



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 05:21 am GMT

PDB ID : 7QCO  
EMDB ID : EMD-13898  
Title : The structure of Photosystem I tetramer from *Chroococcidiopsis* TS-821, a thermophilic, unicellular, non-heterocyst-forming cyanobacterium  
Authors : Semchonok, D.A.; Mondal, J.; Cooper, J.C.; Schlum, K.; Li, M.; Amin, M.; Sorzano, C.O.S.; Ramirez-Aportela, E.; Kastiris, P.L.; Boekema, E.J.; Guskov, A.; Bruce, B.D.  
Deposited on : 2021-11-24  
Resolution : 3.70 Å(reported)  
Based on initial model : 1JB0

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:

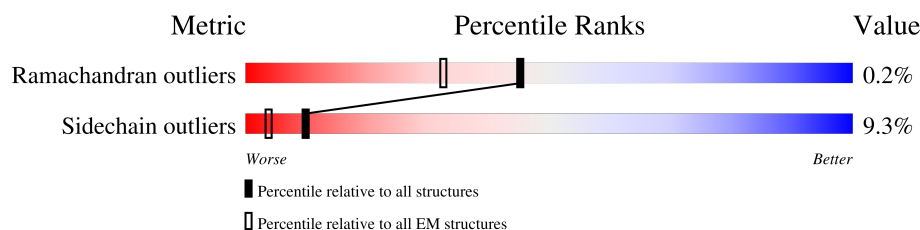
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 3.70 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	752	
1	E	752	
1	a	752	
1	e	752	
2	B	737	
2	G	737	
2	b	737	
2	g	737	

*Continued on next page...*



Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	82	
3	H	82	
3	c	82	
3	h	82	
4	D	168	
4	N	168	
4	d	168	
4	n	168	
5	V	126	
5	W	126	
5	v	126	
5	w	126	
6	F	164	
6	O	164	
6	f	164	
6	o	164	
7	I	39	
7	P	39	
7	i	39	
7	p	39	
8	J	49	
8	Q	49	
8	j	49	
8	q	49	
9	K	93	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	R	93	
9	k	93	
9	r	93	
10	L	172	
10	S	172	
10	l	172	
10	s	172	
11	M	31	
11	T	31	
11	m	31	
11	t	31	

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
13	CLA	A	803	X	-	-	-
13	CLA	A	804	X	-	-	-
13	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	809	X	-	-	-
13	CLA	A	810	X	-	-	-
13	CLA	A	811	X	-	-	-
13	CLA	A	812	X	-	-	-
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	-
13	CLA	A	816	X	-	-	-
13	CLA	A	817	X	-	-	-
13	CLA	A	818	X	-	-	-
13	CLA	A	819	X	-	-	-
13	CLA	A	820	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	-
13	CLA	A	823	X	-	-	-
13	CLA	A	824	X	-	-	-
13	CLA	A	825	X	-	-	-
13	CLA	A	826	X	-	-	-
13	CLA	A	827	X	-	-	-
13	CLA	A	828	X	-	-	-
13	CLA	A	829	X	-	-	-
13	CLA	A	830	X	-	-	-
13	CLA	A	831	X	-	-	-
13	CLA	A	832	X	-	-	-
13	CLA	A	833	X	-	-	-
13	CLA	A	834	X	-	-	-
13	CLA	A	835	X	-	-	-
13	CLA	A	836	X	-	-	-
13	CLA	A	838	X	-	-	-
13	CLA	A	839	X	-	-	-
13	CLA	A	840	X	-	-	-
13	CLA	A	841	X	-	-	-
13	CLA	A	842	X	-	-	-
13	CLA	A	843	X	-	-	-
13	CLA	A	844	X	-	-	-
13	CLA	A	845	X	-	-	-
13	CLA	A	853	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	-
13	CLA	B	804	X	-	-	-
13	CLA	B	805	X	-	-	-
13	CLA	B	806	X	-	-	-
13	CLA	B	807	X	-	-	-
13	CLA	B	808	X	-	-	-
13	CLA	B	809	X	-	-	-
13	CLA	B	810	X	-	-	-
13	CLA	B	811	X	-	-	-
13	CLA	B	812	X	-	-	-
13	CLA	B	813	X	-	-	-
13	CLA	B	814	X	-	-	-
13	CLA	B	815	X	-	-	-
13	CLA	B	816	X	-	-	-
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	-
13	CLA	B	821	X	-	-	-
13	CLA	B	822	X	-	-	-
13	CLA	B	823	X	-	-	-
13	CLA	B	824	X	-	-	-
13	CLA	B	825	X	-	-	-
13	CLA	B	826	X	-	-	-
13	CLA	B	827	X	-	-	-
13	CLA	B	828	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	-	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	X	-	-	-
13	CLA	B	834	X	-	-	-
13	CLA	B	835	X	-	-	-
13	CLA	B	836	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	838	X	-	-	-
13	CLA	B	839	X	-	-	-
13	CLA	B	840	X	-	-	-
13	CLA	B	841	X	-	-	-
13	CLA	E	803	X	-	-	-
13	CLA	E	804	X	-	-	-
13	CLA	E	805	X	-	-	-
13	CLA	E	806	X	-	-	-
13	CLA	E	807	X	-	-	-
13	CLA	E	808	X	-	-	-
13	CLA	E	809	X	-	-	-
13	CLA	E	810	X	-	-	-
13	CLA	E	811	X	-	-	-
13	CLA	E	812	X	-	-	-
13	CLA	E	813	X	-	-	-
13	CLA	E	814	X	-	-	-
13	CLA	E	815	X	-	-	-
13	CLA	E	816	X	-	-	-
13	CLA	E	817	X	-	-	-
13	CLA	E	818	X	-	-	-
13	CLA	E	819	X	-	-	-
13	CLA	E	820	X	-	-	-
13	CLA	E	821	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	E	822	X	-	-	-
13	CLA	E	823	X	-	-	-
13	CLA	E	824	X	-	-	-
13	CLA	E	825	X	-	-	-
13	CLA	E	826	X	-	-	-
13	CLA	E	827	X	-	-	-
13	CLA	E	828	X	-	-	-
13	CLA	E	829	X	-	-	-
13	CLA	E	830	X	-	-	-
13	CLA	E	831	X	-	-	-
13	CLA	E	832	X	-	-	-
13	CLA	E	833	X	-	-	-
13	CLA	E	834	X	-	-	-
13	CLA	E	835	X	-	-	-
13	CLA	E	836	X	-	-	-
13	CLA	E	837	X	-	-	-
13	CLA	E	839	X	-	-	-
13	CLA	E	840	X	-	-	-
13	CLA	E	841	X	-	-	-
13	CLA	E	842	X	-	-	-
13	CLA	E	843	X	-	-	-
13	CLA	E	844	X	-	-	-
13	CLA	E	845	X	-	-	-
13	CLA	E	846	X	-	-	-
13	CLA	F	202	X	-	-	-
13	CLA	G	801	X	-	-	-
13	CLA	G	802	X	-	-	-
13	CLA	G	803	X	-	-	-
13	CLA	G	804	X	-	-	-
13	CLA	G	805	X	-	-	-
13	CLA	G	806	X	-	-	-
13	CLA	G	807	X	-	-	-
13	CLA	G	808	X	-	-	-
13	CLA	G	809	X	-	-	-
13	CLA	G	810	X	-	-	-
13	CLA	G	811	X	-	-	-
13	CLA	G	812	X	-	-	-
13	CLA	G	813	X	-	-	-
13	CLA	G	814	X	-	-	-
13	CLA	G	815	X	-	-	-
13	CLA	G	816	X	-	-	-
13	CLA	G	817	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	G	818	X	-	-	-
13	CLA	G	819	X	-	-	-
13	CLA	G	820	X	-	-	-
13	CLA	G	821	X	-	-	-
13	CLA	G	822	X	-	-	-
13	CLA	G	823	X	-	-	-
13	CLA	G	824	X	-	-	-
13	CLA	G	825	X	-	-	-
13	CLA	G	826	X	-	-	-
13	CLA	G	827	X	-	-	-
13	CLA	G	828	X	-	-	-
13	CLA	G	829	X	-	-	-
13	CLA	G	830	X	-	-	-
13	CLA	G	831	X	-	-	-
13	CLA	G	832	X	-	-	-
13	CLA	G	833	X	-	-	-
13	CLA	G	834	X	-	-	-
13	CLA	G	835	X	-	-	-
13	CLA	G	836	X	-	-	-
13	CLA	G	837	X	-	-	-
13	CLA	G	838	X	-	-	-
13	CLA	G	839	X	-	-	-
13	CLA	G	840	X	-	-	-
13	CLA	G	841	X	-	-	-
13	CLA	K	101	X	-	-	-
13	CLA	K	102	X	-	-	-
13	CLA	L	202	X	-	-	-
13	CLA	L	203	X	-	-	-
13	CLA	L	204	X	-	-	-
13	CLA	O	203	X	-	-	-
13	CLA	R	102	X	-	-	-
13	CLA	S	203	X	-	-	-
13	CLA	S	204	X	-	-	-
13	CLA	S	206	X	-	-	-
13	CLA	a	804	X	-	-	-
13	CLA	a	805	X	-	-	-
13	CLA	a	806	X	-	-	-
13	CLA	a	807	X	-	-	-
13	CLA	a	808	X	-	-	-
13	CLA	a	809	X	-	-	-
13	CLA	a	810	X	-	-	-
13	CLA	a	811	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	a	812	X	-	-	-
13	CLA	a	813	X	-	-	-
13	CLA	a	814	X	-	-	-
13	CLA	a	815	X	-	-	-
13	CLA	a	816	X	-	-	-
13	CLA	a	817	X	-	-	-
13	CLA	a	818	X	-	-	-
13	CLA	a	819	X	-	-	-
13	CLA	a	820	X	-	-	-
13	CLA	a	821	X	-	-	-
13	CLA	a	822	X	-	-	-
13	CLA	a	823	X	-	-	-
13	CLA	a	824	X	-	-	-
13	CLA	a	825	X	-	-	-
13	CLA	a	826	X	-	-	-
13	CLA	a	827	X	-	-	-
13	CLA	a	828	X	-	-	-
13	CLA	a	829	X	-	-	-
13	CLA	a	830	X	-	-	-
13	CLA	a	831	X	-	-	-
13	CLA	a	832	X	-	-	-
13	CLA	a	833	X	-	-	-
13	CLA	a	834	X	-	-	-
13	CLA	a	835	X	-	-	-
13	CLA	a	836	X	-	-	-
13	CLA	a	837	X	-	-	-
13	CLA	a	839	X	-	-	-
13	CLA	a	840	X	-	-	-
13	CLA	a	841	X	-	-	-
13	CLA	a	842	X	-	-	-
13	CLA	a	843	X	-	-	-
13	CLA	a	844	X	-	-	-
13	CLA	a	845	X	-	-	-
13	CLA	a	852	X	-	-	-
13	CLA	b	801	X	-	-	-
13	CLA	b	802	X	-	-	-
13	CLA	b	803	X	-	-	-
13	CLA	b	804	X	-	-	-
13	CLA	b	805	X	-	-	-
13	CLA	b	806	X	-	-	-
13	CLA	b	807	X	-	-	-
13	CLA	b	808	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	b	809	X	-	-	-
13	CLA	b	810	X	-	-	-
13	CLA	b	811	X	-	-	-
13	CLA	b	812	X	-	-	-
13	CLA	b	813	X	-	-	-
13	CLA	b	814	X	-	-	-
13	CLA	b	815	X	-	-	-
13	CLA	b	816	X	-	-	-
13	CLA	b	817	X	-	-	-
13	CLA	b	818	X	-	-	-
13	CLA	b	819	X	-	-	-
13	CLA	b	820	X	-	-	-
13	CLA	b	821	X	-	-	-
13	CLA	b	822	X	-	-	-
13	CLA	b	823	X	-	-	-
13	CLA	b	824	X	-	-	-
13	CLA	b	825	X	-	-	-
13	CLA	b	826	X	-	-	-
13	CLA	b	827	X	-	-	-
13	CLA	b	828	X	-	-	-
13	CLA	b	829	X	-	-	-
13	CLA	b	830	X	-	-	-
13	CLA	b	831	X	-	-	-
13	CLA	b	832	X	-	-	-
13	CLA	b	833	X	-	-	-
13	CLA	b	834	X	-	-	-
13	CLA	b	835	X	-	-	-
13	CLA	b	836	X	-	-	-
13	CLA	b	837	X	-	-	-
13	CLA	b	838	X	-	-	-
13	CLA	b	839	X	-	-	-
13	CLA	b	840	X	-	-	-
13	CLA	e	803	X	-	-	-
13	CLA	e	804	X	-	-	-
13	CLA	e	805	X	-	-	-
13	CLA	e	806	X	-	-	-
13	CLA	e	807	X	-	-	-
13	CLA	e	808	X	-	-	-
13	CLA	e	809	X	-	-	-
13	CLA	e	810	X	-	-	-
13	CLA	e	811	X	-	-	-
13	CLA	e	812	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	e	813	X	-	-	-
13	CLA	e	814	X	-	-	-
13	CLA	e	815	X	-	-	-
13	CLA	e	816	X	-	-	-
13	CLA	e	817	X	-	-	-
13	CLA	e	818	X	-	-	-
13	CLA	e	819	X	-	-	-
13	CLA	e	820	X	-	-	-
13	CLA	e	821	X	-	-	-
13	CLA	e	822	X	-	-	-
13	CLA	e	823	X	-	-	-
13	CLA	e	824	X	-	-	-
13	CLA	e	825	X	-	-	-
13	CLA	e	826	X	-	-	-
13	CLA	e	827	X	-	-	-
13	CLA	e	828	X	-	-	-
13	CLA	e	829	X	-	-	-
13	CLA	e	830	X	-	-	-
13	CLA	e	831	X	-	-	-
13	CLA	e	832	X	-	-	-
13	CLA	e	833	X	-	-	-
13	CLA	e	834	X	-	-	-
13	CLA	e	835	X	-	-	-
13	CLA	e	837	X	-	-	-
13	CLA	e	838	X	-	-	-
13	CLA	e	839	X	-	-	-
13	CLA	e	840	X	-	-	-
13	CLA	e	841	X	-	-	-
13	CLA	e	842	X	-	-	-
13	CLA	e	843	X	-	-	-
13	CLA	e	844	X	-	-	-
13	CLA	e	852	X	-	-	-
13	CLA	f	203	X	-	-	-
13	CLA	g	801	X	-	-	-
13	CLA	g	802	X	-	-	-
13	CLA	g	803	X	-	-	-
13	CLA	g	805	X	-	-	-
13	CLA	g	806	X	-	-	-
13	CLA	g	807	X	-	-	-
13	CLA	g	808	X	-	-	-
13	CLA	g	809	X	-	-	-
13	CLA	g	810	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	g	811	X	-	-	-
13	CLA	g	812	X	-	-	-
13	CLA	g	813	X	-	-	-
13	CLA	g	814	X	-	-	-
13	CLA	g	815	X	-	-	-
13	CLA	g	816	X	-	-	-
13	CLA	g	817	X	-	-	-
13	CLA	g	818	X	-	-	-
13	CLA	g	819	X	-	-	-
13	CLA	g	820	X	-	-	-
13	CLA	g	821	X	-	-	-
13	CLA	g	822	X	-	-	-
13	CLA	g	823	X	-	-	-
13	CLA	g	824	X	-	-	-
13	CLA	g	825	X	-	-	-
13	CLA	g	826	X	-	-	-
13	CLA	g	827	X	-	-	-
13	CLA	g	828	X	-	-	-
13	CLA	g	829	X	-	-	-
13	CLA	g	830	X	-	-	-
13	CLA	g	831	X	-	-	-
13	CLA	g	832	X	-	-	-
13	CLA	g	833	X	-	-	-
13	CLA	g	834	X	-	-	-
13	CLA	g	835	X	-	-	-
13	CLA	g	836	X	-	-	-
13	CLA	g	837	X	-	-	-
13	CLA	g	838	X	-	-	-
13	CLA	g	839	X	-	-	-
13	CLA	g	840	X	-	-	-
13	CLA	g	841	X	-	-	-
13	CLA	g	842	X	-	-	-
13	CLA	k	4002	X	-	-	-
13	CLA	l	201	X	-	-	-
13	CLA	l	203	X	-	-	-
13	CLA	l	204	X	-	-	-
13	CLA	l	205	X	-	-	-
13	CLA	o	202	X	-	-	-
13	CLA	r	101	X	-	-	-
13	CLA	r	102	X	-	-	-
13	CLA	s	202	X	-	-	-
13	CLA	s	203	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	s	205	X	-	-	-

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 90396 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	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	E	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	e	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	a	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		
2	G	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		
2	g	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		
2	b	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	81	Total	C	N	O	S	0	0
			605	370	105	119	11		
3	H	81	Total	C	N	O	S	0	0
			605	370	105	119	11		
3	h	81	Total	C	N	O	S	0	0
			605	370	105	119	11		
3	c	81	Total	C	N	O	S	0	0
			605	370	105	119	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	137	Total	C	N	O	S	0	0
			1080	689	189	198	4		
4	N	135	Total	C	N	O	S	0	0
			1066	680	187	195	4		
4	n	137	Total	C	N	O	S	0	0
			1080	689	189	198	4		
4	d	135	Total	C	N	O	S	0	0
			1066	680	187	195	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	V	61	Total	C	N	O	0	0
			494	315	86	93		
5	W	61	Total	C	N	O	0	0
			494	315	86	93		
5	v	61	Total	C	N	O	0	0
			494	315	86	93		
5	w	61	Total	C	N	O	0	0
			494	315	86	93		

- 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
			1093	700	188	202	3		
6	O	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	o	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	f	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	39	Total	C	N	O	S	0	0
			295	199	42	52	2		
7	P	39	Total	C	N	O	S	0	0
			295	199	42	52	2		
7	p	39	Total	C	N	O	S	0	0
			295	199	42	52	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	39	Total	C	N	O	S	0	0
			295	199	42	52	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	37	Total	C	N	O		0	0
			311	218	44	49			
8	Q	37	Total	C	N	O		0	0
			311	218	44	49			
8	q	37	Total	C	N	O		0	0
			311	218	44	49			
8	j	37	Total	C	N	O		0	0
			311	218	44	49			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	65	Total	C	N	O	S	0	0
			474	316	80	77	1		
9	R	65	Total	C	N	O	S	0	0
			474	316	80	77	1		
9	r	65	Total	C	N	O	S	0	0
			474	316	80	77	1		
9	k	65	Total	C	N	O	S	0	0
			474	316	80	77	1		

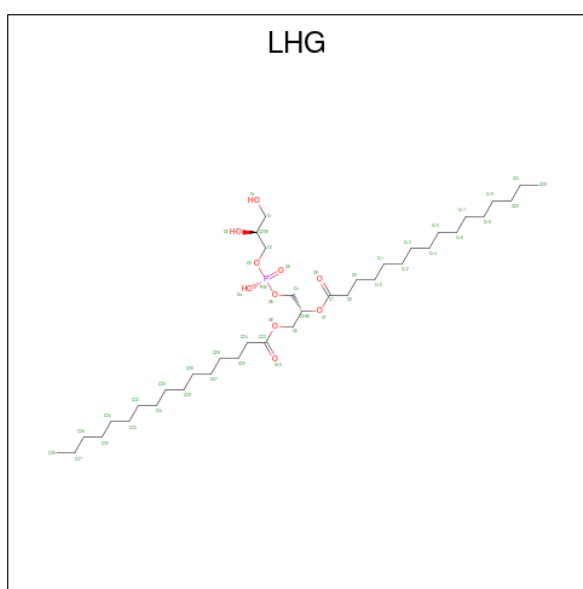
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		
10	S	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		
10	s	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		
10	l	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		

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

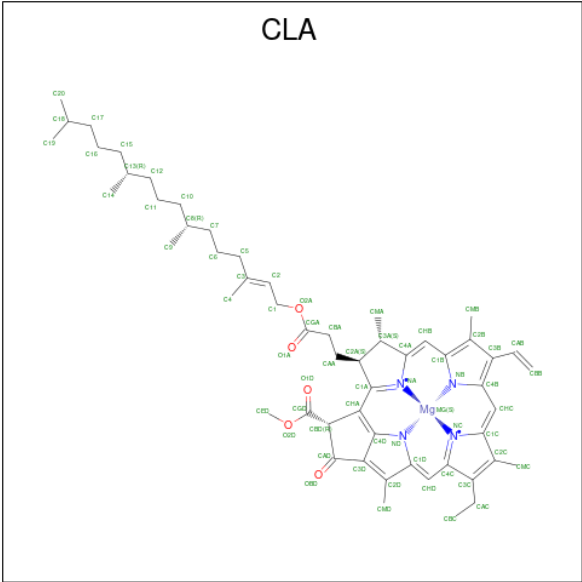
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	T	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	t	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O	P	0
			49	38	10	1	
12	A	1	Total	C	O	P	0
			38	27	10	1	
12	e	1	Total	C	O	P	0
			49	38	10	1	
12	e	1	Total	C	O	P	0
			38	27	10	1	
12	a	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	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
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	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
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	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
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	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
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	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
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	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
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	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
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	G	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
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	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
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	e	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
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	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
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	g	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
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	o	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
13	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	a	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
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	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
13	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	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
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

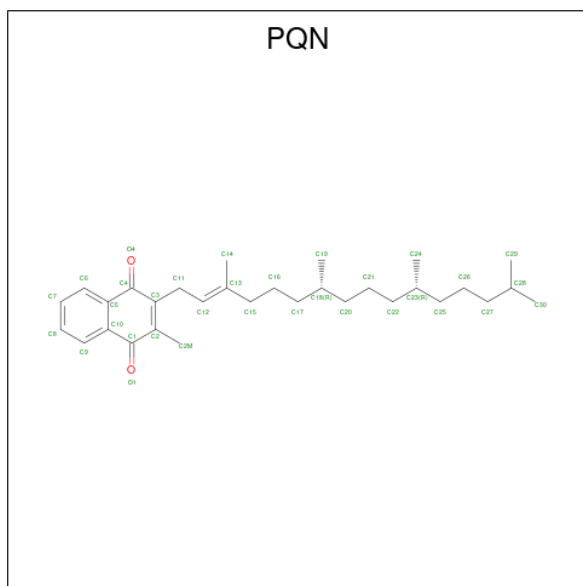
*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



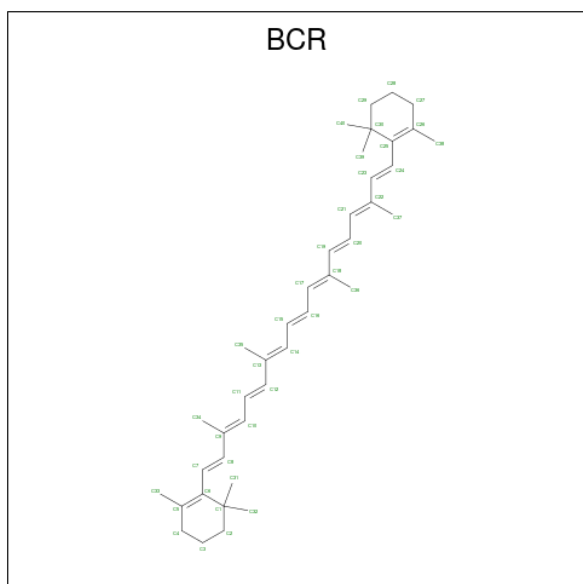
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			33	31	2	
14	B	1	Total	C	O	0
			33	31	2	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
14	E	1	Total	C	O	0
			33	31	2	
14	G	1	Total	C	O	0
			33	31	2	
14	e	1	Total	C	O	0
			33	31	2	
14	g	1	Total	C	O	0
			33	31	2	
14	a	1	Total	C	O	0
			33	31	2	
14	b	1	Total	C	O	0
			33	31	2	

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	O	1	Total C 40 40	0
15	O	1	Total C 40 40	0
15	P	1	Total C 40 40	0
15	Q	1	Total C 40 40	0
15	R	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	T	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0

*Continued on next page...*

*Continued from previous page...*

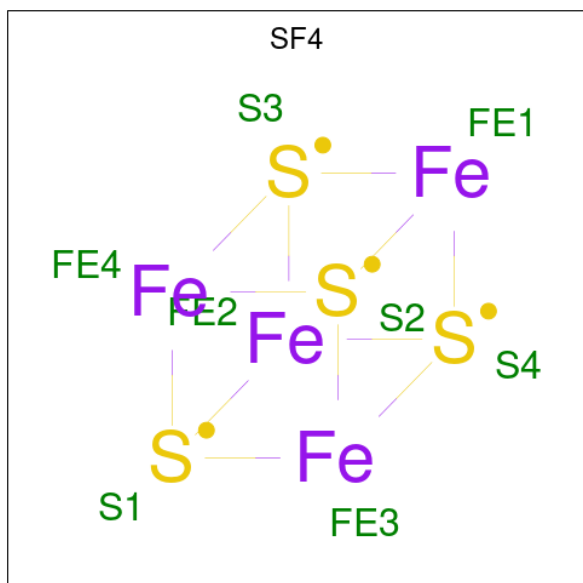
Mol	Chain	Residues	Atoms	AltConf
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	o	1	Total C 40 40	0
15	p	1	Total C 40 40	0
15	q	1	Total C 40 40	0
15	q	1	Total C 40 40	0
15	s	1	Total C 40 40	0
15	s	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0

*Continued on next page...*

Continued from previous page...

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

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total Fe S 8 4 4	0

Continued on next page...

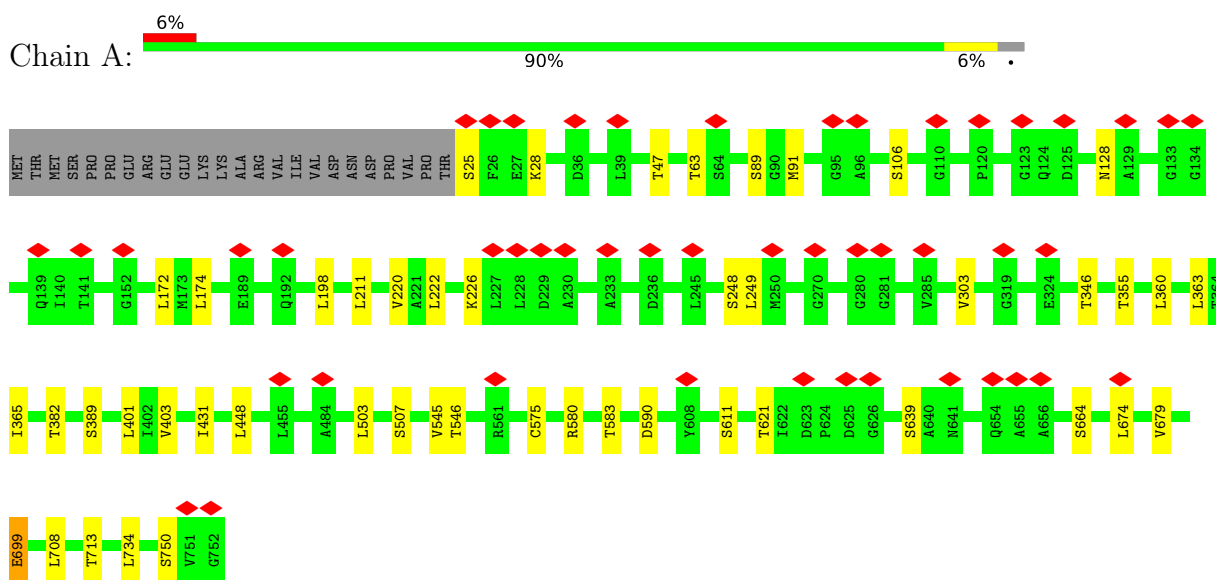
*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
16	C	1	Total 8	Fe 4	S 4	0
16	C	1	Total 8	Fe 4	S 4	0
16	E	1	Total 8	Fe 4	S 4	0
16	H	1	Total 8	Fe 4	S 4	0
16	H	1	Total 8	Fe 4	S 4	0
16	g	1	Total 8	Fe 4	S 4	0
16	h	1	Total 8	Fe 4	S 4	0
16	h	1	Total 8	Fe 4	S 4	0
16	a	1	Total 8	Fe 4	S 4	0
16	c	1	Total 8	Fe 4	S 4	0
16	c	1	Total 8	Fe 4	S 4	0

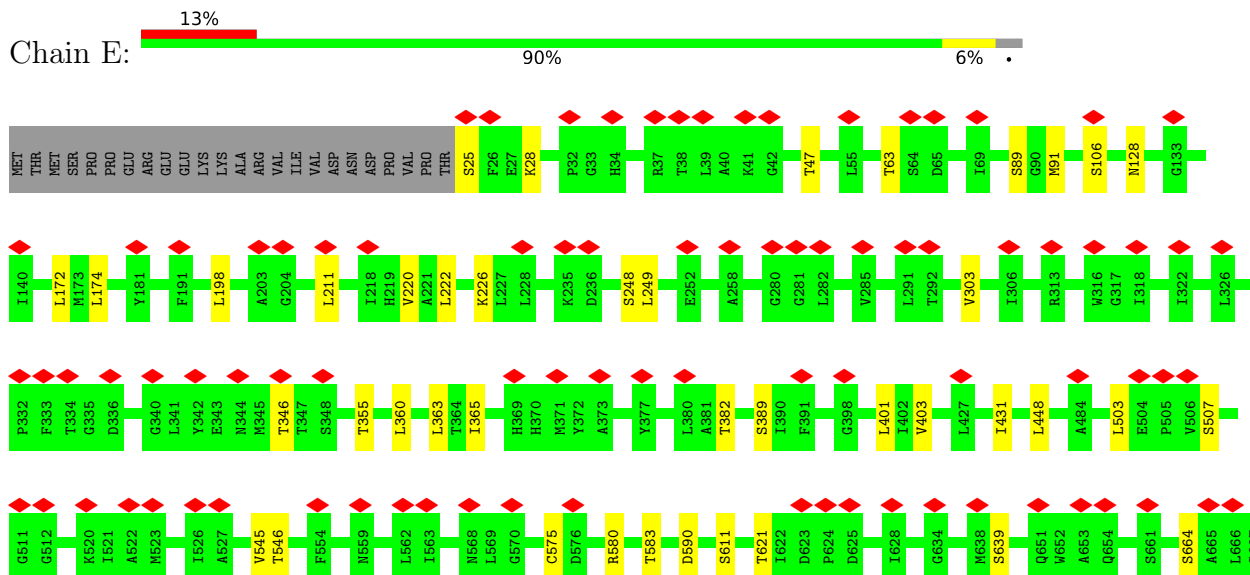
### 3 Residue-property plots

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.

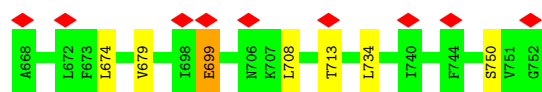
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

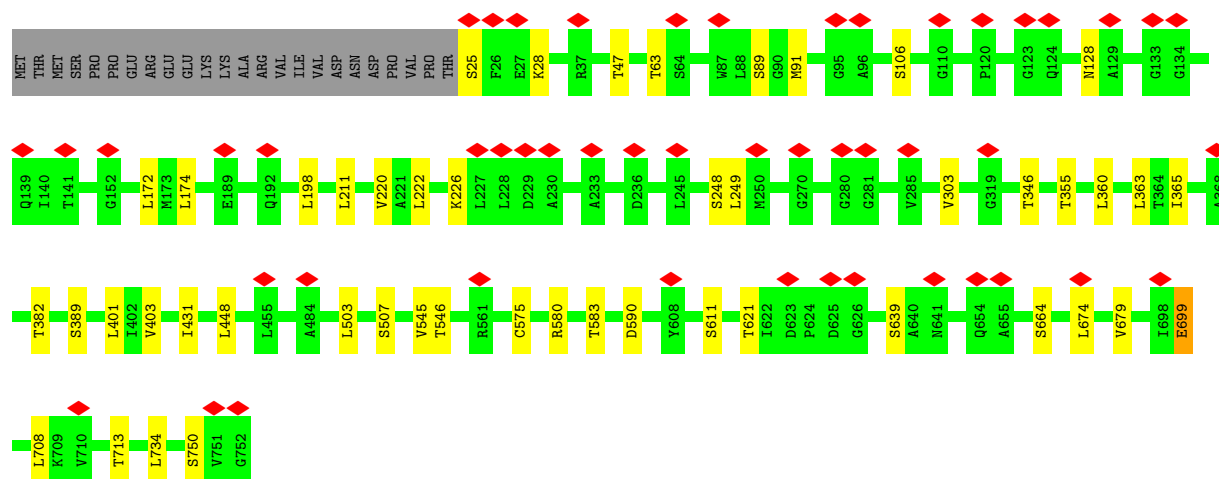






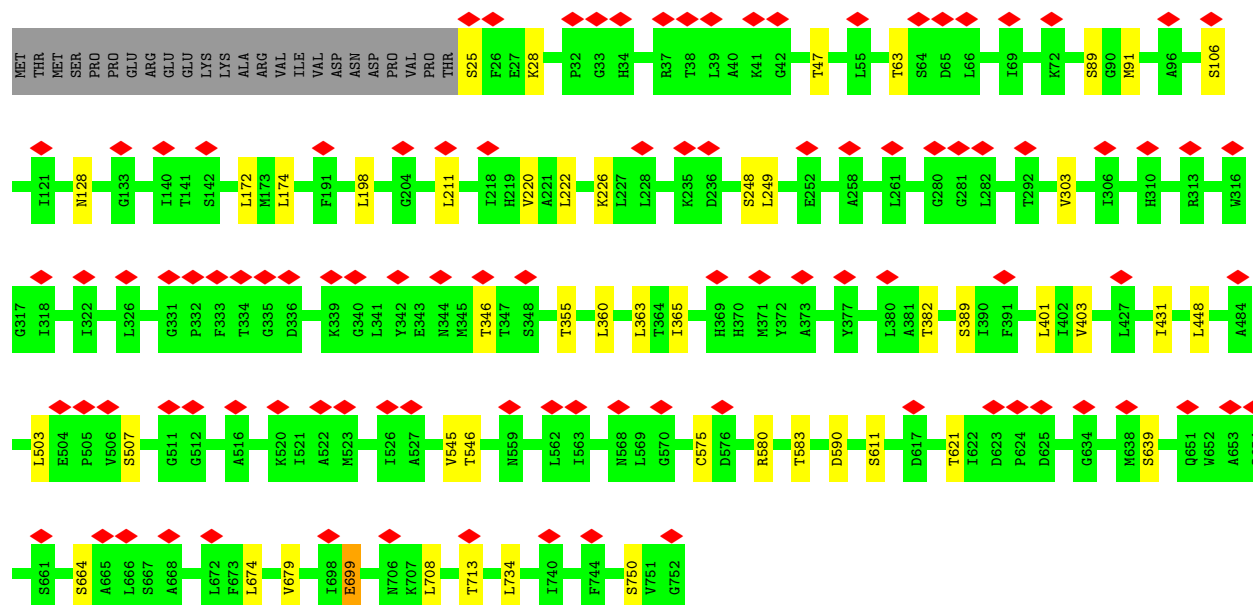
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain e: 7% 90% 6% .



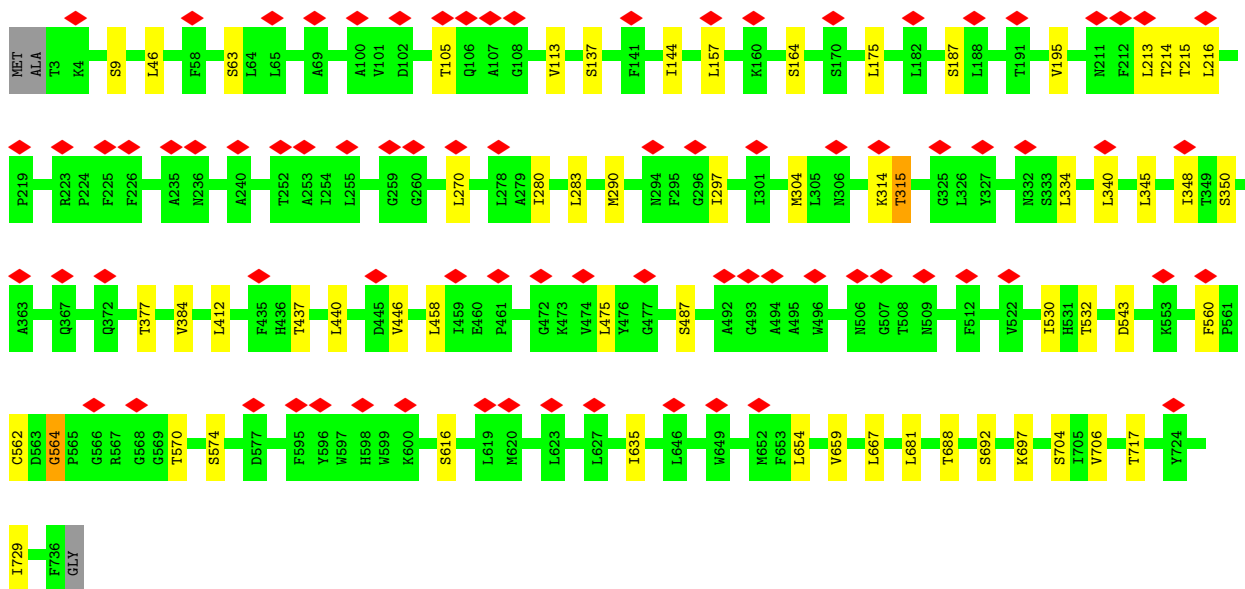
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 13% 90% 6% .

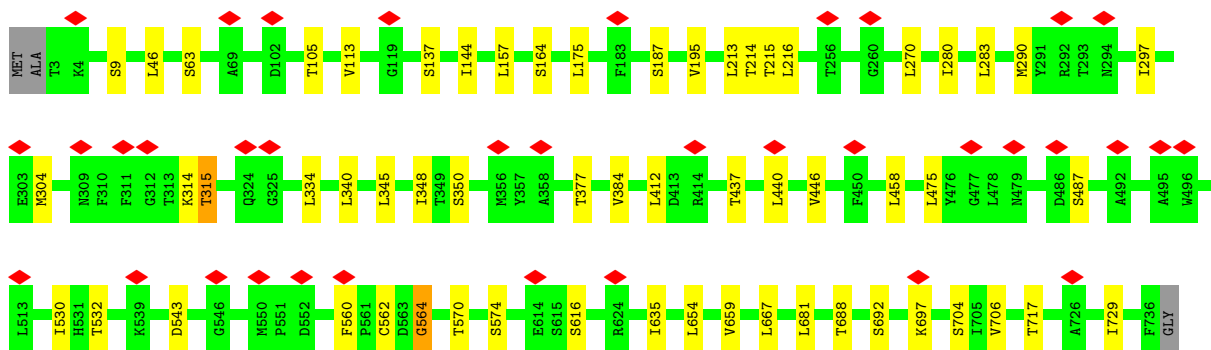


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

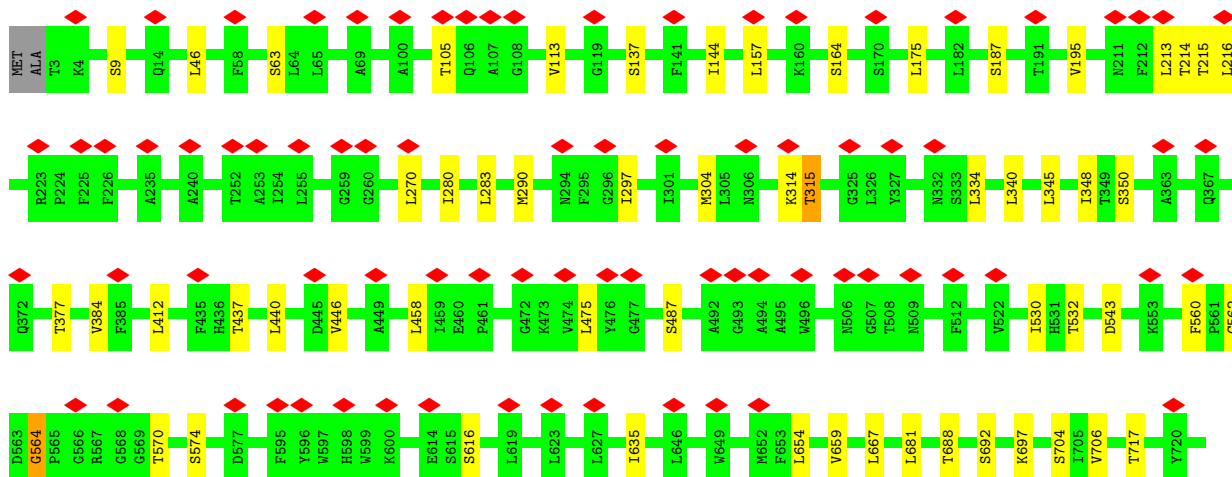
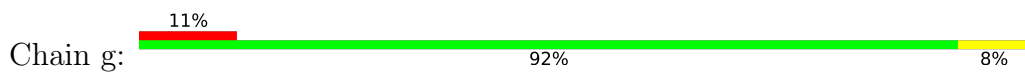
Chain B: 11% 92% 8%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



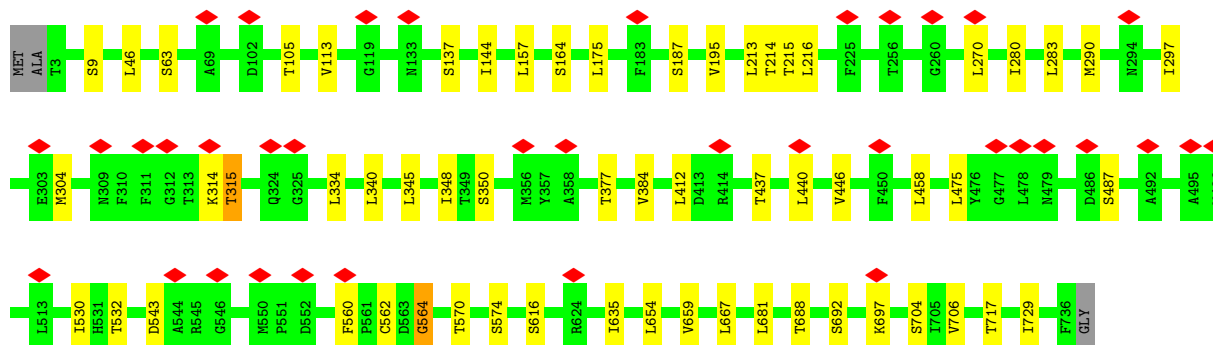
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





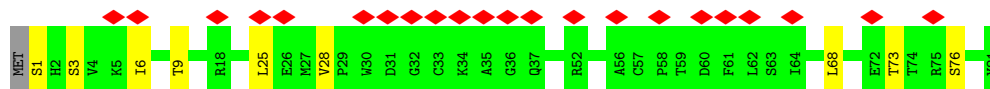
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



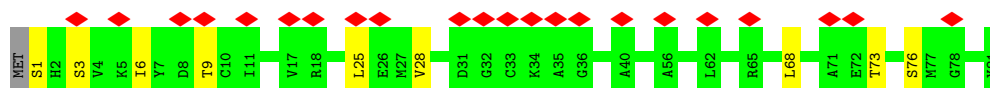
- Molecule 3: Photosystem I iron-sulfur center

Chain C:



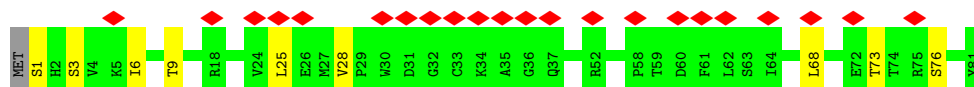
- Molecule 3: Photosystem I iron-sulfur center

Chain H:



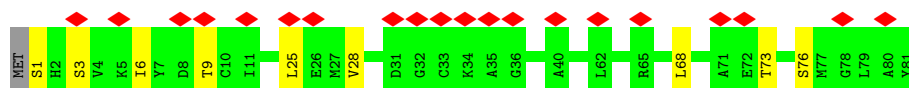
- Molecule 3: Photosystem I iron-sulfur center

Chain h:

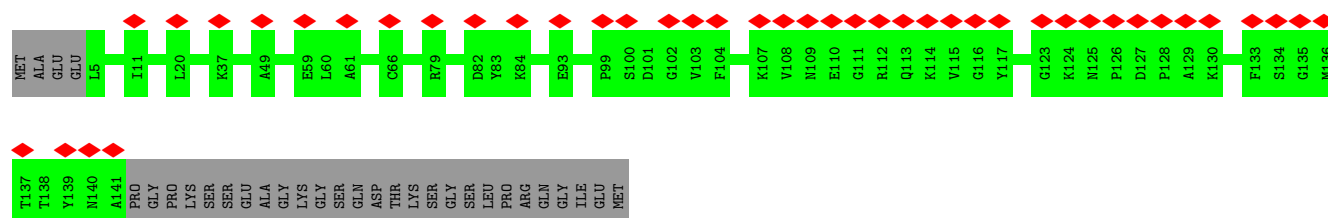
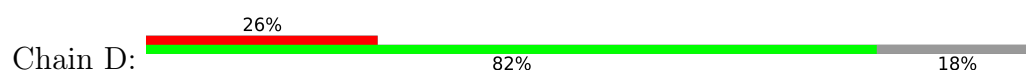


- Molecule 3: Photosystem I iron-sulfur center

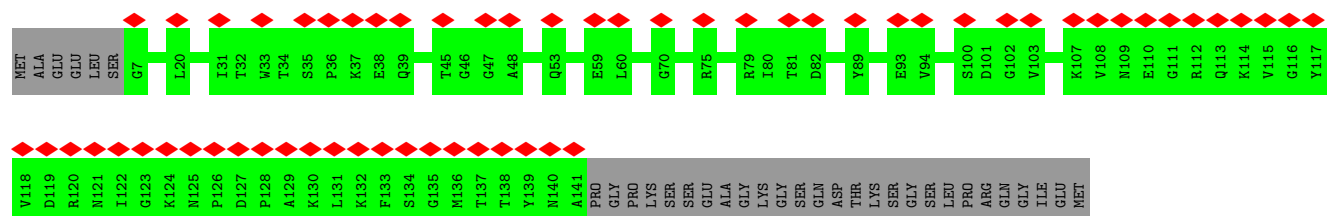
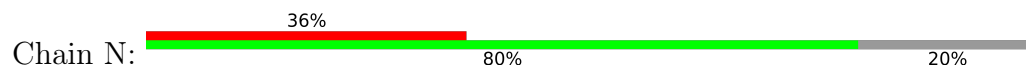
Chain c:



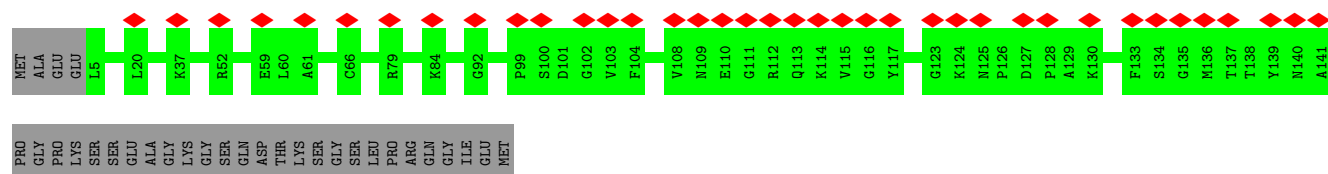
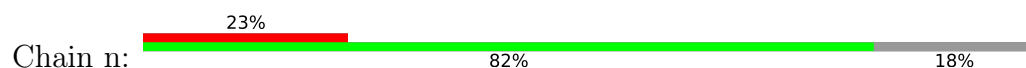
- Molecule 4: Photosystem I reaction center subunit II



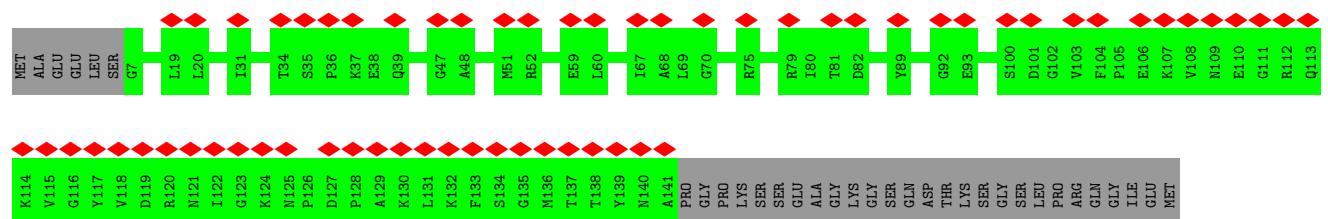
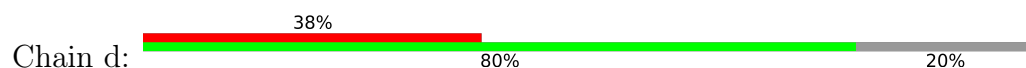
• Molecule 4: Photosystem I reaction center subunit II



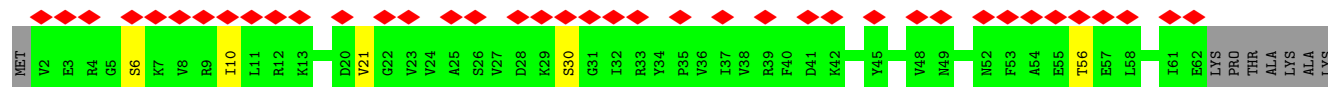
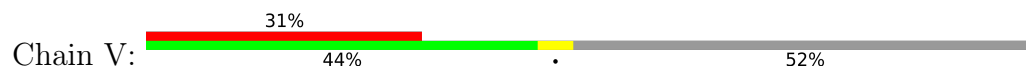
• Molecule 4: Photosystem I reaction center subunit II



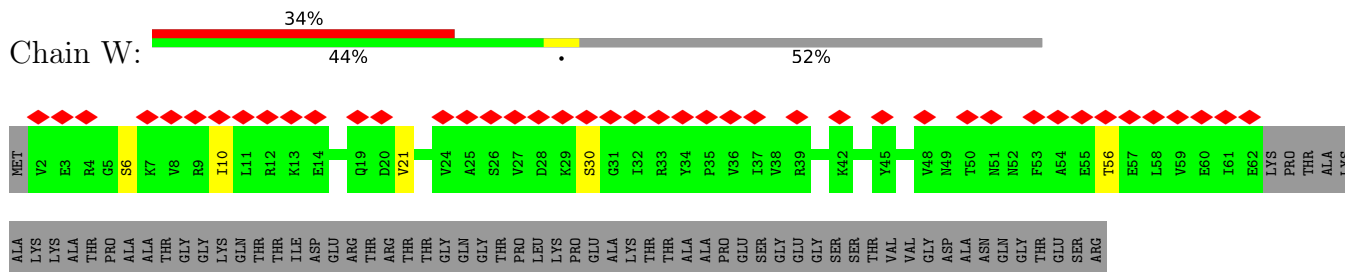
• Molecule 4: Photosystem I reaction center subunit II



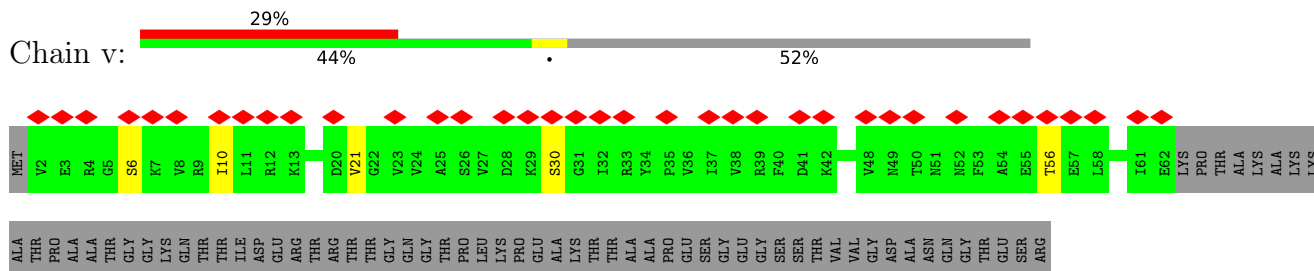
• Molecule 5: Photosystem I reaction center subunit IV



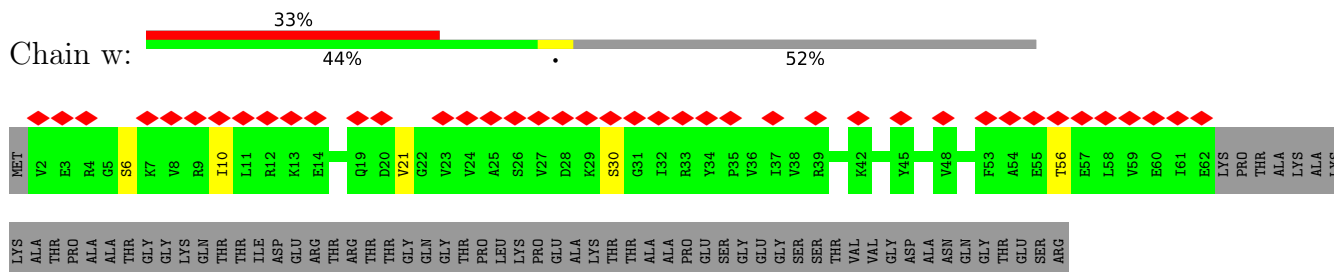
- Molecule 5: Photosystem I reaction center subunit IV



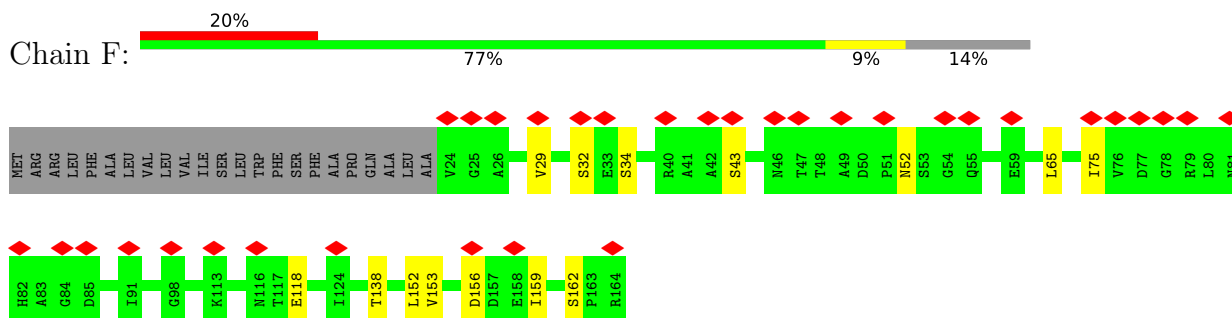
- Molecule 5: Photosystem I reaction center subunit IV



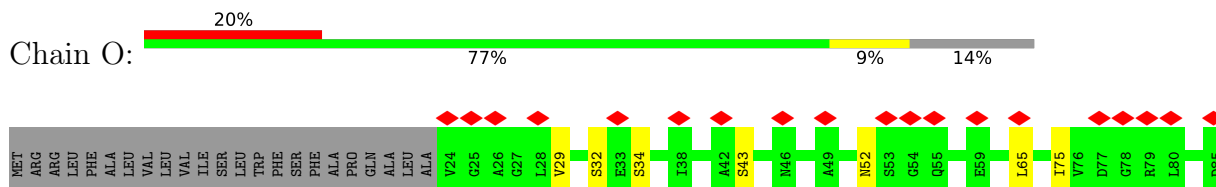
- Molecule 5: Photosystem I reaction center subunit IV

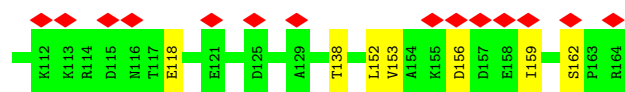


- Molecule 6: Photosystem I reaction center subunit III

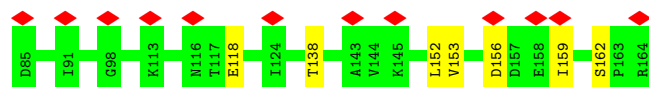
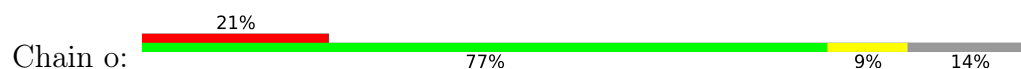


- Molecule 6: Photosystem I reaction center subunit III

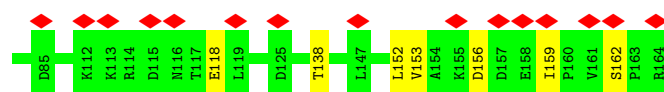
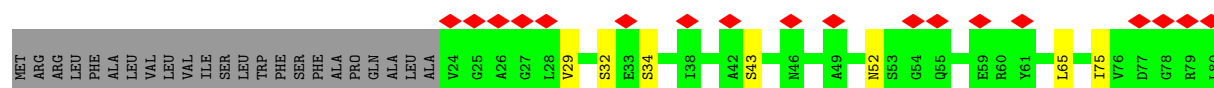
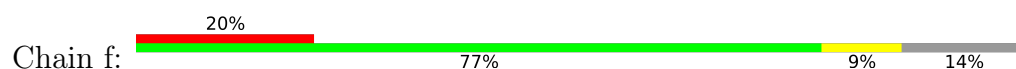




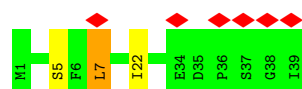
• Molecule 6: Photosystem I reaction center subunit III



• Molecule 6: Photosystem I reaction center subunit III



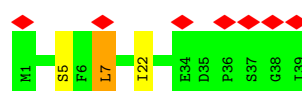
• Molecule 7: Photosystem I reaction center subunit VIII



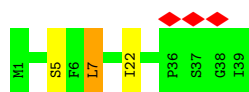
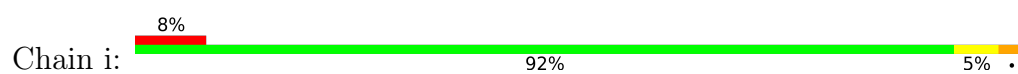
• Molecule 7: Photosystem I reaction center subunit VIII



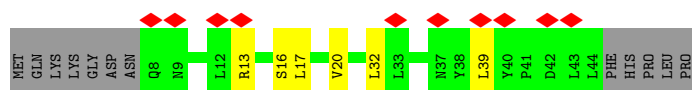
• Molecule 7: Photosystem I reaction center subunit VIII



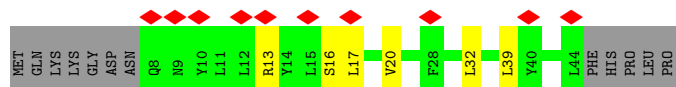
• Molecule 7: Photosystem I reaction center subunit VIII



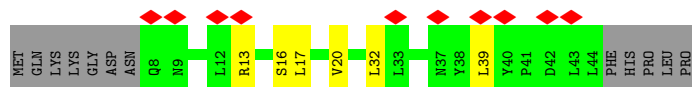
- Molecule 8: Photosystem I reaction center subunit IX



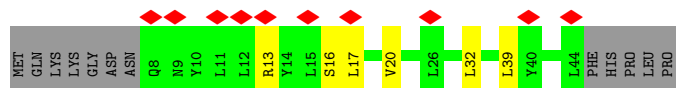
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX

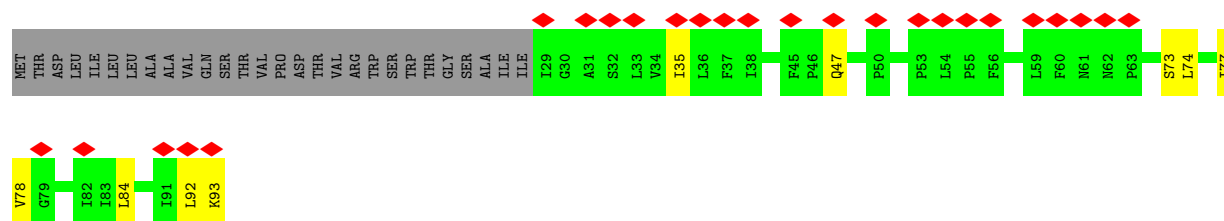


- Molecule 9: Photosystem I reaction center subunit PsaK

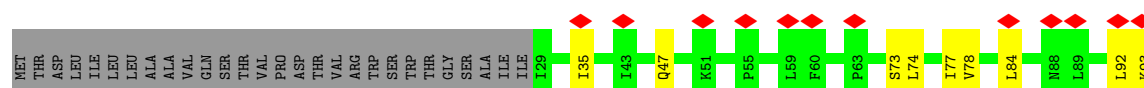


- Molecule 9: Photosystem I reaction center subunit PsaK

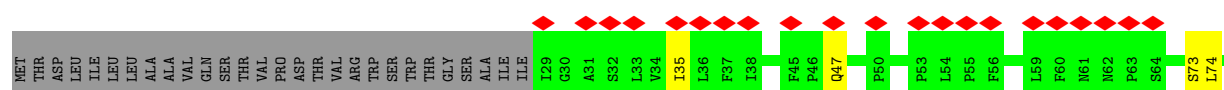




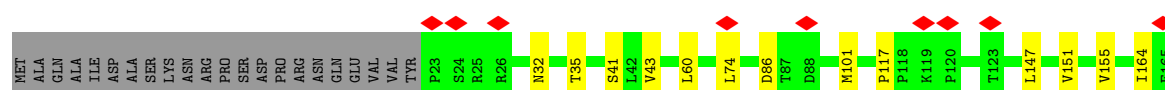
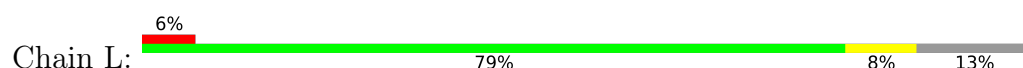
• Molecule 9: Photosystem I reaction center subunit PsaK



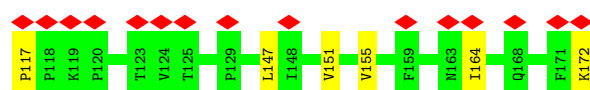
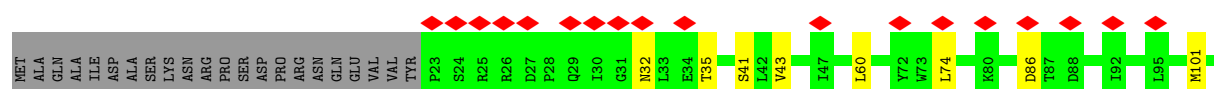
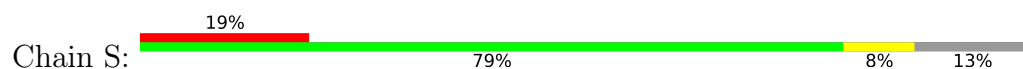
• Molecule 9: Photosystem I reaction center subunit PsaK



• Molecule 10: Photosystem I reaction center subunit XI

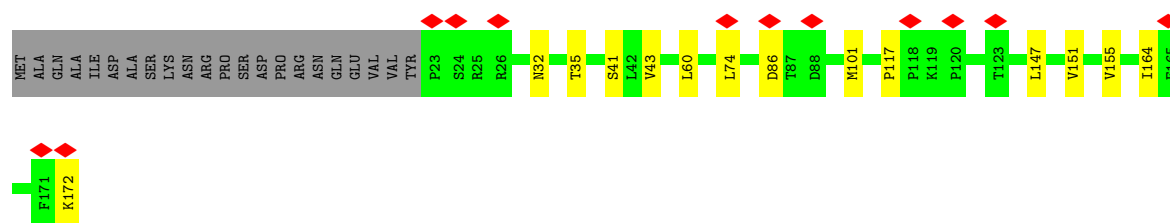
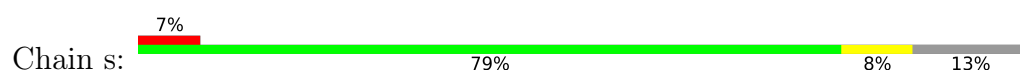


• Molecule 10: Photosystem I reaction center subunit XI

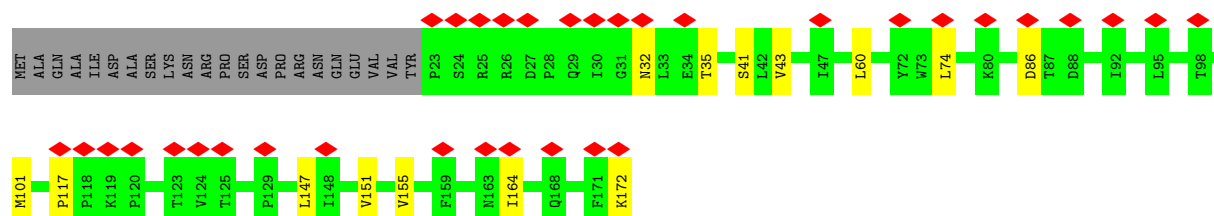
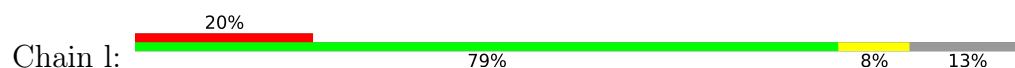


• Molecule 10: Photosystem I reaction center subunit XI

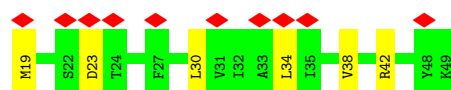
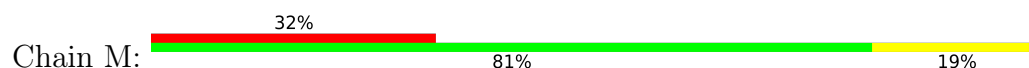




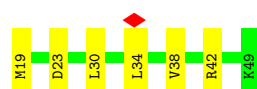
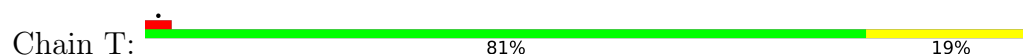
- Molecule 10: Photosystem I reaction center subunit XI



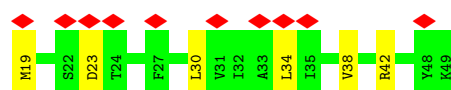
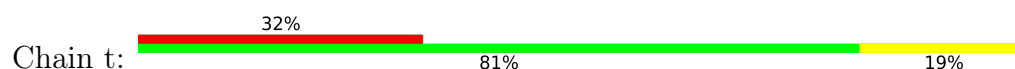
- Molecule 11: Photosystem I reaction center subunit XII



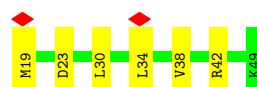
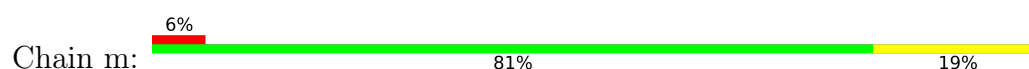
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	66130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	4.3	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	425.47202, 425.47202, 425.47202	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PQN, BCR, SF4, LHG

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	0/5908	0.49	1/8056 (0.0%)
1	E	0.31	0/5908	0.49	1/8056 (0.0%)
1	a	0.31	0/5908	0.49	1/8056 (0.0%)
1	e	0.31	0/5908	0.49	1/8056 (0.0%)
2	B	0.30	0/6072	0.49	0/8301
2	G	0.30	0/6072	0.49	0/8301
2	b	0.30	0/6072	0.49	0/8301
2	g	0.30	0/6072	0.49	0/8301
3	C	0.28	0/615	0.49	0/833
3	H	0.28	0/615	0.49	0/833
3	c	0.28	0/615	0.49	0/833
3	h	0.28	0/615	0.49	0/833
4	D	0.28	0/1105	0.50	0/1489
4	N	0.27	0/1091	0.50	0/1470
4	d	0.28	0/1091	0.51	0/1470
4	n	0.30	0/1105	0.50	0/1489
5	V	0.30	0/502	0.49	0/678
5	W	0.30	0/502	0.49	0/678
5	v	0.29	0/502	0.49	0/678
5	w	0.30	0/502	0.49	0/678
6	F	0.28	0/1119	0.48	0/1522
6	O	0.28	0/1119	0.48	0/1522
6	f	0.28	0/1119	0.48	0/1522
6	o	0.28	0/1119	0.48	0/1522
7	I	0.29	0/302	0.60	1/411 (0.2%)
7	P	0.29	0/302	0.60	1/411 (0.2%)
7	i	0.29	0/302	0.60	1/411 (0.2%)
7	p	0.29	0/302	0.60	1/411 (0.2%)
8	J	0.29	0/321	0.48	0/441
8	Q	0.29	0/321	0.48	0/441
8	j	0.29	0/321	0.48	0/441
8	q	0.29	0/321	0.48	0/441

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	K	0.29	0/484	0.65	1/659 (0.2%)
9	R	0.29	0/484	0.65	1/659 (0.2%)
9	k	0.29	0/484	0.65	1/659 (0.2%)
9	r	0.29	0/484	0.65	1/659 (0.2%)
10	L	0.31	0/1165	0.50	0/1597
10	S	0.31	0/1165	0.50	0/1597
10	l	0.31	0/1165	0.50	0/1597
10	s	0.31	0/1165	0.50	0/1597
11	M	0.33	0/241	0.59	0/326
11	T	0.33	0/241	0.59	0/326
11	m	0.33	0/241	0.59	0/326
11	t	0.34	0/241	0.59	0/326
All	All	0.30	0/71308	0.50	12/97214 (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	3
2	G	0	3
2	b	0	3
2	g	0	3
10	L	0	1
10	S	0	1
10	l	0	1
10	s	0	1
All	All	0	16

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	r	74	LEU	CA-CB-CG	-6.34	100.71	115.30
9	K	74	LEU	CA-CB-CG	-6.34	100.72	115.30
9	k	74	LEU	CA-CB-CG	-6.33	100.74	115.30
9	R	74	LEU	CA-CB-CG	-6.33	100.75	115.30
1	e	699	GLU	CA-CB-CG	6.11	126.85	113.40
1	a	699	GLU	CA-CB-CG	6.11	126.83	113.40
1	A	699	GLU	CA-CB-CG	6.10	126.83	113.40
1	E	699	GLU	CA-CB-CG	6.10	126.83	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	7	LEU	CA-CB-CG	5.42	127.76	115.30
7	p	7	LEU	CA-CB-CG	5.42	127.76	115.30
7	I	7	LEU	CA-CB-CG	5.41	127.74	115.30
7	i	7	LEU	CA-CB-CG	5.39	127.70	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	315	THR	Peptide
2	B	560	PHE	Peptide
2	B	564	GLY	Peptide
2	G	315	THR	Peptide
2	G	560	PHE	Peptide
2	G	564	GLY	Peptide
10	L	117	PRO	Peptide
10	S	117	PRO	Peptide
2	b	315	THR	Peptide
2	b	560	PHE	Peptide
2	b	564	GLY	Peptide
2	g	315	THR	Peptide
2	g	560	PHE	Peptide
2	g	564	GLY	Peptide
10	l	117	PRO	Peptide
10	s	117	PRO	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	726/752 (96%)	625 (86%)	101 (14%)	0	100	100
1	E	726/752 (96%)	625 (86%)	101 (14%)	0	100	100
1	a	726/752 (96%)	625 (86%)	101 (14%)	0	100	100
1	e	726/752 (96%)	626 (86%)	100 (14%)	0	100	100
2	B	732/737 (99%)	642 (88%)	87 (12%)	3 (0%)	30	62
2	G	732/737 (99%)	642 (88%)	87 (12%)	3 (0%)	30	62
2	b	732/737 (99%)	644 (88%)	85 (12%)	3 (0%)	30	62
2	g	732/737 (99%)	642 (88%)	87 (12%)	3 (0%)	30	62
3	C	79/82 (96%)	65 (82%)	14 (18%)	0	100	100
3	H	79/82 (96%)	65 (82%)	14 (18%)	0	100	100
3	c	79/82 (96%)	65 (82%)	14 (18%)	0	100	100
3	h	79/82 (96%)	66 (84%)	13 (16%)	0	100	100
4	D	135/168 (80%)	115 (85%)	20 (15%)	0	100	100
4	N	133/168 (79%)	113 (85%)	20 (15%)	0	100	100
4	d	133/168 (79%)	114 (86%)	19 (14%)	0	100	100
4	n	135/168 (80%)	117 (87%)	18 (13%)	0	100	100
5	V	59/126 (47%)	47 (80%)	12 (20%)	0	100	100
5	W	59/126 (47%)	47 (80%)	12 (20%)	0	100	100
5	v	59/126 (47%)	47 (80%)	12 (20%)	0	100	100
5	w	59/126 (47%)	47 (80%)	12 (20%)	0	100	100
6	F	139/164 (85%)	120 (86%)	19 (14%)	0	100	100
6	O	139/164 (85%)	120 (86%)	19 (14%)	0	100	100
6	f	139/164 (85%)	120 (86%)	19 (14%)	0	100	100
6	o	139/164 (85%)	120 (86%)	19 (14%)	0	100	100
7	I	37/39 (95%)	30 (81%)	7 (19%)	0	100	100
7	P	37/39 (95%)	30 (81%)	7 (19%)	0	100	100
7	i	37/39 (95%)	30 (81%)	7 (19%)	0	100	100
7	p	37/39 (95%)	30 (81%)	7 (19%)	0	100	100
8	J	35/49 (71%)	30 (86%)	5 (14%)	0	100	100
8	Q	35/49 (71%)	30 (86%)	5 (14%)	0	100	100
8	j	35/49 (71%)	30 (86%)	5 (14%)	0	100	100
8	q	35/49 (71%)	30 (86%)	5 (14%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	63/93 (68%)	52 (82%)	11 (18%)	0	100	100
9	R	63/93 (68%)	52 (82%)	11 (18%)	0	100	100
9	k	63/93 (68%)	52 (82%)	11 (18%)	0	100	100
9	r	63/93 (68%)	52 (82%)	11 (18%)	0	100	100
10	L	148/172 (86%)	129 (87%)	19 (13%)	0	100	100
10	S	148/172 (86%)	129 (87%)	19 (13%)	0	100	100
10	l	148/172 (86%)	129 (87%)	19 (13%)	0	100	100
10	s	148/172 (86%)	129 (87%)	19 (13%)	0	100	100
11	M	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	26
11	T	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	26
11	m	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	26
11	t	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	26
All	All	8724/9652 (90%)	7499 (86%)	1209 (14%)	16 (0%)	45	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	314	LYS
2	B	315	THR
2	G	314	LYS
2	G	315	THR
2	g	314	LYS
2	g	315	THR
2	b	314	LYS
2	b	315	THR
11	M	23	ASP
11	T	23	ASP
11	t	23	ASP
11	m	23	ASP
2	B	564	GLY
2	G	564	GLY
2	g	564	GLY
2	b	564	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	578/601 (96%)	530 (92%)	48 (8%)	9	34
1	E	578/601 (96%)	530 (92%)	48 (8%)	9	34
1	a	578/601 (96%)	530 (92%)	48 (8%)	9	34
1	e	578/601 (96%)	530 (92%)	48 (8%)	9	34
2	B	594/595 (100%)	539 (91%)	55 (9%)	7	30
2	G	594/595 (100%)	539 (91%)	55 (9%)	7	30
2	b	594/595 (100%)	539 (91%)	55 (9%)	7	30
2	g	594/595 (100%)	539 (91%)	55 (9%)	7	30
3	C	68/70 (97%)	59 (87%)	9 (13%)	3	18
3	H	68/70 (97%)	59 (87%)	9 (13%)	3	18
3	c	68/70 (97%)	59 (87%)	9 (13%)	3	18
3	h	68/70 (97%)	59 (87%)	9 (13%)	3	18
4	D	113/137 (82%)	113 (100%)	0	100	100
4	N	111/137 (81%)	111 (100%)	0	100	100
4	d	111/137 (81%)	111 (100%)	0	100	100
4	n	113/137 (82%)	113 (100%)	0	100	100
5	V	54/102 (53%)	49 (91%)	5 (9%)	7	30
5	W	54/102 (53%)	49 (91%)	5 (9%)	7	30
5	v	54/102 (53%)	49 (91%)	5 (9%)	7	30
5	w	54/102 (53%)	49 (91%)	5 (9%)	7	30
6	F	116/135 (86%)	102 (88%)	14 (12%)	4	20
6	O	116/135 (86%)	102 (88%)	14 (12%)	4	20
6	f	116/135 (86%)	102 (88%)	14 (12%)	4	20
6	o	116/135 (86%)	102 (88%)	14 (12%)	4	20
7	I	33/33 (100%)	30 (91%)	3 (9%)	7	30
7	P	33/33 (100%)	30 (91%)	3 (9%)	7	30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	i	33/33 (100%)	30 (91%)	3 (9%)	7	30
7	p	33/33 (100%)	30 (91%)	3 (9%)	7	30
8	J	34/45 (76%)	28 (82%)	6 (18%)	1	10
8	Q	34/45 (76%)	28 (82%)	6 (18%)	1	10
8	j	34/45 (76%)	28 (82%)	6 (18%)	1	10
8	q	34/45 (76%)	28 (82%)	6 (18%)	1	10
9	K	53/77 (69%)	45 (85%)	8 (15%)	2	15
9	R	53/77 (69%)	45 (85%)	8 (15%)	2	15
9	k	53/77 (69%)	45 (85%)	8 (15%)	2	15
9	r	53/77 (69%)	45 (85%)	8 (15%)	2	15
10	L	121/140 (86%)	108 (89%)	13 (11%)	5	25
10	S	121/140 (86%)	108 (89%)	13 (11%)	5	25
10	l	121/140 (86%)	108 (89%)	13 (11%)	5	25
10	s	121/140 (86%)	108 (89%)	13 (11%)	5	25
11	M	26/26 (100%)	21 (81%)	5 (19%)	1	8
11	T	26/26 (100%)	21 (81%)	5 (19%)	1	8
11	m	26/26 (100%)	21 (81%)	5 (19%)	1	8
11	t	26/26 (100%)	21 (81%)	5 (19%)	1	8
All	All	7156/7844 (91%)	6492 (91%)	664 (9%)	10	30

All (664) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	28	LYS
1	A	47	THR
1	A	63	THR
1	A	89	SER
1	A	91	MET
1	A	106	SER
1	A	128	ASN
1	A	172	LEU
1	A	174	LEU
1	A	198	LEU
1	A	211	LEU
1	A	220	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	222	LEU
1	A	226	LYS
1	A	248	SER
1	A	249	LEU
1	A	303	VAL
1	A	346	THR
1	A	355	THR
1	A	360	LEU
1	A	363	LEU
1	A	365	ILE
1	A	382	THR
1	A	389	SER
1	A	401	LEU
1	A	403	VAL
1	A	431	ILE
1	A	448	LEU
1	A	503	LEU
1	A	507	SER
1	A	545	VAL
1	A	546	THR
1	A	575	CYS
1	A	580	ARG
1	A	583	THR
1	A	590	ASP
1	A	611	SER
1	A	621	THR
1	A	639	SER
1	A	664	SER
1	A	674	LEU
1	A	679	VAL
1	A	699	GLU
1	A	708	LEU
1	A	713	THR
1	A	734	LEU
1	A	750	SER
2	B	9	SER
2	B	46	LEU
2	B	63	SER
2	B	105	THR
2	B	113	VAL
2	B	137	SER
2	B	144	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	157	LEU
2	B	164	SER
2	B	175	LEU
2	B	187	SER
2	B	195	VAL
2	B	213	LEU
2	B	214	THR
2	B	215	THR
2	B	216	LEU
2	B	270	LEU
2	B	280	ILE
2	B	283	LEU
2	B	290	MET
2	B	297	ILE
2	B	304	MET
2	B	334	LEU
2	B	340	LEU
2	B	345	LEU
2	B	348	ILE
2	B	350	SER
2	B	377	THR
2	B	384	VAL
2	B	412	LEU
2	B	437	THR
2	B	440	LEU
2	B	446	VAL
2	B	458	LEU
2	B	475	LEU
2	B	487	SER
2	B	530	ILE
2	B	532	THR
2	B	543	ASP
2	B	562	CYS
2	B	570	THR
2	B	574	SER
2	B	616	SER
2	B	635	ILE
2	B	654	LEU
2	B	659	VAL
2	B	667	LEU
2	B	681	LEU
2	B	688	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	692	SER
2	B	697	LYS
2	B	704	SER
2	B	706	VAL
2	B	717	THR
2	B	729	ILE
3	C	1	SER
3	C	3	SER
3	C	6	ILE
3	C	9	THR
3	C	25	LEU
3	C	28	VAL
3	C	68	LEU
3	C	73	THR
3	C	76	SER
5	V	6	SER
5	V	10	ILE
5	V	21	VAL
5	V	30	SER
5	V	56	THR
6	F	29	VAL
6	F	32	SER
6	F	34	SER
6	F	43	SER
6	F	52	ASN
6	F	65	LEU
6	F	75	ILE
6	F	118	GLU
6	F	138	THR
6	F	152	LEU
6	F	153	VAL
6	F	156	ASP
6	F	159	ILE
6	F	162	SER
7	I	5	SER
7	I	7	LEU
7	I	22	ILE
8	J	13	ARG
8	J	16	SER
8	J	17	LEU
8	J	20	VAL
8	J	32	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	J	39	LEU
9	K	35	ILE
9	K	47	GLN
9	K	73	SER
9	K	77	ILE
9	K	78	VAL
9	K	84	LEU
9	K	92	LEU
9	K	93	LYS
10	L	32	ASN
10	L	35	THR
10	L	41	SER
10	L	43	VAL
10	L	60	LEU
10	L	74	LEU
10	L	86	ASP
10	L	101	MET
10	L	147	LEU
10	L	151	VAL
10	L	155	VAL
10	L	164	ILE
10	L	172	LYS
11	M	19	MET
11	M	30	LEU
11	M	34	LEU
11	M	38	VAL
11	M	42	ARG
1	E	25	SER
1	E	28	LYS
1	E	47	THR
1	E	63	THR
1	E	89	SER
1	E	91	MET
1	E	106	SER
1	E	128	ASN
1	E	172	LEU
1	E	174	LEU
1	E	198	LEU
1	E	211	LEU
1	E	220	VAL
1	E	222	LEU
1	E	226	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	248	SER
1	E	249	LEU
1	E	303	VAL
1	E	346	THR
1	E	355	THR
1	E	360	LEU
1	E	363	LEU
1	E	365	ILE
1	E	382	THR
1	E	389	SER
1	E	401	LEU
1	E	403	VAL
1	E	431	ILE
1	E	448	LEU
1	E	503	LEU
1	E	507	SER
1	E	545	VAL
1	E	546	THR
1	E	575	CYS
1	E	580	ARG
1	E	583	THR
1	E	590	ASP
1	E	611	SER
1	E	621	THR
1	E	639	SER
1	E	664	SER
1	E	674	LEU
1	E	679	VAL
1	E	699	GLU
1	E	708	LEU
1	E	713	THR
1	E	734	LEU
1	E	750	SER
2	G	9	SER
2	G	46	LEU
2	G	63	SER
2	G	105	THR
2	G	113	VAL
2	G	137	SER
2	G	144	ILE
2	G	157	LEU
2	G	164	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	175	LEU
2	G	187	SER
2	G	195	VAL
2	G	213	LEU
2	G	214	THR
2	G	215	THR
2	G	216	LEU
2	G	270	LEU
2	G	280	ILE
2	G	283	LEU
2	G	290	MET
2	G	297	ILE
2	G	304	MET
2	G	334	LEU
2	G	340	LEU
2	G	345	LEU
2	G	348	ILE
2	G	350	SER
2	G	377	THR
2	G	384	VAL
2	G	412	LEU
2	G	437	THR
2	G	440	LEU
2	G	446	VAL
2	G	458	LEU
2	G	475	LEU
2	G	487	SER
2	G	530	ILE
2	G	532	THR
2	G	543	ASP
2	G	562	CYS
2	G	570	THR
2	G	574	SER
2	G	616	SER
2	G	635	ILE
2	G	654	LEU
2	G	659	VAL
2	G	667	LEU
2	G	681	LEU
2	G	688	THR
2	G	692	SER
2	G	697	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	704	SER
2	G	706	VAL
2	G	717	THR
2	G	729	ILE
3	H	1	SER
3	H	3	SER
3	H	6	ILE
3	H	9	THR
3	H	25	LEU
3	H	28	VAL
3	H	68	LEU
3	H	73	THR
3	H	76	SER
5	W	6	SER
5	W	10	ILE
5	W	21	VAL
5	W	30	SER
5	W	56	THR
6	O	29	VAL
6	O	32	SER
6	O	34	SER
6	O	43	SER
6	O	52	ASN
6	O	65	LEU
6	O	75	ILE
6	O	118	GLU
6	O	138	THR
6	O	152	LEU
6	O	153	VAL
6	O	156	ASP
6	O	159	ILE
6	O	162	SER
7	P	5	SER
7	P	7	LEU
7	P	22	ILE
8	Q	13	ARG
8	Q	16	SER
8	Q	17	LEU
8	Q	20	VAL
8	Q	32	LEU
8	Q	39	LEU
9	R	35	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
9	R	47	GLN
9	R	73	SER
9	R	77	ILE
9	R	78	VAL
9	R	84	LEU
9	R	92	LEU
9	R	93	LYS
10	S	32	ASN
10	S	35	THR
10	S	41	SER
10	S	43	VAL
10	S	60	LEU
10	S	74	LEU
10	S	86	ASP
10	S	101	MET
10	S	147	LEU
10	S	151	VAL
10	S	155	VAL
10	S	164	ILE
10	S	172	LYS
11	T	19	MET
11	T	30	LEU
11	T	34	LEU
11	T	38	VAL
11	T	42	ARG
1	e	25	SER
1	e	28	LYS
1	e	47	THR
1	e	63	THR
1	e	89	SER
1	e	91	MET
1	e	106	SER
1	e	128	ASN
1	e	172	LEU
1	e	174	LEU
1	e	198	LEU
1	e	211	LEU
1	e	220	VAL
1	e	222	LEU
1	e	226	LYS
1	e	248	SER
1	e	249	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	e	303	VAL
1	e	346	THR
1	e	355	THR
1	e	360	LEU
1	e	363	LEU
1	e	365	ILE
1	e	382	THR
1	e	389	SER
1	e	401	LEU
1	e	403	VAL
1	e	431	ILE
1	e	448	LEU
1	e	503	LEU
1	e	507	SER
1	e	545	VAL
1	e	546	THR
1	e	575	CYS
1	e	580	ARG
1	e	583	THR
1	e	590	ASP
1	e	611	SER
1	e	621	THR
1	e	639	SER
1	e	664	SER
1	e	674	LEU
1	e	679	VAL
1	e	699	GLU
1	e	708	LEU
1	e	713	THR
1	e	734	LEU
1	e	750	SER
2	g	9	SER
2	g	46	LEU
2	g	63	SER
2	g	105	THR
2	g	113	VAL
2	g	137	SER
2	g	144	ILE
2	g	157	LEU
2	g	164	SER
2	g	175	LEU
2	g	187	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	g	195	VAL
2	g	213	LEU
2	g	214	THR
2	g	215	THR
2	g	216	LEU
2	g	270	LEU
2	g	280	ILE
2	g	283	LEU
2	g	290	MET
2	g	297	ILE
2	g	304	MET
2	g	334	LEU
2	g	340	LEU
2	g	345	LEU
2	g	348	ILE
2	g	350	SER
2	g	377	THR
2	g	384	VAL
2	g	412	LEU
2	g	437	THR
2	g	440	LEU
2	g	446	VAL
2	g	458	LEU
2	g	475	LEU
2	g	487	SER
2	g	530	ILE
2	g	532	THR
2	g	543	ASP
2	g	562	CYS
2	g	570	THR
2	g	574	SER
2	g	616	SER
2	g	635	ILE
2	g	654	LEU
2	g	659	VAL
2	g	667	LEU
2	g	681	LEU
2	g	688	THR
2	g	692	SER
2	g	697	LYS
2	g	704	SER
2	g	706	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	g	717	THR
2	g	729	ILE
3	h	1	SER
3	h	3	SER
3	h	6	ILE
3	h	9	THR
3	h	25	LEU
3	h	28	VAL
3	h	68	LEU
3	h	73	THR
3	h	76	SER
5	v	6	SER
5	v	10	ILE
5	v	21	VAL
5	v	30	SER
5	v	56	THR
6	o	29	VAL
6	o	32	SER
6	o	34	SER
6	o	43	SER
6	o	52	ASN
6	o	65	LEU
6	o	75	ILE
6	o	118	GLU
6	o	138	THR
6	o	152	LEU
6	o	153	VAL
6	o	156	ASP
6	o	159	ILE
6	o	162	SER
7	p	5	SER
7	p	7	LEU
7	p	22	ILE
8	q	13	ARG
8	q	16	SER
8	q	17	LEU
8	q	20	VAL
8	q	32	LEU
8	q	39	LEU
9	r	35	ILE
9	r	47	GLN
9	r	73	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	r	77	ILE
9	r	78	VAL
9	r	84	LEU
9	r	92	LEU
9	r	93	LYS
10	s	32	ASN
10	s	35	THR
10	s	41	SER
10	s	43	VAL
10	s	60	LEU
10	s	74	LEU
10	s	86	ASP
10	s	101	MET
10	s	147	LEU
10	s	151	VAL
10	s	155	VAL
10	s	164	ILE
10	s	172	LYS
11	t	19	MET
11	t	30	LEU
11	t	34	LEU
11	t	38	VAL
11	t	42	ARG
1	a	25	SER
1	a	28	LYS
1	a	47	THR
1	a	63	THR
1	a	89	SER
1	a	91	MET
1	a	106	SER
1	a	128	ASN
1	a	172	LEU
1	a	174	LEU
1	a	198	LEU
1	a	211	LEU
1	a	220	VAL
1	a	222	LEU
1	a	226	LYS
1	a	248	SER
1	a	249	LEU
1	a	303	VAL
1	a	346	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	a	355	THR
1	a	360	LEU
1	a	363	LEU
1	a	365	ILE
1	a	382	THR
1	a	389	SER
1	a	401	LEU
1	a	403	VAL
1	a	431	ILE
1	a	448	LEU
1	a	503	LEU
1	a	507	SER
1	a	545	VAL
1	a	546	THR
1	a	575	CYS
1	a	580	ARG
1	a	583	THR
1	a	590	ASP
1	a	611	SER
1	a	621	THR
1	a	639	SER
1	a	664	SER
1	a	674	LEU
1	a	679	VAL
1	a	699	GLU
1	a	708	LEU
1	a	713	THR
1	a	734	LEU
1	a	750	SER
2	b	9	SER
2	b	46	LEU
2	b	63	SER
2	b	105	THR
2	b	113	VAL
2	b	137	SER
2	b	144	ILE
2	b	157	LEU
2	b	164	SER
2	b	175	LEU
2	b	187	SER
2	b	195	VAL
2	b	213	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	b	214	THR
2	b	215	THR
2	b	216	LEU
2	b	270	LEU
2	b	280	ILE
2	b	283	LEU
2	b	290	MET
2	b	297	ILE
2	b	304	MET
2	b	334	LEU
2	b	340	LEU
2	b	345	LEU
2	b	348	ILE
2	b	350	SER
2	b	377	THR
2	b	384	VAL
2	b	412	LEU
2	b	437	THR
2	b	440	LEU
2	b	446	VAL
2	b	458	LEU
2	b	475	LEU
2	b	487	SER
2	b	530	ILE
2	b	532	THR
2	b	543	ASP
2	b	562	CYS
2	b	570	THR
2	b	574	SER
2	b	616	SER
2	b	635	ILE
2	b	654	LEU
2	b	659	VAL
2	b	667	LEU
2	b	681	LEU
2	b	688	THR
2	b	692	SER
2	b	697	LYS
2	b	704	SER
2	b	706	VAL
2	b	717	THR
2	b	729	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	c	1	SER
3	c	3	SER
3	c	6	ILE
3	c	9	THR
3	c	25	LEU
3	c	28	VAL
3	c	68	LEU
3	c	73	THR
3	c	76	SER
5	w	6	SER
5	w	10	ILE
5	w	21	VAL
5	w	30	SER
5	w	56	THR
6	f	29	VAL
6	f	32	SER
6	f	34	SER
6	f	43	SER
6	f	52	ASN
6	f	65	LEU
6	f	75	ILE
6	f	118	GLU
6	f	138	THR
6	f	152	LEU
6	f	153	VAL
6	f	156	ASP
6	f	159	ILE
6	f	162	SER
7	i	5	SER
7	i	7	LEU
7	i	22	ILE
8	j	13	ARG
8	j	16	SER
8	j	17	LEU
8	j	20	VAL
8	j	32	LEU
8	j	39	LEU
9	k	35	ILE
9	k	47	GLN
9	k	73	SER
9	k	77	ILE
9	k	78	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
9	k	84	LEU
9	k	92	LEU
9	k	93	LYS
10	l	32	ASN
10	l	35	THR
10	l	41	SER
10	l	43	VAL
10	l	60	LEU
10	l	74	LEU
10	l	86	ASP
10	l	101	MET
10	l	147	LEU
10	l	151	VAL
10	l	155	VAL
10	l	164	ILE
10	l	172	LYS
11	m	19	MET
11	m	30	LEU
11	m	34	LEU
11	m	38	VAL
11	m	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	116	GLN
1	A	199	ASN
1	A	296	HIS
1	A	328	ASN
1	A	369	HIS
1	A	440	HIS
1	A	458	HIS
1	A	459	ASN
1	A	478	GLN
1	A	480	GLN
1	A	491	HIS
1	A	591	HIS
1	A	615	GLN
1	A	657	GLN
2	B	10	GLN
2	B	34	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	41	ASN
2	B	242	HIS
2	B	275	HIS
2	B	276	HIS
2	B	306	ASN
2	B	309	ASN
2	B	332	ASN
2	B	355	HIS
2	B	367	GLN
2	B	378	HIS
2	B	436	HIS
2	B	444	ASN
2	B	456	GLN
2	B	471	HIS
2	B	531	HIS
2	B	613	ASN
2	B	636	ASN
2	B	685	HIS
4	D	73	GLN
4	D	121	ASN
6	F	55	GLN
6	F	73	HIS
8	J	37	ASN
9	K	76	HIS
10	L	70	HIS
1	E	80	GLN
1	E	116	GLN
1	E	199	ASN
1	E	296	HIS
1	E	328	ASN
1	E	369	HIS
1	E	423	GLN
1	E	440	HIS
1	E	458	HIS
1	E	459	ASN
1	E	478	GLN
1	E	480	GLN
1	E	491	HIS
1	E	568	ASN
1	E	591	HIS
1	E	615	GLN
1	E	657	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	10	GLN
2	G	34	HIS
2	G	41	ASN
2	G	242	HIS
2	G	275	HIS
2	G	276	HIS
2	G	306	ASN
2	G	309	ASN
2	G	332	ASN
2	G	355	HIS
2	G	367	GLN
2	G	378	HIS
2	G	436	HIS
2	G	444	ASN
2	G	456	GLN
2	G	471	HIS
2	G	531	HIS
2	G	613	ASN
2	G	685	HIS
4	N	8	GLN
4	N	56	ASN
4	N	72	GLN
4	N	98	HIS
4	N	140	ASN
6	O	55	GLN
6	O	73	HIS
8	Q	37	ASN
9	R	76	HIS
10	S	70	HIS
1	e	80	GLN
1	e	116	GLN
1	e	199	ASN
1	e	296	HIS
1	e	328	ASN
1	e	369	HIS
1	e	440	HIS
1	e	458	HIS
1	e	459	ASN
1	e	478	GLN
1	e	480	GLN
1	e	491	HIS
1	e	591	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	e	615	GLN
1	e	657	GLN
2	g	10	GLN
2	g	34	HIS
2	g	41	ASN
2	g	242	HIS
2	g	275	HIS
2	g	276	HIS
2	g	306	ASN
2	g	309	ASN
2	g	332	ASN
2	g	355	HIS
2	g	367	GLN
2	g	378	HIS
2	g	436	HIS
2	g	444	ASN
2	g	456	GLN
2	g	471	HIS
2	g	531	HIS
2	g	613	ASN
2	g	636	ASN
2	g	685	HIS
4	n	73	GLN
4	n	95	GLN
4	n	113	GLN
4	n	121	ASN
4	n	140	ASN
6	o	55	GLN
6	o	73	HIS
8	q	37	ASN
9	r	76	HIS
10	s	70	HIS
1	a	80	GLN
1	a	116	GLN
1	a	199	ASN
1	a	296	HIS
1	a	328	ASN
1	a	369	HIS
1	a	440	HIS
1	a	458	HIS
1	a	459	ASN
1	a	478	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	a	480	GLN
1	a	491	HIS
1	a	591	HIS
1	a	615	GLN
1	a	657	GLN
2	b	10	GLN
2	b	34	HIS
2	b	41	ASN
2	b	242	HIS
2	b	275	HIS
2	b	276	HIS
2	b	306	ASN
2	b	309	ASN
2	b	332	ASN
2	b	355	HIS
2	b	367	GLN
2	b	378	HIS
2	b	436	HIS
2	b	444	ASN
2	b	456	GLN
2	b	471	HIS
2	b	531	HIS
2	b	613	ASN
2	b	685	HIS
3	c	37	GLN
4	d	56	ASN
4	d	72	GLN
4	d	73	GLN
4	d	95	GLN
6	f	55	GLN
6	f	73	HIS
8	j	37	ASN
10	l	70	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

462 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
13	CLA	E	845	-	50,58,73	1.66	7 (14%)	58,95,113	1.51	8 (13%)
13	CLA	A	837	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	E	807	-	50,58,73	1.63	6 (12%)	58,95,113	1.55	8 (13%)
13	CLA	B	804	-	50,58,73	1.65	7 (14%)	58,95,113	1.46	8 (13%)
13	CLA	G	832	-	49,57,73	1.68	7 (14%)	55,93,113	1.53	7 (12%)
15	BCR	S	202	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	6 (10%)
13	CLA	a	805	-	50,58,73	1.63	8 (16%)	58,95,113	1.45	7 (12%)
14	PQN	G	842	-	34,34,34	1.64	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	G	840	-	50,58,73	1.68	9 (18%)	58,95,113	1.52	8 (13%)
13	CLA	E	808	-	50,58,73	1.66	6 (12%)	58,95,113	1.62	8 (13%)
13	CLA	e	803	-	50,58,73	1.65	6 (12%)	58,95,113	1.48	9 (15%)
13	CLA	g	838	-	50,58,73	1.64	6 (12%)	58,95,113	1.57	8 (13%)
13	CLA	l	203	10	50,58,73	1.64	6 (12%)	58,95,113	1.54	9 (15%)
13	CLA	e	825	-	50,58,73	1.68	7 (14%)	58,95,113	1.54	9 (15%)
13	CLA	l	204	-	45,53,73	1.75	7 (15%)	52,89,113	1.63	7 (13%)
13	CLA	G	803	-	50,58,73	1.65	7 (14%)	58,95,113	1.46	8 (13%)
13	CLA	g	820	-	50,58,73	1.65	7 (14%)	58,95,113	1.53	6 (10%)
13	CLA	G	841	-	50,58,73	1.66	8 (16%)	58,95,113	1.57	7 (12%)
15	BCR	A	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
13	CLA	G	838	-	50,58,73	1.65	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	a	812	1	50,58,73	1.67	5 (10%)	58,95,113	1.55	8 (13%)
13	CLA	A	819	-	49,57,73	1.71	7 (14%)	55,93,113	1.55	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	e	814	-	50,58,73	1.65	6 (12%)	58,95,113	1.55	7 (12%)
15	BCR	Q	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	g	837	-	45,53,73	1.76	6 (13%)	52,89,113	1.70	7 (13%)
13	CLA	g	823	-	45,53,73	1.74	7 (15%)	52,89,113	1.68	7 (13%)
13	CLA	g	801	-	50,58,73	1.63	7 (14%)	58,95,113	1.45	7 (12%)
13	CLA	B	811	2	50,58,73	1.67	8 (16%)	58,95,113	1.56	8 (13%)
13	CLA	g	818	-	50,58,73	1.68	6 (12%)	58,95,113	1.47	8 (13%)
13	CLA	E	838	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	G	812	-	45,53,73	1.77	7 (15%)	52,89,113	1.50	7 (13%)
13	CLA	B	816	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
13	CLA	B	828	-	50,58,73	1.66	8 (16%)	58,95,113	1.47	8 (13%)
13	CLA	a	822	-	50,58,73	1.67	7 (14%)	58,95,113	1.47	8 (13%)
15	BCR	I	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.18	2 (3%)
13	CLA	e	819	-	50,58,73	1.67	7 (14%)	58,95,113	1.57	9 (15%)
15	BCR	R	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.43	7 (12%)
13	CLA	B	833	-	50,58,73	1.73	8 (16%)	58,95,113	1.46	9 (15%)
13	CLA	E	823	-	50,58,73	1.65	8 (16%)	58,95,113	1.46	6 (10%)
13	CLA	A	842	-	50,58,73	1.64	7 (14%)	58,95,113	1.59	9 (15%)
13	CLA	b	827	-	50,58,73	1.67	8 (16%)	58,95,113	1.47	8 (13%)
13	CLA	e	829	-	50,58,73	1.68	7 (14%)	58,95,113	1.54	8 (13%)
13	CLA	e	836	-	50,58,73	1.69	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	A	820	-	50,58,73	1.66	7 (14%)	58,95,113	1.58	8 (13%)
13	CLA	e	834	-	50,58,73	1.72	8 (16%)	58,95,113	1.66	9 (15%)
13	CLA	G	836	-	45,53,73	1.76	6 (13%)	52,89,113	1.69	7 (13%)
16	SF4	a	846	-	0,12,12	-	-	-	-	-
13	CLA	B	835	-	45,53,73	1.81	7 (15%)	52,89,113	1.54	7 (13%)
13	CLA	G	813	-	45,53,73	1.79	8 (17%)	52,89,113	1.52	7 (13%)
15	BCR	G	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	5 (8%)
13	CLA	E	814	-	50,58,73	1.70	7 (14%)	58,95,113	1.51	7 (12%)
13	CLA	B	807	-	50,58,73	1.66	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	b	822	2	50,58,73	1.69	8 (16%)	58,95,113	1.56	8 (13%)
13	CLA	g	809	-	50,58,73	1.67	9 (18%)	58,95,113	1.50	8 (13%)
13	CLA	b	824	-	50,58,73	1.63	6 (12%)	58,95,113	1.63	8 (13%)
15	BCR	m	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.33	9 (16%)
13	CLA	E	834	-	50,58,73	1.64	9 (18%)	58,95,113	1.48	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	B	813	-	45,53,73	1.79	6 (13%)	52,89,113	1.53	7 (13%)
13	CLA	E	826	-	50,58,73	1.69	7 (14%)	58,95,113	1.53	9 (15%)
13	CLA	g	839	-	50,58,73	1.65	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	e	804	-	50,58,73	1.61	7 (14%)	58,95,113	1.60	8 (13%)
13	CLA	B	801	-	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
13	CLA	A	815	-	50,58,73	1.66	6 (12%)	58,95,113	1.55	7 (12%)
15	BCR	k	4001	-	41,41,41	1.17	3 (7%)	56,56,56	1.59	10 (17%)
13	CLA	a	836	-	50,58,73	1.71	8 (16%)	58,95,113	1.66	8 (13%)
15	BCR	s	201	-	41,41,41	1.24	3 (7%)	56,56,56	1.16	5 (8%)
13	CLA	a	817	-	50,58,73	1.73	7 (14%)	58,95,113	1.51	8 (13%)
13	CLA	e	810	-	50,58,73	1.67	7 (14%)	58,95,113	1.52	9 (15%)
15	BCR	G	845	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	G	824	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
13	CLA	b	832	-	50,58,73	1.72	8 (16%)	58,95,113	1.46	9 (15%)
13	CLA	b	834	-	45,53,73	1.81	7 (15%)	52,89,113	1.54	7 (13%)
15	BCR	A	851	-	41,41,41	1.25	2 (4%)	56,56,56	1.26	7 (12%)
15	BCR	b	842	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
13	CLA	G	811	-	50,58,73	1.68	6 (12%)	58,95,113	1.50	7 (12%)
13	CLA	e	840	-	47,55,73	1.72	8 (17%)	54,91,113	1.55	6 (11%)
16	SF4	g	804	-	0,12,12	-	-	-	-	-
15	BCR	b	843	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	E	824	-	50,58,73	1.66	6 (12%)	58,95,113	1.58	8 (13%)
13	CLA	e	841	-	50,58,73	1.62	6 (12%)	58,95,113	1.60	9 (15%)
15	BCR	O	202	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	A	818	-	45,53,73	1.76	6 (13%)	52,89,113	1.61	6 (11%)
13	CLA	A	822	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	8 (13%)
13	CLA	E	827	-	50,58,73	1.69	7 (14%)	58,95,113	1.50	9 (15%)
15	BCR	G	847	-	41,41,41	1.21	3 (7%)	56,56,56	1.17	6 (10%)
13	CLA	e	837	1	45,53,73	1.75	6 (13%)	52,89,113	1.66	8 (15%)
13	CLA	B	819	-	50,58,73	1.66	6 (12%)	58,95,113	1.53	7 (12%)
13	CLA	g	812	2	50,58,73	1.68	7 (14%)	58,95,113	1.56	8 (13%)
13	CLA	A	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
13	CLA	G	805	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
13	CLA	b	802	-	50,58,73	1.64	7 (14%)	58,95,113	1.57	9 (15%)
13	CLA	E	836	-	50,58,73	1.72	8 (16%)	58,95,113	1.66	8 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	LHG	e	801	-	48,48,48	0.67	1 (2%)	51,54,54	1.30	7 (13%)
14	PQN	E	848	-	34,34,34	1.63	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	b	808	-	50,58,73	1.71	7 (14%)	58,95,113	1.48	7 (12%)
13	CLA	b	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	g	826	-	50,58,73	1.64	7 (14%)	58,95,113	1.63	8 (13%)
13	CLA	E	828	-	50,58,73	1.64	6 (12%)	58,95,113	1.58	9 (15%)
13	CLA	G	820	-	50,58,73	1.67	8 (16%)	58,95,113	1.56	7 (12%)
13	CLA	g	807	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
15	BCR	q	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	L	203	-	45,53,73	1.76	7 (15%)	52,89,113	1.63	7 (13%)
13	CLA	g	806	-	50,58,73	1.64	9 (18%)	58,95,113	1.60	8 (13%)
13	CLA	e	818	-	49,57,73	1.72	6 (12%)	55,93,113	1.55	7 (12%)
13	CLA	g	813	-	50,58,73	1.68	6 (12%)	58,95,113	1.50	7 (12%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-
13	CLA	B	827	-	50,58,73	1.70	6 (12%)	58,95,113	1.45	8 (13%)
13	CLA	g	833	-	49,57,73	1.68	7 (14%)	55,93,113	1.53	7 (12%)
13	CLA	b	837	-	50,58,73	1.65	6 (12%)	58,95,113	1.55	9 (15%)
13	CLA	b	825	-	46,54,73	1.71	7 (15%)	53,90,113	1.63	7 (13%)
13	CLA	E	841	-	50,58,73	1.64	9 (18%)	58,95,113	1.53	8 (13%)
15	BCR	E	852	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	A	838	1	45,53,73	1.75	6 (13%)	52,89,113	1.67	8 (15%)
15	BCR	g	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	5 (8%)
13	CLA	E	840	-	50,58,73	1.65	6 (12%)	58,95,113	1.62	9 (15%)
13	CLA	E	846	-	42,49,73	1.81	7 (16%)	48,83,113	1.71	7 (14%)
15	BCR	E	801	-	41,41,41	1.17	3 (7%)	56,56,56	1.26	8 (14%)
13	CLA	b	818	-	50,58,73	1.66	7 (14%)	58,95,113	1.53	6 (10%)
13	CLA	k	4002	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	9 (17%)
13	CLA	G	837	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)
13	CLA	g	825	-	45,53,73	1.77	6 (13%)	52,89,113	1.61	7 (13%)
13	CLA	b	836	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)
13	CLA	e	805	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
13	CLA	a	818	-	45,53,73	1.76	6 (13%)	52,89,113	1.61	6 (11%)
15	BCR	f	202	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	7 (12%)
15	BCR	e	847	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	5 (8%)
13	CLA	G	818	-	50,58,73	1.69	7 (14%)	58,95,113	1.55	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	o	202	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
15	BCR	e	846	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
15	BCR	A	850	-	41,41,41	1.20	3 (7%)	56,56,56	1.26	8 (14%)
13	CLA	L	202	10	50,58,73	1.66	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	E	833	-	50,58,73	1.62	6 (12%)	58,95,113	1.64	7 (12%)
13	CLA	a	844	-	50,58,73	1.66	7 (14%)	58,95,113	1.54	7 (12%)
13	CLA	e	820	-	50,58,73	1.69	8 (16%)	58,95,113	1.50	9 (15%)
13	CLA	A	832	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	9 (15%)
13	CLA	F	202	-	45,53,73	1.75	5 (11%)	52,89,113	1.58	6 (11%)
13	CLA	A	843	-	50,58,73	1.66	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	a	852	-	50,58,73	1.65	5 (10%)	58,95,113	1.55	9 (15%)
15	BCR	b	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.17	6 (10%)
13	CLA	B	840	-	50,58,73	1.68	9 (18%)	58,95,113	1.53	8 (13%)
13	CLA	B	841	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
16	SF4	B	803	-	0,12,12	-	-	-	-	-
13	CLA	l	205	-	50,58,73	2.51	11 (22%)	58,95,113	3.07	15 (25%)
15	BCR	e	849	-	41,41,41	1.19	3 (7%)	56,56,56	1.27	9 (16%)
13	CLA	A	853	-	50,58,73	1.65	7 (14%)	58,95,113	1.56	9 (15%)
15	BCR	g	846	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	e	828	-	50,58,73	1.70	9 (18%)	58,95,113	1.49	6 (10%)
13	CLA	a	814	-	45,53,73	1.79	7 (15%)	52,89,113	1.58	7 (13%)
13	CLA	E	822	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	8 (13%)
15	BCR	e	850	-	41,41,41	1.22	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	f	203	-	45,53,73	1.75	7 (15%)	52,89,113	1.70	6 (11%)
16	SF4	h	101	-	0,12,12	-	-	-	-	-
13	CLA	b	823	-	45,53,73	1.78	6 (13%)	52,89,113	1.62	7 (13%)
13	CLA	G	830	-	50,58,73	1.64	7 (14%)	58,95,113	1.61	8 (13%)
13	CLA	G	827	-	50,58,73	1.70	6 (12%)	58,95,113	1.46	8 (13%)
15	BCR	B	847	-	41,41,41	1.21	2 (4%)	56,56,56	1.17	6 (10%)
15	BCR	B	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	8 (14%)
13	CLA	a	845	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	8 (13%)
13	CLA	b	828	-	50,58,73	1.66	7 (14%)	58,95,113	1.51	8 (13%)
13	CLA	a	821	-	50,58,73	1.69	8 (16%)	58,95,113	1.50	9 (15%)
13	CLA	G	831	-	45,53,73	1.77	6 (13%)	52,89,113	1.54	8 (15%)
15	BCR	a	803	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	e	827	-	50,58,73	1.64	7 (14%)	58,95,113	1.59	9 (15%)
13	CLA	a	815	-	50,58,73	1.65	6 (12%)	58,95,113	1.55	7 (12%)
13	CLA	G	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	E	819	-	49,57,73	1.71	6 (12%)	55,93,113	1.55	7 (12%)
13	CLA	G	801	-	50,58,73	1.68	8 (16%)	58,95,113	1.57	9 (15%)
14	PQN	a	847	-	34,34,34	1.63	2 (5%)	42,45,45	1.18	4 (9%)
13	CLA	a	839	1	45,53,73	1.75	6 (13%)	52,89,113	1.67	8 (15%)
13	CLA	A	824	-	50,58,73	1.66	6 (12%)	58,95,113	1.57	8 (13%)
13	CLA	g	835	-	50,58,73	1.67	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	G	828	-	50,58,73	1.66	8 (16%)	58,95,113	1.46	8 (13%)
13	CLA	b	826	-	50,58,73	1.71	6 (12%)	58,95,113	1.46	8 (13%)
13	CLA	A	845	12	50,58,73	1.65	6 (12%)	58,95,113	1.63	7 (12%)
13	CLA	g	832	-	45,53,73	1.77	6 (13%)	52,89,113	1.54	8 (15%)
13	CLA	a	831	-	50,58,73	1.69	7 (14%)	58,95,113	1.57	9 (15%)
13	CLA	a	841	-	50,58,73	1.64	9 (18%)	58,95,113	1.52	8 (13%)
13	CLA	a	838	-	50,58,73	1.69	6 (12%)	58,95,113	1.55	9 (15%)
13	CLA	e	806	-	50,58,73	1.63	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	b	807	-	50,58,73	1.66	9 (18%)	58,95,113	1.48	8 (13%)
13	CLA	B	831	-	45,53,73	1.77	6 (13%)	52,89,113	1.53	8 (15%)
13	CLA	a	820	-	50,58,73	1.67	7 (14%)	58,95,113	1.58	9 (15%)
13	CLA	A	829	-	50,58,73	1.70	9 (18%)	58,95,113	1.49	6 (10%)
13	CLA	K	102	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	8 (15%)
13	CLA	A	805	-	50,58,73	1.64	7 (14%)	58,95,113	1.45	7 (12%)
13	CLA	G	819	-	50,58,73	1.66	7 (14%)	58,95,113	1.53	7 (12%)
13	CLA	B	836	-	45,53,73	1.76	6 (13%)	52,89,113	1.69	7 (13%)
13	CLA	a	823	-	50,58,73	1.66	8 (16%)	58,95,113	1.45	6 (10%)
13	CLA	E	809	1	50,58,73	1.68	8 (16%)	58,95,113	1.48	6 (10%)
13	CLA	g	814	-	45,53,73	1.78	6 (13%)	52,89,113	1.52	7 (13%)
13	CLA	G	834	-	50,58,73	1.67	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	a	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
14	PQN	e	845	-	34,34,34	1.63	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	E	810	-	50,58,73	1.69	6 (12%)	58,95,113	1.50	8 (13%)
13	CLA	B	830	-	50,58,73	1.64	6 (12%)	58,95,113	1.61	8 (13%)
13	CLA	a	809	1	50,58,73	1.68	8 (16%)	58,95,113	1.48	7 (12%)
13	CLA	e	831	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	a	840	-	50,58,73	1.64	7 (14%)	58,95,113	1.62	9 (15%)
13	CLA	B	838	-	50,58,73	1.65	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	B	820	-	50,58,73	1.67	7 (14%)	58,95,113	1.55	7 (12%)
13	CLA	g	841	-	50,58,73	1.68	9 (18%)	58,95,113	1.53	8 (13%)
13	CLA	e	821	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	8 (13%)
15	BCR	A	852	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	7 (12%)
13	CLA	e	832	-	50,58,73	1.62	6 (12%)	58,95,113	1.63	7 (12%)
15	BCR	j	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	5 (8%)
13	CLA	g	842	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
15	BCR	g	848	-	41,41,41	1.21	2 (4%)	56,56,56	1.17	6 (10%)
15	BCR	e	851	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	b	829	-	50,58,73	1.65	6 (12%)	58,95,113	1.61	8 (13%)
15	BCR	J	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	B	837	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)
13	CLA	b	812	-	45,53,73	1.78	7 (15%)	52,89,113	1.53	7 (13%)
15	BCR	T	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	4 (7%)
13	CLA	E	832	-	50,58,73	1.67	7 (14%)	58,95,113	1.48	9 (15%)
13	CLA	g	831	-	50,58,73	1.64	6 (12%)	58,95,113	1.62	8 (13%)
13	CLA	e	830	-	50,58,73	1.69	7 (14%)	58,95,113	1.57	9 (15%)
15	BCR	G	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	B	818	-	50,58,73	1.69	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	G	829	-	50,58,73	1.67	7 (14%)	58,95,113	1.52	8 (13%)
13	CLA	e	815	-	50,58,73	1.67	6 (12%)	58,95,113	1.55	9 (15%)
13	CLA	e	842	-	50,58,73	1.67	7 (14%)	58,95,113	1.53	8 (13%)
13	CLA	E	825	-	49,57,73	1.66	7 (14%)	55,93,113	1.59	9 (16%)
13	CLA	b	835	-	45,53,73	1.76	6 (13%)	52,89,113	1.69	7 (13%)
13	CLA	g	810	-	50,58,73	1.69	7 (14%)	58,95,113	1.48	7 (12%)
13	CLA	r	102	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	8 (15%)
15	BCR	B	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	g	840	-	47,55,73	1.71	7 (14%)	54,91,113	1.60	6 (11%)
13	CLA	E	842	-	47,55,73	1.73	8 (17%)	54,91,113	1.56	6 (11%)
13	CLA	e	852	-	50,58,73	1.65	7 (14%)	58,95,113	1.56	9 (15%)
13	CLA	G	815	-	50,58,73	1.68	7 (14%)	58,95,113	1.56	7 (12%)
13	CLA	E	820	-	50,58,73	1.67	7 (14%)	58,95,113	1.58	9 (15%)
14	PQN	g	843	-	34,34,34	1.63	2 (5%)	42,45,45	1.19	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	g	803	-	50,58,73	1.67	8 (16%)	58,95,113	1.54	7 (12%)
13	CLA	a	830	-	50,58,73	1.69	7 (14%)	58,95,113	1.54	8 (13%)
15	BCR	E	802	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
13	CLA	G	835	-	45,53,73	1.81	7 (15%)	52,89,113	1.54	7 (13%)
15	BCR	S	201	-	41,41,41	1.19	2 (4%)	56,56,56	1.13	3 (5%)
15	BCR	l	202	-	41,41,41	1.19	2 (4%)	56,56,56	1.16	5 (8%)
12	LHG	e	802	13	37,37,48	0.74	1 (2%)	40,43,54	1.34	5 (12%)
13	CLA	g	830	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	8 (13%)
13	CLA	E	831	-	50,58,73	1.69	7 (14%)	58,95,113	1.57	9 (15%)
15	BCR	a	802	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	b	817	-	50,58,73	1.69	7 (14%)	58,95,113	1.54	8 (13%)
13	CLA	G	809	-	50,58,73	1.66	6 (12%)	58,95,113	1.64	9 (15%)
13	CLA	g	821	-	50,58,73	1.68	7 (14%)	58,95,113	1.56	7 (12%)
15	BCR	E	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
16	SF4	h	102	3	0,12,12	-	-	-	-	-
13	CLA	A	809	1	50,58,73	1.67	7 (14%)	58,95,113	1.49	6 (10%)
15	BCR	f	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	a	807	-	50,58,73	1.64	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	A	810	-	50,58,73	1.68	7 (14%)	58,95,113	1.51	8 (13%)
13	CLA	A	841	-	47,55,73	1.72	8 (17%)	54,91,113	1.56	6 (11%)
15	BCR	a	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
13	CLA	a	813	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	7 (13%)
13	CLA	A	821	-	50,58,73	1.69	8 (16%)	58,95,113	1.50	9 (15%)
13	CLA	A	812	1	50,58,73	1.67	5 (10%)	58,95,113	1.54	8 (13%)
13	CLA	G	802	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	9 (15%)
13	CLA	b	801	-	42,49,73	1.80	8 (19%)	48,83,113	1.54	6 (12%)
13	CLA	G	808	-	50,58,73	1.69	7 (14%)	58,95,113	1.48	7 (12%)
14	PQN	B	842	-	34,34,34	1.62	2 (5%)	42,45,45	1.18	4 (9%)
13	CLA	b	809	-	50,58,73	1.66	6 (12%)	58,95,113	1.64	9 (15%)
13	CLA	E	830	-	50,58,73	1.68	7 (14%)	58,95,113	1.54	8 (13%)
13	CLA	b	839	-	50,58,73	1.69	9 (18%)	58,95,113	1.52	8 (13%)
15	BCR	o	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	K	101	-	42,49,73	1.80	7 (16%)	48,83,113	1.57	6 (12%)
12	LHG	A	802	13	37,37,48	0.77	1 (2%)	40,43,54	1.33	5 (12%)
15	BCR	p	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.17	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	BCR	A	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	7 (12%)
15	BCR	g	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	g	824	2	50,58,73	1.68	8 (16%)	58,95,113	1.57	8 (13%)
13	CLA	B	832	-	49,57,73	1.68	6 (12%)	55,93,113	1.54	7 (12%)
13	CLA	a	833	-	50,58,73	1.63	6 (12%)	58,95,113	1.63	7 (12%)
15	BCR	l	206	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	E	837	-	50,58,73	1.68	6 (12%)	58,95,113	1.47	8 (13%)
13	CLA	A	817	-	45,53,73	1.83	7 (15%)	52,89,113	1.55	6 (11%)
13	CLA	B	809	-	50,58,73	1.70	7 (14%)	58,95,113	1.47	7 (12%)
13	CLA	s	203	-	50,58,73	2.51	11 (22%)	58,95,113	3.06	16 (27%)
15	BCR	E	851	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	g	836	-	45,53,73	1.82	7 (15%)	52,89,113	1.55	7 (13%)
13	CLA	e	835	-	50,58,73	1.68	7 (14%)	58,95,113	1.47	8 (13%)
13	CLA	A	816	-	50,58,73	1.67	6 (12%)	58,95,113	1.54	9 (15%)
13	CLA	g	834	-	50,58,73	1.73	8 (16%)	58,95,113	1.46	9 (15%)
13	CLA	E	818	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	6 (11%)
15	BCR	b	845	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	5 (8%)
13	CLA	A	826	-	50,58,73	1.68	7 (14%)	58,95,113	1.54	9 (15%)
13	CLA	G	822	-	45,53,73	1.74	5 (11%)	52,89,113	1.67	7 (13%)
15	BCR	g	849	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	a	819	-	49,57,73	1.71	6 (12%)	55,93,113	1.55	7 (12%)
13	CLA	G	817	-	50,58,73	1.68	6 (12%)	58,95,113	1.47	8 (13%)
13	CLA	A	807	-	50,58,73	1.63	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	A	834	-	50,58,73	1.66	9 (18%)	58,95,113	1.48	8 (13%)
15	BCR	L	201	-	41,41,41	1.22	2 (4%)	56,56,56	1.13	3 (5%)
13	CLA	a	827	-	50,58,73	1.68	7 (14%)	58,95,113	1.51	9 (15%)
13	CLA	A	813	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	7 (13%)
13	CLA	S	203	-	45,53,73	1.76	7 (15%)	52,89,113	1.62	7 (13%)
13	CLA	B	808	-	50,58,73	1.67	9 (18%)	58,95,113	1.49	9 (15%)
13	CLA	B	806	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
13	CLA	g	811	-	50,58,73	1.66	7 (14%)	58,95,113	1.64	9 (15%)
13	CLA	G	826	-	46,54,73	1.71	7 (15%)	53,90,113	1.63	7 (13%)
13	CLA	E	805	-	50,58,73	1.64	7 (14%)	58,95,113	1.45	7 (12%)
13	CLA	G	821	-	47,55,73	1.74	7 (14%)	54,91,113	1.53	7 (12%)
13	CLA	e	809	-	50,58,73	1.68	7 (14%)	58,95,113	1.51	8 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	BCR	P	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.17	2 (3%)
13	CLA	b	810	2	50,58,73	1.67	8 (16%)	58,95,113	1.56	8 (13%)
15	BCR	a	850	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	5 (8%)
15	BCR	B	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	5 (8%)
13	CLA	E	821	-	50,58,73	1.69	8 (16%)	58,95,113	1.50	9 (15%)
13	CLA	g	816	-	50,58,73	1.68	7 (14%)	58,95,113	1.56	7 (12%)
15	BCR	s	204	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	8 (14%)
16	SF4	H	101	-	0,12,12	-	-	-	-	-
13	CLA	G	823	2	50,58,73	1.69	8 (16%)	58,95,113	1.57	8 (13%)
13	CLA	B	824	-	45,53,73	1.77	6 (13%)	52,89,113	1.61	7 (13%)
16	SF4	E	847	-	0,12,12	-	-	-	-	-
13	CLA	a	835	-	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
13	CLA	G	825	-	50,58,73	1.64	7 (14%)	58,95,113	1.63	8 (13%)
13	CLA	b	814	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	7 (12%)
13	CLA	B	829	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	8 (13%)
13	CLA	g	828	-	50,58,73	1.70	6 (12%)	58,95,113	1.45	8 (13%)
16	SF4	c	101	-	0,12,12	-	-	-	-	-
13	CLA	A	811	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
13	CLA	s	202	-	45,53,73	1.75	7 (15%)	52,89,113	1.62	7 (13%)
13	CLA	E	844	-	50,58,73	1.66	7 (14%)	58,95,113	1.54	8 (13%)
15	BCR	a	848	-	41,41,41	1.19	3 (7%)	56,56,56	1.74	11 (19%)
13	CLA	g	822	-	47,55,73	1.73	7 (14%)	54,91,113	1.52	7 (12%)
13	CLA	b	838	-	47,55,73	1.70	7 (14%)	54,91,113	1.61	6 (11%)
13	CLA	g	819	-	50,58,73	1.69	7 (14%)	58,95,113	1.56	8 (13%)
13	CLA	S	204	-	45,53,73	2.64	12 (26%)	52,89,113	3.21	15 (28%)
13	CLA	A	828	-	50,58,73	1.64	7 (14%)	58,95,113	1.59	9 (15%)
16	SF4	c	102	3	0,12,12	-	-	-	-	-
15	BCR	J	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	e	824	-	49,57,73	1.67	7 (14%)	55,93,113	1.60	9 (16%)
13	CLA	A	835	-	50,58,73	1.71	7 (14%)	58,95,113	1.66	8 (13%)
13	CLA	E	812	1	50,58,73	1.67	5 (10%)	58,95,113	1.54	8 (13%)
13	CLA	G	807	-	50,58,73	1.66	8 (16%)	58,95,113	1.49	9 (15%)
13	CLA	E	803	-	50,58,73	1.66	5 (10%)	58,95,113	1.47	7 (12%)
13	CLA	g	829	-	50,58,73	1.66	8 (16%)	58,95,113	1.47	8 (13%)
13	CLA	B	815	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	a	810	-	50,58,73	1.68	6 (12%)	58,95,113	1.50	8 (13%)
13	CLA	O	203	-	45,53,73	1.76	7 (15%)	52,89,113	1.68	6 (11%)
13	CLA	a	825	-	49,57,73	1.66	7 (14%)	55,93,113	1.60	9 (16%)
13	CLA	b	819	-	50,58,73	1.67	8 (16%)	58,95,113	1.55	7 (12%)
13	CLA	R	102	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	8 (15%)
15	BCR	A	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	5 (8%)
13	CLA	b	831	-	49,57,73	1.68	6 (12%)	55,93,113	1.54	7 (12%)
13	CLA	a	826	-	50,58,73	1.68	7 (14%)	58,95,113	1.53	9 (15%)
15	BCR	i	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.18	3 (5%)
13	CLA	e	838	-	50,58,73	1.64	7 (14%)	58,95,113	1.60	9 (15%)
13	CLA	e	822	-	50,58,73	1.66	8 (16%)	58,95,113	1.46	6 (10%)
13	CLA	b	811	-	45,53,73	1.77	7 (15%)	52,89,113	1.49	7 (13%)
13	CLA	B	802	-	50,58,73	1.67	8 (16%)	58,95,113	1.53	7 (12%)
13	CLA	e	817	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	6 (11%)
13	CLA	A	844	-	50,58,73	1.65	7 (14%)	58,95,113	1.50	8 (13%)
13	CLA	a	834	-	50,58,73	1.65	9 (18%)	58,95,113	1.47	8 (13%)
15	BCR	F	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	E	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.51	9 (15%)
15	BCR	a	853	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	6 (10%)
13	CLA	l	201	-	45,53,73	1.78	8 (17%)	52,89,113	1.50	7 (13%)
15	BCR	G	843	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
13	CLA	g	827	-	46,54,73	1.71	7 (15%)	53,90,113	1.63	7 (13%)
13	CLA	E	829	-	50,58,73	1.69	9 (18%)	58,95,113	1.50	6 (10%)
13	CLA	E	817	-	45,53,73	1.83	8 (17%)	52,89,113	1.55	6 (11%)
13	CLA	e	826	-	50,58,73	1.69	7 (14%)	58,95,113	1.51	9 (15%)
13	CLA	A	825	-	49,57,73	1.66	7 (14%)	55,93,113	1.60	9 (16%)
13	CLA	a	832	-	50,58,73	1.67	8 (16%)	58,95,113	1.48	9 (15%)
13	CLA	e	843	-	50,58,73	1.66	7 (14%)	58,95,113	1.51	8 (13%)
13	CLA	b	816	-	50,58,73	1.69	6 (12%)	58,95,113	1.48	8 (13%)
13	CLA	b	804	-	50,58,73	1.65	7 (14%)	58,95,113	1.59	8 (13%)
13	CLA	A	803	-	50,58,73	1.65	6 (12%)	58,95,113	1.51	9 (15%)
13	CLA	b	821	-	45,53,73	1.74	6 (13%)	52,89,113	1.68	7 (13%)
13	CLA	e	811	1	50,58,73	1.67	5 (10%)	58,95,113	1.54	8 (13%)
13	CLA	e	813	-	50,58,73	1.71	7 (14%)	58,95,113	1.51	7 (12%)
13	CLA	b	815	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	6 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	A	814	-	50,58,73	1.70	7 (14%)	58,95,113	1.51	7 (12%)
13	CLA	g	817	-	45,53,73	1.76	6 (13%)	52,89,113	1.61	6 (11%)
13	CLA	b	840	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
13	CLA	e	812	-	45,53,73	1.77	6 (13%)	52,89,113	1.55	7 (13%)
13	CLA	G	816	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
15	BCR	b	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	e	839	-	50,58,73	1.65	9 (18%)	58,95,113	1.52	8 (13%)
15	BCR	L	205	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	a	842	-	47,55,73	1.72	8 (17%)	54,91,113	1.56	6 (11%)
13	CLA	e	823	-	50,58,73	1.66	6 (12%)	58,95,113	1.57	8 (13%)
13	CLA	E	811	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
14	PQN	b	841	-	34,34,34	1.64	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	A	808	-	50,58,73	1.66	6 (12%)	58,95,113	1.62	8 (13%)
13	CLA	e	807	-	50,58,73	1.67	6 (12%)	58,95,113	1.62	8 (13%)
13	CLA	a	843	-	50,58,73	1.63	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	g	815	-	50,58,73	1.65	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	A	833	-	50,58,73	1.62	6 (12%)	58,95,113	1.63	7 (12%)
13	CLA	e	808	1	50,58,73	1.67	7 (14%)	58,95,113	1.49	6 (10%)
13	CLA	a	829	-	50,58,73	1.69	9 (18%)	58,95,113	1.49	6 (10%)
13	CLA	E	839	1	45,53,73	1.75	6 (13%)	52,89,113	1.67	8 (15%)
13	CLA	a	824	-	50,58,73	1.65	6 (12%)	58,95,113	1.56	8 (13%)
13	CLA	B	822	-	45,53,73	1.75	7 (15%)	52,89,113	1.68	7 (13%)
13	CLA	G	839	-	47,55,73	1.70	7 (14%)	54,91,113	1.59	6 (11%)
13	CLA	A	804	-	50,58,73	1.62	7 (14%)	58,95,113	1.61	8 (13%)
13	CLA	e	833	-	50,58,73	1.65	9 (18%)	58,95,113	1.47	8 (13%)
13	CLA	a	811	-	50,58,73	1.66	6 (12%)	58,95,113	1.53	9 (15%)
13	CLA	b	833	-	50,58,73	1.68	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	B	810	-	50,58,73	1.65	6 (12%)	58,95,113	1.64	9 (15%)
13	CLA	E	804	-	50,58,73	1.61	7 (14%)	58,95,113	1.61	8 (13%)
13	CLA	B	805	-	50,58,73	1.65	8 (16%)	58,95,113	1.60	8 (13%)
13	CLA	a	837	-	50,58,73	1.68	8 (16%)	58,95,113	1.47	8 (13%)
13	CLA	B	812	-	50,58,73	1.67	6 (12%)	58,95,113	1.49	7 (12%)
13	CLA	G	814	-	50,58,73	1.65	6 (12%)	58,95,113	1.56	8 (13%)
12	LHG	a	801	-	48,48,48	0.64	1 (2%)	51,54,54	1.30	7 (13%)
15	BCR	E	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	E	816	-	50,58,73	1.66	6 (12%)	58,95,113	1.54	9 (15%)
13	CLA	G	833	-	50,58,73	1.73	7 (14%)	58,95,113	1.46	7 (12%)
13	CLA	a	816	-	50,58,73	1.67	7 (14%)	58,95,113	1.54	9 (15%)
14	PQN	A	846	-	34,34,34	1.63	2 (5%)	42,45,45	1.18	4 (9%)
13	CLA	a	804	-	50,58,73	1.61	7 (14%)	58,95,113	1.61	8 (13%)
15	BCR	a	851	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	b	803	-	50,58,73	1.65	6 (12%)	58,95,113	1.45	8 (13%)
13	CLA	g	802	-	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
13	CLA	E	815	-	50,58,73	1.66	6 (12%)	58,95,113	1.55	7 (12%)
13	CLA	A	827	-	50,58,73	1.68	6 (12%)	58,95,113	1.50	9 (15%)
13	CLA	E	843	-	50,58,73	1.63	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	g	808	-	50,58,73	1.65	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	L	204	-	50,58,73	2.51	11 (22%)	58,95,113	3.05	16 (27%)
13	CLA	s	205	-	50,58,73	1.67	6 (12%)	58,95,113	1.50	7 (12%)
13	CLA	a	828	-	50,58,73	1.65	7 (14%)	58,95,113	1.60	9 (15%)
15	BCR	B	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	6 (10%)
13	CLA	E	835	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
15	BCR	O	201	-	41,41,41	1.18	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	A	831	-	50,58,73	1.69	7 (14%)	58,95,113	1.57	8 (13%)
15	BCR	S	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	5 (8%)
13	CLA	E	813	-	45,53,73	1.77	6 (13%)	52,89,113	1.55	7 (13%)
13	CLA	b	813	-	50,58,73	1.64	6 (12%)	58,95,113	1.55	8 (13%)
13	CLA	A	836	-	50,58,73	1.69	8 (16%)	58,95,113	1.48	8 (13%)
15	BCR	q	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	6 (10%)
13	CLA	a	808	-	50,58,73	1.65	6 (12%)	58,95,113	1.63	8 (13%)
13	CLA	B	817	-	50,58,73	1.68	6 (12%)	58,95,113	1.46	8 (13%)
13	CLA	B	825	-	50,58,73	1.63	7 (14%)	58,95,113	1.64	9 (15%)
13	CLA	b	805	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
12	LHG	A	801	-	48,48,48	0.68	1 (2%)	51,54,54	1.31	7 (13%)
13	CLA	B	823	2	50,58,73	1.69	8 (16%)	58,95,113	1.56	8 (13%)
13	CLA	r	101	-	42,49,73	1.81	7 (16%)	48,83,113	1.59	6 (12%)
16	SF4	C	101	-	0,12,12	-	-	-	-	-
15	BCR	e	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	B	826	-	46,54,73	1.71	7 (15%)	53,90,113	1.64	7 (13%)
15	BCR	g	844	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	A	830	-	50,58,73	1.69	7 (14%)	58,95,113	1.54	8 (13%)
15	BCR	G	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	S	206	-	45,53,73	1.78	7 (15%)	52,89,113	1.49	7 (13%)
15	BCR	B	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	B	814	-	50,58,73	1.64	6 (12%)	58,95,113	1.55	8 (13%)
13	CLA	g	805	-	50,58,73	1.65	7 (14%)	58,95,113	1.45	8 (13%)
13	CLA	b	830	-	45,53,73	1.76	6 (13%)	52,89,113	1.53	8 (15%)
13	CLA	B	834	-	50,58,73	1.68	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	B	821	-	47,55,73	1.72	7 (14%)	54,91,113	1.52	7 (12%)
16	SF4	H	102	3	0,12,12	-	-	-	-	-
13	CLA	A	840	-	50,58,73	1.65	9 (18%)	58,95,113	1.52	9 (15%)
13	CLA	A	839	-	50,58,73	1.65	7 (14%)	58,95,113	1.61	9 (15%)
13	CLA	A	823	-	50,58,73	1.65	8 (16%)	58,95,113	1.45	6 (10%)
13	CLA	G	804	-	50,58,73	1.65	8 (16%)	58,95,113	1.59	8 (13%)
13	CLA	e	816	-	45,53,73	1.82	8 (17%)	52,89,113	1.54	6 (11%)
13	CLA	B	839	-	47,55,73	1.71	7 (14%)	54,91,113	1.60	6 (11%)
13	CLA	e	844	12	50,58,73	1.66	7 (14%)	58,95,113	1.63	9 (15%)
15	BCR	b	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	b	820	-	47,55,73	1.72	7 (14%)	54,91,113	1.52	7 (12%)
13	CLA	G	810	2	50,58,73	1.68	7 (14%)	58,95,113	1.55	8 (13%)

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
13	CLA	E	845	-	1/1/12/20	6/19/97/115	-
13	CLA	G	832	-	1/1/11/20	6/18/96/115	-
13	CLA	E	807	-	1/1/12/20	7/19/97/115	-
13	CLA	B	804	-	1/1/12/20	6/19/97/115	-
13	CLA	A	837	-	-	7/19/97/115	-
15	BCR	S	202	-	-	17/29/63/63	0/2/2/2
13	CLA	a	805	-	1/1/12/20	7/19/97/115	-
14	PQN	G	842	-	-	11/23/43/43	0/2/2/2
13	CLA	G	840	-	1/1/12/20	7/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	E	808	-	1/1/12/20	6/19/97/115	-
13	CLA	e	803	-	1/1/12/20	8/19/97/115	-
13	CLA	g	838	-	1/1/12/20	6/19/97/115	-
13	CLA	l	203	10	1/1/12/20	7/19/97/115	-
13	CLA	e	825	-	1/1/12/20	13/19/97/115	-
13	CLA	l	204	-	1/1/11/20	5/13/91/115	-
13	CLA	G	803	-	1/1/12/20	6/19/97/115	-
13	CLA	g	820	-	1/1/12/20	7/19/97/115	-
13	CLA	G	841	-	1/1/12/20	7/19/97/115	-
15	BCR	A	847	-	-	19/29/63/63	0/2/2/2
13	CLA	G	838	-	1/1/12/20	6/19/97/115	-
13	CLA	a	812	1	1/1/12/20	6/19/97/115	-
13	CLA	A	819	-	1/1/11/20	10/18/96/115	-
13	CLA	e	814	-	1/1/12/20	8/19/97/115	-
15	BCR	Q	101	-	-	13/29/63/63	0/2/2/2
13	CLA	g	837	-	1/1/11/20	8/13/91/115	-
13	CLA	g	823	-	1/1/11/20	6/13/91/115	-
13	CLA	g	801	-	1/1/12/20	7/19/97/115	-
13	CLA	B	811	2	1/1/12/20	6/19/97/115	-
13	CLA	g	818	-	1/1/12/20	8/19/97/115	-
13	CLA	E	838	-	-	7/19/97/115	-
13	CLA	G	812	-	1/1/11/20	4/13/91/115	-
13	CLA	B	816	-	1/1/11/20	6/13/91/115	-
13	CLA	B	828	-	1/1/12/20	6/19/97/115	-
13	CLA	a	822	-	1/1/12/20	9/19/97/115	-
15	BCR	I	101	-	-	10/29/63/63	0/2/2/2
13	CLA	e	819	-	1/1/12/20	2/19/97/115	-
15	BCR	R	101	-	-	16/29/63/63	0/2/2/2
13	CLA	B	833	-	1/1/12/20	4/19/97/115	-
13	CLA	E	823	-	1/1/12/20	10/19/97/115	-
13	CLA	A	842	-	1/1/12/20	6/19/97/115	-
13	CLA	b	827	-	1/1/12/20	6/19/97/115	-
13	CLA	e	829	-	1/1/12/20	8/19/97/115	-
13	CLA	e	836	-	-	7/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	820	-	1/1/12/20	2/19/97/115	-
13	CLA	e	834	-	1/1/12/20	6/19/97/115	-
13	CLA	G	836	-	1/1/11/20	8/13/91/115	-
16	SF4	a	846	-	-	-	0/6/5/5
13	CLA	B	835	-	1/1/11/20	7/13/91/115	-
13	CLA	G	813	-	1/1/11/20	5/13/91/115	-
15	BCR	G	846	-	-	22/29/63/63	0/2/2/2
13	CLA	E	814	-	1/1/12/20	3/19/97/115	-
13	CLA	B	807	-	1/1/12/20	10/19/97/115	-
13	CLA	b	822	2	1/1/12/20	7/19/97/115	-
13	CLA	g	809	-	1/1/12/20	4/19/97/115	-
13	CLA	b	824	-	1/1/12/20	6/19/97/115	-
15	BCR	m	101	-	-	11/29/63/63	0/2/2/2
13	CLA	E	834	-	1/1/12/20	6/19/97/115	-
13	CLA	B	813	-	1/1/11/20	5/13/91/115	-
13	CLA	E	826	-	1/1/12/20	13/19/97/115	-
13	CLA	g	839	-	1/1/12/20	6/19/97/115	-
13	CLA	e	804	-	1/1/12/20	8/19/97/115	-
13	CLA	B	801	-	1/1/12/20	5/19/97/115	-
13	CLA	A	815	-	1/1/12/20	8/19/97/115	-
15	BCR	k	4001	-	-	21/29/63/63	0/2/2/2
13	CLA	a	836	-	1/1/12/20	6/19/97/115	-
15	BCR	s	201	-	-	18/29/63/63	0/2/2/2
13	CLA	a	817	-	1/1/12/20	3/19/97/115	-
13	CLA	e	810	-	1/1/12/20	3/19/97/115	-
15	BCR	G	845	-	-	17/29/63/63	0/2/2/2
13	CLA	G	824	-	1/1/11/20	6/13/91/115	-
13	CLA	b	832	-	1/1/12/20	4/19/97/115	-
13	CLA	b	834	-	1/1/11/20	7/13/91/115	-
15	BCR	A	851	-	-	5/29/63/63	0/2/2/2
15	BCR	b	842	-	-	9/29/63/63	0/2/2/2
13	CLA	G	811	-	1/1/12/20	12/19/97/115	-
13	CLA	e	840	-	1/1/11/20	6/16/94/115	-
16	SF4	g	804	-	-	-	0/6/5/5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	b	843	-	-	20/29/63/63	0/2/2/2
13	CLA	E	824	-	1/1/12/20	8/19/97/115	-
13	CLA	e	841	-	1/1/12/20	6/19/97/115	-
15	BCR	O	202	-	-	16/29/63/63	0/2/2/2
13	CLA	A	818	-	1/1/11/20	4/13/91/115	-
13	CLA	A	822	-	1/1/12/20	9/19/97/115	-
13	CLA	E	827	-	1/1/12/20	11/19/97/115	-
15	BCR	G	847	-	-	12/29/63/63	0/2/2/2
13	CLA	e	837	1	1/1/11/20	5/13/91/115	-
13	CLA	B	819	-	1/1/12/20	7/19/97/115	-
13	CLA	g	812	2	1/1/12/20	6/19/97/115	-
13	CLA	A	806	-	1/1/12/20	8/19/97/115	-
13	CLA	G	805	-	1/1/12/20	2/19/97/115	-
13	CLA	b	802	-	1/1/12/20	10/19/97/115	-
13	CLA	E	836	-	1/1/12/20	6/19/97/115	-
12	LHG	e	801	-	-	31/53/53/53	-
14	PQN	E	848	-	-	6/23/43/43	0/2/2/2
13	CLA	b	808	-	1/1/12/20	5/19/97/115	-
13	CLA	b	806	-	1/1/12/20	10/19/97/115	-
13	CLA	g	826	-	1/1/12/20	6/19/97/115	-
13	CLA	E	828	-	1/1/12/20	6/19/97/115	-
13	CLA	G	820	-	1/1/12/20	5/19/97/115	-
13	CLA	g	807	-	1/1/12/20	2/19/97/115	-
15	BCR	q	101	-	-	13/29/63/63	0/2/2/2
13	CLA	L	203	-	1/1/11/20	5/13/91/115	-
13	CLA	g	806	-	1/1/12/20	7/19/97/115	-
13	CLA	e	818	-	1/1/11/20	10/18/96/115	-
13	CLA	g	813	-	1/1/12/20	12/19/97/115	-
16	SF4	C	102	3	-	-	0/6/5/5
13	CLA	B	827	-	1/1/12/20	2/19/97/115	-
13	CLA	g	833	-	1/1/11/20	6/18/96/115	-
13	CLA	b	837	-	1/1/12/20	6/19/97/115	-
13	CLA	b	825	-	1/1/11/20	6/15/93/115	-
13	CLA	E	841	-	1/1/12/20	6/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	E	852	-	-	12/29/63/63	0/2/2/2
13	CLA	A	838	1	1/1/11/20	7/13/91/115	-
15	BCR	g	847	-	-	22/29/63/63	0/2/2/2
13	CLA	E	840	-	1/1/12/20	6/19/97/115	-
13	CLA	E	846	-	1/1/9/20	3/7/81/115	-
15	BCR	E	801	-	-	12/29/63/63	0/2/2/2
13	CLA	b	818	-	1/1/12/20	7/19/97/115	-
13	CLA	k	4002	-	1/1/11/20	6/13/91/115	-
13	CLA	G	837	-	1/1/12/20	6/19/97/115	-
13	CLA	g	825	-	1/1/11/20	6/13/91/115	-
13	CLA	b	836	-	1/1/12/20	6/19/97/115	-
13	CLA	e	805	-	1/1/12/20	8/19/97/115	-
13	CLA	a	818	-	1/1/11/20	4/13/91/115	-
15	BCR	f	202	-	-	14/29/63/63	0/2/2/2
15	BCR	e	847	-	-	13/29/63/63	0/2/2/2
13	CLA	G	818	-	1/1/12/20	10/19/97/115	-
13	CLA	o	202	-	1/1/11/20	5/13/91/115	-
15	BCR	e	846	-	-	19/29/63/63	0/2/2/2
15	BCR	A	850	-	-	21/29/63/63	0/2/2/2
13	CLA	L	202	10	1/1/12/20	6/19/97/115	-
13	CLA	E	833	-	1/1/12/20	6/19/97/115	-
13	CLA	a	844	-	1/1/12/20	7/19/97/115	-
13	CLA	e	820	-	1/1/12/20	7/19/97/115	-
13	CLA	A	832	-	1/1/12/20	4/19/97/115	-
13	CLA	F	202	-	1/1/11/20	5/13/91/115	-
13	CLA	A	843	-	1/1/12/20	7/19/97/115	-
13	CLA	a	852	-	1/1/12/20	8/19/97/115	-
15	BCR	b	846	-	-	12/29/63/63	0/2/2/2
13	CLA	B	840	-	1/1/12/20	7/19/97/115	-
13	CLA	B	841	-	1/1/12/20	7/19/97/115	-
16	SF4	B	803	-	-	-	0/6/5/5
13	CLA	l	205	-	1/1/12/20	8/19/97/115	-
15	BCR	e	849	-	-	20/29/63/63	0/2/2/2
13	CLA	A	853	-	1/1/12/20	10/19/97/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	g	846	-	-	17/29/63/63	0/2/2/2
13	CLA	e	828	-	1/1/12/20	9/19/97/115	-
13	CLA	a	814	-	1/1/11/20	3/13/91/115	-
13	CLA	E	822	-	1/1/12/20	9/19/97/115	-
15	BCR	e	850	-	-	6/29/63/63	0/2/2/2
13	CLA	f	203	-	1/1/11/20	7/13/91/115	-
16	SF4	h	101	-	-	-	0/6/5/5
13	CLA	b	823	-	1/1/11/20	6/13/91/115	-
13	CLA	G	830	-	1/1/12/20	6/19/97/115	-
13	CLA	G	827	-	1/1/12/20	2/19/97/115	-
15	BCR	B	847	-	-	12/29/63/63	0/2/2/2
15	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	a	845	-	1/1/12/20	6/19/97/115	-
13	CLA	b	828	-	1/1/12/20	11/19/97/115	-
13	CLA	a	821	-	1/1/12/20	7/19/97/115	-
13	CLA	G	831	-	1/1/11/20	10/13/91/115	-
15	BCR	a	803	-	-	23/29/63/63	0/2/2/2
13	CLA	e	827	-	1/1/12/20	6/19/97/115	-
13	CLA	a	815	-	1/1/12/20	8/19/97/115	-
13	CLA	G	806	-	1/1/12/20	10/19/97/115	-
13	CLA	E	819	-	1/1/11/20	10/18/96/115	-
13	CLA	G	801	-	1/1/12/20	6/19/97/115	-
14	PQN	a	847	-	-	10/23/43/43	0/2/2/2
13	CLA	a	839	1	1/1/11/20	6/13/91/115	-
13	CLA	A	824	-	1/1/12/20	8/19/97/115	-
13	CLA	g	835	-	1/1/12/20	11/19/97/115	-
13	CLA	G	828	-	1/1/12/20	6/19/97/115	-
13	CLA	b	826	-	1/1/12/20	2/19/97/115	-
13	CLA	a	841	-	1/1/12/20	6/19/97/115	-
13	CLA	A	845	12	1/1/12/20	6/19/97/115	-
13	CLA	g	832	-	1/1/11/20	10/13/91/115	-
13	CLA	a	831	-	1/1/12/20	7/19/97/115	-
13	CLA	a	838	-	-	7/19/97/115	-
13	CLA	e	806	-	1/1/12/20	7/19/97/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	807	-	1/1/12/20	4/19/97/115	-
13	CLA	B	831	-	1/1/11/20	10/13/91/115	-
13	CLA	a	820	-	1/1/12/20	2/19/97/115	-
13	CLA	A	829	-	1/1/12/20	9/19/97/115	-
13	CLA	K	102	-	1/1/11/20	6/13/91/115	-
13	CLA	A	805	-	1/1/12/20	7/19/97/115	-
13	CLA	G	819	-	1/1/12/20	7/19/97/115	-
13	CLA	B	836	-	1/1/11/20	8/13/91/115	-
13	CLA	a	823	-	1/1/12/20	10/19/97/115	-
13	CLA	E	809	1	1/1/12/20	5/19/97/115	-
13	CLA	g	814	-	1/1/11/20	5/13/91/115	-
13	CLA	G	834	-	1/1/12/20	11/19/97/115	-
13	CLA	a	806	-	1/1/12/20	8/19/97/115	-
14	PQN	e	845	-	-	7/23/43/43	0/2/2/2
13	CLA	E	810	-	1/1/12/20	8/19/97/115	-
13	CLA	B	830	-	1/1/12/20	6/19/97/115	-
13	CLA	a	809	1	1/1/12/20	5/19/97/115	-
13	CLA	e	831	-	1/1/12/20	4/19/97/115	-
13	CLA	a	840	-	1/1/12/20	7/19/97/115	-
13	CLA	B	838	-	1/1/12/20	6/19/97/115	-
13	CLA	B	820	-	1/1/12/20	5/19/97/115	-
13	CLA	g	841	-	1/1/12/20	7/19/97/115	-
13	CLA	e	821	-	1/1/12/20	9/19/97/115	-
15	BCR	A	852	-	-	15/29/63/63	0/2/2/2
13	CLA	e	832	-	1/1/12/20	6/19/97/115	-
15	BCR	j	101	-	-	13/29/63/63	0/2/2/2
13	CLA	g	842	-	1/1/12/20	7/19/97/115	-
15	BCR	g	848	-	-	12/29/63/63	0/2/2/2
15	BCR	e	851	-	-	16/29/63/63	0/2/2/2
13	CLA	b	829	-	1/1/12/20	6/19/97/115	-
15	BCR	J	101	-	-	13/29/63/63	0/2/2/2
13	CLA	B	837	-	1/1/12/20	6/19/97/115	-
13	CLA	b	812	-	1/1/11/20	5/13/91/115	-
15	BCR	T	101	-	-	11/29/63/63	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	E	832	-	1/1/12/20	4/19/97/115	-
13	CLA	g	831	-	1/1/12/20	6/19/97/115	-
13	CLA	e	830	-	1/1/12/20	8/19/97/115	-
15	BCR	G	844	-	-	20/29/63/63	0/2/2/2
13	CLA	B	818	-	1/1/12/20	10/19/97/115	-
13	CLA	G	829	-	1/1/12/20	11/19/97/115	-
13	CLA	e	815	-	1/1/12/20	5/19/97/115	-
13	CLA	e	842	-	1/1/12/20	7/19/97/115	-
13	CLA	E	825	-	1/1/11/20	9/18/96/115	-
13	CLA	b	835	-	1/1/11/20	8/13/91/115	-
13	CLA	g	810	-	1/1/12/20	5/19/97/115	-
13	CLA	r	102	-	1/1/11/20	6/13/91/115	-
15	BCR	B	845	-	-	17/29/63/63	0/2/2/2
13	CLA	g	840	-	1/1/11/20	8/16/94/115	-
13	CLA	E	842	-	1/1/11/20	6/16/94/115	-
13	CLA	e	852	-	1/1/12/20	10/19/97/115	-
13	CLA	G	815	-	1/1/12/20	3/19/97/115	-
13	CLA	E	820	-	1/1/12/20	2/19/97/115	-
14	PQN	g	843	-	-	11/23/43/43	0/2/2/2
13	CLA	g	803	-	1/1/12/20	6/19/97/115	-
13	CLA	a	830	-	1/1/12/20	8/19/97/115	-
15	BCR	E	802	-	-	20/29/63/63	0/2/2/2
13	CLA	G	835	-	1/1/11/20	7/13/91/115	-
15	BCR	S	201	-	-	17/29/63/63	0/2/2/2
15	BCR	l	202	-	-	18/29/63/63	0/2/2/2
12	LHG	e	802	13	-	14/42/42/53	-
13	CLA	g	830	-	1/1/12/20	11/19/97/115	-
13	CLA	E	831	-	1/1/12/20	7/19/97/115	-
15	BCR	a	802	-	-	10/29/63/63	0/2/2/2
13	CLA	b	817	-	1/1/12/20	10/19/97/115	-
13	CLA	G	809	-	1/1/12/20	4/19/97/115	-
13	CLA	g	821	-	1/1/12/20	5/19/97/115	-
15	BCR	E	849	-	-	19/29/63/63	0/2/2/2
16	SF4	h	102	3	-	-	0/6/5/5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	809	1	1/1/12/20	5/19/97/115	-
15	BCR	f	201	-	-	8/29/63/63	0/2/2/2
13	CLA	a	807	-	1/1/12/20	7/19/97/115	-
13	CLA	A	810	-	1/1/12/20	8/19/97/115	-
13	CLA	A	841	-	1/1/11/20	6/16/94/115	-
15	BCR	a	849	-	-	19/29/63/63	0/2/2/2
13	CLA	a	813	-	1/1/11/20	4/13/91/115	-
13	CLA	A	821	-	1/1/12/20	7/19/97/115	-
13	CLA	A	812	1	1/1/12/20	6/19/97/115	-
13	CLA	G	802	-	1/1/12/20	10/19/97/115	-
13	CLA	b	801	-	1/1/9/20	2/7/81/115	-
13	CLA	G	808	-	1/1/12/20	5/19/97/115	-
14	PQN	B	842	-	-	11/23/43/43	0/2/2/2
13	CLA	b	809	-	1/1/12/20	4/19/97/115	-
13	CLA	E	830	-	1/1/12/20	8/19/97/115	-
13	CLA	b	839	-	1/1/12/20	7/19/97/115	-
15	BCR	o	201	-	-	8/29/63/63	0/2/2/2
13	CLA	K	101	-	1/1/9/20	3/7/81/115	-
12	LHG	A	802	13	-	17/42/42/53	-
15	BCR	p	101	-	-	10/29/63/63	0/2/2/2
15	BCR	A	849	-	-	8/29/63/63	0/2/2/2
15	BCR	g	845	-	-	20/29/63/63	0/2/2/2
13	CLA	g	824	2	1/1/12/20	6/19/97/115	-
13	CLA	B	832	-	1/1/11/20	6/18/96/115	-
13	CLA	a	833	-	1/1/12/20	6/19/97/115	-
15	BCR	l	206	-	-	17/29/63/63	0/2/2/2
13	CLA	E	837	-	1/1/12/20	10/19/97/115	-
13	CLA	A	817	-	1/1/11/20	5/13/91/115	-
13	CLA	B	809	-	1/1/12/20	5/19/97/115	-
13	CLA	s	203	-	1/1/12/20	8/19/97/115	-
15	BCR	E	851	-	-	8/29/63/63	0/2/2/2
13	CLA	g	836	-	1/1/11/20	7/13/91/115	-
13	CLA	e	835	-	1/1/12/20	10/19/97/115	-
13	CLA	A	816	-	1/1/12/20	5/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	g	834	-	1/1/12/20	4/19/97/115	-
13	CLA	E	818	-	1/1/11/20	4/13/91/115	-
15	BCR	b	845	-	-	22/29/63/63	0/2/2/2
13	CLA	A	826	-	1/1/12/20	13/19/97/115	-
13	CLA	G	822	-	1/1/11/20	6/13/91/115	-
15	BCR	g	849	-	-	16/29/63/63	0/2/2/2
13	CLA	a	819	-	1/1/11/20	10/18/96/115	-
13	CLA	G	817	-	1/1/12/20	7/19/97/115	-
13	CLA	A	807	-	1/1/12/20	7/19/97/115	-
13	CLA	A	834	-	1/1/12/20	6/19/97/115	-
15	BCR	L	201	-	-	17/29/63/63	0/2/2/2
13	CLA	a	827	-	1/1/12/20	11/19/97/115	-
13	CLA	A	813	-	1/1/11/20	4/13/91/115	-
13	CLA	S	203	-	1/1/11/20	5/13/91/115	-
13	CLA	B	808	-	1/1/12/20	4/19/97/115	-
13	CLA	B	806	-	1/1/12/20	2/19/97/115	-
13	CLA	g	811	-	1/1/12/20	4/19/97/115	-
13	CLA	G	826	-	1/1/11/20	6/15/93/115	-
13	CLA	E	805	-	1/1/12/20	7/19/97/115	-
13	CLA	G	821	-	1/1/11/20	8/16/94/115	-
13	CLA	e	809	-	1/1/12/20	8/19/97/115	-
15	BCR	P	101	-	-	10/29/63/63	0/2/2/2
13	CLA	b	810	2	1/1/12/20	6/19/97/115	-
15	BCR	a	850	-	-	13/29/63/63	0/2/2/2
15	BCR	B	846	-	-	22/29/63/63	0/2/2/2
13	CLA	E	821	-	1/1/12/20	7/19/97/115	-
13	CLA	g	816	-	1/1/12/20	3/19/97/115	-
15	BCR	s	204	-	-	12/29/63/63	0/2/2/2
16	SF4	H	101	-	-	-	0/6/5/5
13	CLA	G	823	2	1/1/12/20	6/19/97/115	-
13	CLA	B	824	-	1/1/11/20	6/13/91/115	-
16	SF4	E	847	-	-	-	0/6/5/5
13	CLA	a	835	-	1/1/12/20	5/19/97/115	-
13	CLA	G	825	-	1/1/12/20	6/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	814	-	1/1/12/20	3/19/97/115	-
13	CLA	B	829	-	1/1/12/20	11/19/97/115	-
13	CLA	g	828	-	1/1/12/20	2/19/97/115	-
16	SF4	c	101	-	-	-	0/6/5/5
13	CLA	A	811	-	1/1/12/20	3/19/97/115	-
13	CLA	s	202	-	1/1/11/20	5/13/91/115	-
13	CLA	E	844	-	1/1/12/20	7/19/97/115	-
15	BCR	a	848	-	-	16/29/63/63	0/2/2/2
13	CLA	g	822	-	1/1/11/20	8/16/94/115	-
13	CLA	b	838	-	1/1/11/20	8/16/94/115	-
13	CLA	g	819	-	1/1/12/20	10/19/97/115	-
13	CLA	S	204	-	1/1/11/20	7/13/91/115	-
13	CLA	A	828	-	1/1/12/20	6/19/97/115	-
16	SF4	c	102	3	-	-	0/6/5/5
15	BCR	J	102	-	-	12/29/63/63	0/2/2/2
13	CLA	e	824	-	1/1/11/20	9/18/96/115	-
13	CLA	A	835	-	1/1/12/20	6/19/97/115	-
13	CLA	E	812	1	1/1/12/20	6/19/97/115	-
13	CLA	G	807	-	1/1/12/20	4/19/97/115	-
13	CLA	E	803	-	1/1/12/20	5/19/97/115	-
13	CLA	g	829	-	1/1/12/20	6/19/97/115	-
13	CLA	B	815	-	1/1/12/20	3/19/97/115	-
13	CLA	a	810	-	1/1/12/20	8/19/97/115	-
13	CLA	O	203	-	1/1/11/20	7/13/91/115	-
13	CLA	a	825	-	1/1/11/20	9/18/96/115	-
13	CLA	b	819	-	1/1/12/20	5/19/97/115	-
13	CLA	R	102	-	1/1/11/20	6/13/91/115	-
15	BCR	A	848	-	-	13/29/63/63	0/2/2/2
13	CLA	b	831	-	1/1/11/20	6/18/96/115	-
13	CLA	a	826	-	1/1/12/20	13/19/97/115	-
15	BCR	i	101	-	-	10/29/63/63	0/2/2/2
13	CLA	e	838	-	1/1/12/20	7/19/97/115	-
13	CLA	e	822	-	1/1/12/20	10/19/97/115	-
13	CLA	b	811	-	1/1/11/20	4/13/91/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	802	-	1/1/12/20	6/19/97/115	-
13	CLA	e	817	-	1/1/11/20	4/13/91/115	-
13	CLA	A	844	-	1/1/12/20	6/19/97/115	-
13	CLA	a	834	-	1/1/12/20	6/19/97/115	-
15	BCR	F	201	-	-	8/29/63/63	0/2/2/2
13	CLA	E	806	-	1/1/12/20	8/19/97/115	-
15	BCR	a	853	-	-	12/29/63/63	0/2/2/2
13	CLA	l	201	-	1/1/11/20	4/13/91/115	-
15	BCR	G	843	-	-	9/29/63/63	0/2/2/2
13	CLA	g	827	-	1/1/11/20	6/15/93/115	-
13	CLA	E	829	-	1/1/12/20	9/19/97/115	-
13	CLA	E	817	-	1/1/11/20	5/13/91/115	-
13	CLA	e	826	-	1/1/12/20	11/19/97/115	-
13	CLA	A	825	-	1/1/11/20	9/18/96/115	-
13	CLA	a	832	-	1/1/12/20	4/19/97/115	-
13	CLA	e	843	-	1/1/12/20	6/19/97/115	-
13	CLA	b	816	-	1/1/12/20	8/19/97/115	-
13	CLA	b	804	-	1/1/12/20	7/19/97/115	-
13	CLA	A	803	-	1/1/12/20	8/19/97/115	-
13	CLA	b	821	-	1/1/11/20	6/13/91/115	-
13	CLA	e	811	1	1/1/12/20	6/19/97/115	-
13	CLA	e	813	-	1/1/12/20	3/19/97/115	-
13	CLA	b	815	-	1/1/11/20	6/13/91/115	-
13	CLA	A	814	-	1/1/12/20	3/19/97/115	-
13	CLA	g	817	-	1/1/11/20	6/13/91/115	-
13	CLA	b	840	-	1/1/12/20	7/19/97/115	-
13	CLA	e	812	-	1/1/11/20	4/13/91/115	-
13	CLA	G	816	-	1/1/11/20	6/13/91/115	-
15	BCR	b	847	-	-	16/29/63/63	0/2/2/2
13	CLA	e	839	-	1/1/12/20	6/19/97/115	-
15	BCR	L	205	-	-	13/29/63/63	0/2/2/2
13	CLA	a	842	-	1/1/11/20	6/16/94/115	-
13	CLA	e	823	-	1/1/12/20	8/19/97/115	-
13	CLA	E	811	-	1/1/12/20	3/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PQN	b	841	-	-	11/23/43/43	0/2/2/2
13	CLA	A	808	-	1/1/12/20	6/19/97/115	-
13	CLA	e	807	-	1/1/12/20	6/19/97/115	-
13	CLA	a	843	-	1/1/12/20	6/19/97/115	-
13	CLA	g	815	-	1/1/12/20	5/19/97/115	-
13	CLA	A	833	-	1/1/12/20	6/19/97/115	-
13	CLA	e	808	1	1/1/12/20	5/19/97/115	-
13	CLA	a	829	-	1/1/12/20	9/19/97/115	-
13	CLA	E	839	1	1/1/11/20	6/13/91/115	-
13	CLA	a	824	-	1/1/12/20	8/19/97/115	-
13	CLA	B	822	-	1/1/11/20	6/13/91/115	-
13	CLA	G	839	-	1/1/11/20	7/16/94/115	-
13	CLA	A	804	-	1/1/12/20	8/19/97/115	-
13	CLA	e	833	-	1/1/12/20	6/19/97/115	-
13	CLA	a	811	-	1/1/12/20	3/19/97/115	-
13	CLA	b	833	-	1/1/12/20	11/19/97/115	-
13	CLA	B	810	-	1/1/12/20	4/19/97/115	-
13	CLA	E	804	-	1/1/12/20	8/19/97/115	-
13	CLA	B	805	-	1/1/12/20	7/19/97/115	-
13	CLA	a	837	-	1/1/12/20	10/19/97/115	-
13	CLA	B	812	-	1/1/12/20	12/19/97/115	-
13	CLA	G	814	-	1/1/12/20	5/19/97/115	-
12	LHG	a	801	-	-	32/53/53/53	-
15	BCR	E	850	-	-	13/29/63/63	0/2/2/2
13	CLA	E	816	-	1/1/12/20	5/19/97/115	-
13	CLA	G	833	-	1/1/12/20	4/19/97/115	-
13	CLA	a	816	-	1/1/12/20	5/19/97/115	-
14	PQN	A	846	-	-	11/23/43/43	0/2/2/2
13	CLA	a	804	-	1/1/12/20	8/19/97/115	-
15	BCR	a	851	-	-	8/29/63/63	0/2/2/2
13	CLA	b	803	-	1/1/12/20	6/19/97/115	-
13	CLA	g	802	-	1/1/12/20	5/19/97/115	-
13	CLA	E	815	-	1/1/12/20	8/19/97/115	-
13	CLA	A	827	-	1/1/12/20	11/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	E	843	-	1/1/12/20	6/19/97/115	-
13	CLA	g	808	-	1/1/12/20	10/19/97/115	-
13	CLA	L	204	-	1/1/12/20	8/19/97/115	-
13	CLA	s	205	-	1/1/12/20	12/19/97/115	-
13	CLA	a	828	-	1/1/12/20	6/19/97/115	-
15	BCR	B	848	-	-	16/29/63/63	0/2/2/2
13	CLA	E	835	-	1/1/12/20	5/19/97/115	-
15	BCR	O	201	-	-	8/29/63/63	0/2/2/2
13	CLA	A	831	-	1/1/12/20	7/19/97/115	-
15	BCR	S	205	-	-	16/29/63/63	0/2/2/2
13	CLA	E	813	-	1/1/11/20	4/13/91/115	-
13	CLA	b	813	-	1/1/12/20	5/19/97/115	-
13	CLA	A	836	-	1/1/12/20	10/19/97/115	-
15	BCR	q	102	-	-	12/29/63/63	0/2/2/2
13	CLA	a	808	-	1/1/12/20	6/19/97/115	-
13	CLA	B	817	-	1/1/12/20	8/19/97/115	-
13	CLA	B	825	-	1/1/12/20	6/19/97/115	-
13	CLA	b	805	-	1/1/12/20	2/19/97/115	-
12	LHG	A	801	-	-	32/53/53/53	-
13	CLA	B	823	2	1/1/12/20	6/19/97/115	-
13	CLA	r	101	-	1/1/9/20	4/7/81/115	-
16	SF4	C	101	-	-	-	0/6/5/5
15	BCR	e	848	-	-	8/29/63/63	0/2/2/2
13	CLA	B	826	-	1/1/11/20	6/15/93/115	-
15	BCR	g	844	-	-	9/29/63/63	0/2/2/2
13	CLA	A	830	-	1/1/12/20	8/19/97/115	-
15	BCR	G	848	-	-	16/29/63/63	0/2/2/2
13	CLA	S	206	-	1/1/11/20	4/13/91/115	-
15	BCR	B	844	-	-	20/29/63/63	0/2/2/2
13	CLA	B	814	-	1/1/12/20	5/19/97/115	-
13	CLA	g	805	-	1/1/12/20	6/19/97/115	-
13	CLA	b	830	-	1/1/11/20	10/13/91/115	-
13	CLA	B	834	-	1/1/12/20	11/19/97/115	-
13	CLA	B	821	-	1/1/11/20	8/16/94/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SF4	H	102	3	-	-	0/6/5/5
13	CLA	A	840	-	1/1/12/20	6/19/97/115	-
13	CLA	A	839	-	1/1/12/20	6/19/97/115	-
13	CLA	A	823	-	1/1/12/20	10/19/97/115	-
13	CLA	G	804	-	1/1/12/20	7/19/97/115	-
13	CLA	e	816	-	1/1/11/20	5/13/91/115	-
13	CLA	B	839	-	1/1/11/20	7/16/94/115	-
13	CLA	e	844	12	1/1/12/20	8/19/97/115	-
15	BCR	b	844	-	-	17/29/63/63	0/2/2/2
13	CLA	b	820	-	1/1/11/20	8/16/94/115	-
13	CLA	G	810	2	1/1/12/20	6/19/97/115	-

All (2682) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	204	CLA	MG-ND	9.46	2.24	2.05
13	l	205	CLA	MG-ND	9.45	2.24	2.05
13	L	204	CLA	MG-ND	9.43	2.24	2.05
13	s	203	CLA	MG-ND	9.40	2.24	2.05
13	g	834	CLA	C4B-NB	7.84	1.42	1.35
13	G	833	CLA	C4B-NB	7.83	1.42	1.35
13	B	833	CLA	C4B-NB	7.81	1.42	1.35
13	b	832	CLA	C4B-NB	7.78	1.42	1.35
14	G	842	PQN	C3-C2	7.73	1.49	1.35
14	b	841	PQN	C3-C2	7.73	1.49	1.35
14	E	848	PQN	C3-C2	7.71	1.49	1.35
14	g	843	PQN	C3-C2	7.71	1.49	1.35
13	L	204	CLA	C4B-NB	7.69	1.42	1.35
14	A	846	PQN	C3-C2	7.69	1.49	1.35
13	G	835	CLA	C4B-NB	7.68	1.42	1.35
13	g	836	CLA	C4B-NB	7.67	1.42	1.35
14	B	842	PQN	C3-C2	7.66	1.49	1.35
14	e	845	PQN	C3-C2	7.65	1.49	1.35
14	a	847	PQN	C3-C2	7.65	1.49	1.35
13	l	205	CLA	C4B-NB	7.65	1.42	1.35
13	a	817	CLA	C4B-NB	7.62	1.42	1.35
13	b	834	CLA	C4B-NB	7.62	1.42	1.35
13	B	835	CLA	C4B-NB	7.61	1.42	1.35
13	e	816	CLA	C4B-NB	7.58	1.42	1.35
13	B	813	CLA	C4B-NB	7.57	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	s	203	CLA	C4B-NB	7.57	1.42	1.35
13	A	817	CLA	C4B-NB	7.57	1.42	1.35
13	b	826	CLA	C4B-NB	7.56	1.42	1.35
13	E	817	CLA	C4B-NB	7.56	1.42	1.35
13	G	813	CLA	C4B-NB	7.56	1.42	1.35
13	b	808	CLA	C4B-NB	7.55	1.41	1.35
13	B	827	CLA	C4B-NB	7.53	1.41	1.35
13	e	826	CLA	C4B-NB	7.53	1.41	1.35
13	E	814	CLA	C4B-NB	7.50	1.41	1.35
13	S	204	CLA	C4B-NB	7.50	1.41	1.35
13	e	813	CLA	C4B-NB	7.50	1.41	1.35
13	a	814	CLA	C4B-NB	7.49	1.41	1.35
13	g	814	CLA	C4B-NB	7.48	1.41	1.35
13	G	827	CLA	C4B-NB	7.47	1.41	1.35
13	E	827	CLA	C4B-NB	7.47	1.41	1.35
13	B	809	CLA	C4B-NB	7.46	1.41	1.35
13	A	814	CLA	C4B-NB	7.45	1.41	1.35
13	E	836	CLA	C4B-NB	7.45	1.41	1.35
13	e	834	CLA	C4B-NB	7.44	1.41	1.35
13	G	808	CLA	C4B-NB	7.43	1.41	1.35
13	e	818	CLA	C4B-NB	7.43	1.41	1.35
13	g	810	CLA	C4B-NB	7.43	1.41	1.35
13	g	828	CLA	C4B-NB	7.43	1.41	1.35
13	a	831	CLA	C4B-NB	7.42	1.41	1.35
13	A	827	CLA	C4B-NB	7.42	1.41	1.35
13	a	819	CLA	C4B-NB	7.42	1.41	1.35
13	b	823	CLA	C4B-NB	7.41	1.41	1.35
13	A	835	CLA	C4B-NB	7.41	1.41	1.35
13	g	819	CLA	C4B-NB	7.41	1.41	1.35
13	b	812	CLA	C4B-NB	7.41	1.41	1.35
13	a	836	CLA	C4B-NB	7.40	1.41	1.35
13	A	819	CLA	C4B-NB	7.40	1.41	1.35
13	G	824	CLA	C4B-NB	7.40	1.41	1.35
13	G	823	CLA	C4B-NB	7.39	1.41	1.35
13	A	831	CLA	C4B-NB	7.39	1.41	1.35
13	E	819	CLA	C4B-NB	7.39	1.41	1.35
13	e	830	CLA	C4B-NB	7.38	1.41	1.35
13	B	823	CLA	C4B-NB	7.37	1.41	1.35
13	b	822	CLA	C4B-NB	7.37	1.41	1.35
13	A	836	CLA	C4B-NB	7.36	1.41	1.35
13	a	827	CLA	C4B-NB	7.36	1.41	1.35
13	G	815	CLA	C4B-NB	7.35	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	831	CLA	C4B-NB	7.35	1.41	1.35
13	G	818	CLA	C4B-NB	7.35	1.41	1.35
13	g	825	CLA	C4B-NB	7.34	1.41	1.35
13	B	824	CLA	C4B-NB	7.33	1.41	1.35
13	b	817	CLA	C4B-NB	7.32	1.41	1.35
13	E	826	CLA	C4B-NB	7.31	1.41	1.35
13	a	837	CLA	C4B-NB	7.31	1.41	1.35
13	A	832	CLA	C4B-NB	7.31	1.41	1.35
13	e	831	CLA	C4B-NB	7.30	1.41	1.35
13	g	824	CLA	C4B-NB	7.30	1.41	1.35
13	b	814	CLA	C4B-NB	7.30	1.41	1.35
13	e	835	CLA	C4B-NB	7.29	1.41	1.35
13	B	818	CLA	C4B-NB	7.29	1.41	1.35
13	S	206	CLA	C4B-NB	7.29	1.41	1.35
13	G	821	CLA	C4B-NB	7.29	1.41	1.35
13	E	813	CLA	C4B-NB	7.29	1.41	1.35
13	g	837	CLA	C4B-NB	7.28	1.41	1.35
13	G	809	CLA	C4B-NB	7.28	1.41	1.35
13	e	812	CLA	C4B-NB	7.28	1.41	1.35
13	G	817	CLA	C4B-NB	7.27	1.41	1.35
13	B	831	CLA	C4B-NB	7.27	1.41	1.35
13	a	839	CLA	C4B-NB	7.27	1.41	1.35
13	b	835	CLA	C4B-NB	7.27	1.41	1.35
13	e	821	CLA	C4B-NB	7.26	1.41	1.35
13	e	825	CLA	C4B-NB	7.26	1.41	1.35
13	E	837	CLA	C4B-NB	7.26	1.41	1.35
13	a	820	CLA	C4B-NB	7.26	1.41	1.35
13	e	809	CLA	C4B-NB	7.26	1.41	1.35
13	b	833	CLA	C4B-NB	7.26	1.41	1.35
13	G	836	CLA	C4B-NB	7.25	1.41	1.35
13	e	828	CLA	C4B-NB	7.25	1.41	1.35
13	E	820	CLA	C4B-NB	7.25	1.41	1.35
13	A	838	CLA	C4B-NB	7.25	1.41	1.35
13	E	842	CLA	C4B-NB	7.25	1.41	1.35
13	A	822	CLA	C4B-NB	7.25	1.41	1.35
13	E	810	CLA	C4B-NB	7.25	1.41	1.35
13	a	818	CLA	C4B-NB	7.25	1.41	1.35
13	e	820	CLA	C4B-NB	7.25	1.41	1.35
13	e	836	CLA	C4B-NB	7.25	1.41	1.35
13	g	817	CLA	C4B-NB	7.25	1.41	1.35
13	a	821	CLA	C4B-NB	7.25	1.41	1.35
13	E	812	CLA	C4B-NB	7.25	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	803	CLA	C4B-NB	7.24	1.41	1.35
13	a	810	CLA	C4B-NB	7.24	1.41	1.35
13	B	815	CLA	C4B-NB	7.24	1.41	1.35
13	B	834	CLA	C4B-NB	7.24	1.41	1.35
13	e	819	CLA	C4B-NB	7.24	1.41	1.35
13	E	822	CLA	C4B-NB	7.24	1.41	1.35
13	G	831	CLA	C4B-NB	7.24	1.41	1.35
13	A	821	CLA	C4B-NB	7.23	1.41	1.35
13	O	203	CLA	C4B-NB	7.23	1.41	1.35
13	g	816	CLA	C4B-NB	7.23	1.41	1.35
13	b	816	CLA	C4B-NB	7.23	1.41	1.35
13	e	811	CLA	C4B-NB	7.23	1.41	1.35
13	E	821	CLA	C4B-NB	7.23	1.41	1.35
13	e	837	CLA	C4B-NB	7.23	1.41	1.35
13	E	815	CLA	C4B-NB	7.23	1.41	1.35
13	a	838	CLA	C4B-NB	7.23	1.41	1.35
13	a	812	CLA	C4B-NB	7.23	1.41	1.35
13	A	829	CLA	C4B-NB	7.22	1.41	1.35
13	B	836	CLA	C4B-NB	7.22	1.41	1.35
13	l	201	CLA	C4B-NB	7.22	1.41	1.35
13	R	102	CLA	C4B-NB	7.22	1.41	1.35
13	a	826	CLA	C4B-NB	7.22	1.41	1.35
13	e	829	CLA	C4B-NB	7.22	1.41	1.35
13	A	826	CLA	C4B-NB	7.21	1.41	1.35
13	B	817	CLA	C4B-NB	7.21	1.41	1.35
13	A	813	CLA	C4B-NB	7.21	1.41	1.35
13	g	822	CLA	C4B-NB	7.21	1.41	1.35
13	A	830	CLA	C4B-NB	7.21	1.41	1.35
13	g	833	CLA	C4B-NB	7.21	1.41	1.35
13	G	801	CLA	C4B-NB	7.21	1.41	1.35
13	e	842	CLA	C4B-NB	7.21	1.41	1.35
13	B	832	CLA	C4B-NB	7.21	1.41	1.35
13	A	815	CLA	C4B-NB	7.21	1.41	1.35
13	A	812	CLA	C4B-NB	7.20	1.41	1.35
13	b	815	CLA	C4B-NB	7.20	1.41	1.35
13	r	102	CLA	C4B-NB	7.20	1.41	1.35
13	k	4002	CLA	C4B-NB	7.20	1.41	1.35
13	G	829	CLA	C4B-NB	7.20	1.41	1.35
13	b	811	CLA	C4B-NB	7.20	1.41	1.35
13	A	841	CLA	C4B-NB	7.20	1.41	1.35
13	a	829	CLA	C4B-NB	7.20	1.41	1.35
13	e	840	CLA	C4B-NB	7.19	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	813	CLA	C4B-NB	7.19	1.41	1.35
13	G	840	CLA	C4B-NB	7.19	1.41	1.35
13	E	830	CLA	C4B-NB	7.19	1.41	1.35
13	G	816	CLA	C4B-NB	7.19	1.41	1.35
13	a	852	CLA	C4B-NB	7.19	1.41	1.35
13	E	846	CLA	C4B-NB	7.19	1.41	1.35
13	g	818	CLA	C4B-NB	7.19	1.41	1.35
13	g	835	CLA	C4B-NB	7.19	1.41	1.35
13	a	832	CLA	C4B-NB	7.18	1.41	1.35
13	a	842	CLA	C4B-NB	7.18	1.41	1.35
13	A	818	CLA	C4B-NB	7.18	1.41	1.35
13	e	817	CLA	C4B-NB	7.18	1.41	1.35
13	g	811	CLA	C4B-NB	7.18	1.41	1.35
13	A	824	CLA	C4B-NB	7.18	1.41	1.35
13	G	832	CLA	C4B-NB	7.17	1.41	1.35
13	b	809	CLA	C4B-NB	7.17	1.41	1.35
13	K	102	CLA	C4B-NB	7.17	1.41	1.35
13	G	828	CLA	C4B-NB	7.17	1.41	1.35
13	B	816	CLA	C4B-NB	7.17	1.41	1.35
13	E	844	CLA	C4B-NB	7.17	1.41	1.35
13	G	834	CLA	C4B-NB	7.17	1.41	1.35
13	B	829	CLA	C4B-NB	7.17	1.41	1.35
13	a	816	CLA	C4B-NB	7.17	1.41	1.35
13	a	830	CLA	C4B-NB	7.17	1.41	1.35
13	g	832	CLA	C4B-NB	7.16	1.41	1.35
13	b	839	CLA	C4B-NB	7.16	1.41	1.35
13	E	832	CLA	C4B-NB	7.16	1.41	1.35
13	a	844	CLA	C4B-NB	7.16	1.41	1.35
13	E	818	CLA	C4B-NB	7.16	1.41	1.35
13	g	841	CLA	C4B-NB	7.16	1.41	1.35
13	B	822	CLA	C4B-NB	7.16	1.41	1.35
13	b	820	CLA	C4B-NB	7.16	1.41	1.35
13	b	830	CLA	C4B-NB	7.16	1.41	1.35
13	a	822	CLA	C4B-NB	7.16	1.41	1.35
13	a	815	CLA	C4B-NB	7.15	1.41	1.35
13	A	843	CLA	C4B-NB	7.15	1.41	1.35
13	E	839	CLA	C4B-NB	7.15	1.41	1.35
13	G	810	CLA	C4B-NB	7.15	1.41	1.35
13	e	810	CLA	C4B-NB	7.15	1.41	1.35
13	G	812	CLA	C4B-NB	7.15	1.41	1.35
13	b	831	CLA	C4B-NB	7.15	1.41	1.35
13	A	820	CLA	C4B-NB	7.15	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	809	CLA	C4B-NB	7.15	1.41	1.35
13	E	824	CLA	C4B-NB	7.14	1.41	1.35
13	g	830	CLA	C4B-NB	7.14	1.41	1.35
13	A	810	CLA	C4B-NB	7.14	1.41	1.35
13	B	810	CLA	C4B-NB	7.14	1.41	1.35
13	B	802	CLA	C4B-NB	7.13	1.41	1.35
13	A	853	CLA	C4B-NB	7.13	1.41	1.35
13	B	828	CLA	C4B-NB	7.13	1.41	1.35
13	g	829	CLA	C4B-NB	7.13	1.41	1.35
13	e	815	CLA	C4B-NB	7.13	1.41	1.35
13	A	816	CLA	C4B-NB	7.13	1.41	1.35
13	E	838	CLA	C4B-NB	7.12	1.41	1.35
13	b	801	CLA	C4B-NB	7.12	1.41	1.35
13	B	821	CLA	C4B-NB	7.12	1.41	1.35
13	B	840	CLA	C4B-NB	7.12	1.41	1.35
13	b	836	CLA	C4B-NB	7.11	1.41	1.35
13	f	203	CLA	C4B-NB	7.11	1.41	1.35
13	e	814	CLA	C4B-NB	7.11	1.41	1.35
13	E	829	CLA	C4B-NB	7.11	1.41	1.35
13	E	840	CLA	C4B-NB	7.11	1.41	1.35
13	G	802	CLA	C4B-NB	7.10	1.41	1.35
13	g	813	CLA	C4B-NB	7.10	1.41	1.35
13	G	822	CLA	C4B-NB	7.10	1.41	1.35
13	e	852	CLA	C4B-NB	7.10	1.41	1.35
13	e	838	CLA	C4B-NB	7.10	1.41	1.35
13	b	827	CLA	C4B-NB	7.10	1.41	1.35
13	A	811	CLA	C4B-NB	7.09	1.41	1.35
13	g	809	CLA	C4B-NB	7.09	1.41	1.35
13	g	812	CLA	C4B-NB	7.09	1.41	1.35
13	b	819	CLA	C4B-NB	7.09	1.41	1.35
13	L	202	CLA	C4B-NB	7.09	1.41	1.35
13	G	837	CLA	C4B-NB	7.09	1.41	1.35
13	a	823	CLA	C4B-NB	7.08	1.41	1.35
13	g	823	CLA	C4B-NB	7.08	1.41	1.35
13	g	821	CLA	C4B-NB	7.08	1.41	1.35
13	B	837	CLA	C4B-NB	7.08	1.41	1.35
13	E	811	CLA	C4B-NB	7.08	1.41	1.35
13	A	837	CLA	C4B-NB	7.08	1.41	1.35
13	B	820	CLA	C4B-NB	7.07	1.41	1.35
13	b	821	CLA	C4B-NB	7.07	1.41	1.35
13	a	809	CLA	C4B-NB	7.07	1.41	1.35
13	e	807	CLA	C4B-NB	7.07	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	828	CLA	C4B-NB	7.07	1.41	1.35
13	a	824	CLA	C4B-NB	7.07	1.41	1.35
13	e	844	CLA	C4B-NB	7.07	1.41	1.35
13	E	816	CLA	C4B-NB	7.06	1.41	1.35
13	a	811	CLA	C4B-NB	7.06	1.41	1.35
13	B	811	CLA	C4B-NB	7.06	1.41	1.35
13	G	811	CLA	C4B-NB	7.06	1.41	1.35
13	G	825	CLA	C4B-NB	7.05	1.41	1.35
13	s	205	CLA	C4B-NB	7.05	1.41	1.35
13	b	810	CLA	C4B-NB	7.05	1.41	1.35
13	e	823	CLA	C4B-NB	7.05	1.41	1.35
13	e	822	CLA	C4B-NB	7.05	1.41	1.35
13	b	802	CLA	C4B-NB	7.05	1.41	1.35
13	S	203	CLA	C4B-NB	7.05	1.41	1.35
13	F	202	CLA	C4B-NB	7.04	1.41	1.35
13	a	840	CLA	C4B-NB	7.04	1.41	1.35
13	A	823	CLA	C4B-NB	7.04	1.41	1.35
13	o	202	CLA	C4B-NB	7.03	1.41	1.35
13	l	203	CLA	C4B-NB	7.03	1.41	1.35
13	A	839	CLA	C4B-NB	7.03	1.41	1.35
13	A	809	CLA	C4B-NB	7.03	1.41	1.35
13	e	808	CLA	C4B-NB	7.03	1.41	1.35
13	A	803	CLA	C4B-NB	7.03	1.41	1.35
13	g	826	CLA	C4B-NB	7.03	1.41	1.35
13	g	840	CLA	C4B-NB	7.03	1.41	1.35
13	E	823	CLA	C4B-NB	7.03	1.41	1.35
13	g	838	CLA	C4B-NB	7.03	1.41	1.35
13	G	820	CLA	C4B-NB	7.02	1.41	1.35
13	A	808	CLA	C4B-NB	7.01	1.41	1.35
13	B	838	CLA	C4B-NB	7.01	1.41	1.35
13	B	808	CLA	C4B-NB	7.01	1.41	1.35
13	G	819	CLA	C4B-NB	7.00	1.41	1.35
13	B	825	CLA	C4B-NB	7.00	1.41	1.35
13	E	828	CLA	C4B-NB	7.00	1.41	1.35
13	B	819	CLA	C4B-NB	7.00	1.41	1.35
13	B	812	CLA	C4B-NB	7.00	1.41	1.35
13	g	839	CLA	C4B-NB	7.00	1.41	1.35
13	E	845	CLA	C4B-NB	6.99	1.41	1.35
13	E	806	CLA	C4B-NB	6.99	1.41	1.35
13	G	803	CLA	C4B-NB	6.99	1.41	1.35
13	b	829	CLA	C4B-NB	6.99	1.41	1.35
13	l	204	CLA	C4B-NB	6.99	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	203	CLA	C4B-NB	6.99	1.41	1.35
13	b	840	CLA	C4B-NB	6.99	1.41	1.35
13	A	806	CLA	C4B-NB	6.99	1.41	1.35
13	G	838	CLA	C4B-NB	6.98	1.41	1.35
13	G	841	CLA	C4B-NB	6.98	1.41	1.35
13	b	824	CLA	C4B-NB	6.98	1.41	1.35
13	G	807	CLA	C4B-NB	6.98	1.41	1.35
13	b	806	CLA	C4B-NB	6.98	1.41	1.35
13	b	818	CLA	C4B-NB	6.98	1.41	1.35
13	G	839	CLA	C4B-NB	6.98	1.41	1.35
13	g	827	CLA	C4B-NB	6.98	1.41	1.35
13	E	808	CLA	C4B-NB	6.98	1.41	1.35
13	g	808	CLA	C4B-NB	6.98	1.41	1.35
13	B	826	CLA	C4B-NB	6.97	1.41	1.35
13	b	837	CLA	C4B-NB	6.97	1.41	1.35
13	A	845	CLA	C4B-NB	6.97	1.41	1.35
13	s	202	CLA	C4B-NB	6.97	1.41	1.35
13	G	805	CLA	C4B-NB	6.96	1.41	1.35
13	a	828	CLA	C4B-NB	6.96	1.41	1.35
13	B	806	CLA	C4B-NB	6.96	1.41	1.35
13	a	806	CLA	C4B-NB	6.96	1.41	1.35
13	g	842	CLA	C4B-NB	6.96	1.41	1.35
13	B	839	CLA	C4B-NB	6.96	1.41	1.35
13	B	830	CLA	C4B-NB	6.96	1.41	1.35
13	K	101	CLA	C4B-NB	6.96	1.41	1.35
13	A	834	CLA	C4B-NB	6.95	1.41	1.35
13	g	805	CLA	C4B-NB	6.95	1.41	1.35
13	b	805	CLA	C4B-NB	6.95	1.41	1.35
13	g	831	CLA	C4B-NB	6.95	1.41	1.35
13	b	807	CLA	C4B-NB	6.95	1.41	1.35
13	b	825	CLA	C4B-NB	6.95	1.41	1.35
13	e	843	CLA	C4B-NB	6.94	1.41	1.35
13	b	803	CLA	C4B-NB	6.94	1.41	1.35
13	G	806	CLA	C4B-NB	6.94	1.41	1.35
13	A	828	CLA	C4B-NB	6.93	1.41	1.35
13	B	804	CLA	C4B-NB	6.93	1.41	1.35
13	B	841	CLA	C4B-NB	6.93	1.41	1.35
13	A	844	CLA	C4B-NB	6.93	1.41	1.35
13	e	824	CLA	C4B-NB	6.93	1.41	1.35
13	e	805	CLA	C4B-NB	6.93	1.41	1.35
13	e	827	CLA	C4B-NB	6.93	1.41	1.35
13	B	807	CLA	C4B-NB	6.92	1.41	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	814	CLA	C4B-NB	6.92	1.41	1.35
13	r	101	CLA	C4B-NB	6.92	1.41	1.35
13	e	803	CLA	C4B-NB	6.92	1.41	1.35
13	G	826	CLA	C4B-NB	6.91	1.41	1.35
13	a	834	CLA	C4B-NB	6.91	1.41	1.35
13	g	807	CLA	C4B-NB	6.91	1.41	1.35
13	A	842	CLA	C4B-NB	6.91	1.41	1.35
13	e	833	CLA	C4B-NB	6.91	1.41	1.35
13	b	838	CLA	C4B-NB	6.91	1.41	1.35
13	B	801	CLA	C4B-NB	6.91	1.41	1.35
13	E	843	CLA	C4B-NB	6.91	1.41	1.35
13	a	835	CLA	C4B-NB	6.91	1.41	1.35
13	g	815	CLA	C4B-NB	6.91	1.41	1.35
13	a	808	CLA	C4B-NB	6.91	1.41	1.35
13	E	835	CLA	C4B-NB	6.90	1.41	1.35
13	G	830	CLA	C4B-NB	6.90	1.41	1.35
13	a	843	CLA	C4B-NB	6.90	1.41	1.35
13	E	825	CLA	C4B-NB	6.89	1.41	1.35
13	a	825	CLA	C4B-NB	6.89	1.41	1.35
13	b	813	CLA	C4B-NB	6.89	1.41	1.35
13	a	833	CLA	C4B-NB	6.89	1.41	1.35
13	a	807	CLA	C4B-NB	6.89	1.41	1.35
13	g	802	CLA	C4B-NB	6.87	1.41	1.35
13	g	820	CLA	C4B-NB	6.87	1.41	1.35
13	e	841	CLA	C4B-NB	6.87	1.41	1.35
13	b	804	CLA	C4B-NB	6.86	1.41	1.35
13	A	807	CLA	C4B-NB	6.85	1.41	1.35
13	a	845	CLA	C4B-NB	6.84	1.41	1.35
13	A	825	CLA	C4B-NB	6.84	1.41	1.35
13	E	805	CLA	C4B-NB	6.83	1.41	1.35
13	A	833	CLA	C4B-NB	6.83	1.41	1.35
13	A	805	CLA	C4B-NB	6.83	1.41	1.35
13	E	834	CLA	C4B-NB	6.82	1.41	1.35
13	B	814	CLA	C4B-NB	6.82	1.41	1.35
13	E	807	CLA	C4B-NB	6.82	1.41	1.35
13	e	806	CLA	C4B-NB	6.82	1.41	1.35
13	G	804	CLA	C4B-NB	6.80	1.41	1.35
13	e	832	CLA	C4B-NB	6.78	1.41	1.35
13	g	801	CLA	C4B-NB	6.78	1.41	1.35
13	B	805	CLA	C4B-NB	6.78	1.41	1.35
13	E	833	CLA	C4B-NB	6.74	1.41	1.35
13	g	806	CLA	C4B-NB	6.73	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	805	CLA	C4B-NB	6.71	1.41	1.35
13	E	803	CLA	C4B-NB	6.71	1.41	1.35
13	A	840	CLA	C4B-NB	6.67	1.41	1.35
13	e	839	CLA	C4B-NB	6.67	1.41	1.35
13	a	841	CLA	C4B-NB	6.63	1.41	1.35
13	a	804	CLA	C4B-NB	6.62	1.41	1.35
13	A	804	CLA	C4B-NB	6.60	1.41	1.35
13	E	841	CLA	C4B-NB	6.59	1.41	1.35
13	E	804	CLA	C4B-NB	6.57	1.41	1.35
13	e	804	CLA	C4B-NB	6.53	1.41	1.35
13	s	203	CLA	C1D-ND	6.30	1.45	1.37
13	S	204	CLA	C1D-ND	6.29	1.45	1.37
13	l	205	CLA	C1D-ND	6.24	1.45	1.37
13	L	204	CLA	C1D-ND	6.18	1.45	1.37
14	G	842	PQN	C10-C5	5.08	1.49	1.40
14	b	841	PQN	C10-C5	5.06	1.49	1.40
14	g	843	PQN	C10-C5	5.05	1.49	1.40
14	a	847	PQN	C10-C5	5.05	1.49	1.40
14	E	848	PQN	C10-C5	5.04	1.49	1.40
14	A	846	PQN	C10-C5	5.02	1.49	1.40
14	e	845	PQN	C10-C5	5.02	1.49	1.40
14	B	842	PQN	C10-C5	5.00	1.49	1.40
13	L	204	CLA	C1A-CHA	4.44	1.61	1.43
13	S	204	CLA	C1A-CHA	4.43	1.61	1.43
13	s	203	CLA	C1A-CHA	4.42	1.61	1.43
13	l	205	CLA	C1A-CHA	4.42	1.61	1.43
15	s	201	BCR	C30-C25	-4.11	1.48	1.53
15	e	849	BCR	C1-C6	-4.04	1.48	1.53
15	A	850	BCR	C1-C6	-4.01	1.48	1.53
15	e	850	BCR	C1-C6	-3.98	1.48	1.53
15	L	201	BCR	C30-C25	-3.96	1.48	1.53
15	A	851	BCR	C1-C6	-3.95	1.48	1.53
13	e	836	CLA	C1D-ND	3.91	1.42	1.37
13	E	838	CLA	C1D-ND	3.90	1.42	1.37
13	A	837	CLA	C1D-ND	3.90	1.42	1.37
15	E	802	BCR	C1-C6	-3.85	1.48	1.53
13	E	803	CLA	C1D-ND	3.84	1.42	1.37
15	E	801	BCR	C1-C6	-3.84	1.48	1.53
13	A	803	CLA	C1D-ND	3.84	1.42	1.37
13	a	838	CLA	C1D-ND	3.83	1.42	1.37
15	a	803	BCR	C1-C6	-3.82	1.48	1.53
13	F	202	CLA	C1D-ND	3.82	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	817	CLA	C1D-ND	3.80	1.42	1.37
13	e	803	CLA	C1D-ND	3.80	1.42	1.37
13	A	826	CLA	C1D-ND	3.78	1.42	1.37
13	E	846	CLA	C1D-ND	3.77	1.42	1.37
13	o	202	CLA	C1D-ND	3.77	1.42	1.37
13	a	826	CLA	C1D-ND	3.76	1.42	1.37
13	a	843	CLA	C1D-ND	3.76	1.42	1.37
13	r	101	CLA	C1D-ND	3.76	1.42	1.37
13	B	805	CLA	C1D-ND	3.76	1.42	1.37
13	E	817	CLA	C1D-ND	3.76	1.42	1.37
13	E	821	CLA	C1D-ND	3.76	1.42	1.37
13	b	819	CLA	C1D-ND	3.75	1.42	1.37
13	a	817	CLA	C1D-ND	3.75	1.42	1.37
13	E	826	CLA	C1D-ND	3.75	1.42	1.37
13	G	804	CLA	C1D-ND	3.75	1.42	1.37
13	A	842	CLA	C1D-ND	3.75	1.42	1.37
13	E	808	CLA	C1D-ND	3.74	1.42	1.37
13	G	834	CLA	C1D-ND	3.74	1.42	1.37
13	e	825	CLA	C1D-ND	3.74	1.42	1.37
13	s	203	CLA	C2A-C1A	3.74	1.60	1.52
13	b	833	CLA	C1D-ND	3.74	1.42	1.37
13	L	204	CLA	C2A-C1A	3.74	1.60	1.52
13	a	852	CLA	C1D-ND	3.74	1.42	1.37
13	b	835	CLA	C1D-ND	3.74	1.42	1.37
13	B	820	CLA	C1D-ND	3.73	1.42	1.37
13	e	820	CLA	C1D-ND	3.73	1.42	1.37
13	l	205	CLA	C2A-C1A	3.73	1.60	1.52
13	g	821	CLA	C1D-ND	3.73	1.42	1.37
13	g	806	CLA	C1D-ND	3.73	1.42	1.37
13	E	843	CLA	C1D-ND	3.72	1.42	1.37
13	O	203	CLA	C1D-ND	3.72	1.42	1.37
13	B	836	CLA	C1D-ND	3.72	1.42	1.37
15	l	202	BCR	C1-C6	-3.72	1.48	1.53
13	K	101	CLA	C1D-ND	3.72	1.42	1.37
13	b	804	CLA	C1D-ND	3.72	1.42	1.37
13	B	834	CLA	C1D-ND	3.72	1.42	1.37
13	G	818	CLA	C1D-ND	3.71	1.42	1.37
13	G	820	CLA	C1D-ND	3.71	1.42	1.37
13	e	807	CLA	C1D-ND	3.71	1.42	1.37
13	A	808	CLA	C1D-ND	3.71	1.42	1.37
13	A	821	CLA	C1D-ND	3.71	1.42	1.37
13	b	821	CLA	C1D-ND	3.71	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	808	CLA	C1D-ND	3.71	1.42	1.37
13	e	816	CLA	C1D-ND	3.71	1.42	1.37
13	A	839	CLA	C1D-ND	3.70	1.42	1.37
13	G	836	CLA	C1D-ND	3.70	1.42	1.37
13	S	204	CLA	C2A-C1A	3.70	1.60	1.52
13	g	837	CLA	C1D-ND	3.70	1.42	1.37
13	e	844	CLA	C1D-ND	3.70	1.42	1.37
13	g	835	CLA	C1D-ND	3.69	1.42	1.37
13	e	813	CLA	C1D-ND	3.69	1.42	1.37
13	a	821	CLA	C1D-ND	3.69	1.42	1.37
13	b	817	CLA	C1D-ND	3.69	1.42	1.37
13	E	812	CLA	C1D-ND	3.69	1.42	1.37
15	S	201	BCR	C1-C6	-3.69	1.48	1.53
13	B	823	CLA	C1D-ND	3.68	1.42	1.37
13	A	827	CLA	C1D-ND	3.68	1.42	1.37
13	a	827	CLA	C1D-ND	3.68	1.42	1.37
13	a	812	CLA	C1D-ND	3.68	1.42	1.37
13	G	831	CLA	C1D-ND	3.68	1.42	1.37
13	E	814	CLA	C1D-ND	3.67	1.42	1.37
13	b	830	CLA	C1D-ND	3.67	1.42	1.37
13	e	826	CLA	C1D-ND	3.67	1.42	1.37
13	E	818	CLA	C1D-ND	3.67	1.42	1.37
13	E	827	CLA	C1D-ND	3.67	1.42	1.37
13	A	814	CLA	C1D-ND	3.67	1.42	1.37
13	G	822	CLA	C1D-ND	3.67	1.42	1.37
13	e	815	CLA	C1D-ND	3.67	1.42	1.37
13	e	834	CLA	C4D-ND	-3.67	1.32	1.37
13	b	810	CLA	C1D-ND	3.67	1.42	1.37
13	A	804	CLA	C1D-ND	3.67	1.42	1.37
13	E	816	CLA	C1D-ND	3.67	1.42	1.37
13	e	812	CLA	C1D-ND	3.67	1.42	1.37
13	e	810	CLA	C1D-ND	3.67	1.42	1.37
13	G	823	CLA	C1D-ND	3.66	1.42	1.37
13	e	824	CLA	C1D-ND	3.66	1.42	1.37
13	A	845	CLA	C1D-ND	3.66	1.42	1.37
13	G	837	CLA	C1D-ND	3.66	1.42	1.37
13	g	823	CLA	C1D-ND	3.66	1.42	1.37
13	g	812	CLA	C1D-ND	3.66	1.42	1.37
13	g	838	CLA	C1D-ND	3.66	1.42	1.37
13	B	822	CLA	C1D-ND	3.66	1.42	1.37
13	g	832	CLA	C1D-ND	3.66	1.42	1.37
13	b	815	CLA	C1D-ND	3.66	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	811	CLA	C1D-ND	3.66	1.42	1.37
13	L	204	CLA	MG-NC	3.66	2.15	2.06
13	a	813	CLA	C1D-ND	3.65	1.42	1.37
13	s	203	CLA	MG-NC	3.65	2.14	2.06
13	f	203	CLA	C1D-ND	3.65	1.42	1.37
13	A	816	CLA	C1D-ND	3.65	1.42	1.37
13	b	822	CLA	C1D-ND	3.65	1.42	1.37
13	S	204	CLA	MG-NC	3.65	2.14	2.06
13	e	811	CLA	C1D-ND	3.65	1.42	1.37
13	A	811	CLA	C1D-ND	3.65	1.42	1.37
13	g	819	CLA	C1D-ND	3.65	1.42	1.37
13	E	804	CLA	C1D-ND	3.65	1.42	1.37
13	g	836	CLA	C1D-ND	3.65	1.42	1.37
13	B	837	CLA	C1D-ND	3.64	1.42	1.37
13	b	836	CLA	C1D-ND	3.64	1.42	1.37
13	A	818	CLA	C1D-ND	3.64	1.42	1.37
13	A	835	CLA	C4D-ND	-3.64	1.32	1.37
13	A	810	CLA	C1D-ND	3.64	1.42	1.37
13	A	812	CLA	C1D-ND	3.64	1.42	1.37
13	l	205	CLA	MG-NC	3.64	2.14	2.06
13	b	834	CLA	C1D-ND	3.64	1.42	1.37
13	B	835	CLA	C1D-ND	3.64	1.42	1.37
13	g	824	CLA	C1D-ND	3.64	1.42	1.37
13	e	841	CLA	C1D-ND	3.64	1.42	1.37
13	a	830	CLA	C1D-ND	3.64	1.42	1.37
13	B	818	CLA	C1D-ND	3.64	1.42	1.37
13	E	819	CLA	C1D-ND	3.64	1.42	1.37
13	g	817	CLA	C1D-ND	3.64	1.42	1.37
13	E	840	CLA	C1D-ND	3.63	1.42	1.37
13	R	102	CLA	C1D-ND	3.63	1.42	1.37
13	E	810	CLA	C1D-ND	3.63	1.42	1.37
13	a	814	CLA	C1D-ND	3.63	1.42	1.37
13	a	840	CLA	C1D-ND	3.63	1.42	1.37
13	A	825	CLA	C1D-ND	3.63	1.42	1.37
13	k	4002	CLA	C1D-ND	3.63	1.42	1.37
13	A	819	CLA	C1D-ND	3.62	1.42	1.37
13	a	816	CLA	C1D-ND	3.62	1.42	1.37
13	B	816	CLA	C1D-ND	3.62	1.42	1.37
13	b	812	CLA	C1D-ND	3.62	1.42	1.37
13	B	831	CLA	C1D-ND	3.62	1.42	1.37
13	G	813	CLA	C1D-ND	3.62	1.42	1.37
13	a	836	CLA	C4D-ND	-3.62	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	816	CLA	C1D-ND	3.62	1.42	1.37
13	A	813	CLA	C1D-ND	3.62	1.42	1.37
13	r	102	CLA	C1D-ND	3.62	1.42	1.37
13	a	819	CLA	C1D-ND	3.62	1.42	1.37
13	l	201	CLA	C1D-ND	3.62	1.42	1.37
13	A	830	CLA	C1D-ND	3.61	1.42	1.37
13	B	810	CLA	C1D-ND	3.61	1.42	1.37
13	b	809	CLA	C1D-ND	3.61	1.42	1.37
13	G	816	CLA	C1D-ND	3.61	1.42	1.37
13	E	836	CLA	C1D-ND	3.61	1.42	1.37
13	e	818	CLA	C1D-ND	3.61	1.42	1.37
13	a	811	CLA	C1D-ND	3.61	1.42	1.37
13	e	804	CLA	C1D-ND	3.61	1.42	1.37
15	O	201	BCR	C1-C6	-3.61	1.48	1.53
13	B	814	CLA	C1D-ND	3.61	1.42	1.37
13	E	825	CLA	C1D-ND	3.61	1.42	1.37
13	E	836	CLA	C4D-ND	-3.61	1.32	1.37
13	B	811	CLA	C1D-ND	3.60	1.42	1.37
13	g	811	CLA	C1D-ND	3.60	1.42	1.37
13	S	206	CLA	C1D-ND	3.60	1.42	1.37
13	B	821	CLA	C1D-ND	3.60	1.42	1.37
13	a	804	CLA	C1D-ND	3.60	1.42	1.37
13	B	840	CLA	C1D-ND	3.60	1.42	1.37
13	a	810	CLA	C1D-ND	3.60	1.42	1.37
13	b	823	CLA	C1D-ND	3.60	1.42	1.37
13	E	813	CLA	C1D-ND	3.60	1.42	1.37
13	G	826	CLA	C1D-ND	3.60	1.42	1.37
13	G	824	CLA	C1D-ND	3.59	1.42	1.37
13	G	827	CLA	C1D-ND	3.59	1.42	1.37
13	g	815	CLA	C1D-ND	3.59	1.42	1.37
13	g	827	CLA	C1D-ND	3.59	1.42	1.37
13	G	809	CLA	C1D-ND	3.59	1.42	1.37
13	G	835	CLA	C1D-ND	3.59	1.42	1.37
13	e	829	CLA	C1D-ND	3.59	1.42	1.37
13	B	812	CLA	C1D-ND	3.59	1.42	1.37
15	f	201	BCR	C1-C6	-3.59	1.48	1.53
13	E	830	CLA	C1D-ND	3.59	1.42	1.37
13	e	838	CLA	C1D-ND	3.59	1.42	1.37
15	B	847	BCR	C30-C25	-3.59	1.48	1.53
13	B	826	CLA	C1D-ND	3.59	1.42	1.37
13	E	845	CLA	C1D-ND	3.59	1.42	1.37
13	e	809	CLA	C1D-ND	3.59	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	825	CLA	C1D-ND	3.58	1.42	1.37
15	o	201	BCR	C1-C6	-3.58	1.48	1.53
13	b	826	CLA	C1D-ND	3.58	1.42	1.37
13	b	813	CLA	C1D-ND	3.58	1.42	1.37
13	g	825	CLA	C1D-ND	3.58	1.42	1.37
13	G	814	CLA	C1D-ND	3.58	1.42	1.37
13	b	811	CLA	C1D-ND	3.58	1.42	1.37
13	e	821	CLA	C1D-ND	3.58	1.42	1.37
13	a	825	CLA	C1D-ND	3.58	1.42	1.37
13	A	822	CLA	C1D-ND	3.58	1.42	1.37
13	E	820	CLA	C1D-ND	3.58	1.42	1.37
13	B	824	CLA	C1D-ND	3.58	1.42	1.37
15	T	101	BCR	C1-C6	-3.58	1.48	1.53
13	G	810	CLA	C1D-ND	3.58	1.42	1.37
13	g	840	CLA	C1D-ND	3.57	1.42	1.37
13	g	818	CLA	C1D-ND	3.57	1.42	1.37
13	a	818	CLA	C1D-ND	3.57	1.42	1.37
13	g	814	CLA	C1D-ND	3.57	1.42	1.37
15	q	102	BCR	C1-C6	-3.57	1.48	1.53
13	A	815	CLA	C1D-ND	3.57	1.42	1.37
13	a	845	CLA	C1D-ND	3.57	1.42	1.37
13	g	828	CLA	C1D-ND	3.57	1.42	1.37
13	e	828	CLA	C1D-ND	3.57	1.42	1.37
13	g	826	CLA	C1D-ND	3.56	1.42	1.37
13	b	808	CLA	C1D-ND	3.56	1.42	1.37
13	G	812	CLA	C1D-ND	3.56	1.42	1.37
13	B	804	CLA	C1D-ND	3.56	1.42	1.37
13	b	839	CLA	C1D-ND	3.56	1.42	1.37
13	G	839	CLA	C1D-ND	3.56	1.42	1.37
15	b	846	BCR	C30-C25	-3.56	1.48	1.53
13	A	838	CLA	C1D-ND	3.56	1.42	1.37
13	e	837	CLA	C1D-ND	3.56	1.42	1.37
13	g	822	CLA	C1D-ND	3.56	1.42	1.37
13	a	842	CLA	C1D-ND	3.56	1.42	1.37
13	B	809	CLA	C1D-ND	3.56	1.42	1.37
13	K	102	CLA	C1D-ND	3.56	1.42	1.37
13	e	817	CLA	C1D-ND	3.55	1.42	1.37
15	B	847	BCR	C1-C6	-3.55	1.48	1.53
13	a	839	CLA	C1D-ND	3.55	1.42	1.37
13	A	832	CLA	C1D-ND	3.55	1.42	1.37
15	G	847	BCR	C1-C6	-3.55	1.48	1.53
13	b	803	CLA	C1D-ND	3.55	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	813	CLA	C1D-ND	3.55	1.42	1.37
13	G	811	CLA	C1D-ND	3.55	1.42	1.37
13	B	815	CLA	C1D-ND	3.55	1.42	1.37
15	F	201	BCR	C1-C6	-3.55	1.48	1.53
13	B	827	CLA	C1D-ND	3.54	1.42	1.37
13	B	839	CLA	C1D-ND	3.54	1.42	1.37
13	e	834	CLA	C1D-ND	3.54	1.42	1.37
13	A	809	CLA	C1D-ND	3.54	1.42	1.37
15	J	102	BCR	C1-C6	-3.54	1.48	1.53
13	e	831	CLA	C1D-ND	3.54	1.42	1.37
13	e	852	CLA	C1D-ND	3.54	1.42	1.37
13	a	828	CLA	C1D-ND	3.54	1.42	1.37
13	a	829	CLA	C1D-ND	3.54	1.42	1.37
13	b	838	CLA	C1D-ND	3.54	1.42	1.37
13	e	843	CLA	C1D-ND	3.54	1.42	1.37
13	e	808	CLA	C1D-ND	3.54	1.42	1.37
13	g	813	CLA	C1D-ND	3.54	1.42	1.37
13	E	832	CLA	C1D-ND	3.54	1.42	1.37
13	e	819	CLA	C1D-ND	3.54	1.42	1.37
15	k	4001	BCR	C30-C25	-3.54	1.48	1.53
15	g	848	BCR	C30-C25	-3.53	1.48	1.53
13	B	819	CLA	C1D-ND	3.53	1.42	1.37
13	E	815	CLA	C1D-ND	3.53	1.42	1.37
13	E	844	CLA	C1D-ND	3.53	1.42	1.37
13	b	820	CLA	C1D-ND	3.53	1.42	1.37
15	a	853	BCR	C1-C6	-3.53	1.48	1.53
13	G	817	CLA	C1D-ND	3.53	1.42	1.37
13	s	205	CLA	C1D-ND	3.53	1.42	1.37
13	a	831	CLA	C1D-ND	3.53	1.42	1.37
15	g	848	BCR	C1-C6	-3.53	1.48	1.53
13	G	841	CLA	C1D-ND	3.53	1.42	1.37
13	g	833	CLA	C1D-ND	3.52	1.42	1.37
13	a	832	CLA	C1D-ND	3.52	1.42	1.37
13	e	839	CLA	C1D-ND	3.52	1.42	1.37
13	g	820	CLA	C1D-ND	3.52	1.42	1.37
13	b	814	CLA	C1D-ND	3.52	1.42	1.37
13	G	825	CLA	C1D-ND	3.52	1.42	1.37
13	G	806	CLA	C1D-ND	3.52	1.42	1.37
13	g	841	CLA	C1D-ND	3.52	1.42	1.37
13	A	844	CLA	C1D-ND	3.52	1.42	1.37
13	E	806	CLA	C1D-ND	3.52	1.42	1.37
13	E	809	CLA	C1D-ND	3.52	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	802	CLA	C1D-ND	3.52	1.42	1.37
13	g	816	CLA	C1D-ND	3.52	1.42	1.37
13	e	805	CLA	C1D-ND	3.52	1.42	1.37
13	a	841	CLA	C1D-ND	3.52	1.42	1.37
13	L	203	CLA	C1D-ND	3.52	1.42	1.37
13	A	807	CLA	C1D-ND	3.52	1.42	1.37
13	B	833	CLA	C1D-ND	3.52	1.42	1.37
13	b	824	CLA	C1D-ND	3.52	1.42	1.37
13	a	809	CLA	C1D-ND	3.51	1.42	1.37
13	A	840	CLA	C1D-ND	3.51	1.42	1.37
13	A	843	CLA	C1D-ND	3.51	1.42	1.37
13	G	819	CLA	C1D-ND	3.51	1.42	1.37
13	b	832	CLA	C1D-ND	3.51	1.42	1.37
15	A	851	BCR	C30-C25	-3.51	1.48	1.53
13	B	817	CLA	C1D-ND	3.51	1.42	1.37
13	E	822	CLA	C1D-ND	3.51	1.42	1.37
13	E	839	CLA	C1D-ND	3.51	1.42	1.37
13	e	814	CLA	C1D-ND	3.51	1.42	1.37
13	a	820	CLA	C1D-ND	3.51	1.42	1.37
13	B	841	CLA	C1D-ND	3.51	1.42	1.37
13	e	827	CLA	C1D-ND	3.51	1.42	1.37
13	e	830	CLA	C1D-ND	3.51	1.42	1.37
13	E	829	CLA	C1D-ND	3.51	1.42	1.37
13	a	844	CLA	C1D-ND	3.51	1.42	1.37
13	b	802	CLA	C1D-ND	3.51	1.42	1.37
13	A	829	CLA	C1D-ND	3.51	1.42	1.37
13	A	831	CLA	C1D-ND	3.50	1.42	1.37
13	a	806	CLA	C1D-ND	3.50	1.42	1.37
15	A	852	BCR	C1-C6	-3.50	1.49	1.53
13	a	815	CLA	C1D-ND	3.50	1.42	1.37
13	G	821	CLA	C1D-ND	3.50	1.42	1.37
13	S	203	CLA	C1D-ND	3.50	1.42	1.37
13	a	822	CLA	C1D-ND	3.50	1.42	1.37
13	e	842	CLA	C1D-ND	3.50	1.42	1.37
13	g	831	CLA	C1D-ND	3.50	1.42	1.37
13	b	831	CLA	C1D-ND	3.50	1.42	1.37
13	B	832	CLA	C1D-ND	3.50	1.42	1.37
13	E	807	CLA	C1D-ND	3.50	1.42	1.37
13	G	815	CLA	C1D-ND	3.50	1.42	1.37
13	E	828	CLA	C1D-ND	3.50	1.42	1.37
13	A	820	CLA	C1D-ND	3.50	1.42	1.37
15	E	852	BCR	C1-C6	-3.50	1.49	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	846	BCR	C1-C6	-3.50	1.49	1.53
13	B	825	CLA	C1D-ND	3.49	1.42	1.37
13	g	810	CLA	C1D-ND	3.49	1.42	1.37
13	A	853	CLA	C1D-ND	3.49	1.42	1.37
15	G	847	BCR	C30-C25	-3.49	1.49	1.53
13	a	807	CLA	C1D-ND	3.49	1.42	1.37
13	e	839	CLA	C4D-ND	-3.49	1.32	1.37
13	b	829	CLA	C1D-ND	3.49	1.42	1.37
13	A	835	CLA	C1D-ND	3.49	1.42	1.37
13	E	841	CLA	C1D-ND	3.49	1.42	1.37
13	G	840	CLA	C1D-ND	3.49	1.42	1.37
13	b	806	CLA	C1D-ND	3.48	1.42	1.37
13	G	803	CLA	C1D-ND	3.48	1.42	1.37
13	b	818	CLA	C1D-ND	3.48	1.42	1.37
13	g	842	CLA	C1D-ND	3.48	1.42	1.37
13	A	805	CLA	C1D-ND	3.48	1.42	1.37
13	A	841	CLA	C1D-ND	3.48	1.42	1.37
15	G	846	BCR	C1-C6	-3.48	1.49	1.53
13	B	807	CLA	C1D-ND	3.48	1.42	1.37
13	E	831	CLA	C1D-ND	3.48	1.42	1.37
13	e	840	CLA	C1D-ND	3.48	1.42	1.37
13	a	836	CLA	C1D-ND	3.48	1.42	1.37
15	B	845	BCR	C1-C6	-3.48	1.49	1.53
15	g	849	BCR	C1-C6	-3.47	1.49	1.53
13	A	828	CLA	C1D-ND	3.47	1.42	1.37
13	g	834	CLA	C1D-ND	3.47	1.42	1.37
15	l	202	BCR	C30-C25	-3.47	1.49	1.53
15	b	847	BCR	C1-C6	-3.47	1.49	1.53
13	G	808	CLA	C1D-ND	3.47	1.42	1.37
15	p	101	BCR	C30-C25	-3.47	1.49	1.53
13	E	841	CLA	C4D-ND	-3.47	1.32	1.37
15	g	846	BCR	C1-C6	-3.47	1.49	1.53
13	g	805	CLA	C1D-ND	3.47	1.42	1.37
15	G	848	BCR	C1-C6	-3.47	1.49	1.53
13	A	840	CLA	C4D-ND	-3.47	1.32	1.37
13	e	806	CLA	C1D-ND	3.47	1.42	1.37
13	g	839	CLA	C1D-ND	3.47	1.42	1.37
15	B	848	BCR	C1-C6	-3.47	1.49	1.53
13	a	824	CLA	C1D-ND	3.47	1.42	1.37
13	G	832	CLA	C1D-ND	3.47	1.42	1.37
13	L	204	CLA	C4D-CHA	3.46	1.50	1.38
13	b	827	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)
13	A	806	CLA	C1D-ND	3.46	1.42	1.37
13	g	801	CLA	C1D-ND	3.46	1.42	1.37
15	b	844	BCR	C1-C6	-3.45	1.49	1.53
13	l	203	CLA	C1D-ND	3.45	1.42	1.37
13	a	834	CLA	C1D-ND	3.45	1.42	1.37
13	G	833	CLA	C1D-ND	3.45	1.42	1.37
15	i	101	BCR	C30-C25	-3.45	1.49	1.53
13	B	830	CLA	C1D-ND	3.45	1.42	1.37
13	E	833	CLA	C1D-ND	3.45	1.42	1.37
13	s	203	CLA	C4D-CHA	3.45	1.50	1.38
13	e	822	CLA	C4D-ND	-3.45	1.33	1.37
13	a	823	CLA	C1D-ND	3.44	1.42	1.37
13	l	204	CLA	C1D-ND	3.44	1.42	1.37
13	S	204	CLA	C4D-CHA	3.44	1.50	1.38
13	B	806	CLA	C1D-ND	3.44	1.42	1.37
15	G	845	BCR	C1-C6	-3.44	1.49	1.53
15	s	201	BCR	C1-C6	-3.44	1.49	1.53
13	G	807	CLA	C1D-ND	3.44	1.42	1.37
13	b	840	CLA	C1D-ND	3.44	1.42	1.37
15	B	846	BCR	C1-C6	-3.44	1.49	1.53
13	e	822	CLA	C1D-ND	3.44	1.42	1.37
13	A	823	CLA	C1D-ND	3.44	1.42	1.37
15	P	101	BCR	C30-C25	-3.44	1.49	1.53
15	g	847	BCR	C1-C6	-3.44	1.49	1.53
13	B	838	CLA	C1D-ND	3.43	1.42	1.37
13	E	823	CLA	C4D-ND	-3.43	1.33	1.37
13	E	834	CLA	C1D-ND	3.43	1.42	1.37
13	A	824	CLA	C1D-ND	3.43	1.42	1.37
13	E	824	CLA	C1D-ND	3.43	1.42	1.37
13	G	830	CLA	C1D-ND	3.43	1.42	1.37
13	g	829	CLA	C1D-ND	3.43	1.42	1.37
13	l	205	CLA	C4D-CHA	3.43	1.50	1.38
13	E	823	CLA	C1D-ND	3.43	1.42	1.37
13	E	842	CLA	C1D-ND	3.42	1.42	1.37
15	a	849	BCR	C1-C6	-3.42	1.49	1.53
13	b	837	CLA	C1D-ND	3.42	1.42	1.37
13	B	828	CLA	C1D-ND	3.42	1.42	1.37
15	b	845	BCR	C1-C6	-3.42	1.49	1.53
13	a	841	CLA	C4D-ND	-3.42	1.33	1.37
13	a	830	CLA	C4D-ND	-3.42	1.33	1.37
13	l	205	CLA	MG-NA	3.42	2.14	2.06
15	L	201	BCR	C1-C6	-3.42	1.49	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	s	203	CLA	MG-NA	3.41	2.14	2.06
13	G	828	CLA	C1D-ND	3.41	1.42	1.37
15	S	201	BCR	C30-C25	-3.41	1.49	1.53
13	G	801	CLA	C1D-ND	3.41	1.42	1.37
13	S	204	CLA	MG-NA	3.41	2.14	2.06
13	a	805	CLA	C1D-ND	3.41	1.42	1.37
13	e	835	CLA	C1D-ND	3.41	1.42	1.37
13	g	807	CLA	C1D-ND	3.40	1.42	1.37
13	e	823	CLA	C1D-ND	3.40	1.42	1.37
13	L	202	CLA	C1D-ND	3.40	1.42	1.37
13	g	808	CLA	C1D-ND	3.40	1.42	1.37
15	I	101	BCR	C30-C25	-3.40	1.49	1.53
13	E	835	CLA	C1D-ND	3.40	1.42	1.37
15	E	849	BCR	C1-C6	-3.39	1.49	1.53
13	s	202	CLA	C1D-ND	3.39	1.42	1.37
13	g	809	CLA	C1D-ND	3.39	1.42	1.37
13	A	834	CLA	C1D-ND	3.39	1.42	1.37
13	G	829	CLA	C1D-ND	3.39	1.42	1.37
13	e	833	CLA	C1D-ND	3.39	1.42	1.37
13	B	802	CLA	C1D-ND	3.39	1.42	1.37
13	E	830	CLA	C4D-ND	-3.39	1.33	1.37
15	A	847	BCR	C1-C6	-3.39	1.49	1.53
13	b	828	CLA	C1D-ND	3.39	1.41	1.37
13	A	823	CLA	C4D-ND	-3.39	1.33	1.37
13	b	837	CLA	C4D-ND	-3.39	1.33	1.37
13	G	819	CLA	C4D-ND	-3.39	1.33	1.37
13	b	818	CLA	C4D-ND	-3.38	1.33	1.37
13	L	204	CLA	MG-NA	3.38	2.14	2.06
15	e	851	BCR	C1-C6	-3.38	1.49	1.53
13	G	805	CLA	C1D-ND	3.38	1.41	1.37
13	E	805	CLA	C1D-ND	3.38	1.41	1.37
13	A	833	CLA	C1D-ND	3.38	1.41	1.37
13	G	838	CLA	C1D-ND	3.38	1.41	1.37
13	e	832	CLA	C1D-ND	3.38	1.41	1.37
15	G	844	BCR	C1-C6	-3.38	1.49	1.53
13	B	808	CLA	C1D-ND	3.38	1.41	1.37
13	a	823	CLA	C4D-ND	-3.38	1.33	1.37
13	A	836	CLA	C1D-ND	3.37	1.41	1.37
13	a	837	CLA	C1D-ND	3.37	1.41	1.37
13	e	829	CLA	C4D-ND	-3.37	1.33	1.37
13	b	808	CLA	C4D-ND	-3.37	1.33	1.37
13	E	837	CLA	C1D-ND	3.37	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	101	BCR	C1-C6	-3.37	1.49	1.53
13	g	803	CLA	C1D-ND	3.37	1.41	1.37
15	e	846	BCR	C1-C6	-3.36	1.49	1.53
13	A	830	CLA	C4D-ND	-3.36	1.33	1.37
13	g	810	CLA	C4D-ND	-3.36	1.33	1.37
13	a	833	CLA	C1D-ND	3.36	1.41	1.37
15	b	843	BCR	C1-C6	-3.36	1.49	1.53
13	g	809	CLA	C4D-ND	-3.36	1.33	1.37
13	E	806	CLA	C4D-ND	-3.36	1.33	1.37
13	G	808	CLA	C4D-ND	-3.35	1.33	1.37
13	B	809	CLA	C4D-ND	-3.35	1.33	1.37
13	a	806	CLA	C4D-ND	-3.35	1.33	1.37
13	g	802	CLA	C1D-ND	3.35	1.41	1.37
13	B	808	CLA	C4D-ND	-3.35	1.33	1.37
13	b	805	CLA	C1D-ND	3.35	1.41	1.37
13	g	802	CLA	C4D-ND	-3.35	1.33	1.37
13	G	838	CLA	C4D-ND	-3.35	1.33	1.37
13	g	830	CLA	C1D-ND	3.34	1.41	1.37
13	b	807	CLA	C1D-ND	3.34	1.41	1.37
13	g	839	CLA	C4D-ND	-3.34	1.33	1.37
13	e	805	CLA	C4D-ND	-3.34	1.33	1.37
15	I	101	BCR	C1-C6	-3.34	1.49	1.53
15	B	844	BCR	C1-C6	-3.34	1.49	1.53
13	a	837	CLA	C4D-ND	-3.34	1.33	1.37
13	E	835	CLA	C4D-ND	-3.34	1.33	1.37
13	E	837	CLA	C4D-ND	-3.34	1.33	1.37
13	a	835	CLA	C4D-ND	-3.34	1.33	1.37
13	G	821	CLA	C4D-ND	-3.34	1.33	1.37
13	B	829	CLA	C1D-ND	3.34	1.41	1.37
13	A	836	CLA	C4D-ND	-3.34	1.33	1.37
15	i	101	BCR	C1-C6	-3.33	1.49	1.53
15	G	848	BCR	C30-C25	-3.33	1.49	1.53
13	e	835	CLA	C4D-ND	-3.33	1.33	1.37
13	b	839	CLA	C4D-ND	-3.33	1.33	1.37
15	g	849	BCR	C30-C25	-3.33	1.49	1.53
13	B	819	CLA	C4D-ND	-3.32	1.33	1.37
15	g	844	BCR	C1-C6	-3.32	1.49	1.53
15	B	848	BCR	C30-C25	-3.32	1.49	1.53
13	E	832	CLA	C4D-ND	-3.32	1.33	1.37
15	G	843	BCR	C1-C6	-3.32	1.49	1.53
15	p	101	BCR	C1-C6	-3.32	1.49	1.53
15	S	202	BCR	C30-C25	-3.32	1.49	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	840	CLA	C4D-ND	-3.31	1.33	1.37
13	A	806	CLA	C4D-ND	-3.31	1.33	1.37
13	B	801	CLA	C4D-ND	-3.31	1.33	1.37
13	b	820	CLA	C4D-ND	-3.31	1.33	1.37
13	B	833	CLA	C4D-ND	-3.31	1.33	1.37
13	B	838	CLA	C4D-ND	-3.31	1.33	1.37
15	g	847	BCR	C30-C25	-3.31	1.49	1.53
13	B	801	CLA	C1D-ND	3.31	1.41	1.37
13	G	807	CLA	C4D-ND	-3.31	1.33	1.37
15	a	802	BCR	C1-C6	-3.31	1.49	1.53
13	e	823	CLA	C4D-ND	-3.30	1.33	1.37
15	b	847	BCR	C30-C25	-3.30	1.49	1.53
13	g	822	CLA	C4D-ND	-3.30	1.33	1.37
13	A	832	CLA	C4D-ND	-3.30	1.33	1.37
13	a	832	CLA	C4D-ND	-3.30	1.33	1.37
13	b	806	CLA	C4D-ND	-3.30	1.33	1.37
15	b	842	BCR	C1-C6	-3.30	1.49	1.53
13	b	807	CLA	C4D-ND	-3.30	1.33	1.37
15	A	849	BCR	C30-C25	-3.30	1.49	1.53
15	g	845	BCR	C1-C6	-3.30	1.49	1.53
13	b	801	CLA	C1D-ND	3.30	1.41	1.37
13	G	833	CLA	C4D-ND	-3.30	1.33	1.37
13	a	835	CLA	C1D-ND	3.30	1.41	1.37
15	S	202	BCR	C1-C6	-3.29	1.49	1.53
15	B	846	BCR	C30-C25	-3.29	1.49	1.53
15	l	206	BCR	C1-C6	-3.29	1.49	1.53
13	g	826	CLA	C4D-ND	-3.29	1.33	1.37
13	L	202	CLA	CHC-C1C	3.28	1.43	1.35
13	g	821	CLA	C4D-ND	-3.28	1.33	1.37
15	a	850	BCR	C30-C25	-3.28	1.49	1.53
13	G	832	CLA	C4D-ND	-3.28	1.33	1.37
13	G	840	CLA	C4D-ND	-3.28	1.33	1.37
13	B	821	CLA	C4D-ND	-3.28	1.33	1.37
13	s	202	CLA	C4D-ND	-3.28	1.33	1.37
13	a	829	CLA	C4D-ND	-3.28	1.33	1.37
13	G	806	CLA	C4D-ND	-3.28	1.33	1.37
15	q	101	BCR	C1-C6	-3.28	1.49	1.53
13	l	203	CLA	C4D-ND	-3.27	1.33	1.37
13	b	832	CLA	C4D-ND	-3.27	1.33	1.37
13	g	820	CLA	C4D-ND	-3.27	1.33	1.37
13	B	820	CLA	C4D-ND	-3.27	1.33	1.37
13	E	824	CLA	C4D-ND	-3.27	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	203	CLA	C4D-ND	-3.27	1.33	1.37
13	g	833	CLA	C4D-ND	-3.27	1.33	1.37
13	b	831	CLA	C4D-ND	-3.27	1.33	1.37
13	E	838	CLA	C4D-ND	-3.27	1.33	1.37
13	S	203	CLA	C4D-ND	-3.27	1.33	1.37
13	A	833	CLA	C4D-ND	-3.26	1.33	1.37
15	O	202	BCR	C1-C6	-3.26	1.49	1.53
13	G	820	CLA	C4D-ND	-3.26	1.33	1.37
13	a	828	CLA	C4D-ND	-3.26	1.33	1.37
13	B	807	CLA	C4D-ND	-3.26	1.33	1.37
13	b	819	CLA	C4D-ND	-3.26	1.33	1.37
15	a	851	BCR	C30-C25	-3.26	1.49	1.53
13	B	812	CLA	C4D-ND	-3.26	1.33	1.37
15	E	851	BCR	C30-C25	-3.26	1.49	1.53
13	G	826	CLA	C4D-ND	-3.26	1.33	1.37
13	G	841	CLA	C4D-ND	-3.26	1.33	1.37
13	B	826	CLA	C4D-ND	-3.26	1.33	1.37
13	a	809	CLA	C4D-ND	-3.26	1.33	1.37
15	Q	101	BCR	C1-C6	-3.25	1.49	1.53
15	J	101	BCR	C1-C6	-3.25	1.49	1.53
15	E	850	BCR	C30-C25	-3.25	1.49	1.53
15	a	848	BCR	C1-C6	-3.25	1.49	1.53
15	b	845	BCR	C30-C25	-3.25	1.49	1.53
13	g	834	CLA	C4D-ND	-3.25	1.33	1.37
13	e	832	CLA	C4D-ND	-3.25	1.33	1.37
15	j	101	BCR	C1-C6	-3.25	1.49	1.53
13	B	841	CLA	C4D-ND	-3.25	1.33	1.37
15	B	843	BCR	C1-C6	-3.25	1.49	1.53
13	A	809	CLA	C4D-ND	-3.25	1.33	1.37
13	E	809	CLA	C4D-ND	-3.25	1.33	1.37
13	e	842	CLA	C4D-ND	-3.25	1.33	1.37
13	a	845	CLA	C4D-ND	-3.25	1.33	1.37
13	e	831	CLA	C4D-ND	-3.25	1.33	1.37
13	E	822	CLA	C4D-ND	-3.25	1.33	1.37
15	S	205	BCR	C1-C6	-3.25	1.49	1.53
13	A	824	CLA	C4D-ND	-3.25	1.33	1.37
13	b	838	CLA	C4D-ND	-3.25	1.33	1.37
13	g	840	CLA	C4D-ND	-3.25	1.33	1.37
13	a	834	CLA	C4D-ND	-3.24	1.33	1.37
13	A	828	CLA	C4D-ND	-3.24	1.33	1.37
13	B	825	CLA	C4D-ND	-3.24	1.33	1.37
13	G	805	CLA	C4D-ND	-3.24	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	832	CLA	C4D-ND	-3.24	1.33	1.37
13	s	205	CLA	C4D-ND	-3.24	1.33	1.37
13	a	824	CLA	C4D-ND	-3.24	1.33	1.37
13	e	828	CLA	C4D-ND	-3.24	1.33	1.37
15	a	850	BCR	C1-C6	-3.24	1.49	1.53
13	A	811	CLA	C4D-ND	-3.24	1.33	1.37
13	A	829	CLA	C4D-ND	-3.24	1.33	1.37
13	g	808	CLA	C4D-ND	-3.24	1.33	1.37
13	l	204	CLA	C4D-ND	-3.24	1.33	1.37
13	G	801	CLA	C4D-ND	-3.23	1.33	1.37
13	g	819	CLA	C4D-ND	-3.23	1.33	1.37
13	B	839	CLA	C4D-ND	-3.23	1.33	1.37
13	E	831	CLA	C4D-ND	-3.23	1.33	1.37
13	a	838	CLA	C4D-ND	-3.23	1.33	1.37
13	A	822	CLA	C4D-ND	-3.23	1.33	1.37
13	b	829	CLA	C4D-ND	-3.23	1.33	1.37
13	g	827	CLA	C4D-ND	-3.23	1.33	1.37
13	g	842	CLA	C4D-ND	-3.23	1.33	1.37
13	b	840	CLA	C4D-ND	-3.23	1.33	1.37
13	g	841	CLA	C4D-ND	-3.22	1.33	1.37
13	B	830	CLA	C4D-ND	-3.22	1.33	1.37
13	b	805	CLA	C4D-ND	-3.22	1.33	1.37
13	E	833	CLA	C4D-ND	-3.22	1.33	1.37
13	B	814	CLA	C4D-ND	-3.22	1.33	1.37
13	A	843	CLA	C4D-ND	-3.22	1.33	1.37
13	B	829	CLA	C4D-ND	-3.22	1.33	1.37
13	A	834	CLA	C4D-ND	-3.22	1.33	1.37
13	A	844	CLA	C4D-ND	-3.22	1.33	1.37
13	e	808	CLA	C4D-ND	-3.22	1.33	1.37
13	g	807	CLA	C4D-ND	-3.22	1.33	1.37
13	G	811	CLA	C4D-ND	-3.22	1.33	1.37
13	G	818	CLA	C4D-ND	-3.21	1.33	1.37
13	E	845	CLA	C4D-ND	-3.21	1.33	1.37
13	e	810	CLA	C4D-ND	-3.21	1.33	1.37
13	b	817	CLA	C4D-ND	-3.21	1.33	1.37
13	g	815	CLA	C4D-ND	-3.21	1.33	1.37
13	l	203	CLA	CHC-C1C	3.21	1.43	1.35
13	B	802	CLA	C4D-ND	-3.21	1.33	1.37
13	e	833	CLA	C4D-ND	-3.21	1.33	1.37
13	A	837	CLA	C4D-ND	-3.21	1.33	1.37
13	a	833	CLA	C4D-ND	-3.21	1.33	1.37
13	g	813	CLA	C4D-ND	-3.21	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	848	BCR	C1-C6	-3.21	1.49	1.53
13	B	806	CLA	C4D-ND	-3.20	1.33	1.37
15	T	101	BCR	C30-C25	-3.20	1.49	1.53
13	b	821	CLA	C4D-ND	-3.20	1.33	1.37
13	G	830	CLA	C4D-ND	-3.20	1.33	1.37
15	e	848	BCR	C1-C6	-3.20	1.49	1.53
13	G	825	CLA	C4D-ND	-3.20	1.33	1.37
13	e	827	CLA	C4D-ND	-3.20	1.33	1.37
13	B	828	CLA	C4D-ND	-3.20	1.33	1.37
13	E	811	CLA	C4D-ND	-3.20	1.33	1.37
13	g	803	CLA	C4D-ND	-3.20	1.33	1.37
13	b	825	CLA	C4D-ND	-3.19	1.33	1.37
15	e	847	BCR	C30-C25	-3.19	1.49	1.53
13	E	829	CLA	C4D-ND	-3.19	1.33	1.37
13	G	829	CLA	C4D-ND	-3.19	1.33	1.37
13	b	824	CLA	C4D-ND	-3.19	1.33	1.37
13	E	828	CLA	C4D-ND	-3.19	1.33	1.37
15	E	850	BCR	C1-C6	-3.19	1.49	1.53
15	m	101	BCR	C30-C25	-3.19	1.49	1.53
13	b	827	CLA	C4D-ND	-3.19	1.33	1.37
13	A	808	CLA	C4D-ND	-3.19	1.33	1.37
13	b	816	CLA	C4D-ND	-3.19	1.33	1.37
15	e	847	BCR	C1-C6	-3.19	1.49	1.53
13	B	822	CLA	C4D-ND	-3.19	1.33	1.37
13	E	816	CLA	C4D-ND	-3.19	1.33	1.37
13	E	803	CLA	C4D-ND	-3.19	1.33	1.37
15	G	846	BCR	C30-C25	-3.19	1.49	1.53
13	E	844	CLA	C4D-ND	-3.19	1.33	1.37
13	B	817	CLA	C4D-ND	-3.19	1.33	1.37
13	e	821	CLA	C4D-ND	-3.18	1.33	1.37
13	g	830	CLA	C4D-ND	-3.18	1.33	1.37
15	e	848	BCR	C30-C25	-3.18	1.49	1.53
13	g	831	CLA	C4D-ND	-3.18	1.33	1.37
13	b	813	CLA	C4D-ND	-3.18	1.33	1.37
15	b	844	BCR	C30-C25	-3.18	1.49	1.53
13	E	834	CLA	C4D-ND	-3.18	1.33	1.37
13	a	844	CLA	C4D-ND	-3.18	1.33	1.37
13	e	815	CLA	C4D-ND	-3.18	1.33	1.37
13	E	823	CLA	CHC-C1C	3.18	1.43	1.35
13	g	829	CLA	C4D-ND	-3.18	1.33	1.37
13	e	836	CLA	C4D-ND	-3.18	1.33	1.37
13	G	814	CLA	C4D-ND	-3.18	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	201	BCR	C30-C25	-3.18	1.49	1.53
15	B	845	BCR	C30-C25	-3.18	1.49	1.53
13	a	822	CLA	C4D-ND	-3.17	1.33	1.37
13	b	801	CLA	C4D-ND	-3.17	1.33	1.37
15	e	850	BCR	C30-C25	-3.17	1.49	1.53
13	G	822	CLA	C4D-ND	-3.17	1.33	1.37
13	A	816	CLA	C4D-ND	-3.17	1.33	1.37
13	B	818	CLA	C4D-ND	-3.17	1.33	1.37
13	E	808	CLA	C4D-ND	-3.17	1.33	1.37
13	g	818	CLA	C4D-ND	-3.17	1.33	1.37
13	a	810	CLA	C4D-ND	-3.17	1.33	1.37
15	E	851	BCR	C1-C6	-3.17	1.49	1.53
13	G	813	CLA	C4D-ND	-3.17	1.33	1.37
13	G	828	CLA	C4D-ND	-3.17	1.33	1.37
13	g	805	CLA	C4D-ND	-3.17	1.33	1.37
13	G	839	CLA	C4D-ND	-3.16	1.33	1.37
13	A	831	CLA	C4D-ND	-3.16	1.33	1.37
13	S	206	CLA	C4D-ND	-3.16	1.33	1.37
13	a	831	CLA	C4D-ND	-3.16	1.33	1.37
13	a	823	CLA	CHC-C1C	3.16	1.43	1.35
15	A	848	BCR	C30-C25	-3.16	1.49	1.53
13	e	843	CLA	C4D-ND	-3.16	1.33	1.37
13	a	811	CLA	C4D-ND	-3.16	1.33	1.37
13	b	828	CLA	C4D-ND	-3.16	1.33	1.37
13	e	807	CLA	C4D-ND	-3.16	1.33	1.37
13	e	822	CLA	CHC-C1C	3.16	1.43	1.35
13	G	817	CLA	C4D-ND	-3.16	1.33	1.37
13	g	828	CLA	C4D-ND	-3.16	1.33	1.37
13	b	817	CLA	CHC-C1C	3.16	1.43	1.35
15	O	201	BCR	C30-C25	-3.16	1.49	1.53
13	a	816	CLA	C4D-ND	-3.16	1.33	1.37
13	G	812	CLA	C4D-ND	-3.16	1.33	1.37
13	A	823	CLA	CHC-C1C	3.16	1.43	1.35
13	e	830	CLA	C4D-ND	-3.15	1.33	1.37
13	B	818	CLA	CHC-C1C	3.15	1.43	1.35
13	a	808	CLA	C4D-ND	-3.15	1.33	1.37
13	g	835	CLA	C4D-ND	-3.15	1.33	1.37
13	b	826	CLA	C4D-ND	-3.15	1.33	1.37
13	b	811	CLA	C4D-ND	-3.15	1.33	1.37
13	E	833	CLA	CHC-C1C	3.15	1.43	1.35
13	A	810	CLA	C4D-ND	-3.15	1.33	1.37
13	g	823	CLA	C4D-ND	-3.15	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	818	CLA	CHC-C1C	3.15	1.43	1.35
13	b	815	CLA	C4D-ND	-3.15	1.33	1.37
13	g	837	CLA	CHC-C1C	3.15	1.43	1.35
13	B	836	CLA	CHC-C1C	3.14	1.43	1.35
13	B	804	CLA	C4D-ND	-3.14	1.33	1.37
13	a	805	CLA	C4D-ND	-3.14	1.33	1.37
13	B	834	CLA	C4D-ND	-3.14	1.33	1.37
13	A	842	CLA	CHC-C1C	3.14	1.43	1.35
13	E	843	CLA	CHC-C1C	3.14	1.43	1.35
13	e	841	CLA	CHC-C1C	3.14	1.43	1.35
15	G	845	BCR	C30-C25	-3.14	1.49	1.53
13	A	805	CLA	C4D-ND	-3.14	1.33	1.37
13	g	816	CLA	C4D-ND	-3.14	1.33	1.37
13	G	816	CLA	C4D-ND	-3.14	1.33	1.37
13	E	810	CLA	C4D-ND	-3.14	1.33	1.37
13	g	819	CLA	CHC-C1C	3.14	1.43	1.35
13	G	831	CLA	C4D-ND	-3.13	1.33	1.37
13	b	809	CLA	C4D-ND	-3.13	1.33	1.37
13	b	812	CLA	C4D-ND	-3.13	1.33	1.37
13	e	832	CLA	CHC-C1C	3.13	1.43	1.35
13	e	809	CLA	C4D-ND	-3.13	1.33	1.37
13	B	814	CLA	CHC-C1C	3.13	1.43	1.35
15	g	846	BCR	C30-C25	-3.13	1.49	1.53
13	G	836	CLA	CHC-C1C	3.13	1.43	1.35
13	e	844	CLA	C4D-ND	-3.13	1.33	1.37
13	B	827	CLA	C4D-ND	-3.13	1.33	1.37
15	A	849	BCR	C1-C6	-3.13	1.49	1.53
13	g	811	CLA	C4D-ND	-3.12	1.33	1.37
13	a	833	CLA	CHC-C1C	3.12	1.43	1.35
15	f	202	BCR	C30-C25	-3.12	1.49	1.53
13	G	810	CLA	C4D-ND	-3.12	1.33	1.37
13	g	823	CLA	CHC-C1C	3.12	1.43	1.35
13	g	836	CLA	C4D-ND	-3.12	1.33	1.37
13	g	812	CLA	C4D-ND	-3.12	1.33	1.37
13	b	803	CLA	C4D-ND	-3.12	1.33	1.37
13	A	841	CLA	C4D-ND	-3.12	1.33	1.37
13	B	810	CLA	C4D-ND	-3.12	1.33	1.37
13	E	842	CLA	C4D-ND	-3.12	1.33	1.37
15	F	201	BCR	C30-C25	-3.12	1.49	1.53
15	a	851	BCR	C1-C6	-3.12	1.49	1.53
13	A	815	CLA	CHC-C1C	3.12	1.43	1.35
13	B	816	CLA	C4D-ND	-3.12	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	815	CLA	C4D-ND	-3.12	1.33	1.37
13	g	817	CLA	C4D-ND	-3.12	1.33	1.37
13	a	842	CLA	C4D-ND	-3.12	1.33	1.37
13	G	814	CLA	CHC-C1C	3.12	1.43	1.35
13	A	833	CLA	CHC-C1C	3.12	1.43	1.35
13	B	815	CLA	CHC-C1C	3.12	1.43	1.35
13	b	810	CLA	C4D-ND	-3.11	1.33	1.37
13	G	806	CLA	CHC-C1C	3.11	1.42	1.35
13	e	840	CLA	C4D-ND	-3.11	1.33	1.37
13	g	832	CLA	C4D-ND	-3.11	1.33	1.37
13	a	843	CLA	CHC-C1C	3.11	1.42	1.35
13	L	202	CLA	C4D-ND	-3.11	1.33	1.37
13	E	815	CLA	C4D-ND	-3.11	1.33	1.37
13	e	804	CLA	C4D-ND	-3.11	1.33	1.37
15	g	845	BCR	C30-C25	-3.11	1.49	1.53
13	A	845	CLA	C4D-ND	-3.11	1.33	1.37
13	G	803	CLA	C4D-ND	-3.11	1.33	1.37
13	b	836	CLA	C4D-ND	-3.11	1.33	1.37
13	l	201	CLA	C4D-ND	-3.11	1.33	1.37
13	B	807	CLA	CHC-C1C	3.11	1.42	1.35
13	G	834	CLA	CHC-C1C	3.11	1.42	1.35
13	E	839	CLA	CHC-C1C	3.11	1.42	1.35
13	B	815	CLA	C4D-ND	-3.11	1.33	1.37
13	g	814	CLA	C4D-ND	-3.11	1.33	1.37
13	B	824	CLA	CHC-C1C	3.11	1.42	1.35
13	B	813	CLA	C4D-ND	-3.11	1.33	1.37
13	B	834	CLA	CHC-C1C	3.11	1.42	1.35
13	B	811	CLA	C4D-ND	-3.10	1.33	1.37
13	g	808	CLA	CHC-C1C	3.10	1.42	1.35
13	b	806	CLA	CHC-C1C	3.10	1.42	1.35
13	a	815	CLA	C4D-ND	-3.10	1.33	1.37
13	b	825	CLA	CHC-C1C	3.10	1.42	1.35
13	B	822	CLA	CHC-C1C	3.10	1.42	1.35
15	o	201	BCR	C30-C25	-3.10	1.49	1.53
13	b	833	CLA	C4D-ND	-3.10	1.33	1.37
13	b	814	CLA	CHC-C1C	3.10	1.42	1.35
13	b	814	CLA	C4D-ND	-3.10	1.33	1.37
13	G	838	CLA	CHC-C1C	3.10	1.42	1.35
13	A	839	CLA	C4D-ND	-3.10	1.33	1.37
13	E	840	CLA	C4D-ND	-3.10	1.33	1.37
13	G	827	CLA	C4D-ND	-3.10	1.33	1.37
13	g	801	CLA	C4D-ND	-3.10	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	824	CLA	CHC-C1C	3.10	1.42	1.35
13	A	815	CLA	C4D-ND	-3.10	1.33	1.37
13	b	822	CLA	C4D-ND	-3.10	1.33	1.37
13	b	813	CLA	CHC-C1C	3.10	1.42	1.35
13	e	809	CLA	CHC-C1C	3.09	1.42	1.35
13	G	823	CLA	C4D-ND	-3.09	1.33	1.37
13	b	835	CLA	CHC-C1C	3.09	1.42	1.35
13	E	817	CLA	C4D-ND	-3.09	1.33	1.37
13	b	834	CLA	C4D-ND	-3.09	1.33	1.37
13	g	816	CLA	CHC-C1C	3.09	1.42	1.35
13	a	817	CLA	C4D-ND	-3.09	1.33	1.37
15	G	844	BCR	C30-C25	-3.09	1.49	1.53
13	E	827	CLA	CHC-C1C	3.09	1.42	1.35
13	g	827	CLA	CHC-C1C	3.09	1.42	1.35
13	E	805	CLA	C4D-ND	-3.09	1.33	1.37
13	A	810	CLA	CHC-C1C	3.09	1.42	1.35
13	A	827	CLA	CHC-C1C	3.09	1.42	1.35
13	b	802	CLA	C4D-ND	-3.09	1.33	1.37
13	G	834	CLA	C4D-ND	-3.09	1.33	1.37
13	G	824	CLA	CHC-C1C	3.09	1.42	1.35
15	L	205	BCR	C1-C6	-3.09	1.49	1.53
13	a	815	CLA	CHC-C1C	3.09	1.42	1.35
13	A	806	CLA	CHC-C1C	3.09	1.42	1.35
13	b	836	CLA	CHC-C1C	3.09	1.42	1.35
13	e	837	CLA	CHC-C1C	3.08	1.42	1.35
13	b	821	CLA	CHC-C1C	3.08	1.42	1.35
13	G	826	CLA	CHC-C1C	3.08	1.42	1.35
13	e	826	CLA	CHC-C1C	3.08	1.42	1.35
13	b	819	CLA	CHC-C1C	3.08	1.42	1.35
13	G	822	CLA	CHC-C1C	3.08	1.42	1.35
13	g	815	CLA	CHC-C1C	3.08	1.42	1.35
13	E	815	CLA	CHC-C1C	3.08	1.42	1.35
13	g	814	CLA	CHC-C1C	3.08	1.42	1.35
13	b	812	CLA	CHC-C1C	3.08	1.42	1.35
13	A	817	CLA	C4D-ND	-3.08	1.33	1.37
13	g	825	CLA	CHC-C1C	3.08	1.42	1.35
13	e	814	CLA	C4D-ND	-3.08	1.33	1.37
13	a	827	CLA	CHC-C1C	3.08	1.42	1.35
13	e	816	CLA	C4D-ND	-3.08	1.33	1.37
13	l	201	CLA	CHC-C1C	3.08	1.42	1.35
13	B	813	CLA	CHC-C1C	3.08	1.42	1.35
13	B	835	CLA	C4D-ND	-3.08	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	807	CLA	C4D-ND	-3.07	1.33	1.37
13	a	839	CLA	CHC-C1C	3.07	1.42	1.35
13	B	826	CLA	CHC-C1C	3.07	1.42	1.35
13	E	810	CLA	CHC-C1C	3.07	1.42	1.35
13	b	824	CLA	CHC-C1C	3.07	1.42	1.35
13	b	837	CLA	CHC-C1C	3.07	1.42	1.35
13	E	818	CLA	CHC-C1C	3.07	1.42	1.35
13	a	840	CLA	C4D-ND	-3.07	1.33	1.37
13	G	837	CLA	CHC-C1C	3.07	1.42	1.35
13	a	806	CLA	CHC-C1C	3.07	1.42	1.35
13	a	844	CLA	CHC-C1C	3.07	1.42	1.35
13	O	203	CLA	C4D-ND	-3.07	1.33	1.37
13	E	844	CLA	CHC-C1C	3.07	1.42	1.35
13	G	815	CLA	CHC-C1C	3.07	1.42	1.35
13	e	806	CLA	C4D-ND	-3.07	1.33	1.37
13	G	813	CLA	CHC-C1C	3.07	1.42	1.35
13	e	805	CLA	CHC-C1C	3.07	1.42	1.35
13	e	814	CLA	CHC-C1C	3.07	1.42	1.35
13	G	820	CLA	CHC-C1C	3.07	1.42	1.35
13	A	838	CLA	CHC-C1C	3.07	1.42	1.35
13	B	838	CLA	CHC-C1C	3.07	1.42	1.35
13	e	817	CLA	CHC-C1C	3.07	1.42	1.35
13	a	810	CLA	CHC-C1C	3.07	1.42	1.35
13	b	827	CLA	CHC-C1C	3.07	1.42	1.35
13	b	822	CLA	CHC-C1C	3.06	1.42	1.35
13	B	837	CLA	C4D-ND	-3.06	1.33	1.37
13	b	833	CLA	CHC-C1C	3.06	1.42	1.35
13	A	836	CLA	CHC-C1C	3.06	1.42	1.35
15	b	842	BCR	C30-C25	-3.06	1.49	1.53
13	b	811	CLA	CHC-C1C	3.06	1.42	1.35
13	A	832	CLA	CHC-C1C	3.06	1.42	1.35
13	a	832	CLA	CHC-C1C	3.06	1.42	1.35
13	b	823	CLA	CHC-C1C	3.06	1.42	1.35
13	E	831	CLA	CHC-C1C	3.06	1.42	1.35
13	B	823	CLA	C4D-ND	-3.06	1.33	1.37
13	g	818	CLA	CHC-C1C	3.06	1.42	1.35
13	B	837	CLA	CHC-C1C	3.06	1.42	1.35
13	g	838	CLA	C4D-ND	-3.06	1.33	1.37
13	g	835	CLA	CHC-C1C	3.06	1.42	1.35
13	e	818	CLA	C4D-ND	-3.06	1.33	1.37
13	a	804	CLA	C4D-ND	-3.06	1.33	1.37
15	b	843	BCR	C30-C25	-3.06	1.49	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	830	CLA	C4D-ND	-3.06	1.33	1.37
13	A	818	CLA	CHC-C1C	3.06	1.42	1.35
15	s	204	BCR	C1-C6	-3.06	1.49	1.53
13	A	843	CLA	CHC-C1C	3.06	1.42	1.35
13	L	203	CLA	CHC-C1C	3.06	1.42	1.35
13	b	839	CLA	CHC-C1C	3.06	1.42	1.35
13	E	806	CLA	CHC-C1C	3.06	1.42	1.35
13	e	852	CLA	C4D-ND	-3.06	1.33	1.37
13	O	203	CLA	CHC-C1C	3.06	1.42	1.35
13	e	823	CLA	CHC-C1C	3.06	1.42	1.35
13	a	807	CLA	C4D-ND	-3.06	1.33	1.37
15	O	202	BCR	C30-C25	-3.06	1.49	1.53
15	g	844	BCR	C30-C25	-3.06	1.49	1.53
13	g	817	CLA	CHC-C1C	3.06	1.42	1.35
13	a	818	CLA	CHC-C1C	3.05	1.42	1.35
13	E	807	CLA	C4D-ND	-3.05	1.33	1.37
13	g	829	CLA	CHC-C1C	3.05	1.42	1.35
13	b	832	CLA	CHC-C1C	3.05	1.42	1.35
13	f	203	CLA	CHC-C1C	3.05	1.42	1.35
13	S	203	CLA	CHC-C1C	3.05	1.42	1.35
13	B	831	CLA	C4D-ND	-3.05	1.33	1.37
13	g	839	CLA	CHC-C1C	3.05	1.42	1.35
13	s	205	CLA	CHC-C1C	3.05	1.42	1.35
13	A	804	CLA	C4D-ND	-3.05	1.33	1.37
15	G	843	BCR	C30-C25	-3.05	1.49	1.53
13	E	808	CLA	CHC-C1C	3.05	1.42	1.35
13	S	206	CLA	CHC-C1C	3.05	1.42	1.35
13	g	841	CLA	CHC-C1C	3.05	1.42	1.35
13	b	804	CLA	C4D-ND	-3.05	1.33	1.37
13	G	809	CLA	C4D-ND	-3.05	1.33	1.37
13	G	817	CLA	CHC-C1C	3.05	1.42	1.35
13	G	840	CLA	CHC-C1C	3.05	1.42	1.35
13	g	824	CLA	CHC-C1C	3.05	1.42	1.35
13	l	204	CLA	CHC-C1C	3.05	1.42	1.35
13	E	818	CLA	C4D-ND	-3.05	1.33	1.37
13	e	820	CLA	C4D-ND	-3.05	1.33	1.37
13	e	831	CLA	CHC-C1C	3.05	1.42	1.35
13	g	821	CLA	CHC-C1C	3.05	1.42	1.35
13	A	824	CLA	CHC-C1C	3.04	1.42	1.35
13	e	842	CLA	CHC-C1C	3.04	1.42	1.35
13	E	828	CLA	CHC-C1C	3.04	1.42	1.35
13	G	835	CLA	C4D-ND	-3.04	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	832	CLA	CHC-C1C	3.04	1.42	1.35
13	A	808	CLA	CHC-C1C	3.04	1.42	1.35
13	E	803	CLA	CHC-C1C	3.04	1.42	1.35
13	e	807	CLA	CHC-C1C	3.04	1.42	1.35
13	a	824	CLA	CHC-C1C	3.04	1.42	1.35
13	g	826	CLA	CHC-C1C	3.04	1.42	1.35
13	A	831	CLA	CHC-C1C	3.04	1.42	1.35
13	A	818	CLA	C4D-ND	-3.04	1.33	1.37
13	G	811	CLA	CHC-C1C	3.04	1.42	1.35
13	e	827	CLA	CHC-C1C	3.04	1.42	1.35
13	s	202	CLA	CHC-C1C	3.04	1.42	1.35
13	E	821	CLA	C4D-ND	-3.04	1.33	1.37
13	B	816	CLA	CHC-C1C	3.04	1.42	1.35
13	a	808	CLA	CHC-C1C	3.04	1.42	1.35
15	B	843	BCR	C30-C25	-3.04	1.49	1.53
13	E	827	CLA	C4D-ND	-3.04	1.33	1.37
13	G	823	CLA	CHC-C1C	3.04	1.42	1.35
13	B	817	CLA	CHC-C1C	3.04	1.42	1.35
13	E	811	CLA	CHC-C1C	3.04	1.42	1.35
13	a	837	CLA	CHC-C1C	3.04	1.42	1.35
13	A	827	CLA	C4D-ND	-3.04	1.33	1.37
13	g	838	CLA	CHC-C1C	3.04	1.42	1.35
13	a	845	CLA	CHC-C1C	3.04	1.42	1.35
13	B	820	CLA	CHC-C1C	3.04	1.42	1.35
13	a	831	CLA	CHC-C1C	3.04	1.42	1.35
13	e	819	CLA	CHC-C1C	3.04	1.42	1.35
13	G	825	CLA	CHC-C1C	3.03	1.42	1.35
13	G	804	CLA	C4D-ND	-3.03	1.33	1.37
13	A	828	CLA	CHC-C1C	3.03	1.42	1.35
13	G	805	CLA	CHC-C1C	3.03	1.42	1.35
13	B	806	CLA	CHC-C1C	3.03	1.42	1.35
13	b	816	CLA	CHC-C1C	3.03	1.42	1.35
15	q	101	BCR	C30-C25	-3.03	1.49	1.53
13	r	101	CLA	C4D-ND	-3.03	1.33	1.37
13	B	812	CLA	CHC-C1C	3.03	1.42	1.35
13	B	840	CLA	CHC-C1C	3.03	1.42	1.35
13	G	816	CLA	CHC-C1C	3.03	1.42	1.35
13	g	807	CLA	CHC-C1C	3.03	1.42	1.35
13	g	836	CLA	CHC-C1C	3.03	1.42	1.35
13	a	818	CLA	C4D-ND	-3.03	1.33	1.37
13	G	829	CLA	CHC-C1C	3.03	1.42	1.35
13	g	820	CLA	CHC-C1C	3.03	1.42	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	843	CLA	CHC-C1C	3.03	1.42	1.35
13	A	819	CLA	C4D-ND	-3.03	1.33	1.37
13	K	102	CLA	C4D-ND	-3.03	1.33	1.37
13	a	813	CLA	CHC-C1C	3.03	1.42	1.35
13	E	804	CLA	C4D-ND	-3.03	1.33	1.37
13	A	820	CLA	CHC-C1C	3.03	1.42	1.35
13	g	834	CLA	CHC-C1C	3.03	1.42	1.35
13	G	812	CLA	CHC-C1C	3.03	1.42	1.35
13	B	823	CLA	CHC-C1C	3.03	1.42	1.35
13	a	811	CLA	CHC-C1C	3.03	1.42	1.35
13	B	811	CLA	CHC-C1C	3.03	1.42	1.35
13	A	805	CLA	CHC-C1C	3.02	1.42	1.35
13	A	844	CLA	CHC-C1C	3.02	1.42	1.35
13	e	830	CLA	CHC-C1C	3.02	1.42	1.35
13	B	819	CLA	CHC-C1C	3.02	1.42	1.35
13	B	833	CLA	CHC-C1C	3.02	1.42	1.35
13	G	833	CLA	CHC-C1C	3.02	1.42	1.35
13	b	834	CLA	CHC-C1C	3.02	1.42	1.35
13	g	813	CLA	CHC-C1C	3.02	1.42	1.35
13	E	812	CLA	C4D-ND	-3.02	1.33	1.37
13	e	838	CLA	C4D-ND	-3.02	1.33	1.37
13	g	824	CLA	C4D-ND	-3.02	1.33	1.37
13	a	820	CLA	CHC-C1C	3.02	1.42	1.35
13	E	819	CLA	C4D-ND	-3.02	1.33	1.37
13	E	838	CLA	CHC-C1C	3.02	1.42	1.35
13	b	818	CLA	CHC-C1C	3.02	1.42	1.35
13	B	829	CLA	CHC-C1C	3.02	1.42	1.35
13	E	837	CLA	CHC-C1C	3.02	1.42	1.35
15	a	848	BCR	C30-C25	-3.02	1.49	1.53
13	k	4002	CLA	C4D-ND	-3.02	1.33	1.37
13	A	837	CLA	CHC-C1C	3.02	1.42	1.35
13	B	835	CLA	CHC-C1C	3.02	1.42	1.35
13	G	828	CLA	CHC-C1C	3.02	1.42	1.35
13	b	828	CLA	CHC-C1C	3.02	1.42	1.35
13	g	830	CLA	CHC-C1C	3.02	1.42	1.35
13	g	812	CLA	CHC-C1C	3.02	1.42	1.35
13	b	815	CLA	CHC-C1C	3.02	1.42	1.35
13	A	813	CLA	C4D-ND	-3.02	1.33	1.37
13	G	802	CLA	C4D-ND	-3.02	1.33	1.37
13	A	826	CLA	CHC-C1C	3.02	1.42	1.35
13	E	814	CLA	CHC-C1C	3.02	1.42	1.35
13	A	819	CLA	CHC-C1C	3.02	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	821	CLA	C4D-ND	-3.01	1.33	1.37
13	E	812	CLA	CHC-C1C	3.01	1.42	1.35
13	e	836	CLA	CHC-C1C	3.01	1.42	1.35
13	b	826	CLA	CHC-C1C	3.01	1.42	1.35
13	a	821	CLA	C4D-ND	-3.01	1.33	1.37
13	A	821	CLA	CHC-C1C	3.01	1.42	1.35
13	g	801	CLA	CHC-C1C	3.01	1.42	1.35
13	E	805	CLA	CHC-C1C	3.01	1.42	1.35
13	B	825	CLA	CHC-C1C	3.01	1.42	1.35
13	b	810	CLA	CHC-C1C	3.01	1.42	1.35
13	b	830	CLA	CHC-C1C	3.01	1.42	1.35
13	a	814	CLA	C4D-ND	-3.01	1.33	1.37
13	a	819	CLA	C4D-ND	-3.01	1.33	1.37
13	e	835	CLA	CHC-C1C	3.01	1.42	1.35
13	G	837	CLA	C4D-ND	-3.01	1.33	1.37
13	B	828	CLA	CHC-C1C	3.01	1.42	1.35
13	e	804	CLA	CHC-C1C	3.01	1.42	1.35
13	e	811	CLA	CHC-C1C	3.01	1.42	1.35
13	a	813	CLA	C4D-ND	-3.01	1.33	1.37
13	a	835	CLA	CHC-C1C	3.01	1.42	1.35
13	b	805	CLA	CHC-C1C	3.01	1.42	1.35
15	E	849	BCR	C30-C25	-3.01	1.49	1.53
13	e	818	CLA	CHC-C1C	3.01	1.42	1.35
13	e	852	CLA	CHC-C1C	3.01	1.42	1.35
13	e	810	CLA	CHC-C1C	3.01	1.42	1.35
13	a	827	CLA	C4D-ND	-3.01	1.33	1.37
15	A	847	BCR	C30-C25	-3.01	1.49	1.53
13	E	826	CLA	CHC-C1C	3.01	1.42	1.35
13	g	828	CLA	CHC-C1C	3.01	1.42	1.35
15	B	844	BCR	C30-C25	-3.01	1.49	1.53
13	R	102	CLA	C4D-ND	-3.01	1.33	1.37
13	E	846	CLA	CHC-C1C	3.01	1.42	1.35
13	E	813	CLA	CHC-C1C	3.00	1.42	1.35
13	G	835	CLA	CHC-C1C	3.00	1.42	1.35
13	A	853	CLA	C4D-ND	-3.00	1.33	1.37
13	a	828	CLA	CHC-C1C	3.00	1.42	1.35
13	A	804	CLA	CHC-C1C	3.00	1.42	1.35
13	B	810	CLA	CHC-C1C	3.00	1.42	1.35
13	g	822	CLA	CHC-C1C	3.00	1.42	1.35
13	a	830	CLA	CHC-C1C	3.00	1.42	1.35
13	A	811	CLA	CHC-C1C	3.00	1.42	1.35
13	A	830	CLA	CHC-C1C	3.00	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	819	CLA	CHC-C1C	3.00	1.42	1.35
13	a	812	CLA	CHC-C1C	3.00	1.42	1.35
13	G	810	CLA	CHC-C1C	3.00	1.42	1.35
13	b	820	CLA	CHC-C1C	3.00	1.42	1.35
13	G	831	CLA	CHC-C1C	3.00	1.42	1.35
13	a	821	CLA	CHC-C1C	3.00	1.42	1.35
13	a	826	CLA	CHC-C1C	3.00	1.42	1.35
13	E	804	CLA	CHC-C1C	3.00	1.42	1.35
13	e	820	CLA	CHC-C1C	3.00	1.42	1.35
13	f	203	CLA	C4D-ND	-3.00	1.33	1.37
13	e	825	CLA	CHC-C1C	3.00	1.42	1.35
13	a	812	CLA	C4D-ND	-3.00	1.33	1.37
13	B	827	CLA	CHC-C1C	3.00	1.42	1.35
13	E	819	CLA	CHC-C1C	3.00	1.42	1.35
13	E	840	CLA	CHC-C1C	3.00	1.42	1.35
13	E	830	CLA	CHC-C1C	3.00	1.42	1.35
13	a	805	CLA	CHC-C1C	2.99	1.42	1.35
13	A	853	CLA	CHC-C1C	2.99	1.42	1.35
13	A	813	CLA	CHC-C1C	2.99	1.42	1.35
13	B	805	CLA	C4D-ND	-2.99	1.33	1.37
13	E	820	CLA	CHC-C1C	2.99	1.42	1.35
13	A	817	CLA	CHC-C1C	2.99	1.42	1.35
13	A	826	CLA	C4D-ND	-2.99	1.33	1.37
13	E	839	CLA	C4D-ND	-2.99	1.33	1.37
13	e	811	CLA	C4D-ND	-2.99	1.33	1.37
13	g	806	CLA	C4D-ND	-2.99	1.33	1.37
13	B	821	CLA	CHC-C1C	2.99	1.42	1.35
13	g	832	CLA	CHC-C1C	2.99	1.42	1.35
13	B	832	CLA	CHC-C1C	2.99	1.42	1.35
13	e	829	CLA	CHC-C1C	2.99	1.42	1.35
13	E	817	CLA	CHC-C1C	2.99	1.42	1.35
13	E	825	CLA	C4D-ND	-2.99	1.33	1.37
13	G	802	CLA	CHC-C1C	2.99	1.42	1.35
13	g	802	CLA	CHC-C1C	2.99	1.42	1.35
13	A	812	CLA	CHC-C1C	2.99	1.42	1.35
13	a	804	CLA	CHC-C1C	2.99	1.42	1.35
13	a	819	CLA	CHC-C1C	2.99	1.42	1.35
13	B	801	CLA	CHC-C1C	2.99	1.42	1.35
13	e	824	CLA	C4D-ND	-2.99	1.33	1.37
13	A	839	CLA	CHC-C1C	2.99	1.42	1.35
13	B	802	CLA	CHC-C1C	2.99	1.42	1.35
13	E	821	CLA	CHC-C1C	2.99	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	803	CLA	C4D-ND	-2.98	1.33	1.37
13	r	102	CLA	C4D-ND	-2.98	1.33	1.37
15	E	801	BCR	C30-C25	-2.98	1.49	1.53
13	e	812	CLA	C4D-ND	-2.98	1.33	1.37
13	G	821	CLA	CHC-C1C	2.98	1.42	1.35
13	E	845	CLA	CHC-C1C	2.98	1.42	1.35
13	e	812	CLA	CHC-C1C	2.98	1.42	1.35
13	a	814	CLA	CHC-C1C	2.98	1.42	1.35
13	b	802	CLA	CHC-C1C	2.98	1.42	1.35
13	G	801	CLA	CHC-C1C	2.98	1.42	1.35
13	e	817	CLA	C4D-ND	-2.98	1.33	1.37
13	e	826	CLA	C4D-ND	-2.98	1.33	1.37
13	A	814	CLA	CHC-C1C	2.98	1.42	1.35
13	F	202	CLA	CHC-C1C	2.98	1.42	1.35
13	L	204	CLA	CHC-C1C	2.98	1.42	1.35
13	A	803	CLA	CHC-C1C	2.98	1.42	1.35
13	G	827	CLA	CHC-C1C	2.98	1.42	1.35
13	E	834	CLA	CHC-C1C	2.98	1.42	1.35
13	e	838	CLA	CHC-C1C	2.98	1.42	1.35
13	e	816	CLA	CHC-C1C	2.98	1.42	1.35
13	a	840	CLA	CHC-C1C	2.98	1.42	1.35
13	G	839	CLA	CHC-C1C	2.98	1.42	1.35
13	g	833	CLA	CHC-C1C	2.98	1.42	1.35
13	E	829	CLA	CHC-C1C	2.98	1.42	1.35
13	s	203	CLA	CHC-C1C	2.98	1.42	1.35
13	A	834	CLA	CHC-C1C	2.98	1.42	1.35
13	e	833	CLA	CHC-C1C	2.98	1.42	1.35
13	g	840	CLA	CHC-C1C	2.98	1.42	1.35
13	a	826	CLA	C4D-ND	-2.98	1.33	1.37
13	b	809	CLA	CHC-C1C	2.98	1.42	1.35
13	g	811	CLA	CHC-C1C	2.98	1.42	1.35
13	a	838	CLA	CHC-C1C	2.97	1.42	1.35
13	E	813	CLA	C4D-ND	-2.97	1.33	1.37
13	E	816	CLA	CHC-C1C	2.97	1.42	1.35
13	B	831	CLA	CHC-C1C	2.97	1.42	1.35
13	B	839	CLA	CHC-C1C	2.97	1.42	1.35
13	G	832	CLA	CHC-C1C	2.97	1.42	1.35
13	E	814	CLA	C4D-ND	-2.97	1.33	1.37
13	a	817	CLA	CHC-C1C	2.97	1.42	1.35
13	a	816	CLA	CHC-C1C	2.97	1.42	1.35
13	e	813	CLA	CHC-C1C	2.97	1.42	1.35
13	e	815	CLA	CHC-C1C	2.97	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	834	CLA	CHC-C1C	2.97	1.42	1.35
13	E	835	CLA	CHC-C1C	2.97	1.42	1.35
13	e	828	CLA	CHC-C1C	2.97	1.42	1.35
15	Q	101	BCR	C30-C25	-2.96	1.49	1.53
13	A	829	CLA	CHC-C1C	2.96	1.42	1.35
13	A	809	CLA	CHC-C1C	2.96	1.42	1.35
13	A	814	CLA	C4D-ND	-2.96	1.33	1.37
13	K	101	CLA	C4D-ND	-2.96	1.33	1.37
13	E	826	CLA	C4D-ND	-2.96	1.33	1.37
13	b	801	CLA	CHC-C1C	2.96	1.42	1.35
13	G	809	CLA	CHC-C1C	2.96	1.42	1.35
13	o	202	CLA	CHC-C1C	2.96	1.42	1.35
13	A	825	CLA	C4D-ND	-2.96	1.33	1.37
13	e	837	CLA	C4D-ND	-2.96	1.33	1.37
13	a	825	CLA	CHC-C1C	2.96	1.42	1.35
13	b	831	CLA	CHC-C1C	2.96	1.42	1.35
13	l	205	CLA	CHC-C1C	2.96	1.42	1.35
13	a	825	CLA	C4D-ND	-2.96	1.33	1.37
13	e	808	CLA	CHC-C1C	2.96	1.42	1.35
13	g	842	CLA	CHC-C1C	2.96	1.42	1.35
13	a	809	CLA	CHC-C1C	2.96	1.42	1.35
15	e	846	BCR	C30-C25	-2.96	1.49	1.53
13	G	803	CLA	CHC-C1C	2.96	1.42	1.35
13	S	204	CLA	CHC-C1C	2.96	1.42	1.35
13	e	824	CLA	CHC-C1C	2.96	1.42	1.35
13	K	102	CLA	CHC-C1C	2.96	1.42	1.35
13	k	4002	CLA	CHC-C1C	2.96	1.42	1.35
13	A	842	CLA	C4D-ND	-2.96	1.33	1.37
13	R	102	CLA	CHC-C1C	2.95	1.42	1.35
15	f	202	BCR	C1-C6	-2.95	1.49	1.53
15	a	849	BCR	C30-C25	-2.95	1.49	1.53
13	B	841	CLA	CHC-C1C	2.95	1.42	1.35
13	r	102	CLA	CHC-C1C	2.95	1.42	1.35
13	g	805	CLA	CHC-C1C	2.95	1.42	1.35
13	g	809	CLA	CHC-C1C	2.95	1.42	1.35
13	A	819	CLA	CMB-C2B	-2.95	1.45	1.51
13	e	813	CLA	C4D-ND	-2.95	1.33	1.37
13	A	825	CLA	CHC-C1C	2.95	1.42	1.35
13	B	805	CLA	CHC-C1C	2.95	1.42	1.35
13	e	825	CLA	C4D-ND	-2.95	1.33	1.37
13	A	816	CLA	CHC-C1C	2.95	1.42	1.35
13	e	803	CLA	CHC-C1C	2.95	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	819	CLA	C4D-ND	-2.95	1.33	1.37
15	j	101	BCR	C30-C25	-2.95	1.49	1.53
13	g	806	CLA	CHC-C1C	2.95	1.42	1.35
13	b	803	CLA	CHC-C1C	2.95	1.42	1.35
13	G	804	CLA	CHC-C1C	2.94	1.42	1.35
15	J	101	BCR	C30-C25	-2.94	1.49	1.53
13	A	820	CLA	C4D-ND	-2.94	1.33	1.37
13	E	807	CLA	CHC-C1C	2.94	1.42	1.35
13	g	803	CLA	CHC-C1C	2.94	1.42	1.35
13	G	807	CLA	CHC-C1C	2.94	1.42	1.35
13	b	840	CLA	CHC-C1C	2.94	1.42	1.35
13	A	812	CLA	C4D-ND	-2.94	1.33	1.37
13	e	834	CLA	CHC-C1C	2.94	1.42	1.35
13	A	803	CLA	C4D-ND	-2.94	1.33	1.37
13	E	822	CLA	CHC-C1C	2.94	1.42	1.35
13	e	821	CLA	CHC-C1C	2.94	1.42	1.35
13	a	829	CLA	CHC-C1C	2.94	1.42	1.35
13	E	825	CLA	CHC-C1C	2.94	1.42	1.35
13	a	822	CLA	CHC-C1C	2.94	1.42	1.35
13	G	841	CLA	CHC-C1C	2.93	1.42	1.35
13	A	822	CLA	CHC-C1C	2.93	1.42	1.35
13	A	807	CLA	CHC-C1C	2.93	1.42	1.35
13	E	809	CLA	CHC-C1C	2.93	1.42	1.35
13	A	838	CLA	C4D-ND	-2.93	1.33	1.37
13	b	829	CLA	CHC-C1C	2.93	1.42	1.35
13	a	820	CLA	C4D-ND	-2.93	1.33	1.37
13	B	804	CLA	CHC-C1C	2.93	1.42	1.35
13	b	807	CLA	CHC-C1C	2.92	1.42	1.35
13	b	838	CLA	CHC-C1C	2.92	1.42	1.35
13	E	820	CLA	C4D-ND	-2.92	1.33	1.37
13	a	819	CLA	CMB-C2B	-2.92	1.45	1.51
13	e	818	CLA	CMB-C2B	-2.92	1.45	1.51
13	b	804	CLA	CHC-C1C	2.92	1.42	1.35
13	A	835	CLA	CHC-C1C	2.92	1.42	1.35
15	l	206	BCR	C30-C25	-2.92	1.49	1.53
13	a	836	CLA	CHC-C1C	2.92	1.42	1.35
13	E	819	CLA	CMB-C2B	-2.92	1.45	1.51
13	a	839	CLA	C4D-ND	-2.92	1.33	1.37
13	a	843	CLA	C4D-ND	-2.92	1.33	1.37
13	e	806	CLA	CHC-C1C	2.92	1.42	1.35
13	B	830	CLA	CHC-C1C	2.92	1.42	1.35
13	E	846	CLA	C4D-ND	-2.92	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	807	CLA	CHC-C1C	2.91	1.42	1.35
13	G	830	CLA	CHC-C1C	2.91	1.42	1.35
13	a	841	CLA	CHC-C1C	2.90	1.42	1.35
13	e	839	CLA	CHC-C1C	2.90	1.42	1.35
13	K	101	CLA	CHC-C1C	2.90	1.42	1.35
13	A	845	CLA	CHC-C1C	2.90	1.42	1.35
13	F	202	CLA	C4D-ND	-2.90	1.33	1.37
13	r	101	CLA	CHC-C1C	2.89	1.42	1.35
13	B	808	CLA	CHC-C1C	2.89	1.42	1.35
13	A	840	CLA	CHC-C1C	2.89	1.42	1.35
13	E	843	CLA	C4D-ND	-2.89	1.33	1.37
13	G	836	CLA	C4D-ND	-2.89	1.33	1.37
13	g	825	CLA	C4D-ND	-2.89	1.33	1.37
13	g	837	CLA	C4D-ND	-2.89	1.33	1.37
13	e	844	CLA	CHC-C1C	2.89	1.42	1.35
13	a	852	CLA	C4D-ND	-2.89	1.33	1.37
13	G	824	CLA	C4D-ND	-2.88	1.33	1.37
15	R	101	BCR	C30-C25	-2.88	1.49	1.53
15	a	802	BCR	C30-C25	-2.88	1.49	1.53
13	E	836	CLA	CHC-C1C	2.88	1.42	1.35
15	E	852	BCR	C30-C25	-2.88	1.49	1.53
13	g	831	CLA	CHC-C1C	2.88	1.42	1.35
13	E	841	CLA	CHC-C1C	2.88	1.42	1.35
13	o	202	CLA	C4D-ND	-2.88	1.33	1.37
15	J	102	BCR	C30-C25	-2.88	1.49	1.53
13	A	841	CLA	CHC-C1C	2.87	1.42	1.35
13	B	809	CLA	CHC-C1C	2.87	1.42	1.35
13	B	836	CLA	C4D-ND	-2.87	1.33	1.37
13	b	823	CLA	C4D-ND	-2.87	1.33	1.37
13	e	840	CLA	CHC-C1C	2.87	1.42	1.35
13	b	835	CLA	C4D-ND	-2.87	1.33	1.37
13	E	842	CLA	CHC-C1C	2.86	1.42	1.35
13	e	841	CLA	C4D-ND	-2.86	1.33	1.37
13	G	808	CLA	CHC-C1C	2.85	1.42	1.35
13	a	842	CLA	CHC-C1C	2.85	1.42	1.35
13	B	824	CLA	C4D-ND	-2.85	1.33	1.37
13	b	808	CLA	CHC-C1C	2.84	1.42	1.35
13	g	810	CLA	CHC-C1C	2.84	1.42	1.35
15	a	853	BCR	C30-C25	-2.83	1.49	1.53
15	q	102	BCR	C30-C25	-2.83	1.49	1.53
12	A	801	LHG	O7-C5	-2.83	1.39	1.46
15	L	205	BCR	C30-C25	-2.81	1.49	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	e	801	LHG	O7-C5	-2.78	1.39	1.46
12	e	802	LHG	O7-C5	-2.77	1.39	1.46
13	a	852	CLA	CHC-C1C	2.77	1.42	1.35
15	R	101	BCR	C38-C26	-2.77	1.46	1.50
13	b	834	CLA	CMB-C2B	-2.76	1.45	1.51
15	A	850	BCR	C30-C25	-2.75	1.50	1.53
15	e	849	BCR	C30-C25	-2.74	1.50	1.53
13	B	835	CLA	CMB-C2B	-2.73	1.46	1.51
13	G	835	CLA	CMB-C2B	-2.73	1.46	1.51
13	g	836	CLA	CMB-C2B	-2.73	1.46	1.51
13	E	826	CLA	CMB-C2B	-2.71	1.46	1.51
15	m	101	BCR	C1-C6	-2.71	1.50	1.53
13	b	838	CLA	CMB-C2B	-2.70	1.46	1.51
13	a	826	CLA	CMB-C2B	-2.69	1.46	1.51
13	A	826	CLA	CMB-C2B	-2.69	1.46	1.51
15	S	205	BCR	C30-C25	-2.69	1.50	1.53
13	l	204	CLA	CMB-C2B	-2.69	1.46	1.51
13	G	810	CLA	CMB-C2B	-2.69	1.46	1.51
13	a	816	CLA	CMB-C2B	-2.69	1.46	1.51
12	A	802	LHG	O7-C5	-2.68	1.39	1.46
13	E	816	CLA	CMB-C2B	-2.68	1.46	1.51
13	g	840	CLA	CMB-C2B	-2.68	1.46	1.51
13	e	825	CLA	CMB-C2B	-2.68	1.46	1.51
13	A	816	CLA	CMB-C2B	-2.67	1.46	1.51
13	B	811	CLA	CMB-C2B	-2.67	1.46	1.51
13	s	202	CLA	CMB-C2B	-2.67	1.46	1.51
13	G	839	CLA	CMB-C2B	-2.67	1.46	1.51
13	b	810	CLA	CMB-C2B	-2.66	1.46	1.51
15	e	851	BCR	C30-C25	-2.66	1.50	1.53
13	B	820	CLA	CMB-C2B	-2.65	1.46	1.51
13	E	842	CLA	CMB-C2B	-2.65	1.46	1.51
13	A	840	CLA	CMB-C2B	-2.65	1.46	1.51
13	E	841	CLA	CMB-C2B	-2.65	1.46	1.51
13	g	812	CLA	CMB-C2B	-2.65	1.46	1.51
13	a	824	CLA	CMB-C2B	-2.65	1.46	1.51
13	e	823	CLA	CMB-C2B	-2.65	1.46	1.51
13	B	839	CLA	CMB-C2B	-2.64	1.46	1.51
13	e	815	CLA	CMB-C2B	-2.64	1.46	1.51
13	e	840	CLA	CMB-C2B	-2.64	1.46	1.51
13	L	203	CLA	CMB-C2B	-2.64	1.46	1.51
13	S	203	CLA	CMB-C2B	-2.64	1.46	1.51
13	E	824	CLA	CMB-C2B	-2.63	1.46	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	835	CLA	CMB-C2B	-2.63	1.46	1.51
13	b	819	CLA	CMB-C2B	-2.63	1.46	1.51
15	A	852	BCR	C30-C25	-2.63	1.50	1.53
13	A	845	CLA	CMB-C2B	-2.63	1.46	1.51
13	g	803	CLA	CMB-C2B	-2.63	1.46	1.51
13	B	808	CLA	CMB-C2B	-2.63	1.46	1.51
15	s	204	BCR	C30-C25	-2.62	1.50	1.53
13	B	840	CLA	CMB-C2B	-2.62	1.46	1.51
13	a	842	CLA	CMB-C2B	-2.62	1.46	1.51
13	A	841	CLA	CMB-C2B	-2.62	1.46	1.51
13	g	807	CLA	CMB-C2B	-2.62	1.46	1.51
13	a	845	CLA	CMB-C2B	-2.62	1.46	1.51
13	G	840	CLA	CMB-C2B	-2.62	1.46	1.51
13	b	839	CLA	CMB-C2B	-2.62	1.46	1.51
13	e	844	CLA	CMB-C2B	-2.62	1.46	1.51
13	G	804	CLA	CMB-C2B	-2.62	1.46	1.51
13	a	841	CLA	CMB-C2B	-2.62	1.46	1.51
13	b	805	CLA	CMB-C2B	-2.62	1.46	1.51
13	B	829	CLA	CMB-C2B	-2.62	1.46	1.51
13	E	845	CLA	CMB-C2B	-2.62	1.46	1.51
13	B	802	CLA	CMB-C2B	-2.61	1.46	1.51
13	E	809	CLA	CMB-C2B	-2.61	1.46	1.51
13	b	807	CLA	CMB-C2B	-2.61	1.46	1.51
13	b	828	CLA	CMB-C2B	-2.61	1.46	1.51
13	A	818	CLA	CMB-C2B	-2.61	1.46	1.51
13	e	808	CLA	CMB-C2B	-2.61	1.46	1.51
13	b	801	CLA	CMB-C2B	-2.61	1.46	1.51
13	a	809	CLA	CMB-C2B	-2.61	1.46	1.51
13	b	833	CLA	CMB-C2B	-2.61	1.46	1.51
13	B	834	CLA	CMB-C2B	-2.61	1.46	1.51
13	E	829	CLA	CMB-C2B	-2.61	1.46	1.51
13	b	808	CLA	CMB-C2B	-2.61	1.46	1.51
13	G	820	CLA	CMB-C2B	-2.61	1.46	1.51
13	G	801	CLA	CMB-C2B	-2.61	1.46	1.51
13	g	841	CLA	CMB-C2B	-2.61	1.46	1.51
13	A	831	CLA	CMB-C2B	-2.61	1.46	1.51
13	G	829	CLA	CMB-C2B	-2.61	1.46	1.51
13	e	839	CLA	CMB-C2B	-2.61	1.46	1.51
13	E	831	CLA	CMB-C2B	-2.61	1.46	1.51
13	B	809	CLA	CMB-C2B	-2.60	1.46	1.51
13	B	818	CLA	CMB-C2B	-2.60	1.46	1.51
13	g	810	CLA	CMB-C2B	-2.60	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	840	CLA	CMB-C2B	-2.60	1.46	1.51
13	b	814	CLA	CMB-C2B	-2.60	1.46	1.51
13	A	829	CLA	CMB-C2B	-2.60	1.46	1.51
13	g	814	CLA	CMB-C2B	-2.60	1.46	1.51
13	A	809	CLA	CMB-C2B	-2.60	1.46	1.51
13	g	809	CLA	CMB-C2B	-2.60	1.46	1.51
13	E	818	CLA	CMB-C2B	-2.60	1.46	1.51
13	G	815	CLA	CMB-C2B	-2.60	1.46	1.51
13	a	835	CLA	CMB-C2B	-2.60	1.46	1.51
13	B	806	CLA	CMB-C2B	-2.60	1.46	1.51
13	B	830	CLA	CMB-C2B	-2.60	1.46	1.51
13	b	817	CLA	CMB-C2B	-2.60	1.46	1.51
13	e	843	CLA	CMB-C2B	-2.59	1.46	1.51
13	g	830	CLA	CMB-C2B	-2.59	1.46	1.51
13	a	829	CLA	CMB-C2B	-2.59	1.46	1.51
13	B	805	CLA	CMB-C2B	-2.59	1.46	1.51
13	g	821	CLA	CMB-C2B	-2.59	1.46	1.51
13	G	834	CLA	CMB-C2B	-2.59	1.46	1.51
13	G	808	CLA	CMB-C2B	-2.59	1.46	1.51
13	A	824	CLA	CMB-C2B	-2.59	1.46	1.51
13	B	813	CLA	CMB-C2B	-2.59	1.46	1.51
13	e	830	CLA	CMB-C2B	-2.59	1.46	1.51
13	g	802	CLA	CMB-C2B	-2.58	1.46	1.51
13	g	806	CLA	CMB-C2B	-2.58	1.46	1.51
13	g	831	CLA	CMB-C2B	-2.58	1.46	1.51
13	a	831	CLA	CMB-C2B	-2.58	1.46	1.51
13	E	835	CLA	CMB-C2B	-2.58	1.46	1.51
13	e	817	CLA	CMB-C2B	-2.58	1.46	1.51
13	e	828	CLA	CMB-C2B	-2.57	1.46	1.51
13	g	822	CLA	CMB-C2B	-2.57	1.46	1.51
13	G	807	CLA	CMB-C2B	-2.57	1.46	1.51
13	a	817	CLA	CMB-C2B	-2.57	1.46	1.51
13	B	801	CLA	CMB-C2B	-2.57	1.46	1.51
13	g	819	CLA	CMB-C2B	-2.57	1.46	1.51
13	B	815	CLA	CMB-C2B	-2.57	1.46	1.51
13	g	808	CLA	CMB-C2B	-2.56	1.46	1.51
13	e	824	CLA	CMB-C2B	-2.56	1.46	1.51
13	E	817	CLA	CMB-C2B	-2.56	1.46	1.51
13	G	841	CLA	CMB-C2B	-2.56	1.46	1.51
13	E	805	CLA	CMB-C2B	-2.56	1.46	1.51
13	G	818	CLA	CMB-C2B	-2.56	1.46	1.51
13	b	804	CLA	CMB-C2B	-2.56	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	812	CLA	CMB-C2B	-2.56	1.46	1.51
13	G	813	CLA	CMB-C2B	-2.56	1.46	1.51
13	A	817	CLA	CMB-C2B	-2.56	1.46	1.51
13	B	807	CLA	CMB-C2B	-2.56	1.46	1.51
13	G	821	CLA	CMB-C2B	-2.56	1.46	1.51
13	G	830	CLA	CMB-C2B	-2.55	1.46	1.51
15	k	4001	BCR	C1-C6	-2.55	1.50	1.53
13	g	842	CLA	CMB-C2B	-2.55	1.46	1.51
13	G	805	CLA	CMB-C2B	-2.55	1.46	1.51
13	G	828	CLA	CMB-C2B	-2.55	1.46	1.51
13	b	806	CLA	CMB-C2B	-2.55	1.46	1.51
13	B	841	CLA	CMB-C2B	-2.55	1.46	1.51
13	B	804	CLA	CMB-C2B	-2.55	1.46	1.51
13	g	805	CLA	CMB-C2B	-2.55	1.46	1.51
13	g	816	CLA	CMB-C2B	-2.55	1.46	1.51
13	E	837	CLA	CMB-C2B	-2.55	1.46	1.51
13	G	803	CLA	CMB-C2B	-2.55	1.46	1.51
13	G	827	CLA	CMB-C2B	-2.55	1.46	1.51
13	A	844	CLA	CMB-C2B	-2.55	1.46	1.51
13	a	805	CLA	CMB-C2B	-2.55	1.46	1.51
13	o	202	CLA	CMB-C2B	-2.54	1.46	1.51
13	a	814	CLA	CMB-C2B	-2.54	1.46	1.51
13	e	816	CLA	CMB-C2B	-2.54	1.46	1.51
13	e	835	CLA	CMB-C2B	-2.54	1.46	1.51
13	E	825	CLA	CMB-C2B	-2.54	1.46	1.51
13	e	813	CLA	CMB-C2B	-2.54	1.46	1.51
13	a	837	CLA	CMB-C2B	-2.54	1.46	1.51
13	b	803	CLA	CMB-C2B	-2.54	1.46	1.51
13	g	828	CLA	CMB-C2B	-2.54	1.46	1.51
13	a	812	CLA	CMB-C2B	-2.54	1.46	1.51
13	a	818	CLA	CMB-C2B	-2.54	1.46	1.51
13	e	807	CLA	CMB-C2B	-2.54	1.46	1.51
13	b	820	CLA	CMB-C2B	-2.54	1.46	1.51
13	B	838	CLA	CMB-C2B	-2.54	1.46	1.51
13	g	818	CLA	CMB-C2B	-2.54	1.46	1.51
13	B	827	CLA	CMB-C2B	-2.54	1.46	1.51
13	a	807	CLA	CMB-C2B	-2.54	1.46	1.51
13	e	837	CLA	CMB-C2B	-2.54	1.46	1.51
13	g	801	CLA	CMB-C2B	-2.54	1.46	1.51
13	b	826	CLA	CMB-C2B	-2.54	1.46	1.51
13	e	827	CLA	CMB-C2B	-2.54	1.46	1.51
13	A	804	CLA	CMB-C2B	-2.53	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	828	CLA	CMB-C2B	-2.53	1.46	1.51
13	E	814	CLA	CMB-C2B	-2.53	1.46	1.51
13	E	822	CLA	CMB-C2B	-2.53	1.46	1.51
13	g	829	CLA	CMB-C2B	-2.53	1.46	1.51
13	A	812	CLA	CMB-C2B	-2.53	1.46	1.51
13	B	824	CLA	CMB-C2B	-2.53	1.46	1.51
13	G	832	CLA	CMB-C2B	-2.53	1.46	1.51
13	A	807	CLA	CMB-C2B	-2.53	1.46	1.51
13	b	829	CLA	CMB-C2B	-2.53	1.46	1.51
13	E	807	CLA	CMB-C2B	-2.53	1.46	1.51
13	a	822	CLA	CMB-C2B	-2.53	1.46	1.51
13	B	821	CLA	CMB-C2B	-2.53	1.46	1.51
13	G	806	CLA	CMB-C2B	-2.53	1.46	1.51
13	G	823	CLA	CMB-C2B	-2.53	1.46	1.51
13	e	806	CLA	CMB-C2B	-2.53	1.46	1.51
13	G	817	CLA	CMB-C2B	-2.53	1.46	1.51
13	e	819	CLA	CMB-C2B	-2.53	1.46	1.51
13	A	834	CLA	CMB-C2B	-2.53	1.46	1.51
13	a	852	CLA	CMB-C2B	-2.53	1.46	1.51
13	A	820	CLA	CMB-C2B	-2.52	1.46	1.51
13	s	205	CLA	CMB-C2B	-2.52	1.46	1.51
13	A	808	CLA	CMB-C2B	-2.52	1.46	1.51
13	g	827	CLA	CMB-C2B	-2.52	1.46	1.51
13	b	831	CLA	CMB-C2B	-2.52	1.46	1.51
13	A	805	CLA	CMB-C2B	-2.52	1.46	1.51
13	g	820	CLA	CMB-C2B	-2.52	1.46	1.51
13	g	833	CLA	CMB-C2B	-2.52	1.46	1.51
13	E	815	CLA	CMB-C2B	-2.52	1.46	1.51
13	e	814	CLA	CMB-C2B	-2.52	1.46	1.51
13	e	809	CLA	CMB-C2B	-2.52	1.46	1.51
13	A	814	CLA	CMB-C2B	-2.52	1.46	1.51
13	a	804	CLA	CMB-C2B	-2.52	1.46	1.51
13	A	825	CLA	CMB-C2B	-2.52	1.46	1.51
13	e	833	CLA	CMB-C2B	-2.52	1.46	1.51
13	g	825	CLA	CMB-C2B	-2.52	1.46	1.51
13	E	808	CLA	CMB-C2B	-2.52	1.46	1.51
13	e	811	CLA	CMB-C2B	-2.51	1.46	1.51
13	a	834	CLA	CMB-C2B	-2.51	1.46	1.51
13	b	815	CLA	CMB-C2B	-2.51	1.46	1.51
13	e	829	CLA	CMB-C2B	-2.51	1.46	1.51
13	b	827	CLA	CMB-C2B	-2.51	1.46	1.51
13	E	821	CLA	CMB-C2B	-2.51	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	818	CLA	CMB-C2B	-2.51	1.46	1.51
13	b	825	CLA	CMB-C2B	-2.51	1.46	1.51
13	A	836	CLA	CMB-C2B	-2.51	1.46	1.51
13	G	824	CLA	CMB-C2B	-2.51	1.46	1.51
13	g	832	CLA	CMB-C2B	-2.51	1.46	1.51
13	a	830	CLA	CMB-C2B	-2.51	1.46	1.51
13	E	840	CLA	CMB-C2B	-2.51	1.46	1.51
13	A	828	CLA	CMB-C2B	-2.51	1.46	1.51
13	e	821	CLA	CMB-C2B	-2.51	1.46	1.51
13	A	838	CLA	CMB-C2B	-2.51	1.46	1.51
13	B	823	CLA	CMB-C2B	-2.51	1.46	1.51
13	a	815	CLA	CMB-C2B	-2.51	1.46	1.51
13	A	810	CLA	CMB-C2B	-2.51	1.46	1.51
13	a	810	CLA	CMB-C2B	-2.51	1.46	1.51
13	f	203	CLA	CMB-C2B	-2.51	1.46	1.51
13	E	820	CLA	CMB-C2B	-2.50	1.46	1.51
13	b	816	CLA	CMB-C2B	-2.50	1.46	1.51
15	a	848	BCR	C31-C1	-2.50	1.48	1.53
13	b	823	CLA	CMB-C2B	-2.50	1.46	1.51
13	e	831	CLA	CMB-C2B	-2.50	1.46	1.51
13	F	202	CLA	CMB-C2B	-2.50	1.46	1.51
13	B	826	CLA	CMB-C2B	-2.50	1.46	1.51
13	a	825	CLA	CMB-C2B	-2.50	1.46	1.51
13	a	828	CLA	CMB-C2B	-2.50	1.46	1.51
13	K	101	CLA	CMB-C2B	-2.50	1.46	1.51
13	A	815	CLA	CMB-C2B	-2.50	1.46	1.51
13	g	817	CLA	CMB-C2B	-2.50	1.46	1.51
13	r	101	CLA	CMB-C2B	-2.50	1.46	1.51
13	a	808	CLA	CMB-C2B	-2.50	1.46	1.51
13	E	834	CLA	CMB-C2B	-2.50	1.46	1.51
13	a	811	CLA	CMB-C2B	-2.50	1.46	1.51
13	E	830	CLA	CMB-C2B	-2.50	1.46	1.51
13	G	819	CLA	CMB-C2B	-2.50	1.46	1.51
13	B	817	CLA	CMB-C2B	-2.49	1.46	1.51
13	E	827	CLA	CMB-C2B	-2.49	1.46	1.51
13	e	838	CLA	CMB-C2B	-2.49	1.46	1.51
13	B	832	CLA	CMB-C2B	-2.49	1.46	1.51
13	E	832	CLA	CMB-C2B	-2.49	1.46	1.51
13	E	828	CLA	CMB-C2B	-2.49	1.46	1.51
13	e	804	CLA	CMB-C2B	-2.49	1.46	1.51
13	b	830	CLA	CMB-C2B	-2.49	1.46	1.51
13	A	822	CLA	CMB-C2B	-2.49	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	830	CLA	CMB-C2B	-2.49	1.46	1.51
13	E	812	CLA	CMB-C2B	-2.49	1.46	1.51
13	S	206	CLA	CMB-C2B	-2.49	1.46	1.51
13	a	839	CLA	CMB-C2B	-2.49	1.46	1.51
13	G	811	CLA	CMB-C2B	-2.49	1.46	1.51
13	l	201	CLA	CMB-C2B	-2.49	1.46	1.51
13	E	810	CLA	CMB-C2B	-2.49	1.46	1.51
13	G	826	CLA	CMB-C2B	-2.49	1.46	1.51
13	G	825	CLA	CMB-C2B	-2.49	1.46	1.51
13	a	836	CLA	CMB-C2B	-2.49	1.46	1.51
13	E	804	CLA	CMB-C2B	-2.49	1.46	1.51
13	E	839	CLA	CMB-C2B	-2.49	1.46	1.51
13	e	820	CLA	CMB-C2B	-2.49	1.46	1.51
13	G	831	CLA	CMB-C2B	-2.49	1.46	1.51
13	e	836	CLA	CMB-C2B	-2.48	1.46	1.51
13	e	834	CLA	CMB-C2B	-2.48	1.46	1.51
13	B	831	CLA	CMB-C2B	-2.48	1.46	1.51
13	b	837	CLA	CMB-C2B	-2.48	1.46	1.51
13	B	819	CLA	CMB-C2B	-2.48	1.46	1.51
13	B	816	CLA	CMB-C2B	-2.48	1.46	1.51
13	e	805	CLA	CMB-C2B	-2.48	1.46	1.51
13	g	839	CLA	CMB-C2B	-2.48	1.46	1.51
13	a	820	CLA	CMB-C2B	-2.48	1.46	1.51
13	B	812	CLA	CMB-C2B	-2.48	1.46	1.51
13	g	813	CLA	CMB-C2B	-2.48	1.46	1.51
13	b	822	CLA	CMB-C2B	-2.48	1.46	1.51
13	E	811	CLA	CMB-C2B	-2.48	1.46	1.51
13	e	842	CLA	CMB-C2B	-2.48	1.46	1.51
13	b	811	CLA	CMB-C2B	-2.48	1.46	1.51
13	E	813	CLA	CMB-C2B	-2.48	1.46	1.51
13	e	826	CLA	CMB-C2B	-2.48	1.46	1.51
13	a	821	CLA	CMB-C2B	-2.48	1.46	1.51
13	E	844	CLA	CMB-C2B	-2.47	1.46	1.51
13	e	812	CLA	CMB-C2B	-2.47	1.46	1.51
13	g	811	CLA	CMB-C2B	-2.47	1.46	1.51
13	g	815	CLA	CMB-C2B	-2.47	1.46	1.51
13	A	823	CLA	CMB-C2B	-2.47	1.46	1.51
13	a	832	CLA	CMB-C2B	-2.47	1.46	1.51
13	a	840	CLA	CMB-C2B	-2.47	1.46	1.51
13	A	839	CLA	CMB-C2B	-2.47	1.46	1.51
13	b	824	CLA	CMB-C2B	-2.47	1.46	1.51
13	A	832	CLA	CMB-C2B	-2.47	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	806	CLA	CMB-C2B	-2.47	1.46	1.51
13	G	838	CLA	CMB-C2B	-2.47	1.46	1.51
13	G	809	CLA	CMB-C2B	-2.47	1.46	1.51
13	O	203	CLA	CMB-C2B	-2.47	1.46	1.51
13	b	809	CLA	CMB-C2B	-2.47	1.46	1.51
13	A	811	CLA	CMB-C2B	-2.46	1.46	1.51
13	G	816	CLA	CMB-C2B	-2.46	1.46	1.51
13	e	841	CLA	CMB-C2B	-2.46	1.46	1.51
13	E	843	CLA	CMB-C2B	-2.46	1.46	1.51
13	a	813	CLA	CMB-C2B	-2.46	1.46	1.51
13	g	824	CLA	CMB-C2B	-2.46	1.46	1.51
13	G	812	CLA	CMB-C2B	-2.46	1.46	1.51
13	e	803	CLA	CMB-C2B	-2.46	1.46	1.51
13	k	4002	CLA	CMB-C2B	-2.46	1.46	1.51
13	b	835	CLA	CMB-C2B	-2.46	1.46	1.51
13	b	802	CLA	CMB-C2B	-2.46	1.46	1.51
13	A	827	CLA	CMB-C2B	-2.45	1.46	1.51
13	a	844	CLA	CMB-C2B	-2.45	1.46	1.51
13	A	837	CLA	CMB-C2B	-2.45	1.46	1.51
13	G	814	CLA	CMB-C2B	-2.45	1.46	1.51
13	A	821	CLA	CMB-C2B	-2.45	1.46	1.51
13	B	833	CLA	CMB-C2B	-2.45	1.46	1.51
13	b	813	CLA	CMB-C2B	-2.45	1.46	1.51
13	g	834	CLA	CMB-C2B	-2.45	1.46	1.51
13	A	843	CLA	CMB-C2B	-2.45	1.46	1.51
13	B	825	CLA	CMB-C2B	-2.45	1.46	1.51
13	g	826	CLA	CMB-C2B	-2.45	1.46	1.51
13	r	102	CLA	CMB-C2B	-2.45	1.46	1.51
13	a	827	CLA	CMB-C2B	-2.45	1.46	1.51
13	E	806	CLA	CMB-C2B	-2.45	1.46	1.51
13	A	842	CLA	CMB-C2B	-2.44	1.46	1.51
13	e	832	CLA	CMB-C2B	-2.44	1.46	1.51
13	A	813	CLA	CMB-C2B	-2.44	1.46	1.51
13	a	833	CLA	CMB-C2B	-2.44	1.46	1.51
13	A	835	CLA	CMB-C2B	-2.44	1.46	1.51
13	E	836	CLA	CMB-C2B	-2.44	1.46	1.51
13	e	822	CLA	CMB-C2B	-2.44	1.46	1.51
13	L	204	CLA	CMB-C2B	-2.44	1.46	1.51
13	B	810	CLA	CMB-C2B	-2.44	1.46	1.51
13	G	802	CLA	CMB-C2B	-2.44	1.46	1.51
13	A	803	CLA	CMB-C2B	-2.44	1.46	1.51
13	g	837	CLA	CMB-C2B	-2.44	1.46	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	814	CLA	CMB-C2B	-2.44	1.46	1.51
13	a	838	CLA	CMB-C2B	-2.44	1.46	1.51
13	a	843	CLA	CMB-C2B	-2.44	1.46	1.51
13	G	837	CLA	CMB-C2B	-2.44	1.46	1.51
13	l	205	CLA	CMB-C2B	-2.43	1.46	1.51
13	B	836	CLA	CMB-C2B	-2.43	1.46	1.51
13	e	810	CLA	CMB-C2B	-2.43	1.46	1.51
13	b	832	CLA	CMB-C2B	-2.43	1.46	1.51
13	E	833	CLA	CMB-C2B	-2.43	1.46	1.51
13	G	833	CLA	CMB-C2B	-2.43	1.46	1.51
13	E	829	CLA	C3B-C2B	-2.43	1.37	1.40
13	e	828	CLA	C3B-C2B	-2.43	1.37	1.40
13	A	806	CLA	CMB-C2B	-2.43	1.46	1.51
13	A	853	CLA	CMB-C2B	-2.43	1.46	1.51
13	E	803	CLA	CMB-C2B	-2.42	1.46	1.51
13	G	836	CLA	CMB-C2B	-2.42	1.46	1.51
13	B	822	CLA	CMB-C2B	-2.42	1.46	1.51
13	b	836	CLA	CMB-C2B	-2.42	1.46	1.51
13	a	823	CLA	CMB-C2B	-2.42	1.46	1.51
13	K	102	CLA	CMB-C2B	-2.41	1.46	1.51
13	E	838	CLA	CMB-C2B	-2.41	1.46	1.51
13	A	833	CLA	CMB-C2B	-2.41	1.46	1.51
13	g	823	CLA	CMB-C2B	-2.41	1.46	1.51
13	B	837	CLA	CMB-C2B	-2.41	1.46	1.51
13	s	203	CLA	CMB-C2B	-2.41	1.46	1.51
13	G	822	CLA	CMB-C2B	-2.41	1.46	1.51
13	E	846	CLA	CMB-C2B	-2.40	1.46	1.51
13	e	852	CLA	CMB-C2B	-2.40	1.46	1.51
13	a	820	CLA	CMD-C2D	-2.40	1.45	1.50
13	R	102	CLA	CMB-C2B	-2.40	1.46	1.51
13	S	204	CLA	CMB-C2B	-2.40	1.46	1.51
13	E	820	CLA	CMD-C2D	-2.39	1.45	1.50
15	E	802	BCR	C30-C25	-2.39	1.50	1.53
13	E	823	CLA	CMB-C2B	-2.39	1.46	1.51
13	g	838	CLA	CMB-C2B	-2.39	1.46	1.51
13	A	820	CLA	CMD-C2D	-2.39	1.45	1.50
13	e	819	CLA	CMD-C2D	-2.38	1.45	1.50
13	b	821	CLA	CMB-C2B	-2.38	1.46	1.51
15	R	101	BCR	C1-C6	-2.38	1.50	1.53
13	e	820	CLA	MG-ND	-2.37	2.01	2.05
13	A	821	CLA	MG-ND	-2.37	2.01	2.05
13	L	202	CLA	CMB-C2B	-2.35	1.46	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	829	CLA	C3B-C2B	-2.34	1.37	1.40
13	E	821	CLA	MG-ND	-2.34	2.01	2.05
15	a	803	BCR	C30-C25	-2.33	1.50	1.53
13	a	821	CLA	MG-ND	-2.33	2.01	2.05
13	a	829	CLA	C3B-C2B	-2.32	1.37	1.40
13	l	203	CLA	CMB-C2B	-2.31	1.46	1.51
12	a	801	LHG	O7-C5	-2.29	1.40	1.46
13	a	842	CLA	C3B-C2B	-2.26	1.37	1.40
13	A	841	CLA	C3B-C2B	-2.26	1.37	1.40
13	E	846	CLA	CMC-C2C	-2.25	1.46	1.50
13	G	808	CLA	C3B-C2B	-2.24	1.37	1.40
13	e	824	CLA	CMD-C2D	-2.24	1.46	1.50
13	e	832	CLA	CMD-C2D	-2.23	1.46	1.50
13	E	836	CLA	CMD-C2D	-2.23	1.46	1.50
13	a	844	CLA	CMD-C2D	-2.23	1.46	1.50
13	E	844	CLA	CMD-C2D	-2.22	1.46	1.50
13	e	840	CLA	C3B-C2B	-2.22	1.37	1.40
13	g	816	CLA	CMD-C2D	-2.22	1.46	1.50
13	g	810	CLA	C3B-C2B	-2.22	1.37	1.40
13	a	833	CLA	CMD-C2D	-2.22	1.46	1.50
13	E	833	CLA	CMD-C2D	-2.21	1.46	1.50
13	E	842	CLA	C3B-C2B	-2.21	1.37	1.40
13	G	811	CLA	CMD-C2D	-2.21	1.46	1.50
13	B	815	CLA	CMD-C2D	-2.21	1.46	1.50
13	G	815	CLA	CMD-C2D	-2.21	1.46	1.50
13	A	821	CLA	C3B-CAB	-2.20	1.43	1.47
13	a	823	CLA	CMC-C2C	-2.20	1.46	1.50
13	g	841	CLA	C3B-C2B	-2.20	1.37	1.40
13	b	801	CLA	CMC-C2C	-2.20	1.46	1.50
13	g	830	CLA	CMD-C2D	-2.20	1.46	1.50
13	E	804	CLA	CMC-C2C	-2.20	1.46	1.50
13	a	823	CLA	MG-ND	-2.19	2.01	2.05
13	e	822	CLA	MG-ND	-2.19	2.01	2.05
13	A	835	CLA	CMD-C2D	-2.19	1.46	1.50
13	a	821	CLA	C3B-CAB	-2.19	1.43	1.47
13	b	828	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	833	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	843	CLA	CMD-C2D	-2.19	1.46	1.50
13	g	828	CLA	CMD-C2D	-2.19	1.46	1.50
13	g	813	CLA	CMD-C2D	-2.19	1.46	1.50
13	b	805	CLA	CMD-C2D	-2.19	1.46	1.50
13	B	802	CLA	CMC-C2C	-2.19	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	825	CLA	CMD-C2D	-2.19	1.46	1.50
13	E	814	CLA	C3B-C2B	-2.18	1.37	1.40
13	G	829	CLA	CMD-C2D	-2.18	1.46	1.50
13	L	202	CLA	CMD-C2D	-2.18	1.46	1.50
13	b	808	CLA	C3B-C2B	-2.18	1.37	1.40
13	e	834	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	814	CLA	C3B-C2B	-2.18	1.37	1.40
13	a	825	CLA	CMD-C2D	-2.18	1.46	1.50
13	E	825	CLA	CMD-C2D	-2.18	1.46	1.50
13	e	822	CLA	CMC-C2C	-2.18	1.46	1.50
13	g	803	CLA	CMC-C2C	-2.18	1.46	1.50
13	B	809	CLA	C3B-C2B	-2.18	1.37	1.40
13	e	804	CLA	CMC-C2C	-2.18	1.46	1.50
13	B	827	CLA	CMD-C2D	-2.18	1.46	1.50
13	g	806	CLA	CMD-C2D	-2.17	1.46	1.50
13	A	834	CLA	CMD-C2D	-2.17	1.46	1.50
13	E	824	CLA	CMD-C2D	-2.17	1.46	1.50
13	A	836	CLA	CMD-C2D	-2.17	1.46	1.50
13	e	820	CLA	C3B-CAB	-2.17	1.43	1.47
13	e	829	CLA	CMD-C2D	-2.17	1.46	1.50
13	G	833	CLA	CMD-C2D	-2.17	1.46	1.50
13	B	806	CLA	CMD-C2D	-2.17	1.46	1.50
13	E	837	CLA	CMD-C2D	-2.17	1.46	1.50
13	e	842	CLA	CMD-C2D	-2.17	1.46	1.50
13	b	814	CLA	CMD-C2D	-2.17	1.46	1.50
13	B	829	CLA	CMD-C2D	-2.17	1.46	1.50
13	a	804	CLA	CMC-C2C	-2.17	1.46	1.50
13	b	826	CLA	CMD-C2D	-2.17	1.46	1.50
13	A	823	CLA	CMC-C2C	-2.17	1.46	1.50
13	E	834	CLA	CMD-C2D	-2.17	1.46	1.50
13	b	833	CLA	CMD-C2D	-2.17	1.46	1.50
13	E	823	CLA	MG-ND	-2.17	2.01	2.05
13	B	805	CLA	CMD-C2D	-2.17	1.46	1.50
13	E	823	CLA	CMC-C2C	-2.16	1.46	1.50
13	e	821	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	804	CLA	CMD-C2D	-2.16	1.46	1.50
13	B	840	CLA	C3B-C2B	-2.16	1.37	1.40
13	b	832	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	823	CLA	MG-ND	-2.16	2.01	2.05
13	A	824	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	802	CLA	CMD-C2D	-2.16	1.46	1.50
13	e	813	CLA	C3B-C2B	-2.16	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	807	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	804	CLA	CMD-C2D	-2.16	1.46	1.50
13	a	830	CLA	CMD-C2D	-2.16	1.46	1.50
13	E	835	CLA	CMD-C2D	-2.16	1.46	1.50
13	s	205	CLA	CMD-C2D	-2.16	1.46	1.50
13	E	830	CLA	CMD-C2D	-2.16	1.46	1.50
13	b	807	CLA	CMD-C2D	-2.16	1.46	1.50
13	G	801	CLA	CMC-C2C	-2.16	1.46	1.50
13	e	807	CLA	CMD-C2D	-2.16	1.46	1.50
13	e	804	CLA	CMD-C2D	-2.16	1.46	1.50
13	E	804	CLA	CMD-C2D	-2.15	1.46	1.50
13	G	826	CLA	CMD-C2D	-2.15	1.46	1.50
13	A	804	CLA	CMC-C2C	-2.15	1.46	1.50
13	b	804	CLA	CMC-C2C	-2.15	1.46	1.50
13	A	814	CLA	C3B-C2B	-2.15	1.37	1.40
13	a	835	CLA	CMD-C2D	-2.15	1.46	1.50
13	A	822	CLA	CMD-C2D	-2.15	1.46	1.50
13	a	804	CLA	CMD-C2D	-2.15	1.46	1.50
13	B	801	CLA	CMD-C2D	-2.15	1.46	1.50
13	g	834	CLA	CMD-C2D	-2.15	1.46	1.50
13	b	804	CLA	CMD-C2D	-2.15	1.46	1.50
13	A	814	CLA	CMD-C2D	-2.15	1.46	1.50
13	b	802	CLA	CMD-C2D	-2.15	1.46	1.50
13	B	812	CLA	CMD-C2D	-2.15	1.46	1.50
13	E	843	CLA	CMD-C2D	-2.15	1.46	1.50
13	E	807	CLA	CMD-C2D	-2.15	1.46	1.50
13	E	809	CLA	CMD-C2D	-2.15	1.46	1.50
13	a	836	CLA	CMD-C2D	-2.15	1.46	1.50
13	g	802	CLA	CMD-C2D	-2.15	1.46	1.50
13	B	820	CLA	CMD-C2D	-2.14	1.46	1.50
13	G	835	CLA	C3B-C2B	-2.14	1.37	1.40
13	A	830	CLA	CMD-C2D	-2.14	1.46	1.50
13	a	834	CLA	CMD-C2D	-2.14	1.46	1.50
13	G	827	CLA	CMD-C2D	-2.14	1.46	1.50
13	A	809	CLA	CMD-C2D	-2.14	1.46	1.50
13	A	828	CLA	CMD-C2D	-2.14	1.46	1.50
13	E	822	CLA	CMD-C2D	-2.14	1.46	1.50
13	a	814	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	839	CLA	CMD-C2D	-2.14	1.46	1.50
13	a	822	CLA	CMD-C2D	-2.14	1.46	1.50
13	e	833	CLA	CMD-C2D	-2.14	1.46	1.50
13	b	811	CLA	CMD-C2D	-2.14	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	828	CLA	C3B-CAB	-2.14	1.43	1.47
13	B	818	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	835	CLA	C3B-C2B	-2.14	1.37	1.40
13	A	805	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	833	CLA	CMD-C2D	-2.14	1.46	1.50
13	a	807	CLA	CMD-C2D	-2.14	1.46	1.50
13	b	819	CLA	CMD-C2D	-2.14	1.46	1.50
13	g	842	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	820	CLA	CMD-C2D	-2.13	1.46	1.50
13	S	206	CLA	CMD-C2D	-2.13	1.46	1.50
13	A	837	CLA	CMD-C2D	-2.13	1.46	1.50
13	A	817	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	840	CLA	CMD-C2D	-2.13	1.46	1.50
13	e	821	CLA	CMC-C2C	-2.13	1.46	1.50
13	a	824	CLA	CMD-C2D	-2.13	1.46	1.50
13	E	835	CLA	MG-ND	-2.13	2.01	2.05
13	e	822	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	840	CLA	C3B-C2B	-2.13	1.37	1.40
13	g	824	CLA	CMC-C2C	-2.13	1.46	1.50
13	g	826	CLA	CMD-C2D	-2.13	1.46	1.50
13	b	825	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	801	CLA	C3B-C2B	-2.13	1.37	1.40
13	A	829	CLA	C3B-CAB	-2.13	1.43	1.47
13	A	808	CLA	CMD-C2D	-2.13	1.46	1.50
13	L	202	CLA	CMC-C2C	-2.13	1.46	1.50
13	A	823	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	805	CLA	CMD-C2D	-2.13	1.46	1.50
13	a	829	CLA	C3B-CAB	-2.13	1.43	1.47
13	B	825	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	804	CLA	CMC-C2C	-2.13	1.46	1.50
13	a	806	CLA	CMD-C2D	-2.13	1.46	1.50
13	b	818	CLA	CMD-C2D	-2.13	1.46	1.50
13	g	802	CLA	MG-ND	-2.13	2.01	2.05
13	a	809	CLA	CMD-C2D	-2.13	1.46	1.50
13	B	808	CLA	CMD-C2D	-2.13	1.46	1.50
13	B	811	CLA	CMD-C2D	-2.13	1.46	1.50
13	b	829	CLA	CMD-C2D	-2.13	1.46	1.50
13	b	840	CLA	CMC-C2C	-2.13	1.46	1.50
13	B	841	CLA	CMD-C2D	-2.13	1.46	1.50
13	l	201	CLA	CMD-C2D	-2.13	1.46	1.50
13	A	826	CLA	CMD-C2D	-2.13	1.46	1.50
13	G	810	CLA	CMD-C2D	-2.13	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	r	101	CLA	CMD-C2D	-2.13	1.46	1.50
13	g	806	CLA	CMC-C2C	-2.13	1.46	1.50
13	E	821	CLA	C3B-CAB	-2.13	1.43	1.47
13	e	813	CLA	CMD-C2D	-2.12	1.46	1.50
13	A	853	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	826	CLA	CMD-C2D	-2.12	1.46	1.50
13	E	817	CLA	CMD-C2D	-2.12	1.46	1.50
13	G	830	CLA	CMD-C2D	-2.12	1.46	1.50
13	g	809	CLA	CMD-C2D	-2.12	1.46	1.50
13	a	837	CLA	CMD-C2D	-2.12	1.46	1.50
13	b	822	CLA	CMC-C2C	-2.12	1.46	1.50
13	G	812	CLA	CMD-C2D	-2.12	1.46	1.50
13	G	841	CLA	CMD-C2D	-2.12	1.46	1.50
13	a	817	CLA	CMD-C2D	-2.12	1.46	1.50
13	g	827	CLA	CMD-C2D	-2.12	1.46	1.50
13	A	842	CLA	CMD-C2D	-2.12	1.46	1.50
13	a	826	CLA	CMD-C2D	-2.12	1.46	1.50
13	e	835	CLA	CMD-C2D	-2.12	1.46	1.50
13	l	204	CLA	CMD-C2D	-2.12	1.46	1.50
13	E	808	CLA	CMD-C2D	-2.12	1.46	1.50
13	G	806	CLA	CMD-C2D	-2.12	1.46	1.50
13	b	824	CLA	CMD-C2D	-2.12	1.46	1.50
13	b	830	CLA	CMD-C2D	-2.12	1.46	1.50
13	b	839	CLA	CMC-C2C	-2.12	1.46	1.50
13	G	840	CLA	CMC-C2C	-2.12	1.46	1.50
13	e	816	CLA	CMD-C2D	-2.12	1.46	1.50
13	e	841	CLA	CMD-C2D	-2.12	1.46	1.50
13	e	839	CLA	C3B-C2B	-2.12	1.37	1.40
13	B	802	CLA	CMD-C2D	-2.12	1.46	1.50
13	A	806	CLA	CMD-C2D	-2.12	1.46	1.50
13	G	841	CLA	CMC-C2C	-2.12	1.46	1.50
13	b	834	CLA	C3B-C2B	-2.12	1.37	1.40
13	B	805	CLA	CMC-C2C	-2.12	1.46	1.50
13	B	821	CLA	CMD-C2D	-2.12	1.46	1.50
13	A	807	CLA	CMD-C2D	-2.11	1.46	1.50
13	G	834	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	806	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	836	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	852	CLA	CMD-C2D	-2.11	1.46	1.50
13	g	836	CLA	C3B-C2B	-2.11	1.37	1.40
13	b	839	CLA	C3B-C2B	-2.11	1.37	1.40
13	B	819	CLA	CMD-C2D	-2.11	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	845	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	823	CLA	CMD-C2D	-2.11	1.46	1.50
13	a	841	CLA	C3B-C2B	-2.11	1.37	1.40
13	G	807	CLA	CMD-C2D	-2.11	1.46	1.50
13	g	840	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	828	CLA	CMD-C2D	-2.11	1.46	1.50
13	A	840	CLA	C3B-CAB	-2.11	1.43	1.47
13	g	812	CLA	CMD-C2D	-2.11	1.46	1.50
13	g	817	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	808	CLA	C3B-C2B	-2.11	1.37	1.40
13	a	825	CLA	C3B-C2B	-2.11	1.37	1.40
13	B	830	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	838	CLA	CMD-C2D	-2.11	1.46	1.50
13	E	814	CLA	CMD-C2D	-2.11	1.46	1.50
13	a	845	CLA	CMD-C2D	-2.11	1.46	1.50
13	g	814	CLA	CMD-C2D	-2.11	1.46	1.50
13	G	838	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	822	CLA	CMD-C2D	-2.11	1.46	1.50
13	G	825	CLA	CMD-C2D	-2.11	1.46	1.50
13	E	805	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	823	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	839	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	844	CLA	CMD-C2D	-2.11	1.46	1.50
13	a	841	CLA	CMC-C2C	-2.11	1.46	1.50
13	b	840	CLA	CMD-C2D	-2.11	1.46	1.50
13	E	813	CLA	CMD-C2D	-2.10	1.46	1.50
13	G	807	CLA	C3B-C2B	-2.10	1.37	1.40
13	a	805	CLA	CMD-C2D	-2.10	1.46	1.50
13	G	823	CLA	CMC-C2C	-2.10	1.46	1.50
13	B	831	CLA	CMD-C2D	-2.10	1.46	1.50
13	b	810	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	823	CLA	CMD-C2D	-2.10	1.46	1.50
13	g	821	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	844	CLA	CMC-C2C	-2.10	1.46	1.50
13	E	823	CLA	CMD-C2D	-2.10	1.46	1.50
13	b	812	CLA	CMD-C2D	-2.10	1.46	1.50
13	g	831	CLA	CMD-C2D	-2.10	1.46	1.50
13	g	841	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	808	CLA	C3B-C2B	-2.10	1.37	1.40
13	G	820	CLA	C3B-C2B	-2.10	1.37	1.40
13	b	807	CLA	C3B-C2B	-2.10	1.37	1.40
13	G	817	CLA	CMD-C2D	-2.10	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	803	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	822	CLA	CMC-C2C	-2.10	1.46	1.50
13	b	831	CLA	CMD-C2D	-2.10	1.46	1.50
15	A	850	BCR	C33-C5	-2.10	1.47	1.50
13	B	834	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	823	CLA	CMD-C2D	-2.10	1.46	1.50
13	A	845	CLA	CMD-C2D	-2.10	1.46	1.50
13	L	203	CLA	CMC-C2C	-2.10	1.46	1.50
13	G	818	CLA	CMD-C2D	-2.10	1.46	1.50
13	G	823	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	828	CLA	CMD-C2D	-2.10	1.46	1.50
13	b	827	CLA	CMD-C2D	-2.10	1.46	1.50
13	L	203	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	813	CLA	CMD-C2D	-2.10	1.46	1.50
13	b	801	CLA	C3B-C2B	-2.10	1.37	1.40
13	g	801	CLA	CMD-C2D	-2.10	1.46	1.50
13	g	820	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	840	CLA	CMD-C2D	-2.10	1.46	1.50
13	G	813	CLA	CMD-C2D	-2.10	1.46	1.50
13	s	202	CLA	CMD-C2D	-2.10	1.46	1.50
13	A	822	CLA	CMC-C2C	-2.10	1.46	1.50
13	G	824	CLA	CMD-C2D	-2.10	1.46	1.50
13	A	829	CLA	CMC-C2C	-2.10	1.46	1.50
13	E	841	CLA	C3B-C2B	-2.10	1.37	1.40
13	g	803	CLA	C3B-C2B	-2.10	1.37	1.40
13	g	821	CLA	C3B-C2B	-2.10	1.37	1.40
13	A	844	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	841	CLA	C3B-CAB	-2.10	1.43	1.47
13	G	832	CLA	CMD-C2D	-2.09	1.46	1.50
15	e	849	BCR	C33-C5	-2.09	1.47	1.50
13	A	840	CLA	C3B-C2B	-2.09	1.37	1.40
13	B	816	CLA	CMD-C2D	-2.09	1.46	1.50
13	e	827	CLA	CMD-C2D	-2.09	1.46	1.50
13	B	823	CLA	CMC-C2C	-2.09	1.46	1.50
13	e	805	CLA	CMD-C2D	-2.09	1.46	1.50
13	A	813	CLA	CMD-C2D	-2.09	1.46	1.50
13	g	825	CLA	CMD-C2D	-2.09	1.46	1.50
13	B	840	CLA	CMC-C2C	-2.09	1.46	1.50
13	E	846	CLA	CMD-C2D	-2.09	1.46	1.50
13	E	842	CLA	CMD-C2D	-2.09	1.46	1.50
13	g	842	CLA	CMC-C2C	-2.09	1.46	1.50
13	B	813	CLA	CMD-C2D	-2.09	1.46	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	817	CLA	CMD-C2D	-2.09	1.46	1.50
13	g	841	CLA	CMC-C2C	-2.09	1.46	1.50
13	a	808	CLA	CMD-C2D	-2.09	1.46	1.50
13	g	809	CLA	C3B-C2B	-2.09	1.37	1.40
13	b	803	CLA	CMD-C2D	-2.09	1.46	1.50
13	E	806	CLA	CMD-C2D	-2.09	1.46	1.50
13	E	822	CLA	CMC-C2C	-2.09	1.46	1.50
13	G	801	CLA	CMD-C2D	-2.09	1.46	1.50
13	G	809	CLA	CMD-C2D	-2.09	1.46	1.50
13	g	832	CLA	CMD-C2D	-2.09	1.46	1.50
13	a	835	CLA	MG-ND	-2.09	2.01	2.05
13	e	842	CLA	CMC-C2C	-2.09	1.46	1.50
13	a	840	CLA	CMD-C2D	-2.09	1.46	1.50
13	a	845	CLA	CMC-C2C	-2.08	1.46	1.50
13	b	806	CLA	CMD-C2D	-2.08	1.46	1.50
13	E	829	CLA	C3B-CAB	-2.08	1.43	1.47
13	g	833	CLA	CMD-C2D	-2.08	1.46	1.50
13	e	828	CLA	CMC-C2C	-2.08	1.46	1.50
13	b	817	CLA	CMD-C2D	-2.08	1.46	1.50
13	e	831	CLA	C3B-C2B	-2.08	1.37	1.40
13	G	839	CLA	CMD-C2D	-2.08	1.46	1.50
13	S	203	CLA	CMD-C2D	-2.08	1.46	1.50
13	a	821	CLA	CMD-C2D	-2.08	1.46	1.50
13	e	816	CLA	C3B-C2B	-2.08	1.37	1.40
13	B	807	CLA	CMD-C2D	-2.08	1.46	1.50
13	E	838	CLA	CMD-C2D	-2.08	1.46	1.50
13	G	826	CLA	CMC-C2C	-2.08	1.46	1.50
13	e	825	CLA	CMD-C2D	-2.08	1.46	1.50
13	B	802	CLA	C3B-C2B	-2.08	1.37	1.40
13	B	841	CLA	CMC-C2C	-2.08	1.46	1.50
13	g	805	CLA	CMD-C2D	-2.08	1.46	1.50
13	e	839	CLA	C3B-CAB	-2.08	1.43	1.47
13	b	809	CLA	CMD-C2D	-2.08	1.46	1.50
13	A	826	CLA	C3B-C2B	-2.08	1.37	1.40
13	g	819	CLA	CMD-C2D	-2.08	1.46	1.50
13	E	841	CLA	CMD-C2D	-2.08	1.46	1.50
13	A	832	CLA	C3B-C2B	-2.08	1.37	1.40
13	E	825	CLA	C3B-C2B	-2.08	1.37	1.40
13	G	839	CLA	C3B-C2B	-2.08	1.37	1.40
13	S	204	CLA	C3B-C2B	-2.08	1.37	1.40
13	e	808	CLA	CMD-C2D	-2.08	1.46	1.50
13	e	812	CLA	CMD-C2D	-2.08	1.46	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	830	CLA	CMC-C2C	-2.08	1.46	1.50
13	b	838	CLA	CMD-C2D	-2.08	1.46	1.50
13	g	829	CLA	CMD-C2D	-2.08	1.46	1.50
13	a	829	CLA	CMC-C2C	-2.08	1.46	1.50
13	A	843	CLA	CMC-C2C	-2.07	1.46	1.50
13	g	808	CLA	CMD-C2D	-2.07	1.46	1.50
13	g	818	CLA	CMD-C2D	-2.07	1.46	1.50
13	K	101	CLA	CMD-C2D	-2.07	1.46	1.50
13	g	835	CLA	CMD-C2D	-2.07	1.46	1.50
13	s	202	CLA	CMC-C2C	-2.07	1.46	1.50
13	b	837	CLA	CMD-C2D	-2.07	1.46	1.50
13	B	810	CLA	CMD-C2D	-2.07	1.46	1.50
13	e	843	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	838	CLA	CMD-C2D	-2.07	1.46	1.50
13	E	841	CLA	C3B-CAB	-2.07	1.43	1.47
13	E	829	CLA	CMC-C2C	-2.07	1.46	1.50
13	a	831	CLA	CMC-C2C	-2.07	1.46	1.50
13	G	816	CLA	CMD-C2D	-2.07	1.46	1.50
13	A	803	CLA	CMC-C2C	-2.07	1.46	1.50
13	g	824	CLA	CMD-C2D	-2.07	1.46	1.50
13	B	839	CLA	C3B-C2B	-2.07	1.37	1.40
13	a	826	CLA	C3B-C2B	-2.07	1.37	1.40
13	g	808	CLA	C3B-CAB	-2.07	1.43	1.47
13	B	824	CLA	CMD-C2D	-2.07	1.46	1.50
13	b	813	CLA	CMD-C2D	-2.07	1.46	1.50
13	b	816	CLA	CMD-C2D	-2.07	1.46	1.50
13	K	102	CLA	CMD-C2D	-2.07	1.46	1.50
13	G	837	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	843	CLA	CMD-C2D	-2.07	1.46	1.50
13	A	809	CLA	C3B-C2B	-2.07	1.37	1.40
13	E	821	CLA	CMD-C2D	-2.07	1.46	1.50
13	e	818	CLA	CMD-C2D	-2.07	1.46	1.50
13	B	801	CLA	MG-ND	-2.07	2.01	2.05
13	E	834	CLA	C3B-CAB	-2.07	1.43	1.47
13	A	844	CLA	CMC-C2C	-2.07	1.46	1.50
13	E	845	CLA	CMC-C2C	-2.07	1.46	1.50
13	a	830	CLA	CMC-C2C	-2.07	1.46	1.50
13	G	819	CLA	CMD-C2D	-2.07	1.46	1.50
13	e	803	CLA	CMC-C2C	-2.07	1.46	1.50
13	G	821	CLA	CMD-C2D	-2.07	1.46	1.50
13	e	809	CLA	CMD-C2D	-2.07	1.46	1.50
13	b	808	CLA	CMD-C2D	-2.07	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	k	4002	CLA	CMD-C2D	-2.07	1.46	1.50
13	A	811	CLA	CMD-C2D	-2.07	1.46	1.50
13	E	828	CLA	CMD-C2D	-2.07	1.46	1.50
13	G	836	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	818	CLA	CMD-C2D	-2.07	1.46	1.50
13	A	827	CLA	CMD-C2D	-2.07	1.46	1.50
13	B	814	CLA	CMD-C2D	-2.07	1.46	1.50
13	E	841	CLA	CMC-C2C	-2.07	1.46	1.50
13	a	842	CLA	CMC-C2C	-2.07	1.46	1.50
13	a	834	CLA	C3B-C2B	-2.07	1.37	1.40
13	a	816	CLA	CMD-C2D	-2.07	1.46	1.50
13	e	824	CLA	C3B-C2B	-2.07	1.37	1.40
13	l	204	CLA	CMC-C2C	-2.07	1.46	1.50
13	E	834	CLA	C3B-C2B	-2.06	1.37	1.40
13	B	808	CLA	C3B-CAB	-2.06	1.43	1.47
13	A	841	CLA	CMC-C2C	-2.06	1.46	1.50
13	E	842	CLA	CMC-C2C	-2.06	1.46	1.50
13	b	801	CLA	CMD-C2D	-2.06	1.46	1.50
13	g	829	CLA	C3B-C2B	-2.06	1.37	1.40
13	a	817	CLA	C3B-C2B	-2.06	1.37	1.40
13	E	810	CLA	CMD-C2D	-2.06	1.46	1.50
13	E	830	CLA	CMC-C2C	-2.06	1.46	1.50
13	G	808	CLA	CMD-C2D	-2.06	1.46	1.50
13	A	830	CLA	CMC-C2C	-2.06	1.46	1.50
13	B	809	CLA	CMD-C2D	-2.06	1.46	1.50
13	e	834	CLA	MG-ND	-2.06	2.01	2.05
13	A	816	CLA	CMD-C2D	-2.06	1.46	1.50
13	A	840	CLA	CMC-C2C	-2.06	1.46	1.50
13	B	837	CLA	CMD-C2D	-2.06	1.46	1.50
13	E	839	CLA	CMD-C2D	-2.06	1.46	1.50
13	g	842	CLA	C3B-C2B	-2.06	1.37	1.40
13	A	838	CLA	CMD-C2D	-2.06	1.46	1.50
13	G	803	CLA	CMD-C2D	-2.06	1.46	1.50
13	G	814	CLA	CMD-C2D	-2.06	1.46	1.50
13	e	833	CLA	C3B-C2B	-2.06	1.37	1.40
13	g	836	CLA	CMD-C2D	-2.06	1.46	1.50
13	L	204	CLA	C3B-C2B	-2.06	1.37	1.40
13	G	831	CLA	CMD-C2D	-2.06	1.46	1.50
13	E	826	CLA	CMD-C2D	-2.06	1.46	1.50
13	f	203	CLA	CMD-C2D	-2.06	1.46	1.50
13	b	827	CLA	CMC-C2C	-2.06	1.46	1.50
13	b	839	CLA	C3B-CAB	-2.06	1.43	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	810	CLA	CMD-C2D	-2.06	1.46	1.50
13	E	811	CLA	CMD-C2D	-2.06	1.46	1.50
13	E	829	CLA	CMD-C2D	-2.06	1.46	1.50
13	G	828	CLA	CMD-C2D	-2.06	1.46	1.50
13	b	802	CLA	CMC-C2C	-2.06	1.46	1.50
13	b	815	CLA	CMD-C2D	-2.06	1.46	1.50
13	b	820	CLA	CMD-C2D	-2.06	1.46	1.50
13	a	841	CLA	CMD-C2D	-2.06	1.46	1.50
13	a	811	CLA	CMD-C2D	-2.06	1.46	1.50
13	a	815	CLA	CMD-C2D	-2.06	1.46	1.50
13	g	822	CLA	CMD-C2D	-2.06	1.46	1.50
13	a	820	CLA	CMC-C2C	-2.06	1.46	1.50
13	A	825	CLA	C3B-C2B	-2.06	1.37	1.40
13	e	840	CLA	CMC-C2C	-2.06	1.46	1.50
13	g	811	CLA	CMD-C2D	-2.06	1.46	1.50
13	B	811	CLA	CMC-C2C	-2.06	1.46	1.50
13	E	819	CLA	CMD-C2D	-2.06	1.46	1.50
13	B	835	CLA	CMD-C2D	-2.05	1.46	1.50
13	g	815	CLA	CMD-C2D	-2.05	1.46	1.50
13	g	838	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	819	CLA	CMD-C2D	-2.05	1.46	1.50
13	E	836	CLA	MG-ND	-2.05	2.01	2.05
13	E	844	CLA	CMC-C2C	-2.05	1.46	1.50
13	b	836	CLA	CMD-C2D	-2.05	1.46	1.50
13	G	821	CLA	C3B-C2B	-2.05	1.37	1.40
13	E	836	CLA	CMC-C2C	-2.05	1.46	1.50
13	b	834	CLA	CMD-C2D	-2.05	1.46	1.50
13	g	810	CLA	CMD-C2D	-2.05	1.46	1.50
13	B	805	CLA	C3B-C2B	-2.05	1.37	1.40
13	B	804	CLA	CMD-C2D	-2.05	1.46	1.50
13	B	817	CLA	CMD-C2D	-2.05	1.46	1.50
13	B	820	CLA	C3B-C2B	-2.05	1.37	1.40
13	e	839	CLA	CMD-C2D	-2.05	1.46	1.50
13	A	834	CLA	C3B-CAB	-2.05	1.43	1.47
13	a	834	CLA	C3B-CAB	-2.05	1.43	1.47
13	G	810	CLA	CMC-C2C	-2.05	1.46	1.50
13	g	801	CLA	CMC-C2C	-2.05	1.46	1.50
13	g	840	CLA	C3B-C2B	-2.05	1.37	1.40
13	A	829	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	842	CLA	CMD-C2D	-2.05	1.46	1.50
13	G	806	CLA	C3B-CAB	-2.05	1.43	1.47
15	E	801	BCR	C33-C5	-2.05	1.47	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	836	CLA	CMD-C2D	-2.05	1.46	1.50
13	E	827	CLA	CMC-C2C	-2.05	1.46	1.50
13	e	815	CLA	CMD-C2D	-2.05	1.46	1.50
13	E	809	CLA	C3B-C2B	-2.05	1.37	1.40
13	R	102	CLA	CMD-C2D	-2.05	1.46	1.50
13	G	807	CLA	C3B-CAB	-2.05	1.43	1.47
13	g	809	CLA	C3B-CAB	-2.05	1.43	1.47
13	A	853	CLA	CMC-C2C	-2.05	1.46	1.50
13	b	807	CLA	C3B-CAB	-2.05	1.43	1.47
13	G	841	CLA	C3B-C2B	-2.05	1.37	1.40
13	s	203	CLA	C3B-C2B	-2.05	1.37	1.40
13	b	838	CLA	C3B-C2B	-2.05	1.37	1.40
13	l	205	CLA	C3B-C2B	-2.05	1.37	1.40
13	B	825	CLA	CMC-C2C	-2.05	1.46	1.50
13	O	203	CLA	CMD-C2D	-2.05	1.46	1.50
13	e	834	CLA	CMC-C2C	-2.05	1.46	1.50
13	E	826	CLA	C3B-C2B	-2.05	1.37	1.40
13	A	815	CLA	CMD-C2D	-2.05	1.46	1.50
13	A	819	CLA	CMD-C2D	-2.05	1.46	1.50
13	e	826	CLA	CMD-C2D	-2.05	1.46	1.50
13	r	102	CLA	CMD-C2D	-2.05	1.46	1.50
13	b	825	CLA	CMC-C2C	-2.05	1.46	1.50
13	b	819	CLA	C3B-C2B	-2.05	1.37	1.40
13	A	840	CLA	CMD-C2D	-2.05	1.46	1.50
13	A	835	CLA	CMC-C2C	-2.04	1.46	1.50
13	E	834	CLA	CMC-C2C	-2.04	1.46	1.50
13	e	839	CLA	CMC-C2C	-2.04	1.46	1.50
13	e	840	CLA	CMD-C2D	-2.04	1.46	1.50
13	G	840	CLA	C3B-CAB	-2.04	1.43	1.47
13	e	814	CLA	CMD-C2D	-2.04	1.46	1.50
13	g	823	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	832	CLA	C3B-C2B	-2.04	1.37	1.40
13	B	832	CLA	CMD-C2D	-2.04	1.46	1.50
13	G	818	CLA	CMC-C2C	-2.04	1.46	1.50
13	S	206	CLA	CMC-C2C	-2.04	1.46	1.50
13	b	835	CLA	CMD-C2D	-2.04	1.46	1.50
13	K	101	CLA	CBD-CAD	2.04	1.56	1.51
13	e	837	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	810	CLA	CMD-C2D	-2.04	1.46	1.50
13	E	827	CLA	CMD-C2D	-2.04	1.46	1.50
13	e	805	CLA	CMC-C2C	-2.04	1.46	1.50
13	e	833	CLA	C3B-CAB	-2.04	1.43	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	839	CLA	CMD-C2D	-2.04	1.46	1.50
13	G	802	CLA	CMC-C2C	-2.04	1.46	1.50
13	e	810	CLA	CMD-C2D	-2.04	1.46	1.50
13	a	805	CLA	CMC-C2C	-2.04	1.46	1.50
13	a	828	CLA	CMC-C2C	-2.04	1.46	1.50
13	r	101	CLA	CBD-CAD	2.04	1.56	1.51
13	e	828	CLA	CMD-C2D	-2.04	1.46	1.50
13	A	817	CLA	C3B-C2B	-2.04	1.37	1.40
13	g	824	CLA	C3B-C2B	-2.04	1.37	1.40
13	E	815	CLA	CMD-C2D	-2.04	1.46	1.50
13	E	831	CLA	CMC-C2C	-2.04	1.46	1.50
13	A	841	CLA	CMD-C2D	-2.04	1.46	1.50
13	E	820	CLA	CMC-C2C	-2.04	1.46	1.50
13	e	843	CLA	CMC-C2C	-2.04	1.46	1.50
13	b	817	CLA	CMC-C2C	-2.04	1.46	1.50
13	G	833	CLA	C3B-C2B	-2.04	1.37	1.40
13	E	806	CLA	CMC-C2C	-2.04	1.46	1.50
13	E	818	CLA	CMD-C2D	-2.04	1.46	1.50
13	A	821	CLA	CMD-C2D	-2.04	1.46	1.50
13	S	203	CLA	CMC-C2C	-2.04	1.46	1.50
13	B	828	CLA	C3B-C2B	-2.04	1.37	1.40
13	a	809	CLA	C3B-C2B	-2.04	1.37	1.40
13	A	805	CLA	CMC-C2C	-2.04	1.46	1.50
13	A	818	CLA	CMD-C2D	-2.04	1.46	1.50
13	B	826	CLA	CMC-C2C	-2.04	1.46	1.50
13	a	827	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	810	CLA	CMC-C2C	-2.04	1.46	1.50
13	A	836	CLA	C3B-C2B	-2.04	1.37	1.40
13	g	839	CLA	CMD-C2D	-2.04	1.46	1.50
13	B	823	CLA	C3B-C2B	-2.04	1.37	1.40
13	b	832	CLA	C3B-C2B	-2.04	1.37	1.40
13	A	831	CLA	CMC-C2C	-2.04	1.46	1.50
13	g	820	CLA	CMC-C2C	-2.04	1.46	1.50
13	B	840	CLA	C3B-CAB	-2.04	1.43	1.47
13	e	838	CLA	CMD-C2D	-2.04	1.46	1.50
13	G	835	CLA	CMD-C2D	-2.03	1.46	1.50
13	A	839	CLA	CMC-C2C	-2.03	1.46	1.50
13	a	839	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	822	CLA	C3B-C2B	-2.03	1.37	1.40
15	T	101	BCR	C33-C5	-2.03	1.47	1.50
13	A	807	CLA	CMC-C2C	-2.03	1.46	1.50
13	e	819	CLA	CMC-C2C	-2.03	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	818	CLA	CMC-C2C	-2.03	1.46	1.50
13	g	834	CLA	C3B-C2B	-2.03	1.37	1.40
13	G	803	CLA	CMC-C2C	-2.03	1.46	1.50
13	b	828	CLA	CMC-C2C	-2.03	1.46	1.50
15	k	4001	BCR	C38-C26	-2.03	1.47	1.50
13	E	832	CLA	CMD-C2D	-2.03	1.46	1.50
13	e	829	CLA	CMC-C2C	-2.03	1.46	1.50
13	g	807	CLA	CMC-C2C	-2.03	1.46	1.50
13	G	812	CLA	C3B-C2B	-2.03	1.37	1.40
13	A	806	CLA	CMC-C2C	-2.03	1.46	1.50
13	g	830	CLA	CMC-C2C	-2.03	1.46	1.50
13	g	841	CLA	C3B-CAB	-2.03	1.43	1.47
13	a	835	CLA	CMC-C2C	-2.03	1.46	1.50
13	A	834	CLA	C3B-C2B	-2.03	1.37	1.40
13	B	807	CLA	C3B-CAB	-2.03	1.43	1.47
13	g	829	CLA	CMC-C2C	-2.03	1.46	1.50
13	E	811	CLA	CMC-C2C	-2.03	1.46	1.50
13	G	805	CLA	CMC-C2C	-2.03	1.46	1.50
13	a	807	CLA	CMC-C2C	-2.03	1.46	1.50
13	b	810	CLA	C3B-C2B	-2.03	1.37	1.40
13	b	827	CLA	C3B-C2B	-2.03	1.37	1.40
13	G	828	CLA	C3B-C2B	-2.03	1.37	1.40
13	b	806	CLA	C3B-CAB	-2.03	1.43	1.47
13	a	836	CLA	CMC-C2C	-2.03	1.46	1.50
13	b	805	CLA	CMC-C2C	-2.03	1.46	1.50
13	b	820	CLA	C3B-C2B	-2.03	1.37	1.40
13	e	833	CLA	CMC-C2C	-2.03	1.46	1.50
13	g	805	CLA	CMC-C2C	-2.03	1.46	1.50
13	B	818	CLA	CMC-C2C	-2.03	1.46	1.50
13	e	830	CLA	CMD-C2D	-2.03	1.46	1.50
13	e	838	CLA	CMC-C2C	-2.03	1.46	1.50
13	G	828	CLA	CMC-C2C	-2.03	1.46	1.50
13	B	841	CLA	C3B-C2B	-2.03	1.37	1.40
13	A	834	CLA	CMC-C2C	-2.02	1.46	1.50
13	a	829	CLA	CMD-C2D	-2.02	1.46	1.50
13	E	805	CLA	CMC-C2C	-2.02	1.46	1.50
13	E	816	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	805	CLA	C3B-C2B	-2.02	1.37	1.40
13	b	811	CLA	C3B-C2B	-2.02	1.37	1.40
13	g	827	CLA	CMC-C2C	-2.02	1.46	1.50
13	G	804	CLA	C3B-C2B	-2.02	1.37	1.40
13	e	852	CLA	CMC-C2C	-2.02	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	822	CLA	CMC-C2C	-2.02	1.46	1.50
13	E	817	CLA	O2A-CGA	2.02	1.37	1.30
13	A	819	CLA	C3B-C2B	-2.02	1.37	1.40
13	E	809	CLA	CMC-C2C	-2.02	1.46	1.50
13	E	840	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	834	CLA	CMC-C2C	-2.02	1.46	1.50
13	g	802	CLA	CMC-C2C	-2.02	1.46	1.50
13	e	844	CLA	C3B-C2B	-2.02	1.37	1.40
13	A	820	CLA	CMC-C2C	-2.02	1.46	1.50
13	A	836	CLA	CMC-C2C	-2.02	1.46	1.50
13	e	835	CLA	CMC-C2C	-2.02	1.46	1.50
13	E	835	CLA	CMC-C2C	-2.02	1.46	1.50
13	g	826	CLA	CMC-C2C	-2.02	1.46	1.50
13	E	832	CLA	C3B-C2B	-2.02	1.37	1.40
13	e	825	CLA	C3B-C2B	-2.02	1.37	1.40
13	S	204	CLA	CMD-C2D	-2.02	1.46	1.50
13	e	831	CLA	CMD-C2D	-2.02	1.46	1.50
13	a	832	CLA	CMD-C2D	-2.02	1.46	1.50
13	E	817	CLA	C3B-C2B	-2.02	1.37	1.40
13	g	819	CLA	CMC-C2C	-2.02	1.46	1.50
15	m	101	BCR	C38-C26	-2.02	1.47	1.50
13	a	831	CLA	CMD-C2D	-2.02	1.46	1.50
13	b	819	CLA	C3B-CAB	-2.02	1.43	1.47
13	a	816	CLA	CMC-C2C	-2.02	1.46	1.50
13	E	831	CLA	CMD-C2D	-2.02	1.46	1.50
13	B	833	CLA	C3B-C2B	-2.02	1.37	1.40
13	g	815	CLA	CMC-C2C	-2.02	1.46	1.50
13	b	832	CLA	CMC-C2C	-2.02	1.46	1.50
13	O	203	CLA	CMC-C2C	-2.01	1.46	1.50
13	e	806	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	813	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	829	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	822	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	819	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	808	CLA	CMC-C2C	-2.01	1.46	1.50
13	e	810	CLA	CMC-C2C	-2.01	1.46	1.50
13	g	816	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	820	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	832	CLA	CMC-C2C	-2.01	1.46	1.50
13	o	202	CLA	CMD-C2D	-2.01	1.46	1.50
13	a	827	CLA	CMC-C2C	-2.01	1.46	1.50
13	g	812	CLA	CMC-C2C	-2.01	1.46	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	840	CLA	C3B-CAB	-2.01	1.43	1.47
13	B	804	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	825	CLA	CMC-C2C	-2.01	1.46	1.50
13	e	809	CLA	CMC-C2C	-2.01	1.46	1.50
13	g	823	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	821	CLA	C3B-C2B	-2.01	1.37	1.40
13	A	831	CLA	CMD-C2D	-2.01	1.46	1.50
13	B	822	CLA	CMD-C2D	-2.01	1.46	1.50
13	e	827	CLA	CMC-C2C	-2.01	1.46	1.50
13	g	809	CLA	CMC-C2C	-2.01	1.46	1.50
13	a	837	CLA	CMC-C2C	-2.01	1.46	1.50
13	l	201	CLA	CMC-C2C	-2.01	1.46	1.50
13	G	830	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	801	CLA	CMC-C2C	-2.01	1.46	1.50
13	g	806	CLA	C3B-C2B	-2.01	1.37	1.40
13	A	811	CLA	CMC-C2C	-2.01	1.46	1.50
13	A	828	CLA	CMC-C2C	-2.01	1.46	1.50
13	g	806	CLA	C3B-CAB	-2.01	1.43	1.47
15	s	201	BCR	C38-C26	-2.01	1.47	1.50
13	B	828	CLA	CMC-C2C	-2.01	1.46	1.50
13	e	820	CLA	CMD-C2D	-2.01	1.46	1.50
13	A	832	CLA	CMD-C2D	-2.01	1.46	1.50
13	B	811	CLA	C3B-C2B	-2.01	1.37	1.40
13	B	806	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	833	CLA	CMC-C2C	-2.01	1.46	1.50
13	g	834	CLA	CMC-C2C	-2.01	1.46	1.50
13	a	836	CLA	MG-ND	-2.01	2.01	2.05
13	A	810	CLA	CMC-C2C	-2.01	1.46	1.50
15	G	847	BCR	C38-C26	-2.01	1.47	1.50
13	a	832	CLA	CMC-C2C	-2.01	1.46	1.50
15	b	846	BCR	C38-C26	-2.00	1.47	1.50
13	f	203	CLA	CMC-C2C	-2.00	1.46	1.50
13	b	815	CLA	CMC-C2C	-2.00	1.46	1.50
13	e	816	CLA	O2A-CGA	2.00	1.37	1.30
13	B	829	CLA	CMC-C2C	-2.00	1.46	1.50
13	a	840	CLA	CMC-C2C	-2.00	1.46	1.50
13	g	833	CLA	CMC-C2C	-2.00	1.46	1.50
13	G	823	CLA	C3B-C2B	-2.00	1.37	1.40
13	G	815	CLA	CMC-C2C	-2.00	1.46	1.50
13	e	826	CLA	CMC-C2C	-2.00	1.46	1.50
13	g	811	CLA	CMC-C2C	-2.00	1.46	1.50
13	a	806	CLA	CMC-C2C	-2.00	1.46	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	821	CLA	CMD-C2D	-2.00	1.46	1.50
13	l	203	CLA	CMD-C2D	-2.00	1.46	1.50
13	a	837	CLA	C3B-C2B	-2.00	1.37	1.40
13	a	809	CLA	C3B-CAB	-2.00	1.43	1.47
13	b	812	CLA	CMC-C2C	-2.00	1.46	1.50
13	A	842	CLA	CMC-C2C	-2.00	1.46	1.50
13	b	807	CLA	CMC-C2C	-2.00	1.46	1.50
13	G	813	CLA	C3B-C2B	-2.00	1.37	1.40
13	G	838	CLA	CMC-C2C	-2.00	1.46	1.50
13	g	837	CLA	CMD-C2D	-2.00	1.46	1.50
13	l	201	CLA	C3B-C2B	-2.00	1.37	1.40

All (3352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	l	205	CLA	C4A-NA-C1A	17.39	114.53	106.71
13	s	203	CLA	C4A-NA-C1A	17.36	114.51	106.71
13	S	204	CLA	C4A-NA-C1A	17.31	114.49	106.71
13	L	204	CLA	C4A-NA-C1A	17.27	114.47	106.71
13	E	842	CLA	C4A-NA-C1A	7.38	110.03	106.71
13	l	205	CLA	C2A-C1A-CHA	7.33	136.67	123.86
13	s	203	CLA	C2A-C1A-CHA	7.32	136.67	123.86
13	A	841	CLA	C4A-NA-C1A	7.31	109.99	106.71
13	S	204	CLA	C2A-C1A-CHA	7.31	136.64	123.86
13	L	204	CLA	C2A-C1A-CHA	7.30	136.62	123.86
13	a	842	CLA	C4A-NA-C1A	7.28	109.98	106.71
13	e	840	CLA	C4A-NA-C1A	7.26	109.97	106.71
13	E	841	CLA	C4A-NA-C1A	7.22	109.95	106.71
13	b	838	CLA	C4A-NA-C1A	7.16	109.92	106.71
13	g	824	CLA	C4A-NA-C1A	7.15	109.92	106.71
13	G	823	CLA	C4A-NA-C1A	7.14	109.92	106.71
13	a	841	CLA	C4A-NA-C1A	7.13	109.91	106.71
13	g	840	CLA	C4A-NA-C1A	7.13	109.91	106.71
13	B	823	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	e	839	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	a	839	CLA	C4A-NA-C1A	7.12	109.91	106.71
13	g	837	CLA	C4A-NA-C1A	7.11	109.90	106.71
13	A	840	CLA	C4A-NA-C1A	7.10	109.90	106.71
13	g	811	CLA	C4A-NA-C1A	7.09	109.89	106.71
13	A	845	CLA	C4A-NA-C1A	7.09	109.89	106.71
13	b	822	CLA	C4A-NA-C1A	7.08	109.89	106.71
13	A	838	CLA	C4A-NA-C1A	7.08	109.89	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	839	CLA	C4A-NA-C1A	7.08	109.89	106.71
13	E	839	CLA	C4A-NA-C1A	7.08	109.89	106.71
13	b	809	CLA	C4A-NA-C1A	7.07	109.88	106.71
13	A	835	CLA	C4A-NA-C1A	7.04	109.87	106.71
13	G	809	CLA	C4A-NA-C1A	7.04	109.87	106.71
13	E	836	CLA	C4A-NA-C1A	7.03	109.87	106.71
13	B	810	CLA	C4A-NA-C1A	7.03	109.86	106.71
13	a	820	CLA	C4A-NA-C1A	7.02	109.86	106.71
13	G	836	CLA	C4A-NA-C1A	7.02	109.86	106.71
13	e	834	CLA	C4A-NA-C1A	7.01	109.86	106.71
13	E	824	CLA	C4A-NA-C1A	7.01	109.86	106.71
13	e	837	CLA	C4A-NA-C1A	7.00	109.86	106.71
13	a	836	CLA	C4A-NA-C1A	7.00	109.85	106.71
13	a	840	CLA	C4A-NA-C1A	6.99	109.85	106.71
13	A	820	CLA	C4A-NA-C1A	6.98	109.84	106.71
13	B	836	CLA	C4A-NA-C1A	6.98	109.84	106.71
13	b	835	CLA	C4A-NA-C1A	6.97	109.84	106.71
13	E	840	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	E	820	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	g	830	CLA	C4A-NA-C1A	6.95	109.83	106.71
13	G	839	CLA	C4A-NA-C1A	6.94	109.83	106.71
13	e	844	CLA	C4A-NA-C1A	6.93	109.82	106.71
13	A	824	CLA	C4A-NA-C1A	6.91	109.81	106.71
13	B	815	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	a	828	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	f	203	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	G	829	CLA	C4A-NA-C1A	6.89	109.80	106.71
13	e	819	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	B	830	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	G	815	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	g	816	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	g	831	CLA	C4A-NA-C1A	6.87	109.80	106.71
13	b	814	CLA	C4A-NA-C1A	6.87	109.79	106.71
13	B	829	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	e	823	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	E	833	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	e	813	CLA	C4A-NA-C1A	6.86	109.79	106.71
13	B	819	CLA	C4A-NA-C1A	6.85	109.79	106.71
13	a	824	CLA	C4A-NA-C1A	6.85	109.78	106.71
13	b	818	CLA	C4A-NA-C1A	6.84	109.78	106.71
13	g	839	CLA	C4A-NA-C1A	6.84	109.78	106.71
13	g	841	CLA	C4A-NA-C1A	6.84	109.78	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	815	CLA	C4A-NA-C1A	6.83	109.78	106.71
13	g	820	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	e	838	CLA	C4A-NA-C1A	6.82	109.77	106.71
13	G	830	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	g	821	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	B	838	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	B	825	CLA	C4A-NA-C1A	6.81	109.77	106.71
13	A	839	CLA	C4A-NA-C1A	6.80	109.77	106.71
13	A	814	CLA	C4A-NA-C1A	6.80	109.76	106.71
13	A	833	CLA	C4A-NA-C1A	6.79	109.76	106.71
13	B	816	CLA	C4A-NA-C1A	6.79	109.76	106.71
13	G	820	CLA	C4A-NA-C1A	6.79	109.76	106.71
13	G	840	CLA	C4A-NA-C1A	6.78	109.76	106.71
13	A	828	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	e	827	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	b	829	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	G	819	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	O	203	CLA	C4A-NA-C1A	6.78	109.75	106.71
13	b	815	CLA	C4A-NA-C1A	6.77	109.75	106.71
13	B	840	CLA	C4A-NA-C1A	6.77	109.75	106.71
13	b	828	CLA	C4A-NA-C1A	6.77	109.75	106.71
13	E	816	CLA	C4A-NA-C1A	6.76	109.75	106.71
13	G	816	CLA	C4A-NA-C1A	6.76	109.75	106.71
13	a	833	CLA	C4A-NA-C1A	6.75	109.74	106.71
13	b	839	CLA	C4A-NA-C1A	6.75	109.74	106.71
13	a	816	CLA	C4A-NA-C1A	6.74	109.74	106.71
13	E	814	CLA	C4A-NA-C1A	6.74	109.73	106.71
13	a	814	CLA	C4A-NA-C1A	6.74	109.73	106.71
13	A	816	CLA	C4A-NA-C1A	6.73	109.73	106.71
13	G	825	CLA	C4A-NA-C1A	6.73	109.73	106.71
13	B	820	CLA	C4A-NA-C1A	6.73	109.73	106.71
13	B	805	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	E	828	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	g	817	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	A	809	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	e	808	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	b	824	CLA	C4A-NA-C1A	6.72	109.73	106.71
13	a	811	CLA	C4A-NA-C1A	6.71	109.72	106.71
13	b	837	CLA	C4A-NA-C1A	6.71	109.72	106.71
13	A	817	CLA	C4A-NA-C1A	6.71	109.72	106.71
13	G	838	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	b	823	CLA	C4A-NA-C1A	6.70	109.72	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	819	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	b	836	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	E	807	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	E	817	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	g	826	CLA	C4A-NA-C1A	6.70	109.72	106.71
13	e	832	CLA	C4A-NA-C1A	6.69	109.72	106.71
13	B	826	CLA	C4A-NA-C1A	6.69	109.71	106.71
13	G	837	CLA	C4A-NA-C1A	6.69	109.71	106.71
13	g	827	CLA	C4A-NA-C1A	6.68	109.71	106.71
13	B	837	CLA	C4A-NA-C1A	6.68	109.71	106.71
13	a	809	CLA	C4A-NA-C1A	6.68	109.71	106.71
13	a	817	CLA	C4A-NA-C1A	6.68	109.71	106.71
13	G	826	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	b	825	CLA	C4A-NA-C1A	6.67	109.70	106.71
13	E	809	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	e	806	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	g	825	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	b	804	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	g	806	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	a	807	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	G	821	CLA	C4A-NA-C1A	6.66	109.70	106.71
13	A	843	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	B	822	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	E	846	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	B	824	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	b	820	CLA	C4A-NA-C1A	6.63	109.69	106.71
13	A	811	CLA	C4A-NA-C1A	6.63	109.69	106.71
13	g	823	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	g	838	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	A	807	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	B	813	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	e	810	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	b	801	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	b	821	CLA	C4A-NA-C1A	6.61	109.68	106.71
13	g	822	CLA	C4A-NA-C1A	6.60	109.67	106.71
13	G	841	CLA	C4A-NA-C1A	6.60	109.67	106.71
13	a	844	CLA	C4A-NA-C1A	6.60	109.67	106.71
13	E	811	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	e	816	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	G	824	CLA	C4A-NA-C1A	6.59	109.67	106.71
13	G	804	CLA	C4A-NA-C1A	6.58	109.66	106.71
13	a	845	CLA	C4A-NA-C1A	6.57	109.66	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	812	CLA	C4A-NA-C1A	6.57	109.66	106.71
13	g	803	CLA	C4A-NA-C1A	6.57	109.66	106.71
13	B	821	CLA	C4A-NA-C1A	6.57	109.66	106.71
13	E	829	CLA	C4A-NA-C1A	6.57	109.66	106.71
13	e	825	CLA	C4A-NA-C1A	6.56	109.66	106.71
13	A	826	CLA	C4A-NA-C1A	6.56	109.65	106.71
13	e	843	CLA	C4A-NA-C1A	6.56	109.65	106.71
13	A	825	CLA	C4A-NA-C1A	6.54	109.65	106.71
13	E	826	CLA	C4A-NA-C1A	6.54	109.65	106.71
13	g	814	CLA	C4A-NA-C1A	6.53	109.64	106.71
13	E	845	CLA	C4A-NA-C1A	6.53	109.64	106.71
13	a	815	CLA	C4A-NA-C1A	6.53	109.64	106.71
13	e	828	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	a	812	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	b	840	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	g	842	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	s	205	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	a	829	CLA	C4A-NA-C1A	6.52	109.64	106.71
13	g	812	CLA	C4A-NA-C1A	6.51	109.64	106.71
13	L	203	CLA	C4A-NA-C1A	6.51	109.63	106.71
13	b	810	CLA	C4A-NA-C1A	6.51	109.63	106.71
13	E	815	CLA	C4A-NA-C1A	6.50	109.63	106.71
13	A	815	CLA	C4A-NA-C1A	6.50	109.63	106.71
13	G	813	CLA	C4A-NA-C1A	6.50	109.63	106.71
13	A	829	CLA	C4A-NA-C1A	6.49	109.63	106.71
13	g	802	CLA	C4A-NA-C1A	6.49	109.63	106.71
13	a	826	CLA	C4A-NA-C1A	6.49	109.63	106.71
13	E	830	CLA	C4A-NA-C1A	6.49	109.62	106.71
13	B	802	CLA	C4A-NA-C1A	6.49	109.62	106.71
13	E	812	CLA	C4A-NA-C1A	6.49	109.62	106.71
13	b	831	CLA	C4A-NA-C1A	6.49	109.62	106.71
13	B	841	CLA	C4A-NA-C1A	6.49	109.62	106.71
13	E	844	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	G	822	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	a	825	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	e	814	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	l	204	CLA	C4A-NA-C1A	6.48	109.62	106.71
13	B	801	CLA	C4A-NA-C1A	6.47	109.62	106.71
13	e	842	CLA	C4A-NA-C1A	6.47	109.62	106.71
13	A	844	CLA	C4A-NA-C1A	6.47	109.61	106.71
13	B	832	CLA	C4A-NA-C1A	6.47	109.61	106.71
13	b	806	CLA	C4A-NA-C1A	6.47	109.61	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	806	CLA	C4A-NA-C1A	6.46	109.61	106.71
13	G	801	CLA	C4A-NA-C1A	6.46	109.61	106.71
13	e	824	CLA	C4A-NA-C1A	6.46	109.61	106.71
13	a	835	CLA	C4A-NA-C1A	6.45	109.61	106.71
13	A	812	CLA	C4A-NA-C1A	6.45	109.61	106.71
13	B	811	CLA	C4A-NA-C1A	6.45	109.61	106.71
13	G	832	CLA	C4A-NA-C1A	6.45	109.61	106.71
13	e	811	CLA	C4A-NA-C1A	6.45	109.61	106.71
13	e	829	CLA	C4A-NA-C1A	6.45	109.61	106.71
13	G	811	CLA	C4A-NA-C1A	6.44	109.60	106.71
13	g	836	CLA	C4A-NA-C1A	6.44	109.60	106.71
13	G	805	CLA	C4A-NA-C1A	6.44	109.60	106.71
13	A	830	CLA	C4A-NA-C1A	6.43	109.60	106.71
13	G	810	CLA	C4A-NA-C1A	6.43	109.60	106.71
13	e	809	CLA	C4A-NA-C1A	6.43	109.60	106.71
13	B	835	CLA	C4A-NA-C1A	6.42	109.59	106.71
13	a	808	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	b	805	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	g	809	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	g	807	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	g	813	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	o	202	CLA	C4A-NA-C1A	6.41	109.59	106.71
13	b	834	CLA	C4A-NA-C1A	6.40	109.58	106.71
13	B	807	CLA	C4A-NA-C1A	6.40	109.58	106.71
13	G	807	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	G	802	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	g	808	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	E	813	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	s	202	CLA	C4A-NA-C1A	6.39	109.58	106.71
13	E	825	CLA	C4A-NA-C1A	6.38	109.58	106.71
13	E	835	CLA	C4A-NA-C1A	6.38	109.58	106.71
13	g	832	CLA	C4A-NA-C1A	6.38	109.58	106.71
13	b	802	CLA	C4A-NA-C1A	6.38	109.58	106.71
13	S	203	CLA	C4A-NA-C1A	6.38	109.57	106.71
13	a	830	CLA	C4A-NA-C1A	6.37	109.57	106.71
13	B	812	CLA	C4A-NA-C1A	6.37	109.57	106.71
13	g	833	CLA	C4A-NA-C1A	6.37	109.57	106.71
13	B	806	CLA	C4A-NA-C1A	6.37	109.57	106.71
13	e	812	CLA	C4A-NA-C1A	6.37	109.57	106.71
13	E	810	CLA	C4A-NA-C1A	6.36	109.56	106.71
13	B	834	CLA	C4A-NA-C1A	6.36	109.56	106.71
13	A	810	CLA	C4A-NA-C1A	6.35	109.56	106.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	853	CLA	C4A-NA-C1A	6.34	109.56	106.71
13	e	807	CLA	C4A-NA-C1A	6.34	109.56	106.71
13	g	835	CLA	C4A-NA-C1A	6.34	109.56	106.71
13	G	831	CLA	C4A-NA-C1A	6.34	109.56	106.71
13	G	835	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	b	813	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	G	814	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	A	808	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	E	808	CLA	C4A-NA-C1A	6.33	109.55	106.71
13	G	834	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	a	832	CLA	C4A-NA-C1A	6.32	109.55	106.71
13	E	832	CLA	C4A-NA-C1A	6.31	109.54	106.71
13	g	815	CLA	C4A-NA-C1A	6.31	109.54	106.71
13	a	810	CLA	C4A-NA-C1A	6.31	109.54	106.71
13	B	814	CLA	C4A-NA-C1A	6.31	109.54	106.71
13	A	813	CLA	C4A-NA-C1A	6.30	109.54	106.71
13	A	832	CLA	C4A-NA-C1A	6.30	109.54	106.71
13	G	808	CLA	C4A-NA-C1A	6.30	109.54	106.71
13	b	808	CLA	C4A-NA-C1A	6.30	109.54	106.71
13	b	833	CLA	C4A-NA-C1A	6.29	109.53	106.71
13	e	852	CLA	C4A-NA-C1A	6.28	109.53	106.71
13	a	813	CLA	C4A-NA-C1A	6.28	109.53	106.71
13	b	830	CLA	C4A-NA-C1A	6.28	109.53	106.71
13	e	841	CLA	C4A-NA-C1A	6.28	109.53	106.71
13	g	810	CLA	C4A-NA-C1A	6.27	109.53	106.71
13	E	843	CLA	C4A-NA-C1A	6.26	109.52	106.71
13	B	808	CLA	C4A-NA-C1A	6.26	109.52	106.71
13	B	831	CLA	C4A-NA-C1A	6.25	109.52	106.71
13	A	837	CLA	C4A-NA-C1A	6.24	109.51	106.71
13	e	831	CLA	C4A-NA-C1A	6.24	109.51	106.71
13	e	836	CLA	C4A-NA-C1A	6.24	109.51	106.71
13	b	807	CLA	C4A-NA-C1A	6.24	109.51	106.71
13	a	806	CLA	C4A-NA-C1A	6.23	109.51	106.71
13	g	819	CLA	C4A-NA-C1A	6.23	109.50	106.71
13	G	818	CLA	C4A-NA-C1A	6.22	109.50	106.71
13	B	818	CLA	C4A-NA-C1A	6.20	109.50	106.71
13	A	806	CLA	C4A-NA-C1A	6.20	109.49	106.71
13	B	809	CLA	C4A-NA-C1A	6.19	109.49	106.71
13	E	834	CLA	C4A-NA-C1A	6.19	109.49	106.71
13	E	838	CLA	C4A-NA-C1A	6.19	109.49	106.71
13	r	101	CLA	C4A-NA-C1A	6.19	109.49	106.71
13	a	838	CLA	C4A-NA-C1A	6.18	109.49	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	817	CLA	C4A-NA-C1A	6.17	109.48	106.71
13	a	843	CLA	C4A-NA-C1A	6.15	109.47	106.71
13	E	821	CLA	C4A-NA-C1A	6.14	109.47	106.71
13	e	805	CLA	C4A-NA-C1A	6.13	109.46	106.71
13	E	805	CLA	C4A-NA-C1A	6.13	109.46	106.71
13	A	821	CLA	C4A-NA-C1A	6.13	109.46	106.71
13	e	820	CLA	C4A-NA-C1A	6.13	109.46	106.71
13	e	826	CLA	C4A-NA-C1A	6.13	109.46	106.71
13	B	828	CLA	C4A-NA-C1A	6.12	109.46	106.71
13	a	827	CLA	C4A-NA-C1A	6.12	109.46	106.71
13	A	834	CLA	C4A-NA-C1A	6.11	109.45	106.71
13	a	834	CLA	C4A-NA-C1A	6.11	109.45	106.71
13	E	822	CLA	C4A-NA-C1A	6.11	109.45	106.71
13	g	801	CLA	C4A-NA-C1A	6.11	109.45	106.71
13	e	833	CLA	C4A-NA-C1A	6.11	109.45	106.71
13	a	805	CLA	C4A-NA-C1A	6.10	109.45	106.71
13	a	821	CLA	C4A-NA-C1A	6.10	109.45	106.71
13	F	202	CLA	C4A-NA-C1A	6.10	109.45	106.71
13	e	821	CLA	C4A-NA-C1A	6.10	109.45	106.71
13	A	842	CLA	C4A-NA-C1A	6.09	109.44	106.71
13	K	101	CLA	C4A-NA-C1A	6.09	109.44	106.71
13	g	829	CLA	C4A-NA-C1A	6.09	109.44	106.71
13	G	812	CLA	C4A-NA-C1A	6.08	109.44	106.71
13	A	827	CLA	C4A-NA-C1A	6.08	109.44	106.71
13	l	201	CLA	C4A-NA-C1A	6.08	109.44	106.71
13	A	804	CLA	C4A-NA-C1A	6.07	109.44	106.71
13	b	827	CLA	C4A-NA-C1A	6.07	109.44	106.71
13	b	816	CLA	C4A-NA-C1A	6.07	109.43	106.71
13	A	805	CLA	C4A-NA-C1A	6.06	109.43	106.71
13	E	804	CLA	C4A-NA-C1A	6.06	109.43	106.71
13	S	206	CLA	C4A-NA-C1A	6.04	109.42	106.71
13	E	806	CLA	C4A-NA-C1A	6.04	109.42	106.71
13	a	819	CLA	C4A-NA-C1A	6.04	109.42	106.71
13	G	828	CLA	C4A-NA-C1A	6.03	109.42	106.71
13	E	827	CLA	C4A-NA-C1A	6.02	109.41	106.71
13	a	804	CLA	C4A-NA-C1A	6.02	109.41	106.71
13	A	822	CLA	C4A-NA-C1A	6.01	109.41	106.71
13	b	811	CLA	C4A-NA-C1A	6.01	109.41	106.71
13	A	819	CLA	C4A-NA-C1A	5.98	109.40	106.71
13	E	831	CLA	C4A-NA-C1A	5.98	109.40	106.71
13	G	817	CLA	C4A-NA-C1A	5.98	109.39	106.71
13	e	818	CLA	C4A-NA-C1A	5.97	109.39	106.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	831	CLA	C4A-NA-C1A	5.97	109.39	106.71
13	e	830	CLA	C4A-NA-C1A	5.97	109.39	106.71
13	a	822	CLA	C4A-NA-C1A	5.97	109.39	106.71
13	l	205	CLA	CAA-C2A-C3A	-5.97	96.43	112.78
13	S	204	CLA	CAA-C2A-C3A	-5.97	96.44	112.78
13	E	819	CLA	C4A-NA-C1A	5.96	109.39	106.71
13	e	804	CLA	C4A-NA-C1A	5.96	109.39	106.71
13	L	204	CLA	CAA-C2A-C3A	-5.96	96.47	112.78
13	s	203	CLA	CAA-C2A-C3A	-5.94	96.50	112.78
13	G	827	CLA	C4A-NA-C1A	5.93	109.37	106.71
13	G	833	CLA	C4A-NA-C1A	5.93	109.37	106.71
13	b	826	CLA	C4A-NA-C1A	5.92	109.37	106.71
13	g	818	CLA	C4A-NA-C1A	5.91	109.36	106.71
13	g	834	CLA	C4A-NA-C1A	5.91	109.36	106.71
13	B	817	CLA	C4A-NA-C1A	5.90	109.36	106.71
13	B	833	CLA	C4A-NA-C1A	5.89	109.36	106.71
13	k	4002	CLA	C4A-NA-C1A	5.89	109.36	106.71
13	A	831	CLA	C4A-NA-C1A	5.89	109.35	106.71
13	r	102	CLA	C4A-NA-C1A	5.88	109.35	106.71
13	R	102	CLA	C4A-NA-C1A	5.87	109.34	106.71
13	a	852	CLA	C4A-NA-C1A	5.86	109.34	106.71
13	B	804	CLA	C4A-NA-C1A	5.85	109.34	106.71
13	g	828	CLA	C4A-NA-C1A	5.85	109.33	106.71
13	b	832	CLA	C4A-NA-C1A	5.83	109.33	106.71
13	L	202	CLA	C4A-NA-C1A	5.82	109.32	106.71
13	B	827	CLA	C4A-NA-C1A	5.81	109.32	106.71
13	g	805	CLA	C4A-NA-C1A	5.80	109.31	106.71
13	K	102	CLA	C4A-NA-C1A	5.79	109.31	106.71
13	A	836	CLA	C4A-NA-C1A	5.79	109.31	106.71
13	G	803	CLA	C4A-NA-C1A	5.78	109.31	106.71
13	a	837	CLA	C4A-NA-C1A	5.77	109.30	106.71
13	b	803	CLA	C4A-NA-C1A	5.73	109.28	106.71
13	E	837	CLA	C4A-NA-C1A	5.71	109.27	106.71
13	e	835	CLA	C4A-NA-C1A	5.68	109.26	106.71
13	l	203	CLA	C4A-NA-C1A	5.64	109.24	106.71
13	E	818	CLA	C4A-NA-C1A	5.35	109.11	106.71
13	e	817	CLA	C4A-NA-C1A	5.35	109.11	106.71
13	a	818	CLA	C4A-NA-C1A	5.30	109.09	106.71
13	S	204	CLA	C3A-C2A-C1A	5.25	109.21	101.34
13	A	818	CLA	C4A-NA-C1A	5.25	109.07	106.71
13	l	205	CLA	C3A-C2A-C1A	5.25	109.21	101.34
13	s	203	CLA	C3A-C2A-C1A	5.24	109.19	101.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	204	CLA	C3A-C2A-C1A	5.21	109.15	101.34
13	E	803	CLA	C4A-NA-C1A	5.12	109.01	106.71
13	A	803	CLA	C4A-NA-C1A	4.99	108.95	106.71
15	a	848	BCR	C2-C1-C6	4.98	118.16	110.48
13	e	803	CLA	C4A-NA-C1A	4.92	108.92	106.71
13	e	822	CLA	C4A-NA-C1A	4.91	108.92	106.71
15	a	848	BCR	C34-C9-C10	-4.81	116.18	122.92
13	E	823	CLA	C4A-NA-C1A	4.81	108.87	106.71
13	A	823	CLA	C4A-NA-C1A	4.72	108.83	106.71
13	a	823	CLA	C4A-NA-C1A	4.70	108.82	106.71
13	e	804	CLA	CMB-C2B-C1B	-4.68	121.28	128.46
13	a	804	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
13	E	804	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
13	A	804	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
13	A	818	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
13	a	818	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
13	E	818	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
13	e	817	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
13	E	833	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
13	e	832	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
13	a	833	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
13	A	833	CLA	CMB-C2B-C1B	-4.46	121.62	128.46
15	a	848	BCR	C11-C10-C9	-4.44	120.97	127.31
13	G	822	CLA	CMB-C2B-C1B	-4.41	121.68	128.46
13	b	821	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
13	O	203	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
13	f	203	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
13	g	823	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
13	B	822	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
13	L	202	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
13	l	203	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
13	E	846	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
13	E	843	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
12	A	801	LHG	O4-P-O5	4.34	133.68	112.24
13	e	841	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
13	A	842	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
12	e	801	LHG	O4-P-O5	4.33	133.65	112.24
13	a	819	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
12	a	801	LHG	O4-P-O5	4.32	133.60	112.24
13	e	818	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
13	A	819	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
13	a	843	CLA	CMB-C2B-C1B	-4.30	121.86	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	819	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
13	G	802	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
13	g	826	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
13	G	825	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
13	b	824	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
13	A	853	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
13	B	825	CLA	CMB-C2B-C1B	-4.27	121.89	128.46
13	b	802	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
13	E	823	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
13	e	852	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
13	a	840	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
13	S	203	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
13	L	203	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
13	a	823	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
13	A	839	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
13	e	838	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
13	e	822	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
13	E	840	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
13	l	204	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
13	s	202	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
13	A	823	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
12	e	802	LHG	O4-P-O5	4.17	132.85	112.24
13	G	837	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
13	b	836	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
13	g	838	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
13	g	811	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
13	E	835	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
13	B	837	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
13	B	810	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
12	A	802	LHG	O4-P-O5	4.11	132.58	112.24
13	B	801	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
13	G	809	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
13	A	828	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
13	g	802	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
13	a	835	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
13	a	828	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
13	b	809	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
13	E	828	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
13	e	827	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
15	k	4001	BCR	C24-C23-C22	-4.02	120.16	126.23
13	g	831	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
13	G	834	CLA	CMB-C2B-C1B	-4.01	122.30	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	830	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
13	A	815	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
13	B	830	CLA	CMB-C2B-C1B	-3.99	122.32	128.46
13	b	829	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
13	A	831	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
13	g	835	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
13	b	833	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
13	E	815	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
13	a	815	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
13	B	834	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
13	e	814	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
13	B	818	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
13	a	831	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
13	e	830	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
13	b	825	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
13	G	818	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
13	b	817	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
13	a	804	CLA	CMB-C2B-C3B	3.94	132.04	124.68
13	g	819	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
13	G	836	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
13	e	804	CLA	CMB-C2B-C3B	3.93	132.03	124.68
13	G	826	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
13	B	826	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
13	A	804	CLA	CMB-C2B-C3B	3.93	132.03	124.68
13	E	831	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
13	b	835	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
13	g	837	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
13	g	827	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
13	E	804	CLA	CMB-C2B-C3B	3.92	132.00	124.68
13	l	205	CLA	CHB-C4A-NA	3.91	129.93	124.51
13	L	204	CLA	CHB-C4A-NA	3.91	129.92	124.51
13	a	808	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
13	G	814	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
13	B	836	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
13	b	813	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
15	k	4001	BCR	C36-C18-C19	-3.90	111.93	118.08
13	S	204	CLA	CHB-C4A-NA	3.90	129.91	124.51
13	B	814	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
14	g	843	PQN	C11-C12-C13	-3.90	120.30	126.79
13	E	808	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
13	s	203	CLA	CHB-C4A-NA	3.89	129.89	124.51
13	e	807	CLA	CMB-C2B-C1B	-3.88	122.50	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	841	PQN	C11-C12-C13	-3.87	120.34	126.79
13	g	815	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
13	A	808	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
14	e	845	PQN	C11-C12-C13	-3.84	120.40	126.79
14	E	848	PQN	C11-C12-C13	-3.84	120.40	126.79
13	b	805	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
14	G	842	PQN	C11-C12-C13	-3.84	120.41	126.79
14	B	842	PQN	C11-C12-C13	-3.82	120.42	126.79
13	A	818	CLA	CMB-C2B-C3B	3.80	131.80	124.68
13	B	806	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
13	l	203	CLA	CMB-C2B-C3B	3.80	131.78	124.68
13	E	830	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
13	L	202	CLA	CMB-C2B-C3B	3.80	131.78	124.68
13	G	805	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
13	g	807	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
13	B	805	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
13	E	818	CLA	CMB-C2B-C3B	3.78	131.75	124.68
13	G	804	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
13	b	804	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
13	e	817	CLA	CMB-C2B-C3B	3.78	131.75	124.68
13	e	832	CLA	CMB-C2B-C3B	3.77	131.73	124.68
13	A	830	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
13	e	829	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
13	a	830	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
13	a	818	CLA	CMB-C2B-C3B	3.77	131.72	124.68
14	A	846	PQN	C11-C12-C13	-3.76	120.53	126.79
13	g	806	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
14	a	847	PQN	C11-C12-C13	-3.75	120.54	126.79
13	a	833	CLA	CMB-C2B-C3B	3.75	131.70	124.68
13	b	831	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
13	B	824	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
13	E	833	CLA	CMB-C2B-C3B	3.74	131.68	124.68
13	a	836	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
13	b	815	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
13	G	832	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
13	G	824	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
13	A	835	CLA	CMB-C2B-C1B	-3.73	122.72	128.46
13	g	825	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
13	E	836	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
13	A	833	CLA	CMB-C2B-C3B	3.73	131.66	124.68
13	g	833	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
13	b	823	CLA	O2D-CGD-O1D	-3.73	116.55	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	816	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
13	B	832	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
13	g	817	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
13	E	846	CLA	CMB-C2B-C3B	3.71	131.62	124.68
13	e	834	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
13	B	816	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
13	G	810	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
13	B	811	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
13	b	810	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
13	A	803	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
13	a	839	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
13	E	824	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
13	g	812	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
13	O	203	CLA	CMB-C2B-C3B	3.67	131.55	124.68
13	A	838	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
13	g	823	CLA	CMB-C2B-C3B	3.67	131.54	124.68
13	B	822	CLA	CMB-C2B-C3B	3.66	131.53	124.68
13	e	823	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
13	E	839	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
15	e	846	BCR	C24-C23-C22	-3.66	120.71	126.23
13	G	822	CLA	CMB-C2B-C3B	3.65	131.51	124.68
13	B	815	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
13	e	837	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
13	b	821	CLA	CMB-C2B-C3B	3.64	131.49	124.68
13	a	824	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
13	A	824	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
13	e	805	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
13	g	816	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
13	E	806	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
13	G	815	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
13	E	843	CLA	CMB-C2B-C3B	3.63	131.47	124.68
15	A	847	BCR	C24-C23-C22	-3.63	120.75	126.23
15	a	849	BCR	C24-C23-C22	-3.63	120.75	126.23
13	E	844	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
13	g	826	CLA	CMB-C2B-C3B	3.63	131.46	124.68
13	e	842	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
13	G	809	CLA	CMB-C2B-C3B	3.62	131.46	124.68
13	e	841	CLA	CMB-C2B-C3B	3.62	131.46	124.68
13	b	814	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
15	E	849	BCR	C24-C23-C22	-3.62	120.77	126.23
13	b	824	CLA	CMB-C2B-C3B	3.62	131.44	124.68
13	f	203	CLA	CMB-C2B-C3B	3.61	131.44	124.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	g	842	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
13	g	811	CLA	CMB-C2B-C3B	3.61	131.44	124.68
13	G	825	CLA	CMB-C2B-C3B	3.61	131.44	124.68
13	A	843	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
13	G	841	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
13	B	841	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
13	b	802	CLA	CMB-C2B-C3B	3.61	131.43	124.68
13	A	842	CLA	CMB-C2B-C3B	3.61	131.42	124.68
13	a	807	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
13	A	806	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
13	a	806	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
13	G	802	CLA	CMB-C2B-C3B	3.60	131.41	124.68
13	a	844	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
13	B	810	CLA	CMB-C2B-C3B	3.59	131.40	124.68
13	B	825	CLA	CMB-C2B-C3B	3.59	131.40	124.68
13	b	818	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
13	E	807	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
13	B	839	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
13	b	809	CLA	CMB-C2B-C3B	3.58	131.38	124.68
13	g	840	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
15	R	101	BCR	C28-C27-C26	-3.58	107.68	114.08
13	a	843	CLA	CMB-C2B-C3B	3.58	131.37	124.68
13	A	853	CLA	CMB-C2B-C3B	3.58	131.37	124.68
13	G	839	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
13	b	828	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
13	G	829	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
13	b	840	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
13	b	837	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
13	e	806	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
13	A	807	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
13	a	805	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
13	e	852	CLA	CMB-C2B-C3B	3.56	131.35	124.68
13	G	838	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
13	E	823	CLA	CMB-C2B-C3B	3.56	131.34	124.68
13	r	101	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
13	A	836	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
13	e	822	CLA	CMB-C2B-C3B	3.56	131.33	124.68
13	g	839	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
13	b	838	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
13	A	845	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
13	B	829	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
13	K	101	CLA	CMB-C2B-C1B	-3.55	123.00	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	819	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
13	a	823	CLA	CMB-C2B-C3B	3.55	131.32	124.68
13	G	806	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
13	A	823	CLA	CMB-C2B-C3B	3.54	131.31	124.68
13	g	830	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
13	g	820	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
13	B	838	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
13	e	835	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
13	g	808	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
13	B	819	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
13	B	807	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
13	g	801	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
13	A	805	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
13	E	837	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
13	E	805	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
13	a	837	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
13	b	806	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
13	e	838	CLA	CMB-C2B-C3B	3.50	131.23	124.68
13	b	836	CLA	CMB-C2B-C3B	3.50	131.23	124.68
13	G	837	CLA	CMB-C2B-C3B	3.50	131.23	124.68
13	A	839	CLA	CMB-C2B-C3B	3.50	131.23	124.68
13	E	840	CLA	CMB-C2B-C3B	3.49	131.22	124.68
13	g	838	CLA	CMB-C2B-C3B	3.49	131.21	124.68
13	a	840	CLA	CMB-C2B-C3B	3.49	131.21	124.68
13	F	202	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
13	B	835	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
13	G	835	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
13	A	828	CLA	CMB-C2B-C3B	3.48	131.18	124.68
13	g	836	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
13	B	837	CLA	CMB-C2B-C3B	3.47	131.17	124.68
13	l	204	CLA	CMB-C2B-C3B	3.47	131.17	124.68
13	b	834	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
13	E	828	CLA	CMB-C2B-C3B	3.47	131.16	124.68
13	a	828	CLA	CMB-C2B-C3B	3.47	131.16	124.68
13	e	803	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
13	S	203	CLA	CMB-C2B-C3B	3.46	131.15	124.68
13	L	203	CLA	CMB-C2B-C3B	3.45	131.14	124.68
13	b	808	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
13	g	810	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
13	e	827	CLA	CMB-C2B-C3B	3.45	131.12	124.68
13	G	808	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
13	B	809	CLA	CMB-C2B-C1B	-3.44	123.17	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	813	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
13	E	825	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
13	o	202	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
13	a	825	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
13	s	202	CLA	CMB-C2B-C3B	3.44	131.11	124.68
13	G	813	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
13	A	827	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
13	A	821	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
13	e	824	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
13	o	202	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
13	e	826	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
13	g	814	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
13	A	820	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
13	a	827	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
13	b	812	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
13	a	834	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
13	e	844	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
13	A	826	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
13	e	820	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
13	E	803	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
13	B	808	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
13	e	833	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
13	A	825	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
13	a	826	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
13	b	807	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
13	b	835	CLA	CMB-C2B-C3B	3.41	131.05	124.68
13	e	825	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
13	a	821	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
13	e	813	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
13	e	843	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
13	a	813	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
13	a	845	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
13	E	803	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
13	A	834	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
13	g	809	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
13	a	820	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
13	a	852	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
13	E	814	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
13	e	836	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
13	b	813	CLA	CMB-C2B-C3B	3.40	131.03	124.68
13	G	807	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
13	G	836	CLA	O2D-CGD-O1D	-3.40	117.20	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K	102	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
13	a	838	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
13	e	812	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
13	A	814	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
13	g	837	CLA	CMB-C2B-C3B	3.39	131.02	124.68
13	A	813	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
13	A	844	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
13	a	814	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
13	a	822	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
13	E	821	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
13	E	827	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
13	E	838	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
13	A	837	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
13	g	821	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
13	B	836	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
13	A	822	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
13	g	815	CLA	CMB-C2B-C3B	3.38	131.01	124.68
13	G	814	CLA	CMB-C2B-C3B	3.38	131.01	124.68
13	E	834	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
13	E	845	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
13	B	814	CLA	CMB-C2B-C3B	3.38	131.00	124.68
13	E	820	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
13	b	803	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
13	e	819	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
13	g	803	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
13	g	805	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
13	b	816	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
13	B	836	CLA	CMB-C2B-C3B	3.37	130.99	124.68
13	b	801	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
13	G	836	CLA	CMB-C2B-C3B	3.37	130.99	124.68
13	G	803	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
13	k	4002	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
13	F	202	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
13	E	826	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
13	e	844	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
13	B	817	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
13	a	836	CLA	CMB-C2B-C3B	3.36	130.97	124.68
13	E	816	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
13	G	817	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
13	E	813	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
13	R	102	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
13	r	102	CLA	CMB-C2B-C1B	-3.36	123.30	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	812	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
13	e	815	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
13	E	836	CLA	CMB-C2B-C3B	3.36	130.96	124.68
13	e	811	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
13	b	835	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
13	E	810	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
13	G	801	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
13	A	810	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
13	g	837	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
13	G	820	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
13	G	821	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
13	a	812	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
13	g	818	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
13	E	812	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
13	g	831	CLA	CMB-C2B-C3B	3.34	130.93	124.68
13	e	809	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
13	e	821	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
13	B	802	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
13	B	821	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
13	A	835	CLA	CMB-C2B-C3B	3.34	130.92	124.68
13	B	830	CLA	CMB-C2B-C3B	3.34	130.92	124.68
13	A	816	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
13	G	840	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
13	e	828	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
13	B	820	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
13	g	841	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
13	B	804	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
13	a	816	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
13	B	840	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
13	b	819	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
13	e	834	CLA	CMB-C2B-C3B	3.32	130.90	124.68
13	a	808	CLA	CMB-C2B-C3B	3.32	130.90	124.68
13	a	810	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
13	E	835	CLA	CMB-C2B-C3B	3.32	130.89	124.68
13	G	830	CLA	CMB-C2B-C3B	3.32	130.89	124.68
13	E	822	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
13	E	829	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
13	A	845	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
13	B	818	CLA	CMB-C2B-C3B	3.31	130.87	124.68
13	b	817	CLA	CMB-C2B-C3B	3.31	130.86	124.68
13	E	808	CLA	CMB-C2B-C3B	3.30	130.86	124.68
13	b	839	CLA	CMB-C2B-C1B	-3.30	123.39	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	829	CLA	CMB-C2B-C3B	3.30	130.85	124.68
13	g	822	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
13	b	820	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
13	B	801	CLA	CMB-C2B-C3B	3.30	130.85	124.68
13	e	807	CLA	CMB-C2B-C3B	3.30	130.85	124.68
13	A	829	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
13	A	808	CLA	CMB-C2B-C3B	3.29	130.84	124.68
13	b	825	CLA	CMB-C2B-C3B	3.29	130.84	124.68
13	A	817	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
13	g	802	CLA	CMB-C2B-C3B	3.29	130.83	124.68
13	G	826	CLA	CMB-C2B-C3B	3.29	130.83	124.68
13	A	815	CLA	CMB-C2B-C3B	3.29	130.83	124.68
15	R	101	BCR	C30-C25-C26	-3.29	117.98	122.61
13	a	829	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
13	e	816	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
13	E	817	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
13	a	835	CLA	CMB-C2B-C3B	3.28	130.82	124.68
13	g	827	CLA	CMB-C2B-C3B	3.28	130.82	124.68
13	a	815	CLA	CMB-C2B-C3B	3.28	130.82	124.68
13	G	811	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
13	g	813	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
13	B	826	CLA	CMB-C2B-C3B	3.28	130.82	124.68
13	g	819	CLA	CMB-C2B-C3B	3.28	130.82	124.68
13	B	812	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
13	E	815	CLA	CMB-C2B-C3B	3.28	130.81	124.68
15	R	101	BCR	C3-C4-C5	-3.28	108.22	114.08
13	G	818	CLA	CMB-C2B-C3B	3.27	130.80	124.68
13	B	823	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
13	g	824	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
13	A	842	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
13	a	817	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
13	b	822	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
13	G	823	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
13	s	205	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
13	g	835	CLA	CMB-C2B-C3B	3.25	130.77	124.68
13	b	826	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
13	g	832	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
13	G	833	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
13	B	833	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
13	e	840	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
13	e	814	CLA	CMB-C2B-C3B	3.25	130.75	124.68
13	g	834	CLA	CMB-C2B-C1B	-3.25	123.47	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	833	CLA	CMB-C2B-C3B	3.25	130.75	124.68
13	B	834	CLA	CMB-C2B-C3B	3.25	130.75	124.68
13	G	834	CLA	CMB-C2B-C3B	3.25	130.75	124.68
13	a	843	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
13	b	830	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
13	a	808	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
13	b	832	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
13	e	807	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
13	E	843	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
13	B	831	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
13	b	825	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
13	B	826	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
13	A	808	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
13	E	808	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
13	G	827	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
13	a	842	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
13	g	828	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
13	G	831	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
13	A	841	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
13	g	827	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
13	e	841	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
13	E	832	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
13	A	811	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
13	b	827	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
13	E	842	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
13	e	810	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
13	g	834	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
13	e	831	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
13	E	811	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
13	B	828	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
13	a	811	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
13	b	832	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
13	g	829	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
13	B	833	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
13	A	832	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
13	G	828	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
13	G	812	CLA	CMB-C2B-C1B	-3.19	123.55	128.46
13	a	832	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
13	G	826	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
13	B	827	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
13	A	803	CLA	CMB-C2B-C3B	3.19	130.64	124.68
13	E	803	CLA	CMB-C2B-C3B	3.18	130.64	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	807	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
13	l	201	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
13	b	811	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
13	A	819	CLA	CMB-C2B-C3B	3.18	130.62	124.68
15	a	848	BCR	C1-C6-C5	-3.18	118.14	122.61
13	G	833	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
13	G	806	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
13	A	827	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
13	b	805	CLA	CMB-C2B-C3B	3.17	130.60	124.68
13	g	808	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
13	S	206	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
13	e	829	CLA	CMB-C2B-C3B	3.16	130.59	124.68
13	b	806	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
13	e	830	CLA	CMB-C2B-C3B	3.15	130.58	124.68
13	E	827	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
13	E	830	CLA	CMB-C2B-C3B	3.15	130.57	124.68
13	a	827	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
13	e	818	CLA	CMB-C2B-C3B	3.15	130.57	124.68
13	a	819	CLA	CMB-C2B-C3B	3.15	130.57	124.68
13	g	807	CLA	CMB-C2B-C3B	3.15	130.56	124.68
13	e	826	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
13	a	830	CLA	CMB-C2B-C3B	3.14	130.56	124.68
13	A	831	CLA	CMB-C2B-C3B	3.14	130.55	124.68
13	s	203	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
13	B	806	CLA	CMB-C2B-C3B	3.14	130.55	124.68
13	A	830	CLA	CMB-C2B-C3B	3.13	130.54	124.68
13	a	831	CLA	CMB-C2B-C3B	3.13	130.54	124.68
13	e	841	CLA	C1-C2-C3	-3.13	121.69	126.75
13	G	804	CLA	CMB-C2B-C3B	3.13	130.53	124.68
13	E	819	CLA	CMB-C2B-C3B	3.13	130.53	124.68
13	B	805	CLA	CMB-C2B-C3B	3.13	130.53	124.68
15	m	101	BCR	C2-C1-C6	3.12	115.29	110.48
13	L	204	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
13	A	842	CLA	C1-C2-C3	-3.11	121.71	126.75
13	G	809	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
13	K	101	CLA	CMB-C2B-C3B	3.11	130.50	124.68
13	e	808	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
13	B	824	CLA	O2D-CGD-CBD	3.11	116.79	111.27
13	g	806	CLA	CMB-C2B-C3B	3.11	130.50	124.68
13	l	205	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
13	G	805	CLA	CMB-C2B-C3B	3.11	130.50	124.68
13	b	809	CLA	O2D-CGD-O1D	-3.11	117.76	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	r	101	CLA	CMB-C2B-C3B	3.11	130.49	124.68
13	b	804	CLA	CMB-C2B-C3B	3.11	130.49	124.68
13	G	816	CLA	CMB-C2B-C3B	3.10	130.48	124.68
13	S	204	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
13	b	815	CLA	CMB-C2B-C3B	3.10	130.48	124.68
13	G	824	CLA	O2D-CGD-CBD	3.10	116.77	111.27
13	E	831	CLA	CMB-C2B-C3B	3.10	130.47	124.68
13	b	831	CLA	CMB-C2B-C3B	3.10	130.47	124.68
13	g	817	CLA	CMB-C2B-C3B	3.10	130.47	124.68
13	E	831	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
13	O	203	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
13	g	812	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
13	E	843	CLA	C1-C2-C3	-3.09	121.75	126.75
13	g	811	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
13	e	803	CLA	C1-C2-C3	-3.09	121.76	126.75
13	G	832	CLA	CMB-C2B-C3B	3.09	130.45	124.68
13	g	825	CLA	O2D-CGD-CBD	3.08	116.75	111.27
15	B	843	BCR	C15-C14-C13	-3.08	122.91	127.31
15	e	850	BCR	C11-C10-C9	-3.08	122.91	127.31
13	B	832	CLA	CMB-C2B-C3B	3.08	130.45	124.68
13	a	843	CLA	C1-C2-C3	-3.08	121.77	126.75
15	b	842	BCR	C15-C14-C13	-3.08	122.92	127.31
13	E	809	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
13	B	810	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
15	G	843	BCR	C15-C14-C13	-3.08	122.92	127.31
13	B	811	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
13	E	816	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
13	G	810	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
13	b	823	CLA	O2D-CGD-CBD	3.07	116.73	111.27
13	g	833	CLA	CMB-C2B-C3B	3.07	130.43	124.68
15	k	4001	BCR	C33-C5-C6	-3.07	121.08	124.53
13	B	816	CLA	CMB-C2B-C3B	3.07	130.43	124.68
13	l	205	CLA	C3D-C4D-CHA	3.07	119.75	112.72
13	a	831	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
15	g	844	BCR	C15-C14-C13	-3.07	122.93	127.31
13	b	810	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
13	A	803	CLA	C1-C2-C3	-3.07	121.79	126.75
13	A	809	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
13	a	809	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
13	f	203	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
13	L	204	CLA	C3D-C4D-CHA	3.06	119.72	112.72
13	a	816	CLA	O2D-CGD-O1D	-3.06	117.86	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	830	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
13	A	831	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
13	E	828	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
15	A	851	BCR	C11-C10-C9	-3.05	122.96	127.31
13	S	204	CLA	C3D-C4D-CHA	3.05	119.69	112.72
13	e	815	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
13	A	816	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
13	b	823	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
13	e	805	CLA	CMB-C2B-C3B	3.04	130.36	124.68
13	B	824	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
13	G	824	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
13	B	807	CLA	CMB-C2B-C3B	3.04	130.36	124.68
13	e	837	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
13	G	806	CLA	CMB-C2B-C3B	3.03	130.35	124.68
13	A	828	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
13	e	837	CLA	CMB-C2B-C3B	3.03	130.34	124.68
13	s	203	CLA	CHD-C1D-ND	-3.02	121.67	124.45
13	a	828	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
13	e	804	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
13	g	825	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
13	A	811	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
13	E	806	CLA	CMB-C2B-C3B	3.02	130.33	124.68
13	A	838	CLA	CMB-C2B-C3B	3.02	130.32	124.68
13	b	806	CLA	CMB-C2B-C3B	3.02	130.32	124.68
13	a	839	CLA	CMB-C2B-C3B	3.02	130.32	124.68
13	g	808	CLA	CMB-C2B-C3B	3.01	130.32	124.68
13	s	203	CLA	C3D-C4D-CHA	3.01	119.62	112.72
13	a	839	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
13	E	839	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
13	e	817	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
13	a	805	CLA	CMB-C2B-C3B	3.01	130.31	124.68
13	o	202	CLA	CMB-C2B-C3B	3.01	130.31	124.68
13	g	801	CLA	CMB-C2B-C3B	3.01	130.31	124.68
13	e	827	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
13	l	205	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
15	B	843	BCR	C15-C16-C17	-3.01	117.31	123.47
13	e	825	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
13	E	839	CLA	CMB-C2B-C3B	3.01	130.30	124.68
13	a	823	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
13	e	810	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
13	G	828	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
13	a	804	CLA	O2D-CGD-O1D	-3.00	117.97	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	817	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
13	a	818	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
13	g	829	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
13	a	806	CLA	CMB-C2B-C3B	3.00	130.29	124.68
13	A	804	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
15	G	843	BCR	C15-C16-C17	-3.00	117.34	123.47
13	B	811	CLA	CMB-C2B-C3B	3.00	130.28	124.68
13	e	842	CLA	CMB-C2B-C3B	3.00	130.28	124.68
13	E	818	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
13	E	844	CLA	CMB-C2B-C3B	3.00	130.28	124.68
13	e	803	CLA	CMB-C2B-C3B	2.99	130.28	124.68
13	E	823	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
13	A	838	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
13	B	828	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
13	a	811	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
13	E	811	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
15	g	844	BCR	C15-C16-C17	-2.99	117.35	123.47
13	E	804	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
13	E	818	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
13	b	827	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
13	A	843	CLA	CMB-C2B-C3B	2.99	130.27	124.68
13	E	805	CLA	CMB-C2B-C3B	2.99	130.26	124.68
13	e	822	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
13	E	836	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
13	A	805	CLA	CMB-C2B-C3B	2.98	130.26	124.68
13	s	203	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
13	A	818	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
15	E	801	BCR	C15-C16-C17	-2.98	117.36	123.47
13	b	810	CLA	CMB-C2B-C3B	2.98	130.26	124.68
13	a	818	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
13	G	810	CLA	CMB-C2B-C3B	2.98	130.26	124.68
13	e	836	CLA	CMB-C2B-C3B	2.98	130.26	124.68
13	g	812	CLA	CMB-C2B-C3B	2.98	130.26	124.68
15	J	102	BCR	C15-C14-C13	-2.98	123.06	127.31
13	A	806	CLA	CMB-C2B-C3B	2.98	130.26	124.68
13	e	834	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
13	A	823	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
15	b	842	BCR	C15-C16-C17	-2.98	117.37	123.47
13	A	818	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
13	L	204	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
13	A	835	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
13	A	826	CLA	O2D-CGD-O1D	-2.98	118.02	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	204	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
13	A	837	CLA	CMB-C2B-C3B	2.97	130.24	124.68
13	G	801	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
13	E	825	CLA	CMB-C2B-C3B	2.97	130.24	124.68
15	J	102	BCR	C28-C27-C26	-2.97	108.77	114.08
13	a	838	CLA	CMB-C2B-C3B	2.97	130.24	124.68
15	R	101	BCR	C2-C1-C6	2.97	115.05	110.48
13	g	842	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
13	B	838	CLA	CMB-C2B-C3B	2.97	130.23	124.68
13	a	836	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
15	q	102	BCR	C15-C14-C13	-2.97	123.08	127.31
13	a	826	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
13	B	841	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
13	a	844	CLA	CMB-C2B-C3B	2.96	130.22	124.68
13	e	824	CLA	CMB-C2B-C3B	2.96	130.22	124.68
13	G	841	CLA	CMB-C2B-C3B	2.96	130.22	124.68
15	E	852	BCR	C15-C14-C13	-2.96	123.09	127.31
13	g	810	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
13	E	826	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
13	b	818	CLA	CMB-C2B-C3B	2.96	130.21	124.68
13	B	809	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
13	g	842	CLA	CMB-C2B-C3B	2.96	130.21	124.68
13	a	807	CLA	CMB-C2B-C3B	2.96	130.21	124.68
13	b	822	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
13	E	824	CLA	CMB-C2B-C3B	2.96	130.21	124.68
13	b	837	CLA	CMB-C2B-C3B	2.96	130.21	124.68
13	G	838	CLA	CMB-C2B-C3B	2.95	130.20	124.68
13	G	825	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
13	G	841	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
13	b	840	CLA	CMB-C2B-C3B	2.95	130.20	124.68
13	a	825	CLA	CMB-C2B-C3B	2.95	130.20	124.68
13	b	824	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
13	b	840	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
15	a	848	BCR	C7-C6-C5	2.95	128.60	121.46
15	a	853	BCR	C15-C14-C13	-2.95	123.11	127.31
13	B	841	CLA	CMB-C2B-C3B	2.94	130.19	124.68
13	E	807	CLA	CMB-C2B-C3B	2.94	130.19	124.68
13	g	839	CLA	CMB-C2B-C3B	2.94	130.19	124.68
15	q	102	BCR	C28-C27-C26	-2.94	108.82	114.08
15	E	852	BCR	C28-C27-C26	-2.94	108.82	114.08
13	G	823	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
13	G	819	CLA	CMB-C2B-C3B	2.94	130.18	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	852	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	g	826	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	e	806	CLA	CMB-C2B-C3B	2.94	130.18	124.68
15	a	853	BCR	C28-C27-C26	-2.94	108.83	114.08
13	R	102	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	e	818	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
15	S	205	BCR	C24-C23-C22	-2.94	121.79	126.23
13	K	102	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	g	819	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
13	A	807	CLA	CMB-C2B-C3B	2.94	130.17	124.68
13	E	838	CLA	CMB-C2B-C3B	2.94	130.17	124.68
13	A	825	CLA	CMB-C2B-C3B	2.94	130.17	124.68
13	A	819	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
15	a	802	BCR	C15-C16-C17	-2.93	117.46	123.47
13	B	825	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
13	g	824	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
15	E	850	BCR	C29-C30-C25	2.93	115.00	110.48
13	k	4002	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
13	a	840	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	B	819	CLA	CMB-C2B-C3B	2.93	130.16	124.68
13	r	102	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	G	822	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	G	808	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
13	B	823	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	E	841	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
13	b	808	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
13	a	824	CLA	CMB-C2B-C3B	2.93	130.16	124.68
13	B	801	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	E	840	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	b	821	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
13	e	823	CLA	CMB-C2B-C3B	2.93	130.15	124.68
13	F	202	CLA	CMB-C2B-C3B	2.92	130.15	124.68
13	g	820	CLA	CMB-C2B-C3B	2.92	130.15	124.68
13	E	819	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
15	k	4001	BCR	C38-C26-C25	-2.92	121.25	124.53
15	a	850	BCR	C29-C30-C25	2.92	114.97	110.48
13	b	831	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
13	G	832	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
15	A	848	BCR	C29-C30-C25	2.91	114.97	110.48
13	b	817	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
13	e	821	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
13	a	835	CLA	O2D-CGD-O1D	-2.91	118.14	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	818	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	B	832	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	l	205	CLA	CHD-C1D-ND	-2.91	121.78	124.45
13	E	835	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	a	819	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
13	B	822	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
13	A	839	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
13	B	818	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
13	b	838	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
13	g	833	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
13	G	815	CLA	CMB-C2B-C3B	2.90	130.11	124.68
13	L	204	CLA	CHD-C1D-ND	-2.90	121.79	124.45
13	E	822	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
13	G	839	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	A	843	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	g	802	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	a	844	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
13	G	829	CLA	CMB-C2B-C3B	2.90	130.10	124.68
13	B	815	CLA	CMB-C2B-C3B	2.90	130.10	124.68
13	e	838	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
13	g	840	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
13	l	203	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
15	e	847	BCR	C29-C30-C25	2.89	114.94	110.48
13	A	834	CLA	CMB-C2B-C3B	2.89	130.09	124.68
13	B	839	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	g	823	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
13	a	841	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
13	e	833	CLA	CMB-C2B-C3B	2.89	130.08	124.68
13	g	816	CLA	CMB-C2B-C3B	2.89	130.08	124.68
13	S	204	CLA	CHD-C1D-ND	-2.89	121.80	124.45
13	b	814	CLA	CMB-C2B-C3B	2.89	130.08	124.68
13	e	839	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
13	b	833	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
13	A	840	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
13	A	824	CLA	CMB-C2B-C3B	2.88	130.07	124.68
13	B	834	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
13	a	822	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
13	b	828	CLA	CMB-C2B-C3B	2.88	130.07	124.68
13	g	835	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
13	A	822	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
15	f	202	BCR	C2-C1-C6	2.88	114.91	110.48
13	E	844	CLA	O2D-CGD-O1D	-2.88	118.21	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	802	BCR	C15-C14-C13	-2.88	123.21	127.31
13	g	830	CLA	CMB-C2B-C3B	2.88	130.06	124.68
15	f	202	BCR	C15-C16-C17	-2.88	117.58	123.47
15	A	850	BCR	C33-C5-C6	-2.87	121.30	124.53
13	a	834	CLA	CMB-C2B-C3B	2.87	130.06	124.68
13	A	820	CLA	CMB-C2B-C3B	2.87	130.06	124.68
15	s	204	BCR	C28-C27-C26	-2.87	108.95	114.08
13	E	808	CLA	C1-C2-C3	-2.87	122.11	126.75
13	E	829	CLA	CMB-C2B-C3B	2.87	130.04	124.68
13	A	813	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	a	848	BCR	C24-C23-C22	-2.87	121.91	126.23
13	e	842	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
13	G	834	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
13	L	204	CLA	CMB-C2B-C3B	2.86	130.03	124.68
13	a	822	CLA	CMB-C2B-C3B	2.86	130.03	124.68
13	B	829	CLA	CMB-C2B-C3B	2.86	130.03	124.68
13	E	834	CLA	CMB-C2B-C3B	2.86	130.03	124.68
13	a	808	CLA	C1-C2-C3	-2.86	122.13	126.75
13	g	821	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	B	834	CLA	O2D-CGD-CBD	2.86	116.34	111.27
13	A	822	CLA	CMB-C2B-C3B	2.86	130.02	124.68
13	G	820	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
13	g	835	CLA	O2D-CGD-CBD	2.86	116.34	111.27
15	B	846	BCR	C15-C16-C17	-2.86	117.62	123.47
13	E	822	CLA	CMB-C2B-C3B	2.85	130.01	124.68
13	a	813	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	e	828	CLA	CMB-C2B-C3B	2.85	130.01	124.68
13	G	812	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
13	l	201	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
13	l	205	CLA	CMB-C2B-C3B	2.85	130.00	124.68
15	E	801	BCR	C15-C14-C13	-2.85	123.25	127.31
13	A	808	CLA	C1-C2-C3	-2.85	122.15	126.75
13	e	821	CLA	CMB-C2B-C3B	2.85	130.00	124.68
13	e	812	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
13	S	206	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
13	E	820	CLA	CMB-C2B-C3B	2.84	130.00	124.68
13	a	820	CLA	CMB-C2B-C3B	2.84	130.00	124.68
13	b	835	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	f	202	BCR	C3-C4-C5	-2.84	109.00	114.08
13	g	837	CLA	CHB-C4A-NA	2.84	128.44	124.51
15	g	847	BCR	C15-C16-C17	-2.84	117.66	123.47
15	b	845	BCR	C15-C16-C17	-2.84	117.66	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	833	CLA	O2D-CGD-CBD	2.84	116.31	111.27
13	A	845	CLA	C1-C2-C3	-2.84	122.16	126.75
13	a	829	CLA	CMB-C2B-C3B	2.84	129.99	124.68
13	A	812	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
13	B	820	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
13	a	823	CLA	C1-C2-C3	-2.83	122.17	126.75
13	e	822	CLA	C1-C2-C3	-2.83	122.17	126.75
13	E	813	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
13	g	841	CLA	CMB-C2B-C3B	2.83	129.98	124.68
13	a	845	CLA	CMB-C2B-C3B	2.83	129.98	124.68
13	G	834	CLA	O2D-CGD-CBD	2.83	116.30	111.27
14	g	843	PQN	C14-C13-C15	2.83	120.03	115.27
13	A	829	CLA	CMB-C2B-C3B	2.83	129.97	124.68
13	s	203	CLA	CMB-C2B-C3B	2.83	129.97	124.68
13	A	807	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	b	819	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	J	101	BCR	C15-C16-C17	-2.83	117.68	123.47
13	e	843	CLA	CMB-C2B-C3B	2.83	129.97	124.68
13	A	827	CLA	CMB-C2B-C3B	2.83	129.97	124.68
13	E	807	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	G	840	CLA	CMB-C2B-C3B	2.83	129.97	124.68
13	B	816	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
13	a	807	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
13	G	836	CLA	CHB-C4A-NA	2.82	128.42	124.51
15	G	846	BCR	C15-C16-C17	-2.82	117.69	123.47
15	q	101	BCR	C15-C16-C17	-2.82	117.69	123.47
13	e	811	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
13	B	836	CLA	CHB-C4A-NA	2.82	128.42	124.51
13	B	802	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
15	e	849	BCR	C33-C5-C6	-2.82	121.36	124.53
13	b	811	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
15	O	201	BCR	C15-C16-C17	-2.82	117.69	123.47
15	Q	101	BCR	C15-C16-C17	-2.82	117.69	123.47
13	A	823	CLA	C1-C2-C3	-2.82	122.19	126.75
13	E	823	CLA	C1-C2-C3	-2.82	122.19	126.75
13	S	204	CLA	CMB-C2B-C3B	2.82	129.95	124.68
13	a	812	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	G	842	PQN	C14-C13-C15	2.82	120.01	115.27
13	e	807	CLA	C1-C2-C3	-2.82	122.19	126.75
15	f	202	BCR	C15-C14-C13	-2.82	123.29	127.31
13	e	806	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
13	b	839	CLA	CMB-C2B-C3B	2.82	129.95	124.68

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	846	BCR	C38-C26-C27	-2.82	108.20	113.62
13	a	827	CLA	CMB-C2B-C3B	2.82	129.95	124.68
14	e	845	PQN	C14-C13-C15	2.82	120.01	115.27
13	e	826	CLA	CMB-C2B-C3B	2.82	129.94	124.68
15	F	201	BCR	C15-C16-C17	-2.81	117.71	123.47
14	A	846	PQN	C14-C13-C15	2.81	120.00	115.27
15	o	201	BCR	C15-C16-C17	-2.81	117.71	123.47
13	B	834	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	E	848	PQN	C14-C13-C15	2.81	120.00	115.27
15	a	848	BCR	C32-C1-C31	-2.81	99.91	108.53
15	a	849	BCR	C38-C26-C27	-2.81	108.22	113.62
14	a	847	PQN	C14-C13-C15	2.81	120.00	115.27
13	e	819	CLA	CMB-C2B-C3B	2.81	129.93	124.68
13	E	812	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
13	B	840	CLA	CMB-C2B-C3B	2.81	129.93	124.68
13	a	813	CLA	CMB-C2B-C3B	2.81	129.93	124.68
15	f	201	BCR	C15-C16-C17	-2.81	117.73	123.47
14	b	841	PQN	C14-C13-C15	2.81	119.99	115.27
13	e	844	CLA	CMB-C2B-C3B	2.80	129.93	124.68
15	A	847	BCR	C38-C26-C27	-2.80	108.23	113.62
13	G	804	CLA	C1-C2-C3	-2.80	122.22	126.75
13	A	813	CLA	CMB-C2B-C3B	2.80	129.92	124.68
13	G	834	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
13	b	804	CLA	C1-C2-C3	-2.80	122.22	126.75
13	E	845	CLA	CMB-C2B-C3B	2.80	129.91	124.68
13	G	816	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
13	A	803	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
14	B	842	PQN	C14-C13-C15	2.80	119.98	115.27
13	E	827	CLA	CMB-C2B-C3B	2.80	129.91	124.68
15	j	101	BCR	C15-C16-C17	-2.80	117.75	123.47
13	g	803	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
13	b	815	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
13	g	817	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
13	g	835	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
13	A	836	CLA	CMB-C2B-C3B	2.79	129.91	124.68
13	B	805	CLA	C1-C2-C3	-2.79	122.23	126.75
15	E	849	BCR	C38-C26-C27	-2.79	108.25	113.62
13	a	837	CLA	CMB-C2B-C3B	2.79	129.90	124.68
13	G	814	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
13	b	833	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
15	e	846	BCR	C37-C22-C21	-2.79	119.01	122.92
13	e	835	CLA	CMB-C2B-C3B	2.79	129.90	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	m	101	BCR	C27-C26-C25	2.79	126.78	122.73
13	G	803	CLA	CMB-C2B-C3B	2.79	129.90	124.68
13	b	813	CLA	C1-C2-C3	-2.79	122.24	126.75
13	g	806	CLA	C1-C2-C3	-2.79	122.24	126.75
15	G	848	BCR	C15-C14-C13	-2.79	123.33	127.31
15	E	849	BCR	C37-C22-C21	-2.79	119.02	122.92
13	B	835	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
13	g	805	CLA	CMB-C2B-C3B	2.79	129.89	124.68
15	b	847	BCR	C15-C14-C13	-2.79	123.33	127.31
13	E	813	CLA	CMB-C2B-C3B	2.79	129.89	124.68
13	A	810	CLA	CMB-C2B-C3B	2.78	129.89	124.68
13	B	814	CLA	C1-C2-C3	-2.78	122.25	126.75
13	A	844	CLA	CMB-C2B-C3B	2.78	129.89	124.68
13	l	204	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
13	G	814	CLA	C1-C2-C3	-2.78	122.25	126.75
13	a	808	CLA	CHB-C4A-NA	2.78	128.36	124.51
13	e	809	CLA	CMB-C2B-C3B	2.78	129.88	124.68
13	e	812	CLA	CMB-C2B-C3B	2.78	129.88	124.68
15	e	851	BCR	C15-C16-C17	-2.78	117.78	123.47
13	G	820	CLA	CMB-C2B-C3B	2.78	129.88	124.68
13	G	830	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
13	b	829	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
13	B	830	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
13	g	821	CLA	CMB-C2B-C3B	2.77	129.87	124.68
13	b	808	CLA	CMB-C2B-C3B	2.77	129.87	124.68
13	g	836	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	g	815	CLA	C1-C2-C3	-2.77	122.27	126.75
13	B	831	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
15	g	849	BCR	C15-C14-C13	-2.77	123.36	127.31
13	b	813	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
13	K	101	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
13	A	814	CLA	CMB-C2B-C3B	2.77	129.86	124.68
13	E	815	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	e	813	CLA	CMB-C2B-C3B	2.77	129.86	124.68
13	G	831	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	L	203	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
13	b	807	CLA	CMB-C2B-C3B	2.76	129.85	124.68
13	b	819	CLA	CMB-C2B-C3B	2.76	129.85	124.68
13	B	806	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
13	g	815	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
13	a	815	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
13	b	834	CLA	O2D-CGD-O1D	-2.76	118.43	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	g	809	CLA	CMB-C2B-C3B	2.76	129.85	124.68
13	S	203	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
13	B	809	CLA	CMB-C2B-C3B	2.76	129.84	124.68
13	E	810	CLA	CMB-C2B-C3B	2.76	129.84	124.68
13	E	837	CLA	CMB-C2B-C3B	2.76	129.84	124.68
13	a	810	CLA	CMB-C2B-C3B	2.76	129.84	124.68
13	B	808	CLA	CMB-C2B-C3B	2.76	129.84	124.68
13	s	202	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
15	R	101	BCR	C29-C30-C25	2.76	114.73	110.48
13	B	820	CLA	CMB-C2B-C3B	2.76	129.84	124.68
13	G	817	CLA	CMB-C2B-C3B	2.76	129.84	124.68
13	r	102	CLA	CMB-C2B-C3B	2.76	129.84	124.68
13	a	852	CLA	CMB-C2B-C3B	2.76	129.84	124.68
13	b	803	CLA	CMB-C2B-C3B	2.76	129.84	124.68
15	B	848	BCR	C15-C14-C13	-2.76	123.38	127.31
13	B	837	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
13	g	810	CLA	CMB-C2B-C3B	2.75	129.83	124.68
13	g	813	CLA	CMB-C2B-C3B	2.75	129.83	124.68
13	k	4002	CLA	CMB-C2B-C3B	2.75	129.83	124.68
13	b	816	CLA	CMB-C2B-C3B	2.75	129.83	124.68
13	A	814	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
13	K	102	CLA	CMB-C2B-C3B	2.75	129.83	124.68
13	B	814	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
13	G	805	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
15	a	849	BCR	C37-C22-C21	-2.75	119.07	122.92
13	a	814	CLA	CMB-C2B-C3B	2.75	129.82	124.68
15	E	801	BCR	C33-C5-C6	-2.75	121.44	124.53
13	G	808	CLA	CMB-C2B-C3B	2.75	129.82	124.68
13	g	807	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
13	B	812	CLA	CMB-C2B-C3B	2.75	129.82	124.68
13	a	811	CLA	CMB-C2B-C3B	2.75	129.82	124.68
13	G	835	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
13	e	814	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
13	B	839	CLA	CMB-C2B-C3B	2.75	129.82	124.68
13	G	807	CLA	CMB-C2B-C3B	2.75	129.81	124.68
13	B	804	CLA	CMB-C2B-C3B	2.75	129.81	124.68
13	e	815	CLA	CMB-C2B-C3B	2.74	129.81	124.68
13	A	829	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
13	g	838	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
13	g	831	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
13	B	823	CLA	CMB-C2B-C3B	2.74	129.81	124.68
13	s	205	CLA	CMB-C2B-C3B	2.74	129.81	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	813	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
13	e	836	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
15	S	205	BCR	C28-C27-C26	-2.74	109.18	114.08
14	E	848	PQN	C2M-C2-C3	-2.74	119.93	124.40
13	E	829	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
14	G	842	PQN	C2M-C2-C3	-2.74	119.93	124.40
13	E	808	CLA	CHB-C4A-NA	2.74	128.30	124.51
13	e	807	CLA	CHB-C4A-NA	2.74	128.30	124.51
13	E	814	CLA	CMB-C2B-C3B	2.74	129.80	124.68
13	G	811	CLA	CMB-C2B-C3B	2.74	129.80	124.68
13	A	821	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
13	E	811	CLA	CMB-C2B-C3B	2.74	129.80	124.68
13	A	806	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
13	B	817	CLA	CMB-C2B-C3B	2.74	129.80	124.68
13	e	810	CLA	CMB-C2B-C3B	2.74	129.80	124.68
13	A	845	CLA	CMB-C2B-C3B	2.74	129.80	124.68
13	G	837	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
13	b	836	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
13	g	803	CLA	CMB-C2B-C3B	2.73	129.79	124.68
13	g	840	CLA	CMB-C2B-C3B	2.73	129.79	124.68
13	g	832	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
15	E	802	BCR	C15-C16-C17	-2.73	117.88	123.47
13	b	830	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
13	A	816	CLA	CMB-C2B-C3B	2.73	129.79	124.68
13	A	841	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
13	A	811	CLA	CMB-C2B-C3B	2.73	129.79	124.68
13	R	102	CLA	CMB-C2B-C3B	2.73	129.79	124.68
13	g	818	CLA	CMB-C2B-C3B	2.73	129.79	124.68
13	a	816	CLA	CMB-C2B-C3B	2.73	129.79	124.68
13	E	816	CLA	CMB-C2B-C3B	2.73	129.78	124.68
13	G	839	CLA	CMB-C2B-C3B	2.73	129.78	124.68
13	A	814	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
13	a	829	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
14	b	841	PQN	C2M-C2-C3	-2.73	119.95	124.40
13	b	838	CLA	CMB-C2B-C3B	2.73	129.78	124.68
13	E	812	CLA	C1-C2-C3	-2.73	122.34	126.75
15	A	847	BCR	C37-C22-C21	-2.73	119.10	122.92
13	E	814	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
13	b	805	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
13	G	813	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
13	a	821	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
15	A	851	BCR	C24-C23-C22	-2.73	122.12	126.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	g	843	PQN	C2M-C2-C3	-2.73	119.95	124.40
13	G	823	CLA	CMB-C2B-C3B	2.72	129.78	124.68
13	e	803	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
13	a	842	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	e	805	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	B	842	PQN	C2M-C2-C3	-2.72	119.96	124.40
14	e	845	PQN	C2M-C2-C3	-2.72	119.96	124.40
13	A	815	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	E	814	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
13	A	808	CLA	CHB-C4A-NA	2.72	128.27	124.51
14	a	847	PQN	C2M-C2-C3	-2.72	119.96	124.40
13	r	101	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
13	a	812	CLA	C1-C2-C3	-2.72	122.35	126.75
13	A	837	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	a	838	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
13	E	821	CLA	CMB-C2B-C3B	2.72	129.76	124.68
13	e	820	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
13	e	828	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
15	a	848	BCR	C15-C14-C13	-2.72	123.44	127.31
13	e	844	CLA	C1-C2-C3	-2.72	122.36	126.75
15	a	803	BCR	C28-C27-C26	-2.71	109.23	114.08
13	A	812	CLA	C1-C2-C3	-2.71	122.36	126.75
13	e	811	CLA	C1-C2-C3	-2.71	122.36	126.75
14	A	846	PQN	C2M-C2-C3	-2.71	119.97	124.40
13	e	820	CLA	CMB-C2B-C3B	2.71	129.75	124.68
13	g	824	CLA	CMB-C2B-C3B	2.71	129.75	124.68
13	a	814	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
13	a	806	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	m	101	BCR	C3-C4-C5	-2.71	109.24	114.08
13	a	834	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
13	E	821	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
13	a	814	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
12	a	801	LHG	O8-C23-C24	2.71	120.40	111.91
13	G	809	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
13	E	806	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
13	E	838	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
13	b	801	CLA	CMB-C2B-C3B	2.71	129.74	124.68
13	E	842	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
13	G	829	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
13	A	821	CLA	CMB-C2B-C3B	2.70	129.74	124.68
13	l	201	CLA	CMB-C2B-C3B	2.70	129.74	124.68
13	g	832	CLA	CMB-C2B-C3B	2.70	129.74	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	816	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
13	e	843	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
13	G	801	CLA	CMB-C2B-C3B	2.70	129.73	124.68
13	A	834	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
13	a	817	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
13	f	203	CLA	CHB-C4A-NA	2.70	128.25	124.51
13	G	808	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
13	B	827	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
13	b	822	CLA	CMB-C2B-C3B	2.70	129.73	124.68
13	e	840	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
13	b	825	CLA	CHB-C4A-NA	2.70	128.24	124.51
13	g	810	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
13	a	821	CLA	CMB-C2B-C3B	2.70	129.72	124.68
13	g	811	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
13	a	839	CLA	CHB-C4A-NA	2.70	128.24	124.51
13	b	812	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
13	B	809	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
13	E	845	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
13	a	845	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
13	g	821	CLA	CHB-C4A-NA	2.69	128.24	124.51
13	e	833	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
13	B	810	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
13	b	811	CLA	CMB-C2B-C3B	2.69	129.71	124.68
13	b	830	CLA	CMB-C2B-C3B	2.69	129.71	124.68
13	e	813	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
13	E	839	CLA	CHB-C4A-NA	2.69	128.23	124.51
12	A	802	LHG	O8-C23-C24	2.69	120.34	111.91
13	G	827	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
13	O	203	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	G	812	CLA	CMB-C2B-C3B	2.69	129.71	124.68
13	G	826	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	g	828	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
13	g	830	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
13	b	808	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
13	B	815	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
13	E	817	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
13	g	814	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
13	A	803	CLA	CHD-C1D-ND	-2.68	121.99	124.45
13	S	206	CLA	CMB-C2B-C3B	2.68	129.70	124.68
13	A	844	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
13	b	826	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
13	A	829	CLA	O2D-CGD-O1D	-2.68	118.60	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	831	CLA	CMB-C2B-C3B	2.68	129.69	124.68
13	G	805	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	a	829	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
13	B	802	CLA	CMB-C2B-C3B	2.68	129.69	124.68
13	A	838	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	e	828	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
15	g	845	BCR	C15-C16-C17	-2.68	117.99	123.47
13	E	829	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
13	A	812	CLA	CMB-C2B-C3B	2.68	129.69	124.68
13	B	831	CLA	CMB-C2B-C3B	2.68	129.69	124.68
13	A	817	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
13	g	807	CLA	CHB-C4A-NA	2.68	128.21	124.51
15	G	844	BCR	C15-C16-C17	-2.68	117.99	123.47
13	A	817	CLA	CMB-C2B-C3B	2.68	129.69	124.68
13	e	811	CLA	CMB-C2B-C3B	2.68	129.69	124.68
13	E	834	CLA	C1B-CHB-C4A	-2.68	124.82	130.12
13	A	853	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
13	b	826	CLA	CMB-C2B-C3B	2.67	129.68	124.68
15	e	848	BCR	C15-C16-C17	-2.67	118.00	123.47
13	b	828	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
13	b	805	CLA	CHB-C4A-NA	2.67	128.21	124.51
15	E	849	BCR	C15-C16-C17	-2.67	118.00	123.47
13	B	813	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
13	B	826	CLA	CHB-C4A-NA	2.67	128.21	124.51
13	b	802	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
13	b	814	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
13	a	817	CLA	CMB-C2B-C3B	2.67	129.68	124.68
13	b	809	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
13	a	812	CLA	CMB-C2B-C3B	2.67	129.67	124.68
13	g	820	CLA	CHB-C4A-NA	2.67	128.20	124.51
13	e	852	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
12	A	801	LHG	C11-C10-C9	-2.67	100.88	114.42
15	a	851	BCR	C15-C16-C17	-2.67	118.01	123.47
13	g	818	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
15	g	849	BCR	C27-C26-C25	2.67	126.60	122.73
13	B	829	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
13	G	821	CLA	CMB-C2B-C3B	2.67	129.66	124.68
15	O	201	BCR	C24-C23-C22	-2.67	122.21	126.23
15	B	844	BCR	C15-C16-C17	-2.66	118.02	123.47
15	o	201	BCR	C24-C23-C22	-2.66	122.21	126.23
15	k	4001	BCR	C27-C26-C25	2.66	126.60	122.73
15	E	851	BCR	C15-C16-C17	-2.66	118.02	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	827	CLA	CMB-C2B-C3B	2.66	129.66	124.68
15	b	847	BCR	C27-C26-C25	2.66	126.59	122.73
13	E	833	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	g	827	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	g	822	CLA	CMB-C2B-C3B	2.66	129.66	124.68
13	B	821	CLA	CMB-C2B-C3B	2.66	129.65	124.68
13	A	826	CLA	CMB-C2B-C3B	2.66	129.65	124.68
13	E	812	CLA	CMB-C2B-C3B	2.66	129.65	124.68
15	O	202	BCR	C24-C23-C22	-2.66	122.22	126.23
13	a	811	CLA	CHB-C4A-NA	2.66	128.19	124.51
15	a	849	BCR	C15-C16-C17	-2.66	118.03	123.47
12	e	801	LHG	C11-C10-C9	-2.66	100.93	114.42
15	G	848	BCR	C27-C26-C25	2.66	126.59	122.73
15	b	843	BCR	C15-C16-C17	-2.66	118.03	123.47
13	a	833	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
13	E	824	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	G	812	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
13	S	206	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
13	b	811	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
13	l	201	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
15	F	201	BCR	C24-C23-C22	-2.66	122.22	126.23
15	A	849	BCR	C15-C16-C17	-2.66	118.03	123.47
13	B	806	CLA	CHB-C4A-NA	2.65	128.18	124.51
13	g	816	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
15	f	201	BCR	C24-C23-C22	-2.65	122.22	126.23
13	g	828	CLA	CMB-C2B-C3B	2.65	129.64	124.68
13	e	824	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
13	A	835	CLA	C1-C2-C3	-2.65	122.46	126.75
15	T	101	BCR	C11-C10-C9	-2.65	123.52	127.31
15	e	846	BCR	C15-C16-C17	-2.65	118.04	123.47
13	e	832	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
13	e	816	CLA	CMB-C2B-C3B	2.65	129.64	124.68
13	a	836	CLA	C1-C2-C3	-2.65	122.46	126.75
15	E	802	BCR	C28-C27-C26	-2.65	109.34	114.08
15	e	849	BCR	C24-C23-C22	-2.65	122.23	126.23
13	B	840	CLA	CHB-C4A-NA	2.65	128.18	124.51
13	A	804	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
13	a	825	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
13	G	815	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
13	B	838	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
13	B	834	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
13	e	803	CLA	CHD-C1D-ND	-2.65	122.02	124.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	837	CLA	CHB-C4A-NA	2.65	128.17	124.51
13	g	824	CLA	CHB-C4A-NA	2.65	128.17	124.51
13	E	825	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
13	B	827	CLA	CMB-C2B-C3B	2.65	129.63	124.68
13	E	817	CLA	CMB-C2B-C3B	2.65	129.63	124.68
13	G	834	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
13	g	835	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
13	g	835	CLA	C1-C2-C3	-2.65	122.47	126.75
13	A	833	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
13	A	834	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
13	E	820	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
13	e	823	CLA	CHB-C4A-NA	2.64	128.17	124.51
13	B	820	CLA	CHB-C4A-NA	2.64	128.17	124.51
13	G	819	CLA	CHB-C4A-NA	2.64	128.17	124.51
13	a	833	CLA	CHB-C4A-NA	2.64	128.17	124.51
13	b	818	CLA	CHB-C4A-NA	2.64	128.17	124.51
13	G	802	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
13	A	833	CLA	C1-C2-C3	-2.64	122.48	126.75
13	E	836	CLA	C1-C2-C3	-2.64	122.48	126.75
13	b	833	CLA	C1-C2-C3	-2.64	122.48	126.75
13	e	825	CLA	CMB-C2B-C3B	2.64	129.62	124.68
13	A	825	CLA	CHB-C4A-NA	2.64	128.17	124.51
15	B	847	BCR	C27-C26-C25	2.64	126.57	122.73
13	a	826	CLA	CMB-C2B-C3B	2.64	129.62	124.68
13	B	819	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	g	839	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
13	E	833	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
13	b	838	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	b	833	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
15	s	201	BCR	C27-C26-C25	2.64	126.56	122.73
15	A	850	BCR	C24-C23-C22	-2.64	122.25	126.23
13	l	203	CLA	C1-C2-C3	-2.64	122.48	126.75
13	A	824	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	e	804	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
13	A	824	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
13	b	832	CLA	CMB-C2B-C3B	2.64	129.61	124.68
13	A	833	CLA	CHB-C4A-NA	2.64	128.16	124.51
13	a	838	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
13	b	820	CLA	CMB-C2B-C3B	2.63	129.61	124.68
13	B	817	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
13	G	820	CLA	CHB-C4A-NA	2.63	128.15	124.51
13	b	819	CLA	CHB-C4A-NA	2.63	128.15	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	847	BCR	C15-C16-C17	-2.63	118.08	123.47
13	e	836	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
15	G	847	BCR	C27-C26-C25	2.63	126.55	122.73
13	b	816	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
13	G	833	CLA	CMB-C2B-C3B	2.63	129.60	124.68
13	A	820	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
13	a	833	CLA	C1-C2-C3	-2.63	122.50	126.75
13	E	826	CLA	CMB-C2B-C3B	2.63	129.60	124.68
15	g	848	BCR	C27-C26-C25	2.63	126.55	122.73
13	B	834	CLA	C1-C2-C3	-2.63	122.50	126.75
13	G	817	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
13	B	823	CLA	CHB-C4A-NA	2.63	128.15	124.51
13	G	823	CLA	CHB-C4A-NA	2.63	128.15	124.51
13	e	803	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
13	A	840	CLA	CHB-C4A-NA	2.63	128.15	124.51
13	a	820	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
13	G	803	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
13	G	841	CLA	CHB-C4A-NA	2.63	128.14	124.51
13	b	810	CLA	CHB-C4A-NA	2.63	128.14	124.51
15	B	848	BCR	C27-C26-C25	2.62	126.54	122.73
13	A	837	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
13	A	825	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
13	a	824	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
13	G	834	CLA	C1-C2-C3	-2.62	122.51	126.75
13	g	812	CLA	CHB-C4A-NA	2.62	128.14	124.51
13	e	834	CLA	C1-C2-C3	-2.62	122.51	126.75
13	B	839	CLA	CHB-C4A-NA	2.62	128.14	124.51
13	a	825	CLA	CHB-C4A-NA	2.62	128.14	124.51
13	E	826	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
15	b	845	BCR	C24-C23-C22	-2.62	122.28	126.23
13	G	840	CLA	CHB-C4A-NA	2.62	128.13	124.51
13	e	823	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
13	E	838	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
13	g	841	CLA	CHB-C4A-NA	2.62	128.13	124.51
13	G	838	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
15	S	202	BCR	C27-C26-C25	2.62	126.53	122.73
13	E	804	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
13	a	804	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
13	a	841	CLA	CHB-C4A-NA	2.62	128.13	124.51
13	e	832	CLA	CHB-C4A-NA	2.61	128.13	124.51
13	B	804	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
13	E	811	CLA	CHB-C4A-NA	2.61	128.13	124.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	812	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
13	g	813	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
12	a	801	LHG	C11-C10-C9	-2.61	101.16	114.42
13	e	819	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
13	A	826	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
13	b	822	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	b	837	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
13	g	805	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
13	E	841	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	a	824	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	F	202	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
13	a	826	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
13	e	833	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
13	B	811	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	b	829	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	G	811	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
13	B	841	CLA	CHB-C4A-NA	2.61	128.12	124.51
13	e	839	CLA	CHB-C4A-NA	2.61	128.12	124.51
15	b	846	BCR	C27-C26-C25	2.61	126.52	122.73
15	B	846	BCR	C24-C23-C22	-2.61	122.30	126.23
13	g	840	CLA	CHB-C4A-NA	2.60	128.11	124.51
13	g	834	CLA	CMB-C2B-C3B	2.60	129.55	124.68
13	e	832	CLA	C1-C2-C3	-2.60	122.54	126.75
13	s	205	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
13	g	829	CLA	CMB-C2B-C3B	2.60	129.55	124.68
15	g	847	BCR	C24-C23-C22	-2.60	122.30	126.23
13	A	803	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
13	E	824	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
13	E	817	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
13	E	837	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
13	B	833	CLA	CMB-C2B-C3B	2.60	129.54	124.68
13	a	817	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
13	g	831	CLA	CHB-C4A-NA	2.60	128.11	124.51
13	g	842	CLA	CHB-C4A-NA	2.60	128.11	124.51
13	a	834	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
13	A	817	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
13	G	810	CLA	CHB-C4A-NA	2.60	128.10	124.51
13	A	830	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
13	b	839	CLA	CHB-C4A-NA	2.60	128.10	124.51
13	e	825	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
13	B	830	CLA	CHB-C4A-NA	2.60	128.10	124.51
13	e	824	CLA	CHB-C4A-NA	2.60	128.10	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	202	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
13	A	845	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	A	825	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
13	A	811	CLA	CHB-C4A-NA	2.59	128.10	124.51
13	b	827	CLA	CMB-C2B-C3B	2.59	129.53	124.68
13	E	825	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	B	828	CLA	CMB-C2B-C3B	2.59	129.53	124.68
13	B	825	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	E	842	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	b	840	CLA	CHB-C4A-NA	2.59	128.09	124.51
15	G	846	BCR	C24-C23-C22	-2.59	122.32	126.23
13	E	833	CLA	C1-C2-C3	-2.59	122.56	126.75
13	B	838	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
13	b	803	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
13	A	841	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	B	813	CLA	CMB-C2B-C3B	2.59	129.52	124.68
13	a	825	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
13	a	830	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
13	e	810	CLA	CHB-C4A-NA	2.59	128.09	124.51
15	T	101	BCR	C27-C26-C25	2.59	126.49	122.73
13	E	830	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
13	A	824	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
13	b	837	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
13	E	832	CLA	CMB-C2B-C3B	2.59	129.52	124.68
13	a	828	CLA	CHB-C4A-NA	2.59	128.09	124.51
13	g	825	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
13	B	819	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
13	A	853	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
13	G	824	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
13	E	834	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
15	G	848	BCR	C24-C23-C22	-2.58	122.33	126.23
13	G	825	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	e	816	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
13	e	827	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	g	839	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
13	e	852	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
13	a	842	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	A	821	CLA	CHD-C1D-ND	-2.58	122.09	124.45
13	G	828	CLA	CMB-C2B-C3B	2.58	129.50	124.68
13	b	829	CLA	C1-C2-C3	-2.58	122.58	126.75
15	f	202	BCR	C24-C23-C22	-2.58	122.34	126.23
13	G	802	CLA	C1B-CHB-C4A	-2.57	125.02	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	823	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
13	a	824	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
13	E	820	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
15	A	849	BCR	C15-C14-C13	-2.57	123.64	127.31
13	e	840	CLA	CHB-C4A-NA	2.57	128.07	124.51
15	S	202	BCR	C24-C23-C22	-2.57	122.35	126.23
13	a	852	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
13	g	814	CLA	CMB-C2B-C3B	2.57	129.49	124.68
13	e	829	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
13	e	824	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
15	a	803	BCR	C35-C13-C14	-2.57	119.32	122.92
13	E	824	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
13	G	813	CLA	CMB-C2B-C3B	2.57	129.49	124.68
13	A	836	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
13	b	823	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
13	G	839	CLA	CHB-C4A-NA	2.57	128.06	124.51
13	E	821	CLA	CHD-C1D-ND	-2.57	122.09	124.45
13	g	822	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
13	A	805	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
13	E	846	CLA	CAC-C3C-C4C	2.57	128.14	124.81
13	G	830	CLA	C1-C2-C3	-2.57	122.60	126.75
13	A	832	CLA	CMB-C2B-C3B	2.57	129.48	124.68
13	b	802	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
15	B	848	BCR	C24-C23-C22	-2.57	122.36	126.23
13	B	824	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
13	A	822	CLA	O2D-CGD-O1D	-2.56	118.82	123.84
13	G	821	CLA	O2D-CGD-O1D	-2.56	118.82	123.84
13	a	845	CLA	CHB-C4A-NA	2.56	128.06	124.51
15	a	802	BCR	C11-C10-C9	-2.56	123.65	127.31
13	e	820	CLA	CHD-C1D-ND	-2.56	122.10	124.45
12	e	802	LHG	C11-C10-C9	-2.56	101.41	114.42
13	G	830	CLA	CHB-C4A-NA	2.56	128.06	124.51
15	g	849	BCR	C24-C23-C22	-2.56	122.36	126.23
13	G	819	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
13	e	821	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
13	a	809	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
13	g	801	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
15	k	4001	BCR	C20-C21-C22	-2.56	123.65	127.31
13	A	816	CLA	CHB-C4A-NA	2.56	128.05	124.51
15	g	849	BCR	C33-C5-C6	-2.56	121.65	124.53
13	a	822	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
13	g	831	CLA	C1-C2-C3	-2.56	122.61	126.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	831	CLA	CMB-C2B-C3B	2.56	129.47	124.68
13	b	812	CLA	CMB-C2B-C3B	2.56	129.47	124.68
13	A	810	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
13	E	809	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
15	b	847	BCR	C33-C5-C6	-2.56	121.65	124.53
13	e	808	CLA	CHB-C4A-NA	2.56	128.05	124.51
15	E	851	BCR	C15-C14-C13	-2.56	123.66	127.31
13	A	809	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
13	E	820	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	E	822	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
13	A	828	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	e	835	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
15	a	803	BCR	C15-C14-C13	-2.56	123.66	127.31
13	a	837	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
13	a	821	CLA	CHD-C1D-ND	-2.56	122.11	124.45
13	e	830	CLA	C1-C2-C3	-2.56	122.62	126.75
13	g	820	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
13	G	838	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
13	a	805	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
13	g	826	CLA	CHB-C4A-NA	2.55	128.04	124.51
13	b	818	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
13	E	825	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
13	e	809	CLA	CHB-C4A-NA	2.55	128.04	124.51
13	e	815	CLA	CHB-C4A-NA	2.55	128.04	124.51
13	a	852	CLA	C1-C2-C3	-2.55	122.62	126.75
13	B	821	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
13	e	811	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
15	G	845	BCR	C15-C16-C17	-2.55	118.25	123.47
13	a	820	CLA	CHB-C4A-NA	2.55	128.04	124.51
13	G	809	CLA	CHB-C4A-NA	2.55	128.04	124.51
13	E	815	CLA	C1-C2-C3	-2.55	122.62	126.75
15	m	101	BCR	C15-C14-C13	-2.55	123.67	127.31
15	b	847	BCR	C15-C16-C17	-2.55	118.25	123.47
13	B	830	CLA	C1-C2-C3	-2.55	122.63	126.75
15	e	850	BCR	C33-C5-C6	-2.55	121.67	124.53
13	b	820	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
13	g	817	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	l	206	BCR	C27-C26-C25	2.55	126.43	122.73
15	e	848	BCR	C15-C14-C13	-2.55	123.67	127.31
13	A	805	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
15	g	849	BCR	C15-C16-C17	-2.55	118.25	123.47
15	E	801	BCR	C27-C26-C25	2.55	126.43	122.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	809	CLA	CHB-C4A-NA	2.55	128.03	124.51
13	G	803	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
13	G	811	CLA	CHB-C4A-NA	2.55	128.03	124.51
13	o	202	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
13	s	205	CLA	CHB-C4A-NA	2.55	128.03	124.51
13	E	805	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
13	b	827	CLA	C1-C2-C3	-2.55	122.63	126.75
15	a	851	BCR	C15-C14-C13	-2.54	123.68	127.31
13	b	824	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	e	808	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
13	a	821	CLA	C1-C2-C3	-2.54	122.64	126.75
13	A	844	CLA	CHB-C4A-NA	2.54	128.03	124.51
15	b	847	BCR	C24-C23-C22	-2.54	122.39	126.23
13	g	819	CLA	C1-C2-C3	-2.54	122.64	126.75
13	E	805	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
13	E	828	CLA	CHB-C4A-NA	2.54	128.03	124.51
13	a	820	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
15	B	848	BCR	C33-C5-C6	-2.54	121.67	124.53
15	G	844	BCR	C28-C27-C26	-2.54	109.54	114.08
13	G	801	CLA	C1-C2-C3	-2.54	122.64	126.75
13	e	809	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
13	g	801	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
15	b	844	BCR	C15-C16-C17	-2.54	118.28	123.47
13	a	805	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
15	G	848	BCR	C33-C5-C6	-2.54	121.68	124.53
13	g	802	CLA	CHB-C4A-NA	2.54	128.02	124.51
13	b	815	CLA	CHB-C4A-NA	2.54	128.02	124.51
13	g	839	CLA	C1-C2-C3	-2.54	122.65	126.75
15	g	846	BCR	C15-C16-C17	-2.53	118.28	123.47
13	B	828	CLA	C1-C2-C3	-2.53	122.65	126.75
13	E	809	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	B	814	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	e	808	CLA	CMB-C2B-C3B	2.53	129.41	124.68
13	a	810	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
13	A	812	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
15	m	101	BCR	C15-C16-C17	-2.53	118.29	123.47
13	B	832	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
13	g	817	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
13	G	814	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	g	805	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
15	B	845	BCR	C15-C16-C17	-2.53	118.29	123.47
15	m	101	BCR	C7-C8-C9	-2.53	122.41	126.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	837	CLA	C1-C2-C3	-2.53	122.66	126.75
13	e	819	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
13	E	809	CLA	CMB-C2B-C3B	2.53	129.41	124.68
15	B	844	BCR	C28-C27-C26	-2.53	109.56	114.08
13	B	807	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	a	835	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	B	801	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	g	811	CLA	CHB-C4A-NA	2.53	128.01	124.51
13	a	808	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
13	a	812	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
13	b	809	CLA	CHB-C4A-NA	2.53	128.00	124.51
15	G	848	BCR	C15-C16-C17	-2.53	118.30	123.47
13	A	810	CLA	CHB-C4A-NA	2.53	128.00	124.51
13	E	816	CLA	CHB-C4A-NA	2.53	128.00	124.51
13	E	845	CLA	CHB-C4A-NA	2.53	128.00	124.51
13	b	806	CLA	CHB-C4A-NA	2.53	128.00	124.51
13	A	820	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	A	820	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
13	E	803	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
13	g	813	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	b	819	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
15	L	201	BCR	C27-C26-C25	2.52	126.39	122.73
13	A	840	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
13	b	815	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
13	G	816	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	a	832	CLA	CMB-C2B-C3B	2.52	129.40	124.68
13	g	833	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
13	b	810	CLA	C1-C2-C3	-2.52	122.67	126.75
13	B	840	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
13	g	812	CLA	C1-C2-C3	-2.52	122.67	126.75
13	B	805	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	e	840	CLA	CMB-C2B-C3B	2.52	129.39	124.68
13	b	832	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
13	B	810	CLA	CHB-C4A-NA	2.52	128.00	124.51
13	B	804	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
13	a	841	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
13	E	840	CLA	CHB-C4A-NA	2.52	127.99	124.51
13	B	812	CLA	CHB-C4A-NA	2.52	127.99	124.51
13	a	810	CLA	CHB-C4A-NA	2.52	127.99	124.51
13	a	816	CLA	CHB-C4A-NA	2.52	127.99	124.51
13	g	821	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
13	e	820	CLA	C1-C2-C3	-2.52	122.68	126.75

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	843	CLA	CHB-C4A-NA	2.52	127.99	124.51
13	b	812	CLA	CHB-C4A-NA	2.52	127.99	124.51
15	O	202	BCR	C15-C16-C17	-2.52	118.32	123.47
13	E	819	CLA	C1B-CHB-C4A	-2.52	125.14	130.12
15	b	844	BCR	C33-C5-C6	-2.51	121.70	124.53
13	G	832	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
13	B	816	CLA	CHB-C4A-NA	2.51	127.99	124.51
13	E	810	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
13	G	838	CLA	C1-C2-C3	-2.51	122.69	126.75
13	e	844	CLA	CHB-C4A-NA	2.51	127.99	124.51
13	G	816	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
13	A	821	CLA	C1-C2-C3	-2.51	122.69	126.75
13	G	828	CLA	C1-C2-C3	-2.51	122.69	126.75
13	g	808	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	E	812	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
13	A	831	CLA	C1-C2-C3	-2.51	122.69	126.75
15	b	843	BCR	C28-C27-C26	-2.51	109.60	114.08
13	b	837	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	B	838	CLA	C1-C2-C3	-2.51	122.69	126.75
15	B	848	BCR	C15-C16-C17	-2.51	118.33	123.47
13	B	813	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	b	804	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	E	842	CLA	CMB-C2B-C3B	2.51	129.37	124.68
13	E	831	CLA	C1-C2-C3	-2.51	122.69	126.75
13	a	831	CLA	C1-C2-C3	-2.51	122.69	126.75
13	B	838	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	E	835	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	g	815	CLA	CHB-C4A-NA	2.51	127.98	124.51
15	e	851	BCR	C33-C5-C6	-2.51	121.71	124.53
13	E	807	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	e	844	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
13	e	804	CLA	C1-C2-C3	-2.51	122.70	126.75
13	G	820	CLA	C1B-CHB-C4A	-2.51	125.16	130.12
15	I	101	BCR	C27-C26-C25	2.51	126.37	122.73
13	A	807	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	e	819	CLA	CHB-C4A-NA	2.51	127.98	124.51
13	G	818	CLA	C1-C2-C3	-2.50	122.70	126.75
13	a	809	CLA	CHB-C4A-NA	2.50	127.97	124.51
13	B	818	CLA	C1-C2-C3	-2.50	122.70	126.75
13	E	804	CLA	C1-C2-C3	-2.50	122.70	126.75
13	g	826	CLA	C1-C2-C3	-2.50	122.70	126.75
13	E	810	CLA	CHB-C4A-NA	2.50	127.97	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	851	BCR	C33-C5-C6	-2.50	121.72	124.53
12	A	802	LHG	C11-C10-C9	-2.50	101.72	114.42
15	g	845	BCR	C28-C27-C26	-2.50	109.61	114.08
13	G	813	CLA	CHB-C4A-NA	2.50	127.97	124.51
13	g	839	CLA	CHB-C4A-NA	2.50	127.97	124.51
13	A	844	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
13	G	840	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
13	a	845	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
13	G	825	CLA	C1-C2-C3	-2.50	122.71	126.75
13	a	807	CLA	CHB-C4A-NA	2.50	127.97	124.51
13	a	815	CLA	C1-C2-C3	-2.50	122.71	126.75
13	a	809	CLA	CMB-C2B-C3B	2.50	129.35	124.68
13	b	831	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
13	g	803	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
13	g	829	CLA	C1-C2-C3	-2.50	122.71	126.75
13	A	808	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
13	b	813	CLA	CHB-C4A-NA	2.50	127.96	124.51
15	G	845	BCR	C33-C5-C6	-2.50	121.72	124.53
13	L	202	CLA	C1-C2-C3	-2.50	122.71	126.75
13	G	806	CLA	CHB-C4A-NA	2.50	127.96	124.51
13	B	821	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
13	g	819	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
13	b	803	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
13	B	840	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
13	b	814	CLA	CHB-C4A-NA	2.49	127.96	124.51
13	A	809	CLA	CMB-C2B-C3B	2.49	129.34	124.68
13	a	842	CLA	CMB-C2B-C3B	2.49	129.34	124.68
13	B	816	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
13	l	203	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
13	G	818	CLA	CHB-C4A-NA	2.49	127.96	124.51
13	g	806	CLA	CHB-C4A-NA	2.49	127.96	124.51
13	G	821	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
13	A	815	CLA	C1-C2-C3	-2.49	122.72	126.75
13	e	807	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
13	G	837	CLA	CHB-C4A-NA	2.49	127.96	124.51
13	B	833	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
13	e	806	CLA	CHB-C4A-NA	2.49	127.95	124.51
13	e	843	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
13	A	819	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
13	e	839	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
15	b	843	BCR	C15-C14-C13	-2.49	123.76	127.31
13	g	841	CLA	O2D-CGD-O1D	-2.49	118.97	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	815	CLA	CHB-C4A-NA	2.49	127.95	124.51
15	T	101	BCR	C33-C5-C6	-2.49	121.73	124.53
13	e	814	CLA	CHB-C4A-NA	2.49	127.95	124.51
13	g	841	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
13	A	841	CLA	CMB-C2B-C3B	2.49	129.33	124.68
15	E	802	BCR	C33-C5-C6	-2.49	121.73	124.53
13	b	824	CLA	C1-C2-C3	-2.49	122.73	126.75
13	a	840	CLA	CHB-C4A-NA	2.49	127.95	124.51
13	b	839	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
13	b	817	CLA	C1-C2-C3	-2.49	122.73	126.75
13	b	820	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
13	g	834	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
13	E	821	CLA	C1-C2-C3	-2.49	122.73	126.75
13	b	801	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
15	B	845	BCR	C33-C5-C6	-2.49	121.74	124.53
13	B	820	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
13	G	804	CLA	CHB-C4A-NA	2.48	127.95	124.51
13	G	833	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
13	g	814	CLA	CHB-C4A-NA	2.48	127.95	124.51
13	e	814	CLA	C1-C2-C3	-2.48	122.73	126.75
15	g	846	BCR	C33-C5-C6	-2.48	121.74	124.53
13	L	203	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
13	e	831	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
13	G	840	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
13	g	838	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	b	817	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
13	o	202	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	E	808	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
13	b	822	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
13	l	204	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
13	a	832	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
13	g	822	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
13	b	810	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
15	G	845	BCR	C15-C14-C13	-2.48	123.77	127.31
13	g	819	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	a	831	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
13	a	838	CLA	C1-C2-C3	-2.48	122.74	126.75
13	a	841	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
13	E	841	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
13	e	839	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
13	B	802	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
13	G	804	CLA	O2A-CGA-O1A	-2.48	117.34	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	840	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
13	E	841	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
13	G	810	CLA	C1-C2-C3	-2.48	122.75	126.75
13	G	818	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
15	a	851	BCR	C27-C26-C25	2.47	126.32	122.73
15	i	101	BCR	C27-C26-C25	2.47	126.32	122.73
13	A	806	CLA	CHB-C4A-NA	2.47	127.93	124.51
15	B	844	BCR	C15-C14-C13	-2.47	123.78	127.31
12	e	801	LHG	C5-O7-C7	-2.47	111.70	117.79
13	B	811	CLA	C1-C2-C3	-2.47	122.75	126.75
13	B	807	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
13	b	839	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
13	a	804	CLA	C1-C2-C3	-2.47	122.75	126.75
15	e	851	BCR	C24-C23-C22	-2.47	122.50	126.23
12	e	802	LHG	O8-C23-C24	2.47	119.67	111.91
15	A	847	BCR	C20-C21-C22	-2.47	123.78	127.31
13	S	203	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
13	g	806	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
13	B	823	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
15	A	850	BCR	C11-C10-C9	-2.47	123.78	127.31
13	A	839	CLA	CHB-C4A-NA	2.47	127.93	124.51
13	E	845	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
13	a	819	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
13	b	806	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
13	B	805	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
15	E	851	BCR	C27-C26-C25	2.47	126.32	122.73
13	E	841	CLA	CMB-C2B-C3B	2.47	129.30	124.68
13	B	818	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
15	P	101	BCR	C27-C26-C25	2.47	126.31	122.73
15	q	102	BCR	C33-C5-C6	-2.47	121.76	124.53
13	a	827	CLA	CHB-C4A-NA	2.47	127.92	124.51
13	a	815	CLA	CHB-C4A-NA	2.47	127.92	124.51
13	G	838	CLA	CHB-C4A-NA	2.47	127.92	124.51
15	G	844	BCR	C15-C14-C13	-2.47	123.79	127.31
13	g	808	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
13	A	804	CLA	C1-C2-C3	-2.47	122.76	126.75
13	B	825	CLA	C1-C2-C3	-2.47	122.76	126.75
13	e	818	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
13	A	832	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
13	B	815	CLA	CHB-C4A-NA	2.47	127.92	124.51
15	a	853	BCR	C33-C5-C6	-2.46	121.76	124.53
13	E	815	CLA	CHB-C4A-NA	2.46	127.92	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	817	CLA	CHB-C4A-NA	2.46	127.92	124.51
13	G	801	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
15	a	849	BCR	C20-C21-C22	-2.46	123.79	127.31
13	g	824	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
15	l	202	BCR	C35-C13-C14	-2.46	119.47	122.92
13	G	823	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
13	A	815	CLA	CHB-C4A-NA	2.46	127.92	124.51
13	A	826	CLA	CHB-C4A-NA	2.46	127.92	124.51
13	A	837	CLA	C1-C2-C3	-2.46	122.77	126.75
13	e	836	CLA	C1-C2-C3	-2.46	122.77	126.75
13	B	807	CLA	C1-C2-C3	-2.46	122.77	126.75
13	A	830	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
15	e	848	BCR	C27-C26-C25	2.46	126.30	122.73
13	s	202	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
13	g	816	CLA	CHB-C4A-NA	2.46	127.91	124.51
13	a	806	CLA	CHB-C4A-NA	2.46	127.91	124.51
13	B	841	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
13	L	202	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
13	A	831	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
13	B	808	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
13	b	836	CLA	CHB-C4A-NA	2.46	127.91	124.51
13	B	826	CLA	O2D-CGD-CBD	2.46	115.63	111.27
15	b	843	BCR	C11-C10-C9	-2.46	123.81	127.31
15	J	102	BCR	C33-C5-C6	-2.46	121.77	124.53
13	e	836	CLA	CHD-C1D-ND	-2.45	122.20	124.45
13	g	812	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
15	e	849	BCR	C15-C14-C13	-2.45	123.81	127.31
13	B	811	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
13	G	807	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
13	G	806	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
13	b	825	CLA	O2D-CGD-CBD	2.45	115.63	111.27
13	g	809	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
13	b	823	CLA	CMB-C2B-C3B	2.45	129.27	124.68
13	e	811	CLA	CHB-C4A-NA	2.45	127.90	124.51
15	G	846	BCR	C27-C26-C25	2.45	126.29	122.73
15	A	852	BCR	C24-C23-C22	-2.45	122.53	126.23
13	b	804	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
13	g	813	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
13	E	832	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
13	E	831	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
15	g	845	BCR	C11-C10-C9	-2.45	123.81	127.31
13	E	838	CLA	C1-C2-C3	-2.45	122.79	126.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	g	845	BCR	C15-C14-C13	-2.45	123.81	127.31
13	E	830	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
15	R	101	BCR	C33-C5-C6	-2.45	121.78	124.53
13	s	205	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
13	e	838	CLA	CHB-C4A-NA	2.45	127.90	124.51
13	a	826	CLA	CHB-C4A-NA	2.45	127.90	124.51
13	g	842	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
15	b	844	BCR	C15-C14-C13	-2.45	123.81	127.31
13	g	806	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
13	G	841	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
15	A	849	BCR	C27-C26-C25	2.45	126.29	122.73
15	l	202	BCR	C27-C26-C25	2.45	126.28	122.73
13	B	818	CLA	CHB-C4A-NA	2.45	127.90	124.51
15	B	845	BCR	C15-C14-C13	-2.45	123.82	127.31
13	B	805	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
13	B	837	CLA	CHB-C4A-NA	2.45	127.89	124.51
13	b	840	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
13	E	846	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
13	E	826	CLA	CHB-C4A-NA	2.44	127.89	124.51
12	A	801	LHG	C5-O7-C7	-2.44	111.77	117.79
13	A	812	CLA	CHB-C4A-NA	2.44	127.89	124.51
13	e	829	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
13	A	810	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
13	E	806	CLA	CHB-C4A-NA	2.44	127.89	124.51
13	e	805	CLA	CHB-C4A-NA	2.44	127.89	124.51
13	e	841	CLA	CHB-C4A-NA	2.44	127.89	124.51
15	i	101	BCR	C33-C5-C6	-2.44	121.78	124.53
13	B	827	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
13	E	833	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
13	G	827	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
13	e	839	CLA	CMB-C2B-C3B	2.44	129.25	124.68
13	e	809	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
15	B	844	BCR	C11-C10-C9	-2.44	123.83	127.31
13	G	810	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
15	E	802	BCR	C35-C13-C14	-2.44	119.50	122.92
13	B	805	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
15	g	846	BCR	C15-C14-C13	-2.44	123.83	127.31
15	B	846	BCR	C27-C26-C25	2.44	126.28	122.73
13	E	830	CLA	CHB-C4A-NA	2.44	127.89	124.51
13	G	804	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
13	b	835	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
13	G	826	CLA	O2D-CGD-CBD	2.44	115.60	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	o	201	BCR	C33-C5-C6	-2.44	121.79	124.53
15	a	848	BCR	C27-C26-C25	2.44	126.27	122.73
13	a	810	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
13	b	804	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
13	G	805	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
13	G	811	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
13	g	807	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
13	E	843	CLA	CHB-C4A-NA	2.44	127.88	124.51
13	e	826	CLA	CHB-C4A-NA	2.44	127.88	124.51
13	B	812	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
13	e	830	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
13	e	804	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
13	E	827	CLA	CHB-C4A-NA	2.44	127.88	124.51
13	g	827	CLA	O2D-CGD-CBD	2.43	115.59	111.27
13	E	846	CLA	CHB-C4A-NA	2.43	127.88	124.51
15	E	852	BCR	C33-C5-C6	-2.43	121.80	124.53
13	b	804	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
13	b	807	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
13	A	833	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
13	a	841	CLA	CMB-C2B-C3B	2.43	129.23	124.68
15	k	4001	BCR	C16-C17-C18	2.43	130.78	127.31
13	a	812	CLA	CHB-C4A-NA	2.43	127.88	124.51
13	B	815	CLA	C1-C2-C3	-2.43	122.82	126.75
13	G	806	CLA	C1-C2-C3	-2.43	122.82	126.75
15	E	849	BCR	C20-C21-C22	-2.43	123.84	127.31
13	g	816	CLA	C1-C2-C3	-2.43	122.82	126.75
15	p	101	BCR	C27-C26-C25	2.43	126.26	122.73
13	B	824	CLA	CMB-C2B-C3B	2.43	129.22	124.68
15	G	844	BCR	C11-C10-C9	-2.43	123.84	127.31
13	E	812	CLA	CHB-C4A-NA	2.43	127.87	124.51
13	e	825	CLA	CHB-C4A-NA	2.43	127.87	124.51
13	g	837	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
15	F	201	BCR	C33-C5-C6	-2.43	121.80	124.53
13	e	832	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
15	e	846	BCR	C20-C21-C22	-2.43	123.85	127.31
13	B	806	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
13	G	824	CLA	CMB-C2B-C3B	2.43	129.22	124.68
15	E	801	BCR	C11-C10-C9	-2.43	123.85	127.31
13	B	836	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
15	O	201	BCR	C33-C5-C6	-2.43	121.80	124.53
13	A	806	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
13	g	806	CLA	C1B-CHB-C4A	-2.43	125.31	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	101	BCR	C33-C5-C6	-2.42	121.81	124.53
15	T	101	BCR	C24-C23-C22	-2.42	122.57	126.23
13	A	837	CLA	CHD-C1D-ND	-2.42	122.23	124.45
13	a	833	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
15	g	847	BCR	C27-C26-C25	2.42	126.25	122.73
15	f	201	BCR	C33-C5-C6	-2.42	121.81	124.53
13	l	203	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
13	A	827	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	E	821	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	b	805	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
13	G	801	CLA	O2D-CGD-CBD	2.42	115.57	111.27
13	g	828	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
13	r	102	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
13	a	830	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
13	G	817	CLA	C1-C2-C3	-2.42	122.84	126.75
13	g	823	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	b	807	CLA	C1-C2-C3	-2.42	122.84	126.75
13	k	4002	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
12	A	801	LHG	O8-C23-C24	2.42	119.50	111.91
13	g	825	CLA	CMB-C2B-C3B	2.42	129.20	124.68
13	G	815	CLA	C1-C2-C3	-2.42	122.84	126.75
13	E	810	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
12	e	801	LHG	O8-C23-C24	2.42	119.50	111.91
13	A	821	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	e	836	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	b	846	BCR	C33-C5-C6	-2.42	121.81	124.53
13	A	804	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
13	A	840	CLA	CMB-C2B-C3B	2.42	129.20	124.68
13	E	804	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
13	a	804	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
13	b	814	CLA	C1-C2-C3	-2.42	122.84	126.75
13	e	829	CLA	CHB-C4A-NA	2.42	127.85	124.51
13	B	817	CLA	C1-C2-C3	-2.42	122.84	126.75
15	E	851	BCR	C24-C23-C22	-2.41	122.59	126.23
13	a	843	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
13	A	830	CLA	CHB-C4A-NA	2.41	127.85	124.51
13	a	828	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
13	b	829	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
13	b	816	CLA	C1-C2-C3	-2.41	122.85	126.75
15	b	845	BCR	C27-C26-C25	2.41	126.23	122.73
13	L	203	CLA	CHB-C4A-NA	2.41	127.85	124.51
13	K	102	CLA	C1B-CHB-C4A	-2.41	125.34	130.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	827	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
13	G	836	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
13	A	842	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
15	A	850	BCR	C15-C14-C13	-2.41	123.87	127.31
13	g	808	CLA	C1-C2-C3	-2.41	122.85	126.75
13	a	843	CLA	CHB-C4A-NA	2.41	127.84	124.51
13	G	804	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
13	e	812	CLA	CHB-C4A-NA	2.41	127.84	124.51
13	b	826	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
13	E	806	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
13	L	202	CLA	CHB-C4A-NA	2.41	127.84	124.51
13	G	831	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
13	G	825	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
13	g	831	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
15	g	848	BCR	C33-C5-C6	-2.40	121.83	124.53
13	a	821	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	E	828	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
13	g	832	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
13	a	813	CLA	CHB-C4A-NA	2.40	127.83	124.51
15	A	850	BCR	C35-C13-C14	-2.40	119.56	122.92
13	E	843	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
13	e	805	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
13	g	823	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
13	E	838	CLA	CHD-C1D-ND	-2.40	122.25	124.45
13	R	102	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
13	B	825	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
13	e	820	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	g	809	CLA	C1-C2-C3	-2.40	122.87	126.75
15	O	201	BCR	C15-C14-C13	-2.40	123.89	127.31
15	A	849	BCR	C24-C23-C22	-2.40	122.61	126.23
13	b	816	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
13	G	826	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
12	e	802	LHG	C20-C19-C18	-2.40	102.26	114.42
13	b	825	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
15	e	849	BCR	C11-C10-C9	-2.39	123.89	127.31
13	b	806	CLA	C1-C2-C3	-2.39	122.88	126.75
13	G	814	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
13	E	813	CLA	CHB-C4A-NA	2.39	127.82	124.51
13	G	807	CLA	C1-C2-C3	-2.39	122.88	126.75
13	A	836	CLA	CHB-C4A-NA	2.39	127.82	124.51
13	A	837	CLA	CHB-C4A-NA	2.39	127.82	124.51
13	B	822	CLA	CHB-C4A-NA	2.39	127.82	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	838	CLA	CHB-C4A-NA	2.39	127.82	124.51
13	e	835	CLA	CHB-C4A-NA	2.39	127.82	124.51
13	f	203	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
13	B	801	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
15	s	204	BCR	C29-C30-C25	2.39	114.16	110.48
13	b	830	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
13	l	204	CLA	CHB-C4A-NA	2.39	127.82	124.51
13	B	808	CLA	C1-C2-C3	-2.39	122.88	126.75
15	e	849	BCR	C35-C13-C14	-2.39	119.58	122.92
13	B	829	CLA	C1-C2-C3	-2.39	122.89	126.75
13	g	818	CLA	C1-C2-C3	-2.39	122.89	126.75
13	a	835	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
13	g	802	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
13	G	830	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
13	a	838	CLA	CHD-C1D-ND	-2.39	122.26	124.45
13	A	828	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
13	e	841	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
13	A	842	CLA	CHB-C4A-NA	2.38	127.81	124.51
13	B	831	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
13	G	817	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
15	P	101	BCR	C33-C5-C6	-2.38	121.85	124.53
13	O	203	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
13	e	835	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
13	A	816	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
13	a	806	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
13	e	841	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
15	G	843	BCR	C27-C26-C25	2.38	126.19	122.73
15	j	101	BCR	C27-C26-C25	2.38	126.19	122.73
13	a	844	CLA	C1-C2-C3	-2.38	122.90	126.75
13	E	843	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
15	a	851	BCR	C24-C23-C22	-2.38	122.64	126.23
13	G	829	CLA	C1-C2-C3	-2.38	122.90	126.75
13	B	822	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
15	f	201	BCR	C15-C14-C13	-2.38	123.92	127.31
13	a	837	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
15	e	848	BCR	C24-C23-C22	-2.38	122.64	126.23
15	g	847	BCR	C33-C5-C6	-2.38	121.86	124.53
15	a	803	BCR	C33-C5-C6	-2.38	121.86	124.53
15	p	101	BCR	C33-C5-C6	-2.38	121.86	124.53
13	B	826	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
13	g	830	CLA	C1-C2-C3	-2.38	122.91	126.75
13	e	821	CLA	CHB-C4A-NA	2.38	127.80	124.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	817	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
13	g	818	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
13	g	827	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
13	E	837	CLA	CHB-C4A-NA	2.38	127.80	124.51
13	b	821	CLA	CHB-C4A-NA	2.38	127.80	124.51
13	B	814	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
13	B	830	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
13	E	844	CLA	C1-C2-C3	-2.37	122.91	126.75
13	G	809	CLA	C1-C2-C3	-2.37	122.91	126.75
13	a	843	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
15	G	847	BCR	C33-C5-C6	-2.37	121.86	124.53
15	s	204	BCR	C35-C13-C14	-2.37	119.60	122.92
13	A	836	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	E	835	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	E	839	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	e	840	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	g	826	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	E	832	CLA	CHB-C4A-NA	2.37	127.79	124.51
13	E	808	CLA	CHD-C1D-ND	-2.37	122.28	124.45
13	a	830	CLA	CHB-C4A-NA	2.37	127.79	124.51
13	a	837	CLA	CHB-C4A-NA	2.37	127.79	124.51
13	g	815	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	A	845	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	b	824	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	E	821	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
15	b	842	BCR	C27-C26-C25	2.37	126.17	122.73
13	A	843	CLA	CHB-C4A-NA	2.37	127.79	124.51
13	e	815	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
13	G	822	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
13	A	821	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
13	E	822	CLA	CHB-C4A-NA	2.37	127.79	124.51
13	A	838	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
13	r	101	CLA	CHB-C4A-NA	2.37	127.78	124.51
13	a	832	CLA	CHB-C4A-NA	2.37	127.78	124.51
15	J	101	BCR	C27-C26-C25	2.37	126.17	122.73
13	b	813	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
13	b	821	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
13	r	102	CLA	CHB-C4A-NA	2.37	127.78	124.51
13	a	808	CLA	CHD-C1D-ND	-2.37	122.28	124.45
13	e	813	CLA	CHB-C4A-NA	2.37	127.78	124.51
13	a	838	CLA	CHB-C4A-NA	2.37	127.78	124.51
12	a	801	LHG	C20-C19-C18	-2.36	102.42	114.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	827	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
15	J	101	BCR	C24-C23-C22	-2.36	122.66	126.23
15	Q	101	BCR	C24-C23-C22	-2.36	122.66	126.23
13	a	852	CLA	CHB-C4A-NA	2.36	127.78	124.51
13	E	837	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
13	A	839	CLA	C1-C2-C3	-2.36	122.93	126.75
13	A	813	CLA	CHB-C4A-NA	2.36	127.78	124.51
13	E	816	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
15	B	843	BCR	C27-C26-C25	2.36	126.16	122.73
15	B	847	BCR	C33-C5-C6	-2.36	121.88	124.53
13	G	822	CLA	CHB-C4A-NA	2.36	127.78	124.51
13	S	203	CLA	CHB-C4A-NA	2.36	127.78	124.51
13	F	202	CLA	CHB-C4A-NA	2.36	127.78	124.51
13	G	835	CLA	CMB-C2B-C3B	2.36	129.09	124.68
13	g	809	CLA	CHB-C4A-NA	2.36	127.78	124.51
13	g	836	CLA	CHB-C4A-NA	2.36	127.77	124.51
13	A	842	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
13	A	832	CLA	C1-C2-C3	-2.36	122.94	126.75
13	s	202	CLA	CHB-C4A-NA	2.36	127.77	124.51
13	a	844	CLA	CHB-C4A-NA	2.36	127.77	124.51
13	A	814	CLA	CHB-C4A-NA	2.36	127.77	124.51
13	a	821	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
15	a	802	BCR	C27-C26-C25	2.36	126.15	122.73
13	e	820	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
13	G	828	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
13	A	822	CLA	CHB-C4A-NA	2.36	127.77	124.51
13	b	828	CLA	C1-C2-C3	-2.36	122.94	126.75
13	G	831	CLA	CHB-C4A-NA	2.36	127.77	124.51
15	G	846	BCR	C33-C5-C6	-2.35	121.88	124.53
15	a	848	BCR	C37-C22-C21	-2.35	119.62	122.92
15	e	846	BCR	C27-C26-C25	2.35	126.15	122.73
13	K	102	CLA	CHB-C4A-NA	2.35	127.77	124.51
13	a	831	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
13	a	842	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
13	B	835	CLA	CHB-C4A-NA	2.35	127.77	124.51
13	B	829	CLA	CHB-C4A-NA	2.35	127.77	124.51
13	G	829	CLA	CHB-C4A-NA	2.35	127.77	124.51
13	a	814	CLA	CHB-C4A-NA	2.35	127.77	124.51
13	E	811	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
15	S	202	BCR	C33-C5-C6	-2.35	121.89	124.53
13	A	832	CLA	CHB-C4A-NA	2.35	127.76	124.51
13	a	832	CLA	C1-C2-C3	-2.35	122.95	126.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	839	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
13	b	838	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
13	A	843	CLA	C1-C2-C3	-2.35	122.95	126.75
15	E	849	BCR	C27-C26-C25	2.35	126.14	122.73
13	B	835	CLA	CMB-C2B-C3B	2.35	129.08	124.68
13	a	811	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
15	A	847	BCR	C27-C26-C25	2.35	126.14	122.73
13	E	814	CLA	CHB-C4A-NA	2.35	127.76	124.51
13	R	102	CLA	CHB-C4A-NA	2.35	127.76	124.51
15	F	201	BCR	C15-C14-C13	-2.35	123.96	127.31
13	A	841	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
13	a	840	CLA	C1-C2-C3	-2.35	122.95	126.75
13	e	831	CLA	CHB-C4A-NA	2.35	127.76	124.51
13	g	830	CLA	CHB-C4A-NA	2.35	127.76	124.51
13	e	807	CLA	CHD-C1D-ND	-2.35	122.30	124.45
13	b	834	CLA	CMB-C2B-C3B	2.35	129.07	124.68
15	L	205	BCR	C35-C13-C14	-2.35	119.64	122.92
13	A	831	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
13	E	831	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
13	e	842	CLA	C1-C2-C3	-2.35	122.95	126.75
13	G	821	CLA	CHB-C4A-NA	2.35	127.76	124.51
15	a	849	BCR	C27-C26-C25	2.35	126.14	122.73
13	e	837	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
13	a	816	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
15	E	852	BCR	C29-C30-C25	2.35	114.09	110.48
15	E	852	BCR	C15-C16-C17	-2.35	118.67	123.47
15	j	101	BCR	C15-C14-C13	-2.35	123.96	127.31
13	A	808	CLA	CHD-C1D-ND	-2.34	122.30	124.45
13	E	839	CLA	O2D-CGD-CBD	2.34	115.43	111.27
13	E	832	CLA	C1-C2-C3	-2.34	122.96	126.75
13	e	831	CLA	C1-C2-C3	-2.34	122.96	126.75
15	g	844	BCR	C27-C26-C25	2.34	126.13	122.73
13	E	840	CLA	C1-C2-C3	-2.34	122.96	126.75
13	g	842	CLA	C1-C2-C3	-2.34	122.96	126.75
13	b	840	CLA	C1-C2-C3	-2.34	122.96	126.75
13	G	801	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
15	E	802	BCR	C15-C14-C13	-2.34	123.97	127.31
13	g	811	CLA	C1-C2-C3	-2.34	122.96	126.75
13	a	822	CLA	CHB-C4A-NA	2.34	127.75	124.51
13	k	4002	CLA	CHB-C4A-NA	2.34	127.75	124.51
13	b	809	CLA	C1-C2-C3	-2.34	122.97	126.75
15	a	853	BCR	C29-C30-C25	2.34	114.08	110.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	202	BCR	C27-C26-C25	2.34	126.13	122.73
13	G	835	CLA	CHB-C4A-NA	2.34	127.75	124.51
13	g	832	CLA	CHB-C4A-NA	2.34	127.75	124.51
13	a	839	CLA	O2D-CGD-CBD	2.34	115.42	111.27
13	E	842	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
15	B	846	BCR	C33-C5-C6	-2.34	121.90	124.53
15	e	848	BCR	C11-C10-C9	-2.34	123.97	127.31
13	g	836	CLA	CMB-C2B-C3B	2.34	129.05	124.68
15	q	101	BCR	C27-C26-C25	2.34	126.12	122.73
15	b	845	BCR	C33-C5-C6	-2.34	121.90	124.53
15	a	850	BCR	C11-C10-C9	-2.34	123.97	127.31
13	A	811	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
15	F	201	BCR	C7-C8-C9	-2.34	122.70	126.23
15	A	849	BCR	C11-C10-C9	-2.34	123.97	127.31
15	a	849	BCR	C33-C5-C6	-2.34	121.90	124.53
13	e	814	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
13	g	829	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
13	l	203	CLA	CHB-C4A-NA	2.34	127.74	124.51
13	A	838	CLA	CHD-C1D-ND	-2.34	122.31	124.45
15	e	846	BCR	C33-C5-C6	-2.34	121.91	124.53
15	k	4001	BCR	C1-C6-C5	-2.34	119.32	122.61
13	e	826	CLA	O2D-CGD-CBD	2.34	115.42	111.27
13	e	830	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
13	g	803	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
15	A	847	BCR	C33-C5-C6	-2.33	121.91	124.53
13	B	808	CLA	CHB-C4A-NA	2.33	127.74	124.51
13	B	821	CLA	CHB-C4A-NA	2.33	127.74	124.51
13	E	844	CLA	CHB-C4A-NA	2.33	127.74	124.51
12	A	802	LHG	C20-C19-C18	-2.33	102.58	114.42
15	j	101	BCR	C24-C23-C22	-2.33	122.71	126.23
15	q	102	BCR	C29-C30-C25	2.33	114.07	110.48
13	e	810	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
15	m	101	BCR	C11-C10-C9	-2.33	123.98	127.31
13	e	806	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
13	E	807	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
15	O	201	BCR	C7-C8-C9	-2.33	122.71	126.23
15	Q	101	BCR	C27-C26-C25	2.33	126.11	122.73
13	A	804	CLA	CHB-C4A-NA	2.33	127.73	124.51
15	q	101	BCR	C24-C23-C22	-2.33	122.72	126.23
13	B	841	CLA	C1-C2-C3	-2.33	122.98	126.75
13	G	807	CLA	CHB-C4A-NA	2.33	127.73	124.51
15	a	851	BCR	C11-C10-C9	-2.33	123.99	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	831	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
13	e	837	CLA	O2D-CGD-CBD	2.33	115.40	111.27
15	f	201	BCR	C7-C8-C9	-2.33	122.72	126.23
13	G	841	CLA	C1-C2-C3	-2.33	122.99	126.75
13	b	830	CLA	CHB-C4A-NA	2.33	127.73	124.51
13	B	839	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
13	E	832	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
15	a	853	BCR	C15-C16-C17	-2.33	118.71	123.47
13	b	820	CLA	CHB-C4A-NA	2.33	127.73	124.51
13	e	838	CLA	C1-C2-C3	-2.33	122.99	126.75
15	l	206	BCR	C24-C23-C22	-2.33	122.72	126.23
13	A	838	CLA	O2D-CGD-CBD	2.33	115.40	111.27
13	B	810	CLA	C1-C2-C3	-2.33	122.99	126.75
15	A	848	BCR	C11-C10-C9	-2.33	123.99	127.31
15	o	201	BCR	C7-C8-C9	-2.33	122.72	126.23
13	A	843	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
13	B	828	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
13	B	802	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
13	E	827	CLA	O2D-CGD-CBD	2.33	115.40	111.27
13	a	807	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
13	E	804	CLA	CHB-C4A-NA	2.32	127.73	124.51
13	b	828	CLA	CHB-C4A-NA	2.32	127.73	124.51
15	J	102	BCR	C29-C30-C25	2.32	114.06	110.48
13	a	827	CLA	O2D-CGD-CBD	2.32	115.40	111.27
15	G	847	BCR	C24-C23-C22	-2.32	122.72	126.23
13	K	101	CLA	CHB-C4A-NA	2.32	127.72	124.51
15	s	204	BCR	C2-C1-C6	2.32	114.06	110.48
13	g	840	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
13	A	832	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
13	G	802	CLA	CHB-C4A-NA	2.32	127.72	124.51
15	J	102	BCR	C15-C16-C17	-2.32	118.72	123.47
15	J	101	BCR	C15-C14-C13	-2.32	124.00	127.31
15	A	851	BCR	C27-C26-C25	2.32	126.10	122.73
15	B	847	BCR	C24-C23-C22	-2.32	122.73	126.23
13	b	834	CLA	CHB-C4A-NA	2.32	127.72	124.51
13	a	832	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
13	a	844	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
13	A	827	CLA	O2D-CGD-CBD	2.32	115.38	111.27
13	b	814	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
13	G	822	CLA	CHD-C1D-ND	-2.32	122.33	124.45
13	B	831	CLA	CHB-C4A-NA	2.32	127.71	124.51
15	m	101	BCR	C38-C26-C25	-2.32	121.93	124.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	o	201	BCR	C27-C26-C25	2.31	126.09	122.73
15	O	201	BCR	C27-C26-C25	2.31	126.09	122.73
15	q	102	BCR	C15-C16-C17	-2.31	118.73	123.47
15	E	851	BCR	C11-C10-C9	-2.31	124.01	127.31
13	A	807	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
13	A	853	CLA	CHB-C4A-NA	2.31	127.71	124.51
15	g	848	BCR	C24-C23-C22	-2.31	122.74	126.23
13	g	822	CLA	CHB-C4A-NA	2.31	127.71	124.51
15	e	851	BCR	C15-C14-C13	-2.31	124.01	127.31
13	e	835	CLA	C1-C2-C3	-2.31	123.01	126.75
13	A	815	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
13	G	839	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
13	g	838	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
13	b	801	CLA	CHB-C4A-NA	2.31	127.71	124.51
15	f	201	BCR	C27-C26-C25	2.31	126.08	122.73
13	G	815	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
13	e	842	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
15	o	201	BCR	C15-C14-C13	-2.31	124.02	127.31
13	a	837	CLA	C1-C2-C3	-2.31	123.02	126.75
13	E	815	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
13	E	844	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
13	e	852	CLA	CHB-C4A-NA	2.31	127.70	124.51
13	b	821	CLA	CHD-C1D-ND	-2.31	122.33	124.45
13	E	830	CLA	C1-C2-C3	-2.31	123.02	126.75
13	e	842	CLA	CHB-C4A-NA	2.30	127.70	124.51
13	a	834	CLA	CHB-C4A-NA	2.30	127.70	124.51
15	E	849	BCR	C33-C5-C6	-2.30	121.94	124.53
15	b	846	BCR	C24-C23-C22	-2.30	122.75	126.23
13	E	837	CLA	C1-C2-C3	-2.30	123.03	126.75
13	a	815	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
13	b	809	CLA	O2D-CGD-CBD	2.30	115.36	111.27
13	b	803	CLA	C1-C2-C3	-2.30	123.03	126.75
12	e	801	LHG	C20-C19-C18	-2.30	102.74	114.42
13	b	812	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
13	G	809	CLA	O2D-CGD-CBD	2.30	115.36	111.27
13	a	830	CLA	C1-C2-C3	-2.30	123.03	126.75
13	B	823	CLA	C1-C2-C3	-2.30	123.03	126.75
13	G	837	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
15	F	201	BCR	C27-C26-C25	2.30	126.07	122.73
13	G	827	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
13	B	804	CLA	C1-C2-C3	-2.30	123.03	126.75
13	b	836	CLA	C1B-CHB-C4A	-2.30	125.57	130.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	g	803	CLA	CHB-C4A-NA	2.30	127.69	124.51
13	g	805	CLA	C1-C2-C3	-2.30	123.04	126.75
13	E	829	CLA	CHB-C4A-NA	2.30	127.69	124.51
13	b	802	CLA	CHB-C4A-NA	2.30	127.69	124.51
15	S	201	BCR	C33-C5-C6	-2.29	121.95	124.53
13	g	811	CLA	O2D-CGD-CBD	2.29	115.34	111.27
13	B	815	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
15	E	850	BCR	C11-C10-C9	-2.29	124.04	127.31
15	e	847	BCR	C15-C14-C13	-2.29	124.04	127.31
13	g	816	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
12	A	801	LHG	C20-C19-C18	-2.29	102.79	114.42
13	A	834	CLA	CHB-C4A-NA	2.29	127.68	124.51
13	G	827	CLA	CHB-C4A-NA	2.29	127.68	124.51
15	f	202	BCR	C27-C26-C25	2.29	126.06	122.73
13	B	822	CLA	CHD-C1D-ND	-2.29	122.35	124.45
13	e	837	CLA	CHD-C1D-ND	-2.29	122.35	124.45
15	S	205	BCR	C15-C14-C13	-2.29	124.04	127.31
13	A	830	CLA	C1-C2-C3	-2.29	123.05	126.75
15	b	847	BCR	C38-C26-C25	-2.29	121.96	124.53
13	A	807	CLA	C1-C2-C3	-2.29	123.05	126.75
13	a	807	CLA	C1-C2-C3	-2.29	123.05	126.75
13	B	802	CLA	CHB-C4A-NA	2.29	127.68	124.51
13	B	810	CLA	O2D-CGD-CBD	2.29	115.33	111.27
13	a	812	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
13	g	823	CLA	CHD-C1D-ND	-2.29	122.35	124.45
13	g	814	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
13	b	807	CLA	CHB-C4A-NA	2.29	127.68	124.51
15	G	844	BCR	C33-C5-C6	-2.29	121.96	124.53
13	G	813	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
15	Q	101	BCR	C15-C14-C13	-2.28	124.05	127.31
13	a	804	CLA	CHB-C4A-NA	2.28	127.67	124.51
13	e	804	CLA	CHB-C4A-NA	2.28	127.67	124.51
13	e	838	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
15	G	843	BCR	C11-C10-C9	-2.28	124.05	127.31
13	e	811	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
13	a	839	CLA	CHD-C1D-ND	-2.28	122.36	124.45
13	a	831	CLA	CHB-C4A-NA	2.28	127.67	124.51
13	E	840	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
13	B	827	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
13	E	824	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
13	e	823	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
13	A	829	CLA	CHB-C4A-NA	2.28	127.67	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	843	BCR	C33-C5-C6	-2.28	121.97	124.53
13	e	805	CLA	C1-C2-C3	-2.28	123.06	126.75
15	q	101	BCR	C15-C14-C13	-2.28	124.06	127.31
13	G	803	CLA	C1-C2-C3	-2.28	123.06	126.75
13	A	836	CLA	C1-C2-C3	-2.28	123.06	126.75
13	B	837	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
13	B	813	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
13	E	812	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
13	g	828	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
13	G	819	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
13	e	829	CLA	C1-C2-C3	-2.28	123.07	126.75
13	g	824	CLA	C1-C2-C3	-2.28	123.07	126.75
13	G	824	CLA	CHB-C4A-NA	2.28	127.66	124.51
13	b	816	CLA	CHB-C4A-NA	2.28	127.66	124.51
13	b	822	CLA	C1-C2-C3	-2.27	123.07	126.75
13	g	825	CLA	CHB-C4A-NA	2.27	127.66	124.51
13	a	827	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
13	e	833	CLA	CHB-C4A-NA	2.27	127.66	124.51
13	A	820	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
13	L	204	CLA	CHD-C4C-NC	2.27	127.78	124.20
13	A	839	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
13	a	824	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
13	G	801	CLA	CHB-C4A-NA	2.27	127.65	124.51
13	b	823	CLA	CHB-C4A-NA	2.27	127.65	124.51
13	B	829	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
13	b	826	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
13	a	840	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
13	G	832	CLA	CHB-C4A-NA	2.27	127.65	124.51
15	B	844	BCR	C33-C5-C6	-2.27	121.98	124.53
13	A	824	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
13	a	806	CLA	C1-C2-C3	-2.27	123.08	126.75
13	G	829	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
13	E	827	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
13	G	823	CLA	C1-C2-C3	-2.27	123.08	126.75
15	E	850	BCR	C33-C5-C6	-2.27	121.98	124.53
15	e	847	BCR	C11-C10-C9	-2.27	124.07	127.31
13	E	836	CLA	CHD-C1D-ND	-2.27	122.37	124.45
15	j	101	BCR	C33-C5-C6	-2.27	121.98	124.53
13	g	830	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
13	l	205	CLA	CHD-C4C-NC	2.27	127.78	124.20
15	g	845	BCR	C33-C5-C6	-2.27	121.98	124.53
13	g	820	CLA	C1B-CHB-C4A	-2.27	125.63	130.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	806	CLA	C1-C2-C3	-2.27	123.09	126.75
15	E	850	BCR	C15-C14-C13	-2.27	124.08	127.31
13	A	812	CLA	O2A-CGA-O1A	-2.27	117.88	123.59
15	A	848	BCR	C33-C5-C6	-2.26	121.98	124.53
13	A	827	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
13	b	828	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
13	e	830	CLA	CHB-C4A-NA	2.26	127.64	124.51
13	e	819	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
13	a	820	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
13	b	826	CLA	CHB-C4A-NA	2.26	127.64	124.51
13	a	829	CLA	CHB-C4A-NA	2.26	127.64	124.51
13	E	806	CLA	C1-C2-C3	-2.26	123.10	126.75
13	s	203	CLA	CHD-C4C-NC	2.26	127.76	124.20
15	Q	101	BCR	C33-C5-C6	-2.26	121.99	124.53
15	l	202	BCR	C33-C5-C6	-2.26	121.99	124.53
13	E	807	CLA	C1-C2-C3	-2.26	123.10	126.75
13	e	826	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
13	E	841	CLA	C1-C2-C3	-2.26	123.10	126.75
13	A	835	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
13	A	831	CLA	CHB-C4A-NA	2.25	127.63	124.51
13	B	817	CLA	CHB-C4A-NA	2.25	127.63	124.51
13	E	834	CLA	CHB-C4A-NA	2.25	127.63	124.51
13	g	828	CLA	CHB-C4A-NA	2.25	127.63	124.51
15	a	848	BCR	C35-C13-C14	-2.25	119.77	122.92
13	b	831	CLA	CHB-C4A-NA	2.25	127.63	124.51
13	S	204	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
15	G	846	BCR	C15-C14-C13	-2.25	124.09	127.31
13	L	204	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
13	B	832	CLA	CHB-C4A-NA	2.25	127.63	124.51
13	l	205	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
14	G	842	PQN	C2M-C2-C1	2.25	120.00	116.27
13	E	820	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
15	B	846	BCR	C15-C14-C13	-2.25	124.10	127.31
13	E	831	CLA	CHB-C4A-NA	2.25	127.62	124.51
13	G	817	CLA	CHB-C4A-NA	2.25	127.62	124.51
13	b	818	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
13	E	835	CLA	C1-C2-C3	-2.25	123.11	126.75
13	e	834	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
13	E	825	CLA	C2D-C1D-ND	-2.25	108.45	110.10
13	e	824	CLA	C2D-C1D-ND	-2.25	108.45	110.10
15	S	201	BCR	C37-C22-C21	-2.25	119.77	122.92
15	A	848	BCR	C15-C14-C13	-2.25	124.10	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	806	CLA	C1-C2-C3	-2.25	123.12	126.75
13	a	825	CLA	C2D-C1D-ND	-2.25	108.45	110.10
15	a	850	BCR	C15-C14-C13	-2.25	124.10	127.31
15	A	852	BCR	C33-C5-C6	-2.25	122.00	124.53
15	J	101	BCR	C33-C5-C6	-2.25	122.00	124.53
15	G	845	BCR	C27-C26-C25	2.25	125.99	122.73
15	k	4001	BCR	C35-C13-C14	-2.25	119.78	122.92
15	B	843	BCR	C11-C10-C9	-2.25	124.10	127.31
13	a	832	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
13	B	824	CLA	CHB-C4A-NA	2.25	127.62	124.51
15	G	848	BCR	C38-C26-C25	-2.24	122.01	124.53
13	g	809	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
13	B	827	CLA	CHB-C4A-NA	2.24	127.61	124.51
13	S	204	CLA	CHD-C4C-NC	2.24	127.74	124.20
13	a	835	CLA	C1-C2-C3	-2.24	123.12	126.75
13	B	819	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
13	b	801	CLA	O2A-CGA-O1A	-2.24	117.71	123.30
13	g	802	CLA	C1-C2-C3	-2.24	123.12	126.75
13	e	828	CLA	CHB-C4A-NA	2.24	127.61	124.51
15	g	849	BCR	C38-C26-C25	-2.24	122.01	124.53
13	E	838	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
13	g	833	CLA	CHB-C4A-NA	2.24	127.61	124.51
13	s	203	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
13	E	839	CLA	CHD-C1D-ND	-2.24	122.39	124.45
13	A	810	CLA	CHD-C1D-ND	-2.24	122.40	124.45
13	g	818	CLA	CHB-C4A-NA	2.24	127.61	124.51
15	g	844	BCR	C11-C10-C9	-2.24	124.11	127.31
15	a	850	BCR	C33-C5-C6	-2.24	122.02	124.53
14	E	848	PQN	C2M-C2-C1	2.24	119.98	116.27
13	A	809	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
13	B	801	CLA	C1-C2-C3	-2.24	123.14	126.75
13	a	838	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
13	e	827	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
15	e	847	BCR	C33-C5-C6	-2.23	122.02	124.53
13	l	205	CLA	C4D-CHA-C1A	2.23	123.97	121.25
15	q	101	BCR	C33-C5-C6	-2.23	122.02	124.53
15	B	845	BCR	C27-C26-C25	2.23	125.97	122.73
13	A	825	CLA	C2D-C1D-ND	-2.23	108.46	110.10
15	A	847	BCR	C29-C30-C25	2.23	113.92	110.48
15	E	849	BCR	C29-C30-C25	2.23	113.92	110.48
15	L	205	BCR	C27-C26-C25	2.23	125.97	122.73
13	e	810	CLA	C1-C2-C3	-2.23	123.14	126.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	832	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
13	E	819	CLA	CHB-C4A-NA	2.23	127.60	124.51
13	A	832	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
13	G	812	CLA	CHB-C4A-NA	2.23	127.59	124.51
15	s	204	BCR	C15-C14-C13	-2.23	124.13	127.31
13	A	840	CLA	C1-C2-C3	-2.23	123.15	126.75
15	a	802	BCR	C33-C5-C6	-2.23	122.03	124.53
14	A	846	PQN	C2M-C2-C1	2.23	119.96	116.27
13	G	835	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
13	e	839	CLA	C1-C2-C3	-2.23	123.15	126.75
13	e	808	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
13	B	808	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
15	e	846	BCR	C29-C30-C25	2.23	113.91	110.48
13	g	801	CLA	CHB-C4A-NA	2.23	127.59	124.51
13	e	831	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
13	a	805	CLA	CHB-C4A-NA	2.22	127.59	124.51
15	b	842	BCR	C33-C5-C6	-2.22	122.03	124.53
13	A	839	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
13	b	827	CLA	CHB-C4A-NA	2.22	127.59	124.51
13	B	835	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
15	B	848	BCR	C38-C26-C25	-2.22	122.03	124.53
15	g	846	BCR	C27-C26-C25	2.22	125.96	122.73
15	l	202	BCR	C37-C22-C21	-2.22	119.81	122.92
13	E	809	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
13	a	809	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
13	a	836	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
13	g	836	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
13	e	836	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
13	A	828	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
15	g	847	BCR	C15-C14-C13	-2.22	124.14	127.31
15	b	845	BCR	C15-C14-C13	-2.22	124.14	127.31
13	A	837	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
13	E	816	CLA	C1-C2-C3	-2.22	123.16	126.75
13	S	206	CLA	CHB-C4A-NA	2.22	127.58	124.51
13	g	813	CLA	CHD-C1D-ND	-2.22	122.42	124.45
13	A	819	CLA	CHB-C4A-NA	2.22	127.58	124.51
13	G	811	CLA	CHD-C1D-ND	-2.22	122.42	124.45
13	A	805	CLA	CHB-C4A-NA	2.22	127.58	124.51
13	a	816	CLA	C1-C2-C3	-2.22	123.17	126.75
12	A	802	LHG	C18-C17-C16	-2.22	103.18	114.42
13	a	819	CLA	CHB-C4A-NA	2.22	127.58	124.51
13	l	201	CLA	CHB-C4A-NA	2.22	127.58	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	801	LHG	C5-O7-C7	-2.21	112.34	117.79
13	a	828	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
13	a	852	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
14	b	841	PQN	C2M-C2-C1	2.21	119.94	116.27
15	A	852	BCR	C15-C14-C13	-2.21	124.15	127.31
15	e	851	BCR	C35-C13-C14	-2.21	119.82	122.92
13	E	836	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
13	a	824	CLA	C1-C2-C3	-2.21	123.17	126.75
13	b	807	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
15	R	101	BCR	C1-C6-C5	-2.21	119.50	122.61
13	g	829	CLA	CHB-C4A-NA	2.21	127.57	124.51
15	b	842	BCR	C11-C10-C9	-2.21	124.15	127.31
15	O	202	BCR	C15-C14-C13	-2.21	124.16	127.31
14	a	847	PQN	C2M-C2-C1	2.21	119.93	116.27
13	e	823	CLA	C1-C2-C3	-2.21	123.18	126.75
13	a	840	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
13	G	828	CLA	CHB-C4A-NA	2.21	127.57	124.51
13	B	833	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
13	a	810	CLA	CHD-C1D-ND	-2.21	122.42	124.45
13	a	841	CLA	C1-C2-C3	-2.21	123.18	126.75
13	G	807	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
13	a	830	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
13	g	835	CLA	CHB-C4A-NA	2.21	127.56	124.51
13	g	811	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
15	b	844	BCR	C27-C26-C25	2.21	125.94	122.73
15	a	849	BCR	C29-C30-C25	2.21	113.88	110.48
13	b	809	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
14	B	842	PQN	C2M-C2-C1	2.21	119.93	116.27
13	G	809	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
13	b	834	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
13	B	834	CLA	CHB-C4A-NA	2.20	127.56	124.51
13	a	843	CLA	O2D-CGD-CBD	2.20	115.19	111.27
13	G	833	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
13	B	828	CLA	CHB-C4A-NA	2.20	127.56	124.51
13	E	811	CLA	C1-C2-C3	-2.20	123.19	126.75
13	A	842	CLA	O2D-CGD-CBD	2.20	115.18	111.27
13	b	811	CLA	CHB-C4A-NA	2.20	127.56	124.51
13	A	835	CLA	CHD-C1D-ND	-2.20	122.43	124.45
13	E	828	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
14	g	843	PQN	C2M-C2-C1	2.20	119.92	116.27
13	a	813	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
13	E	840	CLA	O2A-CGA-O1A	-2.20	118.04	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	805	CLA	CHB-C4A-NA	2.20	127.55	124.51
13	e	812	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
13	A	824	CLA	C1-C2-C3	-2.20	123.19	126.75
13	A	811	CLA	C1-C2-C3	-2.20	123.19	126.75
13	e	841	CLA	O2D-CGD-CBD	2.20	115.17	111.27
15	l	206	BCR	C15-C14-C13	-2.20	124.17	127.31
13	A	816	CLA	C1-C2-C3	-2.20	123.20	126.75
13	e	834	CLA	CHD-C1D-ND	-2.20	122.44	124.45
15	s	201	BCR	C33-C5-C6	-2.20	122.06	124.53
13	S	204	CLA	C4D-CHA-C1A	2.20	123.92	121.25
13	E	837	CLA	CHD-C1D-ND	-2.20	122.44	124.45
13	B	810	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
13	A	830	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
13	g	834	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
13	a	811	CLA	C1-C2-C3	-2.19	123.20	126.75
13	E	830	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
13	a	836	CLA	CHD-C1D-ND	-2.19	122.44	124.45
13	b	837	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
15	B	843	BCR	C33-C5-C6	-2.19	122.07	124.53
13	L	204	CLA	C4D-CHA-C1A	2.19	123.92	121.25
13	G	838	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
13	e	809	CLA	CHD-C1D-ND	-2.19	122.44	124.45
13	e	815	CLA	C1-C2-C3	-2.19	123.21	126.75
13	b	803	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
14	e	845	PQN	C2M-C2-C1	2.19	119.90	116.27
13	E	822	CLA	C1-C2-C3	-2.19	123.21	126.75
13	E	824	CLA	C1-C2-C3	-2.19	123.21	126.75
13	e	829	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
15	a	803	BCR	C15-C16-C17	-2.19	119.00	123.47
12	e	801	LHG	C18-C17-C16	-2.18	103.33	114.42
13	B	837	CLA	C1-C2-C3	-2.18	123.22	126.75
12	A	801	LHG	C27-C26-C25	-2.18	103.35	114.42
13	a	837	CLA	CHD-C1D-ND	-2.18	122.45	124.45
13	a	818	CLA	O2D-CGD-CBD	2.18	115.14	111.27
15	O	202	BCR	C33-C5-C6	-2.18	122.08	124.53
13	B	812	CLA	CHD-C1D-ND	-2.18	122.45	124.45
13	B	804	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
12	a	801	LHG	C18-C17-C16	-2.18	103.36	114.42
13	b	832	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
13	b	833	CLA	CHB-C4A-NA	2.18	127.52	124.51
13	g	839	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
13	A	813	CLA	C1B-CHB-C4A	-2.18	125.81	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	813	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
13	e	818	CLA	CHB-C4A-NA	2.18	127.52	124.51
15	A	852	BCR	C35-C13-C14	-2.18	119.88	122.92
13	e	838	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
13	a	826	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
12	A	801	LHG	C18-C17-C16	-2.17	103.39	114.42
12	e	801	LHG	C27-C26-C25	-2.17	103.39	114.42
13	B	838	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
13	g	838	CLA	C1-C2-C3	-2.17	123.24	126.75
13	e	825	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
13	e	838	CLA	CHD-C1D-ND	-2.17	122.46	124.45
13	a	822	CLA	C1-C2-C3	-2.17	123.24	126.75
13	E	843	CLA	O2D-CGD-CBD	2.17	115.13	111.27
13	e	817	CLA	O2D-CGD-CBD	2.17	115.12	111.27
13	E	803	CLA	CHD-C1D-ND	-2.17	122.46	124.45
13	s	205	CLA	CHD-C1D-ND	-2.17	122.46	124.45
13	s	203	CLA	C4D-CHA-C1A	2.17	123.89	121.25
13	b	836	CLA	C1-C2-C3	-2.17	123.25	126.75
13	e	844	CLA	O2D-CGD-CBD	2.17	115.12	111.27
13	B	833	CLA	C1-C2-C3	-2.17	123.25	126.75
13	E	810	CLA	CHD-C1D-ND	-2.17	122.46	124.45
15	S	205	BCR	C35-C13-C14	-2.17	119.89	122.92
15	s	201	BCR	C38-C26-C25	-2.16	122.10	124.53
13	A	826	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
13	b	839	CLA	CHD-C1D-ND	-2.16	122.47	124.45
13	a	832	CLA	CHD-C1D-ND	-2.16	122.47	124.45
15	S	202	BCR	C15-C16-C17	-2.16	119.04	123.47
13	G	834	CLA	CHB-C4A-NA	2.16	127.50	124.51
13	g	805	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
13	A	836	CLA	CHD-C1D-ND	-2.16	122.47	124.45
13	B	840	CLA	CHD-C1D-ND	-2.16	122.47	124.45
15	a	851	BCR	C33-C5-C6	-2.16	122.10	124.53
13	E	826	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
13	B	806	CLA	CHD-C1D-ND	-2.16	122.47	124.45
13	E	826	CLA	C1-C2-C3	-2.16	123.26	126.75
13	e	825	CLA	C1-C2-C3	-2.16	123.26	126.75
13	e	806	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
13	A	818	CLA	O2D-CGD-CBD	2.16	115.10	111.27
15	A	851	BCR	C16-C15-C14	-2.16	119.06	123.47
13	A	825	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
13	A	822	CLA	C1-C2-C3	-2.16	123.27	126.75
13	e	820	CLA	O2A-CGA-O1A	-2.15	118.16	123.59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	807	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
13	a	807	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
13	A	839	CLA	CHD-C1D-ND	-2.15	122.47	124.45
13	g	841	CLA	CHD-C1D-ND	-2.15	122.47	124.45
15	e	850	BCR	C16-C15-C14	-2.15	119.06	123.47
13	A	807	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
13	g	810	CLA	CHB-C4A-NA	2.15	127.49	124.51
13	E	821	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
13	E	832	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	G	840	CLA	CHD-C1D-ND	-2.15	122.48	124.45
15	g	844	BCR	C2-C1-C6	2.15	113.79	110.48
15	G	843	BCR	C2-C1-C6	2.15	113.79	110.48
13	G	803	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
13	G	837	CLA	C1-C2-C3	-2.15	123.27	126.75
13	a	821	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
13	a	825	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
13	A	832	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	g	807	CLA	CHD-C1D-ND	-2.15	122.48	124.45
15	G	843	BCR	C33-C5-C6	-2.15	122.11	124.53
13	A	821	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
13	a	826	CLA	C1-C2-C3	-2.15	123.28	126.75
13	G	833	CLA	C1-C2-C3	-2.15	123.28	126.75
13	a	840	CLA	CHD-C1D-ND	-2.15	122.48	124.45
13	e	810	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
15	e	849	BCR	C27-C26-C25	2.15	125.85	122.73
15	e	848	BCR	C33-C5-C6	-2.15	122.12	124.53
15	A	849	BCR	C33-C5-C6	-2.15	122.12	124.53
13	e	831	CLA	CHD-C1D-ND	-2.14	122.48	124.45
13	A	844	CLA	C1-C2-C3	-2.14	123.28	126.75
15	b	842	BCR	C2-C1-C6	2.14	113.78	110.48
13	e	852	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
13	E	825	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
13	E	814	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
13	g	808	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
13	E	818	CLA	O2D-CGD-CBD	2.14	115.08	111.27
13	b	806	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
13	A	826	CLA	C1-C2-C3	-2.14	123.29	126.75
13	e	821	CLA	C1-C2-C3	-2.14	123.29	126.75
15	E	851	BCR	C33-C5-C6	-2.14	122.12	124.53
13	a	852	CLA	C2A-C1A-CHA	2.14	127.60	123.86
15	E	851	BCR	C7-C8-C9	-2.14	123.00	126.23
13	a	845	CLA	C1-C2-C3	-2.14	123.29	126.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	832	CLA	C1-C2-C3	-2.14	123.29	126.75
13	e	835	CLA	CHD-C1D-ND	-2.14	122.49	124.45
13	G	827	CLA	C1-C2-C3	-2.14	123.29	126.75
15	J	102	BCR	C8-C7-C6	-2.14	121.20	127.20
13	G	810	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
15	s	204	BCR	C15-C16-C17	-2.14	119.10	123.47
13	B	827	CLA	C1-C2-C3	-2.14	123.30	126.75
13	G	806	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
15	e	848	BCR	C7-C8-C9	-2.14	123.01	126.23
13	E	806	CLA	CHD-C1D-ND	-2.14	122.49	124.45
13	e	824	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
15	L	201	BCR	C33-C5-C6	-2.13	122.13	124.53
15	L	205	BCR	C2-C1-C6	2.13	113.77	110.48
15	s	204	BCR	C3-C4-C5	-2.13	110.27	114.08
13	e	813	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
13	E	827	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
12	e	802	LHG	C18-C17-C16	-2.13	103.60	114.42
13	E	840	CLA	CHD-C1D-ND	-2.13	122.50	124.45
13	b	805	CLA	CHD-C1D-ND	-2.13	122.50	124.45
13	g	828	CLA	C1-C2-C3	-2.13	123.30	126.75
13	b	810	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
13	E	828	CLA	O2D-CGD-CBD	2.13	115.06	111.27
13	a	828	CLA	O2D-CGD-CBD	2.13	115.06	111.27
13	L	202	CLA	CHD-C1D-ND	-2.13	122.50	124.45
15	E	852	BCR	C8-C7-C6	-2.13	121.22	127.20
13	A	814	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
15	a	851	BCR	C7-C8-C9	-2.13	123.02	126.23
15	g	844	BCR	C33-C5-C6	-2.13	122.14	124.53
12	a	801	LHG	C27-C26-C25	-2.13	103.63	114.42
13	e	826	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
13	e	827	CLA	O2D-CGD-CBD	2.13	115.05	111.27
15	G	847	BCR	C38-C26-C25	-2.13	122.14	124.53
13	b	802	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
15	s	204	BCR	C24-C23-C22	-2.13	123.02	126.23
15	l	206	BCR	C35-C13-C14	-2.12	119.95	122.92
13	B	811	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
13	g	834	CLA	C1-C2-C3	-2.12	123.31	126.75
15	B	843	BCR	C2-C1-C6	2.12	113.75	110.48
15	m	101	BCR	C35-C13-C14	-2.12	119.95	122.92
15	a	853	BCR	C8-C7-C6	-2.12	121.24	127.20
15	b	846	BCR	C38-C26-C25	-2.12	122.14	124.53
13	A	828	CLA	O2D-CGD-CBD	2.12	115.04	111.27

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	831	CLA	CHD-C1D-ND	-2.12	122.50	124.45
13	A	827	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
13	A	853	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
15	g	848	BCR	C38-C26-C25	-2.12	122.15	124.53
15	q	102	BCR	C8-C7-C6	-2.12	121.25	127.20
15	f	201	BCR	C2-C1-C6	2.12	113.74	110.48
13	B	809	CLA	CHB-C4A-NA	2.12	127.44	124.51
13	B	838	CLA	CHD-C1D-ND	-2.12	122.51	124.45
13	B	807	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
15	A	850	BCR	C27-C26-C25	2.12	125.81	122.73
13	b	808	CLA	CHB-C4A-NA	2.12	127.44	124.51
13	G	802	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
13	G	830	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
13	A	835	CLA	C2A-C1A-CHA	2.11	127.55	123.86
13	a	811	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
13	E	811	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
13	A	811	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
13	a	827	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
13	e	834	CLA	C2A-C1A-CHA	2.11	127.55	123.86
13	G	802	CLA	C1-C2-C3	-2.11	123.34	126.75
15	B	847	BCR	C38-C26-C25	-2.11	122.16	124.53
15	S	201	BCR	C27-C26-C25	2.11	125.79	122.73
15	a	802	BCR	C24-C23-C22	-2.11	123.05	126.23
15	A	849	BCR	C7-C8-C9	-2.11	123.05	126.23
13	a	817	CLA	C1-O2A-CGA	2.11	121.97	116.44
15	f	202	BCR	C7-C8-C9	-2.11	123.05	126.23
13	E	836	CLA	C2A-C1A-CHA	2.11	127.54	123.86
15	E	802	BCR	C8-C7-C6	-2.11	121.29	127.20
13	g	839	CLA	CHD-C1D-ND	-2.11	122.52	124.45
13	g	812	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
15	O	201	BCR	C2-C1-C6	2.11	113.72	110.48
13	l	204	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
13	S	203	CLA	O2A-CGA-O1A	-2.10	118.05	123.30
15	e	850	BCR	C7-C8-C9	-2.10	123.06	126.23
15	B	847	BCR	C15-C16-C17	-2.10	119.17	123.47
13	e	805	CLA	CHD-C1D-ND	-2.10	122.52	124.45
13	G	828	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
13	b	829	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
13	G	808	CLA	CHB-C4A-NA	2.10	127.42	124.51
13	G	837	CLA	CHD-C1D-ND	-2.10	122.52	124.45
15	a	802	BCR	C7-C8-C9	-2.10	123.06	126.23
13	e	809	CLA	C1-C2-C3	-2.10	123.35	126.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	814	CLA	CHD-C1D-ND	-2.10	122.53	124.45
13	E	845	CLA	C1-C2-C3	-2.10	123.36	126.75
13	b	831	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
13	a	836	CLA	C2A-C1A-CHA	2.10	127.53	123.86
13	b	826	CLA	C1-C2-C3	-2.10	123.36	126.75
15	L	205	BCR	C15-C14-C13	-2.10	124.32	127.31
13	G	835	CLA	O2A-CGA-O1A	-2.10	118.08	123.30
13	A	828	CLA	C2A-C1A-CHA	2.10	127.52	123.86
15	S	202	BCR	C7-C8-C9	-2.10	123.07	126.23
13	e	843	CLA	C1-C2-C3	-2.09	123.36	126.75
13	g	831	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
15	g	848	BCR	C15-C16-C17	-2.09	119.19	123.47
13	G	803	CLA	CHB-C4A-NA	2.09	127.41	124.51
13	G	813	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
13	g	815	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	o	201	BCR	C2-C1-C6	2.09	113.70	110.48
13	A	803	CLA	C3C-C4C-NC	-2.09	108.22	110.57
13	g	833	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
13	a	810	CLA	C1-C2-C3	-2.09	123.37	126.75
13	E	817	CLA	CHB-C4A-NA	2.09	127.40	124.51
13	e	844	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
13	G	832	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
13	b	837	CLA	CHD-C1D-ND	-2.09	122.53	124.45
13	g	836	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
13	s	202	CLA	O2A-CGA-O1A	-2.09	118.09	123.30
15	A	852	BCR	C15-C16-C17	-2.09	119.20	123.47
13	g	824	CLA	O2D-CGD-CBD	2.09	114.98	111.27
13	A	810	CLA	C1-C2-C3	-2.09	123.37	126.75
15	F	201	BCR	C2-C1-C6	2.09	113.69	110.48
13	L	203	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
13	a	845	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
15	b	846	BCR	C15-C16-C17	-2.09	119.20	123.47
13	a	841	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
13	E	810	CLA	C1-C2-C3	-2.09	123.38	126.75
13	g	829	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
13	B	830	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
13	A	806	CLA	CHD-C1D-ND	-2.08	122.54	124.45
13	A	817	CLA	CHB-C4A-NA	2.08	127.39	124.51
15	G	847	BCR	C15-C16-C17	-2.08	119.20	123.47
13	e	839	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
15	E	801	BCR	C24-C23-C22	-2.08	123.09	126.23
13	b	822	CLA	O2D-CGD-CBD	2.08	114.97	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	828	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
13	E	828	CLA	C2A-C1A-CHA	2.08	127.50	123.86
13	r	101	CLA	C2D-C1D-ND	-2.08	108.57	110.10
13	B	832	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
13	a	828	CLA	C2A-C1A-CHA	2.08	127.50	123.86
13	b	827	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
13	g	805	CLA	CHB-C4A-NA	2.08	127.39	124.51
13	g	821	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
13	E	845	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
13	b	803	CLA	CHB-C4A-NA	2.08	127.38	124.51
13	b	834	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
13	B	837	CLA	CHD-C1D-ND	-2.08	122.55	124.45
13	G	807	CLA	CHD-C1D-ND	-2.08	122.55	124.45
13	e	852	CLA	CHD-C1D-ND	-2.08	122.55	124.45
13	E	841	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
13	b	819	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
13	E	846	CLA	CHD-C1D-ND	-2.08	122.55	124.45
13	l	203	CLA	CHD-C1D-ND	-2.08	122.55	124.45
15	b	846	BCR	C8-C7-C6	-2.08	121.37	127.20
13	s	203	CLA	CAA-C2A-C1A	2.08	118.78	111.97
13	e	843	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
13	G	823	CLA	O2D-CGD-CBD	2.07	114.95	111.27
13	G	831	CLA	CHD-C1D-ND	-2.07	122.55	124.45
13	B	820	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
13	a	834	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
13	G	802	CLA	CHD-C1D-ND	-2.07	122.55	124.45
13	B	806	CLA	C1-C2-C3	-2.07	123.40	126.75
13	e	827	CLA	C2A-C1A-CHA	2.07	127.48	123.86
13	E	803	CLA	C3C-C4C-NC	-2.07	108.25	110.57
13	A	844	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
13	B	814	CLA	CHD-C1D-ND	-2.07	122.55	124.45
15	e	851	BCR	C28-C27-C26	-2.07	110.38	114.08
13	S	204	CLA	CAA-C2A-C1A	2.07	118.76	111.97
13	a	817	CLA	CHB-C4A-NA	2.07	127.38	124.51
13	a	817	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
13	B	818	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
13	G	805	CLA	C1-C2-C3	-2.07	123.40	126.75
13	B	804	CLA	CHB-C4A-NA	2.07	127.37	124.51
15	A	851	BCR	C7-C8-C9	-2.07	123.11	126.23
13	e	833	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
13	g	819	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
13	B	835	CLA	O2A-CGA-O1A	-2.07	118.14	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	816	CLA	O2D-CGD-CBD	2.07	114.94	111.27
13	b	817	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
13	G	820	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
13	L	204	CLA	CAA-C2A-C1A	2.07	118.75	111.97
13	G	805	CLA	CHD-C1D-ND	-2.07	122.56	124.45
13	B	809	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
13	K	102	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
13	B	813	CLA	O2A-CGA-O1A	-2.07	118.15	123.30
13	l	205	CLA	CAA-C2A-C1A	2.06	118.74	111.97
13	b	802	CLA	C1-C2-C3	-2.06	123.41	126.75
13	S	204	CLA	C3C-C4C-NC	-2.06	108.26	110.57
13	s	203	CLA	C3C-C4C-NC	-2.06	108.26	110.57
13	K	101	CLA	C2D-C1D-ND	-2.06	108.58	110.10
13	A	826	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	E	816	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
15	B	847	BCR	C8-C7-C6	-2.06	121.41	127.20
13	b	812	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
13	b	824	CLA	O2D-CGD-CBD	2.06	114.93	111.27
13	b	813	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	E	820	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
13	A	806	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
13	A	840	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
13	g	841	CLA	C1-C2-C3	-2.06	123.42	126.75
13	E	819	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
13	E	834	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
13	e	818	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
13	k	4002	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
13	G	818	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
13	b	836	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	r	102	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
13	e	815	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
15	a	802	BCR	C35-C13-C14	-2.06	120.04	122.92
13	a	816	CLA	O2D-CGD-CBD	2.06	114.92	111.27
13	g	807	CLA	C1-C2-C3	-2.06	123.43	126.75
13	b	830	CLA	CHD-C1D-ND	-2.06	122.56	124.45
13	R	102	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
15	g	848	BCR	C8-C7-C6	-2.06	121.43	127.20
13	G	808	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
15	G	847	BCR	C8-C7-C6	-2.05	121.43	127.20
13	B	808	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	a	806	CLA	CHD-C1D-ND	-2.05	122.57	124.45
15	l	206	BCR	C38-C26-C25	-2.05	122.22	124.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	852	CLA	C1-C2-C3	-2.05	123.43	126.75
13	b	835	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
13	a	806	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
13	B	823	CLA	O2D-CGD-CBD	2.05	114.92	111.27
13	e	815	CLA	O2D-CGD-CBD	2.05	114.92	111.27
13	A	853	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	b	805	CLA	C1-C2-C3	-2.05	123.43	126.75
13	A	816	CLA	O2D-CGD-CBD	2.05	114.91	111.27
13	A	834	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
13	g	814	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
13	e	812	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
13	g	809	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	a	826	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	e	805	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
13	G	825	CLA	O2D-CGD-CBD	2.05	114.91	111.27
13	e	816	CLA	CHB-C4A-NA	2.05	127.34	124.51
13	G	836	CLA	O2A-CGA-O1A	-2.05	118.20	123.30
13	a	813	CLA	O2A-CGA-O1A	-2.05	118.20	123.30
15	L	201	BCR	C38-C26-C25	-2.05	122.23	124.53
13	e	819	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
13	A	816	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
13	g	832	CLA	CHD-C1D-ND	-2.05	122.57	124.45
13	E	806	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
13	a	816	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
15	E	850	BCR	C24-C23-C22	-2.04	123.14	126.23
13	e	819	CLA	C2D-C1D-ND	-2.04	108.60	110.10
13	a	820	CLA	C2D-C1D-ND	-2.04	108.60	110.10
13	g	810	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
15	S	202	BCR	C11-C10-C9	-2.04	124.39	127.31
13	B	825	CLA	O2D-CGD-CBD	2.04	114.90	111.27
13	g	830	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
13	a	820	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
13	g	826	CLA	O2D-CGD-CBD	2.04	114.90	111.27
13	g	834	CLA	CHB-C4A-NA	2.04	127.33	124.51
13	A	853	CLA	C1-C2-C3	-2.04	123.45	126.75
13	A	813	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
13	E	813	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
13	B	836	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
13	a	819	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
15	E	801	BCR	C38-C26-C25	-2.04	122.24	124.53
13	E	826	CLA	CHD-C1D-ND	-2.04	122.58	124.45
15	g	846	BCR	C8-C7-C6	-2.04	121.47	127.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	843	BCR	C7-C8-C9	-2.04	123.15	126.23
13	A	820	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
13	L	202	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
13	E	822	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
15	B	845	BCR	C8-C7-C6	-2.04	121.48	127.20
15	L	205	BCR	C38-C26-C25	-2.04	122.24	124.53
13	L	204	CLA	C3C-C4C-NC	-2.04	108.28	110.57
13	G	840	CLA	C1-C2-C3	-2.04	123.45	126.75
13	b	808	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
13	E	811	CLA	CHD-C1D-ND	-2.04	122.58	124.45
13	A	822	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
15	a	850	BCR	C24-C23-C22	-2.04	123.16	126.23
13	G	812	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
15	B	843	BCR	C24-C23-C22	-2.04	123.16	126.23
13	B	829	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
13	g	818	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
15	G	845	BCR	C8-C7-C6	-2.04	121.48	127.20
13	E	805	CLA	C1-C2-C3	-2.04	123.46	126.75
13	a	814	CLA	O2A-CGA-O1A	-2.04	118.23	123.30
13	B	817	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
13	g	837	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
13	b	807	CLA	CHD-C1D-ND	-2.03	122.58	124.45
13	a	805	CLA	C1-C2-C3	-2.03	123.46	126.75
13	K	102	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
15	k	4001	BCR	C40-C30-C29	-2.03	100.77	108.91
13	B	840	CLA	C1-C2-C3	-2.03	123.46	126.75
15	s	201	BCR	C16-C15-C14	-2.03	119.31	123.47
13	A	819	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
13	l	205	CLA	C3C-C4C-NC	-2.03	108.29	110.57
13	A	825	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
13	E	831	CLA	CAC-C3C-C4C	2.03	127.45	124.81
13	e	833	CLA	C1-C2-C3	-2.03	123.46	126.75
13	A	803	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
13	e	822	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
13	A	827	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	r	102	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
13	e	824	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
13	b	816	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	l	206	BCR	C33-C5-C6	-2.03	122.25	124.53
13	b	828	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	s	201	BCR	C24-C23-C22	-2.03	123.17	126.23
15	E	801	BCR	C8-C7-C6	-2.03	121.50	127.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	g	834	CLA	C2A-C1A-CHA	2.03	127.41	123.86
13	l	201	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
13	A	834	CLA	C1-C2-C3	-2.03	123.47	126.75
13	a	823	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
13	g	801	CLA	C1-C2-C3	-2.03	123.47	126.75
15	A	848	BCR	C24-C23-C22	-2.03	123.17	126.23
13	E	823	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
15	E	802	BCR	C29-C30-C25	2.03	113.60	110.48
13	G	831	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
13	R	102	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
13	G	838	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	B	808	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
15	b	844	BCR	C8-C7-C6	-2.03	121.51	127.20
13	b	839	CLA	C1-C2-C3	-2.03	123.47	126.75
13	S	206	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
15	e	850	BCR	C27-C26-C25	2.03	125.67	122.73
13	a	831	CLA	CAC-C3C-C4C	2.03	127.44	124.81
13	A	811	CLA	CHD-C1D-ND	-2.03	122.59	124.45
13	e	803	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
13	a	822	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
13	G	829	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
15	B	843	BCR	C7-C8-C9	-2.03	123.17	126.23
13	e	810	CLA	CHD-C1D-ND	-2.03	122.59	124.45
15	A	850	BCR	C15-C16-C17	-2.02	119.33	123.47
13	g	822	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
13	E	844	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
15	b	842	BCR	C7-C8-C9	-2.02	123.18	126.23
15	g	844	BCR	C7-C8-C9	-2.02	123.18	126.23
13	G	817	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
13	e	821	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
13	k	4002	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
13	A	823	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
15	g	844	BCR	C24-C23-C22	-2.02	123.18	126.23
13	a	825	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
15	l	202	BCR	C38-C26-C25	-2.02	122.26	124.53
13	e	842	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
15	A	852	BCR	C28-C27-C26	-2.02	110.47	114.08
13	E	825	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
15	J	102	BCR	C11-C10-C9	-2.02	124.43	127.31
15	e	849	BCR	C28-C27-C26	-2.02	110.47	114.08
13	e	803	CLA	C3C-C4C-NC	-2.02	108.31	110.57
13	B	819	CLA	O2A-CGA-O1A	-2.02	118.50	123.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	807	CLA	O2D-CGD-CBD	2.02	114.85	111.27
13	e	830	CLA	CAC-C3C-C4C	2.02	127.43	124.81
15	S	205	BCR	C29-C30-C25	2.02	113.59	110.48
13	B	833	CLA	CHB-C4A-NA	2.02	127.30	124.51
13	B	821	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	A	805	CLA	C1-C2-C3	-2.02	123.49	126.75
15	E	852	BCR	C11-C10-C9	-2.02	124.43	127.31
13	a	834	CLA	C1-C2-C3	-2.02	123.49	126.75
13	G	806	CLA	O2D-CGD-CBD	2.02	114.85	111.27
13	b	820	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
15	e	847	BCR	C24-C23-C22	-2.01	123.19	126.23
15	A	850	BCR	C8-C7-C6	-2.01	121.55	127.20
13	B	825	CLA	CHD-C1D-ND	-2.01	122.60	124.45
15	J	101	BCR	C11-C10-C9	-2.01	124.44	127.31
13	a	811	CLA	CHD-C1D-ND	-2.01	122.61	124.45
13	b	830	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
13	G	819	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
15	b	842	BCR	C24-C23-C22	-2.01	123.20	126.23
13	a	827	CLA	CHD-C1D-ND	-2.01	122.61	124.45
13	b	832	CLA	C2A-C1A-CHA	2.01	127.37	123.86
15	A	852	BCR	C11-C10-C9	-2.01	124.44	127.31
15	i	101	BCR	C15-C16-C17	-2.01	119.36	123.47
13	b	811	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
15	G	843	BCR	C24-C23-C22	-2.01	123.20	126.23
13	s	203	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
13	b	832	CLA	CHB-C4A-NA	2.01	127.29	124.51
13	A	843	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
13	G	807	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
13	B	833	CLA	C2A-C1A-CHA	2.01	127.37	123.86
13	g	808	CLA	O2D-CGD-CBD	2.01	114.84	111.27
13	E	827	CLA	CHD-C1D-ND	-2.01	122.61	124.45
15	e	849	BCR	C8-C7-C6	-2.01	121.56	127.20
13	k	4002	CLA	C2D-C1D-ND	-2.01	108.62	110.10
15	Q	101	BCR	C11-C10-C9	-2.01	124.45	127.31
13	e	826	CLA	CHD-C1D-ND	-2.01	122.61	124.45
13	L	204	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
15	A	851	BCR	C38-C26-C25	-2.01	122.28	124.53
13	B	831	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
13	E	820	CLA	C2D-C1D-ND	-2.01	108.63	110.10
13	e	825	CLA	CHD-C1D-ND	-2.01	122.61	124.45
13	g	838	CLA	CHD-C1D-ND	-2.01	122.61	124.45
15	q	101	BCR	C11-C10-C9	-2.00	124.45	127.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	802	CLA	CHD-C1D-ND	-2.00	122.61	124.45
13	a	809	CLA	C1-C2-C3	-2.00	123.51	126.75
13	A	840	CLA	CHD-C1D-ND	-2.00	122.61	124.45
13	g	832	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
13	e	834	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
15	e	849	BCR	C15-C16-C17	-2.00	119.38	123.47
13	G	821	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (355) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	803	CLA	ND
13	A	804	CLA	ND
13	A	805	CLA	ND
13	A	806	CLA	ND
13	A	807	CLA	ND
13	A	808	CLA	ND
13	A	809	CLA	ND
13	A	810	CLA	ND
13	A	811	CLA	ND
13	A	812	CLA	ND
13	A	813	CLA	ND
13	A	814	CLA	ND
13	A	815	CLA	ND
13	A	816	CLA	ND
13	A	817	CLA	ND
13	A	818	CLA	ND
13	A	819	CLA	ND
13	A	820	CLA	ND
13	A	821	CLA	ND
13	A	822	CLA	ND
13	A	823	CLA	ND
13	A	824	CLA	ND
13	A	825	CLA	ND
13	A	826	CLA	ND
13	A	827	CLA	ND
13	A	828	CLA	ND
13	A	829	CLA	ND
13	A	830	CLA	ND
13	A	831	CLA	ND
13	A	832	CLA	ND
13	A	833	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
13	A	834	CLA	ND
13	A	835	CLA	ND
13	A	836	CLA	ND
13	A	838	CLA	ND
13	A	839	CLA	ND
13	A	840	CLA	ND
13	A	841	CLA	ND
13	A	842	CLA	ND
13	A	843	CLA	ND
13	A	844	CLA	ND
13	A	845	CLA	ND
13	A	853	CLA	ND
13	B	801	CLA	ND
13	B	802	CLA	ND
13	B	804	CLA	ND
13	B	805	CLA	ND
13	B	806	CLA	ND
13	B	807	CLA	ND
13	B	808	CLA	ND
13	B	809	CLA	ND
13	B	810	CLA	ND
13	B	811	CLA	ND
13	B	812	CLA	ND
13	B	813	CLA	ND
13	B	814	CLA	ND
13	B	815	CLA	ND
13	B	816	CLA	ND
13	B	817	CLA	ND
13	B	818	CLA	ND
13	B	819	CLA	ND
13	B	820	CLA	ND
13	B	821	CLA	ND
13	B	822	CLA	ND
13	B	823	CLA	ND
13	B	824	CLA	ND
13	B	825	CLA	ND
13	B	826	CLA	ND
13	B	827	CLA	ND
13	B	828	CLA	ND
13	B	829	CLA	ND
13	B	830	CLA	ND
13	B	831	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
13	B	832	CLA	ND
13	B	833	CLA	ND
13	B	834	CLA	ND
13	B	835	CLA	ND
13	B	836	CLA	ND
13	B	837	CLA	ND
13	B	838	CLA	ND
13	B	839	CLA	ND
13	B	840	CLA	ND
13	B	841	CLA	ND
13	F	202	CLA	ND
13	K	101	CLA	ND
13	K	102	CLA	ND
13	L	202	CLA	ND
13	L	203	CLA	ND
13	L	204	CLA	ND
13	E	803	CLA	ND
13	E	804	CLA	ND
13	E	805	CLA	ND
13	E	806	CLA	ND
13	E	807	CLA	ND
13	E	808	CLA	ND
13	E	809	CLA	ND
13	E	810	CLA	ND
13	E	811	CLA	ND
13	E	812	CLA	ND
13	E	813	CLA	ND
13	E	814	CLA	ND
13	E	815	CLA	ND
13	E	816	CLA	ND
13	E	817	CLA	ND
13	E	818	CLA	ND
13	E	819	CLA	ND
13	E	820	CLA	ND
13	E	821	CLA	ND
13	E	822	CLA	ND
13	E	823	CLA	ND
13	E	824	CLA	ND
13	E	825	CLA	ND
13	E	826	CLA	ND
13	E	827	CLA	ND
13	E	828	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
13	E	829	CLA	ND
13	E	830	CLA	ND
13	E	831	CLA	ND
13	E	832	CLA	ND
13	E	833	CLA	ND
13	E	834	CLA	ND
13	E	835	CLA	ND
13	E	836	CLA	ND
13	E	837	CLA	ND
13	E	839	CLA	ND
13	E	840	CLA	ND
13	E	841	CLA	ND
13	E	842	CLA	ND
13	E	843	CLA	ND
13	E	844	CLA	ND
13	E	845	CLA	ND
13	E	846	CLA	ND
13	G	801	CLA	ND
13	G	802	CLA	ND
13	G	803	CLA	ND
13	G	804	CLA	ND
13	G	805	CLA	ND
13	G	806	CLA	ND
13	G	807	CLA	ND
13	G	808	CLA	ND
13	G	809	CLA	ND
13	G	810	CLA	ND
13	G	811	CLA	ND
13	G	812	CLA	ND
13	G	813	CLA	ND
13	G	814	CLA	ND
13	G	815	CLA	ND
13	G	816	CLA	ND
13	G	817	CLA	ND
13	G	818	CLA	ND
13	G	819	CLA	ND
13	G	820	CLA	ND
13	G	821	CLA	ND
13	G	822	CLA	ND
13	G	823	CLA	ND
13	G	824	CLA	ND
13	G	825	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
13	G	826	CLA	ND
13	G	827	CLA	ND
13	G	828	CLA	ND
13	G	829	CLA	ND
13	G	830	CLA	ND
13	G	831	CLA	ND
13	G	832	CLA	ND
13	G	833	CLA	ND
13	G	834	CLA	ND
13	G	835	CLA	ND
13	G	836	CLA	ND
13	G	837	CLA	ND
13	G	838	CLA	ND
13	G	839	CLA	ND
13	G	840	CLA	ND
13	G	841	CLA	ND
13	O	203	CLA	ND
13	R	102	CLA	ND
13	S	203	CLA	ND
13	S	204	CLA	ND
13	S	206	CLA	ND
13	e	803	CLA	ND
13	e	804	CLA	ND
13	e	805	CLA	ND
13	e	806	CLA	ND
13	e	807	CLA	ND
13	e	808	CLA	ND
13	e	809	CLA	ND
13	e	810	CLA	ND
13	e	811	CLA	ND
13	e	812	CLA	ND
13	e	813	CLA	ND
13	e	814	CLA	ND
13	e	815	CLA	ND
13	e	816	CLA	ND
13	e	817	CLA	ND
13	e	818	CLA	ND
13	e	819	CLA	ND
13	e	820	CLA	ND
13	e	821	CLA	ND
13	e	822	CLA	ND
13	e	823	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
13	e	824	CLA	ND
13	e	825	CLA	ND
13	e	826	CLA	ND
13	e	827	CLA	ND
13	e	828	CLA	ND
13	e	829	CLA	ND
13	e	830	CLA	ND
13	e	831	CLA	ND
13	e	832	CLA	ND
13	e	833	CLA	ND
13	e	834	CLA	ND
13	e	835	CLA	ND
13	e	837	CLA	ND
13	e	838	CLA	ND
13	e	839	CLA	ND
13	e	840	CLA	ND
13	e	841	CLA	ND
13	e	842	CLA	ND
13	e	843	CLA	ND
13	e	844	CLA	ND
13	e	852	CLA	ND
13	g	801	CLA	ND
13	g	802	CLA	ND
13	g	803	CLA	ND
13	g	805	CLA	ND
13	g	806	CLA	ND
13	g	807	CLA	ND
13	g	808	CLA	ND
13	g	809	CLA	ND
13	g	810	CLA	ND
13	g	811	CLA	ND
13	g	812	CLA	ND
13	g	813	CLA	ND
13	g	814	CLA	ND
13	g	815	CLA	ND
13	g	816	CLA	ND
13	g	817	CLA	ND
13	g	818	CLA	ND
13	g	819	CLA	ND
13	g	820	CLA	ND
13	g	821	CLA	ND
13	g	822	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
13	g	823	CLA	ND
13	g	824	CLA	ND
13	g	825	CLA	ND
13	g	826	CLA	ND
13	g	827	CLA	ND
13	g	828	CLA	ND
13	g	829	CLA	ND
13	g	830	CLA	ND
13	g	831	CLA	ND
13	g	832	CLA	ND
13	g	833	CLA	ND
13	g	834	CLA	ND
13	g	835	CLA	ND
13	g	836	CLA	ND
13	g	837	CLA	ND
13	g	838	CLA	ND
13	g	839	CLA	ND
13	g	840	CLA	ND
13	g	841	CLA	ND
13	g	842	CLA	ND
13	o	202	CLA	ND
13	r	101	CLA	ND
13	r	102	CLA	ND
13	s	202	CLA	ND
13	s	203	CLA	ND
13	s	205	CLA	ND
13	a	804	CLA	ND
13	a	805	CLA	ND
13	a	806	CLA	ND
13	a	807	CLA	ND
13	a	808	CLA	ND
13	a	809	CLA	ND
13	a	810	CLA	ND
13	a	811	CLA	ND
13	a	812	CLA	ND
13	a	813	CLA	ND
13	a	814	CLA	ND
13	a	815	CLA	ND
13	a	816	CLA	ND
13	a	817	CLA	ND
13	a	818	CLA	ND
13	a	819	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
13	a	820	CLA	ND
13	a	821	CLA	ND
13	a	822	CLA	ND
13	a	823	CLA	ND
13	a	824	CLA	ND
13	a	825	CLA	ND
13	a	826	CLA	ND
13	a	827	CLA	ND
13	a	828	CLA	ND
13	a	829	CLA	ND
13	a	830	CLA	ND
13	a	831	CLA	ND
13	a	832	CLA	ND
13	a	833	CLA	ND
13	a	834	CLA	ND
13	a	835	CLA	ND
13	a	836	CLA	ND
13	a	837	CLA	ND
13	a	839	CLA	ND
13	a	840	CLA	ND
13	a	841	CLA	ND
13	a	842	CLA	ND
13	a	843	CLA	ND
13	a	844	CLA	ND
13	a	845	CLA	ND
13	a	852	CLA	ND
13	b	801	CLA	ND
13	b	802	CLA	ND
13	b	803	CLA	ND
13	b	804	CLA	ND
13	b	805	CLA	ND
13	b	806	CLA	ND
13	b	807	CLA	ND
13	b	808	CLA	ND
13	b	809	CLA	ND
13	b	810	CLA	ND
13	b	811	CLA	ND
13	b	812	CLA	ND
13	b	813	CLA	ND
13	b	814	CLA	ND
13	b	815	CLA	ND
13	b	816	CLA	ND

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
13	b	817	CLA	ND
13	b	818	CLA	ND
13	b	819	CLA	ND
13	b	820	CLA	ND
13	b	821	CLA	ND
13	b	822	CLA	ND
13	b	823	CLA	ND
13	b	824	CLA	ND
13	b	825	CLA	ND
13	b	826	CLA	ND
13	b	827	CLA	ND
13	b	828	CLA	ND
13	b	829	CLA	ND
13	b	830	CLA	ND
13	b	831	CLA	ND
13	b	832	CLA	ND
13	b	833	CLA	ND
13	b	834	CLA	ND
13	b	835	CLA	ND
13	b	836	CLA	ND
13	b	837	CLA	ND
13	b	838	CLA	ND
13	b	839	CLA	ND
13	b	840	CLA	ND
13	f	203	CLA	ND
13	k	4002	CLA	ND
13	l	201	CLA	ND
13	l	203	CLA	ND
13	l	204	CLA	ND
13	l	205	CLA	ND

All (3682) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	801	LHG	O1-C1-C2-C3
12	A	801	LHG	C3-O3-P-O4
12	A	801	LHG	C3-O3-P-O6
12	A	801	LHG	C4-O6-P-O5
12	A	802	LHG	C3-O3-P-O4
12	A	802	LHG	C3-O3-P-O5
12	A	802	LHG	C3-O3-P-O6
12	e	801	LHG	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
12	e	801	LHG	C3-O3-P-O4
12	e	801	LHG	C4-O6-P-O5
12	e	801	LHG	O7-C5-C6-O8
12	e	802	LHG	C3-O3-P-O4
12	e	802	LHG	C3-O3-P-O5
12	e	802	LHG	C3-O3-P-O6
12	a	801	LHG	O1-C1-C2-C3
12	a	801	LHG	C3-O3-P-O4
12	a	801	LHG	C4-O6-P-O3
12	a	801	LHG	C4-O6-P-O5
13	A	803	CLA	CBD-CGD-O2D-CED
13	A	804	CLA	CHA-CBD-CGD-O1D
13	A	804	CLA	CHA-CBD-CGD-O2D
13	A	804	CLA	CAD-CBD-CGD-O1D
13	A	805	CLA	C1A-C2A-CAA-CBA
13	A	805	CLA	C3A-C2A-CAA-CBA
13	A	805	CLA	CHA-CBD-CGD-O1D
13	A	805	CLA	CHA-CBD-CGD-O2D
13	A	807	CLA	C1A-C2A-CAA-CBA
13	A	807	CLA	C3A-C2A-CAA-CBA
13	A	807	CLA	CBD-CGD-O2D-CED
13	A	807	CLA	O1D-CGD-O2D-CED
13	A	808	CLA	CAD-CBD-CGD-O1D
13	A	808	CLA	CAD-CBD-CGD-O2D
13	A	809	CLA	C3A-C2A-CAA-CBA
13	A	811	CLA	C3A-C2A-CAA-CBA
13	A	812	CLA	CBD-CGD-O2D-CED
13	A	813	CLA	CHA-CBD-CGD-O1D
13	A	813	CLA	CHA-CBD-CGD-O2D
13	A	815	CLA	CHA-CBD-CGD-O1D
13	A	815	CLA	CHA-CBD-CGD-O2D
13	A	815	CLA	CBD-CGD-O2D-CED
13	A	817	CLA	C1A-C2A-CAA-CBA
13	A	817	CLA	C3A-C2A-CAA-CBA
13	A	818	CLA	CBD-CGD-O2D-CED
13	A	819	CLA	C1A-C2A-CAA-CBA
13	A	819	CLA	C3A-C2A-CAA-CBA
13	A	820	CLA	CBD-CGD-O2D-CED
13	A	821	CLA	C3A-C2A-CAA-CBA
13	A	822	CLA	C1A-C2A-CAA-CBA
13	A	822	CLA	C3A-C2A-CAA-CBA
13	A	823	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	823	CLA	CHA-CBD-CGD-O1D
13	A	823	CLA	CHA-CBD-CGD-O2D
13	A	823	CLA	CAD-CBD-CGD-O1D
13	A	824	CLA	CBD-CGD-O2D-CED
13	A	826	CLA	CHA-CBD-CGD-O1D
13	A	826	CLA	CHA-CBD-CGD-O2D
13	A	826	CLA	CAD-CBD-CGD-O1D
13	A	826	CLA	CAD-CBD-CGD-O2D
13	A	826	CLA	CBD-CGD-O2D-CED
13	A	828	CLA	C1A-C2A-CAA-CBA
13	A	828	CLA	C3A-C2A-CAA-CBA
13	A	829	CLA	CBD-CGD-O2D-CED
13	A	830	CLA	CBA-CGA-O2A-C1
13	A	831	CLA	CBA-CGA-O2A-C1
13	A	831	CLA	O1A-CGA-O2A-C1
13	A	831	CLA	CHA-CBD-CGD-O1D
13	A	831	CLA	CHA-CBD-CGD-O2D
13	A	832	CLA	CBD-CGD-O2D-CED
13	A	835	CLA	C1A-C2A-CAA-CBA
13	A	835	CLA	CBD-CGD-O2D-CED
13	A	836	CLA	C1A-C2A-CAA-CBA
13	A	836	CLA	C3A-C2A-CAA-CBA
13	A	837	CLA	C1A-C2A-CAA-CBA
13	A	838	CLA	CHA-CBD-CGD-O2D
13	A	839	CLA	C3A-C2A-CAA-CBA
13	A	840	CLA	CHA-CBD-CGD-O1D
13	A	842	CLA	C1A-C2A-CAA-CBA
13	A	842	CLA	C3A-C2A-CAA-CBA
13	A	843	CLA	CBD-CGD-O2D-CED
13	A	843	CLA	O1D-CGD-O2D-CED
13	A	844	CLA	C1A-C2A-CAA-CBA
13	A	844	CLA	C3A-C2A-CAA-CBA
13	A	845	CLA	C1A-C2A-CAA-CBA
13	A	845	CLA	C3A-C2A-CAA-CBA
13	A	845	CLA	C2A-CAA-CBA-CGA
13	A	853	CLA	C1A-C2A-CAA-CBA
13	A	853	CLA	C3A-C2A-CAA-CBA
13	B	801	CLA	C1A-C2A-CAA-CBA
13	B	801	CLA	C3A-C2A-CAA-CBA
13	B	801	CLA	CHA-CBD-CGD-O1D
13	B	801	CLA	CHA-CBD-CGD-O2D
13	B	804	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	B	804	CLA	CHA-CBD-CGD-O2D
13	B	804	CLA	CBD-CGD-O2D-CED
13	B	805	CLA	CHA-CBD-CGD-O1D
13	B	805	CLA	CHA-CBD-CGD-O2D
13	B	807	CLA	C3A-C2A-CAA-CBA
13	B	808	CLA	CBD-CGD-O2D-CED
13	B	810	CLA	CBD-CGD-O2D-CED
13	B	813	CLA	C1A-C2A-CAA-CBA
13	B	813	CLA	C3A-C2A-CAA-CBA
13	B	815	CLA	C2A-CAA-CBA-CGA
13	B	815	CLA	CBD-CGD-O2D-CED
13	B	815	CLA	O1D-CGD-O2D-CED
13	B	816	CLA	C1A-C2A-CAA-CBA
13	B	816	CLA	C3A-C2A-CAA-CBA
13	B	817	CLA	CBD-CGD-O2D-CED
13	B	817	CLA	O1D-CGD-O2D-CED
13	B	818	CLA	C1A-C2A-CAA-CBA
13	B	818	CLA	C3A-C2A-CAA-CBA
13	B	819	CLA	C1A-C2A-CAA-CBA
13	B	819	CLA	C3A-C2A-CAA-CBA
13	B	821	CLA	CHA-CBD-CGD-O1D
13	B	821	CLA	CHA-CBD-CGD-O2D
13	B	821	CLA	CAD-CBD-CGD-O1D
13	B	821	CLA	CAD-CBD-CGD-O2D
13	B	821	CLA	CBD-CGD-O2D-CED
13	B	822	CLA	CAD-CBD-CGD-O1D
13	B	822	CLA	CAD-CBD-CGD-O2D
13	B	823	CLA	CHA-CBD-CGD-O1D
13	B	823	CLA	CHA-CBD-CGD-O2D
13	B	823	CLA	CBD-CGD-O2D-CED
13	B	826	CLA	C1A-C2A-CAA-CBA
13	B	826	CLA	CBD-CGD-O2D-CED
13	B	828	CLA	CBA-CGA-O2A-C1
13	B	829	CLA	C3A-C2A-CAA-CBA
13	B	829	CLA	CHA-CBD-CGD-O1D
13	B	829	CLA	CHA-CBD-CGD-O2D
13	B	830	CLA	CBD-CGD-O2D-CED
13	B	831	CLA	C3A-C2A-CAA-CBA
13	B	834	CLA	C1A-C2A-CAA-CBA
13	B	834	CLA	C3A-C2A-CAA-CBA
13	B	834	CLA	CBD-CGD-O2D-CED
13	B	836	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	B	836	CLA	C3A-C2A-CAA-CBA
13	B	836	CLA	CAD-CBD-CGD-O1D
13	B	836	CLA	CAD-CBD-CGD-O2D
13	B	837	CLA	CHA-CBD-CGD-O1D
13	B	837	CLA	CHA-CBD-CGD-O2D
13	B	837	CLA	CAD-CBD-CGD-O1D
13	B	837	CLA	CBD-CGD-O2D-CED
13	B	839	CLA	C1A-C2A-CAA-CBA
13	B	839	CLA	C3A-C2A-CAA-CBA
13	B	840	CLA	CHA-CBD-CGD-O1D
13	B	840	CLA	CHA-CBD-CGD-O2D
13	B	840	CLA	CBD-CGD-O2D-CED
13	B	840	CLA	O1D-CGD-O2D-CED
13	F	202	CLA	CAD-CBD-CGD-O1D
13	F	202	CLA	CAD-CBD-CGD-O2D
13	L	202	CLA	C1A-C2A-CAA-CBA
13	L	202	CLA	C3A-C2A-CAA-CBA
13	L	204	CLA	C3A-C2A-CAA-CBA
13	E	803	CLA	CBD-CGD-O2D-CED
13	E	804	CLA	CHA-CBD-CGD-O1D
13	E	804	CLA	CHA-CBD-CGD-O2D
13	E	804	CLA	CAD-CBD-CGD-O1D
13	E	805	CLA	C1A-C2A-CAA-CBA
13	E	805	CLA	C3A-C2A-CAA-CBA
13	E	805	CLA	CHA-CBD-CGD-O1D
13	E	805	CLA	CHA-CBD-CGD-O2D
13	E	807	CLA	C1A-C2A-CAA-CBA
13	E	807	CLA	C3A-C2A-CAA-CBA
13	E	807	CLA	CBD-CGD-O2D-CED
13	E	807	CLA	O1D-CGD-O2D-CED
13	E	808	CLA	CAD-CBD-CGD-O1D
13	E	808	CLA	CAD-CBD-CGD-O2D
13	E	809	CLA	C3A-C2A-CAA-CBA
13	E	811	CLA	C3A-C2A-CAA-CBA
13	E	812	CLA	CBD-CGD-O2D-CED
13	E	813	CLA	CHA-CBD-CGD-O1D
13	E	813	CLA	CHA-CBD-CGD-O2D
13	E	815	CLA	CHA-CBD-CGD-O1D
13	E	815	CLA	CHA-CBD-CGD-O2D
13	E	815	CLA	CBD-CGD-O2D-CED
13	E	817	CLA	C1A-C2A-CAA-CBA
13	E	817	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	E	818	CLA	CBD-CGD-O2D-CED
13	E	819	CLA	C1A-C2A-CAA-CBA
13	E	819	CLA	C3A-C2A-CAA-CBA
13	E	820	CLA	CBD-CGD-O2D-CED
13	E	821	CLA	C1A-C2A-CAA-CBA
13	E	821	CLA	C3A-C2A-CAA-CBA
13	E	822	CLA	C1A-C2A-CAA-CBA
13	E	822	CLA	C3A-C2A-CAA-CBA
13	E	823	CLA	C3A-C2A-CAA-CBA
13	E	823	CLA	CHA-CBD-CGD-O1D
13	E	823	CLA	CHA-CBD-CGD-O2D
13	E	823	CLA	CAD-CBD-CGD-O1D
13	E	824	CLA	CBD-CGD-O2D-CED
13	E	826	CLA	CHA-CBD-CGD-O1D
13	E	826	CLA	CHA-CBD-CGD-O2D
13	E	826	CLA	CAD-CBD-CGD-O1D
13	E	826	CLA	CAD-CBD-CGD-O2D
13	E	826	CLA	CBD-CGD-O2D-CED
13	E	828	CLA	C1A-C2A-CAA-CBA
13	E	828	CLA	C3A-C2A-CAA-CBA
13	E	829	CLA	CBD-CGD-O2D-CED
13	E	830	CLA	CBA-CGA-O2A-C1
13	E	831	CLA	CBA-CGA-O2A-C1
13	E	831	CLA	O1A-CGA-O2A-C1
13	E	831	CLA	CHA-CBD-CGD-O1D
13	E	831	CLA	CHA-CBD-CGD-O2D
13	E	832	CLA	CBD-CGD-O2D-CED
13	E	835	CLA	C1A-C2A-CAA-CBA
13	E	835	CLA	C3A-C2A-CAA-CBA
13	E	835	CLA	CHA-CBD-CGD-O1D
13	E	835	CLA	CHA-CBD-CGD-O2D
13	E	836	CLA	C1A-C2A-CAA-CBA
13	E	836	CLA	CBD-CGD-O2D-CED
13	E	837	CLA	C1A-C2A-CAA-CBA
13	E	837	CLA	C3A-C2A-CAA-CBA
13	E	838	CLA	C1A-C2A-CAA-CBA
13	E	839	CLA	CHA-CBD-CGD-O2D
13	E	840	CLA	C3A-C2A-CAA-CBA
13	E	841	CLA	CHA-CBD-CGD-O1D
13	E	843	CLA	C1A-C2A-CAA-CBA
13	E	843	CLA	C3A-C2A-CAA-CBA
13	E	844	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	E	844	CLA	O1D-CGD-O2D-CED
13	E	845	CLA	C1A-C2A-CAA-CBA
13	E	845	CLA	C3A-C2A-CAA-CBA
13	G	802	CLA	C1A-C2A-CAA-CBA
13	G	802	CLA	C3A-C2A-CAA-CBA
13	G	803	CLA	CHA-CBD-CGD-O1D
13	G	803	CLA	CHA-CBD-CGD-O2D
13	G	803	CLA	CBD-CGD-O2D-CED
13	G	804	CLA	CHA-CBD-CGD-O1D
13	G	804	CLA	CHA-CBD-CGD-O2D
13	G	806	CLA	C3A-C2A-CAA-CBA
13	G	807	CLA	CBD-CGD-O2D-CED
13	G	809	CLA	CBD-CGD-O2D-CED
13	G	812	CLA	CBD-CGD-O2D-CED
13	G	813	CLA	C1A-C2A-CAA-CBA
13	G	813	CLA	C3A-C2A-CAA-CBA
13	G	815	CLA	C2A-CAA-CBA-CGA
13	G	815	CLA	CBD-CGD-O2D-CED
13	G	815	CLA	O1D-CGD-O2D-CED
13	G	816	CLA	C1A-C2A-CAA-CBA
13	G	816	CLA	C3A-C2A-CAA-CBA
13	G	817	CLA	CBD-CGD-O2D-CED
13	G	817	CLA	O1D-CGD-O2D-CED
13	G	818	CLA	C1A-C2A-CAA-CBA
13	G	818	CLA	C3A-C2A-CAA-CBA
13	G	819	CLA	C1A-C2A-CAA-CBA
13	G	819	CLA	C3A-C2A-CAA-CBA
13	G	821	CLA	CHA-CBD-CGD-O1D
13	G	821	CLA	CHA-CBD-CGD-O2D
13	G	821	CLA	CAD-CBD-CGD-O1D
13	G	821	CLA	CAD-CBD-CGD-O2D
13	G	821	CLA	CBD-CGD-O2D-CED
13	G	822	CLA	CAD-CBD-CGD-O1D
13	G	822	CLA	CAD-CBD-CGD-O2D
13	G	823	CLA	CHA-CBD-CGD-O1D
13	G	823	CLA	CHA-CBD-CGD-O2D
13	G	823	CLA	CBD-CGD-O2D-CED
13	G	826	CLA	C1A-C2A-CAA-CBA
13	G	826	CLA	CBD-CGD-O2D-CED
13	G	828	CLA	CBA-CGA-O2A-C1
13	G	829	CLA	C3A-C2A-CAA-CBA
13	G	829	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	G	829	CLA	CHA-CBD-CGD-O2D
13	G	830	CLA	CBD-CGD-O2D-CED
13	G	831	CLA	C3A-C2A-CAA-CBA
13	G	832	CLA	C2A-CAA-CBA-CGA
13	G	834	CLA	C1A-C2A-CAA-CBA
13	G	834	CLA	C3A-C2A-CAA-CBA
13	G	834	CLA	CBD-CGD-O2D-CED
13	G	836	CLA	C1A-C2A-CAA-CBA
13	G	836	CLA	C3A-C2A-CAA-CBA
13	G	836	CLA	CAD-CBD-CGD-O1D
13	G	836	CLA	CAD-CBD-CGD-O2D
13	G	837	CLA	CHA-CBD-CGD-O1D
13	G	837	CLA	CHA-CBD-CGD-O2D
13	G	837	CLA	CAD-CBD-CGD-O1D
13	G	837	CLA	CBD-CGD-O2D-CED
13	G	839	CLA	C1A-C2A-CAA-CBA
13	G	839	CLA	C3A-C2A-CAA-CBA
13	G	840	CLA	CHA-CBD-CGD-O1D
13	G	840	CLA	CHA-CBD-CGD-O2D
13	G	840	CLA	CBD-CGD-O2D-CED
13	G	840	CLA	O1D-CGD-O2D-CED
13	O	203	CLA	CAD-CBD-CGD-O1D
13	O	203	CLA	CAD-CBD-CGD-O2D
13	S	204	CLA	C3A-C2A-CAA-CBA
13	S	206	CLA	CBD-CGD-O2D-CED
13	e	803	CLA	CBD-CGD-O2D-CED
13	e	804	CLA	CHA-CBD-CGD-O1D
13	e	804	CLA	CHA-CBD-CGD-O2D
13	e	804	CLA	CAD-CBD-CGD-O1D
13	e	806	CLA	C1A-C2A-CAA-CBA
13	e	806	CLA	C3A-C2A-CAA-CBA
13	e	806	CLA	CBD-CGD-O2D-CED
13	e	806	CLA	O1D-CGD-O2D-CED
13	e	807	CLA	CAD-CBD-CGD-O1D
13	e	807	CLA	CAD-CBD-CGD-O2D
13	e	808	CLA	C3A-C2A-CAA-CBA
13	e	810	CLA	C3A-C2A-CAA-CBA
13	e	811	CLA	CBD-CGD-O2D-CED
13	e	812	CLA	CHA-CBD-CGD-O1D
13	e	812	CLA	CHA-CBD-CGD-O2D
13	e	814	CLA	CHA-CBD-CGD-O1D
13	e	814	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	e	814	CLA	CBD-CGD-O2D-CED
13	e	816	CLA	C1A-C2A-CAA-CBA
13	e	816	CLA	C3A-C2A-CAA-CBA
13	e	817	CLA	CBD-CGD-O2D-CED
13	e	818	CLA	C1A-C2A-CAA-CBA
13	e	818	CLA	C3A-C2A-CAA-CBA
13	e	819	CLA	CBD-CGD-O2D-CED
13	e	820	CLA	C1A-C2A-CAA-CBA
13	e	820	CLA	C3A-C2A-CAA-CBA
13	e	821	CLA	C1A-C2A-CAA-CBA
13	e	821	CLA	C3A-C2A-CAA-CBA
13	e	822	CLA	C3A-C2A-CAA-CBA
13	e	822	CLA	CHA-CBD-CGD-O1D
13	e	822	CLA	CHA-CBD-CGD-O2D
13	e	822	CLA	CAD-CBD-CGD-O1D
13	e	823	CLA	CBD-CGD-O2D-CED
13	e	825	CLA	CHA-CBD-CGD-O1D
13	e	825	CLA	CHA-CBD-CGD-O2D
13	e	825	CLA	CAD-CBD-CGD-O1D
13	e	825	CLA	CAD-CBD-CGD-O2D
13	e	825	CLA	CBD-CGD-O2D-CED
13	e	827	CLA	C1A-C2A-CAA-CBA
13	e	827	CLA	C3A-C2A-CAA-CBA
13	e	828	CLA	CBD-CGD-O2D-CED
13	e	829	CLA	CBA-CGA-O2A-C1
13	e	830	CLA	CBA-CGA-O2A-C1
13	e	830	CLA	O1A-CGA-O2A-C1
13	e	830	CLA	CHA-CBD-CGD-O1D
13	e	830	CLA	CHA-CBD-CGD-O2D
13	e	831	CLA	CBD-CGD-O2D-CED
13	e	834	CLA	C1A-C2A-CAA-CBA
13	e	834	CLA	CBD-CGD-O2D-CED
13	e	835	CLA	C1A-C2A-CAA-CBA
13	e	835	CLA	C3A-C2A-CAA-CBA
13	e	836	CLA	C1A-C2A-CAA-CBA
13	e	837	CLA	CHA-CBD-CGD-O2D
13	e	838	CLA	C3A-C2A-CAA-CBA
13	e	839	CLA	CHA-CBD-CGD-O1D
13	e	841	CLA	C1A-C2A-CAA-CBA
13	e	841	CLA	C3A-C2A-CAA-CBA
13	e	842	CLA	CBD-CGD-O2D-CED
13	e	842	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	e	843	CLA	C1A-C2A-CAA-CBA
13	e	843	CLA	C3A-C2A-CAA-CBA
13	e	844	CLA	C1A-C2A-CAA-CBA
13	e	844	CLA	C3A-C2A-CAA-CBA
13	e	844	CLA	CHA-CBD-CGD-O1D
13	e	844	CLA	CHA-CBD-CGD-O2D
13	e	844	CLA	CAD-CBD-CGD-O1D
13	e	852	CLA	C1A-C2A-CAA-CBA
13	e	852	CLA	C3A-C2A-CAA-CBA
13	g	801	CLA	C1A-C2A-CAA-CBA
13	g	801	CLA	C3A-C2A-CAA-CBA
13	g	801	CLA	CHA-CBD-CGD-O1D
13	g	801	CLA	CHA-CBD-CGD-O2D
13	g	802	CLA	C1A-C2A-CAA-CBA
13	g	802	CLA	C3A-C2A-CAA-CBA
13	g	802	CLA	CHA-CBD-CGD-O1D
13	g	802	CLA	CHA-CBD-CGD-O2D
13	g	805	CLA	CHA-CBD-CGD-O1D
13	g	805	CLA	CHA-CBD-CGD-O2D
13	g	805	CLA	CBD-CGD-O2D-CED
13	g	806	CLA	CHA-CBD-CGD-O1D
13	g	806	CLA	CHA-CBD-CGD-O2D
13	g	808	CLA	C3A-C2A-CAA-CBA
13	g	809	CLA	CBD-CGD-O2D-CED
13	g	811	CLA	CBD-CGD-O2D-CED
13	g	814	CLA	C1A-C2A-CAA-CBA
13	g	814	CLA	C3A-C2A-CAA-CBA
13	g	816	CLA	C2A-CAA-CBA-CGA
13	g	816	CLA	CBD-CGD-O2D-CED
13	g	816	CLA	O1D-CGD-O2D-CED
13	g	817	CLA	C1A-C2A-CAA-CBA
13	g	817	CLA	C3A-C2A-CAA-CBA
13	g	818	CLA	CBD-CGD-O2D-CED
13	g	818	CLA	O1D-CGD-O2D-CED
13	g	819	CLA	C1A-C2A-CAA-CBA
13	g	819	CLA	C3A-C2A-CAA-CBA
13	g	820	CLA	C1A-C2A-CAA-CBA
13	g	820	CLA	C3A-C2A-CAA-CBA
13	g	822	CLA	CHA-CBD-CGD-O1D
13	g	822	CLA	CHA-CBD-CGD-O2D
13	g	822	CLA	CAD-CBD-CGD-O1D
13	g	822	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	g	822	CLA	CBD-CGD-O2D-CED
13	g	823	CLA	CAD-CBD-CGD-O1D
13	g	823	CLA	CAD-CBD-CGD-O2D
13	g	824	CLA	CHA-CBD-CGD-O1D
13	g	824	CLA	CHA-CBD-CGD-O2D
13	g	824	CLA	CBD-CGD-O2D-CED
13	g	827	CLA	C1A-C2A-CAA-CBA
13	g	827	CLA	CBD-CGD-O2D-CED
13	g	829	CLA	CBA-CGA-O2A-C1
13	g	830	CLA	C3A-C2A-CAA-CBA
13	g	830	CLA	CHA-CBD-CGD-O1D
13	g	830	CLA	CHA-CBD-CGD-O2D
13	g	831	CLA	CBD-CGD-O2D-CED
13	g	832	CLA	C3A-C2A-CAA-CBA
13	g	835	CLA	C1A-C2A-CAA-CBA
13	g	835	CLA	C3A-C2A-CAA-CBA
13	g	835	CLA	CBD-CGD-O2D-CED
13	g	837	CLA	C1A-C2A-CAA-CBA
13	g	837	CLA	C3A-C2A-CAA-CBA
13	g	837	CLA	CAD-CBD-CGD-O1D
13	g	837	CLA	CAD-CBD-CGD-O2D
13	g	838	CLA	CHA-CBD-CGD-O1D
13	g	838	CLA	CHA-CBD-CGD-O2D
13	g	838	CLA	CAD-CBD-CGD-O1D
13	g	838	CLA	CBD-CGD-O2D-CED
13	g	840	CLA	C1A-C2A-CAA-CBA
13	g	840	CLA	C3A-C2A-CAA-CBA
13	g	841	CLA	CHA-CBD-CGD-O1D
13	g	841	CLA	CHA-CBD-CGD-O2D
13	g	841	CLA	CBD-CGD-O2D-CED
13	g	841	CLA	O1D-CGD-O2D-CED
13	o	202	CLA	CAD-CBD-CGD-O1D
13	o	202	CLA	CAD-CBD-CGD-O2D
13	o	202	CLA	CBD-CGD-O2D-CED
13	s	203	CLA	C3A-C2A-CAA-CBA
13	a	804	CLA	CHA-CBD-CGD-O1D
13	a	804	CLA	CHA-CBD-CGD-O2D
13	a	804	CLA	CAD-CBD-CGD-O1D
13	a	805	CLA	C1A-C2A-CAA-CBA
13	a	805	CLA	C3A-C2A-CAA-CBA
13	a	805	CLA	CHA-CBD-CGD-O1D
13	a	805	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	a	807	CLA	C1A-C2A-CAA-CBA
13	a	807	CLA	C3A-C2A-CAA-CBA
13	a	807	CLA	CBD-CGD-O2D-CED
13	a	807	CLA	O1D-CGD-O2D-CED
13	a	808	CLA	CAD-CBD-CGD-O1D
13	a	808	CLA	CAD-CBD-CGD-O2D
13	a	809	CLA	C1A-C2A-CAA-CBA
13	a	809	CLA	C3A-C2A-CAA-CBA
13	a	811	CLA	C3A-C2A-CAA-CBA
13	a	812	CLA	CBD-CGD-O2D-CED
13	a	813	CLA	CHA-CBD-CGD-O1D
13	a	813	CLA	CHA-CBD-CGD-O2D
13	a	815	CLA	CHA-CBD-CGD-O1D
13	a	815	CLA	CHA-CBD-CGD-O2D
13	a	815	CLA	CBD-CGD-O2D-CED
13	a	817	CLA	C1A-C2A-CAA-CBA
13	a	817	CLA	C3A-C2A-CAA-CBA
13	a	818	CLA	CBD-CGD-O2D-CED
13	a	819	CLA	C1A-C2A-CAA-CBA
13	a	819	CLA	C3A-C2A-CAA-CBA
13	a	820	CLA	CBD-CGD-O2D-CED
13	a	821	CLA	C1A-C2A-CAA-CBA
13	a	821	CLA	C3A-C2A-CAA-CBA
13	a	822	CLA	C1A-C2A-CAA-CBA
13	a	822	CLA	C3A-C2A-CAA-CBA
13	a	823	CLA	C3A-C2A-CAA-CBA
13	a	823	CLA	CHA-CBD-CGD-O1D
13	a	823	CLA	CHA-CBD-CGD-O2D
13	a	823	CLA	CAD-CBD-CGD-O1D
13	a	824	CLA	CBD-CGD-O2D-CED
13	a	826	CLA	CHA-CBD-CGD-O1D
13	a	826	CLA	CHA-CBD-CGD-O2D
13	a	826	CLA	CAD-CBD-CGD-O1D
13	a	826	CLA	CAD-CBD-CGD-O2D
13	a	826	CLA	CBD-CGD-O2D-CED
13	a	828	CLA	C1A-C2A-CAA-CBA
13	a	828	CLA	C3A-C2A-CAA-CBA
13	a	829	CLA	CBD-CGD-O2D-CED
13	a	830	CLA	CBA-CGA-O2A-C1
13	a	831	CLA	CBA-CGA-O2A-C1
13	a	831	CLA	O1A-CGA-O2A-C1
13	a	831	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	a	831	CLA	CHA-CBD-CGD-O2D
13	a	832	CLA	CBD-CGD-O2D-CED
13	a	835	CLA	C1A-C2A-CAA-CBA
13	a	835	CLA	C3A-C2A-CAA-CBA
13	a	835	CLA	CHA-CBD-CGD-O1D
13	a	835	CLA	CHA-CBD-CGD-O2D
13	a	836	CLA	C1A-C2A-CAA-CBA
13	a	836	CLA	CBD-CGD-O2D-CED
13	a	837	CLA	C1A-C2A-CAA-CBA
13	a	837	CLA	C3A-C2A-CAA-CBA
13	a	838	CLA	C1A-C2A-CAA-CBA
13	a	839	CLA	CHA-CBD-CGD-O2D
13	a	840	CLA	C3A-C2A-CAA-CBA
13	a	841	CLA	CHA-CBD-CGD-O1D
13	a	843	CLA	C1A-C2A-CAA-CBA
13	a	843	CLA	C3A-C2A-CAA-CBA
13	a	844	CLA	CBD-CGD-O2D-CED
13	a	844	CLA	O1D-CGD-O2D-CED
13	a	845	CLA	C1A-C2A-CAA-CBA
13	a	845	CLA	C3A-C2A-CAA-CBA
13	a	852	CLA	CBD-CGD-O2D-CED
13	b	802	CLA	C1A-C2A-CAA-CBA
13	b	802	CLA	C3A-C2A-CAA-CBA
13	b	803	CLA	CHA-CBD-CGD-O1D
13	b	803	CLA	CHA-CBD-CGD-O2D
13	b	803	CLA	CBD-CGD-O2D-CED
13	b	804	CLA	CHA-CBD-CGD-O1D
13	b	804	CLA	CHA-CBD-CGD-O2D
13	b	806	CLA	C3A-C2A-CAA-CBA
13	b	807	CLA	CBD-CGD-O2D-CED
13	b	809	CLA	CBD-CGD-O2D-CED
13	b	811	CLA	CBD-CGD-O2D-CED
13	b	812	CLA	C1A-C2A-CAA-CBA
13	b	812	CLA	C3A-C2A-CAA-CBA
13	b	814	CLA	C2A-CAA-CBA-CGA
13	b	814	CLA	CBD-CGD-O2D-CED
13	b	814	CLA	O1D-CGD-O2D-CED
13	b	815	CLA	C1A-C2A-CAA-CBA
13	b	815	CLA	C3A-C2A-CAA-CBA
13	b	816	CLA	CBD-CGD-O2D-CED
13	b	816	CLA	O1D-CGD-O2D-CED
13	b	817	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	b	817	CLA	C3A-C2A-CAA-CBA
13	b	818	CLA	C1A-C2A-CAA-CBA
13	b	818	CLA	C3A-C2A-CAA-CBA
13	b	820	CLA	CHA-CBD-CGD-O1D
13	b	820	CLA	CHA-CBD-CGD-O2D
13	b	820	CLA	CAD-CBD-CGD-O1D
13	b	820	CLA	CAD-CBD-CGD-O2D
13	b	820	CLA	CBD-CGD-O2D-CED
13	b	821	CLA	CAD-CBD-CGD-O1D
13	b	821	CLA	CAD-CBD-CGD-O2D
13	b	822	CLA	CHA-CBD-CGD-O1D
13	b	822	CLA	CHA-CBD-CGD-O2D
13	b	822	CLA	CBD-CGD-O2D-CED
13	b	825	CLA	C1A-C2A-CAA-CBA
13	b	825	CLA	CBD-CGD-O2D-CED
13	b	827	CLA	CBA-CGA-O2A-C1
13	b	828	CLA	C3A-C2A-CAA-CBA
13	b	828	CLA	CHA-CBD-CGD-O1D
13	b	828	CLA	CHA-CBD-CGD-O2D
13	b	829	CLA	CBD-CGD-O2D-CED
13	b	830	CLA	C3A-C2A-CAA-CBA
13	b	833	CLA	C1A-C2A-CAA-CBA
13	b	833	CLA	C3A-C2A-CAA-CBA
13	b	833	CLA	CBD-CGD-O2D-CED
13	b	835	CLA	C1A-C2A-CAA-CBA
13	b	835	CLA	C3A-C2A-CAA-CBA
13	b	835	CLA	CAD-CBD-CGD-O1D
13	b	835	CLA	CAD-CBD-CGD-O2D
13	b	836	CLA	CHA-CBD-CGD-O1D
13	b	836	CLA	CHA-CBD-CGD-O2D
13	b	836	CLA	CAD-CBD-CGD-O1D
13	b	836	CLA	CBD-CGD-O2D-CED
13	b	838	CLA	C1A-C2A-CAA-CBA
13	b	838	CLA	C3A-C2A-CAA-CBA
13	b	839	CLA	CHA-CBD-CGD-O1D
13	b	839	CLA	CHA-CBD-CGD-O2D
13	b	839	CLA	CBD-CGD-O2D-CED
13	b	839	CLA	O1D-CGD-O2D-CED
13	f	203	CLA	CAD-CBD-CGD-O1D
13	f	203	CLA	CAD-CBD-CGD-O2D
13	l	201	CLA	CBD-CGD-O2D-CED
13	l	203	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	l	203	CLA	C3A-C2A-CAA-CBA
13	l	205	CLA	C3A-C2A-CAA-CBA
13	l	205	CLA	C2-C1-O2A-CGA
14	A	846	PQN	C12-C11-C3-C4
14	A	846	PQN	C12-C13-C15-C16
14	A	846	PQN	C14-C13-C15-C16
14	E	848	PQN	C12-C13-C15-C16
14	E	848	PQN	C14-C13-C15-C16
15	A	847	BCR	C6-C7-C8-C9
15	A	847	BCR	C7-C8-C9-C10
15	A	847	BCR	C7-C8-C9-C34
15	A	847	BCR	C9-C10-C11-C12
15	A	847	BCR	C11-C12-C13-C14
15	A	847	BCR	C11-C12-C13-C35
15	A	847	BCR	C16-C17-C18-C36
15	A	847	BCR	C37-C22-C23-C24
15	A	847	BCR	C22-C23-C24-C25
15	A	849	BCR	C7-C8-C9-C10
15	A	849	BCR	C7-C8-C9-C34
15	A	850	BCR	C7-C8-C9-C10
15	A	850	BCR	C11-C12-C13-C35
15	A	850	BCR	C14-C15-C16-C17
15	A	850	BCR	C15-C16-C17-C18
15	A	850	BCR	C16-C17-C18-C19
15	A	850	BCR	C16-C17-C18-C36
15	A	850	BCR	C20-C21-C22-C23
15	A	850	BCR	C20-C21-C22-C37
15	A	850	BCR	C21-C22-C23-C24
15	A	850	BCR	C37-C22-C23-C24
15	A	851	BCR	C7-C8-C9-C34
15	A	852	BCR	C7-C8-C9-C34
15	A	852	BCR	C11-C10-C9-C8
15	A	852	BCR	C10-C11-C12-C13
15	A	852	BCR	C11-C12-C13-C35
15	A	852	BCR	C21-C22-C23-C24
15	B	843	BCR	C6-C7-C8-C9
15	B	843	BCR	C22-C23-C24-C25
15	B	844	BCR	C7-C8-C9-C10
15	B	844	BCR	C10-C11-C12-C13
15	B	844	BCR	C17-C18-C19-C20
15	B	844	BCR	C36-C18-C19-C20
15	B	844	BCR	C18-C19-C20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	B	844	BCR	C21-C22-C23-C24
15	B	844	BCR	C37-C22-C23-C24
15	B	845	BCR	C1-C6-C7-C8
15	B	845	BCR	C6-C7-C8-C9
15	B	845	BCR	C11-C10-C9-C8
15	B	845	BCR	C11-C10-C9-C34
15	B	845	BCR	C16-C17-C18-C19
15	B	845	BCR	C16-C17-C18-C36
15	B	845	BCR	C22-C23-C24-C25
15	B	846	BCR	C7-C8-C9-C10
15	B	846	BCR	C7-C8-C9-C34
15	B	846	BCR	C9-C10-C11-C12
15	B	846	BCR	C10-C11-C12-C13
15	B	846	BCR	C11-C12-C13-C14
15	B	846	BCR	C16-C17-C18-C36
15	B	846	BCR	C20-C21-C22-C37
15	B	847	BCR	C16-C17-C18-C36
15	B	847	BCR	C37-C22-C23-C24
15	B	847	BCR	C22-C23-C24-C25
15	B	847	BCR	C23-C24-C25-C30
15	B	848	BCR	C1-C6-C7-C8
15	B	848	BCR	C7-C8-C9-C10
15	B	848	BCR	C10-C11-C12-C13
15	B	848	BCR	C21-C22-C23-C24
15	B	848	BCR	C37-C22-C23-C24
15	B	848	BCR	C23-C24-C25-C26
15	F	201	BCR	C7-C8-C9-C10
15	F	201	BCR	C37-C22-C23-C24
15	I	101	BCR	C18-C19-C20-C21
15	J	101	BCR	C7-C8-C9-C10
15	J	101	BCR	C7-C8-C9-C34
15	J	101	BCR	C18-C19-C20-C21
15	J	102	BCR	C1-C6-C7-C8
15	J	102	BCR	C7-C8-C9-C10
15	J	102	BCR	C7-C8-C9-C34
15	J	102	BCR	C22-C23-C24-C25
15	J	102	BCR	C23-C24-C25-C26
15	J	102	BCR	C23-C24-C25-C30
15	L	201	BCR	C7-C8-C9-C10
15	L	201	BCR	C7-C8-C9-C34
15	L	201	BCR	C17-C18-C19-C20
15	L	201	BCR	C18-C19-C20-C21

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	L	201	BCR	C19-C20-C21-C22
15	L	201	BCR	C20-C21-C22-C23
15	L	201	BCR	C20-C21-C22-C37
15	L	201	BCR	C21-C22-C23-C24
15	L	205	BCR	C7-C8-C9-C10
15	L	205	BCR	C11-C10-C9-C8
15	L	205	BCR	C10-C11-C12-C13
15	L	205	BCR	C11-C12-C13-C35
15	L	205	BCR	C18-C19-C20-C21
15	L	205	BCR	C37-C22-C23-C24
15	E	801	BCR	C6-C7-C8-C9
15	E	801	BCR	C16-C17-C18-C19
15	E	802	BCR	C6-C7-C8-C9
15	E	802	BCR	C7-C8-C9-C34
15	E	802	BCR	C11-C10-C9-C34
15	E	802	BCR	C10-C11-C12-C13
15	E	802	BCR	C16-C17-C18-C19
15	E	802	BCR	C16-C17-C18-C36
15	E	802	BCR	C36-C18-C19-C20
15	E	802	BCR	C18-C19-C20-C21
15	E	802	BCR	C20-C21-C22-C23
15	E	802	BCR	C20-C21-C22-C37
15	E	802	BCR	C37-C22-C23-C24
15	E	802	BCR	C22-C23-C24-C25
15	E	802	BCR	C23-C24-C25-C26
15	E	802	BCR	C23-C24-C25-C30
15	E	849	BCR	C6-C7-C8-C9
15	E	849	BCR	C7-C8-C9-C10
15	E	849	BCR	C7-C8-C9-C34
15	E	849	BCR	C9-C10-C11-C12
15	E	849	BCR	C11-C12-C13-C14
15	E	849	BCR	C11-C12-C13-C35
15	E	849	BCR	C16-C17-C18-C36
15	E	849	BCR	C37-C22-C23-C24
15	E	849	BCR	C22-C23-C24-C25
15	E	851	BCR	C7-C8-C9-C10
15	E	851	BCR	C7-C8-C9-C34
15	E	852	BCR	C1-C6-C7-C8
15	E	852	BCR	C7-C8-C9-C10
15	E	852	BCR	C7-C8-C9-C34
15	E	852	BCR	C22-C23-C24-C25
15	E	852	BCR	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	E	852	BCR	C23-C24-C25-C30
15	G	843	BCR	C6-C7-C8-C9
15	G	843	BCR	C22-C23-C24-C25
15	G	844	BCR	C7-C8-C9-C10
15	G	844	BCR	C10-C11-C12-C13
15	G	844	BCR	C17-C18-C19-C20
15	G	844	BCR	C36-C18-C19-C20
15	G	844	BCR	C18-C19-C20-C21
15	G	844	BCR	C21-C22-C23-C24
15	G	844	BCR	C37-C22-C23-C24
15	G	845	BCR	C1-C6-C7-C8
15	G	845	BCR	C6-C7-C8-C9
15	G	845	BCR	C11-C10-C9-C8
15	G	845	BCR	C11-C10-C9-C34
15	G	845	BCR	C16-C17-C18-C19
15	G	845	BCR	C16-C17-C18-C36
15	G	845	BCR	C22-C23-C24-C25
15	G	846	BCR	C7-C8-C9-C10
15	G	846	BCR	C7-C8-C9-C34
15	G	846	BCR	C9-C10-C11-C12
15	G	846	BCR	C10-C11-C12-C13
15	G	846	BCR	C11-C12-C13-C14
15	G	846	BCR	C16-C17-C18-C36
15	G	846	BCR	C20-C21-C22-C37
15	G	847	BCR	C16-C17-C18-C36
15	G	847	BCR	C37-C22-C23-C24
15	G	847	BCR	C22-C23-C24-C25
15	G	847	BCR	C23-C24-C25-C30
15	G	848	BCR	C1-C6-C7-C8
15	G	848	BCR	C7-C8-C9-C10
15	G	848	BCR	C10-C11-C12-C13
15	G	848	BCR	C21-C22-C23-C24
15	G	848	BCR	C37-C22-C23-C24
15	G	848	BCR	C23-C24-C25-C26
15	O	201	BCR	C7-C8-C9-C10
15	O	201	BCR	C37-C22-C23-C24
15	O	202	BCR	C10-C11-C12-C13
15	O	202	BCR	C12-C13-C14-C15
15	O	202	BCR	C14-C15-C16-C17
15	O	202	BCR	C16-C17-C18-C36
15	O	202	BCR	C23-C24-C25-C30
15	P	101	BCR	C18-C19-C20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	Q	101	BCR	C7-C8-C9-C10
15	Q	101	BCR	C7-C8-C9-C34
15	Q	101	BCR	C18-C19-C20-C21
15	R	101	BCR	C6-C7-C8-C9
15	R	101	BCR	C7-C8-C9-C10
15	R	101	BCR	C13-C14-C15-C16
15	R	101	BCR	C14-C15-C16-C17
15	R	101	BCR	C16-C17-C18-C19
15	R	101	BCR	C16-C17-C18-C36
15	S	201	BCR	C7-C8-C9-C10
15	S	201	BCR	C7-C8-C9-C34
15	S	201	BCR	C12-C13-C14-C15
15	S	201	BCR	C35-C13-C14-C15
15	S	201	BCR	C17-C18-C19-C20
15	S	201	BCR	C36-C18-C19-C20
15	S	201	BCR	C18-C19-C20-C21
15	S	201	BCR	C20-C21-C22-C23
15	S	201	BCR	C20-C21-C22-C37
15	S	202	BCR	C6-C7-C8-C9
15	S	202	BCR	C7-C8-C9-C34
15	S	202	BCR	C10-C11-C12-C13
15	S	202	BCR	C11-C12-C13-C14
15	S	202	BCR	C12-C13-C14-C15
15	S	202	BCR	C35-C13-C14-C15
15	S	205	BCR	C10-C11-C12-C13
15	S	205	BCR	C11-C12-C13-C14
15	S	205	BCR	C11-C12-C13-C35
15	S	205	BCR	C20-C21-C22-C23
15	S	205	BCR	C20-C21-C22-C37
15	S	205	BCR	C21-C22-C23-C24
15	S	205	BCR	C37-C22-C23-C24
15	T	101	BCR	C11-C12-C13-C35
15	T	101	BCR	C14-C15-C16-C17
15	T	101	BCR	C20-C21-C22-C37
15	e	846	BCR	C6-C7-C8-C9
15	e	846	BCR	C7-C8-C9-C10
15	e	846	BCR	C7-C8-C9-C34
15	e	846	BCR	C9-C10-C11-C12
15	e	846	BCR	C11-C12-C13-C14
15	e	846	BCR	C11-C12-C13-C35
15	e	846	BCR	C16-C17-C18-C36
15	e	846	BCR	C37-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	e	846	BCR	C22-C23-C24-C25
15	e	848	BCR	C7-C8-C9-C10
15	e	848	BCR	C7-C8-C9-C34
15	e	849	BCR	C7-C8-C9-C10
15	e	849	BCR	C11-C12-C13-C35
15	e	849	BCR	C14-C15-C16-C17
15	e	849	BCR	C15-C16-C17-C18
15	e	849	BCR	C16-C17-C18-C19
15	e	849	BCR	C16-C17-C18-C36
15	e	849	BCR	C20-C21-C22-C23
15	e	849	BCR	C20-C21-C22-C37
15	e	849	BCR	C21-C22-C23-C24
15	e	849	BCR	C37-C22-C23-C24
15	e	850	BCR	C7-C8-C9-C34
15	e	851	BCR	C1-C6-C7-C8
15	e	851	BCR	C11-C12-C13-C35
15	e	851	BCR	C12-C13-C14-C15
15	e	851	BCR	C35-C13-C14-C15
15	e	851	BCR	C14-C15-C16-C17
15	e	851	BCR	C20-C21-C22-C23
15	e	851	BCR	C21-C22-C23-C24
15	e	851	BCR	C22-C23-C24-C25
15	g	844	BCR	C6-C7-C8-C9
15	g	844	BCR	C22-C23-C24-C25
15	g	845	BCR	C7-C8-C9-C10
15	g	845	BCR	C10-C11-C12-C13
15	g	845	BCR	C17-C18-C19-C20
15	g	845	BCR	C36-C18-C19-C20
15	g	845	BCR	C18-C19-C20-C21
15	g	845	BCR	C21-C22-C23-C24
15	g	845	BCR	C37-C22-C23-C24
15	g	846	BCR	C1-C6-C7-C8
15	g	846	BCR	C6-C7-C8-C9
15	g	846	BCR	C11-C10-C9-C8
15	g	846	BCR	C11-C10-C9-C34
15	g	846	BCR	C16-C17-C18-C19
15	g	846	BCR	C16-C17-C18-C36
15	g	846	BCR	C22-C23-C24-C25
15	g	847	BCR	C7-C8-C9-C10
15	g	847	BCR	C7-C8-C9-C34
15	g	847	BCR	C9-C10-C11-C12
15	g	847	BCR	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	g	847	BCR	C11-C12-C13-C14
15	g	847	BCR	C16-C17-C18-C36
15	g	847	BCR	C20-C21-C22-C37
15	g	848	BCR	C16-C17-C18-C36
15	g	848	BCR	C37-C22-C23-C24
15	g	848	BCR	C22-C23-C24-C25
15	g	848	BCR	C23-C24-C25-C30
15	g	849	BCR	C1-C6-C7-C8
15	g	849	BCR	C7-C8-C9-C10
15	g	849	BCR	C10-C11-C12-C13
15	g	849	BCR	C21-C22-C23-C24
15	g	849	BCR	C37-C22-C23-C24
15	g	849	BCR	C23-C24-C25-C26
15	o	201	BCR	C7-C8-C9-C10
15	o	201	BCR	C37-C22-C23-C24
15	p	101	BCR	C18-C19-C20-C21
15	q	101	BCR	C7-C8-C9-C10
15	q	101	BCR	C7-C8-C9-C34
15	q	101	BCR	C18-C19-C20-C21
15	q	102	BCR	C1-C6-C7-C8
15	q	102	BCR	C7-C8-C9-C10
15	q	102	BCR	C7-C8-C9-C34
15	q	102	BCR	C22-C23-C24-C25
15	q	102	BCR	C23-C24-C25-C26
15	q	102	BCR	C23-C24-C25-C30
15	s	201	BCR	C7-C8-C9-C34
15	s	201	BCR	C11-C12-C13-C35
15	s	201	BCR	C17-C18-C19-C20
15	s	201	BCR	C36-C18-C19-C20
15	s	201	BCR	C18-C19-C20-C21
15	s	201	BCR	C19-C20-C21-C22
15	s	201	BCR	C20-C21-C22-C23
15	s	201	BCR	C20-C21-C22-C37
15	s	201	BCR	C21-C22-C23-C24
15	s	204	BCR	C6-C7-C8-C9
15	s	204	BCR	C11-C10-C9-C8
15	s	204	BCR	C10-C11-C12-C13
15	s	204	BCR	C11-C12-C13-C35
15	s	204	BCR	C18-C19-C20-C21
15	s	204	BCR	C21-C22-C23-C24
15	s	204	BCR	C37-C22-C23-C24
15	s	204	BCR	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	s	204	BCR	C23-C24-C25-C30
15	a	802	BCR	C6-C7-C8-C9
15	a	803	BCR	C1-C6-C7-C8
15	a	803	BCR	C6-C7-C8-C9
15	a	803	BCR	C7-C8-C9-C10
15	a	803	BCR	C7-C8-C9-C34
15	a	803	BCR	C11-C10-C9-C8
15	a	803	BCR	C10-C11-C12-C13
15	a	803	BCR	C11-C12-C13-C14
15	a	803	BCR	C12-C13-C14-C15
15	a	803	BCR	C14-C15-C16-C17
15	a	803	BCR	C18-C19-C20-C21
15	a	803	BCR	C20-C21-C22-C37
15	a	803	BCR	C22-C23-C24-C25
15	a	803	BCR	C23-C24-C25-C26
15	a	803	BCR	C23-C24-C25-C30
15	a	848	BCR	C5-C6-C7-C8
15	a	848	BCR	C11-C12-C13-C14
15	a	848	BCR	C16-C17-C18-C19
15	a	848	BCR	C16-C17-C18-C36
15	a	848	BCR	C20-C21-C22-C23
15	a	848	BCR	C20-C21-C22-C37
15	a	848	BCR	C22-C23-C24-C25
15	a	849	BCR	C6-C7-C8-C9
15	a	849	BCR	C7-C8-C9-C10
15	a	849	BCR	C7-C8-C9-C34
15	a	849	BCR	C9-C10-C11-C12
15	a	849	BCR	C11-C12-C13-C14
15	a	849	BCR	C11-C12-C13-C35
15	a	849	BCR	C16-C17-C18-C36
15	a	849	BCR	C37-C22-C23-C24
15	a	849	BCR	C22-C23-C24-C25
15	a	851	BCR	C7-C8-C9-C10
15	a	851	BCR	C7-C8-C9-C34
15	a	853	BCR	C1-C6-C7-C8
15	a	853	BCR	C7-C8-C9-C10
15	a	853	BCR	C7-C8-C9-C34
15	a	853	BCR	C22-C23-C24-C25
15	a	853	BCR	C23-C24-C25-C26
15	a	853	BCR	C23-C24-C25-C30
15	b	842	BCR	C6-C7-C8-C9
15	b	842	BCR	C22-C23-C24-C25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	b	843	BCR	C7-C8-C9-C10
15	b	843	BCR	C10-C11-C12-C13
15	b	843	BCR	C17-C18-C19-C20
15	b	843	BCR	C36-C18-C19-C20
15	b	843	BCR	C18-C19-C20-C21
15	b	843	BCR	C21-C22-C23-C24
15	b	843	BCR	C37-C22-C23-C24
15	b	844	BCR	C1-C6-C7-C8
15	b	844	BCR	C6-C7-C8-C9
15	b	844	BCR	C11-C10-C9-C8
15	b	844	BCR	C11-C10-C9-C34
15	b	844	BCR	C16-C17-C18-C19
15	b	844	BCR	C16-C17-C18-C36
15	b	844	BCR	C22-C23-C24-C25
15	b	845	BCR	C7-C8-C9-C10
15	b	845	BCR	C7-C8-C9-C34
15	b	845	BCR	C9-C10-C11-C12
15	b	845	BCR	C10-C11-C12-C13
15	b	845	BCR	C11-C12-C13-C14
15	b	845	BCR	C16-C17-C18-C36
15	b	845	BCR	C20-C21-C22-C37
15	b	846	BCR	C16-C17-C18-C36
15	b	846	BCR	C37-C22-C23-C24
15	b	846	BCR	C22-C23-C24-C25
15	b	846	BCR	C23-C24-C25-C30
15	b	847	BCR	C1-C6-C7-C8
15	b	847	BCR	C7-C8-C9-C10
15	b	847	BCR	C10-C11-C12-C13
15	b	847	BCR	C21-C22-C23-C24
15	b	847	BCR	C37-C22-C23-C24
15	b	847	BCR	C23-C24-C25-C26
15	f	201	BCR	C7-C8-C9-C10
15	f	201	BCR	C37-C22-C23-C24
15	f	202	BCR	C10-C11-C12-C13
15	f	202	BCR	C14-C15-C16-C17
15	f	202	BCR	C16-C17-C18-C36
15	f	202	BCR	C23-C24-C25-C30
15	i	101	BCR	C18-C19-C20-C21
15	j	101	BCR	C7-C8-C9-C10
15	j	101	BCR	C7-C8-C9-C34
15	j	101	BCR	C18-C19-C20-C21
15	k	4001	BCR	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	k	4001	BCR	C7-C8-C9-C10
15	k	4001	BCR	C11-C12-C13-C14
15	k	4001	BCR	C15-C16-C17-C18
15	k	4001	BCR	C16-C17-C18-C19
15	k	4001	BCR	C16-C17-C18-C36
15	k	4001	BCR	C18-C19-C20-C21
15	k	4001	BCR	C20-C21-C22-C23
15	k	4001	BCR	C20-C21-C22-C37
15	k	4001	BCR	C22-C23-C24-C25
15	k	4001	BCR	C23-C24-C25-C30
15	l	202	BCR	C7-C8-C9-C10
15	l	202	BCR	C12-C13-C14-C15
15	l	202	BCR	C35-C13-C14-C15
15	l	202	BCR	C18-C19-C20-C21
15	l	202	BCR	C20-C21-C22-C23
15	l	202	BCR	C20-C21-C22-C37
15	l	202	BCR	C21-C22-C23-C24
15	l	202	BCR	C23-C24-C25-C30
15	l	206	BCR	C10-C11-C12-C13
15	l	206	BCR	C11-C12-C13-C14
15	l	206	BCR	C11-C12-C13-C35
15	l	206	BCR	C18-C19-C20-C21
15	l	206	BCR	C20-C21-C22-C23
15	l	206	BCR	C20-C21-C22-C37
15	l	206	BCR	C21-C22-C23-C24
15	l	206	BCR	C37-C22-C23-C24
15	l	206	BCR	C22-C23-C24-C25
15	l	206	BCR	C23-C24-C25-C30
15	m	101	BCR	C19-C20-C21-C22
15	m	101	BCR	C20-C21-C22-C23
15	m	101	BCR	C20-C21-C22-C37
15	m	101	BCR	C37-C22-C23-C24
15	m	101	BCR	C22-C23-C24-C25
15	m	101	BCR	C23-C24-C25-C26
15	m	101	BCR	C23-C24-C25-C30
13	A	810	CLA	O1D-CGD-O2D-CED
13	A	812	CLA	O1D-CGD-O2D-CED
13	A	825	CLA	O1D-CGD-O2D-CED
13	A	832	CLA	O1D-CGD-O2D-CED
13	A	834	CLA	O1D-CGD-O2D-CED
13	A	836	CLA	O1D-CGD-O2D-CED
13	B	804	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	B	808	CLA	O1D-CGD-O2D-CED
13	B	816	CLA	O1D-CGD-O2D-CED
13	B	821	CLA	O1D-CGD-O2D-CED
13	B	830	CLA	O1D-CGD-O2D-CED
13	L	204	CLA	O1D-CGD-O2D-CED
13	E	810	CLA	O1D-CGD-O2D-CED
13	E	812	CLA	O1D-CGD-O2D-CED
13	E	825	CLA	O1D-CGD-O2D-CED
13	E	832	CLA	O1D-CGD-O2D-CED
13	E	834	CLA	O1D-CGD-O2D-CED
13	E	837	CLA	O1D-CGD-O2D-CED
13	G	803	CLA	O1D-CGD-O2D-CED
13	G	807	CLA	O1D-CGD-O2D-CED
13	G	812	CLA	O1D-CGD-O2D-CED
13	G	816	CLA	O1D-CGD-O2D-CED
13	G	821	CLA	O1D-CGD-O2D-CED
13	G	830	CLA	O1D-CGD-O2D-CED
13	S	204	CLA	O1D-CGD-O2D-CED
13	S	206	CLA	O1D-CGD-O2D-CED
13	e	809	CLA	O1D-CGD-O2D-CED
13	e	811	CLA	O1D-CGD-O2D-CED
13	e	824	CLA	O1D-CGD-O2D-CED
13	e	831	CLA	O1D-CGD-O2D-CED
13	e	833	CLA	O1D-CGD-O2D-CED
13	e	835	CLA	O1D-CGD-O2D-CED
13	g	805	CLA	O1D-CGD-O2D-CED
13	g	809	CLA	O1D-CGD-O2D-CED
13	g	817	CLA	O1D-CGD-O2D-CED
13	g	822	CLA	O1D-CGD-O2D-CED
13	g	831	CLA	O1D-CGD-O2D-CED
13	s	203	CLA	O1D-CGD-O2D-CED
13	a	810	CLA	O1D-CGD-O2D-CED
13	a	812	CLA	O1D-CGD-O2D-CED
13	a	825	CLA	O1D-CGD-O2D-CED
13	a	832	CLA	O1D-CGD-O2D-CED
13	a	834	CLA	O1D-CGD-O2D-CED
13	a	837	CLA	O1D-CGD-O2D-CED
13	b	803	CLA	O1D-CGD-O2D-CED
13	b	807	CLA	O1D-CGD-O2D-CED
13	b	811	CLA	O1D-CGD-O2D-CED
13	b	815	CLA	O1D-CGD-O2D-CED
13	b	820	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	b	829	CLA	O1D-CGD-O2D-CED
13	l	201	CLA	O1D-CGD-O2D-CED
13	l	205	CLA	O1D-CGD-O2D-CED
13	A	815	CLA	O1D-CGD-O2D-CED
13	A	816	CLA	O1D-CGD-O2D-CED
13	A	824	CLA	O1D-CGD-O2D-CED
13	A	829	CLA	O1D-CGD-O2D-CED
13	A	835	CLA	O1D-CGD-O2D-CED
13	B	833	CLA	O1D-CGD-O2D-CED
13	E	803	CLA	O1D-CGD-O2D-CED
13	E	815	CLA	O1D-CGD-O2D-CED
13	E	816	CLA	O1D-CGD-O2D-CED
13	E	824	CLA	O1D-CGD-O2D-CED
13	E	829	CLA	O1D-CGD-O2D-CED
13	E	836	CLA	O1D-CGD-O2D-CED
13	G	833	CLA	O1D-CGD-O2D-CED
13	e	814	CLA	O1D-CGD-O2D-CED
13	e	815	CLA	O1D-CGD-O2D-CED
13	e	823	CLA	O1D-CGD-O2D-CED
13	e	828	CLA	O1D-CGD-O2D-CED
13	e	834	CLA	O1D-CGD-O2D-CED
13	g	834	CLA	O1D-CGD-O2D-CED
13	a	815	CLA	O1D-CGD-O2D-CED
13	a	816	CLA	O1D-CGD-O2D-CED
13	a	824	CLA	O1D-CGD-O2D-CED
13	a	829	CLA	O1D-CGD-O2D-CED
13	a	836	CLA	O1D-CGD-O2D-CED
13	a	852	CLA	O1D-CGD-O2D-CED
13	b	832	CLA	O1D-CGD-O2D-CED
13	A	810	CLA	CBD-CGD-O2D-CED
13	A	816	CLA	CBD-CGD-O2D-CED
13	A	822	CLA	CBD-CGD-O2D-CED
13	A	825	CLA	CBD-CGD-O2D-CED
13	A	834	CLA	CBD-CGD-O2D-CED
13	A	836	CLA	CBD-CGD-O2D-CED
13	A	837	CLA	CBD-CGD-O2D-CED
13	B	802	CLA	CBD-CGD-O2D-CED
13	B	809	CLA	CBD-CGD-O2D-CED
13	B	816	CLA	CBD-CGD-O2D-CED
13	B	820	CLA	CBD-CGD-O2D-CED
13	B	822	CLA	CBD-CGD-O2D-CED
13	B	824	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	B	827	CLA	CBD-CGD-O2D-CED
13	B	828	CLA	CBD-CGD-O2D-CED
13	B	833	CLA	CBD-CGD-O2D-CED
13	B	841	CLA	CBD-CGD-O2D-CED
13	F	202	CLA	CBD-CGD-O2D-CED
13	L	202	CLA	CBD-CGD-O2D-CED
13	L	204	CLA	CBD-CGD-O2D-CED
13	E	810	CLA	CBD-CGD-O2D-CED
13	E	816	CLA	CBD-CGD-O2D-CED
13	E	822	CLA	CBD-CGD-O2D-CED
13	E	825	CLA	CBD-CGD-O2D-CED
13	E	834	CLA	CBD-CGD-O2D-CED
13	E	837	CLA	CBD-CGD-O2D-CED
13	E	838	CLA	CBD-CGD-O2D-CED
13	G	808	CLA	CBD-CGD-O2D-CED
13	G	816	CLA	CBD-CGD-O2D-CED
13	G	820	CLA	CBD-CGD-O2D-CED
13	G	822	CLA	CBD-CGD-O2D-CED
13	G	824	CLA	CBD-CGD-O2D-CED
13	G	827	CLA	CBD-CGD-O2D-CED
13	G	828	CLA	CBD-CGD-O2D-CED
13	G	833	CLA	CBD-CGD-O2D-CED
13	G	841	CLA	CBD-CGD-O2D-CED
13	O	203	CLA	CBD-CGD-O2D-CED
13	S	204	CLA	CBD-CGD-O2D-CED
13	e	809	CLA	CBD-CGD-O2D-CED
13	e	815	CLA	CBD-CGD-O2D-CED
13	e	821	CLA	CBD-CGD-O2D-CED
13	e	824	CLA	CBD-CGD-O2D-CED
13	e	833	CLA	CBD-CGD-O2D-CED
13	e	835	CLA	CBD-CGD-O2D-CED
13	e	836	CLA	CBD-CGD-O2D-CED
13	g	803	CLA	CBD-CGD-O2D-CED
13	g	810	CLA	CBD-CGD-O2D-CED
13	g	817	CLA	CBD-CGD-O2D-CED
13	g	821	CLA	CBD-CGD-O2D-CED
13	g	823	CLA	CBD-CGD-O2D-CED
13	g	825	CLA	CBD-CGD-O2D-CED
13	g	828	CLA	CBD-CGD-O2D-CED
13	g	829	CLA	CBD-CGD-O2D-CED
13	g	834	CLA	CBD-CGD-O2D-CED
13	g	842	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	s	203	CLA	CBD-CGD-O2D-CED
13	a	810	CLA	CBD-CGD-O2D-CED
13	a	816	CLA	CBD-CGD-O2D-CED
13	a	822	CLA	CBD-CGD-O2D-CED
13	a	825	CLA	CBD-CGD-O2D-CED
13	a	834	CLA	CBD-CGD-O2D-CED
13	a	837	CLA	CBD-CGD-O2D-CED
13	a	838	CLA	CBD-CGD-O2D-CED
13	b	808	CLA	CBD-CGD-O2D-CED
13	b	815	CLA	CBD-CGD-O2D-CED
13	b	819	CLA	CBD-CGD-O2D-CED
13	b	821	CLA	CBD-CGD-O2D-CED
13	b	823	CLA	CBD-CGD-O2D-CED
13	b	826	CLA	CBD-CGD-O2D-CED
13	b	827	CLA	CBD-CGD-O2D-CED
13	b	832	CLA	CBD-CGD-O2D-CED
13	b	840	CLA	CBD-CGD-O2D-CED
13	f	203	CLA	CBD-CGD-O2D-CED
13	l	203	CLA	CBD-CGD-O2D-CED
13	l	205	CLA	CBD-CGD-O2D-CED
13	A	824	CLA	O1A-CGA-O2A-C1
13	A	830	CLA	O1A-CGA-O2A-C1
13	A	835	CLA	O1A-CGA-O2A-C1
13	B	828	CLA	O1A-CGA-O2A-C1
13	E	824	CLA	O1A-CGA-O2A-C1
13	E	830	CLA	O1A-CGA-O2A-C1
13	E	836	CLA	O1A-CGA-O2A-C1
13	G	828	CLA	O1A-CGA-O2A-C1
13	e	823	CLA	O1A-CGA-O2A-C1
13	e	829	CLA	O1A-CGA-O2A-C1
13	e	834	CLA	O1A-CGA-O2A-C1
13	g	829	CLA	O1A-CGA-O2A-C1
13	a	824	CLA	O1A-CGA-O2A-C1
13	a	830	CLA	O1A-CGA-O2A-C1
13	a	836	CLA	O1A-CGA-O2A-C1
13	b	827	CLA	O1A-CGA-O2A-C1
13	A	803	CLA	O1D-CGD-O2D-CED
13	B	809	CLA	O1D-CGD-O2D-CED
13	B	826	CLA	O1D-CGD-O2D-CED
13	B	827	CLA	O1D-CGD-O2D-CED
13	B	834	CLA	O1D-CGD-O2D-CED
13	G	808	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	G	826	CLA	O1D-CGD-O2D-CED
13	G	827	CLA	O1D-CGD-O2D-CED
13	G	834	CLA	O1D-CGD-O2D-CED
13	g	810	CLA	O1D-CGD-O2D-CED
13	g	827	CLA	O1D-CGD-O2D-CED
13	g	828	CLA	O1D-CGD-O2D-CED
13	g	835	CLA	O1D-CGD-O2D-CED
13	b	808	CLA	O1D-CGD-O2D-CED
13	b	825	CLA	O1D-CGD-O2D-CED
13	b	826	CLA	O1D-CGD-O2D-CED
13	b	833	CLA	O1D-CGD-O2D-CED
13	f	203	CLA	O1D-CGD-O2D-CED
13	A	818	CLA	O1D-CGD-O2D-CED
13	A	822	CLA	O1D-CGD-O2D-CED
13	A	826	CLA	O1D-CGD-O2D-CED
13	A	837	CLA	O1D-CGD-O2D-CED
13	B	820	CLA	O1D-CGD-O2D-CED
13	B	823	CLA	O1D-CGD-O2D-CED
13	E	818	CLA	O1D-CGD-O2D-CED
13	E	822	CLA	O1D-CGD-O2D-CED
13	E	826	CLA	O1D-CGD-O2D-CED
13	E	838	CLA	O1D-CGD-O2D-CED
13	G	820	CLA	O1D-CGD-O2D-CED
13	G	823	CLA	O1D-CGD-O2D-CED
13	O	203	CLA	O1D-CGD-O2D-CED
13	e	803	CLA	O1D-CGD-O2D-CED
13	e	817	CLA	O1D-CGD-O2D-CED
13	e	821	CLA	O1D-CGD-O2D-CED
13	e	825	CLA	O1D-CGD-O2D-CED
13	e	836	CLA	O1D-CGD-O2D-CED
13	g	811	CLA	O1D-CGD-O2D-CED
13	g	821	CLA	O1D-CGD-O2D-CED
13	g	824	CLA	O1D-CGD-O2D-CED
13	a	818	CLA	O1D-CGD-O2D-CED
13	a	822	CLA	O1D-CGD-O2D-CED
13	a	826	CLA	O1D-CGD-O2D-CED
13	a	838	CLA	O1D-CGD-O2D-CED
13	b	819	CLA	O1D-CGD-O2D-CED
13	b	822	CLA	O1D-CGD-O2D-CED
13	b	836	CLA	O1D-CGD-O2D-CED
12	A	801	LHG	C24-C23-O8-C6
12	e	801	LHG	C24-C23-O8-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	835	CLA	CBA-CGA-O2A-C1
13	E	836	CLA	CBA-CGA-O2A-C1
13	G	801	CLA	CBA-CGA-O2A-C1
13	e	834	CLA	CBA-CGA-O2A-C1
13	a	836	CLA	CBA-CGA-O2A-C1
13	B	814	CLA	CBD-CGD-O2D-CED
13	B	838	CLA	CBD-CGD-O2D-CED
13	G	801	CLA	CBD-CGD-O2D-CED
13	G	814	CLA	CBD-CGD-O2D-CED
13	G	838	CLA	CBD-CGD-O2D-CED
13	e	844	CLA	CBD-CGD-O2D-CED
13	g	815	CLA	CBD-CGD-O2D-CED
13	g	839	CLA	CBD-CGD-O2D-CED
13	b	813	CLA	CBD-CGD-O2D-CED
13	b	837	CLA	CBD-CGD-O2D-CED
12	A	801	LHG	O10-C23-O8-C6
12	e	801	LHG	O10-C23-O8-C6
12	a	801	LHG	O10-C23-O8-C6
13	A	812	CLA	O1A-CGA-O2A-C1
13	A	821	CLA	O1A-CGA-O2A-C1
13	A	825	CLA	O1A-CGA-O2A-C1
13	A	827	CLA	O1A-CGA-O2A-C1
13	A	837	CLA	O1A-CGA-O2A-C1
13	B	802	CLA	O1A-CGA-O2A-C1
13	B	807	CLA	O1A-CGA-O2A-C1
13	B	812	CLA	O1A-CGA-O2A-C1
13	B	817	CLA	O1A-CGA-O2A-C1
13	B	821	CLA	O1A-CGA-O2A-C1
13	B	840	CLA	O1A-CGA-O2A-C1
13	L	204	CLA	O1A-CGA-O2A-C1
13	E	812	CLA	O1A-CGA-O2A-C1
13	E	821	CLA	O1A-CGA-O2A-C1
13	E	825	CLA	O1A-CGA-O2A-C1
13	E	827	CLA	O1A-CGA-O2A-C1
13	E	838	CLA	O1A-CGA-O2A-C1
13	G	801	CLA	O1A-CGA-O2A-C1
13	G	806	CLA	O1A-CGA-O2A-C1
13	G	811	CLA	O1A-CGA-O2A-C1
13	G	817	CLA	O1A-CGA-O2A-C1
13	G	821	CLA	O1A-CGA-O2A-C1
13	G	840	CLA	O1A-CGA-O2A-C1
13	e	811	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	e	820	CLA	O1A-CGA-O2A-C1
13	e	824	CLA	O1A-CGA-O2A-C1
13	e	826	CLA	O1A-CGA-O2A-C1
13	e	836	CLA	O1A-CGA-O2A-C1
13	g	803	CLA	O1A-CGA-O2A-C1
13	g	808	CLA	O1A-CGA-O2A-C1
13	g	813	CLA	O1A-CGA-O2A-C1
13	g	818	CLA	O1A-CGA-O2A-C1
13	g	822	CLA	O1A-CGA-O2A-C1
13	g	841	CLA	O1A-CGA-O2A-C1
13	s	203	CLA	O1A-CGA-O2A-C1
13	s	205	CLA	O1A-CGA-O2A-C1
13	a	812	CLA	O1A-CGA-O2A-C1
13	a	821	CLA	O1A-CGA-O2A-C1
13	a	825	CLA	O1A-CGA-O2A-C1
13	a	827	CLA	O1A-CGA-O2A-C1
13	a	838	CLA	O1A-CGA-O2A-C1
13	a	852	CLA	O1A-CGA-O2A-C1
13	b	806	CLA	O1A-CGA-O2A-C1
13	b	816	CLA	O1A-CGA-O2A-C1
13	b	820	CLA	O1A-CGA-O2A-C1
13	b	839	CLA	O1A-CGA-O2A-C1
13	l	205	CLA	O1A-CGA-O2A-C1
13	A	820	CLA	O1D-CGD-O2D-CED
13	B	810	CLA	O1D-CGD-O2D-CED
13	B	837	CLA	O1D-CGD-O2D-CED
13	E	820	CLA	O1D-CGD-O2D-CED
13	G	809	CLA	O1D-CGD-O2D-CED
13	G	837	CLA	O1D-CGD-O2D-CED
13	e	819	CLA	O1D-CGD-O2D-CED
13	g	838	CLA	O1D-CGD-O2D-CED
13	a	820	CLA	O1D-CGD-O2D-CED
13	b	809	CLA	O1D-CGD-O2D-CED
13	o	202	CLA	O1D-CGD-O2D-CED
13	g	803	CLA	O1D-CGD-O2D-CED
14	B	842	PQN	C13-C15-C16-C17
14	G	842	PQN	C13-C15-C16-C17
14	g	843	PQN	C13-C15-C16-C17
14	b	841	PQN	C13-C15-C16-C17
12	a	801	LHG	C24-C23-O8-C6
13	A	812	CLA	CBA-CGA-O2A-C1
13	A	821	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	824	CLA	CBA-CGA-O2A-C1
13	A	825	CLA	CBA-CGA-O2A-C1
13	A	827	CLA	CBA-CGA-O2A-C1
13	B	802	CLA	CBA-CGA-O2A-C1
13	B	812	CLA	CBA-CGA-O2A-C1
13	B	817	CLA	CBA-CGA-O2A-C1
13	B	821	CLA	CBA-CGA-O2A-C1
13	B	840	CLA	CBA-CGA-O2A-C1
13	L	204	CLA	CBA-CGA-O2A-C1
13	E	812	CLA	CBA-CGA-O2A-C1
13	E	821	CLA	CBA-CGA-O2A-C1
13	E	824	CLA	CBA-CGA-O2A-C1
13	E	825	CLA	CBA-CGA-O2A-C1
13	E	827	CLA	CBA-CGA-O2A-C1
13	G	811	CLA	CBA-CGA-O2A-C1
13	G	821	CLA	CBA-CGA-O2A-C1
13	G	840	CLA	CBA-CGA-O2A-C1
13	e	811	CLA	CBA-CGA-O2A-C1
13	e	820	CLA	CBA-CGA-O2A-C1
13	e	823	CLA	CBA-CGA-O2A-C1
13	e	824	CLA	CBA-CGA-O2A-C1
13	e	826	CLA	CBA-CGA-O2A-C1
13	g	803	CLA	CBA-CGA-O2A-C1
13	g	813	CLA	CBA-CGA-O2A-C1
13	g	818	CLA	CBA-CGA-O2A-C1
13	g	822	CLA	CBA-CGA-O2A-C1
13	g	841	CLA	CBA-CGA-O2A-C1
13	s	203	CLA	CBA-CGA-O2A-C1
13	s	205	CLA	CBA-CGA-O2A-C1
13	a	812	CLA	CBA-CGA-O2A-C1
13	a	821	CLA	CBA-CGA-O2A-C1
13	a	824	CLA	CBA-CGA-O2A-C1
13	a	825	CLA	CBA-CGA-O2A-C1
13	a	827	CLA	CBA-CGA-O2A-C1
13	b	820	CLA	CBA-CGA-O2A-C1
13	b	839	CLA	CBA-CGA-O2A-C1
13	l	205	CLA	CBA-CGA-O2A-C1
13	B	802	CLA	O1D-CGD-O2D-CED
13	l	203	CLA	O1D-CGD-O2D-CED
13	A	833	CLA	CBD-CGD-O2D-CED
13	E	833	CLA	CBD-CGD-O2D-CED
13	e	832	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	a	833	CLA	CBD-CGD-O2D-CED
13	A	853	CLA	CBD-CGD-O2D-CED
13	G	802	CLA	CBD-CGD-O2D-CED
13	e	852	CLA	CBD-CGD-O2D-CED
13	b	802	CLA	CBD-CGD-O2D-CED
13	A	811	CLA	C2A-CAA-CBA-CGA
13	A	822	CLA	C2A-CAA-CBA-CGA
13	A	823	CLA	C2A-CAA-CBA-CGA
13	A	832	CLA	C2A-CAA-CBA-CGA
13	A	843	CLA	C2A-CAA-CBA-CGA
13	B	818	CLA	C2A-CAA-CBA-CGA
13	B	832	CLA	C2A-CAA-CBA-CGA
13	F	202	CLA	C2A-CAA-CBA-CGA
13	E	811	CLA	C2A-CAA-CBA-CGA
13	E	822	CLA	C2A-CAA-CBA-CGA
13	E	823	CLA	C2A-CAA-CBA-CGA
13	E	832	CLA	C2A-CAA-CBA-CGA
13	E	844	CLA	C2A-CAA-CBA-CGA
13	G	818	CLA	C2A-CAA-CBA-CGA
13	e	810	CLA	C2A-CAA-CBA-CGA
13	e	821	CLA	C2A-CAA-CBA-CGA
13	e	822	CLA	C2A-CAA-CBA-CGA
13	e	831	CLA	C2A-CAA-CBA-CGA
13	e	842	CLA	C2A-CAA-CBA-CGA
13	g	819	CLA	C2A-CAA-CBA-CGA
13	g	833	CLA	C2A-CAA-CBA-CGA
13	o	202	CLA	C2A-CAA-CBA-CGA
13	a	811	CLA	C2A-CAA-CBA-CGA
13	a	822	CLA	C2A-CAA-CBA-CGA
13	a	823	CLA	C2A-CAA-CBA-CGA
13	a	832	CLA	C2A-CAA-CBA-CGA
13	a	844	CLA	C2A-CAA-CBA-CGA
13	b	817	CLA	C2A-CAA-CBA-CGA
13	b	831	CLA	C2A-CAA-CBA-CGA
13	B	838	CLA	O1A-CGA-O2A-C1
13	G	838	CLA	O1A-CGA-O2A-C1
13	g	839	CLA	O1A-CGA-O2A-C1
13	b	837	CLA	O1A-CGA-O2A-C1
13	A	807	CLA	CBA-CGA-O2A-C1
13	A	822	CLA	CBA-CGA-O2A-C1
13	A	837	CLA	CBA-CGA-O2A-C1
13	A	843	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	B	807	CLA	CBA-CGA-O2A-C1
13	B	838	CLA	CBA-CGA-O2A-C1
13	E	807	CLA	CBA-CGA-O2A-C1
13	E	822	CLA	CBA-CGA-O2A-C1
13	E	838	CLA	CBA-CGA-O2A-C1
13	E	844	CLA	CBA-CGA-O2A-C1
13	G	806	CLA	CBA-CGA-O2A-C1
13	G	817	CLA	CBA-CGA-O2A-C1
13	G	838	CLA	CBA-CGA-O2A-C1
13	e	806	CLA	CBA-CGA-O2A-C1
13	e	821	CLA	CBA-CGA-O2A-C1
13	e	836	CLA	CBA-CGA-O2A-C1
13	e	842	CLA	CBA-CGA-O2A-C1
13	g	808	CLA	CBA-CGA-O2A-C1
13	g	839	CLA	CBA-CGA-O2A-C1
13	a	807	CLA	CBA-CGA-O2A-C1
13	a	838	CLA	CBA-CGA-O2A-C1
13	a	844	CLA	CBA-CGA-O2A-C1
13	a	852	CLA	CBA-CGA-O2A-C1
13	b	806	CLA	CBA-CGA-O2A-C1
13	b	816	CLA	CBA-CGA-O2A-C1
13	b	837	CLA	CBA-CGA-O2A-C1
13	g	812	CLA	CBD-CGD-O2D-CED
13	L	202	CLA	O1D-CGD-O2D-CED
13	A	807	CLA	O1A-CGA-O2A-C1
13	A	810	CLA	O1A-CGA-O2A-C1
13	A	815	CLA	O1A-CGA-O2A-C1
13	A	822	CLA	O1A-CGA-O2A-C1
13	A	843	CLA	O1A-CGA-O2A-C1
13	B	819	CLA	O1A-CGA-O2A-C1
13	E	807	CLA	O1A-CGA-O2A-C1
13	E	810	CLA	O1A-CGA-O2A-C1
13	E	815	CLA	O1A-CGA-O2A-C1
13	E	822	CLA	O1A-CGA-O2A-C1
13	E	844	CLA	O1A-CGA-O2A-C1
13	G	819	CLA	O1A-CGA-O2A-C1
13	e	806	CLA	O1A-CGA-O2A-C1
13	e	809	CLA	O1A-CGA-O2A-C1
13	e	814	CLA	O1A-CGA-O2A-C1
13	e	821	CLA	O1A-CGA-O2A-C1
13	e	842	CLA	O1A-CGA-O2A-C1
13	g	820	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	a	807	CLA	O1A-CGA-O2A-C1
13	a	810	CLA	O1A-CGA-O2A-C1
13	a	815	CLA	O1A-CGA-O2A-C1
13	a	822	CLA	O1A-CGA-O2A-C1
13	a	844	CLA	O1A-CGA-O2A-C1
13	b	818	CLA	O1A-CGA-O2A-C1
15	B	845	BCR	C9-C10-C11-C12
15	B	846	BCR	C19-C20-C21-C22
15	G	845	BCR	C9-C10-C11-C12
15	G	846	BCR	C19-C20-C21-C22
15	S	202	BCR	C13-C14-C15-C16
15	e	849	BCR	C19-C20-C21-C22
15	g	846	BCR	C9-C10-C11-C12
15	g	847	BCR	C19-C20-C21-C22
15	a	848	BCR	C19-C20-C21-C22
15	b	844	BCR	C9-C10-C11-C12
15	b	845	BCR	C19-C20-C21-C22
13	A	806	CLA	CBD-CGD-O2D-CED
13	A	828	CLA	CBD-CGD-O2D-CED
13	A	830	CLA	CBD-CGD-O2D-CED
13	A	842	CLA	CBD-CGD-O2D-CED
13	B	811	CLA	CBD-CGD-O2D-CED
13	B	829	CLA	CBD-CGD-O2D-CED
13	E	806	CLA	CBD-CGD-O2D-CED
13	E	828	CLA	CBD-CGD-O2D-CED
13	E	830	CLA	CBD-CGD-O2D-CED
13	E	843	CLA	CBD-CGD-O2D-CED
13	G	810	CLA	CBD-CGD-O2D-CED
13	G	829	CLA	CBD-CGD-O2D-CED
13	e	805	CLA	CBD-CGD-O2D-CED
13	e	827	CLA	CBD-CGD-O2D-CED
13	e	829	CLA	CBD-CGD-O2D-CED
13	e	841	CLA	CBD-CGD-O2D-CED
13	g	830	CLA	CBD-CGD-O2D-CED
13	a	806	CLA	CBD-CGD-O2D-CED
13	a	828	CLA	CBD-CGD-O2D-CED
13	a	830	CLA	CBD-CGD-O2D-CED
13	a	843	CLA	CBD-CGD-O2D-CED
13	b	810	CLA	CBD-CGD-O2D-CED
13	b	828	CLA	CBD-CGD-O2D-CED
13	B	822	CLA	O1D-CGD-O2D-CED
13	G	822	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	g	823	CLA	O1D-CGD-O2D-CED
13	b	821	CLA	O1D-CGD-O2D-CED
14	A	846	PQN	C13-C15-C16-C17
13	A	805	CLA	CBA-CGA-O2A-C1
13	A	810	CLA	CBA-CGA-O2A-C1
13	A	815	CLA	CBA-CGA-O2A-C1
13	A	826	CLA	CBA-CGA-O2A-C1
13	A	845	CLA	CBA-CGA-O2A-C1
13	B	819	CLA	CBA-CGA-O2A-C1
13	B	825	CLA	CBA-CGA-O2A-C1
13	E	805	CLA	CBA-CGA-O2A-C1
13	E	810	CLA	CBA-CGA-O2A-C1
13	E	815	CLA	CBA-CGA-O2A-C1
13	E	826	CLA	CBA-CGA-O2A-C1
13	G	819	CLA	CBA-CGA-O2A-C1
13	G	825	CLA	CBA-CGA-O2A-C1
13	e	809	CLA	CBA-CGA-O2A-C1
13	e	814	CLA	CBA-CGA-O2A-C1
13	e	825	CLA	CBA-CGA-O2A-C1
13	g	801	CLA	CBA-CGA-O2A-C1
13	g	820	CLA	CBA-CGA-O2A-C1
13	g	826	CLA	CBA-CGA-O2A-C1
13	a	805	CLA	CBA-CGA-O2A-C1
13	a	810	CLA	CBA-CGA-O2A-C1
13	a	815	CLA	CBA-CGA-O2A-C1
13	a	822	CLA	CBA-CGA-O2A-C1
13	a	826	CLA	CBA-CGA-O2A-C1
13	b	818	CLA	CBA-CGA-O2A-C1
13	b	824	CLA	CBA-CGA-O2A-C1
13	A	845	CLA	O1A-CGA-O2A-C1
13	B	825	CLA	O1A-CGA-O2A-C1
13	G	825	CLA	O1A-CGA-O2A-C1
13	g	826	CLA	O1A-CGA-O2A-C1
13	b	824	CLA	O1A-CGA-O2A-C1
13	B	824	CLA	O1D-CGD-O2D-CED
13	G	824	CLA	O1D-CGD-O2D-CED
13	g	825	CLA	O1D-CGD-O2D-CED
13	b	823	CLA	O1D-CGD-O2D-CED
13	A	808	CLA	CBD-CGD-O2D-CED
13	B	813	CLA	CBD-CGD-O2D-CED
13	B	818	CLA	CBD-CGD-O2D-CED
13	B	825	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	B	836	CLA	CBD-CGD-O2D-CED
13	E	808	CLA	CBD-CGD-O2D-CED
13	G	813	CLA	CBD-CGD-O2D-CED
13	G	818	CLA	CBD-CGD-O2D-CED
13	G	825	CLA	CBD-CGD-O2D-CED
13	G	836	CLA	CBD-CGD-O2D-CED
13	e	807	CLA	CBD-CGD-O2D-CED
13	g	814	CLA	CBD-CGD-O2D-CED
13	g	819	CLA	CBD-CGD-O2D-CED
13	g	826	CLA	CBD-CGD-O2D-CED
13	g	837	CLA	CBD-CGD-O2D-CED
13	a	808	CLA	CBD-CGD-O2D-CED
13	b	812	CLA	CBD-CGD-O2D-CED
13	b	817	CLA	CBD-CGD-O2D-CED
13	b	824	CLA	CBD-CGD-O2D-CED
13	b	835	CLA	CBD-CGD-O2D-CED
13	F	202	CLA	O1D-CGD-O2D-CED
13	G	841	CLA	O1D-CGD-O2D-CED
13	b	840	CLA	O1D-CGD-O2D-CED
13	B	833	CLA	CBA-CGA-O2A-C1
13	G	833	CLA	CBA-CGA-O2A-C1
13	g	834	CLA	CBA-CGA-O2A-C1
13	b	832	CLA	CBA-CGA-O2A-C1
13	B	828	CLA	O1D-CGD-O2D-CED
13	B	841	CLA	O1D-CGD-O2D-CED
13	G	828	CLA	O1D-CGD-O2D-CED
13	g	829	CLA	O1D-CGD-O2D-CED
13	g	842	CLA	O1D-CGD-O2D-CED
13	b	827	CLA	O1D-CGD-O2D-CED
13	A	805	CLA	O1A-CGA-O2A-C1
13	E	805	CLA	O1A-CGA-O2A-C1
13	g	801	CLA	O1A-CGA-O2A-C1
13	a	805	CLA	O1A-CGA-O2A-C1
13	B	807	CLA	C2A-CAA-CBA-CGA
13	G	806	CLA	C2A-CAA-CBA-CGA
13	g	808	CLA	C2A-CAA-CBA-CGA
13	b	806	CLA	C2A-CAA-CBA-CGA
13	f	203	CLA	C2A-CAA-CBA-CGA
13	A	826	CLA	O1A-CGA-O2A-C1
13	E	826	CLA	O1A-CGA-O2A-C1
13	A	806	CLA	CBA-CGA-O2A-C1
13	A	853	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	E	806	CLA	CBA-CGA-O2A-C1
13	E	814	CLA	CBA-CGA-O2A-C1
13	G	802	CLA	CBA-CGA-O2A-C1
13	e	805	CLA	CBA-CGA-O2A-C1
13	e	852	CLA	CBA-CGA-O2A-C1
13	a	806	CLA	CBA-CGA-O2A-C1
13	b	802	CLA	CBA-CGA-O2A-C1
13	B	838	CLA	O1D-CGD-O2D-CED
13	G	838	CLA	O1D-CGD-O2D-CED
13	g	839	CLA	O1D-CGD-O2D-CED
13	b	837	CLA	O1D-CGD-O2D-CED
13	B	833	CLA	O1A-CGA-O2A-C1
13	G	833	CLA	O1A-CGA-O2A-C1
13	e	825	CLA	O1A-CGA-O2A-C1
13	g	834	CLA	O1A-CGA-O2A-C1
13	a	826	CLA	O1A-CGA-O2A-C1
13	b	832	CLA	O1A-CGA-O2A-C1
13	A	806	CLA	O1A-CGA-O2A-C1
13	A	829	CLA	O1A-CGA-O2A-C1
13	A	853	CLA	O1A-CGA-O2A-C1
13	E	829	CLA	O1A-CGA-O2A-C1
13	G	802	CLA	O1A-CGA-O2A-C1
13	e	805	CLA	O1A-CGA-O2A-C1
13	e	828	CLA	O1A-CGA-O2A-C1
13	e	852	CLA	O1A-CGA-O2A-C1
13	a	806	CLA	O1A-CGA-O2A-C1
13	a	829	CLA	O1A-CGA-O2A-C1
13	b	802	CLA	O1A-CGA-O2A-C1
13	A	814	CLA	CBA-CGA-O2A-C1
13	A	823	CLA	CBA-CGA-O2A-C1
13	A	829	CLA	CBA-CGA-O2A-C1
13	B	806	CLA	CBA-CGA-O2A-C1
13	E	823	CLA	CBA-CGA-O2A-C1
13	E	829	CLA	CBA-CGA-O2A-C1
13	G	805	CLA	CBA-CGA-O2A-C1
13	e	813	CLA	CBA-CGA-O2A-C1
13	e	822	CLA	CBA-CGA-O2A-C1
13	e	828	CLA	CBA-CGA-O2A-C1
13	g	807	CLA	CBA-CGA-O2A-C1
13	a	823	CLA	CBA-CGA-O2A-C1
13	a	829	CLA	CBA-CGA-O2A-C1
13	b	805	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	L	203	CLA	CBD-CGD-O2D-CED
13	S	203	CLA	CBD-CGD-O2D-CED
13	s	202	CLA	CBD-CGD-O2D-CED
13	l	204	CLA	CBD-CGD-O2D-CED
15	A	847	BCR	C13-C14-C15-C16
15	A	850	BCR	C19-C20-C21-C22
15	B	848	BCR	C15-C16-C17-C18
15	E	849	BCR	C13-C14-C15-C16
15	G	848	BCR	C15-C16-C17-C18
15	S	201	BCR	C19-C20-C21-C22
15	e	846	BCR	C13-C14-C15-C16
15	g	849	BCR	C15-C16-C17-C18
15	a	849	BCR	C13-C14-C15-C16
15	b	847	BCR	C15-C16-C17-C18
14	e	845	PQN	C25-C26-C27-C28
13	E	806	CLA	O1A-CGA-O2A-C1
12	A	801	LHG	C23-C24-C25-C26
12	A	801	LHG	O7-C5-C6-O8
13	B	806	CLA	O1A-CGA-O2A-C1
13	G	805	CLA	O1A-CGA-O2A-C1
13	g	807	CLA	O1A-CGA-O2A-C1
13	b	805	CLA	O1A-CGA-O2A-C1
14	a	847	PQN	C19-C18-C20-C21
13	e	844	CLA	O1D-CGD-O2D-CED
13	b	813	CLA	O1D-CGD-O2D-CED
15	A	850	BCR	C7-C8-C9-C34
15	B	843	BCR	C7-C8-C9-C34
15	B	843	BCR	C37-C22-C23-C24
15	B	844	BCR	C7-C8-C9-C34
15	B	844	BCR	C11-C12-C13-C35
15	B	845	BCR	C11-C12-C13-C35
15	B	846	BCR	C11-C12-C13-C35
15	B	848	BCR	C7-C8-C9-C34
15	F	201	BCR	C7-C8-C9-C34
15	J	102	BCR	C11-C12-C13-C35
15	L	201	BCR	C36-C18-C19-C20
15	L	201	BCR	C37-C22-C23-C24
15	E	802	BCR	C11-C12-C13-C35
15	E	852	BCR	C11-C12-C13-C35
15	G	843	BCR	C7-C8-C9-C34
15	G	843	BCR	C37-C22-C23-C24
15	G	844	BCR	C7-C8-C9-C34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	G	844	BCR	C11-C12-C13-C35
15	G	845	BCR	C11-C12-C13-C35
15	G	846	BCR	C11-C12-C13-C35
15	G	848	BCR	C7-C8-C9-C34
15	O	201	BCR	C7-C8-C9-C34
15	O	202	BCR	C7-C8-C9-C34
15	R	101	BCR	C7-C8-C9-C34
15	S	201	BCR	C37-C22-C23-C24
15	S	202	BCR	C11-C12-C13-C35
15	S	205	BCR	C7-C8-C9-C34
15	e	849	BCR	C7-C8-C9-C34
15	g	844	BCR	C7-C8-C9-C34
15	g	844	BCR	C37-C22-C23-C24
15	g	845	BCR	C7-C8-C9-C34
15	g	845	BCR	C11-C12-C13-C35
15	g	846	BCR	C11-C12-C13-C35
15	g	847	BCR	C11-C12-C13-C35
15	g	849	BCR	C7-C8-C9-C34
15	o	201	BCR	C7-C8-C9-C34
15	q	102	BCR	C11-C12-C13-C35
15	s	204	BCR	C7-C8-C9-C34
15	a	803	BCR	C11-C12-C13-C35
15	a	848	BCR	C7-C8-C9-C34
15	a	848	BCR	C11-C12-C13-C35
15	a	853	BCR	C11-C12-C13-C35
15	b	842	BCR	C7-C8-C9-C34
15	b	842	BCR	C37-C22-C23-C24
15	b	843	BCR	C7-C8-C9-C34
15	b	843	BCR	C11-C12-C13-C35
15	b	844	BCR	C11-C12-C13-C35
15	b	845	BCR	C11-C12-C13-C35
15	b	847	BCR	C7-C8-C9-C34
15	f	201	BCR	C7-C8-C9-C34
15	f	202	BCR	C7-C8-C9-C34
15	k	4001	BCR	C7-C8-C9-C34
15	k	4001	BCR	C11-C12-C13-C35
15	l	202	BCR	C7-C8-C9-C34
15	l	206	BCR	C7-C8-C9-C34
15	A	847	BCR	C21-C22-C23-C24
15	A	848	BCR	C7-C8-C9-C10
15	B	843	BCR	C7-C8-C9-C10
15	B	844	BCR	C11-C12-C13-C14

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	B	845	BCR	C11-C12-C13-C14
15	B	848	BCR	C11-C12-C13-C14
15	J	101	BCR	C11-C12-C13-C14
15	J	102	BCR	C11-C12-C13-C14
15	L	205	BCR	C21-C22-C23-C24
15	E	802	BCR	C11-C12-C13-C14
15	E	849	BCR	C21-C22-C23-C24
15	E	850	BCR	C7-C8-C9-C10
15	E	852	BCR	C11-C12-C13-C14
15	G	843	BCR	C7-C8-C9-C10
15	G	844	BCR	C11-C12-C13-C14
15	G	845	BCR	C11-C12-C13-C14
15	G	848	BCR	C11-C12-C13-C14
15	Q	101	BCR	C11-C12-C13-C14
15	R	101	BCR	C11-C12-C13-C14
15	S	201	BCR	C21-C22-C23-C24
15	e	846	BCR	C21-C22-C23-C24
15	e	847	BCR	C7-C8-C9-C10
15	g	844	BCR	C7-C8-C9-C10
15	g	845	BCR	C11-C12-C13-C14
15	g	846	BCR	C11-C12-C13-C14
15	g	849	BCR	C11-C12-C13-C14
15	q	101	BCR	C11-C12-C13-C14
15	q	102	BCR	C11-C12-C13-C14
15	s	204	BCR	C7-C8-C9-C10
15	a	848	BCR	C7-C8-C9-C10
15	a	849	BCR	C21-C22-C23-C24
15	a	850	BCR	C7-C8-C9-C10
15	a	853	BCR	C11-C12-C13-C14
15	b	842	BCR	C7-C8-C9-C10
15	b	843	BCR	C11-C12-C13-C14
15	b	844	BCR	C11-C12-C13-C14
15	b	847	BCR	C11-C12-C13-C14
15	j	101	BCR	C11-C12-C13-C14
15	k	4001	BCR	C17-C18-C19-C20
13	B	814	CLA	O1D-CGD-O2D-CED
13	G	814	CLA	O1D-CGD-O2D-CED
13	g	815	CLA	O1D-CGD-O2D-CED
14	e	845	PQN	C23-C25-C26-C27
13	B	818	CLA	CBA-CGA-O2A-C1
13	G	818	CLA	CBA-CGA-O2A-C1
12	A	802	LHG	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	S	202	BCR	C14-C15-C16-C17
13	A	814	CLA	O1A-CGA-O2A-C1
13	e	813	CLA	O1A-CGA-O2A-C1
14	B	842	PQN	C25-C26-C27-C28
14	G	842	PQN	C25-C26-C27-C28
14	g	843	PQN	C25-C26-C27-C28
14	b	841	PQN	C25-C26-C27-C28
13	B	830	CLA	CBA-CGA-O2A-C1
13	B	841	CLA	CBA-CGA-O2A-C1
13	G	830	CLA	CBA-CGA-O2A-C1
13	G	841	CLA	CBA-CGA-O2A-C1
13	g	819	CLA	CBA-CGA-O2A-C1
13	g	831	CLA	CBA-CGA-O2A-C1
13	g	842	CLA	CBA-CGA-O2A-C1
13	b	817	CLA	CBA-CGA-O2A-C1
13	b	829	CLA	CBA-CGA-O2A-C1
13	b	840	CLA	CBA-CGA-O2A-C1
13	G	801	CLA	O1D-CGD-O2D-CED
13	L	204	CLA	C2-C1-O2A-CGA
13	s	203	CLA	C2-C1-O2A-CGA
12	e	801	LHG	C23-C24-C25-C26
12	e	802	LHG	C23-C24-C25-C26
13	A	823	CLA	O1A-CGA-O2A-C1
13	E	823	CLA	O1A-CGA-O2A-C1
13	e	822	CLA	O1A-CGA-O2A-C1
13	a	823	CLA	O1A-CGA-O2A-C1
15	A	848	BCR	C9-C10-C11-C12
15	A	848	BCR	C19-C20-C21-C22
15	B	845	BCR	C15-C16-C17-C18
15	B	848	BCR	C9-C10-C11-C12
15	E	850	BCR	C9-C10-C11-C12
15	E	850	BCR	C19-C20-C21-C22
15	G	845	BCR	C15-C16-C17-C18
15	G	848	BCR	C9-C10-C11-C12
15	e	847	BCR	C9-C10-C11-C12
15	e	847	BCR	C19-C20-C21-C22
15	e	851	BCR	C13-C14-C15-C16
15	g	846	BCR	C15-C16-C17-C18
15	g	849	BCR	C9-C10-C11-C12
15	a	803	BCR	C13-C14-C15-C16
15	a	850	BCR	C9-C10-C11-C12
15	a	850	BCR	C19-C20-C21-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	b	844	BCR	C15-C16-C17-C18
15	b	847	BCR	C9-C10-C11-C12
15	l	202	BCR	C19-C20-C21-C22
13	B	802	CLA	C2A-CAA-CBA-CGA
13	B	830	CLA	C2A-CAA-CBA-CGA
13	G	830	CLA	C2A-CAA-CBA-CGA
13	O	203	CLA	C2A-CAA-CBA-CGA
13	g	831	CLA	C2A-CAA-CBA-CGA
13	b	829	CLA	C2A-CAA-CBA-CGA
15	A	852	BCR	C22-C23-C24-C25
15	L	205	BCR	C6-C7-C8-C9
15	A	848	BCR	C10-C11-C12-C13
15	A	848	BCR	C18-C19-C20-C21
15	A	852	BCR	C18-C19-C20-C21
15	B	846	BCR	C18-C19-C20-C21
15	J	102	BCR	C10-C11-C12-C13
15	E	850	BCR	C10-C11-C12-C13
15	E	850	BCR	C18-C19-C20-C21
15	E	852	BCR	C10-C11-C12-C13
15	G	846	BCR	C18-C19-C20-C21
15	R	101	BCR	C10-C11-C12-C13
15	S	205	BCR	C18-C19-C20-C21
15	e	847	BCR	C10-C11-C12-C13
15	e	847	BCR	C18-C19-C20-C21
15	e	851	BCR	C18-C19-C20-C21
15	g	847	BCR	C18-C19-C20-C21
15	q	102	BCR	C10-C11-C12-C13
15	a	848	BCR	C10-C11-C12-C13
15	a	850	BCR	C10-C11-C12-C13
15	a	850	BCR	C18-C19-C20-C21
15	a	853	BCR	C10-C11-C12-C13
15	b	845	BCR	C18-C19-C20-C21
15	l	202	BCR	C10-C11-C12-C13
15	m	101	BCR	C10-C11-C12-C13
14	B	842	PQN	C15-C16-C17-C18
14	G	842	PQN	C15-C16-C17-C18
14	g	843	PQN	C15-C16-C17-C18
14	b	841	PQN	C15-C16-C17-C18
13	E	814	CLA	O1A-CGA-O2A-C1
14	a	847	PQN	C15-C16-C17-C18
13	A	833	CLA	O1D-CGD-O2D-CED
13	E	833	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	e	832	CLA	O1D-CGD-O2D-CED
13	a	833	CLA	O1D-CGD-O2D-CED
12	A	801	LHG	C4-O6-P-O3
12	e	801	LHG	C3-O3-P-O6
12	e	801	LHG	C4-O6-P-O3
12	a	801	LHG	C3-O3-P-O6
13	A	815	CLA	C2A-CAA-CBA-CGA
13	B	801	CLA	C2A-CAA-CBA-CGA
13	B	834	CLA	C2A-CAA-CBA-CGA
13	E	815	CLA	C2A-CAA-CBA-CGA
13	E	835	CLA	C2A-CAA-CBA-CGA
13	G	801	CLA	C2A-CAA-CBA-CGA
13	G	834	CLA	C2A-CAA-CBA-CGA
13	e	814	CLA	C2A-CAA-CBA-CGA
13	g	802	CLA	C2A-CAA-CBA-CGA
13	g	803	CLA	C2A-CAA-CBA-CGA
13	g	835	CLA	C2A-CAA-CBA-CGA
13	a	815	CLA	C2A-CAA-CBA-CGA
13	a	835	CLA	C2A-CAA-CBA-CGA
13	b	801	CLA	C2A-CAA-CBA-CGA
13	b	833	CLA	C2A-CAA-CBA-CGA
14	e	845	PQN	C26-C27-C28-C30
13	A	803	CLA	CBA-CGA-O2A-C1
13	G	802	CLA	O1D-CGD-O2D-CED
13	e	852	CLA	O1D-CGD-O2D-CED
13	b	802	CLA	O1D-CGD-O2D-CED
15	B	846	BCR	C13-C14-C15-C16
15	G	846	BCR	C13-C14-C15-C16
15	S	202	BCR	C9-C10-C11-C12
15	g	847	BCR	C13-C14-C15-C16
15	b	845	BCR	C13-C14-C15-C16
15	k	4001	BCR	C13-C14-C15-C16
15	A	847	BCR	C11-C10-C9-C34
15	A	847	BCR	C35-C13-C14-C15
15	A	847	BCR	C20-C21-C22-C37
15	A	848	BCR	C20-C21-C22-C37
15	A	850	BCR	C35-C13-C14-C15
15	A	852	BCR	C11-C10-C9-C34
15	B	846	BCR	C35-C13-C14-C15
15	B	848	BCR	C20-C21-C22-C37
15	I	101	BCR	C20-C21-C22-C37
15	E	801	BCR	C16-C17-C18-C36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	E	849	BCR	C11-C10-C9-C34
15	E	849	BCR	C35-C13-C14-C15
15	E	849	BCR	C20-C21-C22-C37
15	E	850	BCR	C20-C21-C22-C37
15	G	846	BCR	C35-C13-C14-C15
15	G	848	BCR	C20-C21-C22-C37
15	O	202	BCR	C35-C13-C14-C15
15	P	101	BCR	C20-C21-C22-C37
15	R	101	BCR	C20-C21-C22-C37
15	e	846	BCR	C11-C10-C9-C34
15	e	846	BCR	C35-C13-C14-C15
15	e	846	BCR	C20-C21-C22-C37
15	e	847	BCR	C20-C21-C22-C37
15	e	849	BCR	C35-C13-C14-C15
15	e	850	BCR	C20-C21-C22-C37
15	e	851	BCR	C20-C21-C22-C37
15	g	847	BCR	C35-C13-C14-C15
15	g	849	BCR	C20-C21-C22-C37
15	p	101	BCR	C20-C21-C22-C37
15	a	802	BCR	C16-C17-C18-C36
15	a	803	BCR	C11-C10-C9-C34
15	a	803	BCR	C16-C17-C18-C36
15	a	849	BCR	C11-C10-C9-C34
15	a	849	BCR	C35-C13-C14-C15
15	a	849	BCR	C20-C21-C22-C37
15	a	850	BCR	C20-C21-C22-C37
15	b	845	BCR	C35-C13-C14-C15
15	b	847	BCR	C20-C21-C22-C37
15	i	101	BCR	C20-C21-C22-C37
12	a	801	LHG	C34-C35-C36-C37
13	A	853	CLA	O1D-CGD-O2D-CED
14	E	848	PQN	C26-C27-C28-C29
13	e	803	CLA	CBA-CGA-O2A-C1
12	A	801	LHG	C30-C31-C32-C33
12	e	801	LHG	C30-C31-C32-C33
12	a	801	LHG	C33-C34-C35-C36
13	B	818	CLA	O1A-CGA-O2A-C1
13	G	818	CLA	O1A-CGA-O2A-C1
13	g	819	CLA	O1A-CGA-O2A-C1
13	g	842	CLA	O1A-CGA-O2A-C1
13	b	817	CLA	O1A-CGA-O2A-C1
12	A	801	LHG	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
12	A	801	LHG	C13-C14-C15-C16
13	B	811	CLA	O1D-CGD-O2D-CED
13	G	810	CLA	O1D-CGD-O2D-CED
13	g	812	CLA	O1D-CGD-O2D-CED
13	b	810	CLA	O1D-CGD-O2D-CED
15	A	847	BCR	C11-C10-C9-C8
15	A	847	BCR	C16-C17-C18-C19
15	A	848	BCR	C11-C10-C9-C8
15	A	850	BCR	C11-C10-C9-C8
15	A	852	BCR	C12-C13-C14-C15
15	A	852	BCR	C20-C21-C22-C23
15	B	844	BCR	C11-C10-C9-C8
15	B	846	BCR	C11-C10-C9-C8
15	B	846	BCR	C16-C17-C18-C19
15	I	101	BCR	C12-C13-C14-C15
15	I	101	BCR	C20-C21-C22-C23
15	E	849	BCR	C11-C10-C9-C8
15	E	849	BCR	C16-C17-C18-C19
15	E	850	BCR	C11-C10-C9-C8
15	G	844	BCR	C11-C10-C9-C8
15	G	846	BCR	C11-C10-C9-C8
15	G	846	BCR	C16-C17-C18-C19
15	O	202	BCR	C16-C17-C18-C19
15	O	202	BCR	C20-C21-C22-C23
15	P	101	BCR	C12-C13-C14-C15
15	P	101	BCR	C20-C21-C22-C23
15	S	202	BCR	C20-C21-C22-C23
15	S	205	BCR	C11-C10-C9-C8
15	T	101	BCR	C12-C13-C14-C15
15	T	101	BCR	C20-C21-C22-C23
15	e	846	BCR	C11-C10-C9-C8
15	e	846	BCR	C16-C17-C18-C19
15	e	847	BCR	C11-C10-C9-C8
15	e	849	BCR	C11-C10-C9-C8
15	g	845	BCR	C11-C10-C9-C8
15	g	846	BCR	C12-C13-C14-C15
15	g	847	BCR	C11-C10-C9-C8
15	g	847	BCR	C16-C17-C18-C19
15	p	101	BCR	C12-C13-C14-C15
15	p	101	BCR	C20-C21-C22-C23
15	a	802	BCR	C16-C17-C18-C19
15	a	803	BCR	C20-C21-C22-C23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	a	849	BCR	C11-C10-C9-C8
15	a	849	BCR	C16-C17-C18-C19
15	a	850	BCR	C11-C10-C9-C8
15	b	843	BCR	C11-C10-C9-C8
15	b	844	BCR	C12-C13-C14-C15
15	b	845	BCR	C11-C10-C9-C8
15	b	845	BCR	C16-C17-C18-C19
15	f	202	BCR	C16-C17-C18-C19
15	f	202	BCR	C20-C21-C22-C23
15	i	101	BCR	C12-C13-C14-C15
15	i	101	BCR	C20-C21-C22-C23
15	k	4001	BCR	C11-C10-C9-C8
15	l	206	BCR	C11-C10-C9-C8
13	B	830	CLA	O1A-CGA-O2A-C1
13	B	841	CLA	O1A-CGA-O2A-C1
13	G	830	CLA	O1A-CGA-O2A-C1
13	G	841	CLA	O1A-CGA-O2A-C1
13	g	831	CLA	O1A-CGA-O2A-C1
13	b	829	CLA	O1A-CGA-O2A-C1
13	b	840	CLA	O1A-CGA-O2A-C1
14	e	845	PQN	C26-C27-C28-C29
13	A	830	CLA	O1D-CGD-O2D-CED
13	E	830	CLA	O1D-CGD-O2D-CED
13	e	829	CLA	O1D-CGD-O2D-CED
13	a	830	CLA	O1D-CGD-O2D-CED
12	e	801	LHG	C10-C11-C12-C13
12	e	801	LHG	C13-C14-C15-C16
14	e	845	PQN	C18-C20-C21-C22
13	B	805	CLA	C2A-CAA-CBA-CGA
13	B	835	CLA	C2A-CAA-CBA-CGA
13	G	804	CLA	C2A-CAA-CBA-CGA
13	G	835	CLA	C2A-CAA-CBA-CGA
13	g	806	CLA	C2A-CAA-CBA-CGA
13	g	836	CLA	C2A-CAA-CBA-CGA
13	b	804	CLA	C2A-CAA-CBA-CGA
13	b	834	CLA	C2A-CAA-CBA-CGA
15	A	848	BCR	C7-C8-C9-C34
15	B	848	BCR	C11-C12-C13-C35
15	J	101	BCR	C11-C12-C13-C35
15	L	205	BCR	C7-C8-C9-C34
15	E	850	BCR	C7-C8-C9-C34
15	G	848	BCR	C11-C12-C13-C35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	Q	101	BCR	C11-C12-C13-C35
15	R	101	BCR	C11-C12-C13-C35
15	e	847	BCR	C7-C8-C9-C34
15	g	849	BCR	C11-C12-C13-C35
15	q	101	BCR	C11-C12-C13-C35
15	a	848	BCR	C37-C22-C23-C24
15	a	850	BCR	C7-C8-C9-C34
15	b	847	BCR	C11-C12-C13-C35
15	j	101	BCR	C11-C12-C13-C35
12	A	802	LHG	O1-C1-C2-C3
15	B	843	BCR	C21-C22-C23-C24
15	G	843	BCR	C21-C22-C23-C24
15	O	202	BCR	C7-C8-C9-C10
15	S	205	BCR	C7-C8-C9-C10
15	g	844	BCR	C21-C22-C23-C24
15	a	848	BCR	C21-C22-C23-C24
15	b	842	BCR	C21-C22-C23-C24
15	f	202	BCR	C7-C8-C9-C10
15	l	206	BCR	C7-C8-C9-C10
12	e	801	LHG	C32-C33-C34-C35
12	a	801	LHG	C12-C13-C14-C15
14	E	848	PQN	C26-C27-C28-C30
12	a	801	LHG	C32-C33-C34-C35
12	a	801	LHG	C11-C10-C9-C8
14	a	847	PQN	C13-C15-C16-C17
13	E	828	CLA	O1D-CGD-O2D-CED
13	A	808	CLA	C3A-C2A-CAA-CBA
13	A	830	CLA	C3A-C2A-CAA-CBA
13	A	837	CLA	C3A-C2A-CAA-CBA
13	B	835	CLA	C3A-C2A-CAA-CBA
13	K	102	CLA	C3A-C2A-CAA-CBA
13	E	808	CLA	C3A-C2A-CAA-CBA
13	E	830	CLA	C3A-C2A-CAA-CBA
13	E	838	CLA	C3A-C2A-CAA-CBA
13	G	835	CLA	C3A-C2A-CAA-CBA
13	R	102	CLA	C3A-C2A-CAA-CBA
13	e	807	CLA	C3A-C2A-CAA-CBA
13	e	829	CLA	C3A-C2A-CAA-CBA
13	e	836	CLA	C3A-C2A-CAA-CBA
13	g	836	CLA	C3A-C2A-CAA-CBA
13	r	102	CLA	C3A-C2A-CAA-CBA
13	a	808	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	a	830	CLA	C3A-C2A-CAA-CBA
13	a	838	CLA	C3A-C2A-CAA-CBA
13	a	852	CLA	C3A-C2A-CAA-CBA
13	b	834	CLA	C3A-C2A-CAA-CBA
13	k	4002	CLA	C3A-C2A-CAA-CBA
12	A	801	LHG	C32-C33-C34-C35
13	A	806	CLA	O1D-CGD-O2D-CED
13	A	828	CLA	O1D-CGD-O2D-CED
13	E	806	CLA	O1D-CGD-O2D-CED
13	e	805	CLA	O1D-CGD-O2D-CED
13	e	827	CLA	O1D-CGD-O2D-CED
13	a	806	CLA	O1D-CGD-O2D-CED
13	a	828	CLA	O1D-CGD-O2D-CED
12	e	801	LHG	C27-C28-C29-C30
13	G	811	CLA	C2C-C3C-CAC-CBC
13	B	829	CLA	O1D-CGD-O2D-CED
13	b	828	CLA	O1D-CGD-O2D-CED
15	B	845	BCR	C14-C15-C16-C17
15	J	101	BCR	C14-C15-C16-C17
15	G	845	BCR	C14-C15-C16-C17
15	Q	101	BCR	C14-C15-C16-C17
15	g	846	BCR	C14-C15-C16-C17
15	q	101	BCR	C14-C15-C16-C17
15	b	844	BCR	C14-C15-C16-C17
15	j	101	BCR	C14-C15-C16-C17
15	k	4001	BCR	C14-C15-C16-C17
13	g	830	CLA	O1D-CGD-O2D-CED
13	g	813	CLA	C2C-C3C-CAC-CBC
13	s	205	CLA	C2C-C3C-CAC-CBC
12	e	801	LHG	C15-C16-C17-C18
13	B	812	CLA	C2C-C3C-CAC-CBC
13	G	829	CLA	O1D-CGD-O2D-CED
12	A	801	LHG	O1-C1-C2-O2
12	e	801	LHG	O1-C1-C2-O2
12	a	801	LHG	O1-C1-C2-O2
12	a	801	LHG	C31-C32-C33-C34
12	a	801	LHG	O2-C2-C3-O3
12	A	801	LHG	C27-C28-C29-C30
13	B	807	CLA	C2-C1-O2A-CGA
13	B	829	CLA	C2-C1-O2A-CGA
13	G	806	CLA	C2-C1-O2A-CGA
13	G	829	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	g	808	CLA	C2-C1-O2A-CGA
13	g	830	CLA	C2-C1-O2A-CGA
13	b	806	CLA	C2-C1-O2A-CGA
13	b	828	CLA	C2-C1-O2A-CGA
13	A	803	CLA	O1A-CGA-O2A-C1
15	A	850	BCR	C1-C6-C7-C8
15	A	850	BCR	C5-C6-C7-C8
15	A	850	BCR	C23-C24-C25-C26
15	A	850	BCR	C23-C24-C25-C30
15	A	852	BCR	C23-C24-C25-C26
15	A	852	BCR	C23-C24-C25-C30
15	B	845	BCR	C5-C6-C7-C8
15	B	847	BCR	C1-C6-C7-C8
15	B	847	BCR	C23-C24-C25-C26
15	B	848	BCR	C5-C6-C7-C8
15	B	848	BCR	C23-C24-C25-C30
15	J	102	BCR	C5-C6-C7-C8
15	L	201	BCR	C23-C24-C25-C26
15	L	201	BCR	C23-C24-C25-C30
15	L	205	BCR	C23-C24-C25-C26
15	L	205	BCR	C23-C24-C25-C30
15	E	802	BCR	C1-C6-C7-C8
15	E	802	BCR	C5-C6-C7-C8
15	E	852	BCR	C5-C6-C7-C8
15	G	845	BCR	C5-C6-C7-C8
15	G	847	BCR	C1-C6-C7-C8
15	G	847	BCR	C23-C24-C25-C26
15	G	848	BCR	C5-C6-C7-C8
15	G	848	BCR	C23-C24-C25-C30
15	O	202	BCR	C23-C24-C25-C26
15	S	205	BCR	C23-C24-C25-C26
15	S	205	BCR	C23-C24-C25-C30
15	e	849	BCR	C1-C6-C7-C8
15	e	849	BCR	C5-C6-C7-C8
15	e	849	BCR	C23-C24-C25-C26
15	e	849	BCR	C23-C24-C25-C30
15	e	851	BCR	C5-C6-C7-C8
15	e	851	BCR	C23-C24-C25-C26
15	e	851	BCR	C23-C24-C25-C30
15	g	846	BCR	C5-C6-C7-C8
15	g	848	BCR	C1-C6-C7-C8
15	g	848	BCR	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	g	849	BCR	C5-C6-C7-C8
15	g	849	BCR	C23-C24-C25-C30
15	q	102	BCR	C5-C6-C7-C8
15	s	201	BCR	C23-C24-C25-C26
15	s	201	BCR	C23-C24-C25-C30
15	a	803	BCR	C5-C6-C7-C8
15	a	848	BCR	C1-C6-C7-C8
15	a	853	BCR	C5-C6-C7-C8
15	b	844	BCR	C5-C6-C7-C8
15	b	846	BCR	C23-C24-C25-C26
15	b	847	BCR	C5-C6-C7-C8
15	b	847	BCR	C23-C24-C25-C30
15	f	202	BCR	C23-C24-C25-C26
15	k	4001	BCR	C23-C24-C25-C26
15	l	202	BCR	C23-C24-C25-C26
15	l	206	BCR	C23-C24-C25-C26
14	B	842	PQN	C23-C25-C26-C27
14	G	842	PQN	C23-C25-C26-C27
14	g	843	PQN	C23-C25-C26-C27
14	b	841	PQN	C23-C25-C26-C27
13	e	803	CLA	O1A-CGA-O2A-C1
12	A	801	LHG	C33-C34-C35-C36
13	A	808	CLA	O1D-CGD-O2D-CED
13	E	808	CLA	O1D-CGD-O2D-CED
13	e	807	CLA	O1D-CGD-O2D-CED
13	a	808	CLA	O1D-CGD-O2D-CED
14	a	847	PQN	C21-C22-C23-C25
12	e	801	LHG	C33-C34-C35-C36
15	J	101	BCR	C19-C20-C21-C22
15	Q	101	BCR	C19-C20-C21-C22
15	S	202	BCR	C19-C20-C21-C22
15	q	101	BCR	C19-C20-C21-C22
15	a	803	BCR	C9-C10-C11-C12
15	j	101	BCR	C19-C20-C21-C22
13	A	842	CLA	O1D-CGD-O2D-CED
13	E	843	CLA	O1D-CGD-O2D-CED
13	e	841	CLA	O1D-CGD-O2D-CED
13	a	843	CLA	O1D-CGD-O2D-CED
13	A	804	CLA	C2A-CAA-CBA-CGA
13	A	844	CLA	C2A-CAA-CBA-CGA
13	B	811	CLA	C2A-CAA-CBA-CGA
13	E	804	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	E	846	CLA	C2A-CAA-CBA-CGA
13	G	810	CLA	C2A-CAA-CBA-CGA
13	e	804	CLA	C2A-CAA-CBA-CGA
13	e	843	CLA	C2A-CAA-CBA-CGA
13	g	812	CLA	C2A-CAA-CBA-CGA
13	a	804	CLA	C2A-CAA-CBA-CGA
13	a	845	CLA	C2A-CAA-CBA-CGA
13	b	810	CLA	C2A-CAA-CBA-CGA
13	B	818	CLA	O1D-CGD-O2D-CED
13	g	819	CLA	O1D-CGD-O2D-CED
13	B	813	CLA	O1D-CGD-O2D-CED
13	G	813	CLA	O1D-CGD-O2D-CED
13	G	818	CLA	O1D-CGD-O2D-CED
13	g	814	CLA	O1D-CGD-O2D-CED
13	b	812	CLA	O1D-CGD-O2D-CED
13	b	817	CLA	O1D-CGD-O2D-CED
13	B	825	CLA	O1D-CGD-O2D-CED
13	B	836	CLA	O1D-CGD-O2D-CED
13	b	835	CLA	O1D-CGD-O2D-CED
12	A	801	LHG	C15-C16-C17-C18
13	G	825	CLA	O1D-CGD-O2D-CED
13	G	836	CLA	O1D-CGD-O2D-CED
13	g	826	CLA	O1D-CGD-O2D-CED
13	b	824	CLA	O1D-CGD-O2D-CED
15	J	101	BCR	C22-C23-C24-C25
15	Q	101	BCR	C22-C23-C24-C25
15	q	101	BCR	C22-C23-C24-C25
15	j	101	BCR	C22-C23-C24-C25
13	A	816	CLA	CBA-CGA-O2A-C1
13	E	816	CLA	CBA-CGA-O2A-C1
13	e	815	CLA	CBA-CGA-O2A-C1
13	a	816	CLA	CBA-CGA-O2A-C1
14	A	846	PQN	C26-C27-C28-C30
13	g	837	CLA	O1D-CGD-O2D-CED
12	A	801	LHG	C8-C7-O7-C5
12	e	801	LHG	C8-C7-O7-C5
12	a	801	LHG	C8-C7-O7-C5
15	I	101	BCR	C14-C15-C16-C17
15	P	101	BCR	C14-C15-C16-C17
15	p	101	BCR	C14-C15-C16-C17
15	i	101	BCR	C14-C15-C16-C17
12	a	801	LHG	O7-C5-C6-O8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	a	847	PQN	C20-C21-C22-C23
14	a	847	PQN	C21-C22-C23-C24
12	e	801	LHG	C31-C32-C33-C34
13	A	810	CLA	C2A-CAA-CBA-CGA
13	A	829	CLA	C2A-CAA-CBA-CGA
13	A	836	CLA	C2A-CAA-CBA-CGA
13	E	810	CLA	C2A-CAA-CBA-CGA
13	E	829	CLA	C2A-CAA-CBA-CGA
13	E	837	CLA	C2A-CAA-CBA-CGA
13	E	845	CLA	C2A-CAA-CBA-CGA
13	e	809	CLA	C2A-CAA-CBA-CGA
13	e	828	CLA	C2A-CAA-CBA-CGA
13	e	835	CLA	C2A-CAA-CBA-CGA
13	a	810	CLA	C2A-CAA-CBA-CGA
13	a	829	CLA	C2A-CAA-CBA-CGA
13	a	837	CLA	C2A-CAA-CBA-CGA
12	A	801	LHG	C31-C32-C33-C34
13	A	808	CLA	C1A-C2A-CAA-CBA
13	A	809	CLA	C1A-C2A-CAA-CBA
13	A	811	CLA	C1A-C2A-CAA-CBA
13	A	821	CLA	C1A-C2A-CAA-CBA
13	A	823	CLA	C1A-C2A-CAA-CBA
13	A	827	CLA	C1A-C2A-CAA-CBA
13	A	829	CLA	C1A-C2A-CAA-CBA
13	A	830	CLA	C1A-C2A-CAA-CBA
13	A	831	CLA	C1A-C2A-CAA-CBA
13	A	832	CLA	C1A-C2A-CAA-CBA
13	A	839	CLA	C1A-C2A-CAA-CBA
13	B	807	CLA	C1A-C2A-CAA-CBA
13	B	812	CLA	C1A-C2A-CAA-CBA
13	B	829	CLA	C1A-C2A-CAA-CBA
13	B	831	CLA	C1A-C2A-CAA-CBA
13	B	832	CLA	C1A-C2A-CAA-CBA
13	B	835	CLA	C1A-C2A-CAA-CBA
13	B	840	CLA	C1A-C2A-CAA-CBA
13	K	102	CLA	C1A-C2A-CAA-CBA
13	L	204	CLA	C1A-C2A-CAA-CBA
13	E	808	CLA	C1A-C2A-CAA-CBA
13	E	809	CLA	C1A-C2A-CAA-CBA
13	E	811	CLA	C1A-C2A-CAA-CBA
13	E	823	CLA	C1A-C2A-CAA-CBA
13	E	827	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	E	829	CLA	C1A-C2A-CAA-CBA
13	E	830	CLA	C1A-C2A-CAA-CBA
13	E	831	CLA	C1A-C2A-CAA-CBA
13	E	832	CLA	C1A-C2A-CAA-CBA
13	E	840	CLA	C1A-C2A-CAA-CBA
13	G	806	CLA	C1A-C2A-CAA-CBA
13	G	811	CLA	C1A-C2A-CAA-CBA
13	G	829	CLA	C1A-C2A-CAA-CBA
13	G	831	CLA	C1A-C2A-CAA-CBA
13	G	832	CLA	C1A-C2A-CAA-CBA
13	G	835	CLA	C1A-C2A-CAA-CBA
13	G	840	CLA	C1A-C2A-CAA-CBA
13	R	102	CLA	C1A-C2A-CAA-CBA
13	S	204	CLA	C1A-C2A-CAA-CBA
13	e	807	CLA	C1A-C2A-CAA-CBA
13	e	808	CLA	C1A-C2A-CAA-CBA
13	e	810	CLA	C1A-C2A-CAA-CBA
13	e	822	CLA	C1A-C2A-CAA-CBA
13	e	826	CLA	C1A-C2A-CAA-CBA
13	e	828	CLA	C1A-C2A-CAA-CBA
13	e	829	CLA	C1A-C2A-CAA-CBA
13	e	830	CLA	C1A-C2A-CAA-CBA
13	e	831	CLA	C1A-C2A-CAA-CBA
13	e	838	CLA	C1A-C2A-CAA-CBA
13	g	808	CLA	C1A-C2A-CAA-CBA
13	g	813	CLA	C1A-C2A-CAA-CBA
13	g	830	CLA	C1A-C2A-CAA-CBA
13	g	832	CLA	C1A-C2A-CAA-CBA
13	g	833	CLA	C1A-C2A-CAA-CBA
13	g	836	CLA	C1A-C2A-CAA-CBA
13	g	841	CLA	C1A-C2A-CAA-CBA
13	r	102	CLA	C1A-C2A-CAA-CBA
13	s	203	CLA	C1A-C2A-CAA-CBA
13	s	205	CLA	C1A-C2A-CAA-CBA
13	a	808	CLA	C1A-C2A-CAA-CBA
13	a	811	CLA	C1A-C2A-CAA-CBA
13	a	823	CLA	C1A-C2A-CAA-CBA
13	a	827	CLA	C1A-C2A-CAA-CBA
13	a	829	CLA	C1A-C2A-CAA-CBA
13	a	830	CLA	C1A-C2A-CAA-CBA
13	a	831	CLA	C1A-C2A-CAA-CBA
13	a	832	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	a	840	CLA	C1A-C2A-CAA-CBA
13	a	852	CLA	C1A-C2A-CAA-CBA
13	b	806	CLA	C1A-C2A-CAA-CBA
13	b	828	CLA	C1A-C2A-CAA-CBA
13	b	830	CLA	C1A-C2A-CAA-CBA
13	b	831	CLA	C1A-C2A-CAA-CBA
13	b	834	CLA	C1A-C2A-CAA-CBA
13	b	839	CLA	C1A-C2A-CAA-CBA
13	k	4002	CLA	C1A-C2A-CAA-CBA
13	l	205	CLA	C1A-C2A-CAA-CBA
15	e	851	BCR	C15-C16-C17-C18
15	a	803	BCR	C19-C20-C21-C22
15	l	202	BCR	C15-C16-C17-C18
14	B	842	PQN	C18-C20-C21-C22
14	b	841	PQN	C18-C20-C21-C22
13	B	831	CLA	CBD-CGD-O2D-CED
13	b	830	CLA	CBD-CGD-O2D-CED
14	g	843	PQN	C18-C20-C21-C22
12	A	802	LHG	O6-C4-C5-C6
14	G	842	PQN	C18-C20-C21-C22
13	g	832	CLA	CBD-CGD-O2D-CED
13	S	203	CLA	O1D-CGD-O2D-CED
13	L	203	CLA	O1D-CGD-O2D-CED
13	s	202	CLA	O1D-CGD-O2D-CED
13	l	204	CLA	O1D-CGD-O2D-CED
12	e	801	LHG	C4-C5-C6-O8
14	A	846	PQN	C12-C11-C3-C2
13	G	831	CLA	CBD-CGD-O2D-CED
13	l	203	CLA	CAA-CBA-CGA-O2A
13	e	815	CLA	O1A-CGA-O2A-C1
12	e	801	LHG	C34-C35-C36-C37
12	a	801	LHG	C26-C27-C28-C29
13	A	816	CLA	O1A-CGA-O2A-C1
13	E	816	CLA	O1A-CGA-O2A-C1
13	a	816	CLA	O1A-CGA-O2A-C1
15	L	201	BCR	C35-C13-C14-C15
13	B	805	CLA	CBA-CGA-O2A-C1
13	B	829	CLA	CBA-CGA-O2A-C1
13	G	804	CLA	CBA-CGA-O2A-C1
13	G	829	CLA	CBA-CGA-O2A-C1
13	g	806	CLA	CBA-CGA-O2A-C1
13	g	830	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	b	804	CLA	CBA-CGA-O2A-C1
13	b	828	CLA	CBA-CGA-O2A-C1
12	a	801	LHG	C17-C18-C19-C20
13	E	803	CLA	CBA-CGA-O2A-C1
12	A	801	LHG	C34-C35-C36-C37
15	B	845	BCR	C12-C13-C14-C15
15	B	847	BCR	C16-C17-C18-C19
15	J	102	BCR	C11-C10-C9-C8
15	E	852	BCR	C11-C10-C9-C8
15	G	845	BCR	C12-C13-C14-C15
15	G	847	BCR	C16-C17-C18-C19
15	g	848	BCR	C16-C17-C18-C19
15	q	102	BCR	C11-C10-C9-C8
15	a	853	BCR	C11-C10-C9-C8
15	b	846	BCR	C16-C17-C18-C19
15	f	202	BCR	C12-C13-C14-C15
12	A	802	LHG	O7-C5-C6-O8
12	e	801	LHG	C26-C27-C28-C29
14	A	846	PQN	C21-C22-C23-C25
14	B	842	PQN	C21-C22-C23-C25
14	G	842	PQN	C21-C22-C23-C25
14	g	843	PQN	C21-C22-C23-C25
14	b	841	PQN	C21-C22-C23-C25
12	A	801	LHG	C12-C13-C14-C15
14	B	842	PQN	C16-C17-C18-C19
14	G	842	PQN	C16-C17-C18-C19
14	g	843	PQN	C16-C17-C18-C19
14	b	841	PQN	C16-C17-C18-C19
15	B	848	BCR	C14-C15-C16-C17
15	G	848	BCR	C14-C15-C16-C17
15	g	849	BCR	C14-C15-C16-C17
15	b	847	BCR	C14-C15-C16-C17
12	e	802	LHG	C24-C23-O8-C6
13	A	841	CLA	CBA-CGA-O2A-C1
13	E	842	CLA	CBA-CGA-O2A-C1
13	e	840	CLA	CBA-CGA-O2A-C1
13	a	842	CLA	CBA-CGA-O2A-C1
13	A	819	CLA	C2A-CAA-CBA-CGA
13	A	827	CLA	C2A-CAA-CBA-CGA
13	E	819	CLA	C2A-CAA-CBA-CGA
13	E	827	CLA	C2A-CAA-CBA-CGA
13	e	818	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	e	826	CLA	C2A-CAA-CBA-CGA
13	a	819	CLA	C2A-CAA-CBA-CGA
13	a	827	CLA	C2A-CAA-CBA-CGA
15	l	202	BCR	C36-C18-C19-C20
15	l	202	BCR	C17-C18-C19-C20
12	e	801	LHG	C17-C18-C19-C20
13	B	829	CLA	O1A-CGA-O2A-C1
13	G	829	CLA	O1A-CGA-O2A-C1
13	g	830	CLA	O1A-CGA-O2A-C1
13	B	820	CLA	CBA-CGA-O2A-C1
13	G	820	CLA	CBA-CGA-O2A-C1
13	g	821	CLA	CBA-CGA-O2A-C1
12	A	801	LHG	C26-C27-C28-C29
12	A	802	LHG	C9-C10-C11-C12
13	B	812	CLA	C4C-C3C-CAC-CBC
13	g	813	CLA	C4C-C3C-CAC-CBC
15	F	201	BCR	C22-C23-C24-C25
15	O	201	BCR	C22-C23-C24-C25
15	S	201	BCR	C22-C23-C24-C25
15	o	201	BCR	C22-C23-C24-C25
15	f	201	BCR	C22-C23-C24-C25
13	b	828	CLA	O1A-CGA-O2A-C1
13	G	811	CLA	C4C-C3C-CAC-CBC
13	s	205	CLA	C4C-C3C-CAC-CBC
12	e	801	LHG	C12-C13-C14-C15
13	b	819	CLA	CBA-CGA-O2A-C1
12	e	802	LHG	C7-C8-C9-C10
13	G	804	CLA	O1A-CGA-O2A-C1
13	g	806	CLA	O1A-CGA-O2A-C1
12	a	801	LHG	C30-C31-C32-C33
13	A	833	CLA	CBA-CGA-O2A-C1
13	e	832	CLA	CBA-CGA-O2A-C1
13	a	833	CLA	CBA-CGA-O2A-C1
12	A	802	LHG	C11-C12-C13-C14
13	B	805	CLA	O1A-CGA-O2A-C1
13	A	824	CLA	C3A-C2A-CAA-CBA
13	A	835	CLA	C3A-C2A-CAA-CBA
13	B	812	CLA	C3A-C2A-CAA-CBA
13	B	826	CLA	C3A-C2A-CAA-CBA
13	E	824	CLA	C3A-C2A-CAA-CBA
13	E	836	CLA	C3A-C2A-CAA-CBA
13	G	811	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	G	826	CLA	C3A-C2A-CAA-CBA
13	e	823	CLA	C3A-C2A-CAA-CBA
13	e	834	CLA	C3A-C2A-CAA-CBA
13	g	813	CLA	C3A-C2A-CAA-CBA
13	g	827	CLA	C3A-C2A-CAA-CBA
13	s	205	CLA	C3A-C2A-CAA-CBA
13	a	824	CLA	C3A-C2A-CAA-CBA
13	a	836	CLA	C3A-C2A-CAA-CBA
13	b	825	CLA	C3A-C2A-CAA-CBA
15	B	844	BCR	C9-C10-C11-C12
15	I	101	BCR	C19-C20-C21-C22
15	G	844	BCR	C9-C10-C11-C12
15	P	101	BCR	C19-C20-C21-C22
15	S	201	BCR	C15-C16-C17-C18
15	g	845	BCR	C9-C10-C11-C12
15	p	101	BCR	C19-C20-C21-C22
15	b	843	BCR	C9-C10-C11-C12
15	i	101	BCR	C19-C20-C21-C22
13	b	804	CLA	O1A-CGA-O2A-C1
13	E	833	CLA	CBA-CGA-O2A-C1
14	E	848	PQN	C20-C21-C22-C23
14	a	847	PQN	C23-C25-C26-C27
12	A	801	LHG	C4-C5-C6-O8
12	A	801	LHG	C9-C10-C11-C12
13	E	803	CLA	O1A-CGA-O2A-C1
12	a	801	LHG	C16-C17-C18-C19
13	A	834	CLA	CBA-CGA-O2A-C1
13	E	834	CLA	CBA-CGA-O2A-C1
13	e	833	CLA	CBA-CGA-O2A-C1
13	a	834	CLA	CBA-CGA-O2A-C1
13	A	831	CLA	C2C-C3C-CAC-CBC
13	a	831	CLA	C2C-C3C-CAC-CBC
13	A	841	CLA	O1A-CGA-O2A-C1
13	E	842	CLA	O1A-CGA-O2A-C1
13	e	840	CLA	O1A-CGA-O2A-C1
13	a	842	CLA	O1A-CGA-O2A-C1
14	a	847	PQN	C26-C27-C28-C30
13	E	831	CLA	C2C-C3C-CAC-CBC
13	e	830	CLA	C2C-C3C-CAC-CBC
12	A	801	LHG	C17-C18-C19-C20
14	A	846	PQN	C26-C27-C28-C29
12	e	801	LHG	C9-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
12	a	801	LHG	C19-C20-C21-C22
14	e	845	PQN	C16-C17-C18-C19
13	B	812	CLA	CBD-CGD-O2D-CED
13	G	811	CLA	CBD-CGD-O2D-CED
13	s	205	CLA	CBD-CGD-O2D-CED
12	A	802	LHG	C5-C4-O6-P
12	A	802	LHG	C24-C25-C26-C27
13	A	812	CLA	C2A-CAA-CBA-CGA
13	E	812	CLA	C2A-CAA-CBA-CGA
13	e	811	CLA	C2A-CAA-CBA-CGA
13	a	812	CLA	C2A-CAA-CBA-CGA
13	g	813	CLA	CBD-CGD-O2D-CED
15	A	849	BCR	C23-C24-C25-C26
15	A	849	BCR	C23-C24-C25-C30
15	A	851	BCR	C1-C6-C7-C8
15	A	851	BCR	C5-C6-C7-C8
15	A	851	BCR	C23-C24-C25-C26
15	A	851	BCR	C23-C24-C25-C30
15	A	852	BCR	C1-C6-C7-C8
15	A	852	BCR	C5-C6-C7-C8
15	B	844	BCR	C1-C6-C7-C8
15	B	844	BCR	C5-C6-C7-C8
15	B	845	BCR	C23-C24-C25-C26
15	B	845	BCR	C23-C24-C25-C30
15	B	846	BCR	C5-C6-C7-C8
15	B	847	BCR	C5-C6-C7-C8
15	E	801	BCR	C1-C6-C7-C8
15	E	801	BCR	C23-C24-C25-C30
15	E	851	BCR	C23-C24-C25-C26
15	E	851	BCR	C23-C24-C25-C30
15	G	844	BCR	C1-C6-C7-C8
15	G	844	BCR	C5-C6-C7-C8
15	G	845	BCR	C23-C24-C25-C26
15	G	846	BCR	C5-C6-C7-C8
15	G	847	BCR	C5-C6-C7-C8
15	S	202	BCR	C1-C6-C7-C8
15	S	202	BCR	C5-C6-C7-C8
15	S	202	BCR	C23-C24-C25-C26
15	e	848	BCR	C23-C24-C25-C26
15	e	848	BCR	C23-C24-C25-C30
15	e	850	BCR	C1-C6-C7-C8
15	e	850	BCR	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	g	845	BCR	C1-C6-C7-C8
15	g	845	BCR	C5-C6-C7-C8
15	g	846	BCR	C23-C24-C25-C26
15	g	847	BCR	C5-C6-C7-C8
15	g	848	BCR	C5-C6-C7-C8
15	s	201	BCR	C1-C6-C7-C8
15	s	201	BCR	C5-C6-C7-C8
15	a	802	BCR	C23-C24-C25-C26
15	a	802	BCR	C23-C24-C25-C30
15	a	851	BCR	C23-C24-C25-C26
15	a	851	BCR	C23-C24-C25-C30
15	b	843	BCR	C1-C6-C7-C8
15	b	843	BCR	C5-C6-C7-C8
15	b	844	BCR	C23-C24-C25-C26
15	b	844	BCR	C23-C24-C25-C30
15	b	845	BCR	C5-C6-C7-C8
15	b	846	BCR	C1-C6-C7-C8
15	b	846	BCR	C5-C6-C7-C8
15	f	202	BCR	C1-C6-C7-C8
15	f	202	BCR	C5-C6-C7-C8
13	B	818	CLA	CAA-CBA-CGA-O2A
13	G	818	CLA	CAA-CBA-CGA-O2A
13	g	819	CLA	CAA-CBA-CGA-O2A
13	b	817	CLA	CAA-CBA-CGA-O2A
15	s	201	BCR	C7-C8-C9-C10
15	B	847	BCR	C14-C15-C16-C17
15	J	102	BCR	C14-C15-C16-C17
15	E	852	BCR	C14-C15-C16-C17
15	G	847	BCR	C14-C15-C16-C17
15	g	848	BCR	C14-C15-C16-C17
15	q	102	BCR	C14-C15-C16-C17
15	a	853	BCR	C14-C15-C16-C17
15	b	846	BCR	C14-C15-C16-C17
12	a	801	LHG	O6-C4-C5-C6
14	B	842	PQN	C22-C23-C25-C26
14	G	842	PQN	C22-C23-C25-C26
14	g	843	PQN	C22-C23-C25-C26
14	b	841	PQN	C22-C23-C25-C26
15	B	847	BCR	C13-C14-C15-C16
15	J	101	BCR	C15-C16-C17-C18
15	E	801	BCR	C15-C16-C17-C18
15	G	847	BCR	C13-C14-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	Q	101	BCR	C15-C16-C17-C18
15	T	101	BCR	C13-C14-C15-C16
15	g	848	BCR	C13-C14-C15-C16
15	q	101	BCR	C15-C16-C17-C18
15	a	803	BCR	C15-C16-C17-C18
15	b	846	BCR	C13-C14-C15-C16
15	j	101	BCR	C15-C16-C17-C18
15	l	206	BCR	C13-C14-C15-C16
13	K	101	CLA	C2A-CAA-CBA-CGA
13	K	102	CLA	C2A-CAA-CBA-CGA
13	R	102	CLA	C2A-CAA-CBA-CGA
13	r	102	CLA	C2A-CAA-CBA-CGA
13	k	4002	CLA	C2A-CAA-CBA-CGA
12	a	801	LHG	C27-C28-C29-C30
15	A	852	BCR	C20-C21-C22-C37
15	B	844	BCR	C16-C17-C18-C36
15	B	846	BCR	C11-C10-C9-C34
15	B	848	BCR	C35-C13-C14-C15
15	I	101	BCR	C35-C13-C14-C15
15	G	844	BCR	C16-C17-C18-C36
15	G	846	BCR	C11-C10-C9-C34
15	G	848	BCR	C35-C13-C14-C15
15	P	101	BCR	C35-C13-C14-C15
15	g	845	BCR	C16-C17-C18-C36
15	g	847	BCR	C11-C10-C9-C34
15	g	849	BCR	C35-C13-C14-C15
15	p	101	BCR	C35-C13-C14-C15
15	b	843	BCR	C16-C17-C18-C36
15	b	845	BCR	C11-C10-C9-C34
15	b	847	BCR	C35-C13-C14-C15
15	i	101	BCR	C35-C13-C14-C15
15	l	202	BCR	C11-C10-C9-C34
13	E	839	CLA	CBD-CGD-O2D-CED
13	B	808	CLA	CBA-CGA-O2A-C1
13	G	807	CLA	CBA-CGA-O2A-C1
13	g	809	CLA	CBA-CGA-O2A-C1
13	b	807	CLA	CBA-CGA-O2A-C1
12	A	801	LHG	C11-C10-C9-C8
13	A	838	CLA	CBD-CGD-O2D-CED
13	e	837	CLA	CBD-CGD-O2D-CED
13	A	804	CLA	CAD-CBD-CGD-O2D
13	A	816	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	818	CLA	CAD-CBD-CGD-O2D
13	A	823	CLA	CAD-CBD-CGD-O2D
13	A	824	CLA	CAD-CBD-CGD-O2D
13	A	841	CLA	CAD-CBD-CGD-O2D
13	A	844	CLA	CAD-CBD-CGD-O2D
13	B	825	CLA	CAD-CBD-CGD-O2D
13	B	837	CLA	CAD-CBD-CGD-O2D
13	K	102	CLA	CAD-CBD-CGD-O2D
13	E	804	CLA	CAD-CBD-CGD-O2D
13	E	816	CLA	CAD-CBD-CGD-O2D
13	E	818	CLA	CAD-CBD-CGD-O2D
13	E	823	CLA	CAD-CBD-CGD-O2D
13	E	824	CLA	CAD-CBD-CGD-O2D
13	E	842	CLA	CAD-CBD-CGD-O2D
13	E	845	CLA	CAD-CBD-CGD-O2D
13	G	825	CLA	CAD-CBD-CGD-O2D
13	G	837	CLA	CAD-CBD-CGD-O2D
13	R	102	CLA	CAD-CBD-CGD-O2D
13	e	804	CLA	CAD-CBD-CGD-O2D
13	e	815	CLA	CAD-CBD-CGD-O2D
13	e	817	CLA	CAD-CBD-CGD-O2D
13	e	822	CLA	CAD-CBD-CGD-O2D
13	e	823	CLA	CAD-CBD-CGD-O2D
13	e	840	CLA	CAD-CBD-CGD-O2D
13	e	843	CLA	CAD-CBD-CGD-O2D
13	g	826	CLA	CAD-CBD-CGD-O2D
13	g	838	CLA	CAD-CBD-CGD-O2D
13	r	102	CLA	CAD-CBD-CGD-O2D
13	a	804	CLA	CAD-CBD-CGD-O2D
13	a	816	CLA	CAD-CBD-CGD-O2D
13	a	818	CLA	CAD-CBD-CGD-O2D
13	a	823	CLA	CAD-CBD-CGD-O2D
13	a	824	CLA	CAD-CBD-CGD-O2D
13	a	842	CLA	CAD-CBD-CGD-O2D
13	a	845	CLA	CAD-CBD-CGD-O2D
13	b	824	CLA	CAD-CBD-CGD-O2D
13	b	836	CLA	CAD-CBD-CGD-O2D
13	k	4002	CLA	CAD-CBD-CGD-O2D
15	I	101	BCR	C22-C23-C24-C25
15	P	101	BCR	C22-C23-C24-C25
15	p	101	BCR	C22-C23-C24-C25
15	i	101	BCR	C22-C23-C24-C25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	a	839	CLA	CBD-CGD-O2D-CED
12	e	801	LHG	C28-C29-C30-C31
13	G	834	CLA	C2C-C3C-CAC-CBC
13	A	834	CLA	O1A-CGA-O2A-C1
13	B	808	CLA	O1A-CGA-O2A-C1
13	E	834	CLA	O1A-CGA-O2A-C1
13	G	807	CLA	O1A-CGA-O2A-C1
13	e	833	CLA	O1A-CGA-O2A-C1
13	g	809	CLA	O1A-CGA-O2A-C1
13	a	834	CLA	O1A-CGA-O2A-C1
13	b	807	CLA	O1A-CGA-O2A-C1
12	A	801	LHG	O6-C4-C5-O7
12	A	802	LHG	O6-C4-C5-O7
12	e	801	LHG	O6-C4-C5-O7
13	B	804	CLA	CAA-CBA-CGA-O2A
13	G	803	CLA	CAA-CBA-CGA-O2A
13	g	805	CLA	CAA-CBA-CGA-O2A
13	b	803	CLA	CAA-CBA-CGA-O2A
13	g	835	CLA	C2C-C3C-CAC-CBC
13	A	825	CLA	C2A-CAA-CBA-CGA
13	A	840	CLA	C2A-CAA-CBA-CGA
13	E	825	CLA	C2A-CAA-CBA-CGA
13	E	841	CLA	C2A-CAA-CBA-CGA
13	e	824	CLA	C2A-CAA-CBA-CGA
13	e	839	CLA	C2A-CAA-CBA-CGA
13	r	101	CLA	C2A-CAA-CBA-CGA
13	a	825	CLA	C2A-CAA-CBA-CGA
13	a	841	CLA	C2A-CAA-CBA-CGA
12	e	801	LHG	C11-C10-C9-C8
13	B	834	CLA	C2C-C3C-CAC-CBC
13	A	803	CLA	CHA-CBD-CGD-O1D
13	A	803	CLA	CHA-CBD-CGD-O2D
13	A	806	CLA	CHA-CBD-CGD-O1D
13	A	806	CLA	CHA-CBD-CGD-O2D
13	A	810	CLA	CHA-CBD-CGD-O1D
13	A	810	CLA	CHA-CBD-CGD-O2D
13	A	827	CLA	CHA-CBD-CGD-O1D
13	A	833	CLA	CHA-CBD-CGD-O1D
13	A	833	CLA	CHA-CBD-CGD-O2D
13	A	836	CLA	CHA-CBD-CGD-O1D
13	A	836	CLA	CHA-CBD-CGD-O2D
13	A	838	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	840	CLA	CHA-CBD-CGD-O2D
13	A	843	CLA	CHA-CBD-CGD-O1D
13	A	843	CLA	CHA-CBD-CGD-O2D
13	B	814	CLA	CHA-CBD-CGD-O1D
13	B	819	CLA	CHA-CBD-CGD-O1D
13	B	819	CLA	CHA-CBD-CGD-O2D
13	B	824	CLA	CHA-CBD-CGD-O1D
13	B	824	CLA	CHA-CBD-CGD-O2D
13	B	831	CLA	CHA-CBD-CGD-O1D
13	B	831	CLA	CHA-CBD-CGD-O2D
13	B	832	CLA	CHA-CBD-CGD-O1D
13	B	832	CLA	CHA-CBD-CGD-O2D
13	E	806	CLA	CHA-CBD-CGD-O1D
13	E	806	CLA	CHA-CBD-CGD-O2D
13	E	810	CLA	CHA-CBD-CGD-O1D
13	E	810	CLA	CHA-CBD-CGD-O2D
13	E	827	CLA	CHA-CBD-CGD-O1D
13	E	833	CLA	CHA-CBD-CGD-O1D
13	E	833	CLA	CHA-CBD-CGD-O2D
13	E	837	CLA	CHA-CBD-CGD-O1D
13	E	837	CLA	CHA-CBD-CGD-O2D
13	E	839	CLA	CHA-CBD-CGD-O1D
13	E	841	CLA	CHA-CBD-CGD-O2D
13	E	844	CLA	CHA-CBD-CGD-O1D
13	E	844	CLA	CHA-CBD-CGD-O2D
13	G	814	CLA	CHA-CBD-CGD-O1D
13	G	819	CLA	CHA-CBD-CGD-O1D
13	G	819	CLA	CHA-CBD-CGD-O2D
13	G	824	CLA	CHA-CBD-CGD-O1D
13	G	824	CLA	CHA-CBD-CGD-O2D
13	G	831	CLA	CHA-CBD-CGD-O1D
13	G	831	CLA	CHA-CBD-CGD-O2D
13	G	832	CLA	CHA-CBD-CGD-O1D
13	G	832	CLA	CHA-CBD-CGD-O2D
13	e	803	CLA	CHA-CBD-CGD-O1D
13	e	803	CLA	CHA-CBD-CGD-O2D
13	e	805	CLA	CHA-CBD-CGD-O1D
13	e	805	CLA	CHA-CBD-CGD-O2D
13	e	809	CLA	CHA-CBD-CGD-O1D
13	e	809	CLA	CHA-CBD-CGD-O2D
13	e	826	CLA	CHA-CBD-CGD-O1D
13	e	832	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	e	832	CLA	CHA-CBD-CGD-O2D
13	e	835	CLA	CHA-CBD-CGD-O1D
13	e	835	CLA	CHA-CBD-CGD-O2D
13	e	837	CLA	CHA-CBD-CGD-O1D
13	e	839	CLA	CHA-CBD-CGD-O2D
13	e	842	CLA	CHA-CBD-CGD-O1D
13	e	842	CLA	CHA-CBD-CGD-O2D
13	g	815	CLA	CHA-CBD-CGD-O1D
13	g	820	CLA	CHA-CBD-CGD-O1D
13	g	820	CLA	CHA-CBD-CGD-O2D
13	g	825	CLA	CHA-CBD-CGD-O1D
13	g	825	CLA	CHA-CBD-CGD-O2D
13	g	832	CLA	CHA-CBD-CGD-O1D
13	g	832	CLA	CHA-CBD-CGD-O2D
13	g	833	CLA	CHA-CBD-CGD-O1D
13	g	833	CLA	CHA-CBD-CGD-O2D
13	a	806	CLA	CHA-CBD-CGD-O1D
13	a	806	CLA	CHA-CBD-CGD-O2D
13	a	810	CLA	CHA-CBD-CGD-O1D
13	a	810	CLA	CHA-CBD-CGD-O2D
13	a	827	CLA	CHA-CBD-CGD-O1D
13	a	833	CLA	CHA-CBD-CGD-O1D
13	a	833	CLA	CHA-CBD-CGD-O2D
13	a	837	CLA	CHA-CBD-CGD-O1D
13	a	837	CLA	CHA-CBD-CGD-O2D
13	a	839	CLA	CHA-CBD-CGD-O1D
13	a	841	CLA	CHA-CBD-CGD-O2D
13	a	844	CLA	CHA-CBD-CGD-O1D
13	a	844	CLA	CHA-CBD-CGD-O2D
13	a	852	CLA	CHA-CBD-CGD-O1D
13	a	852	CLA	CHA-CBD-CGD-O2D
13	b	813	CLA	CHA-CBD-CGD-O1D
13	b	818	CLA	CHA-CBD-CGD-O1D
13	b	818	CLA	CHA-CBD-CGD-O2D
13	b	823	CLA	CHA-CBD-CGD-O1D
13	b	823	CLA	CHA-CBD-CGD-O2D
13	b	830	CLA	CHA-CBD-CGD-O1D
13	b	830	CLA	CHA-CBD-CGD-O2D
13	b	831	CLA	CHA-CBD-CGD-O1D
13	b	831	CLA	CHA-CBD-CGD-O2D
13	B	820	CLA	O1A-CGA-O2A-C1
13	E	833	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	G	820	CLA	O1A-CGA-O2A-C1
13	e	832	CLA	O1A-CGA-O2A-C1
13	g	821	CLA	O1A-CGA-O2A-C1
13	a	833	CLA	O1A-CGA-O2A-C1
13	b	819	CLA	O1A-CGA-O2A-C1
12	a	801	LHG	C24-C25-C26-C27
15	B	844	BCR	C16-C17-C18-C19
15	B	846	BCR	C20-C21-C22-C23
15	B	847	BCR	C20-C21-C22-C23
15	E	801	BCR	C12-C13-C14-C15
15	G	844	BCR	C16-C17-C18-C19
15	G	846	BCR	C20-C21-C22-C23
15	G	847	BCR	C20-C21-C22-C23
15	R	101	BCR	C11-C10-C9-C8
15	g	845	BCR	C16-C17-C18-C19
15	g	847	BCR	C20-C21-C22-C23
15	g	848	BCR	C20-C21-C22-C23
15	a	802	BCR	C11-C10-C9-C8
15	b	843	BCR	C16-C17-C18-C19
15	b	845	BCR	C20-C21-C22-C23
15	b	846	BCR	C20-C21-C22-C23
12	A	801	LHG	C35-C36-C37-C38
12	e	801	LHG	C35-C36-C37-C38
13	b	833	CLA	C2C-C3C-CAC-CBC
13	A	833	CLA	O1A-CGA-O2A-C1
12	A	802	LHG	O1-C1-C2-O2
12	A	801	LHG	C28-C29-C30-C31
13	A	813	CLA	C2A-CAA-CBA-CGA
13	e	812	CLA	C2A-CAA-CBA-CGA
13	a	813	CLA	C2A-CAA-CBA-CGA
15	L	201	BCR	C11-C12-C13-C35
15	e	849	BCR	C36-C18-C19-C20
15	s	201	BCR	C37-C22-C23-C24
15	l	206	BCR	C36-C18-C19-C20
15	A	850	BCR	C11-C12-C13-C14
15	L	205	BCR	C11-C12-C13-C14
15	S	202	BCR	C7-C8-C9-C10
15	e	849	BCR	C11-C12-C13-C14
15	s	204	BCR	C11-C12-C13-C14
13	A	824	CLA	C1A-C2A-CAA-CBA
13	B	802	CLA	C1A-C2A-CAA-CBA
13	B	828	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	E	824	CLA	C1A-C2A-CAA-CBA
13	G	801	CLA	C1A-C2A-CAA-CBA
13	G	812	CLA	C1A-C2A-CAA-CBA
13	G	828	CLA	C1A-C2A-CAA-CBA
13	S	206	CLA	C1A-C2A-CAA-CBA
13	e	823	CLA	C1A-C2A-CAA-CBA
13	g	803	CLA	C1A-C2A-CAA-CBA
13	g	829	CLA	C1A-C2A-CAA-CBA
13	a	824	CLA	C1A-C2A-CAA-CBA
13	b	801	CLA	C1A-C2A-CAA-CBA
13	b	811	CLA	C1A-C2A-CAA-CBA
13	b	827	CLA	C1A-C2A-CAA-CBA
13	l	201	CLA	C1A-C2A-CAA-CBA
13	A	804	CLA	CBA-CGA-O2A-C1
13	a	804	CLA	CBA-CGA-O2A-C1
15	J	101	BCR	C9-C10-C11-C12
15	Q	101	BCR	C9-C10-C11-C12
15	q	101	BCR	C9-C10-C11-C12
15	f	202	BCR	C15-C16-C17-C18
15	j	101	BCR	C9-C10-C11-C12
13	G	811	CLA	O1D-CGD-O2D-CED
13	s	205	CLA	O1D-CGD-O2D-CED
13	B	812	CLA	O1D-CGD-O2D-CED
13	g	813	CLA	O1D-CGD-O2D-CED
13	e	843	CLA	CBD-CGD-O2D-CED
13	a	845	CLA	CBD-CGD-O2D-CED
13	b	830	CLA	O1D-CGD-O2D-CED
13	A	819	CLA	O2A-C1-C2-C3
13	E	819	CLA	O2A-C1-C2-C3
13	e	818	CLA	O2A-C1-C2-C3
13	a	819	CLA	O2A-C1-C2-C3
13	E	804	CLA	CBA-CGA-O2A-C1
13	e	804	CLA	CBA-CGA-O2A-C1
13	A	844	CLA	CBD-CGD-O2D-CED
13	E	845	CLA	CBD-CGD-O2D-CED
12	A	801	LHG	O6-C4-C5-C6
12	e	801	LHG	O6-C4-C5-C6
12	e	802	LHG	C18-C19-C20-C21
13	E	813	CLA	C2A-CAA-CBA-CGA
13	B	831	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	CAD-CBD-CGD-O1D
13	A	810	CLA	CAD-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	829	CLA	CAD-CBD-CGD-O1D
13	A	831	CLA	CAD-CBD-CGD-O1D
13	A	836	CLA	CAD-CBD-CGD-O1D
13	A	840	CLA	CAD-CBD-CGD-O1D
13	B	819	CLA	CAD-CBD-CGD-O1D
13	B	831	CLA	CAD-CBD-CGD-O1D
13	E	806	CLA	CAD-CBD-CGD-O1D
13	E	810	CLA	CAD-CBD-CGD-O1D
13	E	829	CLA	CAD-CBD-CGD-O1D
13	E	831	CLA	CAD-CBD-CGD-O1D
13	E	837	CLA	CAD-CBD-CGD-O1D
13	E	841	CLA	CAD-CBD-CGD-O1D
13	G	819	CLA	CAD-CBD-CGD-O1D
13	G	831	CLA	CAD-CBD-CGD-O1D
13	e	805	CLA	CAD-CBD-CGD-O1D
13	e	809	CLA	CAD-CBD-CGD-O1D
13	e	828	CLA	CAD-CBD-CGD-O1D
13	e	830	CLA	CAD-CBD-CGD-O1D
13	e	835	CLA	CAD-CBD-CGD-O1D
13	e	839	CLA	CAD-CBD-CGD-O1D
13	g	820	CLA	CAD-CBD-CGD-O1D
13	g	832	CLA	CAD-CBD-CGD-O1D
13	a	806	CLA	CAD-CBD-CGD-O1D
13	a	810	CLA	CAD-CBD-CGD-O1D
13	a	829	CLA	CAD-CBD-CGD-O1D
13	a	831	CLA	CAD-CBD-CGD-O1D
13	a	837	CLA	CAD-CBD-CGD-O1D
13	a	841	CLA	CAD-CBD-CGD-O1D
13	b	818	CLA	CAD-CBD-CGD-O1D
13	b	830	CLA	CAD-CBD-CGD-O1D
13	G	831	CLA	O1D-CGD-O2D-CED
13	L	202	CLA	CAA-CBA-CGA-O2A
13	g	832	CLA	O1D-CGD-O2D-CED
12	a	801	LHG	C10-C11-C12-C13
12	a	801	LHG	O6-C4-C5-O7
14	a	847	PQN	C17-C18-C20-C21
12	e	802	LHG	C13-C14-C15-C16
15	s	201	BCR	C15-C16-C17-C18
13	e	837	CLA	O1D-CGD-O2D-CED
12	a	801	LHG	C4-C5-C6-O8
13	E	804	CLA	O1A-CGA-O2A-C1
13	a	804	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	e	803	CLA	CAA-CBA-CGA-O2A
13	A	838	CLA	O1D-CGD-O2D-CED
13	a	839	CLA	O1D-CGD-O2D-CED
13	A	804	CLA	O1A-CGA-O2A-C1
13	e	804	CLA	O1A-CGA-O2A-C1
13	E	839	CLA	O1D-CGD-O2D-CED
13	B	829	CLA	CAA-CBA-CGA-O2A
13	G	829	CLA	CAA-CBA-CGA-O2A
13	g	830	CLA	CAA-CBA-CGA-O2A
13	b	828	CLA	CAA-CBA-CGA-O2A
14	A	846	PQN	C16-C17-C18-C19
14	B	842	PQN	C24-C23-C25-C26
14	G	842	PQN	C24-C23-C25-C26
14	g	843	PQN	C24-C23-C25-C26
14	b	841	PQN	C24-C23-C25-C26
15	a	848	BCR	C6-C7-C8-C9
15	S	205	BCR	C13-C14-C15-C16
13	A	803	CLA	CAA-CBA-CGA-O2A
13	A	825	CLA	C1-C2-C3-C4
13	B	832	CLA	C1-C2-C3-C4
13	E	825	CLA	C1-C2-C3-C4
13	G	832	CLA	C1-C2-C3-C4
13	e	824	CLA	C1-C2-C3-C4
13	g	833	CLA	C1-C2-C3-C4
13	a	825	CLA	C1-C2-C3-C4
13	b	831	CLA	C1-C2-C3-C4
13	B	809	CLA	C2A-CAA-CBA-CGA
13	B	812	CLA	C2A-CAA-CBA-CGA
13	B	831	CLA	C2A-CAA-CBA-CGA
13	G	808	CLA	C2A-CAA-CBA-CGA
13	G	811	CLA	C2A-CAA-CBA-CGA
13	G	831	CLA	C2A-CAA-CBA-CGA
13	g	810	CLA	C2A-CAA-CBA-CGA
13	g	813	CLA	C2A-CAA-CBA-CGA
13	g	832	CLA	C2A-CAA-CBA-CGA
13	s	205	CLA	C2A-CAA-CBA-CGA
13	b	808	CLA	C2A-CAA-CBA-CGA
13	b	830	CLA	C2A-CAA-CBA-CGA
13	A	805	CLA	C2-C1-O2A-CGA
13	A	812	CLA	C2-C1-O2A-CGA
13	A	834	CLA	C2-C1-O2A-CGA
13	E	805	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	E	812	CLA	C2-C1-O2A-CGA
13	E	834	CLA	C2-C1-O2A-CGA
13	e	811	CLA	C2-C1-O2A-CGA
13	e	833	CLA	C2-C1-O2A-CGA
13	g	801	CLA	C2-C1-O2A-CGA
13	a	805	CLA	C2-C1-O2A-CGA
13	a	812	CLA	C2-C1-O2A-CGA
13	a	834	CLA	C2-C1-O2A-CGA
13	G	830	CLA	CAA-CBA-CGA-O2A
13	g	831	CLA	CAA-CBA-CGA-O2A
13	b	829	CLA	CAA-CBA-CGA-O2A
12	e	801	LHG	C29-C30-C31-C32
13	B	830	CLA	CAA-CBA-CGA-O2A
13	E	804	CLA	CAA-CBA-CGA-O2A
13	e	804	CLA	CAA-CBA-CGA-O2A
13	a	804	CLA	CAA-CBA-CGA-O2A
15	A	848	BCR	C23-C24-C25-C30
15	B	846	BCR	C1-C6-C7-C8
15	B	846	BCR	C23-C24-C25-C26
15	B	846	BCR	C23-C24-C25-C30
15	J	101	BCR	C1-C6-C7-C8
15	J	101	BCR	C5-C6-C7-C8
15	L	201	BCR	C1-C6-C7-C8
15	L	201	BCR	C5-C6-C7-C8
15	E	801	BCR	C5-C6-C7-C8
15	E	801	BCR	C23-C24-C25-C26
15	E	850	BCR	C23-C24-C25-C30
15	G	845	BCR	C23-C24-C25-C30
15	G	846	BCR	C1-C6-C7-C8
15	G	846	BCR	C23-C24-C25-C26
15	G	846	BCR	C23-C24-C25-C30
15	Q	101	BCR	C1-C6-C7-C8
15	Q	101	BCR	C5-C6-C7-C8
15	S	202	BCR	C23-C24-C25-C30
15	T	101	BCR	C1-C6-C7-C8
15	T	101	BCR	C5-C6-C7-C8
15	T	101	BCR	C23-C24-C25-C26
15	T	101	BCR	C23-C24-C25-C30
15	e	847	BCR	C23-C24-C25-C30
15	e	850	BCR	C23-C24-C25-C30
15	g	846	BCR	C23-C24-C25-C30
15	g	847	BCR	C1-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	g	847	BCR	C23-C24-C25-C26
15	g	847	BCR	C23-C24-C25-C30
15	q	101	BCR	C1-C6-C7-C8
15	q	101	BCR	C5-C6-C7-C8
15	a	802	BCR	C1-C6-C7-C8
15	a	802	BCR	C5-C6-C7-C8
15	a	850	BCR	C23-C24-C25-C30
15	b	845	BCR	C1-C6-C7-C8
15	b	845	BCR	C23-C24-C25-C26
15	b	845	BCR	C23-C24-C25-C30
15	j	101	BCR	C1-C6-C7-C8
15	j	101	BCR	C5-C6-C7-C8
13	A	804	CLA	CAA-CBA-CGA-O2A
12	A	802	LHG	C10-C11-C12-C13
12	e	802	LHG	C24-C25-C26-C27
13	a	845	CLA	O1D-CGD-O2D-CED
15	A	847	BCR	C12-C13-C14-C15
15	E	801	BCR	C11-C10-C9-C8
15	E	849	BCR	C12-C13-C14-C15
15	R	101	BCR	C20-C21-C22-C23
15	e	846	BCR	C12-C13-C14-C15
15	a	849	BCR	C12-C13-C14-C15
13	e	843	CLA	O1D-CGD-O2D-CED
13	A	844	CLA	O1D-CGD-O2D-CED
12	A	802	LHG	C4-C5-C6-O8
13	E	845	CLA	O1D-CGD-O2D-CED
14	B	842	PQN	C16-C17-C18-C20
14	G	842	PQN	C16-C17-C18-C20
14	g	843	PQN	C16-C17-C18-C20
14	b	841	PQN	C16-C17-C18-C20
14	B	842	PQN	C21-C22-C23-C24
14	G	842	PQN	C21-C22-C23-C24
14	g	843	PQN	C21-C22-C23-C24
14	b	841	PQN	C21-C22-C23-C24
12	A	802	LHG	C18-C19-C20-C21
12	A	801	LHG	C29-C30-C31-C32
14	A	846	PQN	C23-C25-C26-C27
13	L	203	CLA	CAA-CBA-CGA-O2A
13	S	203	CLA	CAA-CBA-CGA-O2A
13	s	202	CLA	CAA-CBA-CGA-O2A
13	l	204	CLA	CAA-CBA-CGA-O2A
13	A	806	CLA	C2C-C3C-CAC-CBC

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	e	805	CLA	C2C-C3C-CAC-CBC
15	E	801	BCR	C19-C20-C21-C22
15	E	802	BCR	C15-C16-C17-C18
13	E	806	CLA	C2C-C3C-CAC-CBC
13	a	806	CLA	C2C-C3C-CAC-CBC
15	T	101	BCR	C18-C19-C20-C21
13	l	203	CLA	CAA-CBA-CGA-O1A
13	E	827	CLA	CBD-CGD-O2D-CED
13	A	815	CLA	C2-C1-O2A-CGA
13	B	828	CLA	C2-C1-O2A-CGA
13	E	815	CLA	C2-C1-O2A-CGA
13	G	828	CLA	C2-C1-O2A-CGA
13	e	814	CLA	C2-C1-O2A-CGA
13	g	829	CLA	C2-C1-O2A-CGA
13	a	815	CLA	C2-C1-O2A-CGA
13	b	827	CLA	C2-C1-O2A-CGA
14	a	847	PQN	C26-C27-C28-C29
13	e	826	CLA	CBD-CGD-O2D-CED
12	A	802	LHG	C11-C10-C9-C8
13	A	826	CLA	C2A-CAA-CBA-CGA
13	A	841	CLA	C2A-CAA-CBA-CGA
13	B	838	CLA	C2A-CAA-CBA-CGA
13	E	826	CLA	C2A-CAA-CBA-CGA
13	E	842	CLA	C2A-CAA-CBA-CGA
13	G	838	CLA	C2A-CAA-CBA-CGA
13	e	825	CLA	C2A-CAA-CBA-CGA
13	e	840	CLA	C2A-CAA-CBA-CGA
13	g	839	CLA	C2A-CAA-CBA-CGA
13	a	826	CLA	C2A-CAA-CBA-CGA
13	a	842	CLA	C2A-CAA-CBA-CGA
13	b	837	CLA	C2A-CAA-CBA-CGA
13	a	827	CLA	CBD-CGD-O2D-CED
13	B	810	CLA	C3A-C2A-CAA-CBA
13	G	809	CLA	C3A-C2A-CAA-CBA
13	g	811	CLA	C3A-C2A-CAA-CBA
13	b	809	CLA	C3A-C2A-CAA-CBA
13	A	827	CLA	CBD-CGD-O2D-CED
15	m	101	BCR	C9-C10-C11-C12
15	R	101	BCR	C11-C10-C9-C34
15	s	201	BCR	C16-C17-C18-C36
15	k	4001	BCR	C11-C10-C9-C34
13	R	102	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	r	102	CLA	CAA-CBA-CGA-O1A
13	A	839	CLA	C2A-CAA-CBA-CGA
13	E	840	CLA	C2A-CAA-CBA-CGA
13	e	838	CLA	C2A-CAA-CBA-CGA
13	a	840	CLA	C2A-CAA-CBA-CGA
13	K	102	CLA	CAA-CBA-CGA-O1A
13	k	4002	CLA	CAA-CBA-CGA-O1A
15	k	4001	BCR	C36-C18-C19-C20
13	B	841	CLA	C1A-C2A-CAA-CBA
13	G	841	CLA	C1A-C2A-CAA-CBA
13	g	842	CLA	C1A-C2A-CAA-CBA
13	b	840	CLA	C1A-C2A-CAA-CBA
15	B	845	BCR	C13-C14-C15-C16
15	E	802	BCR	C9-C10-C11-C12
15	G	845	BCR	C13-C14-C15-C16
15	g	846	BCR	C13-C14-C15-C16
15	b	844	BCR	C13-C14-C15-C16
13	B	829	CLA	C2A-CAA-CBA-CGA
13	L	203	CLA	C2A-CAA-CBA-CGA
13	G	829	CLA	C2A-CAA-CBA-CGA
13	S	203	CLA	C2A-CAA-CBA-CGA
13	g	830	CLA	C2A-CAA-CBA-CGA
13	s	202	CLA	C2A-CAA-CBA-CGA
13	b	828	CLA	C2A-CAA-CBA-CGA
13	l	204	CLA	C2A-CAA-CBA-CGA
13	E	803	CLA	CAA-CBA-CGA-O2A
13	S	203	CLA	CAA-CBA-CGA-O1A
13	s	202	CLA	CAA-CBA-CGA-O1A
13	l	204	CLA	CAA-CBA-CGA-O1A
13	L	203	CLA	CAA-CBA-CGA-O1A
15	B	844	BCR	C20-C21-C22-C23
15	G	844	BCR	C20-C21-C22-C23
15	g	845	BCR	C20-C21-C22-C23
15	b	843	BCR	C20-C21-C22-C23
13	A	836	CLA	CBA-CGA-O2A-C1
13	E	837	CLA	CBA-CGA-O2A-C1
13	e	835	CLA	CBA-CGA-O2A-C1
13	a	837	CLA	CBA-CGA-O2A-C1
12	a	801	LHG	C29-C30-C31-C32
15	A	849	BCR	C19-C20-C21-C22
15	L	201	BCR	C15-C16-C17-C18
15	E	851	BCR	C19-C20-C21-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	O	202	BCR	C15-C16-C17-C18
15	R	101	BCR	C9-C10-C11-C12
15	e	848	BCR	C19-C20-C21-C22
15	a	851	BCR	C19-C20-C21-C22
15	L	205	BCR	C22-C23-C24-C25
13	K	102	CLA	CAA-CBA-CGA-O2A
13	R	102	CLA	CAA-CBA-CGA-O2A
13	r	102	CLA	CAA-CBA-CGA-O2A
13	k	4002	CLA	CAA-CBA-CGA-O2A
13	A	827	CLA	O1D-CGD-O2D-CED
12	e	802	LHG	C8-C7-O7-C5
13	L	204	CLA	C2A-CAA-CBA-CGA
13	S	204	CLA	C2A-CAA-CBA-CGA
13	s	203	CLA	C2A-CAA-CBA-CGA
13	l	203	CLA	C2A-CAA-CBA-CGA
13	l	205	CLA	C2A-CAA-CBA-CGA
13	A	836	CLA	O1A-CGA-O2A-C1
13	E	837	CLA	O1A-CGA-O2A-C1
13	e	835	CLA	O1A-CGA-O2A-C1
13	a	837	CLA	O1A-CGA-O2A-C1
15	A	847	BCR	C1-C6-C7-C8
15	A	848	BCR	C1-C6-C7-C8
15	A	848	BCR	C23-C24-C25-C26
15	A	849	BCR	C1-C6-C7-C8
15	A	849	BCR	C5-C6-C7-C8
15	B	843	BCR	C1-C6-C7-C8
15	B	843	BCR	C5-C6-C7-C8
15	B	844	BCR	C23-C24-C25-C30
15	F	201	BCR	C1-C6-C7-C8
15	F	201	BCR	C23-C24-C25-C30
15	I	101	BCR	C1-C6-C7-C8
15	I	101	BCR	C5-C6-C7-C8
15	J	101	BCR	C23-C24-C25-C30
15	E	849	BCR	C1-C6-C7-C8
15	E	850	BCR	C1-C6-C7-C8
15	E	850	BCR	C23-C24-C25-C26
15	E	851	BCR	C1-C6-C7-C8
15	E	851	BCR	C5-C6-C7-C8
15	G	843	BCR	C1-C6-C7-C8
15	G	843	BCR	C5-C6-C7-C8
15	G	844	BCR	C23-C24-C25-C30
15	O	201	BCR	C1-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	O	201	BCR	C23-C24-C25-C26
15	O	201	BCR	C23-C24-C25-C30
15	O	202	BCR	C1-C6-C7-C8
15	P	101	BCR	C1-C6-C7-C8
15	P	101	BCR	C5-C6-C7-C8
15	Q	101	BCR	C23-C24-C25-C30
15	S	201	BCR	C1-C6-C7-C8
15	S	201	BCR	C23-C24-C25-C30
15	e	846	BCR	C1-C6-C7-C8
15	e	847	BCR	C1-C6-C7-C8
15	e	847	BCR	C23-C24-C25-C26
15	e	848	BCR	C1-C6-C7-C8
15	e	850	BCR	C23-C24-C25-C26
15	g	844	BCR	C1-C6-C7-C8
15	g	844	BCR	C5-C6-C7-C8
15	g	845	BCR	C23-C24-C25-C30
15	o	201	BCR	C1-C6-C7-C8
15	o	201	BCR	C23-C24-C25-C26
15	o	201	BCR	C23-C24-C25-C30
15	p	101	BCR	C1-C6-C7-C8
15	p	101	BCR	C5-C6-C7-C8
15	q	101	BCR	C23-C24-C25-C30
15	a	849	BCR	C1-C6-C7-C8
15	a	850	BCR	C1-C6-C7-C8
15	a	850	BCR	C23-C24-C25-C26
15	a	851	BCR	C1-C6-C7-C8
15	a	851	BCR	C5-C6-C7-C8
15	b	842	BCR	C1-C6-C7-C8
15	b	842	BCR	C5-C6-C7-C8
15	b	843	BCR	C23-C24-C25-C30
15	f	201	BCR	C1-C6-C7-C8
15	f	201	BCR	C23-C24-C25-C26
15	f	201	BCR	C23-C24-C25-C30
15	i	101	BCR	C1-C6-C7-C8
15	i	101	BCR	C5-C6-C7-C8
15	j	101	BCR	C23-C24-C25-C30
15	l	202	BCR	C1-C6-C7-C8
15	l	202	BCR	C5-C6-C7-C8
15	m	101	BCR	C1-C6-C7-C8
14	e	845	PQN	C15-C16-C17-C18
13	E	827	CLA	O1D-CGD-O2D-CED
13	a	827	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	S	205	BCR	C19-C20-C21-C22
15	a	802	BCR	C15-C16-C17-C18
15	a	802	BCR	C19-C20-C21-C22
15	E	801	BCR	C14-C15-C16-C17
13	e	826	CLA	O1D-CGD-O2D-CED
13	S	204	CLA	CAA-CBA-CGA-O2A
13	K	101	CLA	CAA-CBA-CGA-O2A
13	r	101	CLA	CAA-CBA-CGA-O2A
13	f	203	CLA	CAA-CBA-CGA-O2A
13	E	846	CLA	CAA-CBA-CGA-O2A
14	E	848	PQN	C13-C15-C16-C17
13	B	834	CLA	C4C-C3C-CAC-CBC
13	g	835	CLA	C4C-C3C-CAC-CBC
15	B	847	BCR	C19-C20-C21-C22
15	G	847	BCR	C19-C20-C21-C22
15	g	848	BCR	C19-C20-C21-C22
15	b	846	BCR	C19-C20-C21-C22
13	G	834	CLA	C4C-C3C-CAC-CBC
13	b	833	CLA	C4C-C3C-CAC-CBC
15	A	849	BCR	C20-C21-C22-C37
15	B	843	BCR	C20-C21-C22-C37
15	B	844	BCR	C20-C21-C22-C37
15	E	851	BCR	C20-C21-C22-C37
15	G	843	BCR	C20-C21-C22-C37
15	G	844	BCR	C20-C21-C22-C37
15	O	202	BCR	C20-C21-C22-C37
15	e	848	BCR	C20-C21-C22-C37
15	g	844	BCR	C20-C21-C22-C37
15	g	845	BCR	C20-C21-C22-C37
15	s	201	BCR	C35-C13-C14-C15
15	b	842	BCR	C20-C21-C22-C37
15	b	843	BCR	C20-C21-C22-C37
15	m	101	BCR	C11-C10-C9-C34
13	A	826	CLA	C3A-C2A-CAA-CBA
13	E	826	CLA	C3A-C2A-CAA-CBA
13	e	825	CLA	C3A-C2A-CAA-CBA
13	a	826	CLA	C3A-C2A-CAA-CBA
13	B	824	CLA	CAA-CBA-CGA-O2A
13	G	824	CLA	CAA-CBA-CGA-O2A
13	g	825	CLA	CAA-CBA-CGA-O2A
13	b	823	CLA	CAA-CBA-CGA-O2A
13	A	807	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	814	CLA	CAD-CBD-CGD-O2D
13	A	817	CLA	CAD-CBD-CGD-O2D
13	A	828	CLA	CAD-CBD-CGD-O2D
13	A	834	CLA	CAD-CBD-CGD-O2D
13	A	837	CLA	CAD-CBD-CGD-O2D
13	B	807	CLA	CAD-CBD-CGD-O2D
13	B	811	CLA	CAD-CBD-CGD-O2D
13	B	826	CLA	CAD-CBD-CGD-O2D
13	B	834	CLA	CAD-CBD-CGD-O2D
13	B	839	CLA	CAD-CBD-CGD-O2D
13	E	807	CLA	CAD-CBD-CGD-O2D
13	E	814	CLA	CAD-CBD-CGD-O2D
13	E	817	CLA	CAD-CBD-CGD-O2D
13	E	828	CLA	CAD-CBD-CGD-O2D
13	E	834	CLA	CAD-CBD-CGD-O2D
13	E	838	CLA	CAD-CBD-CGD-O2D
13	G	806	CLA	CAD-CBD-CGD-O2D
13	G	810	CLA	CAD-CBD-CGD-O2D
13	G	812	CLA	CAD-CBD-CGD-O2D
13	G	826	CLA	CAD-CBD-CGD-O2D
13	G	834	CLA	CAD-CBD-CGD-O2D
13	G	839	CLA	CAD-CBD-CGD-O2D
13	S	206	CLA	CAD-CBD-CGD-O2D
13	e	806	CLA	CAD-CBD-CGD-O2D
13	e	813	CLA	CAD-CBD-CGD-O2D
13	e	816	CLA	CAD-CBD-CGD-O2D
13	e	827	CLA	CAD-CBD-CGD-O2D
13	e	833	CLA	CAD-CBD-CGD-O2D
13	e	836	CLA	CAD-CBD-CGD-O2D
13	e	844	CLA	CAD-CBD-CGD-O2D
13	g	808	CLA	CAD-CBD-CGD-O2D
13	g	812	CLA	CAD-CBD-CGD-O2D
13	g	827	CLA	CAD-CBD-CGD-O2D
13	g	835	CLA	CAD-CBD-CGD-O2D
13	g	840	CLA	CAD-CBD-CGD-O2D
13	a	807	CLA	CAD-CBD-CGD-O2D
13	a	814	CLA	CAD-CBD-CGD-O2D
13	a	817	CLA	CAD-CBD-CGD-O2D
13	a	828	CLA	CAD-CBD-CGD-O2D
13	a	834	CLA	CAD-CBD-CGD-O2D
13	a	838	CLA	CAD-CBD-CGD-O2D
13	b	806	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	b	810	CLA	CAD-CBD-CGD-O2D
13	b	811	CLA	CAD-CBD-CGD-O2D
13	b	825	CLA	CAD-CBD-CGD-O2D
13	b	833	CLA	CAD-CBD-CGD-O2D
13	b	838	CLA	CAD-CBD-CGD-O2D
13	l	201	CLA	CAD-CBD-CGD-O2D
15	A	850	BCR	C6-C7-C8-C9
15	R	101	BCR	C22-C23-C24-C25
15	S	205	BCR	C22-C23-C24-C25
13	K	101	CLA	CAA-CBA-CGA-O1A
13	E	846	CLA	CAA-CBA-CGA-O1A
13	S	204	CLA	CAA-CBA-CGA-O1A
13	r	101	CLA	CAA-CBA-CGA-O1A
13	f	203	CLA	CAA-CBA-CGA-O1A
12	a	801	LHG	C9-C10-C11-C12
13	B	841	CLA	CAA-CBA-CGA-O2A
13	E	826	CLA	CAA-CBA-CGA-O2A
13	G	841	CLA	CAA-CBA-CGA-O2A
13	e	825	CLA	CAA-CBA-CGA-O2A
13	g	842	CLA	CAA-CBA-CGA-O2A
13	a	826	CLA	CAA-CBA-CGA-O2A
13	b	840	CLA	CAA-CBA-CGA-O2A
13	A	822	CLA	CAA-CBA-CGA-O2A
13	A	826	CLA	CAA-CBA-CGA-O2A
13	E	822	CLA	CAA-CBA-CGA-O2A
13	e	821	CLA	CAA-CBA-CGA-O2A
13	a	822	CLA	CAA-CBA-CGA-O2A
13	a	814	CLA	CAA-CBA-CGA-O2A
13	A	828	CLA	O2A-C1-C2-C3
13	B	812	CLA	O2A-C1-C2-C3
13	B	818	CLA	O2A-C1-C2-C3
13	E	828	CLA	O2A-C1-C2-C3
13	G	811	CLA	O2A-C1-C2-C3
13	G	818	CLA	O2A-C1-C2-C3
13	e	827	CLA	O2A-C1-C2-C3
13	g	813	CLA	O2A-C1-C2-C3
13	g	819	CLA	O2A-C1-C2-C3
13	s	205	CLA	O2A-C1-C2-C3
13	a	828	CLA	O2A-C1-C2-C3
13	b	817	CLA	O2A-C1-C2-C3
13	b	822	CLA	O2A-C1-C2-C3
13	B	813	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	G	813	CLA	C2A-CAA-CBA-CGA
13	g	814	CLA	C2A-CAA-CBA-CGA
13	b	812	CLA	C2A-CAA-CBA-CGA
15	B	844	BCR	C14-C15-C16-C17
15	G	844	BCR	C14-C15-C16-C17
15	g	845	BCR	C14-C15-C16-C17
15	b	843	BCR	C14-C15-C16-C17
13	A	827	CLA	CAA-CBA-CGA-O2A
13	E	827	CLA	CAA-CBA-CGA-O2A
13	e	826	CLA	CAA-CBA-CGA-O2A
13	a	827	CLA	CAA-CBA-CGA-O2A
13	A	817	CLA	CAA-CBA-CGA-O1A
13	E	817	CLA	CAA-CBA-CGA-O1A
13	E	817	CLA	CAA-CBA-CGA-O2A
13	O	203	CLA	CAA-CBA-CGA-O2A
13	e	816	CLA	CAA-CBA-CGA-O1A
13	e	816	CLA	CAA-CBA-CGA-O2A
13	A	809	CLA	CHA-CBD-CGD-O1D
13	A	809	CLA	CHA-CBD-CGD-O2D
13	A	819	CLA	CHA-CBD-CGD-O1D
13	A	819	CLA	CHA-CBD-CGD-O2D
13	A	821	CLA	CHA-CBD-CGD-O2D
13	A	827	CLA	CHA-CBD-CGD-O2D
13	A	839	CLA	CHA-CBD-CGD-O1D
13	A	839	CLA	CHA-CBD-CGD-O2D
13	A	842	CLA	CHA-CBD-CGD-O1D
13	A	842	CLA	CHA-CBD-CGD-O2D
13	A	853	CLA	CHA-CBD-CGD-O1D
13	A	853	CLA	CHA-CBD-CGD-O2D
13	B	807	CLA	CHA-CBD-CGD-O1D
13	B	812	CLA	CHA-CBD-CGD-O1D
13	B	814	CLA	CHA-CBD-CGD-O2D
13	B	817	CLA	CHA-CBD-CGD-O1D
13	B	817	CLA	CHA-CBD-CGD-O2D
13	B	822	CLA	CHA-CBD-CGD-O1D
13	B	822	CLA	CHA-CBD-CGD-O2D
13	B	834	CLA	CHA-CBD-CGD-O2D
13	B	835	CLA	CHA-CBD-CGD-O1D
13	B	835	CLA	CHA-CBD-CGD-O2D
13	B	839	CLA	CHA-CBD-CGD-O1D
13	E	809	CLA	CHA-CBD-CGD-O1D
13	E	809	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	E	819	CLA	CHA-CBD-CGD-O1D
13	E	819	CLA	CHA-CBD-CGD-O2D
13	E	821	CLA	CHA-CBD-CGD-O2D
13	E	827	CLA	CHA-CBD-CGD-O2D
13	E	840	CLA	CHA-CBD-CGD-O1D
13	E	840	CLA	CHA-CBD-CGD-O2D
13	E	843	CLA	CHA-CBD-CGD-O1D
13	E	843	CLA	CHA-CBD-CGD-O2D
13	G	802	CLA	CHA-CBD-CGD-O1D
13	G	802	CLA	CHA-CBD-CGD-O2D
13	G	806	CLA	CHA-CBD-CGD-O1D
13	G	811	CLA	CHA-CBD-CGD-O1D
13	G	814	CLA	CHA-CBD-CGD-O2D
13	G	817	CLA	CHA-CBD-CGD-O1D
13	G	817	CLA	CHA-CBD-CGD-O2D
13	G	822	CLA	CHA-CBD-CGD-O1D
13	G	822	CLA	CHA-CBD-CGD-O2D
13	G	834	CLA	CHA-CBD-CGD-O2D
13	G	835	CLA	CHA-CBD-CGD-O1D
13	G	835	CLA	CHA-CBD-CGD-O2D
13	G	839	CLA	CHA-CBD-CGD-O1D
13	e	808	CLA	CHA-CBD-CGD-O1D
13	e	808	CLA	CHA-CBD-CGD-O2D
13	e	818	CLA	CHA-CBD-CGD-O1D
13	e	818	CLA	CHA-CBD-CGD-O2D
13	e	820	CLA	CHA-CBD-CGD-O2D
13	e	826	CLA	CHA-CBD-CGD-O2D
13	e	838	CLA	CHA-CBD-CGD-O1D
13	e	838	CLA	CHA-CBD-CGD-O2D
13	e	841	CLA	CHA-CBD-CGD-O1D
13	e	841	CLA	CHA-CBD-CGD-O2D
13	e	852	CLA	CHA-CBD-CGD-O1D
13	e	852	CLA	CHA-CBD-CGD-O2D
13	g	808	CLA	CHA-CBD-CGD-O1D
13	g	813	CLA	CHA-CBD-CGD-O1D
13	g	815	CLA	CHA-CBD-CGD-O2D
13	g	818	CLA	CHA-CBD-CGD-O1D
13	g	818	CLA	CHA-CBD-CGD-O2D
13	g	823	CLA	CHA-CBD-CGD-O1D
13	g	823	CLA	CHA-CBD-CGD-O2D
13	g	835	CLA	CHA-CBD-CGD-O2D
13	g	836	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	g	836	CLA	CHA-CBD-CGD-O2D
13	g	840	CLA	CHA-CBD-CGD-O1D
13	s	205	CLA	CHA-CBD-CGD-O1D
13	a	809	CLA	CHA-CBD-CGD-O1D
13	a	809	CLA	CHA-CBD-CGD-O2D
13	a	819	CLA	CHA-CBD-CGD-O1D
13	a	819	CLA	CHA-CBD-CGD-O2D
13	a	821	CLA	CHA-CBD-CGD-O2D
13	a	827	CLA	CHA-CBD-CGD-O2D
13	a	840	CLA	CHA-CBD-CGD-O1D
13	a	840	CLA	CHA-CBD-CGD-O2D
13	a	843	CLA	CHA-CBD-CGD-O1D
13	a	843	CLA	CHA-CBD-CGD-O2D
13	b	802	CLA	CHA-CBD-CGD-O1D
13	b	802	CLA	CHA-CBD-CGD-O2D
13	b	806	CLA	CHA-CBD-CGD-O1D
13	b	813	CLA	CHA-CBD-CGD-O2D
13	b	816	CLA	CHA-CBD-CGD-O1D
13	b	816	CLA	CHA-CBD-CGD-O2D
13	b	821	CLA	CHA-CBD-CGD-O1D
13	b	821	CLA	CHA-CBD-CGD-O2D
13	b	833	CLA	CHA-CBD-CGD-O2D
13	b	834	CLA	CHA-CBD-CGD-O1D
13	b	834	CLA	CHA-CBD-CGD-O2D
13	b	838	CLA	CHA-CBD-CGD-O1D
13	A	817	CLA	CAA-CBA-CGA-O2A
13	a	814	CLA	CAA-CBA-CGA-O1A
13	A	819	CLA	CAA-CBA-CGA-O2A
13	B	807	CLA	CAA-CBA-CGA-O2A
13	E	819	CLA	CAA-CBA-CGA-O2A
13	G	806	CLA	CAA-CBA-CGA-O2A
13	e	818	CLA	CAA-CBA-CGA-O2A
13	g	808	CLA	CAA-CBA-CGA-O2A
13	a	819	CLA	CAA-CBA-CGA-O2A
13	b	806	CLA	CAA-CBA-CGA-O2A
12	e	802	LHG	C15-C16-C17-C18
15	B	846	BCR	C12-C13-C14-C15
15	G	846	BCR	C12-C13-C14-C15
15	g	847	BCR	C12-C13-C14-C15
15	b	845	BCR	C12-C13-C14-C15
15	k	4001	BCR	C12-C13-C14-C15
13	O	203	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	825	CLA	CAA-CBA-CGA-O2A
13	E	825	CLA	CAA-CBA-CGA-O2A
13	a	825	CLA	CAA-CBA-CGA-O2A
13	e	820	CLA	O1D-CGD-O2D-CED
13	B	824	CLA	CAA-CBA-CGA-O1A
13	g	825	CLA	CAA-CBA-CGA-O1A
13	b	823	CLA	CAA-CBA-CGA-O1A
13	A	853	CLA	CAA-CBA-CGA-O2A
13	G	802	CLA	CAA-CBA-CGA-O2A
13	e	824	CLA	CAA-CBA-CGA-O2A
13	e	852	CLA	CAA-CBA-CGA-O2A
13	b	802	CLA	CAA-CBA-CGA-O2A
13	b	804	CLA	CAA-CBA-CGA-O2A
13	A	819	CLA	O1D-CGD-O2D-CED
13	A	821	CLA	C2A-CAA-CBA-CGA
13	B	814	CLA	C2A-CAA-CBA-CGA
13	E	821	CLA	C2A-CAA-CBA-CGA
13	G	814	CLA	C2A-CAA-CBA-CGA
13	G	823	CLA	C2A-CAA-CBA-CGA
13	e	820	CLA	C2A-CAA-CBA-CGA
13	g	815	CLA	C2A-CAA-CBA-CGA
13	g	824	CLA	C2A-CAA-CBA-CGA
13	a	821	CLA	C2A-CAA-CBA-CGA
13	b	813	CLA	C2A-CAA-CBA-CGA
13	b	822	CLA	C2A-CAA-CBA-CGA
13	B	835	CLA	CAA-CBA-CGA-O2A
13	G	816	CLA	CAA-CBA-CGA-O2A
13	G	835	CLA	CAA-CBA-CGA-O2A
13	g	836	CLA	CAA-CBA-CGA-O2A
13	b	834	CLA	CAA-CBA-CGA-O2A
13	b	817	CLA	CAA-CBA-CGA-O1A
13	B	805	CLA	CAA-CBA-CGA-O2A
13	B	811	CLA	CAA-CBA-CGA-O2A
13	G	804	CLA	CAA-CBA-CGA-O2A
13	G	810	CLA	CAA-CBA-CGA-O2A
13	g	806	CLA	CAA-CBA-CGA-O2A
13	g	812	CLA	CAA-CBA-CGA-O2A
13	b	810	CLA	CAA-CBA-CGA-O2A
13	G	824	CLA	CAA-CBA-CGA-O1A
12	e	802	LHG	C14-C15-C16-C17
12	a	801	LHG	C14-C15-C16-C17
13	A	821	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	a	821	CLA	O1D-CGD-O2D-CED
13	E	819	CLA	O1D-CGD-O2D-CED
13	g	819	CLA	CAA-CBA-CGA-O1A
13	E	821	CLA	O1D-CGD-O2D-CED
13	r	101	CLA	C2C-C3C-CAC-CBC
13	B	816	CLA	CAA-CBA-CGA-O2A
13	g	817	CLA	CAA-CBA-CGA-O2A
13	b	815	CLA	CAA-CBA-CGA-O2A
13	B	818	CLA	CAA-CBA-CGA-O1A
13	G	818	CLA	CAA-CBA-CGA-O1A
13	B	823	CLA	C2A-CAA-CBA-CGA
13	a	819	CLA	O1D-CGD-O2D-CED
15	A	848	BCR	C11-C12-C13-C14
15	E	850	BCR	C11-C12-C13-C14
15	O	202	BCR	C11-C12-C13-C14
15	e	847	BCR	C11-C12-C13-C14
15	a	850	BCR	C11-C12-C13-C14
13	A	803	CLA	C1A-C2A-CAA-CBA
13	A	826	CLA	C1A-C2A-CAA-CBA
13	B	810	CLA	C1A-C2A-CAA-CBA
13	E	826	CLA	C1A-C2A-CAA-CBA
13	G	809	CLA	C1A-C2A-CAA-CBA
13	e	825	CLA	C1A-C2A-CAA-CBA
13	g	811	CLA	C1A-C2A-CAA-CBA
13	a	826	CLA	C1A-C2A-CAA-CBA
13	b	809	CLA	C1A-C2A-CAA-CBA
13	A	822	CLA	CAA-CBA-CGA-O1A
13	e	821	CLA	CAA-CBA-CGA-O1A
13	a	822	CLA	CAA-CBA-CGA-O1A
13	g	837	CLA	CAA-CBA-CGA-O2A
13	b	835	CLA	CAA-CBA-CGA-O2A
13	e	818	CLA	O1D-CGD-O2D-CED
13	B	841	CLA	CAA-CBA-CGA-O1A
13	E	822	CLA	CAA-CBA-CGA-O1A
13	G	841	CLA	CAA-CBA-CGA-O1A
13	e	818	CLA	CAA-CBA-CGA-O1A
13	g	842	CLA	CAA-CBA-CGA-O1A
13	a	819	CLA	CAA-CBA-CGA-O1A
13	b	840	CLA	CAA-CBA-CGA-O1A
13	B	836	CLA	CAA-CBA-CGA-O2A
13	G	831	CLA	CAA-CBA-CGA-O2A
13	G	836	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	g	832	CLA	CAA-CBA-CGA-O2A
13	B	834	CLA	CAA-CBA-CGA-O2A
13	g	835	CLA	CAA-CBA-CGA-O2A
13	b	833	CLA	CAA-CBA-CGA-O2A
13	A	809	CLA	C2A-CAA-CBA-CGA
13	E	809	CLA	C2A-CAA-CBA-CGA
13	e	808	CLA	C2A-CAA-CBA-CGA
13	a	809	CLA	C2A-CAA-CBA-CGA
12	e	802	LHG	O9-C7-C8-C9
13	A	819	CLA	CAA-CBA-CGA-O1A
13	b	830	CLA	CAA-CBA-CGA-O2A
13	B	809	CLA	CAA-CBA-CGA-O2A
13	G	808	CLA	CAA-CBA-CGA-O2A
13	G	834	CLA	CAA-CBA-CGA-O2A
13	g	810	CLA	CAA-CBA-CGA-O2A
13	b	808	CLA	CAA-CBA-CGA-O2A
13	B	807	CLA	CAA-CBA-CGA-O1A
13	E	819	CLA	CAA-CBA-CGA-O1A
13	g	808	CLA	CAA-CBA-CGA-O1A
13	b	806	CLA	CAA-CBA-CGA-O1A
15	e	851	BCR	C6-C7-C8-C9
13	G	806	CLA	CAA-CBA-CGA-O1A
15	a	851	BCR	C20-C21-C22-C37
15	f	202	BCR	C20-C21-C22-C37
13	A	813	CLA	CAA-CBA-CGA-O2A
13	B	831	CLA	CAA-CBA-CGA-O2A
13	E	813	CLA	CAA-CBA-CGA-O2A
13	e	812	CLA	CAA-CBA-CGA-O2A
13	a	813	CLA	CAA-CBA-CGA-O2A
15	A	847	BCR	C5-C6-C7-C8
15	A	848	BCR	C5-C6-C7-C8
15	F	201	BCR	C5-C6-C7-C8
15	F	201	BCR	C23-C24-C25-C26
15	E	849	BCR	C5-C6-C7-C8
15	E	850	BCR	C5-C6-C7-C8
15	O	201	BCR	C5-C6-C7-C8
15	O	202	BCR	C5-C6-C7-C8
15	S	201	BCR	C5-C6-C7-C8
15	e	846	BCR	C5-C6-C7-C8
15	e	847	BCR	C5-C6-C7-C8
15	e	848	BCR	C5-C6-C7-C8
15	o	201	BCR	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	a	849	BCR	C5-C6-C7-C8
15	a	850	BCR	C5-C6-C7-C8
15	f	201	BCR	C5-C6-C7-C8
13	A	826	CLA	CAA-CBA-CGA-O1A
13	A	827	CLA	CAA-CBA-CGA-O1A
13	E	826	CLA	CAA-CBA-CGA-O1A
13	E	827	CLA	CAA-CBA-CGA-O1A
13	e	825	CLA	CAA-CBA-CGA-O1A
13	e	826	CLA	CAA-CBA-CGA-O1A
13	a	826	CLA	CAA-CBA-CGA-O1A
13	a	827	CLA	CAA-CBA-CGA-O1A
13	g	840	CLA	CBD-CGD-O2D-CED
12	a	801	LHG	O9-C7-O7-C5
15	A	850	BCR	C18-C19-C20-C21
13	G	804	CLA	CAA-CBA-CGA-O1A
13	A	841	CLA	CAA-CBA-CGA-O2A
13	E	842	CLA	CAA-CBA-CGA-O2A
13	e	840	CLA	CAA-CBA-CGA-O2A
13	a	842	CLA	CAA-CBA-CGA-O2A
13	G	839	CLA	O1D-CGD-O2D-CED
13	G	839	CLA	CBD-CGD-O2D-CED
13	B	805	CLA	CAA-CBA-CGA-O1A
13	g	806	CLA	CAA-CBA-CGA-O1A
13	b	838	CLA	O1D-CGD-O2D-CED
13	A	827	CLA	CAD-CBD-CGD-O1D
13	A	841	CLA	CAD-CBD-CGD-O1D
13	A	845	CLA	CAD-CBD-CGD-O1D
13	B	812	CLA	CAD-CBD-CGD-O1D
13	B	820	CLA	CAD-CBD-CGD-O1D
13	E	827	CLA	CAD-CBD-CGD-O1D
13	E	842	CLA	CAD-CBD-CGD-O1D
13	G	811	CLA	CAD-CBD-CGD-O1D
13	G	820	CLA	CAD-CBD-CGD-O1D
13	e	803	CLA	CAD-CBD-CGD-O1D
13	e	826	CLA	CAD-CBD-CGD-O1D
13	e	840	CLA	CAD-CBD-CGD-O1D
13	g	813	CLA	CAD-CBD-CGD-O1D
13	g	821	CLA	CAD-CBD-CGD-O1D
13	s	205	CLA	CAD-CBD-CGD-O1D
13	a	827	CLA	CAD-CBD-CGD-O1D
13	a	842	CLA	CAD-CBD-CGD-O1D
13	b	819	CLA	CAD-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	E	819	CLA	CBD-CGD-O2D-CED
13	b	838	CLA	CBD-CGD-O2D-CED
13	B	839	CLA	O1A-CGA-O2A-C1
13	g	840	CLA	O1A-CGA-O2A-C1
13	b	838	CLA	O1A-CGA-O2A-C1
13	B	811	CLA	CAA-CBA-CGA-O1A
13	B	834	CLA	CAA-CBA-CGA-O1A
13	G	834	CLA	CAA-CBA-CGA-O1A
13	g	835	CLA	CAA-CBA-CGA-O1A
13	b	810	CLA	CAA-CBA-CGA-O1A
13	b	833	CLA	CAA-CBA-CGA-O1A
13	g	840	CLA	O1D-CGD-O2D-CED
13	B	831	CLA	CAA-CBA-CGA-O1A
13	B	835	CLA	CAA-CBA-CGA-O1A
13	G	831	CLA	CAA-CBA-CGA-O1A
13	G	835	CLA	CAA-CBA-CGA-O1A
13	g	836	CLA	CAA-CBA-CGA-O1A
13	b	834	CLA	CAA-CBA-CGA-O1A
13	G	839	CLA	O1A-CGA-O2A-C1
13	B	804	CLA	CAA-CBA-CGA-O1A
13	G	810	CLA	CAA-CBA-CGA-O1A
13	e	824	CLA	CAA-CBA-CGA-O1A
13	g	812	CLA	CAA-CBA-CGA-O1A
13	b	804	CLA	CAA-CBA-CGA-O1A
13	A	824	CLA	CAA-CBA-CGA-O2A
13	A	829	CLA	CAA-CBA-CGA-O2A
13	A	839	CLA	CAA-CBA-CGA-O2A
13	E	824	CLA	CAA-CBA-CGA-O2A
13	E	829	CLA	CAA-CBA-CGA-O2A
13	E	840	CLA	CAA-CBA-CGA-O2A
13	G	823	CLA	CAA-CBA-CGA-O2A
13	e	823	CLA	CAA-CBA-CGA-O2A
13	e	828	CLA	CAA-CBA-CGA-O2A
13	e	838	CLA	CAA-CBA-CGA-O2A
13	a	824	CLA	CAA-CBA-CGA-O2A
13	a	829	CLA	CAA-CBA-CGA-O2A
13	a	840	CLA	CAA-CBA-CGA-O2A
13	b	822	CLA	CAA-CBA-CGA-O2A
13	g	832	CLA	CAA-CBA-CGA-O1A
13	b	830	CLA	CAA-CBA-CGA-O1A
13	E	825	CLA	CAA-CBA-CGA-O1A
13	G	803	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	g	805	CLA	CAA-CBA-CGA-O1A
13	a	825	CLA	CAA-CBA-CGA-O1A
13	b	803	CLA	CAA-CBA-CGA-O1A
13	A	819	CLA	CBD-CGD-O2D-CED
13	B	839	CLA	CBD-CGD-O2D-CED
13	A	830	CLA	C2A-CAA-CBA-CGA
13	B	825	CLA	C2A-CAA-CBA-CGA
13	E	830	CLA	C2A-CAA-CBA-CGA
13	G	825	CLA	C2A-CAA-CBA-CGA
13	e	829	CLA	C2A-CAA-CBA-CGA
13	g	826	CLA	C2A-CAA-CBA-CGA
13	a	830	CLA	C2A-CAA-CBA-CGA
13	b	824	CLA	C2A-CAA-CBA-CGA
13	A	823	CLA	CAA-CBA-CGA-O2A
13	A	830	CLA	CAA-CBA-CGA-O2A
13	B	823	CLA	CAA-CBA-CGA-O2A
13	E	830	CLA	CAA-CBA-CGA-O2A
13	e	829	CLA	CAA-CBA-CGA-O2A
13	g	824	CLA	CAA-CBA-CGA-O2A
13	a	830	CLA	CAA-CBA-CGA-O2A
13	A	838	CLA	CAA-CBA-CGA-O2A
13	a	839	CLA	CAA-CBA-CGA-O2A
13	A	825	CLA	CAA-CBA-CGA-O1A
13	e	818	CLA	CBD-CGD-O2D-CED
14	A	846	PQN	C16-C17-C18-C20
13	A	829	CLA	CAA-CBA-CGA-O1A
13	A	853	CLA	CAA-CBA-CGA-O1A
13	G	802	CLA	CAA-CBA-CGA-O1A
13	e	828	CLA	CAA-CBA-CGA-O1A
13	a	829	CLA	CAA-CBA-CGA-O1A
13	B	816	CLA	CAA-CBA-CGA-O1A
13	E	839	CLA	CAA-CBA-CGA-O2A
13	e	837	CLA	CAA-CBA-CGA-O2A
13	g	817	CLA	CAA-CBA-CGA-O1A
12	e	802	LHG	O7-C7-C8-C9
13	A	840	CLA	CAA-CBA-CGA-O2A
13	B	817	CLA	CAA-CBA-CGA-O2A
13	B	826	CLA	CAA-CBA-CGA-O2A
13	E	823	CLA	CAA-CBA-CGA-O2A
13	E	841	CLA	CAA-CBA-CGA-O2A
13	G	817	CLA	CAA-CBA-CGA-O2A
13	e	839	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	g	818	CLA	CAA-CBA-CGA-O2A
13	a	841	CLA	CAA-CBA-CGA-O2A
13	b	816	CLA	CAA-CBA-CGA-O2A
13	b	837	CLA	CAA-CBA-CGA-O2A
12	A	801	LHG	C24-C25-C26-C27
13	A	825	CLA	O2A-C1-C2-C3
13	E	825	CLA	O2A-C1-C2-C3
13	e	824	CLA	O2A-C1-C2-C3
13	a	825	CLA	O2A-C1-C2-C3
15	B	846	BCR	C21-C22-C23-C24
15	G	846	BCR	C21-C22-C23-C24
15	g	847	BCR	C21-C22-C23-C24
15	b	845	BCR	C21-C22-C23-C24
15	l	206	BCR	C17-C18-C19-C20
13	E	829	CLA	CAA-CBA-CGA-O1A
13	G	808	CLA	CAA-CBA-CGA-O1A
13	e	852	CLA	CAA-CBA-CGA-O1A
13	g	810	CLA	CAA-CBA-CGA-O1A
13	b	802	CLA	CAA-CBA-CGA-O1A
13	G	816	CLA	CAA-CBA-CGA-O1A
13	b	815	CLA	CAA-CBA-CGA-O1A
13	B	838	CLA	CAA-CBA-CGA-O2A
13	G	838	CLA	CAA-CBA-CGA-O2A
13	e	822	CLA	CAA-CBA-CGA-O2A
13	g	827	CLA	CAA-CBA-CGA-O2A
13	g	839	CLA	CAA-CBA-CGA-O2A
13	a	823	CLA	CAA-CBA-CGA-O2A
13	b	825	CLA	CAA-CBA-CGA-O2A
13	L	202	CLA	O1A-CGA-O2A-C1
13	B	809	CLA	CAA-CBA-CGA-O1A
13	B	817	CLA	CAA-CBA-CGA-O1A
13	g	818	CLA	CAA-CBA-CGA-O1A
13	b	808	CLA	CAA-CBA-CGA-O1A
13	B	839	CLA	O1D-CGD-O2D-CED
13	B	836	CLA	CAA-CBA-CGA-O1A
13	G	836	CLA	CAA-CBA-CGA-O1A
13	B	832	CLA	CAA-CBA-CGA-O2A
13	G	826	CLA	CAA-CBA-CGA-O2A
13	G	832	CLA	CAA-CBA-CGA-O2A
13	g	833	CLA	CAA-CBA-CGA-O2A
13	b	831	CLA	CAA-CBA-CGA-O2A
13	a	819	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

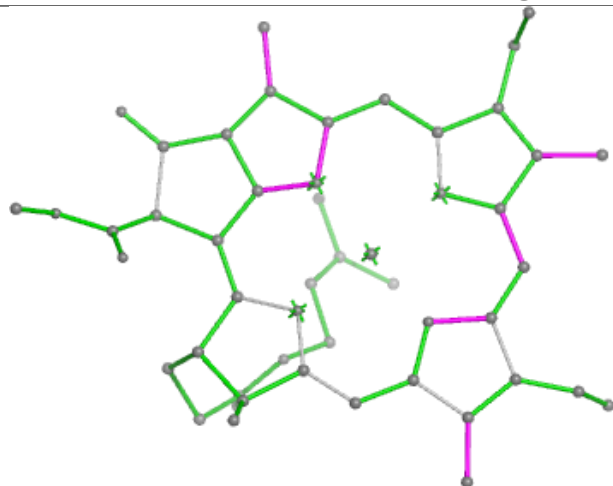
Mol	Chain	Res	Type	Atoms
13	A	838	CLA	C2A-CAA-CBA-CGA
13	g	837	CLA	CAA-CBA-CGA-O1A
13	a	818	CLA	CAA-CBA-CGA-O2A
13	b	835	CLA	CAA-CBA-CGA-O1A
13	g	840	CLA	CBA-CGA-O2A-C1
13	b	838	CLA	CBA-CGA-O2A-C1
13	A	840	CLA	CAA-CBA-CGA-O1A
13	E	841	CLA	CAA-CBA-CGA-O1A
13	e	838	CLA	CAA-CBA-CGA-O1A
13	e	839	CLA	CAA-CBA-CGA-O1A
13	a	840	CLA	CAA-CBA-CGA-O1A
13	a	841	CLA	CAA-CBA-CGA-O1A
13	b	816	CLA	CAA-CBA-CGA-O1A
13	e	830	CLA	C4C-C3C-CAC-CBC
13	A	818	CLA	CAA-CBA-CGA-O2A
13	A	838	CLA	CAA-CBA-CGA-O1A
13	E	818	CLA	CAA-CBA-CGA-O2A
13	E	839	CLA	CAA-CBA-CGA-O1A
13	e	817	CLA	CAA-CBA-CGA-O2A
13	a	839	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

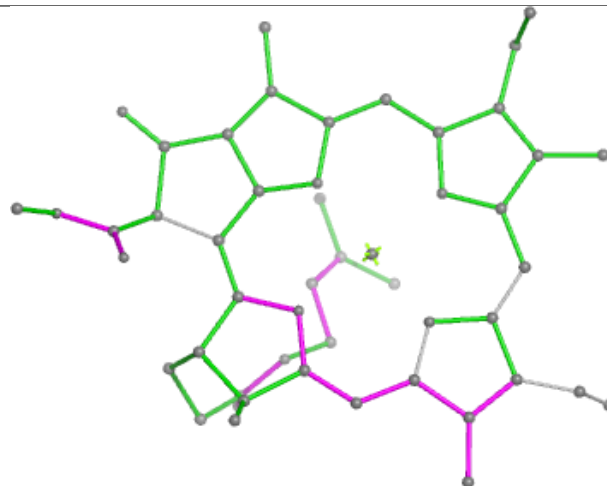
No monomer is involved in short contacts.

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.

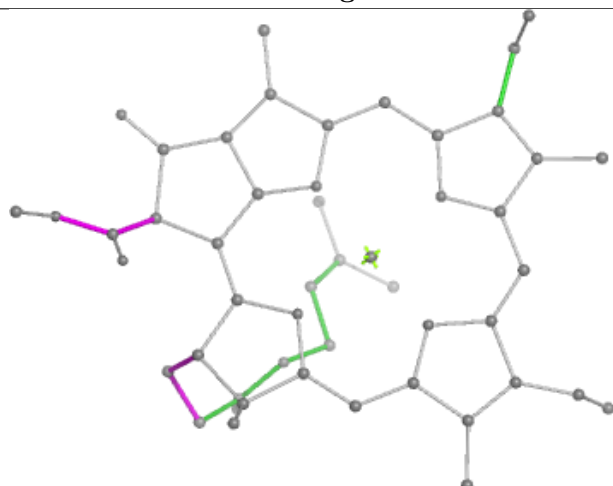
## Ligand CLA E 845



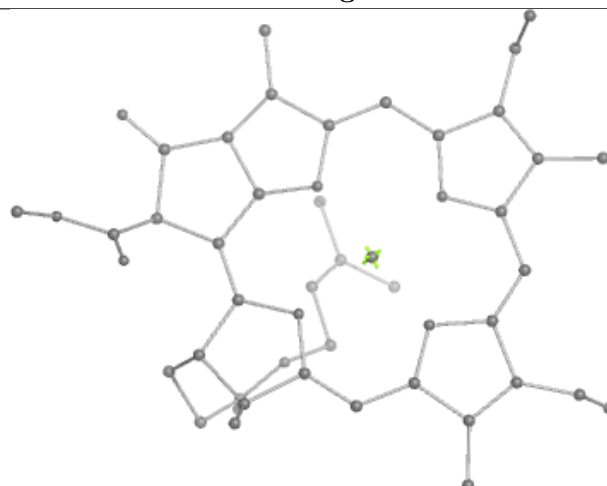
Bond lengths



Bond angles

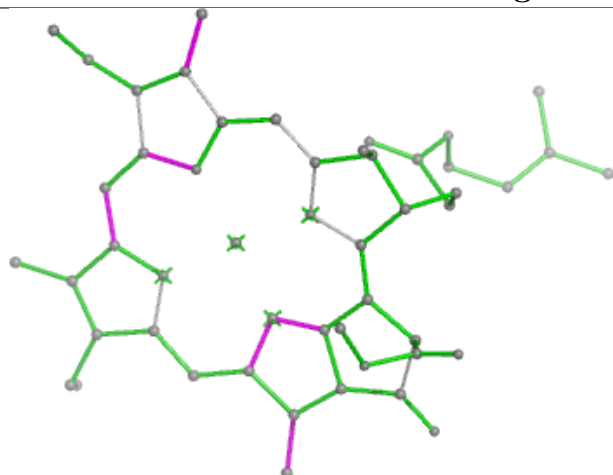


Torsions

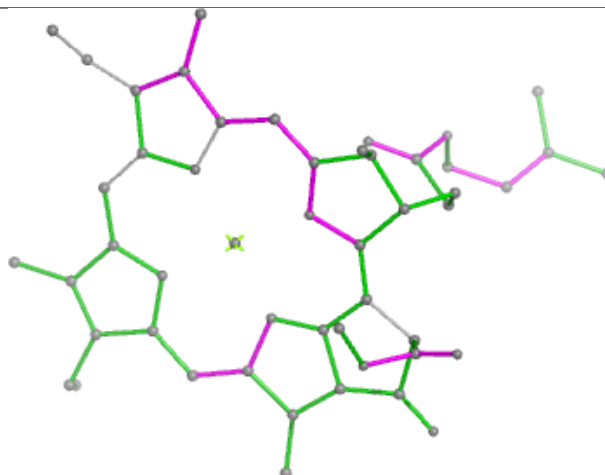


Rings

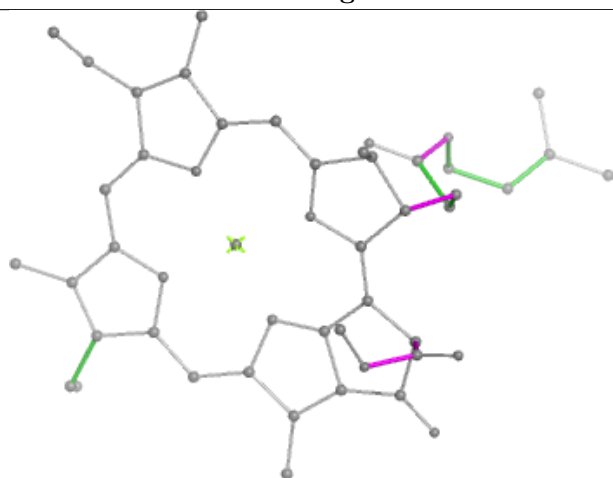
## Ligand CLA A 837



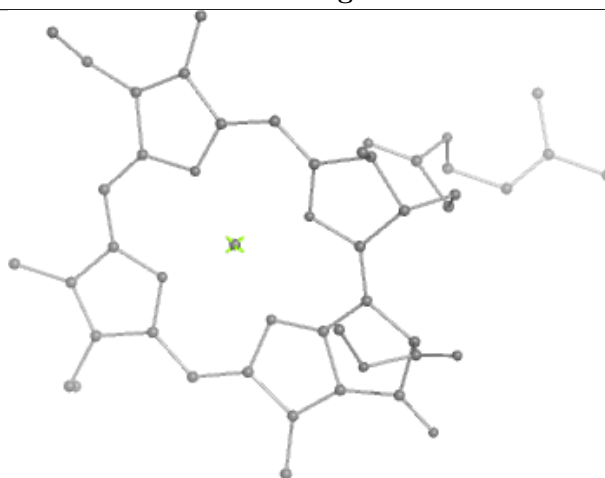
Bond lengths



Bond angles

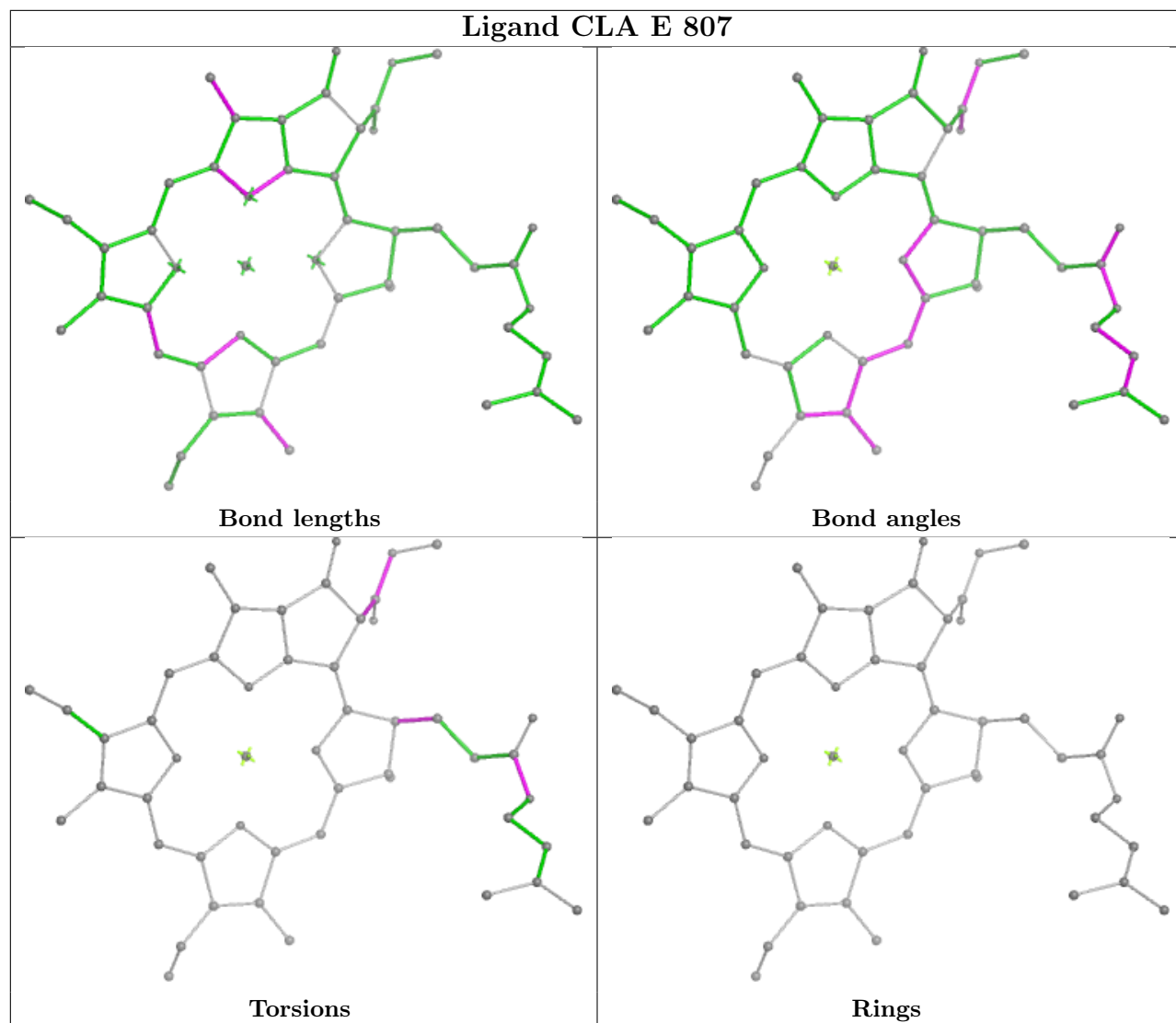


Torsions

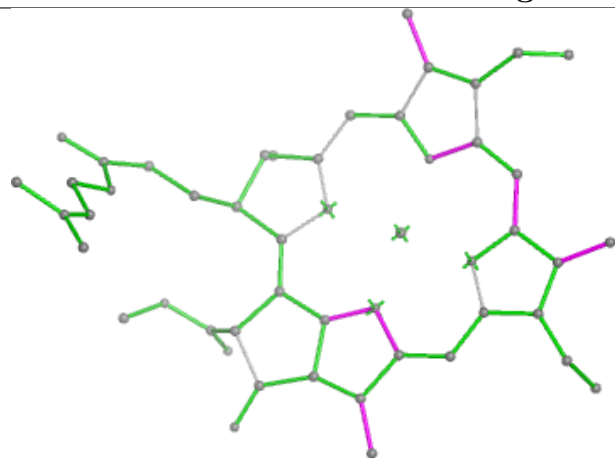


Rings

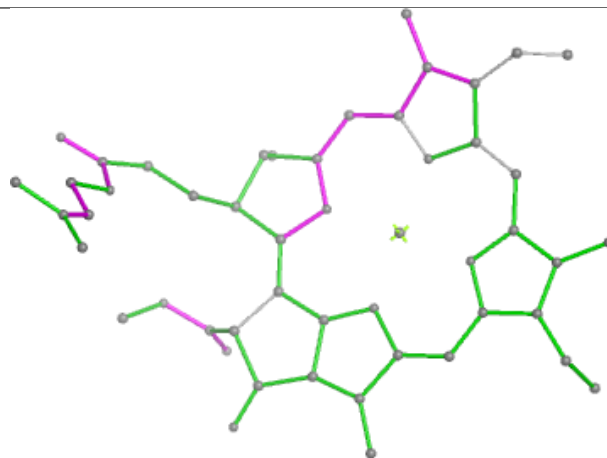
## Ligand CLA E 807



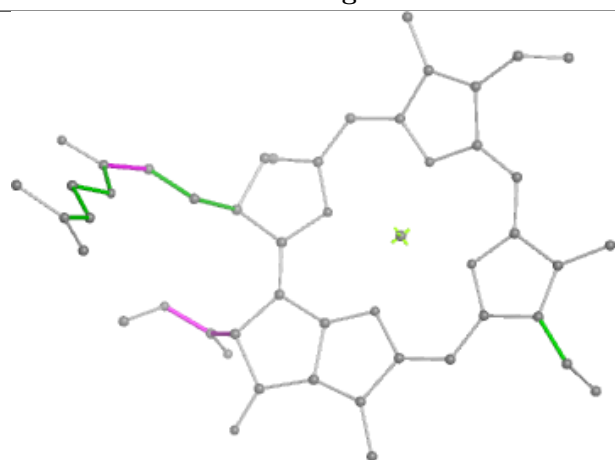
## Ligand CLA B 804



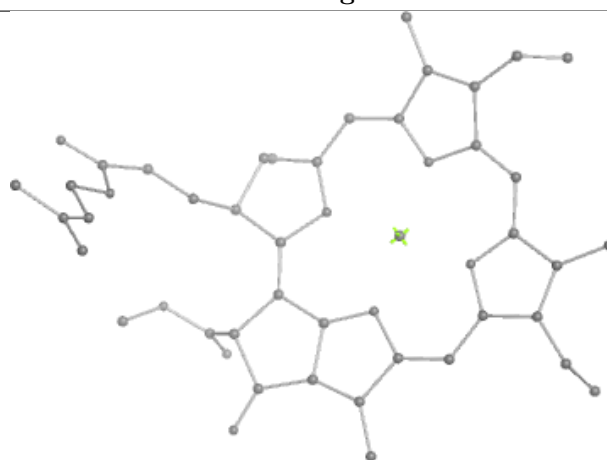
Bond lengths



Bond angles

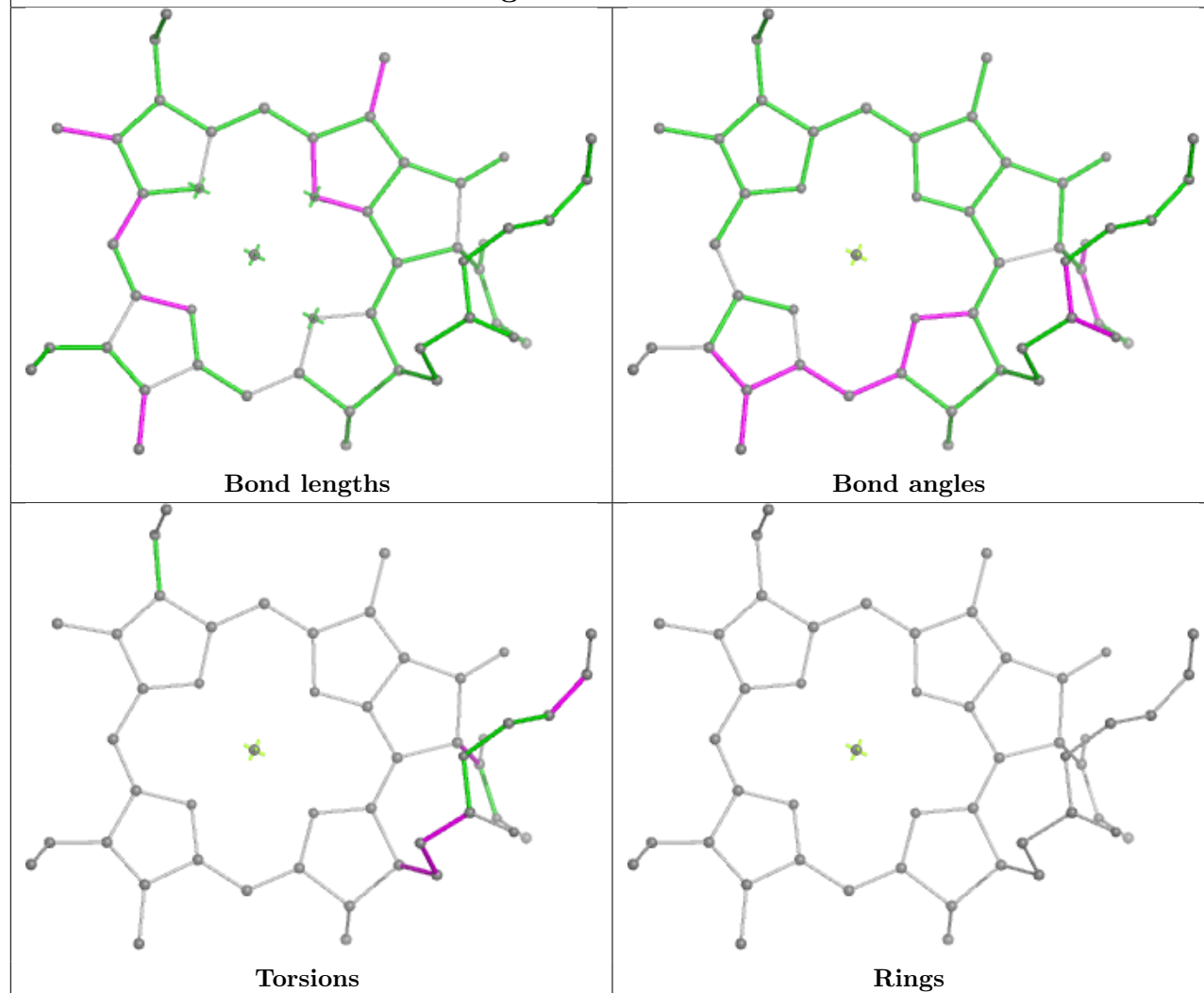


Torsions

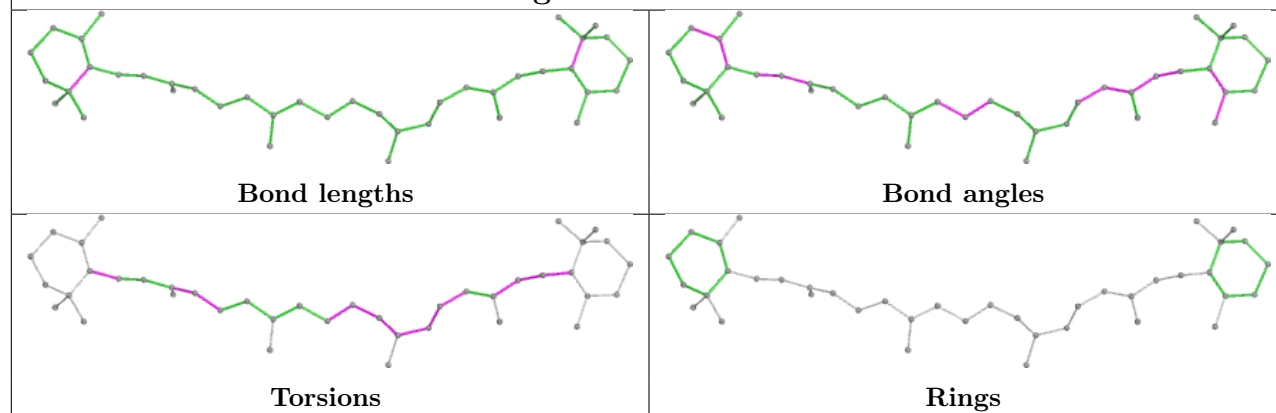


Rings

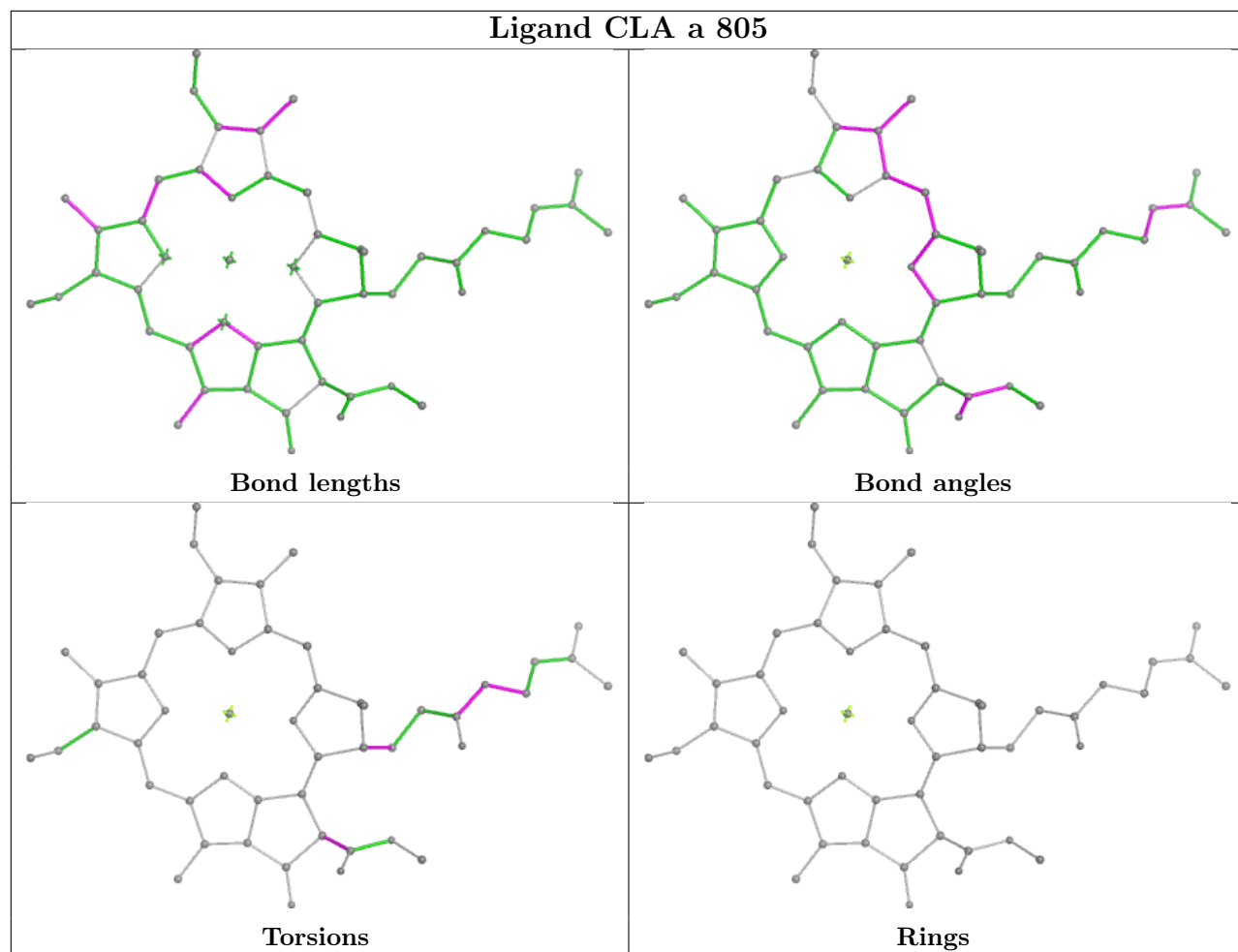
## Ligand CLA G 832



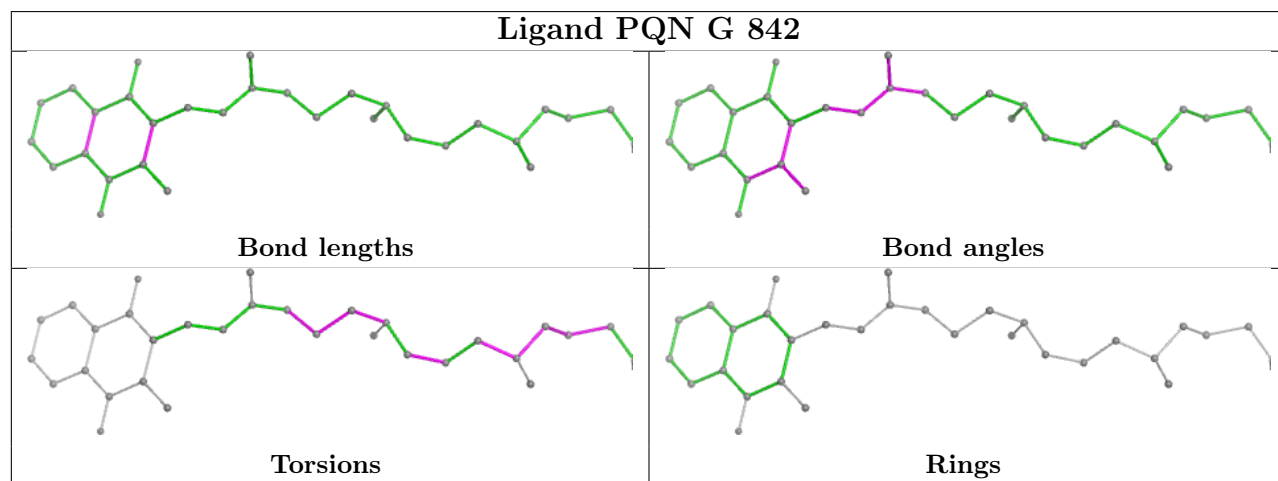
## Ligand BCR S 202

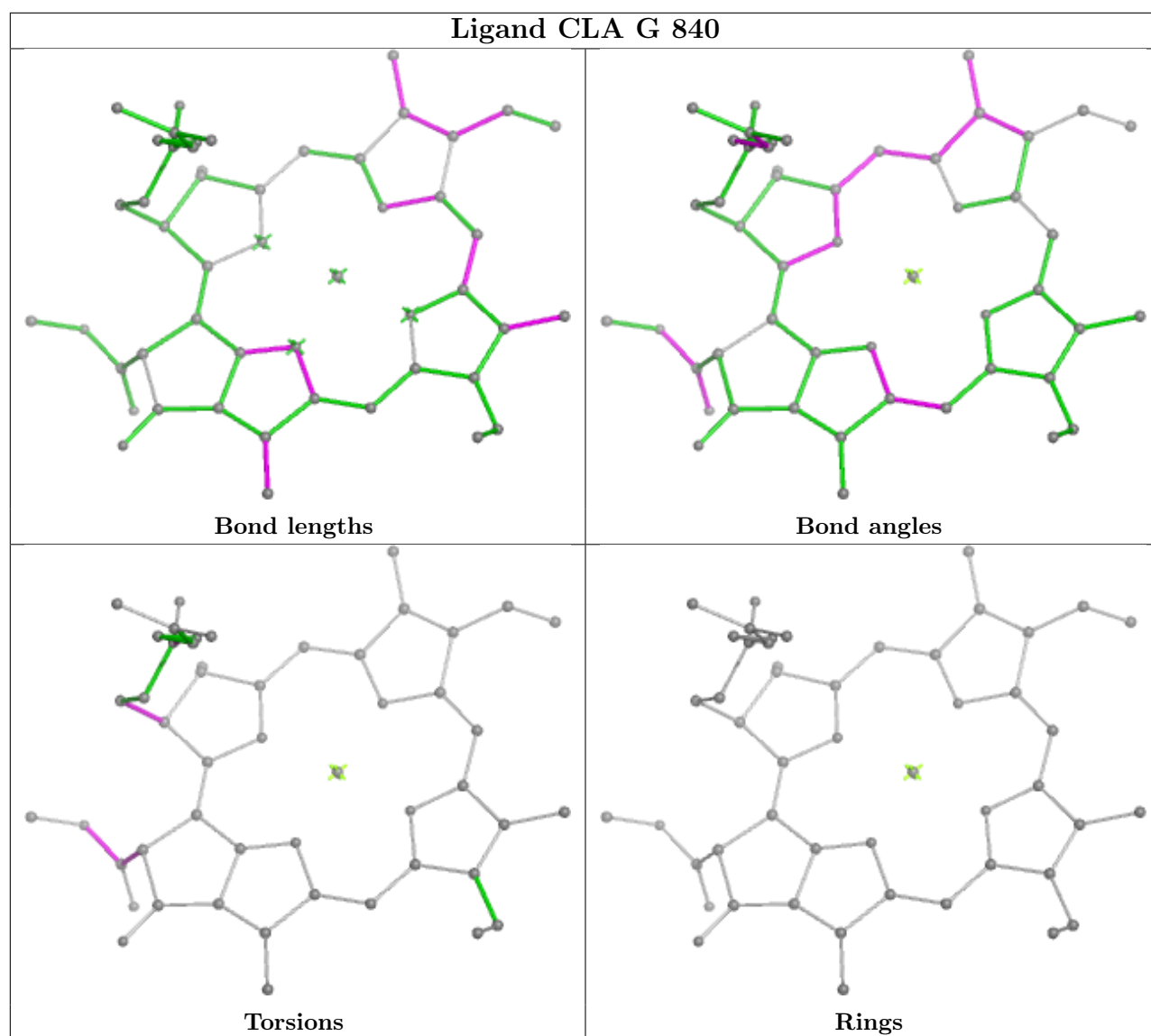


## Ligand CLA a 805

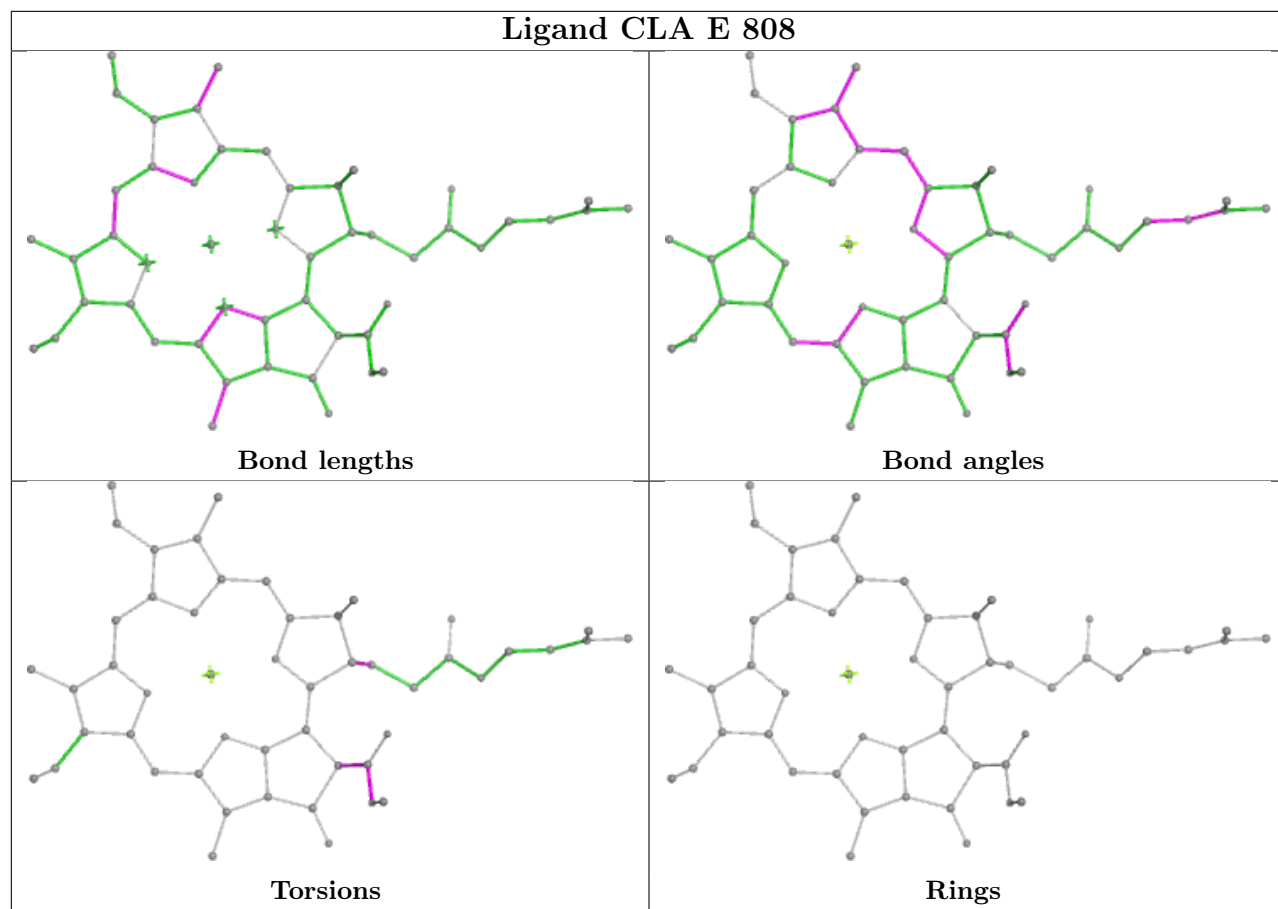


## Ligand PQN G 842

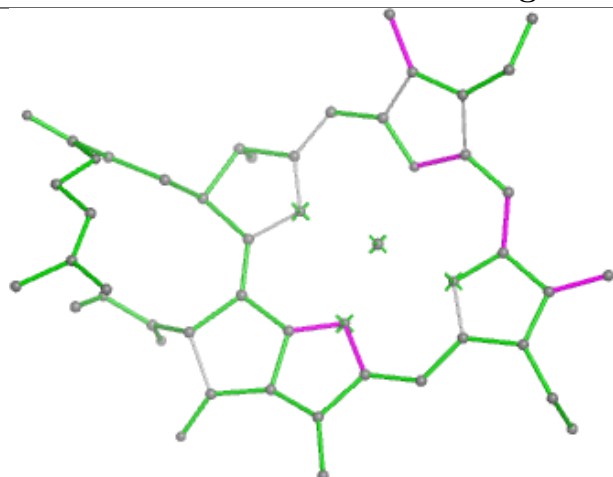




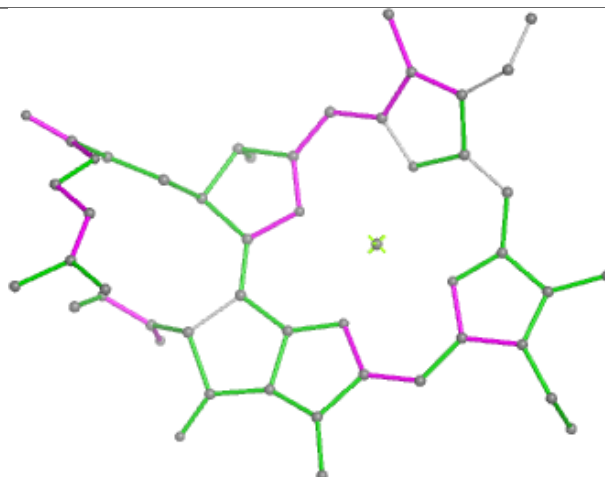




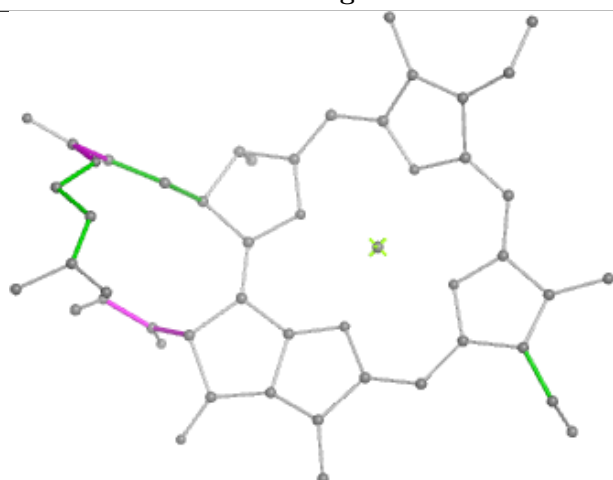
## Ligand CLA e 803



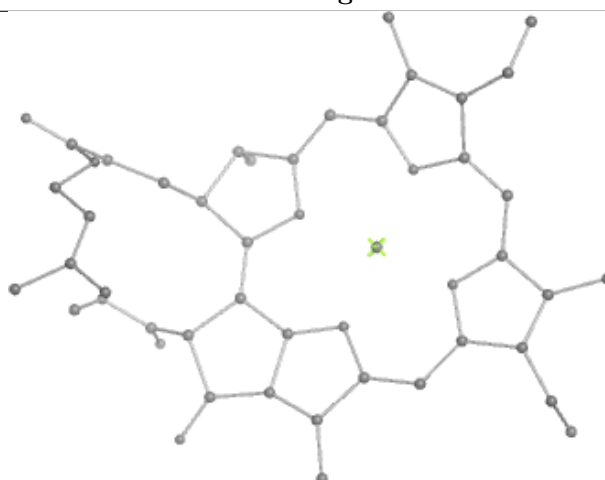
Bond lengths



Bond angles

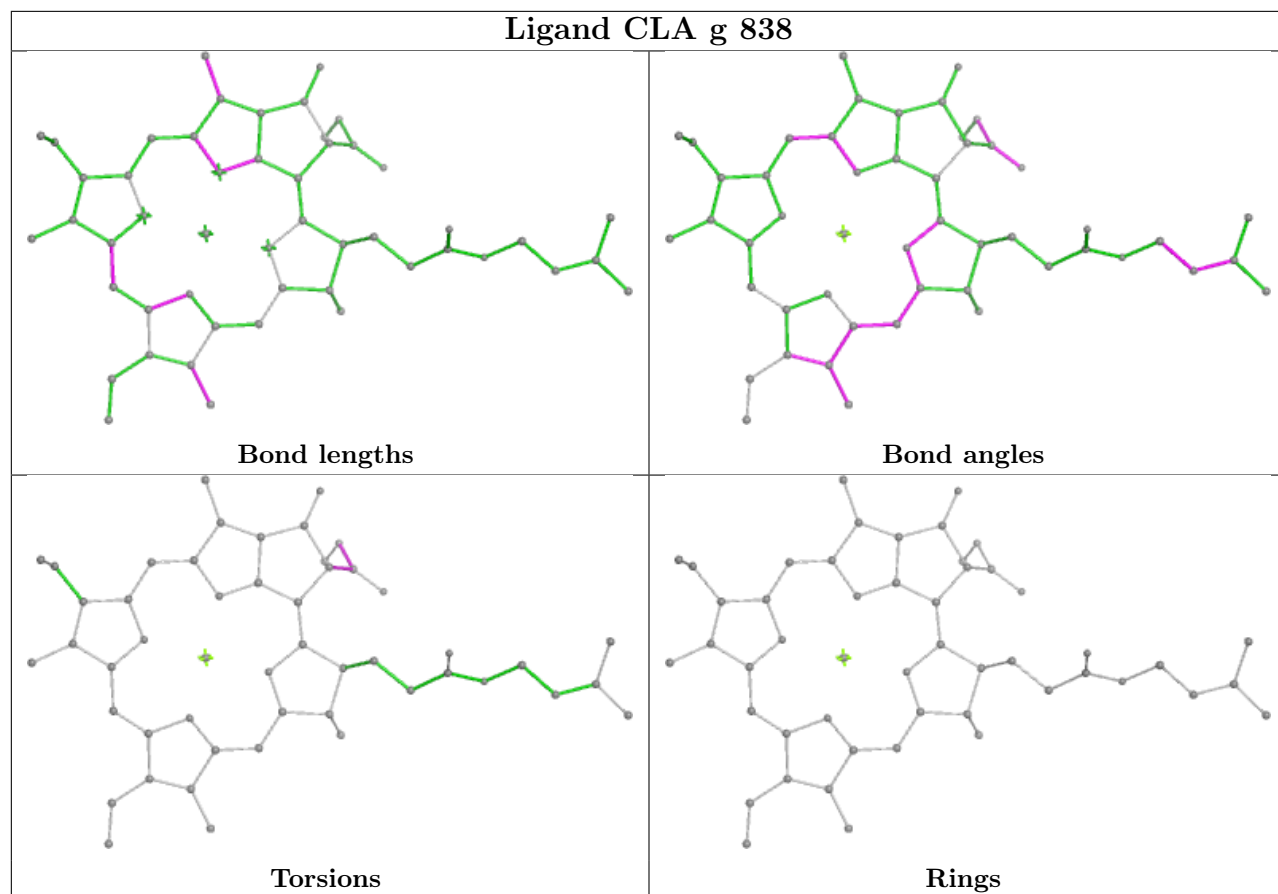


Torsions

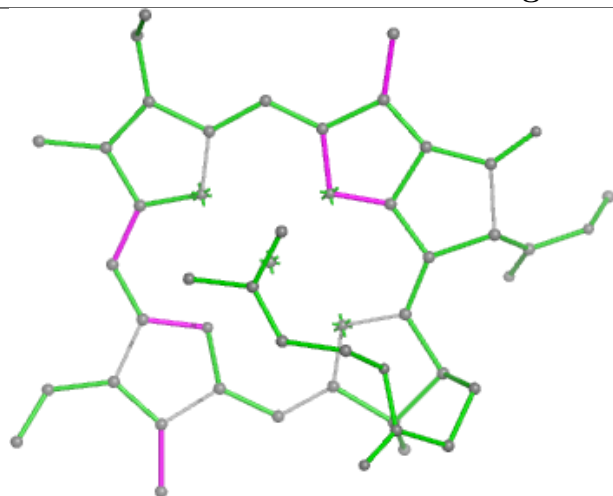


Rings

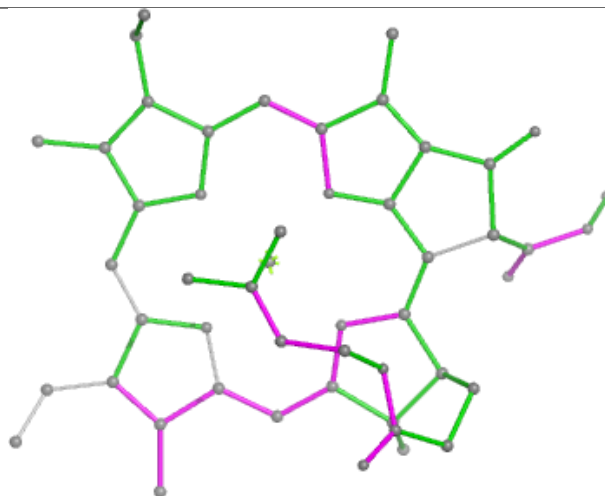
## Ligand CLA g 838



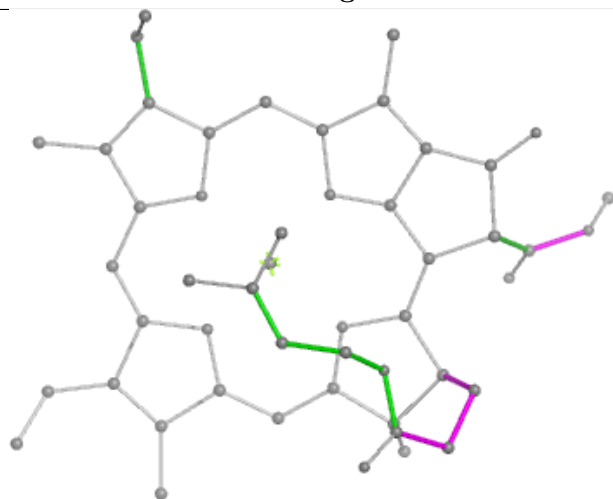
## Ligand CLA 1 203



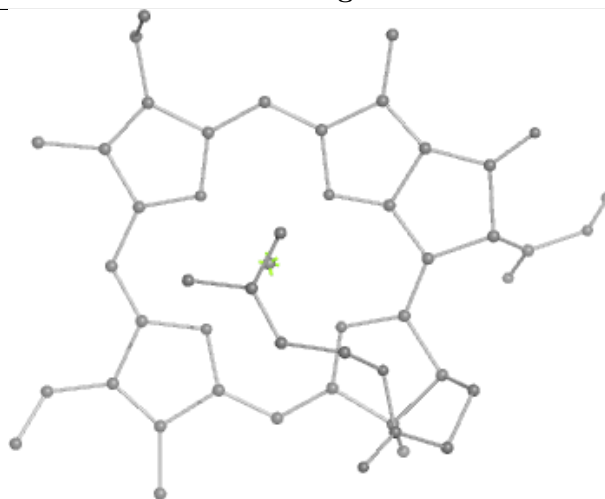
Bond lengths



Bond angles

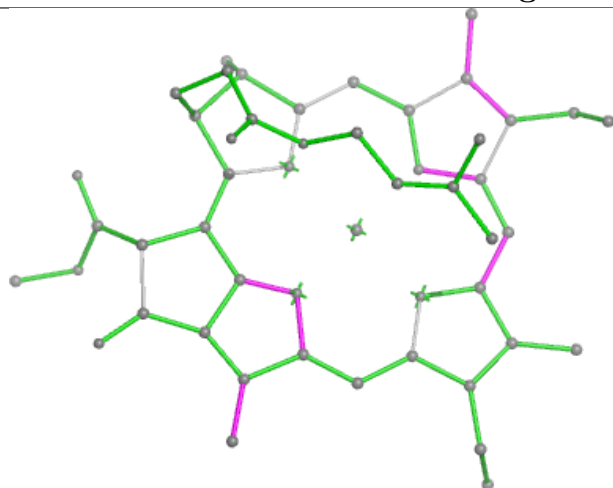


Torsions

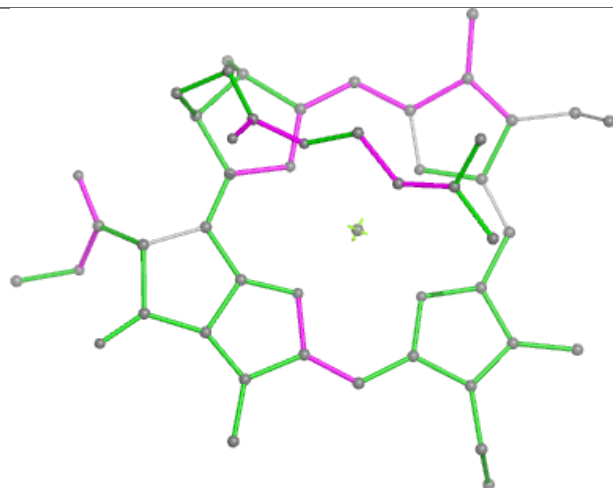


Rings

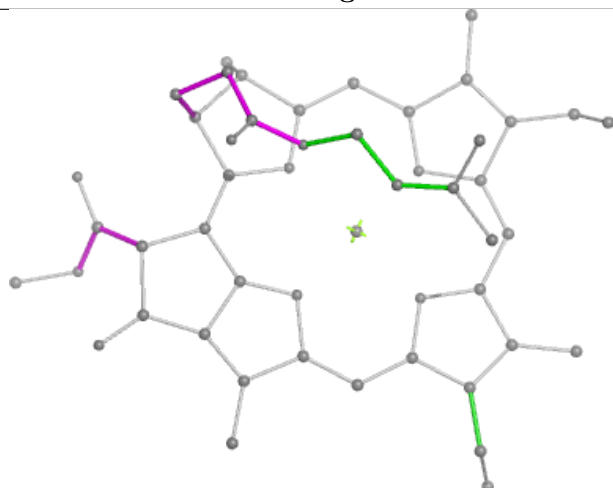
## Ligand CLA e 825



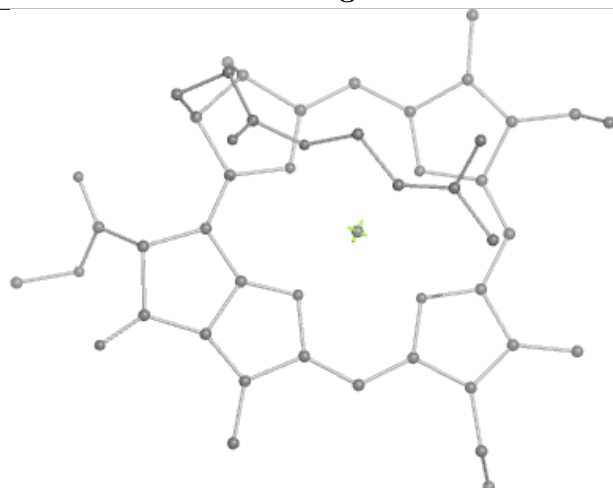
Bond lengths



Bond angles

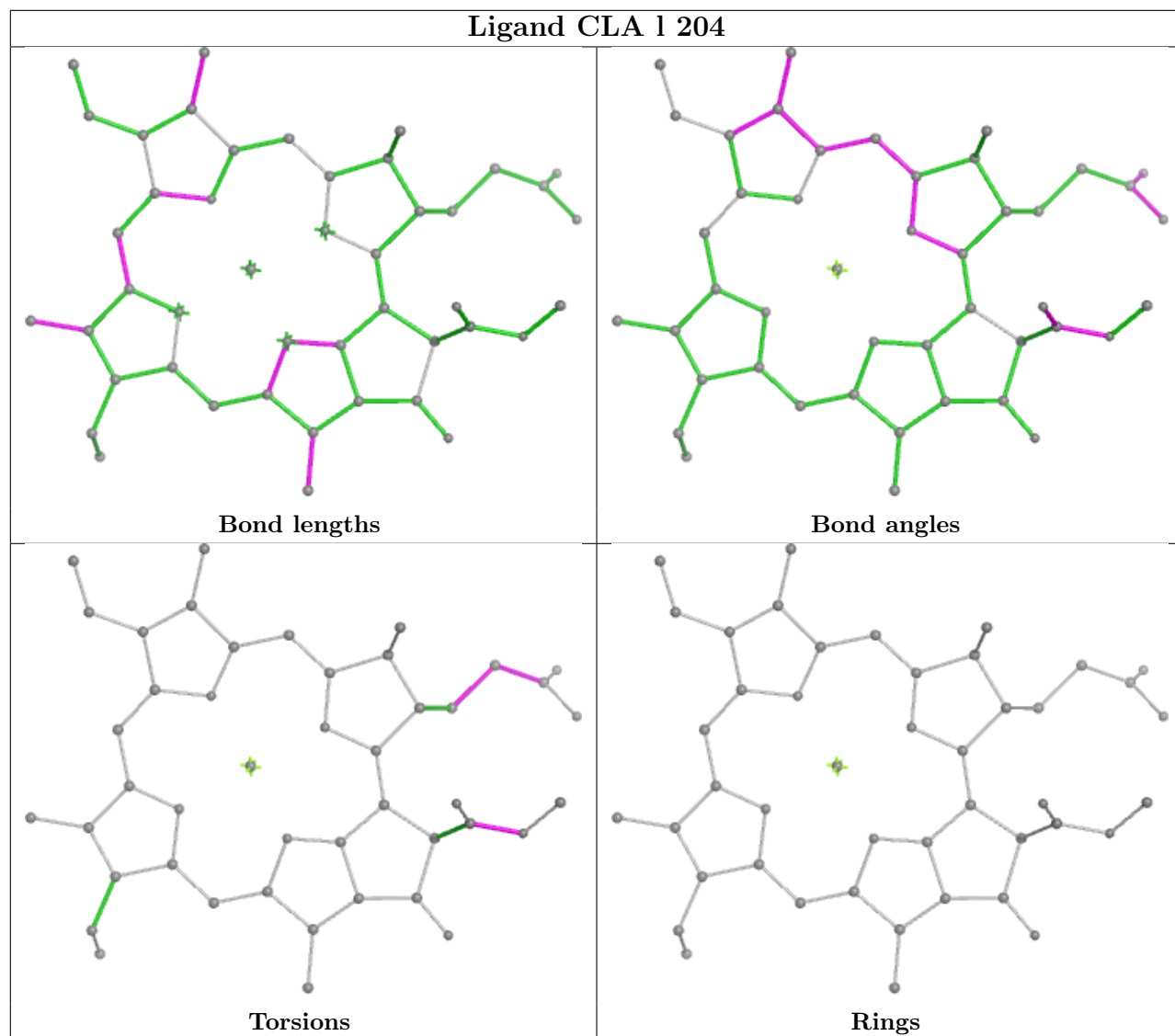


Torsions

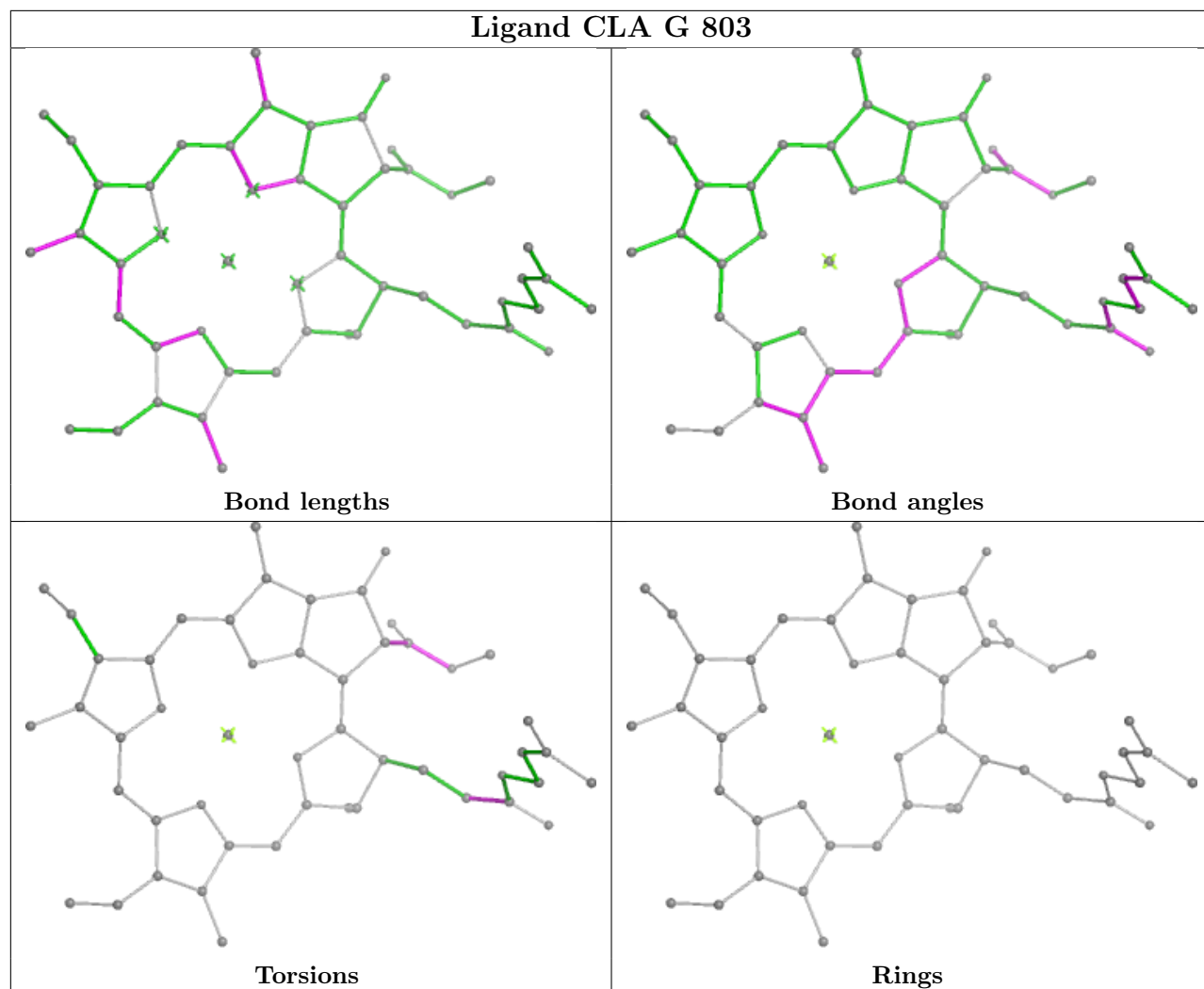


Rings

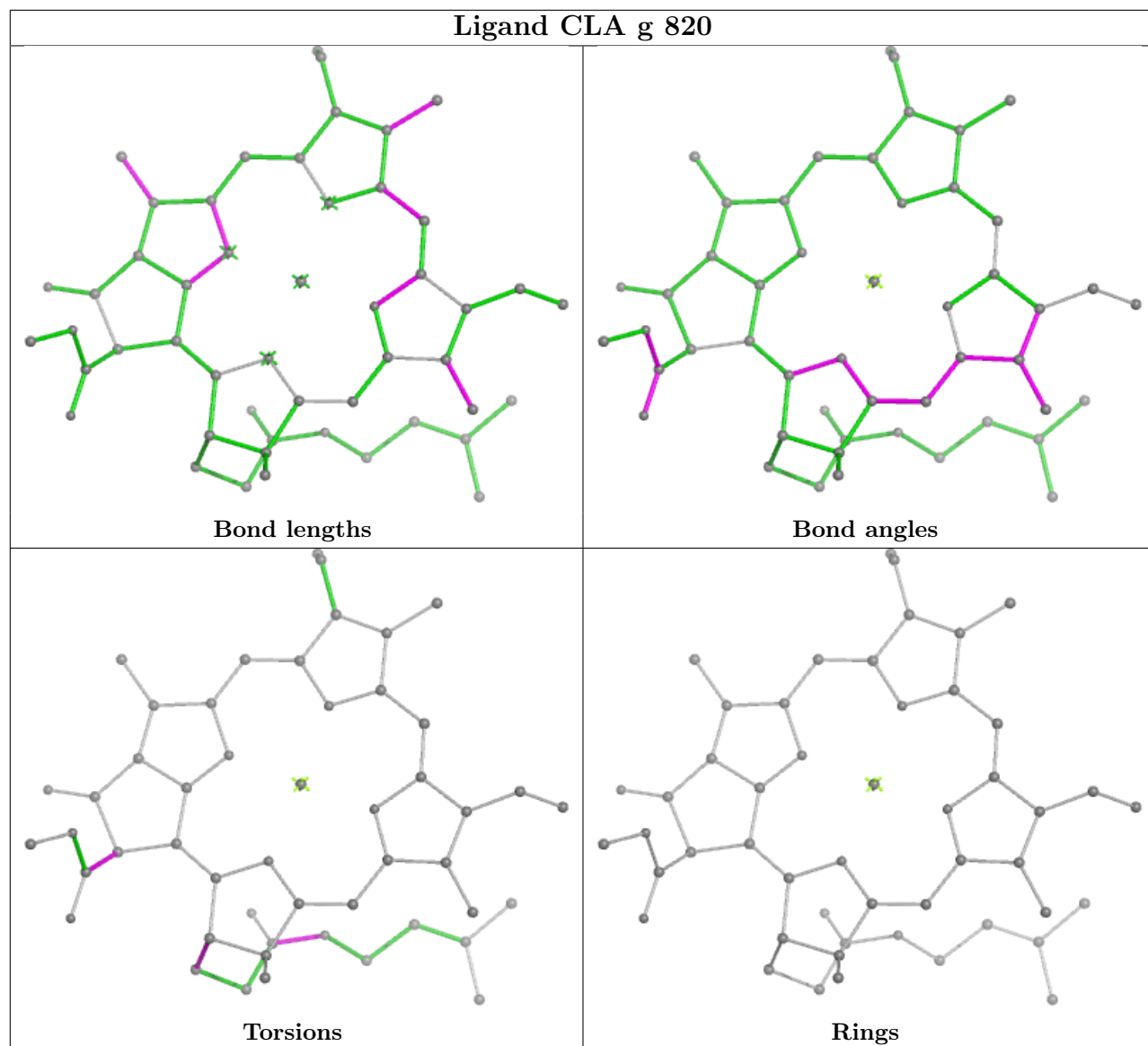
## Ligand CLA 1 204



## Ligand CLA G 803

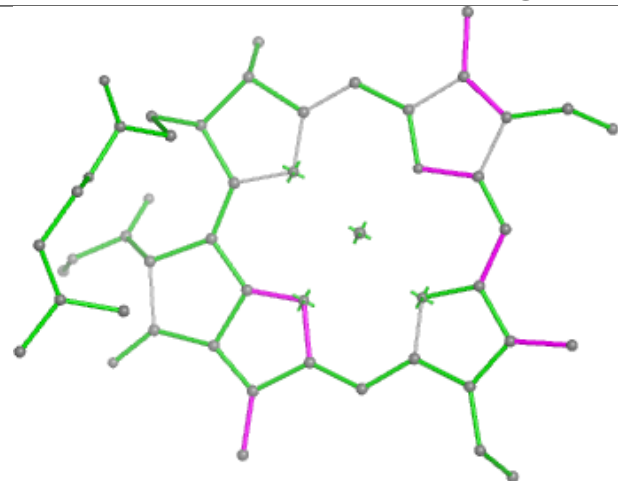


## Ligand CLA g 820

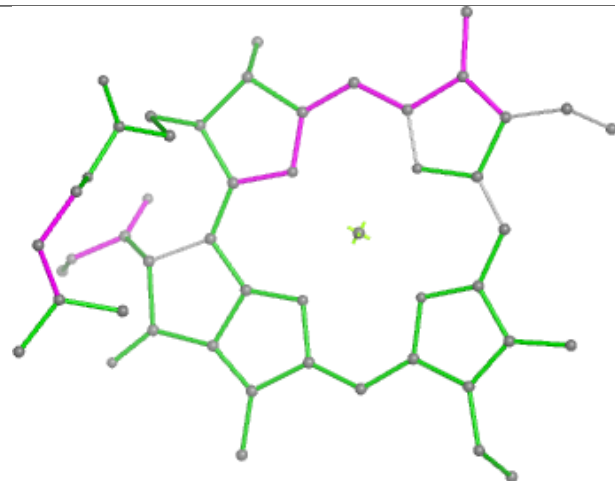




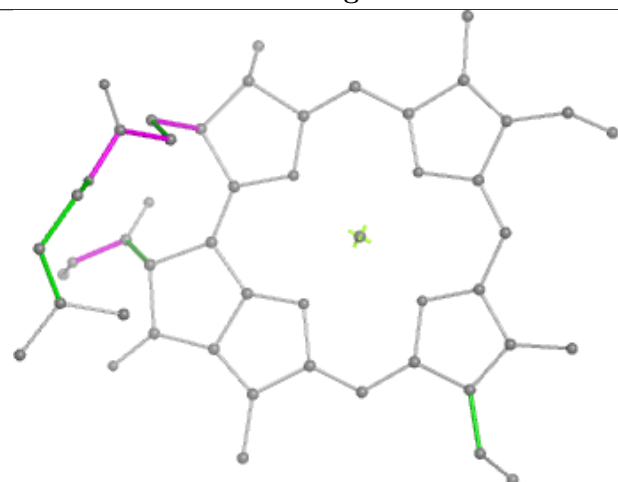
## Ligand CLA G 841



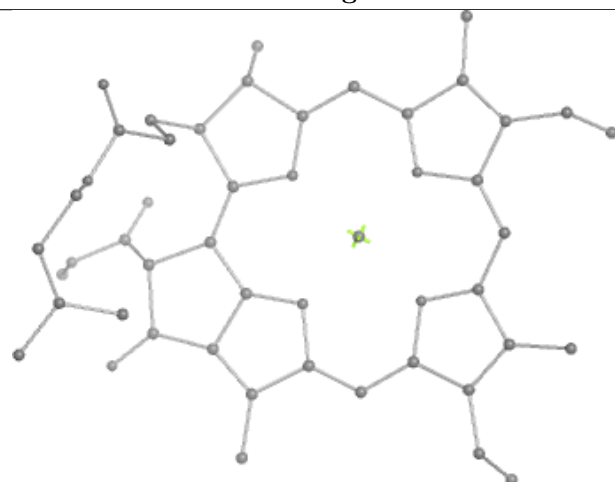
Bond lengths



Bond angles

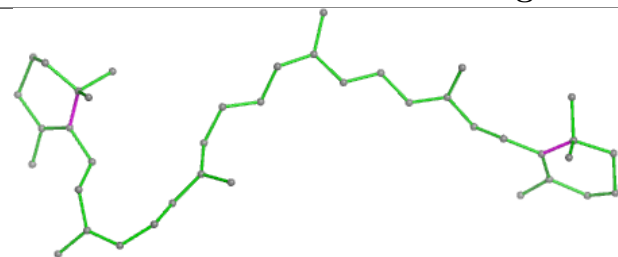


Torsions

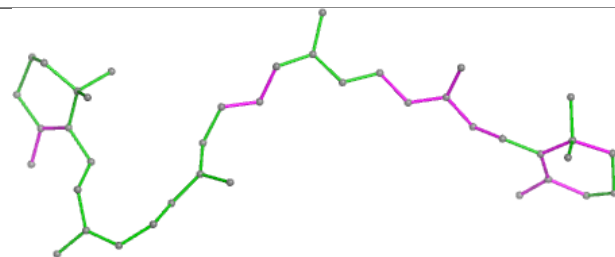


Rings

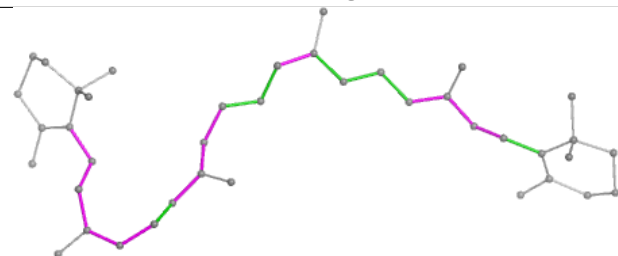
## Ligand BCR A 847



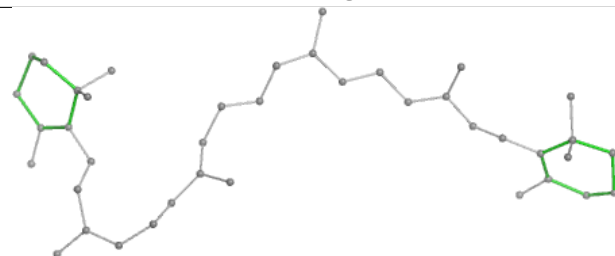
Bond lengths



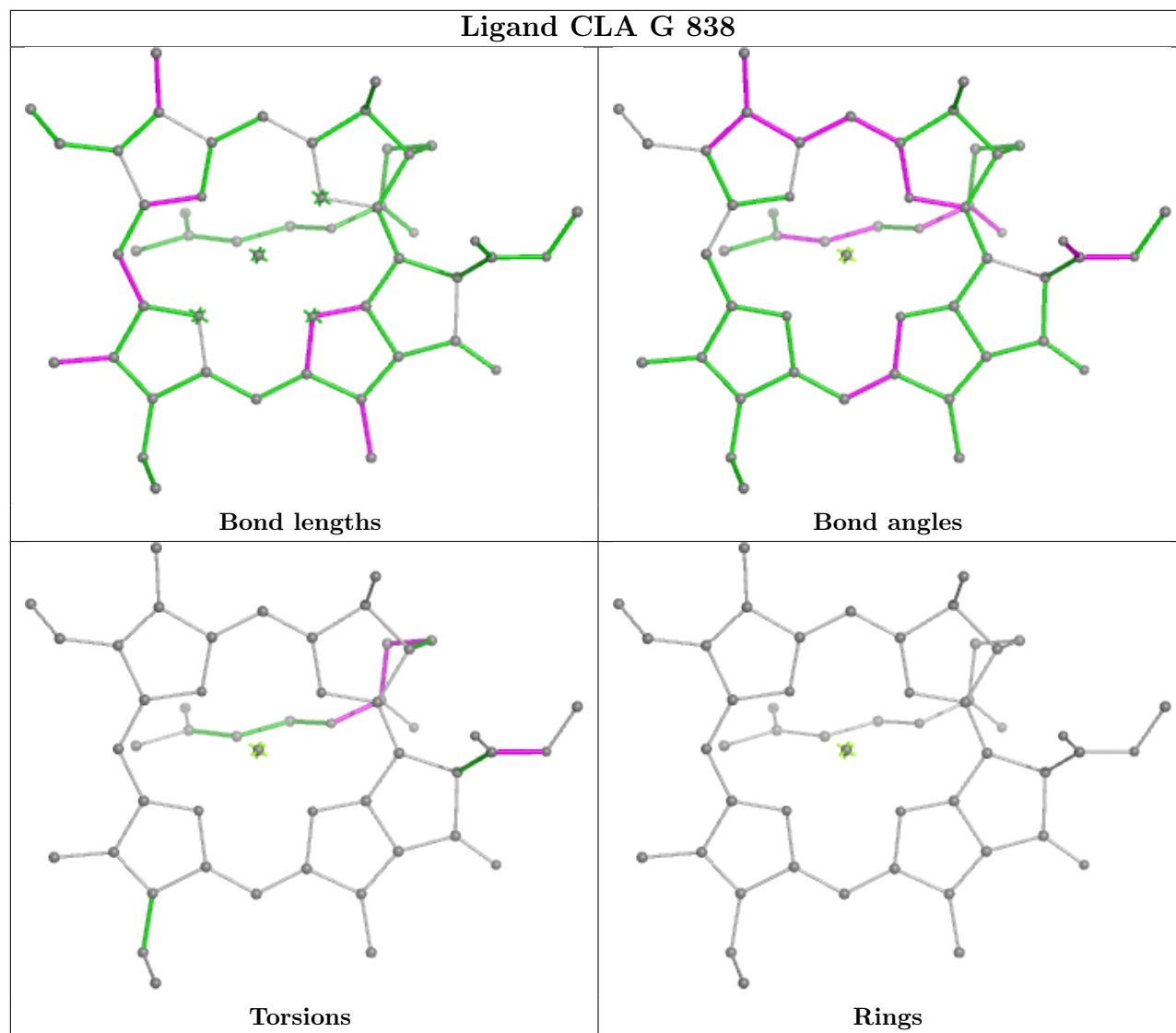
Bond angles



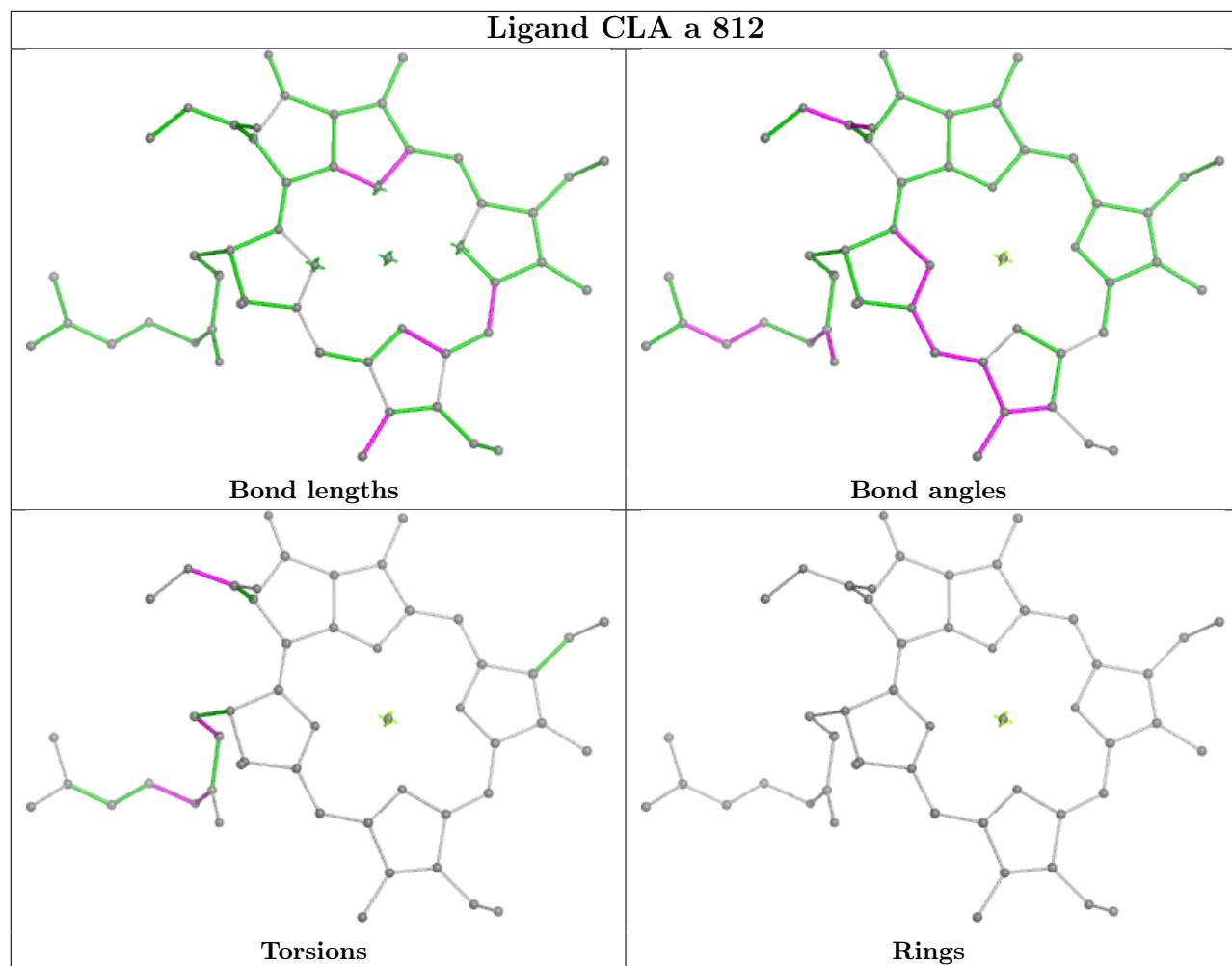
Torsions



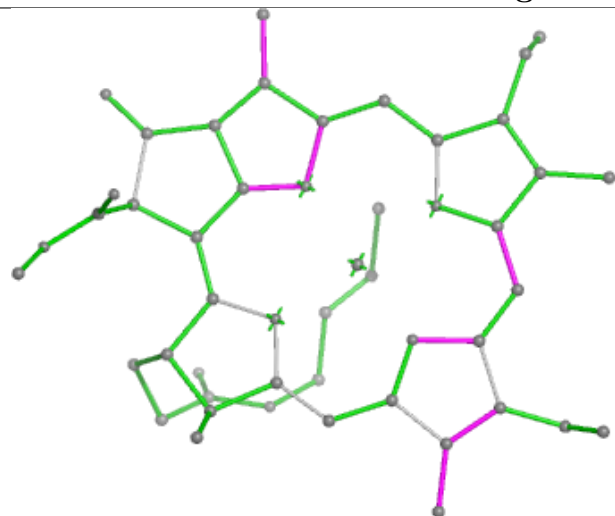
Rings



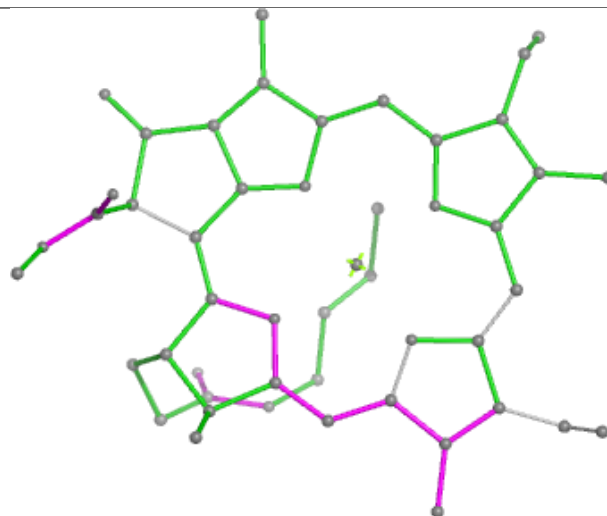
## Ligand CLA a 812



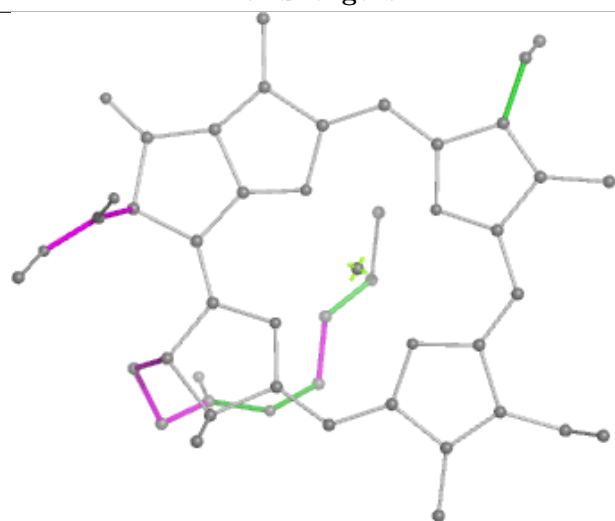
## Ligand CLA A 819



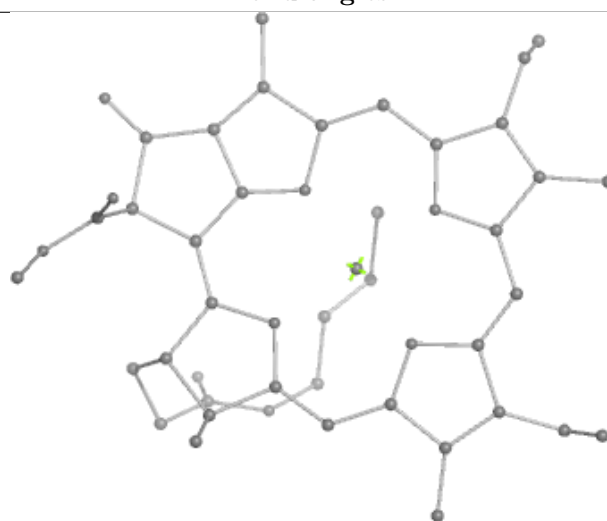
Bond lengths



Bond angles

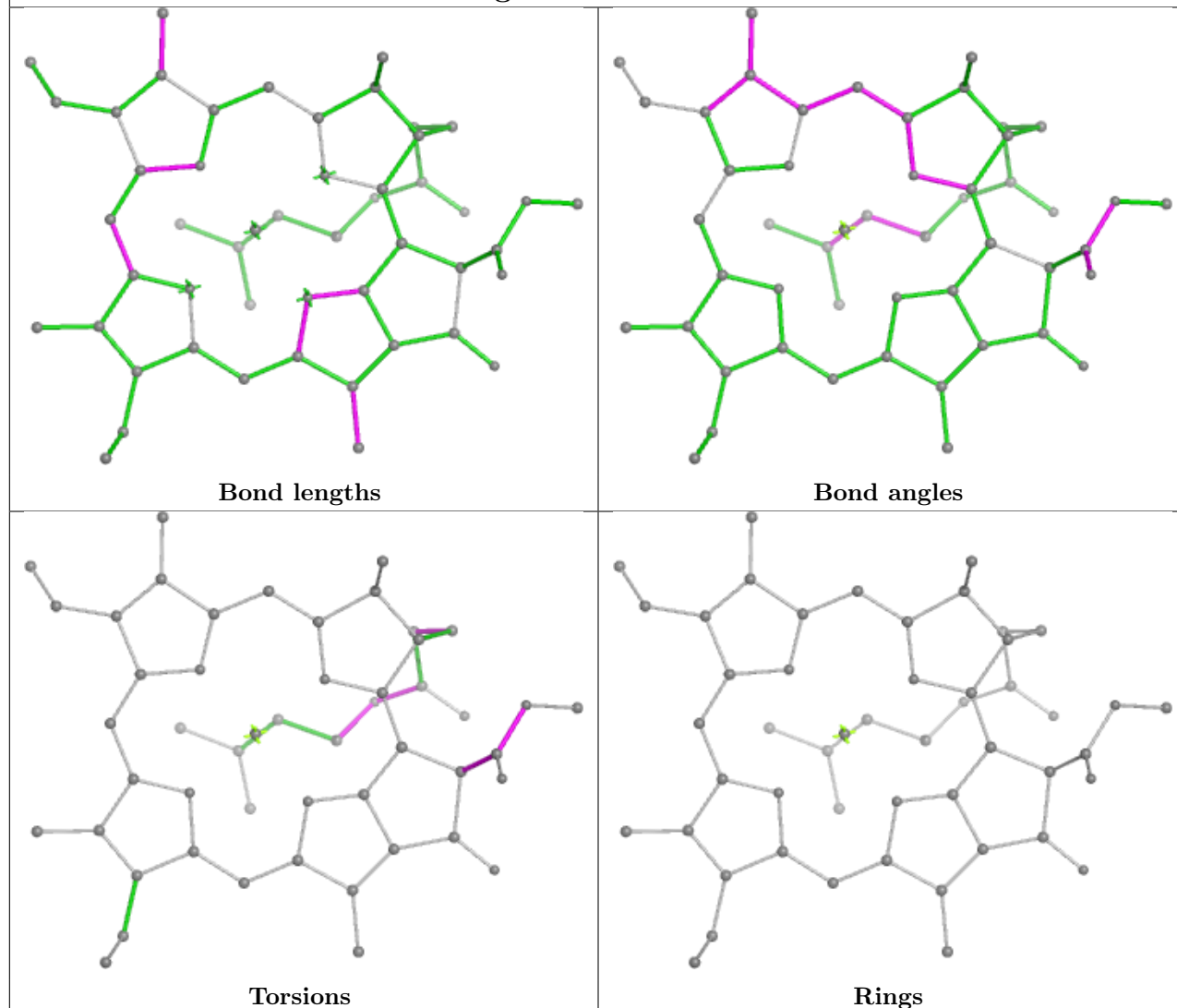


Torsions

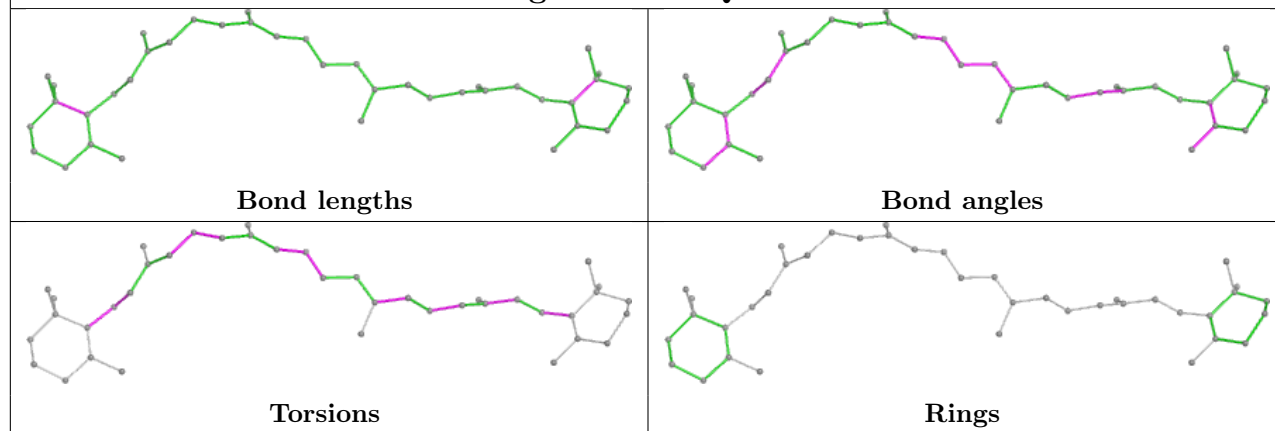


Rings

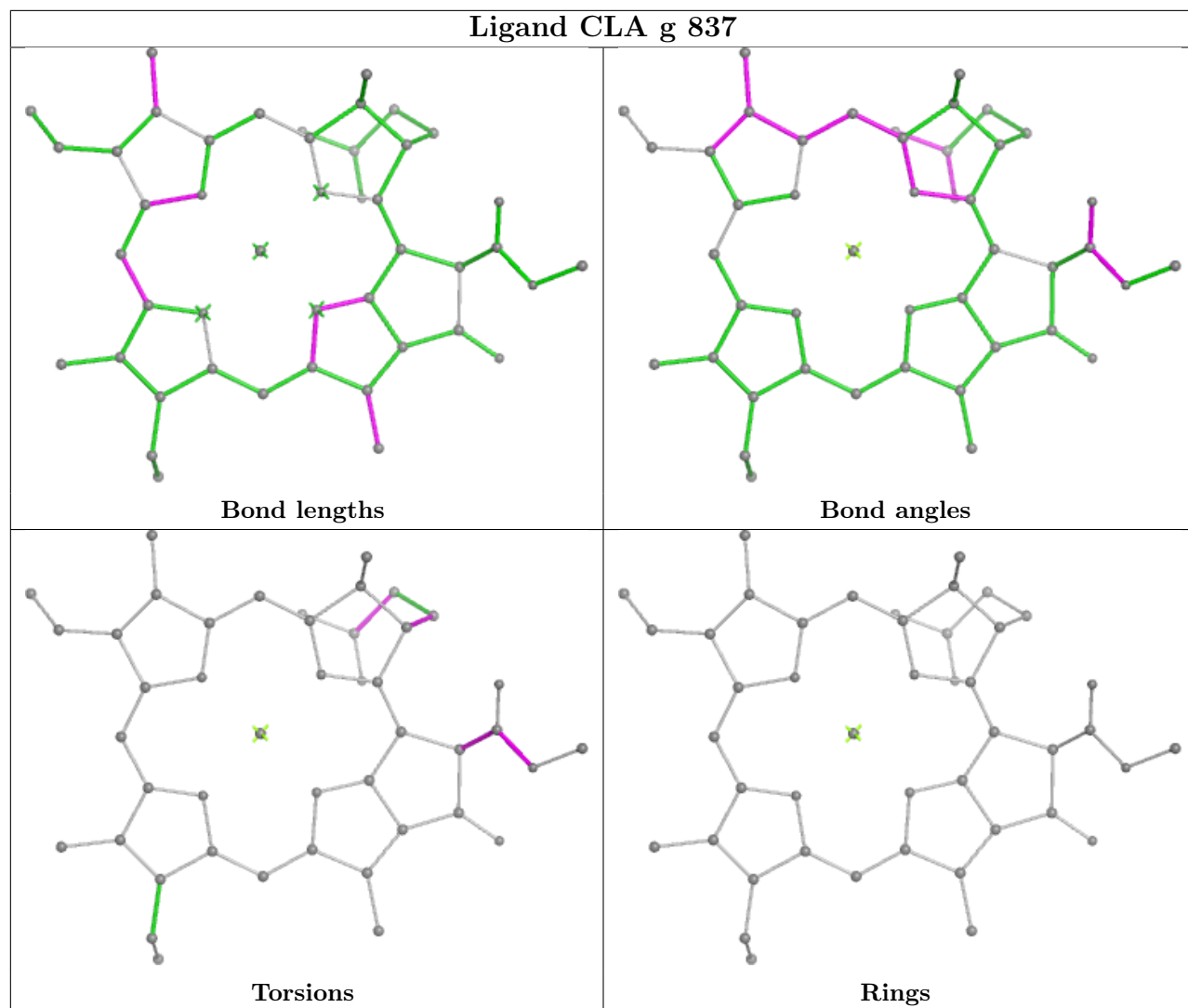
## Ligand CLA e 814



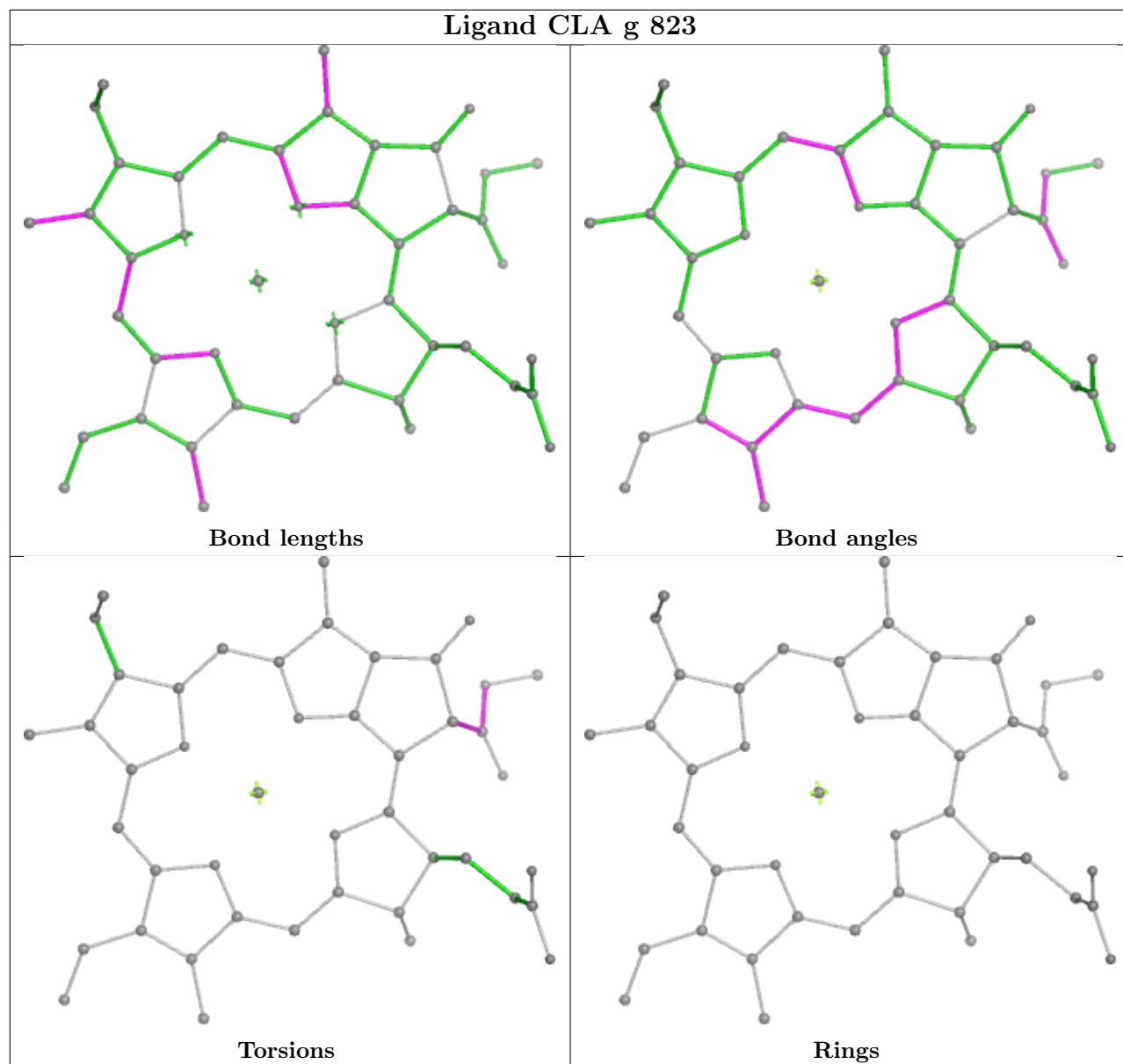
## Ligand BCR Q 101

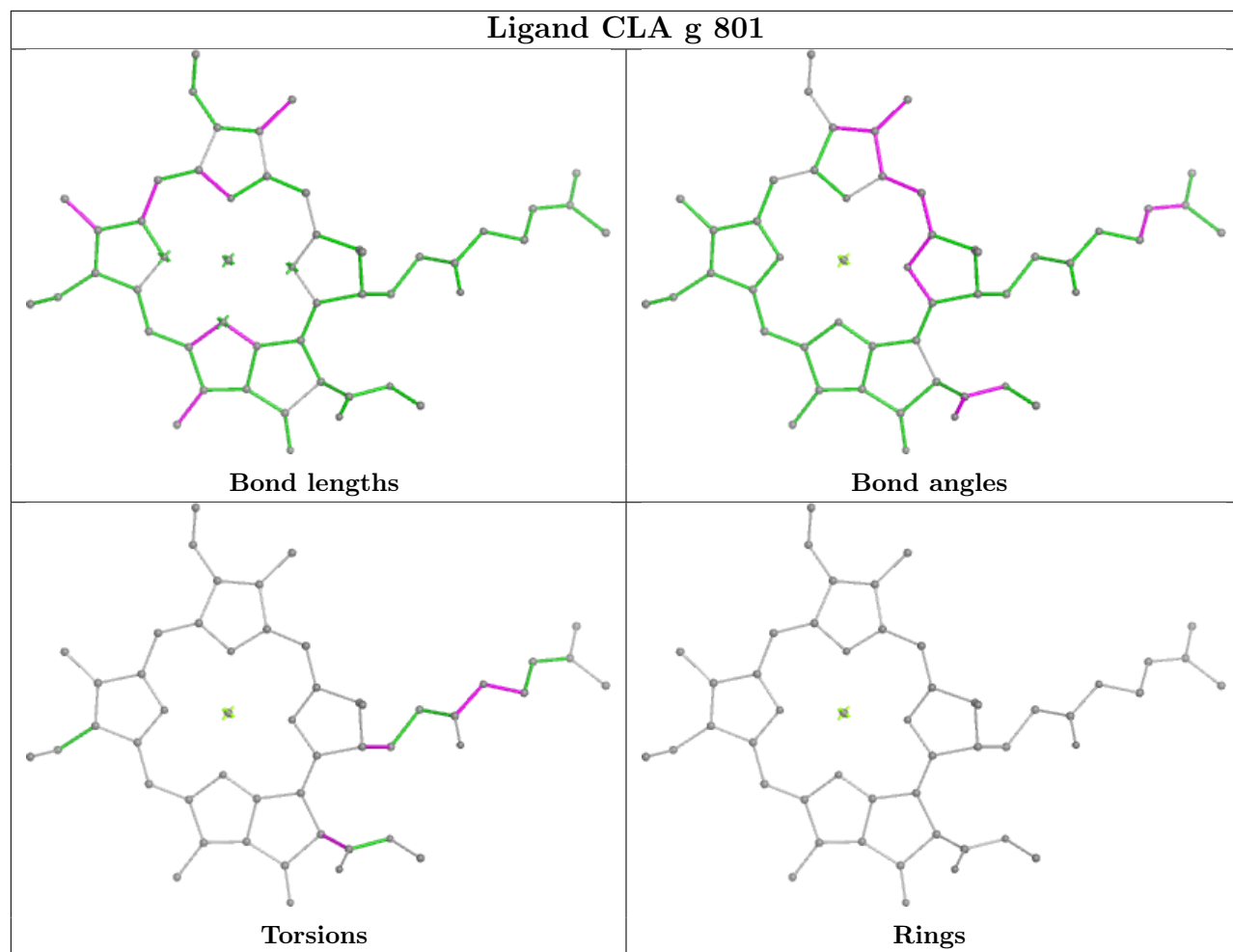


## Ligand CLA g 837



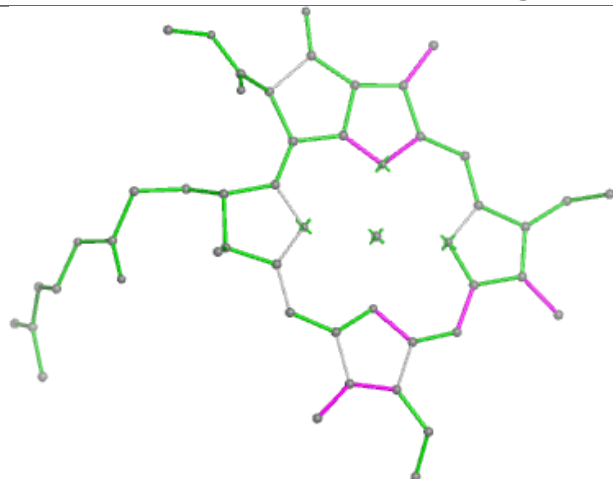
## Ligand CLA g 823



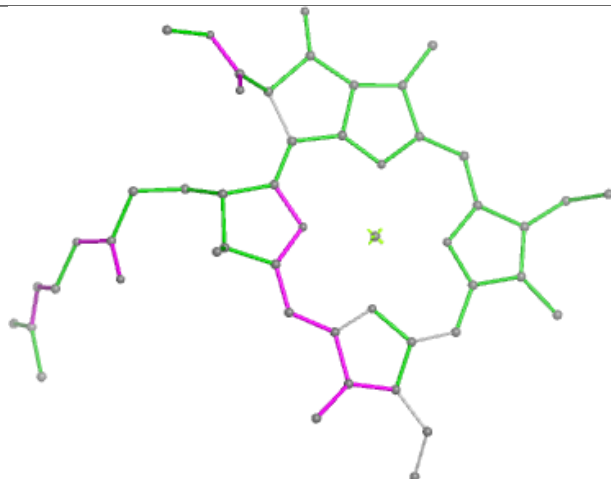




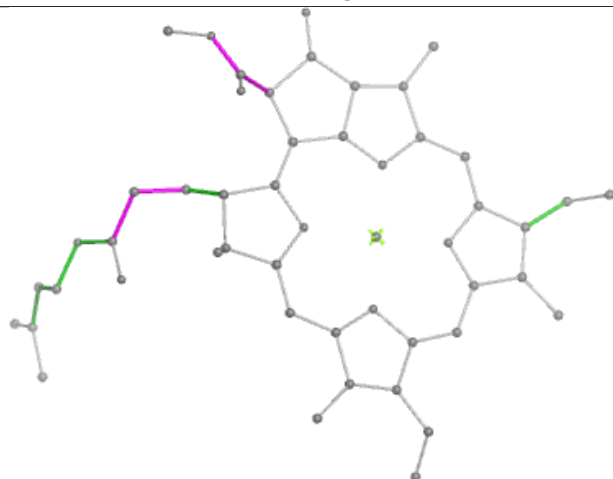
## Ligand CLA B 811



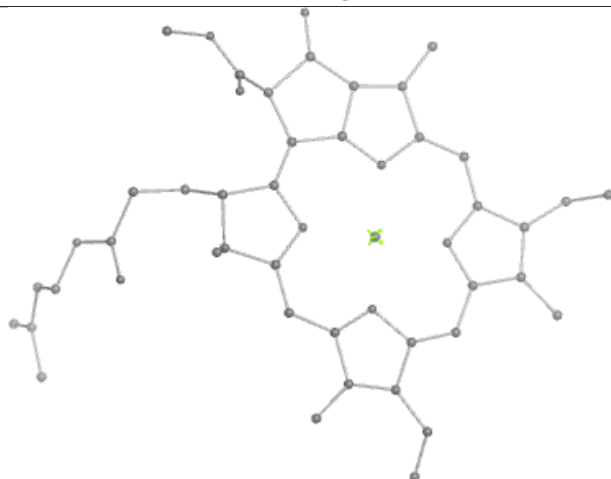
Bond lengths



Bond angles

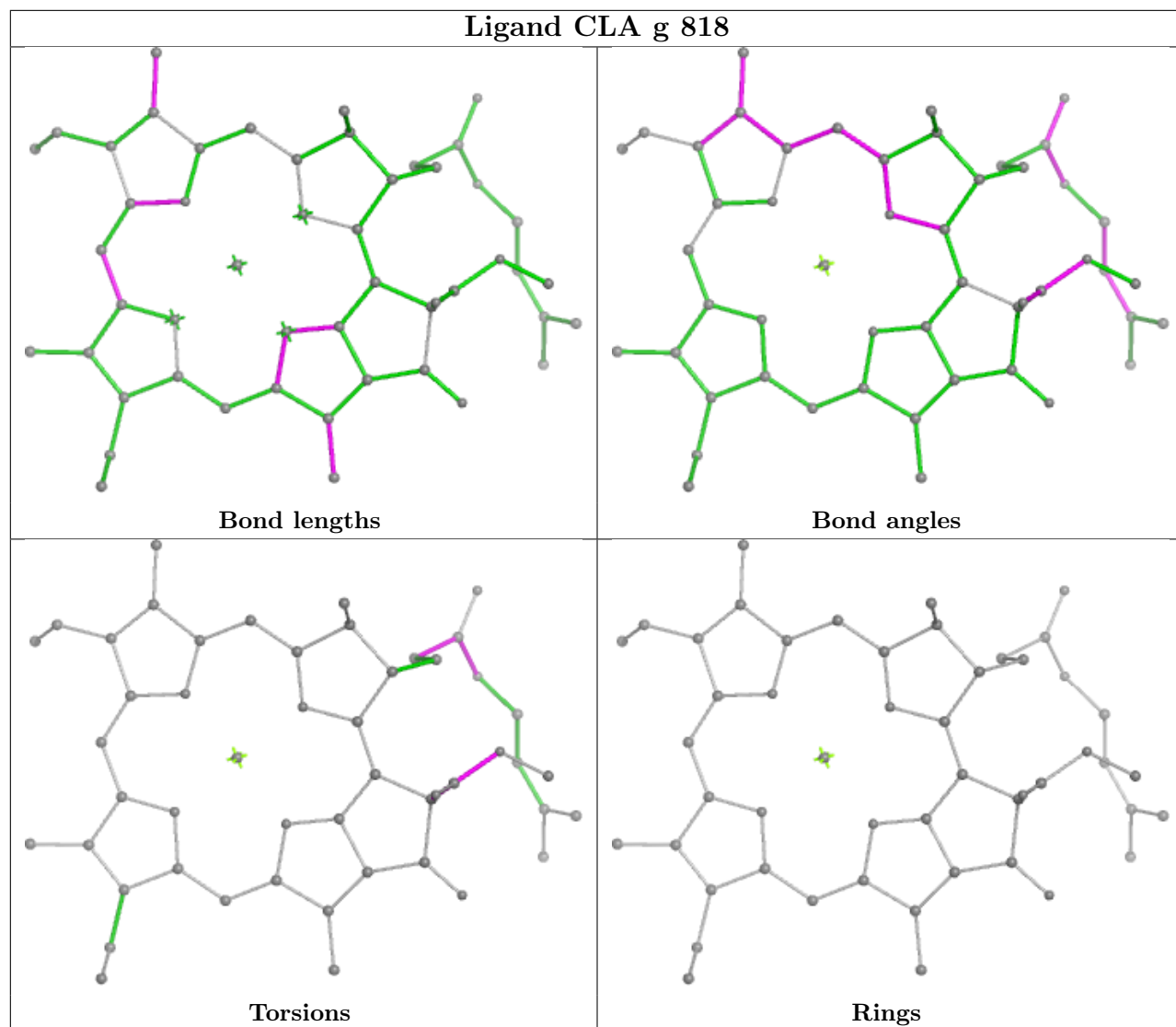


Torsions

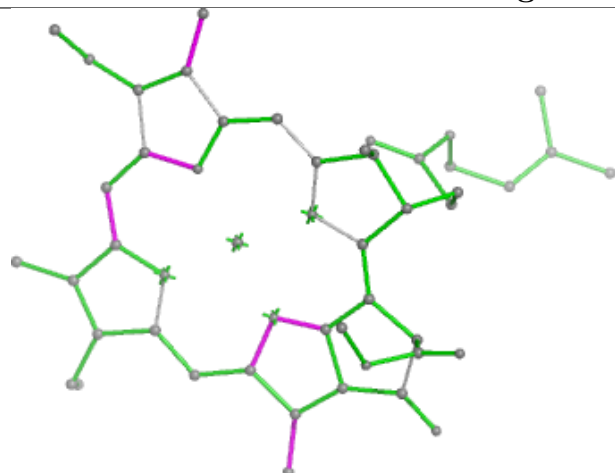


Rings

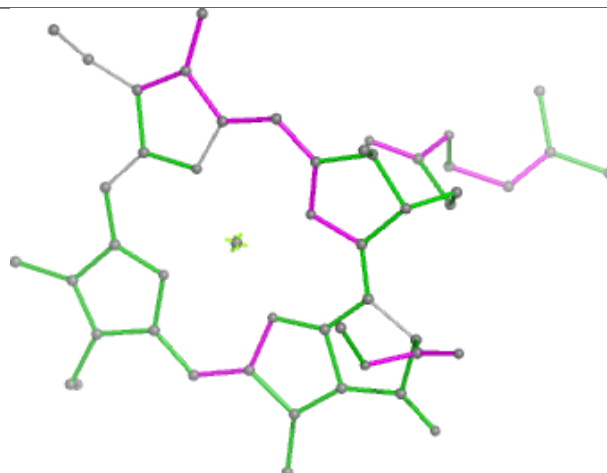
## Ligand CLA g 818



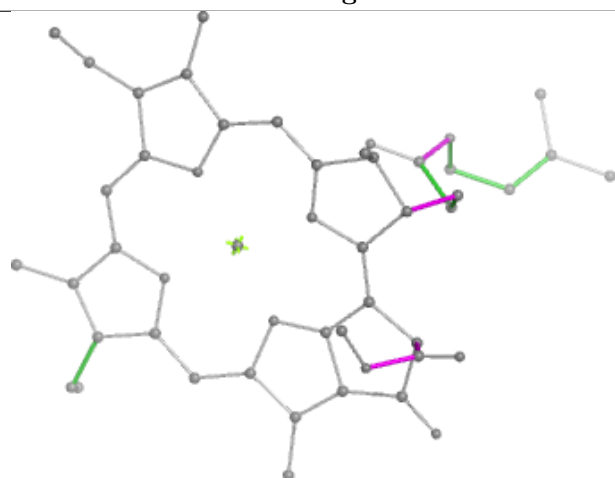
## Ligand CLA E 838



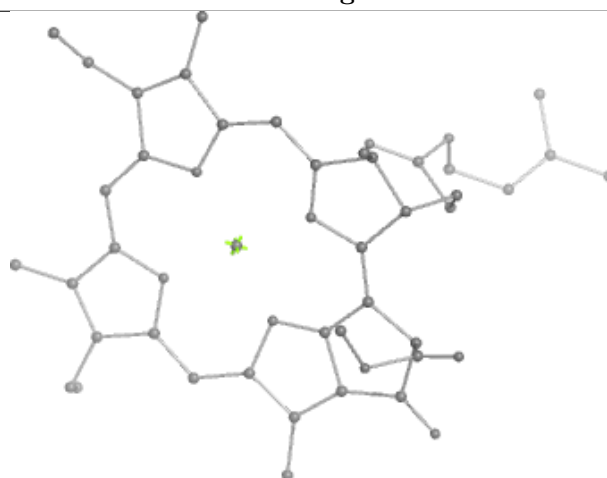
Bond lengths



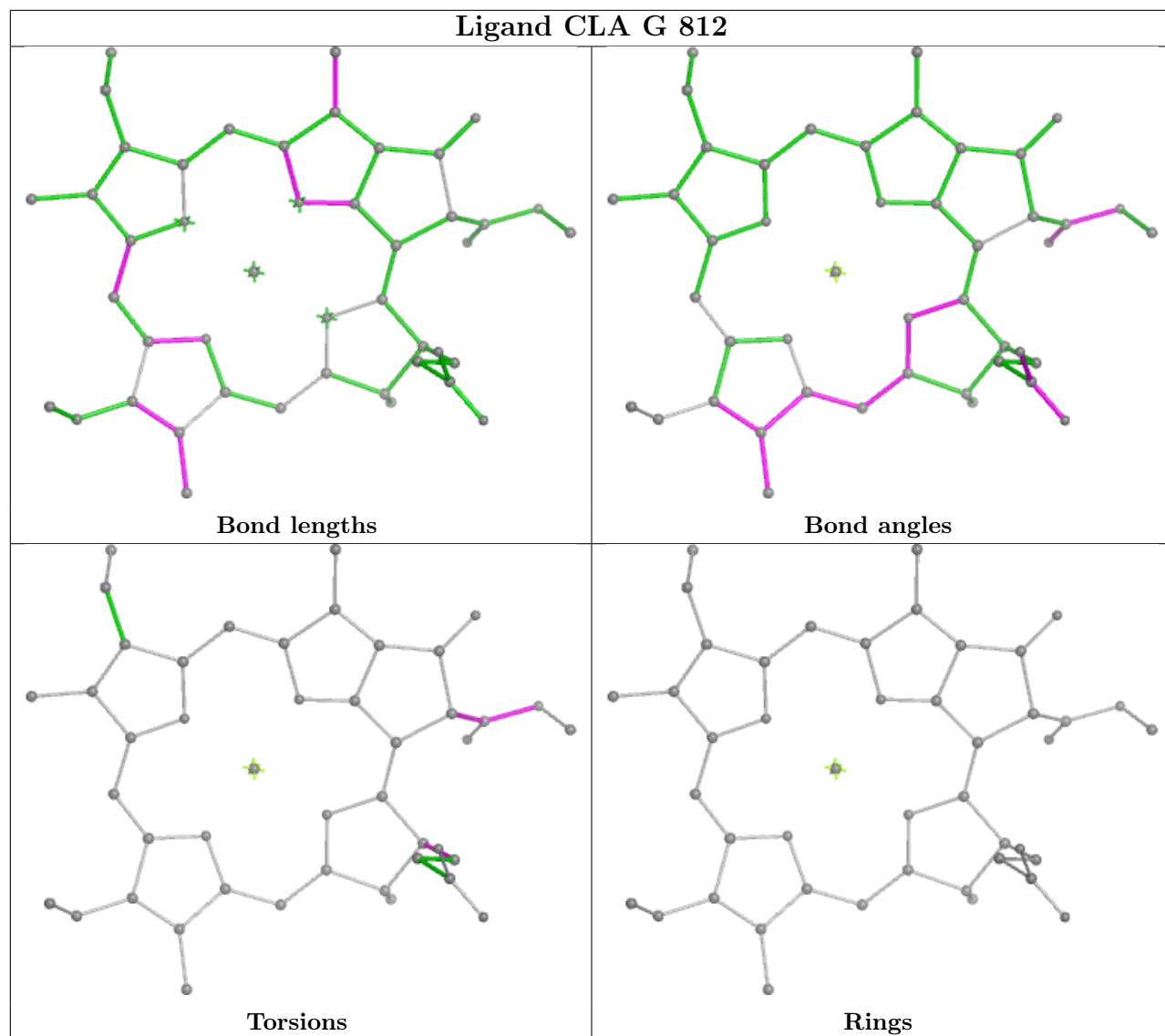
Bond angles



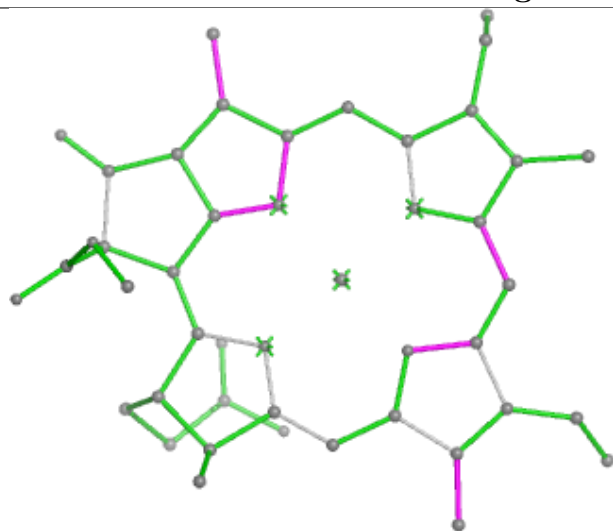
Torsions



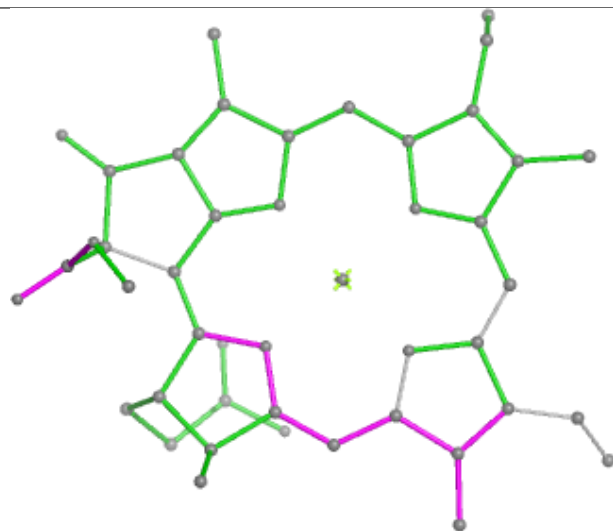
Rings



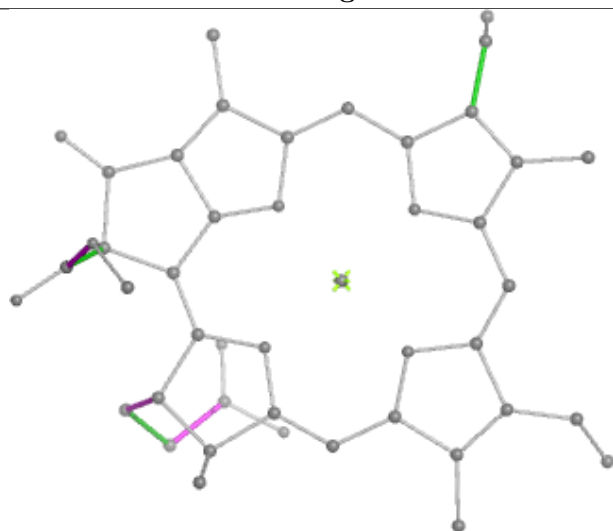
## Ligand CLA B 816



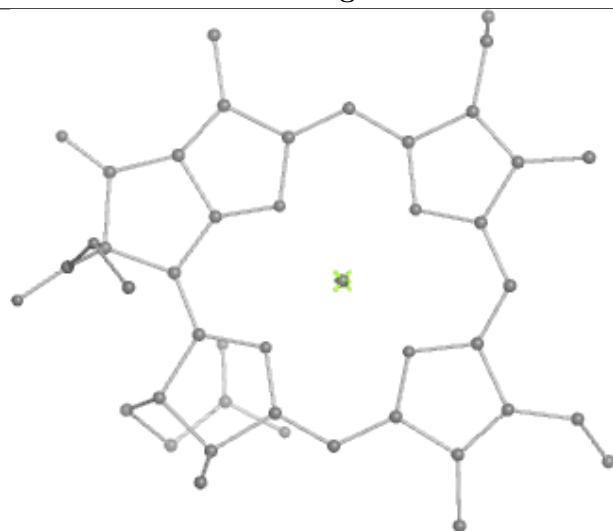
Bond lengths



Bond angles

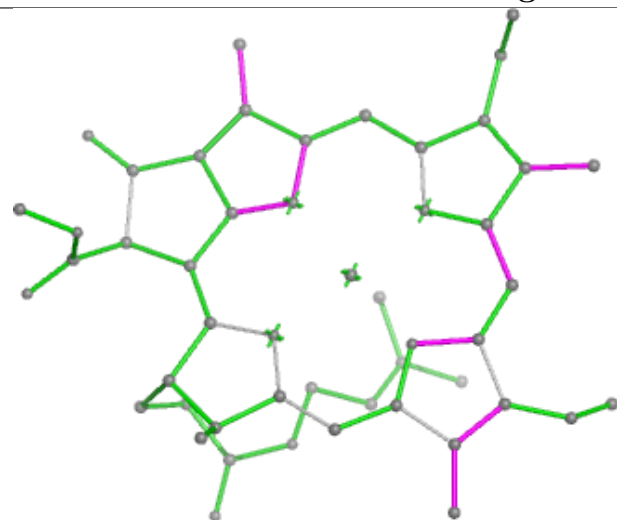


Torsions

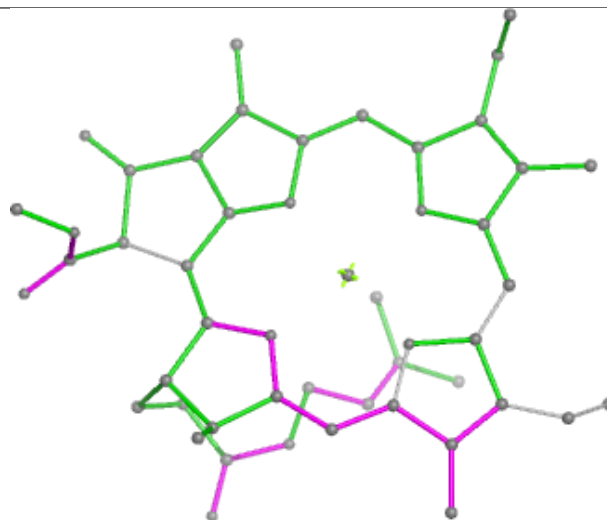


Rings

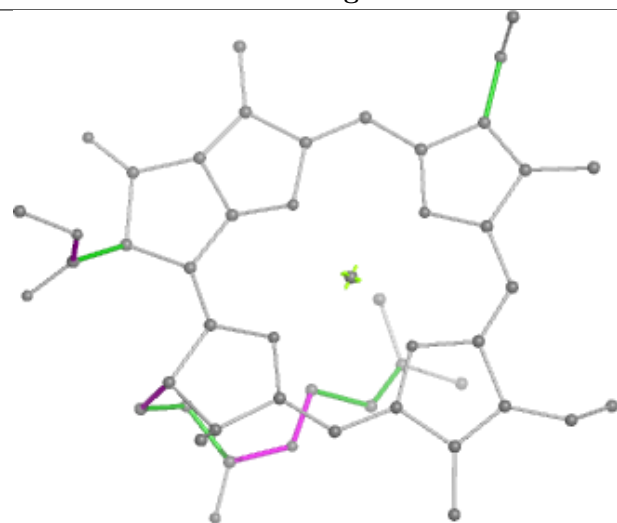
## Ligand CLA B 828



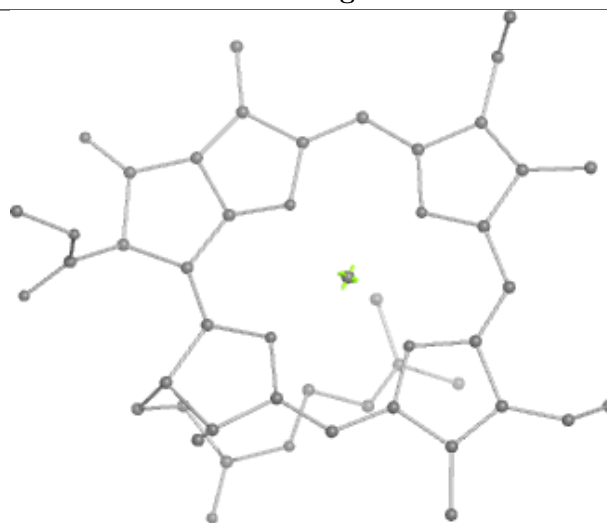
Bond lengths



Bond angles

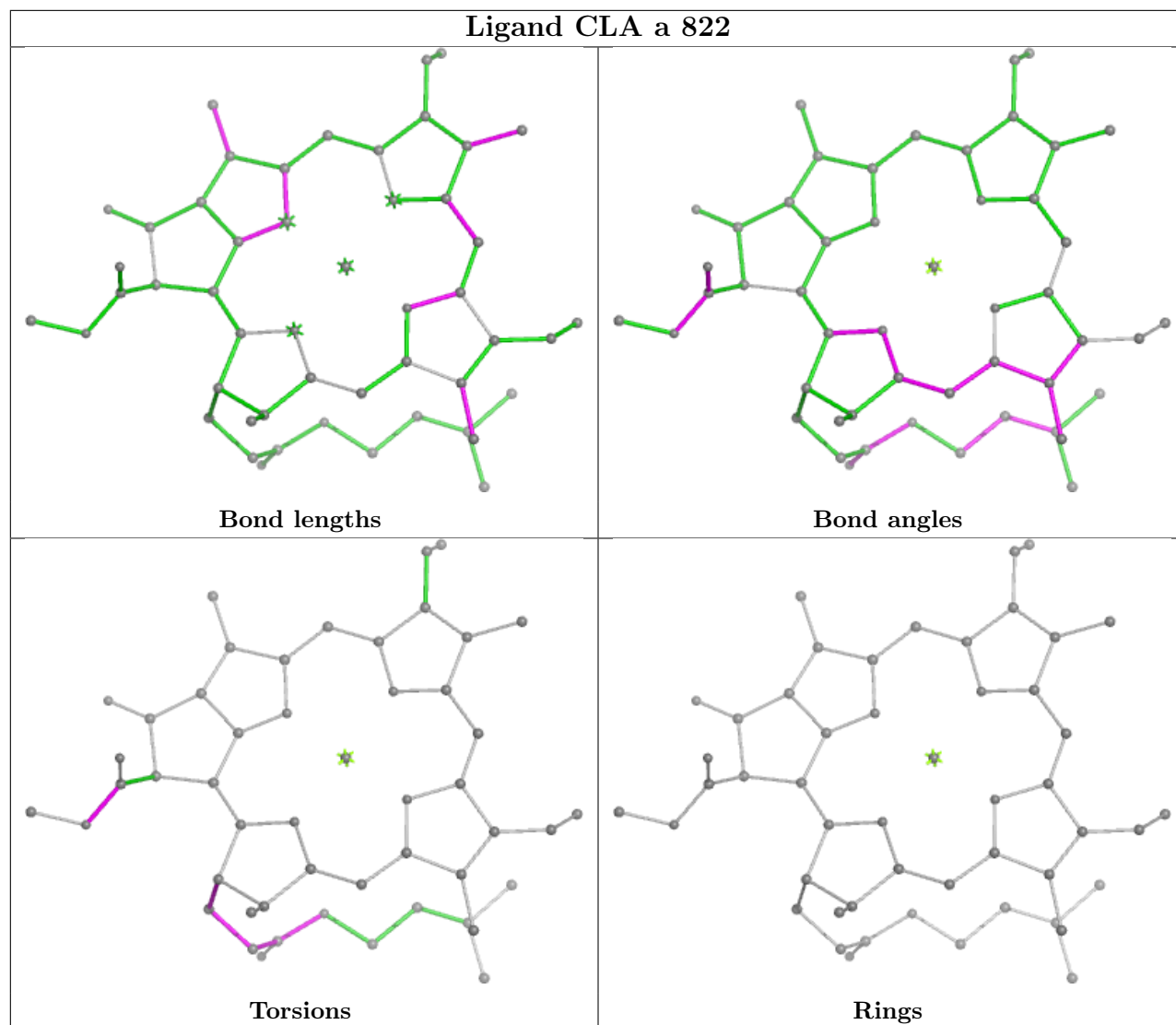


Torsions

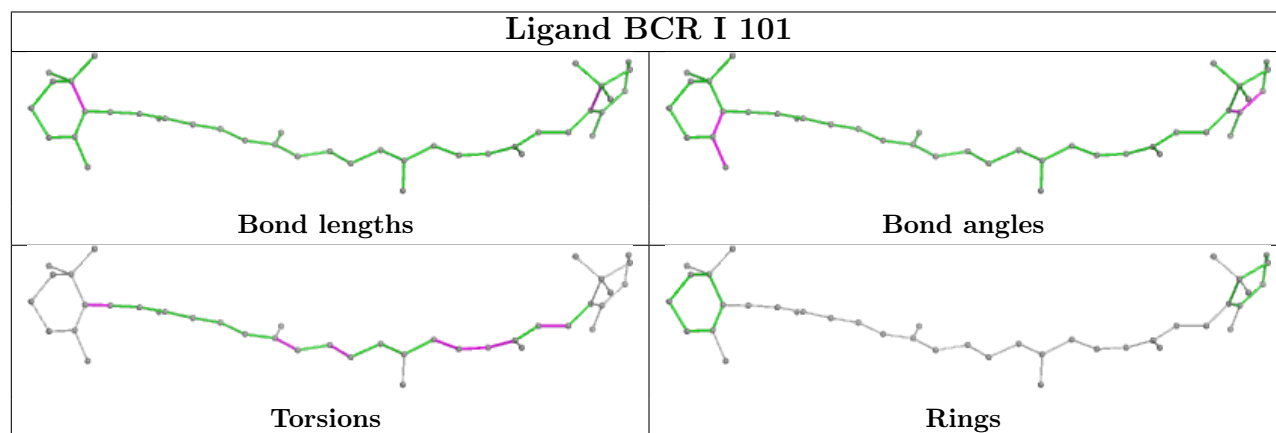


Rings

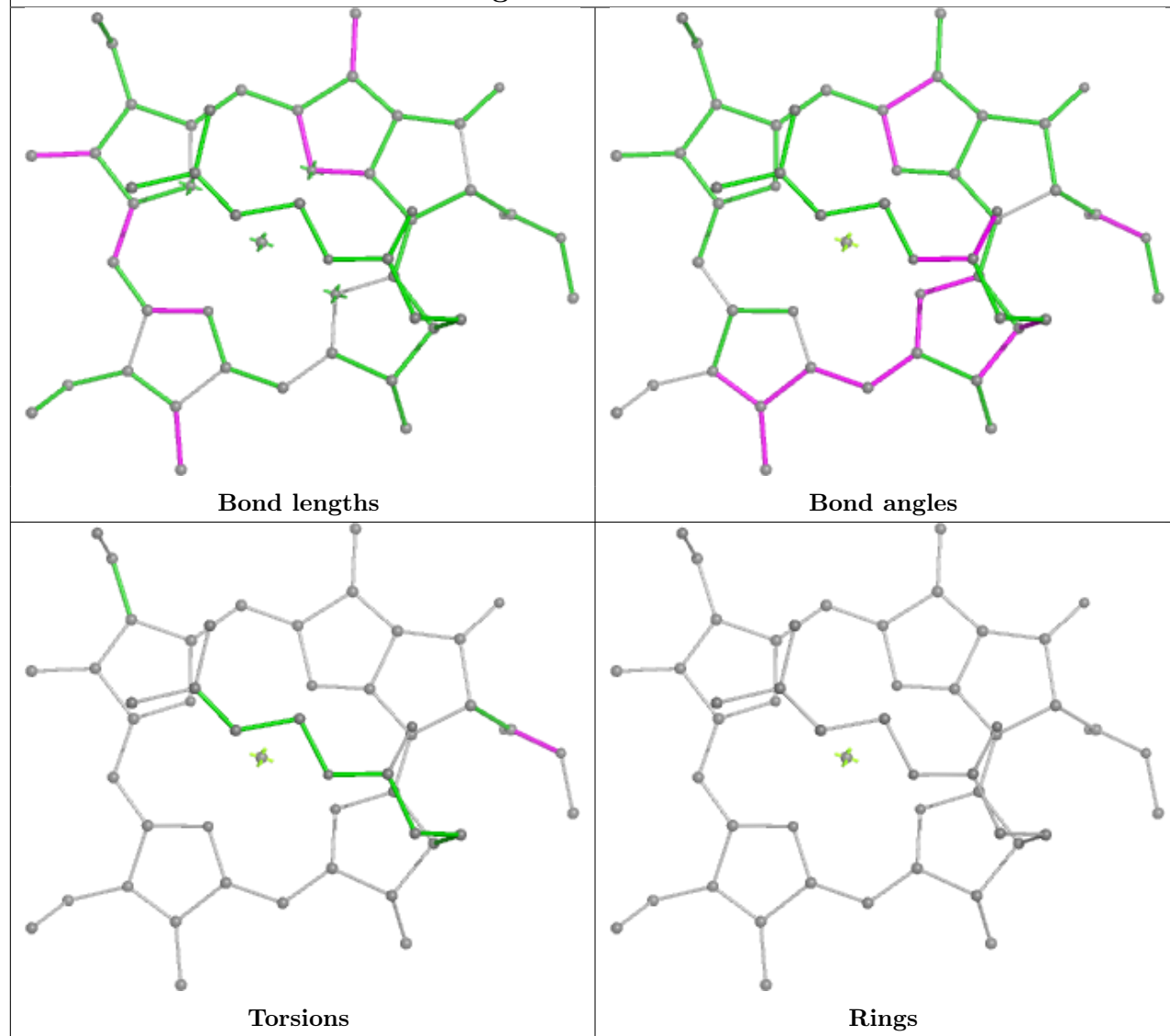
## Ligand CLA a 822



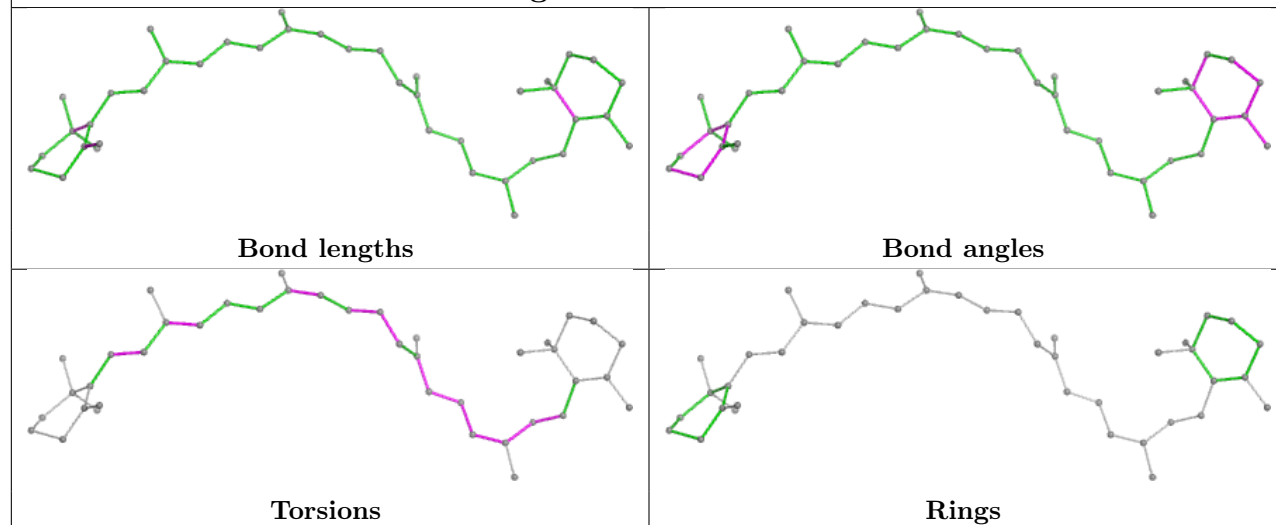
## Ligand BCR I 101



## Ligand CLA e 819

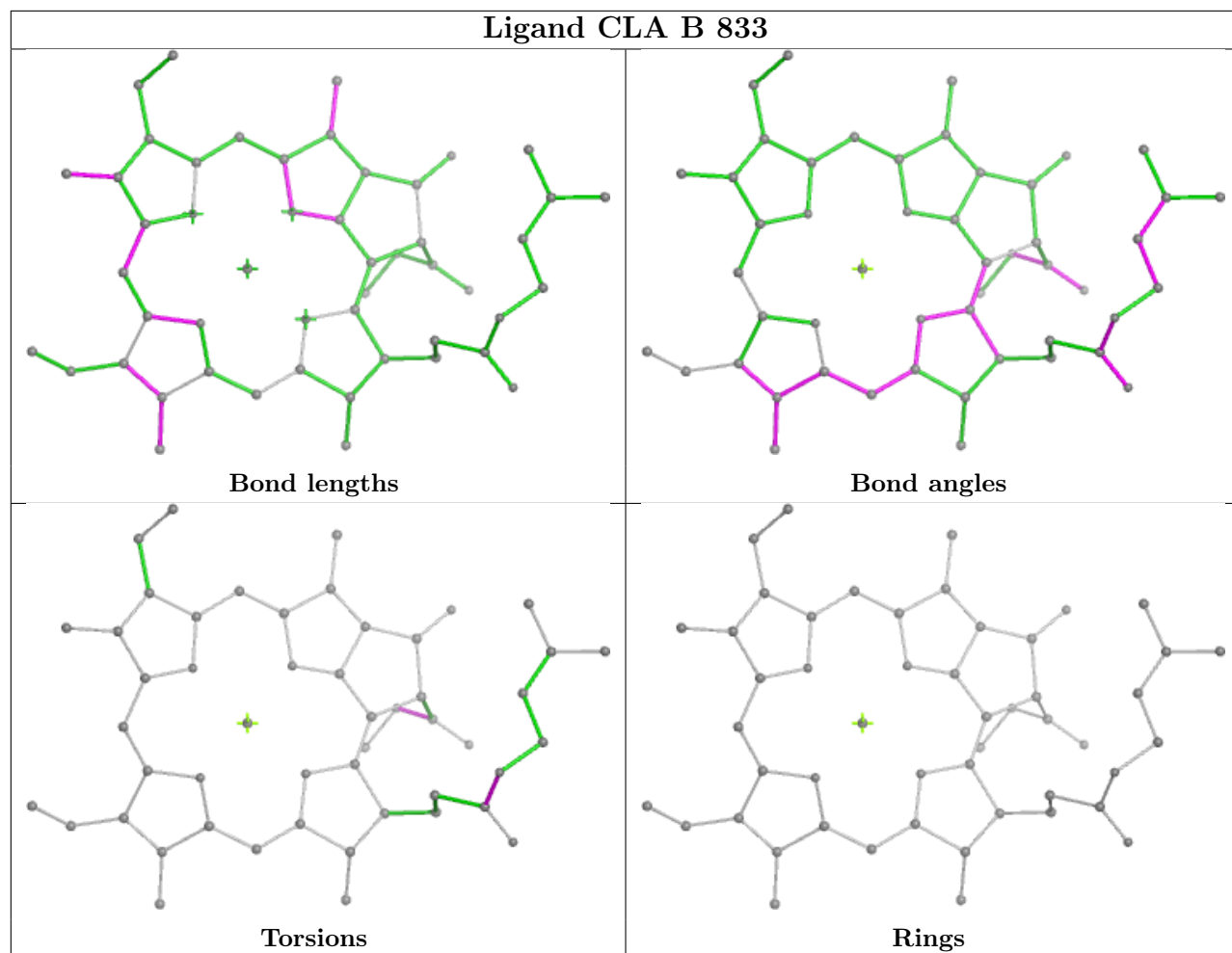


## Ligand BCR R 101

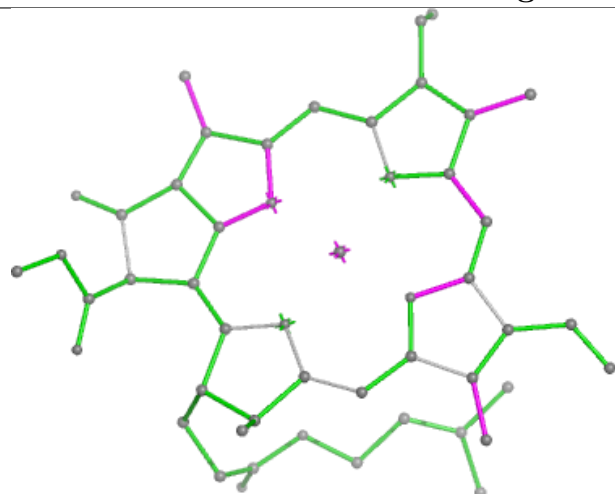




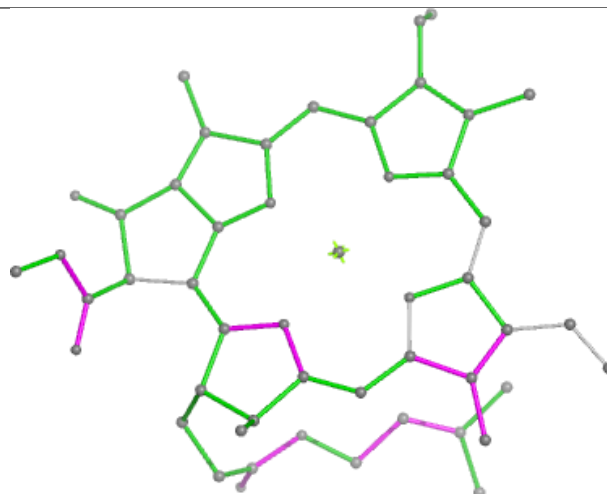
## Ligand CLA B 833



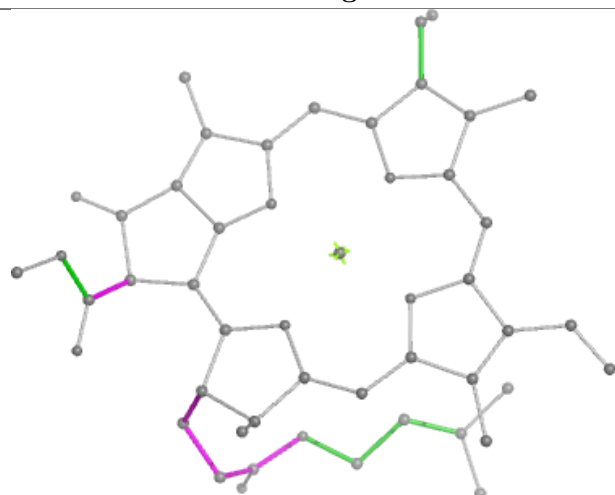
## Ligand CLA E 823



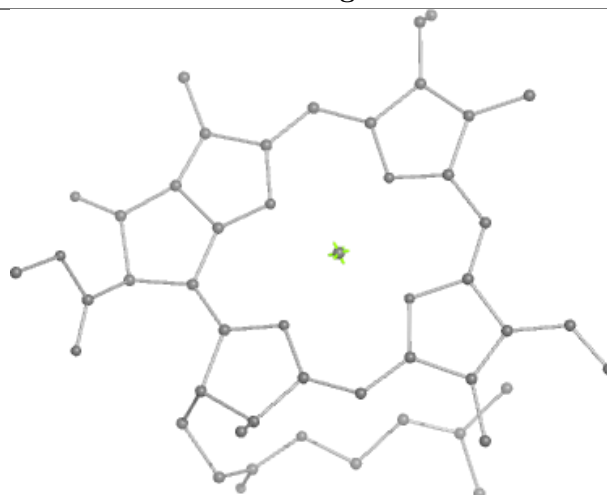
Bond lengths



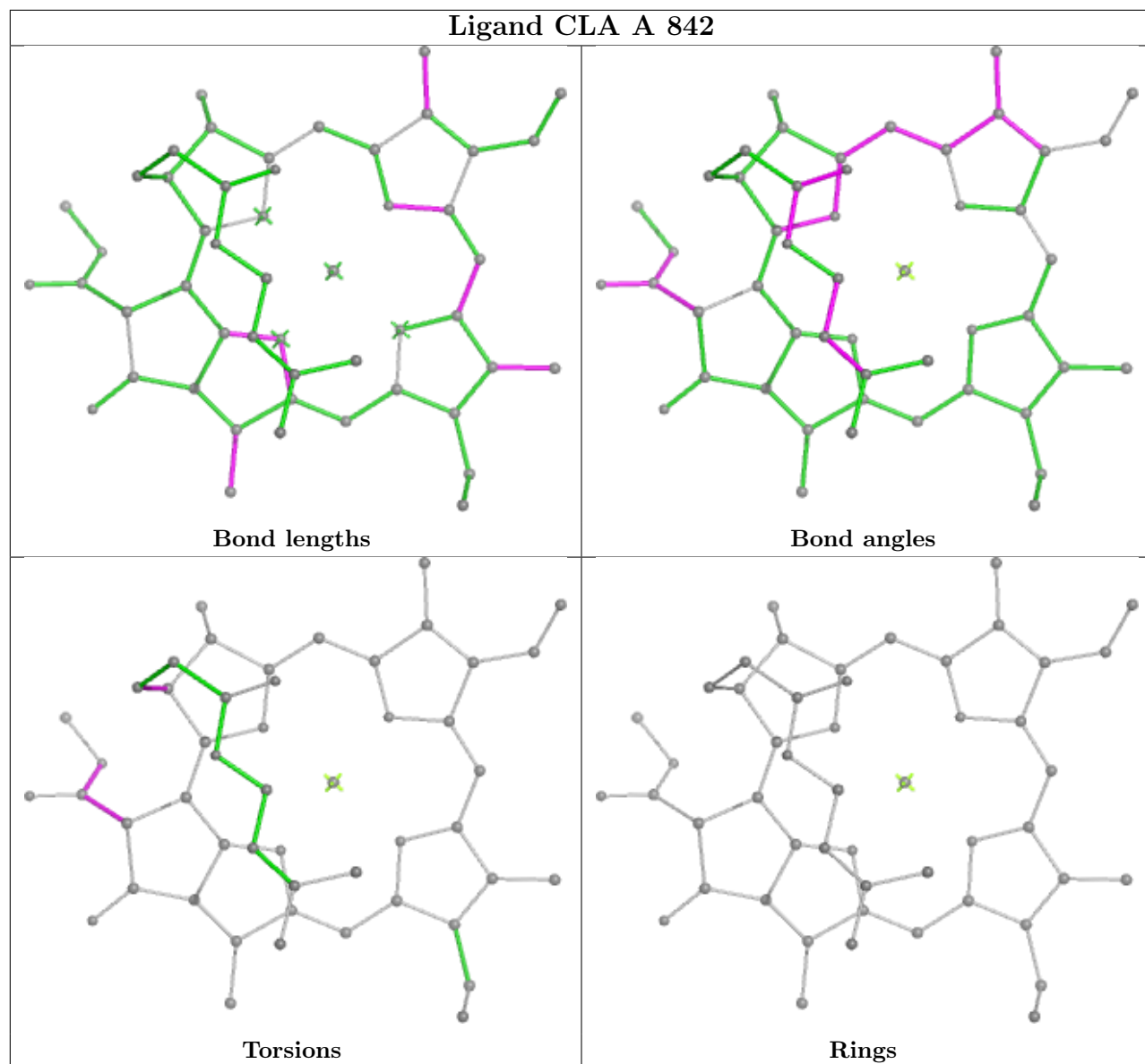
Bond angles



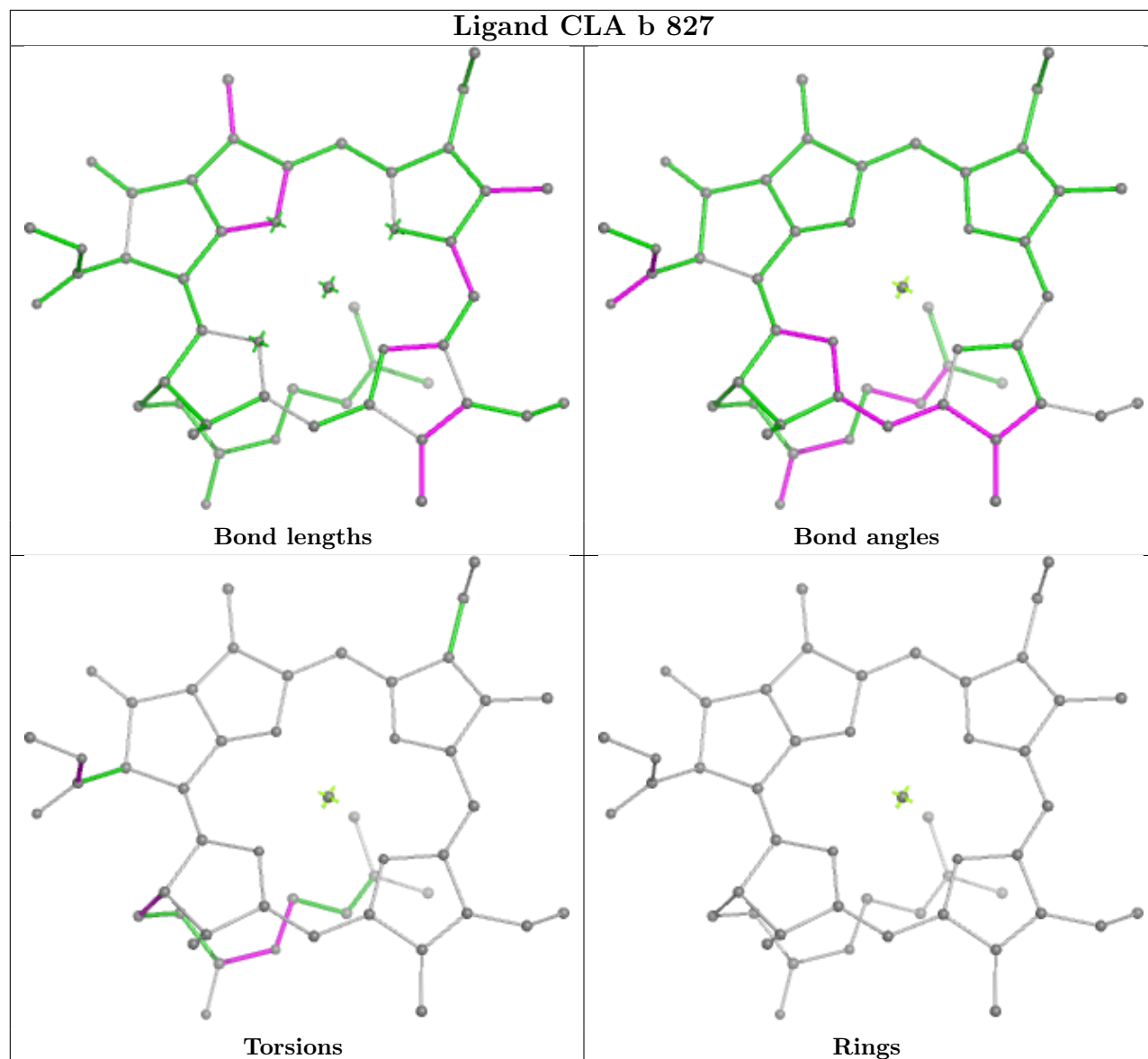
Torsions



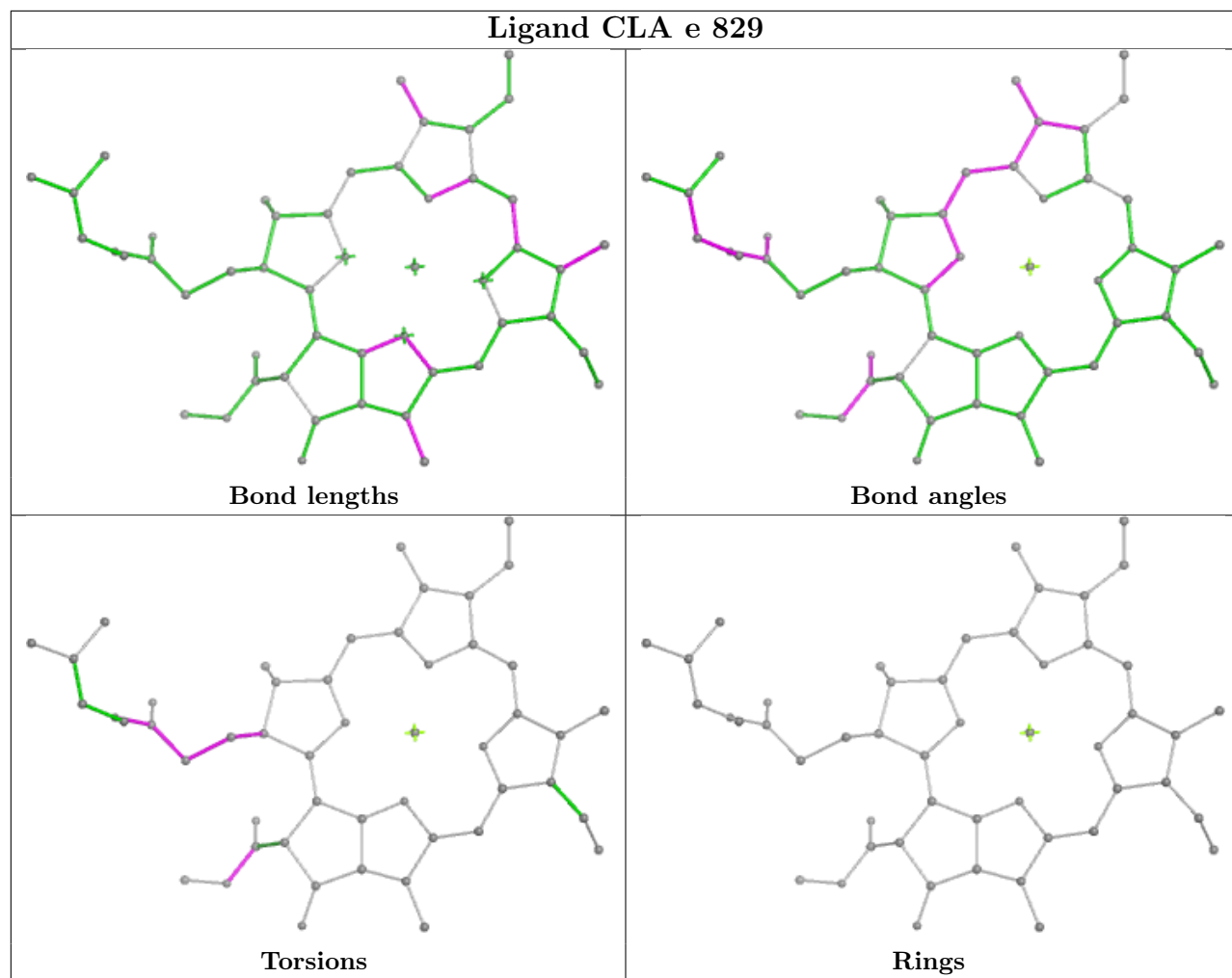
Rings



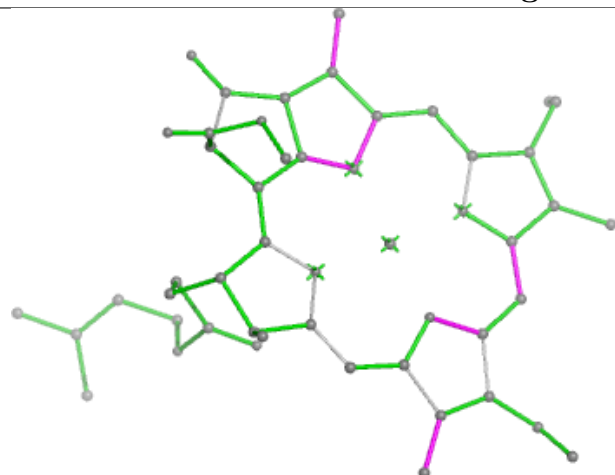
## Ligand CLA b 827



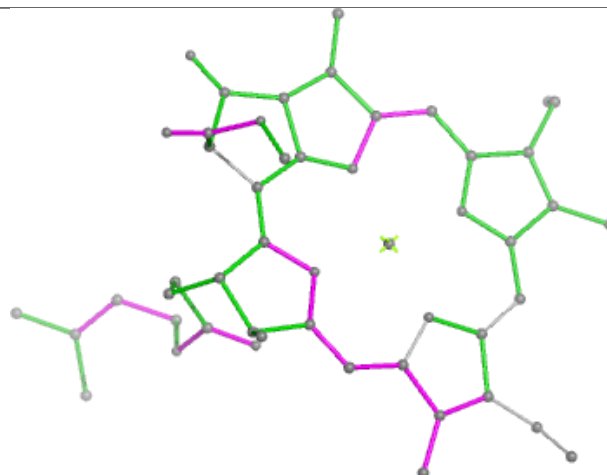
## Ligand CLA e 829



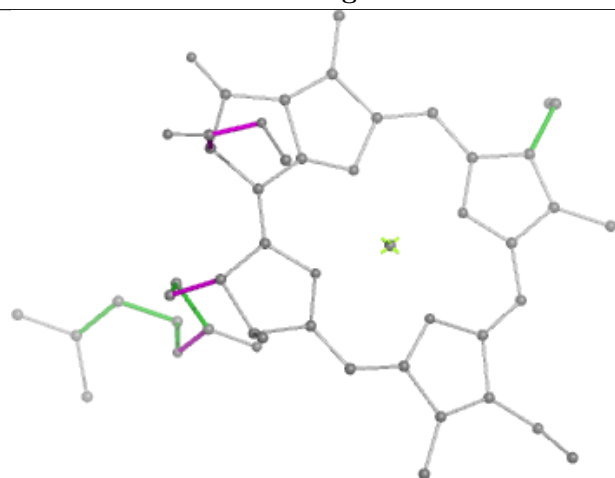
## Ligand CLA e 836



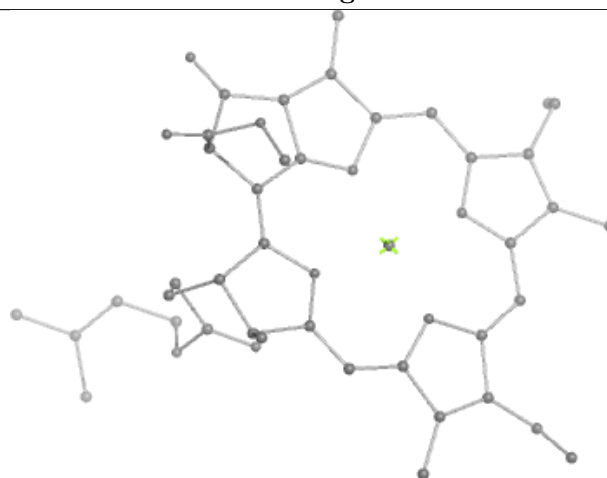
Bond lengths



Bond angles

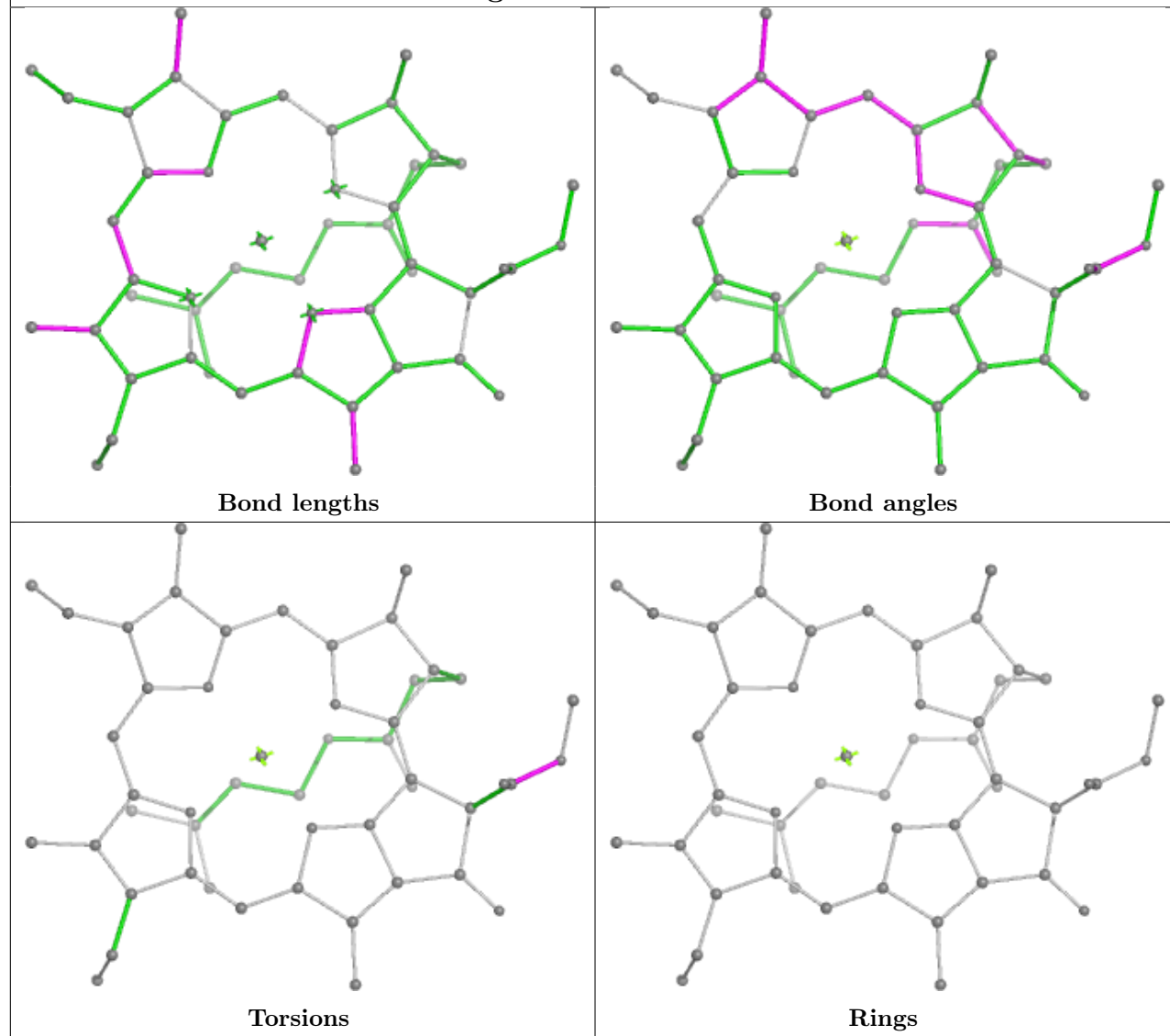


Torsions

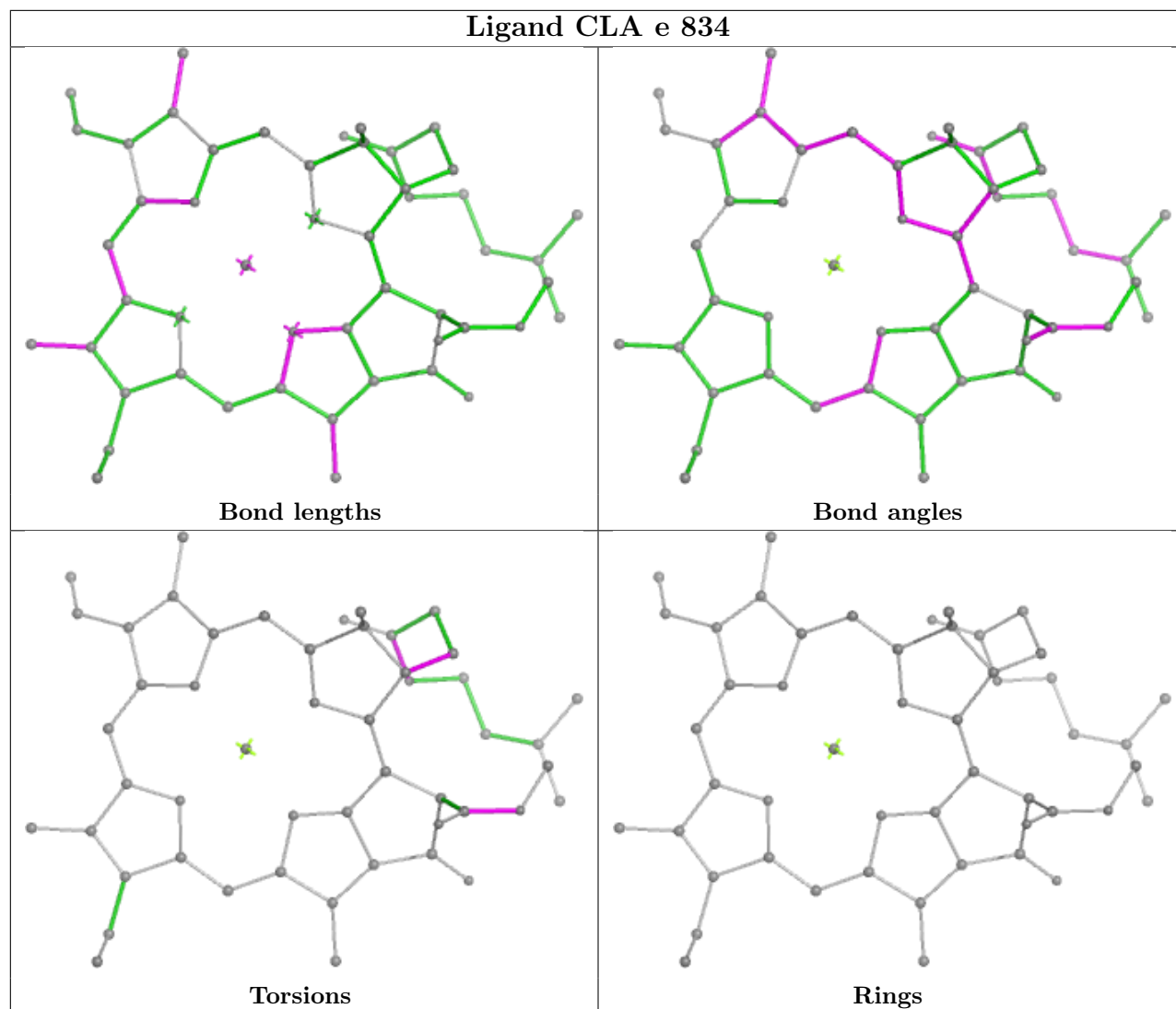


Rings

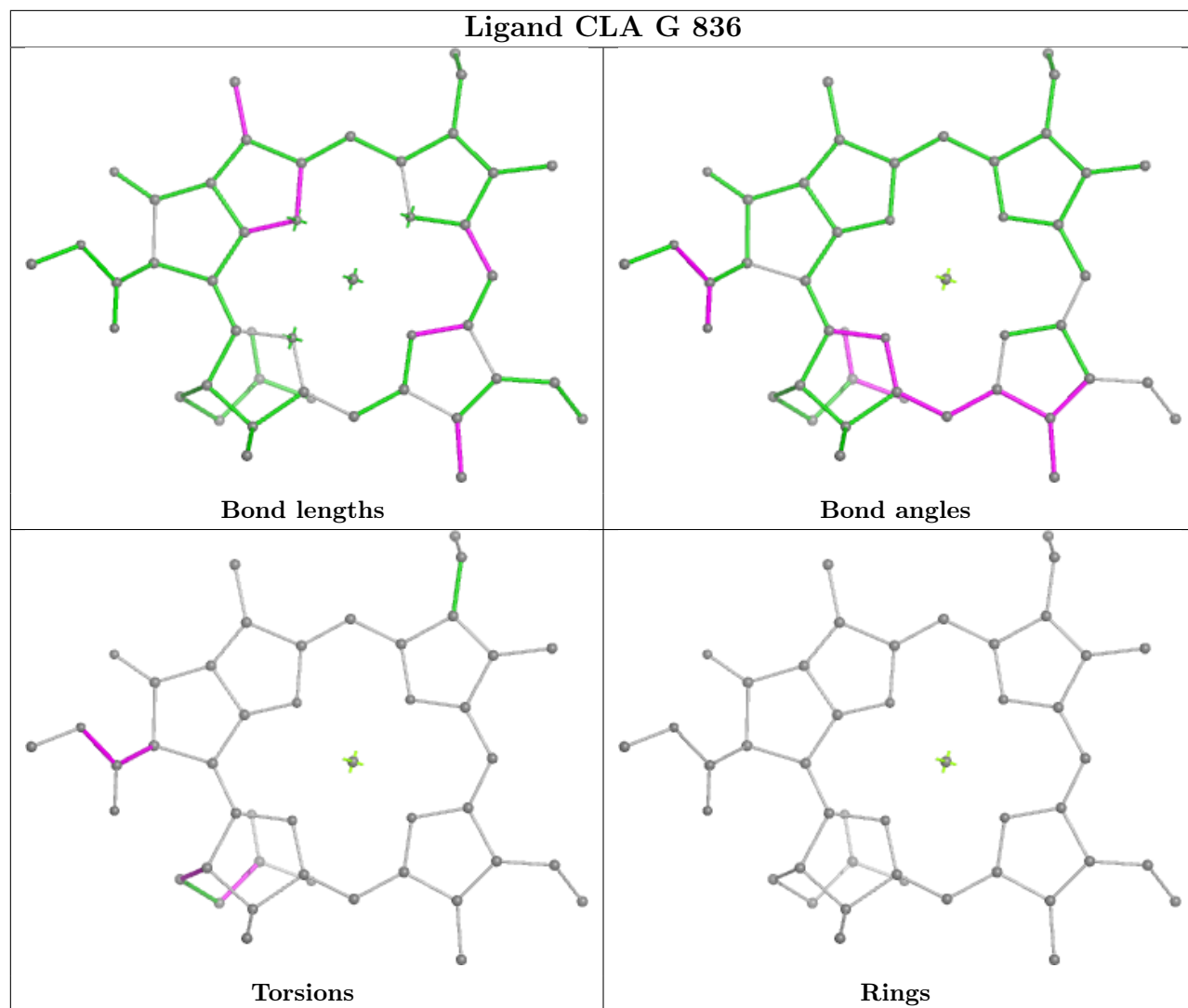
## Ligand CLA A 820



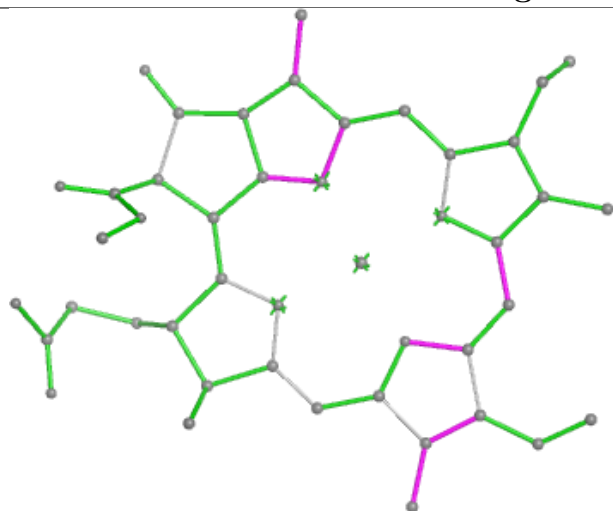
## Ligand CLA e 834



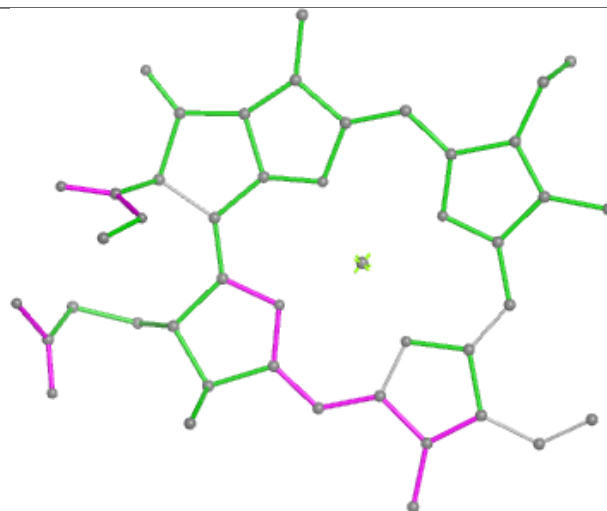




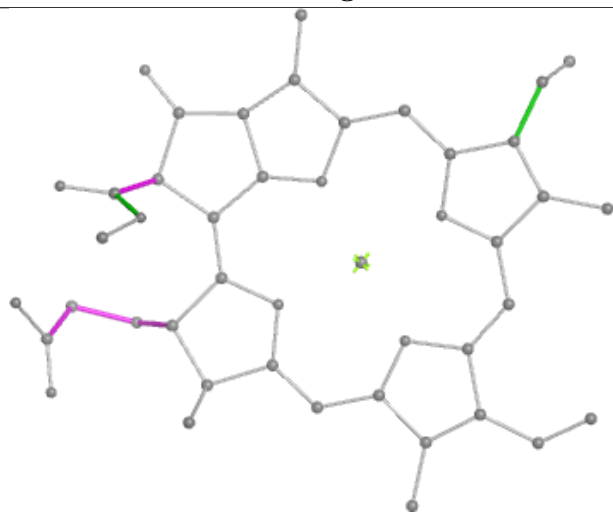
## Ligand CLA B 835



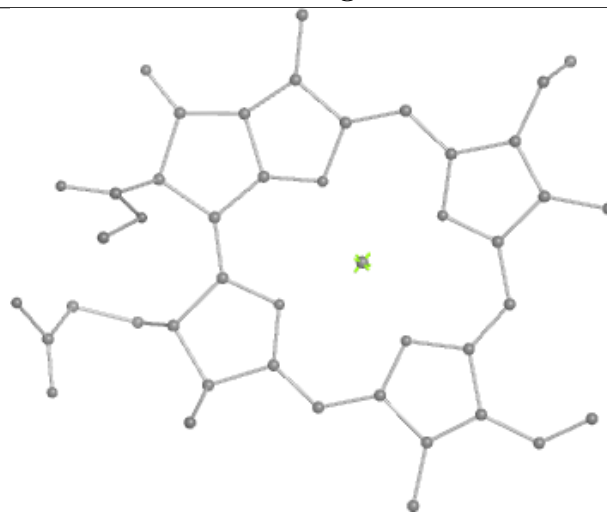
Bond lengths



Bond angles

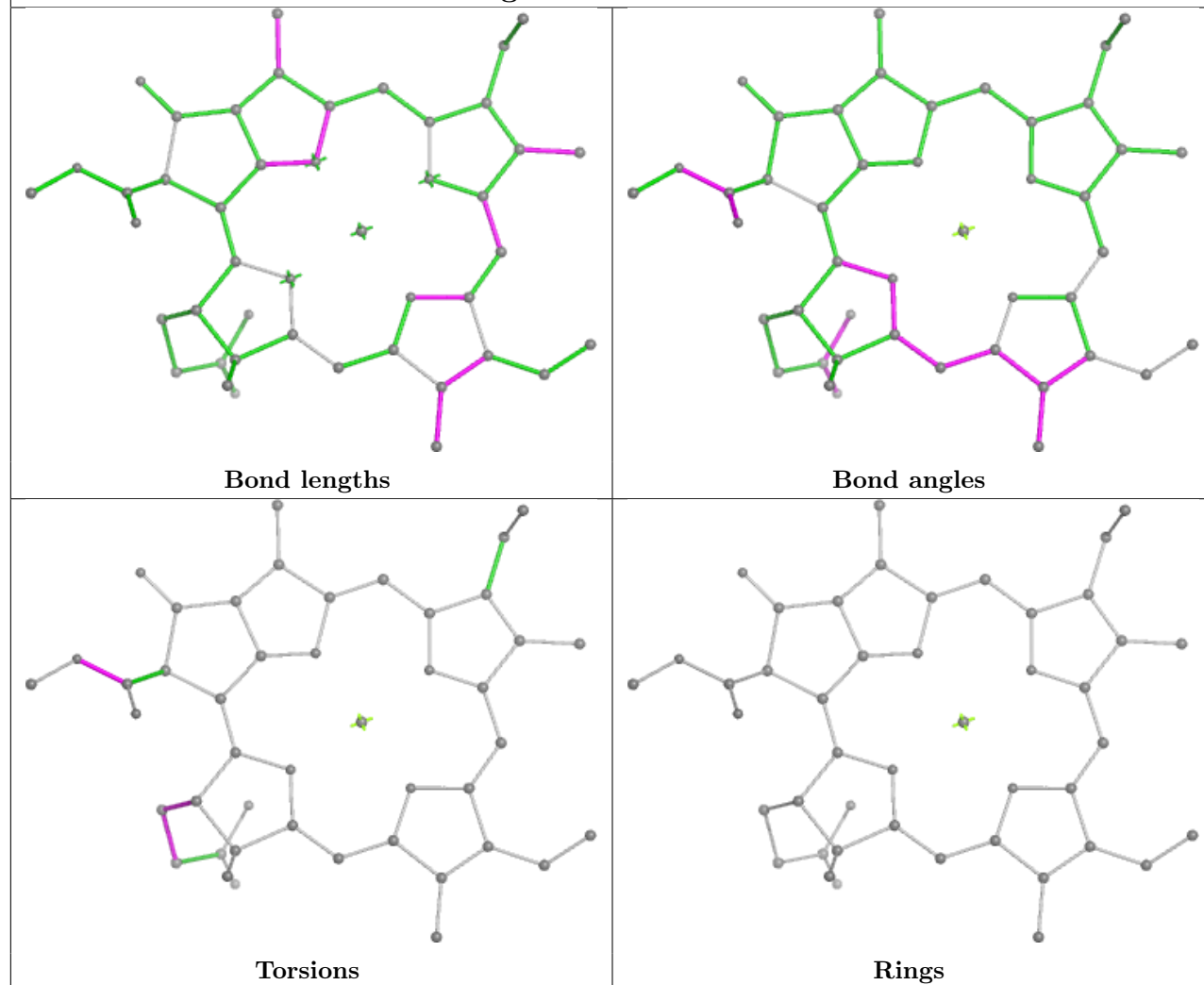


Torsions

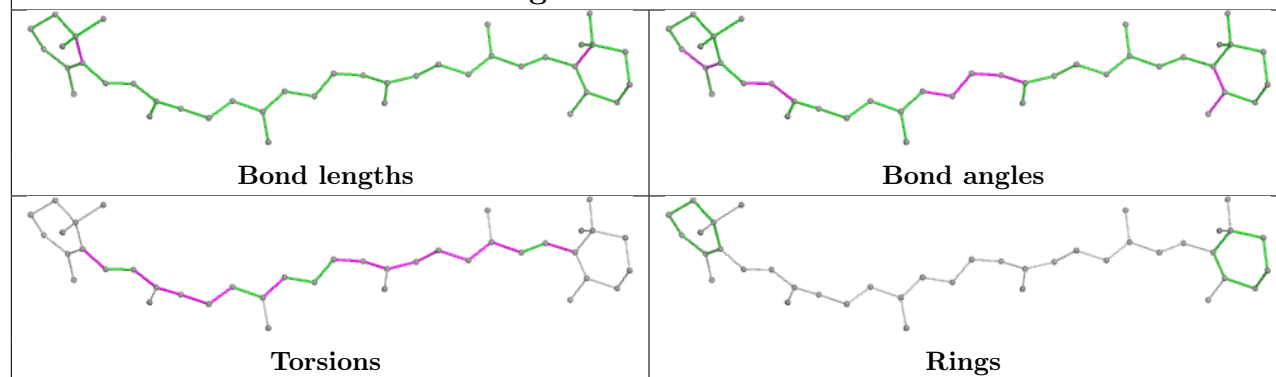


Rings

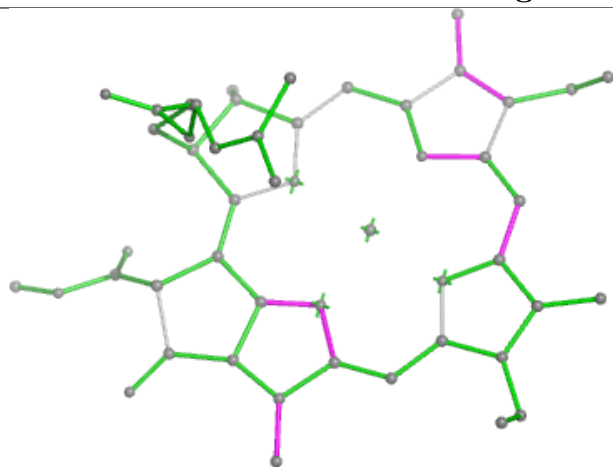
## Ligand CLA G 813



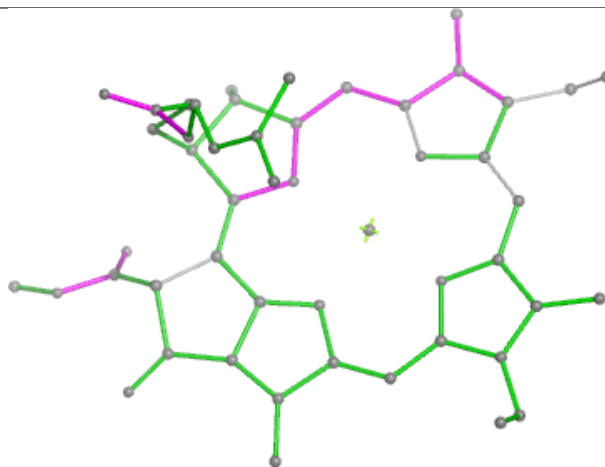
## Ligand BCR G 846



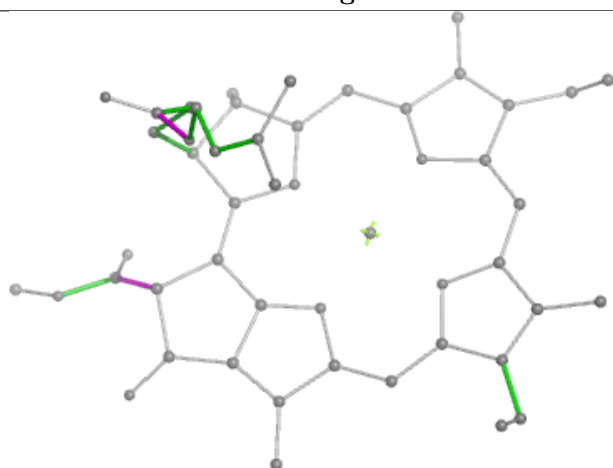
## Ligand CLA E 814



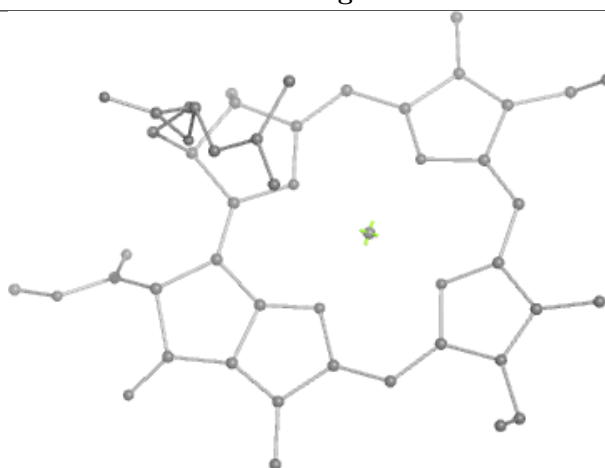
Bond lengths



Bond angles

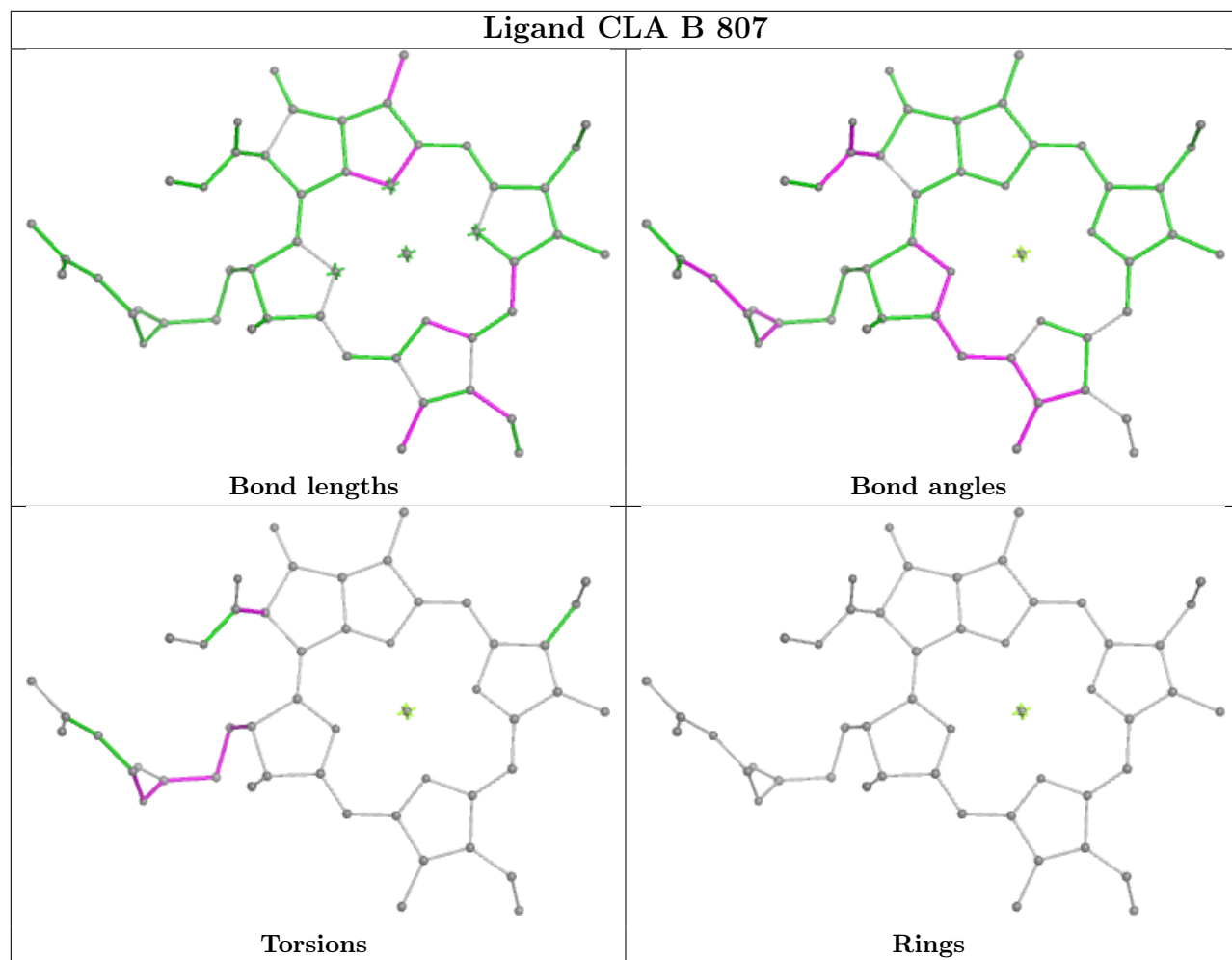


Torsions

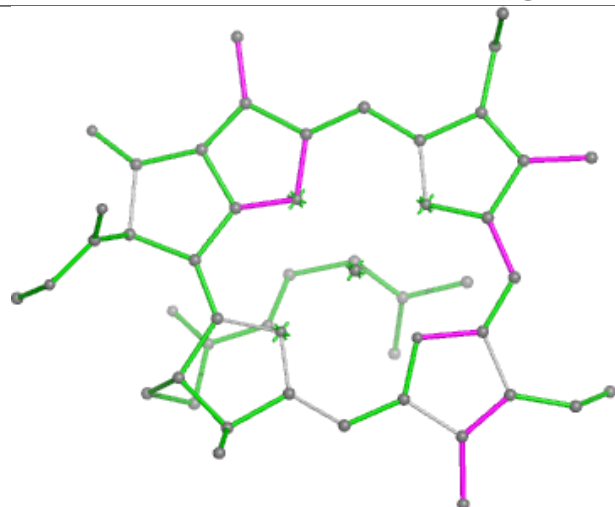


Rings

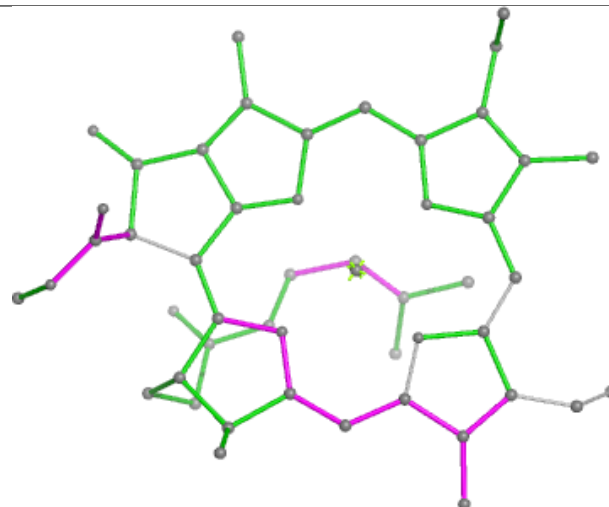
## Ligand CLA B 807



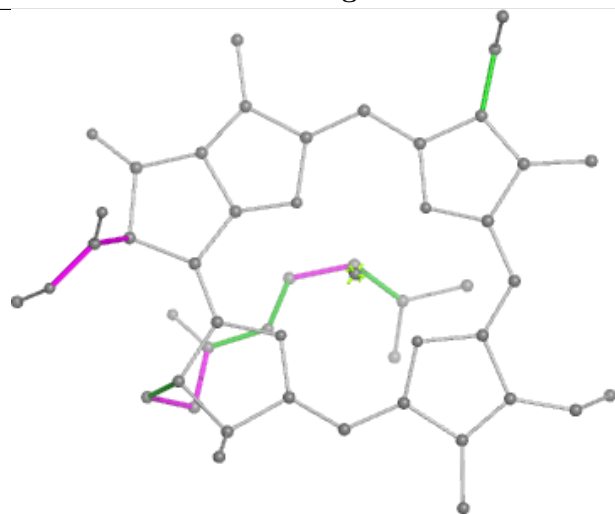
## Ligand CLA b 822



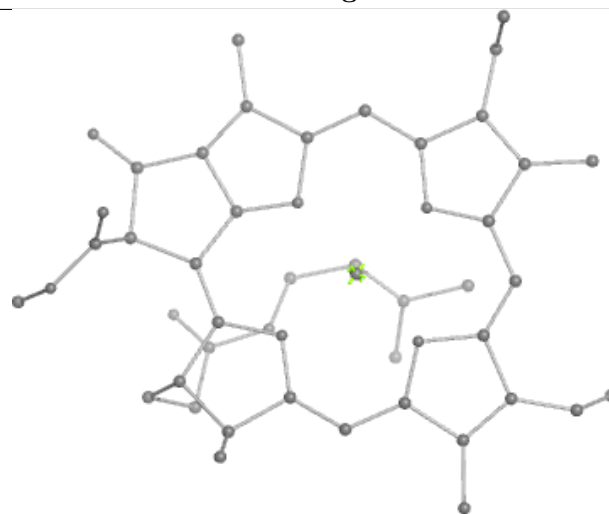
Bond lengths



Bond angles

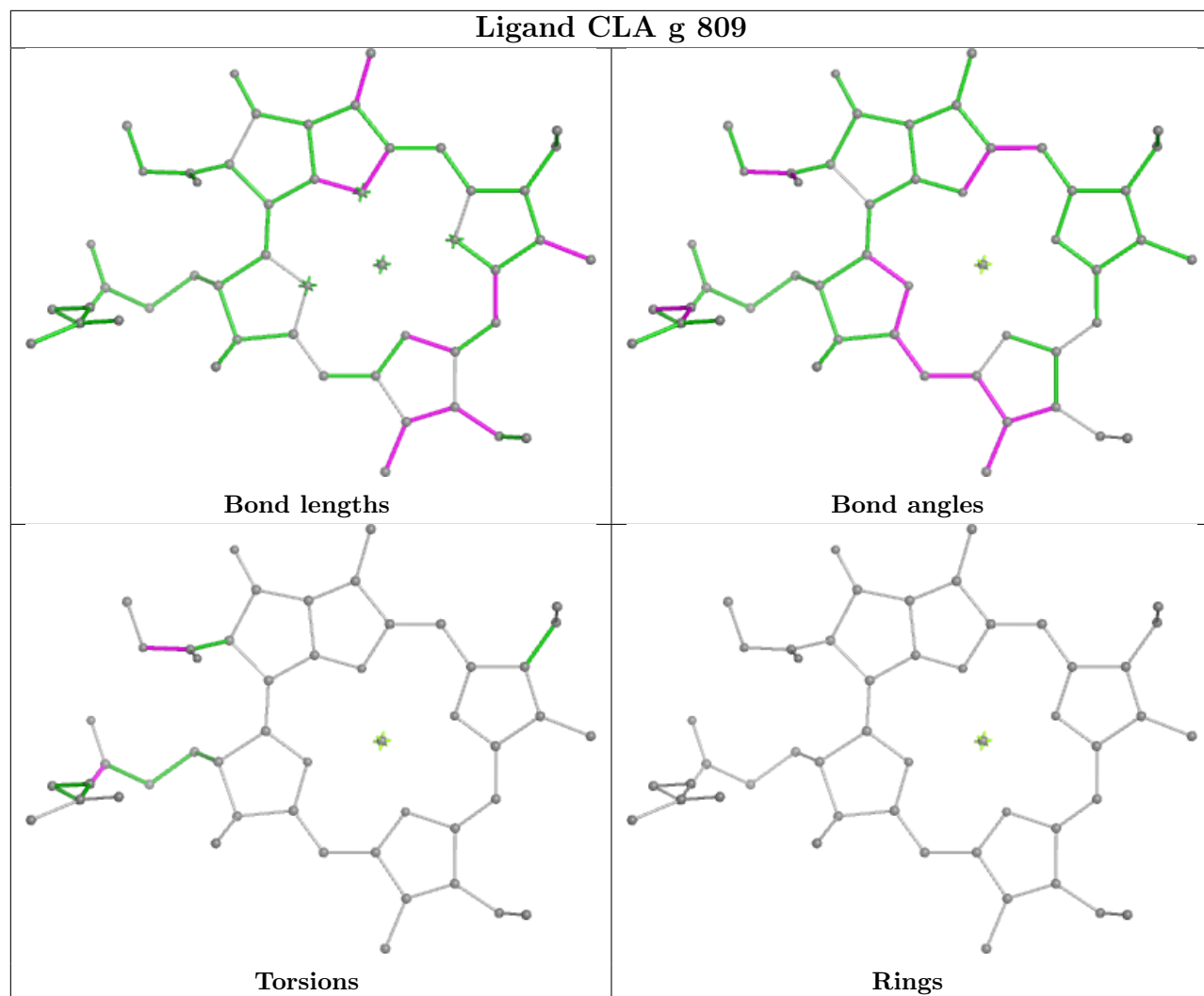


Torsions

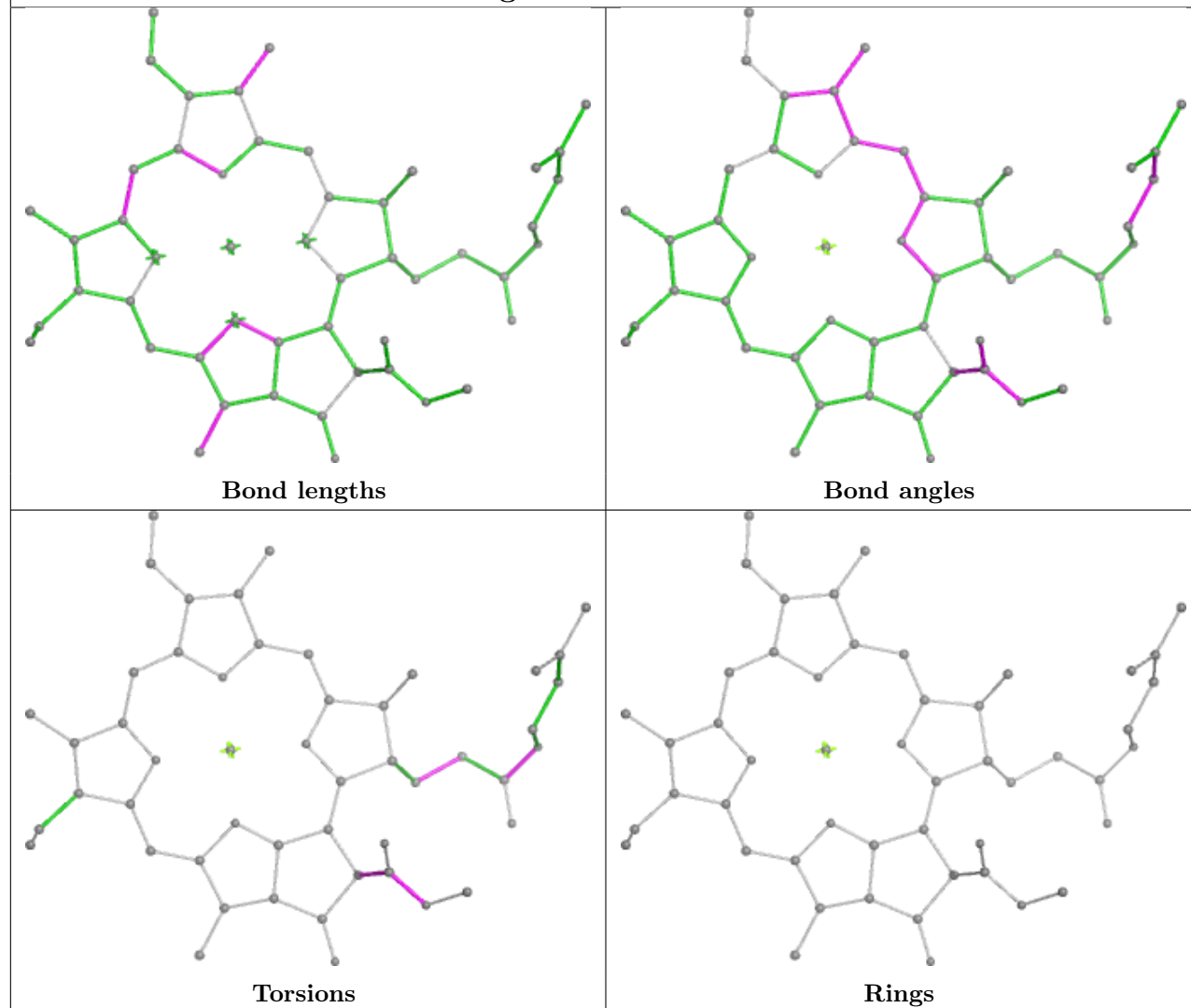


Rings

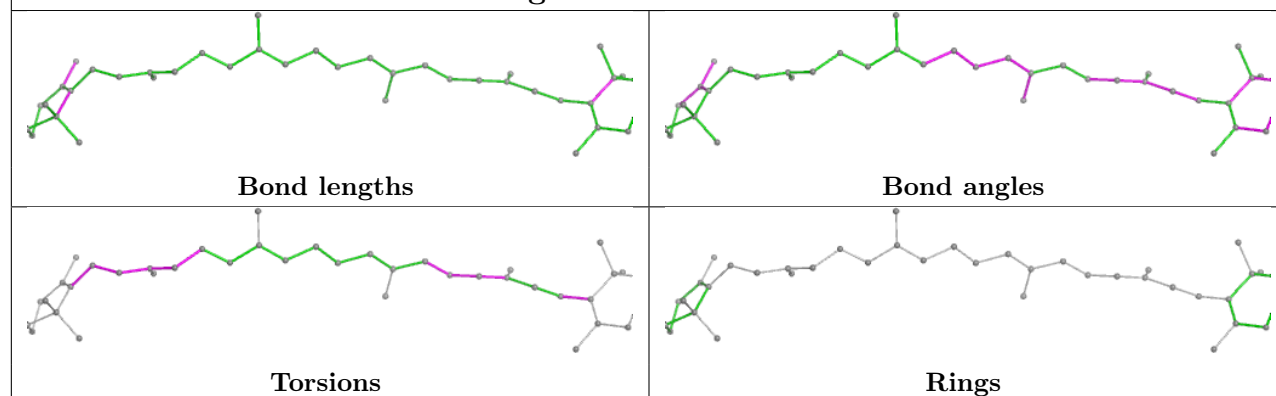
## Ligand CLA g 809



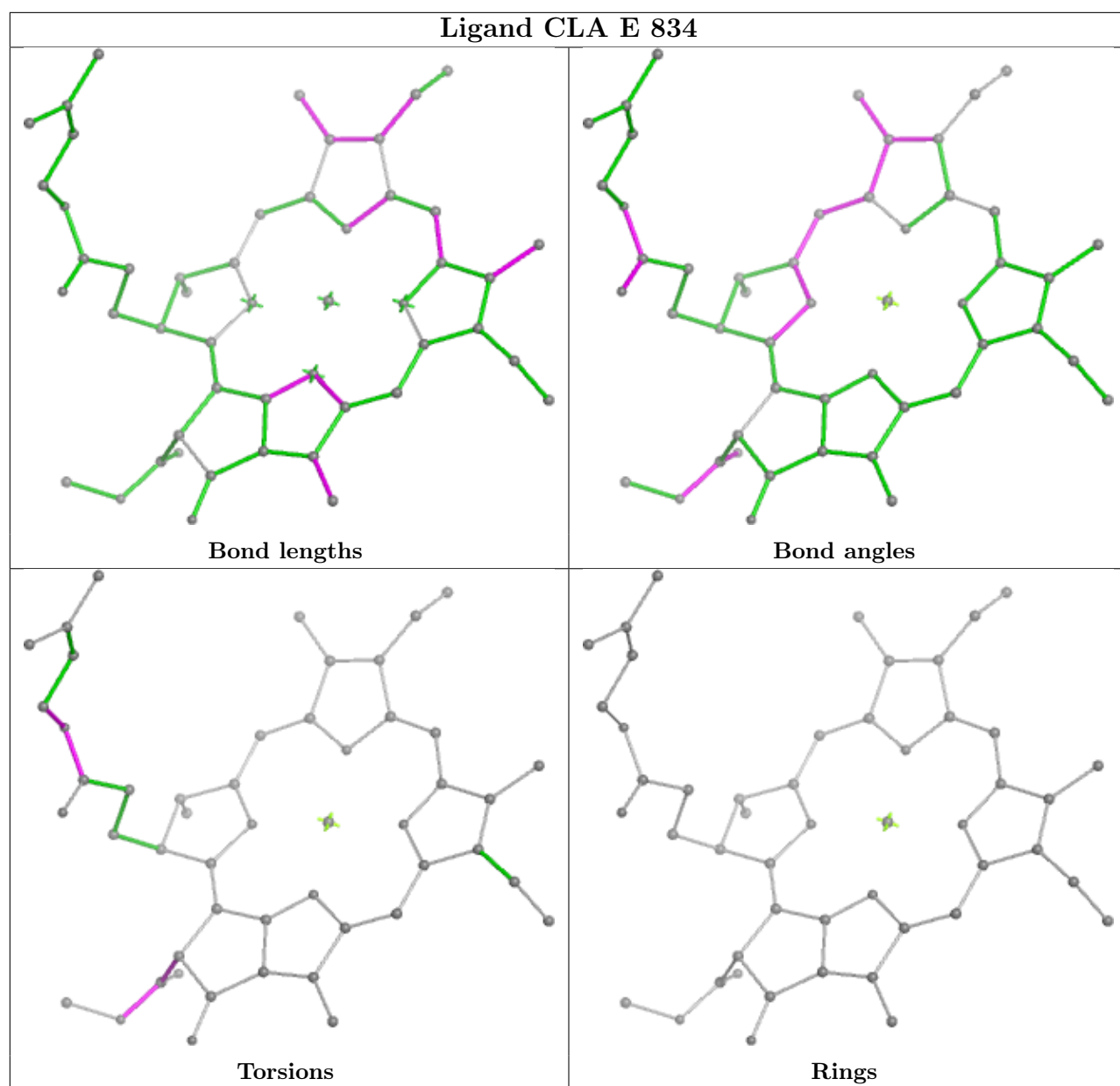
## Ligand CLA b 824



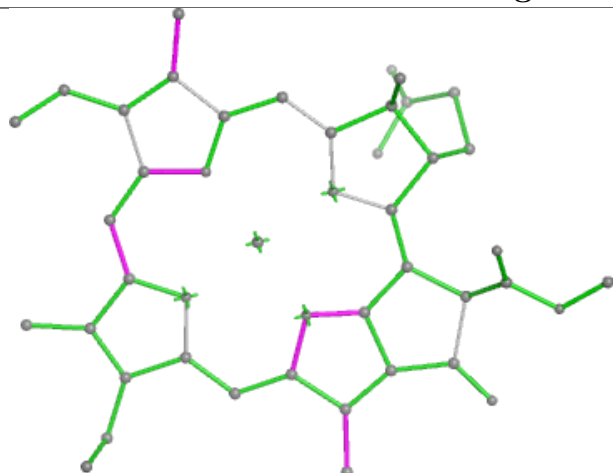
## Ligand BCR m 101



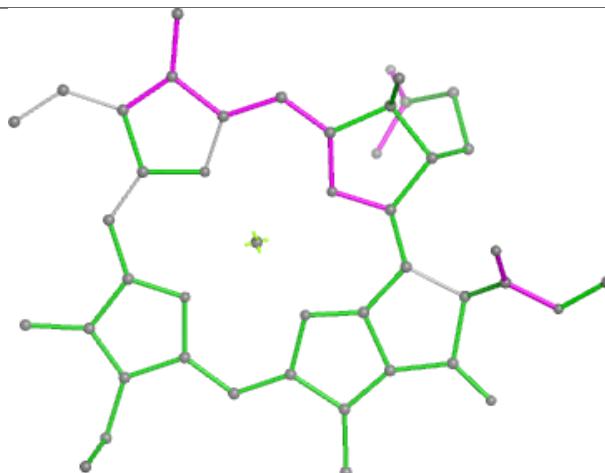




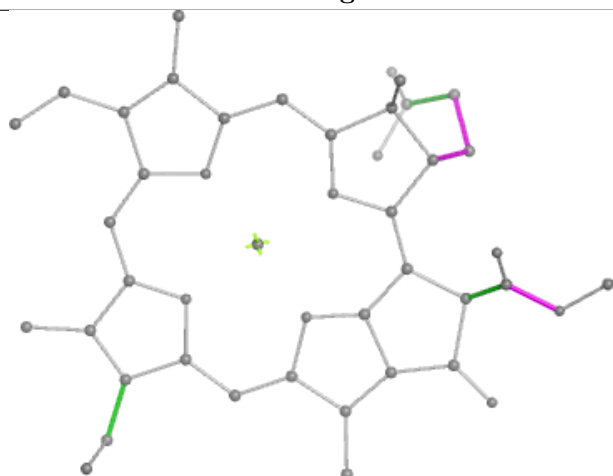
## Ligand CLA B 813



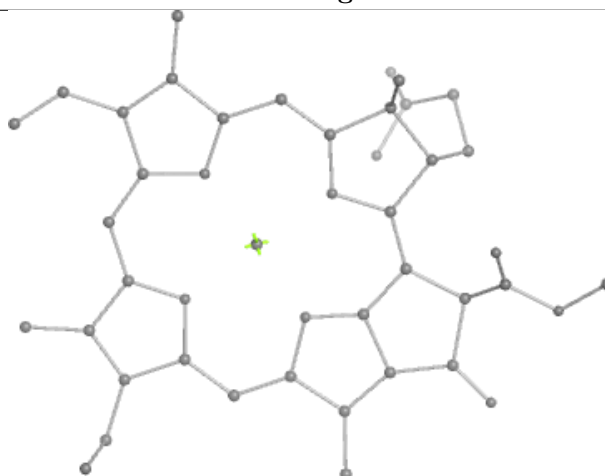
Bond lengths



Bond angles

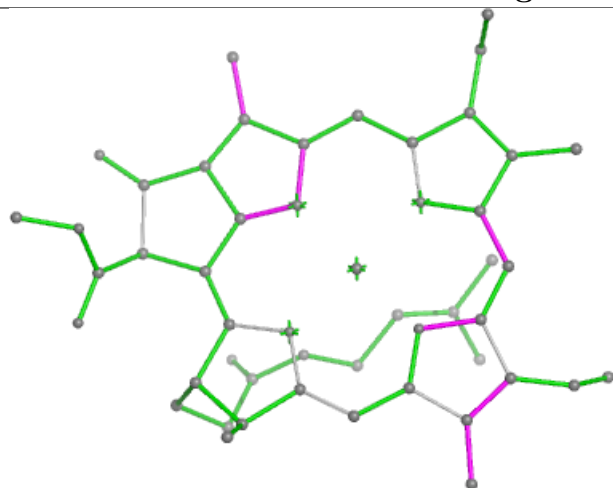


Torsions

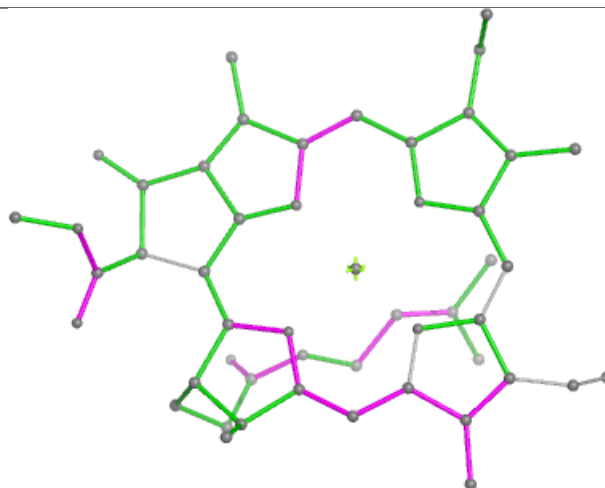


Rings

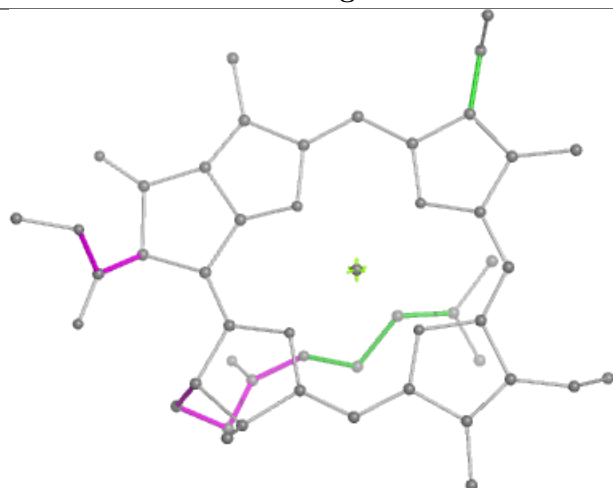
## Ligand CLA E 826



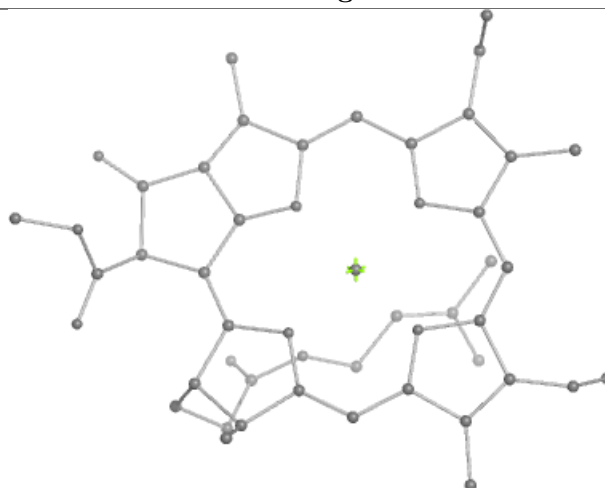
Bond lengths



Bond angles

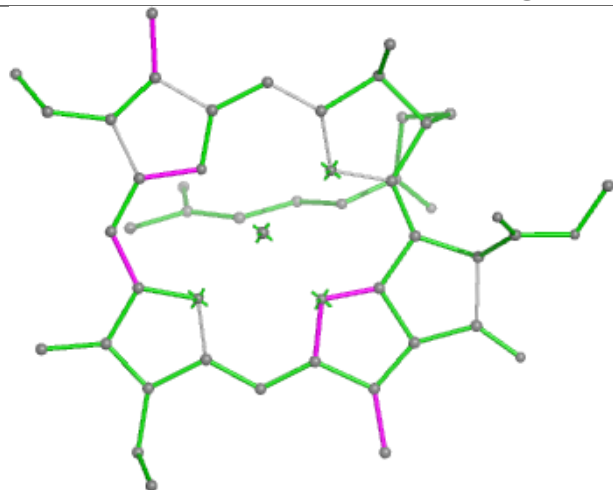


Torsions

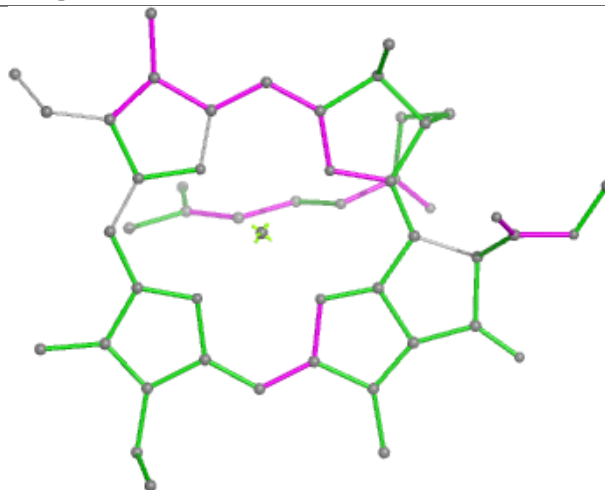


Rings

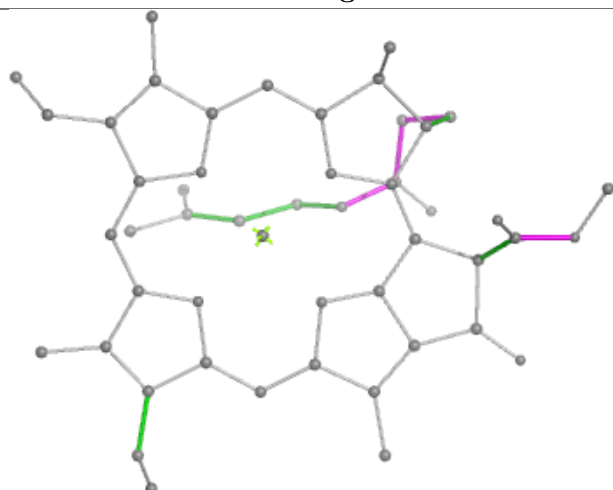
## Ligand CLA g 839



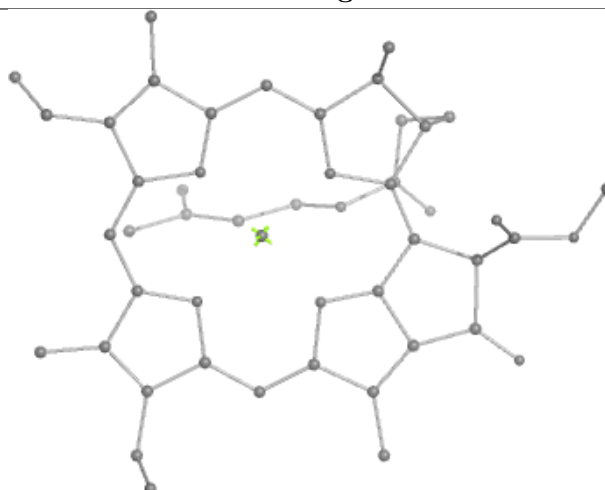
Bond lengths



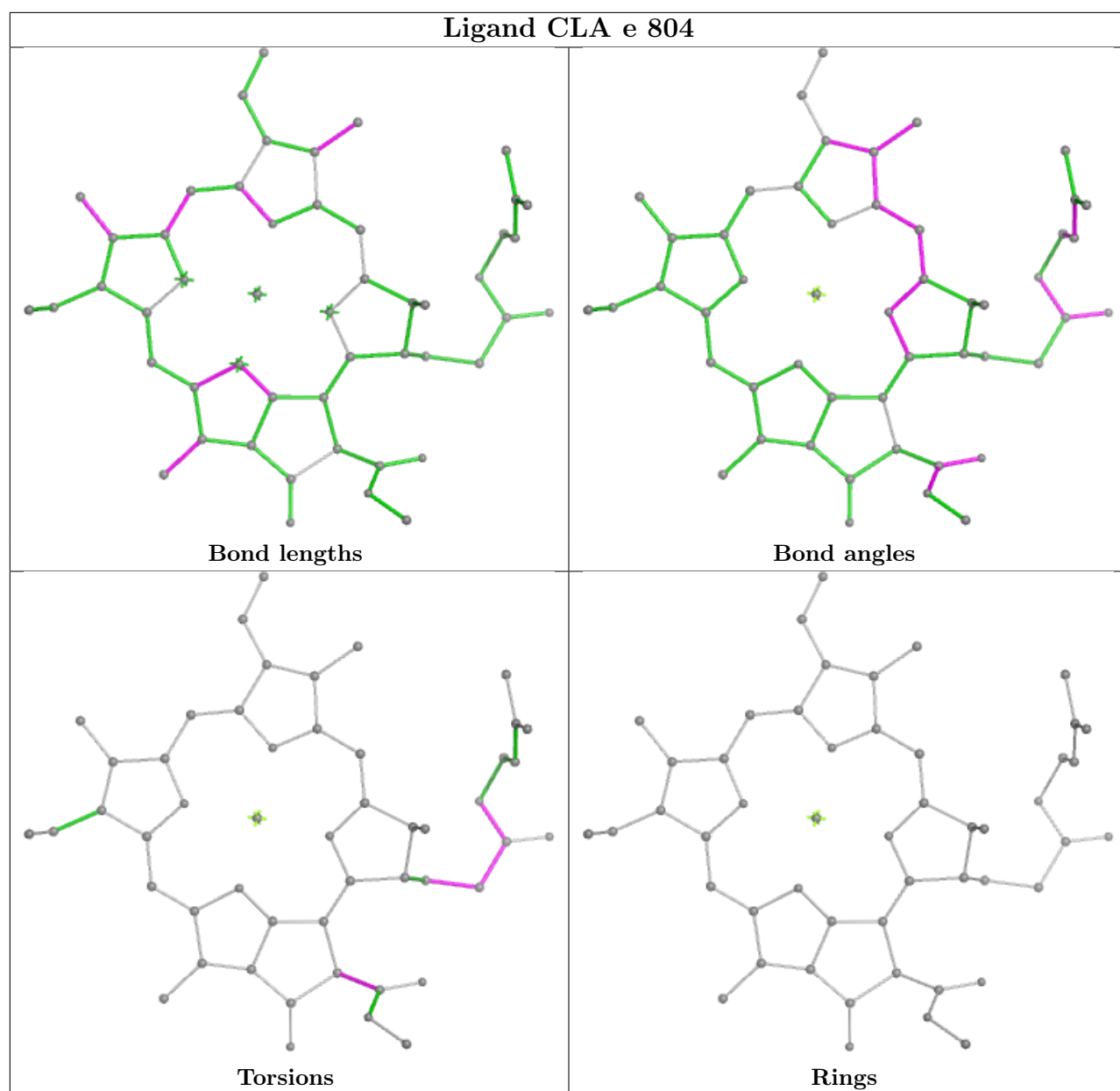
Bond angles



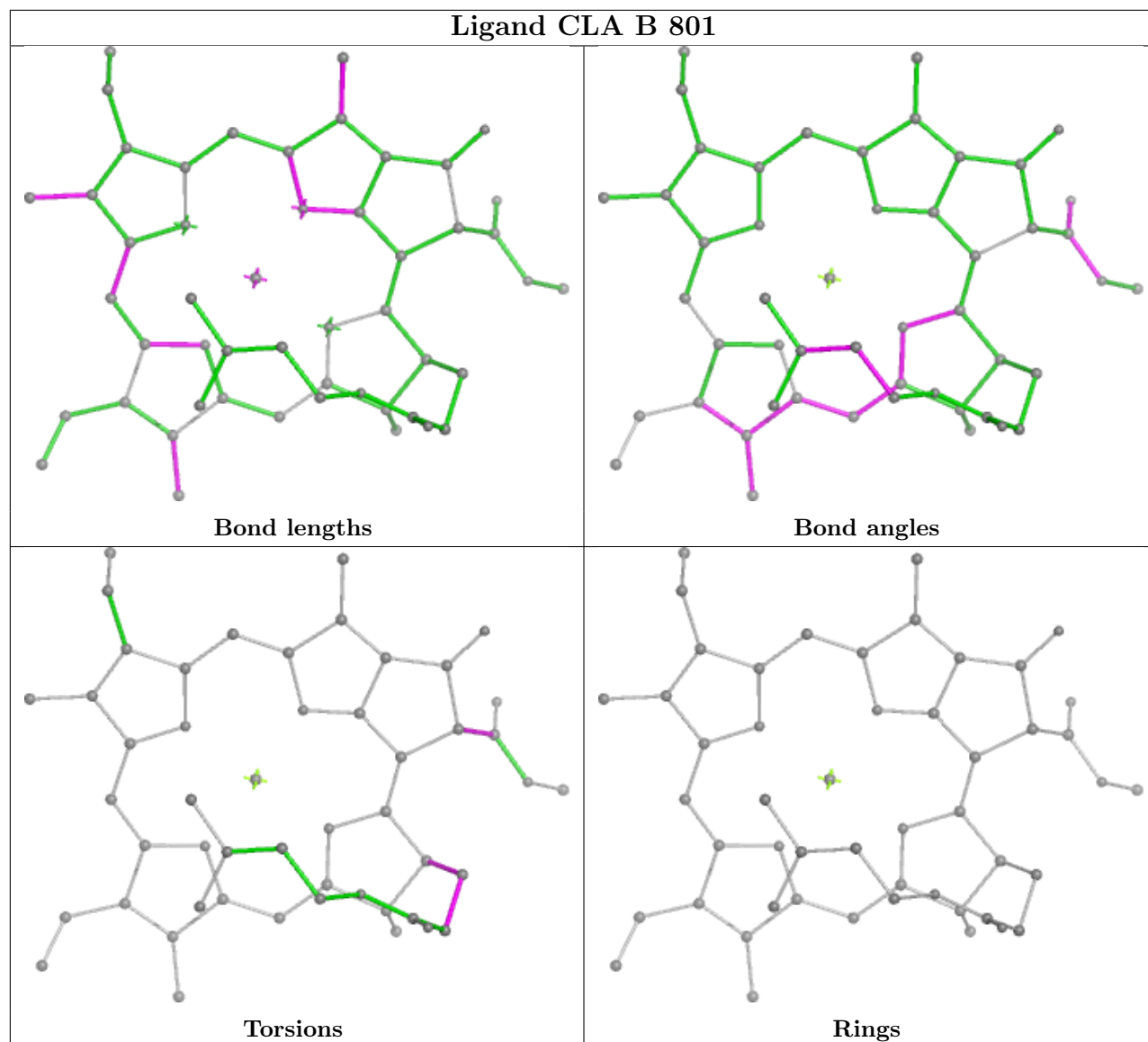
Torsions

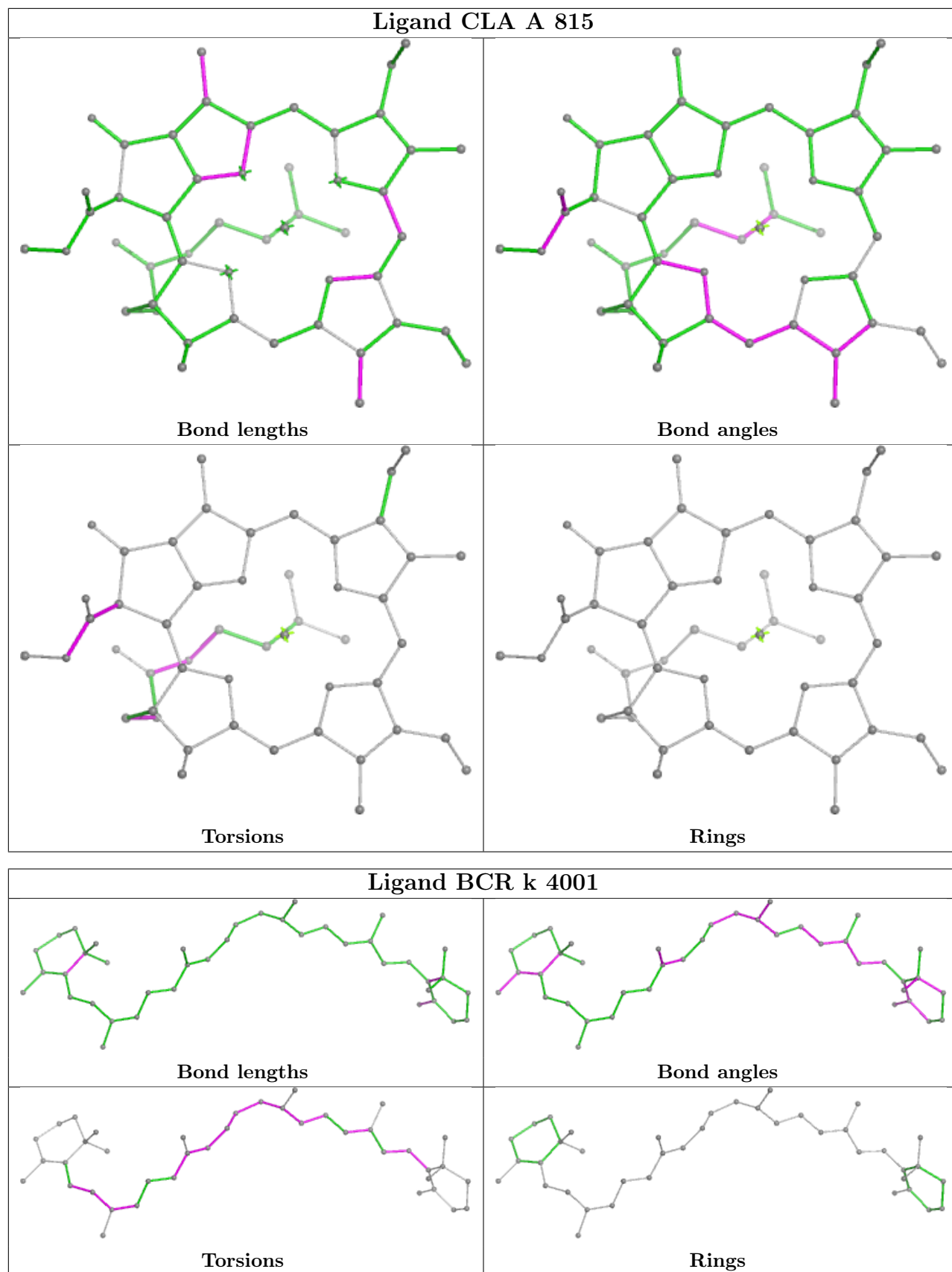


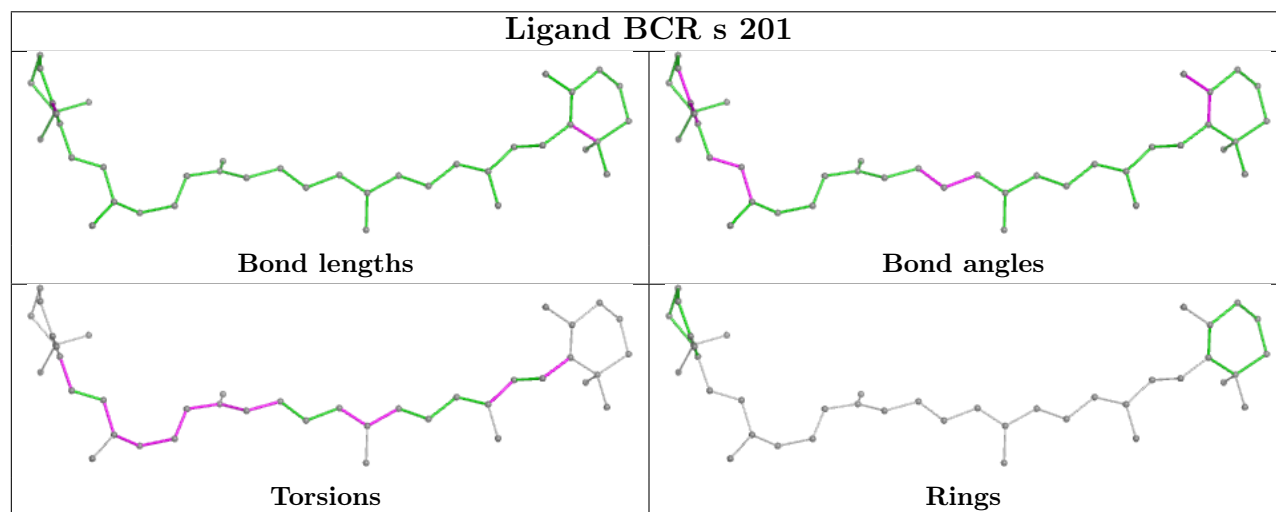
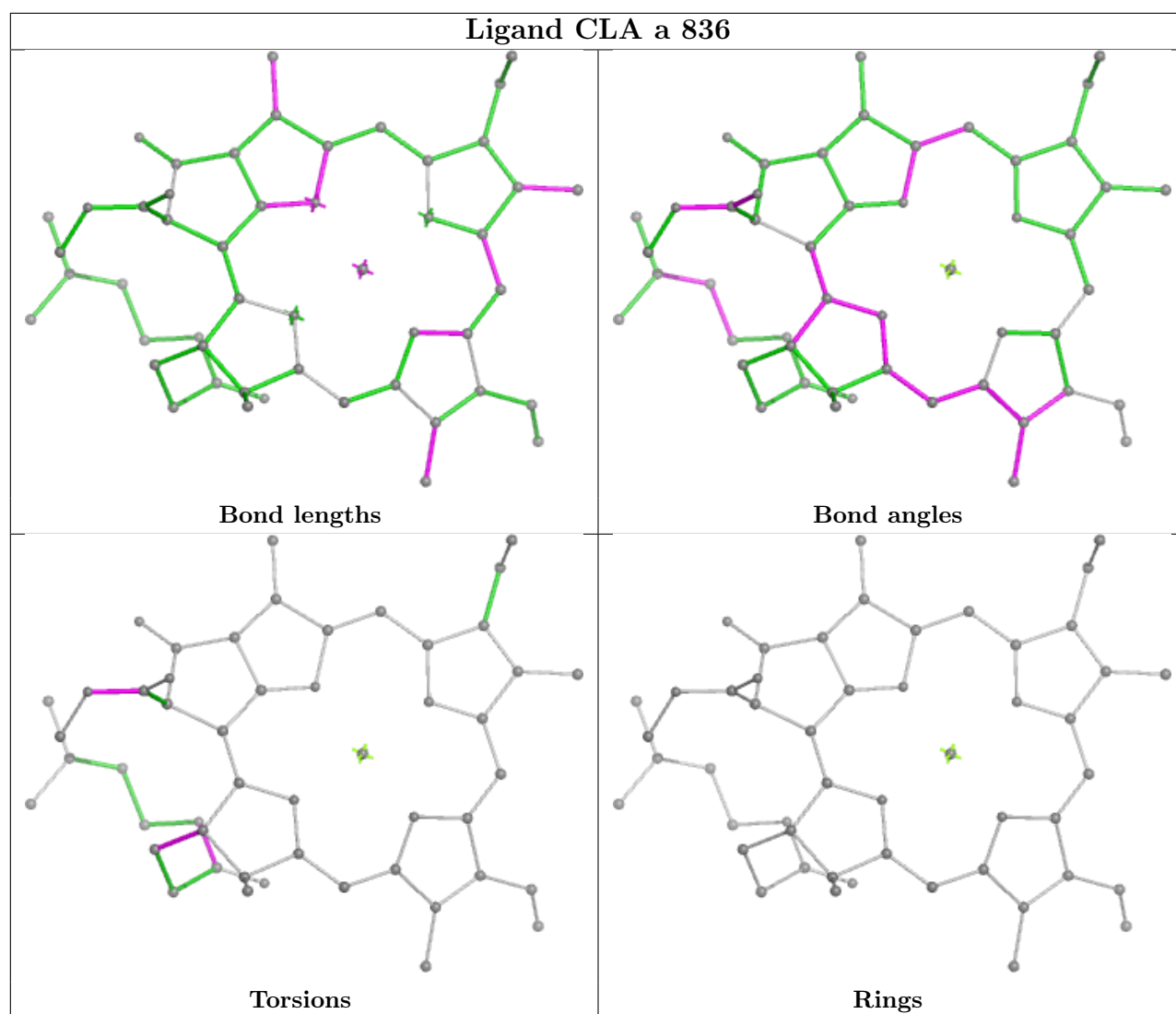
Rings



## Ligand CLA B 801

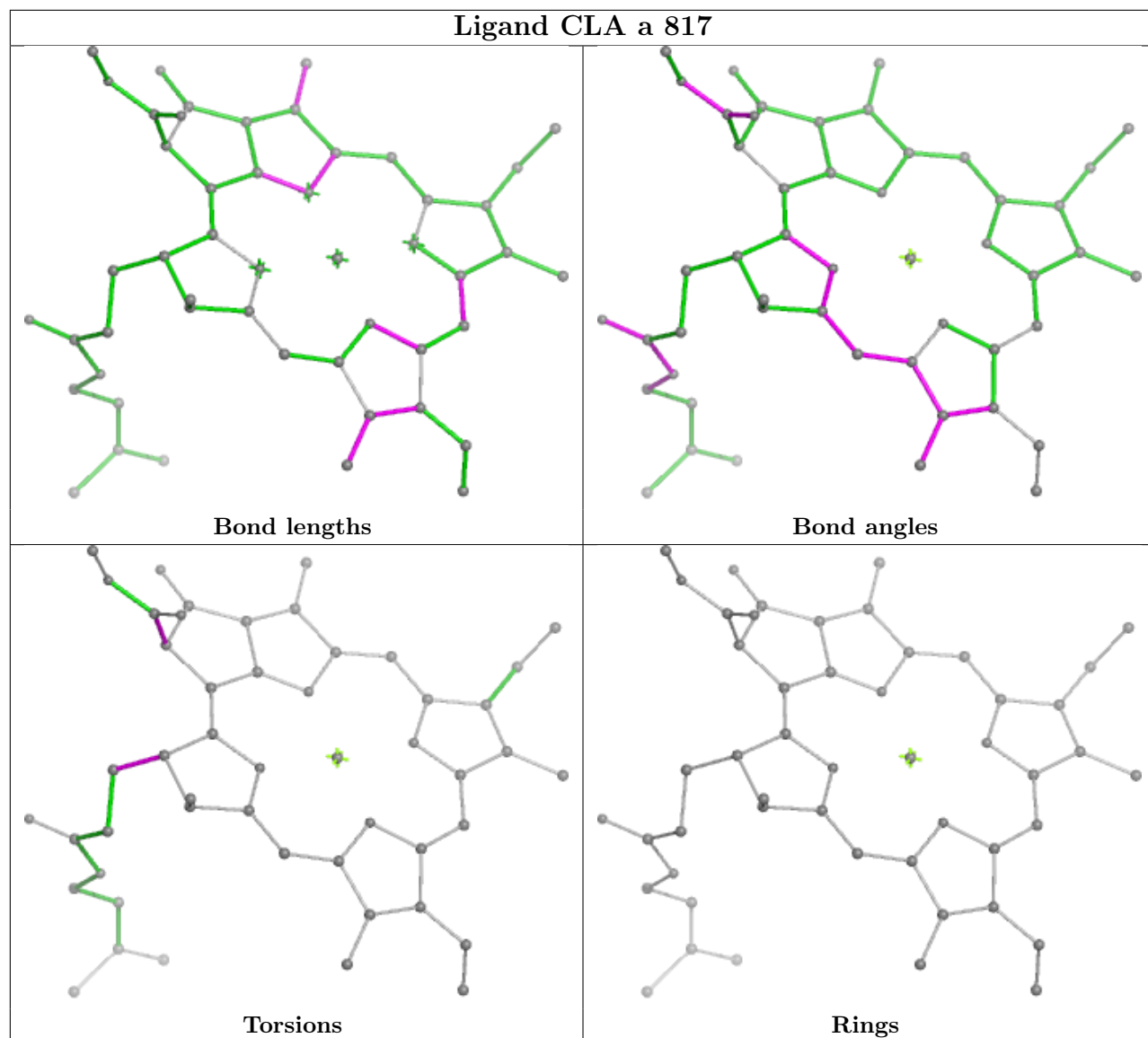




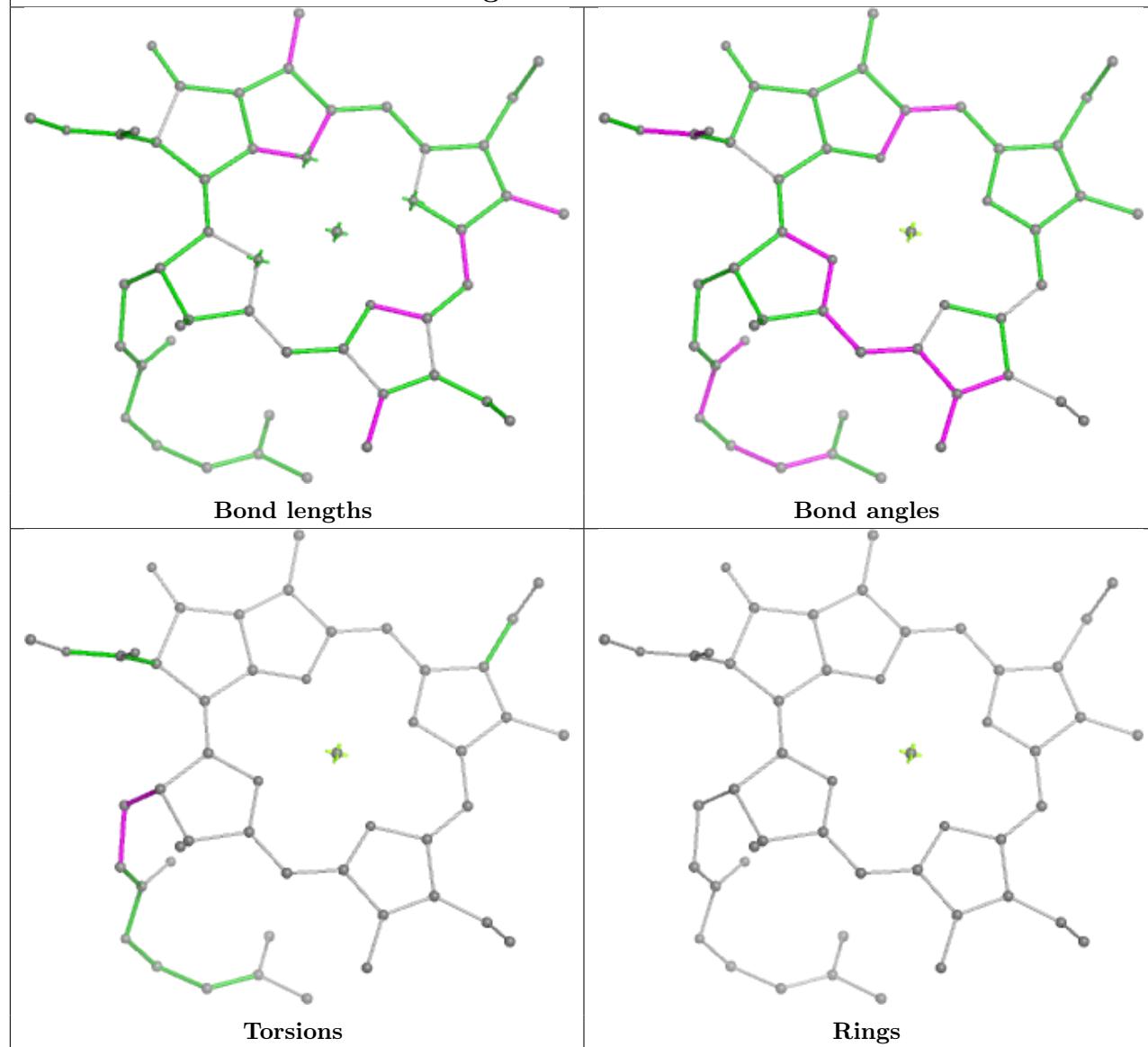




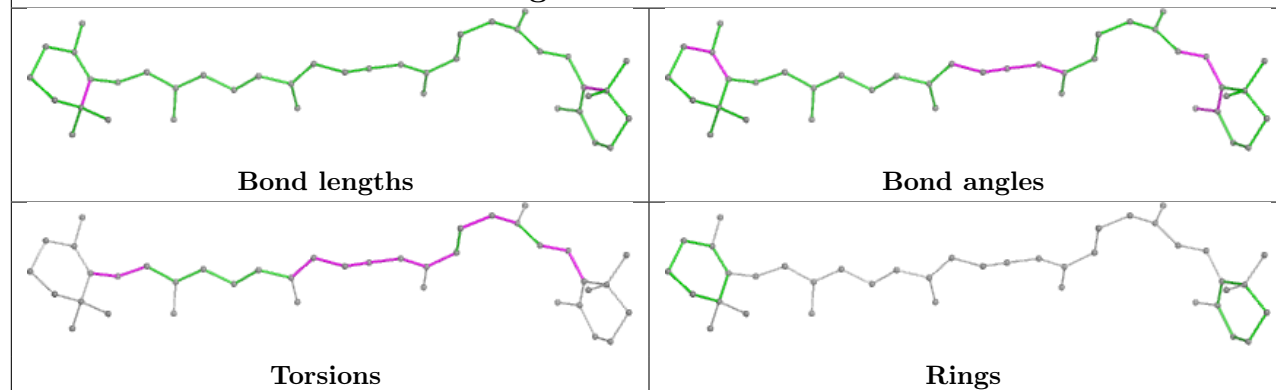
## Ligand CLA a 817



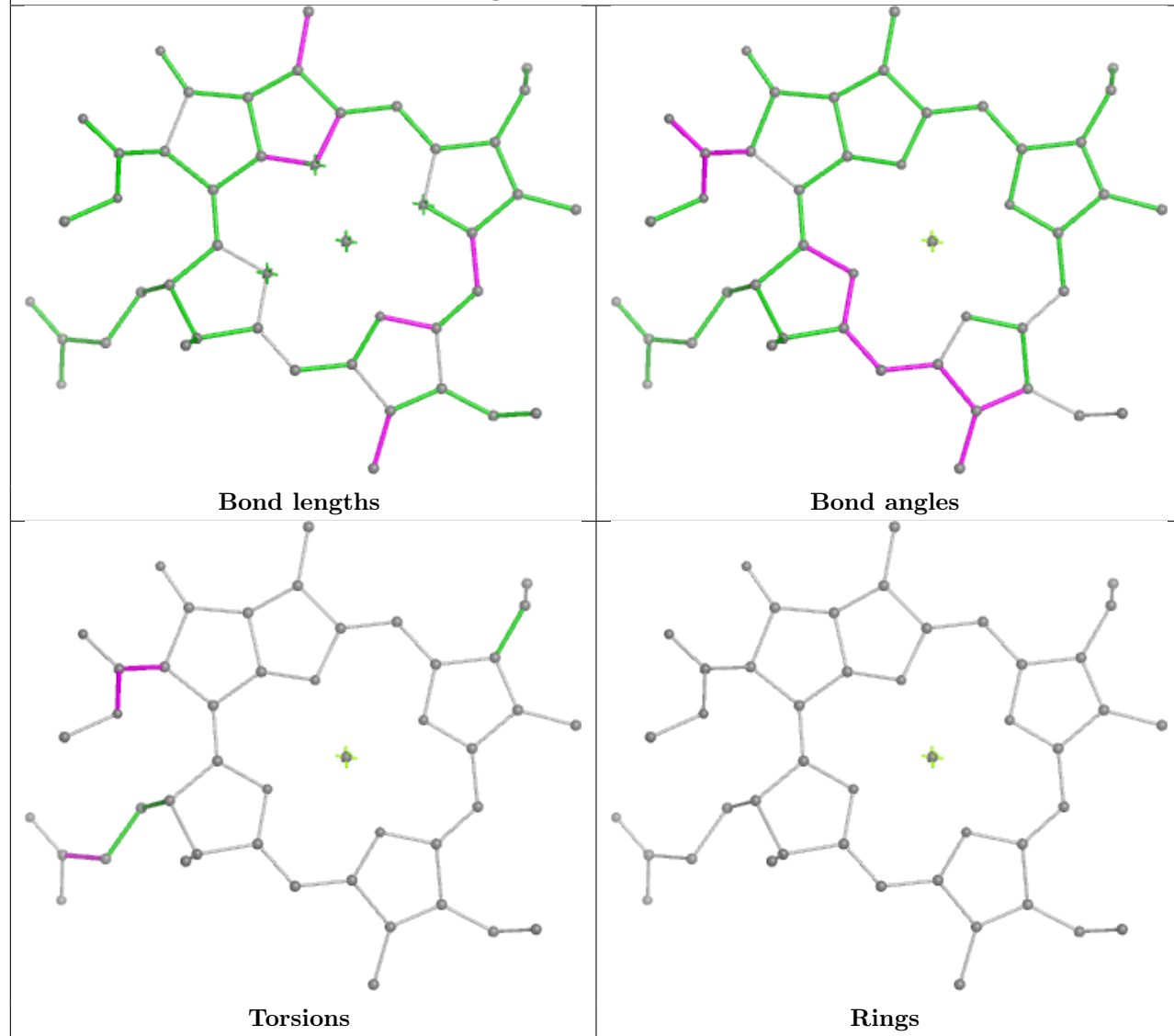
## Ligand CLA e 810



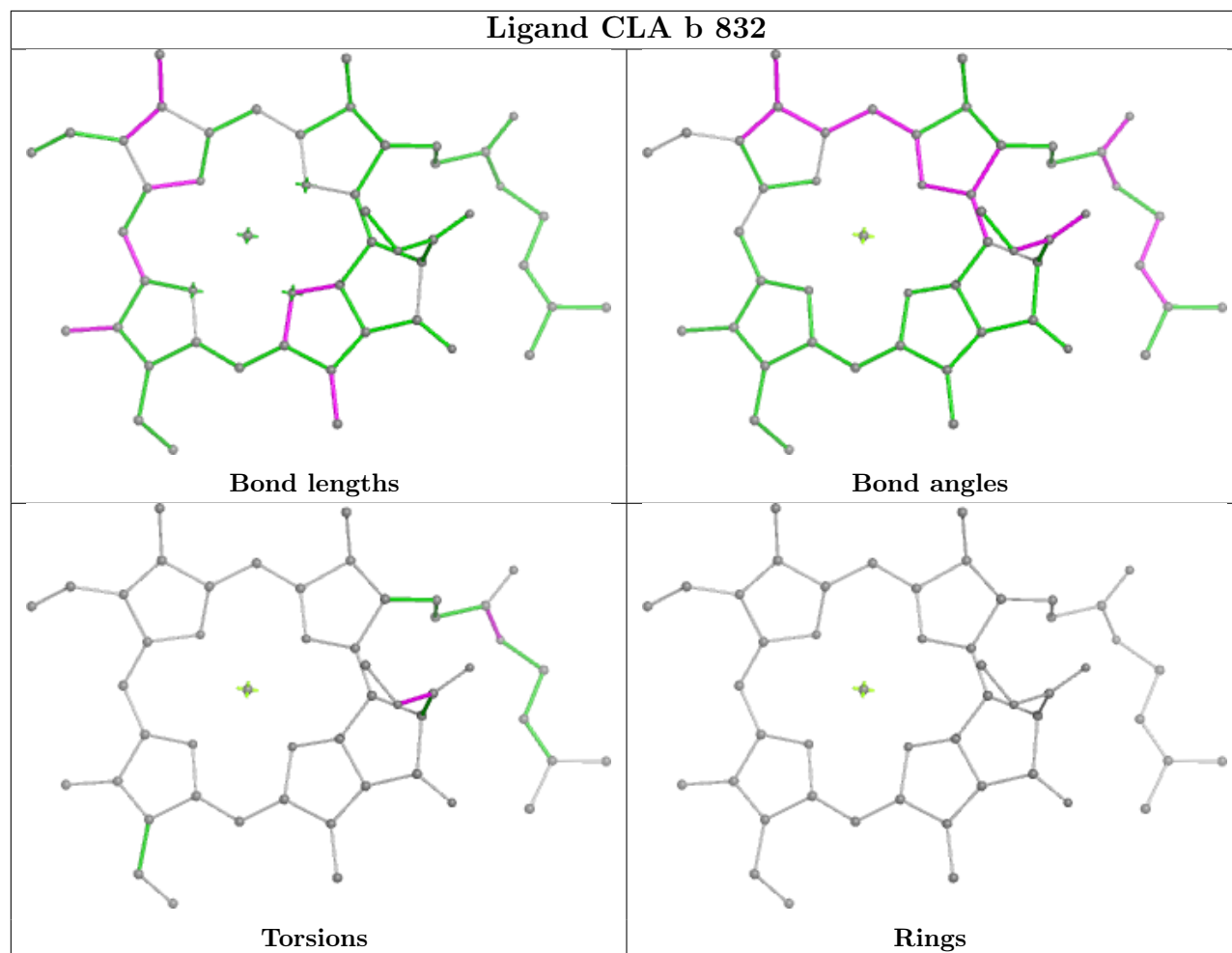
## Ligand BCR G 845



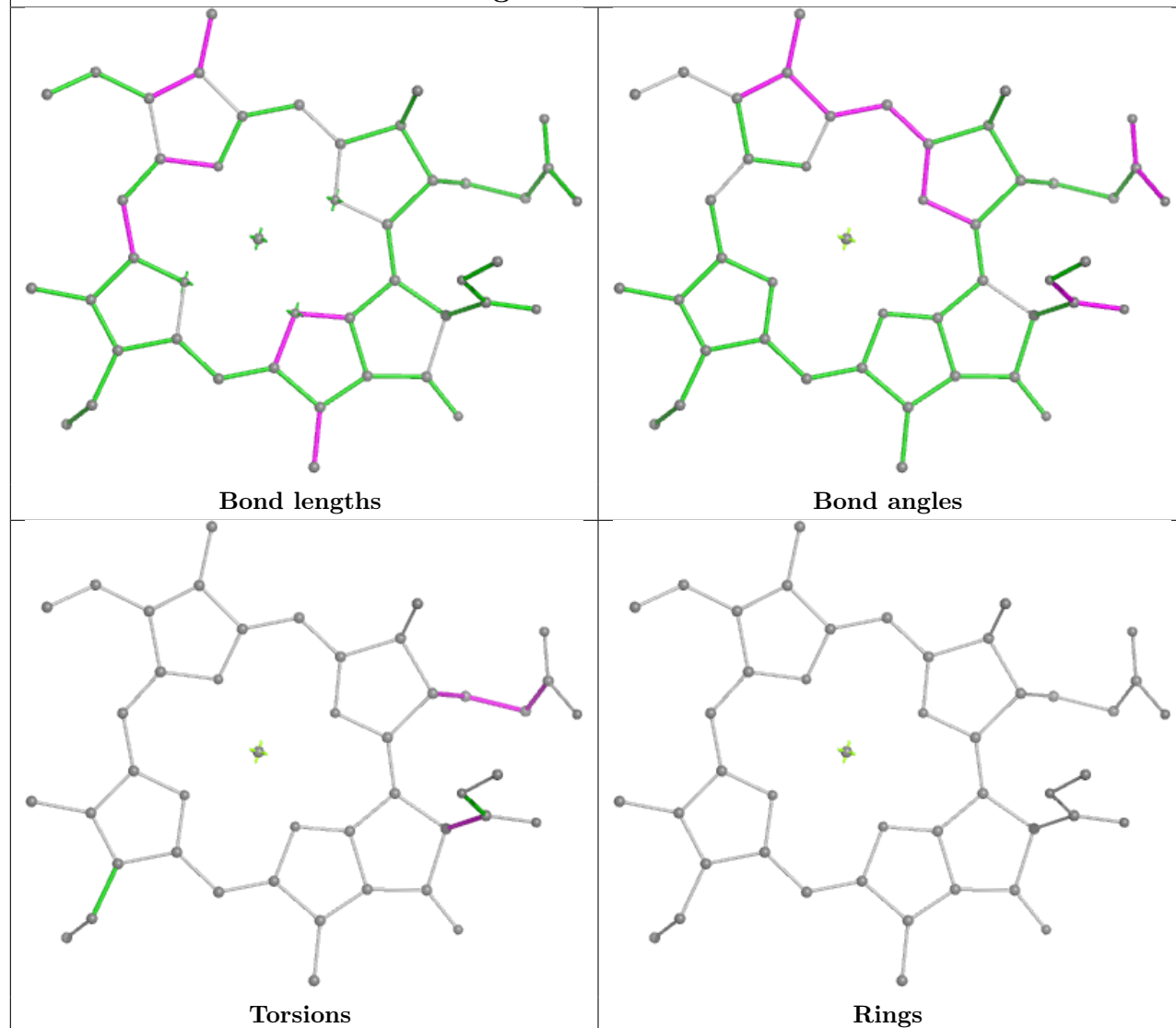
## Ligand CLA G 824



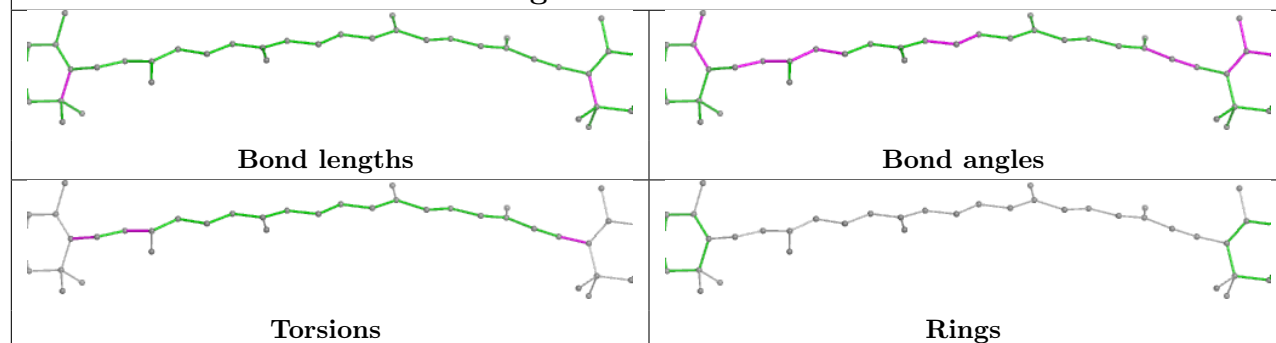
## Ligand CLA b 832

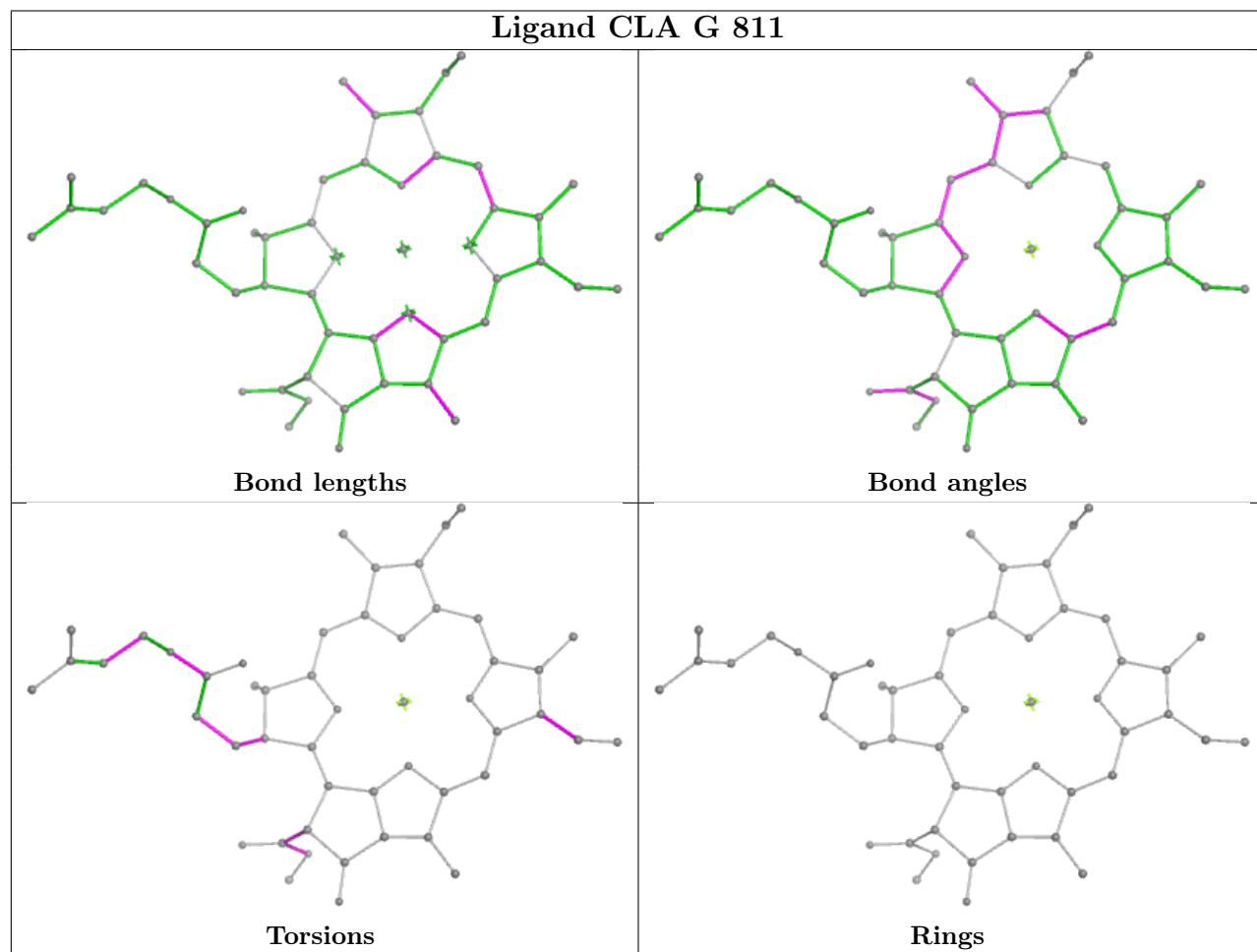
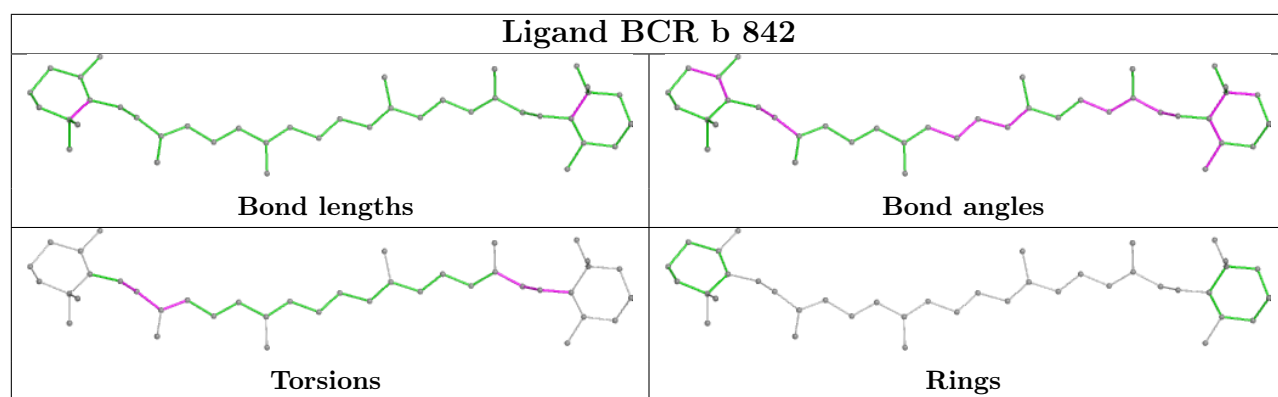


## Ligand CLA b 834

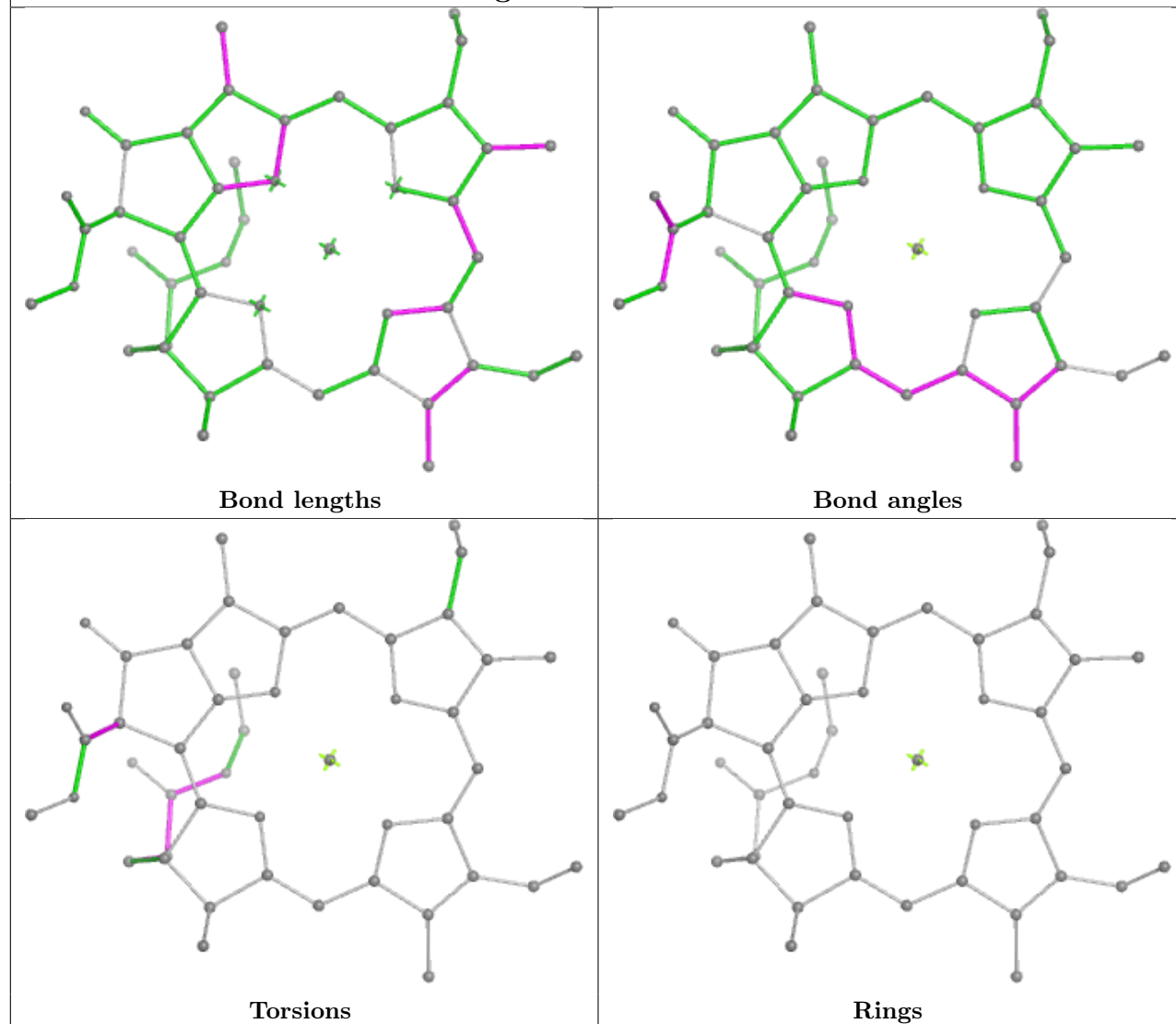


## Ligand BCR A 851

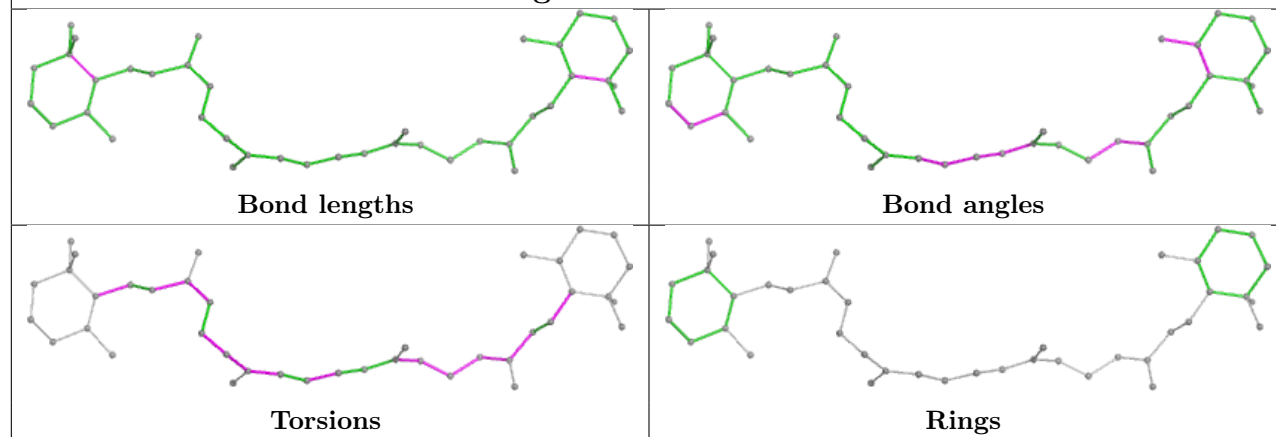




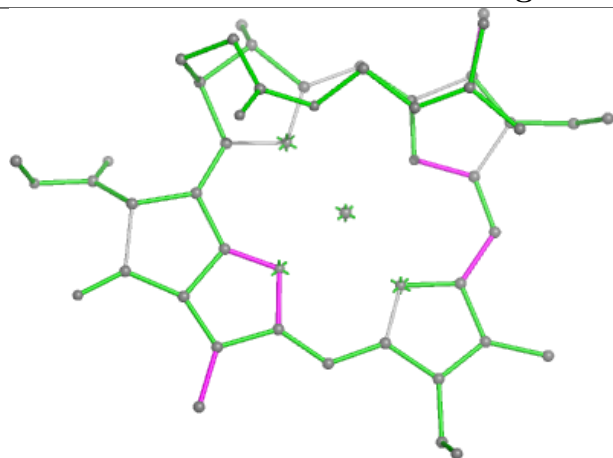
## Ligand CLA e 840



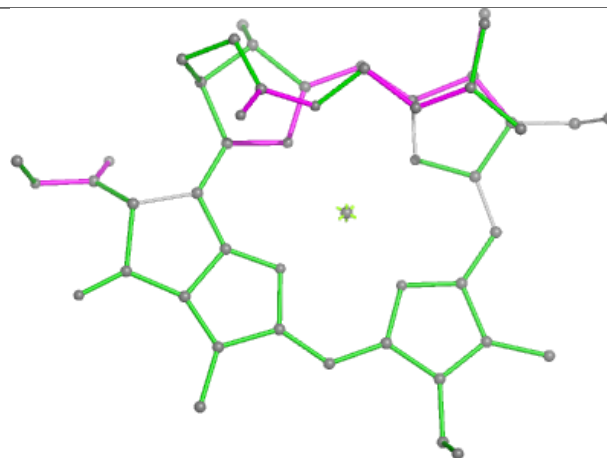
## Ligand BCR b 843



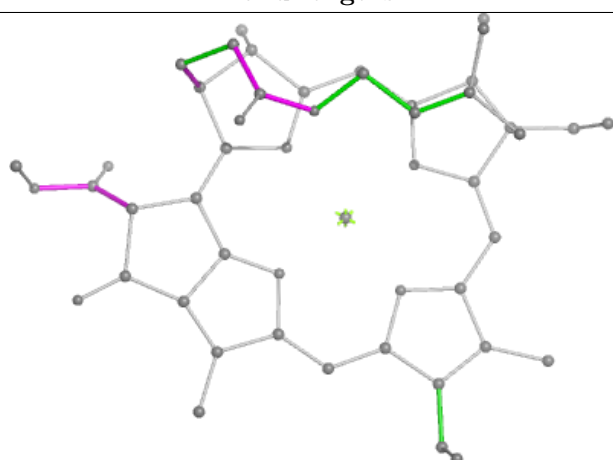
## Ligand CLA E 824



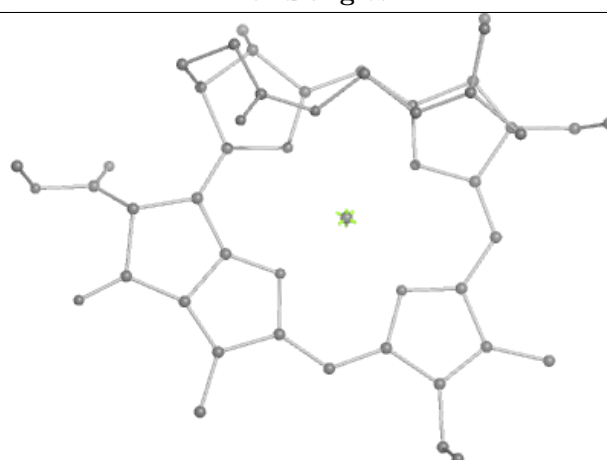
Bond lengths



Bond angles

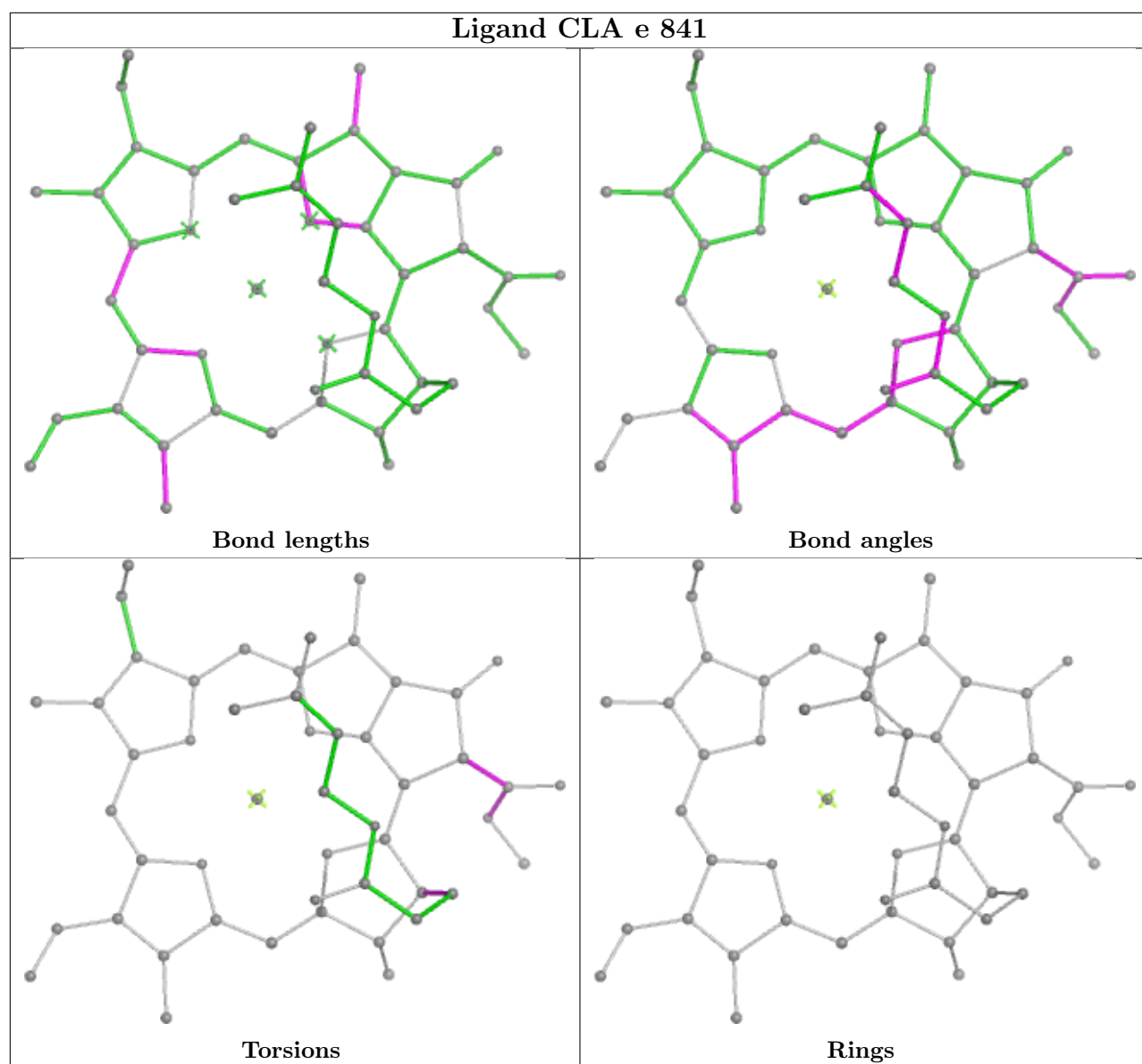


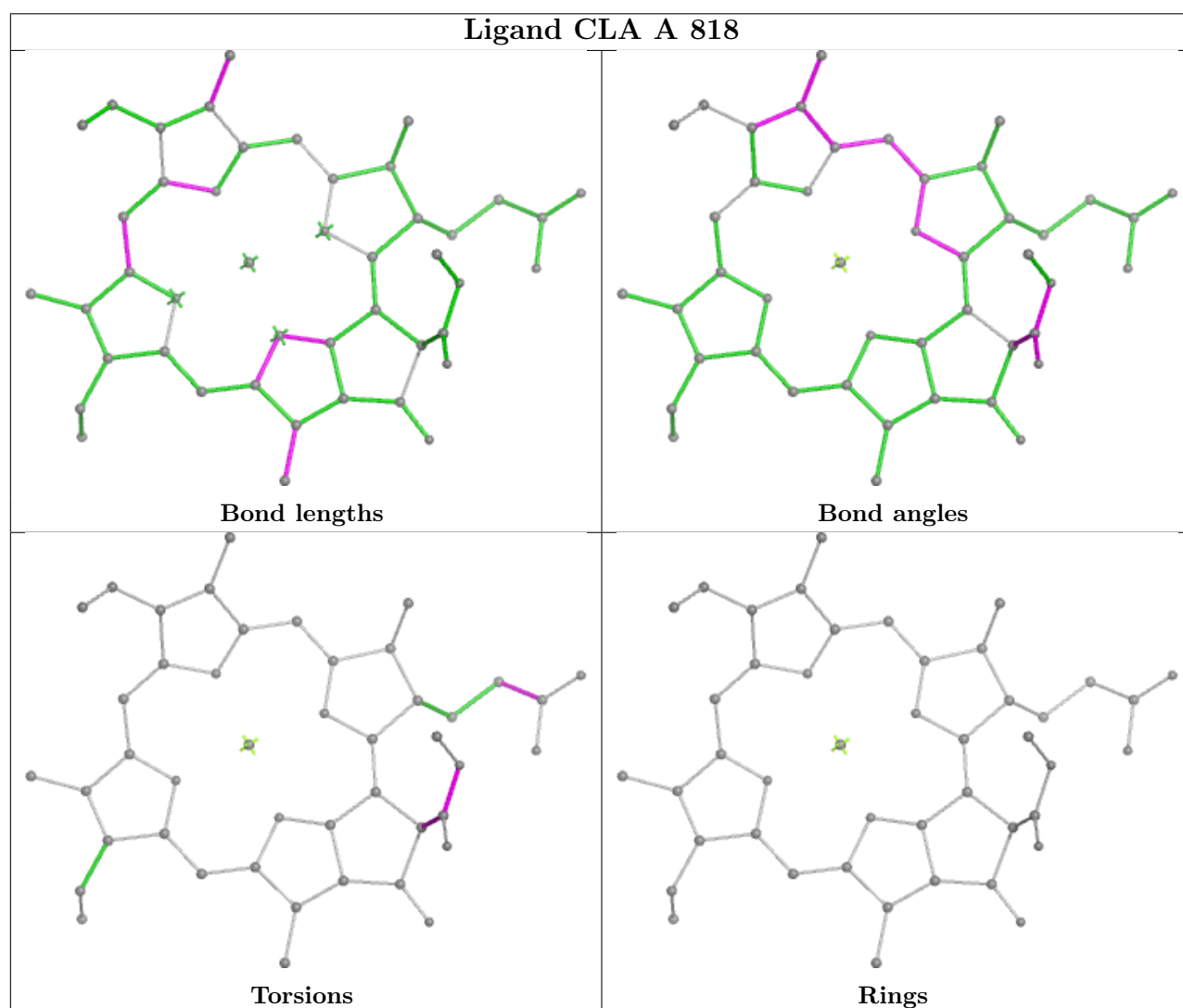
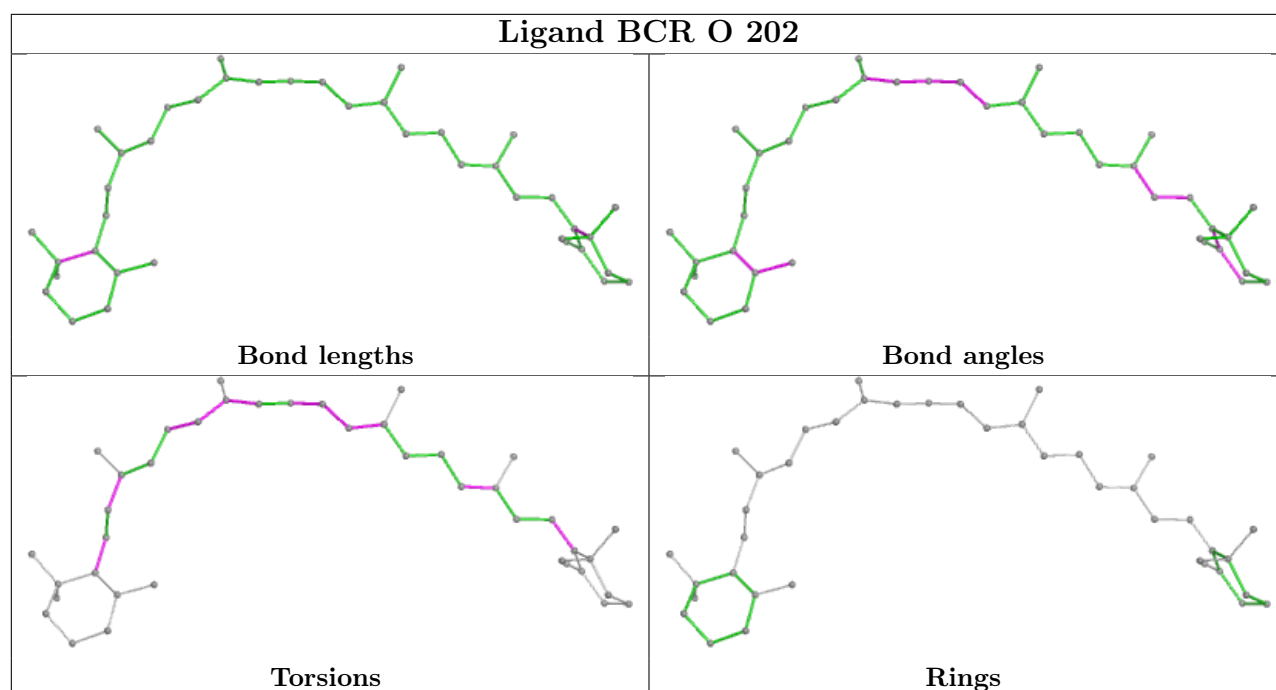
Torsions



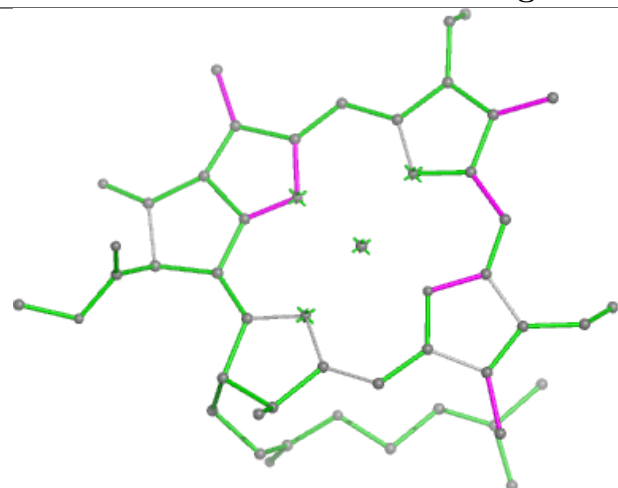
Rings



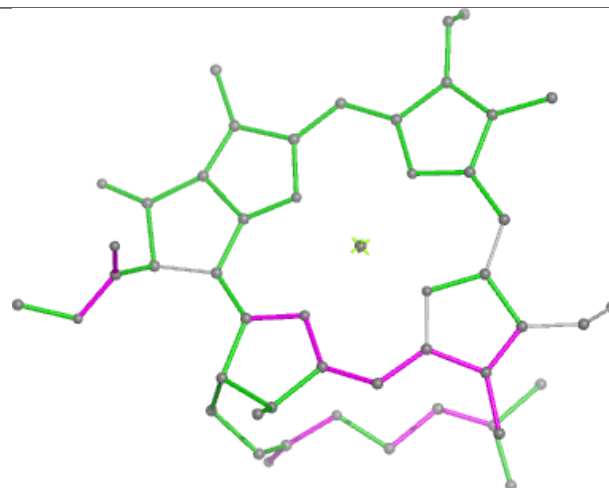




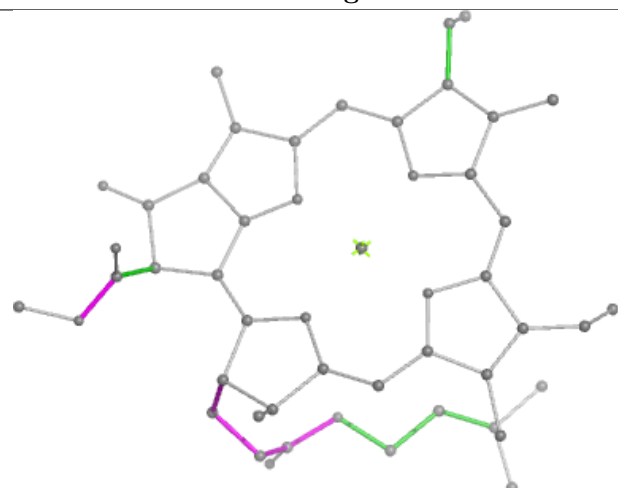
## Ligand CLA A 822



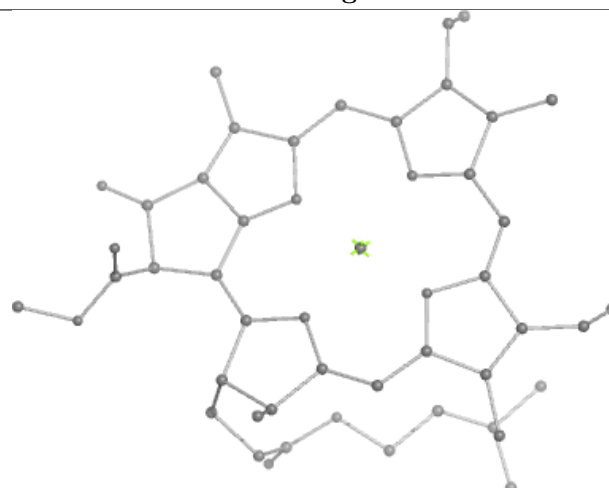
Bond lengths



Bond angles

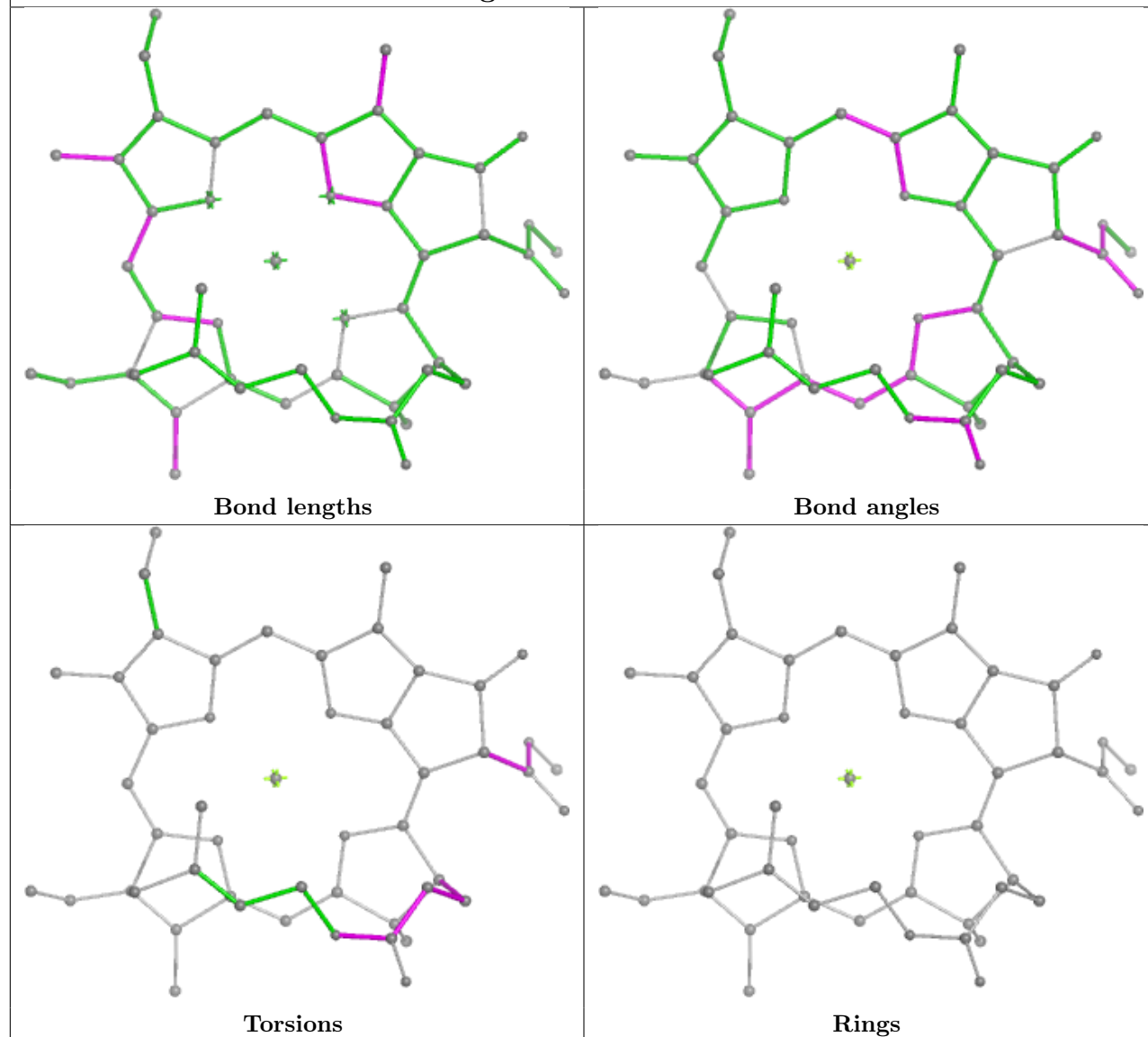


Torsions

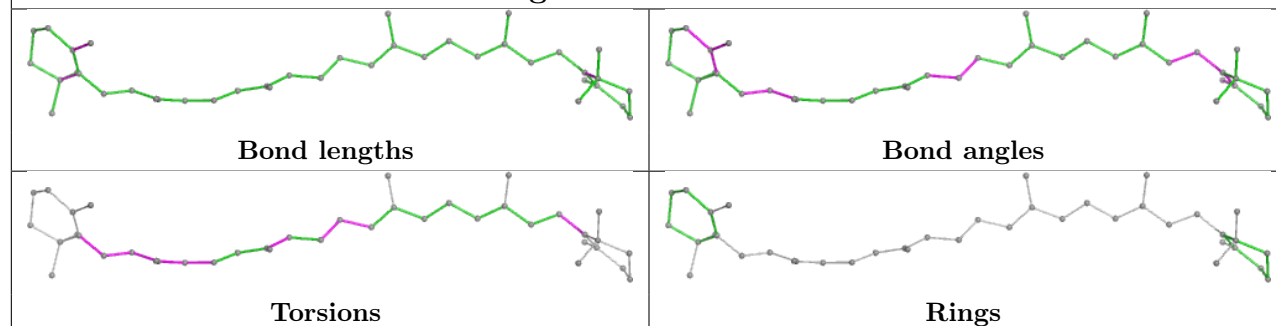


Rings

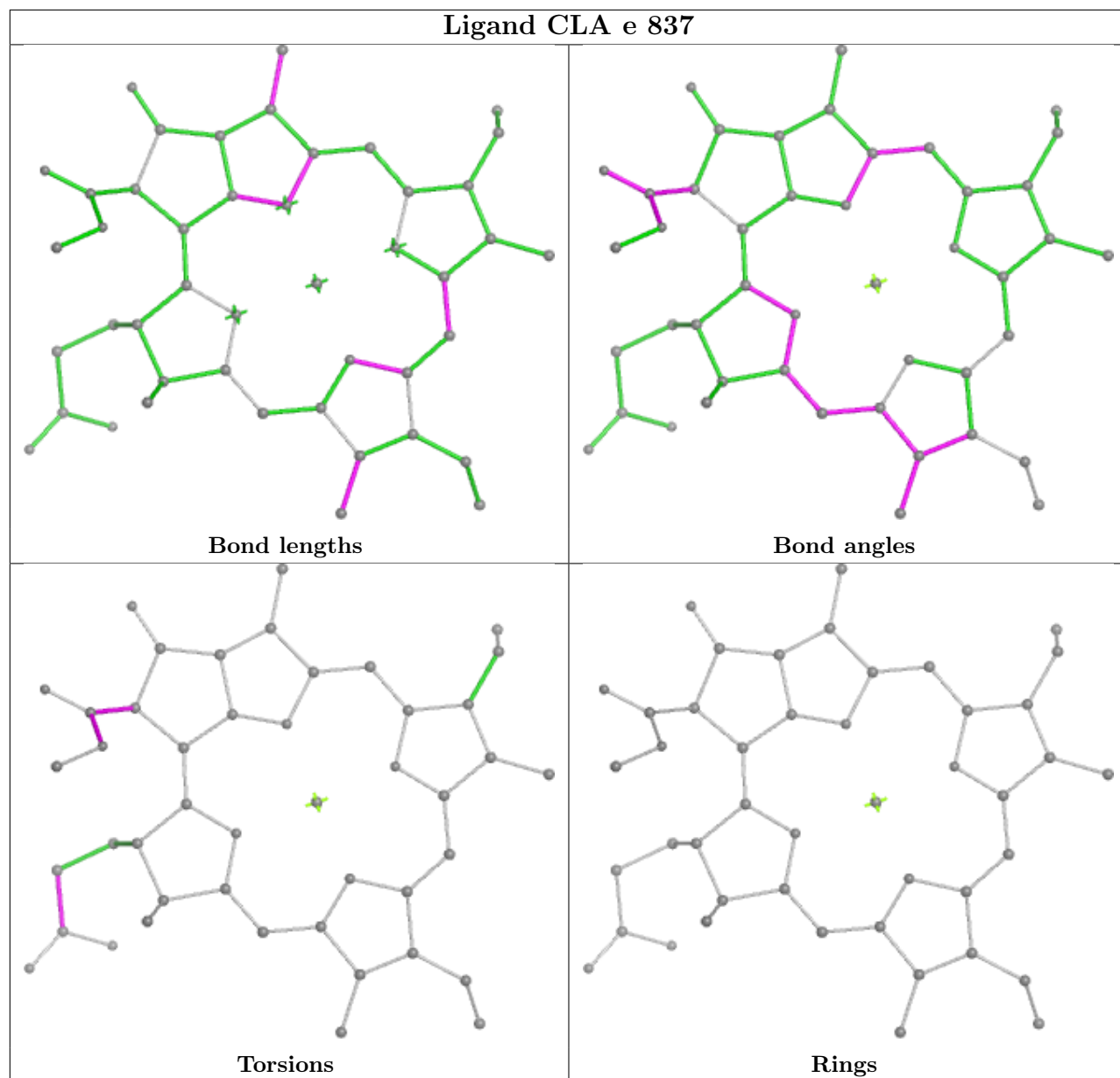
## Ligand CLA E 827

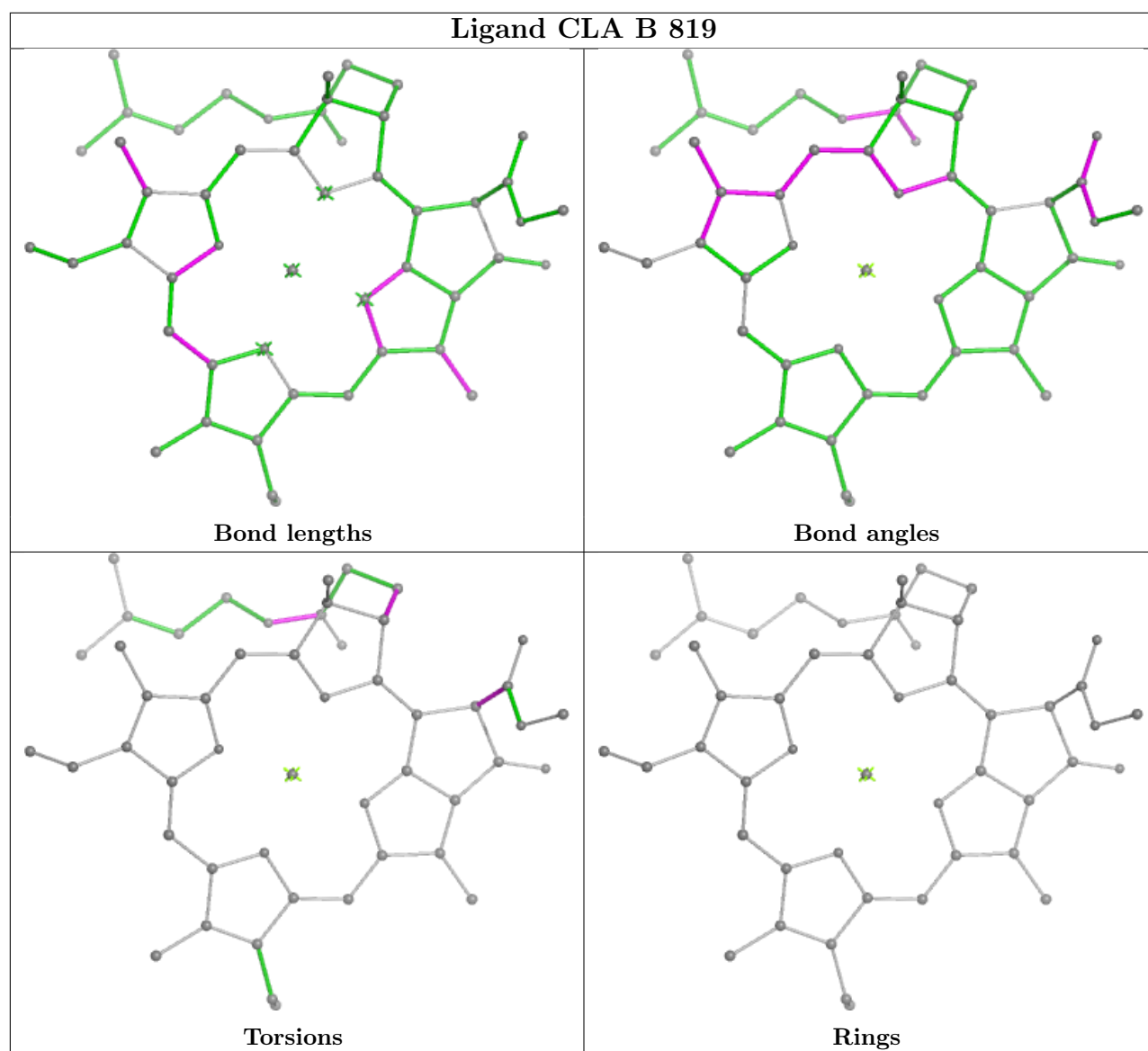


## Ligand BCR G 847

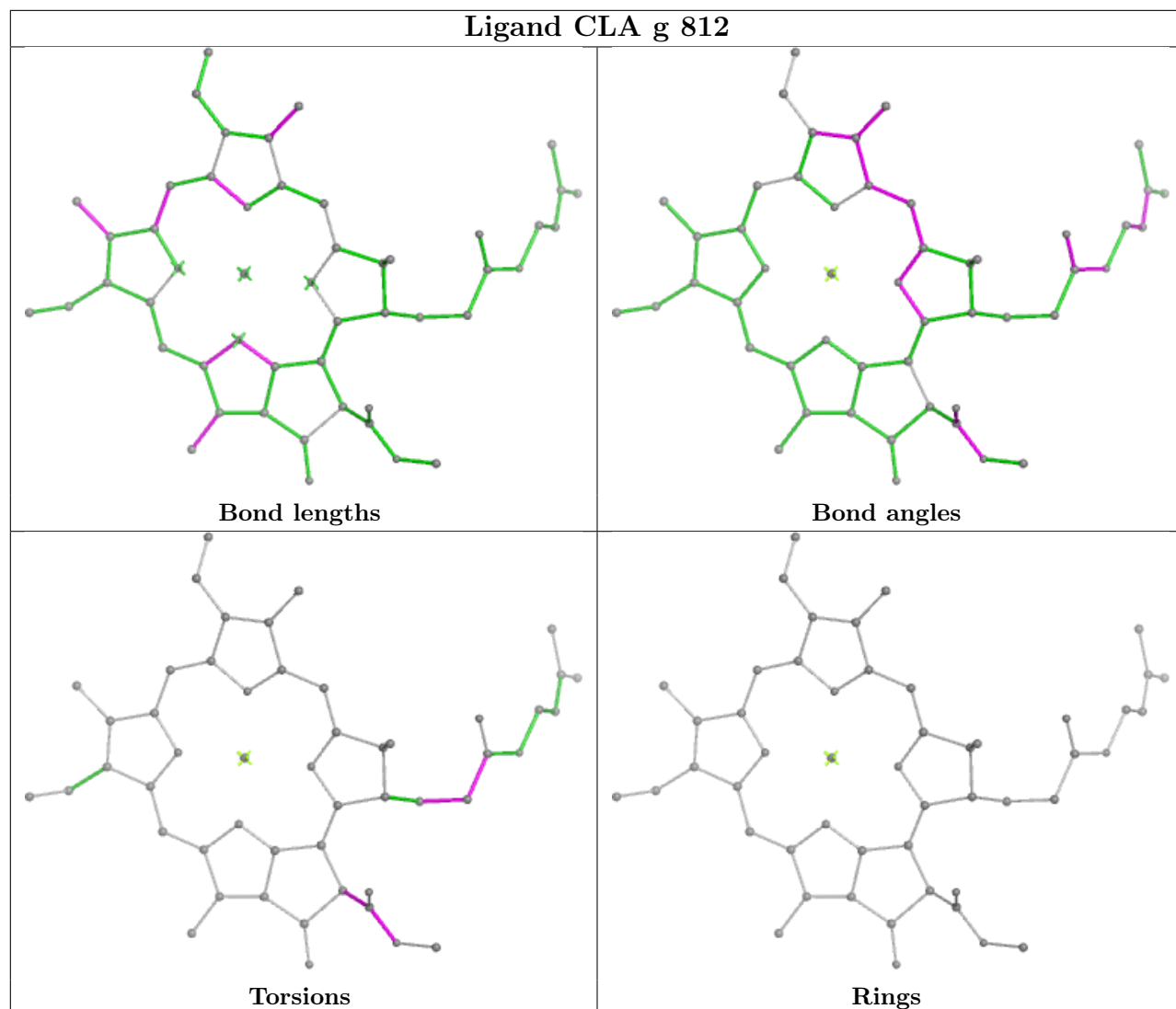


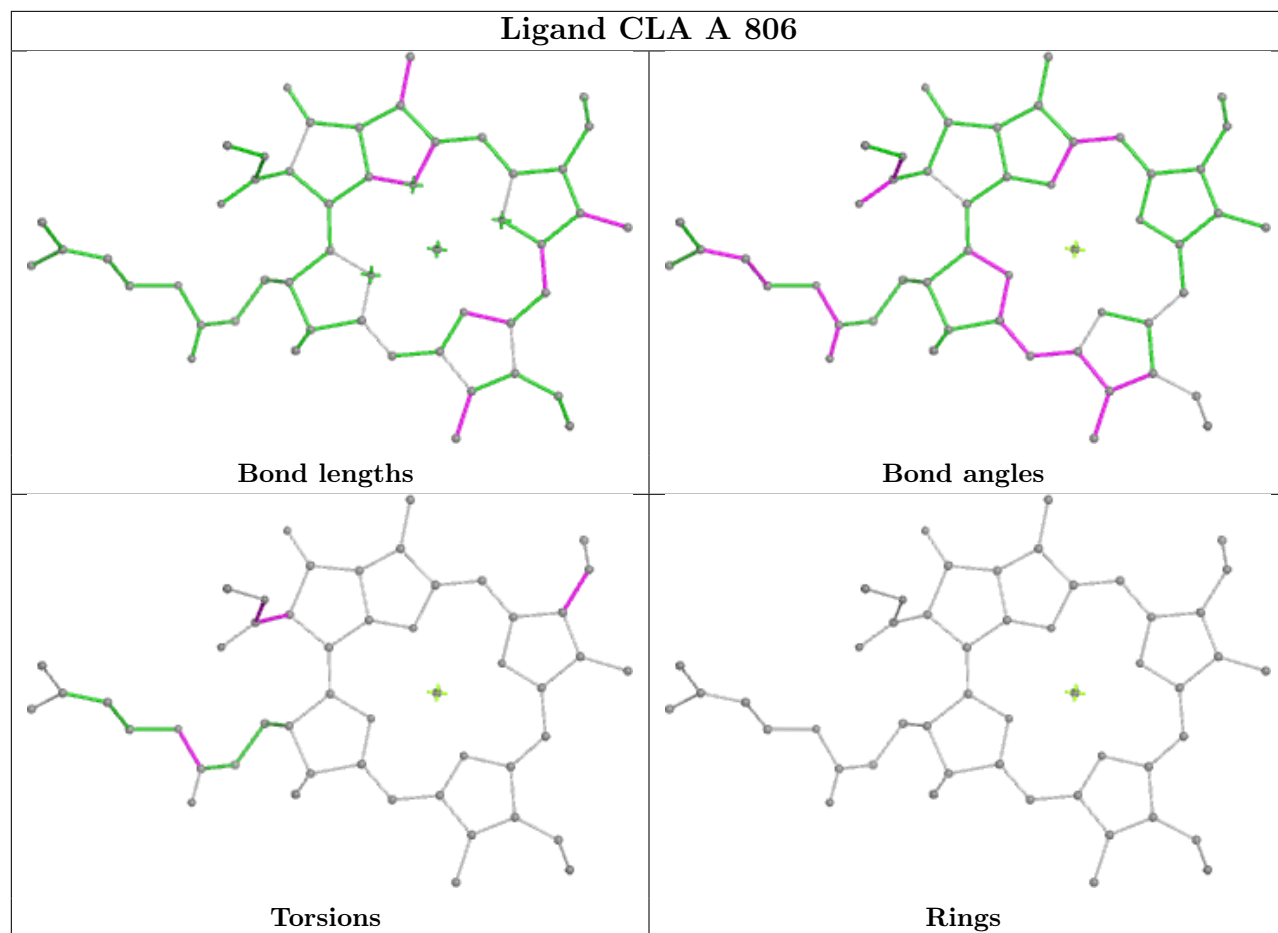
## Ligand CLA e 837



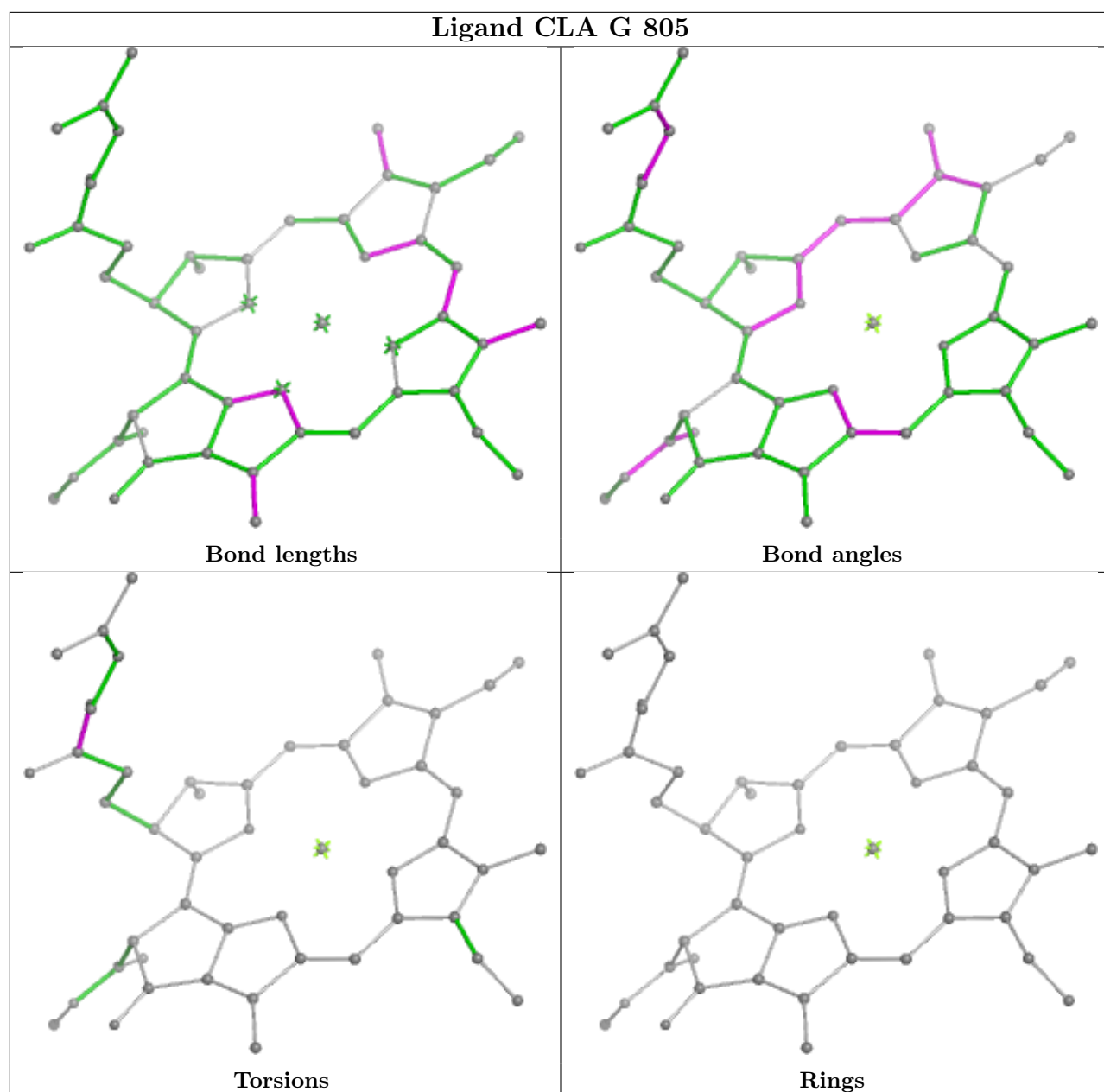


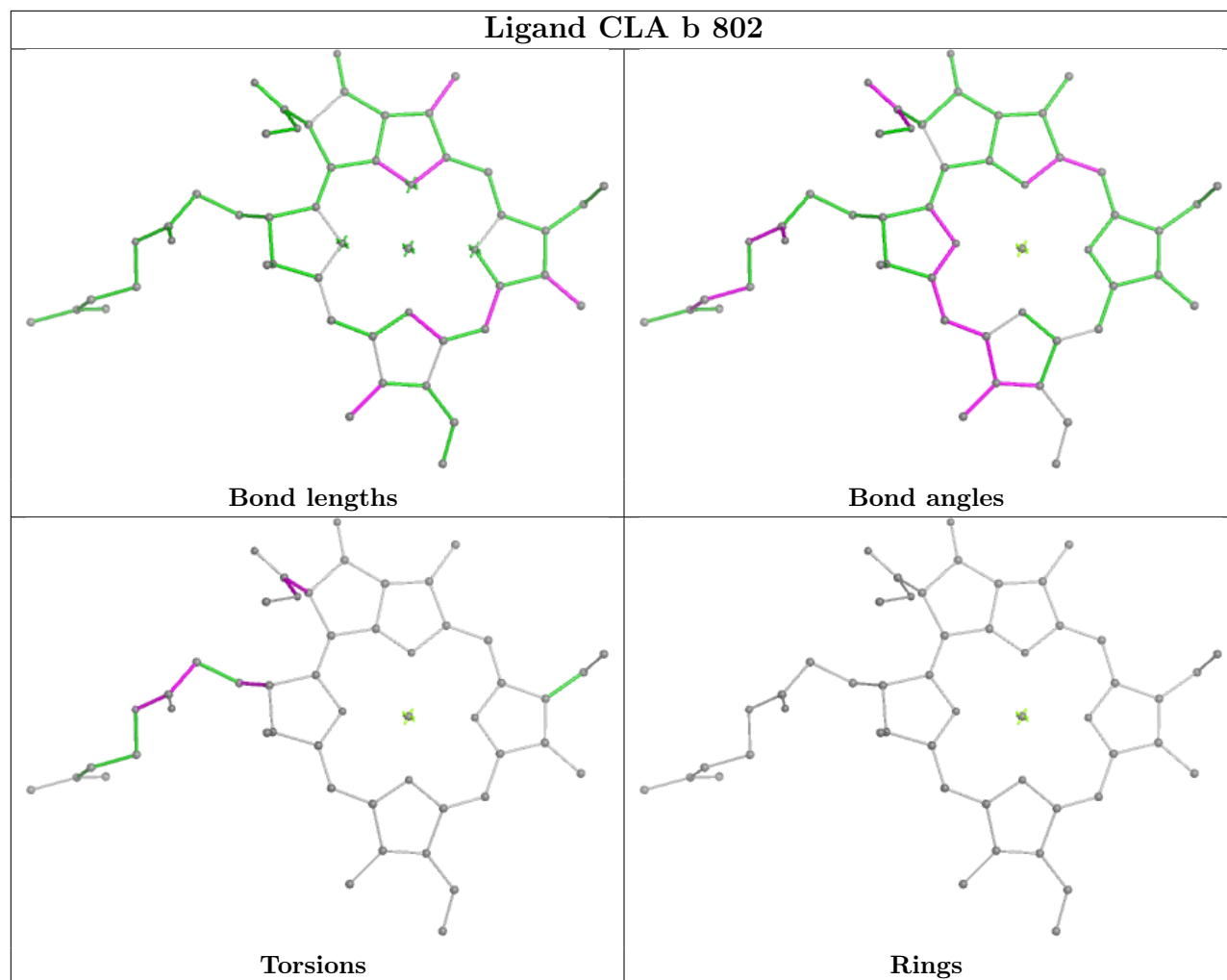
## Ligand CLA g 812



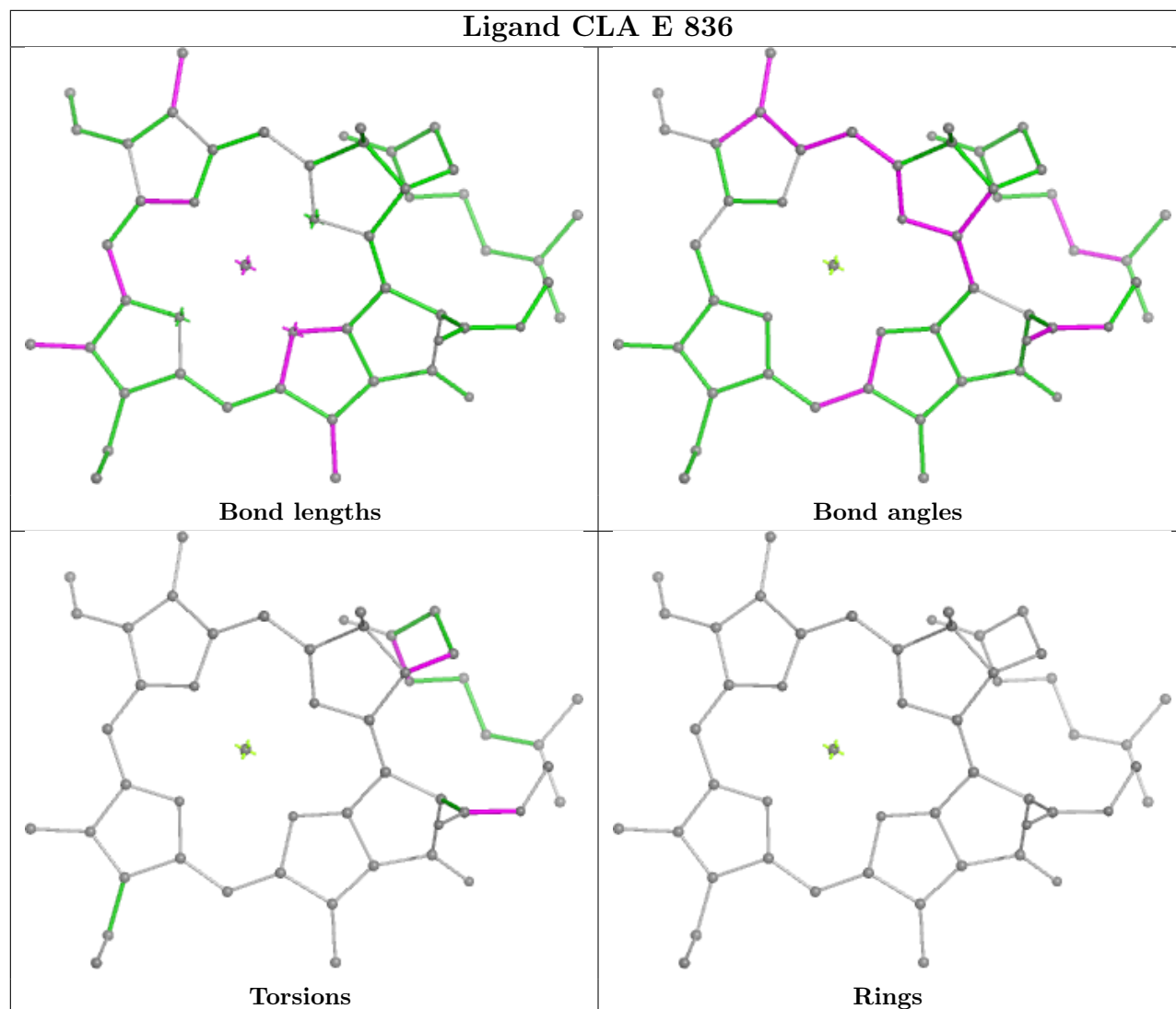




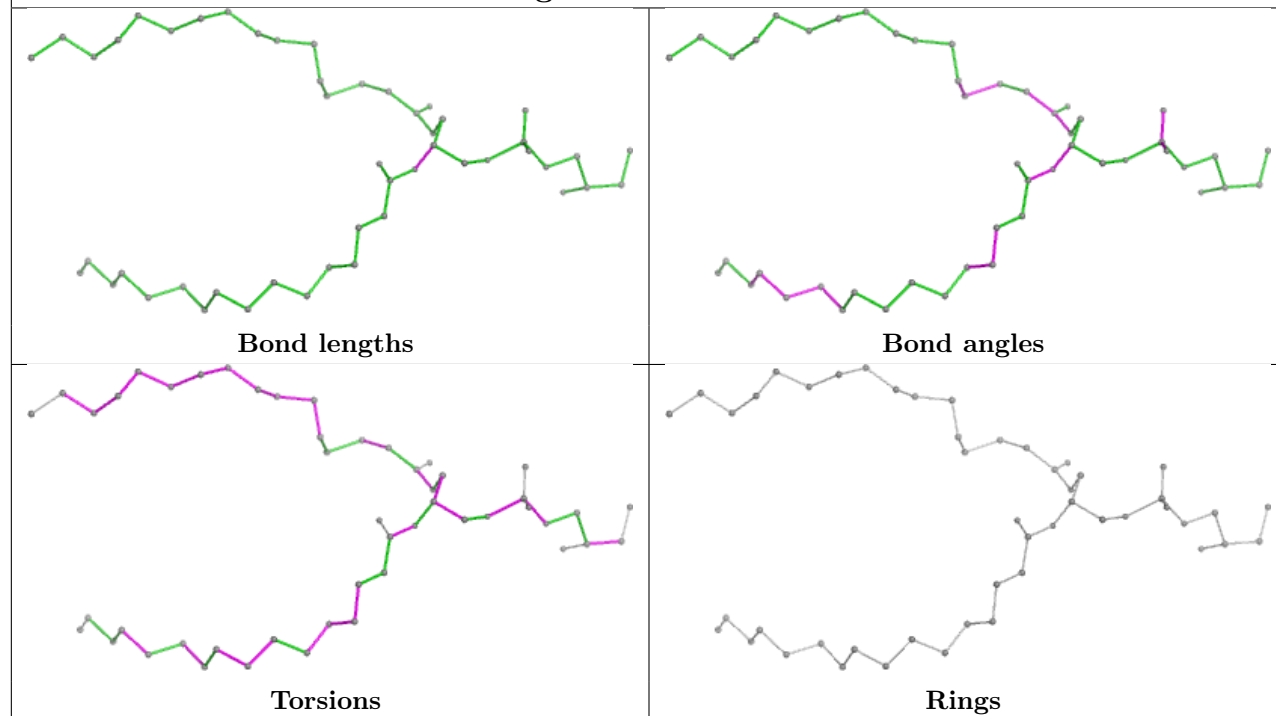




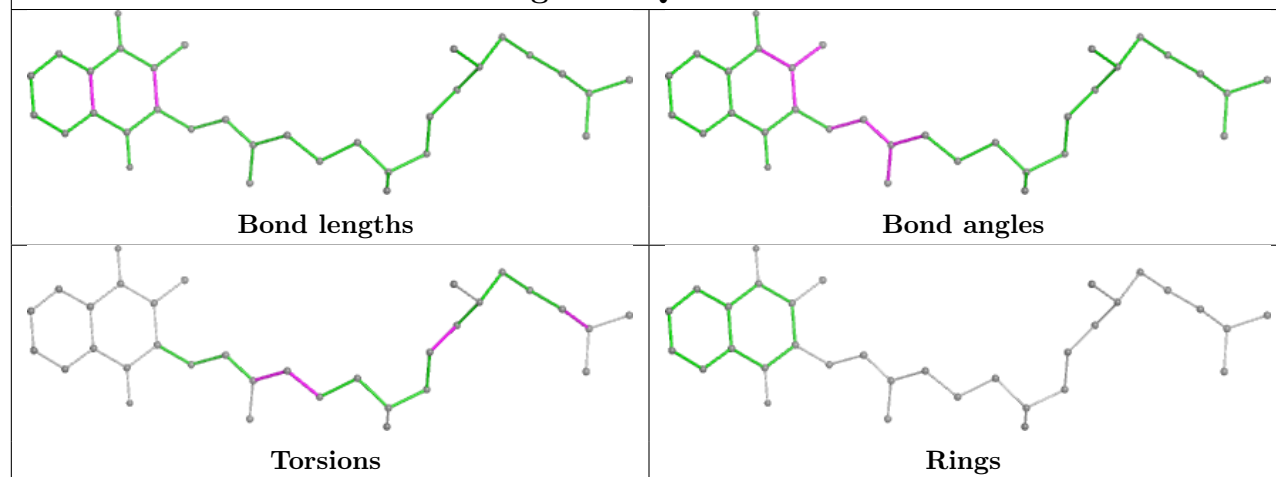
## Ligand CLA E 836



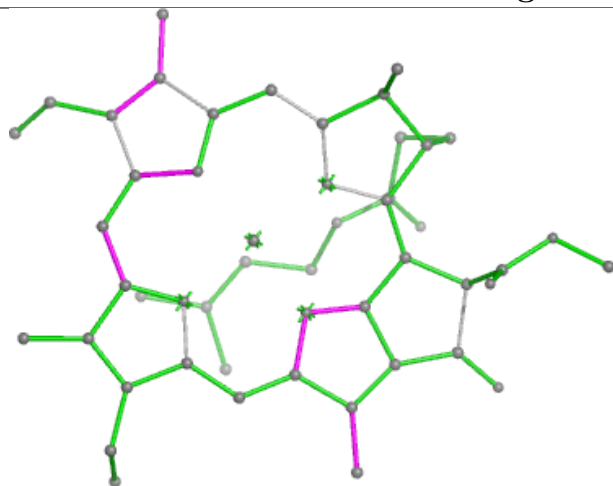
## Ligand LHG e 801



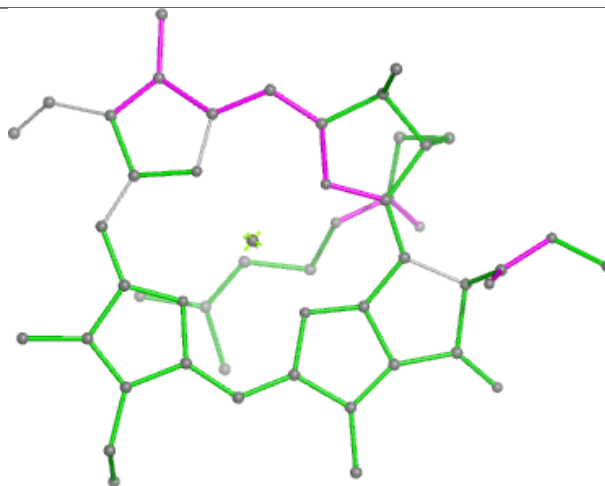
## Ligand PQN E 848



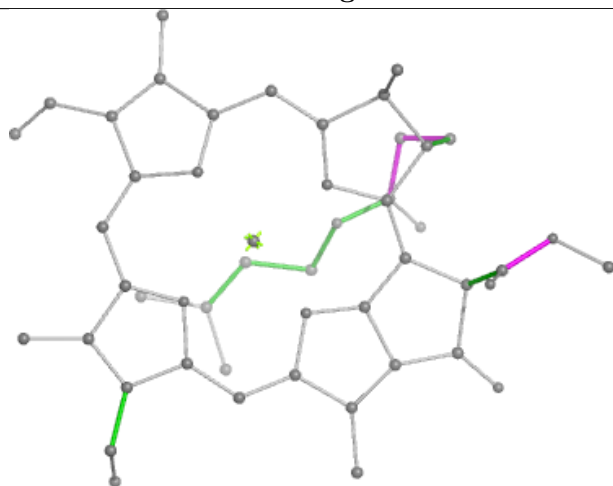
## Ligand CLA b 808



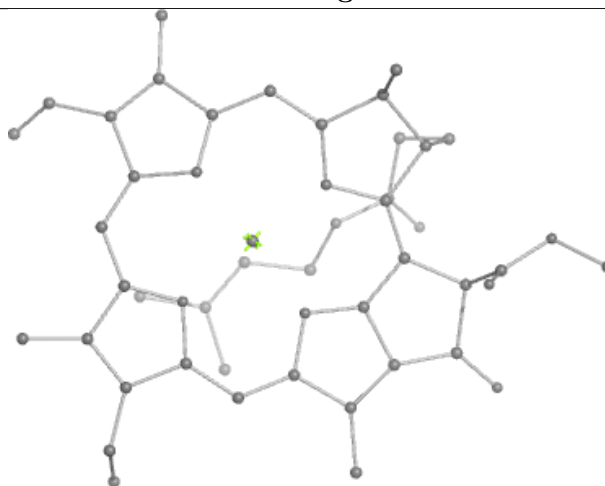
Bond lengths



Bond angles

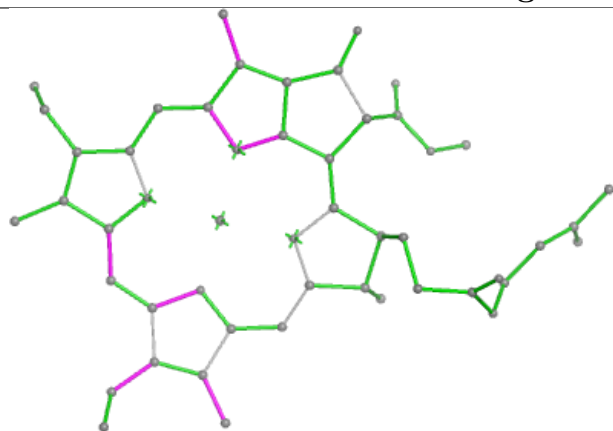


Torsions

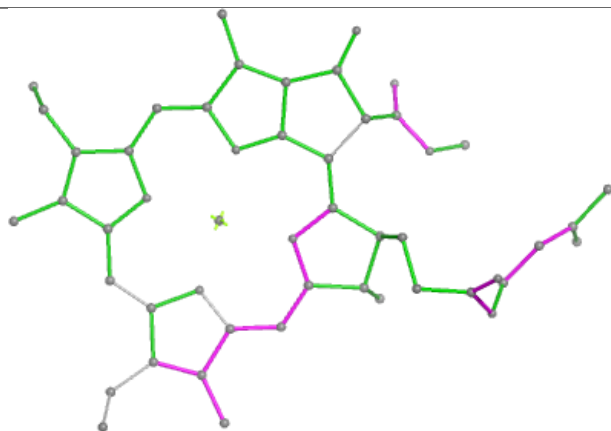


Rings

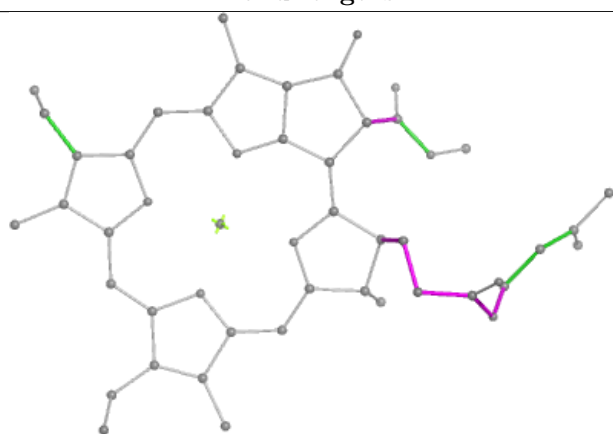
## Ligand CLA b 806



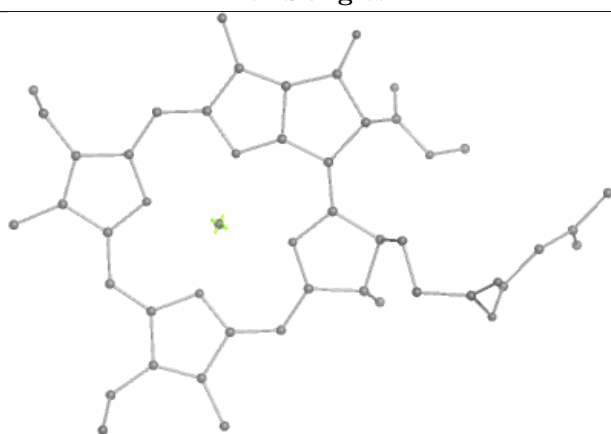
Bond lengths



Bond angles

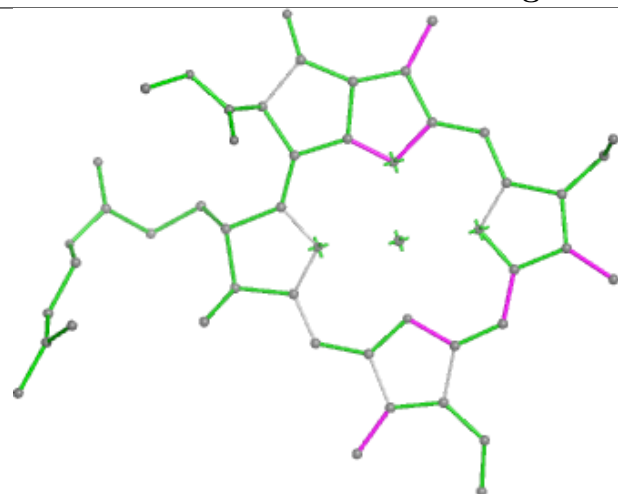


Torsions

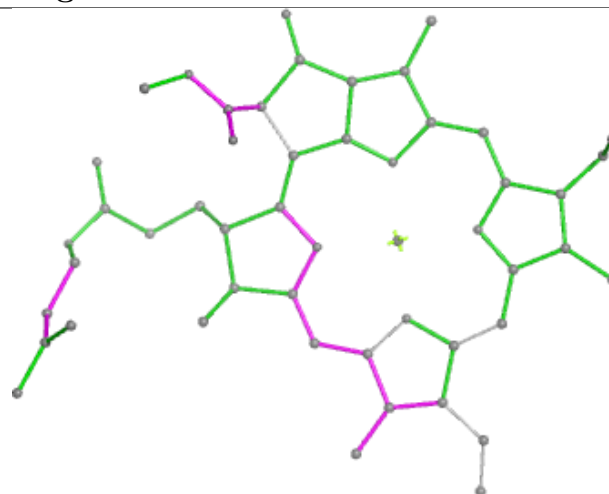


Rings

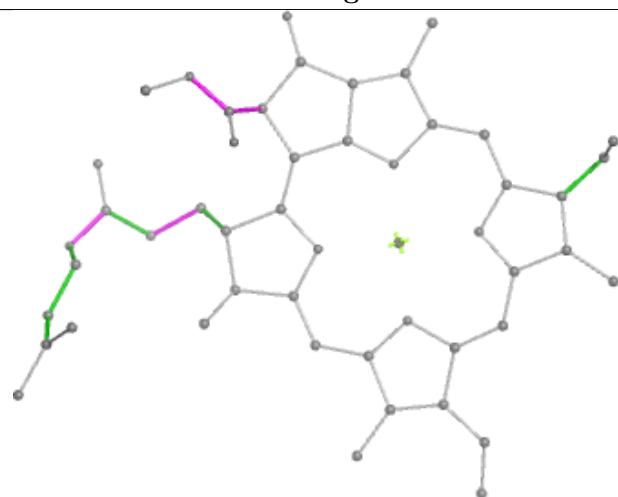
## Ligand CLA g 826



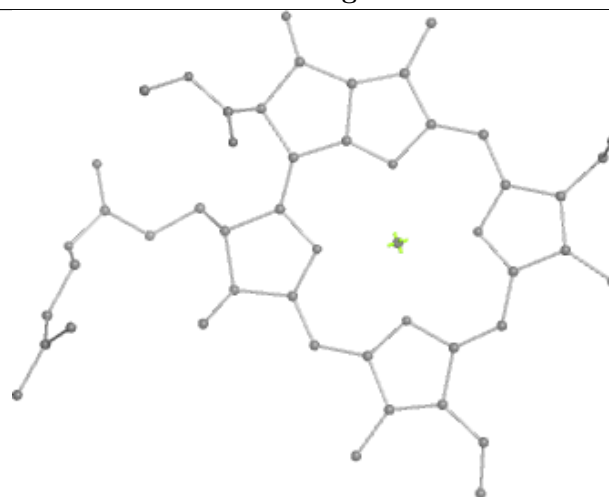
Bond lengths



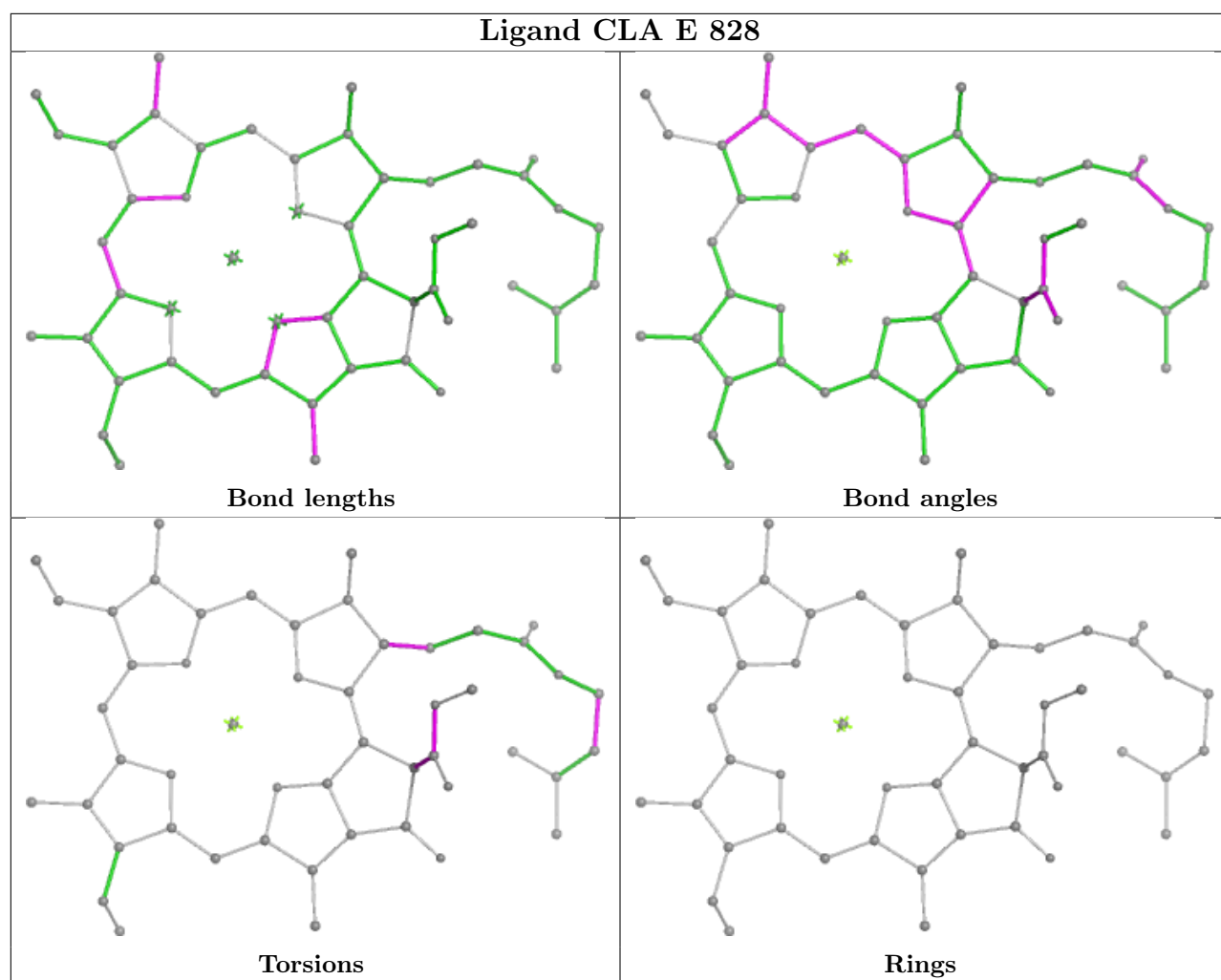
Bond angles



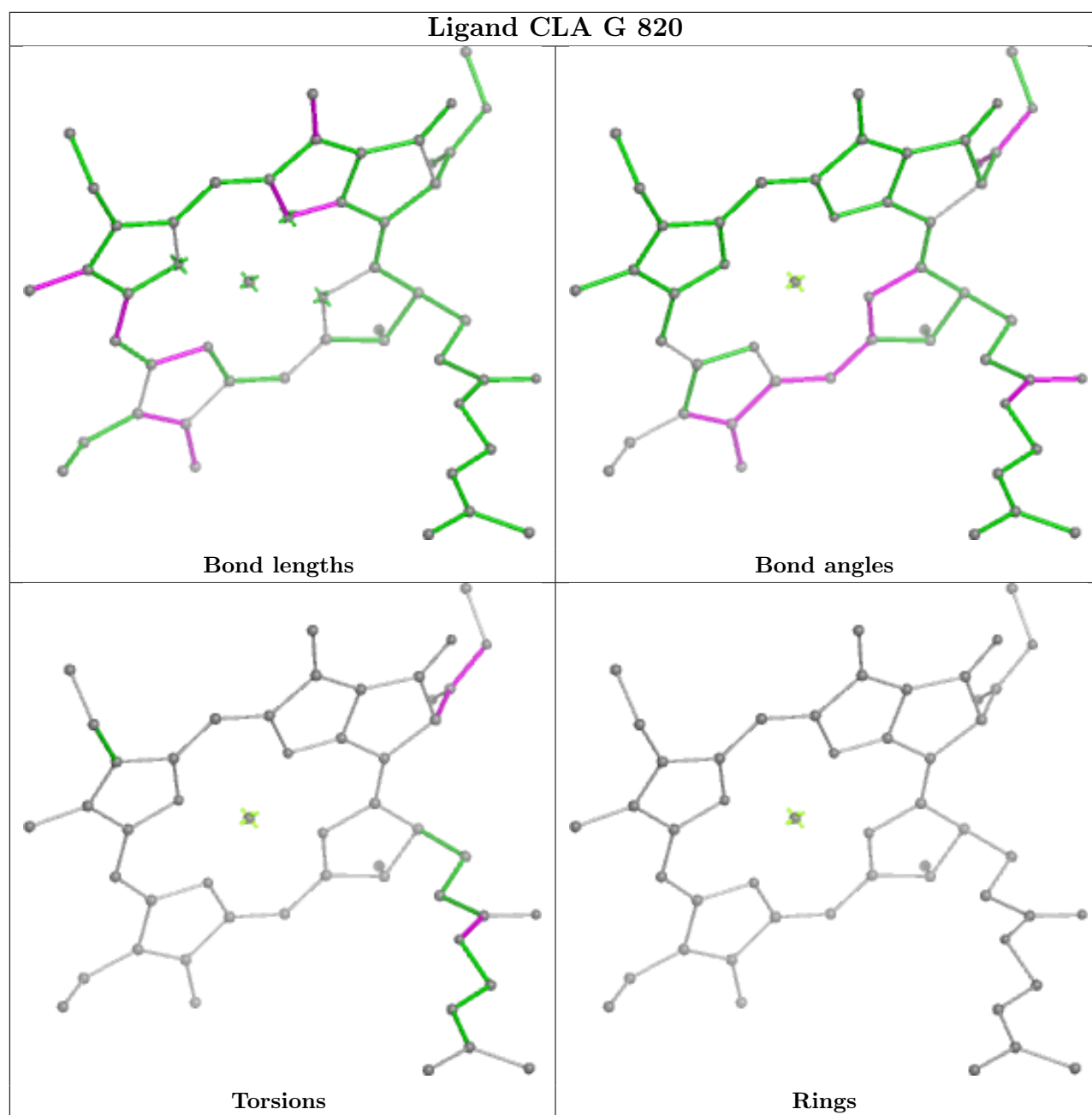
Torsions



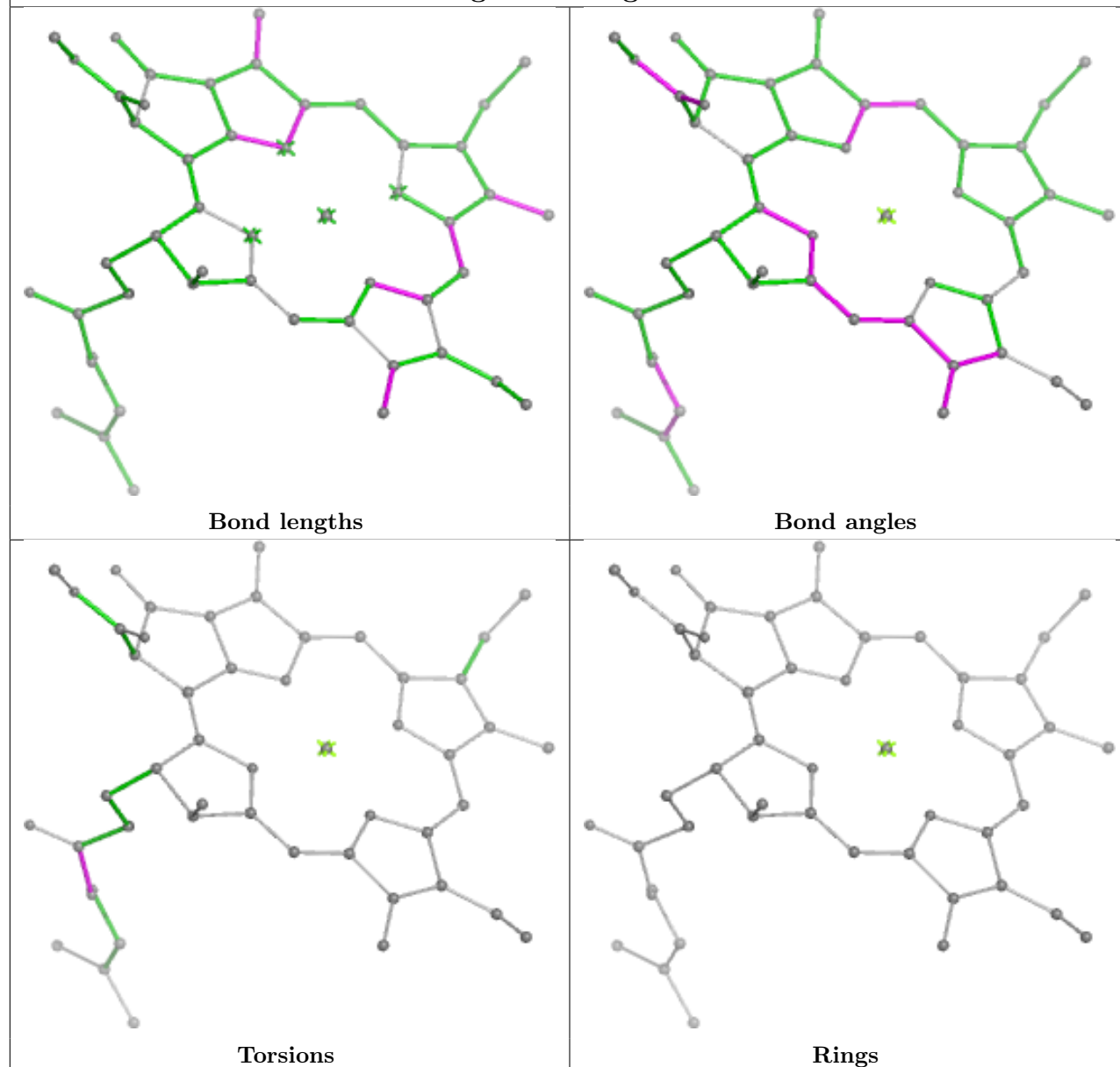
Rings



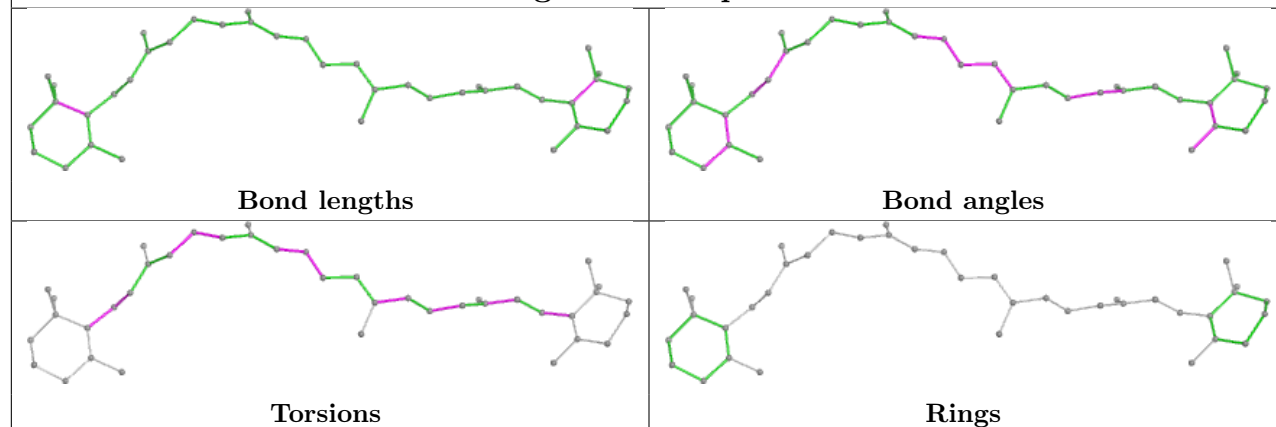




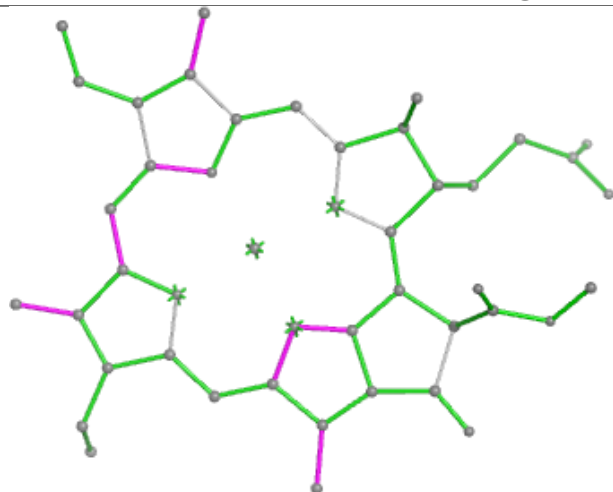
## Ligand CLA g 807



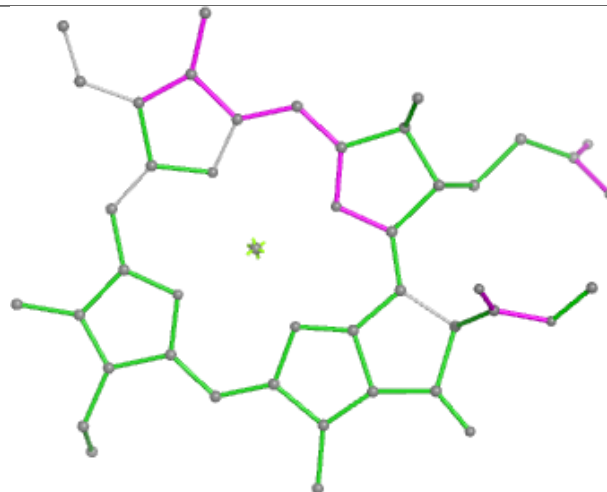
## Ligand BCR q 101



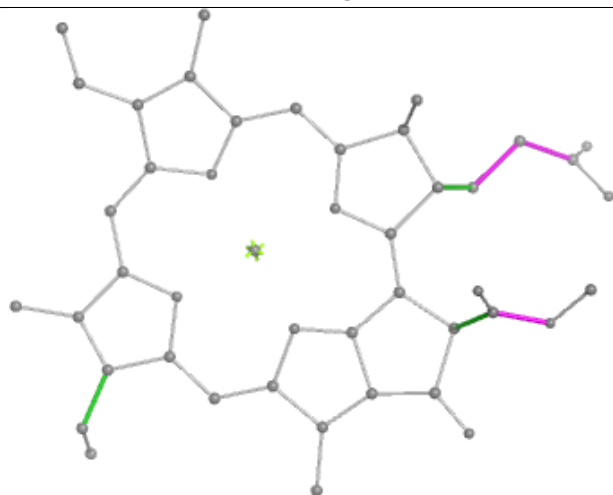
## Ligand CLA L 203



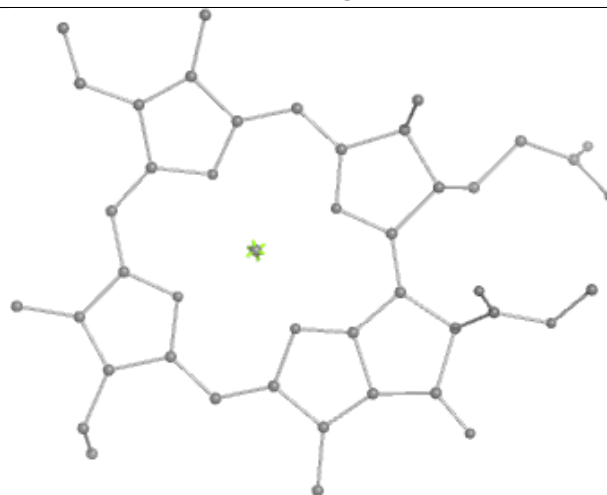
Bond lengths



Bond angles

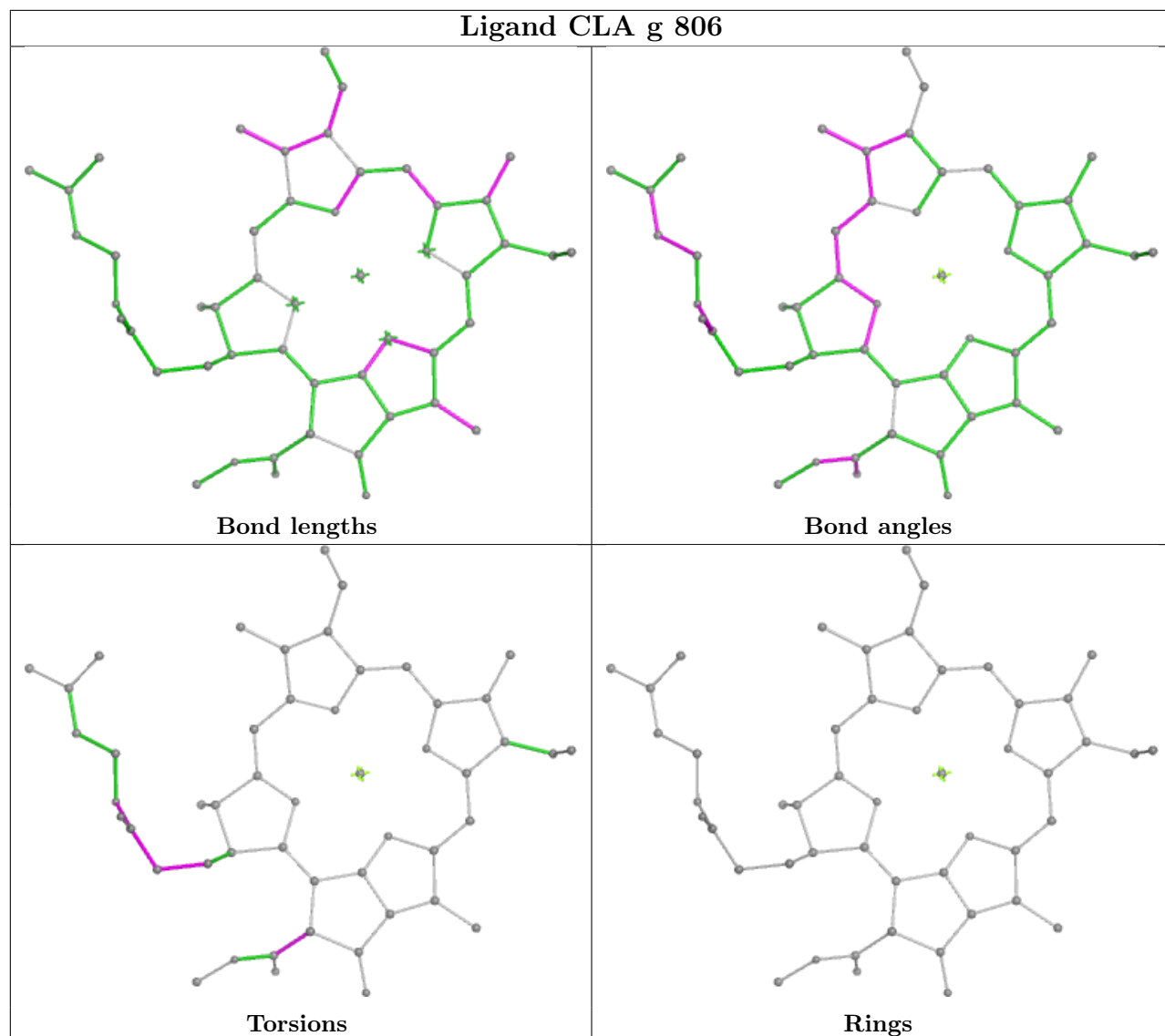


Torsions

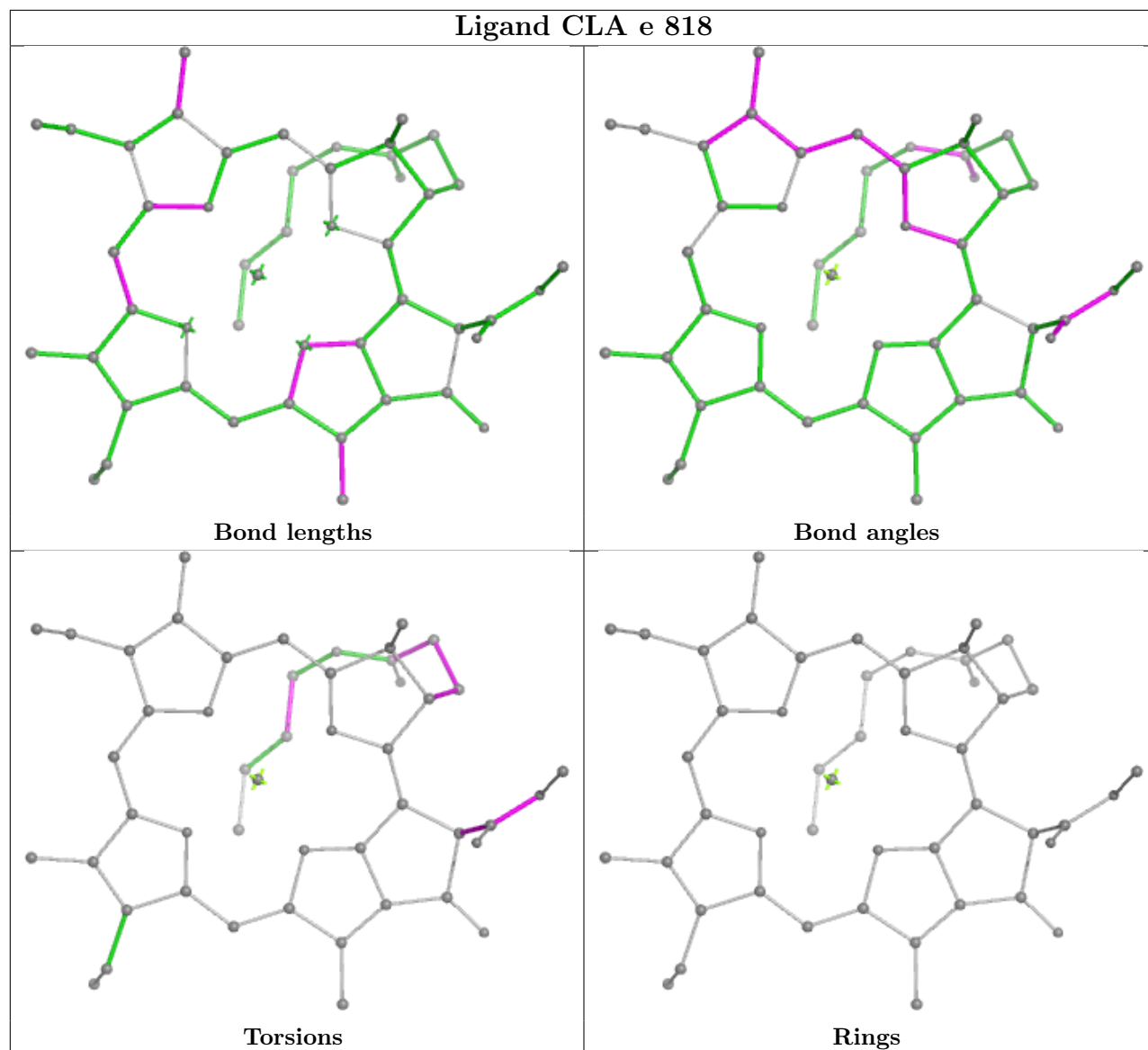


Rings

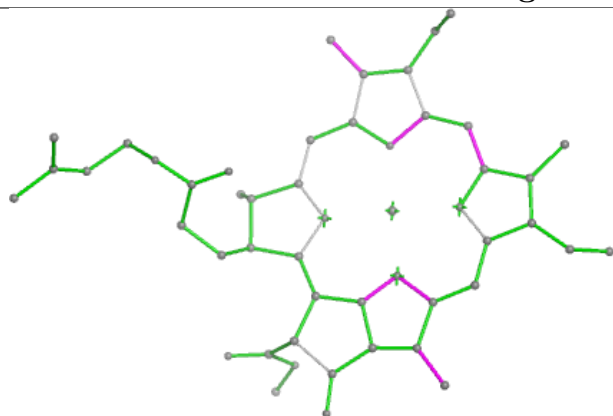
## Ligand CLA g 806



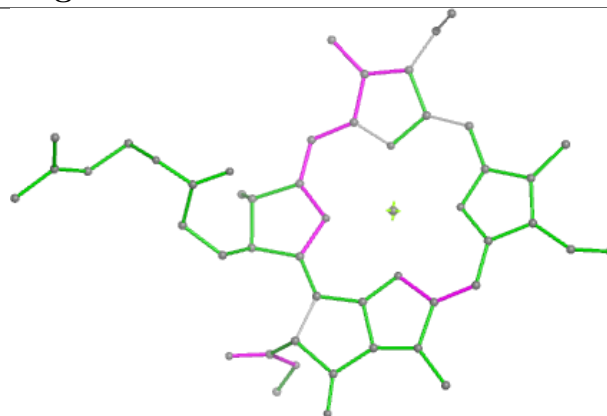
## Ligand CLA e 818



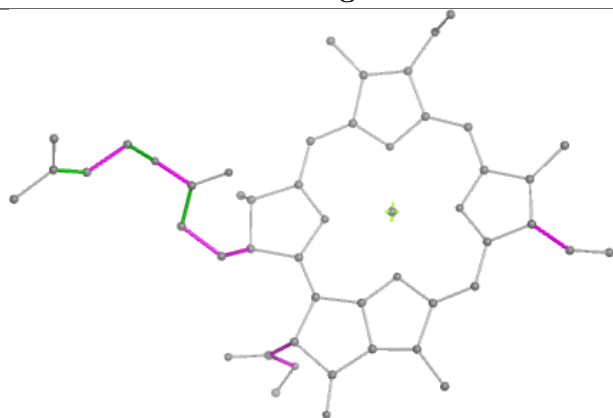
## Ligand CLA g 813



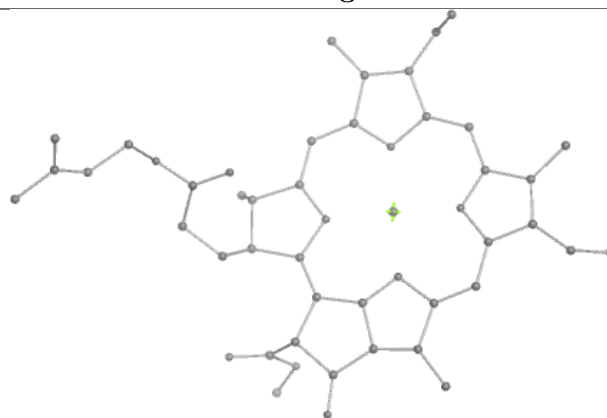
Bond lengths



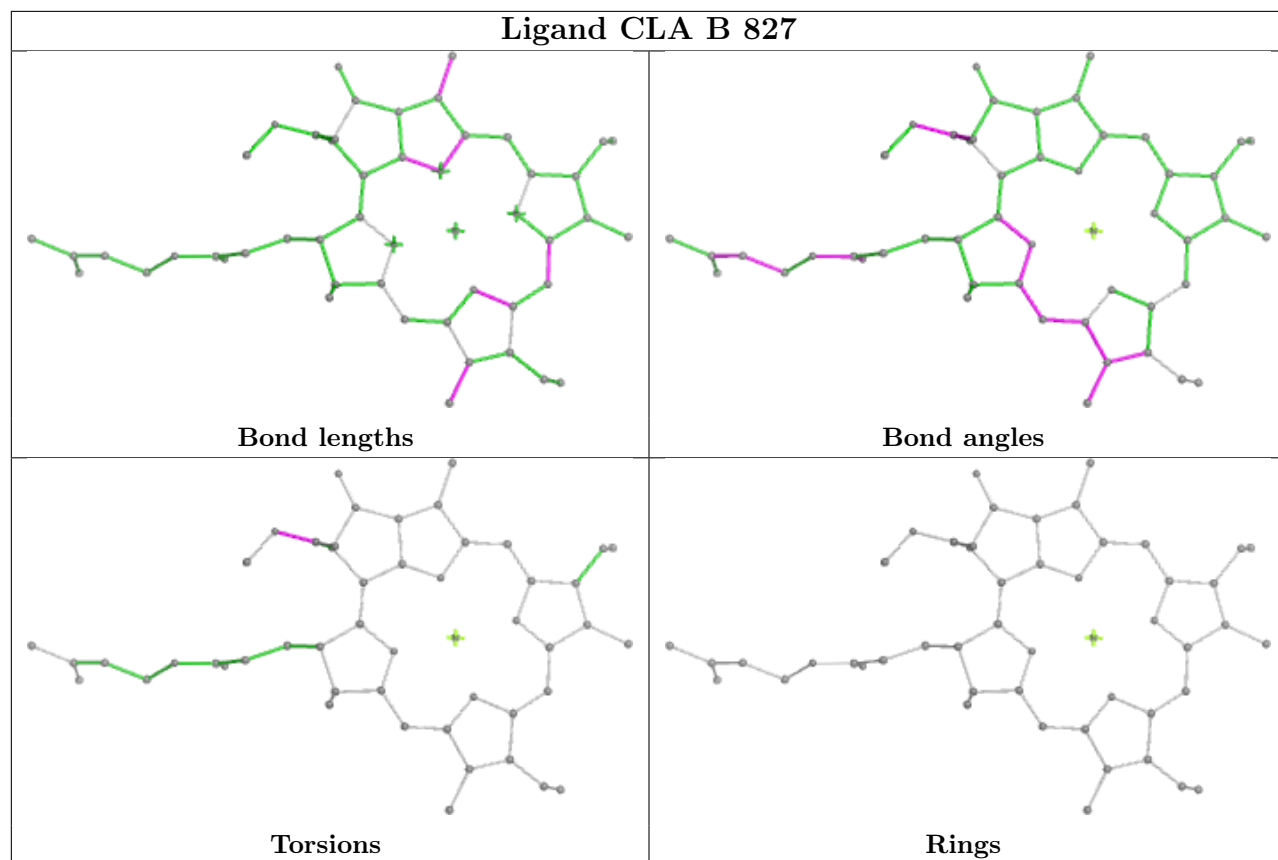
Bond angles



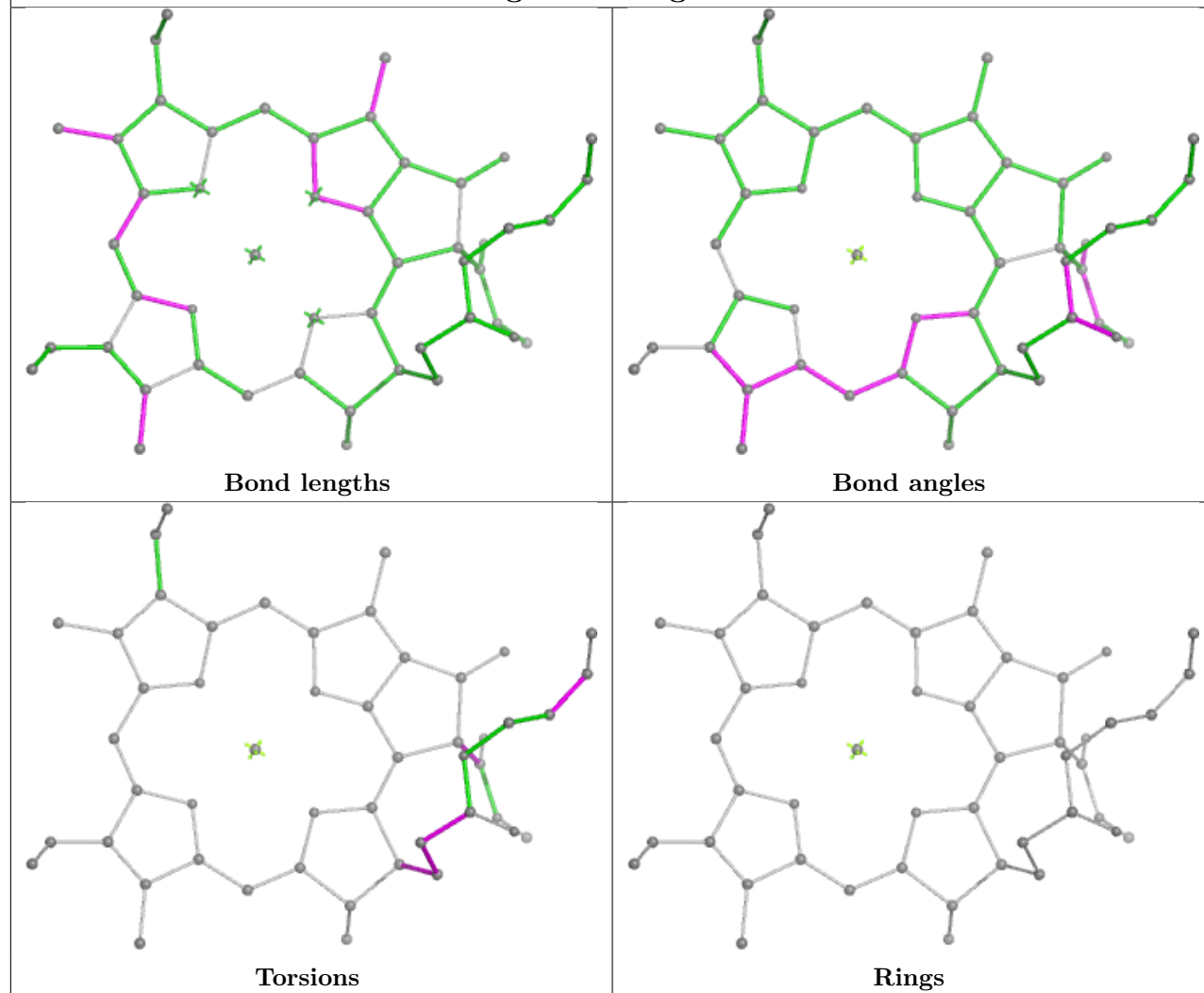
Torsions



Rings

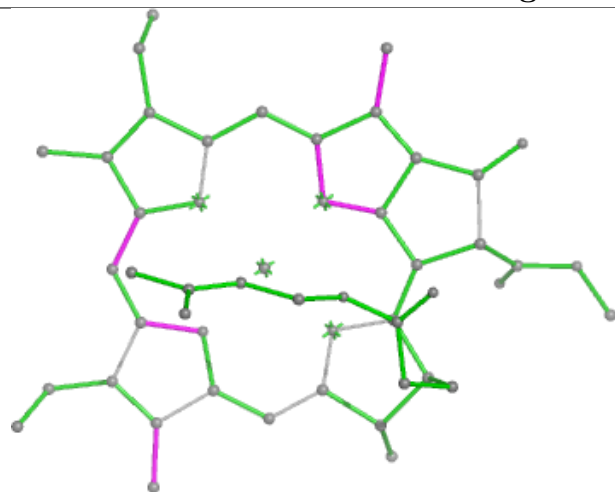


## Ligand CLA g 833

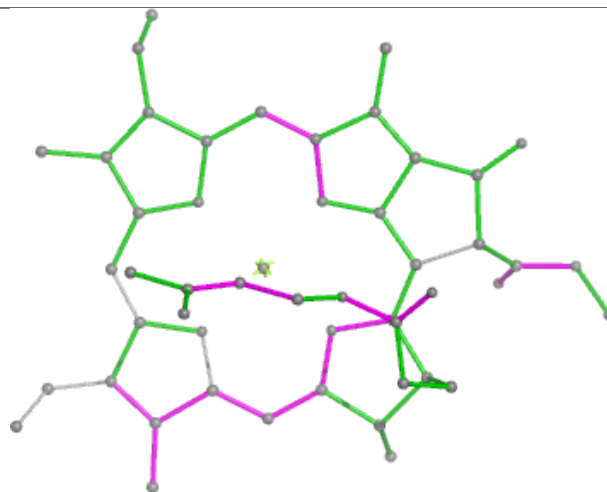




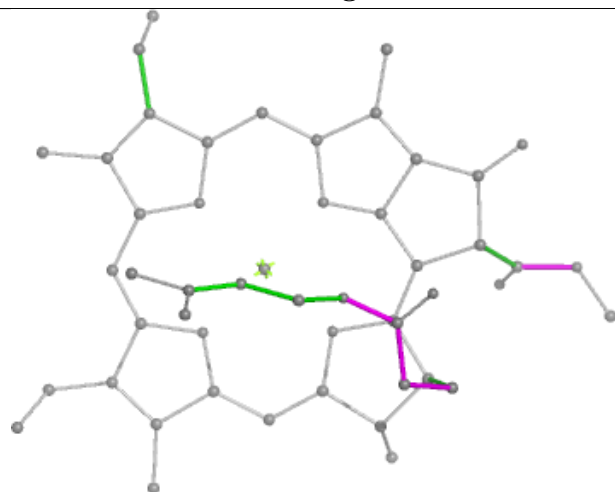
## Ligand CLA b 837



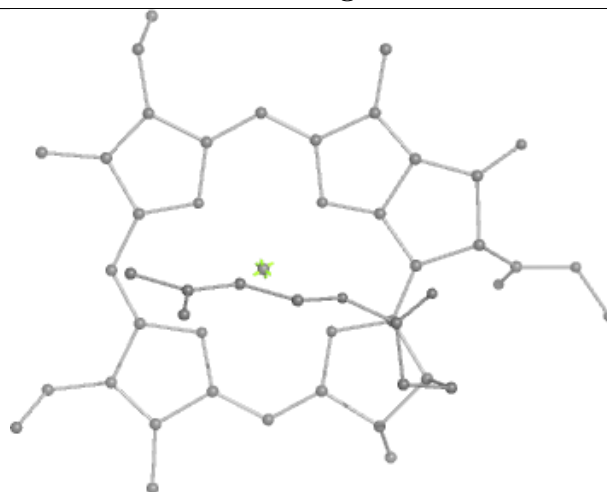
Bond lengths



Bond angles

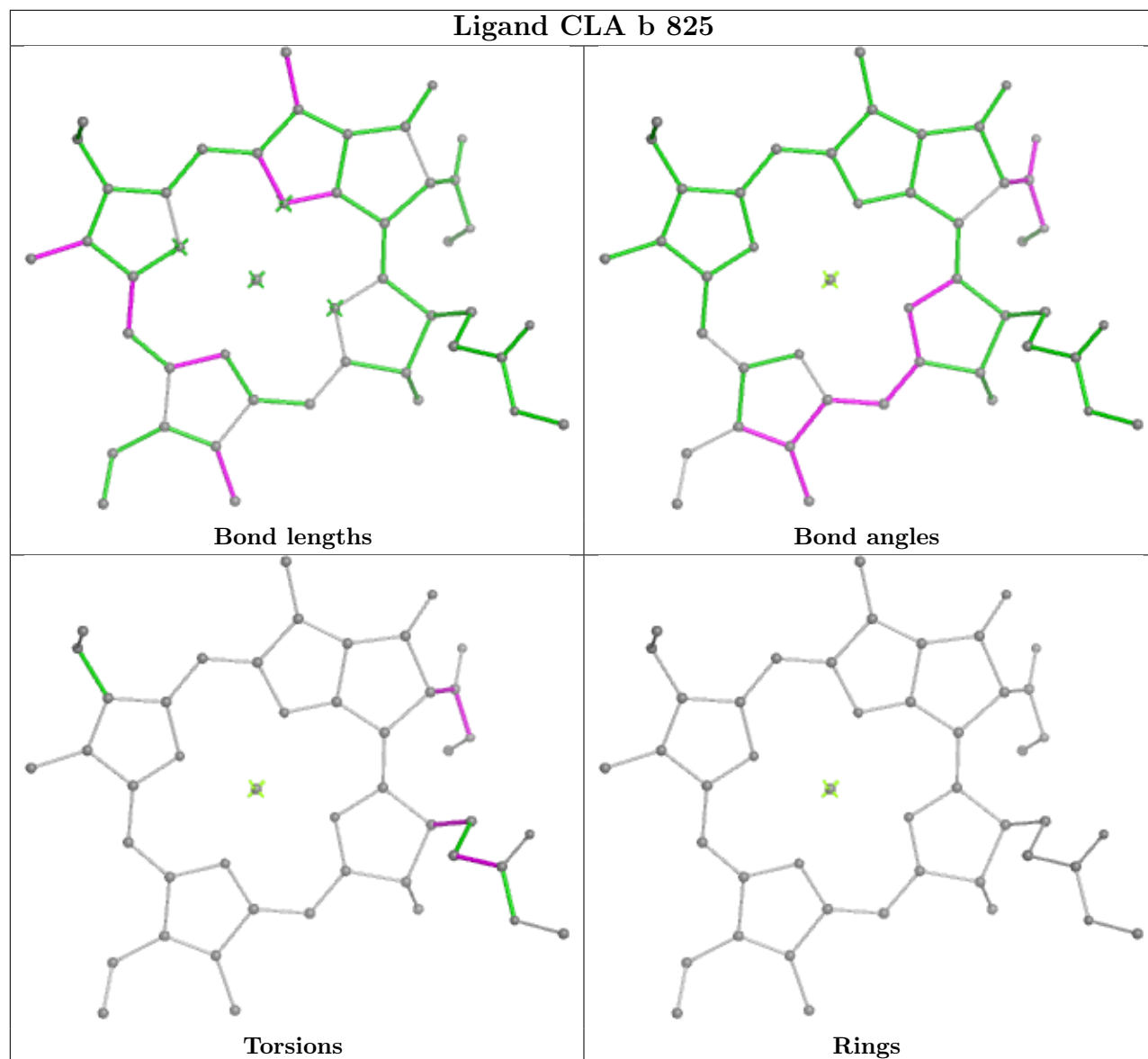


Torsions

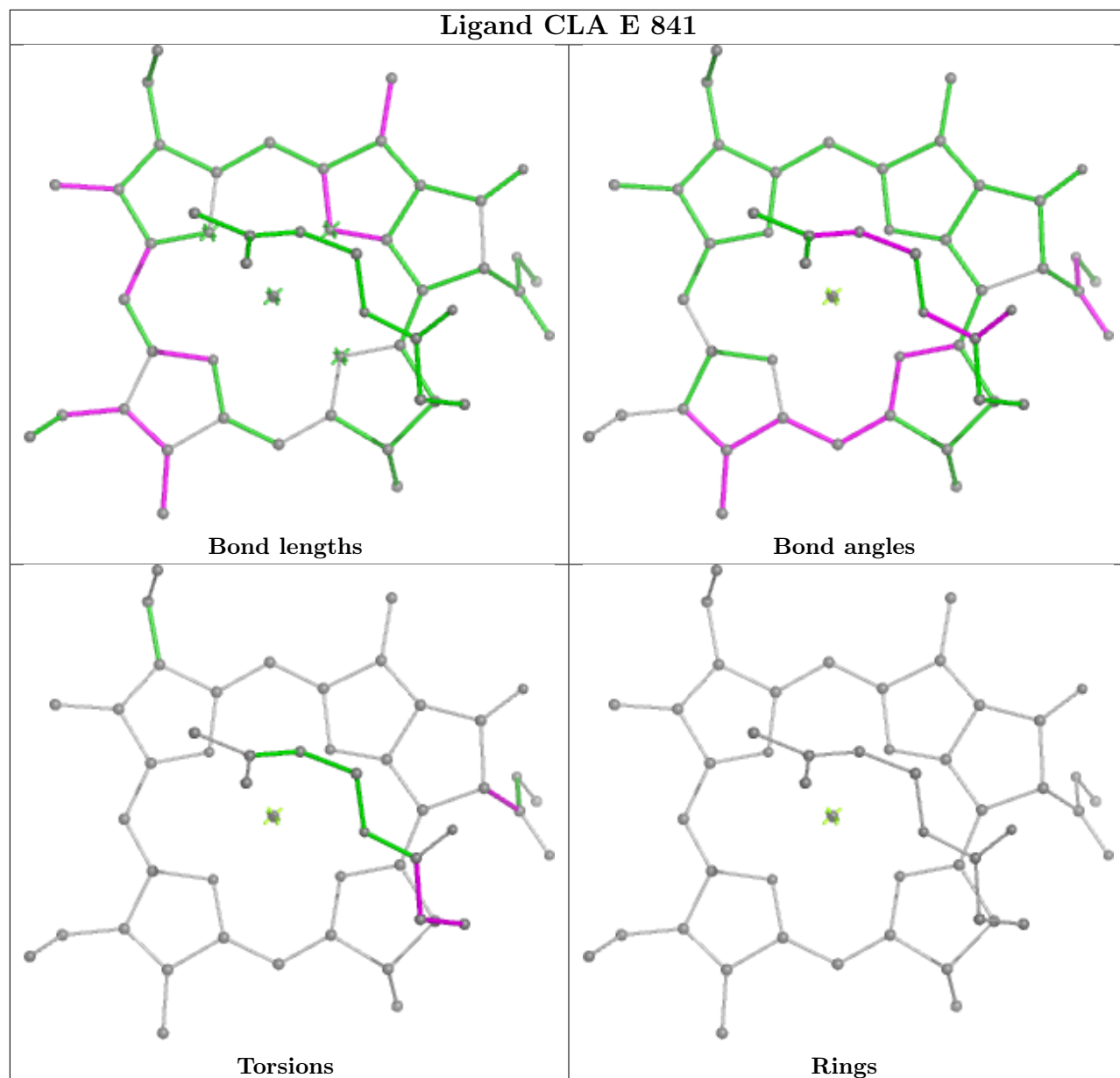


Rings

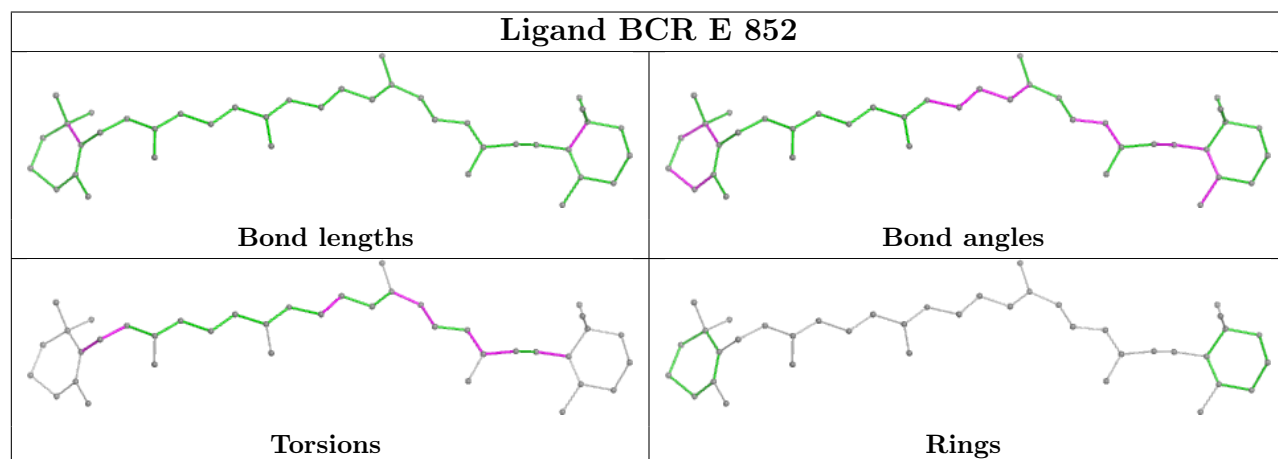
## Ligand CLA b 825



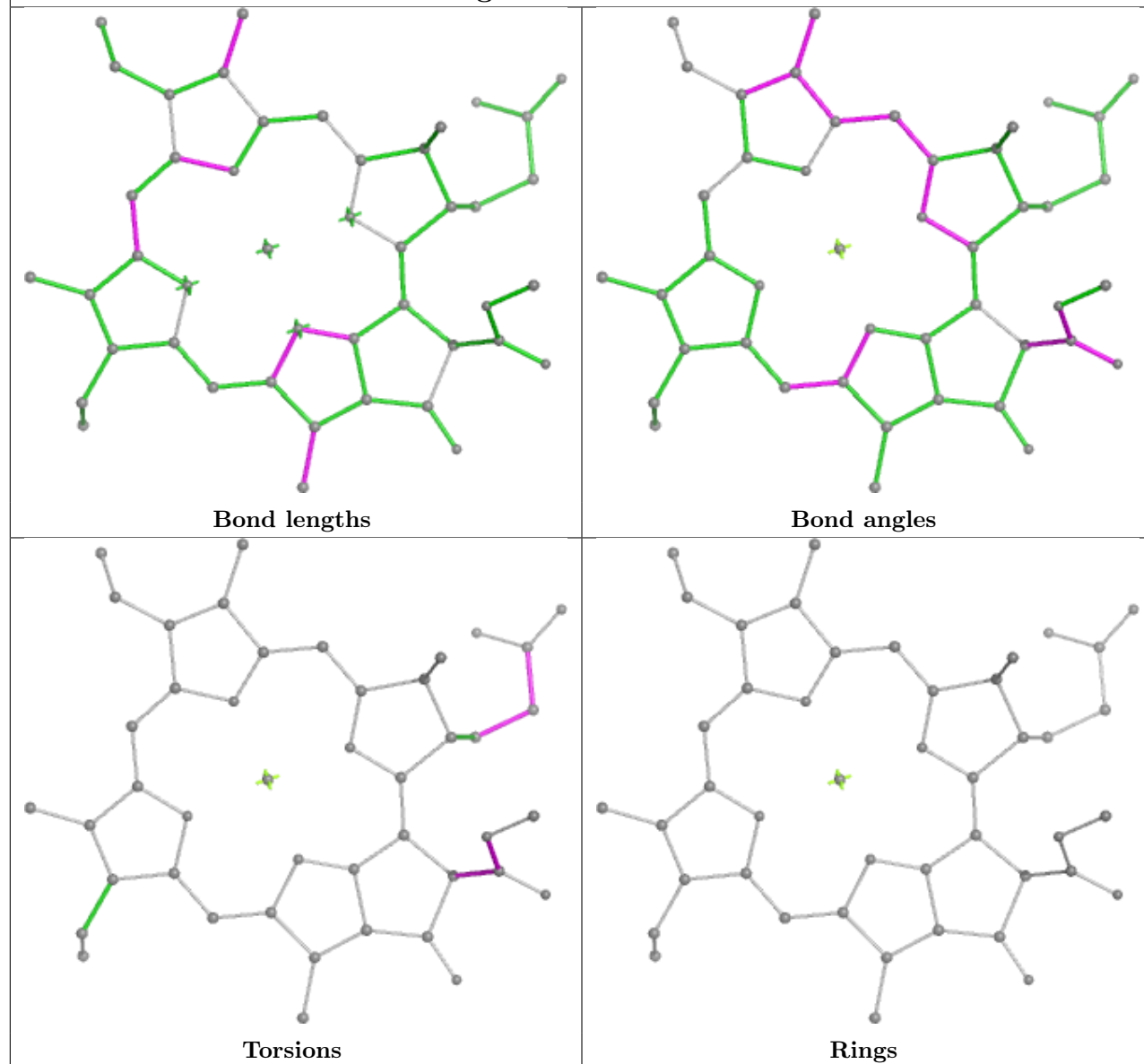
## Ligand CLA E 841



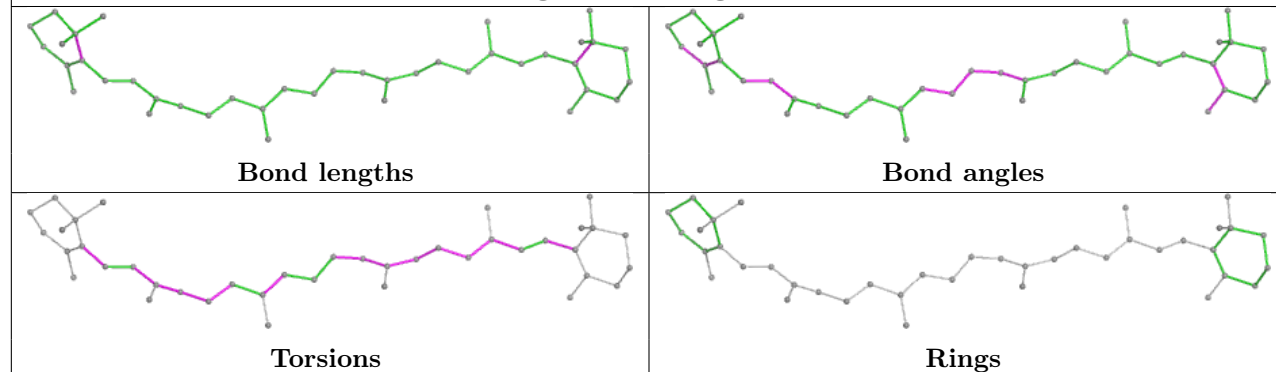
## Ligand BCR E 852

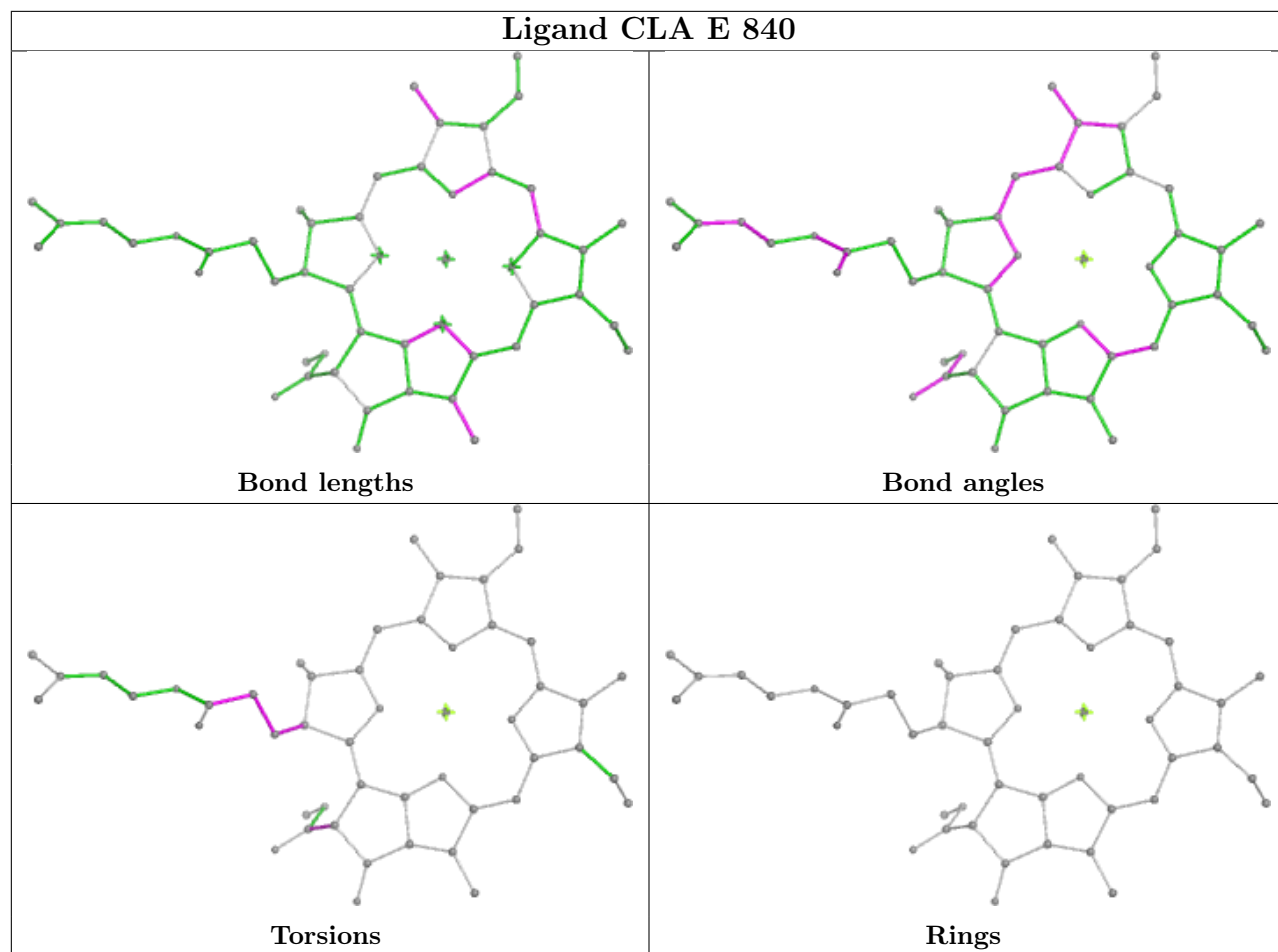


## Ligand CLA A 838

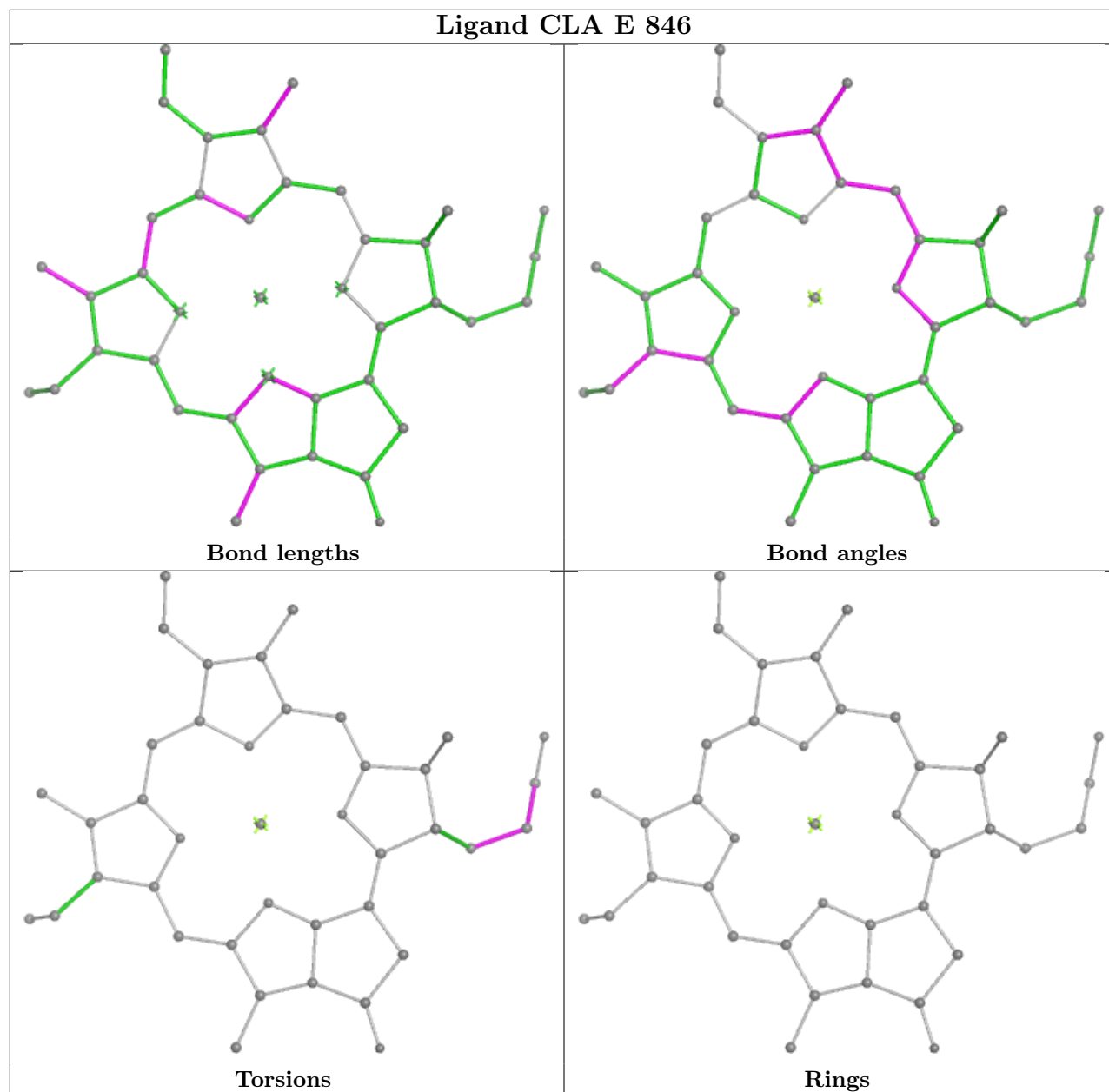


## Ligand BCR g 847

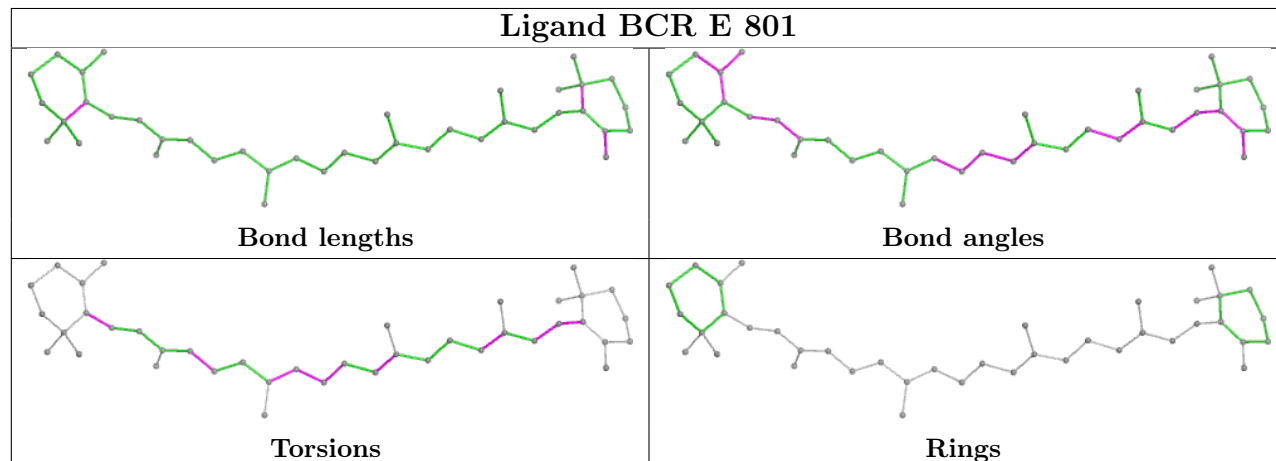




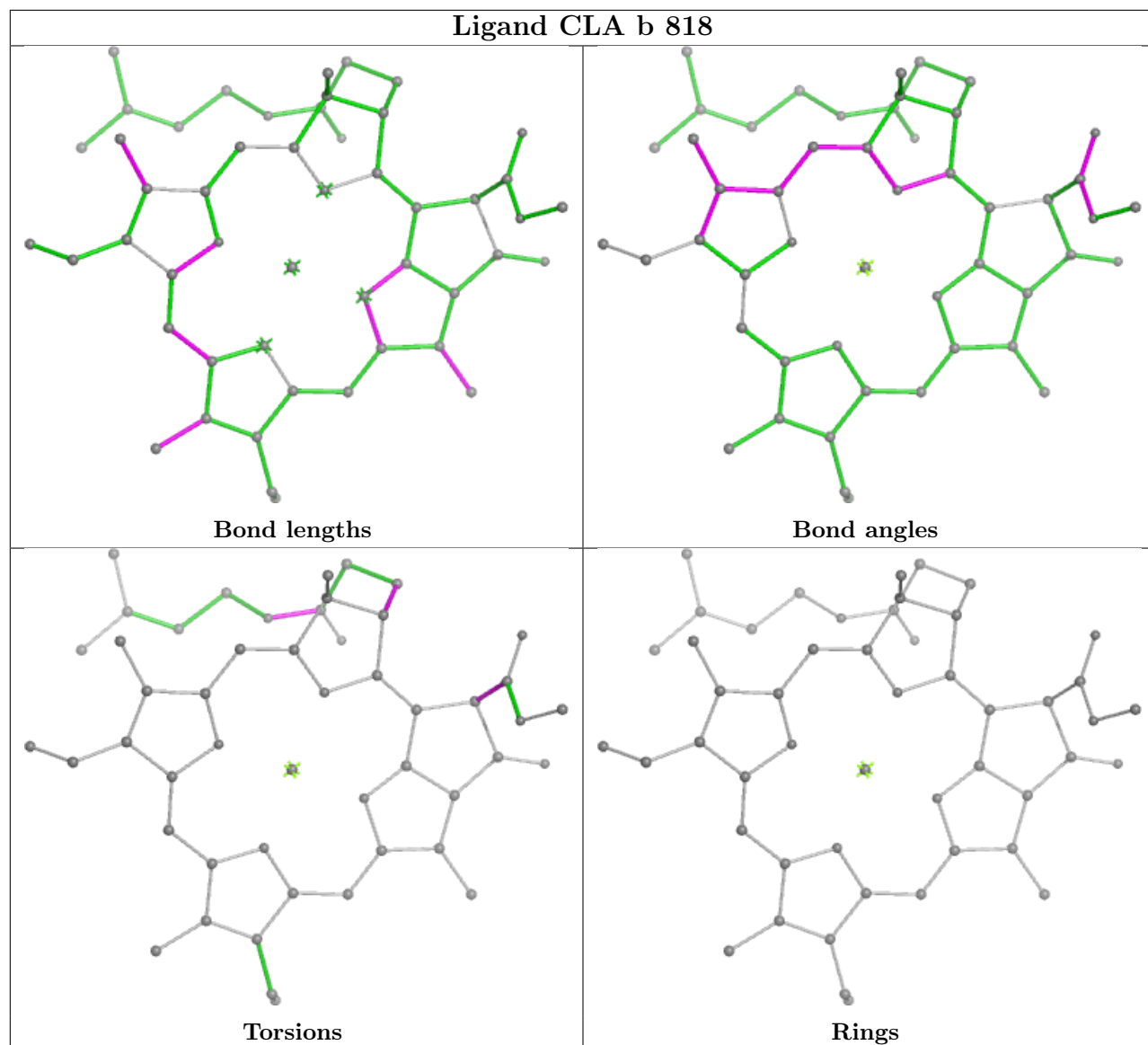
## Ligand CLA E 846

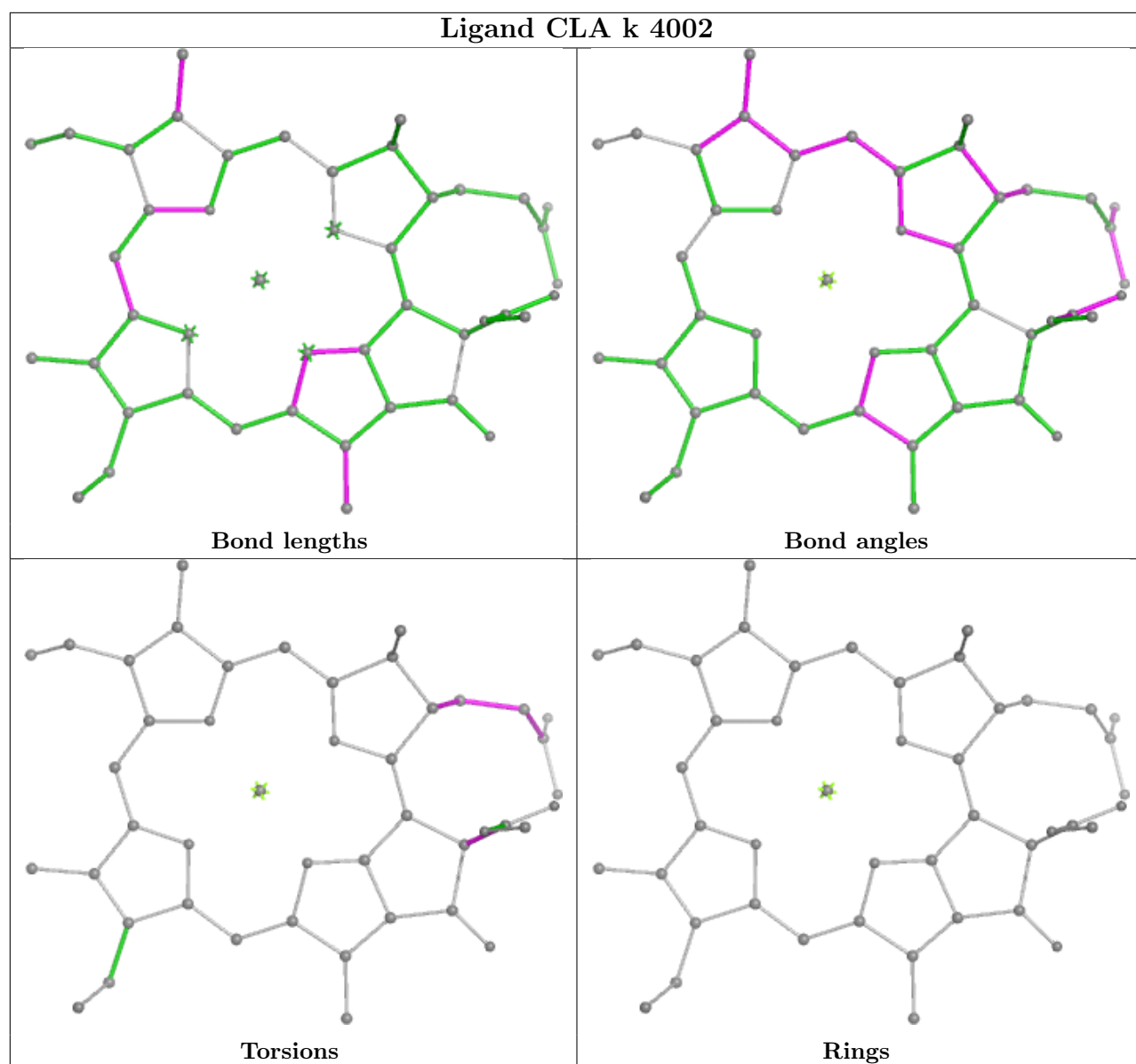


## Ligand BCR E 801

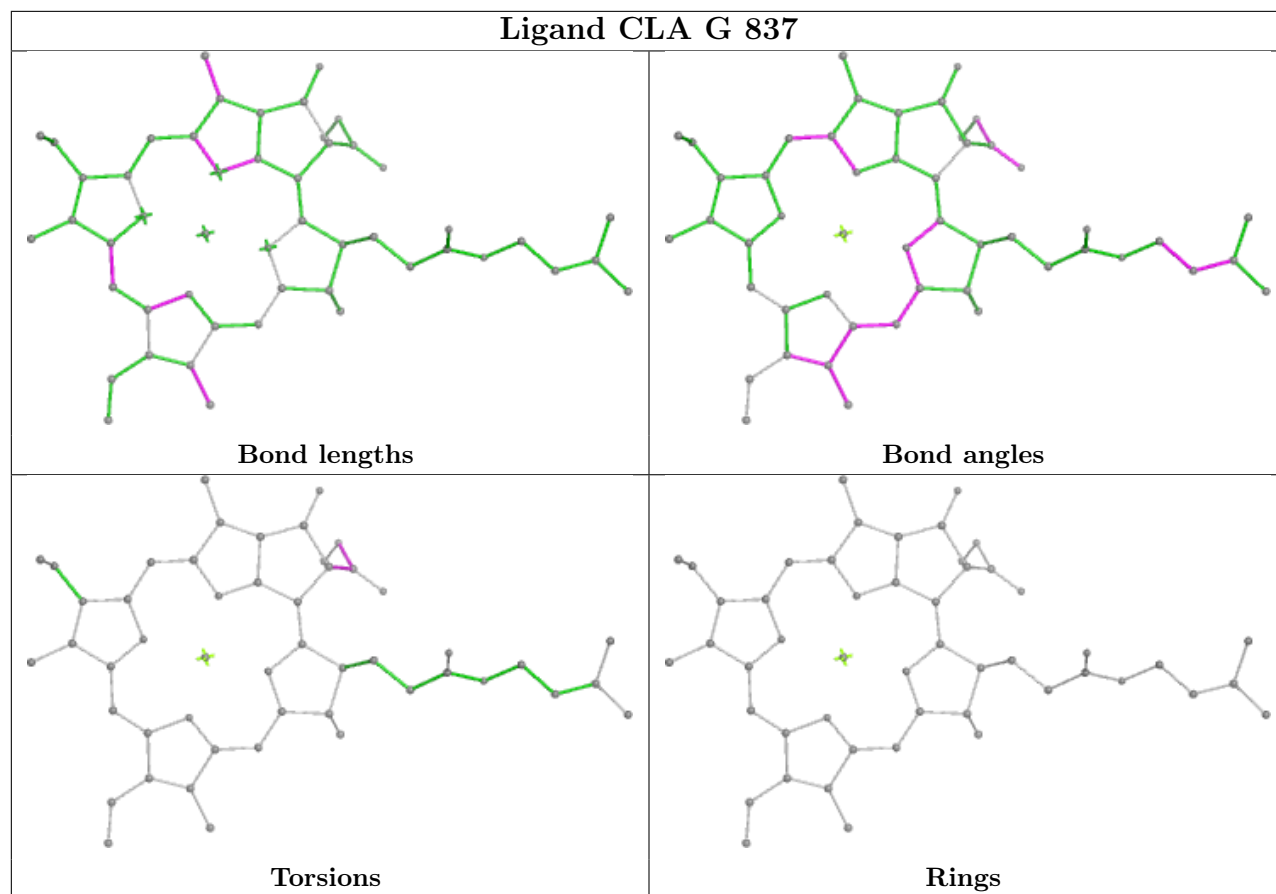


## Ligand CLA b 818

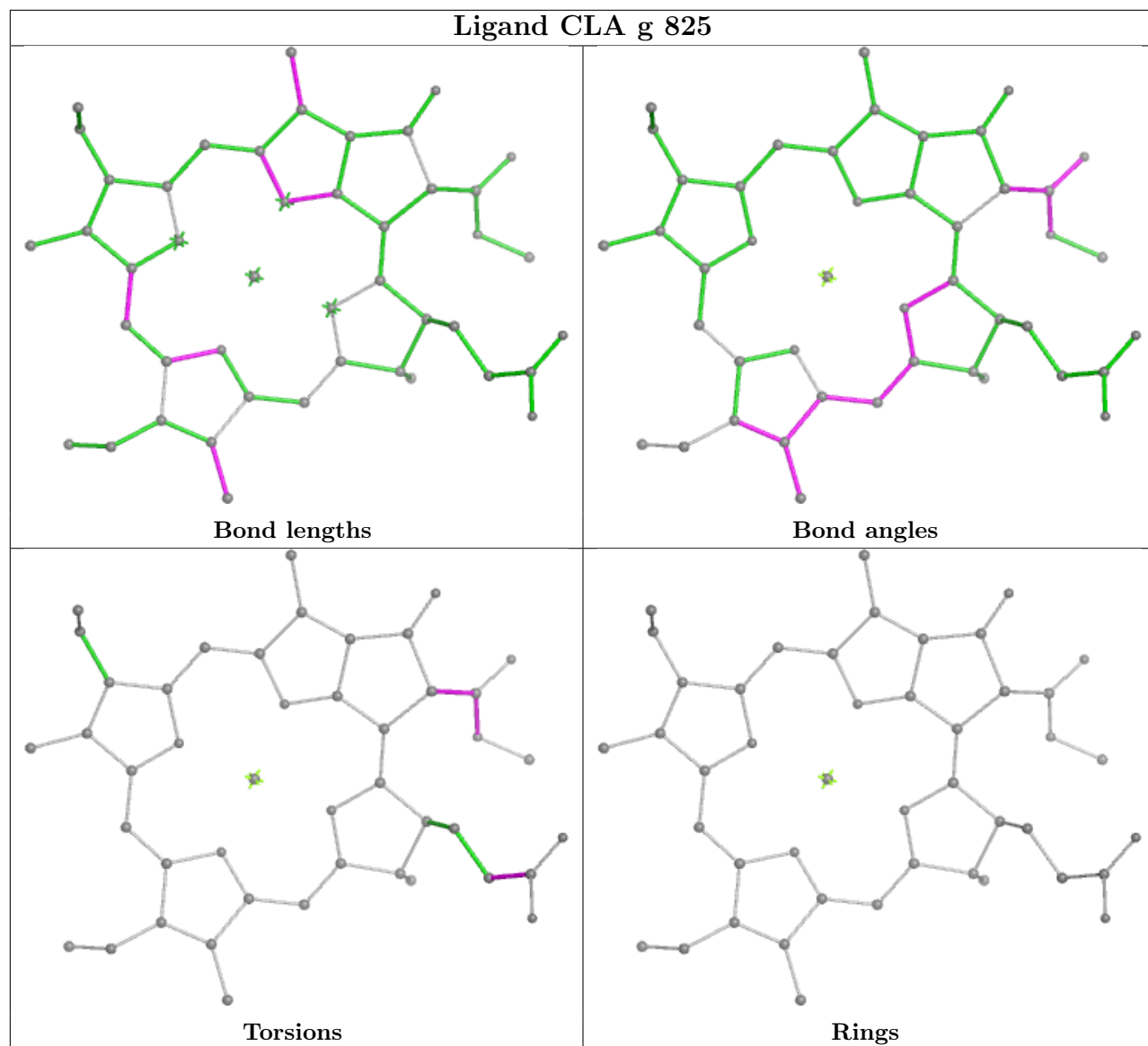


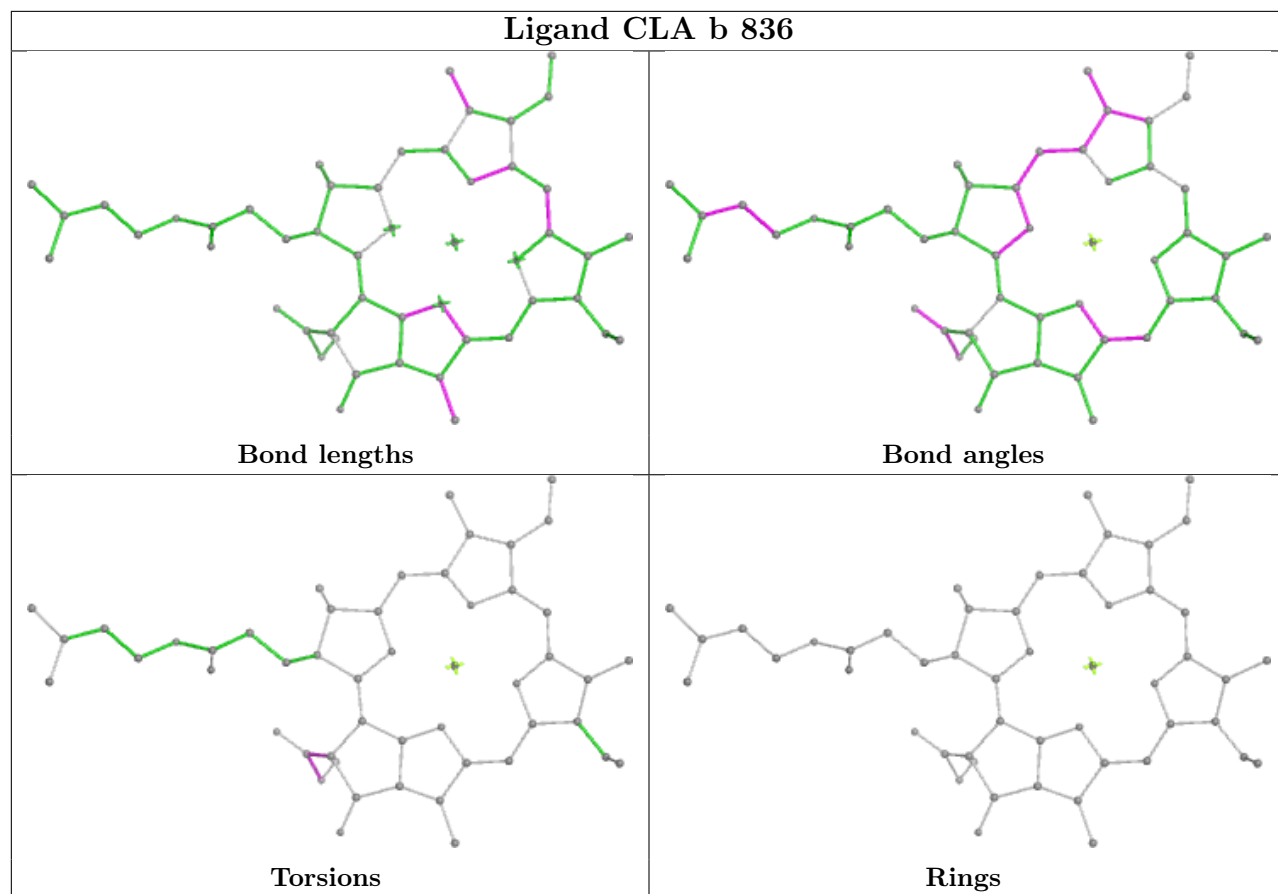




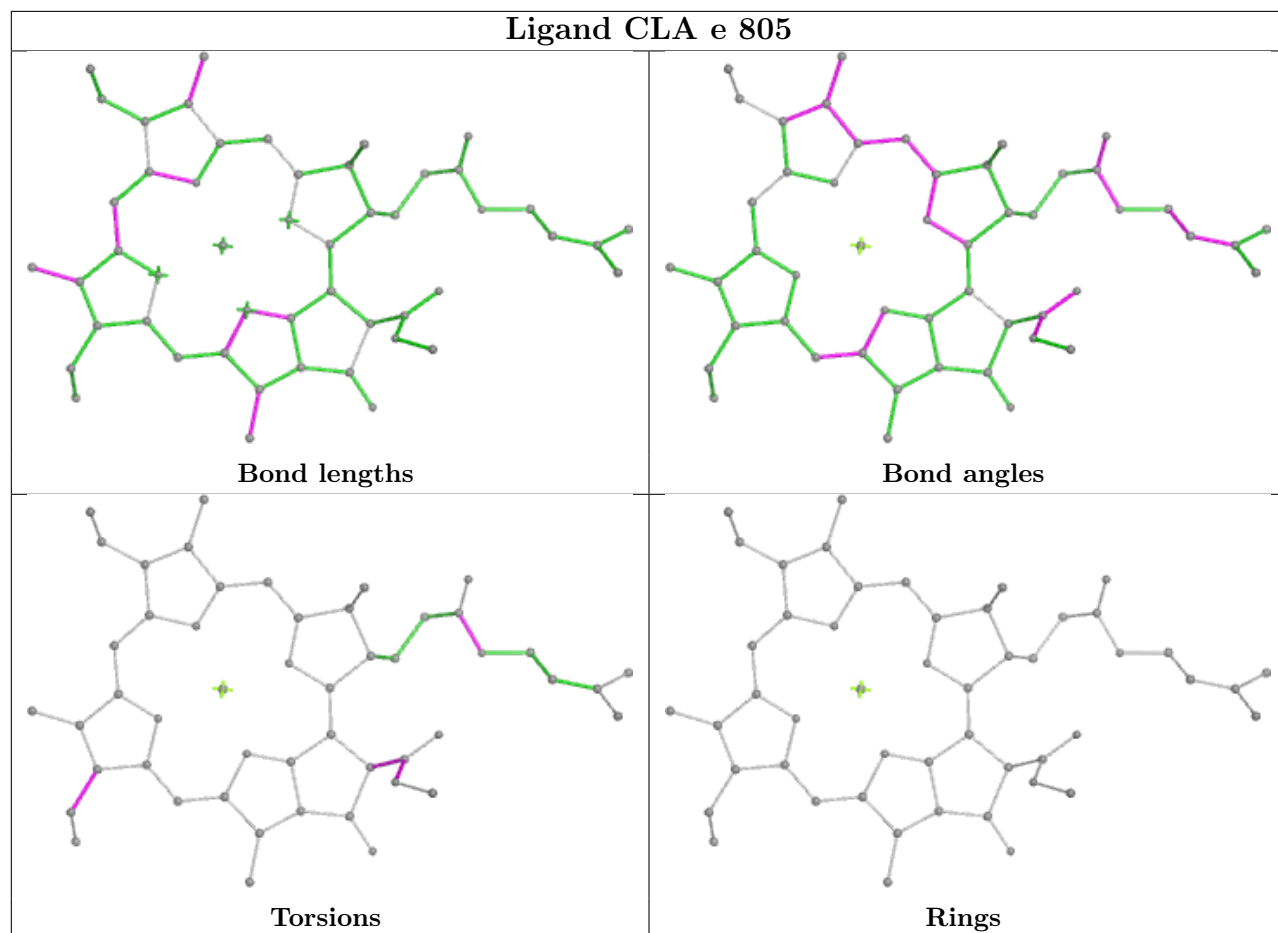


## Ligand CLA g 825

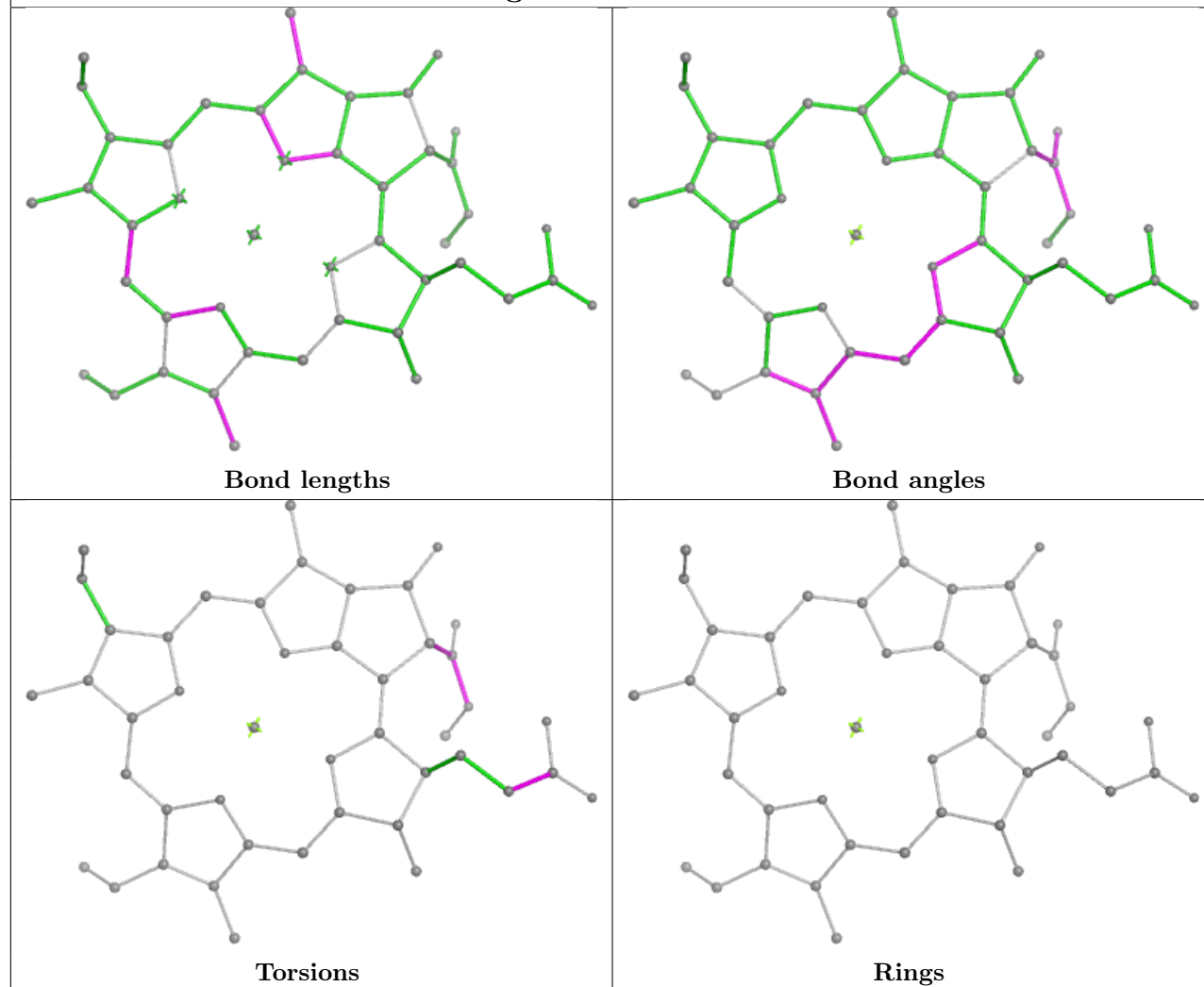




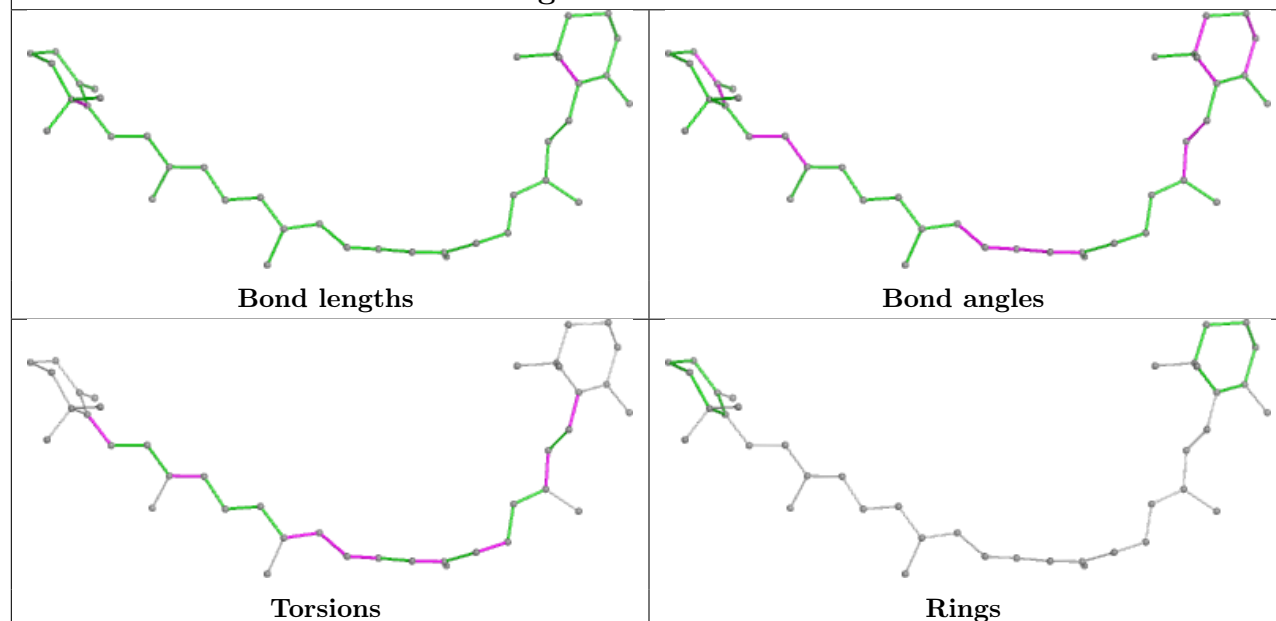
## Ligand CLA e 805



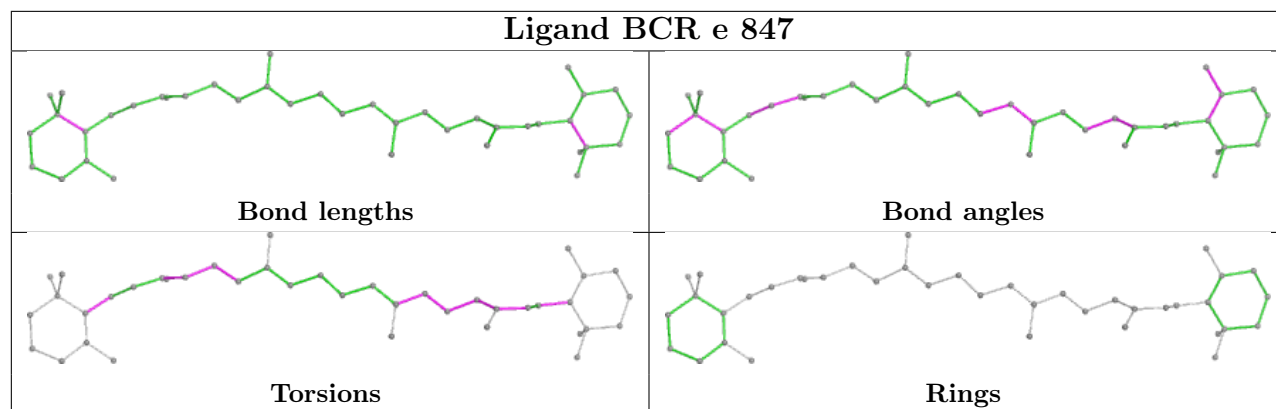
## Ligand CLA a 818



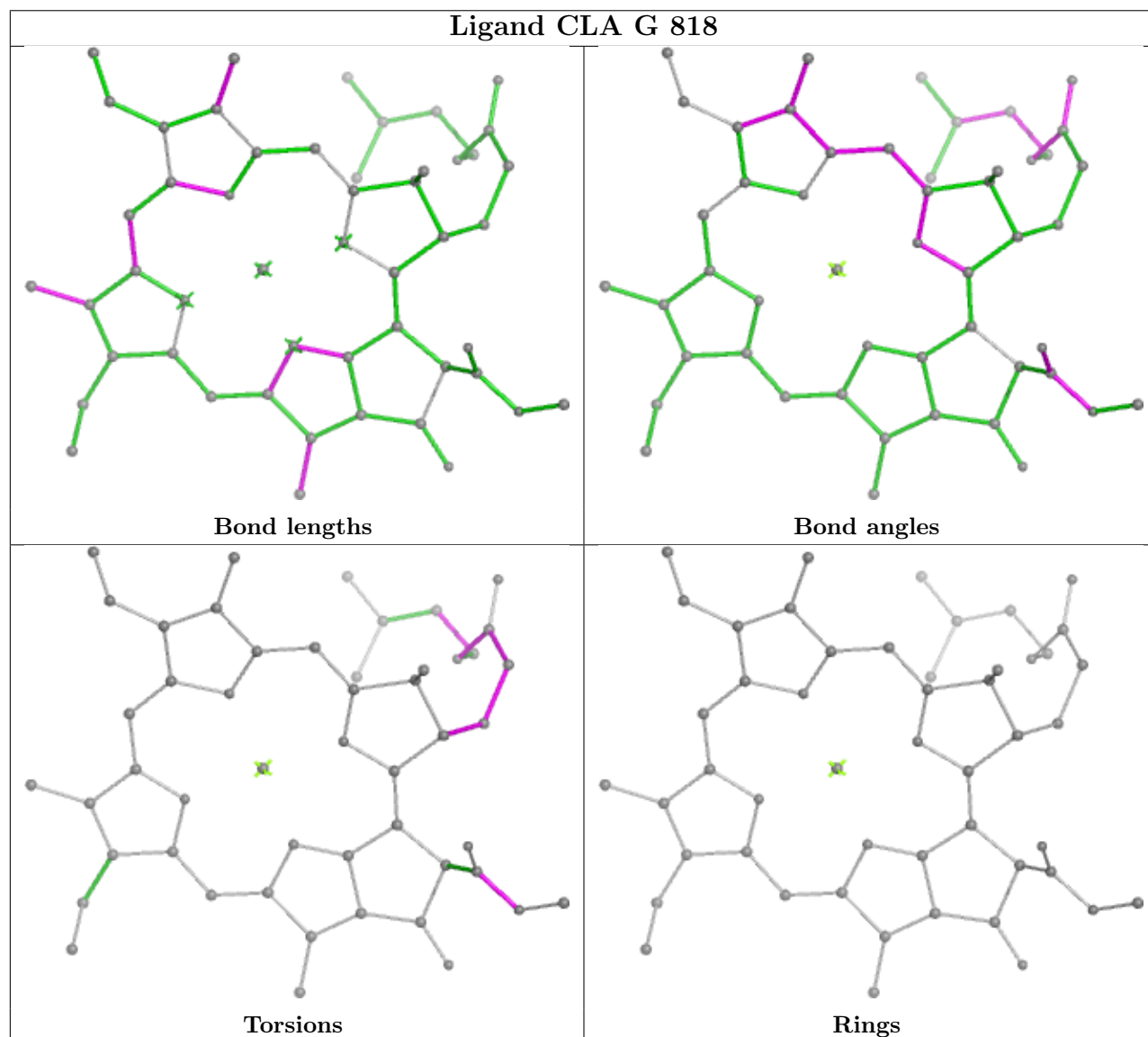
## Ligand BCR f 202



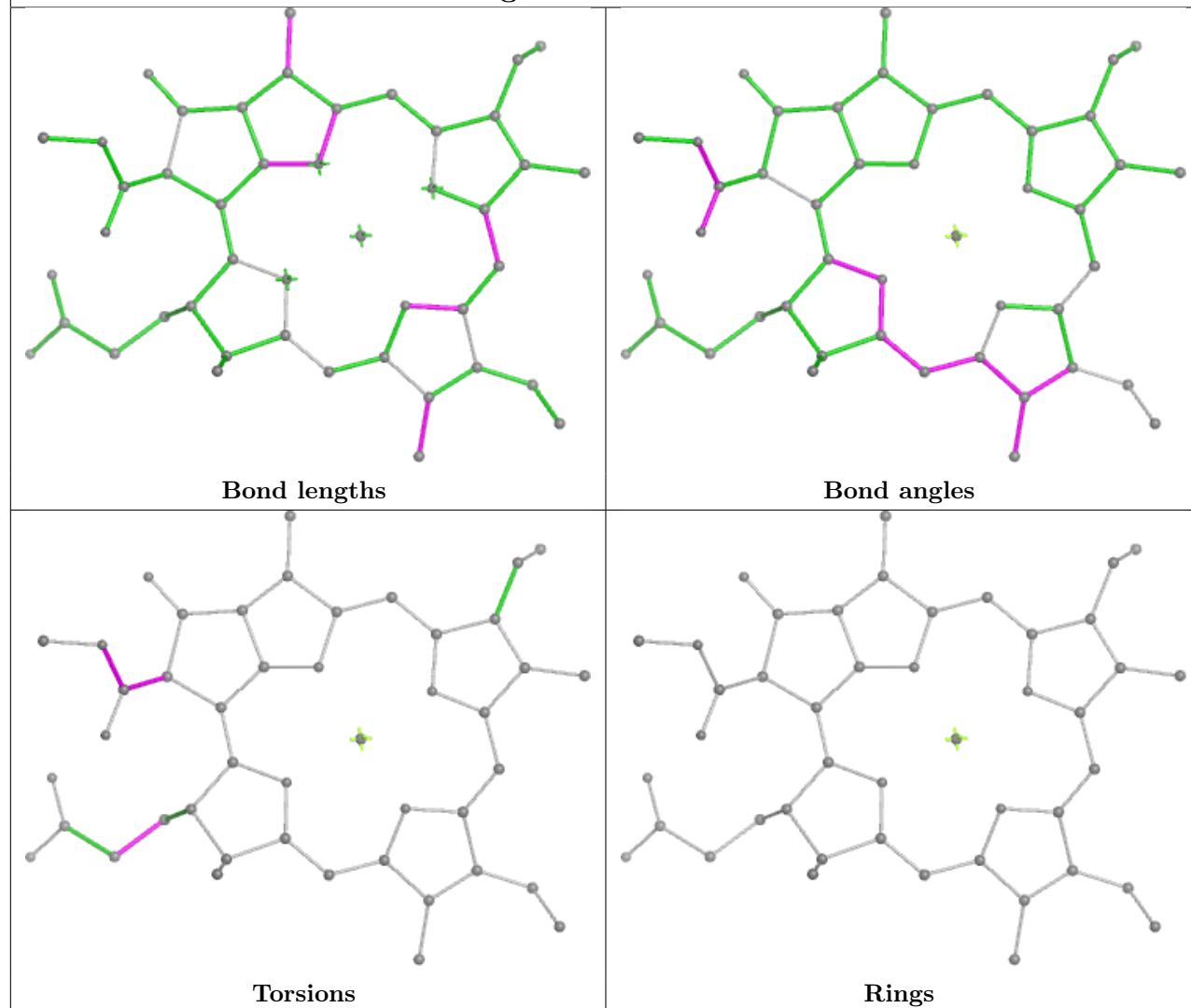
## Ligand BCR e 847



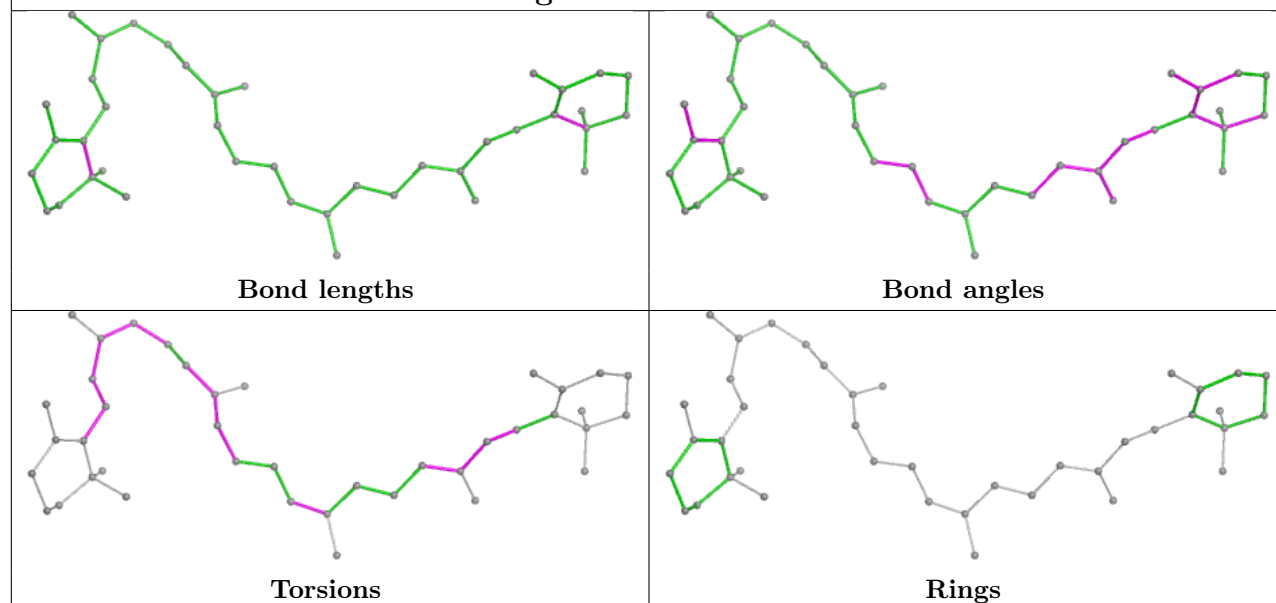
## Ligand CLA G 818

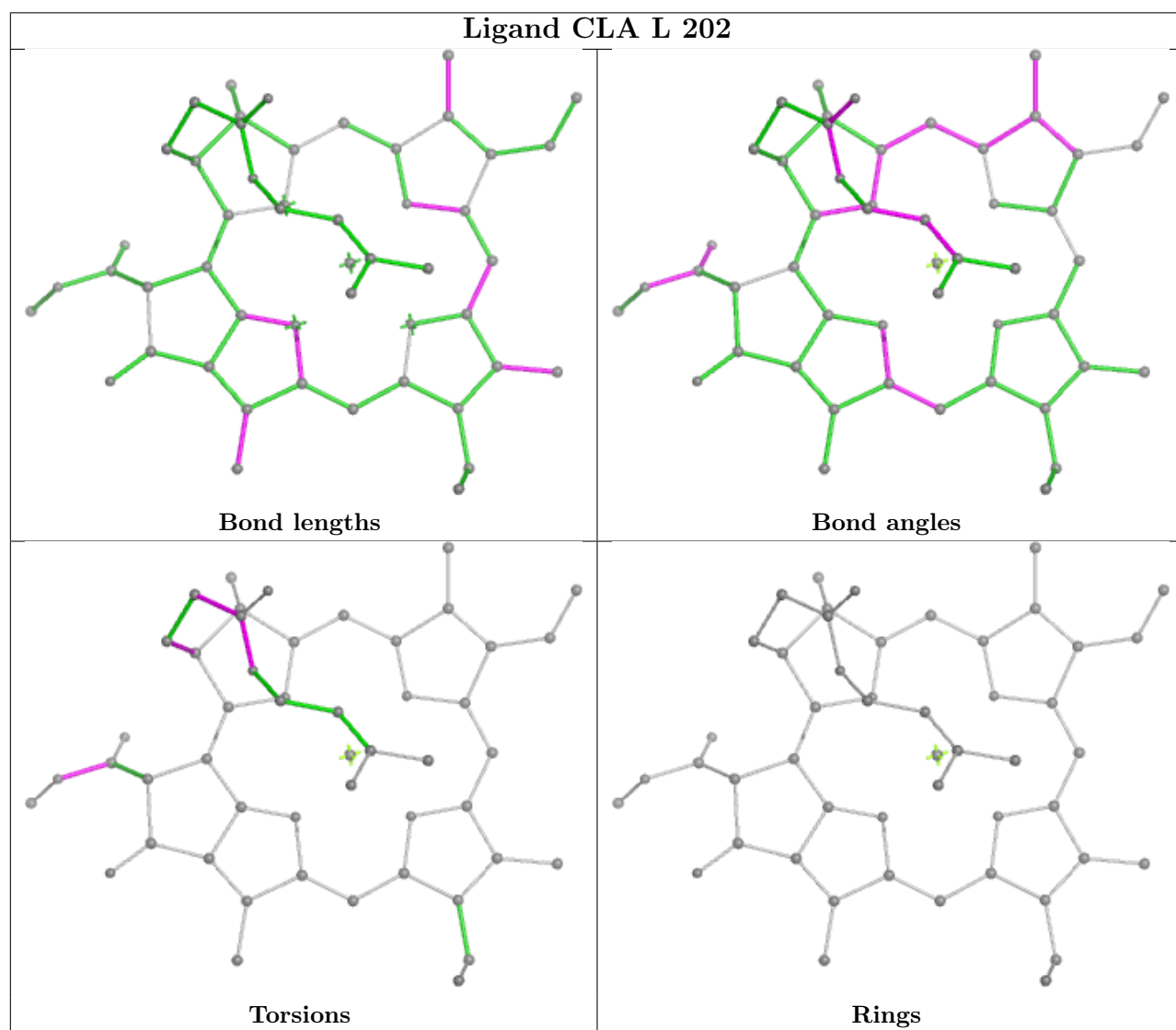
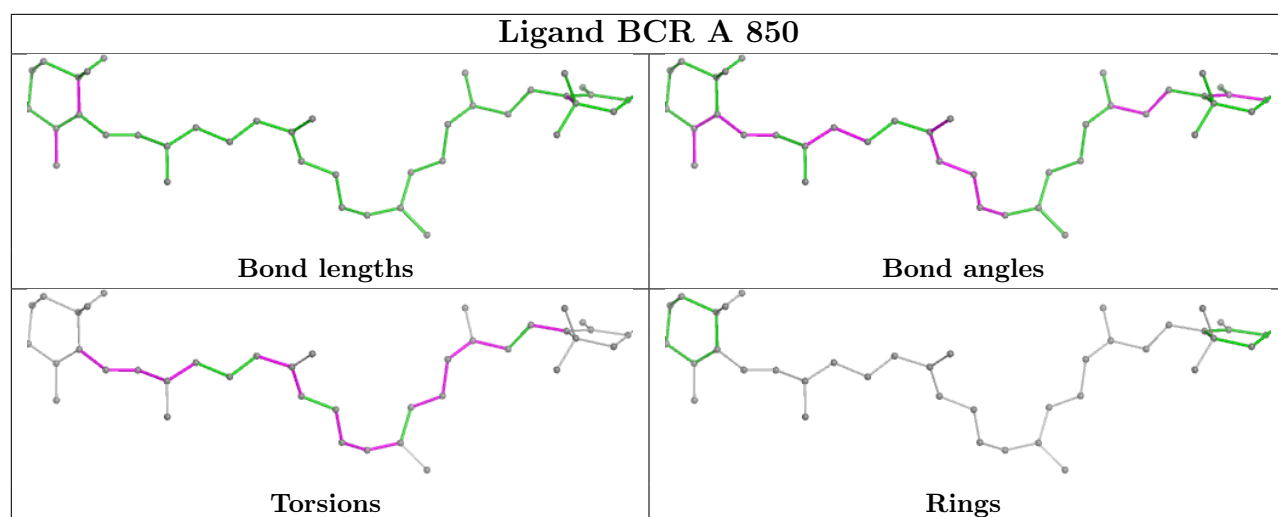


## Ligand CLA o 202



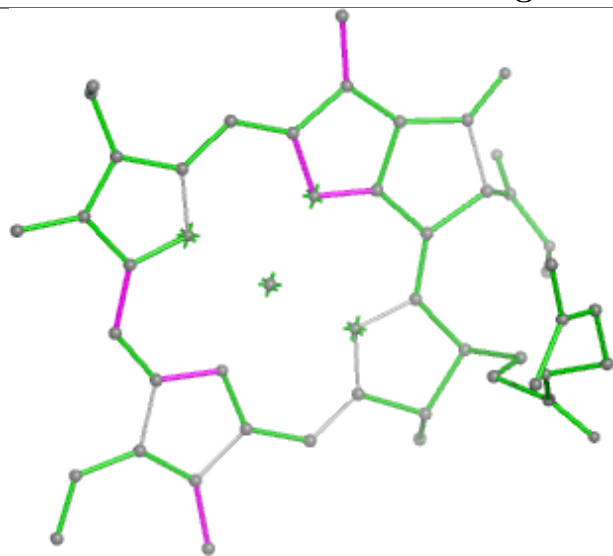
## Ligand BCR e 846



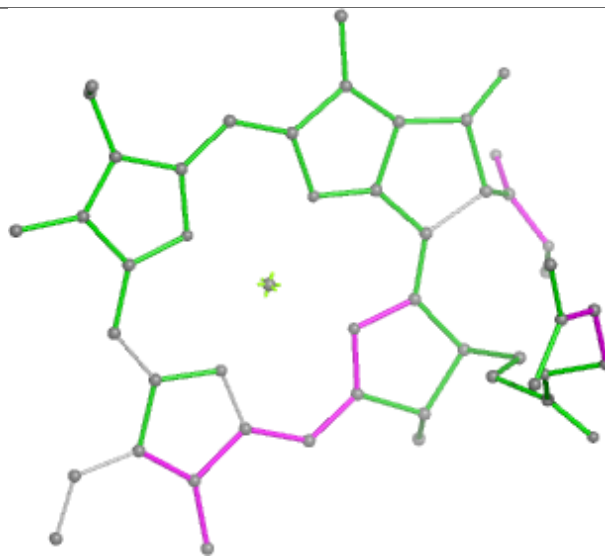




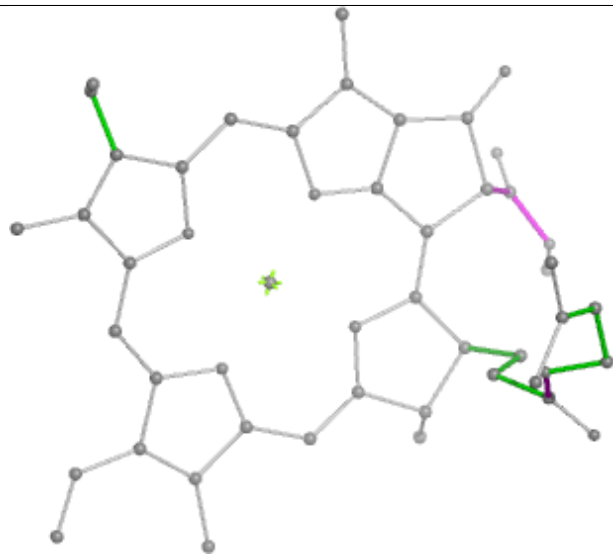
## Ligand CLA E 833



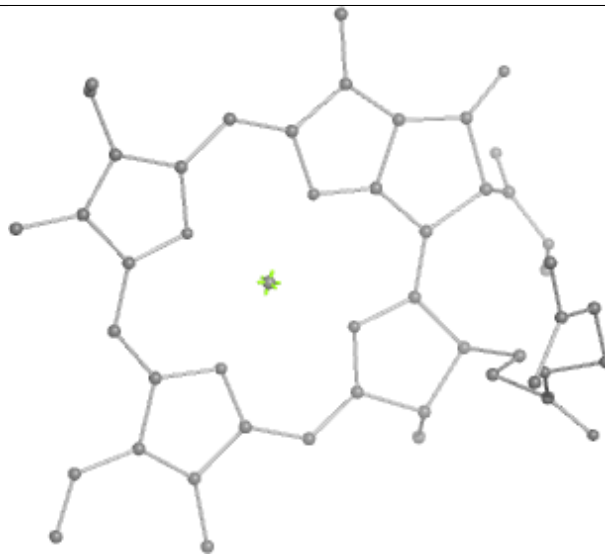
Bond lengths



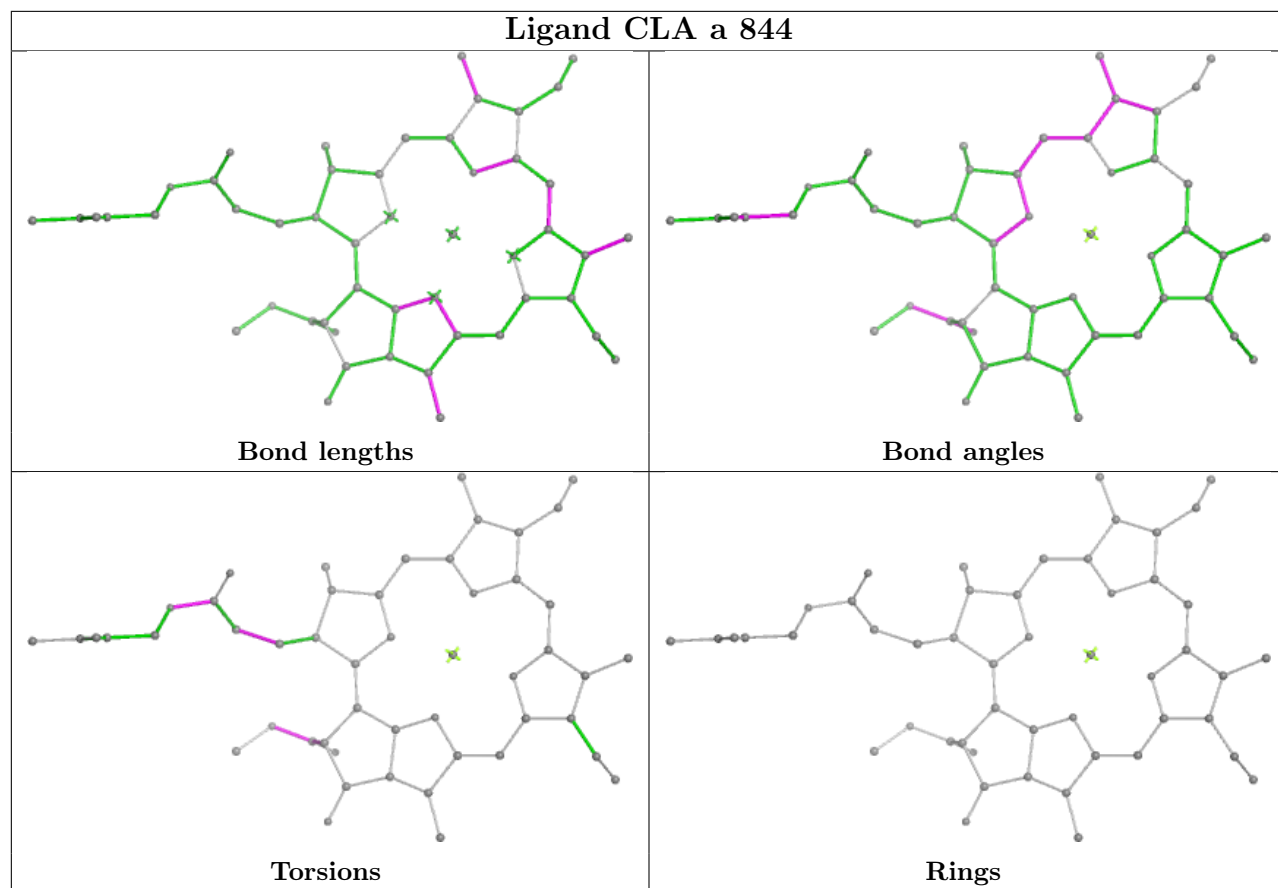
Bond angles



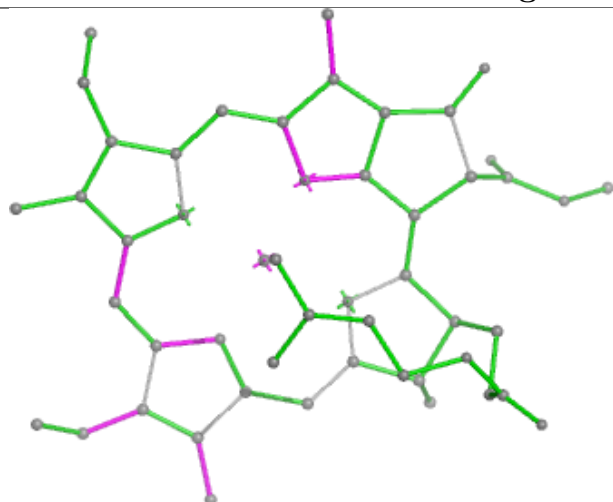
Torsions



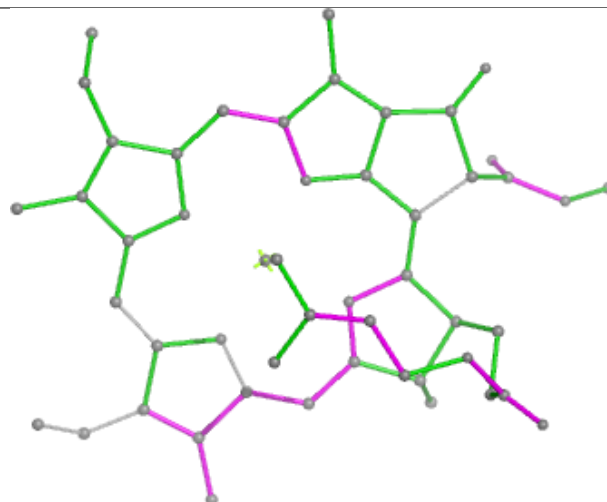
Rings



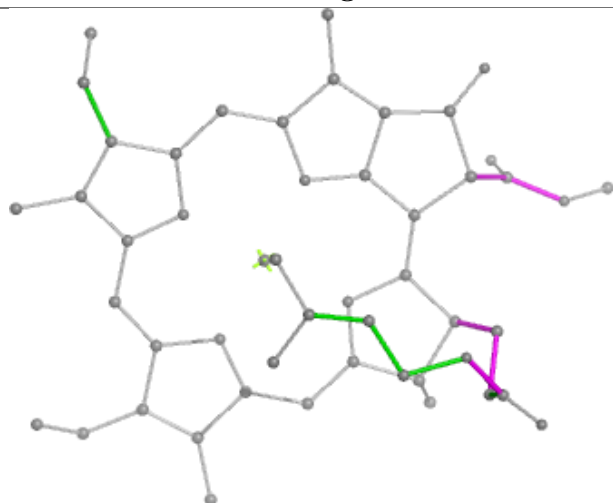
## Ligand CLA e 820



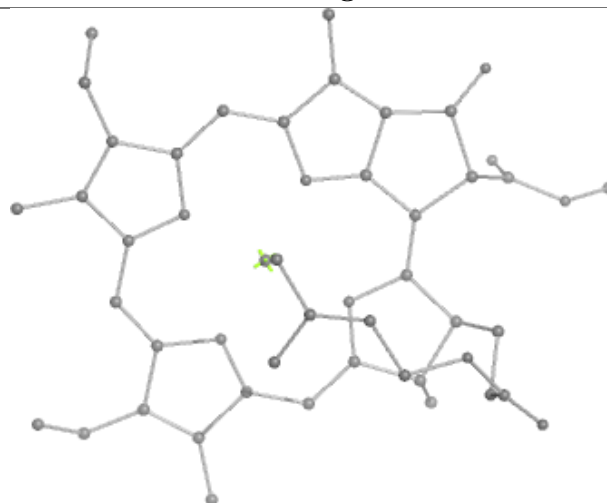
Bond lengths



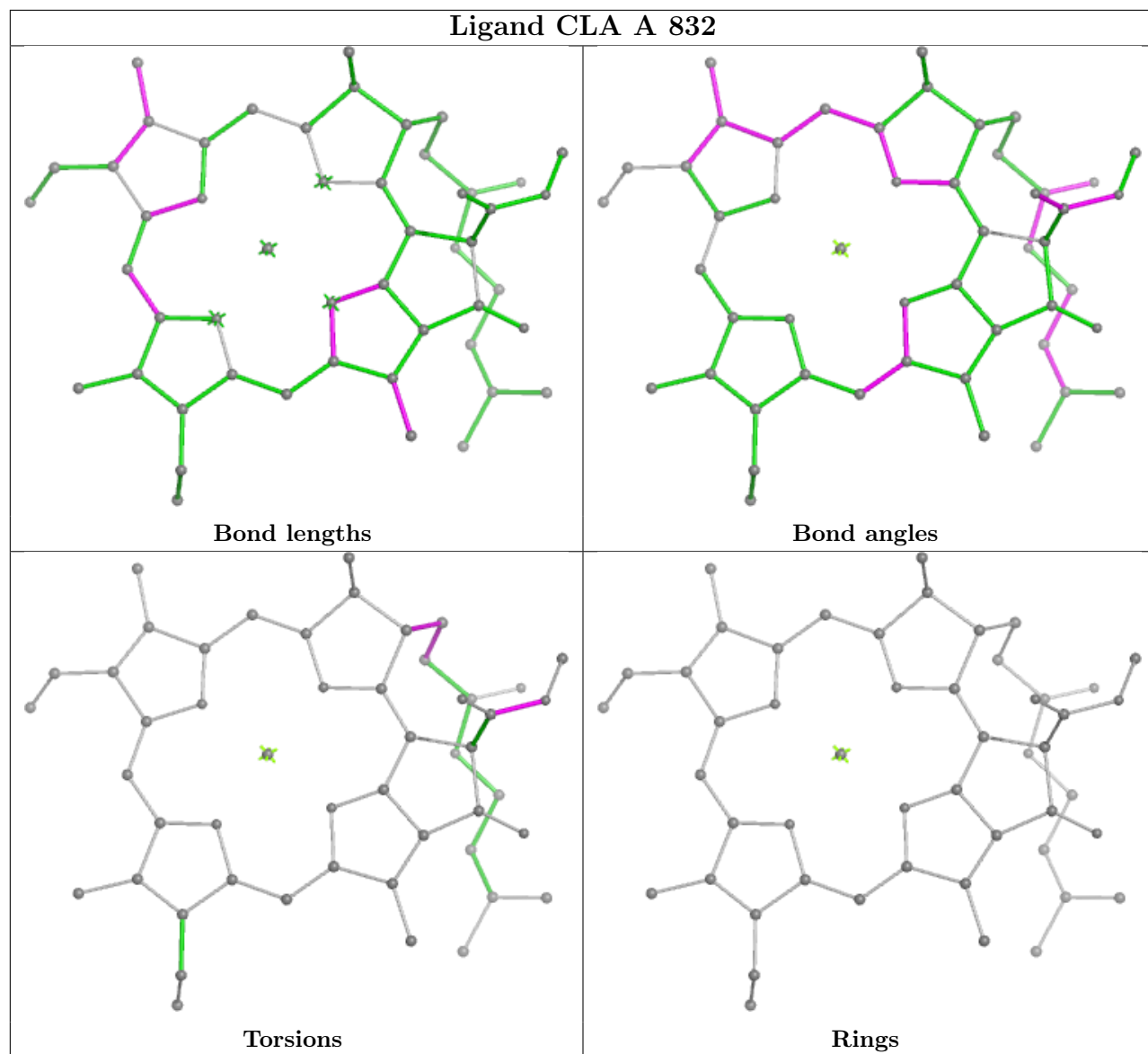
Bond angles



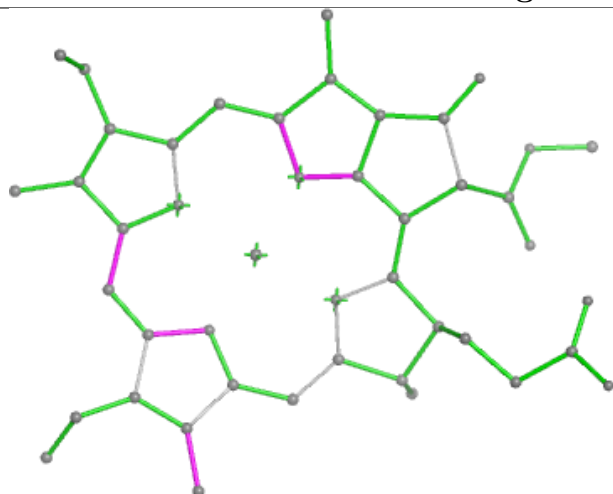
Torsions



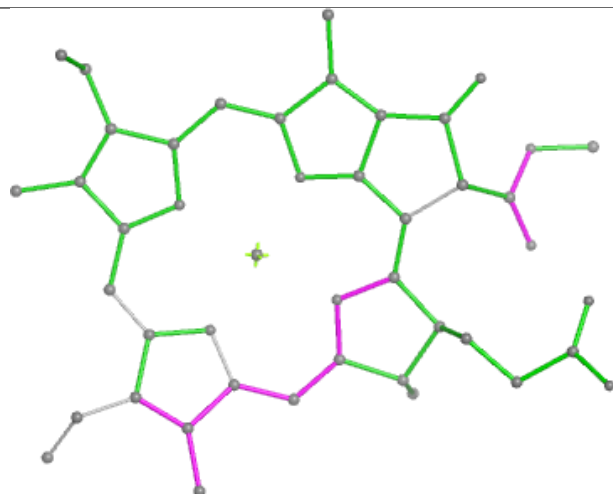
Rings



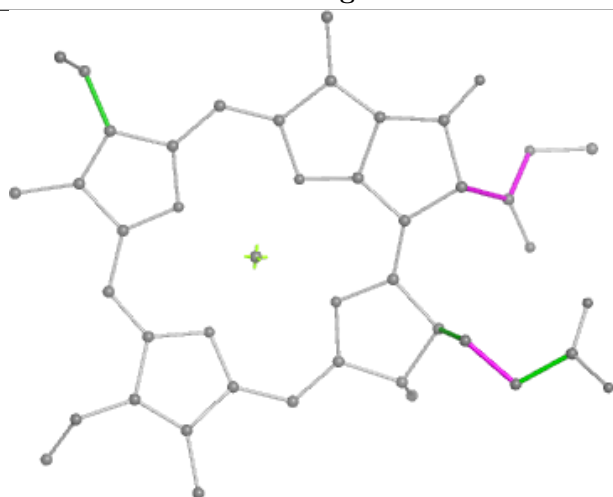
## Ligand CLA F 202



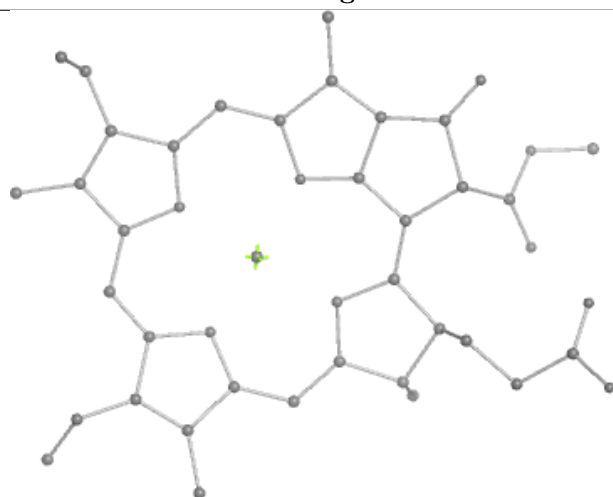
Bond lengths



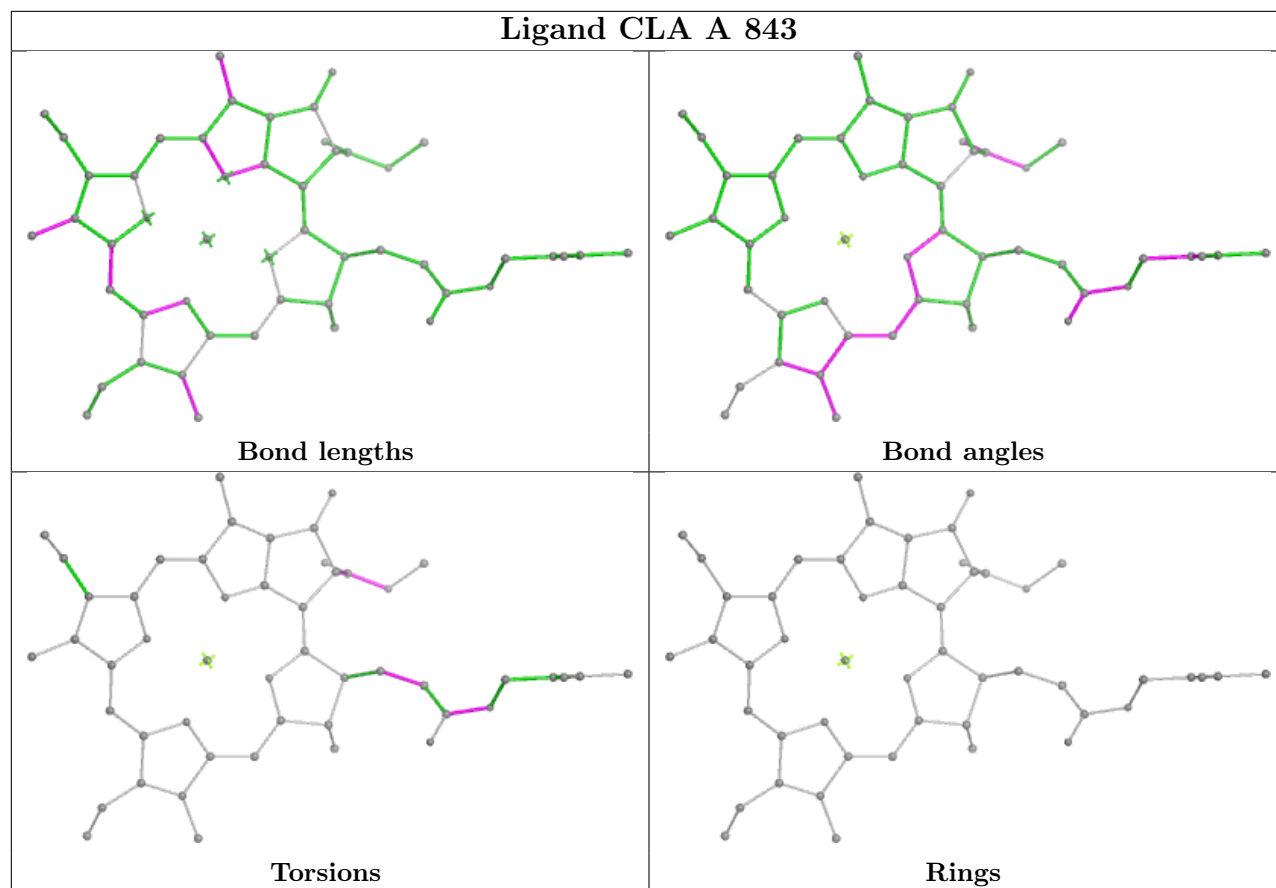
Bond angles



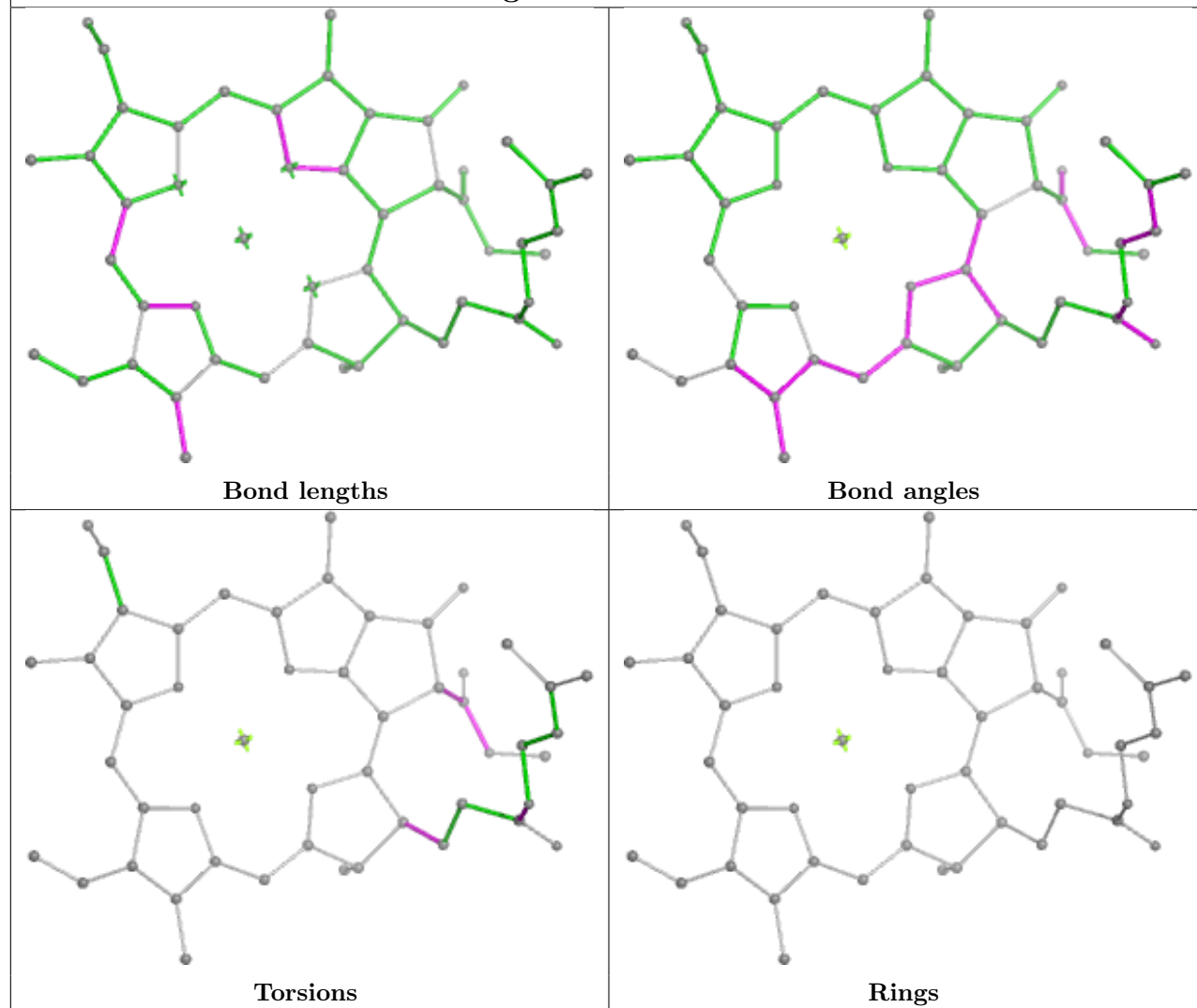
Torsions



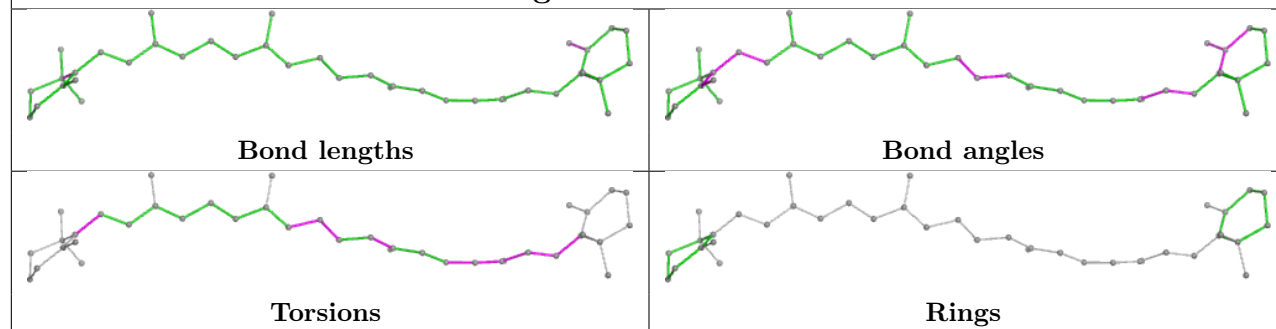
Rings

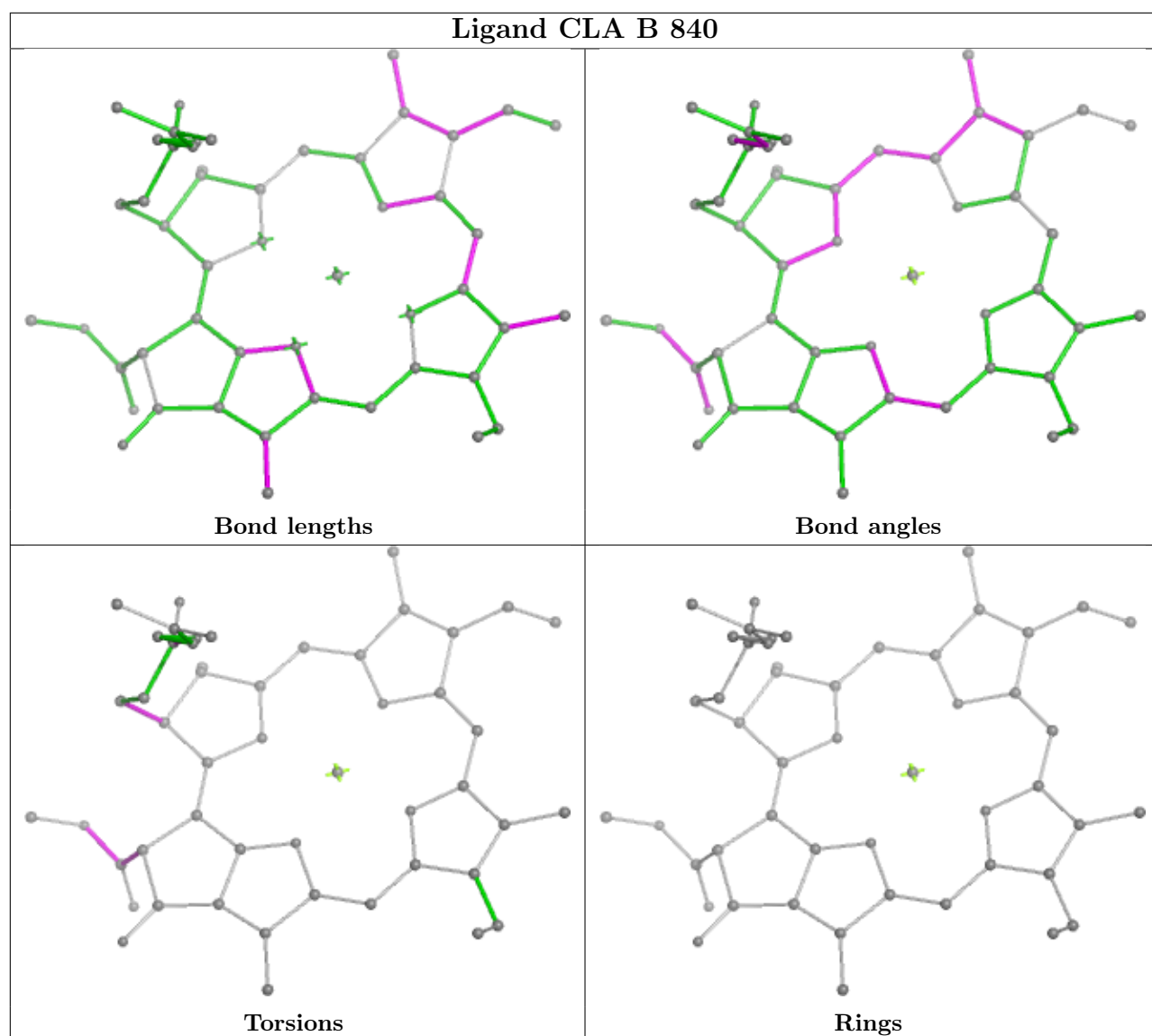


## Ligand CLA a 852



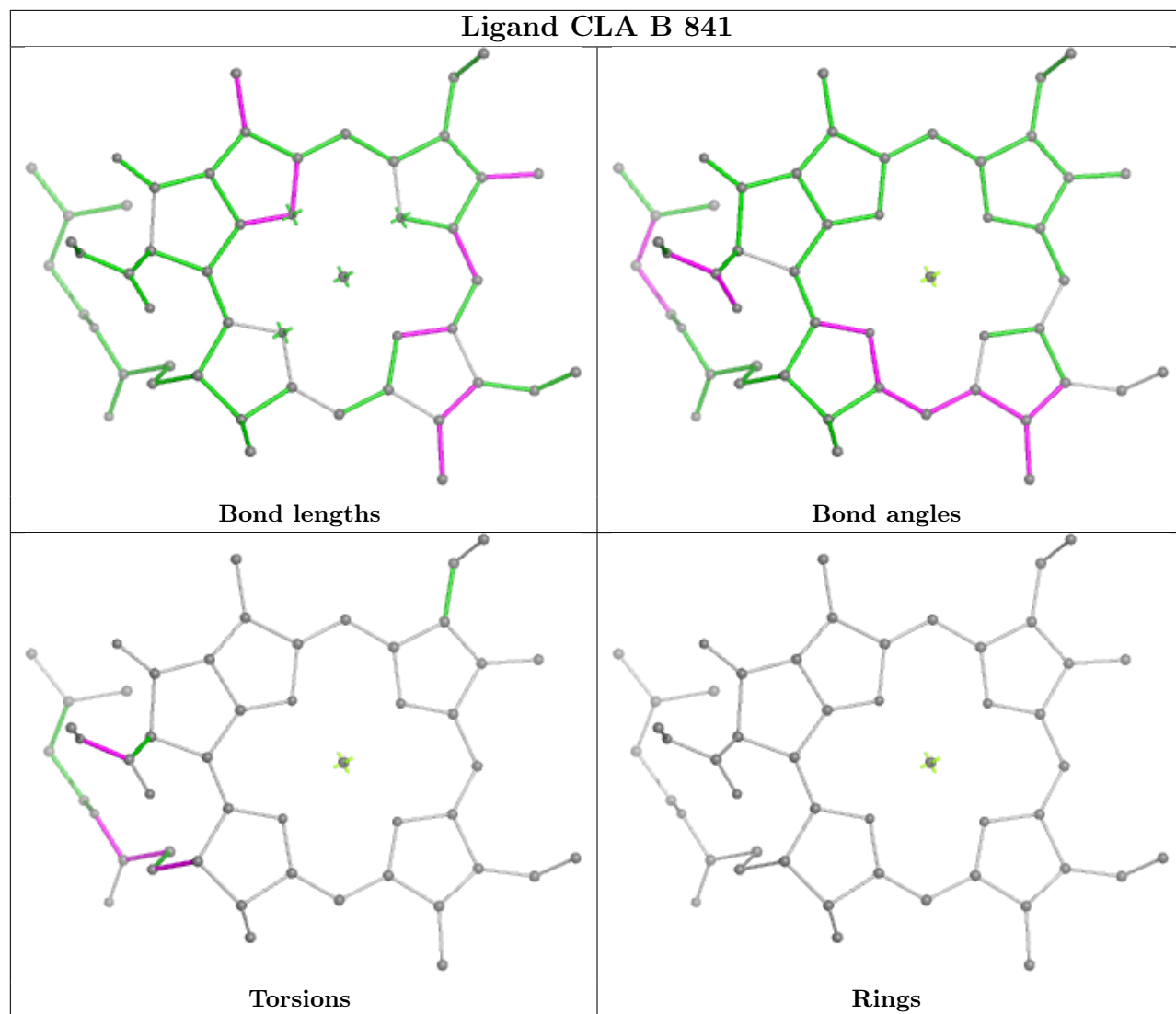
## Ligand BCR b 846



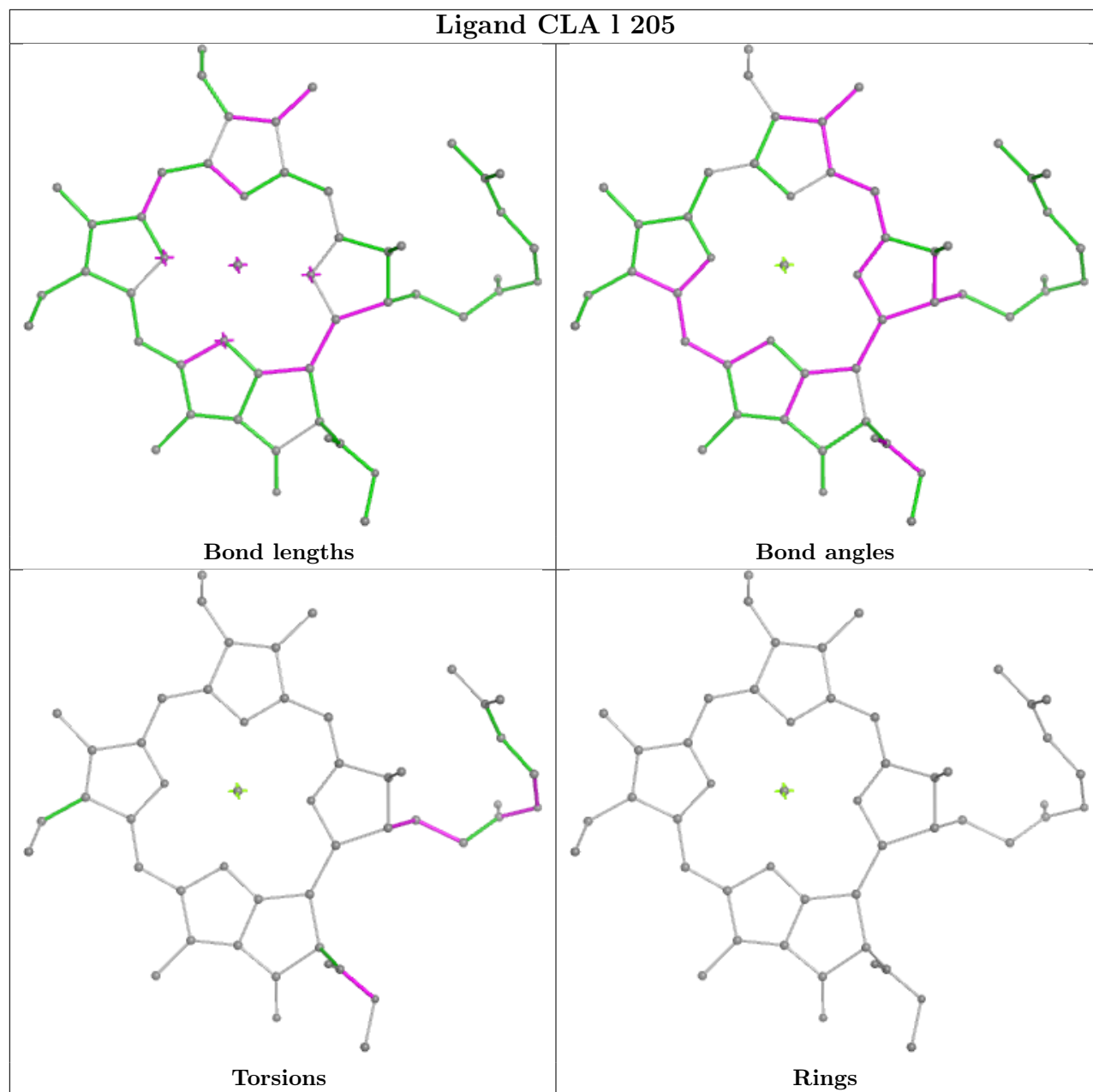




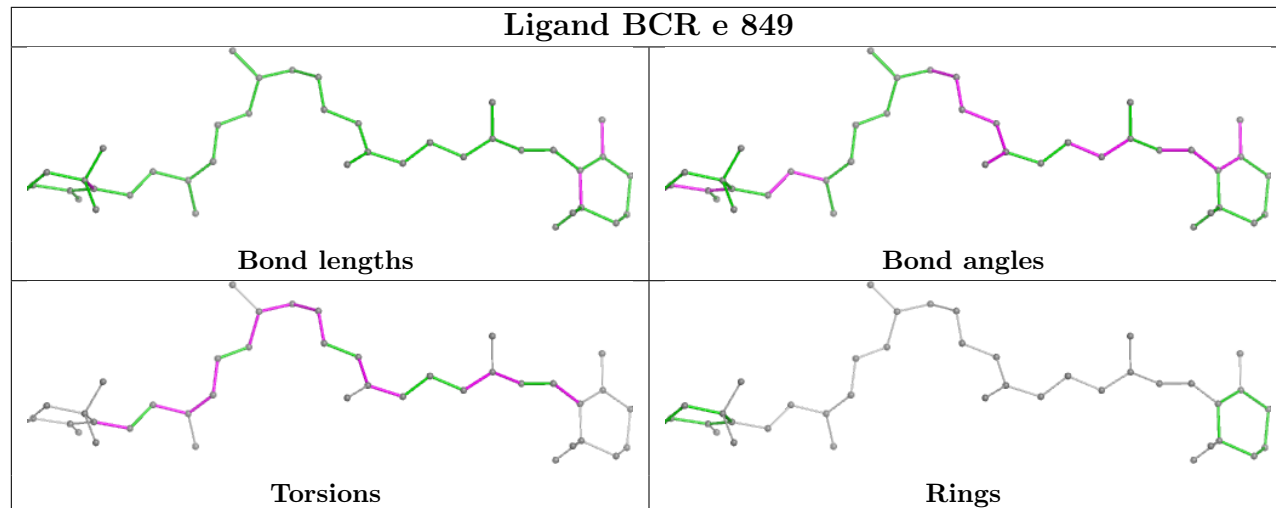
## Ligand CLA B 841



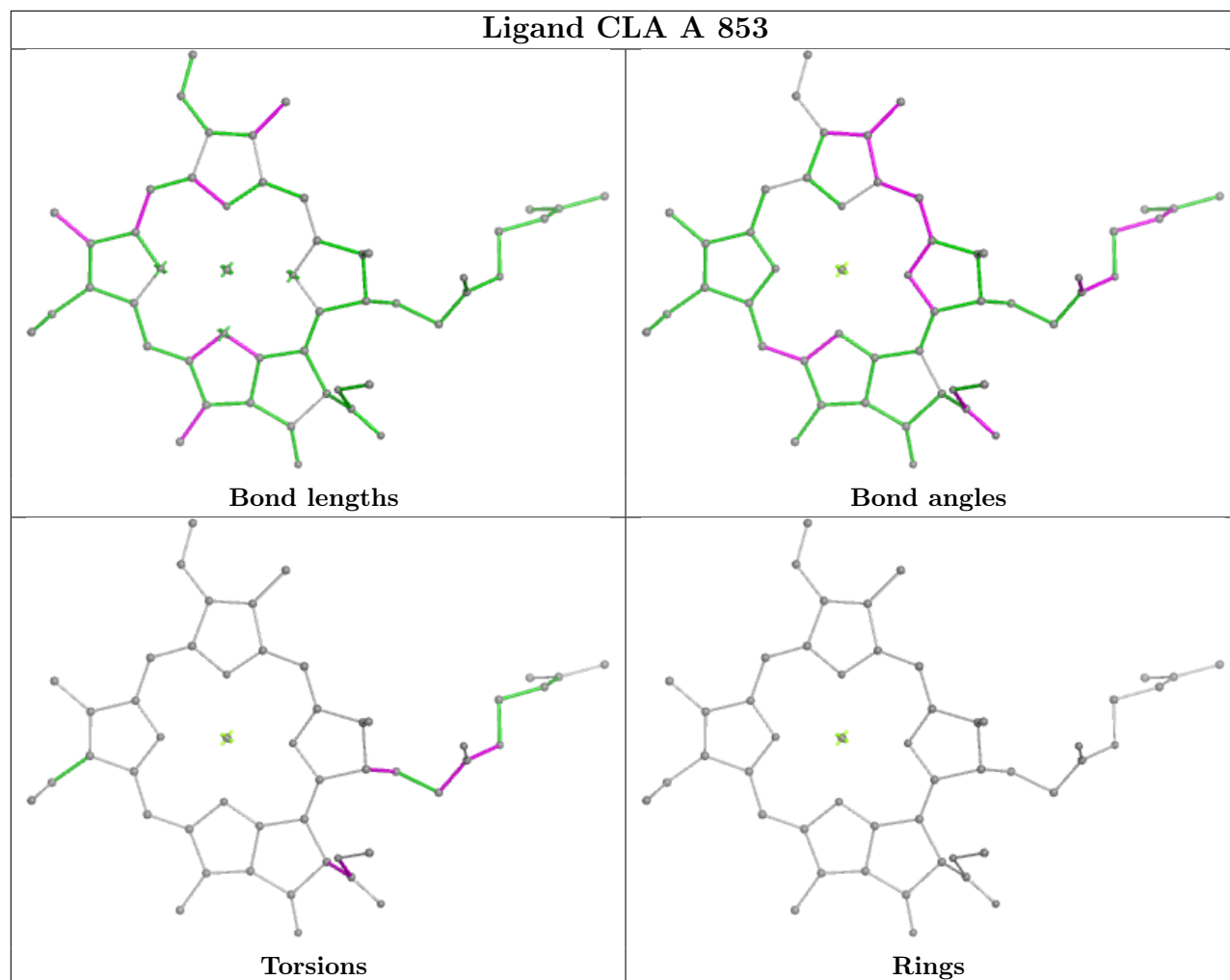
## Ligand CLA 1 205



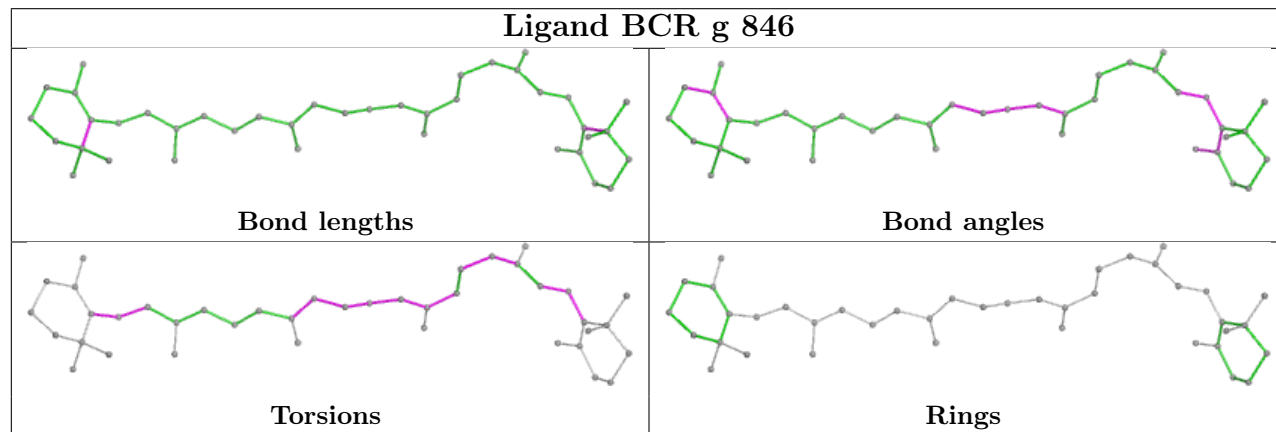
## Ligand BCR e 849



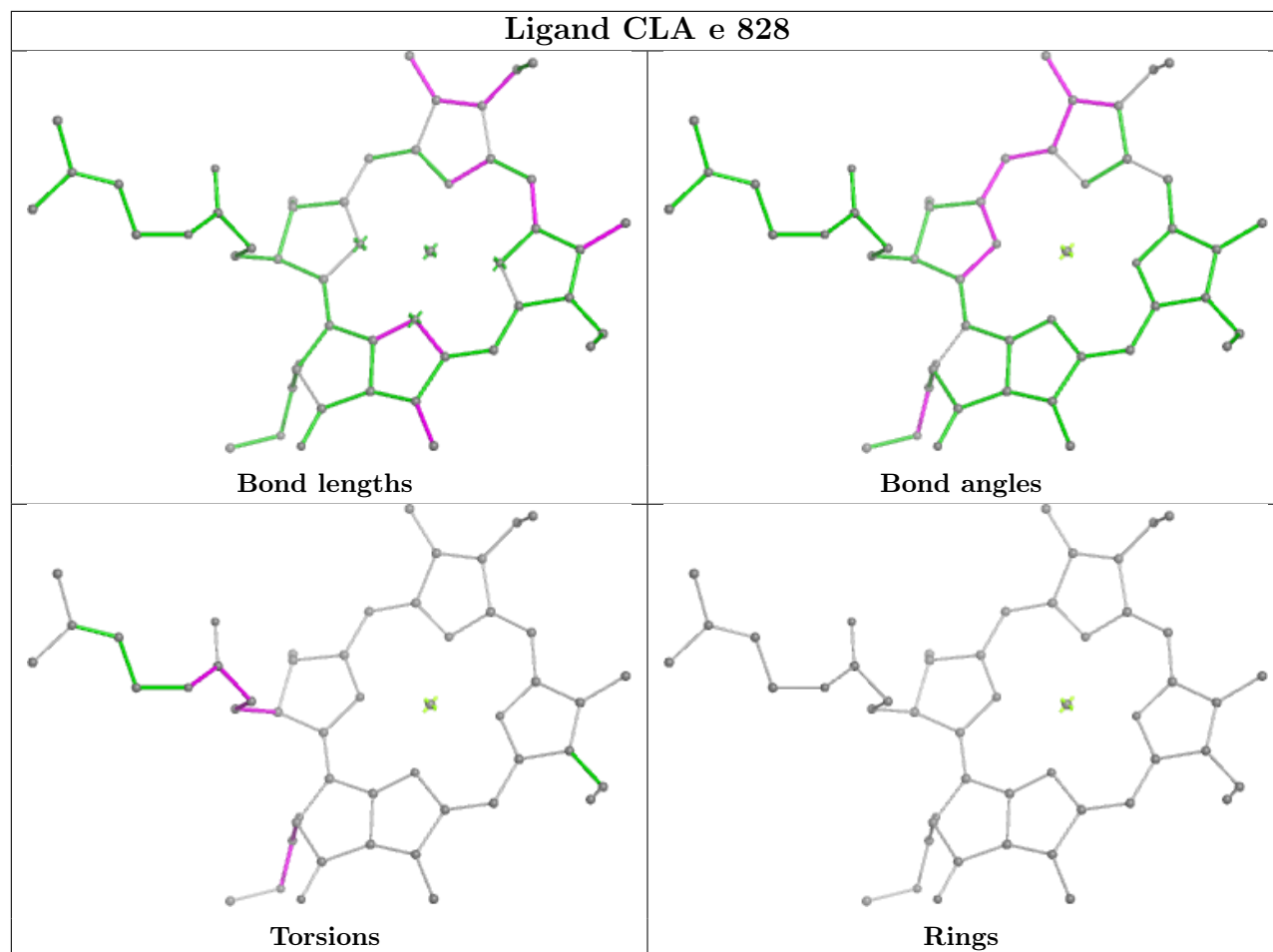
## Ligand CLA A 853



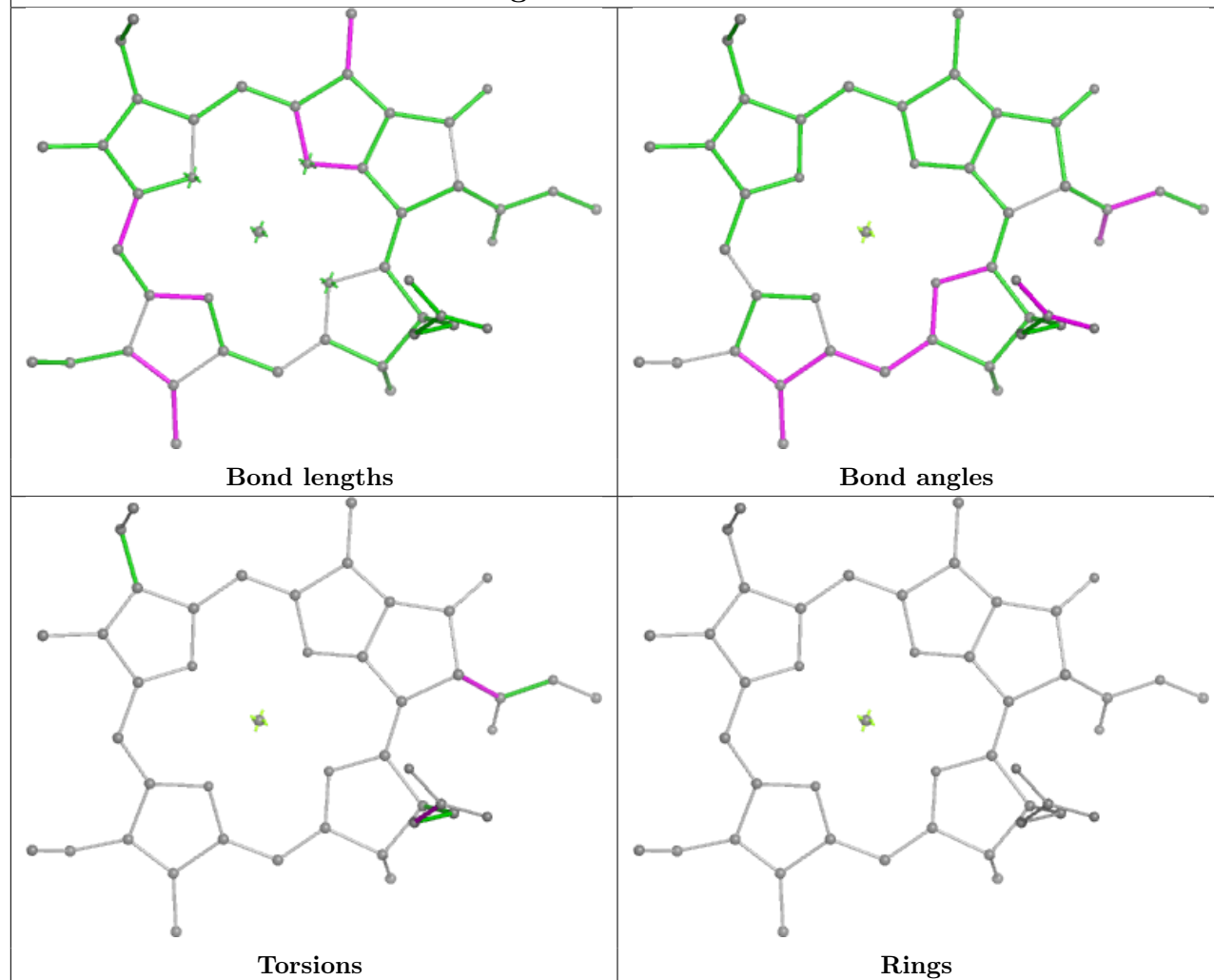
## Ligand BCR g 846



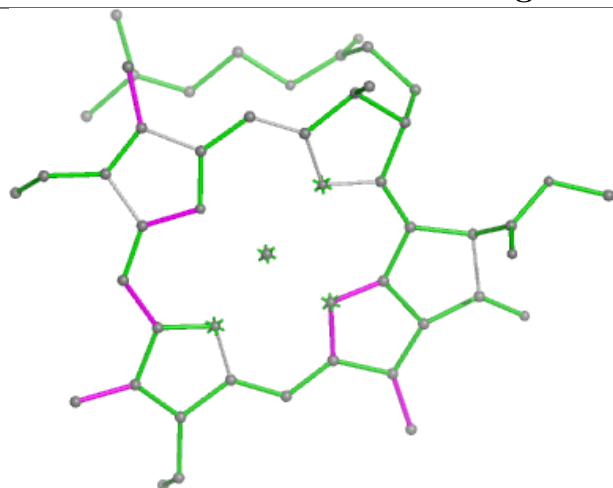
## Ligand CLA e 828



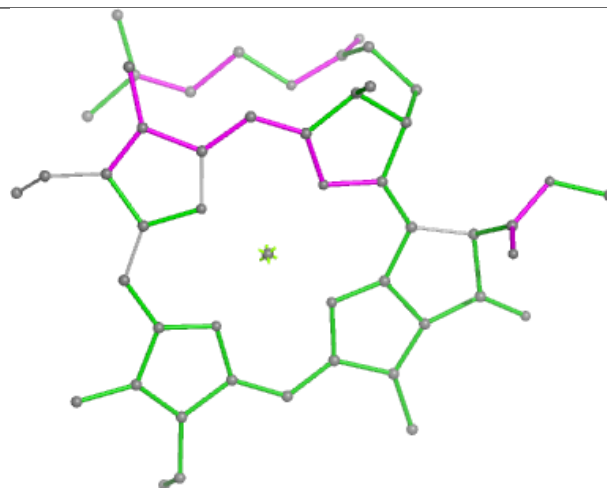
## Ligand CLA a 814



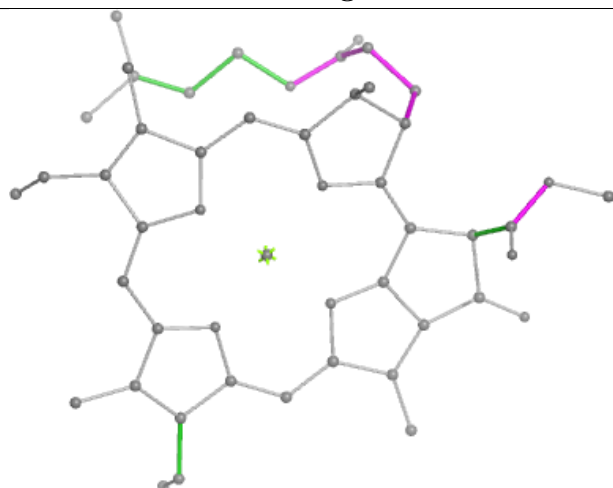
## Ligand CLA E 822



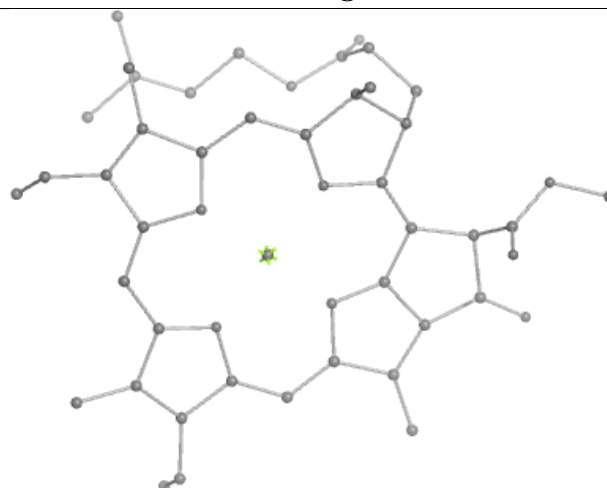
Bond lengths



Bond angles

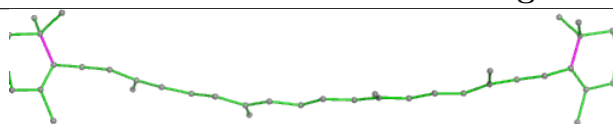


Torsions

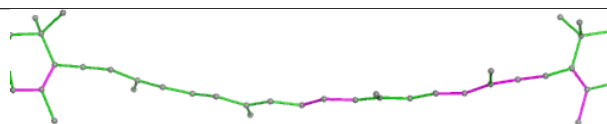


Rings

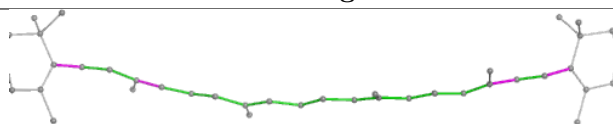
## Ligand BCR e 850



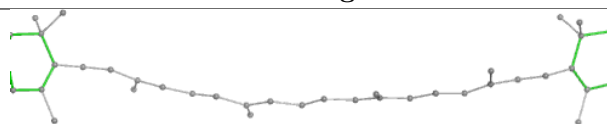
Bond lengths



Bond angles

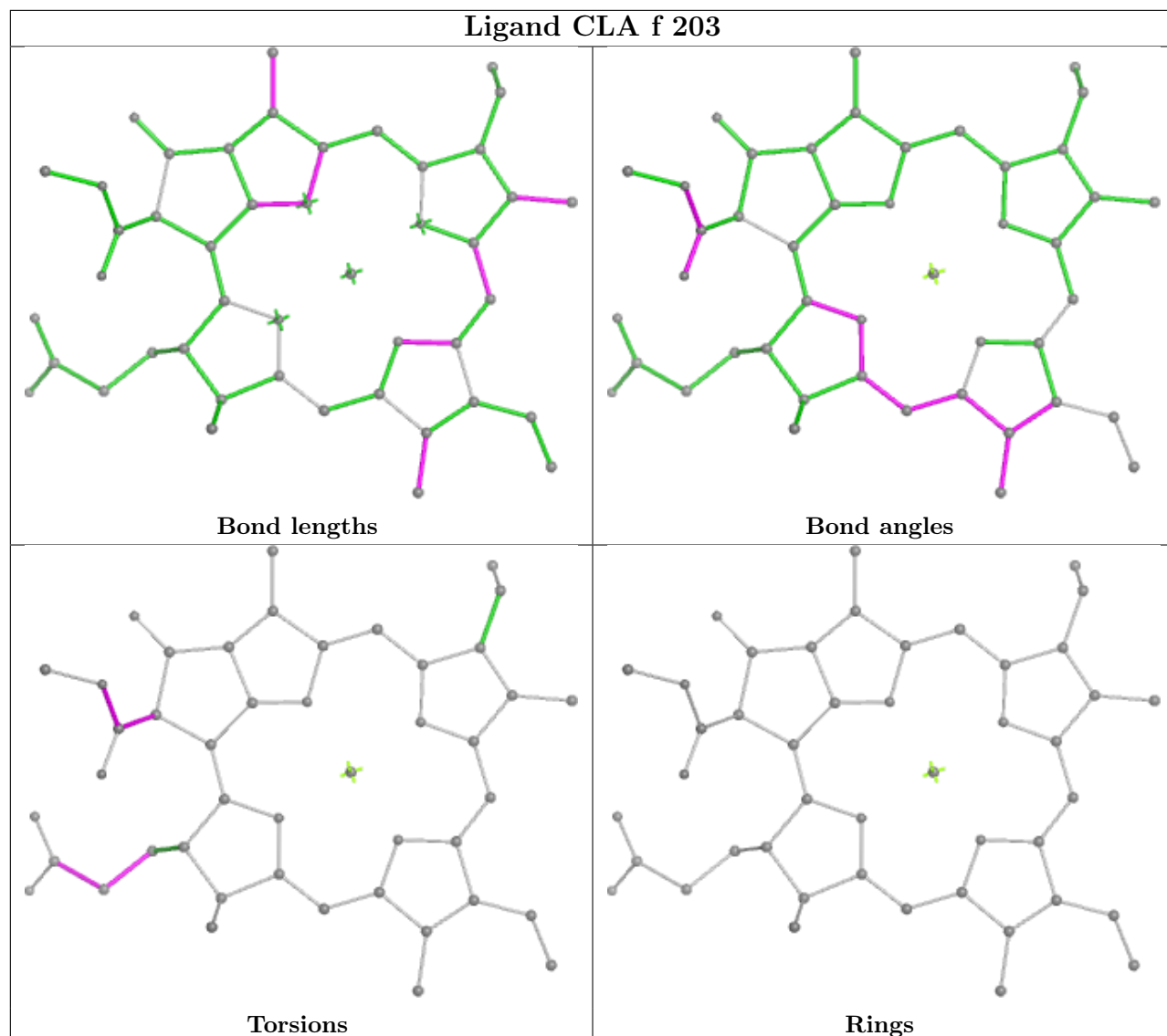


Torsions

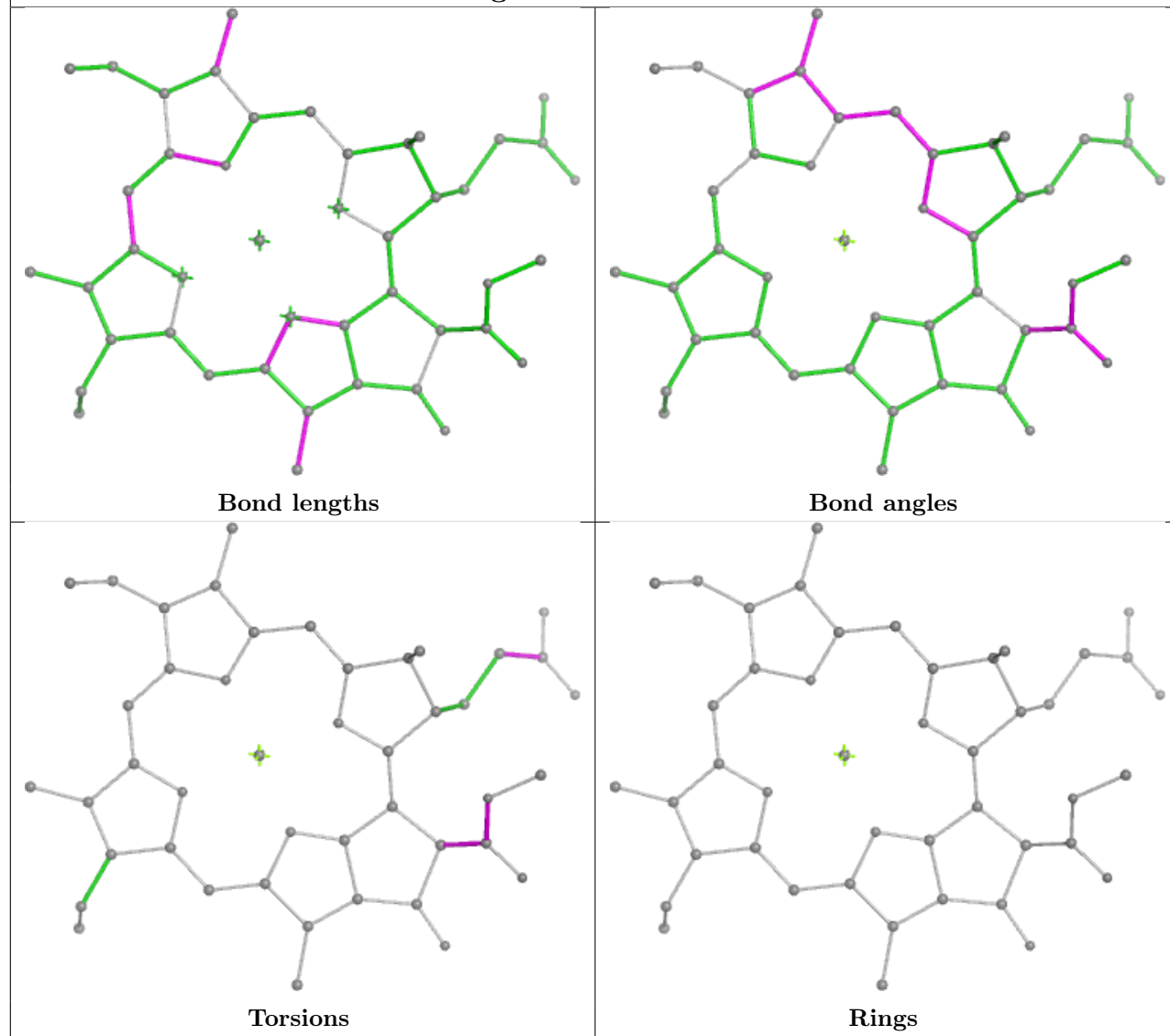


Rings

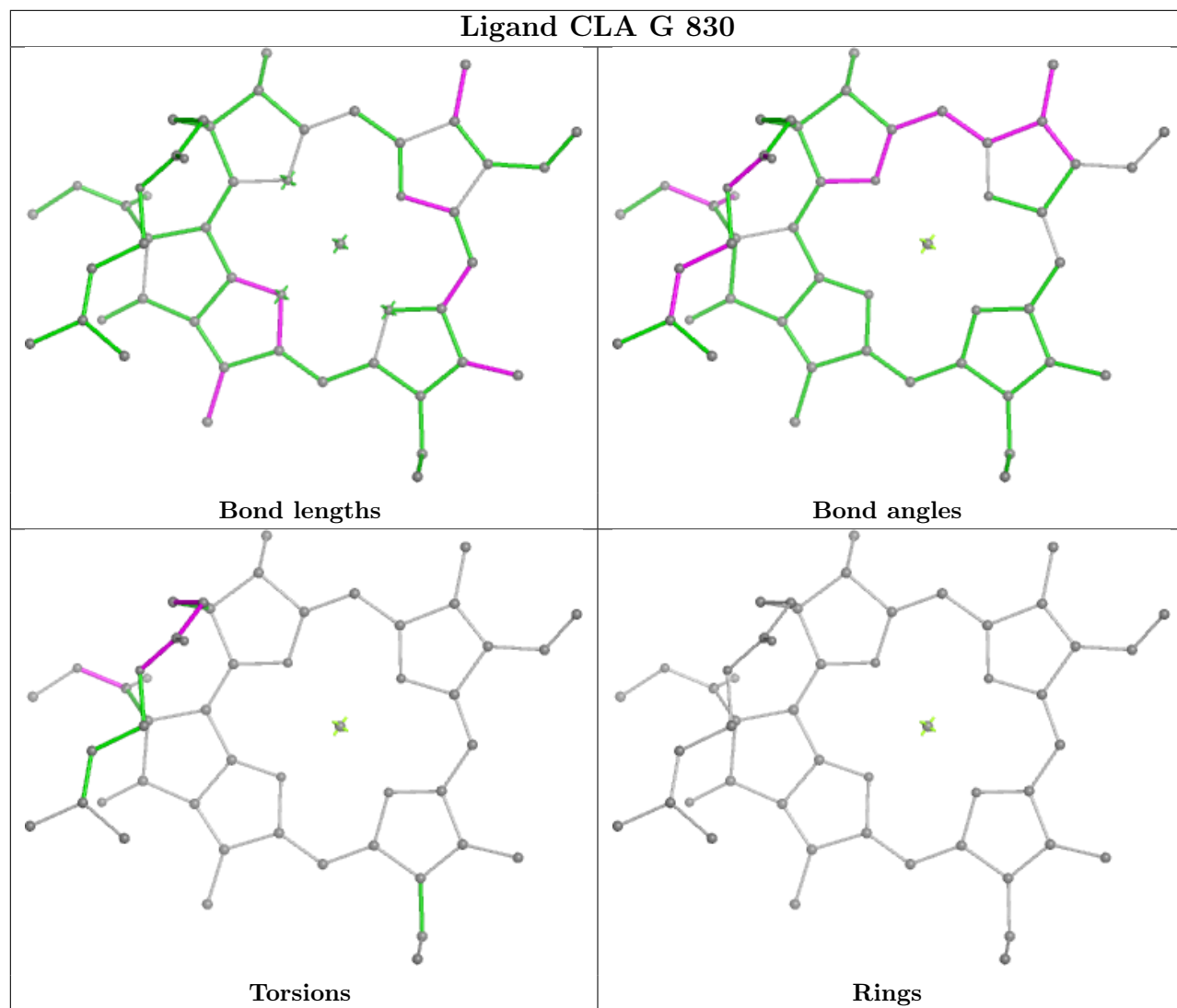
## Ligand CLA f 203

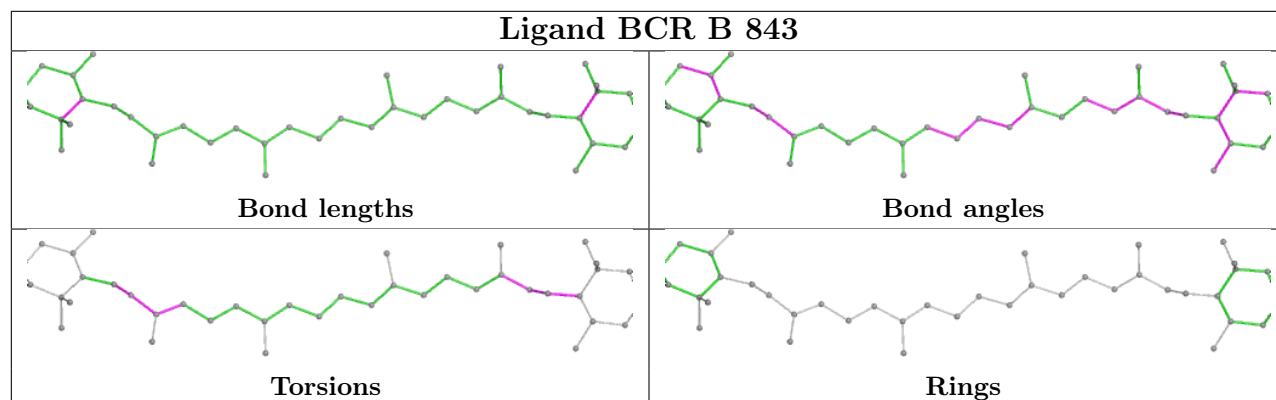
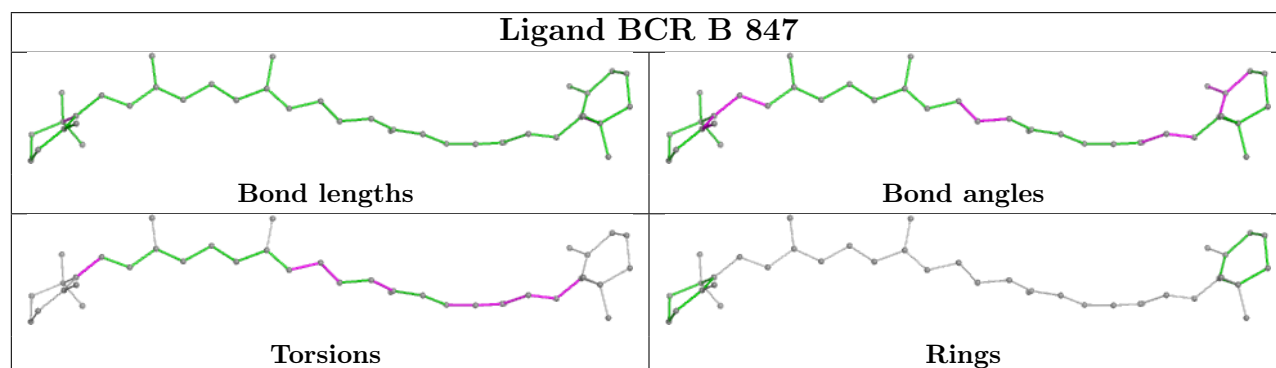
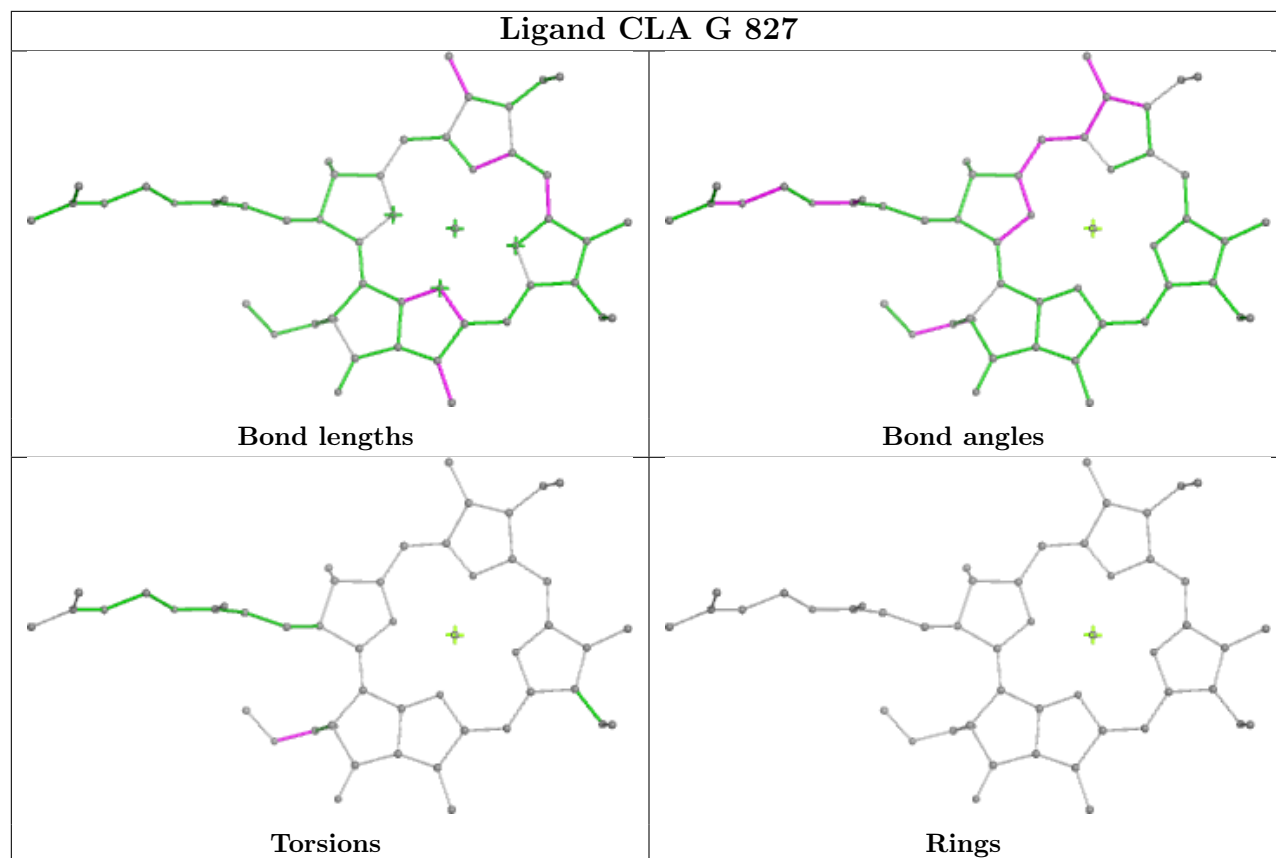


## Ligand CLA b 823

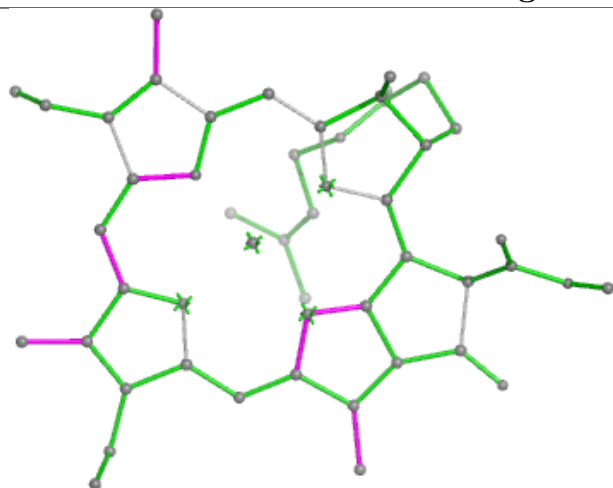




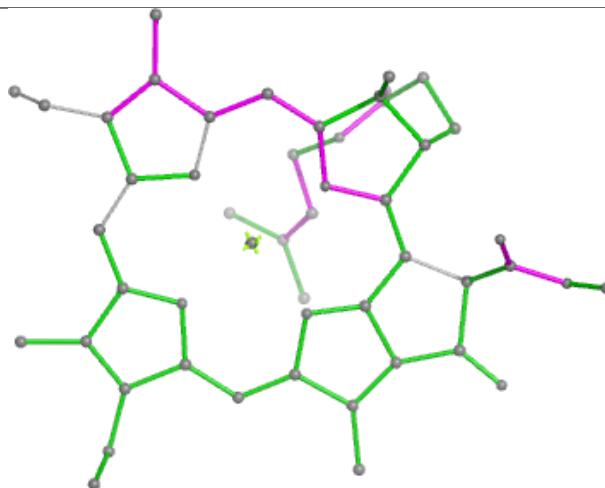




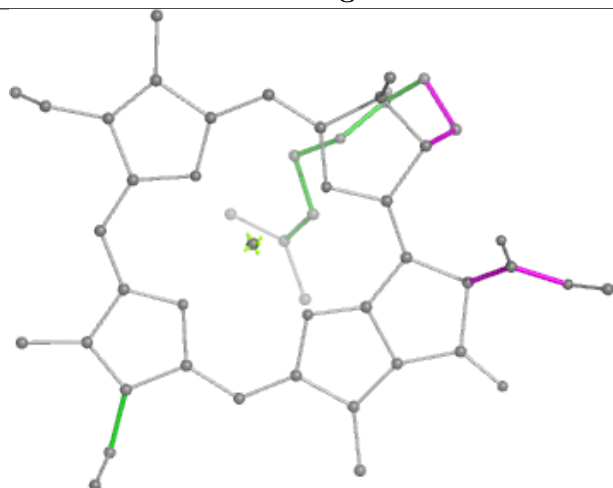
## Ligand CLA a 845



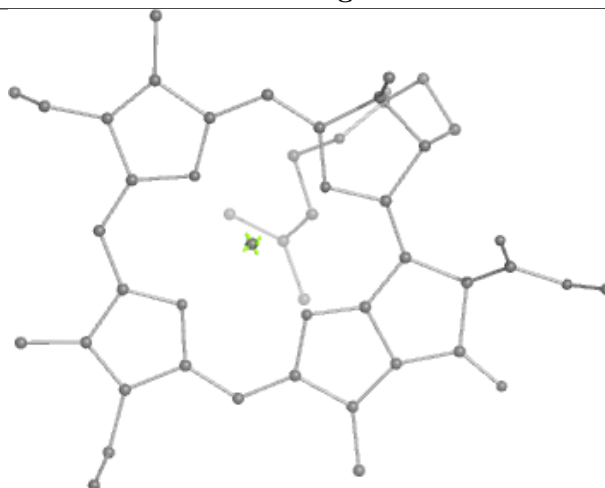
Bond lengths



Bond angles

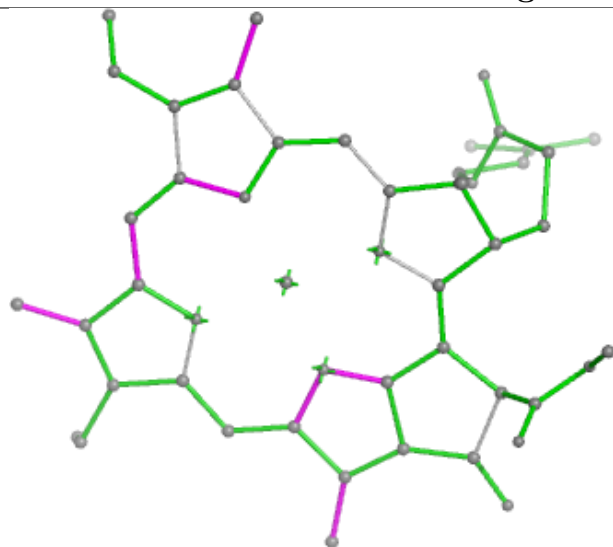


Torsions

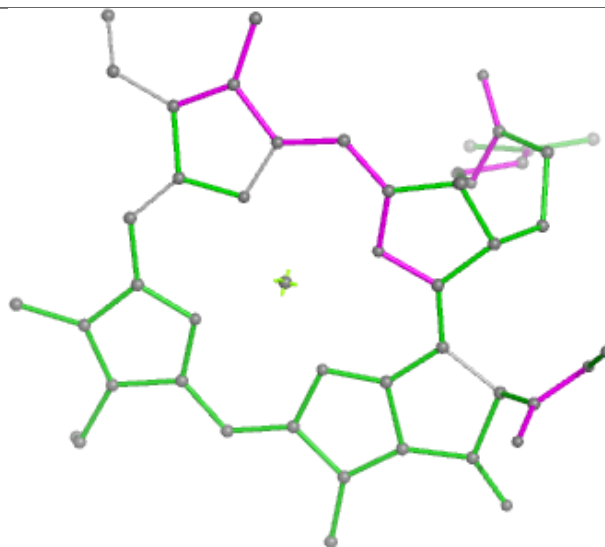


Rings

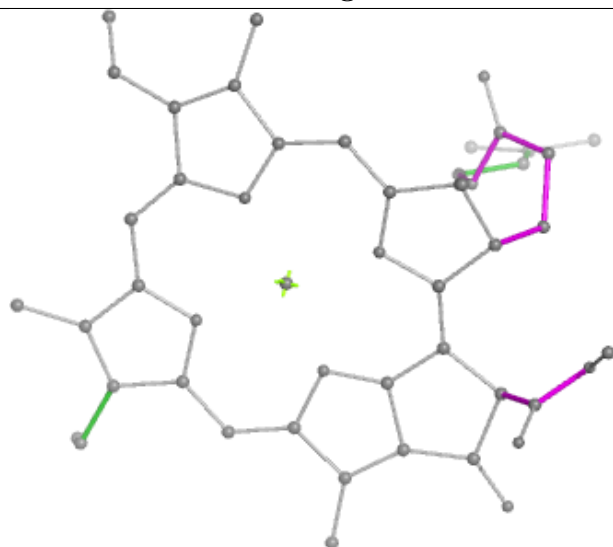
## Ligand CLA b 828



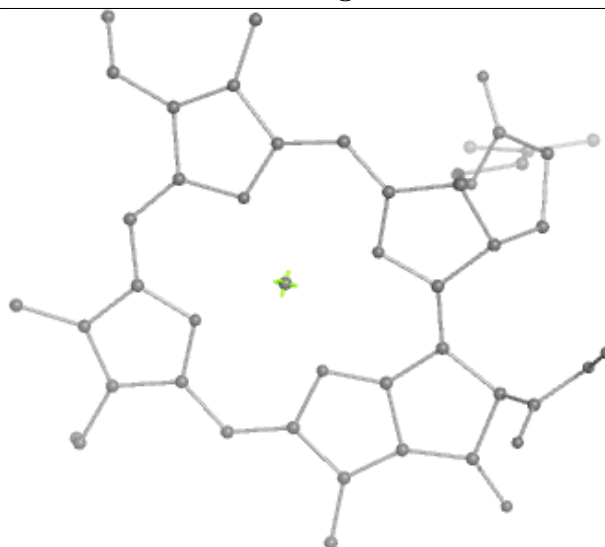
Bond lengths



Bond angles

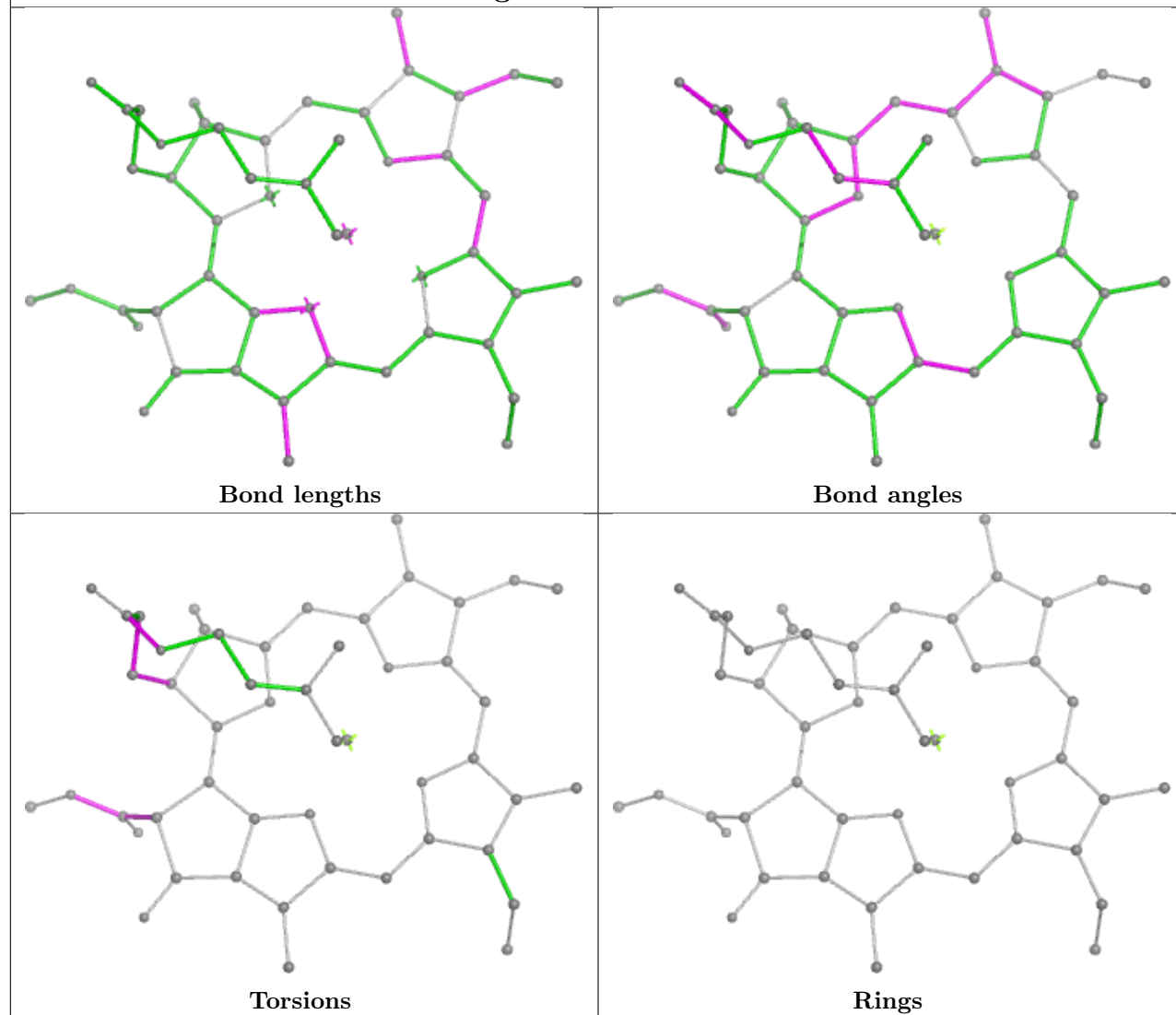


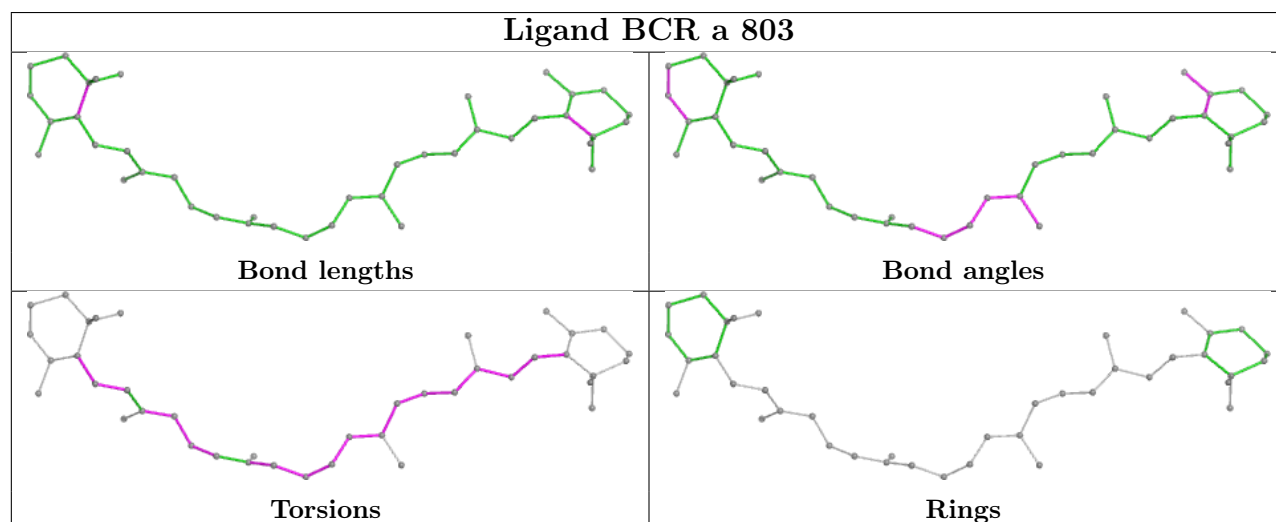
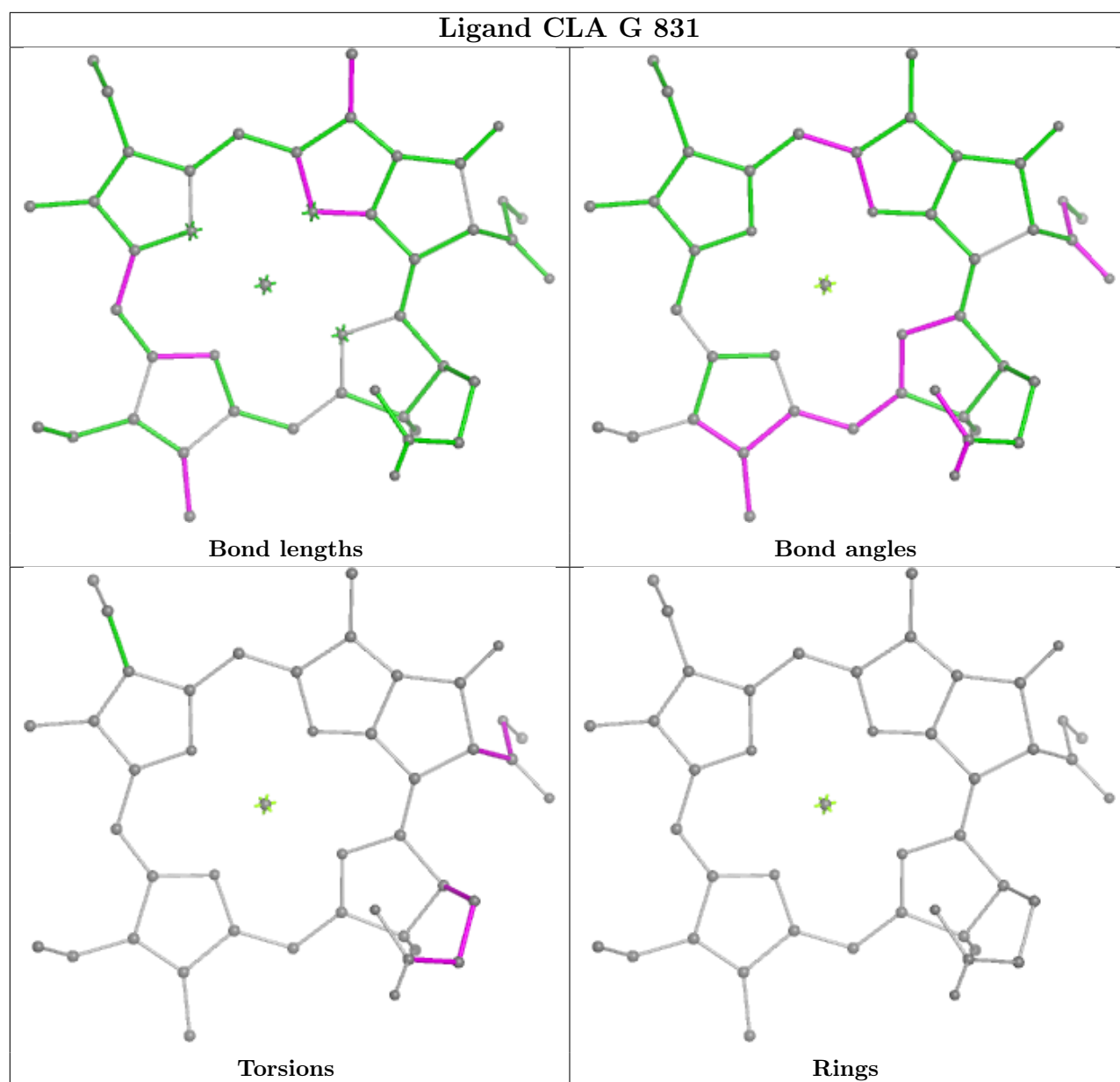
Torsions

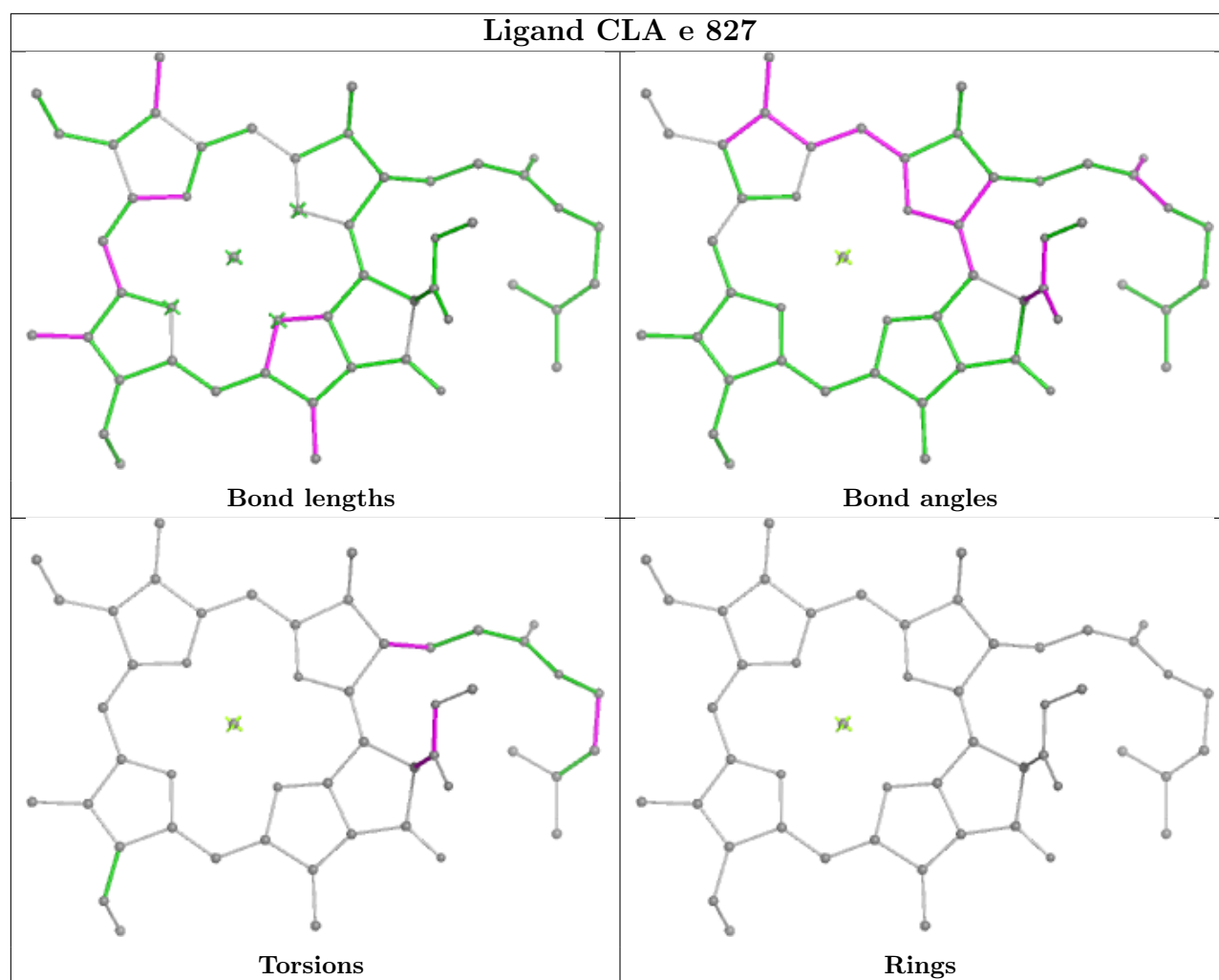


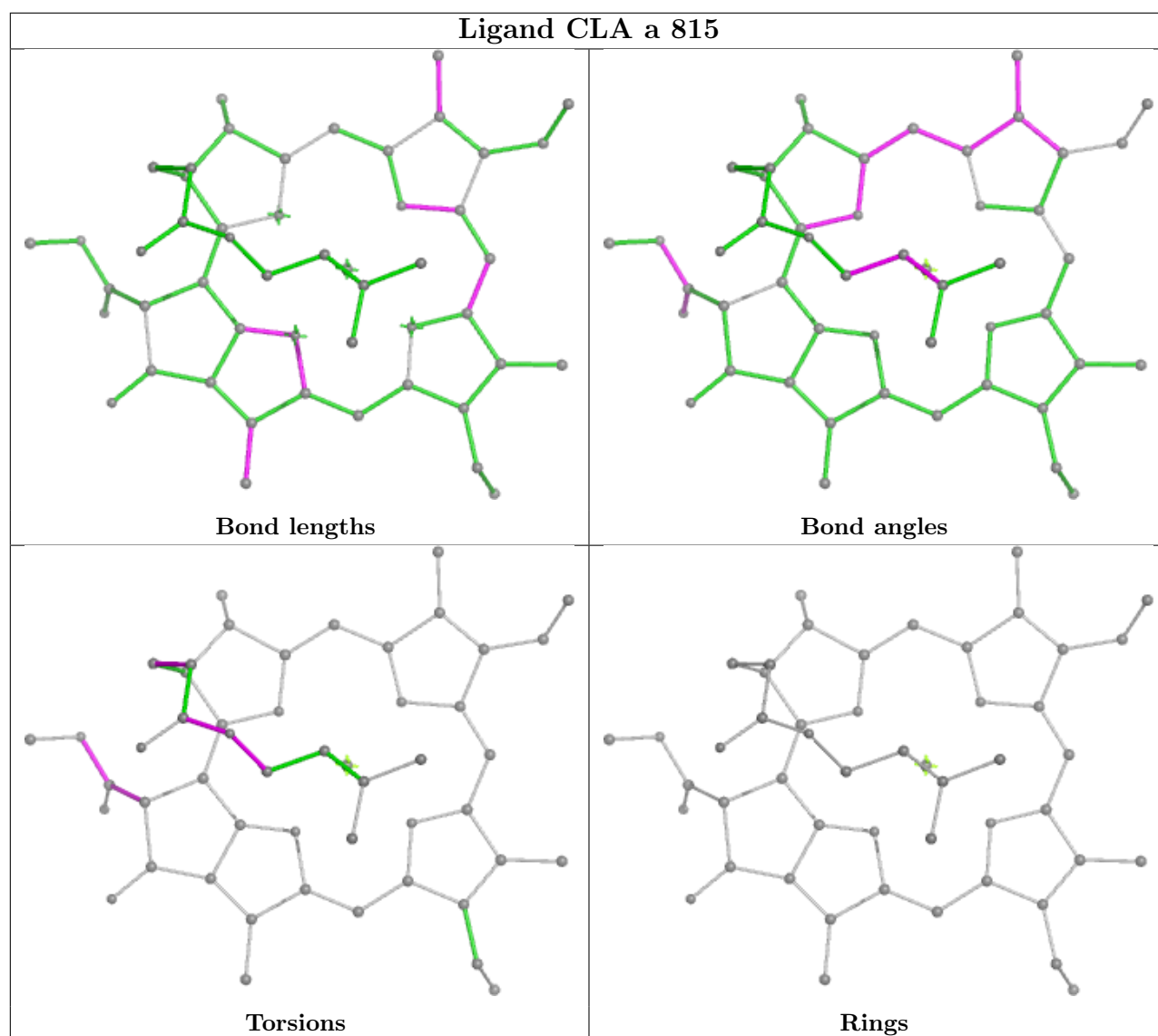
Rings

## Ligand CLA a 821

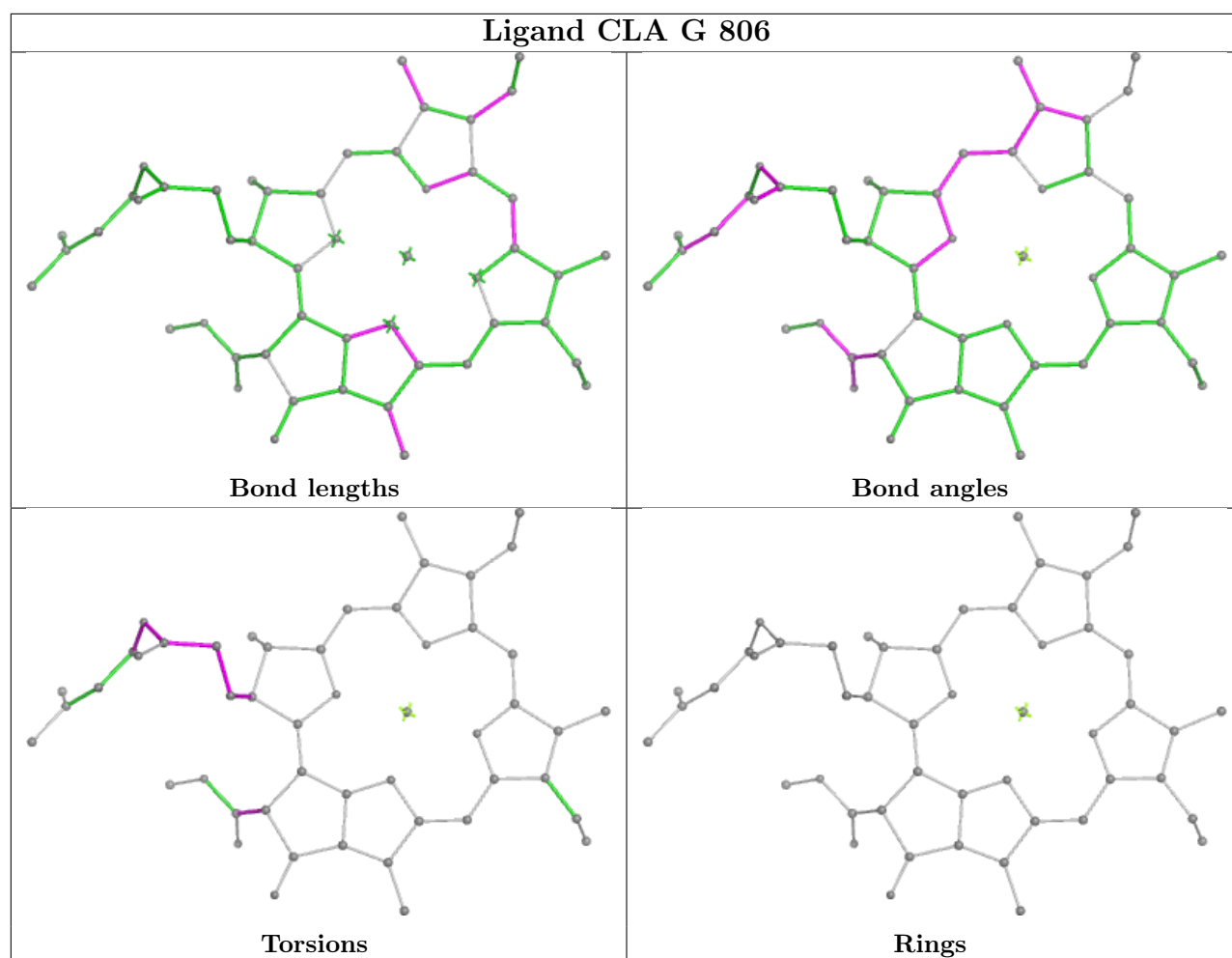




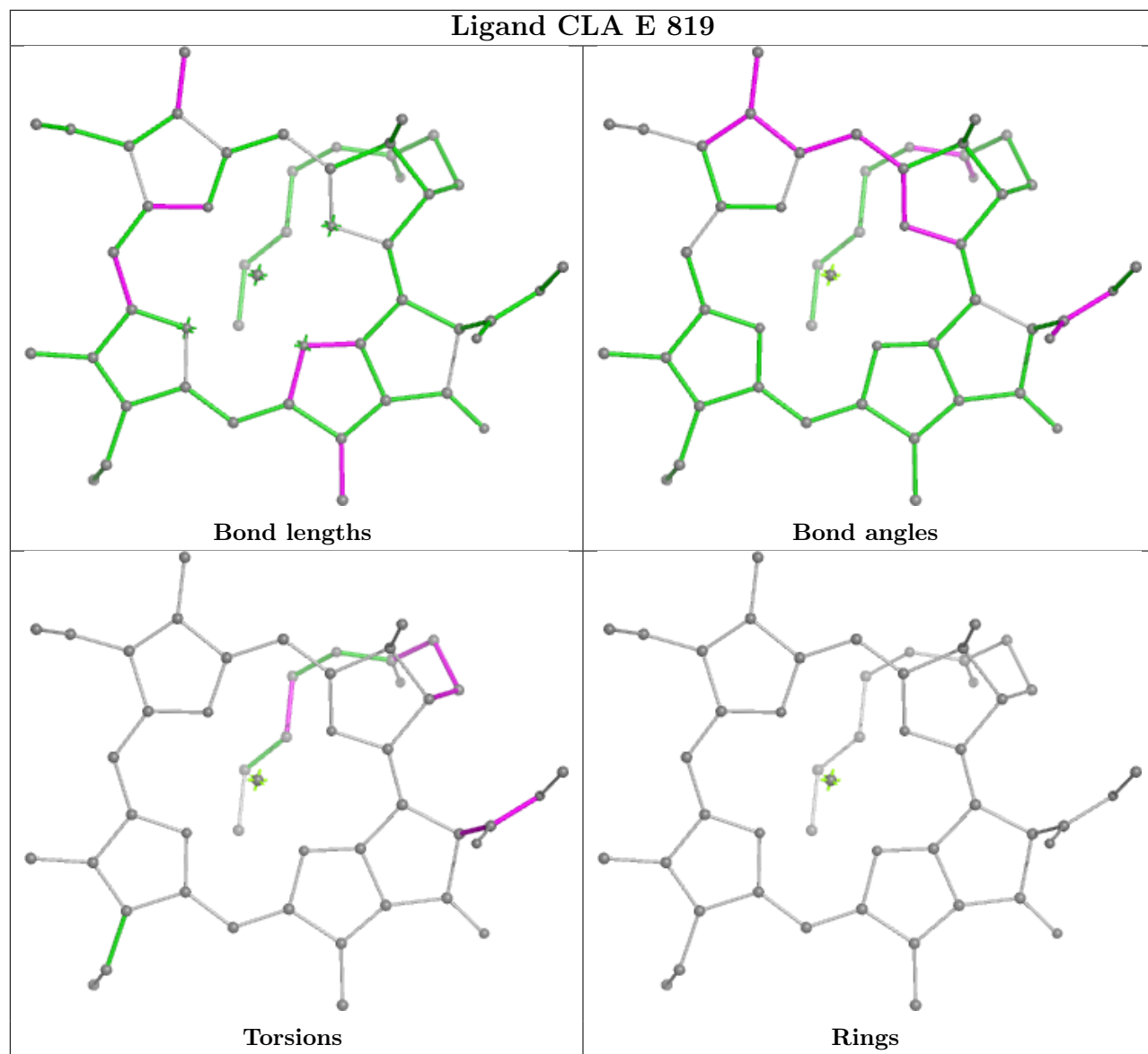




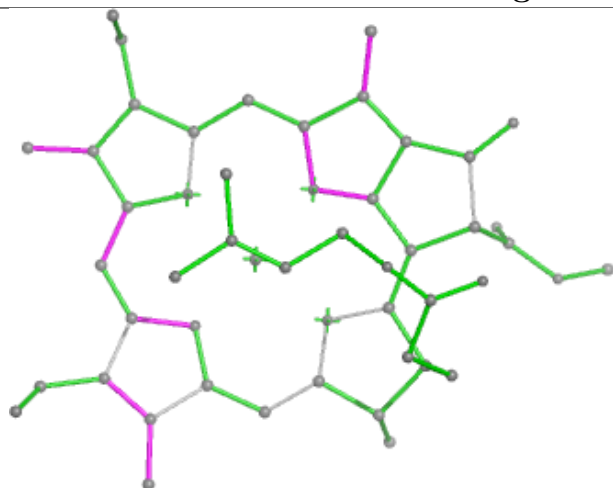




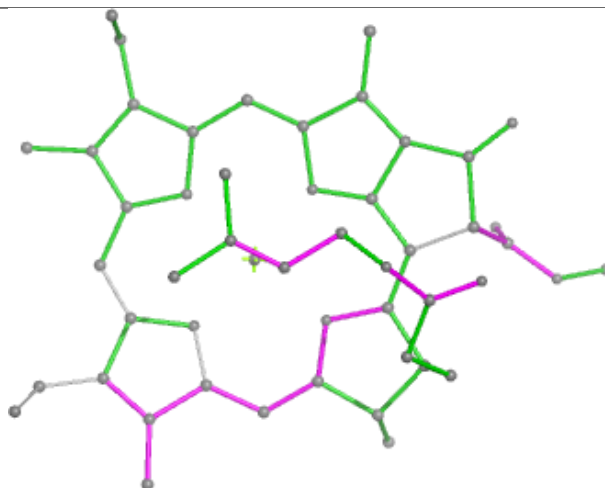
## Ligand CLA E 819



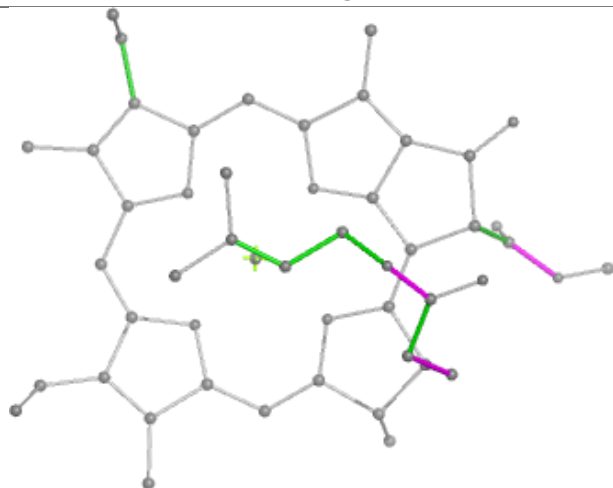
## Ligand CLA G 801



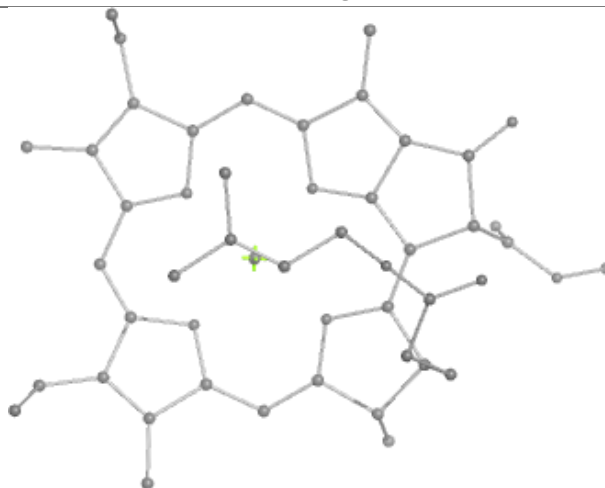
Bond lengths



Bond angles

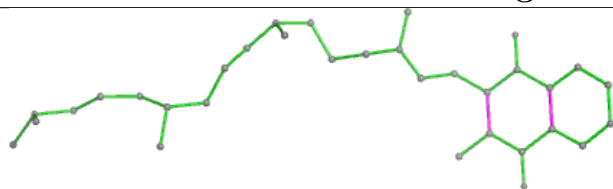


Torsions

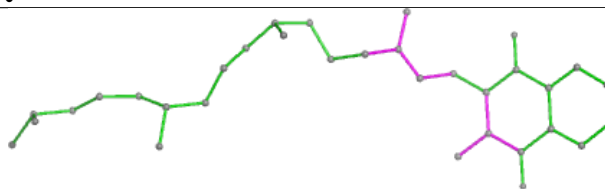


Rings

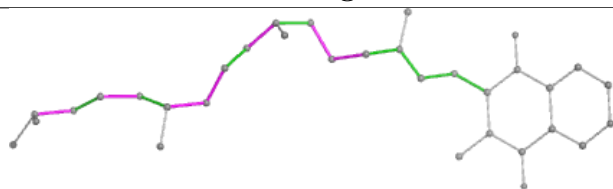
## Ligand PQN a 847



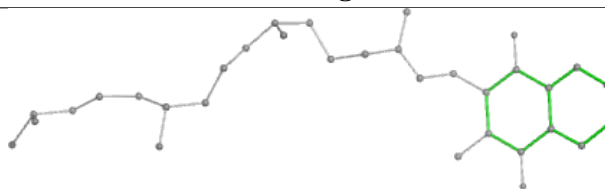
Bond lengths



Bond angles

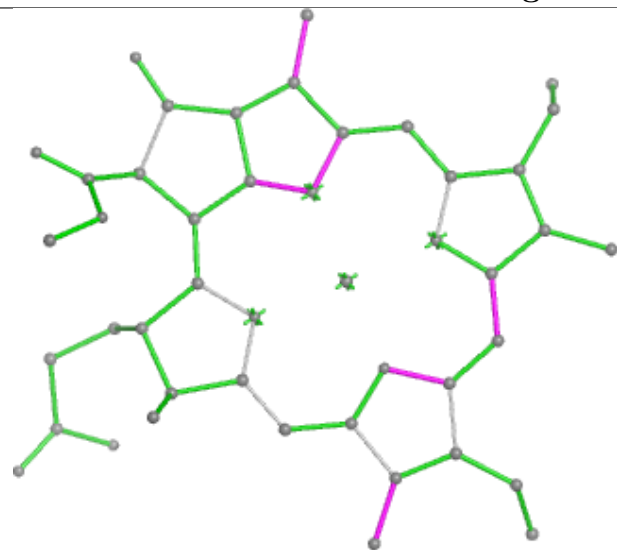


Torsions

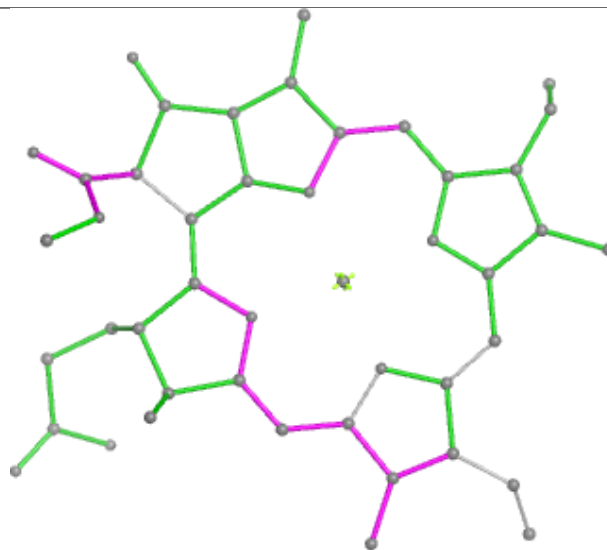


Rings

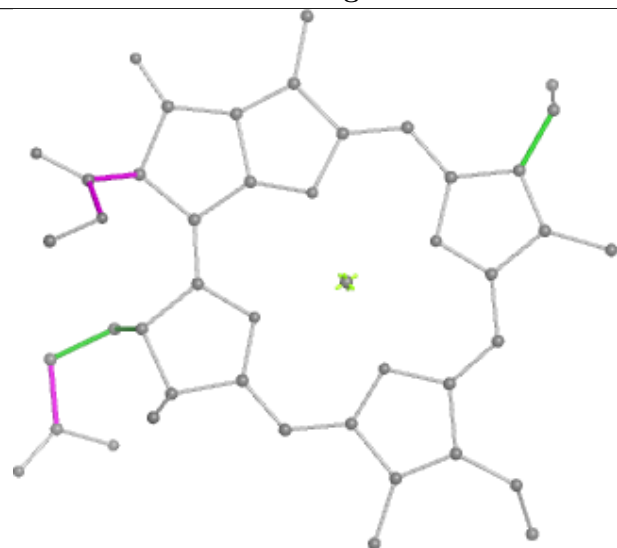
## Ligand CLA a 839



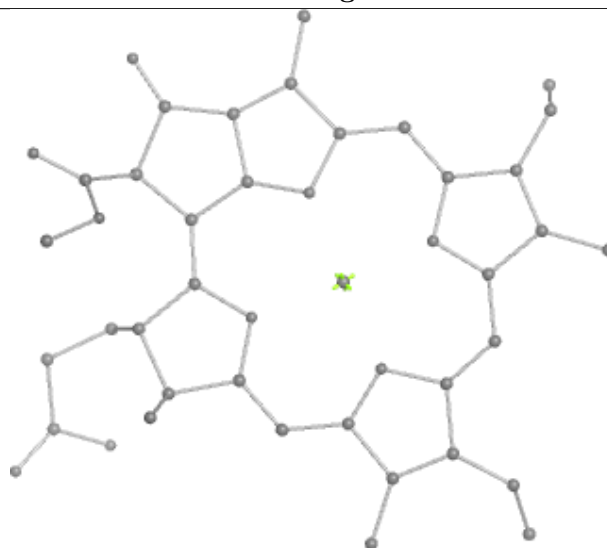
Bond lengths



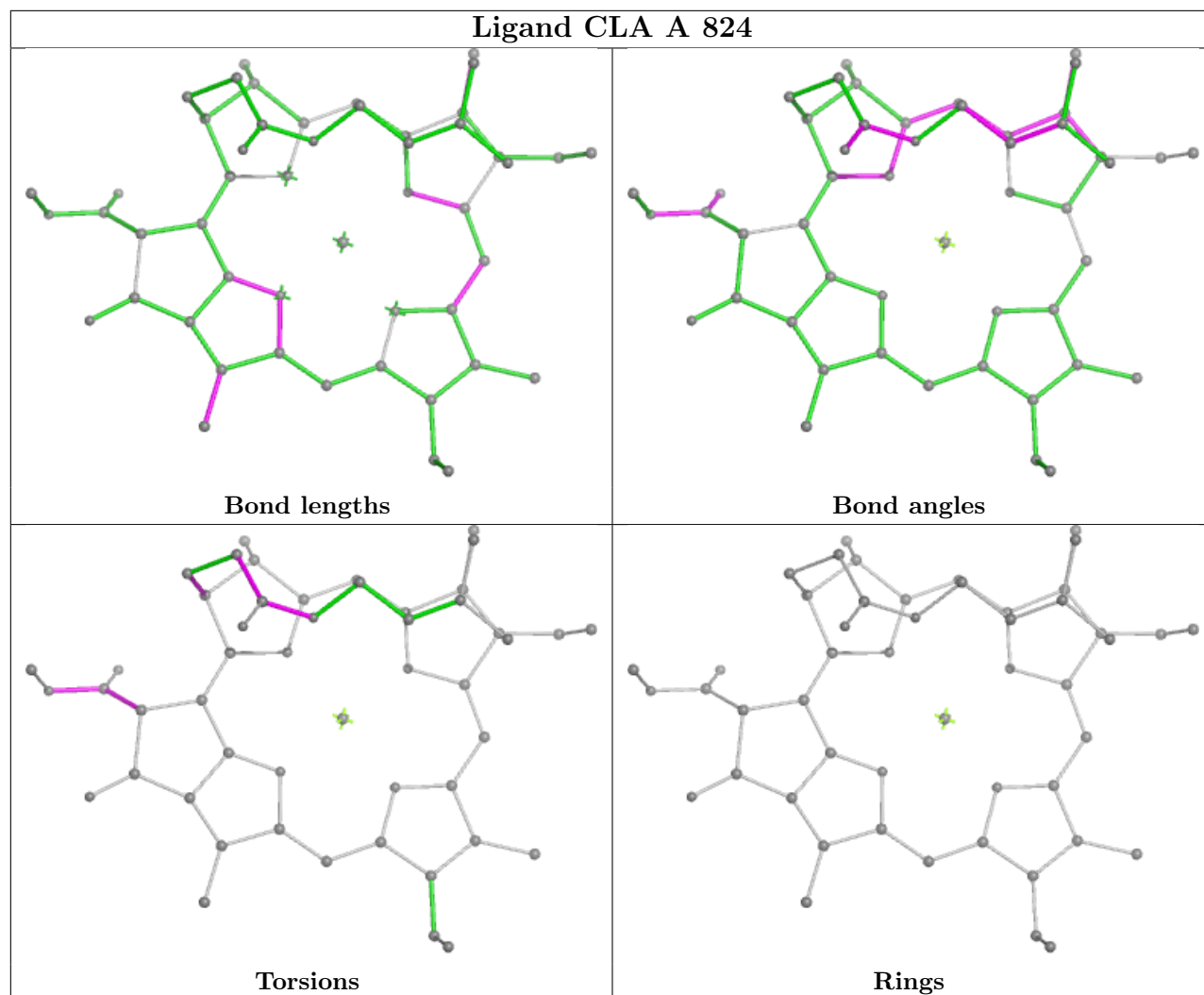
Bond angles



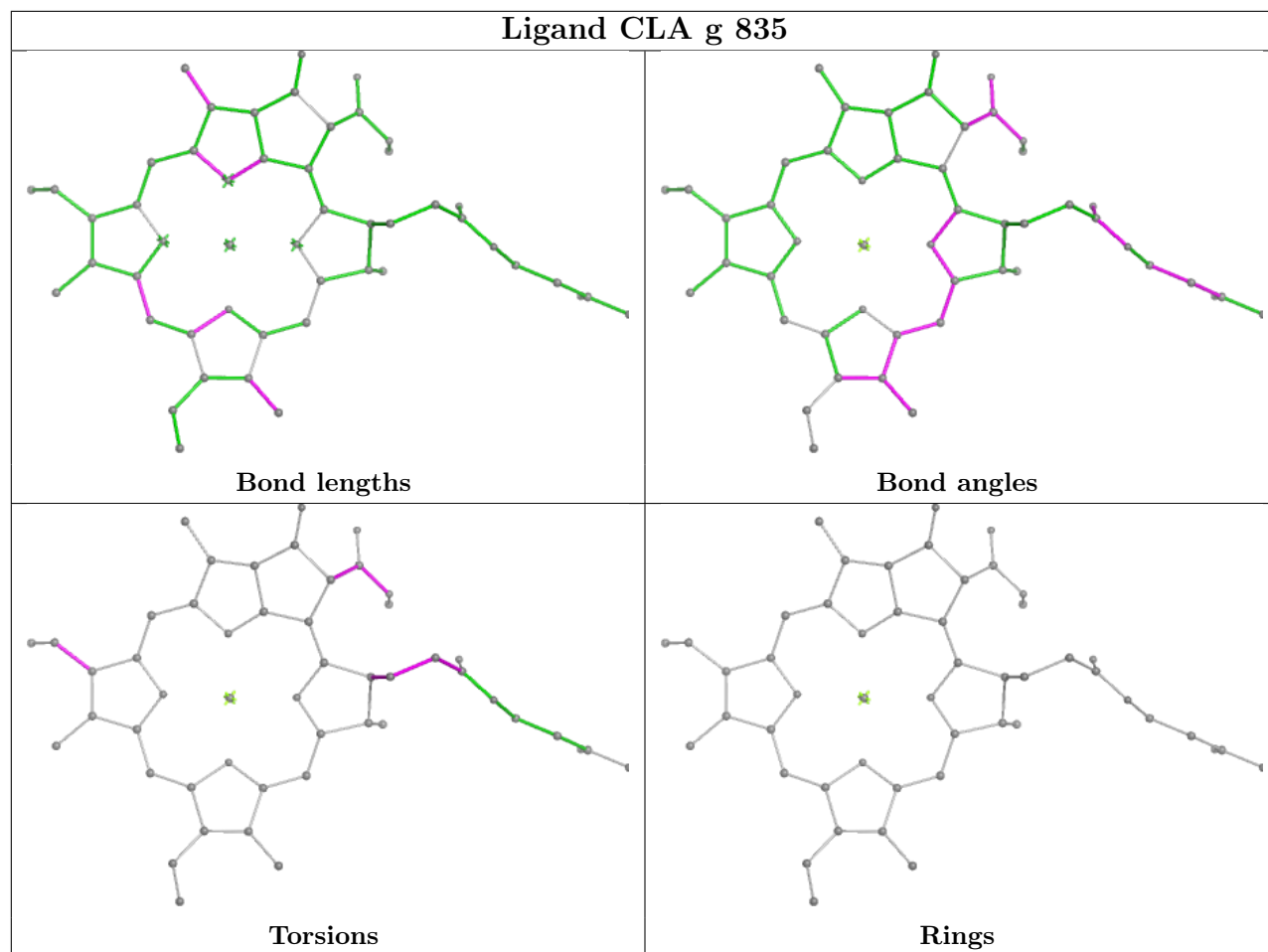
Torsions

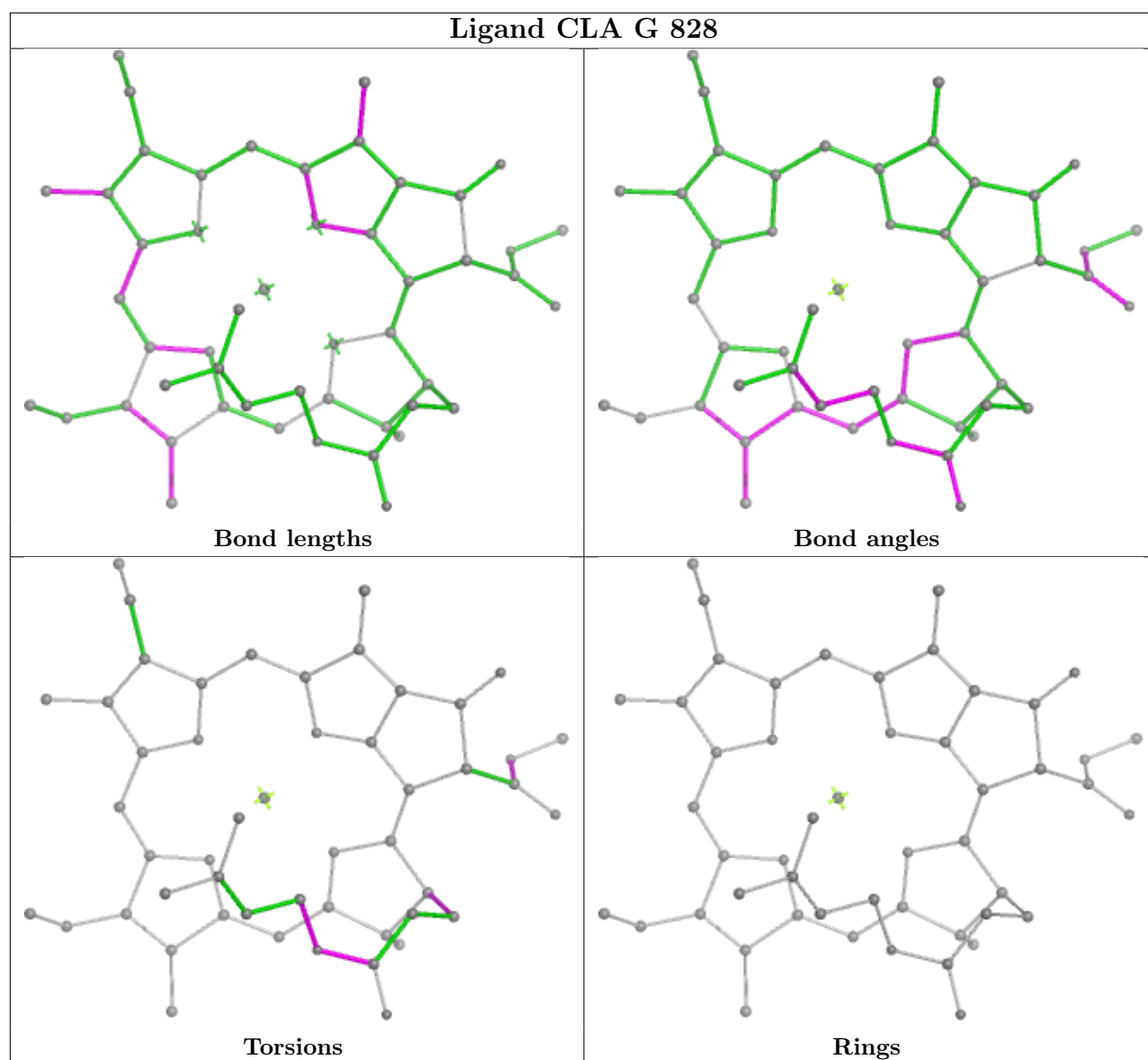


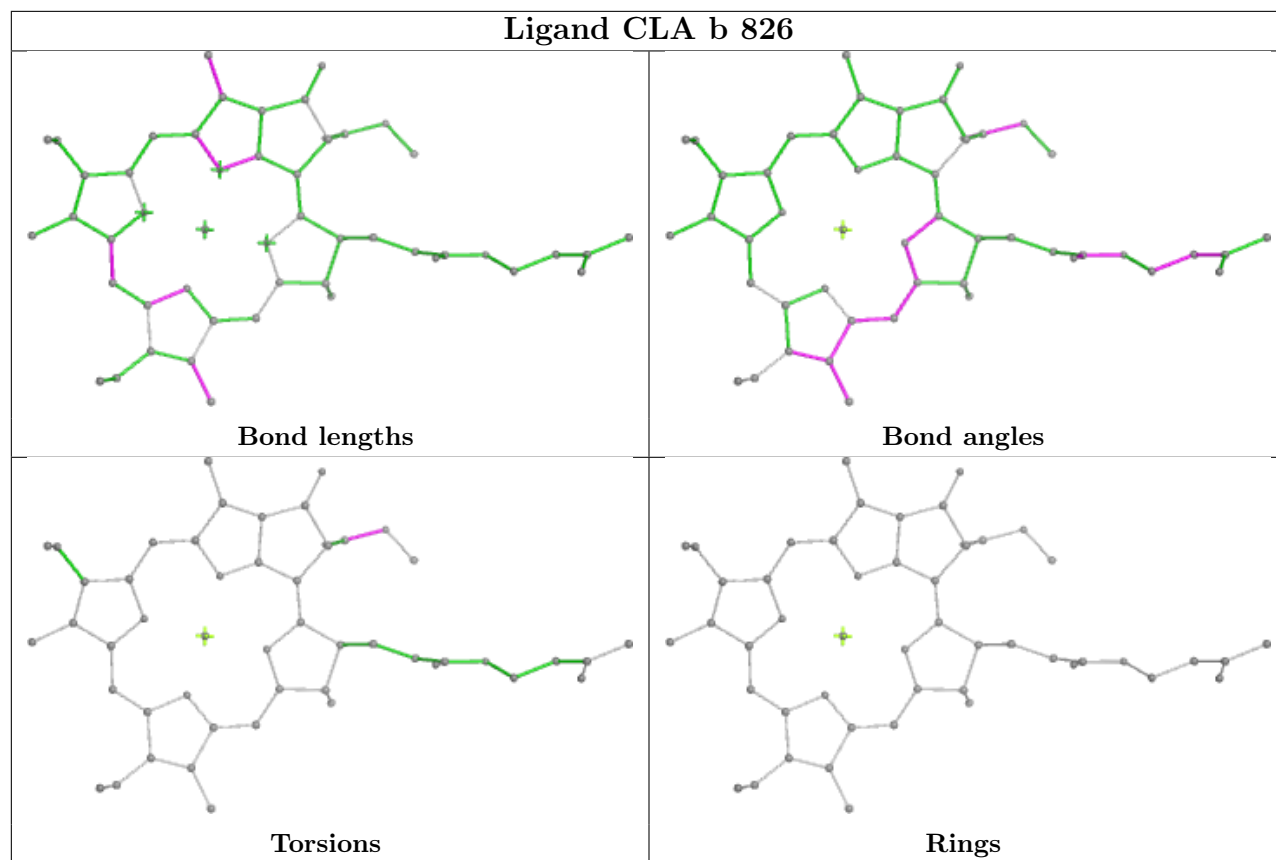
Rings



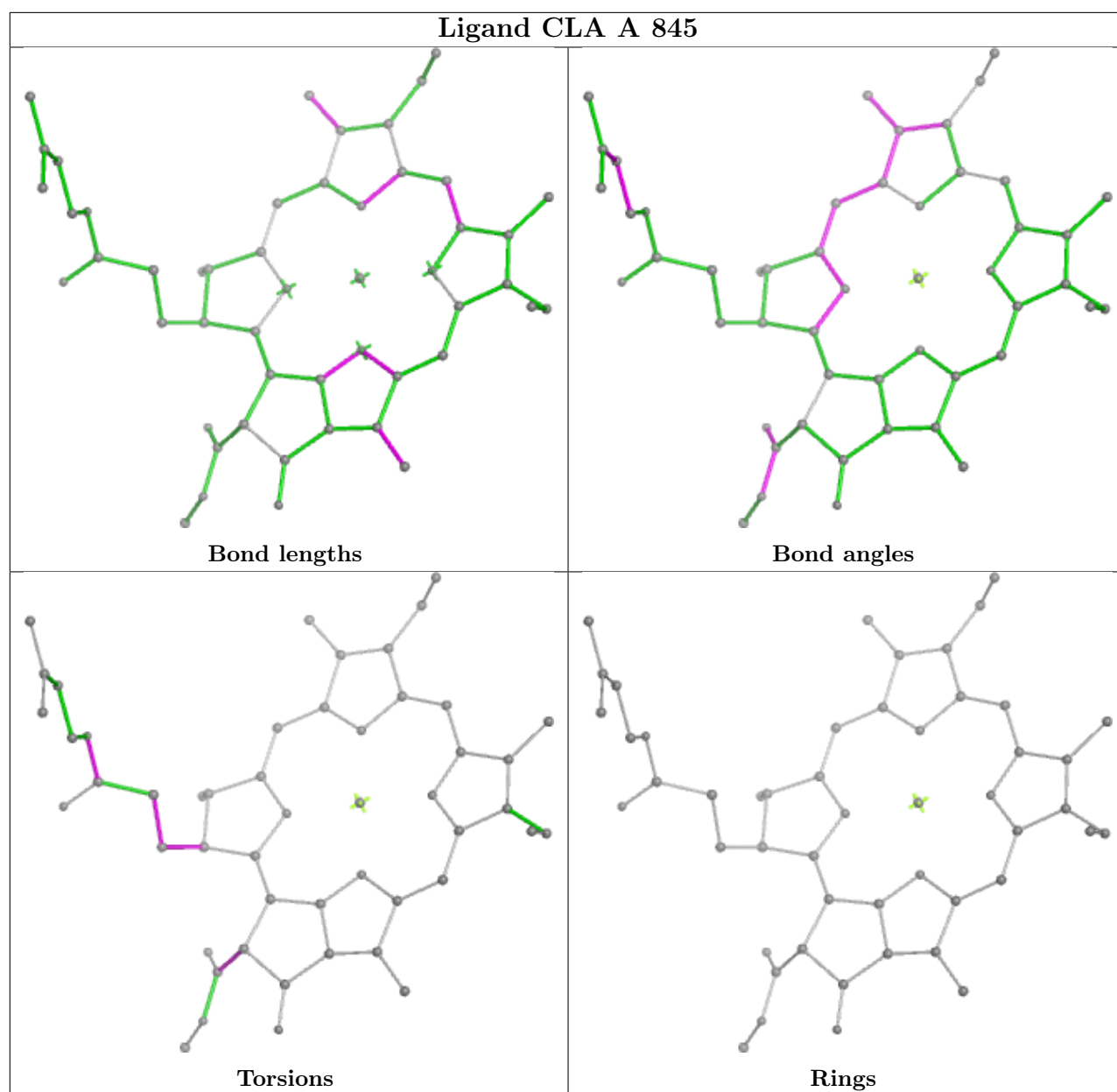
## Ligand CLA g 835



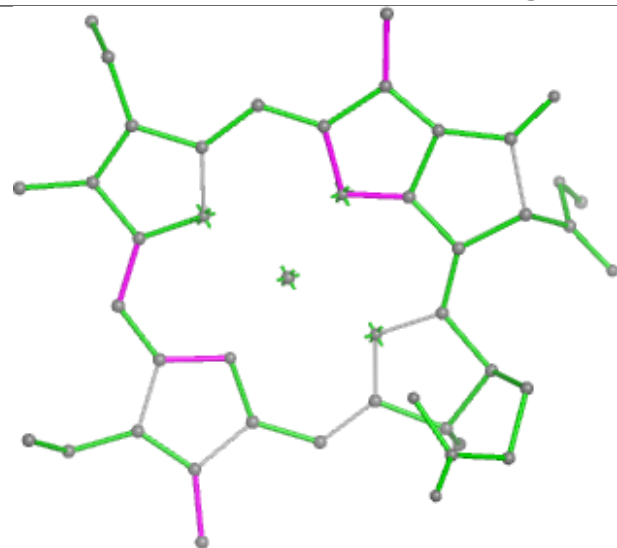




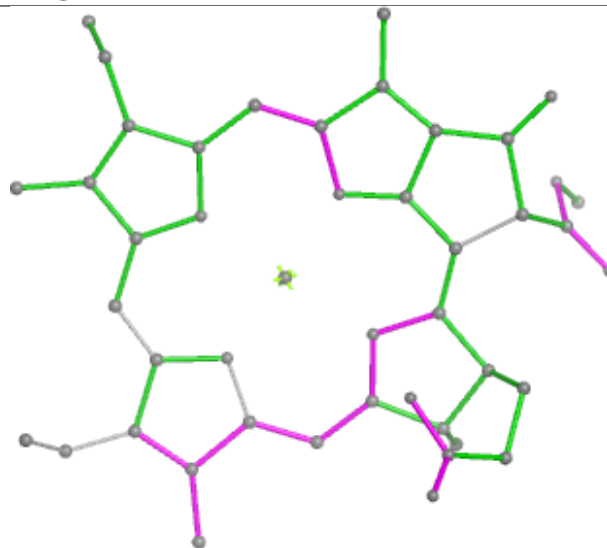




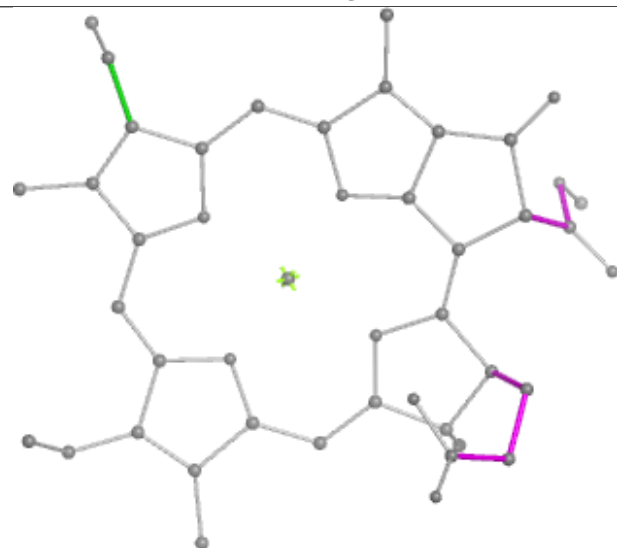
## Ligand CLA g 832



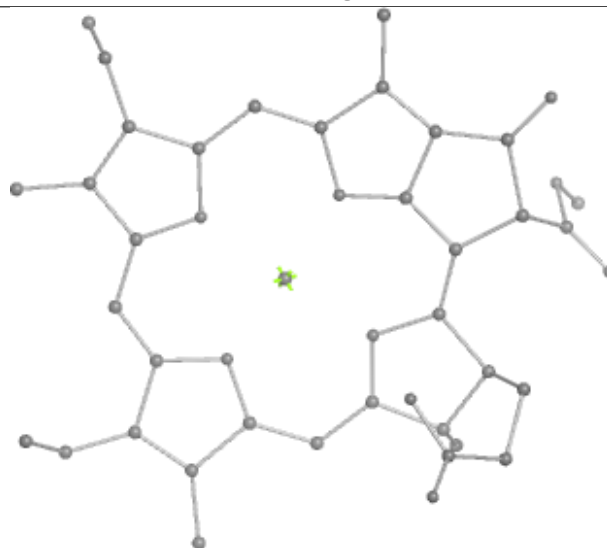
Bond lengths



Bond angles

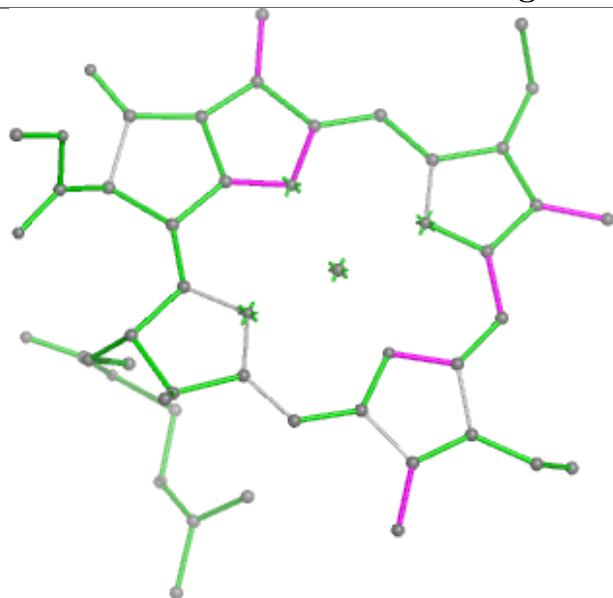


Torsions

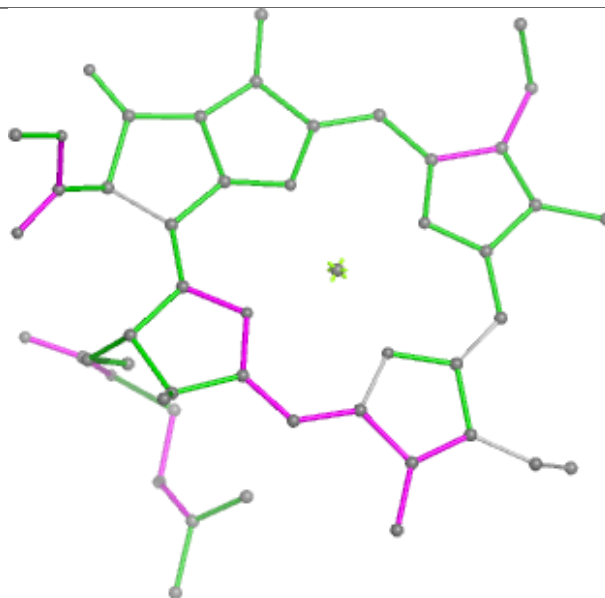


Rings

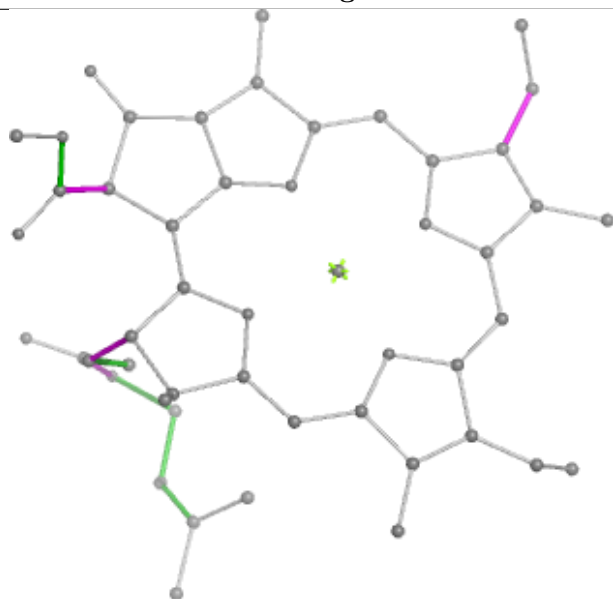
## Ligand CLA a 831



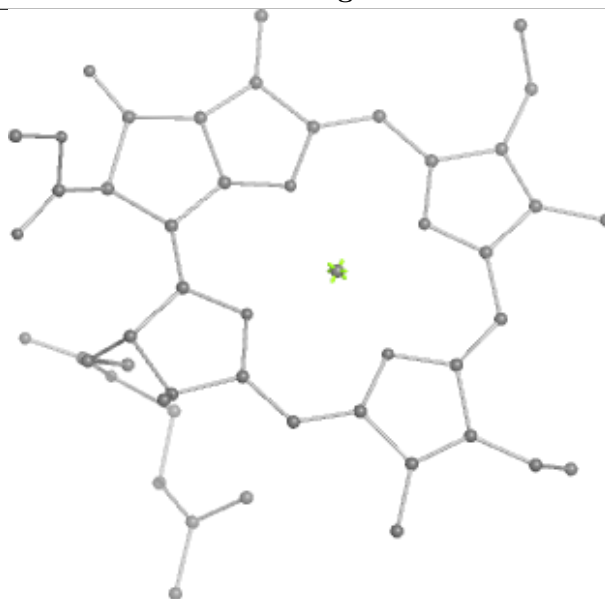
Bond lengths



Bond angles

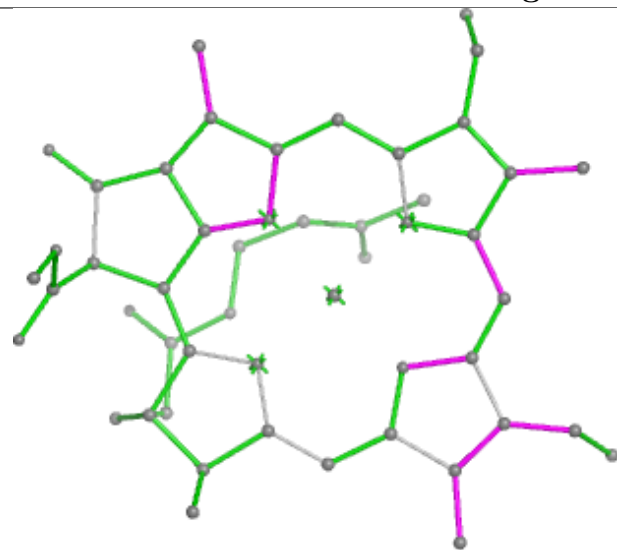


Torsions

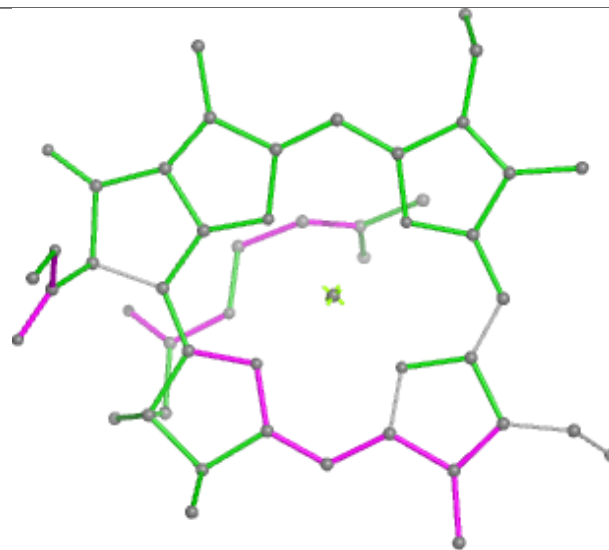


Rings

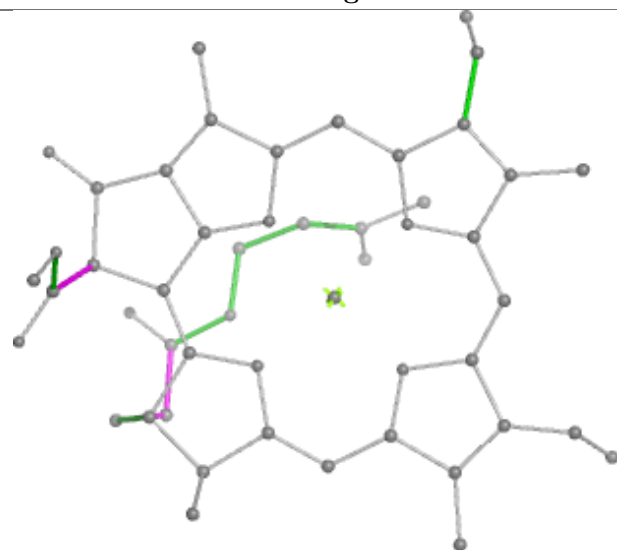
## Ligand CLA a 841



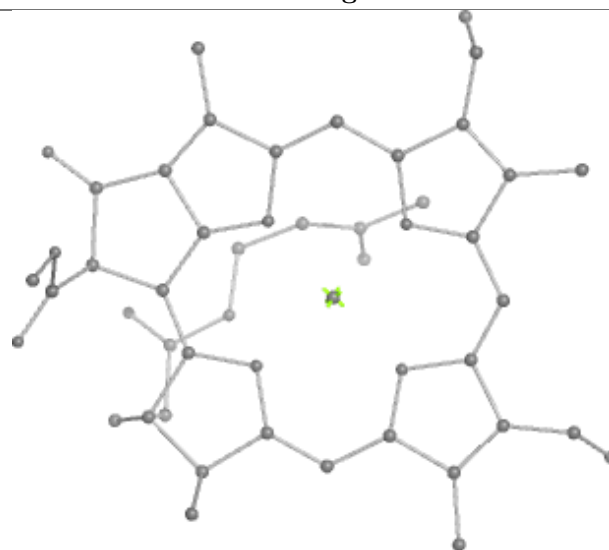
Bond lengths



Bond angles

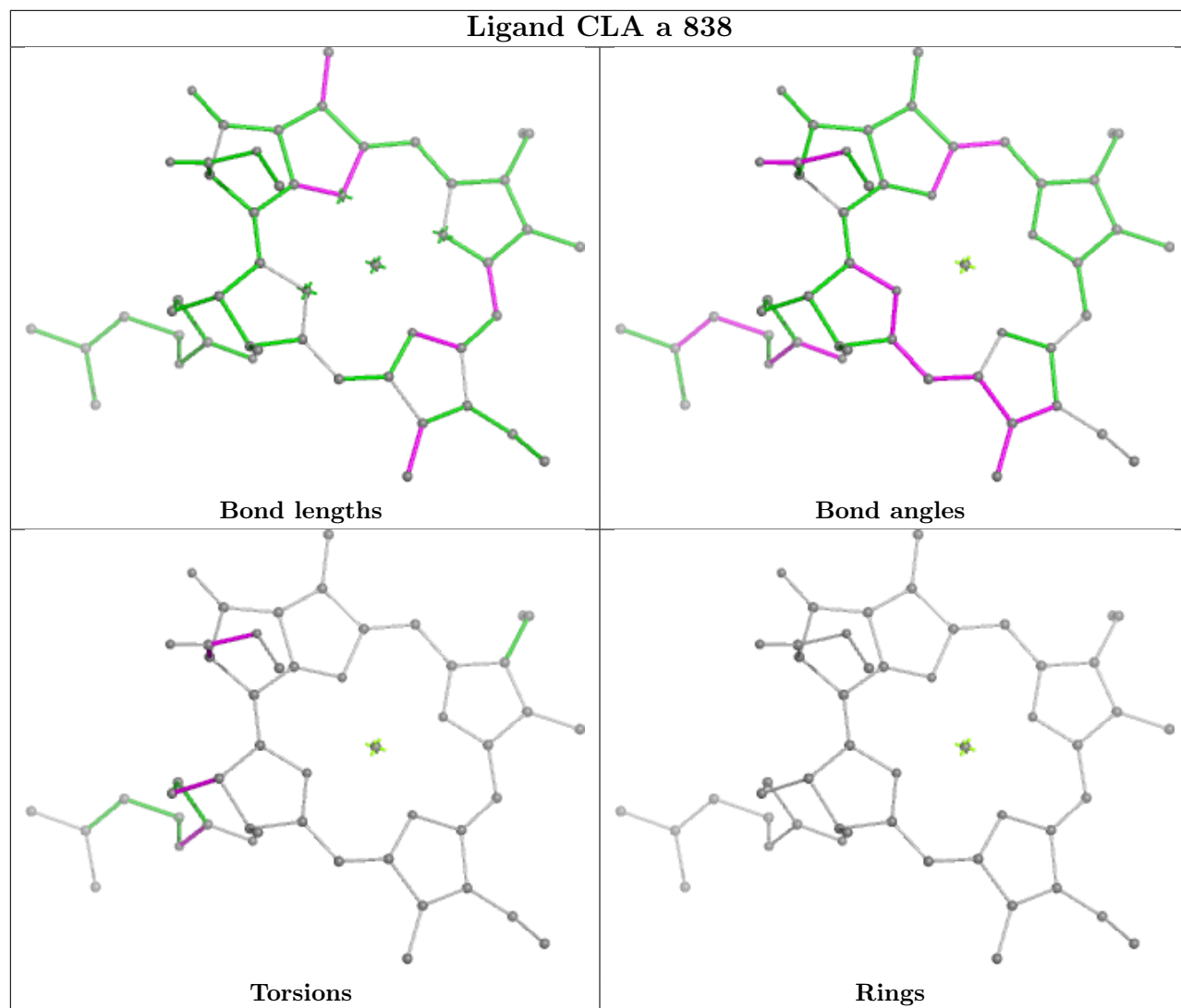


Torsions

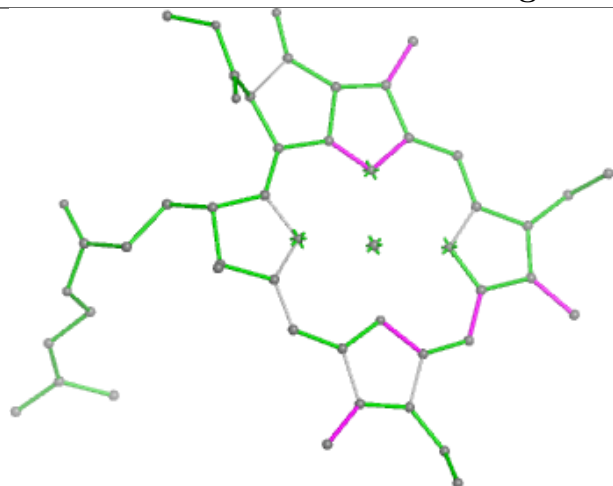


Rings

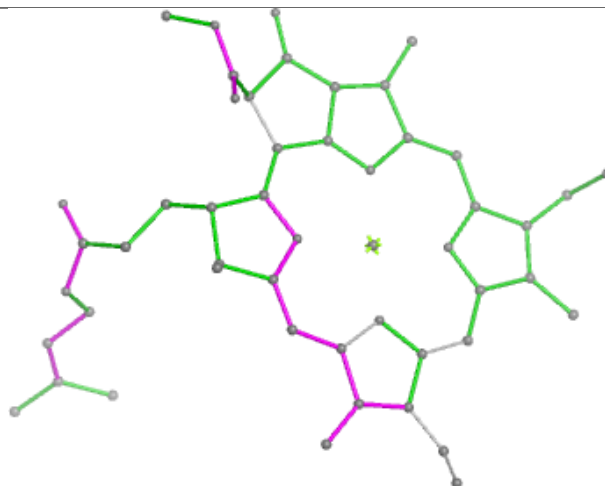
## Ligand CLA a 838



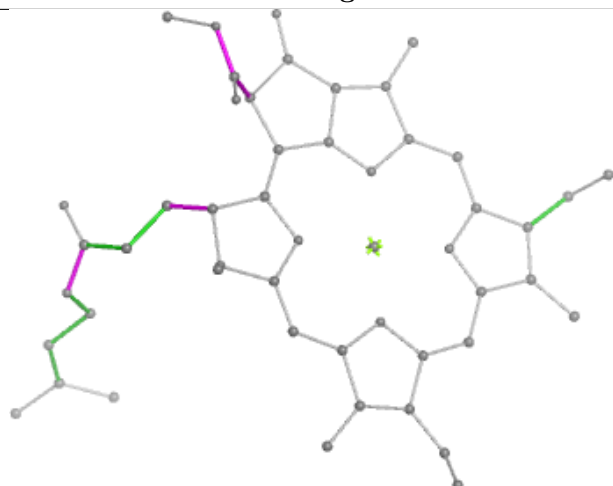
## Ligand CLA e 806



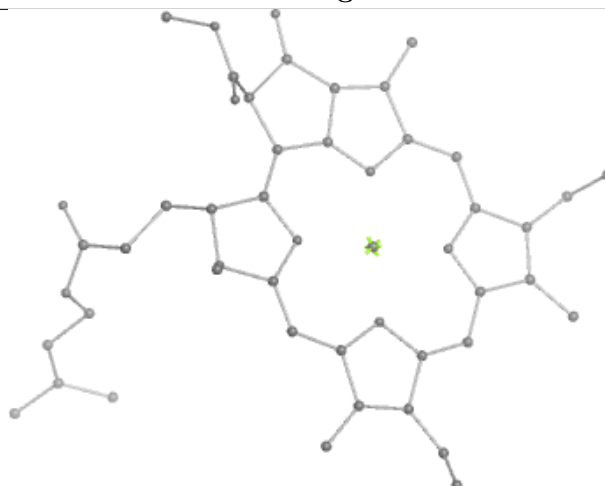
Bond lengths



Bond angles

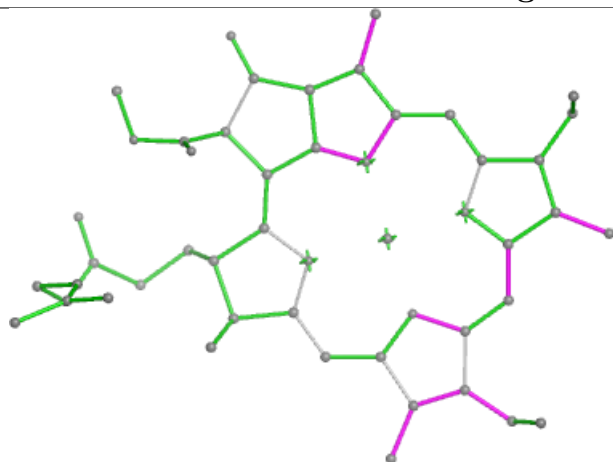


Torsions

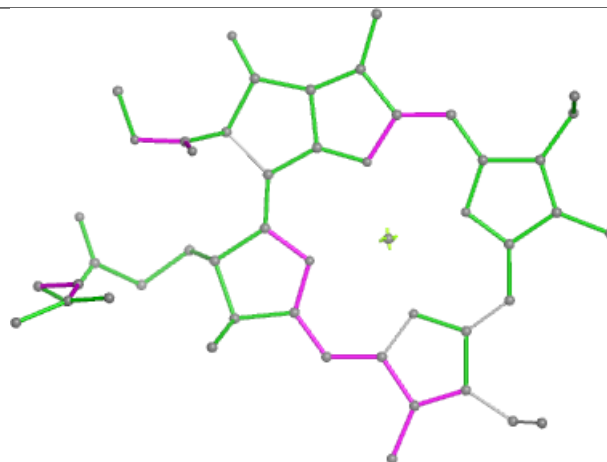


Rings

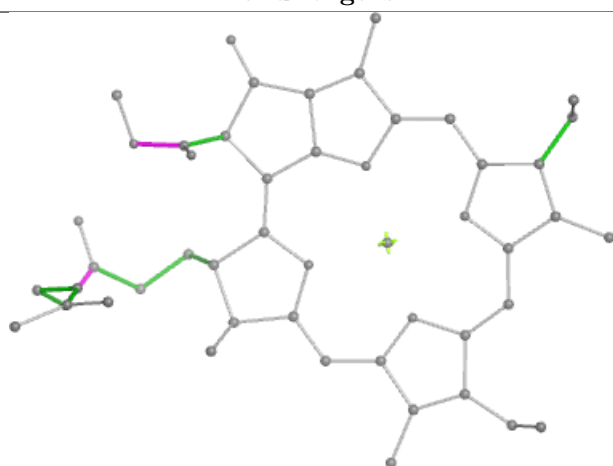
## Ligand CLA b 807



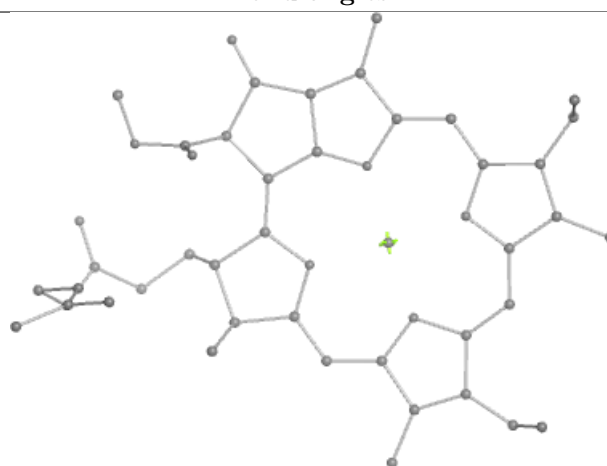
Bond lengths



Bond angles

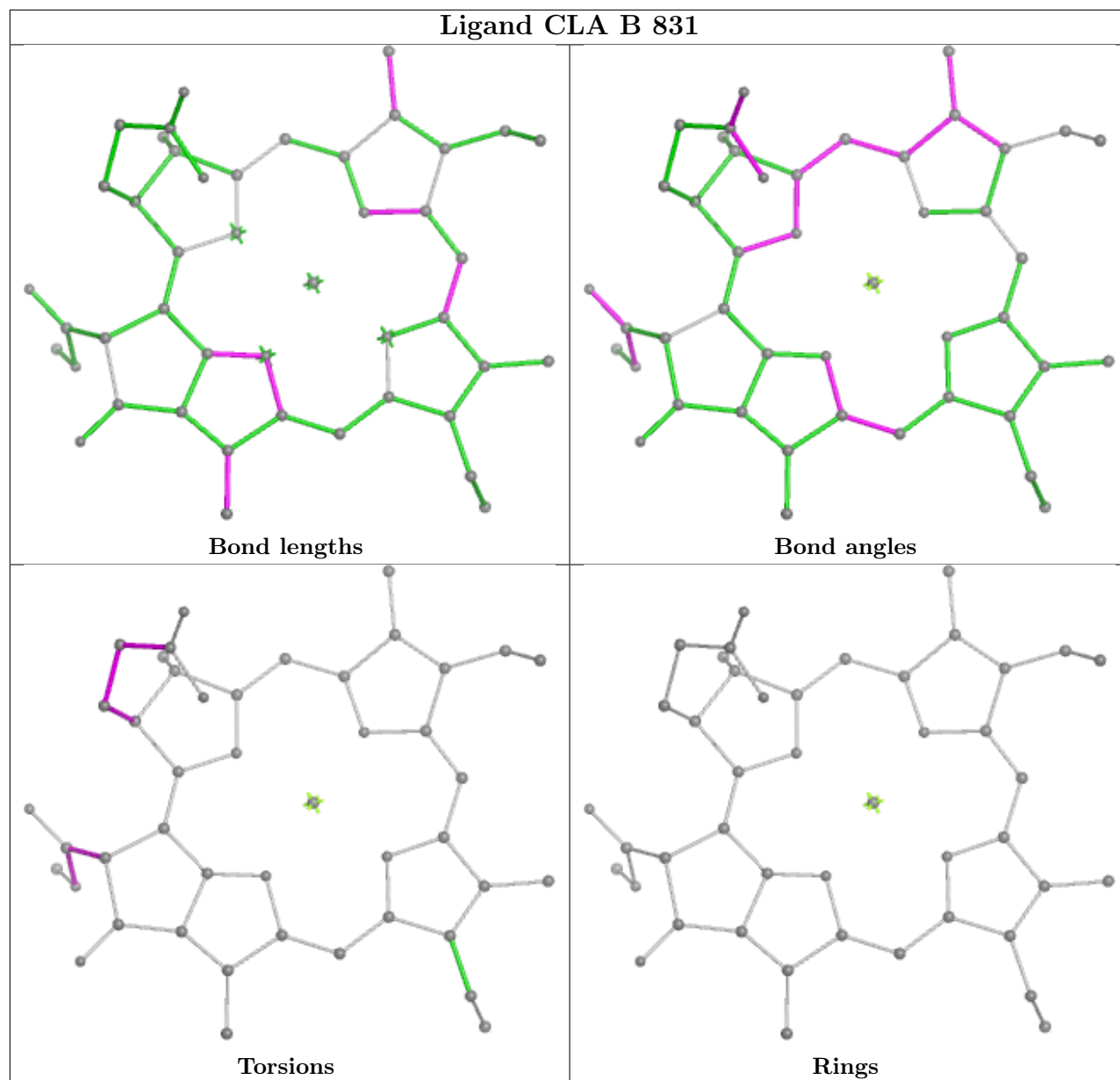


Torsions



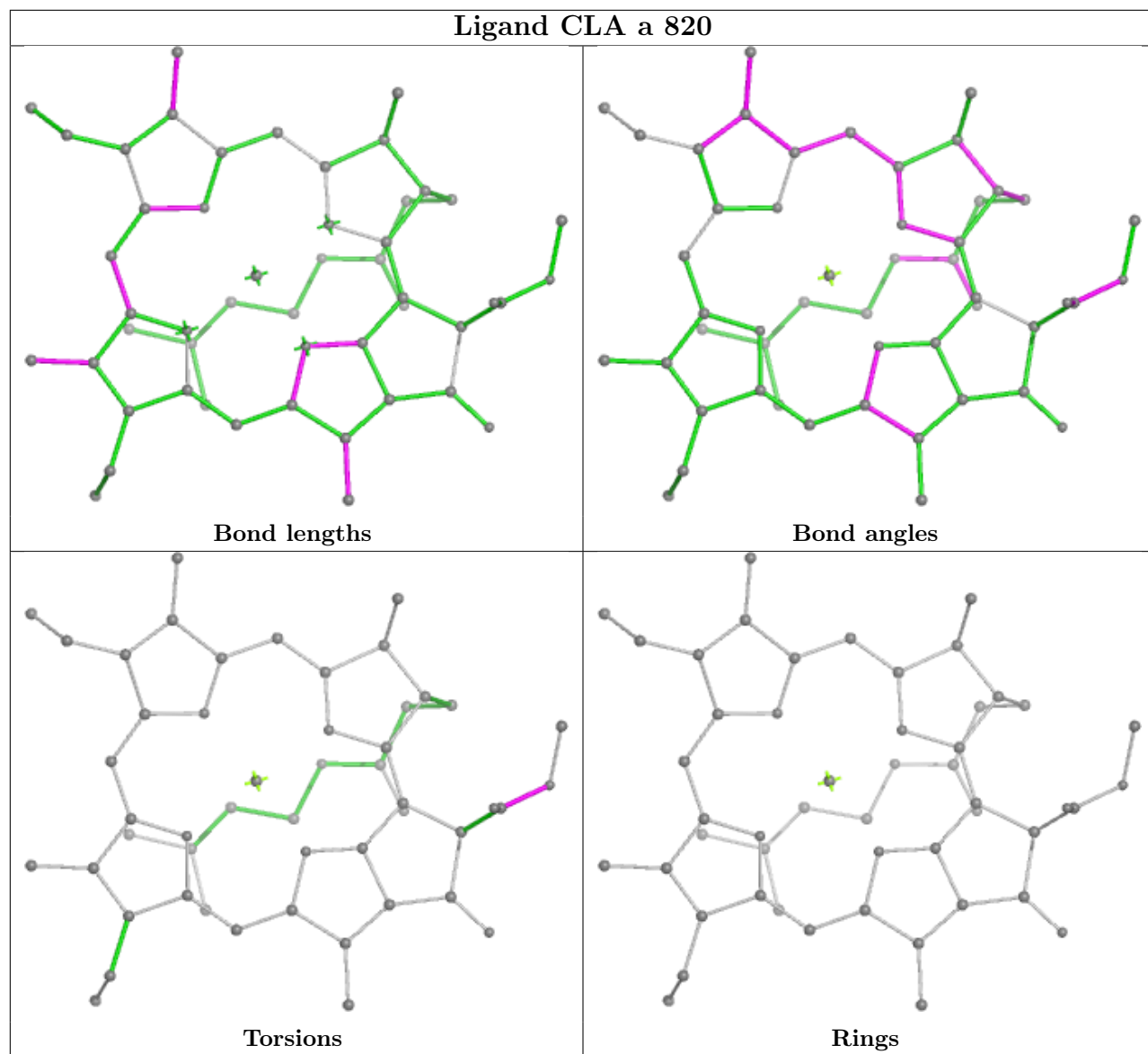
Rings

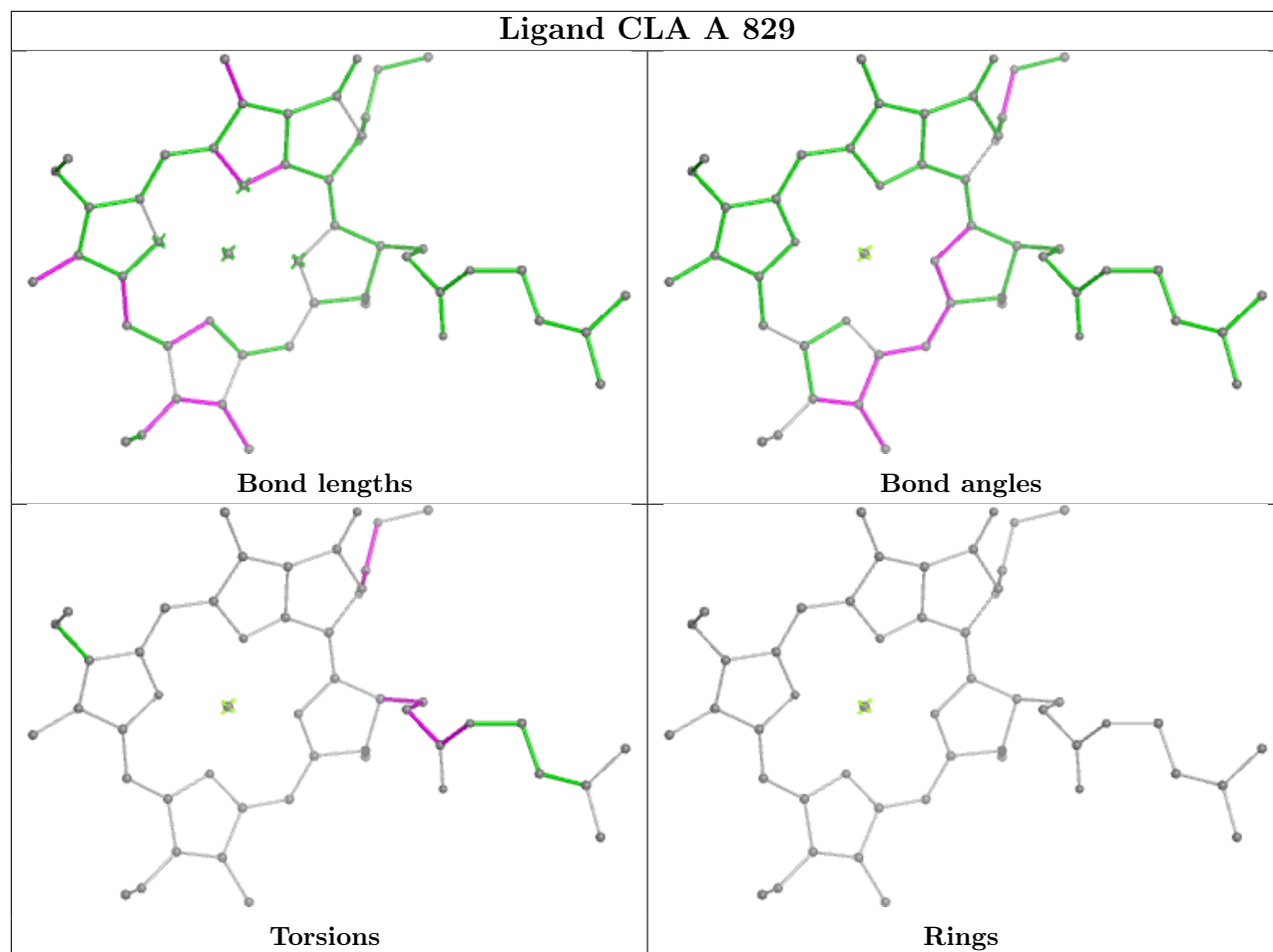
## Ligand CLA B 831

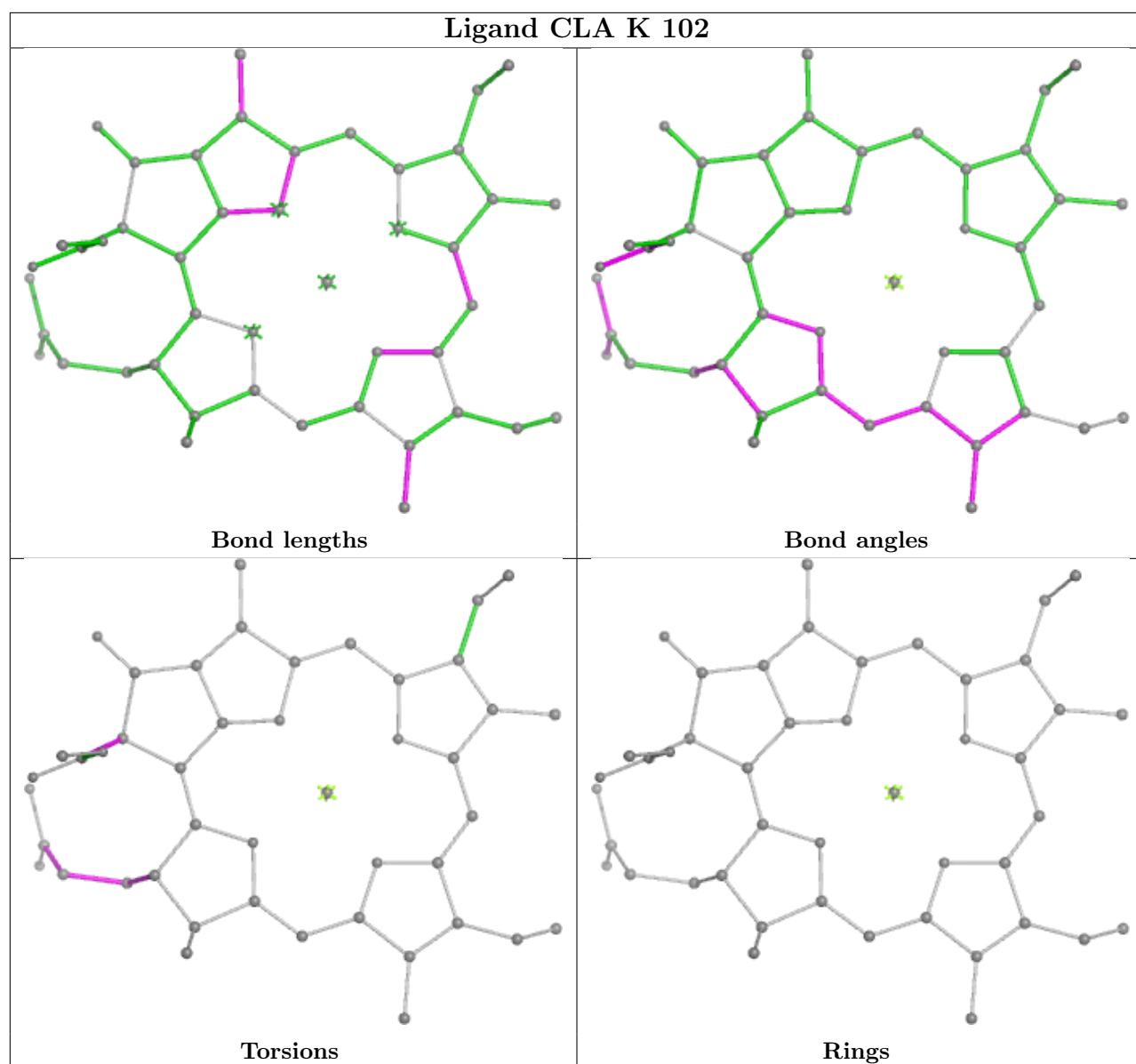


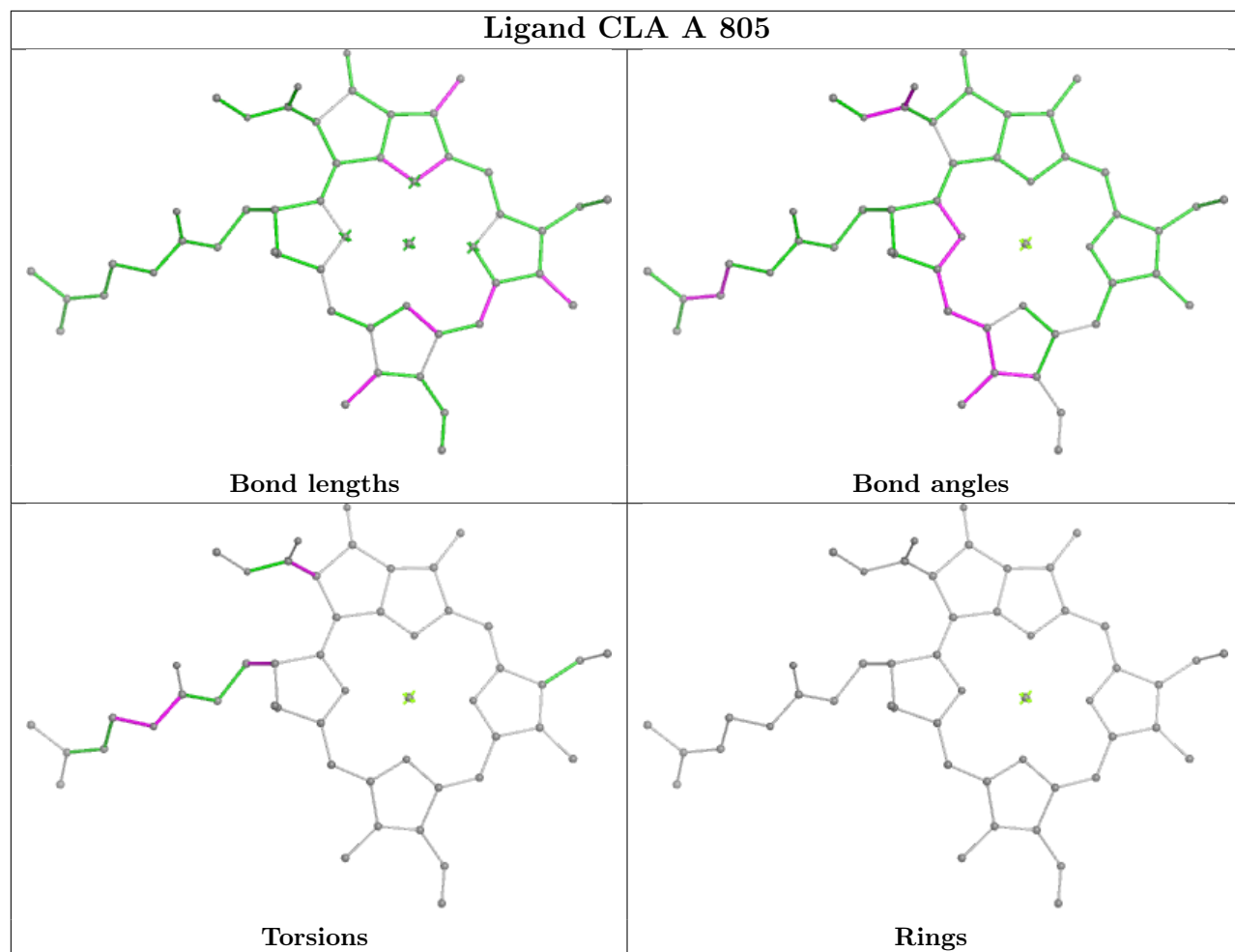


## Ligand CLA a 820

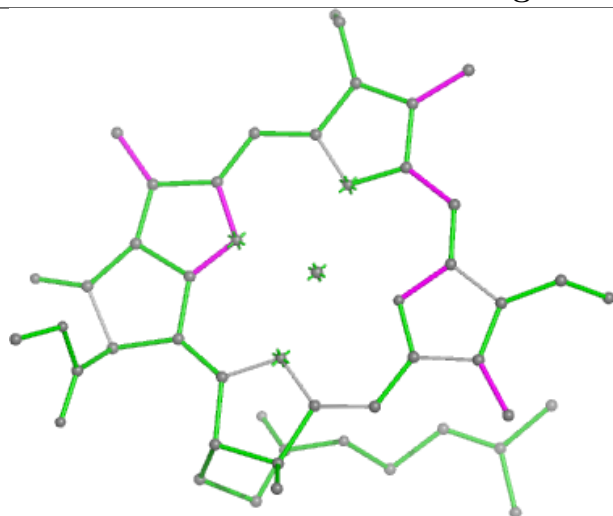




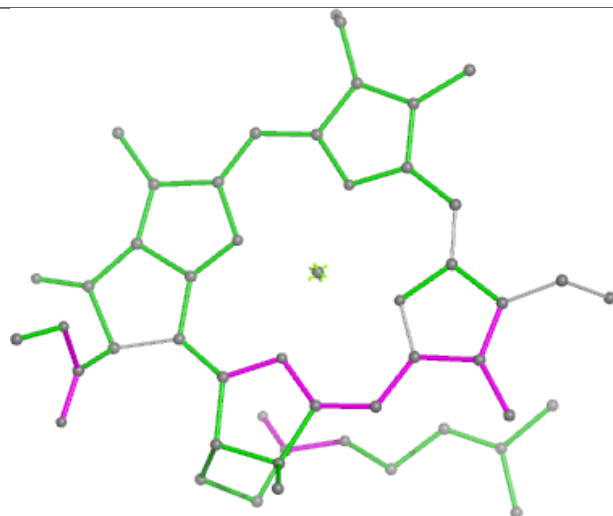




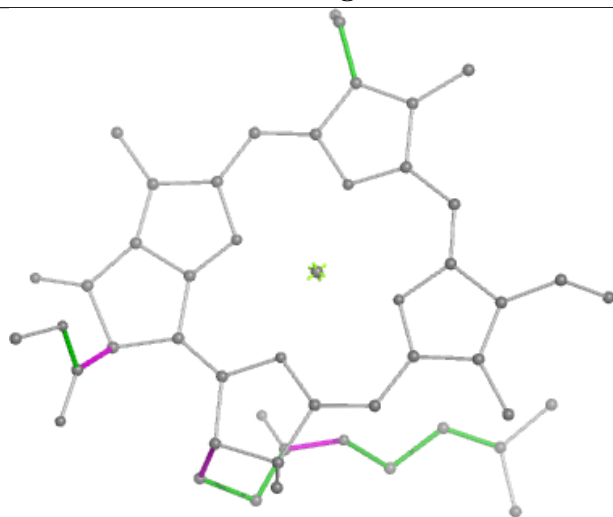
## Ligand CLA G 819



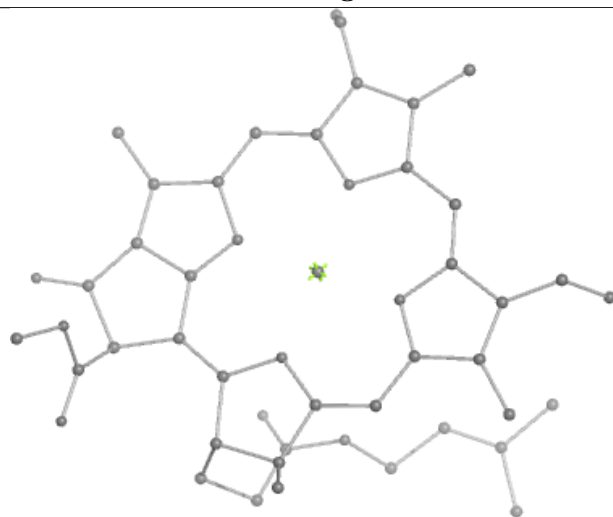
Bond lengths



Bond angles

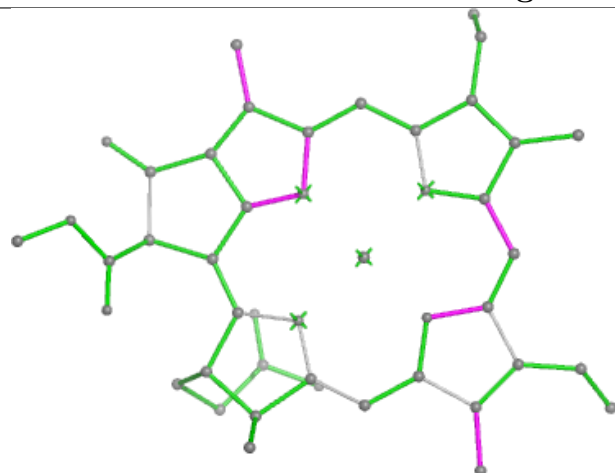


Torsions

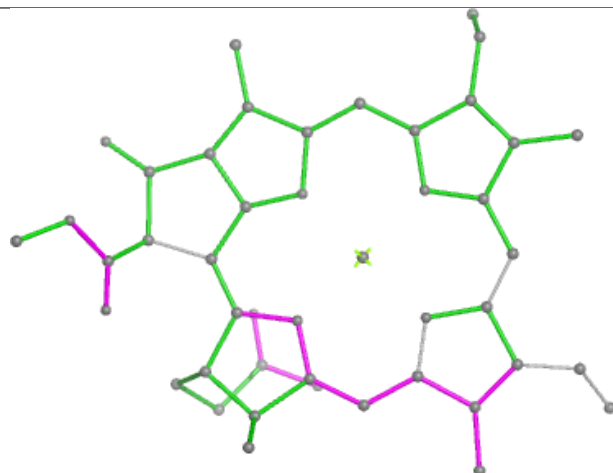


Rings

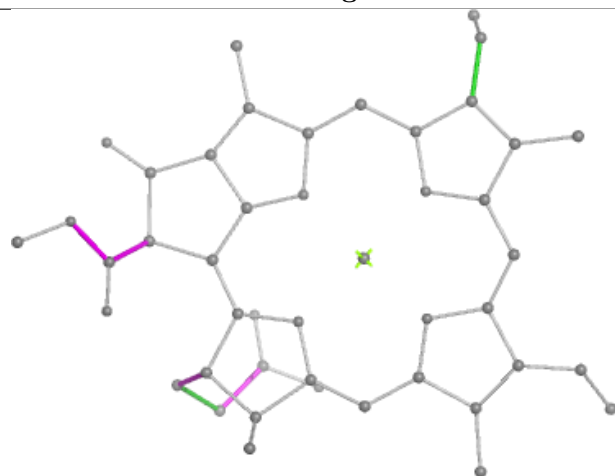
## Ligand CLA B 836



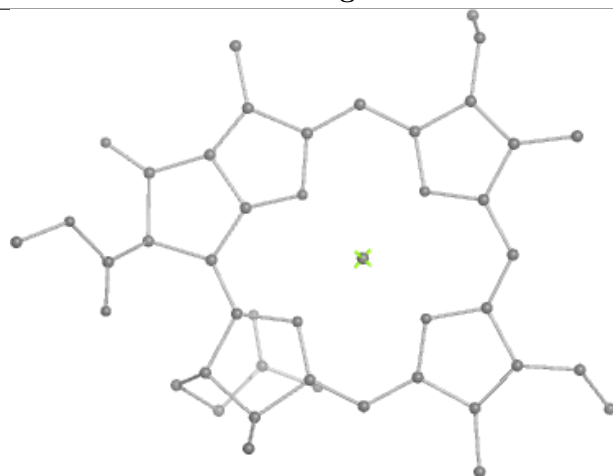
Bond lengths



Bond angles

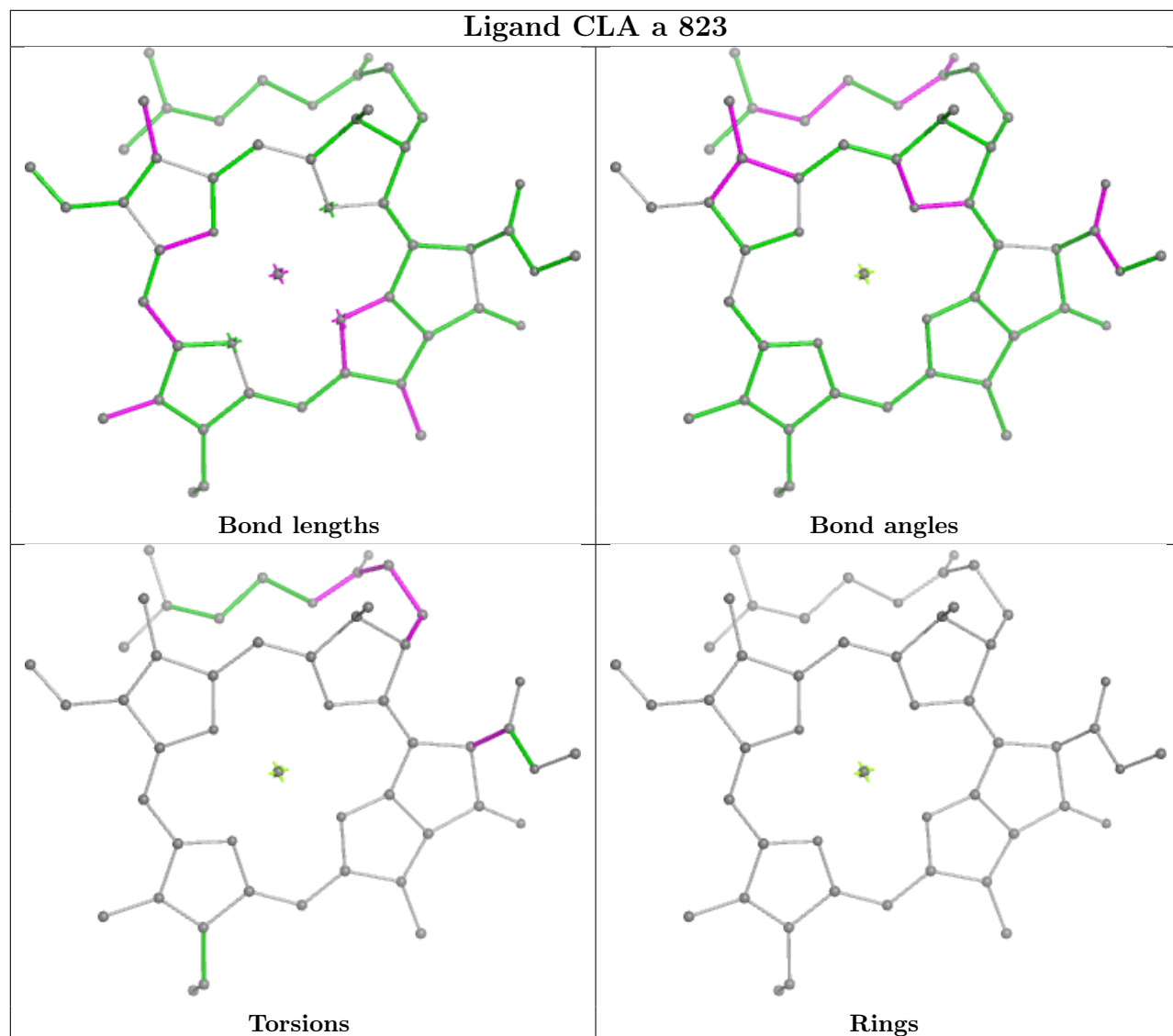


Torsions

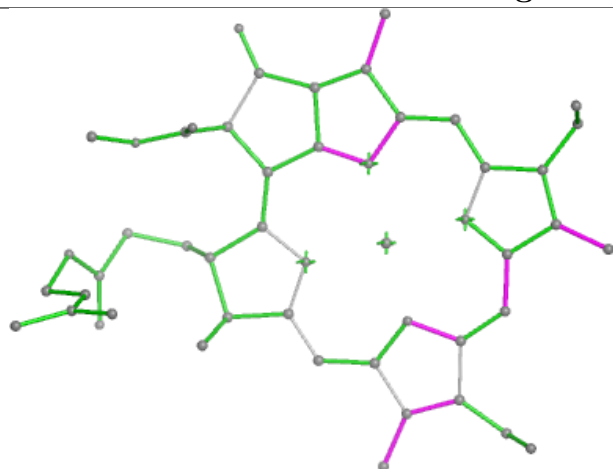


Rings

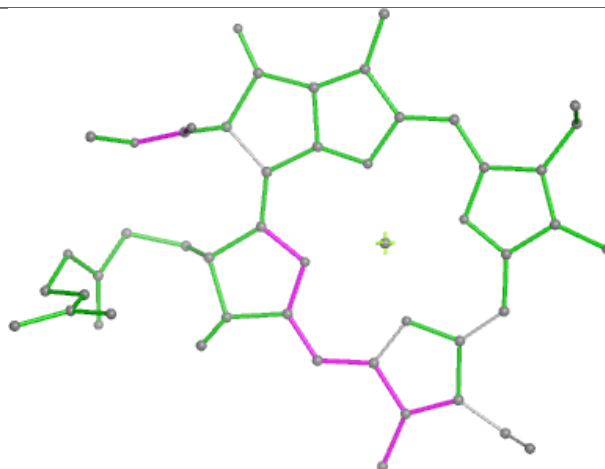
## Ligand CLA a 823



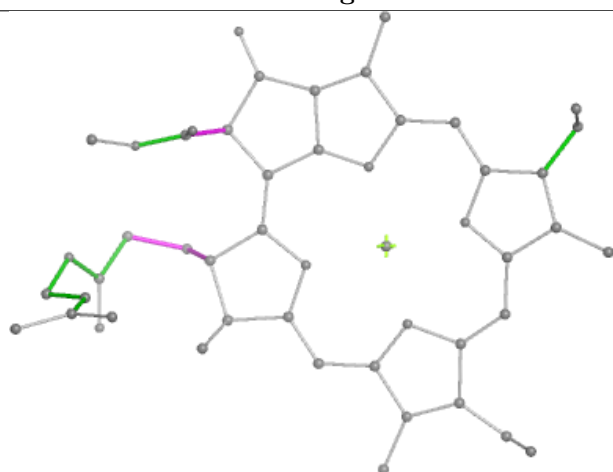
## Ligand CLA E 809



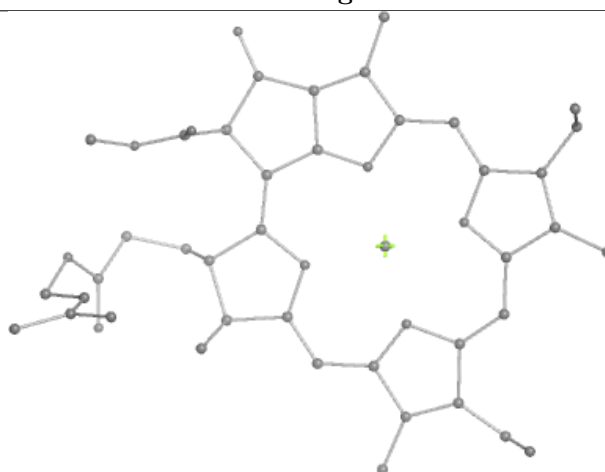
Bond lengths



Bond angles

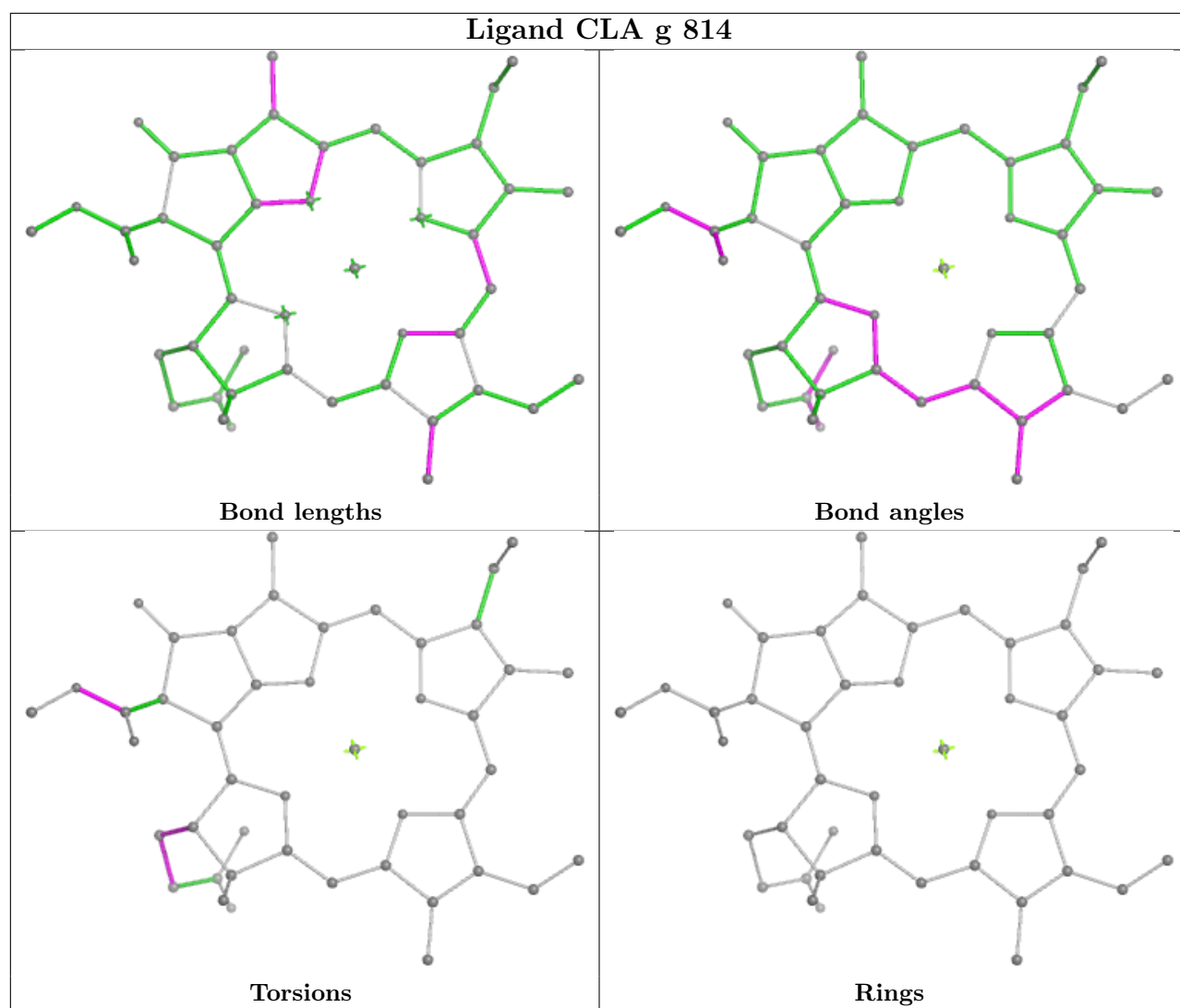


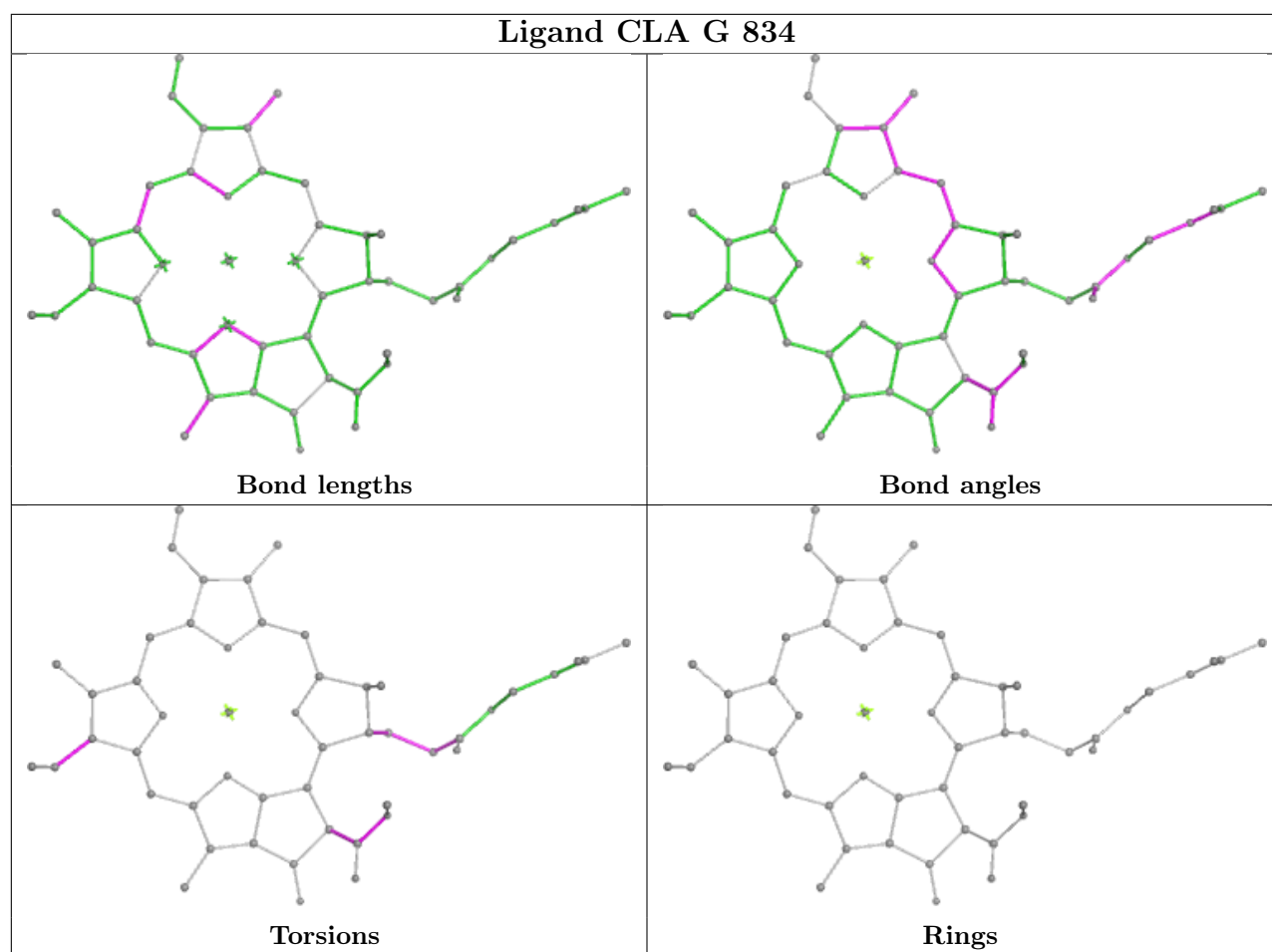
Torsions



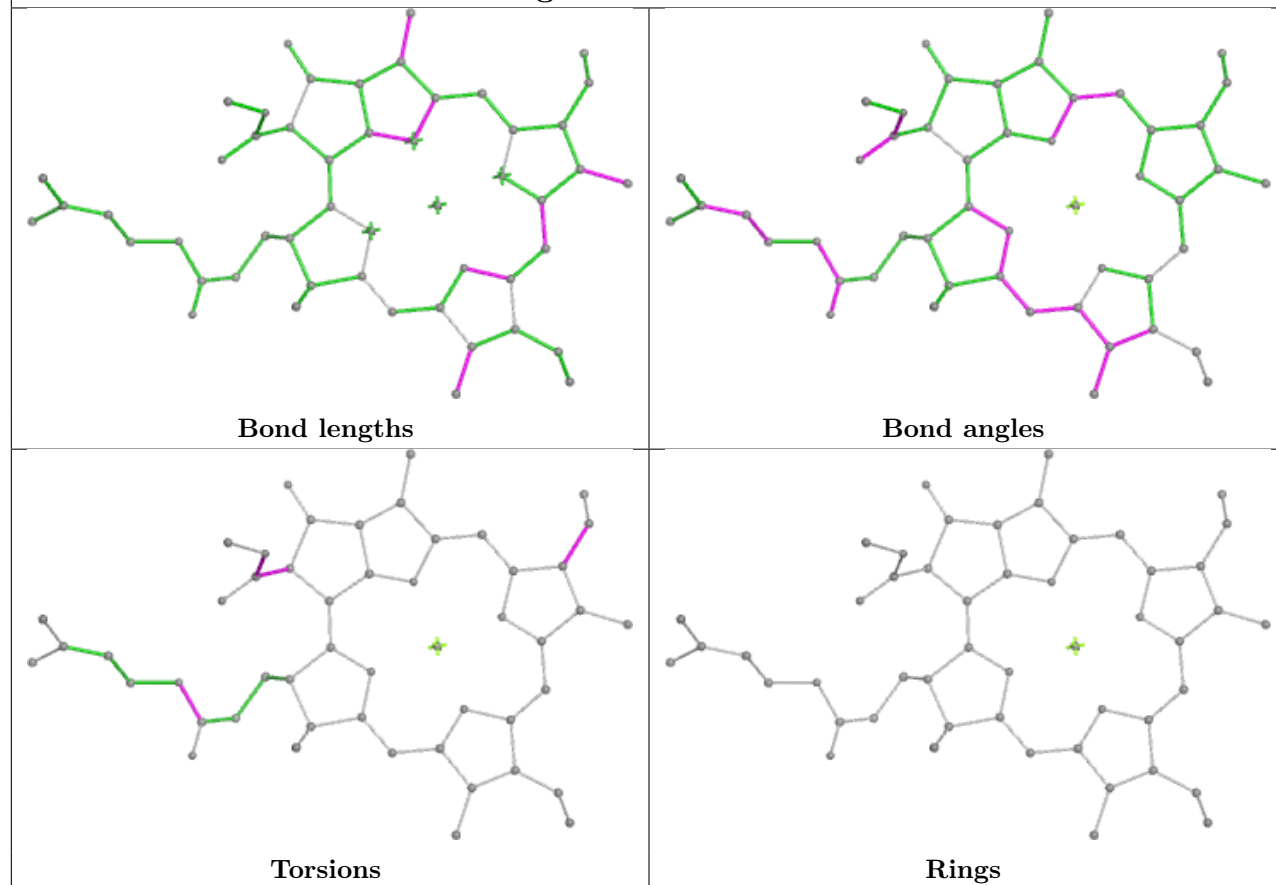
Rings



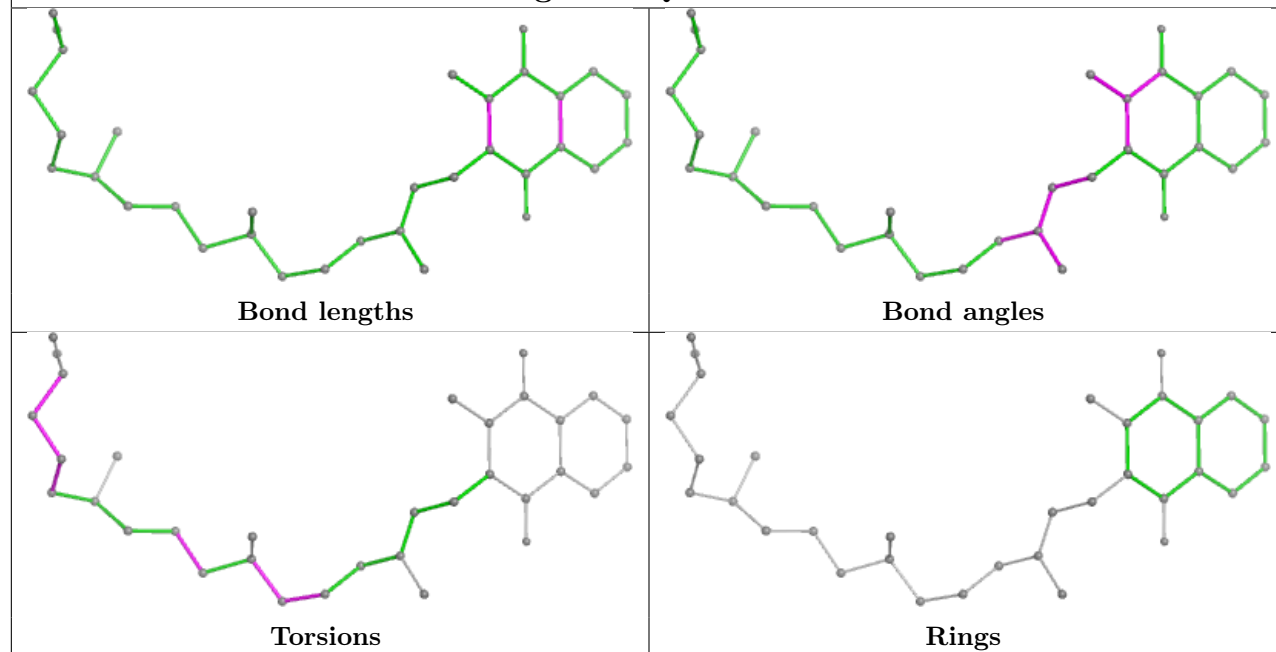




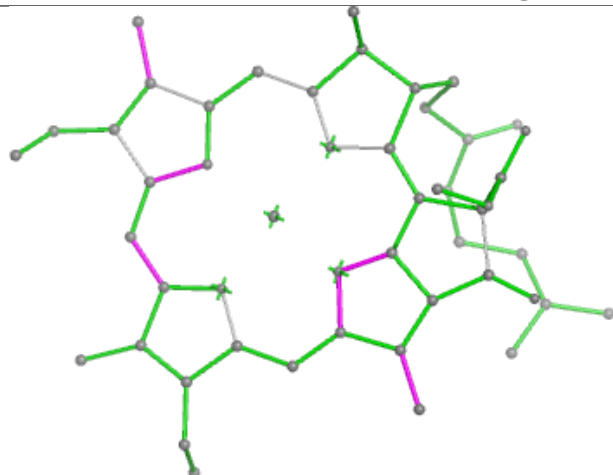
## Ligand CLA a 806



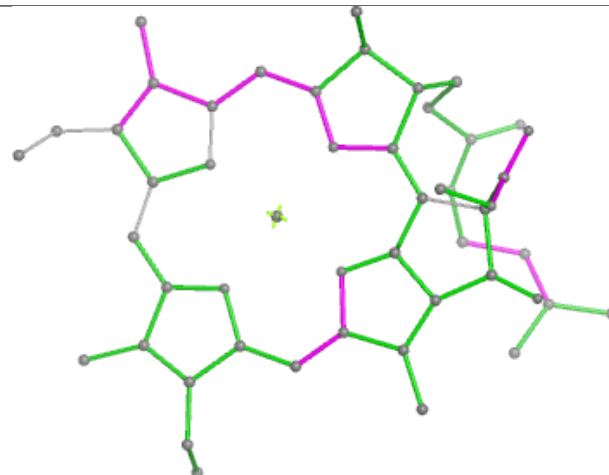
## Ligand PQN e 845



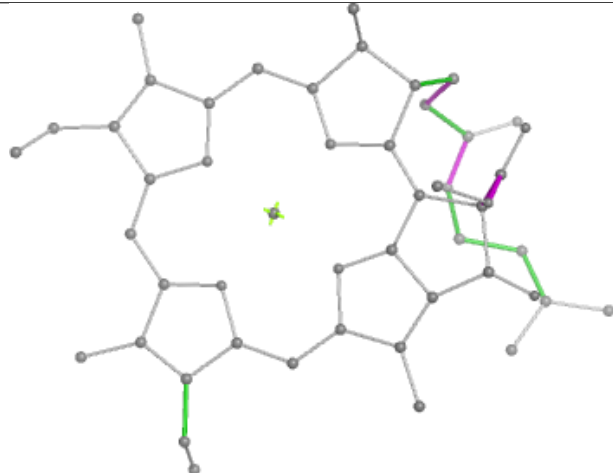
## Ligand CLA E 810



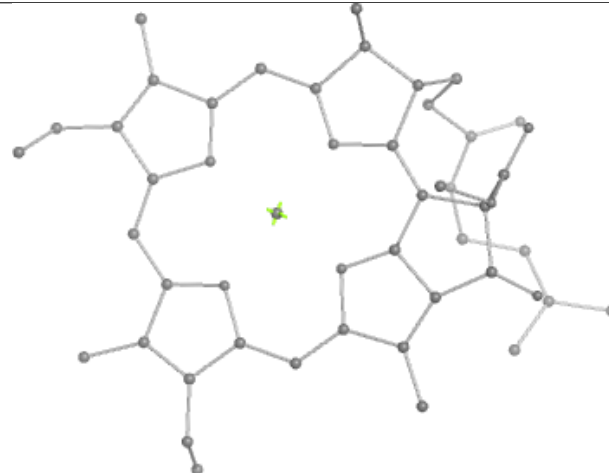
Bond lengths



Bond angles

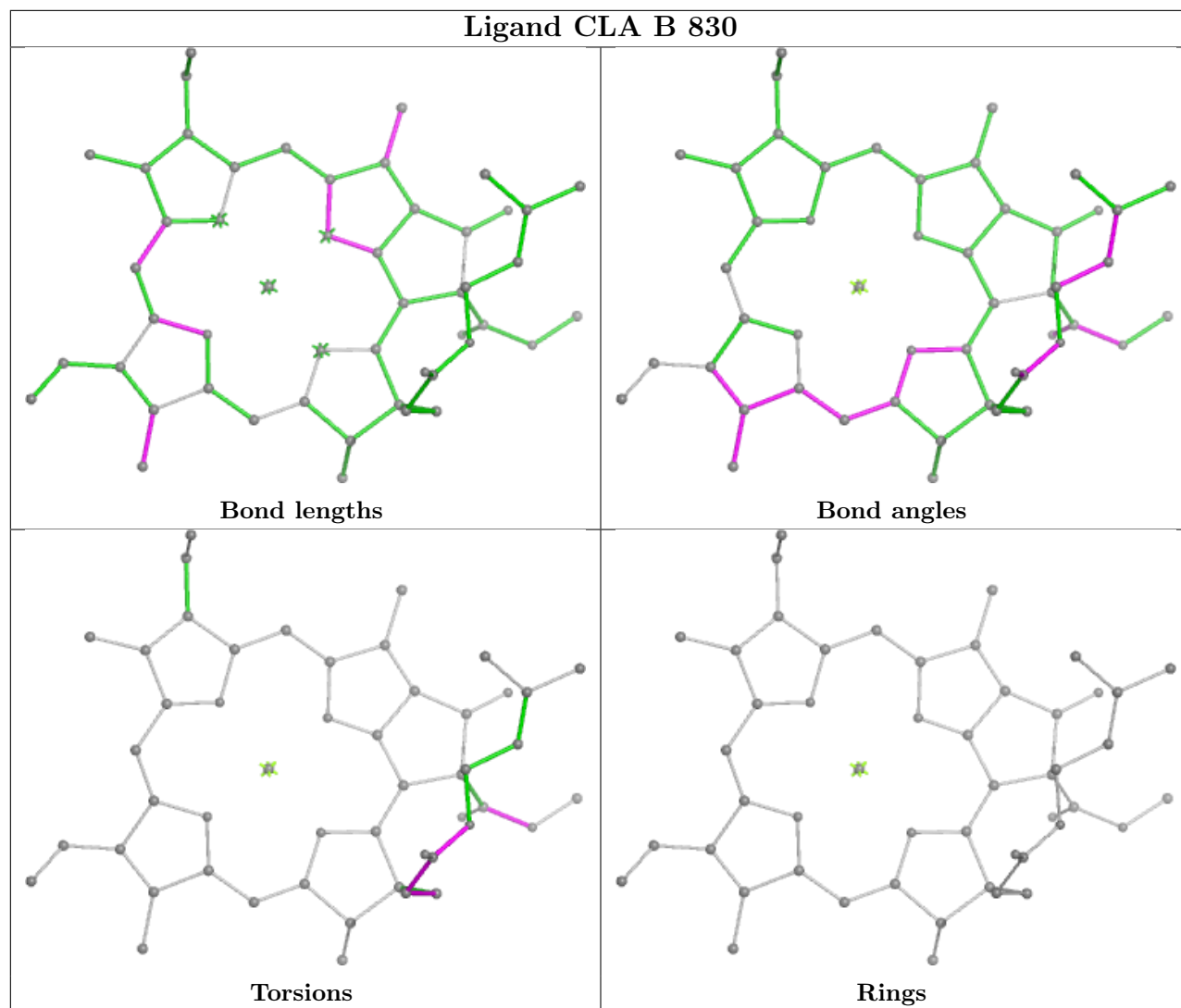


Torsions

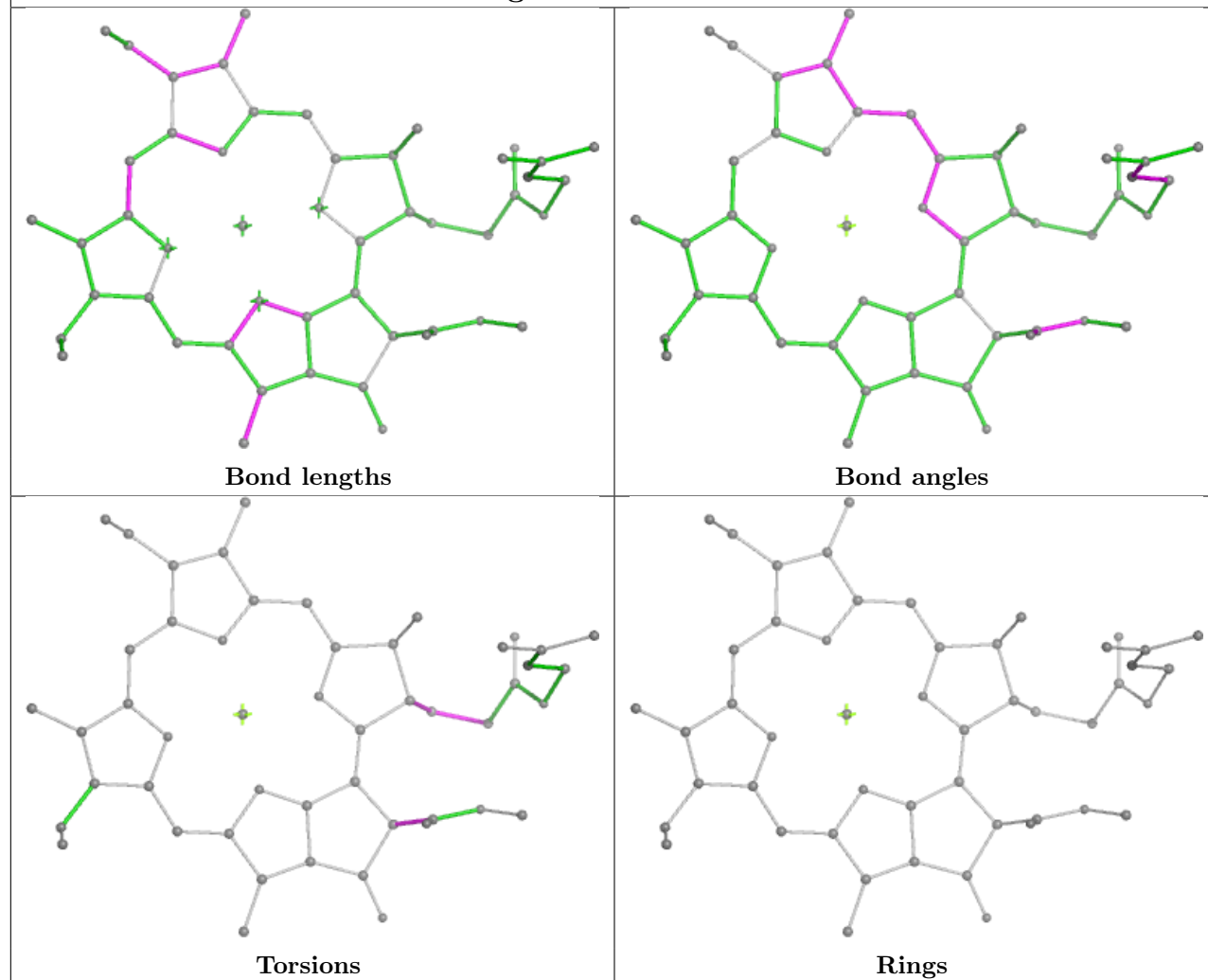


Rings

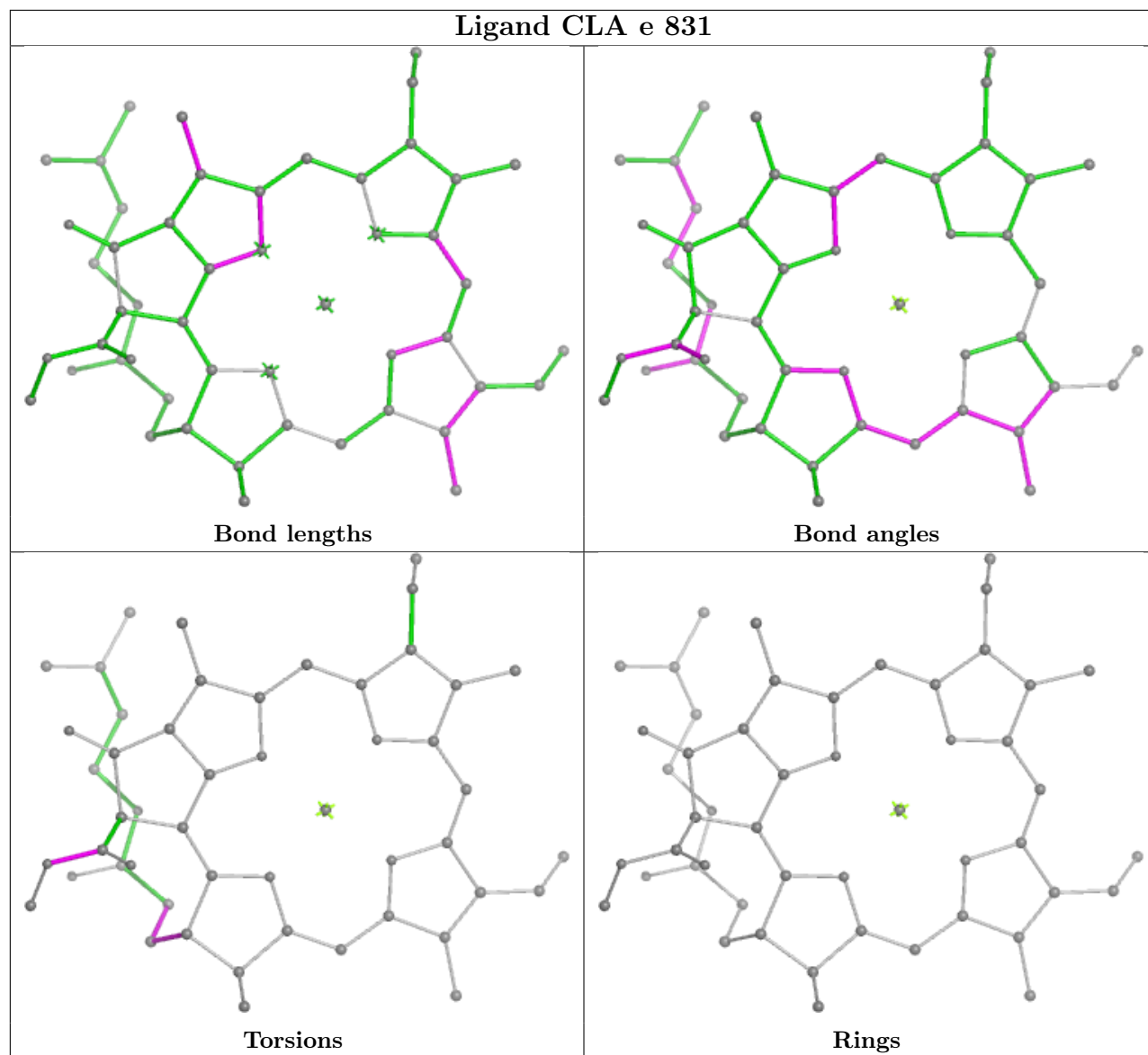
## Ligand CLA B 830



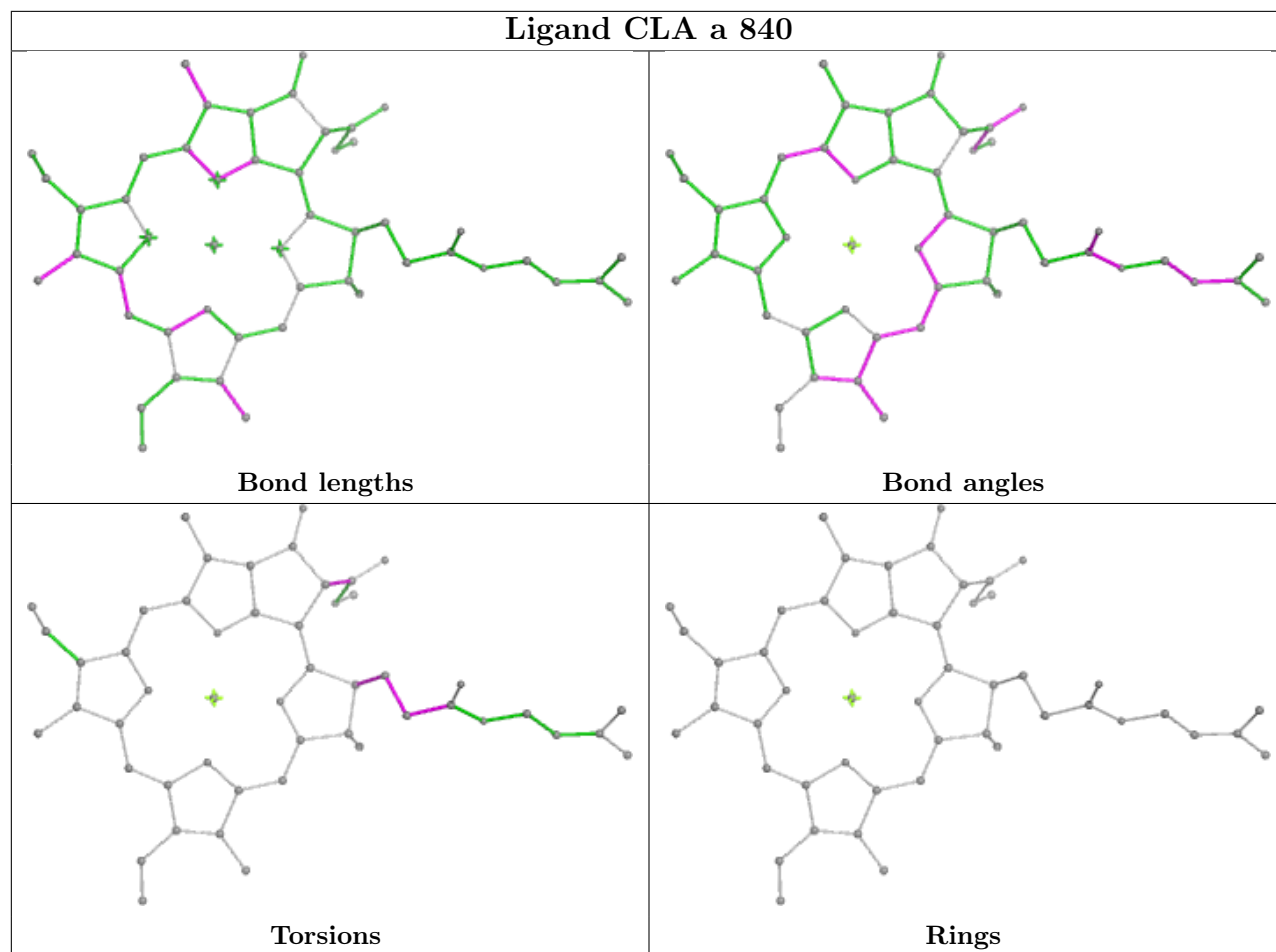
## Ligand CLA a 809



## Ligand CLA e 831

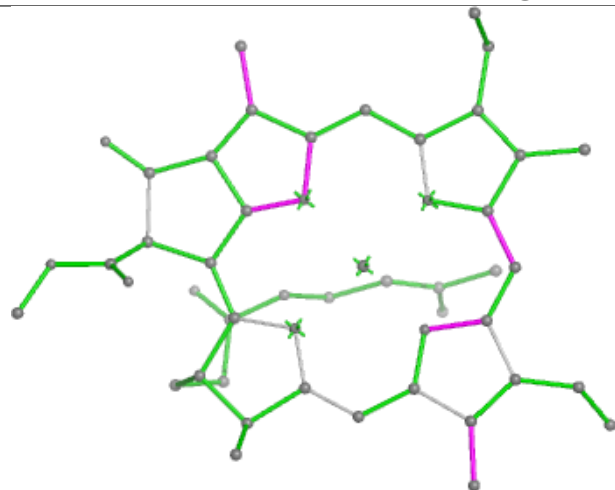


## Ligand CLA a 840

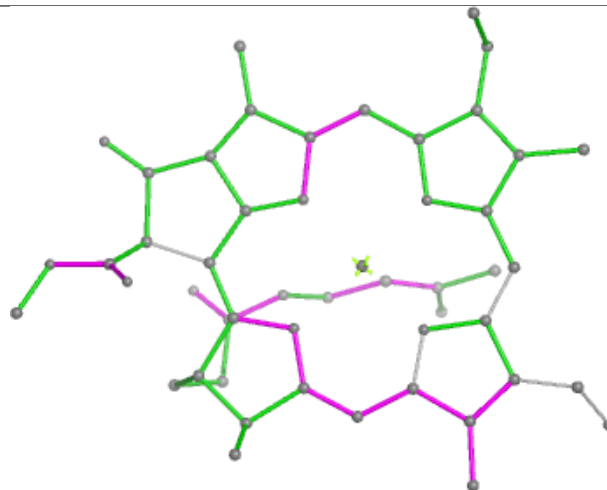




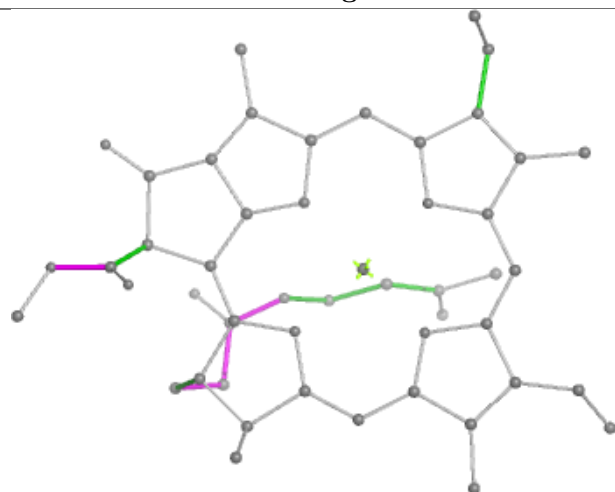
## Ligand CLA B 838



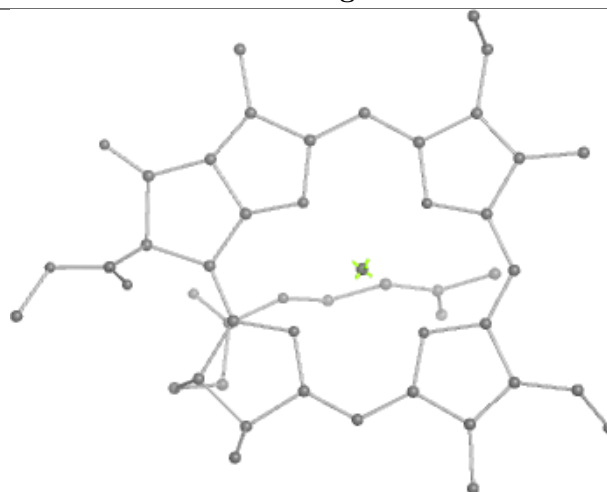
Bond lengths



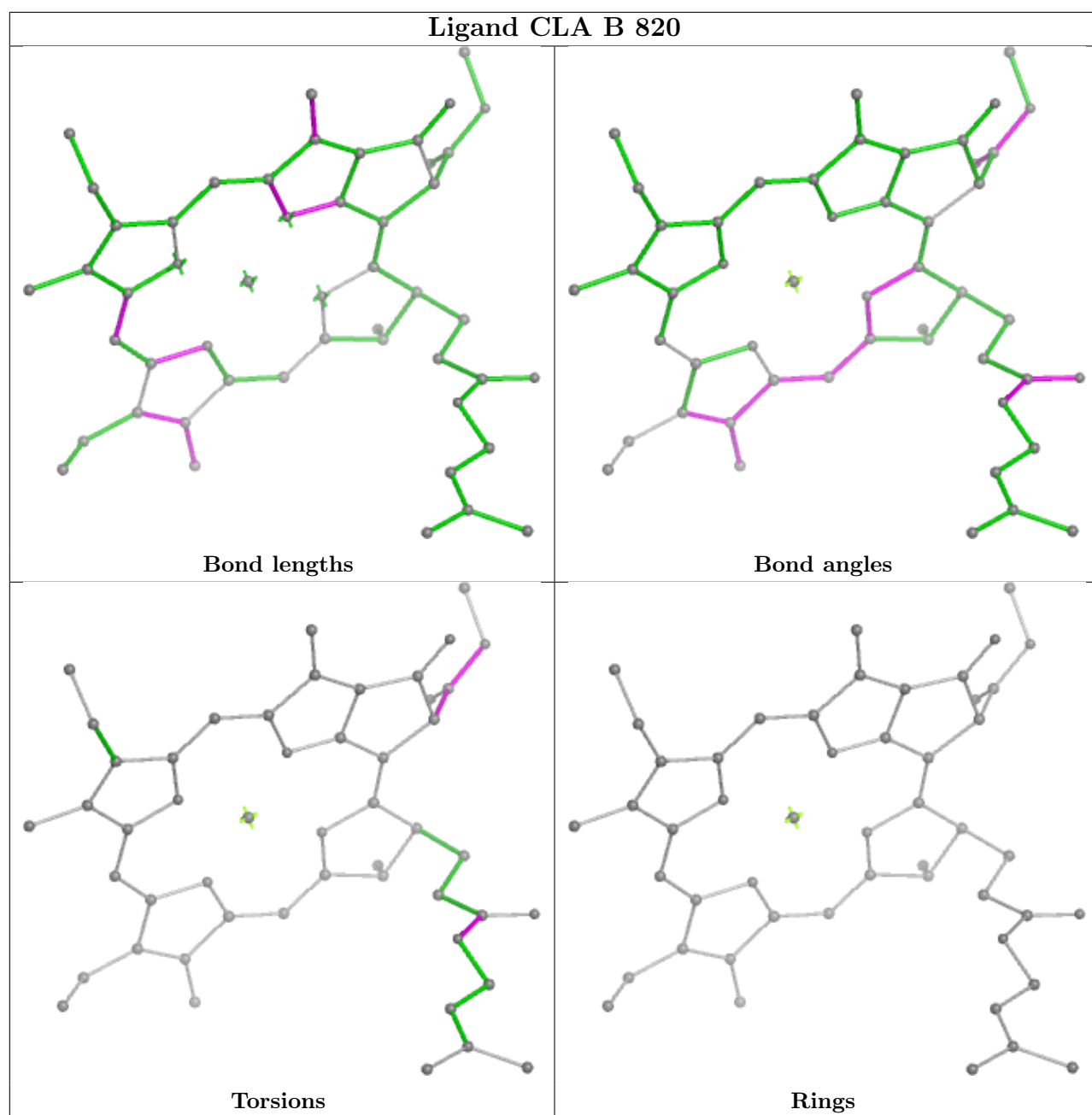
Bond angles



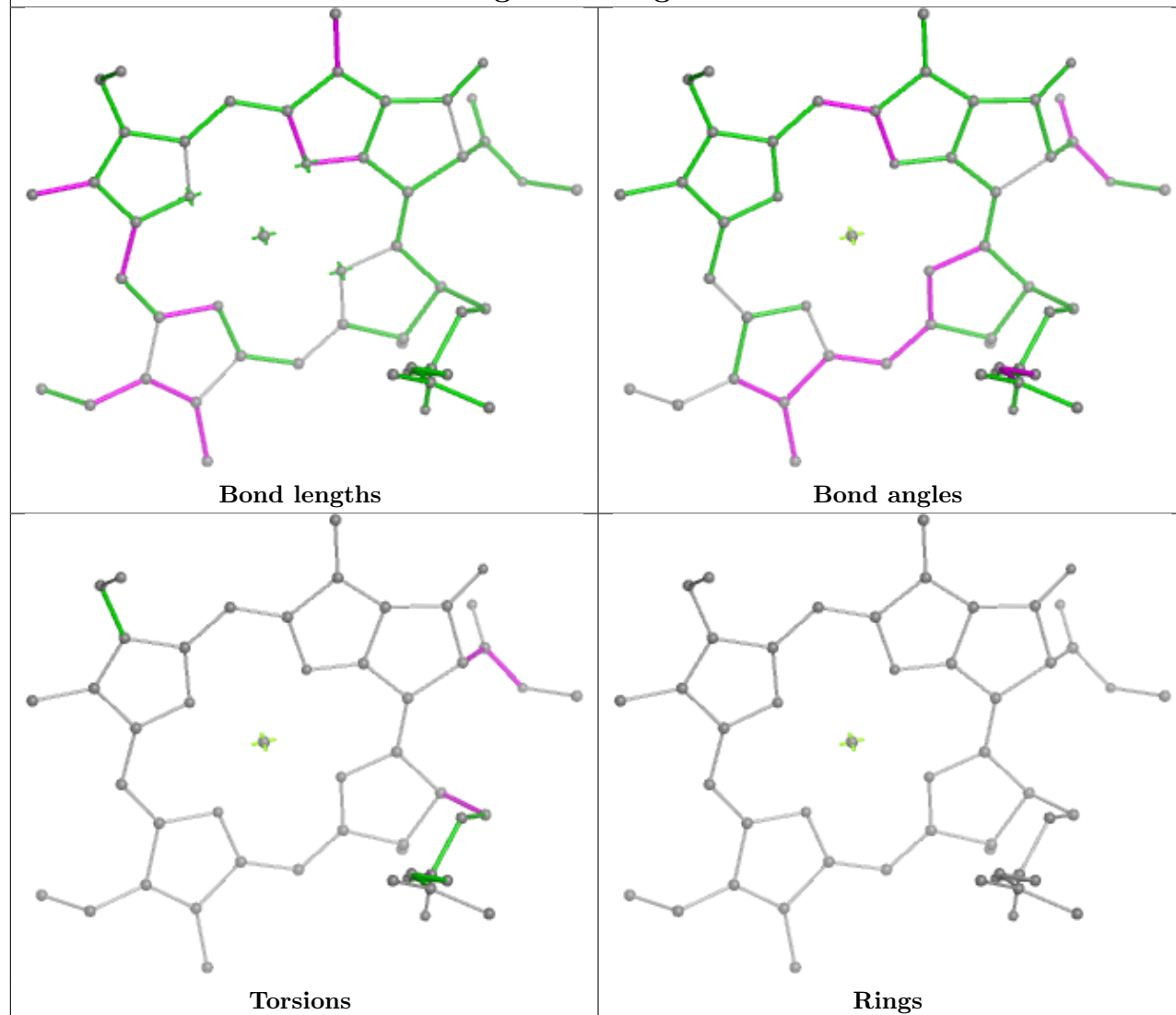
Torsions



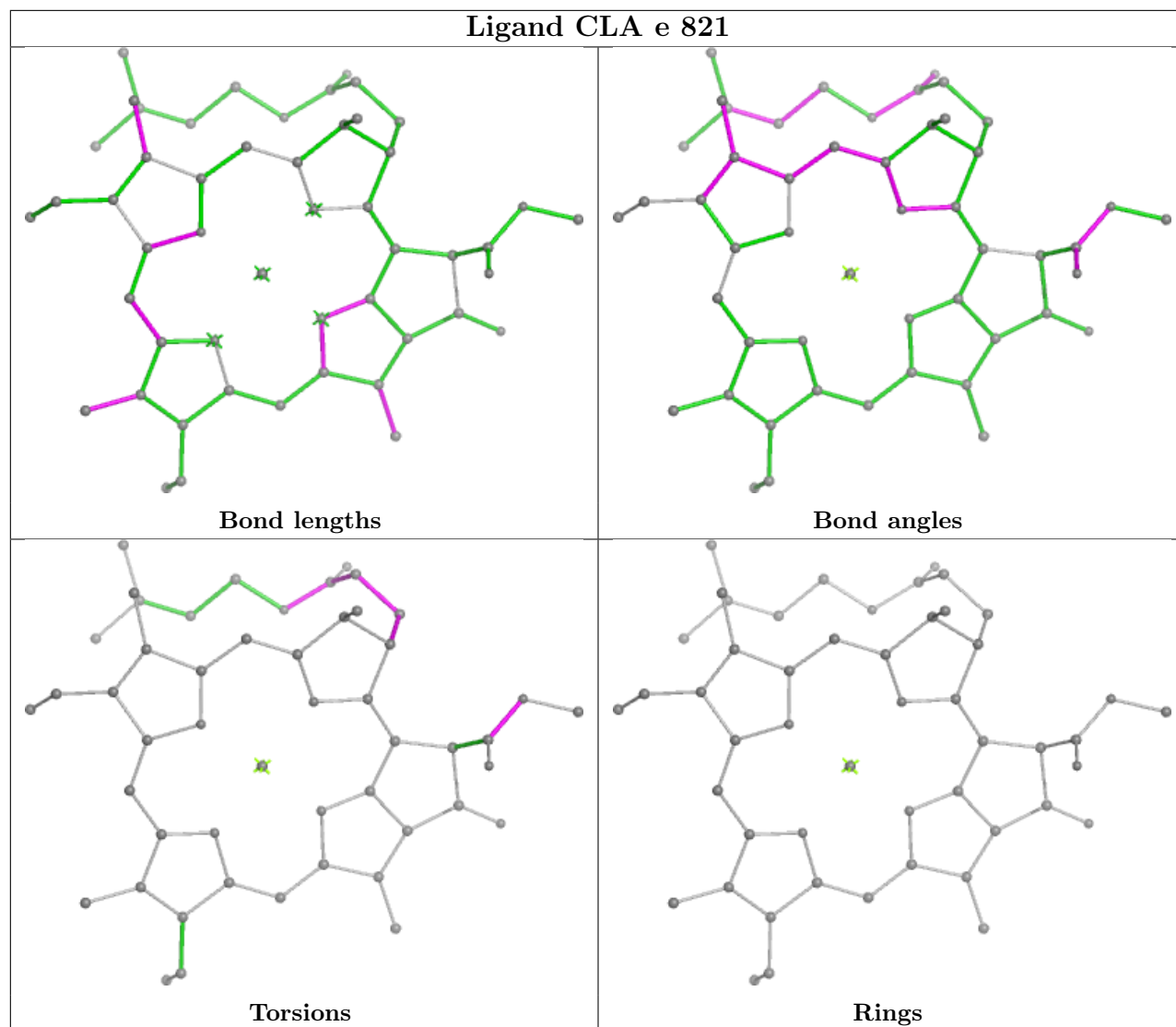
Rings



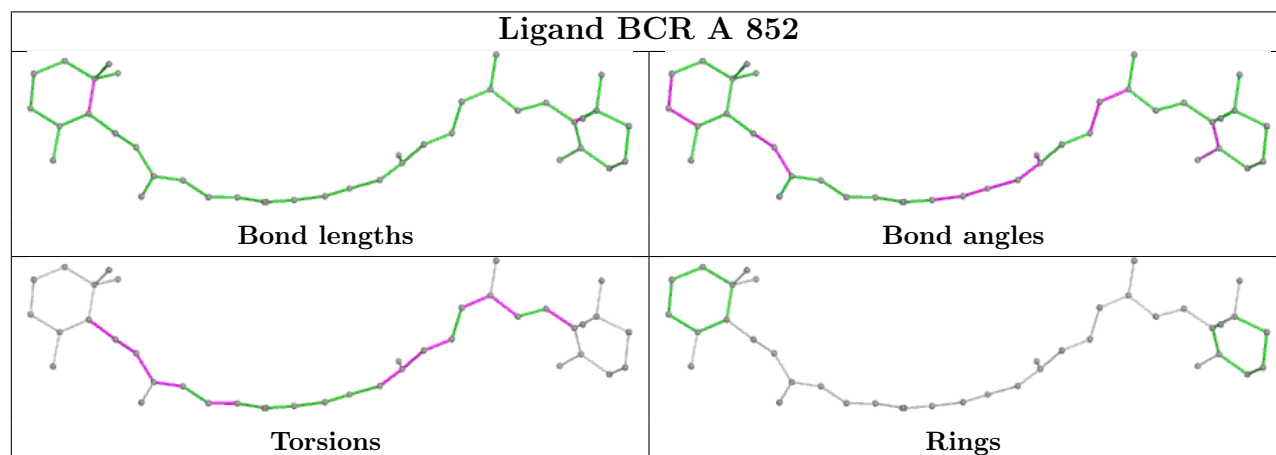
## Ligand CLA g 841



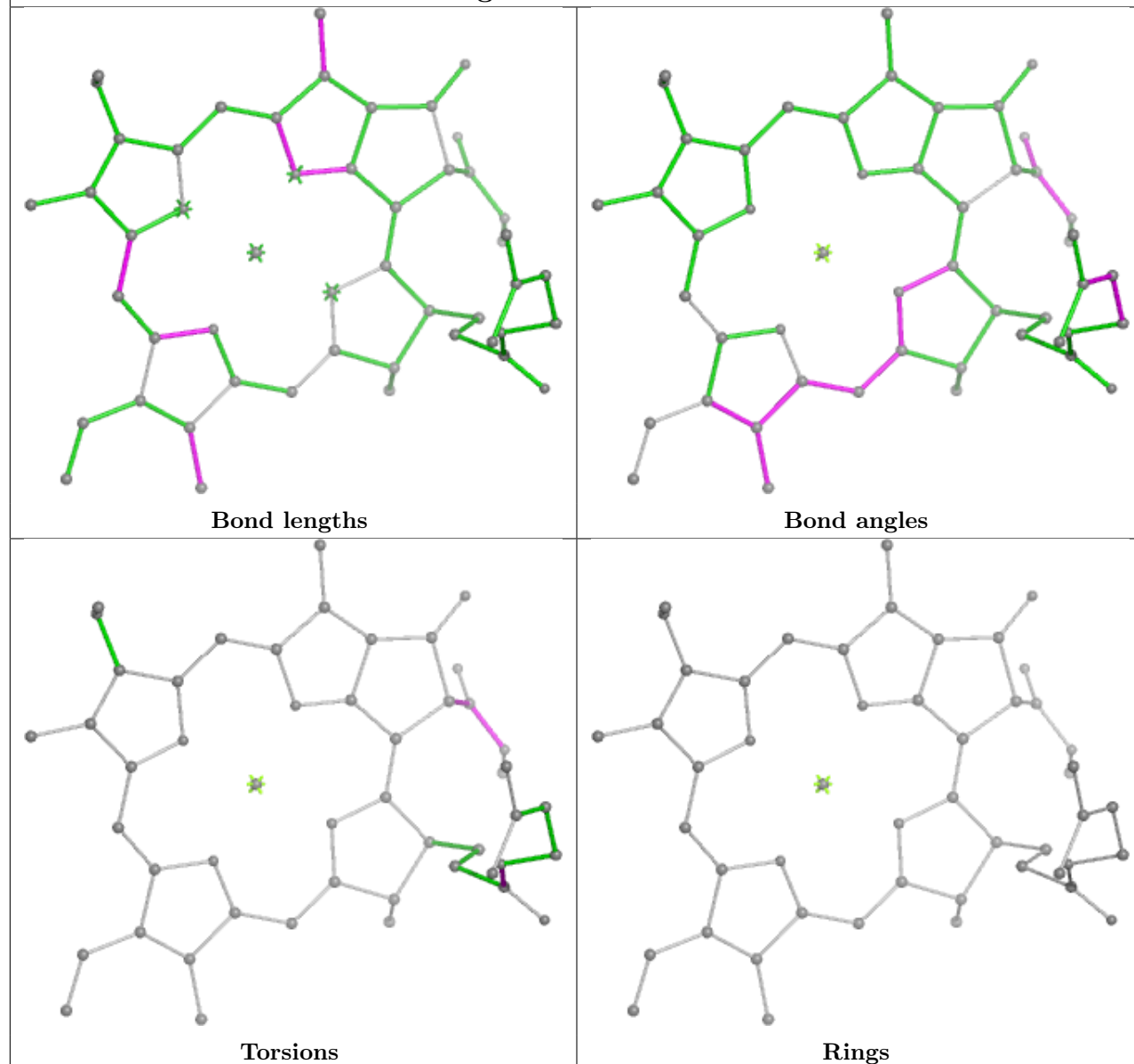
## Ligand CLA e 821



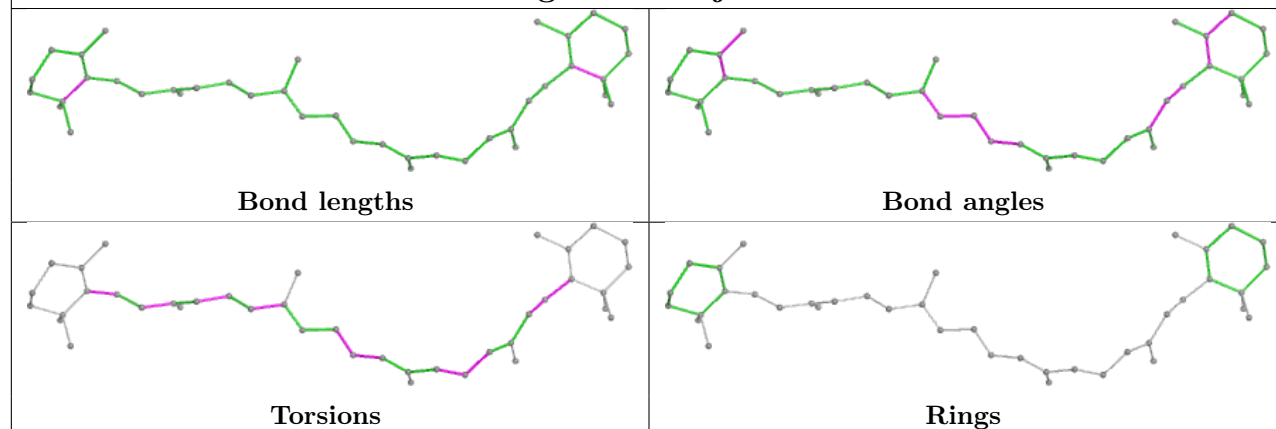
## Ligand BCR A 852



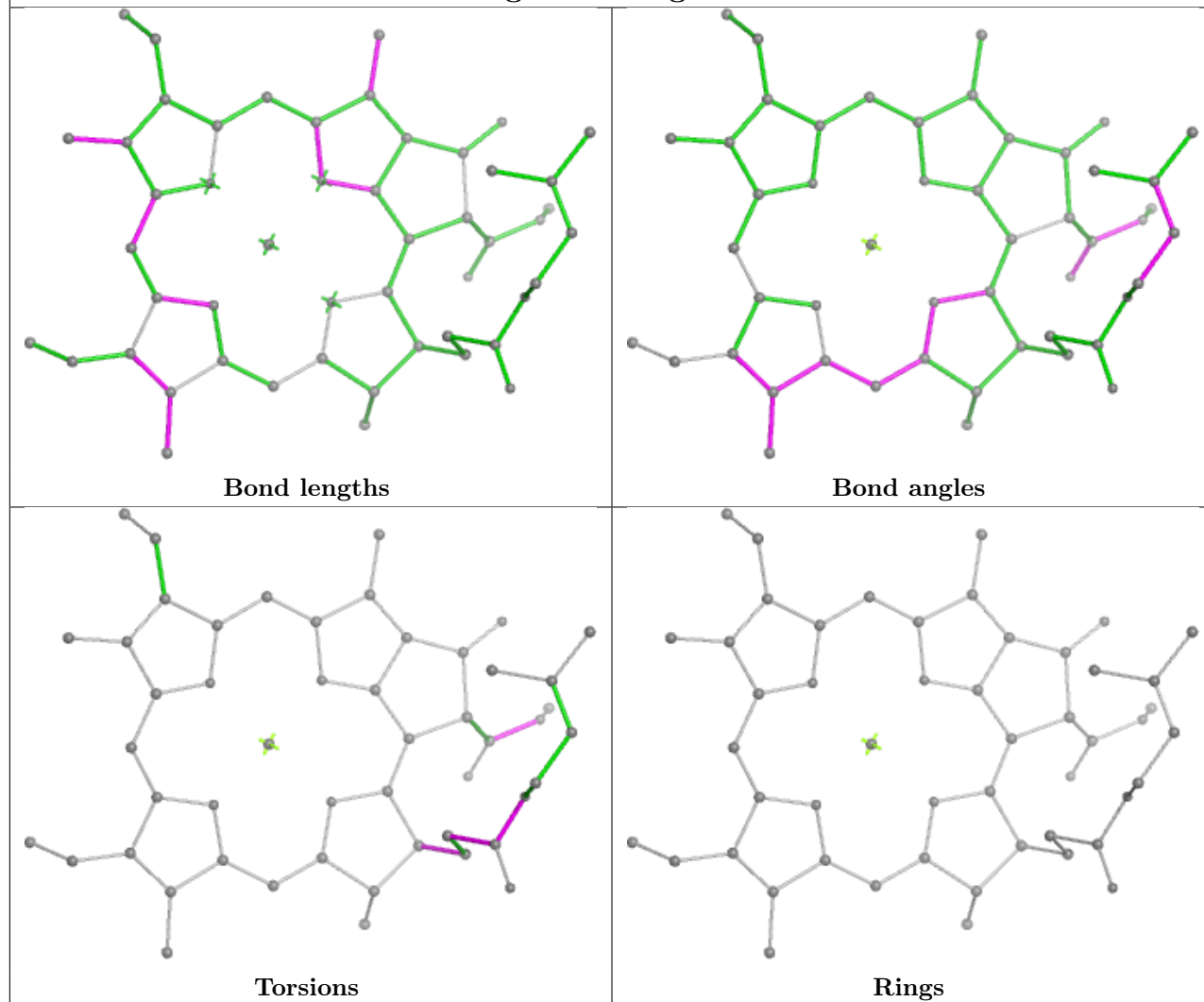
## Ligand CLA e 832



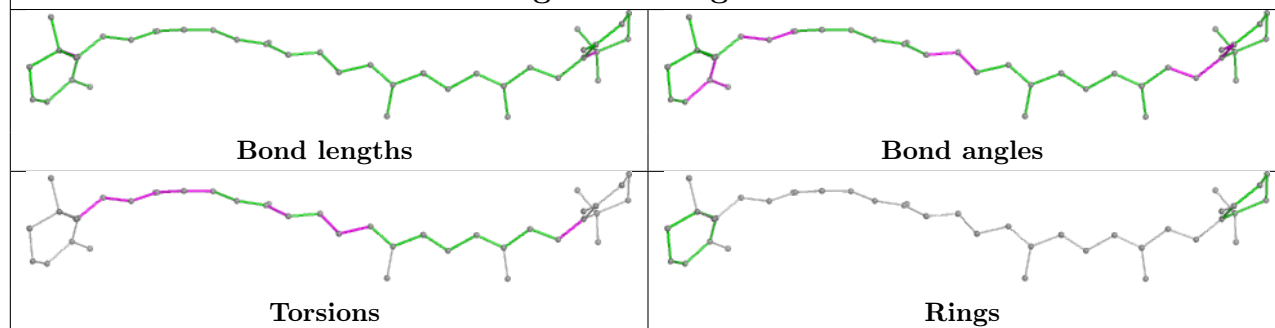
## Ligand BCR j 101

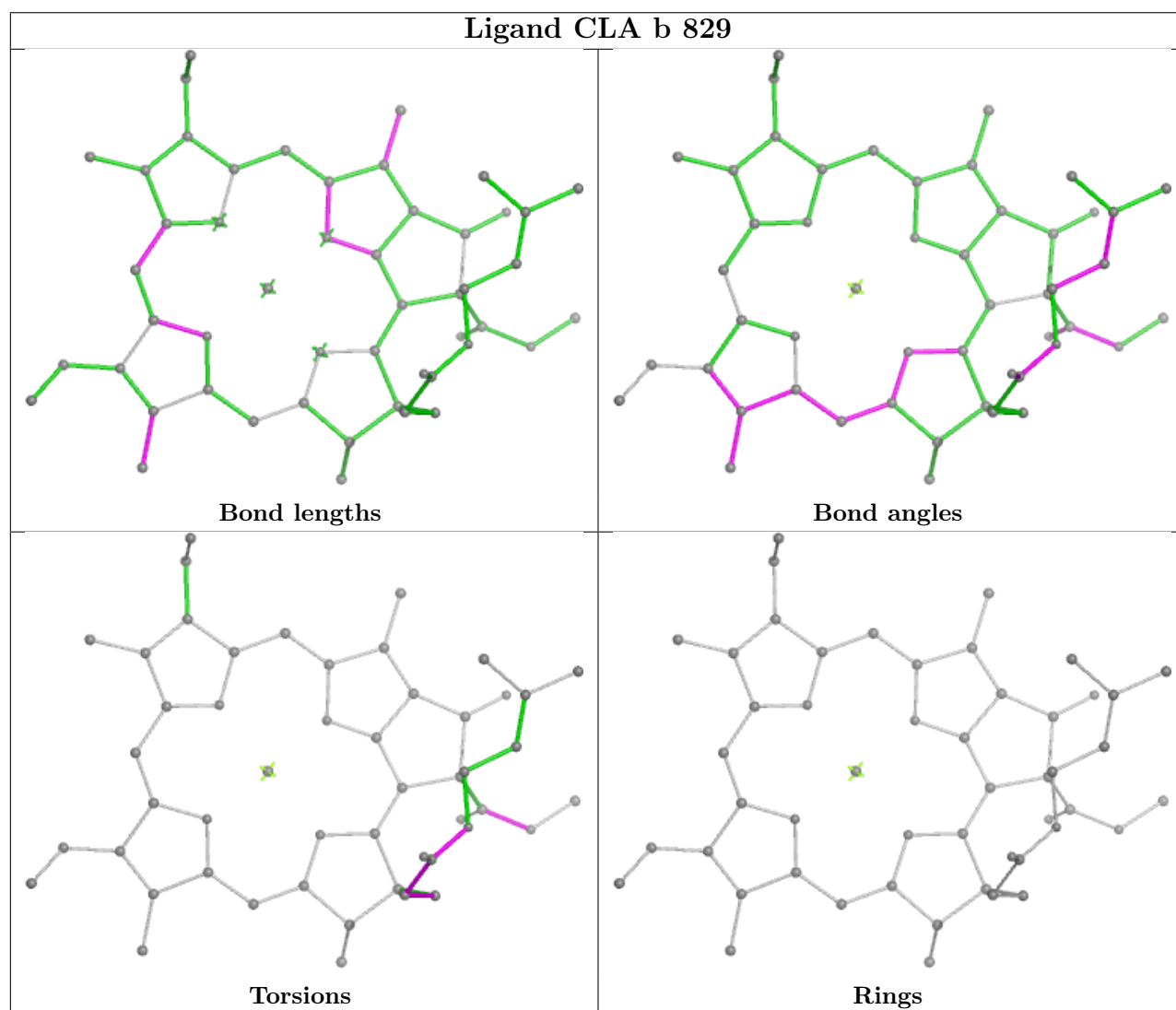
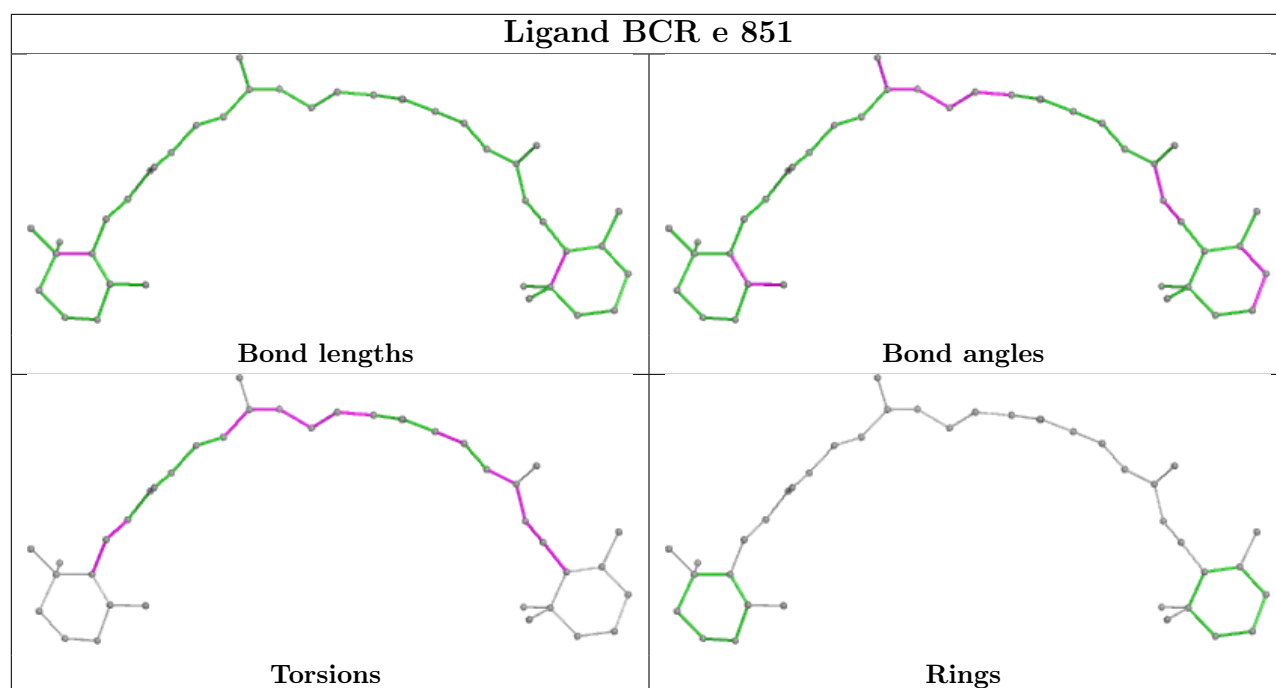


## Ligand CLA g 842

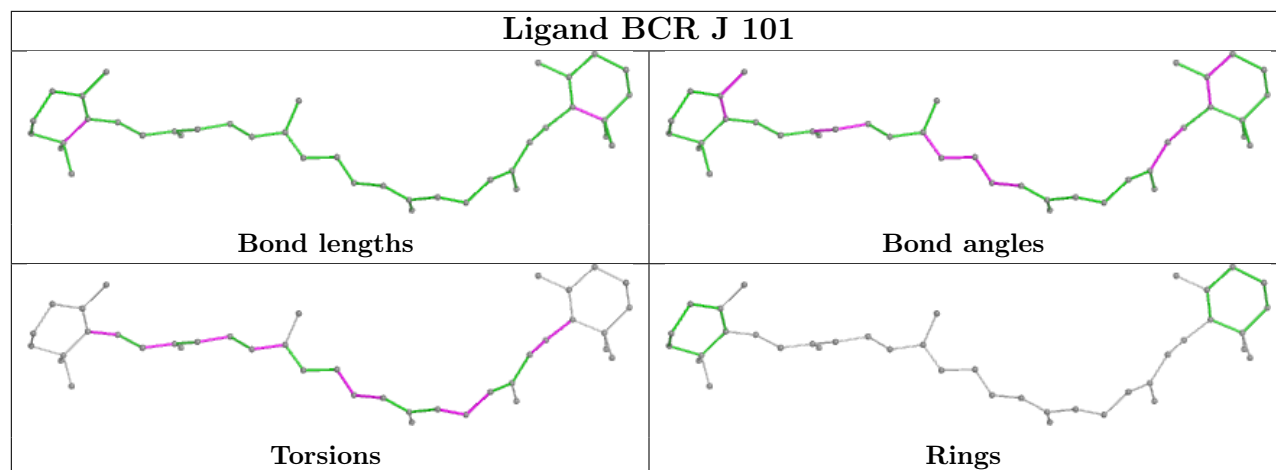


## Ligand BCR g 848

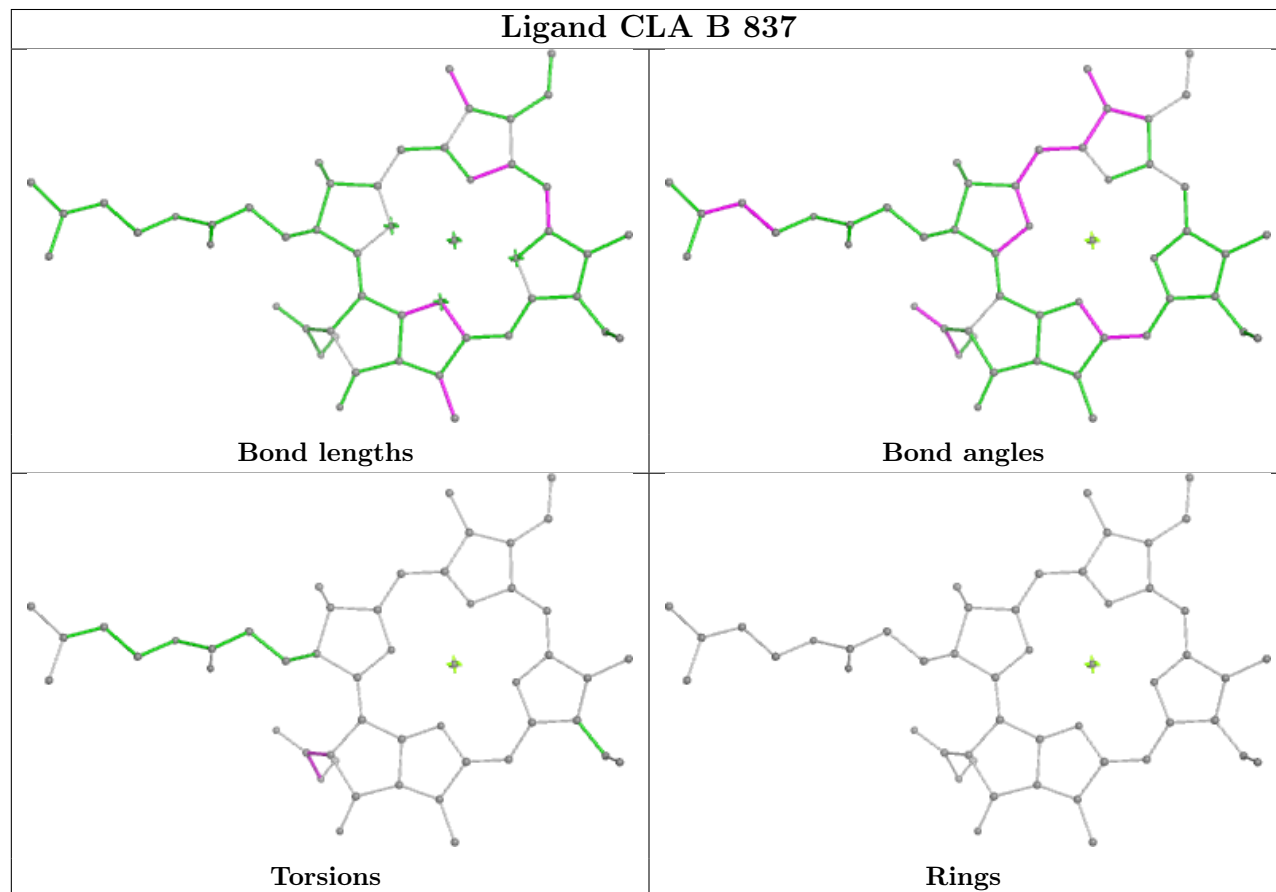




## Ligand BCR J 101

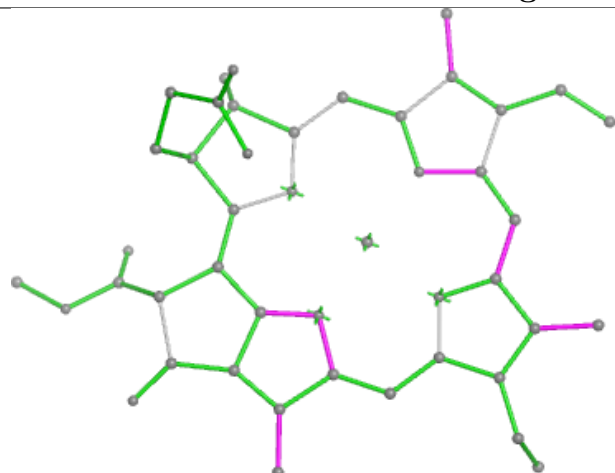


## Ligand CLA B 837

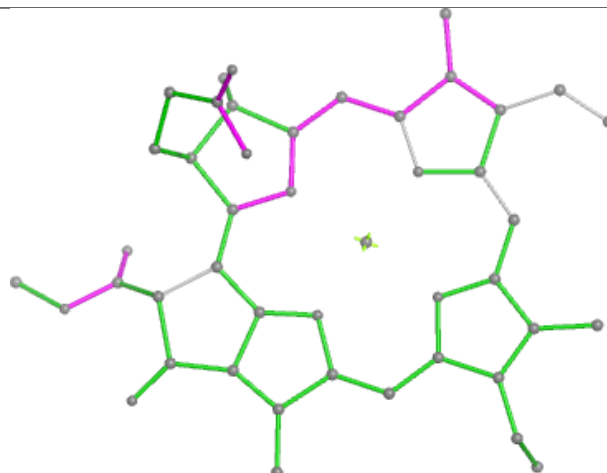




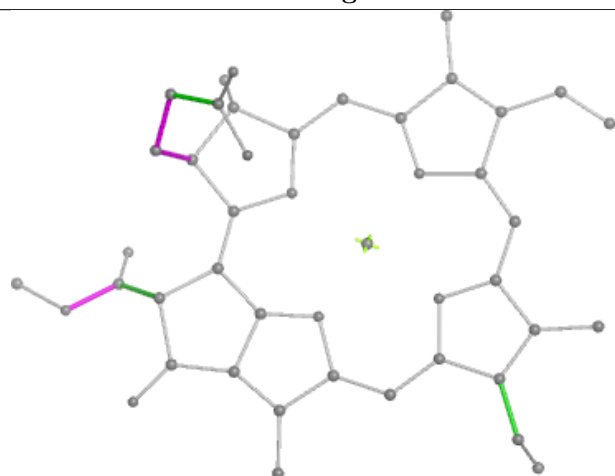
## Ligand CLA b 812



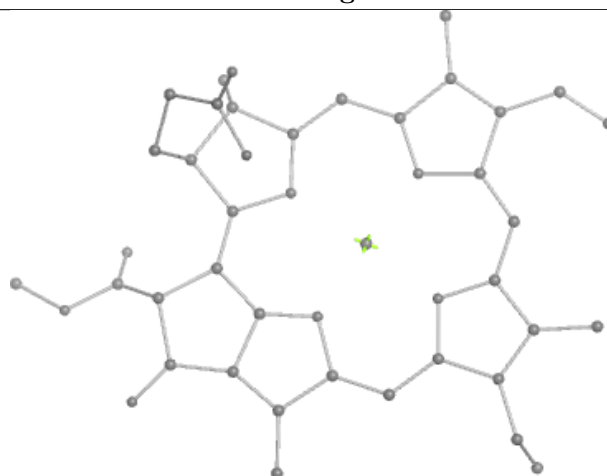
Bond lengths



Bond angles

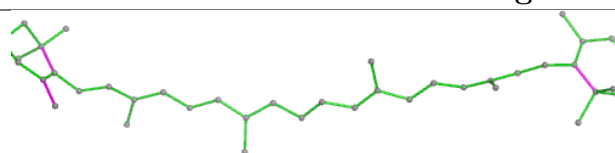


Torsions

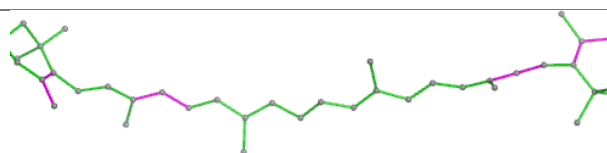


Rings

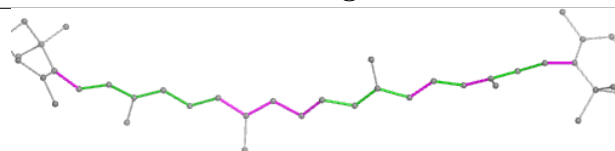
## Ligand BCR T 101



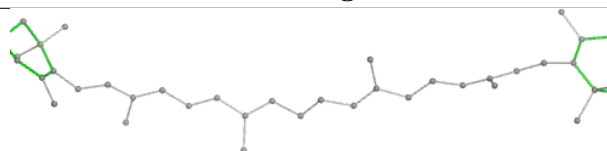
Bond lengths



Bond angles

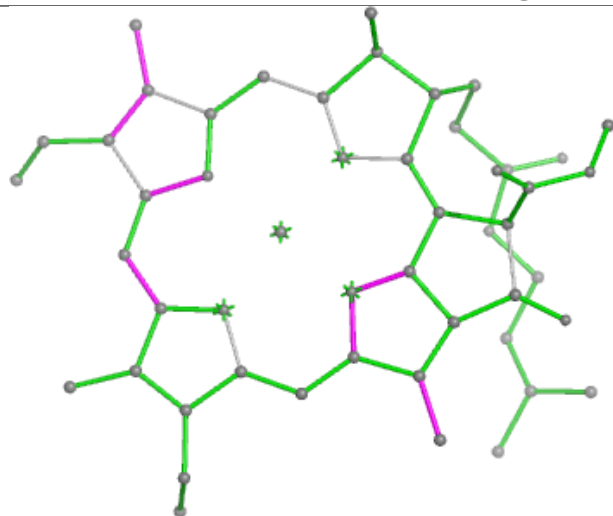


Torsions

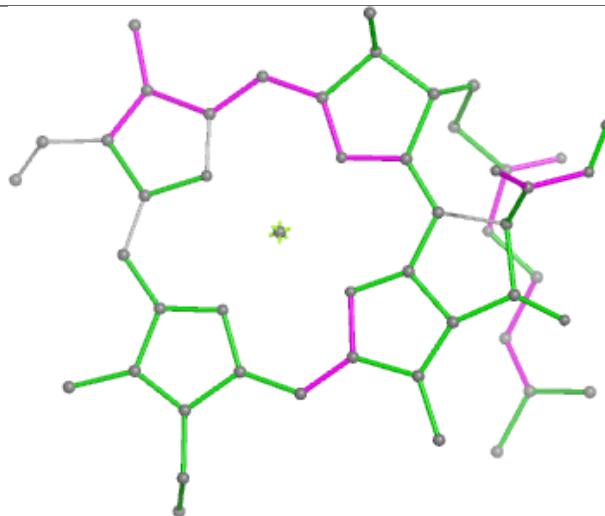


Rings

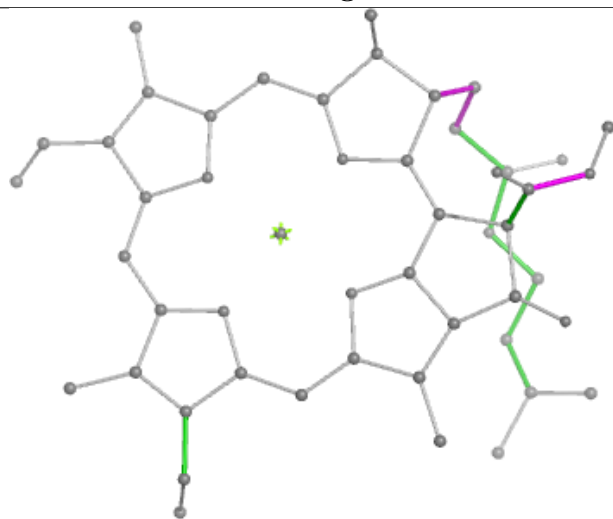
## Ligand CLA E 832



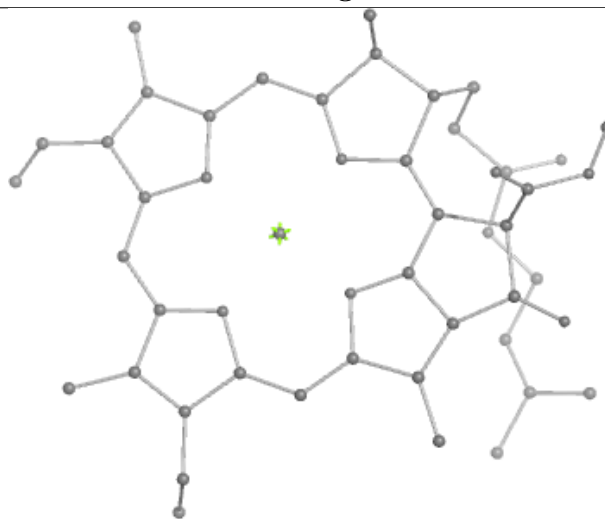
Bond lengths



Bond angles

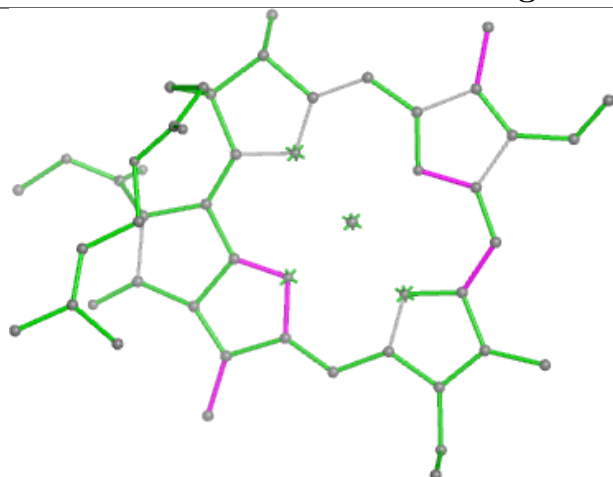


Torsions

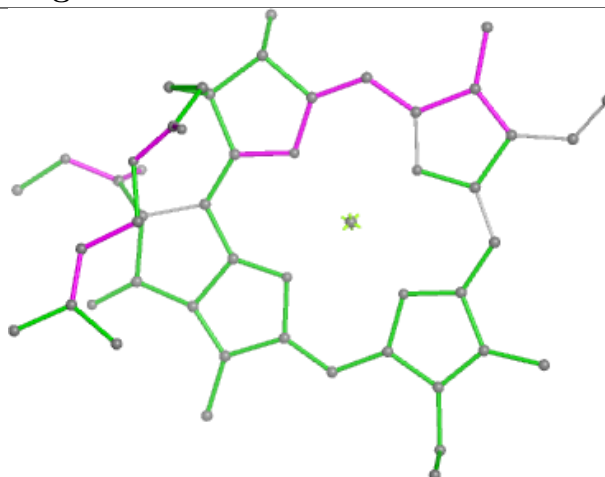


Rings

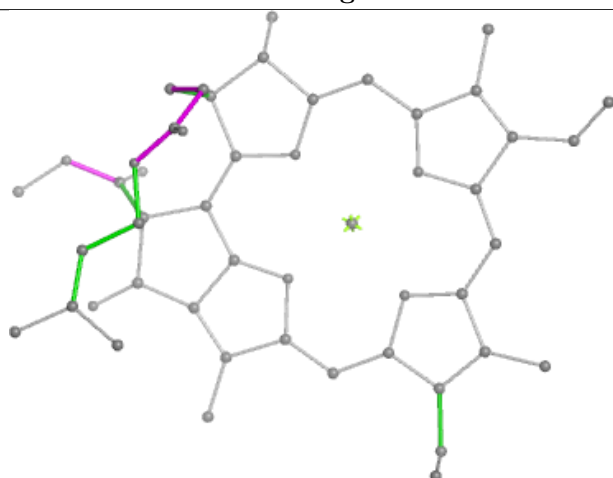
## Ligand CLA g 831



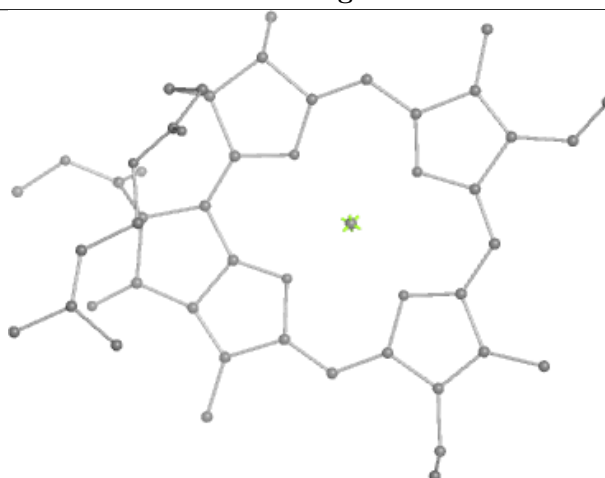
Bond lengths



Bond angles

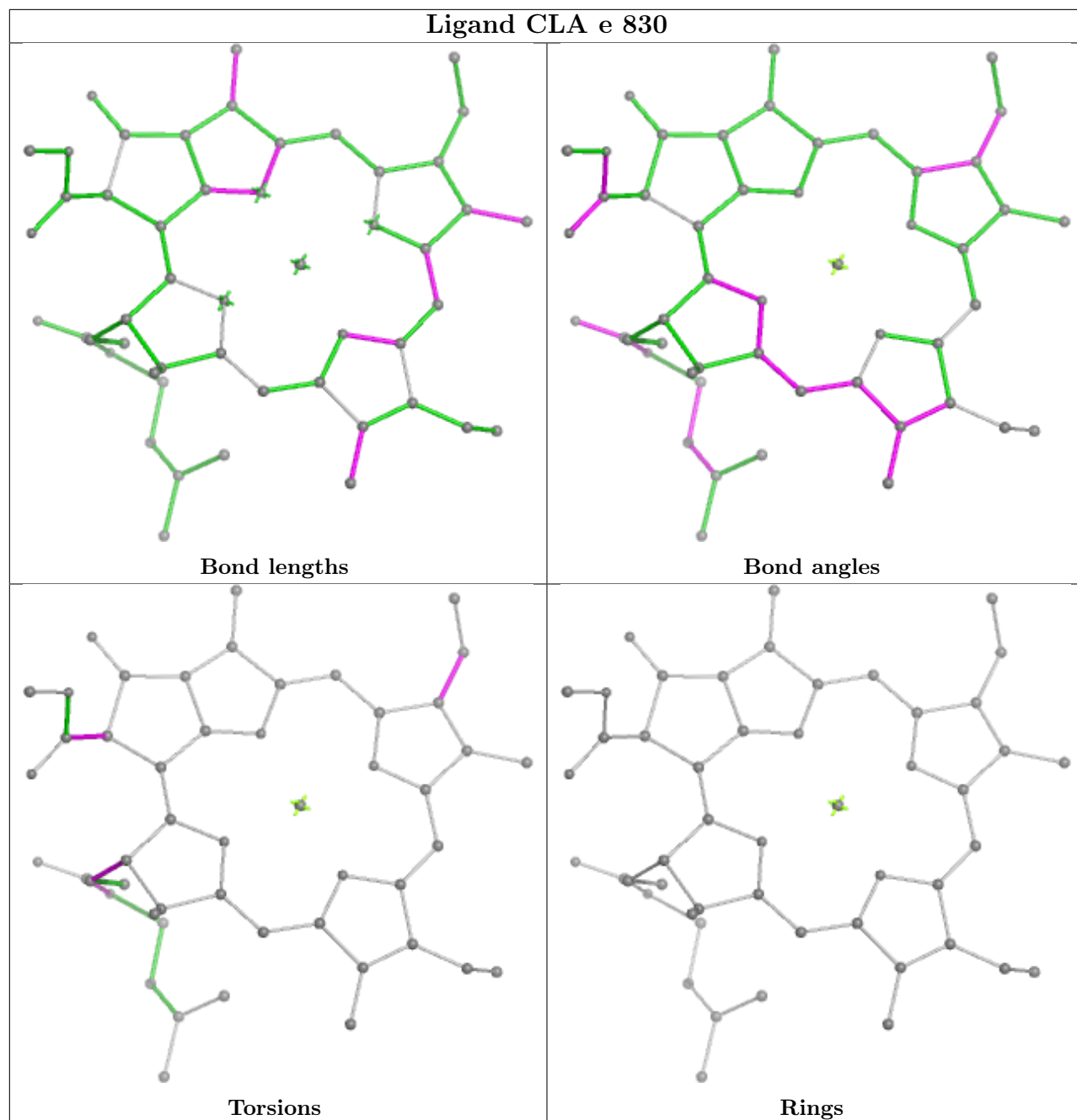


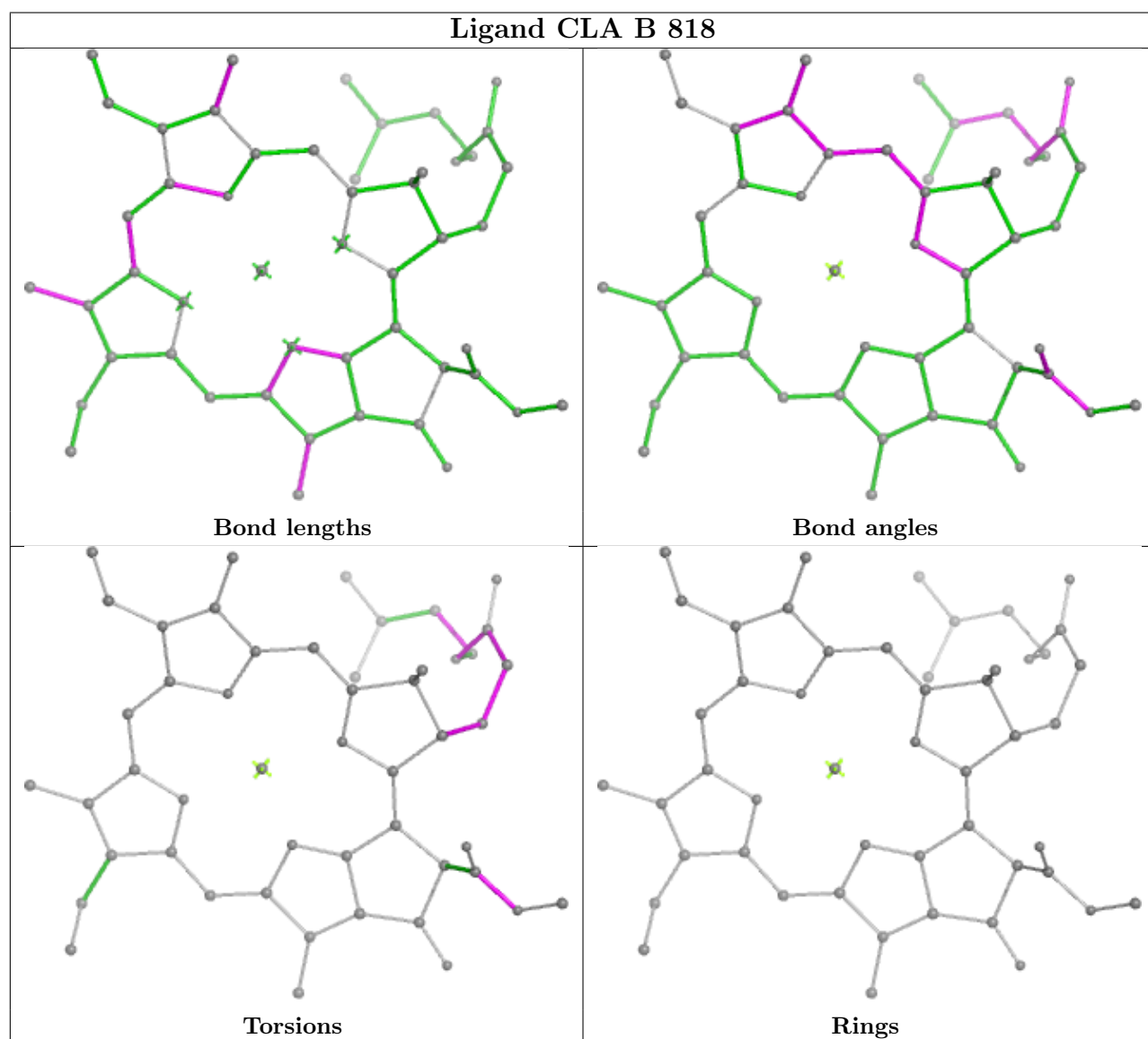
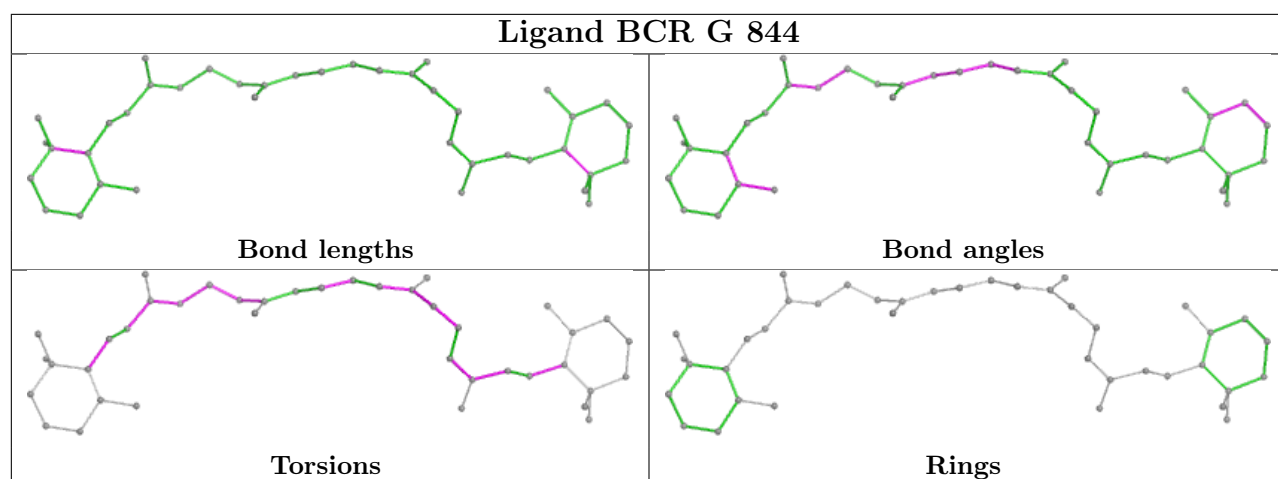
Torsions

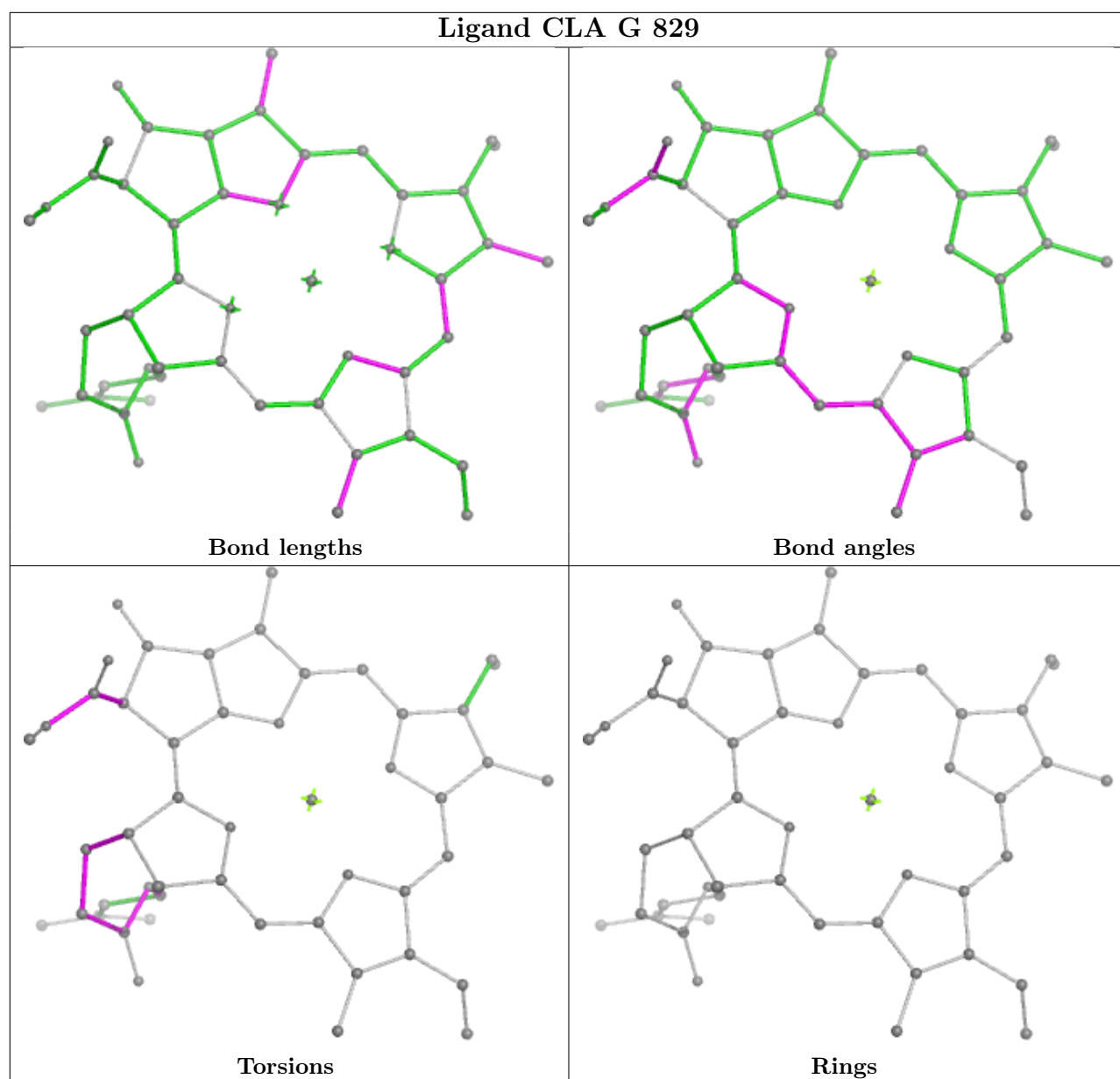


Rings

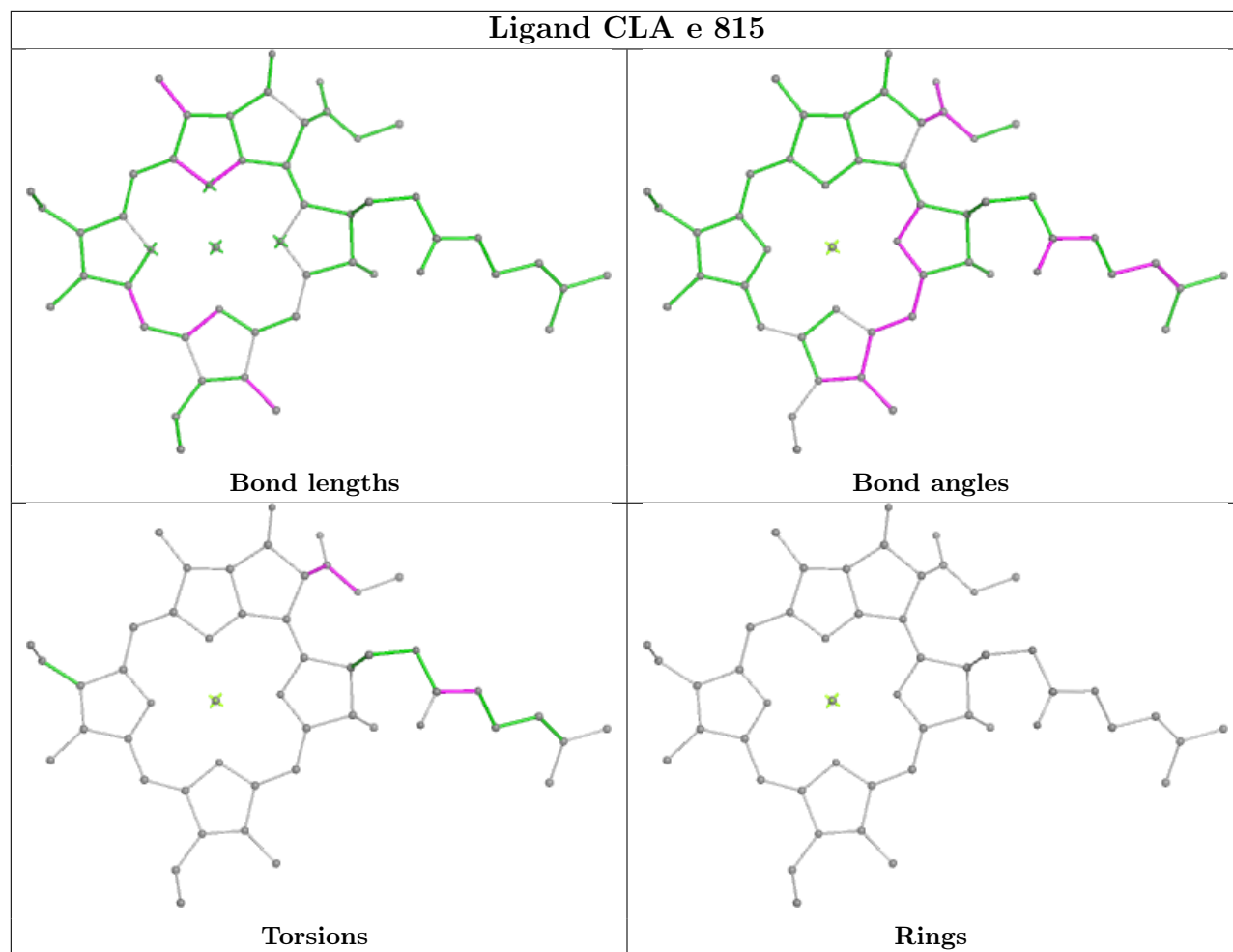
## Ligand CLA e 830

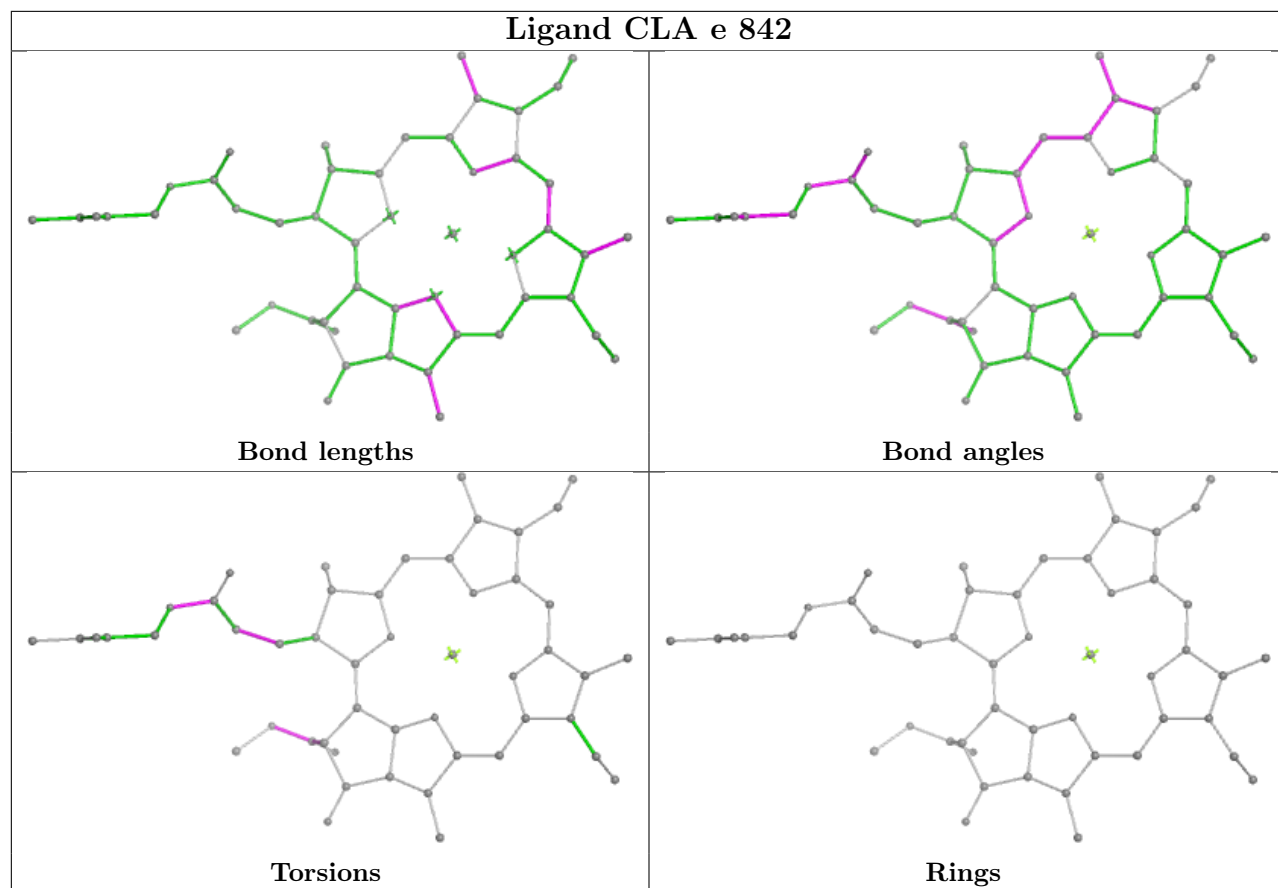




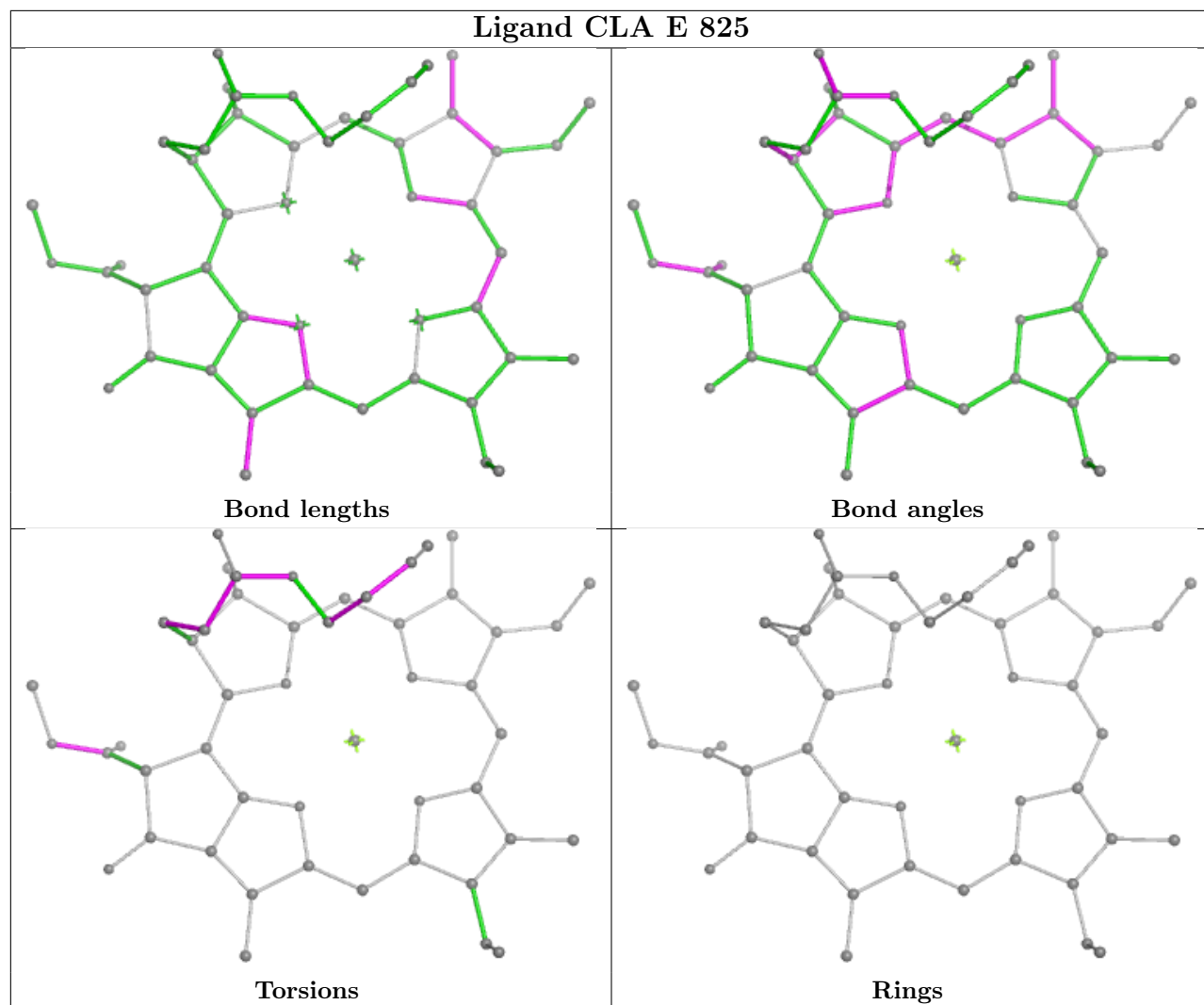


## Ligand CLA e 815

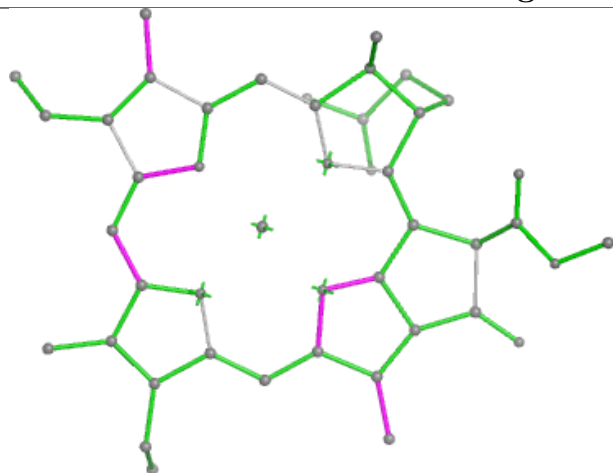




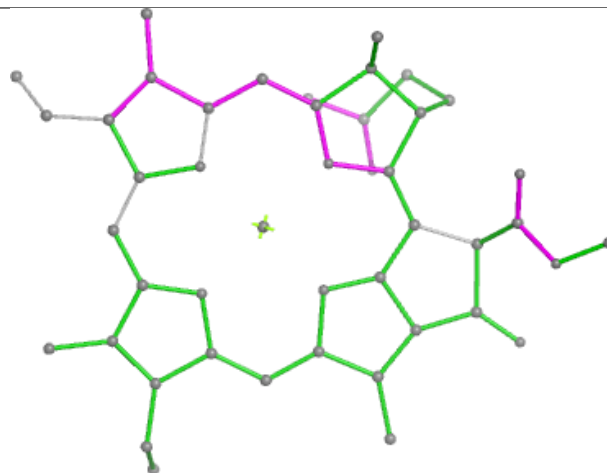




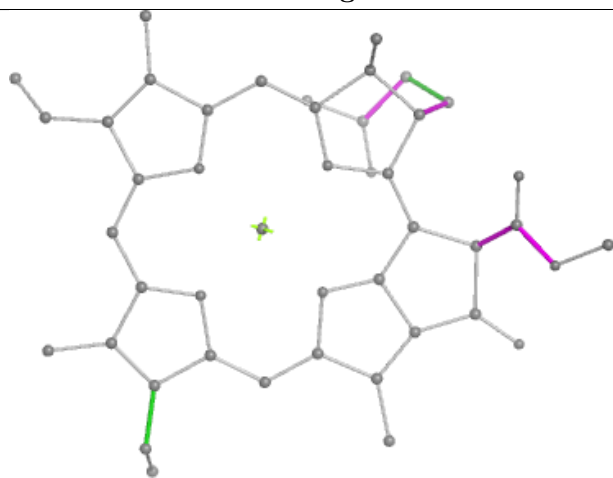
## Ligand CLA b 835



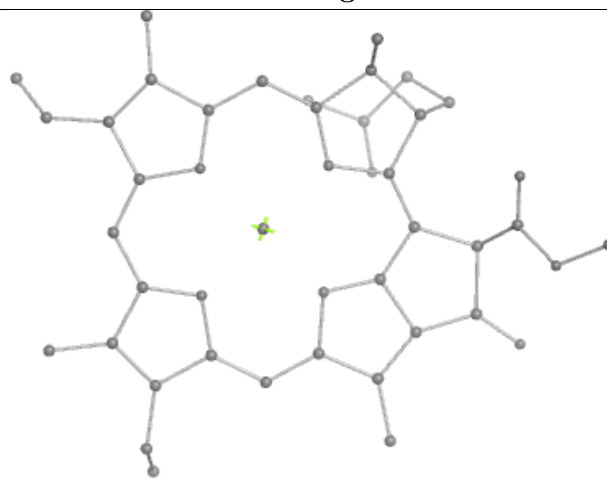
Bond lengths



Bond angles

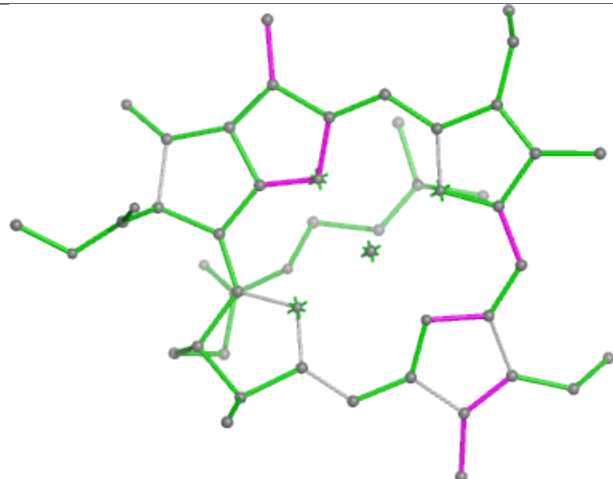


Torsions

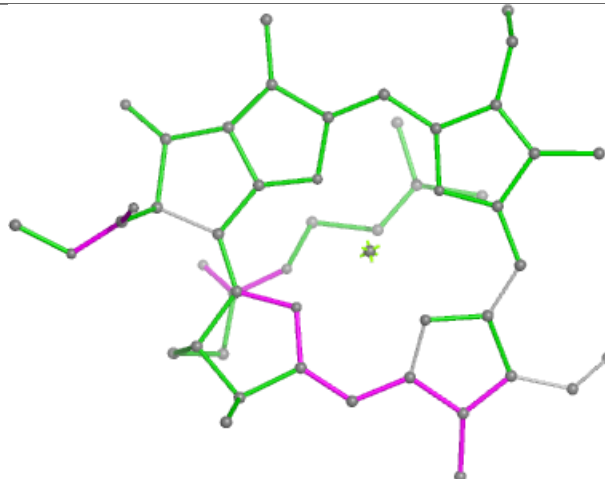


Rings

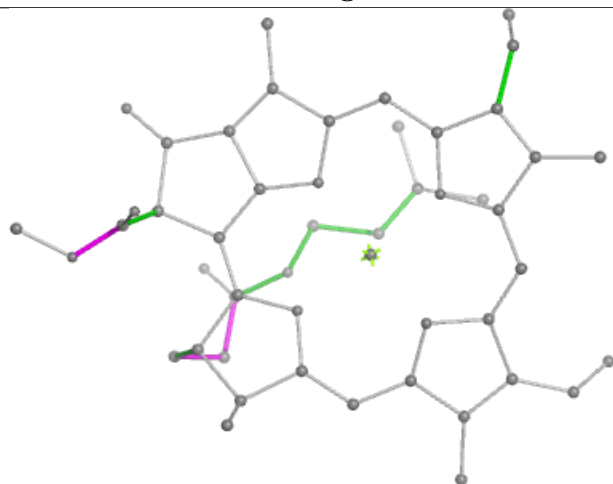
## Ligand CLA g 810



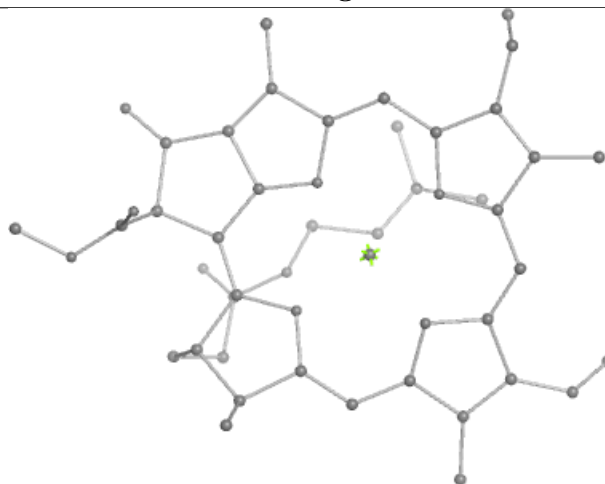
Bond lengths



Bond angles

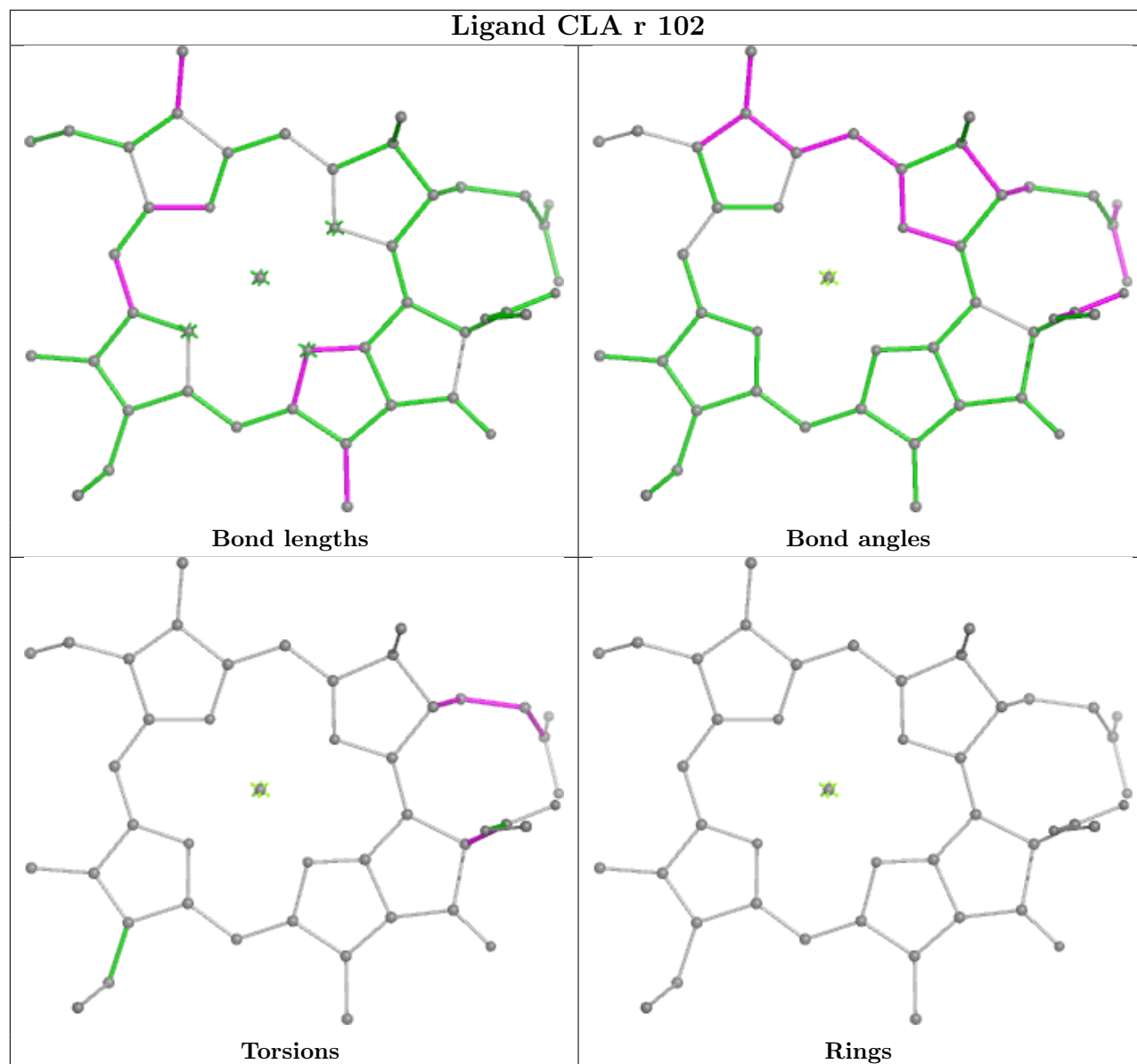


Torsions

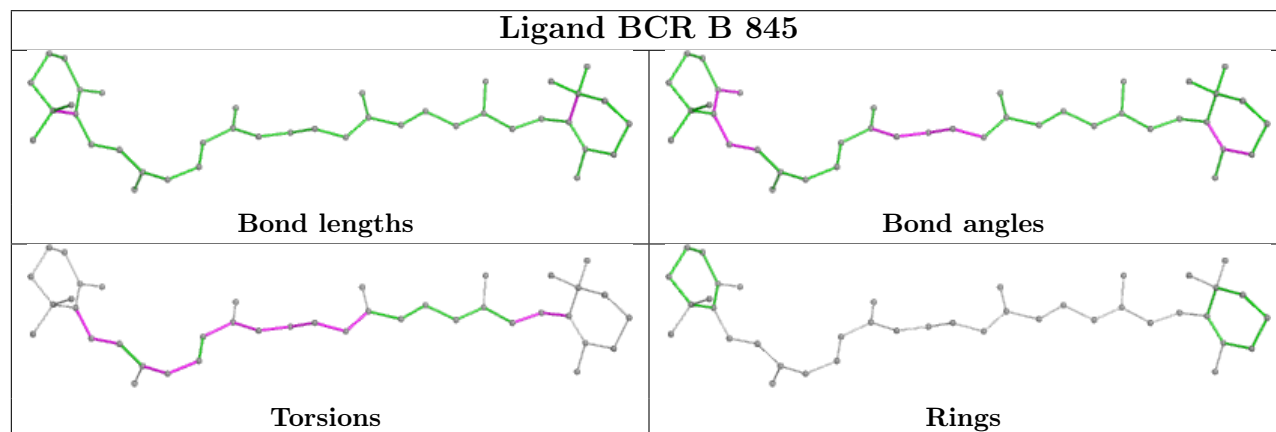


Rings

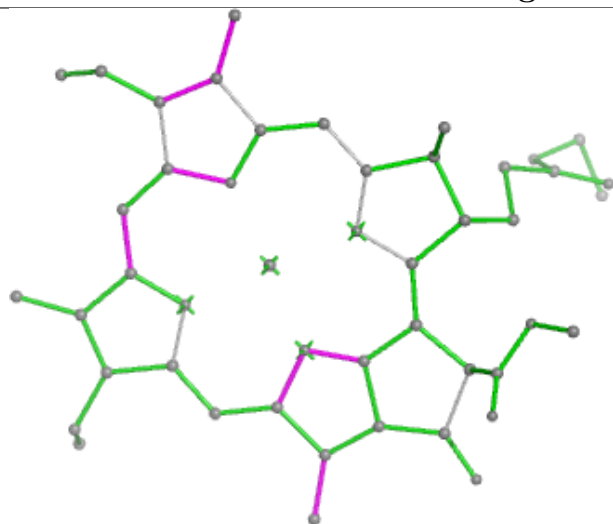
## Ligand CLA r 102



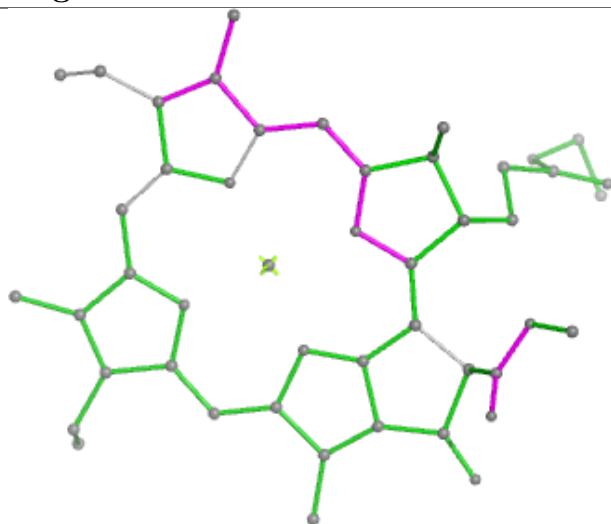
## Ligand BCR B 845



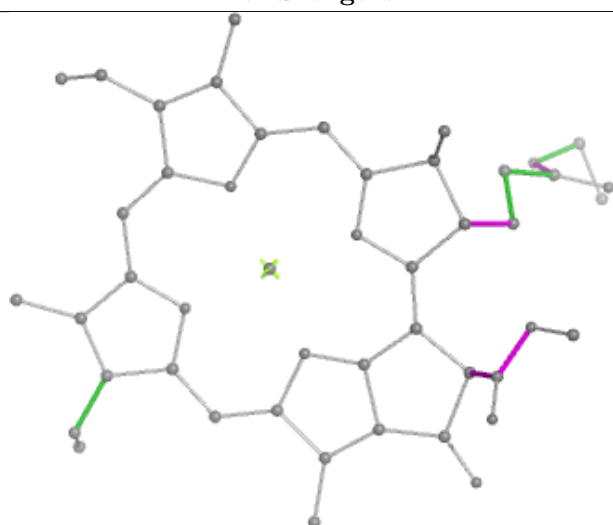
## Ligand CLA g 840



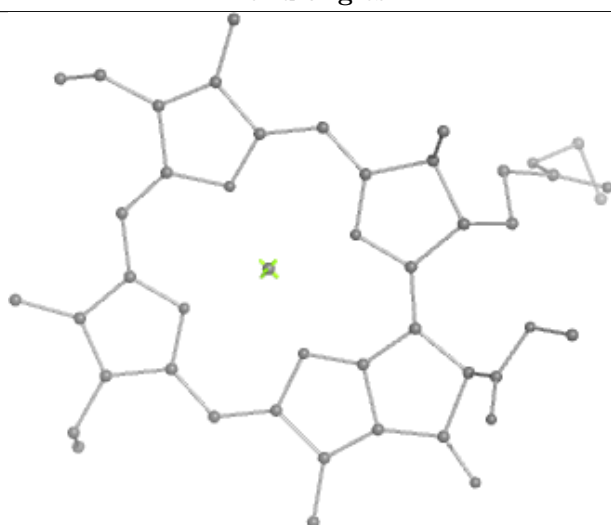
Bond lengths



Bond angles

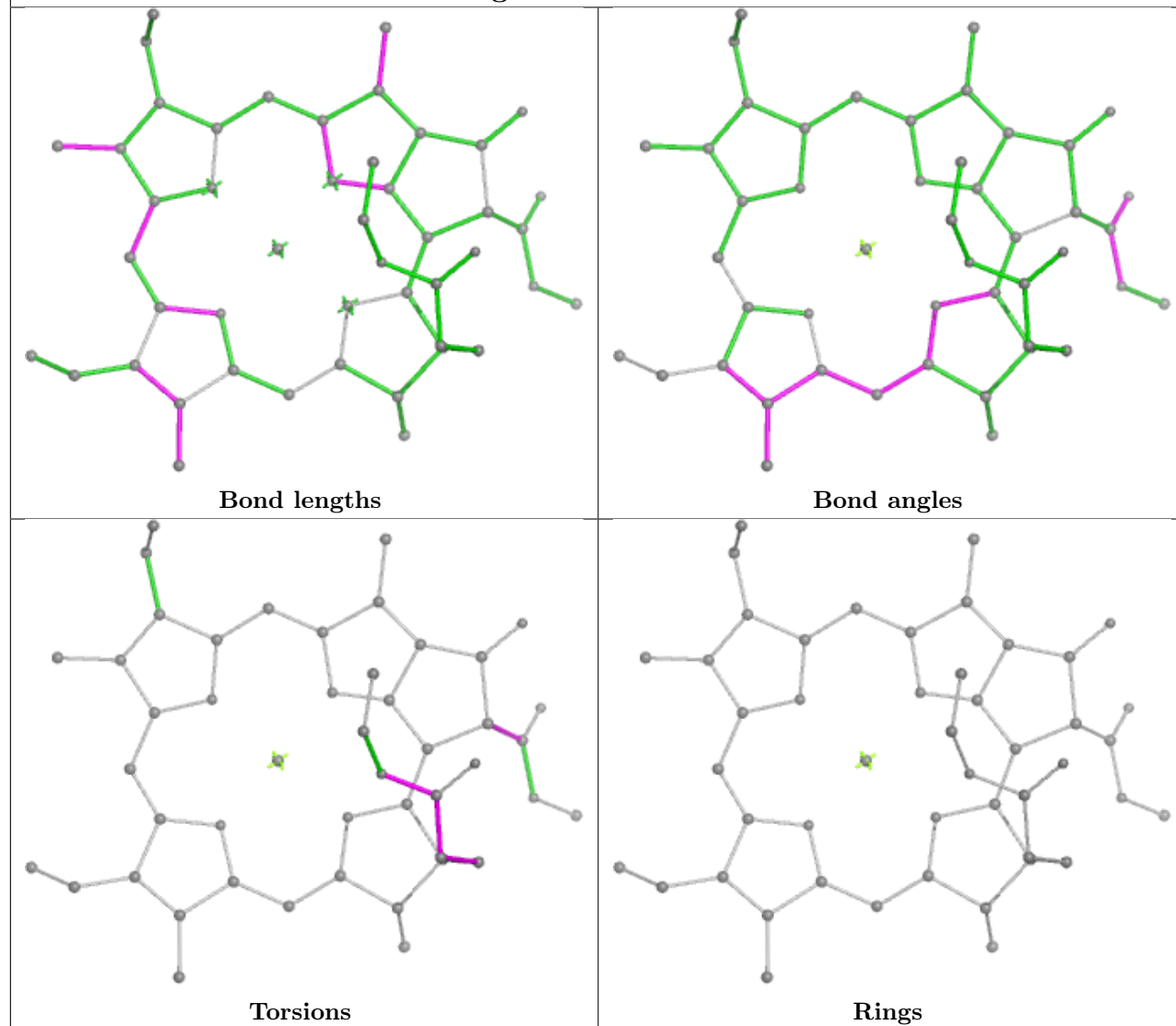


Torsions

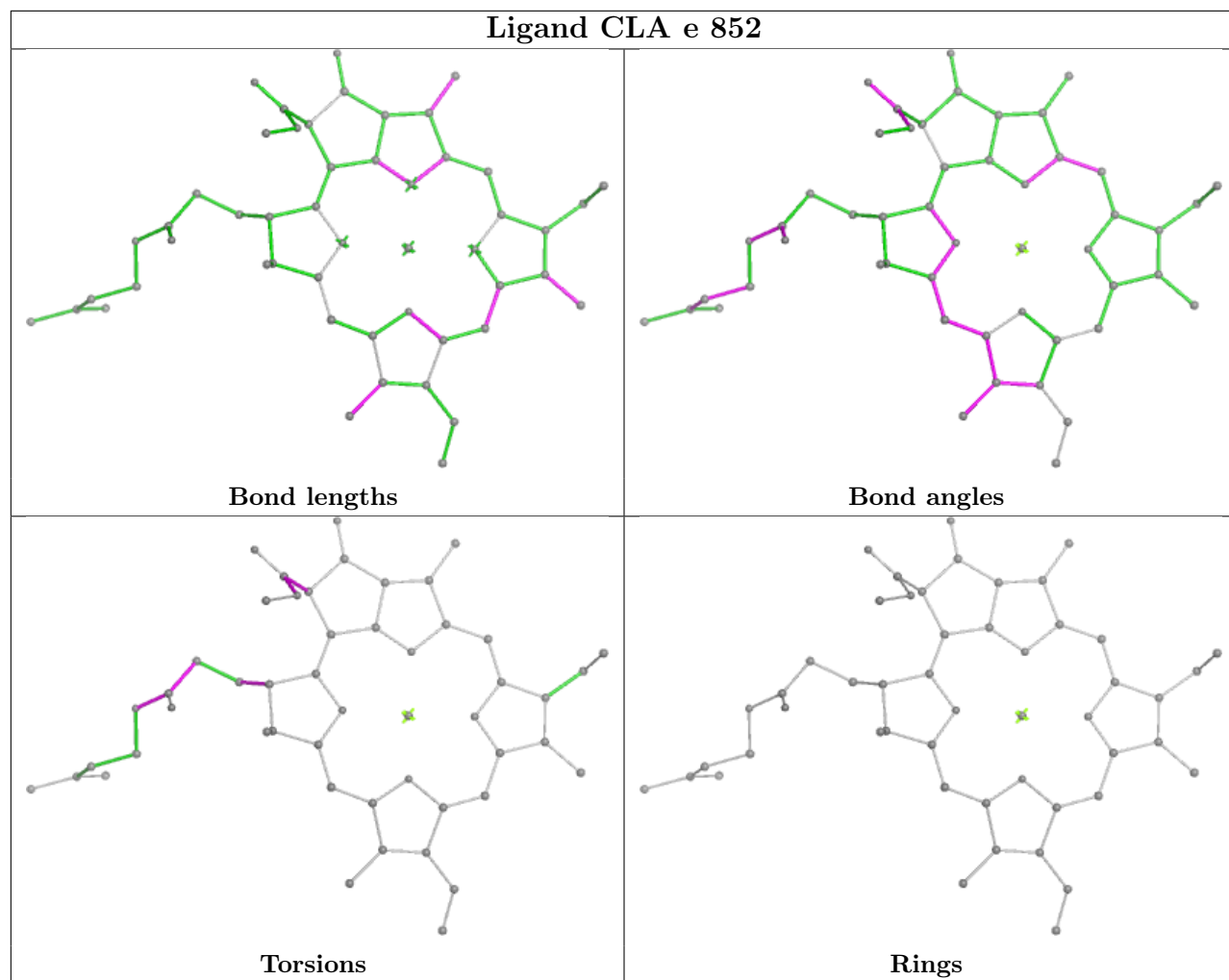


Rings

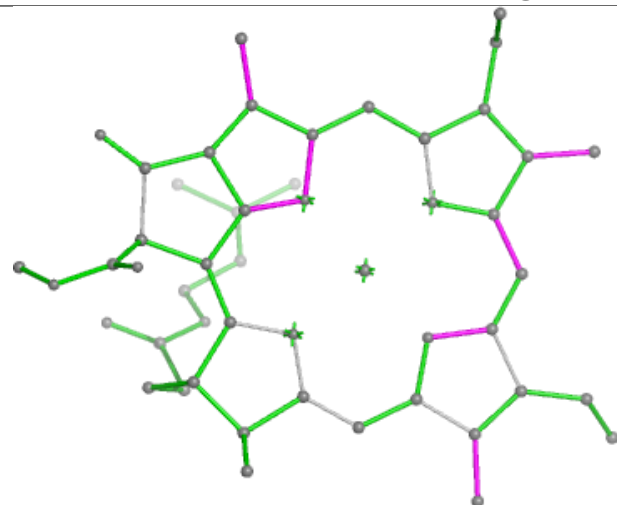
## Ligand CLA E 842



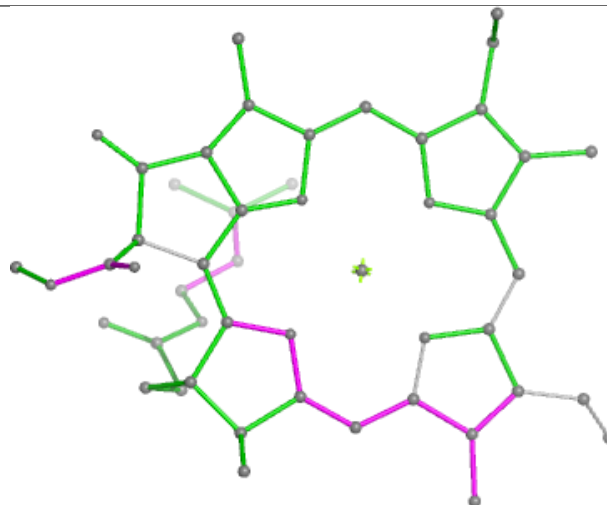
## Ligand CLA e 852



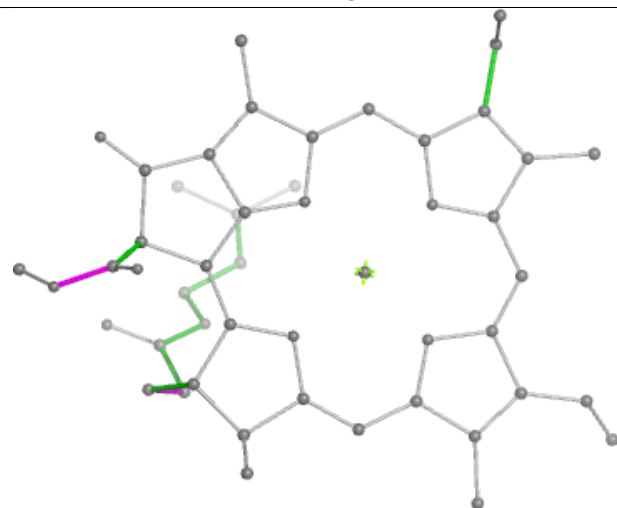
## Ligand CLA G 815



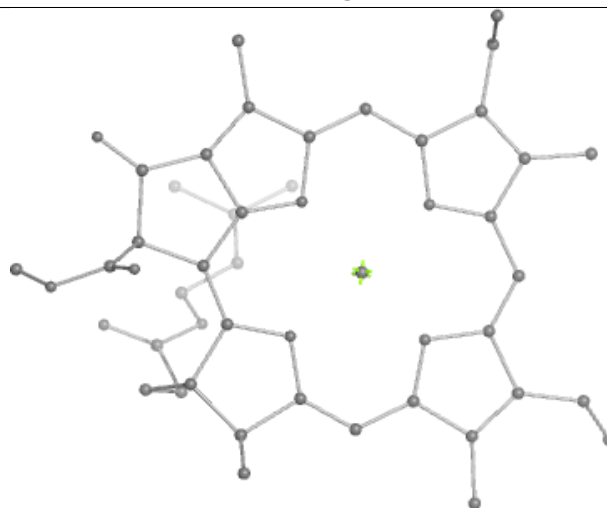
Bond lengths



Bond angles



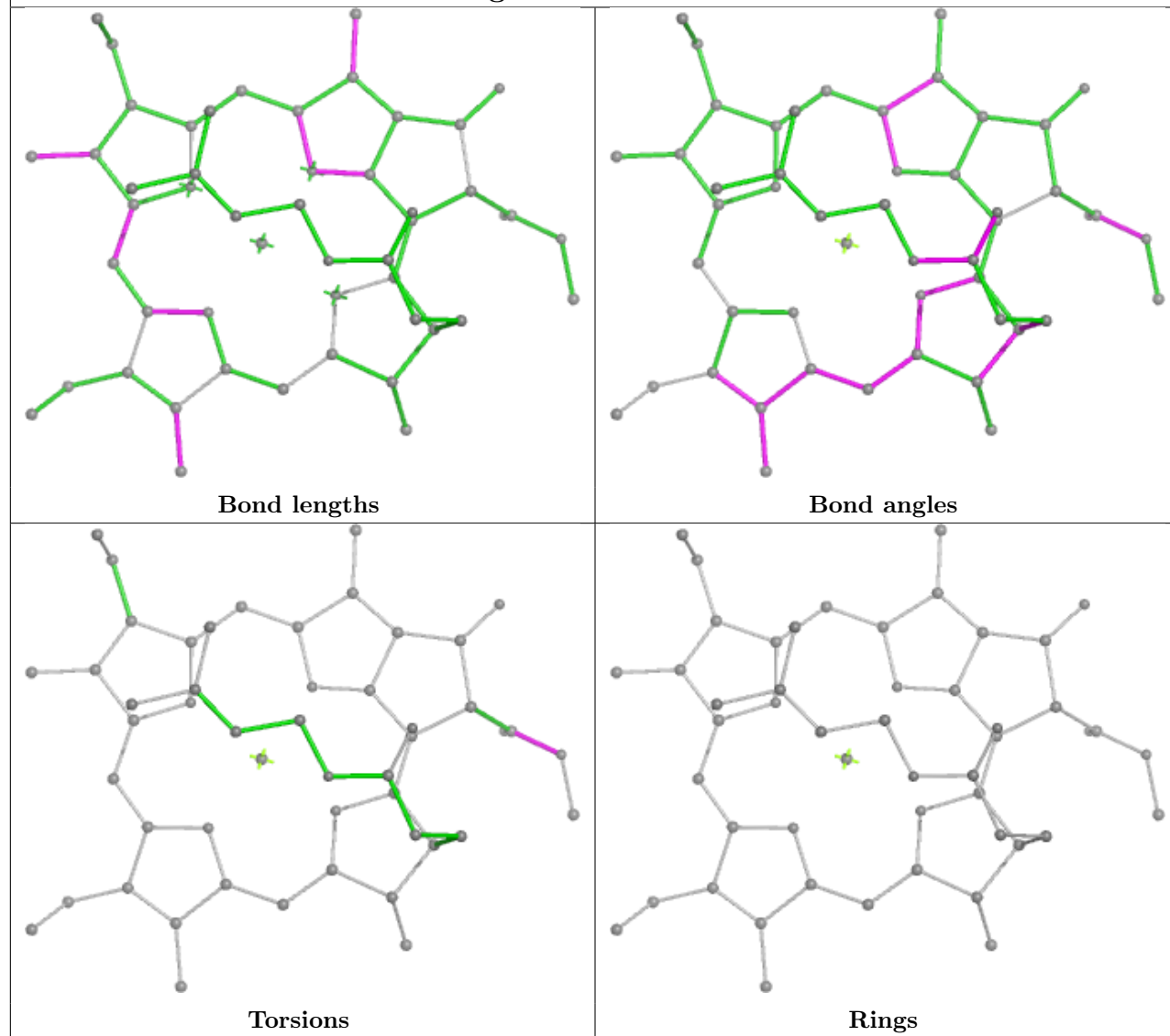
Torsions



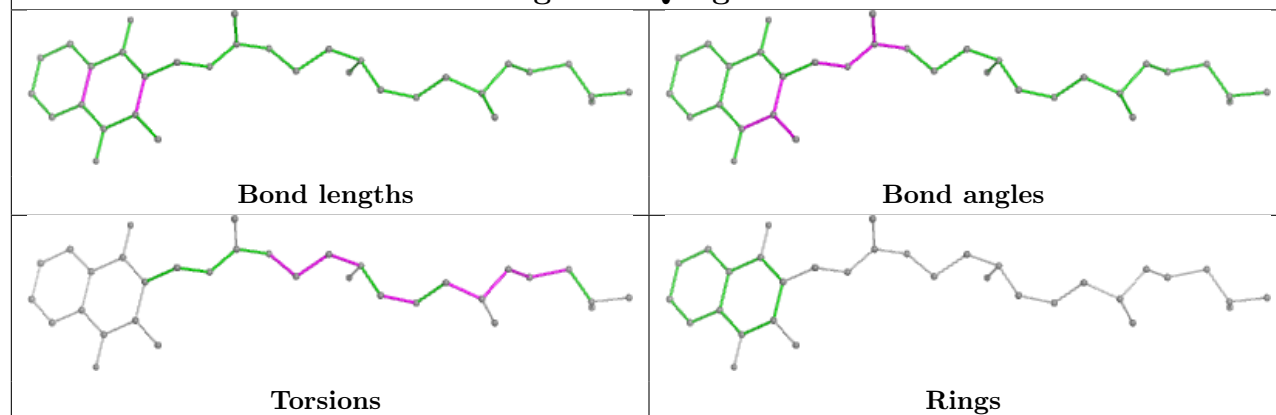
Rings

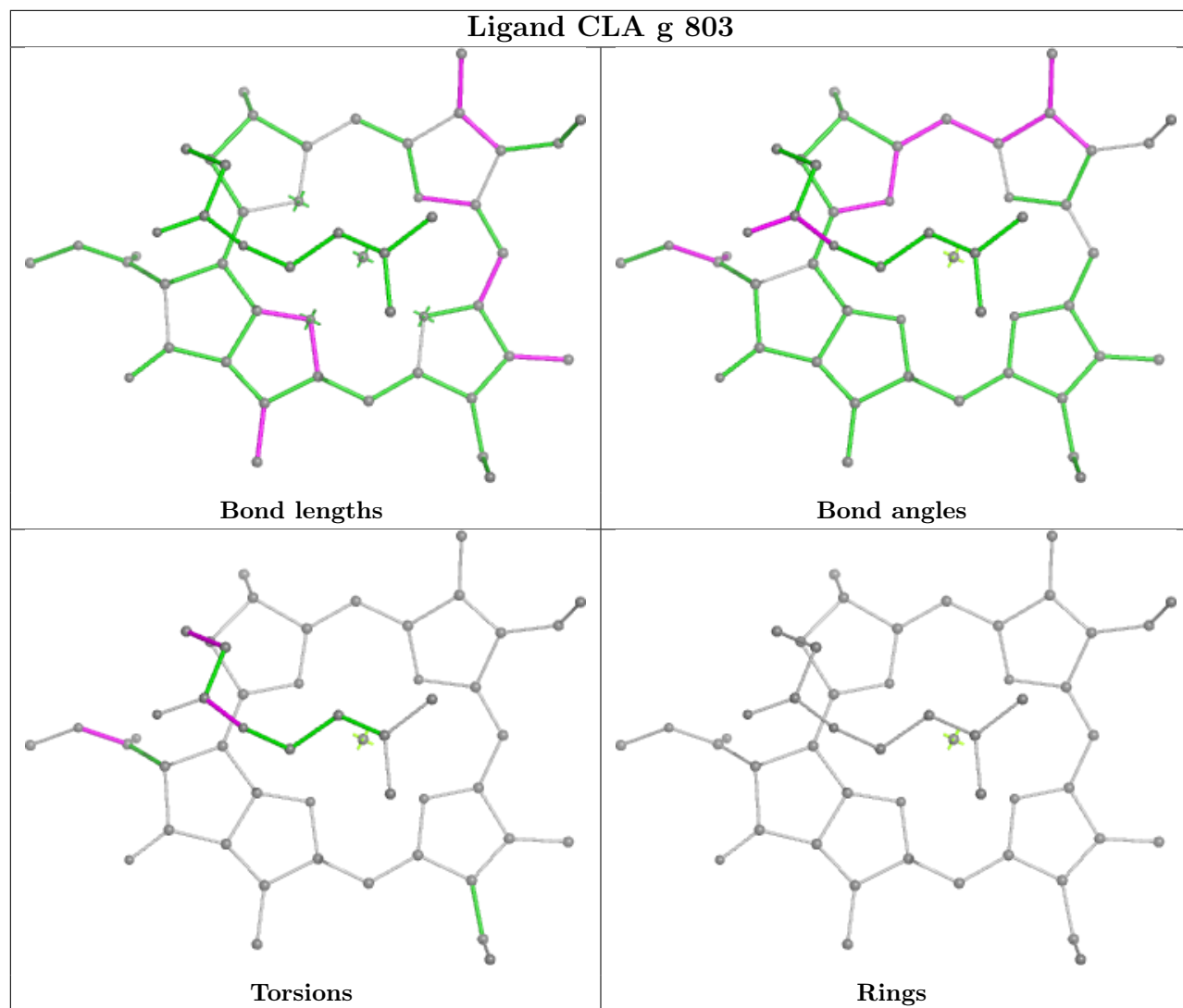


## Ligand CLA E 820

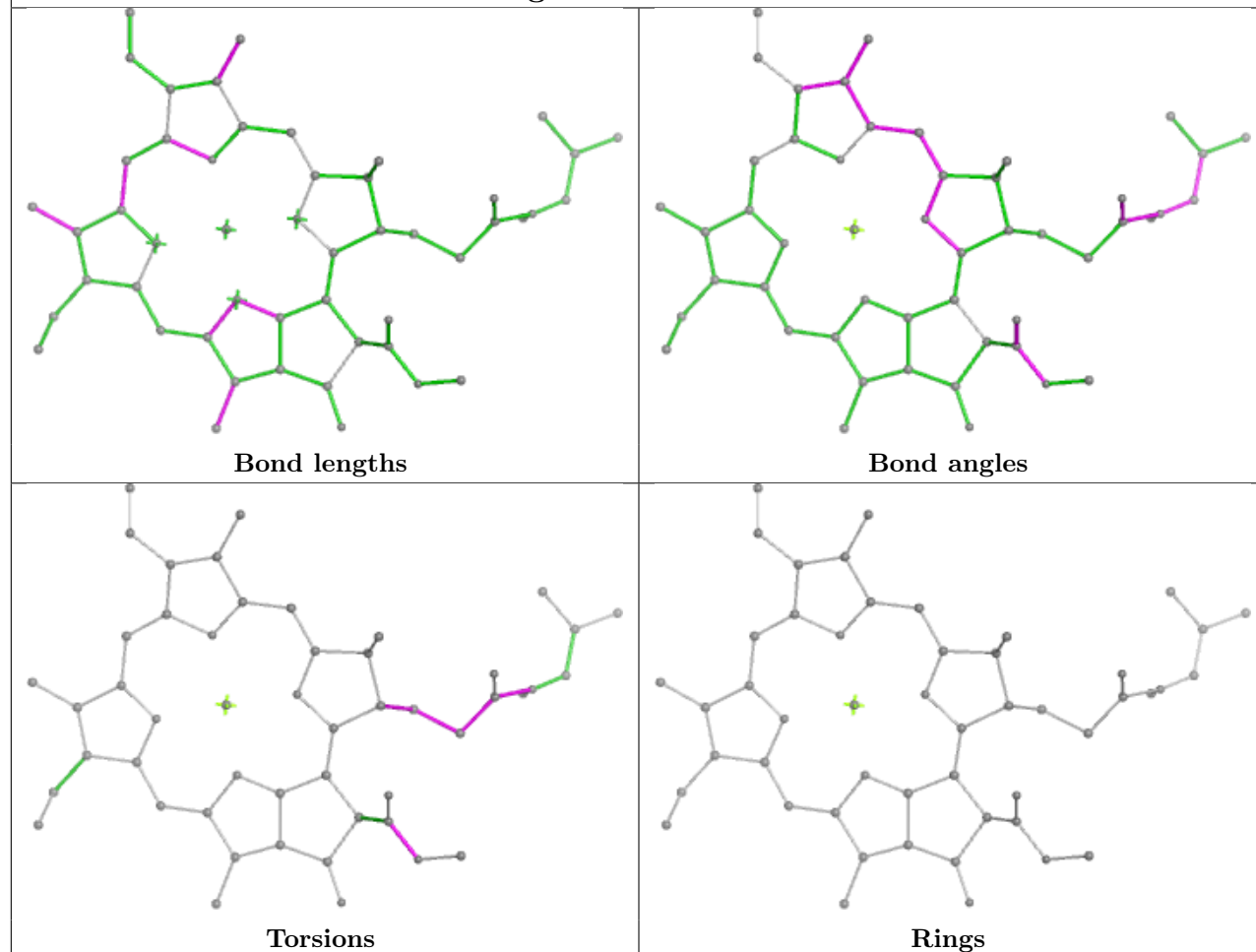


## Ligand PQN g 843

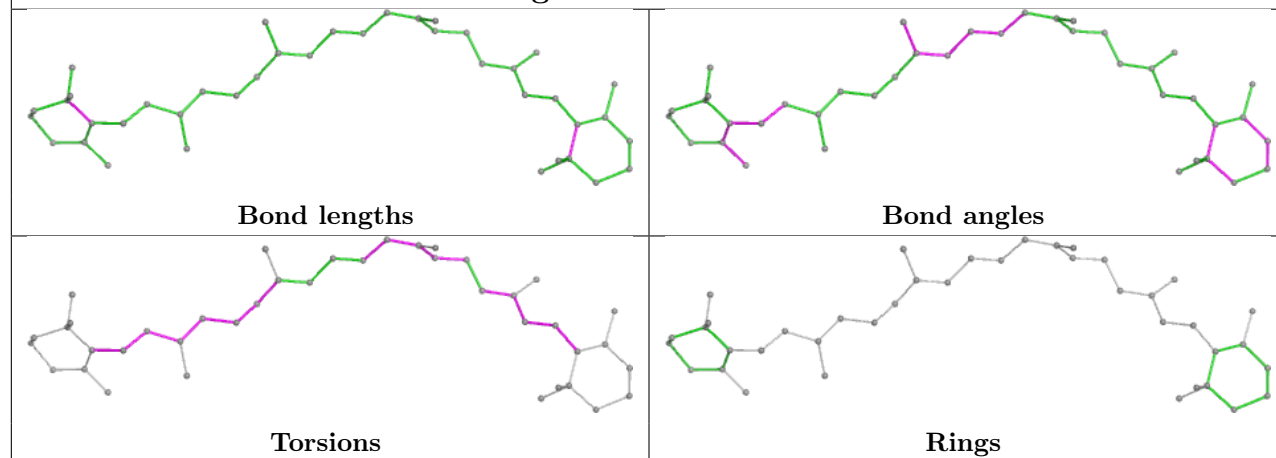




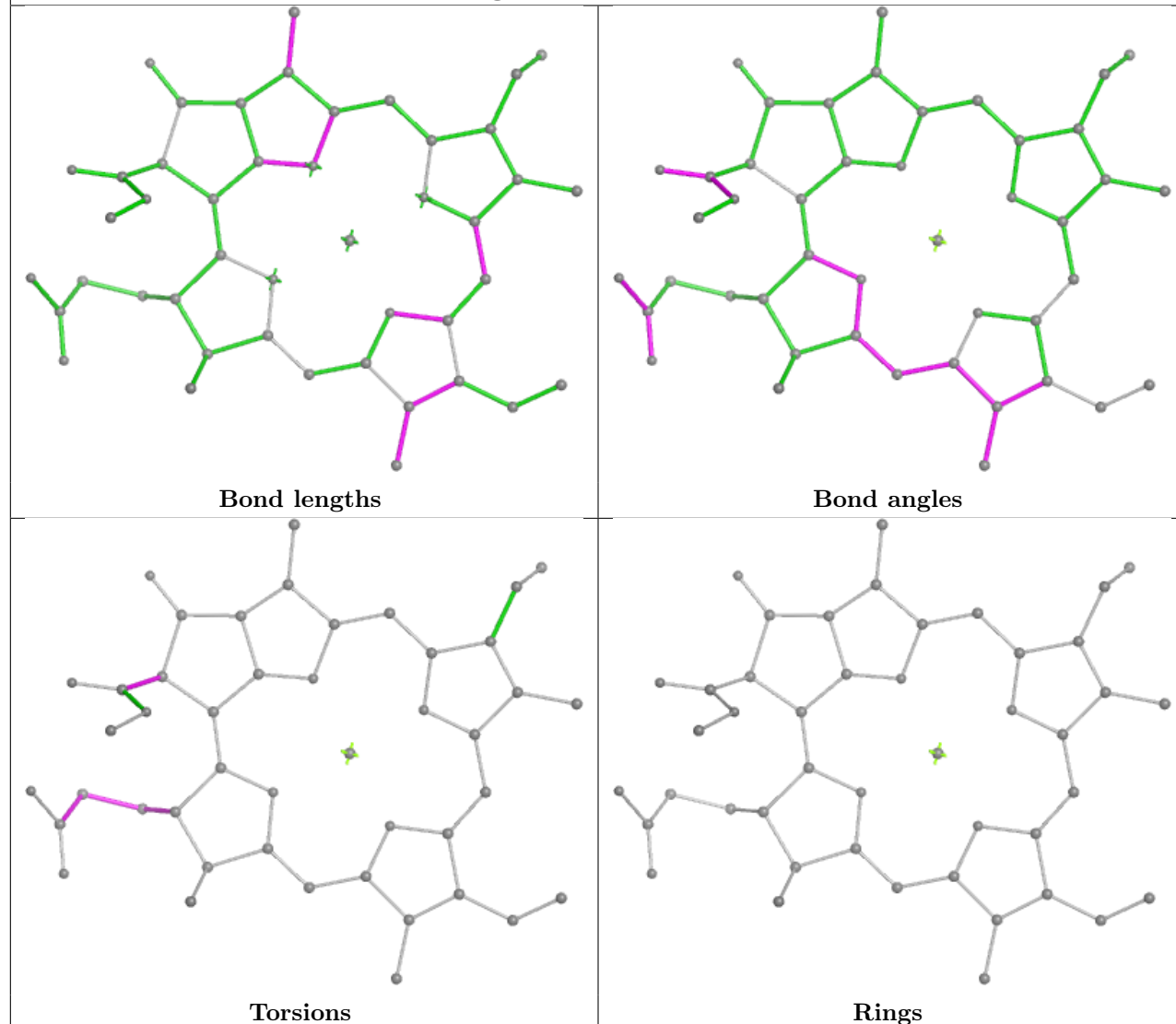
## Ligand CLA a 830



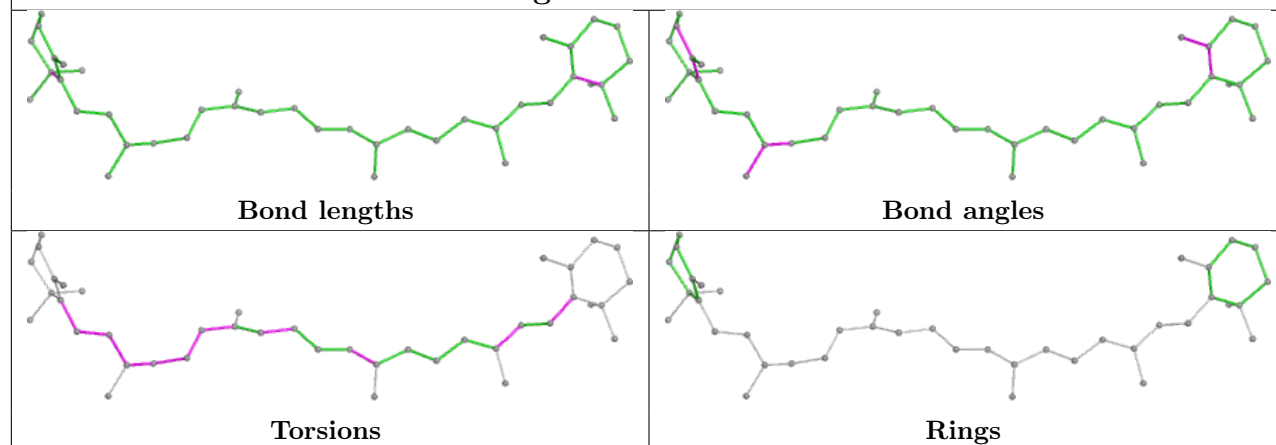
## Ligand BCR E 802

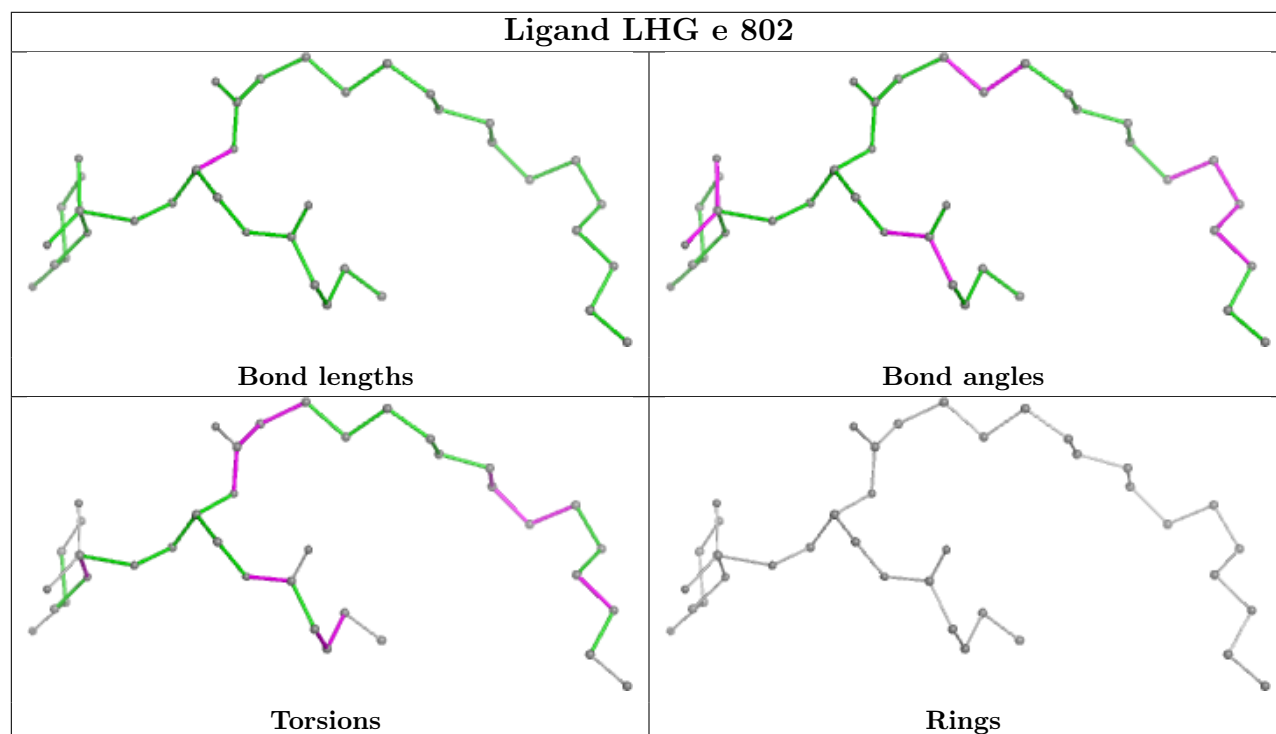
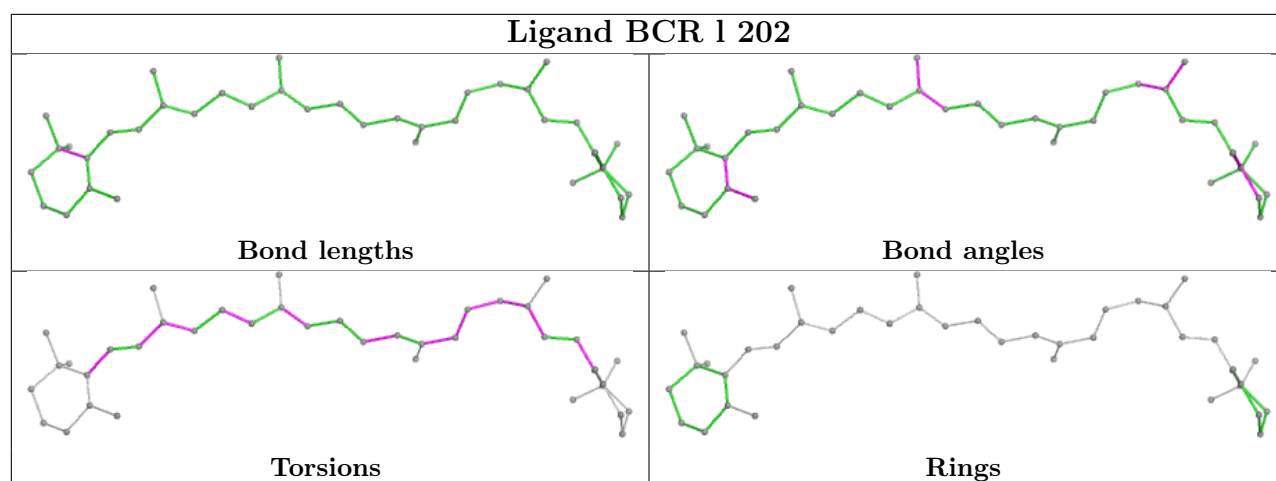


## Ligand CLA G 835

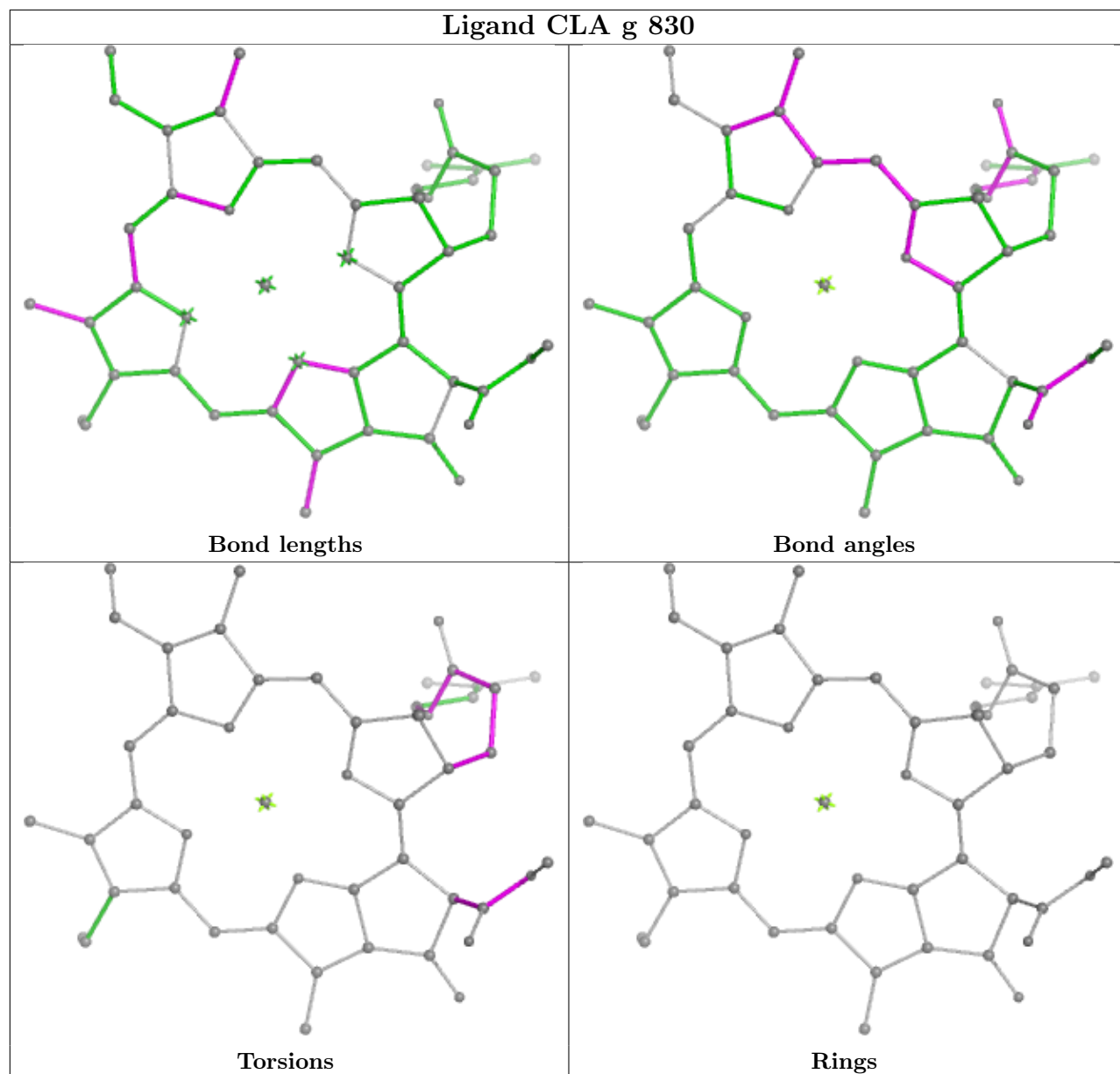


## Ligand BCR S 201

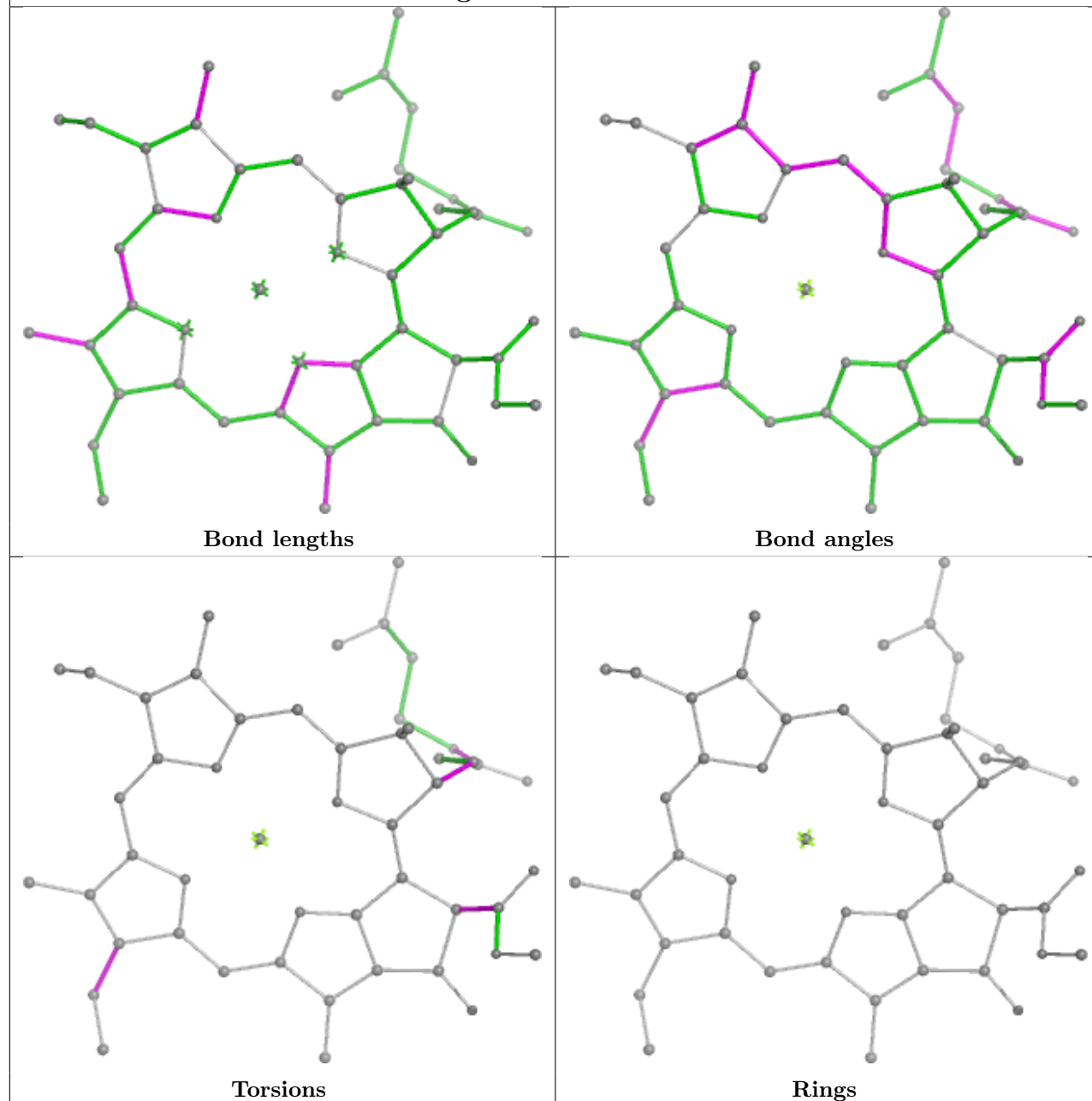




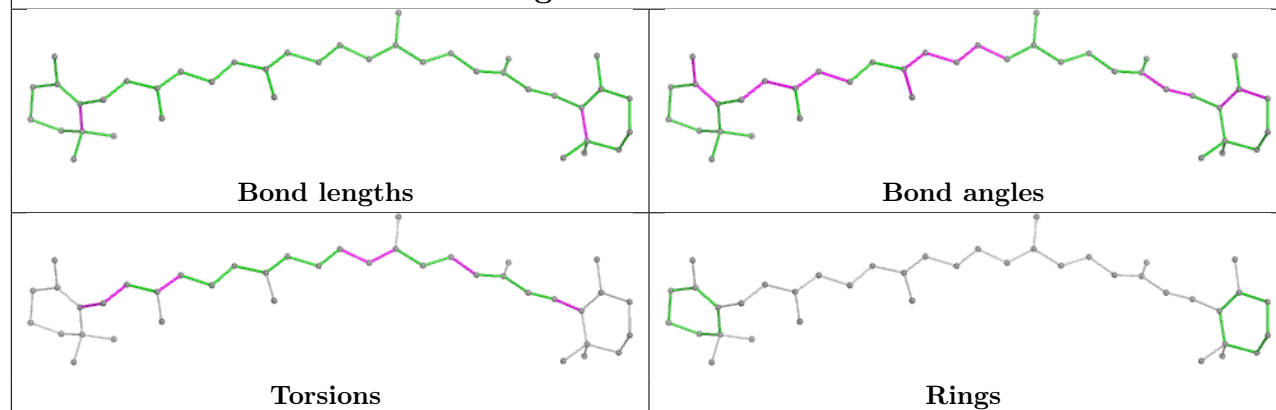
## Ligand CLA g 830



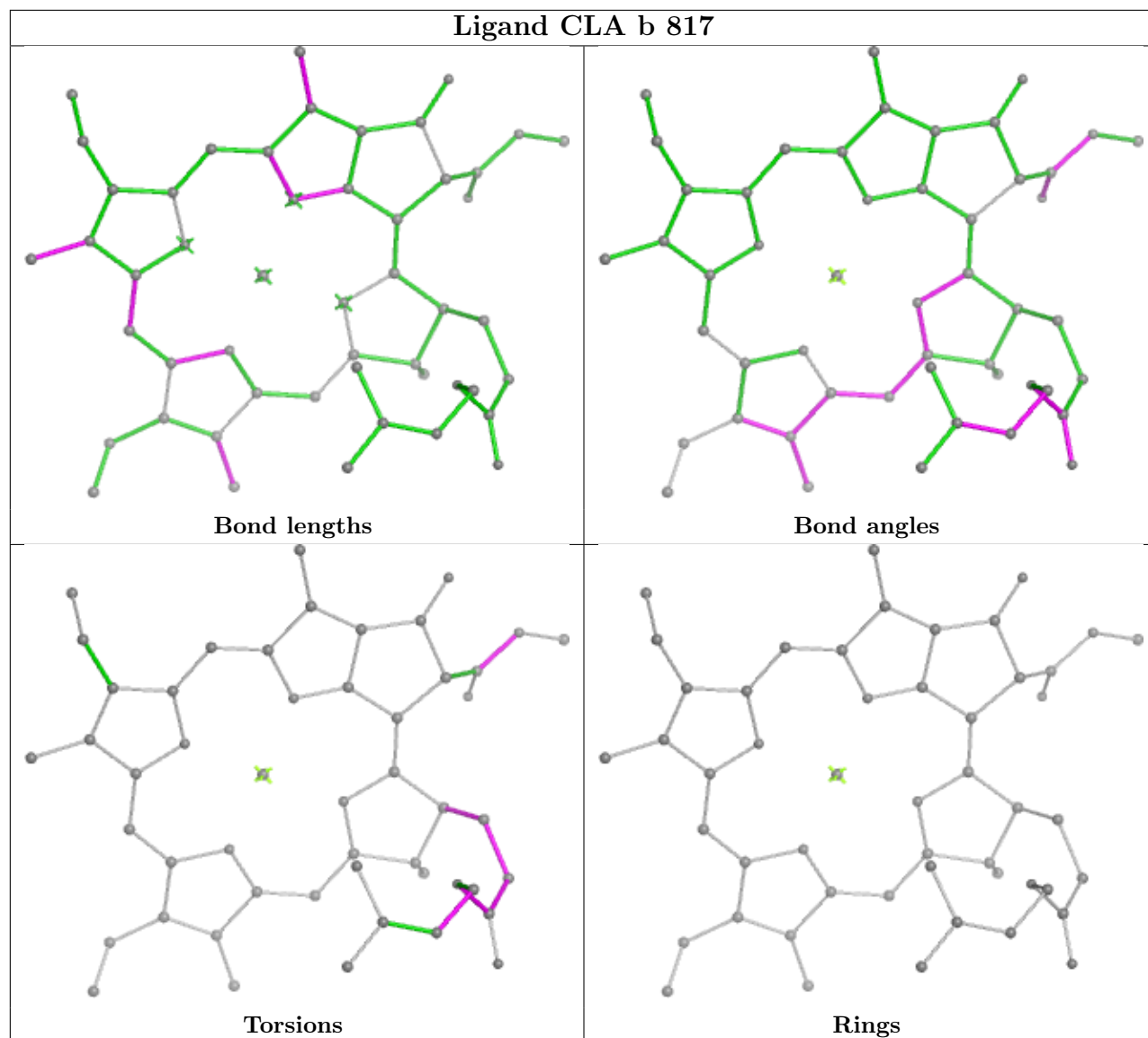
## Ligand CLA E 831



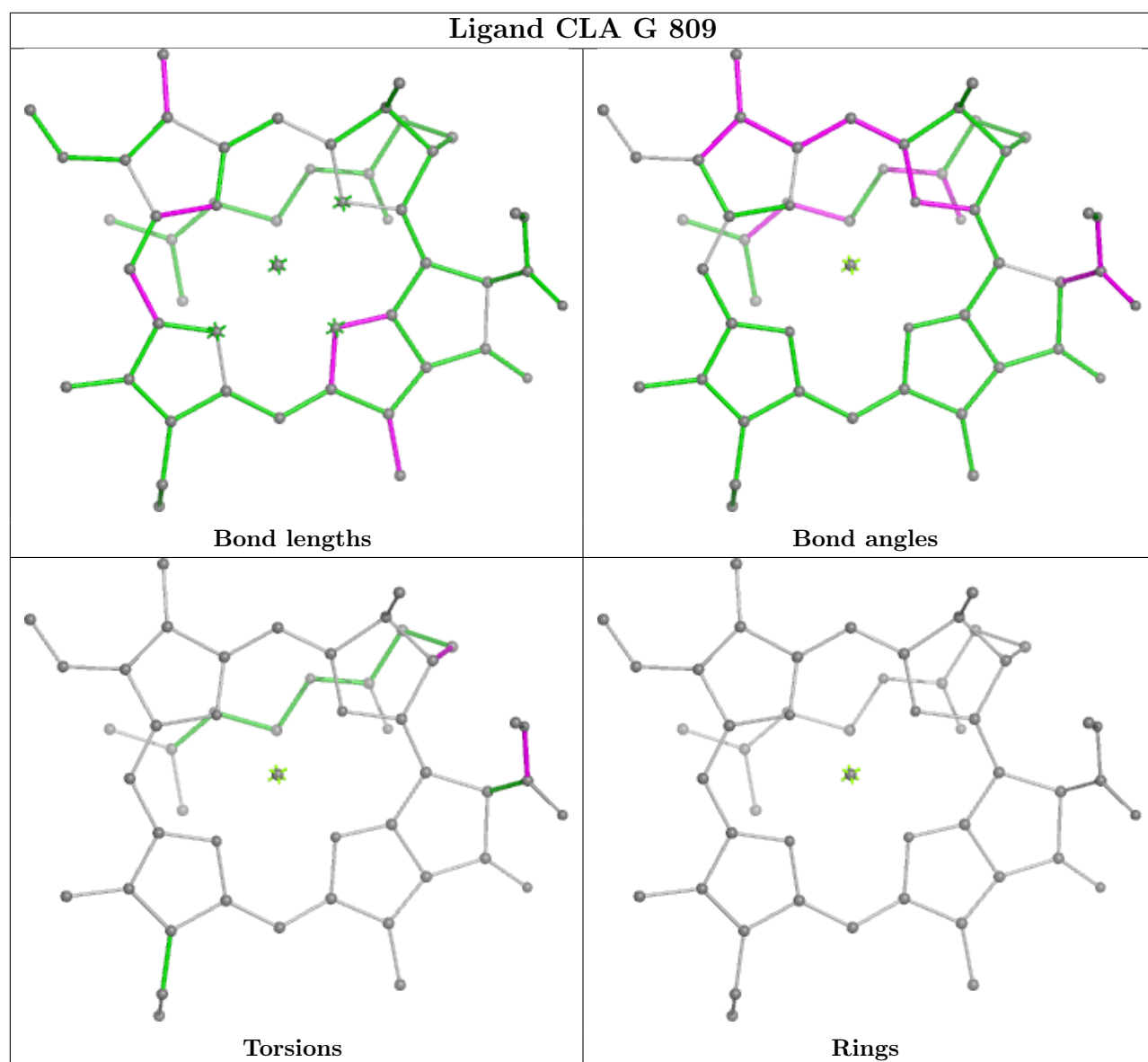
## Ligand BCR a 802

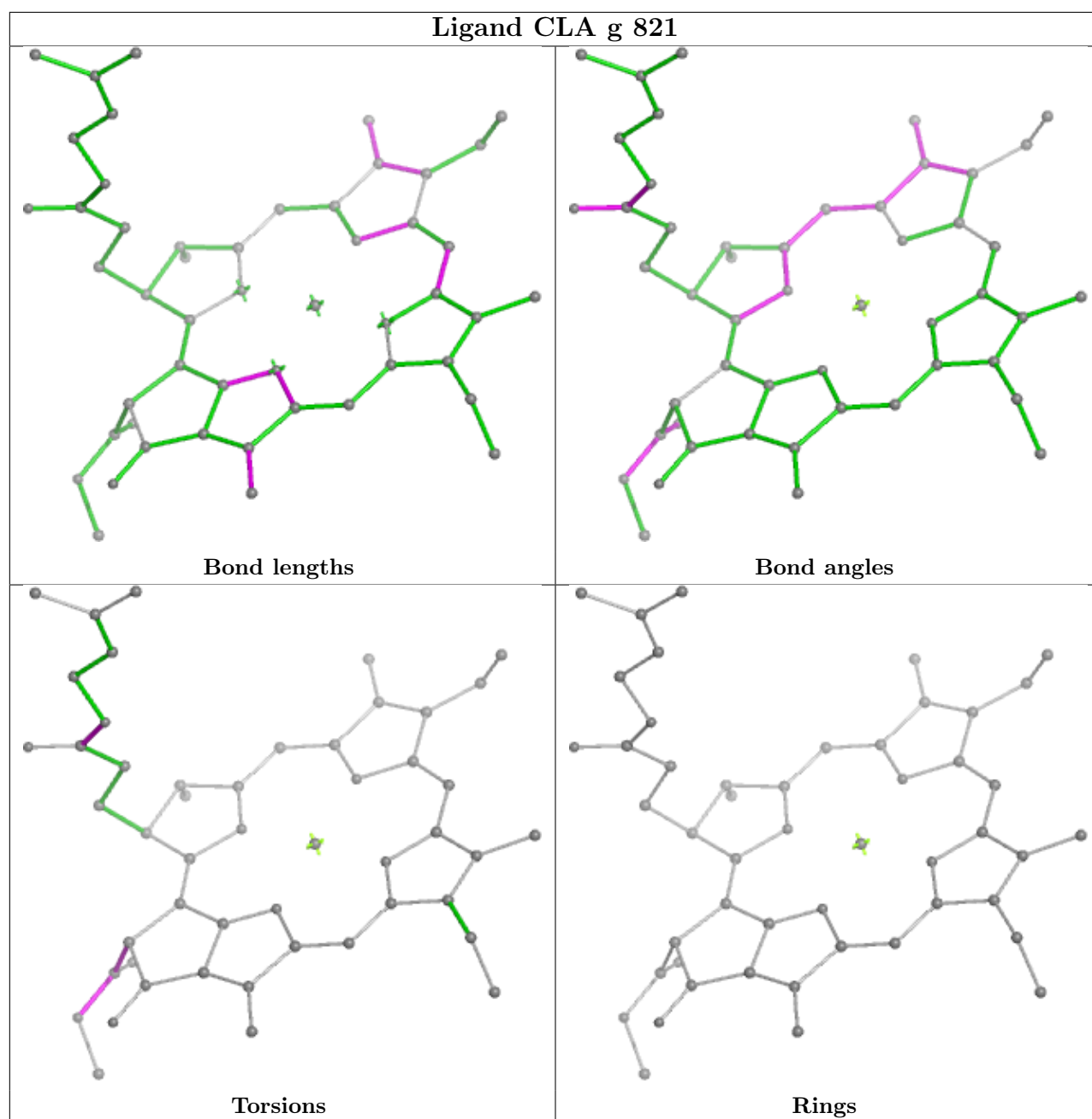


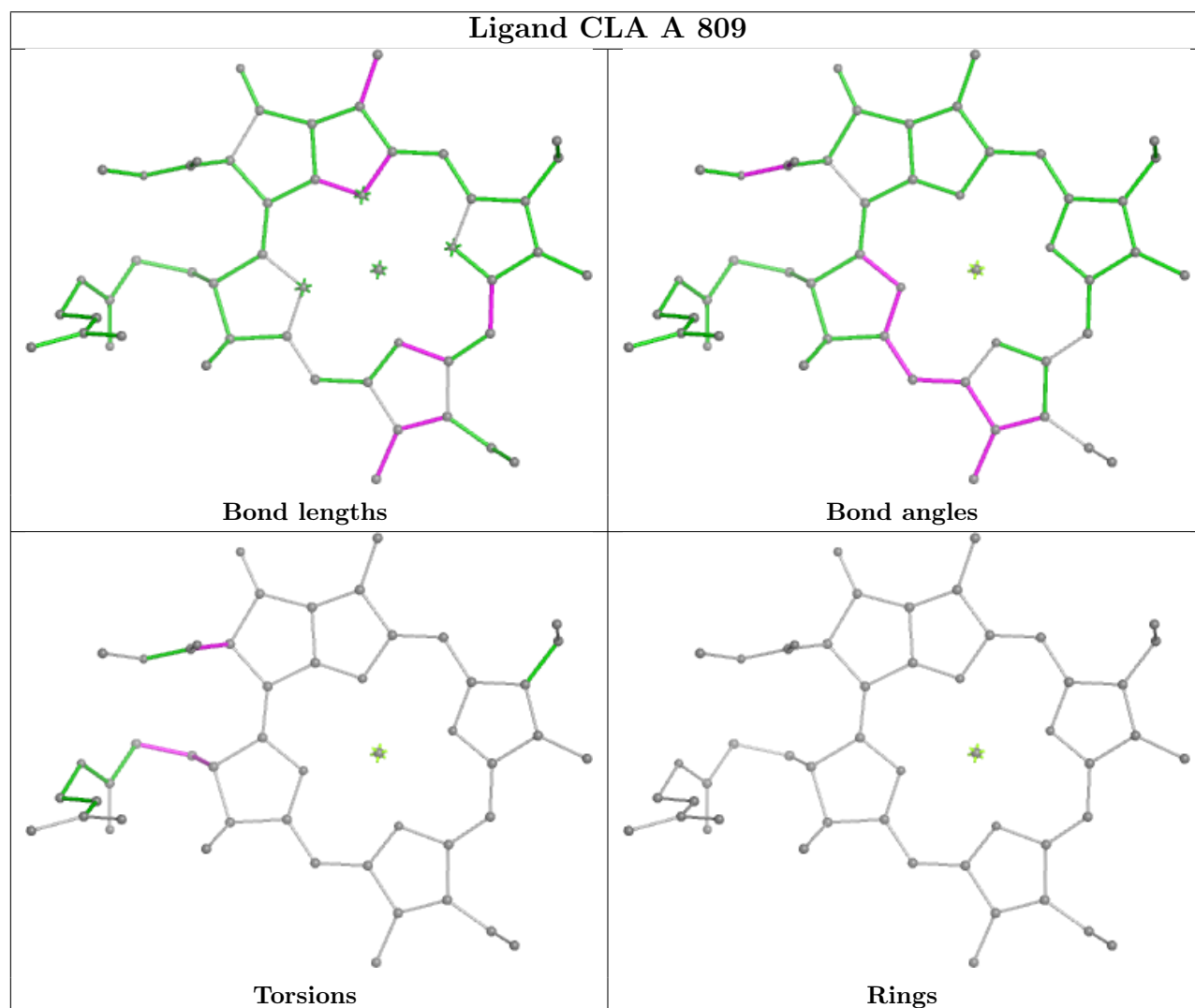
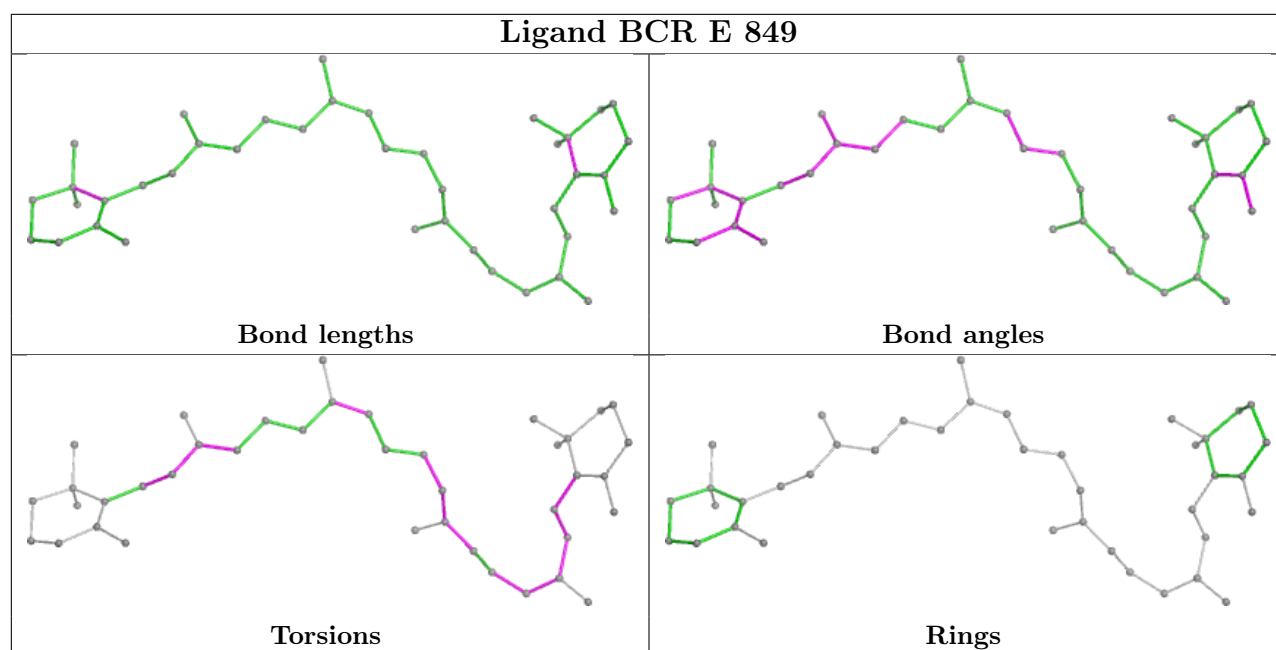
## Ligand CLA b 817

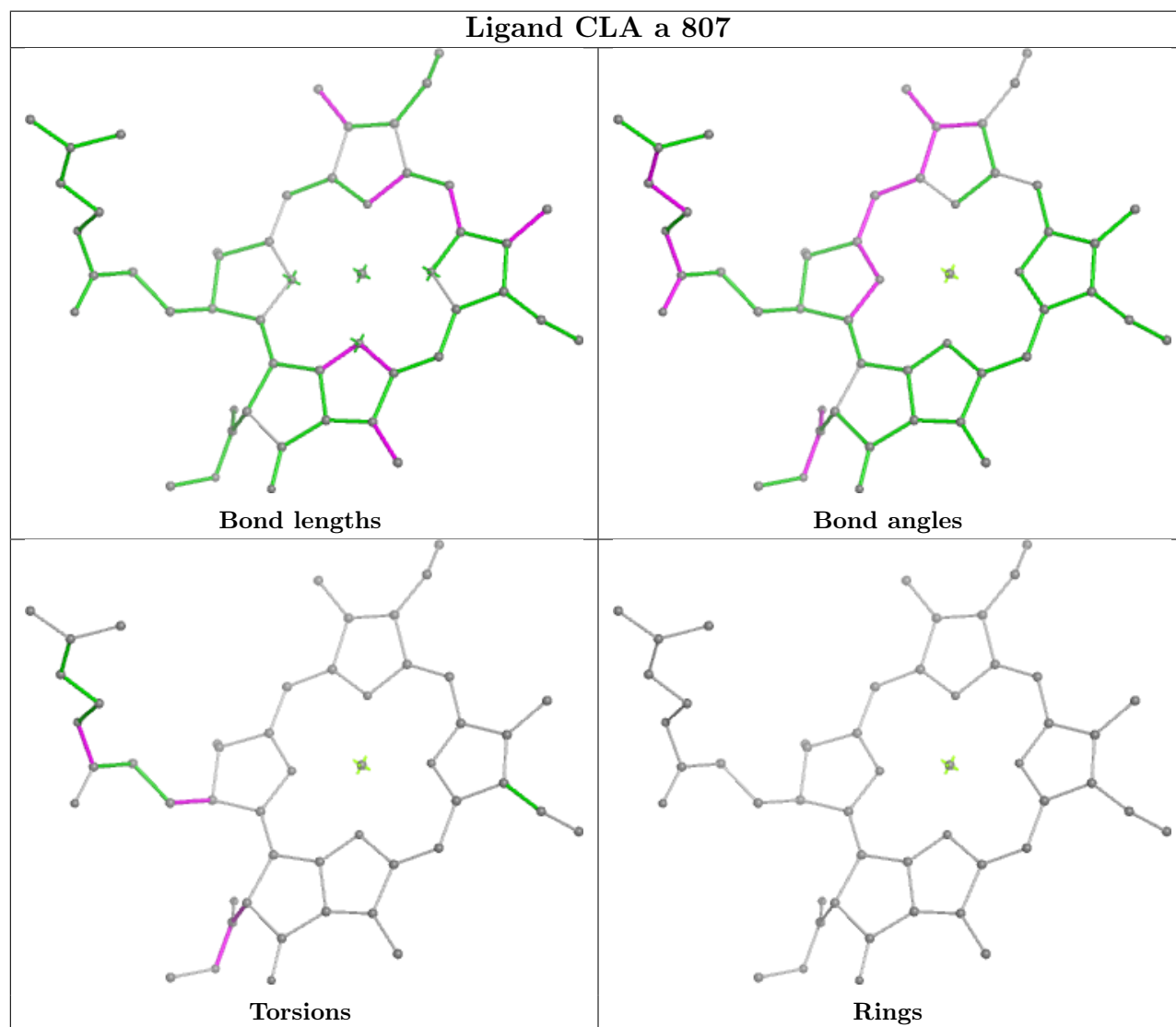
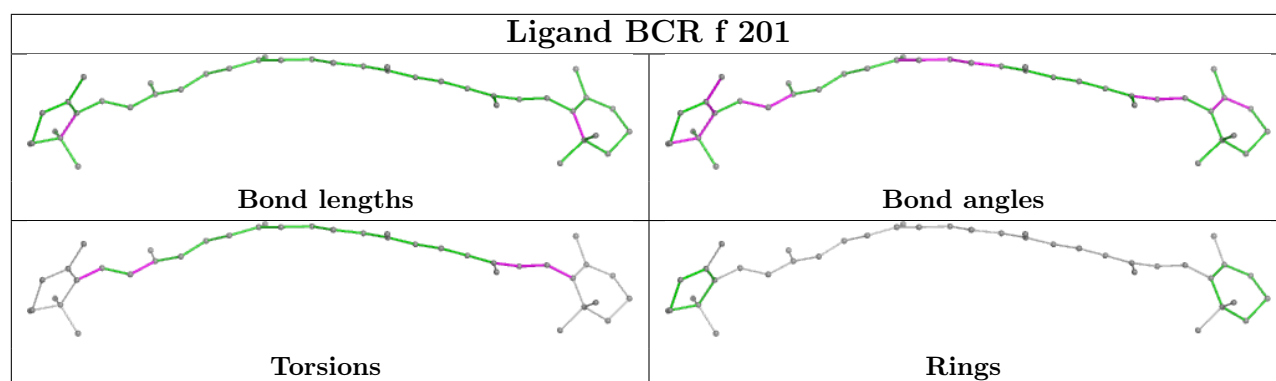




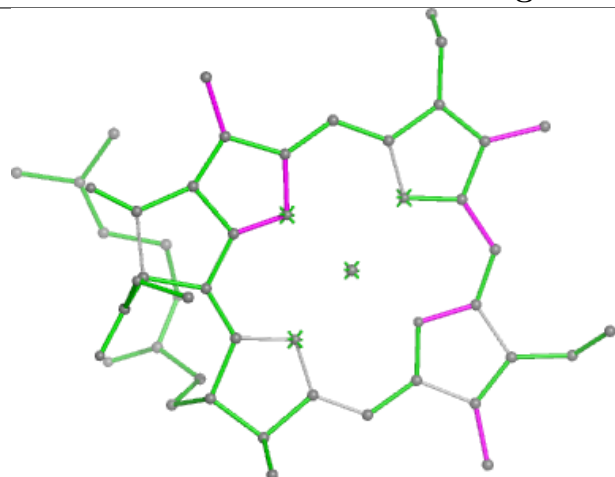




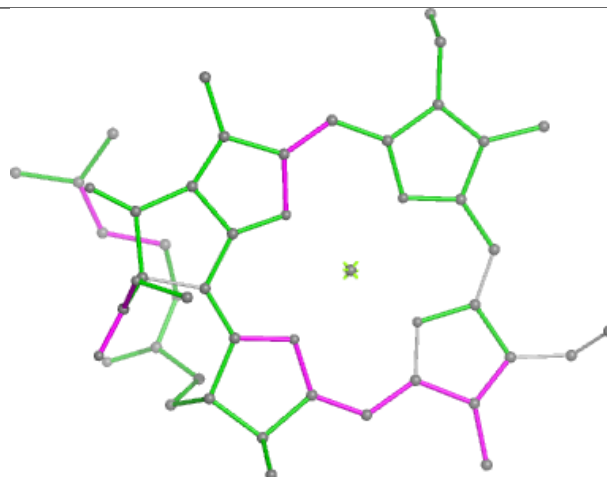




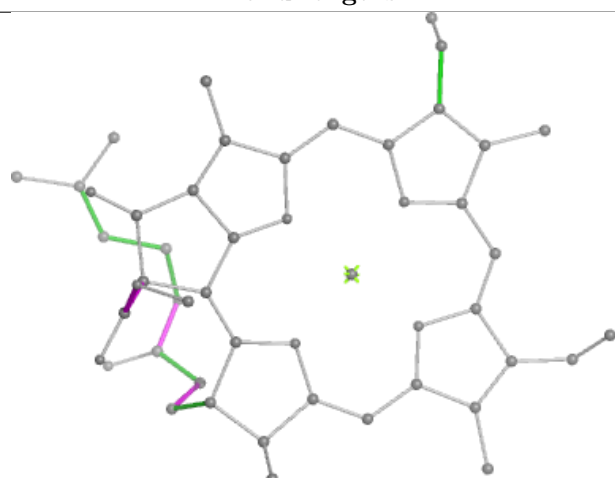
## Ligand CLA A 810



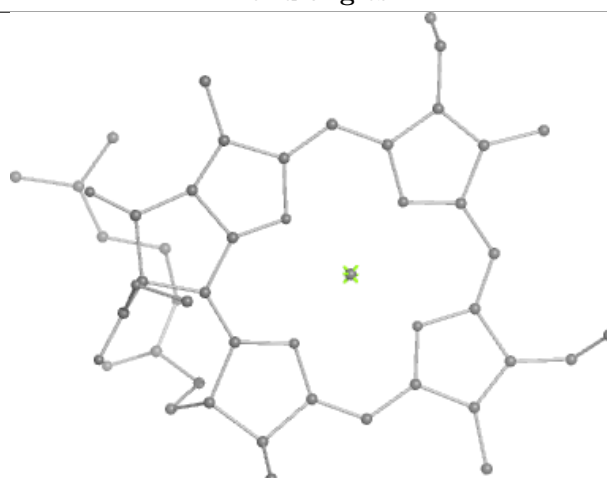
Bond lengths



Bond angles

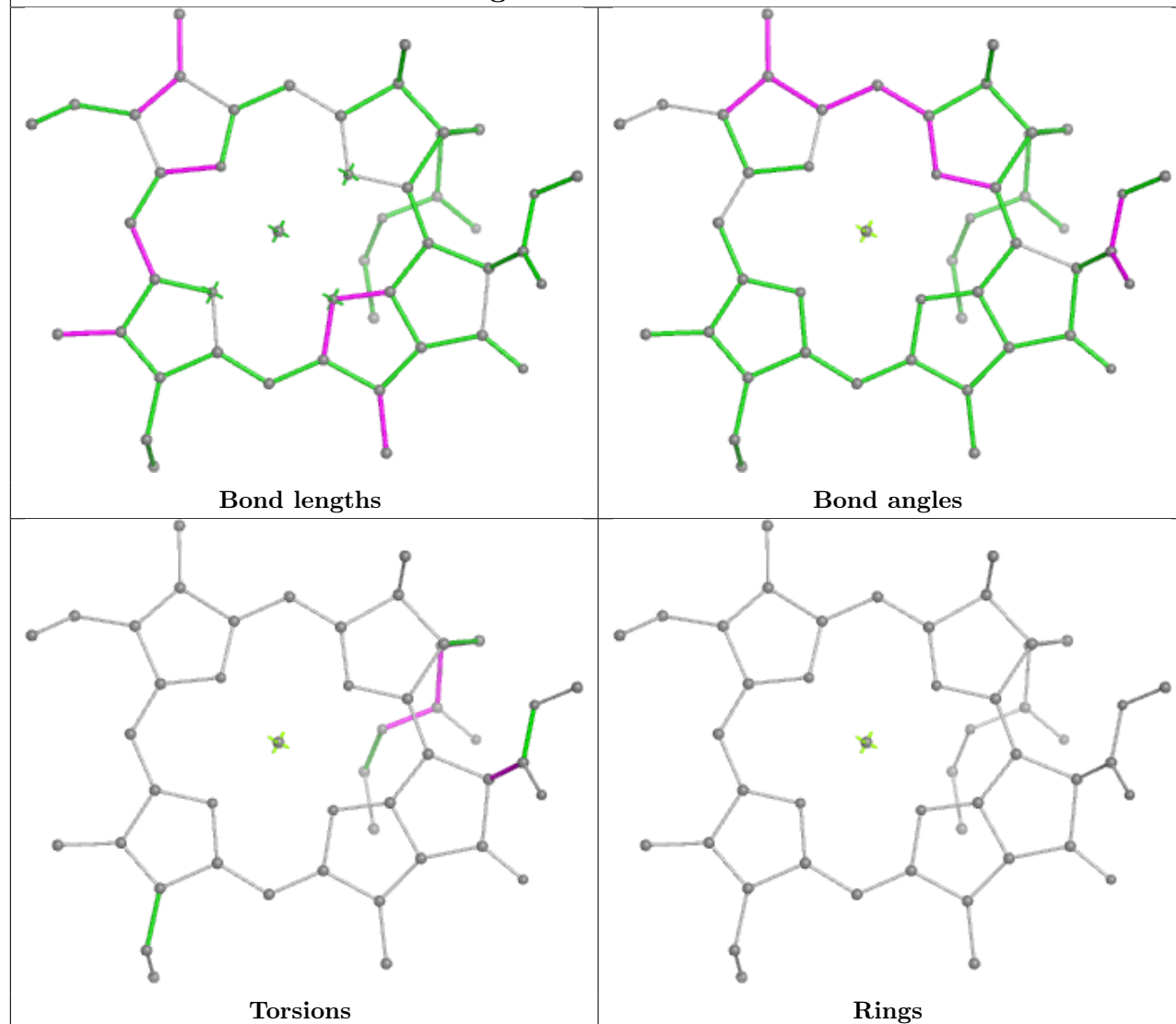


Torsions

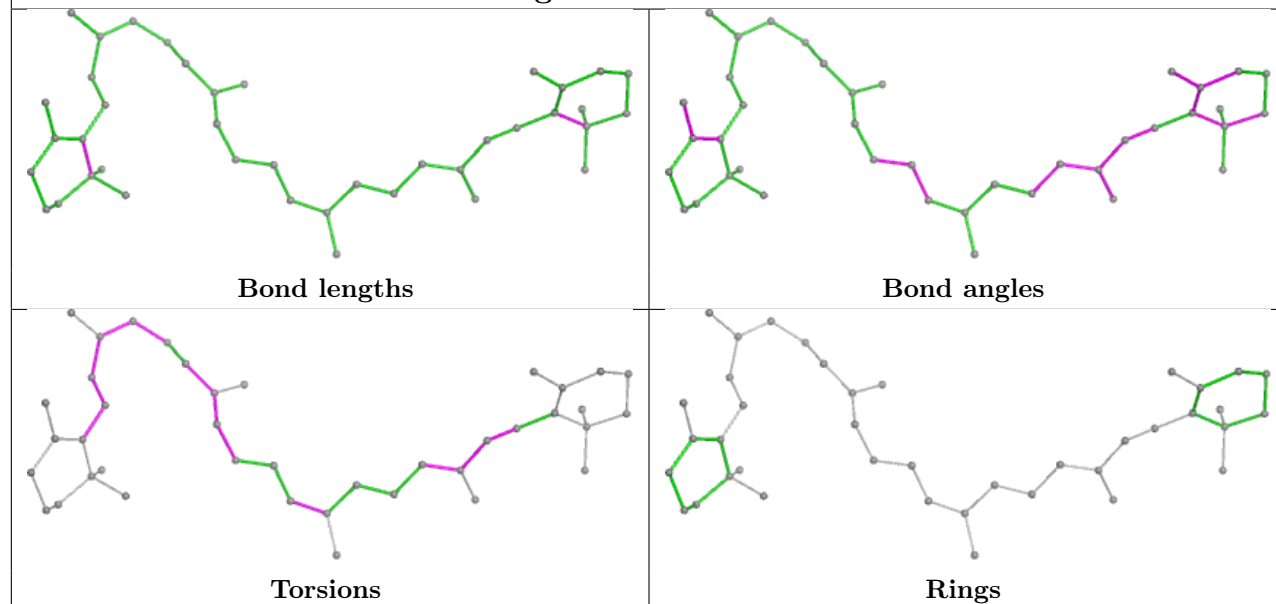


Rings

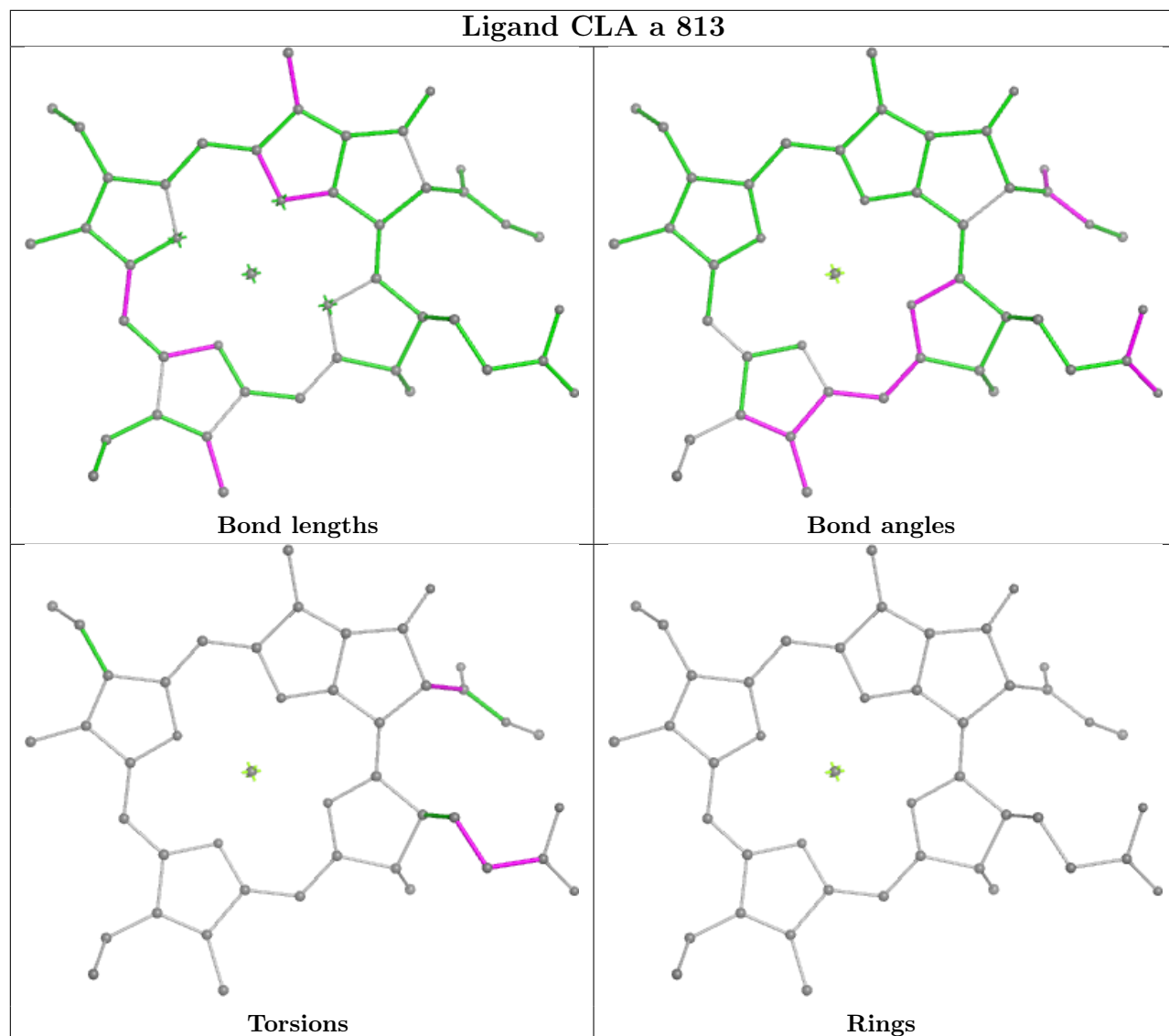
## Ligand CLA A 841



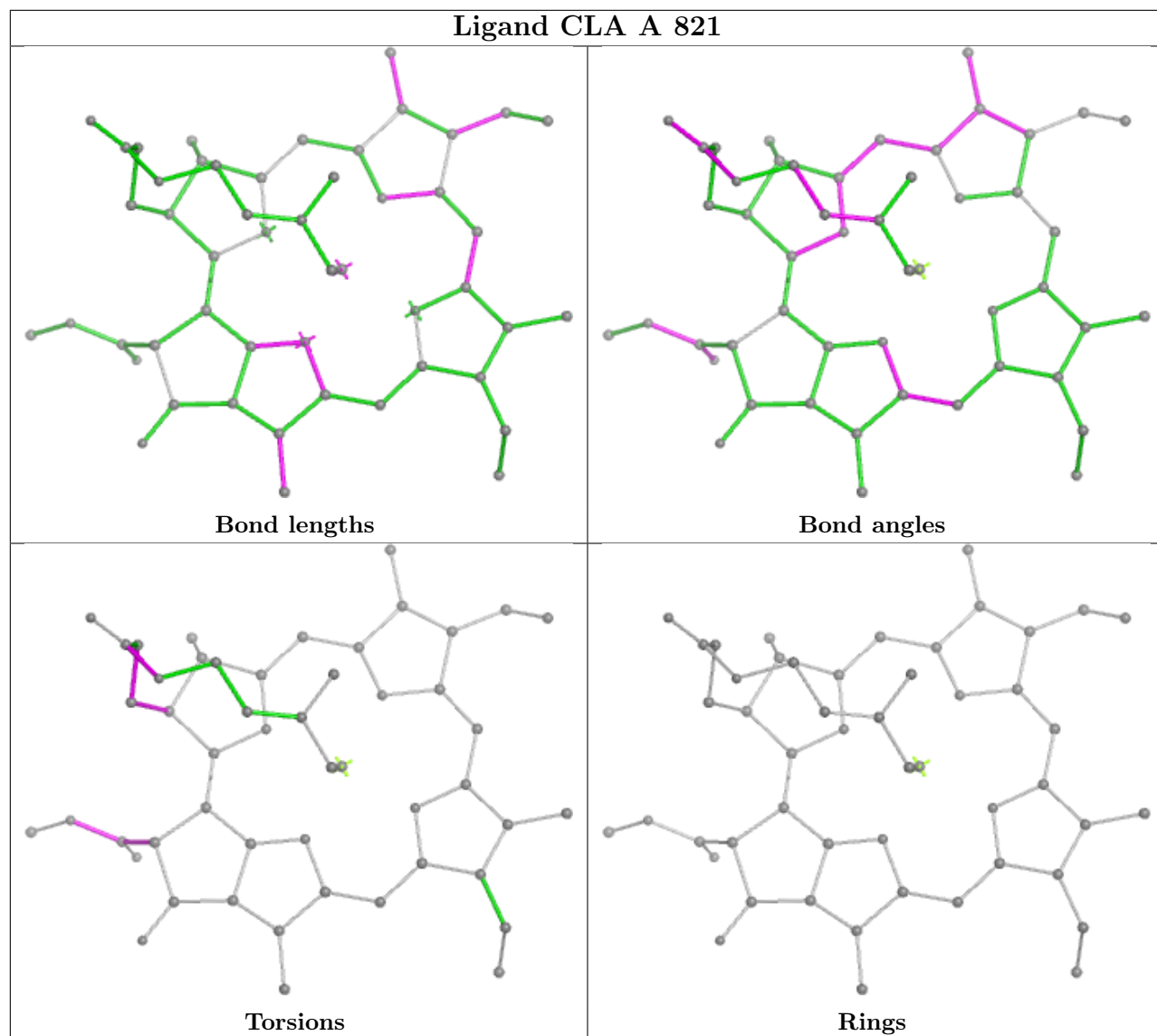
## Ligand BCR a 849



## Ligand CLA a 813

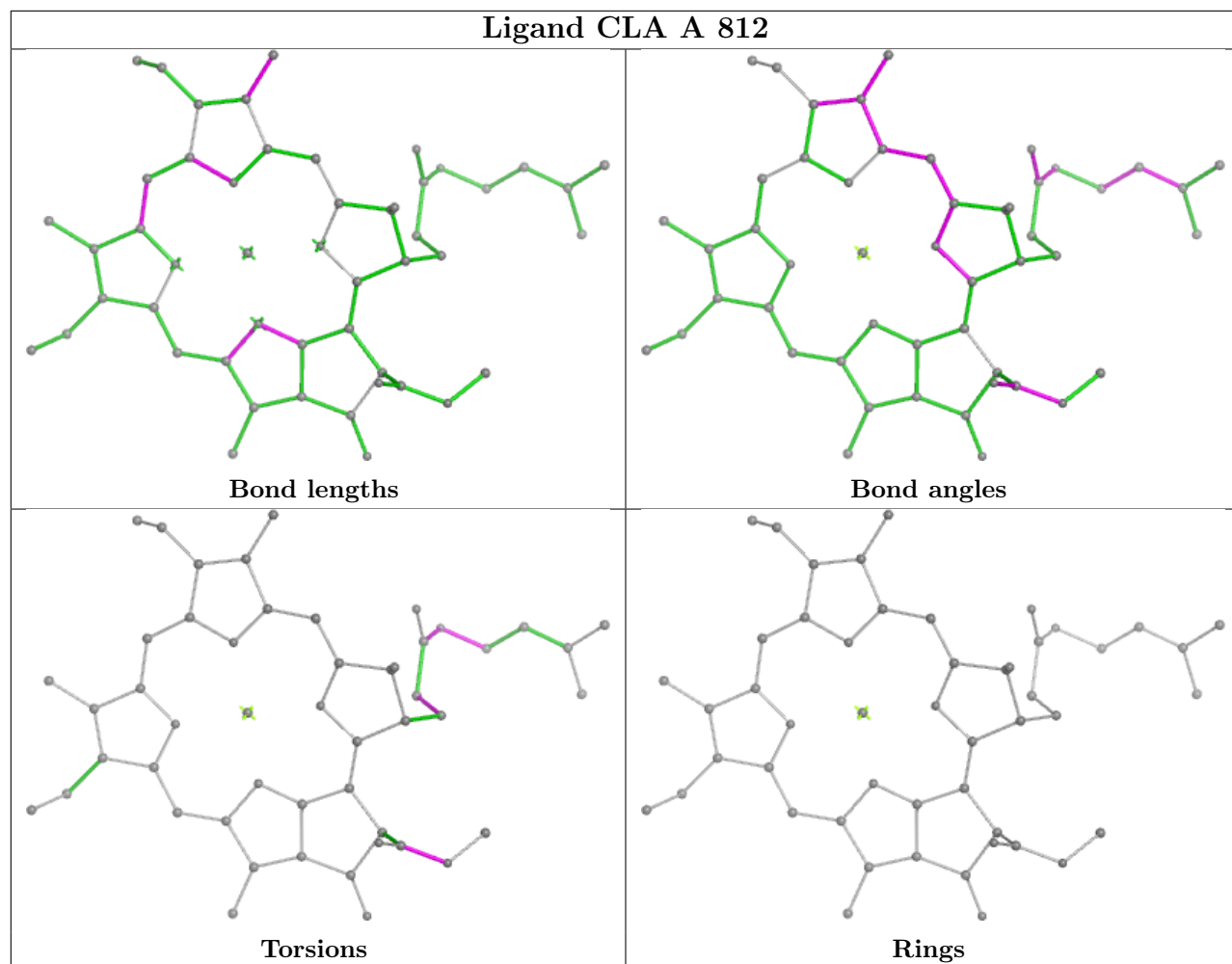


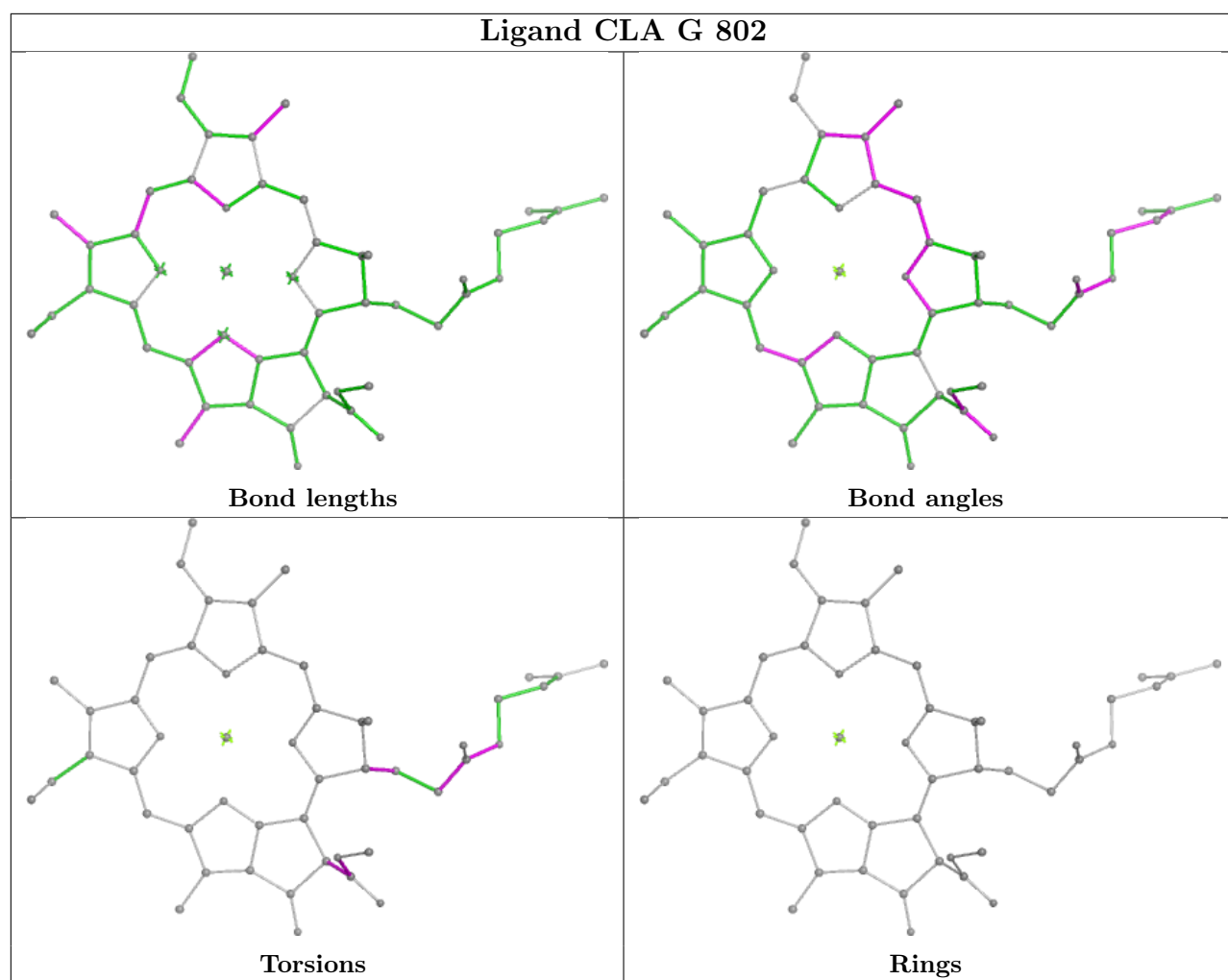
## Ligand CLA A 821



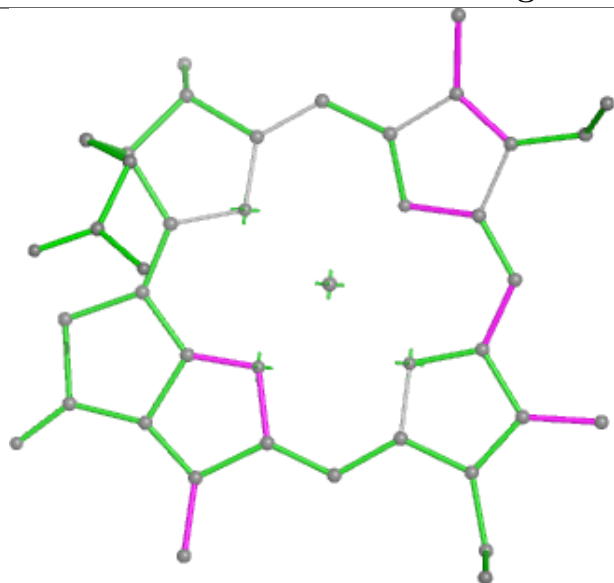


## Ligand CLA A 812

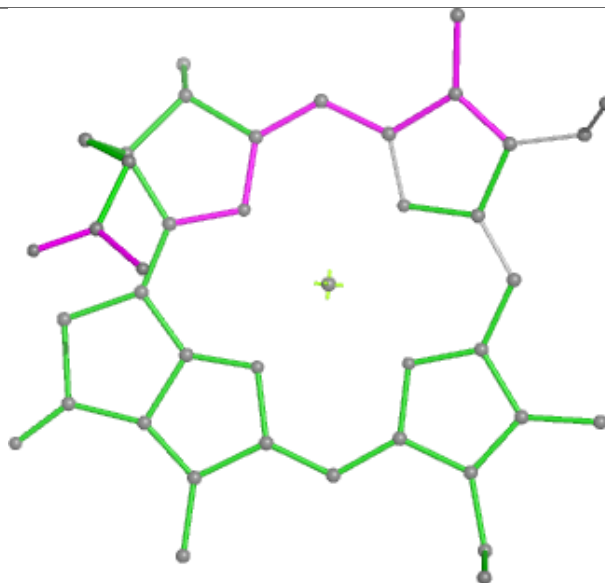




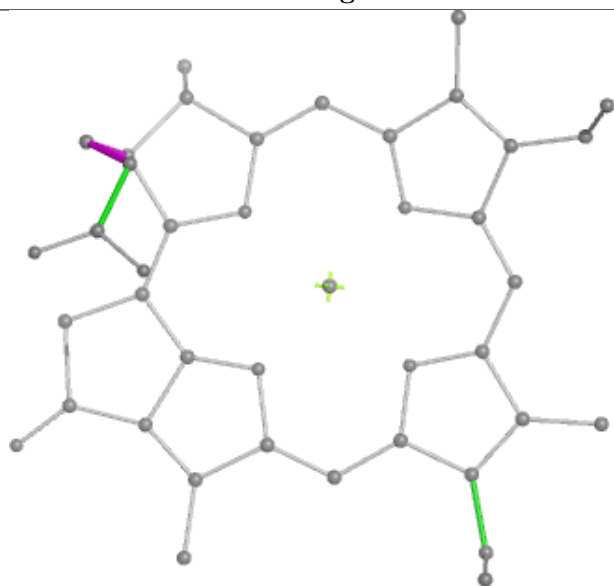
## Ligand CLA b 801



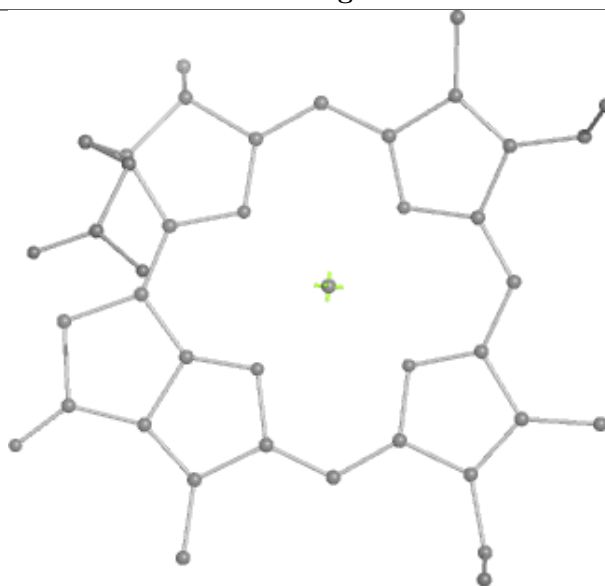
Bond lengths



Bond angles

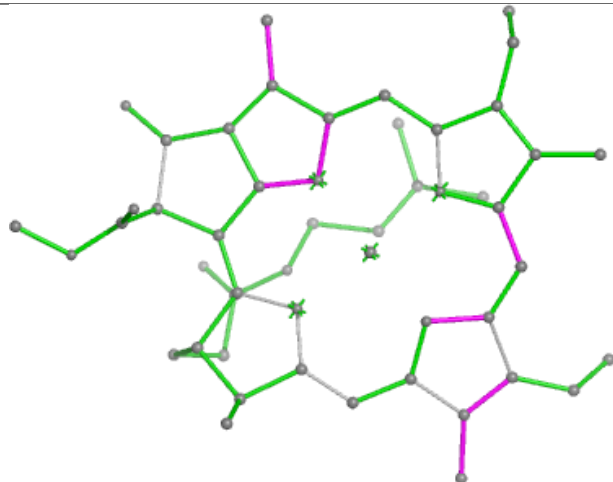


Torsions

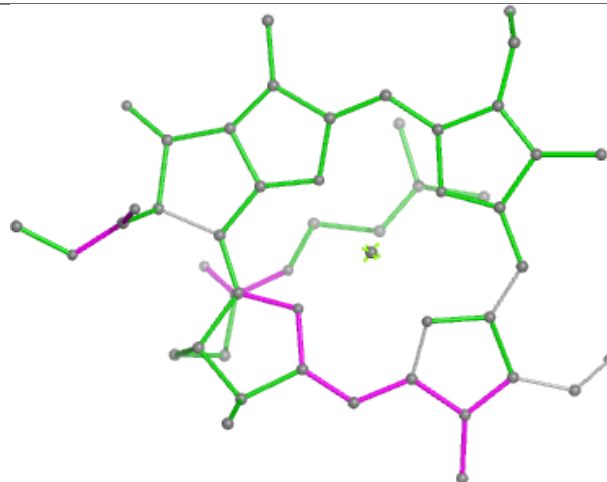


Rings

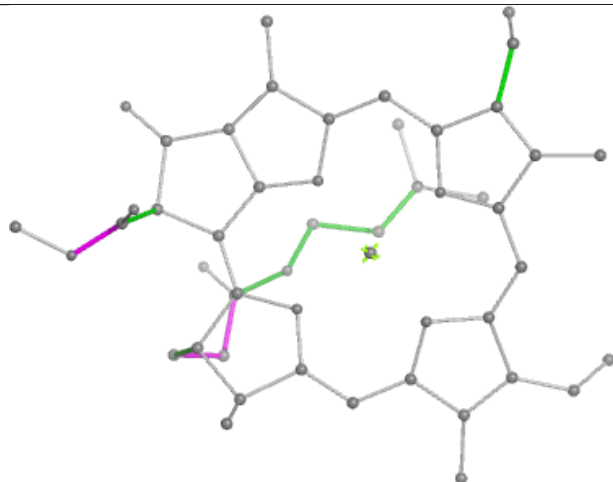
## Ligand CLA G 808



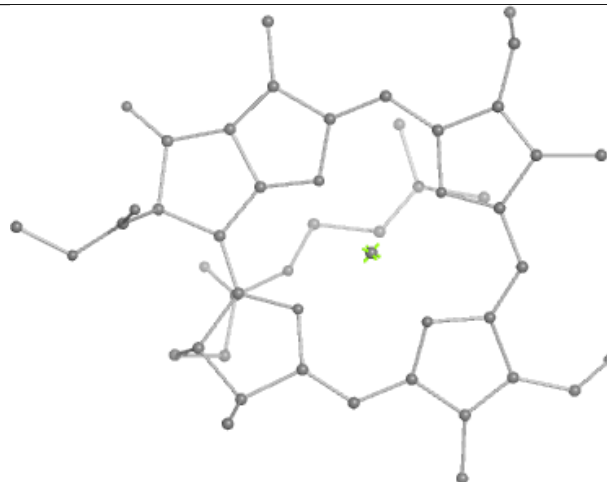
Bond lengths



Bond angles

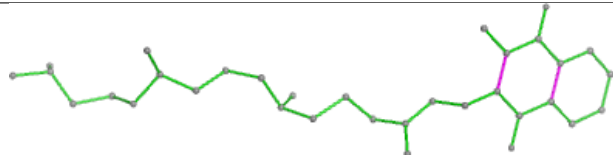


Torsions

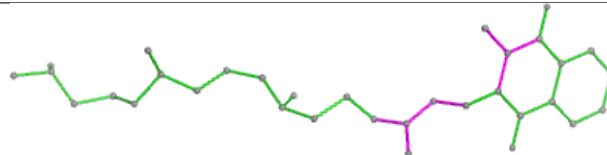


Rings

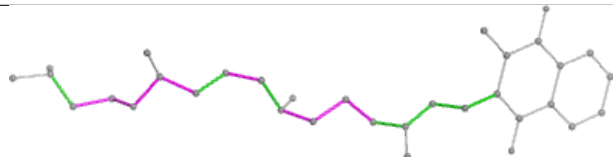
## Ligand PQN B 842



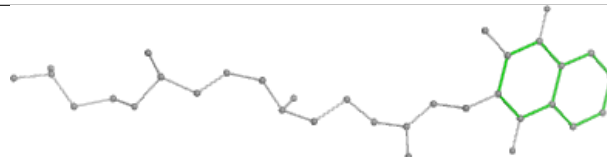
Bond lengths



Bond angles

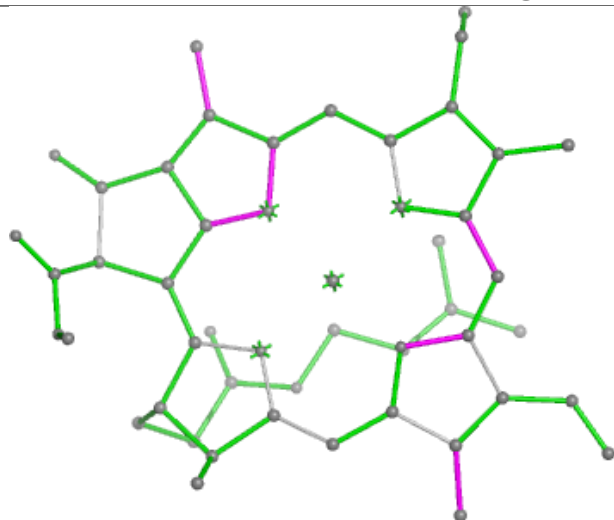


Torsions

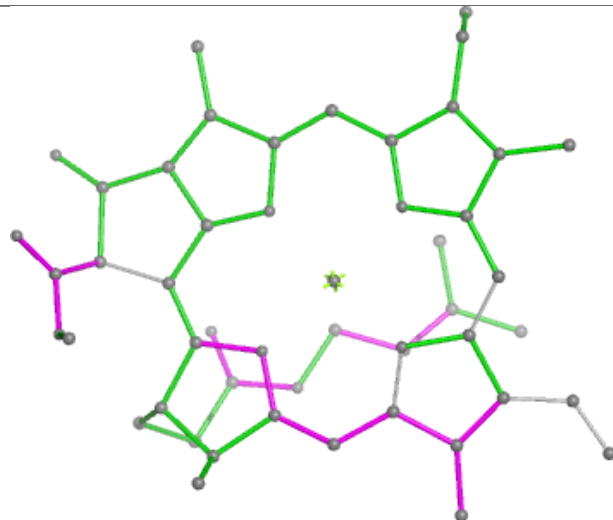


Rings

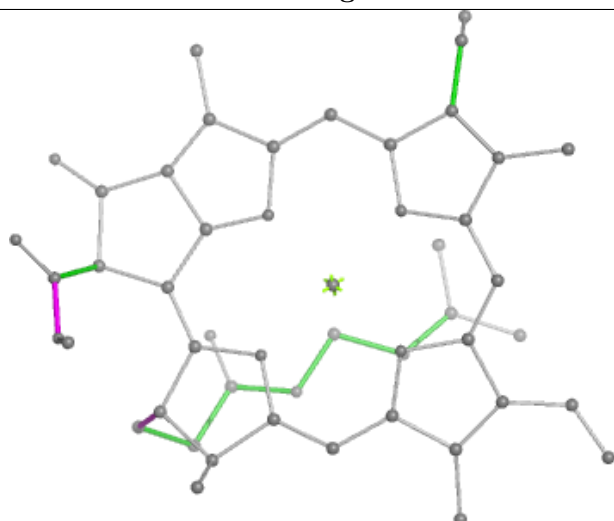
## Ligand CLA b 809



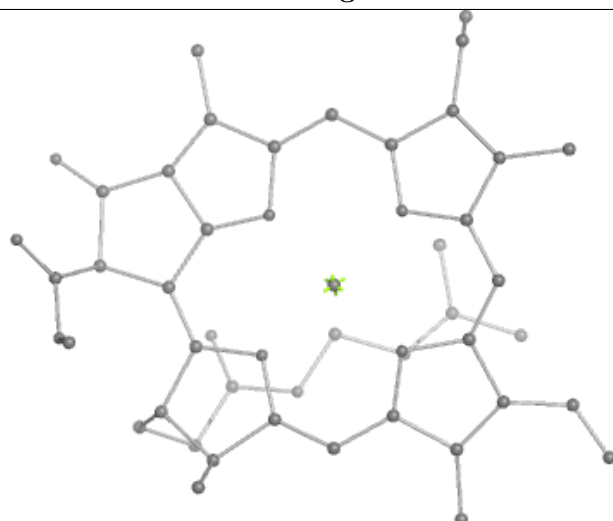
Bond lengths



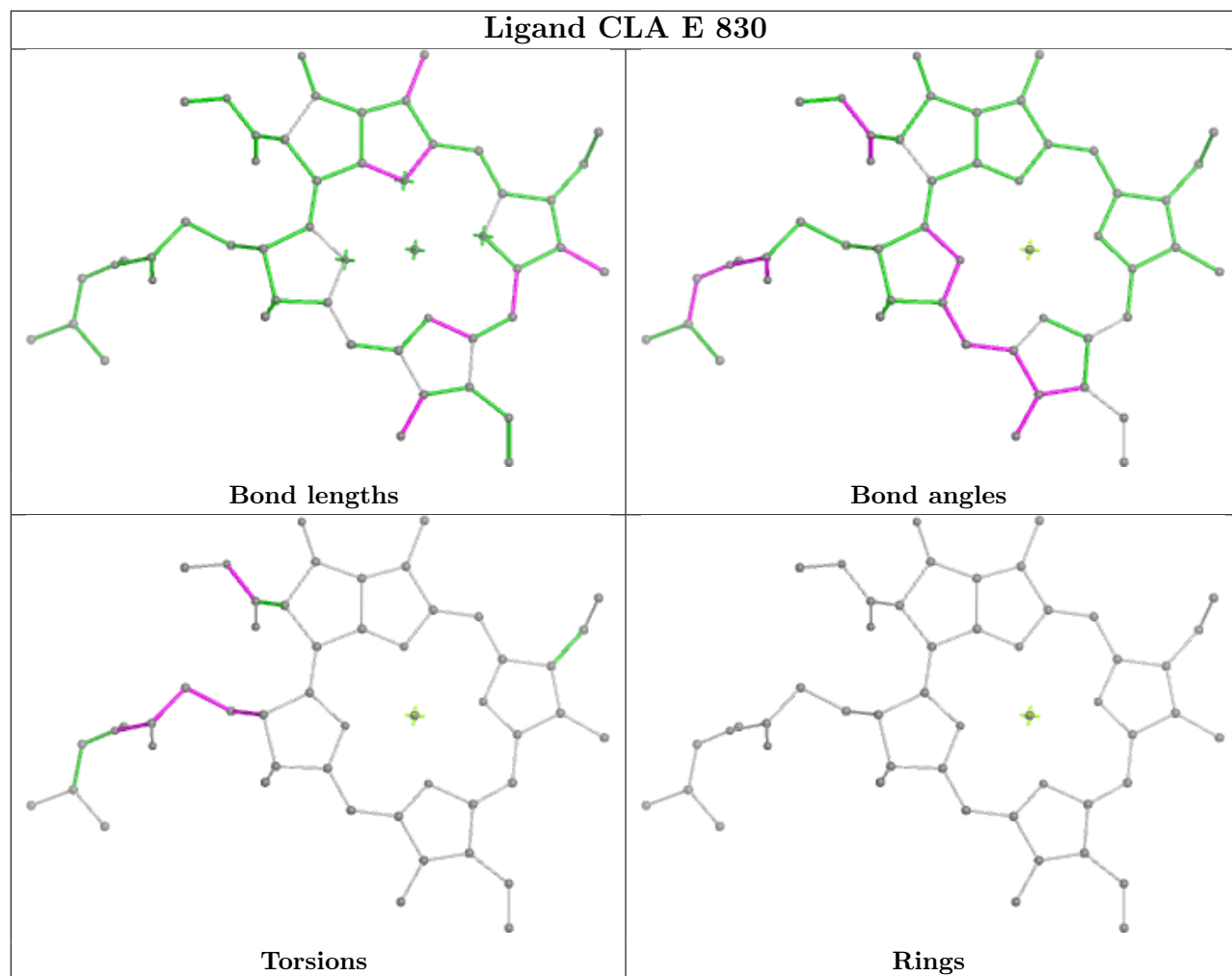
Bond angles



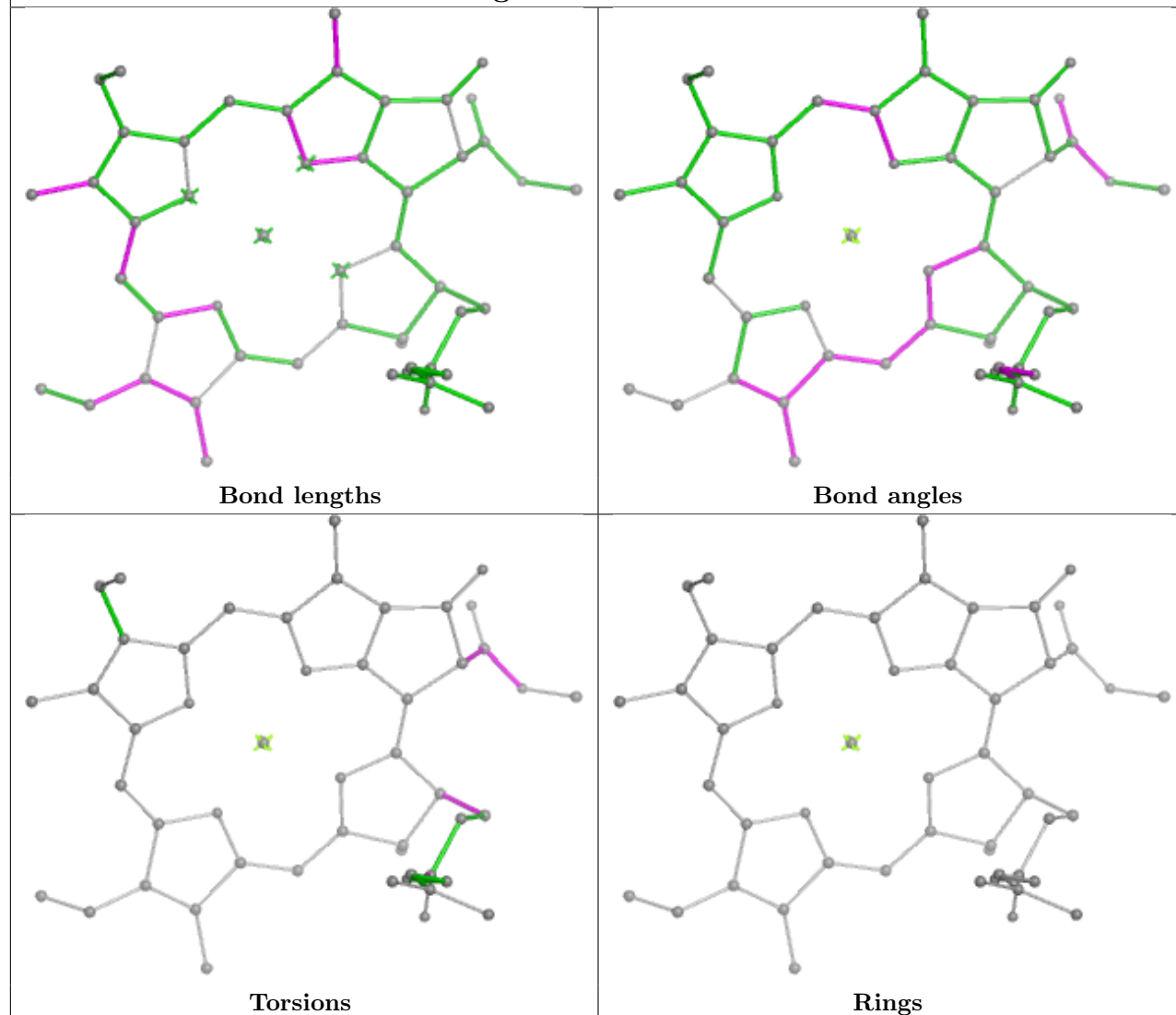
Torsions



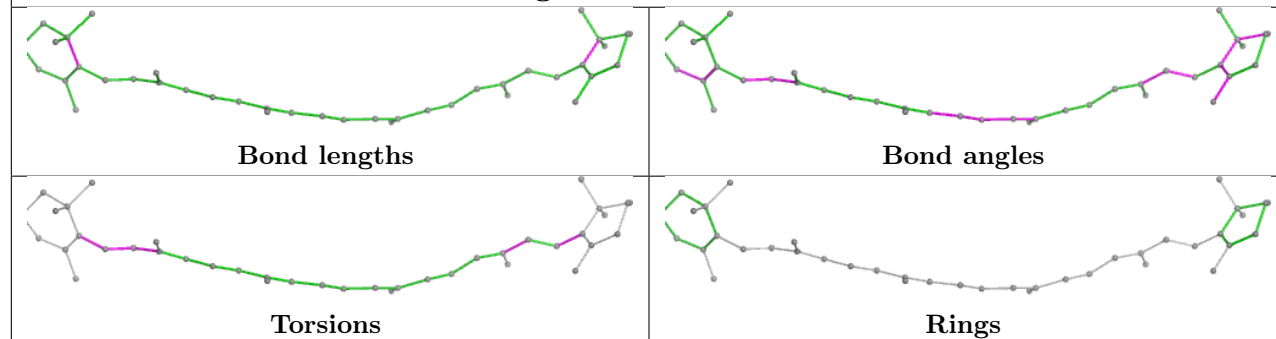
Rings



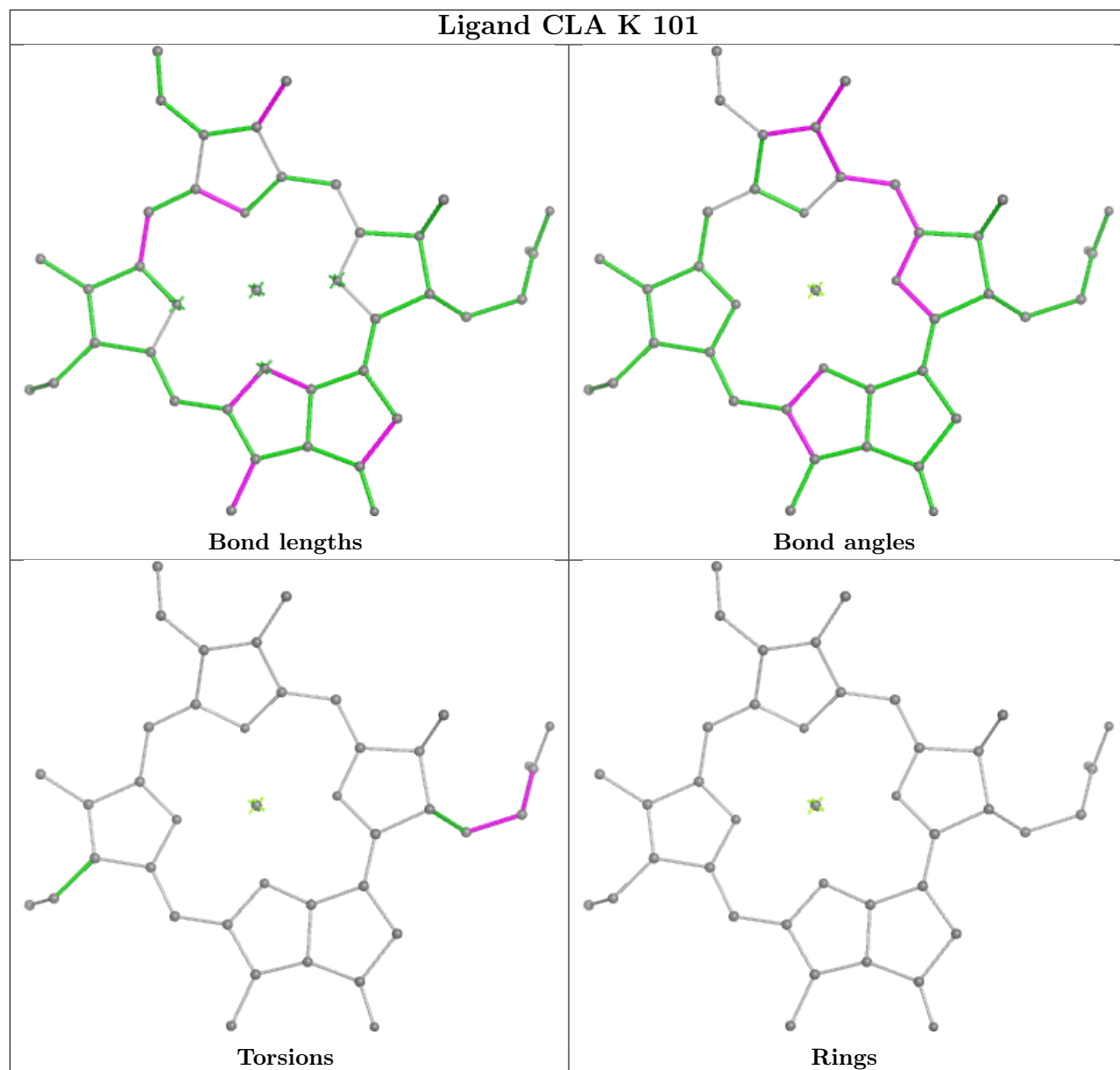
## Ligand CLA b 839



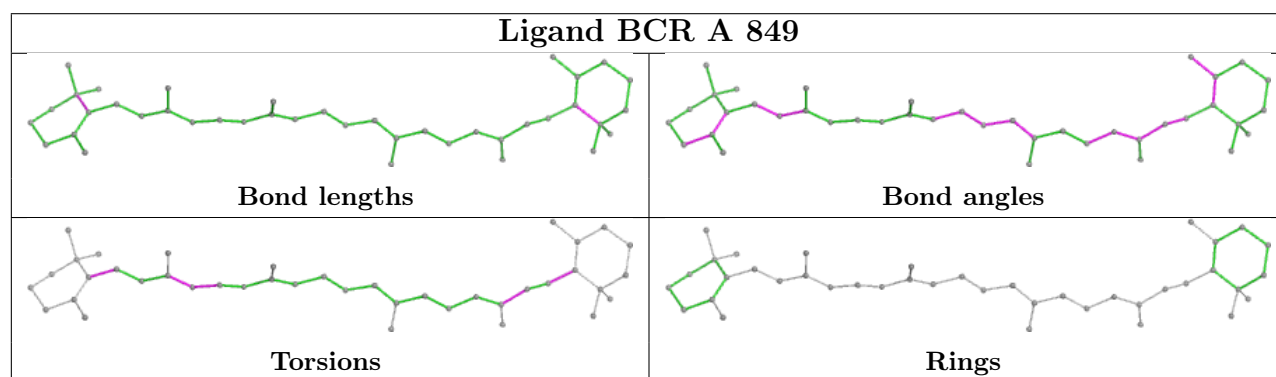
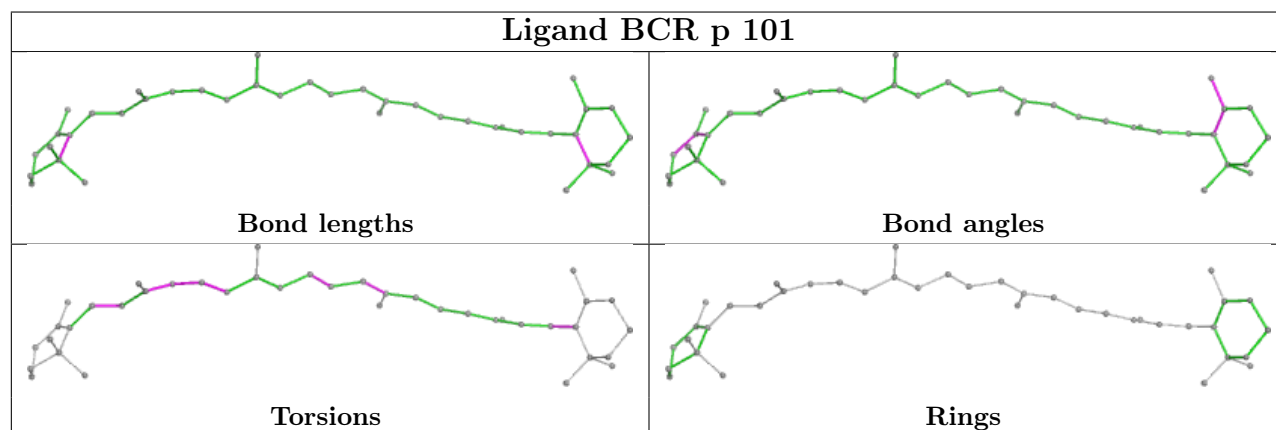
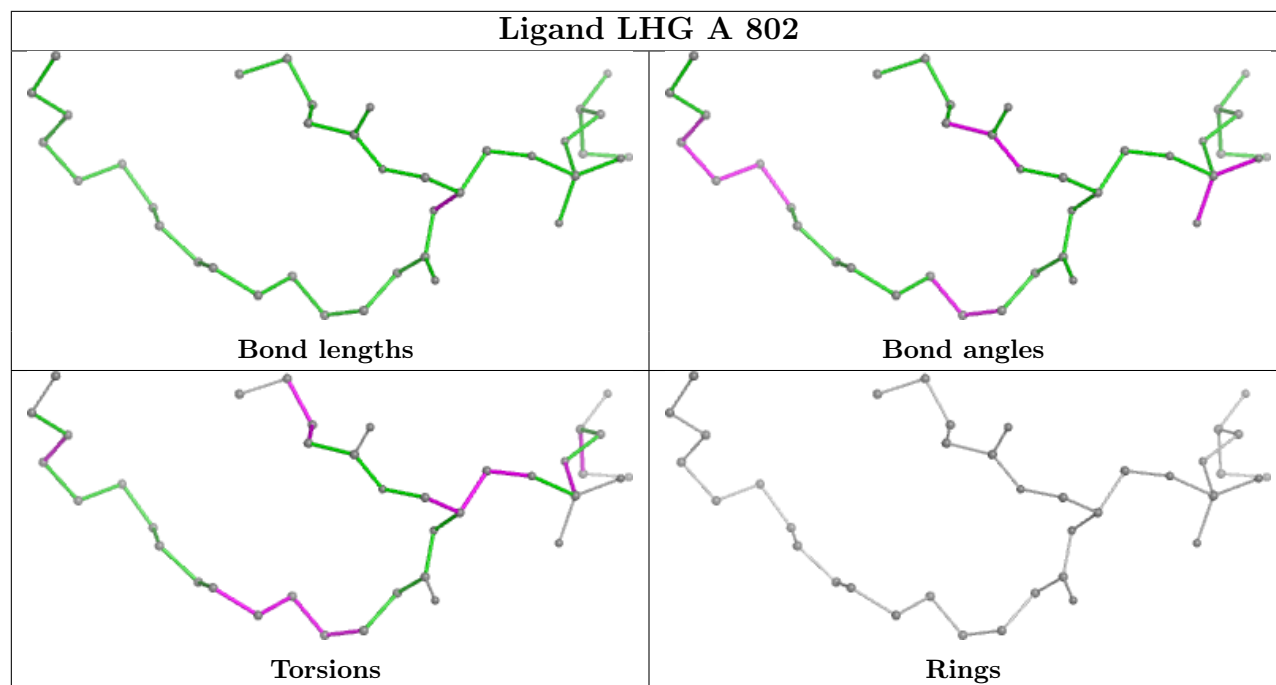
## Ligand BCR o 201

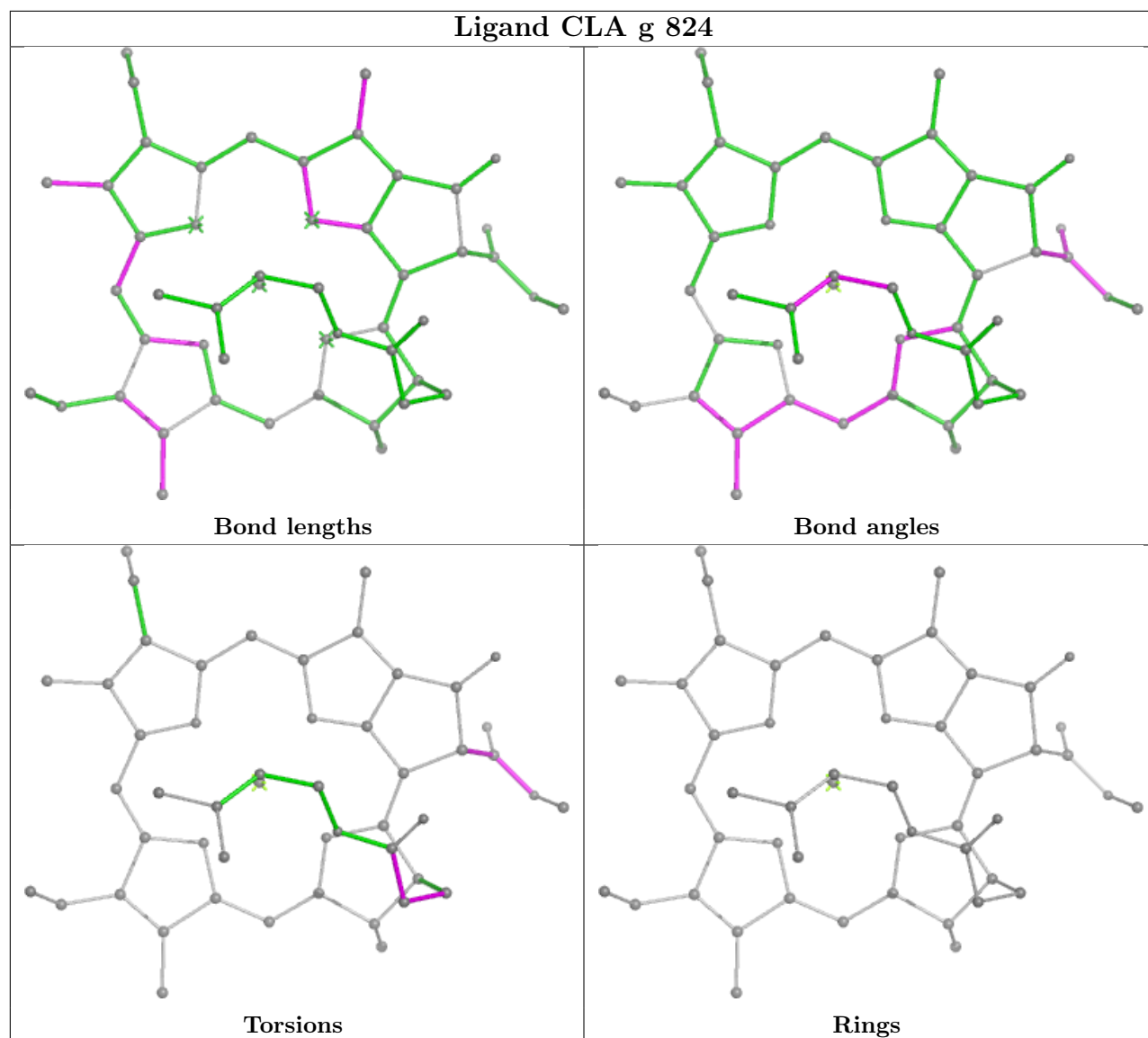
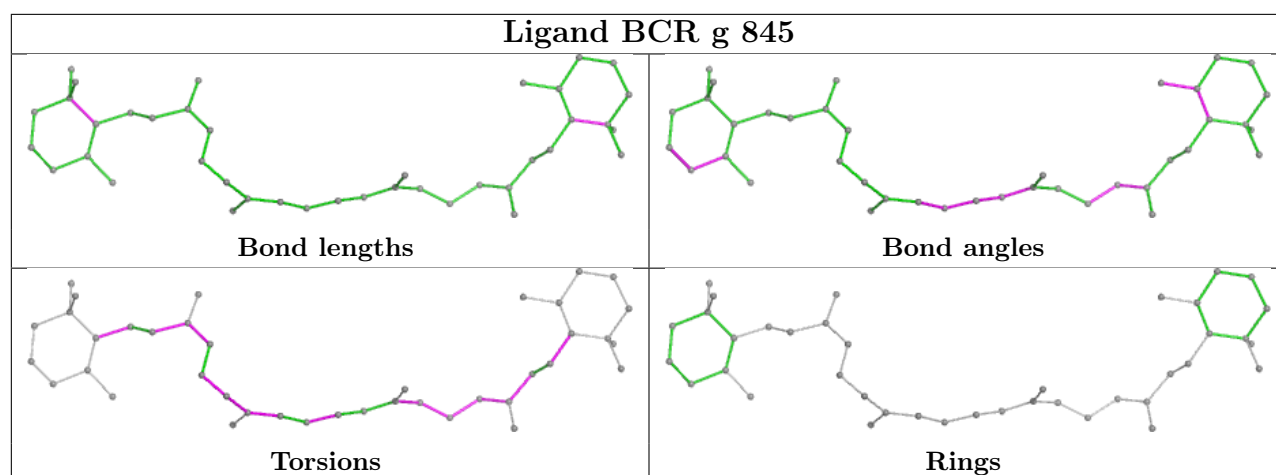


## Ligand CLA K 101

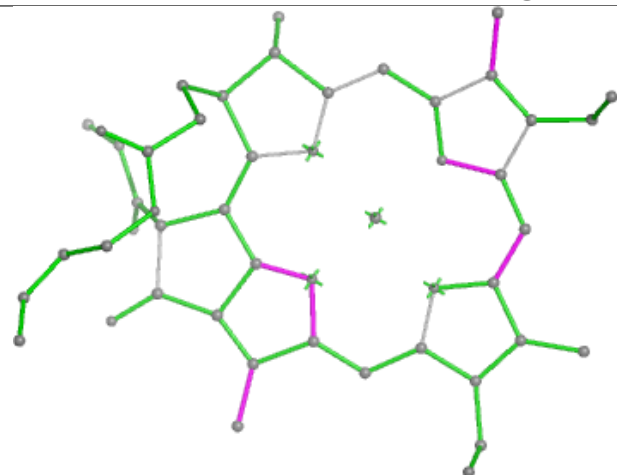




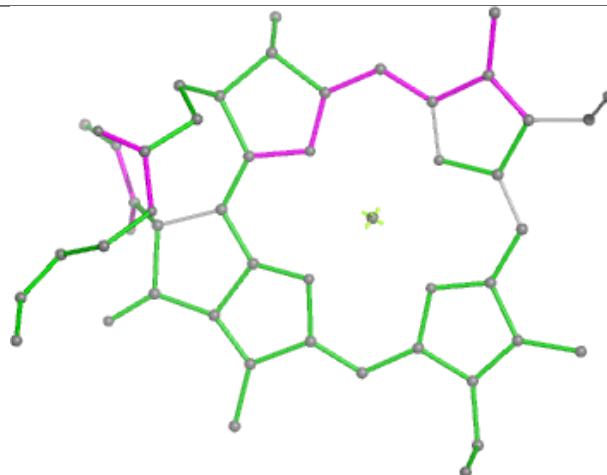




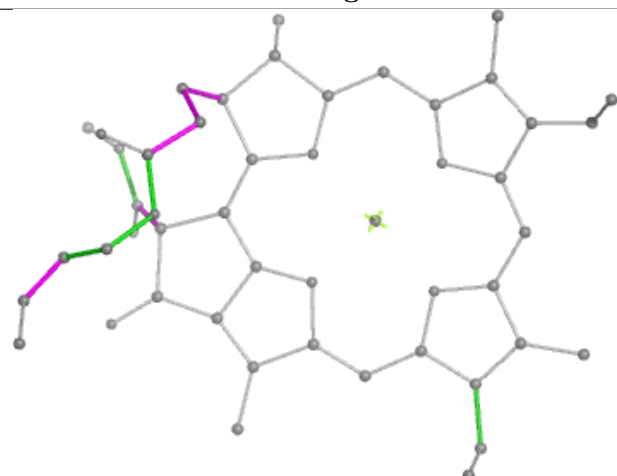
## Ligand CLA B 832



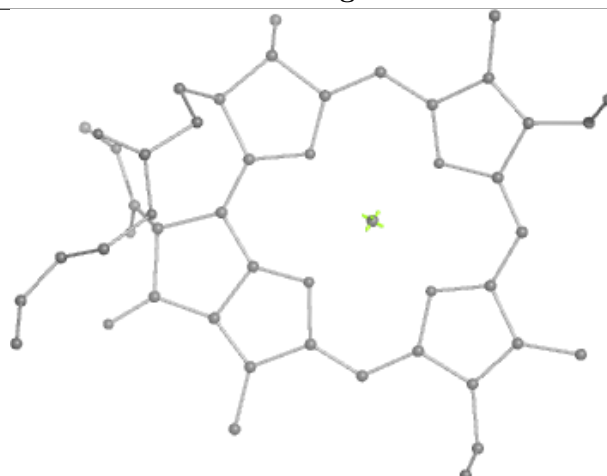
Bond lengths



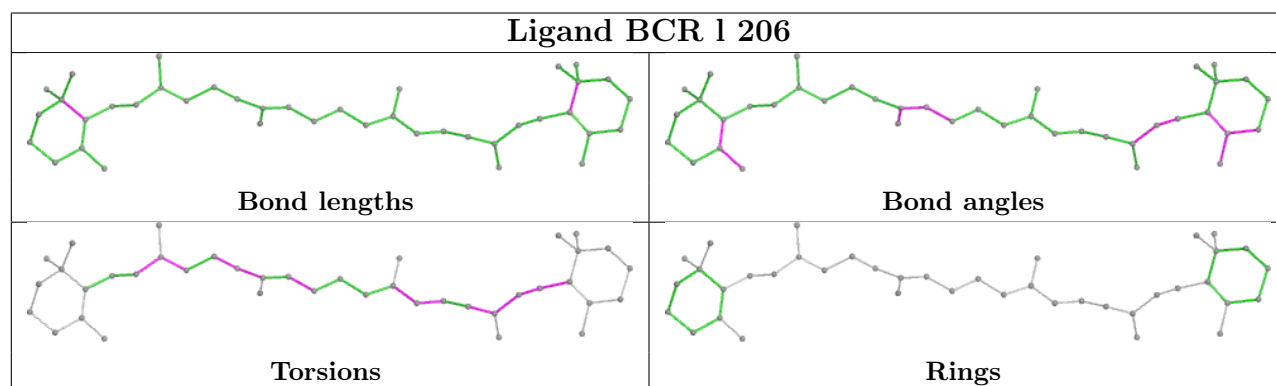
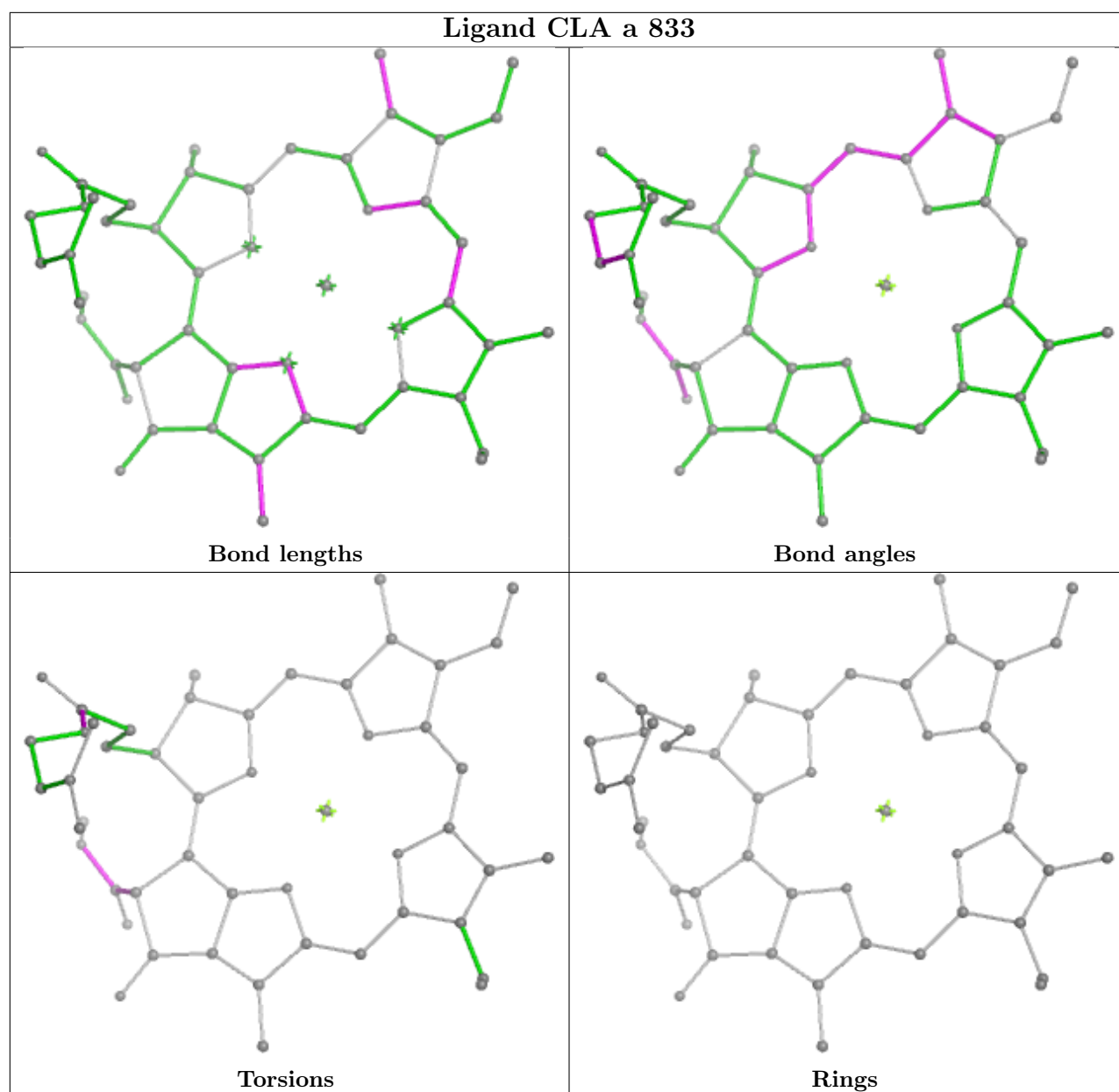
Bond angles



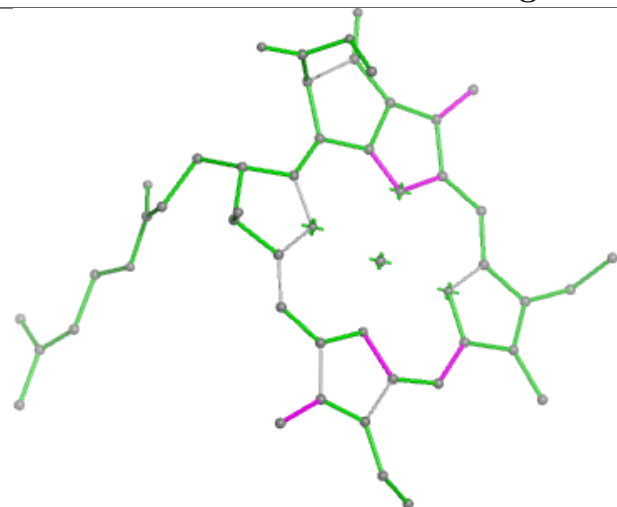
Torsions



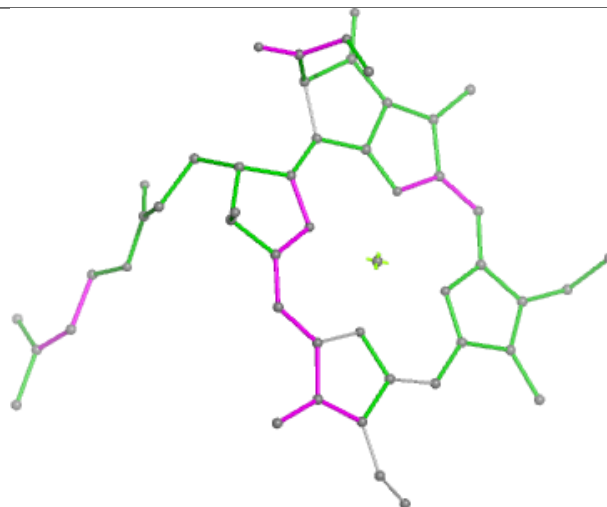
Rings



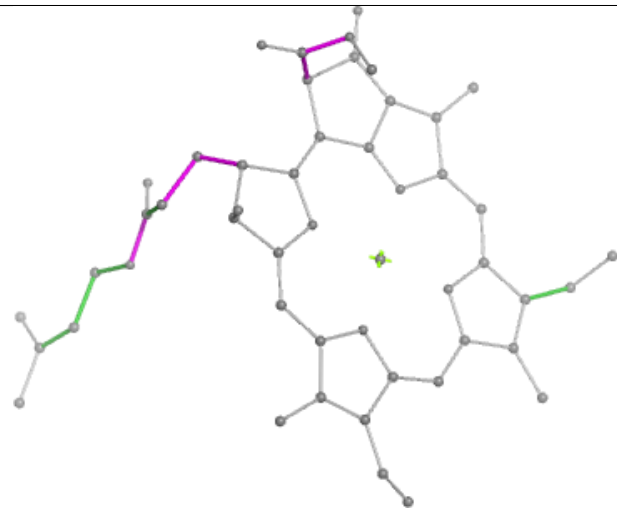
## Ligand CLA E 837



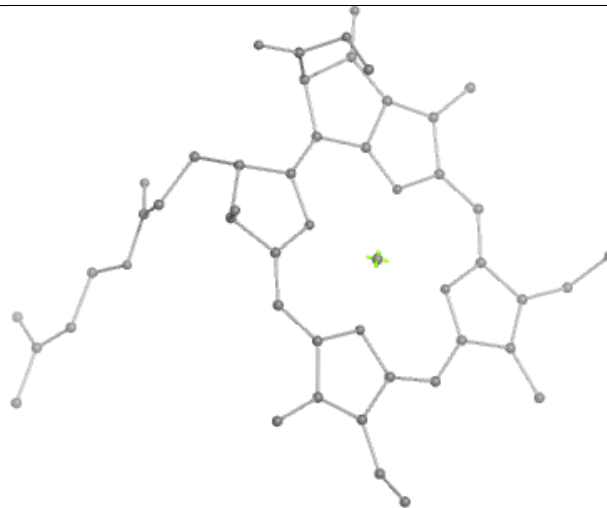
Bond lengths



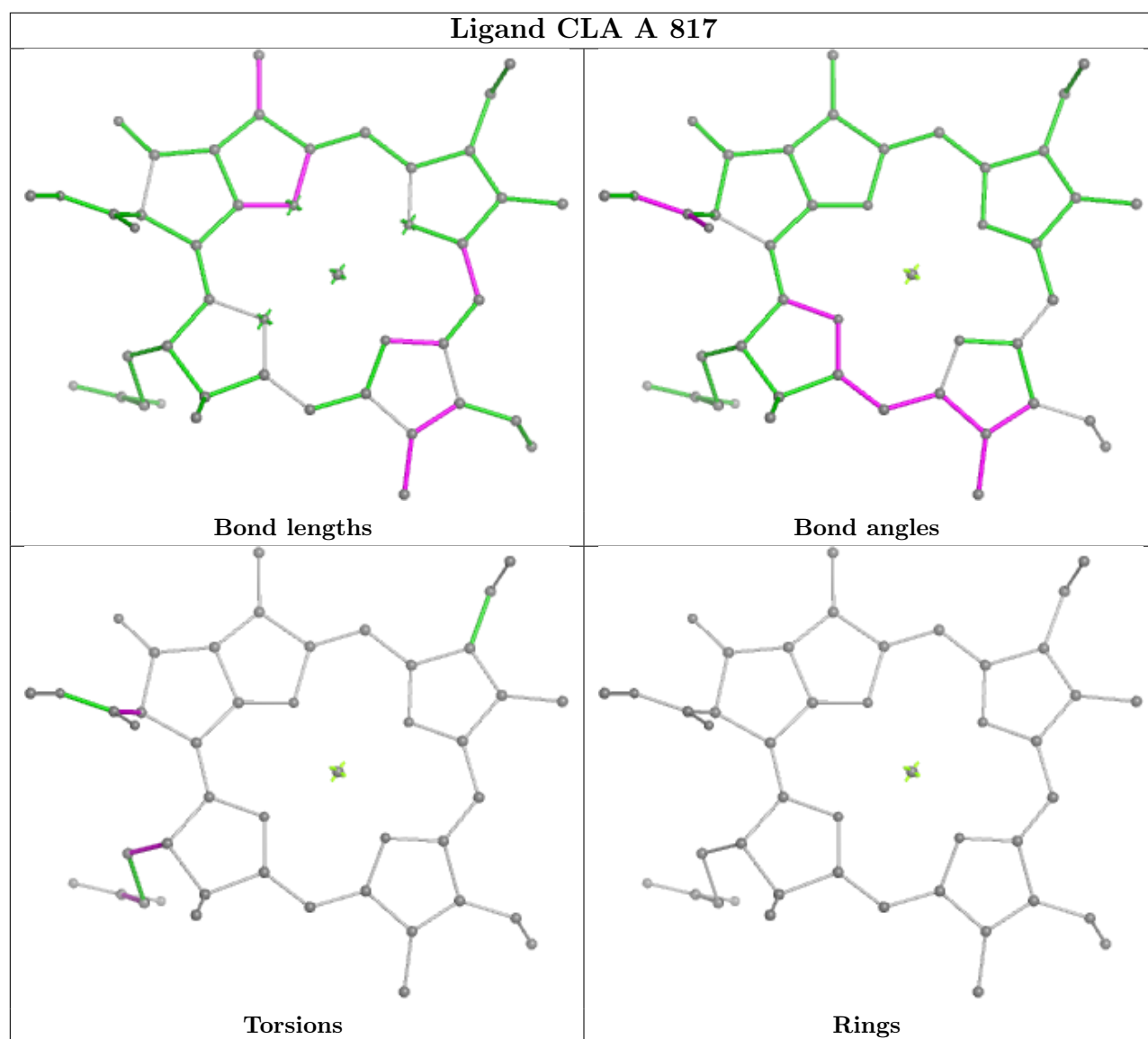
Bond angles



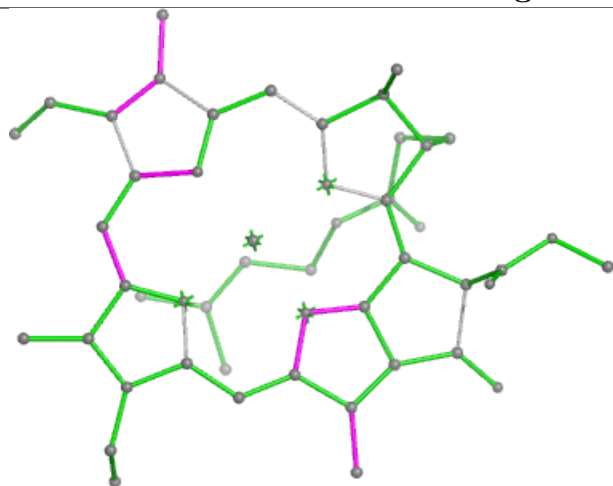
Torsions



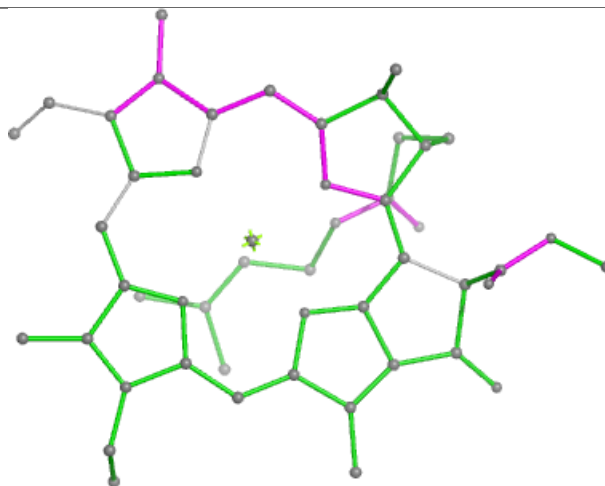
Rings



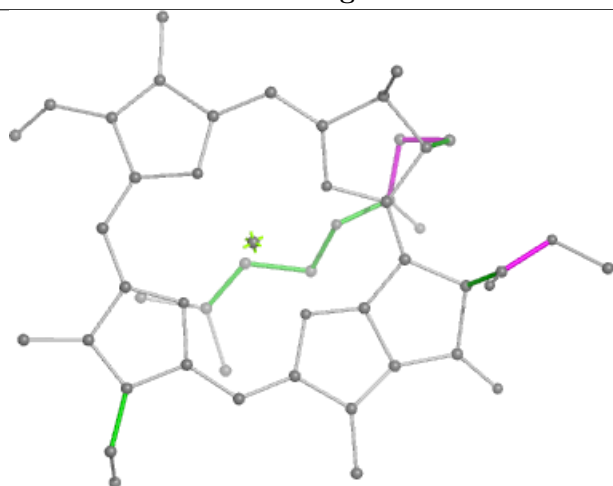
## Ligand CLA B 809



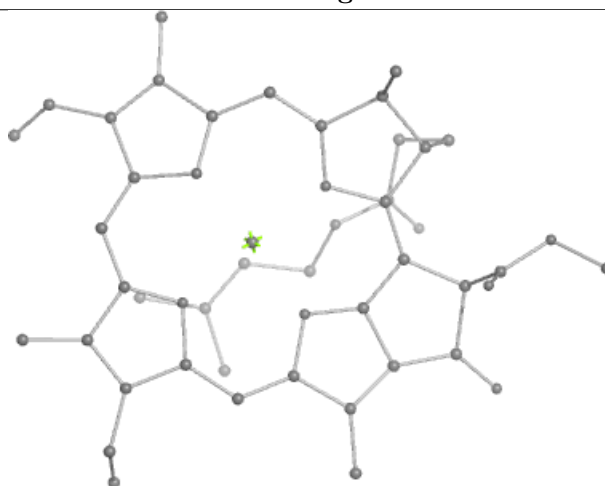
Bond lengths



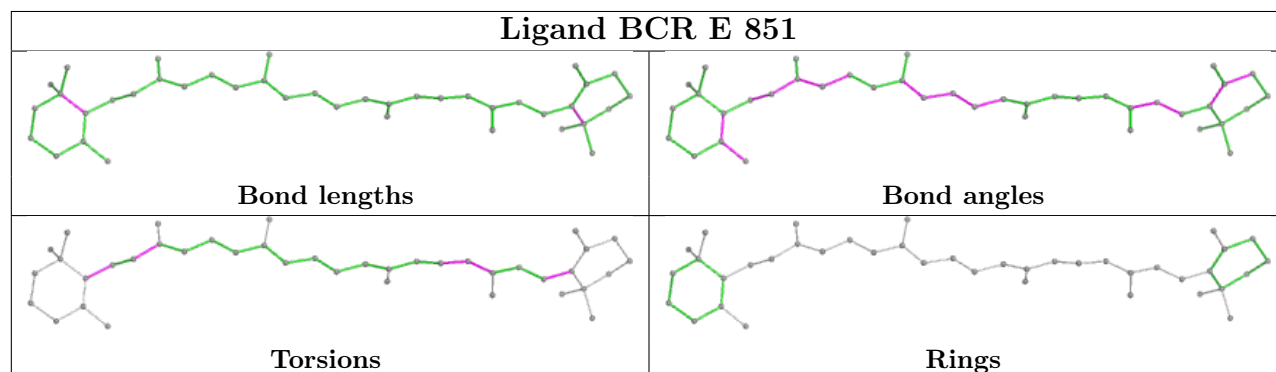
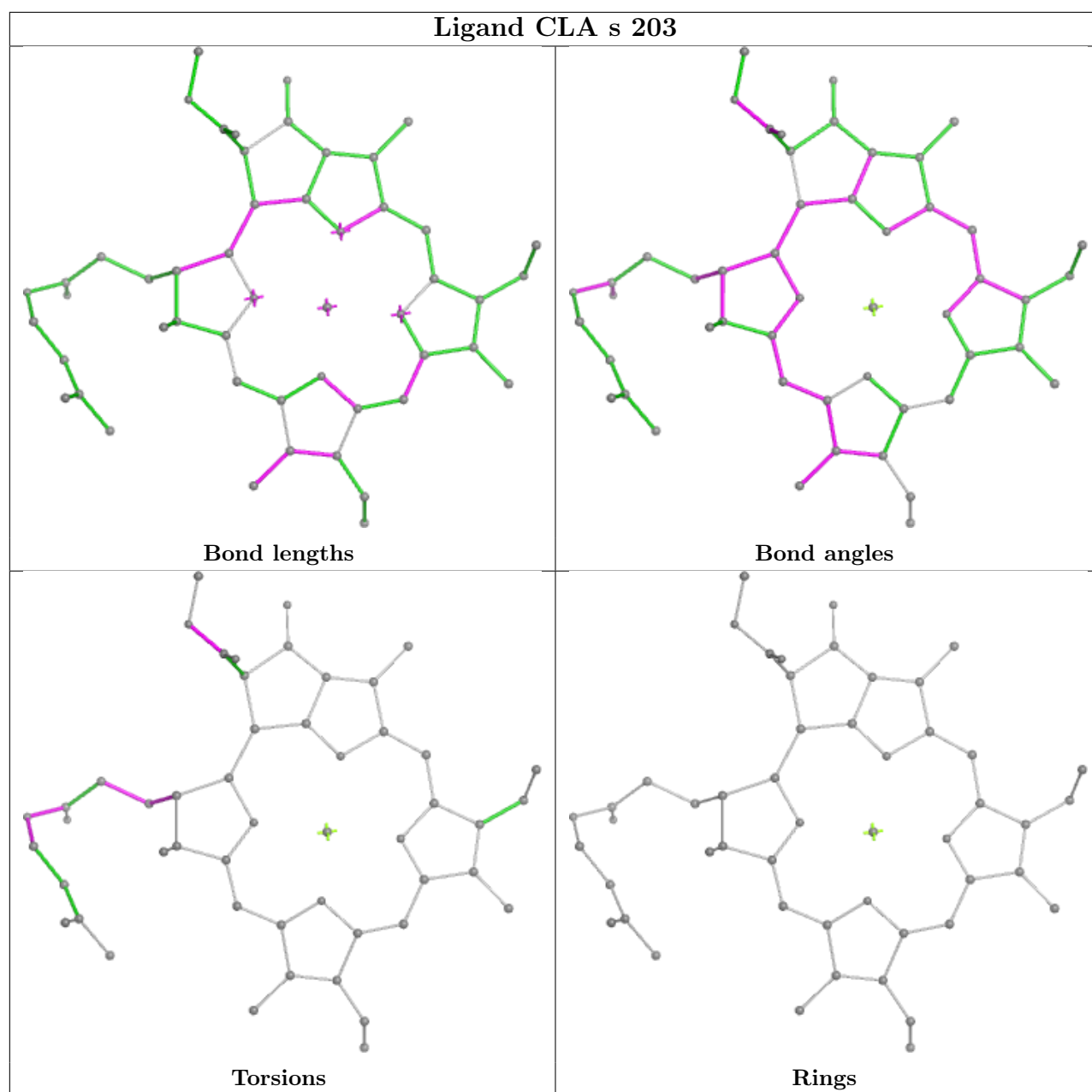
Bond angles



Torsions

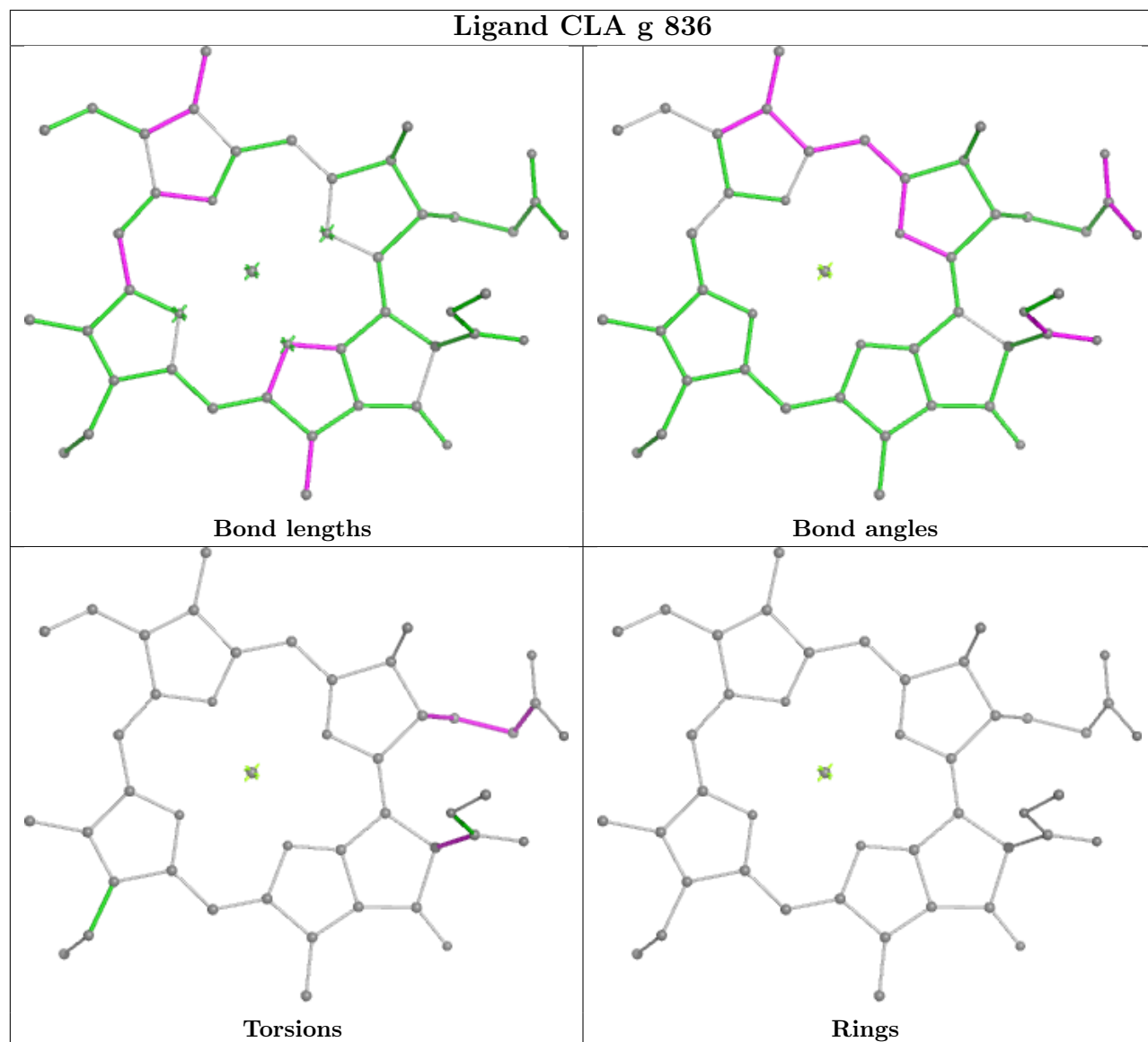


Rings

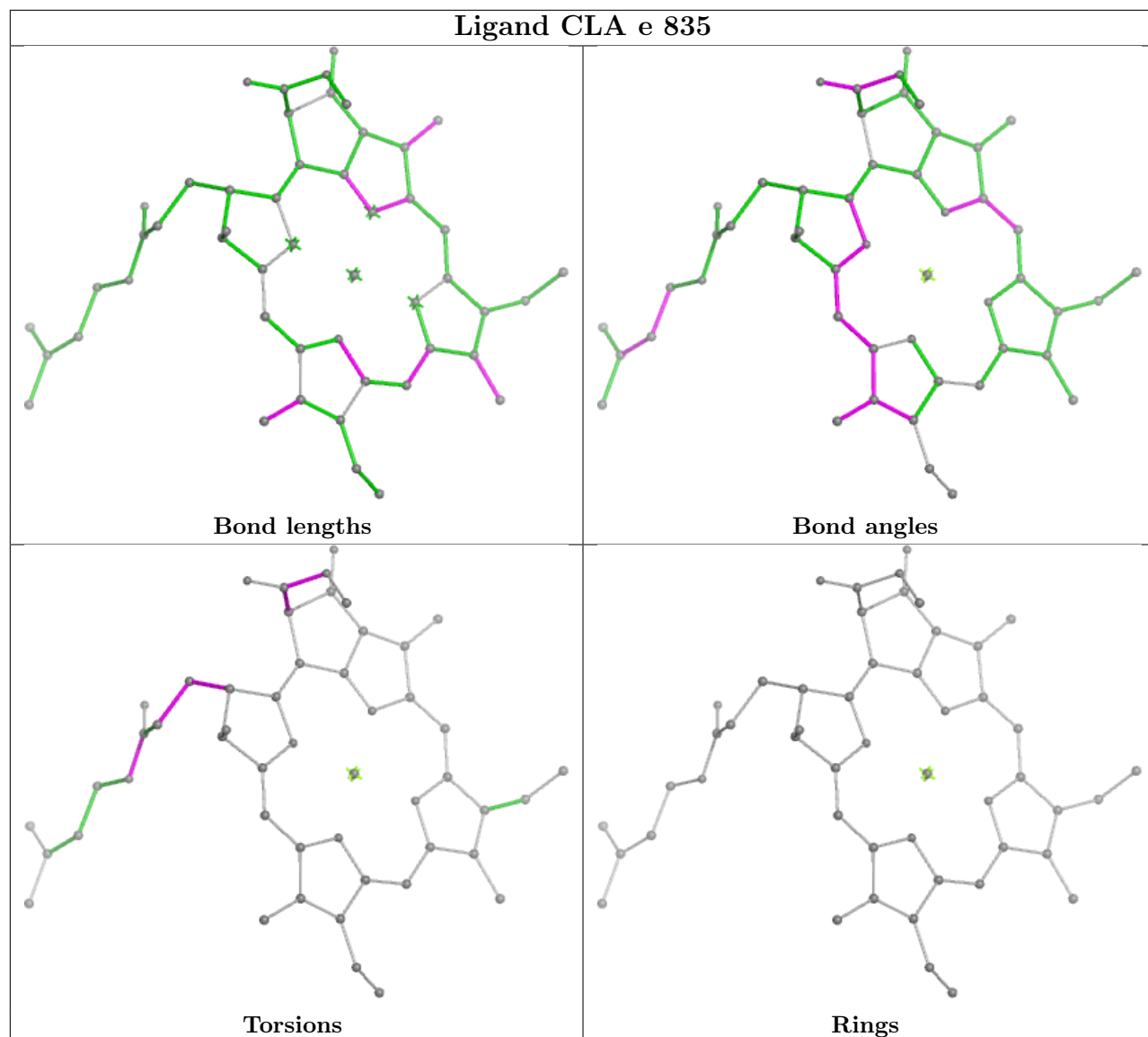


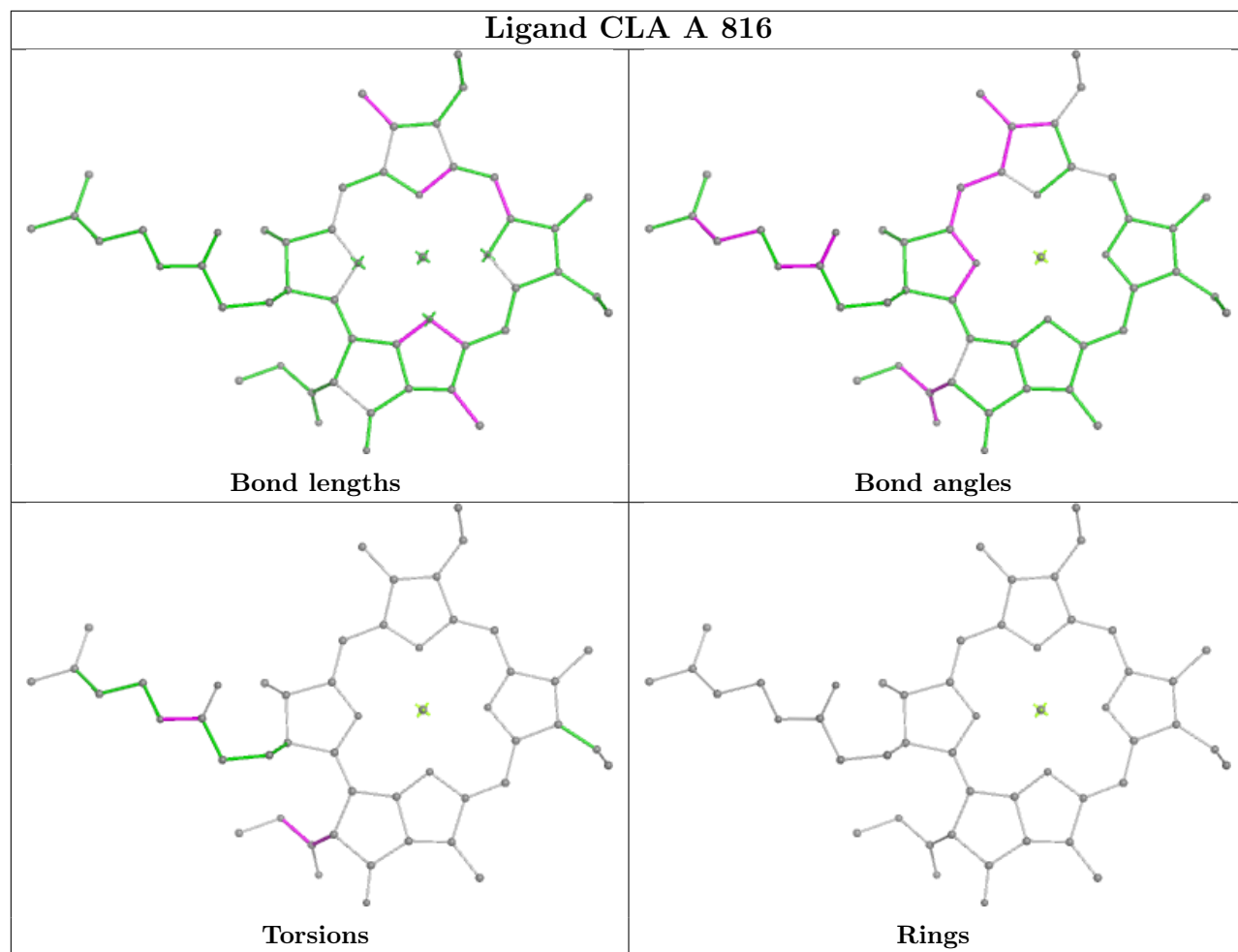


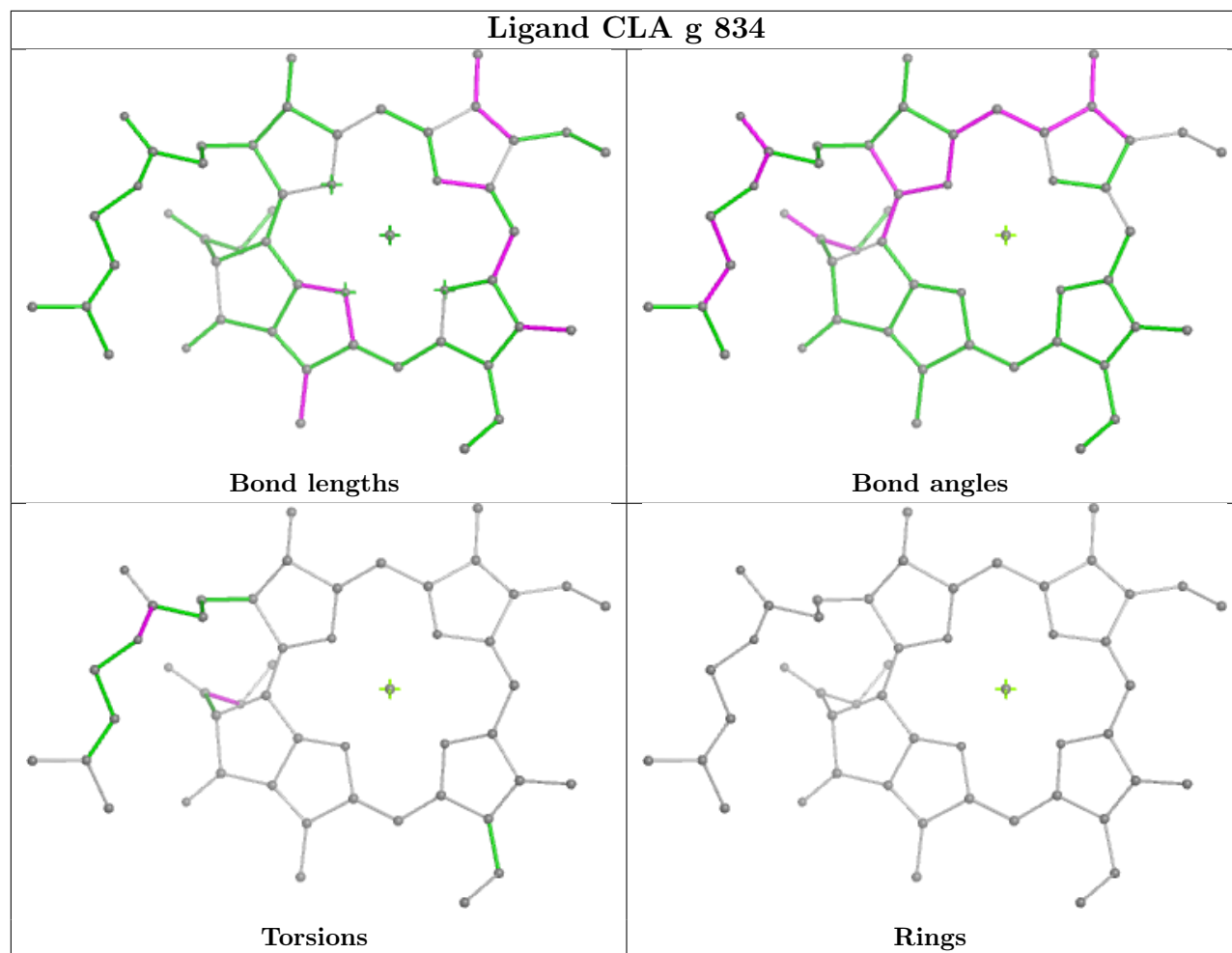
## Ligand CLA g 836



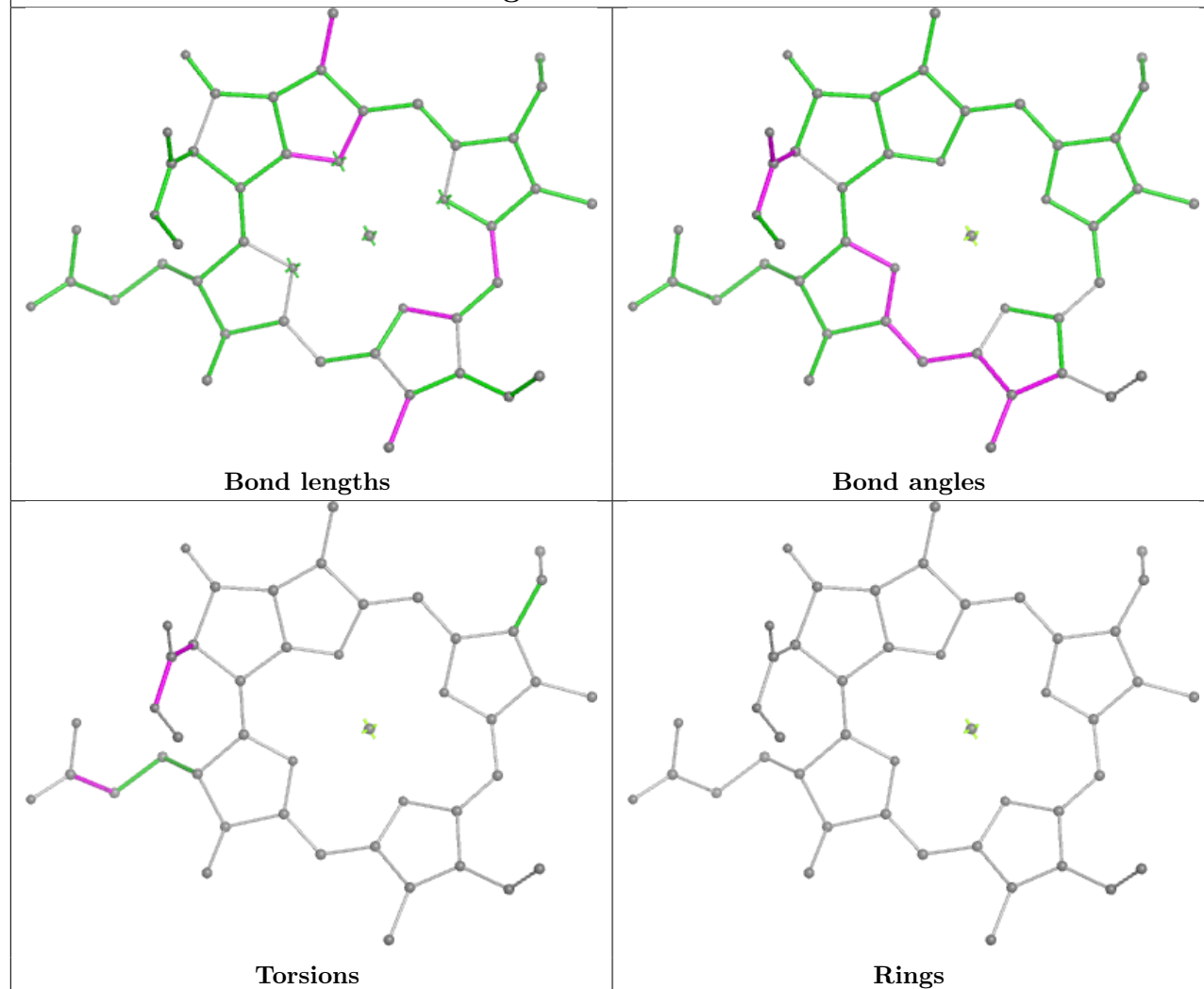
## Ligand CLA e 835



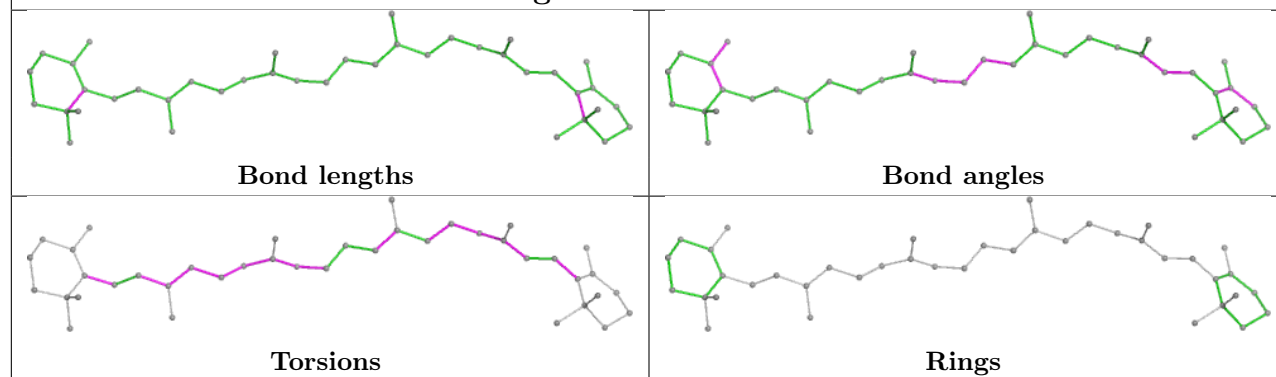




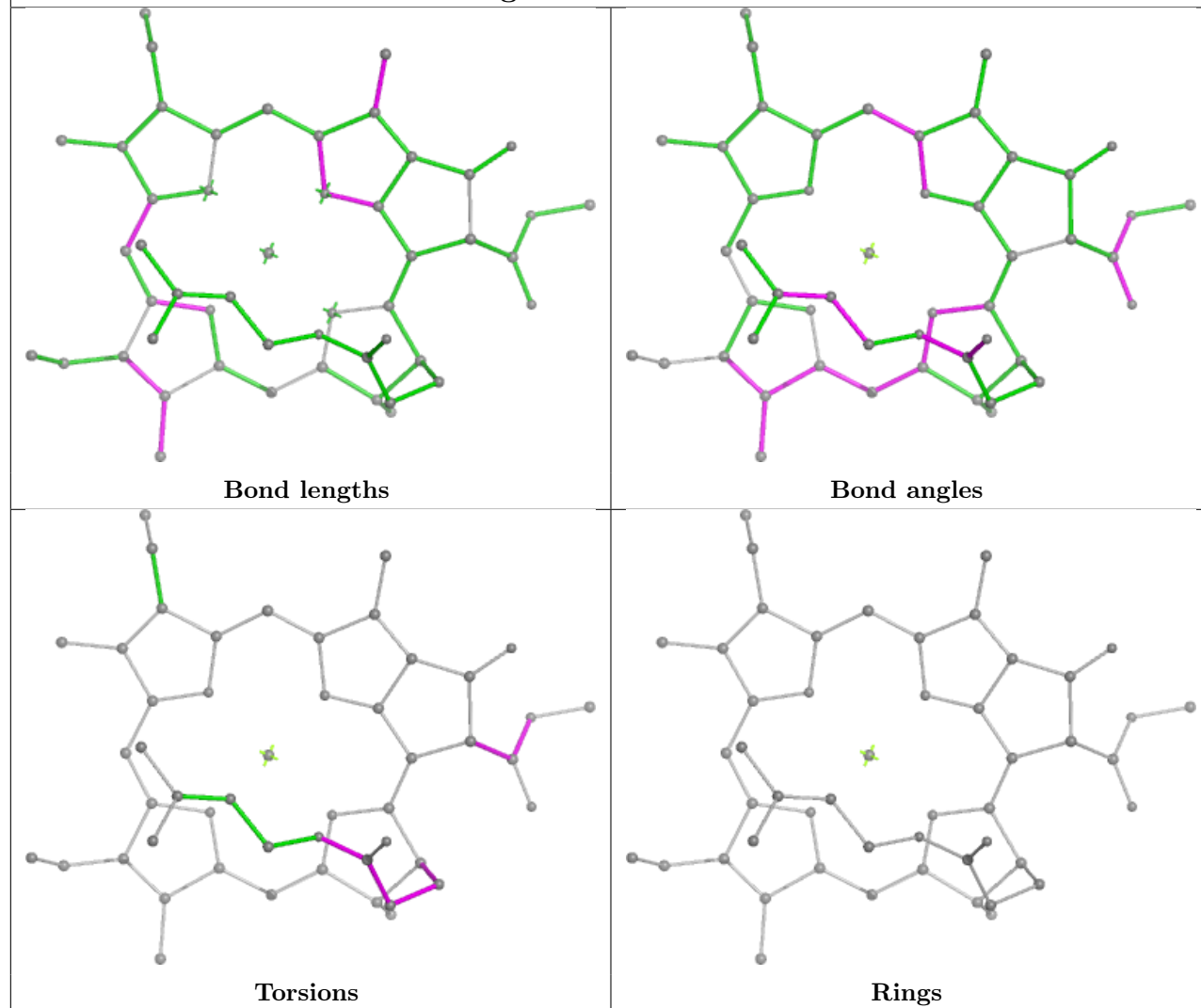
## Ligand CLA E 818

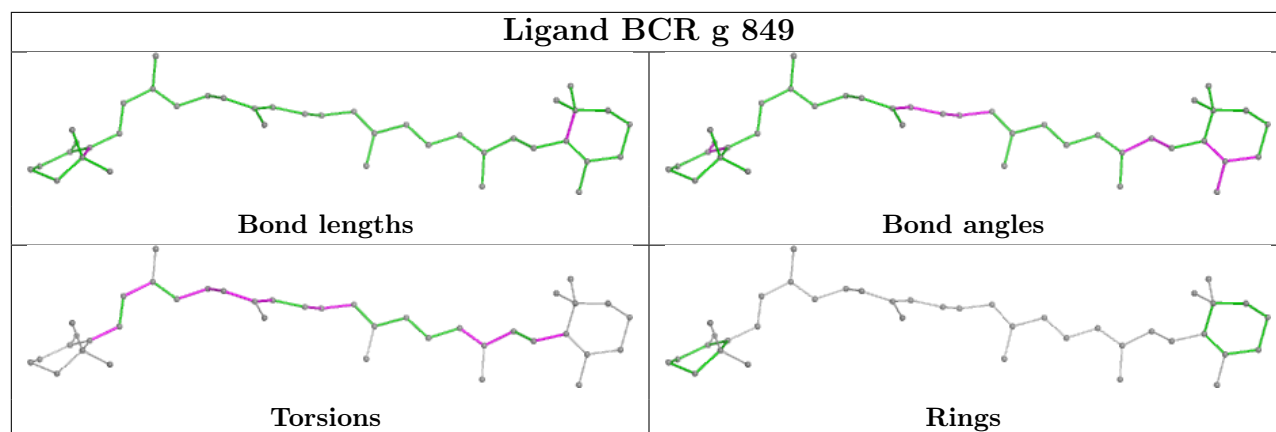
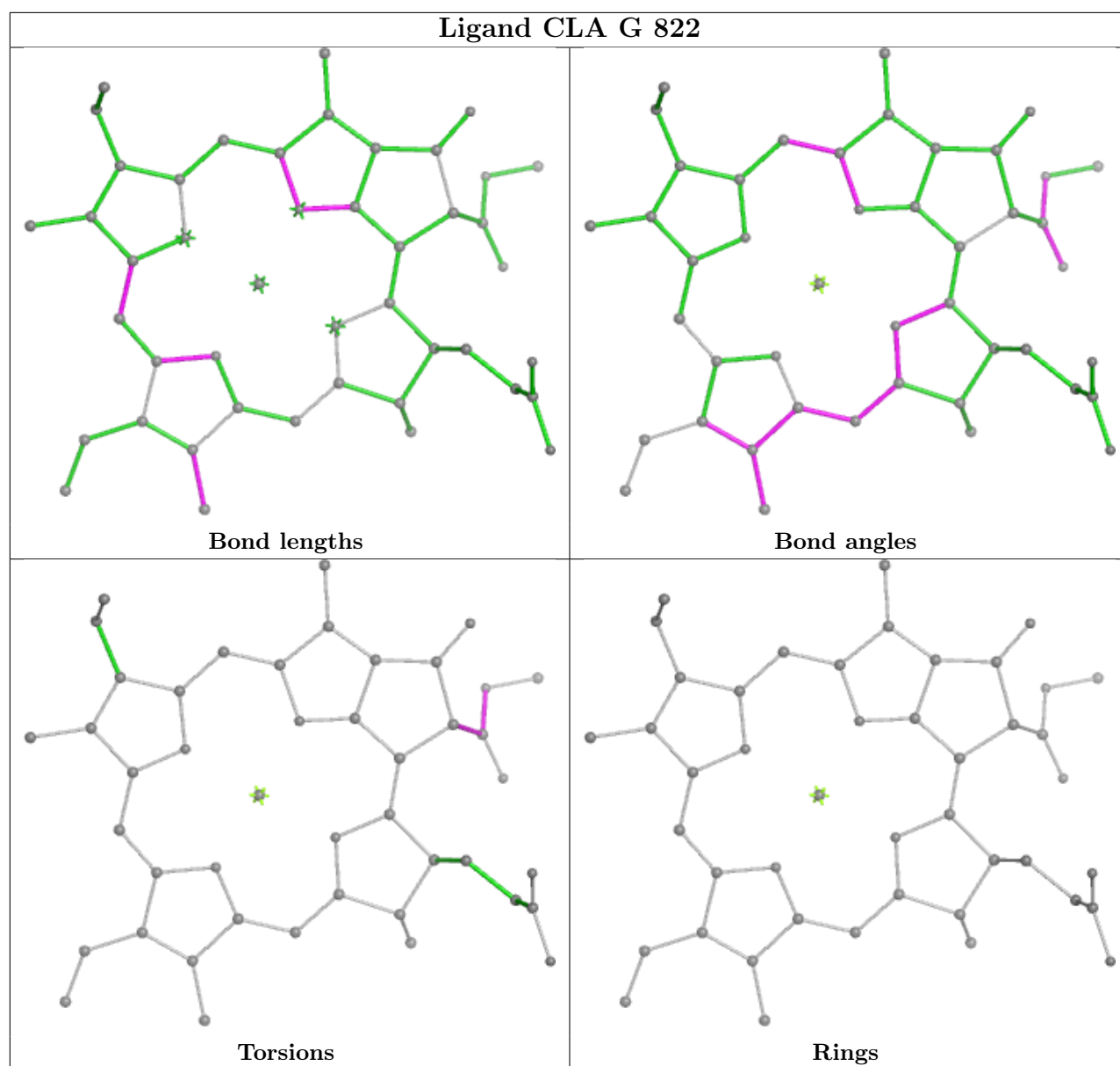


## Ligand BCR b 845

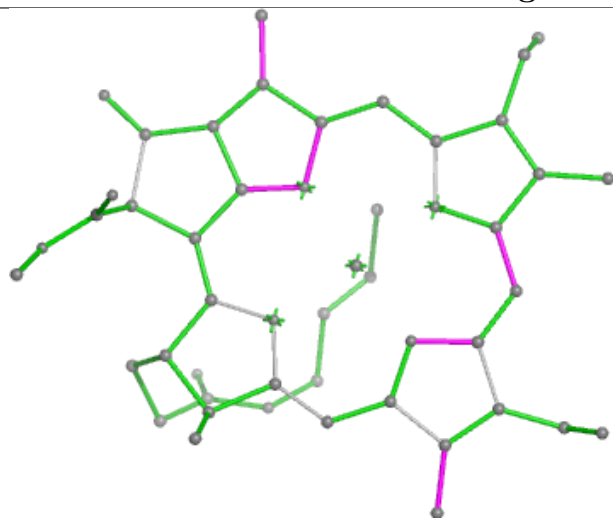


## Ligand CLA A 826

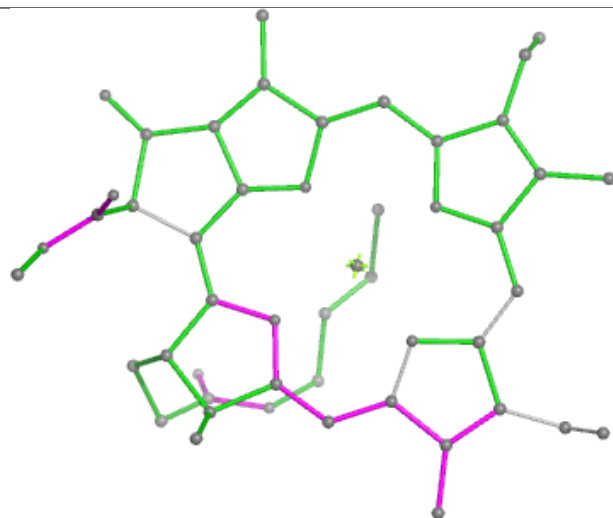




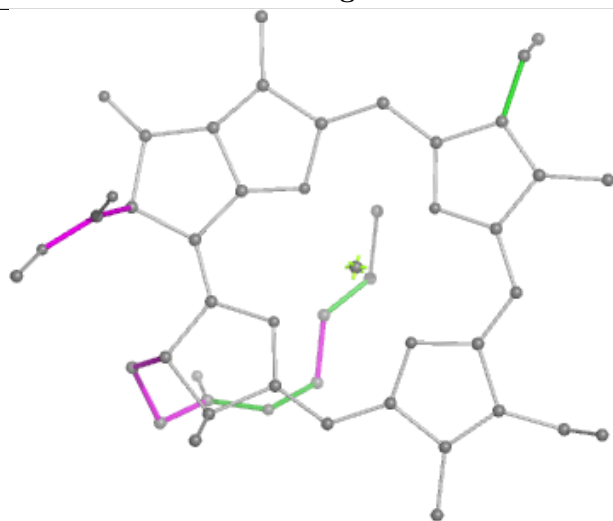
## Ligand CLA a 819



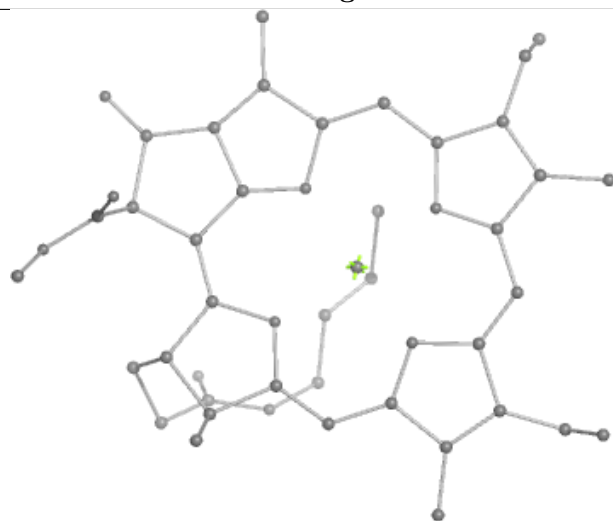
Bond lengths



Bond angles

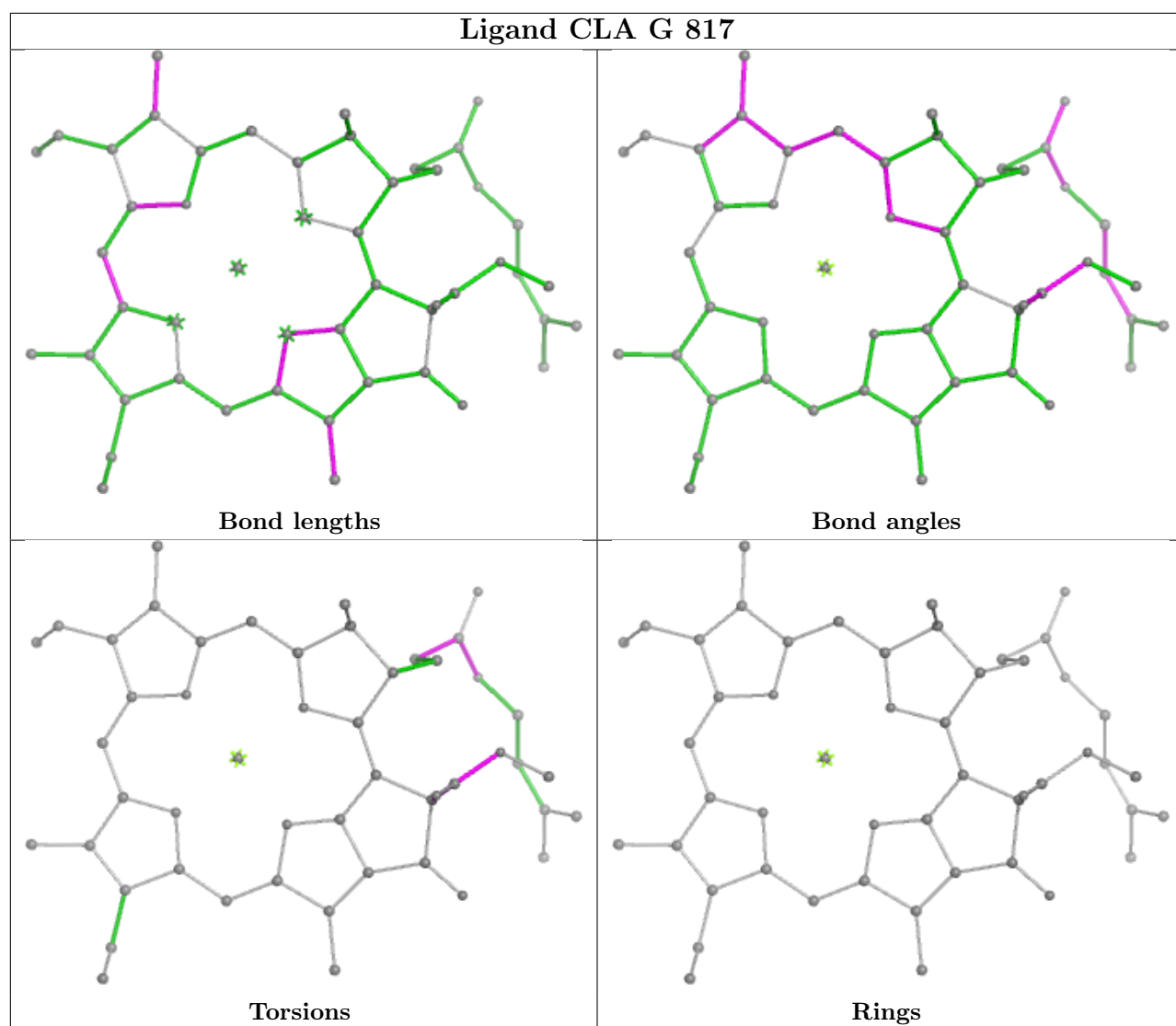


Torsions

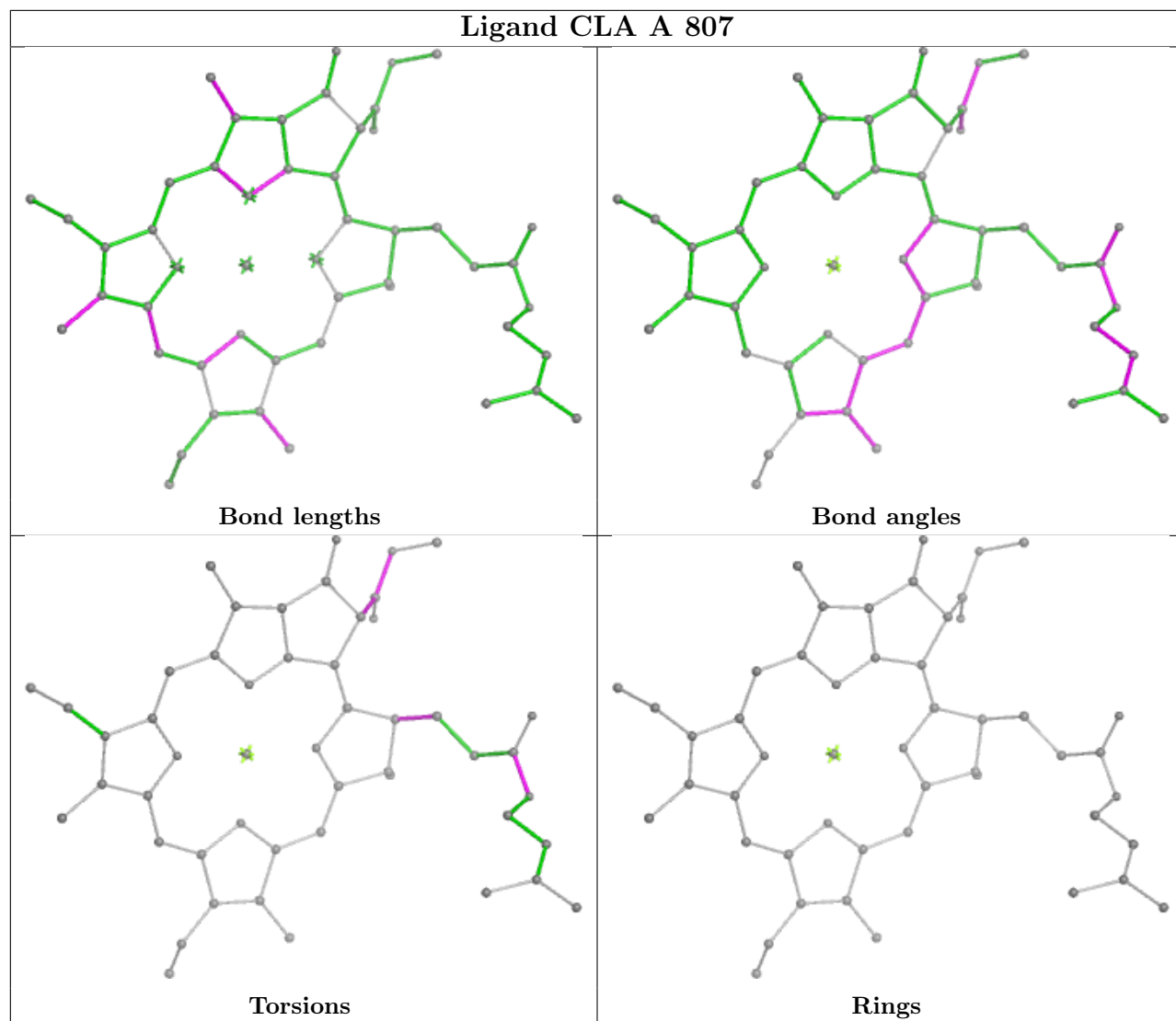


Rings

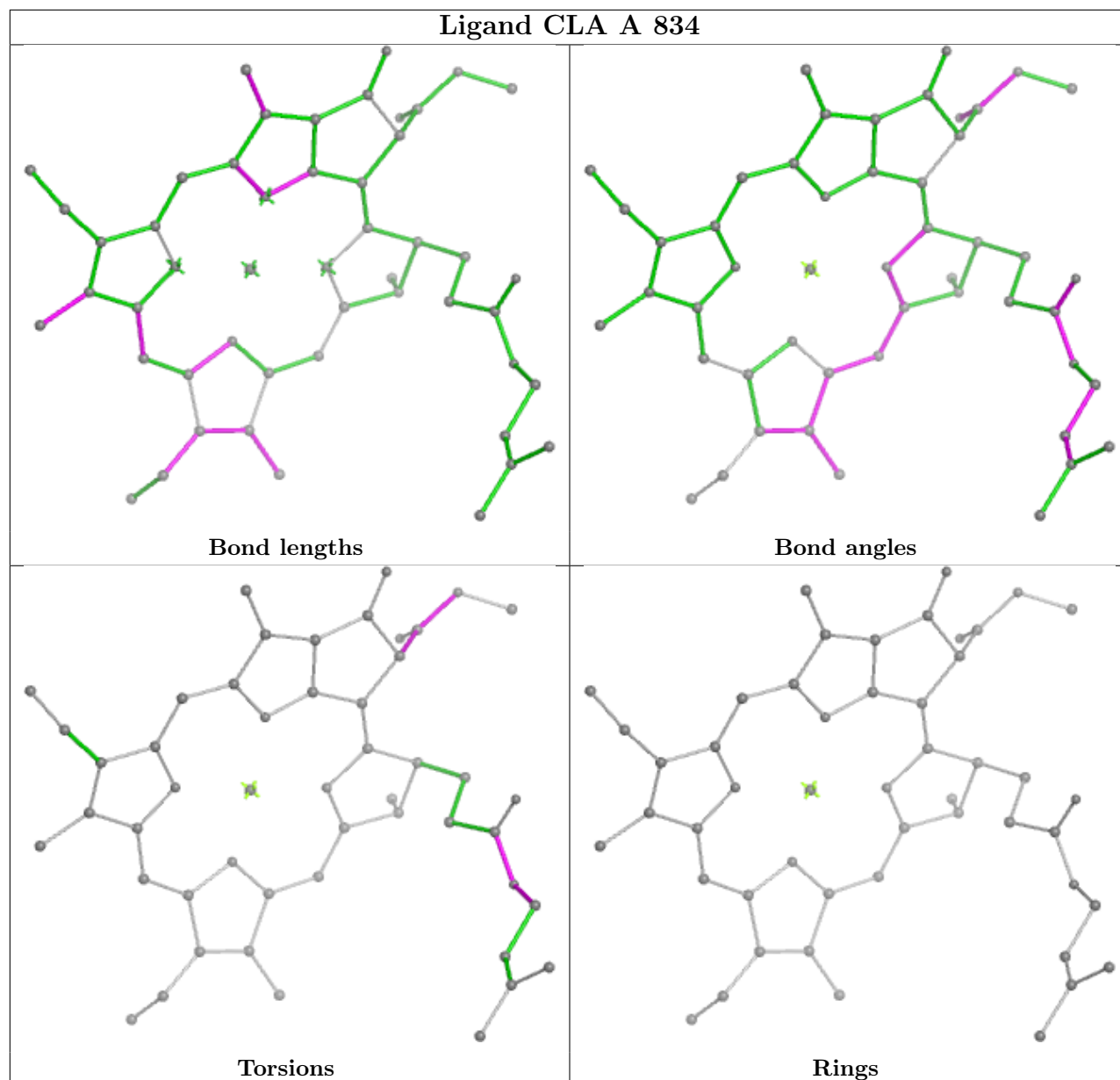




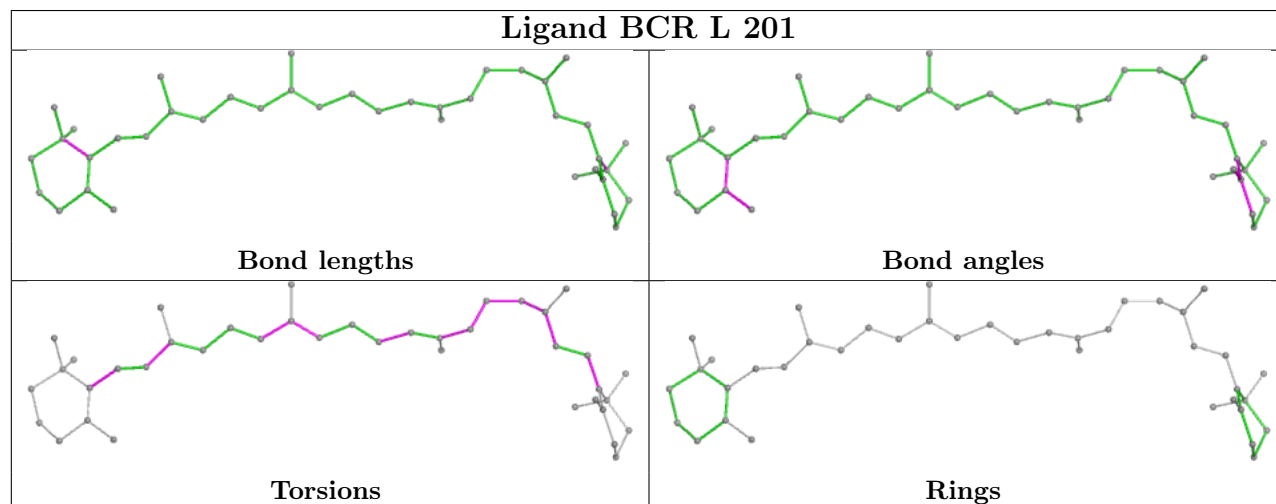
## Ligand CLA A 807



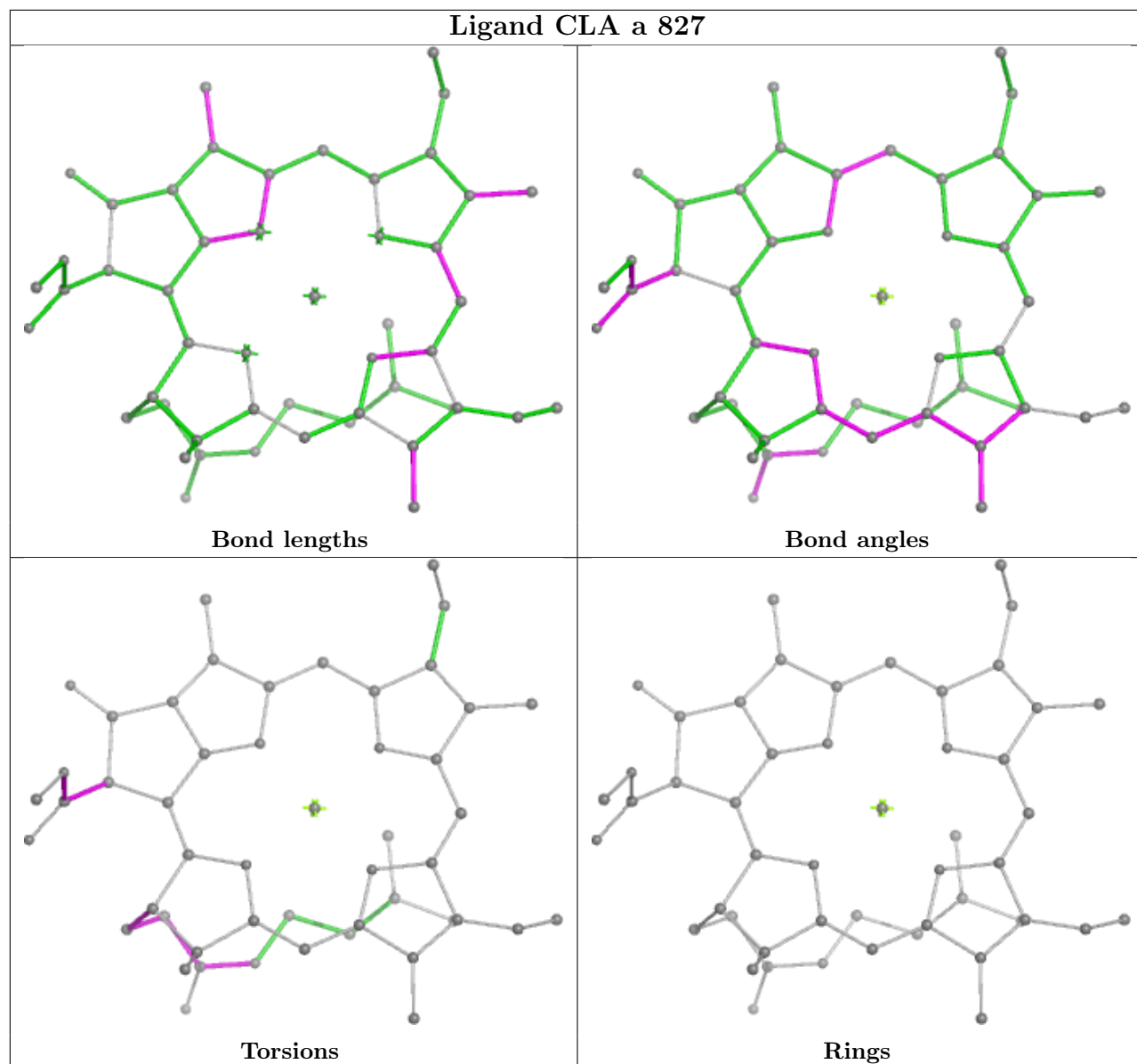
## Ligand CLA A 834



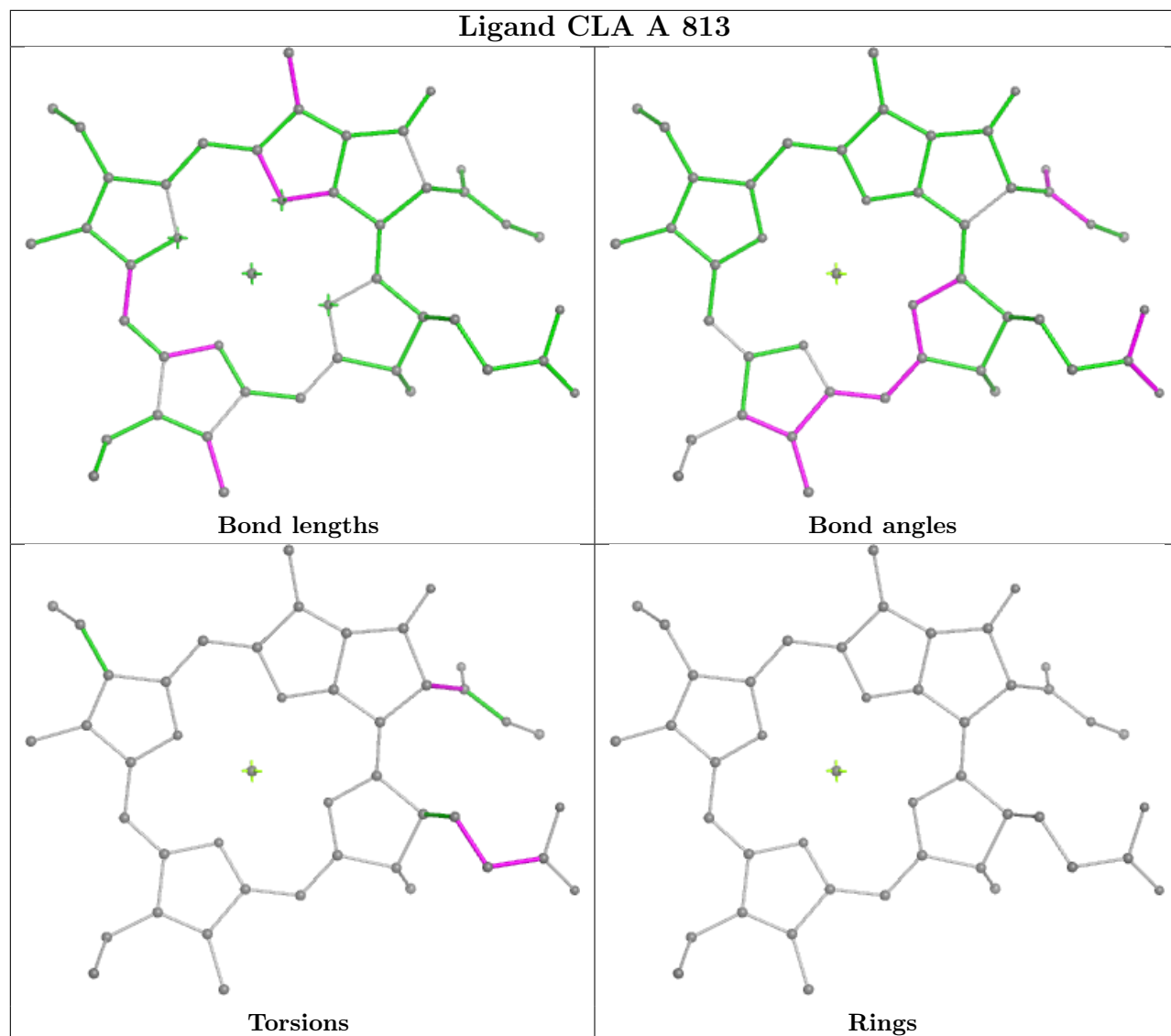
## Ligand BCR L 201



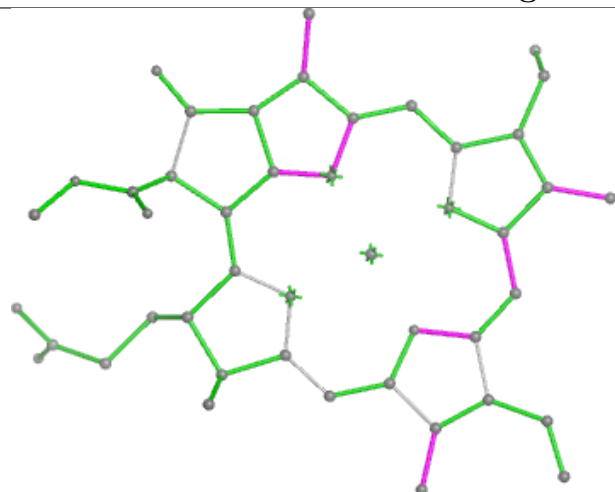
## Ligand CLA a 827



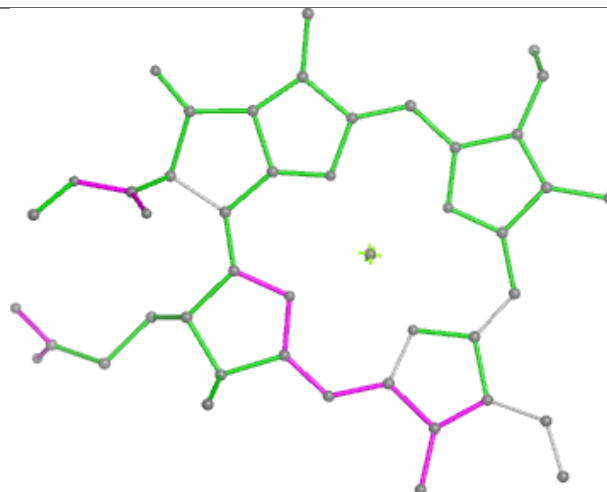
## Ligand CLA A 813



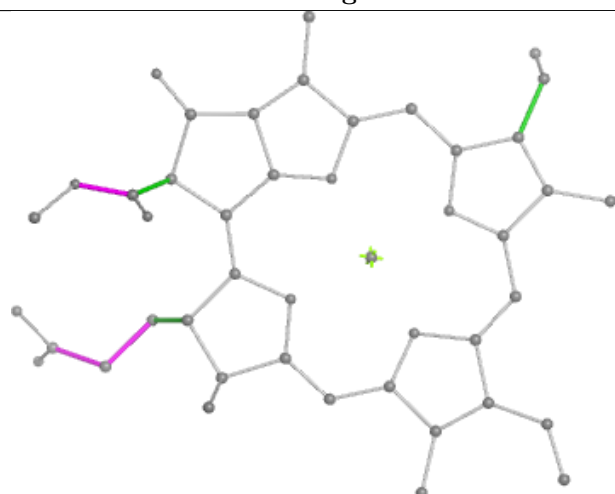
## Ligand CLA S 203



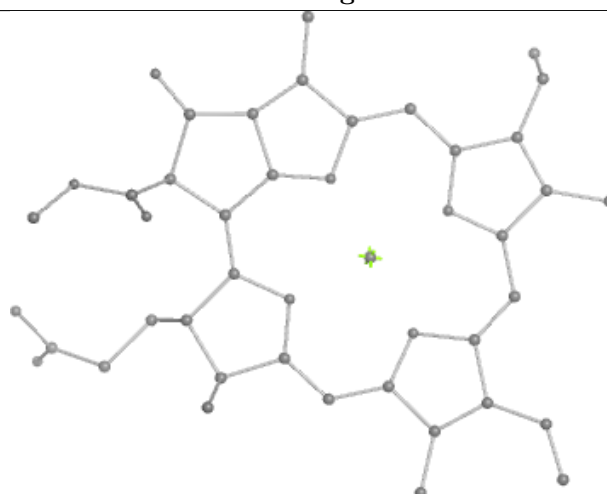
Bond lengths



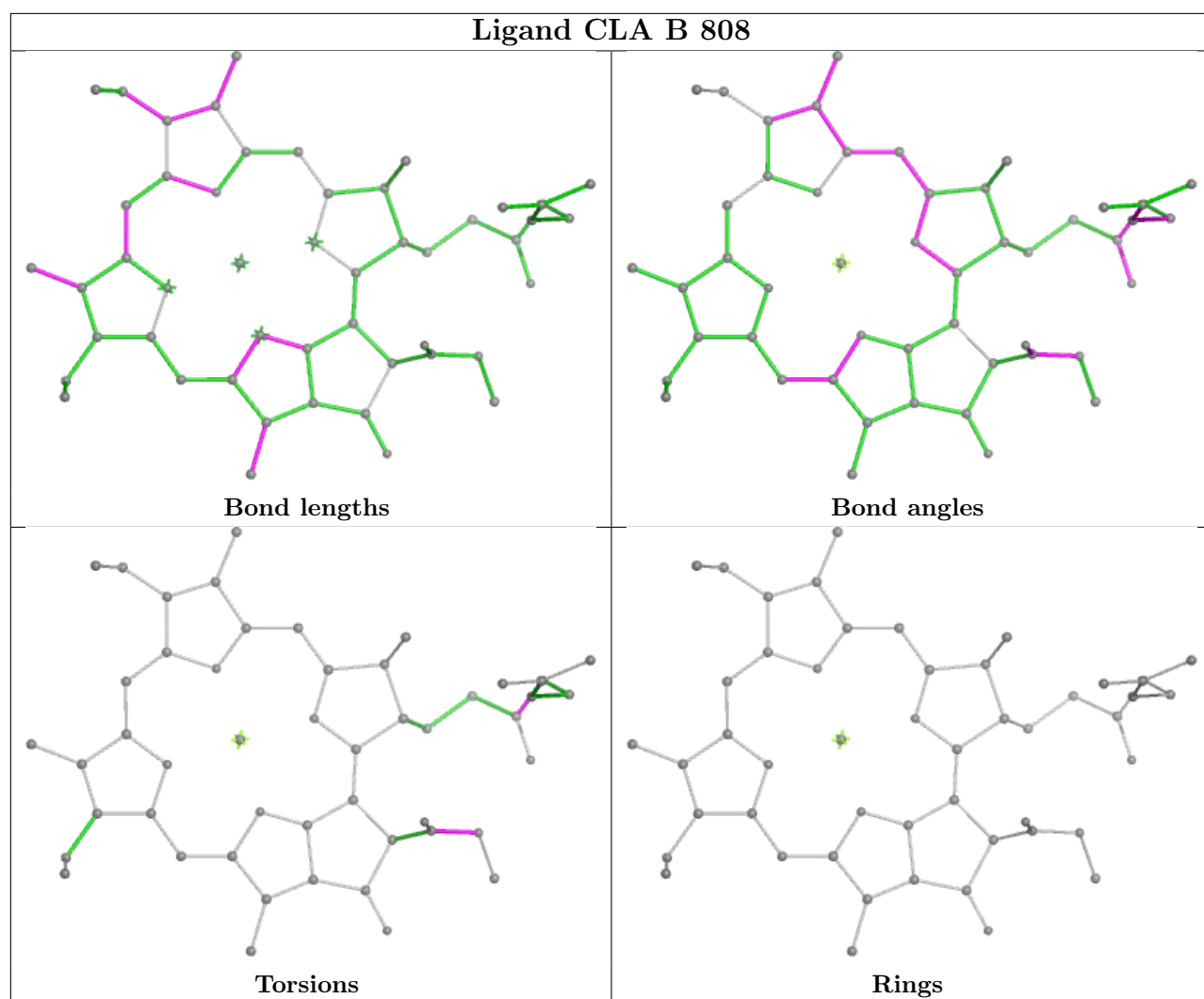
Bond angles



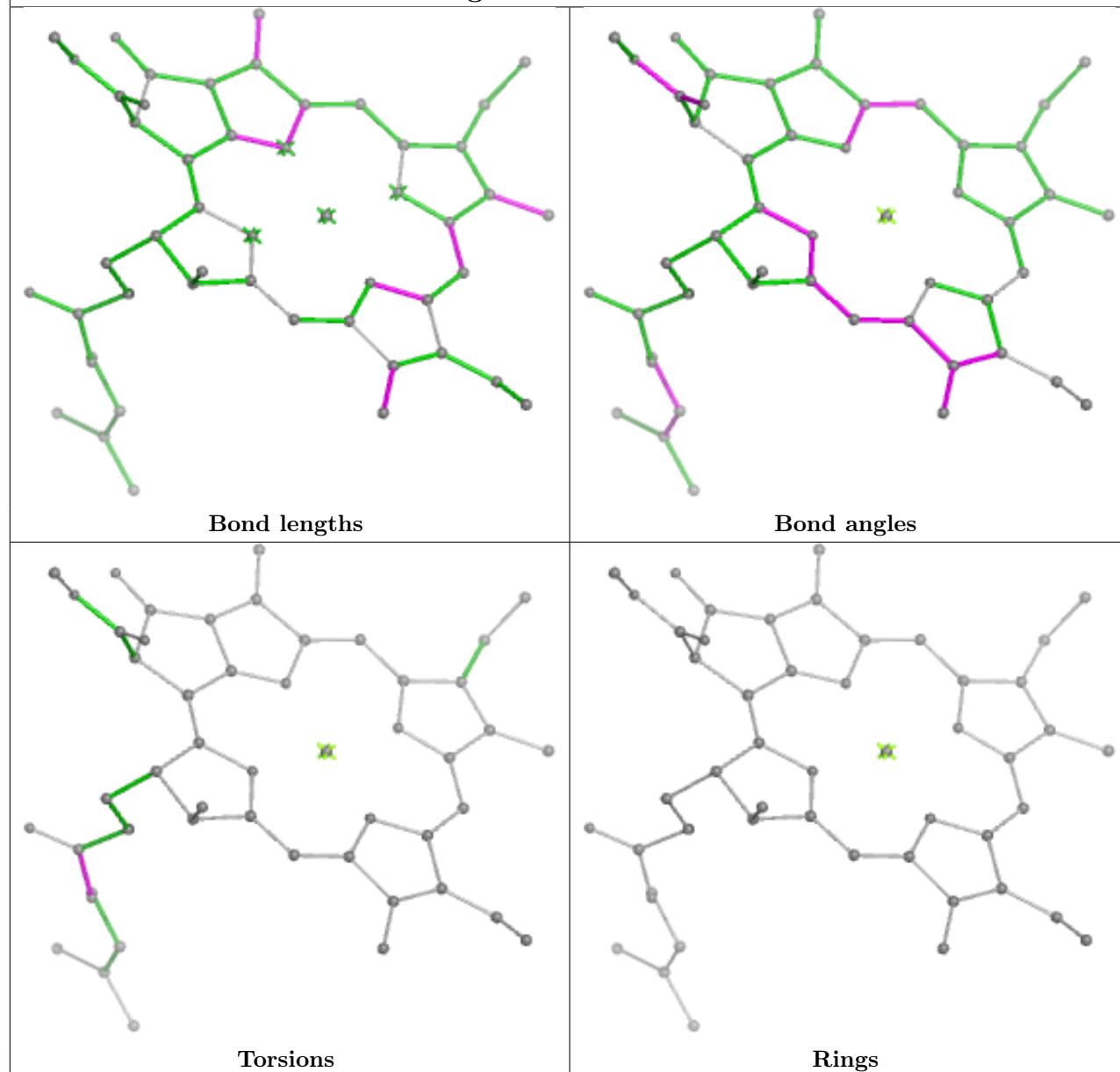
Torsions



Rings

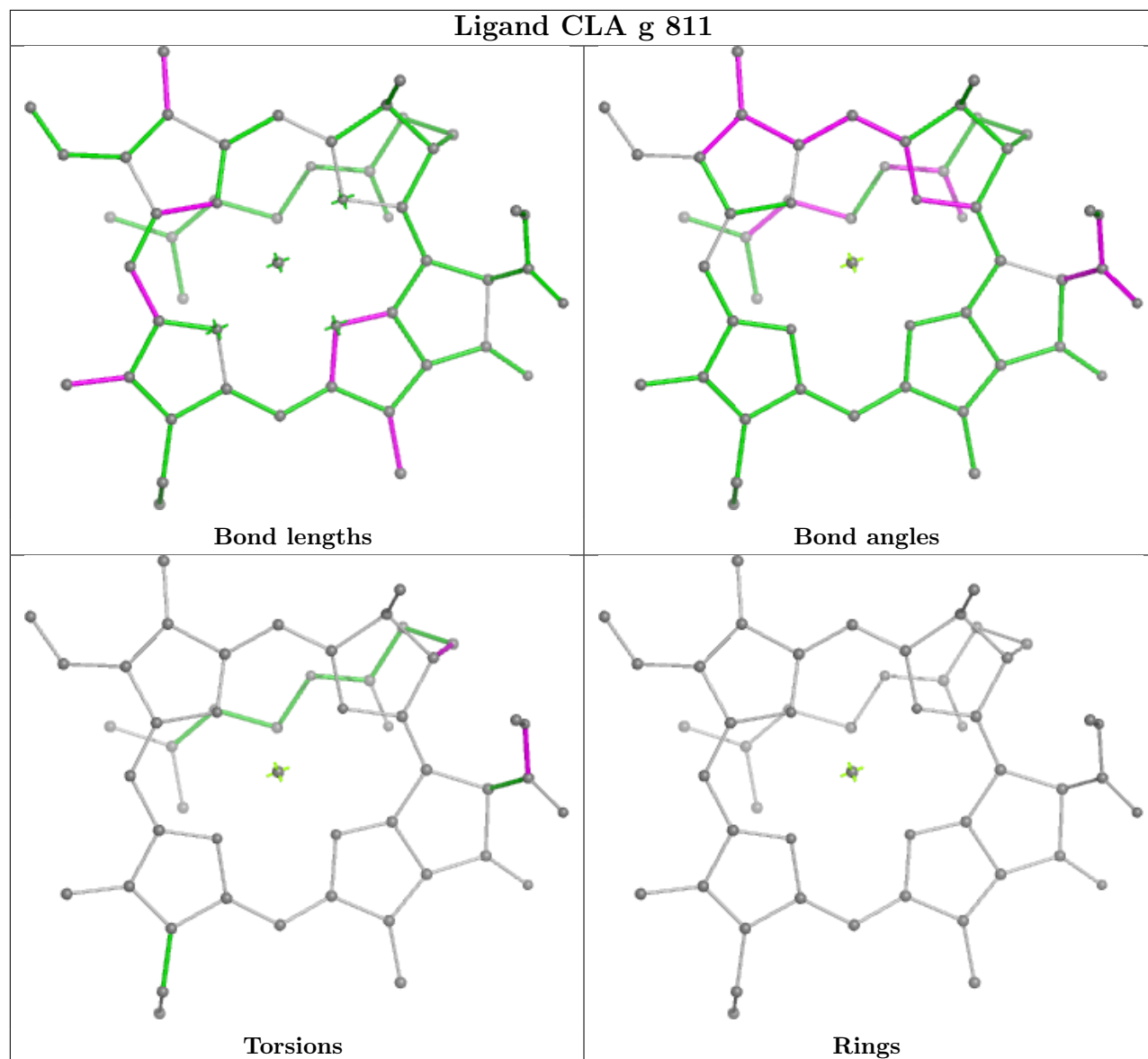


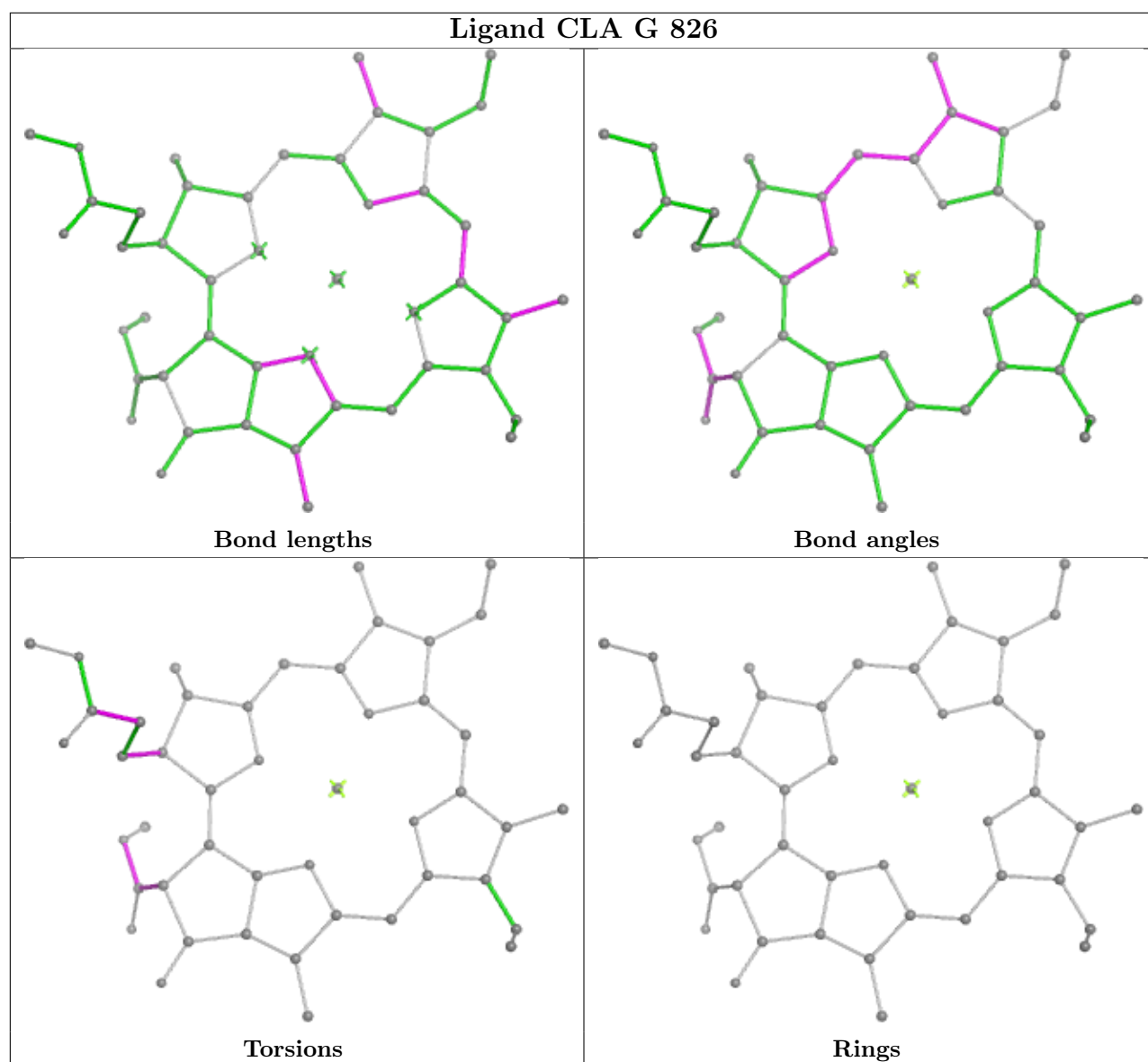
## Ligand CLA B 806

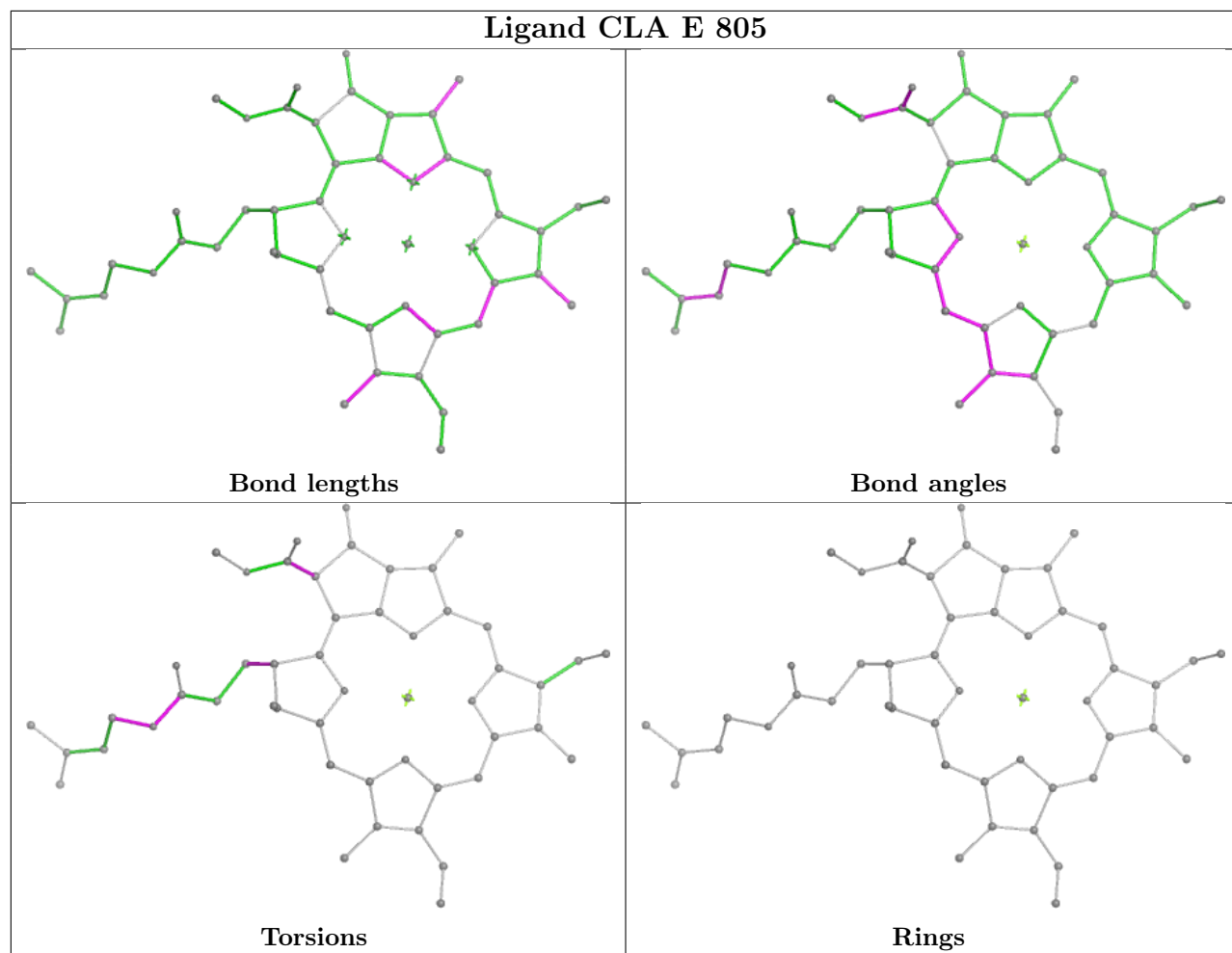


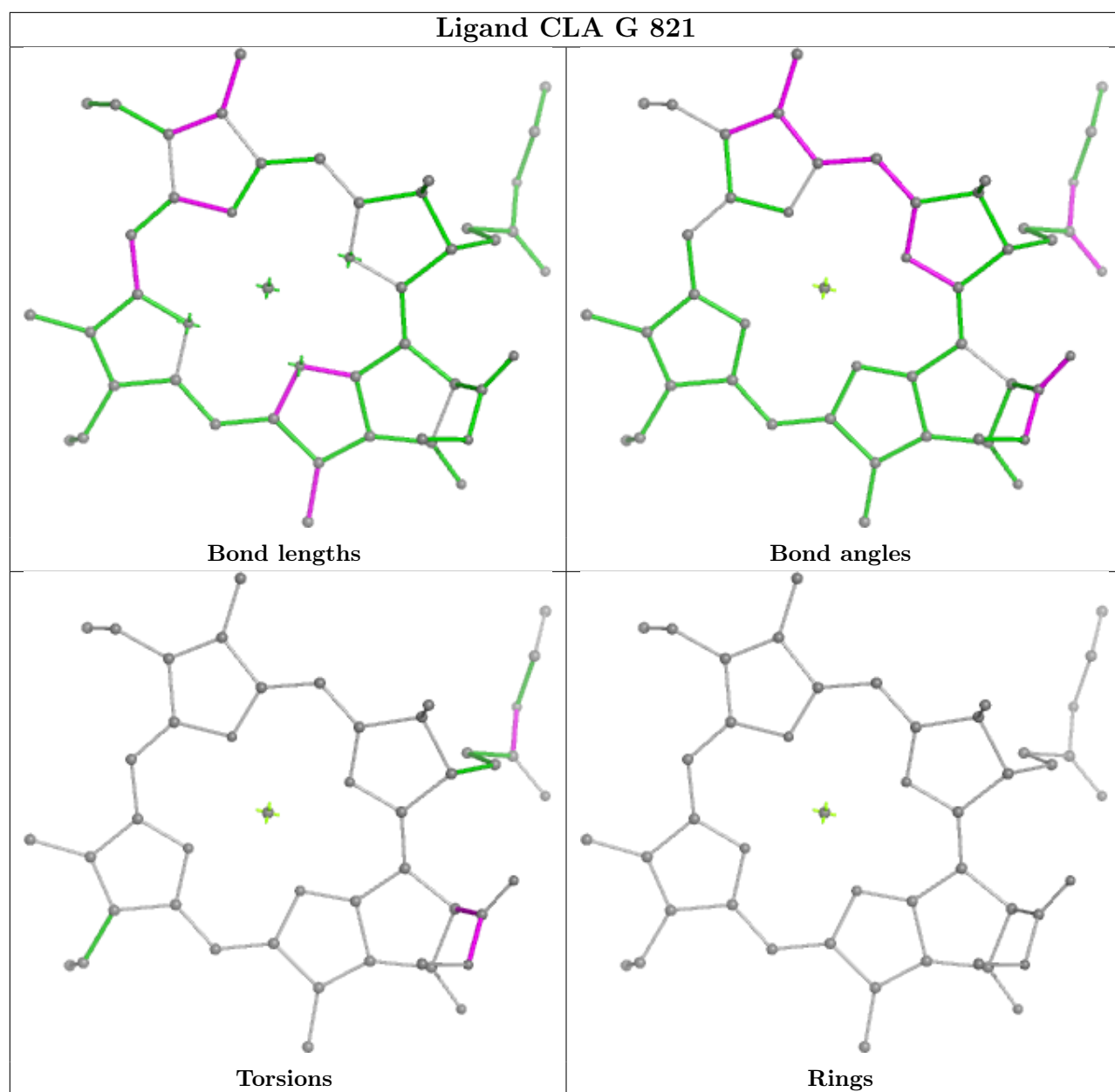


## Ligand CLA g 811

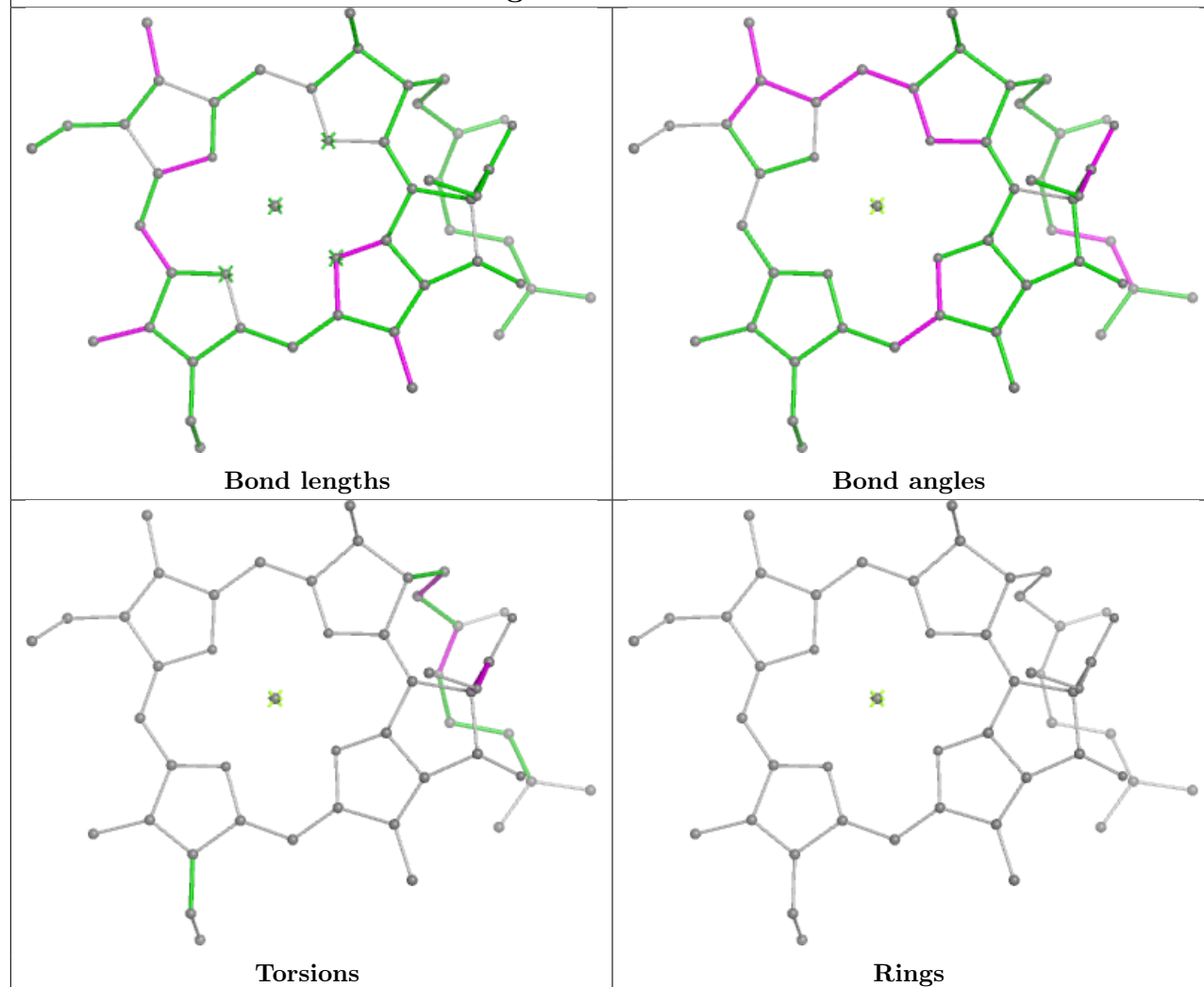




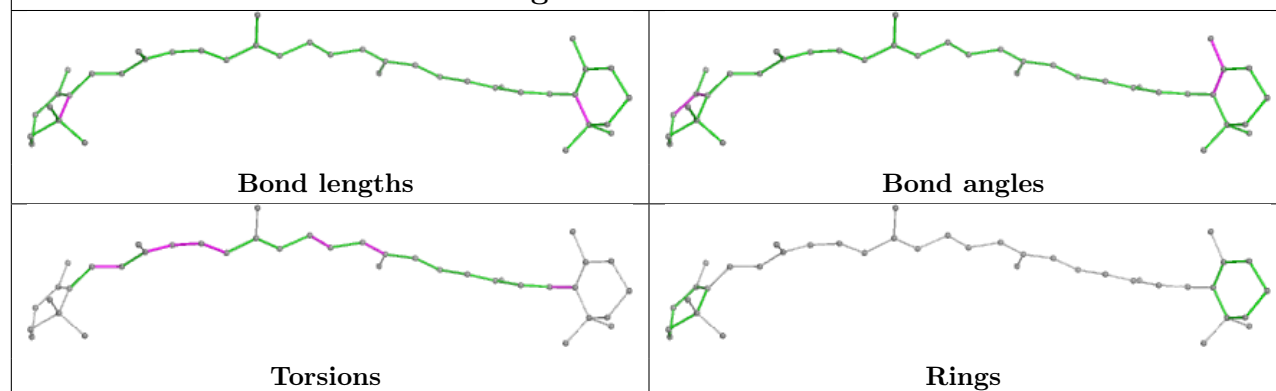




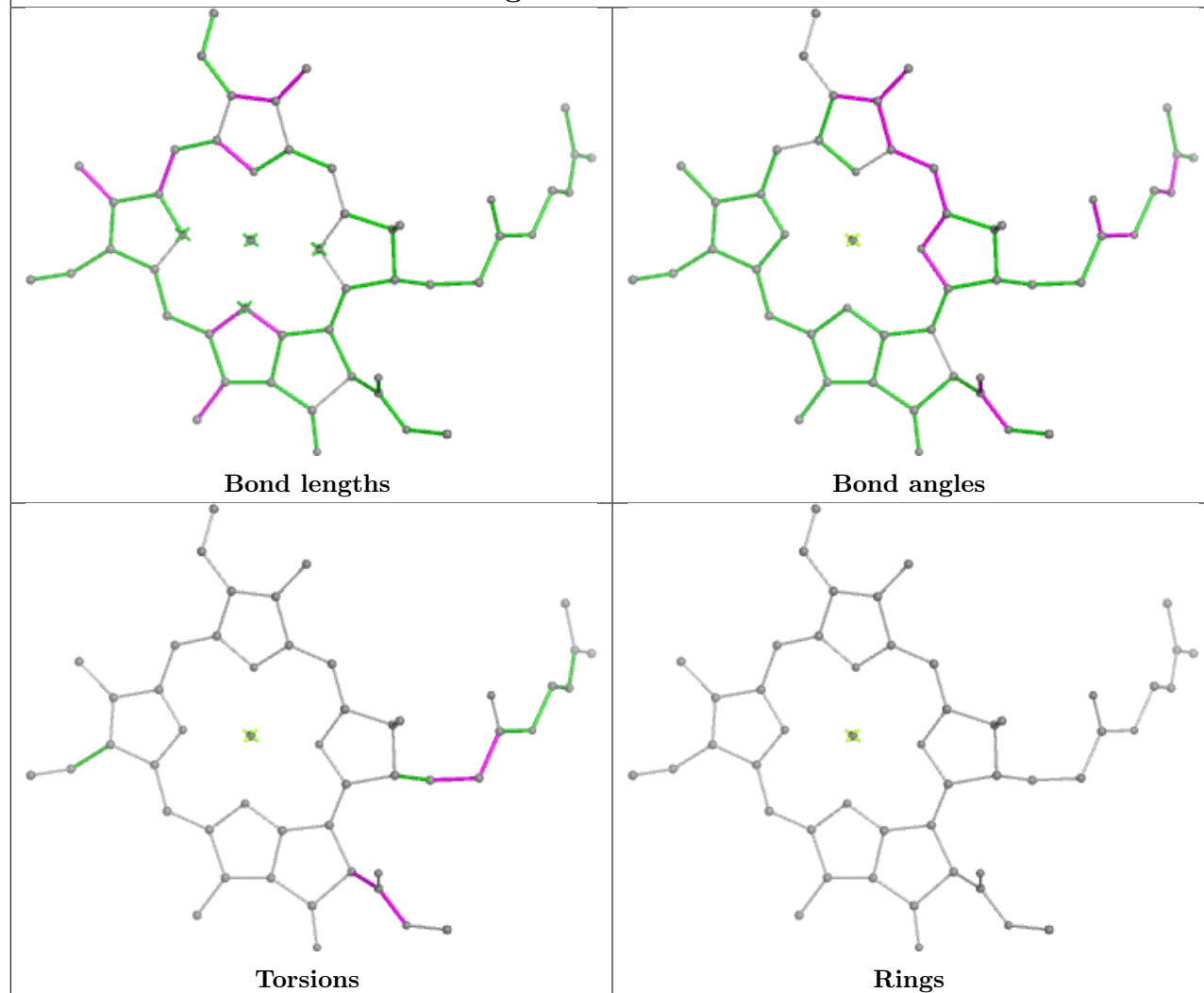
## Ligand CLA e 809



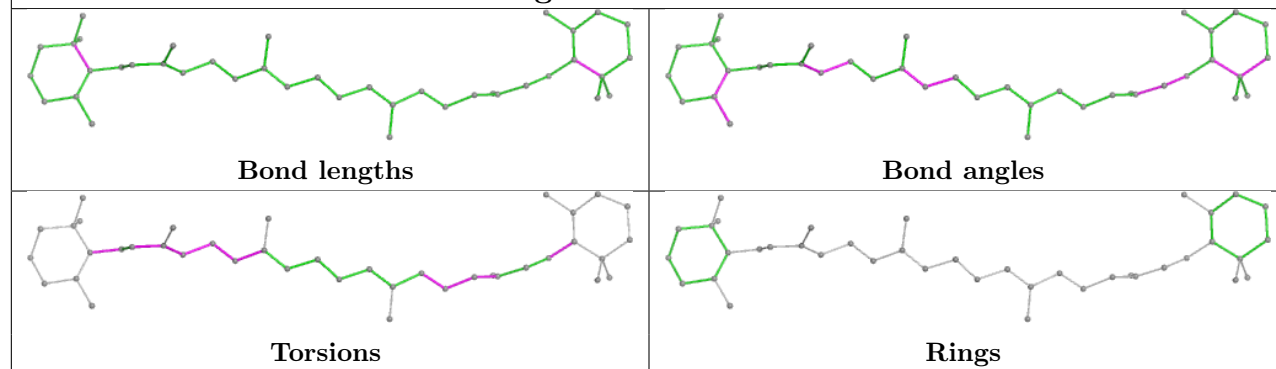
## Ligand BCR P 101

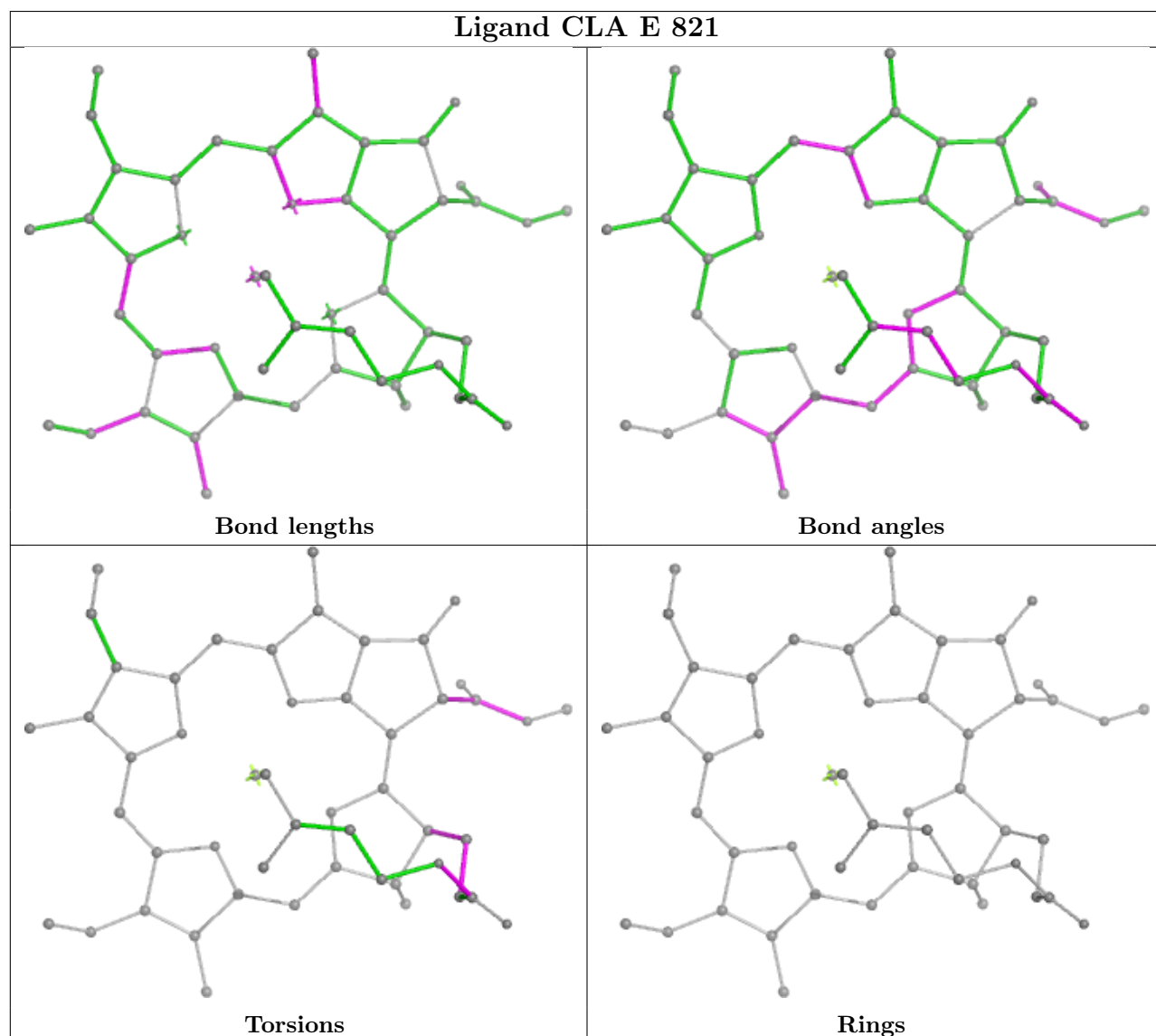
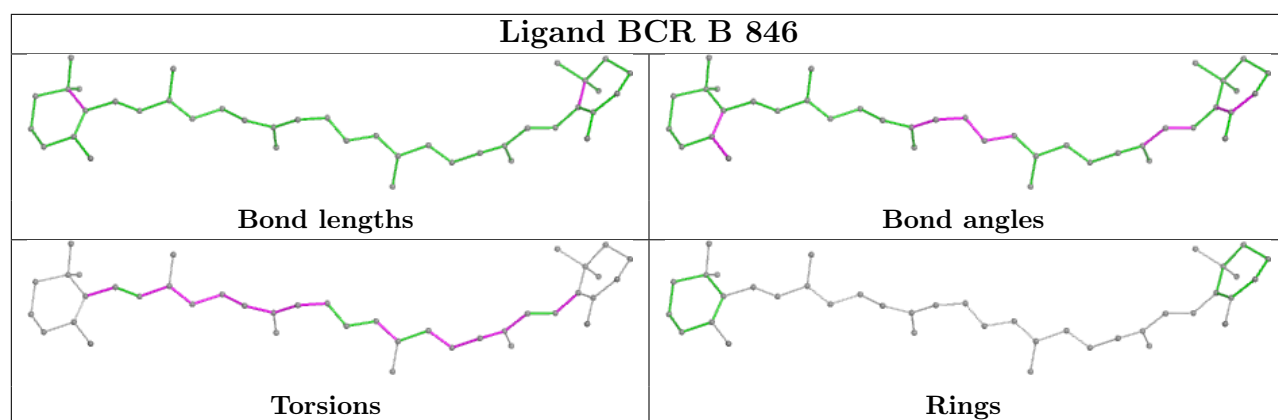


## Ligand CLA b 810

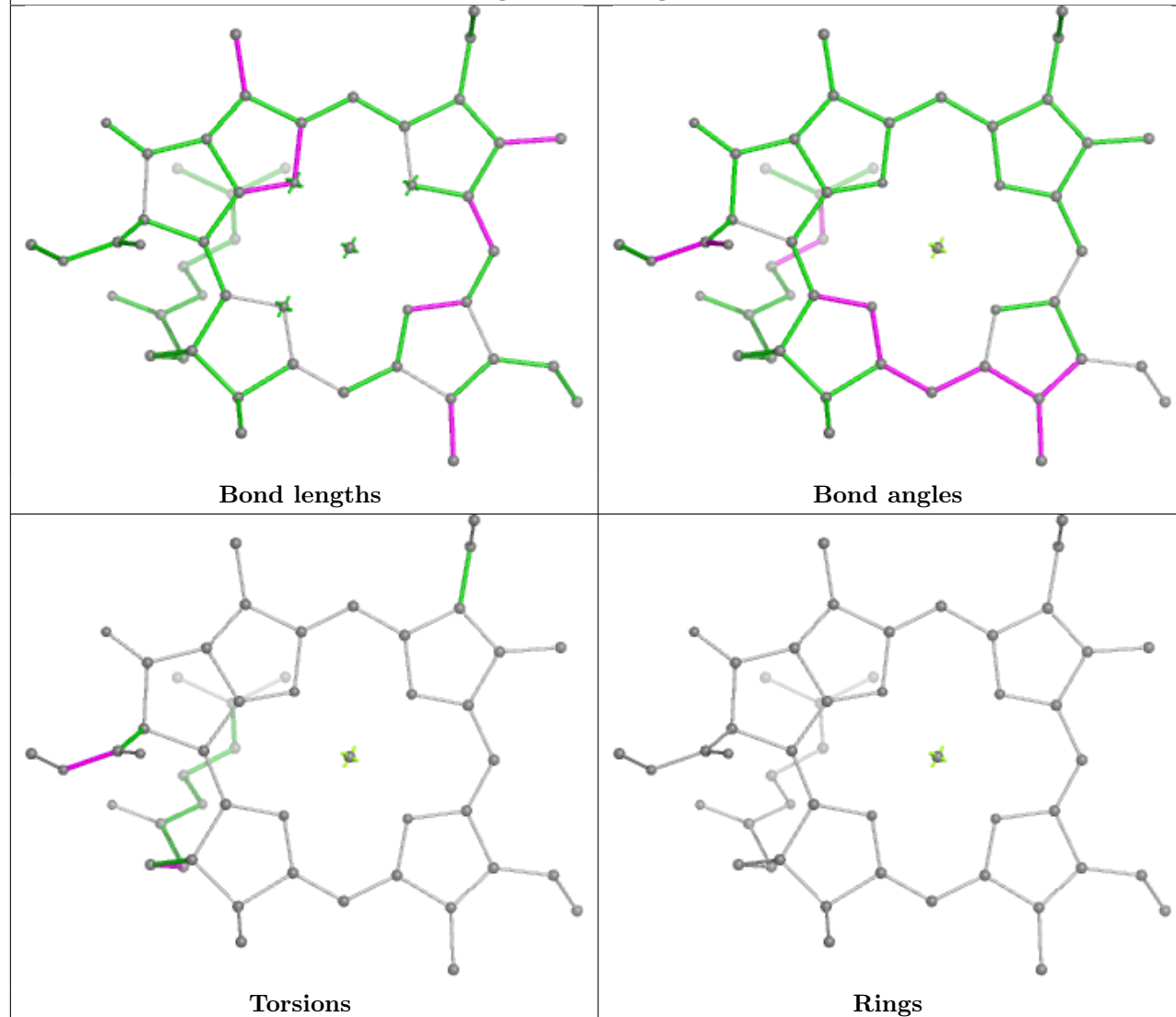


## Ligand BCR a 850

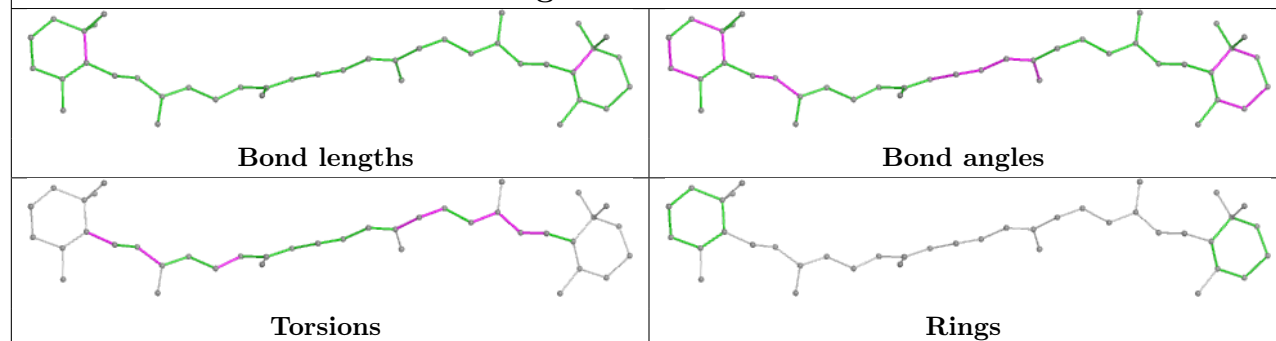




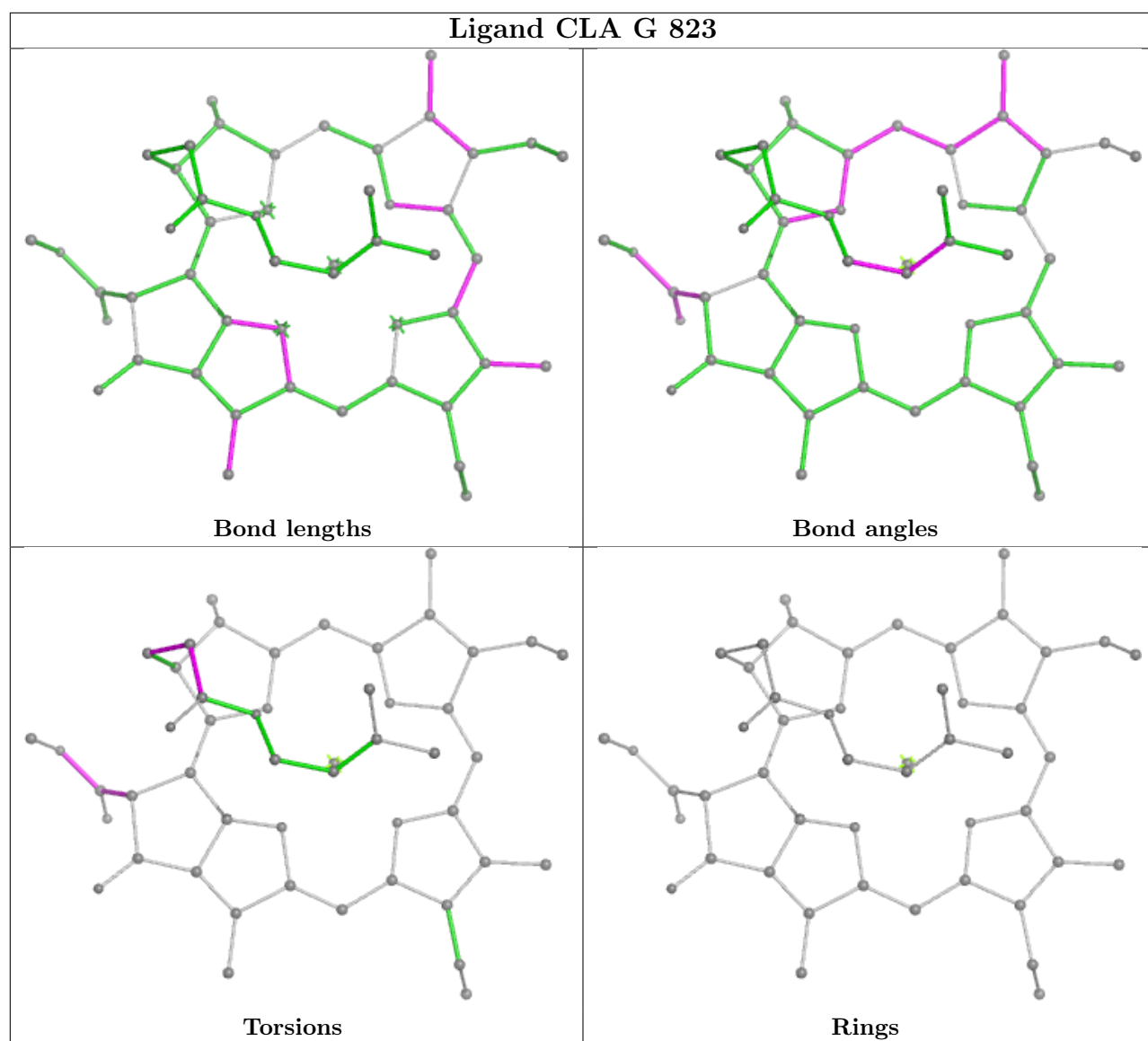
## Ligand CLA g 816



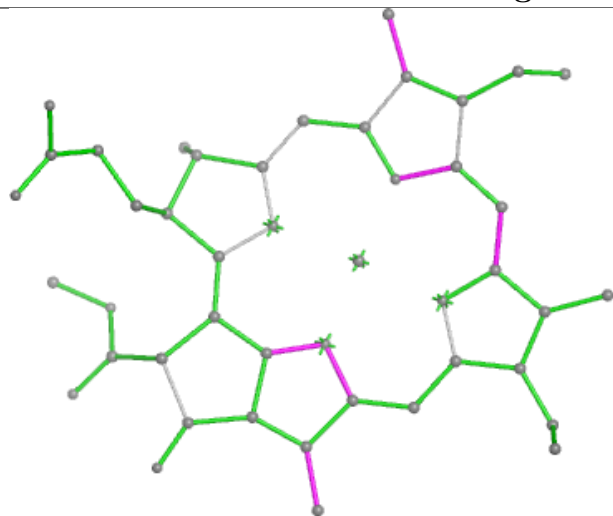
## Ligand BCR s 204



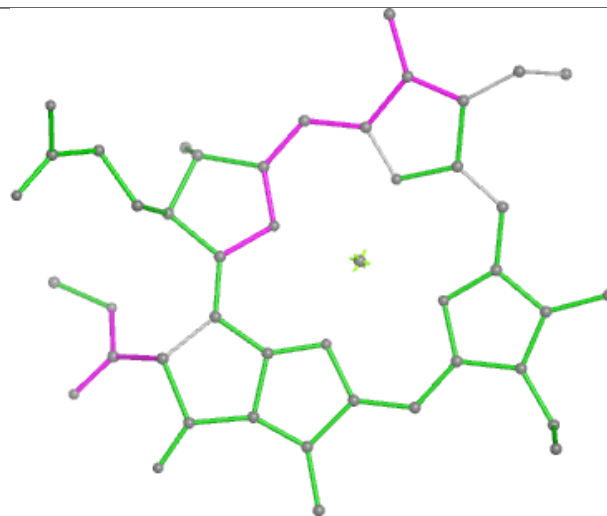




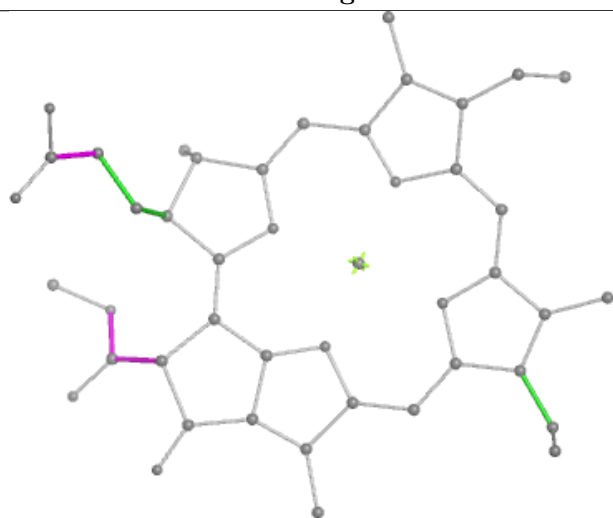
## Ligand CLA B 824



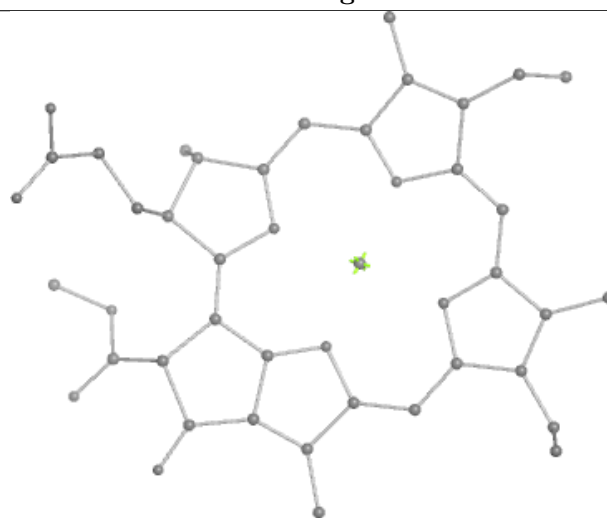
Bond lengths



Bond angles

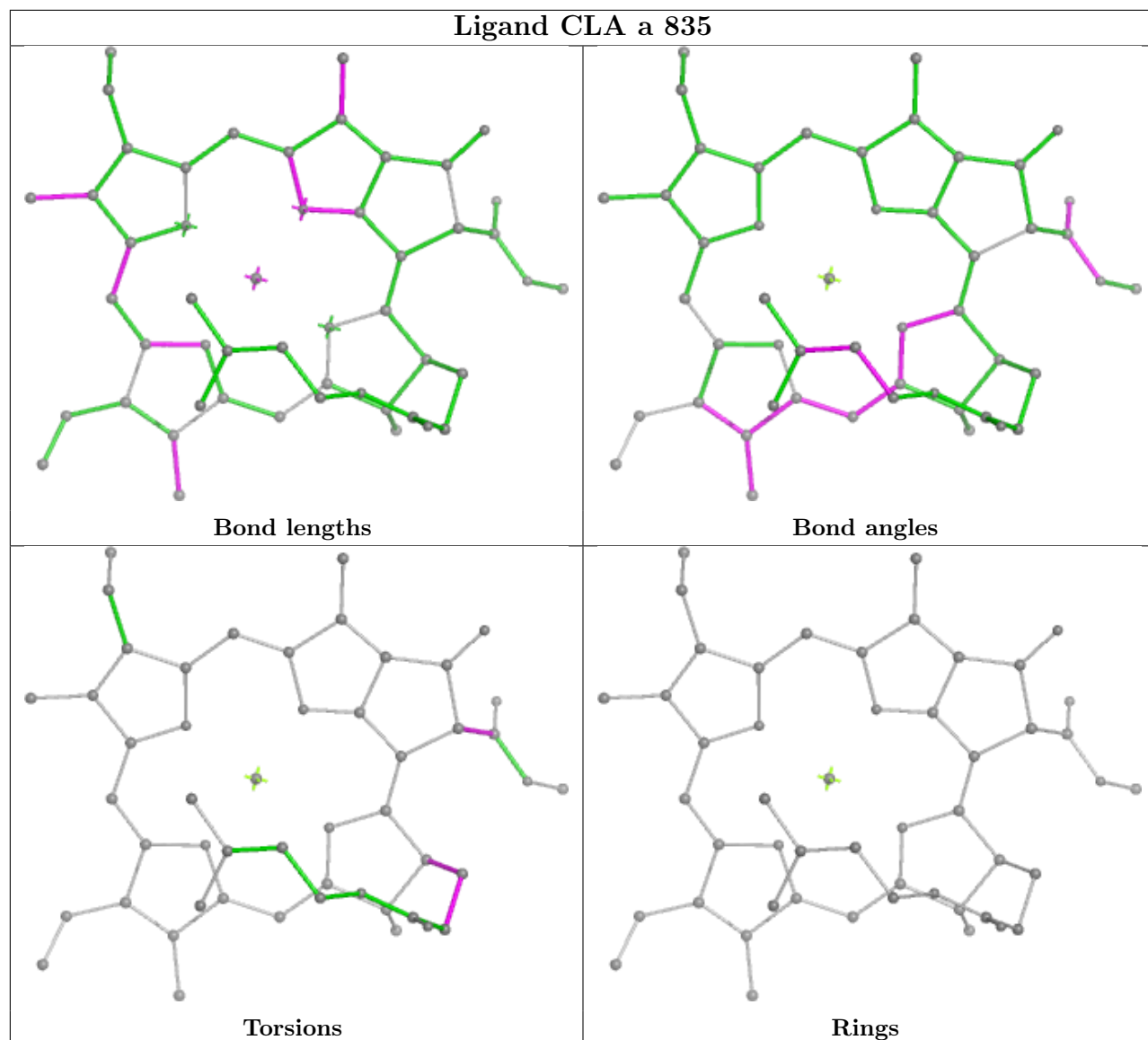


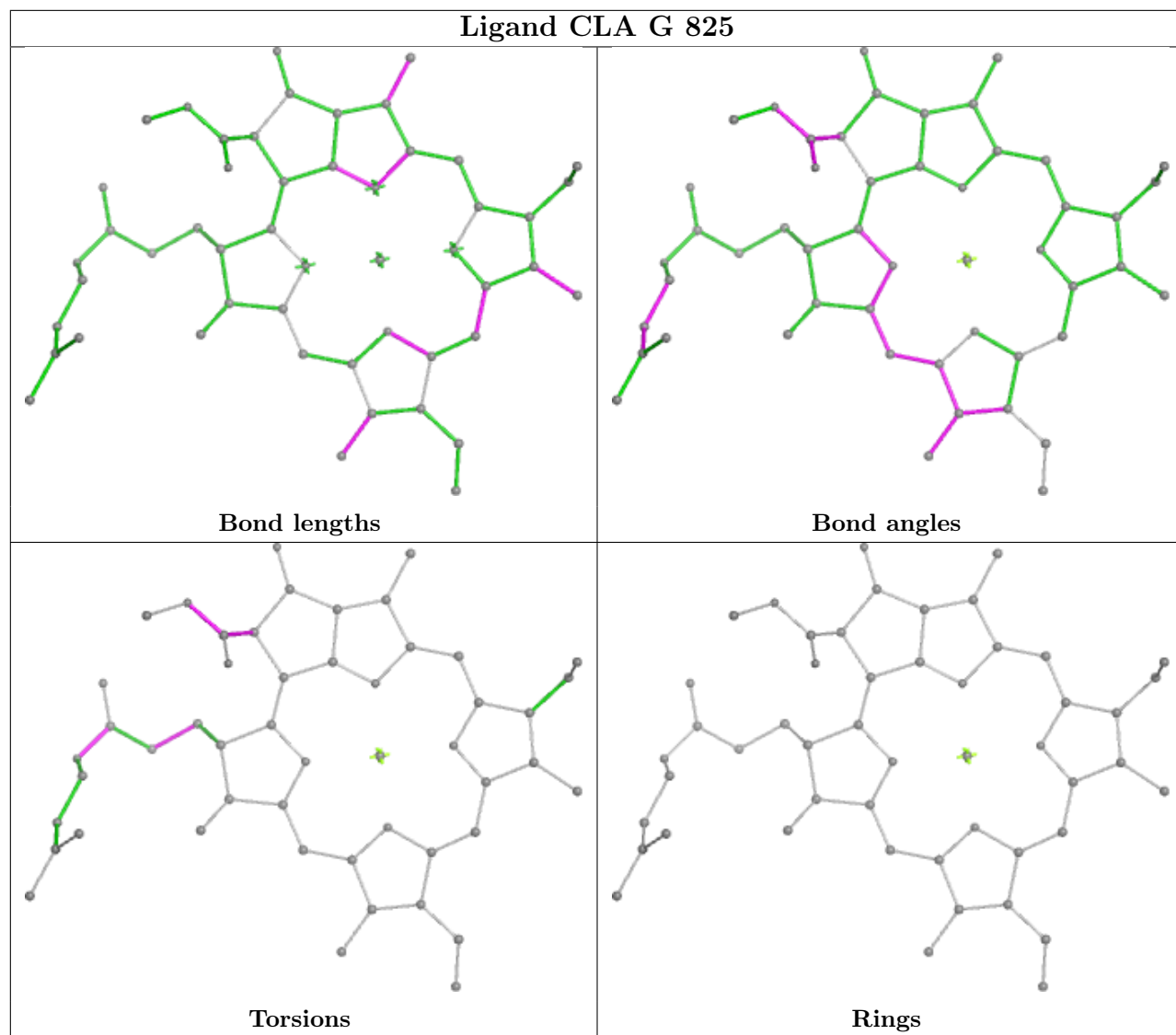
Torsions



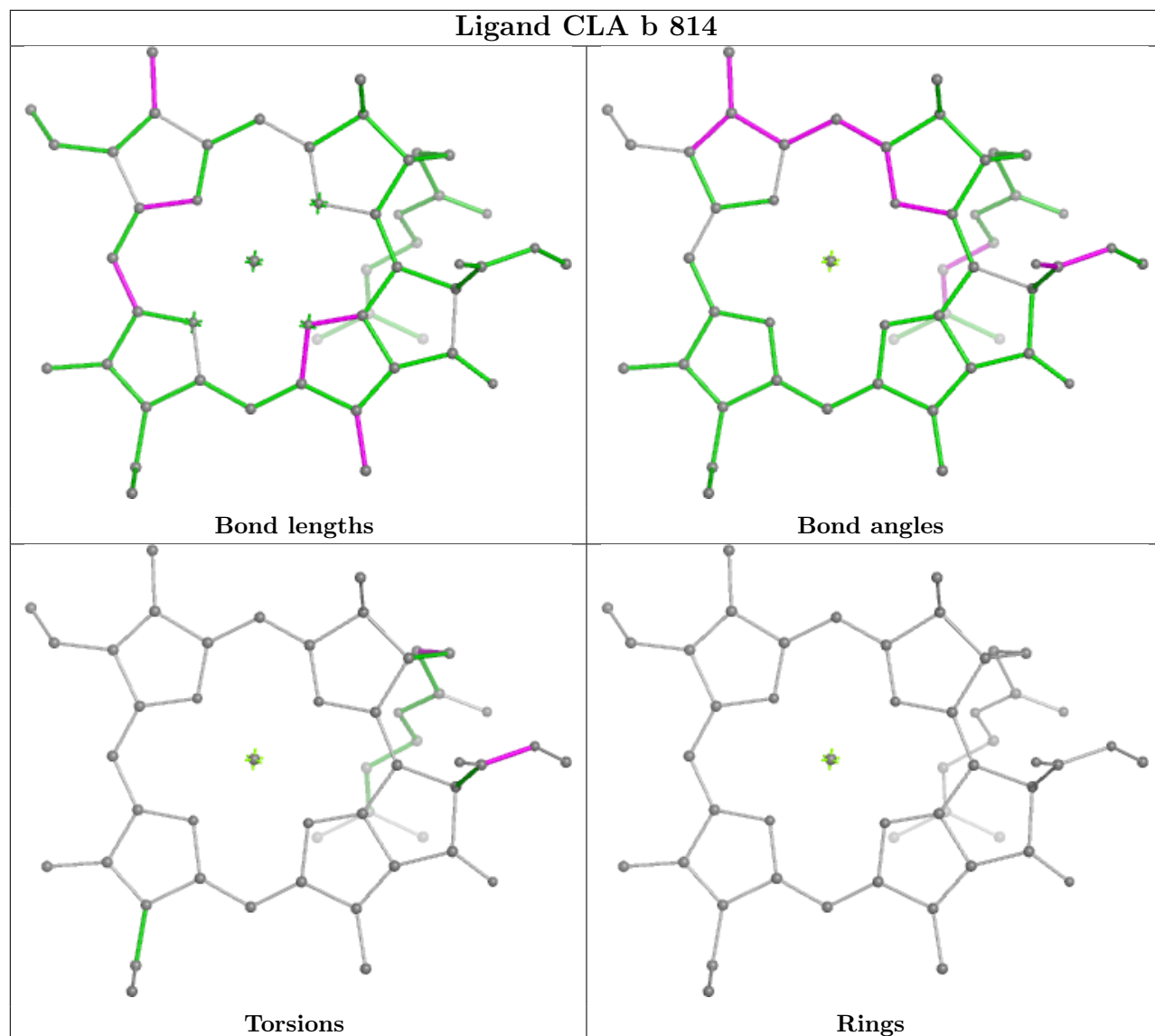
Rings

## Ligand CLA a 835

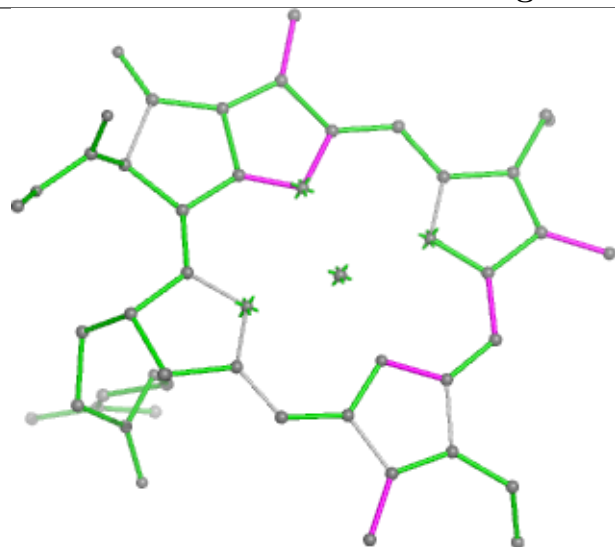




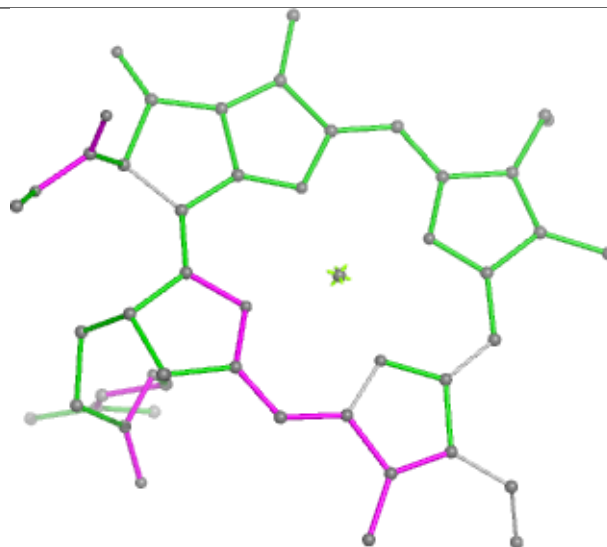
## Ligand CLA b 814



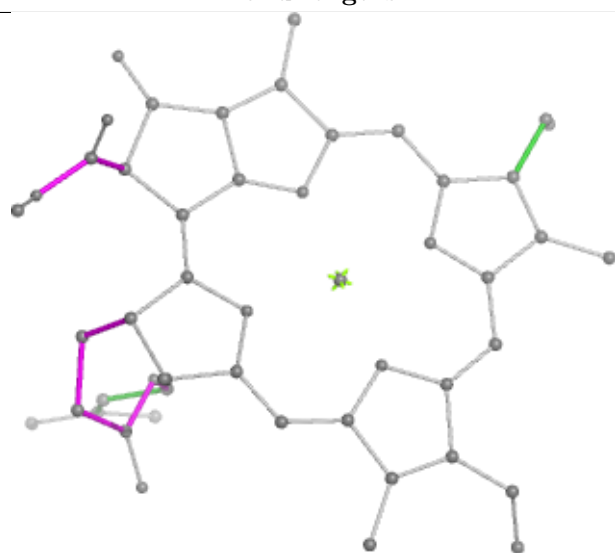
## Ligand CLA B 829



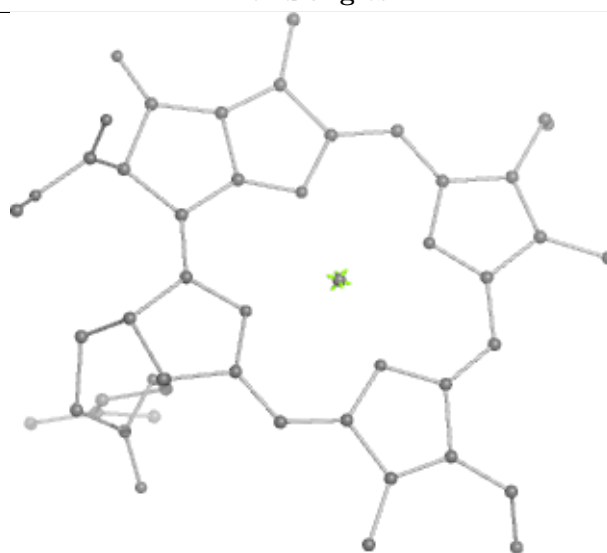
Bond lengths



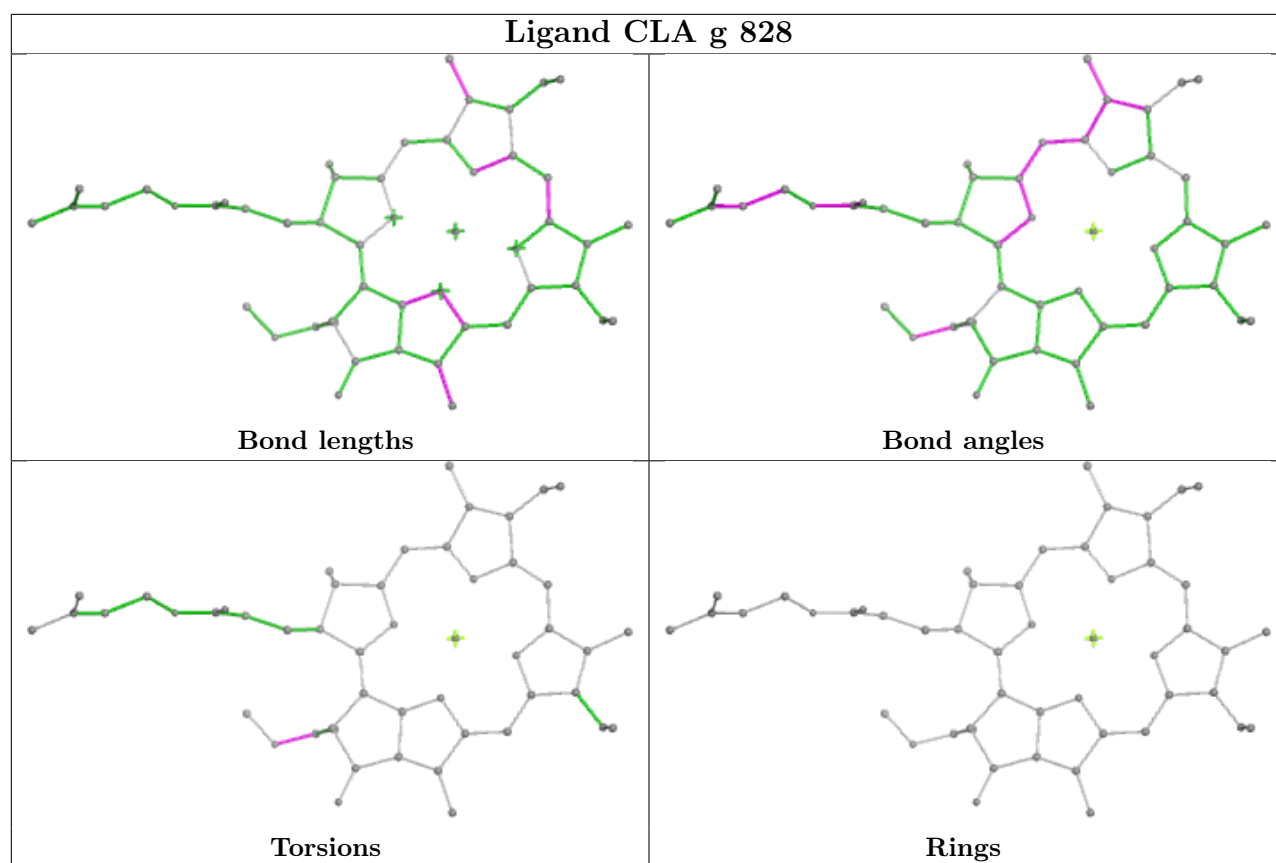
Bond angles



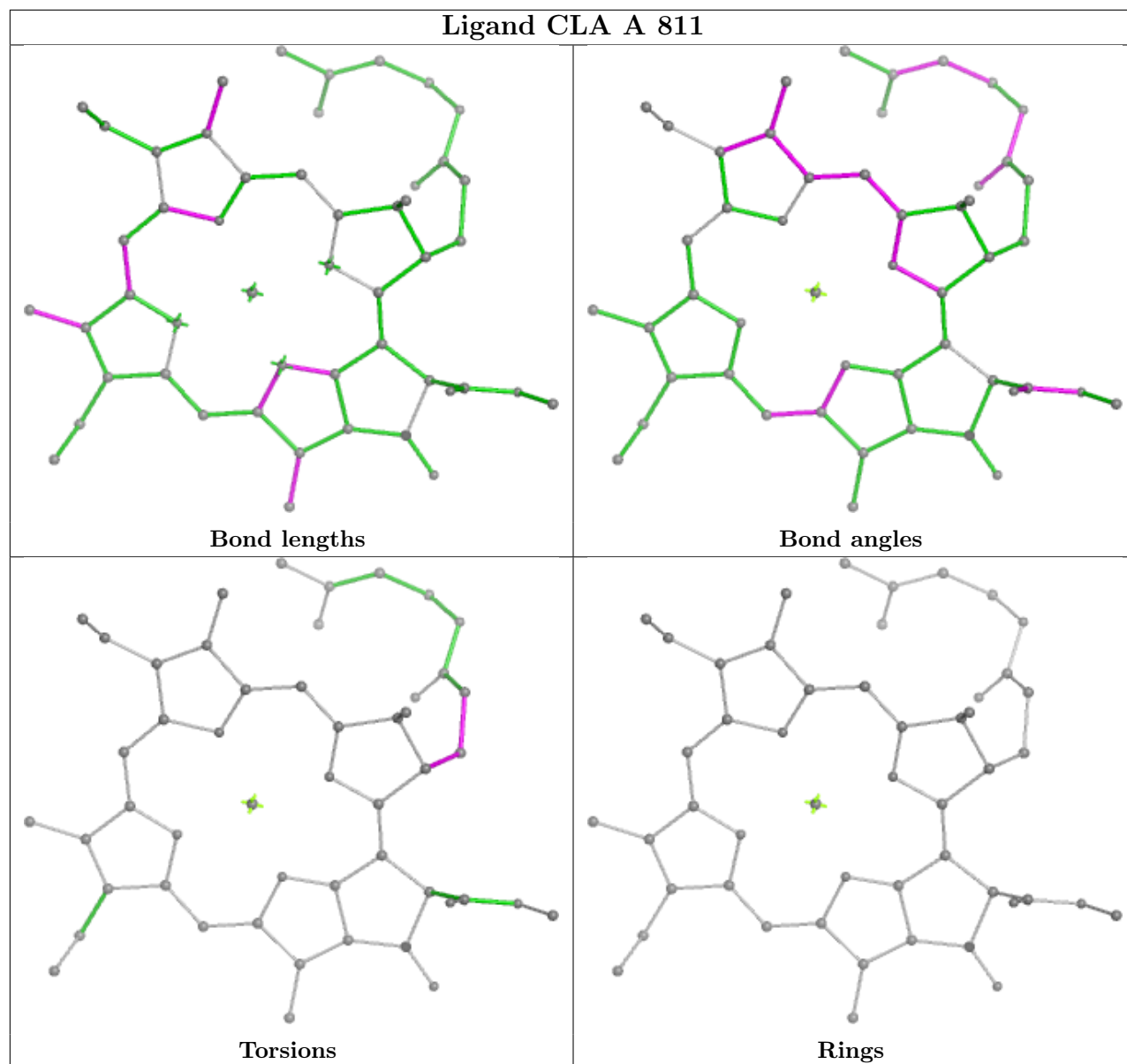
Torsions



Rings

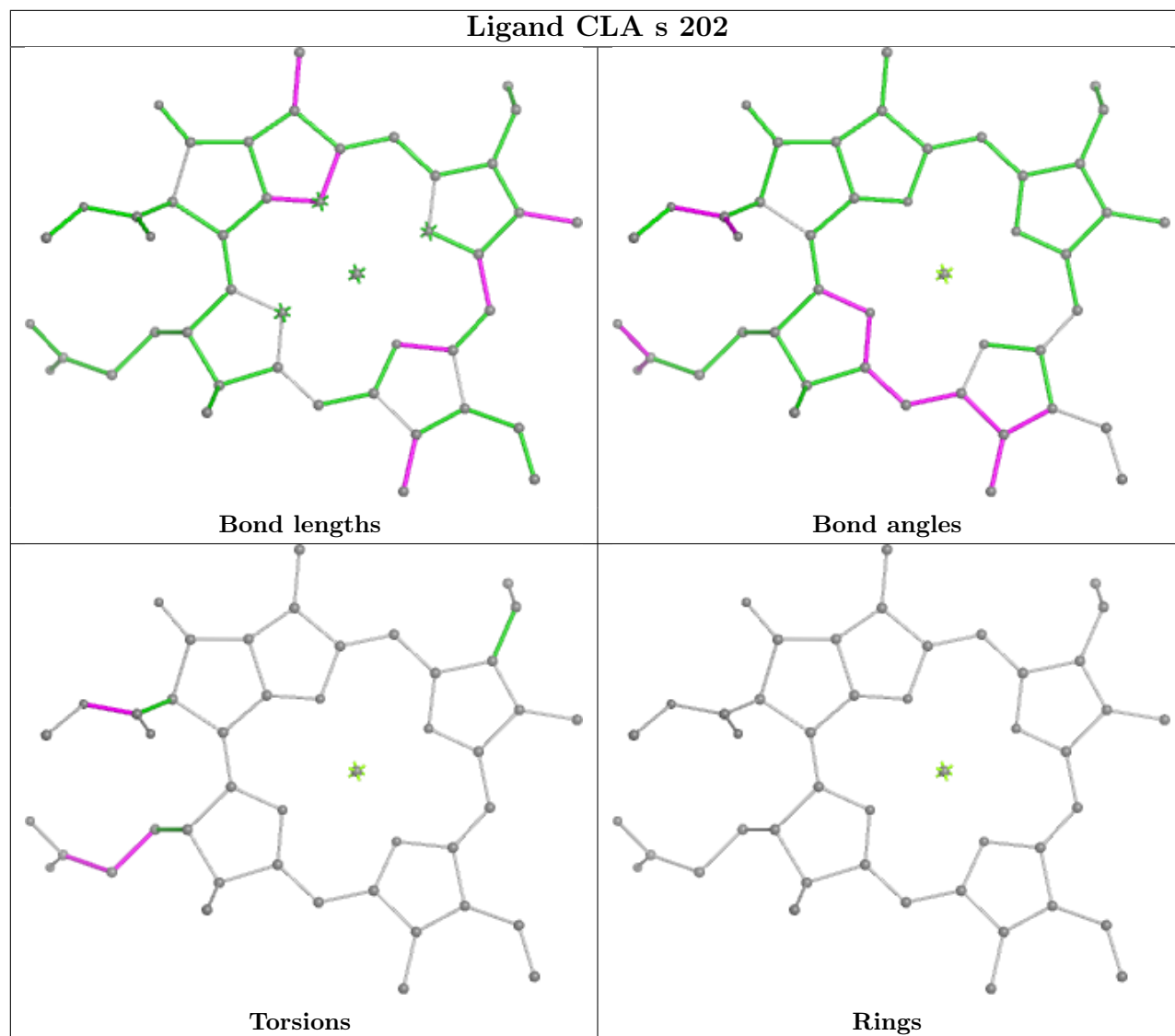


## Ligand CLA A 811

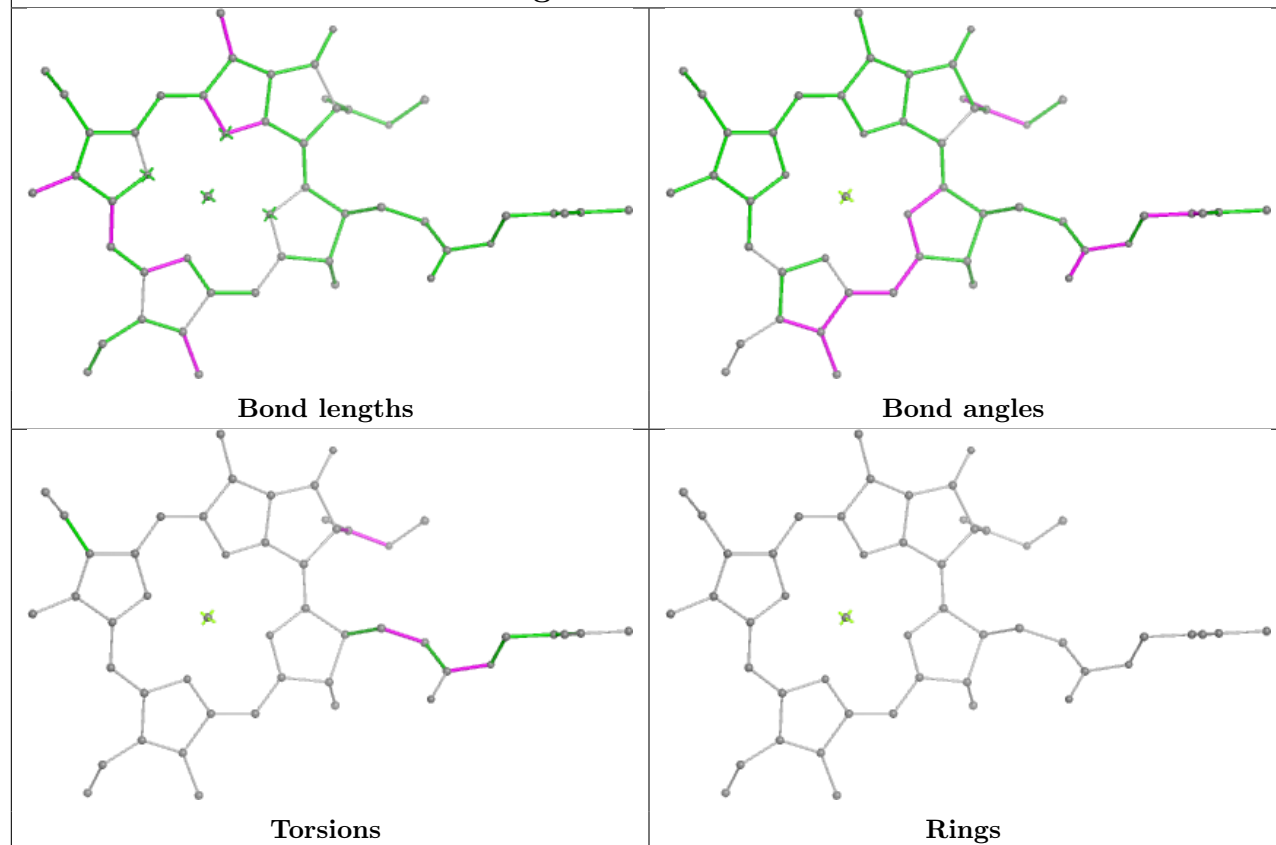




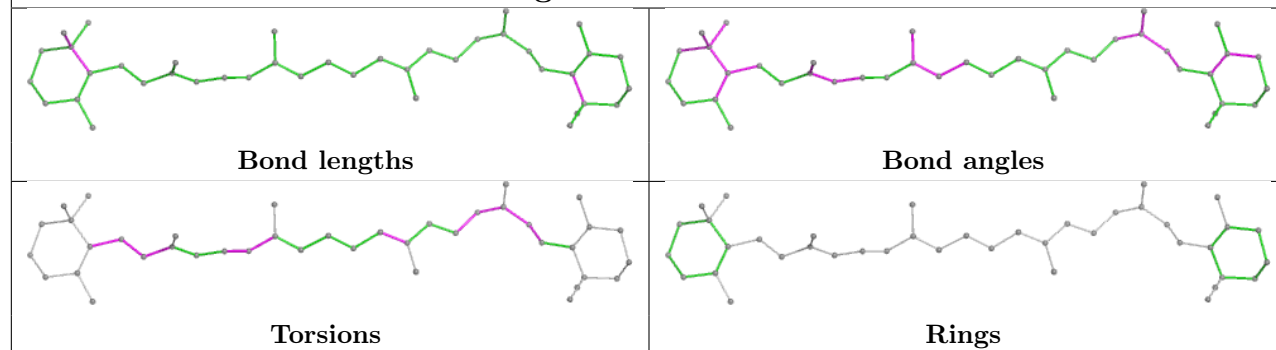
## Ligand CLA s 202



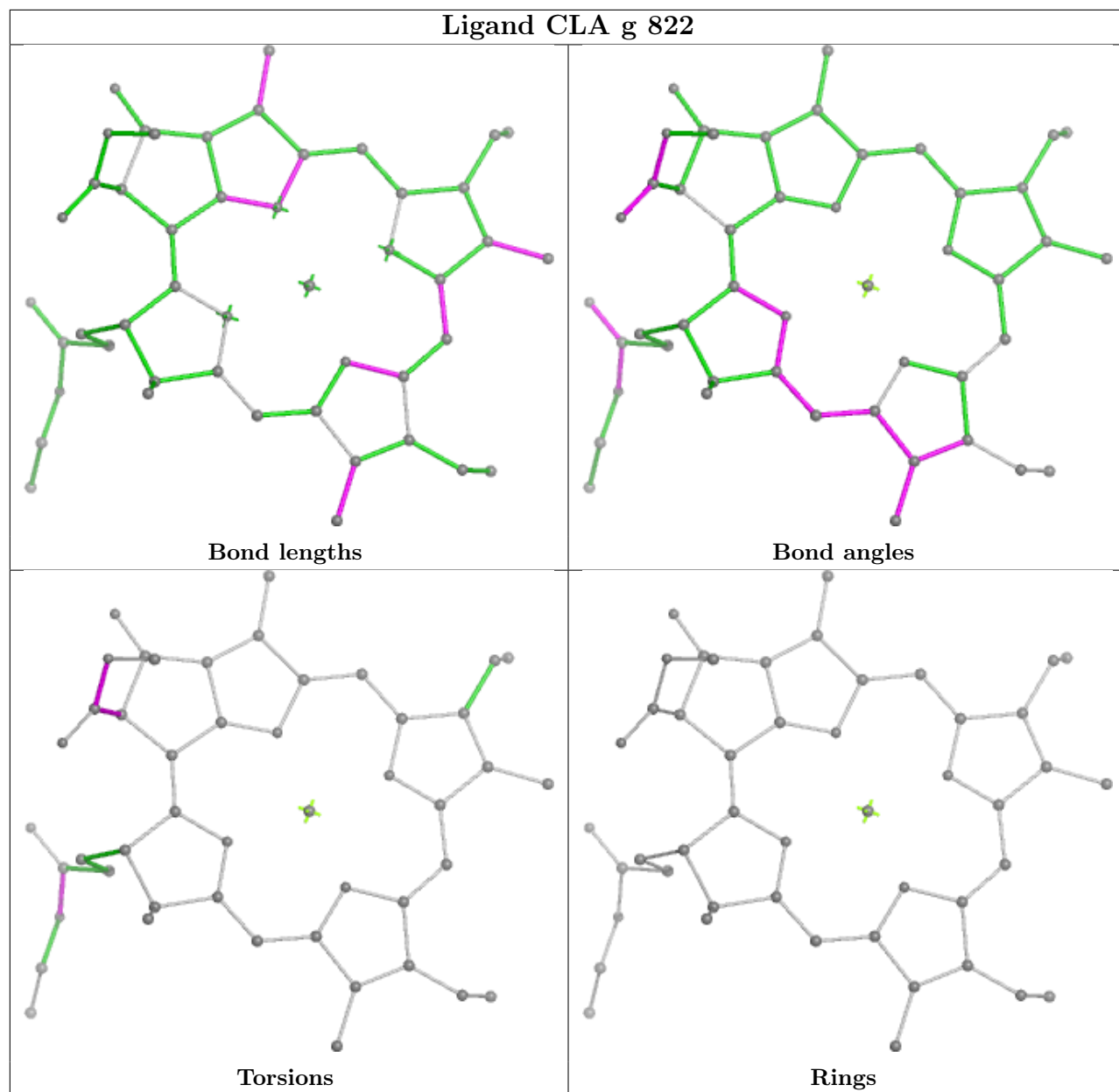
## Ligand CLA E 844



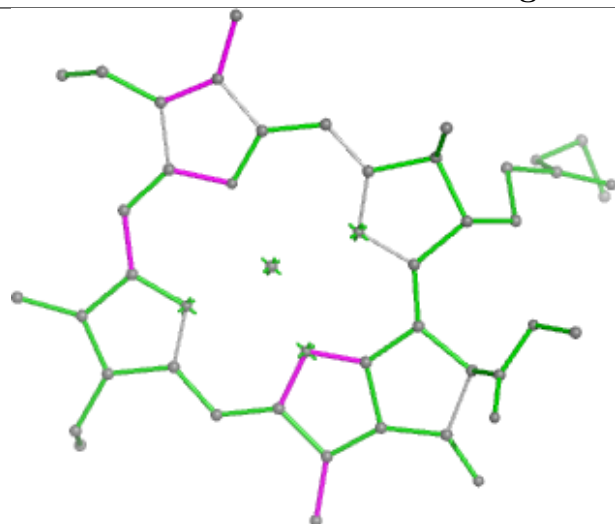
## Ligand BCR a 848



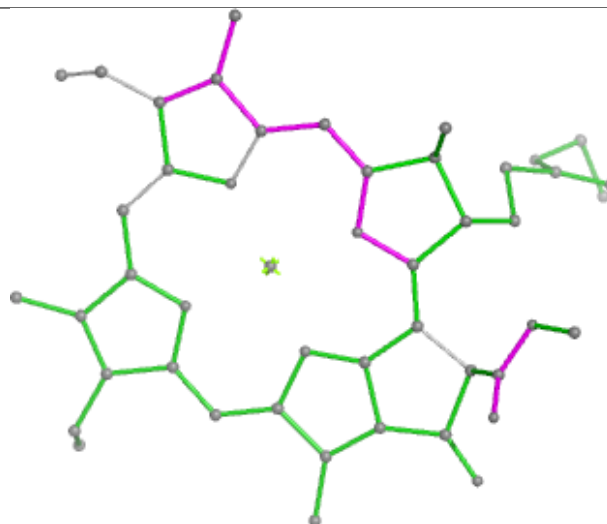
## Ligand CLA g 822



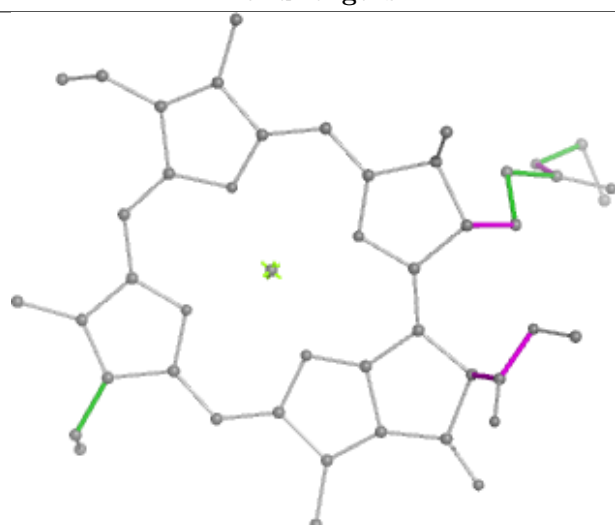
## Ligand CLA b 838



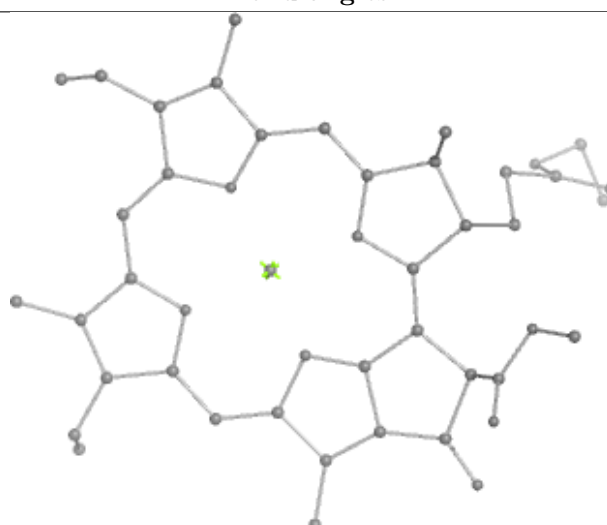
Bond lengths



Bond angles

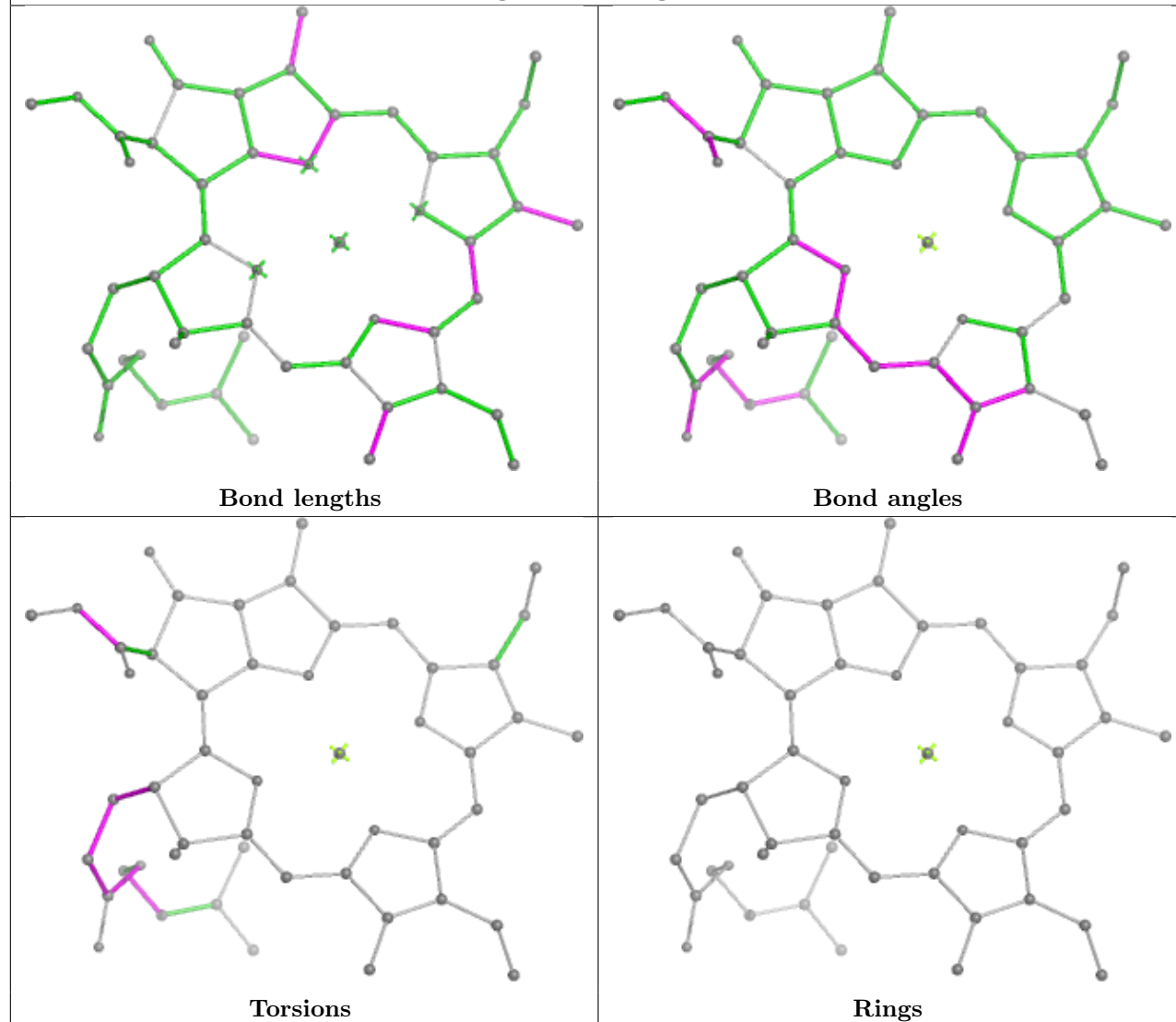


Torsions

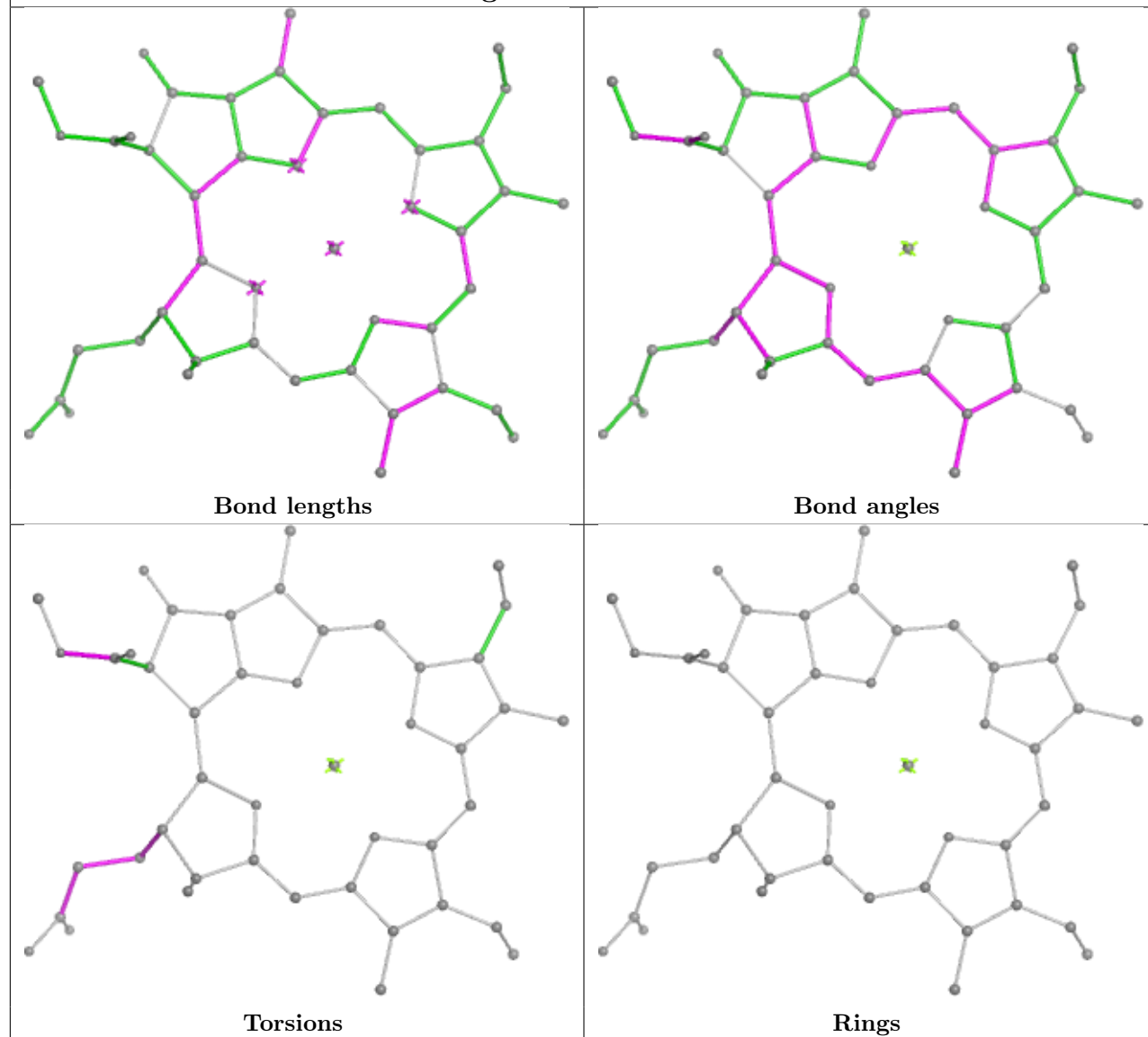


Rings

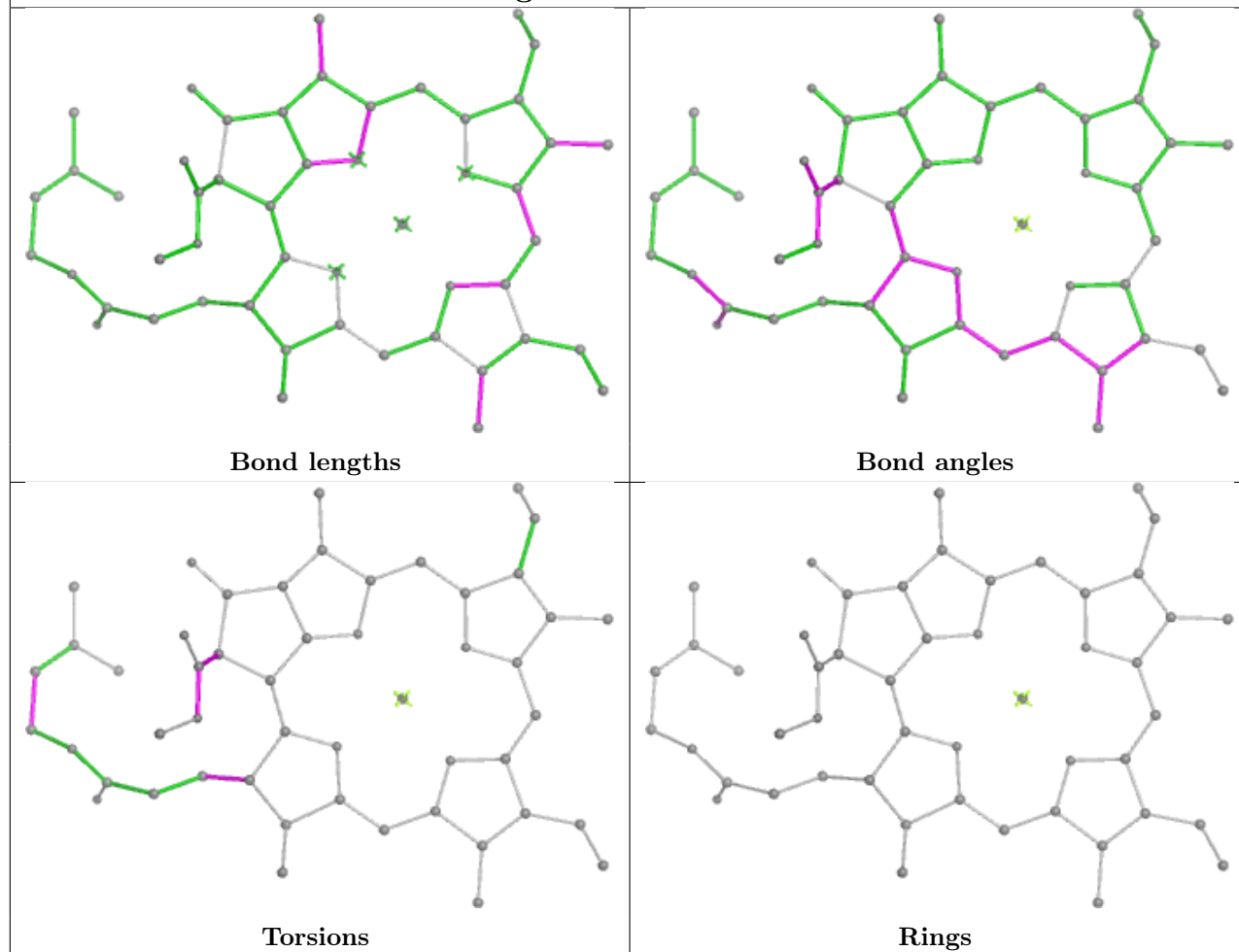
## Ligand CLA g 819



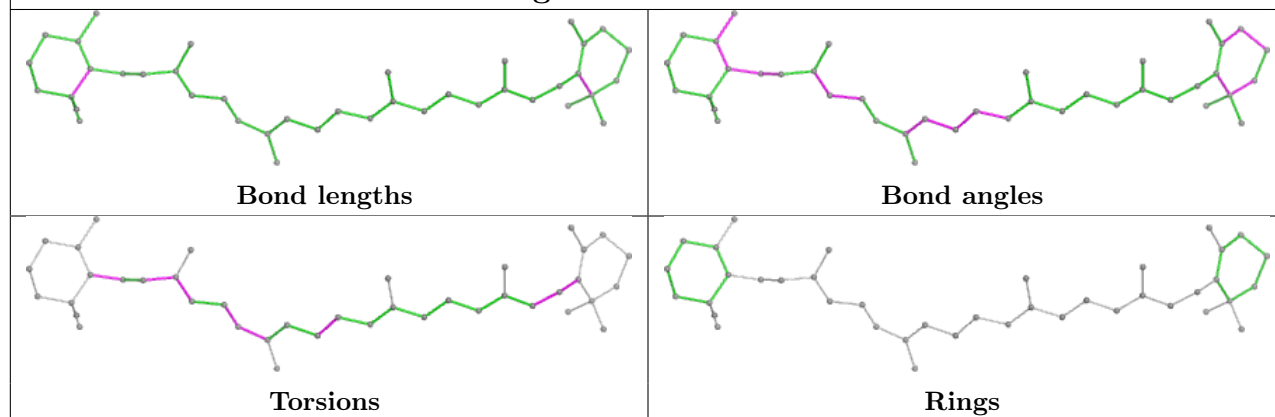
## Ligand CLA S 204



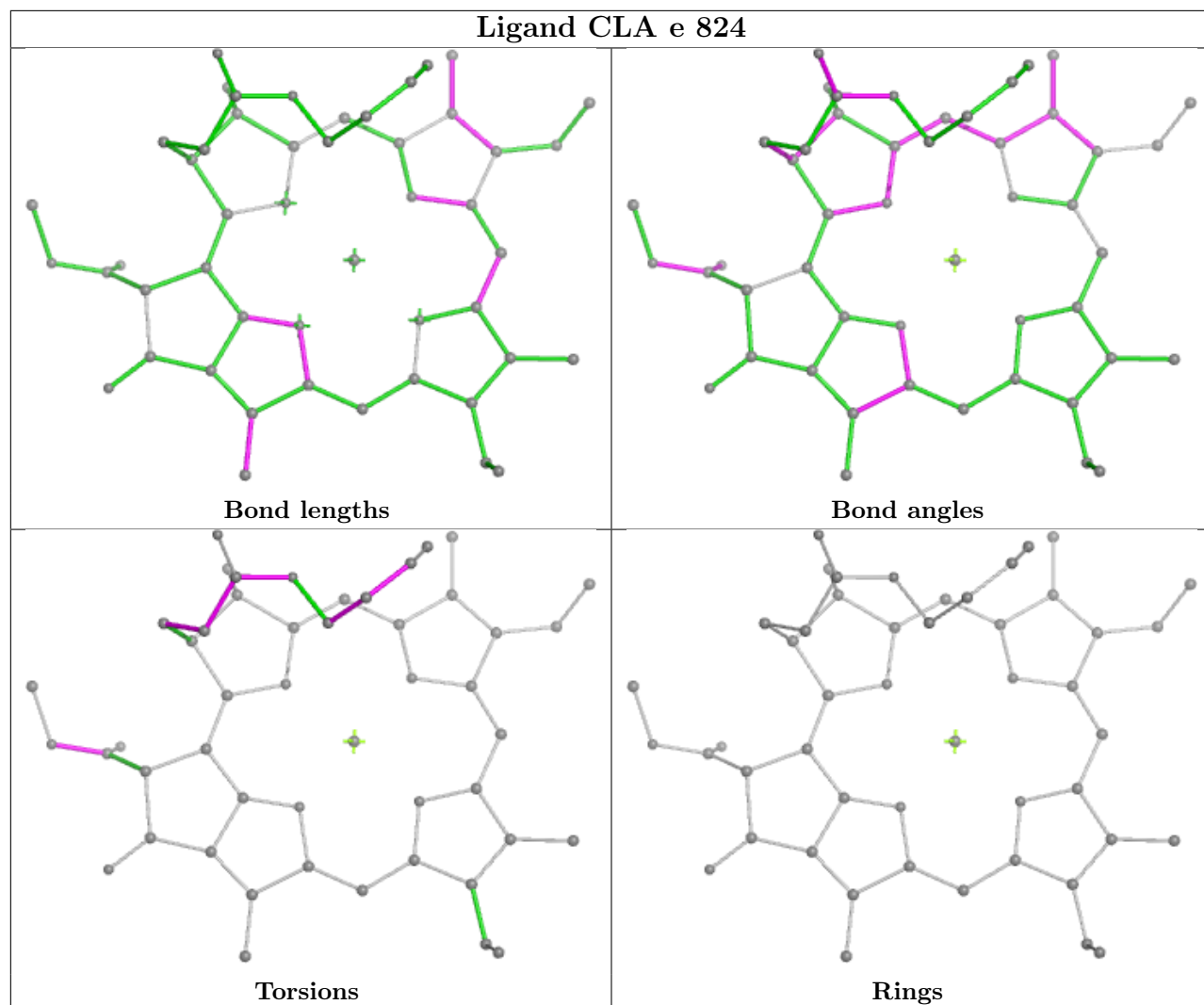
## Ligand CLA A 828



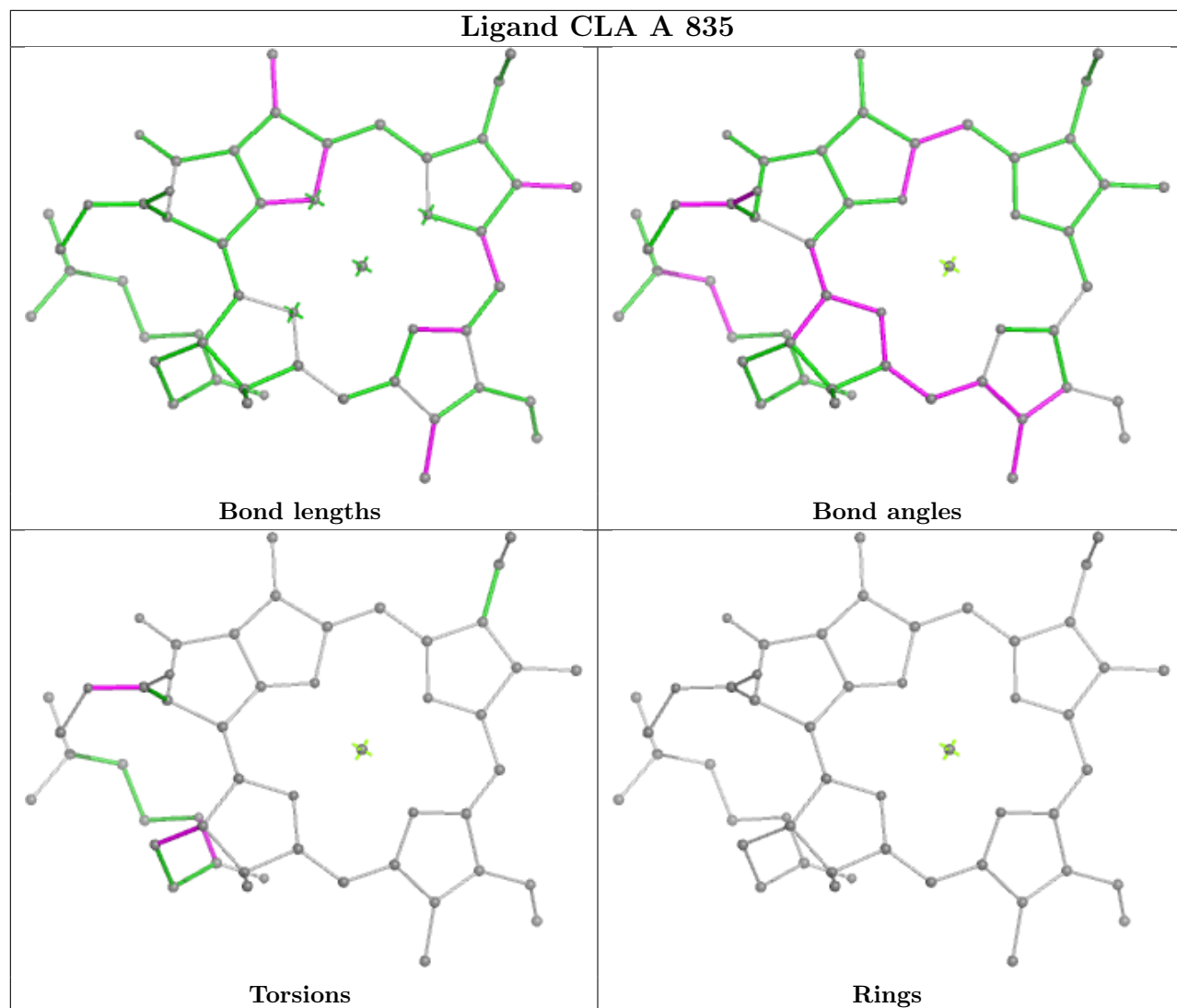
## Ligand BCR J 102

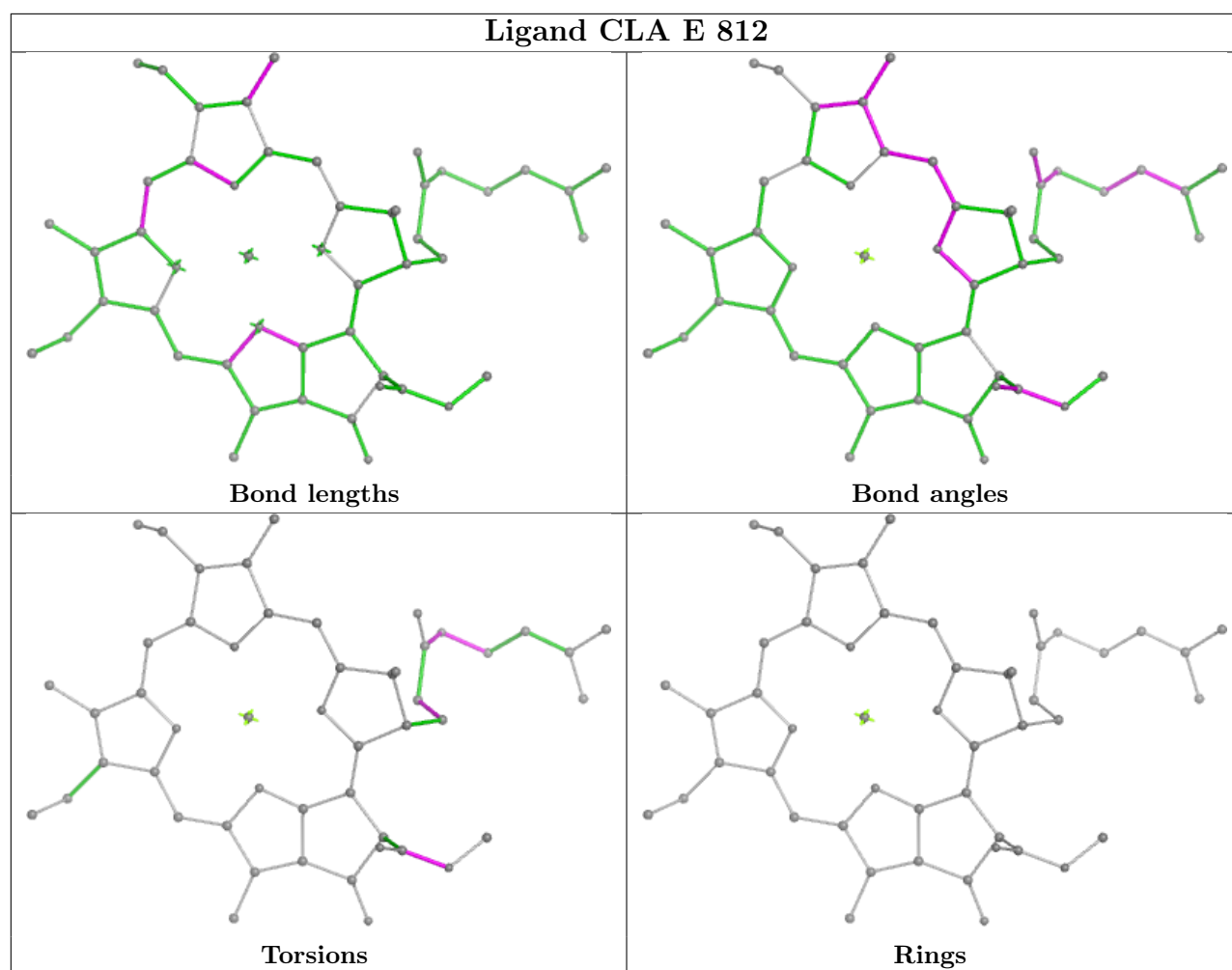


## Ligand CLA e 824

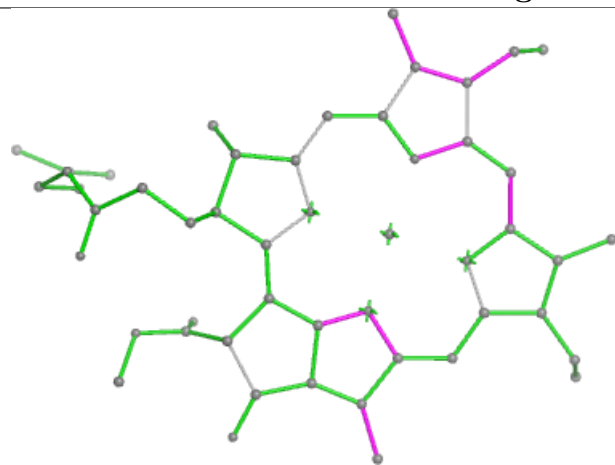




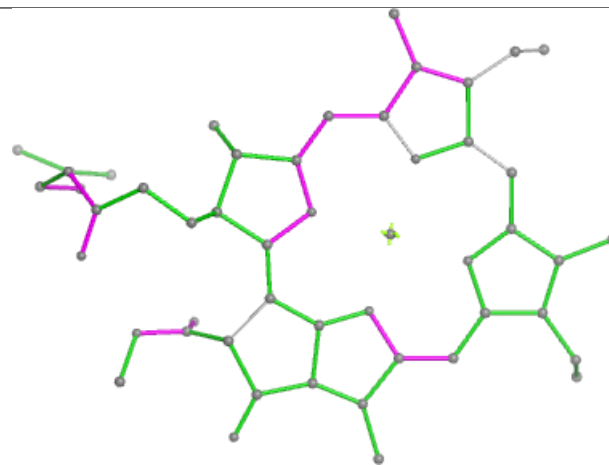




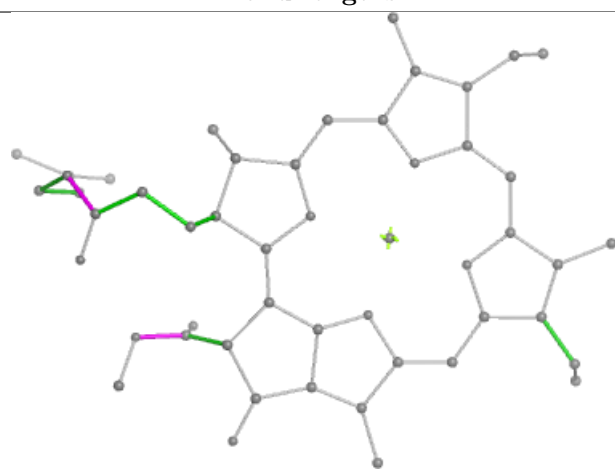
## Ligand CLA G 807



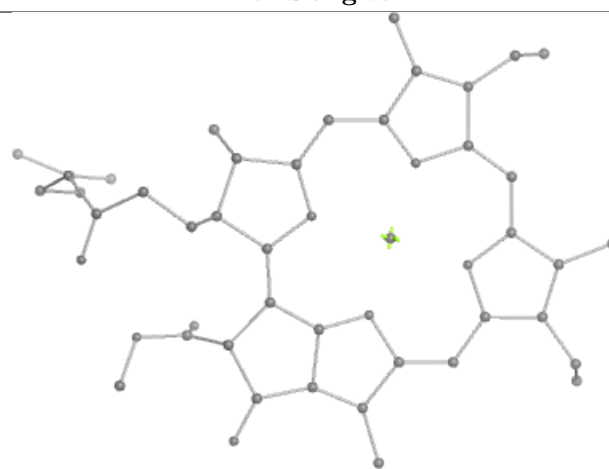
Bond lengths



Bond angles

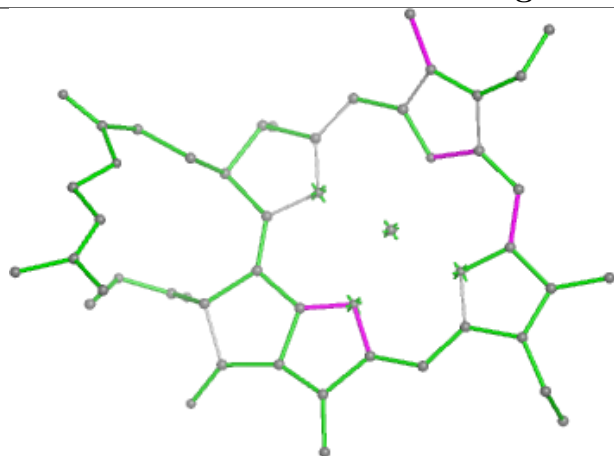


Torsions

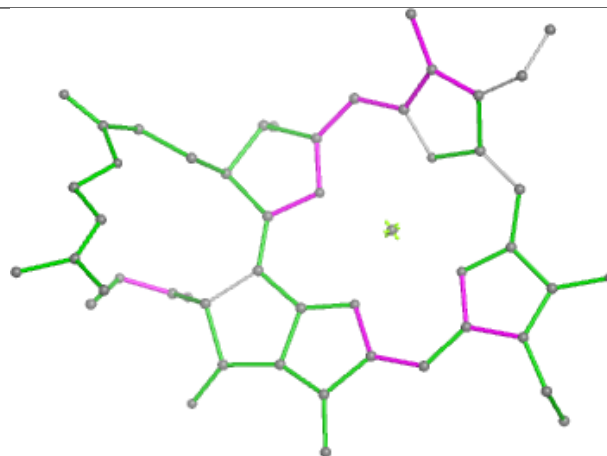


Rings

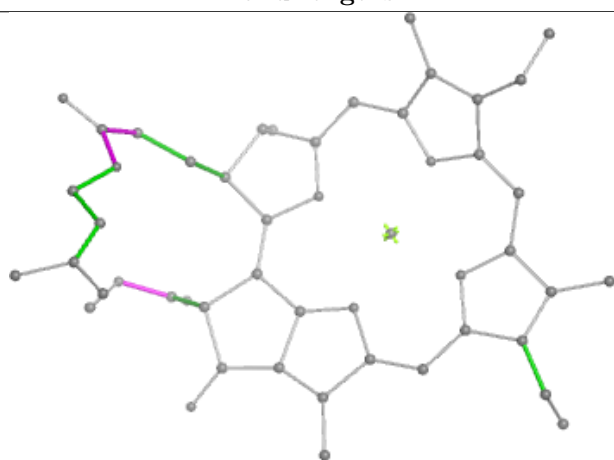
## Ligand CLA E 803



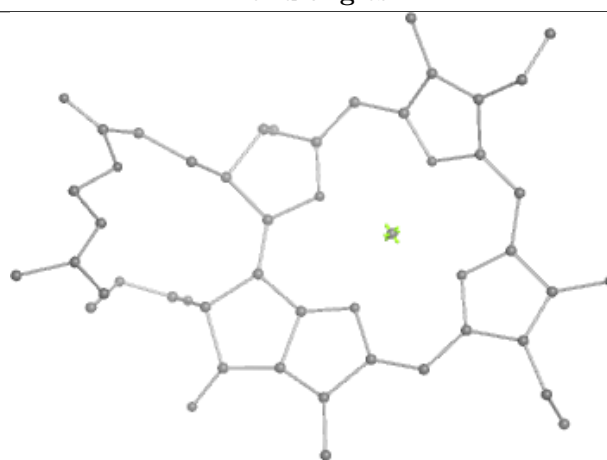
Bond lengths



Bond angles

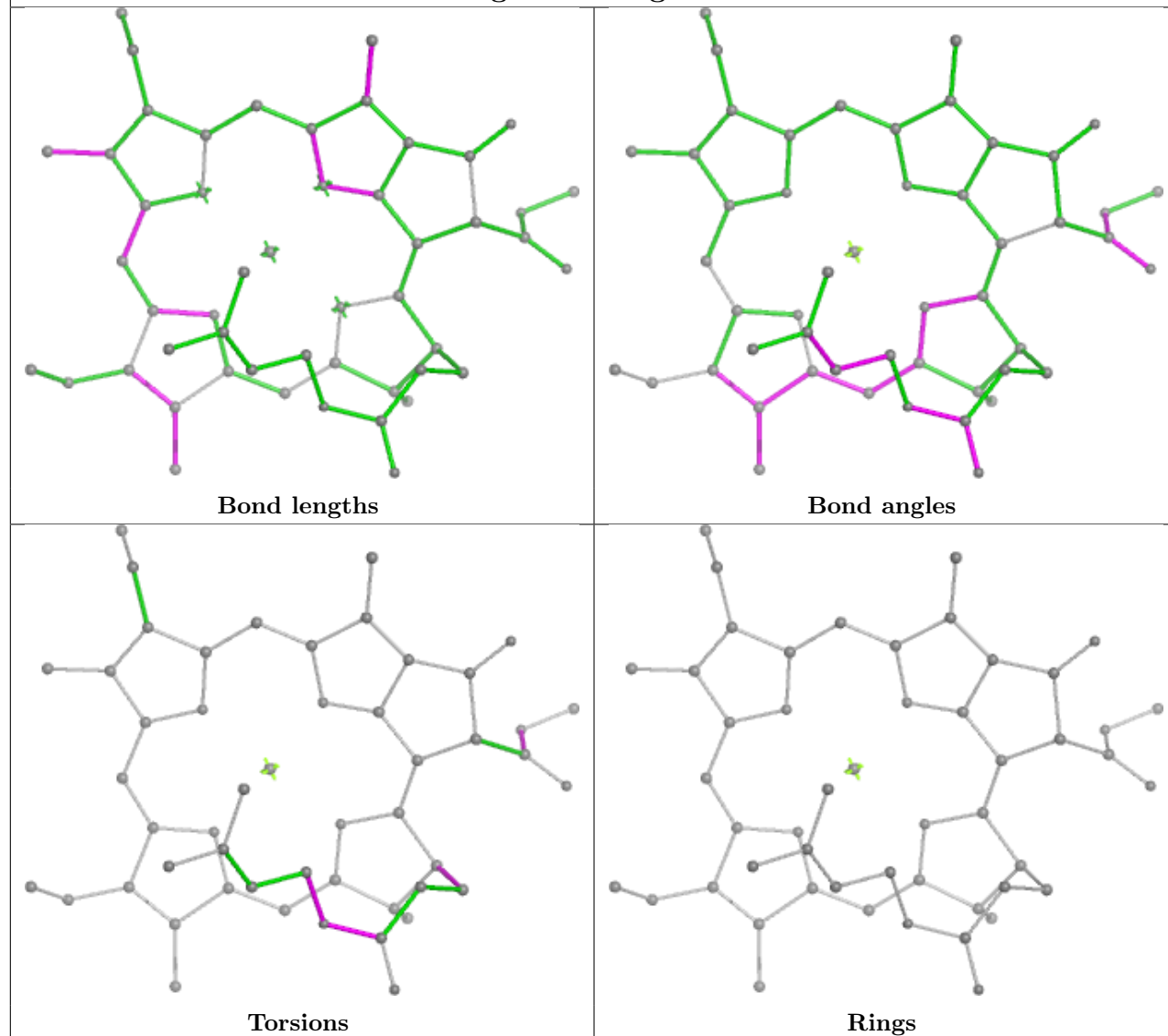


Torsions

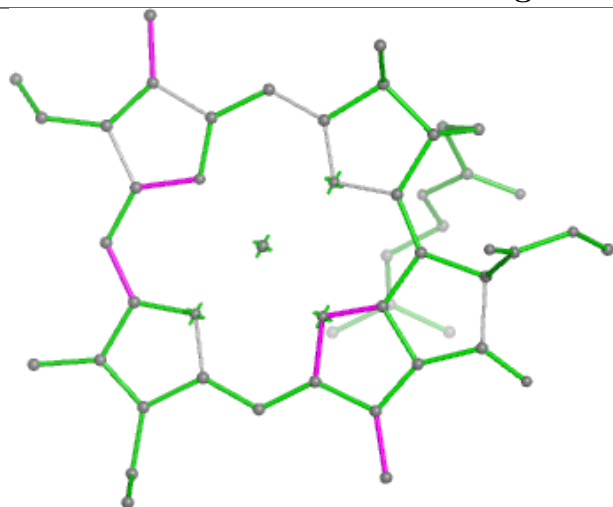


Rings

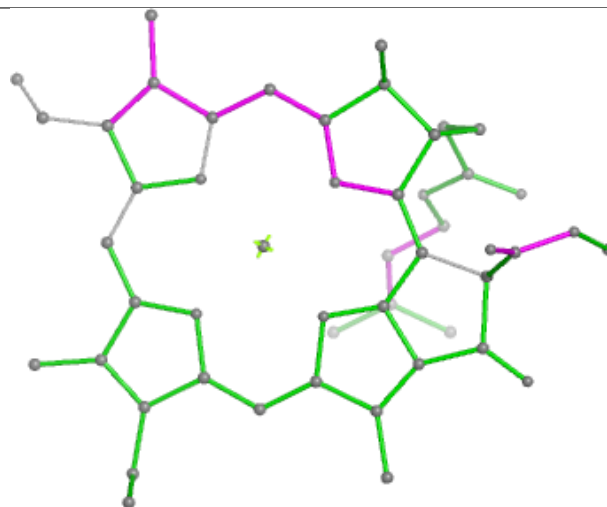
## Ligand CLA g 829



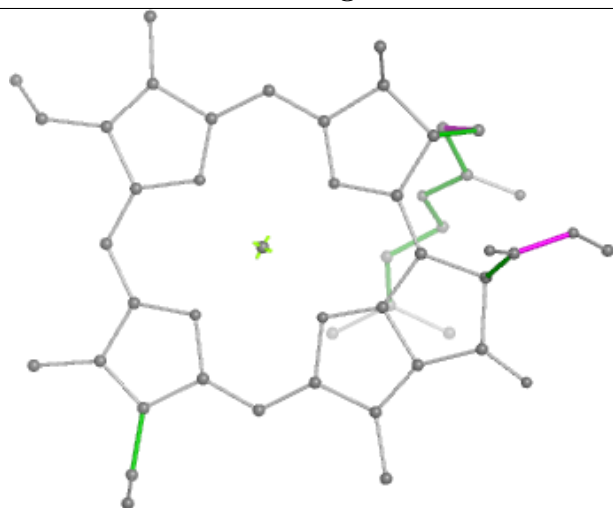
## Ligand CLA B 815



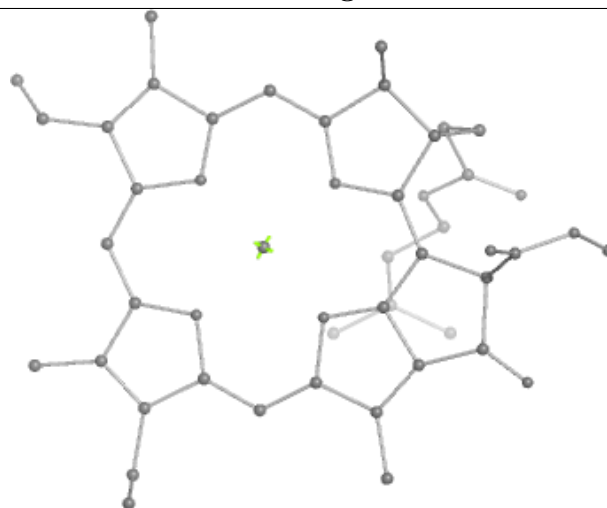
Bond lengths



Bond angles

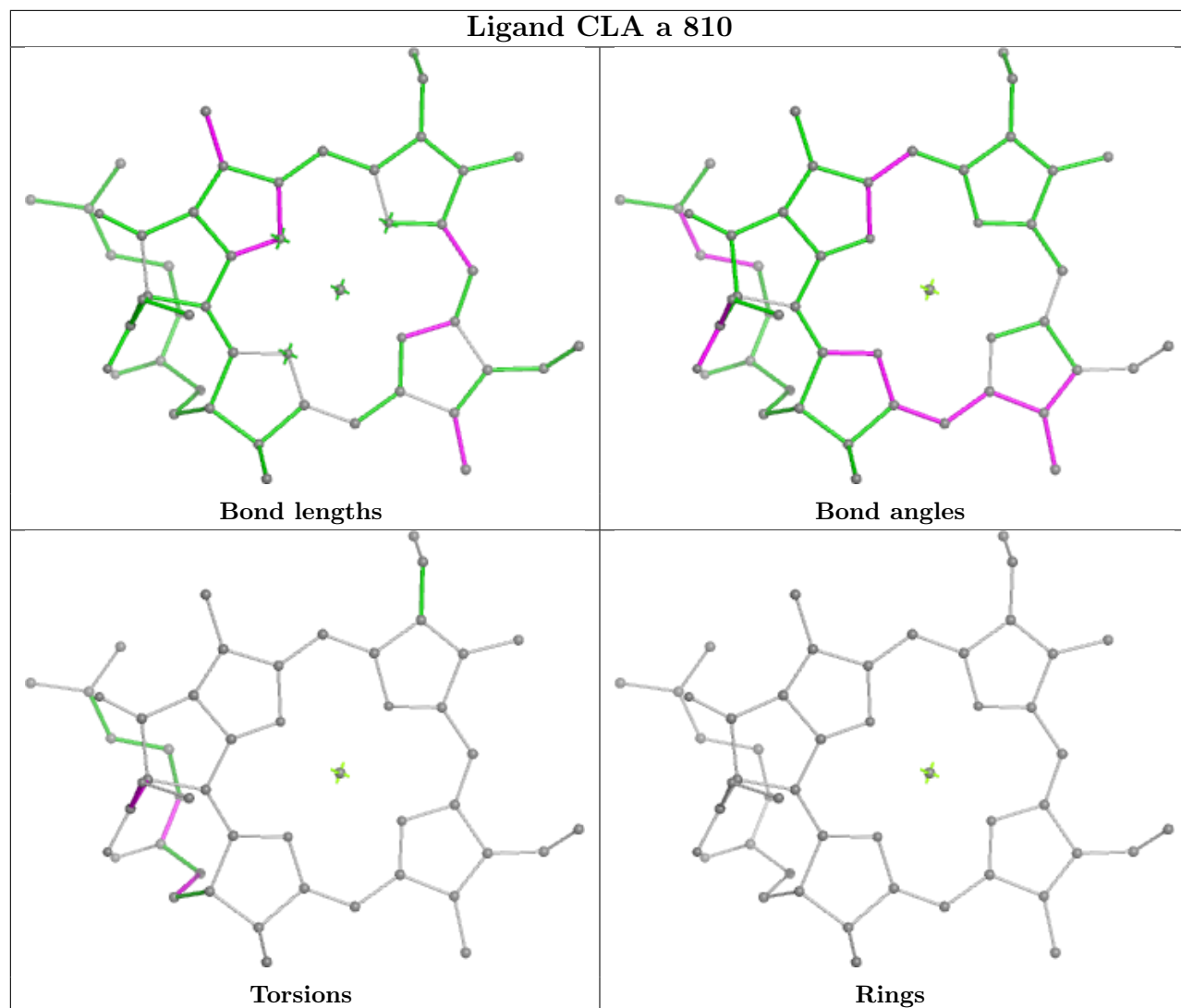


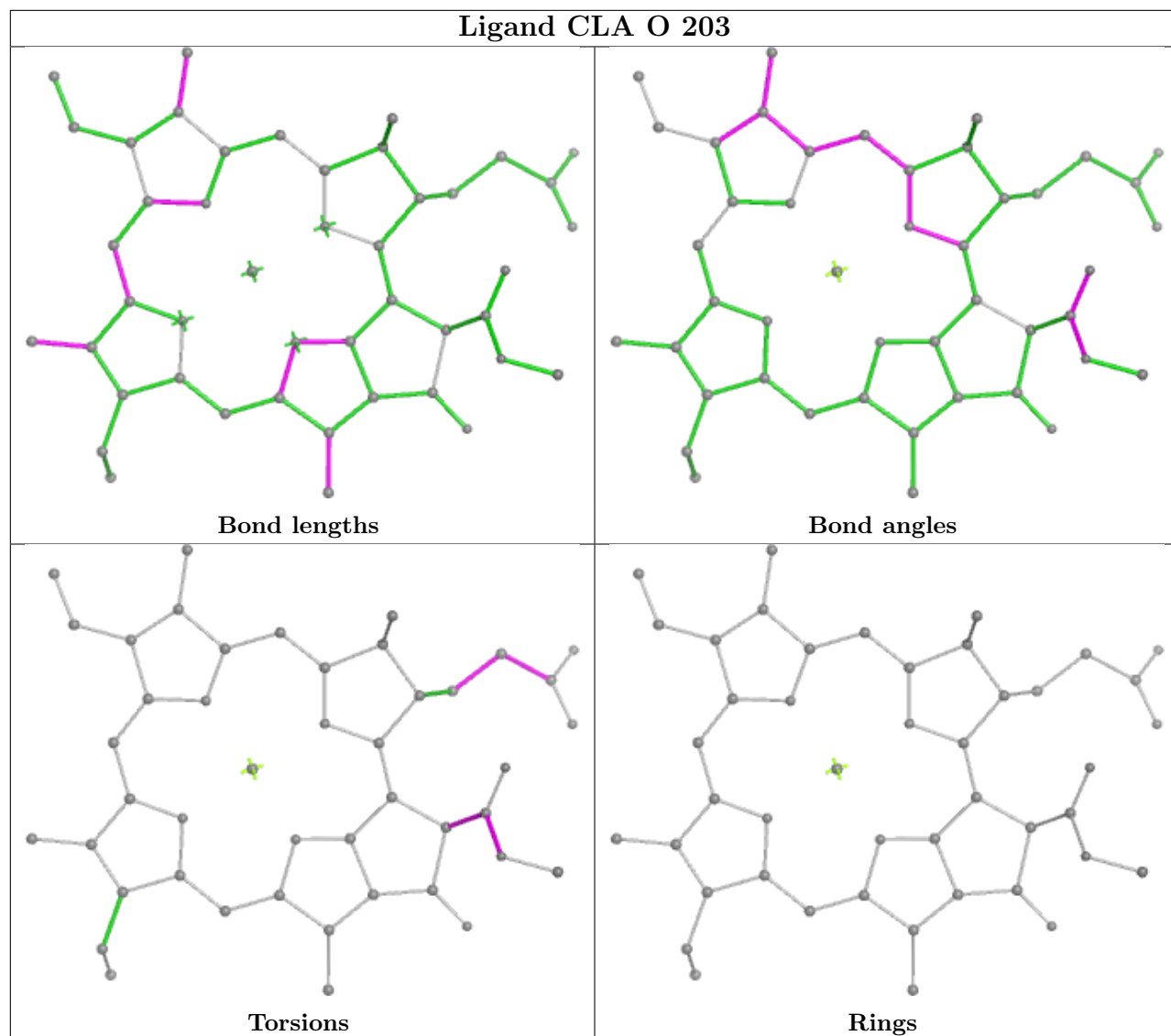
Torsions



Rings

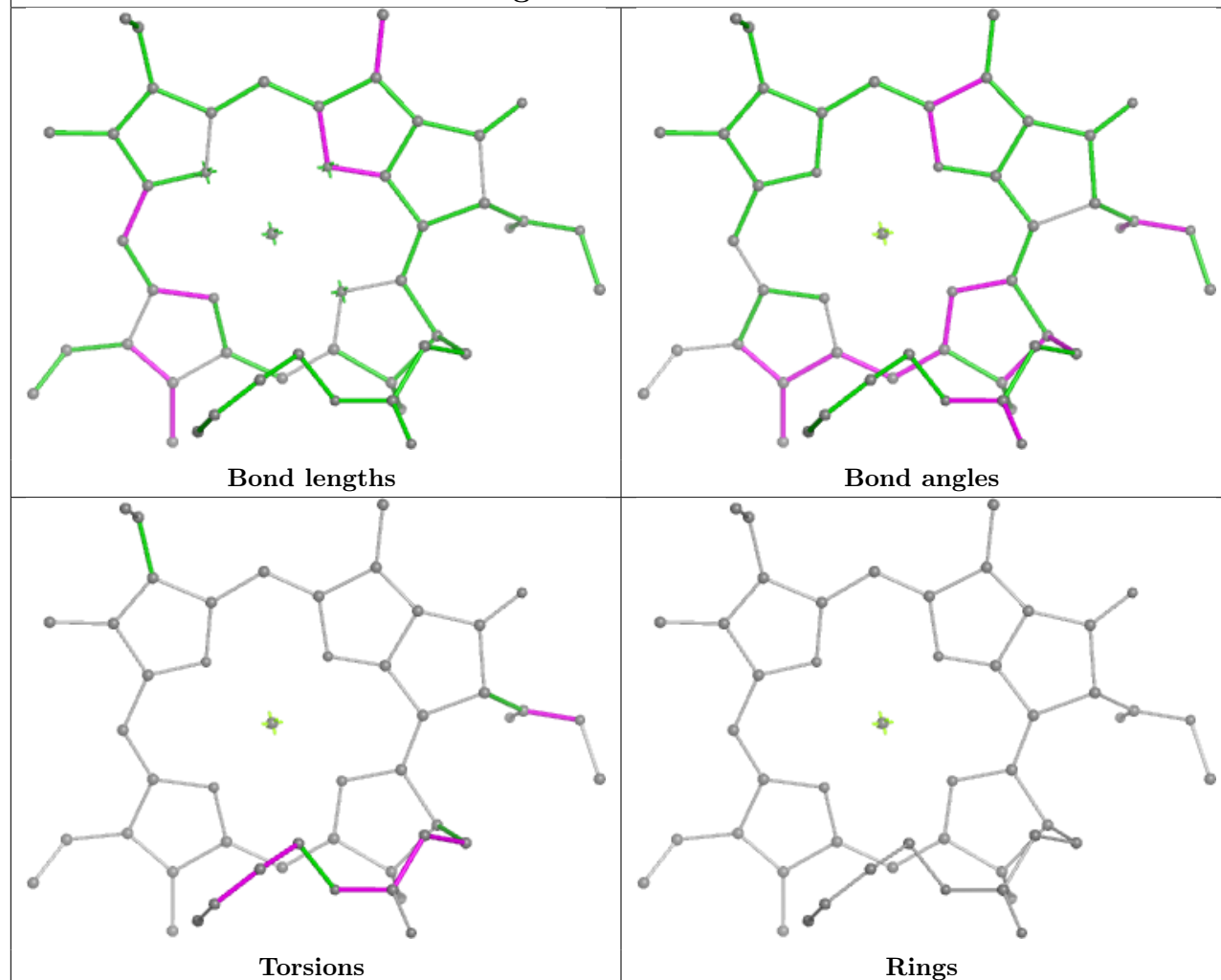
## Ligand CLA a 810

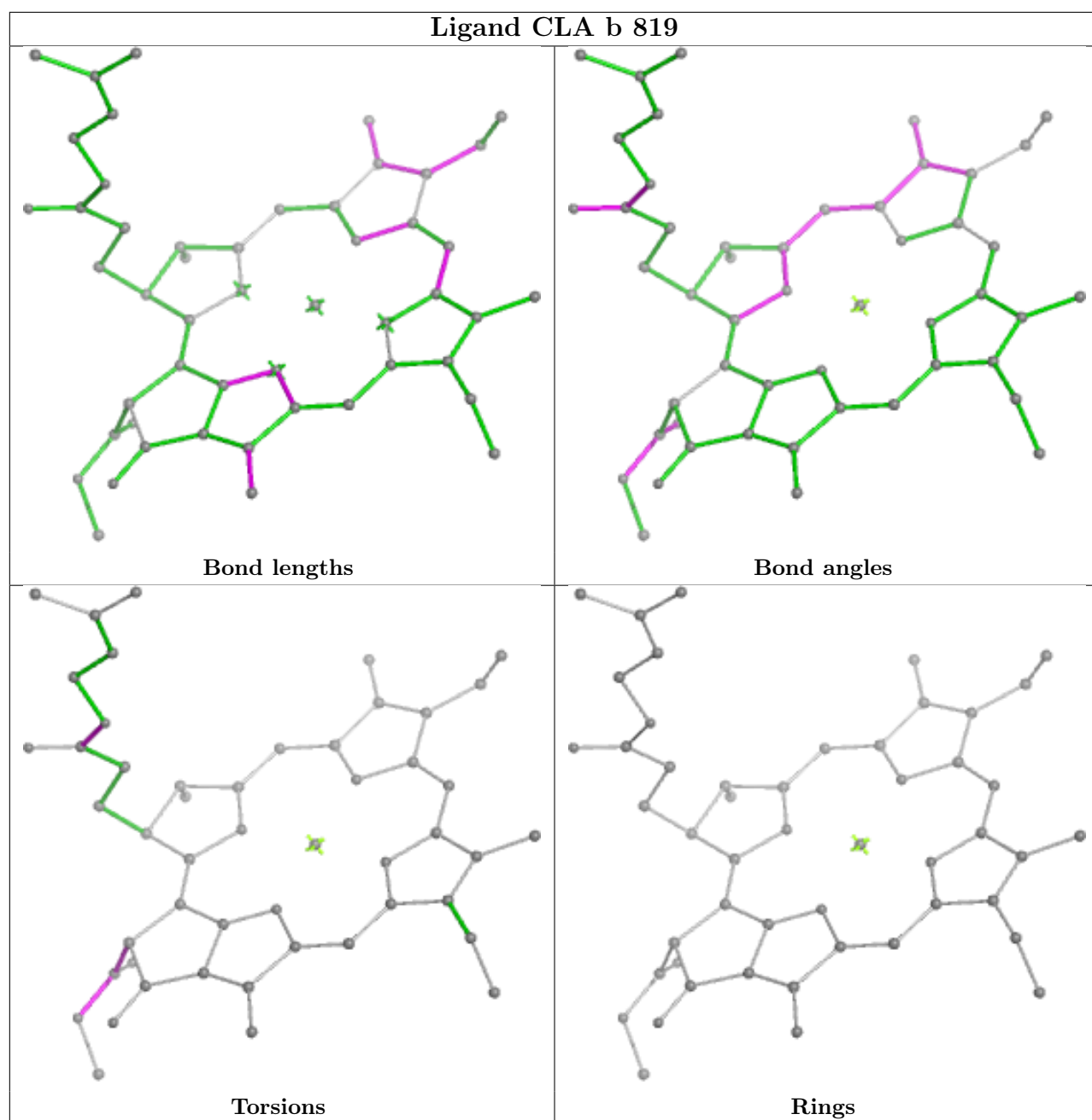




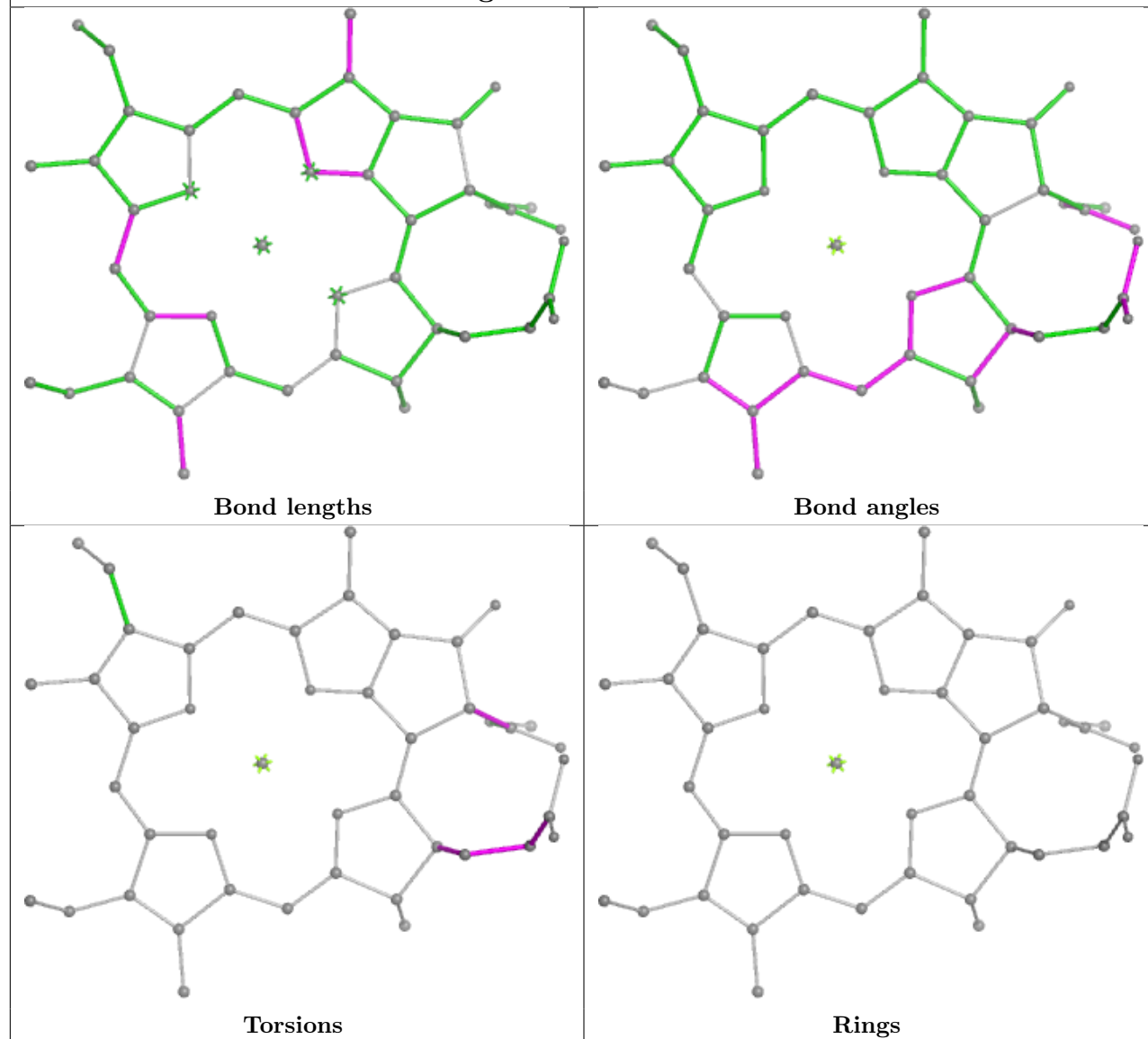


## Ligand CLA a 825

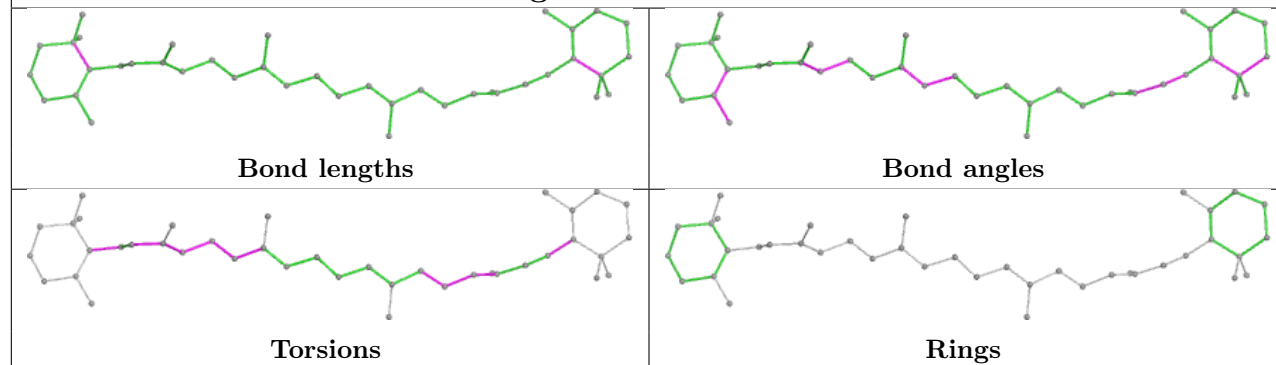




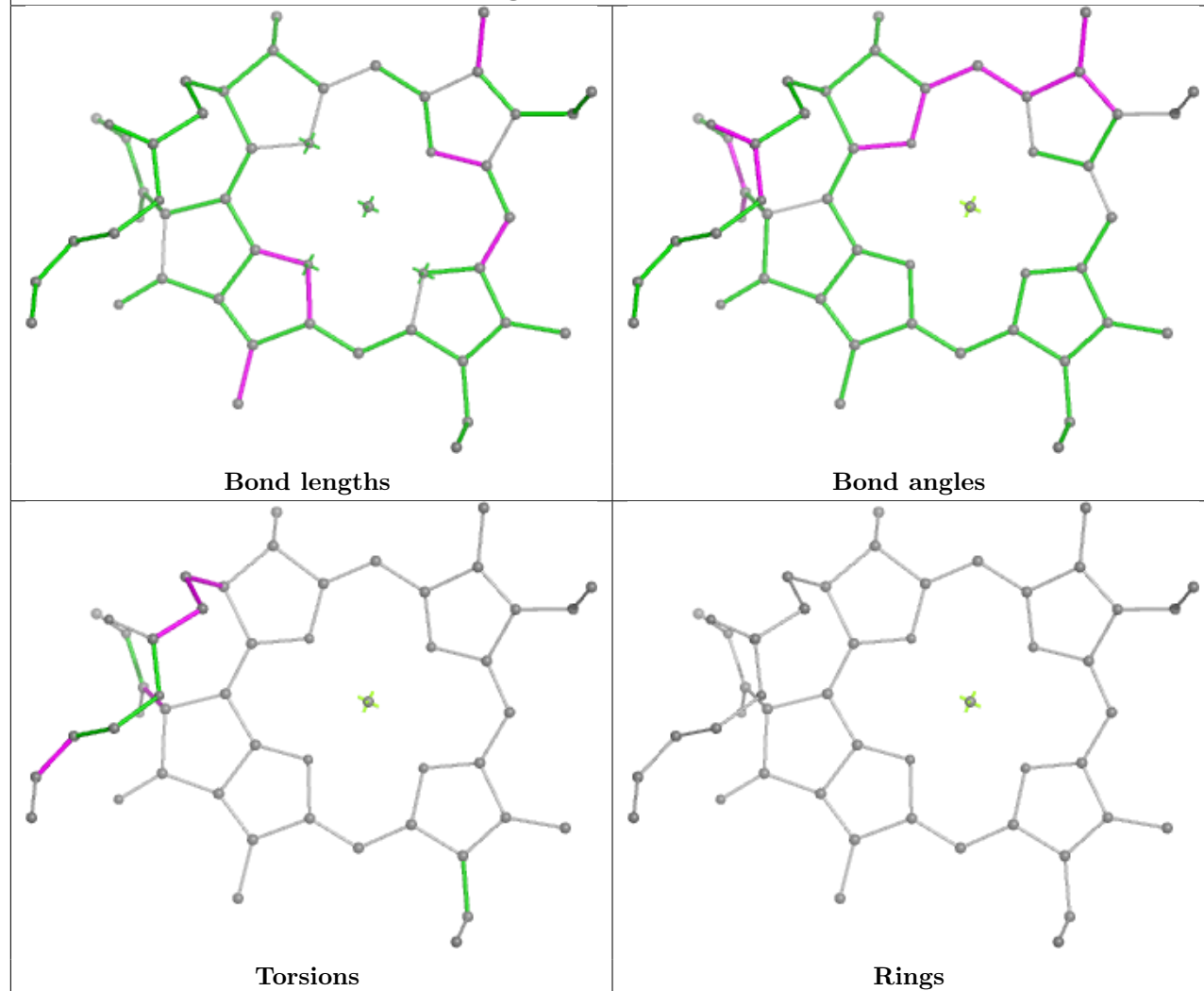
## Ligand CLA R 102



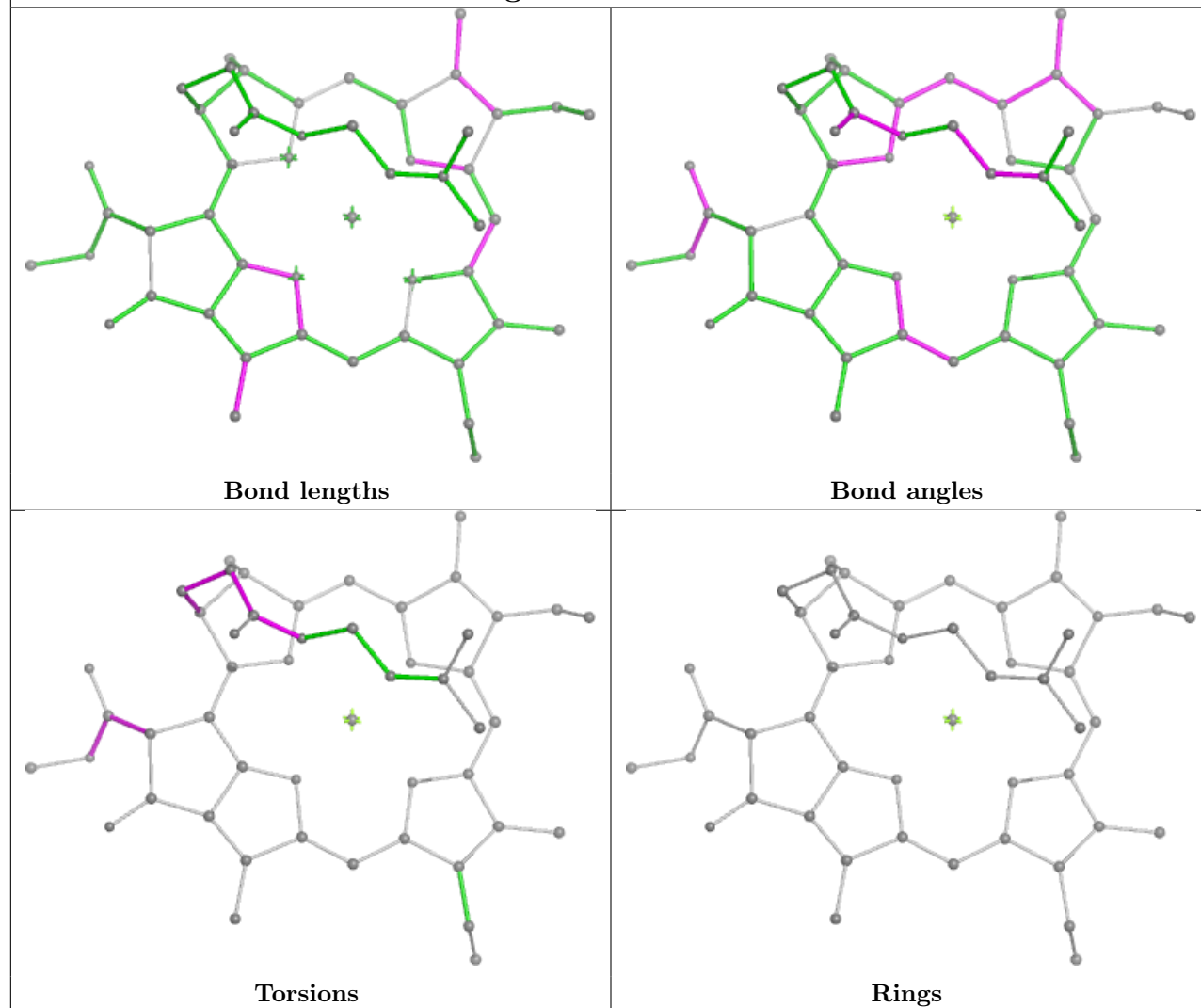
## Ligand BCR A 848



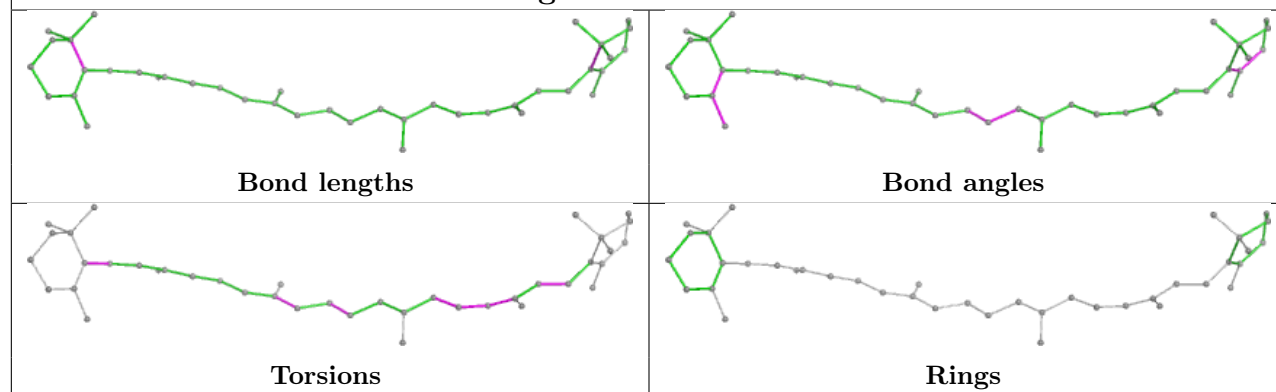
## Ligand CLA b 831

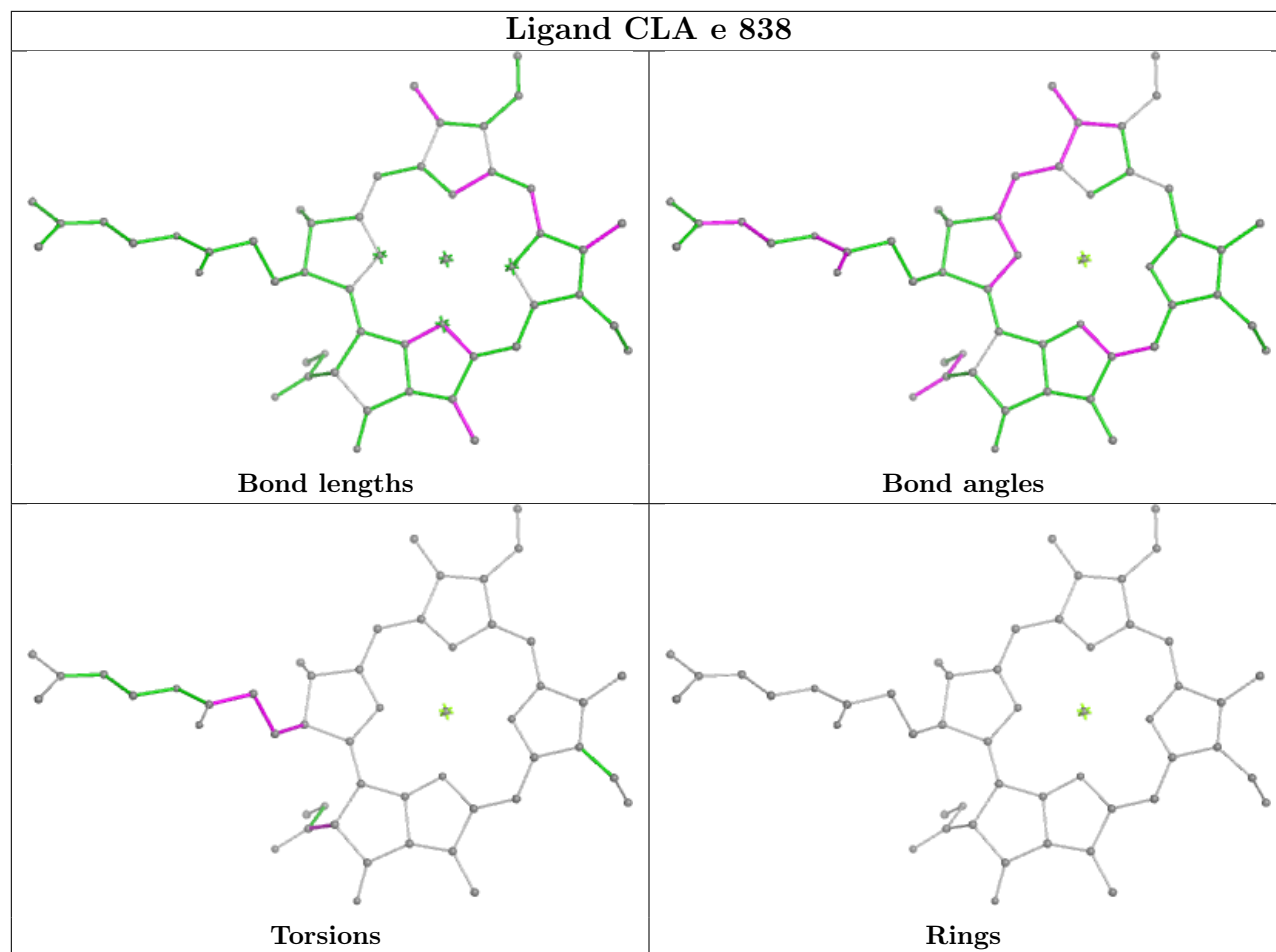


## Ligand CLA a 826

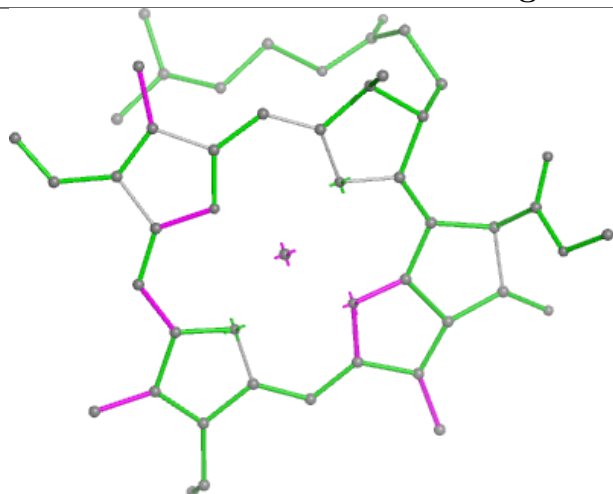


## Ligand BCR i 101

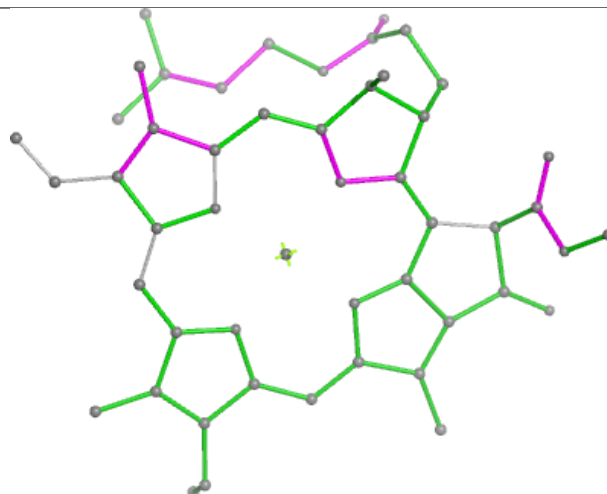




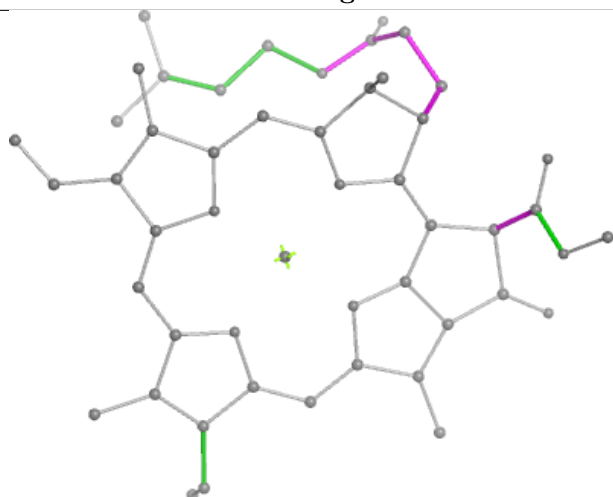
## Ligand CLA e 822



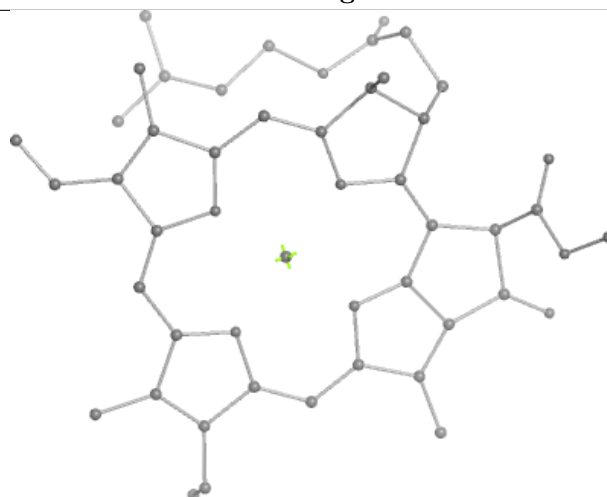
Bond lengths



Bond angles

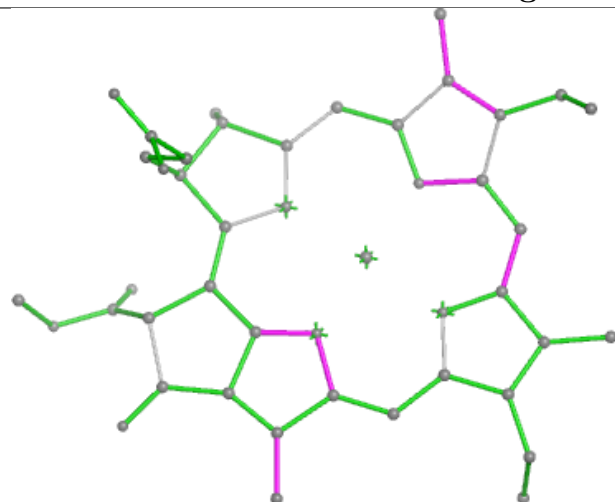


Torsions

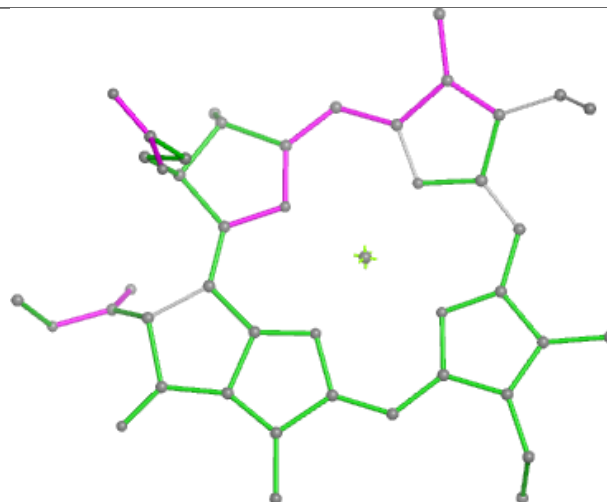


Rings

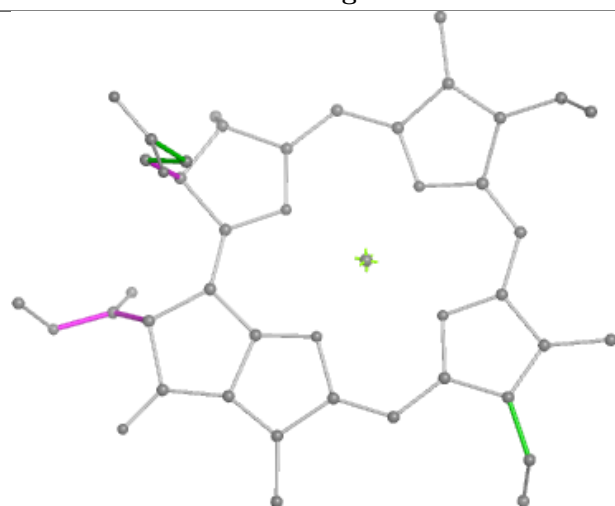
## Ligand CLA b 811



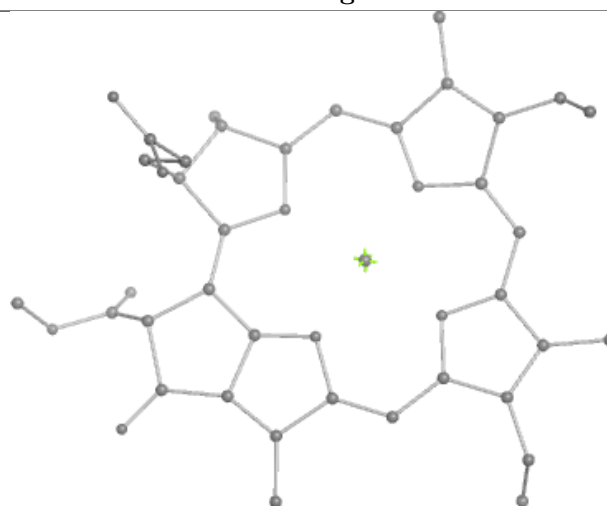
Bond lengths



Bond angles



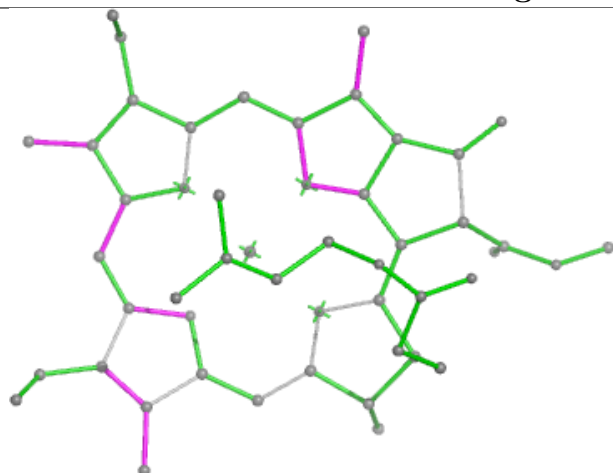
Torsions



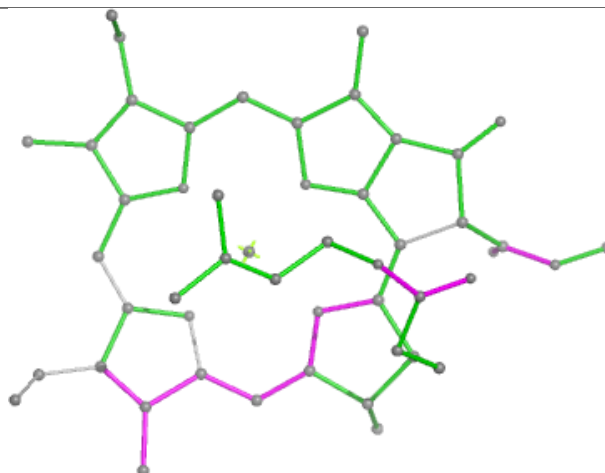
Rings



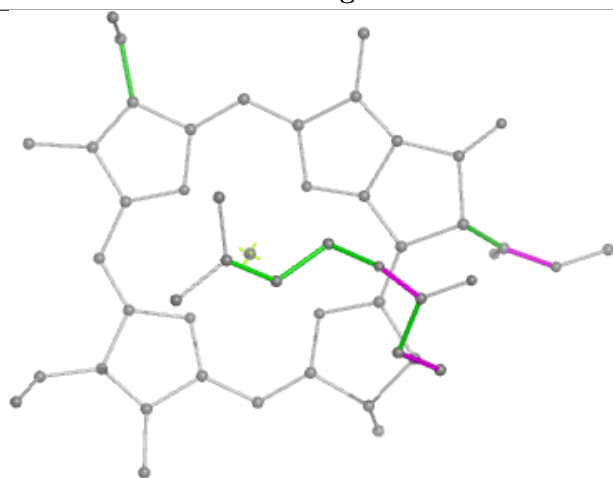
## Ligand CLA B 802



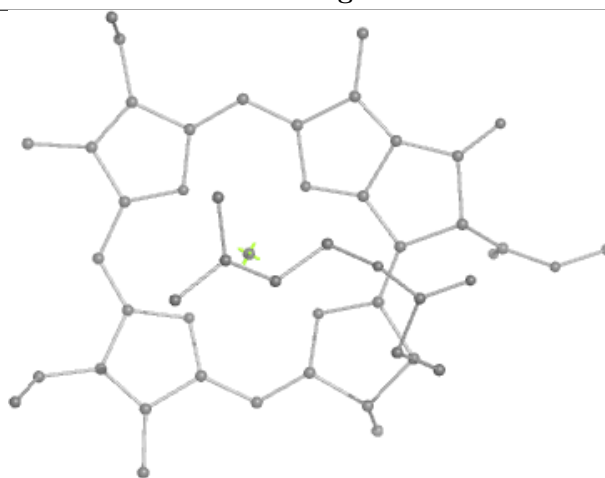
Bond lengths



Bond angles

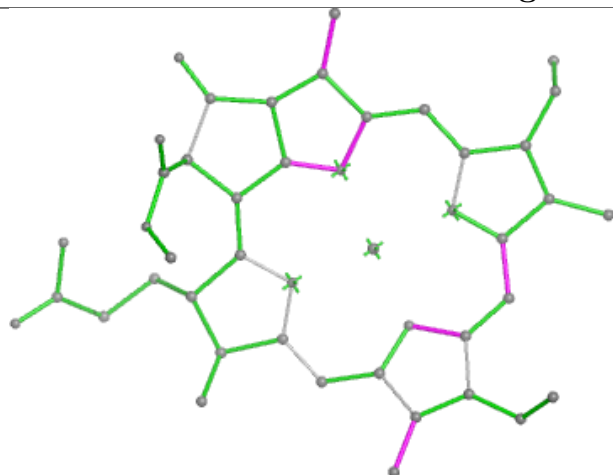


Torsions

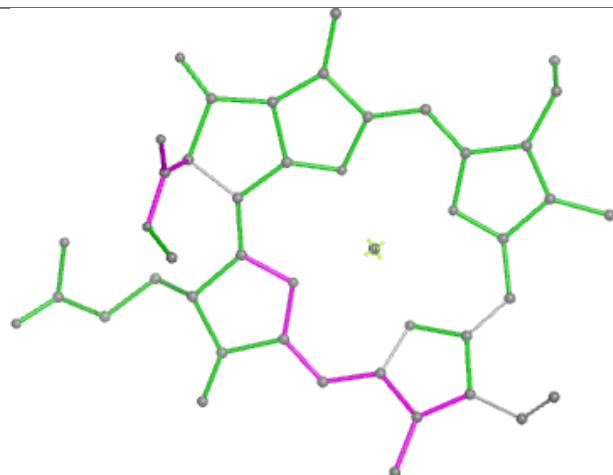


Rings

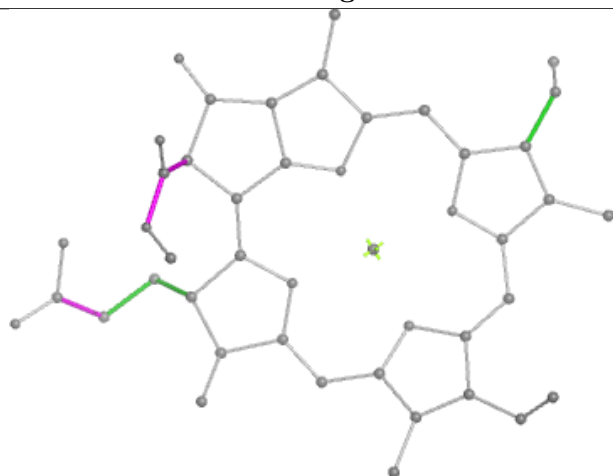
## Ligand CLA e 817



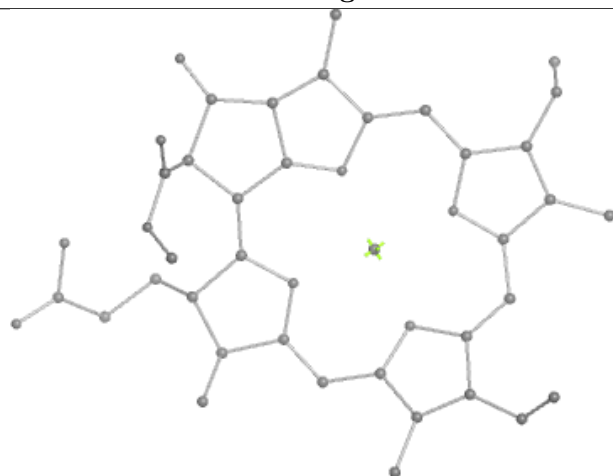
Bond lengths



Bond angles

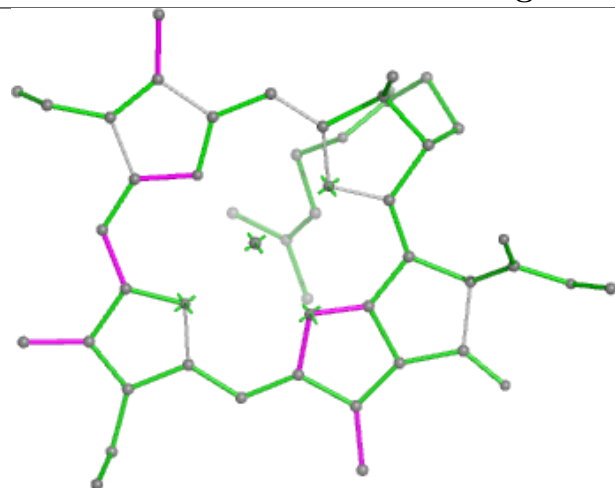


Torsions

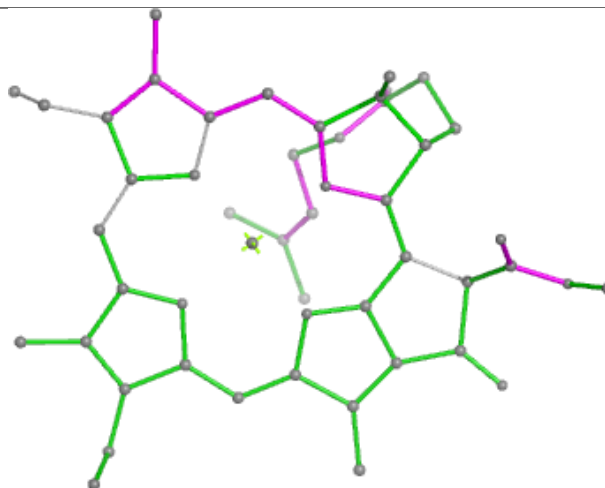


Rings

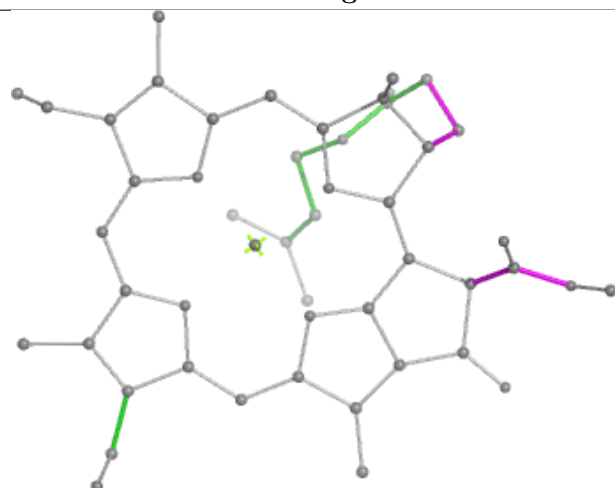
## Ligand CLA A 844



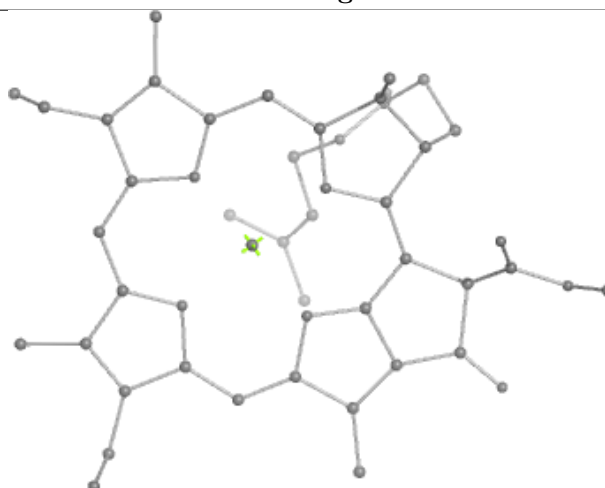
Bond lengths



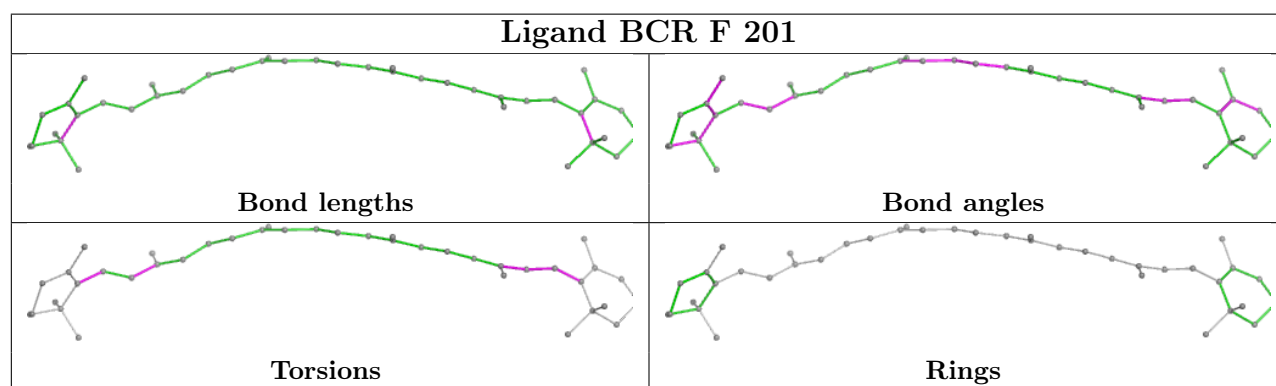
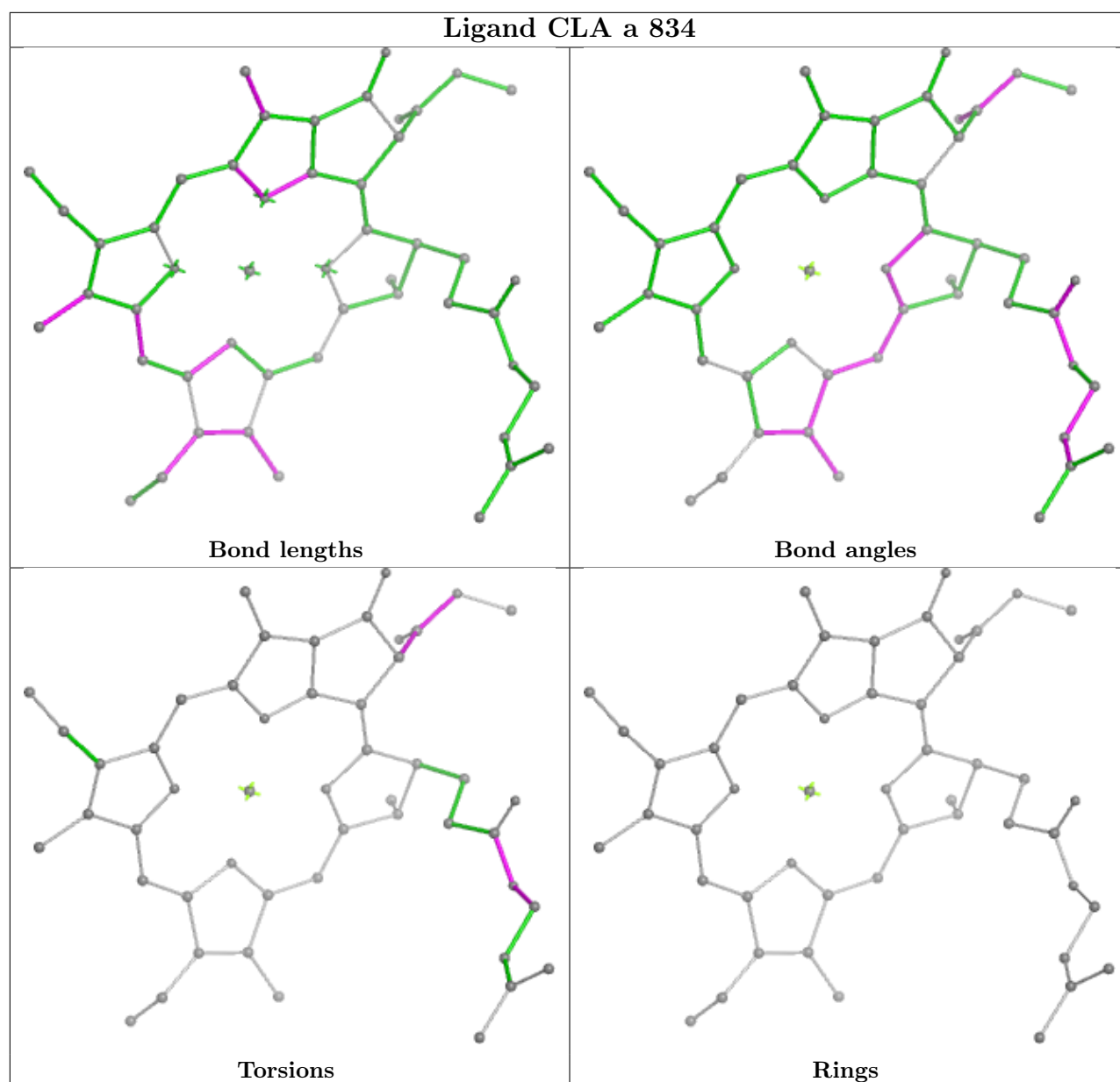
Bond angles



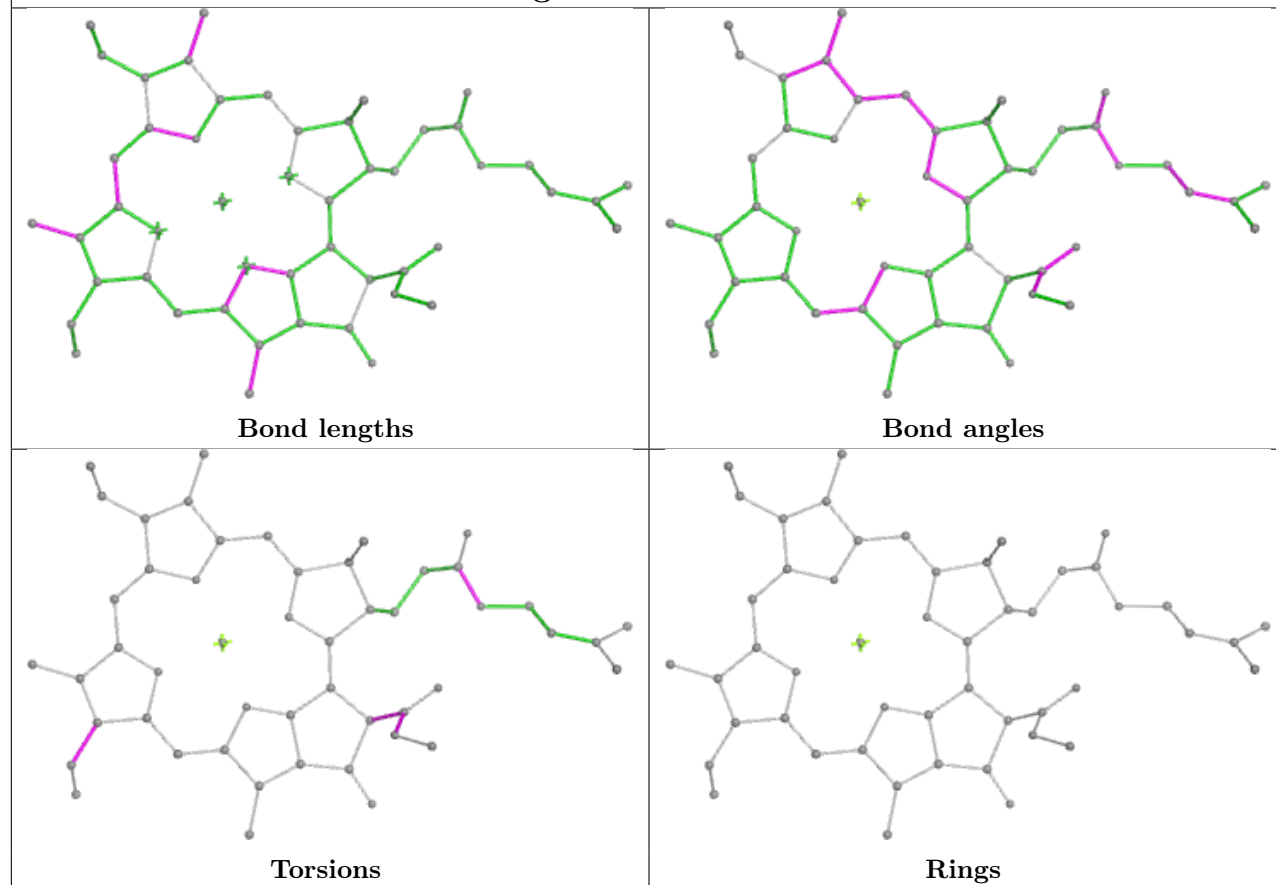
Torsions



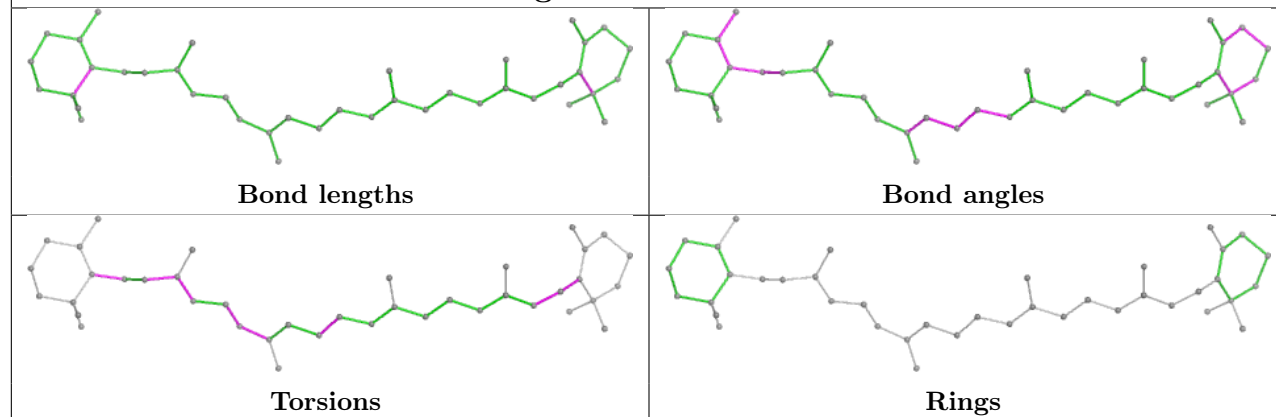
Rings



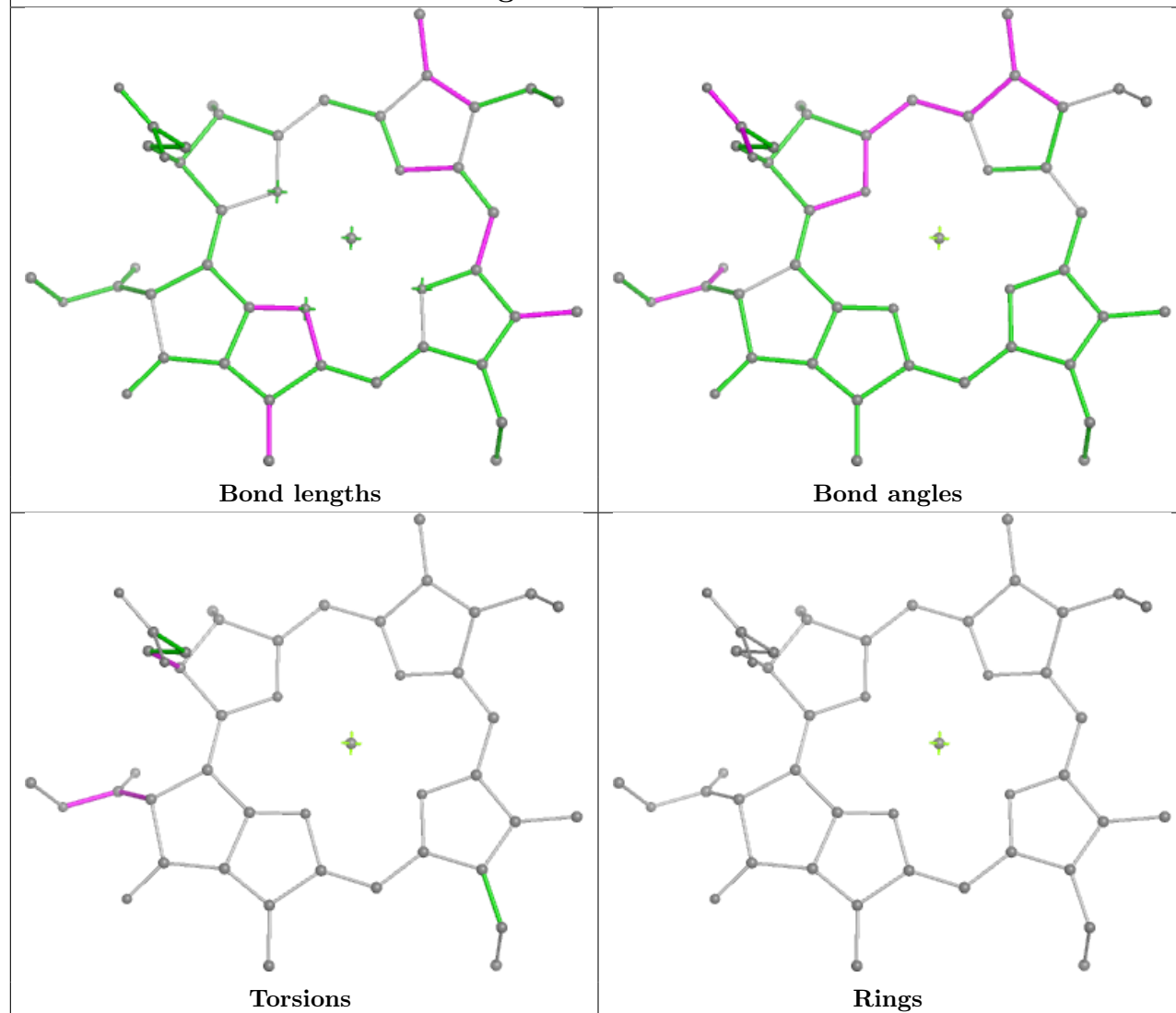
## Ligand CLA E 806



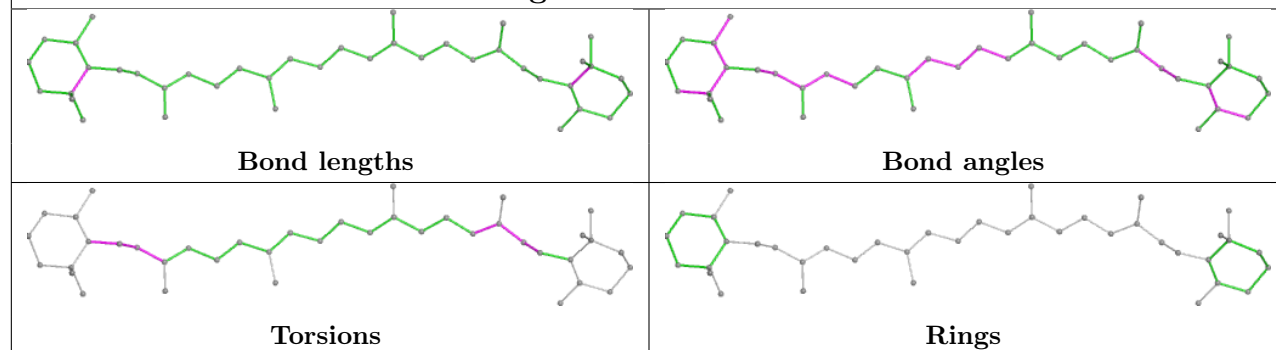
## Ligand BCR a 853



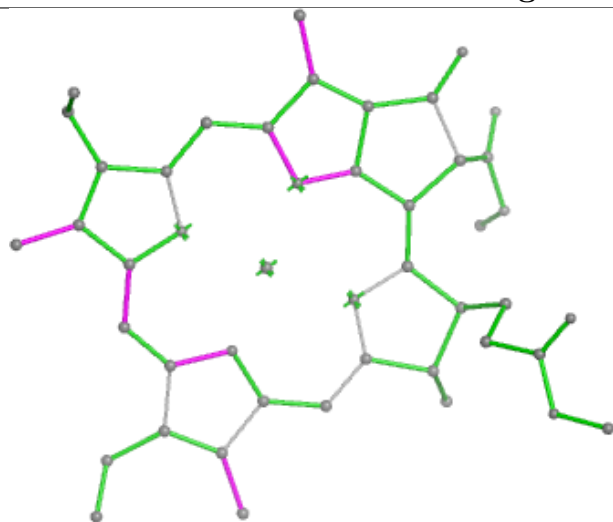
## Ligand CLA I 201



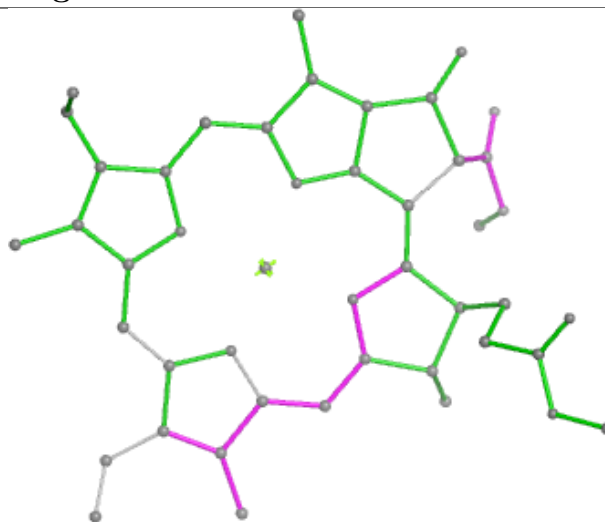
## Ligand BCR G 843



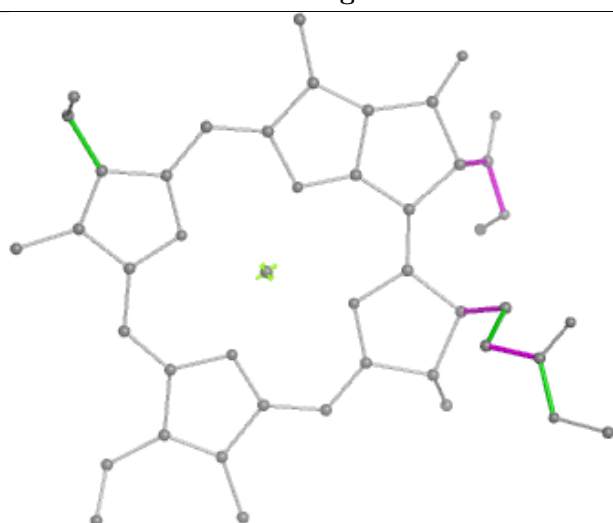
## Ligand CLA g 827



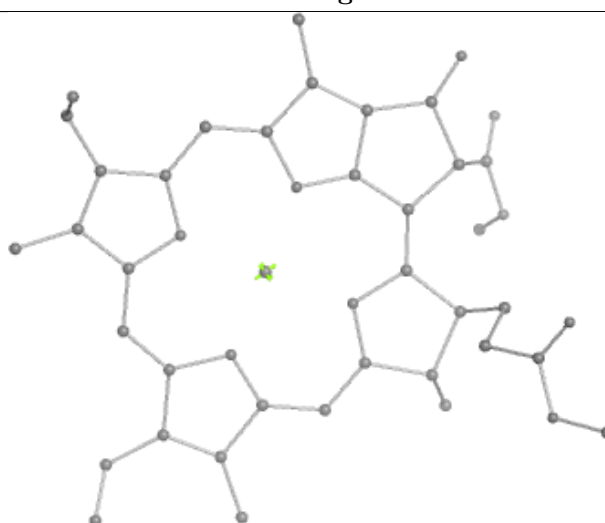
Bond lengths



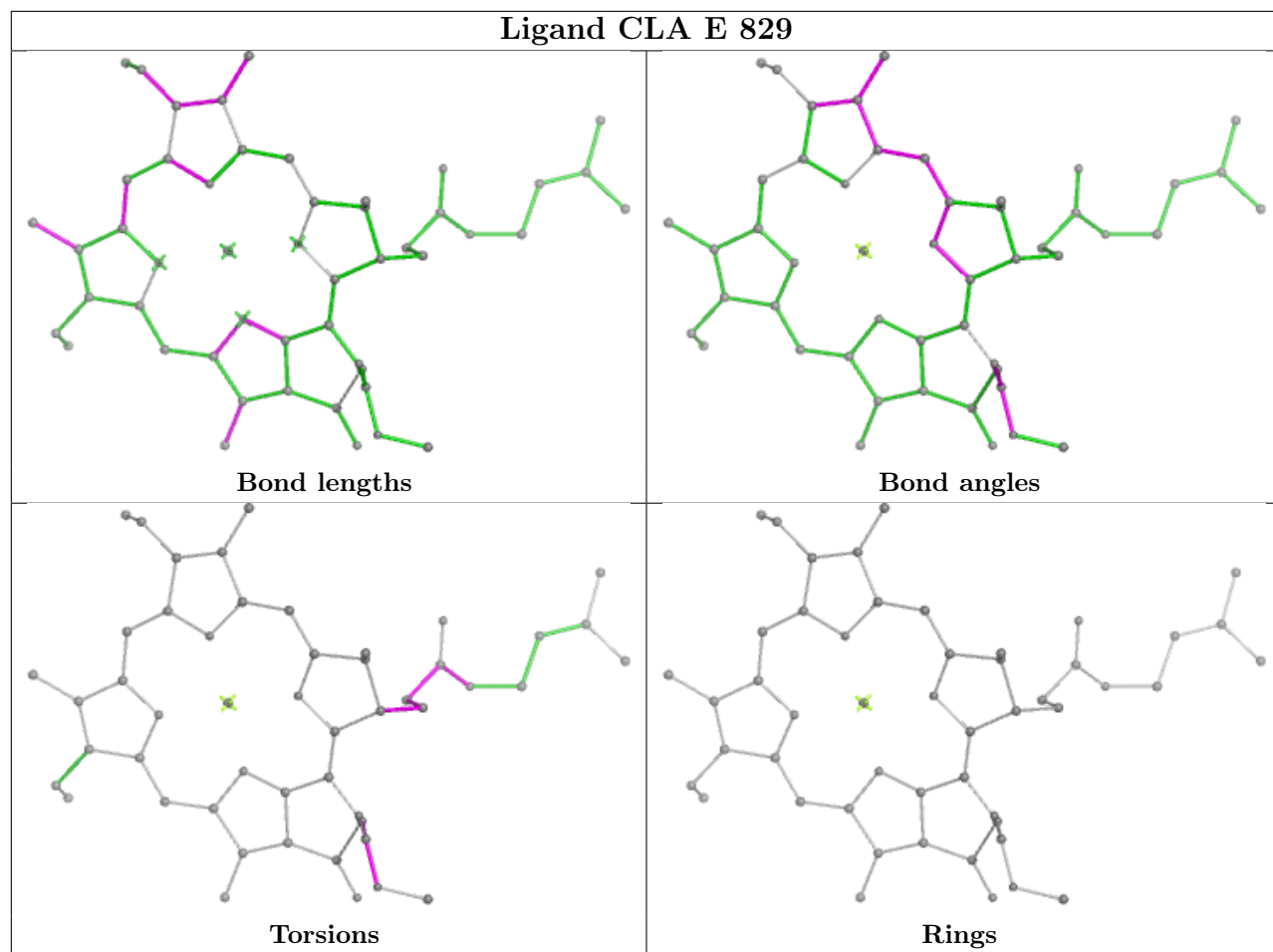
Bond angles



Torsions

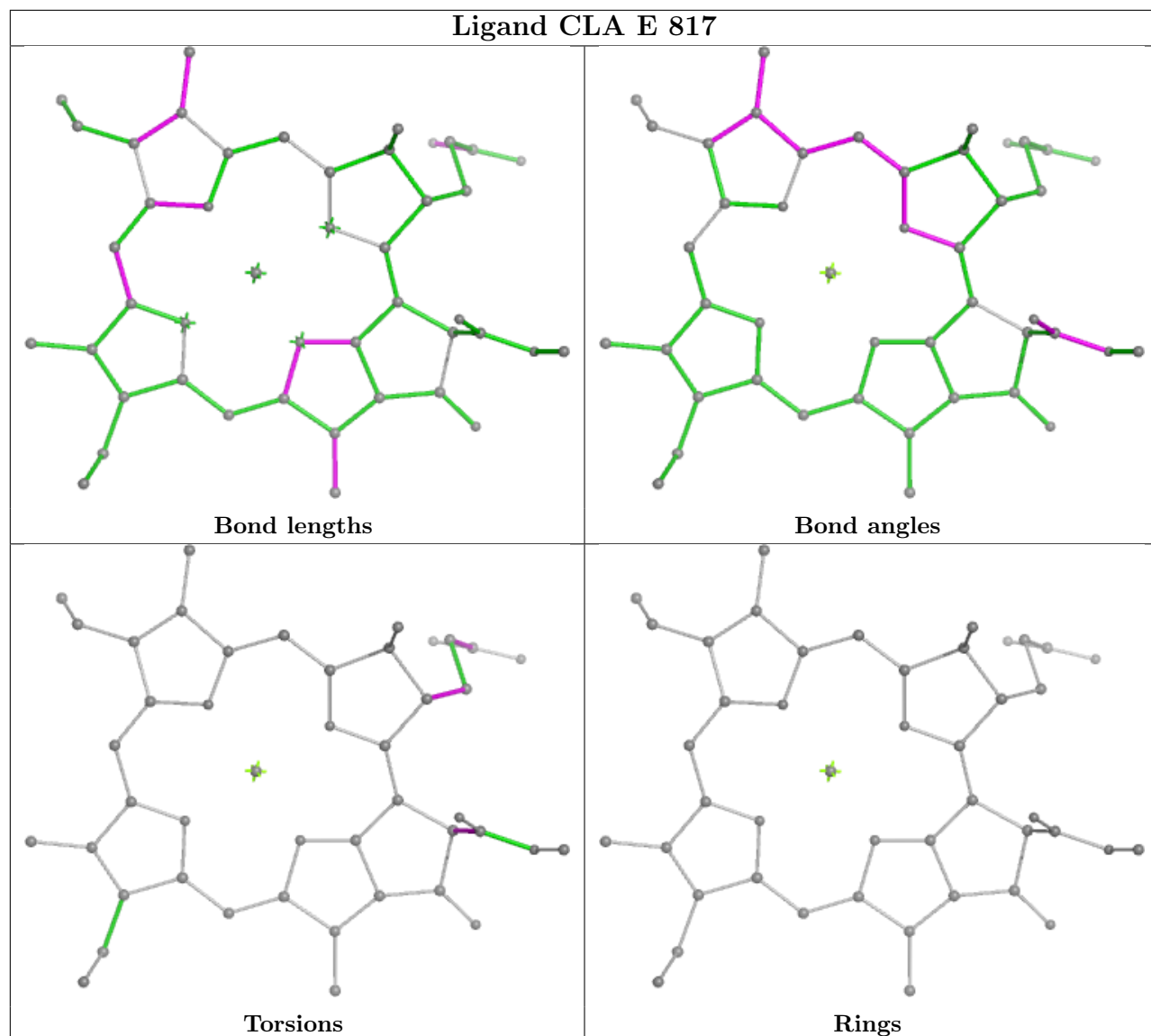


Rings

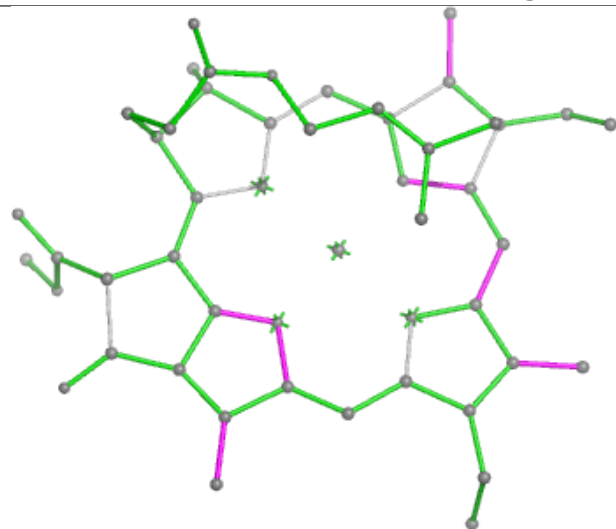




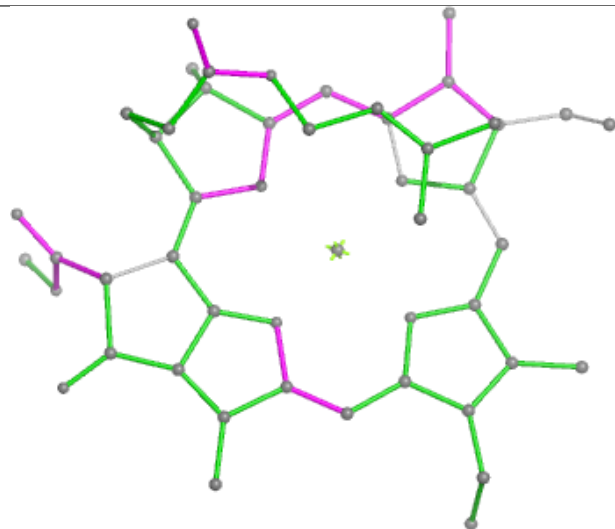
## Ligand CLA E 817



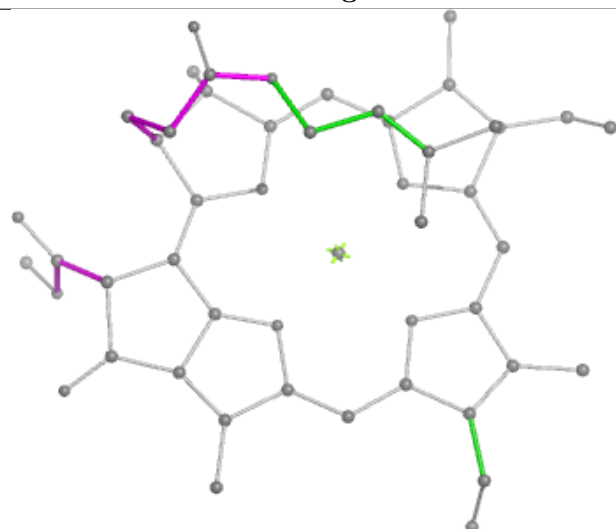
## Ligand CLA e 826



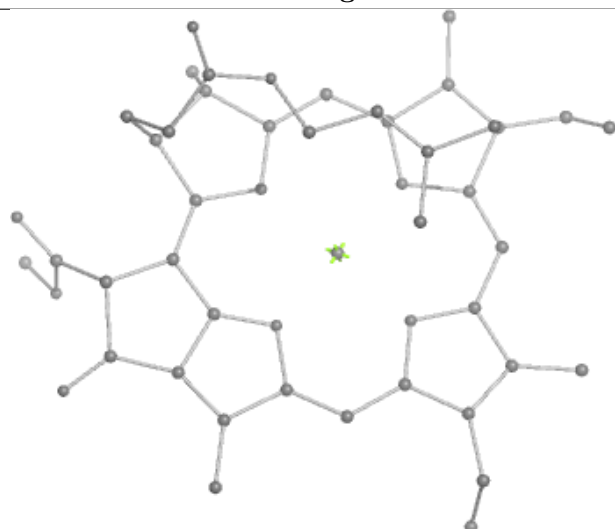
Bond lengths



Bond angles

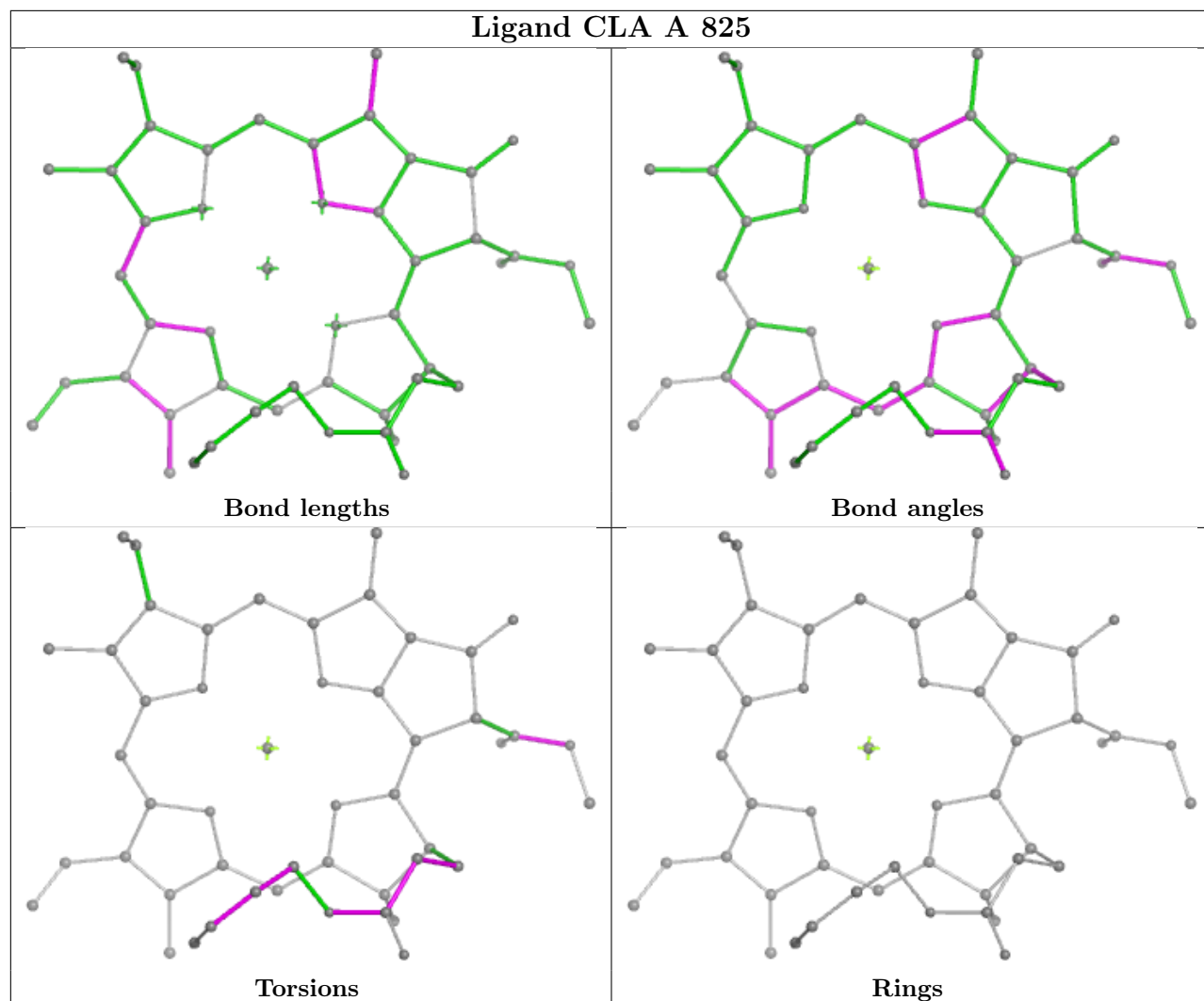


Torsions

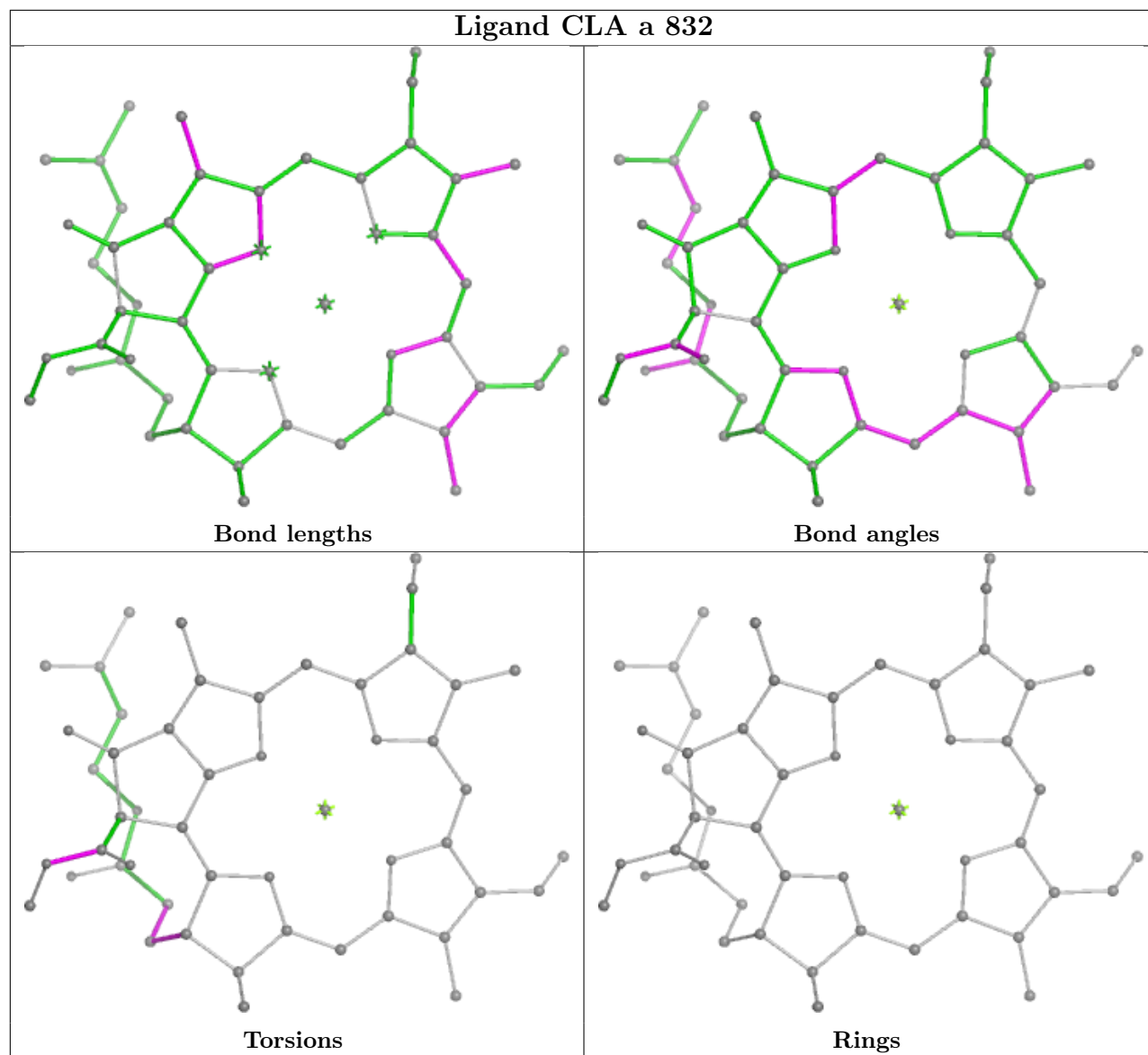


Rings

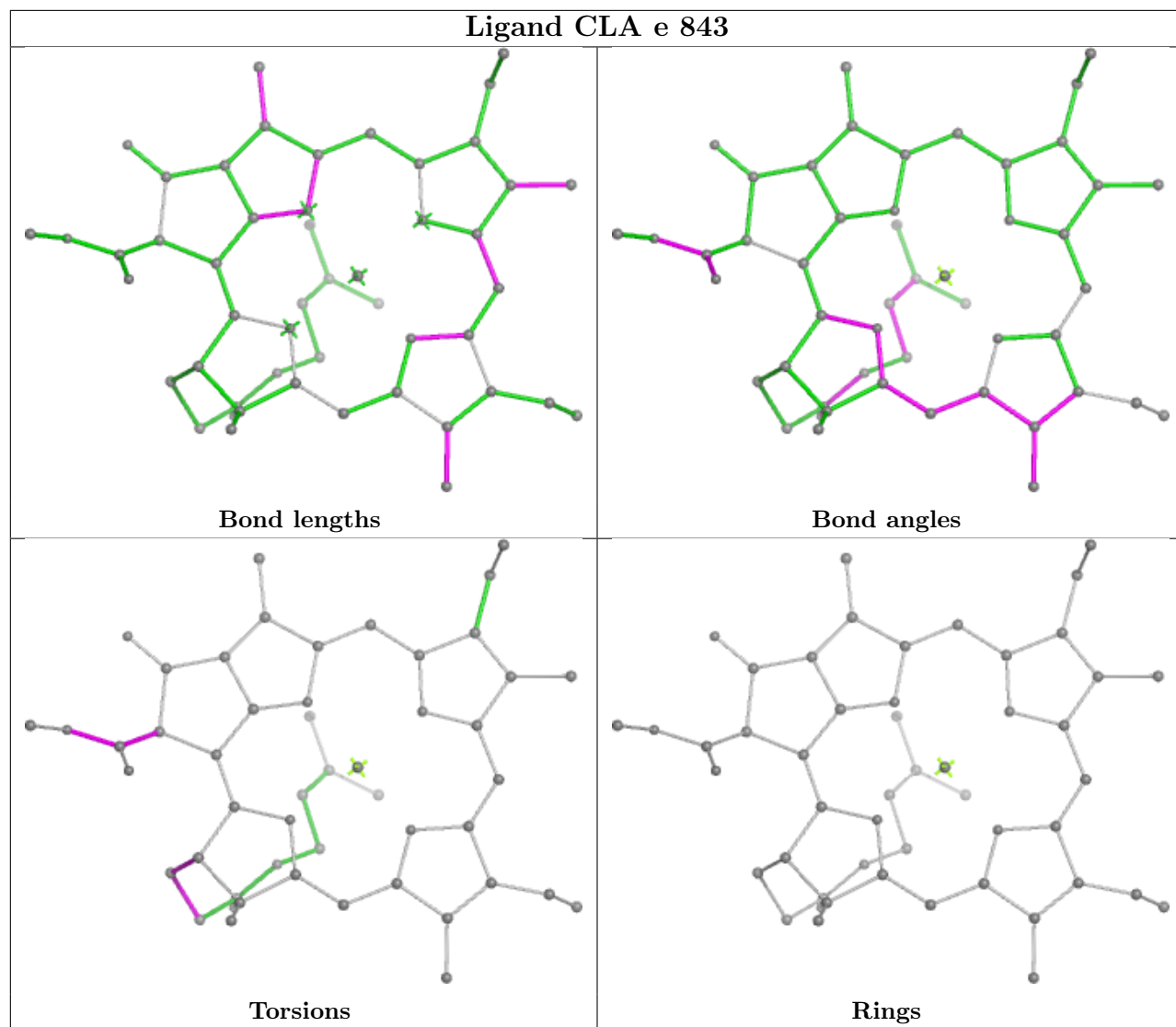
## Ligand CLA A 825



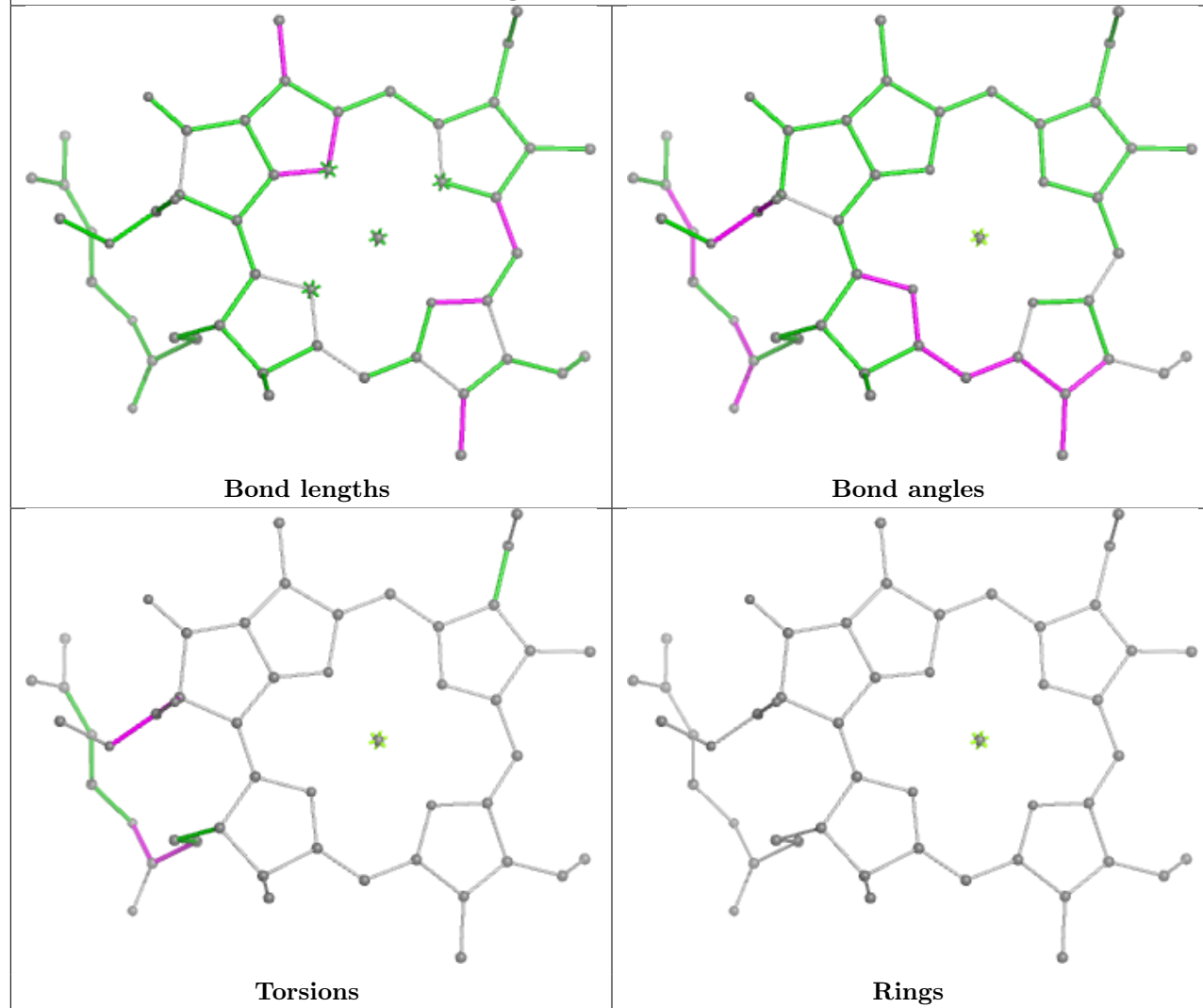
## Ligand CLA a 832



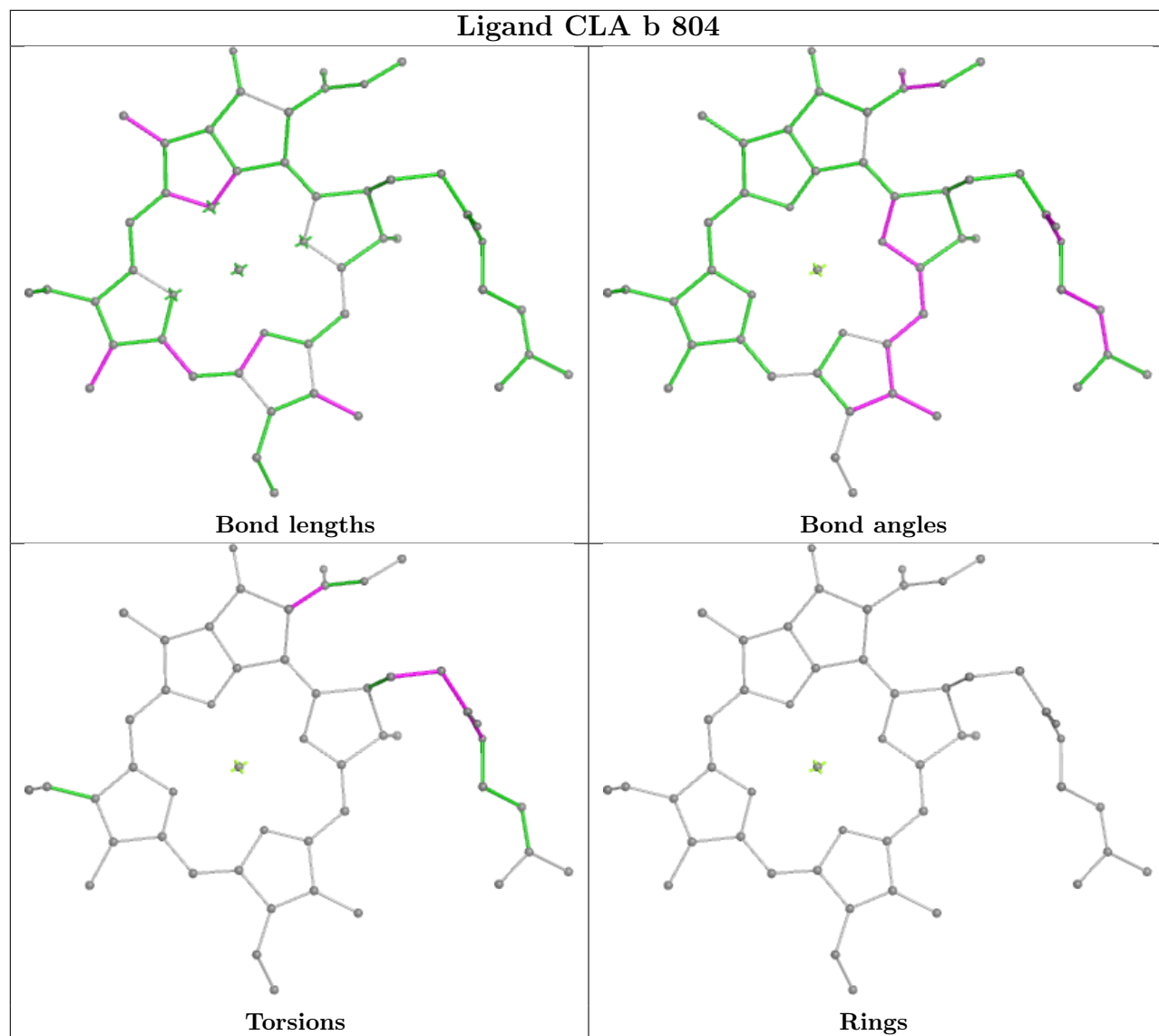
## Ligand CLA e 843



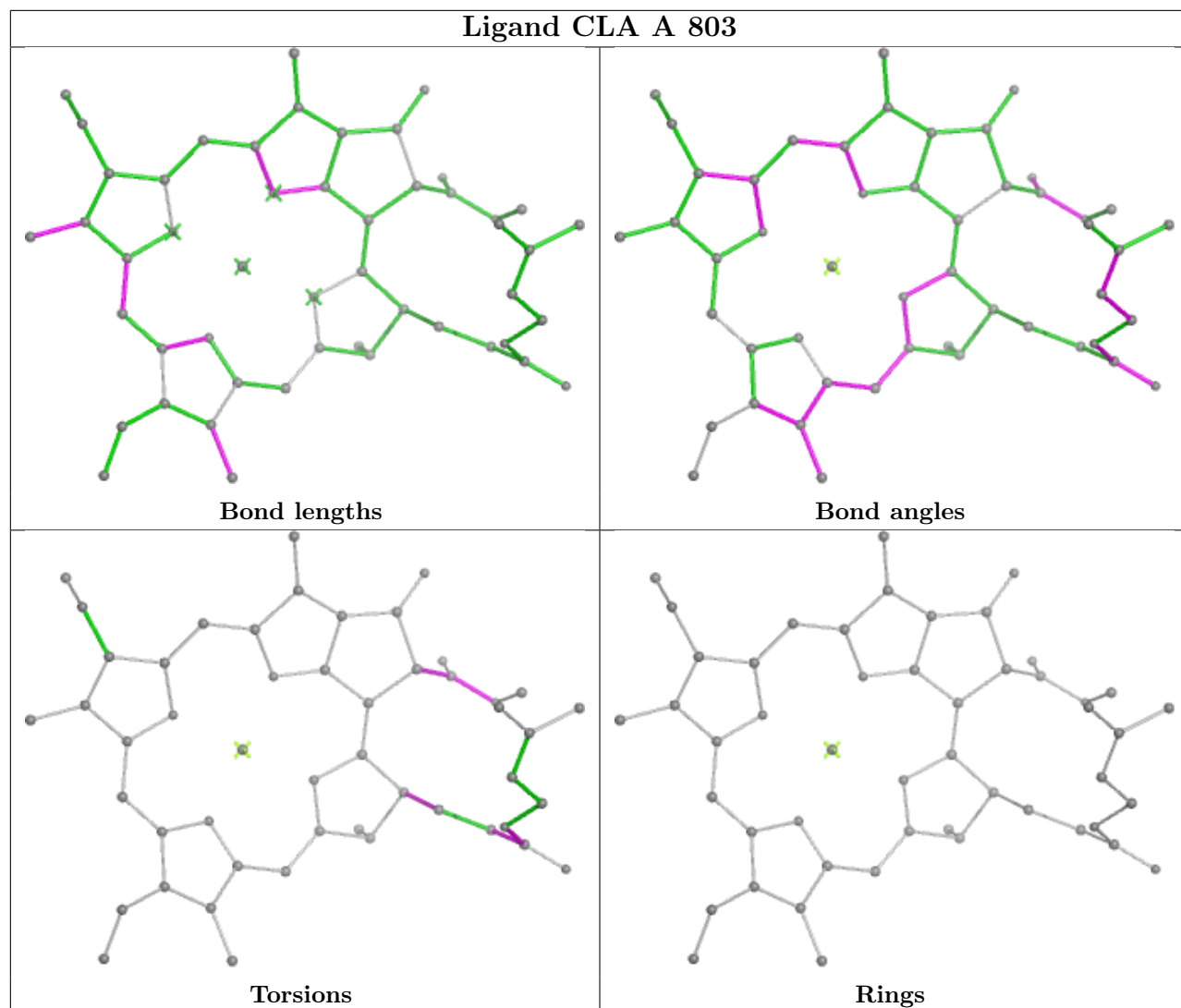
## Ligand CLA b 816



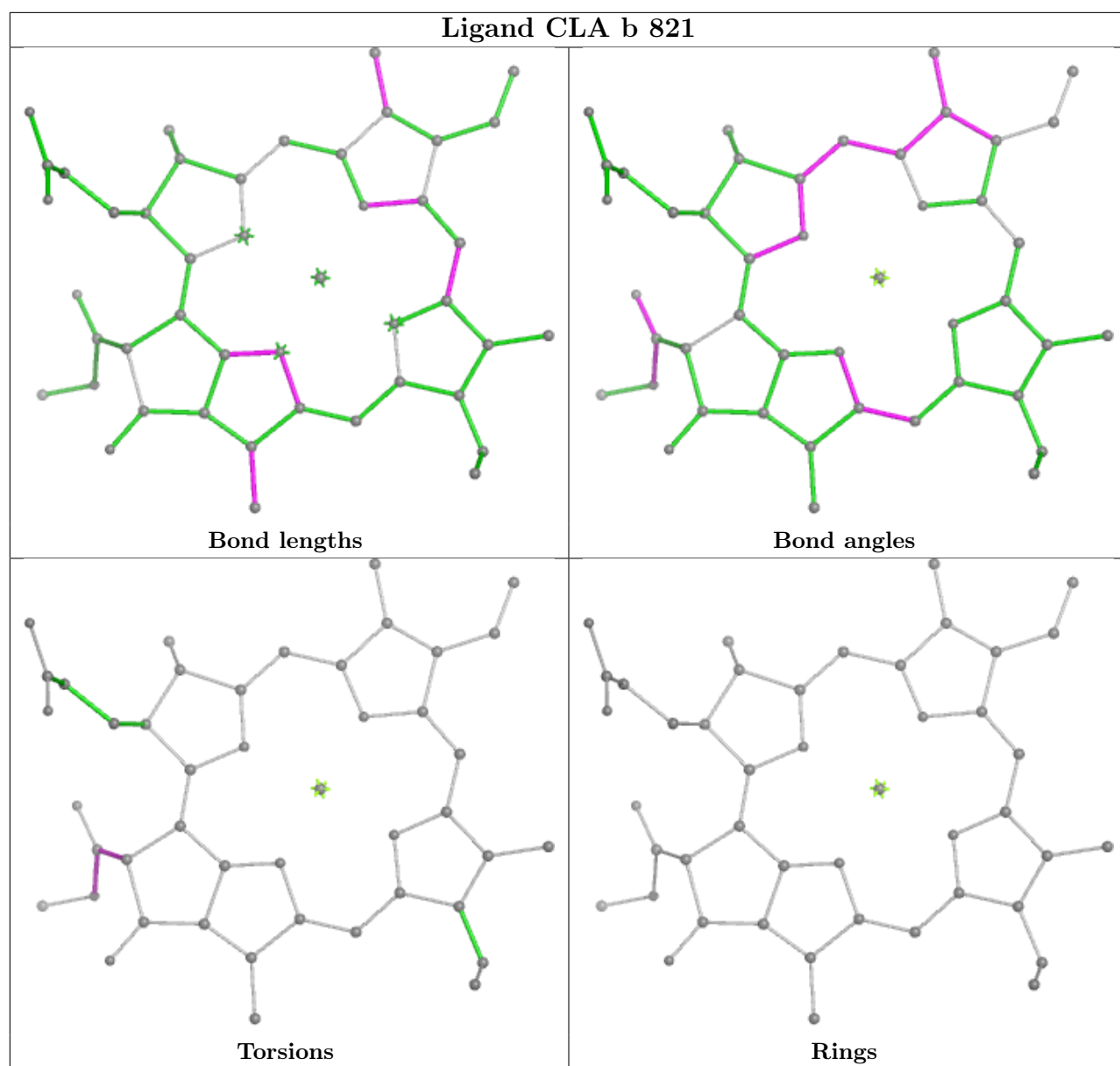
## Ligand CLA b 804



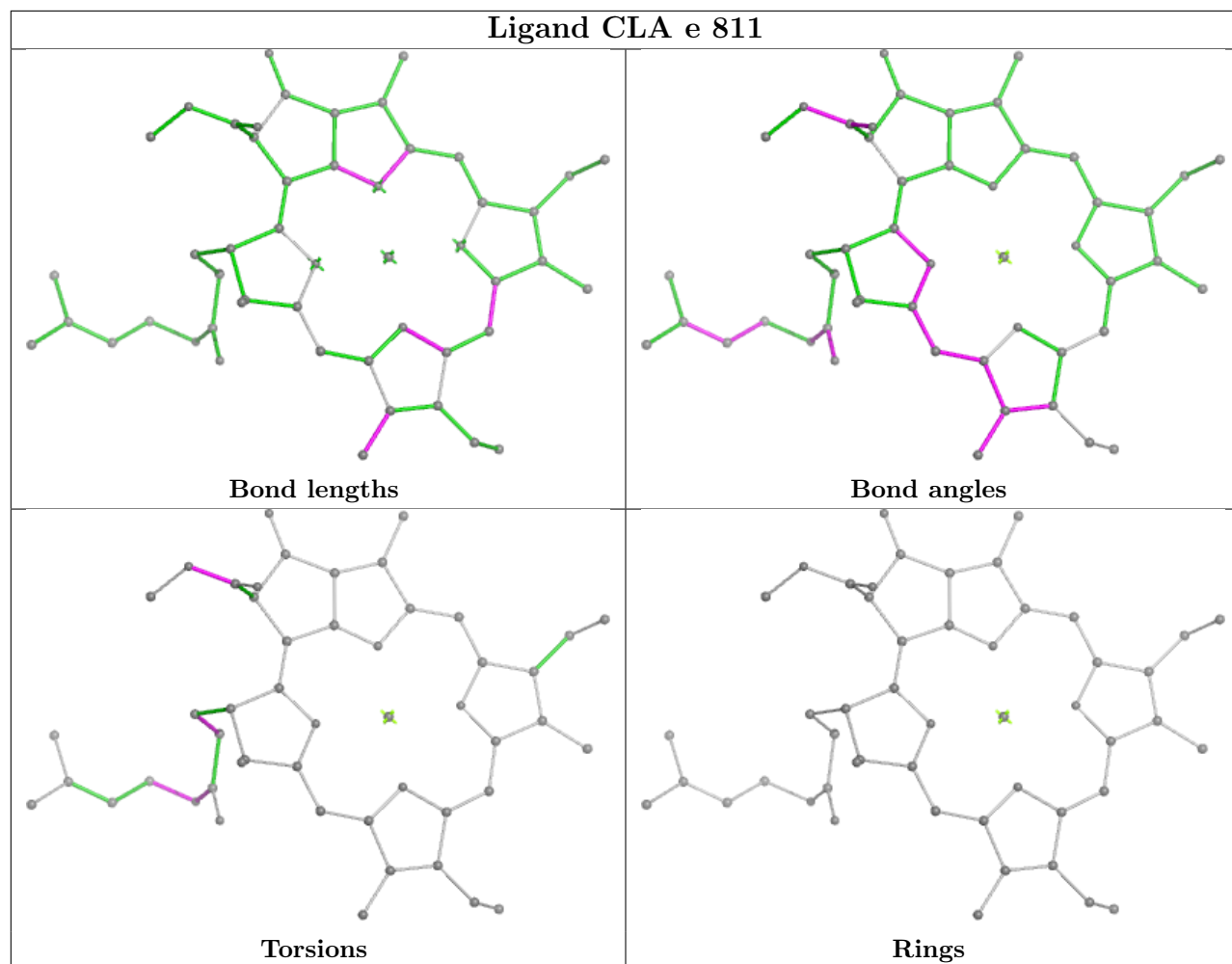
## Ligand CLA A 803



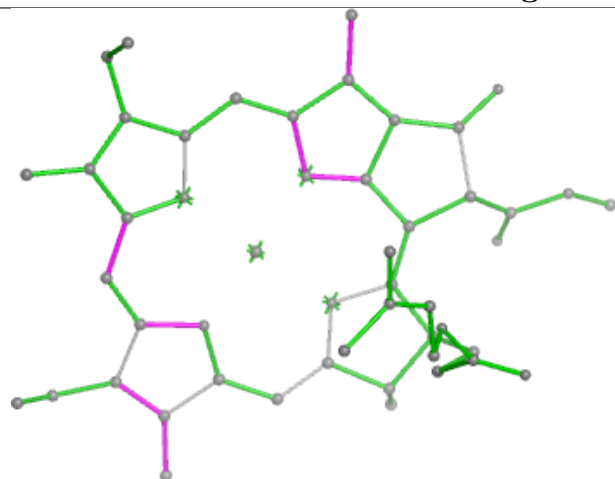




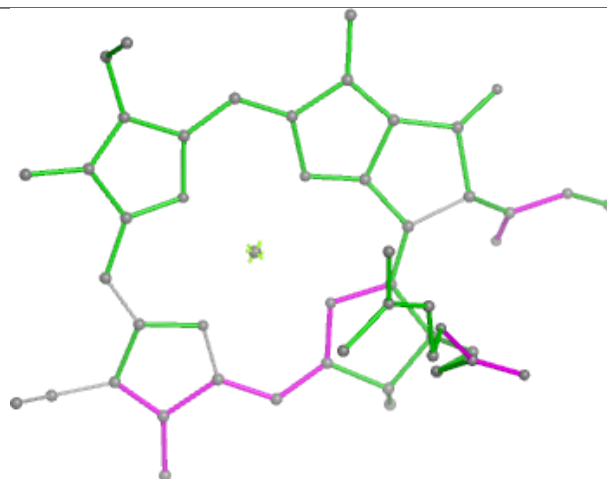
## Ligand CLA e 811



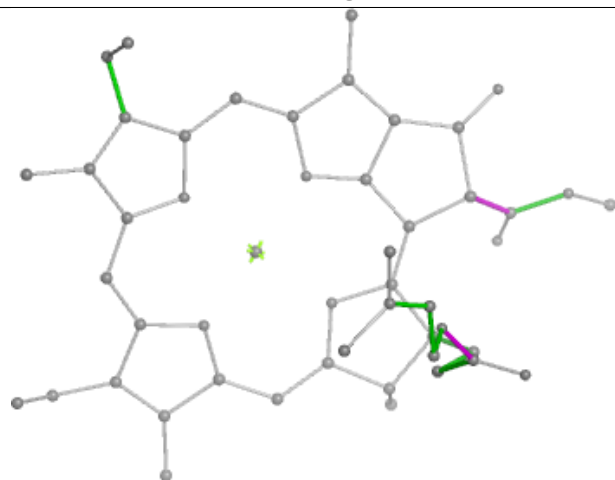
## Ligand CLA e 813



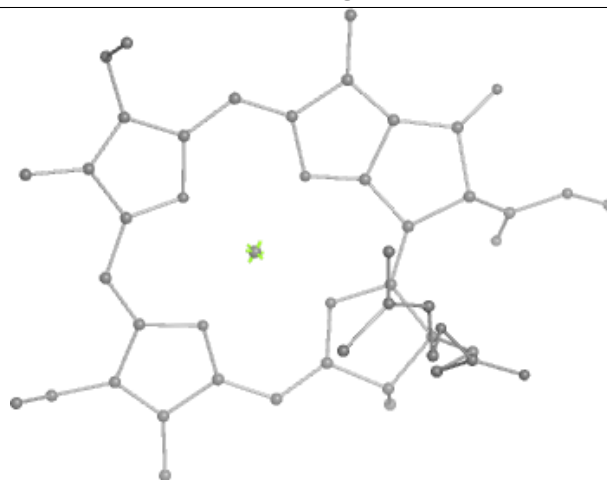
Bond lengths



Bond angles

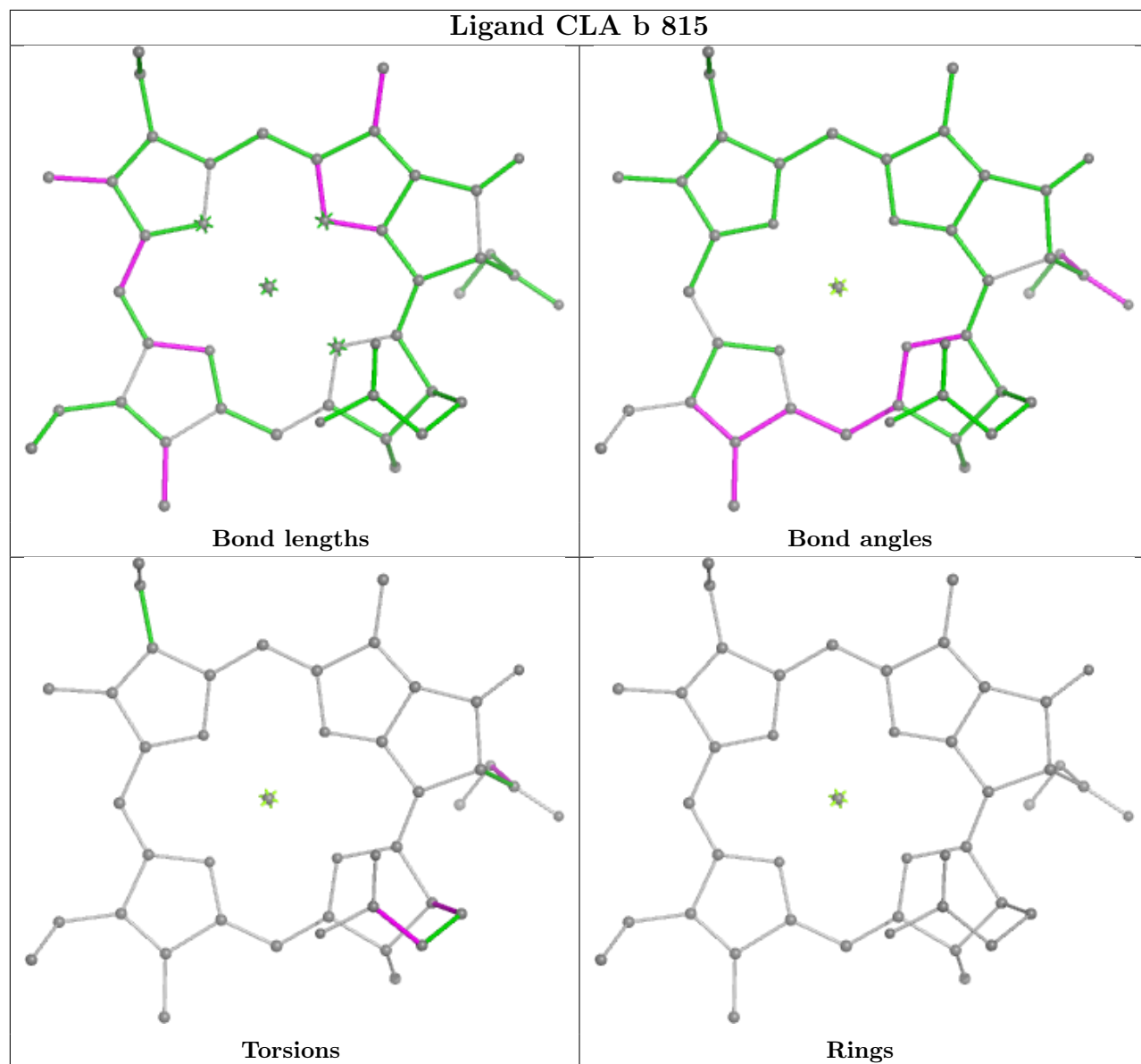


Torsions

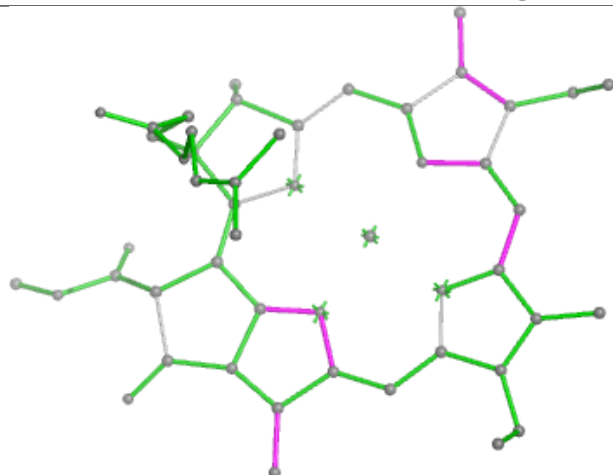


Rings

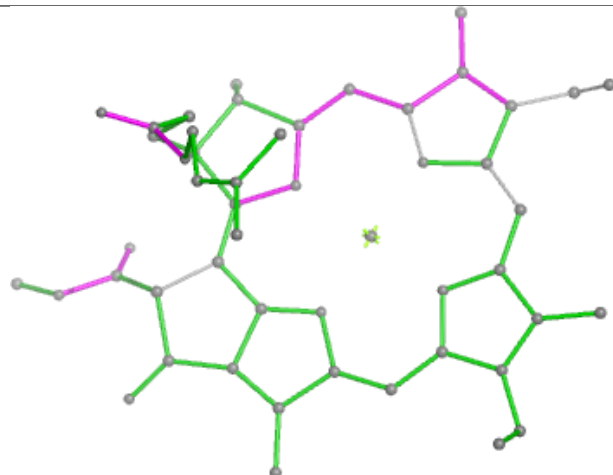
## Ligand CLA b 815



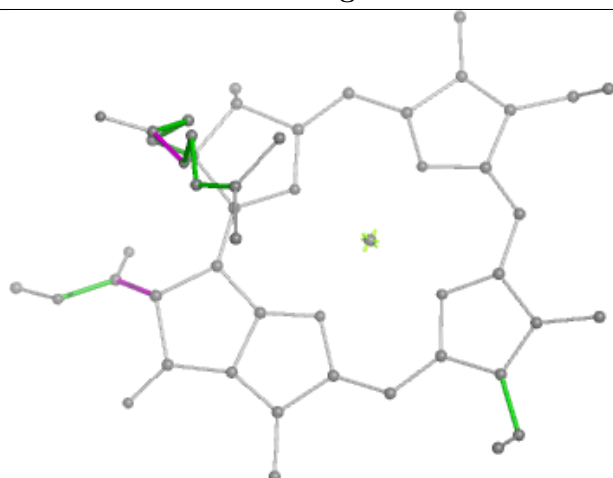
## Ligand CLA A 814



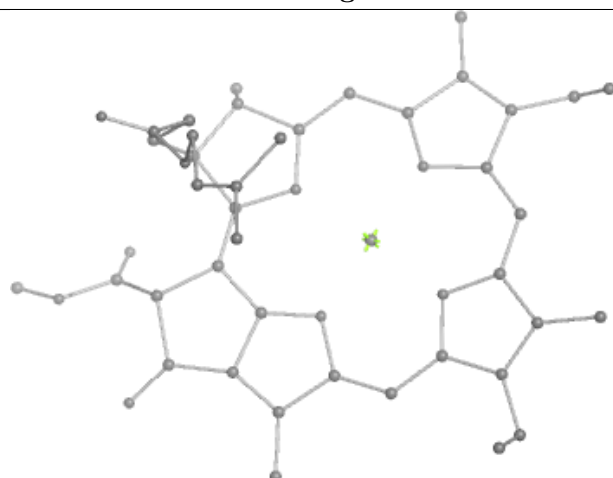
Bond lengths



Bond angles

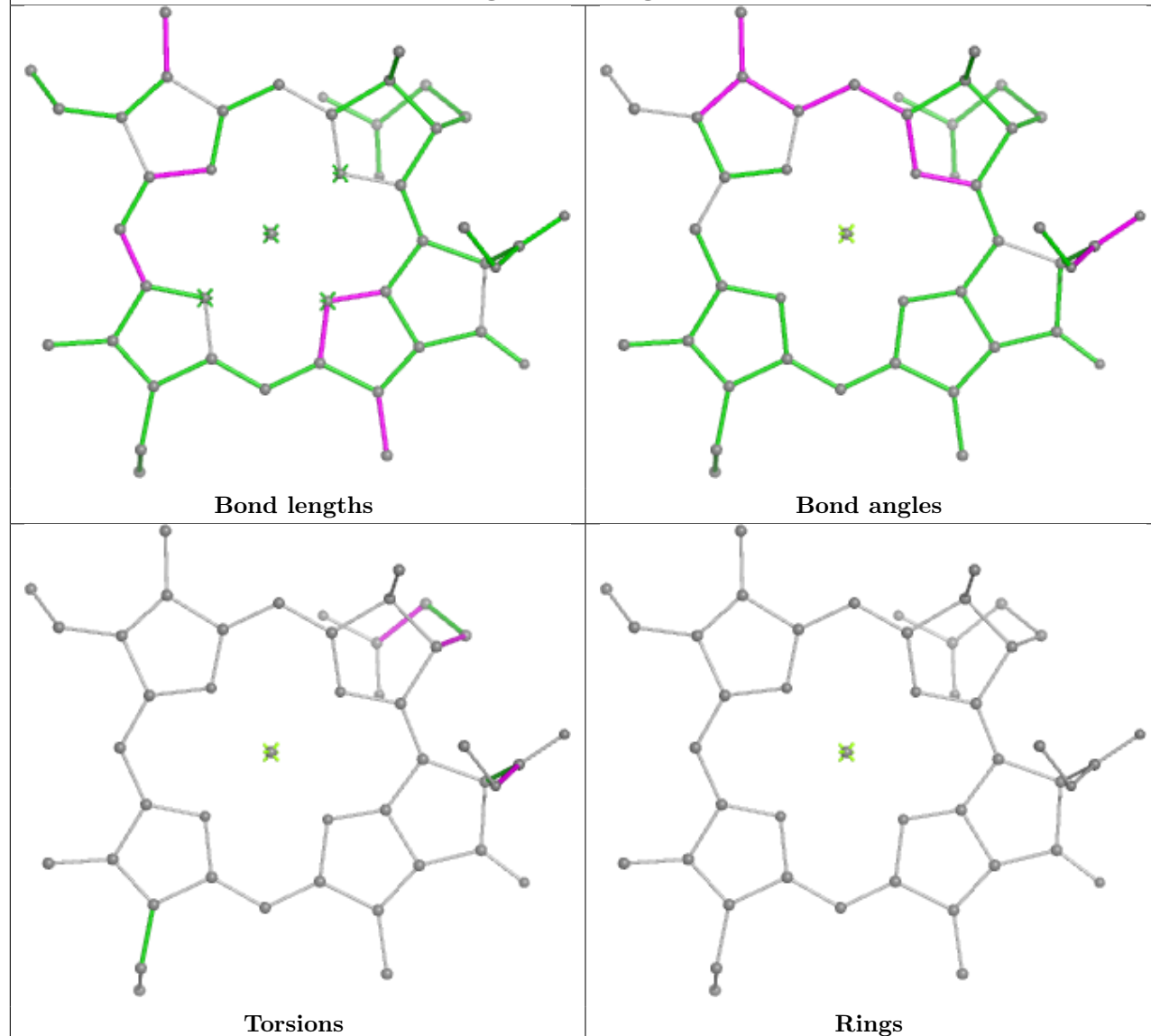


Torsions

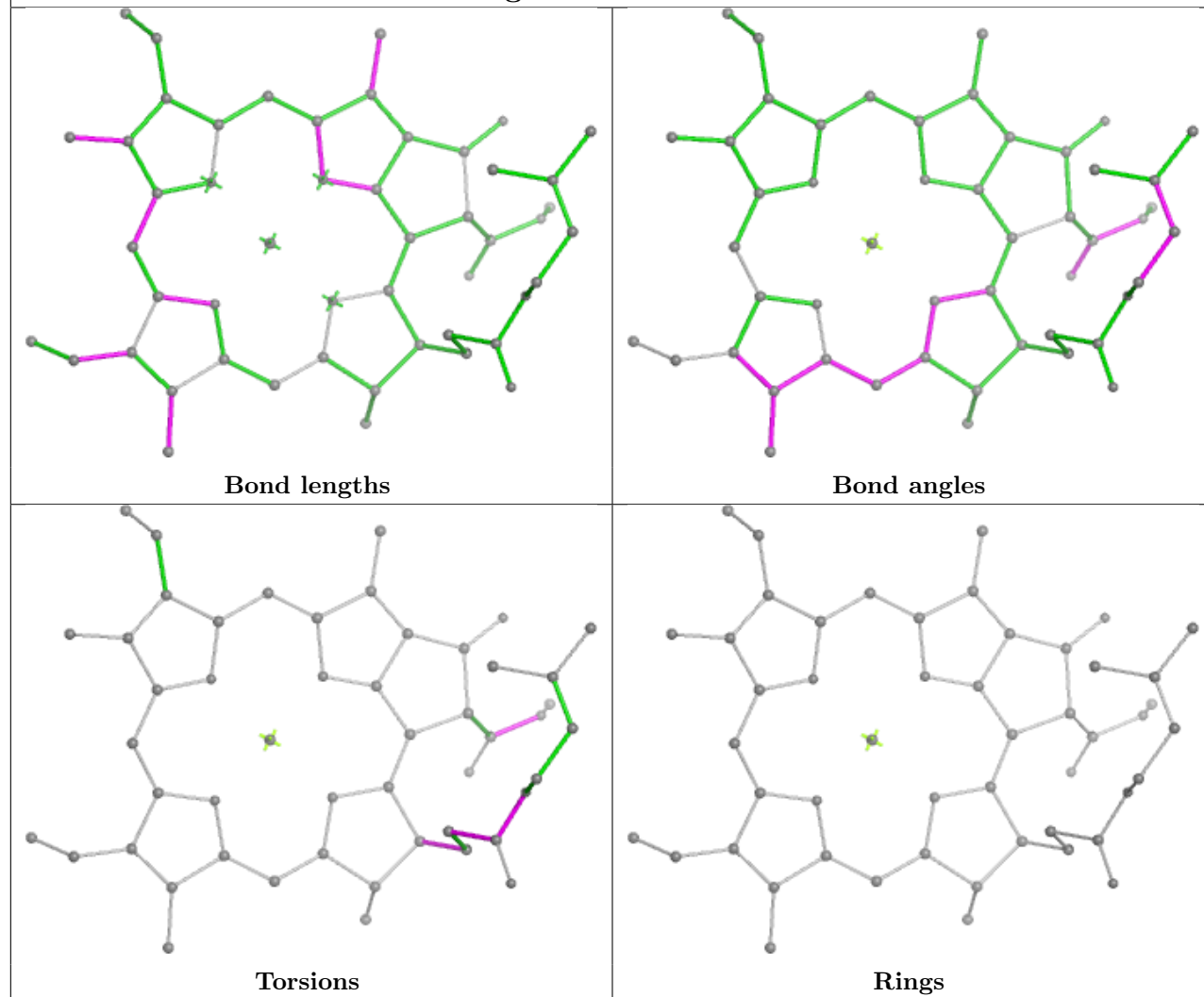


Rings

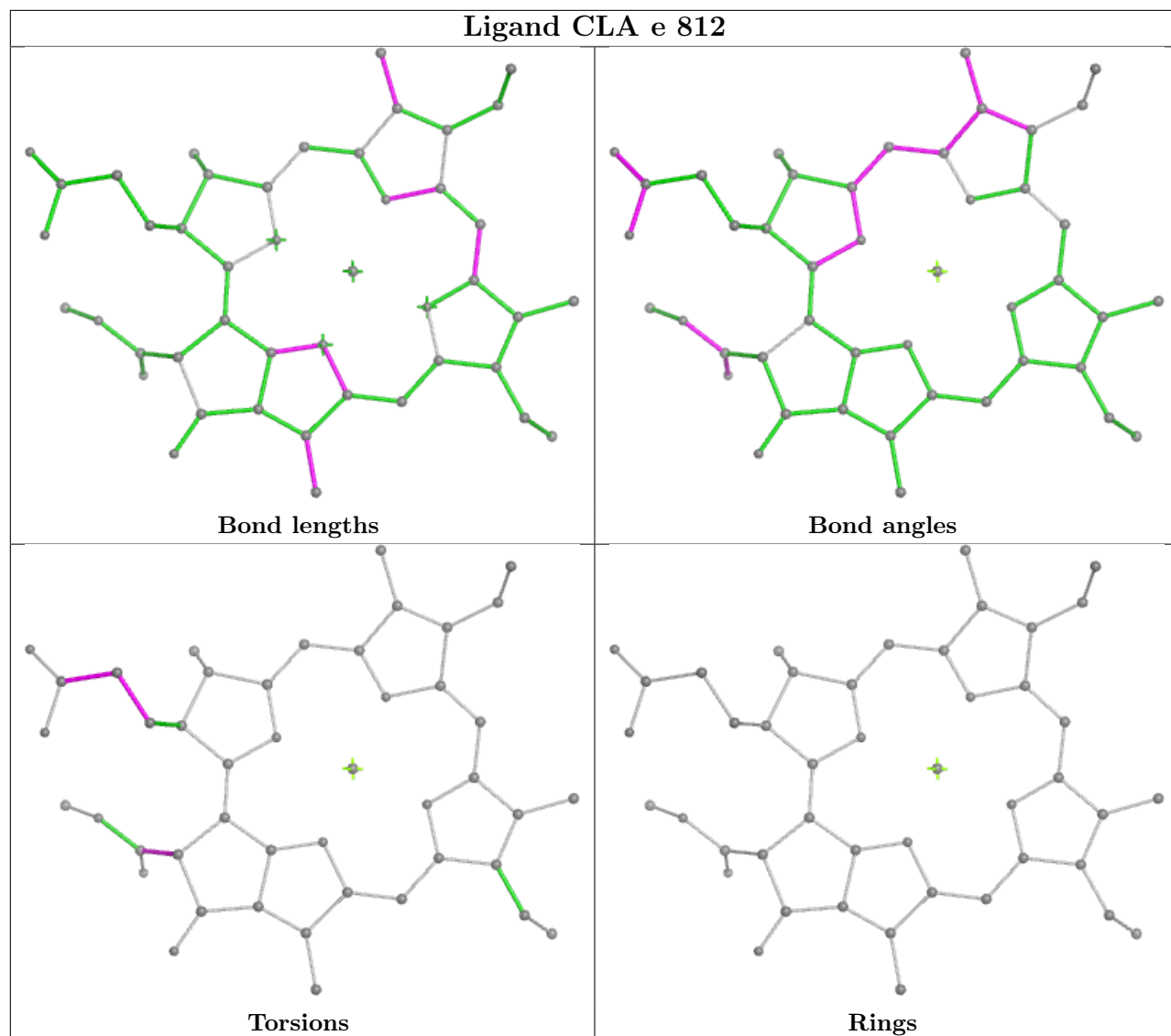
## Ligand CLA g 817



## Ligand CLA b 840

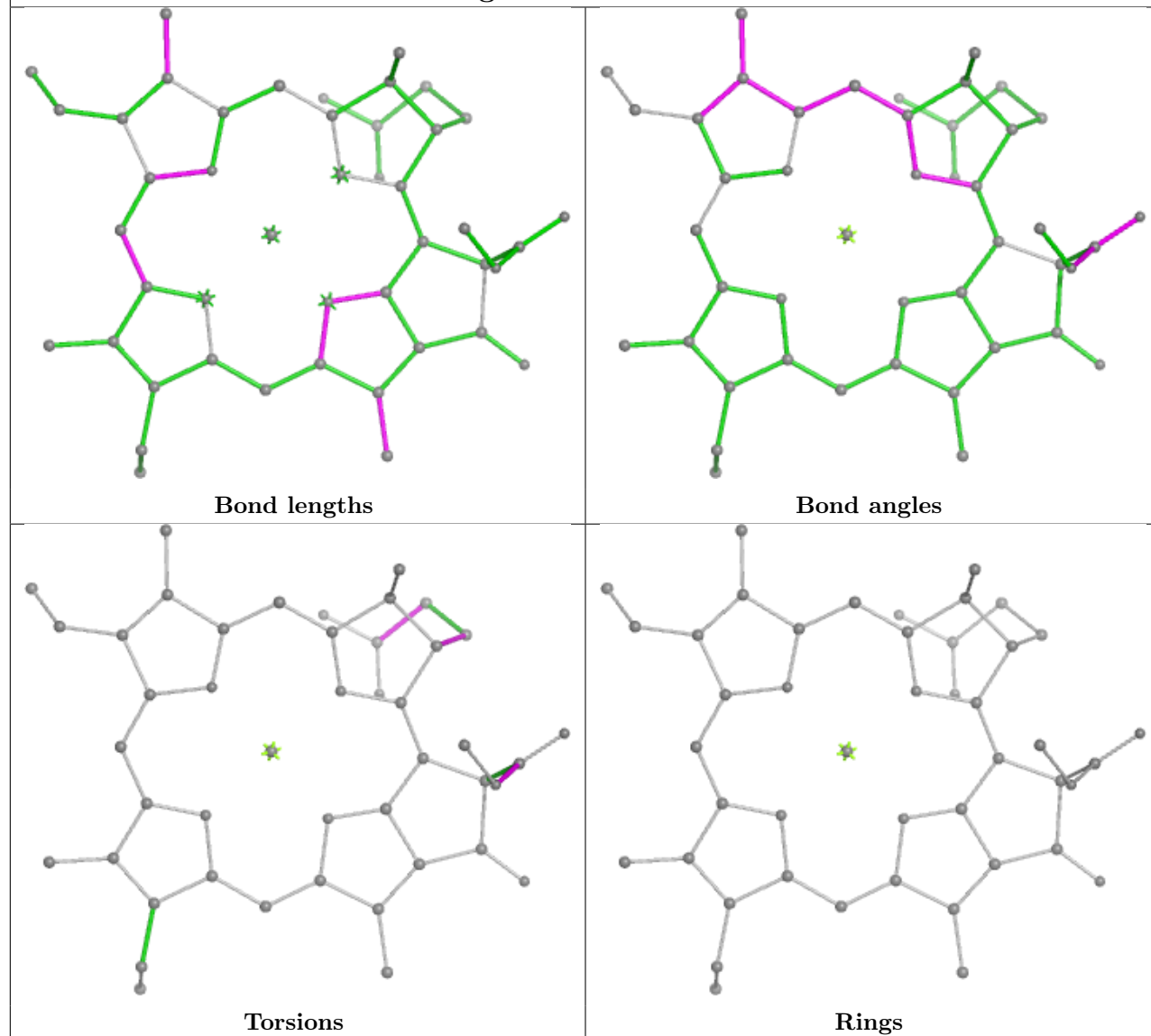


## Ligand CLA e 812

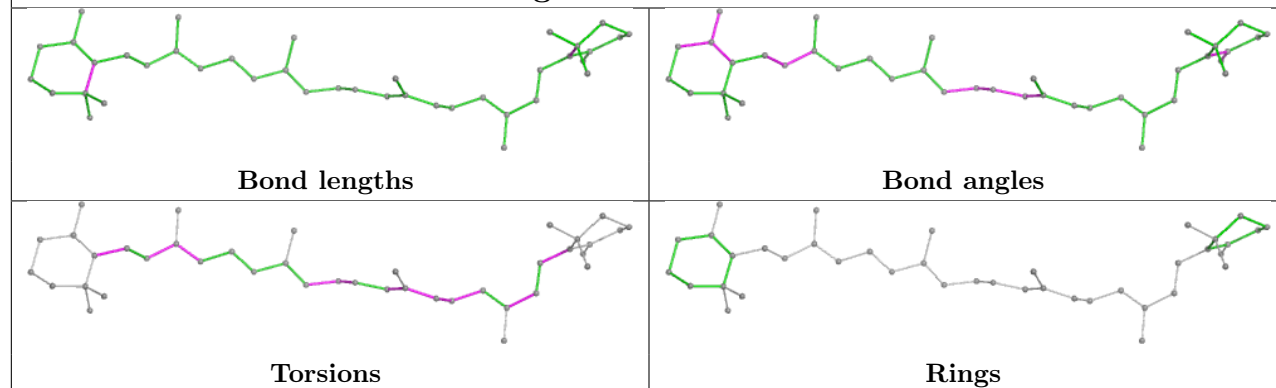




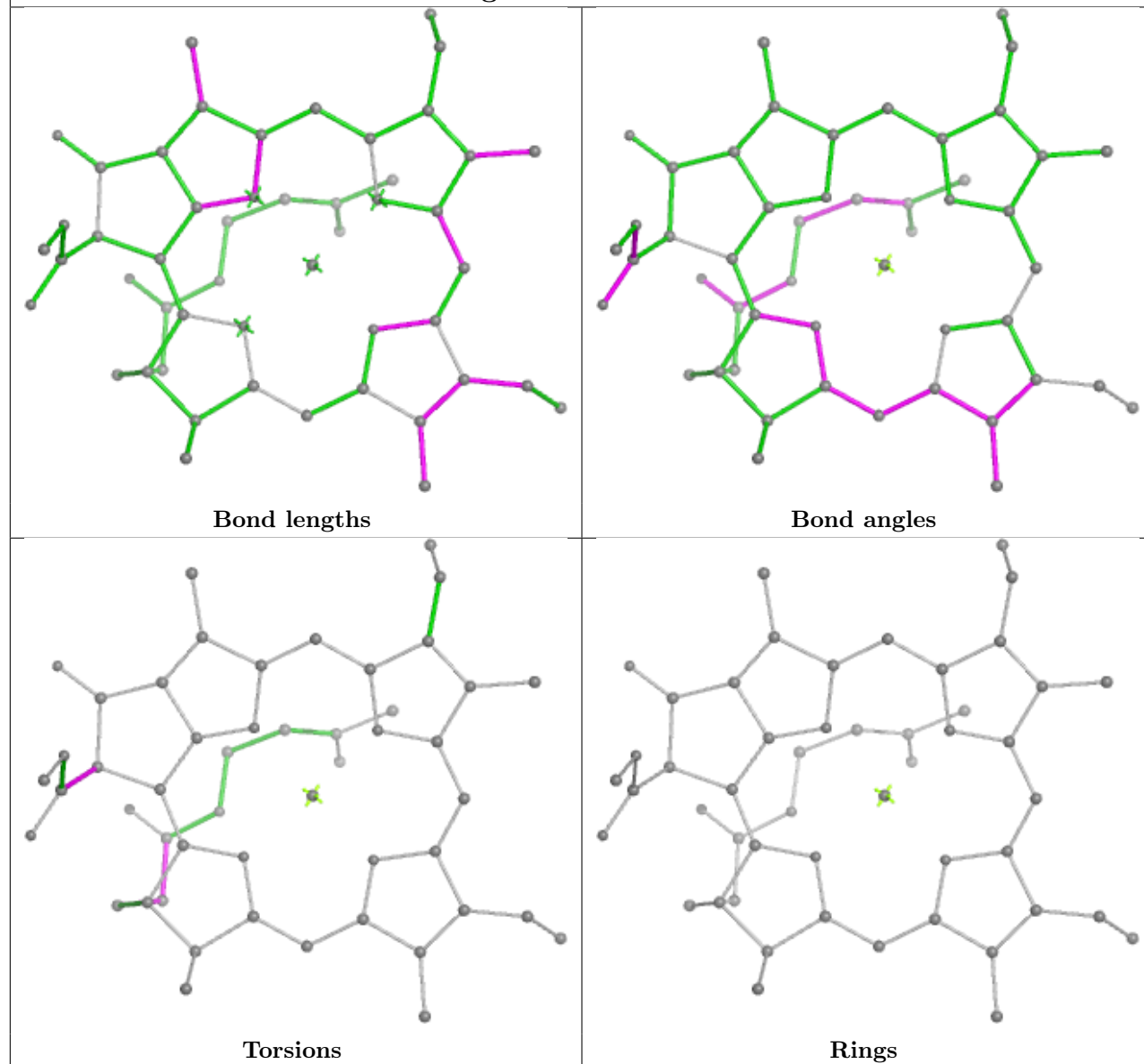
## Ligand CLA G 816



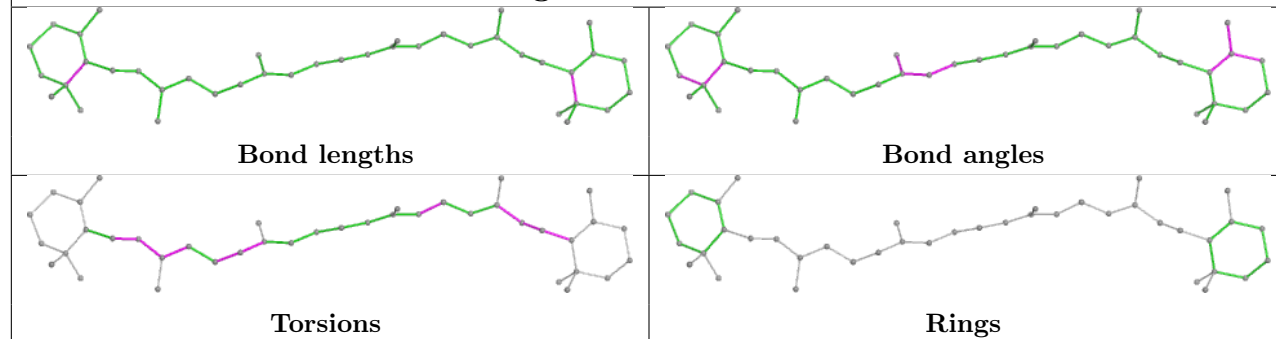
## Ligand BCR b 847



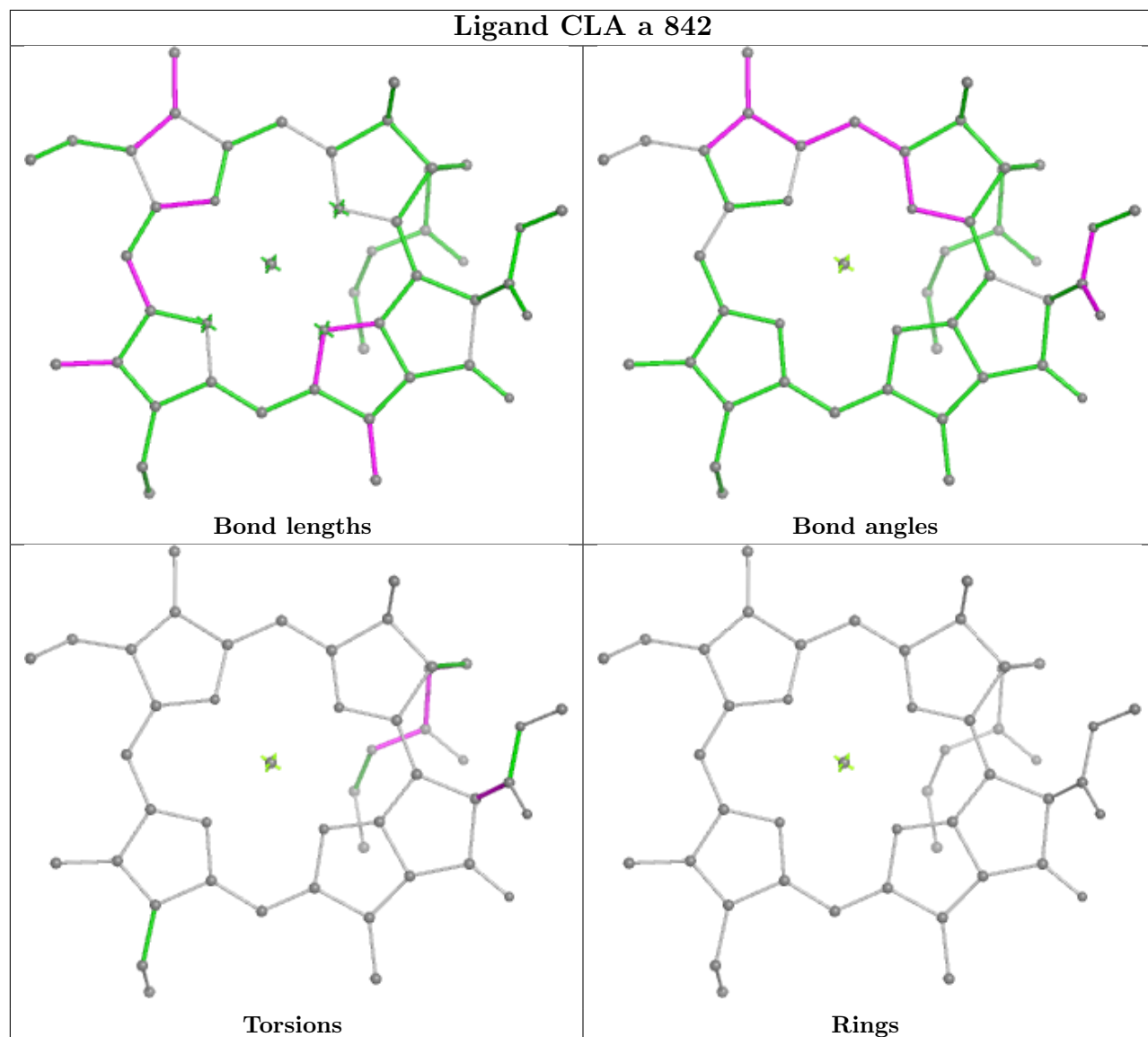
## Ligand CLA e 839



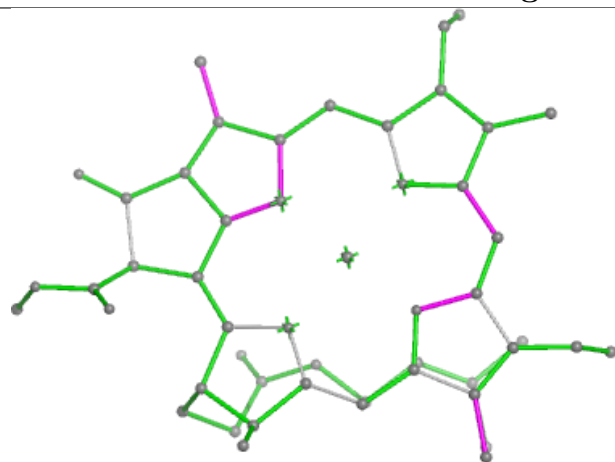
## Ligand BCR L 205



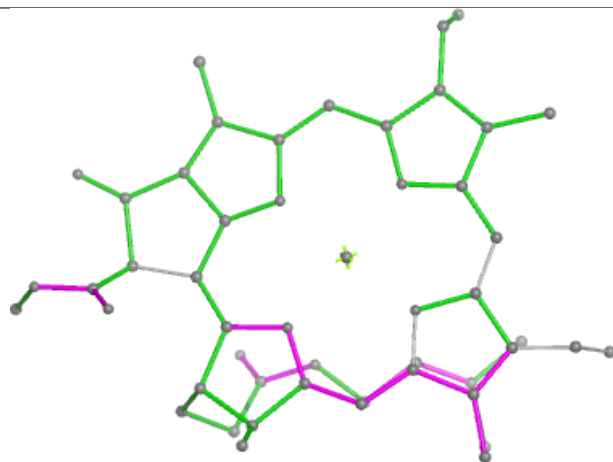
## Ligand CLA a 842



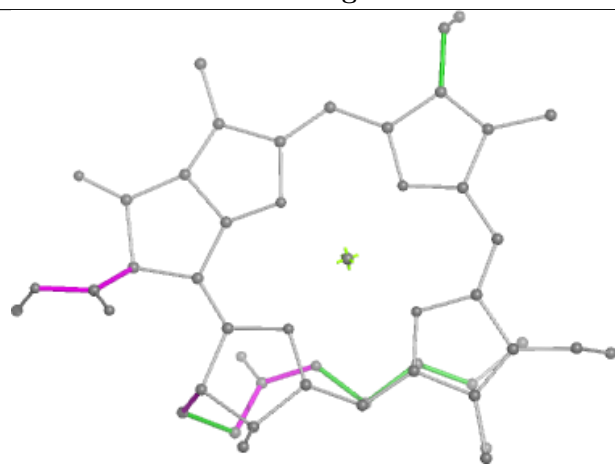
## Ligand CLA e 823



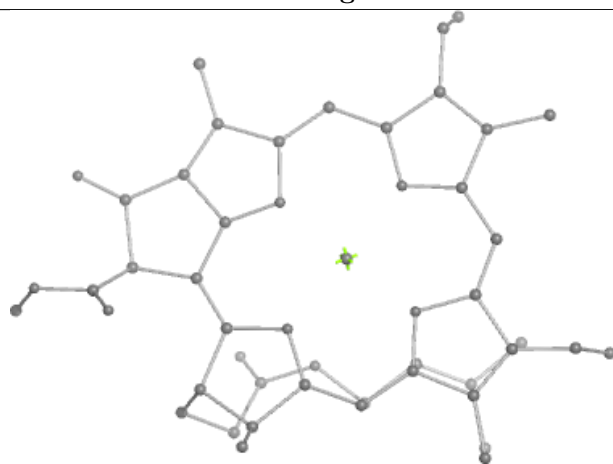
Bond lengths



Bond angles

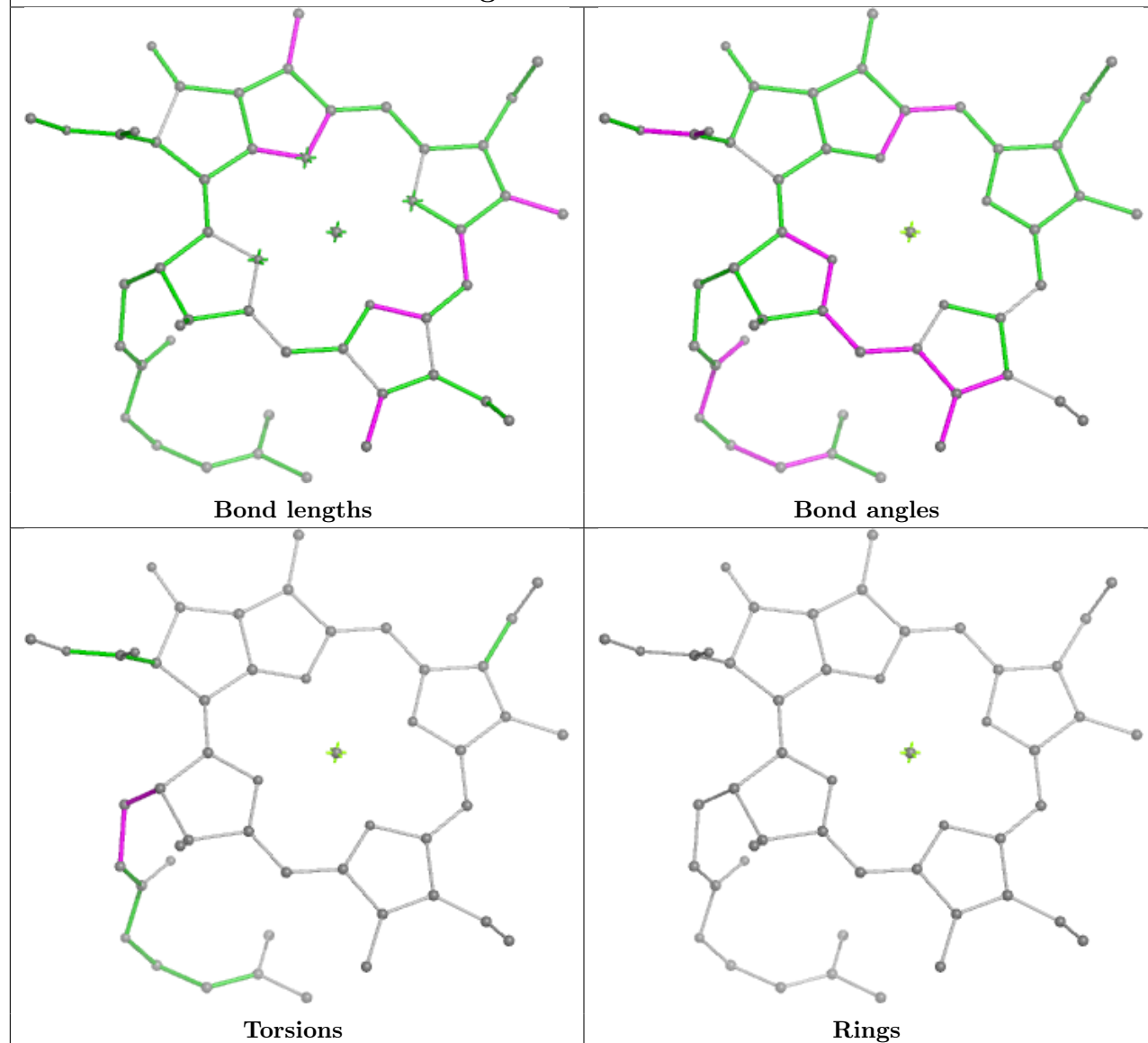


Torsions

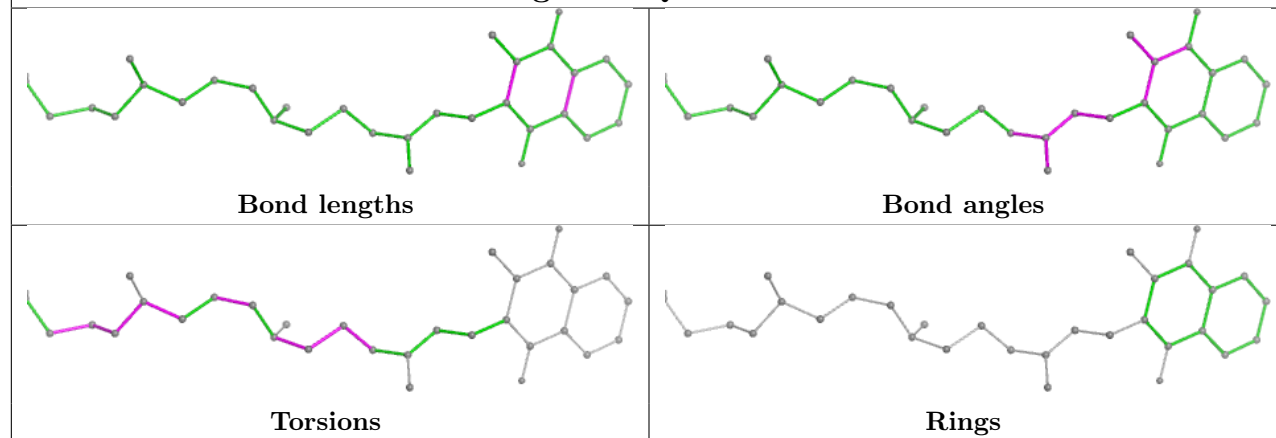


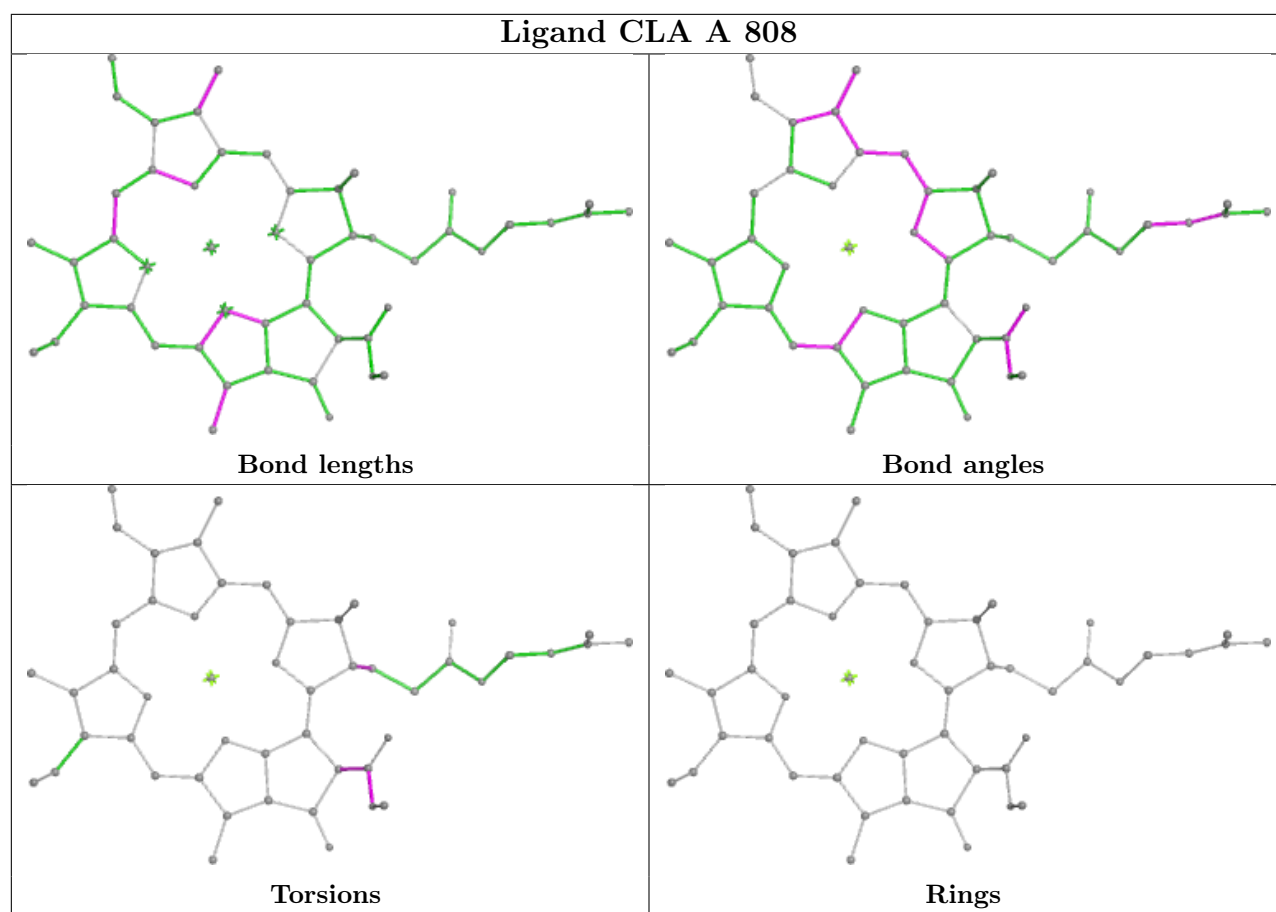
Rings

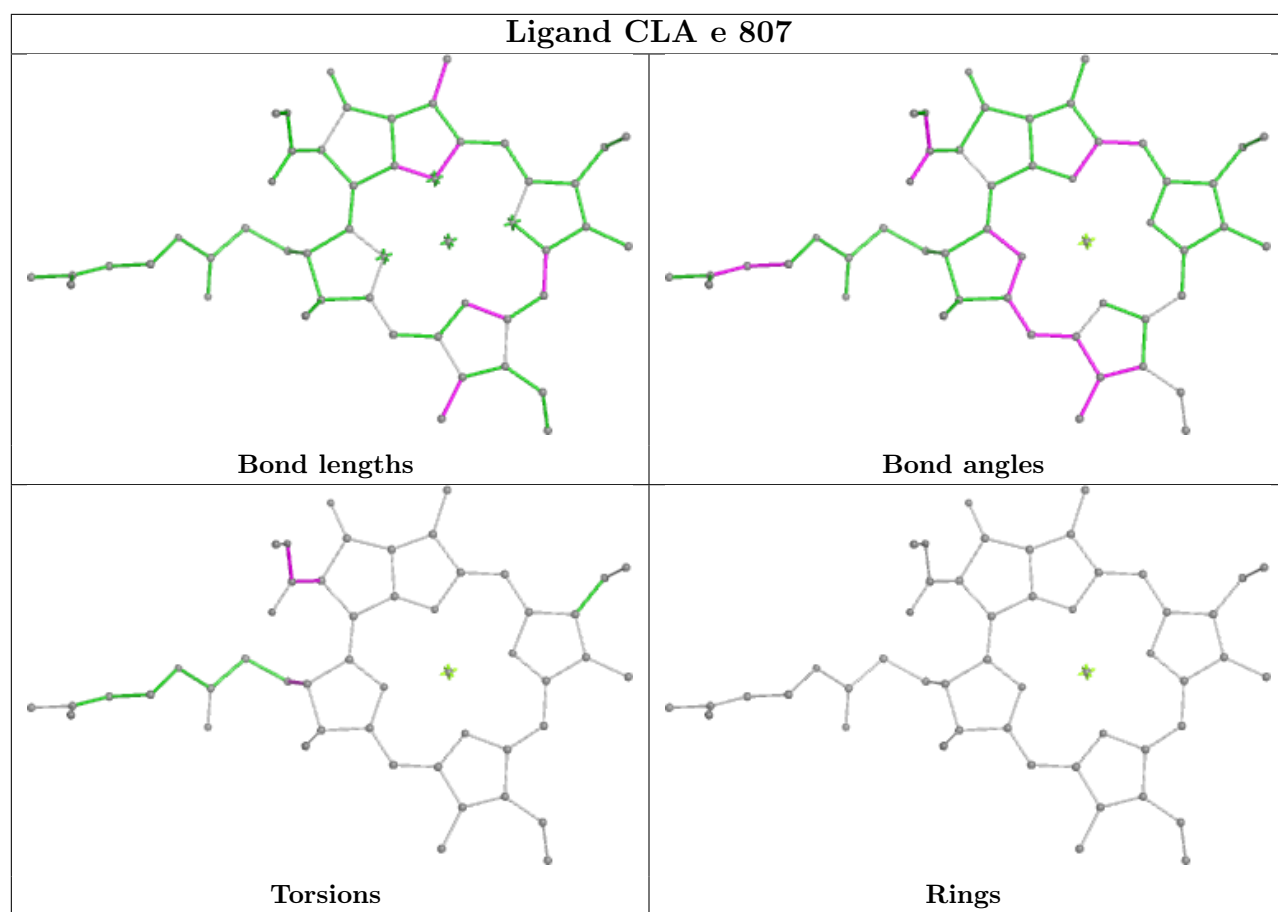
## Ligand CLA E 811



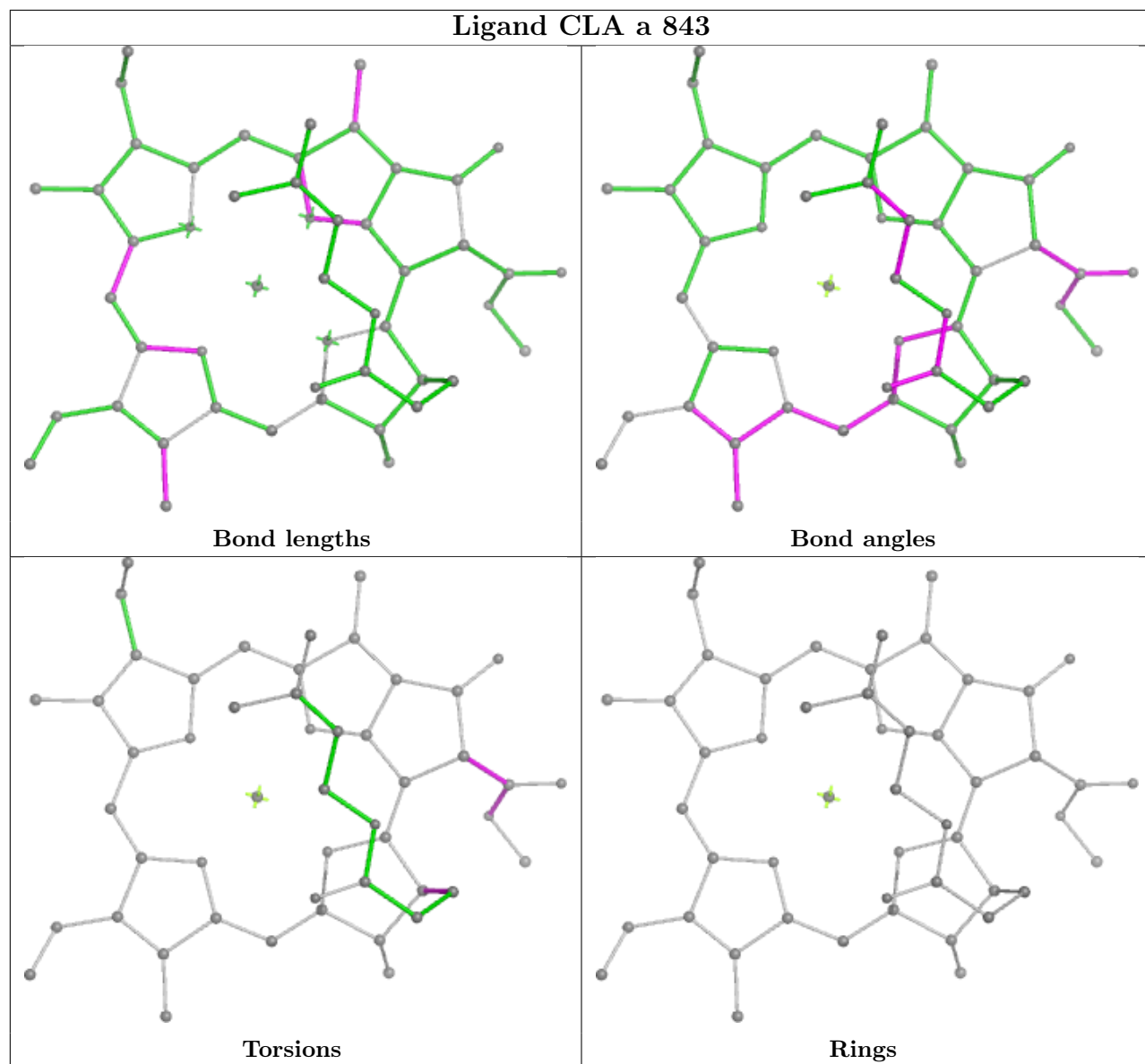
## Ligand PQN b 841





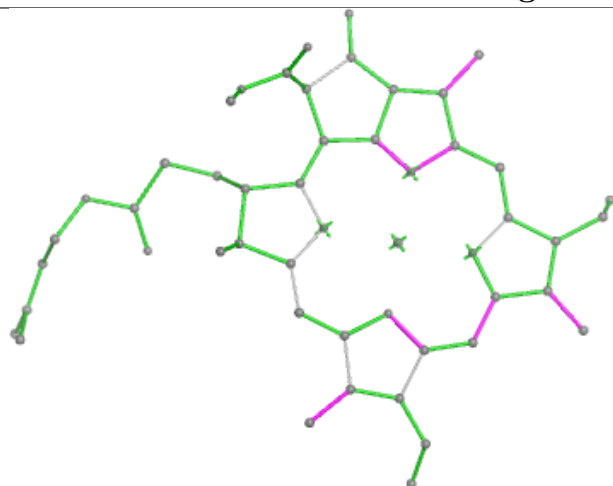


## Ligand CLA a 843

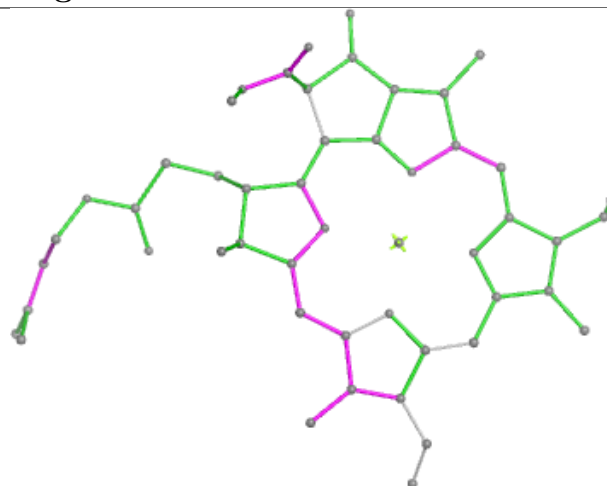




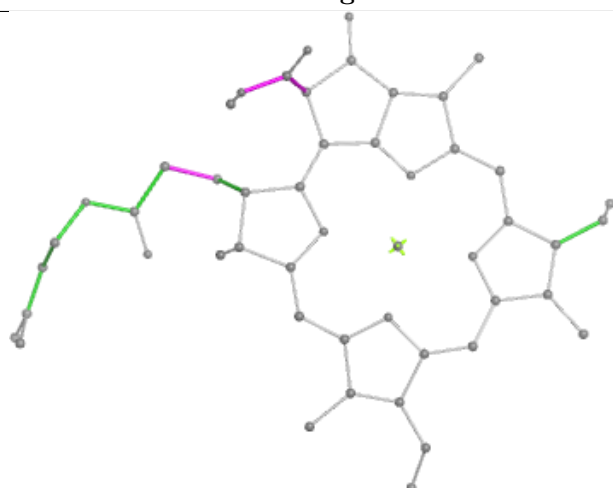
## Ligand CLA g 815



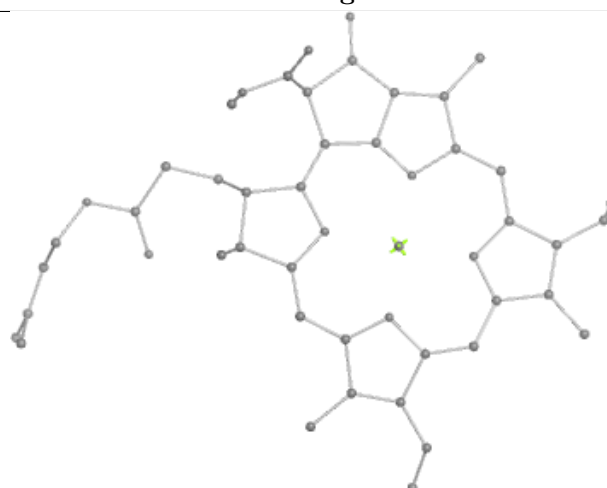
Bond lengths



Bond angles

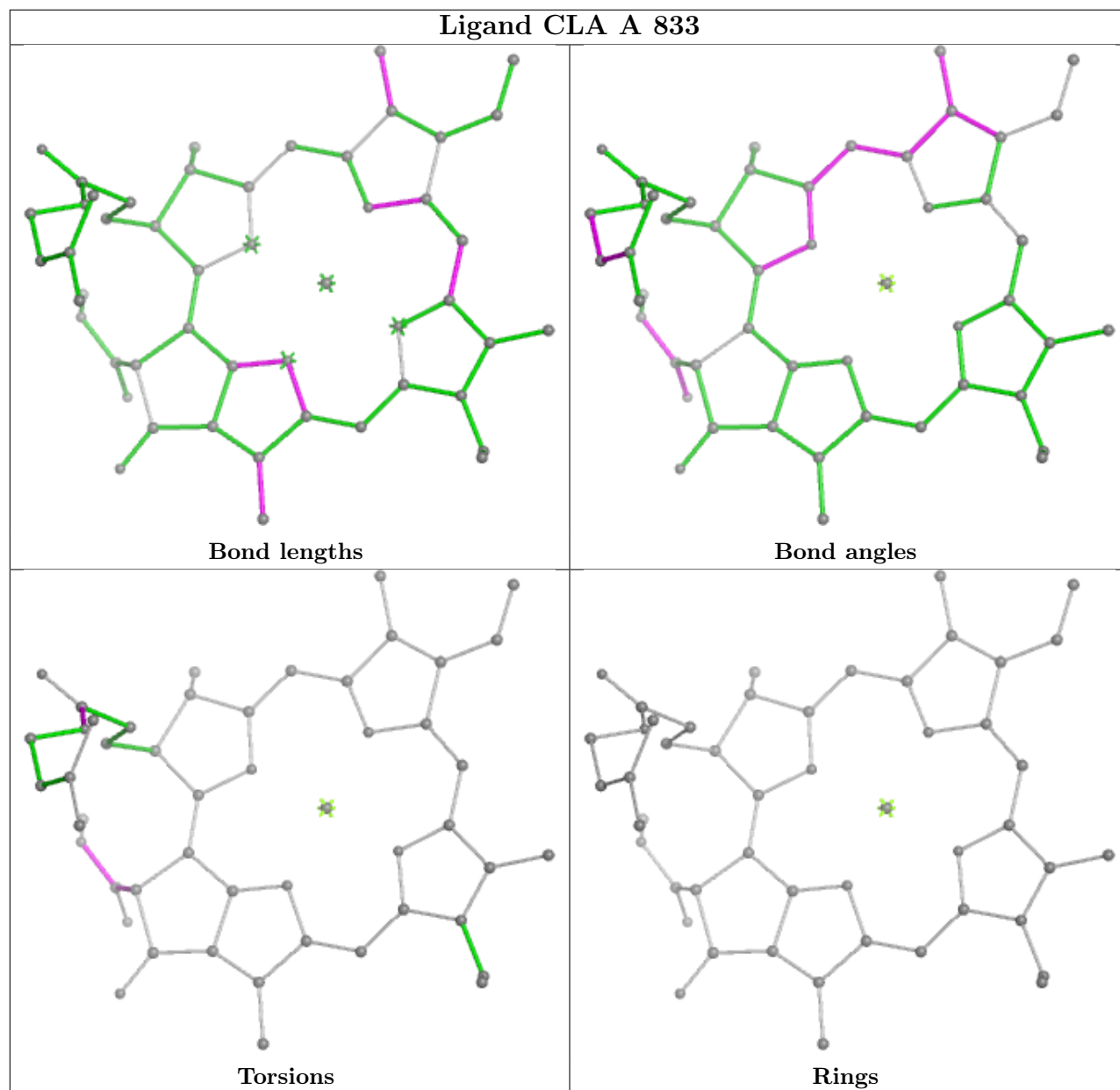


Torsions

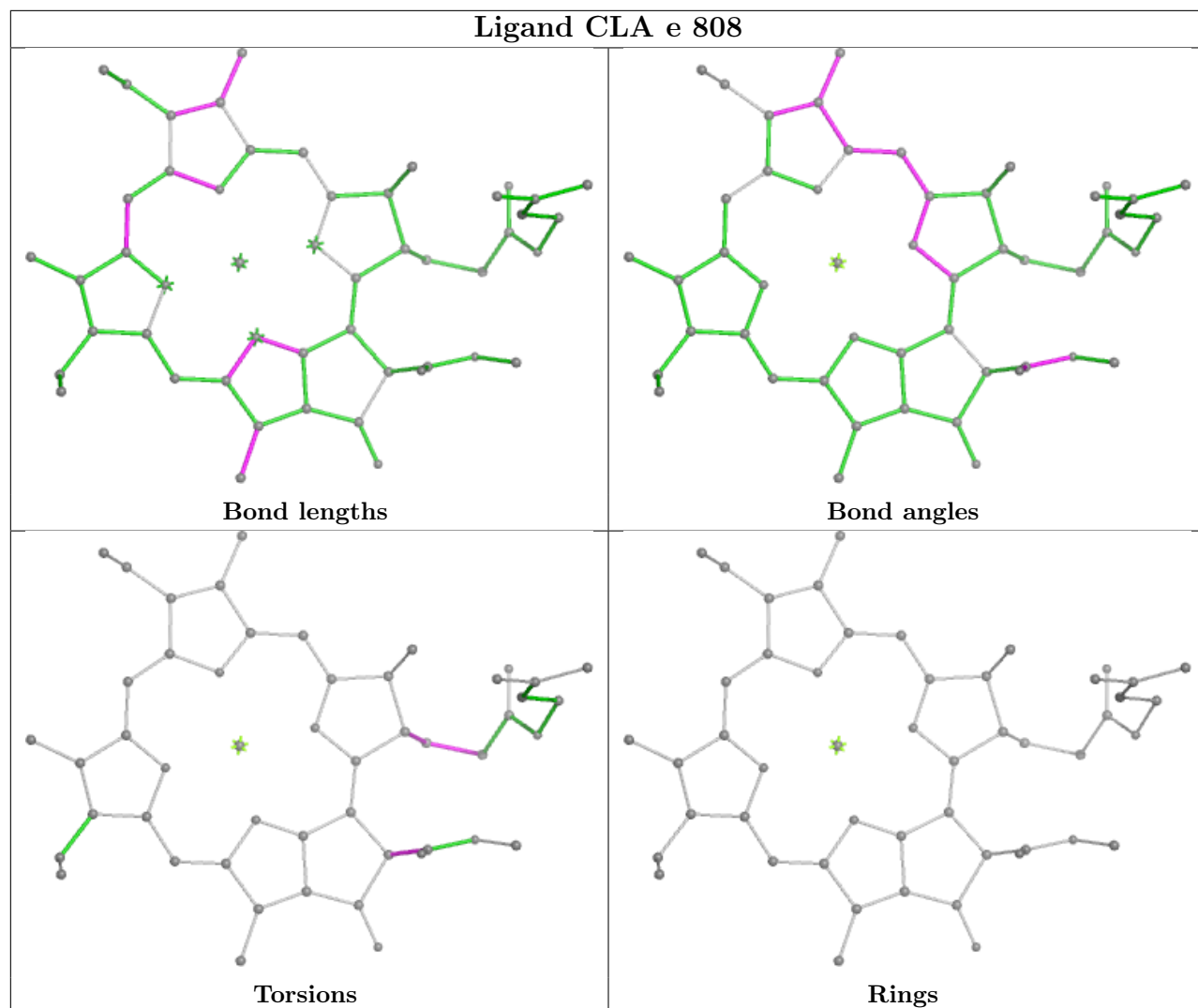


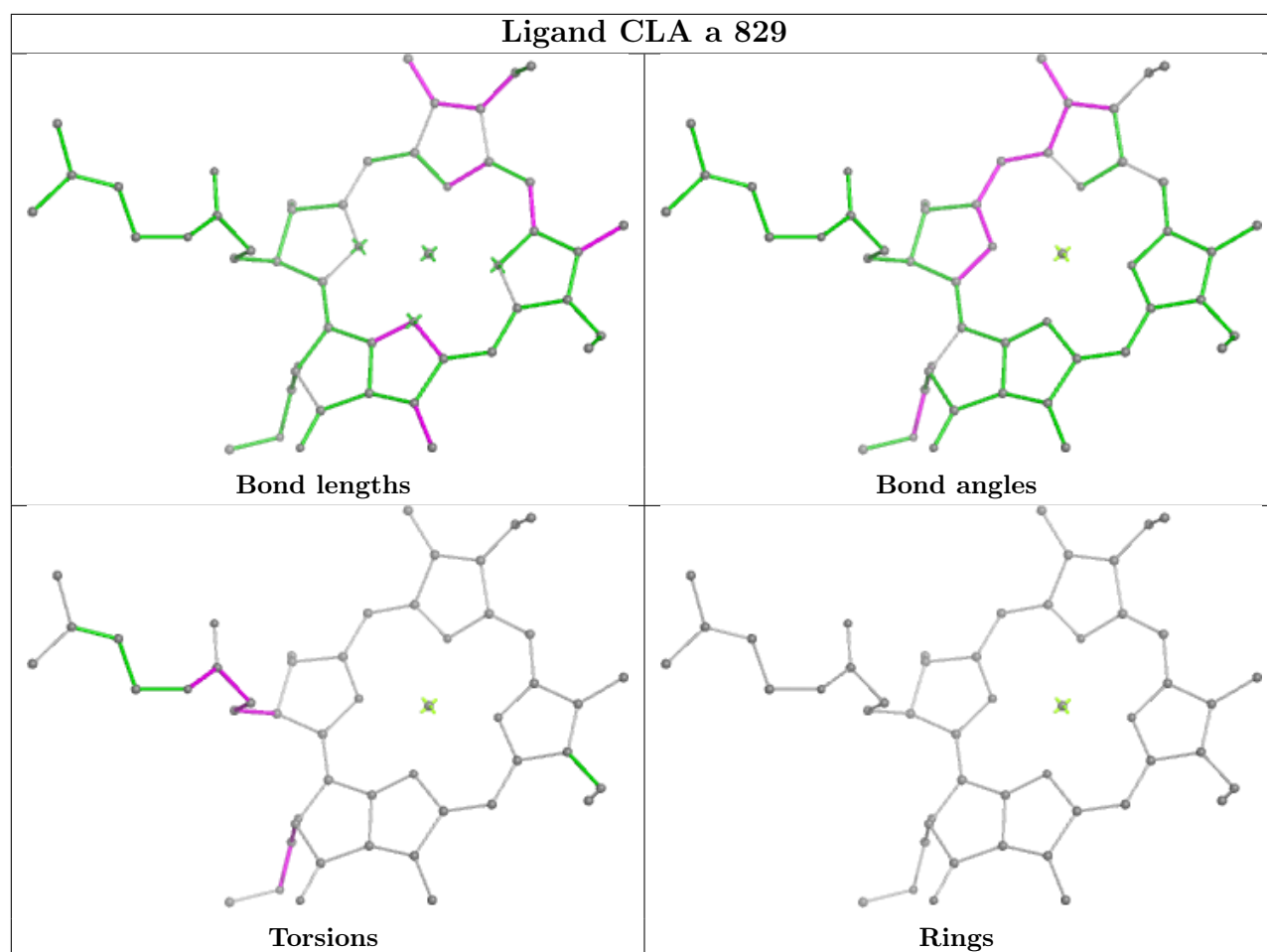
Rings

## Ligand CLA A 833

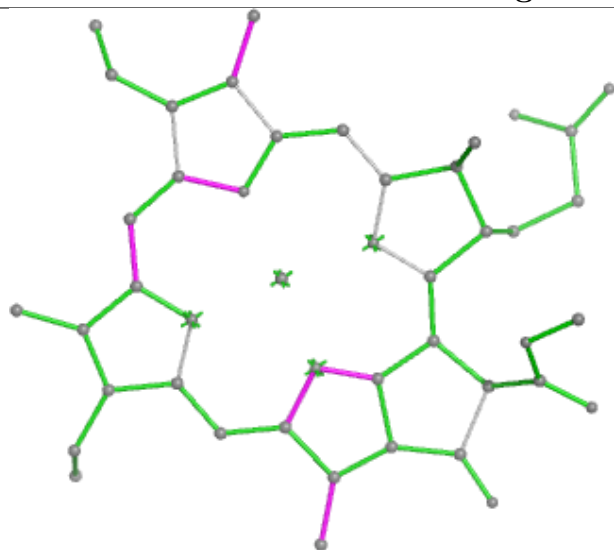


## Ligand CLA e 808

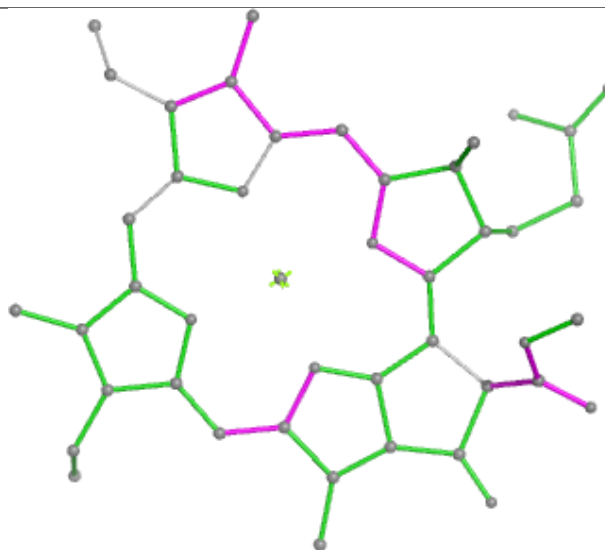




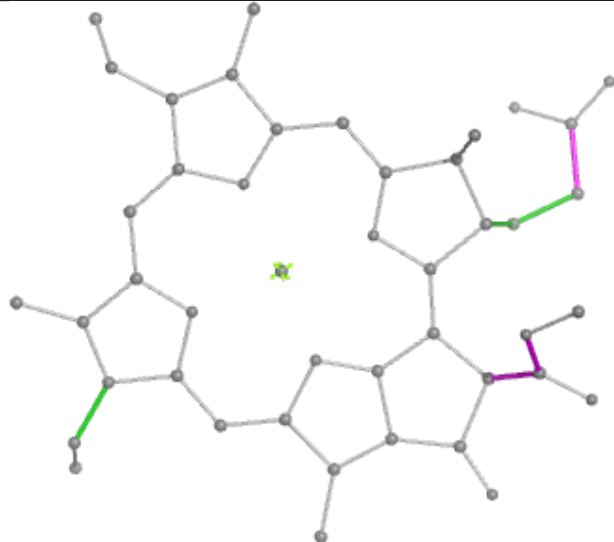
## Ligand CLA E 839



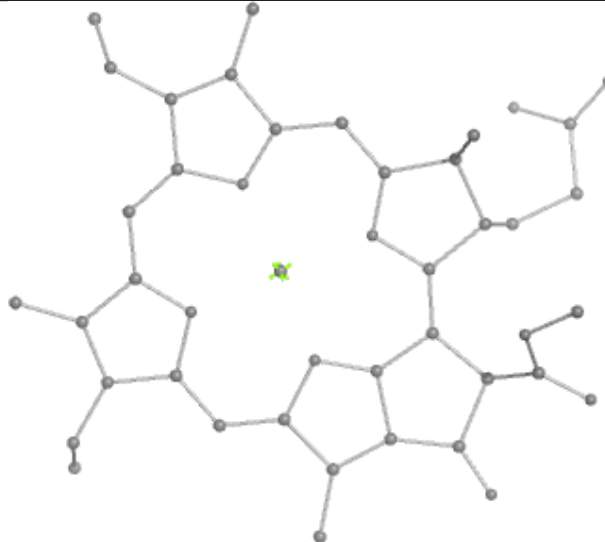
Bond lengths



Bond angles

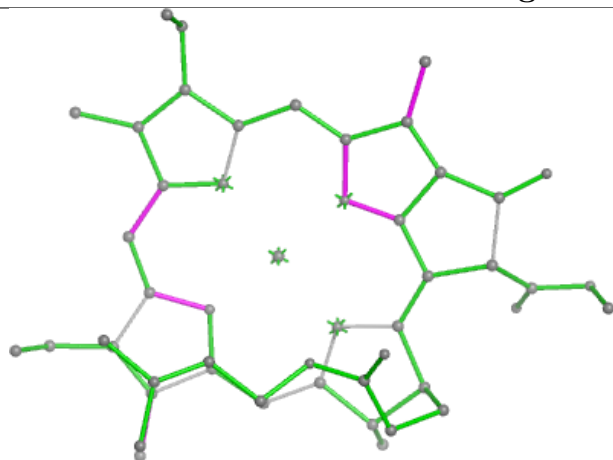


Torsions

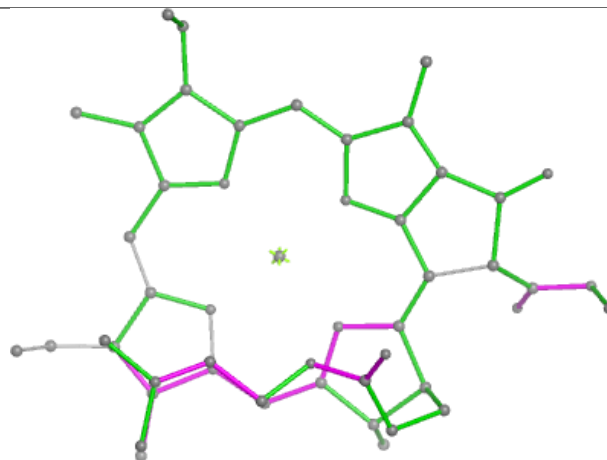


Rings

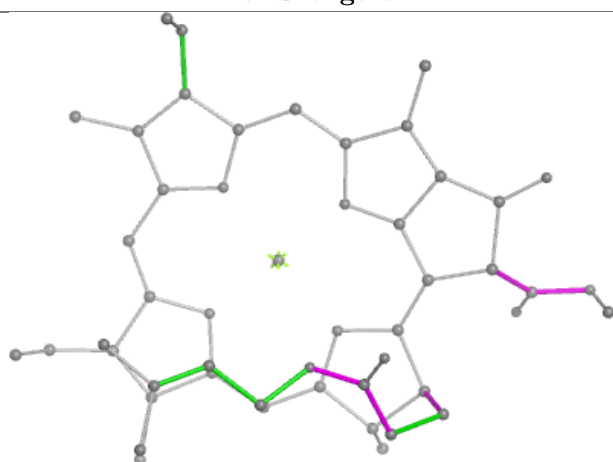
## Ligand CLA a 824



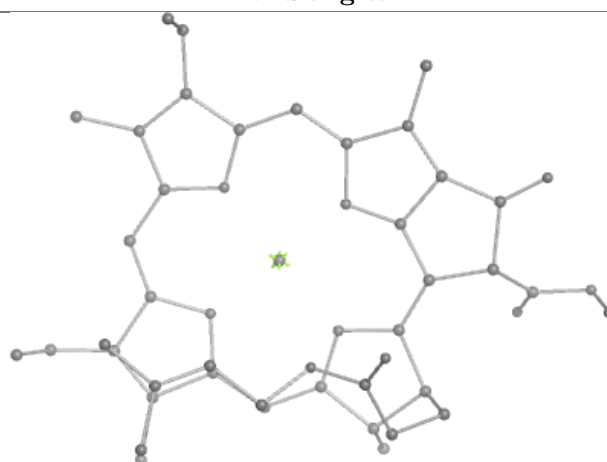
Bond lengths



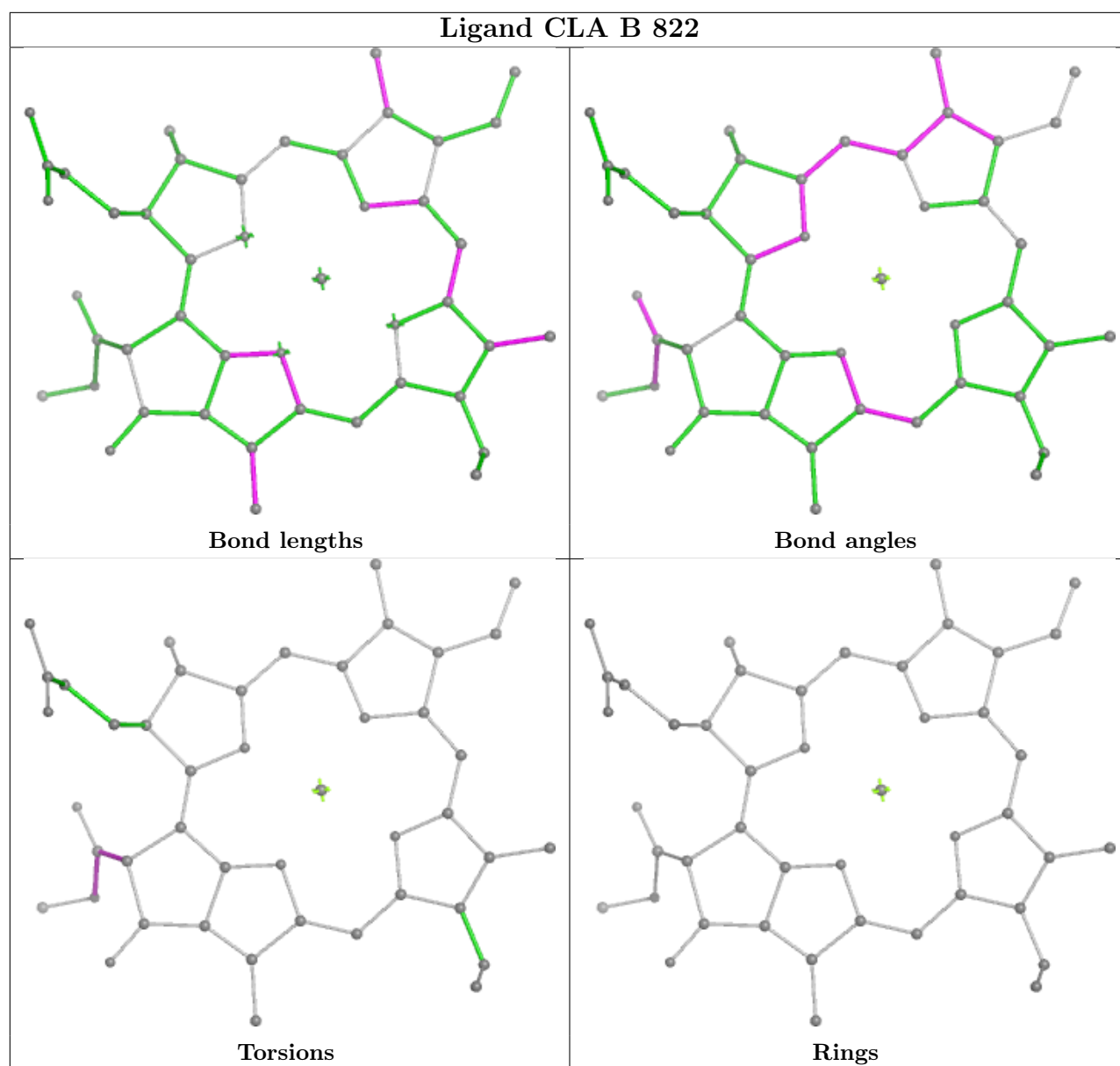
Bond angles

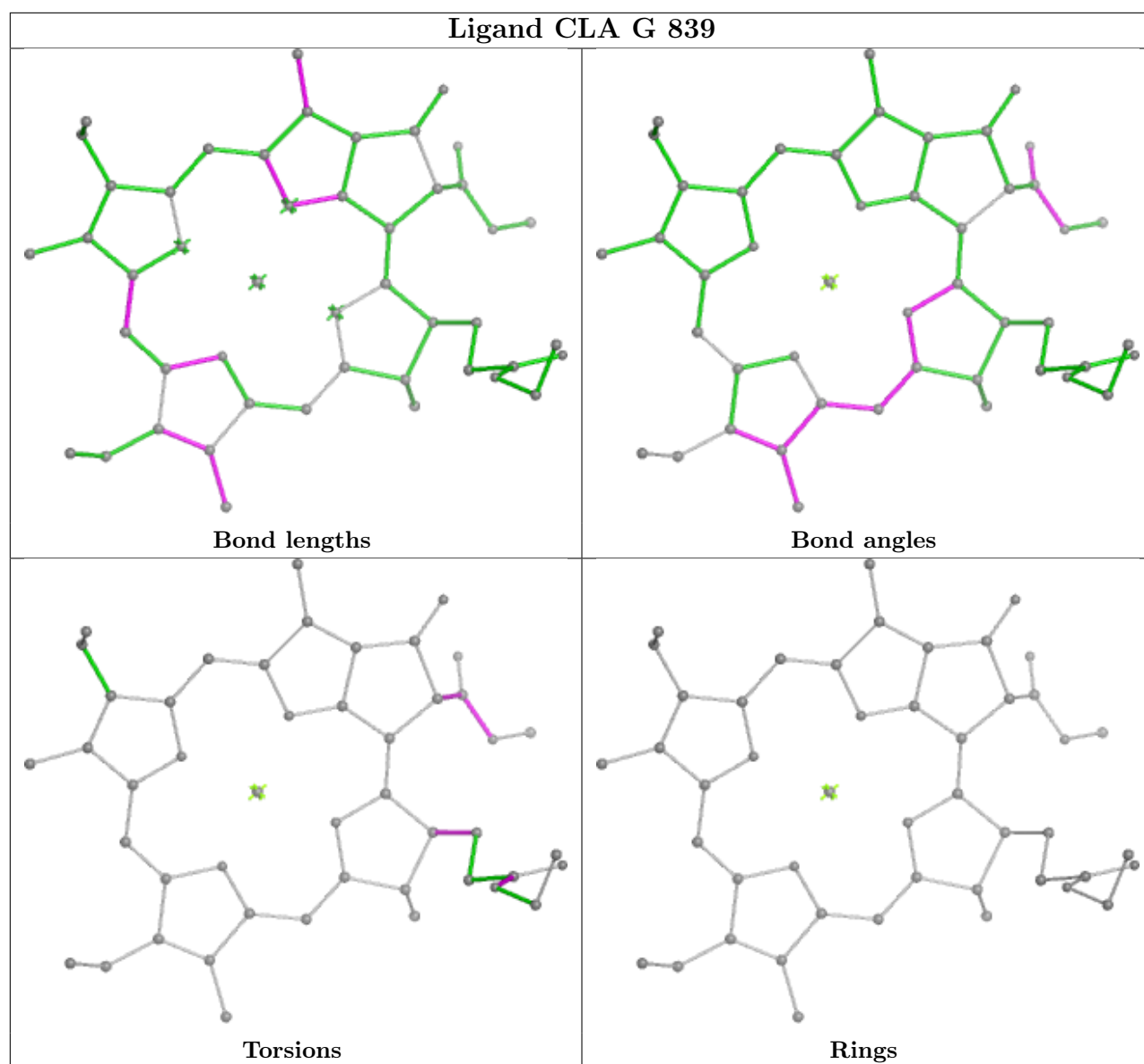


Torsions

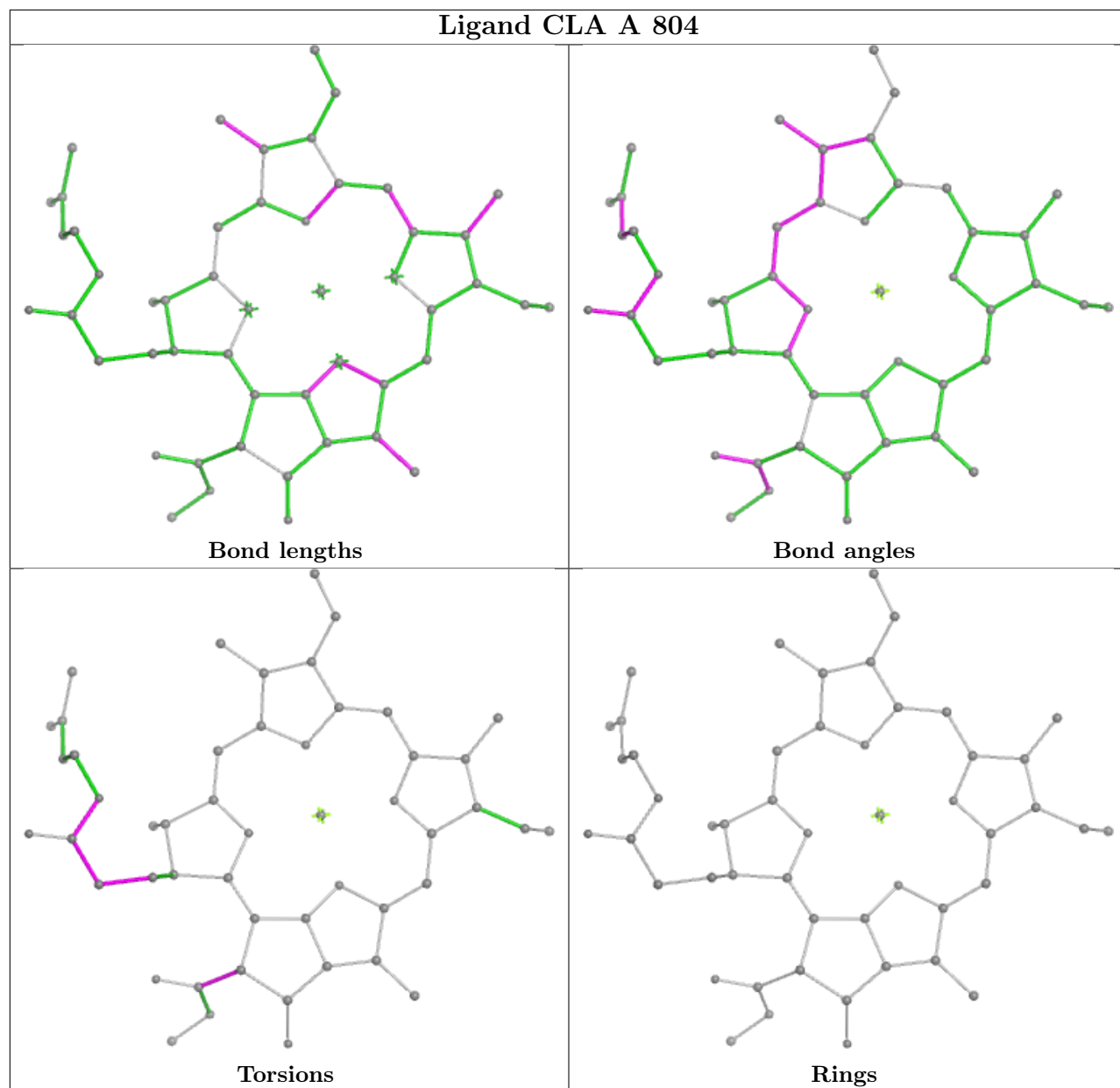


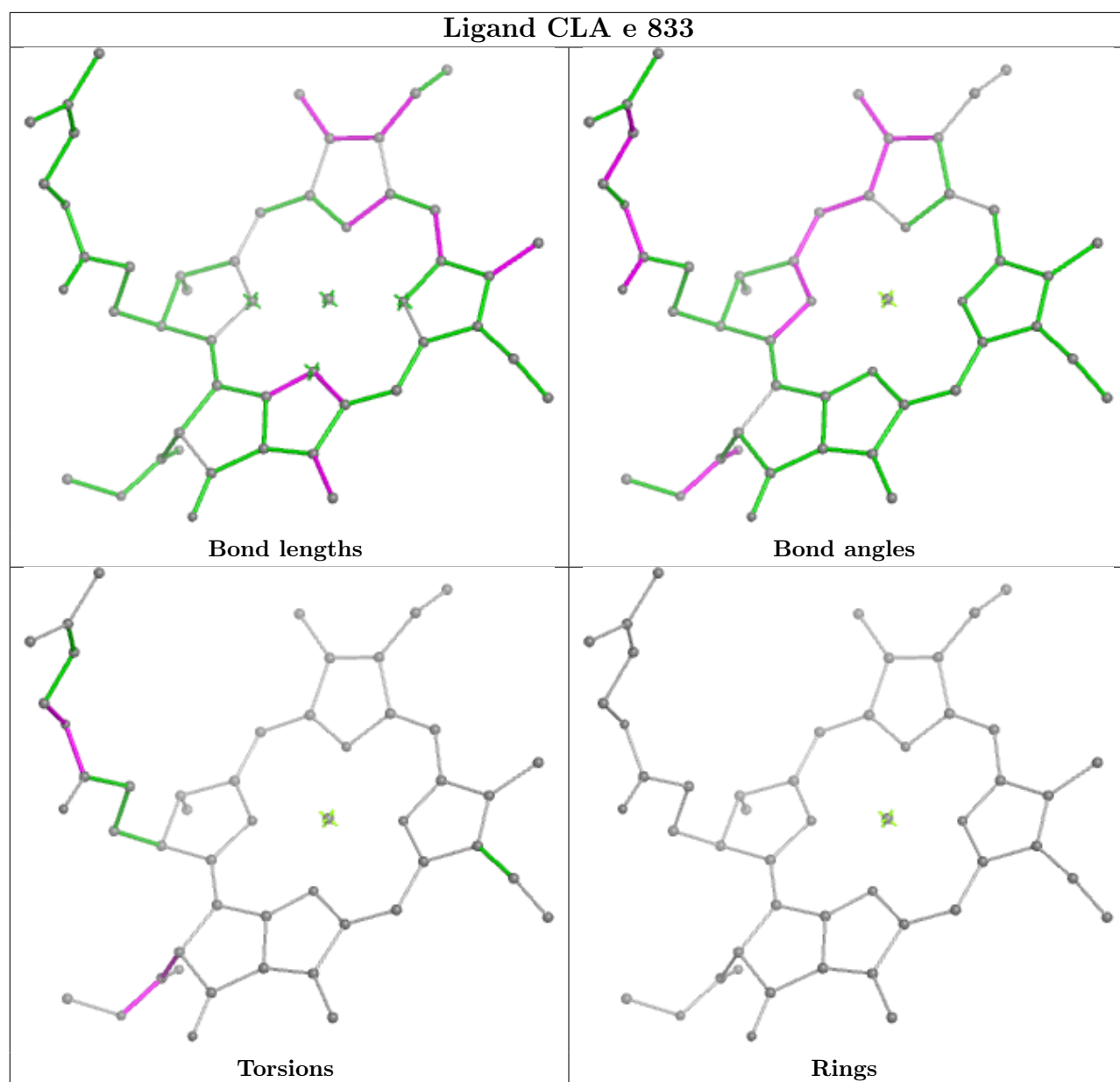
Rings



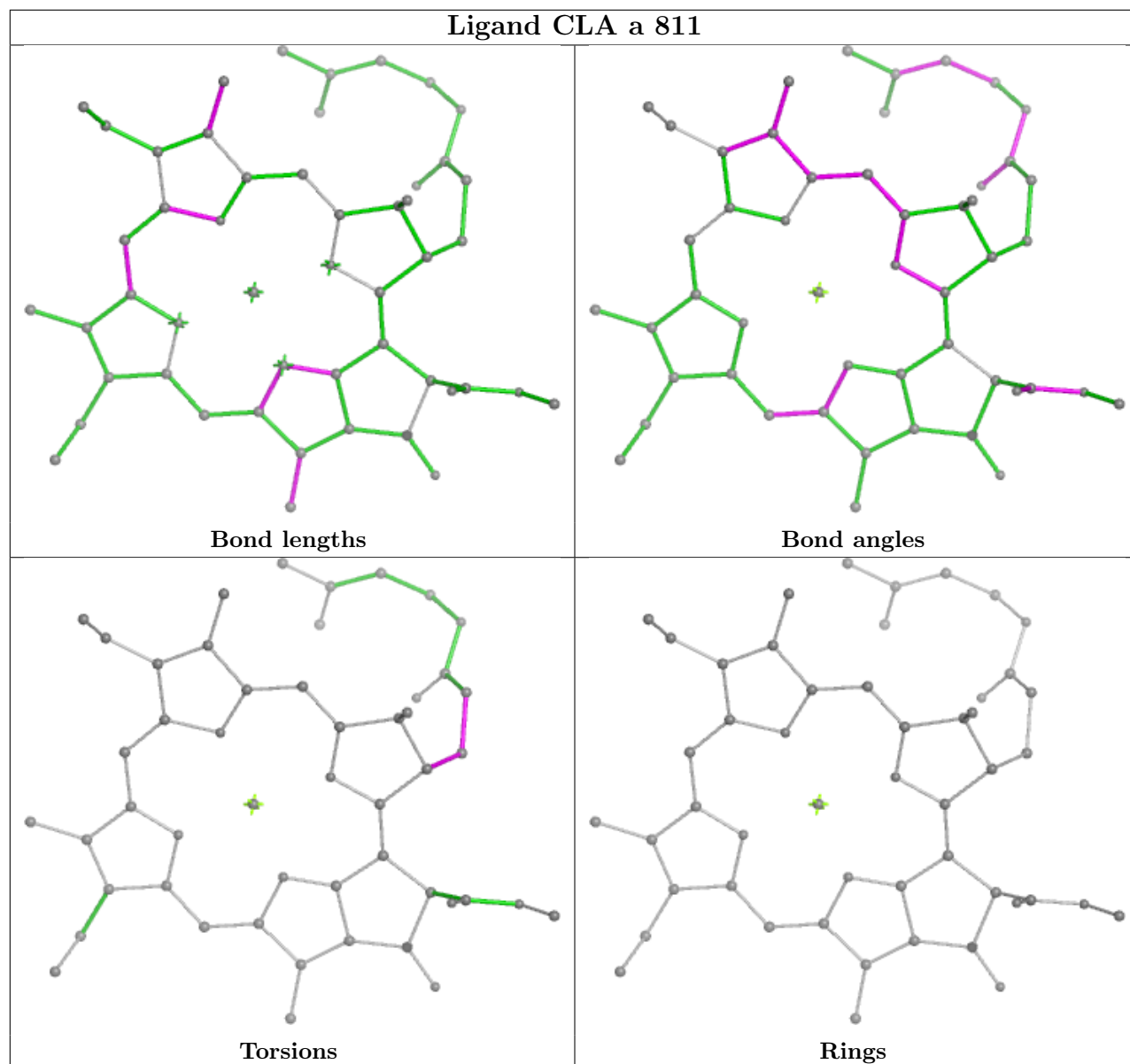




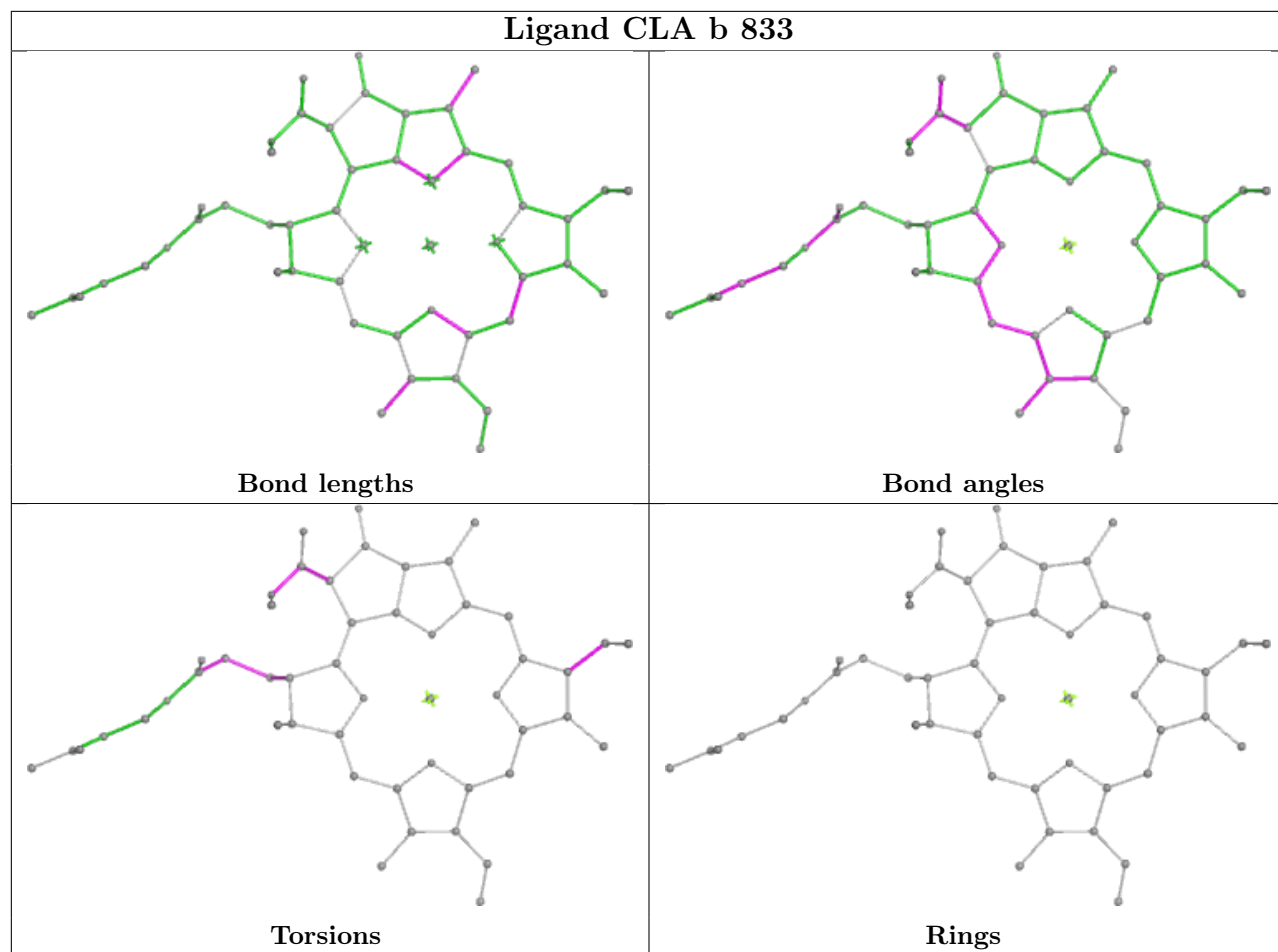




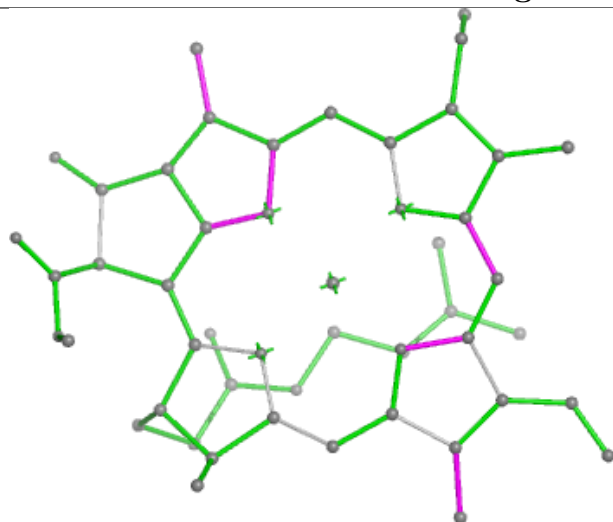
## Ligand CLA a 811



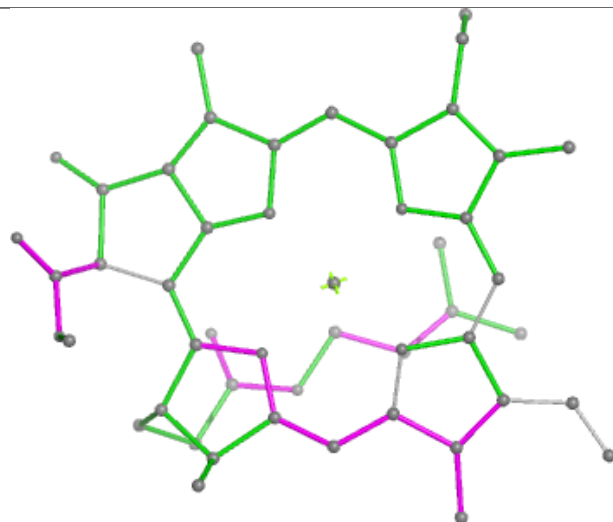
## Ligand CLA b 833



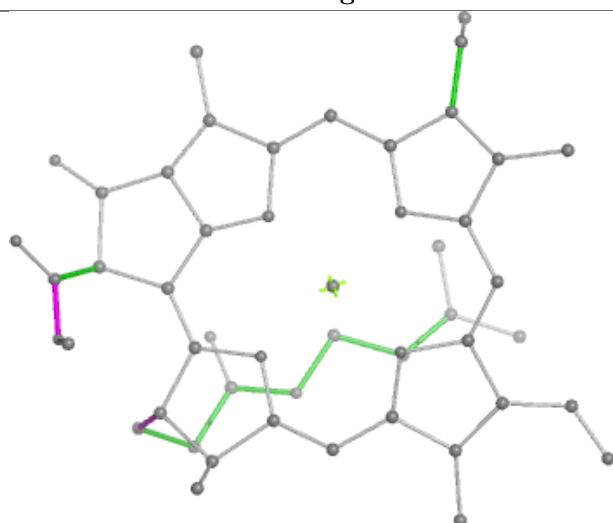
## Ligand CLA B 810



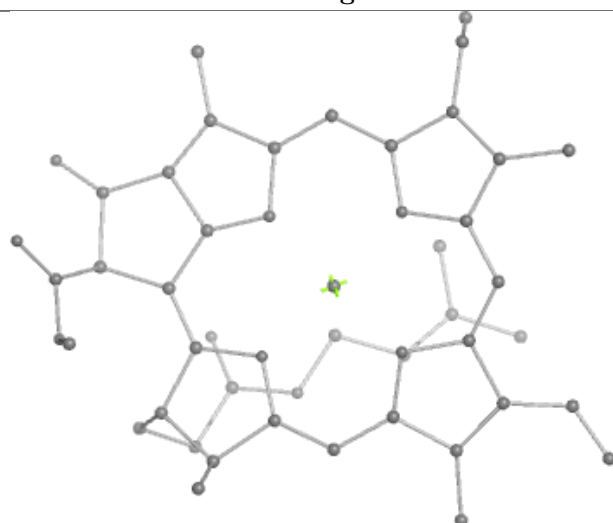
Bond lengths



Bond angles

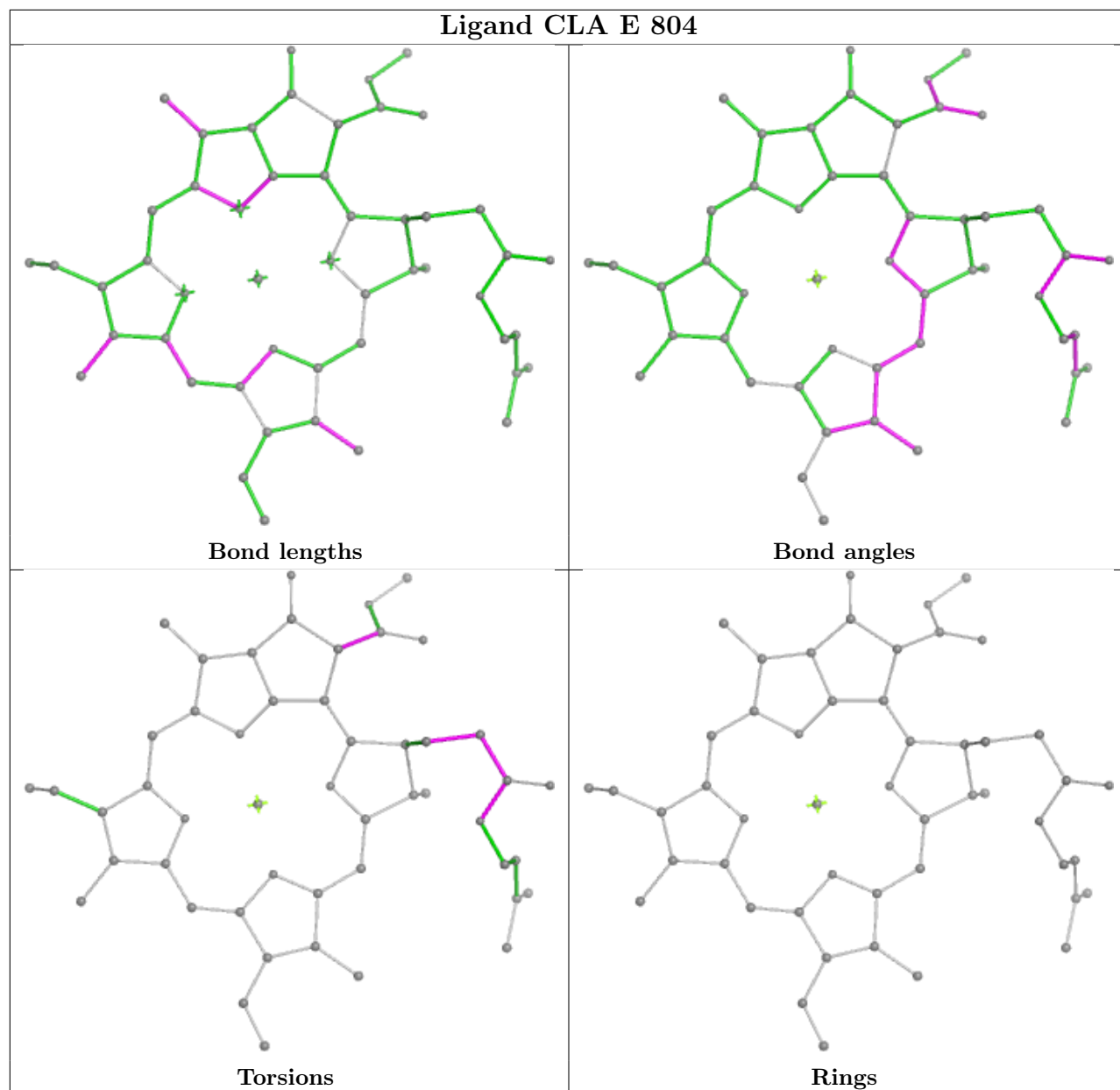


Torsions

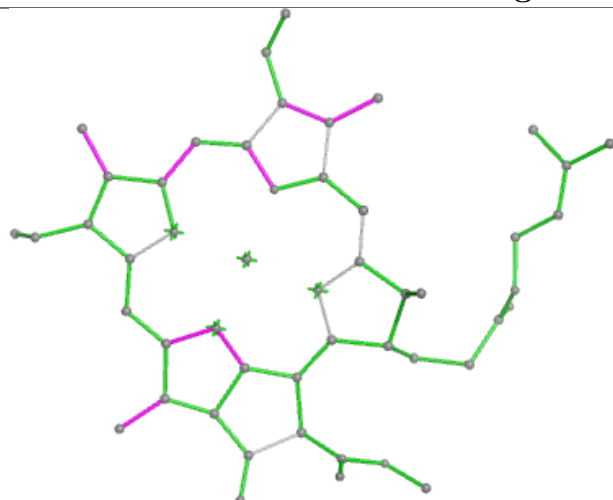


Rings

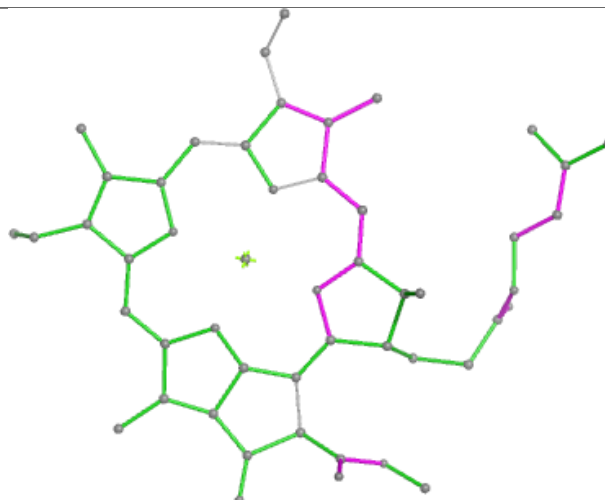
## Ligand CLA E 804



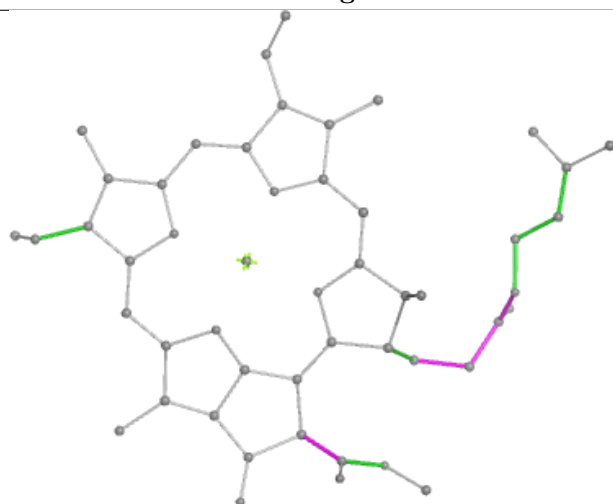
## Ligand CLA B 805



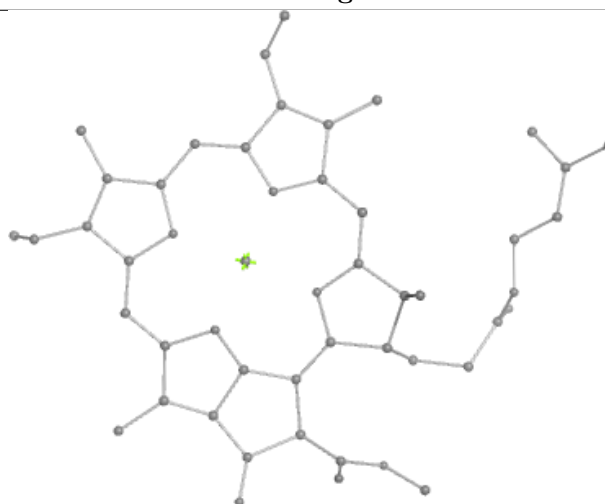
Bond lengths



Bond angles

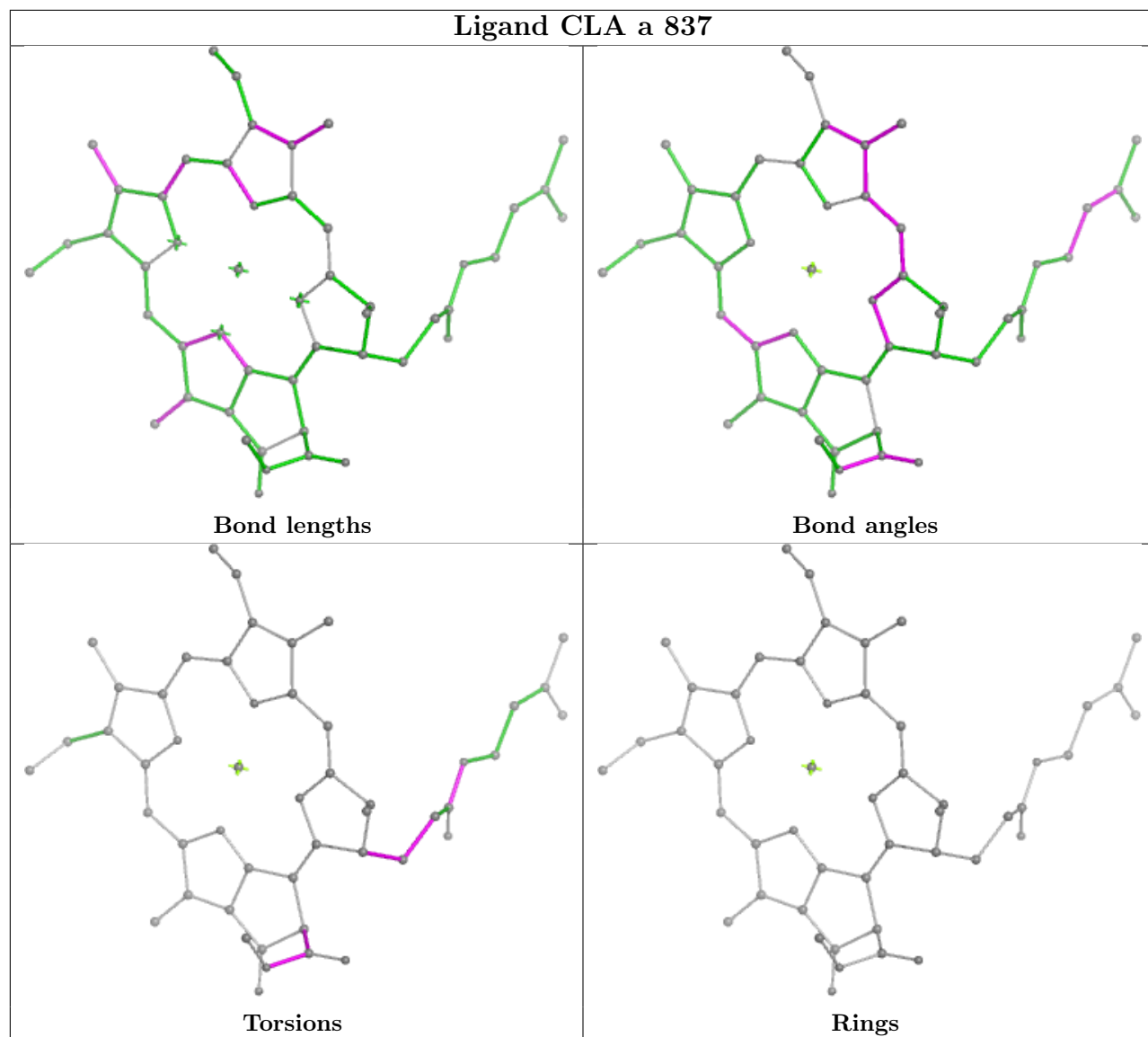


Torsions



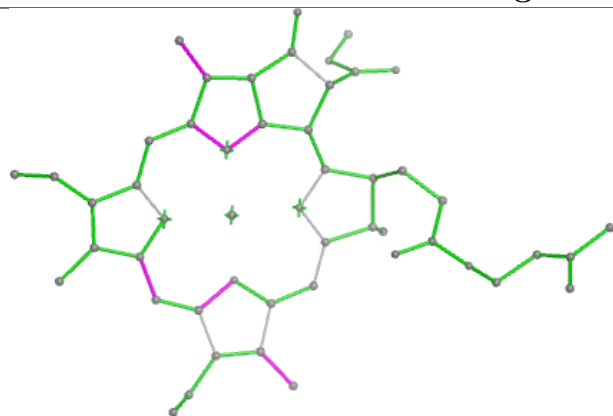
Rings

## Ligand CLA a 837

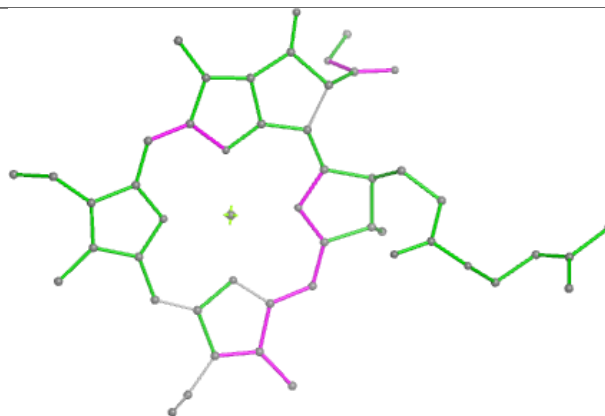




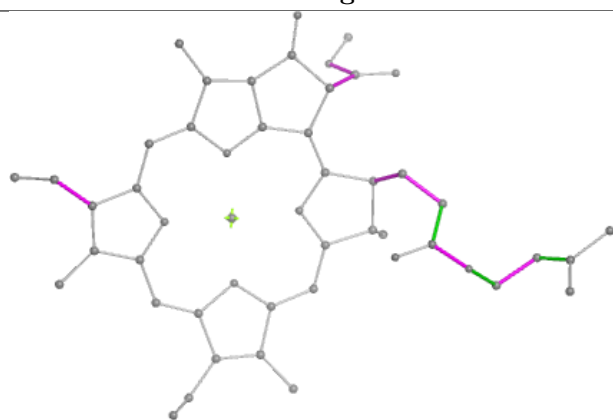
## Ligand CLA B 812



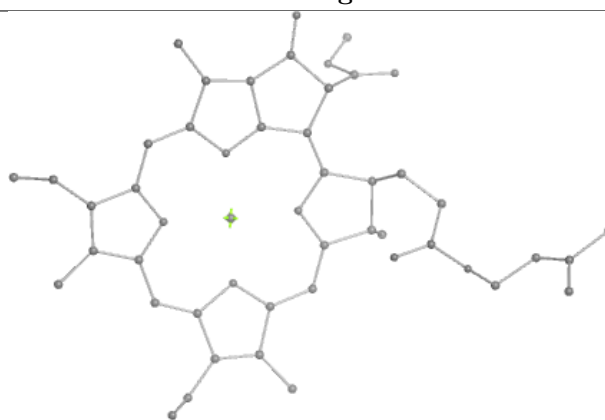
Bond lengths



Bond angles

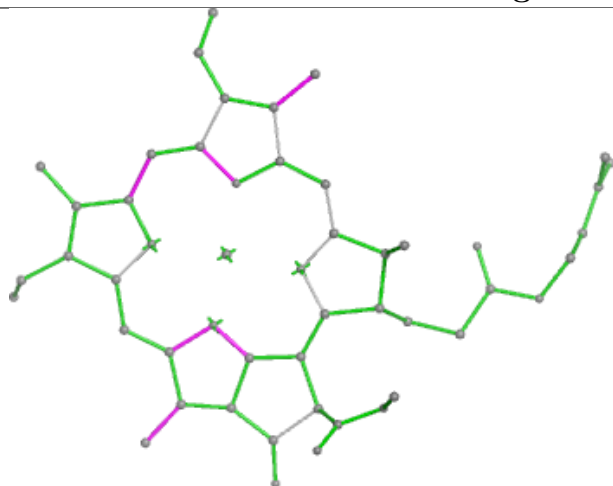


Torsions

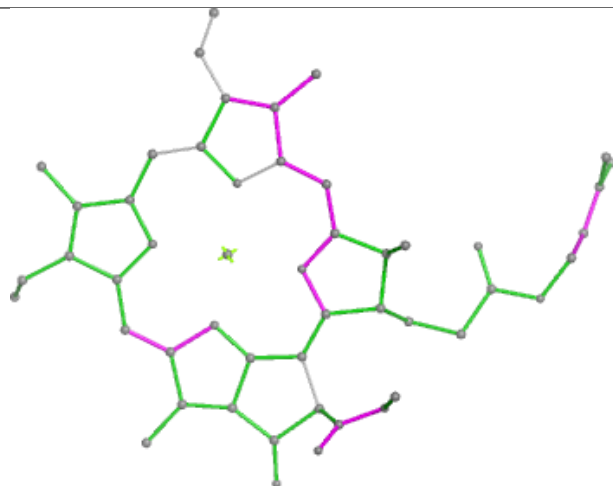


Rings

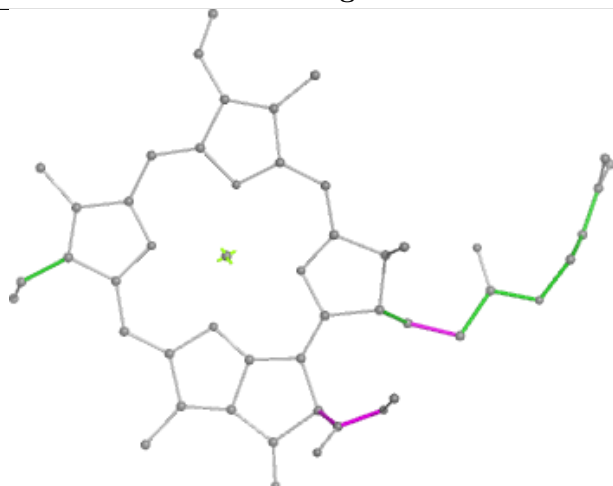
## Ligand CLA G 814



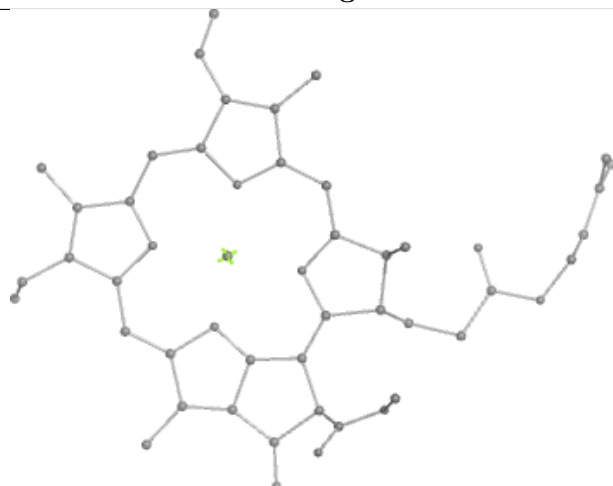
Bond lengths



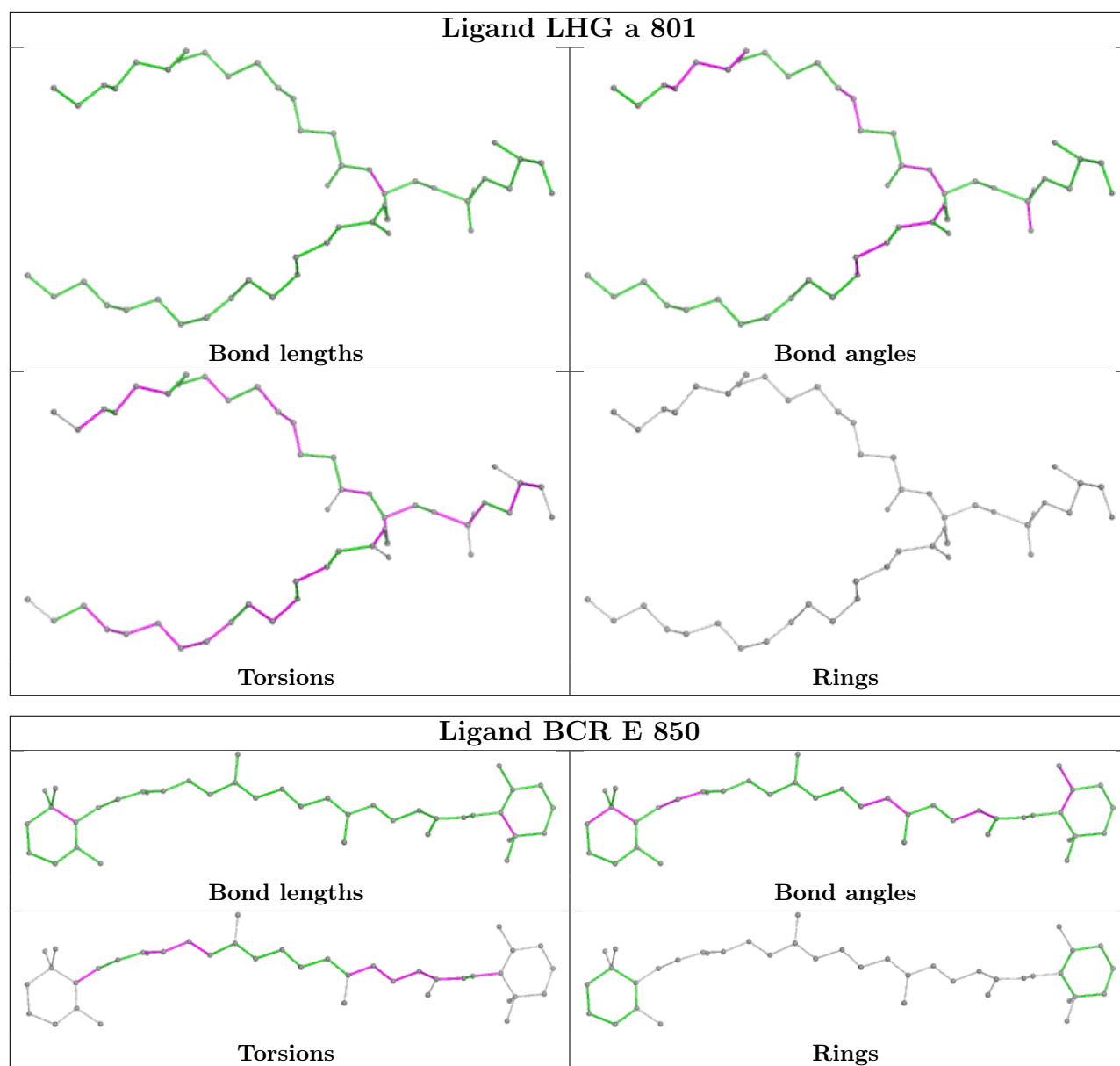
Bond angles



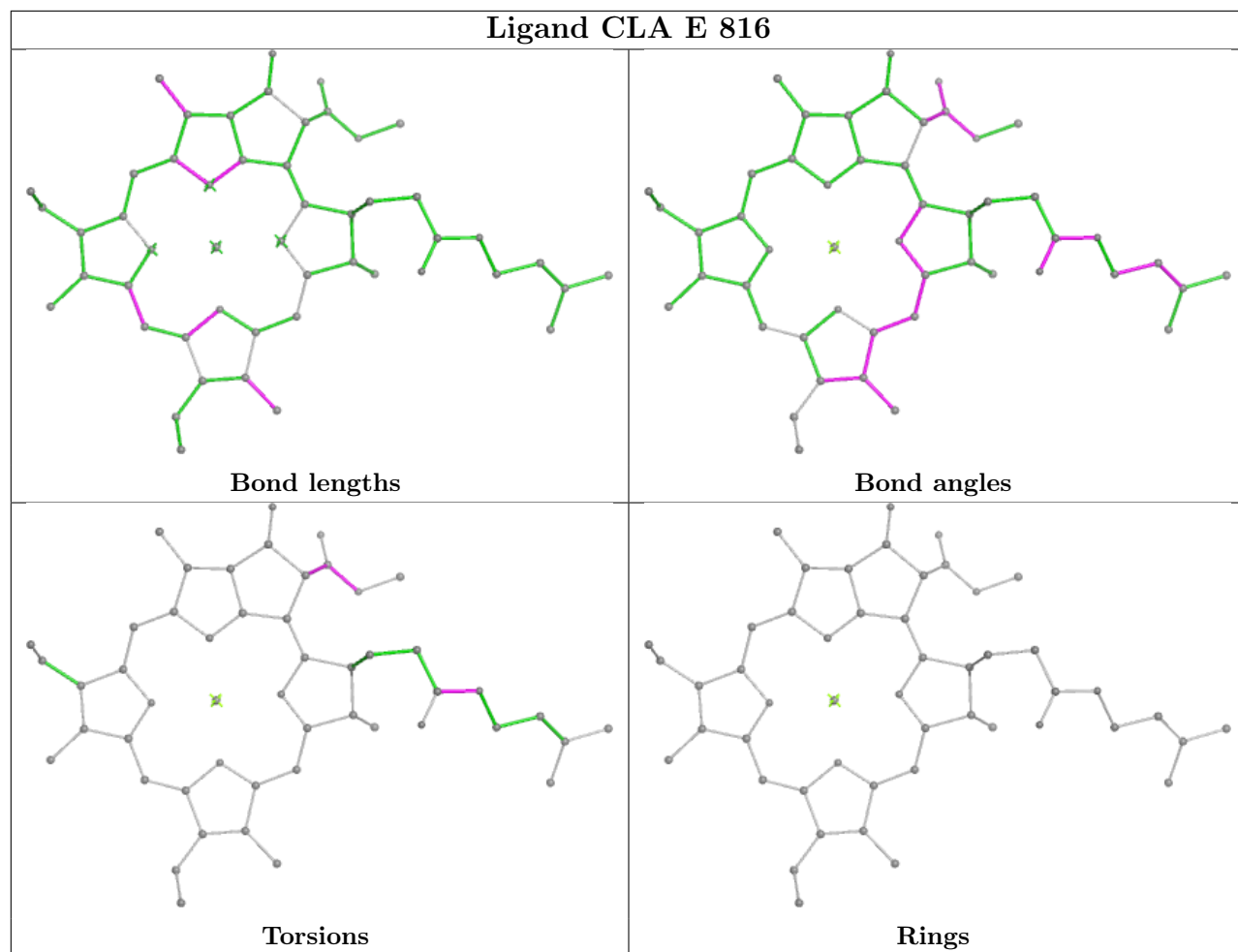
Torsions

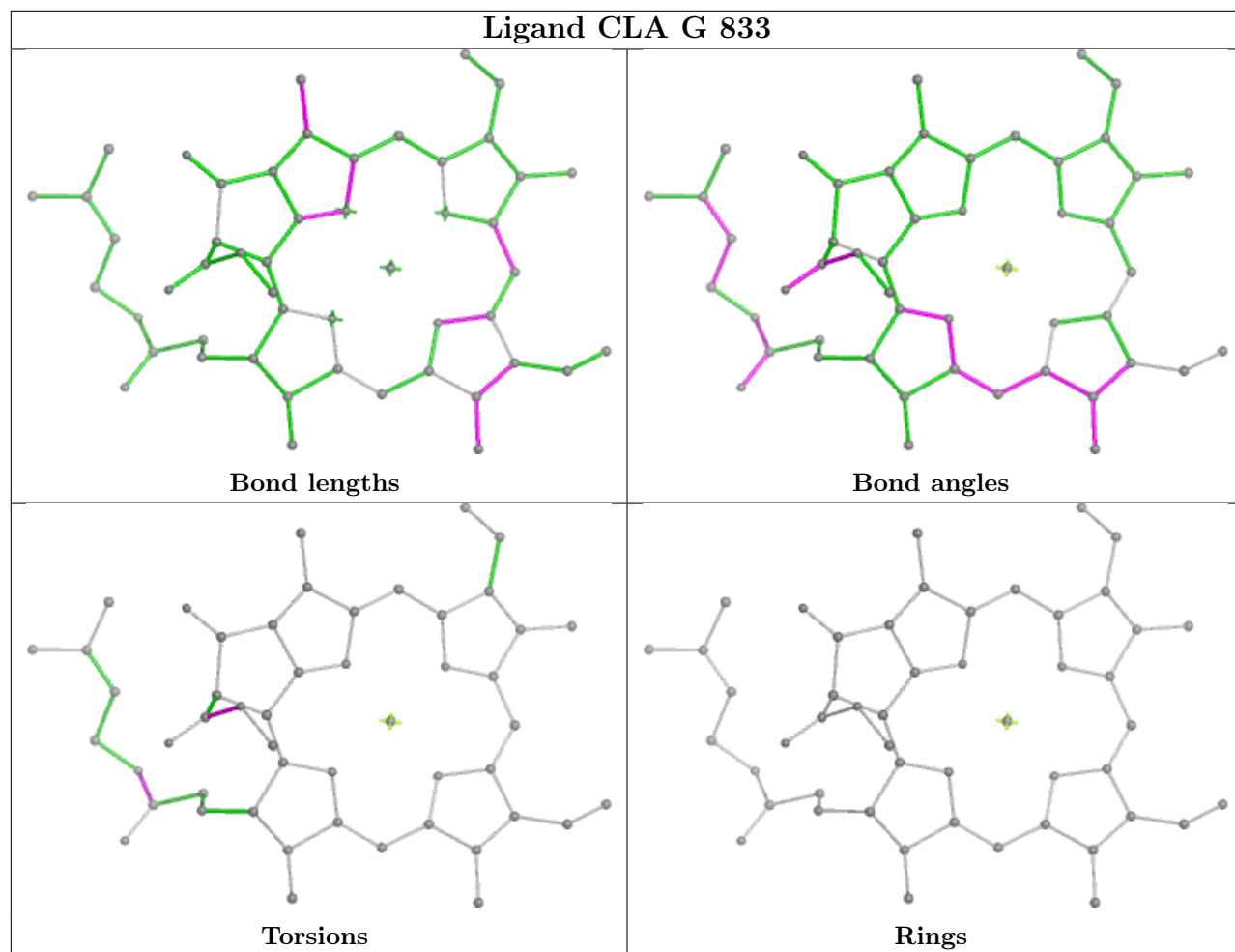


Rings

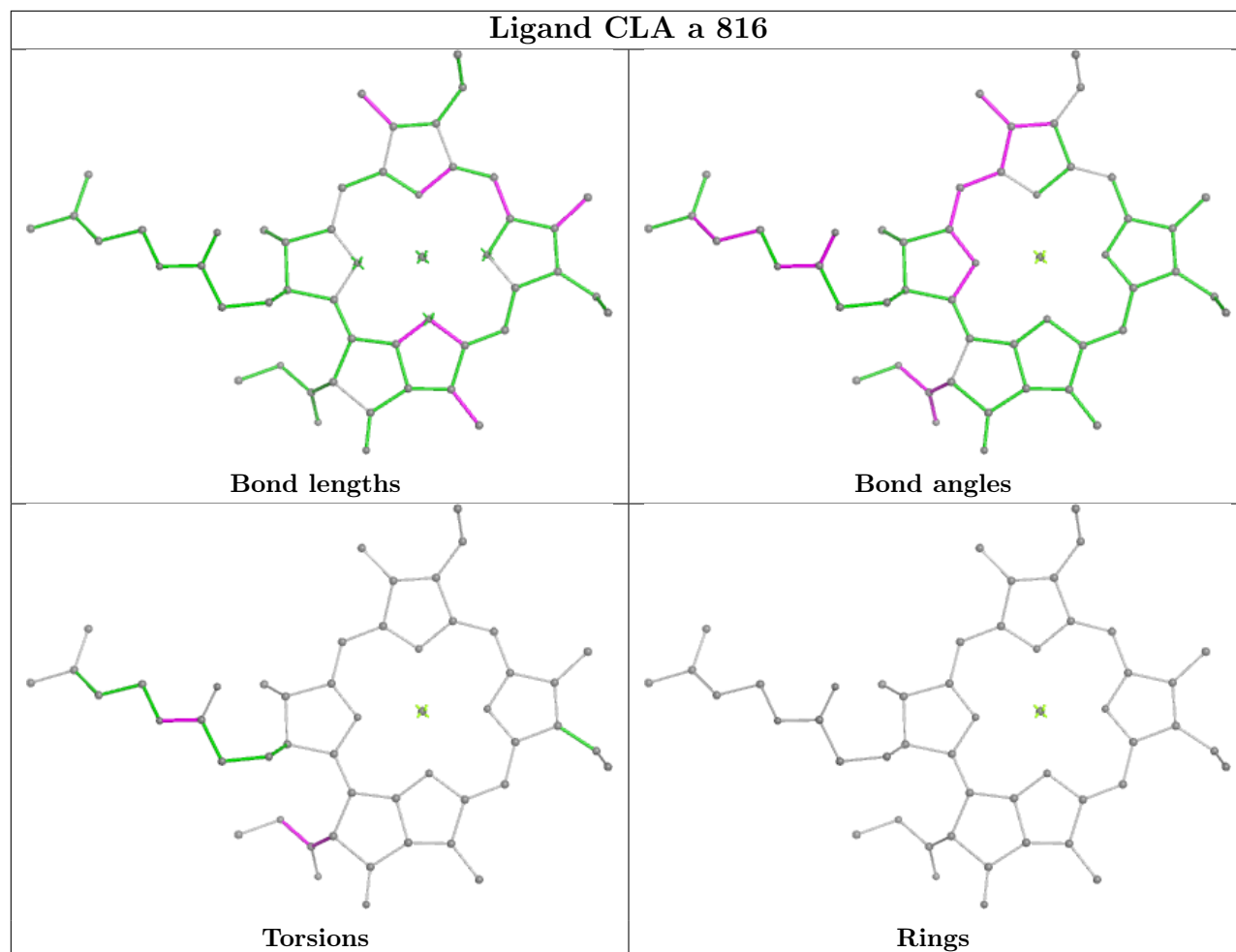


## Ligand CLA E 816

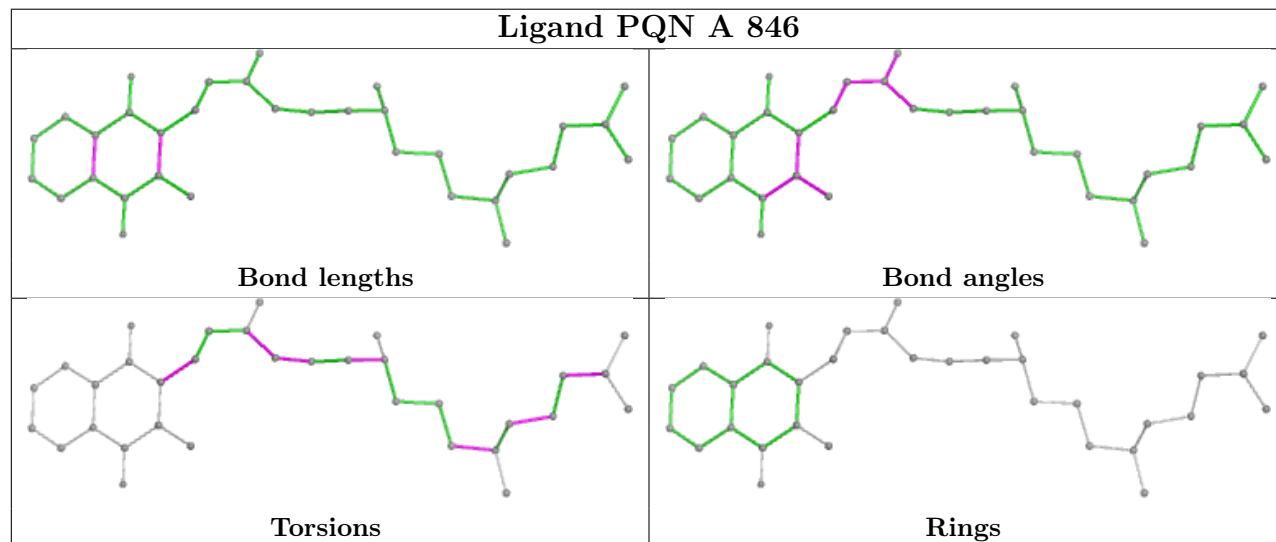




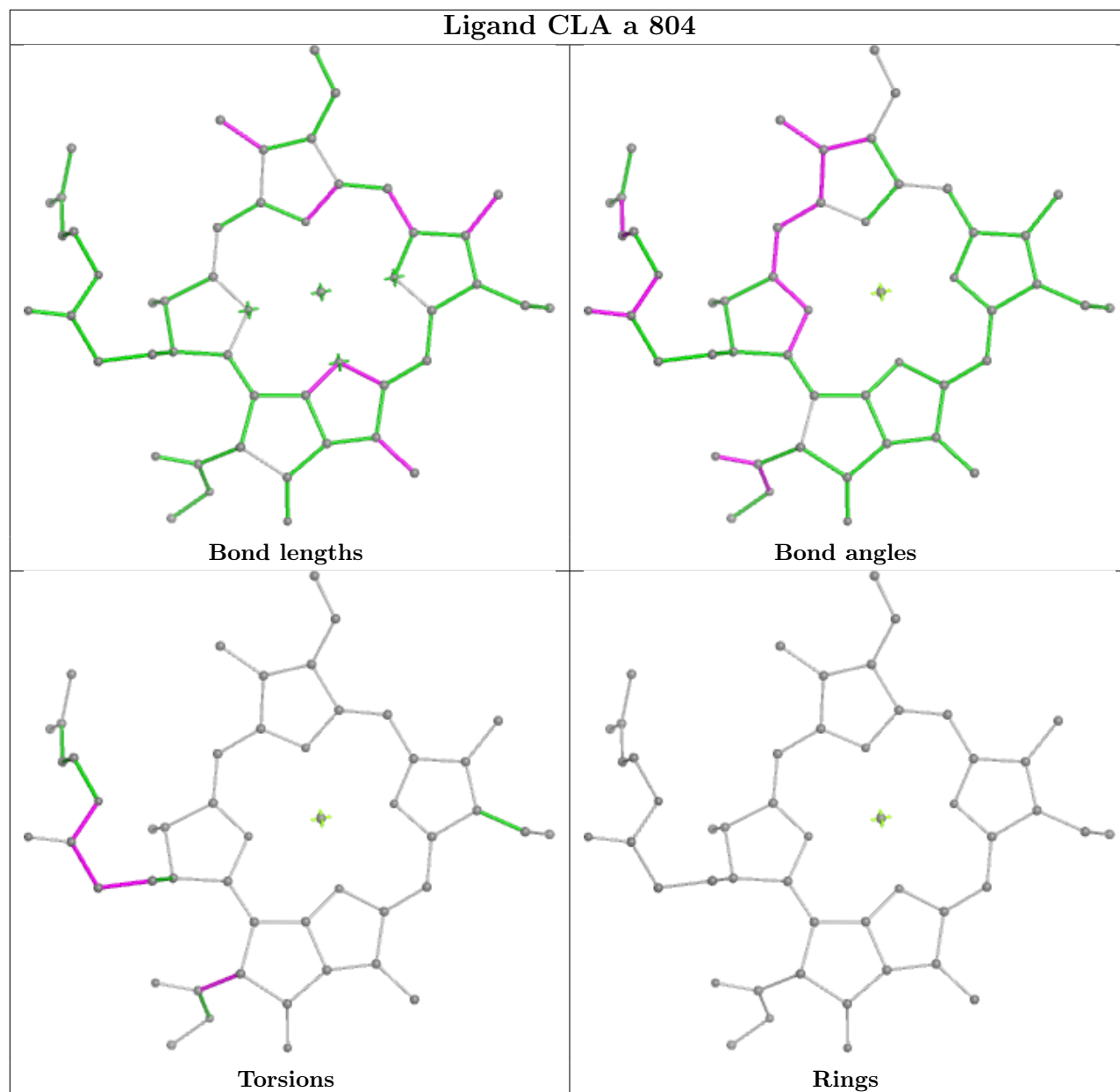
## Ligand CLA a 816



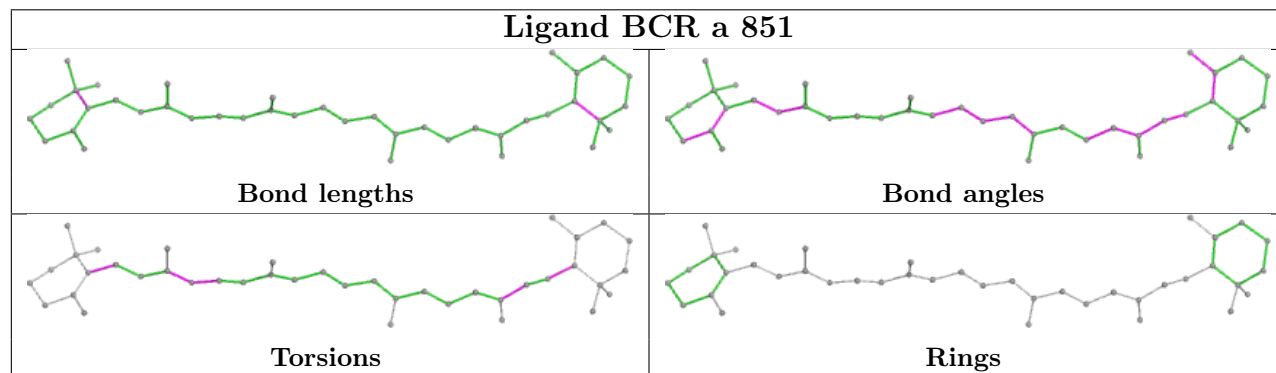
## Ligand PQN A 846



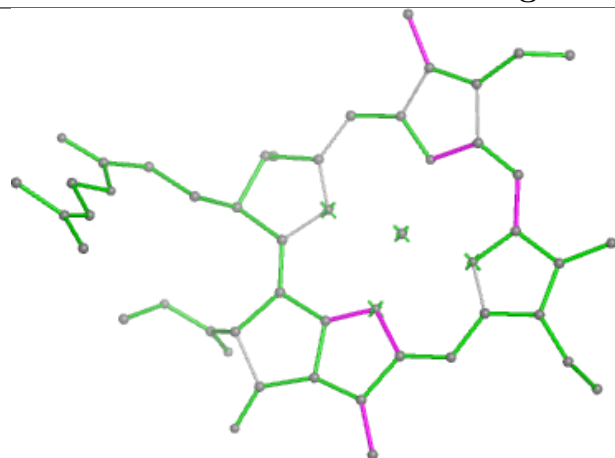
## Ligand CLA a 804



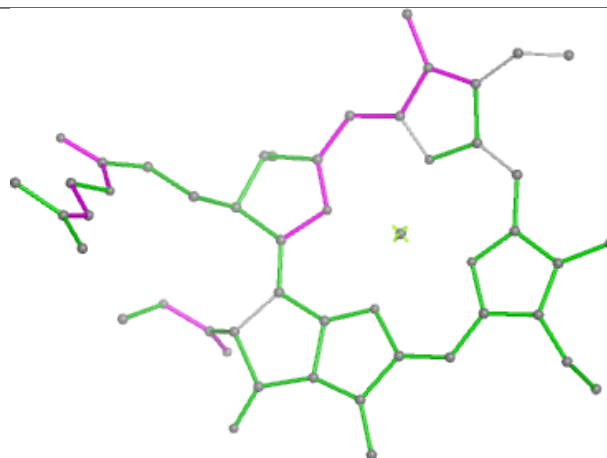
## Ligand BCR a 851



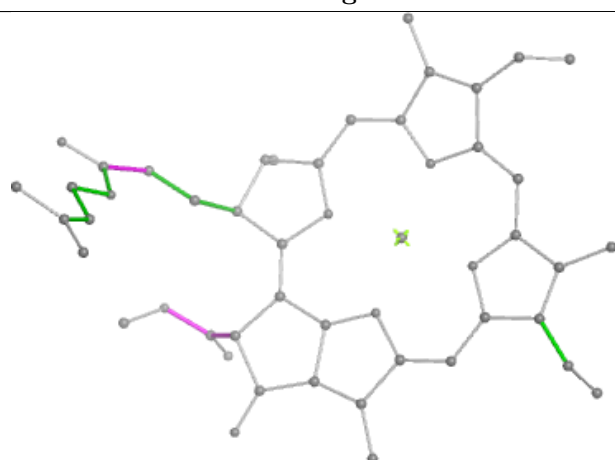
## Ligand CLA b 803



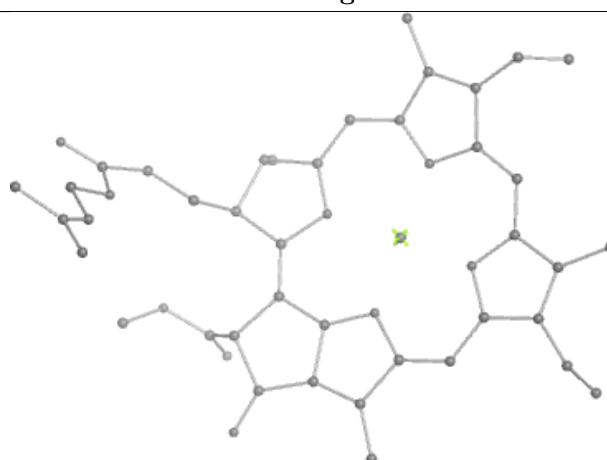
Bond lengths



Bond angles



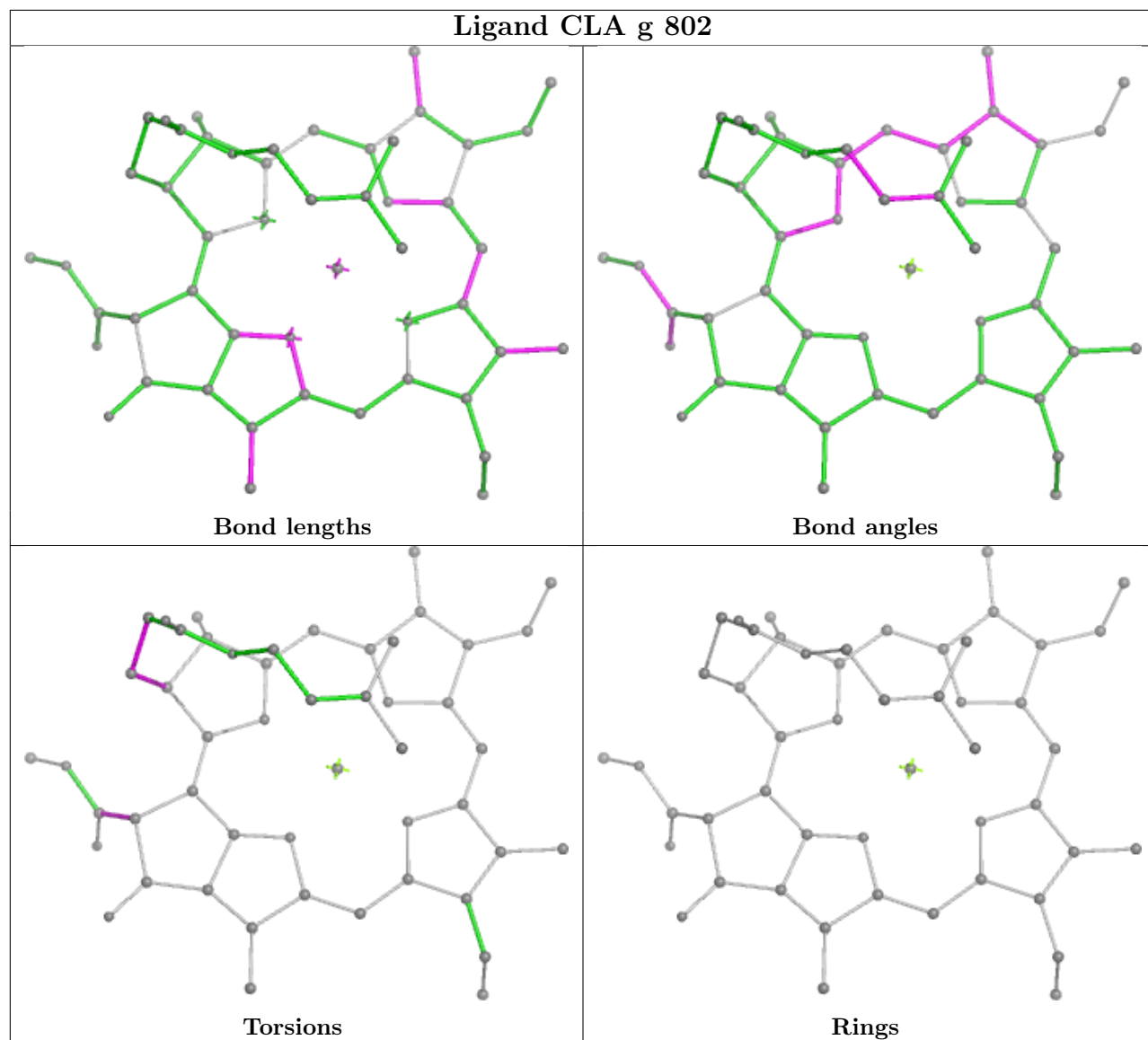
Torsions



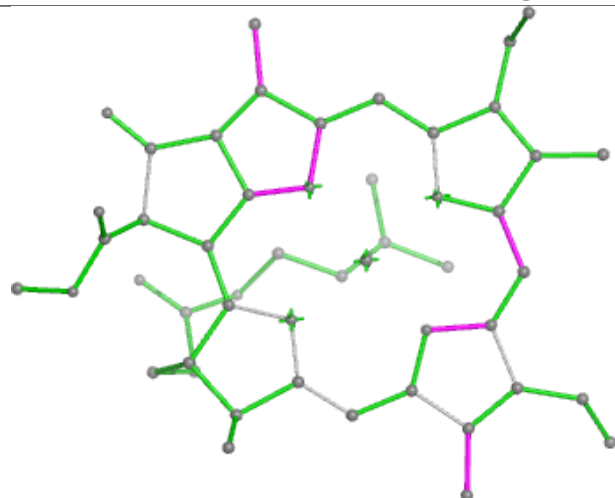
Rings



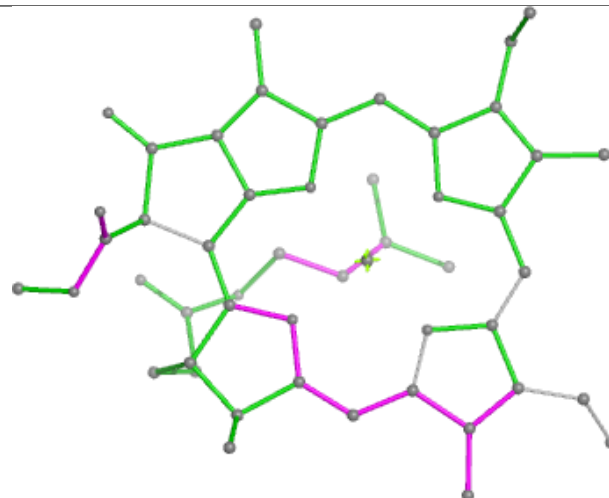
## Ligand CLA g 802



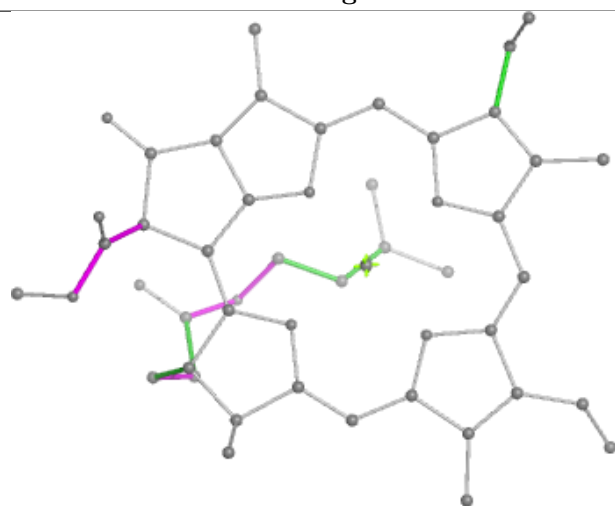
## Ligand CLA E 815



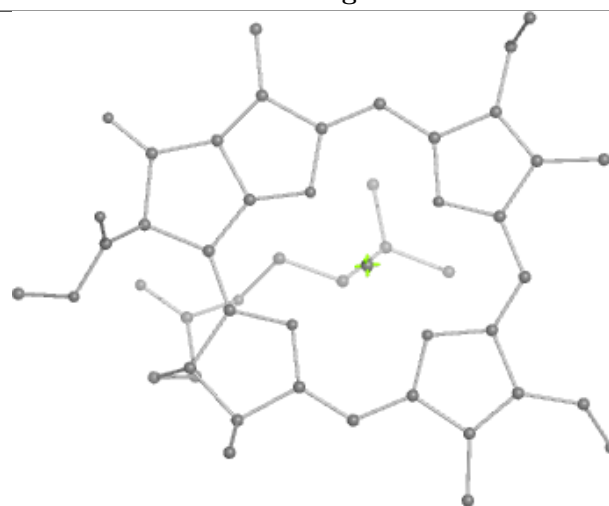
Bond lengths



Bond angles

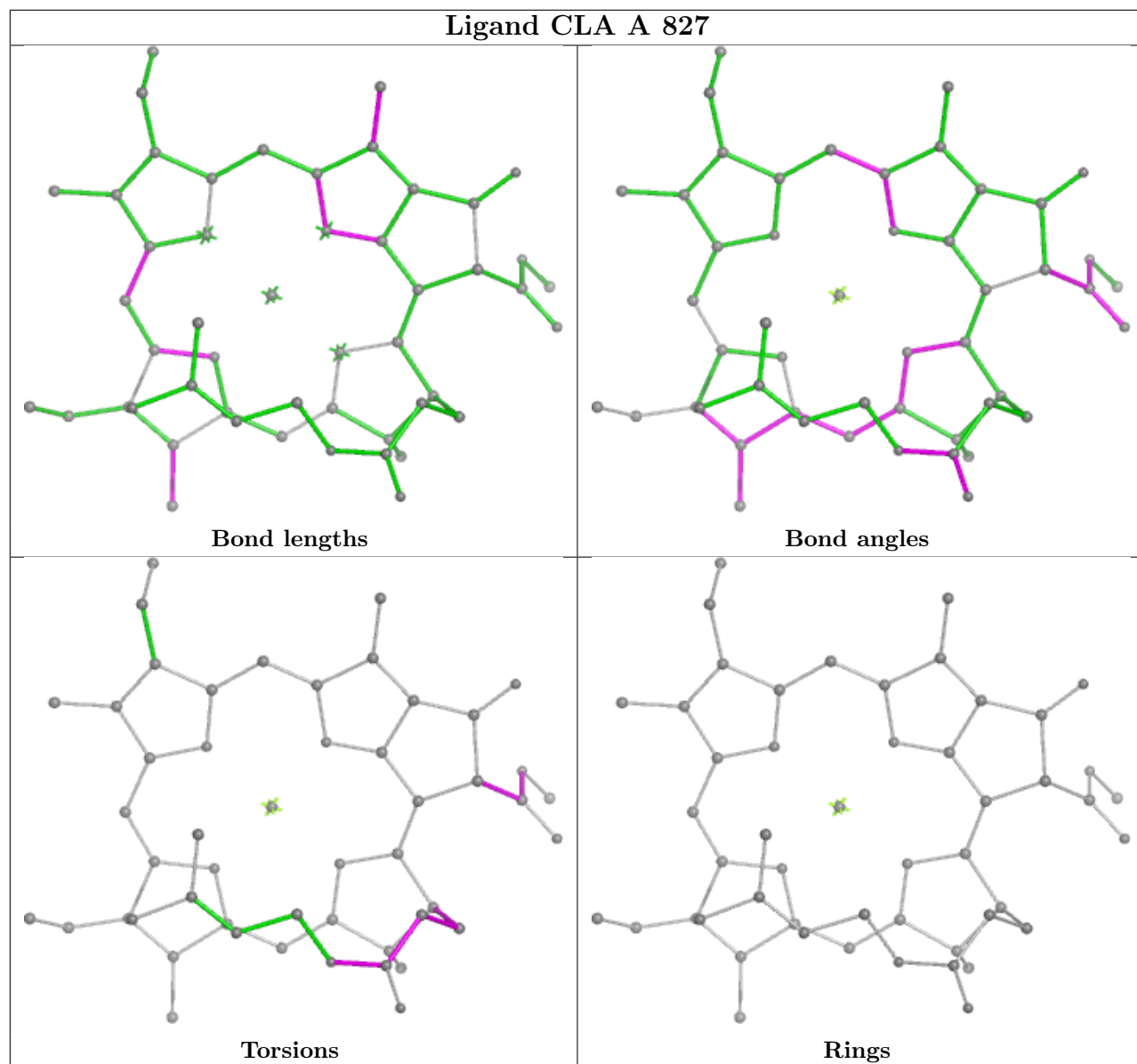


Torsions

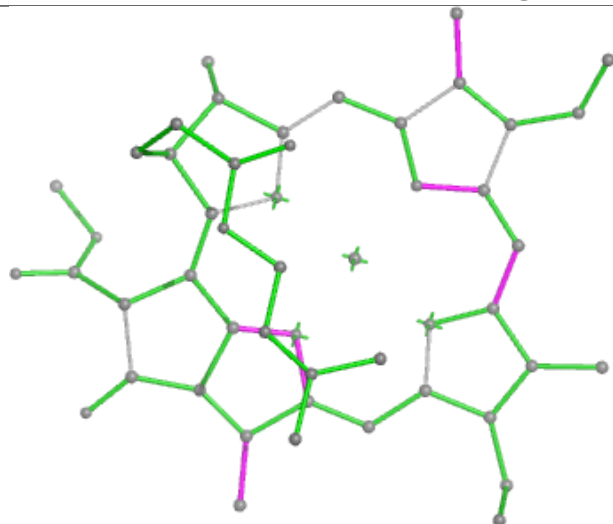


Rings

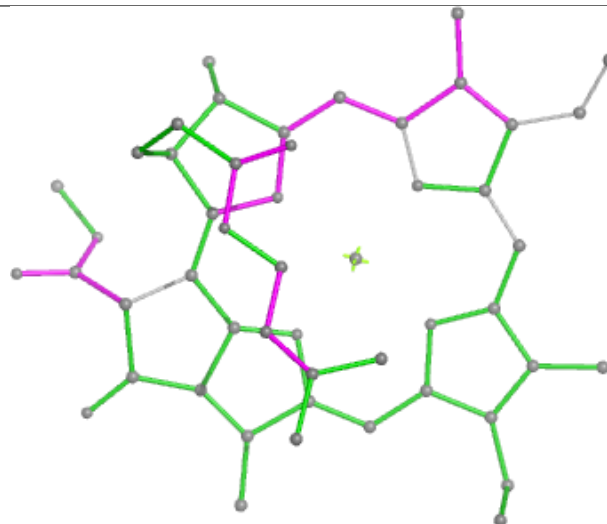
## Ligand CLA A 827



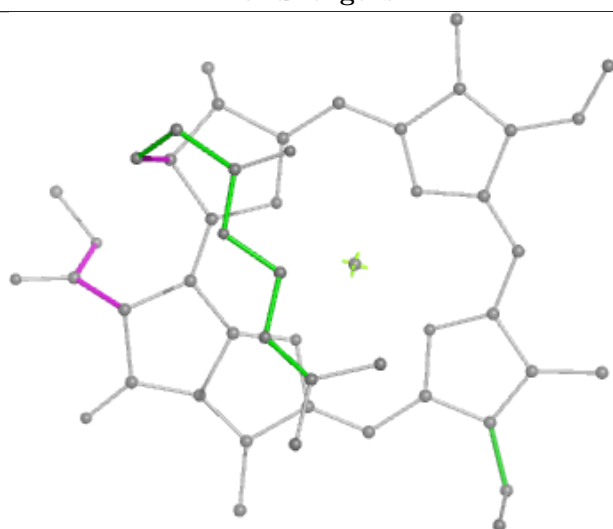
## Ligand CLA E 843



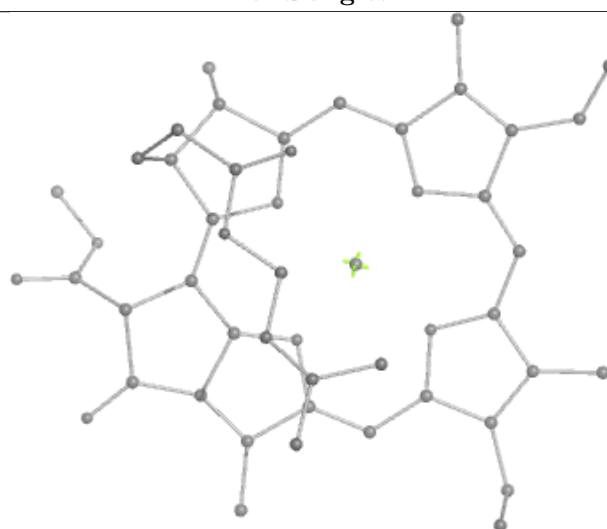
Bond lengths



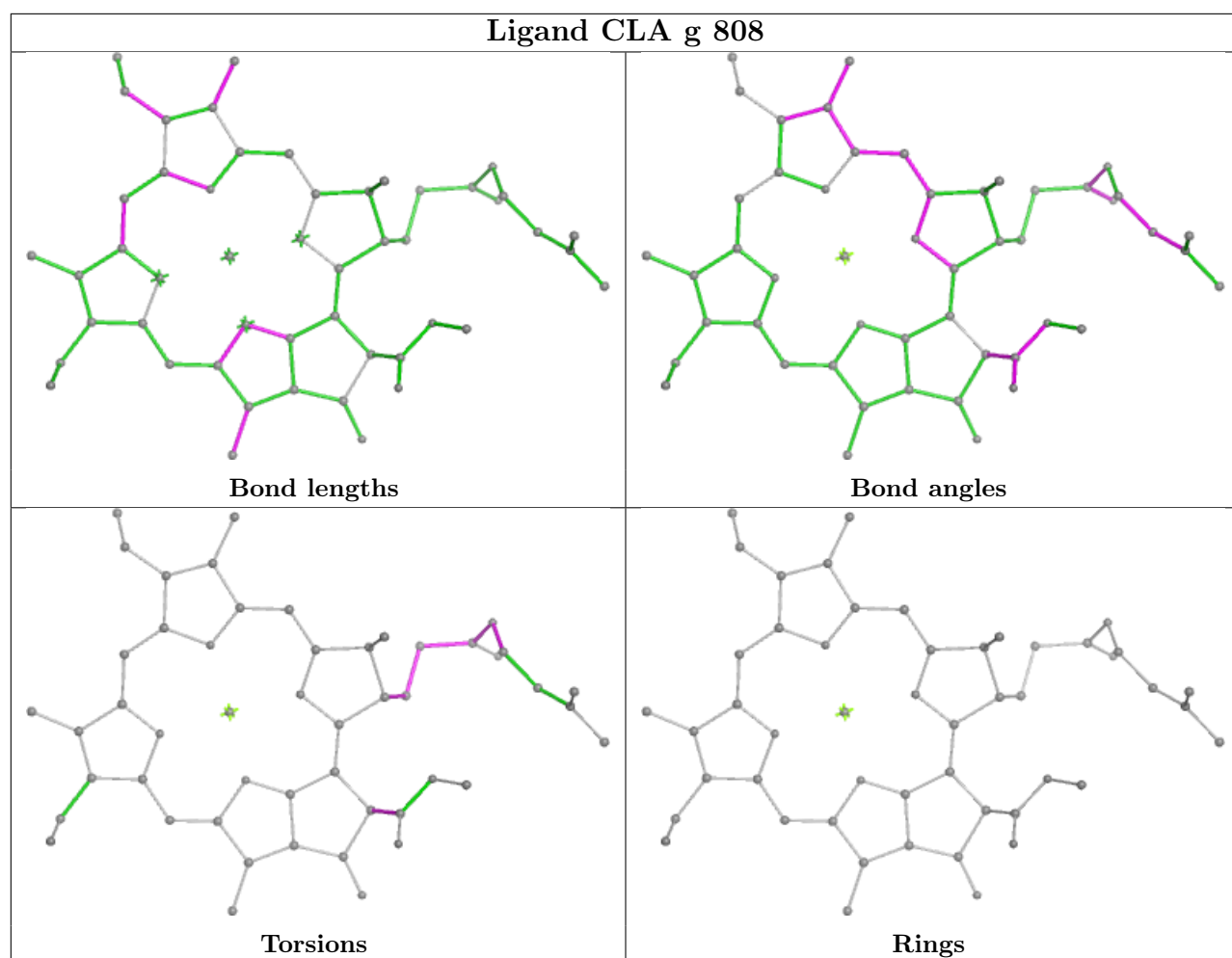
Bond angles



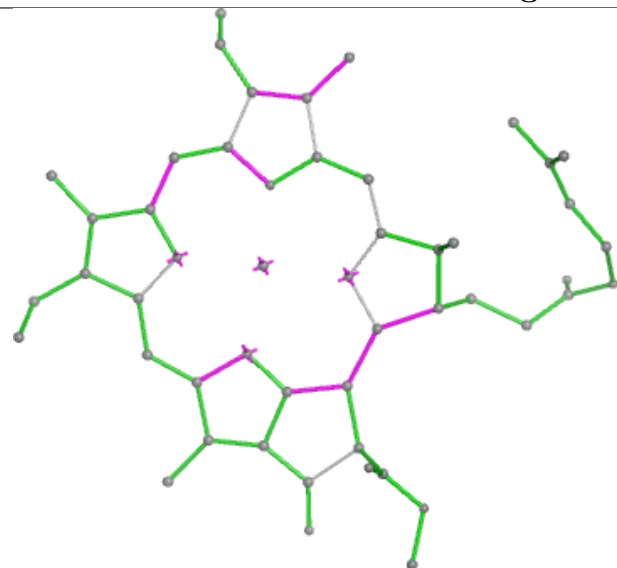
Torsions



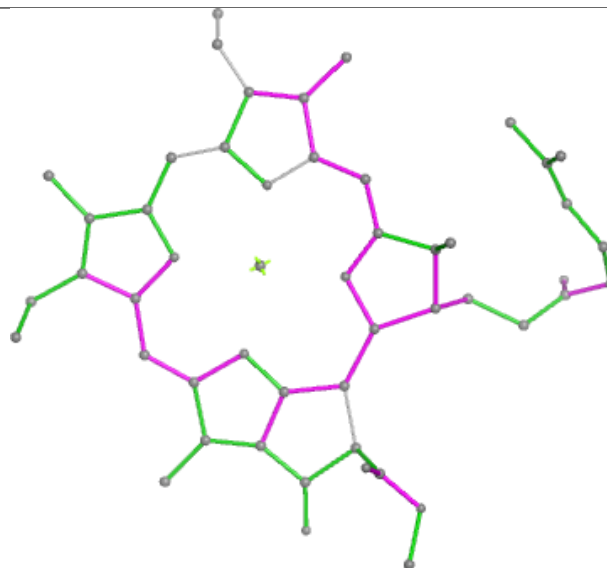
Rings



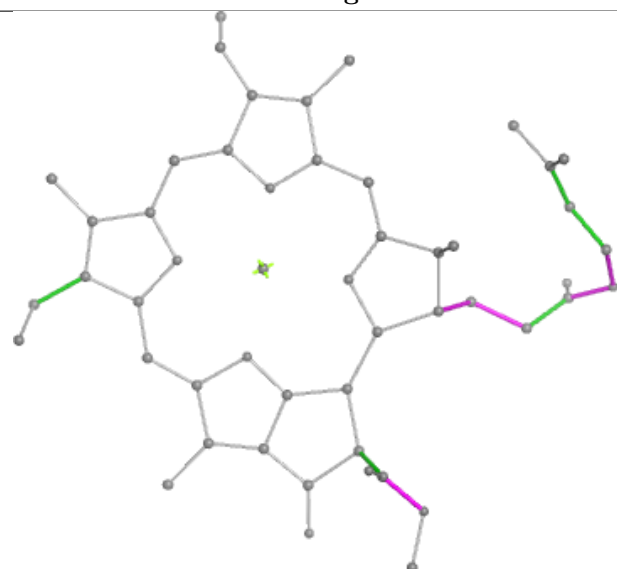
## Ligand CLA L 204



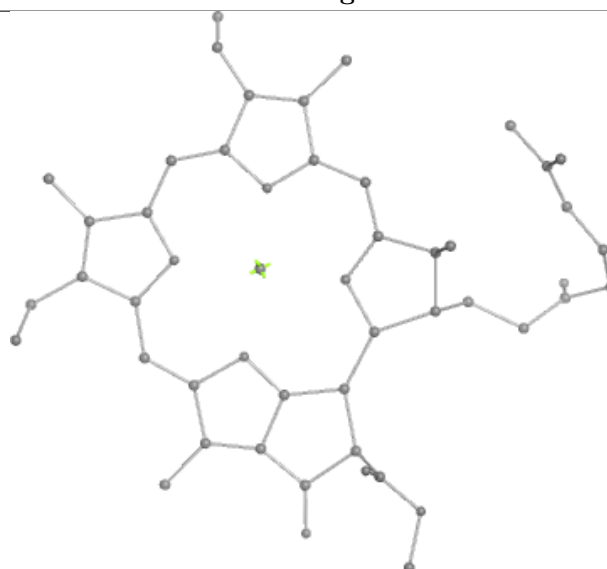
Bond lengths



Bond angles

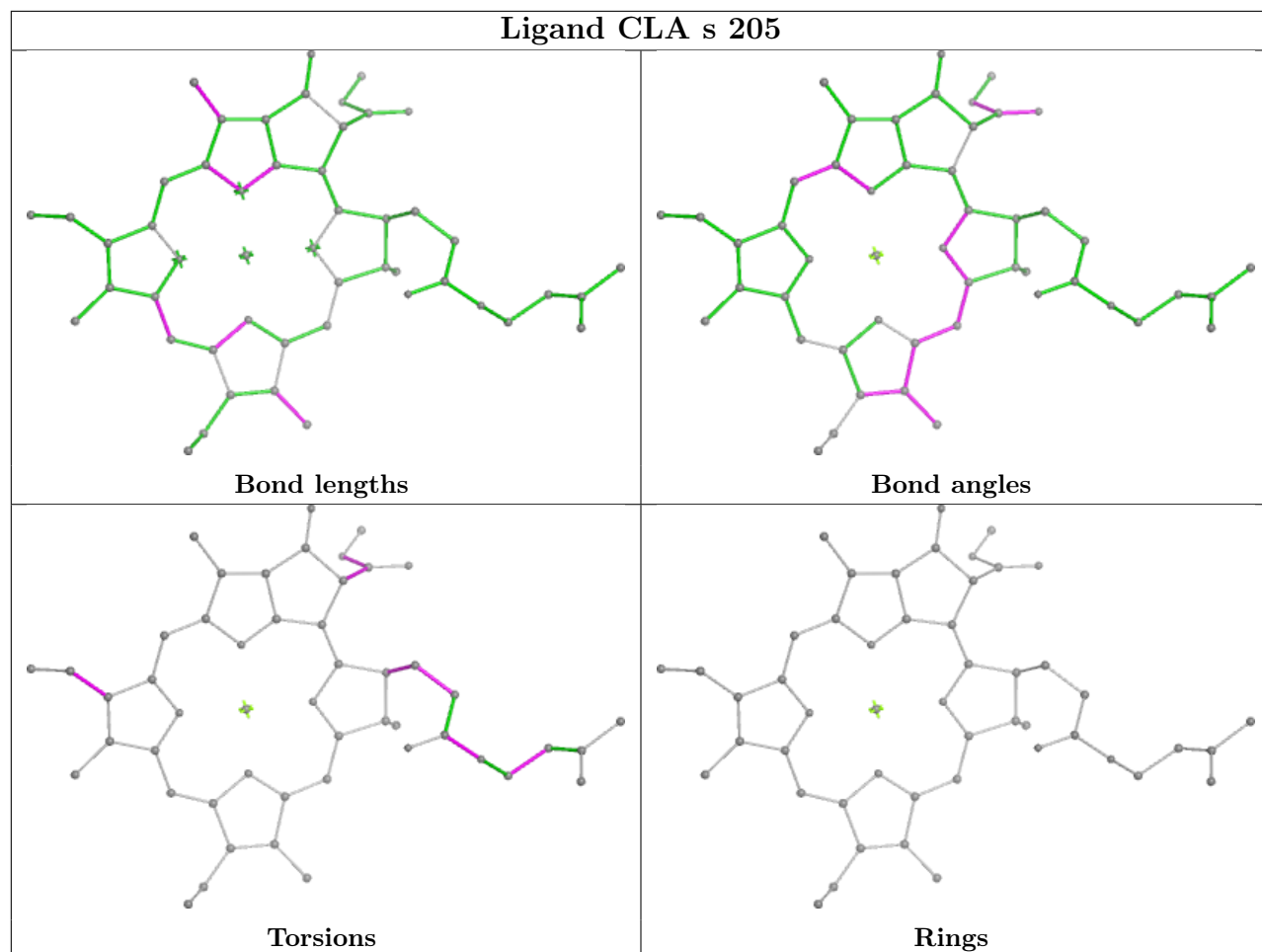


Torsions

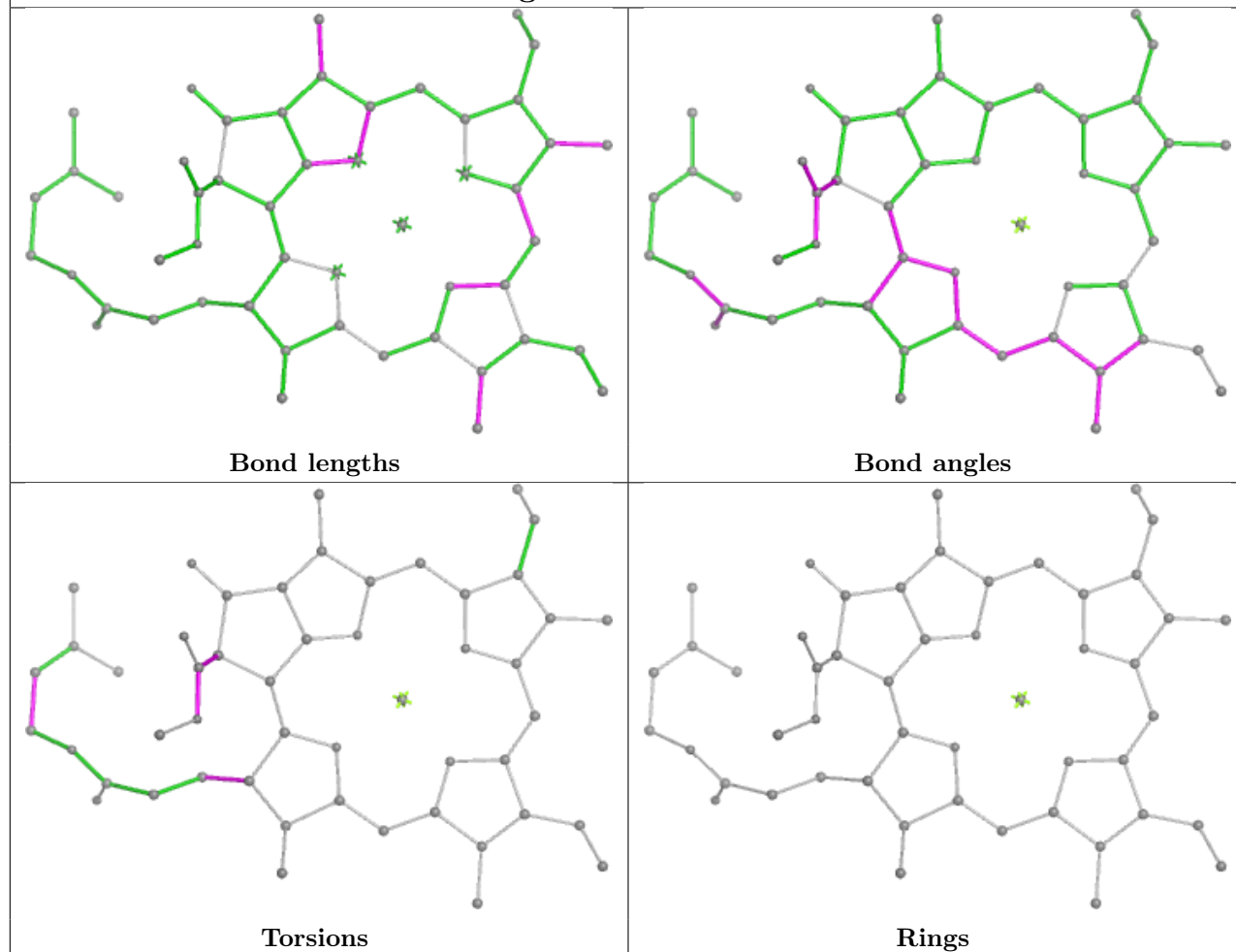


Rings

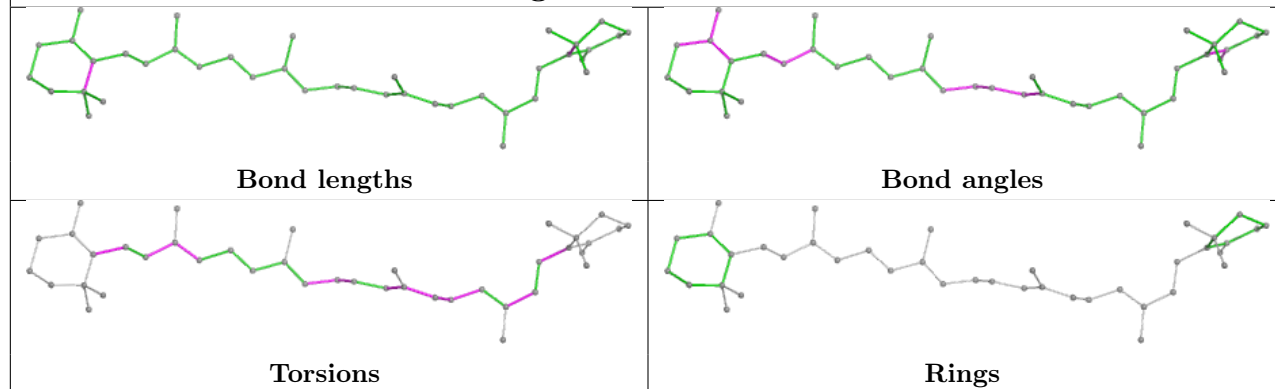
## Ligand CLA s 205



## Ligand CLA a 828

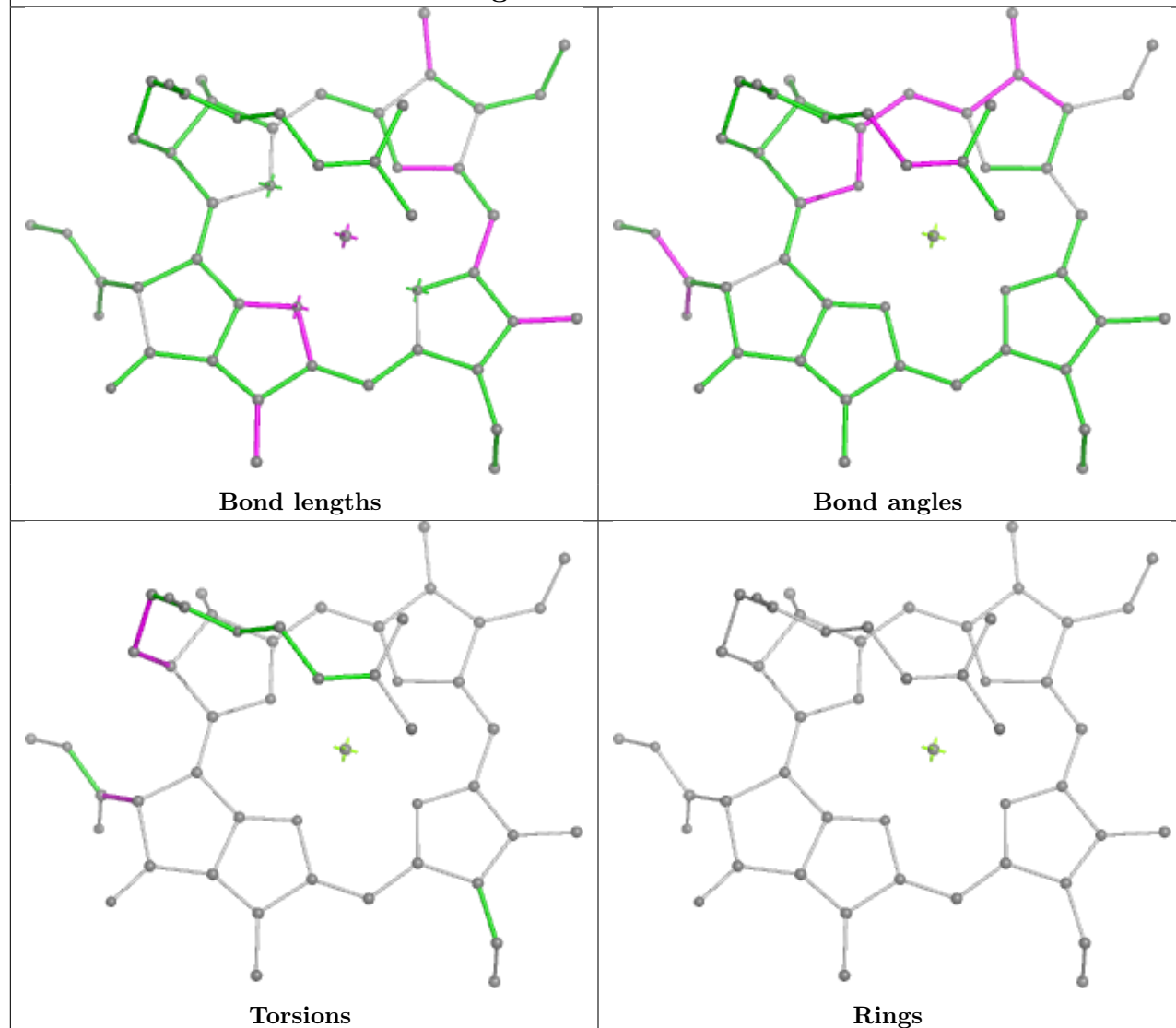


## Ligand BCR B 848

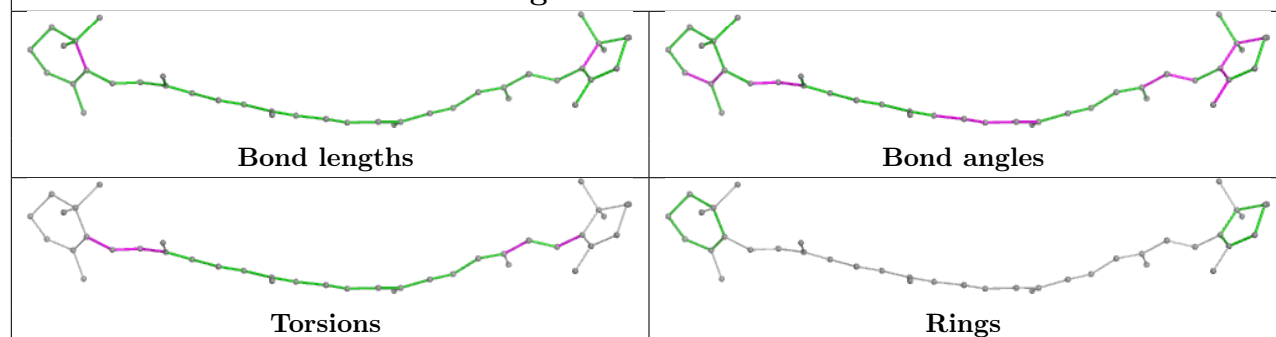




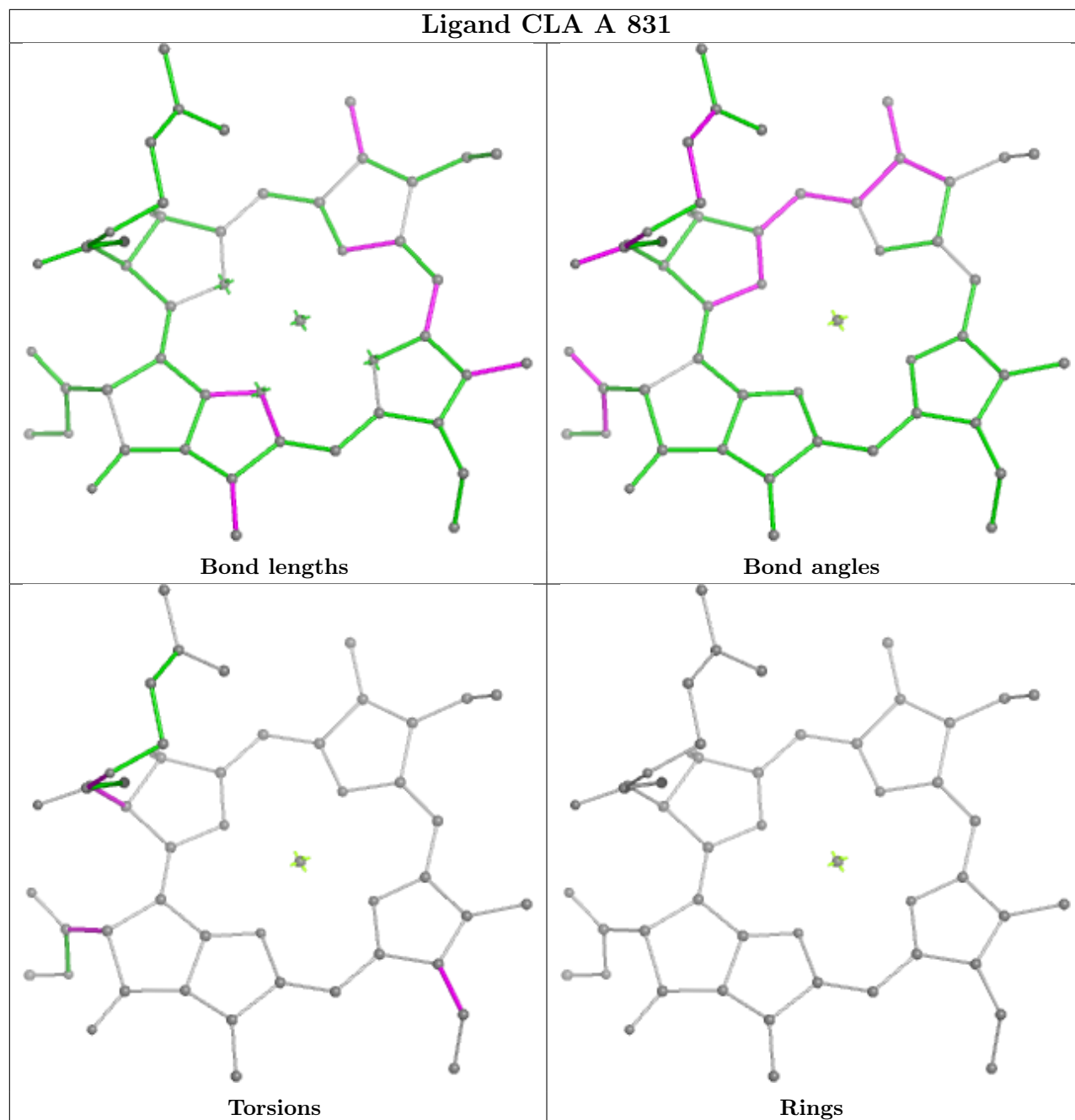
## Ligand CLA E 835



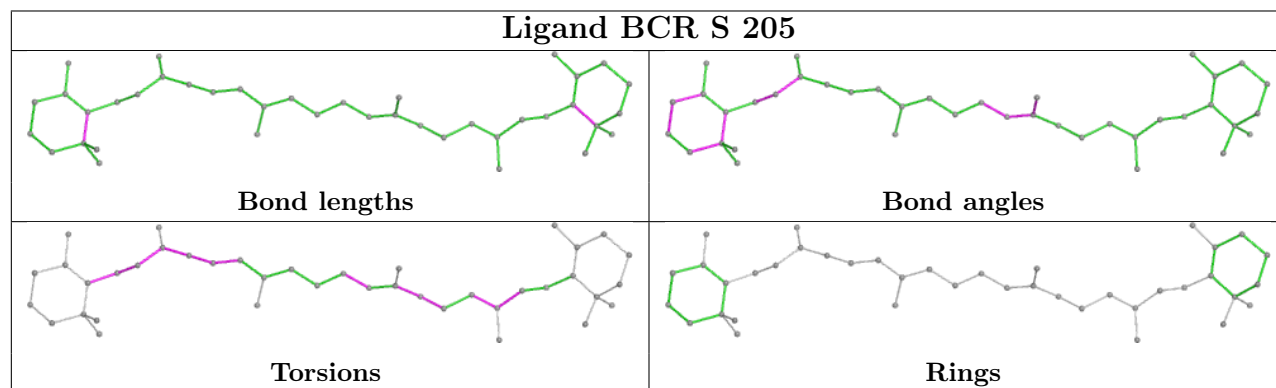
## Ligand BCR O 201



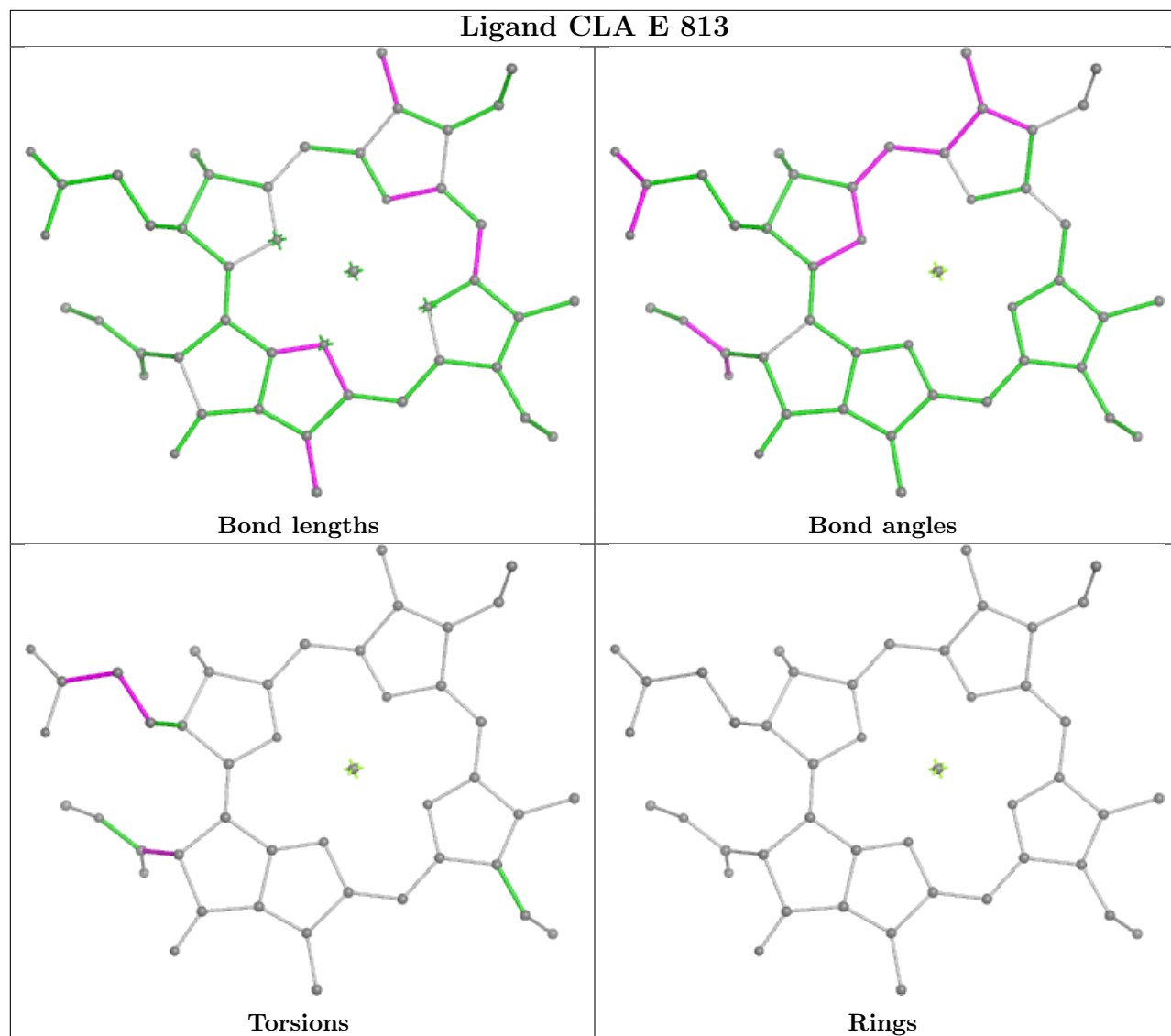
## Ligand CLA A 831



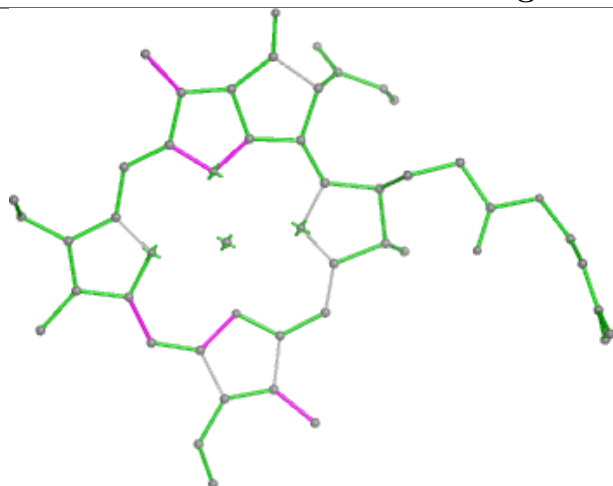
## Ligand BCR S 205



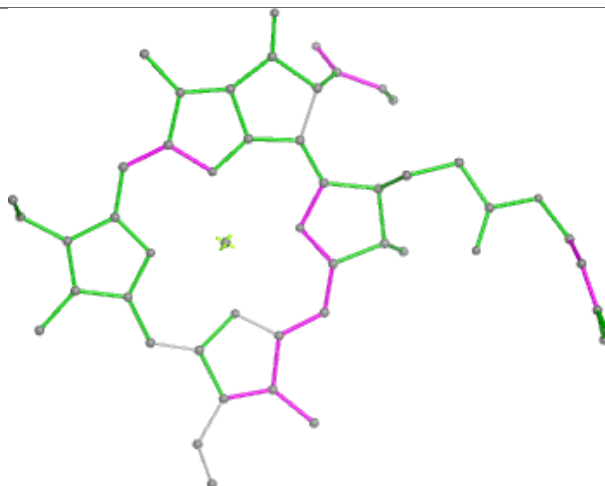
## Ligand CLA E 813



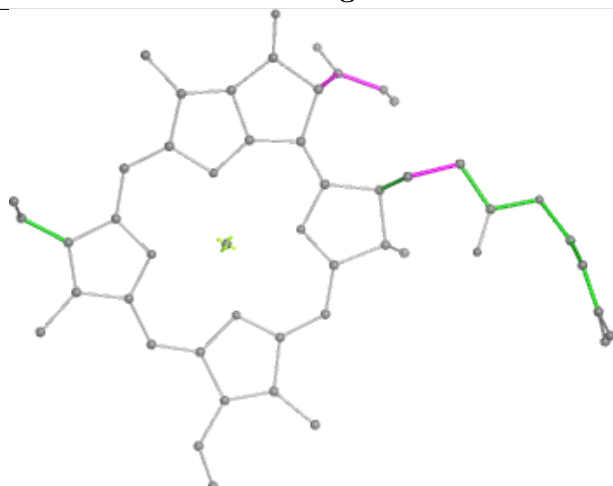
## Ligand CLA b 813



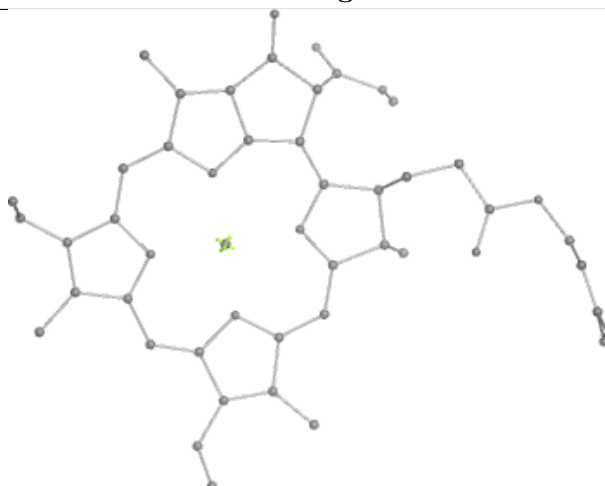
Bond lengths



Bond angles

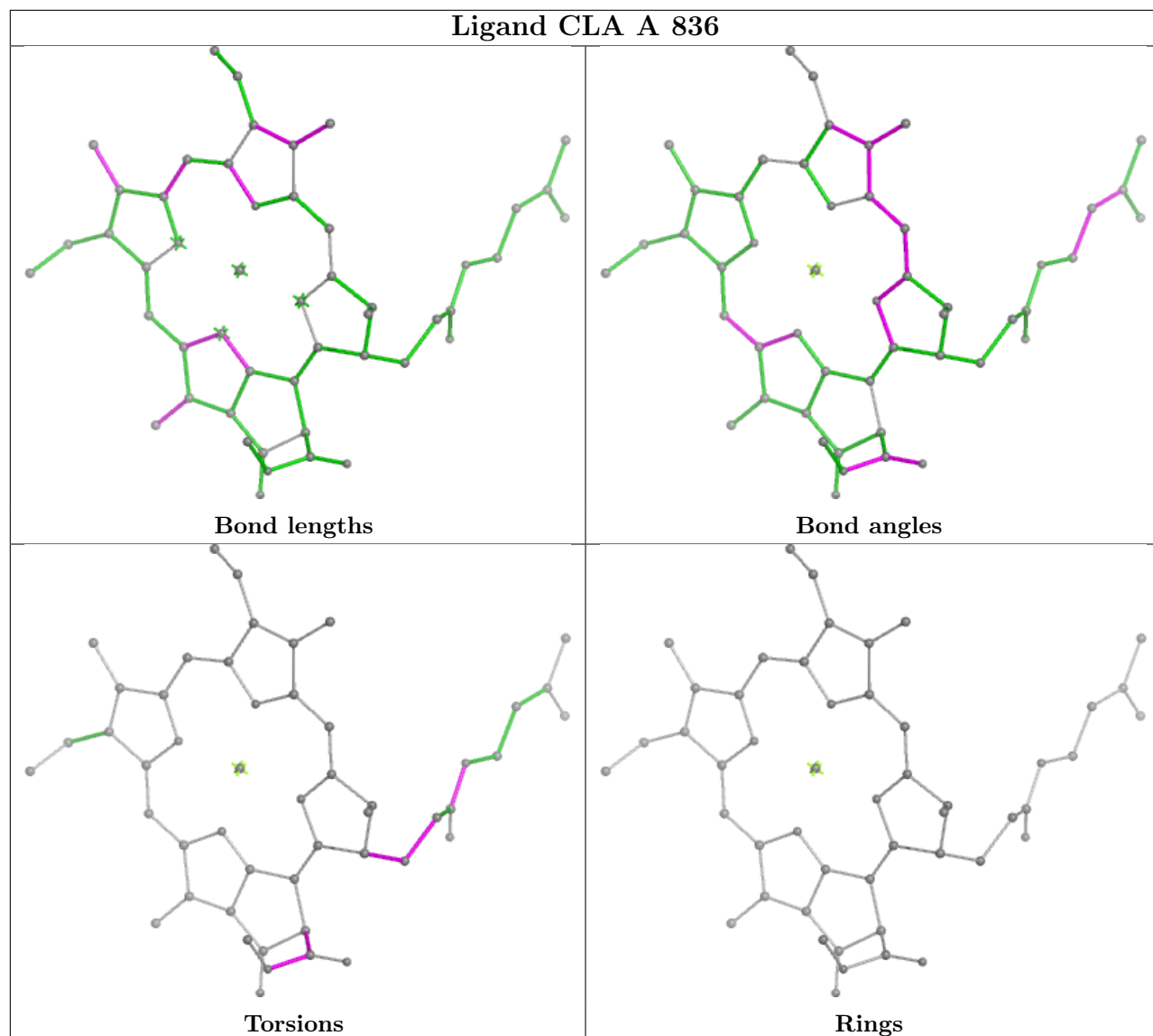


Torsions

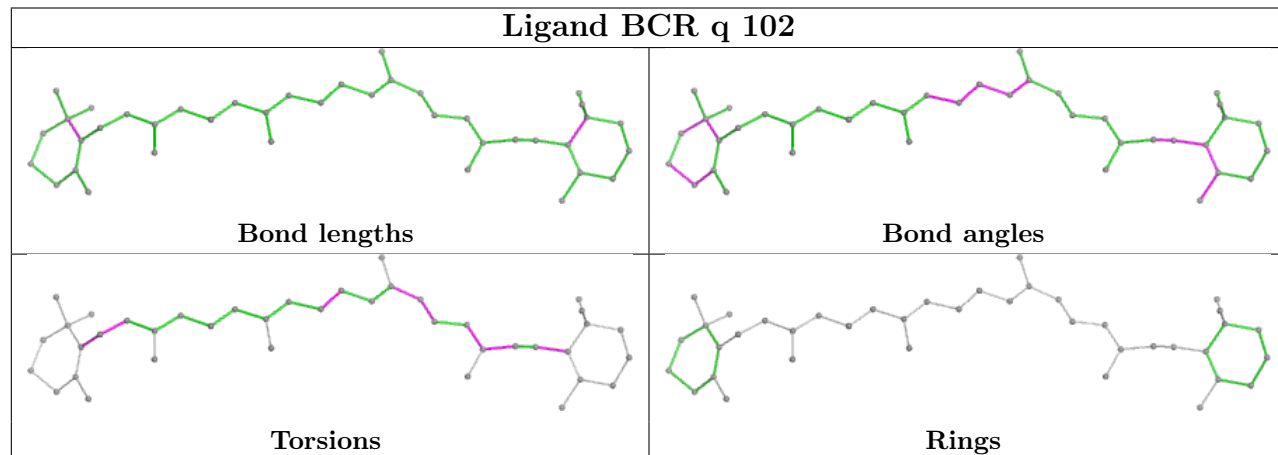


Rings

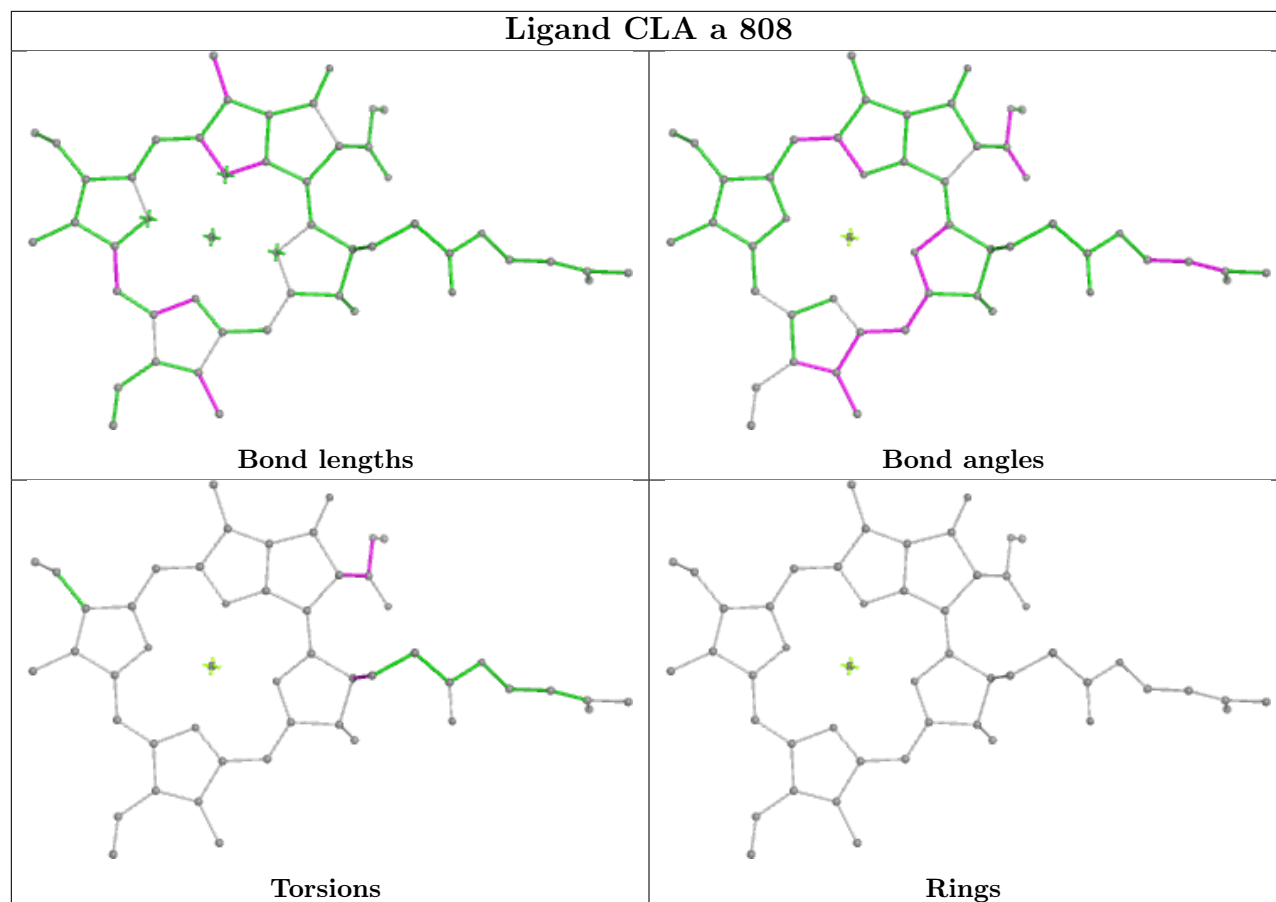
## Ligand CLA A 836



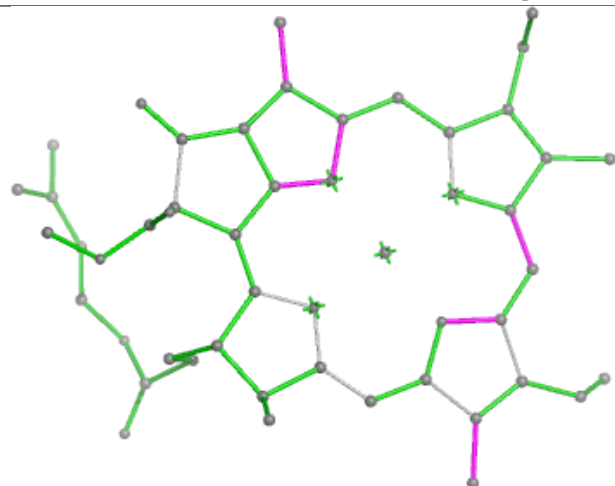
## Ligand BCR q 102



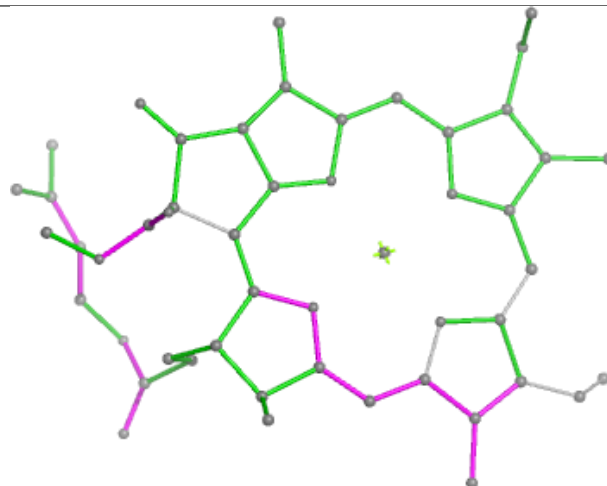
## Ligand CLA a 808



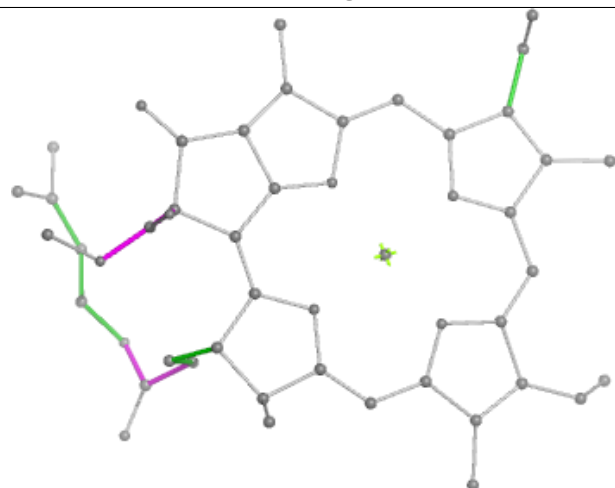
## Ligand CLA B 817



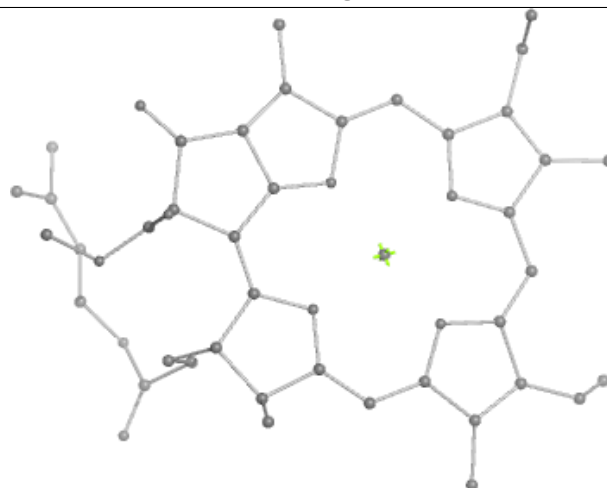
Bond lengths



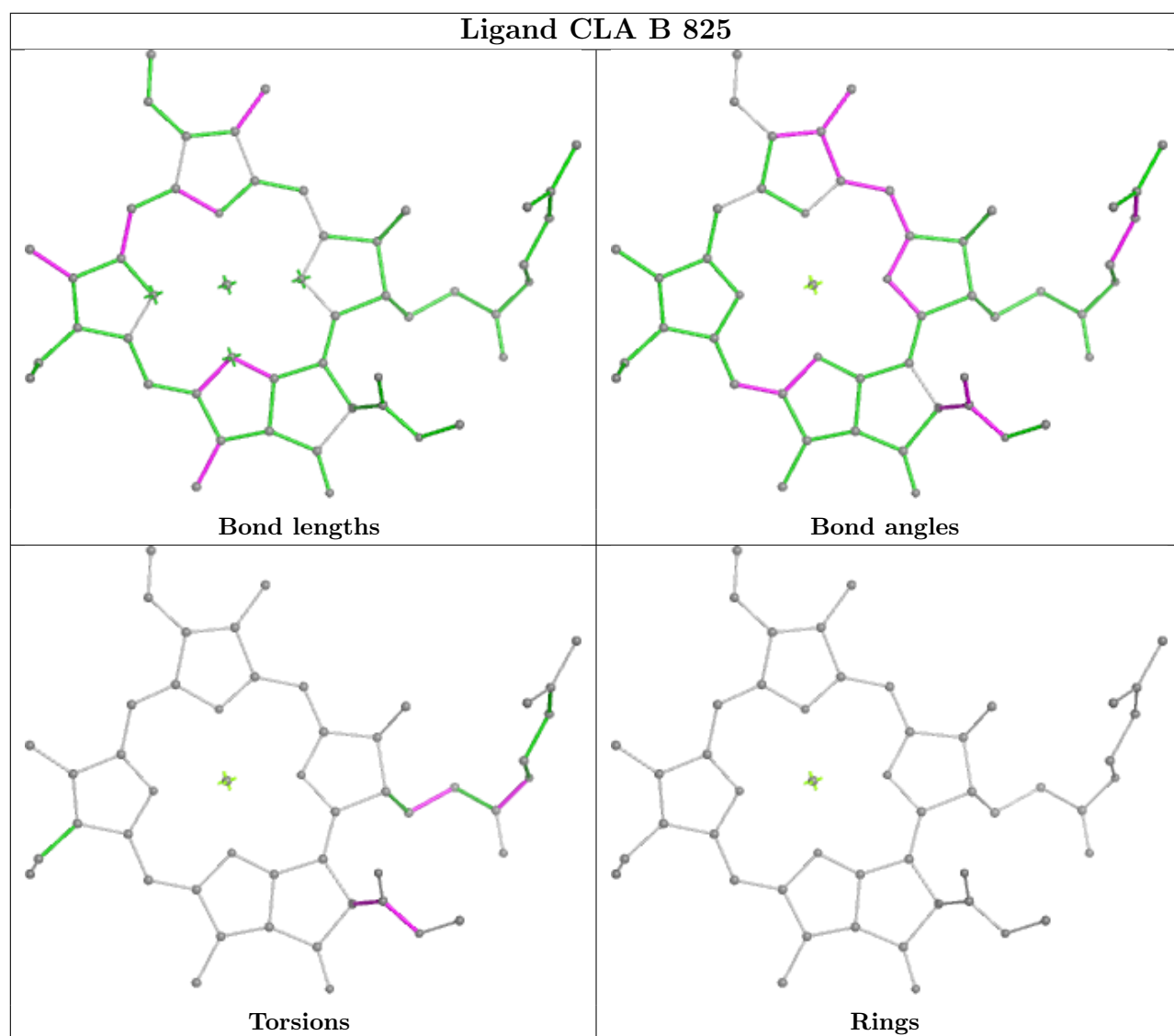
Bond angles



Torsions

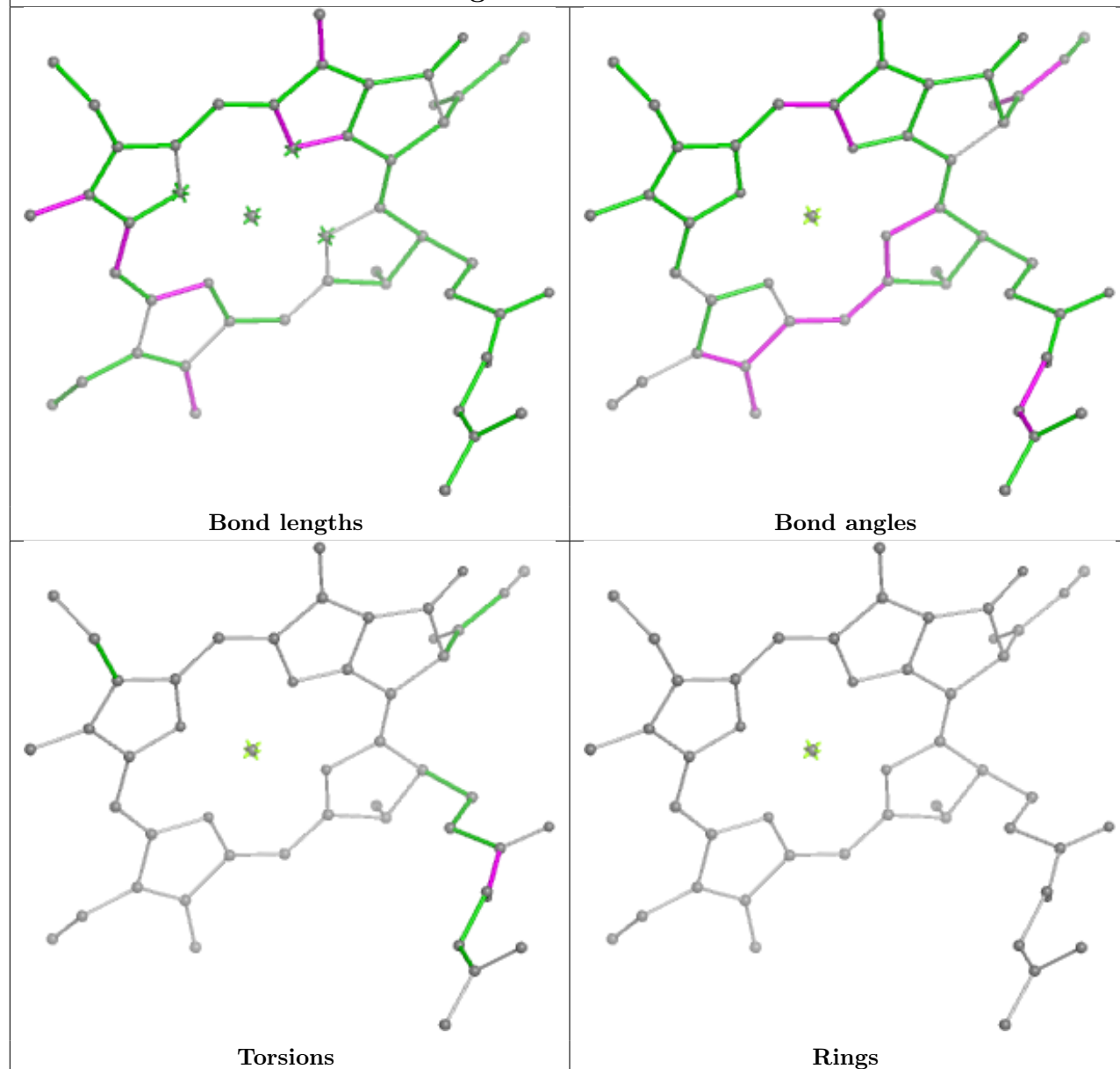


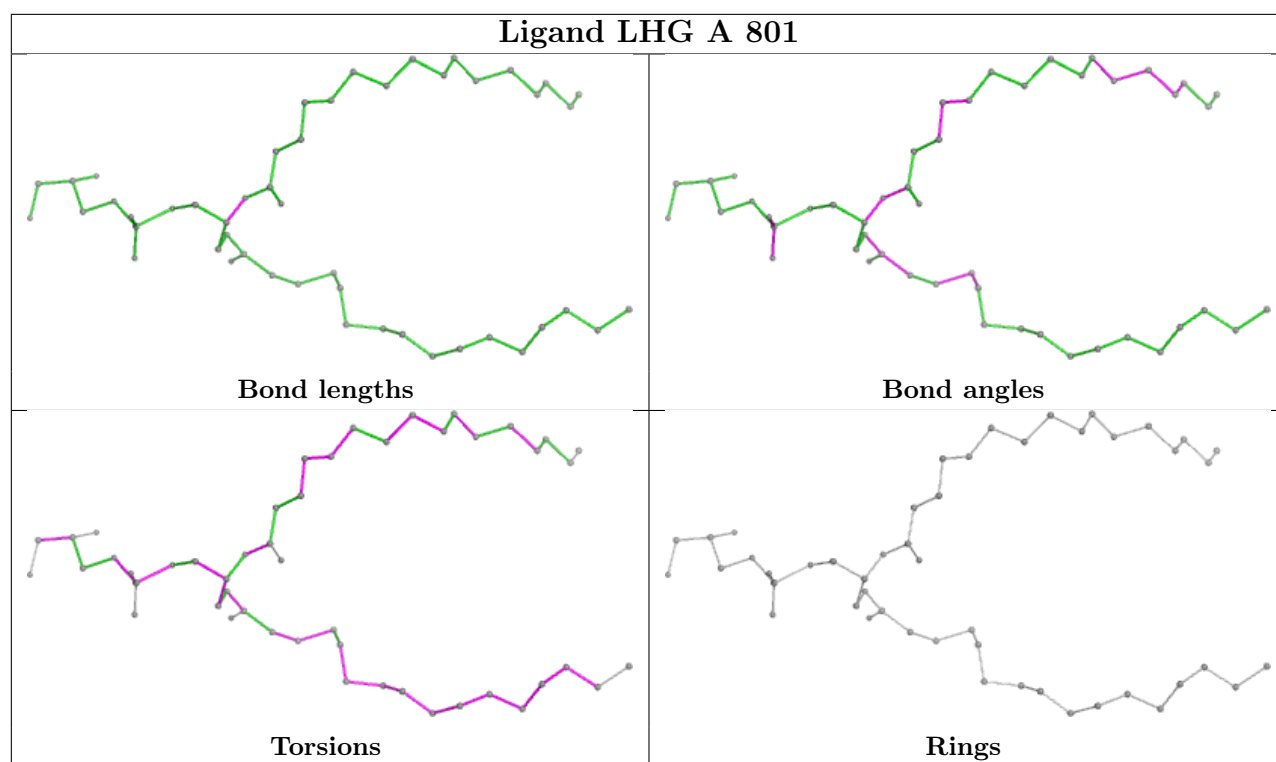
Rings



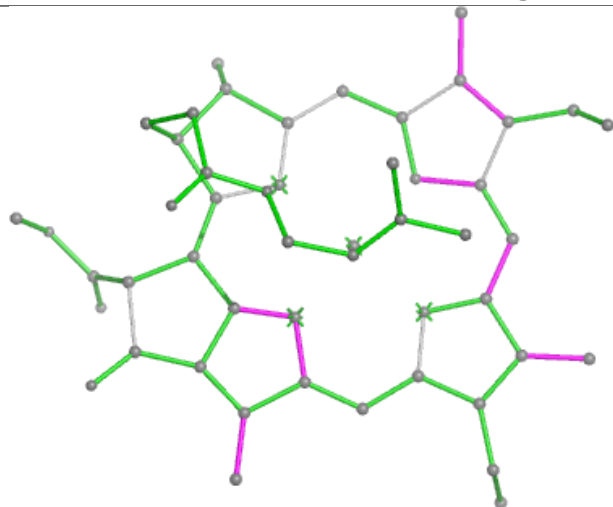


## Ligand CLA b 805

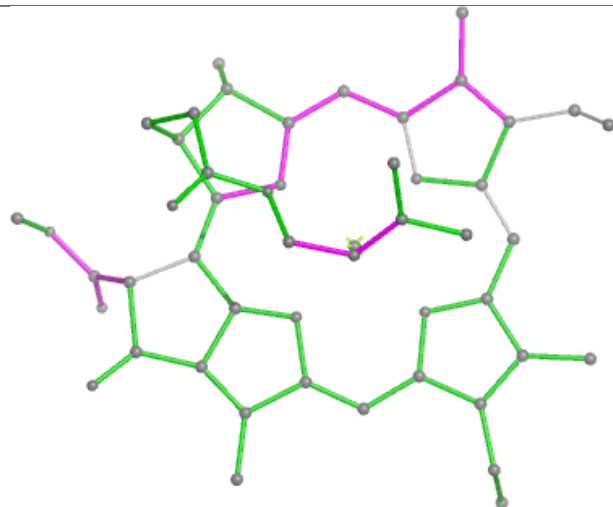




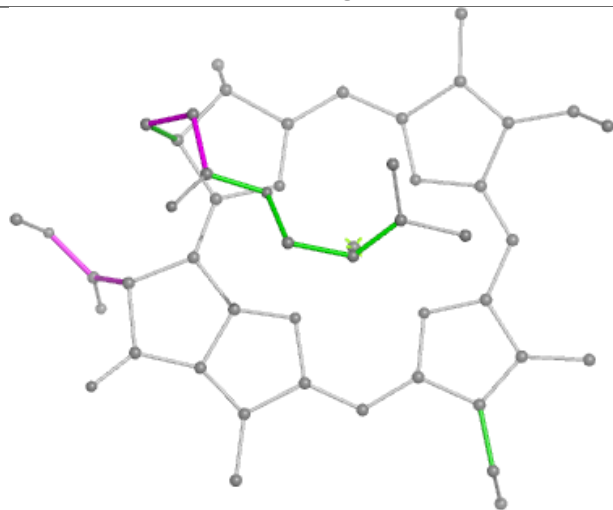
## Ligand CLA B 823



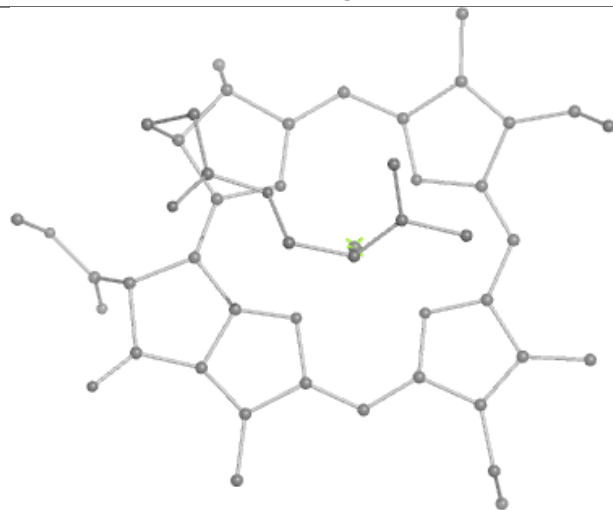
Bond lengths



Bond angles

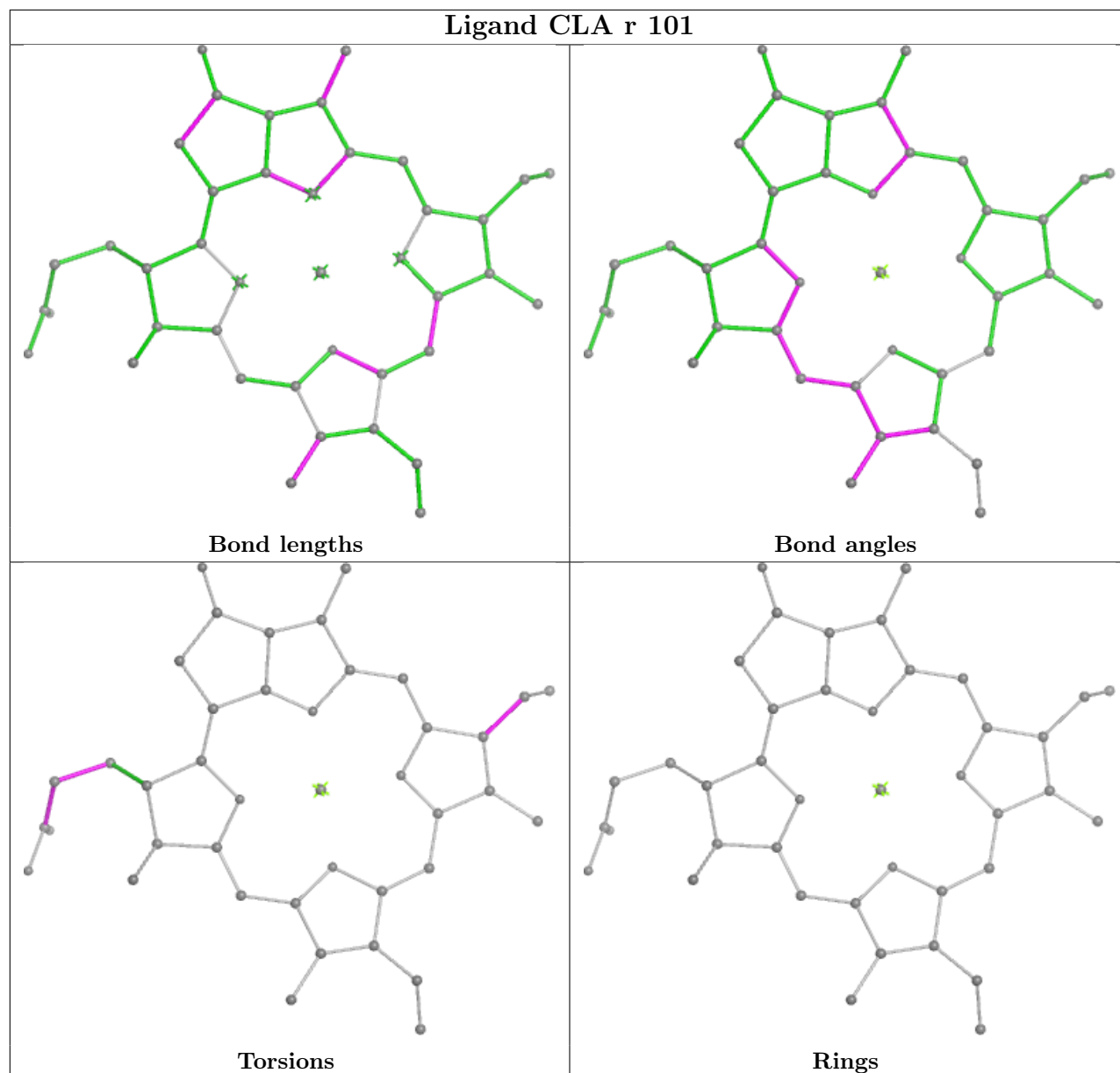


Torsions

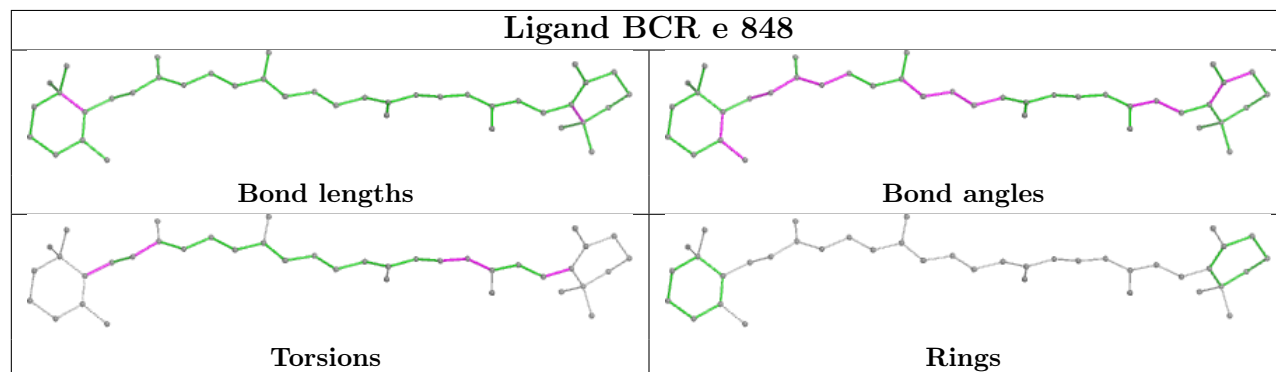


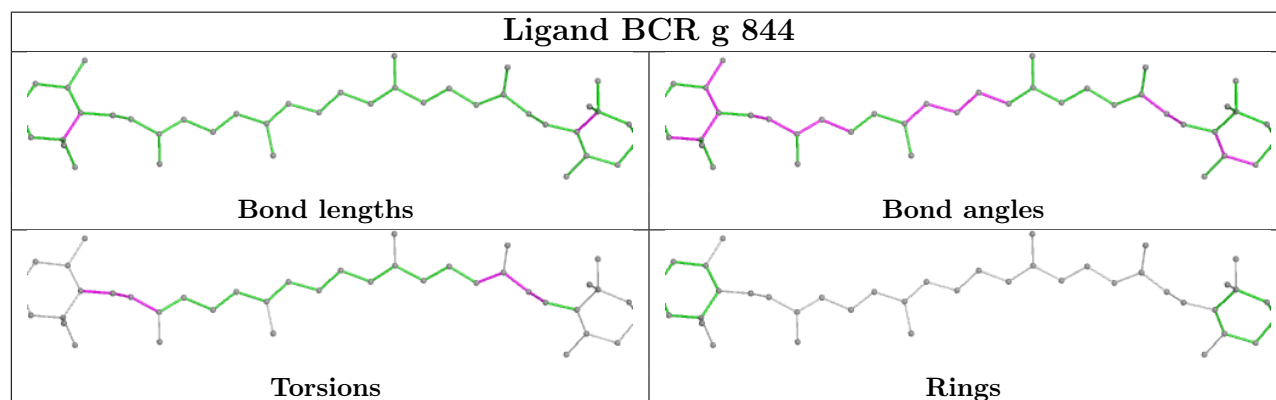
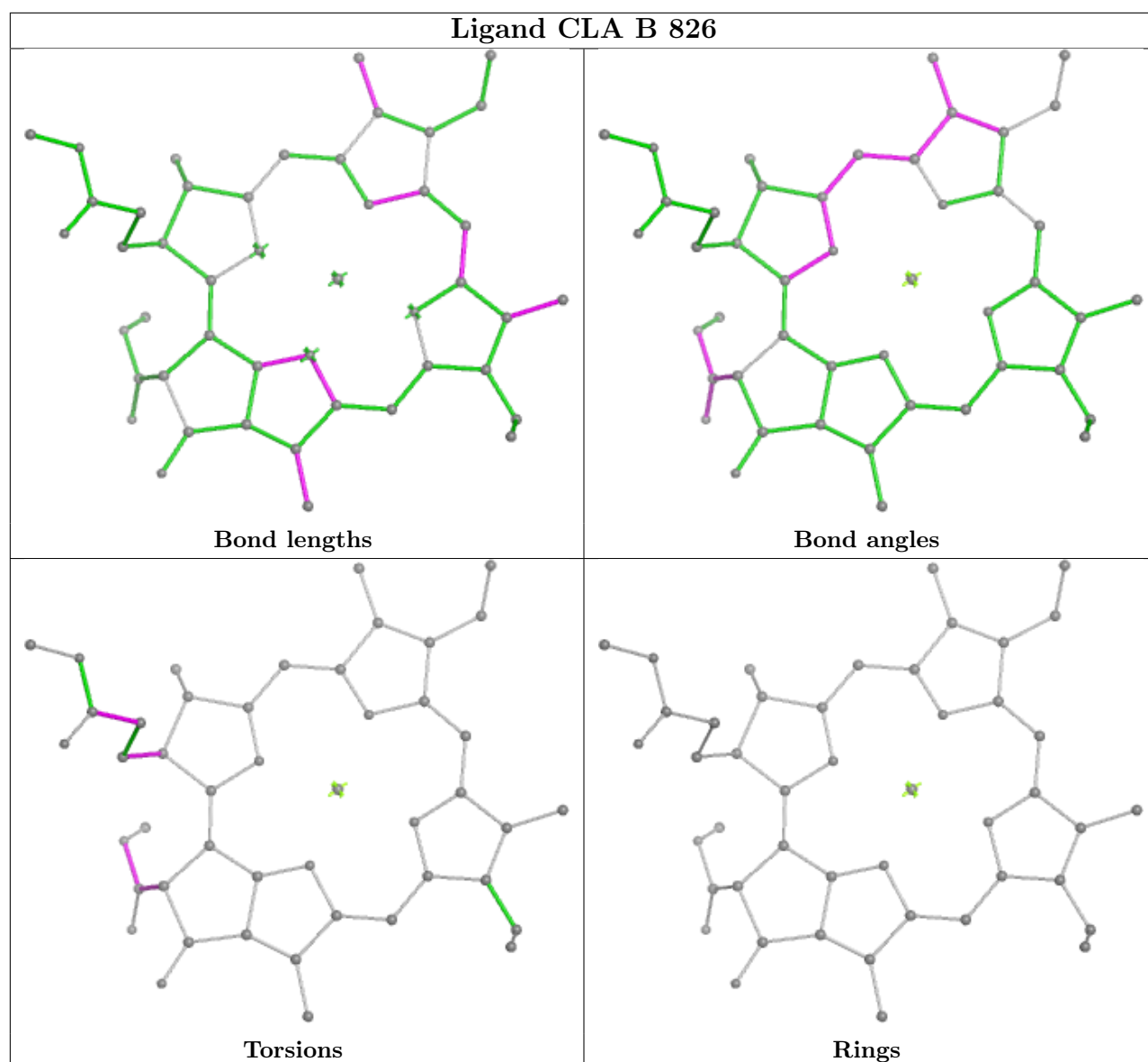
Rings

## Ligand CLA r 101

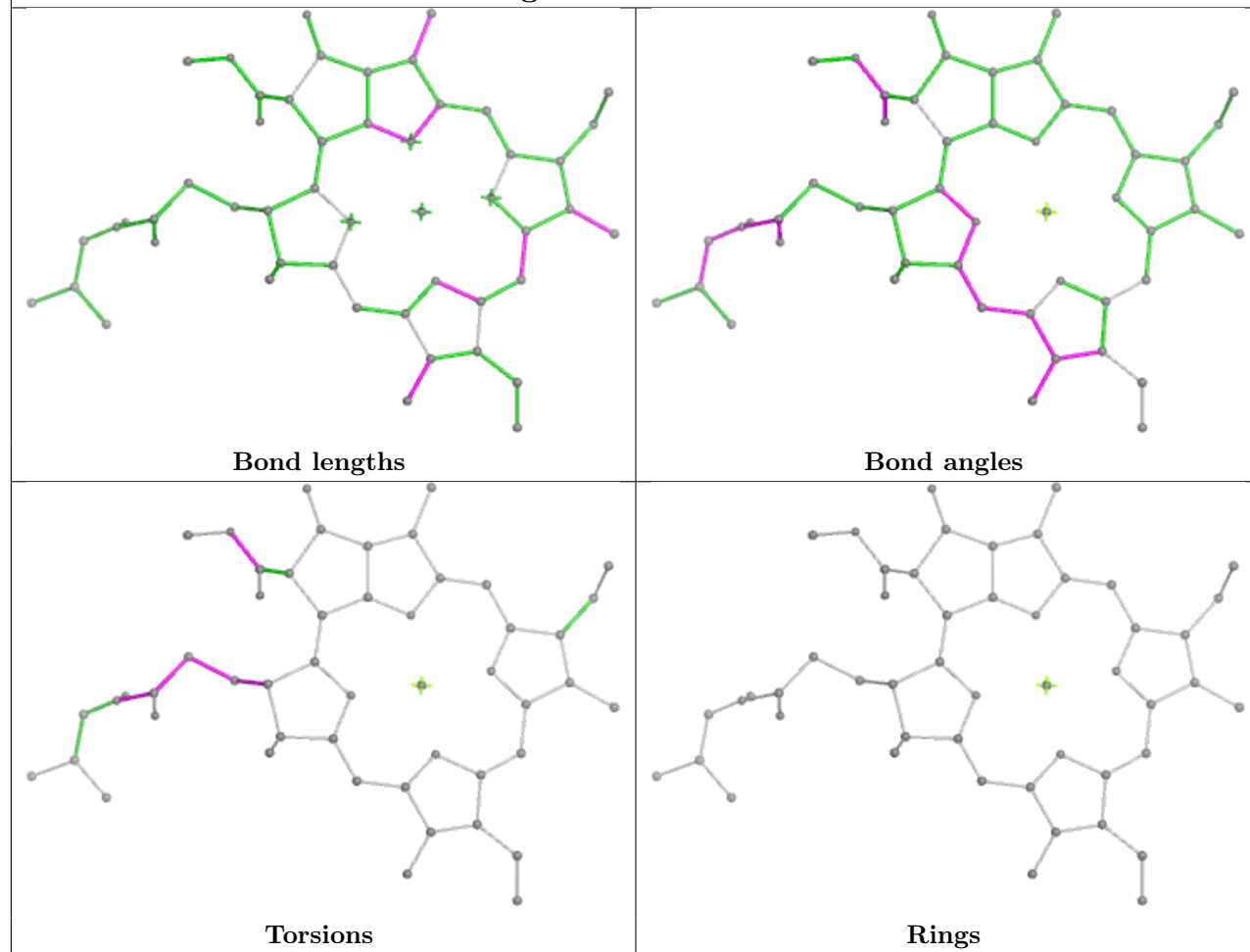


## Ligand BCR e 848

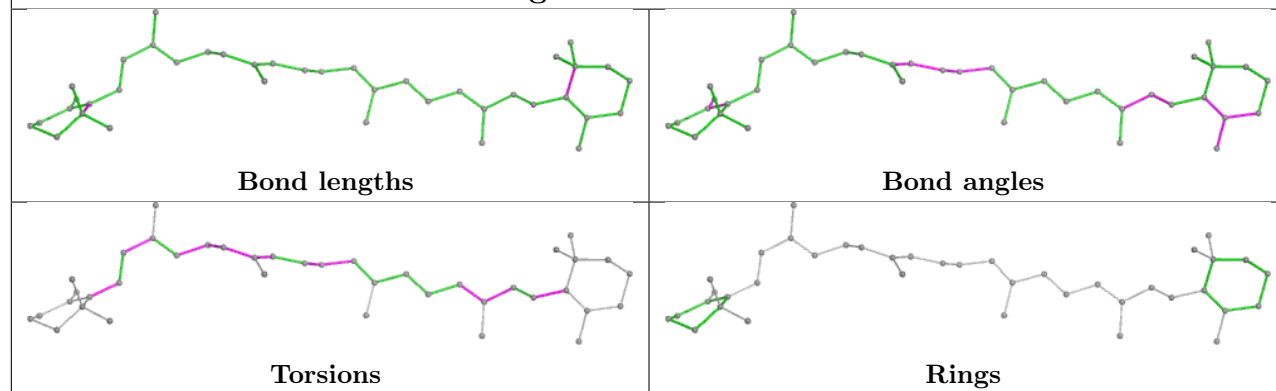




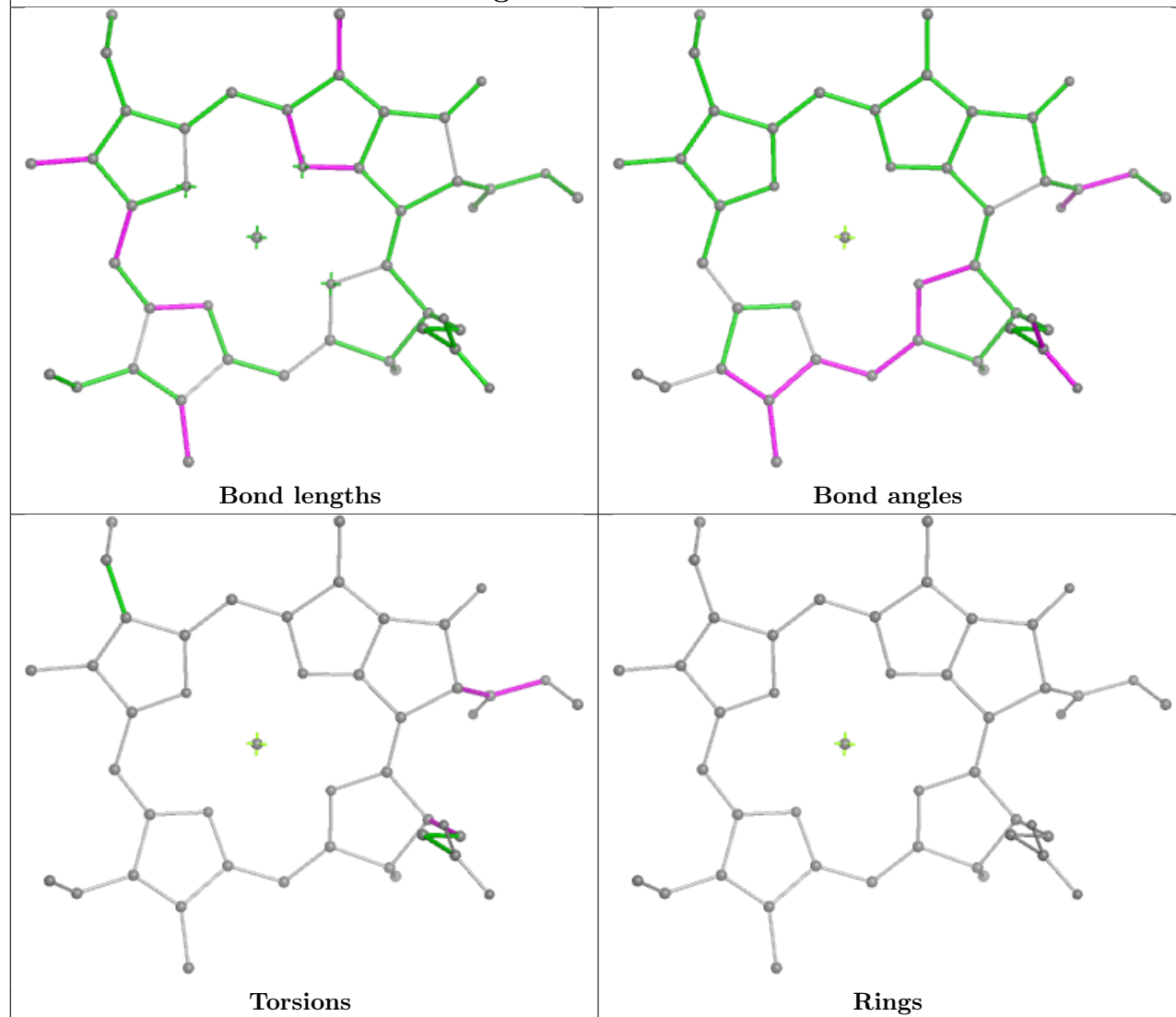
## Ligand CLA A 830



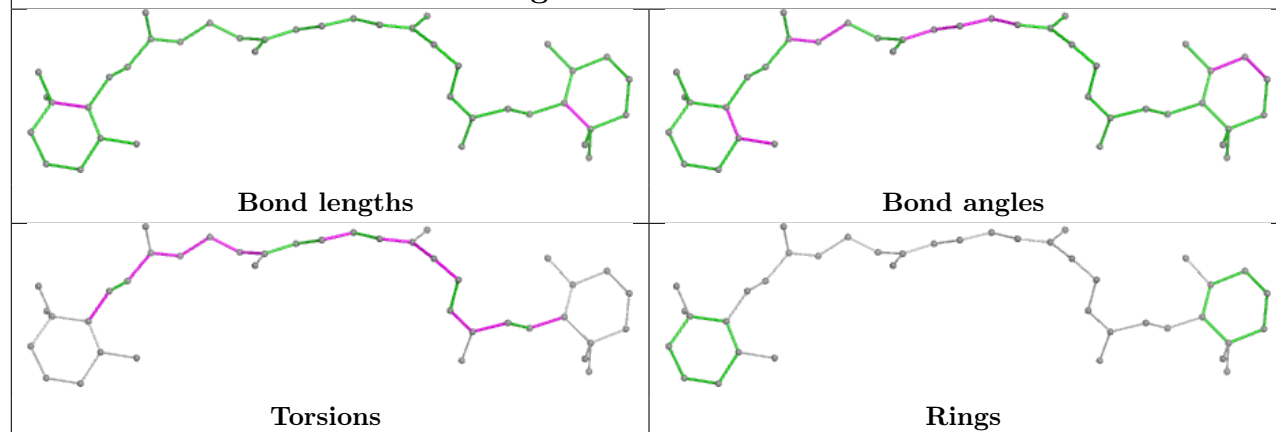
## Ligand BCR G 848



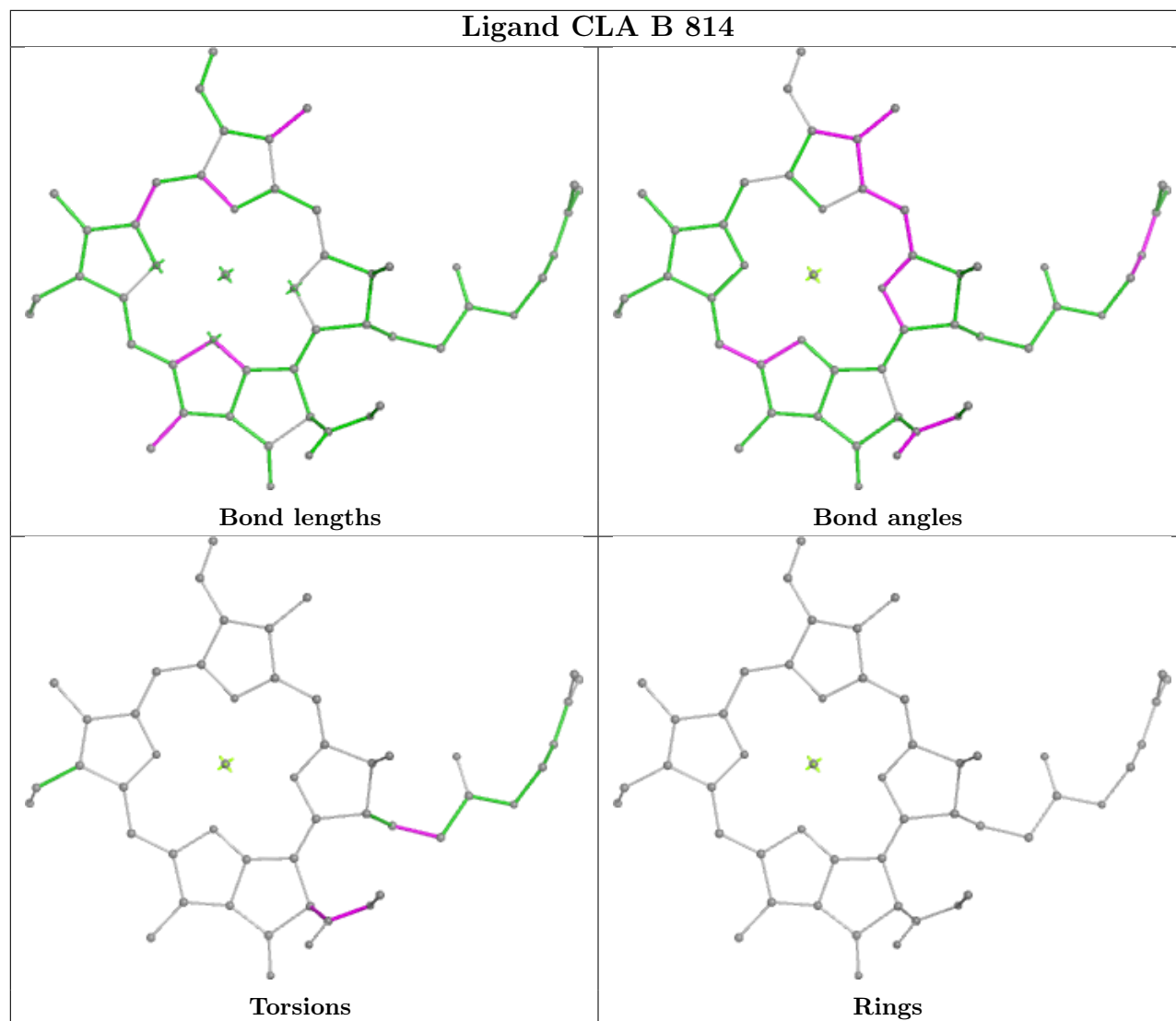
## Ligand CLA S 206



## Ligand BCR B 844

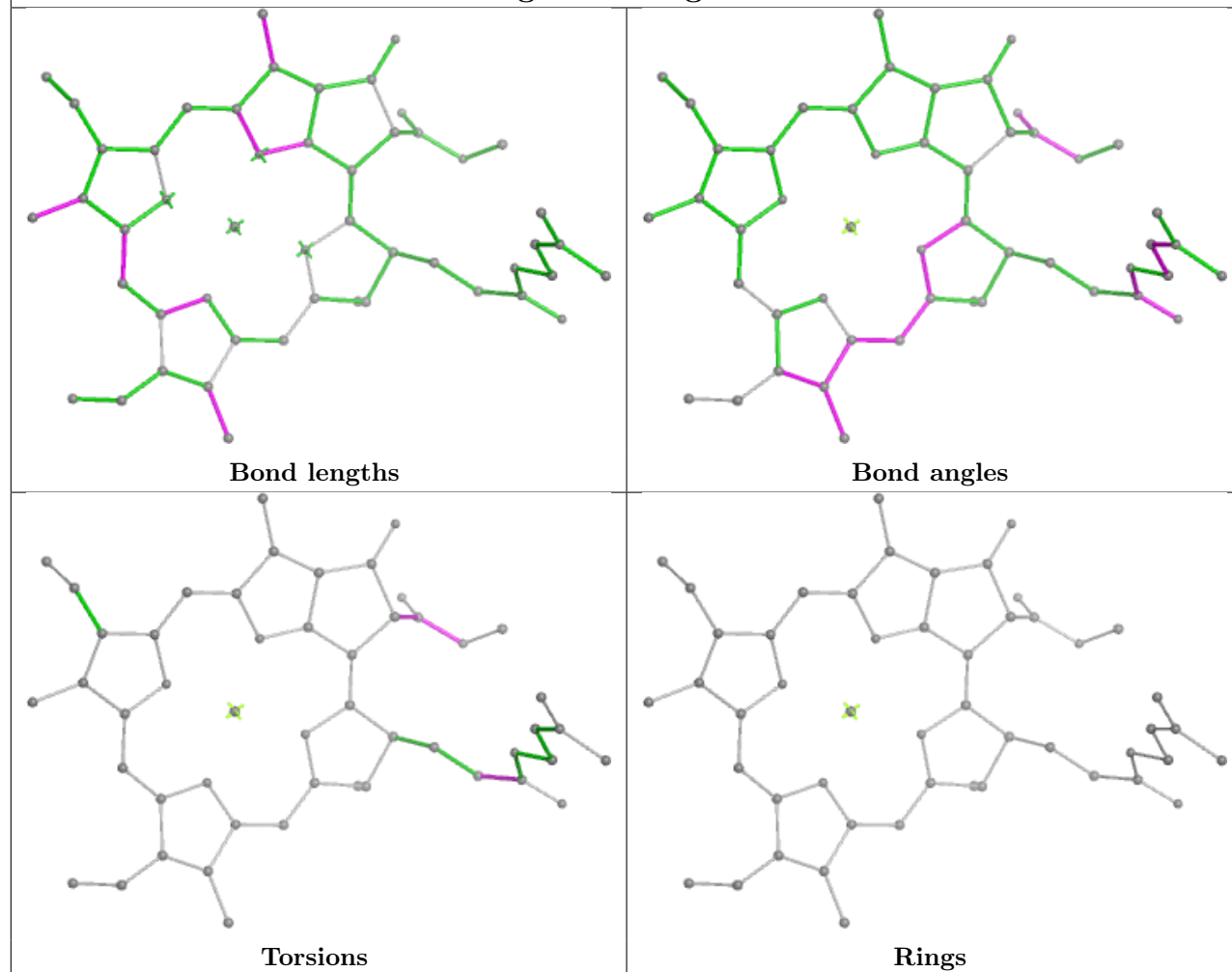


## Ligand CLA B 814

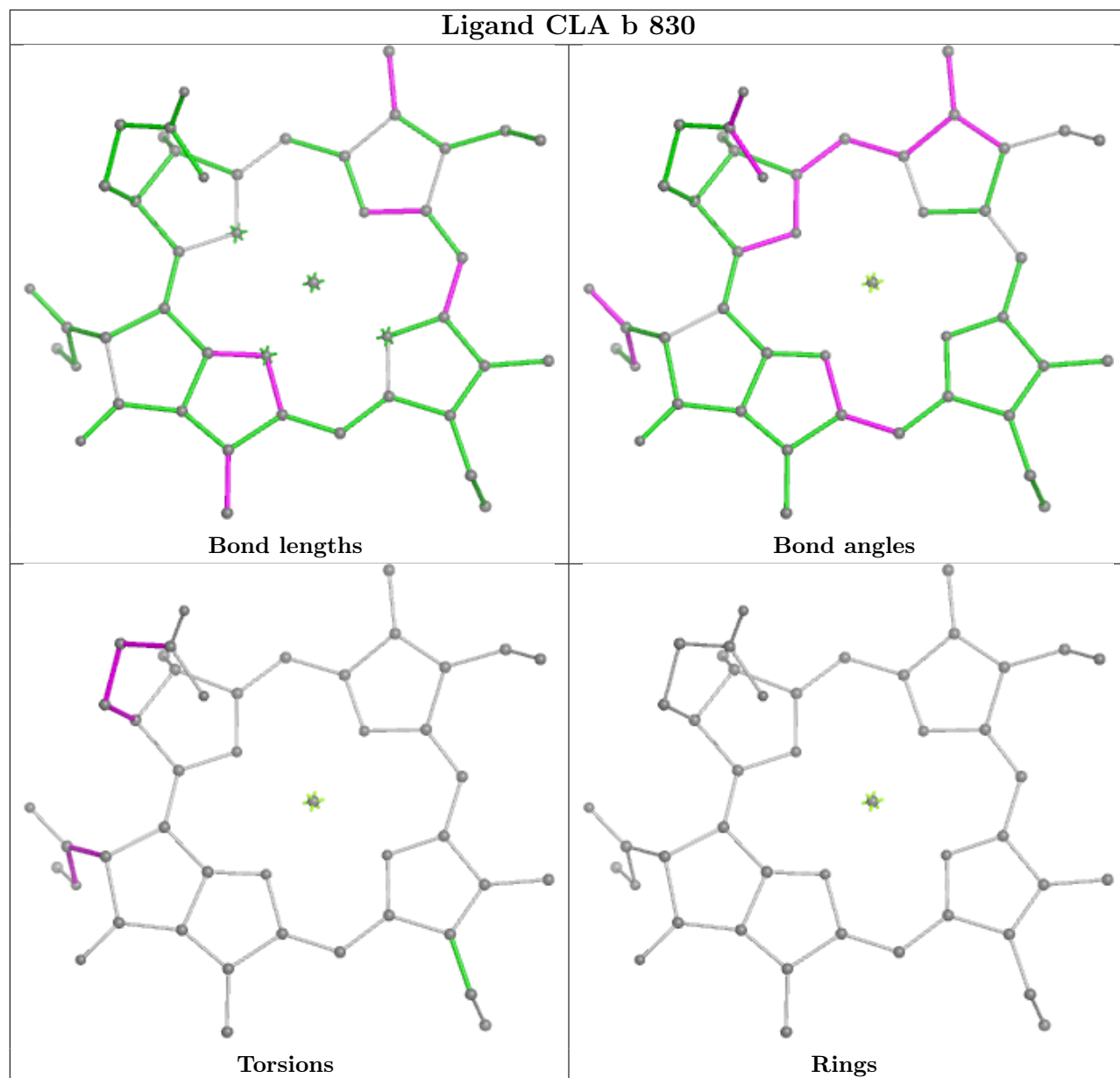




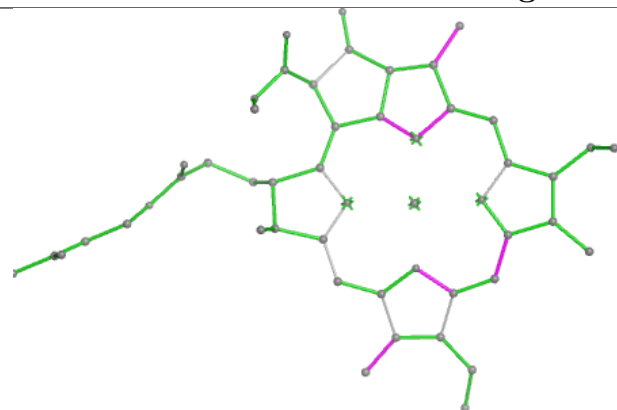
## Ligand CLA g 805



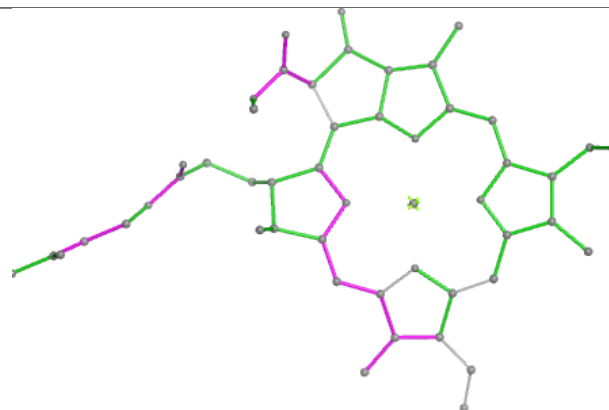
## Ligand CLA b 830



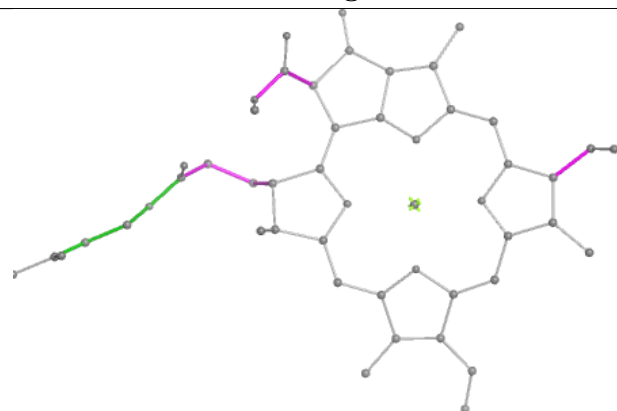
## Ligand CLA B 834



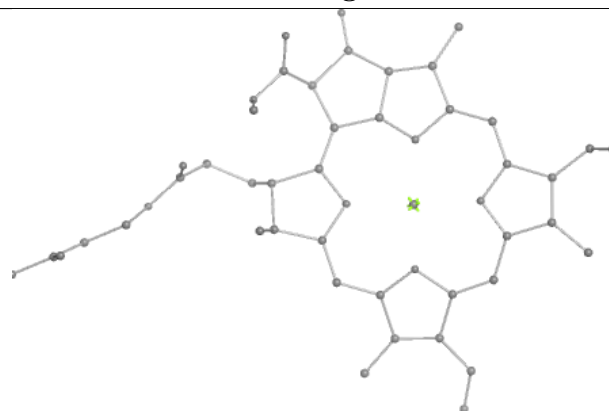
Bond lengths



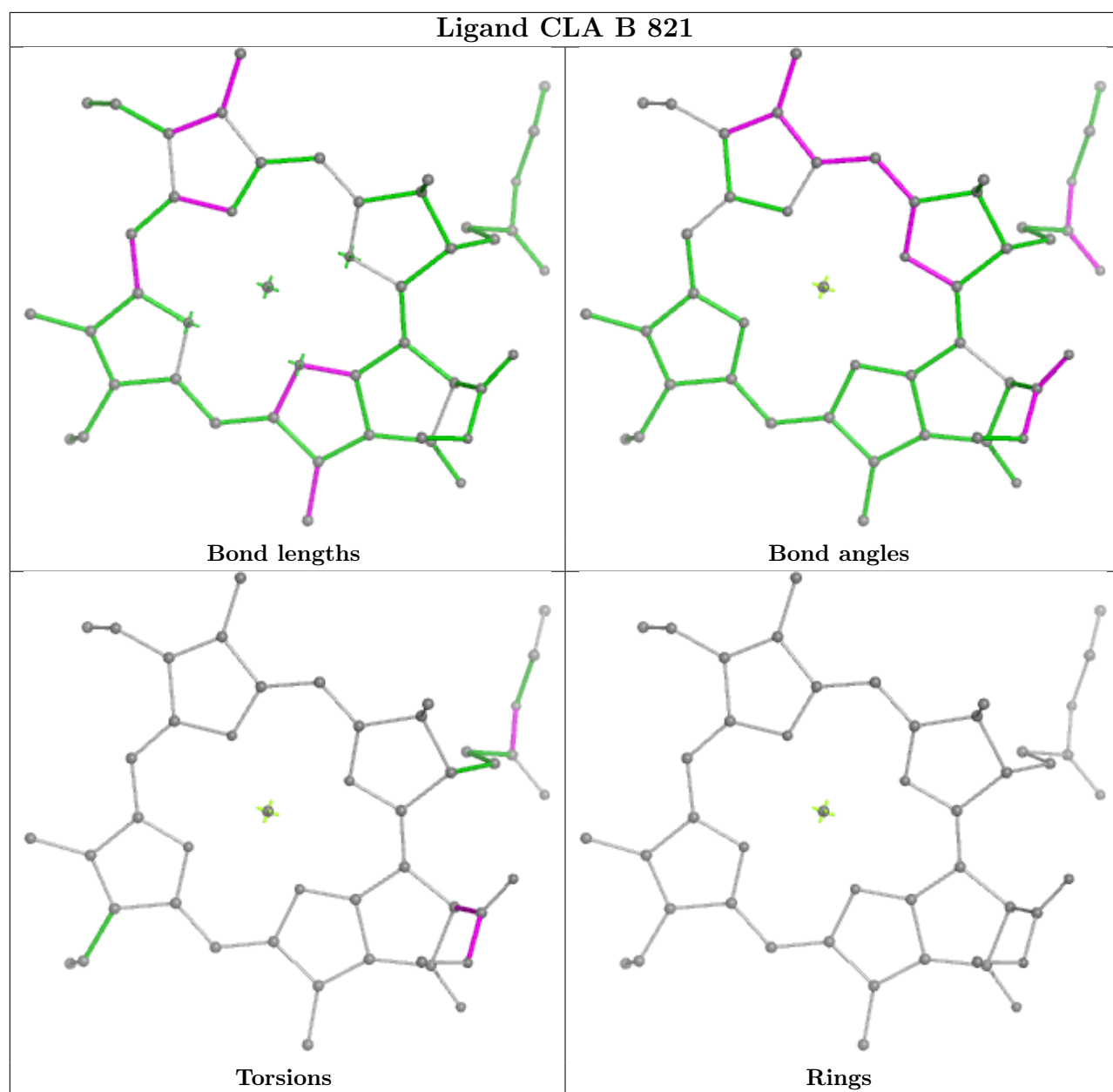
Bond angles



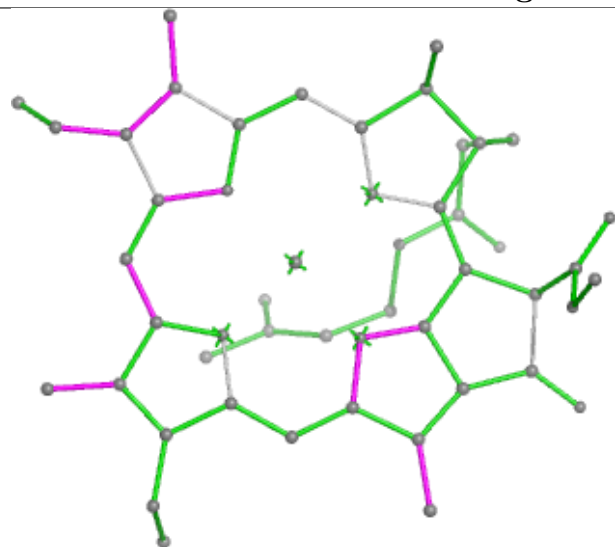
Torsions



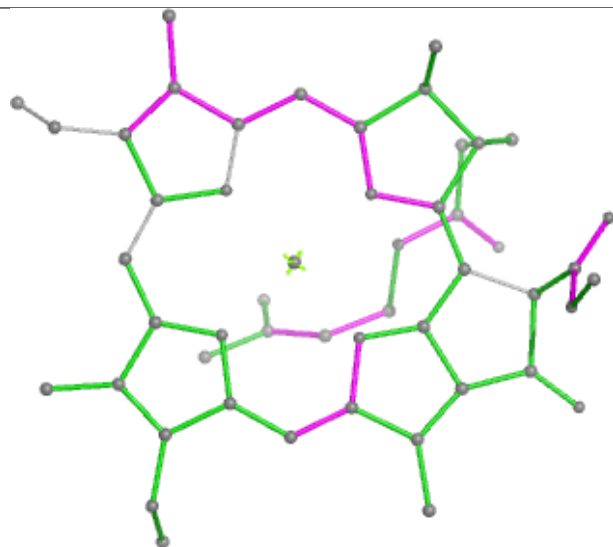
Rings



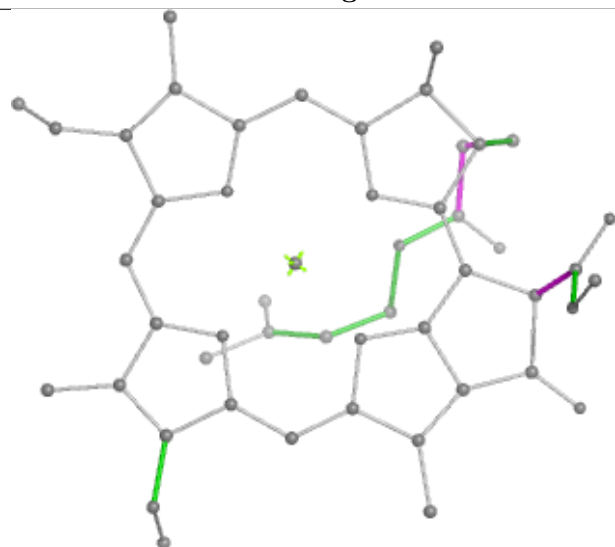
## Ligand CLA A 840



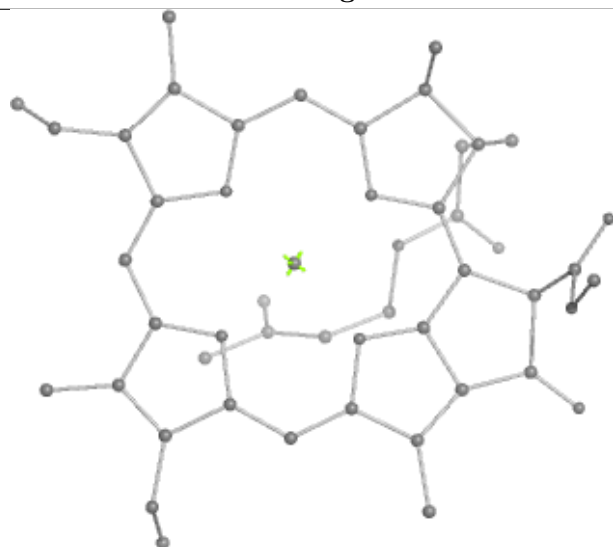
Bond lengths



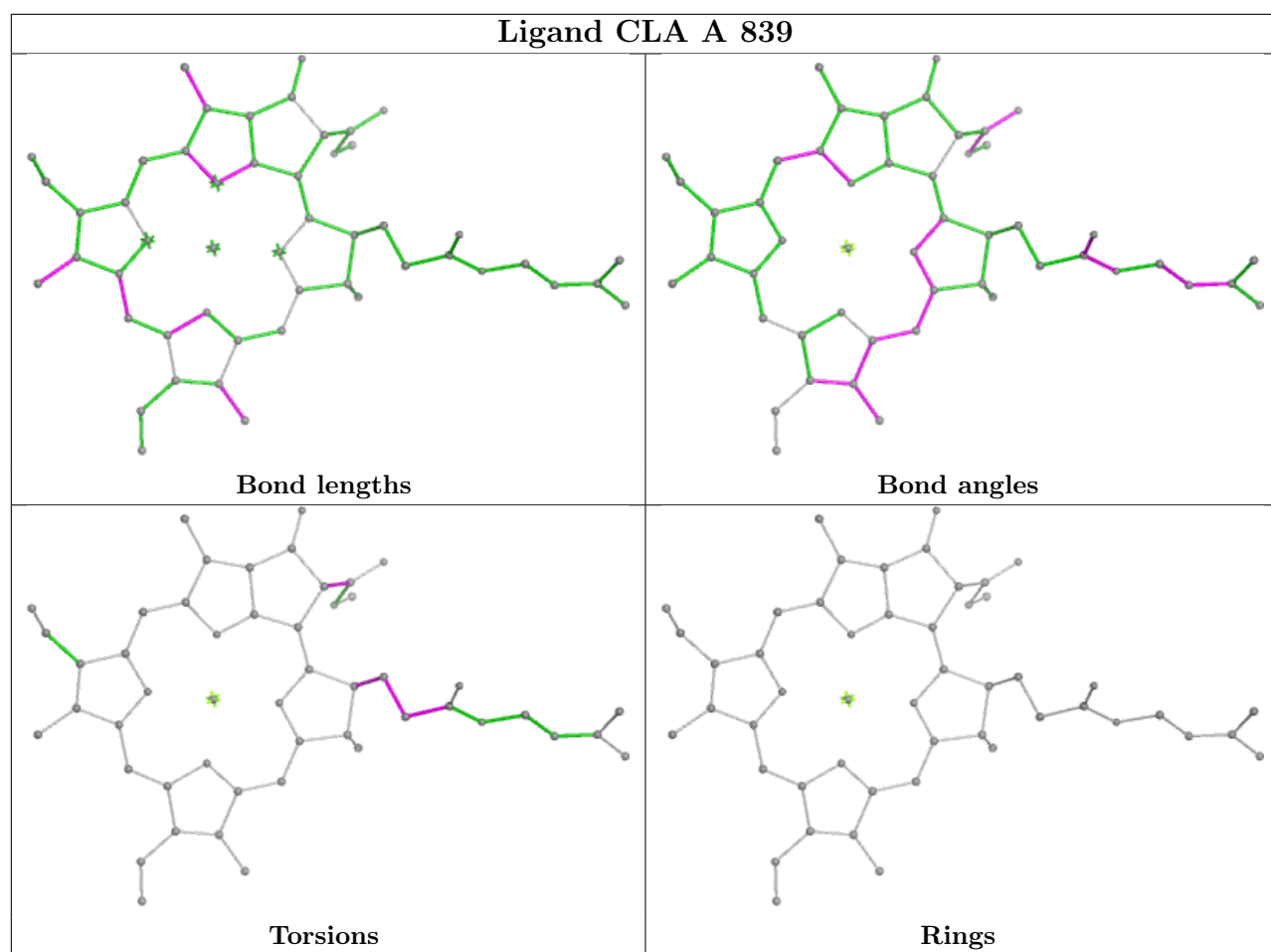
Bond angles



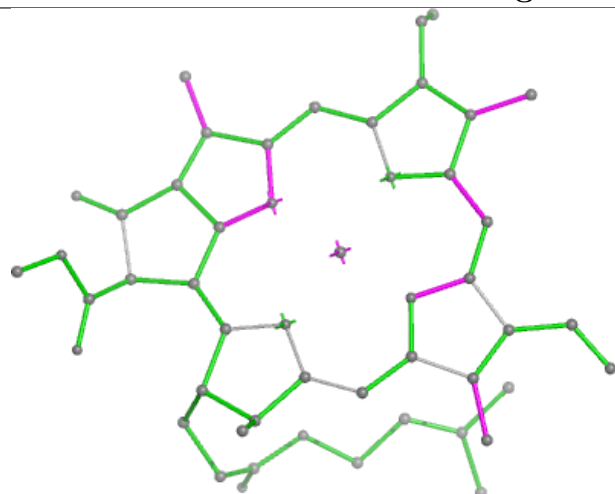
Torsions



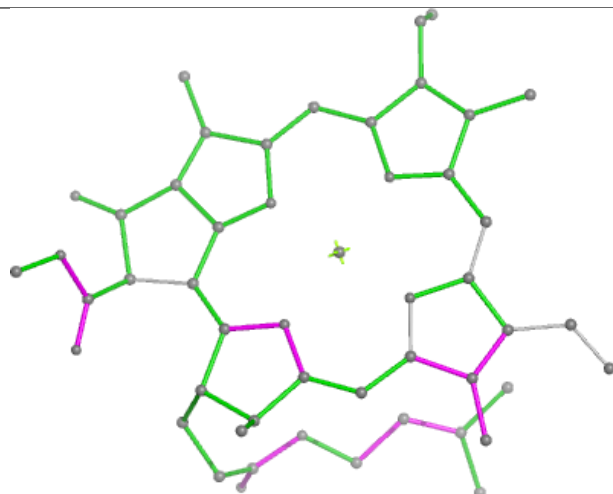
Rings



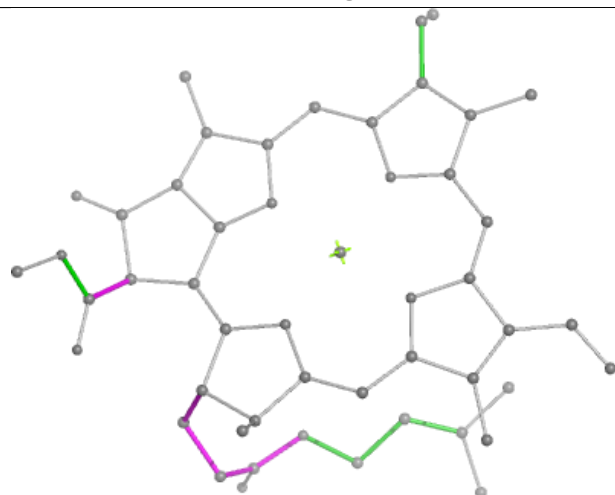
## Ligand CLA A 823



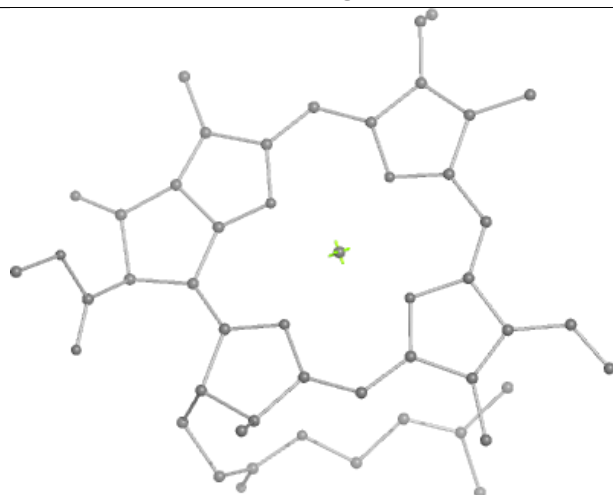
Bond lengths



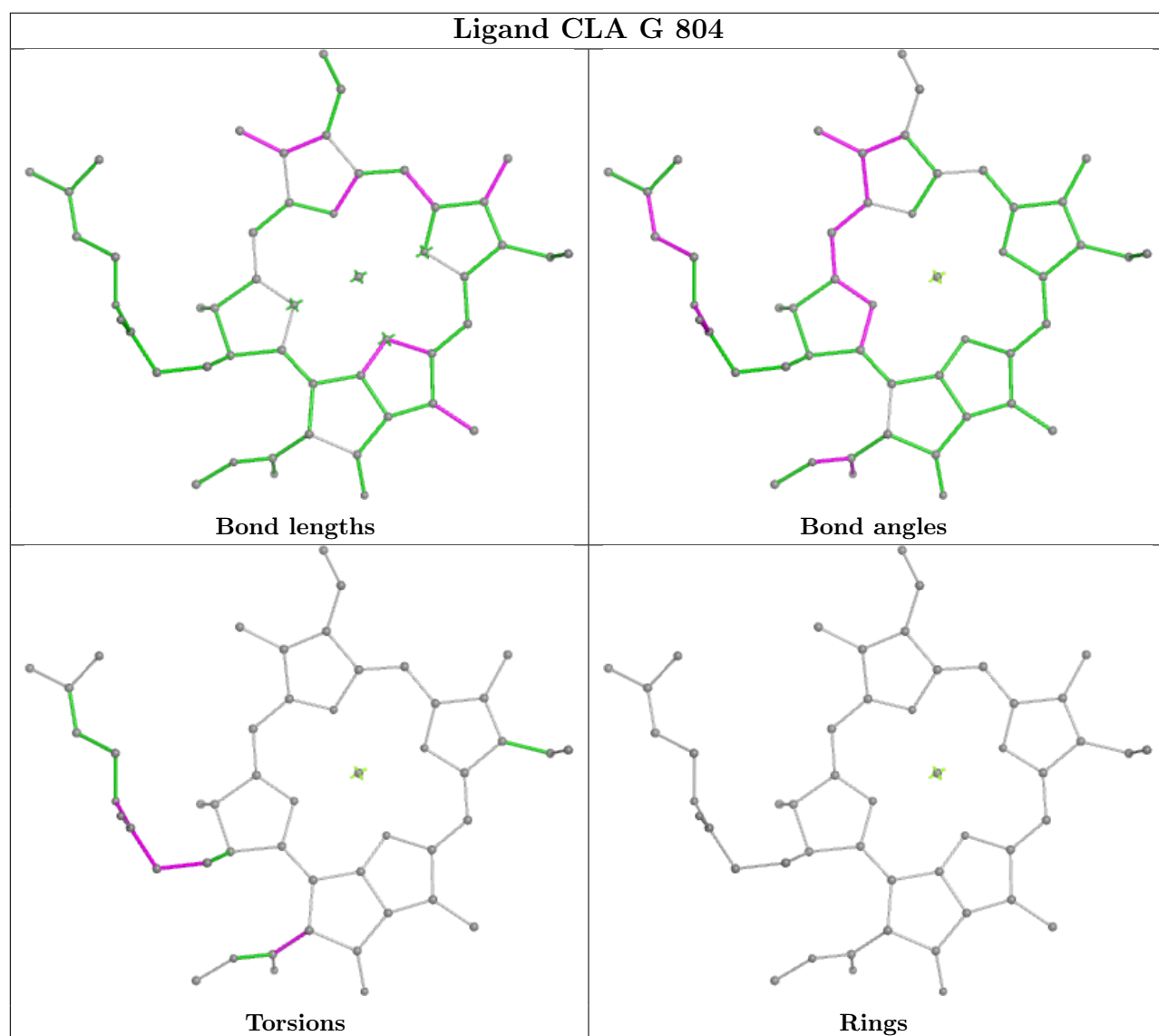
Bond angles



Torsions

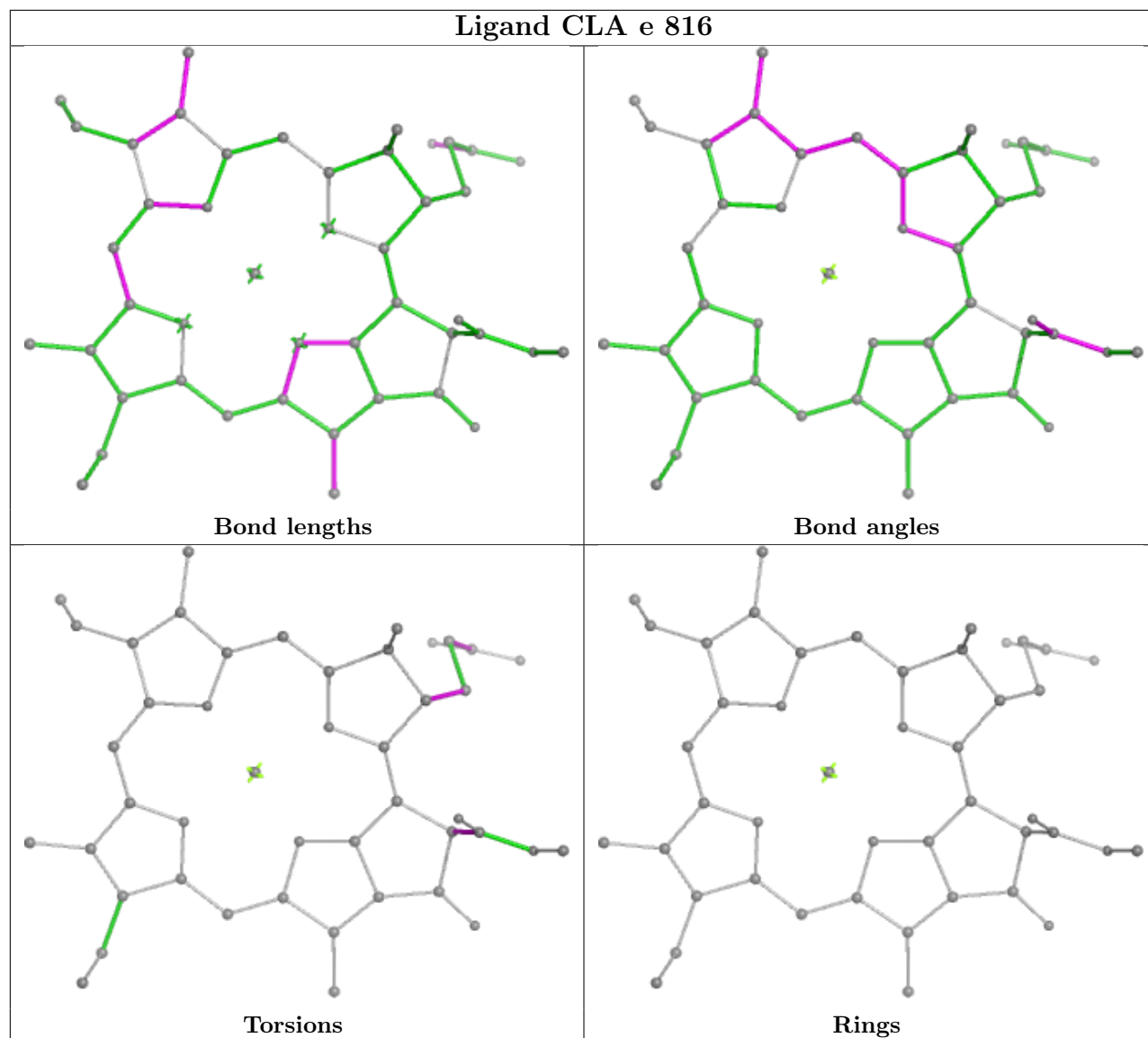


Rings

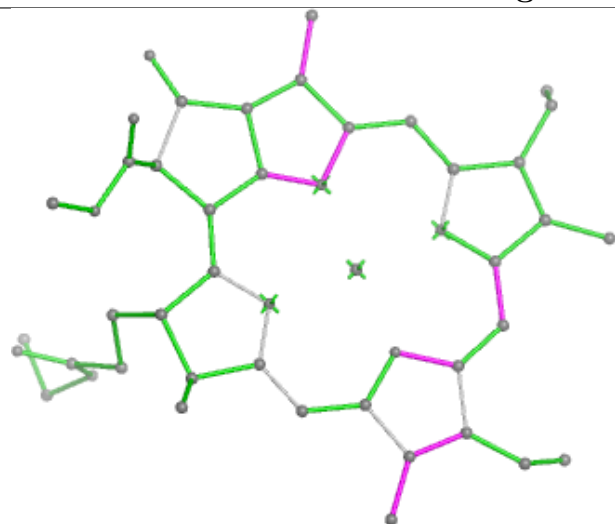




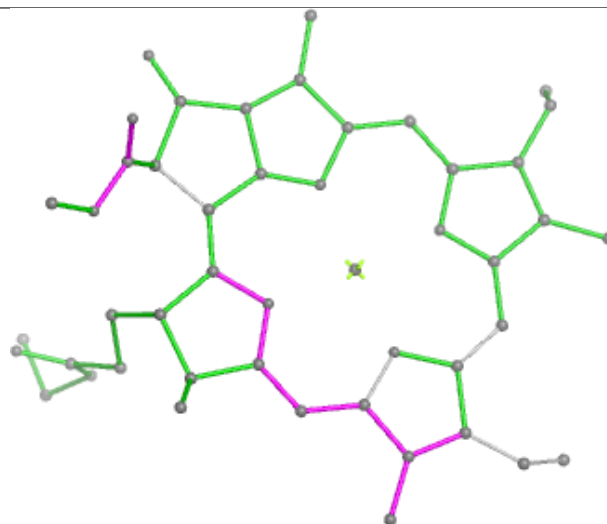
## Ligand CLA e 816



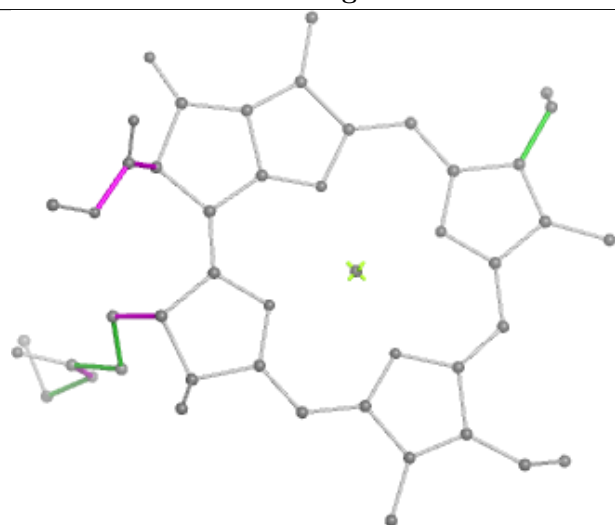
## Ligand CLA B 839



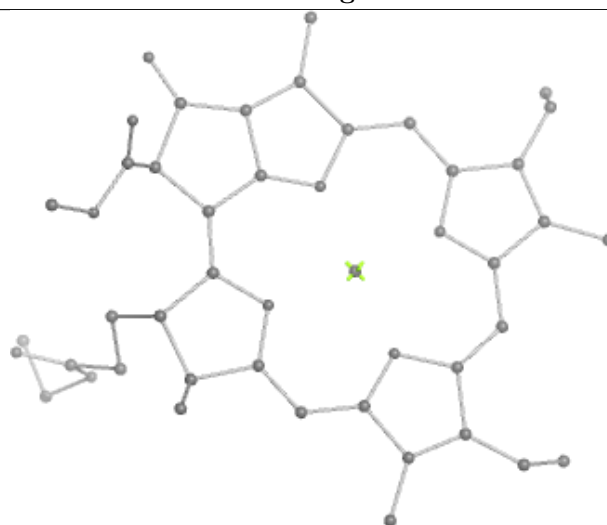
Bond lengths



Bond angles

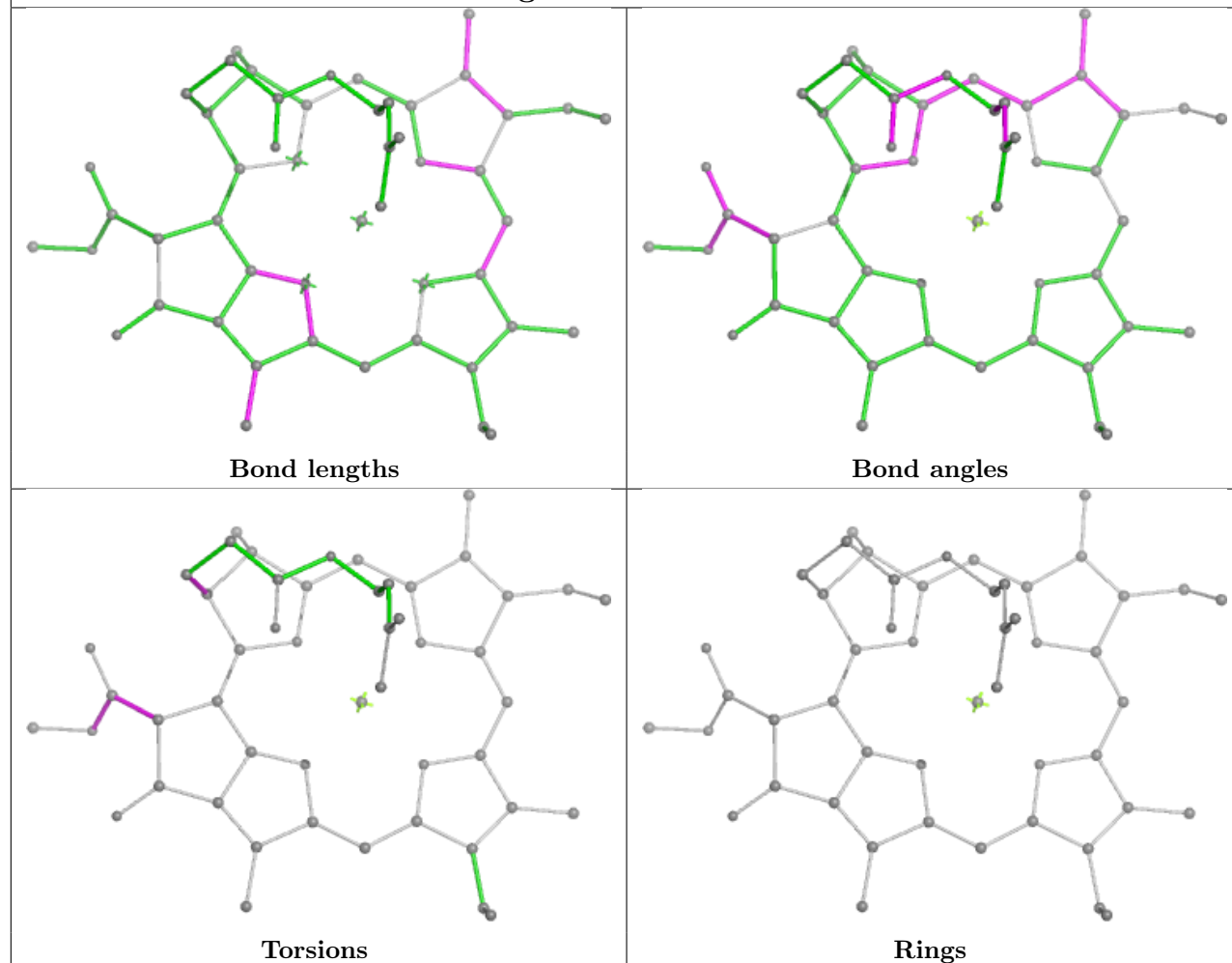


Torsions

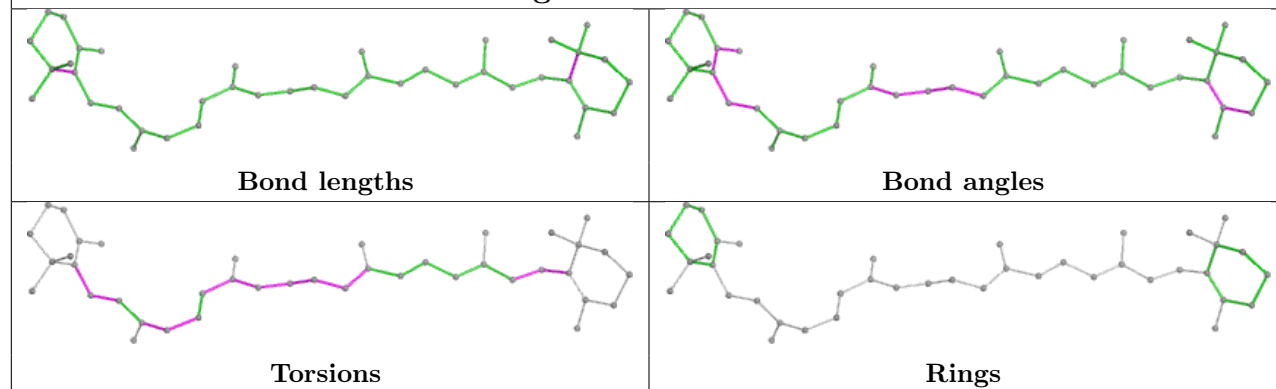


Rings

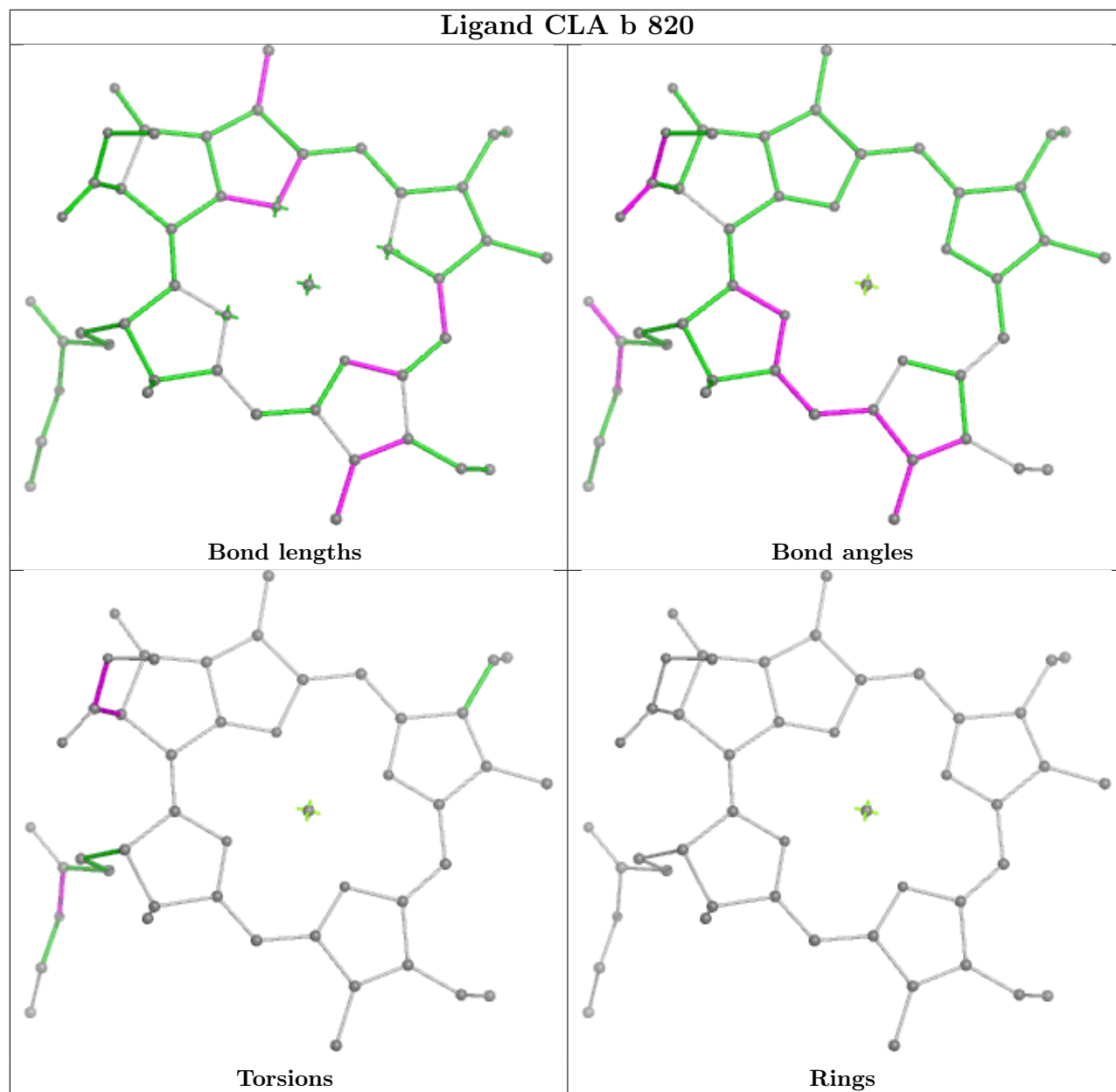
## Ligand CLA e 844

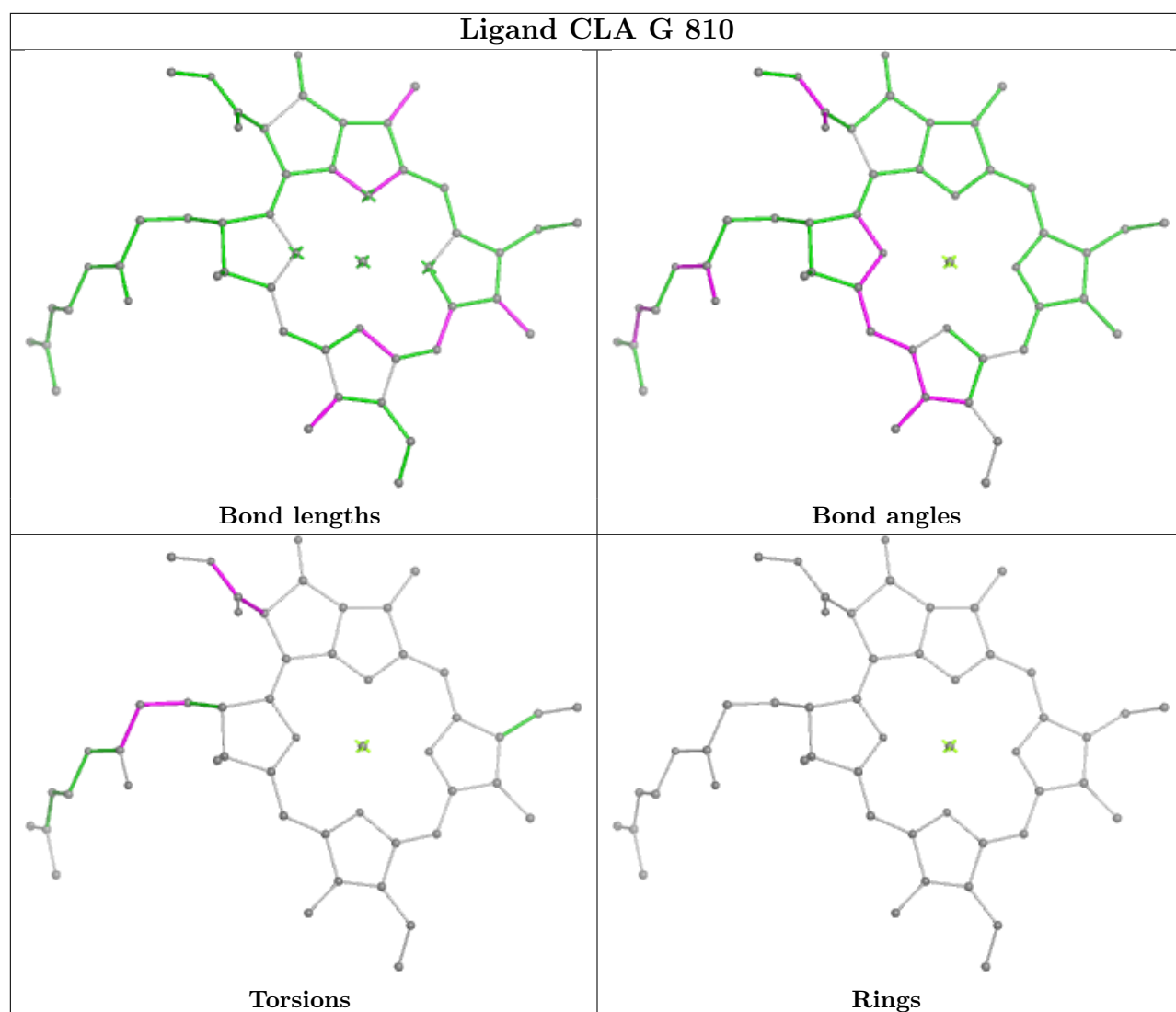


## Ligand BCR b 844



## Ligand CLA b 820





## 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.

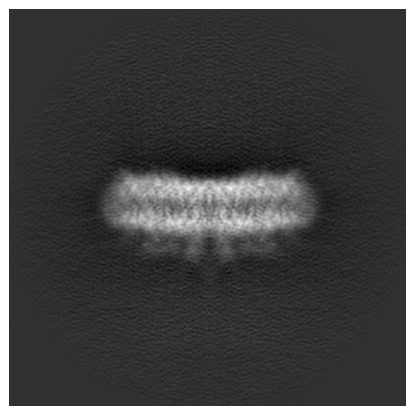
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13898. These allow visual inspection of the internal detail of the map and identification of artifacts.

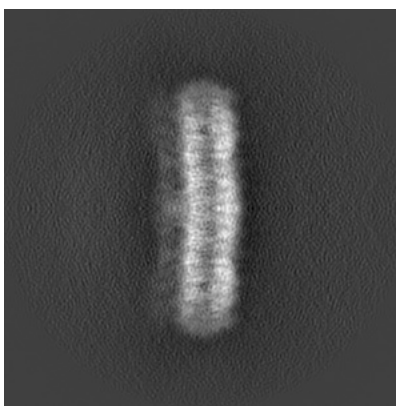
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

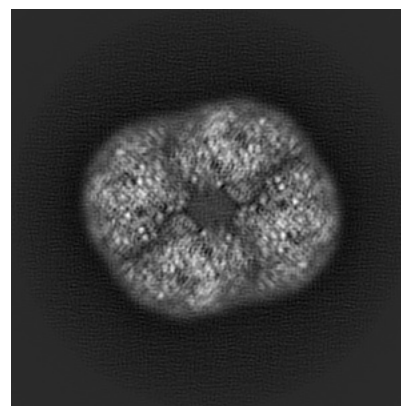
#### 6.1.1 Primary map



X

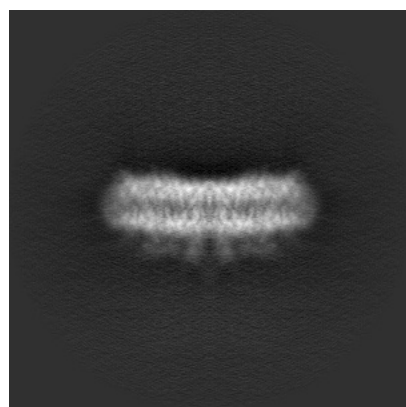


Y

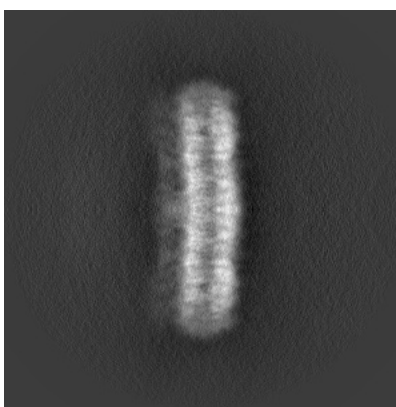


Z

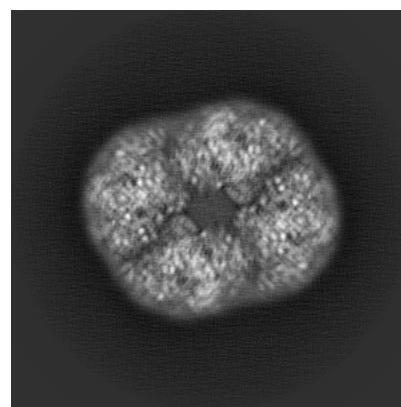
#### 6.1.2 Raw map



X



Y

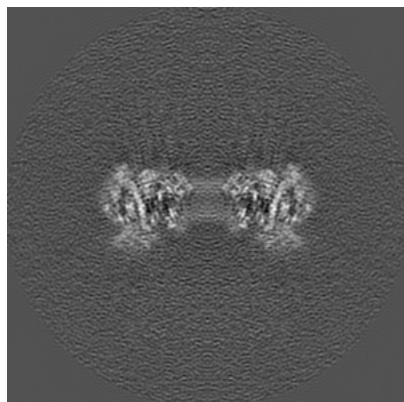


Z

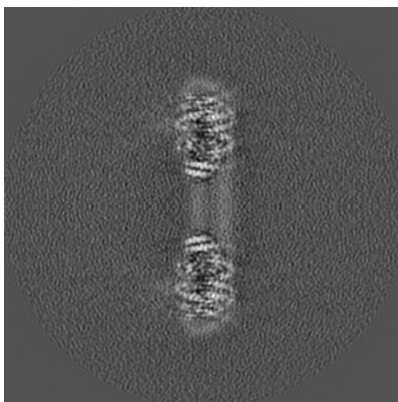
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

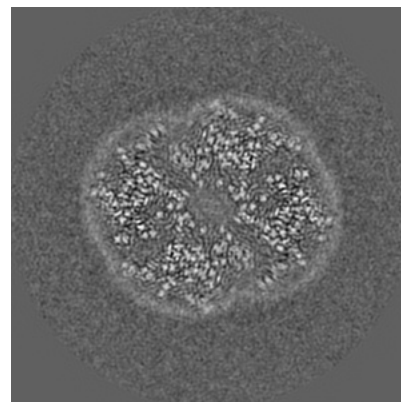
### 6.2.1 Primary map



X Index: 192

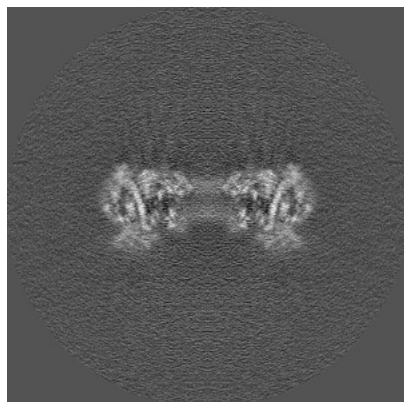


Y Index: 192

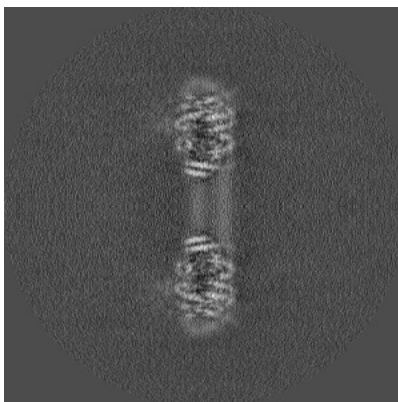


Z Index: 192

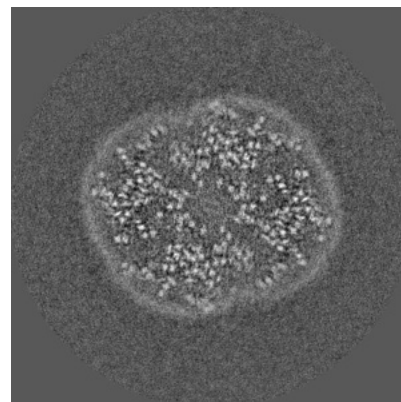
### 6.2.2 Raw map



X Index: 192



Y Index: 192



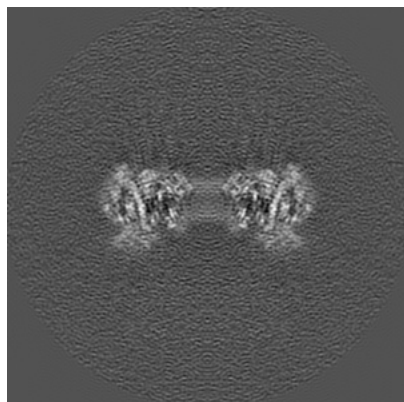
Z Index: 192

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

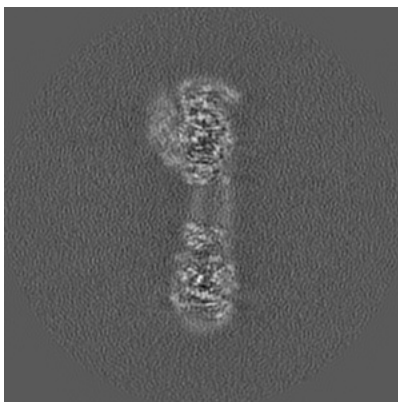


## 6.3 Largest variance slices [i](#)

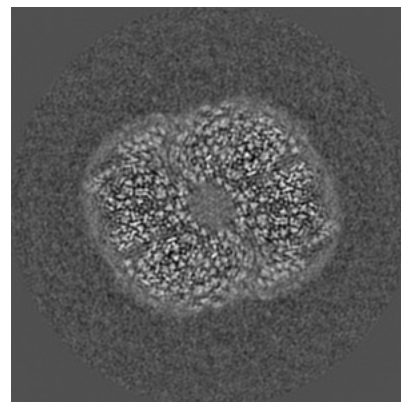
### 6.3.1 Primary map



X Index: 192

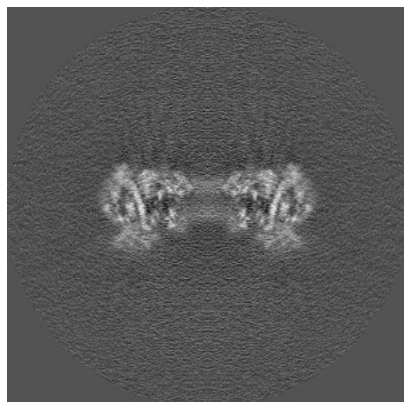


Y Index: 180

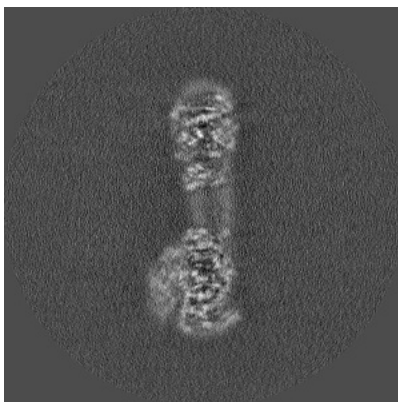


Z Index: 184

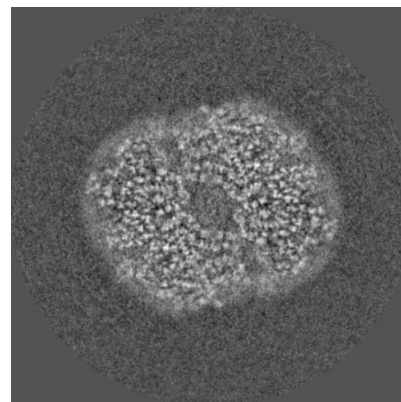
### 6.3.2 Raw map



X Index: 192



Y Index: 204



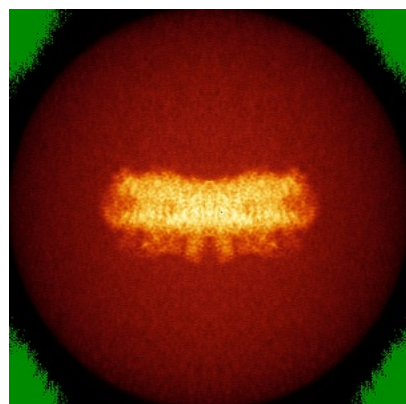
Z Index: 180

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

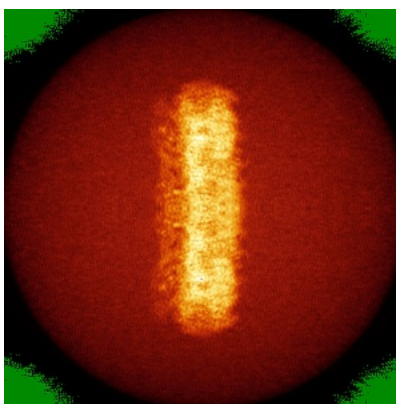


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

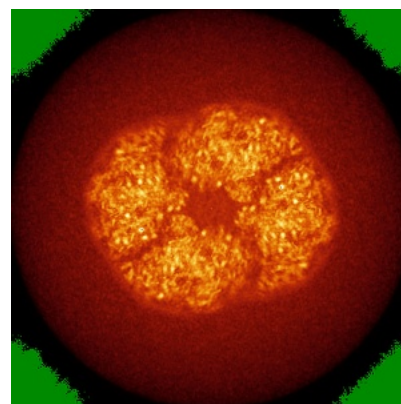
### 6.4.1 Primary map



X

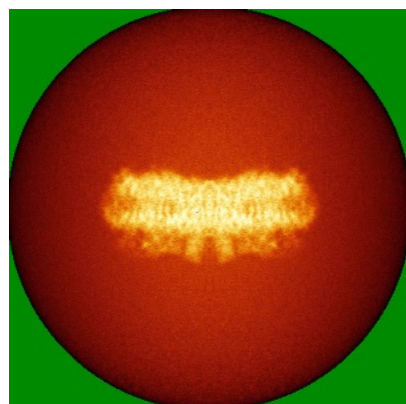


Y

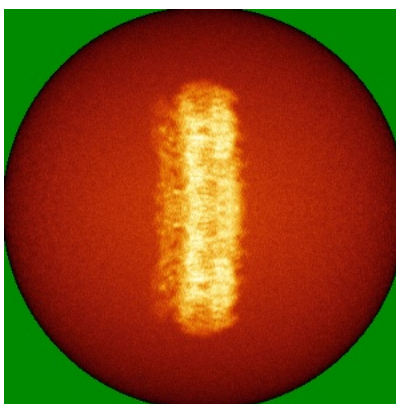


Z

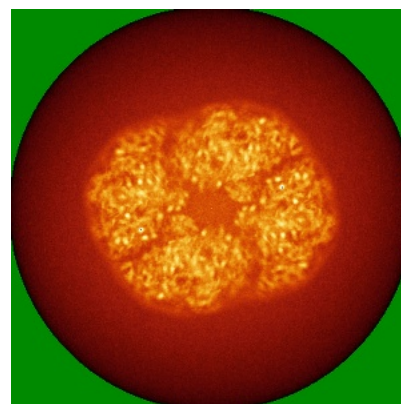
### 6.4.2 Raw map



X



Y

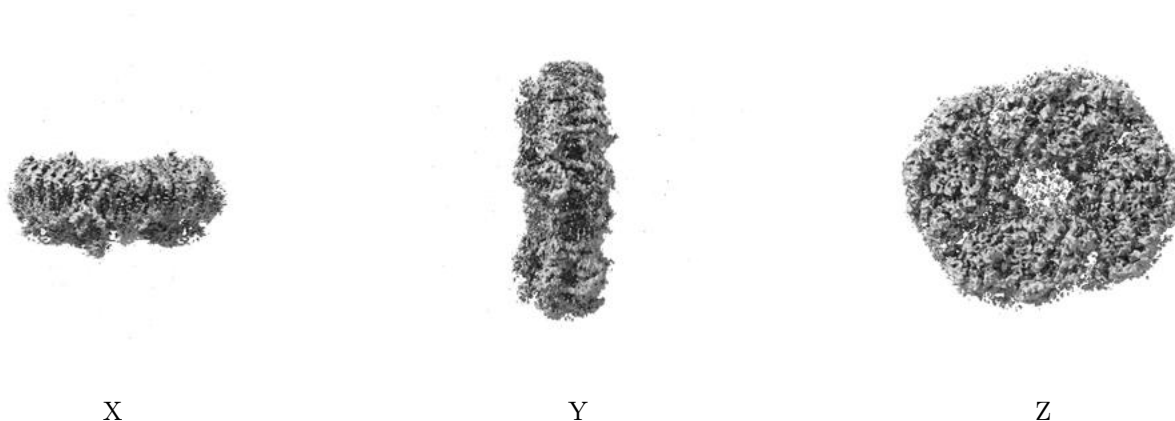


Z

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

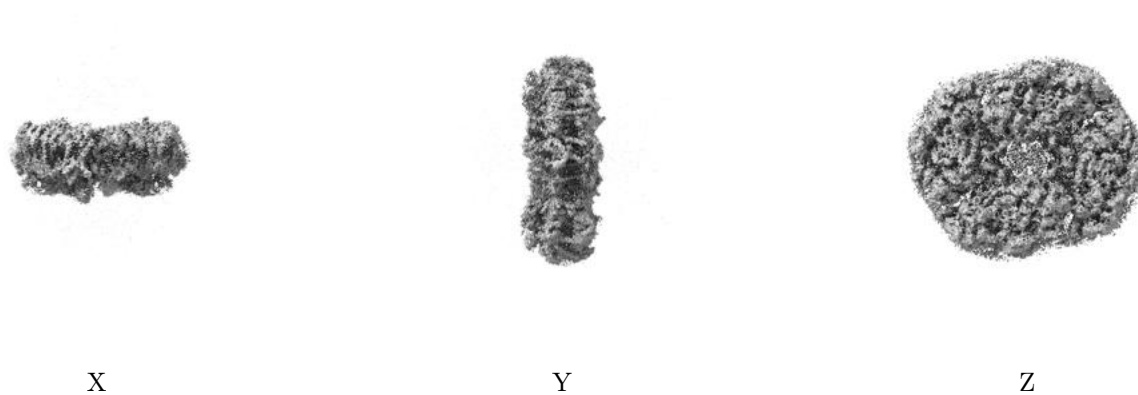
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

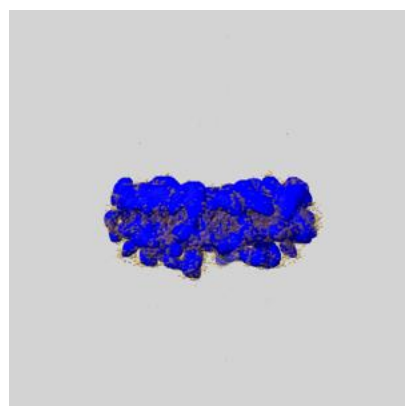
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

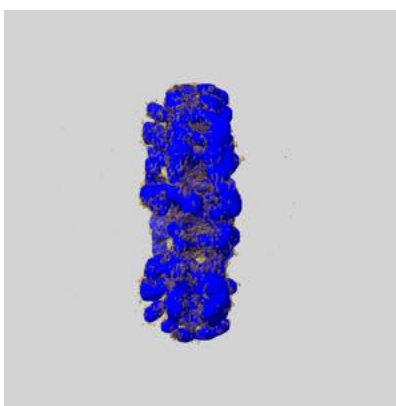
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

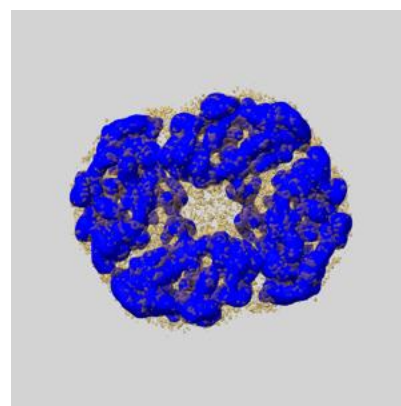
### 6.6.1 emd\_13898\_msk\_1.map [i](#)



X



Y

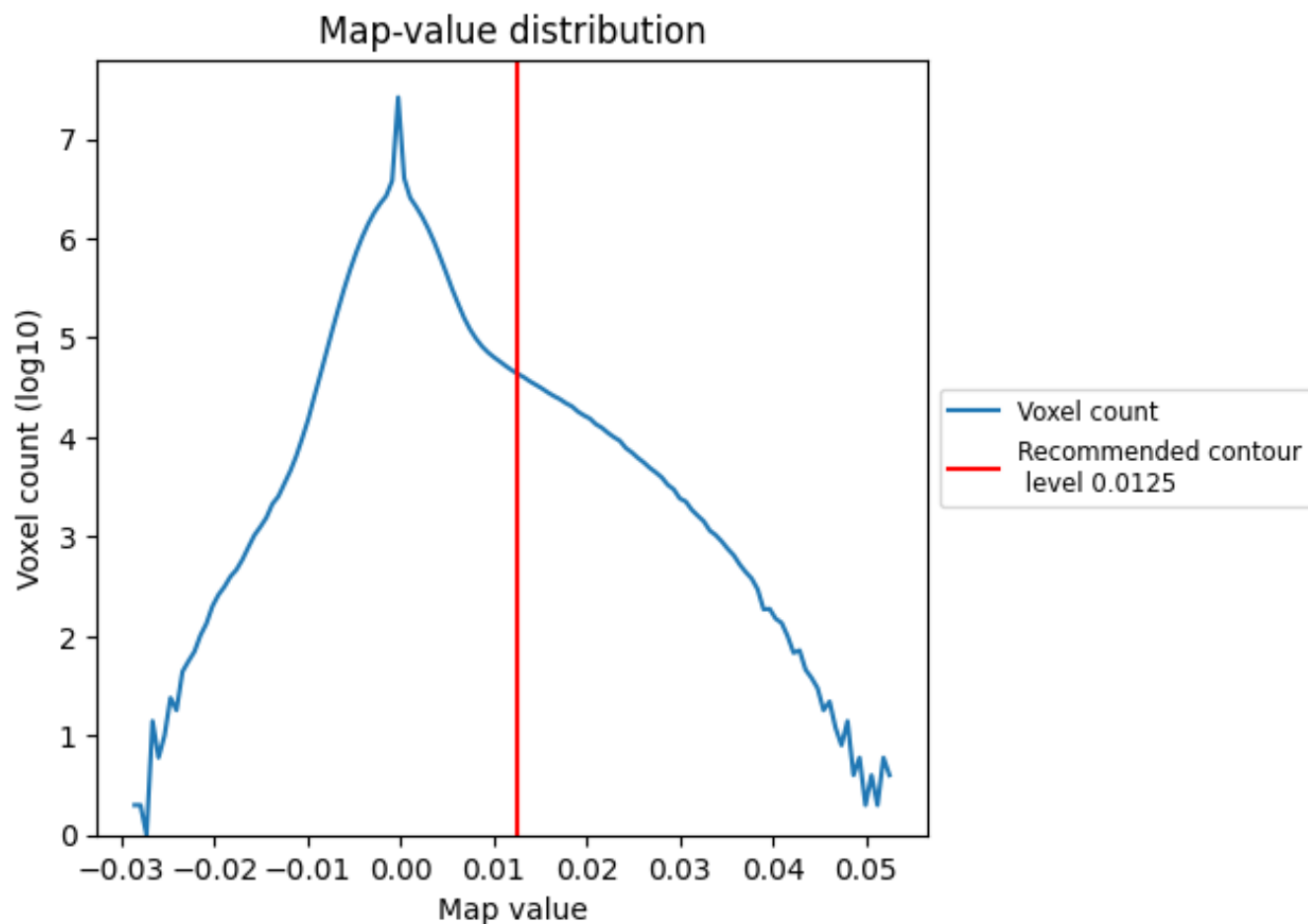


Z

## 7 Map analysis [i](#)

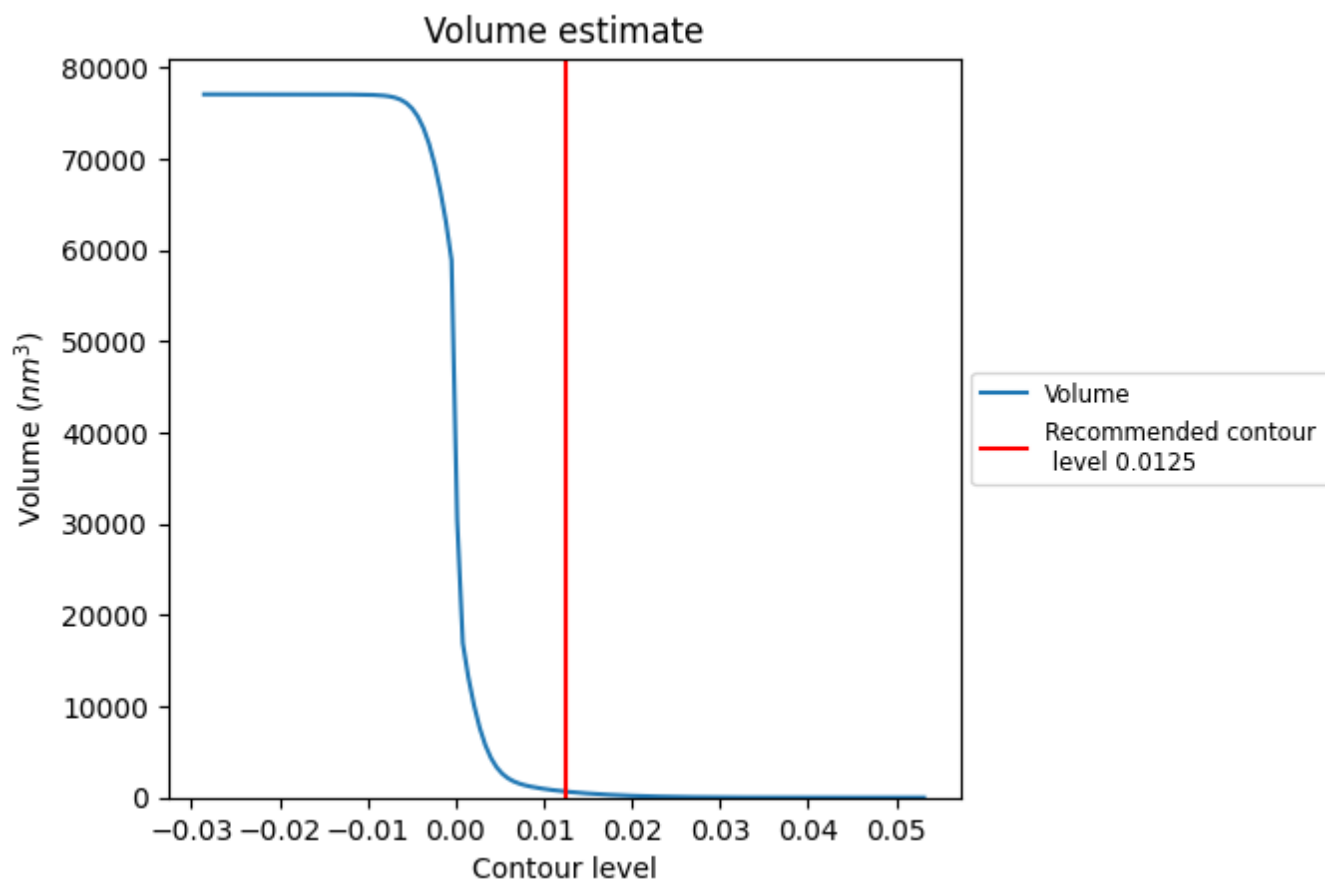
This section contains the results of statistical analysis of the map.

### 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.

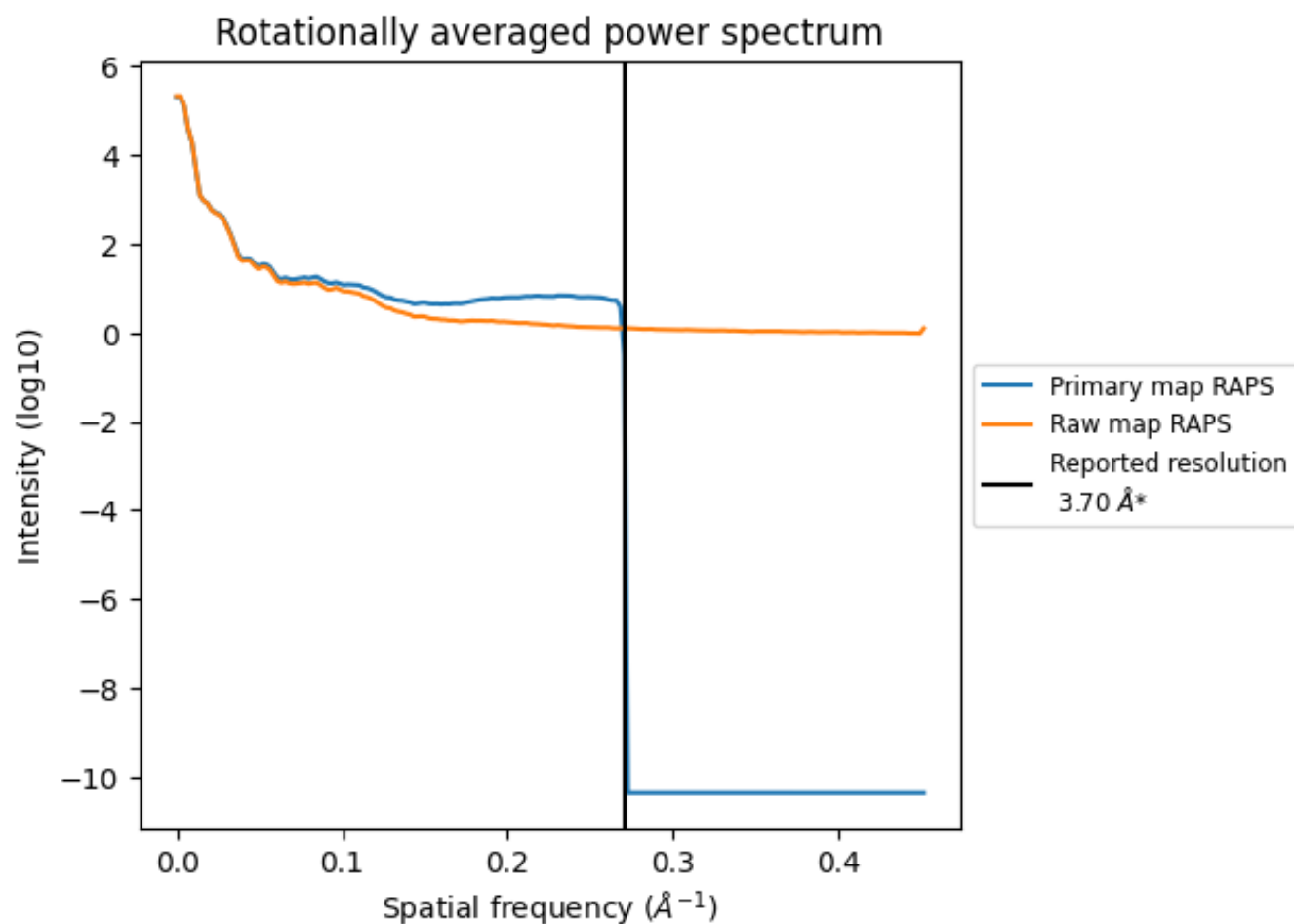
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 658 nm<sup>3</sup>; 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 ⓘ

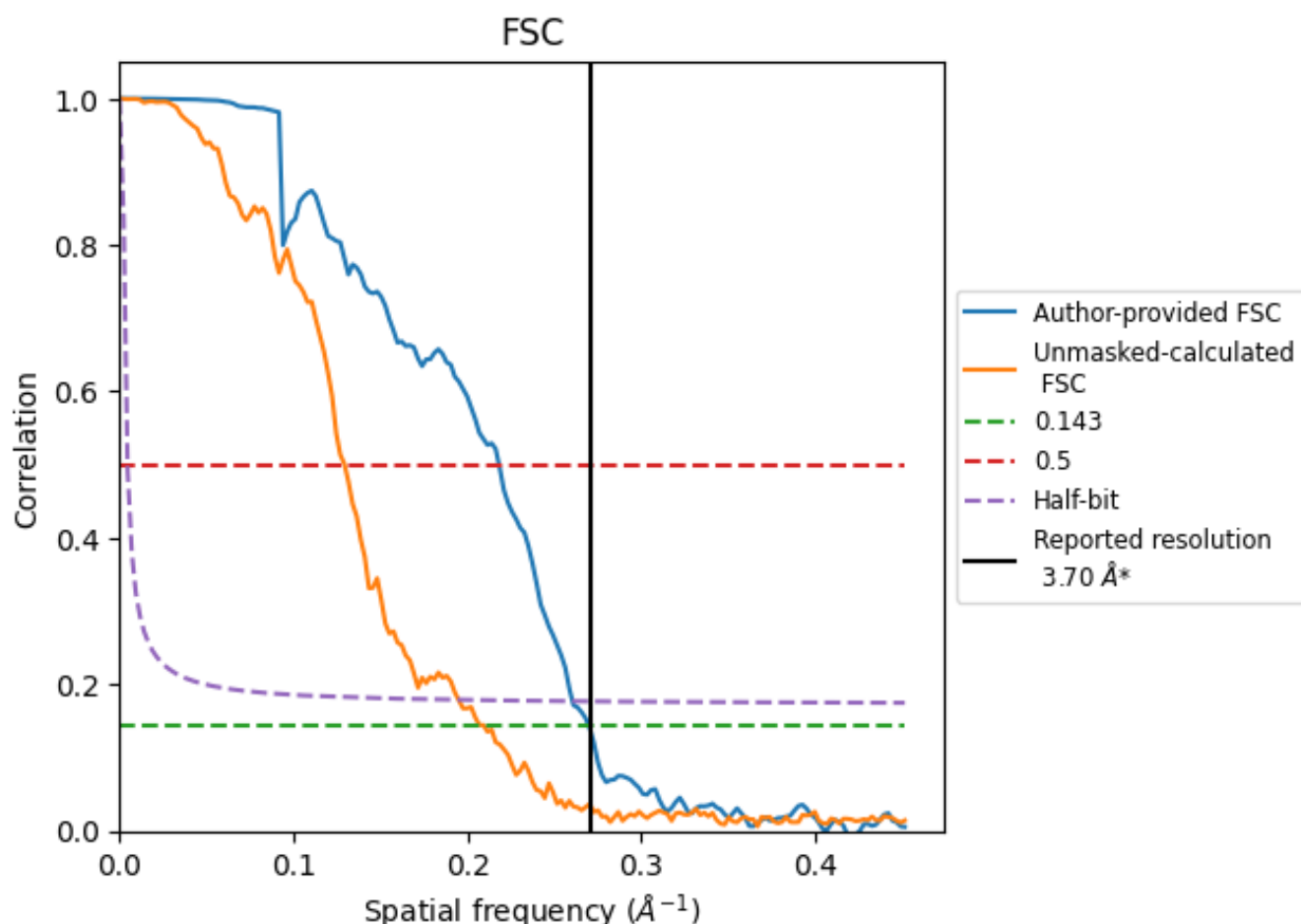


\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.59	3.84
Unmasked-calculated*	4.77	7.73	5.13

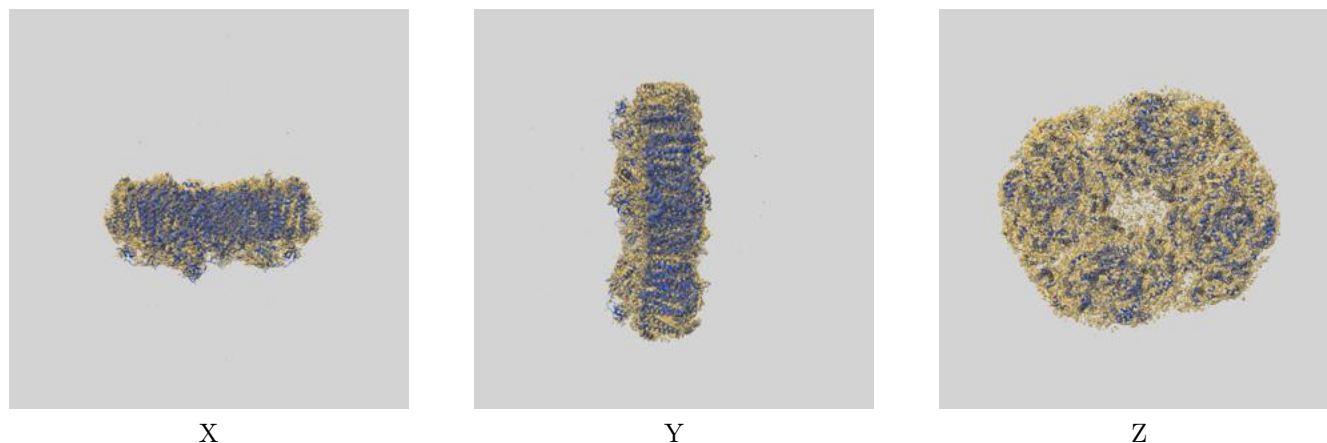
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.77 differs from the reported value 3.7 by more than 10 %



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

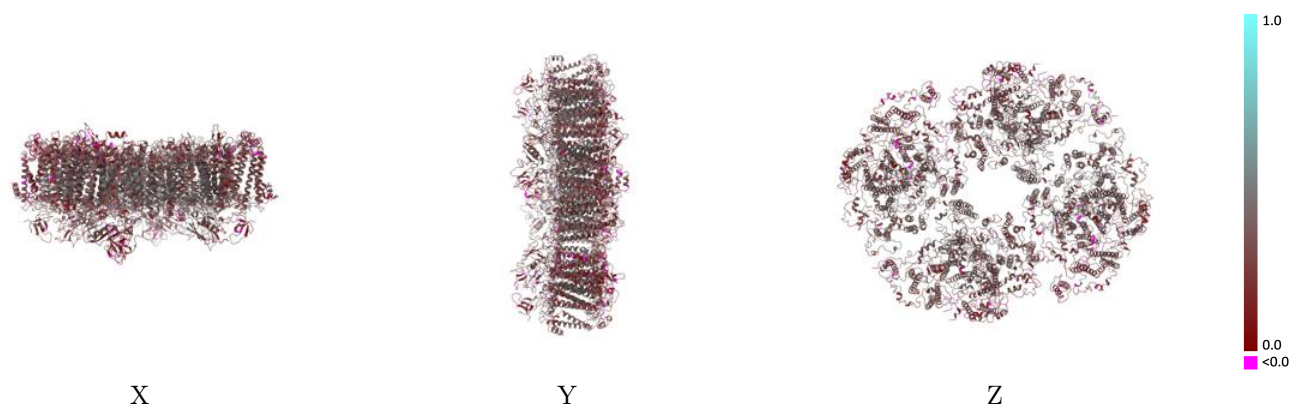
This section contains information regarding the fit between EMDB map EMD-13898 and PDB model 7QCO. Per-residue inclusion information can be found in [section 3](#) on [page 42](#).

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



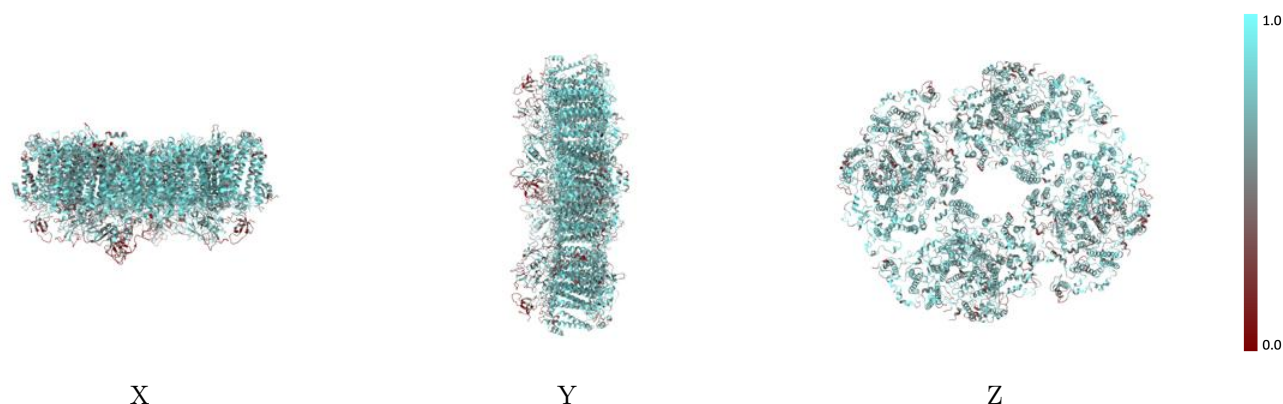
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



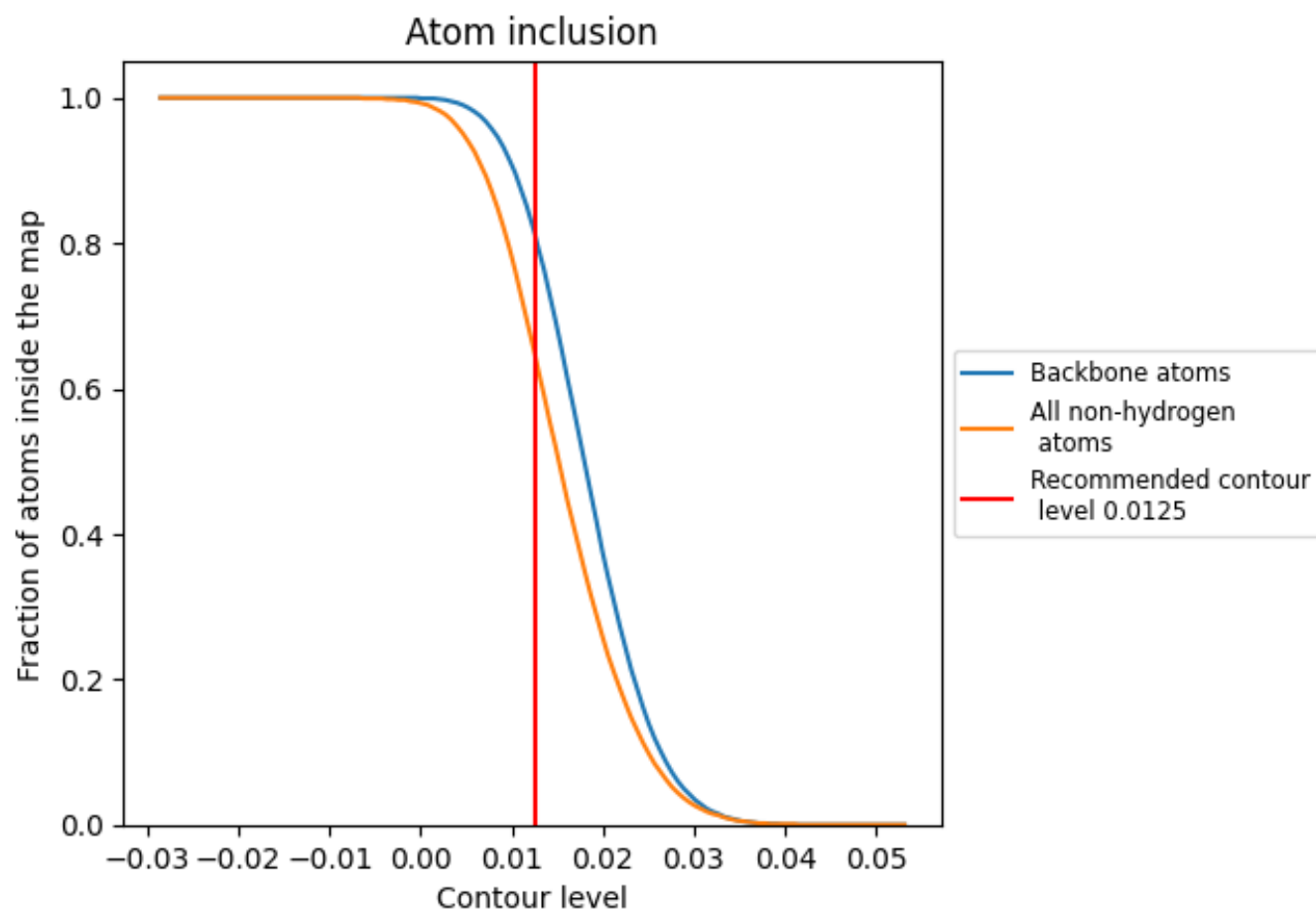
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0125).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6500	 0.3260
A	 0.7060	 0.3530
B	 0.6540	 0.3250
C	 0.6330	 0.2920
D	 0.5610	 0.3410
E	 0.6410	 0.2980
F	 0.6020	 0.2680
G	 0.7410	 0.3840
H	 0.6010	 0.2430
I	 0.5870	 0.3220
J	 0.4660	 0.2660
K	 0.6510	 0.2800
L	 0.7000	 0.3730
M	 0.5400	 0.2970
N	 0.4420	 0.3070
O	 0.5780	 0.3140
P	 0.6930	 0.3780
Q	 0.4970	 0.3000
R	 0.4300	 0.1660
S	 0.5970	 0.3020
T	 0.6760	 0.3850
V	 0.3020	 0.1980
W	 0.2600	 0.1520
a	 0.6340	 0.2930
b	 0.7440	 0.3820
c	 0.6000	 0.2430
d	 0.4280	 0.3040
e	 0.7080	 0.3510
f	 0.5790	 0.3130
g	 0.6580	 0.3250
h	 0.6160	 0.2860
i	 0.6870	 0.3730
j	 0.5170	 0.3010
k	 0.4300	 0.1650
l	 0.5960	 0.3030



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
m	 0.6650	 0.3820
n	 0.5660	 0.3430
o	 0.6020	 0.2660
p	 0.5720	 0.3100
q	 0.4690	 0.2620
r	 0.6460	 0.2780
s	 0.6880	 0.3610
t	 0.5530	 0.3010
v	 0.3650	 0.2490
w	 0.2600	 0.1690