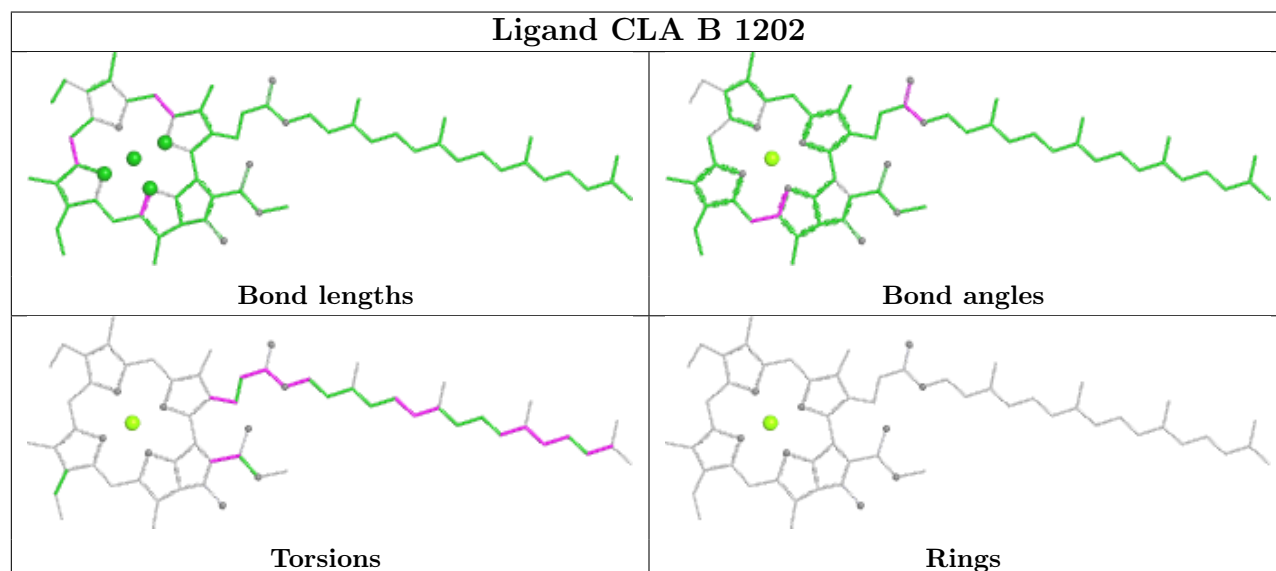
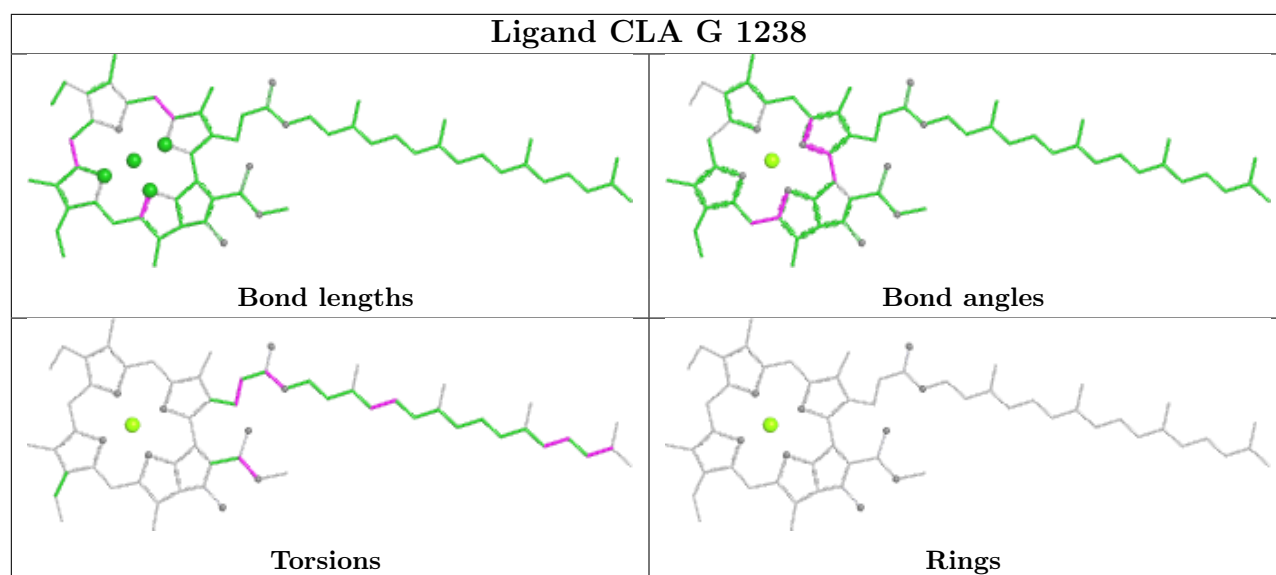


Rings

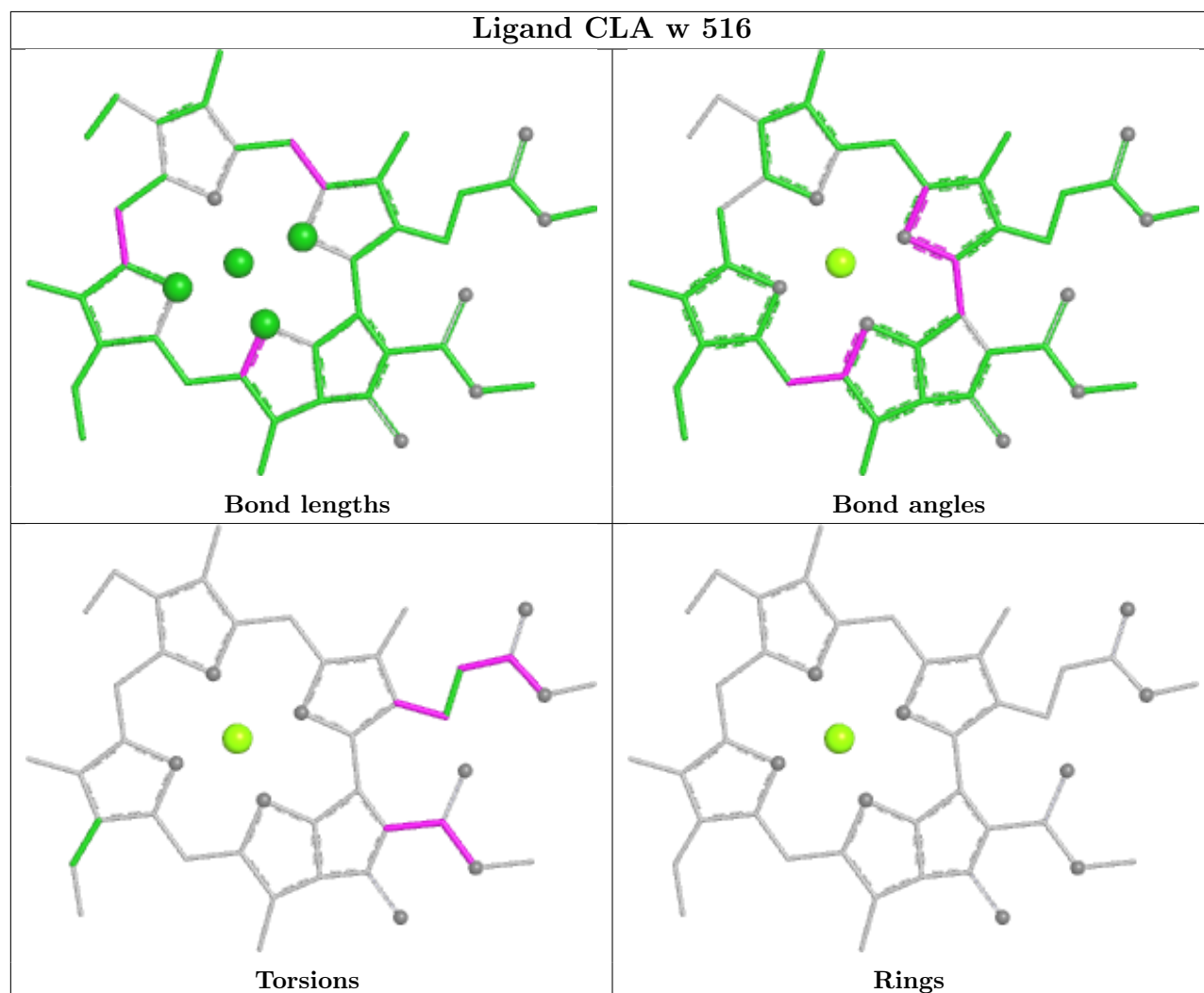
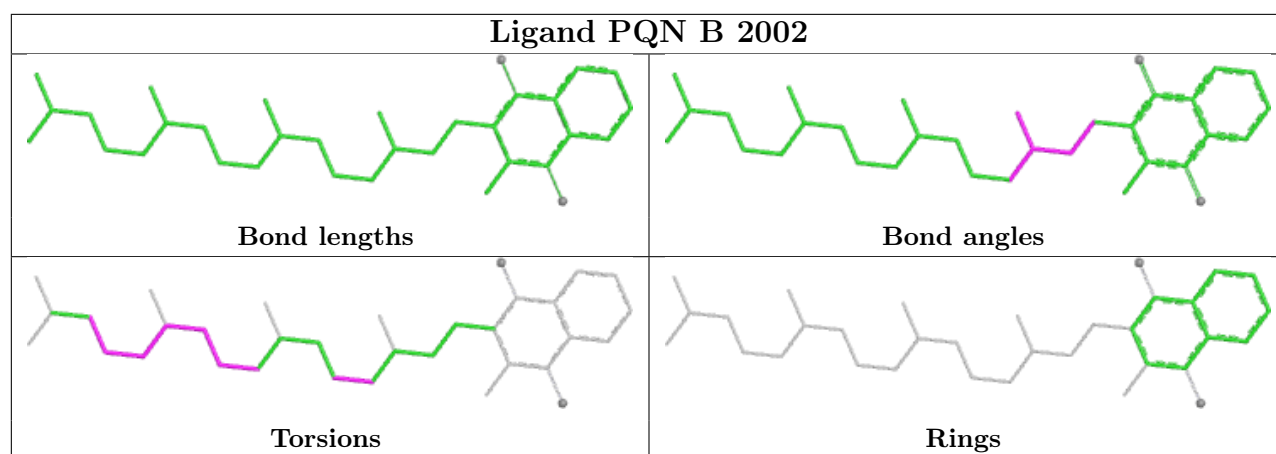




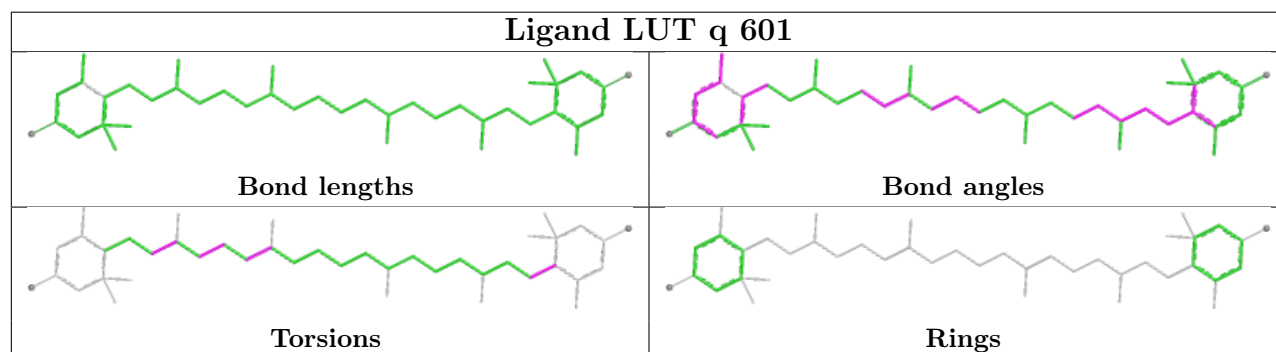
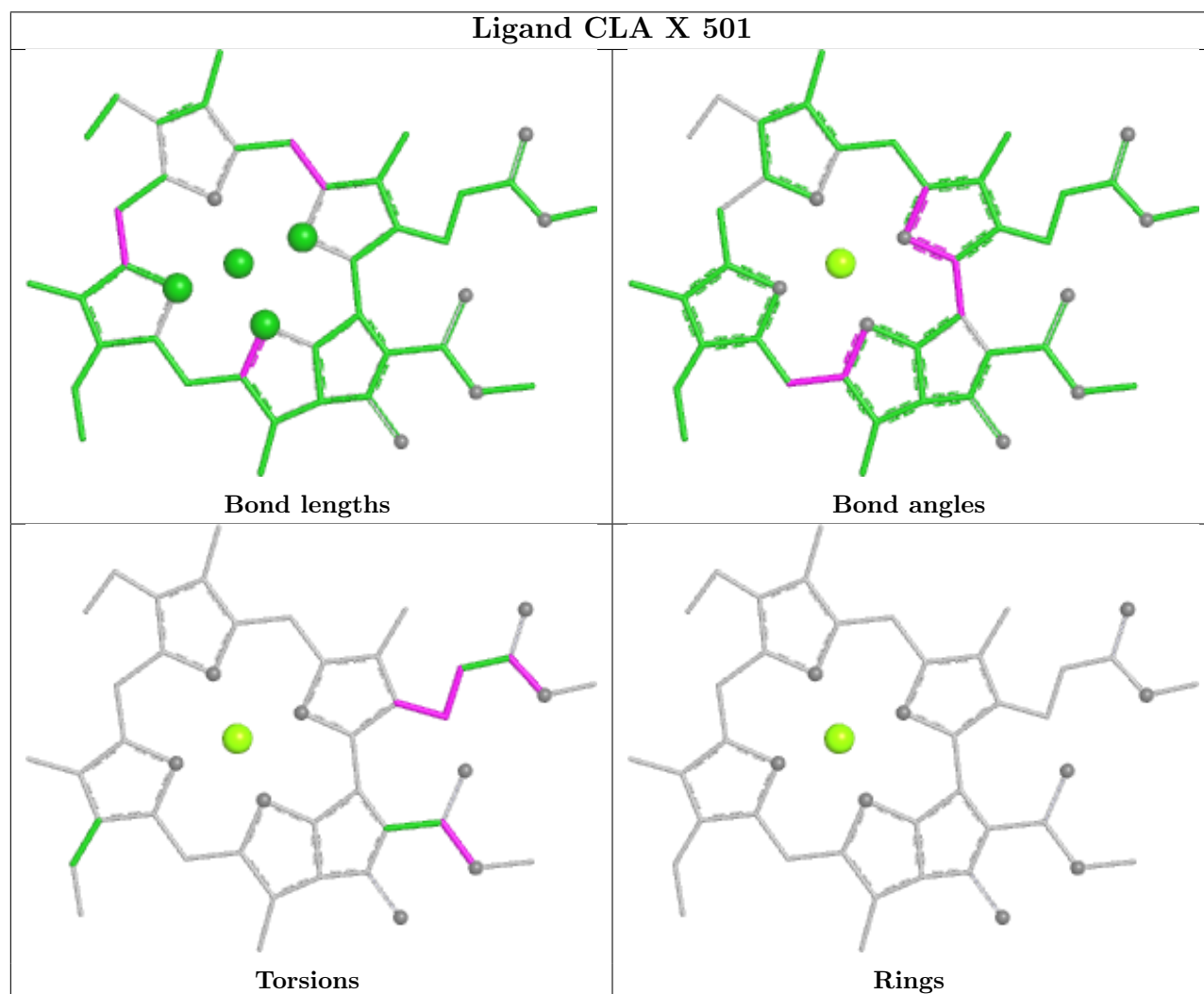
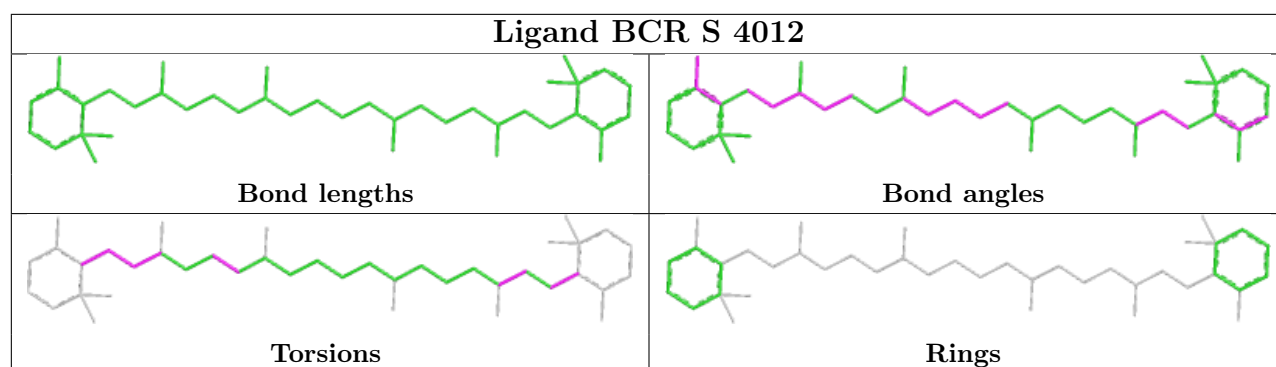






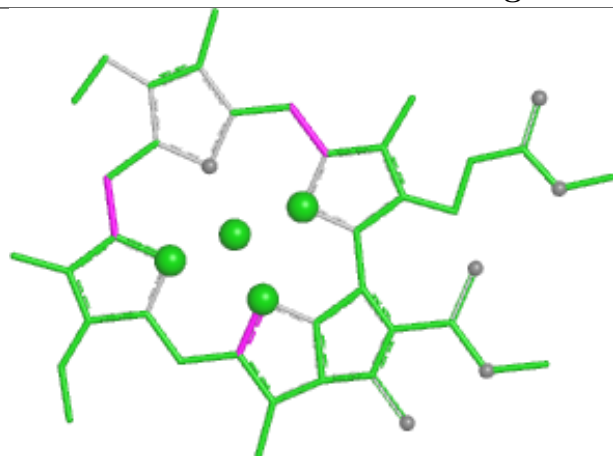




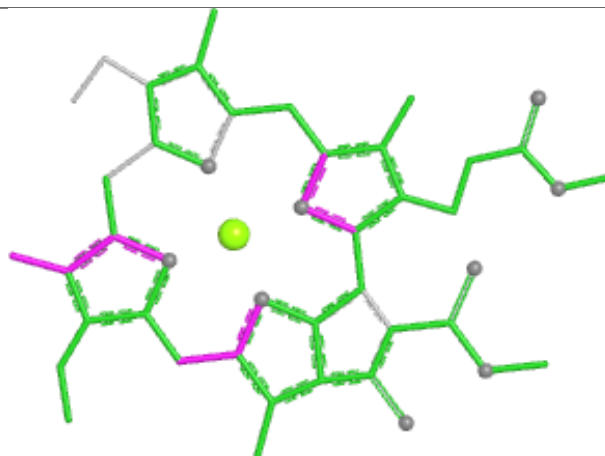




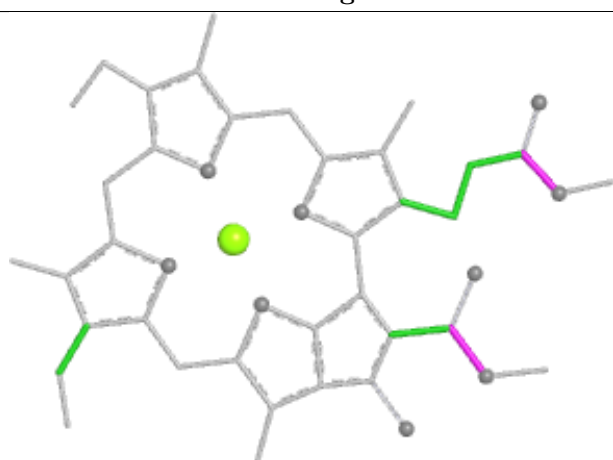
## Ligand CLA G 1240



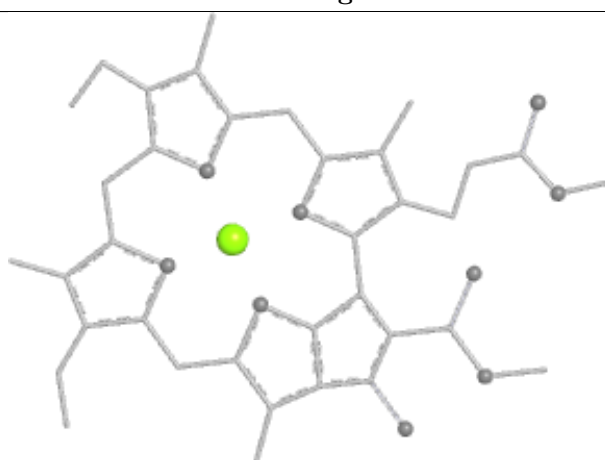
Bond lengths



Bond angles

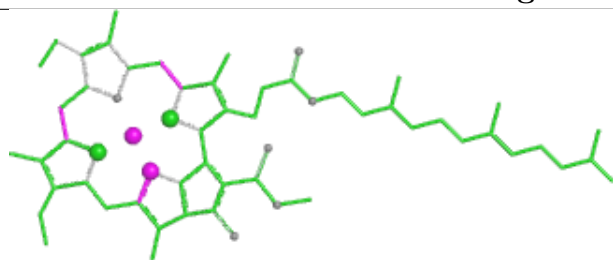


Torsions

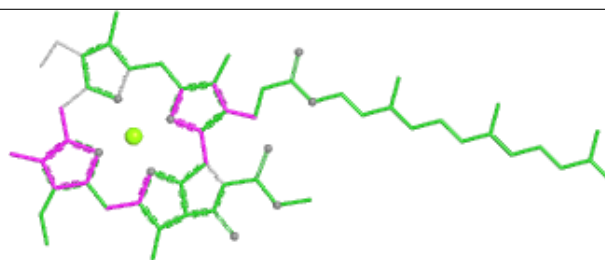


Rings

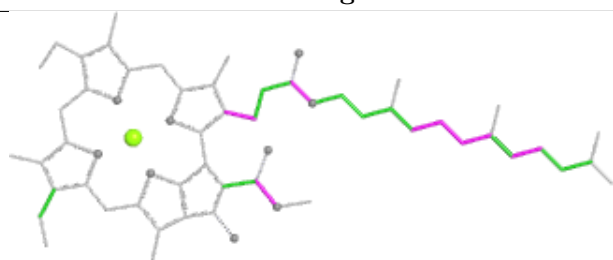
## Ligand CLA u 506



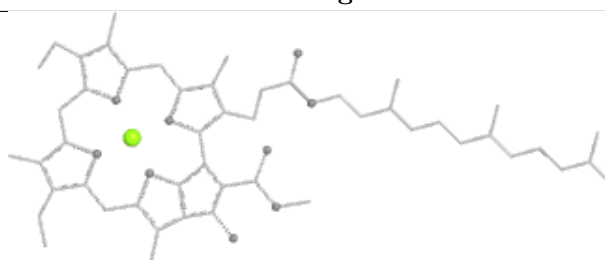
Bond lengths



Bond angles

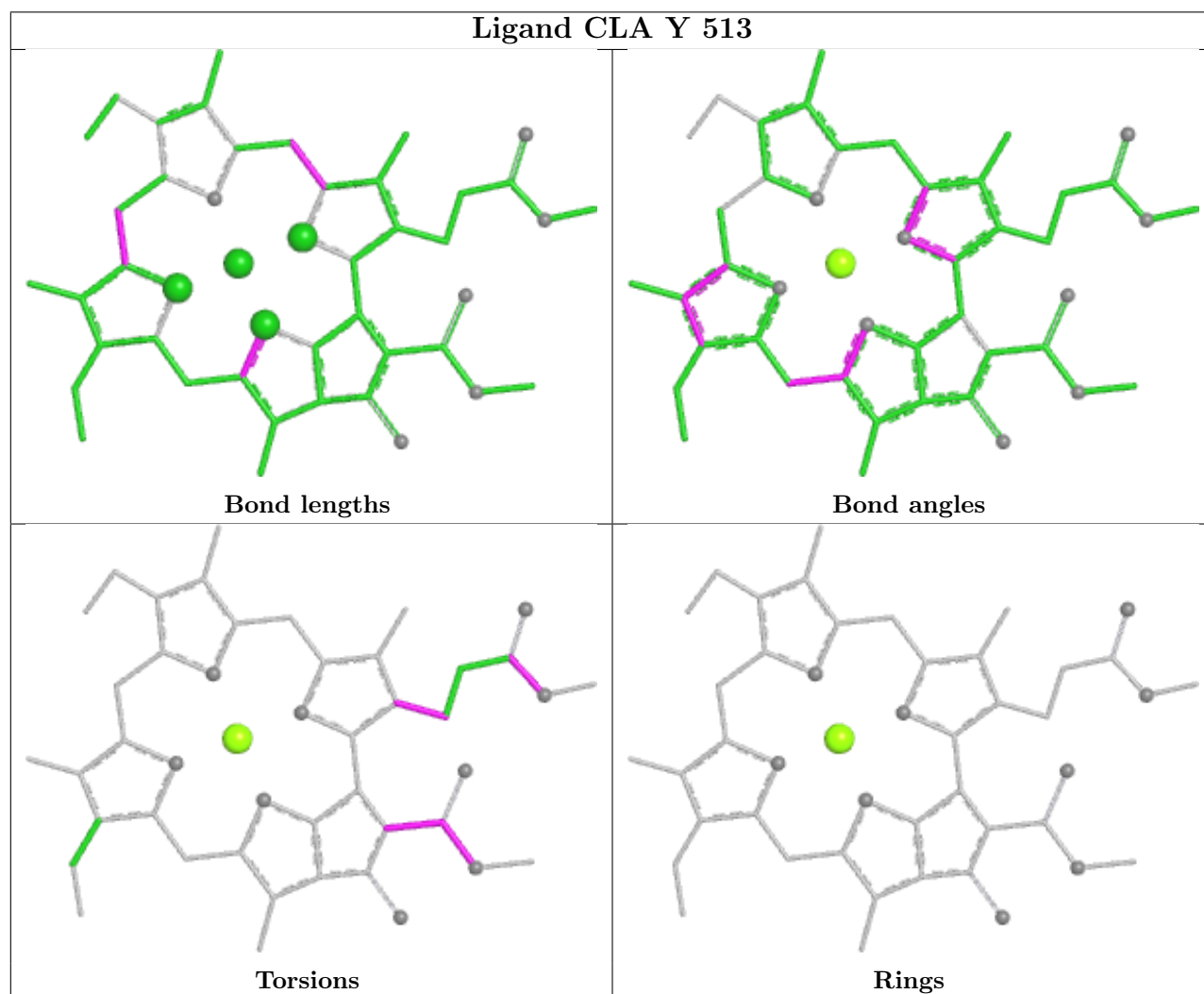
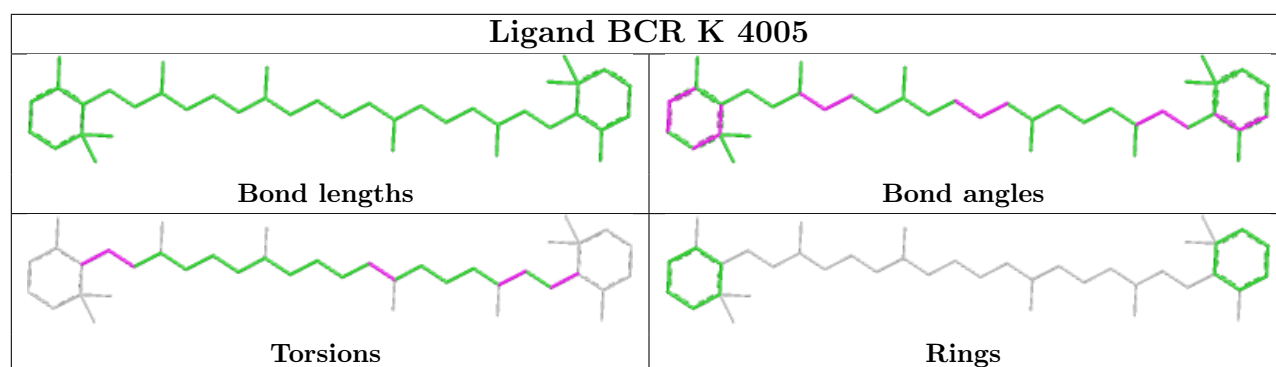


Torsions



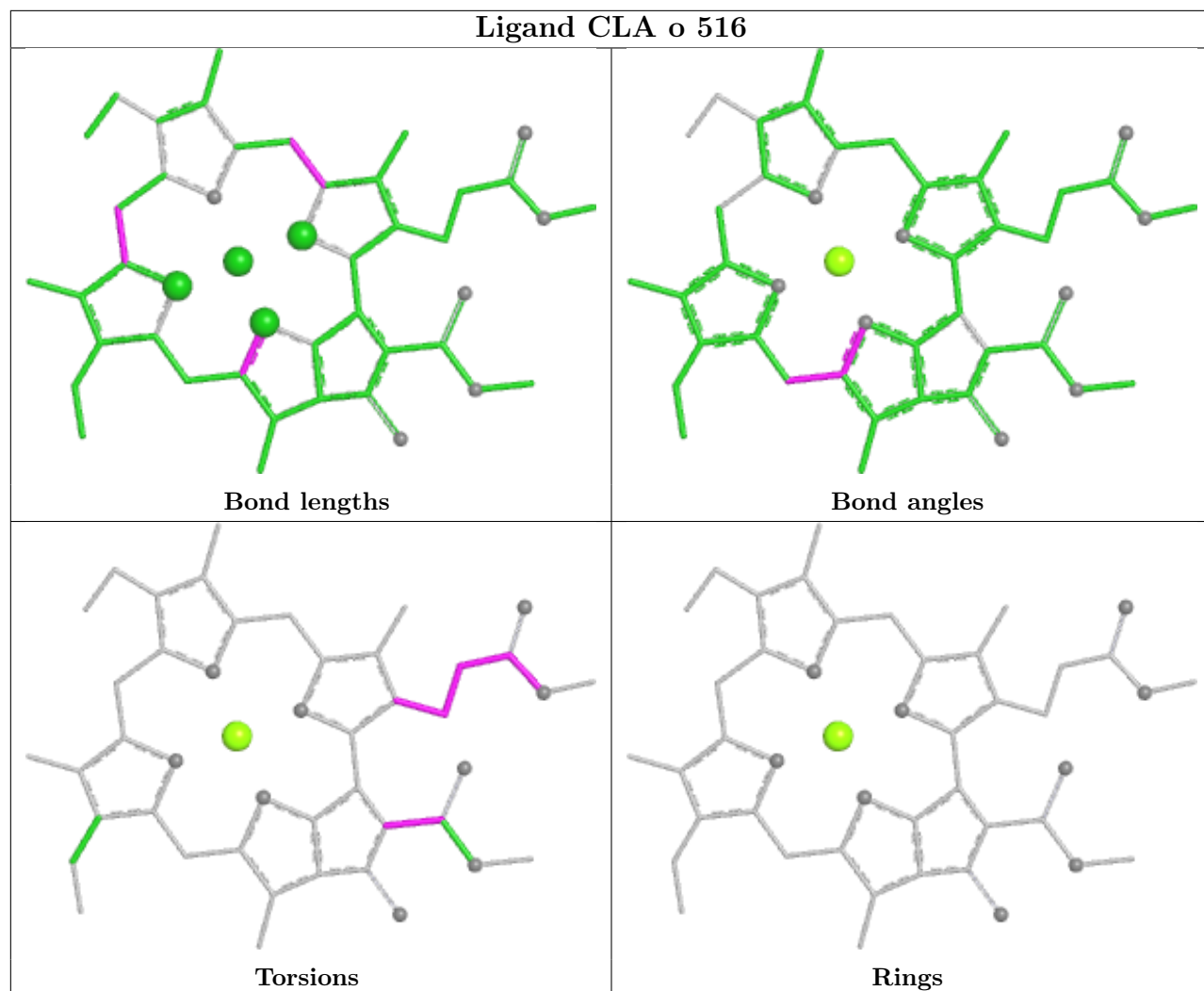
Rings



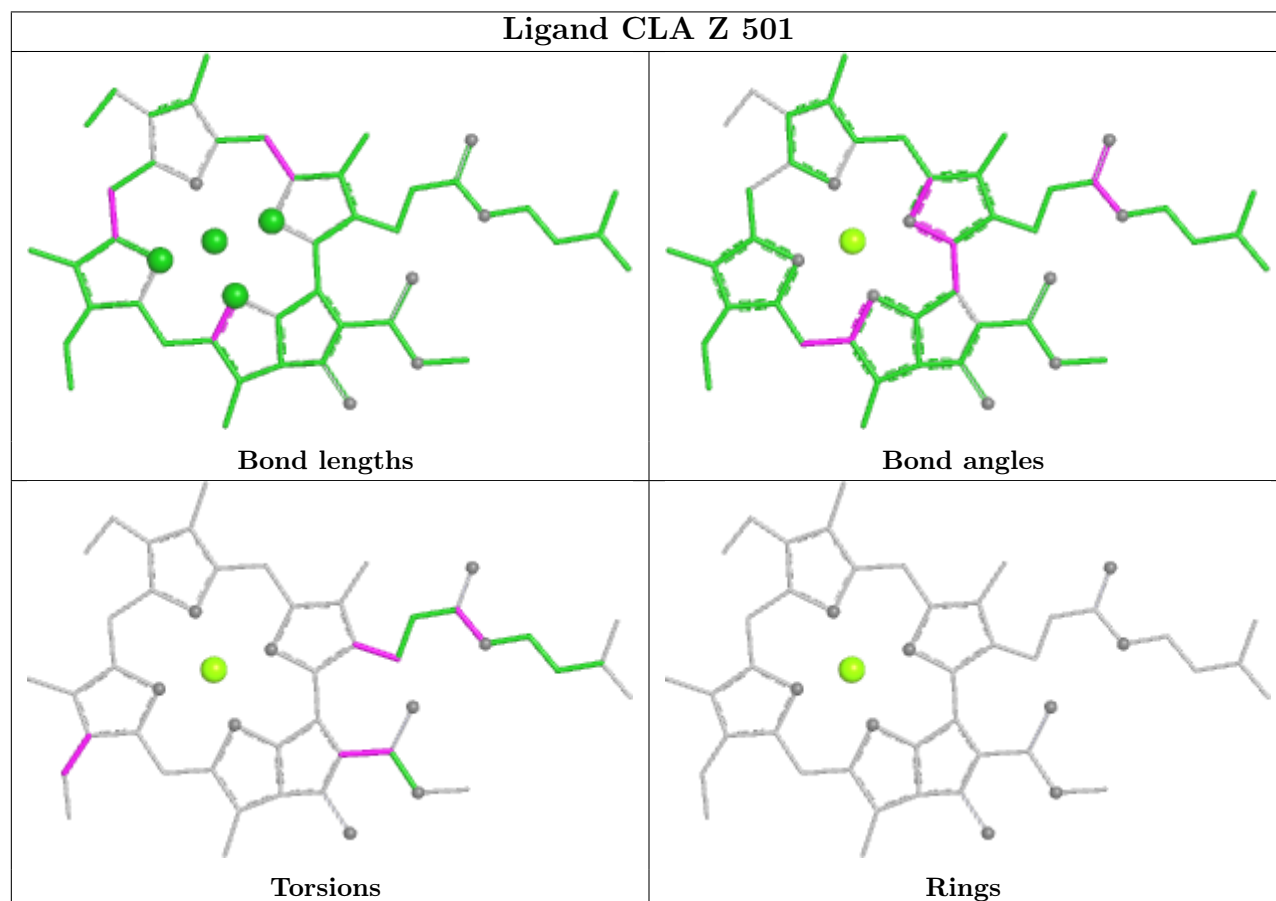
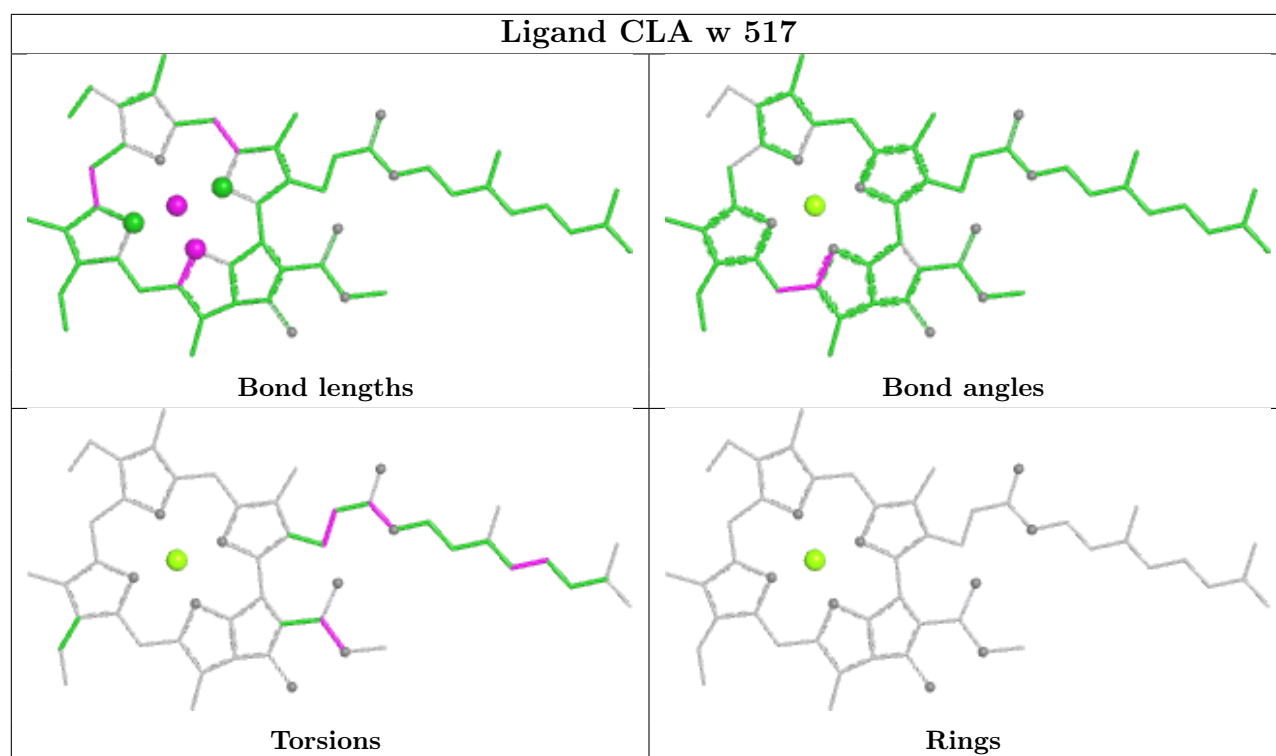




## Ligand CLA o 516

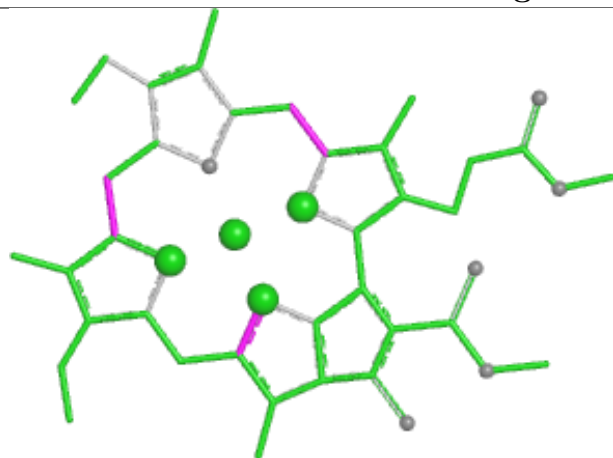




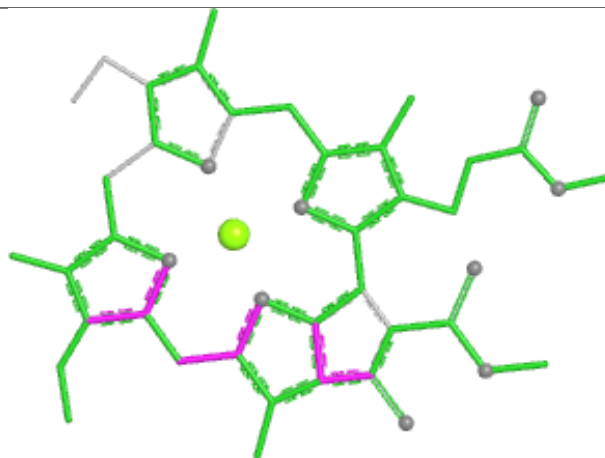




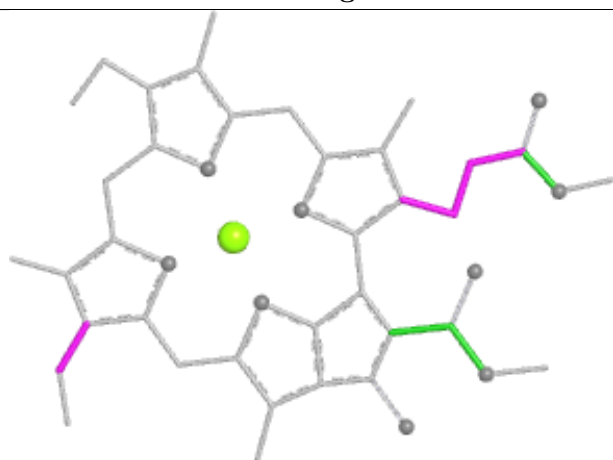
## Ligand CLA Y 503



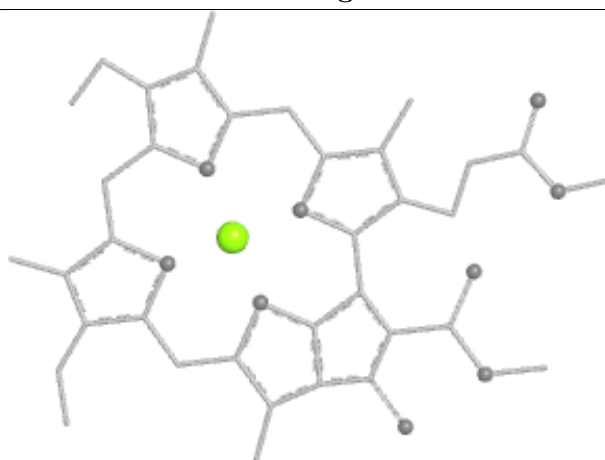
Bond lengths



Bond angles

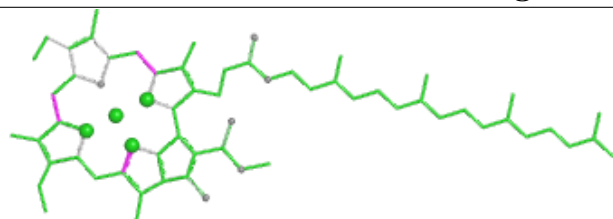


Torsions

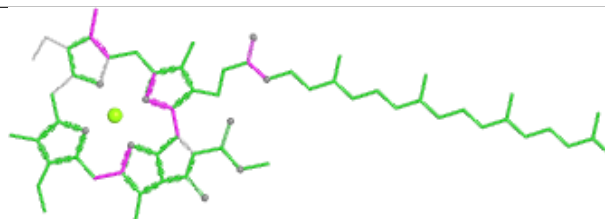


Rings

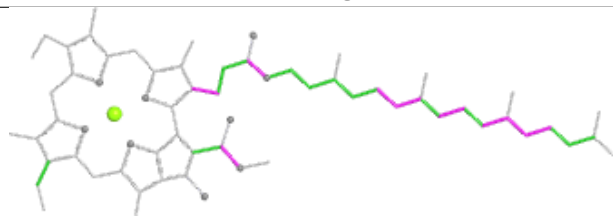
## Ligand CLA Y 511



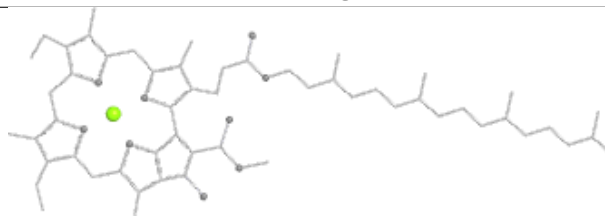
Bond lengths



Bond angles

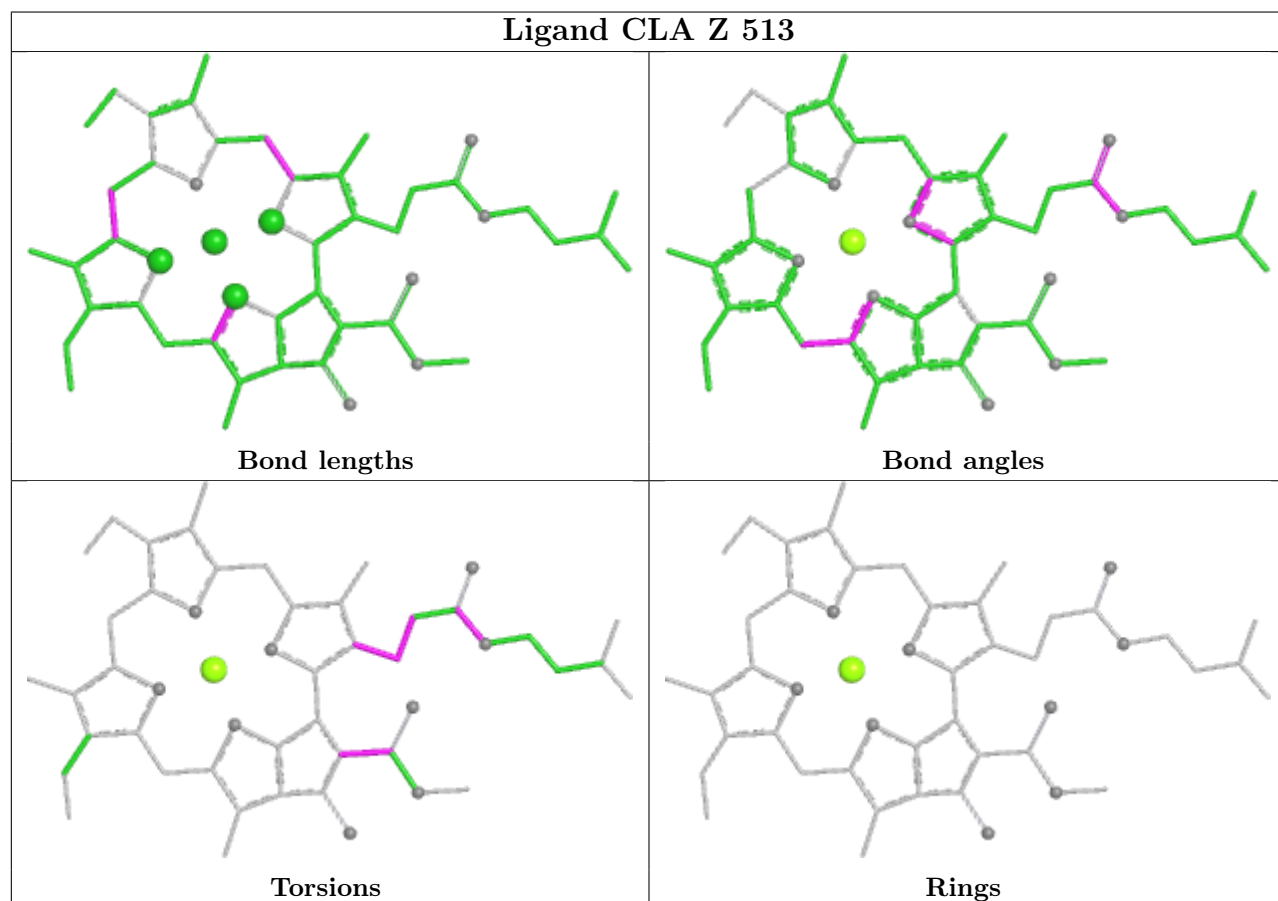
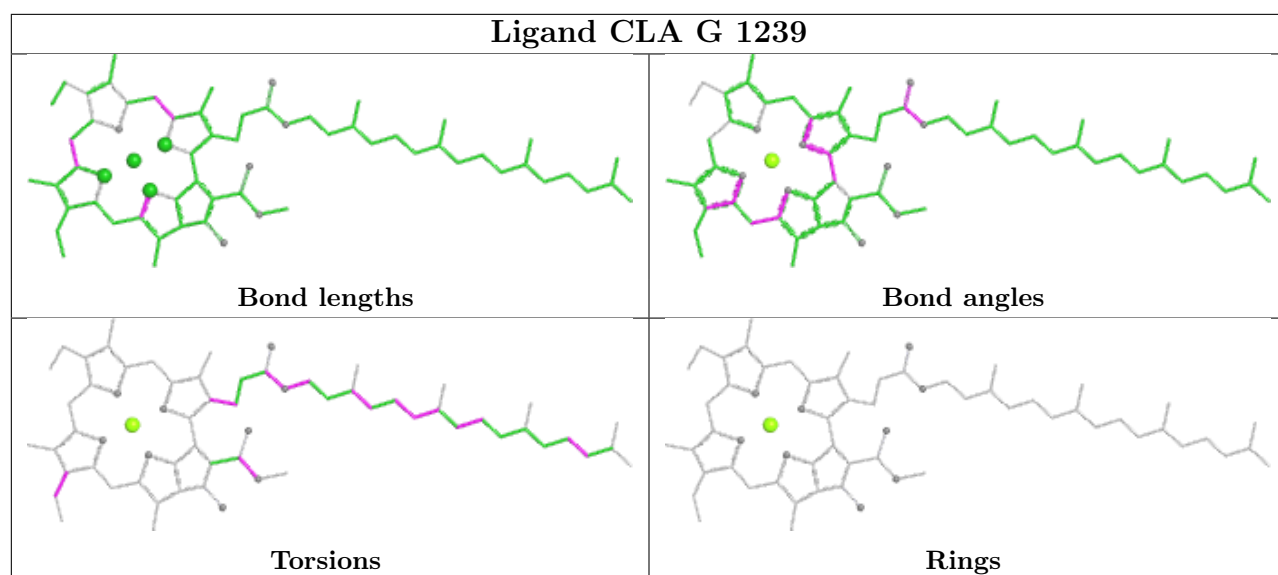


Torsions



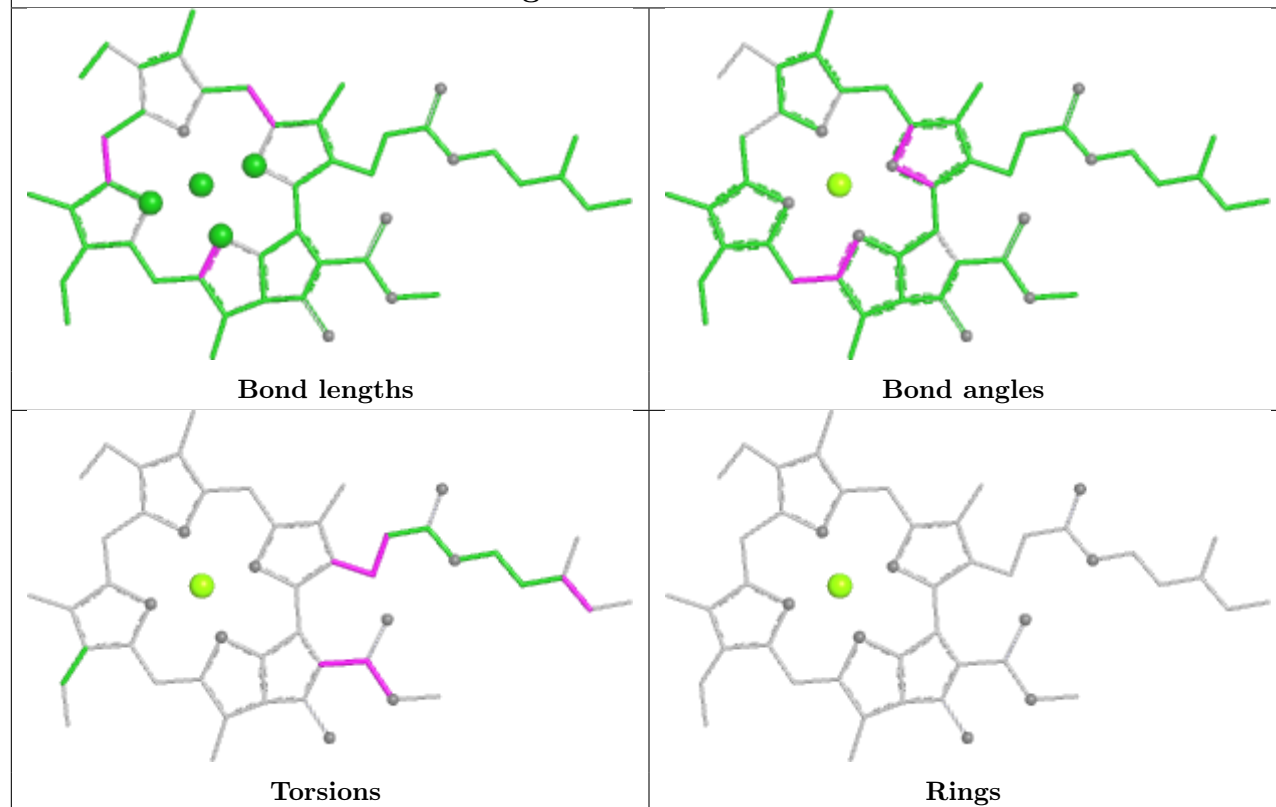
Rings



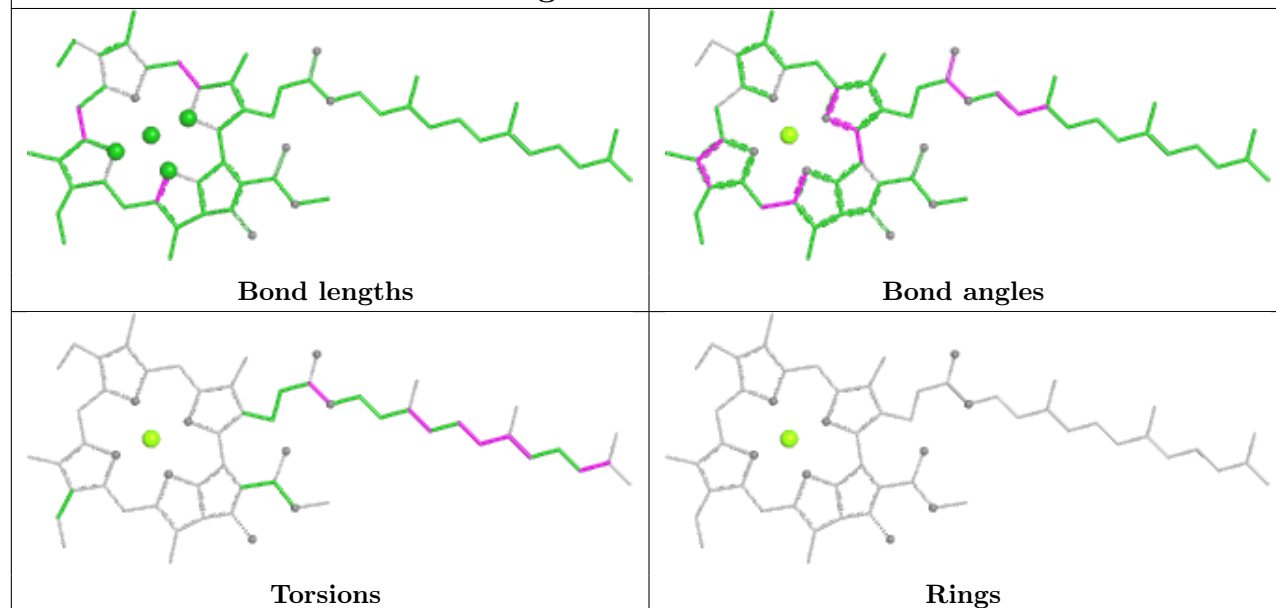




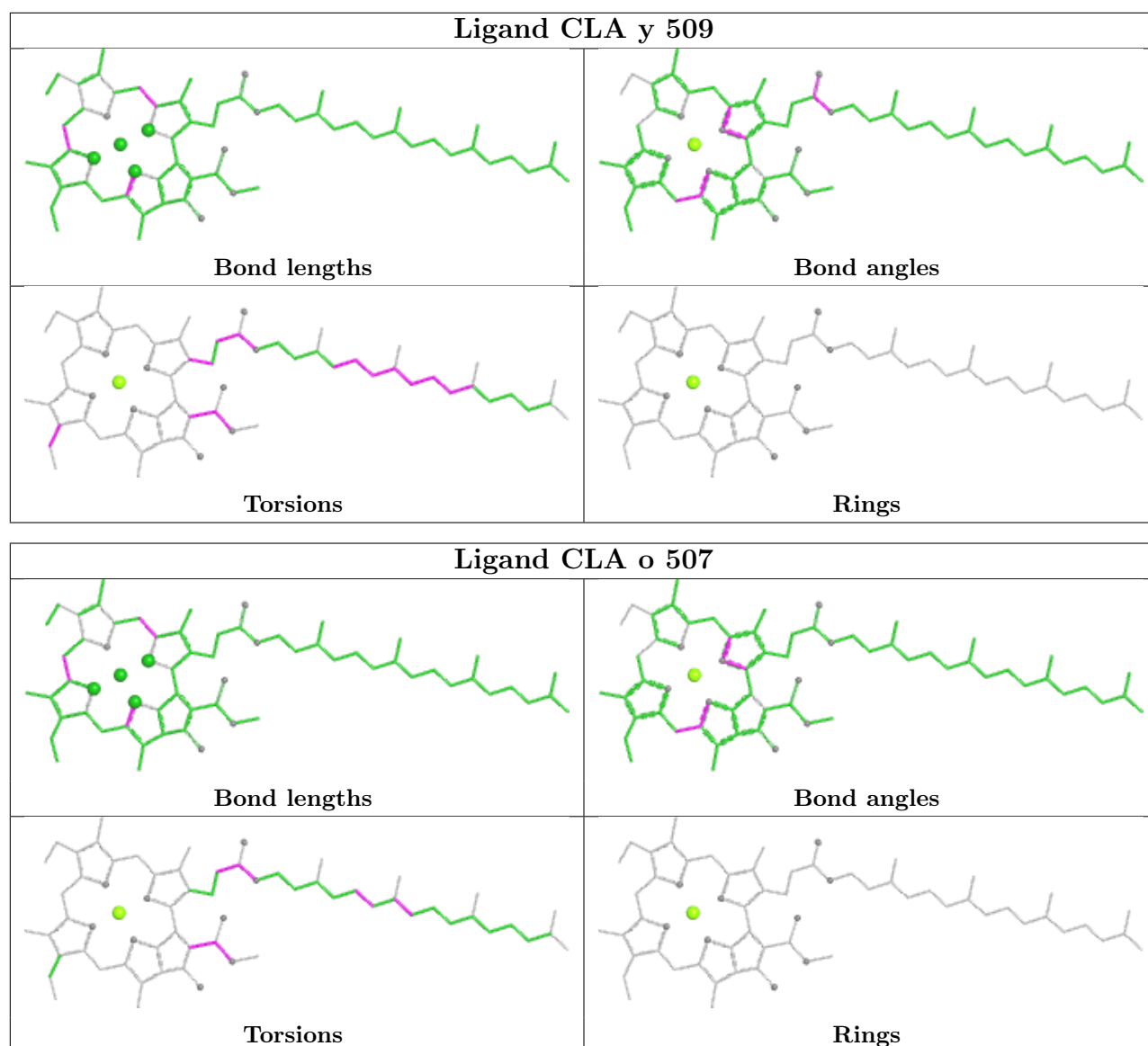
## Ligand CLA H 1121



## Ligand CLA r 506

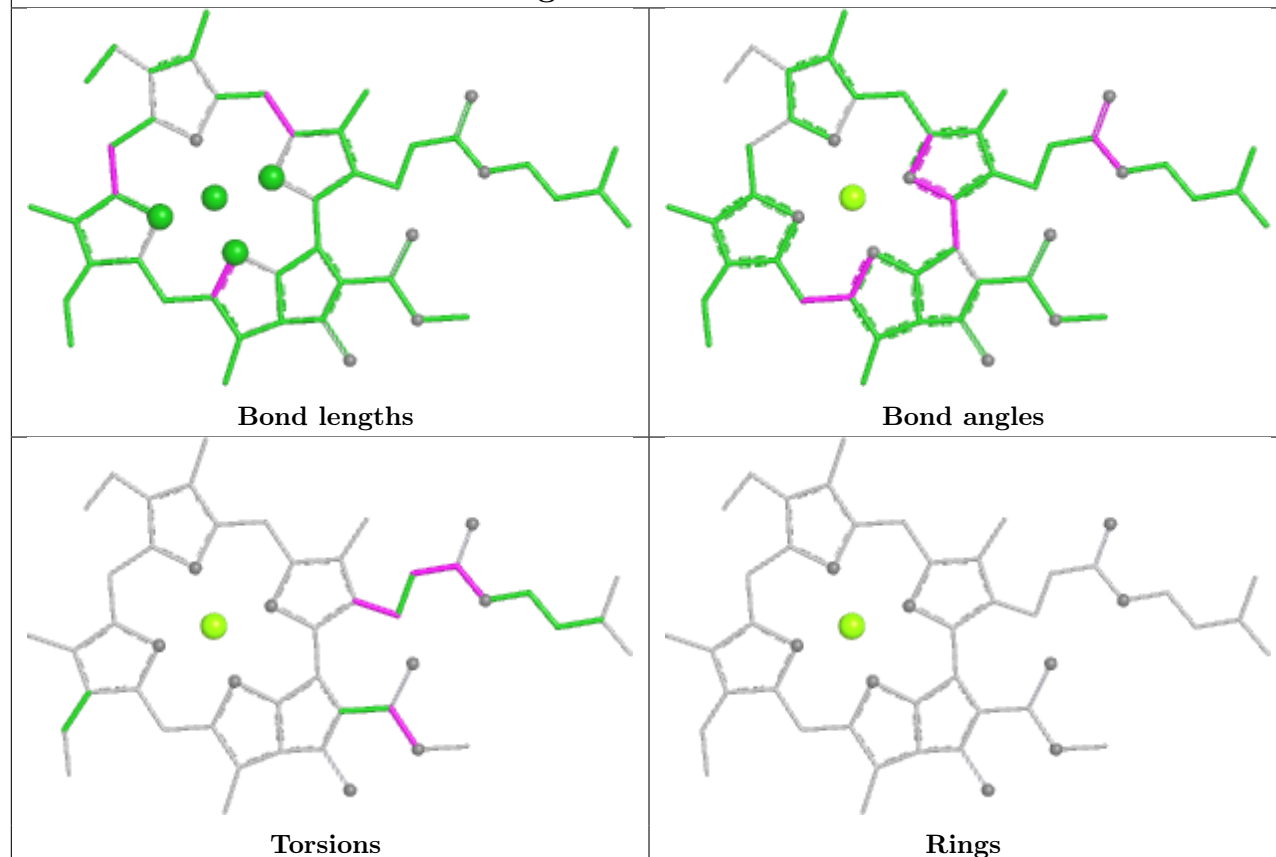




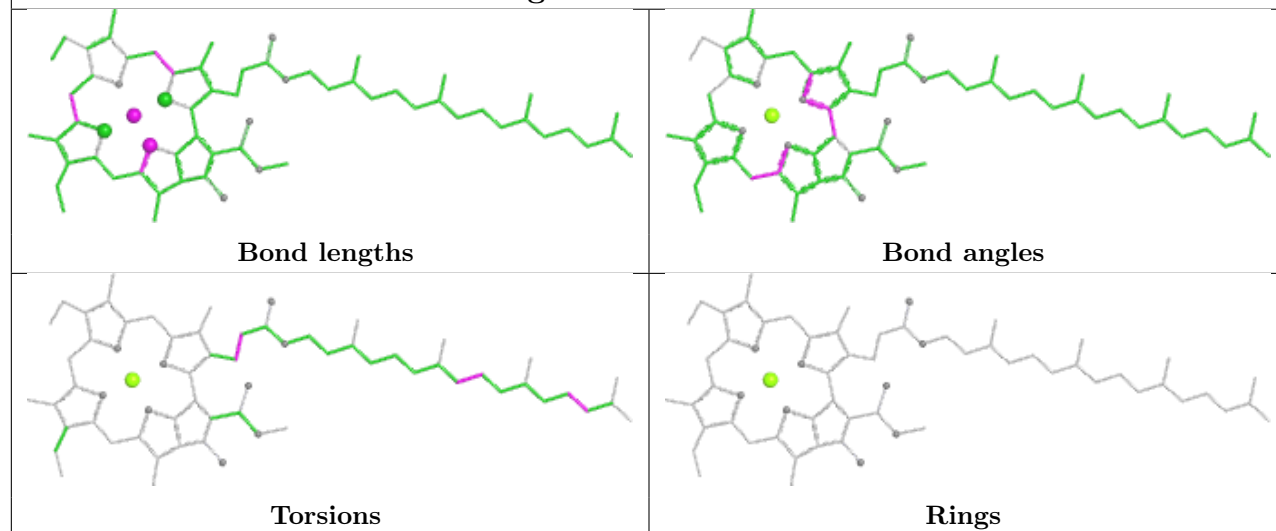




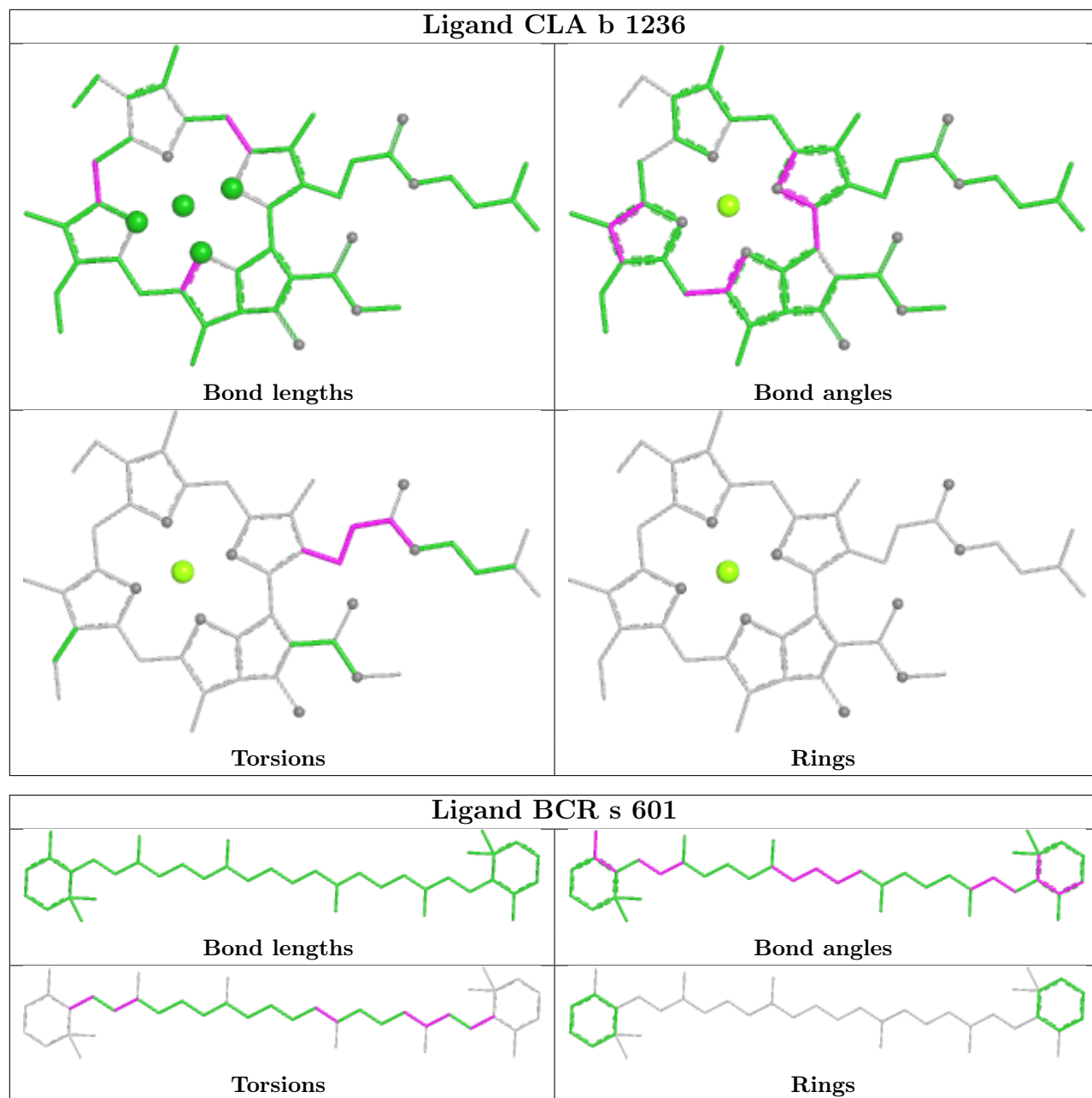
## Ligand CLA s 514



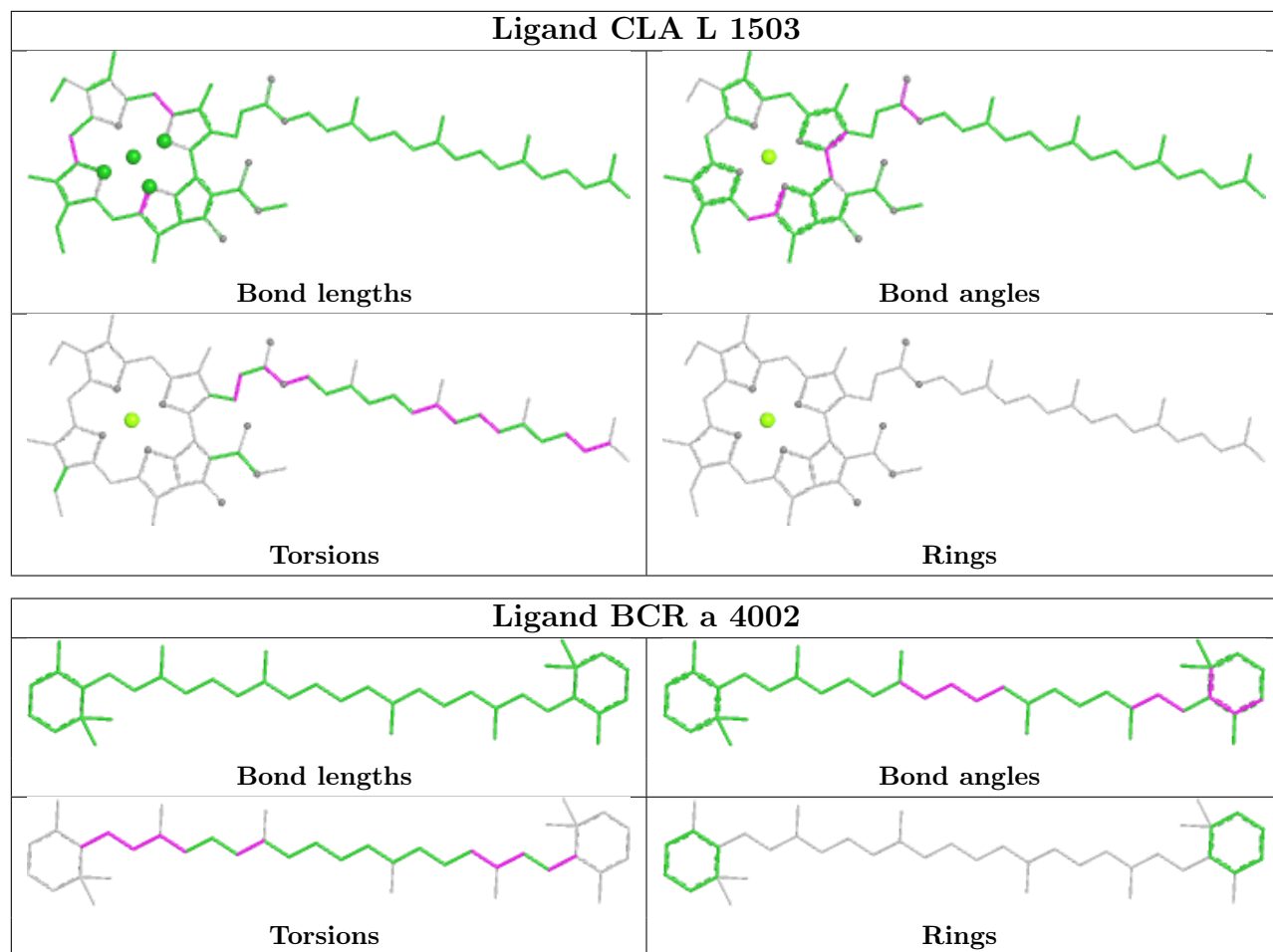
## Ligand CLA a 1127



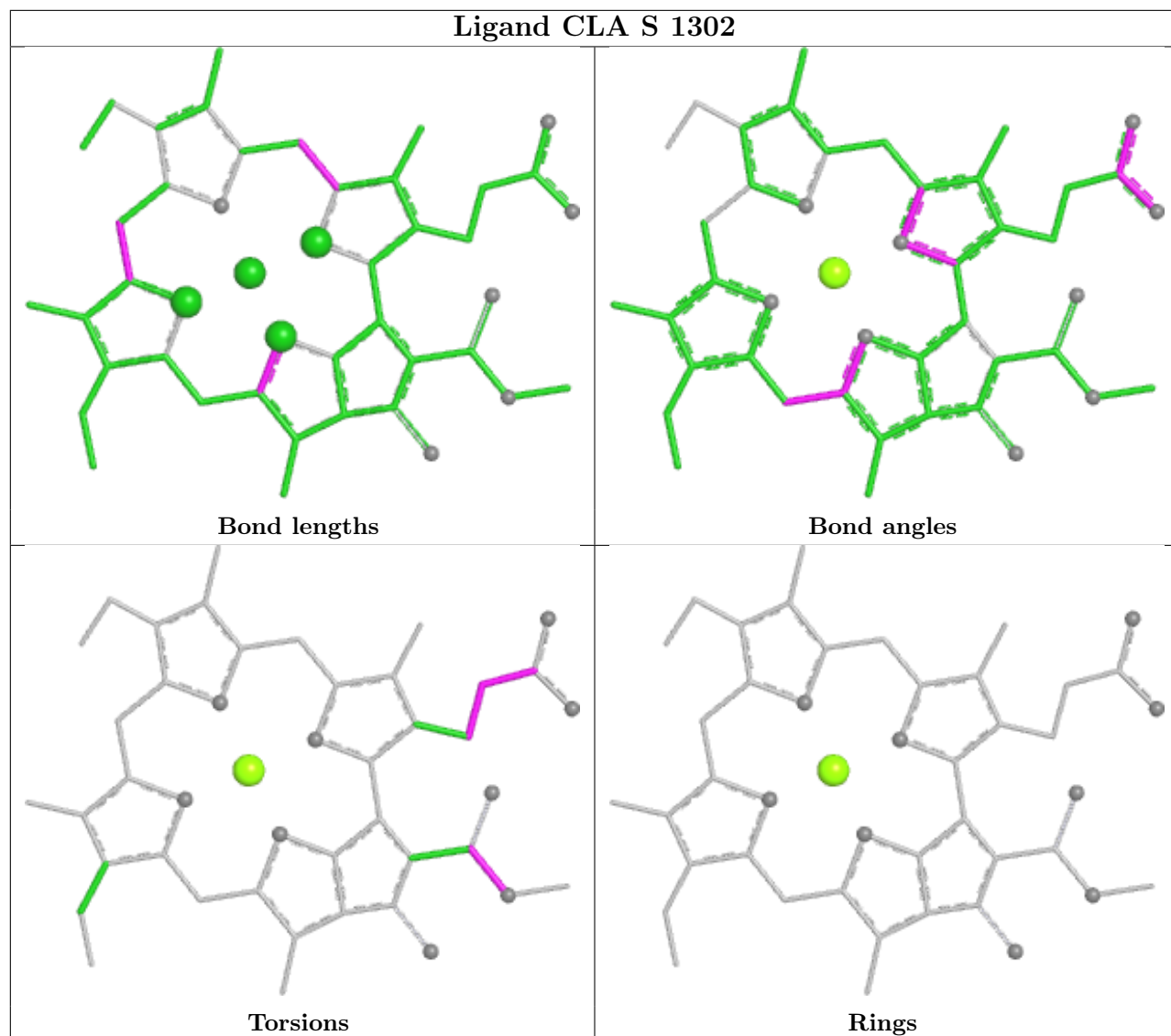






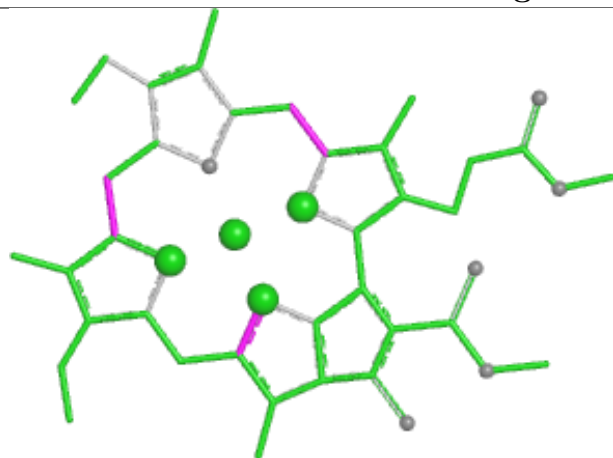




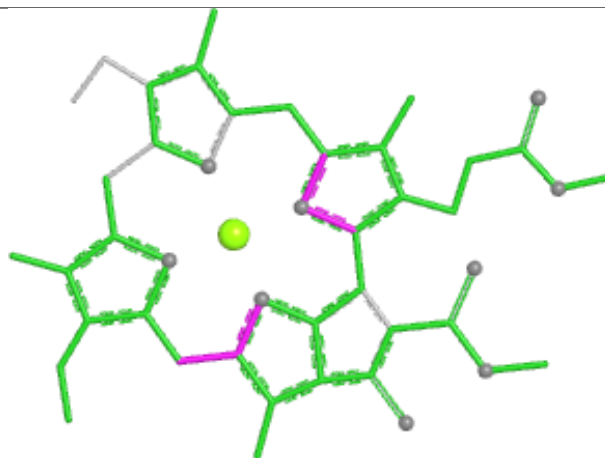




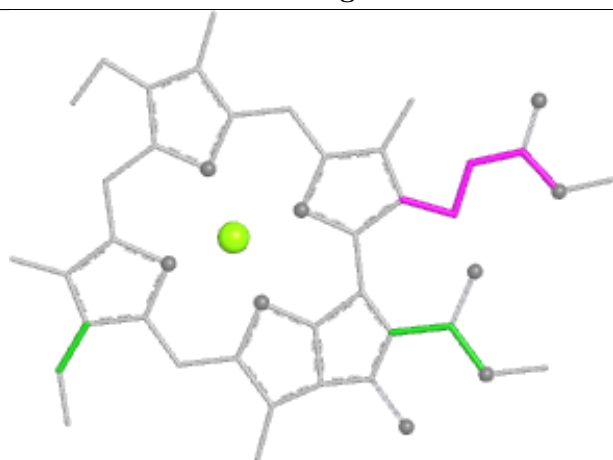
## Ligand CLA X 516



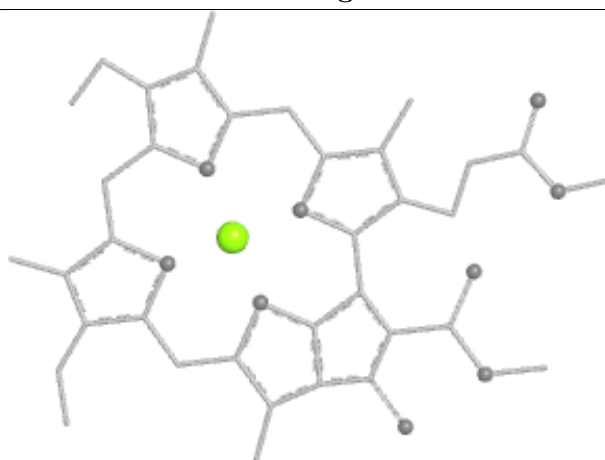
Bond lengths



Bond angles

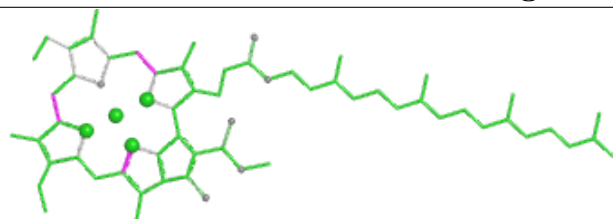


Torsions

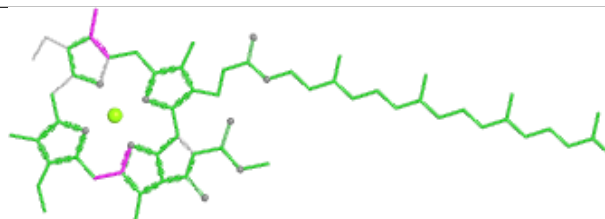


Rings

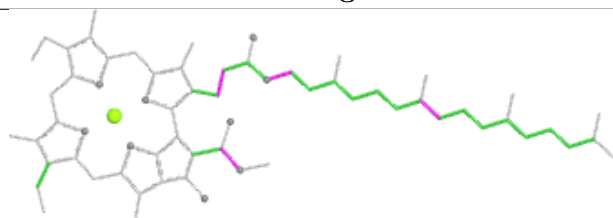
## Ligand CLA r 511



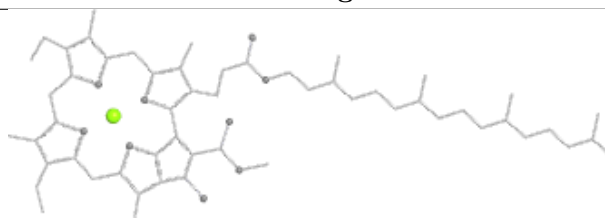
Bond lengths



Bond angles

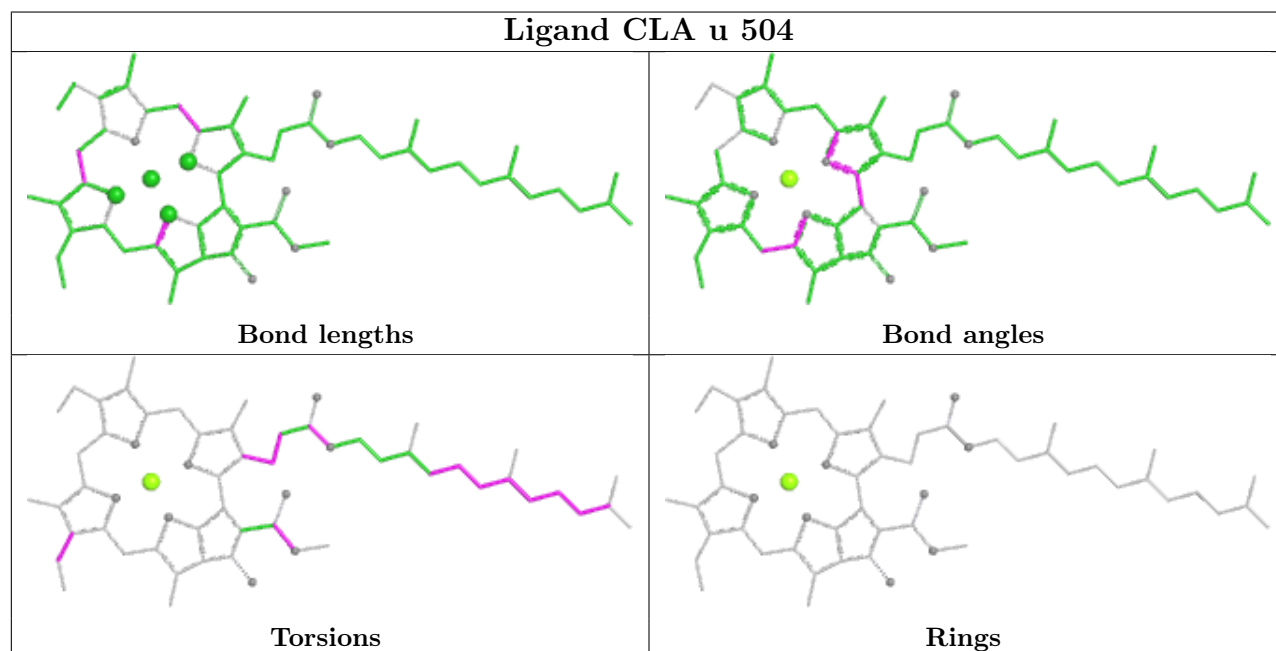
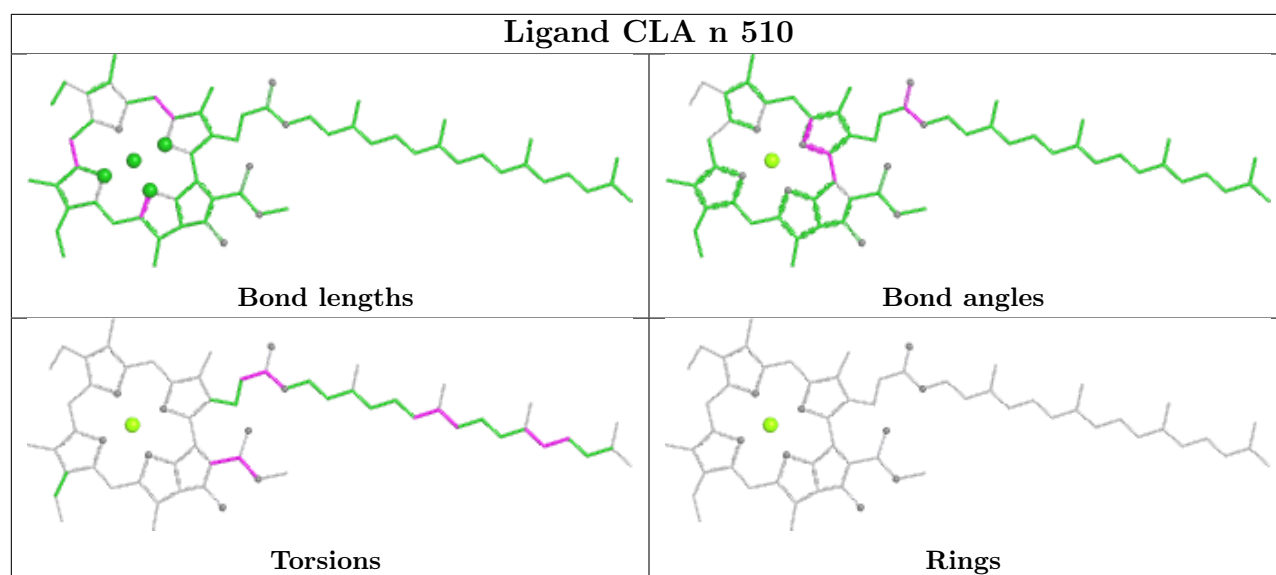


Torsions

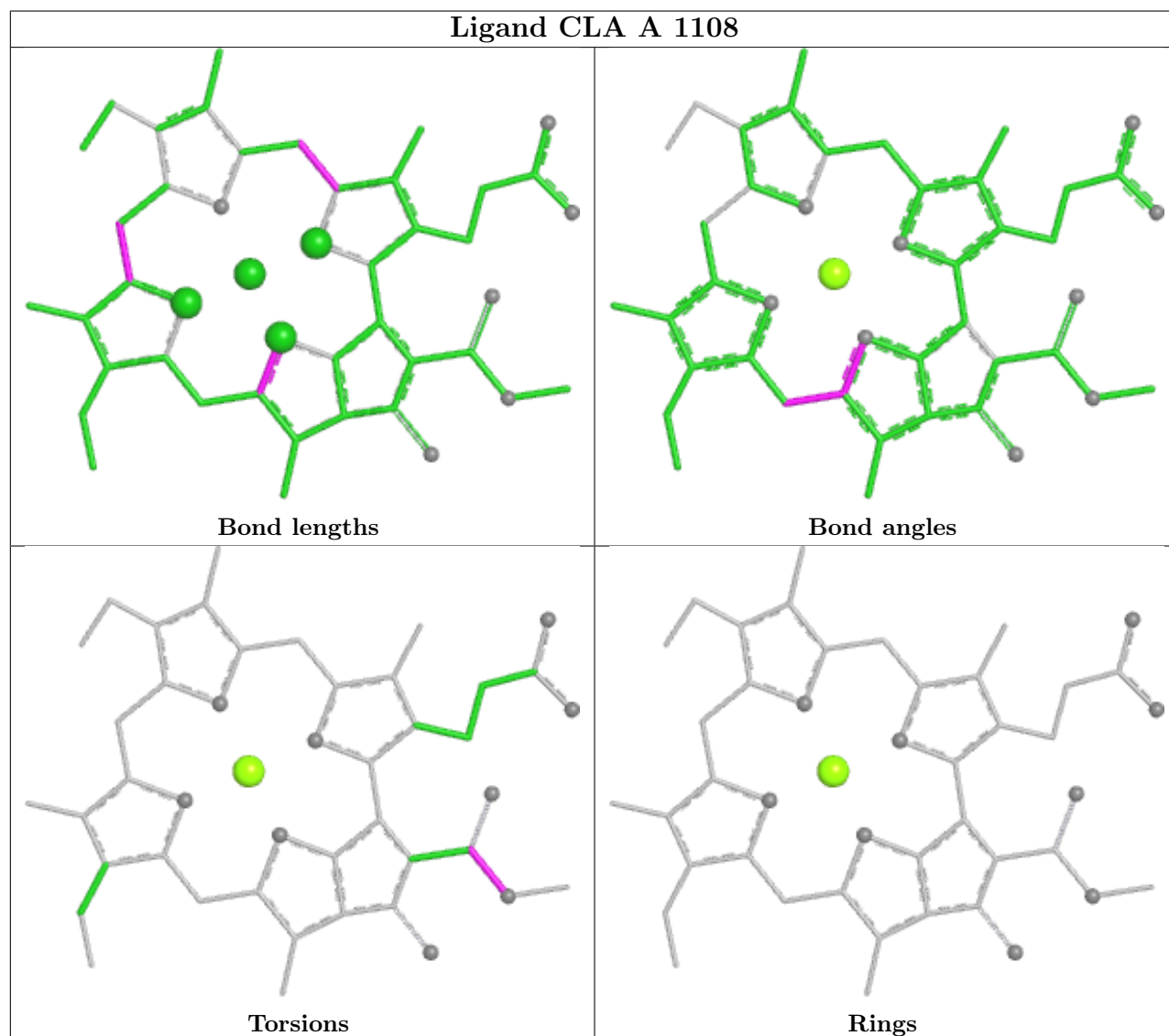
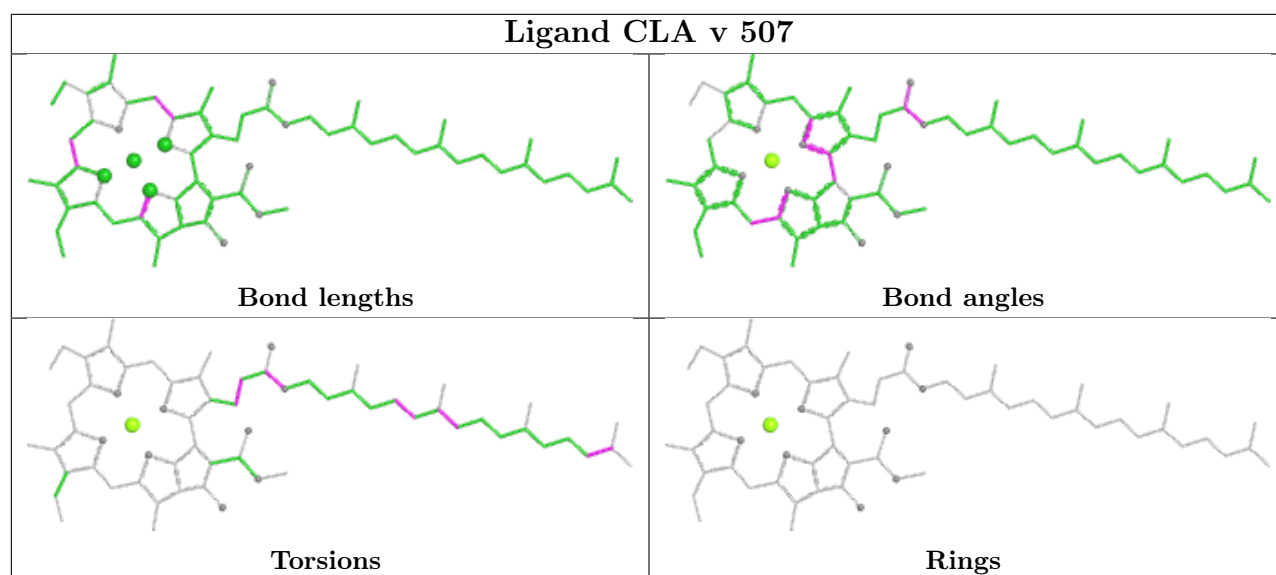


Rings

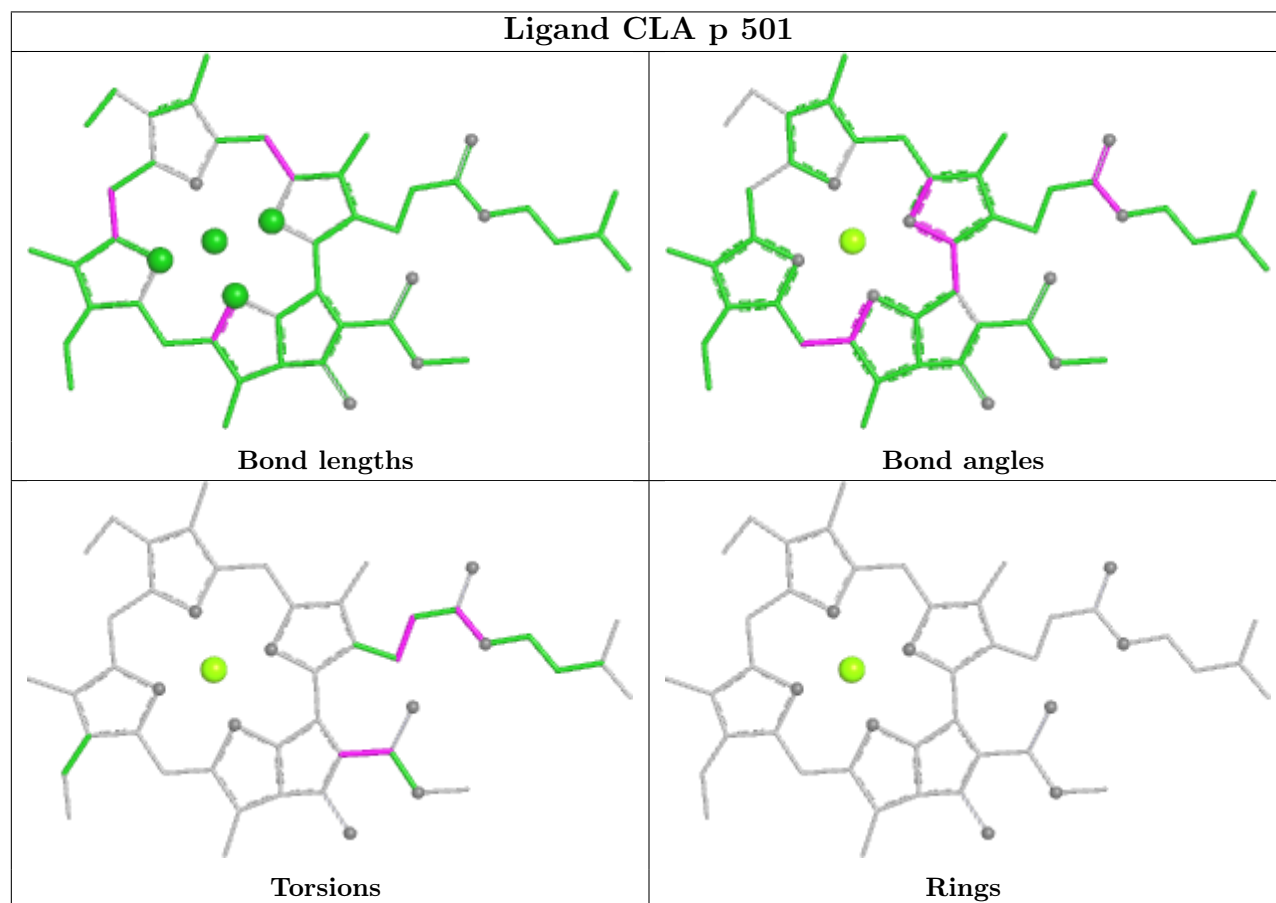
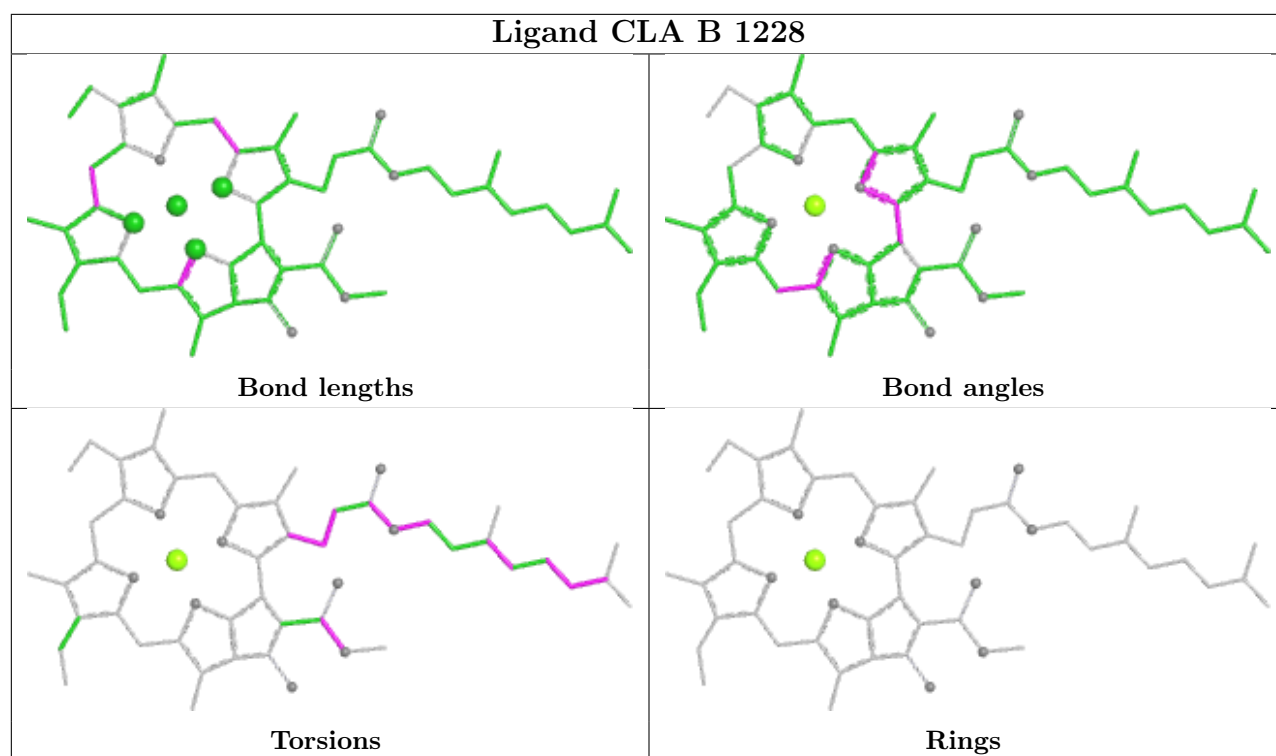




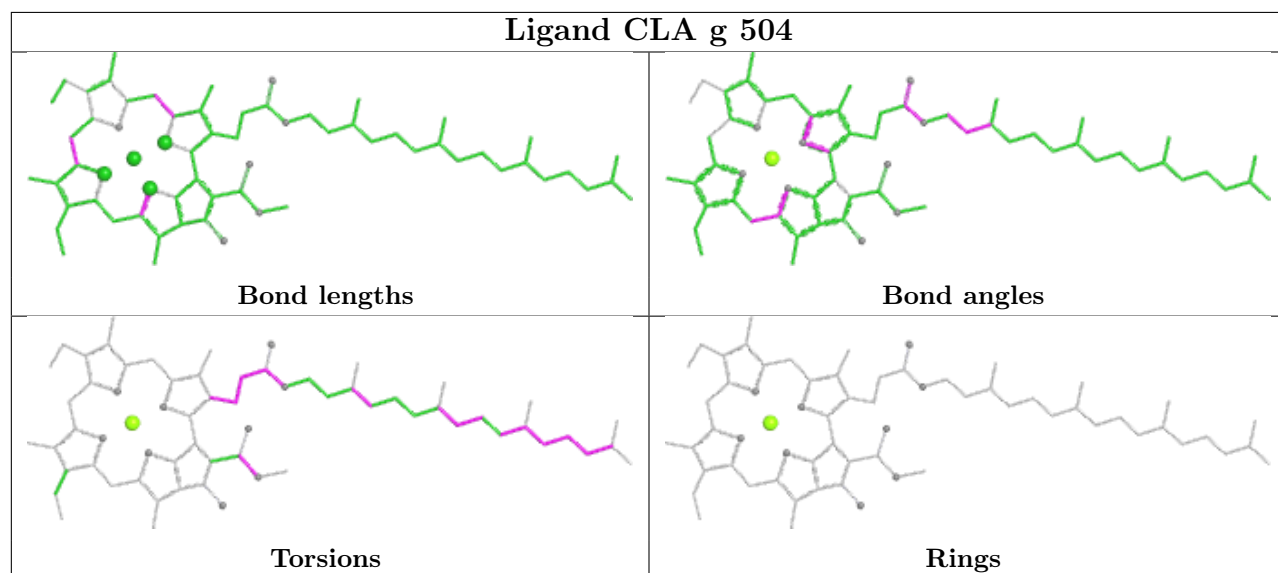
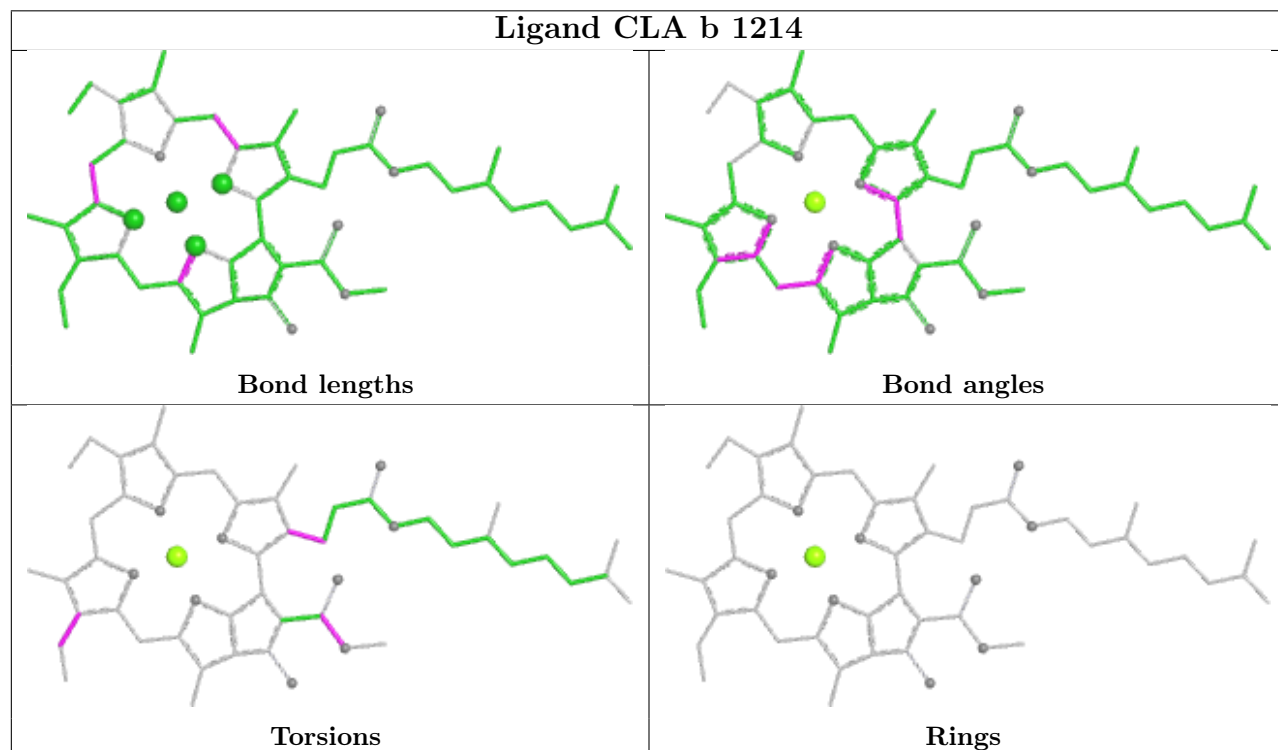
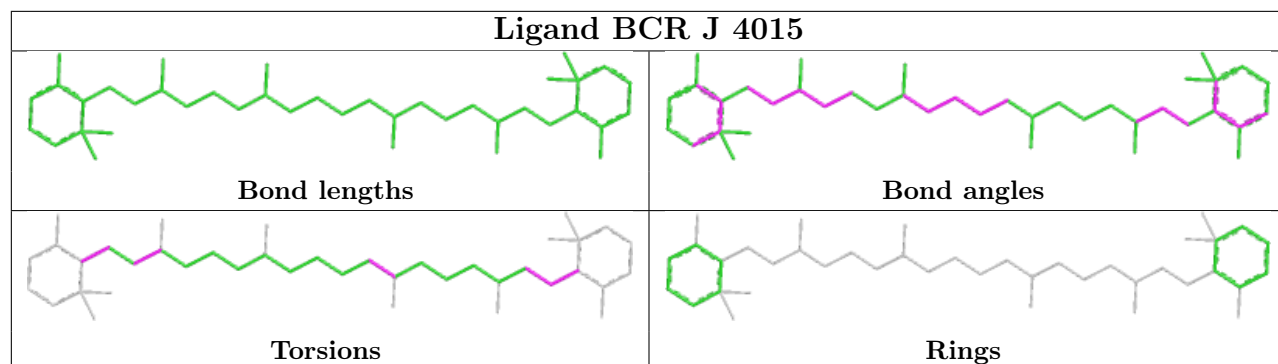




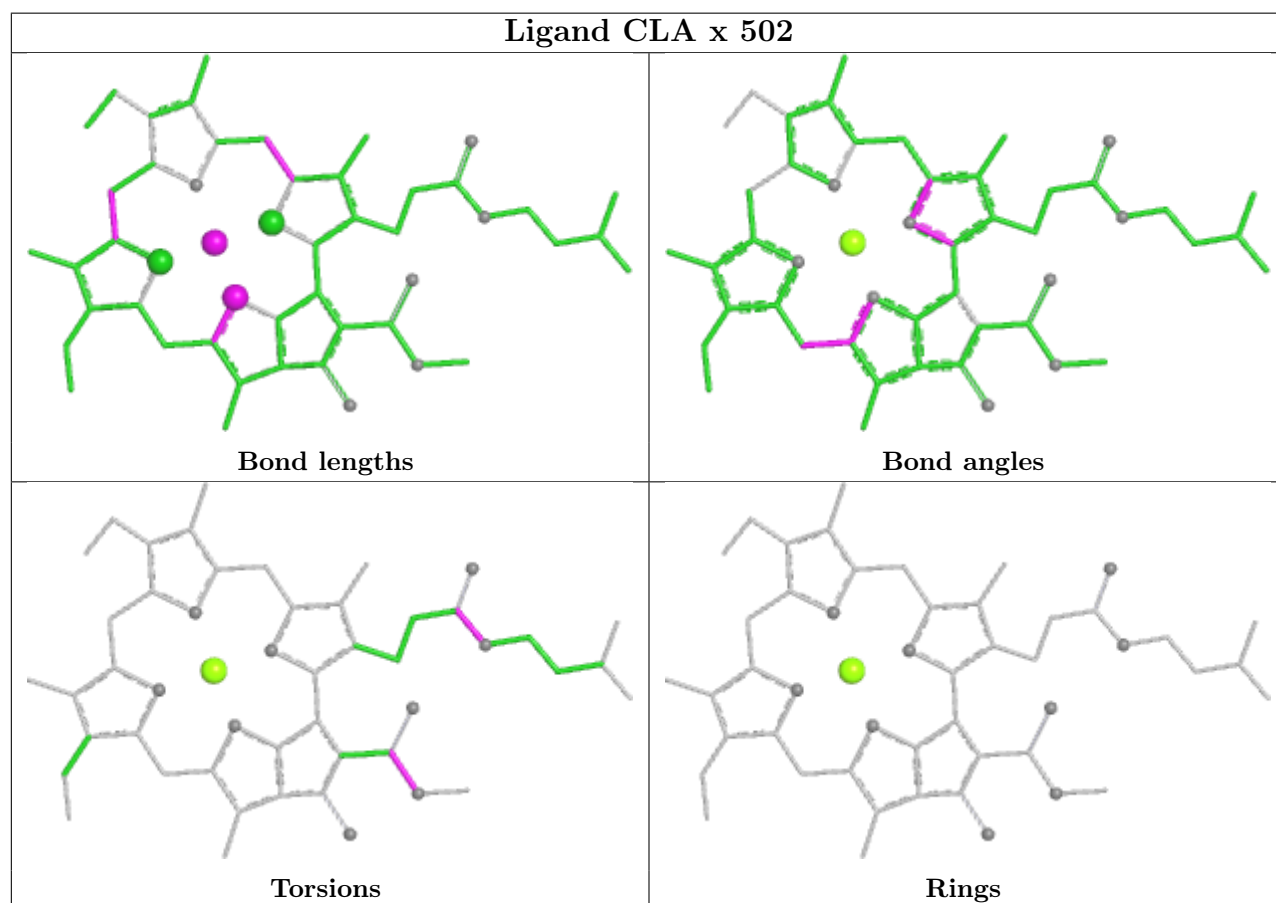
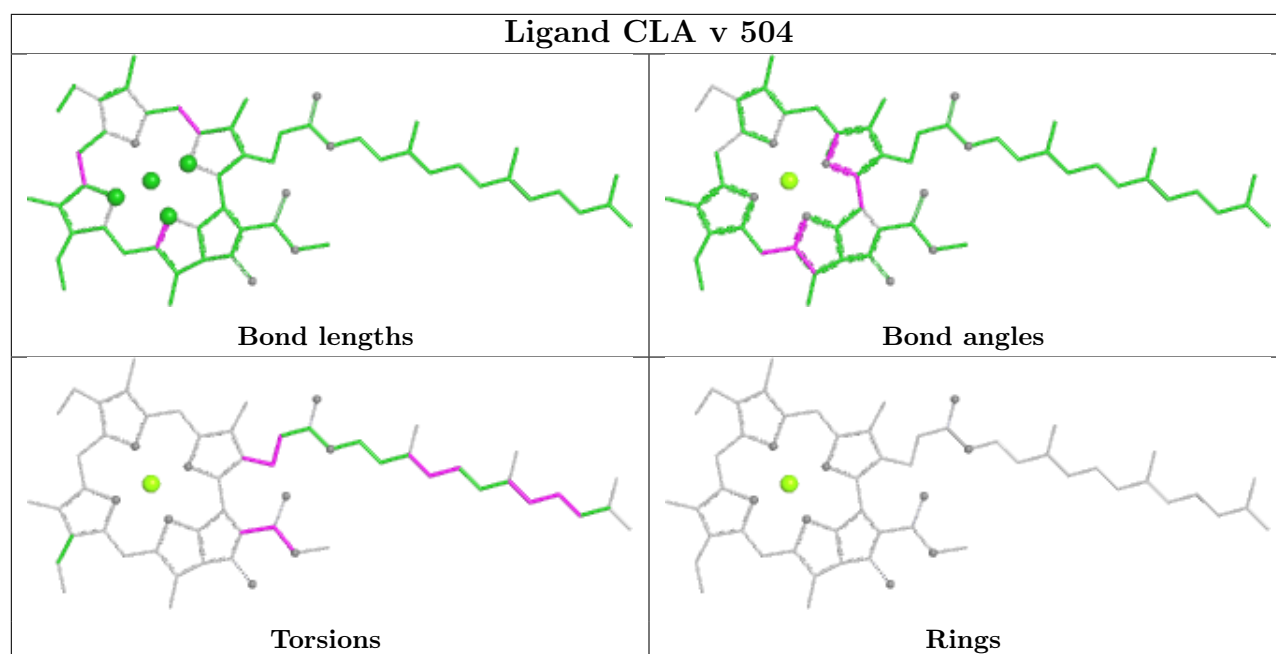




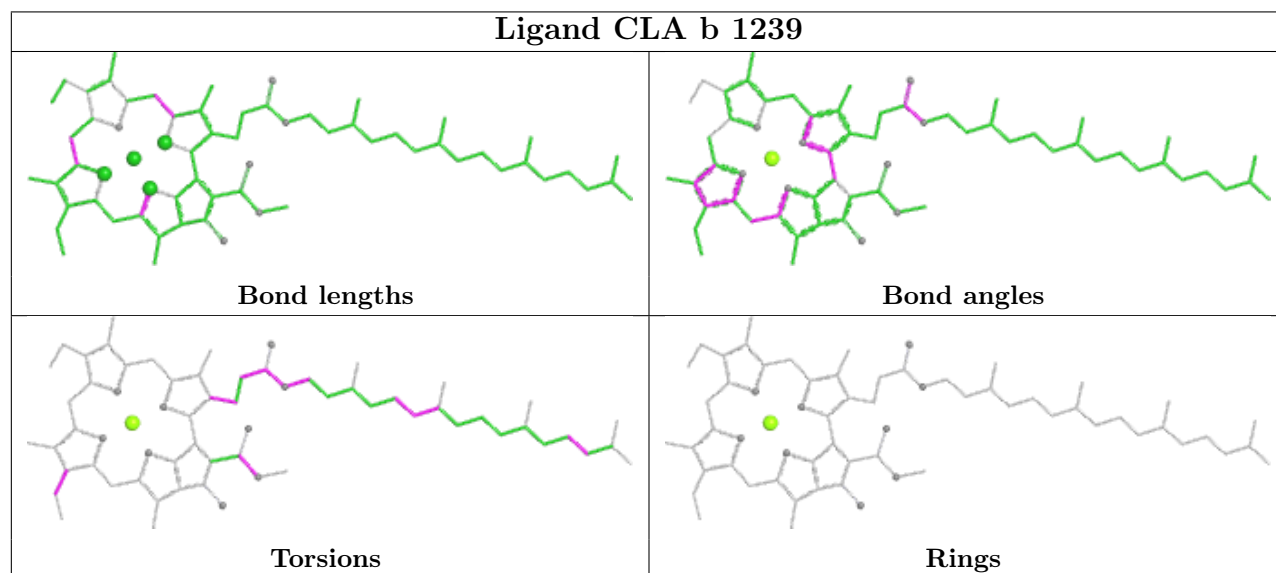
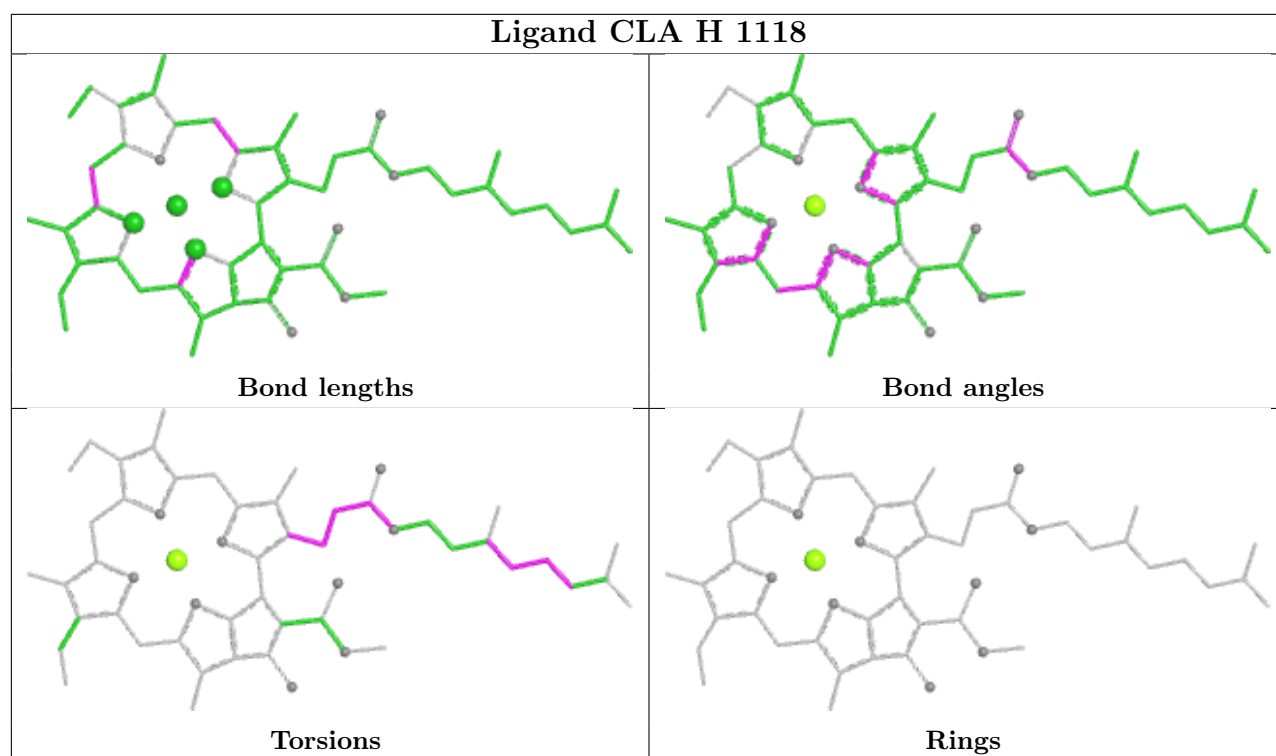






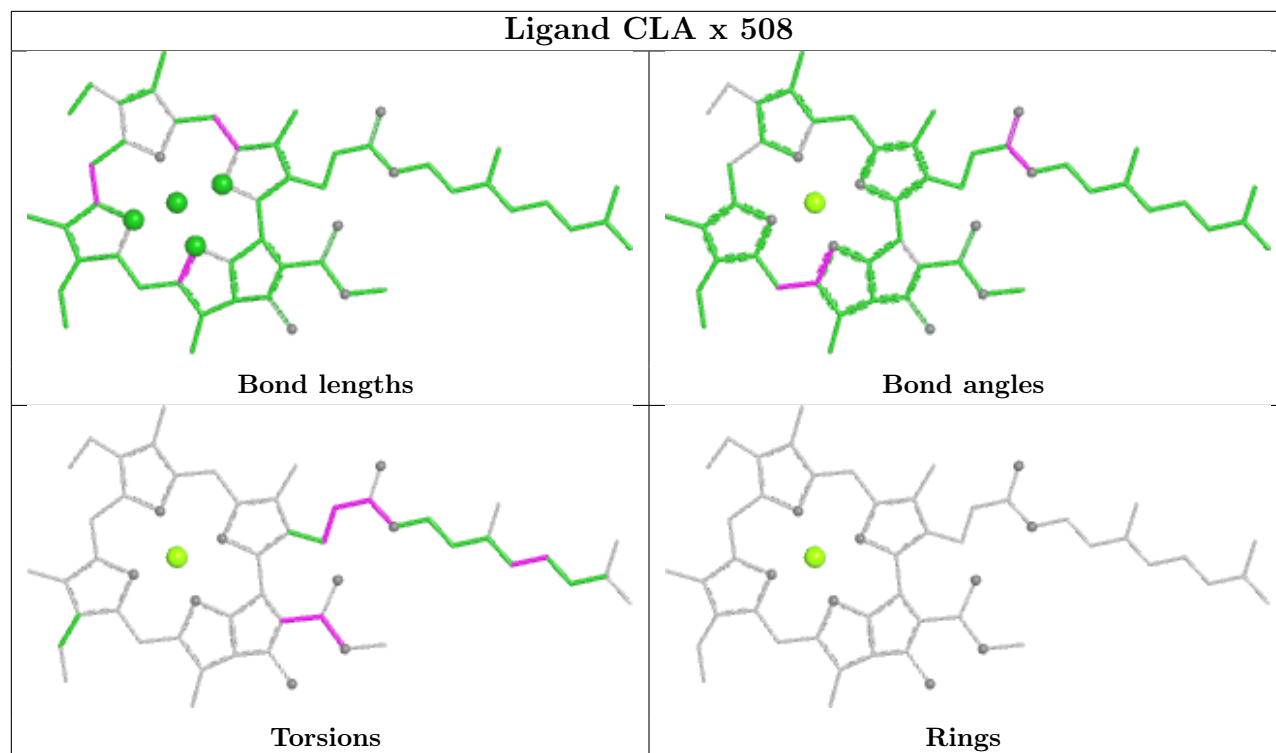




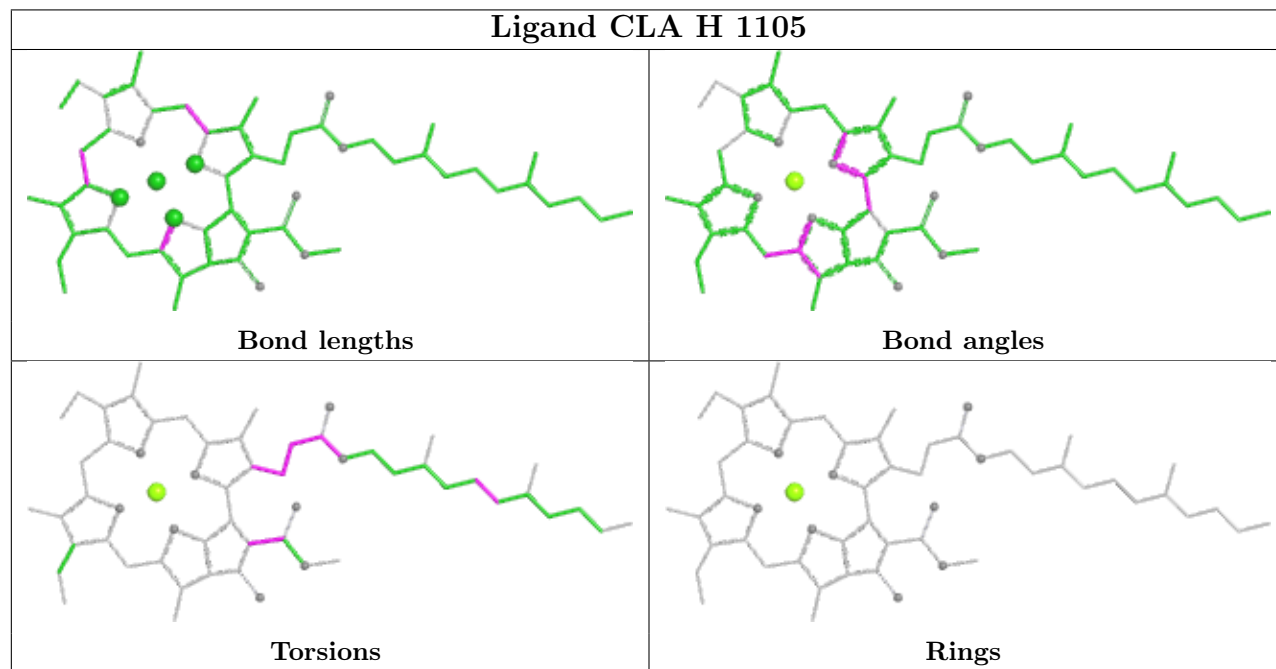




## Ligand CLA x 508

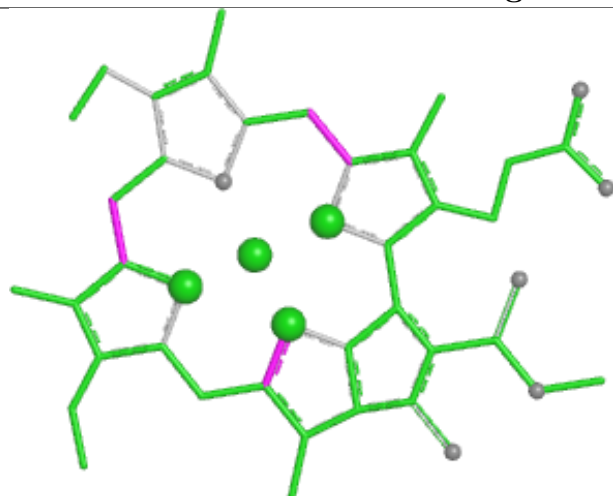


## Ligand CLA H 1105

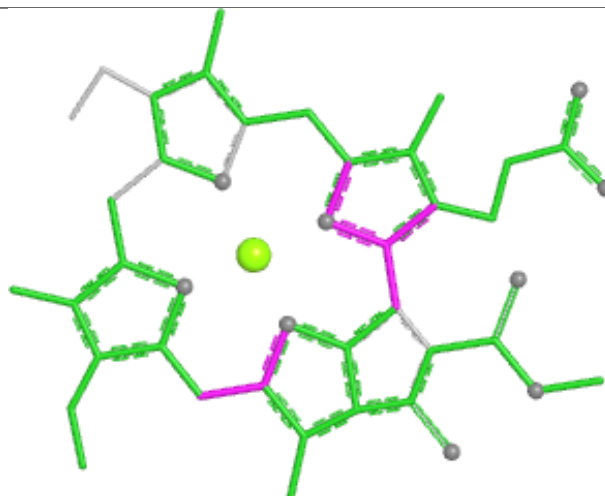




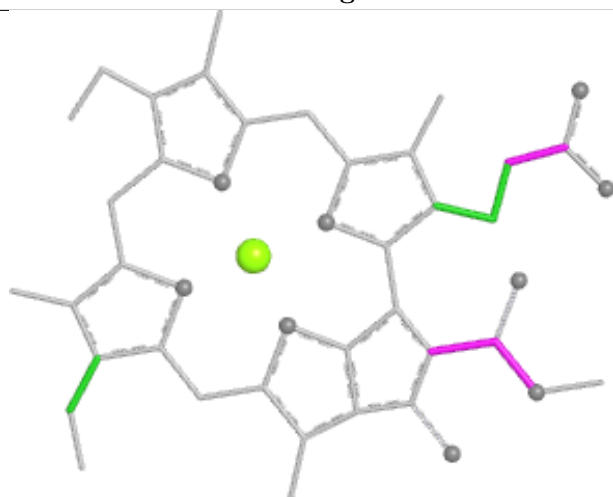
## Ligand CLA B 1232



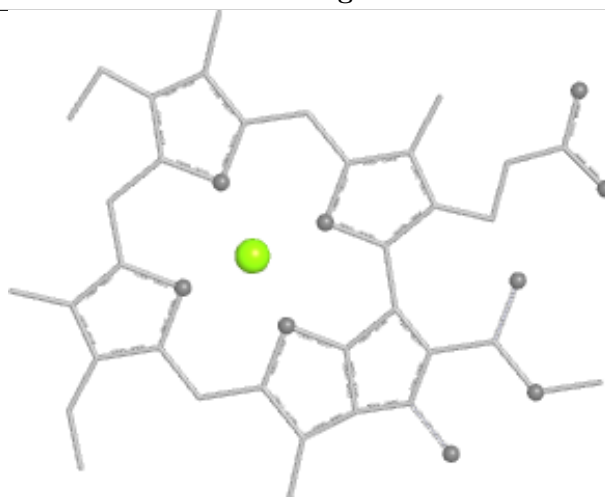
Bond lengths



Bond angles

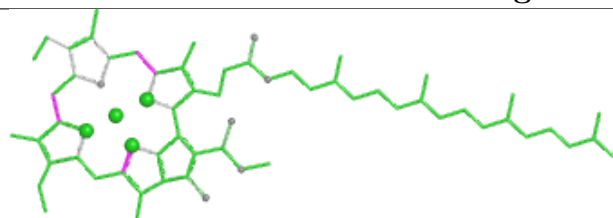


Torsions

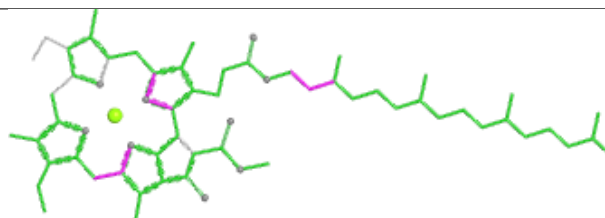


Rings

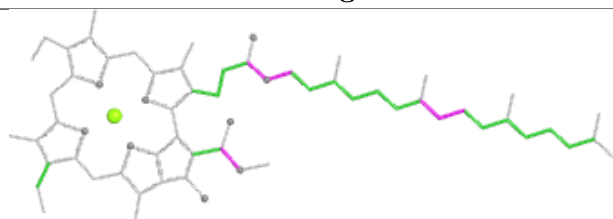
## Ligand CLA Y 507



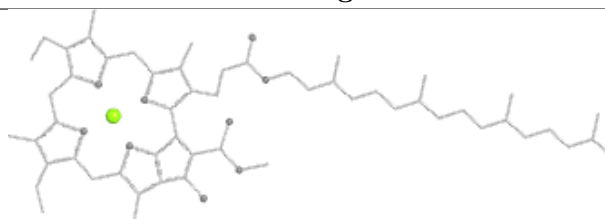
Bond lengths



Bond angles

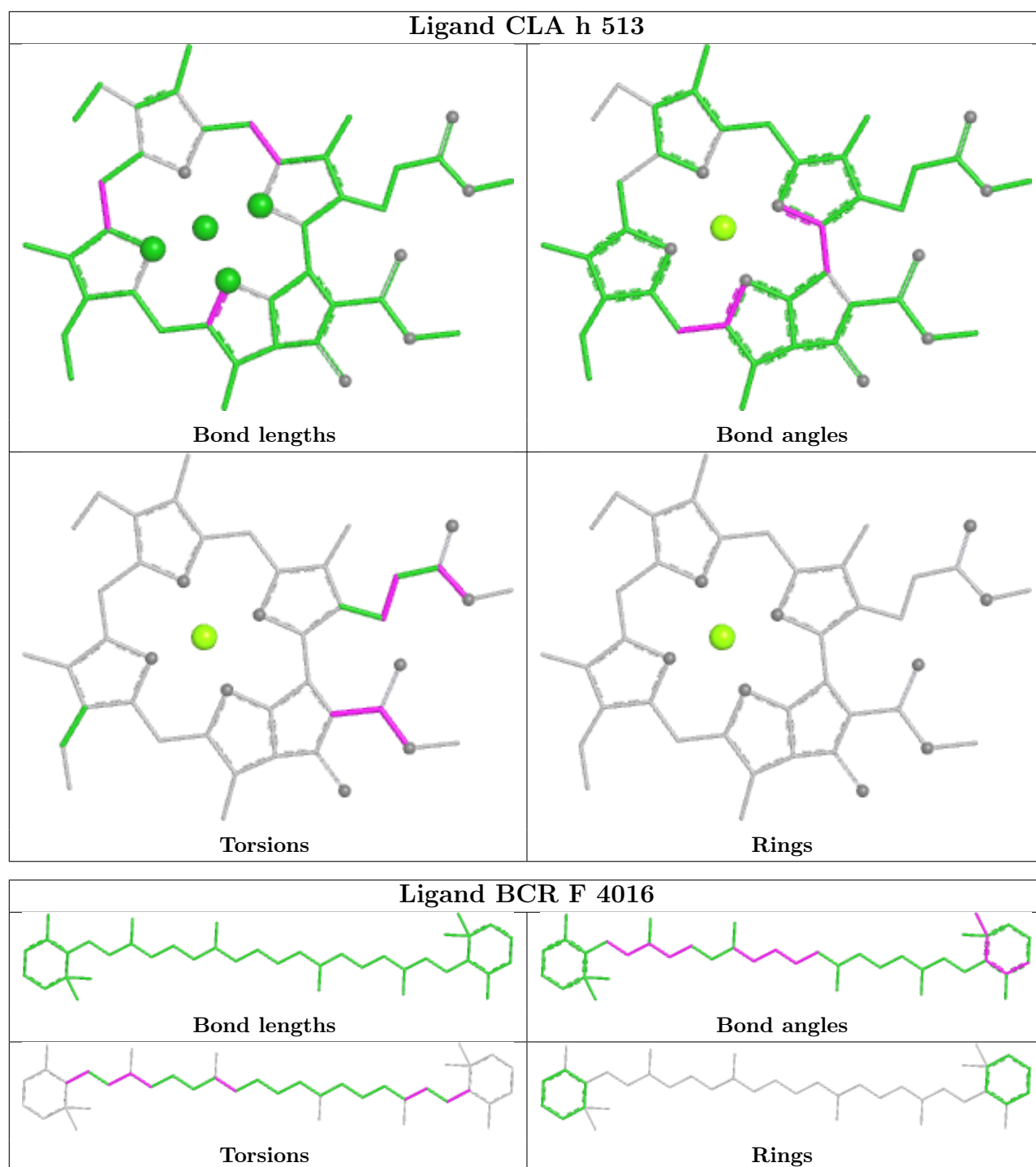


Torsions

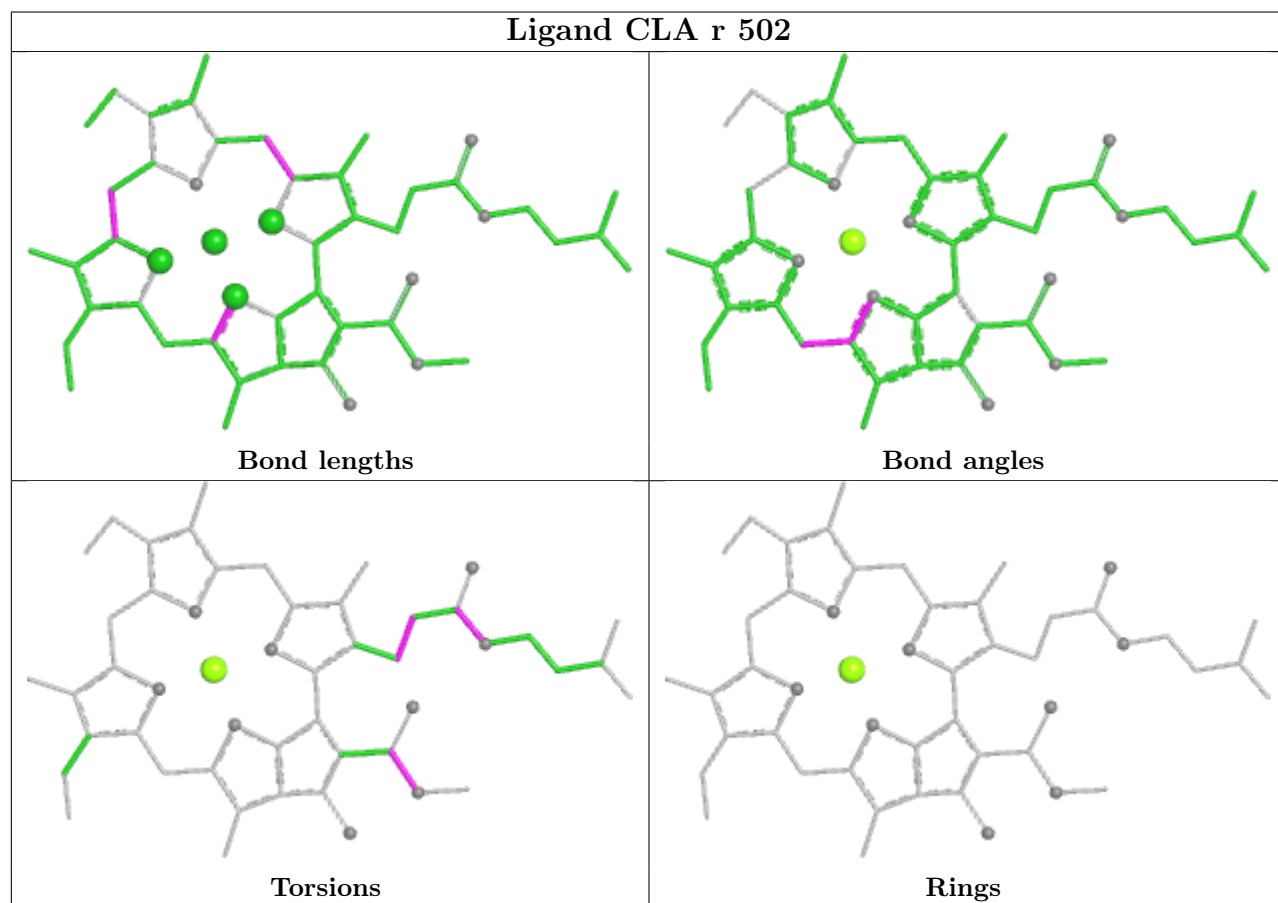
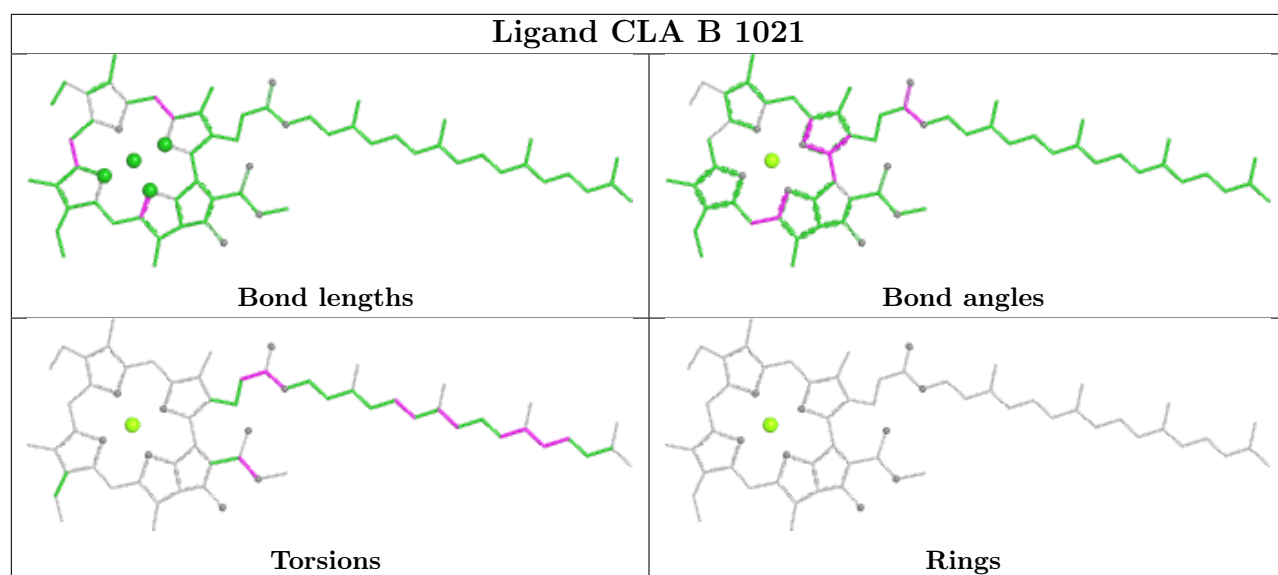


Rings

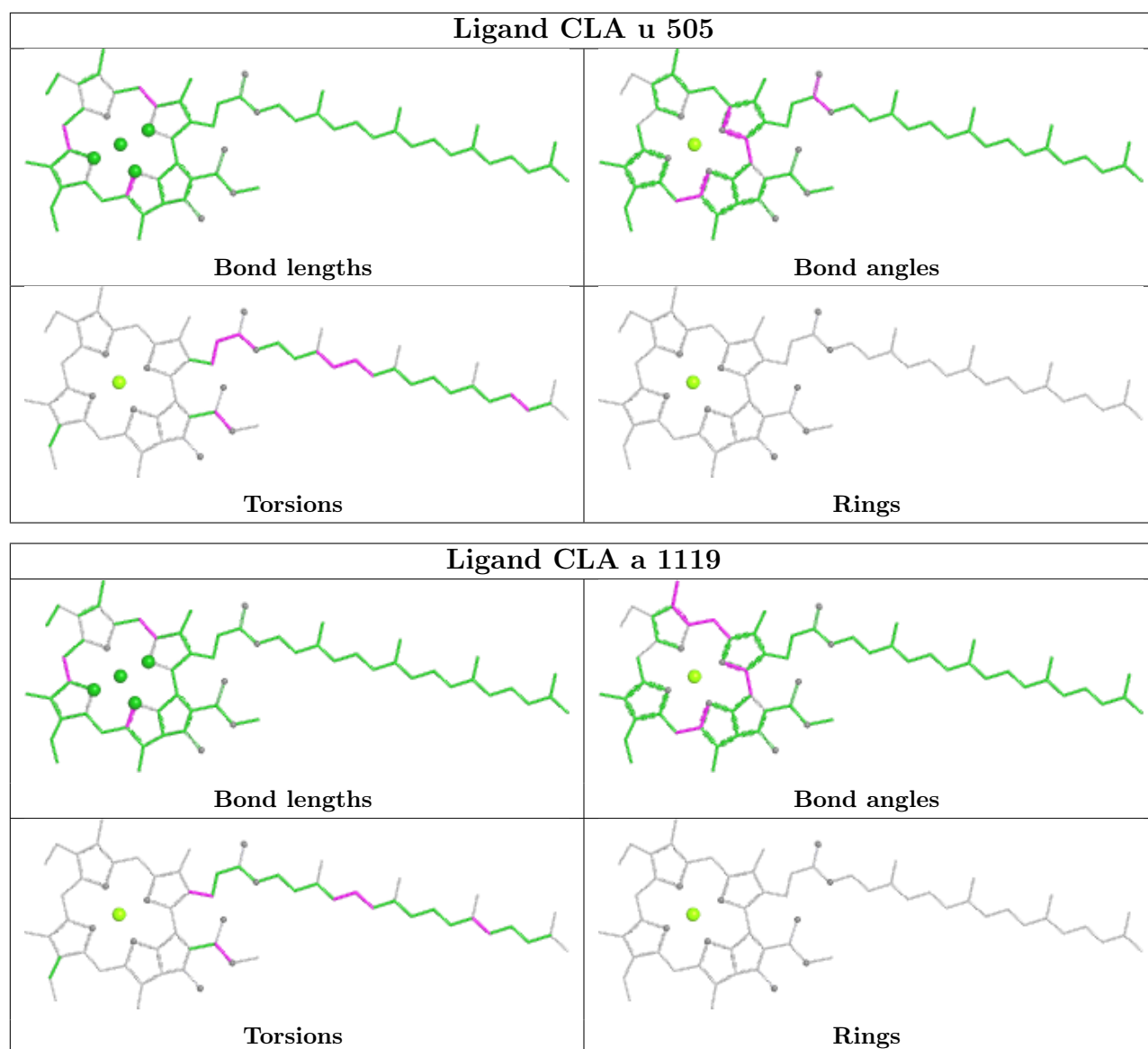






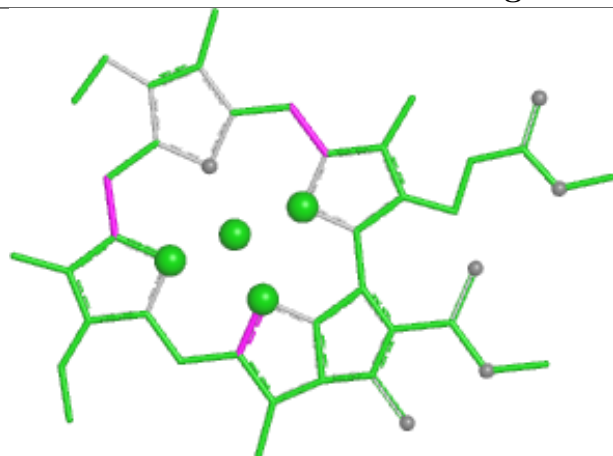




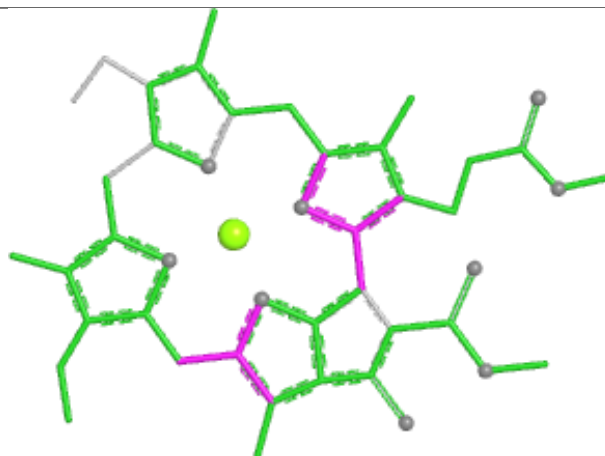




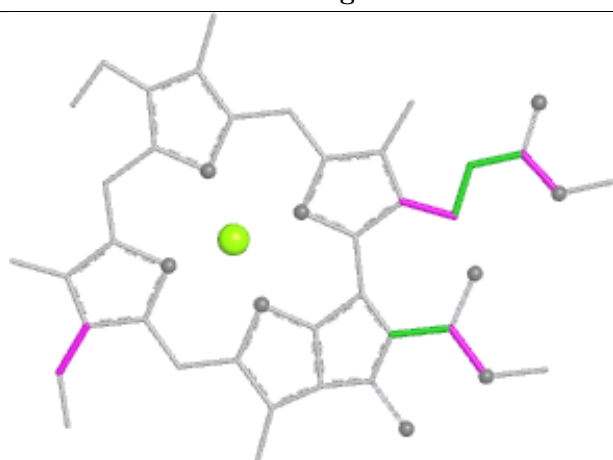
## Ligand CLA H 1114



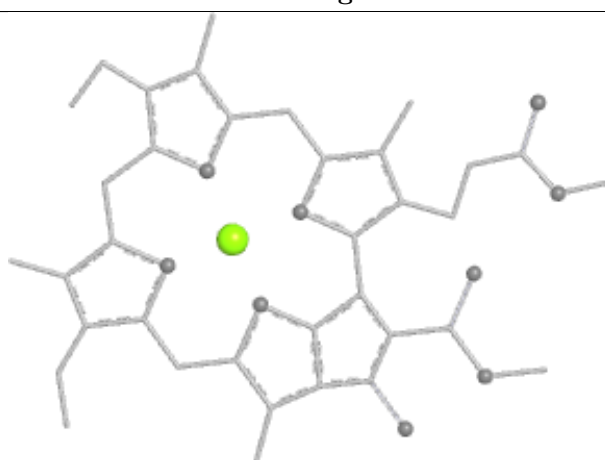
Bond lengths



Bond angles

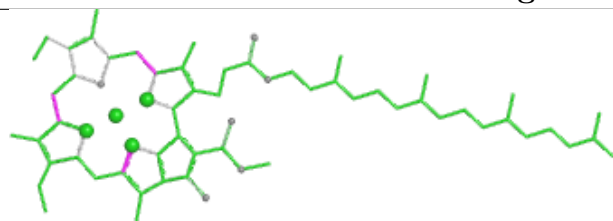


Torsions

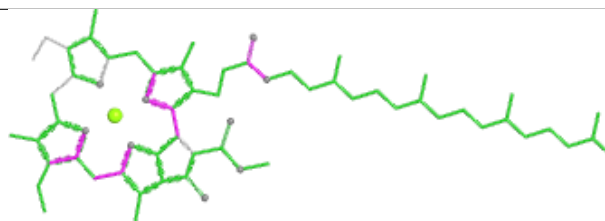


Rings

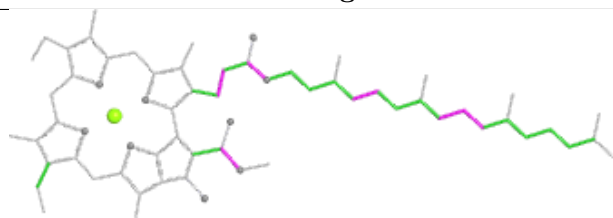
## Ligand CLA x 505



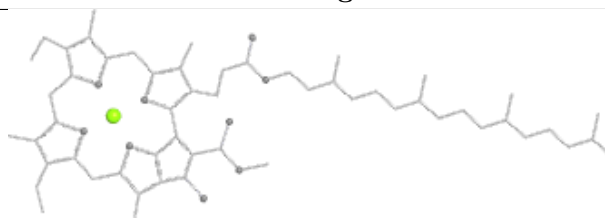
Bond lengths



Bond angles

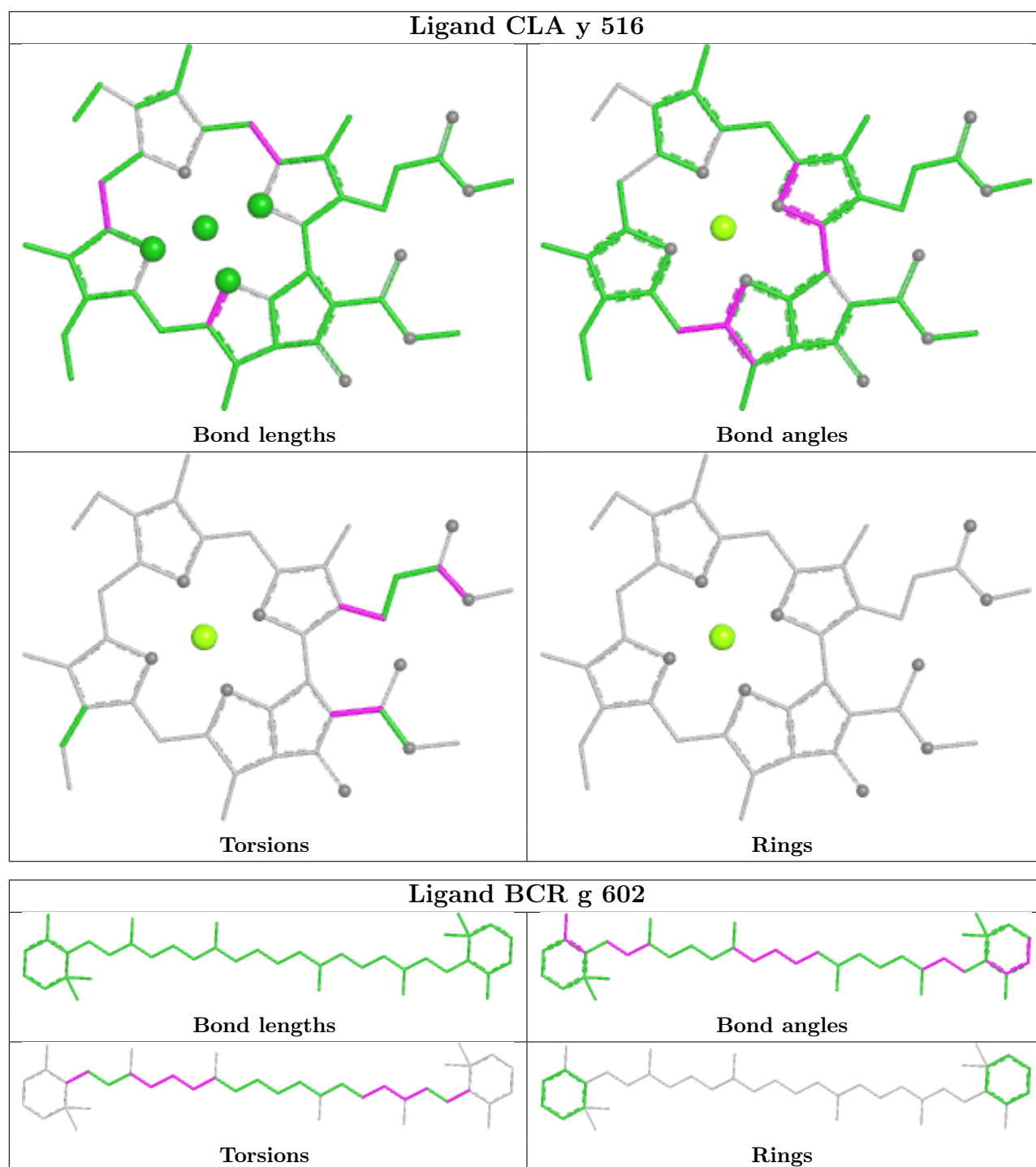


Torsions



Rings





## 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.



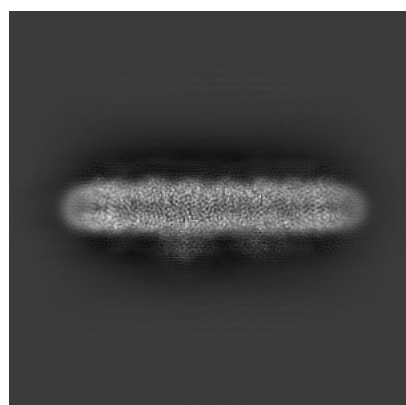
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26601. These allow visual inspection of the internal detail of the map and identification of artifacts.

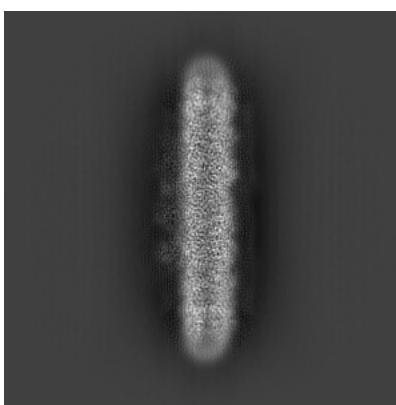
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

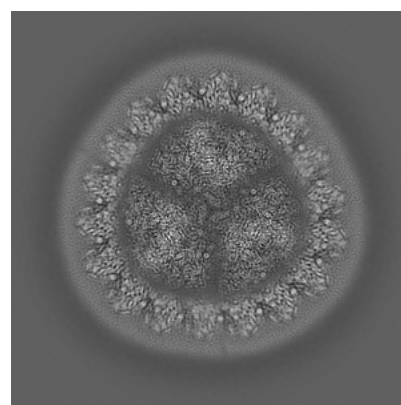
#### 6.1.1 Primary map



X



Y

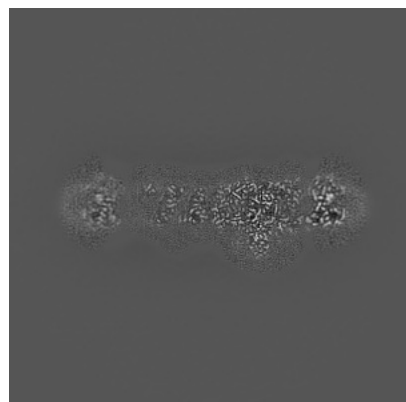


Z

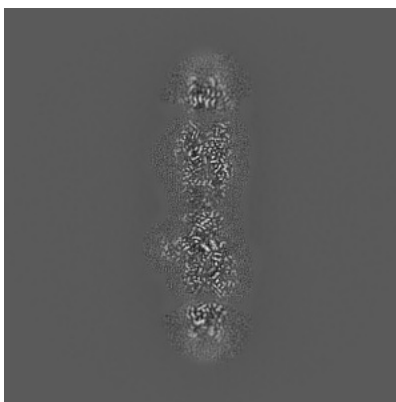
The images above show the map projected in three orthogonal directions.

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

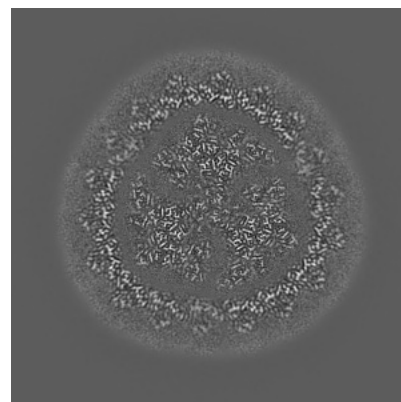
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



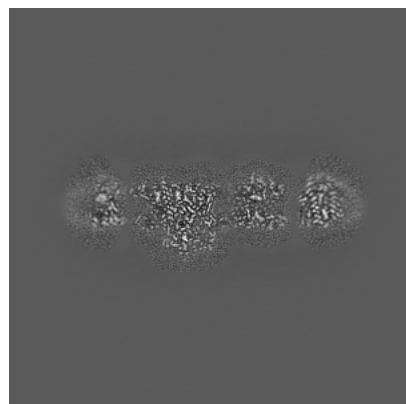
Z Index: 200



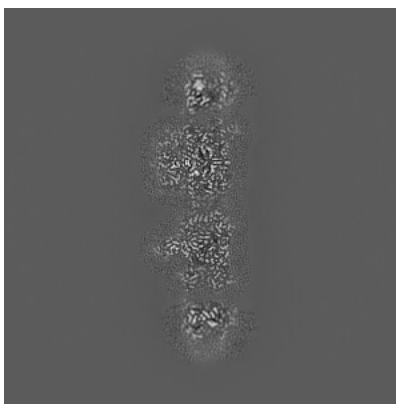
The images above show central slices of the map in three orthogonal directions.

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

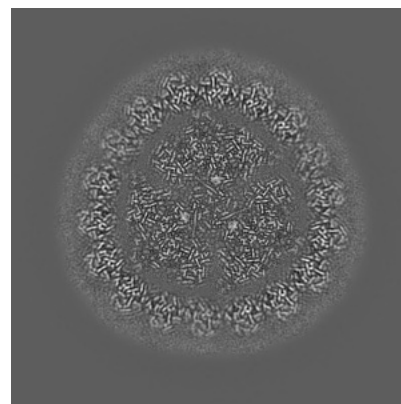
### 6.3.1 Primary map



X Index: 160



Y Index: 177

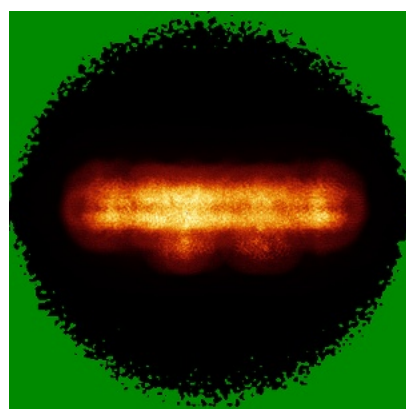


Z Index: 193

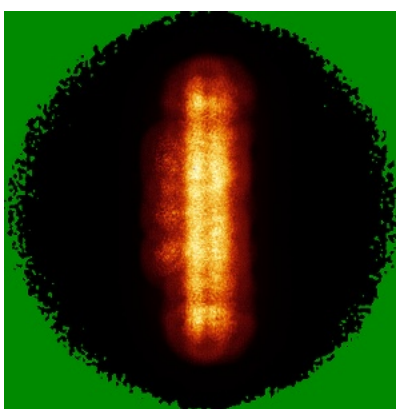
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



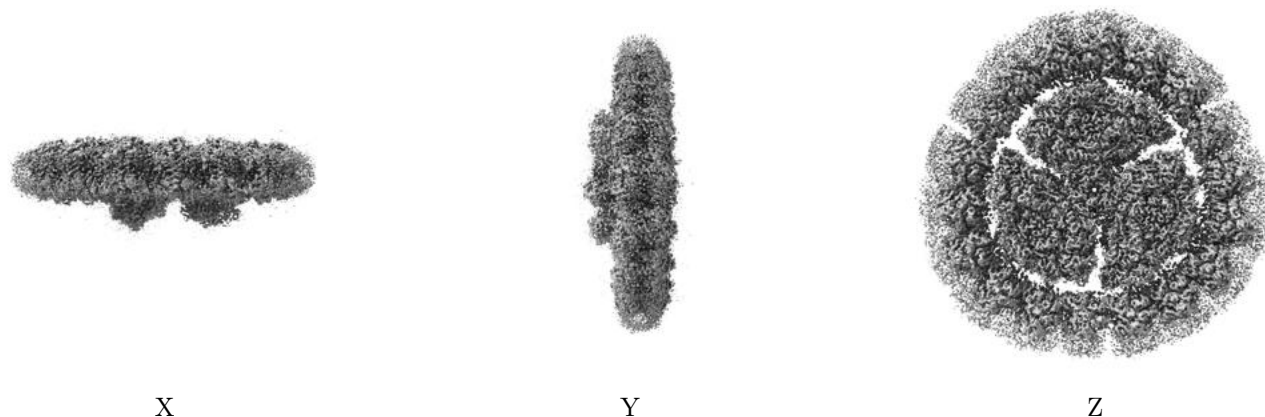
Z

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



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 9.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

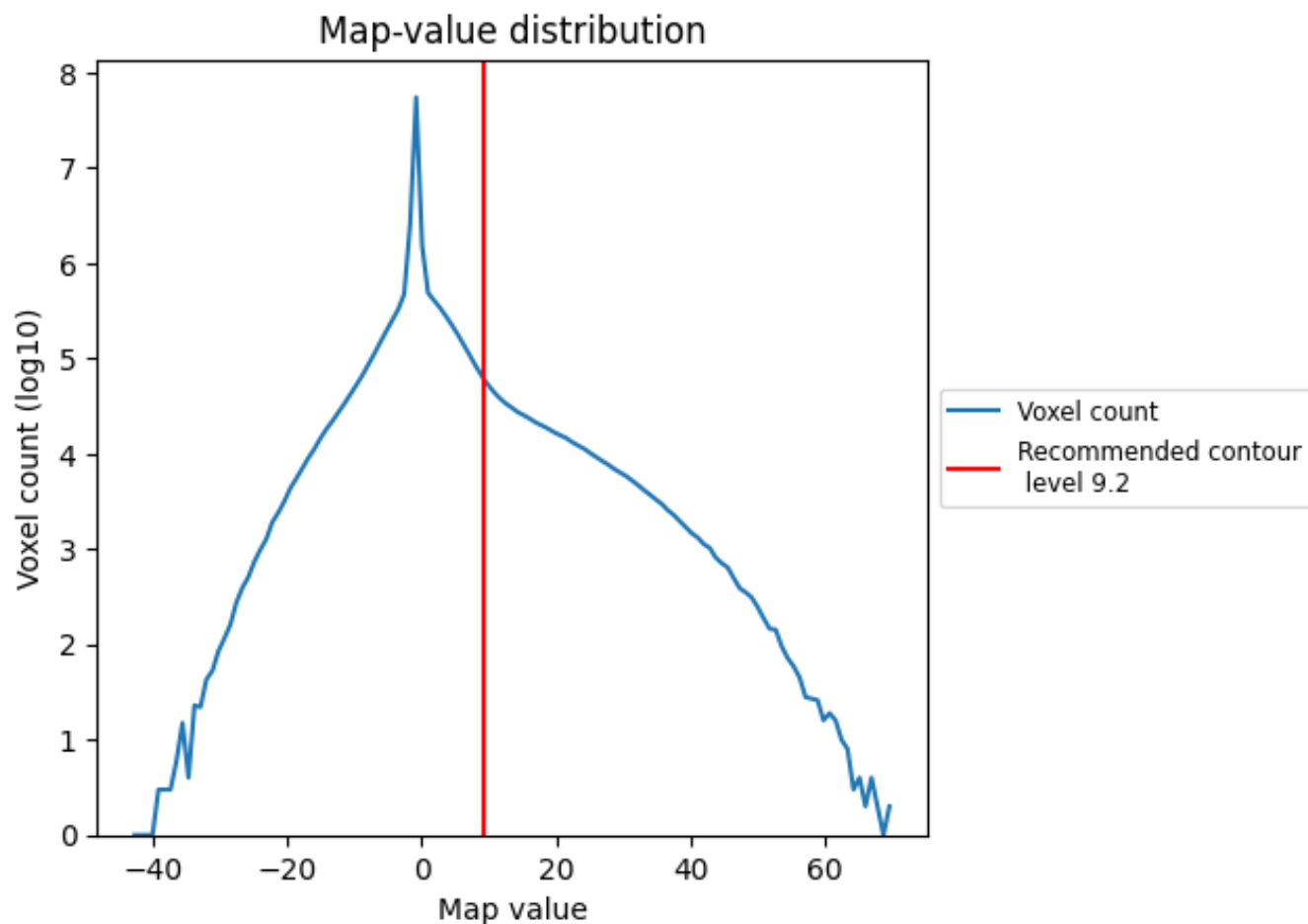
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

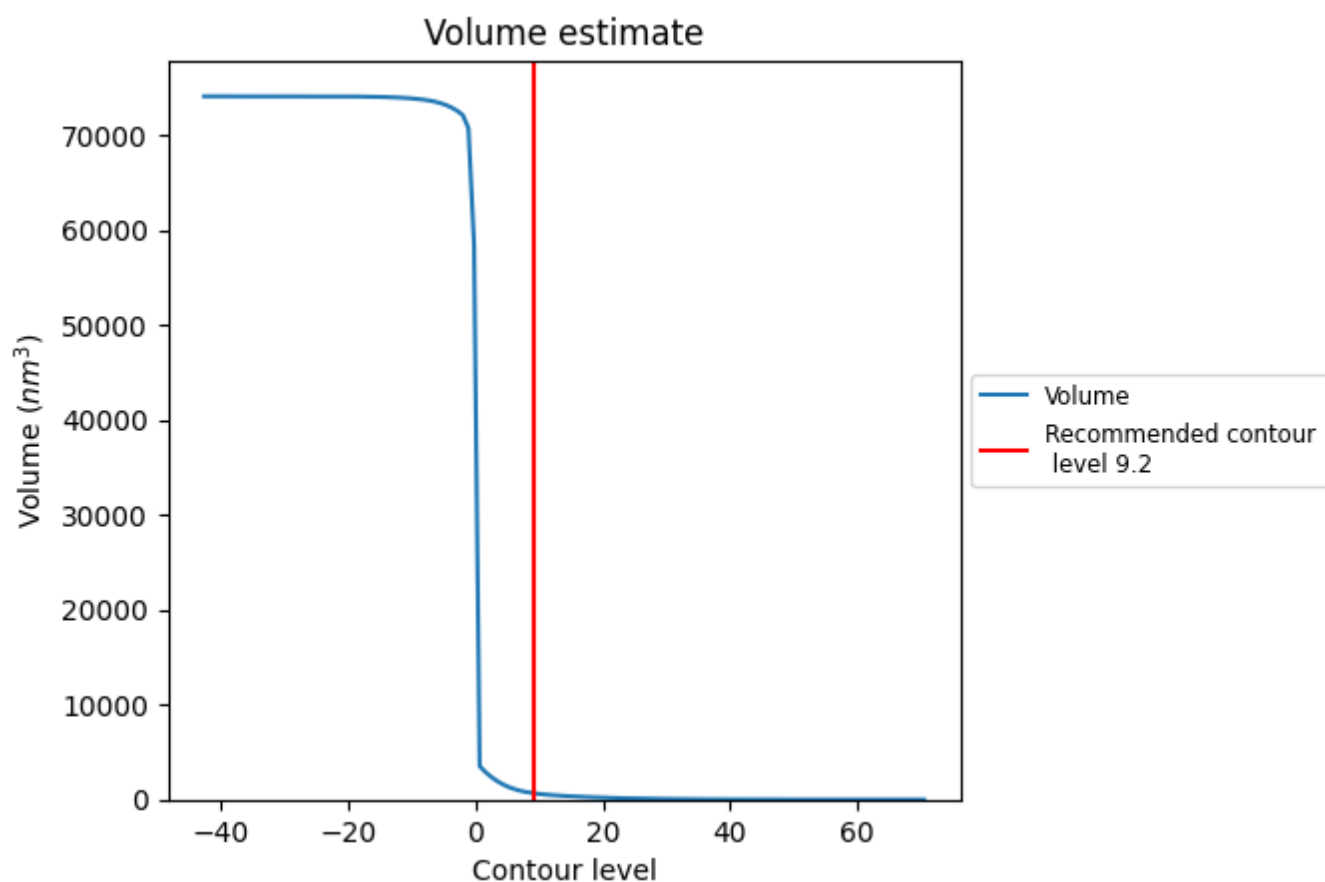
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

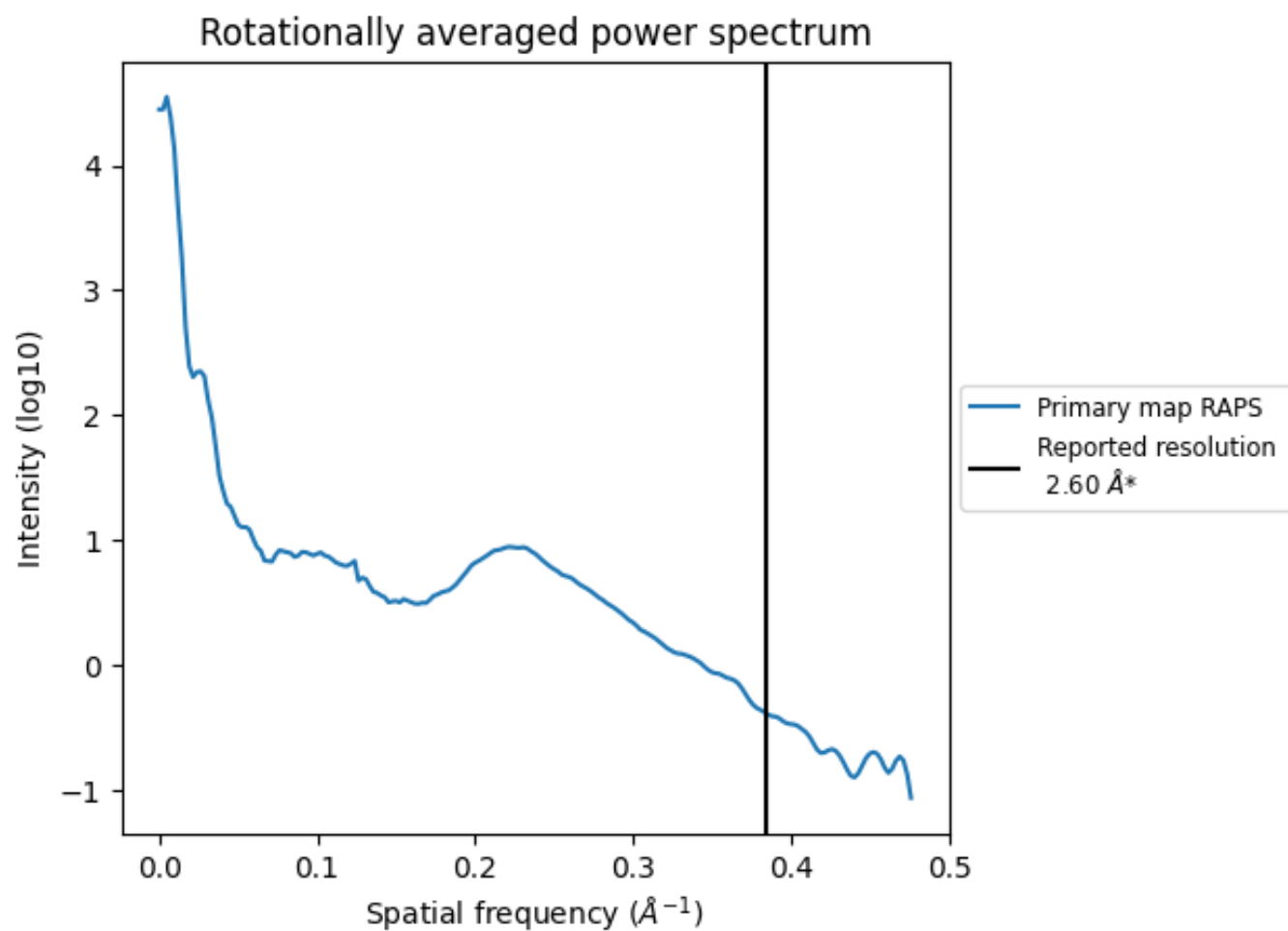


The volume at the recommended contour level is 657  $\text{nm}^3$ ; this corresponds to an approximate mass of 594 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>



## 8 Fourier-Shell correlation

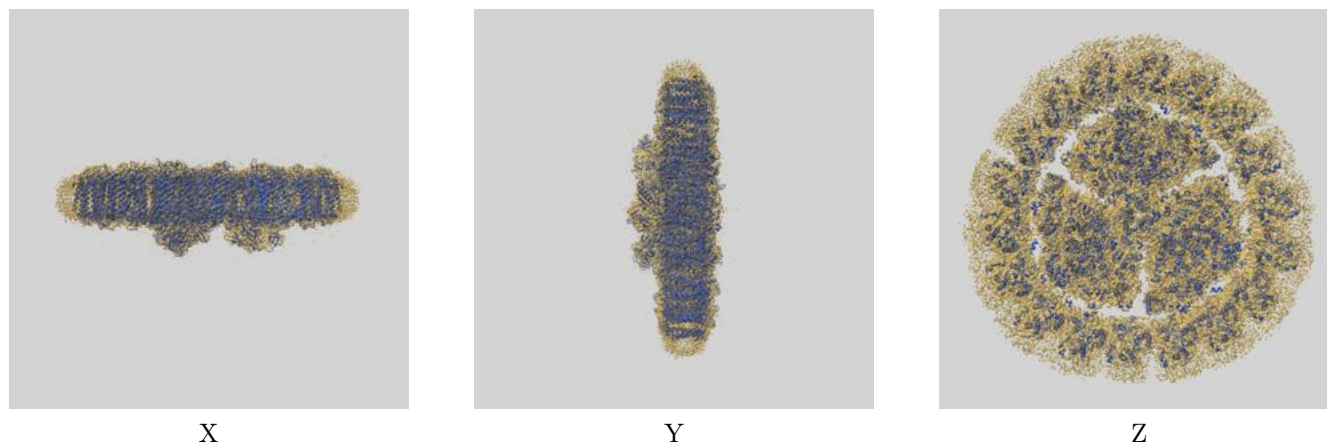
This section was not generated. No FSC curve or half-maps provided.



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

This section contains information regarding the fit between EMDB map EMD-26601 and PDB model 7UMH. Per-residue inclusion information can be found in section [3](#) on page [64](#).

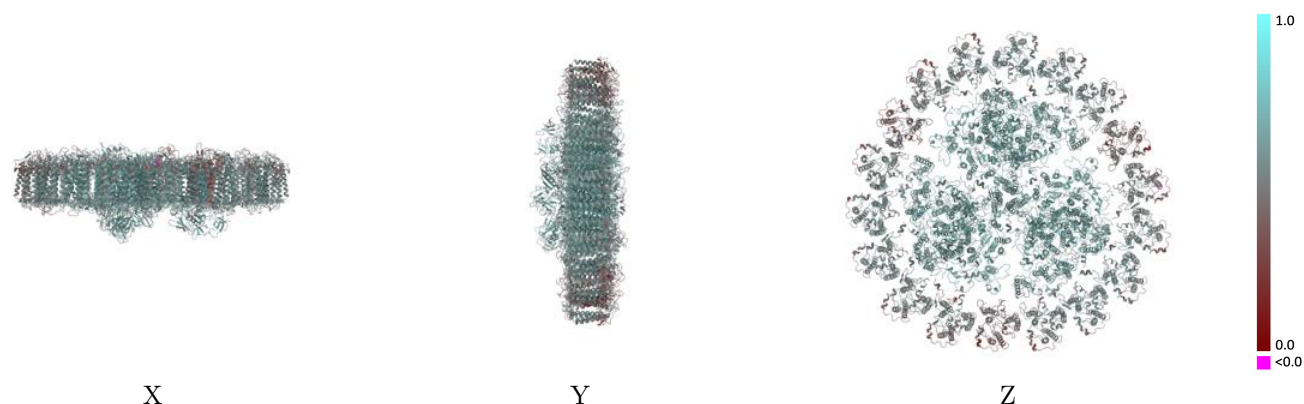
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 9.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

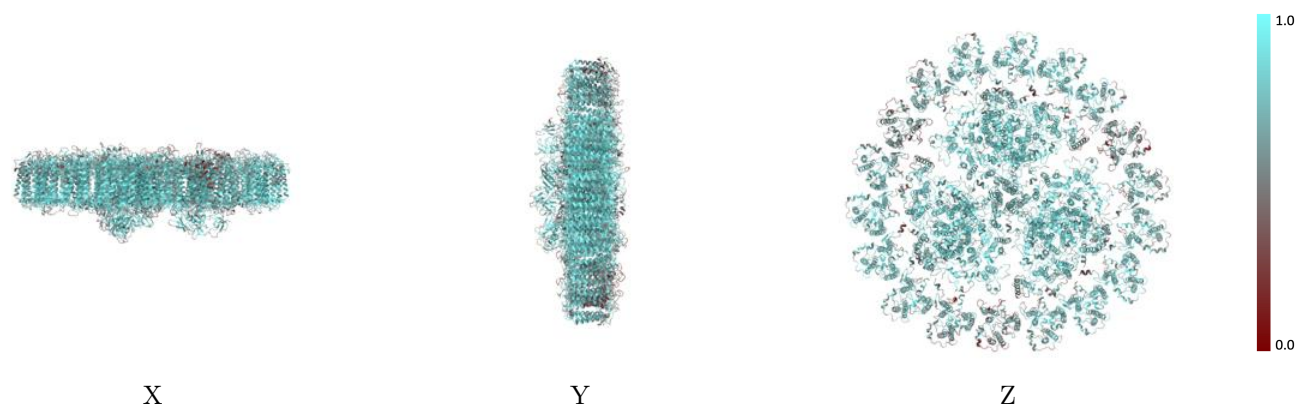


## 9.2 Q-score mapped to coordinate model [i](#)



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

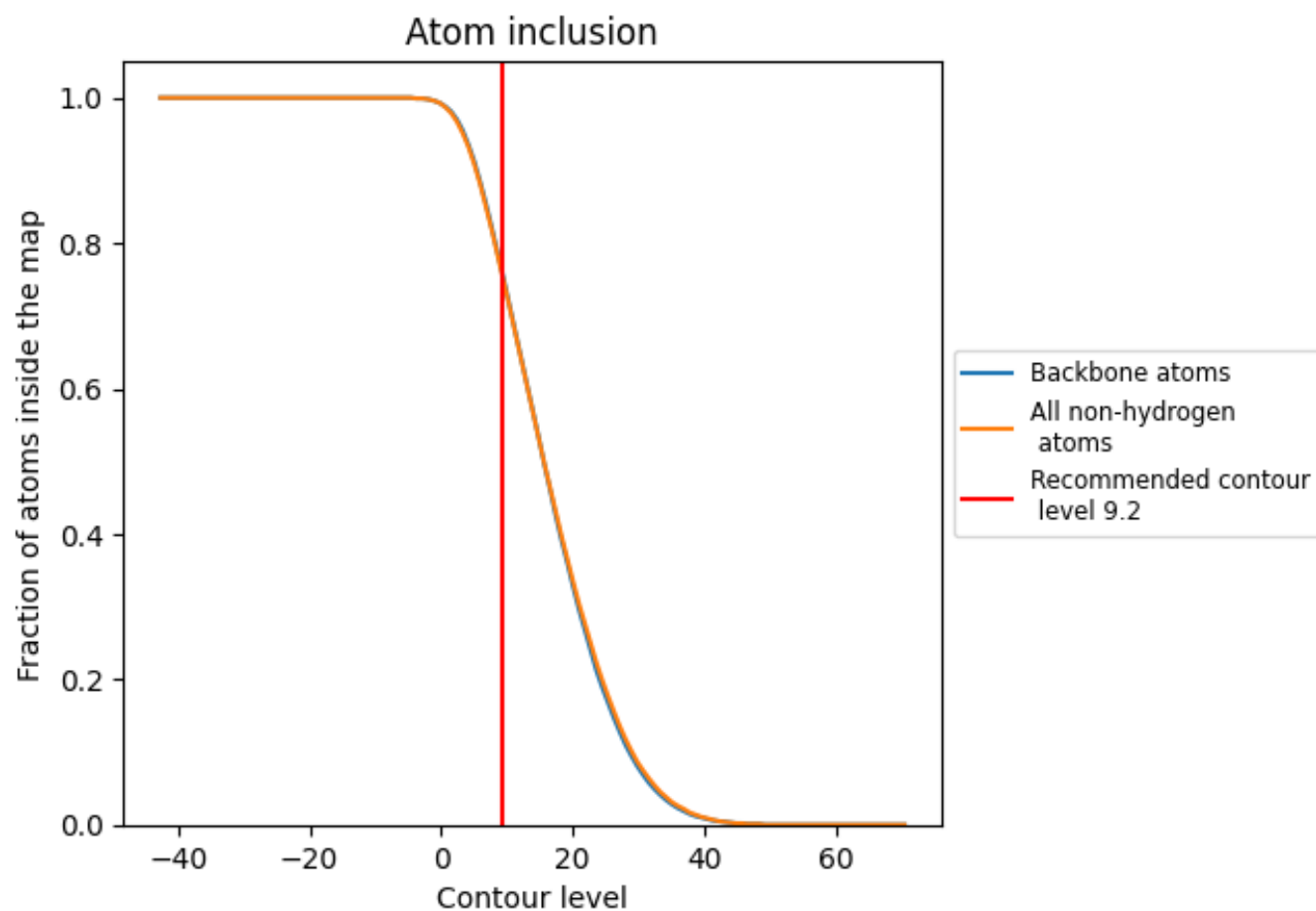
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (9.2).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 76% 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 (9.2) and Q-score for the entire model and for each chain.



































Chain	Atom inclusion	Q-score
All	 0.7600	 0.5830
A	 0.8500	 0.6590
B	 0.8530	 0.6580
C	 0.8720	 0.6440
D	 0.7320	 0.6010
E	 0.7110	 0.5910
F	 0.6610	 0.6030
G	 0.8570	 0.6580
H	 0.8550	 0.6590
I	 0.7320	 0.6300
J	 0.7310	 0.6300
K	 0.5930	 0.5910
L	 0.7710	 0.6360
M	 0.7140	 0.6350
N	 0.8740	 0.6450
O	 0.6800	 0.5860
P	 0.7240	 0.6040
Q	 0.6700	 0.6070
R	 0.7320	 0.6350
S	 0.7270	 0.6340
T	 0.6090	 0.5850
U	 0.7720	 0.6400
V	 0.6770	 0.6170
W	 0.6650	 0.5000
X	 0.7490	 0.5360
Y	 0.7840	 0.5560
Z	 0.7720	 0.5460
a	 0.8490	 0.6620
b	 0.8570	 0.6610
c	 0.8700	 0.6500
d	 0.7210	 0.6020
e	 0.6720	 0.5800
f	 0.6720	 0.6070
g	 0.7050	 0.5260
h	 0.5270	 0.4200



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.7370	 0.6290
j	 0.7590	 0.6360
k	 0.6030	 0.5890
l	 0.7650	 0.6350
m	 0.7140	 0.6350
n	 0.6720	 0.5010
o	 0.7400	 0.5370
p	 0.7770	 0.5570
q	 0.7590	 0.5430
r	 0.6990	 0.5170
s	 0.7750	 0.5550
t	 0.6620	 0.4980
u	 0.7400	 0.5300
v	 0.5460	 0.4350
w	 0.7620	 0.5450
x	 0.6830	 0.5150
y	 0.5320	 0.4260