



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 07:58 AM JST

PDB ID : 7WFD  
EMDB ID : EMD-32462  
Title : Left PSI in the cyclic electron transport supercomplex NDH-PSI from Arabidopsis  
Authors : Pan, X.; Li, M.  
Deposited on : 2021-12-26  
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

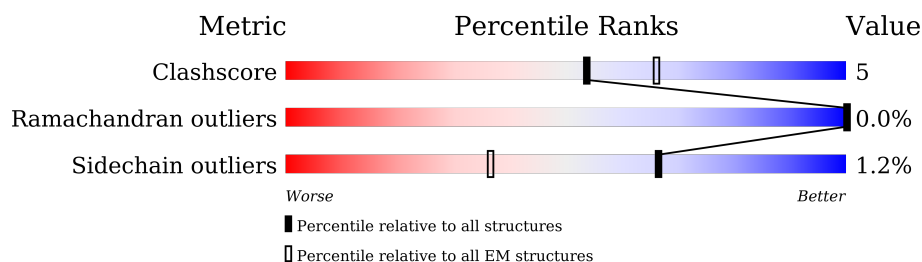
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.25 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)
Clashscore	210492	15764
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	AA	750	 88% 11% .
2	AB	734	 85% 15%
3	AC	81	 78% 21% .
4	AD	204	 60% 9% 31%
5	AE	143	 42% 5% 53%
6	AF	221	 62% 7% 31%
7	AG	160	 55% 6% 39%
8	AH	145	 59% 6% 34%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	AI	37	
10	AJ	44	
11	AK	130	
12	AL	219	
13	A1	241	
14	A3	273	
15	A4	251	
16	A6	270	

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
17	CLA	A1	304	X	-	-	-
17	CLA	A1	305	X	-	-	-
17	CLA	A1	306	X	-	-	-
17	CLA	A1	307	X	-	-	-
17	CLA	A1	309	X	-	-	-
17	CLA	A1	310	X	-	-	-
17	CLA	A1	311	X	-	-	-
17	CLA	A1	312	X	-	-	-
17	CLA	A1	313	X	-	-	-
17	CLA	A1	314	X	-	-	-
17	CLA	A1	315	X	-	-	-
17	CLA	A1	316	X	-	-	-
17	CLA	A3	302	X	-	-	-
17	CLA	A3	303	X	-	-	-
17	CLA	A3	304	X	-	-	-
17	CLA	A3	305	X	-	-	-
17	CLA	A3	306	X	-	-	-
17	CLA	A3	308	X	-	-	-
17	CLA	A3	309	X	-	-	-
17	CLA	A3	310	X	-	-	-
17	CLA	A3	311	X	-	-	-
17	CLA	A3	312	X	-	-	-
17	CLA	A3	314	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A3	315	X	-	-	-
17	CLA	A4	301	X	-	-	-
17	CLA	A4	302	X	-	-	-
17	CLA	A4	303	X	-	-	-
17	CLA	A4	307	X	-	-	-
17	CLA	A4	308	X	-	-	-
17	CLA	A4	309	X	-	-	-
17	CLA	A4	310	X	-	-	-
17	CLA	A4	311	X	-	-	-
17	CLA	A4	312	X	-	-	-
17	CLA	A4	313	X	-	-	-
17	CLA	A6	601	X	-	-	-
17	CLA	A6	602	X	-	-	-
17	CLA	A6	603	X	-	-	-
17	CLA	A6	604	X	-	-	-
17	CLA	A6	608	X	-	-	-
17	CLA	A6	609	X	-	-	-
17	CLA	A6	610	X	-	-	-
17	CLA	A6	611	X	-	-	-
17	CLA	A6	612	X	-	-	-
17	CLA	A6	613	X	-	-	-
17	CLA	AA	801	X	-	-	-
17	CLA	AA	802	X	-	-	-
17	CLA	AA	803	X	-	-	-
17	CLA	AA	805	X	-	-	-
17	CLA	AA	806	X	-	-	-
17	CLA	AA	807	X	-	-	-
17	CLA	AA	808	X	-	-	-
17	CLA	AA	809	X	-	-	-
17	CLA	AA	810	X	-	-	-
17	CLA	AA	811	X	-	-	-
17	CLA	AA	812	X	-	-	-
17	CLA	AA	813	X	-	-	-
17	CLA	AA	814	X	-	-	-
17	CLA	AA	816	X	-	-	-
17	CLA	AA	817	X	-	-	-
17	CLA	AA	819	X	-	-	-
17	CLA	AA	820	X	-	-	-
17	CLA	AA	821	X	-	-	-
17	CLA	AA	822	X	-	-	-
17	CLA	AA	823	X	-	-	-
17	CLA	AA	824	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	AA	825	X	-	-	-
17	CLA	AA	826	X	-	-	-
17	CLA	AA	827	X	-	-	-
17	CLA	AA	828	X	-	-	-
17	CLA	AA	829	X	-	-	-
17	CLA	AA	830	X	-	-	-
17	CLA	AA	831	X	-	-	-
17	CLA	AA	832	X	-	-	-
17	CLA	AA	833	X	-	-	-
17	CLA	AA	835	X	-	-	-
17	CLA	AA	837	X	-	-	-
17	CLA	AA	840	X	-	-	-
17	CLA	AA	842	X	-	-	-
17	CLA	AB	801	X	-	-	-
17	CLA	AB	802	X	-	-	-
17	CLA	AB	803	X	-	-	-
17	CLA	AB	804	X	-	-	-
17	CLA	AB	805	X	-	-	-
17	CLA	AB	806	X	-	-	-
17	CLA	AB	807	X	-	-	-
17	CLA	AB	809	X	-	-	-
17	CLA	AB	810	X	-	-	-
17	CLA	AB	811	X	-	-	-
17	CLA	AB	812	X	-	-	-
17	CLA	AB	813	X	-	-	-
17	CLA	AB	814	X	-	-	-
17	CLA	AB	815	X	-	-	-
17	CLA	AB	816	X	-	-	-
17	CLA	AB	817	X	-	-	-
17	CLA	AB	818	X	-	-	-
17	CLA	AB	819	X	-	-	-
17	CLA	AB	820	X	-	-	-
17	CLA	AB	821	X	-	-	-
17	CLA	AB	822	X	-	-	-
17	CLA	AB	824	X	-	-	-
17	CLA	AB	825	X	-	-	-
17	CLA	AB	826	X	-	-	-
17	CLA	AB	827	X	-	-	-
17	CLA	AB	828	X	-	-	-
17	CLA	AB	829	X	-	-	-
17	CLA	AB	830	X	-	-	-
17	CLA	AB	831	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	AB	833	X	-	-	-
17	CLA	AB	834	X	-	-	-
17	CLA	AB	837	X	-	-	-
17	CLA	AB	839	X	-	-	-
17	CLA	AB	840	X	-	-	-
17	CLA	AB	841	X	-	-	-
17	CLA	AB	842	X	-	-	-
17	CLA	AF	802	X	-	-	-
17	CLA	AF	803	X	-	-	-
17	CLA	AF	804	X	-	-	-
17	CLA	AG	201	X	-	-	-
17	CLA	AG	203	X	-	-	-
17	CLA	AG	204	X	-	-	-
17	CLA	AH	201	X	-	-	-
17	CLA	AJ	102	X	-	-	-
17	CLA	AK	201	X	-	-	-
17	CLA	AK	203	X	-	-	-
17	CLA	AK	204	X	-	-	-
17	CLA	AL	302	X	-	-	-
17	CLA	AL	304	X	-	-	-
26	CHL	A1	303	X	-	-	-
26	CHL	A1	308	X	-	-	-
26	CHL	A3	307	X	-	-	-
26	CHL	A3	320	X	-	-	-
26	CHL	A4	304	X	-	-	-
26	CHL	A4	305	X	-	-	-
26	CHL	A4	306	X	-	-	-
26	CHL	A4	314	X	-	-	-
26	CHL	A6	605	X	-	-	-
26	CHL	A6	606	X	-	-	-
26	CHL	A6	607	X	-	-	-

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 35603 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	AA	742	Total	C	N	O	S	0	0
			5839	3826	992	1003	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	734	Total	C	N	O	S	0	0
			5862	3847	999	1001	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	141	Total	C	N	O	S	0	0
			1112	712	193	203	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AE	67	Total	C	N	O	0	0
			530	341	94	95		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	153	Total	C	N	O	S	0	0
			1213	792	208	210	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AG	98	Total	C	N	O	0	0
			767	499	125	143		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AH	95	Total	C	N	O	0	0
			730	476	119	135		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	33	Total	C	N	O	S	0	0
			257	175	41	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	42	Total	C	N	O	S	0	0
			338	230	51	56	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	65	Total	C	N	O	S	0	0
			451	290	74	84	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	157	Total	C	N	O	S	0	0
			1173	775	187	209	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	196	Total	C	N	O	S	0	0
			1511	984	251	271	5		

- Molecule 14 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A3	219	Total	C	N	O	S	0	0
			1675	1096	272	302	5		

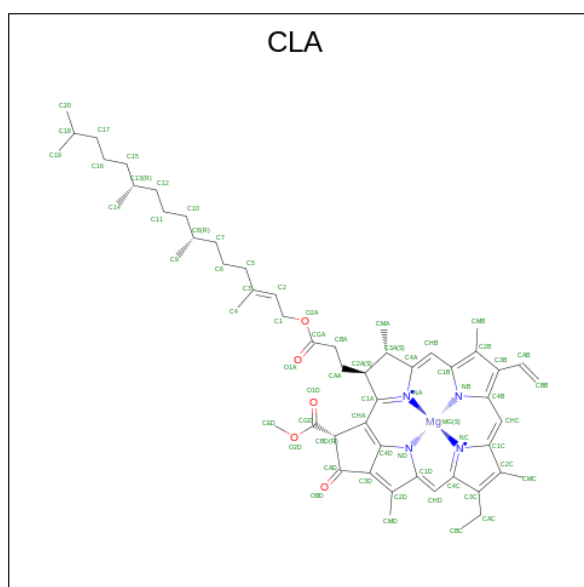
- Molecule 15 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A4	197	Total	C	N	O	S	0	0
			1562	1022	254	283	3		

- Molecule 16 is a protein called Photosystem I chlorophyll a/b-binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A6	212	Total	C	N	O	S	0	0
			1671	1088	272	299	12		

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	AA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	AA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
17	AA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
17	AB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			51	42	1	4	4	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	AB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
17	AB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	AB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	AF	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	AF	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	AF	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	AG	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
17	AG	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	AG	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AH	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	AJ	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	AK	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
17	AK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	AK	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	AL	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	AL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	AL	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	A1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	

*Continued on next page...*

*Continued from previous page...*

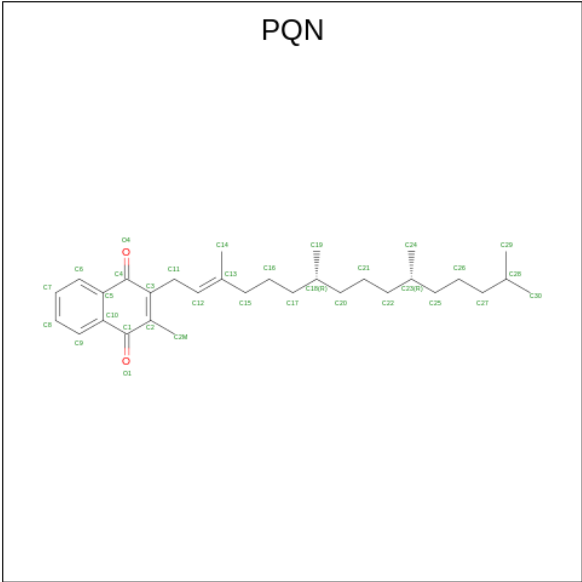
Mol	Chain	Residues	Atoms					AltConf
17	A1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
17	A3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A3	1	Total	C	Mg	N	O	0
			42	32	1	4	5	
17	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
17	A3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	A3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	A3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
17	A3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

*Continued on next page...*

*Continued from previous page...*

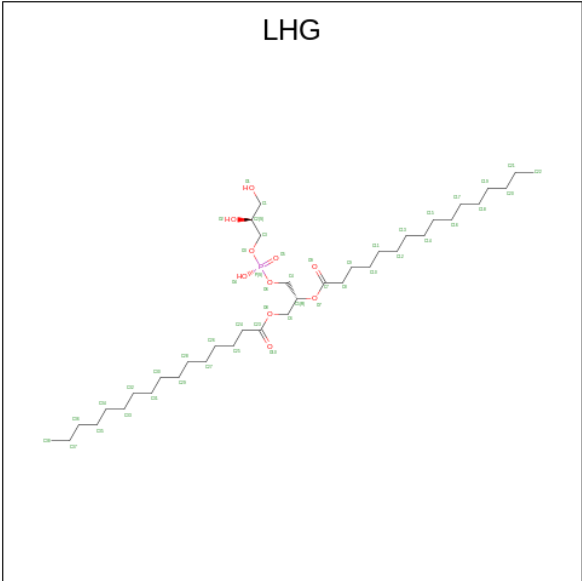
Mol	Chain	Residues	Atoms					AltConf
17	A4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	A6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	A6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
17	A6	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
17	A6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	AA	1	Total	C	O	0
			33	31	2	
18	AB	1	Total	C	O	0
			33	31	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



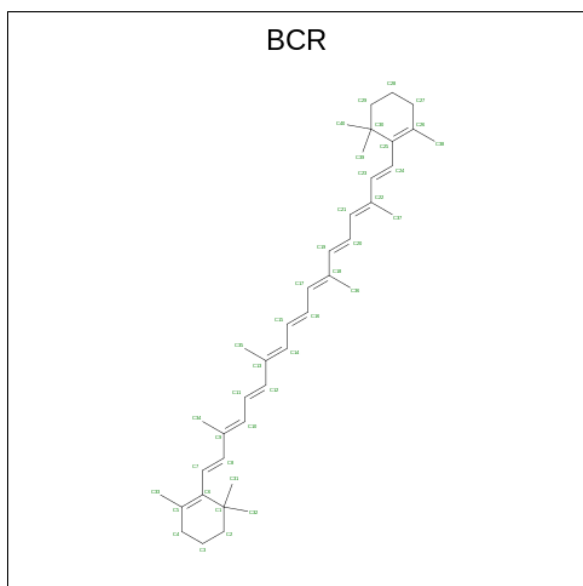
Mol	Chain	Residues	Atoms				AltConf
19	AA	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
19	AJ	1	Total	C	O	P	0
			40	29	10	1	
19	A1	1	Total	C	O	P	0
			38	27	10	1	
19	A1	1	Total	C	O	P	0
			36	25	10	1	
19	A1	1	Total	C	O	P	0
			49	38	10	1	
19	A3	1	Total	C	O	P	0
			36	25	10	1	
19	A3	1	Total	C	O	P	0
			23	12	10	1	
19	A6	1	Total	C	O	P	0
			36	25	10	1	

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
20	AA	1	Total	C	0
			40	40	
20	AA	1	Total	C	0
			40	40	
20	AA	1	Total	C	0
			40	40	
20	AA	1	Total	C	0
			40	40	

*Continued on next page...*

*Continued from previous page...*

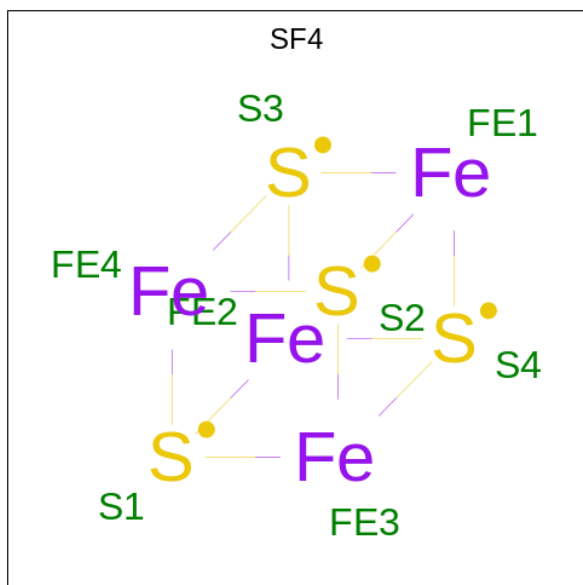
Mol	Chain	Residues	Atoms	AltConf
20	AA	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AB	1	Total C 40 40	0
20	AF	1	Total C 40 40	0
20	AF	1	Total C 40 40	0
20	AG	1	Total C 40 40	0
20	AI	1	Total C 40 40	0
20	AI	1	Total C 40 40	0
20	AJ	1	Total C 40 40	0
20	AJ	1	Total C 40 40	0
20	AK	1	Total C 40 40	0
20	AK	1	Total C 40 40	0
20	AL	1	Total C 40 40	0
20	AL	1	Total C 40 40	0
20	A1	1	Total C 40 40	0
20	A3	1	Total C 40 40	0
20	A4	1	Total C 40 40	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
20	A6	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).

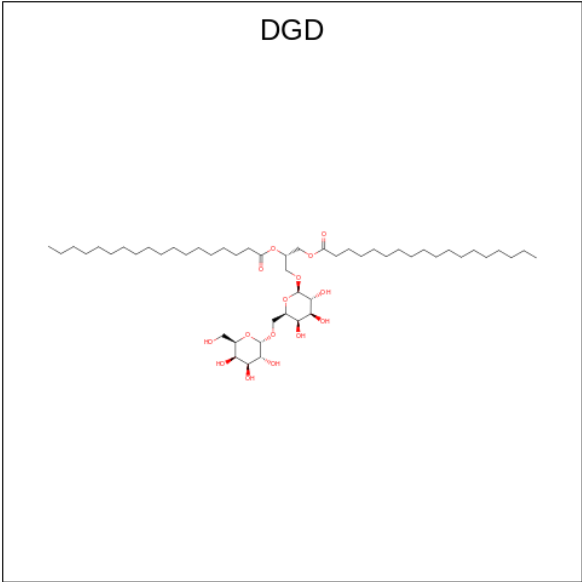


Mol	Chain	Residues	Atoms	AltConf
21	AA	1	Total Fe S 8 4 4	0
21	AC	1	Total Fe S 8 4 4	0
21	AC	1	Total Fe S 8 4 4	0

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $\text{C}_{24}\text{H}_{46}\text{O}_{11}$ ).

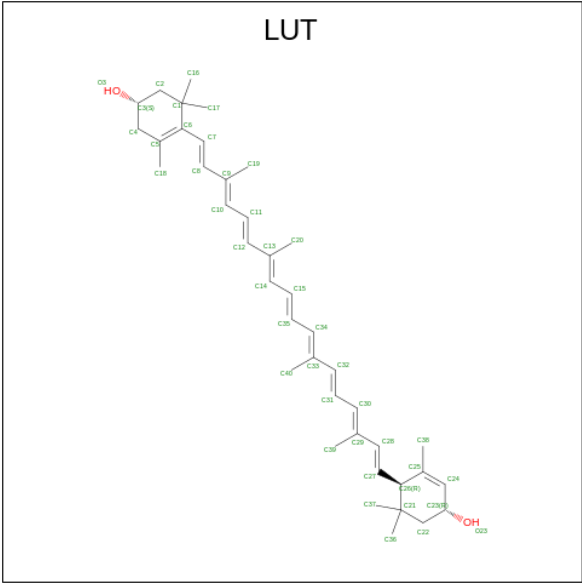


- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
23	AB	1	Total	C	O	0
			66	51	15	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



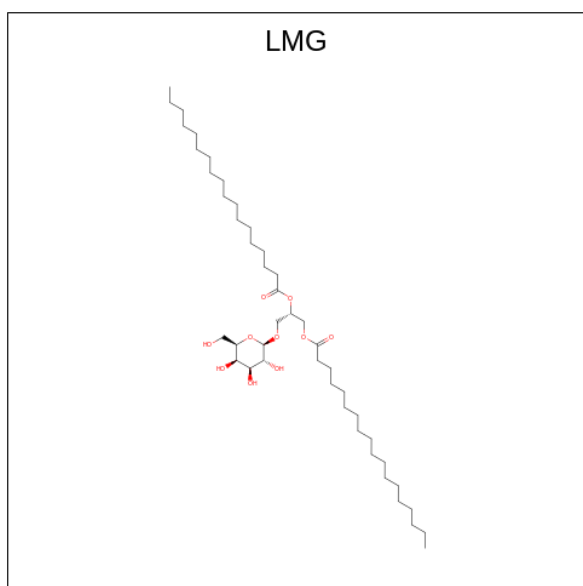
Mol	Chain	Residues	Atoms			AltConf
24	AF	1	Total	C	O	0
			42	40	2	
24	A1	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

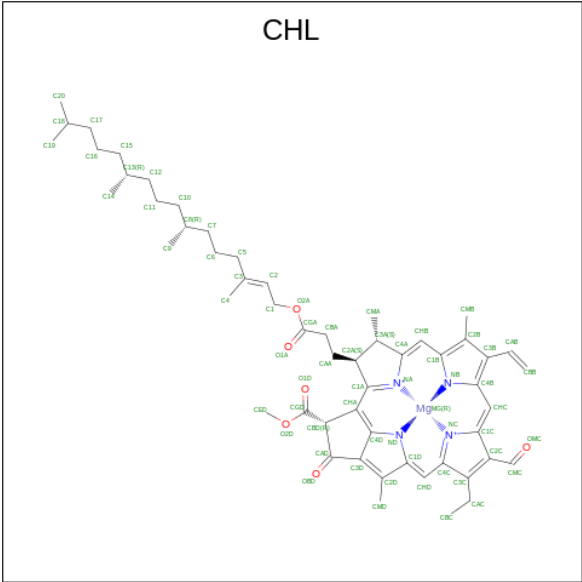
Mol	Chain	Residues	Atoms			AltConf
24	A3	1	Total	C	O	0
			42	40	2	
24	A4	1	Total	C	O	0
			42	40	2	
24	A6	1	Total	C	O	0
			42	40	2	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



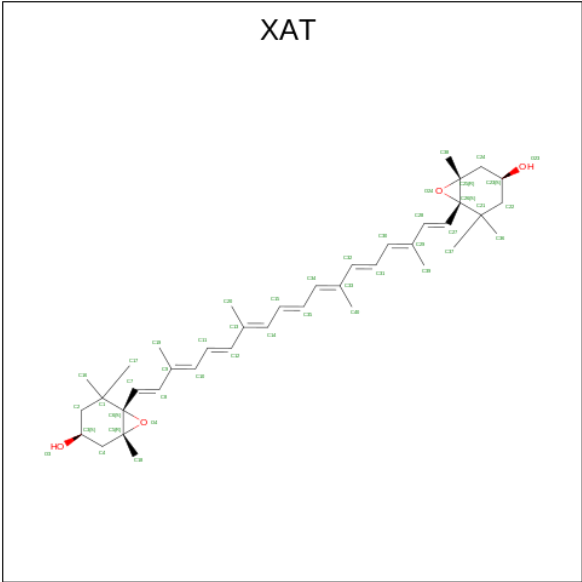
Mol	Chain	Residues	Atoms			AltConf
25	AG	1	Total	C	O	0
			38	28	10	
25	A1	1	Total	C	O	0
			44	34	10	
25	A4	1	Total	C	O	0
			39	29	10	

- Molecule 26 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	A1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
26	A1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
26	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	A3	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
26	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
26	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	A4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
26	A6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
26	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
26	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

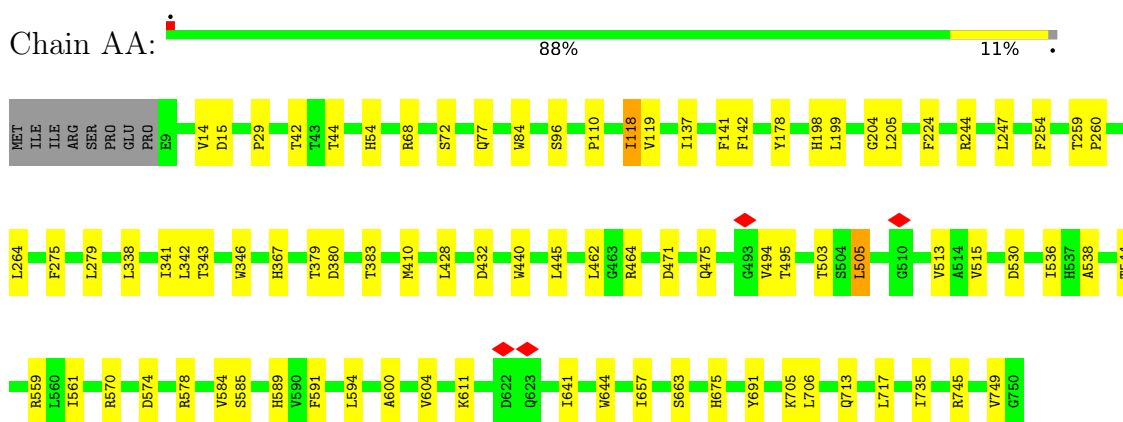


Mol	Chain	Residues	Atoms			AltConf
27	A1	1	Total	C	O	0
			44	40	4	
27	A3	1	Total	C	O	0
			44	40	4	
27	A4	1	Total	C	O	0
			44	40	4	
27	A6	1	Total	C	O	0
			44	40	4	

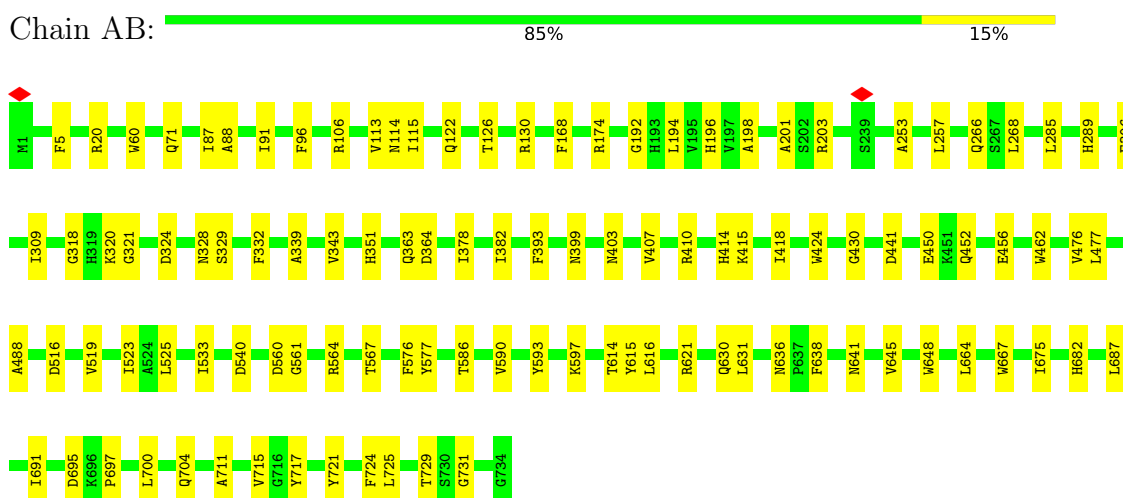
### 3 Residue-property plots

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

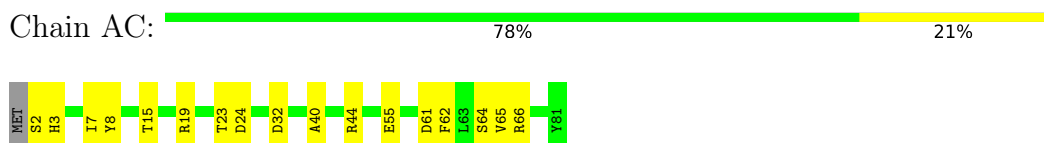
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2




- Molecule 3: Photosystem I iron-sulfur center






- Molecule 9: Photosystem I reaction center subunit VIII

Chain AI:  89% 11%



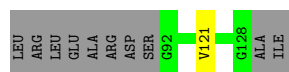
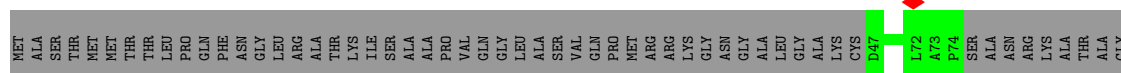
- Molecule 10: Photosystem I reaction center subunit IX

Chain AJ:  84% 11% 5%



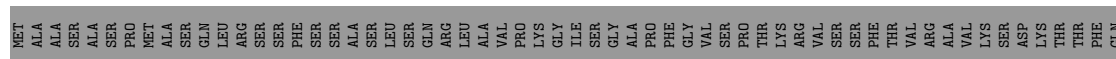
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain AK:  49% 50%



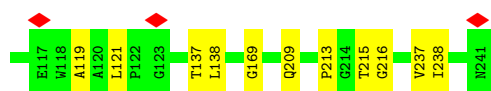
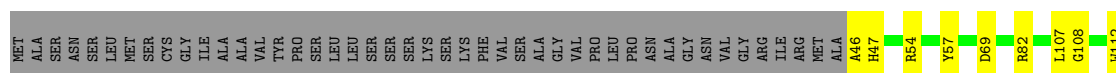
- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

Chain AL:  64% 7% 28%




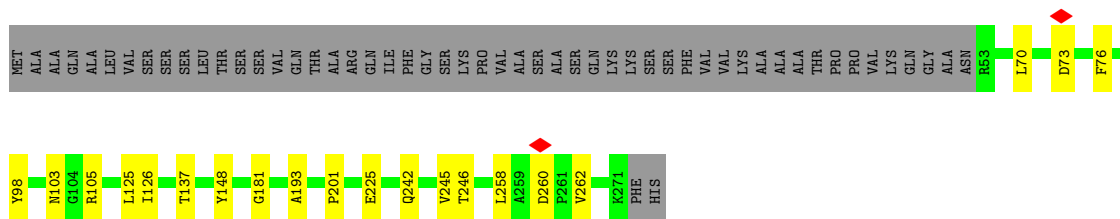
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain A1:  73% 8% 19%



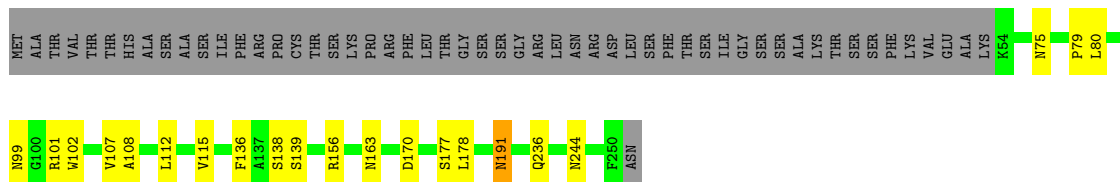
- Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

Chain A3:  73% 7% 20%



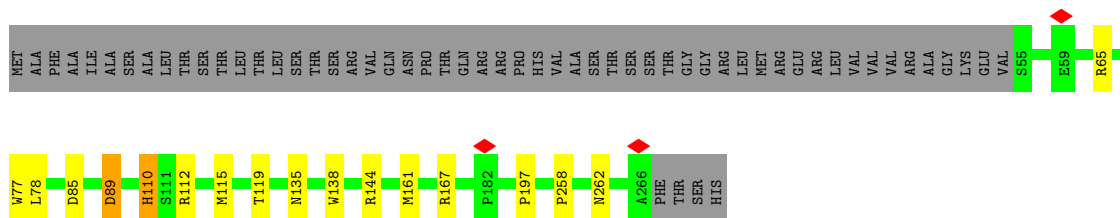
- Molecule 15: Chlorophyll a-b binding protein 4, chloroplastic

Chain A4: 70% 8% 22%



- Molecule 16: Photosystem I chlorophyll a/b-binding protein 6, chloroplastic

Chain A6: 72% 6% 21%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136022	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 ( $e^-/\text{\AA}^2$ )	60.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.422	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, LMU, CLA, CHL, SF4, LHG, DGD, LUT, LMG, PQN, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.38	0/6037	0.53	0/8236
2	AB	0.36	0/6073	0.53	0/8291
3	AC	0.34	0/628	0.59	0/852
4	AD	0.31	0/1140	0.58	0/1542
5	AE	0.32	0/542	0.50	0/736
6	AF	0.31	0/1243	0.53	0/1677
7	AG	0.36	0/787	0.51	0/1067
8	AH	0.32	0/751	0.52	0/1018
9	AI	0.30	0/264	0.45	0/359
10	AJ	0.33	0/348	0.56	0/474
11	AK	0.29	0/456	0.51	0/617
12	AL	0.31	0/1208	0.52	0/1650
13	A1	0.31	0/1562	0.51	0/2131
14	A3	0.31	0/1726	0.51	0/2347
15	A4	0.33	0/1611	0.52	0/2194
16	A6	0.31	0/1732	0.54	0/2363
All	All	0.34	0/26108	0.53	0/35554

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	5839	0	5683	71	0
2	AB	5862	0	5649	92	0
3	AC	615	0	592	14	0
4	AD	1112	0	1122	10	0
5	AE	530	0	536	11	0
6	AF	1213	0	1243	11	0
7	AG	767	0	746	10	0
8	AH	730	0	720	7	0
9	AI	257	0	274	0	0
10	AJ	338	0	351	4	0
11	AK	451	0	462	1	0
12	AL	1173	0	1162	15	0
13	A1	1511	0	1464	13	0
14	A3	1675	0	1647	14	0
15	A4	1562	0	1516	16	0
16	A6	1671	0	1599	16	0
17	A1	575	0	447	6	0
17	A3	575	0	420	3	0
17	A4	480	0	376	5	0
17	A6	485	0	399	4	0
17	AA	2411	0	2371	43	0
17	AB	2452	0	2461	38	0
17	AF	140	0	113	0	0
17	AG	131	0	94	4	0
17	AH	60	0	59	0	0
17	AJ	42	0	31	0	0
17	AK	126	0	88	0	0
17	AL	143	0	119	1	0
18	AA	33	0	46	3	0
18	AB	33	0	46	2	0
19	A1	123	0	162	0	0
19	A3	59	0	58	1	0
19	A6	36	0	42	1	0
19	AA	49	0	74	1	0
19	AJ	40	0	53	0	0
20	A1	40	0	56	3	0
20	A3	40	0	56	3	0
20	A4	40	0	56	0	0
20	A6	40	0	56	3	0
20	AA	200	0	280	6	0
20	AB	240	0	336	10	0
20	AF	80	0	112	6	0
20	AG	40	0	56	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AI	80	0	112	1	0
20	AJ	80	0	112	2	0
20	AK	80	0	112	1	0
20	AL	80	0	112	1	0
21	AA	8	0	0	0	0
21	AC	16	0	0	2	0
22	AA	35	0	46	0	0
22	AB	105	0	138	0	0
22	AL	34	0	41	1	0
23	AB	66	0	96	0	0
24	A1	42	0	56	0	0
24	A3	42	0	56	0	0
24	A4	42	0	56	2	0
24	A6	42	0	56	1	0
24	AF	42	0	56	2	0
25	A1	44	0	58	1	0
25	A4	39	0	48	4	0
25	AG	38	0	46	0	0
26	A1	92	0	60	3	0
26	A3	97	0	68	4	0
26	A4	169	0	100	3	0
26	A6	135	0	89	3	0
27	A1	44	0	56	1	0
27	A3	44	0	56	3	0
27	A4	44	0	56	2	0
27	A6	44	0	56	4	0
All	All	35603	0	34975	354	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (354) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:87:ILE:HG23	2:AB:113:VAL:CG1	1.58	1.33
2:AB:87:ILE:CG2	2:AB:113:VAL:HG11	1.78	1.14
7:AG:76:LEU:HD13	17:AG:204:CLA:CMB	1.81	1.09
2:AB:106:ARG:CZ	2:AB:115:ILE:HG12	1.83	1.08
2:AB:687:LEU:HD21	12:AL:91:LEU:HD11	1.34	1.06
2:AB:87:ILE:HG23	2:AB:113:VAL:HG11	1.16	1.06
2:AB:476:VAL:HG12	2:AB:477:LEU:H	1.20	1.00

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:76:LEU:CD1	17:AG:204:CLA:HMB1	1.89	1.00
1:AA:247:LEU:HD21	1:AA:254:PHE:CE2	1.98	0.99
7:AG:76:LEU:HD13	17:AG:204:CLA:HMB1	0.95	0.95
3:AC:7:ILE:HD12	3:AC:40:ALA:O	1.68	0.93
1:AA:72:SER:OG	17:AA:811:CLA:HMD3	1.66	0.93
2:AB:87:ILE:CG2	2:AB:113:VAL:CG1	2.42	0.91
5:AE:87:VAL:HG21	5:AE:138:VAL:CG1	2.04	0.87
17:AA:801:CLA:HAA2	17:AA:801:CLA:HED2	1.60	0.83
3:AC:7:ILE:CD1	3:AC:40:ALA:O	2.28	0.81
2:AB:476:VAL:HG12	2:AB:477:LEU:N	1.95	0.80
2:AB:476:VAL:CG1	2:AB:477:LEU:H	1.94	0.80
5:AE:87:VAL:CG2	5:AE:138:VAL:CG1	2.65	0.73
4:AD:107:GLU:O	4:AD:137:ARG:NH1	2.21	0.73
1:AA:570:ARG:NH1	19:AA:844:LHG:O10	2.23	0.71
7:AG:88:ARG:NH2	7:AG:131:ASP:OD2	2.24	0.71
1:AA:713:GLN:NE2	5:AE:95:TYR:OH	2.23	0.71
3:AC:7:ILE:HG12	3:AC:65:VAL:HA	1.74	0.70
8:AH:71:TRP:HD1	12:AL:169:LEU:HD11	1.55	0.70
1:AA:118:ILE:HD13	1:AA:119:VAL:HG13	1.73	0.70
1:AA:247:LEU:CD2	1:AA:254:PHE:CE2	2.76	0.68
2:AB:106:ARG:CZ	2:AB:115:ILE:CG1	2.68	0.68
1:AA:247:LEU:CD2	1:AA:254:PHE:CD2	2.78	0.67
1:AA:96:SER:OG	1:AA:142:PHE:HZ	1.79	0.66
15:A4:101:ARG:NH2	26:A4:306:CHL:OBD	2.29	0.66
25:A4:318:LMG:H292	20:A6:616:BCR:H332	1.77	0.66
3:AC:55:GLU:OE2	3:AC:66:ARG:NH2	2.30	0.65
1:AA:338:LEU:HD23	1:AA:341:ILE:HD11	1.79	0.65
2:AB:87:ILE:HG23	2:AB:113:VAL:HG13	1.73	0.65
17:AB:834:CLA:O1A	10:AJ:30:ASN:ND2	2.29	0.65
2:AB:113:VAL:HG12	2:AB:114:ASN:N	2.10	0.65
2:AB:523:ILE:HG12	2:AB:590:VAL:HG12	1.78	0.64
13:A1:209:GLN:NE2	13:A1:213:PRO:O	2.30	0.64
26:A1:303:CHL:HMB2	17:A4:313:CLA:O1D	1.97	0.64
2:AB:456:GLU:OE1	6:AF:137:HIS:ND1	2.31	0.64
26:A4:304:CHL:HMB1	26:A4:304:CHL:HBB1	1.81	0.62
2:AB:87:ILE:HG21	2:AB:113:VAL:HG11	1.77	0.62
1:AA:96:SER:OG	1:AA:142:PHE:CZ	2.53	0.62
2:AB:106:ARG:NH2	2:AB:115:ILE:HG12	2.15	0.62
1:AA:247:LEU:HD21	1:AA:254:PHE:CD2	2.35	0.61
4:AD:98:TRP:NE1	4:AD:116:MET:SD	2.72	0.61
2:AB:87:ILE:HD12	2:AB:113:VAL:HG11	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:494:VAL:HG13	1:AA:495:THR:HG23	1.81	0.61
1:AA:536:ILE:HG23	17:AA:801:CLA:H193	1.83	0.61
2:AB:106:ARG:NH1	2:AB:115:ILE:HG12	2.15	0.61
1:AA:594:LEU:HD21	17:AA:830:CLA:HBC1	1.83	0.60
17:AB:801:CLA:O1D	20:AF:801:BCR:H401	2.00	0.60
2:AB:351:HIS:ND1	17:AB:818:CLA:OBD	2.35	0.60
2:AB:687:LEU:HD21	12:AL:91:LEU:CD1	2.20	0.60
13:A1:237:VAL:O	17:A1:316:CLA:NB	2.35	0.59
2:AB:87:ILE:HD12	2:AB:113:VAL:CG1	2.32	0.59
17:AB:822:CLA:CAD	20:AB:844:BCR:H312	2.33	0.59
5:AE:87:VAL:HG21	5:AE:138:VAL:HG12	1.84	0.59
16:A6:135:ASN:O	16:A6:144:ARG:NH2	2.36	0.59
1:AA:538:ALA:HB1	17:AA:838:CLA:HMB3	1.85	0.59
1:AA:735:ILE:HG21	17:AA:828:CLA:HMC2	1.85	0.59
7:AG:120:LYS:HG2	7:AG:120:LYS:O	2.03	0.59
1:AA:84:TRP:HZ3	20:AA:846:BCR:H322	1.68	0.58
13:A1:119:ALA:HB1	13:A1:138:LEU:HD13	1.85	0.58
8:AH:117:TYR:O	8:AH:121:ASN:ND2	2.36	0.58
13:A1:237:VAL:HG23	13:A1:238:ILE:HD12	1.86	0.58
5:AE:87:VAL:CG2	5:AE:138:VAL:HG12	2.33	0.58
17:AA:801:CLA:HMB3	17:AB:802:CLA:OBD	2.04	0.57
6:AF:143:ASP:OD2	6:AF:145:ARG:NE	2.36	0.57
1:AA:259:THR:HG23	1:AA:260:PRO:HD3	1.84	0.57
20:AA:847:BCR:H383	20:AA:847:BCR:H23C	1.87	0.57
2:AB:122:GLN:NE2	2:AB:364:ASP:OD2	2.37	0.57
13:A1:46:ALA:O	13:A1:54:ARG:NH2	2.38	0.57
2:AB:266:GLN:OE1	2:AB:363:GLN:NE2	2.38	0.56
2:AB:450:GLU:OE2	6:AF:119:ARG:NE	2.38	0.56
17:AA:828:CLA:H11	20:AA:849:BCR:H323	1.88	0.56
2:AB:418:ILE:HG23	17:AB:839:CLA:CBB	2.36	0.56
12:AL:169:LEU:HD12	12:AL:170:THR:O	2.05	0.56
26:A1:303:CHL:OBD	15:A4:156:ARG:NH2	2.37	0.56
17:A6:612:CLA:CHB	17:A6:613:CLA:HMD3	2.36	0.56
1:AA:675:HIS:HD1	17:AB:802:CLA:HED2	1.69	0.56
14:A3:245:VAL:HG13	14:A3:246:THR:HG23	1.86	0.56
17:AB:834:CLA:H41	10:AJ:26:LEU:HD23	1.88	0.56
15:A4:75:ASN:HD21	25:A4:318:LMG:HC61	1.69	0.56
12:AL:169:LEU:CD1	12:AL:170:THR:O	2.54	0.56
4:AD:203:ASP:O	4:AD:204:LEU:HG	2.04	0.56
19:A3:301:LHG:O3	19:A3:301:LHG:O1	2.22	0.55
17:AB:827:CLA:H142	20:AB:847:BCR:C21	2.36	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A1:169:GLY:N	17:A1:311:CLA:OBD	2.39	0.55
14:A3:103:ASN:ND2	17:A3:308:CLA:OBD	2.40	0.55
2:AB:113:VAL:CG1	2:AB:114:ASN:N	2.70	0.55
2:AB:87:ILE:HG23	2:AB:113:VAL:HG12	1.76	0.55
1:AA:464:ARG:NH2	17:AA:834:CLA:O1D	2.41	0.54
1:AA:503:THR:HG21	17:AA:835:CLA:HMA2	1.90	0.54
20:AK:205:BCR:H383	20:AK:205:BCR:H23C	1.88	0.54
13:A1:107:LEU:HD12	13:A1:108:GLY:N	2.23	0.54
2:AB:415:LYS:NZ	2:AB:540:ASP:OD1	2.32	0.54
1:AA:247:LEU:HD23	1:AA:254:PHE:CD2	2.43	0.54
2:AB:418:ILE:HG23	17:AB:839:CLA:HBB2	1.90	0.54
2:AB:615:TYR:OH	2:AB:621:ARG:NH2	2.40	0.54
3:AC:7:ILE:HG22	3:AC:8:TYR:N	2.22	0.54
1:AA:244:ARG:NH2	17:AA:815:CLA:OBD	2.41	0.54
13:A1:82:ARG:NH1	17:A1:305:CLA:O1A	2.41	0.53
1:AA:471:ASP:O	1:AA:475:GLN:NE2	2.42	0.53
8:AH:74:TYR:OH	12:AL:79:THR:OG1	2.25	0.53
4:AD:100:SER:OG	4:AD:102:LYS:O	2.27	0.53
2:AB:71:GLN:NE2	17:AB:808:CLA:O1D	2.40	0.53
2:AB:122:GLN:O	2:AB:126:THR:OG1	2.22	0.53
3:AC:64:SER:OG	21:AC:102:SF4:S3	2.67	0.53
15:A4:99:ASN:ND2	17:A4:307:CLA:OBD	2.42	0.52
15:A4:138:SER:OG	15:A4:139:SER:N	2.41	0.52
1:AA:247:LEU:HD21	1:AA:254:PHE:CZ	2.44	0.52
17:AB:833:CLA:CGA	20:AF:801:BCR:H353	2.39	0.52
16:A6:65:ARG:NH2	16:A6:78:LEU:O	2.43	0.52
2:AB:324:ASP:O	2:AB:328:ASN:ND2	2.43	0.52
3:AC:61:ASP:OD2	5:AE:91:ARG:NH1	2.42	0.52
2:AB:399:ASN:O	2:AB:403:ASN:ND2	2.43	0.52
2:AB:441:ASP:OD1	2:AB:616:LEU:N	2.42	0.52
12:AL:93:GLY:N	17:AL:303:CLA:OBD	2.42	0.52
20:A3:318:BCR:HC21	26:A3:320:CHL:HMD2	1.91	0.52
1:AA:279:LEU:HD22	1:AA:505:LEU:HD11	1.91	0.52
17:AA:801:CLA:HMB3	17:AB:802:CLA:CAD	2.40	0.52
12:AL:121:LYS:O	22:AL:301:LMU:O3'	2.27	0.51
17:AA:832:CLA:HBB1	17:AA:832:CLA:HMB1	1.93	0.51
2:AB:641:ASN:OD1	2:AB:641:ASN:N	2.43	0.51
3:AC:15:THR:O	3:AC:19:ARG:NH2	2.43	0.51
1:AA:342:LEU:HD13	17:AA:825:CLA:HMC2	1.92	0.51
2:AB:168:PHE:O	2:AB:174:ARG:NH1	2.41	0.51
2:AB:519:VAL:HG21	2:AB:593:TYR:HB2	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:15:ASP:OD2	1:AA:68:ARG:NH2	2.44	0.51
17:AA:834:CLA:HBC3	17:AA:834:CLA:HMC1	1.93	0.51
2:AB:257:LEU:HD13	17:AB:818:CLA:HMB2	1.92	0.51
1:AA:110:PRO:O	1:AA:137:ILE:N	2.44	0.50
2:AB:328:ASN:ND2	7:AG:100:ASN:OD1	2.44	0.50
2:AB:418:ILE:HG21	20:AB:847:BCR:H282	1.93	0.50
2:AB:452:GLN:NE2	2:AB:614:THR:OG1	2.43	0.50
5:AE:87:VAL:CG2	5:AE:138:VAL:HG13	2.39	0.50
20:AB:845:BCR:H382	20:AB:845:BCR:H23C	1.92	0.50
14:A3:105:ARG:NH1	26:A3:307:CHL:OBD	2.42	0.50
17:A3:304:CLA:NB	20:A3:318:BCR:H392	2.27	0.50
1:AA:644:TRP:HB3	17:AA:801:CLA:H101	1.94	0.50
15:A4:102:TRP:CE2	26:A4:306:CHL:HED2	2.46	0.50
2:AB:318:GLY:O	2:AB:407:VAL:N	2.42	0.50
17:AB:824:CLA:HAB	17:AB:831:CLA:HMD2	1.94	0.50
2:AB:130:ARG:NH1	2:AB:201:ALA:O	2.40	0.50
15:A4:163:ASN:OD1	15:A4:163:ASN:N	2.44	0.50
8:AH:100:ARG:HD2	12:AL:155:ILE:HG13	1.94	0.50
17:AB:840:CLA:HAB	18:AB:843:PQN:H141	1.94	0.49
2:AB:476:VAL:CG1	2:AB:477:LEU:N	2.62	0.49
1:AA:544:THR:CG2	17:AA:826:CLA:HMC1	2.43	0.49
2:AB:410:ARG:O	2:AB:414:HIS:ND1	2.41	0.49
2:AB:630:GLN:NE2	2:AB:731:GLY:O	2.46	0.49
20:AB:846:BCR:H383	20:AB:846:BCR:H23C	1.94	0.49
1:AA:54:HIS:ND1	17:AA:806:CLA:O1A	2.38	0.49
2:AB:113:VAL:CG1	2:AB:114:ASN:H	2.26	0.49
13:A1:137:THR:HG23	13:A1:138:LEU:H	1.76	0.49
14:A3:181:GLY:HA3	14:A3:193:ALA:HB2	1.95	0.49
14:A3:258:LEU:HD21	17:A3:313:CLA:HMC3	1.95	0.49
16:A6:119:THR:OG1	24:A6:614:LUT:H401	2.13	0.49
2:AB:339:ALA:HB2	20:AB:848:BCR:H372	1.94	0.49
1:AA:644:TRP:CZ2	17:AA:801:CLA:H142	2.48	0.48
14:A3:137:THR:HG21	27:A3:317:XAT:O3	2.12	0.48
16:A6:115:MET:O	16:A6:119:THR:OG1	2.28	0.48
1:AA:410:MET:HE1	1:AA:428:LEU:HD11	1.94	0.48
20:AJ:101:BCR:H23C	20:AJ:101:BCR:H403	1.96	0.48
3:AC:2:SER:OG	3:AC:3:HIS:N	2.46	0.48
2:AB:488:ALA:HB2	7:AG:158:PHE:CE1	2.49	0.48
2:AB:700:LEU:HD21	18:AB:843:PQN:H152	1.94	0.48
1:AA:367:HIS:ND1	17:AA:818:CLA:OBD	2.47	0.48
2:AB:586:THR:O	2:AB:590:VAL:HG13	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AI:102:BCR:HC8	20:AI:102:BCR:H311	1.95	0.48
3:AC:7:ILE:CG2	3:AC:8:TYR:N	2.77	0.48
8:AH:131:ARG:NE	8:AH:134:GLN:OE1	2.46	0.48
15:A4:191:ASN:ND2	17:A4:308:CLA:HBD	2.29	0.48
3:AC:61:ASP:OD1	3:AC:62:PHE:N	2.45	0.47
15:A4:177:SER:OG	15:A4:178:LEU:N	2.47	0.47
2:AB:462:TRP:NE1	2:AB:476:VAL:HG21	2.29	0.47
20:AF:805:BCR:H383	20:AF:805:BCR:H23C	1.96	0.47
13:A1:57:TYR:OH	13:A1:69:ASP:OD2	2.25	0.47
20:AF:801:BCR:H383	20:AF:801:BCR:H23C	1.96	0.47
1:AA:198:HIS:ND1	17:AA:825:CLA:OBD	2.47	0.47
6:AF:70:SER:OG	6:AF:70:SER:O	2.31	0.47
26:A3:320:CHL:HAB	19:A6:617:LHG:H301	1.96	0.47
16:A6:110:HIS:CE1	17:A6:603:CLA:NB	2.83	0.47
1:AA:205:LEU:HD21	17:AA:820:CLA:HMC1	1.97	0.47
1:AA:561:ILE:HD12	1:AA:584:VAL:HG11	1.96	0.47
2:AB:106:ARG:NH1	2:AB:115:ILE:CG1	2.77	0.47
2:AB:462:TRP:CD1	2:AB:476:VAL:HG21	2.50	0.47
3:AC:32:ASP:N	3:AC:32:ASP:OD1	2.44	0.47
1:AA:14:VAL:HG11	17:AA:810:CLA:HED3	1.96	0.47
2:AB:91:ILE:HD12	17:AB:810:CLA:C2D	2.45	0.47
12:AL:188:ALA:O	12:AL:191:THR:OG1	2.26	0.47
2:AB:700:LEU:HD22	2:AB:704:GLN:NE2	2.31	0.47
16:A6:138:TRP:HE3	27:A6:615:XAT:H173	1.81	0.47
2:AB:60:TRP:NE1	17:AB:828:CLA:OBD	2.48	0.46
20:AL:305:BCR:H392	20:AL:305:BCR:H23C	1.97	0.46
12:AL:63:GLN:O	12:AL:75:GLU:N	2.48	0.46
1:AA:544:THR:HG22	17:AA:826:CLA:HMC1	1.97	0.46
4:AD:138:LEU:HD22	4:AD:144:ILE:HD11	1.97	0.46
2:AB:519:VAL:HG23	17:AB:803:CLA:H141	1.98	0.46
17:AA:801:CLA:HED3	17:AA:801:CLA:HBD	1.58	0.46
20:AB:844:BCR:H383	20:AB:844:BCR:H23C	1.97	0.46
16:A6:138:TRP:CE3	27:A6:615:XAT:H173	2.50	0.46
1:AA:440:TRP:NE1	17:AA:833:CLA:OBD	2.46	0.46
5:AE:87:VAL:HG22	5:AE:138:VAL:CG1	2.45	0.46
1:AA:346:TRP:HE3	17:AA:805:CLA:HMD2	1.80	0.46
20:AA:849:BCR:H362	17:AB:802:CLA:H43	1.96	0.46
1:AA:343:THR:O	17:AA:825:CLA:H192	2.16	0.46
25:A4:318:LMG:C29	20:A6:616:BCR:H332	2.46	0.46
1:AA:574:ASP:OD2	1:AA:578:ARG:NH2	2.45	0.46
20:AG:205:BCR:H383	20:AG:205:BCR:H23C	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:87:VAL:HG22	5:AE:138:VAL:HG13	1.98	0.46
16:A6:77:TRP:NE1	16:A6:89:ASP:OD2	2.45	0.46
1:AA:538:ALA:HB2	17:AA:838:CLA:HMA1	1.98	0.45
3:AC:23:THR:OG1	21:AC:101:SF4:S1	2.74	0.45
1:AA:706:LEU:HD21	20:AF:805:BCR:C34	2.46	0.45
20:AA:848:BCR:H392	20:AA:848:BCR:H23C	1.97	0.45
2:AB:636:ASN:OD1	2:AB:636:ASN:N	2.47	0.45
17:AB:834:CLA:O1D	10:AJ:36:ALA:N	2.49	0.45
17:AB:841:CLA:HMB2	20:AB:849:BCR:H12C	1.97	0.45
1:AA:462:LEU:HG	17:AB:810:CLA:HMC3	1.99	0.45
2:AB:516:ASP:OD2	2:AB:597:LYS:NZ	2.42	0.45
14:A3:137:THR:OG1	14:A3:148:TYR:OH	2.32	0.45
17:AB:805:CLA:HMC3	17:AB:807:CLA:OBD	2.16	0.45
1:AA:561:ILE:CD1	1:AA:584:VAL:HG11	2.47	0.45
17:AB:827:CLA:H142	20:AB:847:BCR:C22	2.46	0.45
17:AA:801:CLA:H102	17:AA:801:CLA:H62	1.69	0.45
8:AH:66:ASN:HA	8:AH:71:TRP:HE1	1.82	0.45
1:AA:264:LEU:HD13	11:AK:121:VAL:HG21	1.98	0.45
2:AB:561:GLY:O	2:AB:567:THR:OG1	2.34	0.45
8:AH:100:ARG:NH1	12:AL:154:GLY:O	2.50	0.45
2:AB:560:ASP:OD2	2:AB:564:ARG:NH1	2.49	0.45
5:AE:89:ILE:HG22	5:AE:91:ARG:H	1.81	0.45
15:A4:107:VAL:HG11	24:A4:315:LUT:H12	1.99	0.45
12:AL:91:LEU:HD12	12:AL:93:GLY:H	1.81	0.44
17:A1:311:CLA:HBB1	17:A1:311:CLA:HMB1	1.99	0.44
15:A4:75:ASN:N	17:A4:301:CLA:OBD	2.50	0.44
17:A4:309:CLA:HBC3	25:A4:318:LMG:H112	1.99	0.44
17:AA:801:CLA:HAA1	17:AB:803:CLA:HMB1	1.99	0.44
2:AB:645:VAL:HG21	17:AB:809:CLA:HAC1	1.98	0.44
13:A1:121:LEU:HD12	13:A1:121:LEU:O	2.16	0.44
2:AB:113:VAL:HG12	2:AB:114:ASN:H	1.79	0.44
6:AF:133:ASP:OD1	6:AF:133:ASP:N	2.50	0.44
17:AA:827:CLA:HBB1	17:AA:827:CLA:HMB1	1.99	0.44
15:A4:80:LEU:HD12	27:A4:316:XAT:H372	1.98	0.44
15:A4:191:ASN:HD22	15:A4:191:ASN:HA	1.64	0.44
2:AB:174:ARG:HB2	17:AB:814:CLA:HBC2	1.99	0.44
2:AB:343:VAL:CG2	20:AB:848:BCR:H362	2.47	0.44
4:AD:85:LEU:O	4:AD:89:GLN:NE2	2.51	0.44
1:AA:380:ASP:OD2	1:AA:383:THR:OG1	2.21	0.44
2:AB:721:TYR:HB2	17:AB:803:CLA:HED3	1.99	0.44
12:AL:169:LEU:HD12	12:AL:169:LEU:C	2.38	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A3:260:ASP:O	14:A3:262:VAL:N	2.47	0.44
2:AB:664:LEU:O	2:AB:667:TRP:NE1	2.51	0.44
17:AB:836:CLA:HMD1	7:AG:158:PHE:HE1	1.82	0.44
27:A6:615:XAT:H35	27:A6:615:XAT:H401	1.87	0.44
17:AA:825:CLA:HBB1	17:AA:825:CLA:HMB1	2.00	0.43
2:AB:268:LEU:HD13	17:AB:818:CLA:HMA2	2.00	0.43
2:AB:675:ILE:HG21	2:AB:697:PRO:O	2.18	0.43
24:AF:806:LUT:H373	25:A1:321:LMG:C28	2.48	0.43
10:AJ:7:TYR:O	10:AJ:10:VAL:HG12	2.17	0.43
13:A1:215:THR:OG1	13:A1:216:GLY:N	2.50	0.43
15:A4:236:GLN:O	15:A4:244:ASN:ND2	2.50	0.43
2:AB:20:ARG:NH2	2:AB:695:ASP:OD1	2.48	0.43
2:AB:88:ALA:N	2:AB:114:ASN:O	2.46	0.43
7:AG:99:GLN:N	7:AG:102:LYS:O	2.51	0.43
17:A1:306:CLA:C1B	20:A1:319:BCR:H392	2.48	0.43
1:AA:72:SER:OG	17:AA:811:CLA:CMD	2.53	0.43
1:AA:379:THR:HG21	1:AA:515:VAL:HG22	2.00	0.43
1:AA:585:SER:O	1:AA:589:HIS:ND1	2.43	0.43
1:AA:717:LEU:HD11	17:AA:841:CLA:HMD3	2.01	0.43
2:AB:717:TYR:CE1	17:AB:803:CLA:HED1	2.54	0.43
4:AD:132:LEU:HD23	4:AD:132:LEU:O	2.18	0.43
16:A6:197:PRO:HB3	26:A6:607:CHL:HBC2	2.00	0.43
14:A3:105:ARG:NH2	14:A3:225:GLU:OE2	2.51	0.43
1:AA:432:ASP:OD2	1:AA:559:ARG:NH2	2.48	0.43
6:AF:118:ARG:O	6:AF:122:ASN:ND2	2.48	0.43
17:AA:841:CLA:H143	18:AA:843:PQN:H291	2.00	0.43
2:AB:203:ARG:NH1	2:AB:253:ALA:O	2.47	0.43
14:A3:201:PRO:HD3	26:A3:307:CHL:HMD2	2.00	0.43
1:AA:29:PRO:HA	17:AA:803:CLA:HBC1	2.01	0.43
20:A6:616:BCR:H321	20:A6:616:BCR:HC8	2.00	0.43
17:AB:801:CLA:HMB1	17:AB:801:CLA:HBB1	2.01	0.43
1:AA:536:ILE:HD12	17:AA:801:CLA:H172	2.01	0.43
1:AA:705:LYS:NZ	6:AF:220:ASP:OD2	2.51	0.43
1:AA:745:ARG:O	1:AA:749:VAL:HG22	2.19	0.43
20:A1:319:BCR:H382	20:A1:319:BCR:H23C	2.01	0.43
14:A3:125:LEU:O	14:A3:126:ILE:HG23	2.18	0.43
27:A4:316:XAT:C28	27:A4:316:XAT:H381	2.49	0.43
1:AA:530:ASP:OD2	1:AA:611:LYS:NZ	2.44	0.43
2:AB:631:LEU:HD22	2:AB:724:PHE:HA	1.99	0.43
5:AE:137:GLU:C	5:AE:138:VAL:HG23	2.39	0.43
14:A3:76:PHE:CE2	27:A3:317:XAT:H383	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AA:801:CLA:H2	17:AA:802:CLA:O1D	2.20	0.42
2:AB:378:ILE:HG22	2:AB:382:ILE:HD12	2.02	0.42
1:AA:445:LEU:HD11	17:AA:838:CLA:HMB1	2.00	0.42
2:AB:309:ILE:HD11	2:AB:320:LYS:HB2	2.01	0.42
27:A3:317:XAT:H31	27:A3:317:XAT:H391	1.95	0.42
1:AA:199:LEU:O	1:AA:204:GLY:N	2.53	0.42
1:AA:513:VAL:HG23	1:AA:513:VAL:O	2.20	0.42
2:AB:285:LEU:O	2:AB:289:HIS:ND1	2.51	0.42
2:AB:351:HIS:CE1	17:AB:827:CLA:NB	2.88	0.42
2:AB:430:GLY:HA2	2:AB:525:LEU:HD22	2.00	0.42
18:AA:843:PQN:H193	20:AF:801:BCR:H383	2.02	0.42
2:AB:725:LEU:O	2:AB:729:THR:OG1	2.29	0.42
14:A3:70:LEU:N	14:A3:73:ASP:OD2	2.49	0.42
1:AA:42:THR:HG1	1:AA:44:THR:HG1	1.63	0.42
2:AB:519:VAL:HG11	2:AB:593:TYR:CD1	2.54	0.42
6:AF:104:ALA:HB3	6:AF:105:PRO:HD3	2.02	0.42
14:A3:242:GLN:HA	14:A3:245:VAL:HG12	2.02	0.42
16:A6:161:MET:HG3	26:A6:605:CHL:HMB3	2.01	0.42
15:A4:112:LEU:HA	15:A4:115:VAL:HG22	2.01	0.42
7:AG:120:LYS:O	7:AG:120:LYS:CG	2.68	0.41
13:A1:119:ALA:HB3	26:A1:308:CHL:HMD3	2.01	0.41
16:A6:112:ARG:NH1	26:A6:607:CHL:OBD	2.50	0.41
1:AA:178:TYR:OH	17:AA:811:CLA:O2D	2.38	0.41
1:AA:717:LEU:HD21	18:AA:843:PQN:C15	2.50	0.41
2:AB:306:GLU:OE1	2:AB:321:GLY:N	2.46	0.41
17:AB:824:CLA:HMA1	17:AB:842:CLA:O2D	2.20	0.41
1:AA:641:ILE:HG23	17:AA:801:CLA:H91	2.02	0.41
2:AB:424:TRP:NE1	17:AB:833:CLA:OBD	2.43	0.41
1:AA:600:ALA:O	1:AA:604:VAL:HG23	2.20	0.41
1:AA:691:TYR:OH	2:AB:533:ILE:HA	2.21	0.41
4:AD:161:HIS:HB3	4:AD:162:PRO:HD3	2.02	0.41
20:A3:318:BCR:H382	20:A3:318:BCR:H23C	2.03	0.41
16:A6:65:ARG:NH2	16:A6:85:ASP:OD1	2.53	0.41
16:A6:110:HIS:HD1	27:A6:615:XAT:H201	1.85	0.41
6:AF:141:ASN:OD1	6:AF:142:GLY:N	2.53	0.41
1:AA:77:GLN:HB2	17:AA:805:CLA:HMB2	2.03	0.41
2:AB:329:SER:HG	2:AB:393:PHE:HD1	1.67	0.41
17:AB:830:CLA:HMB1	17:AB:830:CLA:HBB1	2.02	0.41
4:AD:74:SER:O	4:AD:117:ARG:NE	2.49	0.41
2:AB:682:HIS:NE2	2:AB:691:ILE:O	2.49	0.41
2:AB:711:ALA:O	2:AB:715:VAL:HG23	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:127:ARG:NH2	4:AD:129:GLU:OE1	2.50	0.41
15:A4:108:ALA:HB2	24:A4:315:LUT:H401	2.02	0.41
16:A6:258:PRO:O	16:A6:262:ASN:ND2	2.47	0.41
2:AB:192:GLY:O	2:AB:196:HIS:ND1	2.43	0.41
16:A6:167:ARG:NE	17:A6:601:CLA:OBD	2.52	0.41
1:AA:657:ILE:HD12	2:AB:621:ARG:HG3	2.03	0.41
20:AA:848:BCR:H23C	20:AA:848:BCR:H403	2.02	0.41
24:AF:806:LUT:H31	24:AF:806:LUT:H391	1.93	0.41
17:AG:203:CLA:HMC1	20:AG:205:BCR:H332	2.03	0.41
12:AL:150:LEU:HB3	12:AL:191:THR:HG22	2.03	0.41
3:AC:24:ASP:O	3:AC:44:ARG:NE	2.49	0.41
27:A1:318:XAT:H35	27:A1:318:XAT:H401	1.92	0.41
6:AF:77:ASP:O	6:AF:79:LYS:NZ	2.49	0.40
2:AB:194:LEU:HA	2:AB:198:ALA:HB3	2.03	0.40
6:AF:68:ASP:N	6:AF:68:ASP:OD1	2.54	0.40
20:AJ:103:BCR:H23C	20:AJ:103:BCR:H382	2.04	0.40
17:AB:825:CLA:H71	17:AB:827:CLA:H42	2.03	0.40
16:A6:110:HIS:HE1	17:A6:603:CLA:NC	2.20	0.40
17:A1:306:CLA:NB	20:A1:319:BCR:H392	2.37	0.40

There are no symmetry-related clashes.

## 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	AA	740/750 (99%)	688 (93%)	51 (7%)	1 (0%)	48	77
2	AB	732/734 (100%)	695 (95%)	37 (5%)	0	100	100
3	AC	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	AD	139/204 (68%)	126 (91%)	13 (9%)	0	100	100
5	AE	65/143 (46%)	58 (89%)	7 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	151/221 (68%)	144 (95%)	7 (5%)	0	100	100
7	AG	96/160 (60%)	88 (92%)	8 (8%)	0	100	100
8	AH	93/145 (64%)	90 (97%)	3 (3%)	0	100	100
9	AI	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
10	AJ	40/44 (91%)	38 (95%)	2 (5%)	0	100	100
11	AK	61/130 (47%)	57 (93%)	4 (7%)	0	100	100
12	AL	155/219 (71%)	145 (94%)	10 (6%)	0	100	100
13	A1	194/241 (80%)	178 (92%)	16 (8%)	0	100	100
14	A3	217/273 (80%)	191 (88%)	26 (12%)	0	100	100
15	A4	195/251 (78%)	185 (95%)	10 (5%)	0	100	100
16	A6	210/270 (78%)	198 (94%)	12 (6%)	0	100	100
All	All	3197/3903 (82%)	2983 (93%)	213 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	663	SER

### 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	AA	600/610 (98%)	594 (99%)	6 (1%)	73	82
2	AB	598/600 (100%)	591 (99%)	7 (1%)	67	79
3	AC	70/71 (99%)	70 (100%)	0	100	100
4	AD	120/170 (71%)	120 (100%)	0	100	100
5	AE	56/114 (49%)	55 (98%)	1 (2%)	54	72
6	AF	125/185 (68%)	124 (99%)	1 (1%)	79	86
7	AG	83/133 (62%)	81 (98%)	2 (2%)	44	66

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	77/113 (68%)	75 (97%)	2 (3%)	41	64
9	AI	29/33 (88%)	29 (100%)	0	100	100
10	AJ	37/39 (95%)	37 (100%)	0	100	100
11	AK	47/95 (50%)	47 (100%)	0	100	100
12	AL	119/174 (68%)	116 (98%)	3 (2%)	42	65
13	A1	151/190 (80%)	149 (99%)	2 (1%)	65	78
14	A3	168/211 (80%)	167 (99%)	1 (1%)	84	89
15	A4	164/210 (78%)	160 (98%)	4 (2%)	44	66
16	A6	177/226 (78%)	175 (99%)	2 (1%)	70	81
All	All	2621/3174 (83%)	2590 (99%)	31 (1%)	66	79

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	118	ILE
1	AA	141	PHE
1	AA	224	PHE
1	AA	275	PHE
1	AA	505	LEU
1	AA	591	PHE
2	AB	5	PHE
2	AB	96	PHE
2	AB	332	PHE
2	AB	576	PHE
2	AB	577	TYR
2	AB	638	PHE
2	AB	648	TRP
5	AE	129	SER
6	AF	145	ARG
7	AG	109	ASP
7	AG	127	PHE
8	AH	71	TRP
8	AH	73	VAL
12	AL	114	PHE
12	AL	126	ARG
12	AL	158	PHE
13	A1	47	HIS
13	A1	112	TRP
14	A3	98	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	A4	79	PRO
15	A4	136	PHE
15	A4	170	ASP
15	A4	191	ASN
16	A6	89	ASP
16	A6	110	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	628	HIS
1	AA	713	GLN
2	AB	452	GLN
6	AF	213	ASN
7	AG	90	ASN
8	AH	86	GLN
8	AH	121	ASN
11	AK	54	ASN
12	AL	66	ASN
13	A1	208	GLN
13	A1	209	GLN
14	A3	242	GLN
15	A4	75	ASN
15	A4	191	ASN
15	A4	248	GLN
16	A6	250	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

211 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$
26	CHL	A6	607	-	50,58,74	2.26	16 (32%)	58,95,114	2.64	21 (36%)
17	CLA	A6	609	16	55,63,73	1.67	9 (16%)	64,101,113	1.33	10 (15%)
17	CLA	AB	807	2	65,73,73	1.45	10 (15%)	76,113,113	1.35	8 (10%)
17	CLA	A3	305	-	40,49,73	1.90	7 (17%)	45,84,113	1.45	7 (15%)
17	CLA	AB	831	-	43,51,73	1.84	9 (20%)	49,86,113	1.33	8 (16%)
17	CLA	A6	613	-	43,51,73	1.89	6 (13%)	49,86,113	1.47	7 (14%)
17	CLA	AB	839	-	47,55,73	1.74	8 (17%)	54,91,113	1.56	7 (12%)
17	CLA	AB	808	-	51,59,73	1.67	9 (17%)	58,95,113	1.45	7 (12%)
17	CLA	AA	803	-	65,73,73	1.47	10 (15%)	76,113,113	1.36	11 (14%)
17	CLA	A3	311	14	43,51,73	1.82	5 (11%)	49,86,113	1.48	7 (14%)
17	CLA	AA	842	-	65,73,73	1.48	8 (12%)	76,113,113	1.41	11 (14%)
17	CLA	AA	813	-	65,73,73	1.47	9 (13%)	76,113,113	1.38	8 (10%)
17	CLA	AB	823	-	65,73,73	1.50	9 (13%)	76,113,113	1.31	9 (11%)
17	CLA	AA	809	1	50,58,73	1.77	9 (18%)	58,95,113	1.48	11 (18%)
17	CLA	AB	812	-	54,62,73	1.66	8 (14%)	67,100,113	1.52	12 (17%)
17	CLA	A6	604	-	43,51,73	1.83	8 (18%)	48,86,113	1.40	7 (14%)
17	CLA	AA	827	-	65,73,73	1.48	7 (10%)	76,113,113	1.34	8 (10%)
17	CLA	AB	801	-	65,73,73	1.47	9 (13%)	76,113,113	1.59	14 (18%)
17	CLA	A3	310	19	36,45,73	1.97	6 (16%)	43,79,113	1.48	8 (18%)
17	CLA	AA	811	-	65,73,73	1.49	7 (10%)	76,113,113	1.31	8 (10%)
17	CLA	AB	820	-	55,63,73	1.70	8 (14%)	64,101,113	1.28	6 (9%)
17	CLA	AB	815	-	65,73,73	1.46	8 (12%)	76,113,113	1.39	9 (11%)
17	CLA	AA	830	-	65,73,73	1.52	9 (13%)	76,113,113	1.31	8 (10%)
17	CLA	AF	802	-	57,65,73	1.58	11 (19%)	66,103,113	1.43	9 (13%)
17	CLA	AB	802	-	64,72,73	1.60	8 (12%)	79,112,113	1.34	9 (11%)
19	LHG	A1	301	17	37,37,48	1.07	2 (5%)	40,43,54	0.97	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	AA	801	-	65,73,73	1.50	7 (10%)	76,113,113	1.27	8 (10%)
17	CLA	AA	840	-	65,73,73	1.51	8 (12%)	76,113,113	1.31	10 (13%)
17	CLA	A4	302	15	44,52,73	1.85	8 (18%)	55,88,113	1.61	9 (16%)
25	LMG	A1	321	-	44,44,55	1.03	2 (4%)	52,52,63	1.19	5 (9%)
17	CLA	A3	314	-	37,44,73	1.97	8 (21%)	42,77,113	1.42	7 (16%)
19	LHG	A1	320	17	48,48,48	0.93	2 (4%)	51,54,54	0.84	2 (3%)
26	CHL	A1	303	13	50,59,74	2.22	15 (30%)	53,96,114	2.68	24 (45%)
17	CLA	AA	806	1	65,73,73	1.49	9 (13%)	76,113,113	1.38	8 (10%)
22	LMU	AB	852	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
17	CLA	A1	309	-	43,52,73	1.87	6 (13%)	49,88,113	1.42	9 (18%)
17	CLA	AG	204	7	45,53,73	1.84	7 (15%)	52,89,113	1.46	7 (13%)
17	CLA	A4	307	15	45,53,73	1.85	7 (15%)	52,89,113	1.36	7 (13%)
17	CLA	AB	838	-	65,73,73	1.46	7 (10%)	76,113,113	1.34	8 (10%)
17	CLA	AK	203	-	45,53,73	1.82	6 (13%)	52,89,113	1.41	7 (13%)
26	CHL	A3	320	16	51,60,74	2.19	16 (31%)	54,97,114	2.65	20 (37%)
17	CLA	AB	805	-	41,49,73	1.81	6 (14%)	47,84,113	1.55	8 (17%)
17	CLA	AB	828	-	65,73,73	1.46	8 (12%)	76,113,113	1.43	8 (10%)
17	CLA	AB	827	-	62,70,73	1.50	7 (11%)	72,109,113	1.50	9 (12%)
17	CLA	AA	834	-	65,73,73	1.47	10 (15%)	76,113,113	1.48	14 (18%)
17	CLA	AK	201	11	37,43,73	2.45	10 (27%)	45,75,113	1.48	8 (17%)
20	BCR	A3	318	-	41,41,41	0.98	1 (2%)	56,56,56	2.77	20 (35%)
17	CLA	A3	303	14	55,63,73	1.67	9 (16%)	64,101,113	1.46	9 (14%)
20	BCR	AA	845	-	41,41,41	1.03	2 (4%)	56,56,56	1.91	13 (23%)
17	CLA	AG	203	-	42,50,73	1.85	6 (14%)	48,85,113	1.44	7 (14%)
17	CLA	AB	830	-	56,64,73	1.62	9 (16%)	65,102,113	1.39	7 (10%)
21	SF4	AC	101	3	0,12,12	-	-	-	-	-
18	PQN	AA	843	-	34,34,34	3.42	10 (29%)	42,45,45	1.74	8 (19%)
17	CLA	AA	837	-	51,59,73	1.62	7 (13%)	59,96,113	1.59	9 (15%)
17	CLA	A1	316	13	43,51,73	1.89	7 (16%)	54,87,113	1.63	9 (16%)
17	CLA	AA	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.40	12 (15%)
20	BCR	AB	847	-	41,41,41	0.87	0	56,56,56	2.02	14 (25%)
19	LHG	AA	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.89	2 (3%)
17	CLA	AB	803	-	65,73,73	1.49	8 (12%)	76,113,113	1.23	7 (9%)
20	BCR	AB	848	-	41,41,41	0.89	1 (2%)	56,56,56	1.97	18 (32%)
17	CLA	AA	841	-	65,73,73	1.50	9 (13%)	76,113,113	1.34	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	AJ	102	10	42,50,73	1.84	5 (11%)	48,85,113	1.48	7 (14%)
24	LUT	A3	316	-	42,43,43	0.84	0	51,60,60	1.78	14 (27%)
20	BCR	AL	305	-	41,41,41	0.86	0	56,56,56	2.54	18 (32%)
17	CLA	AA	816	-	45,53,73	1.82	9 (20%)	52,89,113	1.58	9 (17%)
17	CLA	AA	817	-	60,68,73	1.55	6 (10%)	70,107,113	1.36	9 (12%)
17	CLA	AB	822	-	47,55,73	1.77	7 (14%)	54,91,113	1.35	7 (12%)
17	CLA	AA	804	-	52,60,73	1.65	8 (15%)	60,97,113	1.54	7 (11%)
19	LHG	A1	302	-	35,35,48	1.10	2 (5%)	38,41,54	1.04	2 (5%)
17	CLA	A4	301	15	60,68,73	1.55	9 (15%)	70,107,113	1.33	10 (14%)
17	CLA	A6	610	19	38,45,73	2.96	10 (26%)	41,76,113	1.56	10 (24%)
20	BCR	AA	846	-	41,41,41	0.82	0	56,56,56	2.12	21 (37%)
21	SF4	AA	850	2,1	0,12,12	-	-	-	-	-
17	CLA	A3	304	-	41,50,73	1.94	7 (17%)	51,86,113	1.50	9 (17%)
17	CLA	AB	829	-	65,73,73	1.50	9 (13%)	76,113,113	1.33	9 (11%)
17	CLA	AF	804	-	41,49,73	1.87	7 (17%)	47,84,113	1.59	8 (17%)
17	CLA	AA	812	-	54,62,73	1.61	9 (16%)	62,99,113	1.51	8 (12%)
17	CLA	AA	822	-	42,50,73	1.86	6 (14%)	48,85,113	1.50	8 (16%)
17	CLA	A3	313	-	39,48,73	1.91	7 (17%)	44,83,113	1.46	8 (18%)
20	BCR	A6	616	-	41,41,41	0.99	2 (4%)	56,56,56	2.01	16 (28%)
17	CLA	AA	832	-	56,64,73	1.60	6 (10%)	65,102,113	1.36	10 (15%)
17	CLA	AB	809	-	65,73,73	1.52	8 (12%)	76,113,113	1.36	10 (13%)
26	CHL	A4	305	-	41,49,74	2.25	13 (31%)	51,84,114	2.78	20 (39%)
26	CHL	A6	606	-	43,51,74	2.34	16 (37%)	45,86,114	2.83	19 (42%)
17	CLA	AB	816	-	43,51,73	1.80	7 (16%)	49,86,113	1.42	6 (12%)
17	CLA	AB	825	-	65,73,73	1.49	10 (15%)	76,113,113	1.34	9 (11%)
17	CLA	AA	818	-	59,67,73	1.58	9 (15%)	68,105,113	1.33	8 (11%)
17	CLA	A1	310	13	40,48,73	1.92	7 (17%)	50,83,113	1.65	10 (20%)
22	LMU	AA	851	-	36,36,36	1.16	2 (5%)	47,47,47	1.04	2 (4%)
17	CLA	AA	824	-	53,62,73	1.68	8 (15%)	61,100,113	1.50	11 (18%)
17	CLA	A1	304	13	60,68,73	1.52	9 (15%)	69,106,113	1.33	8 (11%)
20	BCR	AJ	103	-	41,41,41	0.74	0	56,56,56	2.38	22 (39%)
20	BCR	AI	101	-	41,41,41	0.92	1 (2%)	56,56,56	2.05	20 (35%)
17	CLA	AA	825	-	65,73,73	1.48	6 (9%)	76,113,113	1.33	6 (7%)
20	BCR	AF	805	-	41,41,41	0.81	0	56,56,56	1.86	14 (25%)
23	DGD	AB	851	-	67,67,67	0.80	2 (2%)	81,81,81	0.99	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	AB	818	-	59,67,73	1.58	8 (13%)	68,105,113	1.34	10 (14%)
17	CLA	AL	303	-	60,68,73	1.57	9 (15%)	70,107,113	1.41	10 (14%)
17	CLA	AA	839	-	52,60,73	1.66	8 (15%)	60,97,113	1.37	7 (11%)
17	CLA	A6	603	-	41,50,73	1.90	6 (14%)	46,85,113	1.60	7 (15%)
20	BCR	AA	847	-	41,41,41	1.00	2 (4%)	56,56,56	2.28	24 (42%)
17	CLA	AA	808	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	9 (11%)
17	CLA	AB	821	-	50,58,73	1.70	8 (16%)	58,95,113	1.49	8 (13%)
17	CLA	AA	823	-	41,49,73	1.93	7 (17%)	47,84,113	1.46	8 (17%)
17	CLA	AB	810	2	65,73,73	1.48	11 (16%)	76,113,113	1.38	6 (7%)
20	BCR	AA	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.12	20 (35%)
22	LMU	AB	850	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
17	CLA	AA	815	-	40,49,73	1.79	5 (12%)	44,83,113	1.62	8 (18%)
17	CLA	A1	312	19	37,46,73	2.01	7 (18%)	46,81,113	1.43	10 (21%)
17	CLA	AA	802	-	65,73,73	1.53	10 (15%)	76,113,113	1.42	6 (7%)
27	XAT	A4	316	-	39,47,47	0.95	2 (5%)	54,74,74	2.29	16 (29%)
17	CLA	A4	308	15	54,62,73	1.67	8 (14%)	62,99,113	1.29	9 (14%)
17	CLA	A4	310	15	40,49,73	1.90	8 (20%)	45,84,113	1.47	7 (15%)
17	CLA	A3	308	14	45,53,73	1.80	8 (17%)	52,89,113	1.43	8 (15%)
17	CLA	A4	311	-	55,64,73	1.64	7 (12%)	63,102,113	1.31	7 (11%)
17	CLA	A3	312	-	53,62,73	1.67	7 (13%)	61,100,113	1.39	8 (13%)
17	CLA	A6	611	16	44,52,73	1.84	7 (15%)	51,88,113	1.37	6 (11%)
24	LUT	A4	315	-	42,43,43	0.95	2 (4%)	51,60,60	1.84	15 (29%)
20	BCR	AG	205	-	41,41,41	0.93	0	56,56,56	2.00	18 (32%)
17	CLA	AB	842	19	65,73,73	1.46	8 (12%)	76,113,113	1.37	10 (13%)
17	CLA	AB	833	-	65,73,73	1.49	9 (13%)	76,113,113	1.18	7 (9%)
17	CLA	A6	608	16	45,53,73	1.80	7 (15%)	52,89,113	1.42	7 (13%)
17	CLA	A1	313	13	45,53,73	1.78	7 (15%)	52,89,113	1.57	7 (13%)
17	CLA	A1	305	-	55,63,73	1.63	7 (12%)	64,101,113	1.60	10 (15%)
21	SF4	AC	102	3	0,12,12	-	-	-	-	-
17	CLA	AB	811	-	65,73,73	1.46	8 (12%)	76,113,113	1.48	10 (13%)
17	CLA	A1	311	13	59,67,73	1.57	7 (11%)	69,106,113	1.27	8 (11%)
22	LMU	AL	301	-	35,35,36	1.23	2 (5%)	46,46,47	1.05	5 (10%)
26	CHL	A1	308	13	40,49,74	2.48	18 (45%)	41,84,114	2.86	17 (41%)
20	BCR	AB	844	-	41,41,41	0.86	0	56,56,56	2.28	23 (41%)
17	CLA	AA	838	-	55,63,73	1.61	9 (16%)	64,101,113	1.29	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	AA	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.56	9 (11%)
17	CLA	AB	840	-	65,73,73	1.54	9 (13%)	76,113,113	1.25	7 (9%)
17	CLA	A4	312	-	45,53,73	1.81	7 (15%)	52,89,113	1.40	7 (13%)
19	LHG	A6	617	17	35,35,48	1.05	2 (5%)	38,41,54	0.97	2 (5%)
17	CLA	AK	204	-	46,54,73	1.78	9 (19%)	53,90,113	1.47	7 (13%)
20	BCR	AB	849	-	41,41,41	0.83	0	56,56,56	2.41	24 (42%)
25	LMG	AG	202	-	38,38,55	1.14	3 (7%)	46,46,63	1.07	2 (4%)
22	LMU	AB	853	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	2 (4%)
17	CLA	A4	309	-	42,50,73	1.79	5 (11%)	48,85,113	1.53	7 (14%)
17	CLA	A1	307	-	39,48,73	1.89	9 (23%)	45,82,113	1.74	11 (24%)
17	CLA	AA	807	-	50,58,73	1.69	8 (16%)	58,95,113	1.43	6 (10%)
17	CLA	AA	814	-	45,53,73	1.81	9 (20%)	52,89,113	1.45	8 (15%)
17	CLA	AB	806	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	9 (11%)
17	CLA	A3	306	14	41,49,73	1.90	7 (17%)	51,84,113	1.67	9 (17%)
17	CLA	AB	813	-	43,51,73	1.78	6 (13%)	49,86,113	1.44	8 (16%)
17	CLA	AB	814	-	65,73,73	1.49	10 (15%)	76,113,113	1.30	7 (9%)
17	CLA	A4	303	-	43,51,73	1.86	7 (16%)	54,87,113	1.59	9 (16%)
17	CLA	AG	201	-	43,52,73	1.87	7 (16%)	49,88,113	1.48	7 (14%)
20	BCR	AB	846	-	41,41,41	0.86	0	56,56,56	2.07	16 (28%)
17	CLA	AB	826	-	62,70,73	1.52	9 (14%)	72,109,113	1.32	7 (9%)
24	LUT	A1	317	-	42,43,43	0.94	1 (2%)	51,60,60	1.88	13 (25%)
17	CLA	AB	817	-	55,63,73	1.63	8 (14%)	64,101,113	1.34	7 (10%)
24	LUT	A6	614	-	42,43,43	0.90	1 (2%)	51,60,60	1.59	12 (23%)
26	CHL	A4	314	15	40,49,74	2.26	13 (32%)	45,84,114	2.77	17 (37%)
17	CLA	A6	601	15	46,54,73	1.73	8 (17%)	53,90,113	1.46	8 (15%)
20	BCR	AL	306	-	41,41,41	0.94	1 (2%)	56,56,56	2.01	21 (37%)
19	LHG	A3	301	-	35,35,48	1.09	2 (5%)	38,41,54	1.01	2 (5%)
17	CLA	AB	834	-	65,73,73	1.49	9 (13%)	76,113,113	1.23	9 (11%)
17	CLA	AA	820	-	45,53,73	1.78	8 (17%)	52,89,113	1.46	7 (13%)
17	CLA	A1	314	-	63,72,73	1.52	8 (12%)	73,112,113	1.30	9 (12%)
20	BCR	AK	202	-	41,41,41	0.94	2 (4%)	56,56,56	2.19	17 (30%)
17	CLA	A1	306	-	49,57,73	1.71	7 (14%)	55,93,113	1.45	8 (14%)
17	CLA	AA	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	9 (11%)
17	CLA	AB	804	-	65,73,73	1.45	10 (15%)	76,113,113	1.69	15 (19%)
19	LHG	AJ	104	-	39,39,48	1.06	2 (5%)	42,45,54	0.92	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	PQN	AB	843	-	34,34,34	3.39	11 (32%)	42,45,45	1.83	6 (14%)
26	CHL	A4	306	-	46,54,74	2.32	17 (36%)	49,90,114	2.85	21 (42%)
17	CLA	A1	315	-	37,46,73	1.99	7 (18%)	46,81,113	1.69	11 (23%)
17	CLA	AA	829	-	65,73,73	1.46	9 (13%)	76,113,113	1.49	11 (14%)
17	CLA	AB	837	-	50,58,73	1.69	9 (18%)	58,95,113	1.51	8 (13%)
20	BCR	AI	102	-	41,41,41	0.78	0	56,56,56	2.22	22 (39%)
20	BCR	AK	205	-	41,41,41	1.02	3 (7%)	56,56,56	2.06	14 (25%)
17	CLA	AH	201	-	60,68,73	1.60	7 (11%)	70,107,113	1.36	10 (14%)
17	CLA	AA	831	-	47,55,73	1.78	9 (19%)	54,91,113	1.43	7 (12%)
17	CLA	AA	835	-	43,52,73	1.85	8 (18%)	49,88,113	1.47	7 (14%)
17	CLA	A3	302	14	60,68,73	1.57	8 (13%)	70,107,113	1.22	9 (12%)
17	CLA	AA	819	-	65,73,73	1.48	10 (15%)	76,113,113	1.43	9 (11%)
17	CLA	AB	835	-	60,68,73	1.55	8 (13%)	70,107,113	1.37	8 (11%)
17	CLA	AF	803	-	42,50,73	1.88	8 (19%)	48,85,113	1.57	8 (16%)
17	CLA	A3	315	-	39,48,73	1.86	6 (15%)	44,83,113	1.42	7 (15%)
20	BCR	AA	848	-	41,41,41	0.77	1 (2%)	56,56,56	1.97	16 (28%)
20	BCR	AJ	101	-	41,41,41	0.89	1 (2%)	56,56,56	1.98	16 (28%)
20	BCR	A4	317	-	41,41,41	0.82	0	56,56,56	2.37	23 (41%)
17	CLA	AB	819	-	60,68,73	1.53	9 (15%)	70,107,113	1.64	12 (17%)
25	LMG	A4	318	-	39,39,55	1.00	2 (5%)	47,47,63	1.40	7 (14%)
17	CLA	A6	602	16	65,73,73	1.51	9 (13%)	76,113,113	1.29	9 (11%)
20	BCR	AB	845	-	41,41,41	0.85	1 (2%)	56,56,56	1.93	17 (30%)
27	XAT	A3	317	-	39,47,47	0.97	1 (2%)	54,74,74	2.31	19 (35%)
17	CLA	AL	302	12	41,49,73	1.91	7 (17%)	47,84,113	1.46	8 (17%)
27	XAT	A6	615	-	39,47,47	0.98	2 (5%)	54,74,74	2.49	21 (38%)
20	BCR	A1	319	-	41,41,41	0.90	1 (2%)	56,56,56	3.13	20 (35%)
20	BCR	AF	801	-	41,41,41	0.86	1 (2%)	56,56,56	1.56	10 (17%)
17	CLA	A6	612	16	64,72,73	1.53	8 (12%)	74,111,113	1.28	7 (9%)
26	CHL	A6	605	-	42,50,74	2.35	15 (35%)	45,85,114	2.88	20 (44%)
17	CLA	AA	826	-	59,67,73	1.56	9 (15%)	68,105,113	1.28	8 (11%)
17	CLA	A4	313	-	50,58,73	1.72	8 (16%)	58,95,113	1.47	10 (17%)
17	CLA	AA	821	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	9 (11%)
17	CLA	AB	832	-	65,73,73	1.50	10 (15%)	76,113,113	1.30	9 (11%)
26	CHL	A4	304	-	40,49,74	2.45	16 (40%)	42,84,114	2.82	20 (47%)
27	XAT	A1	318	-	39,47,47	0.91	2 (5%)	54,74,74	2.42	24 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	AA	836	1	45,53,73	1.85	7 (15%)	52,89,113	1.47	8 (15%)
17	CLA	A3	309	14	41,49,73	1.88	8 (19%)	47,84,113	1.49	10 (21%)
24	LUT	AF	806	-	42,43,43	1.03	3 (7%)	51,60,60	1.72	12 (23%)
17	CLA	AA	810	-	65,72,73	1.55	9 (13%)	71,111,113	1.29	7 (9%)
19	LHG	A3	319	17	22,22,48	1.44	2 (9%)	25,28,54	1.27	2 (8%)
26	CHL	A3	307	-	45,53,74	2.29	16 (35%)	52,89,114	2.69	21 (40%)
17	CLA	AB	836	-	42,50,73	1.86	7 (16%)	48,85,113	1.52	7 (14%)
17	CLA	AB	841	-	65,73,73	1.54	9 (13%)	76,113,113	1.22	6 (7%)
17	CLA	AB	824	-	43,51,73	1.77	10 (23%)	49,86,113	1.57	8 (16%)
17	CLA	AL	304	-	42,50,73	1.85	8 (19%)	48,85,113	1.57	8 (16%)

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
26	CHL	A6	607	-	3/3/17/26	8/19/117/137	-
17	CLA	A6	609	16	1/1/13/20	4/25/103/115	-
17	CLA	AB	807	2	1/1/15/20	11/37/115/115	-
17	CLA	A3	305	-	1/1/10/20	4/8/86/115	-
17	CLA	AB	831	-	1/1/10/20	3/11/89/115	-
17	CLA	A6	613	-	1/1/10/20	2/11/89/115	-
17	CLA	AB	839	-	1/1/11/20	3/16/94/115	-
17	CLA	AB	808	-	-	5/20/98/115	-
17	CLA	AA	803	-	1/1/15/20	15/37/115/115	-
17	CLA	A3	311	14	1/1/10/20	0/11/89/115	-
17	CLA	AA	842	-	1/1/15/20	18/37/115/115	-
17	CLA	AA	813	-	1/1/15/20	17/37/115/115	-
17	CLA	AB	823	-	-	19/37/115/115	-
17	CLA	AA	809	1	1/1/12/20	5/19/97/115	-
17	CLA	AB	812	-	1/1/13/20	8/25/101/115	-
17	CLA	A6	604	-	1/1/10/20	1/9/88/115	-
17	CLA	AA	827	-	1/1/15/20	18/37/115/115	-
17	CLA	AB	801	-	1/1/15/20	17/37/115/115	-
17	CLA	A3	310	19	1/1/9/20	0/0/78/115	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AA	811	-	1/1/15/20	11/37/115/115	-
17	CLA	AB	820	-	1/1/13/20	8/25/103/115	-
17	CLA	AB	815	-	1/1/15/20	17/37/115/115	-
17	CLA	AA	830	-	1/1/15/20	14/37/115/115	-
17	CLA	AF	802	-	1/1/13/20	10/28/106/115	-
17	CLA	AB	802	-	1/1/15/20	16/37/113/115	-
19	LHG	A1	301	17	-	11/42/42/53	-
17	CLA	AA	801	-	1/1/15/20	13/37/115/115	-
17	CLA	AA	840	-	1/1/15/20	14/37/115/115	-
17	CLA	A4	302	15	1/1/11/20	5/13/89/115	-
25	LMG	A1	321	-	-	17/39/59/70	0/1/1/1
17	CLA	A3	314	-	1/1/8/20	0/0/74/115	-
26	CHL	A1	303	13	3/3/17/26	4/21/119/137	-
19	LHG	A1	320	17	-	16/53/53/53	-
17	CLA	AA	806	1	1/1/15/20	13/37/115/115	-
22	LMU	AB	852	-	-	9/21/61/61	0/2/2/2
17	CLA	A1	309	-	1/1/11/20	5/11/89/115	-
17	CLA	AG	204	7	1/1/11/20	4/13/91/115	-
17	CLA	A4	307	15	1/1/11/20	1/13/91/115	-
17	CLA	AK	203	-	1/1/11/20	5/13/91/115	-
17	CLA	AB	838	-	-	7/37/115/115	-
26	CHL	A3	320	16	3/3/17/26	6/22/120/137	-
17	CLA	AB	805	-	1/1/10/20	2/8/86/115	-
17	CLA	AB	828	-	1/1/15/20	13/37/115/115	-
17	CLA	AB	827	-	1/1/14/20	14/34/112/115	-
17	CLA	AA	834	-	-	15/37/115/115	-
17	CLA	AK	201	11	1/1/8/20	0/2/74/115	-
20	BCR	A3	318	-	-	4/29/63/63	0/2/2/2
17	CLA	A3	303	14	1/1/13/20	8/25/103/115	-
20	BCR	AA	845	-	-	2/29/63/63	0/2/2/2
17	CLA	AG	203	-	1/1/10/20	3/10/88/115	-
17	CLA	AB	830	-	1/1/13/20	10/27/105/115	-
21	SF4	AC	101	3	-	-	0/6/5/5
18	PQN	AA	843	-	-	6/23/43/43	0/2/2/2
17	CLA	AA	837	-	1/1/12/20	6/21/99/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A1	316	13	1/1/11/20	9/11/87/115	-
17	CLA	AA	805	-	1/1/15/20	17/37/115/115	-
20	BCR	AB	847	-	-	0/29/63/63	0/2/2/2
19	LHG	AA	844	-	-	18/53/53/53	-
17	CLA	AB	803	-	1/1/15/20	17/37/115/115	-
20	BCR	AB	848	-	-	2/29/63/63	0/2/2/2
17	CLA	AA	841	-	-	10/37/115/115	-
17	CLA	AJ	102	10	1/1/10/20	3/10/88/115	-
24	LUT	A3	316	-	-	0/29/67/67	0/2/2/2
20	BCR	AL	305	-	-	3/29/63/63	0/2/2/2
17	CLA	AA	816	-	1/1/11/20	6/13/91/115	-
17	CLA	AA	817	-	1/1/14/20	6/31/109/115	-
17	CLA	AB	822	-	1/1/11/20	5/16/94/115	-
17	CLA	AA	804	-	-	7/22/100/115	-
19	LHG	A1	302	-	-	15/40/40/53	-
17	CLA	A4	301	15	1/1/14/20	8/31/109/115	-
17	CLA	A6	610	19	1/1/7/20	5/10/70/115	-
20	BCR	AA	846	-	-	6/29/63/63	0/2/2/2
21	SF4	AA	850	2,1	-	-	0/6/5/5
17	CLA	A3	304	-	1/1/11/20	0/9/85/115	-
17	CLA	AB	829	-	1/1/15/20	15/37/115/115	-
17	CLA	AF	804	-	1/1/10/20	2/8/86/115	-
17	CLA	AA	812	-	1/1/12/20	9/24/102/115	-
17	CLA	AA	822	-	1/1/10/20	3/10/88/115	-
17	CLA	A3	313	-	-	1/6/84/115	-
20	BCR	A6	616	-	-	2/29/63/63	0/2/2/2
17	CLA	AA	832	-	1/1/13/20	7/27/105/115	-
17	CLA	AB	809	-	1/1/15/20	16/37/115/115	-
26	CHL	A4	305	-	3/3/15/26	0/10/106/137	-
26	CHL	A6	606	-	3/3/15/26	2/12/110/137	-
17	CLA	AB	816	-	1/1/10/20	4/11/89/115	-
17	CLA	AB	825	-	1/1/15/20	14/37/115/115	-
17	CLA	AA	818	-	-	7/30/108/115	-
17	CLA	A1	310	13	1/1/10/20	2/8/84/115	-
22	LMU	AA	851	-	-	10/21/61/61	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AA	824	-	1/1/13/20	7/23/101/115	-
17	CLA	A1	304	13	1/1/13/20	11/31/109/115	-
20	BCR	AJ	103	-	-	5/29/63/63	0/2/2/2
20	BCR	AI	101	-	-	7/29/63/63	0/2/2/2
17	CLA	AA	825	-	1/1/15/20	10/37/115/115	-
20	BCR	AF	805	-	-	6/29/63/63	0/2/2/2
23	DGD	AB	851	-	-	21/55/95/95	0/2/2/2
17	CLA	AB	818	-	1/1/13/20	10/30/108/115	-
17	CLA	AL	303	-	-	9/31/109/115	-
17	CLA	AA	839	-	-	6/22/100/115	-
17	CLA	A6	603	-	1/1/10/20	2/9/87/115	-
20	BCR	AA	847	-	-	13/29/63/63	0/2/2/2
17	CLA	AA	808	1	1/1/15/20	10/37/115/115	-
17	CLA	AB	821	-	1/1/12/20	7/19/97/115	-
17	CLA	AA	823	-	1/1/10/20	4/8/86/115	-
17	CLA	AB	810	2	1/1/15/20	16/37/115/115	-
20	BCR	AA	849	-	-	8/29/63/63	0/2/2/2
22	LMU	AB	850	-	-	9/21/61/61	0/2/2/2
17	CLA	AA	815	-	-	3/10/88/115	-
17	CLA	A1	312	19	1/1/10/20	0/4/80/115	-
17	CLA	AA	802	-	1/1/15/20	8/37/115/115	-
27	XAT	A4	316	-	-	0/31/93/93	0/4/4/4
17	CLA	A4	308	15	1/1/12/20	4/24/102/115	-
17	CLA	A4	310	15	1/1/10/20	5/8/86/115	-
17	CLA	A3	308	14	1/1/11/20	5/13/91/115	-
17	CLA	A4	311	-	1/1/13/20	7/26/104/115	-
17	CLA	A3	312	-	1/1/13/20	11/23/101/115	-
17	CLA	A6	611	16	1/1/11/20	6/11/89/115	-
24	LUT	A4	315	-	-	1/29/67/67	0/2/2/2
20	BCR	AG	205	-	-	2/29/63/63	0/2/2/2
17	CLA	AB	842	19	1/1/15/20	18/37/115/115	-
17	CLA	AB	833	-	1/1/15/20	10/37/115/115	-
17	CLA	A6	608	16	1/1/11/20	3/13/91/115	-
17	CLA	A1	313	13	1/1/11/20	4/13/91/115	-
17	CLA	A1	305	-	1/1/13/20	7/25/103/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	SF4	AC	102	3	-	-	0/6/5/5
17	CLA	AB	811	-	1/1/15/20	15/37/115/115	-
17	CLA	A1	311	13	1/1/14/20	3/29/107/115	-
22	LMU	AL	301	-	-	11/20/60/61	0/2/2/2
26	CHL	A1	308	13	3/3/15/26	2/8/106/137	-
20	BCR	AB	844	-	-	5/29/63/63	0/2/2/2
17	CLA	AA	838	-	-	6/25/103/115	-
17	CLA	AA	828	-	1/1/15/20	15/37/115/115	-
17	CLA	AB	840	-	1/1/15/20	7/37/115/115	-
17	CLA	A4	312	-	1/1/11/20	4/13/91/115	-
19	LHG	A6	617	17	-	17/40/40/53	-
17	CLA	AK	204	-	1/1/11/20	7/15/93/115	-
20	BCR	AB	849	-	-	5/29/63/63	0/2/2/2
25	LMG	AG	202	-	-	5/33/53/70	0/1/1/1
22	LMU	AB	853	-	-	13/21/61/61	0/2/2/2
17	CLA	A4	309	-	1/1/10/20	3/10/88/115	-
17	CLA	A1	307	-	1/1/9/20	4/8/82/115	-
17	CLA	AA	807	-	1/1/12/20	4/19/97/115	-
17	CLA	AA	814	-	1/1/11/20	5/13/91/115	-
17	CLA	AB	806	-	1/1/15/20	15/37/115/115	-
17	CLA	A3	306	14	1/1/10/20	0/10/86/115	-
17	CLA	AB	813	-	1/1/10/20	3/11/89/115	-
17	CLA	AB	814	-	1/1/15/20	14/37/115/115	-
17	CLA	A4	303	-	1/1/11/20	4/11/87/115	-
17	CLA	AG	201	-	1/1/11/20	3/11/89/115	-
20	BCR	AB	846	-	-	6/29/63/63	0/2/2/2
17	CLA	AB	826	-	1/1/14/20	6/34/112/115	-
24	LUT	A1	317	-	-	0/29/67/67	0/2/2/2
17	CLA	AB	817	-	1/1/13/20	8/25/103/115	-
26	CHL	A4	314	15	3/3/15/26	0/10/106/137	-
24	LUT	A6	614	-	-	0/29/67/67	0/2/2/2
17	CLA	A6	601	15	1/1/11/20	2/15/93/115	-
20	BCR	AL	306	-	-	5/29/63/63	0/2/2/2
19	LHG	A3	301	-	-	11/40/40/53	-
17	CLA	AB	834	-	1/1/15/20	16/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	AA	820	-	1/1/11/20	3/13/91/115	-
17	CLA	A1	314	-	1/1/15/20	12/35/113/115	-
20	BCR	AK	202	-	-	5/29/63/63	0/2/2/2
17	CLA	A1	306	-	1/1/11/20	9/18/96/115	-
17	CLA	AA	833	-	1/1/15/20	19/37/115/115	-
17	CLA	AB	804	-	1/1/15/20	16/37/115/115	-
19	LHG	AJ	104	-	-	16/44/44/53	-
18	PQN	AB	843	-	-	8/23/43/43	0/2/2/2
26	CHL	A4	306	-	3/3/16/26	2/15/113/137	-
17	CLA	A1	315	-	1/1/10/20	0/4/80/115	-
17	CLA	AA	829	-	1/1/15/20	18/37/115/115	-
17	CLA	AB	837	-	1/1/12/20	7/19/97/115	-
20	BCR	AI	102	-	-	5/29/63/63	0/2/2/2
20	BCR	AK	205	-	-	6/29/63/63	0/2/2/2
17	CLA	AH	201	-	1/1/14/20	10/31/109/115	-
17	CLA	AA	831	-	1/1/11/20	7/16/94/115	-
17	CLA	AA	835	-	1/1/11/20	0/11/89/115	-
17	CLA	A3	302	14	1/1/14/20	6/31/109/115	-
17	CLA	AA	819	-	1/1/15/20	14/37/115/115	-
17	CLA	AF	803	-	1/1/10/20	2/10/88/115	-
17	CLA	A3	315	-	1/1/10/20	0/6/84/115	-
17	CLA	AB	835	-	-	7/31/109/115	-
20	BCR	AA	848	-	-	4/29/63/63	0/2/2/2
20	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
20	BCR	A4	317	-	-	2/29/63/63	0/2/2/2
17	CLA	AB	819	-	1/1/14/20	14/31/109/115	-
25	LMG	A4	318	-	-	15/34/54/70	0/1/1/1
17	CLA	A6	602	16	1/1/15/20	9/37/115/115	-
20	BCR	AB	845	-	-	6/29/63/63	0/2/2/2
27	XAT	A3	317	-	-	0/31/93/93	0/4/4/4
17	CLA	AL	302	12	1/1/10/20	5/8/86/115	-
27	XAT	A6	615	-	-	0/31/93/93	0/4/4/4
20	BCR	A1	319	-	-	4/29/63/63	0/2/2/2
20	BCR	AF	801	-	-	2/29/63/63	0/2/2/2
17	CLA	A6	612	16	1/1/14/20	7/35/113/115	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	A6	605	-	3/3/15/26	2/10/108/137	-
17	CLA	AA	826	-	1/1/13/20	11/30/108/115	-
17	CLA	A4	313	-	1/1/12/20	9/19/97/115	-
17	CLA	AA	821	-	1/1/15/20	15/37/115/115	-
17	CLA	AB	832	-	-	7/37/115/115	-
26	CHL	A4	304	-	3/3/15/26	1/8/106/137	-
27	XAT	A1	318	-	-	0/31/93/93	0/4/4/4
17	CLA	AA	836	1	-	7/13/91/115	-
17	CLA	A3	309	14	1/1/10/20	3/8/86/115	-
24	LUT	AF	806	-	-	0/29/67/67	0/2/2/2
17	CLA	AA	810	-	1/1/14/20	10/37/111/115	-
19	LHG	A3	319	17	-	14/26/26/53	-
26	CHL	A3	307	-	3/3/16/26	4/13/111/137	-
17	CLA	AB	836	-	-	2/10/88/115	-
17	CLA	AB	841	-	1/1/15/20	7/37/115/115	-
17	CLA	AB	824	-	1/1/10/20	4/11/89/115	-
17	CLA	AL	304	-	1/1/10/20	5/10/88/115	-

All (1393) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A6	610	CLA	C1A-NA	12.69	1.40	1.29
18	AA	843	PQN	C12-C13	9.56	1.55	1.33
18	AB	843	PQN	C12-C13	9.36	1.55	1.33
17	AK	201	CLA	C3B-C4B	8.50	1.49	1.39
17	A6	613	CLA	C4B-NB	7.99	1.42	1.35
17	AK	201	CLA	C4B-NB	7.91	1.42	1.35
17	AF	803	CLA	C4B-NB	7.87	1.42	1.35
17	AG	204	CLA	C4B-NB	7.86	1.42	1.35
17	AH	201	CLA	C4B-NB	7.84	1.42	1.35
17	AA	822	CLA	C4B-NB	7.83	1.42	1.35
18	AB	843	PQN	O4-C4	7.78	1.39	1.23
18	AA	843	PQN	O4-C4	7.78	1.39	1.23
17	AA	836	CLA	C4B-NB	7.77	1.42	1.35
17	A4	307	CLA	C4B-NB	7.76	1.42	1.35
17	A4	308	CLA	C4B-NB	7.76	1.42	1.35
17	AB	809	CLA	C4B-NB	7.75	1.42	1.35
17	AK	203	CLA	C4B-NB	7.71	1.42	1.35
17	A1	309	CLA	C4B-NB	7.71	1.42	1.35

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AA	823	CLA	C4B-NB	7.69	1.42	1.35
17	AB	822	CLA	C4B-NB	7.69	1.42	1.35
17	AB	820	CLA	C4B-NB	7.69	1.42	1.35
17	AA	809	CLA	C4B-NB	7.68	1.42	1.35
17	AG	201	CLA	C4B-NB	7.67	1.42	1.35
17	A6	603	CLA	C4B-NB	7.67	1.42	1.35
17	A6	610	CLA	C4B-NB	7.67	1.42	1.35
17	AL	302	CLA	C4B-NB	7.67	1.42	1.35
17	AG	203	CLA	C4B-NB	7.67	1.42	1.35
17	A1	311	CLA	C4B-NB	7.65	1.42	1.35
17	AA	824	CLA	C4B-NB	7.65	1.42	1.35
17	A4	311	CLA	C4B-NB	7.63	1.42	1.35
17	A3	304	CLA	C4B-NB	7.62	1.42	1.35
17	A1	305	CLA	C4B-NB	7.62	1.42	1.35
17	A6	609	CLA	C4B-NB	7.61	1.42	1.35
17	A3	314	CLA	C4B-NB	7.60	1.42	1.35
17	A4	310	CLA	C4B-NB	7.60	1.42	1.35
17	A3	311	CLA	C4B-NB	7.57	1.42	1.35
17	A3	305	CLA	C4B-NB	7.57	1.42	1.35
17	A3	310	CLA	C4B-NB	7.56	1.42	1.35
17	A6	612	CLA	C4B-NB	7.56	1.42	1.35
17	AJ	102	CLA	C4B-NB	7.55	1.41	1.35
17	AA	831	CLA	C4B-NB	7.55	1.41	1.35
17	A6	611	CLA	C4B-NB	7.54	1.41	1.35
17	AA	808	CLA	C4B-NB	7.54	1.41	1.35
17	A1	310	CLA	C4B-NB	7.53	1.41	1.35
17	A4	313	CLA	C4B-NB	7.53	1.41	1.35
17	A3	303	CLA	C4B-NB	7.52	1.41	1.35
17	AL	304	CLA	C4B-NB	7.51	1.41	1.35
17	AF	804	CLA	C4B-NB	7.50	1.41	1.35
18	AB	843	PQN	O1-C1	7.50	1.39	1.23
17	AA	801	CLA	C4B-NB	7.49	1.41	1.35
17	A4	312	CLA	C4B-NB	7.49	1.41	1.35
17	AB	830	CLA	C4B-NB	7.48	1.41	1.35
17	AB	840	CLA	C4B-NB	7.48	1.41	1.35
17	A3	306	CLA	C4B-NB	7.48	1.41	1.35
17	AA	810	CLA	C4B-NB	7.48	1.41	1.35
17	AB	802	CLA	C4B-NB	7.48	1.41	1.35
17	AB	836	CLA	C4B-NB	7.47	1.41	1.35
17	A1	306	CLA	C4B-NB	7.47	1.41	1.35
17	A1	315	CLA	C4B-NB	7.47	1.41	1.35
17	AA	816	CLA	C4B-NB	7.44	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A3	312	CLA	C4B-NB	7.42	1.41	1.35
17	A3	313	CLA	C4B-NB	7.42	1.41	1.35
17	AA	811	CLA	C4B-NB	7.41	1.41	1.35
17	AA	833	CLA	C4B-NB	7.40	1.41	1.35
17	A4	309	CLA	C4B-NB	7.39	1.41	1.35
17	AA	817	CLA	C4B-NB	7.39	1.41	1.35
17	AA	827	CLA	C4B-NB	7.38	1.41	1.35
17	AA	830	CLA	C4B-NB	7.38	1.41	1.35
17	A1	312	CLA	C4B-NB	7.38	1.41	1.35
17	A6	608	CLA	C4B-NB	7.38	1.41	1.35
17	A6	604	CLA	C4B-NB	7.36	1.41	1.35
17	AA	815	CLA	C4B-NB	7.36	1.41	1.35
17	AB	803	CLA	C4B-NB	7.35	1.41	1.35
17	AB	837	CLA	C4B-NB	7.35	1.41	1.35
17	A3	309	CLA	C4B-NB	7.35	1.41	1.35
17	AA	821	CLA	C4B-NB	7.35	1.41	1.35
17	A1	313	CLA	C4B-NB	7.34	1.41	1.35
17	AB	812	CLA	C4B-NB	7.34	1.41	1.35
17	AB	821	CLA	C4B-NB	7.34	1.41	1.35
17	AK	204	CLA	C4B-NB	7.34	1.41	1.35
18	AA	843	PQN	O1-C1	7.34	1.38	1.23
17	A1	307	CLA	C4B-NB	7.32	1.41	1.35
17	AA	825	CLA	C4B-NB	7.32	1.41	1.35
17	AB	834	CLA	C4B-NB	7.32	1.41	1.35
17	A1	316	CLA	C4B-NB	7.31	1.41	1.35
17	AA	835	CLA	C4B-NB	7.31	1.41	1.35
17	AA	820	CLA	C4B-NB	7.31	1.41	1.35
17	AB	841	CLA	C4B-NB	7.30	1.41	1.35
17	AA	814	CLA	C4B-NB	7.30	1.41	1.35
17	A4	303	CLA	C4B-NB	7.28	1.41	1.35
17	A3	302	CLA	C4B-NB	7.28	1.41	1.35
17	A4	302	CLA	C4B-NB	7.27	1.41	1.35
17	AB	831	CLA	C4B-NB	7.27	1.41	1.35
18	AA	843	PQN	C9-C10	7.26	1.51	1.39
17	AA	802	CLA	C4B-NB	7.24	1.41	1.35
17	AA	828	CLA	C4B-NB	7.23	1.41	1.35
17	AB	816	CLA	C4B-NB	7.22	1.41	1.35
17	A3	308	CLA	C4B-NB	7.21	1.41	1.35
17	AB	823	CLA	C4B-NB	7.21	1.41	1.35
17	AB	838	CLA	C4B-NB	7.20	1.41	1.35
17	AB	835	CLA	C4B-NB	7.19	1.41	1.35
17	A4	301	CLA	C4B-NB	7.18	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AB	813	CLA	C4B-NB	7.17	1.41	1.35
17	AA	804	CLA	C4B-NB	7.17	1.41	1.35
17	AB	827	CLA	C4B-NB	7.16	1.41	1.35
17	A1	314	CLA	C4B-NB	7.15	1.41	1.35
17	A6	602	CLA	C4B-NB	7.15	1.41	1.35
17	AA	832	CLA	C4B-NB	7.14	1.41	1.35
17	AB	826	CLA	C4B-NB	7.14	1.41	1.35
17	AB	839	CLA	C4B-NB	7.13	1.41	1.35
17	AB	817	CLA	C4B-NB	7.13	1.41	1.35
17	AA	839	CLA	C4B-NB	7.12	1.41	1.35
17	AA	838	CLA	C4B-NB	7.11	1.41	1.35
17	AA	803	CLA	C4B-NB	7.11	1.41	1.35
17	AB	825	CLA	C4B-NB	7.08	1.41	1.35
17	A3	315	CLA	C4B-NB	7.07	1.41	1.35
17	AA	807	CLA	C4B-NB	7.07	1.41	1.35
17	AA	841	CLA	C4B-NB	7.06	1.41	1.35
17	AA	842	CLA	C4B-NB	7.03	1.41	1.35
17	AB	806	CLA	C4B-NB	7.03	1.41	1.35
17	AB	832	CLA	C4B-NB	7.02	1.41	1.35
17	AB	805	CLA	C4B-NB	7.01	1.41	1.35
17	AB	815	CLA	C4B-NB	7.00	1.41	1.35
17	AB	828	CLA	C4B-NB	6.99	1.41	1.35
17	AB	818	CLA	C4B-NB	6.98	1.41	1.35
17	AA	826	CLA	C4B-NB	6.98	1.41	1.35
17	AB	819	CLA	C4B-NB	6.97	1.41	1.35
18	AA	843	PQN	C6-C5	6.96	1.51	1.39
17	AA	818	CLA	C4B-NB	6.96	1.41	1.35
17	AB	801	CLA	C4B-NB	6.95	1.41	1.35
17	AA	806	CLA	C4B-NB	6.94	1.41	1.35
17	AB	808	CLA	C4B-NB	6.92	1.41	1.35
17	A1	304	CLA	C4B-NB	6.90	1.41	1.35
17	AB	833	CLA	C4B-NB	6.89	1.41	1.35
17	AA	805	CLA	C4B-NB	6.88	1.41	1.35
18	AB	843	PQN	C6-C5	6.88	1.50	1.39
18	AB	843	PQN	C9-C10	6.88	1.50	1.39
17	AL	303	CLA	C4B-NB	6.87	1.41	1.35
17	AB	824	CLA	C4B-NB	6.83	1.41	1.35
17	AF	802	CLA	C4B-NB	6.81	1.41	1.35
17	AB	811	CLA	C4B-NB	6.80	1.41	1.35
17	AB	829	CLA	C4B-NB	6.80	1.41	1.35
17	AA	840	CLA	C4B-NB	6.80	1.41	1.35
17	AA	813	CLA	C4B-NB	6.79	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AA	834	CLA	C4B-NB	6.78	1.41	1.35
17	AA	812	CLA	C4B-NB	6.77	1.41	1.35
17	AA	837	CLA	C4B-NB	6.75	1.41	1.35
17	AB	842	CLA	C4B-NB	6.73	1.41	1.35
17	A6	601	CLA	C4B-NB	6.73	1.41	1.35
18	AB	843	PQN	C10-C5	-6.68	1.29	1.40
17	AA	819	CLA	C4B-NB	6.65	1.41	1.35
17	AB	814	CLA	C4B-NB	6.64	1.41	1.35
17	AB	807	CLA	C4B-NB	6.58	1.41	1.35
18	AA	843	PQN	C10-C5	-6.56	1.29	1.40
17	AB	810	CLA	C4B-NB	6.49	1.41	1.35
17	AB	804	CLA	C4B-NB	6.35	1.40	1.35
17	AA	829	CLA	C4B-NB	5.98	1.40	1.35
26	A4	304	CHL	C3B-C2B	5.84	1.48	1.40
26	A6	607	CHL	C3B-C2B	5.53	1.48	1.40
26	A6	606	CHL	C3B-C2B	5.35	1.47	1.40
26	A6	605	CHL	C3B-C2B	5.23	1.47	1.40
26	A3	320	CHL	C2C-C3C	5.21	1.47	1.36
26	A4	306	CHL	C3B-C2B	5.19	1.47	1.40
26	A4	305	CHL	O2D-CGD	5.18	1.45	1.33
26	A6	606	CHL	O2D-CGD	5.16	1.45	1.33
26	A6	605	CHL	O2D-CGD	5.13	1.45	1.33
26	A4	314	CHL	C2C-C3C	5.09	1.47	1.36
26	A6	607	CHL	O2D-CGD	5.08	1.45	1.33
26	A4	306	CHL	CHC-C1C	5.08	1.48	1.35
26	A3	320	CHL	C3B-C2B	5.05	1.47	1.40
26	A4	304	CHL	C2C-C3C	5.05	1.47	1.37
26	A1	303	CHL	C2C-C3C	5.03	1.47	1.36
26	A4	306	CHL	O2D-CGD	5.00	1.45	1.33
26	A3	307	CHL	O2D-CGD	4.95	1.45	1.33
26	A1	308	CHL	C2C-C3C	4.93	1.47	1.36
26	A1	308	CHL	C3B-C2B	4.91	1.47	1.40
26	A4	305	CHL	C3C-C2C	4.90	1.47	1.36
26	A1	303	CHL	C3B-C2B	4.89	1.47	1.40
26	A3	307	CHL	C3B-C2B	4.88	1.47	1.40
26	A1	303	CHL	CHC-C1C	4.83	1.47	1.35
26	A6	605	CHL	CHC-C1C	4.83	1.47	1.35
26	A4	314	CHL	CHC-C1C	4.83	1.47	1.35
26	A3	320	CHL	CHC-C1C	4.80	1.47	1.35
26	A6	606	CHL	C2C-C3C	4.80	1.47	1.36
26	A6	607	CHL	C3C-C2C	4.80	1.46	1.36
26	A6	605	CHL	C2C-C3C	4.77	1.46	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A1	308	CHL	CHC-C1C	4.76	1.47	1.35
26	A6	607	CHL	CHC-C1C	4.75	1.47	1.35
26	A4	305	CHL	CHC-C1C	4.75	1.47	1.35
19	A3	319	LHG	O7-C7	4.72	1.45	1.35
26	A4	306	CHL	C2C-C3C	4.71	1.46	1.36
26	A4	304	CHL	CHC-C1C	4.67	1.47	1.35
26	A4	314	CHL	O2D-CGD	4.66	1.45	1.30
26	A3	307	CHL	C3C-C2C	4.65	1.46	1.36
26	A4	304	CHL	O2D-CGD	4.63	1.45	1.30
26	A1	308	CHL	O2D-CGD	4.63	1.45	1.30
26	A6	606	CHL	CHC-C1C	4.62	1.46	1.35
26	A1	303	CHL	O2D-CGD	4.57	1.45	1.30
26	A4	306	CHL	O2A-CGA	4.51	1.45	1.30
26	A1	303	CHL	O2A-CGA	4.48	1.46	1.33
26	A3	307	CHL	O2A-CGA	4.47	1.45	1.30
26	A3	320	CHL	O2D-CGD	4.47	1.45	1.30
26	A1	303	CHL	C1D-ND	-4.42	1.32	1.37
25	AG	202	LMG	O7-C10	4.38	1.46	1.34
26	A3	307	CHL	CHC-C1C	4.38	1.46	1.35
26	A1	308	CHL	CHD-C1D	4.38	1.46	1.38
26	A4	314	CHL	CHD-C1D	4.37	1.46	1.38
26	A1	308	CHL	C3A-C2A	-4.36	1.50	1.54
26	A3	320	CHL	CHD-C1D	4.35	1.46	1.38
19	AJ	104	LHG	O8-C23	4.29	1.45	1.33
25	AG	202	LMG	O8-C28	4.28	1.45	1.33
26	A4	305	CHL	CHD-C1D	4.28	1.46	1.38
26	A6	607	CHL	O2A-CGA	4.28	1.45	1.33
19	A1	301	LHG	O7-C7	4.27	1.46	1.34
19	A1	302	LHG	O8-C23	4.27	1.45	1.33
26	A6	607	CHL	CHD-C1D	4.26	1.46	1.38
19	AA	844	LHG	O8-C23	4.26	1.45	1.33
19	AJ	104	LHG	O7-C7	4.26	1.46	1.34
19	A3	301	LHG	O8-C23	4.25	1.45	1.33
19	A1	320	LHG	O8-C23	4.24	1.45	1.33
26	A6	606	CHL	CHD-C1D	4.24	1.46	1.38
26	A4	304	CHL	CHD-C1D	4.23	1.46	1.38
25	A1	321	LMG	O8-C28	4.22	1.45	1.33
17	A6	610	CLA	CHB-C4A	4.21	1.38	1.34
25	A1	321	LMG	O7-C10	4.19	1.46	1.34
26	A3	307	CHL	CHD-C1D	4.18	1.46	1.38
26	A3	320	CHL	O2A-CGA	4.17	1.45	1.33
26	A6	605	CHL	CHD-C1D	4.17	1.46	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A1	308	CHL	C1D-ND	-4.14	1.32	1.37
19	A1	302	LHG	O7-C7	4.13	1.46	1.34
19	A3	301	LHG	O7-C7	4.11	1.45	1.34
26	A3	320	CHL	C1D-ND	-4.11	1.32	1.37
19	A1	301	LHG	O8-C23	4.09	1.45	1.33
19	A3	319	LHG	O8-C23	4.09	1.45	1.33
23	AB	851	DGD	O1G-C1A	4.06	1.45	1.33
19	A1	320	LHG	O7-C7	4.06	1.45	1.34
26	A4	314	CHL	CHD-C4C	4.02	1.48	1.39
17	AA	823	CLA	C1D-ND	4.02	1.42	1.37
26	A4	304	CHL	C1D-ND	-4.01	1.32	1.37
19	A6	617	LHG	O7-C7	4.00	1.45	1.34
26	A1	303	CHL	CHD-C1D	3.99	1.46	1.38
17	A6	613	CLA	C1D-ND	3.99	1.42	1.37
26	A4	306	CHL	C1D-ND	-3.97	1.32	1.37
19	A6	617	LHG	O8-C23	3.96	1.44	1.33
26	A4	304	CHL	CHD-C4C	3.93	1.48	1.39
26	A6	605	CHL	C1D-ND	-3.91	1.33	1.37
17	AB	802	CLA	CAB-C3B	-3.90	1.43	1.51
17	AA	801	CLA	C1D-ND	3.90	1.42	1.37
26	A4	314	CHL	C1D-ND	-3.89	1.33	1.37
25	A4	318	LMG	O8-C28	3.89	1.44	1.33
19	AA	844	LHG	O7-C7	3.89	1.45	1.34
26	A6	607	CHL	C1D-ND	-3.88	1.33	1.37
17	AK	201	CLA	C4B-CHC	-3.88	1.36	1.43
17	A3	311	CLA	C1D-ND	3.88	1.42	1.37
26	A3	320	CHL	CHD-C4C	3.87	1.48	1.39
17	A4	302	CLA	C1D-ND	3.85	1.42	1.37
23	AB	851	DGD	O2G-C1B	3.85	1.45	1.34
17	A3	313	CLA	C1D-ND	3.84	1.42	1.37
26	A4	305	CHL	CHD-C4C	3.83	1.48	1.39
26	A6	606	CHL	C1D-ND	-3.82	1.33	1.37
17	AK	201	CLA	C1D-ND	3.82	1.42	1.37
17	A3	312	CLA	C1D-ND	3.81	1.42	1.37
26	A4	305	CHL	C1D-ND	-3.81	1.33	1.37
17	A1	316	CLA	C1D-ND	3.81	1.42	1.37
26	A6	606	CHL	CHD-C4C	3.80	1.47	1.39
17	AL	303	CLA	C1D-ND	3.80	1.42	1.37
17	A1	305	CLA	C1D-ND	3.80	1.42	1.37
17	AH	201	CLA	C1D-ND	3.80	1.42	1.37
17	A1	312	CLA	CAB-C3B	-3.79	1.43	1.51
17	AB	836	CLA	C1D-ND	3.79	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AF	804	CLA	C1D-ND	3.79	1.42	1.37
17	A1	313	CLA	C1D-ND	3.78	1.42	1.37
26	A4	305	CHL	OBD-CAD	3.78	1.29	1.22
17	AG	204	CLA	C1D-ND	3.78	1.42	1.37
26	A1	308	CHL	CHD-C4C	3.77	1.47	1.39
17	AA	836	CLA	C1D-ND	3.77	1.42	1.37
17	AA	816	CLA	C1D-ND	3.77	1.42	1.37
17	A3	303	CLA	C1D-ND	3.77	1.42	1.37
17	AB	817	CLA	C1D-ND	3.76	1.42	1.37
26	A4	306	CHL	CHD-C1D	3.75	1.45	1.38
26	A6	607	CHL	CHD-C4C	3.75	1.47	1.39
17	AA	812	CLA	C1D-ND	3.74	1.42	1.37
17	A6	612	CLA	C1D-ND	3.74	1.42	1.37
17	A1	309	CLA	C1D-ND	3.74	1.42	1.37
26	A1	308	CHL	OBD-CAD	3.74	1.28	1.22
17	A1	307	CLA	C1D-ND	3.74	1.42	1.37
17	AK	204	CLA	C1D-ND	3.73	1.42	1.37
26	A3	307	CHL	C1D-ND	-3.73	1.33	1.37
17	AK	203	CLA	C1D-ND	3.73	1.42	1.37
17	A3	306	CLA	C1D-ND	3.72	1.42	1.37
26	A6	605	CHL	CHD-C4C	3.72	1.47	1.39
26	A1	303	CHL	CHD-C4C	3.71	1.47	1.39
17	A1	306	CLA	C1D-ND	3.71	1.42	1.37
26	A6	606	CHL	OBD-CAD	3.71	1.28	1.22
17	A4	310	CLA	C1D-ND	3.71	1.42	1.37
17	A3	305	CLA	C1D-ND	3.71	1.42	1.37
17	A1	315	CLA	C1D-ND	3.70	1.42	1.37
26	A6	605	CHL	OBD-CAD	3.69	1.28	1.22
17	AG	201	CLA	C1D-ND	3.69	1.42	1.37
17	A4	312	CLA	C1D-ND	3.69	1.42	1.37
17	AB	808	CLA	C1D-ND	3.69	1.42	1.37
26	A4	314	CHL	OBD-CAD	3.69	1.28	1.22
17	AJ	102	CLA	C1D-ND	3.68	1.42	1.37
17	AA	822	CLA	C1D-ND	3.68	1.42	1.37
17	AA	832	CLA	C1D-ND	3.67	1.42	1.37
17	A6	604	CLA	C1D-ND	3.67	1.42	1.37
17	AL	304	CLA	C1D-ND	3.67	1.42	1.37
22	AL	301	LMU	O5B-C1B	3.67	1.51	1.41
17	A3	314	CLA	C1D-ND	3.66	1.42	1.37
17	AA	835	CLA	C1D-ND	3.65	1.42	1.37
17	A3	310	CLA	C1D-ND	3.65	1.42	1.37
26	A3	320	CHL	C3D-C2D	3.65	1.49	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A4	304	CHL	OBD-CAD	3.65	1.28	1.22
17	AA	819	CLA	C1D-ND	3.65	1.42	1.37
26	A4	306	CHL	CHD-C4C	3.64	1.47	1.39
17	A4	308	CLA	C1D-ND	3.64	1.42	1.37
17	A3	304	CLA	CAB-C3B	-3.63	1.44	1.51
26	A6	607	CHL	OBD-CAD	3.61	1.28	1.22
17	A6	610	CLA	CAB-C3B	-3.61	1.44	1.51
17	A4	303	CLA	C1D-ND	3.61	1.42	1.37
17	AA	802	CLA	C4D-ND	-3.61	1.32	1.37
17	AB	841	CLA	C1D-ND	3.60	1.42	1.37
17	A3	309	CLA	C1D-ND	3.59	1.42	1.37
17	A4	307	CLA	C1D-ND	3.59	1.42	1.37
17	AB	827	CLA	C1D-ND	3.59	1.42	1.37
17	AA	807	CLA	C1D-ND	3.59	1.42	1.37
17	A4	303	CLA	CAB-C3B	-3.58	1.44	1.51
17	A1	311	CLA	C1D-ND	3.58	1.42	1.37
17	A3	304	CLA	C1D-ND	3.58	1.42	1.37
17	A4	302	CLA	CAB-C3B	-3.57	1.44	1.51
17	AA	809	CLA	C1D-ND	3.57	1.42	1.37
17	AA	820	CLA	C1D-ND	3.57	1.42	1.37
17	AB	812	CLA	C1D-ND	3.57	1.42	1.37
17	AB	816	CLA	C1D-ND	3.57	1.42	1.37
17	AB	819	CLA	C1D-ND	3.57	1.42	1.37
17	A4	309	CLA	C1D-ND	3.57	1.42	1.37
17	AB	832	CLA	C1D-ND	3.57	1.42	1.37
17	AA	806	CLA	C1D-ND	3.57	1.42	1.37
17	AL	302	CLA	C1D-ND	3.56	1.42	1.37
17	A6	609	CLA	C1D-ND	3.56	1.42	1.37
17	A6	610	CLA	C1D-ND	3.56	1.42	1.37
17	A1	310	CLA	CAB-C3B	-3.56	1.44	1.51
17	AA	828	CLA	C1D-ND	3.55	1.42	1.37
17	A6	611	CLA	C1D-ND	3.55	1.42	1.37
17	A1	316	CLA	CAB-C3B	-3.55	1.44	1.51
17	A4	311	CLA	C1D-ND	3.55	1.42	1.37
25	A4	318	LMG	O7-C10	3.54	1.44	1.34
17	A1	312	CLA	C1D-ND	3.54	1.42	1.37
17	AB	812	CLA	CAB-C3B	-3.54	1.44	1.51
17	AA	803	CLA	C1D-ND	3.54	1.42	1.37
17	AA	827	CLA	C1D-ND	3.53	1.42	1.37
17	A4	313	CLA	C1D-ND	3.53	1.42	1.37
17	A6	601	CLA	C1D-ND	3.53	1.42	1.37
26	A3	307	CHL	CHD-C4C	3.53	1.47	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AB	818	CLA	C1D-ND	3.53	1.42	1.37
26	A4	305	CHL	C3D-C2D	3.52	1.48	1.39
17	AA	813	CLA	C1D-ND	3.52	1.42	1.37
17	A6	603	CLA	C1D-ND	3.52	1.42	1.37
17	AA	811	CLA	C1D-ND	3.52	1.42	1.37
17	AB	842	CLA	C1D-ND	3.52	1.42	1.37
17	AA	839	CLA	C1D-ND	3.52	1.42	1.37
17	A3	306	CLA	CAB-C3B	-3.52	1.44	1.51
17	AA	807	CLA	C4D-ND	-3.51	1.32	1.37
17	AA	814	CLA	C1D-ND	3.51	1.42	1.37
26	A3	307	CHL	OBD-CAD	3.50	1.28	1.22
17	A3	308	CLA	C1D-ND	3.50	1.42	1.37
17	A1	314	CLA	C1D-ND	3.50	1.42	1.37
26	A6	606	CHL	C3D-C2D	3.50	1.48	1.39
17	AA	831	CLA	C1D-ND	3.49	1.42	1.37
17	AF	803	CLA	C1D-ND	3.49	1.42	1.37
26	A4	314	CHL	C3D-C2D	3.49	1.48	1.39
17	AB	806	CLA	C1D-ND	3.49	1.42	1.37
22	AL	301	LMU	O5'-C1'	3.48	1.50	1.41
17	AB	837	CLA	C1D-ND	3.48	1.42	1.37
17	A6	608	CLA	C1D-ND	3.48	1.42	1.37
26	A6	605	CHL	C3D-C2D	3.48	1.48	1.39
17	AA	826	CLA	C4D-ND	-3.48	1.32	1.37
17	AA	837	CLA	C1D-ND	3.47	1.42	1.37
17	AB	821	CLA	C1D-ND	3.47	1.42	1.37
17	A1	315	CLA	CAB-C3B	-3.47	1.44	1.51
17	AA	821	CLA	C1D-ND	3.46	1.42	1.37
26	A1	303	CHL	C3D-C2D	3.46	1.48	1.39
17	AB	811	CLA	C1D-ND	3.45	1.42	1.37
26	A1	308	CHL	C3D-C2D	3.45	1.48	1.39
17	AB	828	CLA	C1D-ND	3.45	1.42	1.37
17	A3	302	CLA	C1D-ND	3.44	1.42	1.37
22	AB	852	LMU	O5B-C1B	3.44	1.50	1.41
17	AA	818	CLA	C1D-ND	3.44	1.42	1.37
17	AB	802	CLA	C1D-ND	3.43	1.42	1.37
17	A1	310	CLA	C1D-ND	3.43	1.42	1.37
17	AA	805	CLA	C1D-ND	3.41	1.42	1.37
17	AA	810	CLA	C1D-ND	3.41	1.42	1.37
17	AG	203	CLA	C1D-ND	3.40	1.42	1.37
26	A4	304	CHL	C3D-C2D	3.40	1.48	1.39
26	A6	607	CHL	C3D-C2D	3.39	1.48	1.39
17	AB	826	CLA	C1D-ND	3.39	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	AB	843	PQN	C11-C12	3.39	1.55	1.50
17	AB	811	CLA	C4D-ND	-3.39	1.33	1.37
17	AA	804	CLA	C1D-ND	3.38	1.41	1.37
17	A6	602	CLA	C1D-ND	3.37	1.41	1.37
22	AB	853	LMU	O5'-C1'	3.37	1.50	1.41
26	A3	307	CHL	C3D-C2D	3.37	1.48	1.39
17	AB	833	CLA	C1D-ND	3.37	1.41	1.37
17	AB	835	CLA	C1D-ND	3.37	1.41	1.37
26	A1	303	CHL	OBD-CAD	3.37	1.28	1.22
17	AB	833	CLA	C4D-ND	-3.37	1.33	1.37
17	AB	820	CLA	C4D-ND	-3.36	1.33	1.37
17	AA	842	CLA	C1D-ND	3.36	1.41	1.37
17	AA	829	CLA	C1D-ND	3.36	1.41	1.37
18	AA	843	PQN	C11-C12	3.35	1.55	1.50
17	AB	823	CLA	C1D-ND	3.35	1.41	1.37
17	A4	301	CLA	C4D-ND	-3.35	1.33	1.37
17	AB	822	CLA	C1D-ND	3.34	1.41	1.37
22	AA	851	LMU	O5'-C1'	3.34	1.50	1.41
17	A6	610	CLA	C4D-ND	-3.34	1.33	1.37
17	AB	805	CLA	C1D-ND	3.34	1.41	1.37
17	AB	814	CLA	C4D-ND	-3.34	1.33	1.37
26	A4	306	CHL	OBD-CAD	3.34	1.28	1.22
22	AB	853	LMU	O5B-C1B	3.33	1.50	1.41
17	AA	824	CLA	C1D-ND	3.32	1.41	1.37
17	AA	841	CLA	C1D-ND	3.32	1.41	1.37
17	AB	802	CLA	C4D-ND	-3.31	1.33	1.37
26	A4	306	CHL	C3D-C2D	3.31	1.48	1.39
17	AA	817	CLA	C1D-ND	3.31	1.41	1.37
17	AB	803	CLA	C1D-ND	3.31	1.41	1.37
17	AB	826	CLA	C4D-ND	-3.31	1.33	1.37
17	AB	820	CLA	C1D-ND	3.31	1.41	1.37
22	AB	850	LMU	O5'-C1'	3.29	1.50	1.41
17	AA	838	CLA	C4D-ND	-3.29	1.33	1.37
17	AB	829	CLA	C4D-ND	-3.29	1.33	1.37
17	AB	813	CLA	C1D-ND	3.29	1.41	1.37
17	AB	814	CLA	C1D-ND	3.29	1.41	1.37
17	AA	813	CLA	C4D-ND	-3.29	1.33	1.37
17	AA	838	CLA	C1D-ND	3.28	1.41	1.37
17	AA	819	CLA	C4D-ND	-3.28	1.33	1.37
17	AA	804	CLA	C4D-ND	-3.28	1.33	1.37
17	AB	838	CLA	C4D-ND	-3.27	1.33	1.37
17	AA	808	CLA	C1D-ND	3.27	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A6	602	CLA	C4D-ND	-3.27	1.33	1.37
17	AA	834	CLA	C1D-ND	3.27	1.41	1.37
17	AA	830	CLA	CMB-C2B	-3.27	1.44	1.51
17	A3	315	CLA	C1D-ND	3.26	1.41	1.37
17	AA	802	CLA	C1D-ND	3.26	1.41	1.37
17	AB	807	CLA	C4D-ND	-3.26	1.33	1.37
17	AB	810	CLA	C4D-ND	-3.25	1.33	1.37
17	AA	832	CLA	C4D-ND	-3.25	1.33	1.37
17	A3	302	CLA	C4D-ND	-3.25	1.33	1.37
17	AK	204	CLA	C4D-ND	-3.25	1.33	1.37
17	AB	809	CLA	C4D-ND	-3.24	1.33	1.37
17	AB	829	CLA	C1D-ND	3.24	1.41	1.37
17	AL	303	CLA	C4D-ND	-3.24	1.33	1.37
17	AF	803	CLA	C4D-ND	-3.23	1.33	1.37
17	AB	810	CLA	C1D-ND	3.23	1.41	1.37
17	AB	815	CLA	C4D-ND	-3.23	1.33	1.37
17	AB	804	CLA	C4D-ND	-3.23	1.33	1.37
17	AB	841	CLA	C4D-ND	-3.23	1.33	1.37
17	A6	603	CLA	C4D-ND	-3.23	1.33	1.37
17	AA	826	CLA	C1D-ND	3.22	1.41	1.37
17	AA	840	CLA	C1D-ND	3.22	1.41	1.37
17	AB	831	CLA	C1D-ND	3.22	1.41	1.37
17	AB	820	CLA	CMB-C2B	-3.22	1.44	1.51
17	A6	603	CLA	CHC-C1C	3.22	1.43	1.35
17	AB	839	CLA	CMD-C2D	-3.21	1.44	1.50
17	AB	825	CLA	C4D-ND	-3.21	1.33	1.37
17	AA	833	CLA	CMB-C2B	-3.21	1.45	1.51
17	AA	833	CLA	C1D-ND	3.21	1.41	1.37
17	AF	802	CLA	CMB-C2B	-3.21	1.45	1.51
17	AB	817	CLA	C4D-ND	-3.21	1.33	1.37
17	AB	801	CLA	C4D-ND	-3.21	1.33	1.37
17	A6	601	CLA	C4D-ND	-3.21	1.33	1.37
17	A3	308	CLA	C4D-ND	-3.20	1.33	1.37
17	AA	825	CLA	C1D-ND	3.20	1.41	1.37
22	AB	852	LMU	O5'-C1'	3.20	1.50	1.41
17	A6	613	CLA	CHC-C1C	3.20	1.43	1.35
17	AB	840	CLA	C4D-ND	-3.20	1.33	1.37
17	AA	839	CLA	C4D-ND	-3.19	1.33	1.37
17	AB	824	CLA	C4D-ND	-3.19	1.33	1.37
17	AA	842	CLA	C4D-ND	-3.19	1.33	1.37
17	AB	823	CLA	C4D-ND	-3.19	1.33	1.37
17	AA	810	CLA	C4D-ND	-3.19	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AA	830	CLA	C4D-ND	-3.19	1.33	1.37
17	AB	815	CLA	C1D-ND	3.18	1.41	1.37
17	AA	829	CLA	C4D-ND	-3.18	1.33	1.37
17	AA	821	CLA	C4D-ND	-3.18	1.33	1.37
17	AF	802	CLA	C4D-ND	-3.18	1.33	1.37
22	AB	850	LMU	O5B-C1B	3.18	1.49	1.41
22	AA	851	LMU	O5B-C1B	3.18	1.49	1.41
17	A6	608	CLA	C4D-ND	-3.18	1.33	1.37
17	AA	805	CLA	C4D-ND	-3.17	1.33	1.37
17	AB	829	CLA	CMB-C2B	-3.17	1.45	1.51
17	AA	834	CLA	C4D-ND	-3.17	1.33	1.37
17	AA	830	CLA	C1D-ND	3.17	1.41	1.37
17	AA	814	CLA	C4D-ND	-3.16	1.33	1.37
17	AB	822	CLA	C4D-ND	-3.16	1.33	1.37
17	A3	312	CLA	C4D-ND	-3.16	1.33	1.37
17	A1	304	CLA	C1D-ND	3.16	1.41	1.37
17	A6	609	CLA	CHC-C1C	3.16	1.43	1.35
17	AB	841	CLA	C3B-C2B	-3.15	1.36	1.40
17	AA	829	CLA	CMD-C2D	-3.15	1.44	1.50
17	AA	809	CLA	C4D-ND	-3.15	1.33	1.37
17	AB	802	CLA	CHC-C1C	3.15	1.43	1.35
17	AB	835	CLA	C4D-ND	-3.15	1.33	1.37
17	A4	313	CLA	C4D-ND	-3.15	1.33	1.37
17	AB	839	CLA	C1D-ND	3.15	1.41	1.37
17	AB	842	CLA	C4D-ND	-3.15	1.33	1.37
17	A1	310	CLA	C4D-ND	-3.14	1.33	1.37
17	AA	808	CLA	C4D-ND	-3.14	1.33	1.37
17	A3	302	CLA	CHC-C1C	3.14	1.43	1.35
17	AB	817	CLA	CHC-C1C	3.14	1.43	1.35
17	A1	311	CLA	C4D-ND	-3.13	1.33	1.37
17	AB	830	CLA	CMB-C2B	-3.13	1.45	1.51
17	AA	819	CLA	CMB-C2B	-3.13	1.45	1.51
17	AB	824	CLA	C1D-ND	3.13	1.41	1.37
17	AA	841	CLA	C4D-ND	-3.13	1.33	1.37
17	AB	837	CLA	C4D-ND	-3.13	1.33	1.37
17	AA	827	CLA	CHC-C1C	3.12	1.43	1.35
17	AB	840	CLA	CMB-C2B	-3.12	1.45	1.51
17	A3	315	CLA	CHC-C1C	3.12	1.43	1.35
17	AG	203	CLA	CHC-C1C	3.12	1.43	1.35
17	AA	806	CLA	C4D-ND	-3.12	1.33	1.37
17	AB	816	CLA	C4D-ND	-3.12	1.33	1.37
17	A4	307	CLA	CHC-C1C	3.12	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AB	826	CLA	CHC-C1C	3.12	1.43	1.35
17	A1	312	CLA	CHC-C1C	3.12	1.43	1.35
17	AA	818	CLA	C4D-ND	-3.12	1.33	1.37
17	AB	814	CLA	CHC-C1C	3.12	1.43	1.35
17	AB	834	CLA	C1D-ND	3.12	1.41	1.37
17	A6	604	CLA	C4D-ND	-3.12	1.33	1.37
17	AB	808	CLA	C4D-ND	-3.12	1.33	1.37
17	AB	821	CLA	C4D-ND	-3.12	1.33	1.37
17	AB	832	CLA	C4D-ND	-3.11	1.33	1.37
17	AG	203	CLA	C4D-ND	-3.11	1.33	1.37
17	AB	840	CLA	C1D-ND	3.11	1.41	1.37
17	AB	825	CLA	CHC-C1C	3.11	1.42	1.35
17	AB	810	CLA	CMB-C2B	-3.11	1.45	1.51
17	AB	819	CLA	C4D-ND	-3.11	1.33	1.37
17	AA	837	CLA	C4D-ND	-3.10	1.33	1.37
17	AB	834	CLA	C4D-ND	-3.10	1.33	1.37
17	AL	302	CLA	C4D-ND	-3.10	1.33	1.37
17	AG	201	CLA	C4D-ND	-3.10	1.33	1.37
17	AB	831	CLA	C4D-ND	-3.10	1.33	1.37
17	A6	601	CLA	CHC-C1C	3.09	1.42	1.35
17	AB	807	CLA	C1D-ND	3.09	1.41	1.37
17	AB	815	CLA	CHC-C1C	3.09	1.42	1.35
17	A4	310	CLA	CHC-C1C	3.09	1.42	1.35
17	AB	828	CLA	C4D-ND	-3.09	1.33	1.37
17	AB	827	CLA	CHC-C1C	3.09	1.42	1.35
17	A3	306	CLA	C4D-ND	-3.09	1.33	1.37
17	A3	304	CLA	CHC-C1C	3.09	1.42	1.35
17	A1	304	CLA	C4D-ND	-3.08	1.33	1.37
17	AB	813	CLA	C4D-ND	-3.08	1.33	1.37
17	AB	830	CLA	C4D-ND	-3.08	1.33	1.37
17	A4	312	CLA	CHC-C1C	3.08	1.42	1.35
17	AB	809	CLA	C1D-ND	3.07	1.41	1.37
17	AB	838	CLA	C1D-ND	3.07	1.41	1.37
17	AA	831	CLA	C4D-ND	-3.07	1.33	1.37
17	A4	308	CLA	CHC-C1C	3.07	1.42	1.35
17	A3	309	CLA	CHC-C1C	3.07	1.42	1.35
17	AA	812	CLA	C4D-ND	-3.07	1.33	1.37
17	A4	312	CLA	C4D-ND	-3.06	1.33	1.37
17	A1	312	CLA	C4D-ND	-3.05	1.33	1.37
17	AG	204	CLA	CHC-C1C	3.05	1.42	1.35
17	A1	306	CLA	C4D-ND	-3.05	1.33	1.37
17	A3	309	CLA	C4D-ND	-3.05	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AA	840	CLA	C3B-C2B	-3.05	1.36	1.40
17	AA	823	CLA	CHC-C1C	3.05	1.42	1.35
17	AK	201	CLA	CHC-C1C	3.05	1.42	1.35
17	A3	315	CLA	C4D-ND	-3.04	1.33	1.37
17	AA	817	CLA	C4D-ND	-3.04	1.33	1.37
17	AB	803	CLA	C4D-ND	-3.04	1.33	1.37
17	A3	303	CLA	C4D-ND	-3.04	1.33	1.37
17	AB	818	CLA	CHC-C1C	3.04	1.42	1.35
17	AK	203	CLA	CHC-C1C	3.04	1.42	1.35
17	A1	314	CLA	C4D-ND	-3.04	1.33	1.37
17	AA	822	CLA	CHC-C1C	3.04	1.42	1.35
17	AA	826	CLA	CHC-C1C	3.04	1.42	1.35
17	AF	802	CLA	C1D-ND	3.04	1.41	1.37
17	AB	804	CLA	CHC-C1C	3.04	1.42	1.35
17	A1	309	CLA	CHC-C1C	3.03	1.42	1.35
17	AB	838	CLA	CHC-C1C	3.03	1.42	1.35
17	A3	313	CLA	CHC-C1C	3.03	1.42	1.35
17	AA	824	CLA	C4D-ND	-3.03	1.33	1.37
17	AA	804	CLA	CHC-C1C	3.03	1.42	1.35
17	AA	806	CLA	CHC-C1C	3.03	1.42	1.35
17	AB	813	CLA	CHC-C1C	3.03	1.42	1.35
17	A3	312	CLA	CHC-C1C	3.03	1.42	1.35
17	A1	311	CLA	CHC-C1C	3.03	1.42	1.35
17	AB	806	CLA	CHC-C1C	3.03	1.42	1.35
17	AJ	102	CLA	CHC-C1C	3.02	1.42	1.35
17	AA	805	CLA	CHC-C1C	3.02	1.42	1.35
17	A4	311	CLA	C4D-ND	-3.02	1.33	1.37
17	A6	612	CLA	C4D-ND	-3.02	1.33	1.37
17	A4	311	CLA	CHC-C1C	3.02	1.42	1.35
17	AA	821	CLA	CHC-C1C	3.02	1.42	1.35
17	AL	304	CLA	C4D-ND	-3.02	1.33	1.37
17	AA	836	CLA	CMB-C2B	-3.01	1.45	1.51
17	AA	803	CLA	C4D-ND	-3.01	1.33	1.37
17	AA	840	CLA	C4D-ND	-3.01	1.33	1.37
17	AB	805	CLA	C4D-ND	-3.01	1.33	1.37
17	AA	807	CLA	CHC-C1C	3.01	1.42	1.35
17	AB	806	CLA	C4D-ND	-3.01	1.33	1.37
17	AB	842	CLA	CHC-C1C	3.01	1.42	1.35
17	A6	610	CLA	CHC-C1C	3.00	1.42	1.35
17	AA	841	CLA	CHC-C1C	3.00	1.42	1.35
17	A6	611	CLA	CHC-C1C	3.00	1.42	1.35
17	AA	809	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)
17	AB	828	CLA	CHC-C1C	3.00	1.42	1.35
17	AG	201	CLA	CHC-C1C	3.00	1.42	1.35
17	A3	314	CLA	CHC-C1C	3.00	1.42	1.35
17	AB	827	CLA	C4D-ND	-3.00	1.33	1.37
17	AA	810	CLA	CAD-C3D	-3.00	1.45	1.50
17	A3	305	CLA	CHC-C1C	2.99	1.42	1.35
17	AA	831	CLA	CHC-C1C	2.99	1.42	1.35
17	A3	306	CLA	CHC-C1C	2.99	1.42	1.35
17	AB	839	CLA	C4D-ND	-2.99	1.33	1.37
17	AA	840	CLA	CHC-C1C	2.99	1.42	1.35
17	AA	820	CLA	CHC-C1C	2.99	1.42	1.35
17	A4	303	CLA	CHC-C1C	2.99	1.42	1.35
17	A6	602	CLA	CHC-C1C	2.99	1.42	1.35
17	A6	611	CLA	C4D-ND	-2.99	1.33	1.37
17	A1	307	CLA	CHC-C1C	2.99	1.42	1.35
17	AB	801	CLA	CMB-C2B	-2.99	1.45	1.51
17	AK	203	CLA	C4D-ND	-2.98	1.33	1.37
17	AB	831	CLA	CHC-C1C	2.98	1.42	1.35
17	A1	316	CLA	C4D-ND	-2.98	1.33	1.37
17	AA	811	CLA	C4D-ND	-2.98	1.33	1.37
17	AA	808	CLA	CHC-C1C	2.98	1.42	1.35
17	A3	310	CLA	CHC-C1C	2.98	1.42	1.35
17	AB	836	CLA	C4D-ND	-2.98	1.33	1.37
17	A1	313	CLA	CHC-C1C	2.98	1.42	1.35
17	AB	803	CLA	CHC-C1C	2.97	1.42	1.35
17	A3	311	CLA	CHC-C1C	2.97	1.42	1.35
17	A4	307	CLA	C4D-ND	-2.97	1.33	1.37
17	AA	835	CLA	CHC-C1C	2.97	1.42	1.35
17	AA	833	CLA	C4D-ND	-2.97	1.33	1.37
17	A3	314	CLA	C4D-ND	-2.97	1.33	1.37
17	AA	824	CLA	CHC-C1C	2.97	1.42	1.35
17	AL	302	CLA	CMB-C2B	-2.96	1.45	1.51
17	A1	314	CLA	CHC-C1C	2.96	1.42	1.35
17	AF	804	CLA	C4D-ND	-2.96	1.33	1.37
17	AK	204	CLA	CHC-C1C	2.96	1.42	1.35
17	AB	831	CLA	CMB-C2B	-2.96	1.45	1.51
17	A6	608	CLA	CHC-C1C	2.96	1.42	1.35
17	AF	803	CLA	CHC-C1C	2.96	1.42	1.35
17	A1	306	CLA	CHC-C1C	2.96	1.42	1.35
17	A4	301	CLA	CHC-C1C	2.96	1.42	1.35
17	AB	812	CLA	CHC-C1C	2.96	1.42	1.35
17	AB	818	CLA	C4D-ND	-2.95	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AJ	102	CLA	C4D-ND	-2.95	1.33	1.37
17	A4	301	CLA	C1D-ND	2.95	1.41	1.37
17	AF	804	CLA	CHC-C1C	2.95	1.42	1.35
17	A3	310	CLA	C4D-ND	-2.95	1.33	1.37
17	A1	309	CLA	C4D-ND	-2.95	1.33	1.37
17	A3	304	CLA	C4D-ND	-2.95	1.33	1.37
17	AA	832	CLA	CHC-C1C	2.95	1.42	1.35
17	A1	310	CLA	CHC-C1C	2.95	1.42	1.35
17	AA	835	CLA	C4D-ND	-2.95	1.33	1.37
17	A1	316	CLA	CHC-C1C	2.95	1.42	1.35
17	A1	315	CLA	CHC-C1C	2.95	1.42	1.35
17	AA	827	CLA	C4D-ND	-2.94	1.33	1.37
17	AA	815	CLA	C2D-C1D	2.94	1.48	1.42
17	A6	613	CLA	C4D-ND	-2.94	1.33	1.37
17	AB	822	CLA	CHC-C1C	2.94	1.42	1.35
17	AB	812	CLA	C4D-ND	-2.94	1.33	1.37
17	AA	828	CLA	C4D-ND	-2.93	1.33	1.37
26	A3	320	CHL	MG-NA	-2.93	1.99	2.06
17	AL	303	CLA	CHC-C1C	2.93	1.42	1.35
17	AA	829	CLA	CMB-C2B	-2.93	1.45	1.51
17	A6	609	CLA	C4D-ND	-2.93	1.33	1.37
17	AB	836	CLA	CMB-C2B	-2.93	1.45	1.51
17	AA	836	CLA	CHC-C1C	2.93	1.42	1.35
17	AA	817	CLA	CHC-C1C	2.92	1.42	1.35
17	AB	830	CLA	C1D-ND	2.92	1.41	1.37
17	AB	808	CLA	CHC-C1C	2.92	1.42	1.35
17	AB	820	CLA	CHC-C1C	2.92	1.42	1.35
17	A4	302	CLA	C4D-ND	-2.92	1.33	1.37
17	AA	820	CLA	C4D-ND	-2.92	1.33	1.37
17	AH	201	CLA	C4D-ND	-2.92	1.33	1.37
17	AA	825	CLA	C4D-ND	-2.92	1.33	1.37
17	AB	834	CLA	CHC-C1C	2.92	1.42	1.35
17	AA	816	CLA	CHC-C1C	2.91	1.42	1.35
17	AB	839	CLA	CHC-C1C	2.91	1.42	1.35
17	A6	604	CLA	CHC-C1C	2.91	1.42	1.35
17	AB	805	CLA	CHC-C1C	2.90	1.42	1.35
17	AB	816	CLA	CHC-C1C	2.90	1.42	1.35
17	AA	813	CLA	CHC-C1C	2.90	1.42	1.35
17	AL	302	CLA	CHC-C1C	2.90	1.42	1.35
17	A3	303	CLA	CHC-C1C	2.90	1.42	1.35
17	AA	818	CLA	CHC-C1C	2.90	1.42	1.35
17	AA	810	CLA	CHC-C1C	2.90	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A4	303	CLA	C4D-ND	-2.89	1.33	1.37
17	AB	830	CLA	CMD-C2D	-2.89	1.44	1.50
17	AL	304	CLA	CHC-C1C	2.89	1.42	1.35
17	A4	308	CLA	C4D-ND	-2.89	1.33	1.37
17	AA	815	CLA	C4D-ND	-2.89	1.33	1.37
17	AA	816	CLA	C4D-ND	-2.89	1.33	1.37
17	AA	815	CLA	CHC-C1C	2.89	1.42	1.35
17	AB	801	CLA	CHC-C1C	2.89	1.42	1.35
17	AB	821	CLA	CHC-C1C	2.89	1.42	1.35
17	AB	840	CLA	CHC-C1C	2.88	1.42	1.35
17	AA	829	CLA	C3B-CAB	-2.88	1.42	1.47
17	AA	802	CLA	CHC-C1C	2.88	1.42	1.35
17	AA	801	CLA	C4D-ND	-2.88	1.33	1.37
17	AA	823	CLA	C4D-ND	-2.88	1.33	1.37
17	AA	811	CLA	CHC-C1C	2.87	1.42	1.35
17	AA	842	CLA	CHC-C1C	2.87	1.42	1.35
17	AA	825	CLA	CMD-C2D	-2.87	1.44	1.50
17	AB	821	CLA	CMB-C2B	-2.87	1.45	1.51
17	AA	838	CLA	CHC-C1C	2.86	1.42	1.35
26	A3	320	CHL	OBD-CAD	2.86	1.27	1.22
17	A1	313	CLA	C4D-ND	-2.86	1.33	1.37
17	A6	612	CLA	CHC-C1C	2.86	1.42	1.35
17	AA	840	CLA	CMB-C2B	-2.86	1.45	1.51
17	AB	819	CLA	CMB-C2B	-2.86	1.45	1.51
17	AH	201	CLA	CHC-C1C	2.85	1.42	1.35
20	A3	318	BCR	C40-C30	2.85	1.59	1.53
17	AB	814	CLA	CMB-C2B	-2.85	1.45	1.51
17	A1	315	CLA	C4D-ND	-2.85	1.33	1.37
17	AA	809	CLA	CMB-C2B	-2.85	1.45	1.51
17	AA	822	CLA	C4D-ND	-2.85	1.33	1.37
17	AA	816	CLA	CMB-C2B	-2.85	1.45	1.51
17	A1	304	CLA	CHC-C1C	2.85	1.42	1.35
17	A4	302	CLA	CHC-C1C	2.85	1.42	1.35
17	A4	310	CLA	C4D-ND	-2.85	1.33	1.37
26	A4	305	CHL	MG-NA	-2.84	1.99	2.06
17	AA	818	CLA	CMB-C2B	-2.84	1.45	1.51
17	AA	836	CLA	C4D-ND	-2.84	1.33	1.37
17	AL	303	CLA	CMB-C2B	-2.84	1.45	1.51
17	AA	821	CLA	CMB-C2B	-2.84	1.45	1.51
17	AB	811	CLA	CHC-C1C	2.84	1.42	1.35
17	A3	305	CLA	C4D-ND	-2.84	1.33	1.37
17	AA	802	CLA	CMD-C2D	-2.84	1.44	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AB	829	CLA	CHC-C1C	2.84	1.42	1.35
17	AB	835	CLA	CHC-C1C	2.84	1.42	1.35
17	AA	834	CLA	CHC-C1C	2.83	1.42	1.35
17	A3	313	CLA	C4D-ND	-2.83	1.33	1.37
17	A4	309	CLA	C4D-ND	-2.83	1.33	1.37
17	AA	831	CLA	CMB-C2B	-2.83	1.45	1.51
17	AA	812	CLA	CHC-C1C	2.83	1.42	1.35
20	AA	849	BCR	C30-C25	-2.83	1.49	1.53
17	AK	201	CLA	C4D-ND	-2.83	1.33	1.37
17	AB	841	CLA	CMB-C2B	-2.83	1.45	1.51
18	AA	843	PQN	C10-C1	2.83	1.53	1.48
17	AA	814	CLA	CHC-C1C	2.82	1.42	1.35
17	A4	313	CLA	CHC-C1C	2.81	1.42	1.35
17	A3	308	CLA	CHC-C1C	2.81	1.42	1.35
17	A1	307	CLA	C4D-ND	-2.81	1.33	1.37
17	A3	311	CLA	C4D-ND	-2.81	1.33	1.37
17	AA	837	CLA	CHC-C1C	2.81	1.42	1.35
17	AA	842	CLA	CMB-C2B	-2.81	1.45	1.51
17	AB	833	CLA	CHC-C1C	2.80	1.42	1.35
17	AA	812	CLA	CMB-C2B	-2.80	1.45	1.51
17	AF	803	CLA	CMB-C2B	-2.79	1.45	1.51
17	AB	840	CLA	CMD-C2D	-2.79	1.44	1.50
17	A3	303	CLA	CMB-C2B	-2.79	1.45	1.51
17	AA	825	CLA	CHC-C1C	2.79	1.42	1.35
17	AB	837	CLA	CMB-C2B	-2.78	1.45	1.51
17	AB	836	CLA	CHC-C1C	2.78	1.42	1.35
17	AA	841	CLA	CMC-C2C	-2.78	1.44	1.50
17	A1	304	CLA	CMB-C2B	-2.78	1.45	1.51
17	AA	803	CLA	CHC-C1C	2.77	1.42	1.35
17	AB	835	CLA	CMB-C2B	-2.77	1.45	1.51
17	A3	308	CLA	CMB-C2B	-2.77	1.45	1.51
17	A4	309	CLA	CHC-C1C	2.76	1.42	1.35
17	AA	835	CLA	CMB-C2B	-2.76	1.45	1.51
17	AA	819	CLA	CHC-C1C	2.76	1.42	1.35
17	AA	834	CLA	CMB-C2B	-2.76	1.45	1.51
17	AB	824	CLA	CHC-C1C	2.76	1.42	1.35
17	AG	204	CLA	CMB-C2B	-2.76	1.45	1.51
17	AB	837	CLA	CHC-C1C	2.75	1.42	1.35
17	AB	809	CLA	CHC-C1C	2.75	1.42	1.35
17	A6	612	CLA	CMB-C2B	-2.75	1.45	1.51
17	AB	801	CLA	CMD-C2D	-2.75	1.45	1.50
17	AA	839	CLA	CHC-C1C	2.75	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AA	829	CLA	CHC-C1C	2.74	1.42	1.35
17	AB	825	CLA	CMD-C2D	-2.74	1.45	1.50
17	AB	825	CLA	C1D-ND	2.74	1.41	1.37
17	A1	305	CLA	C4D-ND	-2.74	1.33	1.37
17	AB	810	CLA	C3B-C2B	-2.74	1.36	1.40
17	AA	825	CLA	CMB-C2B	-2.74	1.46	1.51
17	AB	832	CLA	CMB-C2B	-2.74	1.46	1.51
17	AA	833	CLA	CHC-C1C	2.73	1.42	1.35
17	A6	609	CLA	C3B-C2B	-2.73	1.36	1.40
20	AA	847	BCR	C8-C9	2.73	1.51	1.45
17	AG	204	CLA	C4D-ND	-2.73	1.33	1.37
17	AA	830	CLA	CHC-C1C	2.72	1.41	1.35
17	AA	801	CLA	CHC-C1C	2.72	1.41	1.35
17	AA	813	CLA	CMB-C2B	-2.72	1.46	1.51
17	AB	805	CLA	CMB-C2B	-2.72	1.46	1.51
17	AB	824	CLA	CMB-C2B	-2.72	1.46	1.51
26	A1	308	CHL	C4C-C3C	2.72	1.49	1.45
17	AB	809	CLA	CMB-C2B	-2.72	1.46	1.51
17	AB	818	CLA	CMB-C2B	-2.72	1.46	1.51
17	AB	841	CLA	CHC-C1C	2.71	1.41	1.35
17	AB	831	CLA	C3B-C2B	-2.71	1.36	1.40
17	AA	801	CLA	CMB-C2B	-2.71	1.46	1.51
17	AA	802	CLA	CMB-C2B	-2.71	1.46	1.51
17	AB	829	CLA	CMD-C2D	-2.71	1.45	1.50
17	A6	603	CLA	CMB-C2B	-2.71	1.46	1.51
17	A1	316	CLA	CMB-C2B	-2.70	1.46	1.51
17	AA	811	CLA	CMB-C2B	-2.70	1.46	1.51
17	AA	814	CLA	CMB-C2B	-2.69	1.46	1.51
17	A4	307	CLA	CMB-C2B	-2.69	1.46	1.51
17	A3	315	CLA	CMD-C2D	-2.69	1.45	1.50
17	AB	814	CLA	C3B-C2B	-2.69	1.36	1.40
17	AA	808	CLA	CMB-C2B	-2.69	1.46	1.51
17	AA	823	CLA	CMB-C2B	-2.69	1.46	1.51
17	AF	802	CLA	C3B-C2B	-2.68	1.36	1.40
17	AB	805	CLA	CMD-C2D	-2.68	1.45	1.50
17	AB	832	CLA	CHC-C1C	2.68	1.41	1.35
17	AB	823	CLA	CMB-C2B	-2.68	1.46	1.51
17	AA	805	CLA	CMB-C2B	-2.68	1.46	1.51
27	A6	615	XAT	O4-C5	-2.68	1.42	1.46
17	A6	604	CLA	CMB-C2B	-2.68	1.46	1.51
17	AB	819	CLA	CHC-C1C	2.67	1.41	1.35
17	AB	813	CLA	CMB-C2B	-2.67	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AA	840	CLA	C3B-CAB	-2.67	1.42	1.47
17	AB	803	CLA	CMB-C2B	-2.66	1.46	1.51
17	A1	314	CLA	CMB-C2B	-2.66	1.46	1.51
18	AA	843	PQN	C5-C4	2.65	1.53	1.48
17	A6	610	CLA	CMB-C2B	-2.65	1.46	1.51
17	AB	810	CLA	C3B-CAB	-2.65	1.42	1.47
26	A6	606	CHL	C4C-C3C	2.65	1.49	1.45
17	AA	830	CLA	CMC-C2C	-2.65	1.45	1.50
17	A1	305	CLA	CHC-C1C	2.65	1.41	1.35
17	A6	601	CLA	CMB-C2B	-2.64	1.46	1.51
17	A6	609	CLA	CMB-C2B	-2.64	1.46	1.51
17	AB	818	CLA	C3B-C2B	-2.63	1.36	1.40
17	AL	304	CLA	CMB-C2B	-2.63	1.46	1.51
17	AB	807	CLA	CHC-C1C	2.63	1.41	1.35
17	AB	822	CLA	CMB-C2B	-2.63	1.46	1.51
17	AB	807	CLA	CMB-C2B	-2.63	1.46	1.51
17	AB	812	CLA	CMB-C2B	-2.63	1.46	1.51
17	AA	838	CLA	CMB-C2B	-2.63	1.46	1.51
26	A4	304	CHL	MG-NA	-2.62	2.00	2.06
17	A6	602	CLA	CMB-C2B	-2.62	1.46	1.51
17	AB	804	CLA	CMB-C2B	-2.62	1.46	1.51
17	AA	828	CLA	CHC-C1C	2.62	1.41	1.35
17	A6	611	CLA	CMB-C2B	-2.62	1.46	1.51
17	AA	810	CLA	CMB-C2B	-2.62	1.46	1.51
17	AB	804	CLA	CMD-C2D	-2.62	1.45	1.50
17	AB	820	CLA	C3B-C2B	-2.62	1.36	1.40
18	AB	843	PQN	C5-C4	2.62	1.53	1.48
17	AB	842	CLA	CMB-C2B	-2.62	1.46	1.51
17	A4	313	CLA	CMB-C2B	-2.62	1.46	1.51
17	AG	201	CLA	CMB-C2B	-2.61	1.46	1.51
26	A6	607	CHL	MG-NA	-2.61	2.00	2.06
26	A4	314	CHL	MG-NA	-2.61	2.00	2.06
17	A4	301	CLA	CMB-C2B	-2.61	1.46	1.51
17	AA	828	CLA	CMB-C2B	-2.61	1.46	1.51
17	AB	808	CLA	CMB-C2B	-2.61	1.46	1.51
17	A6	608	CLA	CMB-C2B	-2.60	1.46	1.51
17	A6	601	CLA	CMC-C2C	-2.60	1.45	1.50
17	A3	309	CLA	CMB-C2B	-2.60	1.46	1.51
17	AA	818	CLA	CMD-C2D	-2.60	1.45	1.50
17	AA	841	CLA	CMB-C2B	-2.60	1.46	1.51
26	A6	606	CHL	MG-NA	-2.60	2.00	2.06
26	A1	303	CHL	MG-NA	-2.60	2.00	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A4	306	CHL	MG-NA	-2.59	2.00	2.06
17	AB	818	CLA	C3B-CAB	-2.59	1.42	1.47
17	AF	804	CLA	CMB-C2B	-2.59	1.46	1.51
17	AB	811	CLA	CMB-C2B	-2.58	1.46	1.51
17	A3	305	CLA	CMB-C2B	-2.58	1.46	1.51
17	AB	823	CLA	CHC-C1C	2.58	1.41	1.35
17	AB	838	CLA	CMB-C2B	-2.58	1.46	1.51
17	A4	312	CLA	CMB-C2B	-2.57	1.46	1.51
17	A3	314	CLA	CMB-C2B	-2.57	1.46	1.51
17	AA	840	CLA	CMD-C2D	-2.57	1.45	1.50
17	AA	826	CLA	CMB-C2B	-2.57	1.46	1.51
26	A3	307	CHL	MG-NA	-2.57	2.00	2.06
17	AB	815	CLA	CMB-C2B	-2.56	1.46	1.51
17	AB	809	CLA	C3B-C2B	-2.56	1.36	1.40
26	A1	308	CHL	MG-NA	-2.56	2.00	2.06
26	A6	605	CHL	MG-NA	-2.56	2.00	2.06
17	A1	315	CLA	CMB-C2B	-2.56	1.46	1.51
17	AB	832	CLA	C3B-C2B	-2.55	1.36	1.40
17	A4	303	CLA	CMB-C2B	-2.55	1.46	1.51
17	A3	312	CLA	CMB-C2B	-2.55	1.46	1.51
17	AA	817	CLA	CMB-C2B	-2.55	1.46	1.51
17	AA	806	CLA	CMB-C2B	-2.55	1.46	1.51
17	AB	801	CLA	C1D-ND	2.55	1.40	1.37
17	AB	828	CLA	CMB-C2B	-2.55	1.46	1.51
17	AB	807	CLA	CMD-C2D	-2.55	1.45	1.50
17	AB	834	CLA	CMB-C2B	-2.55	1.46	1.51
17	AA	824	CLA	CMB-C2B	-2.55	1.46	1.51
17	A1	312	CLA	CMB-C2B	-2.53	1.46	1.51
26	A4	304	CHL	C4C-C3C	2.53	1.49	1.44
26	A4	314	CHL	C4C-C3C	2.53	1.49	1.45
17	AA	820	CLA	CMB-C2B	-2.53	1.46	1.51
17	AA	815	CLA	CMB-C2B	-2.53	1.46	1.51
17	A1	306	CLA	CMB-C2B	-2.53	1.46	1.51
17	A3	306	CLA	CMB-C2B	-2.53	1.46	1.51
17	A1	313	CLA	CMB-C2B	-2.53	1.46	1.51
17	AB	810	CLA	CHC-C1C	2.53	1.41	1.35
17	AA	809	CLA	C3B-C2B	-2.53	1.36	1.40
17	AB	829	CLA	C3B-CAB	-2.53	1.42	1.47
17	A4	308	CLA	CMB-C2B	-2.52	1.46	1.51
26	A6	607	CHL	C4C-C3C	2.52	1.49	1.45
17	AB	823	CLA	C3B-C2B	-2.52	1.36	1.40
17	AA	837	CLA	CMB-C2B	-2.52	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AH	201	CLA	CMB-C2B	-2.52	1.46	1.51
17	AB	842	CLA	CMD-C2D	-2.52	1.45	1.50
17	A1	311	CLA	CMC-C2C	-2.52	1.45	1.50
26	A4	305	CHL	C4C-C3C	2.52	1.49	1.45
17	AB	833	CLA	CMB-C2B	-2.52	1.46	1.51
17	AA	839	CLA	CMB-C2B	-2.51	1.46	1.51
17	A4	310	CLA	CMB-C2B	-2.51	1.46	1.51
17	A4	302	CLA	CMB-C2B	-2.51	1.46	1.51
17	AA	803	CLA	CMB-C2B	-2.50	1.46	1.51
17	AB	825	CLA	CMB-C2B	-2.50	1.46	1.51
17	AA	839	CLA	CMD-C2D	-2.50	1.45	1.50
17	A1	309	CLA	CMB-C2B	-2.50	1.46	1.51
17	A3	303	CLA	C3B-C2B	-2.50	1.36	1.40
17	A4	307	CLA	CMD-C2D	-2.50	1.45	1.50
17	AA	818	CLA	C3B-CAB	-2.50	1.42	1.47
20	AA	847	BCR	C12-C13	2.50	1.51	1.45
17	AA	829	CLA	C3B-C2B	-2.50	1.36	1.40
17	A3	304	CLA	CMB-C2B	-2.49	1.46	1.51
17	AG	203	CLA	CMB-C2B	-2.49	1.46	1.51
17	A6	602	CLA	C3B-C2B	-2.49	1.36	1.40
17	A3	309	CLA	CMD-C2D	-2.49	1.45	1.50
17	A4	309	CLA	CMB-C2B	-2.49	1.46	1.51
17	AB	816	CLA	CMB-C2B	-2.49	1.46	1.51
17	AA	809	CLA	CMD-C2D	-2.49	1.45	1.50
17	A3	302	CLA	CMB-C2B	-2.48	1.46	1.51
17	AA	830	CLA	C3B-C2B	-2.48	1.36	1.40
17	AA	807	CLA	CMB-C2B	-2.48	1.46	1.51
17	AB	833	CLA	C3B-C2B	-2.48	1.36	1.40
17	A3	302	CLA	C3B-C2B	-2.48	1.36	1.40
17	AB	824	CLA	CMD-C2D	-2.47	1.45	1.50
17	AA	827	CLA	CMD-C2D	-2.47	1.45	1.50
17	AB	829	CLA	C3B-C2B	-2.47	1.36	1.40
17	AB	827	CLA	CMB-C2B	-2.47	1.46	1.51
17	AK	203	CLA	CMB-C2B	-2.47	1.46	1.51
17	A3	313	CLA	CMB-C2B	-2.47	1.46	1.51
17	A1	305	CLA	CMB-C2B	-2.47	1.46	1.51
17	AB	806	CLA	CMB-C2B	-2.46	1.46	1.51
17	AF	802	CLA	CMD-C2D	-2.46	1.45	1.50
17	AA	841	CLA	CMD-C2D	-2.45	1.45	1.50
17	AA	804	CLA	CMB-C2B	-2.45	1.46	1.51
26	A6	605	CHL	C4C-C3C	2.45	1.49	1.44
26	A4	304	CHL	C4B-CHC	2.44	1.47	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A6	608	CLA	CMD-C2D	-2.44	1.45	1.50
17	AB	814	CLA	C3B-CAB	-2.44	1.43	1.47
17	AB	831	CLA	CMD-C2D	-2.44	1.45	1.50
17	A3	310	CLA	CMB-C2B	-2.44	1.46	1.51
17	AB	840	CLA	C3B-C2B	-2.44	1.37	1.40
17	AA	822	CLA	CMB-C2B	-2.44	1.46	1.51
18	AB	843	PQN	C10-C1	2.44	1.52	1.48
17	AB	804	CLA	C1D-ND	2.44	1.40	1.37
17	AA	818	CLA	C3B-C2B	-2.43	1.37	1.40
26	A3	320	CHL	C4D-CHA	2.42	1.47	1.38
17	AA	831	CLA	C3B-C2B	-2.42	1.37	1.40
17	A1	307	CLA	CMB-C2B	-2.42	1.46	1.51
26	A6	607	CHL	C4D-CHA	2.42	1.47	1.38
17	AJ	102	CLA	CMB-C2B	-2.42	1.46	1.51
26	A1	308	CHL	C4B-CHC	2.42	1.47	1.41
26	A4	306	CHL	C4B-CHC	2.42	1.47	1.41
17	AB	830	CLA	CHC-C1C	2.42	1.41	1.35
17	A4	308	CLA	C3B-C2B	-2.42	1.37	1.40
17	AB	801	CLA	CMC-C2C	-2.42	1.45	1.50
17	AB	839	CLA	CMB-C2B	-2.42	1.46	1.51
17	AA	834	CLA	C3B-C2B	-2.41	1.37	1.40
17	AL	303	CLA	C3B-C2B	-2.41	1.37	1.40
17	AB	817	CLA	CMB-C2B	-2.41	1.46	1.51
17	AB	824	CLA	C3B-CAB	-2.41	1.43	1.47
17	A4	311	CLA	CMB-C2B	-2.41	1.46	1.51
26	A4	305	CHL	C4D-CHA	2.41	1.47	1.38
17	AB	804	CLA	CMC-C2C	-2.41	1.45	1.50
24	A4	315	LUT	C8-C9	2.41	1.51	1.45
17	AA	808	CLA	CMD-C2D	-2.40	1.45	1.50
17	A3	308	CLA	CMD-C2D	-2.40	1.45	1.50
26	A4	314	CHL	C4D-CHA	2.40	1.46	1.38
17	AK	204	CLA	CMB-C2B	-2.40	1.46	1.51
26	A1	303	CHL	C4D-CHA	2.39	1.46	1.38
17	AB	821	CLA	CMD-C2D	-2.39	1.45	1.50
17	A1	310	CLA	CMB-C2B	-2.39	1.46	1.51
17	A4	301	CLA	C3B-C2B	-2.39	1.37	1.40
17	A6	613	CLA	CMB-C2B	-2.39	1.46	1.51
17	AB	834	CLA	C3B-C2B	-2.39	1.37	1.40
17	AB	802	CLA	CMB-C2B	-2.38	1.46	1.51
17	AA	813	CLA	C3B-C2B	-2.38	1.37	1.40
24	AF	806	LUT	C12-C13	2.38	1.51	1.45
17	AB	808	CLA	C3B-C2B	-2.38	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A1	304	CLA	CMD-C2D	-2.38	1.45	1.50
26	A1	308	CHL	C4D-CHA	2.38	1.46	1.38
17	AF	802	CLA	CHC-C1C	2.38	1.41	1.35
26	A1	303	CHL	C2C-C1C	2.38	1.49	1.44
17	A3	311	CLA	CMB-C2B	-2.38	1.46	1.51
17	AB	835	CLA	CMD-C2D	-2.37	1.45	1.50
17	AB	834	CLA	CMD-C2D	-2.37	1.45	1.50
26	A6	606	CHL	C4B-CHC	2.37	1.47	1.41
17	A4	301	CLA	CMC-C2C	-2.37	1.45	1.50
17	A1	311	CLA	CMB-C2B	-2.37	1.46	1.51
17	AB	815	CLA	CMD-C2D	-2.37	1.45	1.50
17	AA	802	CLA	C3B-C2B	-2.37	1.37	1.40
17	AB	842	CLA	C3B-CAB	-2.37	1.43	1.47
17	A6	602	CLA	CMD-C2D	-2.37	1.45	1.50
17	AL	302	CLA	C3B-C2B	-2.37	1.37	1.40
17	AA	829	CLA	MG-ND	-2.36	2.01	2.05
17	AA	821	CLA	CMD-C2D	-2.36	1.45	1.50
17	AA	811	CLA	CMD-C2D	-2.36	1.45	1.50
17	AA	826	CLA	CMD-C2D	-2.36	1.45	1.50
26	A6	606	CHL	C4D-CHA	2.36	1.46	1.38
17	AB	809	CLA	CMD-C2D	-2.36	1.45	1.50
17	AA	828	CLA	CMD-C2D	-2.36	1.45	1.50
17	AA	803	CLA	CMC-C2C	-2.35	1.45	1.50
17	AA	832	CLA	CMB-C2B	-2.35	1.46	1.51
26	A1	303	CHL	C4B-CHC	2.35	1.47	1.41
17	AB	820	CLA	CMD-C2D	-2.35	1.45	1.50
17	AB	832	CLA	CMD-C2D	-2.35	1.45	1.50
17	A6	602	CLA	C3B-CAB	-2.35	1.43	1.47
17	AA	806	CLA	CMD-C2D	-2.34	1.45	1.50
17	AA	814	CLA	C3B-C2B	-2.34	1.37	1.40
17	A6	602	CLA	CMC-C2C	-2.34	1.45	1.50
17	AB	801	CLA	C3B-C2B	-2.34	1.37	1.40
17	A4	307	CLA	C3B-C2B	-2.34	1.37	1.40
17	AB	819	CLA	CMD-C2D	-2.34	1.45	1.50
17	A3	302	CLA	C3B-CAB	-2.34	1.43	1.47
17	AB	830	CLA	C3B-C2B	-2.34	1.37	1.40
17	A3	309	CLA	C3B-C2B	-2.33	1.37	1.40
26	A3	307	CHL	C4D-CHA	2.33	1.46	1.38
17	AB	831	CLA	C3B-CAB	-2.33	1.43	1.47
26	A3	307	CHL	C4C-C3C	2.33	1.49	1.45
20	AI	101	BCR	C30-C25	-2.33	1.50	1.53
17	AB	802	CLA	CMD-C2D	-2.33	1.45	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AB	826	CLA	CMD-C2D	-2.33	1.45	1.50
17	AA	814	CLA	C3B-CAB	-2.33	1.43	1.47
17	AA	834	CLA	CMC-C2C	-2.32	1.45	1.50
17	AB	825	CLA	CMC-C2C	-2.32	1.45	1.50
17	AF	803	CLA	CMD-C2D	-2.32	1.45	1.50
17	AB	803	CLA	CMD-C2D	-2.32	1.45	1.50
17	A6	609	CLA	CMD-C2D	-2.32	1.45	1.50
17	AA	812	CLA	CMD-C2D	-2.32	1.45	1.50
17	AB	801	CLA	MG-ND	-2.32	2.01	2.05
26	A6	605	CHL	C2C-C1C	2.32	1.49	1.44
17	AA	827	CLA	CMB-C2B	-2.32	1.46	1.51
17	AA	802	CLA	CMC-C2C	-2.32	1.45	1.50
26	A4	304	CHL	C2C-C1C	2.31	1.49	1.44
26	A1	303	CHL	C4C-C3C	2.31	1.49	1.45
17	AA	820	CLA	CMD-C2D	-2.31	1.45	1.50
17	AA	830	CLA	CMD-C2D	-2.31	1.45	1.50
17	AA	803	CLA	CMD-C2D	-2.31	1.45	1.50
20	A6	616	BCR	C8-C9	2.31	1.50	1.45
17	AA	805	CLA	CMD-C2D	-2.31	1.45	1.50
17	AB	809	CLA	CMC-C2C	-2.31	1.45	1.50
17	AB	827	CLA	CMD-C2D	-2.31	1.45	1.50
26	A6	605	CHL	C4D-CHA	2.31	1.46	1.38
26	A4	306	CHL	C4C-C3C	2.31	1.49	1.45
17	AA	838	CLA	C3B-C2B	-2.31	1.37	1.40
26	A4	304	CHL	C4D-CHA	2.30	1.46	1.38
27	A4	316	XAT	O24-C25	-2.30	1.42	1.46
17	A1	305	CLA	C3B-C2B	-2.30	1.37	1.40
20	AA	849	BCR	C1-C6	-2.30	1.50	1.53
17	AB	838	CLA	CMC-C2C	-2.30	1.45	1.50
17	A6	610	CLA	C1A-CHA	-2.30	1.36	1.40
17	AA	833	CLA	C3B-C2B	-2.30	1.37	1.40
17	AA	824	CLA	CMD-C2D	-2.30	1.45	1.50
17	A1	304	CLA	C3B-C2B	-2.30	1.37	1.40
26	A4	304	CHL	C1B-CHB	2.30	1.47	1.41
25	AG	202	LMG	O1-C1	2.30	1.44	1.40
17	A3	315	CLA	CMB-C2B	-2.30	1.46	1.51
17	AA	838	CLA	CMD-C2D	-2.29	1.45	1.50
17	AB	818	CLA	CMD-C2D	-2.29	1.45	1.50
17	AB	811	CLA	CMD-C2D	-2.29	1.45	1.50
17	AB	815	CLA	C3B-CAB	-2.29	1.43	1.47
17	AB	804	CLA	C3B-CAB	-2.29	1.43	1.47
17	AB	824	CLA	C3B-C2B	-2.29	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AB	804	CLA	MG-ND	-2.29	2.01	2.05
17	AA	814	CLA	CMD-C2D	-2.29	1.46	1.50
26	A1	308	CHL	C2C-C1C	2.28	1.49	1.44
17	AB	810	CLA	CMD-C2D	-2.28	1.46	1.50
17	AK	201	CLA	CMB-C2B	-2.28	1.46	1.51
17	AL	304	CLA	CMD-C2D	-2.28	1.46	1.50
17	AA	816	CLA	C3B-C2B	-2.28	1.37	1.40
17	AB	804	CLA	C3B-C2B	-2.28	1.37	1.40
17	AB	842	CLA	C3B-C2B	-2.27	1.37	1.40
17	A6	611	CLA	CMD-C2D	-2.27	1.46	1.50
27	A1	318	XAT	O24-C25	-2.27	1.43	1.46
17	AB	810	CLA	MG-ND	-2.27	2.01	2.05
17	AB	837	CLA	CMC-C2C	-2.27	1.46	1.50
17	AA	808	CLA	C3B-C2B	-2.27	1.37	1.40
17	AB	817	CLA	CMD-C2D	-2.27	1.46	1.50
17	A1	314	CLA	C3B-C2B	-2.27	1.37	1.40
17	AB	832	CLA	CMC-C2C	-2.26	1.46	1.50
26	A3	307	CHL	C1C-NC	-2.26	1.34	1.37
17	A4	310	CLA	CMD-C2D	-2.26	1.46	1.50
17	AA	819	CLA	C3B-C2B	-2.26	1.37	1.40
17	AB	841	CLA	CMD-C2D	-2.26	1.46	1.50
17	AA	807	CLA	CMC-C2C	-2.26	1.46	1.50
17	AA	823	CLA	CMD-C2D	-2.26	1.46	1.50
26	A1	308	CHL	CMC-C2C	2.26	1.49	1.45
17	AB	814	CLA	CMD-C2D	-2.26	1.46	1.50
17	AA	831	CLA	CMD-C2D	-2.26	1.46	1.50
17	AB	813	CLA	CMD-C2D	-2.25	1.46	1.50
17	AF	803	CLA	CMC-C2C	-2.25	1.46	1.50
17	AA	805	CLA	C3B-C2B	-2.25	1.37	1.40
17	AL	304	CLA	CMC-C2C	-2.25	1.46	1.50
17	A4	301	CLA	C3B-CAB	-2.25	1.43	1.47
17	AB	823	CLA	CMD-C2D	-2.25	1.46	1.50
17	AA	806	CLA	C3B-CAB	-2.25	1.43	1.47
17	AB	816	CLA	CMC-C2C	-2.25	1.46	1.50
17	AB	802	CLA	CMC-C2C	-2.25	1.46	1.50
26	A4	306	CHL	C4D-CHA	2.24	1.46	1.38
17	AA	842	CLA	CMD-C2D	-2.24	1.46	1.50
20	AK	205	BCR	C12-C13	2.24	1.50	1.45
17	AA	837	CLA	CMD-C2D	-2.24	1.46	1.50
17	A4	301	CLA	CMD-C2D	-2.24	1.46	1.50
26	A4	306	CHL	C1B-CHB	2.24	1.47	1.41
26	A6	606	CHL	C2C-C1C	2.23	1.49	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AA	836	CLA	C3B-C2B	-2.23	1.37	1.40
17	AA	804	CLA	CMD-C2D	-2.23	1.46	1.50
26	A6	607	CHL	C4B-CHC	2.23	1.47	1.41
17	AB	830	CLA	CMC-C2C	-2.23	1.46	1.50
17	AA	819	CLA	CMD-C2D	-2.23	1.46	1.50
17	AA	834	CLA	CMD-C2D	-2.23	1.46	1.50
17	AL	303	CLA	CMD-C2D	-2.23	1.46	1.50
17	AA	812	CLA	C4B-CHC	-2.23	1.34	1.41
17	AK	204	CLA	C3B-C2B	-2.22	1.37	1.40
17	AB	807	CLA	CAC-C3C	-2.22	1.45	1.51
17	AA	812	CLA	C3B-C2B	-2.22	1.37	1.40
17	AA	839	CLA	C3B-C2B	-2.22	1.37	1.40
17	AF	802	CLA	C3B-CAB	-2.22	1.43	1.47
17	A1	314	CLA	CMD-C2D	-2.22	1.46	1.50
17	AA	806	CLA	C3B-C2B	-2.22	1.37	1.40
26	A3	307	CHL	C4B-CHC	2.22	1.47	1.41
17	AB	834	CLA	CMC-C2C	-2.22	1.46	1.50
17	A4	313	CLA	CMD-C2D	-2.22	1.46	1.50
17	AA	835	CLA	C3B-C2B	-2.22	1.37	1.40
17	A4	310	CLA	C3B-C2B	-2.22	1.37	1.40
17	AB	812	CLA	CMD-C2D	-2.21	1.46	1.50
27	A6	615	XAT	O24-C25	-2.21	1.43	1.46
17	AB	836	CLA	CMD-C2D	-2.21	1.46	1.50
17	AB	817	CLA	C3B-CAB	-2.21	1.43	1.47
24	A4	315	LUT	C22-C21	-2.21	1.51	1.54
17	AA	823	CLA	C3B-C2B	-2.21	1.37	1.40
17	A3	305	CLA	CMD-C2D	-2.21	1.46	1.50
17	A4	302	CLA	CMD-C2D	-2.21	1.46	1.50
17	AB	808	CLA	CMC-C2C	-2.21	1.46	1.50
17	A1	307	CLA	CMD-C2D	-2.21	1.46	1.50
17	AA	817	CLA	CMD-C2D	-2.20	1.46	1.50
26	A6	607	CHL	C1B-CHB	2.20	1.47	1.41
17	AB	827	CLA	CMC-C2C	-2.20	1.46	1.50
17	AK	204	CLA	CMC-C2C	-2.20	1.46	1.50
17	AB	806	CLA	CMD-C2D	-2.20	1.46	1.50
17	AA	813	CLA	CMC-C2C	-2.20	1.46	1.50
17	AB	817	CLA	C3B-C2B	-2.20	1.37	1.40
17	A1	316	CLA	CMD-C2D	-2.19	1.46	1.50
20	AB	848	BCR	C19-C18	2.19	1.50	1.45
17	AB	816	CLA	CMD-C2D	-2.19	1.46	1.50
17	AB	808	CLA	CMD-C2D	-2.19	1.46	1.50
26	A4	306	CHL	C2C-C1C	2.19	1.49	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A3	305	CLA	C3B-C2B	-2.19	1.37	1.40
17	AB	833	CLA	C3B-CAB	-2.19	1.43	1.47
17	AG	203	CLA	CMD-C2D	-2.19	1.46	1.50
17	A1	307	CLA	C3B-CAB	-2.19	1.43	1.47
17	AL	302	CLA	CMD-C2D	-2.19	1.46	1.50
17	A1	307	CLA	C3B-C2B	-2.19	1.37	1.40
17	A4	308	CLA	CMD-C2D	-2.19	1.46	1.50
17	A6	609	CLA	C3B-CAB	-2.19	1.43	1.47
17	AA	805	CLA	CMC-C2C	-2.19	1.46	1.50
17	A6	603	CLA	CMD-C2D	-2.19	1.46	1.50
17	AA	813	CLA	C3B-CAB	-2.18	1.43	1.47
17	AA	841	CLA	C3B-C2B	-2.18	1.37	1.40
17	AA	835	CLA	CMD-C2D	-2.18	1.46	1.50
17	A3	303	CLA	CMD-C2D	-2.18	1.46	1.50
17	AB	836	CLA	C3B-C2B	-2.18	1.37	1.40
18	AB	843	PQN	C2-C1	2.18	1.52	1.48
17	AB	808	CLA	C3B-CAB	-2.18	1.43	1.47
17	AA	803	CLA	C3B-C2B	-2.18	1.37	1.40
20	AA	845	BCR	C8-C9	2.18	1.50	1.45
17	AB	825	CLA	MG-ND	-2.18	2.01	2.05
17	AA	801	CLA	C3B-C2B	-2.18	1.37	1.40
17	AB	840	CLA	C3B-CAB	-2.18	1.43	1.47
26	A6	605	CHL	C4B-CHC	2.18	1.47	1.41
17	AA	819	CLA	CMC-C2C	-2.18	1.46	1.50
17	A3	306	CLA	CMD-C2D	-2.18	1.46	1.50
17	AB	838	CLA	CMD-C2D	-2.17	1.46	1.50
17	AB	824	CLA	MG-ND	-2.17	2.01	2.05
17	AB	815	CLA	CMC-C2C	-2.17	1.46	1.50
17	AB	841	CLA	CMC-C2C	-2.17	1.46	1.50
17	AB	835	CLA	C3B-CAB	-2.17	1.43	1.47
17	AB	832	CLA	C4B-CHC	-2.17	1.35	1.41
26	A3	320	CHL	C1B-CHB	2.17	1.47	1.41
17	AB	811	CLA	CMC-C2C	-2.17	1.46	1.50
17	AA	838	CLA	C3B-CAB	-2.17	1.43	1.47
17	AB	814	CLA	CMC-C2C	-2.17	1.46	1.50
17	A4	311	CLA	CMD-C2D	-2.17	1.46	1.50
17	AA	832	CLA	CMD-C2D	-2.16	1.46	1.50
17	A4	303	CLA	CMD-C2D	-2.16	1.46	1.50
17	A1	310	CLA	CMD-C2D	-2.16	1.46	1.50
17	AB	810	CLA	C4B-CHC	-2.16	1.35	1.41
17	AG	204	CLA	C3B-C2B	-2.16	1.37	1.40
17	A6	612	CLA	CMD-C2D	-2.16	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AK	201	CLA	CBD-CAD	2.16	1.56	1.51
17	AL	303	CLA	CMC-C2C	-2.16	1.46	1.50
17	AF	802	CLA	MG-ND	-2.16	2.01	2.05
17	AB	826	CLA	CMB-C2B	-2.16	1.47	1.51
17	A6	613	CLA	CMD-C2D	-2.15	1.46	1.50
26	A6	606	CHL	CMC-C2C	2.15	1.49	1.45
17	AB	807	CLA	C4B-CHC	-2.15	1.35	1.41
17	A1	305	CLA	CMD-C2D	-2.15	1.46	1.50
17	AB	839	CLA	C3B-C2B	-2.15	1.37	1.40
26	A4	305	CHL	C1B-CHB	2.15	1.47	1.41
17	AB	837	CLA	C3B-C2B	-2.15	1.37	1.40
17	AA	835	CLA	C3B-CAB	-2.15	1.43	1.47
17	AG	201	CLA	CMD-C2D	-2.15	1.46	1.50
17	AB	841	CLA	C3B-CAB	-2.15	1.43	1.47
17	AF	804	CLA	CMD-C2D	-2.15	1.46	1.50
17	AB	832	CLA	C3B-CAB	-2.14	1.43	1.47
17	A1	313	CLA	CMD-C2D	-2.14	1.46	1.50
20	A1	319	BCR	C40-C30	2.14	1.58	1.53
17	AH	201	CLA	CMD-C2D	-2.14	1.46	1.50
17	A1	312	CLA	CMD-C2D	-2.14	1.46	1.50
17	AK	203	CLA	CMD-C2D	-2.14	1.46	1.50
17	AB	822	CLA	C3B-C2B	-2.14	1.37	1.40
17	AL	304	CLA	C3B-C2B	-2.13	1.37	1.40
17	A4	313	CLA	C3B-C2B	-2.13	1.37	1.40
26	A4	304	CHL	CMC-C2C	2.13	1.49	1.45
17	AA	810	CLA	CMD-C2D	-2.13	1.46	1.50
17	A3	312	CLA	C3B-C2B	-2.13	1.37	1.40
17	AB	822	CLA	CMD-C2D	-2.13	1.46	1.50
17	AB	839	CLA	C3B-CAB	-2.13	1.43	1.47
17	AB	826	CLA	C3B-C2B	-2.13	1.37	1.40
17	A6	604	CLA	CMD-C2D	-2.13	1.46	1.50
17	AB	825	CLA	C3B-CAB	-2.13	1.43	1.47
17	AF	802	CLA	CMC-C2C	-2.12	1.46	1.50
17	AA	833	CLA	CMD-C2D	-2.12	1.46	1.50
17	A3	313	CLA	CMD-C2D	-2.12	1.46	1.50
17	A6	601	CLA	CMD-C2D	-2.12	1.46	1.50
17	AB	833	CLA	CMD-C2D	-2.12	1.46	1.50
20	AK	205	BCR	C8-C9	2.12	1.50	1.45
17	AK	204	CLA	CMD-C2D	-2.12	1.46	1.50
17	A1	309	CLA	CMD-C2D	-2.12	1.46	1.50
27	A3	317	XAT	O24-C25	-2.12	1.43	1.46
17	AB	828	CLA	CMD-C2D	-2.12	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AB	807	CLA	C3B-C2B	-2.12	1.37	1.40
17	AA	821	CLA	CMC-C2C	-2.12	1.46	1.50
17	AA	806	CLA	CMC-C2C	-2.12	1.46	1.50
17	AB	835	CLA	C3B-C2B	-2.11	1.37	1.40
17	A1	307	CLA	CMC-C2C	-2.11	1.46	1.50
17	AA	838	CLA	CMC-C2C	-2.11	1.46	1.50
17	AA	804	CLA	CMC-C2C	-2.11	1.46	1.50
17	A4	311	CLA	C3B-C2B	-2.11	1.37	1.40
17	AB	824	CLA	CMC-C2C	-2.11	1.46	1.50
17	AB	837	CLA	CMD-C2D	-2.11	1.46	1.50
17	AA	816	CLA	CMD-C2D	-2.11	1.46	1.50
17	AH	201	CLA	C3B-C2B	-2.11	1.37	1.40
17	AB	826	CLA	C3B-CAB	-2.10	1.43	1.47
17	AB	825	CLA	C3B-C2B	-2.10	1.37	1.40
17	AA	820	CLA	CMC-C2C	-2.10	1.46	1.50
17	A4	302	CLA	CMC-C2C	-2.10	1.46	1.50
17	AA	809	CLA	C3B-CAB	-2.10	1.43	1.47
17	A3	310	CLA	CMD-C2D	-2.10	1.46	1.50
17	A3	312	CLA	CMC-C2C	-2.10	1.46	1.50
26	A1	308	CHL	C1B-CHB	2.10	1.46	1.41
17	AA	816	CLA	C3B-CAB	-2.10	1.43	1.47
17	AA	828	CLA	CMC-C2C	-2.10	1.46	1.50
17	AA	827	CLA	CMC-C2C	-2.10	1.46	1.50
26	A4	314	CHL	C1B-CHB	2.10	1.46	1.41
17	AA	822	CLA	CMD-C2D	-2.10	1.46	1.50
17	AB	821	CLA	CMC-C2C	-2.10	1.46	1.50
26	A6	607	CHL	C1C-NC	-2.10	1.34	1.37
17	AA	826	CLA	C3B-C2B	-2.10	1.37	1.40
17	A3	313	CLA	C3B-C2B	-2.10	1.37	1.40
17	AA	812	CLA	CMC-C2C	-2.10	1.46	1.50
20	AK	202	BCR	C12-C13	2.09	1.50	1.45
17	A1	306	CLA	CMD-C2D	-2.09	1.46	1.50
17	A4	312	CLA	CMD-C2D	-2.09	1.46	1.50
26	A3	320	CHL	C4B-CHC	2.09	1.46	1.41
17	AA	811	CLA	C3B-C2B	-2.09	1.37	1.40
17	A6	604	CLA	C3B-C2B	-2.09	1.37	1.40
17	AB	829	CLA	MG-ND	-2.09	2.01	2.05
17	AA	802	CLA	C3B-CAB	-2.09	1.43	1.47
17	A1	313	CLA	CMC-C2C	-2.09	1.46	1.50
17	AA	819	CLA	C4B-CHC	-2.09	1.35	1.41
17	AB	807	CLA	CMC-C2C	-2.09	1.46	1.50
17	A3	302	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)
17	AG	204	CLA	CMD-C2D	-2.09	1.46	1.50
17	A6	610	CLA	CMD-C2D	-2.09	1.46	1.50
17	AA	834	CLA	C3B-CAB	-2.09	1.43	1.47
17	A1	311	CLA	CMD-C2D	-2.09	1.46	1.50
17	AA	803	CLA	C4B-CHC	-2.09	1.35	1.41
17	AL	303	CLA	C3B-CAB	-2.09	1.43	1.47
17	A6	612	CLA	CMC-C2C	-2.08	1.46	1.50
17	AA	813	CLA	CMD-C2D	-2.08	1.46	1.50
17	AB	819	CLA	C4B-CHC	-2.08	1.35	1.41
20	AB	845	BCR	C8-C9	2.08	1.50	1.45
17	AA	837	CLA	C3B-CAB	-2.08	1.43	1.47
17	A3	314	CLA	C3B-C2B	-2.08	1.37	1.40
17	AA	842	CLA	C3B-C2B	-2.08	1.37	1.40
17	AB	828	CLA	CMC-C2C	-2.08	1.46	1.50
17	A3	314	CLA	CMD-C2D	-2.07	1.46	1.50
20	AF	801	BCR	C23-C22	2.07	1.50	1.45
24	AF	806	LUT	C8-C9	2.07	1.50	1.45
17	AA	810	CLA	C3B-C2B	-2.07	1.37	1.40
17	A6	601	CLA	C3B-C2B	-2.07	1.37	1.40
17	AB	831	CLA	CMC-C2C	-2.07	1.46	1.50
17	A1	315	CLA	CMD-C2D	-2.07	1.46	1.50
26	A1	308	CHL	C3D-C4D	-2.07	1.39	1.44
17	A6	604	CLA	CMC-C2C	-2.07	1.46	1.50
17	A3	314	CLA	CBD-CAD	2.07	1.56	1.51
17	AA	807	CLA	CMD-C2D	-2.07	1.46	1.50
17	AB	823	CLA	C4B-CHC	-2.06	1.35	1.41
17	A3	309	CLA	C3B-CAB	-2.06	1.43	1.47
17	AB	821	CLA	C3B-C2B	-2.06	1.37	1.40
17	AB	819	CLA	CMC-C2C	-2.06	1.46	1.50
24	A6	614	LUT	C22-C21	-2.06	1.52	1.54
17	AB	811	CLA	C3B-C2B	-2.06	1.37	1.40
17	AA	801	CLA	CMD-C2D	-2.06	1.46	1.50
17	AA	826	CLA	C3B-CAB	-2.06	1.43	1.47
17	AA	831	CLA	C3B-CAB	-2.06	1.43	1.47
17	AB	826	CLA	CMC-C2C	-2.06	1.46	1.50
17	AK	204	CLA	C3B-CAB	-2.06	1.43	1.47
20	AA	845	BCR	C12-C13	2.06	1.50	1.45
17	AB	812	CLA	CMC-C2C	-2.06	1.46	1.50
17	AG	201	CLA	C3B-C2B	-2.06	1.37	1.40
17	A6	611	CLA	C3B-C2B	-2.06	1.37	1.40
27	A4	316	XAT	O4-C5	-2.05	1.43	1.46
26	A4	306	CHL	C3D-C4D	-2.05	1.39	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	AA	810	CLA	CMC-C2C	-2.05	1.46	1.50
17	A3	304	CLA	CMD-C2D	-2.05	1.46	1.50
17	AF	802	CLA	C4B-CHC	-2.05	1.35	1.41
24	AF	806	LUT	C26-C27	2.05	1.53	1.50
17	A4	312	CLA	C3B-C2B	-2.05	1.37	1.40
17	AA	826	CLA	CMC-C2C	-2.05	1.46	1.50
17	A4	310	CLA	CMC-C2C	-2.05	1.46	1.50
17	A3	308	CLA	C3B-C2B	-2.05	1.37	1.40
17	AB	814	CLA	MG-ND	-2.05	2.01	2.05
26	A6	606	CHL	C1B-CHB	2.05	1.46	1.41
17	AA	824	CLA	C3B-C2B	-2.05	1.37	1.40
26	A4	305	CHL	C4B-CHC	2.05	1.46	1.41
17	AA	819	CLA	C3B-CAB	-2.04	1.43	1.47
17	AB	830	CLA	C4B-CHC	-2.04	1.35	1.41
17	AB	803	CLA	C3B-C2B	-2.04	1.37	1.40
20	A6	616	BCR	C12-C13	2.04	1.50	1.45
26	A3	307	CHL	C1B-CHB	2.04	1.46	1.41
17	A3	303	CLA	CMC-C2C	-2.04	1.46	1.50
17	AA	818	CLA	CMC-C2C	-2.04	1.46	1.50
17	AA	834	CLA	C4B-CHC	-2.04	1.35	1.41
17	AF	803	CLA	C3B-C2B	-2.04	1.37	1.40
17	A1	304	CLA	C3B-CAB	-2.04	1.43	1.47
17	AF	804	CLA	C3B-C2B	-2.04	1.37	1.40
17	AB	819	CLA	C3B-C2B	-2.04	1.37	1.40
17	AK	201	CLA	CMC-C2C	-2.04	1.46	1.50
17	AB	820	CLA	C3B-CAB	-2.04	1.43	1.47
17	AA	842	CLA	C4B-CHC	-2.04	1.35	1.41
17	AA	824	CLA	CMC-C2C	-2.04	1.46	1.50
17	AA	802	CLA	MG-ND	-2.03	2.01	2.05
17	AA	831	CLA	CMC-C2C	-2.03	1.46	1.50
17	A4	313	CLA	CMC-C2C	-2.03	1.46	1.50
17	A6	612	CLA	C3B-C2B	-2.03	1.37	1.40
17	A6	609	CLA	CMC-C2C	-2.03	1.46	1.50
24	A1	317	LUT	C22-C21	-2.03	1.52	1.54
17	AA	836	CLA	CMD-C2D	-2.03	1.46	1.50
26	A6	605	CHL	CMC-C2C	2.03	1.49	1.45
17	A1	306	CLA	CMC-C2C	-2.03	1.46	1.50
17	AB	803	CLA	CMC-C2C	-2.03	1.46	1.50
26	A4	314	CHL	C1D-C2D	2.03	1.49	1.45
17	A3	308	CLA	C3B-CAB	-2.03	1.43	1.47
17	A4	308	CLA	CMC-C2C	-2.02	1.46	1.50
20	AA	848	BCR	C1-C6	-2.02	1.51	1.53

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	AJ	101	BCR	C23-C22	2.02	1.50	1.45
20	AK	202	BCR	C23-C22	2.02	1.50	1.45
17	A1	314	CLA	C4B-CHC	-2.02	1.35	1.41
17	A1	304	CLA	C4B-CHC	-2.02	1.35	1.41
26	A3	320	CHL	C4C-C3C	2.02	1.48	1.45
17	A3	303	CLA	C4B-CHC	-2.02	1.35	1.41
17	AA	807	CLA	C3B-C2B	-2.02	1.37	1.40
17	A6	608	CLA	CMC-C2C	-2.02	1.46	1.50
17	AA	803	CLA	C3B-CAB	-2.02	1.43	1.47
17	AA	804	CLA	C3B-CAB	-2.02	1.43	1.47
17	AK	201	CLA	CMD-C2D	-2.01	1.46	1.50
20	AL	306	BCR	C12-C13	2.01	1.50	1.45
18	AA	843	PQN	C2-C1	2.01	1.52	1.48
26	A3	320	CHL	C3D-C4D	-2.01	1.39	1.44
17	AA	809	CLA	CMC-C2C	-2.01	1.46	1.50
17	AA	841	CLA	C3B-CAB	-2.01	1.43	1.47
18	AB	843	PQN	C11-C3	2.01	1.54	1.51
17	AA	839	CLA	CMC-C2C	-2.01	1.46	1.50
17	AB	837	CLA	MG-ND	-2.01	2.01	2.05
17	AA	816	CLA	CMC-C2C	-2.01	1.46	1.50
17	AB	828	CLA	C3B-CAB	-2.01	1.43	1.47
17	AB	834	CLA	C3B-CAB	-2.01	1.43	1.47
17	AB	810	CLA	CMC-C2C	-2.01	1.46	1.50
17	AA	820	CLA	C3B-C2B	-2.01	1.37	1.40
27	A1	318	XAT	O4-C5	-2.01	1.43	1.46
17	AB	840	CLA	CMC-C2C	-2.00	1.46	1.50
17	AB	833	CLA	C4B-CHC	-2.00	1.35	1.41
17	AB	823	CLA	CMC-C2C	-2.00	1.46	1.50
17	AA	814	CLA	CMC-C2C	-2.00	1.46	1.50
20	AK	205	BCR	C19-C18	2.00	1.50	1.45
17	AA	830	CLA	C4B-CHC	-2.00	1.35	1.41

All (2111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A1	319	BCR	C40-C30-C25	-13.95	87.67	110.30
20	A3	318	BCR	C40-C30-C25	-10.15	93.83	110.30
20	AL	305	BCR	C7-C8-C9	-9.80	111.42	126.23
20	A1	319	BCR	C39-C30-C25	9.45	125.63	110.30
27	A4	316	XAT	O4-C5-C4	9.12	120.24	113.38
20	AJ	103	BCR	C28-C27-C26	-8.86	98.26	114.08
27	A1	318	XAT	O4-C5-C4	8.64	119.87	113.38

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A6	615	XAT	O4-C5-C4	8.61	119.85	113.38
20	AB	844	BCR	C3-C4-C5	-8.34	99.18	114.08
27	A3	317	XAT	O4-C5-C4	7.90	119.31	113.38
26	A6	607	CHL	C4D-CHA-C1A	-7.36	112.29	121.25
26	A1	308	CHL	C4D-CHA-C1A	-7.24	112.43	121.25
26	A4	306	CHL	C4D-CHA-C1A	-7.23	112.46	121.25
26	A4	304	CHL	C4D-CHA-C1A	-7.21	112.47	121.25
26	A1	303	CHL	C4D-CHA-C1A	-7.13	112.57	121.25
27	A1	318	XAT	O24-C25-C24	7.10	118.72	113.38
26	A4	305	CHL	C4D-CHA-C1A	-7.06	112.66	121.25
20	AB	846	BCR	C37-C22-C21	-7.05	113.05	122.92
26	A3	320	CHL	C4D-CHA-C1A	-6.99	112.74	121.25
20	A3	318	BCR	C39-C30-C25	6.97	121.60	110.30
26	A4	314	CHL	C4D-CHA-C1A	-6.96	112.78	121.25
26	A6	606	CHL	C4D-CHA-C1A	-6.96	112.78	121.25
26	A6	605	CHL	C4D-CHA-C1A	-6.96	112.78	121.25
20	AK	205	BCR	C28-C27-C26	-6.73	102.06	114.08
17	AB	811	CLA	C4A-NA-C1A	6.63	109.69	106.71
20	AG	205	BCR	C3-C4-C5	-6.59	102.31	114.08
20	A3	318	BCR	C40-C30-C39	-6.58	88.33	108.53
26	A3	307	CHL	C4D-CHA-C1A	-6.54	113.29	121.25
17	A1	305	CLA	C4A-NA-C1A	6.53	109.64	106.71
24	A4	315	LUT	C8-C7-C6	-6.43	109.13	127.20
20	A1	319	BCR	C40-C30-C39	-6.40	88.87	108.53
20	AA	848	BCR	C28-C27-C26	-6.36	102.72	114.08
20	AB	849	BCR	C24-C23-C22	-6.30	116.71	126.23
20	AA	845	BCR	C38-C26-C25	-6.30	117.46	124.53
20	A6	616	BCR	C40-C30-C25	-6.28	100.12	110.30
20	AK	202	BCR	C3-C4-C5	-6.27	102.88	114.08
20	AK	205	BCR	C3-C4-C5	-6.27	102.89	114.08
17	AB	825	CLA	C4A-NA-C1A	6.25	109.52	106.71
17	AL	304	CLA	C4A-NA-C1A	6.25	109.52	106.71
17	AA	841	CLA	C4A-NA-C1A	6.24	109.51	106.71
18	AB	843	PQN	C15-C13-C12	-6.22	108.53	121.12
17	AB	807	CLA	C4A-NA-C1A	6.17	109.48	106.71
20	A4	317	BCR	C28-C27-C26	-6.16	103.08	114.08
17	AB	804	CLA	CAC-C3C-C4C	6.10	132.73	124.81
17	AB	827	CLA	C4A-NA-C1A	6.09	109.45	106.71
24	A1	317	LUT	C17-C1-C6	-6.09	100.43	110.30
20	AB	849	BCR	C3-C4-C5	-6.08	103.22	114.08
17	AA	820	CLA	C4A-NA-C1A	6.04	109.42	106.71
17	AA	813	CLA	C4A-NA-C1A	6.03	109.42	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	828	CLA	CMB-C2B-C1B	-5.98	119.28	128.46
17	AF	802	CLA	C4A-NA-C1A	5.96	109.38	106.71
17	AA	837	CLA	C4A-NA-C1A	5.94	109.38	106.71
18	AA	843	PQN	C15-C13-C12	-5.92	109.15	121.12
17	AB	828	CLA	C4A-NA-C1A	5.90	109.36	106.71
17	AA	806	CLA	C4A-NA-C1A	5.90	109.36	106.71
17	AF	803	CLA	C4A-NA-C1A	5.89	109.36	106.71
26	A6	605	CHL	O2D-CGD-CBD	5.88	121.72	111.27
17	A6	603	CLA	C4A-NA-C1A	5.87	109.34	106.71
17	AB	824	CLA	C4A-NA-C1A	5.84	109.33	106.71
20	AB	849	BCR	C37-C22-C23	5.82	127.24	118.08
17	AB	832	CLA	C4A-NA-C1A	5.81	109.32	106.71
24	A3	316	LUT	C17-C1-C6	-5.80	100.88	110.30
26	A4	306	CHL	C2C-C3C-C4C	-5.79	102.36	106.49
20	AA	849	BCR	C34-C9-C10	-5.78	114.83	122.92
17	AB	839	CLA	C4A-NA-C1A	5.77	109.30	106.71
17	AB	810	CLA	C4A-NA-C1A	5.76	109.30	106.71
20	AL	306	BCR	C38-C26-C25	-5.75	118.07	124.53
17	A1	316	CLA	C4A-NA-C1A	5.73	109.28	106.71
17	AB	842	CLA	C4A-NA-C1A	5.71	109.28	106.71
17	AB	804	CLA	C4A-NA-C1A	5.71	109.27	106.71
20	AI	102	BCR	C28-C27-C26	-5.70	103.90	114.08
26	A3	320	CHL	C1B-CHB-C4A	-5.69	118.85	130.12
17	AA	834	CLA	C4A-NA-C1A	5.65	109.25	106.71
17	AK	204	CLA	C4A-NA-C1A	5.63	109.24	106.71
17	AA	833	CLA	C4A-NA-C1A	5.63	109.23	106.71
17	AB	841	CLA	C4A-NA-C1A	5.62	109.23	106.71
17	AA	808	CLA	C4A-NA-C1A	5.61	109.23	106.71
20	AB	847	BCR	C38-C26-C25	-5.60	118.24	124.53
17	AA	828	CLA	C4A-NA-C1A	5.60	109.22	106.71
26	A4	304	CHL	CHB-C4A-NA	5.59	132.24	124.51
17	AB	837	CLA	C4A-NA-C1A	5.58	109.22	106.71
17	AA	812	CLA	C4A-NA-C1A	5.58	109.21	106.71
17	A1	313	CLA	C4A-NA-C1A	5.57	109.21	106.71
17	A4	313	CLA	C4A-NA-C1A	5.56	109.21	106.71
20	A6	616	BCR	C28-C27-C26	-5.53	104.21	114.08
17	AB	830	CLA	C4A-NA-C1A	5.51	109.18	106.71
26	A6	605	CHL	CHB-C4A-NA	5.50	132.12	124.51
17	AA	842	CLA	C4A-NA-C1A	5.50	109.18	106.71
17	AA	810	CLA	C4A-NA-C1A	5.49	109.17	106.71
20	A3	318	BCR	C30-C25-C26	-5.49	114.88	122.61
18	AB	843	PQN	C11-C12-C13	-5.48	117.67	126.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A3	318	BCR	C3-C4-C5	-5.48	104.29	114.08
26	A4	305	CHL	CHB-C4A-NA	5.48	132.09	124.51
17	AK	201	CLA	C4A-NA-C1A	5.46	109.16	106.71
27	A4	316	XAT	O24-C25-C38	5.46	121.60	115.06
17	AA	814	CLA	C4A-NA-C1A	5.46	109.16	106.71
20	AL	305	BCR	C8-C7-C6	-5.44	111.92	127.20
26	A4	314	CHL	CHB-C4A-NA	5.44	132.03	124.51
17	A3	306	CLA	C4A-NA-C1A	5.43	109.15	106.71
20	AB	845	BCR	C34-C9-C10	-5.43	115.32	122.92
26	A1	303	CHL	C2C-C3C-C4C	-5.41	102.63	106.49
17	AG	203	CLA	C4A-NA-C1A	5.40	109.13	106.71
20	AA	845	BCR	C23-C24-C25	-5.40	112.04	127.20
20	AK	205	BCR	C32-C1-C6	-5.39	101.55	110.30
17	A6	601	CLA	C4A-NA-C1A	5.39	109.13	106.71
20	AA	847	BCR	C7-C8-C9	-5.38	118.11	126.23
17	AA	839	CLA	C4A-NA-C1A	5.37	109.12	106.71
26	A4	306	CHL	CHD-C4C-C3C	-5.36	116.95	124.84
20	A4	317	BCR	C32-C1-C6	5.36	118.99	110.30
17	AB	802	CLA	C4A-NA-C1A	5.35	109.11	106.71
26	A6	606	CHL	CHB-C4A-NA	5.34	131.90	124.51
17	A4	309	CLA	C4A-NA-C1A	5.34	109.11	106.71
17	AG	201	CLA	C4A-NA-C1A	5.33	109.10	106.71
20	AI	102	BCR	C31-C1-C6	5.33	118.94	110.30
17	AA	830	CLA	C4A-NA-C1A	5.32	109.10	106.71
17	AB	814	CLA	C4A-NA-C1A	5.32	109.10	106.71
17	AB	822	CLA	C4A-NA-C1A	5.32	109.10	106.71
20	AB	848	BCR	C23-C24-C25	-5.32	112.27	127.20
26	A3	320	CHL	CHD-C4C-C3C	-5.30	117.05	124.84
17	A1	310	CLA	C4A-NA-C1A	5.30	109.09	106.71
20	AA	847	BCR	C35-C13-C14	-5.30	115.50	122.92
17	AB	821	CLA	C4A-NA-C1A	5.29	109.08	106.71
17	AB	812	CLA	C4A-NA-C1A	5.29	109.08	106.71
20	AA	847	BCR	C28-C27-C26	-5.29	104.64	114.08
20	A4	317	BCR	C1-C6-C5	-5.28	115.18	122.61
26	A1	303	CHL	CHD-C4C-C3C	-5.26	117.11	124.84
17	AJ	102	CLA	C4A-NA-C1A	5.26	109.07	106.71
26	A4	304	CHL	C1B-CHB-C4A	-5.25	119.73	130.12
17	AA	825	CLA	C4A-NA-C1A	5.24	109.06	106.71
20	AI	101	BCR	C38-C26-C25	-5.24	118.65	124.53
20	AA	847	BCR	C31-C1-C6	5.23	118.78	110.30
26	A4	306	CHL	CHB-C4A-NA	5.23	131.74	124.51
17	A1	306	CLA	C4A-NA-C1A	5.22	109.05	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	811	CLA	C4A-NA-C1A	5.22	109.05	106.71
26	A4	306	CHL	OBD-CAD-C3D	-5.21	115.98	128.52
17	AA	822	CLA	C4A-NA-C1A	5.21	109.05	106.71
26	A4	305	CHL	C1B-C2B-C3B	-5.20	102.08	106.92
26	A3	307	CHL	CHD-C4C-C3C	-5.20	117.20	124.84
17	AB	808	CLA	C4A-NA-C1A	5.17	109.03	106.71
26	A1	308	CHL	C1B-CHB-C4A	-5.15	119.91	130.12
26	A1	308	CHL	CHB-C4A-NA	5.15	131.63	124.51
17	AA	805	CLA	C4A-NA-C1A	5.14	109.02	106.71
17	AF	804	CLA	C4A-NA-C1A	5.14	109.02	106.71
26	A4	314	CHL	C1B-C2B-C3B	-5.13	102.15	106.92
27	A3	317	XAT	O24-C25-C38	5.12	121.19	115.06
26	A3	320	CHL	C1D-ND-C4D	5.11	109.96	106.33
17	AA	804	CLA	C4A-NA-C1A	5.10	109.00	106.71
26	A3	307	CHL	CHB-C4A-NA	5.10	131.57	124.51
17	AB	838	CLA	C4A-NA-C1A	5.09	109.00	106.71
20	AA	846	BCR	C36-C18-C19	5.09	126.10	118.08
26	A1	303	CHL	OBD-CAD-C3D	-5.08	116.30	128.52
26	A6	605	CHL	C2C-C3C-C4C	-5.08	102.72	106.49
26	A4	305	CHL	C1B-CHB-C4A	-5.07	120.08	130.12
17	AA	827	CLA	C4A-NA-C1A	5.07	108.98	106.71
26	A4	306	CHL	C2A-C1A-CHA	-5.07	115.00	123.86
17	AA	815	CLA	C4A-NA-C1A	5.06	108.98	106.71
26	A4	314	CHL	C1B-CHB-C4A	-5.05	120.12	130.12
26	A4	304	CHL	C2A-C1A-CHA	-5.03	115.06	123.86
26	A1	303	CHL	CHB-C4A-NA	5.03	131.46	124.51
17	AA	821	CLA	CMB-C2B-C1B	-5.02	120.75	128.46
26	A1	308	CHL	C2C-C3C-C4C	-5.02	102.91	106.49
17	A3	312	CLA	C4A-NA-C1A	5.02	108.96	106.71
20	AJ	103	BCR	C39-C30-C25	-4.99	102.21	110.30
17	A4	302	CLA	C4A-NA-C1A	4.99	108.95	106.71
17	A6	612	CLA	C4A-NA-C1A	4.97	108.94	106.71
17	AB	819	CLA	C4A-NA-C1A	4.96	108.94	106.71
26	A6	606	CHL	C2C-C3C-C4C	-4.96	102.95	106.49
26	A6	605	CHL	CHD-C4C-C3C	-4.96	117.24	124.98
17	A1	307	CLA	C4A-NA-C1A	4.96	108.93	106.71
20	AL	305	BCR	C27-C26-C25	-4.95	115.54	122.73
17	AG	204	CLA	C4A-NA-C1A	4.94	108.93	106.71
20	AF	805	BCR	C35-C13-C14	-4.94	116.01	122.92
26	A4	305	CHL	O2D-CGD-CBD	4.94	120.04	111.27
17	AB	813	CLA	C4A-NA-C1A	4.92	108.92	106.71
17	A4	310	CLA	C4A-NA-C1A	4.92	108.92	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AB	809	CLA	C4A-NA-C1A	4.92	108.92	106.71
26	A3	307	CHL	OBD-CAD-C3D	-4.91	116.69	128.52
17	AA	821	CLA	C4A-NA-C1A	4.91	108.91	106.71
20	AL	305	BCR	C33-C5-C6	4.90	130.03	124.53
26	A3	320	CHL	C2C-C3C-C4C	-4.90	103.00	106.49
26	A6	606	CHL	C1B-CHB-C4A	-4.90	120.42	130.12
26	A4	305	CHL	CHD-C4C-C3C	-4.89	117.65	124.84
26	A4	304	CHL	C2C-C3C-C4C	-4.89	102.86	106.49
26	A3	307	CHL	C1B-CHB-C4A	-4.88	120.46	130.12
26	A6	605	CHL	C2A-C1A-CHA	-4.88	115.33	123.86
26	A4	304	CHL	CHD-C4C-C3C	-4.87	117.36	124.98
20	AK	202	BCR	C36-C18-C19	4.86	125.73	118.08
17	AA	817	CLA	C4A-NA-C1A	4.85	108.89	106.71
20	AB	847	BCR	C28-C27-C26	-4.85	105.42	114.08
17	AA	828	CLA	CMB-C2B-C3B	4.85	133.75	124.68
17	A4	311	CLA	C4A-NA-C1A	4.84	108.88	106.71
26	A4	314	CHL	CHD-C4C-C3C	-4.83	117.74	124.84
17	A3	305	CLA	C4A-NA-C1A	4.83	108.88	106.71
26	A6	607	CHL	OBD-CAD-C3D	-4.82	116.91	128.52
17	AA	816	CLA	C4A-NA-C1A	4.82	108.87	106.71
26	A6	606	CHL	OBD-CAD-C3D	-4.81	116.94	128.52
17	A1	314	CLA	C4A-NA-C1A	4.81	108.87	106.71
17	A3	311	CLA	C4A-NA-C1A	4.81	108.87	106.71
17	AB	801	CLA	C4A-NA-C1A	4.80	108.86	106.71
26	A6	607	CHL	C4A-NA-C1A	-4.80	104.55	106.71
26	A6	605	CHL	C1B-CHB-C4A	-4.80	120.61	130.12
20	AK	202	BCR	C30-C25-C26	-4.80	115.86	122.61
26	A6	607	CHL	CHB-C4A-NA	4.79	131.14	124.51
17	AB	836	CLA	C4A-NA-C1A	4.78	108.85	106.71
26	A6	607	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
26	A4	306	CHL	CAC-C3C-C4C	4.76	130.99	124.81
17	AA	802	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
17	AA	818	CLA	C4A-NA-C1A	4.76	108.84	106.71
26	A4	314	CHL	OBD-CAD-C3D	-4.75	117.08	128.52
26	A3	320	CHL	CHB-C4A-NA	4.74	131.07	124.51
26	A1	308	CHL	OBD-CAD-C3D	-4.74	117.12	128.52
27	A6	615	XAT	O24-C25-C24	4.73	116.94	113.38
26	A4	306	CHL	C1B-CHB-C4A	-4.73	120.75	130.12
26	A4	305	CHL	OBD-CAD-C3D	-4.72	117.15	128.52
27	A1	318	XAT	C6-C7-C8	-4.71	116.04	125.99
26	A6	606	CHL	CHD-C4C-C3C	-4.71	117.92	124.84
17	AB	803	CLA	C4A-NA-C1A	4.70	108.82	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A4	314	CHL	C2C-C3C-C4C	-4.69	103.14	106.49
17	AA	803	CLA	C4A-NA-C1A	4.69	108.81	106.71
26	A1	308	CHL	C1D-ND-C4D	4.69	109.66	106.33
17	AA	801	CLA	C4A-NA-C1A	4.68	108.81	106.71
17	AB	834	CLA	C4A-NA-C1A	4.67	108.81	106.71
20	AB	846	BCR	C34-C9-C10	-4.66	116.39	122.92
20	A4	317	BCR	C40-C30-C25	-4.65	102.75	110.30
26	A6	605	CHL	OBD-CAD-C3D	-4.64	117.36	128.52
17	A3	303	CLA	C4A-NA-C1A	4.64	108.79	106.71
17	AA	835	CLA	C4A-NA-C1A	4.63	108.79	106.71
17	AB	816	CLA	C4A-NA-C1A	4.63	108.79	106.71
27	A6	615	XAT	C6-C7-C8	-4.63	116.21	125.99
17	AA	831	CLA	C4A-NA-C1A	4.63	108.79	106.71
20	A4	317	BCR	C23-C24-C25	-4.62	114.21	127.20
18	AA	843	PQN	C11-C12-C13	-4.61	119.11	126.79
17	A1	315	CLA	C4A-NA-C1A	4.61	108.78	106.71
17	AA	836	CLA	C4A-NA-C1A	4.61	108.78	106.71
26	A4	314	CHL	C2A-C1A-CHA	-4.60	115.82	123.86
20	AJ	101	BCR	C3-C4-C5	-4.59	105.88	114.08
20	A1	319	BCR	C29-C30-C25	4.59	117.55	110.48
26	A6	606	CHL	CAC-C3C-C4C	4.59	130.77	124.81
26	A1	308	CHL	CHD-C4C-C3C	-4.59	118.10	124.84
17	A3	304	CLA	C4A-NA-C1A	4.59	108.77	106.71
20	AK	202	BCR	C28-C27-C26	-4.58	105.89	114.08
17	AA	829	CLA	C4A-NA-C1A	4.58	108.76	106.71
17	AA	809	CLA	C4A-NA-C1A	4.58	108.76	106.71
26	A1	303	CHL	C2A-C1A-CHA	-4.56	115.89	123.86
26	A3	307	CHL	C2A-C1A-CHA	-4.55	115.90	123.86
17	A6	602	CLA	C4A-NA-C1A	4.55	108.75	106.71
17	AB	829	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
17	AH	201	CLA	C4A-NA-C1A	4.53	108.74	106.71
17	A3	310	CLA	C4A-NA-C1A	4.52	108.74	106.71
26	A1	303	CHL	C1B-CHB-C4A	-4.52	121.17	130.12
26	A4	304	CHL	OBD-CAD-C3D	-4.51	117.67	128.52
17	A4	303	CLA	C4A-NA-C1A	4.51	108.73	106.71
17	AA	840	CLA	C4A-NA-C1A	4.50	108.73	106.71
20	AJ	101	BCR	C34-C9-C8	4.49	125.16	118.08
20	AB	847	BCR	C36-C18-C19	4.49	125.16	118.08
17	AK	203	CLA	C4A-NA-C1A	4.49	108.73	106.71
19	A3	319	LHG	O7-C7-C8	4.48	119.34	111.09
27	A6	615	XAT	C18-C5-C6	-4.48	114.76	122.26
20	A6	616	BCR	C3-C4-C5	-4.48	106.08	114.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A1	308	CHL	C2A-C1A-CHA	-4.47	116.04	123.85
26	A3	320	CHL	OBD-CAD-C3D	-4.47	117.76	128.52
20	AL	306	BCR	C33-C5-C6	-4.47	119.51	124.53
17	A4	301	CLA	C4A-NA-C1A	4.47	108.71	106.71
26	A6	606	CHL	O2D-CGD-CBD	4.46	119.19	111.27
26	A6	607	CHL	O2D-CGD-CBD	4.43	119.14	111.27
26	A4	306	CHL	O2D-CGD-CBD	4.43	119.13	111.27
17	AB	819	CLA	C4-C3-C5	4.42	122.70	115.27
20	AB	848	BCR	C33-C5-C6	-4.42	119.57	124.53
20	AI	101	BCR	C36-C18-C19	4.41	125.03	118.08
26	A3	307	CHL	O2D-CGD-CBD	4.41	119.10	111.27
26	A4	305	CHL	C1D-ND-C4D	4.41	109.47	106.33
20	AI	102	BCR	C8-C7-C6	-4.40	114.83	127.20
20	AJ	101	BCR	C32-C1-C6	-4.40	103.16	110.30
26	A6	606	CHL	C2A-C1A-CHA	-4.39	116.17	123.86
17	AA	838	CLA	C4A-NA-C1A	4.39	108.68	106.71
17	AB	819	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
17	AB	815	CLA	C4A-NA-C1A	4.38	108.67	106.71
26	A6	607	CHL	CAC-C3C-C4C	4.38	130.49	124.81
20	AA	845	BCR	C32-C1-C6	-4.36	103.22	110.30
17	AB	827	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
17	A3	313	CLA	C4A-NA-C1A	4.35	108.66	106.71
17	AA	802	CLA	CMB-C2B-C3B	4.34	132.80	124.68
20	AA	846	BCR	C32-C1-C6	4.33	117.33	110.30
20	AA	846	BCR	C24-C23-C22	-4.33	119.69	126.23
20	AA	846	BCR	C3-C4-C5	-4.33	106.35	114.08
17	A6	604	CLA	C4A-NA-C1A	4.32	108.65	106.71
17	A3	308	CLA	C4A-NA-C1A	4.32	108.65	106.71
20	AI	102	BCR	C34-C9-C10	-4.31	116.88	122.92
26	A3	320	CHL	C2A-C1A-CHA	-4.31	116.32	123.86
20	AG	205	BCR	C36-C18-C17	-4.30	116.90	122.92
26	A3	320	CHL	C1D-CHD-C4C	-4.30	116.78	126.06
17	A6	612	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
17	AB	837	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
18	AB	843	PQN	C14-C13-C12	-4.29	112.67	123.68
27	A3	317	XAT	C6-C7-C8	-4.29	116.92	125.99
26	A6	607	CHL	C1D-ND-C4D	4.29	109.38	106.33
20	AK	202	BCR	C37-C22-C23	4.28	124.83	118.08
17	AB	823	CLA	C4A-NA-C1A	4.28	108.63	106.71
26	A6	607	CHL	C1B-CHB-C4A	-4.28	121.64	130.12
24	AF	806	LUT	C40-C33-C32	4.28	124.82	118.08
20	AJ	103	BCR	C36-C18-C19	4.27	124.81	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	819	CLA	C4A-NA-C1A	4.27	108.63	106.71
27	A6	615	XAT	C39-C29-C28	4.27	124.80	118.08
20	AB	844	BCR	C34-C9-C8	4.26	124.80	118.08
17	AB	815	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
17	AA	829	CLA	C4-C3-C5	4.26	122.44	115.27
20	AJ	103	BCR	C32-C1-C6	-4.26	103.39	110.30
20	AG	205	BCR	C28-C27-C26	-4.26	106.47	114.08
26	A4	314	CHL	C1D-ND-C4D	4.26	109.36	106.33
20	AF	805	BCR	C37-C22-C23	4.25	124.77	118.08
26	A3	307	CHL	CMC-C2C-C1C	4.25	131.51	125.04
26	A1	308	CHL	CAC-C3C-C4C	4.25	130.32	124.81
20	A1	319	BCR	C1-C6-C5	-4.25	116.63	122.61
20	AI	102	BCR	C38-C26-C25	-4.24	119.76	124.53
20	A4	317	BCR	C3-C4-C5	-4.24	106.51	114.08
17	AB	840	CLA	C4A-NA-C1A	4.24	108.61	106.71
26	A4	305	CHL	CHC-C1C-NC	4.23	130.62	124.20
17	AB	817	CLA	C4A-NA-C1A	4.22	108.61	106.71
20	AA	848	BCR	C37-C22-C23	4.22	124.72	118.08
20	AF	801	BCR	C37-C22-C23	4.22	124.72	118.08
26	A6	607	CHL	CMC-C2C-C1C	4.22	131.46	125.04
17	AA	824	CLA	C4-C3-C5	4.22	122.36	115.27
17	AA	832	CLA	C4A-NA-C1A	4.20	108.60	106.71
17	AA	825	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
17	A3	314	CLA	C4A-NA-C1A	4.20	108.59	106.71
17	AA	804	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
20	AJ	101	BCR	C37-C22-C23	4.19	124.68	118.08
24	A6	614	LUT	C8-C7-C6	-4.19	115.43	127.20
20	A6	616	BCR	C37-C22-C23	4.19	124.68	118.08
17	AA	807	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
20	AA	849	BCR	C39-C30-C25	-4.19	103.51	110.30
17	A4	312	CLA	C4A-NA-C1A	4.18	108.59	106.71
20	AA	847	BCR	C1-C6-C5	-4.18	116.73	122.61
20	AI	102	BCR	C3-C4-C5	-4.18	106.62	114.08
17	AB	805	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
27	A3	317	XAT	C38-C25-C26	-4.17	115.28	122.26
26	A3	307	CHL	C1D-ND-C4D	4.16	109.29	106.33
24	A1	317	LUT	C3-C4-C5	-4.15	103.58	111.85
20	AL	305	BCR	C40-C30-C25	-4.15	103.57	110.30
20	AJ	103	BCR	C31-C1-C6	4.15	117.02	110.30
20	A4	317	BCR	C36-C18-C19	4.14	124.60	118.08
17	AA	802	CLA	C4A-NA-C1A	4.13	108.56	106.71
24	AF	806	LUT	C39-C29-C28	4.11	124.56	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A4	305	CHL	C2A-C1A-CHA	-4.11	116.67	123.86
20	AB	844	BCR	C38-C26-C25	-4.11	119.91	124.53
17	AA	837	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
17	A1	313	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
17	A1	315	CLA	CAB-C3B-C4B	-4.09	122.18	128.46
20	AB	847	BCR	C37-C22-C23	4.08	124.51	118.08
17	A4	302	CLA	CAB-C3B-C4B	-4.08	122.19	128.46
20	AK	202	BCR	C27-C26-C25	-4.08	116.81	122.73
17	AB	821	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
26	A3	307	CHL	C1D-CHD-C4C	-4.07	117.28	126.06
17	AB	840	CLA	CMB-C2B-C1B	-4.07	122.22	128.46
26	A4	305	CHL	C1D-CHD-C4C	-4.06	117.30	126.06
20	AI	101	BCR	C7-C8-C9	-4.06	120.11	126.23
25	A4	318	LMG	C8-O7-C10	-4.05	107.82	117.79
20	A4	317	BCR	C37-C22-C23	4.05	124.46	118.08
27	A3	317	XAT	O4-C5-C18	4.04	119.90	115.06
17	A3	306	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
26	A6	607	CHL	CHC-C1C-NC	4.04	130.33	124.20
20	AI	101	BCR	C31-C1-C6	-4.04	103.75	110.30
17	A4	303	CLA	CAB-C3B-C4B	-4.03	122.27	128.46
17	AB	805	CLA	C4A-NA-C1A	4.03	108.52	106.71
26	A3	320	CHL	C6-C5-C3	-4.03	108.04	114.62
26	A6	607	CHL	C2A-C1A-CHA	-4.02	116.83	123.86
26	A6	606	CHL	C1D-ND-C4D	4.02	109.19	106.33
19	A3	301	LHG	O7-C7-C8	4.02	120.16	111.50
17	AA	826	CLA	C4A-NA-C1A	4.01	108.51	106.71
27	A4	316	XAT	C39-C29-C28	4.01	124.40	118.08
26	A1	303	CHL	C1D-CHD-C4C	-4.00	117.42	126.06
17	AA	821	CLA	CMB-C2B-C3B	4.00	132.16	124.68
20	AB	847	BCR	C3-C4-C5	-4.00	106.94	114.08
27	A6	615	XAT	C40-C33-C32	4.00	124.37	118.08
26	A3	320	CHL	CHD-C4C-NC	4.00	130.50	124.20
17	AB	820	CLA	CMB-C2B-C1B	-3.99	122.32	128.46
17	A1	316	CLA	CAB-C3B-C4B	-3.99	122.33	128.46
26	A4	306	CHL	C4A-NA-C1A	-3.99	104.91	106.71
19	A1	301	LHG	O7-C7-C8	3.98	120.08	111.50
20	AB	849	BCR	C32-C1-C6	-3.98	103.85	110.30
17	A6	611	CLA	C4A-NA-C1A	3.97	108.49	106.71
20	AJ	103	BCR	C8-C9-C10	-3.97	112.84	118.94
20	AG	205	BCR	C36-C18-C19	3.97	124.33	118.08
27	A6	615	XAT	O24-C25-C38	3.96	119.80	115.06
20	AB	845	BCR	C37-C22-C23	3.95	124.31	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AB	846	BCR	C37-C22-C23	3.95	124.31	118.08
24	A1	317	LUT	C16-C1-C6	3.95	116.71	110.30
17	AB	833	CLA	C4A-NA-C1A	3.95	108.48	106.71
20	AB	846	BCR	C33-C5-C6	-3.94	120.10	124.53
20	A1	319	BCR	C30-C25-C26	-3.94	117.06	122.61
17	AB	835	CLA	C4A-NA-C1A	3.94	108.48	106.71
20	AI	102	BCR	C37-C22-C23	3.94	124.28	118.08
17	A3	306	CLA	CAB-C3B-C4B	-3.93	122.42	128.46
17	AA	807	CLA	C4A-NA-C1A	3.93	108.47	106.71
17	A1	309	CLA	C4A-NA-C1A	3.93	108.47	106.71
20	AL	305	BCR	C28-C27-C26	-3.93	107.06	114.08
20	AL	305	BCR	C1-C6-C5	-3.92	117.09	122.61
20	AA	849	BCR	C36-C18-C17	-3.91	117.44	122.92
20	AA	846	BCR	C38-C26-C25	-3.91	120.14	124.53
20	AA	849	BCR	C37-C22-C23	3.91	124.23	118.08
17	AB	815	CLA	CMB-C2B-C3B	3.91	131.99	124.68
20	AB	845	BCR	C36-C18-C19	3.90	124.23	118.08
17	AB	811	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
17	A4	307	CLA	C4A-NA-C1A	3.90	108.46	106.71
20	A3	318	BCR	C40-C30-C29	-3.90	93.31	108.91
26	A3	307	CHL	CHC-C1C-NC	3.90	130.12	124.20
26	A6	606	CHL	C1D-CHD-C4C	-3.89	117.67	126.06
17	AF	804	CLA	CAA-C2A-C3A	-3.89	107.03	116.10
17	AB	810	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
26	A4	306	CHL	C1D-CHD-C4C	-3.88	117.68	126.06
26	A6	605	CHL	C4A-NA-C1A	-3.88	104.96	106.71
20	A1	319	BCR	C37-C22-C23	3.87	124.17	118.08
26	A1	303	CHL	C1D-ND-C4D	3.86	109.08	106.33
17	A1	304	CLA	C4A-NA-C1A	3.86	108.44	106.71
17	AB	806	CLA	C4A-NA-C1A	3.86	108.44	106.71
17	A1	310	CLA	CAB-C3B-C4B	-3.86	122.54	128.46
17	A1	311	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
19	A1	302	LHG	O7-C7-C8	3.85	119.80	111.50
17	AB	827	CLA	CMB-C2B-C3B	3.85	131.88	124.68
17	A4	308	CLA	C4A-NA-C1A	3.84	108.43	106.71
20	AA	847	BCR	C24-C23-C22	-3.84	120.43	126.23
17	AB	828	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
17	AA	808	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
26	A1	308	CHL	C1D-CHD-C4C	-3.83	117.79	126.06
17	AL	302	CLA	C4A-NA-C1A	3.82	108.42	106.71
17	AL	303	CLA	C4A-NA-C1A	3.82	108.42	106.71
17	AL	303	CLA	CMB-C2B-C1B	-3.82	122.60	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A3	302	CLA	C4A-NA-C1A	3.81	108.42	106.71
20	AF	805	BCR	C7-C8-C9	-3.81	120.48	126.23
17	AB	835	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
17	AB	836	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
26	A6	606	CHL	C4A-NA-C1A	-3.81	105.00	106.71
26	A1	303	CHL	C4A-NA-C1A	-3.80	105.00	106.71
17	A3	315	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
17	AA	837	CLA	CMB-C2B-C3B	3.79	131.76	124.68
26	A4	314	CHL	C1D-CHD-C4C	-3.79	117.89	126.06
17	AA	816	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
17	AA	819	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
23	AB	851	DGD	O2G-C1B-C2B	3.78	119.64	111.50
17	A6	608	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
26	A3	307	CHL	C4A-NA-C1A	-3.76	105.02	106.71
17	AB	812	CLA	CAB-C3B-C4B	-3.76	122.68	128.46
26	A6	607	CHL	C1D-CHD-C4C	-3.76	117.95	126.06
26	A6	605	CHL	C1D-CHD-C4C	-3.75	117.97	126.06
20	A1	319	BCR	C36-C18-C19	3.75	123.98	118.08
17	AA	826	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
27	A6	615	XAT	C8-C9-C10	-3.74	113.20	118.94
17	A4	303	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
17	AA	802	CLA	C1B-CHB-C4A	-3.73	122.74	130.12
17	A6	608	CLA	C4A-NA-C1A	3.72	108.38	106.71
17	A6	613	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
26	A4	304	CHL	C1D-ND-C4D	3.71	108.97	106.33
17	AA	804	CLA	CMB-C2B-C3B	3.71	131.62	124.68
17	AB	838	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
17	AB	829	CLA	CMB-C2B-C3B	3.70	131.60	124.68
17	A3	303	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
17	AA	817	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
26	A1	303	CHL	O2A-CGA-CBA	3.69	123.48	111.91
20	AJ	103	BCR	C1-C6-C5	-3.69	117.42	122.61
26	A1	308	CHL	C4A-NA-C1A	-3.68	105.05	106.71
26	A6	605	CHL	C1D-ND-C4D	3.68	108.95	106.33
17	AB	839	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
26	A4	304	CHL	C4A-NA-C1A	-3.67	105.06	106.71
27	A3	317	XAT	C39-C29-C28	3.67	123.86	118.08
17	AB	806	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
26	A4	306	CHL	CHD-C4C-NC	3.66	129.97	124.20
20	AB	849	BCR	C23-C22-C21	-3.66	113.32	118.94
17	A6	603	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
26	A4	305	CHL	CAC-C3C-C4C	3.66	129.56	124.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AB	819	CLA	CMB-C2B-C3B	3.66	131.52	124.68
26	A4	304	CHL	C1D-CHD-C4C	-3.66	118.17	126.06
17	AB	826	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
17	A1	306	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
17	A1	315	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
23	AB	851	DGD	C2G-O2G-C1B	-3.63	108.84	117.79
20	AL	305	BCR	C37-C22-C23	3.63	123.80	118.08
17	AA	829	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
20	AB	844	BCR	C7-C8-C9	-3.63	120.75	126.23
17	A4	309	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
20	AL	306	BCR	C28-C27-C26	-3.61	107.62	114.08
17	AL	302	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
20	A3	318	BCR	C38-C26-C25	-3.61	120.48	124.53
20	AL	306	BCR	C38-C26-C27	3.60	120.54	113.62
17	A1	309	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
17	AB	816	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
17	AB	826	CLA	CMB-C2B-C3B	3.60	131.41	124.68
25	A1	321	LMG	O7-C10-C11	3.60	119.25	111.50
20	AG	205	BCR	C32-C1-C6	-3.60	104.47	110.30
17	AA	807	CLA	CMB-C2B-C3B	3.60	131.41	124.68
17	AB	812	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
17	AB	818	CLA	C4A-NA-C1A	3.59	108.32	106.71
25	A4	318	LMG	C7-O1-C1	-3.59	106.73	113.74
17	AA	811	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
17	A6	613	CLA	C4A-NA-C1A	3.59	108.32	106.71
20	AK	202	BCR	C37-C22-C21	-3.59	117.90	122.92
17	AA	815	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
20	AL	305	BCR	C30-C25-C26	-3.59	117.56	122.61
20	A3	318	BCR	C39-C30-C29	3.58	123.24	108.91
17	A3	308	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
17	A1	311	CLA	C4A-NA-C1A	3.58	108.31	106.71
27	A1	318	XAT	C8-C9-C10	-3.57	113.46	118.94
17	AA	829	CLA	CMB-C2B-C3B	3.57	131.36	124.68
20	AA	848	BCR	C36-C18-C19	3.57	123.70	118.08
26	A4	314	CHL	CHD-C4C-NC	3.56	129.82	124.20
17	AB	814	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
17	A3	309	CLA	C4A-NA-C1A	3.56	108.31	106.71
20	AB	848	BCR	C36-C18-C19	3.55	123.67	118.08
27	A3	317	XAT	C19-C9-C8	3.55	123.67	118.08
17	AA	803	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
17	AB	828	CLA	CMB-C2B-C3B	3.54	131.30	124.68
25	A4	318	LMG	O7-C10-C11	3.54	119.12	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A3	318	BCR	C1-C6-C5	-3.53	117.64	122.61
18	AB	843	PQN	C11-C3-C4	-3.53	114.72	118.50
17	AB	801	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
17	AB	817	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
17	AA	816	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
17	AA	832	CLA	C4-C3-C5	3.52	121.18	115.27
17	AB	813	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
26	A3	307	CHL	CHD-C4C-NC	3.51	129.73	124.20
17	AA	829	CLA	C6-C5-C3	3.51	122.65	113.45
18	AB	843	PQN	C12-C11-C3	-3.51	102.59	112.05
17	AB	804	CLA	CAC-C3C-C2C	-3.51	121.53	127.53
17	AA	812	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
20	AB	849	BCR	C16-C15-C14	-3.50	116.31	123.47
17	A1	307	CLA	CBD-CHA-C1A	3.49	132.61	128.50
17	AA	835	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
17	AA	830	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
24	AF	806	LUT	C15-C35-C34	-3.48	116.34	123.47
17	AA	818	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
17	A3	313	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
26	A1	303	CHL	CHD-C4C-NC	3.46	129.66	124.20
17	A4	301	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
20	A1	319	BCR	C40-C30-C29	-3.46	95.06	108.91
17	AA	836	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
17	AB	801	CLA	CAA-C2A-C1A	-3.46	100.64	111.97
17	AB	839	CLA	CMB-C2B-C3B	3.46	131.15	124.68
26	A3	307	CHL	CAC-C3C-C4C	3.46	129.29	124.81
17	AB	835	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
17	A4	310	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
26	A6	605	CHL	CHD-C4C-NC	3.45	129.64	124.20
17	A3	311	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
20	AA	849	BCR	C27-C26-C25	-3.45	117.73	122.73
20	AB	848	BCR	C15-C16-C17	-3.44	116.43	123.47
20	AA	846	BCR	C15-C16-C17	-3.44	116.43	123.47
17	AA	822	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
20	AB	847	BCR	C23-C24-C25	-3.44	117.55	127.20
20	AA	849	BCR	C38-C26-C27	3.44	120.22	113.62
17	AB	804	CLA	CHB-C4A-NA	3.43	129.26	124.51
20	A1	319	BCR	C4-C5-C6	-3.43	117.75	122.73
26	A4	305	CHL	CMC-C2C-C1C	3.43	130.26	125.04
17	AF	802	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
26	A4	305	CHL	CHD-C4C-NC	3.43	129.61	124.20
17	AA	824	CLA	CMB-C2B-C1B	-3.43	123.19	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A4	315	LUT	C21-C26-C27	-3.43	108.37	112.70
17	A6	609	CLA	C1B-CHB-C4A	-3.43	123.33	130.12
17	A3	315	CLA	C4A-NA-C1A	3.43	108.25	106.71
17	AB	805	CLA	CMB-C2B-C3B	3.43	131.09	124.68
17	A1	313	CLA	CMB-C2B-C3B	3.43	131.09	124.68
17	AA	827	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
17	AB	810	CLA	CMB-C2B-C3B	3.42	131.08	124.68
17	A1	312	CLA	C4A-NA-C1A	3.42	108.24	106.71
17	AA	813	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
25	AG	202	LMG	O7-C10-C11	3.41	118.86	111.50
26	A3	307	CHL	CHC-C1C-C2C	-3.41	117.28	126.72
20	AJ	101	BCR	C8-C7-C6	-3.41	117.61	127.20
17	AA	837	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
17	AB	811	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
27	A4	316	XAT	C35-C15-C14	-3.41	116.49	123.47
17	AB	823	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
17	A3	304	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
17	AA	840	CLA	C1B-CHB-C4A	-3.41	123.37	130.12
20	AA	847	BCR	C36-C18-C19	3.40	123.44	118.08
20	A6	616	BCR	C23-C24-C25	-3.40	117.65	127.20
17	AB	835	CLA	CMB-C2B-C3B	3.39	131.02	124.68
17	AA	825	CLA	CMB-C2B-C3B	3.39	131.02	124.68
17	AB	830	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
20	AA	849	BCR	C31-C1-C6	-3.38	104.81	110.30
17	A6	609	CLA	C4A-NA-C1A	3.38	108.22	106.71
17	A3	315	CLA	CMB-C2B-C3B	3.38	131.00	124.68
17	A1	311	CLA	CMB-C2B-C3B	3.37	130.99	124.68
20	AA	848	BCR	C30-C25-C24	3.37	125.31	115.78
17	AB	842	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
20	AA	848	BCR	C38-C26-C25	-3.37	120.75	124.53
17	AA	842	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
17	AA	823	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
17	AB	817	CLA	CMB-C2B-C3B	3.36	130.97	124.68
17	AB	819	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
17	A4	307	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
17	AA	826	CLA	CMB-C2B-C3B	3.36	130.96	124.68
17	AB	818	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
20	AB	844	BCR	C37-C22-C23	3.36	123.36	118.08
20	AI	101	BCR	C37-C22-C23	3.35	123.36	118.08
20	AF	805	BCR	C16-C15-C14	-3.35	116.60	123.47
20	AK	202	BCR	C15-C16-C17	-3.35	116.61	123.47
26	A4	304	CHL	CHD-C4C-NC	3.35	129.49	124.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	809	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
17	A6	610	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
17	AB	808	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
20	AL	306	BCR	C30-C25-C24	3.35	125.25	115.78
20	AI	102	BCR	C2-C1-C6	-3.35	105.33	110.48
17	AB	831	CLA	C4A-NA-C1A	3.35	108.21	106.71
17	AB	826	CLA	C1B-CHB-C4A	-3.34	123.49	130.12
17	AG	201	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
17	A6	610	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
20	AI	102	BCR	C35-C13-C12	3.34	123.33	118.08
24	A3	316	LUT	C39-C29-C28	3.33	123.33	118.08
26	A4	306	CHL	CHC-C1C-NC	3.33	129.26	124.20
17	A1	304	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
17	AB	813	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
17	AA	833	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
19	A6	617	LHG	O7-C7-C8	3.33	118.68	111.50
20	AF	801	BCR	C35-C13-C12	3.33	123.32	118.08
17	AA	833	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
20	AB	846	BCR	C36-C18-C19	3.32	123.31	118.08
17	AB	832	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
17	A6	610	CLA	CAB-C3B-C4B	-3.32	123.36	128.46
27	A3	317	XAT	C26-C27-C28	-3.32	118.98	125.99
17	AB	827	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
17	A3	304	CLA	CAB-C3B-C4B	-3.31	123.37	128.46
26	A4	314	CHL	CHC-C1C-NC	3.31	129.23	124.20
20	AB	845	BCR	C8-C7-C6	-3.31	117.91	127.20
17	AF	804	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
17	AB	818	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
26	A4	305	CHL	C4C-C3C-C2C	-3.30	102.08	106.90
27	A1	318	XAT	C18-C5-C6	-3.30	116.73	122.26
17	A3	310	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
20	AL	305	BCR	C30-C25-C24	3.30	125.12	115.78
24	A1	317	LUT	C8-C7-C6	-3.30	117.94	127.20
17	A3	306	CLA	CMB-C2B-C3B	3.30	131.15	124.69
17	AA	827	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
17	A6	612	CLA	CMB-C2B-C3B	3.30	130.84	124.68
17	AB	837	CLA	CMB-C2B-C3B	3.29	130.84	124.68
17	AB	809	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
20	AB	849	BCR	C39-C30-C25	-3.29	104.96	110.30
20	AB	848	BCR	C8-C9-C10	-3.29	113.89	118.94
17	AB	801	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
17	AA	824	CLA	C4A-NA-C1A	3.29	108.18	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A6	611	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
20	AI	101	BCR	C24-C23-C22	-3.28	121.27	126.23
17	A1	314	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
20	AB	844	BCR	C4-C5-C6	-3.28	117.97	122.73
17	AA	819	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
17	A1	312	CLA	CAB-C3B-C4B	-3.28	123.42	128.46
26	A6	607	CHL	CHD-C4C-NC	3.28	129.37	124.20
17	AA	839	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
17	AB	806	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
20	AG	205	BCR	C8-C7-C6	-3.27	118.01	127.20
17	AJ	102	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
20	AB	849	BCR	C24-C25-C26	3.27	129.39	121.46
17	AA	824	CLA	CHD-C1D-ND	-3.27	121.45	124.45
20	AI	101	BCR	C39-C30-C25	-3.27	105.00	110.30
20	AB	845	BCR	C8-C9-C10	3.26	123.95	118.94
27	A4	316	XAT	C6-C7-C8	-3.26	119.10	125.99
17	AB	835	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
17	A6	613	CLA	CMB-C2B-C3B	3.26	130.78	124.68
20	AB	846	BCR	C3-C4-C5	-3.26	108.26	114.08
20	AK	205	BCR	C30-C25-C26	-3.25	118.03	122.61
20	AJ	103	BCR	C15-C16-C17	-3.25	116.81	123.47
17	AB	839	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
17	A1	307	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
17	AA	806	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
20	A1	319	BCR	C38-C26-C25	-3.25	120.88	124.53
17	AF	802	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
17	A4	311	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
17	AB	804	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
17	AB	840	CLA	CMB-C2B-C3B	3.24	130.74	124.68
26	A6	605	CHL	CAC-C3C-C4C	3.24	129.97	125.04
27	A4	316	XAT	C28-C29-C30	-3.24	113.97	118.94
17	AF	803	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
20	AK	205	BCR	C23-C22-C21	3.24	123.91	118.94
17	AA	830	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
17	AA	816	CLA	CMB-C2B-C3B	3.23	130.72	124.68
24	AF	806	LUT	C8-C7-C6	-3.23	118.12	127.20
27	A4	316	XAT	C38-C25-C26	-3.23	116.85	122.26
26	A4	305	CHL	CHC-C1C-C2C	-3.23	117.79	126.72
20	AA	846	BCR	C36-C18-C17	-3.23	118.40	122.92
27	A6	615	XAT	C15-C35-C34	-3.23	116.86	123.47
17	A4	302	CLA	CAB-C3B-C2B	3.23	131.00	124.69
20	AB	848	BCR	C38-C26-C25	-3.22	120.91	124.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A1	315	CLA	CAB-C3B-C2B	3.22	131.00	124.69
17	AK	203	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
20	A4	317	BCR	C33-C5-C6	-3.22	120.91	124.53
17	AA	822	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
26	A3	320	CHL	CHC-C1C-NC	3.22	129.08	124.20
17	A6	608	CLA	CMB-C2B-C3B	3.21	130.69	124.68
26	A6	606	CHL	CHC-C1C-NC	3.21	129.08	124.20
20	AA	849	BCR	C28-C27-C26	-3.21	108.34	114.08
26	A6	606	CHL	CHD-C4C-NC	3.21	129.26	124.20
17	AB	806	CLA	CMB-C2B-C3B	3.21	130.68	124.68
17	AA	827	CLA	CAA-CBA-CGA	-3.21	103.88	113.25
22	AA	851	LMU	O5B-C5B-C4B	3.20	115.51	109.69
27	A3	317	XAT	C35-C15-C14	-3.20	116.91	123.47
17	AB	801	CLA	CMD-C2D-C1D	-3.20	119.07	124.71
20	AA	849	BCR	C8-C9-C10	3.20	123.85	118.94
17	AA	836	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
20	AJ	101	BCR	C4-C5-C6	-3.20	118.09	122.73
26	A6	607	CHL	C4C-C3C-C2C	-3.19	102.24	106.90
17	AA	819	CLA	CMB-C2B-C3B	3.19	130.65	124.68
17	A6	609	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
17	AA	803	CLA	O2D-CGD-CBD	3.19	116.94	111.27
17	AA	811	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
20	AF	801	BCR	C30-C25-C26	-3.19	118.13	122.61
17	AL	303	CLA	CMB-C2B-C3B	3.18	130.63	124.68
17	AB	840	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
17	AA	809	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
20	AB	845	BCR	C3-C4-C5	-3.18	108.40	114.08
17	AA	817	CLA	CMB-C2B-C3B	3.18	130.63	124.68
17	AB	823	CLA	CHD-C1D-ND	-3.18	121.53	124.45
17	AB	816	CLA	CMB-C2B-C3B	3.18	130.62	124.68
26	A6	607	CHL	CHC-C1C-C2C	-3.17	117.94	126.72
17	AL	304	CLA	CMB-C2B-C1B	-3.17	123.58	128.46
17	AA	824	CLA	CBA-CAA-C2A	3.17	123.23	113.86
17	AA	815	CLA	CMB-C2B-C3B	3.17	130.61	124.68
17	A4	308	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
17	A3	309	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
17	A4	313	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
17	AB	821	CLA	CMB-C2B-C3B	3.17	130.60	124.68
17	AB	842	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
17	AA	807	CLA	CHD-C1D-ND	-3.16	121.55	124.45
17	AB	838	CLA	CMB-C2B-C3B	3.16	130.60	124.68
17	AA	819	CLA	C1B-CHB-C4A	-3.16	123.86	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	829	CLA	C2D-C1D-ND	-3.16	107.77	110.10
17	AB	804	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
17	AA	812	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
17	AB	836	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
17	AB	812	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
20	AK	205	BCR	C29-C30-C25	3.16	115.34	110.48
17	AA	818	CLA	CMB-C2B-C3B	3.16	130.58	124.68
18	AA	843	PQN	C14-C13-C12	-3.16	115.58	123.68
26	A4	304	CHL	C1C-C2C-C3C	-3.15	104.61	107.11
17	AG	204	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
17	AA	815	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
27	A1	318	XAT	C40-C33-C32	3.15	123.05	118.08
17	A3	311	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
17	A1	307	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
20	AA	848	BCR	C33-C5-C6	-3.15	120.99	124.53
17	A1	316	CLA	CAB-C3B-C2B	3.15	130.85	124.69
17	AB	801	CLA	CHB-C4A-NA	3.15	128.86	124.51
17	A1	316	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
24	A3	316	LUT	C3-C4-C5	-3.14	105.59	111.85
20	AB	849	BCR	C4-C5-C6	-3.13	118.18	122.73
26	A3	320	CHL	C1-C2-C3	-3.13	120.62	126.04
17	AB	828	CLA	CHB-C4A-NA	3.13	128.84	124.51
17	AB	806	CLA	CHB-C4A-NA	3.13	128.84	124.51
17	AB	817	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
17	AB	825	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
17	AB	808	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
17	AA	823	CLA	C4A-NA-C1A	3.13	108.11	106.71
27	A1	318	XAT	C39-C29-C28	3.12	123.00	118.08
17	AA	834	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
17	A1	310	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
20	AJ	103	BCR	C7-C8-C9	-3.12	121.52	126.23
17	A3	314	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
17	AB	825	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
20	AB	844	BCR	C33-C5-C6	3.12	128.03	124.53
17	A4	303	CLA	CAB-C3B-C2B	3.12	130.79	124.69
17	AB	828	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
17	AB	817	CLA	CHD-C1D-ND	-3.11	121.59	124.45
17	A1	304	CLA	CAC-C3C-C4C	3.11	128.85	124.81
17	AL	303	CLA	CHD-C1D-ND	-3.11	121.60	124.45
17	AA	831	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
17	A6	604	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
17	AB	818	CLA	O2D-CGD-O1D	-3.11	117.77	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A1	308	CHL	C1C-C2C-C3C	-3.10	104.65	107.11
17	AB	817	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
17	A4	303	CLA	CMB-C2B-C3B	3.10	130.76	124.69
17	AA	808	CLA	CMB-C2B-C3B	3.10	130.48	124.68
17	A3	306	CLA	CAB-C3B-C2B	3.10	130.76	124.69
17	AA	834	CLA	C4-C3-C5	3.10	120.48	115.27
17	AB	814	CLA	CMB-C2B-C3B	3.10	130.47	124.68
17	AB	815	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
17	AB	818	CLA	CHB-C4A-NA	3.09	128.78	124.51
17	AA	832	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
20	AA	849	BCR	C2-C3-C4	-3.09	104.48	111.38
17	A4	301	CLA	CMB-C2B-C3B	3.09	130.45	124.68
17	AB	839	CLA	C1B-CHB-C4A	-3.09	124.01	130.12
20	AB	844	BCR	C30-C25-C26	-3.09	118.27	122.61
20	A1	319	BCR	C33-C5-C4	3.08	119.54	113.62
20	AB	846	BCR	C1-C6-C5	-3.08	118.27	122.61
17	AA	841	CLA	CHB-C4A-NA	3.08	128.78	124.51
24	A6	614	LUT	C8-C9-C10	-3.08	114.21	118.94
17	AA	821	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
17	A6	602	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
17	A4	312	CLA	CHD-C1D-ND	-3.08	121.62	124.45
17	AA	813	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
17	A4	301	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
17	AA	828	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
17	A4	312	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
17	AA	804	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
17	A6	608	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
17	AB	810	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
17	AB	818	CLA	CMB-C2B-C3B	3.07	130.43	124.68
17	AB	807	CLA	CHD-C1D-ND	-3.07	121.63	124.45
24	AF	806	LUT	C37-C21-C36	3.07	112.42	107.89
17	A6	601	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
26	A6	607	CHL	CHA-C4D-ND	3.06	138.91	132.50
17	AA	810	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
26	A1	308	CHL	CHD-C4C-NC	3.06	129.03	124.20
17	AA	829	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
17	AA	828	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
17	AA	842	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
20	AK	202	BCR	C36-C18-C17	-3.05	118.65	122.92
17	A6	604	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
17	AB	819	CLA	C6-C5-C3	3.05	121.44	113.45
17	AB	829	CLA	C1B-CHB-C4A	-3.05	124.08	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A3	313	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
20	AB	846	BCR	C8-C9-C10	3.05	123.61	118.94
20	AF	801	BCR	C37-C22-C21	-3.04	118.66	122.92
17	A6	602	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
17	A3	308	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
18	AA	843	PQN	O1-C1-C2	-3.04	116.31	120.25
17	AB	803	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
17	AA	836	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
27	A4	316	XAT	C26-C27-C28	-3.04	119.57	125.99
17	AB	802	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
17	AB	809	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
17	A4	309	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
17	A4	309	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
17	A1	306	CLA	CMB-C2B-C3B	3.03	130.34	124.68
20	AF	805	BCR	C36-C18-C19	3.02	122.84	118.08
20	AL	306	BCR	C36-C18-C19	3.02	122.84	118.08
20	AL	306	BCR	C30-C25-C26	-3.02	118.36	122.61
17	AA	817	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
17	AB	804	CLA	CMB-C2B-C3B	3.02	130.33	124.68
17	AA	807	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
17	AB	808	CLA	CMB-C2B-C3B	3.02	130.33	124.68
20	AJ	101	BCR	C37-C22-C21	-3.02	118.69	122.92
17	AA	834	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
17	A1	314	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
24	A4	315	LUT	C39-C29-C28	3.01	122.83	118.08
17	A1	305	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
20	AB	844	BCR	C32-C1-C6	-3.01	105.42	110.30
26	A1	308	CHL	CHC-C1C-NC	3.01	128.77	124.20
17	AA	805	CLA	CHD-C1D-ND	-3.01	121.69	124.45
26	A6	605	CHL	CHC-C1C-NC	3.01	128.76	124.20
17	A3	309	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
17	A3	313	CLA	CMB-C2B-C3B	3.00	130.30	124.68
20	AJ	101	BCR	C36-C18-C19	3.00	122.81	118.08
17	AA	806	CLA	CHB-C4A-NA	3.00	128.66	124.51
27	A1	318	XAT	C12-C13-C14	-3.00	114.34	118.94
17	AB	819	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
17	AL	304	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
17	AB	803	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
20	AA	848	BCR	C30-C25-C26	-3.00	118.39	122.61
17	A6	603	CLA	CMB-C2B-C3B	3.00	130.28	124.68
17	A1	310	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
17	A3	308	CLA	CMB-C2B-C3B	2.99	130.28	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A3	311	CLA	CMB-C2B-C3B	2.99	130.28	124.68
17	AB	820	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
17	A4	309	CLA	CMB-C2B-C3B	2.99	130.28	124.68
17	A6	610	CLA	O2D-CGD-CBD	2.99	116.58	111.27
17	AA	821	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
17	AA	820	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
17	A4	312	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
17	AL	303	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
17	AH	201	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
26	A6	606	CHL	C1C-C2C-C3C	-2.98	104.75	107.11
17	A3	303	CLA	CMB-C2B-C3B	2.98	130.26	124.68
17	AB	829	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
17	A4	307	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
17	A4	303	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
17	AA	820	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
20	A3	318	BCR	C24-C23-C22	-2.98	121.73	126.23
17	AA	812	CLA	C4-C3-C5	2.98	120.28	115.27
17	AB	842	CLA	CMB-C2B-C3B	2.97	130.24	124.68
17	AA	804	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
17	A3	310	CLA	CBD-CHA-C1A	2.97	132.19	127.43
19	AA	844	LHG	O7-C7-C8	2.97	117.90	111.50
17	AA	841	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
17	AB	811	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
17	AB	812	CLA	CAB-C3B-C2B	2.97	130.50	124.69
20	AI	101	BCR	C38-C26-C27	2.97	119.31	113.62
17	A4	311	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
17	AA	835	CLA	CMB-C2B-C3B	2.97	130.23	124.68
24	A3	316	LUT	C16-C1-C6	2.97	115.11	110.30
17	AB	826	CLA	C4A-NA-C1A	2.96	108.04	106.71
17	A3	305	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
17	AA	805	CLA	CAA-C2A-C1A	-2.96	102.27	111.97
24	A4	315	LUT	C28-C29-C30	-2.96	114.40	118.94
17	AB	825	CLA	CMB-C2B-C3B	2.96	130.22	124.68
17	AA	818	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
17	AA	822	CLA	O2D-CGD-CBD	2.96	116.53	111.27
17	AB	823	CLA	CHB-C4A-NA	2.95	128.60	124.51
26	A4	314	CHL	C4A-NA-C1A	-2.95	105.38	106.71
17	A1	313	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
26	A4	306	CHL	C1D-ND-C4D	2.95	108.43	106.33
17	A3	302	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
17	AA	834	CLA	CHD-C1D-ND	-2.95	121.74	124.45
17	AB	835	CLA	CHD-C1D-ND	-2.95	121.74	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AL	302	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
24	A6	614	LUT	C21-C26-C27	-2.95	108.97	112.70
17	A1	312	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
17	AB	801	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
17	A6	601	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
20	AA	849	BCR	C30-C25-C26	-2.94	118.47	122.61
17	AA	816	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
17	AB	824	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
17	A3	312	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
17	AB	826	CLA	CHD-C1D-ND	-2.94	121.75	124.45
17	AA	813	CLA	CMB-C2B-C3B	2.94	130.17	124.68
17	A1	310	CLA	CAB-C3B-C2B	2.93	130.44	124.69
20	AJ	101	BCR	C16-C15-C14	-2.93	117.46	123.47
20	AK	202	BCR	C24-C23-C22	-2.93	121.80	126.23
17	A1	307	CLA	CMB-C2B-C3B	2.93	130.16	124.68
17	A6	613	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
20	AB	848	BCR	C28-C27-C26	-2.93	108.84	114.08
17	AB	820	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
20	AL	306	BCR	C37-C22-C21	-2.93	118.82	122.92
26	A1	303	CHL	CHC-C1C-NC	2.93	128.65	124.20
27	A4	316	XAT	O4-C5-C18	2.93	118.57	115.06
17	A3	304	CLA	CMB-C2B-C3B	2.93	130.42	124.69
26	A1	308	CHL	CHA-C4D-ND	2.93	138.62	132.50
17	AA	824	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
17	AA	810	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
17	A3	303	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
17	AA	806	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
17	AA	835	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
27	A6	615	XAT	C20-C13-C12	2.92	122.69	118.08
17	AF	802	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
17	AF	803	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
20	AB	849	BCR	C36-C18-C19	2.92	122.68	118.08
17	AA	809	CLA	CHB-C4A-NA	2.92	128.56	124.51
20	AB	846	BCR	C33-C5-C4	2.92	119.23	113.62
17	A1	306	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
17	A1	315	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
17	AA	827	CLA	CMB-C2B-C3B	2.92	130.14	124.68
17	AB	811	CLA	CMB-C2B-C3B	2.92	130.14	124.68
20	AA	847	BCR	C37-C22-C21	-2.92	118.83	122.92
17	A1	309	CLA	CMB-C2B-C3B	2.92	130.14	124.68
20	A4	317	BCR	C15-C16-C17	-2.92	117.50	123.47
26	A4	304	CHL	CHC-C1C-NC	2.92	128.63	124.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	838	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
20	AL	305	BCR	C4-C5-C6	-2.91	118.50	122.73
17	AA	815	CLA	C1B-CHB-C4A	-2.91	124.34	130.12
17	A4	303	CLA	C1B-CHB-C4A	-2.91	124.34	130.12
27	A6	615	XAT	C12-C13-C14	-2.91	114.47	118.94
17	AB	814	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
20	AA	845	BCR	C37-C22-C23	2.91	122.66	118.08
26	A6	607	CHL	C3A-C2A-C1A	-2.91	96.98	101.34
17	A1	315	CLA	CMB-C2B-C3B	2.91	130.38	124.69
17	AA	811	CLA	CMB-C2B-C3B	2.91	130.12	124.68
17	AA	831	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
17	A4	310	CLA	CMB-C2B-C3B	2.91	130.11	124.68
20	A3	318	BCR	C37-C22-C23	2.90	122.65	118.08
17	AB	836	CLA	CMB-C2B-C3B	2.90	130.10	124.68
20	AA	846	BCR	C35-C13-C12	2.90	122.65	118.08
26	A3	307	CHL	C4C-C3C-C2C	-2.90	102.67	106.90
17	A1	305	CLA	C5-C3-C2	2.90	126.99	121.12
17	AA	823	CLA	CHD-C1D-ND	-2.90	121.79	124.45
17	AK	203	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
20	AA	846	BCR	C31-C1-C6	-2.90	105.60	110.30
17	AB	808	CLA	CHD-C1D-ND	-2.90	121.79	124.45
17	AB	812	CLA	CMB-C2B-C3B	2.90	130.36	124.69
17	AB	828	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
17	AJ	102	CLA	CMB-C2B-C3B	2.90	130.10	124.68
17	AK	204	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
20	AB	844	BCR	C16-C15-C14	-2.89	117.54	123.47
17	A1	316	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
17	A6	612	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
17	AB	820	CLA	C4A-NA-C1A	2.89	108.01	106.71
20	AA	847	BCR	C10-C11-C12	2.89	132.24	123.22
20	AJ	101	BCR	C8-C9-C10	-2.89	114.51	118.94
17	AG	203	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
17	AB	834	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
17	A3	310	CLA	CMB-C2B-C3B	2.88	130.07	124.68
17	AB	824	CLA	CBA-CAA-C2A	2.88	120.10	114.02
20	AA	848	BCR	C23-C22-C21	-2.88	114.52	118.94
20	AA	847	BCR	C32-C1-C6	-2.88	105.62	110.30
26	A4	306	CHL	CHA-C4D-ND	2.88	138.53	132.50
22	AA	851	LMU	C3B-C4B-C5B	2.88	115.37	110.24
17	AB	813	CLA	CMB-C2B-C3B	2.88	130.06	124.68
17	AA	813	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
17	A6	604	CLA	C1B-CHB-C4A	-2.88	124.42	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	822	CLA	CMB-C2B-C3B	2.88	130.06	124.68
17	AA	809	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
17	AB	805	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
20	AB	844	BCR	C40-C30-C25	-2.87	105.64	110.30
17	AB	841	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
17	AB	832	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
26	A3	320	CHL	CHA-C4D-ND	2.87	138.51	132.50
20	A6	616	BCR	C1-C6-C5	-2.87	118.57	122.61
27	A3	317	XAT	C8-C9-C10	-2.87	114.54	118.94
17	A1	304	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
17	AA	813	CLA	CHB-C4A-NA	2.86	128.47	124.51
17	AA	826	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
24	A1	317	LUT	C28-C29-C30	-2.86	114.55	118.94
20	AA	849	BCR	C20-C21-C22	-2.86	123.23	127.31
17	AB	816	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
17	AB	802	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
17	AA	823	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
20	A3	318	BCR	C29-C30-C25	2.86	114.88	110.48
17	AA	811	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
17	A1	309	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
20	AJ	103	BCR	C34-C9-C8	2.86	122.58	118.08
17	AB	827	CLA	CHB-C4A-NA	2.86	128.46	124.51
26	A3	320	CHL	O2A-CGA-CBA	2.86	120.87	111.91
17	AA	834	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
17	AB	838	CLA	CHD-C1D-ND	-2.85	121.83	124.45
20	A4	317	BCR	C27-C26-C25	-2.85	118.59	122.73
18	AA	843	PQN	C16-C15-C13	-2.85	105.98	113.45
17	A4	302	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
17	A4	311	CLA	CMB-C2B-C3B	2.85	130.00	124.68
17	AA	824	CLA	CMB-C2B-C3B	2.84	130.00	124.68
17	AB	801	CLA	O2D-CGD-CBD	2.84	116.32	111.27
26	A3	307	CHL	CHA-C4D-ND	2.84	138.45	132.50
17	A3	306	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	A6	607	CHL	O2A-CGA-CBA	2.84	120.83	111.91
17	AA	804	CLA	CHB-C4A-NA	2.84	128.44	124.51
26	A3	320	CHL	C4-C3-C5	2.84	120.05	115.27
17	AB	834	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
17	A1	312	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
17	AA	801	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
17	AB	808	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
17	A6	609	CLA	CMB-C2B-C3B	2.84	129.99	124.68
17	A1	307	CLA	O2D-CGD-CBD	2.84	116.31	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	832	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
17	A3	310	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
26	A4	314	CHL	CHA-C4D-ND	2.83	138.42	132.50
17	A4	301	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
17	AA	828	CLA	C14-C13-C15	2.83	121.52	111.29
26	A3	320	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
24	A6	614	LUT	C28-C29-C30	-2.83	114.61	118.94
17	AJ	102	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
17	AB	834	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
17	AA	831	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
17	AB	831	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
17	AB	838	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
17	AB	825	CLA	CHB-C4A-NA	2.82	128.41	124.51
20	AF	805	BCR	C12-C13-C14	2.82	123.27	118.94
24	A1	317	LUT	C1-C6-C5	-2.82	118.64	122.61
17	AA	812	CLA	CMB-C2B-C3B	2.82	129.95	124.68
17	A6	612	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	A6	605	CHL	CHA-C4D-ND	2.82	138.40	132.50
17	A6	609	CLA	CHB-C4A-NA	2.82	128.41	124.51
17	AB	821	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	AG	204	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
20	AB	847	BCR	C38-C26-C27	2.82	119.03	113.62
25	A1	321	LMG	C8-O7-C10	-2.82	110.86	117.79
17	A3	312	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
20	AB	847	BCR	C15-C16-C17	-2.82	117.70	123.47
17	A4	308	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
17	AB	805	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	A3	307	CHL	C2C-C1C-NC	2.81	112.61	109.97
26	A6	606	CHL	CHA-C4D-ND	2.81	138.38	132.50
17	A4	302	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
17	A6	613	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
20	AB	849	BCR	C16-C17-C18	-2.81	123.30	127.31
17	AA	804	CLA	CHD-C1D-ND	-2.81	121.87	124.45
20	AF	801	BCR	C16-C15-C14	-2.81	117.72	123.47
17	A3	306	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
17	AA	806	CLA	CMB-C2B-C3B	2.81	129.93	124.68
20	AA	848	BCR	C7-C8-C9	-2.80	122.00	126.23
17	AB	807	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	A4	304	CHL	CHA-C4D-ND	2.80	138.36	132.50
17	AL	304	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
17	A3	304	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
17	A3	309	CLA	O2D-CGD-O1D	-2.80	118.36	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A3	312	CLA	O2D-CGD-O1D	-2.80	117.73	124.09
19	AJ	104	LHG	O8-C23-C24	2.80	120.69	111.91
26	A1	303	CHL	O2A-CGA-O1A	-2.80	116.53	123.59
17	AB	829	CLA	C2D-C1D-ND	-2.80	108.04	110.10
26	A1	303	CHL	CHA-C4D-ND	2.80	138.35	132.50
17	AA	842	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
25	A1	321	LMG	C7-O1-C1	2.79	119.20	113.74
17	A6	602	CLA	CMB-C2B-C3B	2.79	129.90	124.68
20	AA	849	BCR	C23-C22-C21	-2.79	114.66	118.94
17	AB	831	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
17	AA	818	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
17	AB	820	CLA	CMB-C2B-C3B	2.79	129.90	124.68
20	AA	845	BCR	C16-C15-C14	-2.79	117.76	123.47
17	AA	831	CLA	CHD-C1D-ND	-2.79	121.89	124.45
17	AB	824	CLA	CMB-C2B-C3B	2.79	129.90	124.68
17	A3	314	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
17	A1	304	CLA	CMB-C2B-C3B	2.79	129.89	124.68
20	AA	846	BCR	C38-C26-C27	2.79	118.97	113.62
17	AB	803	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
20	AA	846	BCR	C40-C30-C25	-2.78	105.78	110.30
17	AG	204	CLA	CHB-C4A-NA	2.78	128.36	124.51
20	AK	205	BCR	C36-C18-C17	-2.78	119.02	122.92
17	AA	805	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
17	AA	810	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
27	A4	316	XAT	C18-C5-C6	-2.78	117.60	122.26
17	A3	312	CLA	CHD-C1D-ND	-2.78	121.90	124.45
17	A4	309	CLA	CHB-C4A-NA	2.78	128.36	124.51
17	A1	310	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
20	AB	849	BCR	C37-C22-C21	-2.78	119.03	122.92
17	A1	304	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	AB	833	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
17	AB	823	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
17	A1	311	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
20	A6	616	BCR	C1-C6-C7	2.77	123.62	115.78
17	A1	315	CLA	O2D-CGD-O1D	-2.77	117.80	124.09
17	A6	602	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
17	AG	201	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
25	AG	202	LMG	O8-C28-C29	2.77	120.60	111.91
20	A3	318	BCR	C36-C18-C19	2.77	122.44	118.08
24	AF	806	LUT	C38-C25-C24	-2.77	117.64	123.56
17	AB	813	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
17	A1	305	CLA	C1B-CHB-C4A	-2.76	124.64	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AK	205	BCR	C40-C30-C25	-2.76	105.82	110.30
17	A1	314	CLA	CMB-C2B-C3B	2.76	129.84	124.68
17	AA	809	CLA	C2A-C1A-CHA	2.76	128.69	123.86
24	A1	317	LUT	C39-C29-C28	2.76	122.43	118.08
17	AA	823	CLA	CMB-C2B-C3B	2.76	129.84	124.68
17	AA	825	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	AK	204	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
26	A4	305	CHL	CHA-C4D-ND	2.76	138.27	132.50
20	A4	317	BCR	C1-C6-C7	2.76	123.58	115.78
17	A4	313	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
19	AJ	104	LHG	O7-C7-C8	2.75	117.44	111.50
17	AB	815	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
17	A3	311	CLA	CHB-C4A-NA	2.75	128.32	124.51
17	A6	602	CLA	CHB-C4A-NA	2.75	128.32	124.51
17	AG	201	CLA	CMB-C2B-C3B	2.75	129.83	124.68
20	AI	101	BCR	C16-C15-C14	-2.75	117.84	123.47
24	A6	614	LUT	C1-C6-C5	-2.75	118.74	122.61
24	A4	315	LUT	C37-C21-C22	-2.75	104.23	109.44
20	AI	101	BCR	C20-C21-C22	-2.75	123.39	127.31
17	AB	801	CLA	C1-O2A-CGA	2.75	123.65	116.44
17	AB	836	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	A4	314	CHL	CAC-C3C-C4C	2.75	128.37	124.81
20	A3	318	BCR	C23-C22-C21	-2.75	114.73	118.94
20	AA	848	BCR	C38-C26-C27	2.75	118.89	113.62
17	AA	812	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
20	A4	317	BCR	C12-C13-C14	-2.74	114.73	118.94
20	AG	205	BCR	C37-C22-C23	2.74	122.40	118.08
17	AA	801	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
24	A3	316	LUT	C40-C33-C32	2.74	122.39	118.08
17	A6	610	CLA	C1A-CHA-C4D	-2.74	121.89	125.72
17	AK	203	CLA	CMB-C2B-C3B	2.74	129.80	124.68
17	A4	312	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
17	AB	822	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
20	AA	847	BCR	C7-C6-C5	2.74	128.09	121.46
17	AB	832	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
17	AA	837	CLA	CHB-C4A-NA	2.74	128.30	124.51
17	AB	821	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
17	AA	809	CLA	CMB-C2B-C3B	2.73	129.79	124.68
17	A1	307	CLA	CAC-C3C-C4C	2.73	128.35	124.81
17	AA	817	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
17	AH	201	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
20	AB	845	BCR	C16-C15-C14	-2.73	117.88	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A3	302	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
17	AA	839	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
20	A1	319	BCR	C23-C22-C21	-2.73	114.75	118.94
17	A3	315	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
17	AF	804	CLA	CMB-C2B-C3B	2.73	129.78	124.68
17	AA	834	CLA	CHB-C4A-NA	2.73	128.28	124.51
17	AF	802	CLA	CMB-C2B-C3B	2.73	129.78	124.68
20	AB	848	BCR	C1-C6-C5	-2.73	118.78	122.61
17	AA	814	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
17	AA	812	CLA	CHD-C1D-ND	-2.72	121.95	124.45
17	A3	305	CLA	CHD-C1D-ND	-2.72	121.95	124.45
20	AF	801	BCR	C8-C9-C10	-2.72	114.77	118.94
22	AB	853	LMU	C2'-C3'-C4'	2.72	115.89	109.68
17	AB	810	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
20	AL	306	BCR	C3-C4-C5	-2.72	109.23	114.08
24	A4	315	LUT	C40-C33-C32	2.72	122.36	118.08
26	A4	314	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
17	A3	305	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
17	AL	302	CLA	CMB-C2B-C3B	2.72	129.76	124.68
17	AA	802	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
20	AB	848	BCR	C8-C7-C6	-2.71	119.59	127.20
17	AK	203	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
17	A6	611	CLA	CMB-C2B-C3B	2.71	129.75	124.68
27	A6	615	XAT	C40-C33-C34	-2.71	119.13	122.92
27	A6	615	XAT	C10-C11-C12	-2.71	114.77	123.22
17	A6	610	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
17	AB	809	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
26	A4	306	CHL	C3D-C2D-C1D	-2.71	102.14	105.83
20	AB	845	BCR	C38-C26-C25	2.70	127.56	124.53
17	AA	842	CLA	CMB-C2B-C3B	2.70	129.74	124.68
27	A4	316	XAT	C8-C9-C10	-2.70	114.79	118.94
20	AB	845	BCR	C30-C25-C26	-2.70	118.81	122.61
20	AB	849	BCR	C30-C25-C26	-2.70	118.81	122.61
17	A6	613	CLA	CHD-C1D-ND	-2.70	121.97	124.45
17	A1	314	CLA	O2D-CGD-O1D	-2.70	117.96	124.09
17	A6	602	CLA	CAC-C3C-C4C	2.70	128.31	124.81
20	AI	101	BCR	C30-C25-C26	-2.70	118.81	122.61
20	A6	616	BCR	C27-C26-C25	-2.70	118.81	122.73
20	AJ	103	BCR	C3-C4-C5	-2.69	109.27	114.08
17	AA	840	CLA	CHB-C4A-NA	2.69	128.24	124.51
17	A6	604	CLA	CMB-C2B-C3B	2.69	129.72	124.68
20	AB	844	BCR	C8-C9-C10	-2.69	114.81	118.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AJ	102	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
27	A1	318	XAT	O24-C25-C38	2.69	118.28	115.06
17	AB	816	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
17	AF	804	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
17	A3	315	CLA	O2D-CGD-O1D	-2.69	117.99	124.09
20	A6	616	BCR	C2-C3-C4	-2.69	105.37	111.38
17	AB	811	CLA	O1D-CGD-CBD	2.69	129.98	124.48
17	AH	201	CLA	C4-C3-C5	2.69	119.79	115.27
17	AA	805	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
22	AB	850	LMU	C3B-C4B-C5B	2.68	115.03	110.24
20	AJ	103	BCR	C7-C6-C5	2.68	127.97	121.46
20	AB	848	BCR	C37-C22-C23	2.68	122.30	118.08
17	AG	201	CLA	CHD-C1D-ND	-2.68	121.99	124.45
17	A1	311	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
17	AA	805	CLA	CMC-C2C-C1C	-2.68	120.96	125.04
20	AL	306	BCR	C37-C22-C23	2.68	122.30	118.08
17	AL	302	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
17	A1	305	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
18	AA	843	PQN	C12-C11-C3	-2.68	104.82	112.05
17	AA	822	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	A6	608	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
17	A1	313	CLA	CHB-C4A-NA	2.68	128.21	124.51
20	AB	849	BCR	C23-C24-C25	2.68	134.72	127.20
20	AA	847	BCR	C35-C13-C12	2.67	122.29	118.08
17	AB	835	CLA	CHB-C4A-NA	2.67	128.21	124.51
17	AA	832	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
22	AL	301	LMU	O5B-C5B-C4B	2.67	114.54	109.69
17	AF	802	CLA	CHB-C4A-NA	2.67	128.20	124.51
17	AB	840	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	AA	840	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
17	A1	309	CLA	O2D-CGD-O1D	-2.67	118.03	124.09
17	AA	833	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
17	A4	310	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
17	A6	601	CLA	CMB-C2B-C3B	2.67	129.67	124.68
17	AA	823	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
17	AA	808	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
17	AA	814	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
17	A3	302	CLA	CMB-C2B-C3B	2.66	129.66	124.68
17	AA	819	CLA	CHB-C4A-NA	2.66	128.19	124.51
17	A3	303	CLA	C5-C3-C2	2.66	126.50	121.12
17	AA	840	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
17	A3	314	CLA	CMB-C2B-C3B	2.66	129.66	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A3	309	CLA	CMB-C2B-C3B	2.66	129.65	124.68
17	AB	837	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
19	A1	320	LHG	O7-C7-C8	2.66	117.23	111.50
17	AG	203	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
17	A1	315	CLA	CHD-C1D-ND	-2.66	122.01	124.45
17	AB	814	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
17	A4	302	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
17	AB	826	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
20	AB	848	BCR	C20-C21-C22	-2.65	123.53	127.31
17	AA	841	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
17	AA	803	CLA	CAC-C3C-C4C	2.65	128.25	124.81
20	AA	848	BCR	C40-C30-C25	-2.65	106.00	110.30
17	AB	842	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
17	A3	303	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
17	AB	802	CLA	CAB-C3B-C4B	-2.64	124.41	128.46
17	AB	829	CLA	C4A-NA-C1A	2.64	107.89	106.71
17	AA	829	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	AB	801	CLA	CMB-C2B-C3B	2.64	129.62	124.68
20	A6	616	BCR	C23-C22-C21	-2.64	114.89	118.94
17	AA	824	CLA	C6-C5-C3	2.64	120.37	113.45
17	A3	302	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
20	AJ	103	BCR	C19-C18-C17	-2.63	114.90	118.94
20	AB	847	BCR	C39-C30-C25	-2.63	106.03	110.30
17	AA	840	CLA	CMB-C2B-C3B	2.63	129.60	124.68
17	AB	822	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
20	AA	846	BCR	C8-C9-C10	-2.63	114.90	118.94
20	AF	805	BCR	C23-C22-C21	-2.63	114.90	118.94
17	AK	201	CLA	CAA-C2A-C3A	-2.63	109.96	116.10
20	AB	848	BCR	C15-C14-C13	-2.63	123.56	127.31
17	AK	201	CLA	C4B-CHC-C1C	-2.63	125.58	129.64
17	A4	311	CLA	O2D-CGD-O1D	-2.63	118.12	124.09
17	AB	830	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
17	AB	824	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
17	AA	824	CLA	O2D-CGD-O1D	-2.63	118.12	124.09
17	A4	307	CLA	CMB-C2B-C3B	2.63	129.59	124.68
17	A3	311	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
17	A4	310	CLA	CHB-C4A-NA	2.63	128.14	124.51
17	A1	314	CLA	CHB-C4A-NA	2.62	128.14	124.51
26	A1	303	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
17	A1	311	CLA	CHB-C4A-NA	2.62	128.14	124.51
17	A4	308	CLA	CHB-C4A-NA	2.62	128.14	124.51
20	AL	305	BCR	C37-C22-C21	-2.62	119.25	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A6	610	CLA	CMB-C2B-C3B	2.62	129.82	124.69
20	AA	847	BCR	C8-C9-C10	-2.62	114.92	118.94
17	AA	842	CLA	CHB-C4A-NA	2.62	128.13	124.51
17	AA	820	CLA	CMB-C2B-C3B	2.62	129.58	124.68
23	AB	851	DGD	O1G-C1A-C2A	2.62	120.13	111.91
20	AA	846	BCR	C20-C21-C22	-2.62	123.57	127.31
27	A6	615	XAT	C39-C29-C30	-2.62	119.26	122.92
24	AF	806	LUT	C1-C6-C5	-2.62	118.93	122.61
17	A6	603	CLA	O2D-CGD-O1D	-2.62	118.15	124.09
17	AA	833	CLA	C4-C3-C2	-2.62	116.96	123.68
17	AL	304	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	AA	847	BCR	C3-C4-C5	-2.62	109.41	114.08
20	AB	844	BCR	C31-C1-C6	2.61	114.54	110.30
17	AA	835	CLA	O2D-CGD-O1D	-2.61	118.15	124.09
17	AA	808	CLA	CHD-C1D-ND	-2.61	122.05	124.45
17	AB	804	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
17	A1	316	CLA	CHD-C1D-ND	-2.61	122.05	124.45
17	A1	313	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
17	AA	828	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	AB	844	BCR	C36-C18-C19	2.61	122.19	118.08
17	AB	801	CLA	CMD-C2D-C3D	2.61	133.62	127.61
17	AA	814	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
20	AI	101	BCR	C36-C18-C17	-2.61	119.27	122.92
26	A6	605	CHL	C1C-C2C-C3C	-2.61	105.05	107.11
19	A1	320	LHG	O8-C23-C24	2.61	120.08	111.91
17	A3	302	CLA	C6-C5-C3	2.60	120.28	113.45
17	A6	611	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
17	AB	808	CLA	O2D-CGD-CBD	2.60	115.89	111.27
17	AK	201	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
17	AB	806	CLA	CHD-C1D-ND	-2.60	122.06	124.45
17	A3	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
17	A3	313	CLA	O2D-CGD-O1D	-2.60	118.19	124.09
17	A4	302	CLA	CAC-C3C-C4C	2.60	128.18	124.81
17	AF	804	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
17	AB	802	CLA	CHB-C4A-NA	2.60	128.10	124.51
20	AA	849	BCR	C24-C23-C22	-2.60	122.31	126.23
17	AA	838	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
17	AB	804	CLA	CBC-CAC-C3C	2.59	119.58	112.43
17	AA	801	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
24	A3	316	LUT	C2-C3-C4	-2.59	106.75	110.30
17	AB	809	CLA	O2D-CGD-CBD	2.59	115.87	111.27
17	A1	314	CLA	CHD-C1D-ND	-2.59	122.07	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A1	316	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
17	AA	827	CLA	CHB-C4A-NA	2.59	128.09	124.51
17	AB	836	CLA	CHD-C1D-ND	-2.59	122.08	124.45
26	A1	303	CHL	C4-C3-C5	2.59	118.94	115.98
17	AB	841	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
17	AA	817	CLA	C4-C3-C2	-2.59	117.05	123.68
17	AA	808	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
17	A3	305	CLA	O2D-CGD-O1D	-2.58	118.22	124.09
17	A1	310	CLA	CMB-C2B-C3B	2.58	129.75	124.69
17	AB	812	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
17	AA	834	CLA	CMC-C2C-C1C	-2.58	121.11	125.04
17	AB	806	CLA	CMC-C2C-C1C	-2.58	121.11	125.04
17	AG	203	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
20	AF	801	BCR	C12-C13-C14	-2.58	114.98	118.94
27	A1	318	XAT	C26-C27-C28	-2.58	120.54	125.99
20	AA	846	BCR	C30-C25-C26	-2.58	118.98	122.61
17	A3	312	CLA	C4-C3-C5	2.58	119.61	115.27
17	AG	204	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
17	AA	803	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
17	AL	303	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
17	AB	830	CLA	C1B-CHB-C4A	-2.58	125.02	130.12
17	AB	842	CLA	C6-C5-C3	2.57	120.21	113.45
20	AF	801	BCR	C24-C25-C26	2.57	127.70	121.46
17	A4	312	CLA	CMB-C2B-C3B	2.57	129.49	124.68
17	AA	812	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	AB	850	LMU	O5B-C5B-C4B	2.57	114.36	109.69
25	A4	318	LMG	O7-C10-O9	-2.57	117.49	123.70
20	AI	101	BCR	C15-C16-C17	-2.57	118.21	123.47
17	AB	811	CLA	CHB-C4A-NA	2.57	128.06	124.51
17	AA	834	CLA	CMB-C2B-C3B	2.57	129.48	124.68
20	AB	847	BCR	C36-C18-C17	-2.57	119.33	122.92
17	A1	307	CLA	CHB-C4A-NA	2.57	128.06	124.51
17	AB	806	CLA	C1B-CHB-C4A	-2.57	125.04	130.12
20	AL	305	BCR	C31-C1-C6	2.56	114.46	110.30
20	AB	849	BCR	C33-C5-C4	2.56	118.54	113.62
17	AA	815	CLA	CHB-C4A-NA	2.56	128.06	124.51
17	A6	601	CLA	CHB-C4A-NA	2.56	128.05	124.51
17	AB	819	CLA	CHD-C1D-ND	-2.56	122.10	124.45
17	AA	840	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
17	A6	611	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
17	AA	832	CLA	CHD-C1D-ND	-2.56	122.11	124.45
24	A3	316	LUT	C38-C25-C24	-2.56	118.09	123.56

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A4	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
17	AL	303	CLA	CBA-CAA-C2A	2.55	121.39	113.86
20	AJ	103	BCR	C38-C26-C25	-2.55	121.66	124.53
17	AB	834	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	AF	805	BCR	C33-C5-C6	-2.55	121.67	124.53
17	A1	306	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
17	AB	831	CLA	CHD-C1D-ND	-2.55	122.11	124.45
17	AB	833	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
17	A1	307	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
27	A3	317	XAT	C36-C21-C22	-2.54	104.57	108.98
20	AB	845	BCR	C19-C18-C17	-2.54	115.04	118.94
17	AA	832	CLA	CMB-C2B-C3B	2.54	129.43	124.68
17	AL	304	CLA	CMB-C2B-C3B	2.54	129.43	124.68
17	AH	201	CLA	CHB-C4A-NA	2.54	128.03	124.51
24	A1	317	LUT	C37-C21-C36	2.54	111.64	107.89
17	AA	813	CLA	O2A-C1-C2	-2.54	101.96	108.64
17	A1	304	CLA	CHD-C1D-ND	-2.54	122.12	124.45
17	AA	819	CLA	CHD-C1D-ND	-2.53	122.13	124.45
20	AA	845	BCR	C34-C9-C10	-2.53	119.38	122.92
20	AA	848	BCR	C15-C16-C17	-2.53	118.29	123.47
17	A4	307	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
17	AA	826	CLA	CHD-C1D-ND	-2.53	122.13	124.45
17	A1	310	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	AA	848	BCR	C31-C1-C6	-2.53	106.20	110.30
17	AG	203	CLA	CMB-C2B-C3B	2.53	129.41	124.68
17	A3	304	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	AB	811	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
17	A4	313	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
20	AL	306	BCR	C1-C6-C5	-2.52	119.06	122.61
20	AF	805	BCR	C29-C28-C27	-2.52	105.74	111.38
20	AL	305	BCR	C2-C3-C4	-2.52	105.74	111.38
24	A1	317	LUT	C21-C26-C27	-2.52	109.51	112.70
24	A3	316	LUT	C28-C29-C30	-2.52	115.07	118.94
17	A4	308	CLA	CMB-C2B-C3B	2.52	129.40	124.68
24	A4	315	LUT	C3-C4-C5	-2.52	106.83	111.85
17	A3	304	CLA	O2D-CGD-O1D	-2.52	118.37	124.09
17	AK	204	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	A1	305	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	AB	831	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
17	AB	832	CLA	CMB-C2B-C3B	2.52	129.39	124.68
17	AF	803	CLA	CHB-C4A-NA	2.52	127.99	124.51
17	A3	302	CLA	CHB-C4A-NA	2.52	127.99	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AF	806	LUT	C32-C33-C34	-2.52	115.08	118.94
20	AB	844	BCR	C15-C16-C17	-2.52	118.32	123.47
17	AB	824	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	AB	838	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
17	A3	305	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	A6	612	CLA	CHD-C1D-ND	-2.51	122.14	124.45
26	A6	605	CHL	O1D-CGD-CBD	-2.51	119.34	124.48
17	AA	830	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
17	AB	824	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
17	A4	301	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	AB	848	BCR	C19-C18-C17	-2.51	115.09	118.94
17	AA	838	CLA	CHD-C1D-ND	-2.51	122.15	124.45
20	A1	319	BCR	C15-C16-C17	-2.51	118.34	123.47
20	AI	102	BCR	C19-C18-C17	-2.51	115.09	118.94
17	A6	609	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
26	A6	605	CHL	O2D-CGD-O1D	-2.51	118.94	123.84
17	A6	610	CLA	CAB-C3B-C2B	2.51	129.60	124.69
17	AB	810	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	AL	301	LMU	O1B-C4'-C3'	2.51	113.95	107.28
17	AB	827	CLA	O2D-CGD-CBD	2.50	115.72	111.27
17	AB	807	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	A1	319	BCR	C23-C24-C25	-2.50	120.17	127.20
17	AB	822	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
17	AA	838	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
17	AK	204	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
20	AK	205	BCR	C36-C18-C19	2.50	122.02	118.08
20	AA	845	BCR	C7-C8-C9	-2.50	122.46	126.23
17	AK	201	CLA	CMB-C2B-C3B	2.50	129.50	124.93
17	AL	304	CLA	O2D-CGD-CBD	2.50	115.70	111.27
17	AB	801	CLA	C4-C3-C5	2.50	119.47	115.27
20	AB	844	BCR	C24-C23-C22	-2.49	122.47	126.23
17	AH	201	CLA	CAA-C2A-C3A	2.49	119.60	112.78
20	AI	102	BCR	C8-C9-C10	2.49	122.76	118.94
17	AA	817	CLA	CHB-C4A-NA	2.49	127.95	124.51
17	A1	305	CLA	CMB-C2B-C3B	2.49	129.34	124.68
17	AB	812	CLA	CHB-C4A-NA	2.49	127.95	124.51
17	AA	839	CLA	O2D-CGD-CBD	2.49	115.69	111.27
20	AG	205	BCR	C16-C15-C14	-2.49	118.38	123.47
25	A1	321	LMG	O8-C28-C29	2.49	119.71	111.91
17	AB	820	CLA	CHD-C1D-ND	-2.49	122.17	124.45
17	AB	821	CLA	CHD-C1D-ND	-2.49	122.17	124.45
20	AI	101	BCR	C34-C9-C8	2.48	121.99	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AL	302	CLA	CHD-C1D-ND	-2.48	122.17	124.45
17	AA	820	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
17	AA	807	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
17	AB	833	CLA	CHD-C1D-ND	-2.48	122.18	124.45
17	AA	836	CLA	CMB-C2B-C3B	2.48	129.31	124.68
20	AI	102	BCR	C38-C26-C27	2.48	118.38	113.62
17	AB	828	CLA	CHD-C1D-ND	-2.48	122.18	124.45
17	A1	304	CLA	CHB-C4A-NA	2.48	127.94	124.51
17	AA	806	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
20	AK	205	BCR	C27-C26-C25	-2.48	119.14	122.73
17	AB	822	CLA	CHD-C1D-ND	-2.48	122.18	124.45
17	AA	834	CLA	C6-C5-C3	2.48	119.95	113.45
17	AA	837	CLA	O2D-CGD-CBD	2.48	115.67	111.27
22	AL	301	LMU	C1B-O5B-C5B	2.48	118.55	113.69
17	AA	831	CLA	CMB-C2B-C3B	2.47	129.31	124.68
17	AA	821	CLA	CHD-C1D-ND	-2.47	122.18	124.45
17	AA	841	CLA	CMB-C2B-C3B	2.47	129.31	124.68
24	A4	315	LUT	C1-C6-C5	-2.47	119.13	122.61
20	AF	805	BCR	C19-C18-C17	-2.47	115.15	118.94
20	AI	101	BCR	C12-C13-C14	-2.47	115.15	118.94
19	A1	302	LHG	O8-C23-C24	2.47	119.66	111.91
27	A3	317	XAT	C12-C13-C14	-2.47	115.15	118.94
17	A4	310	CLA	O2D-CGD-O1D	-2.47	118.48	124.09
17	AB	819	CLA	CHB-C4A-NA	2.47	127.93	124.51
17	A6	603	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
17	A1	316	CLA	CMB-C2B-C3B	2.47	129.52	124.69
17	AA	842	CLA	C4-C3-C5	-2.47	111.12	115.27
17	A4	301	CLA	CAC-C3C-C4C	2.47	128.01	124.81
26	A1	303	CHL	CAC-C3C-C4C	2.47	128.01	124.81
18	AB	843	PQN	C14-C13-C15	-2.47	111.12	115.27
20	A3	318	BCR	C33-C5-C6	-2.46	121.76	124.53
17	AA	810	CLA	CMB-C2B-C3B	2.46	129.28	124.68
24	A3	316	LUT	C8-C7-C6	-2.46	120.29	127.20
27	A6	615	XAT	C36-C21-C26	2.46	116.69	110.05
27	A3	317	XAT	C10-C11-C12	-2.46	115.54	123.22
17	A6	609	CLA	C6-C5-C3	2.46	119.91	113.45
17	A3	306	CLA	CHB-C4A-NA	2.46	127.91	124.51
17	AA	831	CLA	CHB-C4A-NA	2.46	127.91	124.51
17	AA	833	CLA	CMD-C2D-C3D	2.46	133.27	127.61
24	AF	806	LUT	C8-C9-C10	-2.45	115.17	118.94
17	AB	815	CLA	CHB-C4A-NA	2.45	127.91	124.51
17	AF	804	CLA	CHB-C4A-NA	2.45	127.91	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AK	202	BCR	C40-C30-C25	-2.45	106.32	110.30
17	AG	201	CLA	O2D-CGD-O1D	-2.45	118.52	124.09
20	AG	205	BCR	C20-C21-C22	-2.45	123.81	127.31
17	AA	815	CLA	O2D-CGD-CBD	2.45	115.63	111.27
17	A1	312	CLA	O2D-CGD-O1D	-2.45	118.52	124.09
17	AF	803	CLA	CHD-C1D-ND	-2.45	122.20	124.45
17	AB	827	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
17	AB	834	CLA	CHD-C1D-ND	-2.45	122.20	124.45
20	AI	102	BCR	C23-C22-C21	-2.45	115.18	118.94
17	AL	303	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	A6	614	LUT	C39-C29-C28	2.45	121.93	118.08
17	AA	841	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
17	A3	304	CLA	CAB-C3B-C2B	2.45	129.48	124.69
20	AI	102	BCR	C30-C25-C26	-2.45	119.17	122.61
20	AJ	101	BCR	C30-C25-C26	-2.45	119.17	122.61
20	AB	848	BCR	C34-C9-C8	2.45	121.93	118.08
17	A3	306	CLA	CHD-C1D-ND	-2.45	122.21	124.45
17	AB	834	CLA	CMB-C2B-C3B	2.44	129.25	124.68
17	A3	305	CLA	CMB-C2B-C3B	2.44	129.25	124.68
17	AB	804	CLA	CMD-C2D-C1D	-2.44	120.41	124.71
20	AA	846	BCR	C1-C6-C5	-2.44	119.17	122.61
17	AA	805	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
17	AB	842	CLA	CHB-C4A-NA	2.44	127.89	124.51
17	AB	817	CLA	CHB-C4A-NA	2.44	127.89	124.51
17	A6	603	CLA	CHB-C4A-NA	2.44	127.89	124.51
17	AA	811	CLA	CHD-C1D-ND	-2.44	122.21	124.45
20	AB	844	BCR	C12-C13-C14	-2.44	115.20	118.94
20	AA	845	BCR	C16-C17-C18	-2.44	123.83	127.31
20	AB	847	BCR	C30-C25-C26	-2.44	119.18	122.61
17	A1	315	CLA	CHB-C4A-NA	2.44	127.88	124.51
17	AB	831	CLA	CAC-C3C-C4C	2.44	127.97	124.81
17	A3	303	CLA	CAC-C3C-C4C	2.44	127.97	124.81
17	AA	837	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
20	AL	305	BCR	C39-C30-C25	2.43	114.25	110.30
20	AI	101	BCR	C28-C27-C26	-2.43	109.73	114.08
20	AB	849	BCR	C12-C13-C14	-2.43	115.21	118.94
20	AB	844	BCR	C23-C22-C21	-2.43	115.21	118.94
20	A3	318	BCR	C30-C25-C24	2.43	122.64	115.78
17	A1	309	CLA	CHD-C1D-ND	-2.43	122.22	124.45
20	AL	306	BCR	C34-C9-C10	-2.43	119.53	122.92
17	AA	842	CLA	CHD-C1D-ND	-2.42	122.23	124.45
20	AA	849	BCR	C12-C13-C14	-2.42	115.23	118.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A4	317	BCR	C38-C26-C27	2.42	118.26	113.62
20	AB	848	BCR	C24-C23-C22	-2.42	122.58	126.23
26	A6	605	CHL	OMC-CMC-C2C	-2.42	120.22	125.69
26	A3	320	CHL	C4A-NA-C1A	-2.42	105.62	106.71
17	A4	308	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
17	AA	813	CLA	CHD-C1D-ND	-2.41	122.24	124.45
20	AK	202	BCR	C11-C10-C9	-2.41	123.87	127.31
17	AA	818	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
17	AB	815	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
17	AA	810	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	AF	806	LUT	C39-C29-C30	-2.41	119.55	122.92
20	AA	846	BCR	C37-C22-C23	2.41	121.88	118.08
24	A4	315	LUT	C8-C9-C10	-2.41	115.25	118.94
17	AK	204	CLA	CMB-C2B-C3B	2.41	129.18	124.68
17	AB	832	CLA	CHB-C4A-NA	2.41	127.84	124.51
17	A4	303	CLA	CHB-C4A-NA	2.41	127.84	124.51
17	A3	312	CLA	CMB-C2B-C3B	2.41	129.18	124.68
27	A3	317	XAT	O24-C25-C24	2.41	115.19	113.38
17	AA	835	CLA	CHB-C4A-NA	2.40	127.84	124.51
17	AB	805	CLA	CHB-C4A-NA	2.40	127.84	124.51
20	AA	848	BCR	C19-C18-C17	-2.40	115.25	118.94
20	AJ	101	BCR	C12-C13-C14	-2.40	115.25	118.94
20	AA	846	BCR	C15-C14-C13	-2.40	123.88	127.31
17	A4	311	CLA	CHD-C1D-ND	-2.40	122.25	124.45
20	AA	847	BCR	C37-C22-C23	2.40	121.86	118.08
20	AB	848	BCR	C37-C22-C21	-2.40	119.56	122.92
17	AA	801	CLA	C1D-ND-C4D	-2.40	104.63	106.33
17	AA	809	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
17	AA	823	CLA	CAA-C2A-C3A	-2.40	110.50	116.10
20	A6	616	BCR	C36-C18-C19	2.40	121.86	118.08
24	A3	316	LUT	C19-C9-C8	2.40	121.86	118.08
17	A3	304	CLA	CHD-C1D-ND	-2.40	122.25	124.45
17	AA	805	CLA	CBA-CAA-C2A	2.40	120.94	113.86
20	AA	849	BCR	C38-C26-C25	-2.40	121.84	124.53
17	AA	821	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	AB	847	BCR	C19-C18-C17	-2.40	115.26	118.94
27	A6	615	XAT	C38-C25-C26	-2.40	118.25	122.26
17	AB	809	CLA	CBA-CAA-C2A	2.40	120.94	113.86
17	AA	839	CLA	CHB-C4A-NA	2.40	127.82	124.51
17	A1	312	CLA	CMB-C2B-C3B	2.39	129.38	124.69
17	AA	829	CLA	C5-C3-C2	-2.39	116.27	121.12
17	AA	820	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(°)
17	AA	830	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
17	AA	814	CLA	CMB-C2B-C3B	2.39	129.16	124.68
20	AA	845	BCR	C8-C7-C6	-2.39	120.48	127.20
17	AB	819	CLA	O2D-CGD-CBD	2.39	115.52	111.27
17	AB	839	CLA	O2D-CGD-CBD	2.39	115.52	111.27
20	AB	845	BCR	C12-C13-C14	-2.39	115.28	118.94
17	AB	803	CLA	CMB-C2B-C3B	2.39	129.15	124.68
17	AB	816	CLA	CHB-C4A-NA	2.39	127.81	124.51
20	A4	317	BCR	C8-C9-C10	-2.39	115.28	118.94
20	AA	847	BCR	C27-C26-C25	-2.39	119.27	122.73
17	AA	803	CLA	CHB-C4A-NA	2.39	127.81	124.51
24	A4	315	LUT	C35-C15-C14	-2.39	118.59	123.47
17	AA	819	CLA	CBA-CAA-C2A	2.38	120.90	113.86
17	AB	814	CLA	CHB-C4A-NA	2.38	127.81	124.51
17	A4	312	CLA	CHB-C4A-NA	2.38	127.81	124.51
17	AA	836	CLA	CHB-C4A-NA	2.38	127.80	124.51
27	A3	317	XAT	C24-C23-C22	-2.38	106.18	110.77
17	AG	203	CLA	CHD-C1D-ND	-2.38	122.27	124.45
17	A4	311	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	AA	845	BCR	C11-C10-C9	-2.38	123.92	127.31
20	AB	845	BCR	C15-C16-C17	-2.38	118.60	123.47
26	A4	306	CHL	CMD-C2D-C1D	2.38	128.90	124.71
17	AB	807	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
17	AB	823	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
17	A3	313	CLA	CHD-C1D-ND	-2.38	122.27	124.45
20	AB	849	BCR	C8-C9-C10	-2.38	115.30	118.94
17	AA	805	CLA	CMB-C2B-C3B	2.38	129.12	124.68
17	AA	827	CLA	O2D-CGD-CBD	2.37	115.49	111.27
17	A1	306	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
17	AB	825	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
20	AF	801	BCR	C36-C18-C19	2.37	121.81	118.08
17	A4	302	CLA	CMB-C2B-C3B	2.37	129.33	124.69
26	A1	303	CHL	C3C-C4C-NC	2.37	113.23	110.57
17	A6	604	CLA	CHB-C4A-NA	2.37	127.79	124.51
17	AF	803	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
17	AA	835	CLA	CHD-C1D-ND	-2.36	122.28	124.45
17	AG	204	CLA	CMB-C2B-C3B	2.36	129.10	124.68
20	A1	319	BCR	C8-C9-C10	-2.36	115.31	118.94
20	A6	616	BCR	C29-C30-C25	2.36	114.11	110.48
20	AB	849	BCR	C29-C28-C27	-2.36	106.10	111.38
20	A6	616	BCR	C8-C9-C10	-2.36	115.32	118.94
17	AF	803	CLA	CMB-C2B-C3B	2.36	129.09	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	806	CLA	O2D-CGD-CBD	2.36	115.46	111.27
17	AB	829	CLA	CBA-CAA-C2A	2.36	120.82	113.86
26	A4	304	CHL	C3C-C4C-NC	2.36	113.14	110.57
20	AB	845	BCR	C24-C25-C26	2.36	127.17	121.46
17	AK	201	CLA	CHD-C1D-ND	-2.35	122.29	124.45
20	AI	101	BCR	C11-C10-C9	-2.35	123.95	127.31
27	A6	615	XAT	C36-C21-C22	-2.35	104.89	108.98
20	AB	849	BCR	C29-C30-C25	2.35	114.10	110.48
17	A3	314	CLA	CHD-C1D-ND	-2.35	122.29	124.45
17	AA	826	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
17	AA	830	CLA	CMB-C2B-C3B	2.35	129.08	124.68
20	AB	849	BCR	C2-C3-C4	-2.35	106.13	111.38
17	A6	608	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	AA	844	LHG	O8-C23-C24	2.35	119.27	111.91
17	A1	307	CLA	CHD-C1D-ND	-2.35	122.30	124.45
20	AK	202	BCR	C32-C1-C6	-2.35	106.49	110.30
17	A3	312	CLA	CHB-C4A-NA	2.35	127.75	124.51
27	A1	318	XAT	C36-C21-C22	-2.34	104.91	108.98
17	A1	307	CLA	C2A-C1A-CHA	2.34	126.35	122.71
17	AA	803	CLA	C1-C2-C3	-2.34	121.99	126.04
20	AJ	103	BCR	C16-C15-C14	-2.34	118.67	123.47
27	A1	318	XAT	C10-C11-C12	-2.34	115.91	123.22
17	AA	803	CLA	CMB-C2B-C3B	2.34	129.06	124.68
17	AB	818	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
17	AB	842	CLA	O2D-CGD-CBD	2.34	115.43	111.27
17	AB	821	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	A1	317	LUT	C35-C15-C14	-2.34	118.68	123.47
26	A6	605	CHL	C3C-C4C-NC	2.34	113.12	110.57
24	A1	317	LUT	C8-C9-C10	-2.34	115.36	118.94
20	AJ	103	BCR	C10-C11-C12	-2.34	115.92	123.22
20	AK	202	BCR	C29-C30-C25	2.34	114.08	110.48
20	A6	616	BCR	C4-C5-C6	-2.34	119.34	122.73
17	AA	817	CLA	CHD-C1D-ND	-2.33	122.31	124.45
20	AJ	101	BCR	C16-C17-C18	-2.33	123.98	127.31
20	A4	317	BCR	C19-C18-C17	-2.33	115.36	118.94
17	AA	824	CLA	CHB-C4A-NA	2.33	127.74	124.51
20	AB	845	BCR	C37-C22-C21	-2.33	119.66	122.92
17	AB	833	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	AA	847	BCR	C11-C12-C13	2.33	132.96	126.42
17	AB	833	CLA	O2A-C1-C2	-2.33	102.52	108.64
27	A3	317	XAT	C4-C3-C2	-2.33	106.28	110.77
20	AB	845	BCR	C40-C30-C25	-2.33	106.53	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AB	849	BCR	C2-C1-C6	2.33	114.06	110.48
17	AA	832	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	AB	846	BCR	C23-C22-C21	2.33	122.51	118.94
17	AA	838	CLA	C5-C3-C2	2.32	125.82	121.12
26	A4	304	CHL	O2D-CGD-O1D	-2.32	118.82	124.09
17	AB	841	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
17	A1	310	CLA	CAA-C2A-C3A	-2.32	110.69	116.10
17	A6	612	CLA	CHB-C4A-NA	2.32	127.72	124.51
17	AA	814	CLA	O2A-CGA-O1A	-2.32	117.52	123.30
17	AA	841	CLA	CHD-C1D-ND	-2.32	122.32	124.45
17	AA	811	CLA	CHB-C4A-NA	2.32	127.72	124.51
17	AG	201	CLA	CHB-C4A-NA	2.32	127.71	124.51
17	A6	601	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
17	AF	803	CLA	CAA-C2A-C3A	-2.31	108.48	114.26
24	A6	614	LUT	C37-C21-C22	-2.31	105.05	109.44
20	AG	205	BCR	C2-C1-C6	2.31	114.04	110.48
17	A1	305	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
20	AB	849	BCR	C7-C8-C9	-2.31	122.74	126.23
20	AA	847	BCR	C15-C16-C17	-2.31	118.74	123.47
24	A4	315	LUT	C38-C25-C24	-2.31	118.61	123.56
20	A4	317	BCR	C2-C1-C6	-2.31	106.92	110.48
27	A1	318	XAT	C20-C13-C12	2.31	121.72	118.08
17	AH	201	CLA	CBA-CAA-C2A	2.31	120.68	113.86
17	A6	602	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	AB	823	CLA	CBA-CAA-C2A	2.31	120.68	113.86
17	AA	816	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	A1	306	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	AB	838	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
24	A3	316	LUT	C15-C35-C34	-2.31	118.75	123.47
17	AB	827	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
22	AB	852	LMU	C1B-O1B-C4'	-2.30	112.26	117.96
17	A3	310	CLA	CHB-C4A-NA	2.30	127.70	124.51
25	A1	321	LMG	O4-C4-C3	-2.30	105.03	110.35
17	AA	808	CLA	CHB-C4A-NA	2.30	127.69	124.51
17	AA	836	CLA	CHD-C1D-ND	-2.30	122.34	124.45
17	A4	307	CLA	CHD-C1D-ND	-2.30	122.34	124.45
17	AA	836	CLA	O2D-CGD-CBD	2.30	115.36	111.27
26	A1	303	CHL	C1-O2A-CGA	2.30	122.48	116.44
17	A3	308	CLA	CHB-C4A-NA	2.30	127.69	124.51
20	AK	205	BCR	C2-C3-C4	-2.30	106.24	111.38
17	AK	201	CLA	CHB-C4A-NA	2.30	127.69	124.51
17	A1	310	CLA	CMA-C3A-C2A	-2.30	110.74	116.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A4	315	LUT	C19-C9-C8	2.30	121.70	118.08
20	AI	101	BCR	C16-C17-C18	-2.30	124.03	127.31
20	A6	616	BCR	C15-C16-C17	-2.30	118.77	123.47
17	AA	839	CLA	CMB-C2B-C1B	-2.30	124.94	128.46
22	AB	850	LMU	C1'-C2'-C3'	2.29	114.77	110.00
17	AA	841	CLA	CBA-CAA-C2A	2.29	120.63	113.86
17	AA	818	CLA	CHB-C4A-NA	2.29	127.68	124.51
17	AG	203	CLA	CHB-C4A-NA	2.29	127.68	124.51
17	A1	305	CLA	O2A-C1-C2	-2.29	102.61	108.64
20	AB	849	BCR	C21-C20-C19	-2.29	116.07	123.22
17	AB	809	CLA	C11-C10-C8	-2.29	108.52	115.92
17	A3	314	CLA	CHB-C4A-NA	2.29	127.68	124.51
27	A6	615	XAT	C19-C9-C8	2.29	121.68	118.08
20	AA	847	BCR	C29-C30-C25	2.29	114.00	110.48
27	A6	615	XAT	C24-C23-C22	-2.29	106.36	110.77
20	AB	847	BCR	C37-C22-C21	-2.29	119.72	122.92
17	AG	204	CLA	CHD-C1D-ND	-2.29	122.35	124.45
20	AL	305	BCR	C38-C26-C25	2.29	127.09	124.53
20	AK	205	BCR	C7-C8-C9	-2.28	122.78	126.23
27	A4	316	XAT	C35-C34-C33	-2.28	124.05	127.31
17	AB	809	CLA	CHB-C4A-NA	2.28	127.67	124.51
17	AA	829	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
20	AB	845	BCR	C7-C8-C9	-2.28	122.78	126.23
17	AB	804	CLA	CMD-C2D-C3D	2.28	132.87	127.61
17	AB	809	CLA	C5-C3-C2	2.28	125.73	121.12
27	A1	318	XAT	C35-C15-C14	-2.28	118.81	123.47
17	AB	842	CLA	CHD-C1D-ND	-2.28	122.36	124.45
17	AA	833	CLA	CHB-C4A-NA	2.28	127.66	124.51
17	AA	805	CLA	CHB-C4A-NA	2.28	127.66	124.51
17	AB	826	CLA	CHB-C4A-NA	2.28	127.66	124.51
17	A6	613	CLA	CHB-C4A-NA	2.28	127.66	124.51
17	A1	309	CLA	CHB-C4A-NA	2.28	127.66	124.51
17	AA	833	CLA	CMB-C2B-C3B	2.27	128.93	124.68
17	A4	301	CLA	O2D-CGD-CBD	2.27	115.31	111.27
22	AB	850	LMU	C2'-C3'-C4'	2.27	114.87	109.68
20	AI	102	BCR	C2-C3-C4	-2.27	106.30	111.38
17	A1	305	CLA	C4-C3-C2	-2.27	117.85	123.68
18	AA	843	PQN	C17-C16-C15	-2.27	107.19	113.36
17	A1	312	CLA	CAB-C3B-C2B	2.27	129.13	124.69
26	A4	305	CHL	C4A-NA-C1A	-2.27	105.69	106.71
17	AJ	102	CLA	CHB-C4A-NA	2.27	127.65	124.51
17	AA	822	CLA	CHB-C4A-NA	2.27	127.64	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AB	851	DGD	O2G-C1B-O1B	-2.26	118.23	123.70
17	AB	828	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
20	AG	205	BCR	C40-C30-C25	-2.26	106.63	110.30
20	AA	846	BCR	C19-C18-C17	-2.26	115.47	118.94
17	A4	302	CLA	CHB-C4A-NA	2.26	127.64	124.51
26	A4	304	CHL	CAC-C3C-C4C	2.26	128.48	125.04
17	A1	312	CLA	CAA-C2A-C3A	-2.26	110.82	116.10
20	AB	844	BCR	C35-C13-C12	2.26	121.64	118.08
17	AA	802	CLA	C2D-C1D-ND	-2.26	108.44	110.10
17	A3	302	CLA	CHD-C1D-ND	-2.26	122.38	124.45
17	A4	309	CLA	O2D-CGD-CBD	2.26	115.28	111.27
17	A6	601	CLA	CHD-C1D-ND	-2.26	122.38	124.45
17	AB	812	CLA	C5-C3-C2	2.26	125.68	121.12
17	AA	808	CLA	O2D-CGD-CBD	2.25	115.28	111.27
19	A3	319	LHG	O8-C23-C24	2.25	118.98	111.91
20	A4	317	BCR	C21-C20-C19	-2.25	116.19	123.22
17	A3	308	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
27	A1	318	XAT	C19-C9-C8	2.25	121.62	118.08
17	AB	811	CLA	C2A-C1A-CHA	2.25	127.79	123.86
24	A1	317	LUT	C37-C21-C22	-2.25	105.17	109.44
20	AL	305	BCR	C15-C16-C17	-2.25	118.87	123.47
17	AA	816	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	A3	313	CLA	CHB-C4A-NA	2.25	127.62	124.51
27	A1	318	XAT	C36-C21-C26	2.25	116.11	110.05
17	A4	307	CLA	CHB-C4A-NA	2.25	127.62	124.51
20	AL	306	BCR	C35-C13-C12	2.24	121.61	118.08
20	AJ	103	BCR	C24-C23-C22	-2.24	122.85	126.23
17	A4	313	CLA	CMB-C2B-C3B	2.24	128.87	124.68
17	AB	809	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
17	AA	819	CLA	O2D-CGD-CBD	2.24	115.25	111.27
17	AA	833	CLA	CMD-C2D-C1D	-2.24	120.77	124.71
27	A3	317	XAT	O4-C5-C6	-2.24	57.11	58.96
19	A3	301	LHG	O8-C23-C24	2.24	118.92	111.91
26	A4	306	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
17	AA	827	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
20	AJ	101	BCR	C2-C3-C4	-2.24	106.38	111.38
17	AB	841	CLA	CAC-C3C-C4C	2.24	127.71	124.81
20	AI	101	BCR	C32-C1-C6	2.23	113.92	110.30
17	A3	311	CLA	O2D-CGD-CBD	2.23	115.24	111.27
20	AL	306	BCR	C20-C21-C22	-2.23	124.12	127.31
17	A6	611	CLA	CHB-C4A-NA	2.23	127.60	124.51
17	AA	834	CLA	CBC-CAC-C3C	2.23	118.58	112.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AB	807	CLA	C3C-C4C-NC	-2.23	108.07	110.57
17	AA	840	CLA	CHD-C1D-ND	-2.23	122.40	124.45
20	AB	845	BCR	C32-C1-C6	-2.23	106.68	110.30
17	AA	809	CLA	CHA-C1A-NA	-2.23	121.29	126.40
17	AB	837	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
20	AL	305	BCR	C36-C18-C19	2.23	121.59	118.08
17	AB	829	CLA	CHB-C4A-NA	2.23	127.60	124.51
17	AB	802	CLA	O2D-CGD-CBD	2.23	115.23	111.27
17	AB	831	CLA	CMB-C2B-C3B	2.23	128.85	124.68
26	A3	307	CHL	C3C-C4C-NC	2.23	113.07	110.57
17	A3	309	CLA	CMA-C3A-C2A	-2.23	110.90	116.10
26	A4	306	CHL	C3C-C4C-NC	2.23	113.07	110.57
17	AB	827	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
17	A6	601	CLA	CMC-C2C-C1C	-2.23	121.65	125.04
17	AB	832	CLA	O2A-CGA-O1A	-2.23	117.98	123.59
27	A1	318	XAT	C31-C30-C29	-2.22	124.14	127.31
17	AB	830	CLA	CMB-C2B-C3B	2.22	128.84	124.68
17	A3	315	CLA	CHB-C4A-NA	2.22	127.59	124.51
26	A4	306	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
17	AA	803	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
20	AA	848	BCR	C24-C25-C26	-2.22	116.08	121.46
24	A1	317	LUT	C38-C25-C24	-2.22	118.81	123.56
17	AA	821	CLA	O2D-CGD-CBD	2.22	115.21	111.27
17	AB	818	CLA	CHD-C1D-ND	-2.22	122.42	124.45
20	A1	319	BCR	C3-C4-C5	-2.22	110.12	114.08
17	A3	313	CLA	CAA-C2A-C3A	-2.22	110.92	116.10
26	A1	303	CHL	O2D-CGD-O1D	-2.22	119.06	124.09
20	A4	317	BCR	C23-C22-C21	-2.22	115.54	118.94
17	AB	814	CLA	CHD-C1D-ND	-2.22	122.42	124.45
17	AB	839	CLA	CHB-C4A-NA	2.22	127.58	124.51
17	AB	802	CLA	C4-C3-C5	2.21	119.00	115.27
26	A4	306	CHL	O2A-CGA-CBA	2.21	121.14	114.03
24	A3	316	LUT	C1-C6-C5	-2.21	119.50	122.61
17	AK	204	CLA	CHD-C1D-ND	-2.21	122.42	124.45
20	AJ	101	BCR	C1-C6-C5	-2.21	119.50	122.61
17	A4	313	CLA	CHD-C1D-ND	-2.21	122.42	124.45
24	AF	806	LUT	C37-C21-C22	-2.21	105.25	109.44
20	A3	318	BCR	C20-C21-C22	-2.21	124.16	127.31
17	AA	814	CLA	O2D-CGD-CBD	2.21	115.20	111.27
17	AL	302	CLA	CMA-C3A-C2A	-2.21	110.94	116.10
24	A6	614	LUT	C3-C4-C5	-2.21	107.45	111.85
17	A3	315	CLA	CAA-C2A-C3A	-2.21	110.94	116.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AL	306	BCR	C29-C30-C25	-2.21	107.08	110.48
20	AL	306	BCR	C11-C10-C9	-2.21	124.16	127.31
17	A1	315	CLA	CAA-C2A-C3A	-2.21	110.95	116.10
20	AF	805	BCR	C11-C10-C9	-2.21	124.16	127.31
24	A6	614	LUT	C15-C35-C34	-2.21	118.95	123.47
20	AA	846	BCR	C28-C27-C26	-2.21	110.14	114.08
20	AB	844	BCR	C15-C14-C13	-2.20	124.17	127.31
17	AA	838	CLA	CMB-C2B-C3B	2.20	128.80	124.68
17	AA	806	CLA	CHD-C1D-ND	-2.20	122.43	124.45
17	AK	203	CLA	CHD-C1D-ND	-2.20	122.43	124.45
17	AB	804	CLA	CMC-C2C-C1C	-2.20	121.69	125.04
17	AL	302	CLA	CHB-C4A-NA	2.20	127.56	124.51
17	AA	818	CLA	CAA-C2A-C3A	2.20	118.80	112.78
27	A4	316	XAT	C12-C13-C14	-2.20	115.57	118.94
17	AB	802	CLA	CHD-C1D-ND	-2.20	122.43	124.45
20	AK	205	BCR	C20-C21-C22	-2.20	124.17	127.31
27	A4	316	XAT	C32-C33-C34	-2.20	115.57	118.94
26	A6	607	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
17	A1	312	CLA	CHB-C4A-NA	2.20	127.55	124.51
17	AA	834	CLA	O2D-CGD-CBD	2.20	115.17	111.27
17	A6	602	CLA	O1D-CGD-CBD	2.20	128.98	124.48
17	A3	309	CLA	CHD-C1D-ND	-2.20	122.44	124.45
17	AA	817	CLA	C5-C3-C2	2.19	125.56	121.12
26	A4	304	CHL	C3B-C4B-NB	2.19	112.05	109.21
25	A4	318	LMG	C13-C12-C11	-2.19	105.31	113.19
27	A4	316	XAT	C19-C9-C8	2.19	121.53	118.08
22	AL	301	LMU	O5B-C1B-C2B	2.19	114.98	110.35
17	A3	309	CLA	C2D-C1D-ND	-2.19	108.49	110.10
27	A1	318	XAT	C37-C21-C36	-2.19	104.14	107.37
25	A4	318	LMG	O8-C28-C29	2.19	118.78	111.91
17	AH	201	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
17	AB	824	CLA	CAA-C2A-C1A	2.19	119.14	111.97
17	AB	825	CLA	O2D-CGD-CBD	2.18	115.15	111.27
17	AB	813	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	A4	314	CHL	O2D-CGD-O1D	-2.18	119.13	124.09
17	AA	805	CLA	CMC-C2C-C3C	2.18	132.03	126.12
17	AB	831	CLA	CHB-C4A-NA	2.18	127.53	124.51
25	A4	318	LMG	O1-C1-C2	2.18	111.70	108.30
20	AG	205	BCR	C34-C9-C8	2.18	121.51	118.08
24	A3	316	LUT	C32-C33-C34	-2.18	115.60	118.94
17	AB	804	CLA	CHD-C4C-C3C	2.18	128.04	124.84
27	A6	615	XAT	C26-C27-C28	-2.18	121.39	125.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AK	202	BCR	C19-C18-C17	-2.18	115.60	118.94
20	AI	102	BCR	C1-C6-C7	2.17	121.93	115.78
20	AI	102	BCR	C16-C15-C14	-2.17	119.02	123.47
17	AB	837	CLA	CHA-C1A-NA	-2.17	121.42	126.40
20	AA	845	BCR	C36-C18-C17	-2.17	119.88	122.92
20	A3	318	BCR	C33-C5-C4	2.17	117.79	113.62
17	AF	804	CLA	CHD-C1D-ND	-2.17	122.46	124.45
17	A3	308	CLA	O1D-CGD-CBD	2.17	128.92	124.48
24	A6	614	LUT	C17-C1-C6	-2.17	106.78	110.30
17	AB	834	CLA	CAC-C3C-C4C	2.17	127.62	124.81
17	AA	842	CLA	CAA-CBA-CGA	-2.17	106.92	113.25
17	AB	823	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
27	A1	318	XAT	C28-C29-C30	-2.17	115.61	118.94
17	AB	813	CLA	CHB-C4A-NA	2.17	127.51	124.51
17	AB	822	CLA	CHB-C4A-NA	2.17	127.51	124.51
17	AH	201	CLA	CMB-C2B-C1B	-2.17	125.14	128.46
17	AB	842	CLA	C3A-C2A-C1A	2.17	104.58	101.34
20	AA	847	BCR	C29-C28-C27	-2.17	106.54	111.38
20	AA	846	BCR	C37-C22-C21	-2.16	119.89	122.92
17	AB	829	CLA	O2D-CGD-CBD	2.16	115.11	111.27
20	AI	102	BCR	C7-C6-C5	-2.16	116.22	121.46
17	AB	830	CLA	O1D-CGD-CBD	2.16	128.91	124.48
17	AA	816	CLA	CAC-C3C-C4C	2.16	127.61	124.81
20	AJ	103	BCR	C30-C25-C26	-2.16	119.57	122.61
24	A6	614	LUT	C40-C33-C32	2.16	121.48	118.08
17	AA	808	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
17	AB	840	CLA	C2D-C1D-ND	-2.16	108.51	110.10
17	AA	830	CLA	O1D-CGD-CBD	2.16	128.90	124.48
17	AB	805	CLA	CMA-C3A-C2A	-2.15	111.07	116.10
20	AB	846	BCR	C12-C13-C14	-2.15	115.64	118.94
17	A3	302	CLA	O1D-CGD-CBD	2.15	128.89	124.48
24	A3	316	LUT	C35-C15-C14	-2.15	119.06	123.47
26	A3	320	CHL	C3D-C2D-C1D	-2.15	102.89	105.83
17	A6	604	CLA	CHD-C1D-ND	-2.15	122.47	124.45
17	A4	301	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
17	A1	314	CLA	CBC-CAC-C3C	2.15	118.37	112.43
17	AA	809	CLA	CHD-C1D-ND	-2.15	122.48	124.45
27	A4	316	XAT	C10-C11-C12	-2.15	116.50	123.22
17	A1	312	CLA	CHD-C1D-ND	-2.15	122.48	124.45
17	AB	836	CLA	CHB-C4A-NA	2.15	127.49	124.51
20	AB	844	BCR	C20-C21-C22	-2.15	124.24	127.31
20	AF	805	BCR	C28-C27-C26	-2.15	110.24	114.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AJ	102	CLA	CHD-C1D-ND	-2.15	122.48	124.45
17	AB	822	CLA	CMB-C2B-C3B	2.15	128.69	124.68
17	AB	812	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
20	AA	846	BCR	C2-C3-C4	-2.14	106.58	111.38
24	A6	614	LUT	C19-C9-C8	2.14	121.45	118.08
17	AA	809	CLA	O1D-CGD-CBD	2.14	128.87	124.48
20	AB	848	BCR	C38-C26-C27	2.14	117.73	113.62
20	AB	844	BCR	C1-C6-C5	-2.14	119.60	122.61
17	AB	834	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
20	AB	846	BCR	C24-C23-C22	-2.14	123.00	126.23
17	AA	834	CLA	C7-C6-C5	-2.14	107.55	113.36
20	AB	844	BCR	C16-C17-C18	-2.14	124.26	127.31
17	AB	818	CLA	O2D-CGD-CBD	2.14	115.07	111.27
24	A4	315	LUT	C37-C21-C26	2.14	112.78	109.55
20	AA	849	BCR	C19-C18-C17	2.14	122.22	118.94
20	AB	846	BCR	C24-C25-C26	2.14	126.64	121.46
17	A1	311	CLA	CHD-C1D-ND	-2.14	122.49	124.45
20	AJ	103	BCR	C38-C26-C27	2.14	117.72	113.62
20	AK	202	BCR	C20-C21-C22	-2.14	124.26	127.31
17	AB	807	CLA	CMB-C2B-C3B	2.14	128.68	124.68
26	A4	304	CHL	CMB-C2B-C3B	2.14	128.67	124.68
19	A1	301	LHG	O8-C23-C24	2.14	118.61	111.91
17	AA	842	CLA	O2D-CGD-CBD	2.14	115.06	111.27
27	A1	318	XAT	C24-C23-C22	-2.13	106.65	110.77
17	AA	816	CLA	O2D-CGD-CBD	2.13	115.06	111.27
20	AG	205	BCR	C29-C30-C25	2.13	113.76	110.48
27	A3	317	XAT	C28-C29-C30	-2.13	115.67	118.94
19	A1	301	LHG	O8-C23-O10	-2.13	118.22	123.59
17	A1	316	CLA	CHB-C4A-NA	2.13	127.46	124.51
17	AB	825	CLA	C1-O2A-CGA	2.13	122.03	116.44
17	AB	825	CLA	CMA-C3A-C4A	-2.13	106.06	111.77
26	A1	308	CHL	O2D-CGD-O1D	-2.13	119.26	124.09
20	AA	849	BCR	C16-C15-C14	-2.13	119.12	123.47
17	AH	201	CLA	CHD-C1D-ND	-2.13	122.50	124.45
17	AA	805	CLA	O1D-CGD-CBD	2.12	128.83	124.48
20	AA	847	BCR	C12-C13-C14	2.12	122.20	118.94
20	AK	202	BCR	C38-C26-C25	2.12	126.91	124.53
17	AF	802	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
20	AI	102	BCR	C23-C24-C25	-2.12	121.24	127.20
20	AI	101	BCR	C19-C18-C17	-2.12	115.69	118.94
20	AG	205	BCR	C16-C17-C18	-2.12	124.28	127.31
26	A4	305	CHL	O2D-CGD-O1D	-2.12	119.70	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AL	306	BCR	C16-C15-C14	-2.12	119.14	123.47
17	AA	837	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
17	AA	838	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
17	A4	303	CLA	CHD-C1D-ND	-2.11	122.51	124.45
17	A1	306	CLA	CHB-C4A-NA	2.11	127.44	124.51
20	AA	845	BCR	C20-C21-C22	-2.11	124.30	127.31
17	AA	829	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
17	AB	837	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
17	AB	840	CLA	CHB-C4A-NA	2.11	127.43	124.51
26	A3	307	CHL	C3D-C2D-C1D	-2.11	102.95	105.83
17	AB	813	CLA	O2D-CGD-CBD	2.11	115.02	111.27
17	AB	815	CLA	C16-C15-C13	2.11	122.74	115.92
27	A1	318	XAT	C17-C1-C16	-2.11	104.26	107.37
17	AA	834	CLA	CMC-C2C-C3C	2.11	131.84	126.12
20	AF	805	BCR	C40-C30-C25	-2.11	106.88	110.30
27	A1	318	XAT	C35-C34-C33	-2.11	124.30	127.31
17	AB	806	CLA	CMC-C2C-C3C	2.11	131.84	126.12
20	AA	845	BCR	C36-C18-C19	2.11	121.40	118.08
17	AB	805	CLA	CHD-C1D-ND	-2.11	122.52	124.45
17	AB	830	CLA	CHB-C4A-NA	2.11	127.42	124.51
17	AB	802	CLA	CMB-C2B-C3B	2.11	128.81	124.69
17	A6	603	CLA	CHD-C1D-ND	-2.10	122.52	124.45
20	AB	848	BCR	C3-C4-C5	-2.10	110.32	114.08
17	AB	837	CLA	CHB-C4A-NA	2.10	127.42	124.51
20	AL	306	BCR	C29-C28-C27	-2.10	106.68	111.38
17	A6	609	CLA	CHD-C1D-ND	-2.10	122.52	124.45
17	AA	814	CLA	CHB-C4A-NA	2.10	127.41	124.51
20	A4	317	BCR	C37-C22-C21	-2.10	119.99	122.92
17	A4	310	CLA	CHD-C1D-ND	-2.09	122.53	124.45
27	A3	317	XAT	C38-C25-C24	2.09	116.64	114.28
20	AG	205	BCR	C1-C6-C5	-2.09	119.66	122.61
17	AA	826	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
17	AA	803	CLA	CAA-CBA-CGA	-2.09	107.13	113.25
26	A6	607	CHL	C5-C3-C4	2.09	119.23	114.60
17	AL	303	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
17	AA	840	CLA	C1-C2-C3	-2.09	122.42	126.04
17	AB	823	CLA	CMB-C2B-C3B	2.09	128.59	124.68
20	AB	846	BCR	C16-C15-C14	-2.09	119.19	123.47
19	A6	617	LHG	O8-C23-C24	2.09	118.47	111.91
20	A3	318	BCR	C28-C27-C26	-2.09	110.34	114.08
20	AL	306	BCR	C24-C25-C26	-2.09	116.40	121.46
17	AA	815	CLA	CHD-C1D-ND	-2.09	122.50	124.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A4	315	LUT	C36-C21-C26	2.09	112.71	109.55
17	AB	807	CLA	CAA-C2A-C1A	-2.09	105.13	111.97
17	AL	304	CLA	CHD-C1D-ND	-2.09	122.53	124.45
17	AA	842	CLA	CAC-C3C-C4C	2.09	127.52	124.81
17	A3	314	CLA	CAA-C2A-C3A	-2.09	111.23	116.10
17	AA	828	CLA	C16-C15-C13	2.08	122.66	115.92
17	A4	308	CLA	C1D-ND-C4D	-2.08	104.85	106.33
17	AB	804	CLA	C2A-C1A-CHA	2.08	127.50	123.86
17	AB	801	CLA	C2A-C1A-CHA	2.08	127.50	123.86
17	AA	832	CLA	O2D-CGD-CBD	2.08	114.97	111.27
26	A4	305	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
17	AF	802	CLA	CMD-C2D-C3D	2.08	132.40	127.61
20	A3	318	BCR	C15-C16-C17	-2.08	119.21	123.47
20	AJ	101	BCR	C19-C18-C17	-2.08	115.75	118.94
20	AK	205	BCR	C8-C7-C6	-2.08	121.36	127.20
26	A6	606	CHL	CED-O2D-CGD	2.08	120.64	115.94
17	AB	804	CLA	O2D-CGD-CBD	2.08	114.96	111.27
17	A3	303	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
20	AA	849	BCR	C15-C16-C17	-2.08	119.22	123.47
17	AA	838	CLA	CHB-C4A-NA	2.08	127.38	124.51
27	A1	318	XAT	C38-C25-C26	-2.07	118.78	122.26
17	AB	819	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
20	A1	319	BCR	C12-C13-C14	-2.07	115.76	118.94
17	A4	313	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
17	AK	203	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
17	AA	838	CLA	O2D-CGD-CBD	2.07	114.95	111.27
17	A6	610	CLA	C1D-ND-C4D	-2.07	104.86	106.33
20	AI	102	BCR	C20-C21-C22	-2.07	124.35	127.31
20	A1	319	BCR	C20-C21-C22	-2.07	124.35	127.31
26	A3	320	CHL	C4D-C3D-CAD	-2.07	105.66	108.10
17	AA	830	CLA	CHB-C4A-NA	2.07	127.37	124.51
20	AB	847	BCR	C23-C22-C21	-2.07	115.77	118.94
17	AB	818	CLA	CAC-C3C-C4C	2.07	127.49	124.81
17	AB	811	CLA	CHA-C1A-NA	-2.06	121.67	126.40
26	A4	304	CHL	CMA-C3A-C4A	-2.06	106.22	111.77
20	AB	849	BCR	C8-C7-C6	-2.06	121.41	127.20
27	A1	318	XAT	O4-C5-C18	2.06	117.53	115.06
17	A1	311	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
17	A1	314	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
17	AB	819	CLA	CAA-C2A-C3A	2.06	118.43	112.78
20	AJ	103	BCR	C20-C21-C22	-2.06	124.37	127.31
17	A3	309	CLA	CAA-C2A-C3A	-2.06	111.29	116.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AA	847	BCR	C34-C9-C8	2.06	121.32	118.08
17	AB	801	CLA	C3A-C2A-C1A	2.06	104.42	101.34
26	A6	606	CHL	CHC-C1C-C2C	-2.06	118.64	126.11
20	A4	317	BCR	C36-C18-C17	-2.06	120.04	122.92
20	AG	205	BCR	C29-C28-C27	-2.06	106.78	111.38
20	AA	849	BCR	C34-C9-C8	2.06	121.32	118.08
22	AL	301	LMU	C1-O1'-C1'	2.06	117.25	113.84
17	A6	609	CLA	CBA-CAA-C2A	2.06	119.93	113.86
17	AB	821	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
17	AA	821	CLA	C7-C6-C5	-2.05	107.79	113.36
17	AB	832	CLA	CMC-C2C-C3C	2.05	131.68	126.12
20	AJ	103	BCR	C12-C13-C14	-2.05	115.80	118.94
20	AL	306	BCR	C12-C13-C14	-2.05	115.80	118.94
24	A4	315	LUT	C12-C13-C14	-2.05	115.80	118.94
20	AA	848	BCR	C1-C6-C5	-2.05	119.73	122.61
20	AI	102	BCR	C12-C13-C14	-2.05	115.80	118.94
17	AB	833	CLA	C4-C3-C5	2.04	118.71	115.27
17	AA	826	CLA	CHB-C4A-NA	2.04	127.34	124.51
20	A4	317	BCR	C35-C13-C12	2.04	121.30	118.08
26	A1	303	CHL	C3D-C2D-C1D	-2.04	103.04	105.83
20	A6	616	BCR	C30-C25-C26	-2.04	119.74	122.61
20	A1	319	BCR	C36-C18-C17	-2.04	120.07	122.92
17	AA	825	CLA	C2D-C1D-ND	-2.04	108.60	110.10
17	AK	201	CLA	CMA-C3A-C2A	-2.04	111.34	116.10
26	A1	308	CHL	C3C-C4C-NC	2.04	112.85	110.57
17	A1	309	CLA	CAC-C3C-C4C	2.04	127.45	124.81
17	A4	308	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
17	AA	824	CLA	CAA-C2A-C3A	2.03	118.34	112.78
20	AG	205	BCR	C37-C22-C21	-2.03	120.08	122.92
17	AA	801	CLA	O1D-CGD-CBD	2.03	128.64	124.48
17	AA	839	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	A6	610	CLA	C3A-C4A-CHB	-2.03	118.95	124.50
17	AA	832	CLA	C5-C3-C2	-2.03	117.01	121.12
22	AB	853	LMU	O5B-C5B-C4B	2.03	113.38	109.69
17	A1	313	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
17	A4	313	CLA	O2D-CGD-CBD	2.03	114.87	111.27
20	AB	846	BCR	C32-C1-C6	-2.03	107.01	110.30
17	AB	832	CLA	CMC-C2C-C1C	-2.03	121.95	125.04
17	A1	315	CLA	CMA-C3A-C2A	-2.03	111.37	116.10
20	AL	306	BCR	C34-C9-C8	2.02	121.27	118.08
20	AA	847	BCR	C16-C15-C14	-2.02	119.33	123.47
17	AB	803	CLA	O1D-CGD-CBD	2.02	128.62	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	825	CLA	CBA-CAA-C2A	-2.02	107.89	113.86
17	A6	609	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
20	AJ	103	BCR	C27-C26-C25	-2.02	119.80	122.73
17	AA	822	CLA	CHD-C1D-ND	-2.02	122.60	124.45
17	AA	840	CLA	C2D-C1D-ND	-2.02	108.61	110.10
17	A3	310	CLA	CAA-C2A-C3A	-2.02	111.38	116.10
17	AA	811	CLA	O1D-CGD-CBD	2.02	128.62	124.48
17	AA	828	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
17	A4	313	CLA	CBA-CAA-C2A	2.02	119.82	113.86
17	AA	823	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	AB	803	CLA	CHB-C4A-NA	2.02	127.30	124.51
26	A1	303	CHL	CBA-CAA-C2A	2.02	119.81	113.86
17	A4	301	CLA	CHD-C1D-ND	-2.02	122.60	124.45
26	A1	303	CHL	OMC-CMC-C2C	-2.02	121.13	125.69
17	AA	803	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
17	AB	835	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
24	AF	806	LUT	C40-C33-C34	-2.01	120.10	122.92
26	A3	307	CHL	C1C-C2C-C3C	-2.01	104.84	106.96
17	AA	837	CLA	C2A-C1A-CHA	2.01	127.38	123.86
17	A3	303	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	A3	310	CLA	CHD-C1D-ND	-2.01	122.61	124.45
27	A6	615	XAT	C35-C34-C33	-2.01	124.44	127.31
20	AG	205	BCR	C33-C5-C6	-2.01	122.27	124.53
20	AF	801	BCR	C39-C30-C25	-2.01	107.04	110.30
17	AA	820	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
17	AF	802	CLA	O1D-CGD-CBD	2.01	128.59	124.48
17	A4	308	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	A1	309	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
20	AA	847	BCR	C19-C18-C17	-2.01	115.86	118.94
17	AL	303	CLA	CHD-C1D-C2D	2.01	129.69	125.48
17	AB	812	CLA	CHD-C1D-ND	-2.01	122.61	124.45
17	AB	812	CLA	C4-C3-C2	-2.01	118.53	123.68
26	A6	606	CHL	C3D-C2D-C1D	-2.01	103.09	105.83
17	AB	841	CLA	CHD-C1D-ND	-2.01	122.61	124.45
20	AF	805	BCR	C24-C25-C26	2.01	126.32	121.46
20	AB	846	BCR	C15-C16-C17	-2.00	119.37	123.47
17	A6	608	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
18	AA	843	PQN	C21-C22-C23	-2.00	109.44	115.92
17	AB	815	CLA	CHD-C1D-ND	-2.00	122.61	124.45
20	A4	317	BCR	C34-C9-C8	2.00	121.23	118.08
17	AA	801	CLA	CBA-CAA-C2A	-2.00	107.95	113.86
17	A3	308	CLA	CHD-C1D-ND	-2.00	122.61	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AB	838	CLA	CHB-C4A-NA	2.00	127.28	124.51
17	AA	810	CLA	CHD-C1D-ND	-2.00	122.62	124.45
20	AI	102	BCR	C15-C16-C17	-2.00	119.38	123.47
17	AA	801	CLA	CMB-C2B-C3B	2.00	128.42	124.68

All (160) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	AA	801	CLA	ND
17	AA	802	CLA	ND
17	AA	803	CLA	ND
17	AA	805	CLA	ND
17	AA	806	CLA	ND
17	AA	807	CLA	ND
17	AA	808	CLA	ND
17	AA	809	CLA	ND
17	AA	810	CLA	ND
17	AA	811	CLA	ND
17	AA	812	CLA	ND
17	AA	813	CLA	ND
17	AA	814	CLA	ND
17	AA	816	CLA	ND
17	AA	817	CLA	ND
17	AA	819	CLA	ND
17	AA	820	CLA	ND
17	AA	821	CLA	ND
17	AA	822	CLA	ND
17	AA	823	CLA	ND
17	AA	824	CLA	ND
17	AA	825	CLA	ND
17	AA	826	CLA	ND
17	AA	827	CLA	ND
17	AA	828	CLA	ND
17	AA	829	CLA	ND
17	AA	830	CLA	ND
17	AA	831	CLA	ND
17	AA	832	CLA	ND
17	AA	833	CLA	ND
17	AA	835	CLA	ND
17	AA	837	CLA	ND
17	AA	840	CLA	ND
17	AA	842	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
17	AB	801	CLA	ND
17	AB	802	CLA	ND
17	AB	803	CLA	ND
17	AB	804	CLA	ND
17	AB	805	CLA	ND
17	AB	806	CLA	ND
17	AB	807	CLA	ND
17	AB	809	CLA	ND
17	AB	810	CLA	ND
17	AB	811	CLA	ND
17	AB	812	CLA	ND
17	AB	813	CLA	ND
17	AB	814	CLA	ND
17	AB	815	CLA	ND
17	AB	816	CLA	ND
17	AB	817	CLA	ND
17	AB	818	CLA	ND
17	AB	819	CLA	ND
17	AB	820	CLA	ND
17	AB	821	CLA	ND
17	AB	822	CLA	ND
17	AB	824	CLA	ND
17	AB	825	CLA	ND
17	AB	826	CLA	ND
17	AB	827	CLA	ND
17	AB	828	CLA	ND
17	AB	829	CLA	ND
17	AB	830	CLA	ND
17	AB	831	CLA	ND
17	AB	833	CLA	ND
17	AB	834	CLA	ND
17	AB	837	CLA	ND
17	AB	839	CLA	ND
17	AB	840	CLA	ND
17	AB	841	CLA	ND
17	AB	842	CLA	ND
17	AF	802	CLA	ND
17	AF	803	CLA	ND
17	AF	804	CLA	ND
17	AG	201	CLA	ND
17	AG	203	CLA	ND
17	AG	204	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
17	AH	201	CLA	ND
17	AJ	102	CLA	ND
17	AK	201	CLA	ND
17	AK	203	CLA	ND
17	AK	204	CLA	ND
17	AL	302	CLA	ND
17	AL	304	CLA	ND
17	A1	304	CLA	ND
17	A1	305	CLA	ND
17	A1	306	CLA	ND
17	A1	307	CLA	ND
17	A1	309	CLA	ND
17	A1	310	CLA	ND
17	A1	311	CLA	ND
17	A1	312	CLA	ND
17	A1	313	CLA	ND
17	A1	314	CLA	ND
17	A1	315	CLA	ND
17	A1	316	CLA	ND
17	A3	302	CLA	ND
17	A3	303	CLA	ND
17	A3	304	CLA	ND
17	A3	305	CLA	ND
17	A3	306	CLA	ND
17	A3	308	CLA	ND
17	A3	309	CLA	ND
17	A3	310	CLA	ND
17	A3	311	CLA	ND
17	A3	312	CLA	ND
17	A3	314	CLA	ND
17	A3	315	CLA	ND
17	A4	301	CLA	ND
17	A4	302	CLA	ND
17	A4	303	CLA	ND
17	A4	307	CLA	ND
17	A4	308	CLA	ND
17	A4	309	CLA	ND
17	A4	310	CLA	ND
17	A4	311	CLA	ND
17	A4	312	CLA	ND
17	A4	313	CLA	ND
17	A6	601	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
17	A6	602	CLA	ND
17	A6	603	CLA	ND
17	A6	604	CLA	ND
17	A6	608	CLA	ND
17	A6	609	CLA	ND
17	A6	610	CLA	ND
17	A6	611	CLA	ND
17	A6	612	CLA	ND
17	A6	613	CLA	ND
26	A1	303	CHL	NC
26	A1	303	CHL	NA
26	A1	303	CHL	ND
26	A1	308	CHL	NC
26	A1	308	CHL	NA
26	A1	308	CHL	ND
26	A3	307	CHL	NC
26	A3	307	CHL	NA
26	A3	307	CHL	ND
26	A3	320	CHL	NC
26	A3	320	CHL	NA
26	A3	320	CHL	ND
26	A4	304	CHL	NC
26	A4	304	CHL	NA
26	A4	304	CHL	ND
26	A4	305	CHL	NC
26	A4	305	CHL	NA
26	A4	305	CHL	ND
26	A4	306	CHL	NC
26	A4	306	CHL	NA
26	A4	306	CHL	ND
26	A4	314	CHL	NC
26	A4	314	CHL	NA
26	A4	314	CHL	ND
26	A6	605	CHL	NC
26	A6	605	CHL	NA
26	A6	605	CHL	ND
26	A6	606	CHL	NC
26	A6	606	CHL	NA
26	A6	606	CHL	ND
26	A6	607	CHL	NC
26	A6	607	CHL	NA
26	A6	607	CHL	ND

All (1499) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	AA	801	CLA	CBD-CGD-O2D-CED
17	AA	802	CLA	CBD-CGD-O2D-CED
17	AA	804	CLA	C1A-C2A-CAA-CBA
17	AA	804	CLA	C3A-C2A-CAA-CBA
17	AA	805	CLA	CHA-CBD-CGD-O1D
17	AA	805	CLA	CHA-CBD-CGD-O2D
17	AA	813	CLA	CHA-CBD-CGD-O1D
17	AA	813	CLA	CHA-CBD-CGD-O2D
17	AA	813	CLA	CAD-CBD-CGD-O1D
17	AA	814	CLA	CHA-CBD-CGD-O1D
17	AA	816	CLA	CHA-CBD-CGD-O1D
17	AA	816	CLA	CHA-CBD-CGD-O2D
17	AA	816	CLA	CAD-CBD-CGD-O1D
17	AA	818	CLA	C3A-C2A-CAA-CBA
17	AA	819	CLA	C3A-C2A-CAA-CBA
17	AA	822	CLA	C1A-C2A-CAA-CBA
17	AA	824	CLA	C1A-C2A-CAA-CBA
17	AA	824	CLA	C3A-C2A-CAA-CBA
17	AA	825	CLA	C1A-C2A-CAA-CBA
17	AA	828	CLA	CBD-CGD-O2D-CED
17	AA	828	CLA	C14-C13-C15-C16
17	AA	829	CLA	CHA-CBD-CGD-O1D
17	AA	829	CLA	C2-C3-C5-C6
17	AA	829	CLA	C4-C3-C5-C6
17	AA	831	CLA	C1A-C2A-CAA-CBA
17	AA	831	CLA	C3A-C2A-CAA-CBA
17	AA	832	CLA	C2-C3-C5-C6
17	AA	832	CLA	C4-C3-C5-C6
17	AA	833	CLA	CHA-CBD-CGD-O1D
17	AA	833	CLA	CHA-CBD-CGD-O2D
17	AA	833	CLA	CAD-CBD-CGD-O1D
17	AA	833	CLA	CBD-CGD-O2D-CED
17	AA	837	CLA	CHA-CBD-CGD-O1D
17	AA	837	CLA	CHA-CBD-CGD-O2D
17	AA	837	CLA	C4-C3-C5-C6
17	AA	842	CLA	C2A-CAA-CBA-CGA
17	AB	802	CLA	C2-C3-C5-C6
17	AB	802	CLA	C4-C3-C5-C6
17	AB	803	CLA	CHA-CBD-CGD-O1D
17	AB	803	CLA	CHA-CBD-CGD-O2D
17	AB	804	CLA	C1A-C2A-CAA-CBA
17	AB	804	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	804	CLA	C2C-C3C-CAC-CBC
17	AB	804	CLA	C4C-C3C-CAC-CBC
17	AB	804	CLA	CBD-CGD-O2D-CED
17	AB	804	CLA	C11-C10-C8-C7
17	AB	806	CLA	C1A-C2A-CAA-CBA
17	AB	806	CLA	C3A-C2A-CAA-CBA
17	AB	806	CLA	CHA-CBD-CGD-O1D
17	AB	806	CLA	CHA-CBD-CGD-O2D
17	AB	806	CLA	CAD-CBD-CGD-O1D
17	AB	806	CLA	CAD-CBD-CGD-O2D
17	AB	807	CLA	CBD-CGD-O2D-CED
17	AB	808	CLA	CHA-CBD-CGD-O1D
17	AB	808	CLA	CHA-CBD-CGD-O2D
17	AB	809	CLA	C1A-C2A-CAA-CBA
17	AB	809	CLA	C3A-C2A-CAA-CBA
17	AB	810	CLA	C2A-CAA-CBA-CGA
17	AB	810	CLA	CBD-CGD-O2D-CED
17	AB	811	CLA	C1A-C2A-CAA-CBA
17	AB	811	CLA	CHA-CBD-CGD-O1D
17	AB	811	CLA	CHA-CBD-CGD-O2D
17	AB	811	CLA	CAD-CBD-CGD-O1D
17	AB	812	CLA	CBD-CGD-O2D-CED
17	AB	812	CLA	O1D-CGD-O2D-CED
17	AB	814	CLA	C1A-C2A-CAA-CBA
17	AB	814	CLA	C3A-C2A-CAA-CBA
17	AB	815	CLA	CBD-CGD-O2D-CED
17	AB	816	CLA	CBD-CGD-O2D-CED
17	AB	819	CLA	C3A-C2A-CAA-CBA
17	AB	819	CLA	C4-C3-C5-C6
17	AB	824	CLA	C1A-C2A-CAA-CBA
17	AB	824	CLA	C3A-C2A-CAA-CBA
17	AB	824	CLA	CHA-CBD-CGD-O1D
17	AB	828	CLA	C1A-C2A-CAA-CBA
17	AB	829	CLA	C1A-C2A-CAA-CBA
17	AB	834	CLA	CBD-CGD-O2D-CED
17	AB	834	CLA	C6-C7-C8-C9
17	AB	836	CLA	CBD-CGD-O2D-CED
17	AB	839	CLA	CHA-CBD-CGD-O1D
17	AB	839	CLA	CHA-CBD-CGD-O2D
17	AB	841	CLA	C6-C7-C8-C9
17	AF	802	CLA	C3A-C2A-CAA-CBA
17	AF	803	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AF	804	CLA	CHA-CBD-CGD-O1D
17	AG	203	CLA	CBD-CGD-O2D-CED
17	AG	204	CLA	CBD-CGD-O2D-CED
17	AH	201	CLA	C3A-C2A-CAA-CBA
17	AH	201	CLA	CBD-CGD-O2D-CED
17	AJ	102	CLA	C1A-C2A-CAA-CBA
17	AJ	102	CLA	CHA-CBD-CGD-O1D
17	AJ	102	CLA	CHA-CBD-CGD-O2D
17	AK	204	CLA	C1A-C2A-CAA-CBA
17	AK	204	CLA	CBA-CGA-O2A-C1
17	AK	204	CLA	CBD-CGD-O2D-CED
17	AL	302	CLA	CHA-CBD-CGD-O1D
17	AL	302	CLA	CHA-CBD-CGD-O2D
17	AL	304	CLA	C1A-C2A-CAA-CBA
17	AL	304	CLA	CHA-CBD-CGD-O2D
17	A1	306	CLA	CHA-CBD-CGD-O1D
17	A1	306	CLA	CHA-CBD-CGD-O2D
17	A1	306	CLA	CAD-CBD-CGD-O1D
17	A1	306	CLA	CAD-CBD-CGD-O2D
17	A1	306	CLA	CBD-CGD-O2D-CED
17	A1	307	CLA	CBD-CGD-O2D-CED
17	A1	309	CLA	C1A-C2A-CAA-CBA
17	A1	310	CLA	CBD-CGD-O2D-CED
17	A1	313	CLA	CBD-CGD-O2D-CED
17	A1	314	CLA	C11-C10-C8-C9
17	A3	303	CLA	C1A-C2A-CAA-CBA
17	A3	303	CLA	C3A-C2A-CAA-CBA
17	A3	305	CLA	C1A-C2A-CAA-CBA
17	A3	309	CLA	CBD-CGD-O2D-CED
17	A4	301	CLA	CHA-CBD-CGD-O1D
17	A4	301	CLA	CHA-CBD-CGD-O2D
17	A4	302	CLA	CBD-CGD-O2D-CED
17	A4	303	CLA	CBD-CGD-O2D-CED
17	A4	309	CLA	C1A-C2A-CAA-CBA
17	A4	309	CLA	C3A-C2A-CAA-CBA
17	A4	310	CLA	C1A-C2A-CAA-CBA
17	A4	310	CLA	C3A-C2A-CAA-CBA
17	A4	312	CLA	CBD-CGD-O2D-CED
17	A4	313	CLA	C1A-C2A-CAA-CBA
17	A4	313	CLA	CBD-CGD-O2D-CED
17	A6	608	CLA	C1A-C2A-CAA-CBA
17	A6	608	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	A6	610	CLA	CMA-C3A-C4A-NA
18	AB	843	PQN	C19-C18-C20-C21
19	AA	844	LHG	C4-O6-P-O3
19	AJ	104	LHG	C4-O6-P-O3
19	AJ	104	LHG	C4-O6-P-O4
19	AJ	104	LHG	C4-O6-P-O5
19	A1	320	LHG	C4-O6-P-O3
19	A1	320	LHG	C4-O6-P-O4
19	A1	320	LHG	C4-O6-P-O5
19	A3	301	LHG	C3-O3-P-O5
19	A3	301	LHG	C4-O6-P-O3
19	A3	301	LHG	C4-O6-P-O4
19	A3	301	LHG	C4-O6-P-O5
19	A3	319	LHG	C3-O3-P-O4
19	A3	319	LHG	C3-O3-P-O5
19	A3	319	LHG	C3-O3-P-O6
19	A6	617	LHG	C3-O3-P-O4
19	A6	617	LHG	C4-O6-P-O5
20	AA	845	BCR	C7-C8-C9-C10
20	AA	846	BCR	C21-C22-C23-C24
20	AA	846	BCR	C23-C24-C25-C26
20	AA	847	BCR	C5-C6-C7-C8
20	AA	847	BCR	C7-C8-C9-C10
20	AA	847	BCR	C7-C8-C9-C34
20	AA	847	BCR	C21-C22-C23-C24
20	AA	847	BCR	C37-C22-C23-C24
20	AA	849	BCR	C23-C24-C25-C26
20	AB	844	BCR	C5-C6-C7-C8
20	AB	845	BCR	C7-C8-C9-C10
20	AB	845	BCR	C23-C24-C25-C26
20	AB	845	BCR	C23-C24-C25-C30
20	AB	848	BCR	C21-C22-C23-C24
20	AB	848	BCR	C37-C22-C23-C24
20	AB	849	BCR	C21-C22-C23-C24
20	AB	849	BCR	C37-C22-C23-C24
20	AB	849	BCR	C23-C24-C25-C26
20	AB	849	BCR	C23-C24-C25-C30
20	AF	801	BCR	C23-C24-C25-C26
20	AF	801	BCR	C23-C24-C25-C30
20	AF	805	BCR	C7-C8-C9-C10
20	AF	805	BCR	C7-C8-C9-C34
20	AI	101	BCR	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	AI	101	BCR	C7-C8-C9-C34
20	AI	102	BCR	C1-C6-C7-C8
20	AI	102	BCR	C5-C6-C7-C8
20	AJ	103	BCR	C5-C6-C7-C8
20	AK	202	BCR	C23-C24-C25-C26
20	AK	202	BCR	C23-C24-C25-C30
20	AL	305	BCR	C7-C8-C9-C10
20	AL	305	BCR	C7-C8-C9-C34
20	A1	319	BCR	C1-C6-C7-C8
20	A1	319	BCR	C5-C6-C7-C8
20	A3	318	BCR	C21-C22-C23-C24
20	A6	616	BCR	C5-C6-C7-C8
22	AA	851	LMU	O5'-C1'-O1'-C1
22	AB	852	LMU	C2'-C1'-O1'-C1
22	AB	852	LMU	O5'-C1'-O1'-C1
22	AL	301	LMU	C2'-C1'-O1'-C1
23	AB	851	DGD	C2B-C1B-O2G-C2G
23	AB	851	DGD	O2G-C2G-C3G-O3G
24	A4	315	LUT	C1-C6-C7-C8
25	A1	321	LMG	O9-C10-O7-C8
25	A1	321	LMG	C11-C10-O7-C8
25	A4	318	LMG	O6-C1-O1-C7
25	A4	318	LMG	C11-C10-O7-C8
26	A3	307	CHL	CBD-CGD-O2D-CED
26	A3	320	CHL	C1A-C2A-CAA-CBA
26	A3	320	CHL	C3A-C2A-CAA-CBA
26	A3	320	CHL	C2A-CAA-CBA-CGA
26	A6	606	CHL	CBD-CGD-O2D-CED
19	A3	319	LHG	C8-C7-O7-C5
17	AA	823	CLA	O1D-CGD-O2D-CED
17	AB	803	CLA	O1D-CGD-O2D-CED
17	AH	201	CLA	O1D-CGD-O2D-CED
17	AK	204	CLA	O1D-CGD-O2D-CED
17	A1	305	CLA	O1D-CGD-O2D-CED
17	A1	307	CLA	O1D-CGD-O2D-CED
17	A1	310	CLA	O1D-CGD-O2D-CED
17	A1	311	CLA	O1D-CGD-O2D-CED
17	A3	303	CLA	O1D-CGD-O2D-CED
17	AA	802	CLA	O1D-CGD-O2D-CED
17	AA	810	CLA	O1D-CGD-O2D-CED
17	AB	804	CLA	O1D-CGD-O2D-CED
17	AB	807	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	815	CLA	O1D-CGD-O2D-CED
17	AB	830	CLA	O1D-CGD-O2D-CED
17	AB	836	CLA	O1D-CGD-O2D-CED
17	AG	204	CLA	O1D-CGD-O2D-CED
17	A4	303	CLA	O1D-CGD-O2D-CED
17	AA	810	CLA	CBD-CGD-O2D-CED
17	AA	811	CLA	CBD-CGD-O2D-CED
17	AA	813	CLA	CBD-CGD-O2D-CED
17	AA	814	CLA	CBD-CGD-O2D-CED
17	AA	815	CLA	CBD-CGD-O2D-CED
17	AA	823	CLA	CBD-CGD-O2D-CED
17	AA	834	CLA	CBD-CGD-O2D-CED
17	AA	842	CLA	CBD-CGD-O2D-CED
17	AB	801	CLA	CBD-CGD-O2D-CED
17	AB	803	CLA	CBD-CGD-O2D-CED
17	AB	822	CLA	CBD-CGD-O2D-CED
17	AB	823	CLA	CBD-CGD-O2D-CED
17	AB	830	CLA	CBD-CGD-O2D-CED
17	AB	837	CLA	CBD-CGD-O2D-CED
17	AF	802	CLA	CBD-CGD-O2D-CED
17	A1	305	CLA	CBD-CGD-O2D-CED
17	A1	311	CLA	CBD-CGD-O2D-CED
17	A3	302	CLA	CBD-CGD-O2D-CED
17	A3	303	CLA	CBD-CGD-O2D-CED
17	A6	602	CLA	CBD-CGD-O2D-CED
26	A4	306	CHL	CBD-CGD-O2D-CED
26	A6	607	CHL	CBD-CGD-O2D-CED
17	AB	830	CLA	O1A-CGA-O2A-C1
26	A3	320	CHL	O1A-CGA-O2A-C1
17	AA	834	CLA	C4C-C3C-CAC-CBC
17	AA	814	CLA	O1D-CGD-O2D-CED
17	AA	833	CLA	O1D-CGD-O2D-CED
17	AB	801	CLA	O1D-CGD-O2D-CED
17	AG	203	CLA	O1D-CGD-O2D-CED
26	A3	307	CHL	O1D-CGD-O2D-CED
26	A4	306	CHL	O1D-CGD-O2D-CED
17	AA	834	CLA	C2C-C3C-CAC-CBC
17	AA	801	CLA	O1D-CGD-O2D-CED
17	AA	811	CLA	O1D-CGD-O2D-CED
17	AB	816	CLA	O1D-CGD-O2D-CED
17	AF	802	CLA	O1D-CGD-O2D-CED
17	AF	803	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	A1	313	CLA	O1D-CGD-O2D-CED
17	A3	309	CLA	O1D-CGD-O2D-CED
17	A4	302	CLA	O1D-CGD-O2D-CED
17	A4	313	CLA	O1D-CGD-O2D-CED
26	A6	607	CHL	O1D-CGD-O2D-CED
26	A3	320	CHL	CBA-CGA-O2A-C1
17	AA	820	CLA	CBD-CGD-O2D-CED
17	AA	821	CLA	CBD-CGD-O2D-CED
17	AA	826	CLA	CBD-CGD-O2D-CED
17	AA	829	CLA	CBD-CGD-O2D-CED
17	AA	831	CLA	CBD-CGD-O2D-CED
17	AA	836	CLA	CBD-CGD-O2D-CED
17	AB	802	CLA	CBD-CGD-O2D-CED
17	AB	811	CLA	CBD-CGD-O2D-CED
17	AB	820	CLA	CBD-CGD-O2D-CED
17	AB	832	CLA	CBD-CGD-O2D-CED
17	AB	838	CLA	CBD-CGD-O2D-CED
17	AL	304	CLA	CBD-CGD-O2D-CED
17	A4	308	CLA	CBD-CGD-O2D-CED
17	A6	612	CLA	CBD-CGD-O2D-CED
17	AA	817	CLA	O1A-CGA-O2A-C1
17	AA	821	CLA	O1A-CGA-O2A-C1
17	AL	303	CLA	O1A-CGA-O2A-C1
17	A3	303	CLA	O1A-CGA-O2A-C1
19	A1	301	LHG	O10-C23-O8-C6
19	A6	617	LHG	O10-C23-O8-C6
26	A1	303	CHL	O1A-CGA-O2A-C1
17	AA	828	CLA	O1D-CGD-O2D-CED
17	A1	306	CLA	O1D-CGD-O2D-CED
17	A4	312	CLA	O1D-CGD-O2D-CED
26	A6	606	CHL	O1D-CGD-O2D-CED
17	AB	834	CLA	O1D-CGD-O2D-CED
22	AL	301	LMU	O5B-C1B-O1B-C4'
17	AB	825	CLA	CBD-CGD-O2D-CED
17	A6	613	CLA	CBD-CGD-O2D-CED
17	AA	815	CLA	O1D-CGD-O2D-CED
17	AB	810	CLA	O1D-CGD-O2D-CED
23	AB	851	DGD	O1B-C1B-O2G-C2G
17	AA	833	CLA	O1A-CGA-O2A-C1
17	AA	829	CLA	C3-C5-C6-C7
17	AB	810	CLA	C3-C5-C6-C7
17	AB	812	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	820	CLA	C3-C5-C6-C7
17	AB	835	CLA	C3-C5-C6-C7
17	AB	840	CLA	C3-C5-C6-C7
17	AB	841	CLA	C3-C5-C6-C7
17	AH	201	CLA	C3-C5-C6-C7
17	A1	314	CLA	C3-C5-C6-C7
17	A6	602	CLA	C3-C5-C6-C7
17	A6	612	CLA	C3-C5-C6-C7
17	AA	811	CLA	CBA-CGA-O2A-C1
17	AA	812	CLA	CBA-CGA-O2A-C1
17	AA	842	CLA	CBA-CGA-O2A-C1
17	AB	830	CLA	CBA-CGA-O2A-C1
17	AL	303	CLA	CBA-CGA-O2A-C1
17	A1	314	CLA	CBA-CGA-O2A-C1
19	A1	301	LHG	C24-C23-O8-C6
26	A1	303	CHL	CBA-CGA-O2A-C1
17	AB	822	CLA	O1D-CGD-O2D-CED
17	AA	832	CLA	CBD-CGD-O2D-CED
17	AK	204	CLA	O1A-CGA-O2A-C1
17	AA	812	CLA	C4-C3-C5-C6
17	AA	838	CLA	CBD-CGD-O2D-CED
17	A1	304	CLA	CBD-CGD-O2D-CED
17	A1	316	CLA	CBD-CGD-O2D-CED
17	AA	817	CLA	C2A-CAA-CBA-CGA
17	AA	821	CLA	C2A-CAA-CBA-CGA
17	AA	833	CLA	C2A-CAA-CBA-CGA
17	AB	811	CLA	C2A-CAA-CBA-CGA
17	AB	811	CLA	O1A-CGA-O2A-C1
19	A3	319	LHG	O9-C7-O7-C5
17	AB	823	CLA	C3-C5-C6-C7
17	AB	833	CLA	C3-C5-C6-C7
17	AA	817	CLA	CBA-CGA-O2A-C1
17	AA	821	CLA	CBA-CGA-O2A-C1
17	AA	826	CLA	CBA-CGA-O2A-C1
17	AA	832	CLA	CBA-CGA-O2A-C1
17	AA	833	CLA	CBA-CGA-O2A-C1
17	AA	838	CLA	CBA-CGA-O2A-C1
17	AB	817	CLA	CBA-CGA-O2A-C1
17	A1	306	CLA	CBA-CGA-O2A-C1
17	A3	303	CLA	CBA-CGA-O2A-C1
19	A6	617	LHG	C24-C23-O8-C6
22	AB	852	LMU	O5'-C5'-C6'-O6'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	AB	843	PQN	C11-C12-C13-C14
17	AA	812	CLA	CBD-CGD-O2D-CED
17	AA	830	CLA	CBD-CGD-O2D-CED
17	AB	805	CLA	CBD-CGD-O2D-CED
17	AA	813	CLA	O1D-CGD-O2D-CED
25	A4	318	LMG	O9-C10-O7-C8
23	AB	851	DGD	C4E-C5E-C6E-O5E
17	AA	810	CLA	O1A-CGA-O2A-C1
17	AA	811	CLA	O1A-CGA-O2A-C1
17	AA	837	CLA	O1A-CGA-O2A-C1
17	AB	803	CLA	O1A-CGA-O2A-C1
17	AB	842	CLA	O1A-CGA-O2A-C1
17	A1	314	CLA	O1A-CGA-O2A-C1
17	AA	819	CLA	CBD-CGD-O2D-CED
17	AA	840	CLA	CBD-CGD-O2D-CED
17	AB	814	CLA	CBD-CGD-O2D-CED
17	AB	819	CLA	CBD-CGD-O2D-CED
17	AB	840	CLA	CBD-CGD-O2D-CED
17	AB	842	CLA	CBD-CGD-O2D-CED
17	AA	842	CLA	O1D-CGD-O2D-CED
17	AB	823	CLA	O1D-CGD-O2D-CED
19	AJ	104	LHG	O2-C2-C3-O3
17	AA	805	CLA	C3-C5-C6-C7
17	AA	833	CLA	C3-C5-C6-C7
17	AF	802	CLA	C3-C5-C6-C7
17	AA	810	CLA	CBA-CGA-O2A-C1
17	AA	837	CLA	CBA-CGA-O2A-C1
17	AB	827	CLA	CBA-CGA-O2A-C1
19	A3	319	LHG	C24-C23-O8-C6
17	AA	812	CLA	O1A-CGA-O2A-C1
17	AA	842	CLA	O1A-CGA-O2A-C1
17	AB	817	CLA	O1A-CGA-O2A-C1
22	AB	850	LMU	O5'-C5'-C6'-O6'
22	AB	852	LMU	C4'-C5'-C6'-O6'
17	AA	834	CLA	O1D-CGD-O2D-CED
17	A3	302	CLA	O1D-CGD-O2D-CED
17	A6	602	CLA	O1D-CGD-O2D-CED
17	AL	302	CLA	CBD-CGD-O2D-CED
22	AA	851	LMU	O5B-C5B-C6B-O6B
19	A3	319	LHG	O10-C23-O8-C6
22	AB	853	LMU	O5'-C5'-C6'-O6'
22	AB	850	LMU	C4'-C5'-C6'-O6'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AA	828	CLA	C3-C5-C6-C7
17	AB	803	CLA	CBA-CGA-O2A-C1
17	AB	811	CLA	CBA-CGA-O2A-C1
17	AB	815	CLA	CBA-CGA-O2A-C1
17	AB	842	CLA	CBA-CGA-O2A-C1
17	A4	308	CLA	O1D-CGD-O2D-CED
17	AA	826	CLA	O1A-CGA-O2A-C1
17	AA	832	CLA	O1A-CGA-O2A-C1
23	AB	851	DGD	O6E-C5E-C6E-O5E
17	AA	824	CLA	C4-C3-C5-C6
17	AA	824	CLA	C2-C3-C5-C6
17	AB	819	CLA	C2-C3-C5-C6
17	AA	836	CLA	C2A-CAA-CBA-CGA
17	A4	313	CLA	C2A-CAA-CBA-CGA
17	AA	838	CLA	O1A-CGA-O2A-C1
17	AB	819	CLA	O1A-CGA-O2A-C1
17	AB	827	CLA	O1A-CGA-O2A-C1
17	A1	306	CLA	O1A-CGA-O2A-C1
22	AL	301	LMU	O5'-C1'-O1'-C1
23	AB	851	DGD	O6D-C1D-O3G-C3G
17	AA	827	CLA	CBA-CGA-O2A-C1
17	AB	819	CLA	CBA-CGA-O2A-C1
17	AB	832	CLA	CBA-CGA-O2A-C1
17	AB	838	CLA	CBA-CGA-O2A-C1
17	AA	831	CLA	O1D-CGD-O2D-CED
17	AB	832	CLA	O1D-CGD-O2D-CED
17	AB	837	CLA	O1D-CGD-O2D-CED
17	AA	821	CLA	O1D-CGD-O2D-CED
22	AB	853	LMU	C4'-C5'-C6'-O6'
17	AB	815	CLA	O1A-CGA-O2A-C1
17	AB	832	CLA	O1A-CGA-O2A-C1
17	AA	813	CLA	C3-C5-C6-C7
17	AB	838	CLA	O1D-CGD-O2D-CED
17	AA	806	CLA	CBA-CGA-O2A-C1
17	AA	808	CLA	CBA-CGA-O2A-C1
17	AA	819	CLA	CBA-CGA-O2A-C1
17	AA	834	CLA	CBA-CGA-O2A-C1
17	AA	839	CLA	CBA-CGA-O2A-C1
17	AB	812	CLA	CBA-CGA-O2A-C1
17	AB	818	CLA	CBA-CGA-O2A-C1
17	AB	822	CLA	CBA-CGA-O2A-C1
17	AB	829	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	834	CLA	CBA-CGA-O2A-C1
17	AB	841	CLA	CBA-CGA-O2A-C1
17	AF	802	CLA	CBA-CGA-O2A-C1
19	A1	302	LHG	C24-C23-O8-C6
22	AL	301	LMU	C5'-C4'-O1B-C1B
17	AA	827	CLA	C15-C16-C17-C18
17	AA	832	CLA	C5-C6-C7-C8
17	AB	838	CLA	C5-C6-C7-C8
19	A3	319	LHG	O2-C2-C3-O3
22	AA	851	LMU	C2'-C1'-O1'-C1
17	AB	834	CLA	O1A-CGA-O2A-C1
17	AA	812	CLA	C2-C3-C5-C6
17	AA	821	CLA	C11-C10-C8-C9
17	AA	825	CLA	C11-C12-C13-C14
17	AA	827	CLA	C6-C7-C8-C9
17	AA	840	CLA	C11-C12-C13-C14
17	AB	801	CLA	C6-C7-C8-C9
17	AB	804	CLA	C11-C12-C13-C14
17	AB	815	CLA	C14-C13-C15-C16
17	AB	823	CLA	C6-C7-C8-C9
17	AB	829	CLA	C14-C13-C15-C16
17	AB	842	CLA	C14-C13-C15-C16
17	AA	820	CLA	O1D-CGD-O2D-CED
17	AA	829	CLA	O1D-CGD-O2D-CED
17	AA	836	CLA	O1D-CGD-O2D-CED
17	AB	811	CLA	O1D-CGD-O2D-CED
17	A6	612	CLA	O1D-CGD-O2D-CED
17	AA	802	CLA	C2A-CAA-CBA-CGA
17	AB	802	CLA	C2A-CAA-CBA-CGA
17	AB	840	CLA	C2A-CAA-CBA-CGA
20	AA	845	BCR	C7-C8-C9-C34
20	AA	846	BCR	C37-C22-C23-C24
20	AA	847	BCR	C11-C12-C13-C35
20	AB	845	BCR	C7-C8-C9-C34
20	AK	205	BCR	C37-C22-C23-C24
20	AK	205	BCR	C21-C22-C23-C24
17	AA	808	CLA	O1A-CGA-O2A-C1
17	AA	819	CLA	O1A-CGA-O2A-C1
17	AB	812	CLA	O1A-CGA-O2A-C1
17	AB	818	CLA	O1A-CGA-O2A-C1
17	AF	802	CLA	O1A-CGA-O2A-C1
17	AB	807	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	826	CLA	CBA-CGA-O2A-C1
17	A4	311	CLA	CBA-CGA-O2A-C1
17	AA	803	CLA	C15-C16-C17-C18
17	AA	842	CLA	C5-C6-C7-C8
17	AB	801	CLA	C13-C15-C16-C17
17	AB	823	CLA	C8-C10-C11-C12
17	AB	825	CLA	C10-C11-C12-C13
17	AB	825	CLA	C13-C15-C16-C17
17	AB	835	CLA	C8-C10-C11-C12
17	AB	838	CLA	C15-C16-C17-C18
17	AB	802	CLA	O1D-CGD-O2D-CED
17	AB	820	CLA	O1D-CGD-O2D-CED
22	AB	850	LMU	O5B-C1B-O1B-C4'
17	AB	833	CLA	CBD-CGD-O2D-CED
17	AA	806	CLA	C5-C6-C7-C8
17	AA	833	CLA	C15-C16-C17-C18
17	AA	841	CLA	C15-C16-C17-C18
17	AB	801	CLA	C15-C16-C17-C18
17	AB	803	CLA	C10-C11-C12-C13
17	AB	806	CLA	C13-C15-C16-C17
17	AB	815	CLA	C8-C10-C11-C12
17	A6	602	CLA	C13-C15-C16-C17
17	A6	612	CLA	C13-C15-C16-C17
18	AB	843	PQN	C15-C16-C17-C18
17	AA	826	CLA	O1D-CGD-O2D-CED
17	AL	304	CLA	O1D-CGD-O2D-CED
25	A1	321	LMG	C10-C11-C12-C13
25	A1	321	LMG	C28-C29-C30-C31
17	AA	805	CLA	C8-C10-C11-C12
17	AA	810	CLA	C13-C15-C16-C17
17	AA	840	CLA	C5-C6-C7-C8
17	AB	802	CLA	C15-C16-C17-C18
17	AH	201	CLA	CBA-CGA-O2A-C1
22	AL	301	LMU	O5B-C5B-C6B-O6B
17	AA	825	CLA	C2-C1-O2A-CGA
17	AB	803	CLA	C13-C15-C16-C17
17	AB	811	CLA	C8-C10-C11-C12
17	AB	829	CLA	C8-C10-C11-C12
17	A3	302	CLA	C10-C11-C12-C13
18	AA	843	PQN	C25-C26-C27-C28
18	AB	843	PQN	C25-C26-C27-C28
26	A6	605	CHL	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AA	806	CLA	C11-C12-C13-C15
17	AB	826	CLA	C11-C10-C8-C7
17	AB	827	CLA	C3-C5-C6-C7
17	AA	806	CLA	O1A-CGA-O2A-C1
17	AA	827	CLA	O1A-CGA-O2A-C1
17	AA	834	CLA	O1A-CGA-O2A-C1
17	AB	829	CLA	O1A-CGA-O2A-C1
17	AB	841	CLA	O1A-CGA-O2A-C1
19	A1	302	LHG	O10-C23-O8-C6
22	AB	852	LMU	O1'-C1-C2-C3
17	AA	808	CLA	C2A-CAA-CBA-CGA
17	AG	201	CLA	C2A-CAA-CBA-CGA
17	A3	312	CLA	C2A-CAA-CBA-CGA
17	A6	601	CLA	C2A-CAA-CBA-CGA
17	AA	805	CLA	C13-C15-C16-C17
17	AA	827	CLA	C10-C11-C12-C13
17	AB	807	CLA	C13-C15-C16-C17
17	AA	839	CLA	O1A-CGA-O2A-C1
17	AB	822	CLA	O1A-CGA-O2A-C1
18	AA	843	PQN	C13-C15-C16-C17
17	AA	829	CLA	C8-C10-C11-C12
17	AA	829	CLA	C10-C11-C12-C13
17	AA	833	CLA	C5-C6-C7-C8
17	AB	829	CLA	C10-C11-C12-C13
17	AB	832	CLA	C13-C15-C16-C17
17	AB	834	CLA	C15-C16-C17-C18
18	AA	843	PQN	C20-C21-C22-C23
17	AA	830	CLA	CBA-CGA-O2A-C1
17	AB	838	CLA	O1A-CGA-O2A-C1
17	AH	201	CLA	O1A-CGA-O2A-C1
17	A4	311	CLA	O1A-CGA-O2A-C1
22	AB	850	LMU	O1'-C1-C2-C3
17	A6	613	CLA	O1D-CGD-O2D-CED
17	AA	828	CLA	C8-C10-C11-C12
17	AB	808	CLA	CAA-CBA-CGA-O2A
17	AA	813	CLA	C8-C10-C11-C12
17	AA	826	CLA	C5-C6-C7-C8
17	AA	828	CLA	C10-C11-C12-C13
17	AA	841	CLA	C13-C15-C16-C17
17	AB	827	CLA	C5-C6-C7-C8
17	AB	827	CLA	C10-C11-C12-C13
17	AB	834	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	A1	302	LHG	C3-O3-P-O6
19	A1	302	LHG	C4-O6-P-O3
19	A6	617	LHG	C3-O3-P-O6
19	A6	617	LHG	C4-O6-P-O3
17	AB	801	CLA	C3-C5-C6-C7
17	AA	803	CLA	CBA-CGA-O2A-C1
17	A4	308	CLA	CBA-CGA-O2A-C1
17	AA	819	CLA	C13-C15-C16-C17
17	AB	842	CLA	C8-C10-C11-C12
17	AA	838	CLA	O1D-CGD-O2D-CED
17	AB	825	CLA	O1D-CGD-O2D-CED
17	AA	832	CLA	O1D-CGD-O2D-CED
19	AJ	104	LHG	C1-C2-C3-O3
17	AB	815	CLA	C13-C15-C16-C17
17	AA	824	CLA	C2A-CAA-CBA-CGA
17	AA	806	CLA	C16-C17-C18-C19
17	AB	804	CLA	CBA-CGA-O2A-C1
17	AB	823	CLA	CBA-CGA-O2A-C1
17	A4	313	CLA	CBA-CGA-O2A-C1
17	AA	828	CLA	C13-C15-C16-C17
17	AA	806	CLA	C13-C15-C16-C17
17	AA	830	CLA	C8-C10-C11-C12
17	AB	805	CLA	O1D-CGD-O2D-CED
17	A6	612	CLA	C2A-CAA-CBA-CGA
19	AJ	104	LHG	C18-C19-C20-C21
19	A1	320	LHG	C11-C12-C13-C14
25	A4	318	LMG	C12-C13-C14-C15
17	AB	826	CLA	O1A-CGA-O2A-C1
17	AA	830	CLA	O1D-CGD-O2D-CED
17	A1	304	CLA	O1D-CGD-O2D-CED
17	A1	316	CLA	O1D-CGD-O2D-CED
17	AB	810	CLA	C16-C17-C18-C19
17	AB	817	CLA	C6-C7-C8-C10
17	AA	801	CLA	CBA-CGA-O2A-C1
23	AB	851	DGD	CAA-CBA-CCA-CDA
17	AA	812	CLA	O1D-CGD-O2D-CED
25	A4	318	LMG	C13-C14-C15-C16
17	AA	825	CLA	C15-C16-C17-C18
17	AB	832	CLA	C8-C10-C11-C12
19	A1	320	LHG	C33-C34-C35-C36
17	AA	801	CLA	C3-C5-C6-C7
17	AA	809	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	806	CLA	CBA-CGA-O2A-C1
17	A1	305	CLA	CBA-CGA-O2A-C1
19	A1	301	LHG	C24-C25-C26-C27
25	A4	318	LMG	C29-C30-C31-C32
17	AA	828	CLA	C15-C16-C17-C18
17	AA	833	CLA	C13-C15-C16-C17
17	A4	313	CLA	O1A-CGA-O2A-C1
17	AA	819	CLA	C16-C17-C18-C19
17	AA	819	CLA	C16-C17-C18-C20
17	A3	312	CLA	C6-C7-C8-C10
17	A4	301	CLA	C11-C12-C13-C15
17	AA	819	CLA	O1D-CGD-O2D-CED
17	AA	840	CLA	O1D-CGD-O2D-CED
18	AA	843	PQN	C11-C12-C13-C14
19	AA	844	LHG	C10-C11-C12-C13
22	AL	301	LMU	C3'-C4'-O1B-C1B
23	AB	851	DGD	C3A-C4A-C5A-C6A
17	AA	819	CLA	C11-C12-C13-C14
17	AB	803	CLA	C11-C10-C8-C9
17	AB	811	CLA	C14-C13-C15-C16
17	AB	823	CLA	C11-C12-C13-C14
17	A1	314	CLA	C6-C7-C8-C9
22	AA	851	LMU	C4-C5-C6-C7
17	AA	817	CLA	C10-C11-C12-C13
19	AA	844	LHG	C16-C17-C18-C19
19	A3	301	LHG	O1-C1-C2-C3
17	AA	827	CLA	C3-C5-C6-C7
19	A6	617	LHG	C8-C7-O7-C5
19	AJ	104	LHG	C7-C8-C9-C10
17	AB	810	CLA	C16-C17-C18-C20
17	AB	812	CLA	C6-C7-C8-C9
17	AB	817	CLA	C6-C7-C8-C9
17	A6	602	CLA	C10-C11-C12-C13
22	AA	851	LMU	C3-C4-C5-C6
22	AB	852	LMU	C11-C10-C9-C8
23	AB	851	DGD	C9B-CAB-CBB-CCB
17	AB	831	CLA	CBD-CGD-O2D-CED
17	AA	829	CLA	C5-C6-C7-C8
17	AA	804	CLA	CBA-CGA-O2A-C1
17	AB	821	CLA	CBA-CGA-O2A-C1
17	AA	803	CLA	C3A-C2A-CAA-CBA
17	AA	825	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	828	CLA	C3A-C2A-CAA-CBA
17	AB	829	CLA	C3A-C2A-CAA-CBA
17	AB	834	CLA	C3A-C2A-CAA-CBA
17	AK	204	CLA	C3A-C2A-CAA-CBA
17	A1	316	CLA	C3A-C2A-CAA-CBA
17	A6	611	CLA	C3A-C2A-CAA-CBA
17	AB	840	CLA	O1D-CGD-O2D-CED
17	AA	803	CLA	O1A-CGA-O2A-C1
17	AA	830	CLA	O1A-CGA-O2A-C1
17	AB	823	CLA	O1A-CGA-O2A-C1
17	A4	308	CLA	O1A-CGA-O2A-C1
17	AA	808	CLA	C16-C17-C18-C19
17	AB	812	CLA	C6-C7-C8-C10
17	AB	835	CLA	C11-C12-C13-C14
17	AB	835	CLA	C11-C12-C13-C15
17	A4	301	CLA	C11-C12-C13-C14
17	AB	814	CLA	O1D-CGD-O2D-CED
22	AB	853	LMU	O5B-C5B-C6B-O6B
17	AB	821	CLA	CBD-CGD-O2D-CED
17	AB	804	CLA	C5-C6-C7-C8
18	AB	843	PQN	C14-C13-C15-C16
17	AA	831	CLA	CBA-CGA-O2A-C1
19	AA	844	LHG	C33-C34-C35-C36
17	A1	305	CLA	O1A-CGA-O2A-C1
17	AA	805	CLA	C16-C17-C18-C19
22	AB	850	LMU	C1-C2-C3-C4
17	AA	801	CLA	O1A-CGA-O2A-C1
17	AA	809	CLA	O1A-CGA-O2A-C1
17	AB	804	CLA	O1A-CGA-O2A-C1
17	AB	806	CLA	O1A-CGA-O2A-C1
19	A6	617	LHG	O9-C7-O7-C5
17	AB	804	CLA	C2-C1-O2A-CGA
17	AB	821	CLA	O1A-CGA-O2A-C1
17	AA	811	CLA	C3-C5-C6-C7
17	AB	811	CLA	C3-C5-C6-C7
20	AA	846	BCR	C5-C6-C7-C8
20	AA	846	BCR	C23-C24-C25-C30
20	AA	847	BCR	C1-C6-C7-C8
20	AA	847	BCR	C23-C24-C25-C26
20	AA	848	BCR	C1-C6-C7-C8
20	AA	848	BCR	C5-C6-C7-C8
20	AA	849	BCR	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	AA	849	BCR	C23-C24-C25-C30
20	AB	844	BCR	C1-C6-C7-C8
20	AB	844	BCR	C23-C24-C25-C26
20	AB	844	BCR	C23-C24-C25-C30
20	AB	846	BCR	C1-C6-C7-C8
20	AB	846	BCR	C5-C6-C7-C8
20	AF	805	BCR	C1-C6-C7-C8
20	AF	805	BCR	C5-C6-C7-C8
20	AG	205	BCR	C23-C24-C25-C26
20	AI	101	BCR	C23-C24-C25-C26
20	AJ	103	BCR	C1-C6-C7-C8
20	AJ	103	BCR	C23-C24-C25-C26
20	AK	202	BCR	C5-C6-C7-C8
20	AK	205	BCR	C23-C24-C25-C26
20	AK	205	BCR	C23-C24-C25-C30
20	AL	306	BCR	C1-C6-C7-C8
20	AL	306	BCR	C5-C6-C7-C8
20	A3	318	BCR	C1-C6-C7-C8
20	A3	318	BCR	C5-C6-C7-C8
20	A4	317	BCR	C1-C6-C7-C8
20	A4	317	BCR	C5-C6-C7-C8
20	A6	616	BCR	C1-C6-C7-C8
22	AL	301	LMU	C2-C3-C4-C5
17	AA	827	CLA	C8-C10-C11-C12
17	AA	804	CLA	O1A-CGA-O2A-C1
19	A1	301	LHG	C7-C8-C9-C10
19	A1	301	LHG	C23-C24-C25-C26
17	AB	819	CLA	O1D-CGD-O2D-CED
17	AA	827	CLA	C4-C3-C5-C6
17	AB	815	CLA	C4-C3-C5-C6
17	AA	811	CLA	C12-C13-C15-C16
17	AA	813	CLA	C6-C7-C8-C10
17	AA	821	CLA	C2-C3-C5-C6
17	AA	827	CLA	C2-C3-C5-C6
17	AB	815	CLA	C2-C3-C5-C6
17	AB	823	CLA	C11-C12-C13-C15
17	AB	834	CLA	C11-C12-C13-C15
17	AB	842	CLA	C12-C13-C15-C16
17	A4	311	CLA	C6-C7-C8-C10
18	AB	843	PQN	C21-C22-C23-C25
17	AA	803	CLA	C3-C5-C6-C7
17	AA	831	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	802	CLA	C5-C6-C7-C8
17	AB	806	CLA	C8-C10-C11-C12
17	AL	303	CLA	C11-C12-C13-C14
17	AA	812	CLA	C2A-CAA-CBA-CGA
17	AB	814	CLA	C2A-CAA-CBA-CGA
22	AB	850	LMU	C3'-C4'-O1B-C1B
17	AB	842	CLA	O1D-CGD-O2D-CED
17	AL	302	CLA	O1D-CGD-O2D-CED
22	AB	850	LMU	C5'-C4'-O1B-C1B
25	AG	202	LMG	C11-C12-C13-C14
17	AB	835	CLA	CBD-CGD-O2D-CED
17	A3	312	CLA	C6-C7-C8-C9
19	A3	301	LHG	C11-C10-C9-C8
22	AB	850	LMU	C5-C6-C7-C8
25	AG	202	LMG	C10-C11-C12-C13
19	AA	844	LHG	C8-C7-O7-C5
20	AA	847	BCR	C10-C11-C12-C13
19	AJ	104	LHG	C14-C15-C16-C17
19	AA	844	LHG	O9-C7-O7-C5
17	AB	809	CLA	C3-C5-C6-C7
25	AG	202	LMG	C30-C31-C32-C33
22	AB	853	LMU	C2'-C1'-O1'-C1
17	AA	805	CLA	C16-C17-C18-C20
17	AA	806	CLA	C16-C17-C18-C20
17	AA	821	CLA	C4-C3-C5-C6
17	AA	834	CLA	C4-C3-C5-C6
17	AA	826	CLA	C2-C3-C5-C6
17	AA	834	CLA	C2-C3-C5-C6
19	A1	320	LHG	C30-C31-C32-C33
17	AA	803	CLA	C11-C12-C13-C14
17	AA	811	CLA	C14-C13-C15-C16
17	AB	826	CLA	C11-C10-C8-C9
17	A1	304	CLA	C11-C10-C8-C9
17	A4	301	CLA	C11-C10-C8-C9
17	A4	311	CLA	C6-C7-C8-C9
19	A6	617	LHG	C9-C10-C11-C12
17	AB	802	CLA	C3-C5-C6-C7
17	AL	303	CLA	C3-C5-C6-C7
17	A1	314	CLA	C2A-CAA-CBA-CGA
26	A6	607	CHL	C2A-CAA-CBA-CGA
22	AB	852	LMU	C5-C6-C7-C8
20	AA	848	BCR	C7-C8-C9-C34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	A1	314	CLA	C2C-C3C-CAC-CBC
20	AI	101	BCR	C21-C22-C23-C24
20	A1	319	BCR	C21-C22-C23-C24
17	AA	803	CLA	C1A-C2A-CAA-CBA
17	AA	805	CLA	C1A-C2A-CAA-CBA
17	AA	807	CLA	C1A-C2A-CAA-CBA
17	AA	810	CLA	C1A-C2A-CAA-CBA
17	AA	818	CLA	C1A-C2A-CAA-CBA
17	AA	819	CLA	C1A-C2A-CAA-CBA
17	AA	839	CLA	C1A-C2A-CAA-CBA
17	AB	819	CLA	C1A-C2A-CAA-CBA
17	AB	821	CLA	C1A-C2A-CAA-CBA
17	AB	833	CLA	C1A-C2A-CAA-CBA
17	AB	834	CLA	C1A-C2A-CAA-CBA
17	AB	839	CLA	C1A-C2A-CAA-CBA
17	AF	802	CLA	C1A-C2A-CAA-CBA
17	AH	201	CLA	C1A-C2A-CAA-CBA
17	AL	303	CLA	C1A-C2A-CAA-CBA
17	A1	316	CLA	C1A-C2A-CAA-CBA
17	A4	312	CLA	C1A-C2A-CAA-CBA
17	A6	611	CLA	C1A-C2A-CAA-CBA
17	AA	801	CLA	C16-C17-C18-C19
17	AB	815	CLA	C16-C17-C18-C20
17	AB	823	CLA	C16-C17-C18-C20
17	AA	810	CLA	CAD-CBD-CGD-O2D
17	A6	610	CLA	CMA-C3A-C4A-CHB
17	AB	817	CLA	C3-C5-C6-C7
17	AA	803	CLA	C5-C6-C7-C8
17	AA	803	CLA	C10-C11-C12-C13
17	AA	829	CLA	C15-C16-C17-C18
19	A1	301	LHG	C30-C31-C32-C33
23	AB	851	DGD	C9A-CAA-CBA-CCA
17	AA	822	CLA	C3A-C2A-CAA-CBA
17	A3	305	CLA	C3A-C2A-CAA-CBA
22	AB	852	LMU	C4-C5-C6-C7
23	AB	851	DGD	CCA-CDA-CEA-CFA
17	AB	803	CLA	C16-C17-C18-C20
19	A3	301	LHG	C4-C5-C6-O8
25	AG	202	LMG	O1-C7-C8-C9
25	A1	321	LMG	O1-C7-C8-C9
17	A6	603	CLA	C2A-CAA-CBA-CGA
19	A1	320	LHG	C8-C7-O7-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	808	CLA	C2A-CAA-CBA-CGA
17	AA	805	CLA	C4-C3-C5-C6
17	AA	826	CLA	C4-C3-C5-C6
17	AB	809	CLA	C4-C3-C5-C6
17	AB	842	CLA	C4-C3-C5-C6
17	AL	303	CLA	C8-C10-C11-C12
17	AB	829	CLA	C2A-CAA-CBA-CGA
17	A1	314	CLA	C15-C16-C17-C18
17	AB	801	CLA	C2-C1-O2A-CGA
23	AB	851	DGD	CCB-CDB-CEB-CFB
17	AA	842	CLA	C13-C15-C16-C17
17	AB	807	CLA	C5-C6-C7-C8
17	AB	801	CLA	C16-C17-C18-C20
17	AB	823	CLA	C16-C17-C18-C19
17	AL	303	CLA	C11-C12-C13-C15
17	AB	802	CLA	C8-C10-C11-C12
17	A1	314	CLA	C8-C10-C11-C12
17	AB	826	CLA	C10-C11-C12-C13
19	A3	301	LHG	O7-C5-C6-O8
25	A4	318	LMG	O1-C7-C8-O7
17	AB	801	CLA	C5-C6-C7-C8
26	A6	605	CHL	O1D-CGD-O2D-CED
23	AB	851	DGD	CDA-CEA-CFA-CGA
17	AB	808	CLA	C2-C1-O2A-CGA
17	A6	612	CLA	C2-C1-O2A-CGA
17	AA	804	CLA	C4-C3-C5-C6
17	AB	833	CLA	C4-C3-C5-C6
17	AA	801	CLA	C12-C13-C15-C16
17	AA	803	CLA	C11-C12-C13-C15
17	AA	805	CLA	C2-C3-C5-C6
17	AA	813	CLA	C11-C10-C8-C7
17	AA	819	CLA	C6-C7-C8-C10
17	AA	825	CLA	C11-C10-C8-C7
17	AA	827	CLA	C12-C13-C15-C16
17	AA	828	CLA	C6-C7-C8-C10
17	AA	829	CLA	C11-C12-C13-C15
17	AB	802	CLA	C12-C13-C15-C16
17	AB	803	CLA	C6-C7-C8-C10
17	AB	806	CLA	C11-C10-C8-C7
17	AB	807	CLA	C11-C12-C13-C15
17	AB	815	CLA	C11-C10-C8-C7
17	AB	815	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	819	CLA	C11-C10-C8-C7
17	AB	825	CLA	C12-C13-C15-C16
17	AB	841	CLA	C6-C7-C8-C10
17	AB	842	CLA	C2-C3-C5-C6
17	A1	304	CLA	C11-C10-C8-C7
17	A4	301	CLA	C11-C10-C8-C7
17	A6	602	CLA	C11-C12-C13-C15
18	AB	843	PQN	C17-C18-C20-C21
17	AA	803	CLA	C11-C10-C8-C9
17	AA	808	CLA	C11-C12-C13-C14
17	AA	813	CLA	C11-C10-C8-C9
17	AA	813	CLA	C11-C12-C13-C14
17	AA	821	CLA	C11-C12-C13-C14
17	AA	825	CLA	C11-C10-C8-C9
17	AA	827	CLA	C14-C13-C15-C16
17	AA	828	CLA	C6-C7-C8-C9
17	AA	830	CLA	C14-C13-C15-C16
17	AA	842	CLA	C11-C10-C8-C9
17	AB	802	CLA	C14-C13-C15-C16
17	AB	806	CLA	C11-C10-C8-C9
17	AB	807	CLA	C11-C12-C13-C14
17	AB	807	CLA	C14-C13-C15-C16
17	AB	810	CLA	C11-C10-C8-C9
17	AB	814	CLA	C6-C7-C8-C9
17	AB	825	CLA	C14-C13-C15-C16
17	AB	834	CLA	C11-C12-C13-C14
17	AA	825	CLA	CBA-CGA-O2A-C1
17	AB	840	CLA	CBA-CGA-O2A-C1
17	A6	609	CLA	CBA-CGA-O2A-C1
17	A4	311	CLA	C2A-CAA-CBA-CGA
20	A3	318	BCR	C37-C22-C23-C24
17	AB	828	CLA	C10-C11-C12-C13
20	AJ	103	BCR	C7-C8-C9-C10
17	AA	840	CLA	C3-C5-C6-C7
17	AB	833	CLA	O1D-CGD-O2D-CED
17	AB	829	CLA	C5-C6-C7-C8
17	AB	809	CLA	CBA-CGA-O2A-C1
22	AA	851	LMU	C7-C8-C9-C10
19	A1	320	LHG	O6-C4-C5-C6
17	AA	841	CLA	CBA-CGA-O2A-C1
17	AA	805	CLA	C10-C11-C12-C13
17	AF	802	CLA	C4-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AA	804	CLA	C2-C3-C5-C6
17	AB	809	CLA	C2-C3-C5-C6
17	AB	833	CLA	C2-C3-C5-C6
19	A1	320	LHG	O9-C7-O7-C5
23	AB	851	DGD	C4A-C5A-C6A-C7A
17	AB	817	CLA	C5-C6-C7-C8
17	AB	830	CLA	C5-C6-C7-C8
17	AA	824	CLA	CBA-CGA-O2A-C1
17	AB	820	CLA	CBA-CGA-O2A-C1
17	AA	805	CLA	C3A-C2A-CAA-CBA
17	AB	810	CLA	C3A-C2A-CAA-CBA
17	A1	309	CLA	C3A-C2A-CAA-CBA
17	A4	313	CLA	C3A-C2A-CAA-CBA
22	AB	853	LMU	C2-C1-O1'-C1'
22	AB	850	LMU	C9-C10-C11-C12
17	A3	303	CLA	C6-C7-C8-C10
17	AA	829	CLA	CBA-CGA-O2A-C1
26	A6	607	CHL	CBA-CGA-O2A-C1
23	AB	851	DGD	C1G-C2G-C3G-O3G
19	AA	844	LHG	C23-C24-C25-C26
17	AB	809	CLA	O1A-CGA-O2A-C1
19	A3	319	LHG	C4-O6-P-O3
17	AA	801	CLA	CAA-CBA-CGA-O2A
19	A3	301	LHG	O1-C1-C2-O2
17	AA	811	CLA	C13-C15-C16-C17
19	A1	320	LHG	C34-C35-C36-C37
19	A1	320	LHG	O6-C4-C5-O7
17	AA	825	CLA	O1A-CGA-O2A-C1
17	AB	840	CLA	O1A-CGA-O2A-C1
17	AA	801	CLA	C16-C17-C18-C20
17	AB	819	CLA	C11-C12-C13-C15
23	AB	851	DGD	C4B-C5B-C6B-C7B
17	A6	609	CLA	O1A-CGA-O2A-C1
26	A6	607	CHL	O1A-CGA-O2A-C1
17	AB	821	CLA	O1D-CGD-O2D-CED
25	AG	202	LMG	O1-C7-C8-O7
25	A1	321	LMG	O1-C7-C8-O7
25	A1	321	LMG	O7-C8-C9-O8
19	A1	320	LHG	C7-C8-C9-C10
17	A4	301	CLA	CBD-CGD-O2D-CED
17	AA	833	CLA	C2-C1-O2A-CGA
17	AB	829	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	A6	607	CHL	C2-C1-O2A-CGA
17	AF	802	CLA	C2-C3-C5-C6
17	AA	819	CLA	C6-C7-C8-C9
17	AB	803	CLA	C6-C7-C8-C9
17	AB	810	CLA	C11-C12-C13-C14
17	AB	819	CLA	C11-C10-C8-C9
17	AB	827	CLA	C11-C12-C13-C14
17	AB	830	CLA	C6-C7-C8-C9
17	AA	816	CLA	CBD-CGD-O2D-CED
25	A1	321	LMG	C11-C12-C13-C14
17	AB	818	CLA	C8-C10-C11-C12
17	AB	833	CLA	C10-C11-C12-C13
19	A6	617	LHG	C5-C4-O6-P
22	AA	851	LMU	C1-C2-C3-C4
19	A1	320	LHG	C11-C10-C9-C8
23	AB	851	DGD	C7A-C8A-C9A-CAA
17	AA	808	CLA	C16-C17-C18-C20
17	AB	815	CLA	C16-C17-C18-C19
20	AA	847	BCR	C23-C24-C25-C30
20	AI	101	BCR	C5-C6-C7-C8
20	AJ	103	BCR	C23-C24-C25-C30
20	AK	202	BCR	C1-C6-C7-C8
20	AL	305	BCR	C1-C6-C7-C8
17	AA	802	CLA	C15-C16-C17-C18
17	AB	831	CLA	O1D-CGD-O2D-CED
20	AA	847	BCR	C11-C12-C13-C14
20	AA	848	BCR	C7-C8-C9-C10
20	AB	849	BCR	C7-C8-C9-C10
20	AJ	101	BCR	C17-C18-C19-C20
20	AK	205	BCR	C7-C8-C9-C10
17	AB	803	CLA	C16-C17-C18-C19
17	AB	814	CLA	C15-C16-C17-C18
19	AJ	104	LHG	O6-C4-C5-C6
17	AA	803	CLA	C11-C10-C8-C7
17	AA	808	CLA	C11-C12-C13-C15
17	AA	810	CLA	C6-C7-C8-C10
17	AA	813	CLA	C11-C12-C13-C15
17	AA	819	CLA	C11-C12-C13-C15
17	AA	821	CLA	C6-C7-C8-C10
17	AA	827	CLA	C6-C7-C8-C10
17	AA	828	CLA	C12-C13-C15-C16
17	AA	830	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AA	842	CLA	C11-C10-C8-C7
17	AB	801	CLA	C6-C7-C8-C10
17	AB	801	CLA	C11-C10-C8-C7
17	AB	802	CLA	C6-C7-C8-C10
17	AB	803	CLA	C11-C10-C8-C7
17	AB	807	CLA	C12-C13-C15-C16
17	AB	809	CLA	C6-C7-C8-C10
17	AB	810	CLA	C11-C10-C8-C7
17	AB	814	CLA	C6-C7-C8-C10
17	AB	818	CLA	C6-C7-C8-C10
17	AB	823	CLA	C6-C7-C8-C10
17	AB	830	CLA	C6-C7-C8-C10
17	AB	834	CLA	C6-C7-C8-C10
17	A1	314	CLA	C11-C10-C8-C7
23	AB	851	DGD	C5A-C6A-C7A-C8A
17	A6	611	CLA	CBD-CGD-O2D-CED
17	AB	801	CLA	C16-C17-C18-C19
17	A3	303	CLA	C6-C7-C8-C9
22	AL	301	LMU	C1-C2-C3-C4
25	A4	318	LMG	C29-C28-O8-C9
19	A1	301	LHG	C11-C12-C13-C14
17	AA	830	CLA	C5-C6-C7-C8
17	AB	819	CLA	C5-C6-C7-C8
17	AB	826	CLA	C8-C10-C11-C12
17	AA	841	CLA	O1A-CGA-O2A-C1
17	AA	830	CLA	C10-C11-C12-C13
17	AA	840	CLA	CBA-CGA-O2A-C1
17	A1	304	CLA	CBA-CGA-O2A-C1
22	AL	301	LMU	C3-C4-C5-C6
19	AA	844	LHG	C25-C26-C27-C28
22	AL	301	LMU	C5-C6-C7-C8
19	AA	844	LHG	C31-C32-C33-C34
19	A6	617	LHG	C26-C27-C28-C29
17	AA	804	CLA	CAD-CBD-CGD-O2D
17	AA	806	CLA	CAD-CBD-CGD-O2D
17	AA	807	CLA	CAD-CBD-CGD-O2D
17	AA	815	CLA	CAD-CBD-CGD-O2D
17	AA	816	CLA	CAD-CBD-CGD-O2D
17	AA	825	CLA	CAD-CBD-CGD-O2D
17	AA	833	CLA	CAD-CBD-CGD-O2D
17	AA	841	CLA	CAD-CBD-CGD-O2D
17	AB	810	CLA	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	811	CLA	CAD-CBD-CGD-O2D
17	AB	813	CLA	CAD-CBD-CGD-O2D
17	AB	815	CLA	CAD-CBD-CGD-O2D
17	AB	816	CLA	CAD-CBD-CGD-O2D
17	AB	817	CLA	CAD-CBD-CGD-O2D
17	AB	823	CLA	CAD-CBD-CGD-O2D
17	AB	828	CLA	CAD-CBD-CGD-O2D
17	AB	833	CLA	CAD-CBD-CGD-O2D
17	AG	203	CLA	CAD-CBD-CGD-O2D
17	AH	201	CLA	CAD-CBD-CGD-O2D
17	A1	311	CLA	CAD-CBD-CGD-O2D
17	A6	609	CLA	CAD-CBD-CGD-O2D
19	A3	319	LHG	C6-C5-O7-C7
17	AA	834	CLA	C5-C6-C7-C8
17	AH	201	CLA	C5-C6-C7-C8
17	AB	842	CLA	C16-C17-C18-C19
19	AJ	104	LHG	O6-C4-C5-O7
17	AA	805	CLA	C2C-C3C-CAC-CBC
25	A1	321	LMG	C30-C31-C32-C33
19	AA	844	LHG	C30-C31-C32-C33
17	A1	304	CLA	O1A-CGA-O2A-C1
17	AA	808	CLA	CHA-CBD-CGD-O1D
17	AA	808	CLA	CHA-CBD-CGD-O2D
17	AA	814	CLA	CHA-CBD-CGD-O2D
17	AA	829	CLA	CHA-CBD-CGD-O2D
17	AA	834	CLA	CHA-CBD-CGD-O1D
17	AA	834	CLA	CHA-CBD-CGD-O2D
17	AA	836	CLA	CHA-CBD-CGD-O1D
17	AA	836	CLA	CHA-CBD-CGD-O2D
17	AA	839	CLA	CHA-CBD-CGD-O1D
17	AA	839	CLA	CHA-CBD-CGD-O2D
17	AB	802	CLA	CHA-CBD-CGD-O1D
17	AB	802	CLA	CHA-CBD-CGD-O2D
17	AB	809	CLA	CHA-CBD-CGD-O1D
17	AB	809	CLA	CHA-CBD-CGD-O2D
17	AB	814	CLA	CHA-CBD-CGD-O1D
17	AB	821	CLA	CHA-CBD-CGD-O1D
17	AB	824	CLA	CHA-CBD-CGD-O2D
17	AB	825	CLA	CHA-CBD-CGD-O1D
17	AB	825	CLA	CHA-CBD-CGD-O2D
17	AB	827	CLA	CHA-CBD-CGD-O1D
17	AB	827	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AB	837	CLA	CHA-CBD-CGD-O1D
17	AB	842	CLA	CHA-CBD-CGD-O1D
17	AB	842	CLA	CHA-CBD-CGD-O2D
17	AF	804	CLA	CHA-CBD-CGD-O2D
17	AL	304	CLA	CHA-CBD-CGD-O1D
17	A1	305	CLA	CHA-CBD-CGD-O1D
17	A1	305	CLA	CHA-CBD-CGD-O2D
17	A1	316	CLA	CHA-CBD-CGD-O1D
17	A1	316	CLA	CHA-CBD-CGD-O2D
17	A6	610	CLA	CHA-CBD-CGD-O1D
17	A6	610	CLA	CHA-CBD-CGD-O2D
17	AA	829	CLA	O1A-CGA-O2A-C1
17	AB	820	CLA	O1A-CGA-O2A-C1
19	A1	302	LHG	C10-C11-C12-C13
17	AB	835	CLA	O1D-CGD-O2D-CED
19	A6	617	LHG	O7-C5-C6-O8
17	AA	805	CLA	C5-C6-C7-C8
17	AA	824	CLA	O1A-CGA-O2A-C1
17	AA	829	CLA	CAA-CBA-CGA-O2A
19	A1	320	LHG	C25-C26-C27-C28
17	AB	828	CLA	C4-C3-C5-C6
17	AA	840	CLA	C11-C10-C8-C9
17	AB	802	CLA	C6-C7-C8-C9
17	AB	804	CLA	C11-C10-C8-C9
17	AB	814	CLA	C11-C12-C13-C14
17	AB	818	CLA	C6-C7-C8-C9
17	AB	828	CLA	C11-C10-C8-C9
17	A6	612	CLA	CBA-CGA-O2A-C1
17	AB	823	CLA	C5-C6-C7-C8
18	AA	843	PQN	C18-C20-C21-C22
22	AA	851	LMU	C4'-C5'-C6'-O6'
23	AB	851	DGD	C8B-C9B-CAB-CBB
20	AI	101	BCR	C37-C22-C23-C24
20	AK	205	BCR	C7-C8-C9-C34
20	A1	319	BCR	C37-C22-C23-C24
19	AJ	104	LHG	C16-C17-C18-C19
25	A1	321	LMG	C33-C34-C35-C36
17	AA	830	CLA	C1A-C2A-CAA-CBA
17	AB	810	CLA	C1A-C2A-CAA-CBA
17	AB	841	CLA	C1A-C2A-CAA-CBA
17	A3	308	CLA	C1A-C2A-CAA-CBA
17	A4	310	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	AA	828	CLA	C2-C1-O2A-CGA
17	AB	833	CLA	C2-C1-O2A-CGA
19	A1	320	LHG	C3-O3-P-O6
19	A3	301	LHG	C3-O3-P-O6
19	AJ	104	LHG	C2-C3-O3-P
19	A6	617	LHG	C29-C30-C31-C32
22	AB	853	LMU	C3'-C4'-O1B-C1B
25	A4	318	LMG	O10-C28-O8-C9
19	AA	844	LHG	C4-O6-P-O4
19	A1	301	LHG	C3-O3-P-O4
19	A1	302	LHG	C3-O3-P-O5
19	A1	302	LHG	C4-O6-P-O4
19	A1	302	LHG	C4-O6-P-O5
19	A6	617	LHG	C4-O6-P-O4
19	A1	302	LHG	C7-C8-C9-C10
17	AA	813	CLA	CBA-CGA-O2A-C1
17	AA	817	CLA	C5-C6-C7-C8
17	AA	805	CLA	CAD-CBD-CGD-O1D
17	AA	814	CLA	CAD-CBD-CGD-O1D
17	AA	837	CLA	C2-C3-C5-C6
17	AB	814	CLA	CAD-CBD-CGD-O1D
17	AB	827	CLA	CAD-CBD-CGD-O1D
17	AB	837	CLA	CAD-CBD-CGD-O1D
17	AB	842	CLA	CAD-CBD-CGD-O1D
17	AL	302	CLA	CAD-CBD-CGD-O1D
17	A1	305	CLA	CAD-CBD-CGD-O1D
17	A1	316	CLA	CAD-CBD-CGD-O1D
17	A6	610	CLA	CAD-CBD-CGD-O1D
17	AA	818	CLA	CAA-CBA-CGA-O2A
17	AB	828	CLA	CAA-CBA-CGA-O2A
17	AA	816	CLA	O1D-CGD-O2D-CED
17	AA	811	CLA	C6-C7-C8-C10
17	AA	830	CLA	C11-C10-C8-C7
17	AA	840	CLA	C11-C10-C8-C7
17	AA	841	CLA	C11-C10-C8-C7
17	AB	814	CLA	C11-C12-C13-C15
17	AB	815	CLA	C11-C12-C13-C15
17	AB	823	CLA	C11-C10-C8-C7
17	AB	823	CLA	C12-C13-C15-C16
17	AB	825	CLA	C6-C7-C8-C10
17	AB	828	CLA	C11-C10-C8-C7
17	AB	829	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	A3	308	CLA	C3A-C2A-CAA-CBA
17	AB	804	CLA	C15-C16-C17-C18
17	AB	829	CLA	C13-C15-C16-C17
17	AA	813	CLA	O1A-CGA-O2A-C1
22	AL	301	LMU	C2-C1-O1'-C1'
17	AB	833	CLA	CAA-CBA-CGA-O2A
22	AA	851	LMU	C4B-C5B-C6B-O6B
19	AA	844	LHG	C35-C36-C37-C38
17	A3	305	CLA	CAD-CBD-CGD-O1D
19	AA	844	LHG	C29-C30-C31-C32
17	A6	611	CLA	O1D-CGD-O2D-CED
17	AA	826	CLA	C8-C10-C11-C12
17	AA	842	CLA	C4-C3-C5-C6
18	AA	843	PQN	C14-C13-C15-C16
17	AB	837	CLA	CBA-CGA-O2A-C1
23	AB	851	DGD	CBB-CCB-CDB-CEB
17	AB	810	CLA	C8-C10-C11-C12
17	AB	828	CLA	C15-C16-C17-C18
17	AA	810	CLA	C6-C7-C8-C9
17	AB	801	CLA	C11-C10-C8-C9
17	AB	809	CLA	C6-C7-C8-C9
17	AB	809	CLA	C11-C10-C8-C9
17	AB	825	CLA	C6-C7-C8-C9
17	A6	602	CLA	C11-C12-C13-C14
17	AA	840	CLA	O1A-CGA-O2A-C1
17	AB	837	CLA	O1A-CGA-O2A-C1
17	AB	818	CLA	C10-C11-C12-C13
20	AK	202	BCR	C21-C22-C23-C24
19	AA	844	LHG	C32-C33-C34-C35
17	AA	838	CLA	C5-C6-C7-C8
17	A1	306	CLA	C1-C2-C3-C4
17	AA	813	CLA	C2A-CAA-CBA-CGA
17	AB	809	CLA	C2A-CAA-CBA-CGA
17	AB	817	CLA	C2A-CAA-CBA-CGA
19	A1	302	LHG	O9-C7-O7-C5
17	AA	834	CLA	C2-C1-O2A-CGA
17	AA	838	CLA	C2-C1-O2A-CGA
17	AB	812	CLA	C2-C1-O2A-CGA
17	AB	815	CLA	C2-C1-O2A-CGA
17	AB	818	CLA	C2-C1-O2A-CGA
17	AB	828	CLA	C2C-C3C-CAC-CBC
17	AB	818	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	A3	312	CLA	O1A-CGA-O2A-C1
22	AB	853	LMU	C5'-C4'-O1B-C1B
17	AB	829	CLA	C4-C3-C5-C6
20	AA	846	BCR	C1-C6-C7-C8
17	A4	301	CLA	O1D-CGD-O2D-CED
22	AB	853	LMU	C3-C4-C5-C6
17	AB	819	CLA	C11-C12-C13-C14
22	AB	853	LMU	O5'-C1'-O1'-C1
17	A1	304	CLA	C2-C3-C5-C6
17	AB	818	CLA	C5-C6-C7-C8
17	AB	806	CLA	C2C-C3C-CAC-CBC
19	AA	844	LHG	C3-O3-P-O6
19	AJ	104	LHG	C3-O3-P-O6
17	AA	826	CLA	C10-C11-C12-C13
19	AJ	104	LHG	C19-C20-C21-C22
25	A4	318	LMG	O1-C7-C8-C9
17	A3	312	CLA	C4-C3-C5-C6
17	AA	821	CLA	C11-C12-C13-C15
17	AA	842	CLA	C12-C13-C15-C16
17	AB	811	CLA	C12-C13-C15-C16
17	AA	811	CLA	C6-C7-C8-C9
17	AA	829	CLA	C11-C12-C13-C14
17	AA	830	CLA	C11-C10-C8-C9
17	AB	815	CLA	C11-C10-C8-C9
17	AB	823	CLA	C14-C13-C15-C16
17	A1	314	CLA	C14-C13-C15-C16
17	AB	838	CLA	C8-C10-C11-C12
19	A1	302	LHG	C23-C24-C25-C26
17	AA	826	CLA	C11-C12-C13-C14
22	AA	851	LMU	C2-C3-C4-C5
17	AA	842	CLA	C10-C11-C12-C13
17	AB	814	CLA	C5-C6-C7-C8
17	AA	842	CLA	C2-C3-C5-C6
17	A3	312	CLA	CBA-CGA-O2A-C1
25	A1	321	LMG	C31-C32-C33-C34
22	AB	853	LMU	C5-C6-C7-C8
17	A3	312	CLA	C3-C5-C6-C7
19	A1	320	LHG	C15-C16-C17-C18
17	AA	802	CLA	C4-C3-C5-C6
17	AH	201	CLA	C2-C1-O2A-CGA
17	AA	833	CLA	C8-C10-C11-C12
17	AB	842	CLA	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	AB	851	DGD	CBA-CCA-CDA-CEA
17	AA	809	CLA	C3A-C2A-CAA-CBA
17	AB	811	CLA	C3A-C2A-CAA-CBA
17	A1	309	CLA	CAA-CBA-CGA-O2A
17	AA	806	CLA	C4-C3-C5-C6
17	AB	803	CLA	C11-C12-C13-C14
19	A3	319	LHG	C1-C2-C3-O3
20	AA	847	BCR	C35-C13-C14-C15
20	AA	849	BCR	C11-C10-C9-C34
20	AA	849	BCR	C16-C17-C18-C36
20	AB	845	BCR	C11-C10-C9-C34
20	AB	846	BCR	C11-C10-C9-C34
20	AB	846	BCR	C20-C21-C22-C37
20	AF	805	BCR	C35-C13-C14-C15
20	AI	102	BCR	C11-C10-C9-C34
25	A4	318	LMG	C7-C8-C9-O8
17	AB	804	CLA	O2A-C1-C2-C3
17	A3	308	CLA	CAA-CBA-CGA-O1A
17	AB	830	CLA	C4-C3-C5-C6
17	AA	841	CLA	C1A-C2A-CAA-CBA
17	AB	820	CLA	C1A-C2A-CAA-CBA
17	AK	203	CLA	C1A-C2A-CAA-CBA
17	AA	833	CLA	C11-C12-C13-C15
17	AB	827	CLA	C11-C10-C8-C7
17	AB	827	CLA	C11-C12-C13-C15
17	AB	840	CLA	C11-C10-C8-C7
26	A3	320	CHL	C3C-C2C-CMC-OMC
19	A1	302	LHG	C27-C28-C29-C30
17	A1	309	CLA	CAA-CBA-CGA-O1A
17	AA	808	CLA	C15-C16-C17-C18
17	AB	818	CLA	C3-C5-C6-C7
17	AA	806	CLA	C2A-CAA-CBA-CGA
17	AB	828	CLA	C2A-CAA-CBA-CGA
17	AB	841	CLA	C5-C6-C7-C8
17	A6	611	CLA	CAA-CBA-CGA-O2A
19	A3	319	LHG	C23-C24-C25-C26
19	A1	302	LHG	C8-C7-O7-C5
17	AB	802	CLA	C10-C11-C12-C13
17	AB	828	CLA	C2-C3-C5-C6
17	AB	829	CLA	C2-C3-C5-C6
17	A4	311	CLA	C2-C3-C5-C6
17	AB	842	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	AA	847	BCR	C12-C13-C14-C15
20	AA	849	BCR	C11-C10-C9-C8
20	AA	849	BCR	C16-C17-C18-C19
20	AB	845	BCR	C11-C10-C9-C8
20	AB	846	BCR	C11-C10-C9-C8
20	AB	846	BCR	C20-C21-C22-C23
20	AF	805	BCR	C12-C13-C14-C15
20	AI	102	BCR	C11-C10-C9-C8
25	A4	318	LMG	O7-C8-C9-O8
17	A6	611	CLA	CAA-CBA-CGA-O1A
17	AG	204	CLA	CAA-CBA-CGA-O2A
22	AB	852	LMU	C4B-C5B-C6B-O6B
17	AB	813	CLA	O1D-CGD-O2D-CED
17	AB	803	CLA	C4-C3-C5-C6
17	AA	806	CLA	C2-C3-C5-C6
17	A3	312	CLA	C2-C3-C5-C6
17	A3	308	CLA	CAA-CBA-CGA-O2A
17	AA	821	CLA	C13-C15-C16-C17
17	AK	203	CLA	CAA-CBA-CGA-O1A
26	A1	303	CHL	C4-C3-C5-C6
17	AA	809	CLA	C2A-CAA-CBA-CGA
17	AB	842	CLA	C2A-CAA-CBA-CGA
20	AG	205	BCR	C23-C24-C25-C30
20	AI	102	BCR	C23-C24-C25-C26
26	A3	307	CHL	CAA-CBA-CGA-O2A
17	A4	311	CLA	C4-C3-C5-C6
17	AA	828	CLA	C5-C6-C7-C8
17	AA	802	CLA	C2-C3-C5-C6
17	A6	609	CLA	C3-C5-C6-C7
17	A1	316	CLA	CAA-CBA-CGA-O2A
17	AA	801	CLA	CAA-CBA-CGA-O1A
17	AB	809	CLA	C16-C17-C18-C19
17	AG	204	CLA	CAA-CBA-CGA-O1A
17	AA	810	CLA	CAD-CBD-CGD-O1D
17	A6	602	CLA	C2A-CAA-CBA-CGA
25	A1	321	LMG	C34-C35-C36-C37
22	AB	853	LMU	O5B-C1B-O1B-C4'
17	AB	809	CLA	C11-C10-C8-C7
17	AB	830	CLA	C2-C3-C5-C6
17	A1	314	CLA	C6-C7-C8-C10
17	AB	813	CLA	CBD-CGD-O2D-CED
19	A3	319	LHG	O7-C5-C6-O8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	A6	607	CHL	CAA-CBA-CGA-O2A
17	AB	801	CLA	O1A-CGA-O2A-C1
17	AB	825	CLA	C8-C10-C11-C12
17	AA	833	CLA	CAA-CBA-CGA-O2A
17	AB	827	CLA	C4-C3-C5-C6
17	AA	821	CLA	C10-C11-C12-C13
17	AA	836	CLA	CAA-CBA-CGA-O2A
17	AA	818	CLA	C10-C11-C12-C13
19	A3	301	LHG	O7-C7-C8-C9
17	AA	821	CLA	C6-C7-C8-C9
17	AA	833	CLA	C11-C12-C13-C14
17	AA	842	CLA	C14-C13-C15-C16
17	AB	801	CLA	C11-C12-C13-C14
17	AL	303	CLA	C11-C10-C8-C9
17	A3	302	CLA	C6-C7-C8-C9
17	A1	304	CLA	C4C-C3C-CAC-CBC
17	A4	302	CLA	CAA-CBA-CGA-O2A
17	A4	303	CLA	CAA-CBA-CGA-O1A
17	AA	841	CLA	C3A-C2A-CAA-CBA
25	A4	318	LMG	O7-C10-C11-C12
17	AA	813	CLA	CAD-CBD-CGD-O2D
17	AA	818	CLA	CAD-CBD-CGD-O2D
17	AA	821	CLA	CAD-CBD-CGD-O2D
17	AA	826	CLA	CAD-CBD-CGD-O2D
17	AA	842	CLA	CAD-CBD-CGD-O2D
17	AB	820	CLA	CAD-CBD-CGD-O2D
17	AB	821	CLA	CAD-CBD-CGD-O2D
17	AB	822	CLA	CAD-CBD-CGD-O2D
17	AB	834	CLA	CAD-CBD-CGD-O2D
17	AF	802	CLA	CAD-CBD-CGD-O2D
17	A1	304	CLA	CAD-CBD-CGD-O2D
17	A1	307	CLA	CAD-CBD-CGD-O2D
17	A3	308	CLA	CAD-CBD-CGD-O2D
17	A3	309	CLA	CAD-CBD-CGD-O2D
17	A4	309	CLA	CAD-CBD-CGD-O2D
17	A4	312	CLA	CAD-CBD-CGD-O2D
17	A4	313	CLA	CAD-CBD-CGD-O2D
17	A6	601	CLA	CAD-CBD-CGD-O2D
17	A6	602	CLA	CAD-CBD-CGD-O2D
19	A6	617	LHG	C4-C5-O7-C7
17	A1	304	CLA	C2A-CAA-CBA-CGA
17	AA	834	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	AB	844	BCR	C17-C18-C19-C20
20	AL	306	BCR	C7-C8-C9-C10
19	A6	617	LHG	C4-C5-C6-O8
25	A1	321	LMG	C7-C8-C9-O8
17	A1	316	CLA	CAA-CBA-CGA-O1A
26	A3	307	CHL	CAA-CBA-CGA-O1A
17	A3	302	CLA	C8-C10-C11-C12
17	AA	803	CLA	O2A-C1-C2-C3
17	AA	827	CLA	O2A-C1-C2-C3
17	AA	830	CLA	O2A-C1-C2-C3
17	AA	839	CLA	O2A-C1-C2-C3
17	AA	842	CLA	O2A-C1-C2-C3
17	AB	834	CLA	O2A-C1-C2-C3
17	A4	313	CLA	O2A-C1-C2-C3
22	AB	853	LMU	C2-C3-C4-C5
17	AA	829	CLA	C2A-CAA-CBA-CGA
17	AA	803	CLA	CHA-CBD-CGD-O1D
17	AA	803	CLA	CHA-CBD-CGD-O2D
17	AA	820	CLA	CHA-CBD-CGD-O1D
17	AA	822	CLA	CHA-CBD-CGD-O2D
17	AA	823	CLA	CHA-CBD-CGD-O1D
17	AA	823	CLA	CHA-CBD-CGD-O2D
17	AA	827	CLA	CHA-CBD-CGD-O1D
17	AA	831	CLA	CHA-CBD-CGD-O2D
17	AA	840	CLA	CHA-CBD-CGD-O1D
17	AA	840	CLA	CHA-CBD-CGD-O2D
17	AB	814	CLA	CHA-CBD-CGD-O2D
17	AB	816	CLA	CHA-CBD-CGD-O2D
17	AB	837	CLA	CHA-CBD-CGD-O2D
17	AK	203	CLA	CHA-CBD-CGD-O1D
17	AK	204	CLA	CHA-CBD-CGD-O1D
17	AL	303	CLA	CHA-CBD-CGD-O2D
17	A1	307	CLA	CHA-CBD-CGD-O1D
17	A4	302	CLA	CHA-CBD-CGD-O2D
17	A4	302	CLA	CAA-CBA-CGA-O1A
19	A1	302	LHG	O8-C23-C24-C25
19	AA	844	LHG	O6-C4-C5-C6
19	A1	301	LHG	O6-C4-C5-C6
17	AA	827	CLA	CAA-CBA-CGA-O2A
17	AB	806	CLA	CAA-CBA-CGA-O2A
17	AB	834	CLA	CAA-CBA-CGA-O2A
17	A4	303	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	A6	604	CLA	O1D-CGD-O2D-CED
25	A1	321	LMG	O8-C28-C29-C30
17	AB	801	CLA	C2A-CAA-CBA-CGA
17	AA	836	CLA	CAA-CBA-CGA-O1A
17	A1	313	CLA	CAA-CBA-CGA-O2A
17	AA	801	CLA	C11-C10-C8-C7
17	AB	810	CLA	C11-C12-C13-C15
17	AB	827	CLA	C2-C3-C5-C6
17	AA	801	CLA	C11-C10-C8-C9
17	AA	801	CLA	C14-C13-C15-C16
17	AA	806	CLA	C11-C12-C13-C14
17	AA	813	CLA	C6-C7-C8-C9
17	AA	841	CLA	C11-C10-C8-C9
18	AB	843	PQN	C21-C22-C23-C24
17	AG	201	CLA	CAA-CBA-CGA-O2A
19	AJ	104	LHG	C17-C18-C19-C20
17	AK	203	CLA	CAA-CBA-CGA-O2A
19	AA	844	LHG	C12-C13-C14-C15
17	AA	802	CLA	C1A-C2A-CAA-CBA
17	AA	827	CLA	C1A-C2A-CAA-CBA
17	AA	829	CLA	C1A-C2A-CAA-CBA
17	AB	803	CLA	C1A-C2A-CAA-CBA
17	AB	823	CLA	C1A-C2A-CAA-CBA
17	A4	307	CLA	C1A-C2A-CAA-CBA
26	A1	303	CHL	C1A-C2A-CAA-CBA
26	A1	308	CHL	CHA-CBD-CGD-O2D
26	A4	304	CHL	CHA-CBD-CGD-O2D
17	AB	820	CLA	C2-C1-O2A-CGA
17	A3	302	CLA	C5-C6-C7-C8
17	AA	807	CLA	O1D-CGD-O2D-CED
17	AA	833	CLA	CAA-CBA-CGA-O1A
26	A6	607	CHL	CAA-CBA-CGA-O1A
17	AB	842	CLA	C5-C6-C7-C8
17	AA	807	CLA	CBD-CGD-O2D-CED
17	AA	818	CLA	O1A-CGA-O2A-C1
17	AA	834	CLA	C15-C16-C17-C18
17	AB	806	CLA	CAA-CBA-CGA-O1A
17	A6	608	CLA	CAA-CBA-CGA-O2A
19	AJ	104	LHG	C3-O3-P-O5
19	A3	319	LHG	C4-O6-P-O5
17	AB	842	CLA	C16-C17-C18-C20
17	AA	834	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	AA	849	BCR	C1-C6-C7-C8
20	AI	101	BCR	C23-C24-C25-C30
20	AL	306	BCR	C23-C24-C25-C26
20	AL	306	BCR	C23-C24-C25-C30
17	AK	203	CLA	O1D-CGD-O2D-CED
25	A4	318	LMG	O9-C10-C11-C12
17	AA	805	CLA	CAA-CBA-CGA-O2A
19	A6	617	LHG	O8-C23-C24-C25
25	A4	318	LMG	O8-C28-C29-C30
17	AA	840	CLA	C2A-CAA-CBA-CGA
17	AB	825	CLA	C2A-CAA-CBA-CGA
17	AB	828	CLA	C8-C10-C11-C12
17	A1	313	CLA	CAA-CBA-CGA-O1A
17	AB	834	CLA	CAA-CBA-CGA-O1A
17	AA	818	CLA	CBA-CGA-O2A-C1
17	AA	811	CLA	CAD-CBD-CGD-O1D
17	AA	827	CLA	CAD-CBD-CGD-O1D
17	AA	830	CLA	CAD-CBD-CGD-O1D
17	AA	840	CLA	CAD-CBD-CGD-O1D
17	AB	831	CLA	CAD-CBD-CGD-O1D
25	A1	321	LMG	O10-C28-C29-C30
17	AB	825	CLA	C11-C10-C8-C9
17	AB	827	CLA	C11-C10-C8-C9
17	A1	304	CLA	C6-C7-C8-C9
17	AA	806	CLA	C3-C5-C6-C7
17	AB	819	CLA	C3-C5-C6-C7
17	AB	810	CLA	CAA-CBA-CGA-O2A
25	A1	321	LMG	O7-C10-C11-C12
17	AG	201	CLA	CAA-CBA-CGA-O1A
17	AA	828	CLA	C2A-CAA-CBA-CGA
17	AB	807	CLA	CAA-CBA-CGA-O2A
17	AB	829	CLA	CAA-CBA-CGA-O2A
17	AA	805	CLA	C6-C7-C8-C10
17	AA	840	CLA	C12-C13-C15-C16
17	AB	804	CLA	C11-C12-C13-C15
17	AB	823	CLA	C3A-C2A-CAA-CBA
17	AB	825	CLA	C11-C10-C8-C7
17	AB	835	CLA	C3A-C2A-CAA-CBA
17	A1	309	CLA	CHA-CBD-CGD-O1D
17	A3	305	CLA	CAD-CBD-CGD-O2D
17	A3	312	CLA	CHA-CBD-CGD-O1D
17	A3	313	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	A4	310	CLA	CHA-CBD-CGD-O1D
17	A4	310	CLA	CAD-CBD-CGD-O2D
17	A6	603	CLA	CAD-CBD-CGD-O2D
19	A1	301	LHG	O6-C4-C5-O7
26	A1	308	CHL	CAD-CBD-CGD-O2D
19	A1	302	LHG	O10-C23-C24-C25
17	AA	817	CLA	O1D-CGD-O2D-CED
17	AA	812	CLA	CAA-CBA-CGA-O2A
17	AA	828	CLA	CAA-CBA-CGA-O2A
17	AA	841	CLA	CAA-CBA-CGA-O2A
17	AA	842	CLA	CAA-CBA-CGA-O2A
17	AB	801	CLA	CAA-CBA-CGA-O2A
17	AB	809	CLA	C15-C16-C17-C18
17	AA	827	CLA	CAA-CBA-CGA-O1A
17	A3	312	CLA	CAA-CBA-CGA-O1A
17	AA	809	CLA	CAA-CBA-CGA-O2A
17	A3	312	CLA	CAA-CBA-CGA-O2A
17	AA	802	CLA	C8-C10-C11-C12
17	AA	842	CLA	C8-C10-C11-C12
17	AB	832	CLA	C10-C11-C12-C13
19	A1	301	LHG	O9-C7-O7-C5
17	AA	812	CLA	CAA-CBA-CGA-O1A
17	AB	807	CLA	CAA-CBA-CGA-O1A
17	AB	810	CLA	CAA-CBA-CGA-O1A
17	AA	819	CLA	C5-C6-C7-C8
22	AB	853	LMU	C2B-C1B-O1B-C4'
17	AB	830	CLA	C2A-CAA-CBA-CGA
25	A1	321	LMG	C14-C15-C16-C17
19	AA	844	LHG	O7-C7-C8-C9

There are no ring outliers.

110 monomers are involved in 161 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A6	607	CHL	2	0
17	AB	807	CLA	1	0
17	AB	831	CLA	1	0
17	A6	613	CLA	1	0
17	AB	839	CLA	2	0
17	AB	808	CLA	1	0
17	AA	803	CLA	1	0
17	AA	827	CLA	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AB	801	CLA	2	0
17	AA	811	CLA	3	0
17	AA	830	CLA	1	0
17	AB	802	CLA	4	0
17	AA	801	CLA	12	0
25	A1	321	LMG	1	0
26	A1	303	CHL	2	0
17	AA	806	CLA	1	0
17	AG	204	CLA	3	0
17	A4	307	CLA	1	0
26	A3	320	CHL	2	0
17	AB	805	CLA	1	0
17	AB	828	CLA	1	0
17	AB	827	CLA	4	0
17	AA	834	CLA	2	0
20	A3	318	BCR	3	0
17	AG	203	CLA	1	0
17	AB	830	CLA	1	0
21	AC	101	SF4	1	0
18	AA	843	PQN	3	0
17	A1	316	CLA	1	0
17	AA	805	CLA	2	0
20	AB	847	BCR	3	0
19	AA	844	LHG	1	0
17	AB	803	CLA	4	0
20	AB	848	BCR	2	0
17	AA	841	CLA	2	0
20	AL	305	BCR	1	0
17	AB	822	CLA	1	0
17	A4	301	CLA	1	0
20	AA	846	BCR	1	0
17	A3	304	CLA	1	0
17	A3	313	CLA	1	0
20	A6	616	BCR	3	0
17	AA	832	CLA	1	0
17	AB	809	CLA	1	0
17	AB	825	CLA	1	0
17	AA	818	CLA	1	0
20	AJ	103	BCR	1	0
17	AA	825	CLA	4	0
20	AF	805	BCR	2	0
17	AB	818	CLA	3	0

*Continued on next page...*

*Continued from previous page...*

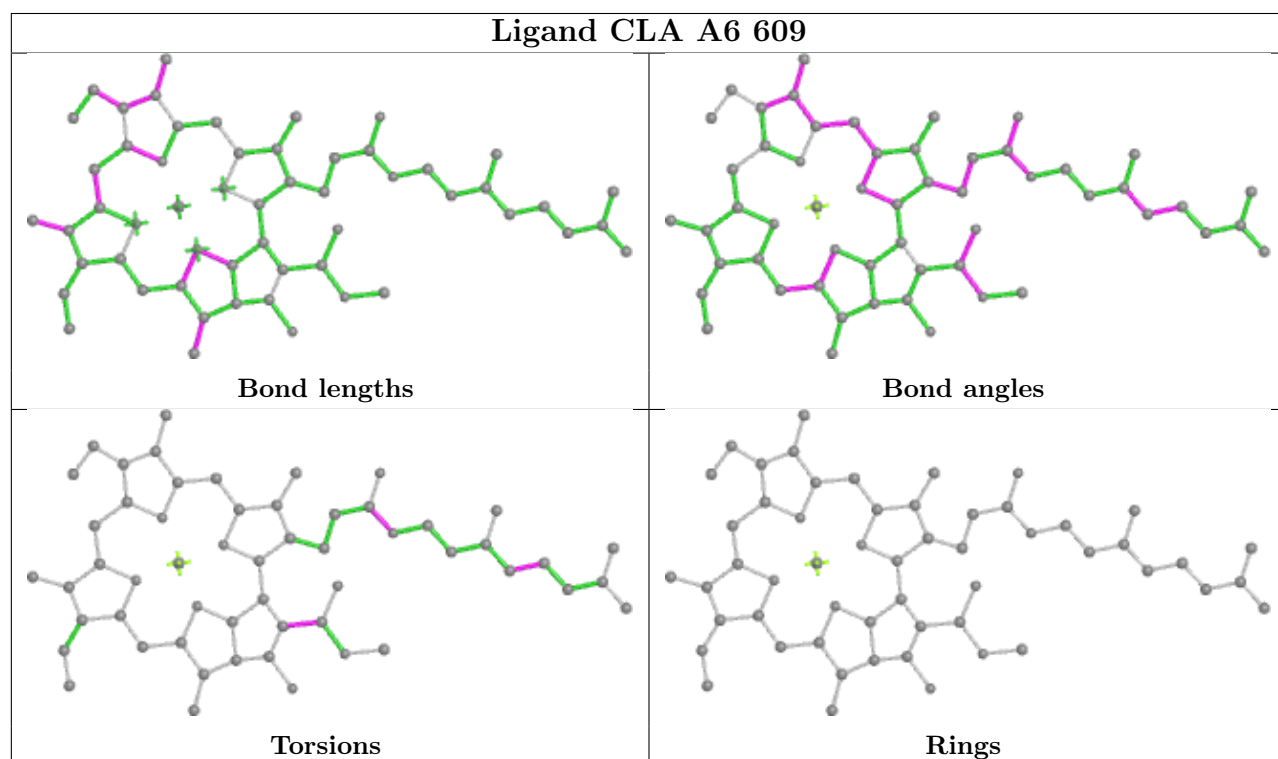
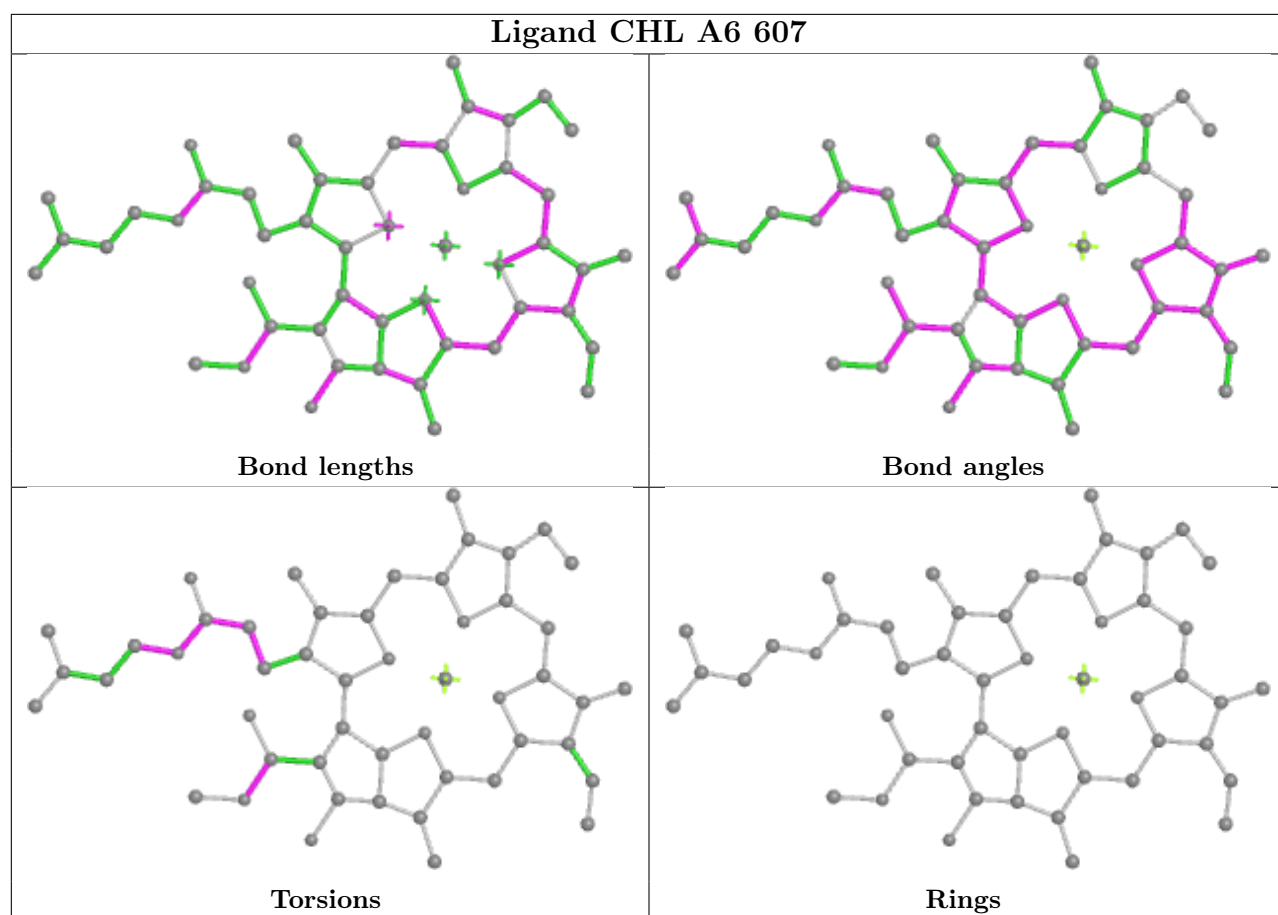
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AL	303	CLA	1	0
17	A6	603	CLA	2	0
20	AA	847	BCR	1	0
17	AB	810	CLA	2	0
20	AA	849	BCR	2	0
17	AA	815	CLA	1	0
17	AA	802	CLA	1	0
27	A4	316	XAT	2	0
17	A4	308	CLA	1	0
17	A3	308	CLA	1	0
24	A4	315	LUT	2	0
20	AG	205	BCR	2	0
17	AB	842	CLA	1	0
17	AB	833	CLA	2	0
17	A1	305	CLA	1	0
21	AC	102	SF4	1	0
17	A1	311	CLA	2	0
22	AL	301	LMU	1	0
26	A1	308	CHL	1	0
20	AB	844	BCR	2	0
17	AA	838	CLA	3	0
17	AA	828	CLA	2	0
17	AB	840	CLA	1	0
19	A6	617	LHG	1	0
20	AB	849	BCR	1	0
17	A4	309	CLA	1	0
17	AB	814	CLA	1	0
20	AB	846	BCR	1	0
24	A6	614	LUT	1	0
17	A6	601	CLA	1	0
19	A3	301	LHG	1	0
17	AB	834	CLA	3	0
17	AA	820	CLA	1	0
17	A1	306	CLA	2	0
17	AA	833	CLA	1	0
18	AB	843	PQN	2	0
26	A4	306	CHL	2	0
20	AI	102	BCR	1	0
20	AK	205	BCR	1	0
17	AA	835	CLA	1	0
20	AA	848	BCR	2	0
20	AJ	101	BCR	1	0

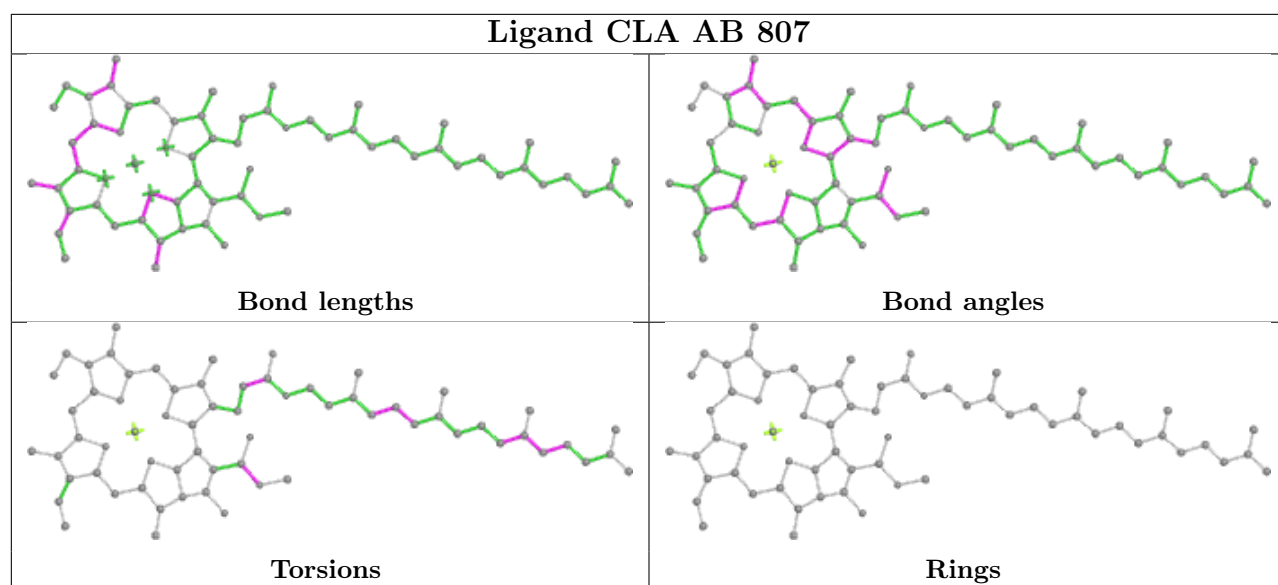
*Continued on next page...*

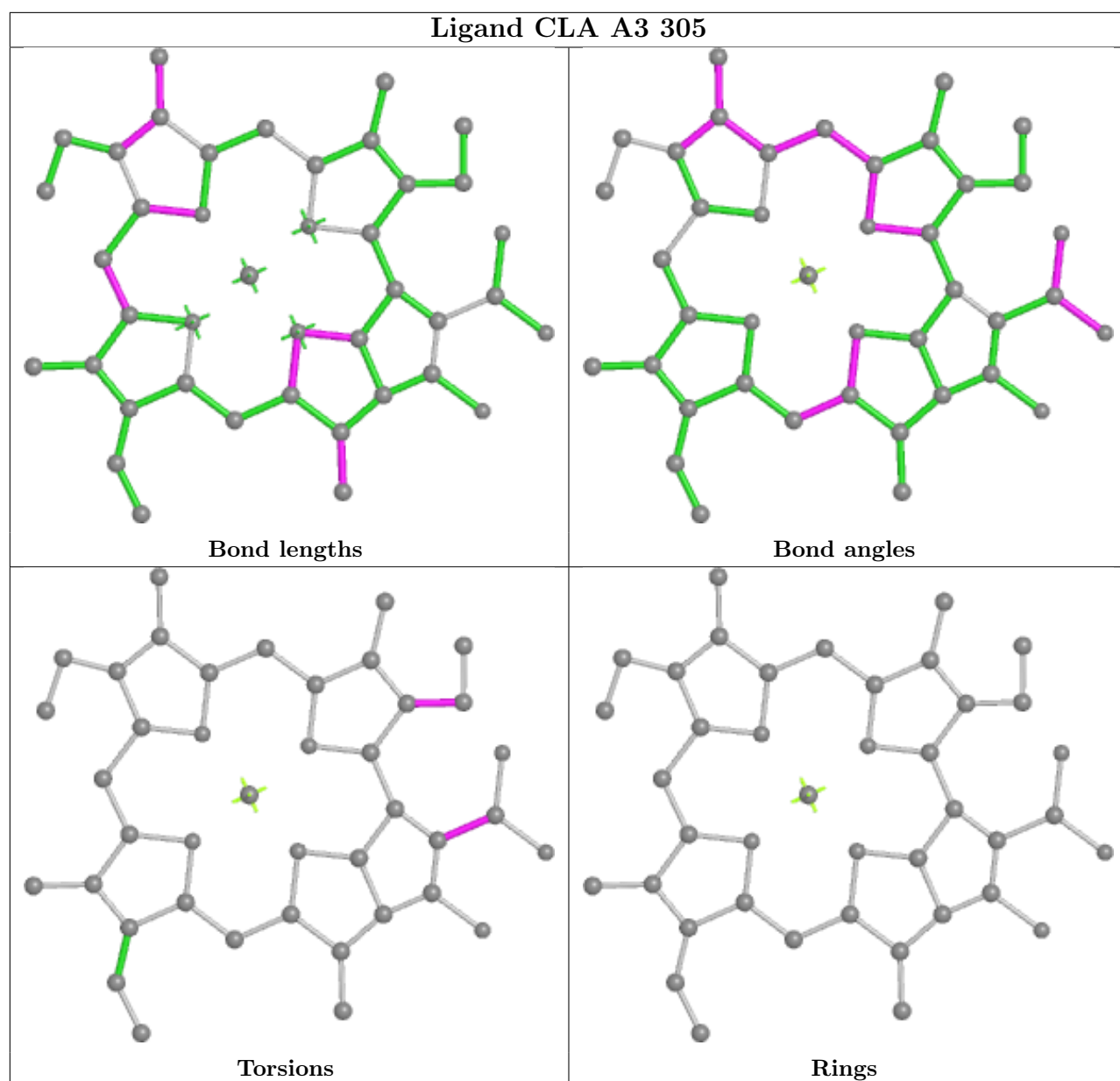
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A4	318	LMG	4	0
20	AB	845	BCR	1	0
27	A3	317	XAT	3	0
27	A6	615	XAT	4	0
20	A1	319	BCR	3	0
20	AF	801	BCR	4	0
17	A6	612	CLA	1	0
26	A6	605	CHL	1	0
17	AA	826	CLA	2	0
17	A4	313	CLA	1	0
26	A4	304	CHL	1	0
27	A1	318	XAT	1	0
24	AF	806	LUT	2	0
17	AA	810	CLA	1	0
26	A3	307	CHL	2	0
17	AB	836	CLA	1	0
17	AB	841	CLA	1	0
17	AB	824	CLA	2	0

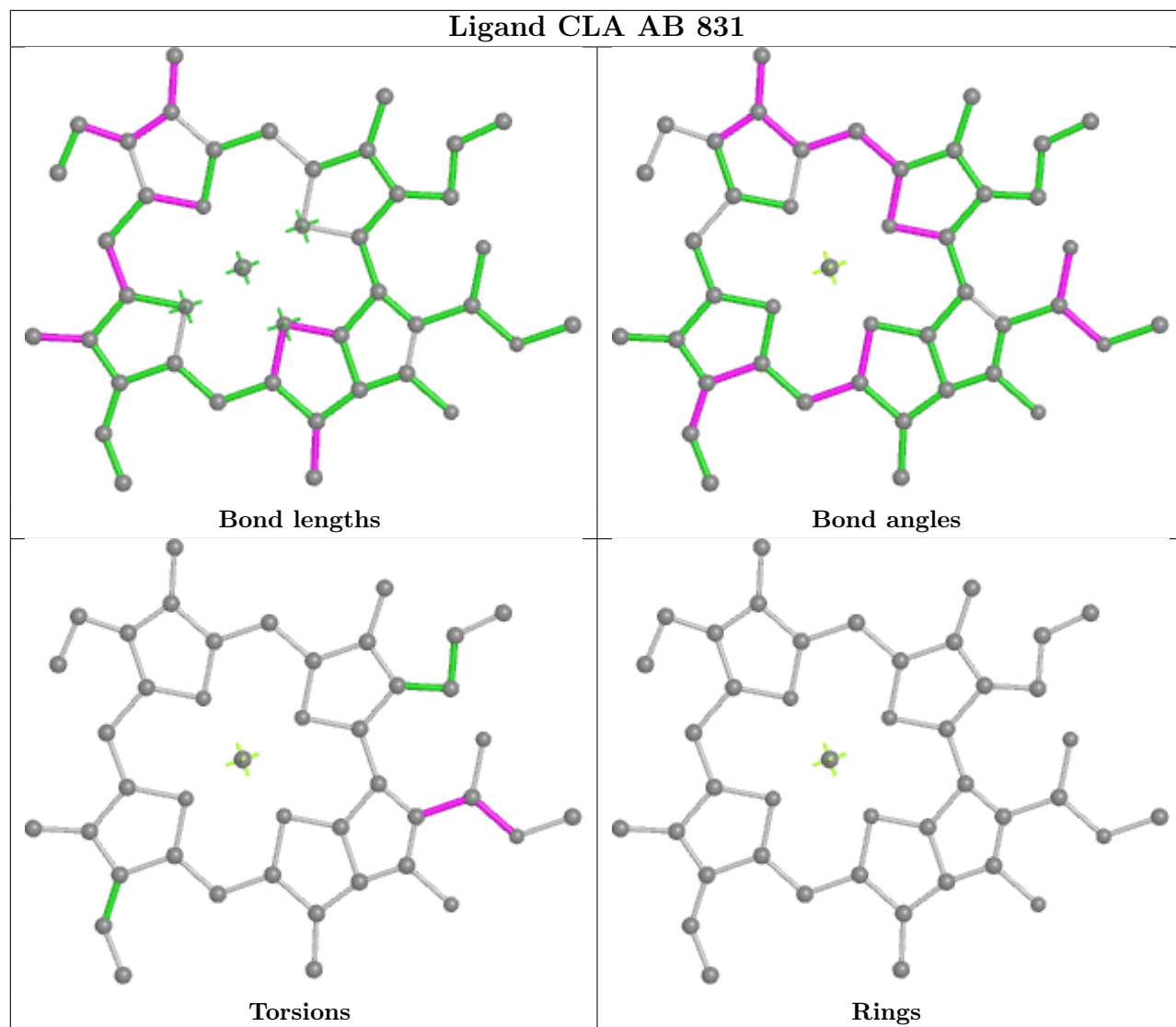
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

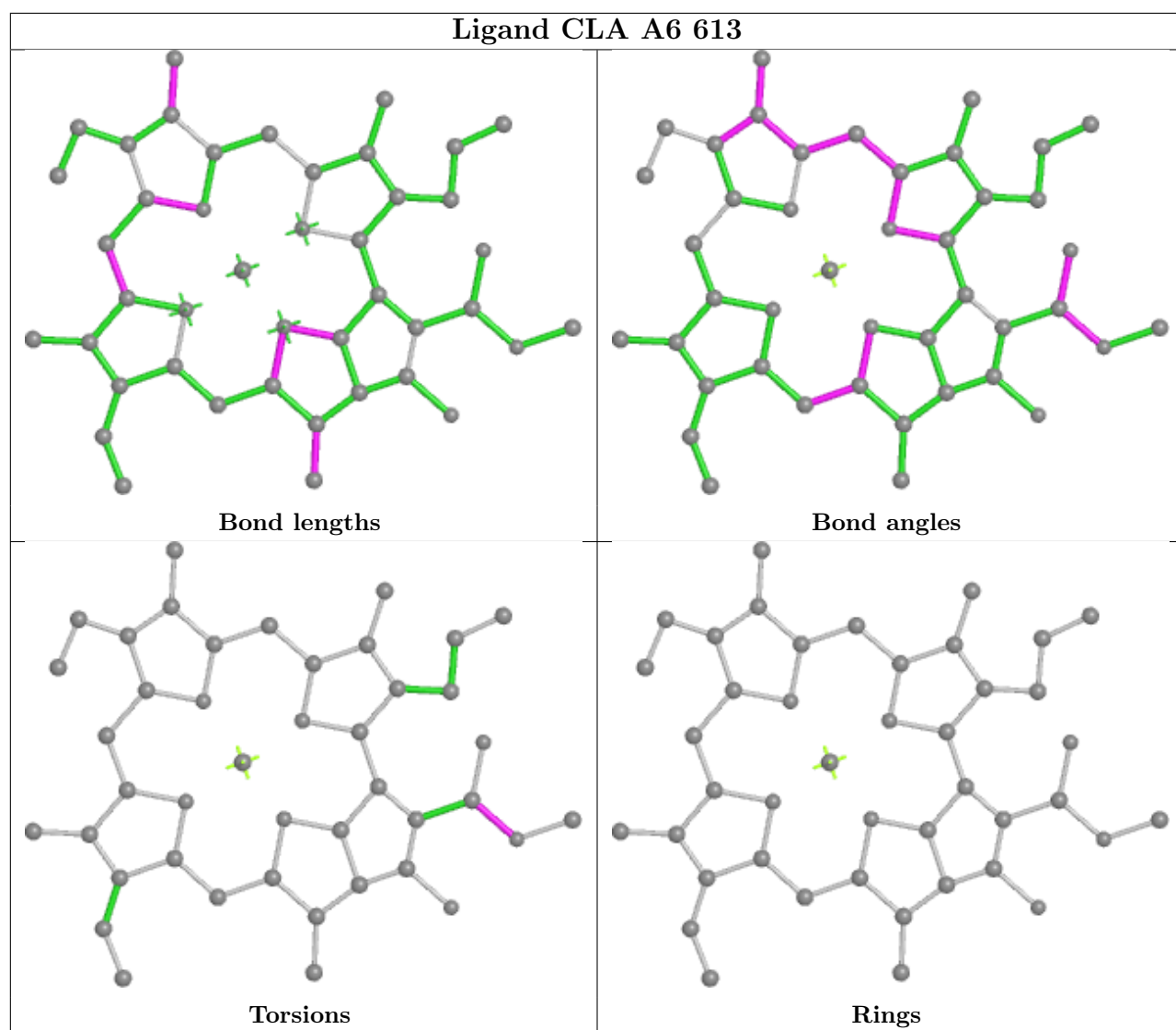




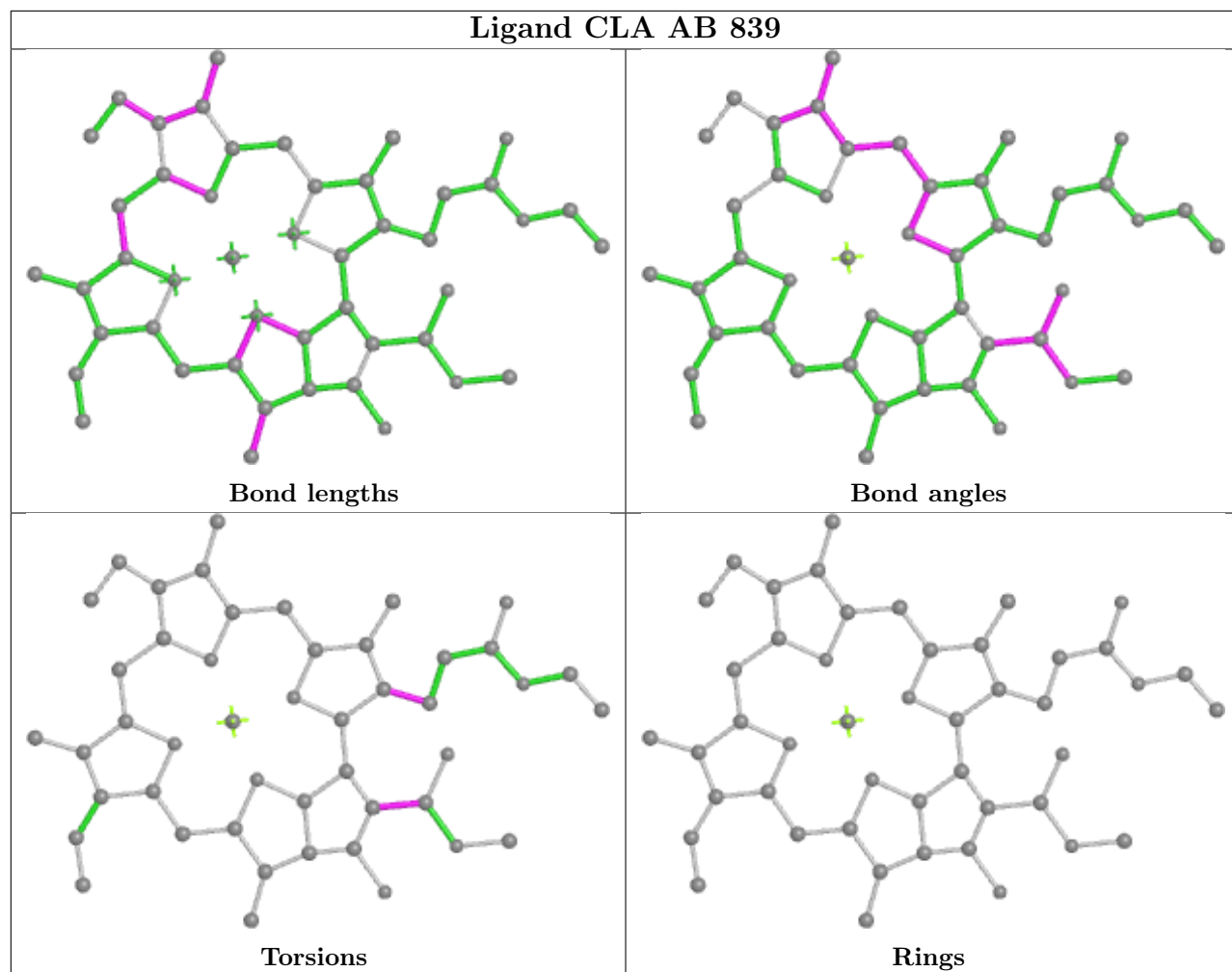


## Ligand CLA AB 831

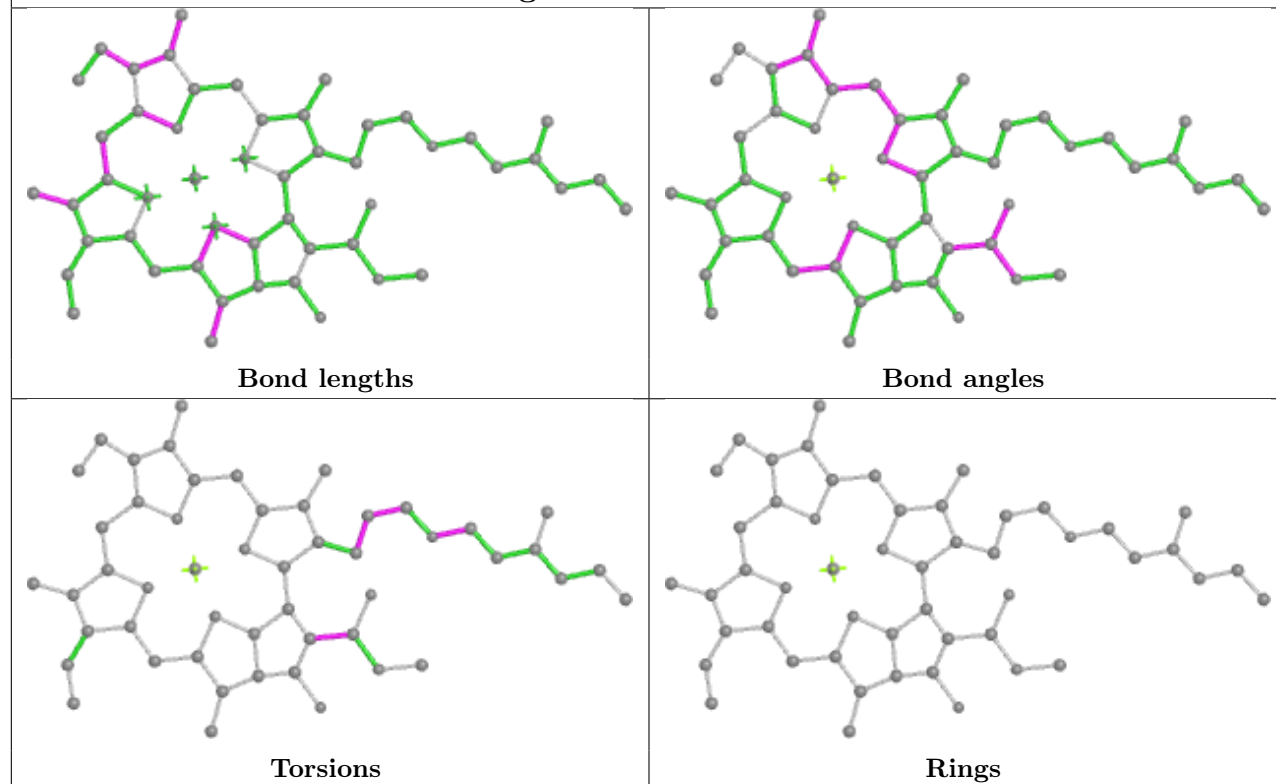




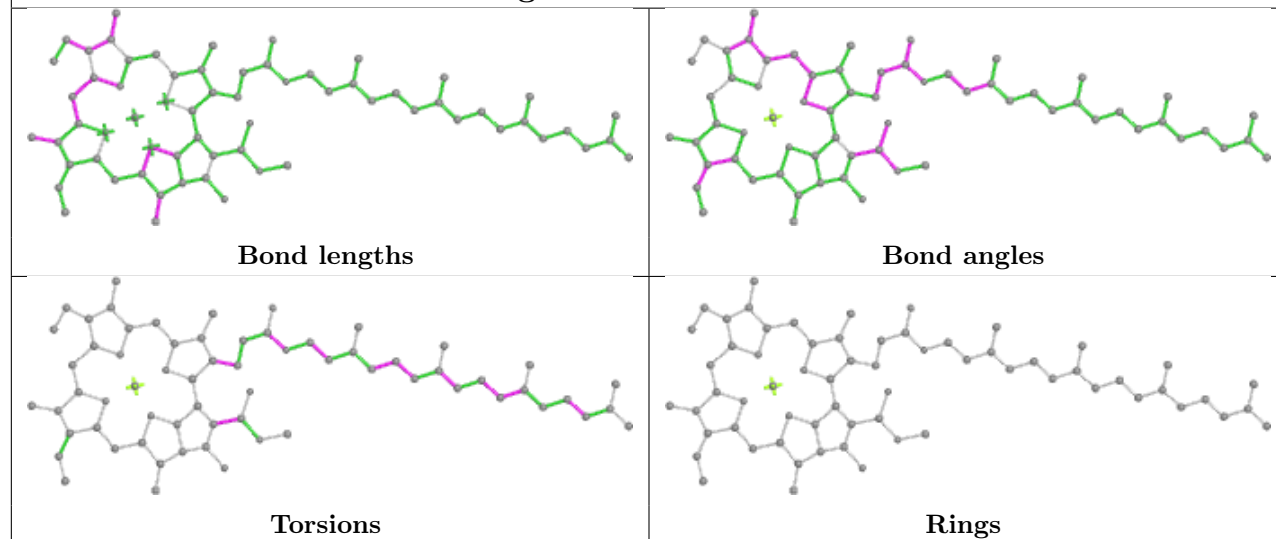
## Ligand CLA AB 839



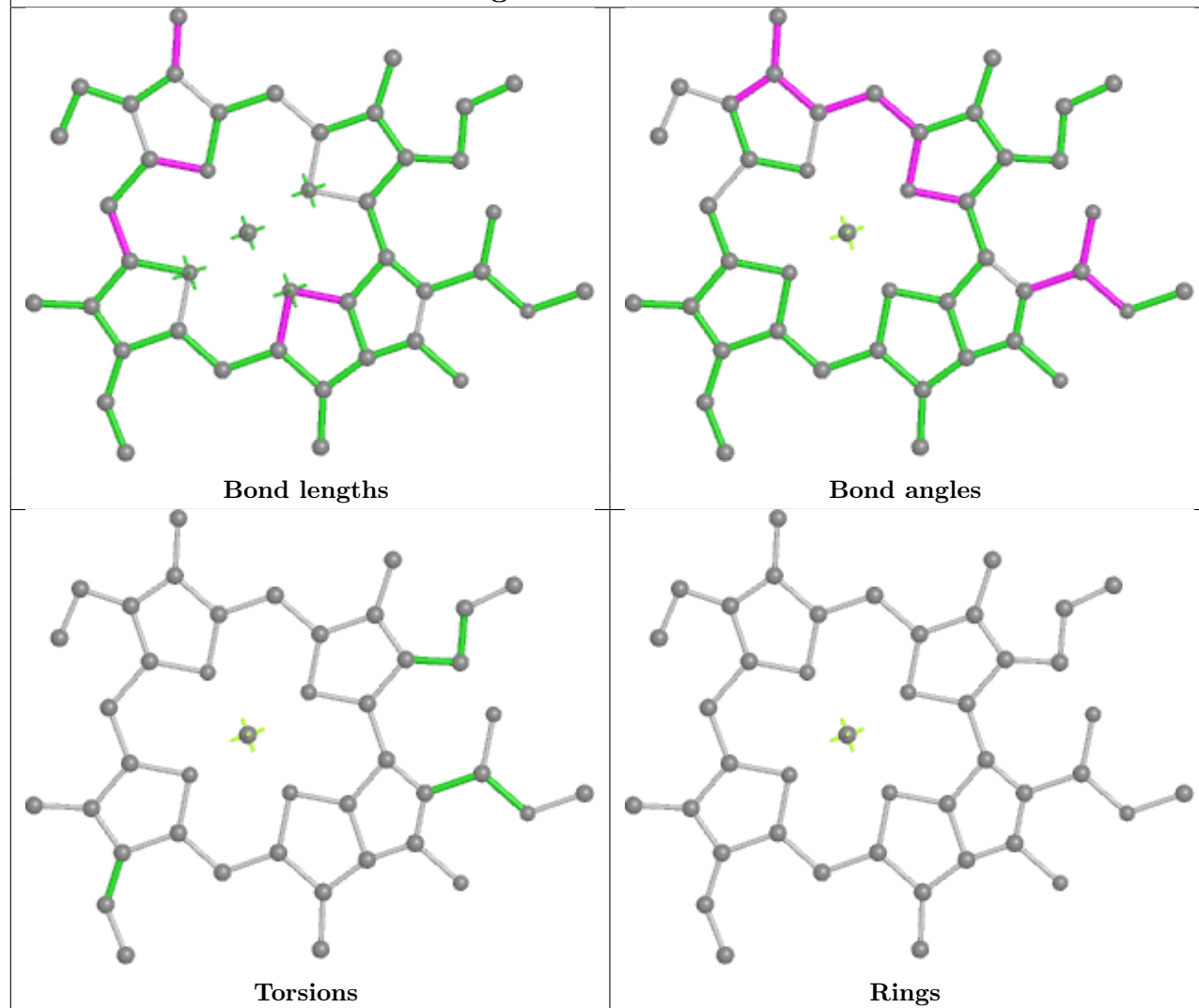
## Ligand CLA AB 808



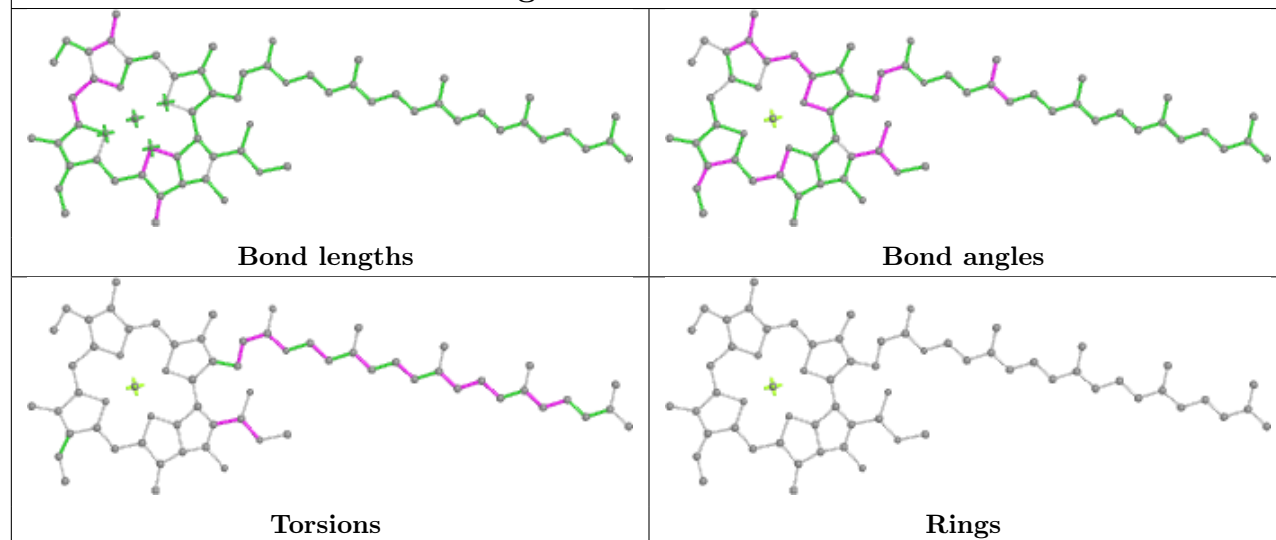
## Ligand CLA AA 803



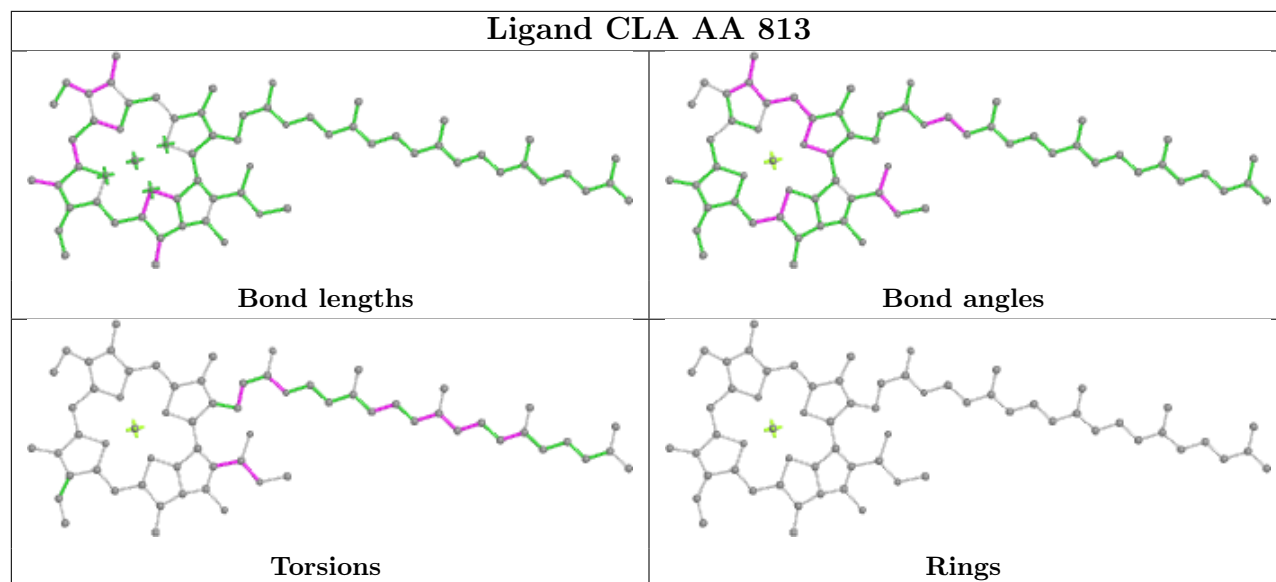
## Ligand CLA A3 311



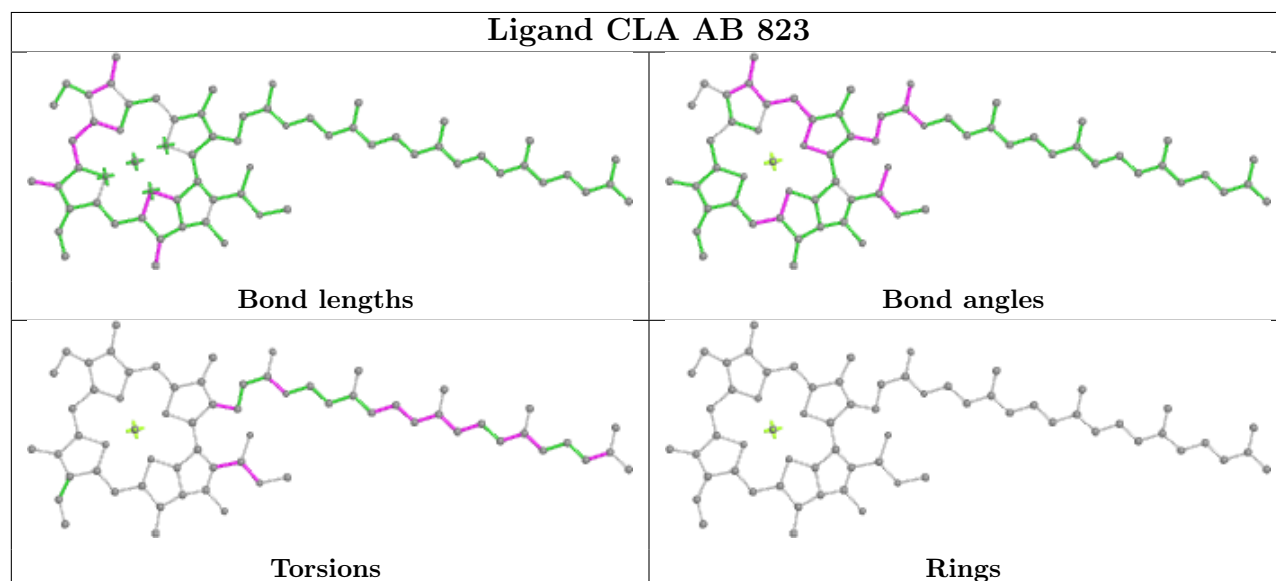
## Ligand CLA AA 842



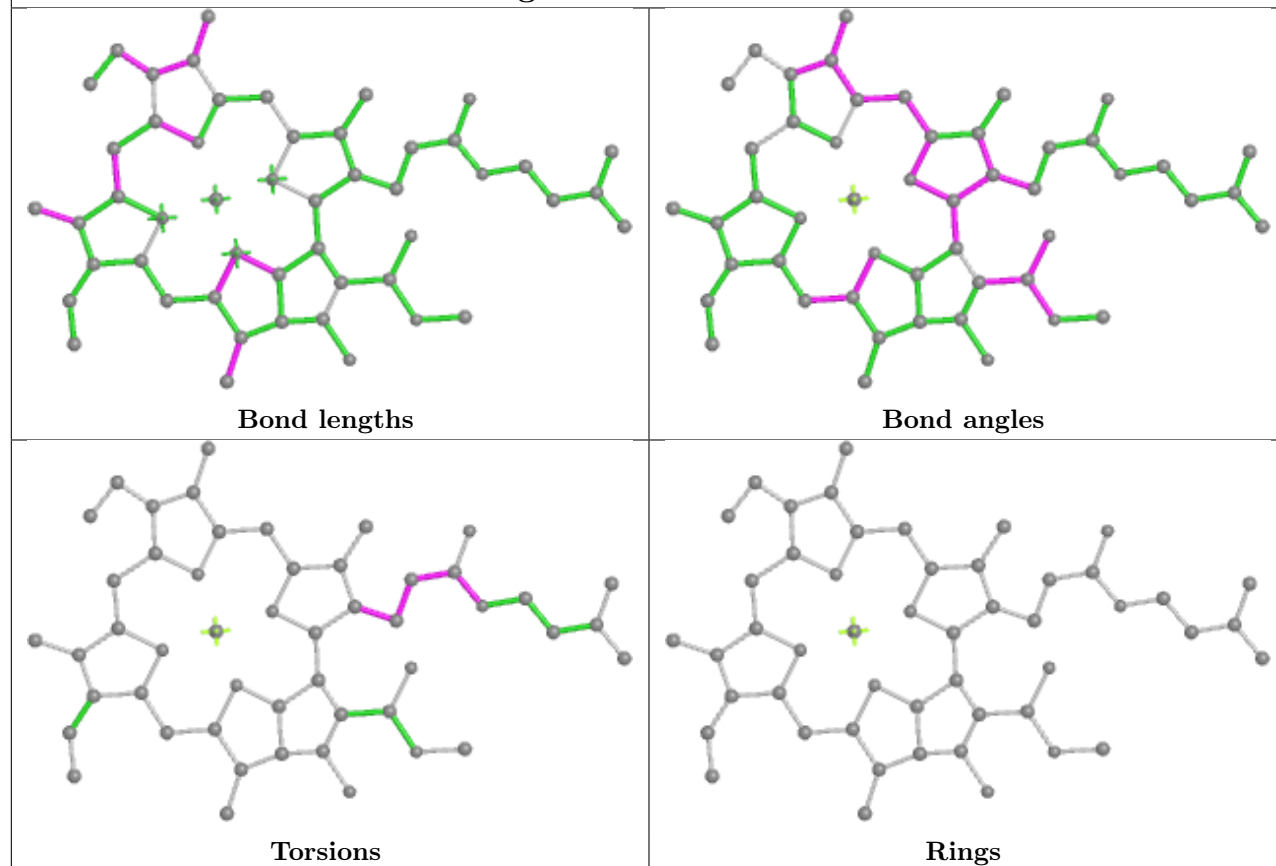
## Ligand CLA AA 813



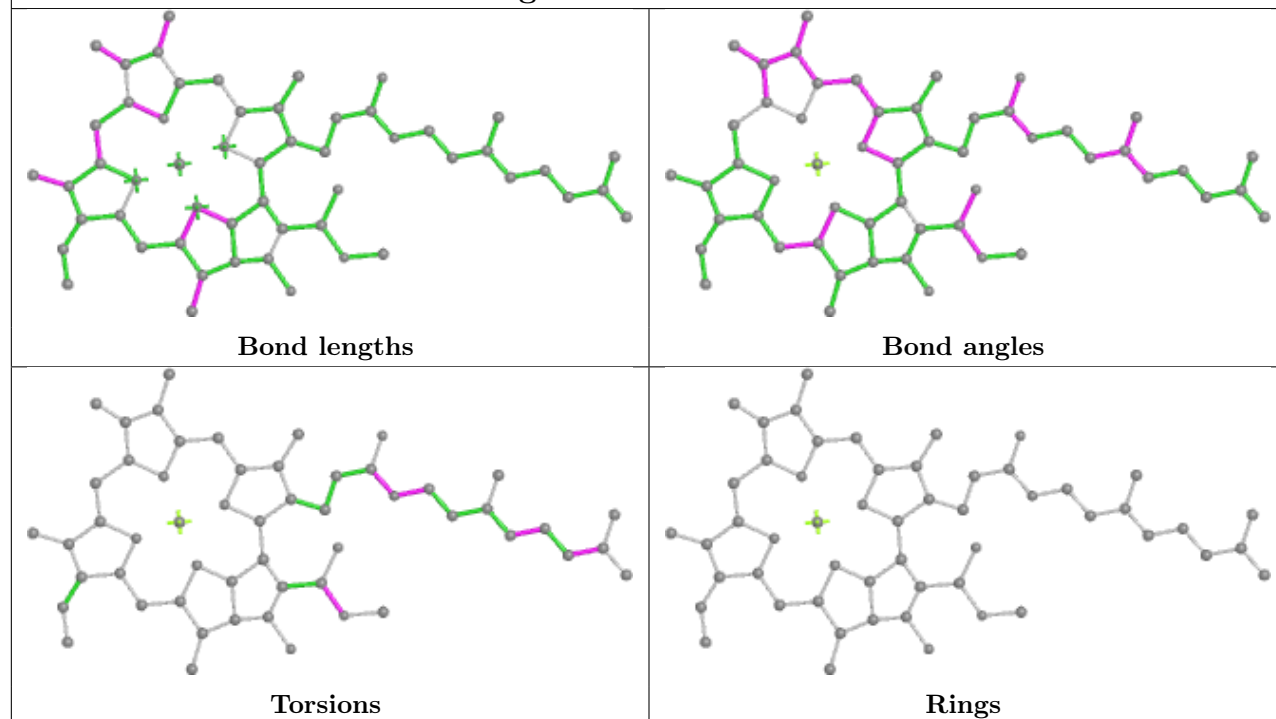
## Ligand CLA AB 823



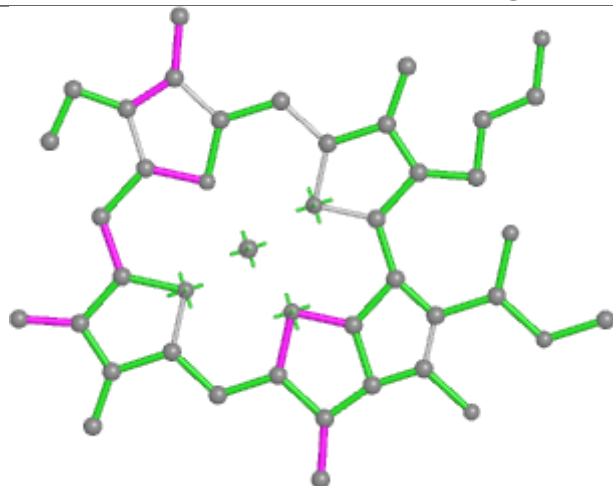
## Ligand CLA AA 809



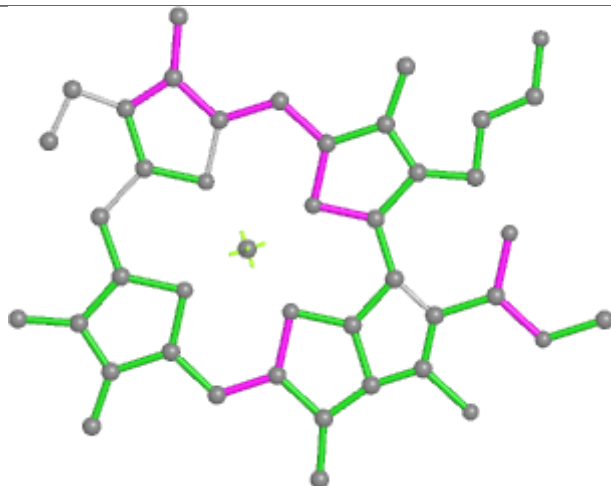
## Ligand CLA AB 812



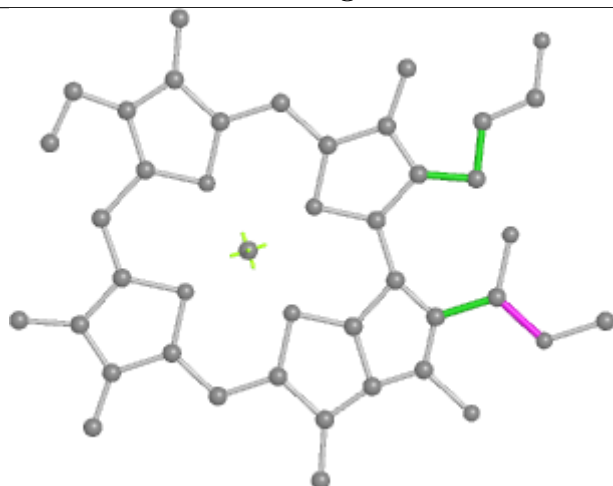
## Ligand CLA A6 604



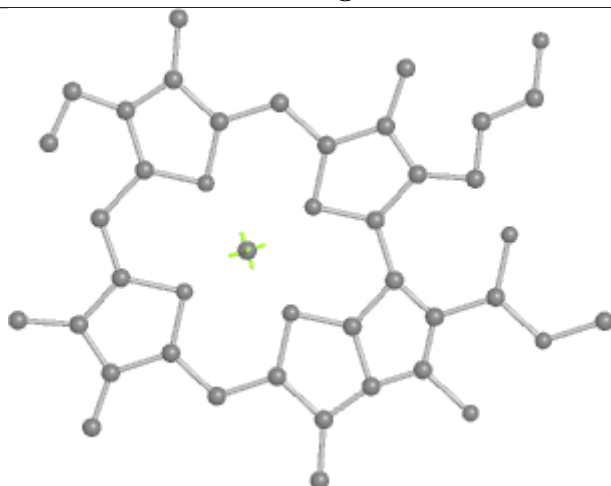
Bond lengths



Bond angles

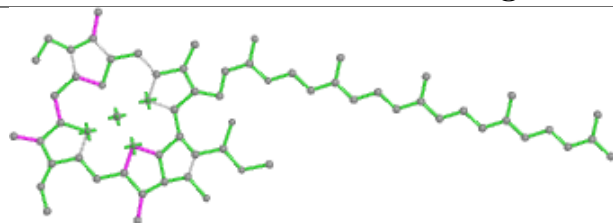


Torsions

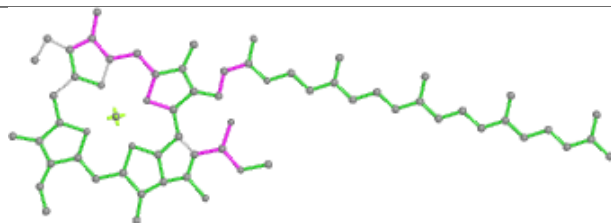


Rings

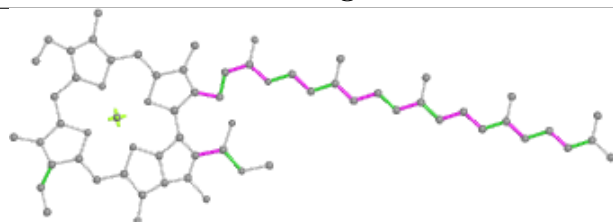
## Ligand CLA AA 827



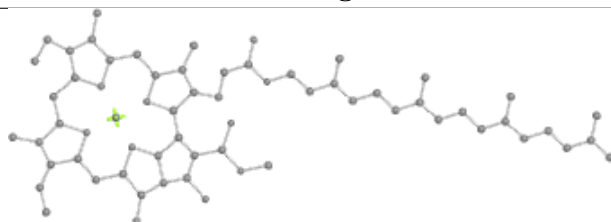
Bond lengths



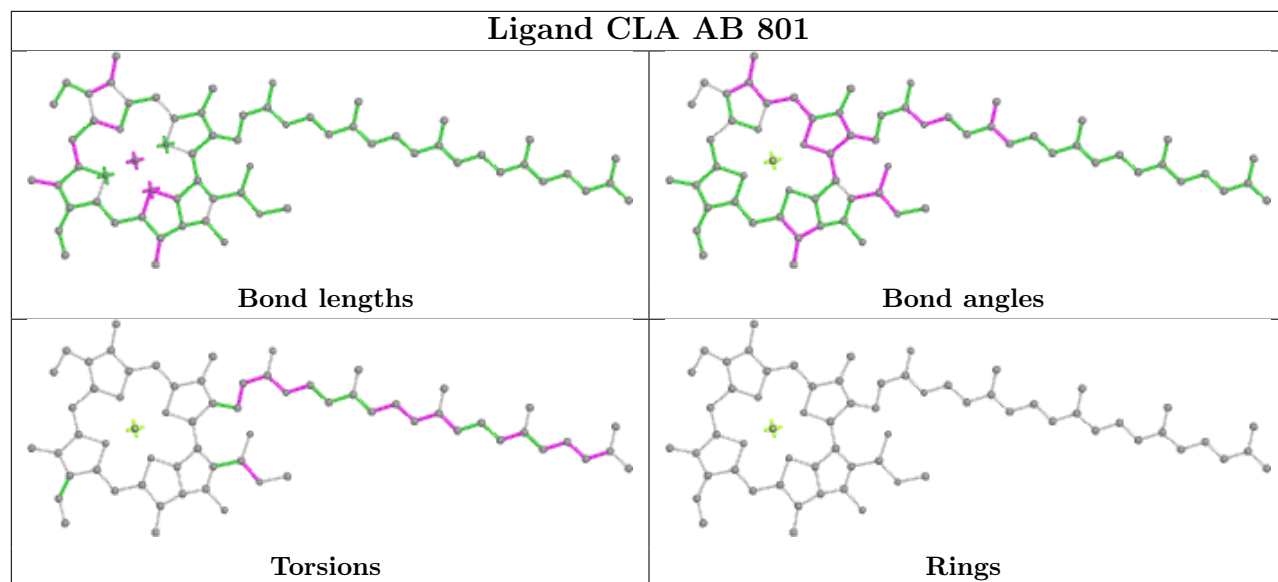
Bond angles



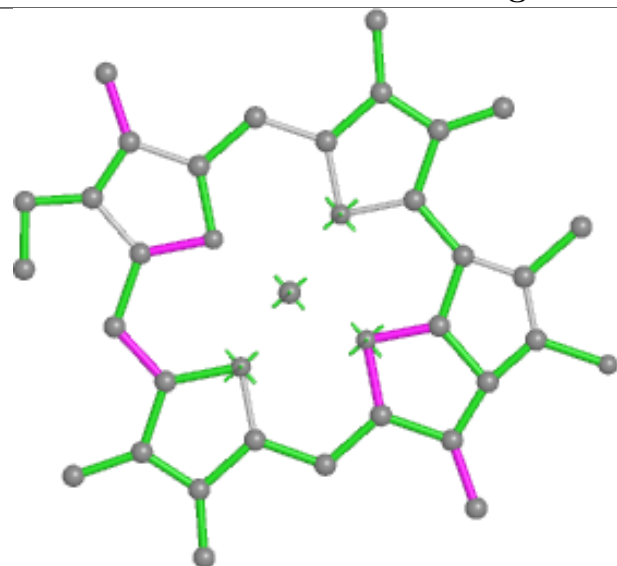
Torsions



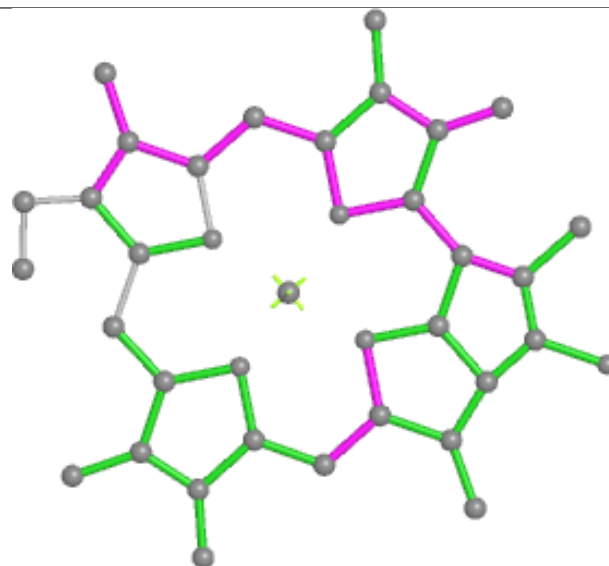
Rings



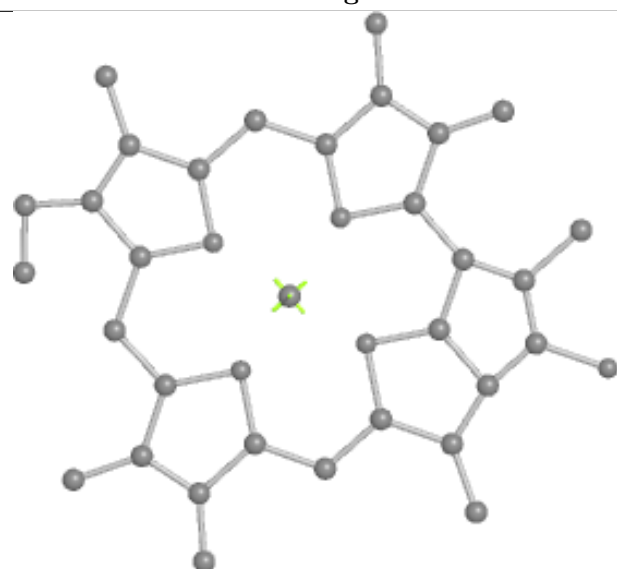
## Ligand CLA A3 310



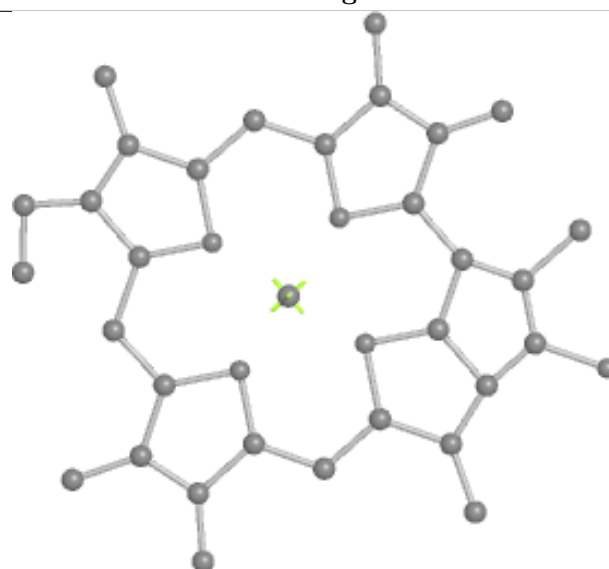
Bond lengths



Bond angles

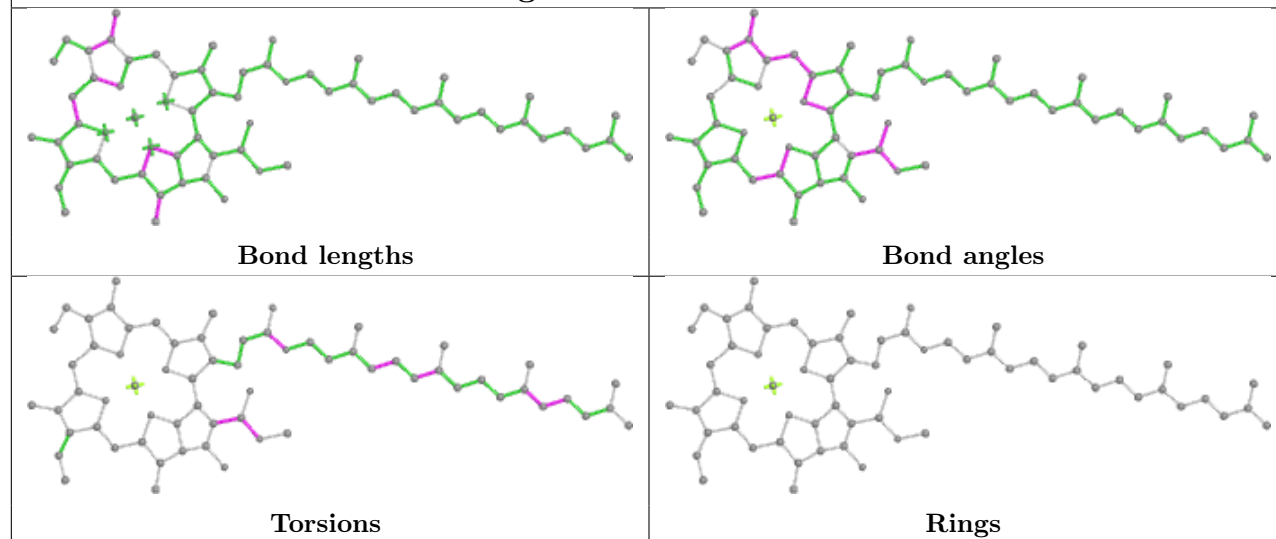


Torsions

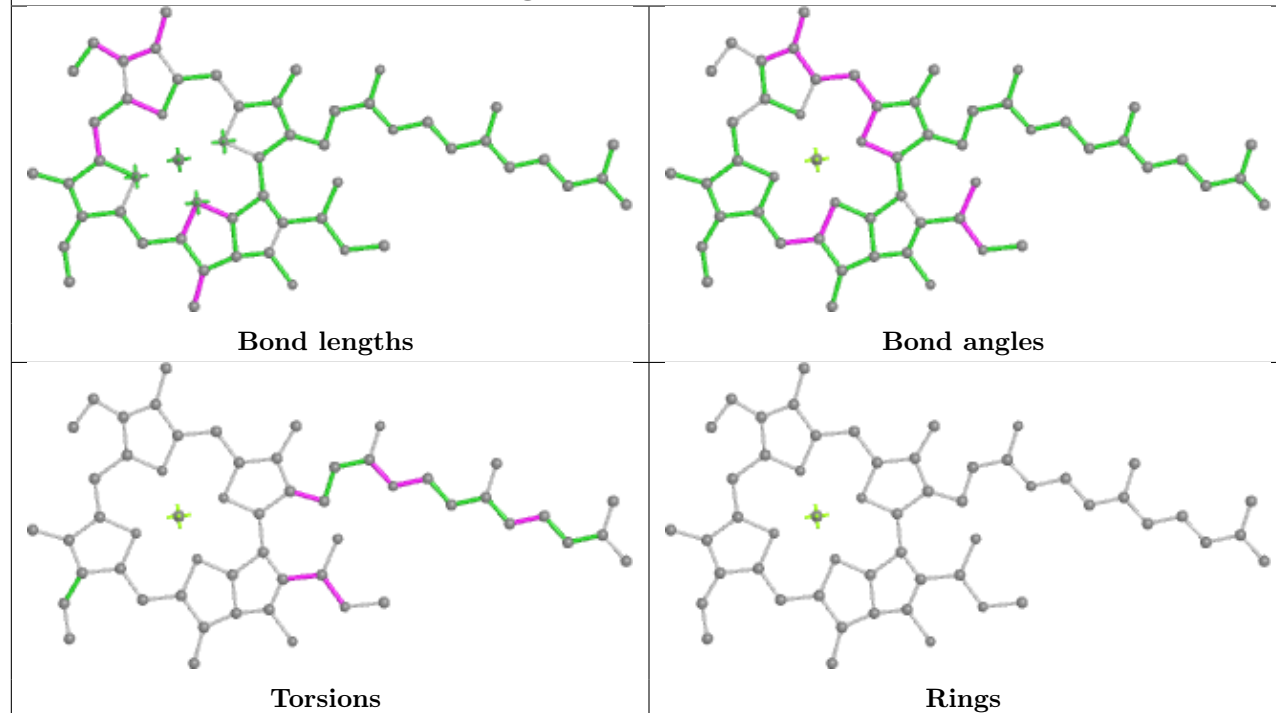


Rings

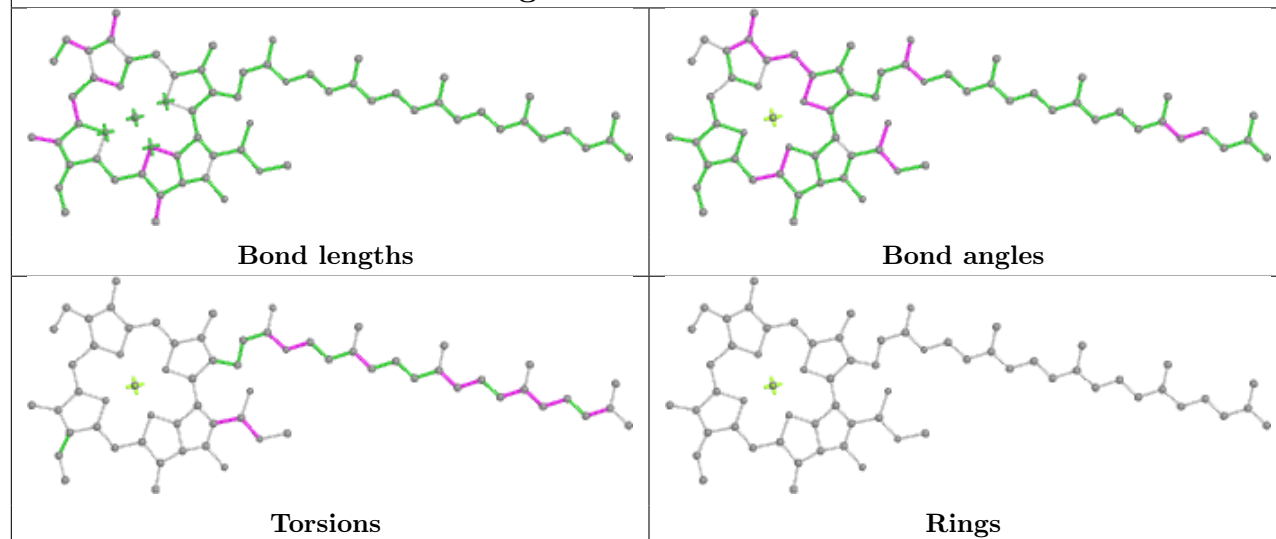
## Ligand CLA AA 811



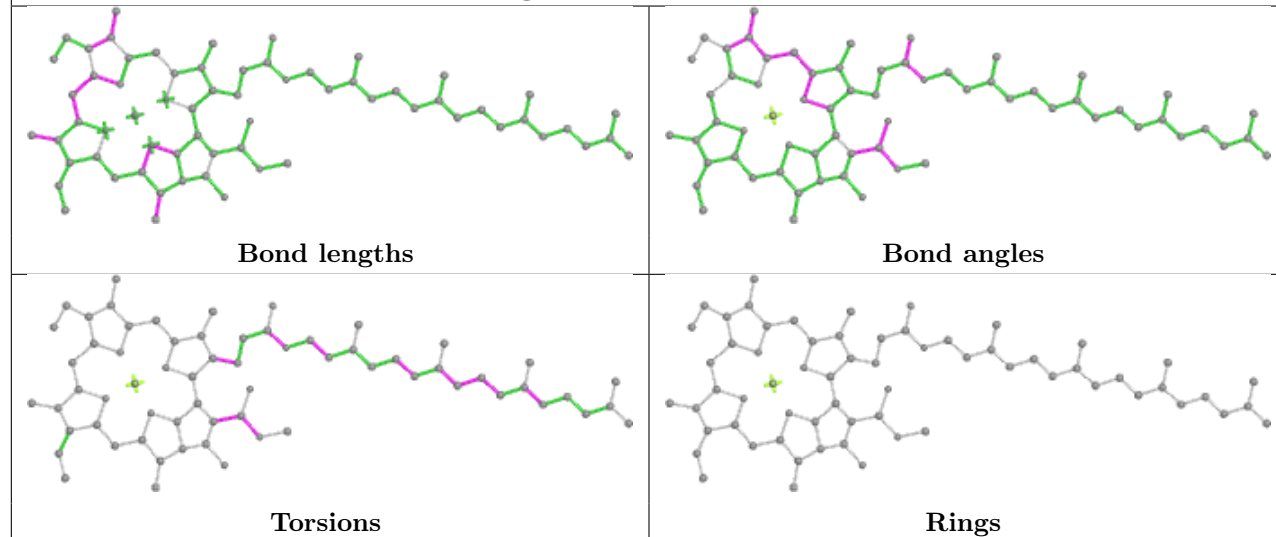
## Ligand CLA AB 820



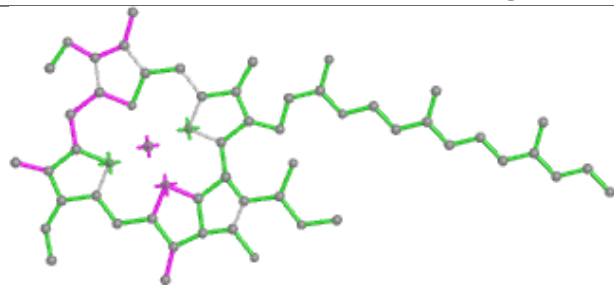
## Ligand CLA AB 815



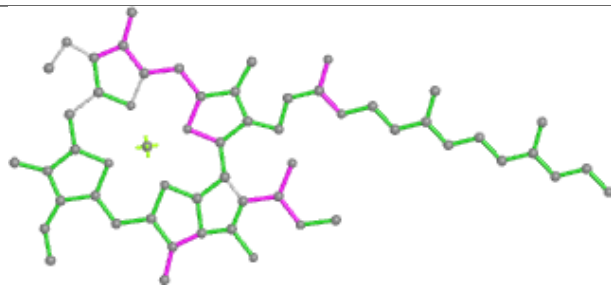
## Ligand CLA AA 830



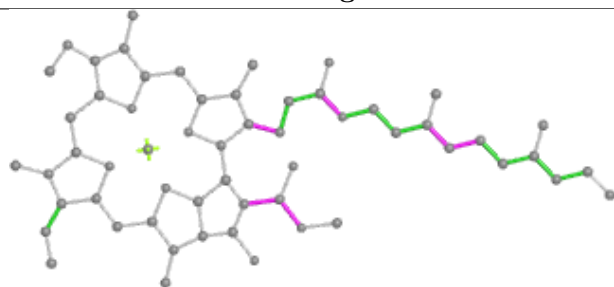
## Ligand CLA AF 802



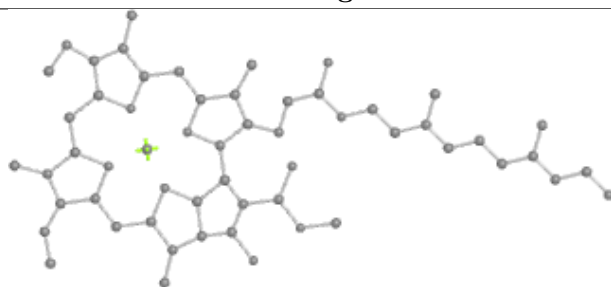
Bond lengths



Bond angles

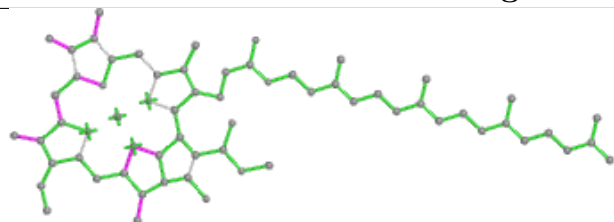


Torsions

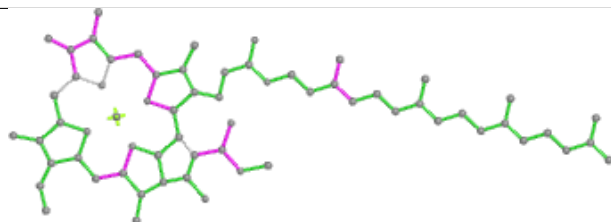


Rings

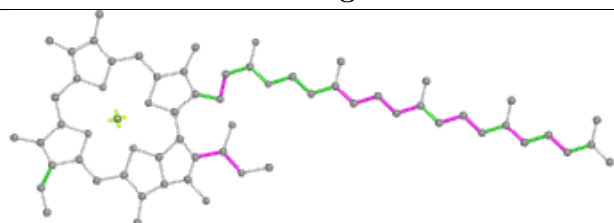
## Ligand CLA AB 802



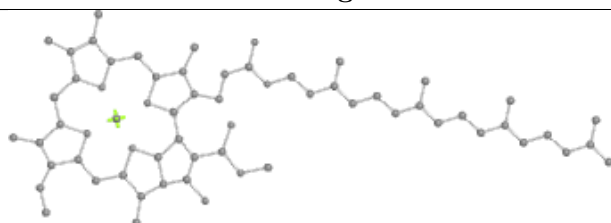
Bond lengths



Bond angles

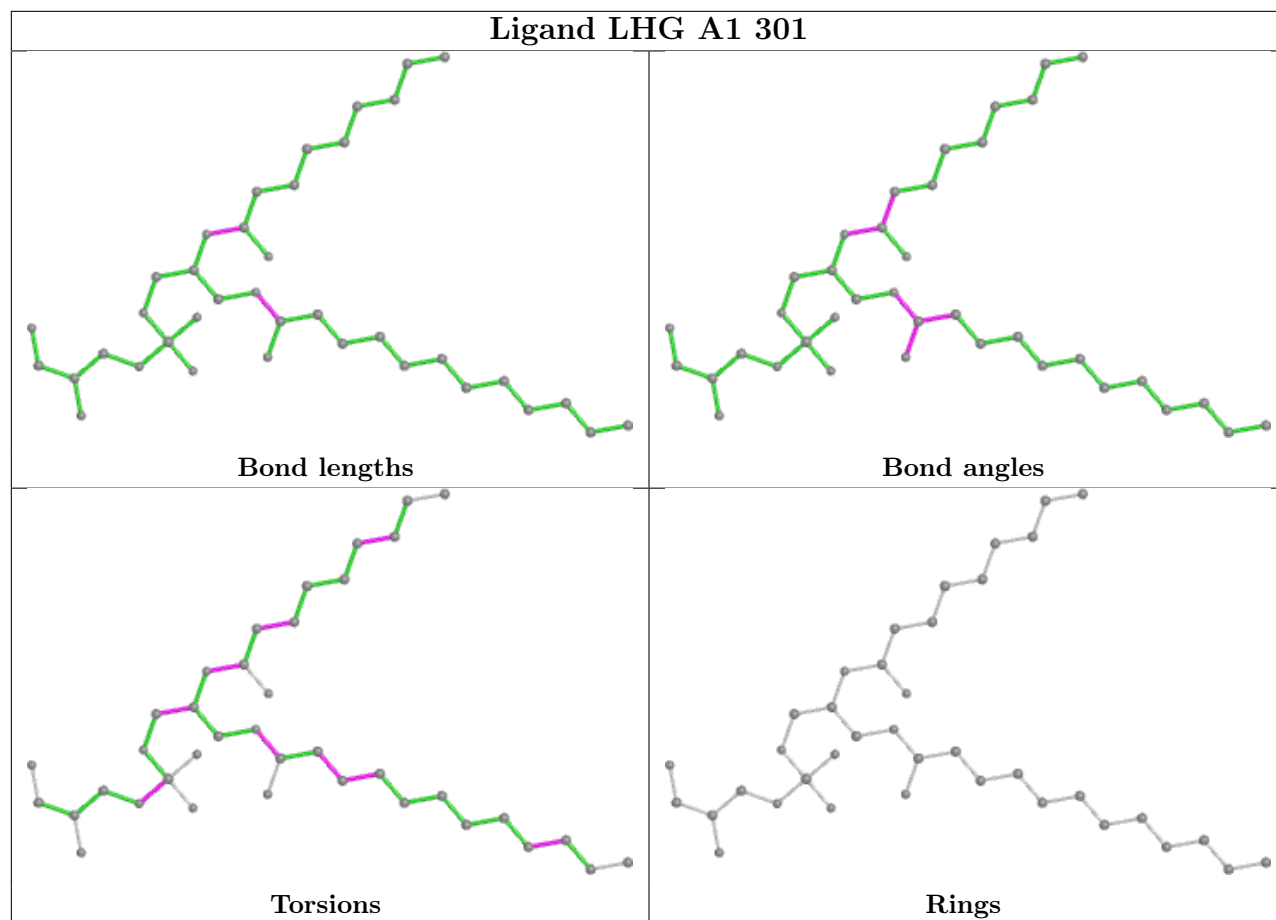


Torsions

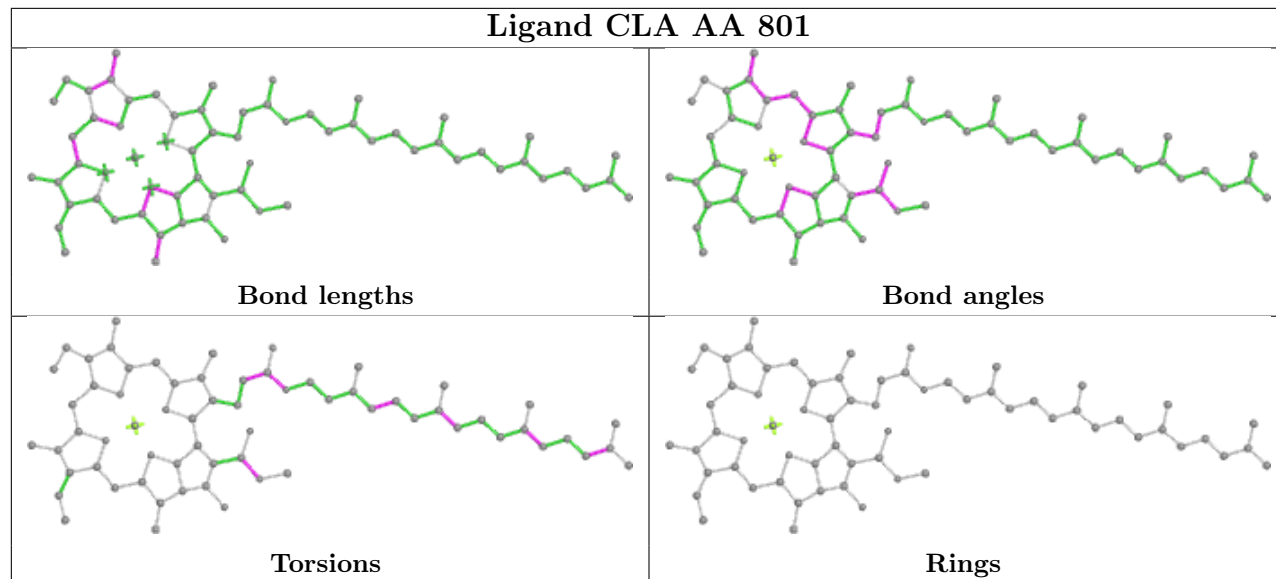


Rings

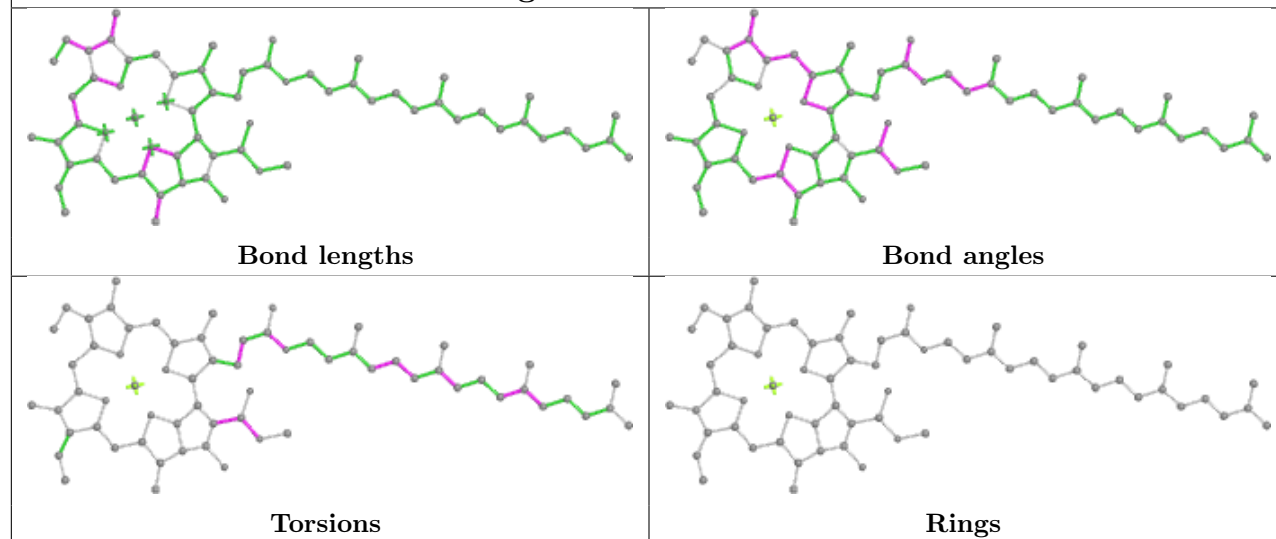
## Ligand LHG A1 301



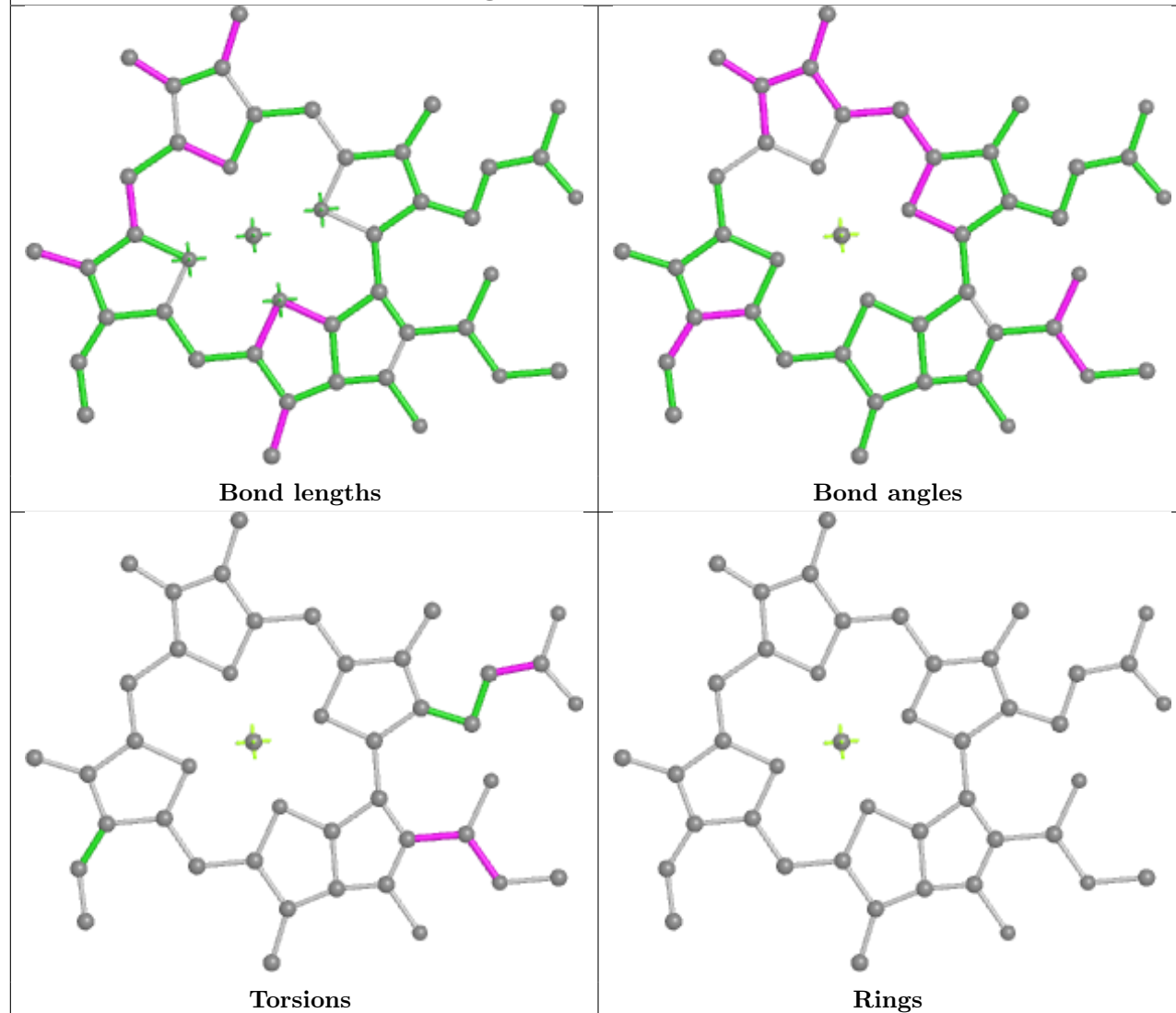
## Ligand CLA AA 801



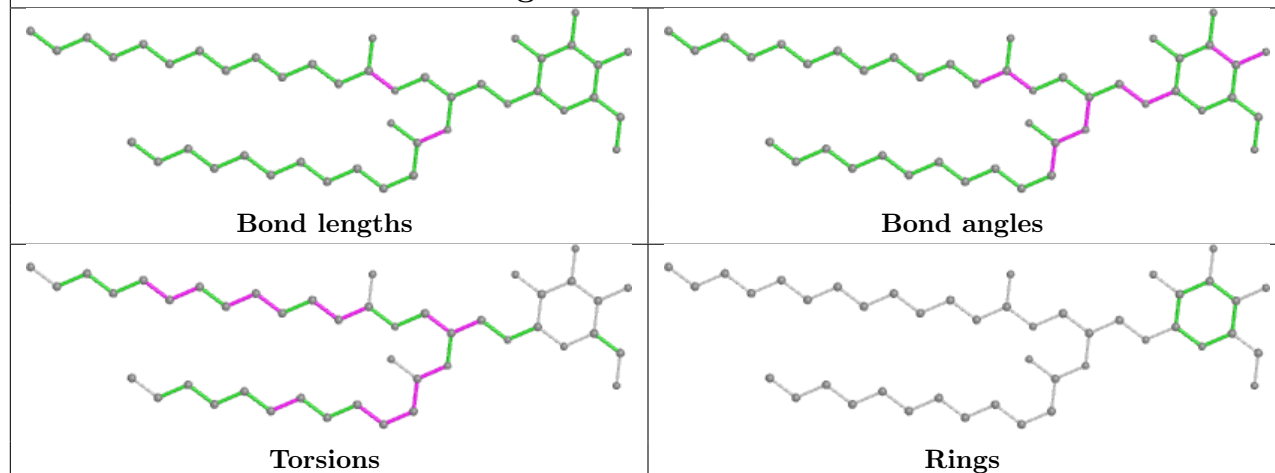
## Ligand CLA AA 840



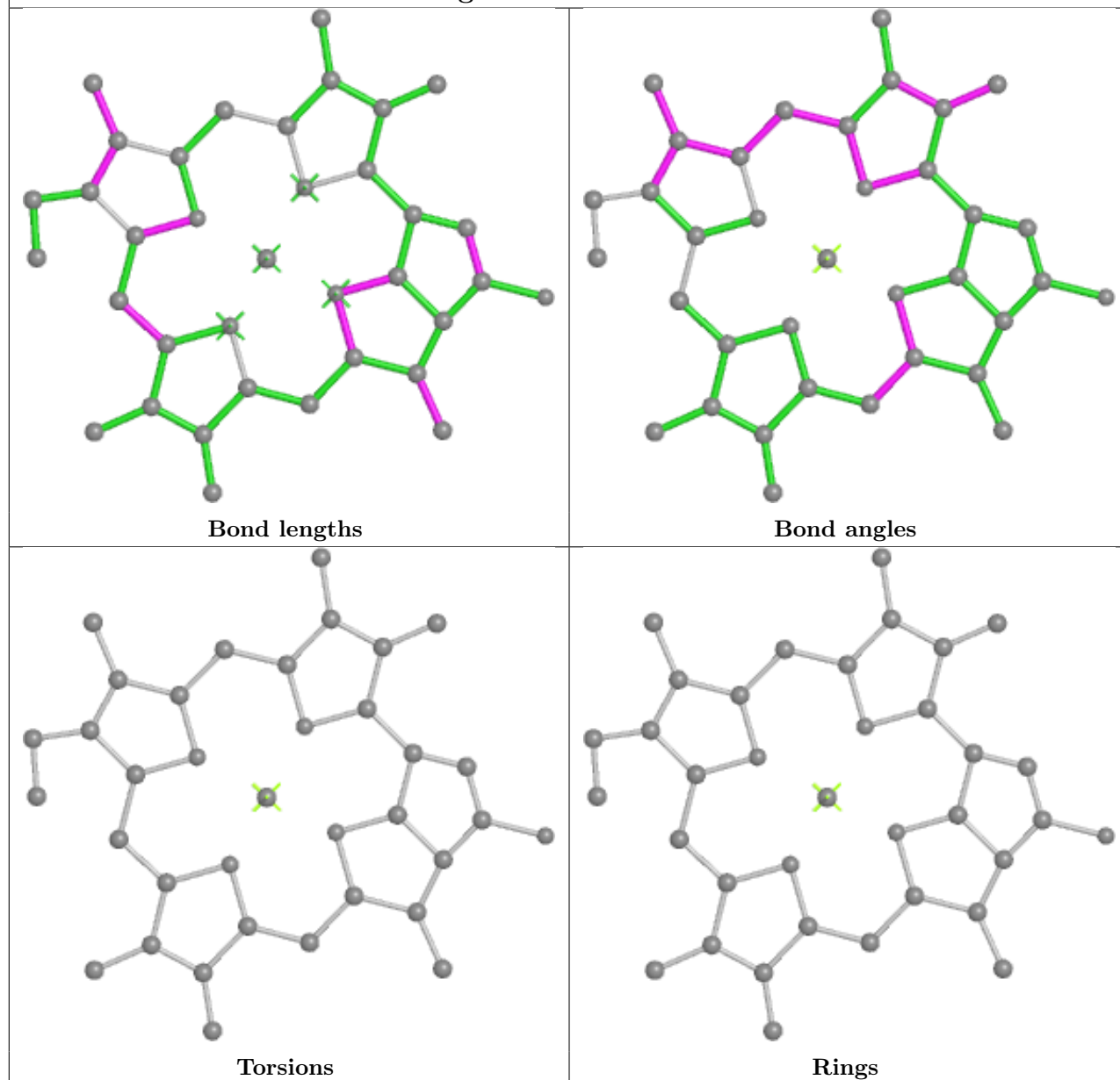
## Ligand CLA A4 302

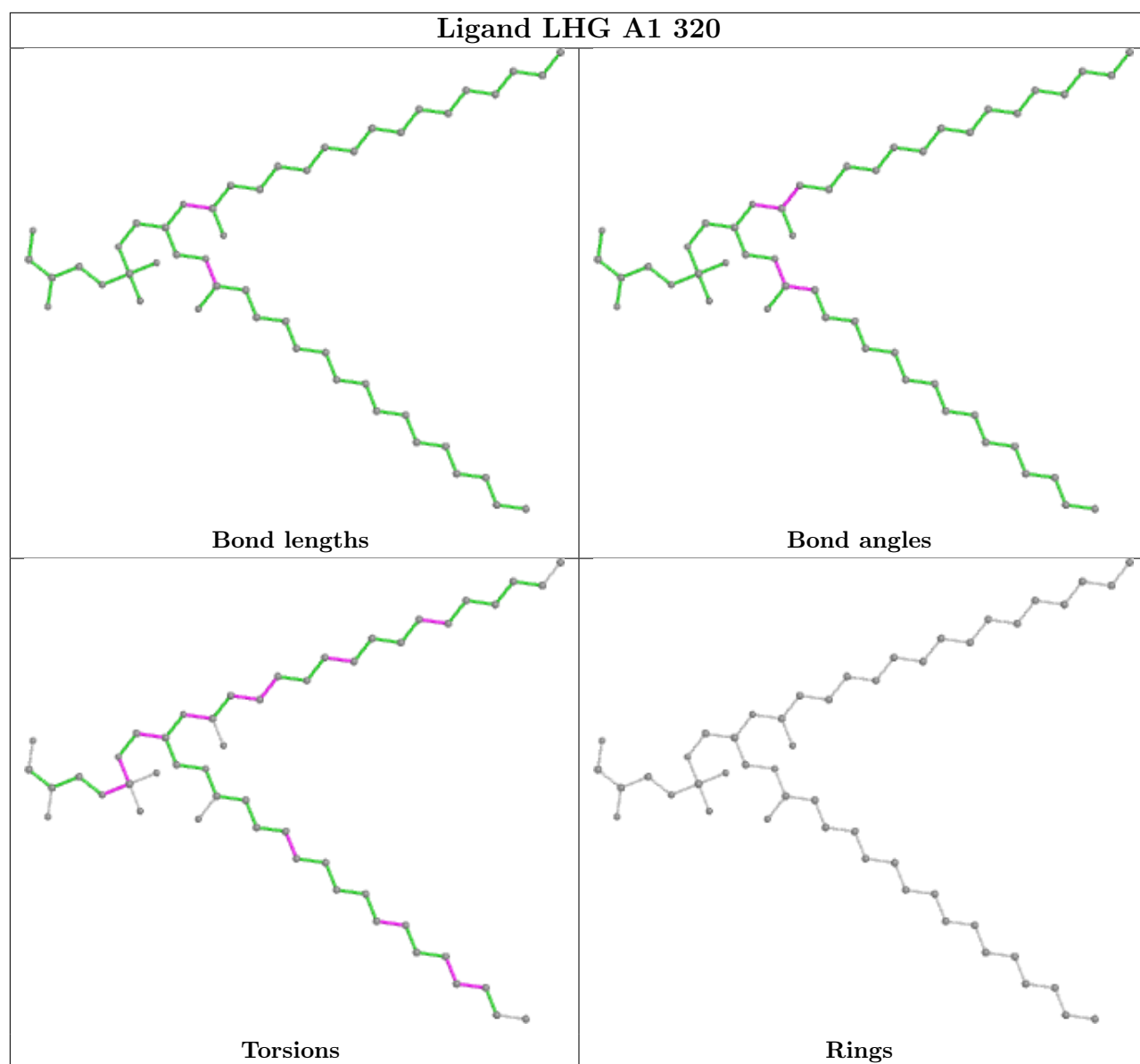


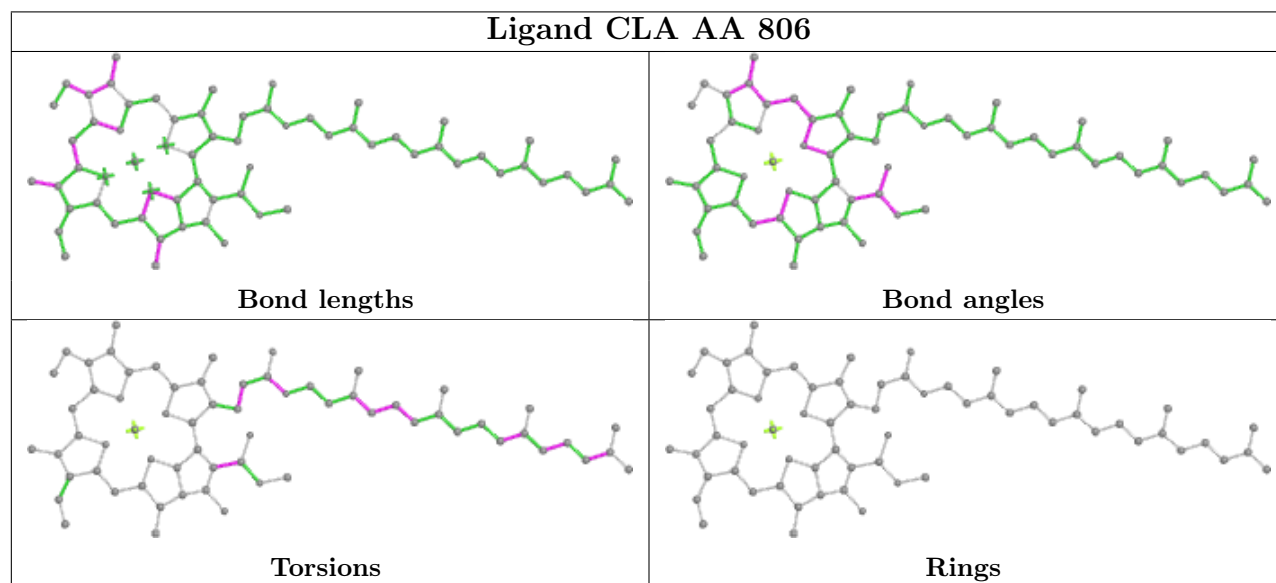
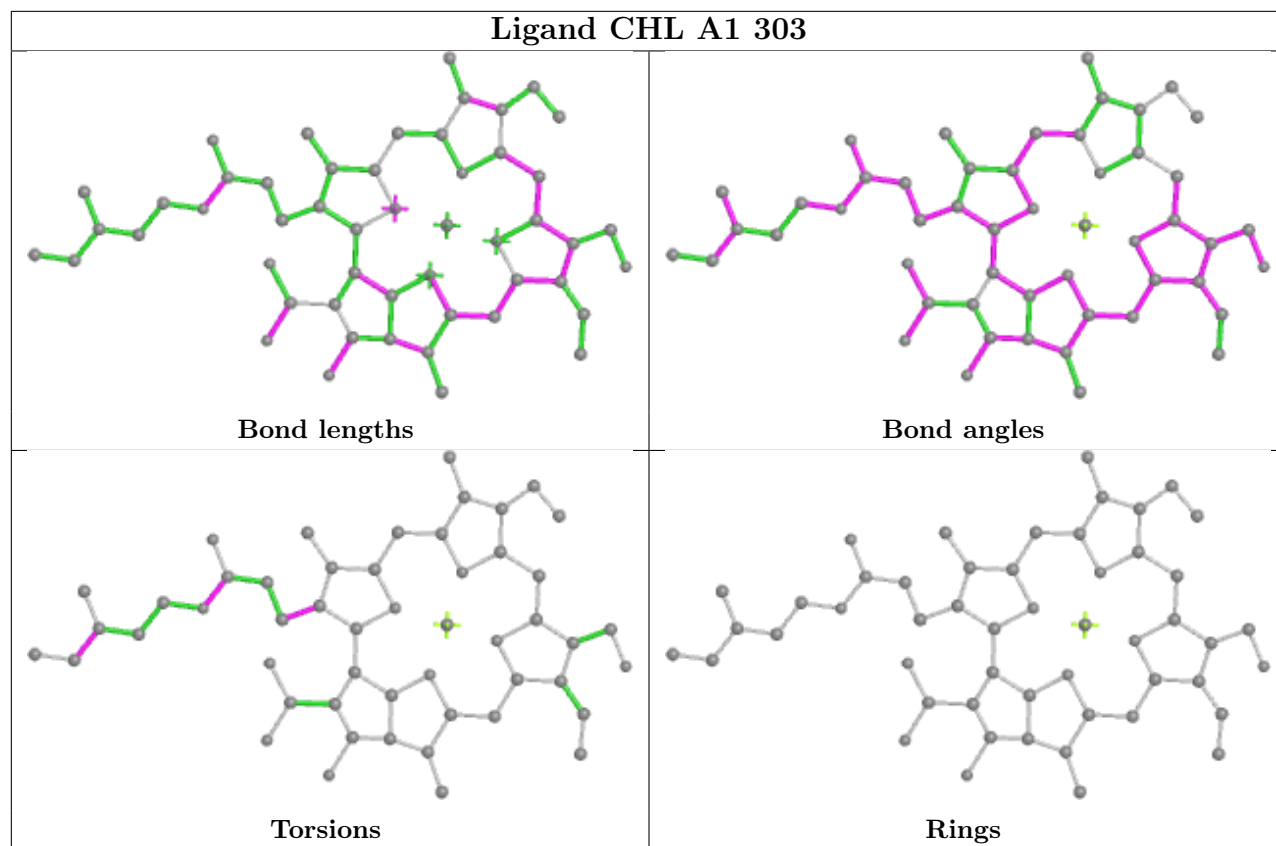
## Ligand LMG A1 321

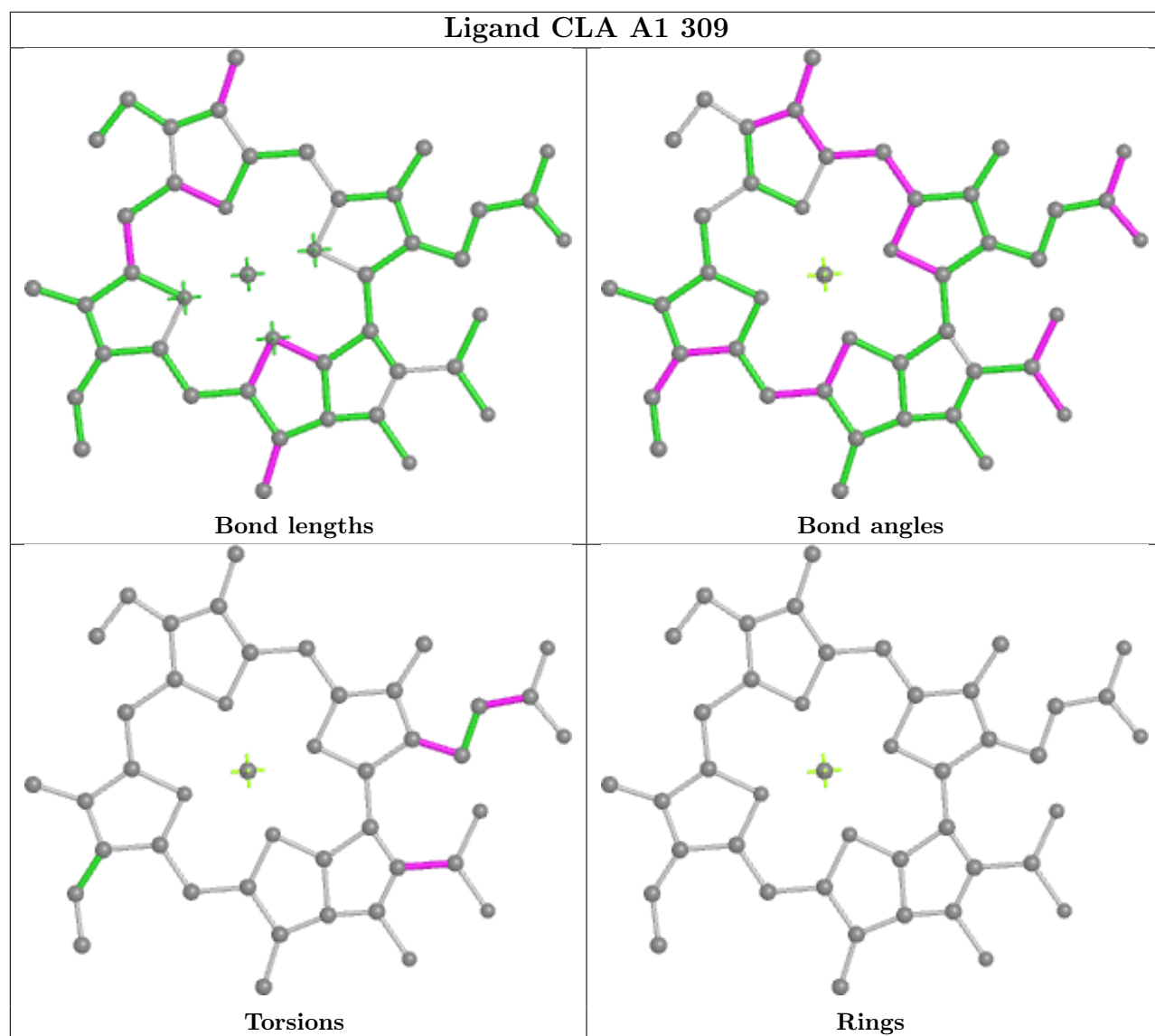
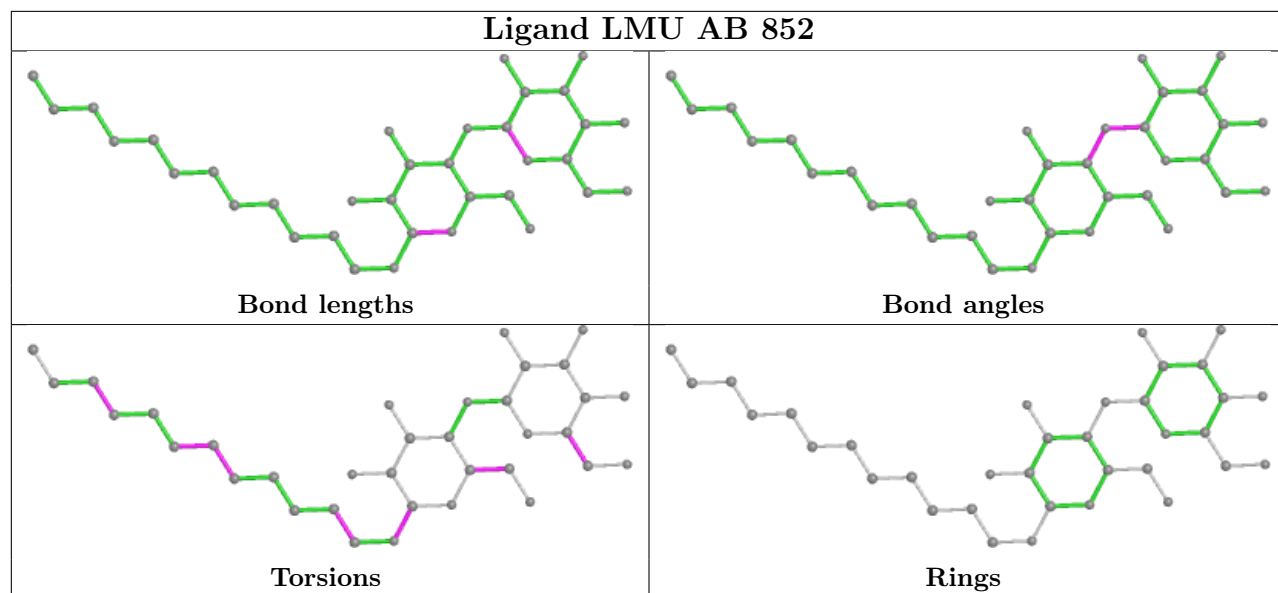


## Ligand CLA A3 314

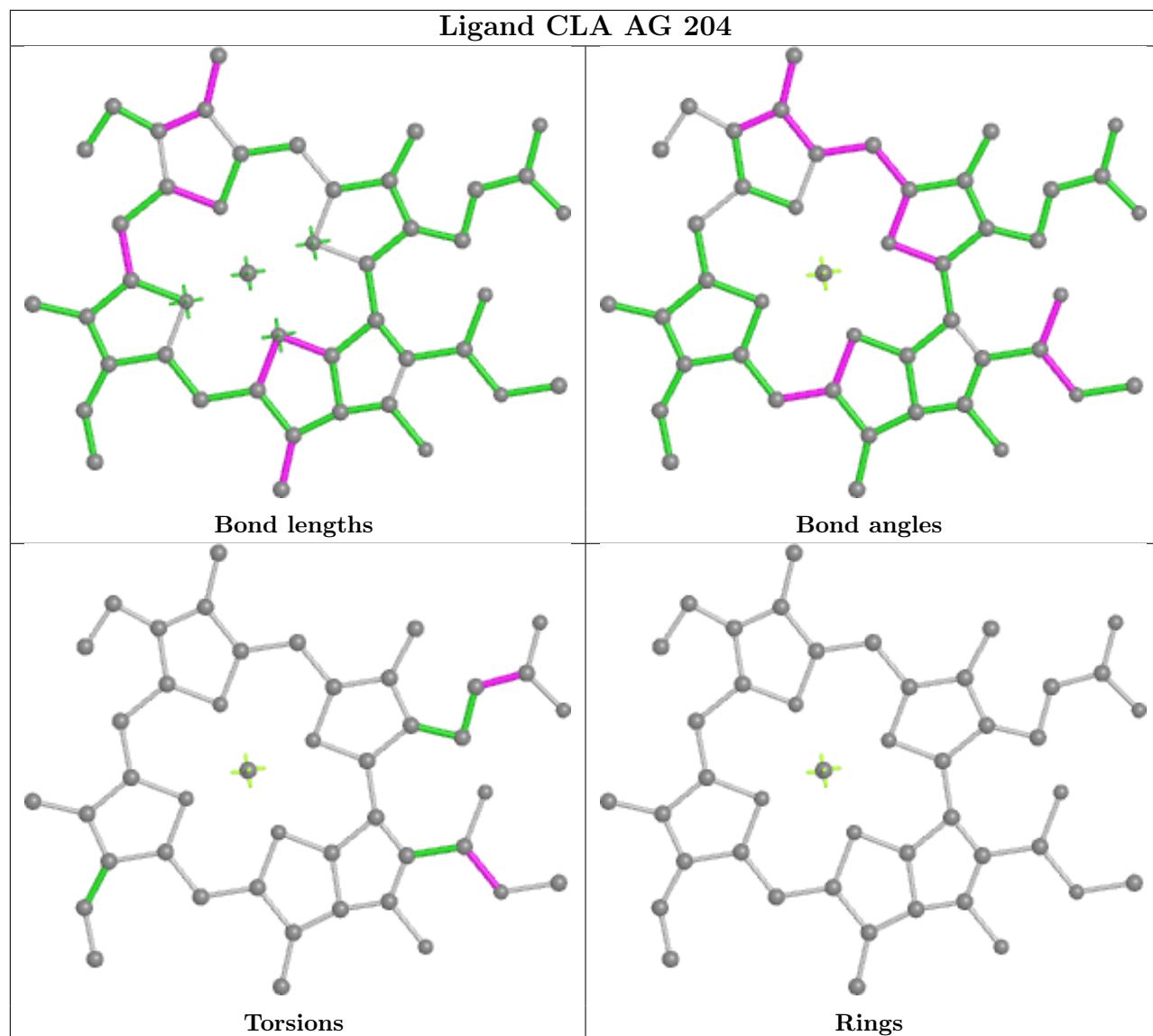




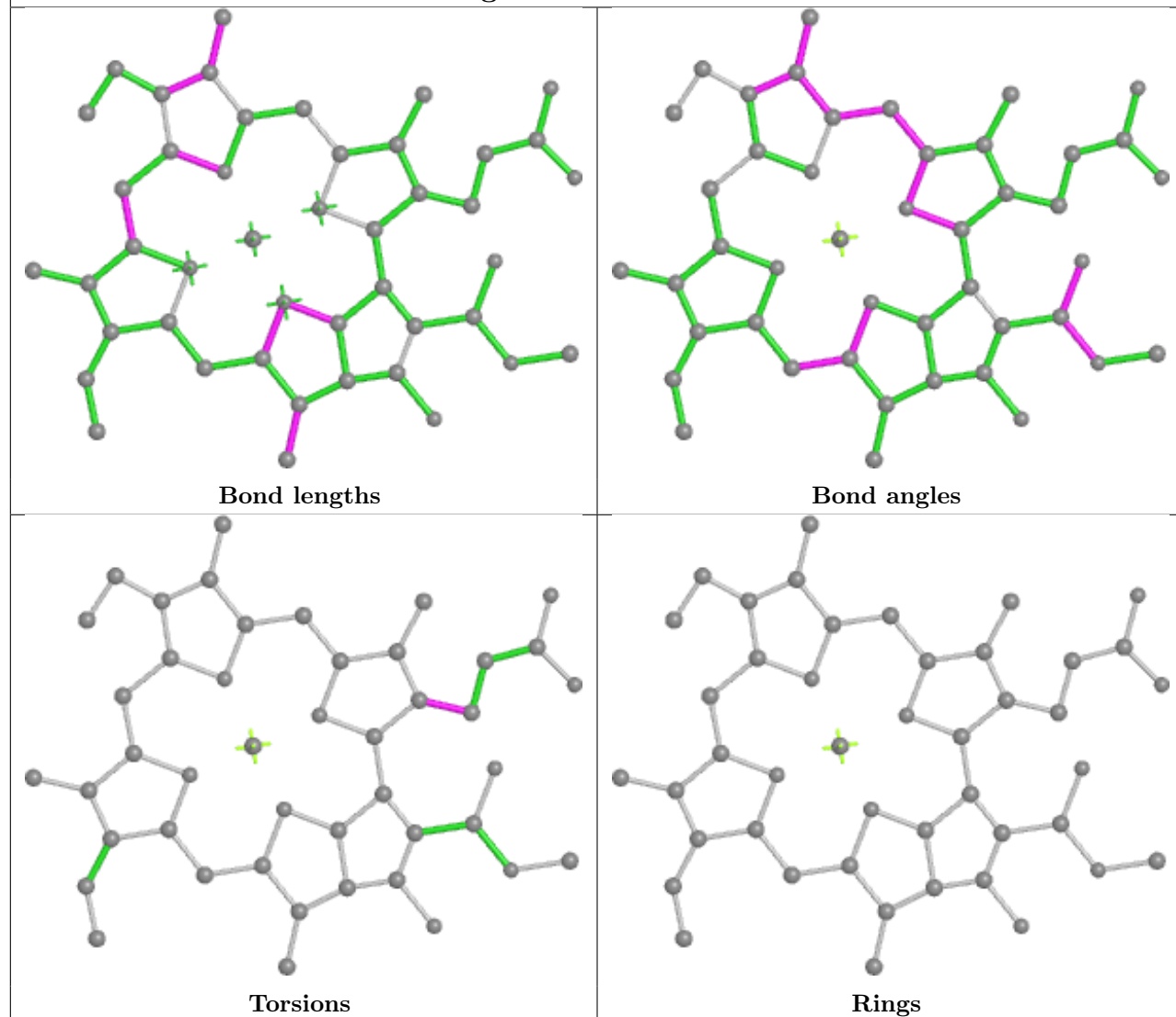




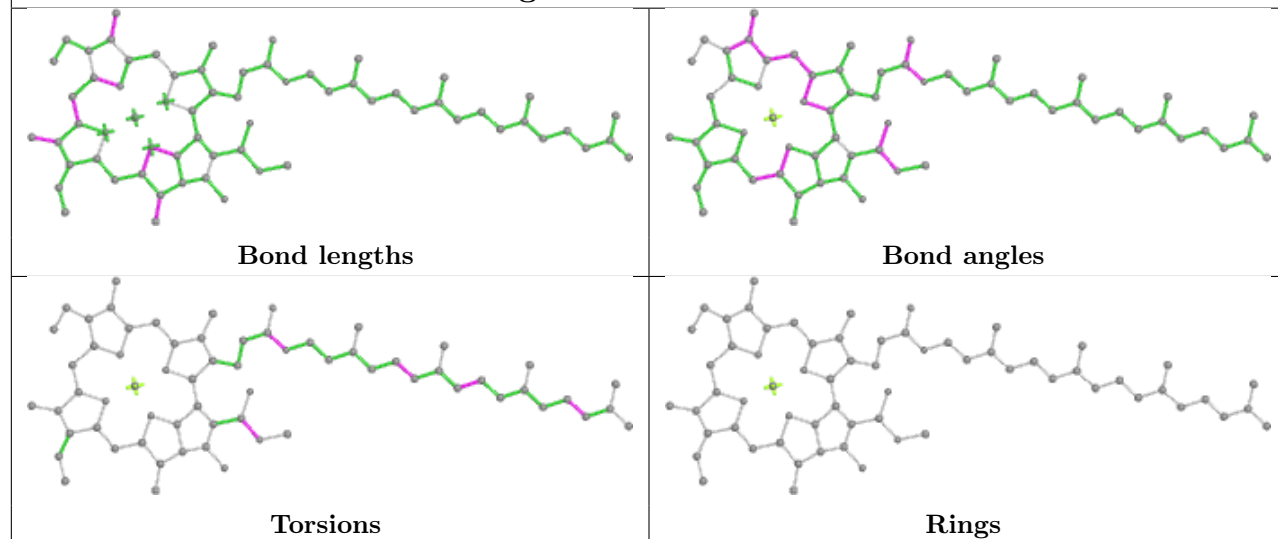
## Ligand CLA AG 204



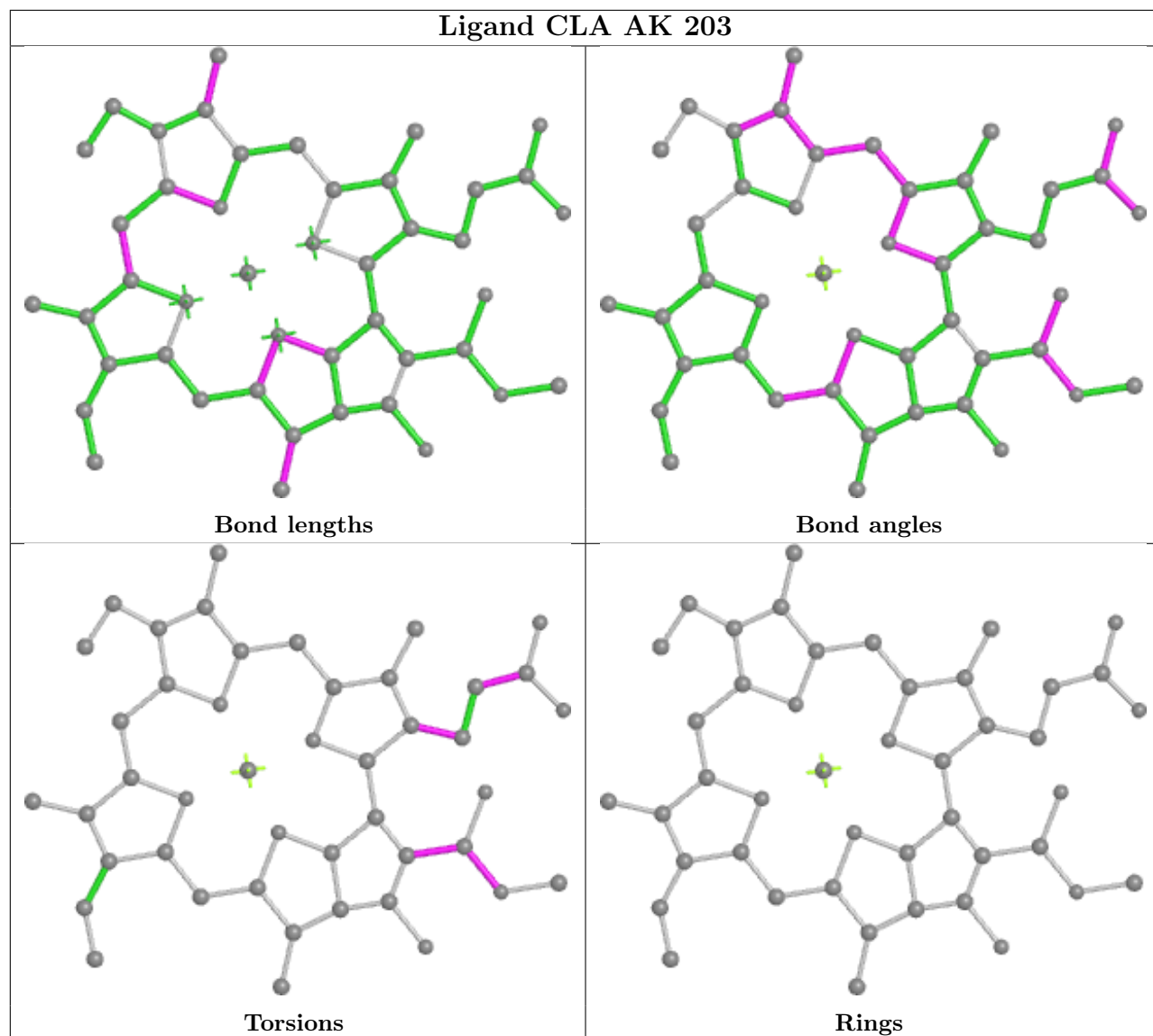
## Ligand CLA A4 307

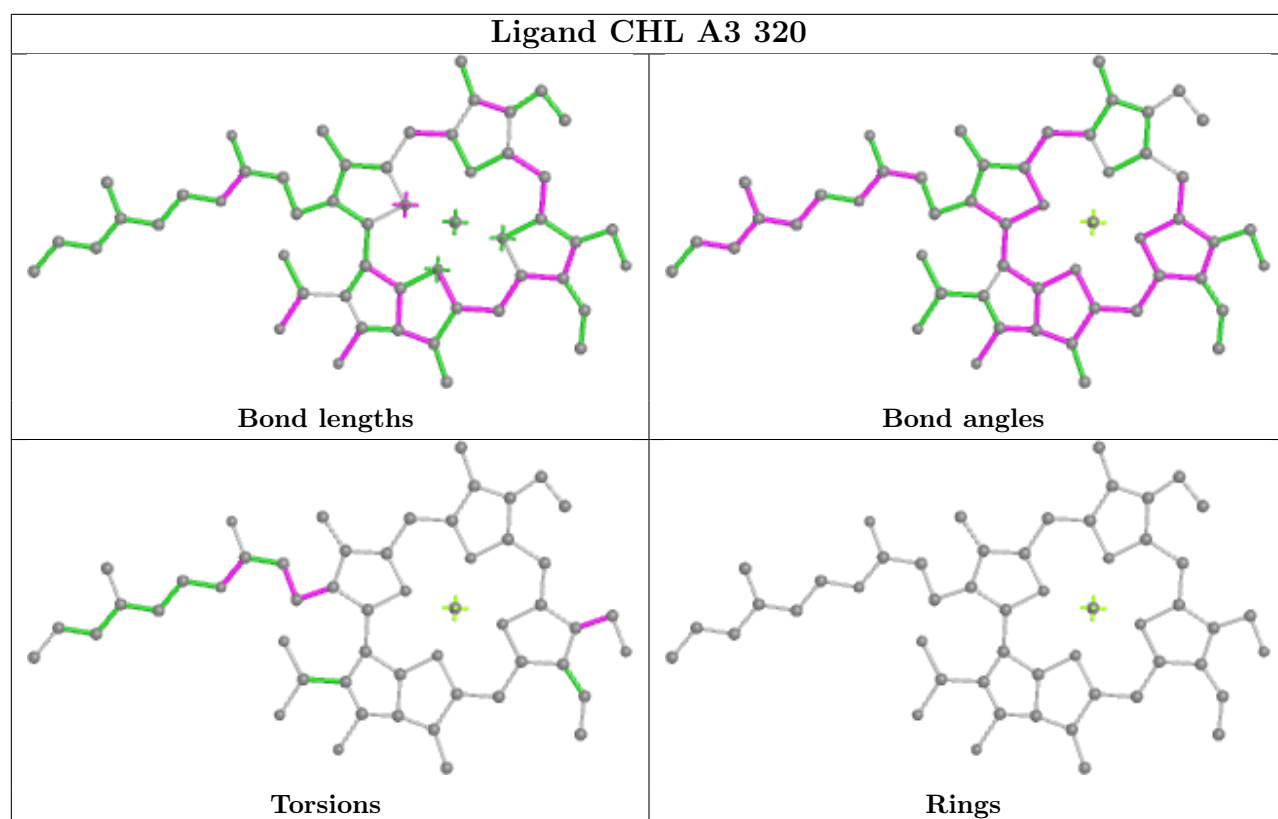


## Ligand CLA AB 838

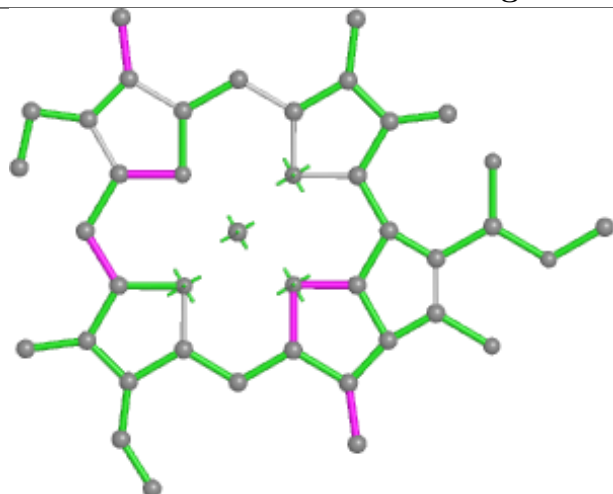


## Ligand CLA AK 203

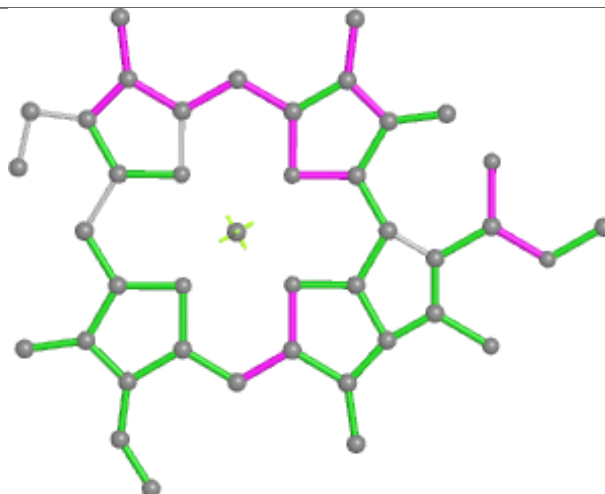




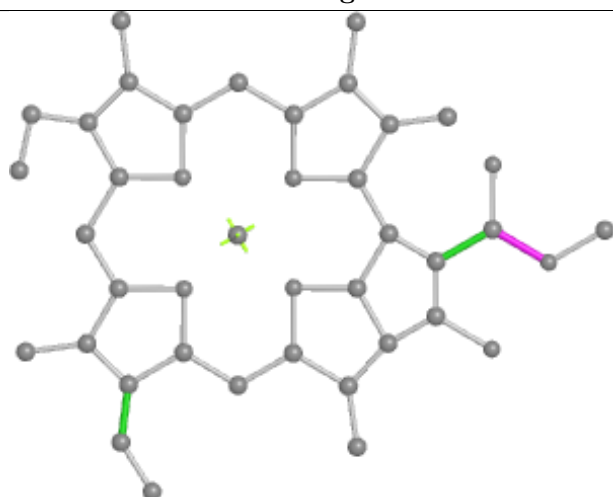
## Ligand CLA AB 805



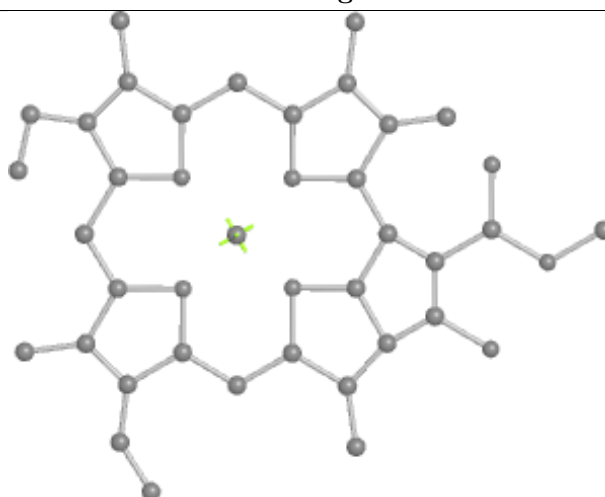
Bond lengths



Bond angles

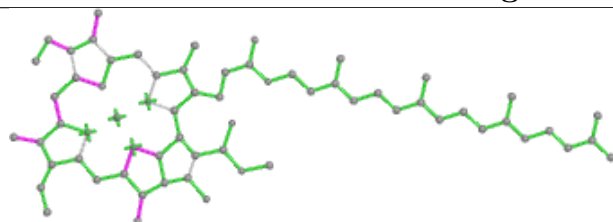


Torsions

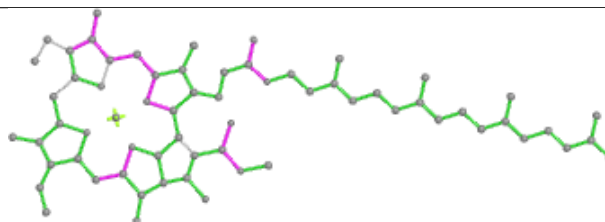


Rings

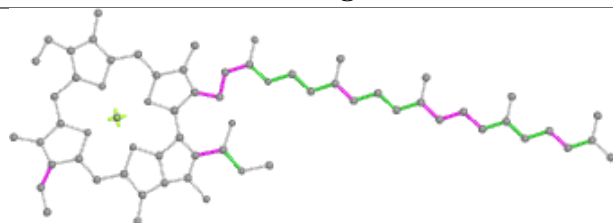
## Ligand CLA AB 828



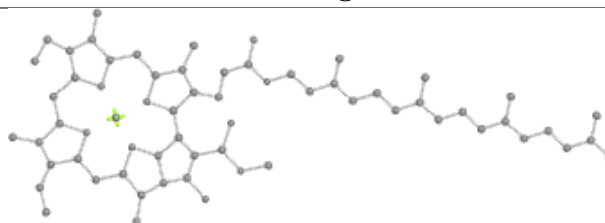
Bond lengths



Bond angles

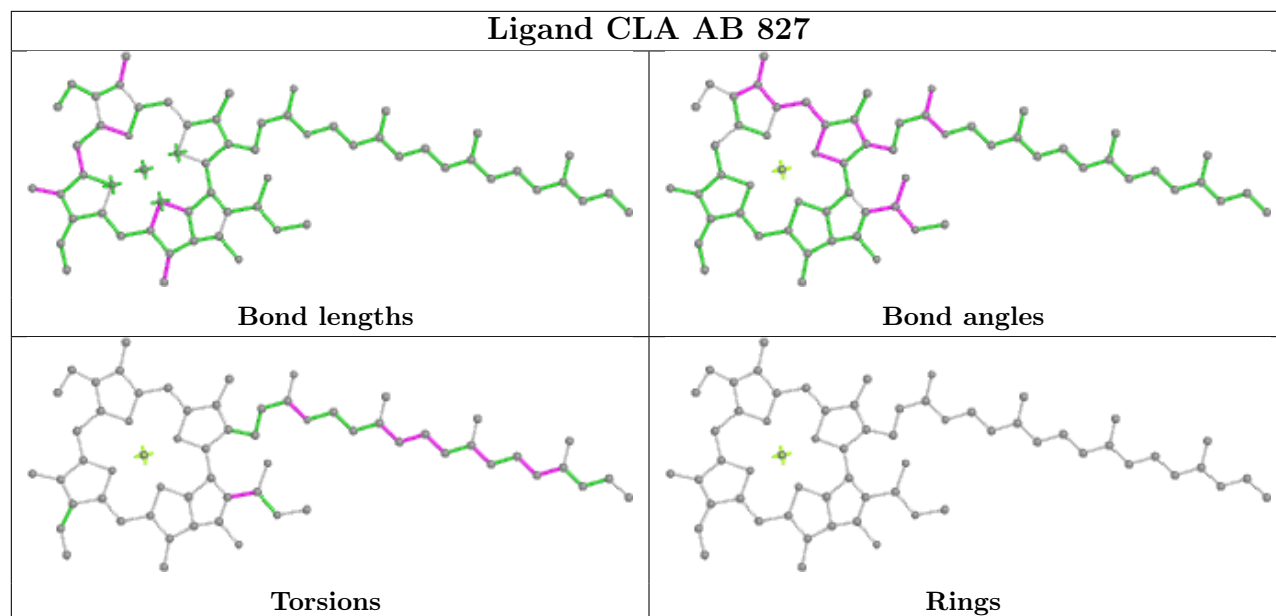


Torsions

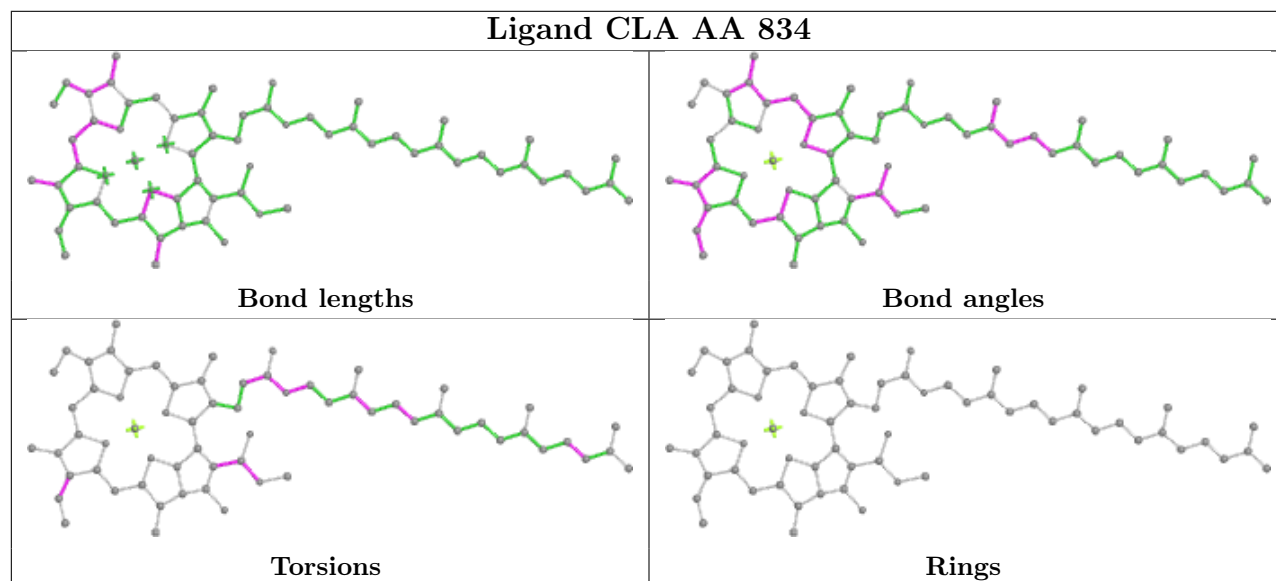


Rings

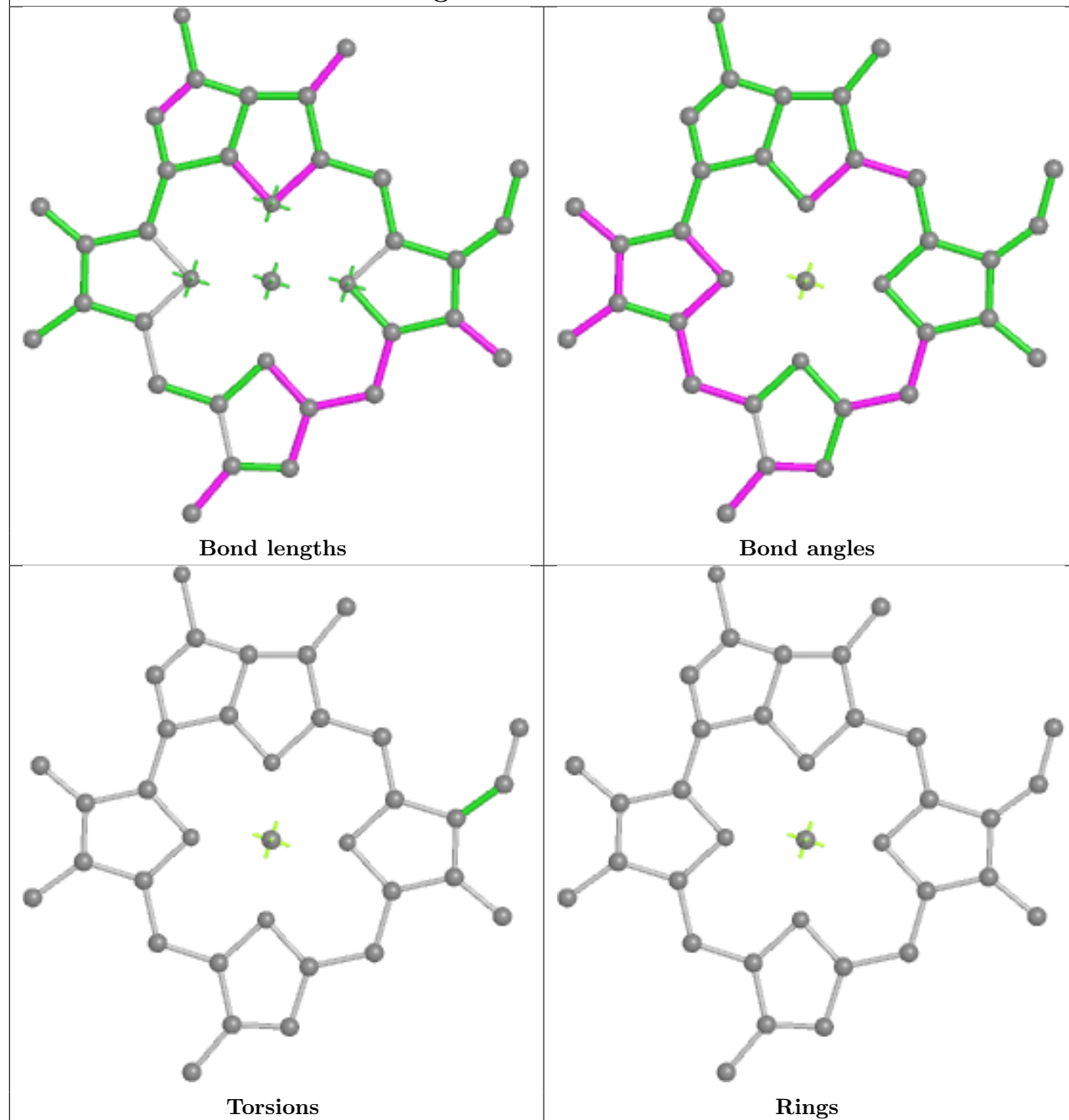
## Ligand CLA AB 827



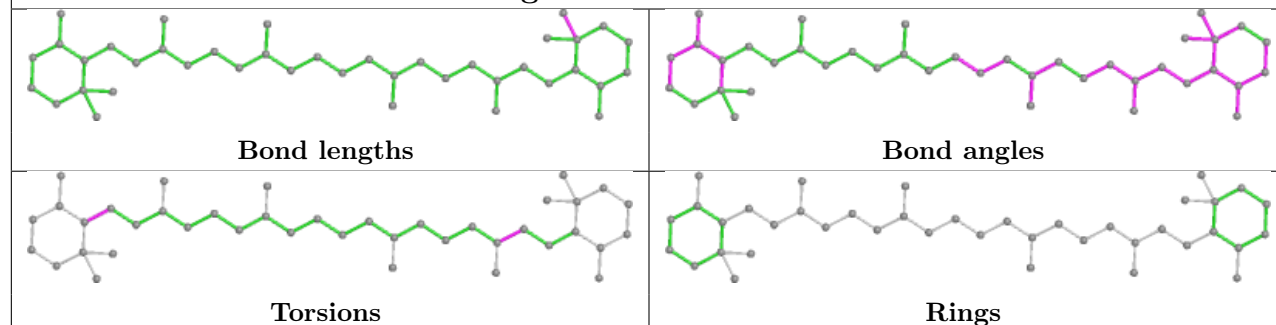
## Ligand CLA AA 834

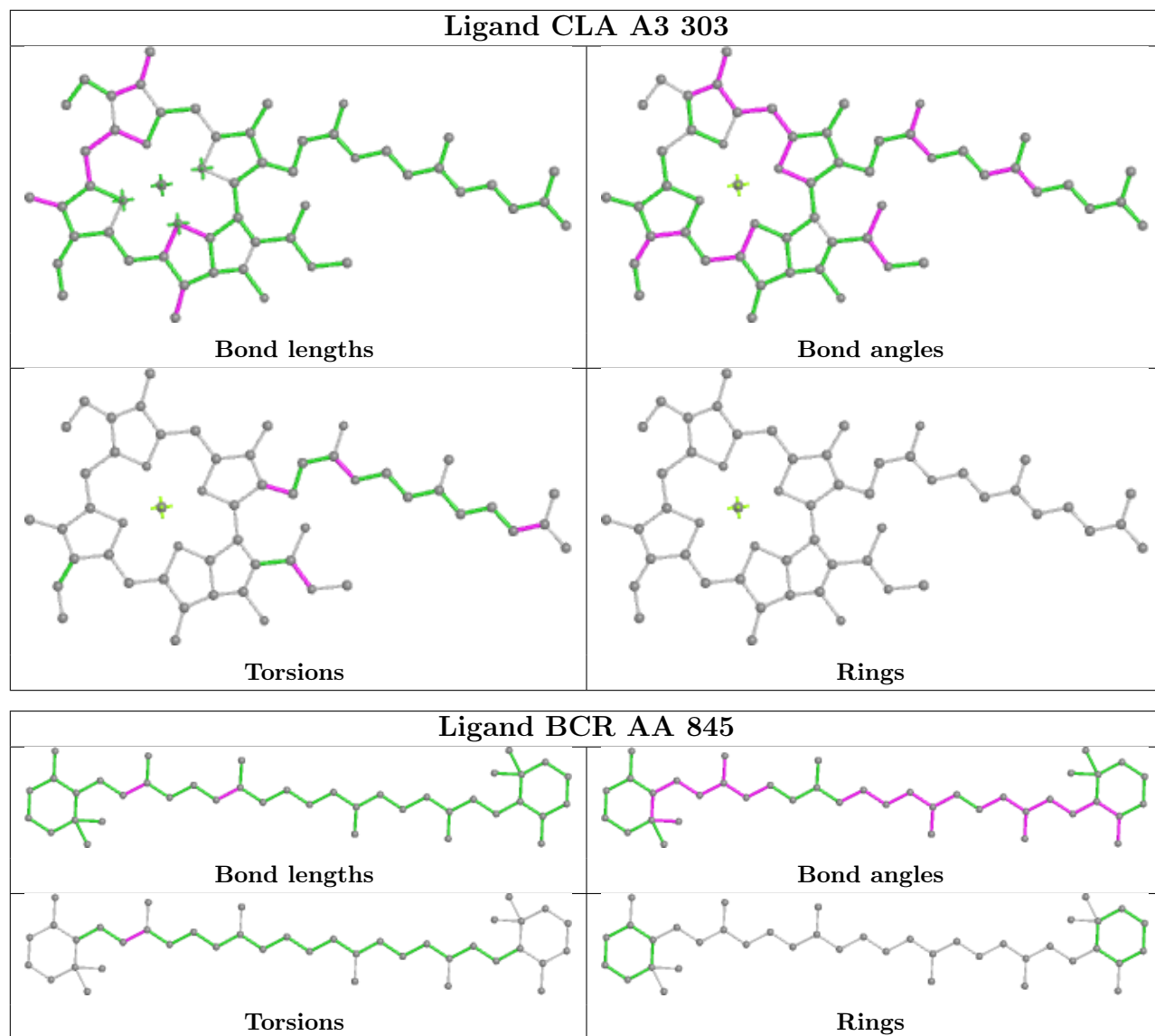


## Ligand CLA AK 201

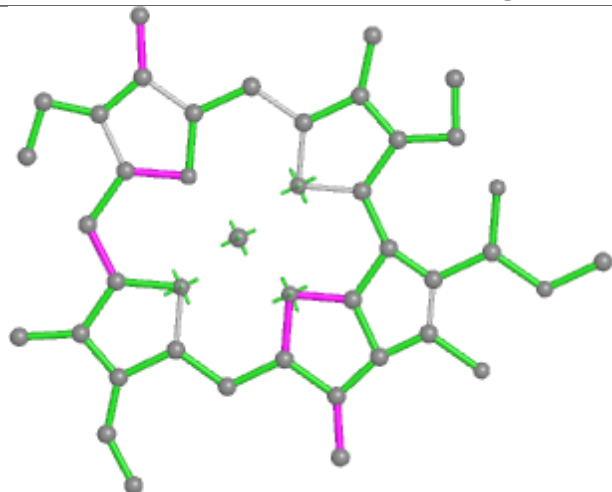


## Ligand BCR A3 318

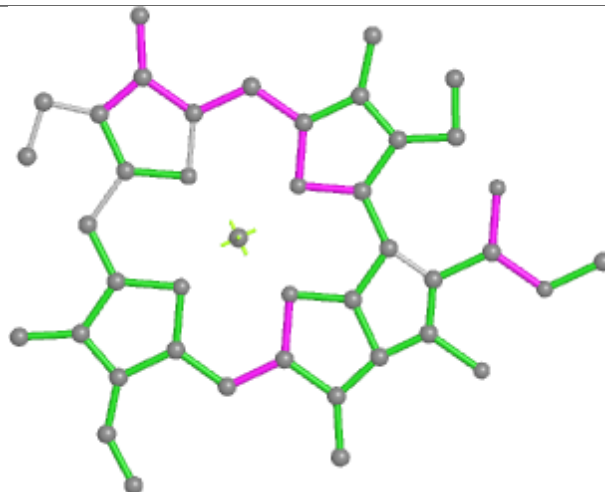




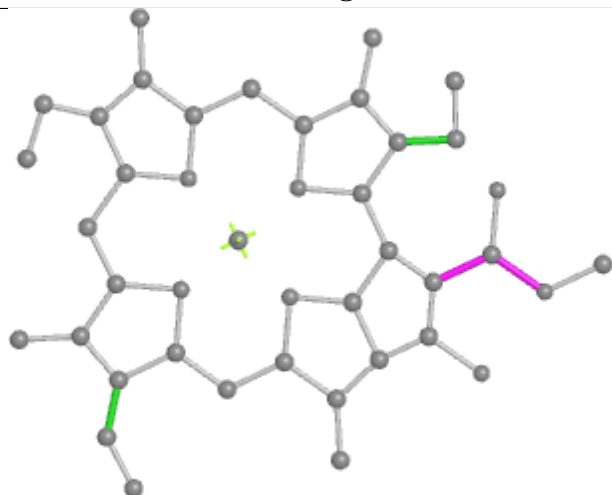
## Ligand CLA AG 203



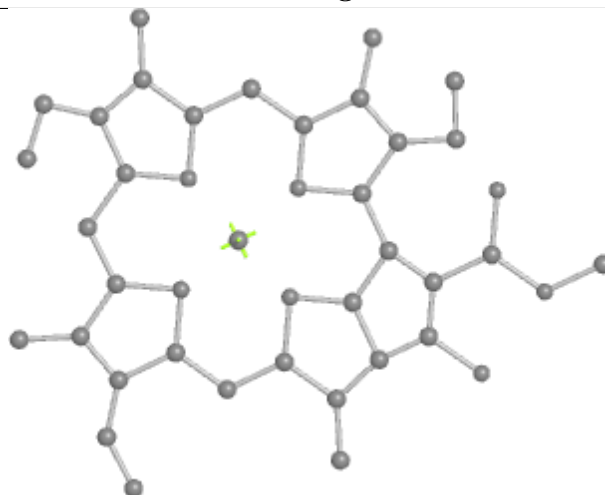
Bond lengths



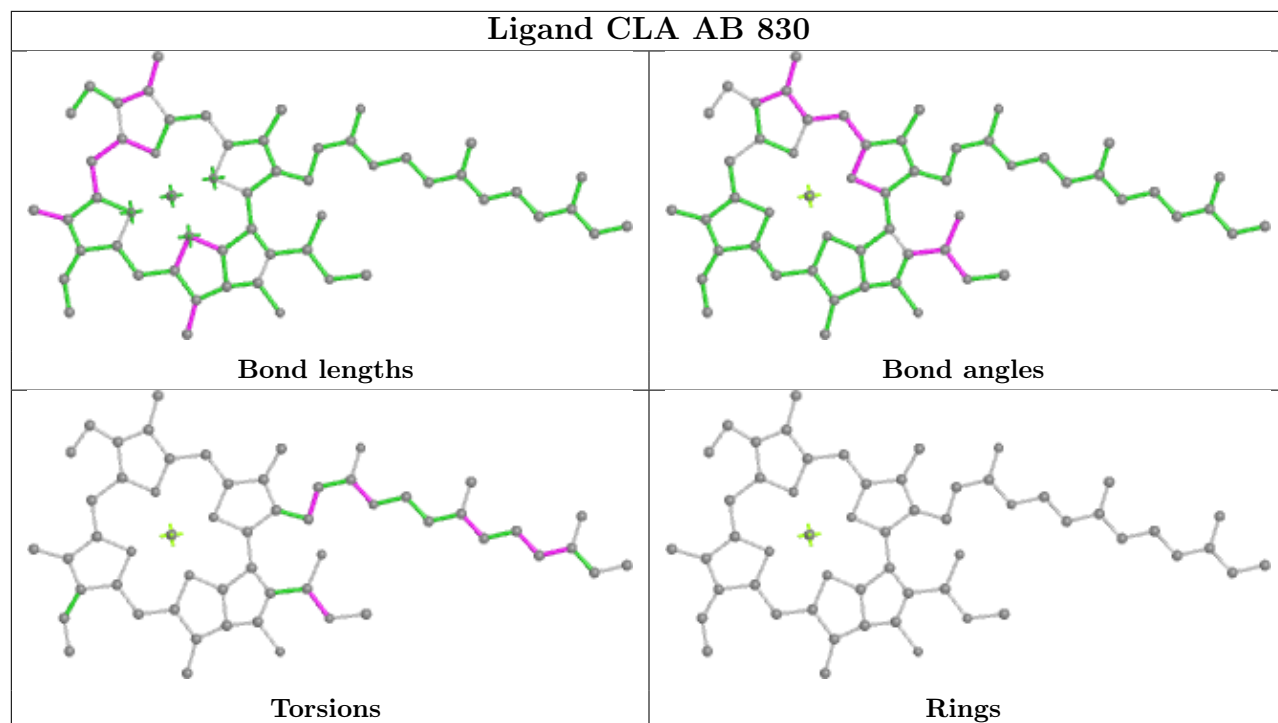
Bond angles

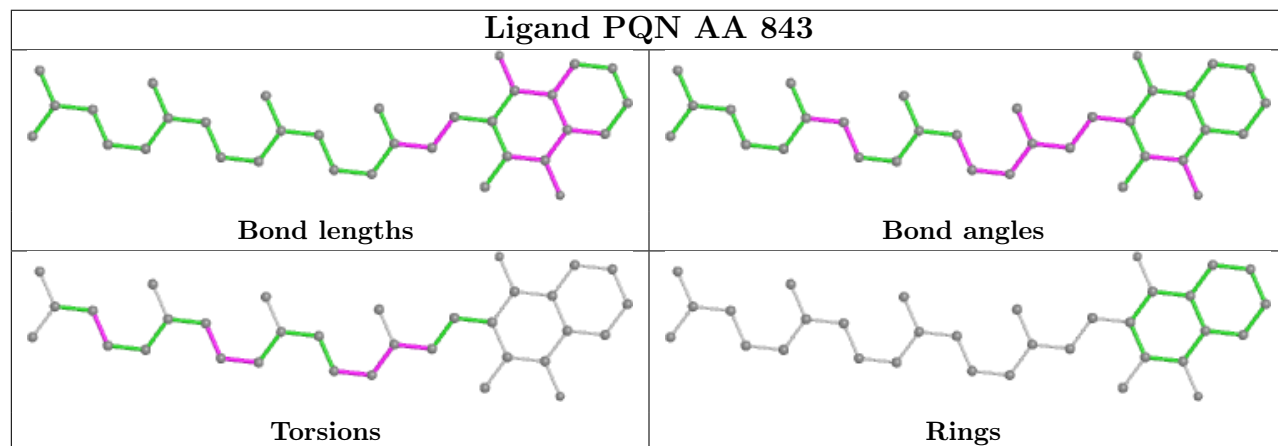
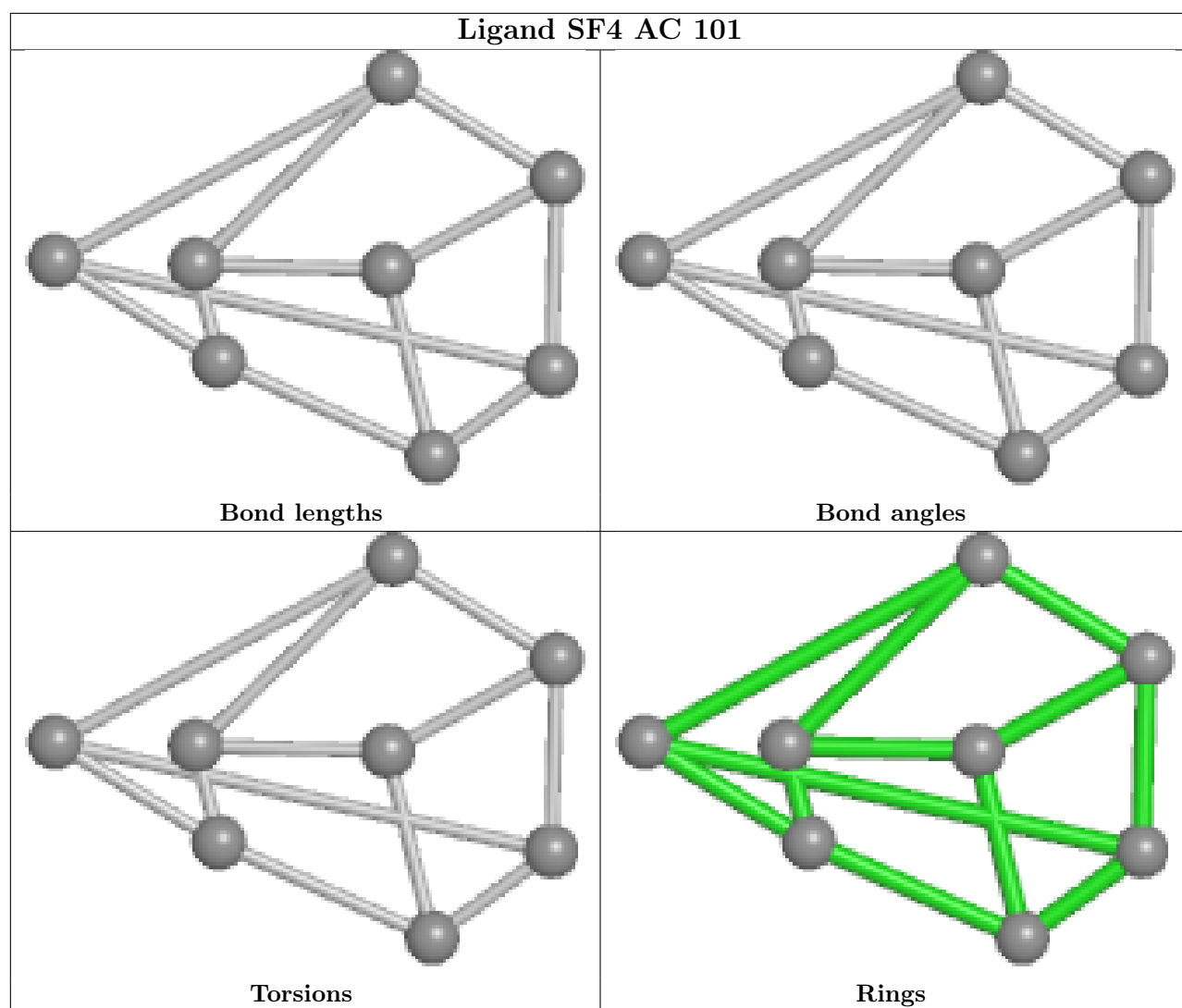


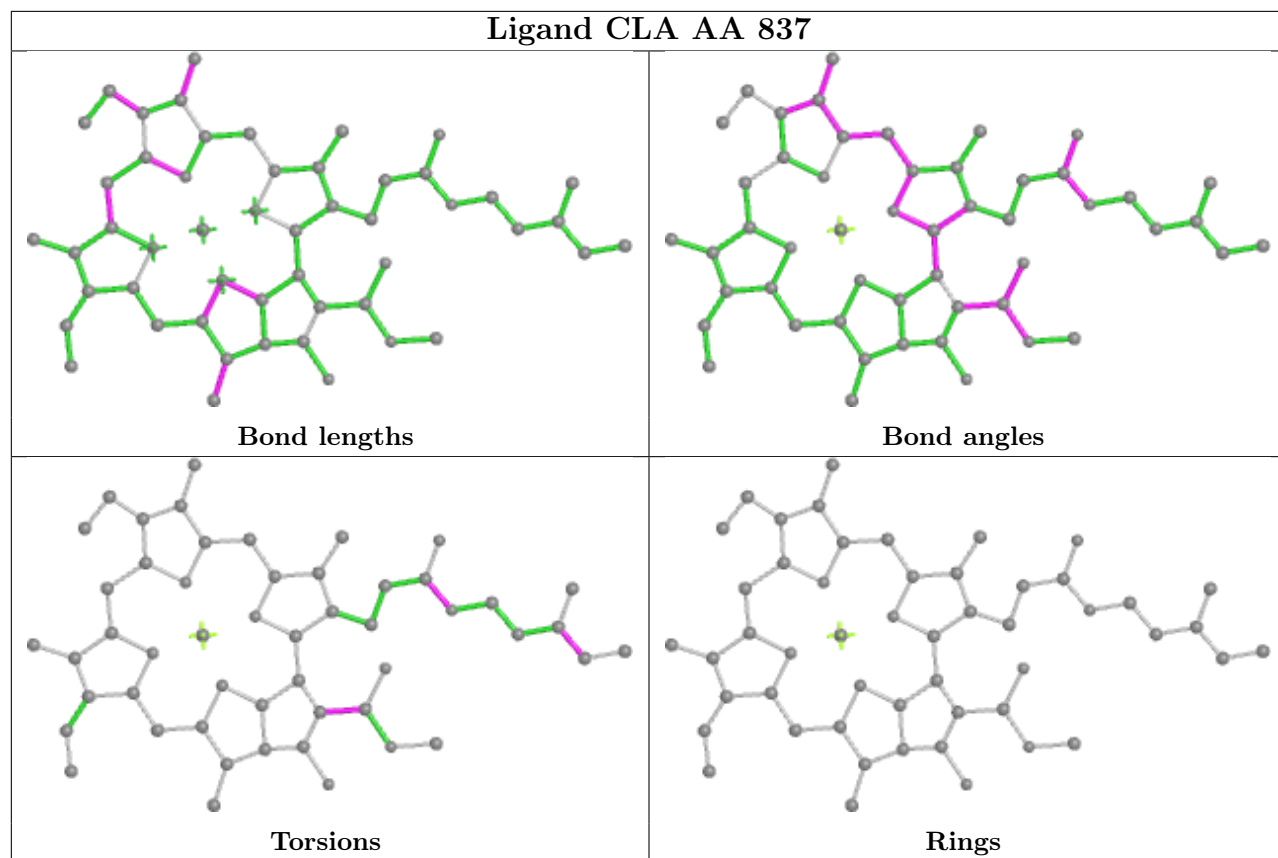
Torsions



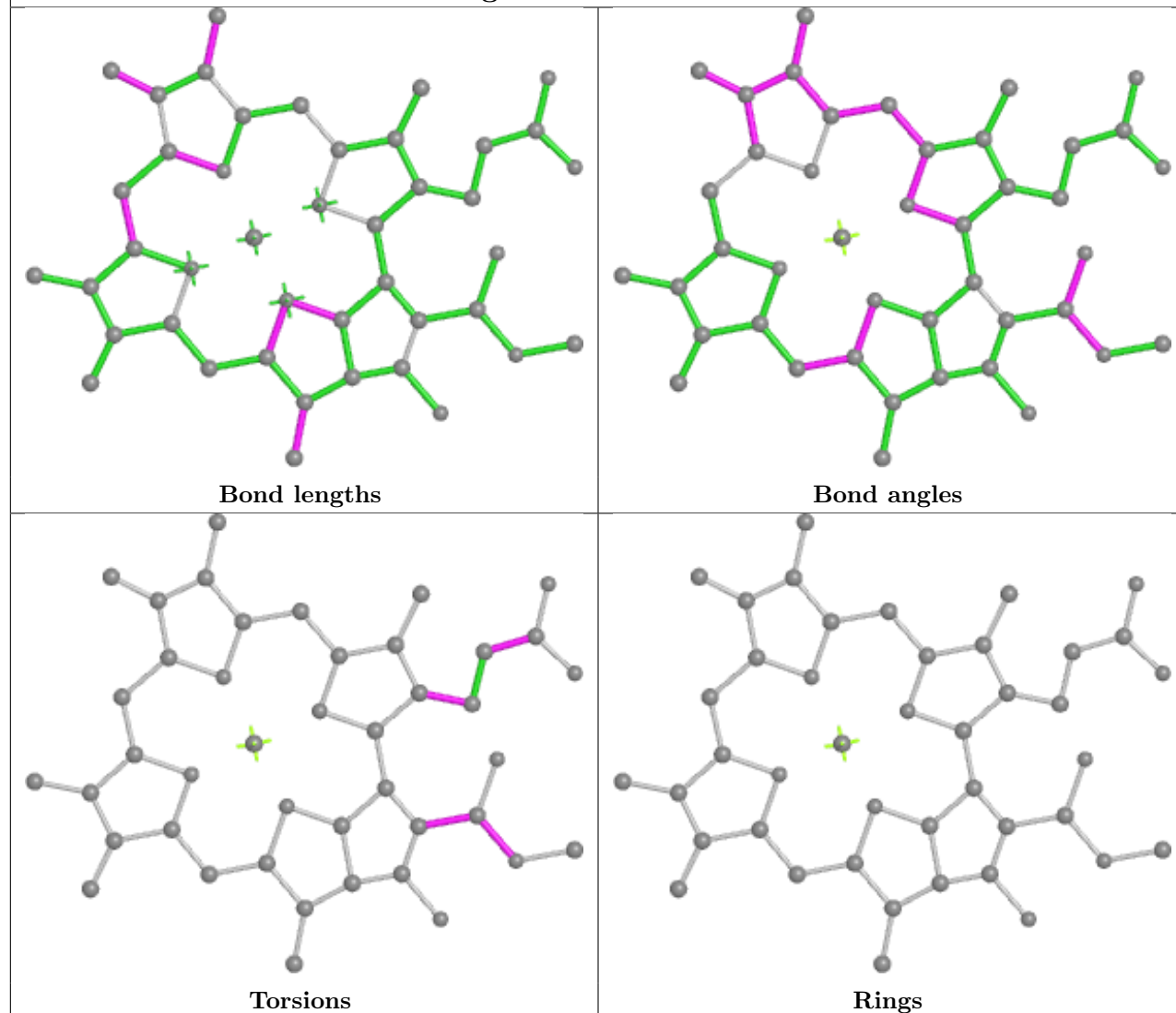
Rings



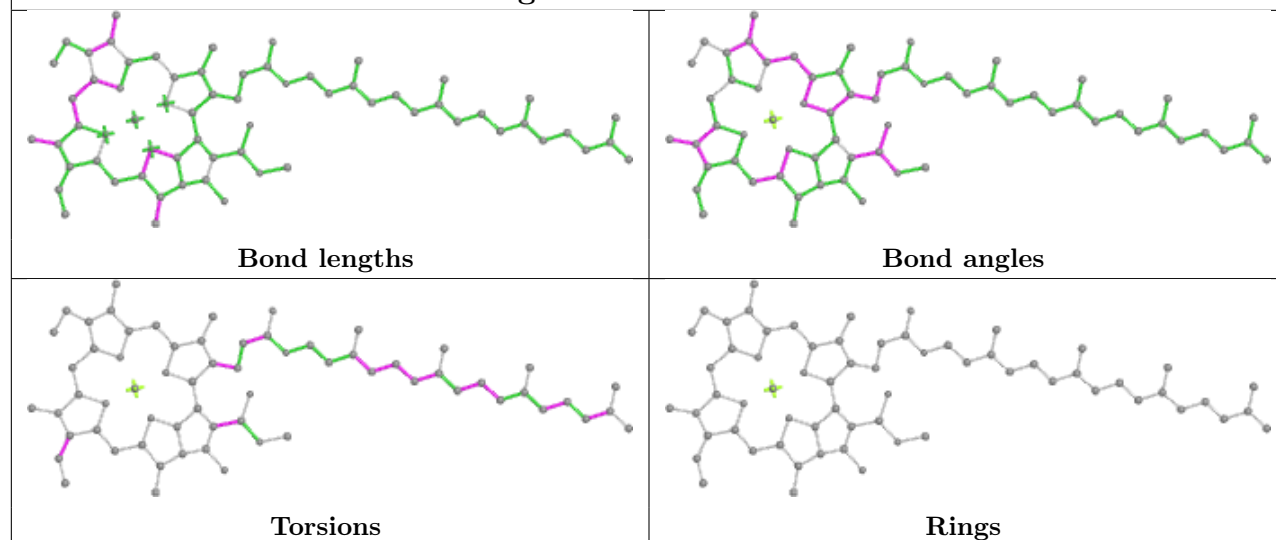


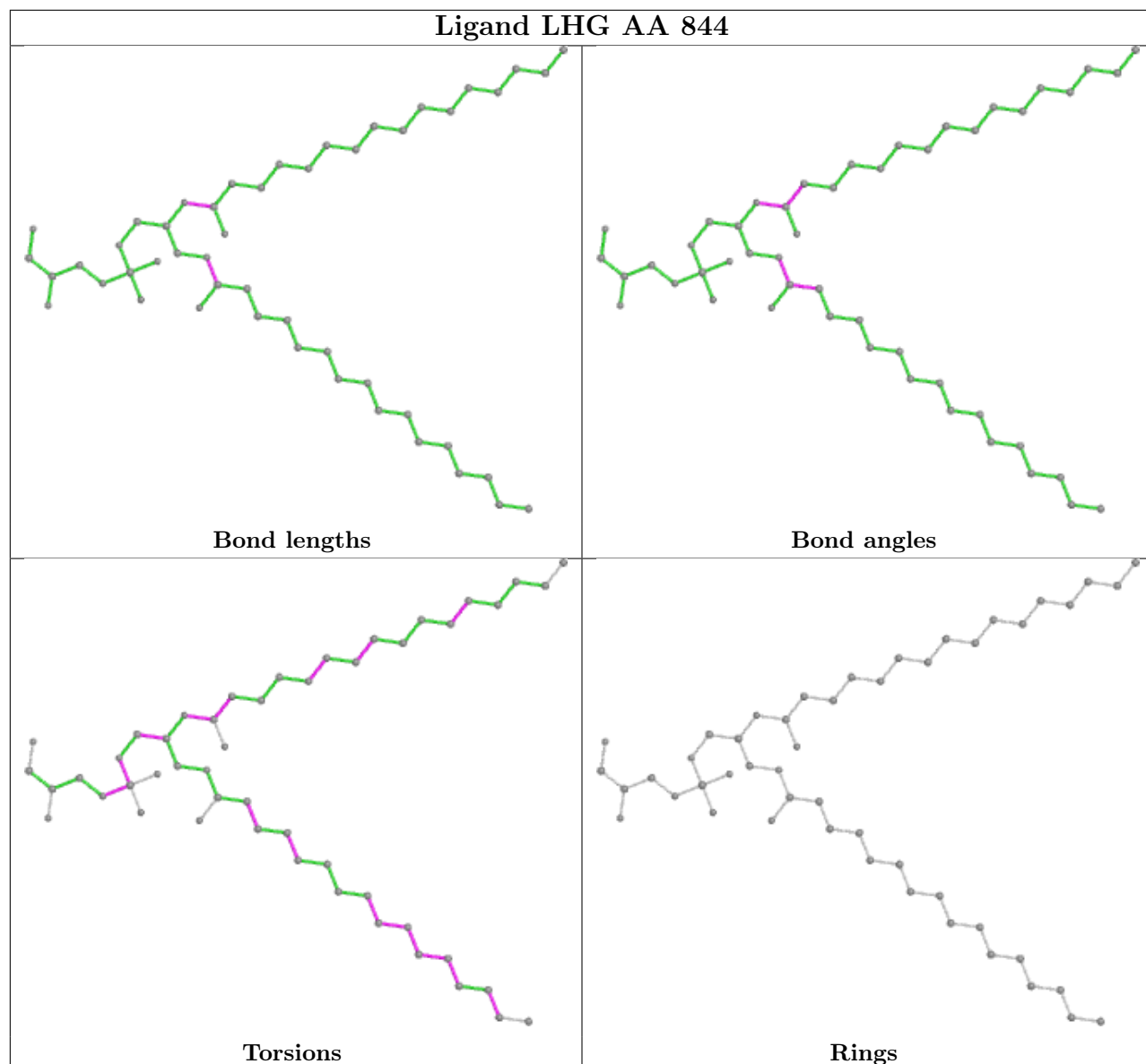
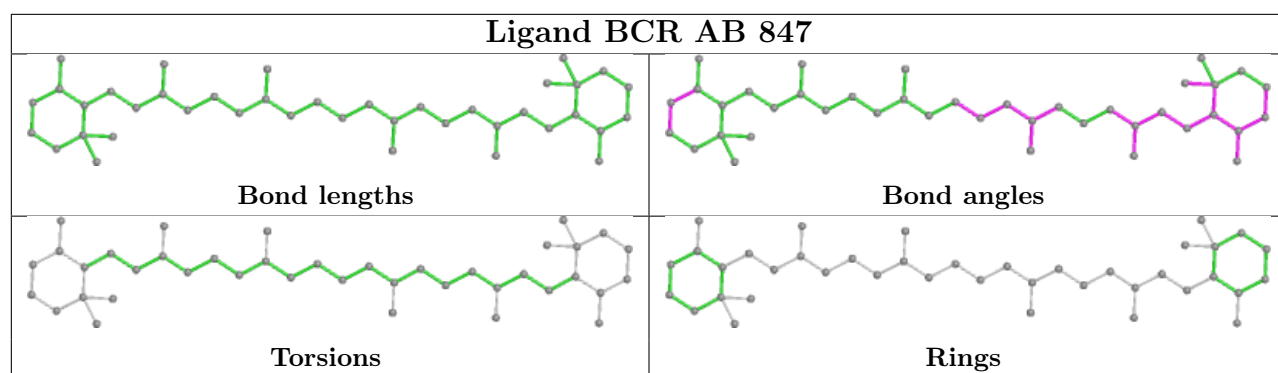


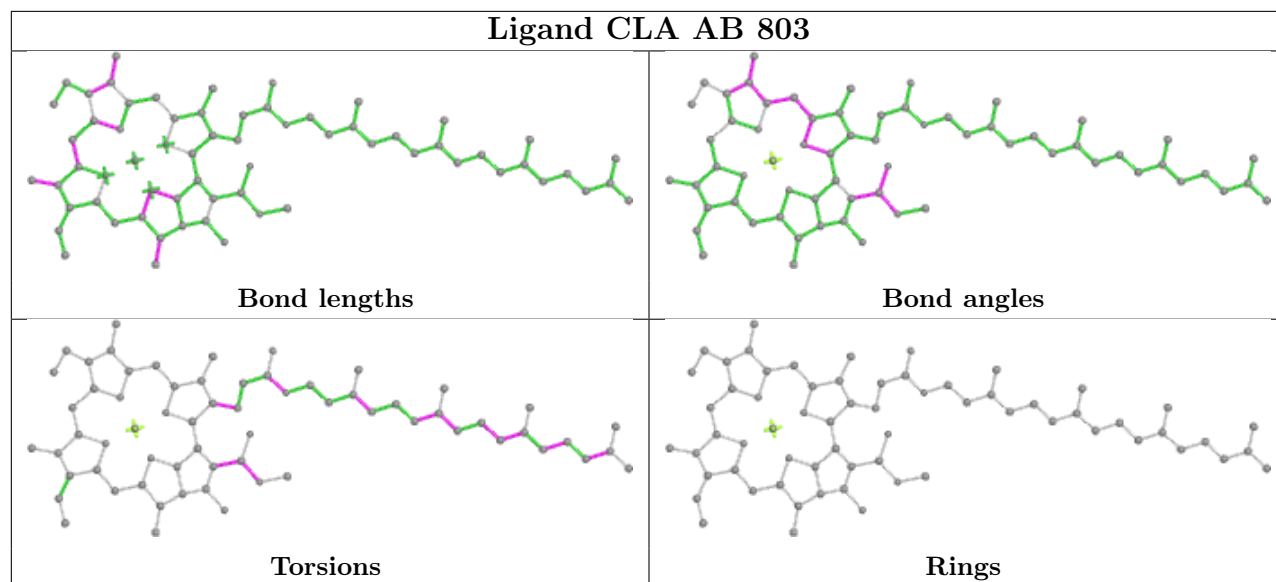
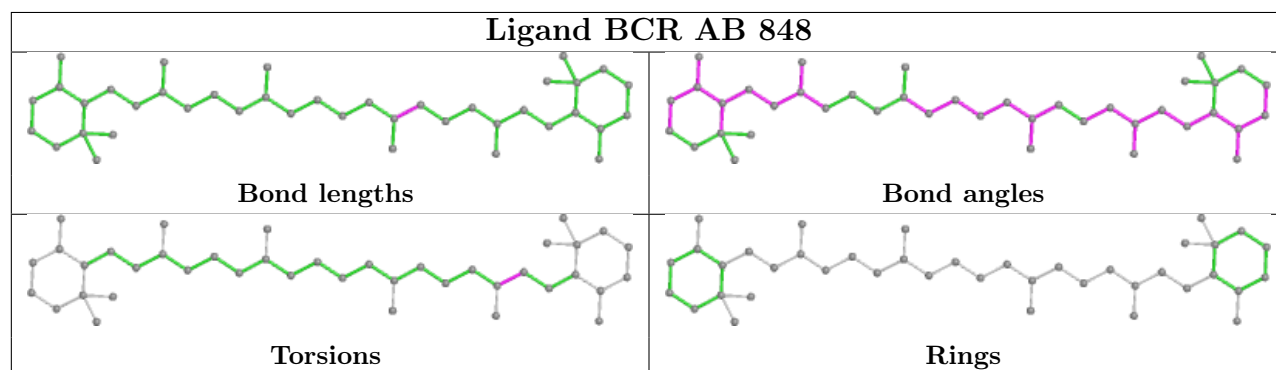
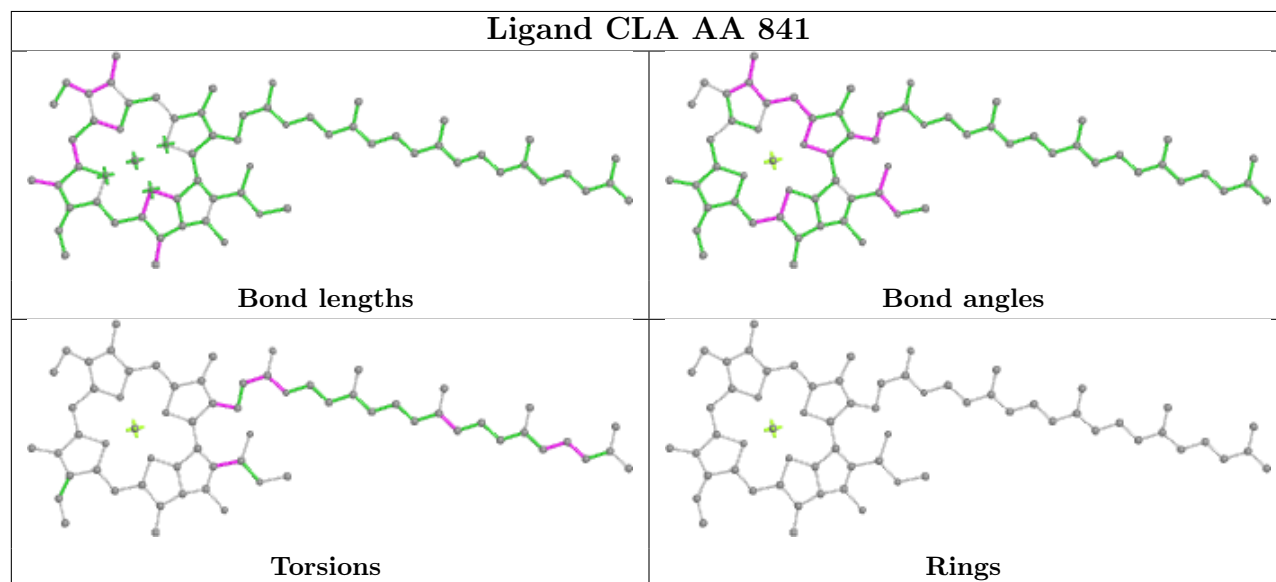
## Ligand CLA A1 316



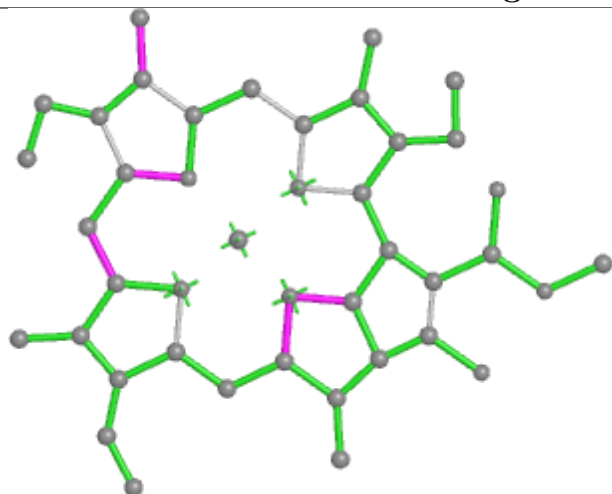
## Ligand CLA AA 805



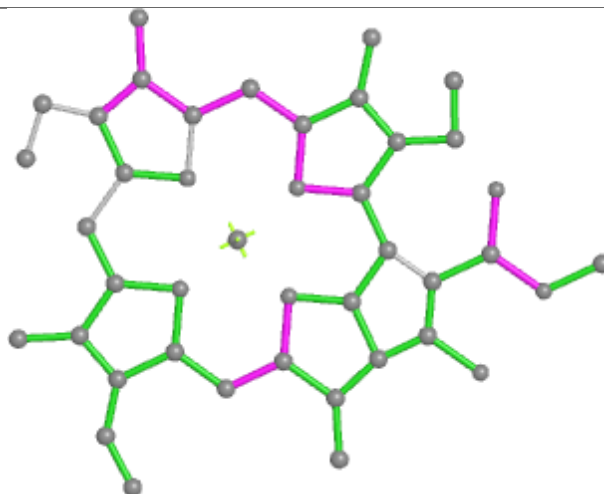


**Ligand CLA AB 803****Ligand BCR AB 848****Ligand CLA AA 841**

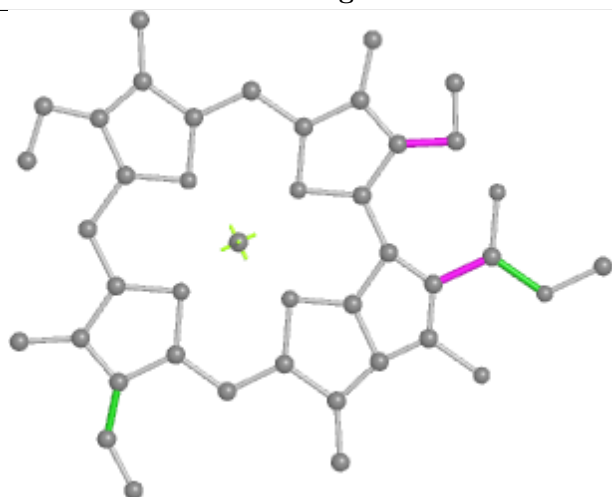
## Ligand CLA AJ 102



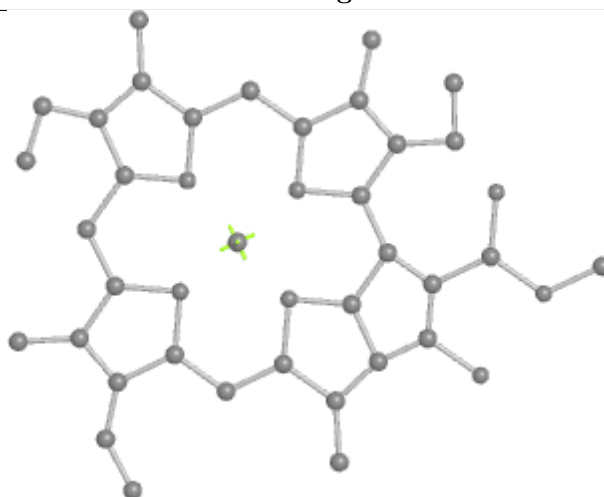
Bond lengths



Bond angles

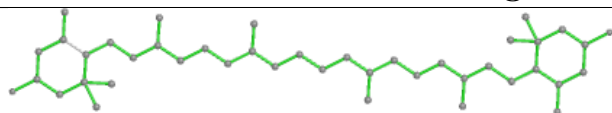


Torsions

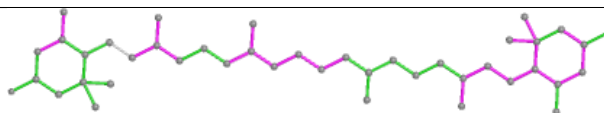


Rings

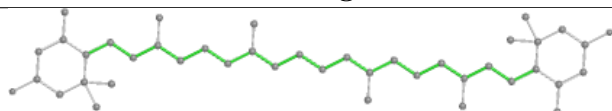
## Ligand LUT A3 316



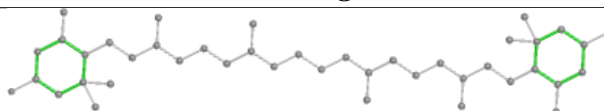
Bond lengths



Bond angles

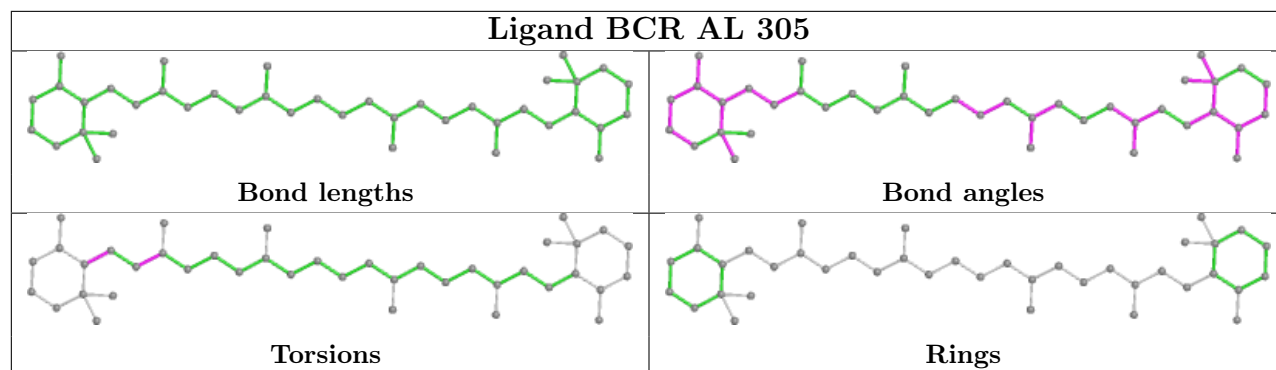


Torsions

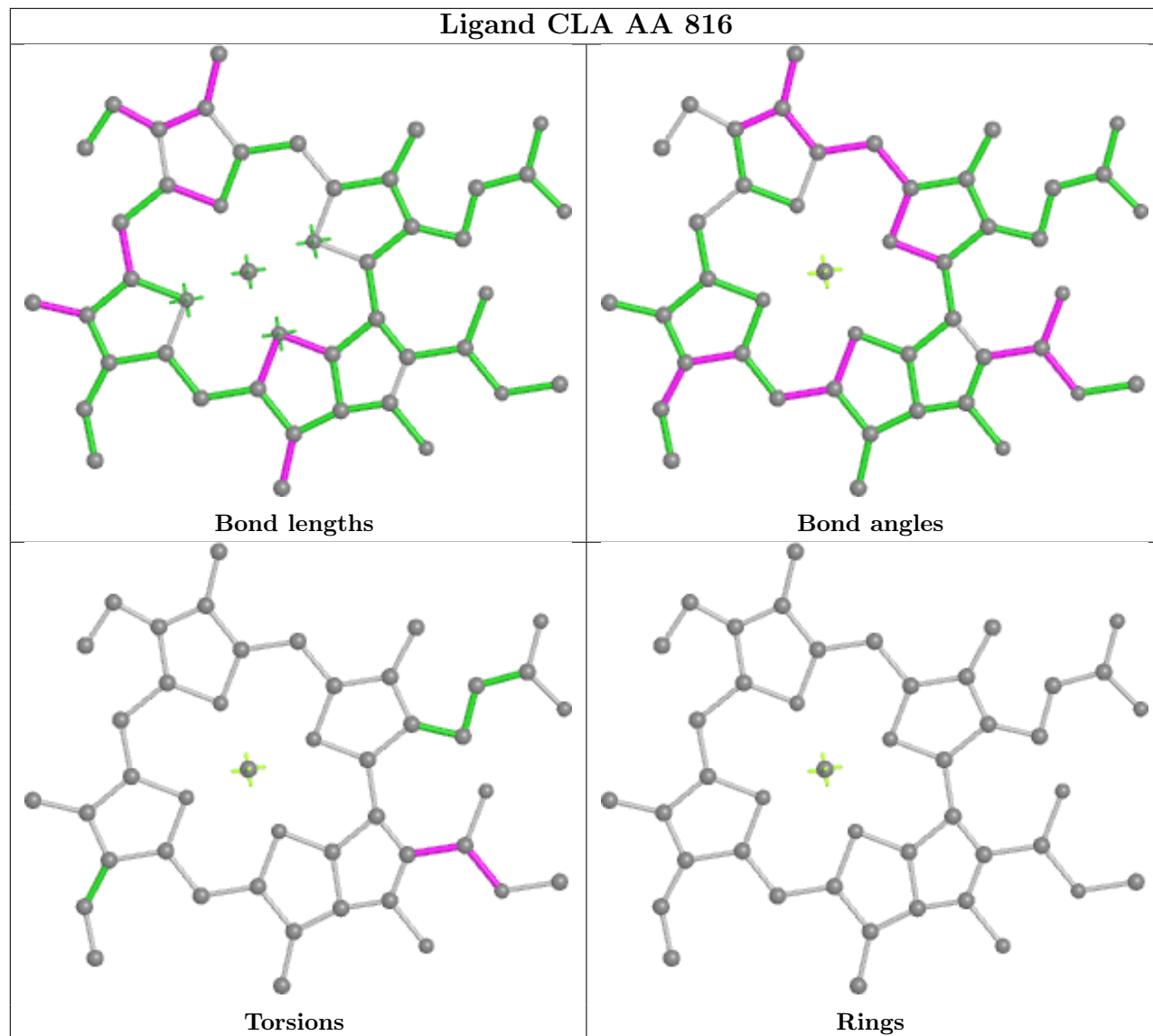


Rings

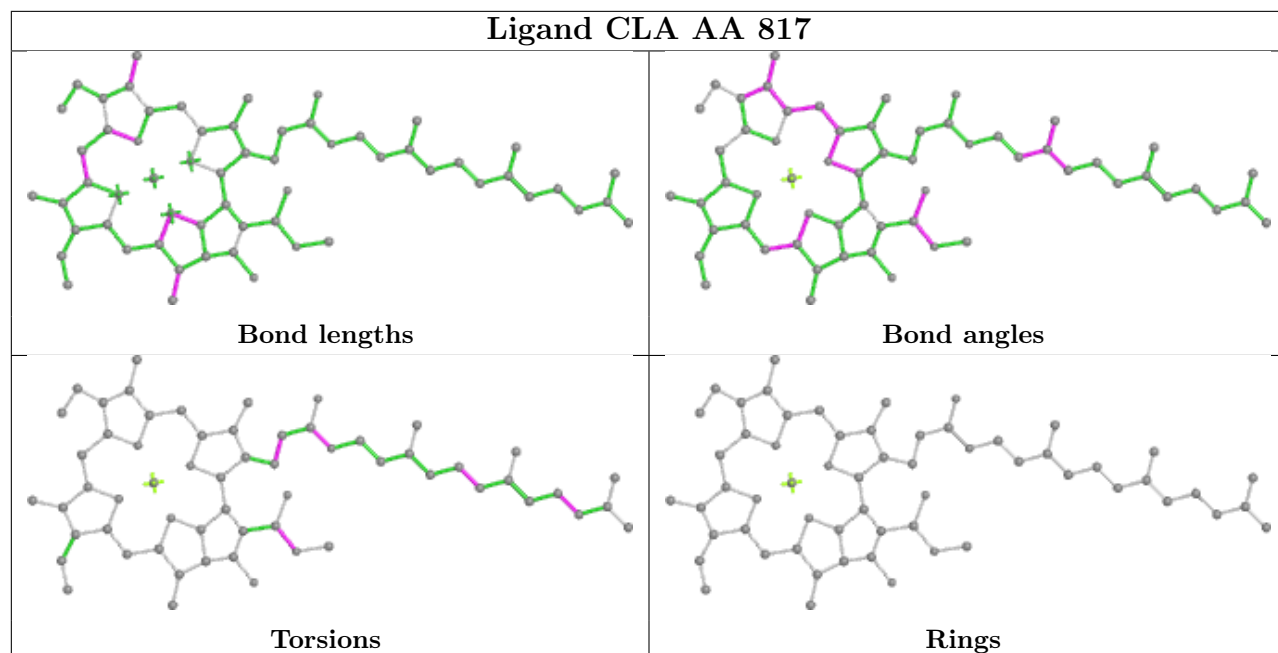
## Ligand BCR AL 305



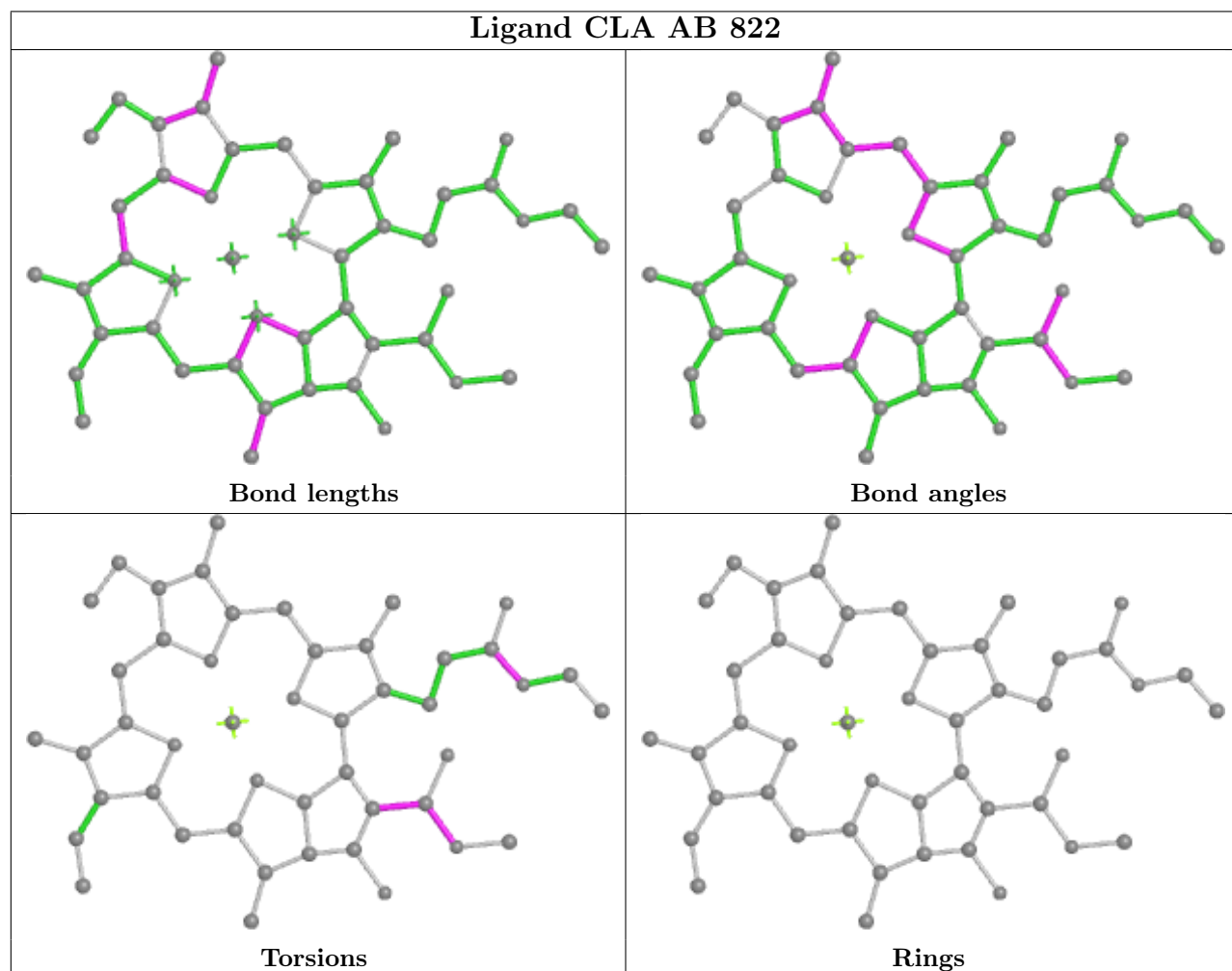
## Ligand CLA AA 816

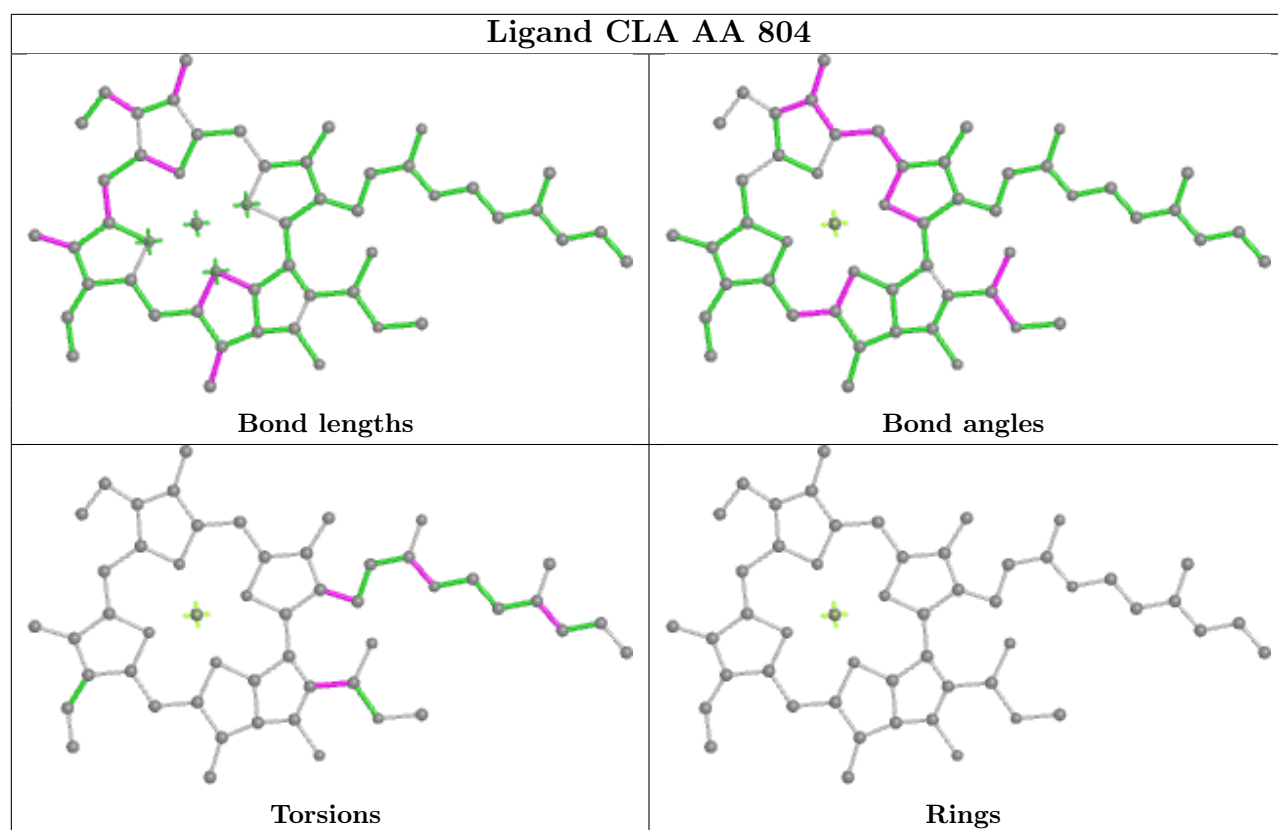


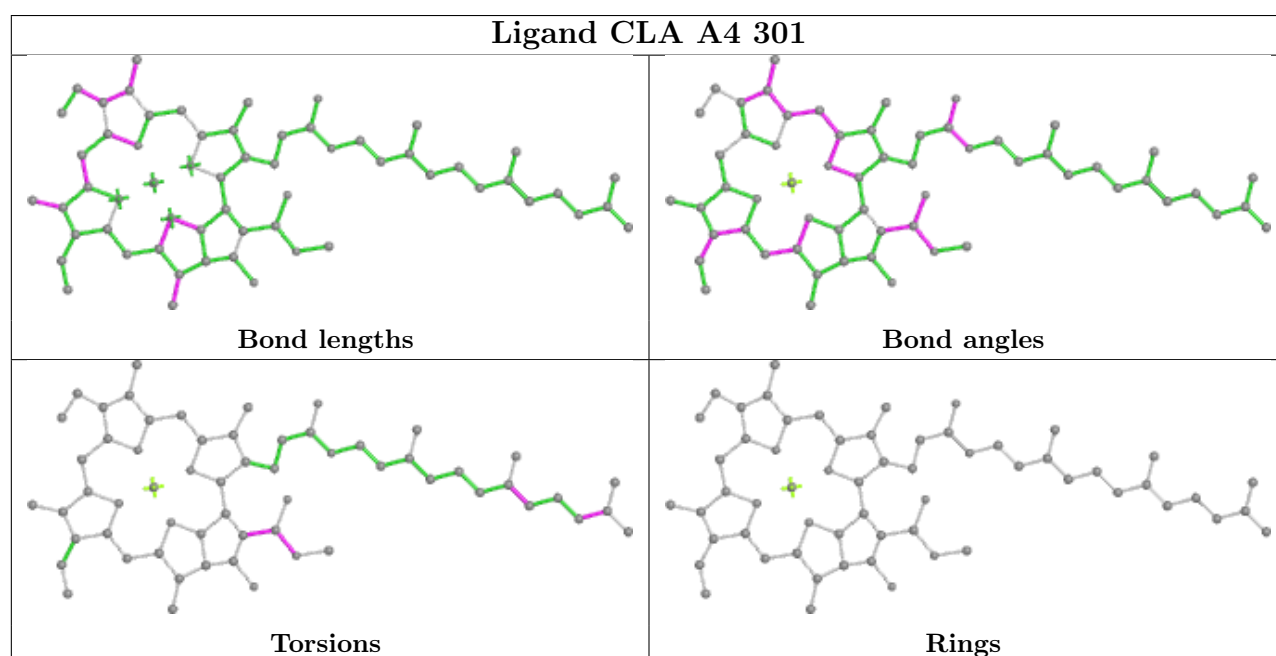
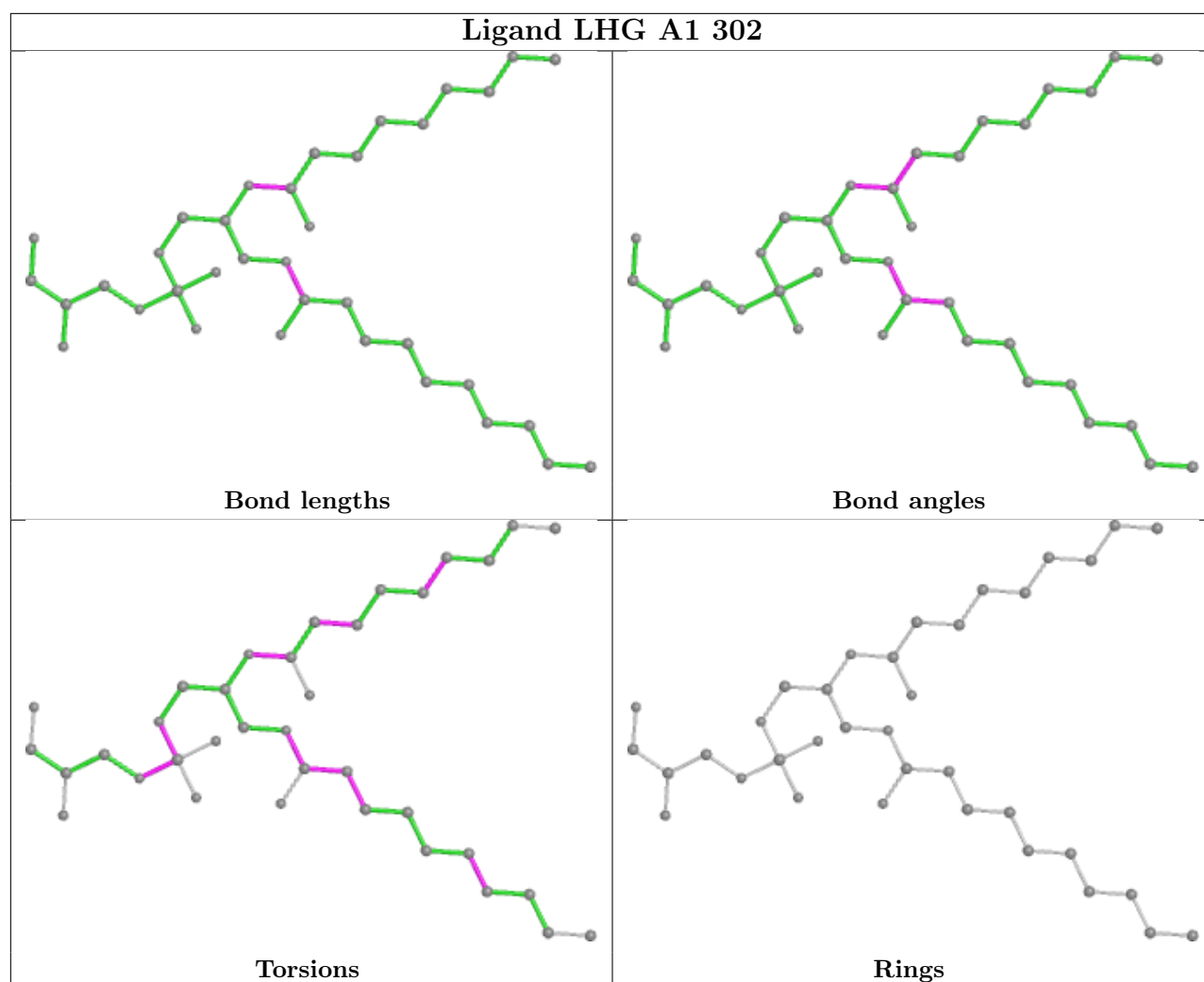
## Ligand CLA AA 817



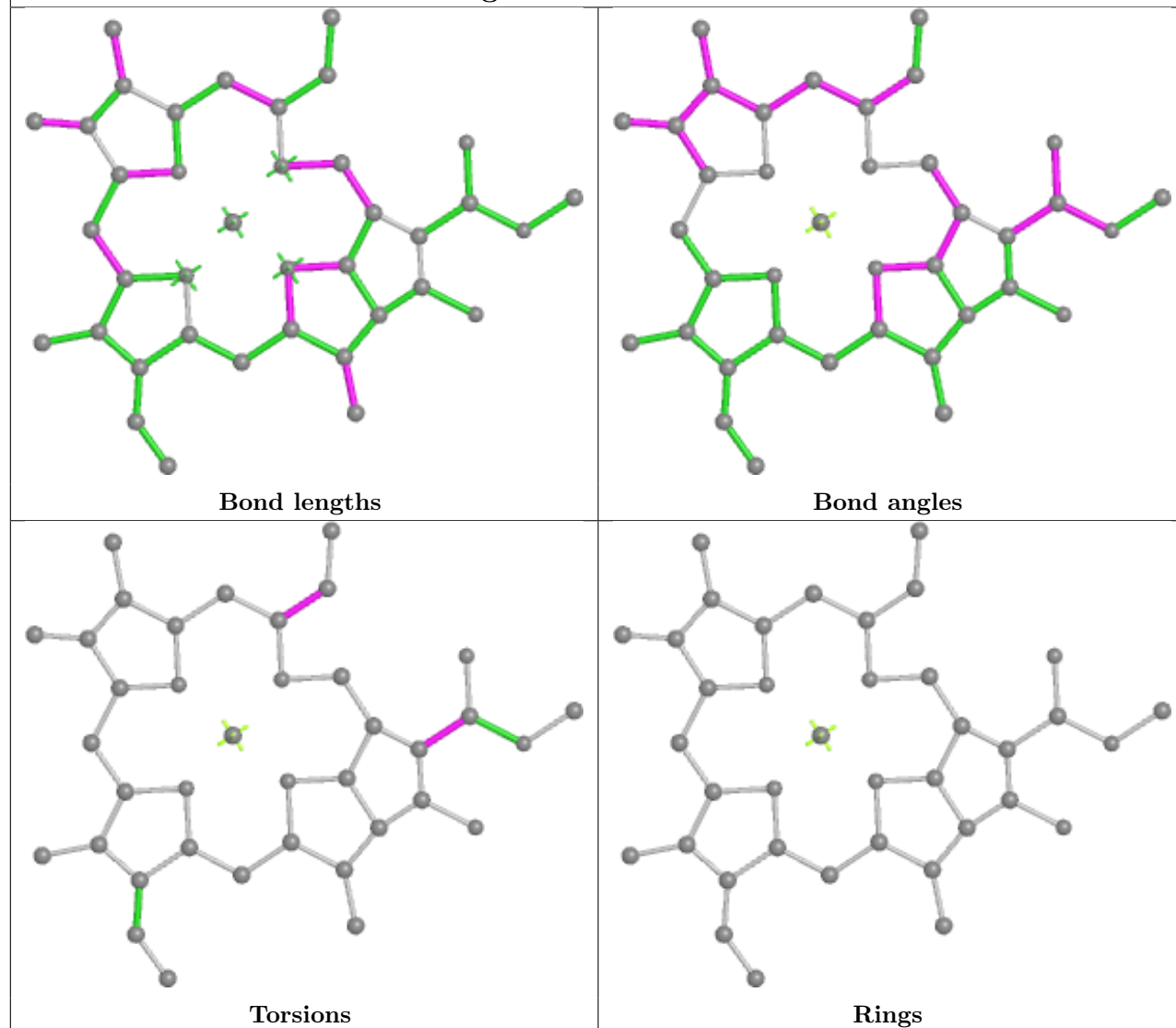
## Ligand CLA AB 822



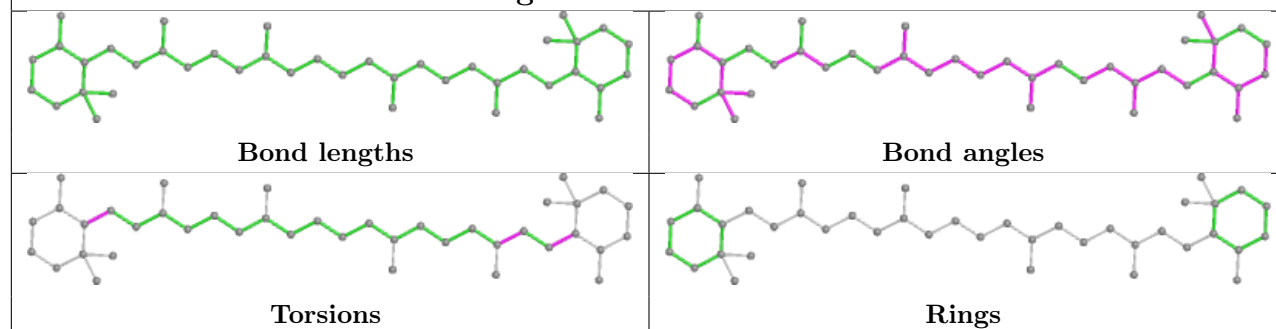


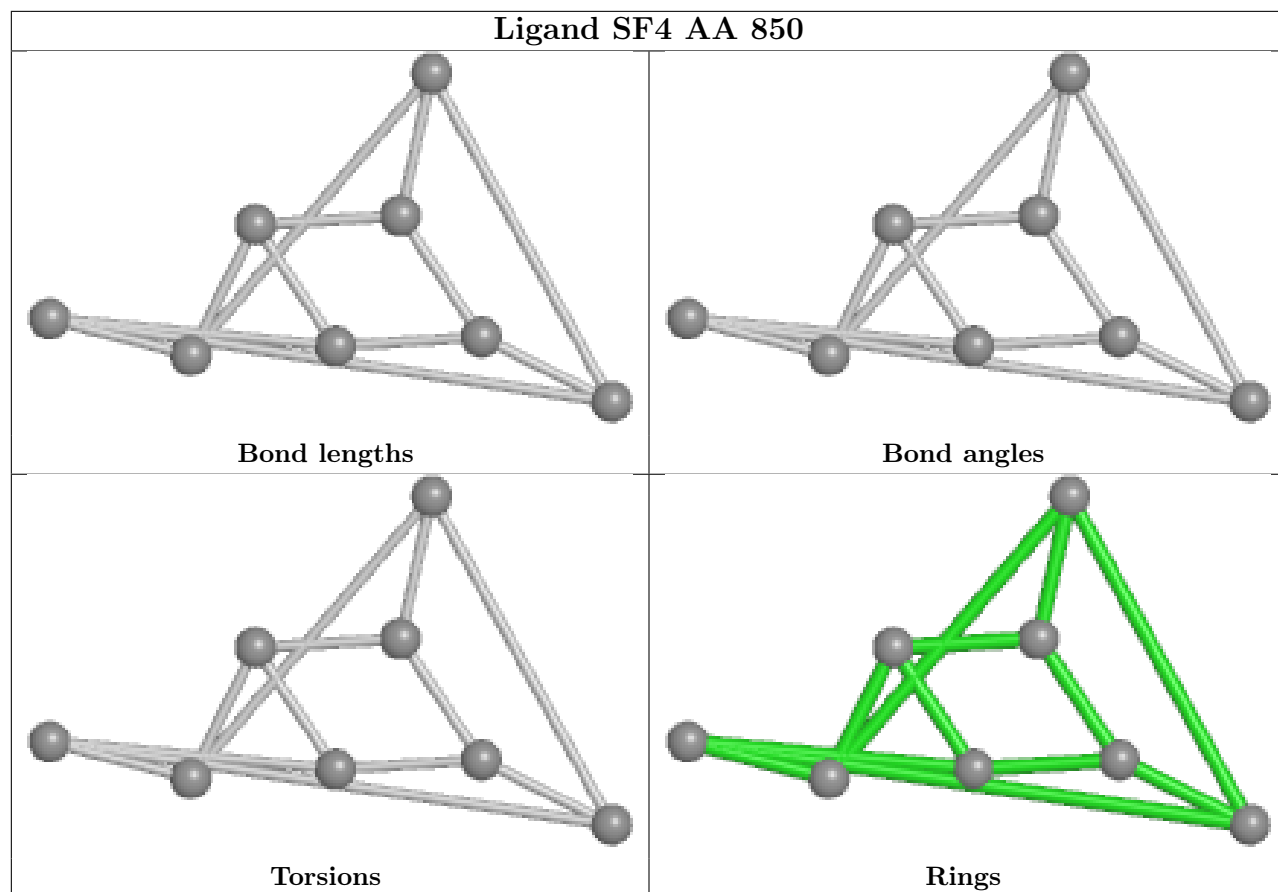


## Ligand CLA A6 610

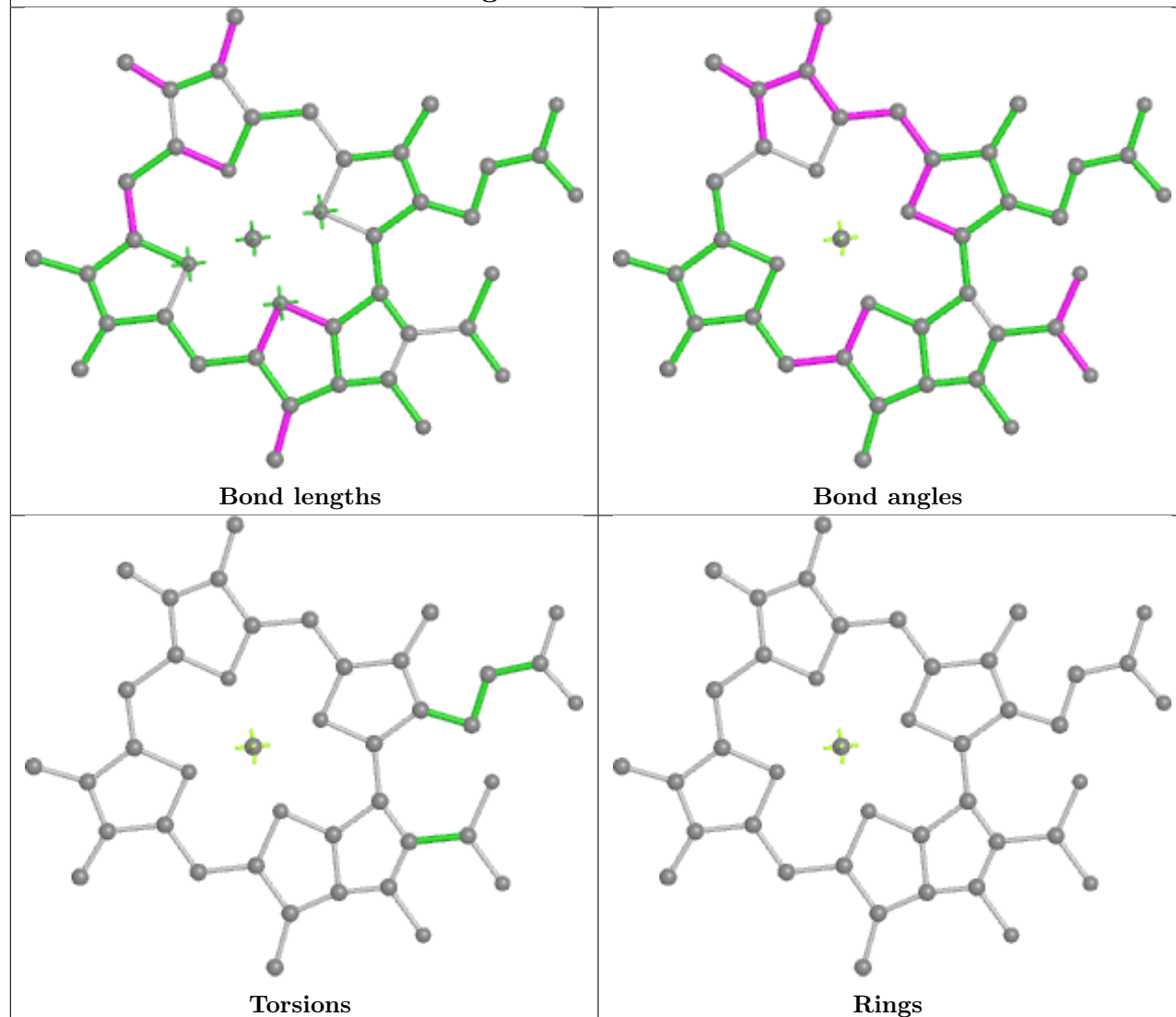


## Ligand BCR AA 846

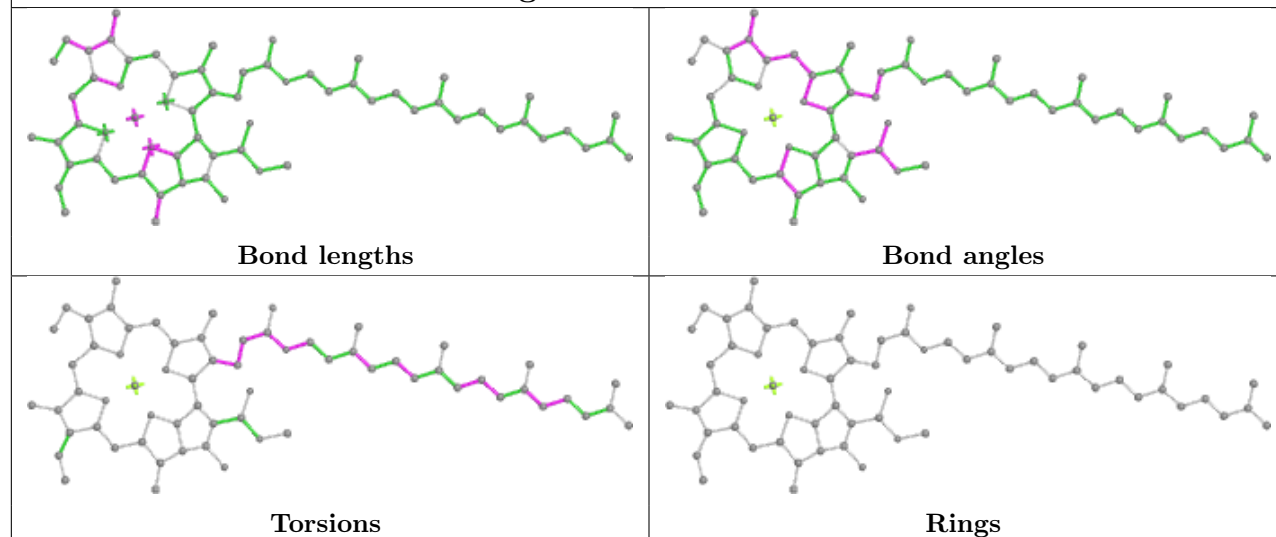


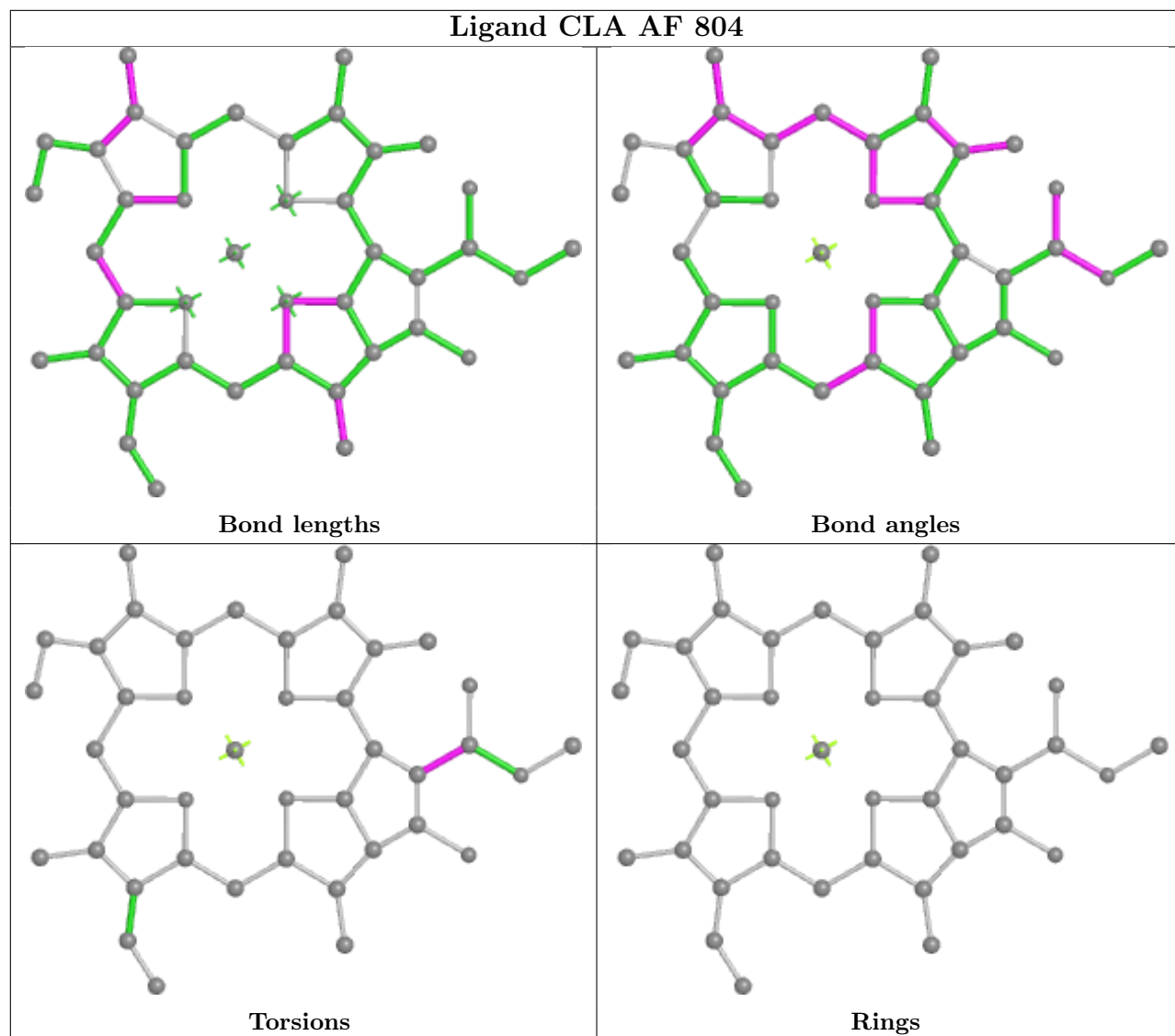


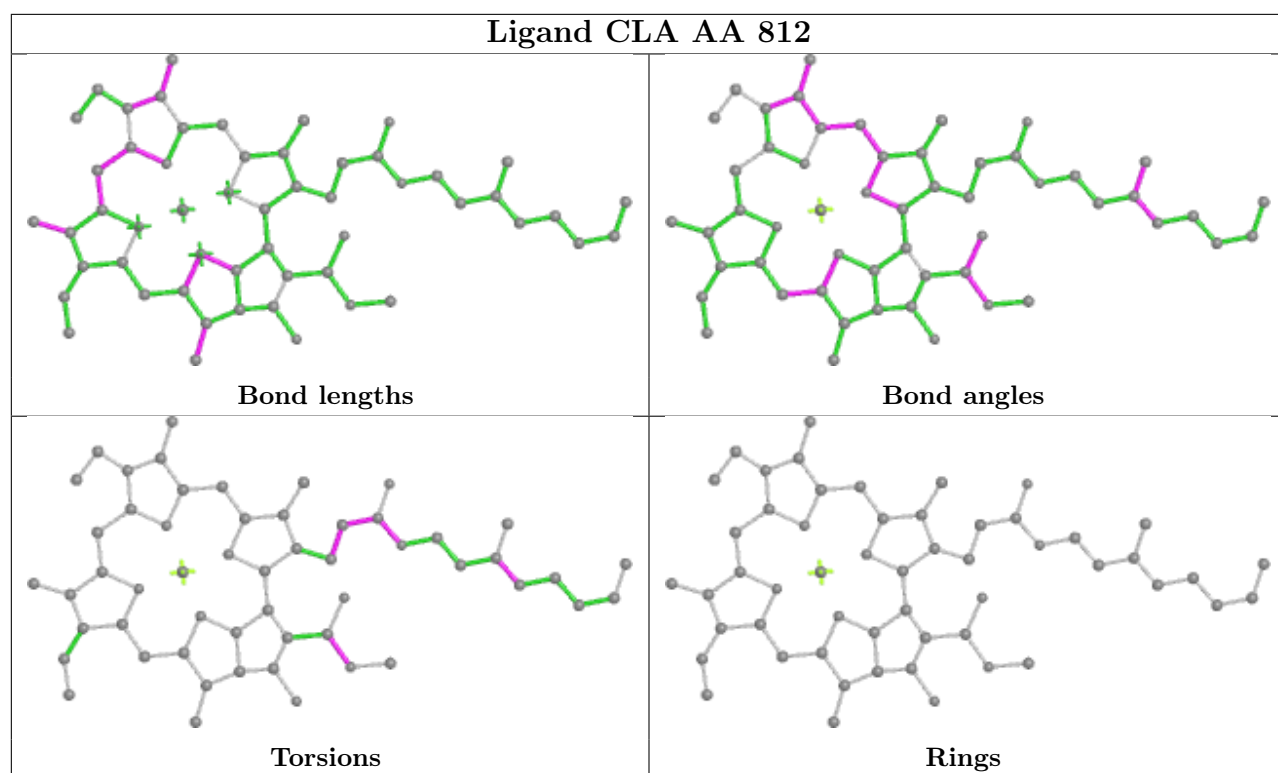
## Ligand CLA A3 304



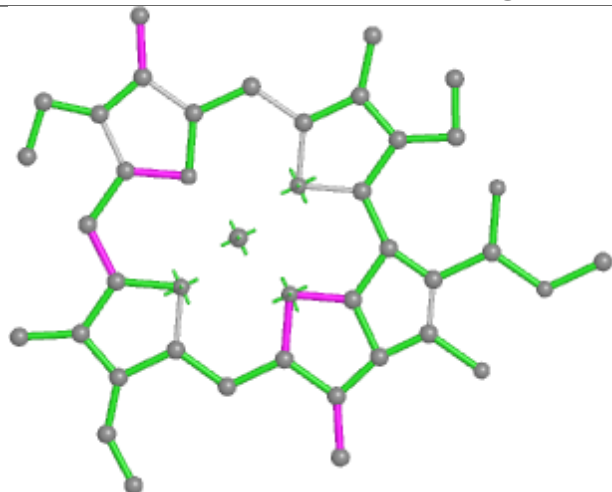
## Ligand CLA AB 829



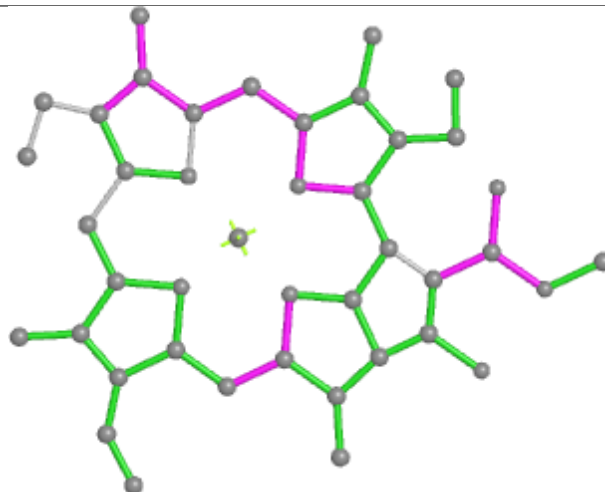




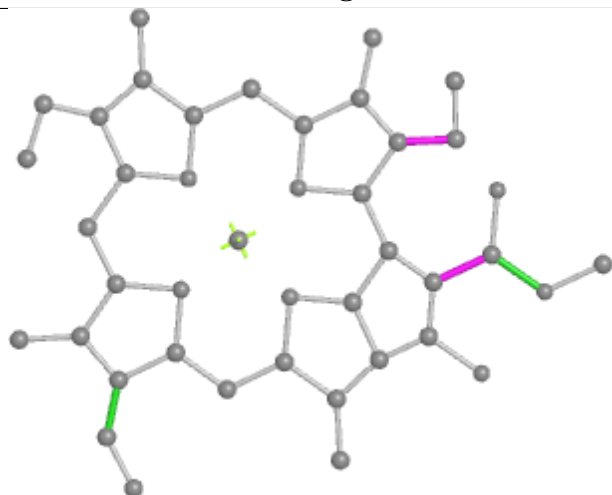
## Ligand CLA AA 822



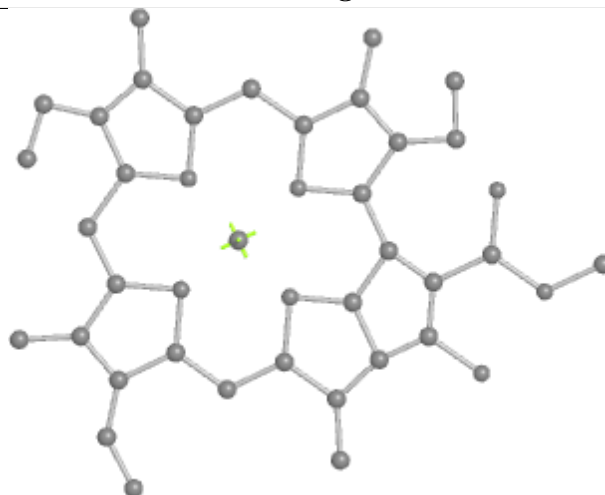
Bond lengths



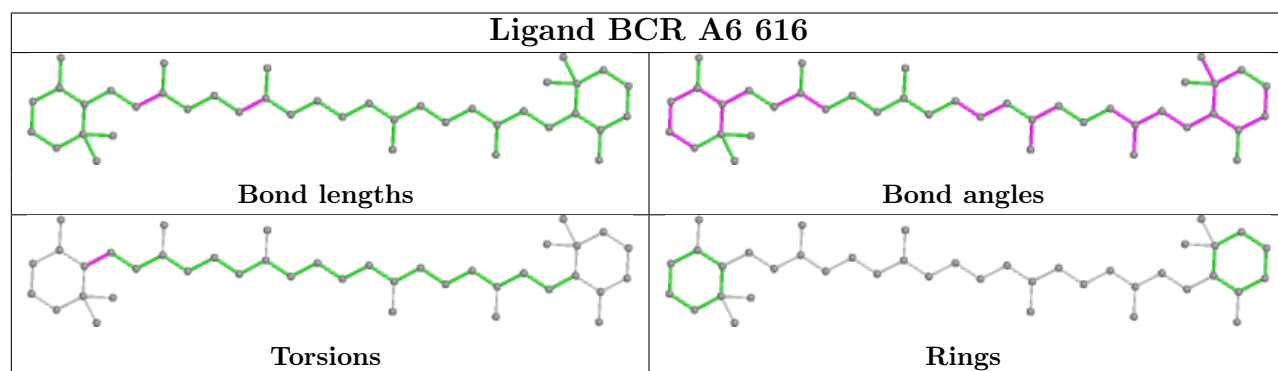
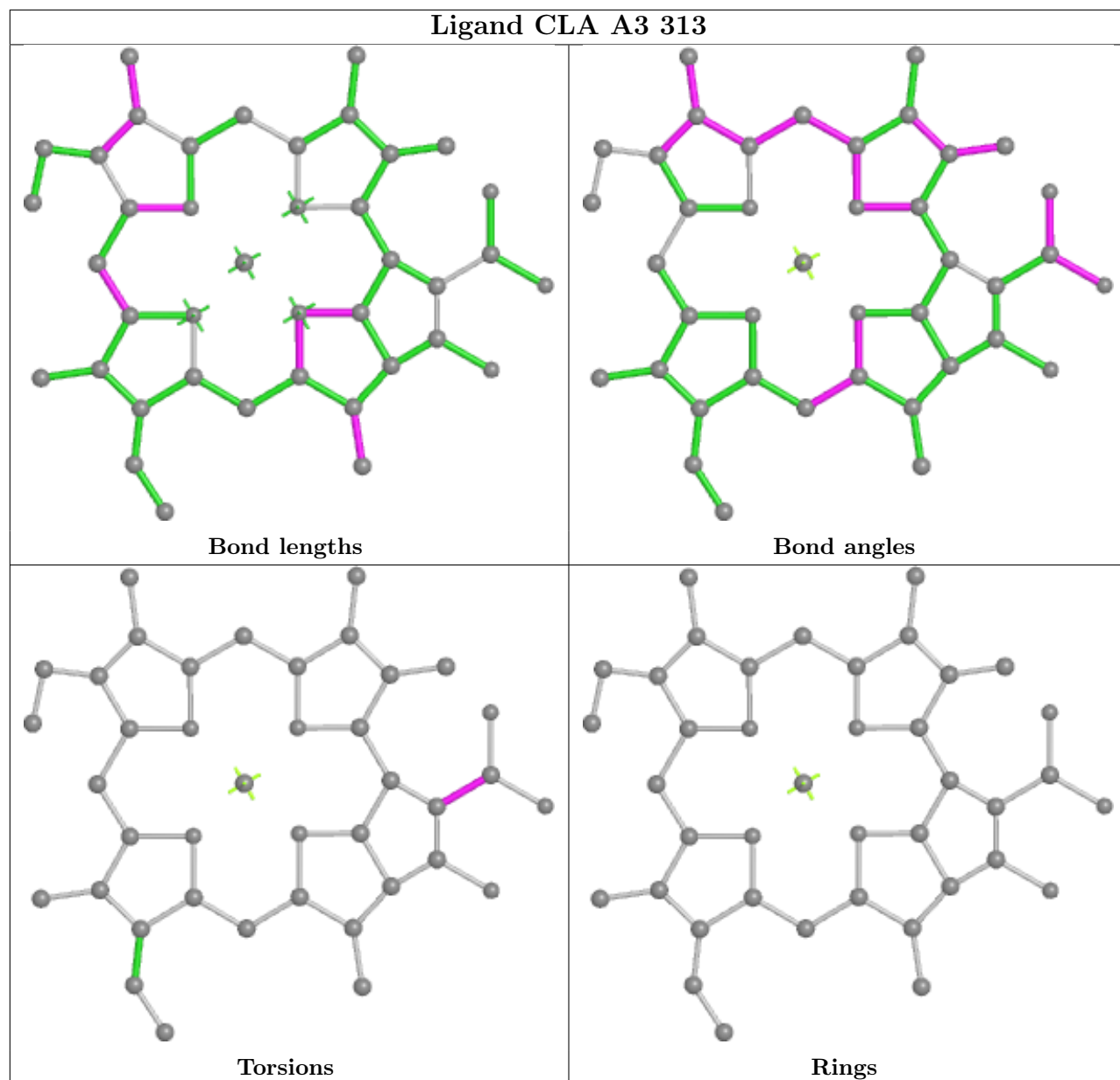
Bond angles



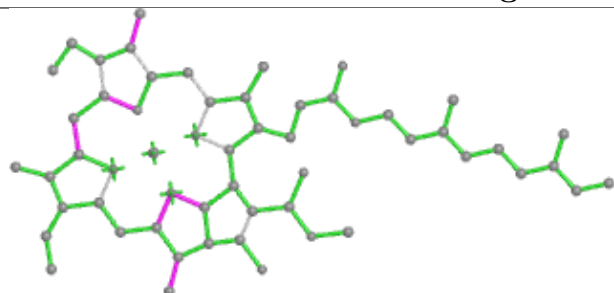
Torsions



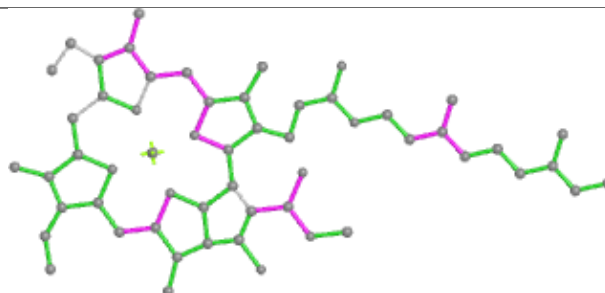
Rings



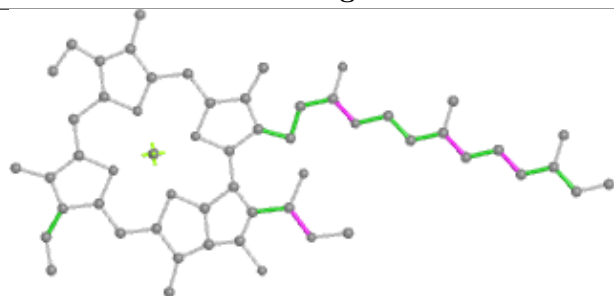
## Ligand CLA AA 832



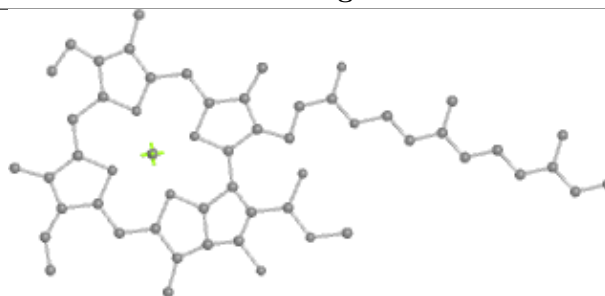
Bond lengths



Bond angles

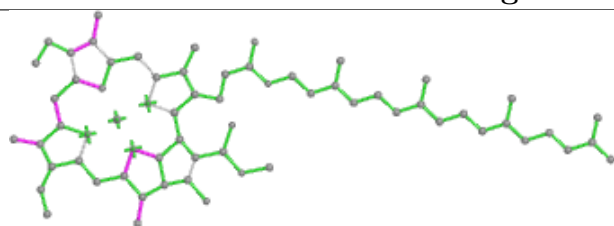


Torsions

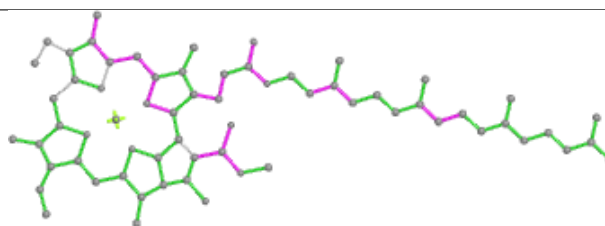


Rings

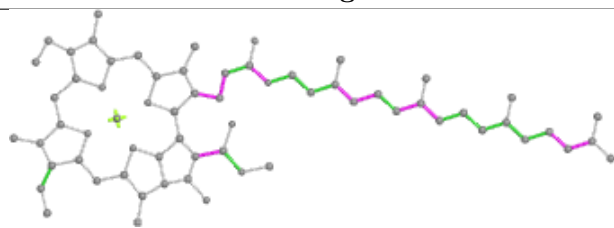
## Ligand CLA AB 809



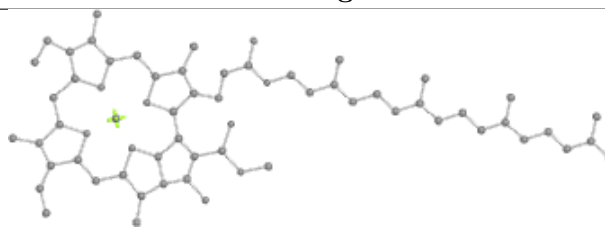
Bond lengths



Bond angles

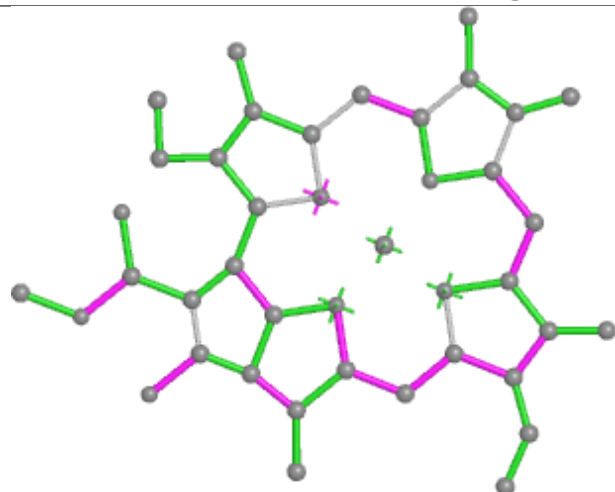


Torsions

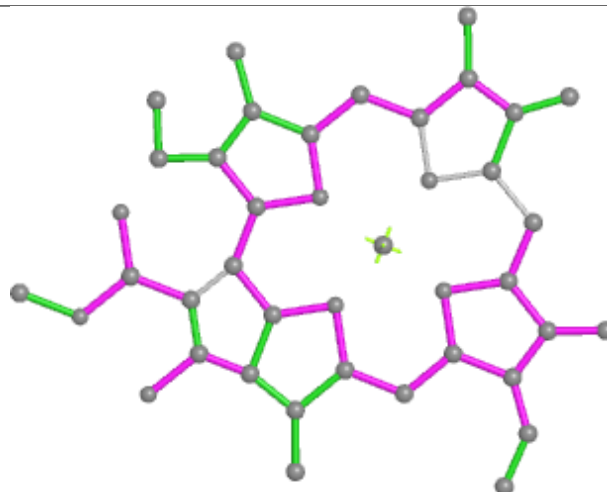


Rings

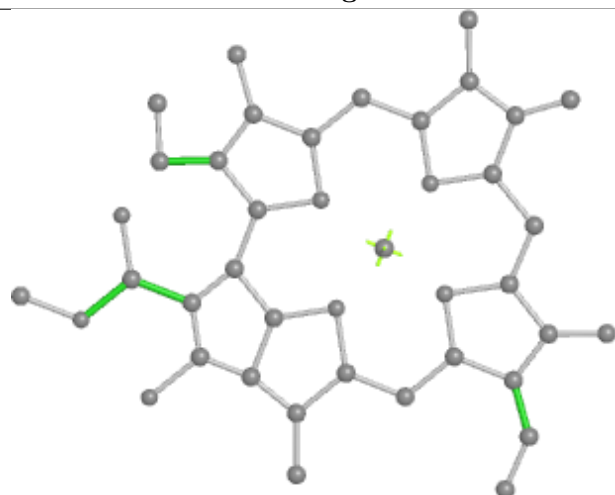
## Ligand CHL A4 305



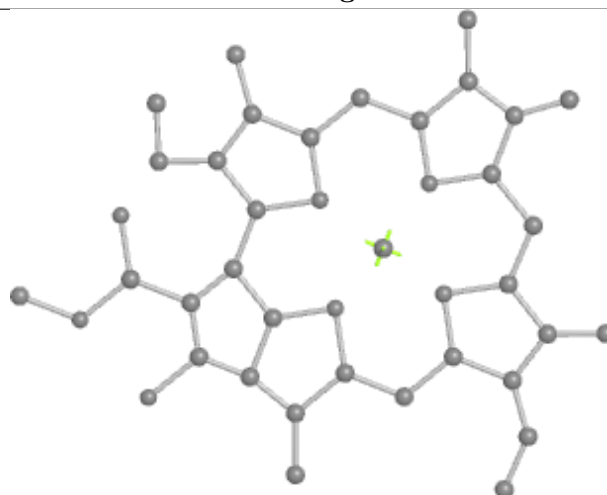
Bond lengths



Bond angles

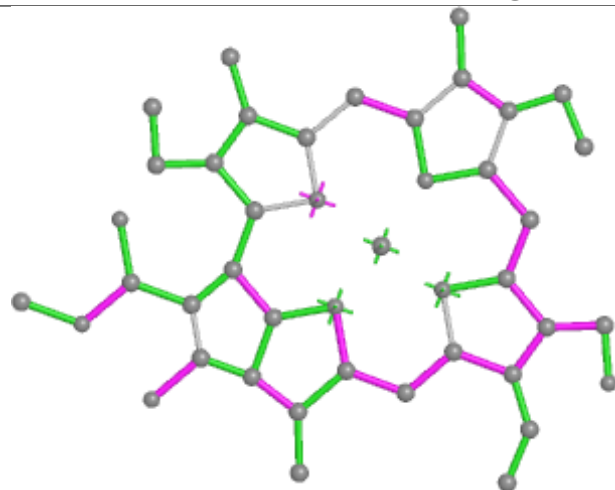


Torsions

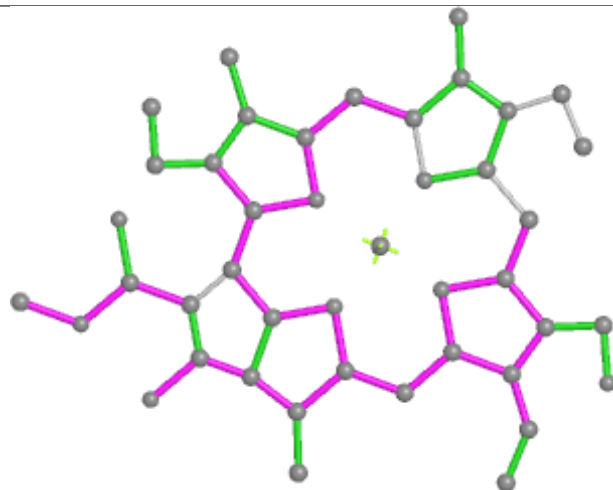


Rings

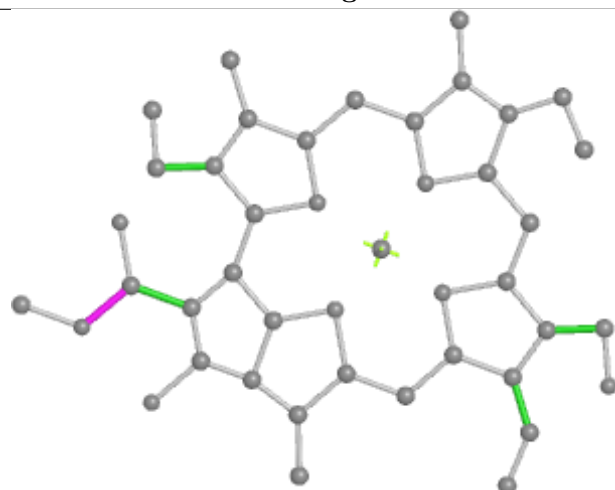
## Ligand CHL A6 606



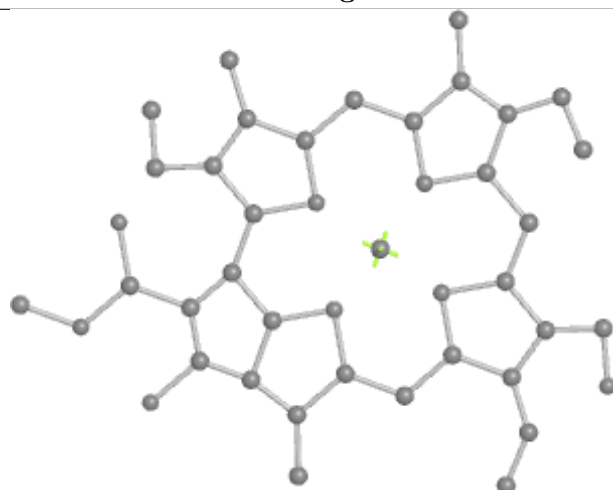
Bond lengths



Bond angles

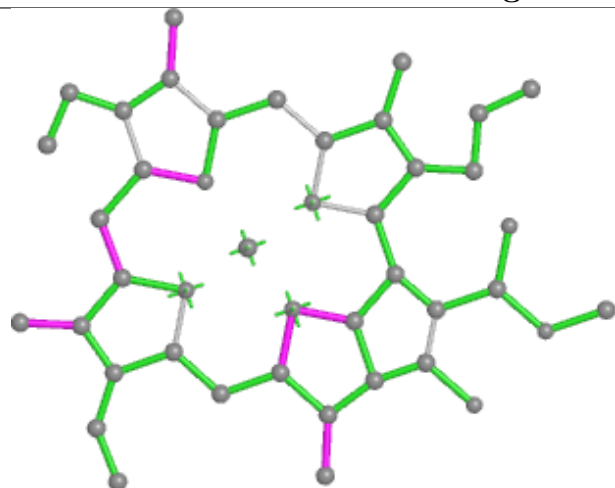


Torsions

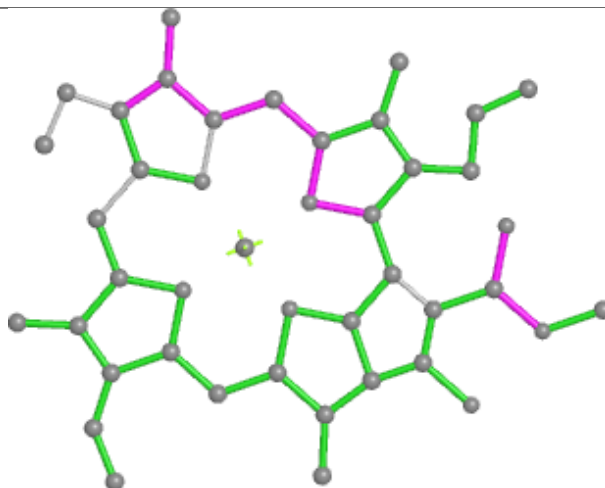


Rings

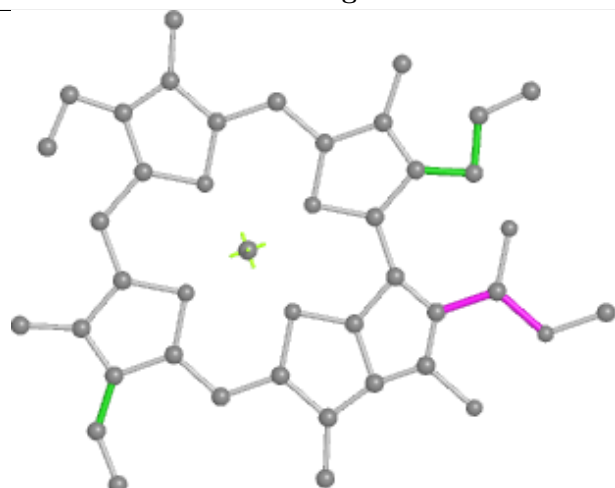
## Ligand CLA AB 816



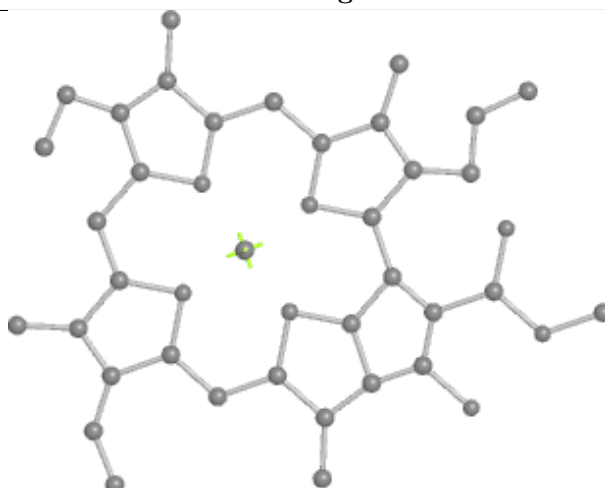
Bond lengths



Bond angles

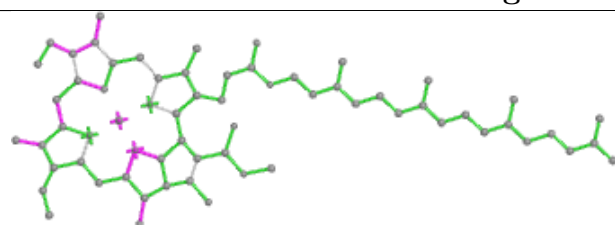


Torsions

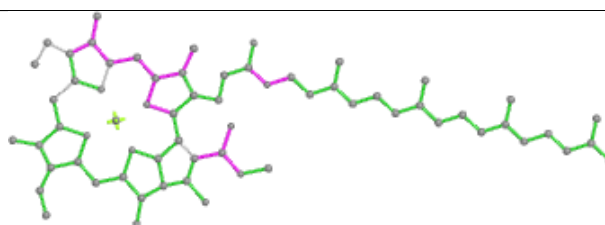


Rings

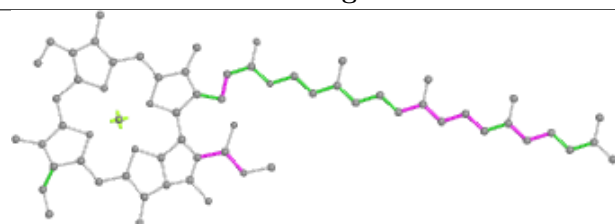
## Ligand CLA AB 825



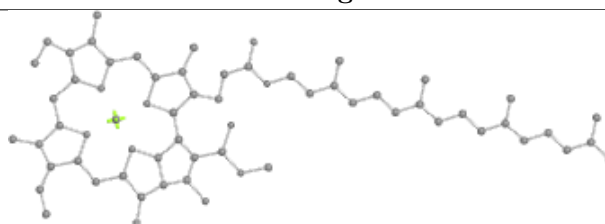
Bond lengths



Bond angles

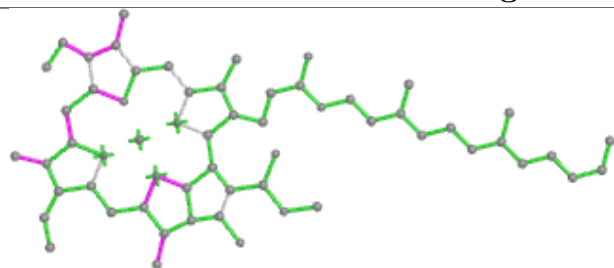


Torsions

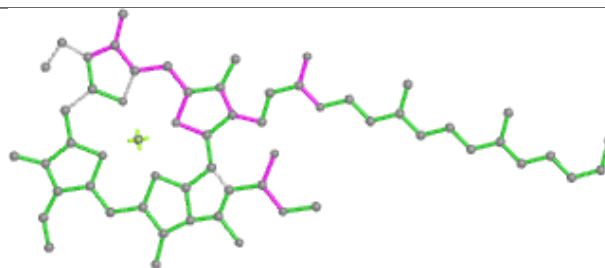


Rings

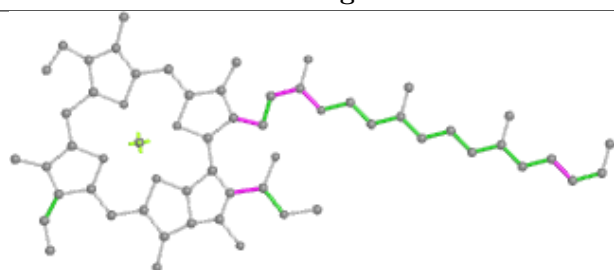
## Ligand CLA AA 818



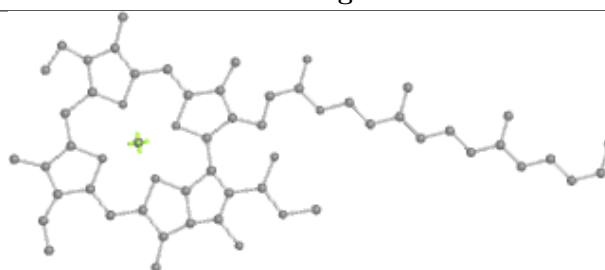
Bond lengths



Bond angles

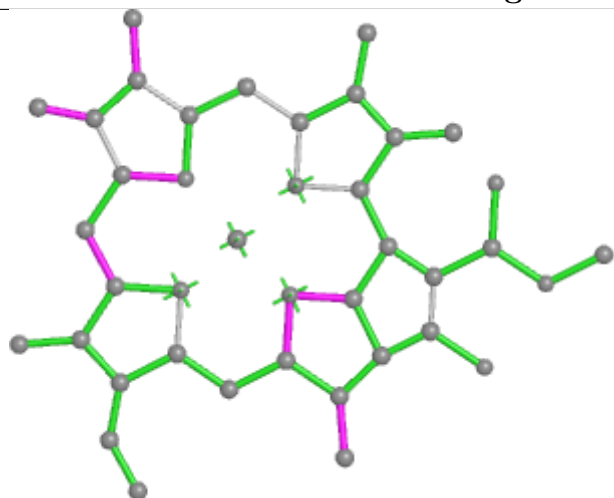


Torsions

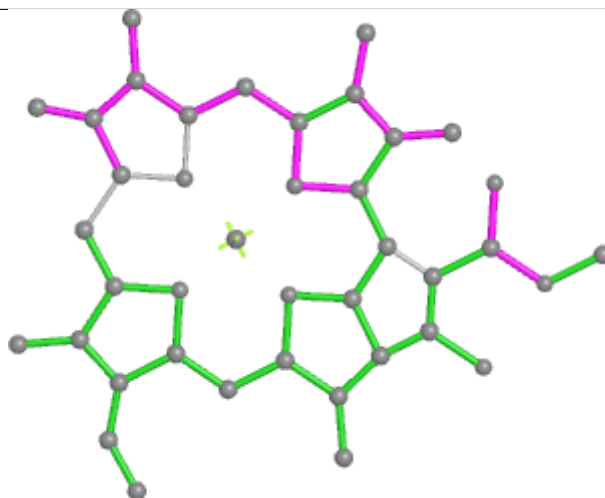


Rings

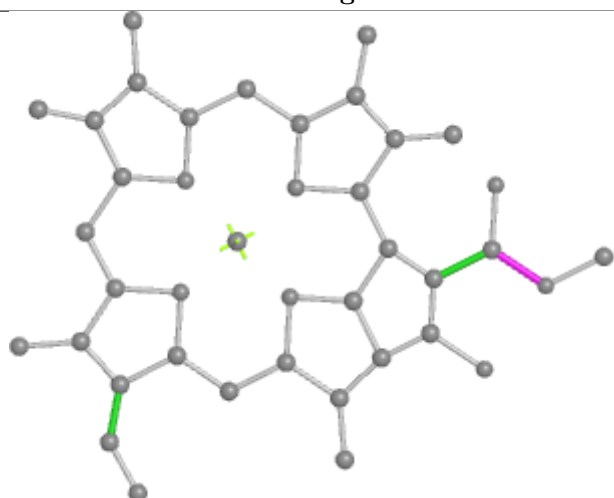
## Ligand CLA A1 310



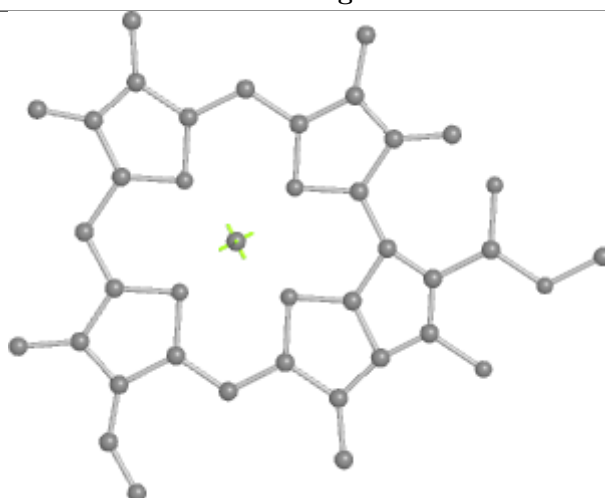
Bond lengths



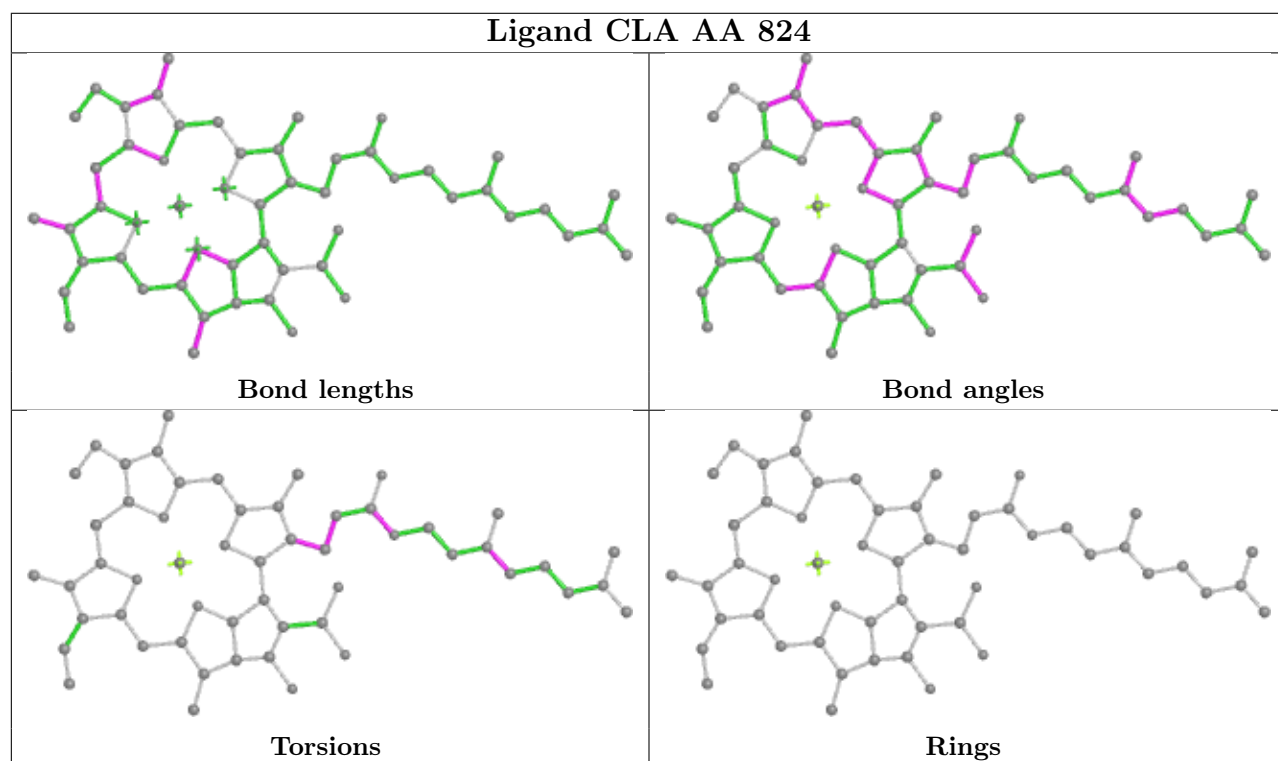
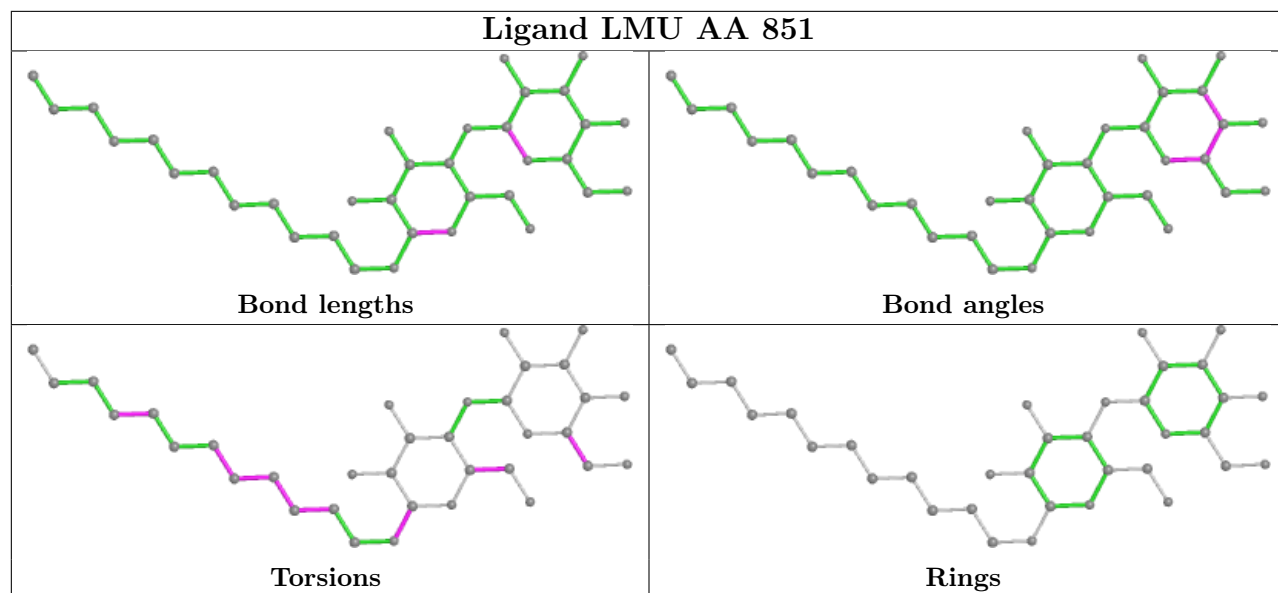
Bond angles

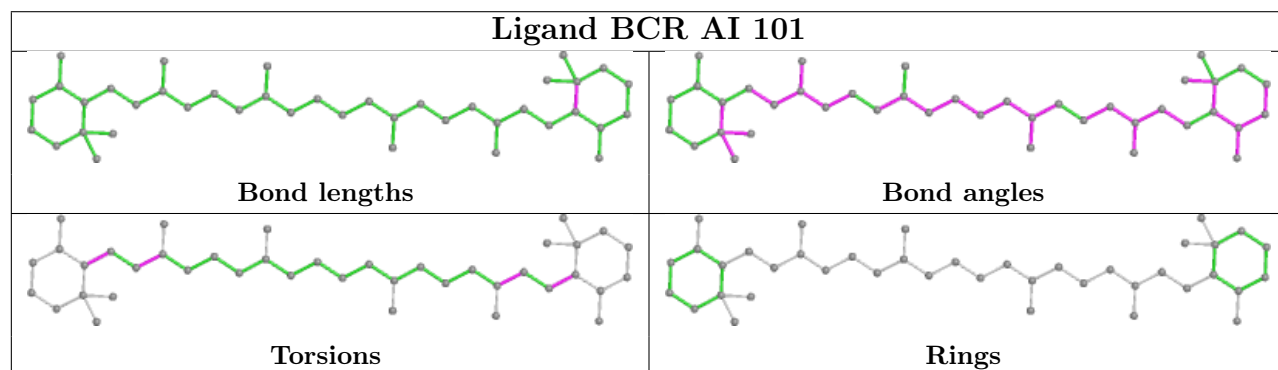
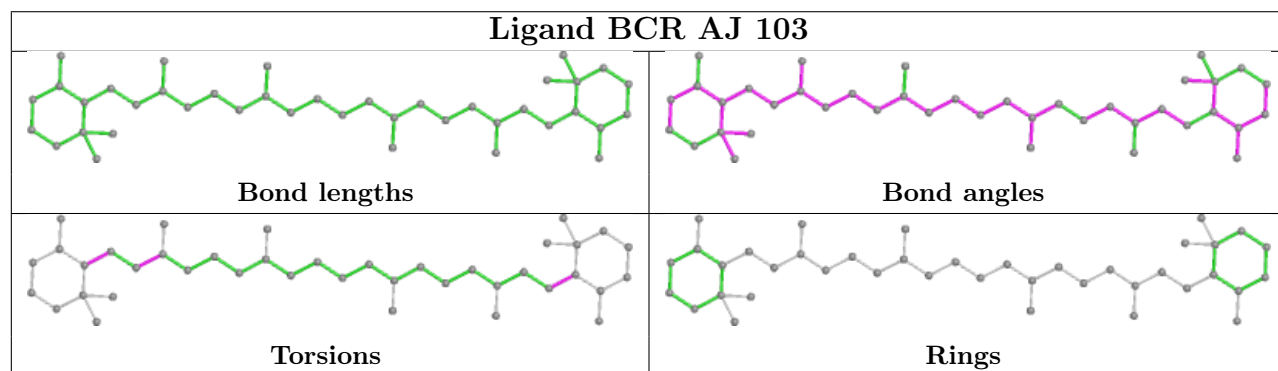
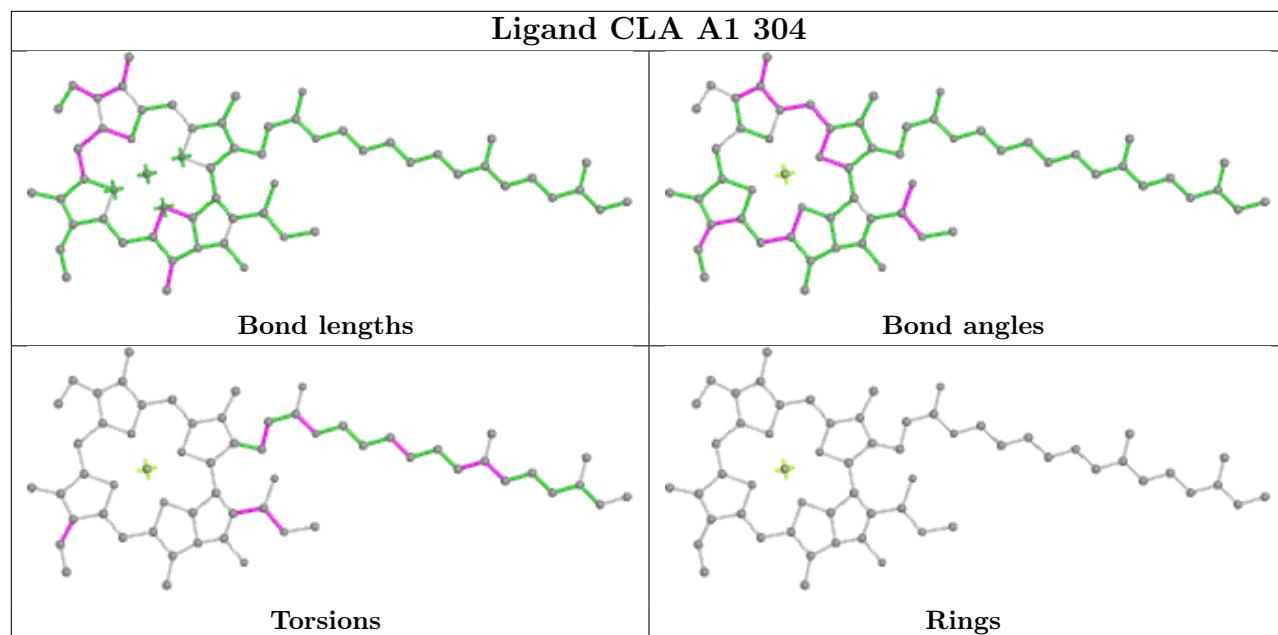


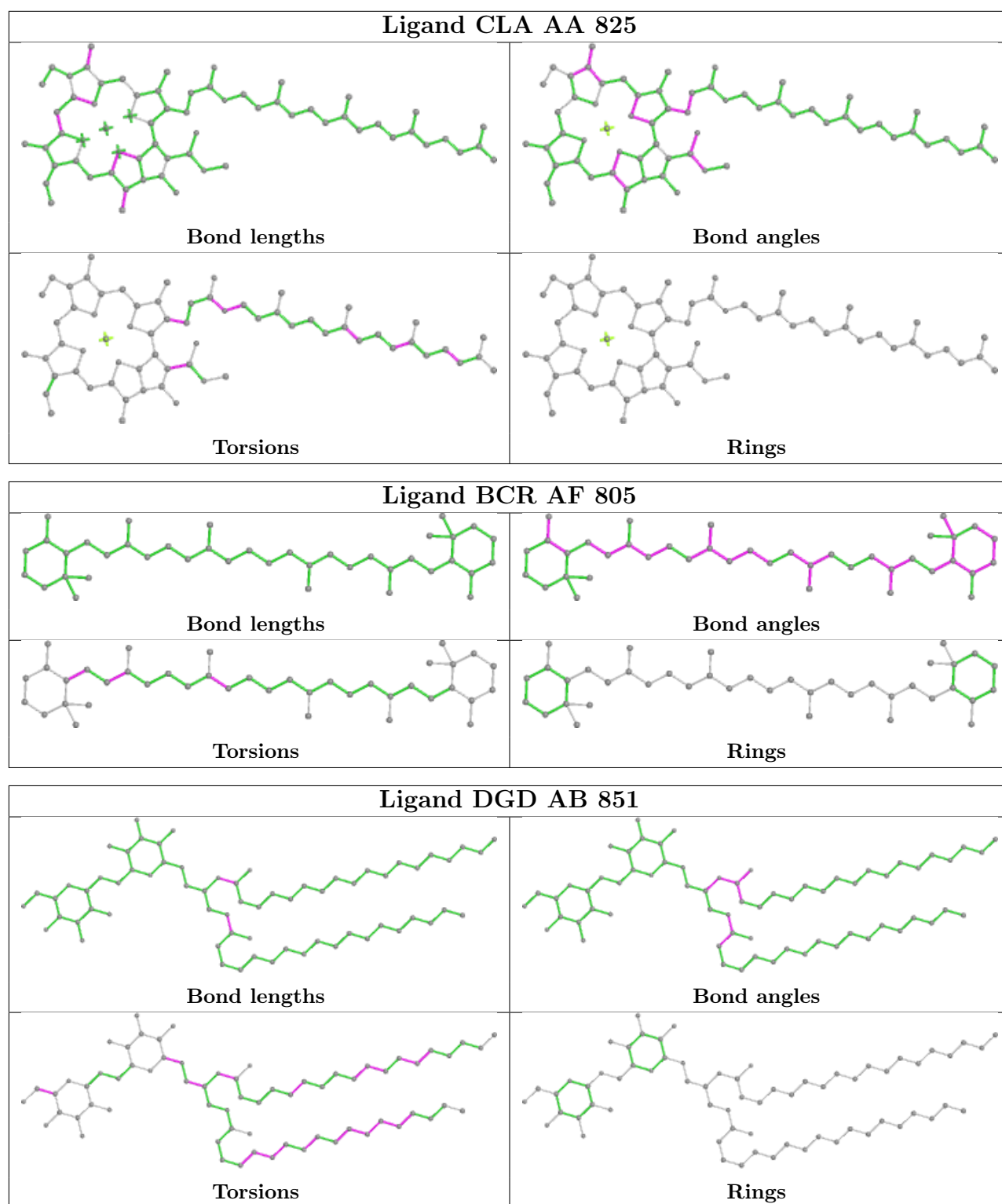
Torsions



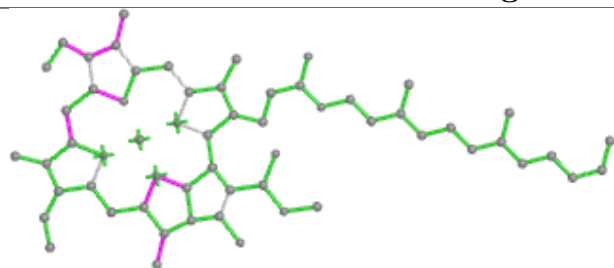
Rings



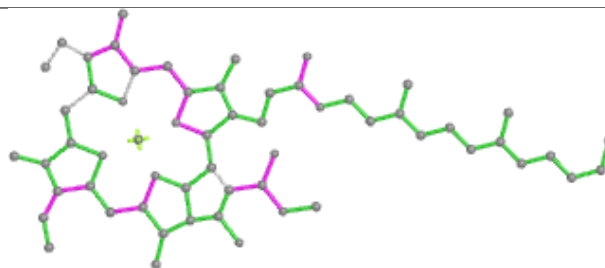




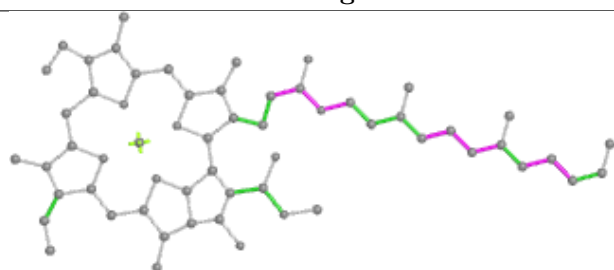
## Ligand CLA AB 818



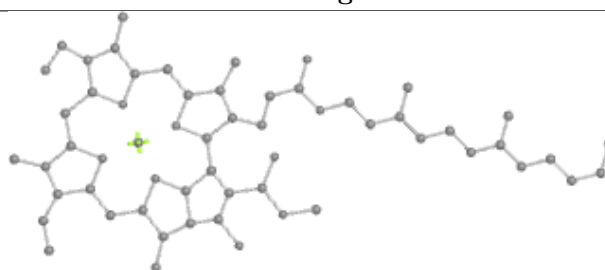
Bond lengths



Bond angles

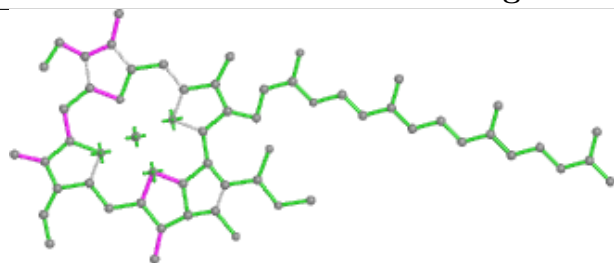


Torsions

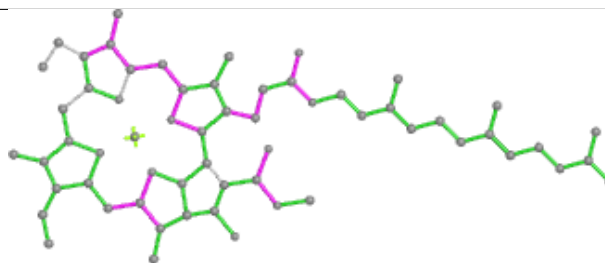


Rings

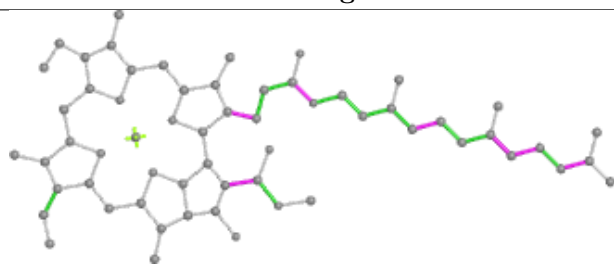
## Ligand CLA AL 303



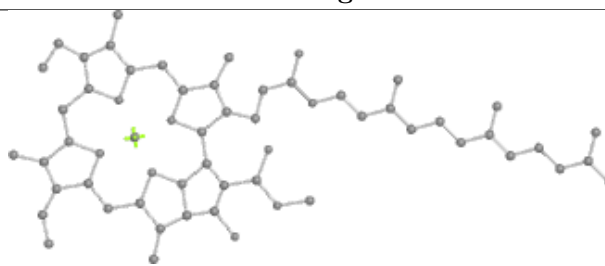
Bond lengths



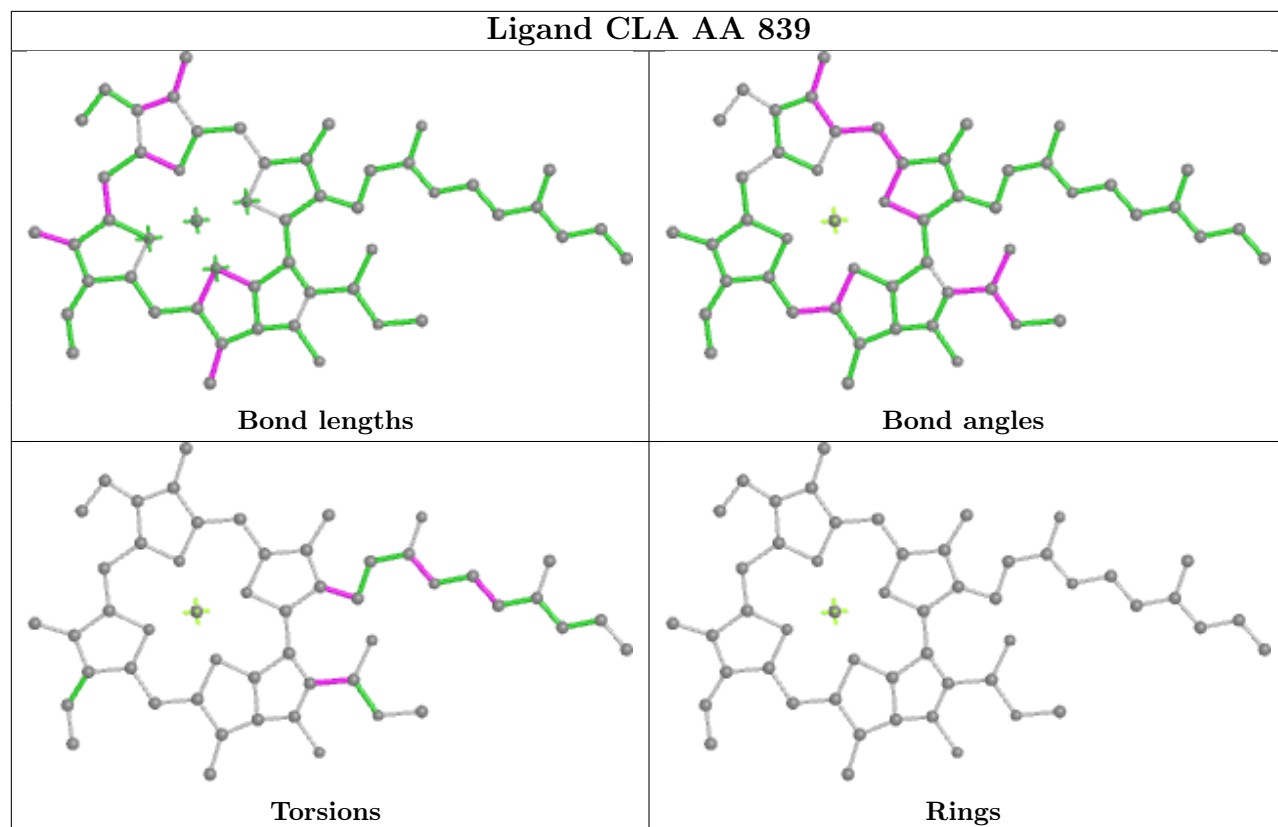
Bond angles

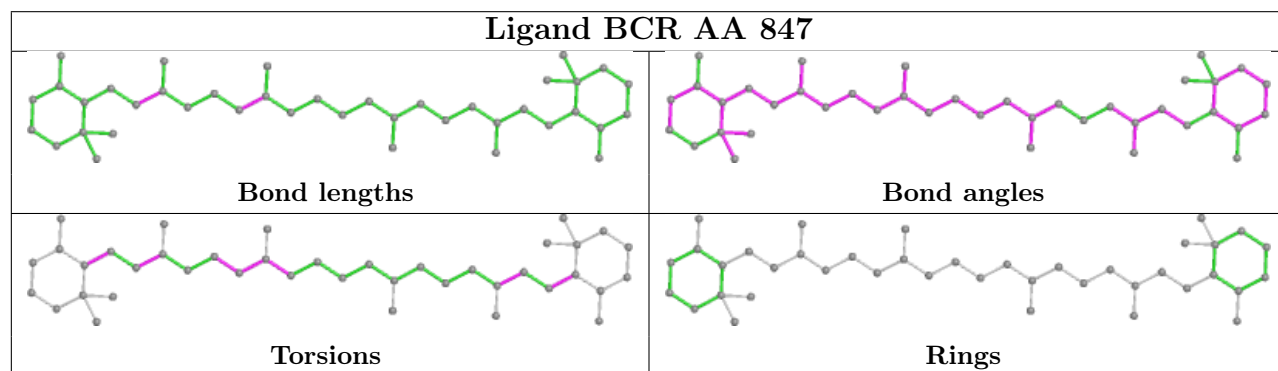
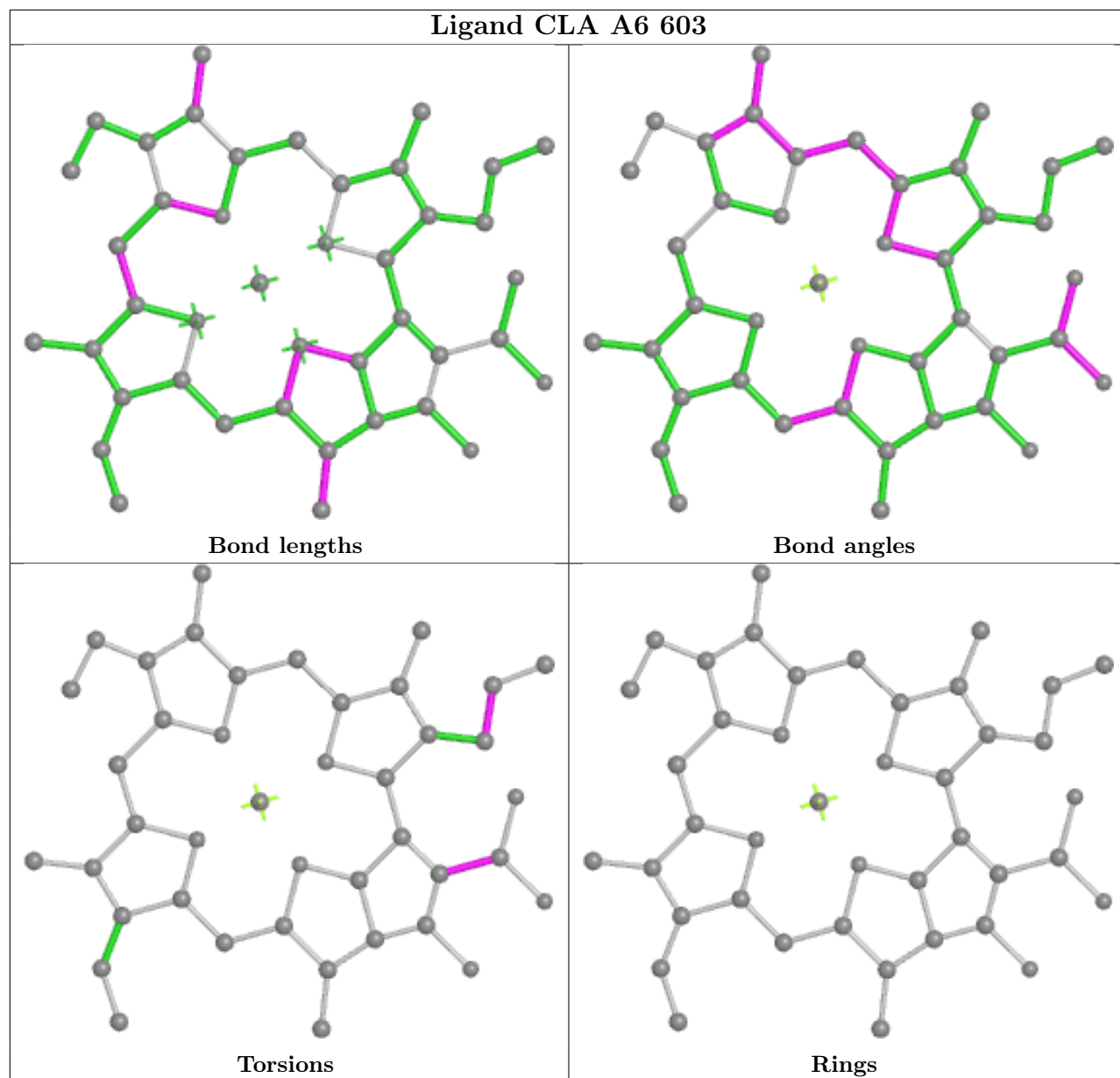


Torsions

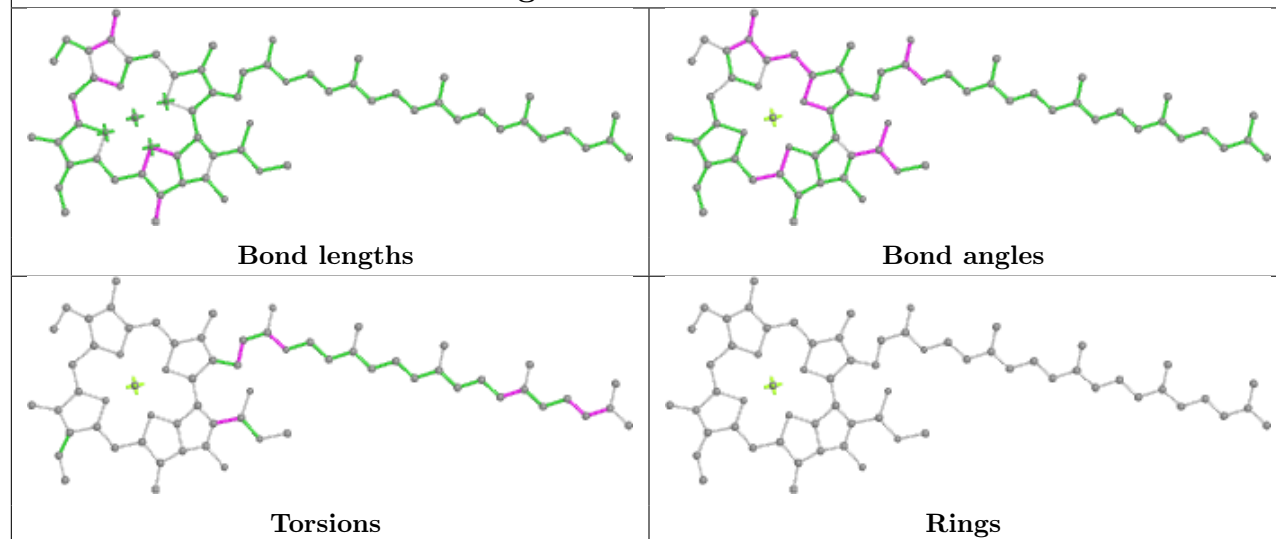


Rings

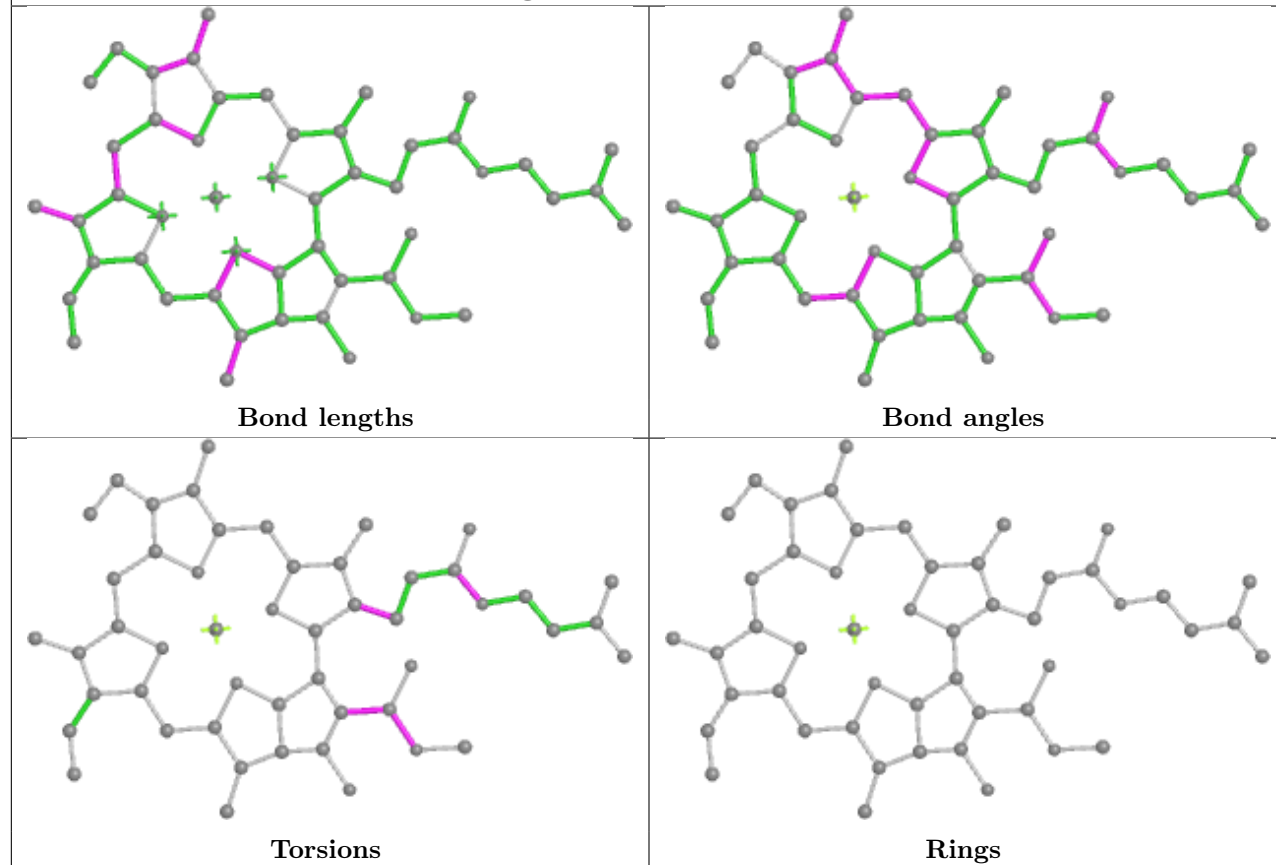




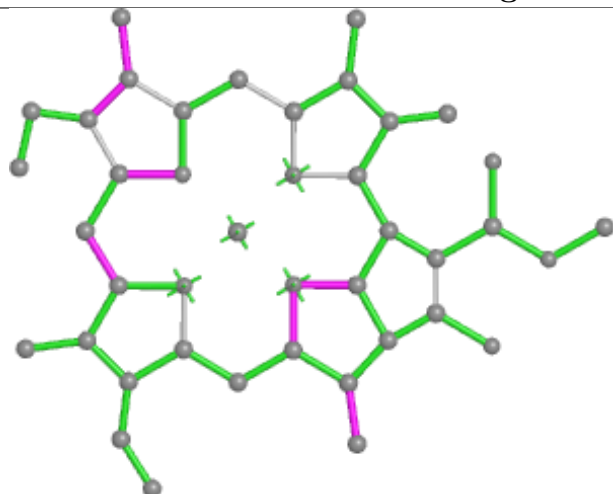
## Ligand CLA AA 808



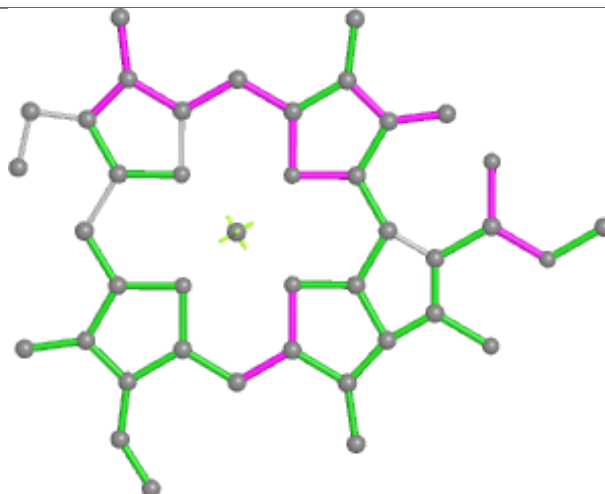
## Ligand CLA AB 821



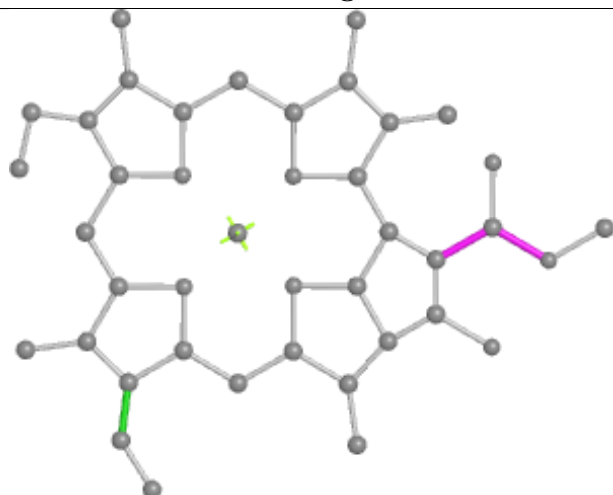
## Ligand CLA AA 823



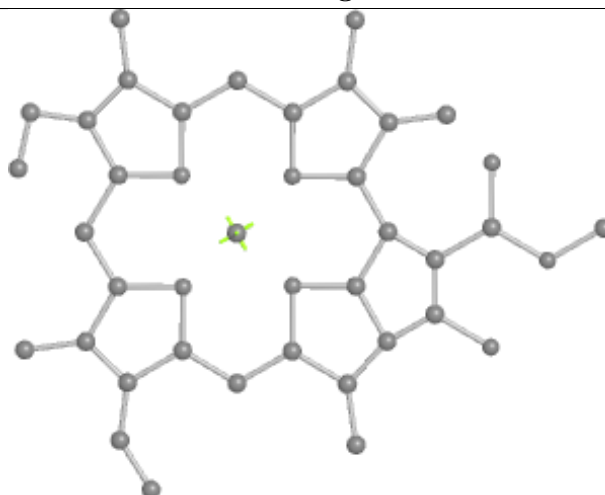
Bond lengths



Bond angles

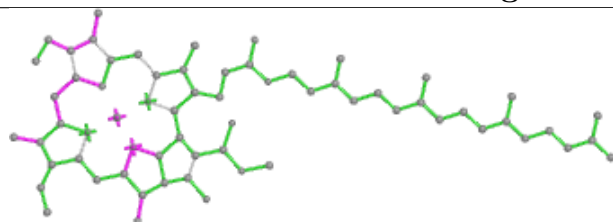


Torsions

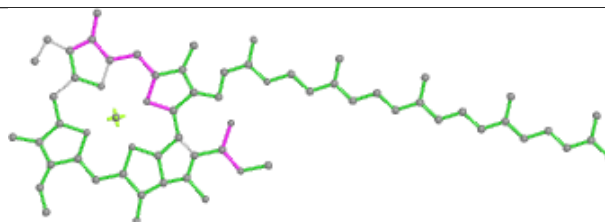


Rings

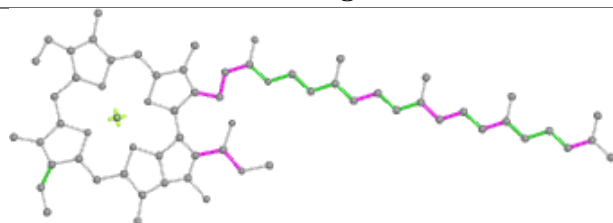
## Ligand CLA AB 810



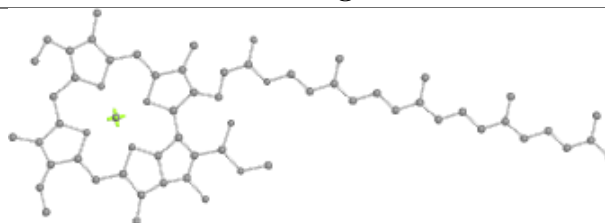
Bond lengths



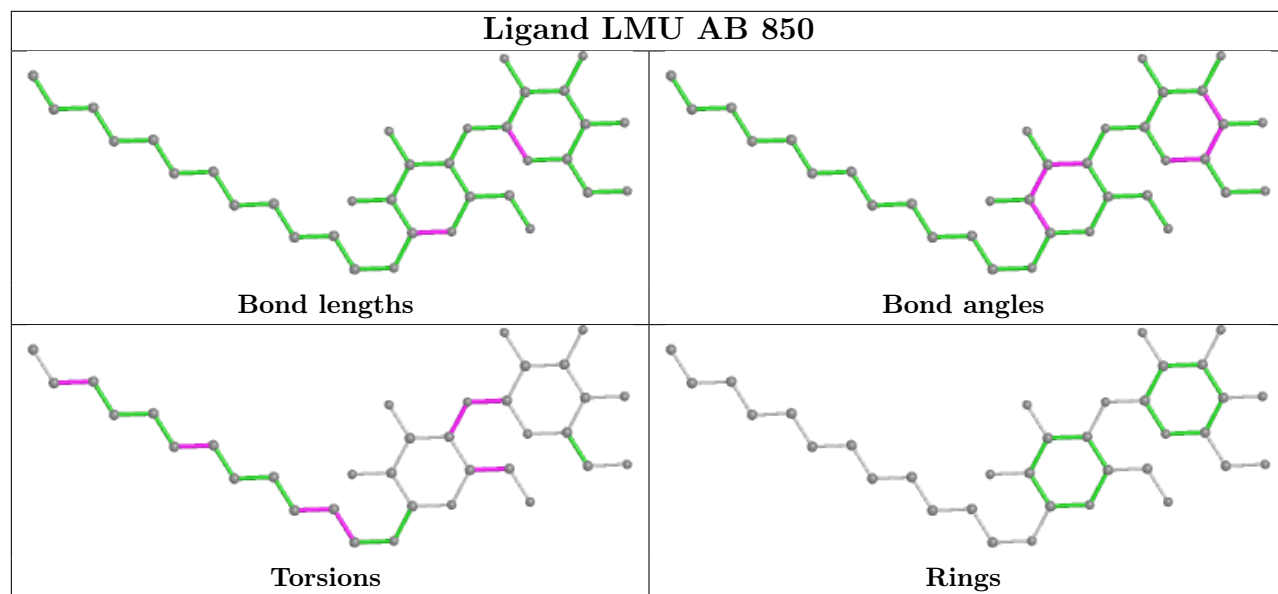
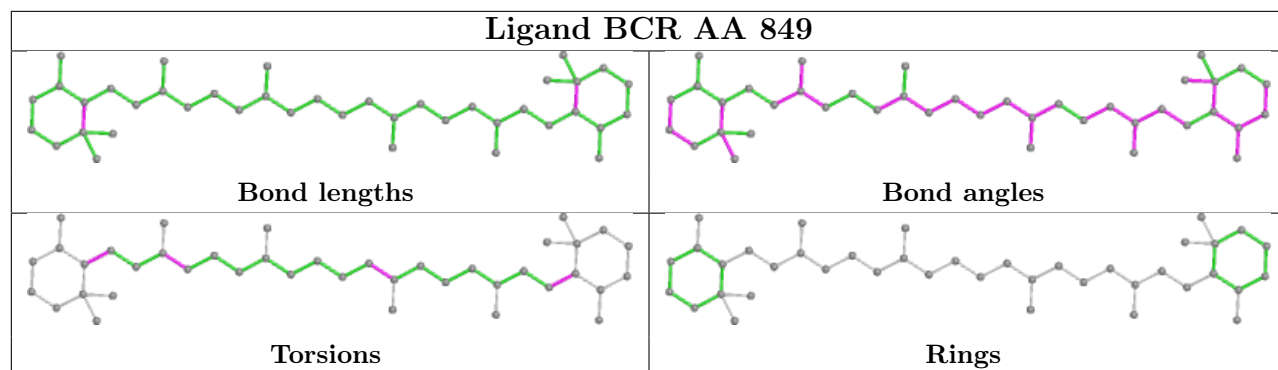
Bond angles



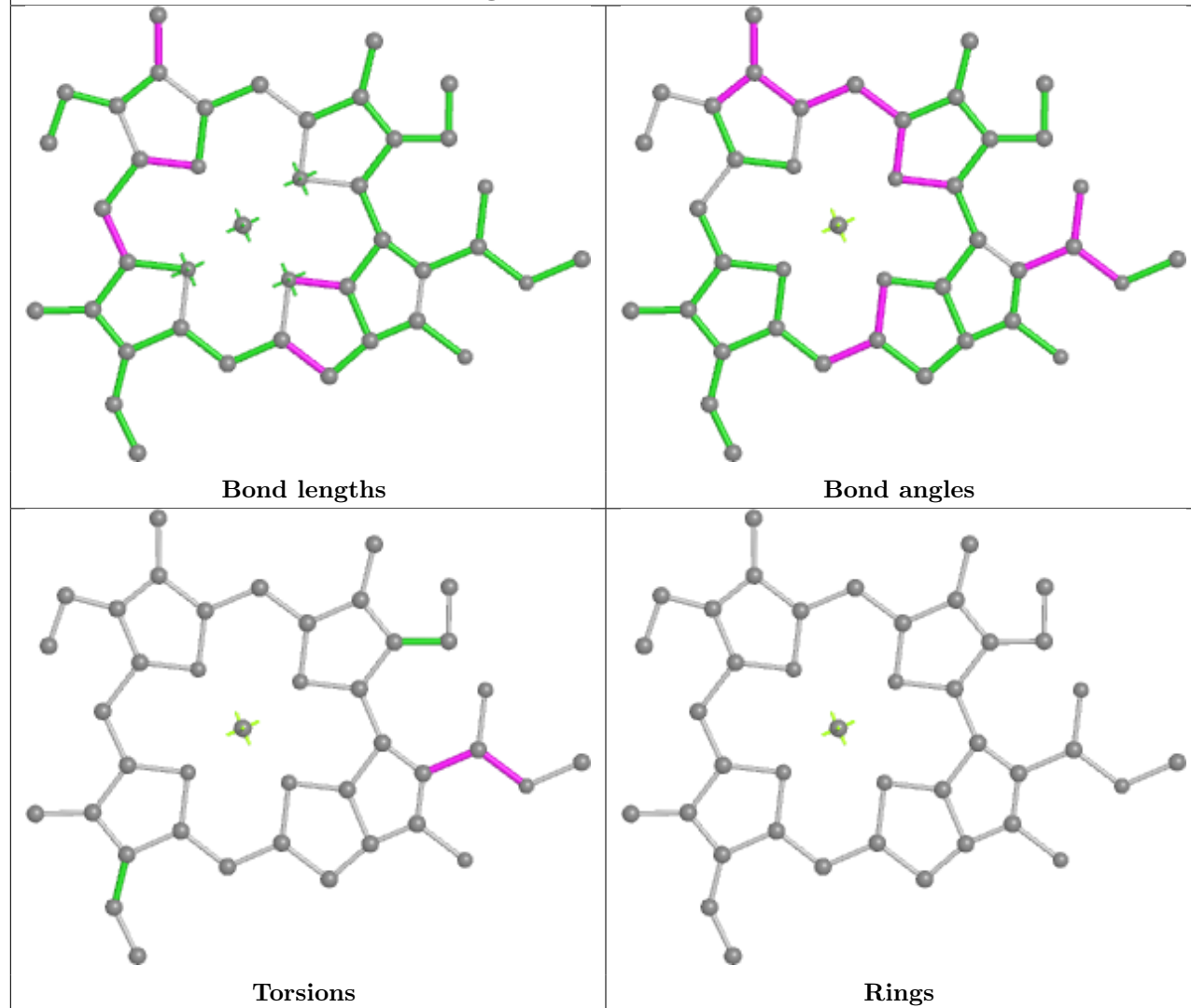
Torsions



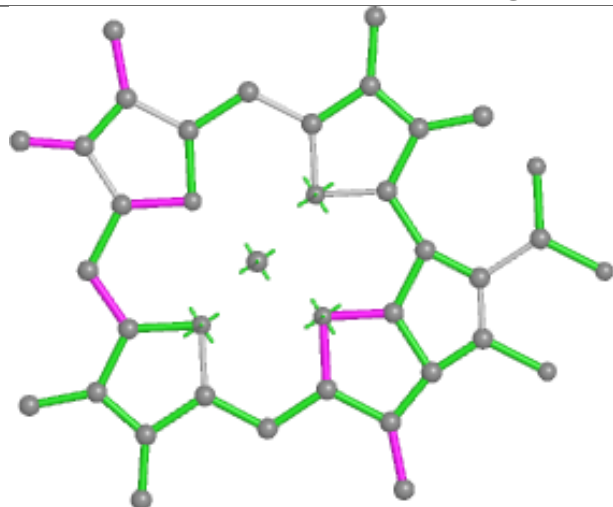
Rings



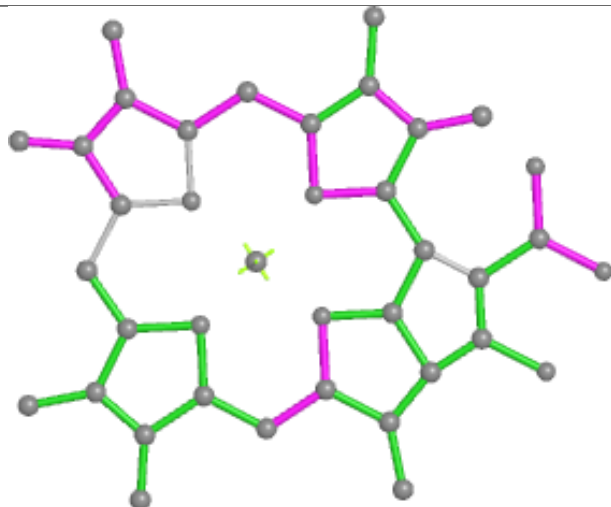
## Ligand CLA AA 815



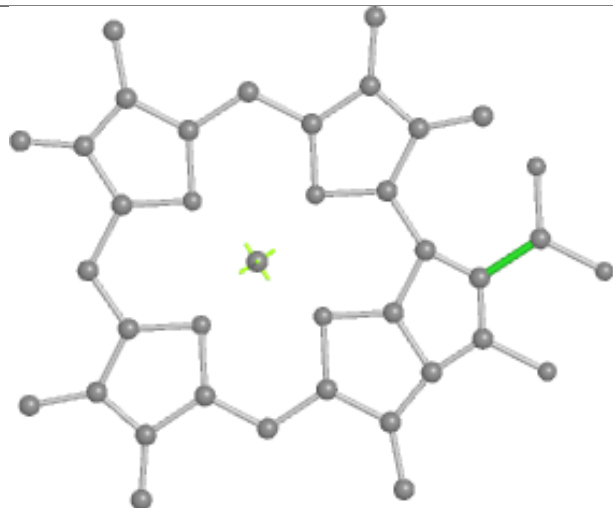
## Ligand CLA A1 312



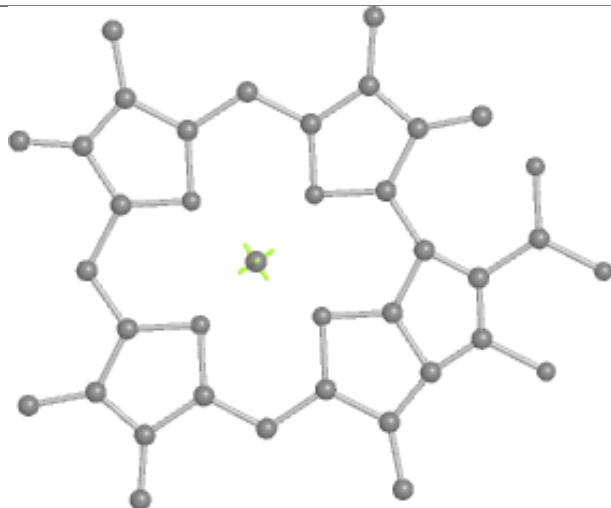
Bond lengths



Bond angles

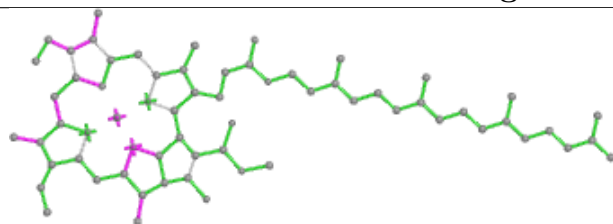


Torsions

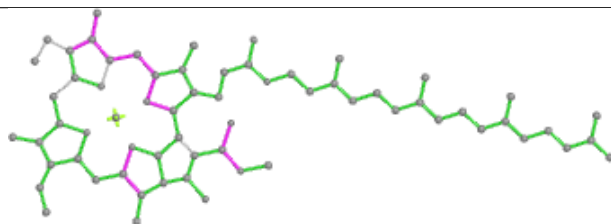


Rings

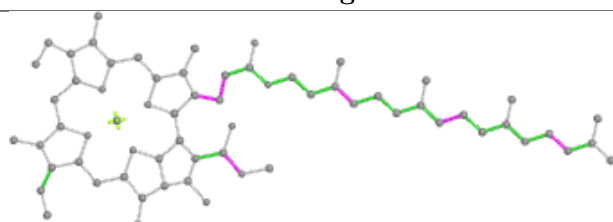
## Ligand CLA AA 802



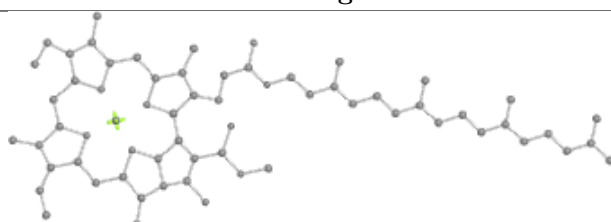
Bond lengths



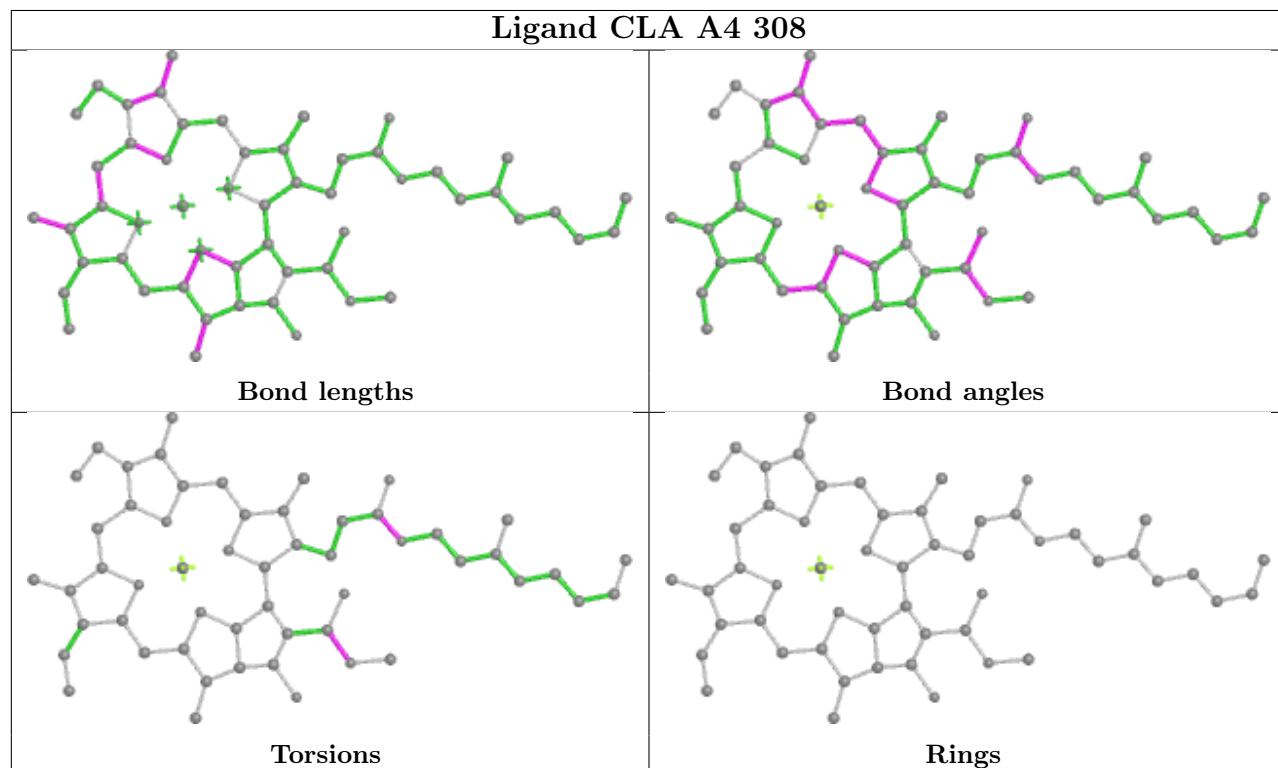
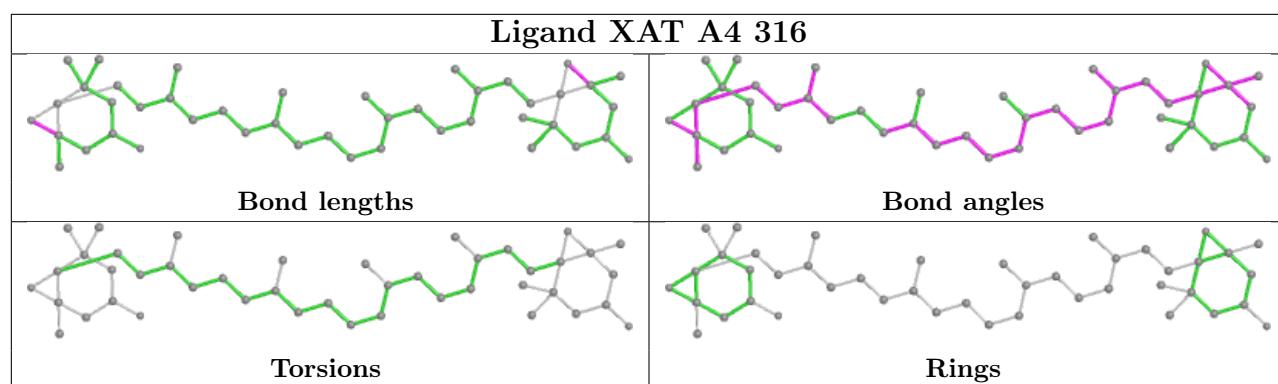
Bond angles

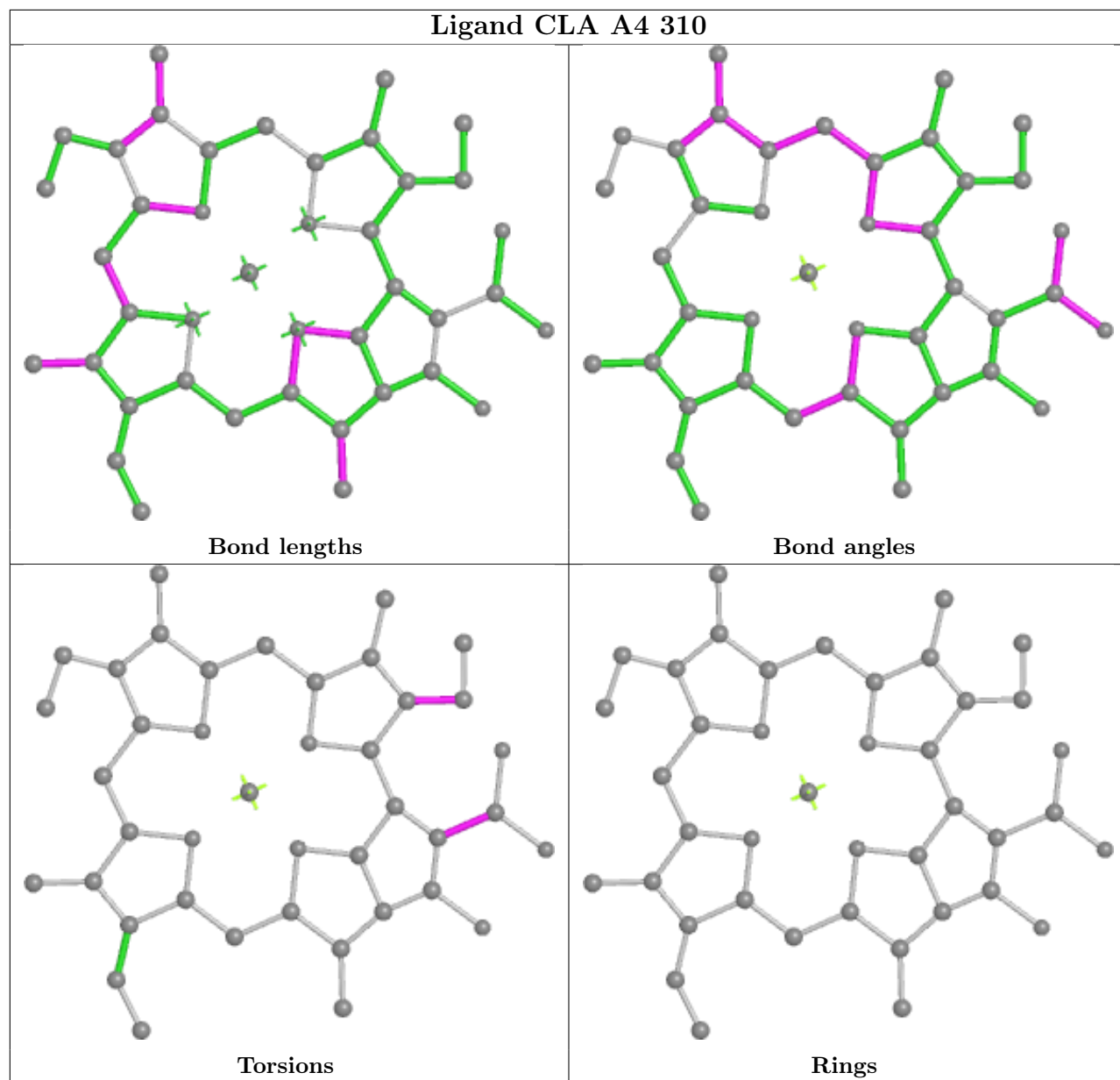


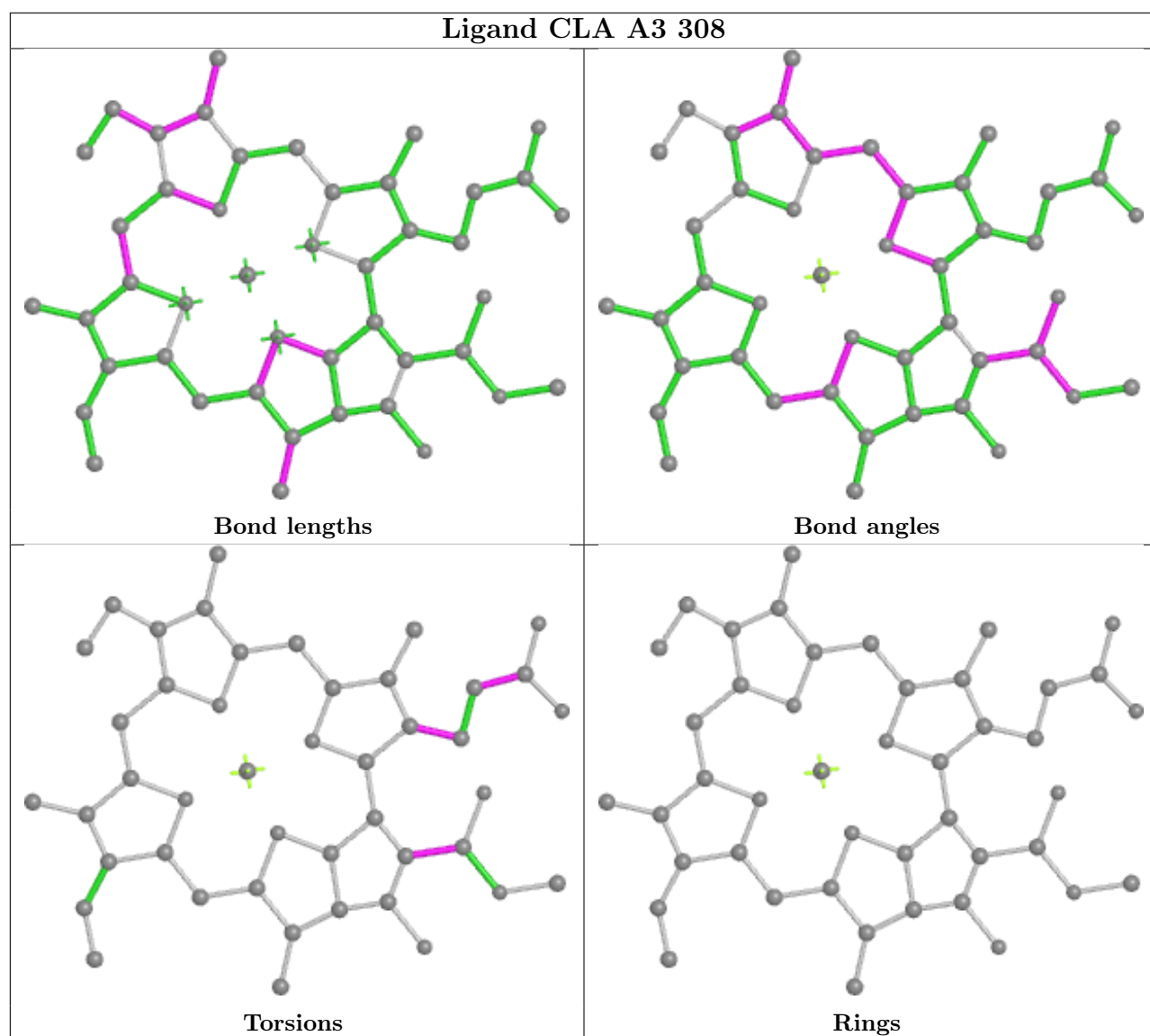
Torsions



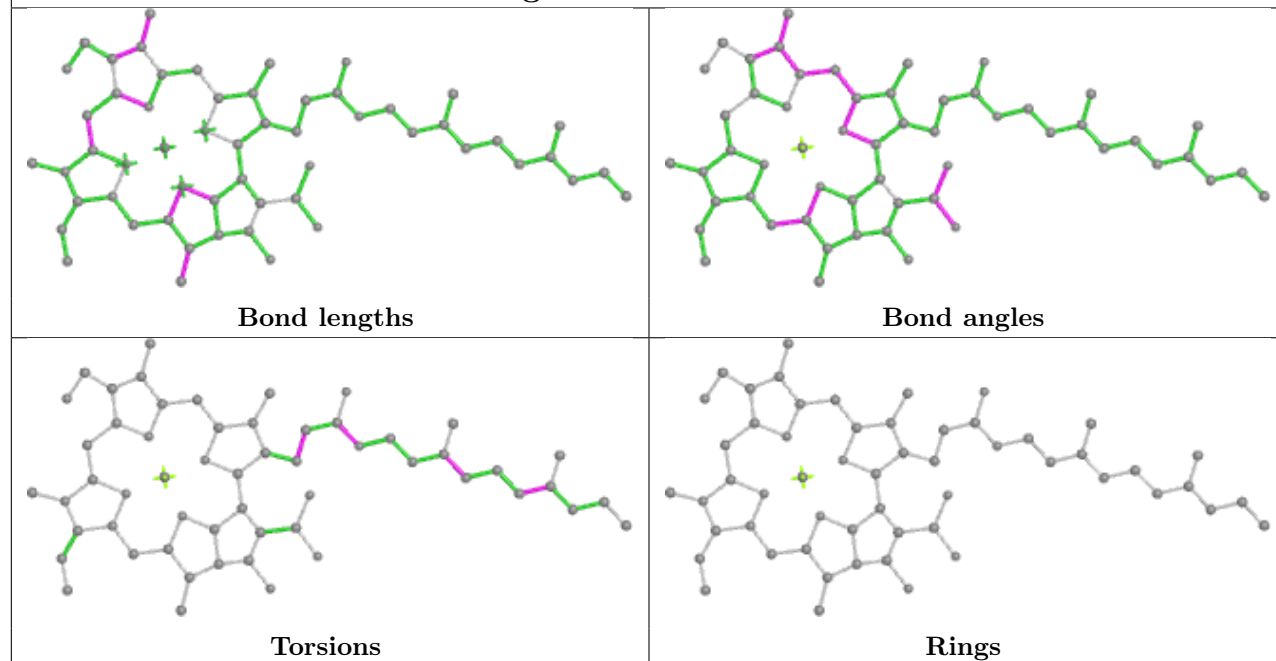
Rings



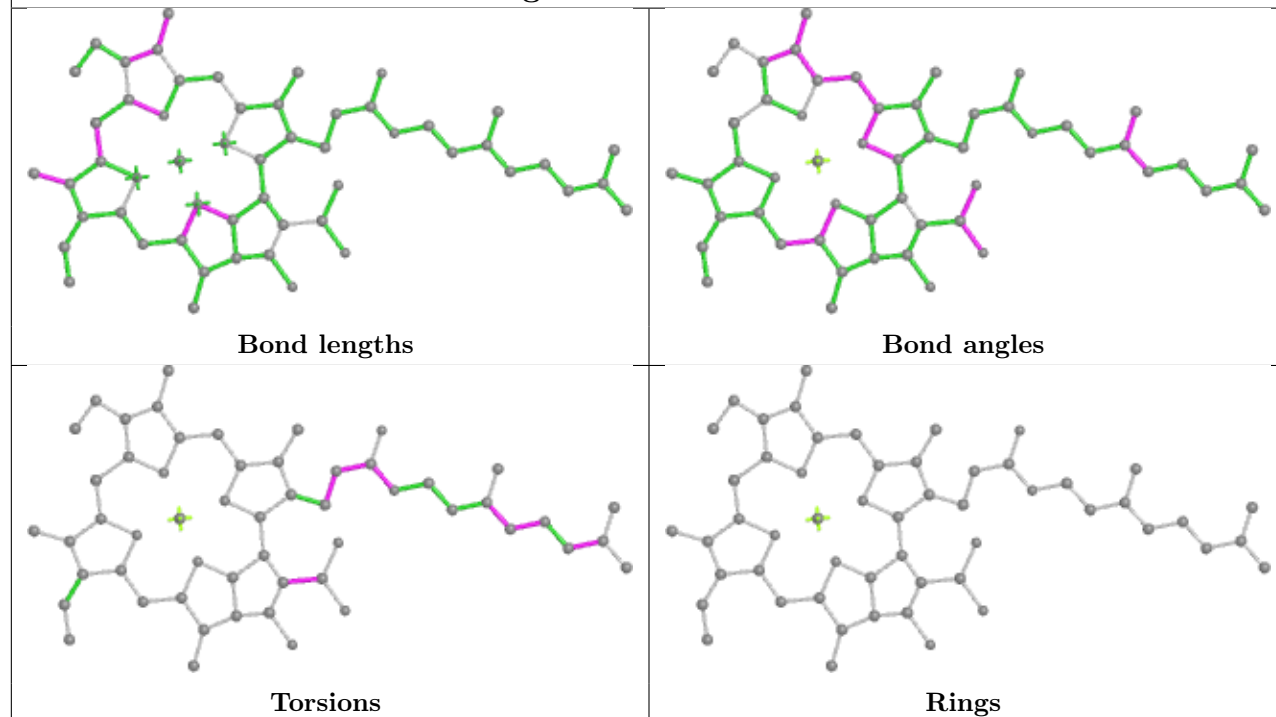




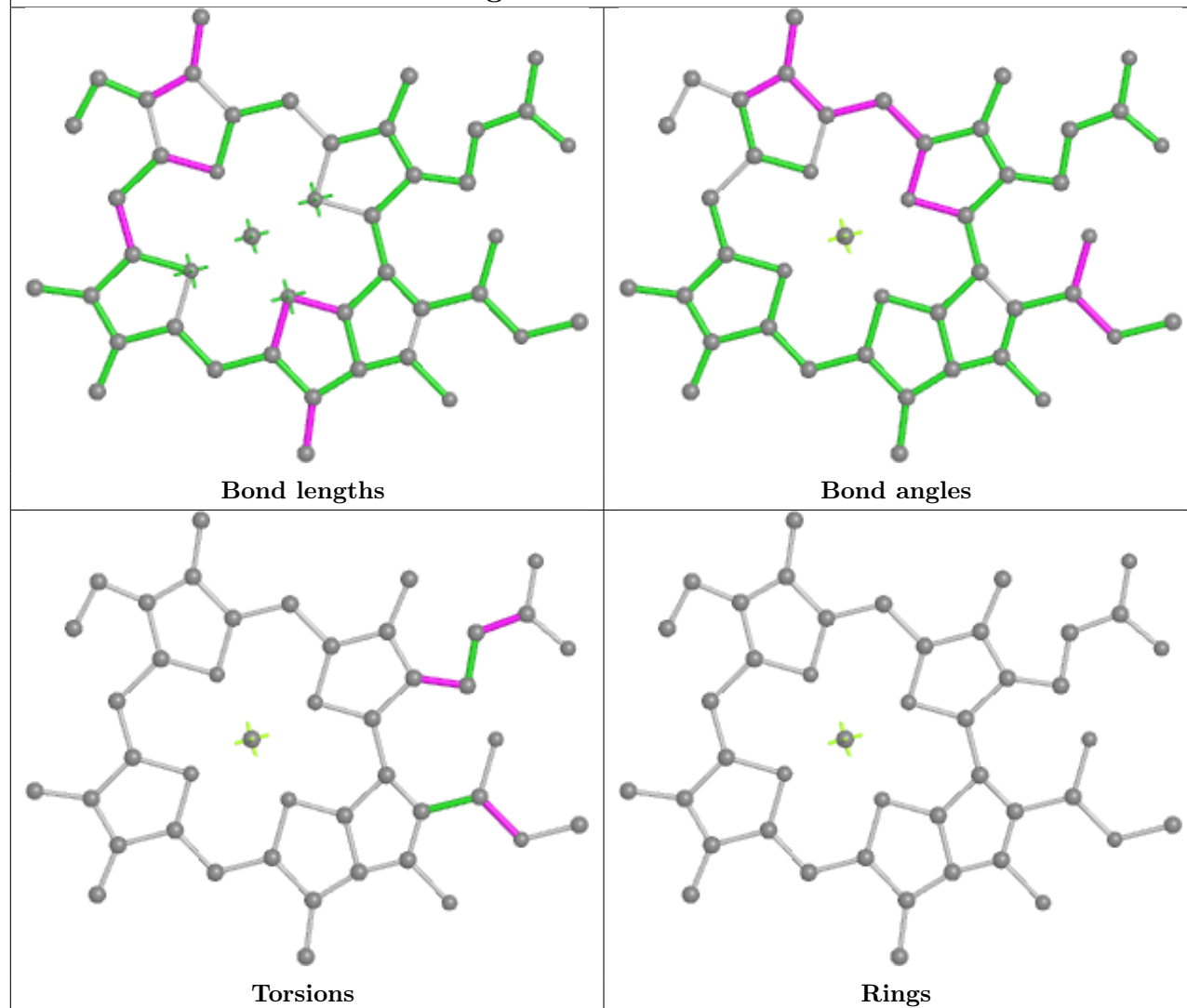
## Ligand CLA A4 311



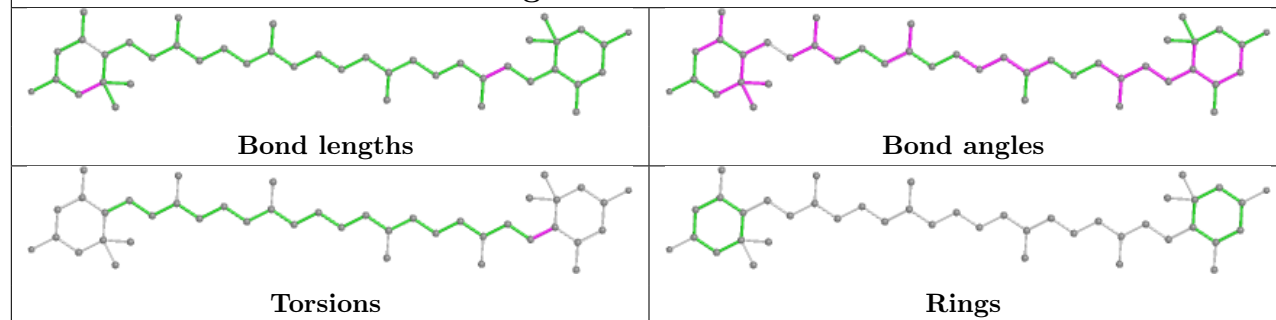
## Ligand CLA A3 312

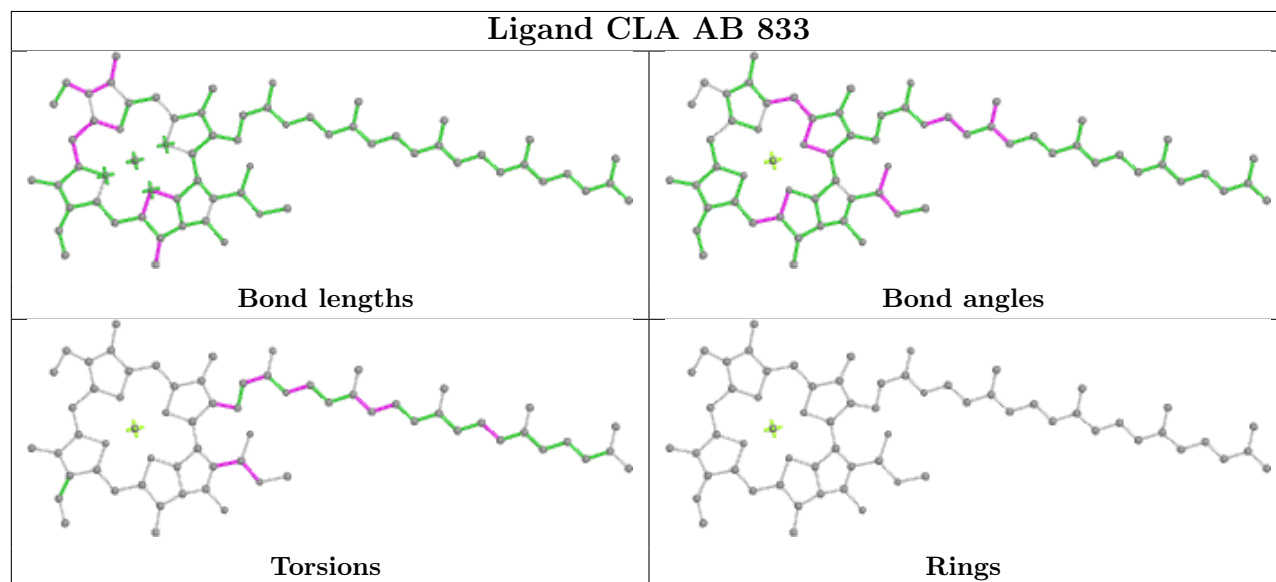
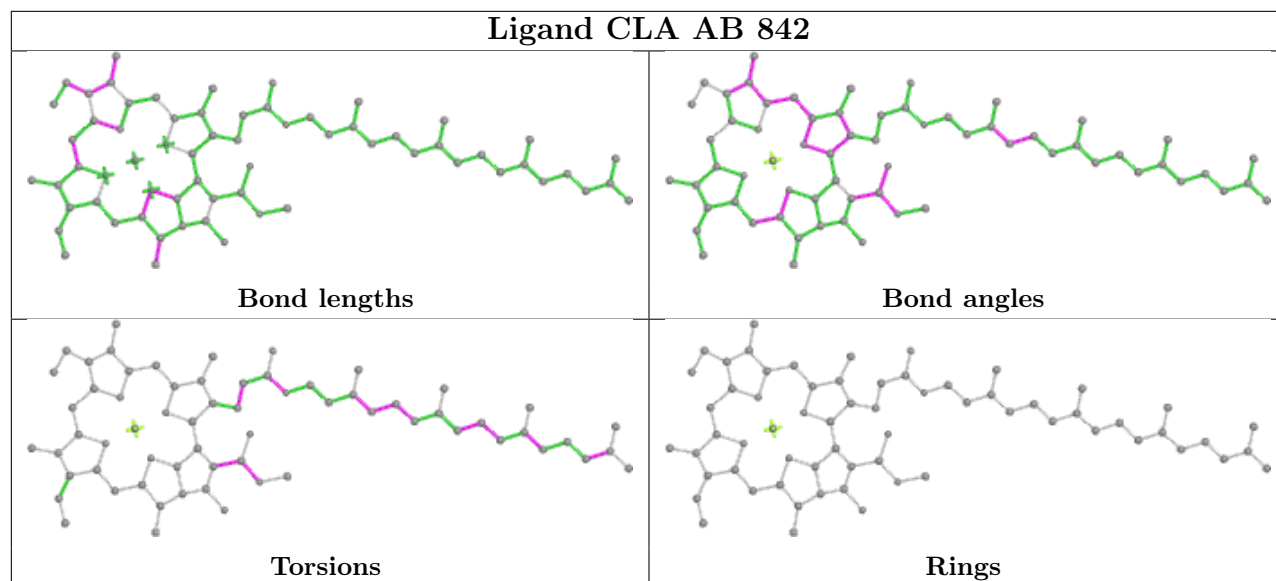
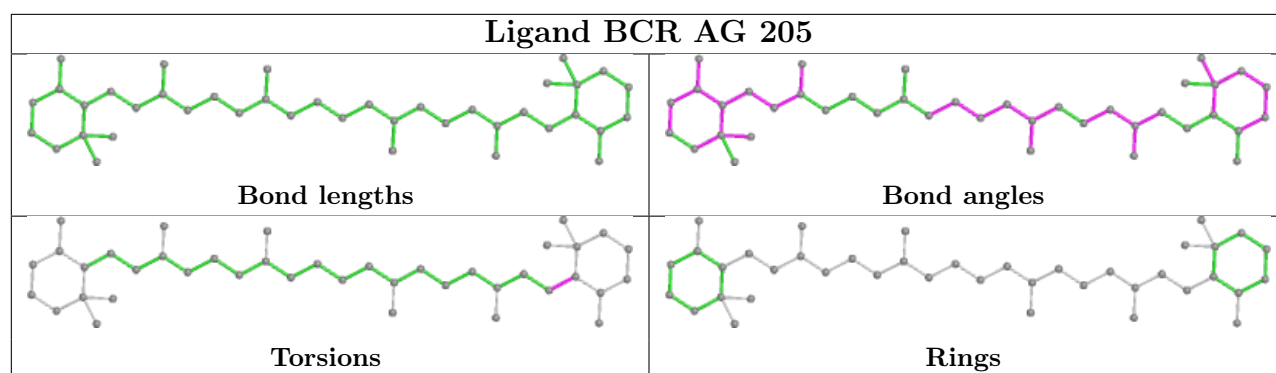


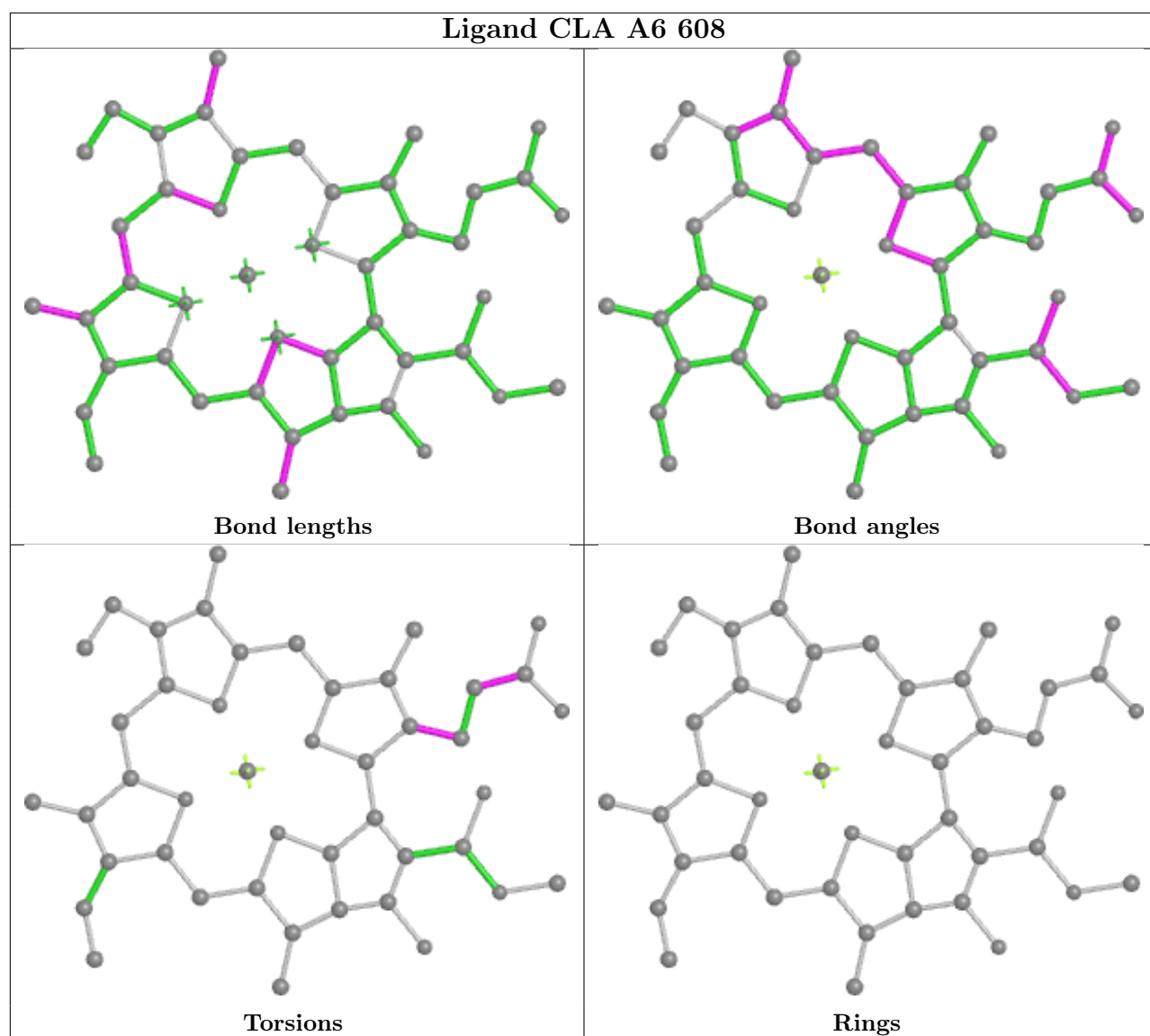
## Ligand CLA A6 611

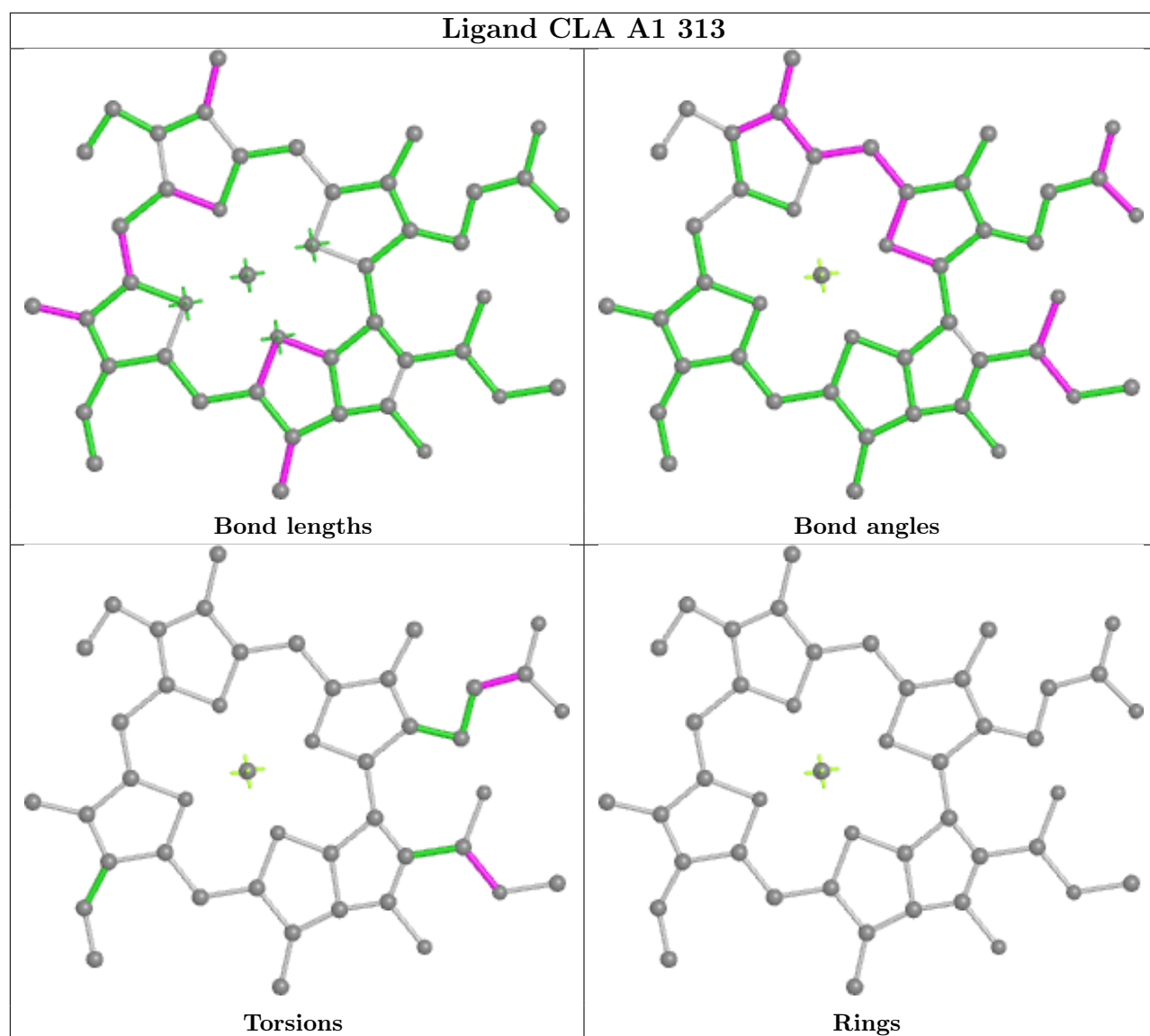


## Ligand LUT A4 315

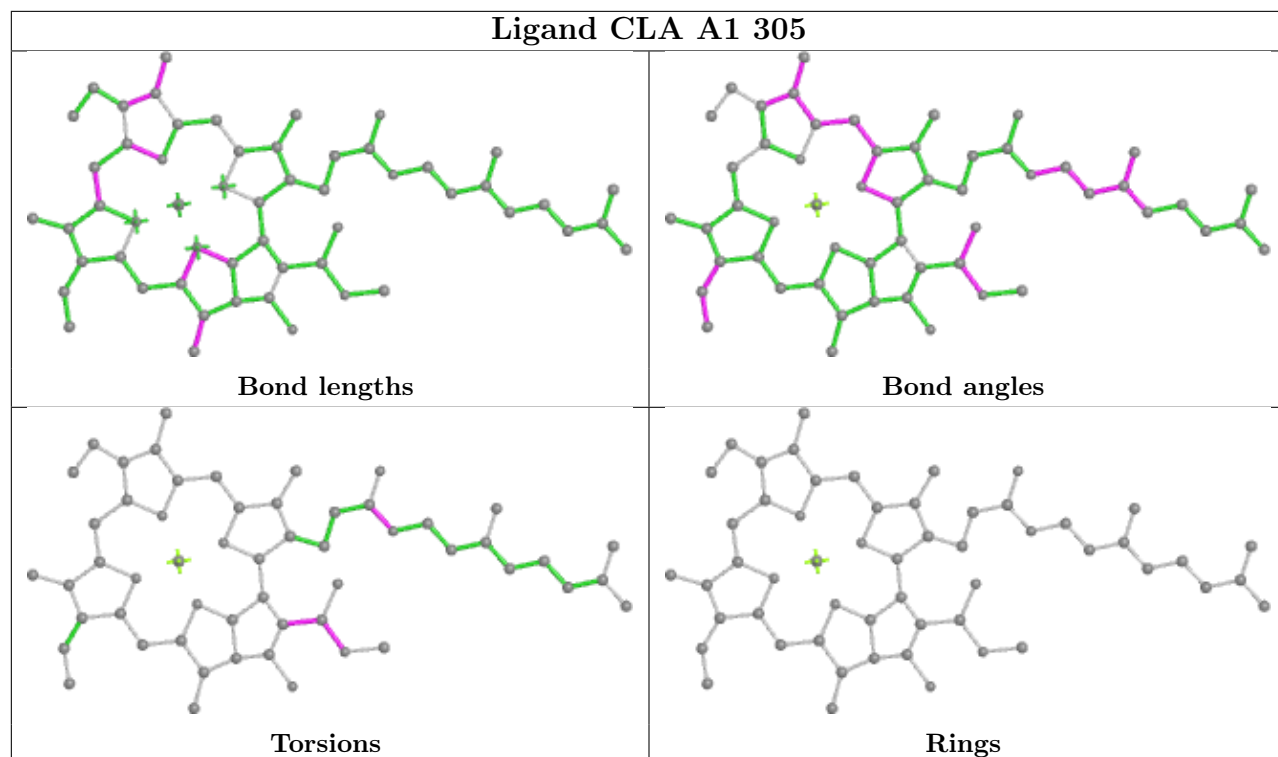




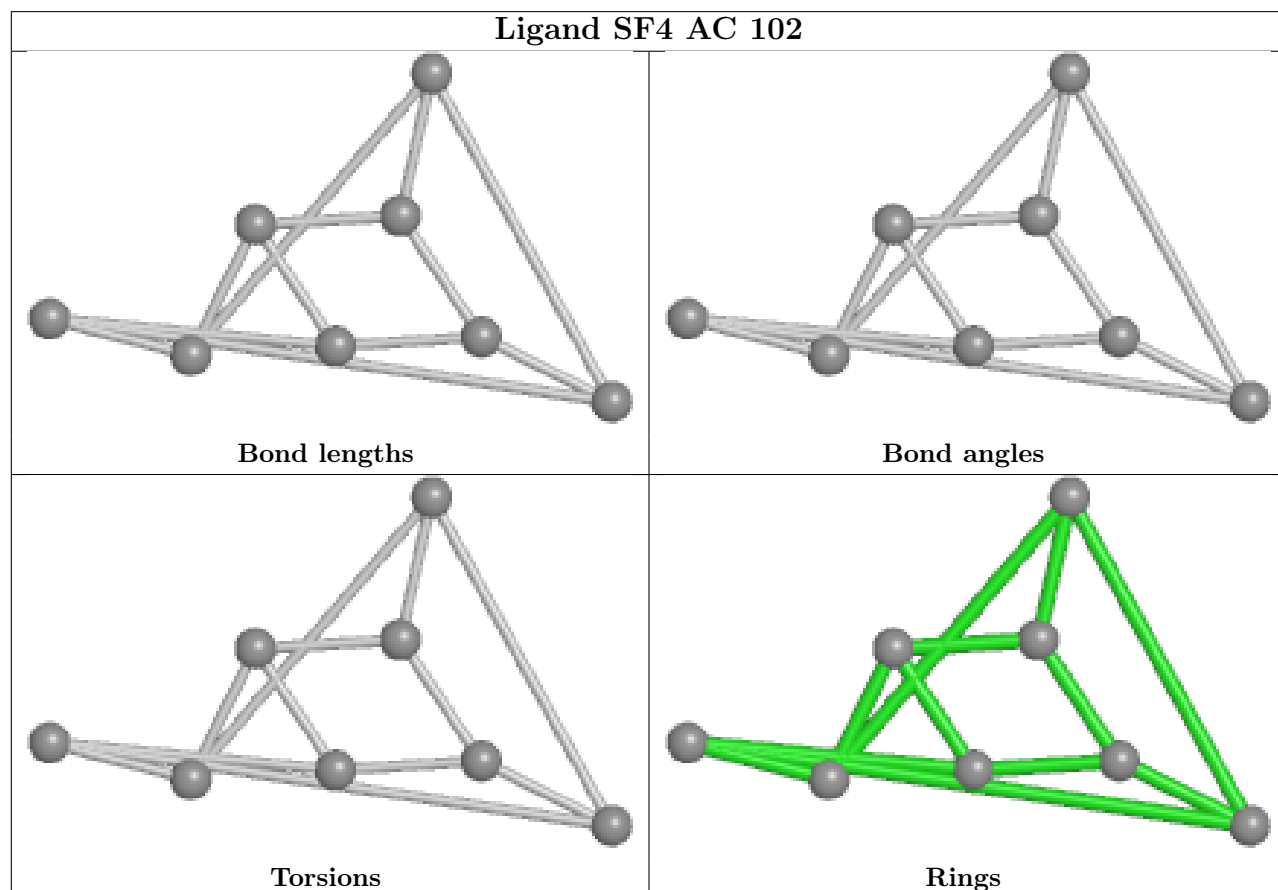




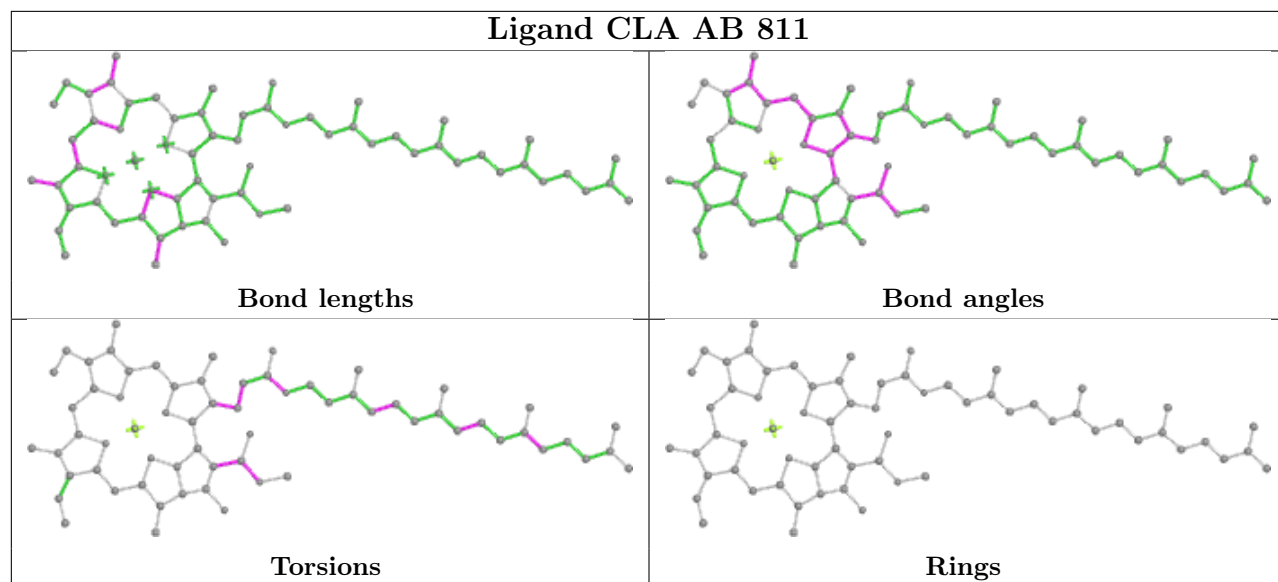
## Ligand CLA A1 305



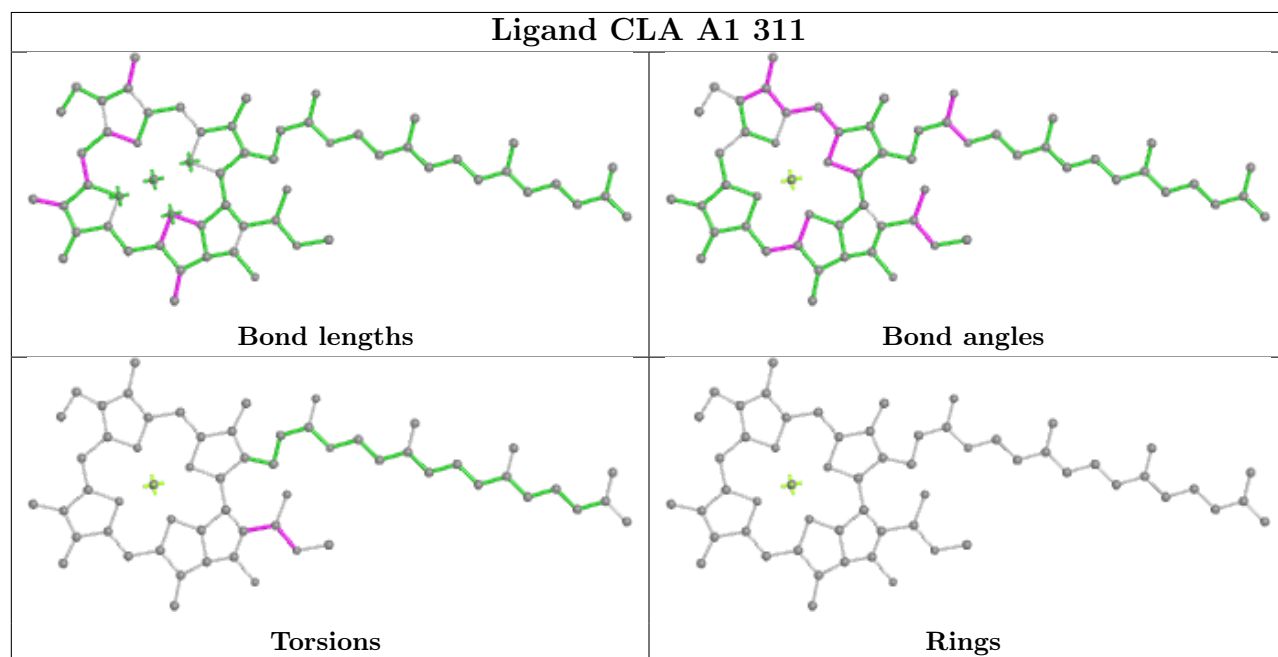
## Ligand SF4 AC 102

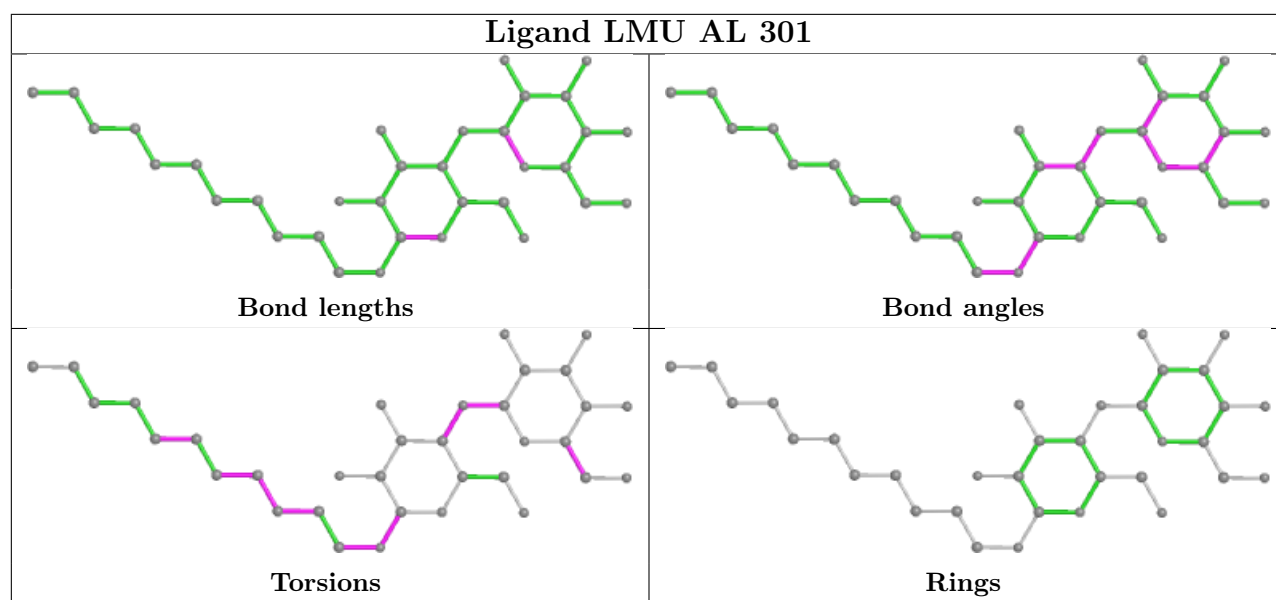


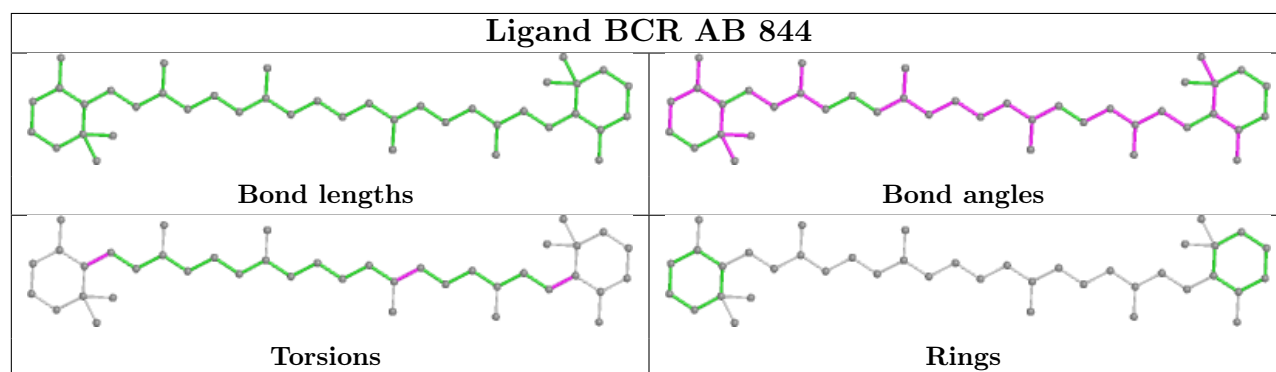
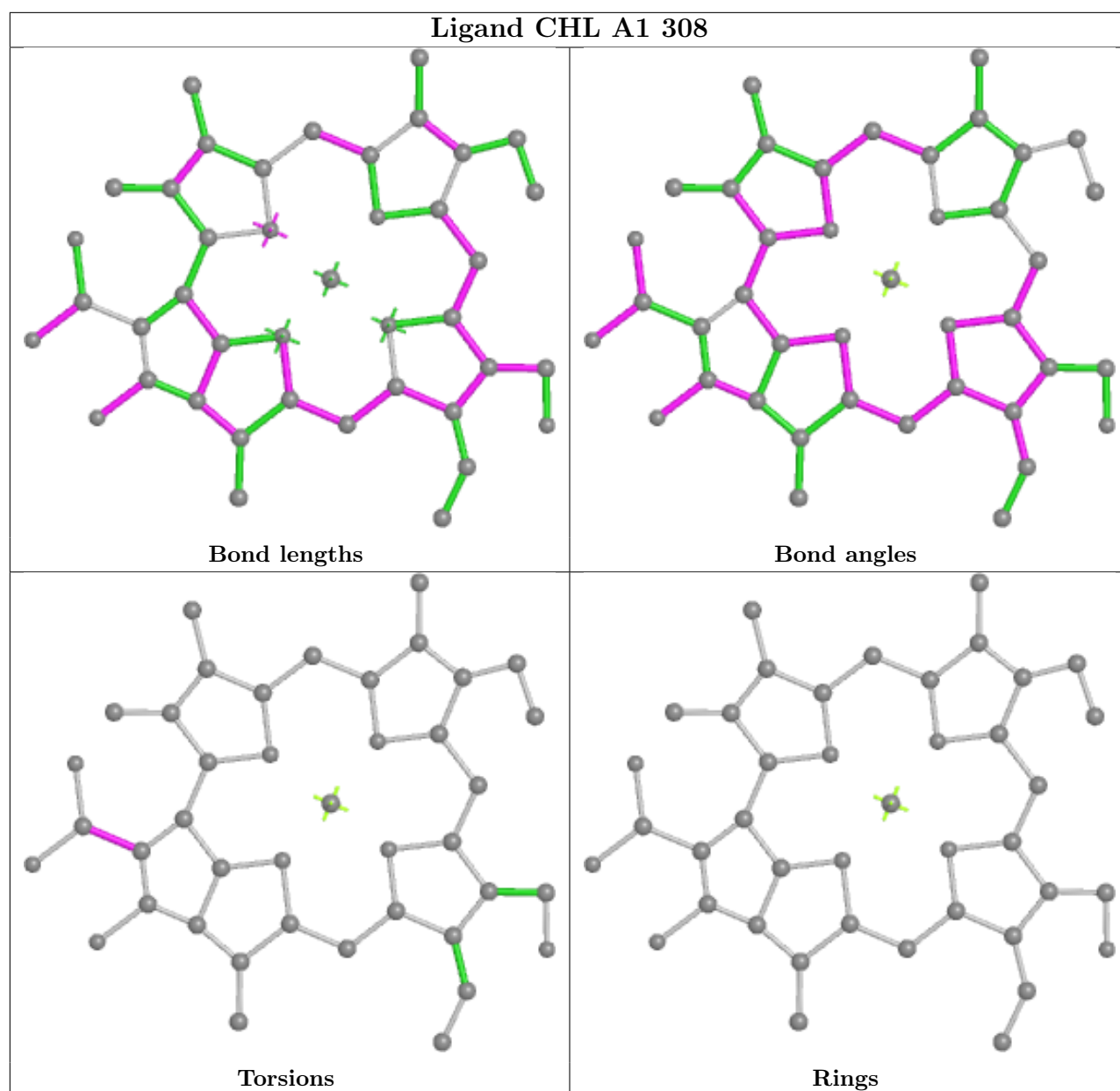
## Ligand CLA AB 811



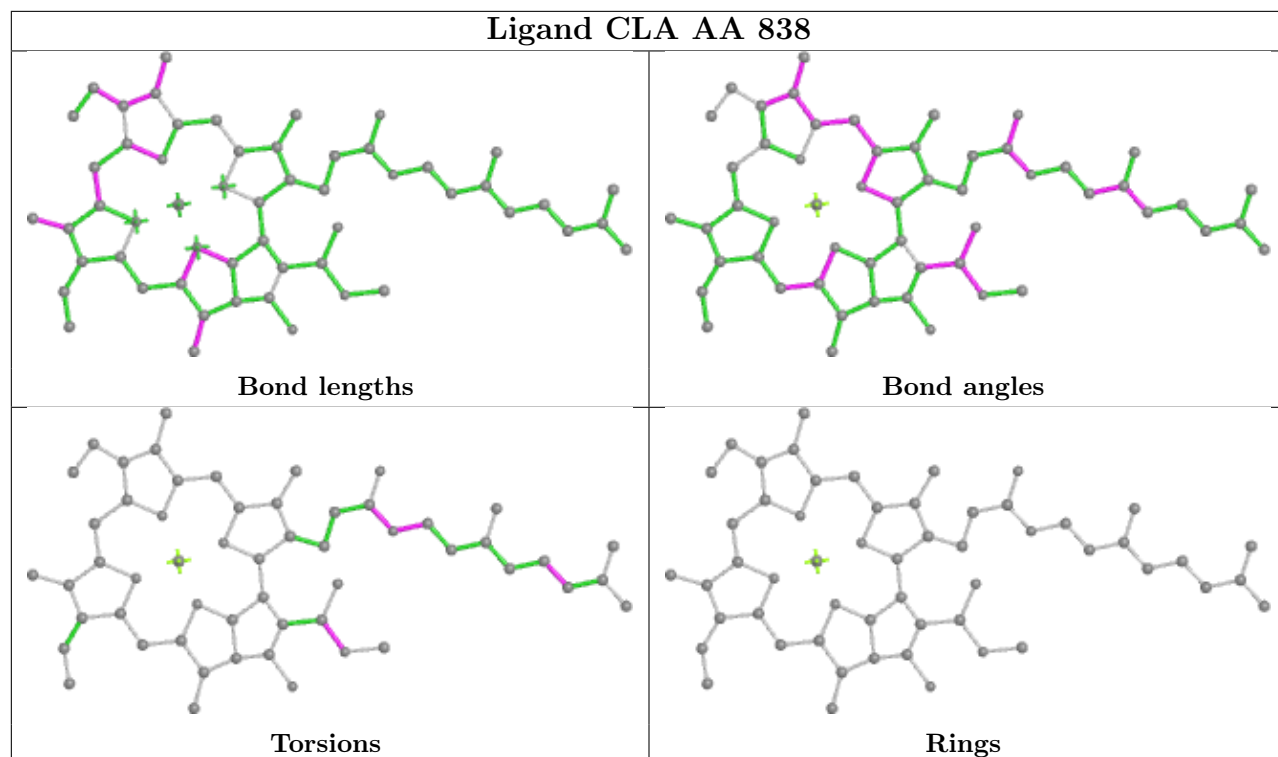
## Ligand CLA A1 311



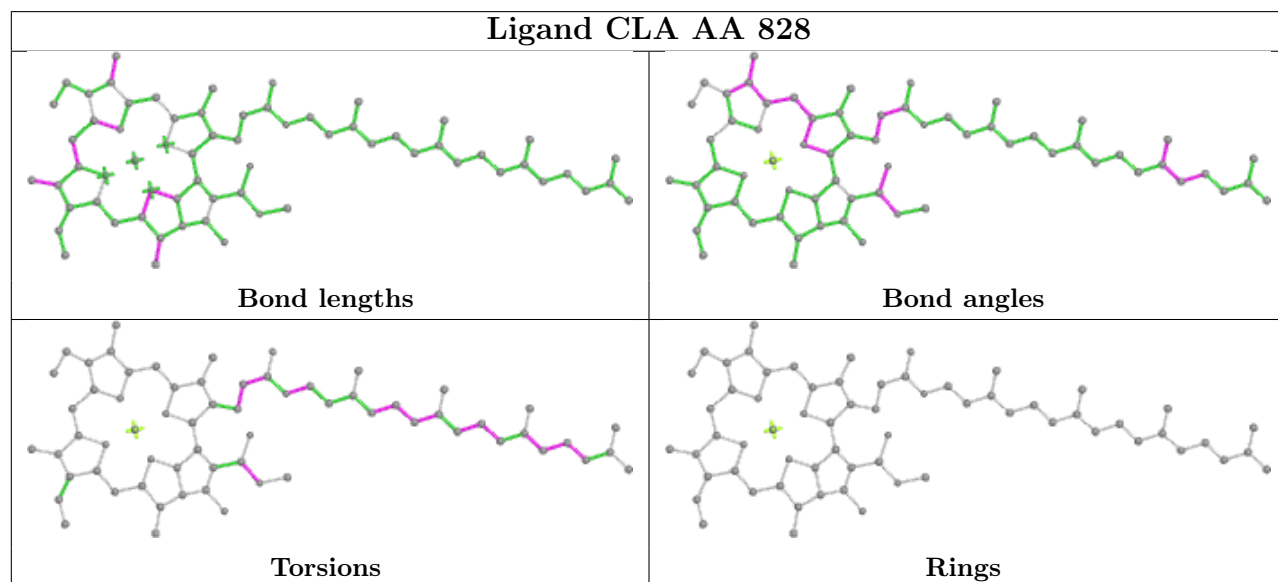




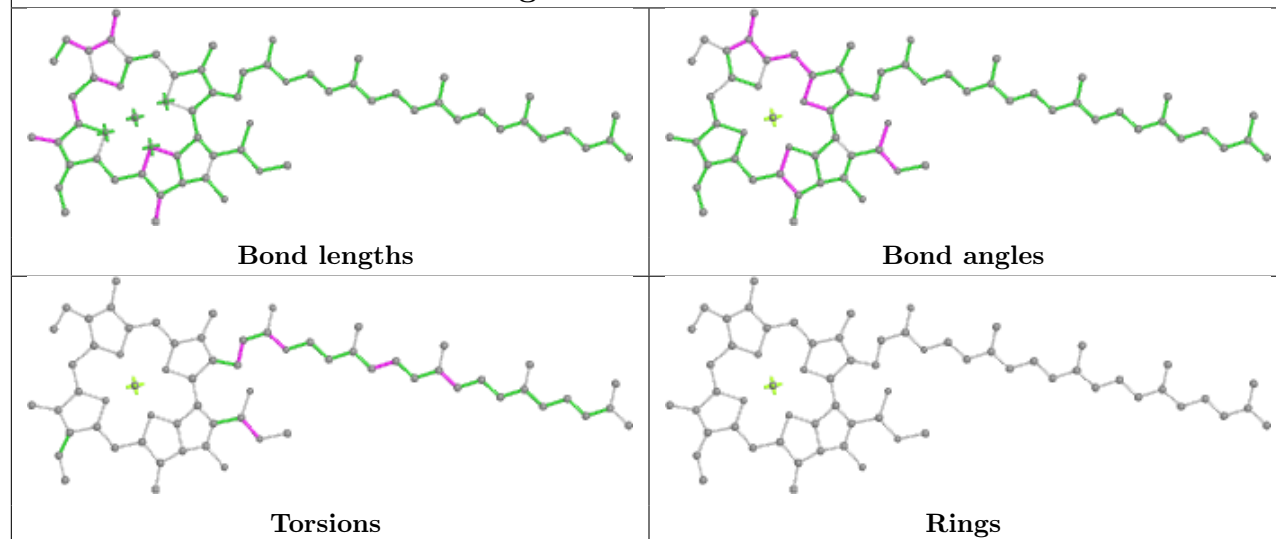
## Ligand CLA AA 838



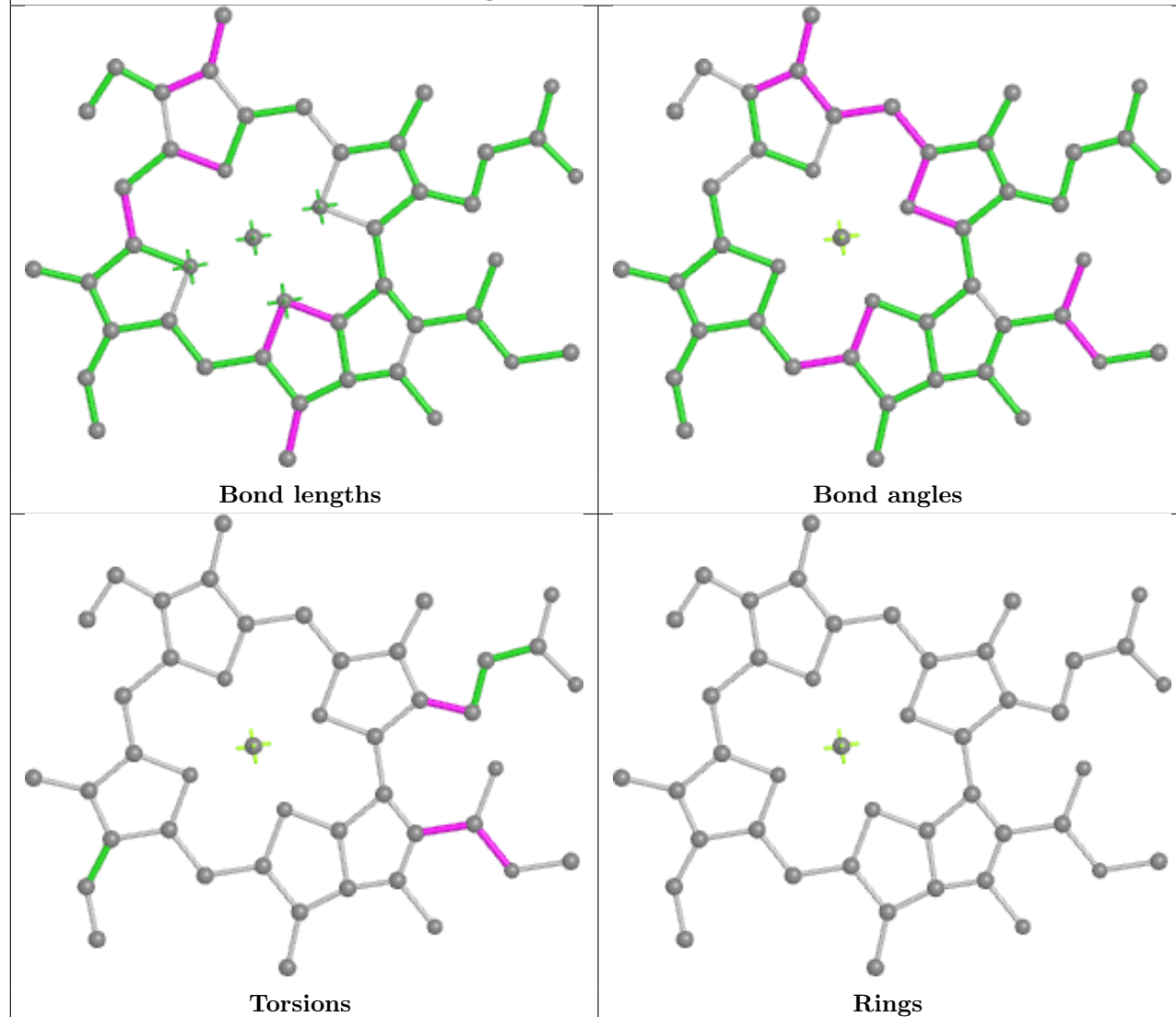
## Ligand CLA AA 828

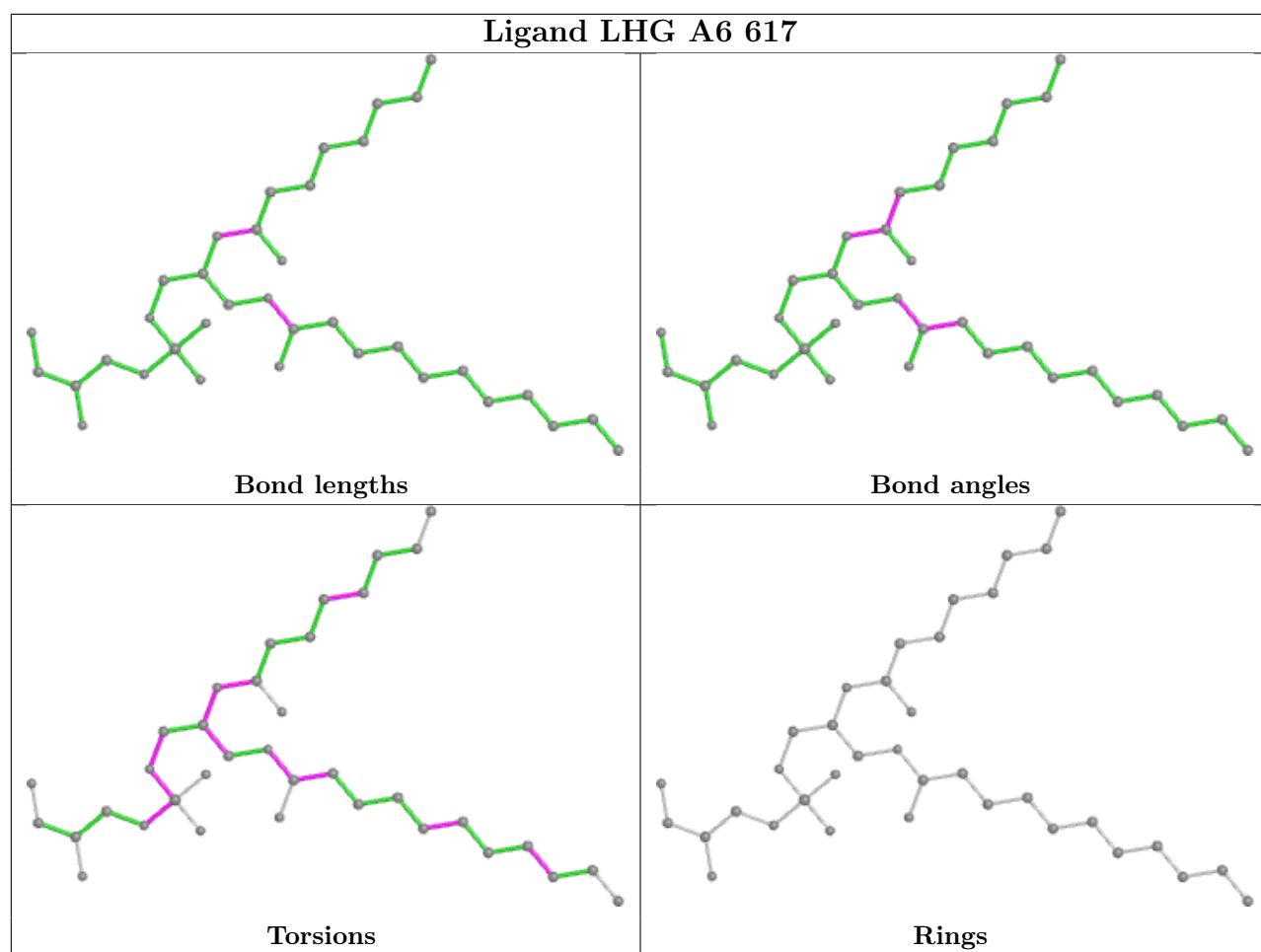


## Ligand CLA AB 840

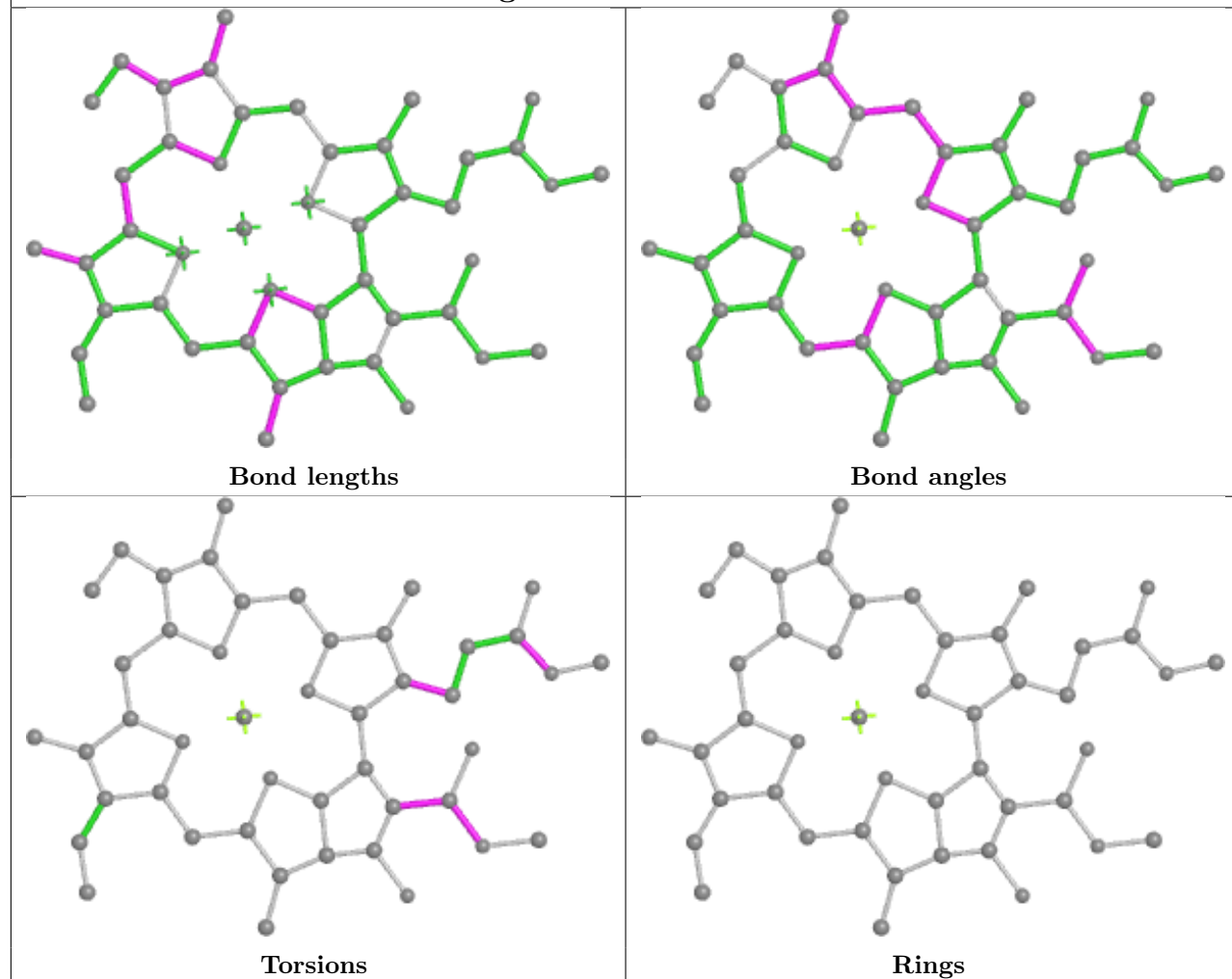


## Ligand CLA A4 312

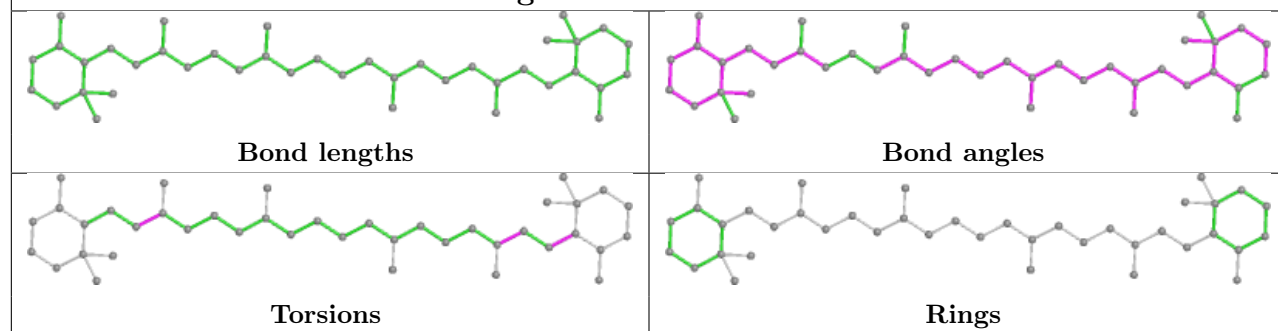


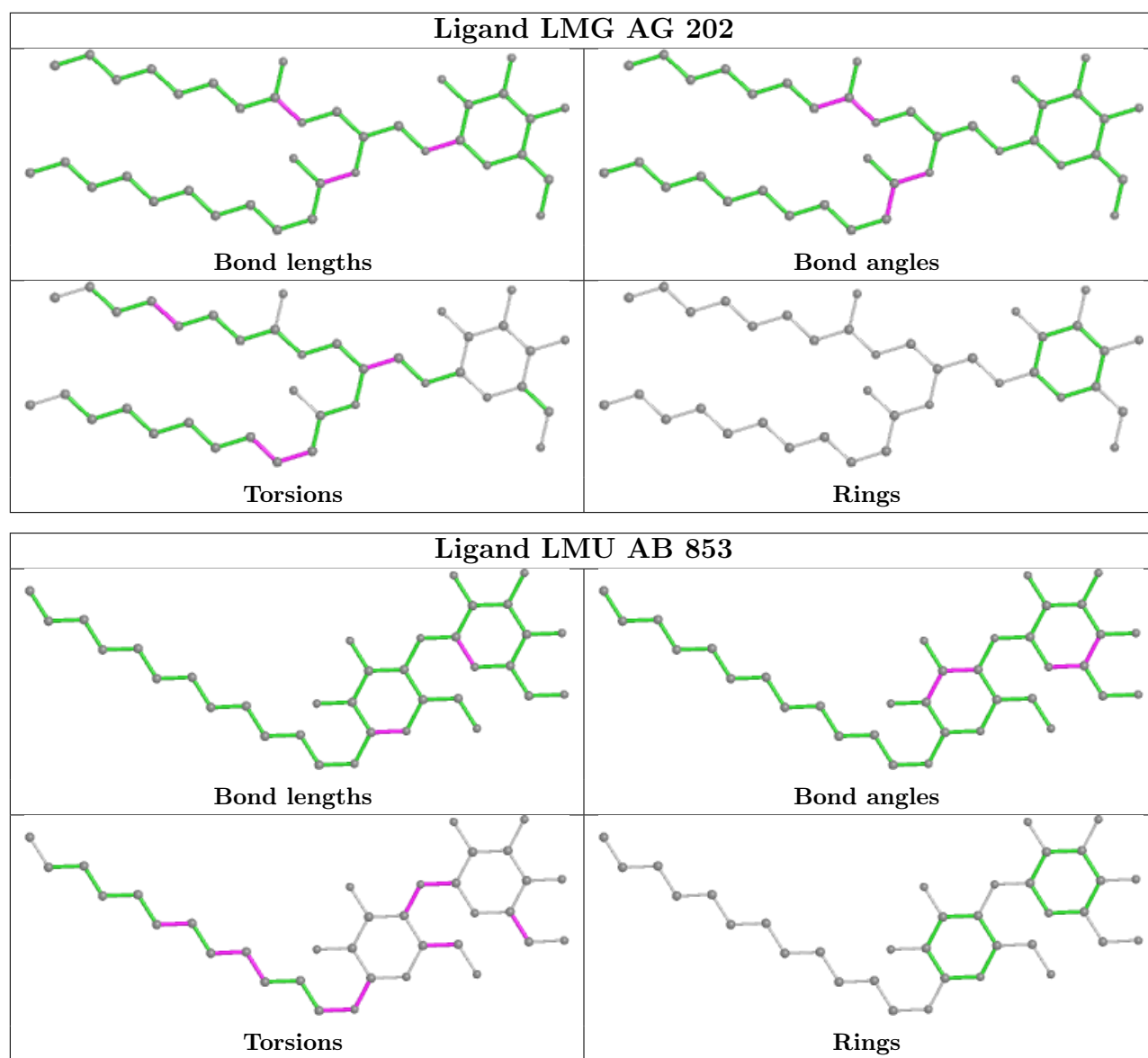


## Ligand CLA AK 204

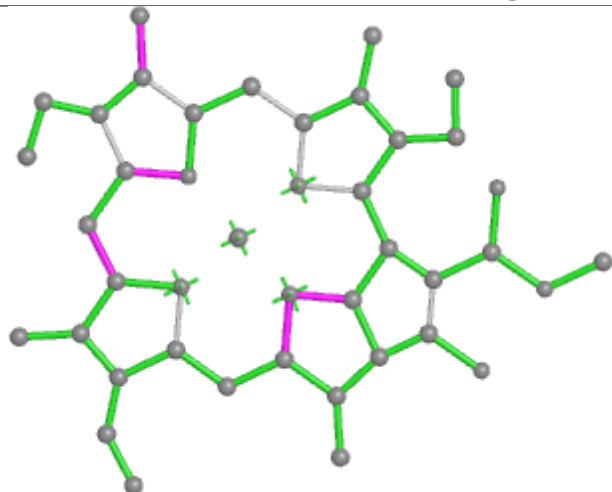


## Ligand BCR AB 849

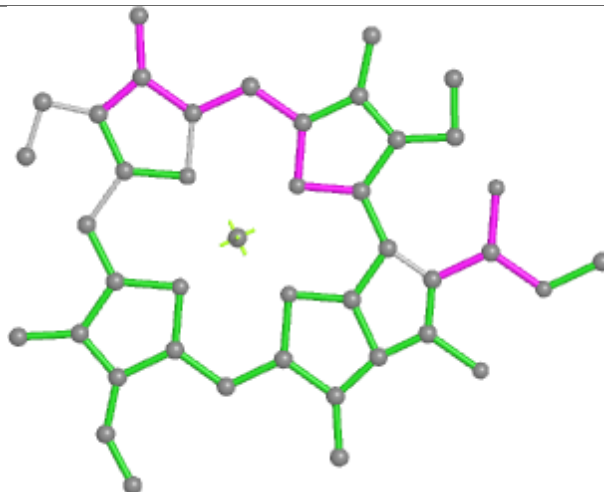




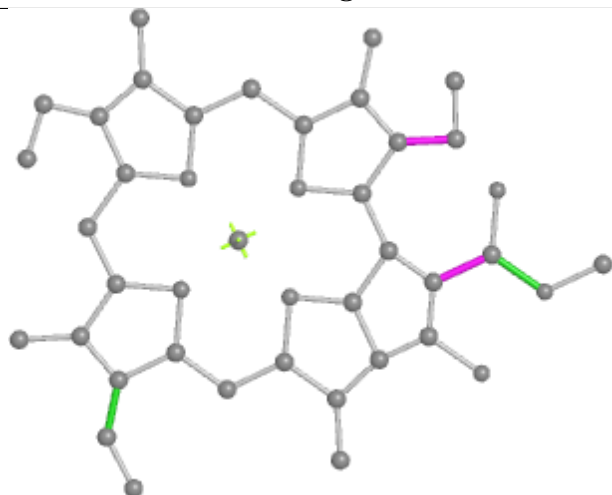
## Ligand CLA A4 309



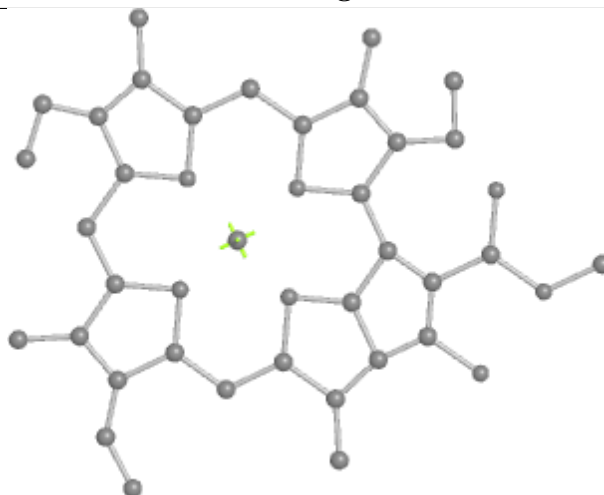
Bond lengths



Bond angles

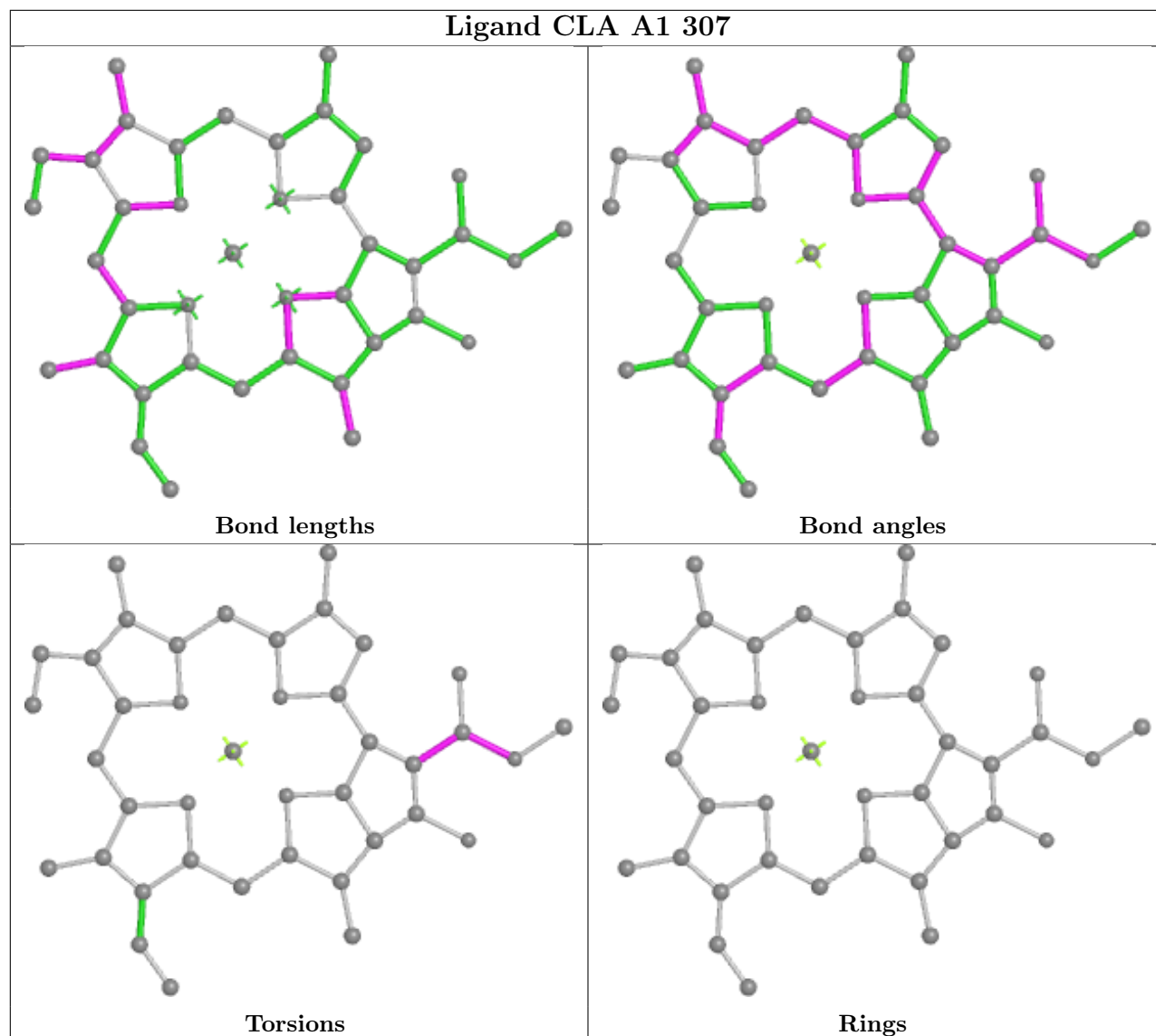


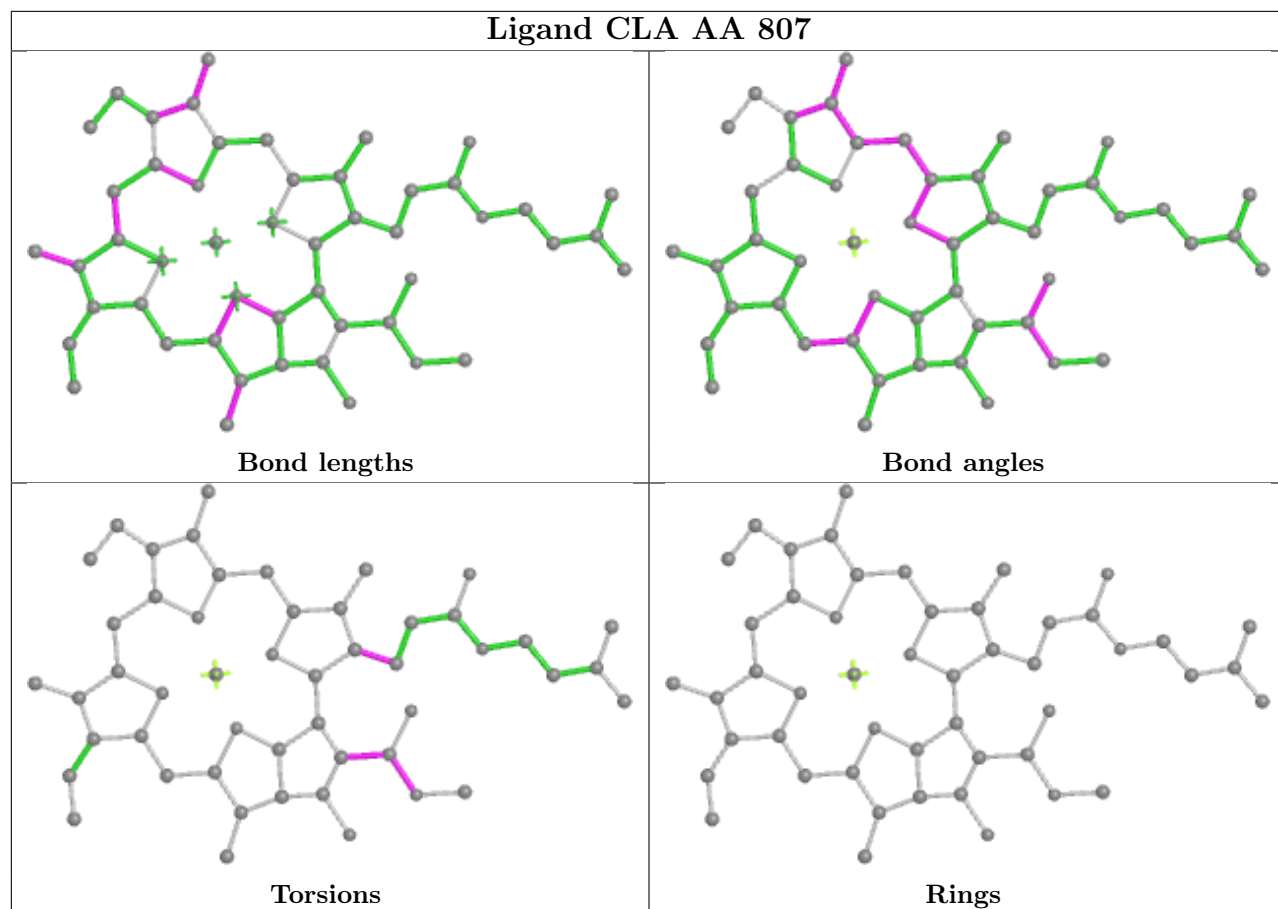
Torsions



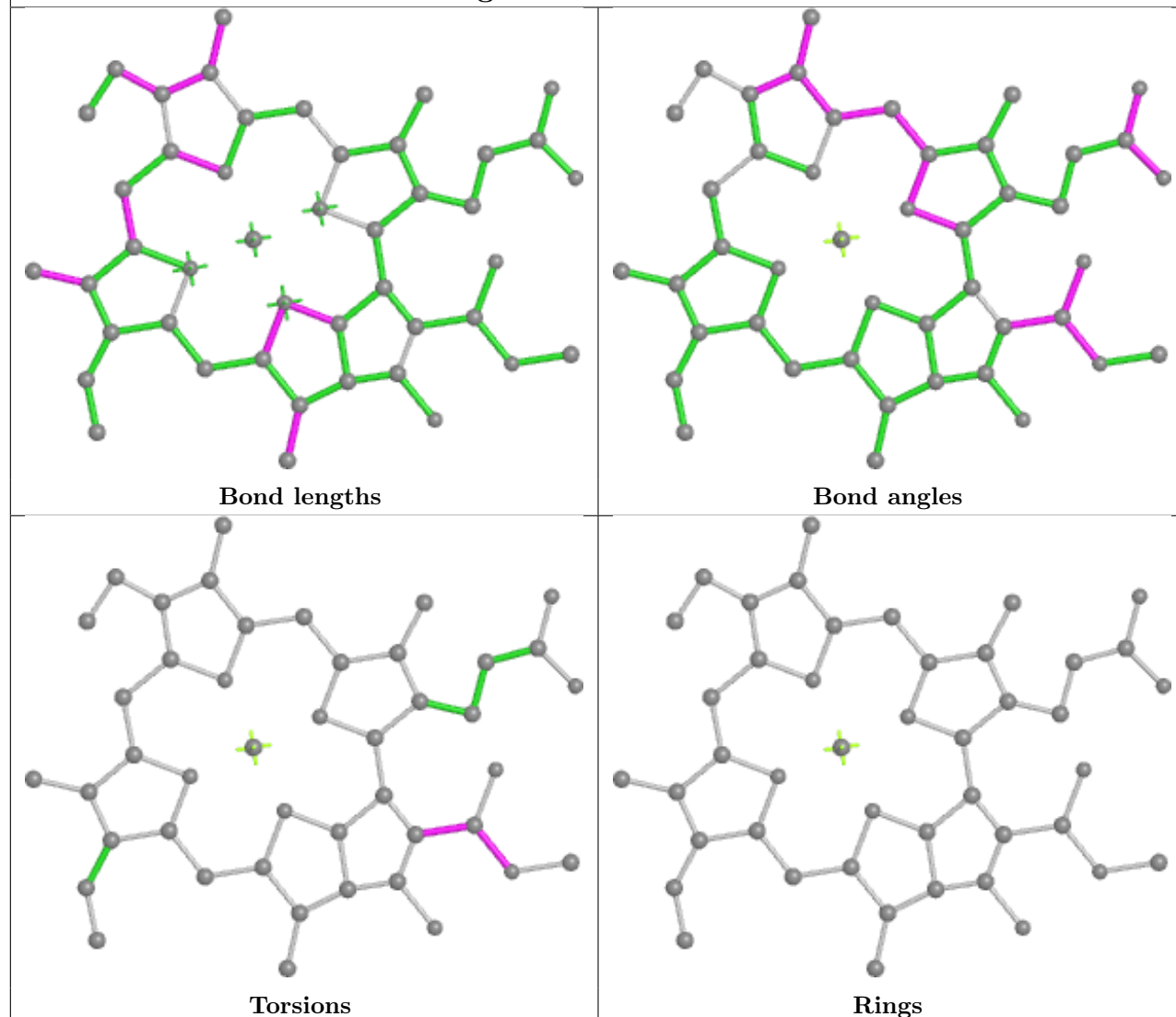
Rings

## Ligand CLA A1 307

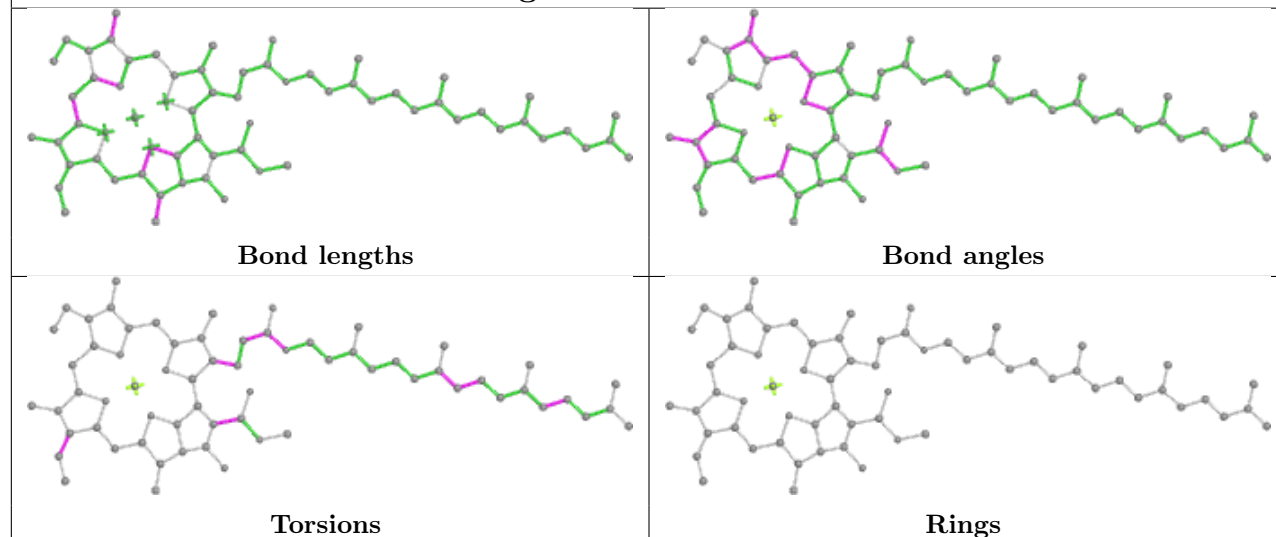




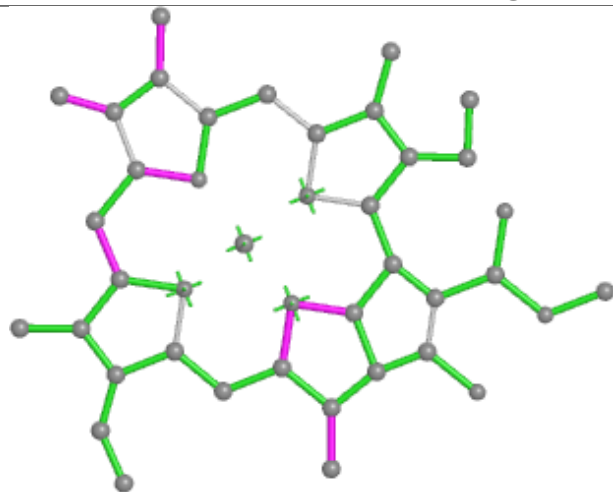
## Ligand CLA AA 814



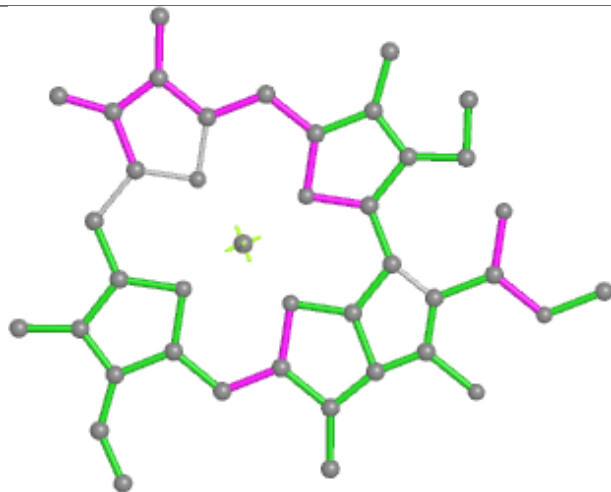
## Ligand CLA AB 806



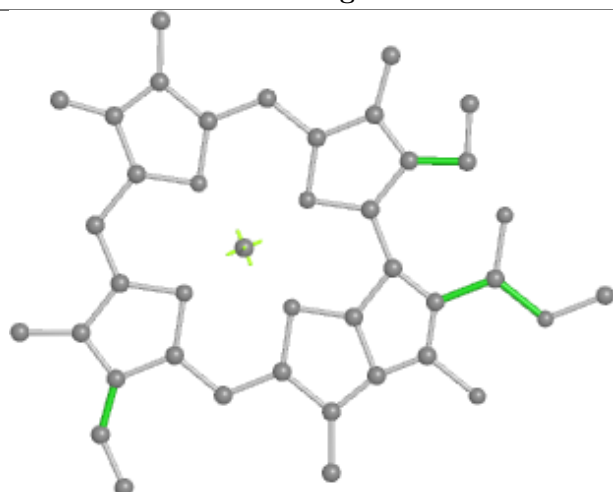
## Ligand CLA A3 306



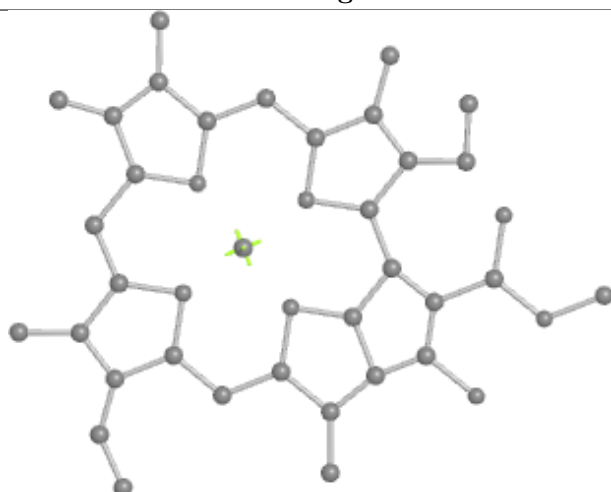
Bond lengths



Bond angles

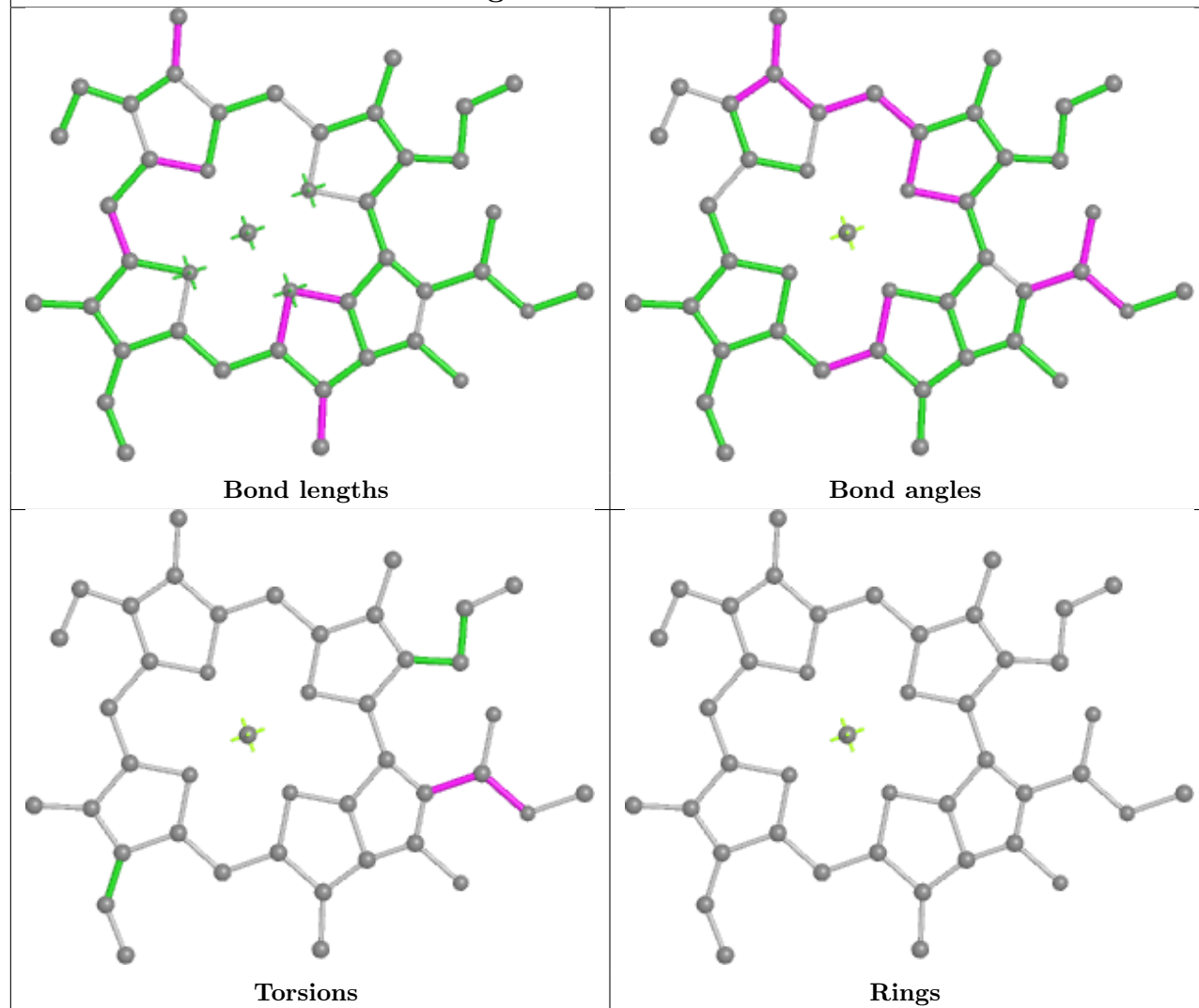


Torsions

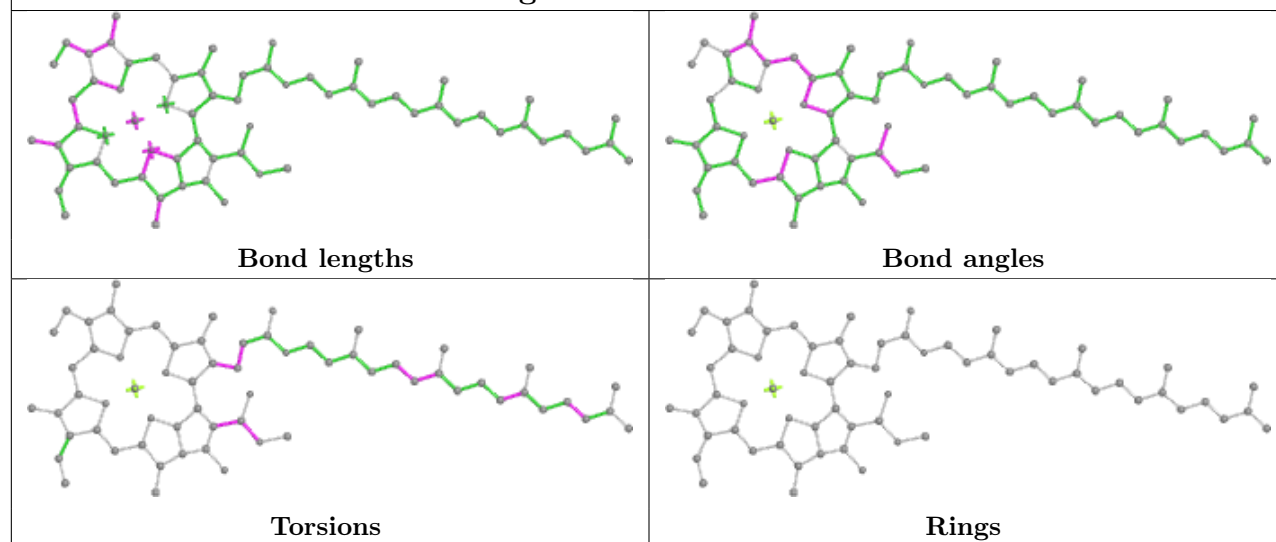


Rings

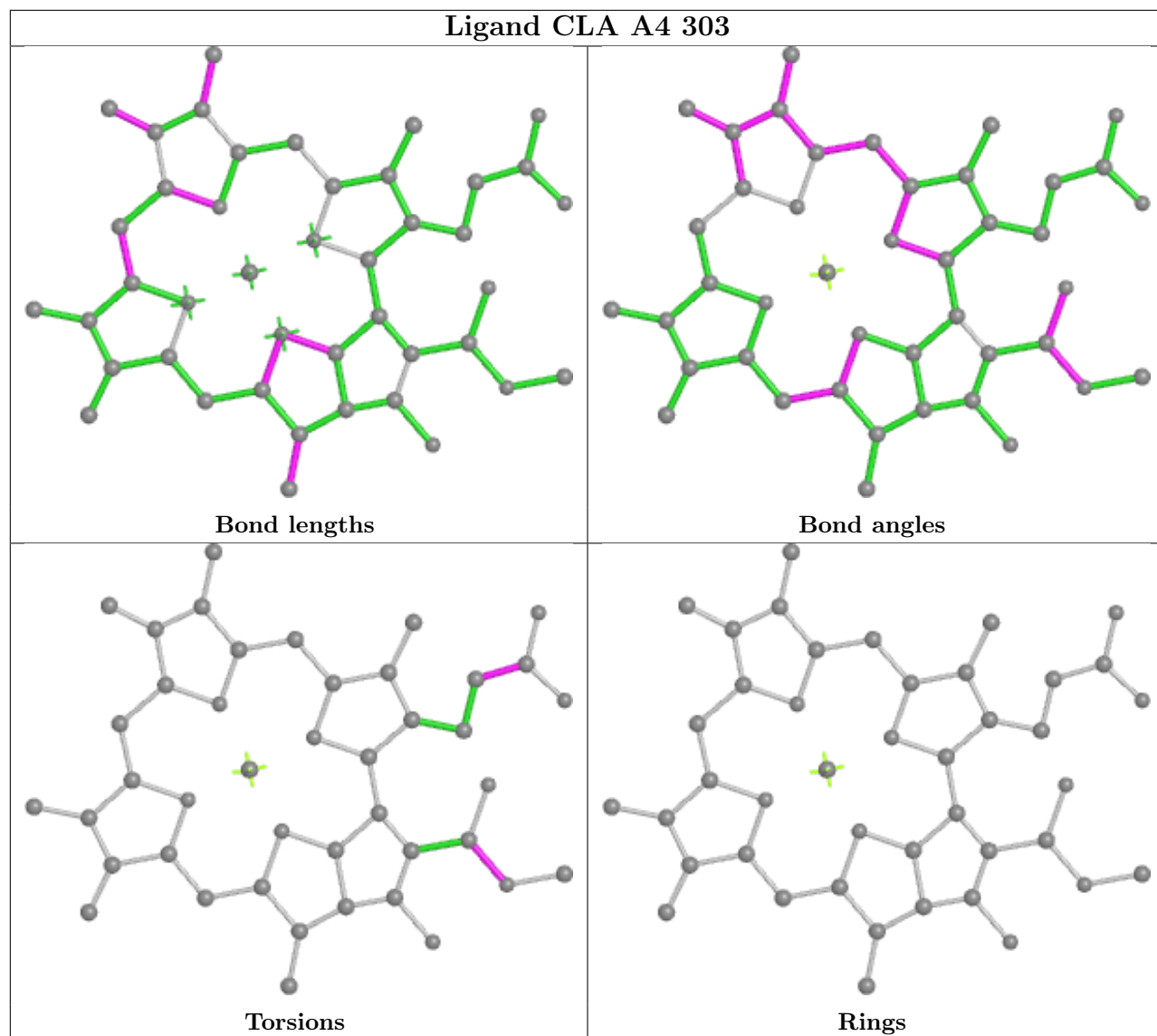
## Ligand CLA AB 813



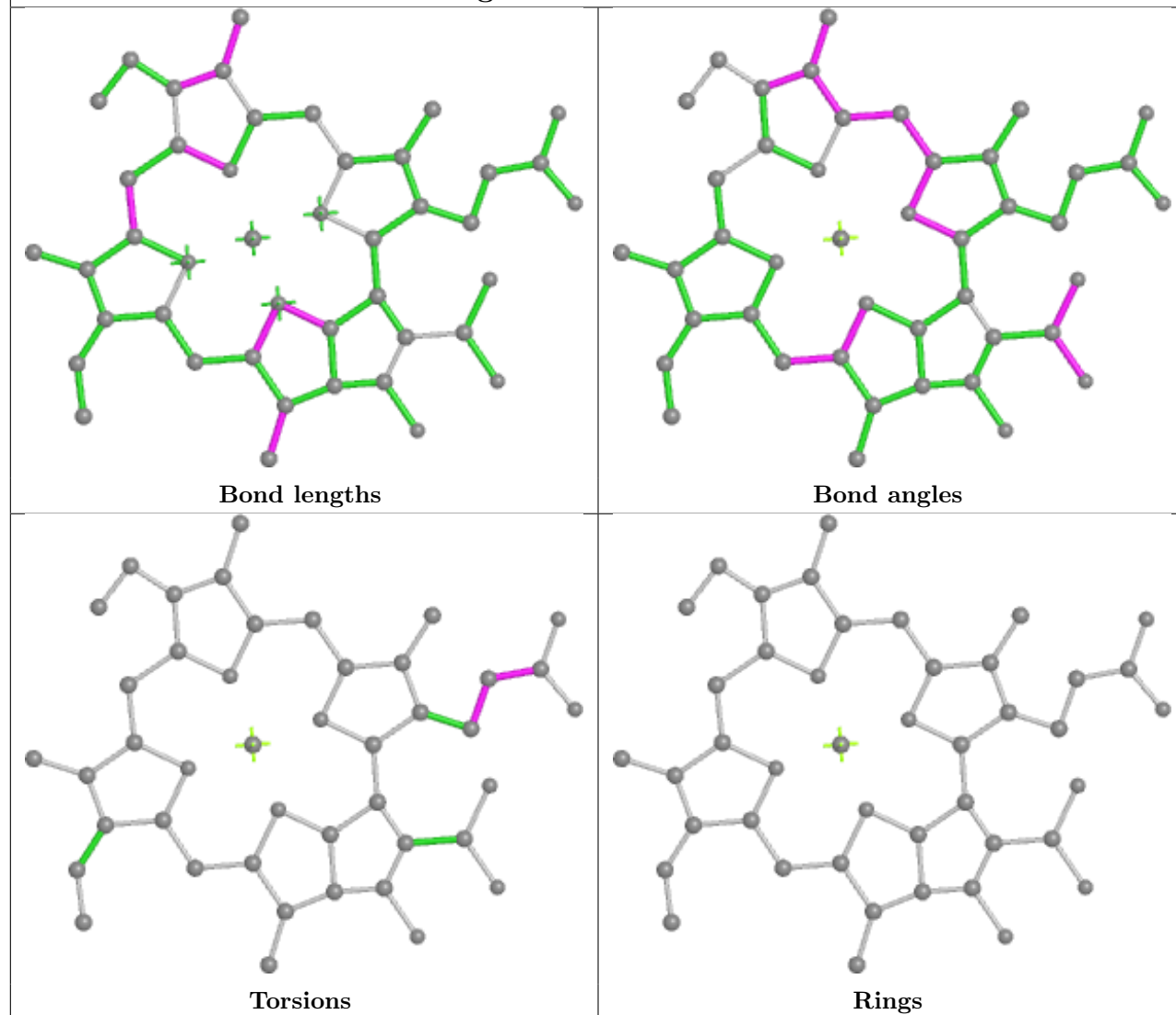
## Ligand CLA AB 814



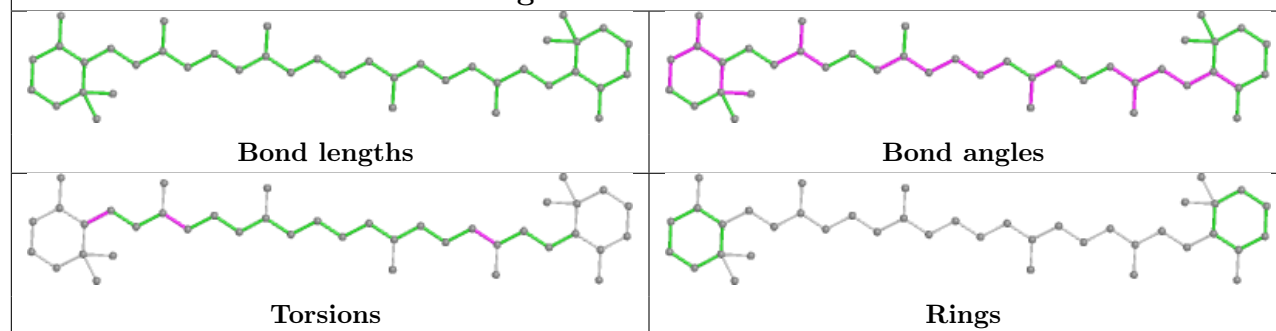
## Ligand CLA A4 303



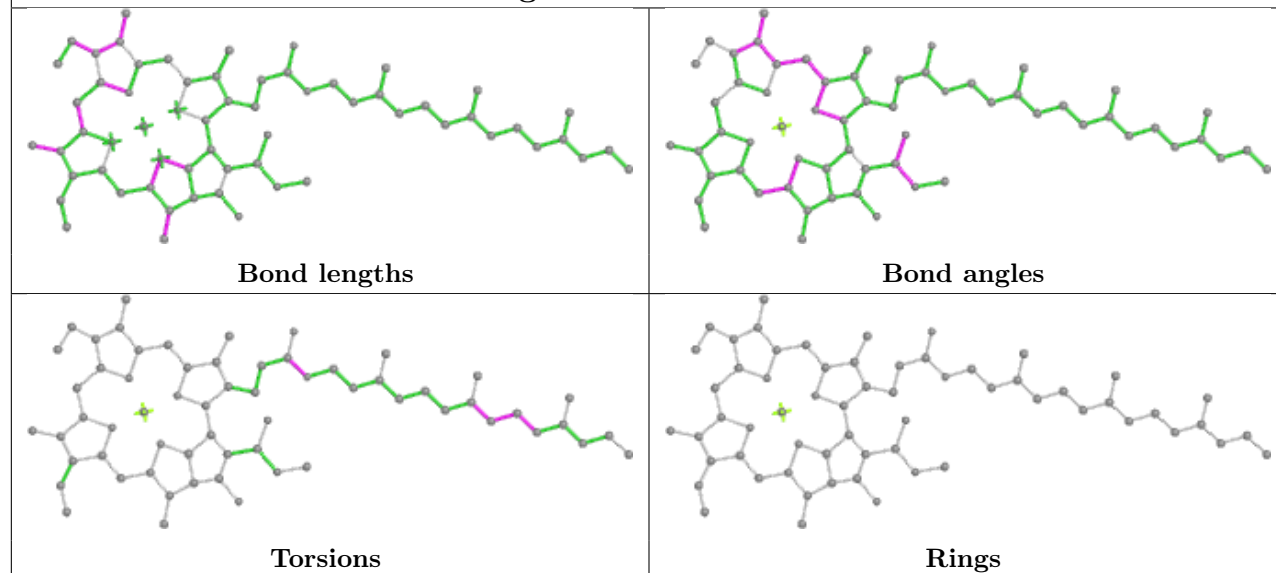
## Ligand CLA AG 201



## Ligand BCR AB 846



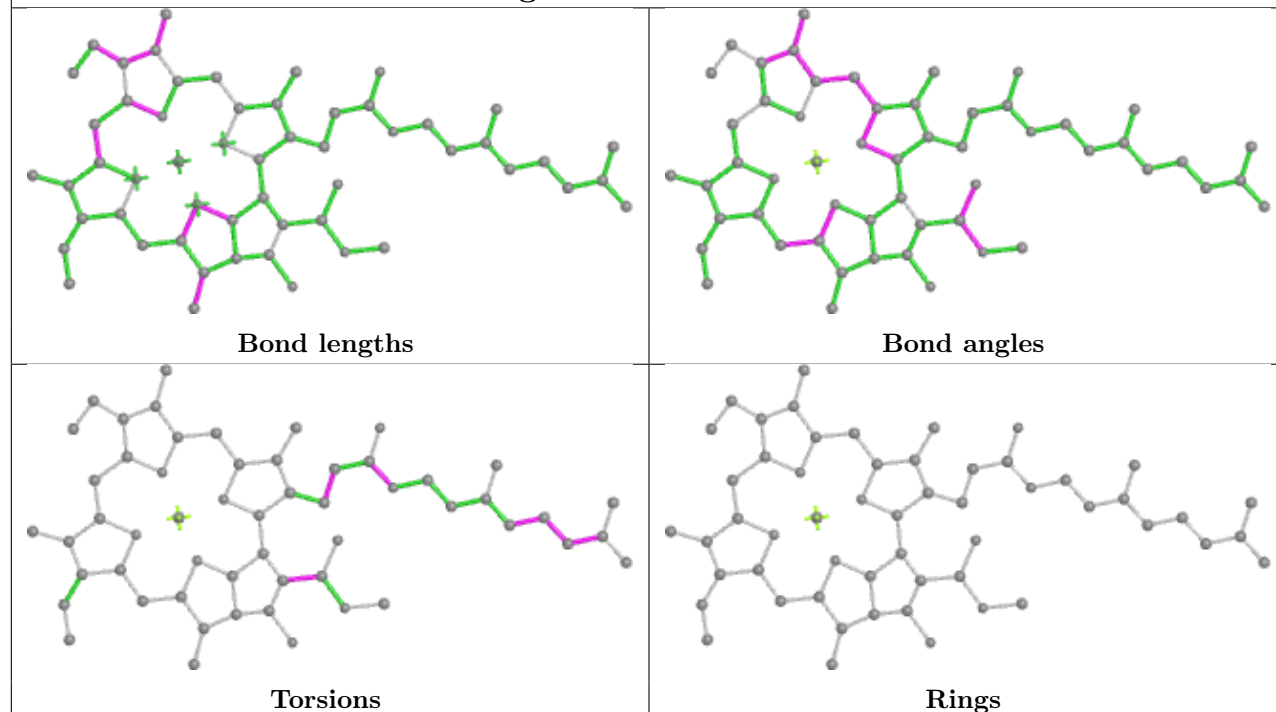
## Ligand CLA AB 826

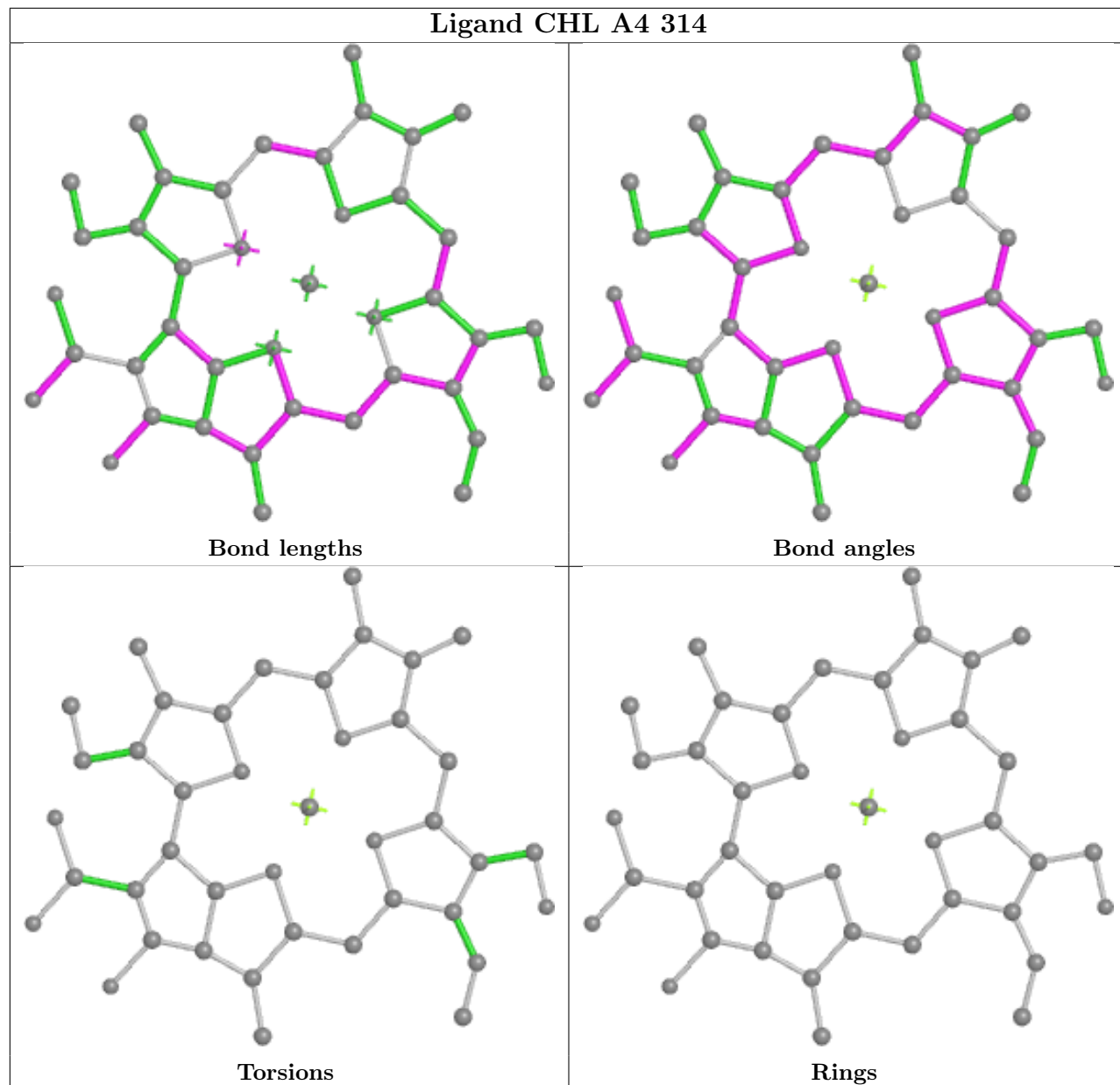
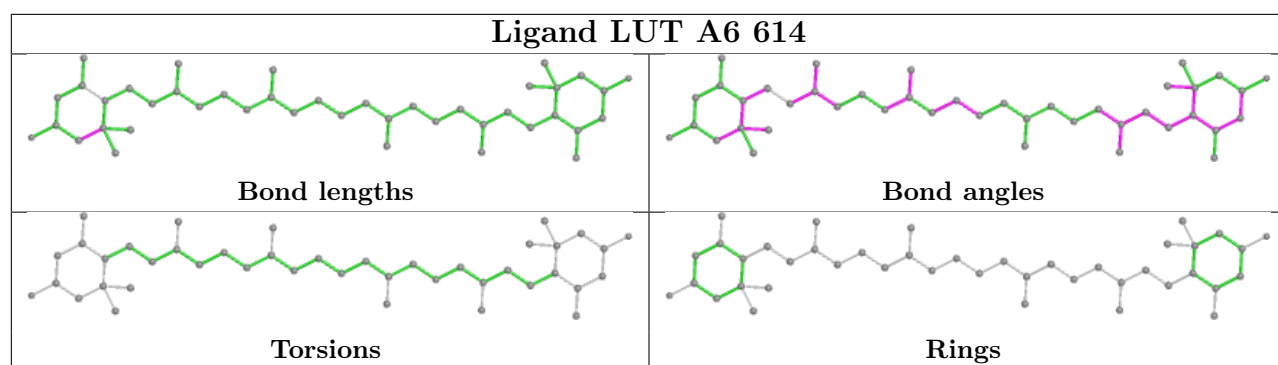


## Ligand LUT A1 317

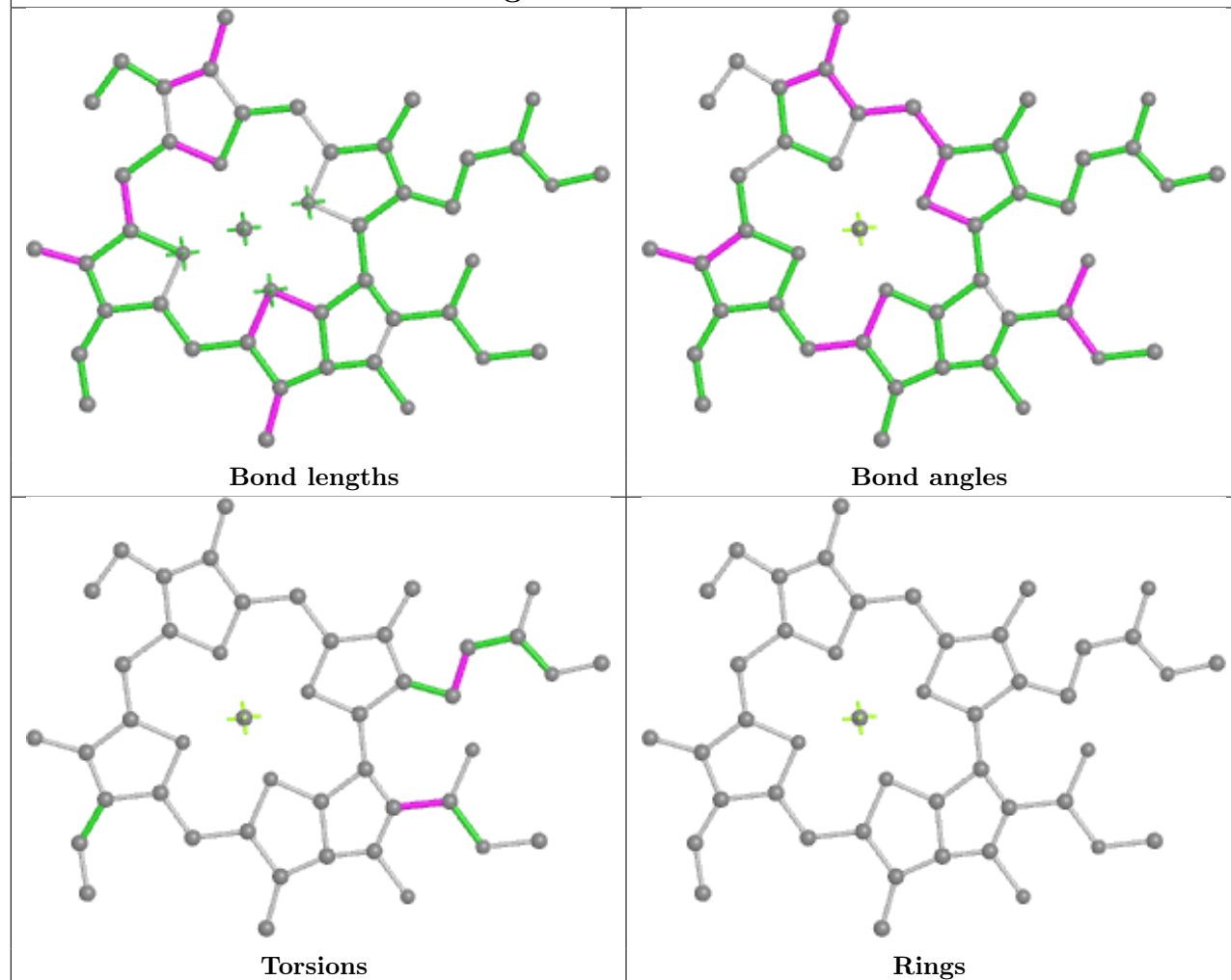


## Ligand CLA AB 817

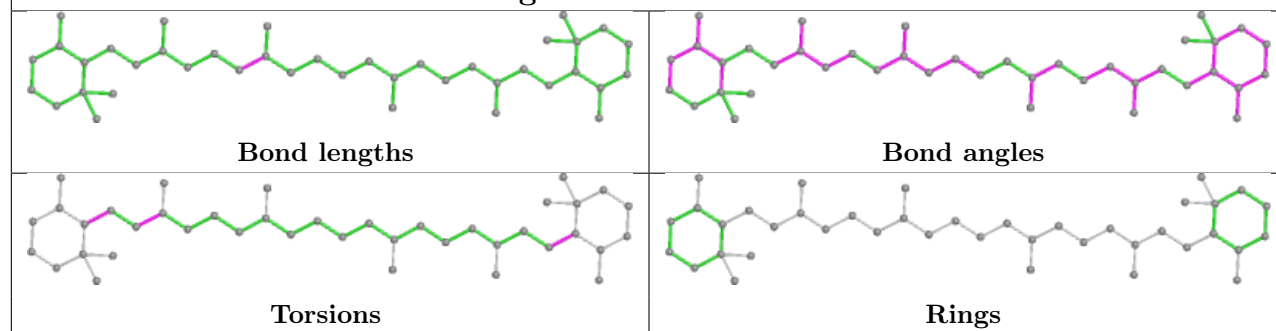




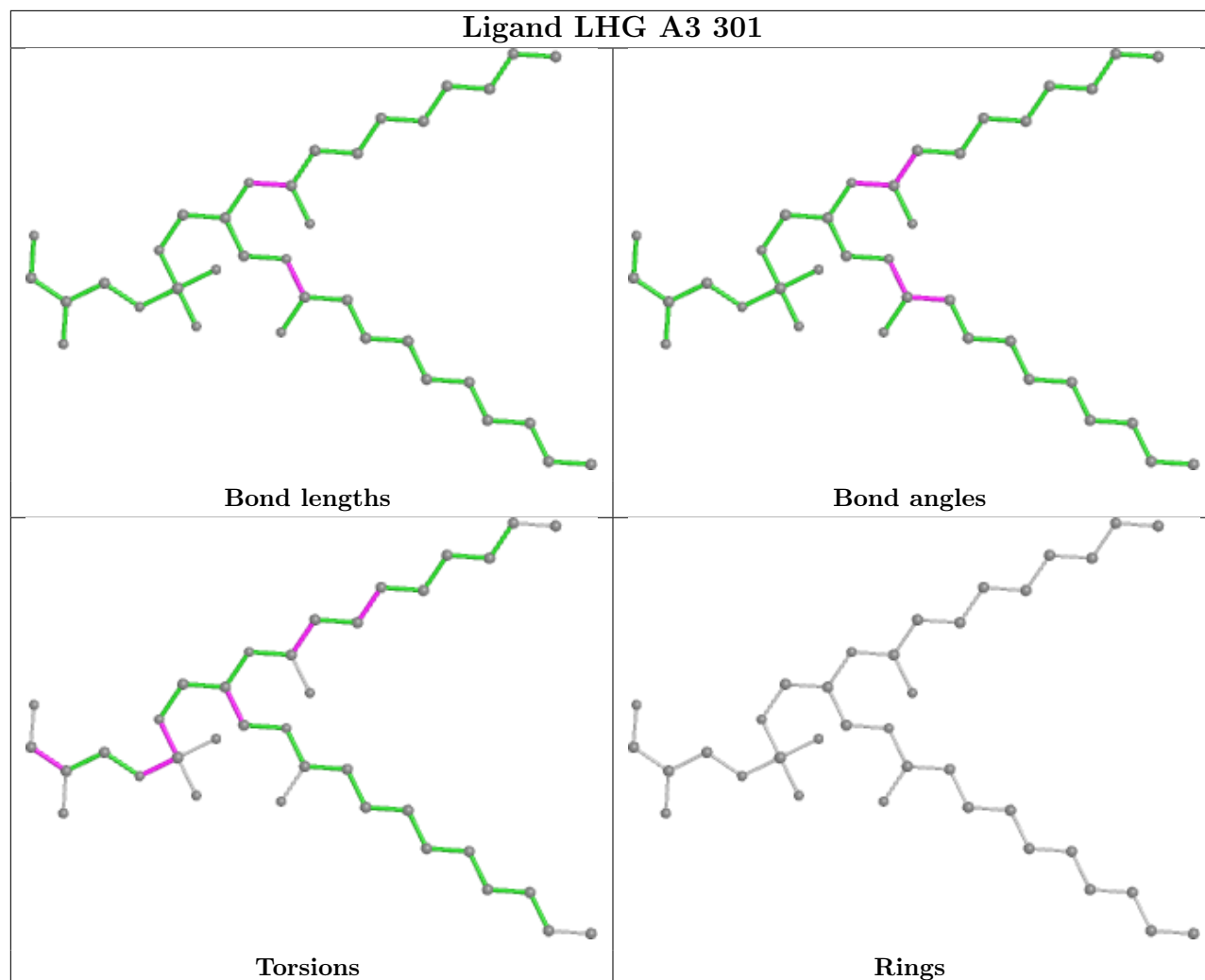
## Ligand CLA A6 601



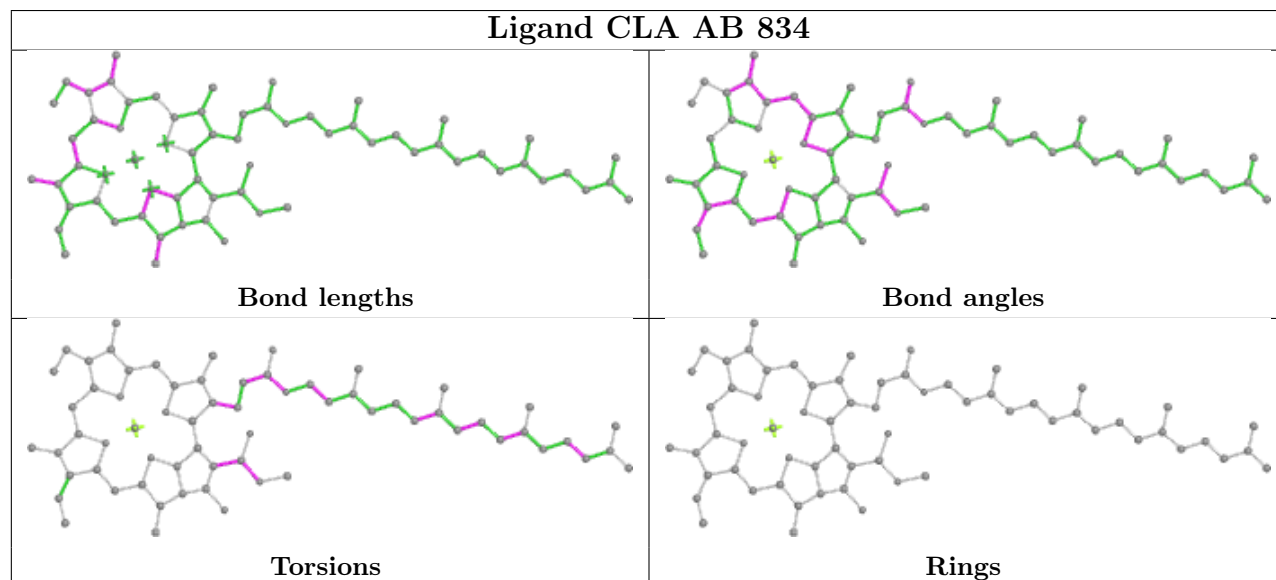
## Ligand BCR AL 306



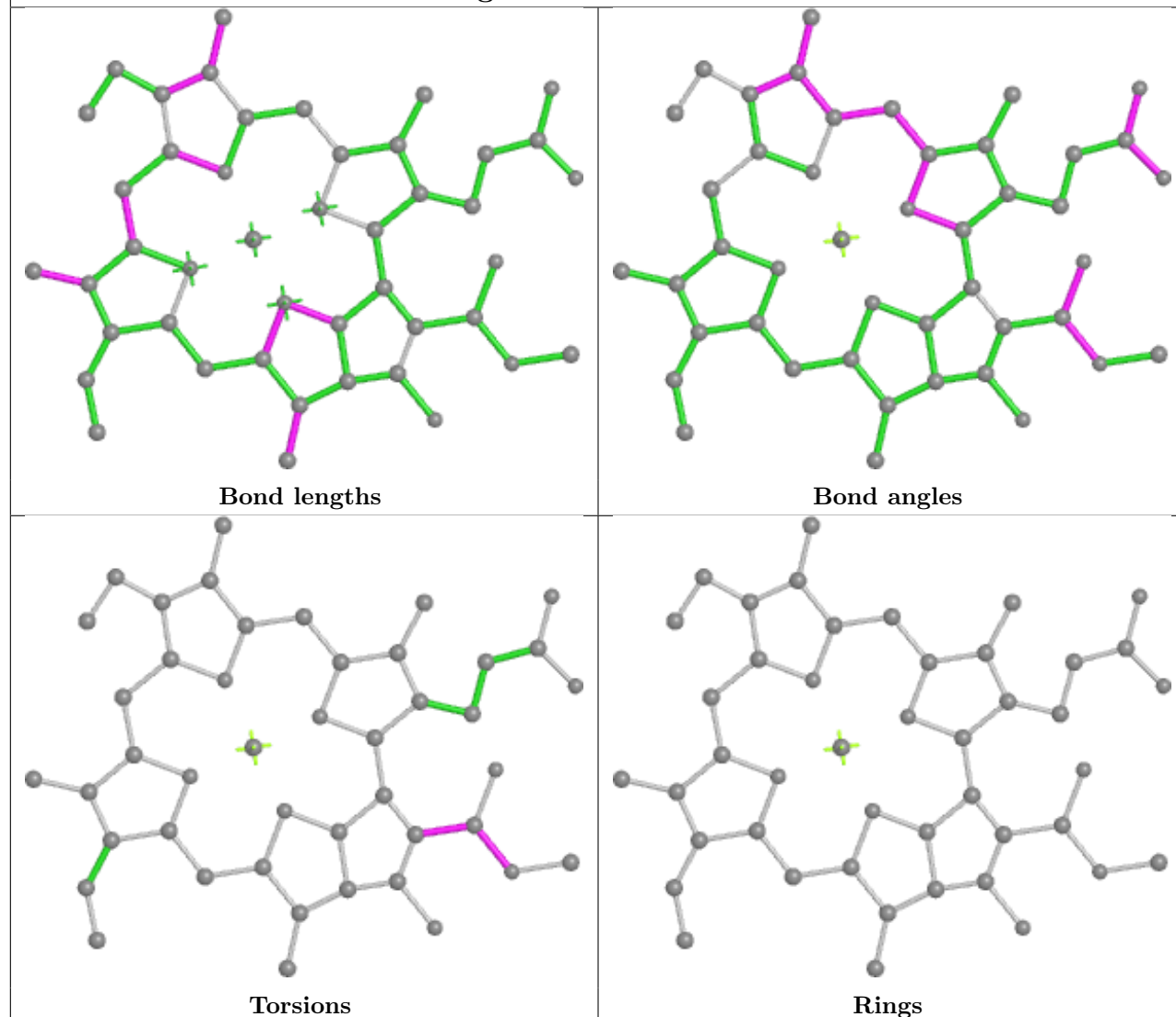
## Ligand LHG A3 301



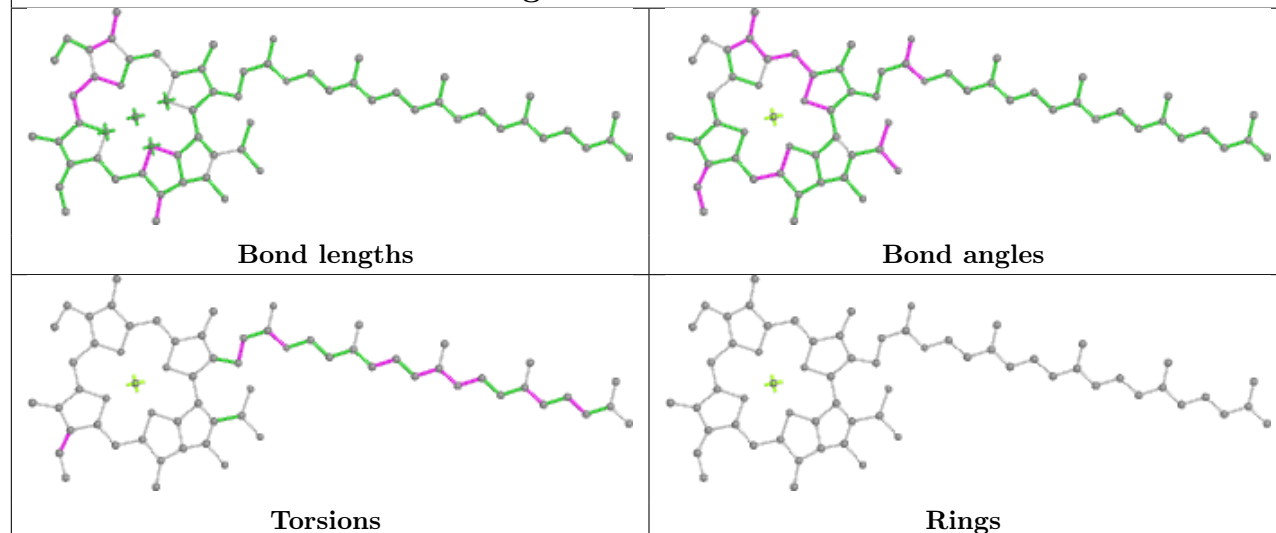
## Ligand CLA AB 834

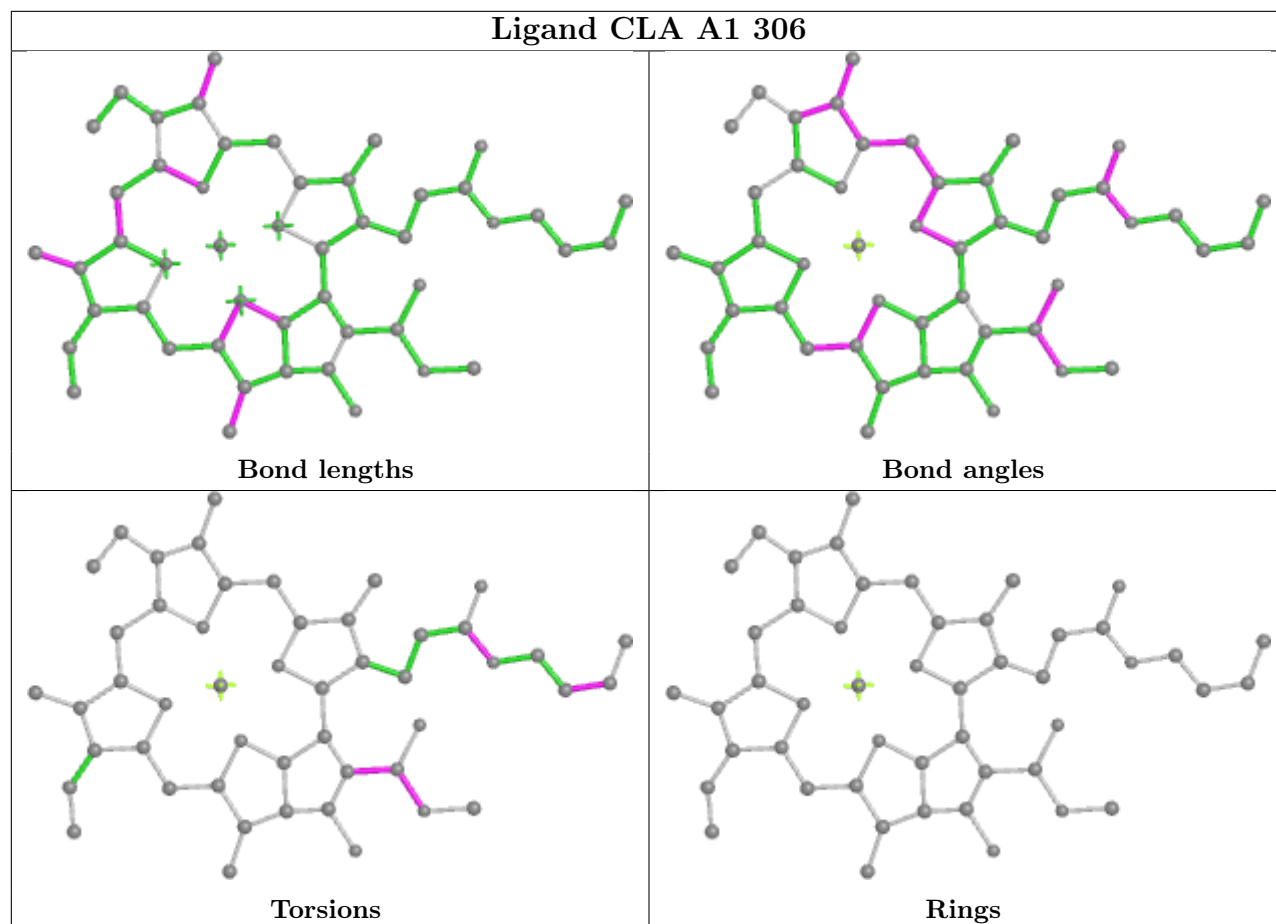
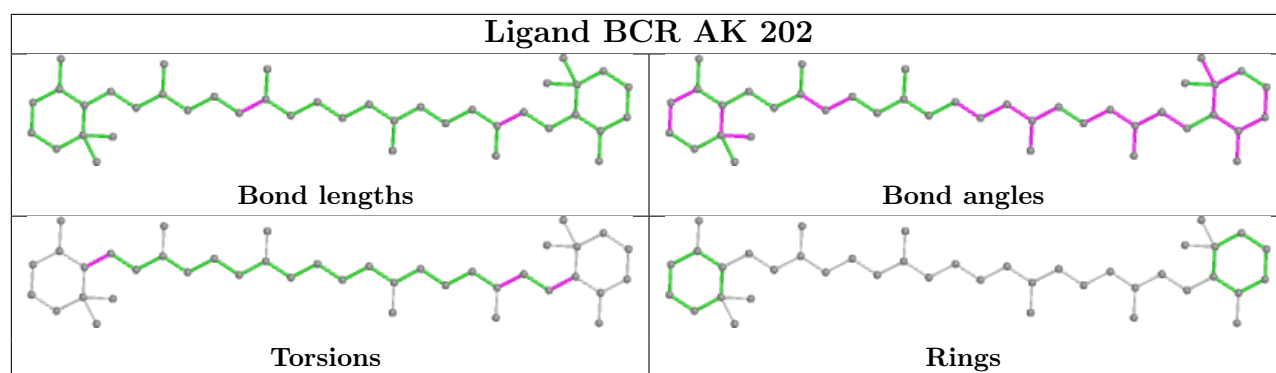


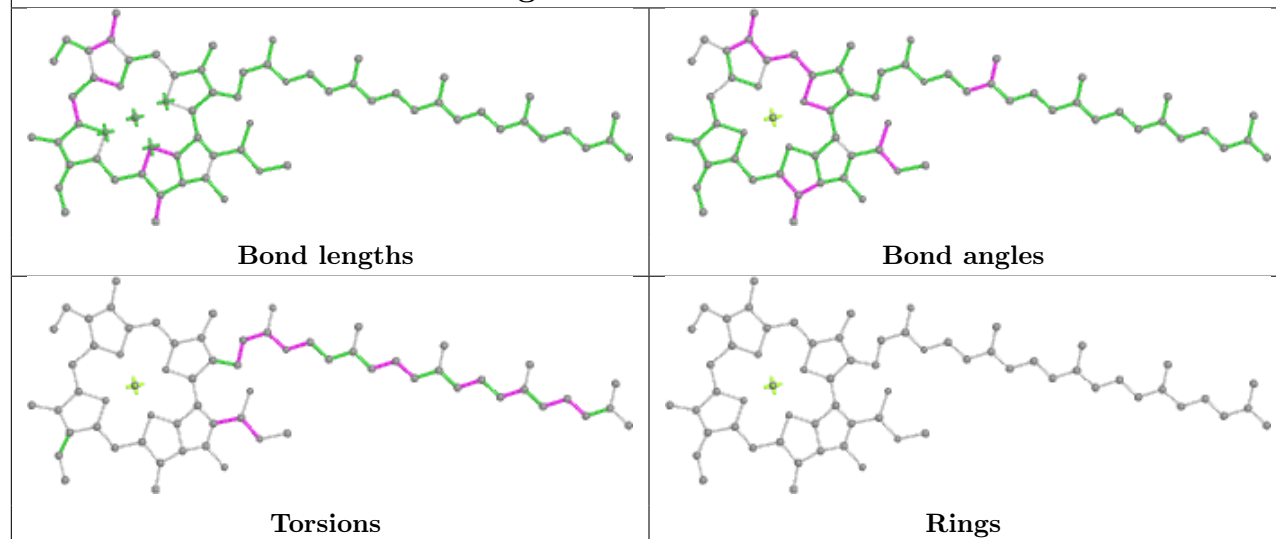
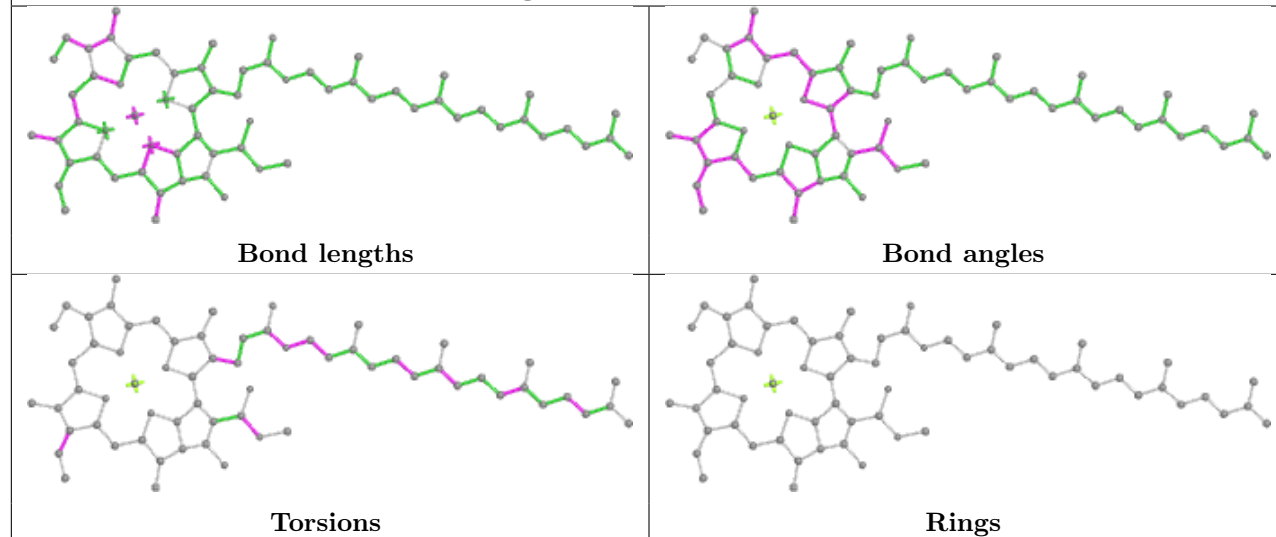
## Ligand CLA AA 820



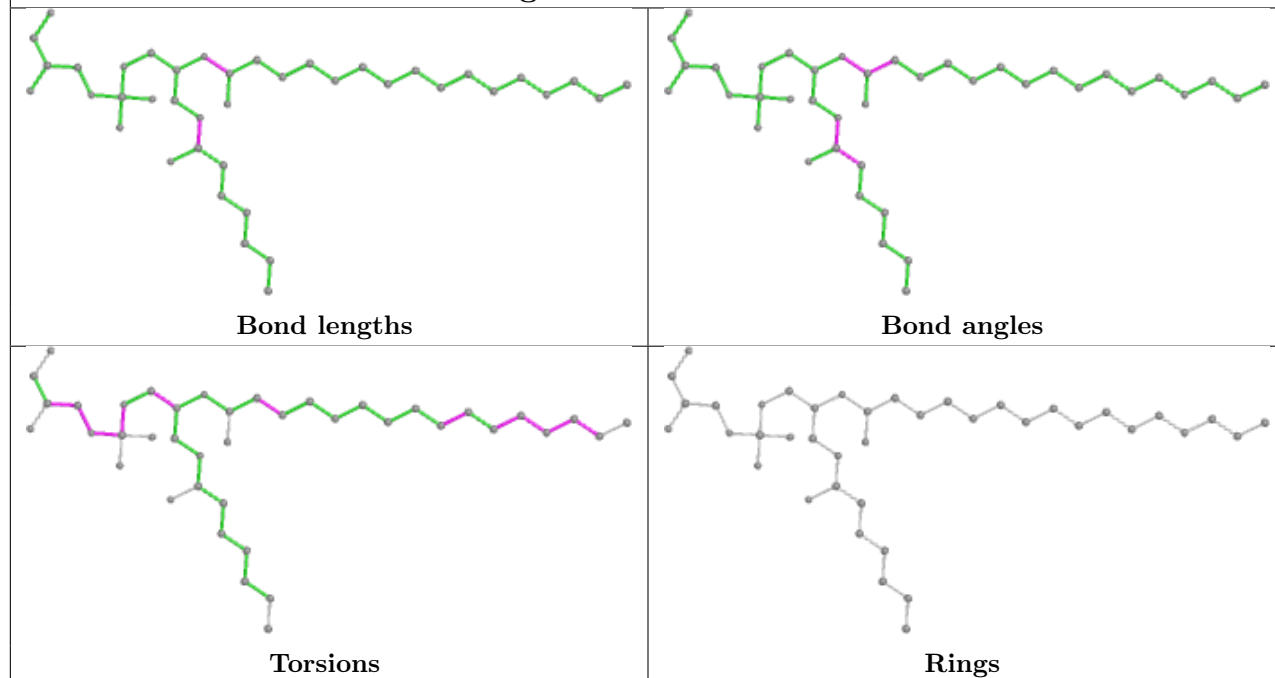
## Ligand CLA A1 314



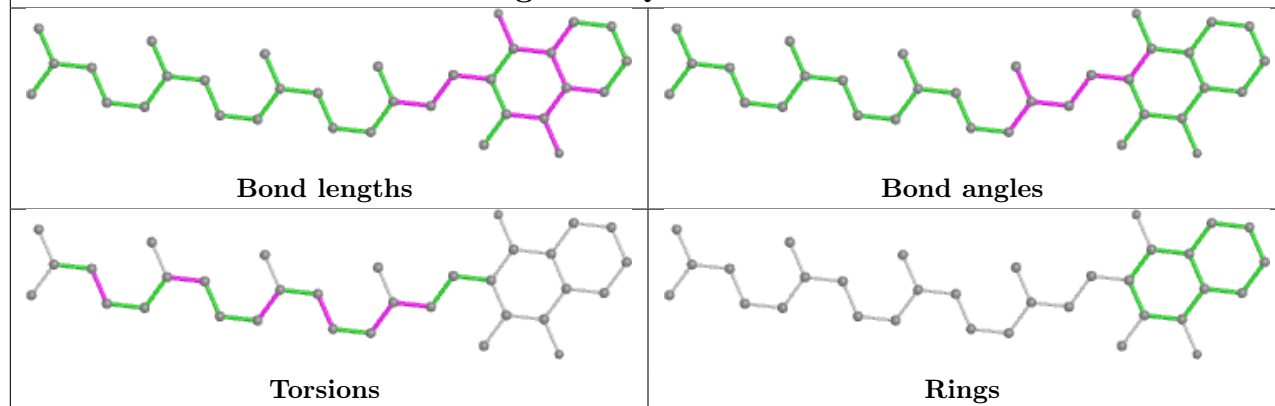


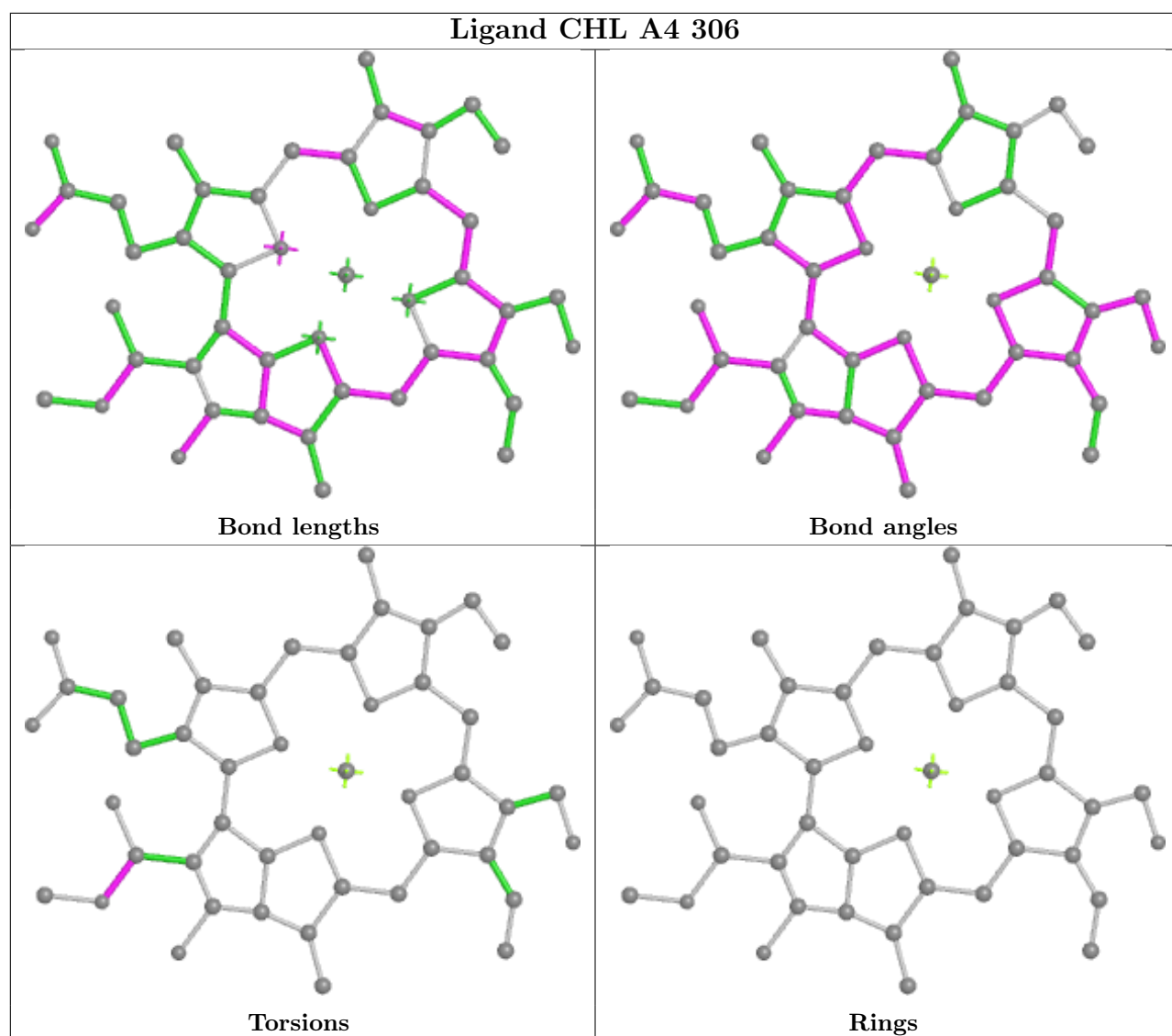
**Ligand CLA AA 833****Ligand CLA AB 804**

## Ligand LHG AJ 104

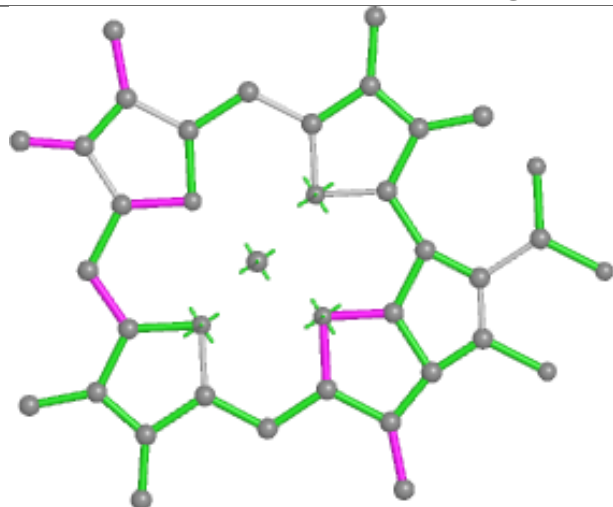


## Ligand PQN AB 843

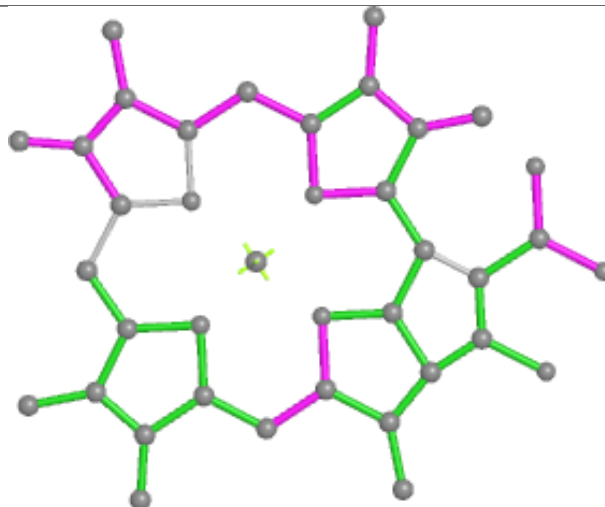




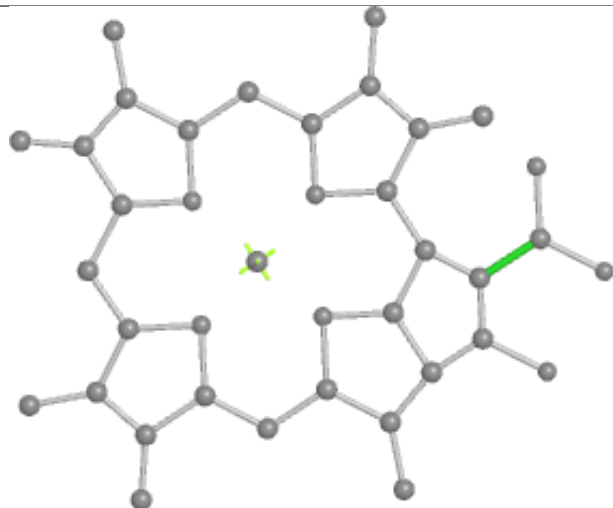
## Ligand CLA A1 315



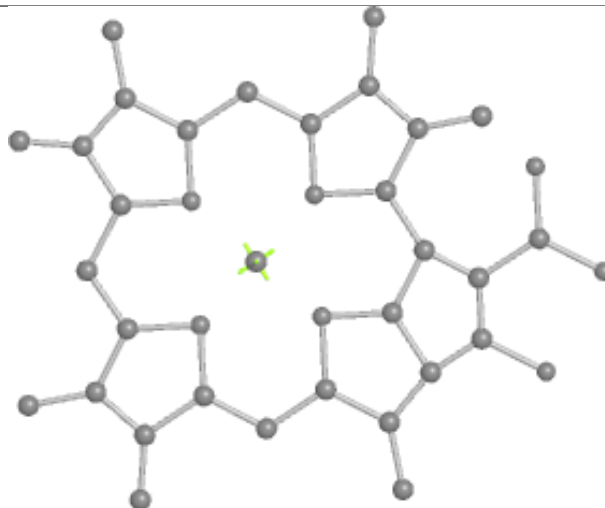
Bond lengths



Bond angles

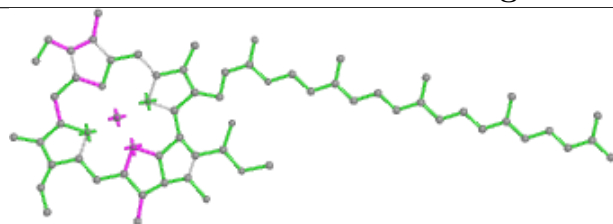


Torsions

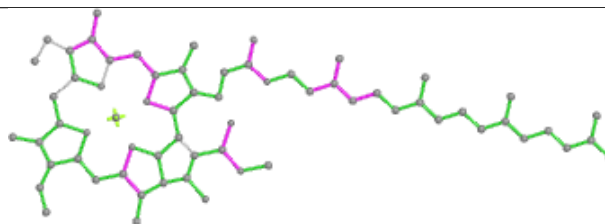


Rings

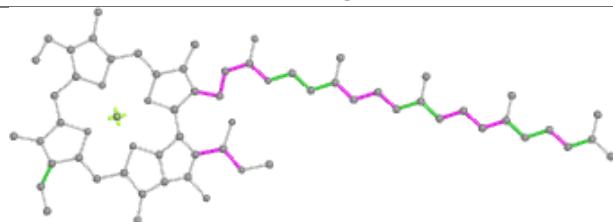
## Ligand CLA AA 829



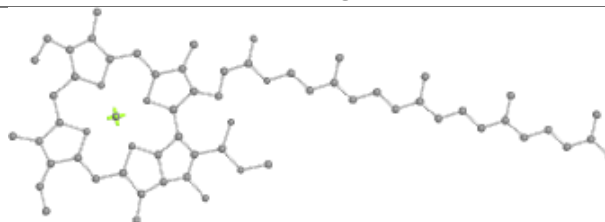
Bond lengths



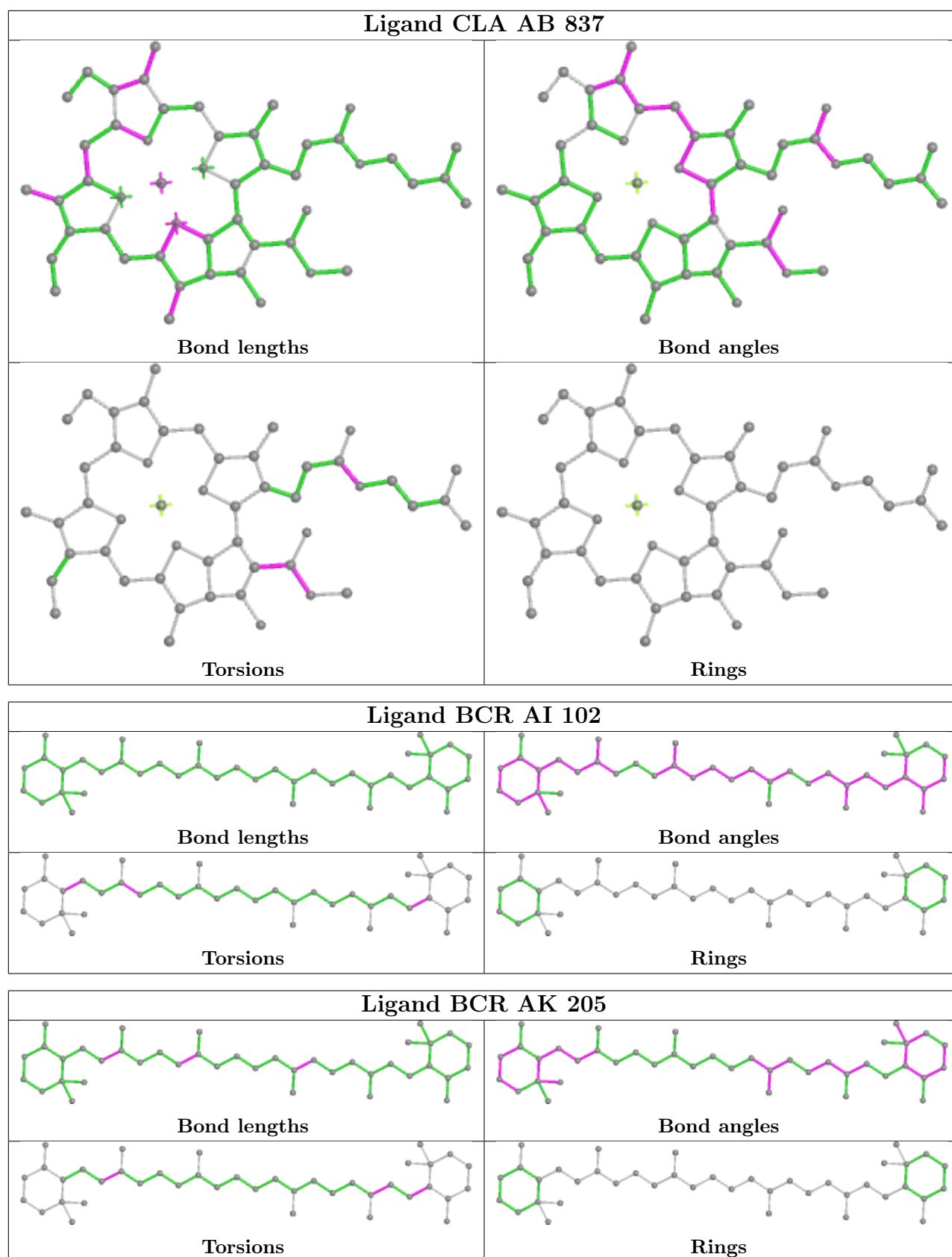
Bond angles



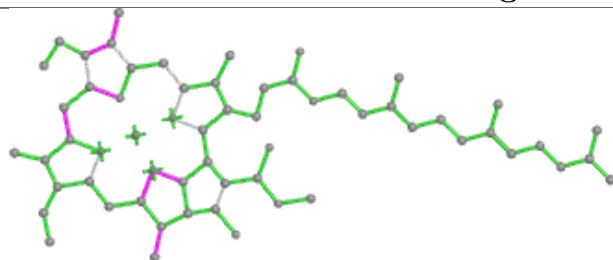
Torsions



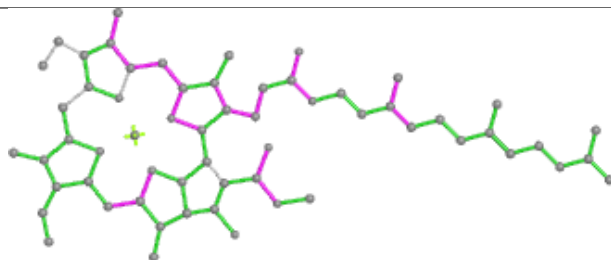
Rings



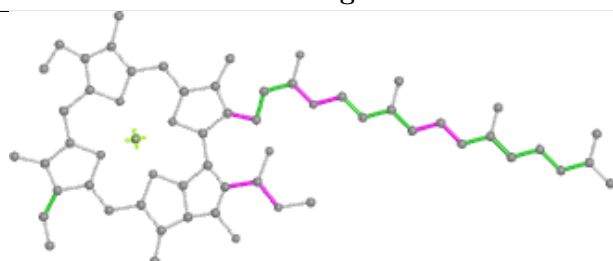
## Ligand CLA AH 201



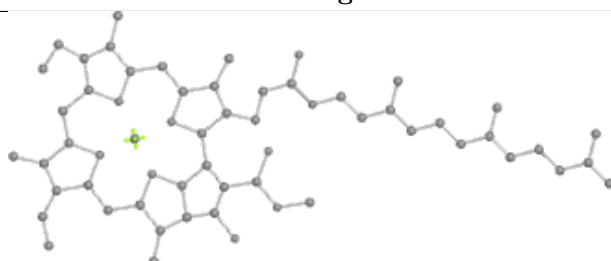
Bond lengths



Bond angles

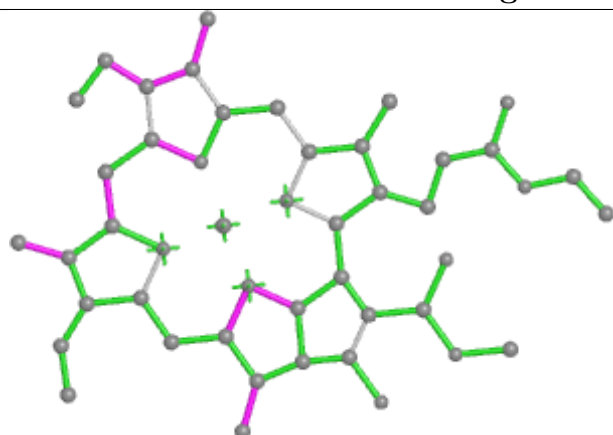


Torsions

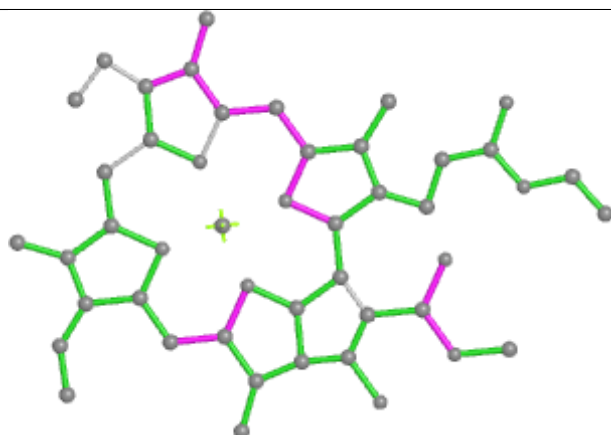


Rings

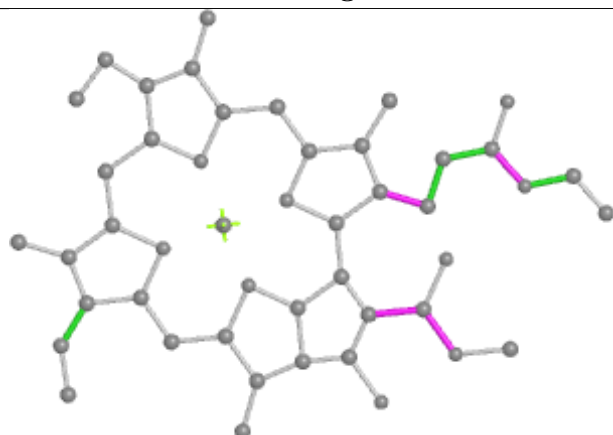
## Ligand CLA AA 831



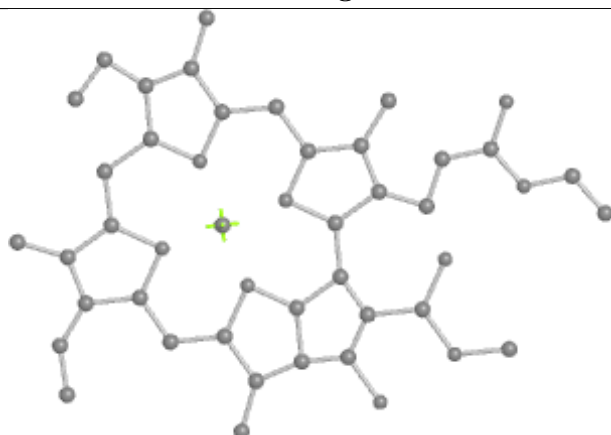
Bond lengths



Bond angles

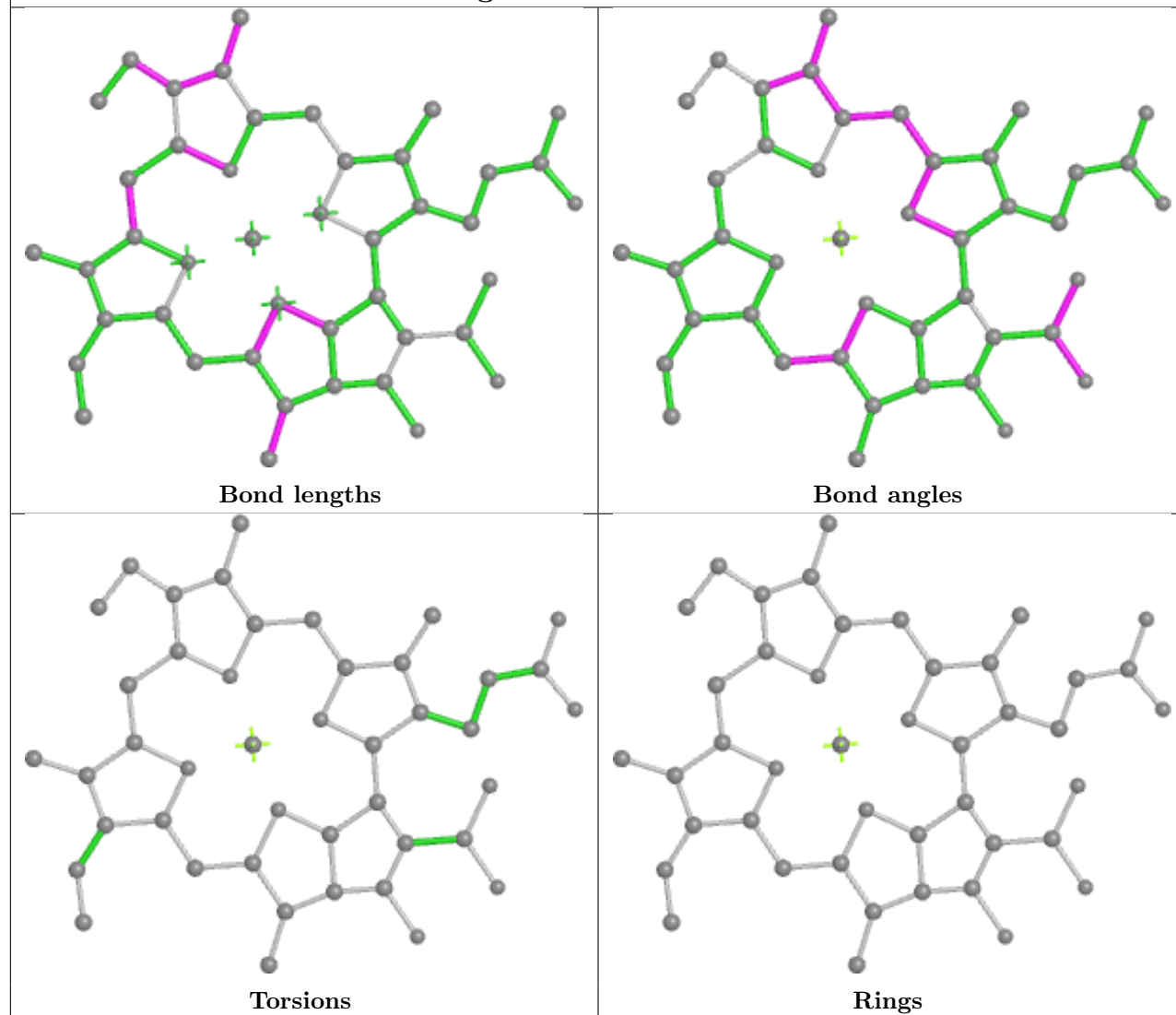


Torsions

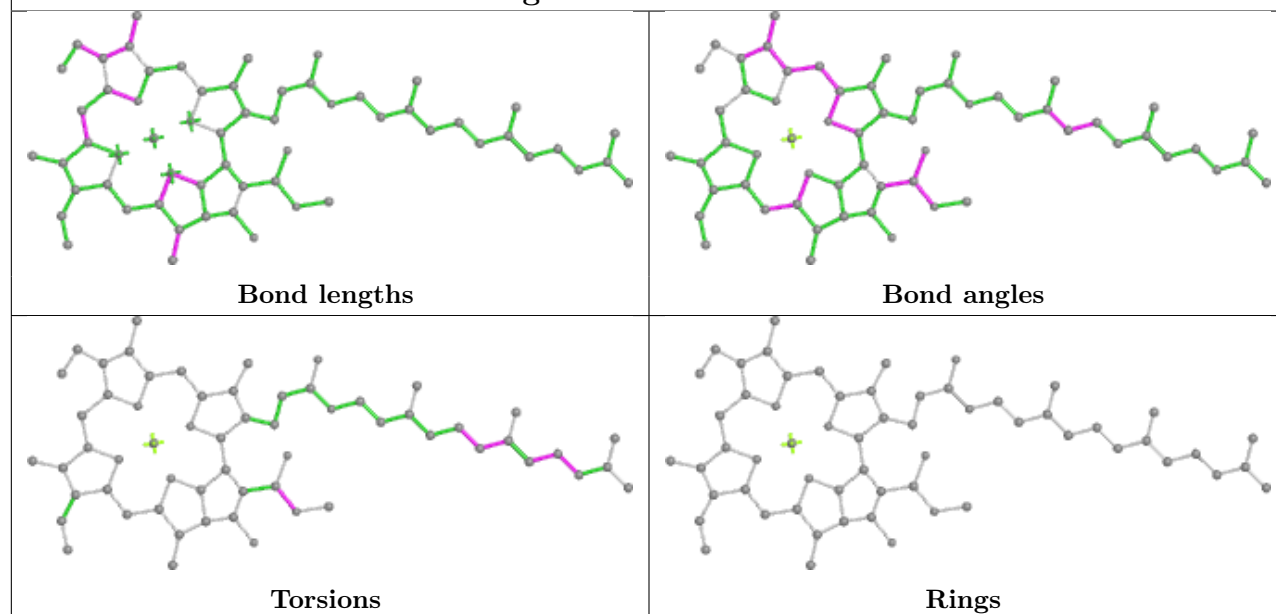


Rings

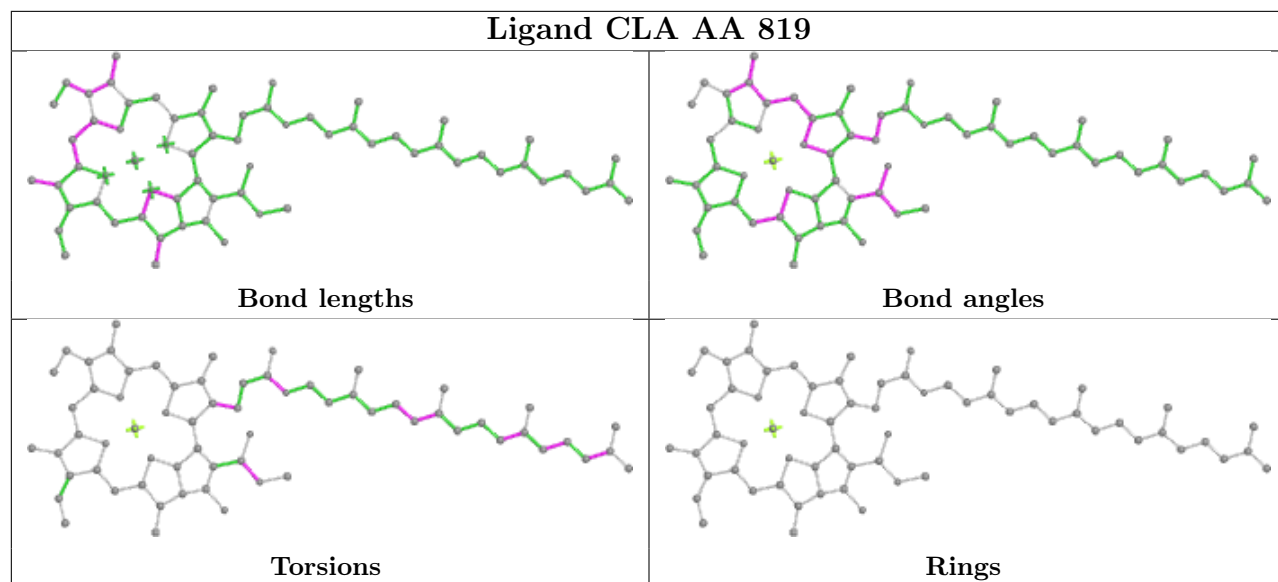
## Ligand CLA AA 835



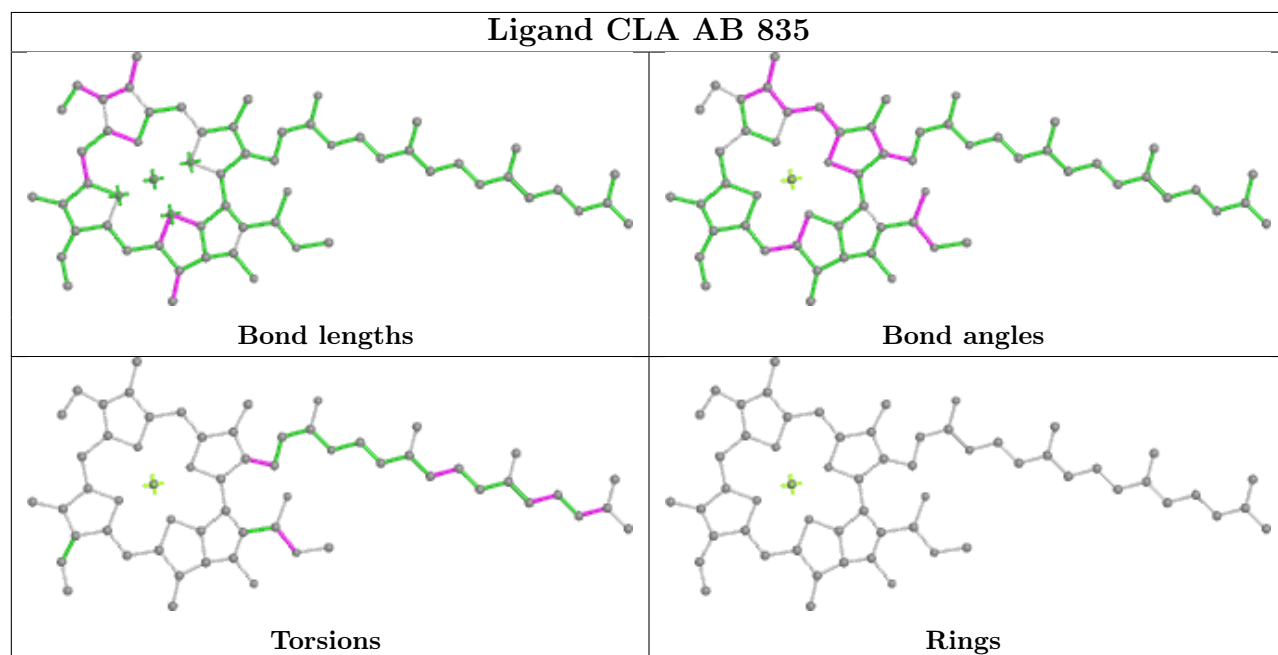
## Ligand CLA A3 302



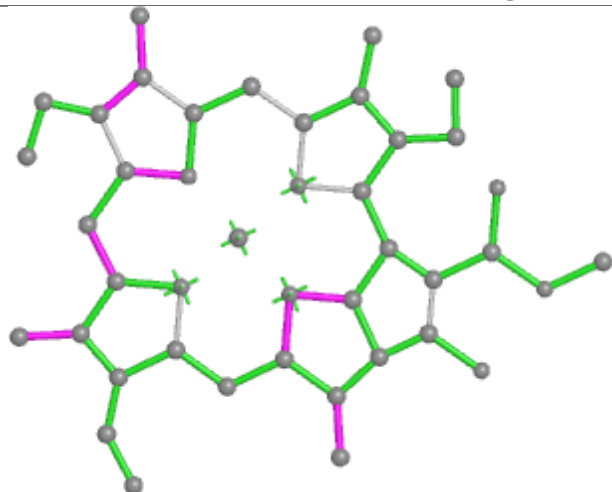
## Ligand CLA AA 819



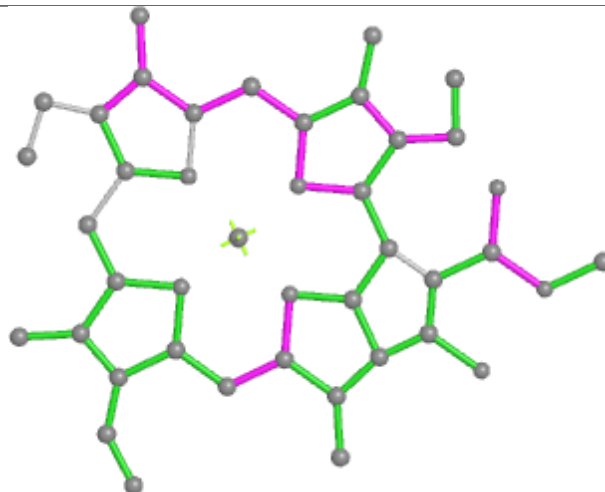
## Ligand CLA AB 835



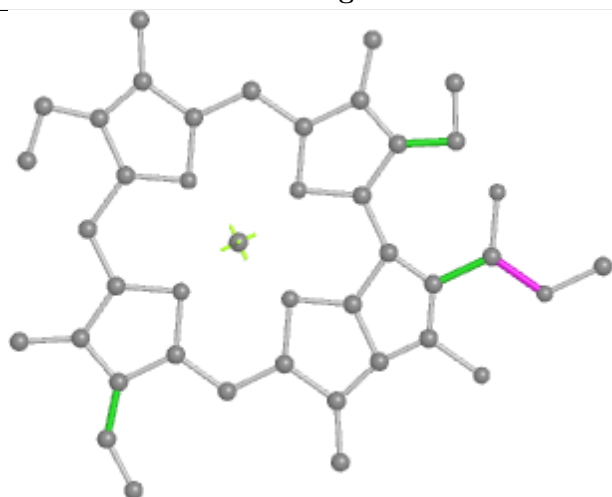
## Ligand CLA AF 803



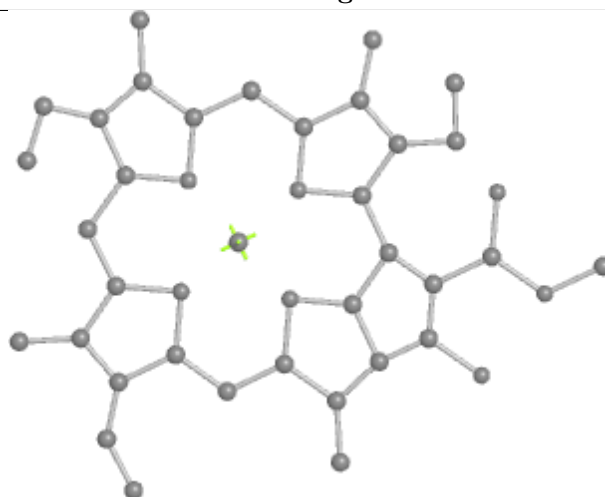
Bond lengths



Bond angles

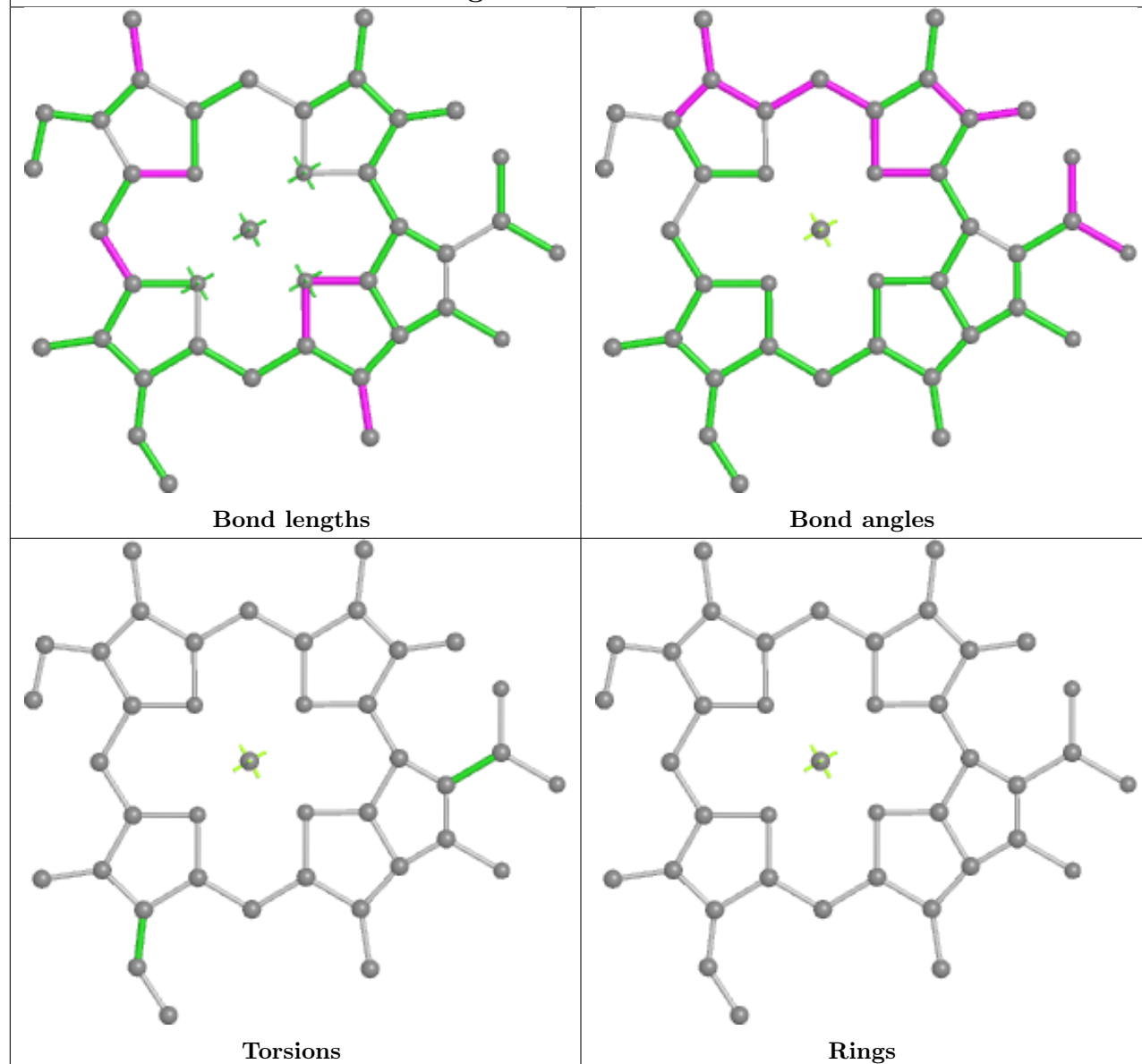


Torsions

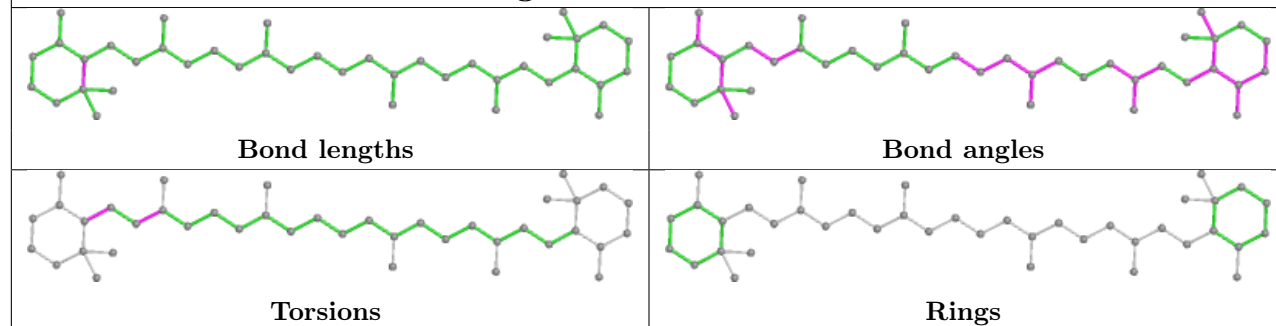


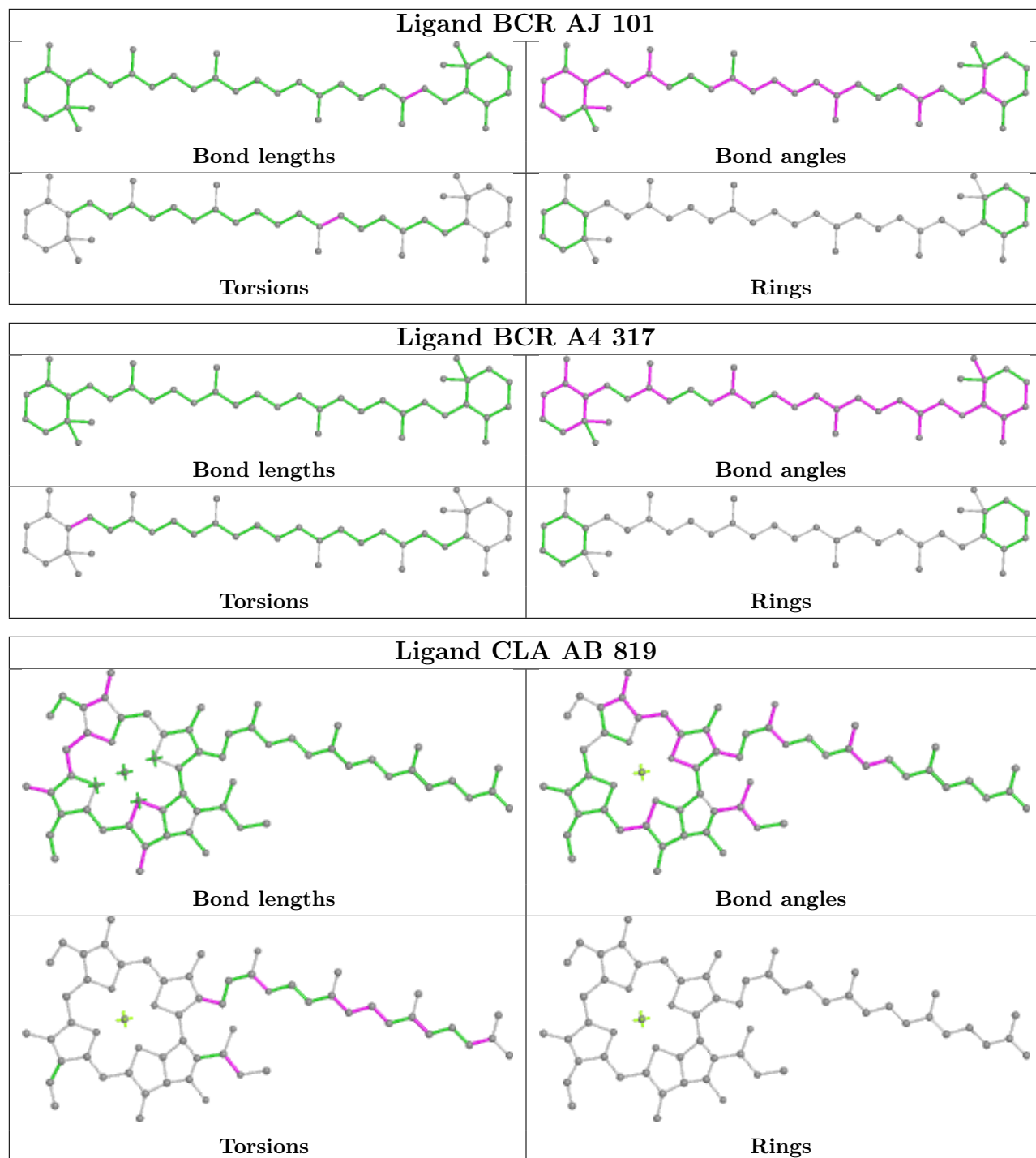
Rings

## Ligand CLA A3 315

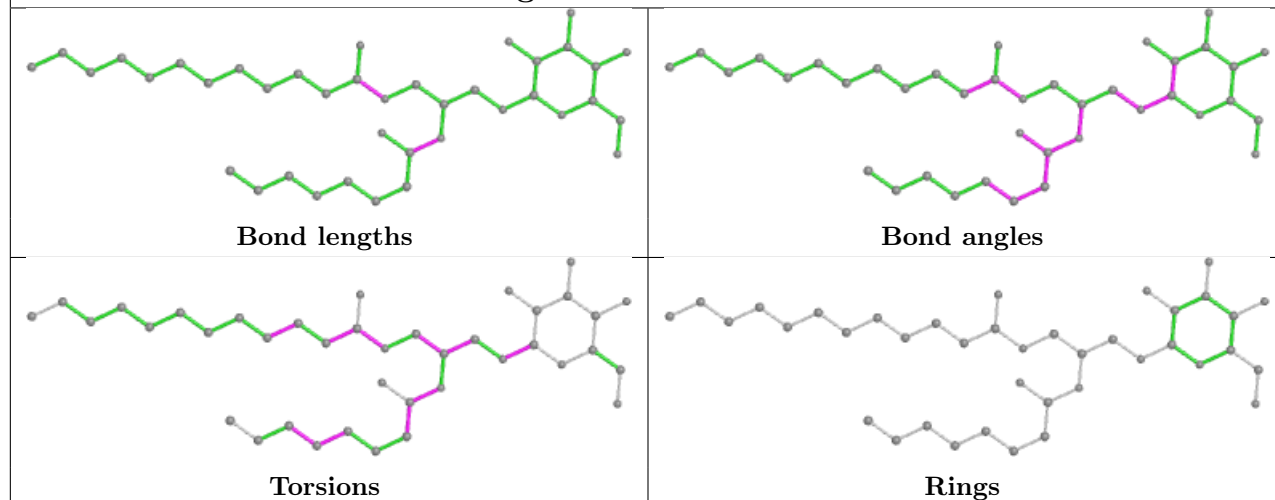


## Ligand BCR AA 848

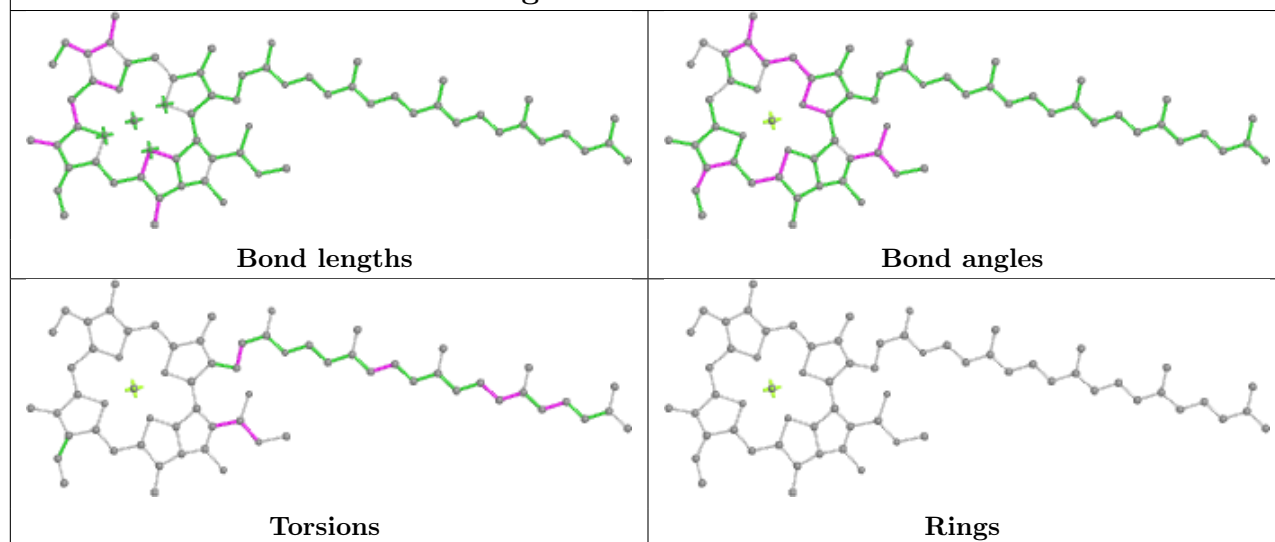




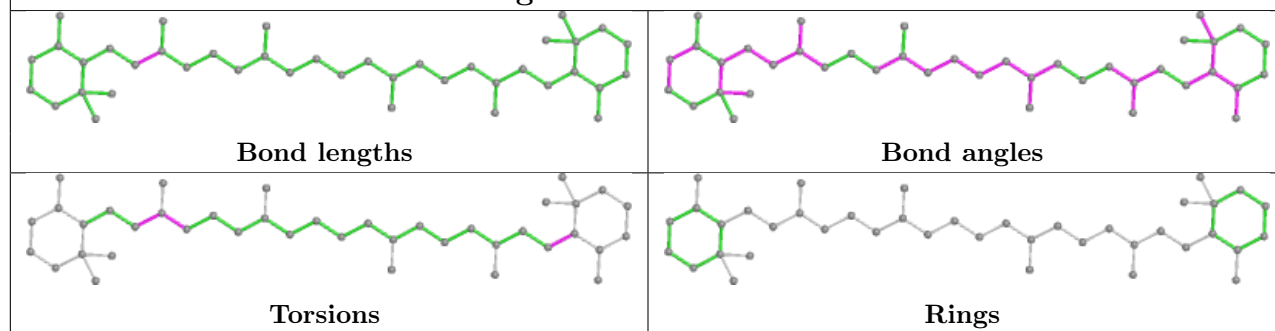
## Ligand LMG A4 318



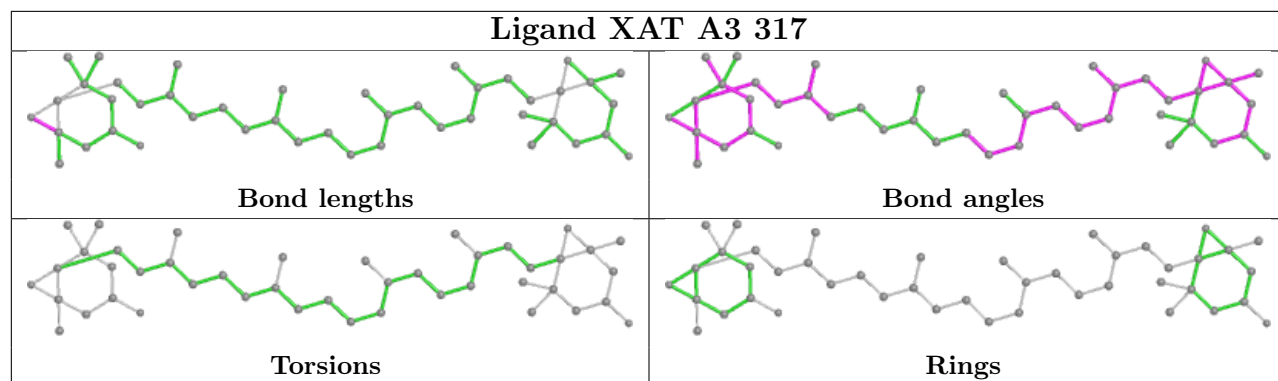
## Ligand CLA A6 602



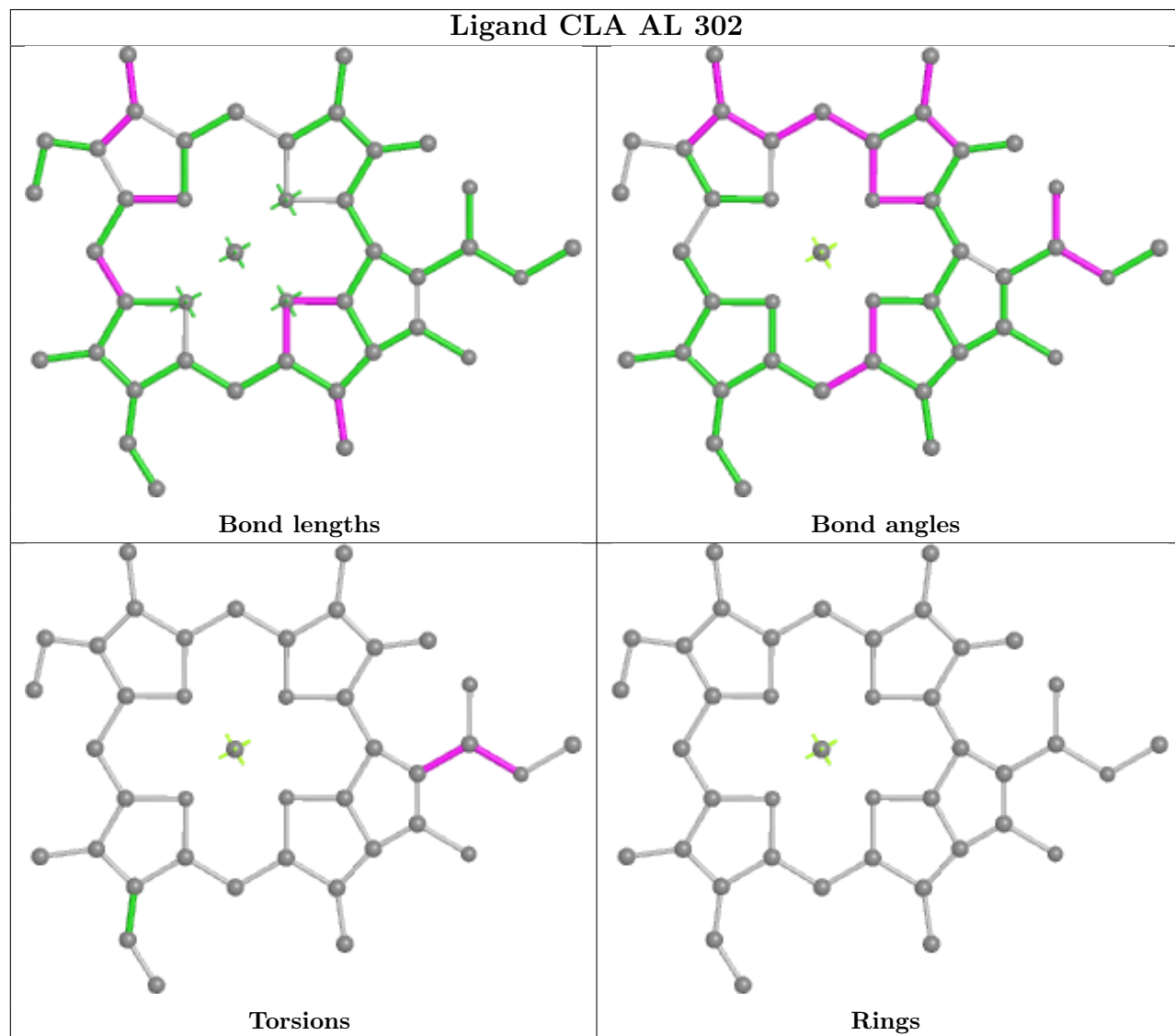
## Ligand BCR AB 845

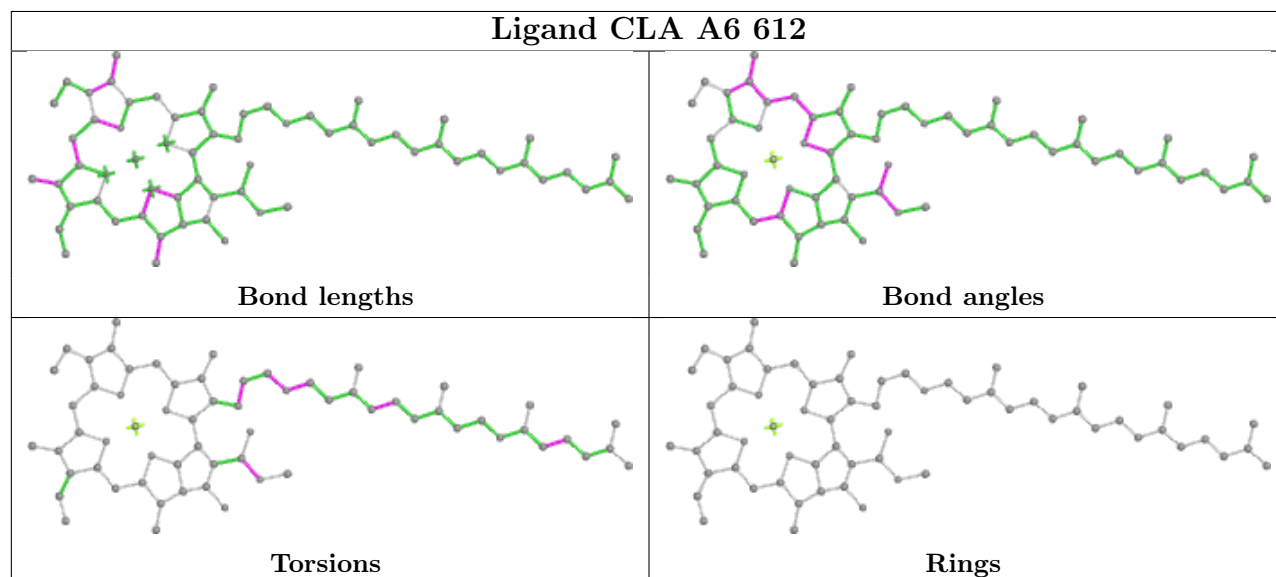
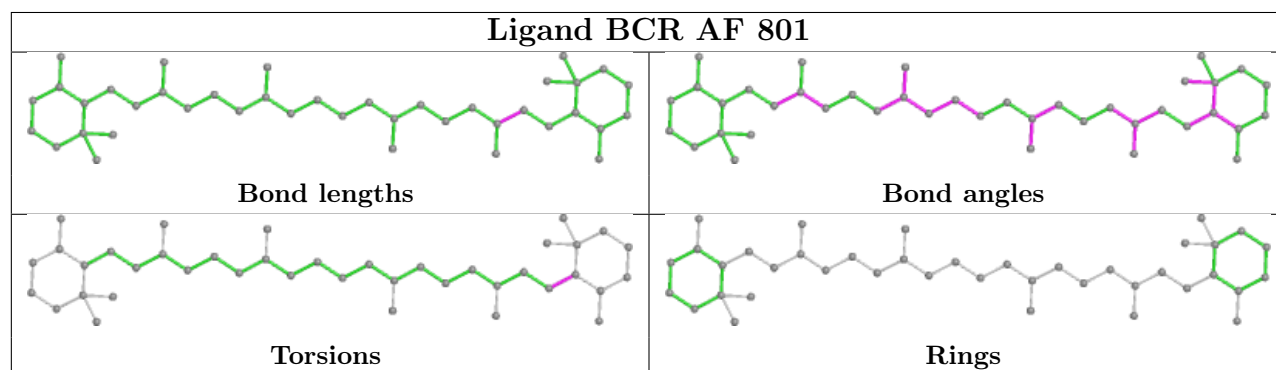
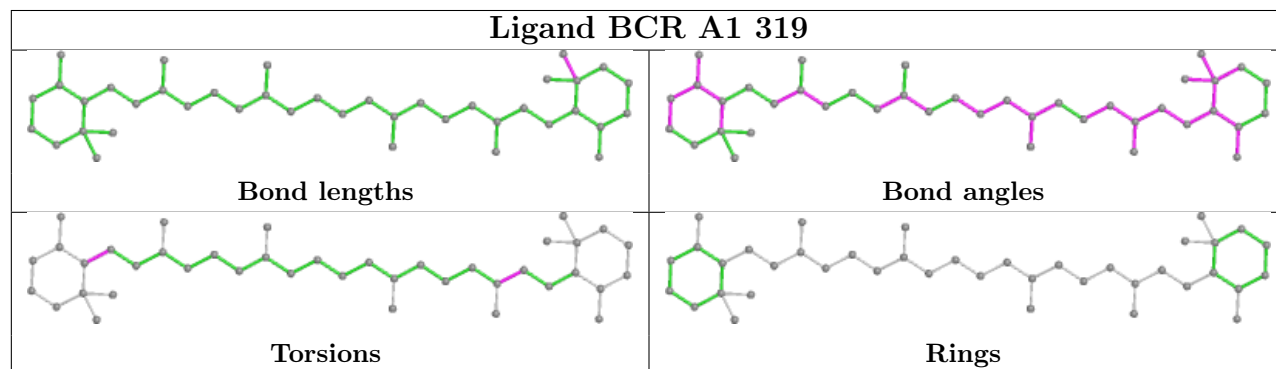
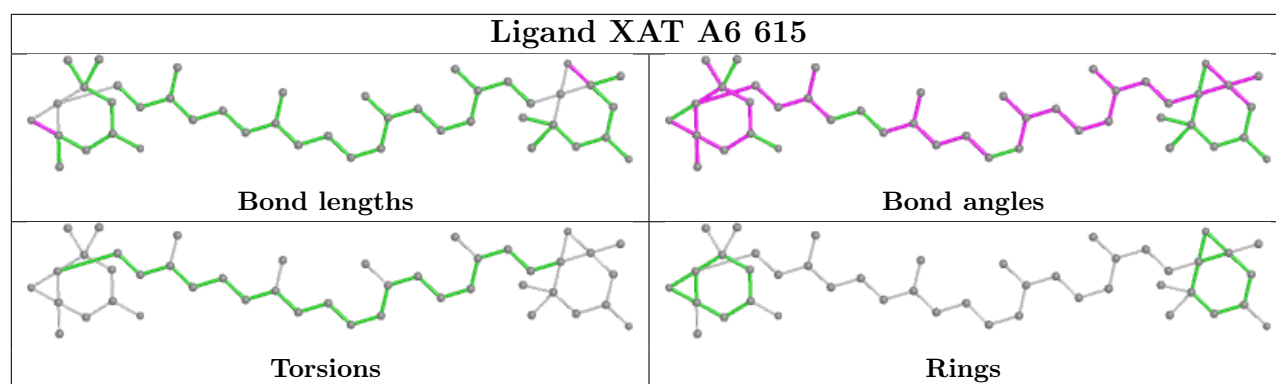


## Ligand XAT A3 317

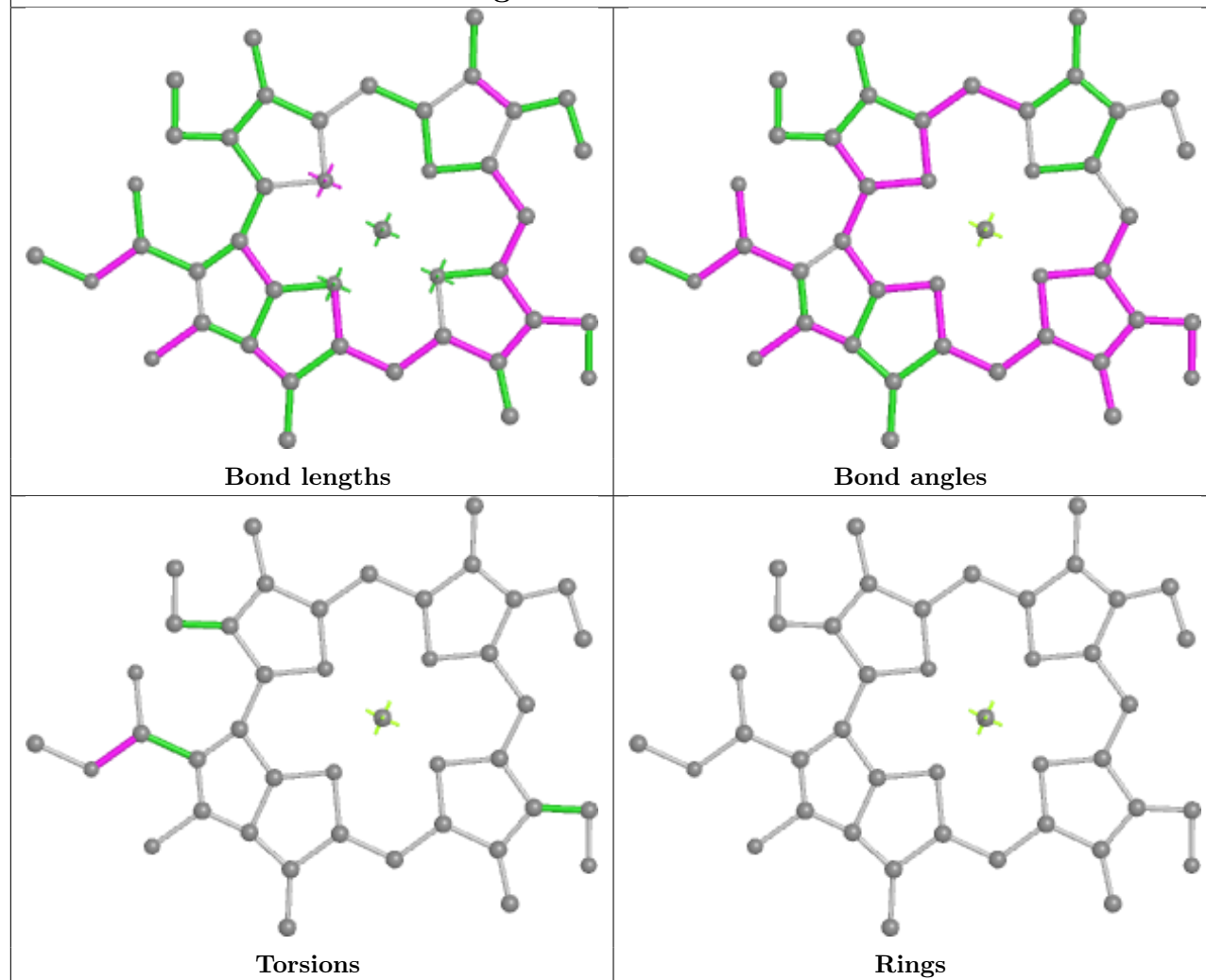


## Ligand CLA AL 302

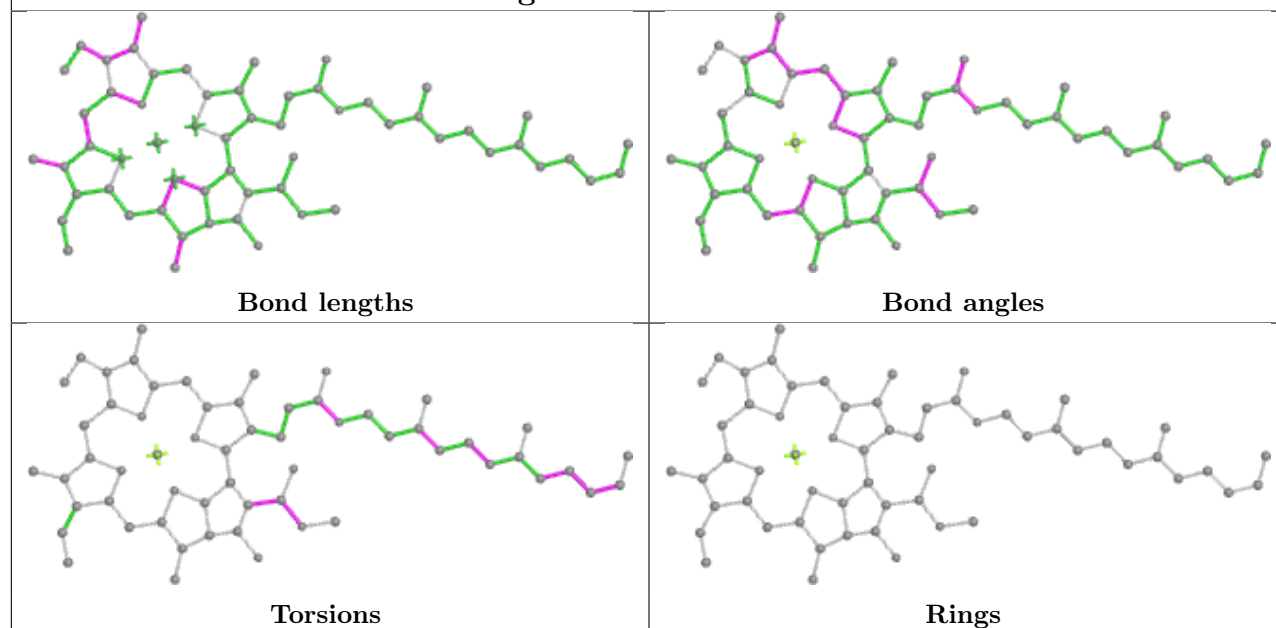




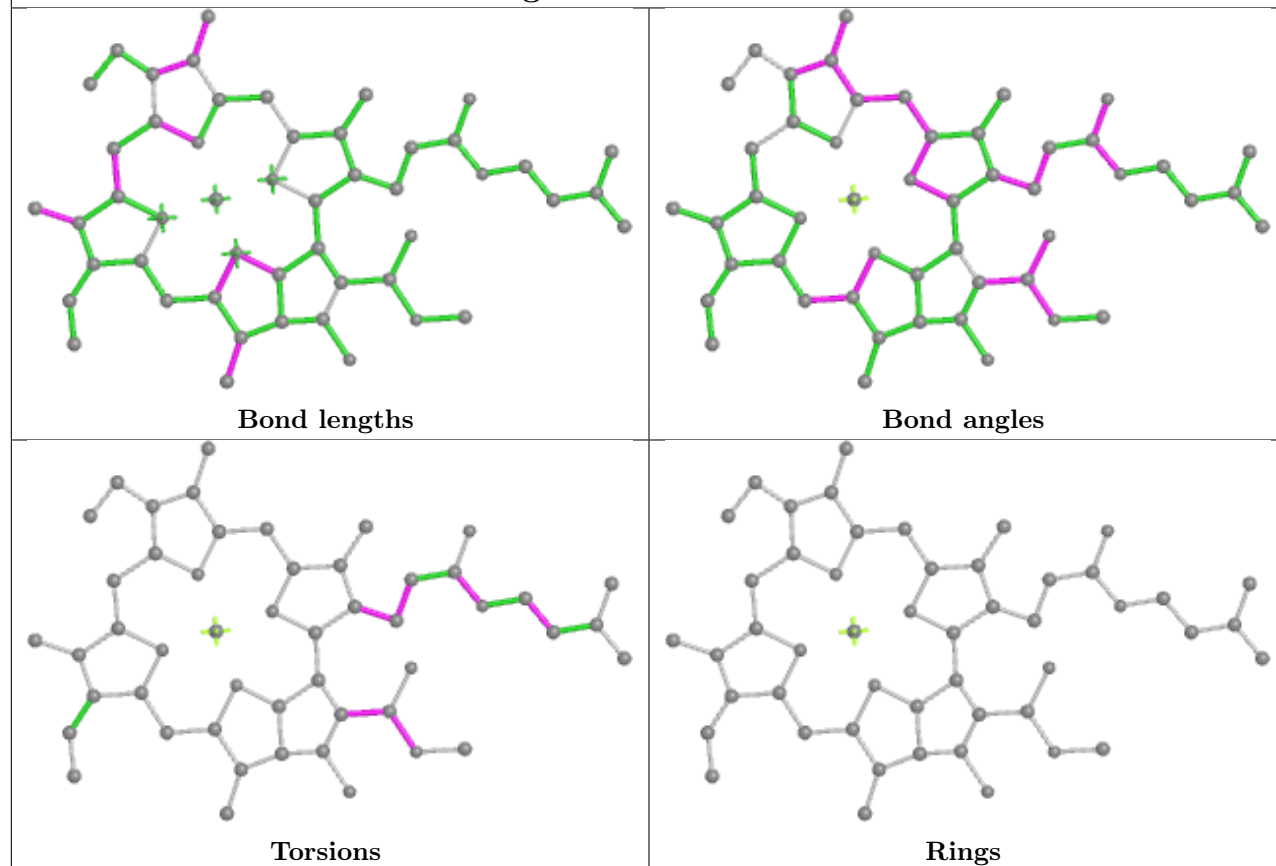
## Ligand CHL A6 605



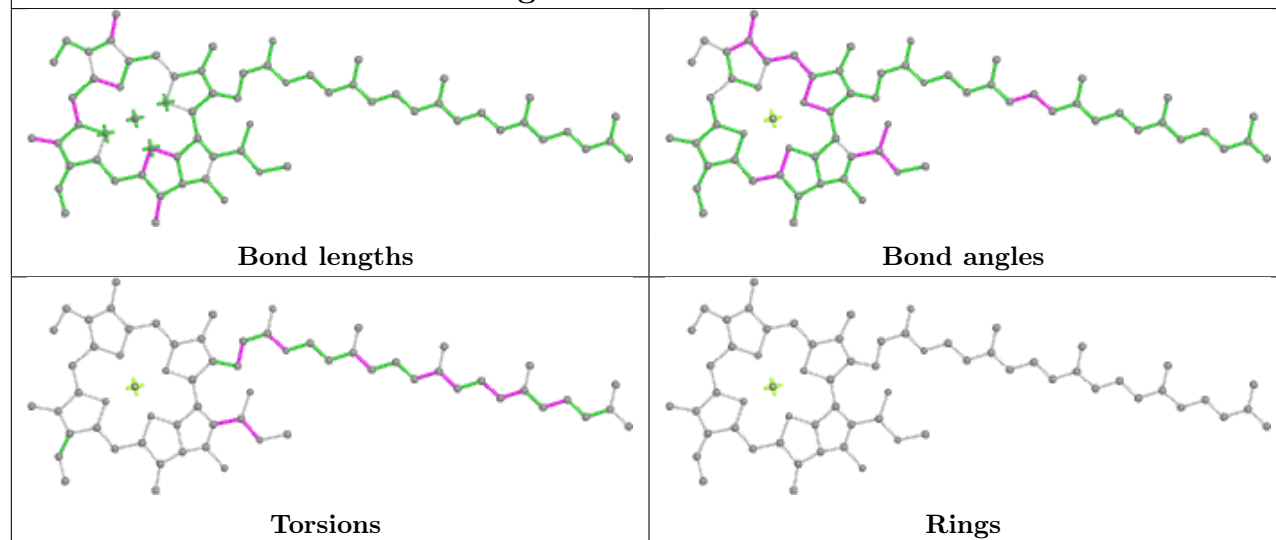
## Ligand CLA AA 826



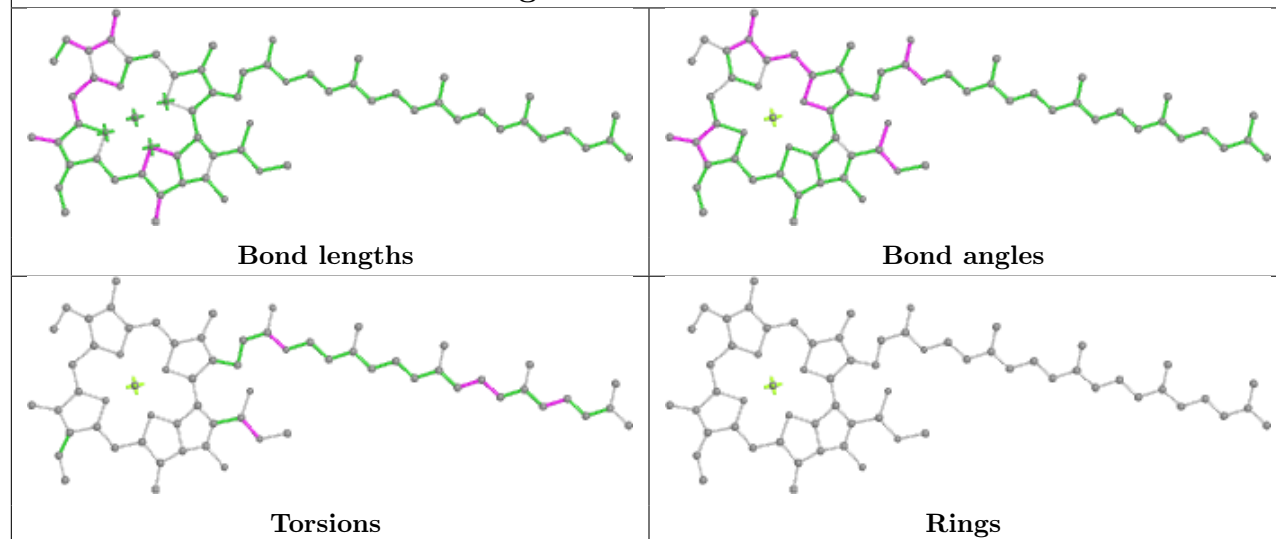
## Ligand CLA A4 313



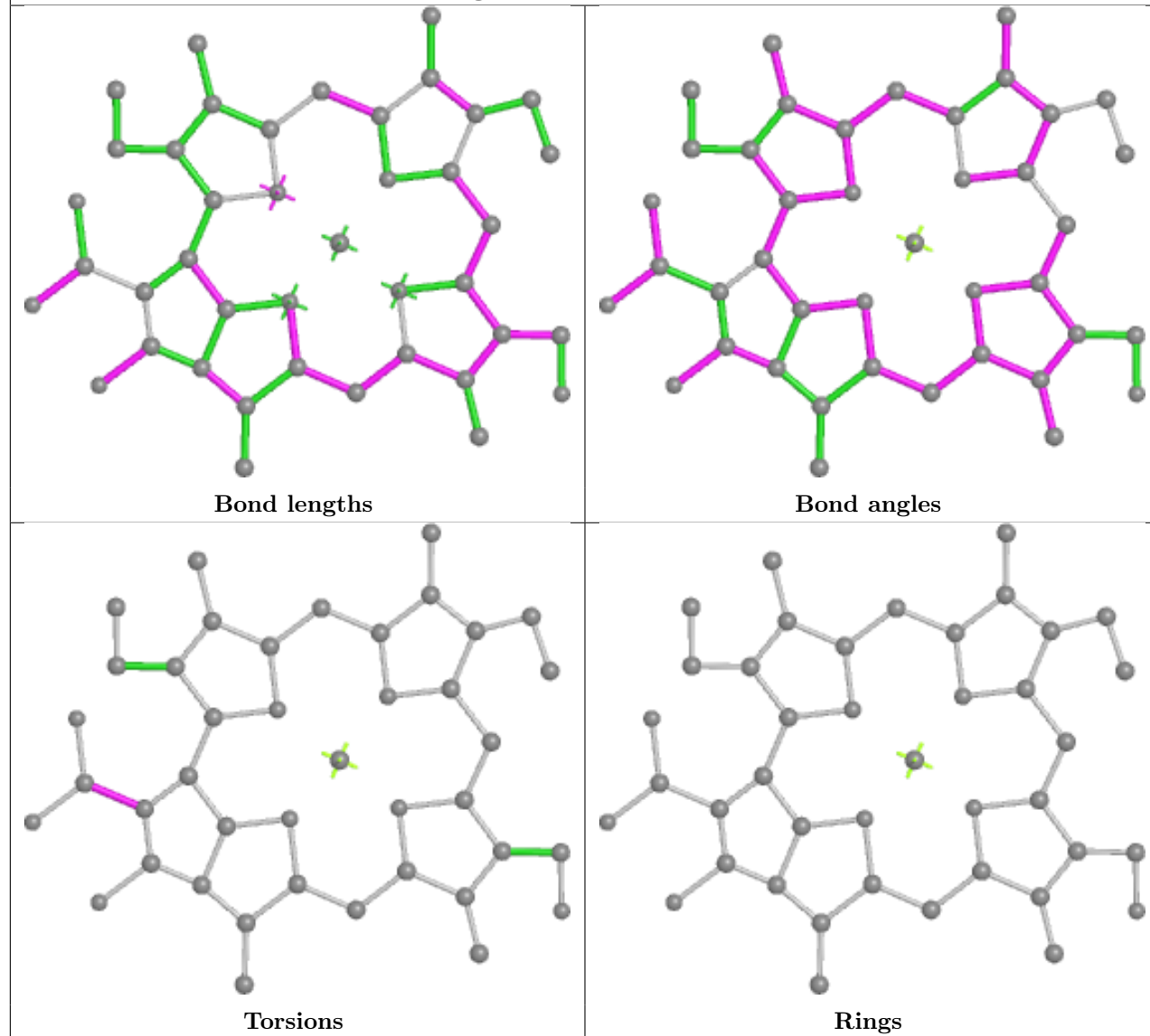
## Ligand CLA AA 821



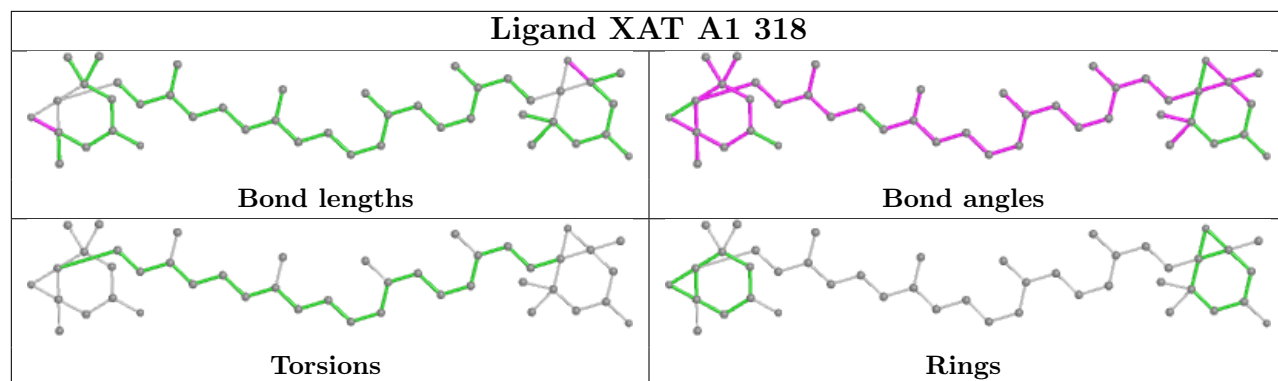
## Ligand CLA AB 832



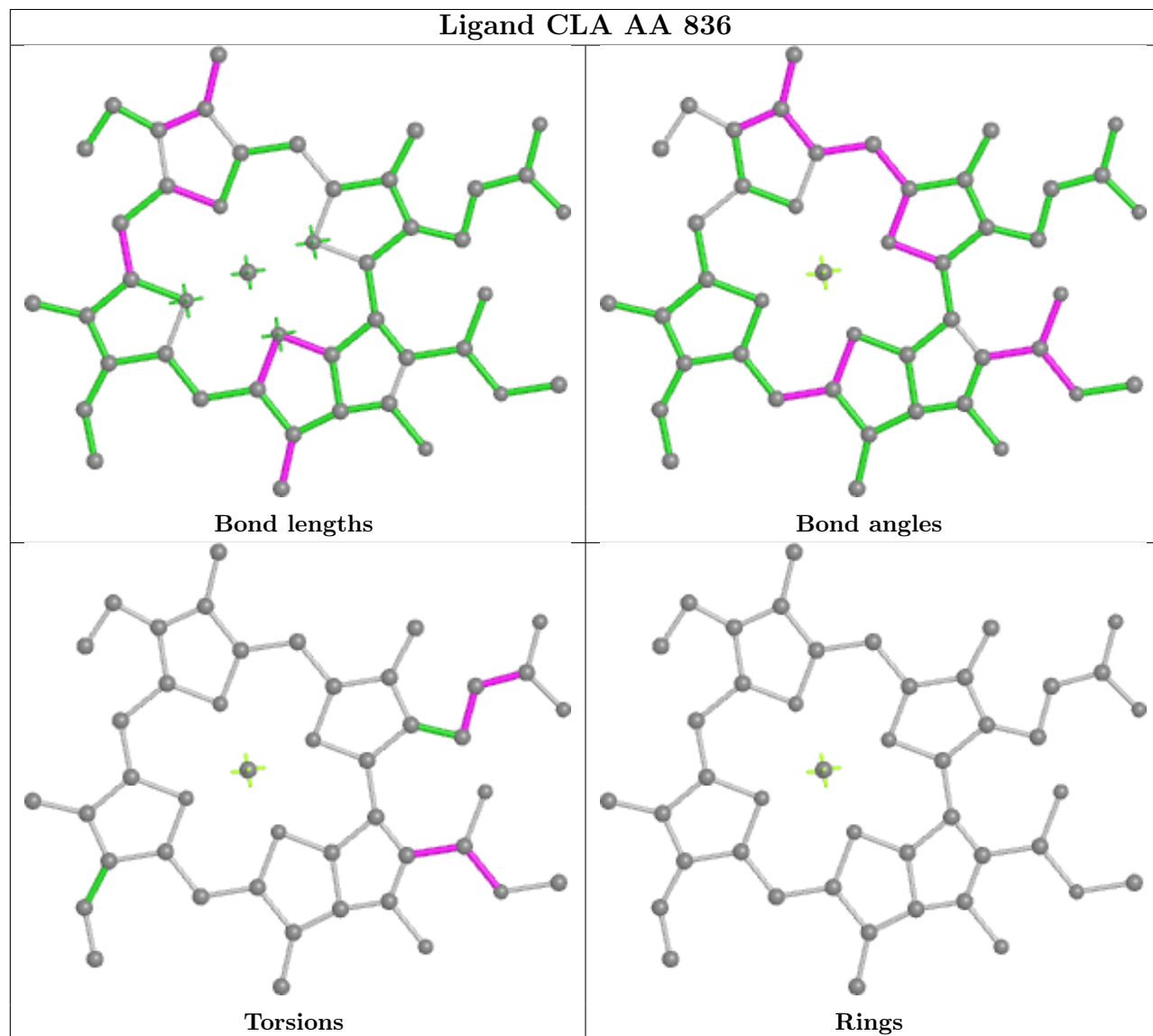
## Ligand CHL A4 304



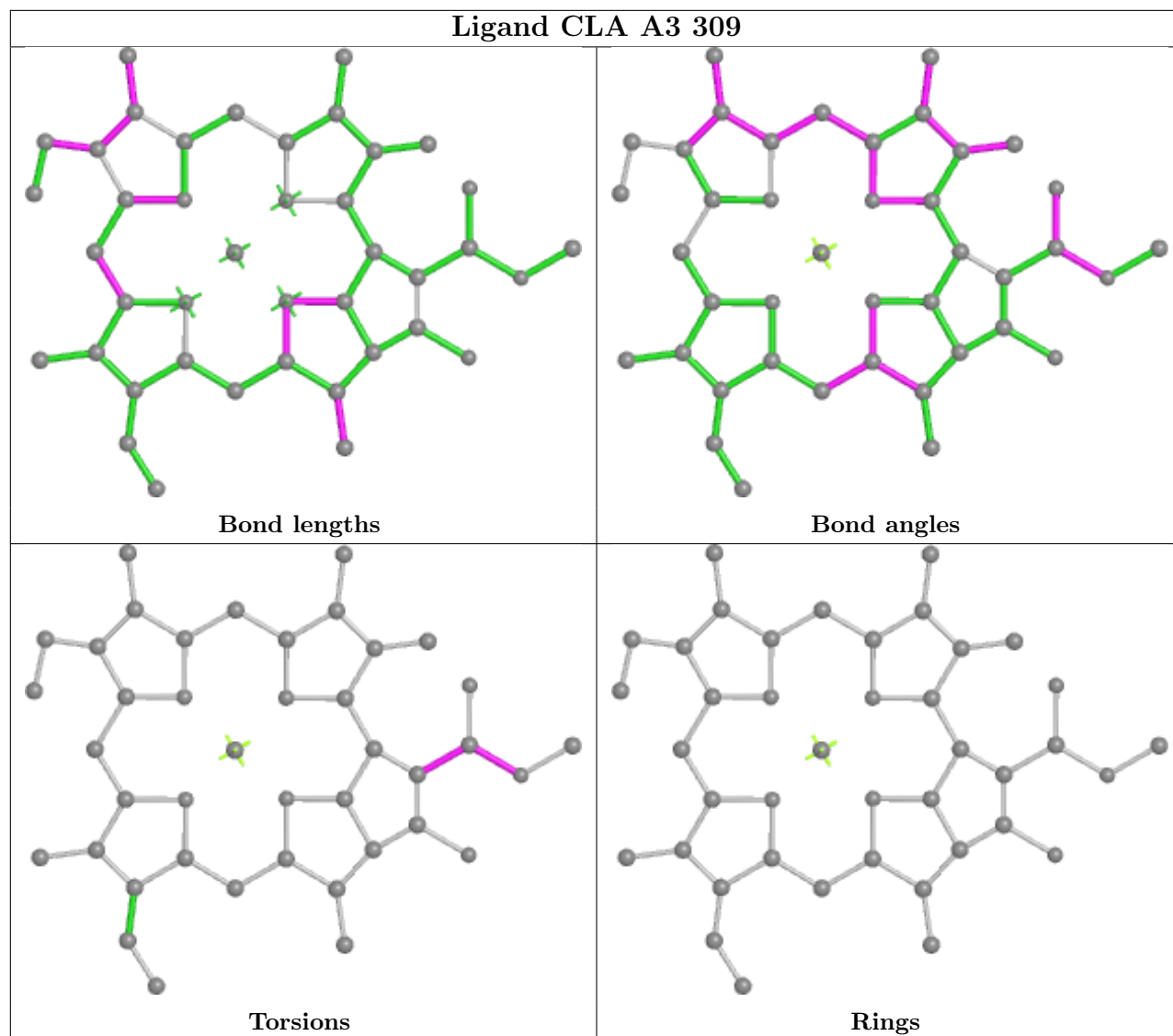
## Ligand XAT A1 318



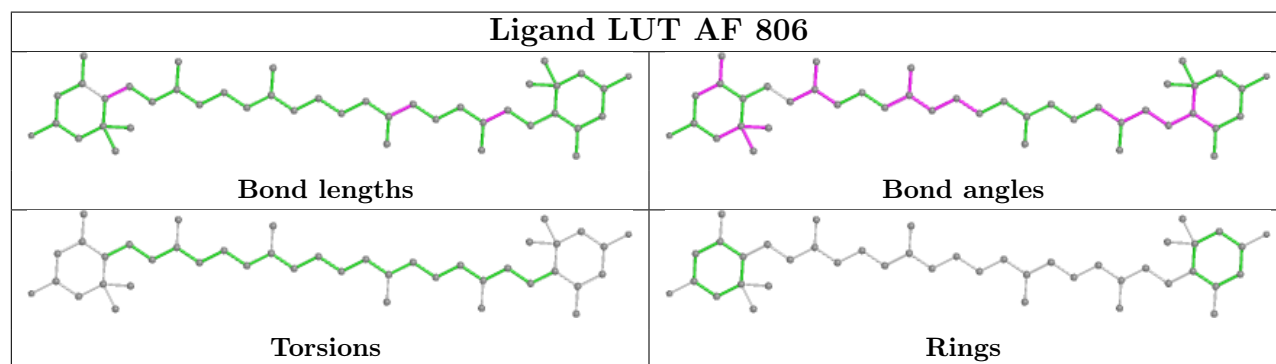
## Ligand CLA AA 836



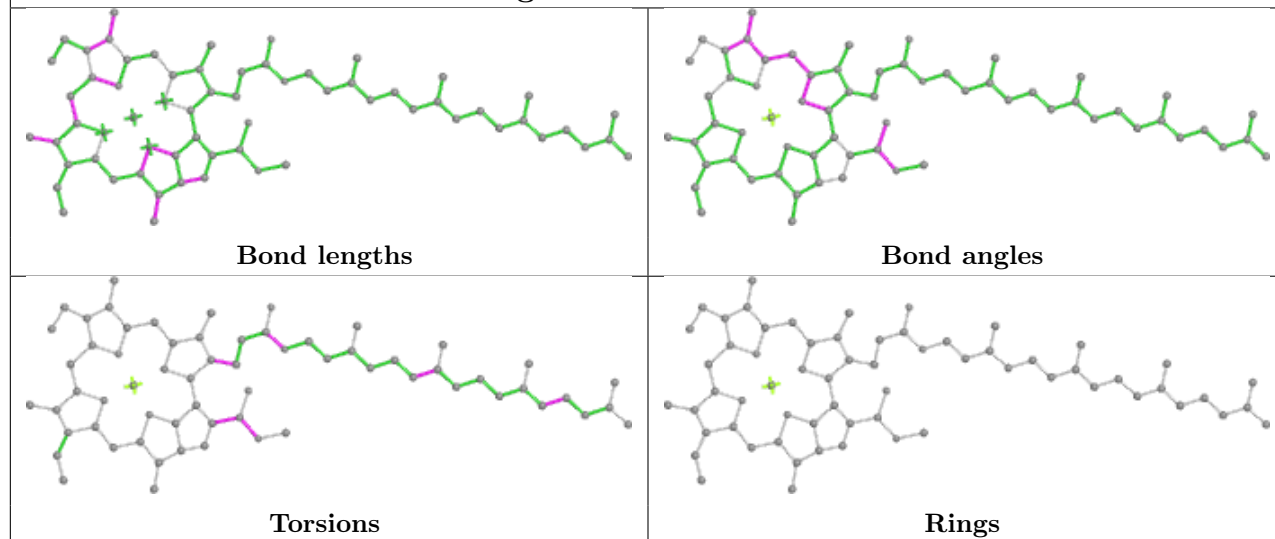
## Ligand CLA A3 309



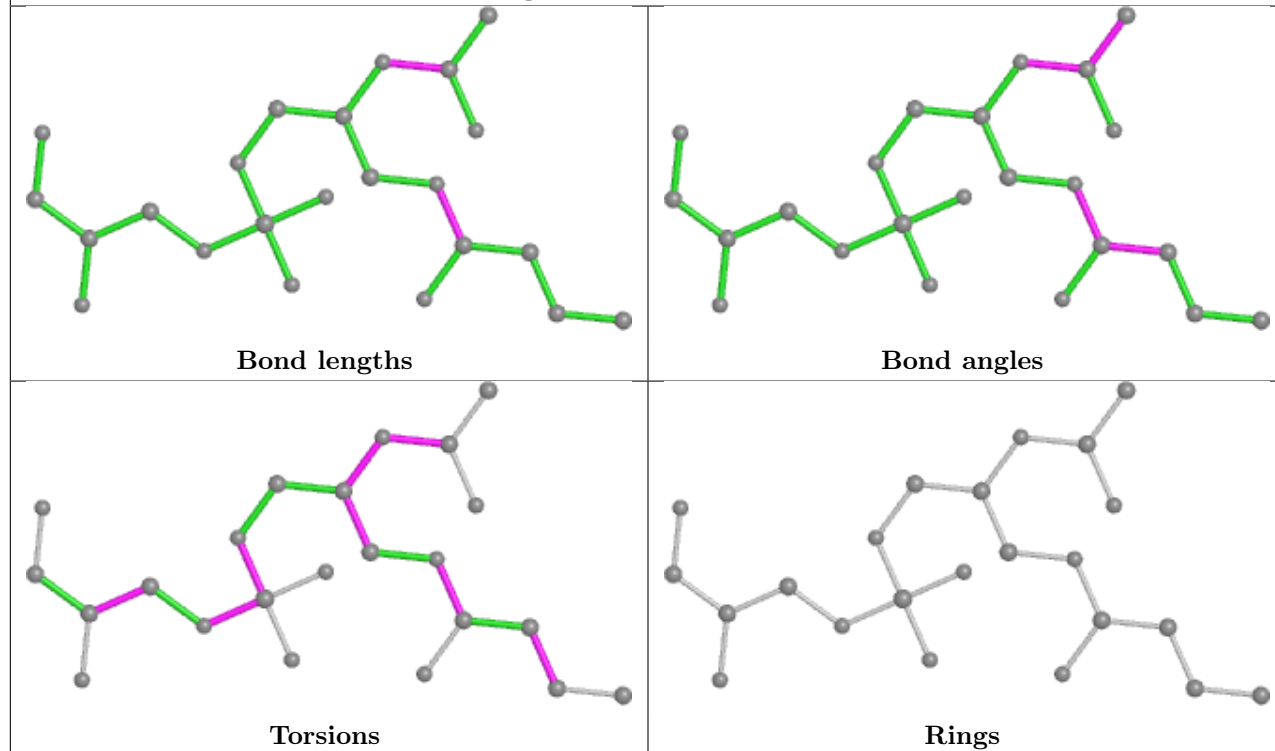
## Ligand LUT AF 806

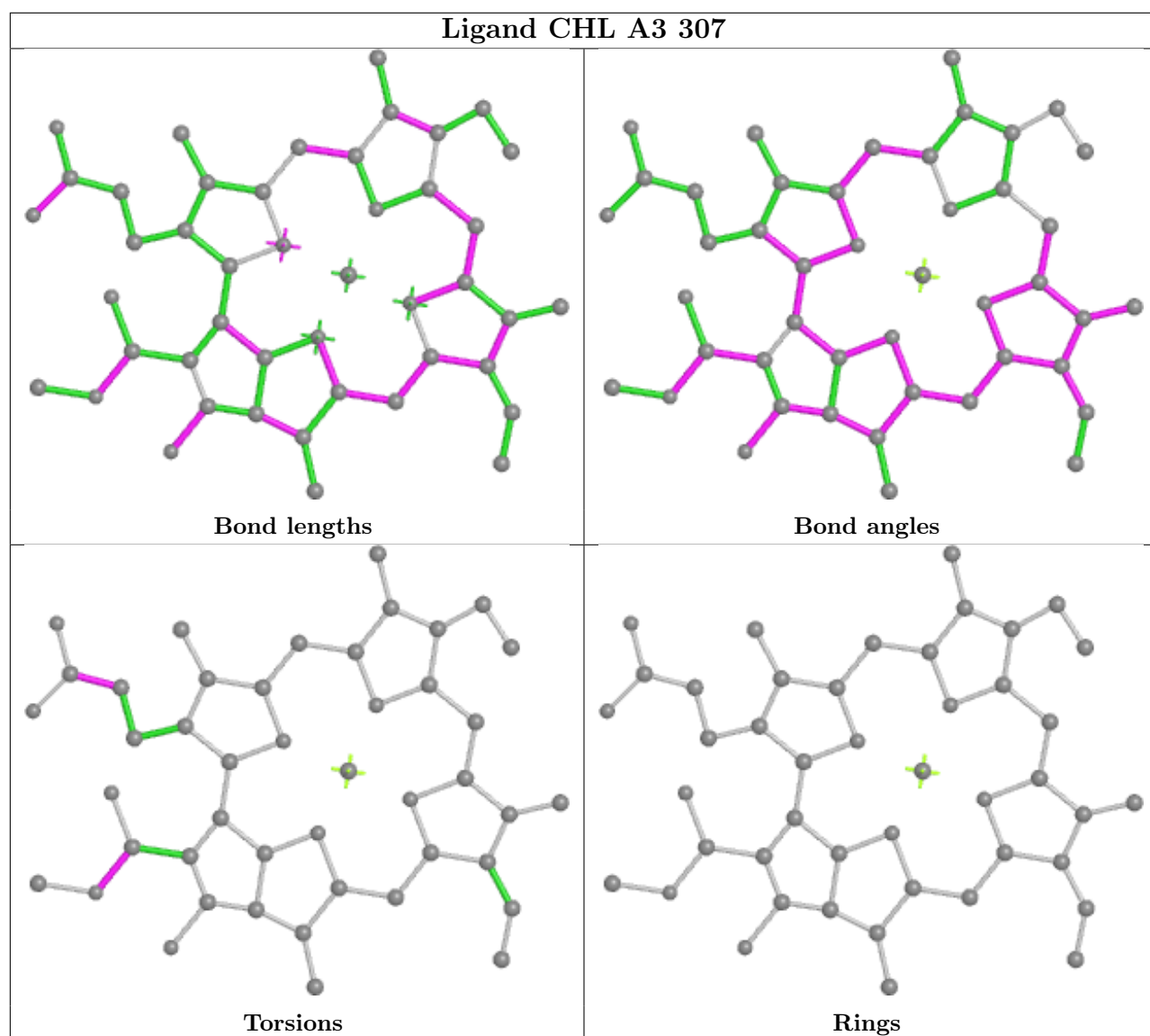


## Ligand CLA AA 810

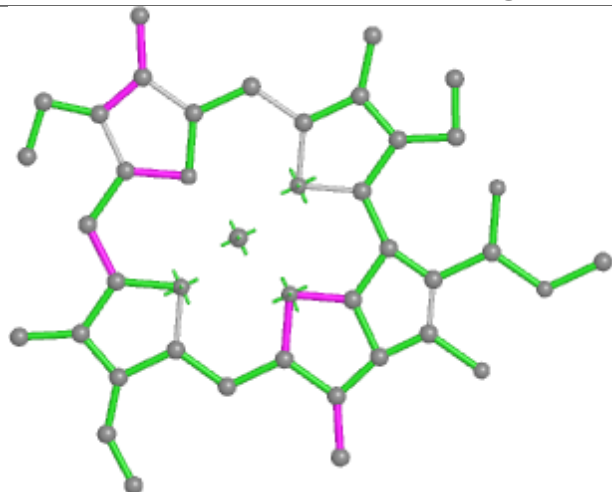


## Ligand LHG A3 319

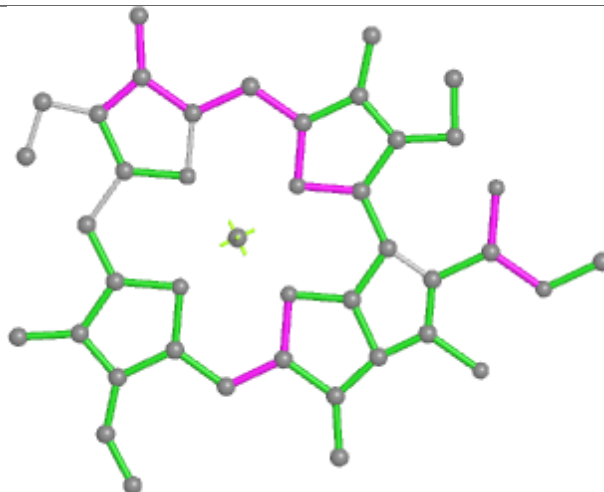




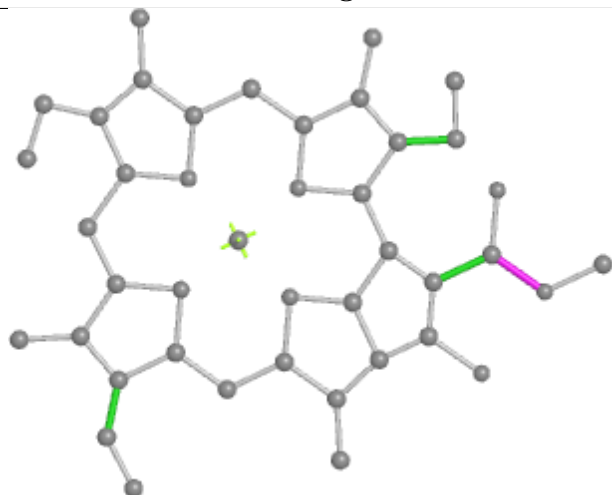
## Ligand CLA AB 836



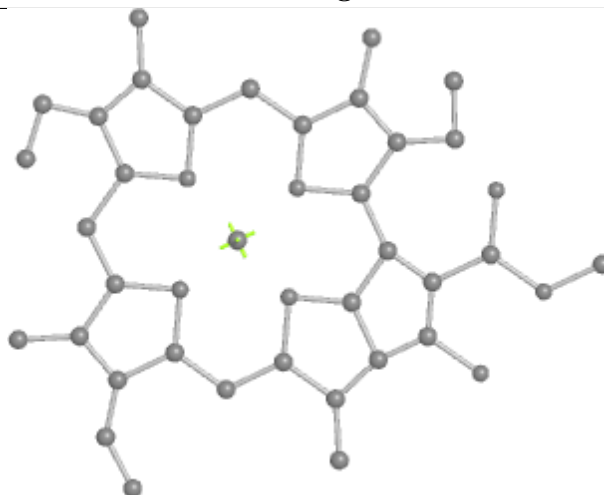
Bond lengths



Bond angles

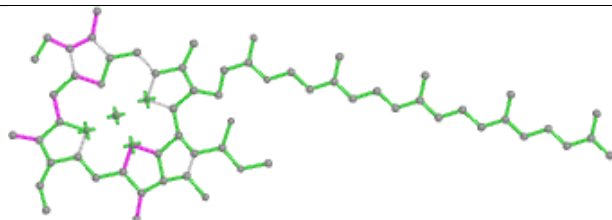


Torsions

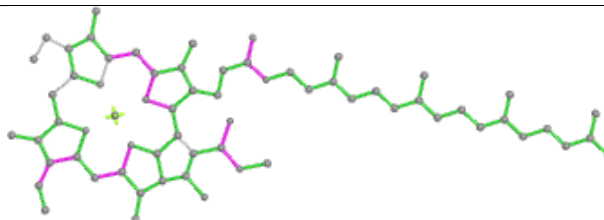


Rings

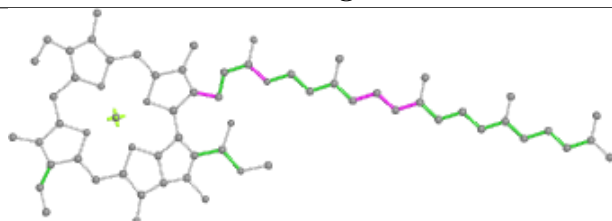
## Ligand CLA AB 841



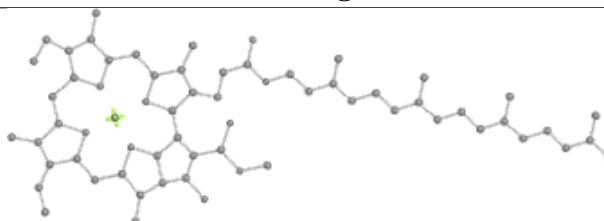
Bond lengths



Bond angles

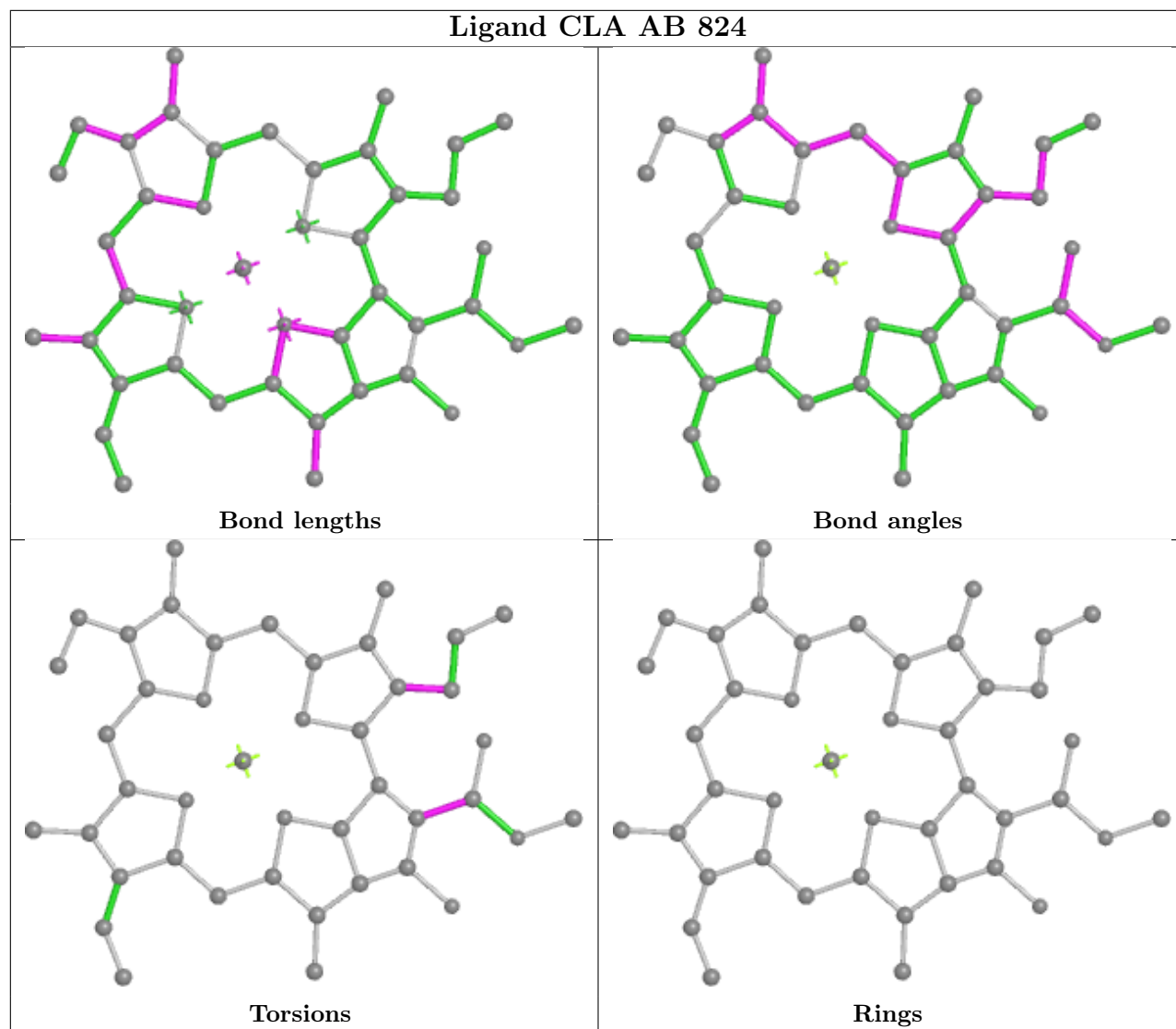


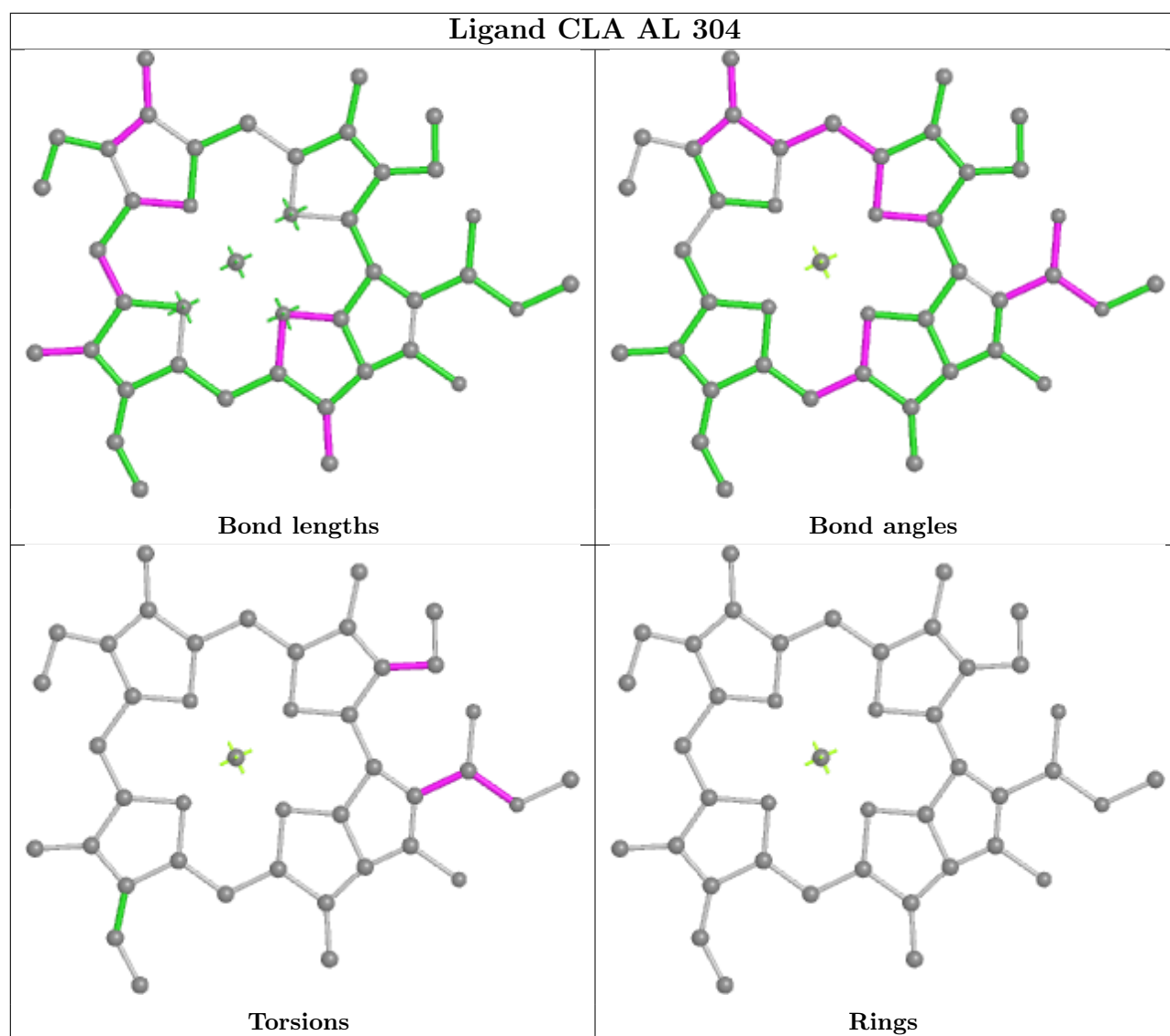
Torsions



Rings

## Ligand CLA AB 824





## 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.

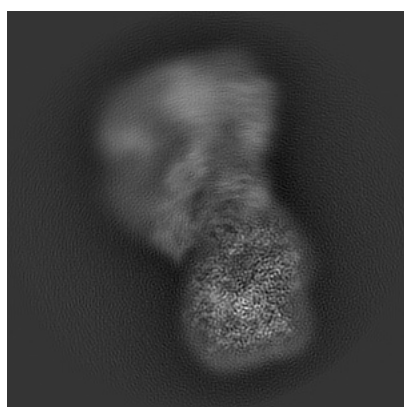
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32462. These allow visual inspection of the internal detail of the map and identification of artifacts.

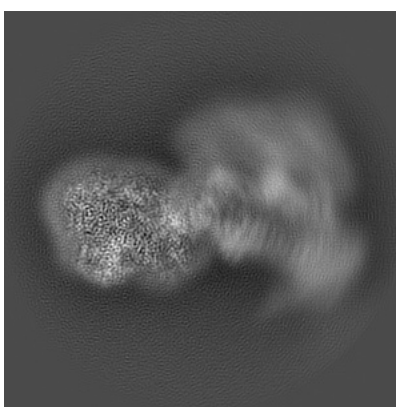
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

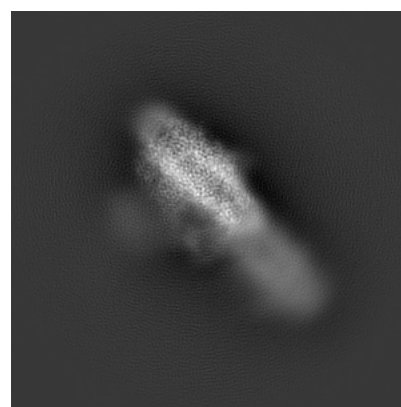
#### 6.1.1 Primary map



X



Y

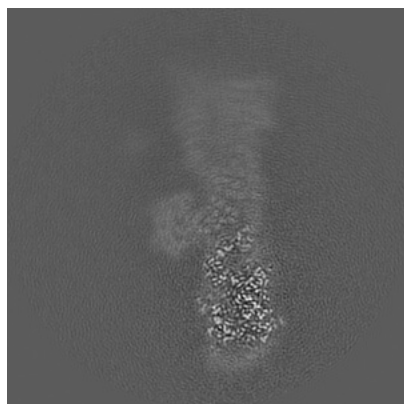


Z

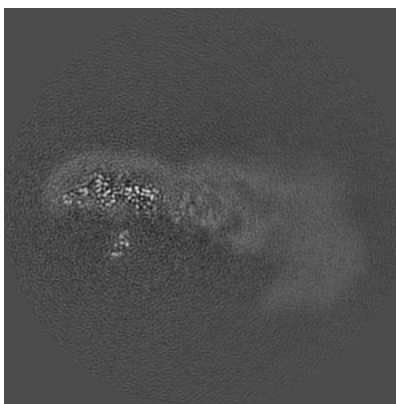
The images above show the map projected in three orthogonal directions.

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

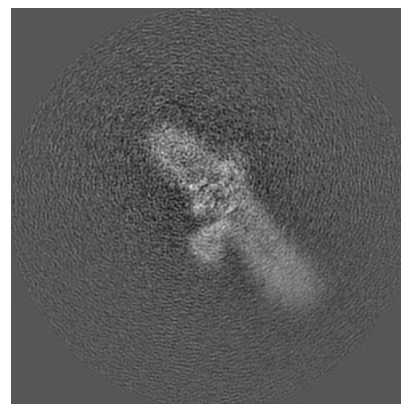
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

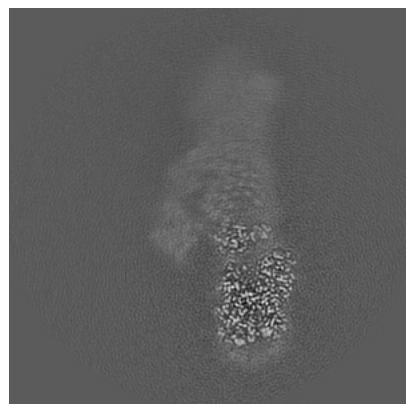


Z Index: 200

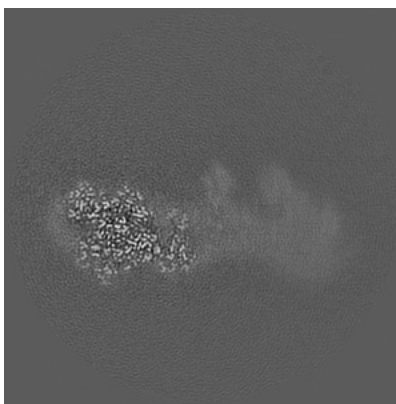
The images above show central slices of the map in three orthogonal directions.

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

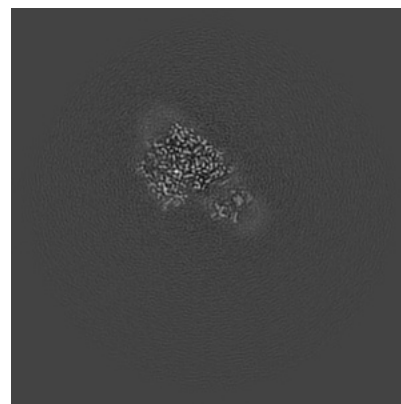
### 6.3.1 Primary map



X Index: 185



Y Index: 251

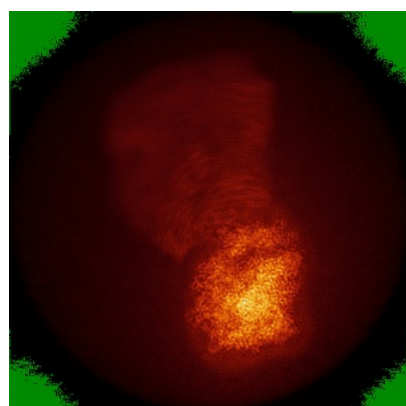


Z Index: 109

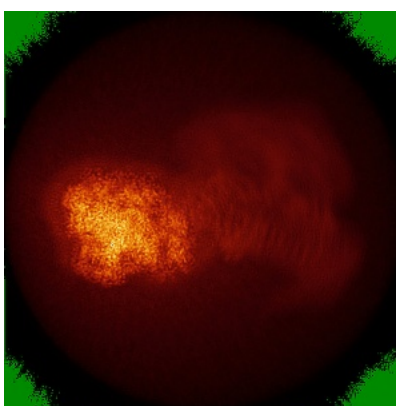
The images above show the largest variance slices of the map in three orthogonal directions.

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

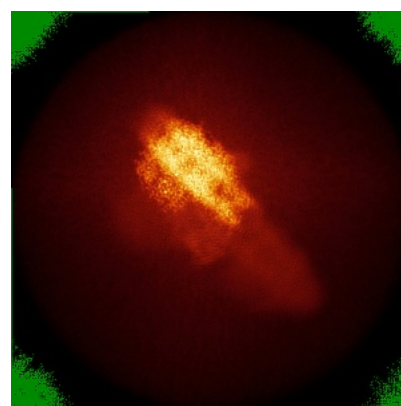
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

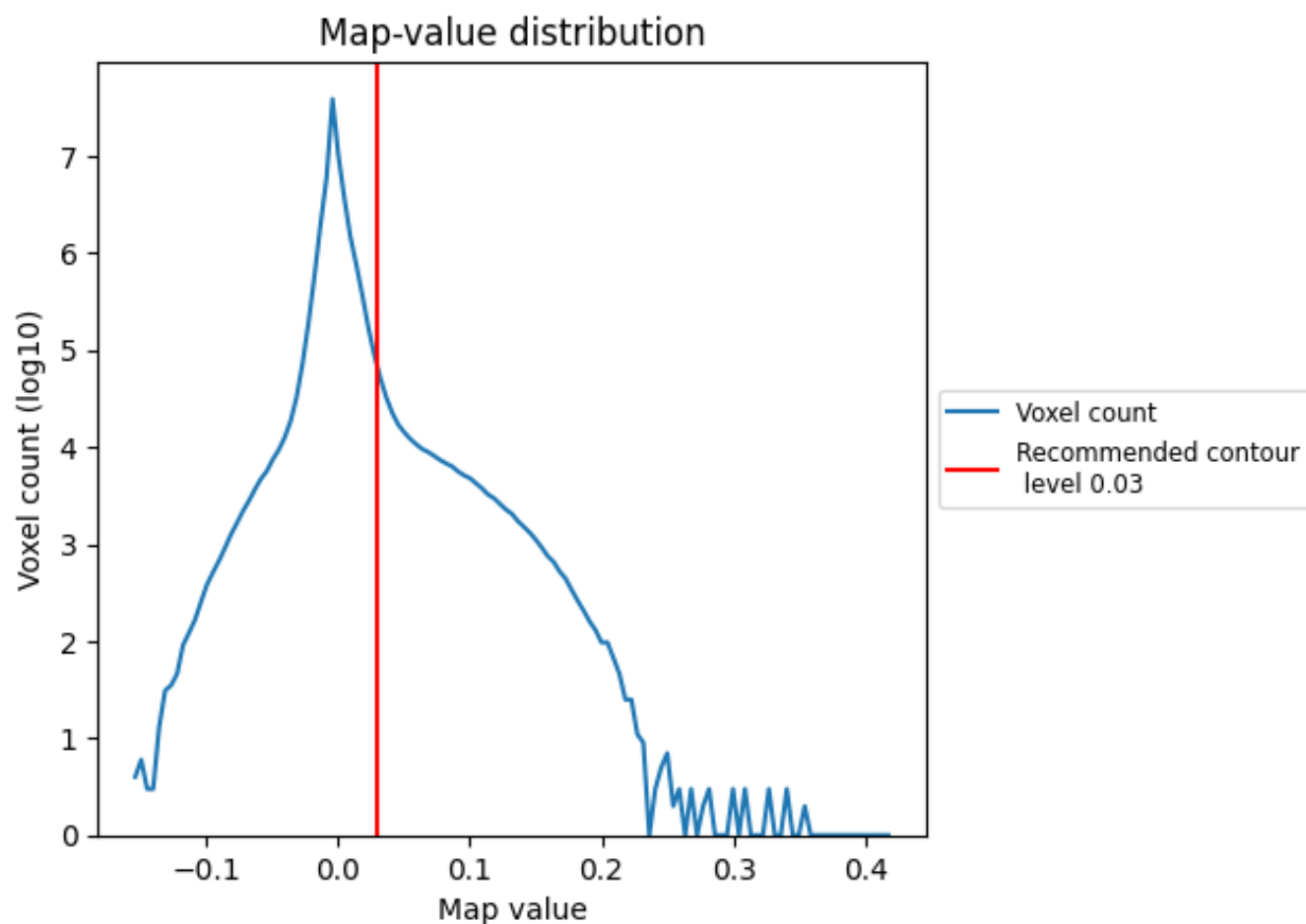
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

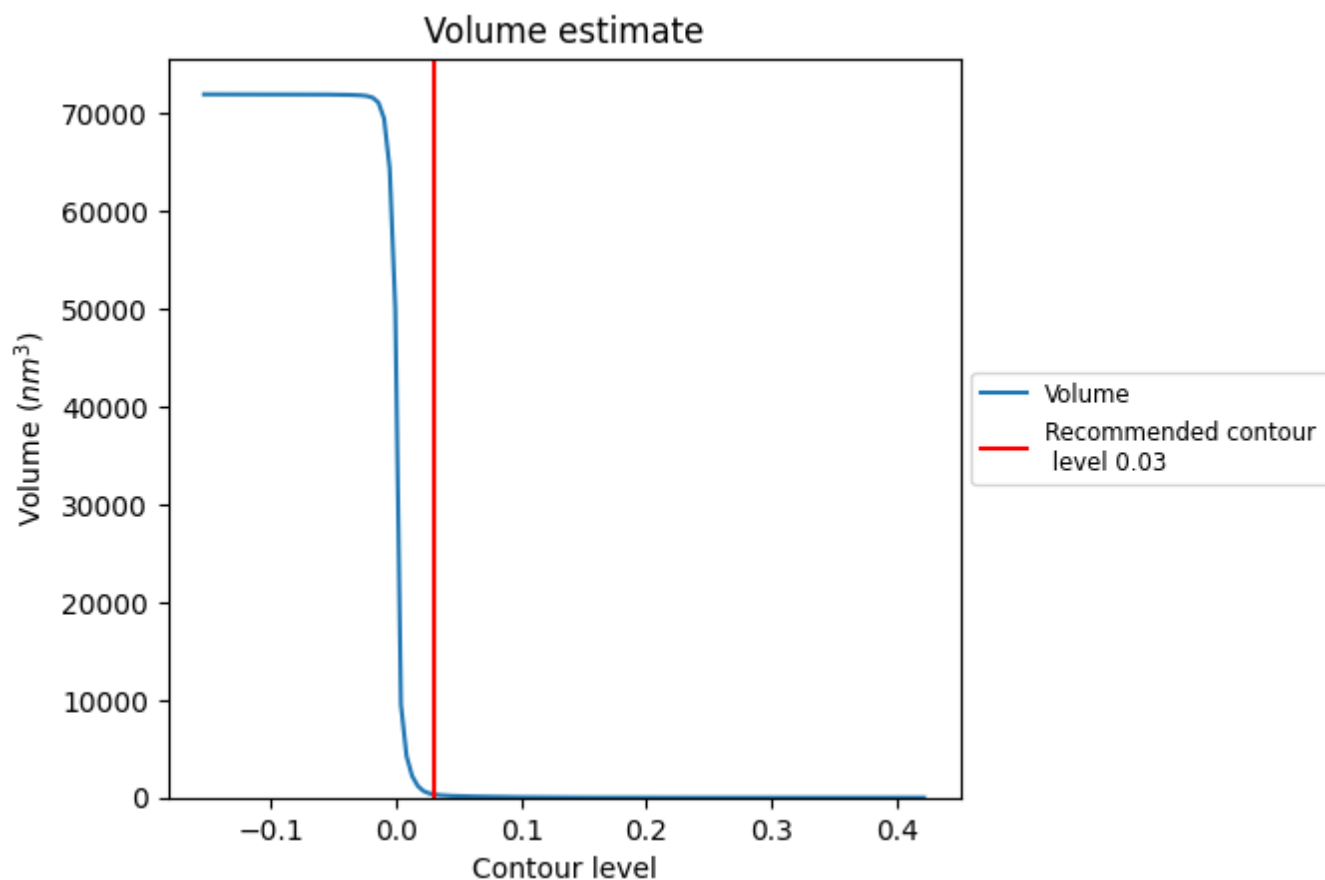
This section contains the results of statistical analysis of the map.

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



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

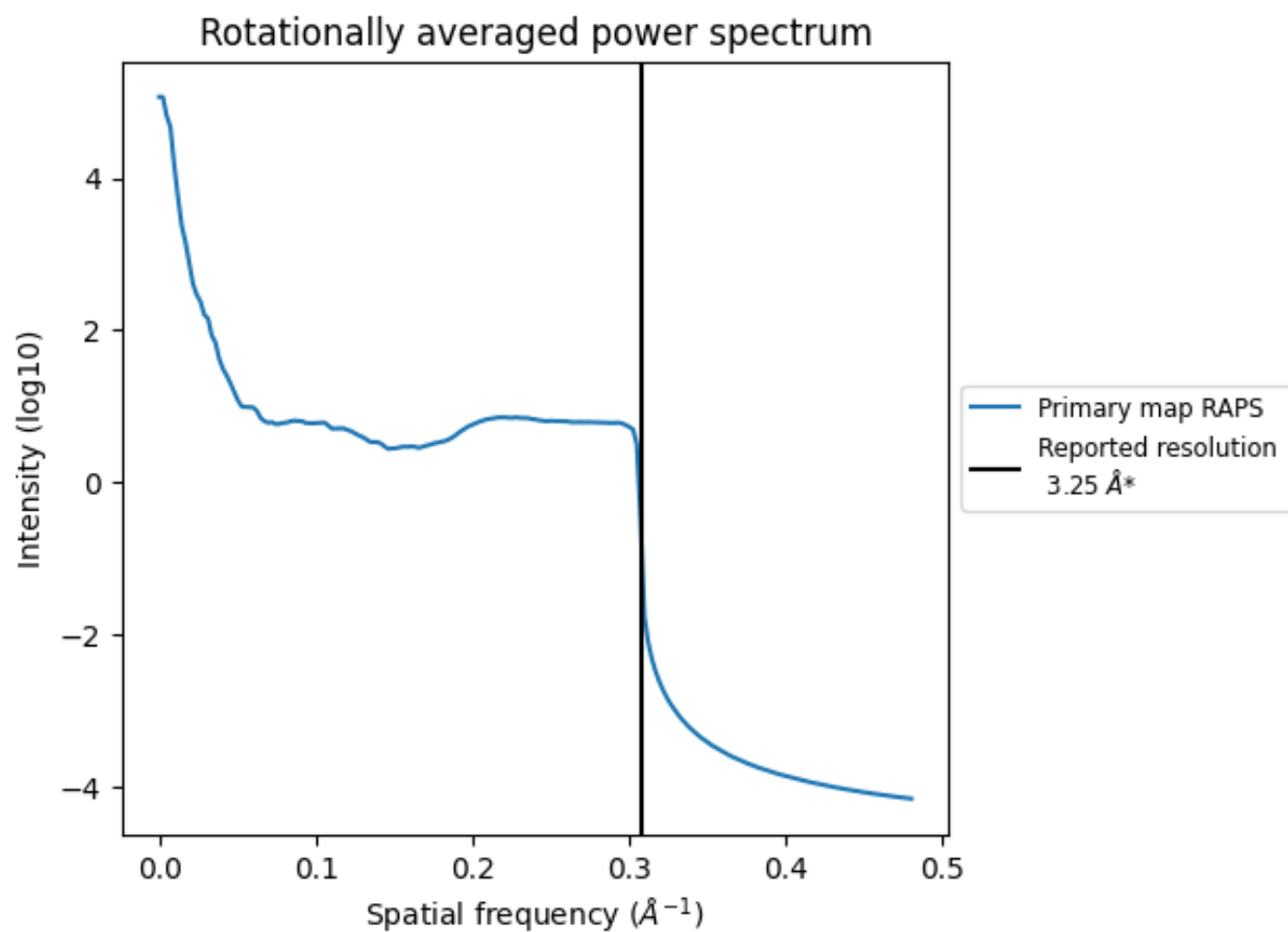
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338  $\text{nm}^3$ ; this corresponds to an approximate mass of 305 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 0.308 Å<sup>-1</sup>

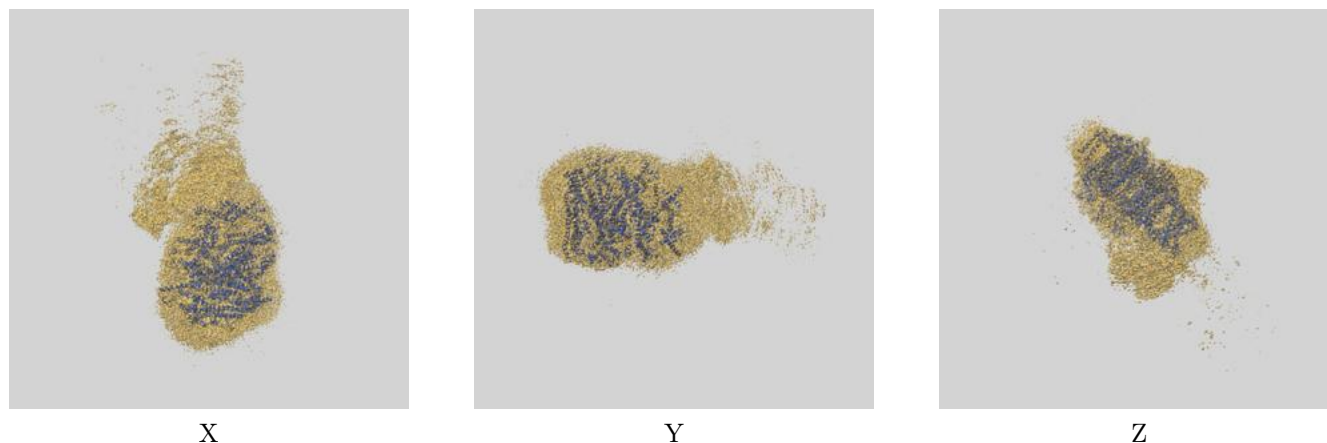
## 8 Fourier-Shell correlation ⓘ

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

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

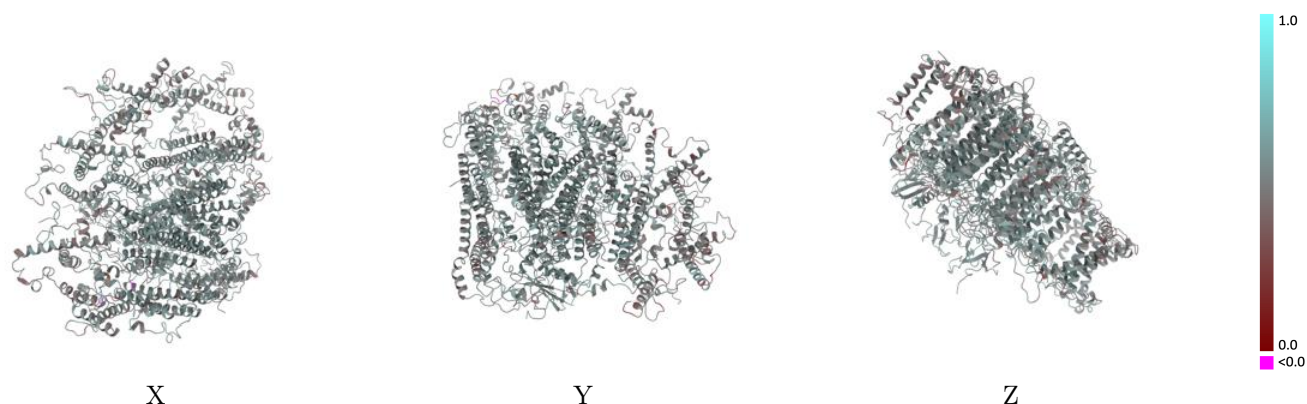
This section contains information regarding the fit between EMDB map EMD-32462 and PDB model 7WFD. Per-residue inclusion information can be found in section [3](#) on page [26](#).

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



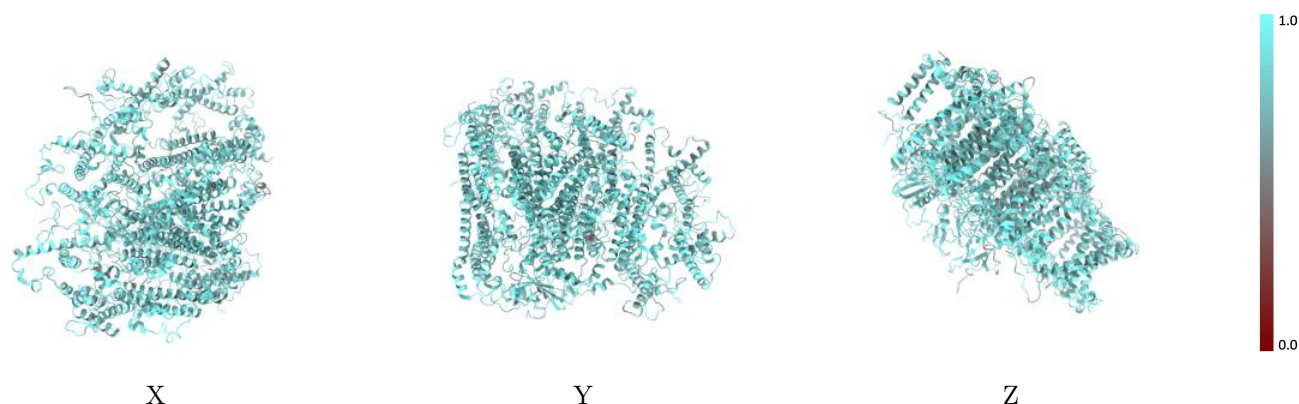
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



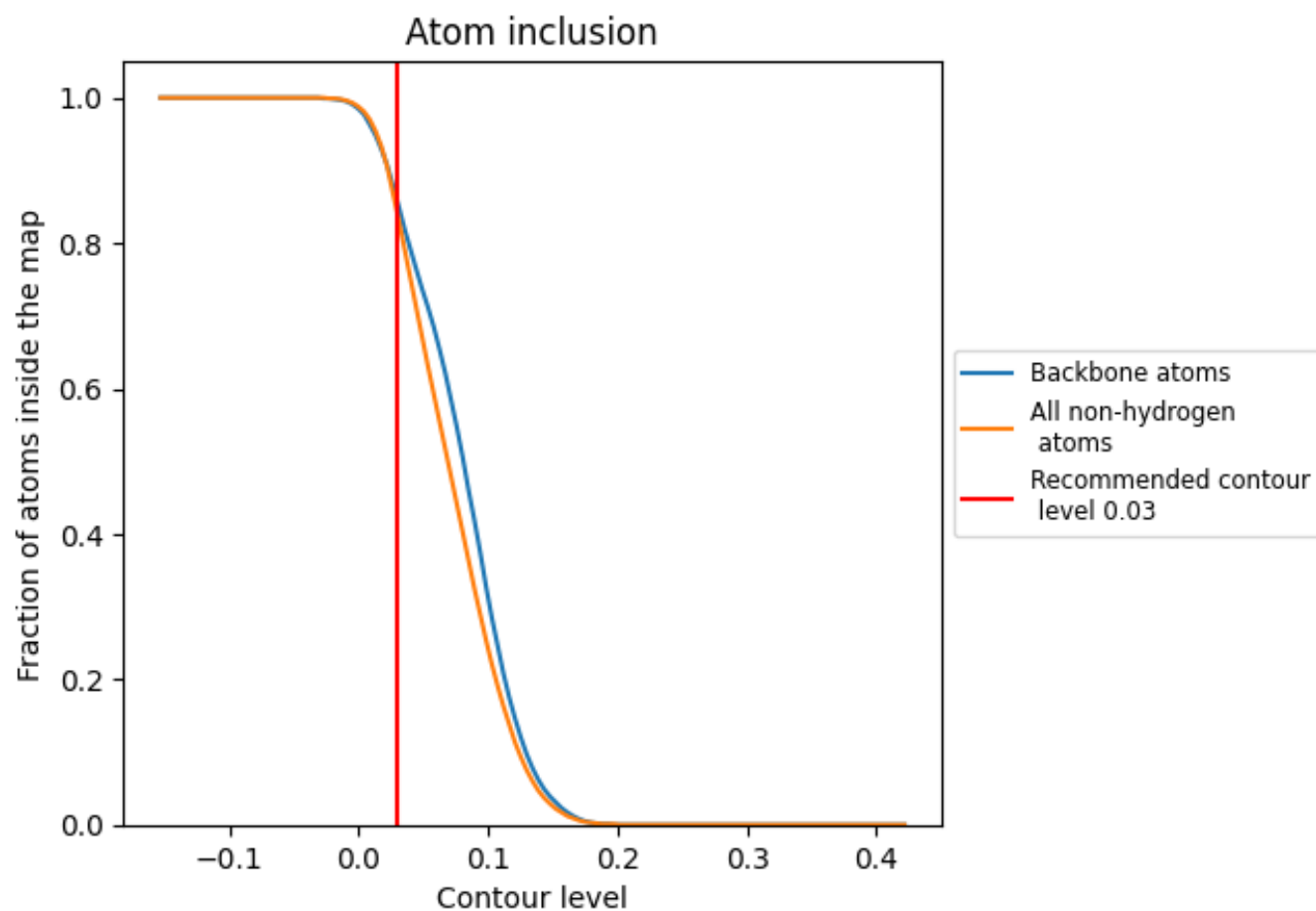
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8400	<div><div></div></div> 0.5260
A1	<div><div></div></div> 0.8080	<div><div></div></div> 0.4950
A3	<div><div></div></div> 0.8200	<div><div></div></div> 0.4920
A4	<div><div></div></div> 0.8260	<div><div></div></div> 0.5120
A6	<div><div></div></div> 0.7940	<div><div></div></div> 0.5080
AA	<div><div></div></div> 0.8520	<div><div></div></div> 0.5410
AB	<div><div></div></div> 0.8730	<div><div></div></div> 0.5510
AC	<div><div></div></div> 0.9040	<div><div></div></div> 0.5380
AD	<div><div></div></div> 0.8780	<div><div></div></div> 0.5350
AE	<div><div></div></div> 0.8330	<div><div></div></div> 0.5360
AF	<div><div></div></div> 0.8530	<div><div></div></div> 0.5450
AG	<div><div></div></div> 0.8030	<div><div></div></div> 0.4910
AH	<div><div></div></div> 0.8220	<div><div></div></div> 0.4920
AI	<div><div></div></div> 0.8040	<div><div></div></div> 0.5050
AJ	<div><div></div></div> 0.7780	<div><div></div></div> 0.5130
AK	<div><div></div></div> 0.7230	<div><div></div></div> 0.4550
AL	<div><div></div></div> 0.8090	<div><div></div></div> 0.5000

1.0

0.0

<0.0