



## Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 05:55 PM JST

PDB ID : 7FIX  
EMDB ID : EMD-31605  
Title : Cryo-EM structure of cyanobacterial photosystem I in the presence of ferredoxin and cytochrome c6  
Authors : Li, J.; Kurisu, G.  
Deposited on : 2021-08-01  
Resolution : 1.97 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>.

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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

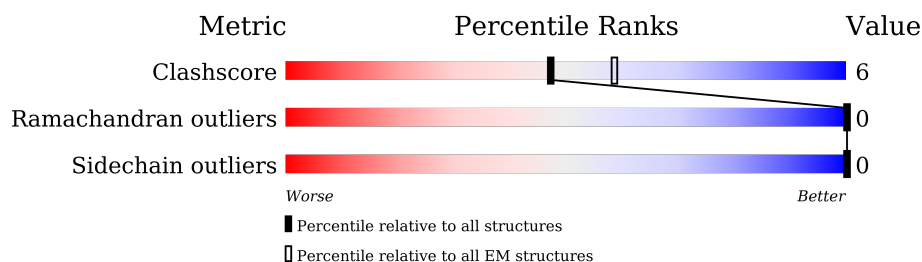
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 1.97 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.




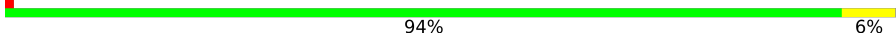

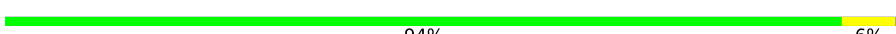


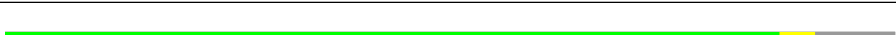
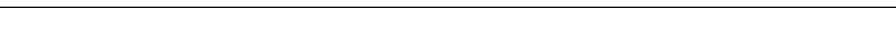
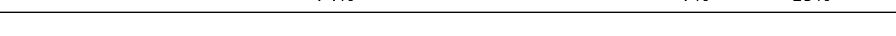
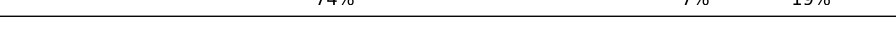
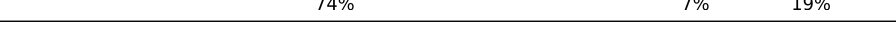
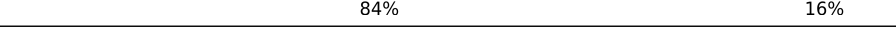












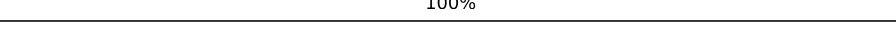
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A1	755	89% 10% .
1	A2	755	89% 10% .
1	A3	755	89% 9% .
2	B1	741	89% 11%
2	B2	741	88% 12%
2	B3	741	89% 11%
3	C1	81	93% 6% .
3	C2	81	91% 7% .

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Mol	Chain	Length	Quality of chain
3	C3	81	
4	D1	139	
4	D2	139	
4	D3	139	
5	E1	76	
5	E2	76	
5	E3	76	
6	F1	174	
6	F2	174	
6	F3	174	
7	I1	38	
7	I2	38	
7	I3	38	
8	J1	41	
8	J2	41	
8	J3	41	
9	K1	83	
9	K2	83	
9	K3	83	
10	L1	155	
10	L2	155	
10	L3	155	
11	M1	31	
11	M2	31	
11	M3	31	

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Mol	Chain	Length	Quality of chain
12	R1	98	
12	R2	98	
12	R3	98	
13	X1	39	
13	X2	39	
13	X3	39	

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
14	CL0	A1	801	X	-	-	-
14	CL0	A2	801	X	-	-	-
14	CL0	A3	801	X	-	-	-
15	CLA	A1	802	X	-	-	-
15	CLA	A1	803	X	-	-	-
15	CLA	A1	804	X	-	-	-
15	CLA	A1	805	X	-	-	-
15	CLA	A1	806	X	-	-	-
15	CLA	A1	807	X	-	-	-
15	CLA	A1	808	X	-	-	-
15	CLA	A1	809	X	-	-	-
15	CLA	A1	810	X	-	-	-
15	CLA	A1	811	X	-	-	-
15	CLA	A1	812	X	-	-	-
15	CLA	A1	813	X	-	-	-
15	CLA	A1	814	X	-	-	-
15	CLA	A1	815	X	-	-	-
15	CLA	A1	816	X	-	-	-
15	CLA	A1	817	X	-	-	-
15	CLA	A1	818	X	-	-	-
15	CLA	A1	819	X	-	-	-
15	CLA	A1	820	X	-	-	-
15	CLA	A1	821	X	-	-	-
15	CLA	A1	822	X	-	-	-
15	CLA	A1	823	X	-	-	-
15	CLA	A1	824	X	-	-	-
15	CLA	A1	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A1	826	X	-	-	-
15	CLA	A1	827	X	-	-	-
15	CLA	A1	828	X	-	-	-
15	CLA	A1	829	X	-	-	-
15	CLA	A1	830	X	-	-	-
15	CLA	A1	831	X	-	-	-
15	CLA	A1	832	X	-	-	-
15	CLA	A1	833	X	-	-	-
15	CLA	A1	834	X	-	-	-
15	CLA	A1	835	X	-	-	-
15	CLA	A1	836	X	-	-	-
15	CLA	A1	837	X	-	-	-
15	CLA	A1	838	X	-	-	-
15	CLA	A1	839	X	-	-	-
15	CLA	A1	840	X	-	-	-
15	CLA	A1	841	X	-	-	-
15	CLA	A1	842	X	-	-	-
15	CLA	A1	843	X	-	-	-
15	CLA	A1	844	X	-	-	-
15	CLA	A1	856	X	-	-	-
15	CLA	A2	802	X	-	-	-
15	CLA	A2	803	X	-	-	-
15	CLA	A2	804	X	-	-	-
15	CLA	A2	805	X	-	-	-
15	CLA	A2	806	X	-	-	-
15	CLA	A2	807	X	-	-	-
15	CLA	A2	808	X	-	-	-
15	CLA	A2	809	X	-	-	-
15	CLA	A2	810	X	-	-	-
15	CLA	A2	811	X	-	-	-
15	CLA	A2	812	X	-	-	-
15	CLA	A2	813	X	-	-	-
15	CLA	A2	814	X	-	-	-
15	CLA	A2	815	X	-	-	-
15	CLA	A2	816	X	-	-	-
15	CLA	A2	817	X	-	-	-
15	CLA	A2	818	X	-	-	-
15	CLA	A2	819	X	-	-	-
15	CLA	A2	820	X	-	-	-
15	CLA	A2	821	X	-	-	-
15	CLA	A2	822	X	-	-	-
15	CLA	A2	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A2	824	X	-	-	-
15	CLA	A2	825	X	-	-	-
15	CLA	A2	826	X	-	-	-
15	CLA	A2	827	X	-	-	-
15	CLA	A2	828	X	-	-	-
15	CLA	A2	829	X	-	-	-
15	CLA	A2	830	X	-	-	-
15	CLA	A2	831	X	-	-	-
15	CLA	A2	832	X	-	-	-
15	CLA	A2	833	X	-	-	-
15	CLA	A2	834	X	-	-	-
15	CLA	A2	835	X	-	-	-
15	CLA	A2	836	X	-	-	-
15	CLA	A2	837	X	-	-	-
15	CLA	A2	838	X	-	-	-
15	CLA	A2	839	X	-	-	-
15	CLA	A2	840	X	-	-	-
15	CLA	A2	841	X	-	-	-
15	CLA	A2	842	X	-	-	-
15	CLA	A2	843	X	-	-	-
15	CLA	A2	844	X	-	-	-
15	CLA	A2	856	X	-	-	-
15	CLA	A3	802	X	-	-	-
15	CLA	A3	803	X	-	-	-
15	CLA	A3	804	X	-	-	-
15	CLA	A3	805	X	-	-	-
15	CLA	A3	806	X	-	-	-
15	CLA	A3	807	X	-	-	-
15	CLA	A3	808	X	-	-	-
15	CLA	A3	809	X	-	-	-
15	CLA	A3	810	X	-	-	-
15	CLA	A3	811	X	-	-	-
15	CLA	A3	812	X	-	-	-
15	CLA	A3	813	X	-	-	-
15	CLA	A3	814	X	-	-	-
15	CLA	A3	815	X	-	-	-
15	CLA	A3	816	X	-	-	-
15	CLA	A3	817	X	-	-	-
15	CLA	A3	818	X	-	-	-
15	CLA	A3	819	X	-	-	-
15	CLA	A3	820	X	-	-	-
15	CLA	A3	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A3	822	X	-	-	-
15	CLA	A3	823	X	-	-	-
15	CLA	A3	824	X	-	-	-
15	CLA	A3	825	X	-	-	-
15	CLA	A3	826	X	-	-	-
15	CLA	A3	827	X	-	-	-
15	CLA	A3	828	X	-	-	-
15	CLA	A3	829	X	-	-	-
15	CLA	A3	830	X	-	-	-
15	CLA	A3	831	X	-	-	-
15	CLA	A3	832	X	-	-	-
15	CLA	A3	833	X	-	-	-
15	CLA	A3	834	X	-	-	-
15	CLA	A3	835	X	-	-	-
15	CLA	A3	836	X	-	-	-
15	CLA	A3	837	X	-	-	-
15	CLA	A3	838	X	-	-	-
15	CLA	A3	839	X	-	-	-
15	CLA	A3	840	X	-	-	-
15	CLA	A3	841	X	-	-	-
15	CLA	A3	842	X	-	-	-
15	CLA	A3	843	X	-	-	-
15	CLA	A3	844	X	-	-	-
15	CLA	A3	856	X	-	-	-
15	CLA	B1	801	X	-	-	-
15	CLA	B1	802	X	-	-	-
15	CLA	B1	803	X	-	-	-
15	CLA	B1	804	X	-	-	-
15	CLA	B1	805	X	-	-	-
15	CLA	B1	806	X	-	-	-
15	CLA	B1	807	X	-	-	-
15	CLA	B1	808	X	-	-	-
15	CLA	B1	809	X	-	-	-
15	CLA	B1	810	X	-	-	-
15	CLA	B1	811	X	-	-	-
15	CLA	B1	812	X	-	-	-
15	CLA	B1	813	X	-	-	-
15	CLA	B1	814	X	-	-	-
15	CLA	B1	815	X	-	-	-
15	CLA	B1	816	X	-	-	-
15	CLA	B1	817	X	-	-	-
15	CLA	B1	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B1	819	X	-	-	-
15	CLA	B1	820	X	-	-	-
15	CLA	B1	821	X	-	-	-
15	CLA	B1	822	X	-	-	-
15	CLA	B1	823	X	-	-	-
15	CLA	B1	824	X	-	-	-
15	CLA	B1	825	X	-	-	-
15	CLA	B1	826	X	-	-	-
15	CLA	B1	827	X	-	-	-
15	CLA	B1	828	X	-	-	-
15	CLA	B1	829	X	-	-	-
15	CLA	B1	830	X	-	-	-
15	CLA	B1	831	X	-	-	-
15	CLA	B1	832	X	-	-	-
15	CLA	B1	833	X	-	-	-
15	CLA	B1	834	X	-	-	-
15	CLA	B1	835	X	-	-	-
15	CLA	B1	836	X	-	-	-
15	CLA	B1	837	X	-	-	-
15	CLA	B1	838	X	-	-	-
15	CLA	B1	839	X	-	-	-
15	CLA	B1	849	X	-	-	-
15	CLA	B2	801	X	-	-	-
15	CLA	B2	802	X	-	-	-
15	CLA	B2	803	X	-	-	-
15	CLA	B2	804	X	-	-	-
15	CLA	B2	805	X	-	-	-
15	CLA	B2	806	X	-	-	-
15	CLA	B2	807	X	-	-	-
15	CLA	B2	808	X	-	-	-
15	CLA	B2	809	X	-	-	-
15	CLA	B2	810	X	-	-	-
15	CLA	B2	811	X	-	-	-
15	CLA	B2	812	X	-	-	-
15	CLA	B2	813	X	-	-	-
15	CLA	B2	814	X	-	-	-
15	CLA	B2	815	X	-	-	-
15	CLA	B2	816	X	-	-	-
15	CLA	B2	817	X	-	-	-
15	CLA	B2	818	X	-	-	-
15	CLA	B2	819	X	-	-	-
15	CLA	B2	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B2	821	X	-	-	-
15	CLA	B2	822	X	-	-	-
15	CLA	B2	823	X	-	-	-
15	CLA	B2	824	X	-	-	-
15	CLA	B2	825	X	-	-	-
15	CLA	B2	826	X	-	-	-
15	CLA	B2	827	X	-	-	-
15	CLA	B2	828	X	-	-	-
15	CLA	B2	829	X	-	-	-
15	CLA	B2	830	X	-	-	-
15	CLA	B2	831	X	-	-	-
15	CLA	B2	832	X	-	-	-
15	CLA	B2	833	X	-	-	-
15	CLA	B2	834	X	-	-	-
15	CLA	B2	835	X	-	-	-
15	CLA	B2	836	X	-	-	-
15	CLA	B2	837	X	-	-	-
15	CLA	B2	838	X	-	-	-
15	CLA	B2	839	X	-	-	-
15	CLA	B2	849	X	-	-	-
15	CLA	B3	801	X	-	-	-
15	CLA	B3	802	X	-	-	-
15	CLA	B3	803	X	-	-	-
15	CLA	B3	804	X	-	-	-
15	CLA	B3	805	X	-	-	-
15	CLA	B3	806	X	-	-	-
15	CLA	B3	807	X	-	-	-
15	CLA	B3	808	X	-	-	-
15	CLA	B3	809	X	-	-	-
15	CLA	B3	810	X	-	-	-
15	CLA	B3	811	X	-	-	-
15	CLA	B3	812	X	-	-	-
15	CLA	B3	813	X	-	-	-
15	CLA	B3	814	X	-	-	-
15	CLA	B3	815	X	-	-	-
15	CLA	B3	816	X	-	-	-
15	CLA	B3	817	X	-	-	-
15	CLA	B3	818	X	-	-	-
15	CLA	B3	819	X	-	-	-
15	CLA	B3	820	X	-	-	-
15	CLA	B3	821	X	-	-	-
15	CLA	B3	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B3	823	X	-	-	-
15	CLA	B3	824	X	-	-	-
15	CLA	B3	825	X	-	-	-
15	CLA	B3	826	X	-	-	-
15	CLA	B3	827	X	-	-	-
15	CLA	B3	828	X	-	-	-
15	CLA	B3	829	X	-	-	-
15	CLA	B3	830	X	-	-	-
15	CLA	B3	831	X	-	-	-
15	CLA	B3	832	X	-	-	-
15	CLA	B3	833	X	-	-	-
15	CLA	B3	834	X	-	-	-
15	CLA	B3	835	X	-	-	-
15	CLA	B3	836	X	-	-	-
15	CLA	B3	837	X	-	-	-
15	CLA	B3	838	X	-	-	-
15	CLA	B3	839	X	-	-	-
15	CLA	B3	849	X	-	-	-
15	CLA	I1	101	X	-	-	-
15	CLA	I2	101	X	-	-	-
15	CLA	I3	101	X	-	-	-
15	CLA	J1	1301	X	-	-	-
15	CLA	J1	1302	X	-	-	-
15	CLA	J1	1303	X	-	-	-
15	CLA	J1	1307	X	-	-	-
15	CLA	J2	1301	X	-	-	-
15	CLA	J2	1302	X	-	-	-
15	CLA	J2	1303	X	-	-	-
15	CLA	J2	1307	X	-	-	-
15	CLA	J3	1301	X	-	-	-
15	CLA	J3	1302	X	-	-	-
15	CLA	J3	1303	X	-	-	-
15	CLA	J3	1307	X	-	-	-
15	CLA	K1	101	X	-	-	-
15	CLA	K1	103	X	-	-	-
15	CLA	K2	101	X	-	-	-
15	CLA	K2	103	X	-	-	-
15	CLA	K3	101	X	-	-	-
15	CLA	K3	103	X	-	-	-
15	CLA	L1	1002	X	-	-	-
15	CLA	L1	1003	X	-	-	-
15	CLA	L1	1004	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	L2	1002	X	-	-	-
15	CLA	L2	1003	X	-	-	-
15	CLA	L2	1004	X	-	-	-
15	CLA	L3	1002	X	-	-	-
15	CLA	L3	1003	X	-	-	-
15	CLA	L3	1004	X	-	-	-
15	CLA	X1	102	X	-	-	-
15	CLA	X2	102	X	-	-	-
15	CLA	X3	102	X	-	-	-

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 73929 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	A1	745	Total	C	N	O	S	0	0
			5676	3708	990	952	26		
1	A2	745	Total	C	N	O	S	0	0
			5676	3708	990	952	26		
1	A3	745	Total	C	N	O	S	0	0
			5676	3708	990	952	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	740	Total	C	N	O	S	0	0
			5853	3853	984	995	21		
2	B2	740	Total	C	N	O	S	0	0
			5853	3853	984	995	21		
2	B3	740	Total	C	N	O	S	0	0
			5853	3853	984	995	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	C2	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	C3	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	138	Total	C	N	O	S	0	0
			1067	677	185	202	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	D2	138	Total	C	N	O	S	0	0
			1067	677	185	202	3		
4	D3	138	Total	C	N	O	S	0	0
			1067	677	185	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	69	Total	C	N	O		0	0
			532	339	93	100			
5	E2	69	Total	C	N	O		0	0
			532	339	93	100			
5	E3	69	Total	C	N	O		0	0
			532	339	93	100			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	141	Total	C	N	O	S	0	0
			1038	667	183	184	4		
6	F2	141	Total	C	N	O	S	0	0
			1038	667	183	184	4		
6	F3	141	Total	C	N	O	S	0	0
			1038	667	183	184	4		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	-9	HIS	-	expression tag	UNP P0A401
F1	-8	HIS	-	expression tag	UNP P0A401
F1	-7	HIS	-	expression tag	UNP P0A401
F1	-6	HIS	-	expression tag	UNP P0A401
F1	-5	HIS	-	expression tag	UNP P0A401
F1	-4	HIS	-	expression tag	UNP P0A401
F1	-3	HIS	-	expression tag	UNP P0A401
F1	-2	HIS	-	expression tag	UNP P0A401
F1	-1	HIS	-	expression tag	UNP P0A401
F1	0	HIS	-	expression tag	UNP P0A401
F2	-9	HIS	-	expression tag	UNP P0A401
F2	-8	HIS	-	expression tag	UNP P0A401
F2	-7	HIS	-	expression tag	UNP P0A401
F2	-6	HIS	-	expression tag	UNP P0A401

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Chain	Residue	Modelled	Actual	Comment	Reference
F2	-5	HIS	-	expression tag	UNP P0A401
F2	-4	HIS	-	expression tag	UNP P0A401
F2	-3	HIS	-	expression tag	UNP P0A401
F2	-2	HIS	-	expression tag	UNP P0A401
F2	-1	HIS	-	expression tag	UNP P0A401
F2	0	HIS	-	expression tag	UNP P0A401
F3	-9	HIS	-	expression tag	UNP P0A401
F3	-8	HIS	-	expression tag	UNP P0A401
F3	-7	HIS	-	expression tag	UNP P0A401
F3	-6	HIS	-	expression tag	UNP P0A401
F3	-5	HIS	-	expression tag	UNP P0A401
F3	-4	HIS	-	expression tag	UNP P0A401
F3	-3	HIS	-	expression tag	UNP P0A401
F3	-2	HIS	-	expression tag	UNP P0A401
F3	-1	HIS	-	expression tag	UNP P0A401
F3	0	HIS	-	expression tag	UNP P0A401

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I1	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	I2	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	I3	38	Total	C	N	O	S	0	0
			301	208	40	48	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J1	41	Total	C	N	O	S	0	0
			337	231	51	53	2		
8	J2	41	Total	C	N	O	S	0	0
			337	231	51	53	2		
8	J3	41	Total	C	N	O	S	0	0
			337	231	51	53	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K1	79	Total	C	N	O	S	0	0
			483	306	84	92	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	K2	79	Total	C	N	O	S	0	0
			483	306	84	92	1		
9	K3	79	Total	C	N	O	S	0	0
			483	306	84	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L1	152	Total	C	N	O	S	0	0
			1121	736	180	201	4		
10	L2	152	Total	C	N	O	S	0	0
			1121	736	180	201	4		
10	L3	152	Total	C	N	O	S	0	0
			1121	736	180	201	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M1	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	M2	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	M3	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Ferredoxin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R1	97	Total	C	N	O	S	0	0
			748	463	116	164	5		
12	R2	97	Total	C	N	O	S	0	0
			748	463	116	164	5		
12	R3	97	Total	C	N	O	S	0	0
			748	463	116	164	5		

- Molecule 13 is a protein called Photosystem I 4.8K protein.

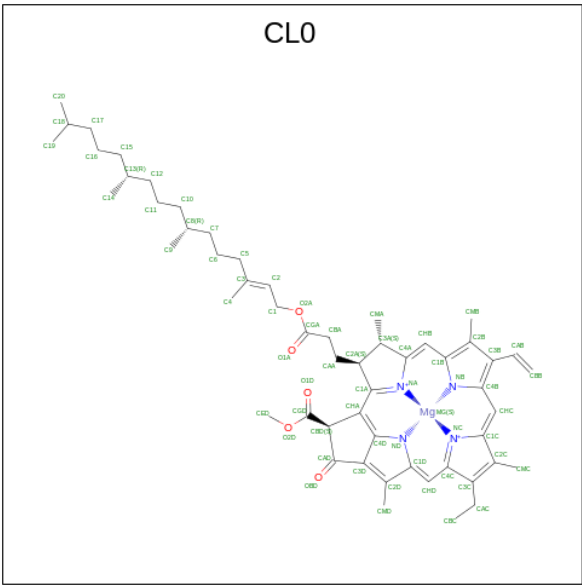
Mol	Chain	Residues	Atoms				AltConf	Trace
13	X1	28	Total	C	N	O	0	0
			225	159	33	33		
13	X2	28	Total	C	N	O	0	0
			225	159	33	33		

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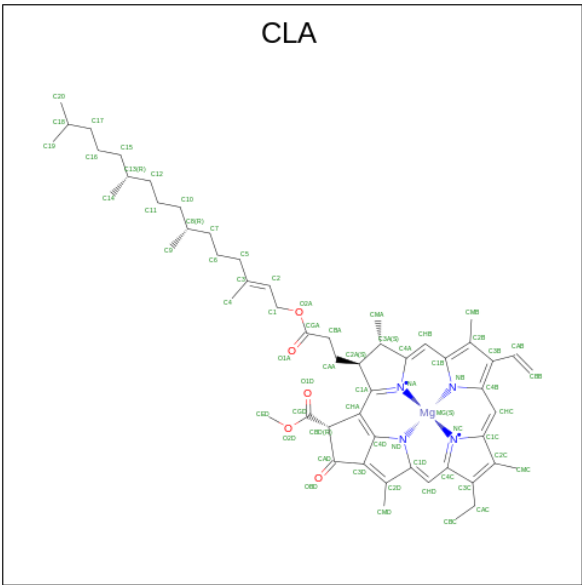
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	X3	28	225	159	33	33	0	0

- Molecule 14 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A3	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	A1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			33	27	1	4	1	
15	A1	1	Total	C	Mg	N	O	0
			36	28	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
15	A1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	A1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	A1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	A1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
15	A1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
15	A1	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	A1	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A1	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A1	1	Total 40	C 32	Mg 1	N 4	O 3	0
15	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B1	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	B1	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B1	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	B1	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B1	1	Total 44	C 34	Mg 1	N 4	O 5	0
15	B1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	B1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
15	B1	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
15	B1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
15	B1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
15	B1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			37	31	1	4	1	

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Mol	Chain	Residues	Atoms					AltConf
15	B1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	I1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	J1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	J1	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
15	J1	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
15	J1	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
15	K1	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
15	K1	1	Total	C	Mg	N	O	0
			32	26	1	4	1	
15	L1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	L1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	L1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	X1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			33	27	1	4	1	
15	A2	1	Total	C	Mg	N	O	0
			36	28	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
15	B2	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
15	B2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
15	B2	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
15	B2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
15	B2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
15	B2	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
15	B2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	B2	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
15	B2	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
15	B2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	I2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	J2	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	J2	1	Total	C	Mg	N	O	0
			35	29	1	4	1	

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Mol	Chain	Residues	Atoms					AltConf
15	J2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
15	J2	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
15	K2	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
15	K2	1	Total	C	Mg	N	O	0
			32	26	1	4	1	
15	L2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	L2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	L2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	X2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			33	27	1	4	1	

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Mol	Chain	Residues	Atoms					AltConf
15	A3	1	Total	C	Mg	N	O	0
			36	28	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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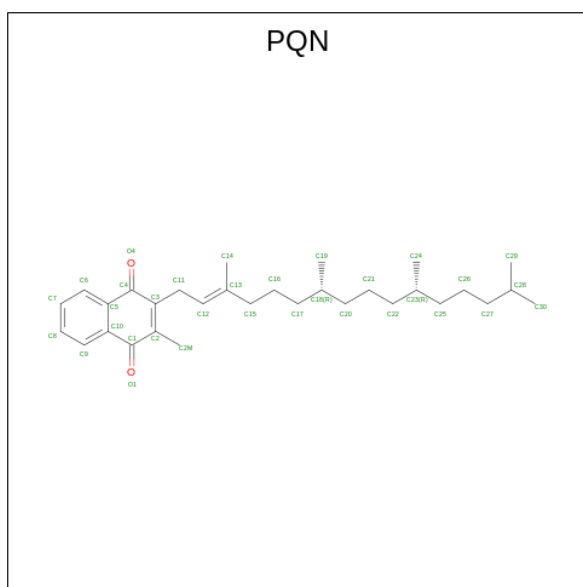
Mol	Chain	Residues	Atoms					AltConf
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
15	B3	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
15	B3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
15	B3	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
15	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
15	B3	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
15	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
15	B3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
15	B3	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
15	B3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	I3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	J3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
15	J3	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
15	J3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
15	J3	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
15	K3	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
15	K3	1	Total	C	Mg	N	O	0
			32	26	1	4	1	
15	L3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	L3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	L3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	X3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

- Molecule 16 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



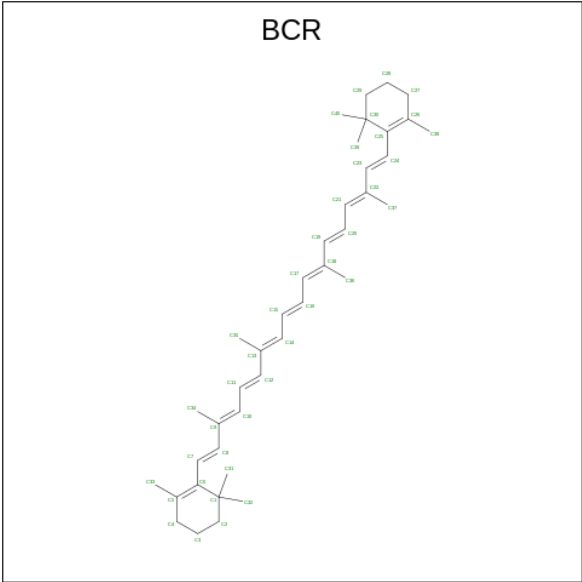
Mol	Chain	Residues	Atoms			AltConf
16	A1	1	Total	C	O	0
			33	31	2	
16	B1	1	Total	C	O	0
			33	31	2	
16	A2	1	Total	C	O	0
			33	31	2	
16	B2	1	Total	C	O	0
			33	31	2	
16	A3	1	Total	C	O	0
			33	31	2	
16	B3	1	Total	C	O	0
			33	31	2	

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	A1	1	Total	Fe	S	0
			8	4	4	
17	C1	1	Total	Fe	S	0
			8	4	4	
17	C1	1	Total	Fe	S	0
			8	4	4	
17	A2	1	Total	Fe	S	0
			8	4	4	
17	C2	1	Total	Fe	S	0
			8	4	4	
17	C2	1	Total	Fe	S	0
			8	4	4	
17	A3	1	Total	Fe	S	0
			8	4	4	
17	C3	1	Total	Fe	S	0
			8	4	4	
17	C3	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
18	A1	1	Total	C	0
			40	40	
18	A1	1	Total	C	0
			40	40	
18	A1	1	Total	C	0
			40	40	
18	A1	1	Total	C	0
			40	40	
18	A1	1	Total	C	0
			40	40	
18	A1	1	Total	C	0
			40	40	
18	A1	1	Total	C	0
			30	30	
18	B1	1	Total	C	0
			40	40	
18	B1	1	Total	C	0
			30	30	
18	B1	1	Total	C	0
			25	25	
18	B1	1	Total	C	0
			40	40	
18	B1	1	Total	C	0
			40	40	
18	B1	1	Total	C	0
			40	40	
18	B1	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
18	F1	1	Total C 40 40	0
18	I1	1	Total C 40 40	0
18	I1	1	Total C 40 40	0
18	J1	1	Total C 40 40	0
18	J1	1	Total C 40 40	0
18	J1	1	Total C 40 40	0
18	K1	1	Total C 25 25	0
18	L1	1	Total C 40 40	0
18	L1	1	Total C 40 40	0
18	L1	1	Total C 40 40	0
18	M1	1	Total C 40 40	0
18	A2	1	Total C 40 40	0
18	A2	1	Total C 40 40	0
18	A2	1	Total C 40 40	0
18	A2	1	Total C 40 40	0
18	A2	1	Total C 40 40	0
18	A2	1	Total C 40 40	0
18	A2	1	Total C 30 30	0
18	B2	1	Total C 40 40	0
18	B2	1	Total C 30 30	0
18	B2	1	Total C 25 25	0

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Mol	Chain	Residues	Atoms	AltConf
18	B2	1	Total C 40 40	0
18	B2	1	Total C 40 40	0
18	B2	1	Total C 40 40	0
18	B2	1	Total C 40 40	0
18	F2	1	Total C 40 40	0
18	I2	1	Total C 40 40	0
18	I2	1	Total C 40 40	0
18	J2	1	Total C 40 40	0
18	J2	1	Total C 40 40	0
18	J2	1	Total C 40 40	0
18	K2	1	Total C 25 25	0
18	L2	1	Total C 40 40	0
18	L2	1	Total C 40 40	0
18	M2	1	Total C 40 40	0
18	A3	1	Total C 40 40	0
18	A3	1	Total C 40 40	0
18	A3	1	Total C 40 40	0
18	A3	1	Total C 40 40	0
18	A3	1	Total C 40 40	0
18	A3	1	Total C 40 40	0
18	A3	1	Total C 30 30	0

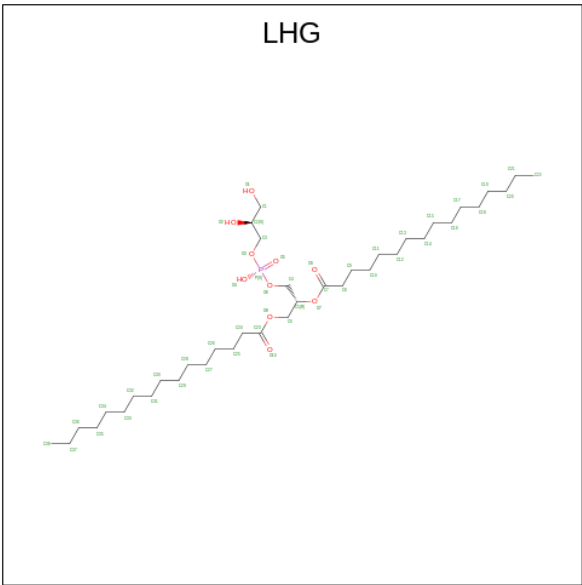
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Mol	Chain	Residues	Atoms	AltConf
18	B3	1	Total C 40 40	0
18	B3	1	Total C 30 30	0
18	B3	1	Total C 25 25	0
18	B3	1	Total C 40 40	0
18	B3	1	Total C 40 40	0
18	B3	1	Total C 40 40	0
18	B3	1	Total C 40 40	0
18	B3	1	Total C 40 40	0
18	F3	1	Total C 40 40	0
18	I3	1	Total C 40 40	0
18	I3	1	Total C 40 40	0
18	J3	1	Total C 40 40	0
18	J3	1	Total C 40 40	0
18	J3	1	Total C 40 40	0
18	K3	1	Total C 25 25	0
18	L3	1	Total C 40 40	0
18	M3	1	Total C 40 40	0

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf
19	A1	1	Total	C	O	P	0
			47	36	10	1	
19	A1	1	Total	C	O	P	0
			35	24	10	1	
19	X1	1	Total	C	O	P	0
			42	31	10	1	
19	A2	1	Total	C	O	P	0
			47	36	10	1	
19	A2	1	Total	C	O	P	0
			35	24	10	1	
19	X2	1	Total	C	O	P	0
			42	31	10	1	
19	A3	1	Total	C	O	P	0
			47	36	10	1	
19	A3	1	Total	C	O	P	0
			35	24	10	1	
19	X3	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 20 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

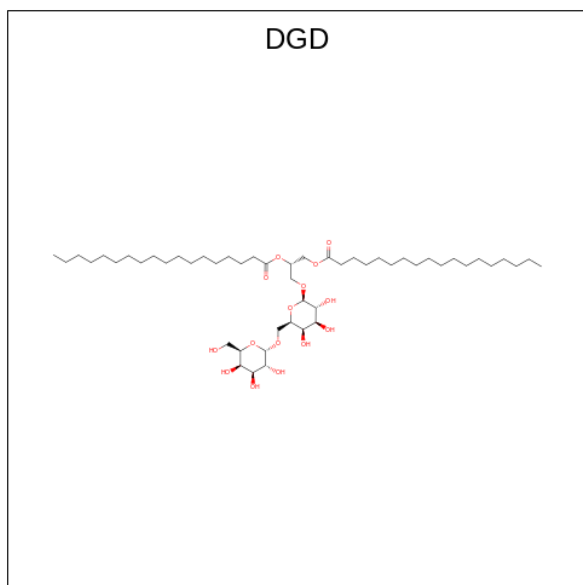
Mol	Chain	Residues	Atoms		AltConf
20	A1	7	Total	C	0
			97	97	
20	I1	4	Total	C	0
			61	61	

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Mol	Chain	Residues	Atoms	AltConf
20	L1	4	Total C 64 64	0
20	M1	2	Total C 32 32	0
20	A2	7	Total C 97 97	0
20	I2	4	Total C 61 61	0
20	L2	4	Total C 64 64	0
20	M2	2	Total C 32 32	0
20	A3	7	Total C 97 97	0
20	I3	4	Total C 61 61	0
20	L3	4	Total C 64 64	0
20	M3	2	Total C 32 32	0

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
21	B1	1	Total C O 66 51 15	0

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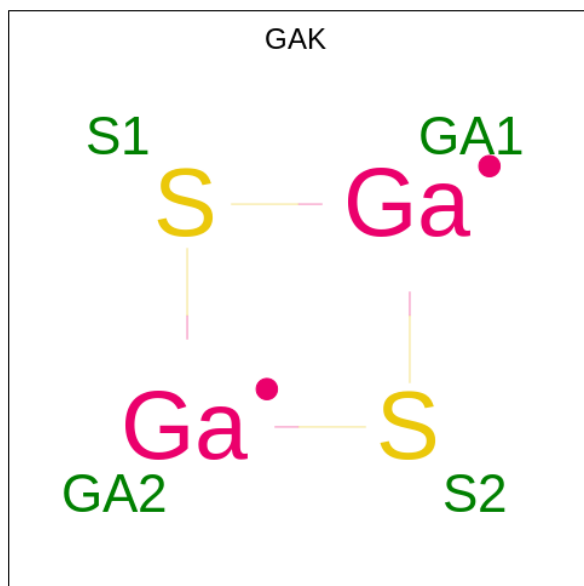
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Mol	Chain	Residues	Atoms			AltConf
21	B2	1	Total	C	O	0
			66	51	15	
21	B3	1	Total	C	O	0
			66	51	15	

- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
22	L1	1	Total	Ca	0
			1	1	
22	L2	1	Total	Ca	0
			1	1	
22	L3	1	Total	Ca	0
			1	1	

- Molecule 23 is [2Ga-2S] cluster (three-letter code: GAK) (formula: Ga<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	R1	1	Total	Ga	S	0
			4	2	2	
23	R2	1	Total	Ga	S	0
			4	2	2	
23	R3	1	Total	Ga	S	0
			4	2	2	

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	A1	26	Total 26	O 26	0
24	B1	42	Total 42	O 42	0
24	C1	13	Total 13	O 13	0
24	D1	7	Total 7	O 7	0
24	E1	1	Total 1	O 1	0
24	I1	1	Total 1	O 1	0
24	L1	22	Total 22	O 22	0
24	R1	4	Total 4	O 4	0
24	A2	26	Total 26	O 26	0
24	B2	42	Total 42	O 42	0
24	C2	13	Total 13	O 13	0
24	D2	7	Total 7	O 7	0
24	E2	1	Total 1	O 1	0
24	I2	1	Total 1	O 1	0
24	L2	22	Total 22	O 22	0
24	R2	4	Total 4	O 4	0
24	A3	26	Total 26	O 26	0
24	B3	42	Total 42	O 42	0
24	C3	13	Total 13	O 13	0
24	D3	7	Total 7	O 7	0
24	E3	1	Total 1	O 1	0

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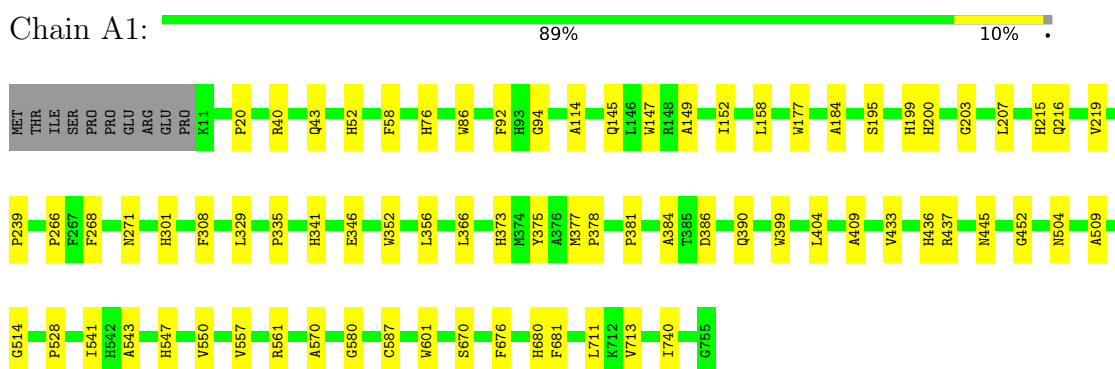
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
24	I3	1	Total 1	O 1	0
24	L3	22	Total 22	O 22	0
24	R3	4	Total 4	O 4	0

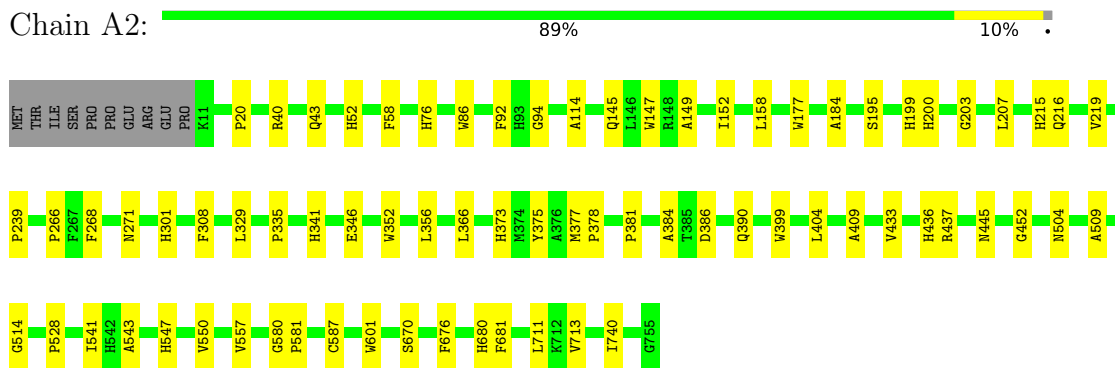
### 3 Residue-property plots [i](#)

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

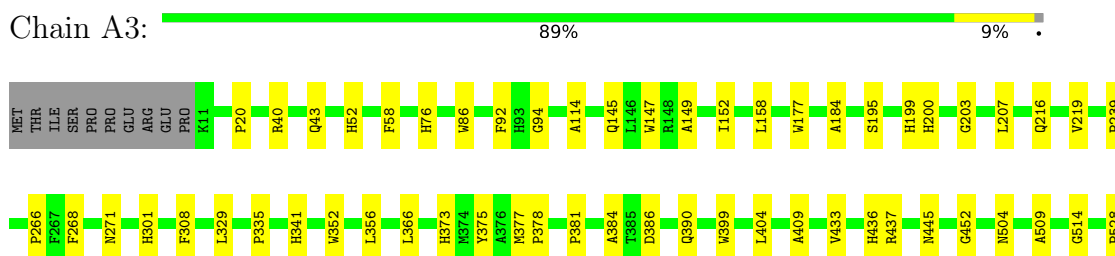
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



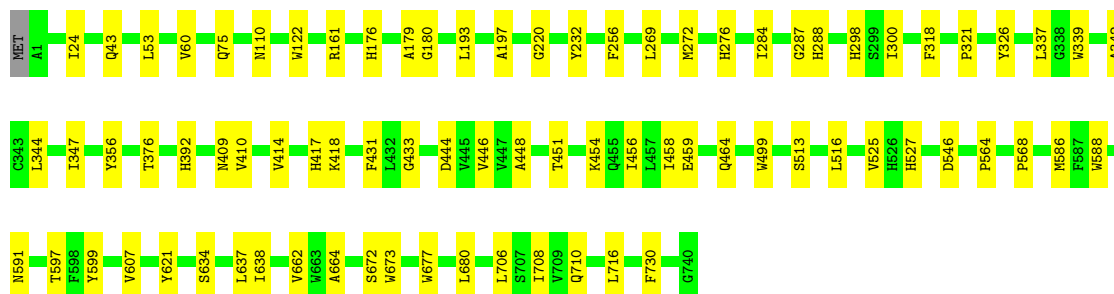
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





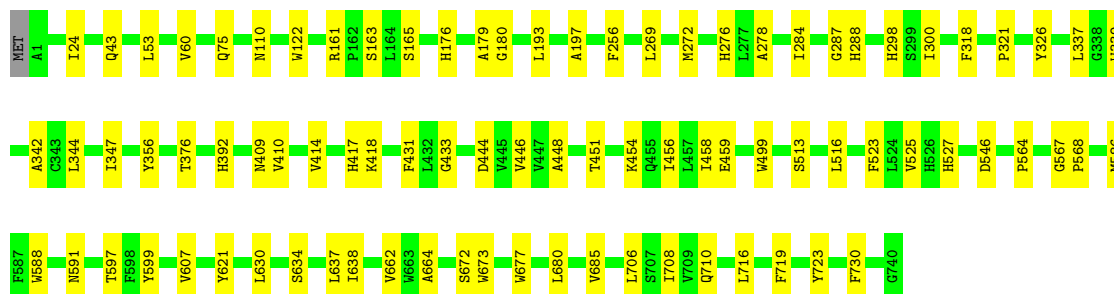
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B1: 89% 11%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B2: 88% 12%



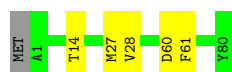
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B3: 89% 11%



- Molecule 3: Photosystem I iron-sulfur center

Chain C1: 93% 6%



- Molecule 3: Photosystem I iron-sulfur center

Chain C2:  91% 7%



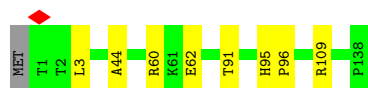
- Molecule 3: Photosystem I iron-sulfur center

Chain C3:  91% 7%



- Molecule 4: Photosystem I reaction center subunit II

Chain D1:  94% 6%



- Molecule 4: Photosystem I reaction center subunit II

Chain D2:  92% 7%




- Molecule 4: Photosystem I reaction center subunit II

Chain D3:  94% 6%




- Molecule 5: Photosystem I reaction center subunit IV

Chain E1:  87% 9%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E2:  87% 9%





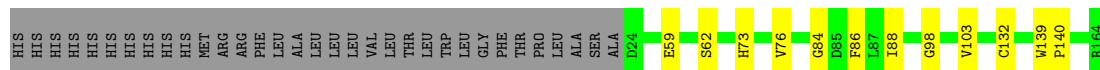
- Molecule 5: Photosystem I reaction center subunit IV

Chain E3:  87% 9%




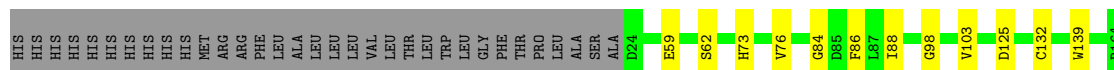
- Molecule 6: Photosystem I reaction center subunit III

Chain F1:  74% 7% 19%




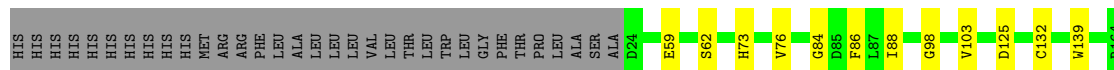
- Molecule 6: Photosystem I reaction center subunit III

Chain F2:  74% 7% 19%




- Molecule 6: Photosystem I reaction center subunit III

Chain F3:  74% 7% 19%




- Molecule 7: Photosystem I reaction center subunit VIII

Chain I1:  84% 16%




- Molecule 7: Photosystem I reaction center subunit VIII

Chain I2:  82% 18%




- Molecule 7: Photosystem I reaction center subunit VIII

Chain I3:  84% 16%




- Molecule 8: Photosystem I reaction center subunit IX

Chain J1:  83% 17%




- Molecule 8: Photosystem I reaction center subunit IX

Chain J2:  78% 22%




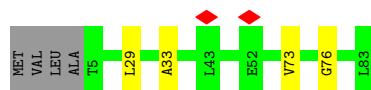
- Molecule 8: Photosystem I reaction center subunit IX

Chain J3:  78% 22%



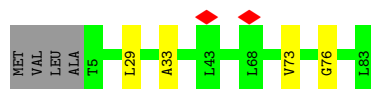
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K1:  90% 5% 5%



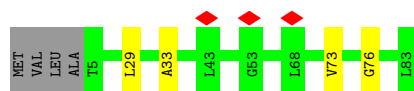
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K2:  90% 5% 5%



- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K3:  90% 5% 5%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L1:  90% 8% .



- Molecule 10: Photosystem I reaction center subunit XI

Chain L2:  91% 7%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L3:  90% 8%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M1:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem I reaction center subunit XII

Chain M2:  100%


There are no outlier residues recorded for this chain.

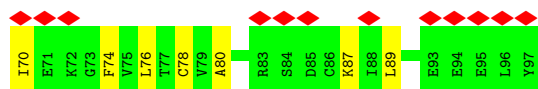
- Molecule 11: Photosystem I reaction center subunit XII

Chain M3:  100%


There are no outlier residues recorded for this chain.

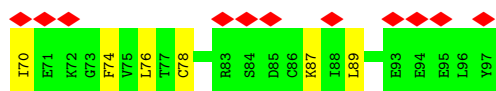
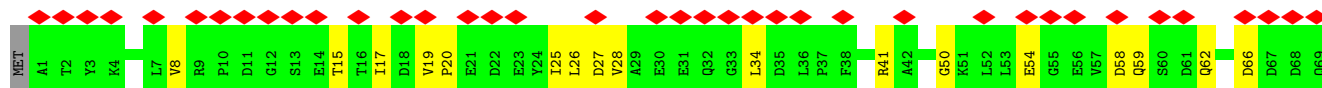
- Molecule 12: Ferredoxin-1

Chain R1:  56% 74% 24%

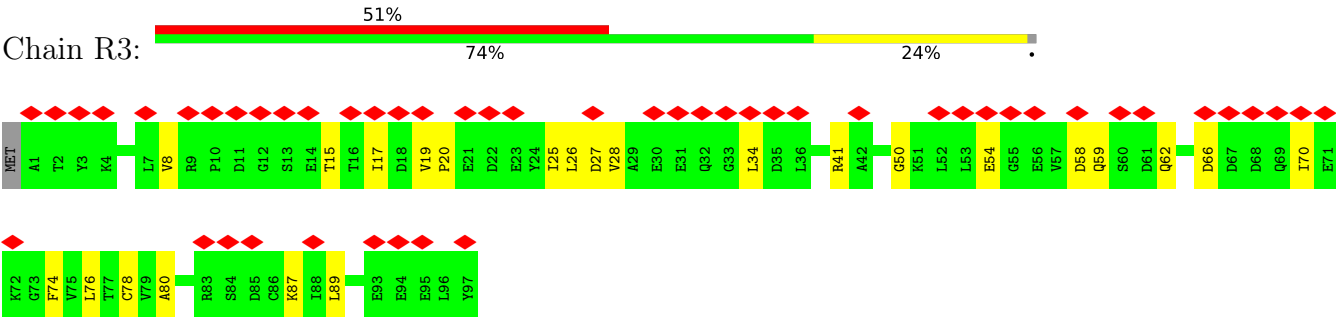


- Molecule 12: Ferredoxin-1

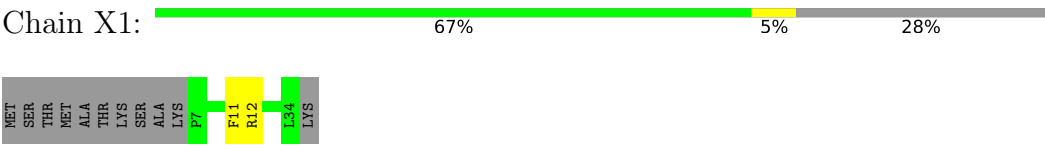
Chain R2:  50% 76% 23%



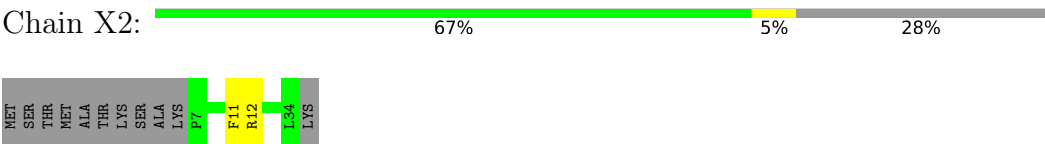
● Molecule 12: Ferredoxin-1



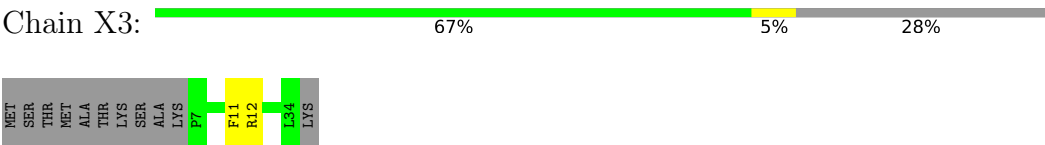
● Molecule 13: Photosystem I 4.8K protein



● Molecule 13: Photosystem I 4.8K protein



● Molecule 13: Photosystem I 4.8K protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	207142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	322.4, 322.4, 322.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.806, 0.806, 0.806	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, SF4, LHG, CLA, BCR, GAK, UNL, CA, PQN, DGD

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	A1	0.26	0/5862	0.43	0/8000
1	A2	0.26	0/5862	0.43	0/8000
1	A3	0.26	0/5862	0.43	0/8000
2	B1	0.26	0/6071	0.42	0/8302
2	B2	0.26	0/6071	0.42	0/8302
2	B3	0.26	0/6071	0.42	0/8302
3	C1	0.25	0/608	0.51	0/824
3	C2	0.25	0/608	0.51	0/824
3	C3	0.25	0/608	0.51	0/824
4	D1	0.26	0/1093	0.49	0/1483
4	D2	0.26	0/1093	0.49	0/1483
4	D3	0.26	0/1093	0.49	0/1483
5	E1	0.26	0/544	0.47	0/741
5	E2	0.26	0/544	0.47	0/741
5	E3	0.26	0/544	0.47	0/741
6	F1	0.24	0/1060	0.46	0/1443
6	F2	0.24	0/1060	0.46	0/1443
6	F3	0.24	0/1060	0.46	0/1443
7	I1	0.26	0/312	0.41	0/425
7	I2	0.26	0/312	0.41	0/425
7	I3	0.26	0/312	0.41	0/425
8	J1	0.27	0/349	0.45	0/476
8	J2	0.27	0/349	0.45	0/476
8	J3	0.27	0/349	0.45	0/476
9	K1	0.25	0/490	0.40	0/674
9	K2	0.25	0/490	0.40	0/674
9	K3	0.25	0/490	0.40	0/674
10	L1	0.26	0/1150	0.40	0/1561
10	L2	0.26	0/1150	0.40	0/1561
10	L3	0.26	0/1150	0.40	0/1561
11	M1	0.24	0/244	0.41	0/332
11	M2	0.24	0/244	0.41	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	M3	0.24	0/244	0.41	0/332
12	R1	0.26	0/758	0.48	0/1029
12	R2	0.26	0/758	0.48	0/1029
12	R3	0.26	0/758	0.48	0/1029
13	X1	0.35	0/234	0.47	0/320
13	X2	0.35	0/234	0.47	0/320
13	X3	0.35	0/234	0.47	0/320
All	All	0.26	0/56325	0.44	0/76830

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	A1	5676	0	5476	67	0
1	A2	5676	0	5476	67	0
1	A3	5676	0	5476	64	0
2	B1	5853	0	5580	64	0
2	B2	5853	0	5580	69	0
2	B3	5853	0	5580	68	0
3	C1	598	0	580	3	0
3	C2	598	0	580	4	0
3	C3	598	0	580	4	0
4	D1	1067	0	1062	5	0
4	D2	1067	0	1062	6	0
4	D3	1067	0	1062	5	0
5	E1	532	0	522	4	0
5	E2	532	0	522	4	0
5	E3	532	0	522	4	0
6	F1	1038	0	1040	7	0
6	F2	1038	0	1040	8	0
6	F3	1038	0	1040	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I1	301	0	306	5	0
7	I2	301	0	306	6	0
7	I3	301	0	306	5	0
8	J1	337	0	344	7	0
8	J2	337	0	344	8	0
8	J3	337	0	344	8	0
9	K1	483	0	409	3	0
9	K2	483	0	409	3	0
9	K3	483	0	409	3	0
10	L1	1121	0	1117	9	0
10	L2	1121	0	1117	8	0
10	L3	1121	0	1117	9	0
11	M1	241	0	264	0	0
11	M2	241	0	264	0	0
11	M3	241	0	264	0	0
12	R1	748	0	705	16	0
12	R2	748	0	705	15	0
12	R3	748	0	705	16	0
13	X1	225	0	213	3	0
13	X2	225	0	213	3	0
13	X3	225	0	213	2	0
14	A1	65	0	72	4	0
14	A2	65	0	72	2	0
14	A3	65	0	72	2	0
15	A1	2328	0	2111	66	0
15	A2	2328	0	2111	67	0
15	A3	2328	0	2111	65	0
15	B1	1961	0	1678	44	0
15	B2	1961	0	1678	50	0
15	B3	1961	0	1678	49	0
15	I1	65	0	72	3	0
15	I2	65	0	72	3	0
15	I3	65	0	72	3	0
15	J1	143	0	75	0	0
15	J2	143	0	75	1	0
15	J3	143	0	75	1	0
15	K1	66	0	30	2	0
15	K2	66	0	30	2	0
15	K3	66	0	30	2	0
15	L1	190	0	203	9	0
15	L2	190	0	203	7	0
15	L3	190	0	203	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	X1	40	0	24	1	0
15	X2	40	0	24	1	0
15	X3	40	0	24	1	0
16	A1	33	0	46	0	0
16	A2	33	0	46	0	0
16	A3	33	0	46	0	0
16	B1	33	0	46	4	0
16	B2	33	0	46	4	0
16	B3	33	0	46	5	0
17	A1	8	0	0	0	0
17	A2	8	0	0	0	0
17	A3	8	0	0	0	0
17	C1	16	0	0	0	0
17	C2	16	0	0	0	0
17	C3	16	0	0	0	0
18	A1	270	0	375	22	0
18	A2	270	0	375	18	0
18	A3	270	0	375	19	0
18	B1	255	0	352	15	0
18	B2	255	0	352	12	0
18	B3	255	0	352	14	0
18	F1	40	0	56	3	0
18	F2	40	0	56	4	0
18	F3	40	0	56	3	0
18	I1	80	0	112	2	0
18	I2	80	0	112	2	0
18	I3	80	0	112	4	0
18	J1	120	0	168	11	0
18	J2	120	0	168	8	0
18	J3	120	0	168	11	0
18	K1	25	0	33	0	0
18	K2	25	0	33	0	0
18	K3	25	0	33	0	0
18	L1	120	0	168	8	0
18	L2	80	0	112	5	0
18	L3	40	0	56	4	0
18	M1	40	0	56	2	0
18	M2	40	0	56	2	0
18	M3	40	0	56	3	0
19	A1	82	0	110	0	0
19	A2	82	0	110	0	0
19	A3	82	0	110	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	X1	42	0	57	5	0
19	X2	42	0	57	5	0
19	X3	42	0	57	4	0
20	A1	97	0	0	0	0
20	A2	97	0	0	0	0
20	A3	97	0	0	0	0
20	I1	61	0	0	0	0
20	I2	61	0	0	0	0
20	I3	61	0	0	0	0
20	L1	64	0	0	0	0
20	L2	64	0	0	0	0
20	L3	64	0	0	0	0
20	M1	32	0	0	0	0
20	M2	32	0	0	0	0
20	M3	32	0	0	0	0
21	B1	66	0	96	0	0
21	B2	66	0	96	0	0
21	B3	66	0	96	0	0
22	L1	1	0	0	0	0
22	L2	1	0	0	0	0
22	L3	1	0	0	0	0
23	R1	4	0	0	0	0
23	R2	4	0	0	0	0
23	R3	4	0	0	0	0
24	A1	26	0	0	1	0
24	A2	26	0	0	1	0
24	A3	26	0	0	1	0
24	B1	42	0	0	1	0
24	B2	42	0	0	1	0
24	B3	42	0	0	1	0
24	C1	13	0	0	0	0
24	C2	13	0	0	0	0
24	C3	13	0	0	0	0
24	D1	7	0	0	0	0
24	D2	7	0	0	0	0
24	D3	7	0	0	0	0
24	E1	1	0	0	0	0
24	E2	1	0	0	0	0
24	E3	1	0	0	0	0
24	I1	1	0	0	0	0
24	I2	1	0	0	0	0
24	I3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	L1	22	0	0	0	0
24	L2	22	0	0	0	0
24	L3	22	0	0	0	0
24	R1	4	0	0	0	0
24	R2	4	0	0	0	0
24	R3	4	0	0	0	0
All	All	73929	0	70506	829	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 6.

All (829) 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)
1:A2:207:LEU:HD11	15:A2:820:CLA:HMC1	1.72	0.72
8:J2:31:ARG:HE	18:J2:1305:BCR:H312	1.55	0.72
1:A1:207:LEU:HD11	15:A1:820:CLA:HMC1	1.72	0.71
1:A3:207:LEU:HD11	15:A3:820:CLA:HMC1	1.72	0.71
8:J3:31:ARG:HE	18:J3:1305:BCR:H312	1.55	0.70
8:J1:31:ARG:HE	18:J1:1305:BCR:H312	1.55	0.70
15:B2:810:CLA:HBB2	15:B2:812:CLA:HMA3	1.76	0.68
15:A3:819:CLA:HAB	15:A3:819:CLA:H8	1.76	0.68
15:B3:810:CLA:HBB2	15:B3:812:CLA:HMA3	1.76	0.67
15:B1:810:CLA:HBB2	15:B1:812:CLA:HMA3	1.76	0.67
15:A2:819:CLA:H8	15:A2:819:CLA:HAB	1.76	0.66
15:A1:819:CLA:HAB	15:A1:819:CLA:H8	1.76	0.66
9:K3:76:GLY:HA3	15:K3:103:CLA:HMA3	1.78	0.66
9:K2:76:GLY:HA3	15:K2:103:CLA:HMA3	1.78	0.66
9:K1:76:GLY:HA3	15:K1:103:CLA:HMA3	1.78	0.65
1:A2:601:TRP:CH2	15:A2:802:CLA:HAB	2.33	0.64
1:A1:86:TRP:HA	15:A1:807:CLA:HBB2	1.80	0.64
1:A1:601:TRP:CH2	15:A1:802:CLA:HAB	2.33	0.64
1:A2:86:TRP:HA	15:A2:807:CLA:HBB2	1.80	0.63
2:B2:60:VAL:HG21	15:B2:827:CLA:H2	1.80	0.63
2:B3:60:VAL:HG21	15:B3:827:CLA:H2	1.80	0.63
15:B1:838:CLA:H18	18:I1:102:BCR:H362	1.80	0.63
1:A3:601:TRP:CH2	15:A3:802:CLA:HAB	2.33	0.63
12:R3:62:GLN:HB2	12:R3:76:LEU:HD12	1.81	0.63
2:B1:60:VAL:HG21	15:B1:827:CLA:H2	1.81	0.63
15:B2:838:CLA:H18	18:I2:102:BCR:H362	1.80	0.63
1:A3:86:TRP:HA	15:A3:807:CLA:HBB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:399:TRP:HB3	15:A3:828:CLA:HMC3	1.81	0.63
13:X2:12:ARG:NH2	19:X2:101:LHG:HC41	2.14	0.63
1:A1:399:TRP:HB3	15:A1:828:CLA:HMC3	1.81	0.62
18:A1:850:BCR:H333	18:A1:851:BCR:H333	1.81	0.62
12:R1:62:GLN:HB2	12:R1:76:LEU:HD12	1.81	0.62
18:A2:850:BCR:H333	18:A2:851:BCR:H333	1.81	0.62
18:A3:850:BCR:H333	18:A3:851:BCR:H333	1.81	0.62
13:X3:12:ARG:NH2	19:X3:101:LHG:HC41	2.14	0.62
1:A2:399:TRP:HB3	15:A2:828:CLA:HMC3	1.81	0.62
12:R2:62:GLN:HB2	12:R2:76:LEU:HD12	1.81	0.62
2:B1:318:PHE:HB2	15:B1:822:CLA:HMA1	1.82	0.62
13:X1:12:ARG:NH2	19:X1:101:LHG:HC41	2.14	0.62
15:B3:838:CLA:H18	18:I3:102:BCR:H362	1.80	0.62
2:B2:318:PHE:HB2	15:B2:822:CLA:HMA1	1.82	0.61
2:B3:499:TRP:HE1	15:B3:832:CLA:HED3	1.65	0.61
1:A2:200:HIS:ND1	15:A2:825:CLA:OBD	2.33	0.61
2:B3:321:PRO:HB2	2:B3:409:ASN:HA	1.83	0.61
1:A2:378:PRO:HG3	1:A2:384:ALA:HB2	1.83	0.61
1:A2:409:ALA:HA	18:A2:851:BCR:HC41	1.83	0.60
1:A3:378:PRO:HG3	1:A3:384:ALA:HB2	1.83	0.60
2:B1:499:TRP:HE1	15:B1:832:CLA:HED3	1.65	0.60
1:A3:409:ALA:HA	18:A3:851:BCR:HC41	1.84	0.60
2:B3:318:PHE:HB2	15:B3:822:CLA:HMA1	1.82	0.60
1:A2:711:LEU:HD21	18:F2:201:BCR:H342	1.84	0.60
1:A3:504:ASN:HB2	15:A3:836:CLA:HED2	1.83	0.60
1:A2:504:ASN:HB2	15:A2:836:CLA:HED2	1.83	0.60
2:B2:321:PRO:HB2	2:B2:409:ASN:HA	1.83	0.60
2:B2:499:TRP:HE1	15:B2:832:CLA:HED3	1.65	0.60
1:A1:378:PRO:HG3	1:A1:384:ALA:HB2	1.83	0.60
1:A3:711:LEU:HD21	18:F3:201:BCR:H342	1.84	0.60
2:B1:321:PRO:HB2	2:B1:409:ASN:HA	1.83	0.60
15:B3:807:CLA:HHB	15:B3:808:CLA:HHB	1.84	0.60
15:B1:807:CLA:HHB	15:B1:808:CLA:HHB	1.84	0.59
2:B2:342:ALA:HB2	18:B2:845:BCR:H372	1.84	0.59
1:A1:711:LEU:HD21	18:F1:201:BCR:H342	1.84	0.59
15:A1:821:CLA:H151	15:A1:831:CLA:HBC1	1.85	0.59
1:A1:409:ALA:HA	18:A1:851:BCR:HC41	1.83	0.59
1:A1:504:ASN:HB2	15:A1:836:CLA:HED2	1.83	0.59
15:B1:831:CLA:HAB	15:B1:849:CLA:HMB2	1.85	0.58
2:B3:342:ALA:HB2	18:B3:845:BCR:H372	1.84	0.58
15:B2:831:CLA:HAB	15:B2:849:CLA:HMB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:342:ALA:HB2	18:B1:845:BCR:H372	1.84	0.58
15:B2:807:CLA:HHB	15:B2:808:CLA:HHB	1.84	0.58
7:I3:19:CYS:HB3	15:I3:101:CLA:HAB	1.86	0.58
15:A2:821:CLA:H151	15:A2:831:CLA:HBC1	1.85	0.58
2:B2:298:HIS:CE1	15:B2:821:CLA:HMD1	2.39	0.57
12:R1:19:VAL:HG11	12:R1:25:ILE:HD13	1.87	0.57
15:A3:821:CLA:H151	15:A3:831:CLA:HBC1	1.85	0.57
15:A3:833:CLA:H102	15:B3:838:CLA:H52	1.86	0.57
7:I1:19:CYS:HB3	15:I1:101:CLA:HAB	1.86	0.57
15:B3:831:CLA:HAB	15:B3:849:CLA:HMB2	1.85	0.57
15:A1:833:CLA:H102	15:B1:838:CLA:H52	1.86	0.57
7:I2:19:CYS:HB3	15:I2:101:CLA:HAB	1.86	0.57
2:B1:298:HIS:CE1	15:B1:821:CLA:HMD1	2.40	0.57
4:D1:3:LEU:HD21	4:D1:91:THR:HG21	1.87	0.57
2:B3:456:ILE:HG22	2:B3:458:ILE:HD11	1.87	0.57
4:D2:3:LEU:HD21	4:D2:91:THR:HG21	1.87	0.56
2:B1:456:ILE:HG22	2:B1:458:ILE:HD11	1.87	0.56
1:A1:200:HIS:ND1	15:A1:825:CLA:OBD	2.33	0.56
2:B3:298:HIS:CE1	15:B3:821:CLA:HMD1	2.40	0.56
1:A2:681:PHE:CG	18:A2:852:BCR:H363	2.41	0.56
15:B3:827:CLA:H8	18:B3:842:BCR:H21C	1.87	0.56
15:A2:833:CLA:H102	15:B2:838:CLA:H52	1.86	0.56
2:B2:456:ILE:HG22	2:B2:458:ILE:HD11	1.87	0.56
1:A3:20:PRO:HG2	1:A3:184:ALA:HB3	1.88	0.56
1:A2:20:PRO:HG2	1:A2:184:ALA:HB3	1.88	0.56
12:R2:19:VAL:HG11	12:R2:25:ILE:HD13	1.87	0.56
18:M1:101:BCR:H321	18:M1:101:BCR:HC8	1.88	0.56
18:M2:101:BCR:HC8	18:M2:101:BCR:H321	1.88	0.56
1:A2:550:VAL:HG11	15:A2:839:CLA:HMB3	1.89	0.55
1:A3:681:PHE:CG	18:A3:852:BCR:H363	2.41	0.55
12:R3:19:VAL:HG11	12:R3:25:ILE:HD13	1.87	0.55
1:A3:266:PRO:HA	1:A3:271:ASN:HB3	1.89	0.55
4:D3:3:LEU:HD21	4:D3:91:THR:HG21	1.87	0.55
1:A1:681:PHE:CG	18:A1:852:BCR:H363	2.41	0.55
7:I1:21:LEU:HB2	15:L3:1004:CLA:H141	1.87	0.55
1:A2:266:PRO:HA	1:A2:271:ASN:HB3	1.89	0.55
1:A1:20:PRO:HG2	1:A1:184:ALA:HB3	1.88	0.55
1:A1:266:PRO:HA	1:A1:271:ASN:HB3	1.89	0.55
15:A3:839:CLA:H92	18:A3:850:BCR:H372	1.89	0.55
15:L1:1004:CLA:H141	7:I2:21:LEU:HB2	1.88	0.55
15:A2:839:CLA:H92	18:A2:850:BCR:H372	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:200:HIS:ND1	15:A3:825:CLA:OBD	2.33	0.55
15:B2:827:CLA:H8	18:B2:842:BCR:H21C	1.88	0.54
15:B2:838:CLA:HBB2	16:B2:840:PQN:H141	1.89	0.54
1:A3:76:HIS:ND1	15:A3:813:CLA:OBD	2.40	0.54
1:A3:550:VAL:HG11	15:A3:839:CLA:HMB3	1.89	0.54
1:A1:40:ARG:HH21	5:E1:53:SER:HA	1.73	0.54
15:A1:839:CLA:H92	18:A1:850:BCR:H372	1.89	0.54
15:L2:1004:CLA:H141	7:I3:21:LEU:HB2	1.87	0.54
1:A1:550:VAL:HG11	15:A1:839:CLA:HMB3	1.89	0.54
15:A1:813:CLA:HAA1	15:A1:825:CLA:H43	1.89	0.54
1:A3:366:LEU:HD21	15:A3:819:CLA:H71	1.90	0.54
1:A1:76:HIS:ND1	15:A1:813:CLA:OBD	2.40	0.54
18:M3:101:BCR:H321	18:M3:101:BCR:HC8	1.88	0.54
12:R3:27:ASP:OD1	12:R3:28:VAL:N	2.41	0.54
12:R1:27:ASP:OD1	12:R1:28:VAL:N	2.41	0.54
1:A2:76:HIS:ND1	15:A2:813:CLA:OBD	2.40	0.54
12:R2:27:ASP:OD1	12:R2:28:VAL:N	2.41	0.54
2:B1:53:LEU:HD12	15:B1:812:CLA:HED1	1.89	0.54
15:B1:827:CLA:H8	18:B1:842:BCR:H21C	1.88	0.54
1:A2:366:LEU:HD21	15:A2:819:CLA:H71	1.90	0.54
15:B3:838:CLA:HBB2	16:B3:840:PQN:H141	1.89	0.54
1:A1:366:LEU:HD21	15:A1:819:CLA:H71	1.90	0.54
15:B1:838:CLA:HBB2	16:B1:840:PQN:H141	1.89	0.54
2:B2:53:LEU:HD12	15:B2:812:CLA:HED1	1.89	0.54
12:R2:19:VAL:HG13	12:R2:28:VAL:HG21	1.89	0.54
1:A3:40:ARG:HH21	5:E3:53:SER:HA	1.73	0.54
1:A2:40:ARG:HH21	5:E2:53:SER:HA	1.73	0.53
15:A2:813:CLA:HAA1	15:A2:825:CLA:H43	1.89	0.53
2:B3:53:LEU:HD12	15:B3:812:CLA:HED1	1.89	0.53
15:A3:813:CLA:HAA1	15:A3:825:CLA:H43	1.89	0.53
1:A2:219:VAL:HG13	1:A2:239:PRO:HB3	1.90	0.53
1:A2:177:TRP:HB2	15:A2:811:CLA:HMC3	1.91	0.53
2:B2:591:ASN:HB2	15:B2:802:CLA:HBC2	1.91	0.53
2:B2:588:TRP:CH2	15:B2:802:CLA:HAB	2.44	0.53
1:A1:177:TRP:HB2	15:A1:811:CLA:HMC3	1.91	0.53
10:L1:131:SER:HA	10:L1:134:VAL:HG12	1.91	0.53
2:B2:193:LEU:HA	2:B2:197:ALA:HB3	1.91	0.53
2:B3:588:TRP:CH2	15:B3:802:CLA:HAB	2.44	0.53
2:B3:591:ASN:HB2	15:B3:802:CLA:HBC2	1.91	0.53
12:R3:19:VAL:HG13	12:R3:28:VAL:HG21	1.89	0.53
2:B1:193:LEU:HA	2:B1:197:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:219:VAL:HG13	1:A3:239:PRO:HB3	1.90	0.53
2:B3:459:GLU:OE2	6:F3:73:HIS:ND1	2.41	0.53
2:B1:588:TRP:CH2	15:B1:802:CLA:HAB	2.44	0.52
2:B3:454:LYS:HE3	8:J3:35:ASP:HA	1.91	0.52
2:B1:176:HIS:CG	15:B1:812:CLA:HMC2	2.44	0.52
10:L2:131:SER:HA	10:L2:134:VAL:HG12	1.91	0.52
24:A3:926:HOH:O	5:E3:53:SER:HB2	2.10	0.52
10:L3:131:SER:HA	10:L3:134:VAL:HG12	1.91	0.52
2:B2:176:HIS:CG	15:B2:812:CLA:HMC2	2.44	0.52
2:B3:193:LEU:HA	2:B3:197:ALA:HB3	1.91	0.52
2:B3:176:HIS:CG	15:B3:812:CLA:HMC2	2.44	0.52
24:A2:926:HOH:O	5:E2:53:SER:HB2	2.10	0.52
15:L3:1002:CLA:C1B	15:L3:1003:CLA:HED1	2.40	0.52
2:B1:444:ASP:OD1	2:B1:621:TYR:HB2	2.10	0.52
10:L2:35:PRO:HG3	15:L2:1003:CLA:HED2	1.92	0.52
1:A3:40:ARG:CZ	1:A3:43:GLN:HG3	2.39	0.52
1:A1:40:ARG:CZ	1:A1:43:GLN:HG3	2.39	0.52
2:B1:454:LYS:HE3	8:J1:35:ASP:HA	1.91	0.52
2:B2:454:LYS:HE3	8:J2:35:ASP:HA	1.91	0.52
24:A1:926:HOH:O	5:E1:53:SER:HB2	2.10	0.52
10:L1:35:PRO:HG3	15:L1:1003:CLA:HED2	1.92	0.52
12:R1:19:VAL:HG13	12:R1:28:VAL:HG21	1.89	0.52
1:A1:219:VAL:HG13	1:A1:239:PRO:HB3	1.90	0.52
2:B2:451:THR:HG22	2:B2:454:LYS:HG2	1.91	0.52
15:L2:1002:CLA:C1B	15:L2:1003:CLA:HED1	2.40	0.52
1:A3:177:TRP:HB2	15:A3:811:CLA:HMC3	1.91	0.51
2:B3:444:ASP:OD1	2:B3:621:TYR:HB2	2.10	0.51
18:B3:846:BCR:HC32	18:J3:1306:BCR:H15C	1.92	0.51
2:B1:459:GLU:OE2	6:F1:73:HIS:ND1	2.41	0.51
1:A2:40:ARG:CZ	1:A2:43:GLN:HG3	2.39	0.51
2:B2:444:ASP:OD1	2:B2:621:TYR:HB2	2.10	0.51
2:B3:662:VAL:HG22	15:B3:839:CLA:HMB3	1.92	0.51
2:B2:662:VAL:HG22	15:B2:839:CLA:HMB3	1.92	0.51
2:B1:662:VAL:HG22	15:B1:839:CLA:HMB3	1.92	0.51
2:B3:451:THR:HG22	2:B3:454:LYS:HG2	1.91	0.51
2:B1:451:THR:HG22	2:B1:454:LYS:HG2	1.91	0.51
2:B2:527:HIS:NE2	18:J2:1306:BCR:H401	2.26	0.51
2:B1:591:ASN:HB2	15:B1:802:CLA:HBC2	1.91	0.51
2:B2:459:GLU:OE2	6:F2:73:HIS:ND1	2.41	0.51
1:A3:543:ALA:HB1	15:A3:838:CLA:HMB3	1.93	0.51
6:F3:59:GLU:O	6:F3:62:SER:OG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:122:TRP:HH2	18:B2:843:BCR:H313	1.75	0.51
10:L3:35:PRO:HG3	15:L3:1003:CLA:HED2	1.92	0.51
1:A2:543:ALA:HB1	15:A2:838:CLA:HMB3	1.93	0.51
18:A3:852:BCR:H362	15:B3:802:CLA:C2	2.42	0.50
15:I3:101:CLA:HAA2	15:I3:101:CLA:HBD	1.94	0.50
15:A1:833:CLA:H11	15:A1:843:CLA:H43	1.93	0.50
15:L1:1002:CLA:C1B	15:L1:1003:CLA:HED1	2.40	0.50
18:A2:852:BCR:H362	15:B2:802:CLA:C2	2.42	0.50
18:B2:846:BCR:HC32	18:J2:1306:BCR:H15C	1.92	0.50
1:A1:713:VAL:HG21	15:A1:840:CLA:HMB3	1.94	0.50
2:B1:122:TRP:HH2	18:B1:843:BCR:H313	1.75	0.50
18:B1:846:BCR:HC32	18:J1:1306:BCR:H15C	1.92	0.50
15:A3:842:CLA:H121	15:B3:801:CLA:H143	1.94	0.50
15:I1:101:CLA:HBD	15:I1:101:CLA:HAA2	1.94	0.50
15:A1:818:CLA:HED3	15:A1:819:CLA:O1A	2.12	0.50
2:B2:433:GLY:HA3	15:B2:801:CLA:O1A	2.12	0.50
2:B3:433:GLY:HA3	15:B3:801:CLA:O1A	2.12	0.50
2:B3:527:HIS:NE2	18:J3:1306:BCR:H401	2.26	0.50
2:B1:433:GLY:HA3	15:B1:801:CLA:O1A	2.12	0.50
15:A2:833:CLA:H11	15:A2:843:CLA:H43	1.93	0.50
15:A2:842:CLA:H121	15:B2:801:CLA:H143	1.94	0.50
1:A1:543:ALA:HB1	15:A1:838:CLA:HMB3	1.93	0.49
2:B2:272:MET:O	2:B2:276:HIS:ND1	2.46	0.49
15:A3:833:CLA:H11	15:A3:843:CLA:H43	1.93	0.49
2:B3:122:TRP:HH2	18:B3:843:BCR:H313	1.75	0.49
18:A1:852:BCR:H362	15:B1:802:CLA:C2	2.42	0.49
18:B2:841:BCR:HC8	18:B2:841:BCR:H311	1.95	0.49
2:B1:527:HIS:NE2	18:J1:1306:BCR:H401	2.26	0.49
2:B2:356:TYR:O	2:B2:513:SER:OG	2.30	0.49
2:B1:272:MET:O	2:B1:276:HIS:ND1	2.45	0.49
15:A2:802:CLA:HBB2	15:A2:856:CLA:HAA1	1.95	0.49
12:R2:15:THR:HG21	12:R2:34:LEU:HD21	1.95	0.49
3:C3:14:THR:HG22	3:C3:27:MET:HG3	1.95	0.49
1:A2:433:VAL:HG23	15:A2:831:CLA:HMD3	1.94	0.49
15:A3:802:CLA:HBB2	15:A3:856:CLA:HAA1	1.95	0.49
15:A3:818:CLA:HED3	15:A3:819:CLA:O1A	2.12	0.49
1:A1:543:ALA:O	1:A1:547:HIS:ND1	2.40	0.49
18:B1:841:BCR:HC8	18:B1:841:BCR:H311	1.95	0.49
3:C1:14:THR:HG22	3:C1:27:MET:HG3	1.95	0.49
1:A2:711:LEU:HD23	18:F2:201:BCR:H321	1.94	0.49
1:A3:433:VAL:HG23	15:A3:831:CLA:HMD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B3:841:BCR:HC8	18:B3:841:BCR:H311	1.95	0.49
1:A1:541:ILE:HD12	14:A1:801:CL0:H63	1.95	0.49
12:R1:15:THR:HG21	12:R1:34:LEU:HD21	1.95	0.49
1:A2:377:MET:HE1	15:A2:827:CLA:HHC	1.95	0.49
2:B2:269:LEU:HD23	2:B2:272:MET:HE3	1.94	0.49
15:I2:101:CLA:HAA2	15:I2:101:CLA:HBD	1.94	0.49
15:B1:839:CLA:HBA2	16:B1:840:PQN:H241	1.95	0.49
15:A2:818:CLA:HED3	15:A2:819:CLA:O1A	2.12	0.49
8:J2:31:ARG:NE	18:J2:1305:BCR:H312	2.26	0.49
2:B3:272:MET:O	2:B3:276:HIS:ND1	2.45	0.49
2:B3:431:PHE:HD2	15:B3:836:CLA:HBB2	1.78	0.49
1:A1:711:LEU:HD23	18:F1:201:BCR:H321	1.94	0.49
15:A1:842:CLA:H121	15:B1:801:CLA:H143	1.94	0.49
1:A2:713:VAL:HG21	15:A2:840:CLA:HMB3	1.94	0.49
6:F2:59:GLU:O	6:F2:62:SER:OG	2.29	0.49
15:B3:839:CLA:HBA2	16:B3:840:PQN:H241	1.95	0.48
1:A1:195:SER:O	1:A1:199:HIS:ND1	2.42	0.48
2:B2:431:PHE:HD2	15:B2:836:CLA:HBB2	1.78	0.48
15:B2:839:CLA:HBA2	16:B2:840:PQN:H241	1.95	0.48
1:A1:377:MET:HE1	15:A1:827:CLA:HHC	1.95	0.48
2:B1:431:PHE:HD2	15:B1:836:CLA:HBB2	1.78	0.48
1:A3:713:VAL:HG21	15:A3:840:CLA:HMB3	1.94	0.48
12:R3:15:THR:HG21	12:R3:34:LEU:HD21	1.95	0.48
13:X3:11:PHE:HB3	19:X3:101:LHG:O2	2.13	0.48
3:C2:14:THR:HG22	3:C2:27:MET:HG3	1.95	0.48
2:B3:339:TRP:HE1	15:B3:823:CLA:C2B	2.27	0.48
15:A1:802:CLA:HBB2	15:A1:856:CLA:HAA1	1.95	0.48
2:B1:256:PHE:HD1	15:B1:816:CLA:HMB2	1.79	0.48
13:X1:11:PHE:HB3	19:X1:101:LHG:O2	2.13	0.48
2:B2:256:PHE:HD1	15:B2:816:CLA:HMB2	1.79	0.48
4:D2:60:ARG:NH2	4:D2:62:GLU:OE1	2.45	0.48
2:B3:256:PHE:HD1	15:B3:816:CLA:HMB2	1.79	0.48
6:F1:59:GLU:O	6:F1:62:SER:OG	2.29	0.48
1:A2:740:ILE:HG21	15:A2:828:CLA:HMC2	1.95	0.48
1:A3:541:ILE:HD12	14:A3:801:CL0:H63	1.95	0.48
1:A1:433:VAL:HG23	15:A1:831:CLA:HMD3	1.94	0.48
2:B1:418:LYS:NZ	2:B1:546:ASP:OD1	2.45	0.48
1:A3:195:SER:O	1:A3:199:HIS:ND1	2.42	0.48
1:A3:740:ILE:HG21	15:A3:828:CLA:HMC2	1.95	0.48
2:B3:256:PHE:CE2	2:B3:499:TRP:HE3	2.32	0.48
2:B3:418:LYS:NZ	2:B3:546:ASP:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:207:LEU:HG	18:A1:848:BCR:H361	1.96	0.48
1:A2:195:SER:O	1:A2:199:HIS:ND1	2.42	0.48
8:J2:3:HIS:O	8:J2:6:THR:OG1	2.28	0.48
1:A3:711:LEU:HD23	18:F3:201:BCR:H321	1.94	0.48
1:A2:207:LEU:HG	18:A2:848:BCR:H361	1.96	0.48
1:A1:268:PHE:HE1	18:A1:848:BCR:H272	1.79	0.47
2:B1:256:PHE:CE2	2:B1:499:TRP:HE3	2.32	0.47
1:A2:268:PHE:HE1	18:A2:848:BCR:H272	1.79	0.47
1:A2:541:ILE:HD12	14:A2:801:CL0:H63	1.95	0.47
15:A3:829:CLA:C1C	18:A3:849:BCR:H271	2.44	0.47
2:B3:591:ASN:OD1	24:B3:901:HOH:O	2.20	0.47
12:R1:58:ASP:OD1	12:R1:59:GLN:N	2.47	0.47
15:A2:829:CLA:C1C	18:A2:849:BCR:H271	2.44	0.47
15:A2:805:CLA:H151	18:A2:848:BCR:H323	1.96	0.47
13:X2:11:PHE:HB3	19:X2:101:LHG:O2	2.13	0.47
1:A3:207:LEU:HG	18:A3:848:BCR:H361	1.95	0.47
1:A3:268:PHE:HE1	18:A3:848:BCR:H272	1.79	0.47
15:A1:829:CLA:C1C	18:A1:849:BCR:H271	2.44	0.47
2:B1:339:TRP:HE1	15:B1:823:CLA:C2B	2.27	0.47
2:B1:414:VAL:HA	2:B1:417:HIS:CE1	2.50	0.47
4:D1:60:ARG:NH2	4:D1:62:GLU:OE1	2.45	0.47
1:A1:335:PRO:HB2	10:L1:4:LEU:HD12	1.97	0.47
2:B2:339:TRP:HE1	15:B2:823:CLA:C2B	2.27	0.47
1:A3:377:MET:HE1	15:A3:827:CLA:HHC	1.95	0.47
2:B3:356:TYR:O	2:B3:513:SER:OG	2.30	0.47
4:D3:60:ARG:NH2	4:D3:62:GLU:OE1	2.45	0.47
1:A1:92:PHE:CG	15:A1:807:CLA:HBC3	2.50	0.47
8:J1:31:ARG:NE	18:J1:1305:BCR:H312	2.26	0.47
2:B2:414:VAL:HA	2:B2:417:HIS:CE1	2.50	0.47
1:A3:58:PHE:CD2	15:A3:805:CLA:HMC2	2.50	0.47
1:A1:58:PHE:CD2	15:A1:805:CLA:HMC2	2.50	0.47
15:A1:828:CLA:HMB1	15:A1:828:CLA:HBB1	1.97	0.47
2:B1:43:GLN:OE1	2:B1:161:ARG:NE	2.47	0.47
2:B2:256:PHE:CE2	2:B2:499:TRP:HE3	2.32	0.47
1:A3:335:PRO:HB2	10:L3:4:LEU:HD12	1.97	0.47
15:A3:805:CLA:H151	18:A3:848:BCR:H323	1.96	0.47
15:A3:828:CLA:HBB1	15:A3:828:CLA:HMB1	1.97	0.47
2:B2:525:VAL:HG21	2:B2:599:TYR:HB2	1.97	0.47
1:A3:543:ALA:O	1:A3:547:HIS:ND1	2.40	0.47
2:B3:24:ILE:HA	15:B3:804:CLA:HMD3	1.97	0.47
2:B1:24:ILE:HA	15:B1:804:CLA:HMD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R1:41:ARG:O	12:R1:41:ARG:HG3	2.15	0.47
15:A2:828:CLA:HMB1	15:A2:828:CLA:HBB1	1.97	0.47
1:A1:740:ILE:HG21	15:A1:828:CLA:HMC2	1.95	0.47
1:A2:58:PHE:CD2	15:A2:805:CLA:HMC2	2.50	0.47
2:B2:418:LYS:NZ	2:B2:546:ASP:OD1	2.45	0.47
6:F2:84:GLY:HA2	6:F2:88:ILE:HD13	1.97	0.47
2:B3:180:GLY:HA3	15:B3:812:CLA:HBB1	1.97	0.47
5:E3:37:ILE:HG21	12:R3:41:ARG:HG2	1.97	0.47
12:R3:41:ARG:HG3	12:R3:41:ARG:O	2.15	0.47
2:B2:180:GLY:HA3	15:B2:812:CLA:HBB1	1.97	0.46
1:A1:375:TYR:HA	1:A1:390:GLN:HE22	1.80	0.46
2:B1:591:ASN:OD1	24:B1:901:HOH:O	2.20	0.46
6:F1:84:GLY:HA2	6:F1:88:ILE:HD13	1.97	0.46
19:X1:101:LHG:H251	19:X1:101:LHG:H282	1.58	0.46
1:A2:375:TYR:HA	1:A2:390:GLN:HE22	1.80	0.46
12:R2:41:ARG:O	12:R2:41:ARG:HG3	2.15	0.46
1:A1:587:CYS:HB2	2:B1:673:TRP:HB3	1.98	0.46
15:A1:805:CLA:H151	18:A1:848:BCR:H323	1.96	0.46
10:L1:144:VAL:HG21	10:L2:76:LEU:HD13	1.97	0.46
1:A2:335:PRO:HB2	10:L2:4:LEU:HD12	1.97	0.46
1:A2:670:SER:HB2	2:B2:448:ALA:HB1	1.98	0.46
2:B2:163:SER:HG	2:B2:165:SER:HG	1.63	0.46
10:L2:144:VAL:HG21	10:L3:76:LEU:HD13	1.97	0.46
1:A3:92:PHE:CG	15:A3:807:CLA:HBC3	2.50	0.46
9:K1:29:LEU:O	9:K1:33:ALA:N	2.48	0.46
1:A2:92:PHE:CG	15:A2:807:CLA:HBC3	2.50	0.46
2:B3:163:SER:HG	2:B3:165:SER:HG	1.63	0.46
2:B3:414:VAL:HA	2:B3:417:HIS:CE1	2.50	0.46
2:B3:525:VAL:HG21	2:B3:599:TYR:HB2	1.97	0.46
1:A2:356:LEU:HB2	15:A2:805:CLA:HMD3	1.98	0.46
12:R3:58:ASP:OD1	12:R3:59:GLN:N	2.47	0.46
1:A1:433:VAL:HA	1:A1:436:HIS:CE1	2.51	0.46
2:B1:356:TYR:O	2:B1:513:SER:OG	2.30	0.46
1:A2:587:CYS:HB2	2:B2:673:TRP:HB3	1.98	0.46
12:R2:58:ASP:OD1	12:R2:59:GLN:N	2.47	0.46
1:A3:433:VAL:HA	1:A3:436:HIS:CE1	2.51	0.46
1:A3:587:CYS:HB2	2:B3:673:TRP:HB3	1.98	0.46
1:A3:670:SER:HB2	2:B3:448:ALA:HB1	1.98	0.46
2:B3:43:GLN:OE1	2:B3:161:ARG:NE	2.47	0.46
6:F3:84:GLY:HA2	6:F3:88:ILE:HD13	1.97	0.46
19:X3:101:LHG:H111	19:X3:101:LHG:HC81	1.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:24:ILE:HA	15:B2:804:CLA:HMD3	1.97	0.46
15:A3:821:CLA:HMB2	15:A3:825:CLA:HMA3	1.98	0.46
2:B1:180:GLY:HA3	15:B1:812:CLA:HBB1	1.97	0.46
5:E1:37:ILE:HG21	12:R1:41:ARG:HG2	1.97	0.46
2:B2:591:ASN:OD1	24:B2:901:HOH:O	2.20	0.46
5:E2:37:ILE:HG21	12:R2:41:ARG:HG2	1.97	0.46
1:A3:601:TRP:HH2	15:A3:802:CLA:HAB	1.80	0.46
1:A3:601:TRP:HE1	15:A3:856:CLA:C1D	2.29	0.46
15:A1:815:CLA:C3B	18:A1:847:BCR:H333	2.46	0.46
10:L1:76:LEU:HD13	10:L3:144:VAL:HG21	1.97	0.46
12:R1:54:GLU:HG3	12:R1:87:LYS:HB3	1.98	0.46
15:A2:821:CLA:HMB2	15:A2:825:CLA:HMA3	1.97	0.46
15:B3:807:CLA:HMC2	15:B3:807:CLA:H92	1.98	0.46
1:A1:356:LEU:HB2	15:A1:805:CLA:HMD3	1.98	0.46
1:A2:216:GLN:OE1	1:A2:301:HIS:ND1	2.49	0.46
10:L3:36:ALA:HB2	15:L3:1003:CLA:HMD1	1.98	0.46
10:L1:20:PRO:HA	10:L1:24:SER:HB3	1.98	0.45
15:A2:815:CLA:C3B	18:A2:847:BCR:H333	2.46	0.45
18:A3:850:BCR:H24C	18:A3:850:BCR:H371	1.80	0.45
9:K3:29:LEU:O	9:K3:33:ALA:N	2.48	0.45
2:B1:525:VAL:HG21	2:B1:599:TYR:HB2	1.97	0.45
15:B1:835:CLA:HMB1	15:B1:835:CLA:HBB1	1.99	0.45
10:L2:36:ALA:HB2	15:L2:1003:CLA:HMD1	1.98	0.45
1:A3:352:TRP:HB3	15:A3:805:CLA:HAC1	1.98	0.45
1:A3:375:TYR:HA	1:A3:390:GLN:HE22	1.80	0.45
15:A3:842:CLA:H102	18:B3:846:BCR:H363	1.99	0.45
12:R3:54:GLU:HG3	12:R3:87:LYS:HB3	1.98	0.45
1:A1:352:TRP:HB3	15:A1:805:CLA:HAC1	1.98	0.45
2:B1:586:MET:HG3	2:B1:716:LEU:HD21	1.99	0.45
10:L1:36:ALA:HB2	15:L1:1003:CLA:HMD1	1.98	0.45
1:A2:543:ALA:O	1:A2:547:HIS:ND1	2.40	0.45
15:B2:835:CLA:HBB1	15:B2:835:CLA:HMB1	1.99	0.45
12:R2:17:ILE:HD11	12:R2:34:LEU:HD23	1.99	0.45
15:A3:811:CLA:H62	15:A3:811:CLA:H41	1.62	0.45
8:J3:31:ARG:NE	18:J3:1305:BCR:H312	2.26	0.45
18:A1:848:BCR:H24C	18:A1:848:BCR:H371	1.83	0.45
1:A2:601:TRP:HE1	15:A2:856:CLA:C1D	2.29	0.45
15:B2:807:CLA:H92	15:B2:807:CLA:HMC2	1.98	0.45
15:A3:826:CLA:HBB2	18:A3:851:BCR:H311	1.98	0.45
2:B3:179:ALA:HB2	2:B3:287:GLY:HA3	1.98	0.45
2:B1:179:ALA:HB2	2:B1:287:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R1:8:VAL:HG13	12:R1:89:LEU:HA	1.99	0.45
1:A2:433:VAL:HA	1:A2:436:HIS:CE1	2.51	0.45
2:B2:586:MET:HG3	2:B2:716:LEU:HD21	1.99	0.45
15:A3:815:CLA:C3B	18:A3:847:BCR:H333	2.46	0.45
15:B3:801:CLA:H62	15:B3:801:CLA:H41	1.75	0.45
15:B3:839:CLA:H171	7:I3:24:THR:HG23	1.99	0.45
12:R3:8:VAL:HG13	12:R3:89:LEU:HA	1.99	0.45
15:A1:819:CLA:H92	15:A1:829:CLA:H91	1.99	0.45
15:A1:821:CLA:HMB2	15:A1:825:CLA:HMA3	1.98	0.45
15:A1:826:CLA:HBB2	18:A1:851:BCR:H311	1.98	0.45
15:I1:101:CLA:HAA2	15:I1:101:CLA:CBD	2.47	0.45
18:A3:848:BCR:H361	18:A3:848:BCR:H20C	1.85	0.45
15:B3:835:CLA:HBB1	15:B3:835:CLA:HMB1	1.98	0.45
2:B1:637:LEU:HD22	2:B1:730:PHE:HA	1.98	0.45
15:B1:839:CLA:H171	7:I1:24:THR:HG23	1.99	0.45
4:D1:95:HIS:HB3	4:D1:96:PRO:HD3	1.98	0.45
2:B2:122:TRP:CH2	18:B2:843:BCR:H313	2.51	0.45
15:B2:801:CLA:HMB2	15:B2:802:CLA:HBB1	1.99	0.45
2:B3:637:LEU:HD22	2:B3:730:PHE:HA	1.98	0.45
1:A1:601:TRP:HE1	15:A1:856:CLA:C1D	2.29	0.45
2:B1:431:PHE:CD2	15:B1:836:CLA:HBB2	2.52	0.45
15:B1:801:CLA:HMB2	15:B1:802:CLA:HBB1	1.99	0.45
15:A2:811:CLA:H62	15:A2:811:CLA:H41	1.62	0.45
15:I2:101:CLA:HAA2	15:I2:101:CLA:CBD	2.47	0.45
15:A2:826:CLA:HBB2	18:A2:851:BCR:H311	1.98	0.45
2:B2:431:PHE:CD2	15:B2:836:CLA:HBB2	2.52	0.45
2:B2:677:TRP:CZ2	16:B2:840:PQN:H2M3	2.52	0.45
9:K2:29:LEU:O	9:K2:33:ALA:N	2.48	0.45
12:R2:54:GLU:HG3	12:R2:87:LYS:HB3	1.98	0.45
1:A3:356:LEU:HB2	15:A3:805:CLA:HMD3	1.98	0.45
15:B3:801:CLA:HMB2	15:B3:802:CLA:HBB1	1.99	0.45
18:L3:1005:BCR:H331	18:L3:1005:BCR:C8	2.47	0.45
1:A1:145:GLN:NE2	1:A1:386:ASP:OD2	2.51	0.45
18:L1:1005:BCR:H331	18:L1:1005:BCR:C8	2.47	0.45
2:B2:43:GLN:OE1	2:B2:161:ARG:NE	2.47	0.45
2:B2:637:LEU:HD22	2:B2:730:PHE:HA	1.98	0.45
12:R2:66:ASP:O	12:R2:70:ILE:HG12	2.17	0.45
15:B3:808:CLA:O1A	15:B3:826:CLA:HBD	2.17	0.45
12:R3:17:ILE:HD11	12:R3:34:LEU:HD23	1.99	0.45
1:A1:670:SER:HB2	2:B1:448:ALA:HB1	1.98	0.44
15:A1:842:CLA:H161	8:J1:19:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:122:TRP:CH2	18:B1:843:BCR:H313	2.51	0.44
19:X2:101:LHG:H111	19:X2:101:LHG:HC81	1.47	0.44
15:A2:819:CLA:H92	15:A2:829:CLA:H91	1.99	0.44
15:L3:1002:CLA:HBA2	15:L3:1002:CLA:H18	1.99	0.44
18:L3:1005:BCR:H23C	18:L3:1005:BCR:H392	2.00	0.44
18:B1:841:BCR:H24C	18:B1:841:BCR:H371	1.83	0.44
1:A2:352:TRP:HB3	15:A2:805:CLA:HAC1	1.98	0.44
4:D2:95:HIS:HB3	4:D2:96:PRO:HD3	1.98	0.44
2:B3:122:TRP:CH2	18:B3:843:BCR:H313	2.52	0.44
2:B3:677:TRP:CZ2	16:B3:840:PQN:H2M3	2.52	0.44
18:I3:103:BCR:H402	15:L3:1003:CLA:H52	2.00	0.44
10:L3:20:PRO:HA	10:L3:24:SER:HB3	1.98	0.44
2:B1:53:LEU:HD23	2:B1:53:LEU:HA	1.85	0.44
2:B1:588:TRP:HH2	15:B1:802:CLA:HAB	1.83	0.44
12:R1:17:ILE:HD11	12:R1:34:LEU:HD23	1.99	0.44
15:B2:808:CLA:O1A	15:B2:826:CLA:HBD	2.17	0.44
18:L2:1005:BCR:H24C	18:L2:1005:BCR:H371	1.83	0.44
2:B3:75:GLN:OE1	2:B3:75:GLN:N	2.49	0.44
15:B3:808:CLA:H8	15:B3:808:CLA:HBB1	2.00	0.44
15:A1:811:CLA:H62	15:A1:811:CLA:H41	1.62	0.44
18:A1:850:BCR:H371	18:A1:850:BCR:H24C	1.79	0.44
2:B1:269:LEU:HD23	2:B1:272:MET:HE1	1.98	0.44
2:B1:376:THR:HG23	2:B1:597:THR:HG21	2.00	0.44
15:B1:807:CLA:H92	15:B1:807:CLA:HMC2	1.98	0.44
15:B1:808:CLA:H8	15:B1:808:CLA:HBB1	2.00	0.44
15:A2:842:CLA:H161	8:J2:19:MET:SD	2.57	0.44
15:B2:827:CLA:ND	18:B2:842:BCR:H282	2.33	0.44
2:B3:431:PHE:CD2	15:B3:836:CLA:HBB2	2.52	0.44
4:D3:95:HIS:HB3	4:D3:96:PRO:HD3	1.99	0.44
18:A1:848:BCR:H361	18:A1:848:BCR:H20C	1.85	0.44
18:A1:852:BCR:H20C	18:A1:852:BCR:H361	1.88	0.44
15:B2:839:CLA:H171	7:I2:24:THR:HG23	1.99	0.44
6:F2:125:ASP:OD1	6:F2:125:ASP:N	2.51	0.44
10:L2:20:PRO:HA	10:L2:24:SER:HB3	1.98	0.44
15:L2:1002:CLA:HBA2	15:L2:1002:CLA:H18	1.99	0.44
12:R3:66:ASP:O	12:R3:70:ILE:HG12	2.17	0.44
1:A1:346:GLU:OE1	1:A1:346:GLU:N	2.47	0.44
15:A1:802:CLA:OBD	15:B1:803:CLA:HMB3	2.18	0.44
2:B1:516:LEU:HD22	2:B1:607:VAL:HG21	2.00	0.44
15:B1:827:CLA:ND	18:B1:842:BCR:H282	2.33	0.44
12:R2:8:VAL:HG13	12:R2:89:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:269:LEU:HD23	2:B3:272:MET:HE3	1.99	0.44
2:B3:586:MET:HG3	2:B3:716:LEU:HD21	1.99	0.44
3:C3:28:VAL:HG12	4:D3:109:ARG:HB3	2.00	0.44
15:I3:101:CLA:HAA2	15:I3:101:CLA:CBD	2.47	0.44
1:A1:216:GLN:OE1	1:A1:301:HIS:ND1	2.49	0.44
15:B1:808:CLA:O1A	15:B1:826:CLA:HBD	2.17	0.44
12:R1:66:ASP:O	12:R1:70:ILE:HG12	2.17	0.44
15:A2:825:CLA:HBB1	15:A2:825:CLA:HMB1	2.00	0.44
15:A3:825:CLA:HBB1	15:A3:825:CLA:HMB1	2.00	0.44
15:A3:842:CLA:H161	8:J3:19:MET:SD	2.57	0.44
15:B3:827:CLA:ND	18:B3:842:BCR:H282	2.33	0.44
15:A1:825:CLA:HMB1	15:A1:825:CLA:HBB1	2.00	0.44
15:B1:817:CLA:HBA2	15:B1:817:CLA:H3A	1.78	0.44
15:A2:802:CLA:OBD	15:B2:803:CLA:HMB3	2.18	0.44
2:B2:75:GLN:OE1	2:B2:75:GLN:N	2.49	0.44
15:B2:808:CLA:H8	15:B2:808:CLA:HBB1	2.00	0.44
3:C2:28:VAL:HG12	4:D2:109:ARG:HB3	2.00	0.44
18:L2:1005:BCR:H331	18:L2:1005:BCR:C8	2.47	0.44
1:A3:308:PHE:HE1	15:A3:821:CLA:HAB	1.83	0.44
18:J3:1306:BCR:H20C	18:J3:1306:BCR:H361	1.88	0.44
19:X3:101:LHG:H282	19:X3:101:LHG:H251	1.58	0.44
1:A1:437:ARG:CZ	4:D1:44:ALA:HB2	2.48	0.43
2:B1:677:TRP:CZ2	16:B1:840:PQN:H2M3	2.52	0.43
7:I1:10:LEU:HD22	7:I1:14:PHE:HE2	1.83	0.43
15:A2:842:CLA:H102	18:B2:846:BCR:H363	1.99	0.43
15:A3:819:CLA:H92	15:A3:829:CLA:H91	1.99	0.43
15:B3:827:CLA:H62	15:B3:827:CLA:H41	1.79	0.43
18:J3:1306:BCR:H371	18:J3:1306:BCR:H24C	1.81	0.43
3:C1:28:VAL:HG12	4:D1:109:ARG:HB3	2.00	0.43
1:A2:40:ARG:HH22	5:E2:43:VAL:HG11	1.83	0.43
2:B2:516:LEU:HD22	2:B2:607:VAL:HG21	2.00	0.43
7:I2:10:LEU:HD22	7:I2:14:PHE:HE2	1.83	0.43
18:I2:103:BCR:H402	15:L2:1003:CLA:H52	2.00	0.43
15:L1:1002:CLA:H111	15:L1:1002:CLA:H152	1.86	0.43
2:B2:179:ALA:HB2	2:B2:287:GLY:HA3	1.98	0.43
2:B2:634:SER:O	2:B2:638:ILE:HG12	2.19	0.43
1:A3:145:GLN:NE2	1:A3:386:ASP:OD2	2.51	0.43
15:A3:818:CLA:H3A	15:A3:818:CLA:HBA2	1.57	0.43
15:A1:813:CLA:CAA	15:A1:825:CLA:H43	2.49	0.43
18:A1:849:BCR:H20C	18:A1:849:BCR:H361	1.90	0.43
15:A2:818:CLA:H3A	15:A2:818:CLA:HBA2	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L2:1005:BCR:H392	18:L2:1005:BCR:H23C	2.00	0.43
1:A3:40:ARG:HH22	5:E3:43:VAL:HG11	1.83	0.43
1:A3:509:ALA:HB2	15:A3:835:CLA:HED3	2.00	0.43
15:A3:837:CLA:HBB1	15:A3:837:CLA:HMB1	2.00	0.43
2:B3:284:ILE:O	2:B3:288:HIS:ND1	2.51	0.43
1:A1:94:GLY:HA3	1:A1:147:TRP:CH2	2.54	0.43
1:A1:308:PHE:HE1	15:A1:821:CLA:HAB	1.83	0.43
15:A1:838:CLA:HAA1	15:A1:838:CLA:HBD	2.00	0.43
18:L1:1005:BCR:H392	18:L1:1005:BCR:H23C	2.00	0.43
1:A2:437:ARG:CZ	4:D2:44:ALA:HB2	2.48	0.43
15:A2:830:CLA:H193	15:A2:842:CLA:HMB2	2.01	0.43
15:A2:837:CLA:HBB1	15:A2:837:CLA:HMB1	2.00	0.43
15:A2:838:CLA:HAA1	15:A2:838:CLA:HBD	2.00	0.43
18:B2:841:BCR:H20C	18:B2:841:BCR:H361	1.88	0.43
2:B3:60:VAL:CG2	15:B3:827:CLA:H2	2.48	0.43
18:F3:201:BCR:H373	15:X3:102:CLA:C4B	2.49	0.43
7:I3:10:LEU:HD22	7:I3:14:PHE:HE2	1.83	0.43
15:A1:842:CLA:H102	18:B1:846:BCR:H363	1.99	0.43
15:L1:1002:CLA:H18	15:L1:1002:CLA:HBA2	1.99	0.43
19:X2:101:LHG:H251	19:X2:101:LHG:H282	1.58	0.43
15:A3:838:CLA:HAA1	15:A3:838:CLA:HBD	2.00	0.43
2:B3:516:LEU:HD22	2:B3:607:VAL:HG21	2.00	0.43
2:B3:634:SER:O	2:B3:638:ILE:HG12	2.19	0.43
18:M3:101:BCR:H24C	18:M3:101:BCR:H371	1.86	0.43
1:A1:509:ALA:HB2	15:A1:835:CLA:HED3	2.00	0.43
18:A2:851:BCR:H24C	18:A2:851:BCR:H371	1.89	0.43
18:F2:201:BCR:H373	15:X2:102:CLA:C4B	2.49	0.43
2:B3:588:TRP:HH2	15:B3:802:CLA:HAB	1.83	0.43
1:A1:40:ARG:HH22	5:E1:43:VAL:HG11	1.83	0.43
18:I1:103:BCR:H402	15:L1:1003:CLA:H52	2.00	0.43
2:B2:706:LEU:HD22	2:B2:710:GLN:NE2	2.34	0.43
8:J2:21:ILE:O	8:J2:25:ILE:HG12	2.19	0.43
9:K2:73:VAL:HA	15:K2:103:CLA:HMA1	2.01	0.43
1:A3:114:ALA:HB3	15:A3:808:CLA:HED3	2.01	0.43
6:F3:103:VAL:HG22	6:F3:132:CYS:O	2.19	0.43
18:J3:1304:BCR:H20C	18:J3:1304:BCR:H361	1.93	0.43
1:A1:114:ALA:HB3	15:A1:808:CLA:HED3	2.01	0.43
15:A1:837:CLA:HMB1	15:A1:837:CLA:HBB1	2.00	0.43
18:L1:1005:BCR:H24C	18:L1:1005:BCR:H371	1.83	0.43
2:B2:630:LEU:O	2:B2:634:SER:OG	2.30	0.43
18:B3:847:BCR:H20C	18:B3:847:BCR:H361	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A1:830:CLA:H193	15:A1:842:CLA:HMB2	2.01	0.43
2:B1:300:ILE:HG21	15:B1:823:CLA:HAC1	2.01	0.43
2:B1:634:SER:O	2:B1:638:ILE:HG12	2.19	0.43
12:R1:20:PRO:HD2	12:R1:28:VAL:HG11	2.01	0.43
15:L2:1002:CLA:H42	18:L2:1010:BCR:H10C	2.01	0.43
1:A3:437:ARG:CZ	4:D3:44:ALA:HB2	2.48	0.43
6:F3:125:ASP:OD1	6:F3:125:ASP:N	2.51	0.43
9:K3:73:VAL:HA	15:K3:103:CLA:HMA1	2.01	0.43
1:A1:399:TRP:CD1	15:A1:828:CLA:HAB	2.54	0.42
15:A1:824:CLA:HBA1	15:A1:824:CLA:H3A	1.85	0.42
2:B1:284:ILE:O	2:B1:288:HIS:ND1	2.51	0.42
2:B1:446:VAL:HB	2:B1:454:LYS:HB2	2.01	0.42
1:A2:308:PHE:HE1	15:A2:821:CLA:HAB	1.83	0.42
1:A2:399:TRP:CD1	15:A2:828:CLA:HAB	2.54	0.42
2:B3:376:THR:HG23	2:B3:597:THR:HG21	2.00	0.42
15:B3:805:CLA:O1D	15:B3:805:CLA:H2	2.19	0.42
18:I3:103:BCR:H20C	18:I3:103:BCR:H361	1.91	0.42
8:J3:8:LEU:HA	8:J3:13:VAL:HG11	2.00	0.42
2:B1:220:GLY:O	2:B1:232:TYR:OH	2.24	0.42
2:B1:706:LEU:HD22	2:B1:710:GLN:NE2	2.34	0.42
15:B1:805:CLA:H2	15:B1:805:CLA:O1D	2.19	0.42
8:J1:31:ARG:HH21	18:J1:1305:BCR:C6	2.32	0.42
18:J1:1306:BCR:H20C	18:J1:1306:BCR:H361	1.88	0.42
9:K1:73:VAL:HA	15:K1:103:CLA:HMA1	2.01	0.42
15:A2:803:CLA:HMC3	15:A2:811:CLA:H52	2.01	0.42
15:A2:830:CLA:H62	15:A2:830:CLA:H41	1.84	0.42
2:B2:376:THR:HG23	2:B2:597:THR:HG21	2.00	0.42
8:J2:8:LEU:HA	8:J2:13:VAL:HG11	2.00	0.42
15:A3:802:CLA:OBD	15:B3:803:CLA:HMB3	2.18	0.42
15:B3:820:CLA:C4C	18:B3:841:BCR:H382	2.50	0.42
2:B1:564:PRO:HB3	2:B1:708:ILE:HB	2.01	0.42
15:A2:802:CLA:H51	15:A2:802:CLA:H12	1.74	0.42
15:B2:801:CLA:H41	15:B2:801:CLA:H62	1.75	0.42
15:A3:802:CLA:H12	15:A3:802:CLA:H51	1.74	0.42
15:A3:808:CLA:HMC3	15:A3:809:CLA:HMD2	2.01	0.42
2:B3:564:PRO:HB3	2:B3:708:ILE:HB	2.01	0.42
8:J3:21:ILE:O	8:J3:25:ILE:HG12	2.19	0.42
12:R3:20:PRO:HD2	12:R3:28:VAL:HG11	2.01	0.42
15:A1:804:CLA:H2	15:A1:811:CLA:H71	2.02	0.42
18:A1:851:BCR:H24C	18:A1:851:BCR:H371	1.89	0.42
8:J1:8:LEU:HA	8:J1:13:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J1:21:ILE:O	8:J1:25:ILE:HG12	2.19	0.42
15:L1:1002:CLA:H42	18:L1:1011:BCR:H10C	2.00	0.42
2:B2:337:LEU:HD23	2:B2:392:HIS:CE1	2.55	0.42
2:B2:446:VAL:HB	2:B2:454:LYS:HB2	2.01	0.42
6:F2:103:VAL:HG22	6:F2:132:CYS:O	2.19	0.42
2:B3:672:SER:O	16:B3:840:PQN:H9	2.20	0.42
18:I3:102:BCR:H24C	18:I3:102:BCR:H371	1.92	0.42
8:J3:31:ARG:HH21	18:J3:1305:BCR:C6	2.32	0.42
15:A1:808:CLA:HMC3	15:A1:809:CLA:HMD2	2.02	0.42
18:A1:847:BCR:H371	18:A1:847:BCR:H24C	1.84	0.42
15:B1:820:CLA:C4C	18:B1:841:BCR:H382	2.50	0.42
6:F1:103:VAL:HG22	6:F1:132:CYS:O	2.19	0.42
18:F1:201:BCR:H373	15:X1:102:CLA:C4B	2.49	0.42
12:R1:50:GLY:O	12:R1:74:PHE:HA	2.20	0.42
2:B2:588:TRP:HH2	15:B2:802:CLA:HAB	1.83	0.42
15:B2:808:CLA:HMC3	15:B2:809:CLA:C3D	2.49	0.42
8:J2:31:ARG:HH21	18:J2:1305:BCR:C6	2.32	0.42
12:R2:20:PRO:HD2	12:R2:28:VAL:HG11	2.01	0.42
15:A3:804:CLA:H2	15:A3:811:CLA:H71	2.02	0.42
18:A3:848:BCR:H371	18:A3:848:BCR:H24C	1.83	0.42
14:A1:801:CL0:O1D	15:B1:803:CLA:HBB2	2.20	0.42
15:B1:808:CLA:HMC3	15:B1:809:CLA:C3D	2.49	0.42
18:J1:1305:BCR:H24C	18:J1:1305:BCR:H371	1.87	0.42
1:A3:94:GLY:HA3	1:A3:147:TRP:CH2	2.54	0.42
15:A3:803:CLA:HMC3	15:A3:811:CLA:H52	2.01	0.42
2:B3:446:VAL:HB	2:B3:454:LYS:HB2	2.01	0.42
2:B1:300:ILE:HB	2:B1:326:TYR:CD1	2.54	0.42
2:B1:672:SER:O	16:B1:840:PQN:H9	2.20	0.42
15:B1:801:CLA:H62	15:B1:801:CLA:H41	1.75	0.42
1:A2:94:GLY:HA3	1:A2:147:TRP:CH2	2.54	0.42
1:A2:557:VAL:HG21	18:A2:851:BCR:HC31	2.02	0.42
15:A2:813:CLA:CAA	15:A2:825:CLA:H43	2.49	0.42
1:A3:557:VAL:HG21	18:A3:851:BCR:HC31	2.02	0.42
15:A3:833:CLA:HAB	15:A3:834:CLA:HHB	2.02	0.42
2:B1:337:LEU:HD23	2:B1:392:HIS:CE1	2.55	0.42
1:A2:145:GLN:NE2	1:A2:386:ASP:OD2	2.51	0.42
1:A2:676:PHE:CZ	1:A2:680:HIS:HE1	2.38	0.42
15:A2:833:CLA:HAB	15:A2:834:CLA:HHB	2.02	0.42
2:B3:300:ILE:HB	2:B3:326:TYR:CD1	2.54	0.42
2:B3:337:LEU:HD23	2:B3:392:HIS:CE1	2.55	0.42
2:B3:706:LEU:HD22	2:B3:710:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B3:842:BCR:H24C	18:B3:842:BCR:H371	1.88	0.42
15:A1:833:CLA:HAB	15:A1:834:CLA:HHB	2.02	0.42
18:L1:1006:BCR:H10C	15:L3:1002:CLA:H42	2.01	0.42
1:A2:509:ALA:HB2	15:A2:835:CLA:HED3	2.00	0.42
18:A2:848:BCR:H361	18:A2:848:BCR:H20C	1.85	0.42
2:B2:300:ILE:HG21	15:B2:823:CLA:HAC1	2.01	0.42
18:B2:846:BCR:H24C	18:B2:846:BCR:H371	1.86	0.42
12:R2:50:GLY:O	12:R2:74:PHE:HA	2.20	0.42
15:A3:813:CLA:CAA	15:A3:825:CLA:H43	2.49	0.42
15:A3:830:CLA:H193	15:A3:842:CLA:HMB2	2.01	0.42
1:A1:452:GLY:HA3	15:A1:856:CLA:O1A	2.20	0.42
14:A1:801:CL0:H49	14:A1:801:CL0:H41	1.84	0.42
15:A1:819:CLA:CAD	15:A1:829:CLA:H41	2.50	0.42
3:C1:60:ASP:HA	3:C1:61:PHE:HA	1.85	0.42
10:L1:23:ASP:O	10:L1:28:LYS:NZ	2.53	0.42
15:B2:805:CLA:O1D	15:B2:805:CLA:H2	2.19	0.42
15:B2:820:CLA:C4C	18:B2:841:BCR:H382	2.50	0.42
6:F2:76:VAL:HG12	6:F2:86:PHE:HB2	2.01	0.42
10:L2:50:VAL:HG13	10:L2:54:HIS:CE1	2.55	0.42
1:A3:373:HIS:HB3	15:A3:818:CLA:HED2	2.02	0.42
2:B3:53:LEU:HD23	2:B3:53:LEU:HA	1.85	0.42
18:B3:841:BCR:H24C	18:B3:841:BCR:H371	1.83	0.42
10:L3:23:ASP:O	10:L3:28:LYS:NZ	2.53	0.42
18:L3:1005:BCR:H24C	18:L3:1005:BCR:H371	1.83	0.42
15:A1:803:CLA:HMC3	15:A1:811:CLA:H52	2.01	0.41
18:B1:841:BCR:H20C	18:B1:841:BCR:H361	1.88	0.41
2:B2:60:VAL:CG2	15:B2:827:CLA:H2	2.48	0.41
2:B2:564:PRO:HB3	2:B2:708:ILE:HB	2.01	0.41
15:B2:827:CLA:H62	15:B2:827:CLA:H41	1.79	0.41
18:F2:201:BCR:H20C	18:F2:201:BCR:H361	1.88	0.41
15:B3:808:CLA:HMC3	15:B3:809:CLA:C3D	2.49	0.41
15:L3:1002:CLA:H152	15:L3:1002:CLA:H111	1.86	0.41
1:A1:52:HIS:HB3	15:A1:804:CLA:HBC1	2.03	0.41
1:A1:199:HIS:CG	15:A1:813:CLA:HMC2	2.55	0.41
14:A1:801:CL0:H33	14:A1:801:CL0:H39	1.80	0.41
2:B1:344:LEU:HD12	2:B1:347:ILE:HD11	2.02	0.41
18:B1:844:BCR:H20C	18:B1:844:BCR:H361	1.93	0.41
18:B1:845:BCR:H24C	18:B1:845:BCR:H371	1.87	0.41
10:L1:50:VAL:HG13	10:L1:54:HIS:CE1	2.55	0.41
1:A2:452:GLY:HA3	15:A2:856:CLA:O1A	2.20	0.41
18:A2:848:BCR:H371	18:A2:848:BCR:H24C	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:672:SER:O	16:B2:840:PQN:H9	2.20	0.41
18:L2:1010:BCR:H20C	18:L2:1010:BCR:H361	1.88	0.41
1:A3:399:TRP:CD1	15:A3:828:CLA:HAB	2.54	0.41
14:A3:801:CL0:O1D	15:B3:803:CLA:HBB2	2.20	0.41
15:A3:819:CLA:CAD	15:A3:829:CLA:H41	2.50	0.41
2:B3:300:ILE:HG21	15:B3:823:CLA:HAC1	2.01	0.41
1:A1:676:PHE:CZ	1:A1:680:HIS:HE1	2.38	0.41
2:B1:75:GLN:OE1	2:B1:75:GLN:N	2.49	0.41
1:A2:601:TRP:HH2	15:A2:802:CLA:HAB	1.80	0.41
2:B3:278:ALA:HA	15:B3:815:CLA:HMC3	2.02	0.41
1:A1:373:HIS:HB3	15:A1:818:CLA:HED2	2.02	0.41
18:A1:849:BCR:H24C	18:A1:849:BCR:H371	1.87	0.41
1:A2:199:HIS:CG	15:A2:813:CLA:HMC2	2.55	0.41
1:A2:346:GLU:OE1	1:A2:346:GLU:N	2.47	0.41
15:B2:849:CLA:HBD	15:B2:849:CLA:HBA1	2.03	0.41
1:A3:199:HIS:CG	15:A3:813:CLA:HMC2	2.55	0.41
1:A3:216:GLN:OE1	1:A3:301:HIS:ND1	2.49	0.41
15:B3:805:CLA:HBA1	15:B3:805:CLA:H3A	1.90	0.41
15:B3:849:CLA:HBD	15:B3:849:CLA:HBA1	2.03	0.41
10:L3:50:VAL:HG13	10:L3:54:HIS:CE1	2.55	0.41
15:A1:830:CLA:H161	15:A1:830:CLA:H122	1.94	0.41
18:A1:852:BCR:H272	18:J1:1304:BCR:H313	2.03	0.41
6:F1:98:GLY:HA3	6:F1:139:TRP:CE2	2.56	0.41
15:A2:803:CLA:HBB1	18:J2:1305:BCR:H271	2.02	0.41
18:A2:855:BCR:H24C	18:A2:855:BCR:H371	1.83	0.41
2:B2:300:ILE:HB	2:B2:326:TYR:CD1	2.55	0.41
2:B2:344:LEU:HD12	2:B2:347:ILE:HD11	2.02	0.41
15:B2:805:CLA:HBA1	15:B2:805:CLA:H3A	1.90	0.41
18:J2:1304:BCR:H371	18:J2:1304:BCR:H24C	1.88	0.41
1:A3:149:ALA:HB2	1:A3:381:PRO:HD2	2.02	0.41
1:A3:452:GLY:HA3	15:A3:856:CLA:O1A	2.20	0.41
2:B3:220:GLY:O	2:B3:232:TYR:OH	2.24	0.41
2:B3:344:LEU:HD12	2:B3:347:ILE:HD11	2.02	0.41
6:F1:76:VAL:HG12	6:F1:86:PHE:HB2	2.01	0.41
1:A2:114:ALA:HB3	15:A2:808:CLA:HED3	2.01	0.41
1:A2:203:GLY:O	1:A2:207:LEU:HB2	2.21	0.41
15:A2:819:CLA:CAD	15:A2:829:CLA:H41	2.50	0.41
2:B2:284:ILE:O	2:B2:288:HIS:ND1	2.51	0.41
6:F2:98:GLY:HA3	6:F2:139:TRP:CE2	2.56	0.41
18:M2:101:BCR:H20C	18:M2:101:BCR:H361	1.91	0.41
12:R2:26:LEU:HB3	12:R2:78:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:203:GLY:O	1:A3:207:LEU:HB2	2.21	0.41
6:F3:76:VAL:HG12	6:F3:86:PHE:HB2	2.02	0.41
18:J3:1305:BCR:H24C	18:J3:1305:BCR:H371	1.87	0.41
12:R3:26:LEU:HB3	12:R3:78:CYS:HA	2.02	0.41
12:R3:50:GLY:O	12:R3:74:PHE:HA	2.20	0.41
18:L1:1006:BCR:H24C	18:L1:1006:BCR:H371	1.82	0.41
6:F2:88:ILE:HG13	15:J2:1303:CLA:HMB3	2.03	0.41
1:A1:514:GLY:HA2	1:A1:528:PRO:HB3	2.03	0.41
18:L1:1005:BCR:H20C	18:L1:1005:BCR:H361	1.92	0.41
18:L1:1011:BCR:H371	18:L1:1011:BCR:H24C	1.82	0.41
15:A2:808:CLA:HMC3	15:A2:809:CLA:HMD2	2.01	0.41
18:A2:852:BCR:H272	18:J2:1304:BCR:H313	2.03	0.41
3:C2:24:VAL:HG21	3:C2:47:CYS:HA	2.03	0.41
18:A3:849:BCR:H24C	18:A3:849:BCR:H371	1.87	0.41
18:A3:852:BCR:H272	18:J3:1304:BCR:H313	2.03	0.41
1:A1:215:HIS:HB2	15:A1:814:CLA:C1C	2.51	0.41
1:A1:266:PRO:HB3	1:A1:271:ASN:O	2.21	0.41
1:A1:329:LEU:O	1:A1:341:HIS:HB2	2.21	0.41
15:A1:802:CLA:H51	15:A1:802:CLA:H12	1.74	0.41
2:B1:410:VAL:O	2:B1:414:VAL:HG23	2.21	0.41
18:J1:1305:BCR:H20C	18:J1:1305:BCR:H361	1.93	0.41
15:L1:1002:CLA:H11	15:L1:1002:CLA:H51	1.84	0.41
13:X1:12:ARG:HH21	19:X1:101:LHG:HC11	1.86	0.41
19:X1:101:LHG:HC81	19:X1:101:LHG:H111	1.47	0.41
1:A2:149:ALA:HB2	1:A2:381:PRO:HD2	2.02	0.41
1:A2:404:LEU:HD21	15:A2:806:CLA:H142	2.02	0.41
1:A2:514:GLY:HA2	1:A2:528:PRO:HB3	2.03	0.41
14:A2:801:CL0:O1D	15:B2:803:CLA:HBB2	2.20	0.41
15:A2:819:CLA:C3D	15:A2:829:CLA:H41	2.51	0.41
18:A2:850:BCR:H371	18:A2:850:BCR:H24C	1.80	0.41
2:B2:278:ALA:HA	15:B2:815:CLA:HMC3	2.02	0.41
1:A3:404:LEU:HD21	15:A3:806:CLA:H142	2.02	0.41
15:A3:830:CLA:H161	15:A3:830:CLA:H122	1.94	0.41
18:B3:844:BCR:H24C	18:B3:844:BCR:H371	1.87	0.41
18:B3:846:BCR:H20C	18:B3:846:BCR:H361	1.88	0.41
12:R3:25:ILE:HG12	12:R3:80:ALA:O	2.21	0.41
1:A1:149:ALA:HB2	1:A1:381:PRO:HD2	2.02	0.41
1:A1:404:LEU:HD21	15:A1:806:CLA:H142	2.02	0.41
15:A1:856:CLA:HBB2	2:B1:664:ALA:HB3	2.03	0.41
2:B1:459:GLU:OE1	2:B1:464:GLN:NE2	2.47	0.41
18:J1:1304:BCR:H20C	18:J1:1304:BCR:H361	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M1:101:BCR:H371	18:M1:101:BCR:H24C	1.86	0.41
15:B2:824:CLA:C2B	15:B2:837:CLA:H3A	2.51	0.41
1:A3:445:ASN:HD22	2:B3:680:LEU:HD11	1.86	0.41
2:B1:110:ASN:HB3	7:I1:3:GLY:HA2	2.03	0.40
18:B1:842:BCR:H20C	18:B1:842:BCR:H361	1.96	0.40
1:A2:215:HIS:HB2	15:A2:814:CLA:C1C	2.51	0.40
1:A2:445:ASN:HD22	2:B2:680:LEU:HD11	1.86	0.40
15:A2:856:CLA:HBB2	2:B2:664:ALA:HB3	2.03	0.40
1:A3:676:PHE:CZ	1:A3:680:HIS:HE1	2.38	0.40
2:B3:110:ASN:HB3	7:I3:3:GLY:HA2	2.03	0.40
2:B3:685:VAL:HG11	3:C3:80:TYR:CG	2.56	0.40
15:B3:827:CLA:H3A	15:B3:827:CLA:HBA2	1.91	0.40
6:F3:88:ILE:HG13	15:J3:1303:CLA:HMB3	2.03	0.40
8:J3:3:HIS:O	8:J3:6:THR:OG1	2.28	0.40
1:A1:557:VAL:HG21	18:A1:851:BCR:HC31	2.02	0.40
1:A1:561:ARG:O	1:A1:570:ALA:N	2.55	0.40
6:F1:139:TRP:CG	6:F1:140:PRO:HD3	2.56	0.40
1:A2:52:HIS:HB3	15:A2:804:CLA:HBC1	2.03	0.40
1:A2:152:ILE:HG21	1:A2:158:LEU:HG	2.03	0.40
1:A2:329:LEU:O	1:A2:341:HIS:HB2	2.21	0.40
1:A2:581:PRO:HD3	2:B2:567:GLY:HA2	2.03	0.40
2:B2:410:VAL:O	2:B2:414:VAL:HG23	2.21	0.40
2:B2:685:VAL:HG11	3:C2:80:TYR:CG	2.56	0.40
13:X2:12:ARG:HH21	19:X2:101:LHG:HC11	1.86	0.40
1:A3:52:HIS:HB3	15:A3:804:CLA:HBC1	2.03	0.40
1:A3:514:GLY:HA2	1:A3:528:PRO:HB3	2.03	0.40
15:A3:803:CLA:HBB1	18:J3:1305:BCR:H271	2.03	0.40
18:A3:849:BCR:H20C	18:A3:849:BCR:H361	1.90	0.40
3:C3:24:VAL:HG21	3:C3:47:CYS:HA	2.03	0.40
1:A1:152:ILE:HG21	1:A1:158:LEU:HG	2.03	0.40
15:B1:827:CLA:H3A	15:B1:827:CLA:HBA2	1.91	0.40
4:D2:30:THR:O	4:D2:80:TYR:HA	2.21	0.40
1:A3:152:ILE:HG21	1:A3:158:LEU:HG	2.03	0.40
1:A3:329:LEU:O	1:A3:341:HIS:HB2	2.21	0.40
15:A3:856:CLA:HBB2	2:B3:664:ALA:HB3	2.03	0.40
2:B3:410:VAL:O	2:B3:414:VAL:HG23	2.21	0.40
15:B3:824:CLA:C2B	15:B3:837:CLA:H3A	2.51	0.40
18:L3:1005:BCR:H20C	18:L3:1005:BCR:H361	1.92	0.40
1:A1:203:GLY:O	1:A1:207:LEU:HB2	2.21	0.40
1:A1:445:ASN:HD22	2:B1:680:LEU:HD11	1.86	0.40
15:A1:819:CLA:C3D	15:A1:829:CLA:H41	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B1:845:BCR:H20C	18:B1:845:BCR:H361	1.97	0.40
15:B1:849:CLA:HBA1	15:B1:849:CLA:HBD	2.03	0.40
12:R1:25:ILE:HG12	12:R1:80:ALA:O	2.21	0.40
12:R1:26:LEU:HB3	12:R1:78:CYS:HA	2.02	0.40
15:A2:804:CLA:H2	15:A2:811:CLA:H71	2.02	0.40
2:B2:719:PHE:O	2:B2:723:TYR:HB2	2.22	0.40
15:B2:808:CLA:H143	15:B2:808:CLA:HBA2	2.04	0.40
15:B2:809:CLA:H201	7:I2:23:PRO:HA	2.04	0.40
2:B3:706:LEU:HD21	16:B3:840:PQN:H151	2.03	0.40
15:B3:808:CLA:HBA2	15:B3:808:CLA:H143	2.04	0.40
18:M3:101:BCR:H20C	18:M3:101:BCR:H361	1.91	0.40
1:A1:580:GLY:HA2	2:B1:568:PRO:HD3	2.04	0.40
15:A1:803:CLA:HBB1	18:J1:1305:BCR:H271	2.03	0.40
18:A1:855:BCR:H20C	18:A1:855:BCR:H361	1.85	0.40
1:A2:373:HIS:HB3	15:A2:818:CLA:HED2	2.02	0.40
1:A2:580:GLY:HA2	2:B2:568:PRO:HD3	2.04	0.40
2:B2:110:ASN:HB3	7:I2:3:GLY:HA2	2.03	0.40
2:B2:458:ILE:HD13	2:B2:523:PHE:CE1	2.57	0.40
15:B2:820:CLA:HMD2	18:B2:841:BCR:H371	2.04	0.40
1:A3:266:PRO:HB3	1:A3:271:ASN:O	2.21	0.40
18:A3:855:BCR:H20C	18:A3:855:BCR:H361	1.85	0.40
2:B3:459:GLU:OE1	2:B3:464:GLN:NE2	2.47	0.40
6:F3:98:GLY:HA3	6:F3:139:TRP:CE2	2.56	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	A1	743/755 (98%)	729 (98%)	14 (2%)	0	100	100
1	A2	743/755 (98%)	729 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A3	743/755 (98%)	729 (98%)	14 (2%)	0	100	100
2	B1	738/741 (100%)	724 (98%)	14 (2%)	0	100	100
2	B2	738/741 (100%)	724 (98%)	14 (2%)	0	100	100
2	B3	738/741 (100%)	724 (98%)	14 (2%)	0	100	100
3	C1	78/81 (96%)	78 (100%)	0	0	100	100
3	C2	78/81 (96%)	78 (100%)	0	0	100	100
3	C3	78/81 (96%)	78 (100%)	0	0	100	100
4	D1	136/139 (98%)	129 (95%)	7 (5%)	0	100	100
4	D2	136/139 (98%)	129 (95%)	7 (5%)	0	100	100
4	D3	136/139 (98%)	129 (95%)	7 (5%)	0	100	100
5	E1	67/76 (88%)	65 (97%)	2 (3%)	0	100	100
5	E2	67/76 (88%)	65 (97%)	2 (3%)	0	100	100
5	E3	67/76 (88%)	65 (97%)	2 (3%)	0	100	100
6	F1	139/174 (80%)	138 (99%)	1 (1%)	0	100	100
6	F2	139/174 (80%)	138 (99%)	1 (1%)	0	100	100
6	F3	139/174 (80%)	138 (99%)	1 (1%)	0	100	100
7	I1	36/38 (95%)	36 (100%)	0	0	100	100
7	I2	36/38 (95%)	36 (100%)	0	0	100	100
7	I3	36/38 (95%)	36 (100%)	0	0	100	100
8	J1	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
8	J2	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
8	J3	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
9	K1	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
9	K2	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
9	K3	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
10	L1	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
10	L2	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
10	L3	150/155 (97%)	148 (99%)	2 (1%)	0	100	100
11	M1	29/31 (94%)	29 (100%)	0	0	100	100
11	M2	29/31 (94%)	29 (100%)	0	0	100	100
11	M3	29/31 (94%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	R1	95/98 (97%)	89 (94%)	6 (6%)	0	100	100
12	R2	95/98 (97%)	89 (94%)	6 (6%)	0	100	100
12	R3	95/98 (97%)	89 (94%)	6 (6%)	0	100	100
13	X1	26/39 (67%)	26 (100%)	0	0	100	100
13	X2	26/39 (67%)	26 (100%)	0	0	100	100
13	X3	26/39 (67%)	26 (100%)	0	0	100	100
All	All	7059/7353 (96%)	6912 (98%)	147 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A1	557/603 (92%)	557 (100%)	0	100	100
1	A2	557/603 (92%)	557 (100%)	0	100	100
1	A3	557/603 (92%)	557 (100%)	0	100	100
2	B1	586/598 (98%)	586 (100%)	0	100	100
2	B2	586/598 (98%)	586 (100%)	0	100	100
2	B3	586/598 (98%)	586 (100%)	0	100	100
3	C1	67/68 (98%)	67 (100%)	0	100	100
3	C2	67/68 (98%)	67 (100%)	0	100	100
3	C3	67/68 (98%)	67 (100%)	0	100	100
4	D1	113/116 (97%)	113 (100%)	0	100	100
4	D2	113/116 (97%)	113 (100%)	0	100	100
4	D3	113/116 (97%)	113 (100%)	0	100	100
5	E1	57/65 (88%)	57 (100%)	0	100	100
5	E2	57/65 (88%)	57 (100%)	0	100	100
5	E3	57/65 (88%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F1	101/138 (73%)	101 (100%)	0	100	100
6	F2	101/138 (73%)	101 (100%)	0	100	100
6	F3	101/138 (73%)	101 (100%)	0	100	100
7	I1	32/32 (100%)	32 (100%)	0	100	100
7	I2	32/32 (100%)	32 (100%)	0	100	100
7	I3	32/32 (100%)	32 (100%)	0	100	100
8	J1	35/36 (97%)	35 (100%)	0	100	100
8	J2	35/36 (97%)	35 (100%)	0	100	100
8	J3	35/36 (97%)	35 (100%)	0	100	100
9	K1	33/61 (54%)	33 (100%)	0	100	100
9	K2	33/61 (54%)	33 (100%)	0	100	100
9	K3	33/61 (54%)	33 (100%)	0	100	100
10	L1	115/120 (96%)	115 (100%)	0	100	100
10	L2	115/120 (96%)	115 (100%)	0	100	100
10	L3	115/120 (96%)	115 (100%)	0	100	100
11	M1	26/26 (100%)	26 (100%)	0	100	100
11	M2	26/26 (100%)	26 (100%)	0	100	100
11	M3	26/26 (100%)	26 (100%)	0	100	100
12	R1	85/86 (99%)	85 (100%)	0	100	100
12	R2	85/86 (99%)	85 (100%)	0	100	100
12	R3	85/86 (99%)	85 (100%)	0	100	100
13	X1	19/31 (61%)	19 (100%)	0	100	100
13	X2	19/31 (61%)	19 (100%)	0	100	100
13	X3	19/31 (61%)	19 (100%)	0	100	100
All	All	5478/5940 (92%)	5478 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	445	ASN
2	B1	105	GLN

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Mol	Chain	Res	Type
1	A2	445	ASN
2	B2	105	GLN
1	A3	445	ASN
2	B3	105	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 444 ligands modelled in this entry, 51 are unknown and 3 are monoatomic - leaving 390 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	CLA	A3	843	24	65,73,73	1.30	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	B1	829	-	35,43,73	1.79	8 (22%)	41,74,113	2.09	13 (31%)
15	CLA	L3	1004	24	65,73,73	1.28	7 (10%)	76,113,113	1.38	10 (13%)
15	CLA	A1	817	-	39,46,73	1.73	10 (25%)	46,80,113	1.76	11 (23%)
18	BCR	B1	845	-	41,41,41	0.14	0	56,56,56	0.38	0
15	CLA	B3	805	-	65,73,73	1.26	7 (10%)	76,113,113	1.31	9 (11%)
15	CLA	A2	824	-	45,53,73	1.51	7 (15%)	52,89,113	1.53	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A3	838	-	55,63,73	1.40	7 (12%)	64,101,113	1.40	9 (14%)
15	CLA	B3	812	-	65,73,73	1.29	7 (10%)	76,113,113	1.38	12 (15%)
15	CLA	B1	817	-	50,58,73	1.44	7 (14%)	58,95,113	1.55	10 (17%)
18	BCR	M2	101	-	41,41,41	0.16	0	56,56,56	0.30	0
15	CLA	A2	808	1	65,73,73	1.29	7 (10%)	76,113,113	1.32	9 (11%)
15	CLA	B1	820	-	36,44,73	1.76	7 (19%)	40,76,113	1.89	10 (25%)
18	BCR	A2	850	-	41,41,41	0.11	0	56,56,56	0.30	0
18	BCR	B2	843	-	25,25,41	0.36	0	33,33,56	0.46	0
18	BCR	J3	1305	-	41,41,41	0.18	0	56,56,56	0.29	0
15	CLA	A2	802	24	65,73,73	1.32	7 (10%)	76,113,113	1.36	7 (9%)
15	CLA	B2	835	-	46,54,73	1.48	7 (15%)	53,90,113	1.61	10 (18%)
18	BCR	A3	848	-	41,41,41	0.13	0	56,56,56	0.31	0
15	CLA	B3	832	-	41,48,73	1.63	6 (14%)	45,82,113	1.97	9 (20%)
15	CLA	B3	811	-	45,53,73	1.48	6 (13%)	52,89,113	1.49	9 (17%)
15	CLA	A3	813	-	44,52,73	1.47	8 (18%)	55,88,113	1.53	11 (20%)
15	CLA	B2	829	-	35,43,73	1.79	8 (22%)	41,74,113	2.08	13 (31%)
15	CLA	B3	823	2	41,49,73	1.70	8 (19%)	47,84,113	1.64	10 (21%)
15	CLA	A1	831	-	50,58,73	1.48	7 (14%)	58,95,113	1.63	10 (17%)
15	CLA	B2	815	-	36,44,73	1.73	7 (19%)	40,76,113	1.82	9 (22%)
15	CLA	A2	806	-	65,73,73	1.26	7 (10%)	76,113,113	1.28	9 (11%)
15	CLA	A3	836	1	41,49,73	1.69	7 (17%)	47,84,113	1.67	8 (17%)
18	BCR	I3	103	-	41,41,41	0.18	0	56,56,56	0.35	0
15	CLA	A1	835	-	45,53,73	1.56	6 (13%)	52,89,113	1.50	8 (15%)
15	CLA	A2	835	-	45,53,73	1.56	6 (13%)	52,89,113	1.50	8 (15%)
15	CLA	B2	818	-	50,58,73	1.43	7 (14%)	58,95,113	1.49	9 (15%)
15	CLA	A2	837	-	50,58,73	1.41	7 (14%)	58,95,113	1.53	12 (20%)
15	CLA	J3	1302	8	33,43,73	1.69	8 (24%)	43,76,113	1.77	9 (20%)
15	CLA	B3	838	24	65,73,73	1.27	7 (10%)	76,113,113	1.30	9 (11%)
15	CLA	K3	101	-	33,42,73	1.72	5 (15%)	35,73,113	2.01	11 (31%)
15	CLA	B1	809	2	65,73,73	1.34	7 (10%)	76,113,113	1.27	10 (13%)
15	CLA	L2	1002	10	65,73,73	1.24	7 (10%)	76,113,113	1.27	10 (13%)
15	CLA	B3	834	-	37,47,73	1.65	7 (18%)	42,81,113	1.79	10 (23%)
15	CLA	B2	809	2	65,73,73	1.34	7 (10%)	76,113,113	1.27	10 (13%)
15	CLA	A3	817	-	39,46,73	1.73	10 (25%)	46,80,113	1.76	11 (23%)
15	CLA	A1	829	-	55,63,73	1.34	7 (12%)	64,101,113	1.45	10 (15%)
15	CLA	A2	842	-	65,73,73	1.30	7 (10%)	76,113,113	1.29	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A2	833	-	65,73,73	1.32	7 (10%)	76,113,113	1.34	10 (13%)
18	BCR	B3	842	-	30,30,41	0.34	0	39,39,56	0.51	0
15	CLA	B3	820	-	36,44,73	1.76	7 (19%)	40,76,113	1.89	10 (25%)
15	CLA	A3	820	-	36,46,73	1.59	8 (22%)	45,80,113	1.76	10 (22%)
15	CLA	B3	803	-	54,62,73	1.45	7 (12%)	62,99,113	1.37	8 (12%)
15	CLA	A1	840	-	65,73,73	1.29	7 (10%)	76,113,113	1.43	9 (11%)
15	CLA	A1	804	-	65,73,73	1.30	7 (10%)	76,113,113	1.37	10 (13%)
18	BCR	A2	852	-	41,41,41	0.16	0	56,56,56	0.38	0
15	CLA	A2	839	-	55,63,73	1.43	7 (12%)	64,101,113	1.39	9 (14%)
15	CLA	B2	826	-	45,53,73	1.56	7 (15%)	52,89,113	1.45	8 (15%)
18	BCR	L2	1010	-	41,41,41	0.16	0	56,56,56	0.33	0
15	CLA	J1	1302	8	33,43,73	1.68	8 (24%)	43,76,113	1.77	10 (23%)
18	BCR	B1	841	-	41,41,41	0.19	0	56,56,56	0.35	0
15	CLA	L2	1004	24	65,73,73	1.28	7 (10%)	76,113,113	1.38	10 (13%)
18	BCR	A1	855	-	30,30,41	0.33	0	39,39,56	0.36	0
15	CLA	B1	837	-	41,49,73	1.73	8 (19%)	47,84,113	1.67	9 (19%)
15	CLA	B3	809	2	65,73,73	1.35	7 (10%)	76,113,113	1.28	10 (13%)
15	CLA	A3	826	24	55,63,73	1.38	6 (10%)	64,101,113	1.50	9 (14%)
15	CLA	B1	830	-	41,49,73	1.72	8 (19%)	47,84,113	1.71	8 (17%)
15	CLA	A2	816	-	41,49,73	1.66	8 (19%)	47,84,113	1.71	9 (19%)
15	CLA	B2	831	-	41,49,73	1.73	8 (19%)	47,84,113	1.74	12 (25%)
15	CLA	B1	816	-	38,46,73	1.84	9 (23%)	40,79,113	1.87	10 (25%)
15	CLA	A3	822	-	45,53,73	1.52	7 (15%)	52,89,113	1.64	9 (17%)
15	CLA	A3	830	-	65,73,73	1.29	6 (9%)	76,113,113	1.28	11 (14%)
19	LHG	A2	853	-	46,46,48	0.24	0	49,52,54	0.24	0
15	CLA	K1	101	-	33,42,73	1.72	5 (15%)	35,73,113	2.00	11 (31%)
18	BCR	J2	1304	-	41,41,41	0.16	0	56,56,56	0.29	0
17	SF4	A1	846	1,2	0,12,12	-	-	-	-	-
18	BCR	A1	849	-	41,41,41	0.12	0	56,56,56	0.29	0
15	CLA	B1	819	-	45,53,73	1.54	7 (15%)	52,89,113	1.70	9 (17%)
15	CLA	A1	834	-	65,73,73	1.27	7 (10%)	76,113,113	1.34	10 (13%)
15	CLA	A2	827	-	60,68,73	1.33	7 (11%)	70,107,113	1.38	6 (8%)
15	CLA	A2	813	-	44,52,73	1.47	8 (18%)	55,88,113	1.53	11 (20%)
15	CLA	A1	842	-	65,73,73	1.30	7 (10%)	76,113,113	1.30	9 (11%)
15	CLA	I1	101	2	65,73,73	1.28	7 (10%)	76,113,113	1.27	11 (14%)
15	CLA	A1	856	-	65,73,73	1.30	6 (9%)	76,113,113	1.20	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A3	819	-	58,67,73	1.40	7 (12%)	67,106,113	1.64	11 (16%)
15	CLA	B3	806	-	50,58,73	1.43	7 (14%)	58,95,113	1.46	11 (18%)
15	CLA	L3	1003	-	60,68,73	1.31	6 (10%)	70,107,113	1.40	11 (15%)
21	DGD	B3	848	-	67,67,67	0.17	0	81,81,81	0.16	0
15	CLA	B1	802	24	65,73,73	1.34	6 (9%)	76,113,113	1.35	7 (9%)
18	BCR	J1	1304	-	41,41,41	0.15	0	56,56,56	0.29	0
15	CLA	B3	817	-	50,58,73	1.44	7 (14%)	58,95,113	1.55	10 (17%)
15	CLA	J1	1307	-	34,42,73	1.97	11 (32%)	41,73,113	2.14	12 (29%)
18	BCR	B1	847	-	41,41,41	0.16	0	56,56,56	0.51	0
17	SF4	C3	102	3	0,12,12	-	-	-	-	-
15	CLA	B3	822	-	39,48,73	1.60	7 (17%)	45,82,113	1.67	7 (15%)
15	CLA	B3	807	-	60,68,73	1.41	6 (10%)	70,107,113	1.64	10 (14%)
15	CLA	B2	823	2	41,49,73	1.71	8 (19%)	47,84,113	1.65	10 (21%)
15	CLA	B3	802	24	65,73,73	1.34	6 (9%)	76,113,113	1.35	7 (9%)
15	CLA	B1	810	-	43,52,73	1.55	7 (16%)	49,88,113	1.59	9 (18%)
16	PQN	B1	840	-	34,34,34	0.22	0	42,45,45	0.53	1 (2%)
15	CLA	A3	821	-	64,72,73	1.28	7 (10%)	75,112,113	1.33	11 (14%)
15	CLA	B3	833	-	37,45,73	1.74	9 (24%)	44,78,113	1.79	10 (22%)
15	CLA	A1	824	-	45,53,73	1.51	7 (15%)	52,89,113	1.53	10 (19%)
15	CLA	K3	103	-	32,40,73	1.80	7 (21%)	38,70,113	2.24	13 (34%)
15	CLA	L1	1004	24	65,73,73	1.28	7 (10%)	76,113,113	1.37	10 (13%)
15	CLA	J2	1302	8	33,43,73	1.69	8 (24%)	43,76,113	1.78	10 (23%)
15	CLA	A2	841	24	39,48,73	1.72	8 (20%)	44,83,113	1.66	11 (25%)
14	CL0	A2	801	-	65,73,73	2.41	7 (10%)	76,113,113	1.18	8 (10%)
15	CLA	B3	849	-	45,53,73	1.61	6 (13%)	52,89,113	1.47	8 (15%)
15	CLA	B1	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.31	9 (11%)
15	CLA	J3	1303	-	35,44,73	1.73	9 (25%)	46,78,113	1.79	11 (23%)
15	CLA	A2	830	-	65,73,73	1.29	6 (9%)	76,113,113	1.28	11 (14%)
15	CLA	A3	834	-	65,73,73	1.27	7 (10%)	76,113,113	1.33	10 (13%)
15	CLA	B1	834	-	37,47,73	1.65	7 (18%)	42,81,113	1.79	10 (23%)
15	CLA	B1	812	-	65,73,73	1.29	7 (10%)	76,113,113	1.38	12 (15%)
15	CLA	A2	832	-	45,53,73	1.59	6 (13%)	52,89,113	1.62	12 (23%)
15	CLA	B2	811	-	45,53,73	1.47	6 (13%)	52,89,113	1.48	9 (17%)
15	CLA	B3	819	-	45,53,73	1.54	7 (15%)	52,89,113	1.70	9 (17%)
18	BCR	J2	1306	-	41,41,41	0.20	0	56,56,56	0.54	0
23	GAK	R2	101	12	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	LHG	X1	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.10	2 (4%)
18	BCR	B3	847	-	41,41,41	0.16	0	56,56,56	0.51	0
15	CLA	I3	101	2	65,73,73	1.28	7 (10%)	76,113,113	1.27	10 (13%)
15	CLA	J3	1307	-	34,42,73	1.96	11 (32%)	41,73,113	2.15	12 (29%)
18	BCR	B2	842	-	30,30,41	0.34	0	39,39,56	0.51	0
19	LHG	A3	854	-	34,34,48	0.22	0	37,40,54	0.31	0
15	CLA	B2	838	24	65,73,73	1.26	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	I2	101	2	65,73,73	1.28	7 (10%)	76,113,113	1.27	11 (14%)
15	CLA	A3	835	-	45,53,73	1.57	6 (13%)	52,89,113	1.51	8 (15%)
15	CLA	A1	809	-	65,73,73	1.27	7 (10%)	76,113,113	1.42	10 (13%)
15	CLA	B1	801	-	65,73,73	1.30	6 (9%)	76,113,113	1.27	8 (10%)
15	CLA	B3	828	-	41,50,73	1.65	6 (14%)	49,85,113	1.66	8 (16%)
15	CLA	K1	103	-	32,40,73	1.80	7 (21%)	38,70,113	2.23	13 (34%)
15	CLA	B1	839	-	65,73,73	1.31	7 (10%)	76,113,113	1.27	9 (11%)
17	SF4	C2	101	3	0,12,12	-	-	-	-	-
15	CLA	A3	829	-	55,63,73	1.35	7 (12%)	64,101,113	1.45	10 (15%)
18	BCR	A1	850	-	41,41,41	0.11	0	56,56,56	0.30	0
15	CLA	A1	828	-	42,50,73	1.54	7 (16%)	48,85,113	1.72	9 (18%)
15	CLA	B3	810	-	43,52,73	1.55	7 (16%)	49,88,113	1.59	9 (18%)
15	CLA	B1	835	-	46,54,73	1.48	7 (15%)	53,90,113	1.60	9 (16%)
15	CLA	B2	803	-	54,62,73	1.45	7 (12%)	62,99,113	1.36	8 (12%)
23	GAK	R1	101	12	0,4,4	-	-	-	-	-
14	CL0	A3	801	-	65,73,73	2.41	7 (10%)	76,113,113	1.19	8 (10%)
15	CLA	B2	801	-	65,73,73	1.30	6 (9%)	76,113,113	1.27	8 (10%)
15	CLA	J3	1301	-	40,46,73	1.71	9 (22%)	48,79,113	1.72	12 (25%)
15	CLA	A3	840	-	65,73,73	1.29	7 (10%)	76,113,113	1.43	9 (11%)
15	CLA	X2	102	-	40,48,73	1.73	8 (20%)	46,83,113	1.72	13 (28%)
18	BCR	A3	850	-	41,41,41	0.12	0	56,56,56	0.30	0
15	CLA	A1	815	-	37,44,73	1.90	10 (27%)	43,76,113	1.98	10 (23%)
15	CLA	B3	821	-	38,47,73	1.72	6 (15%)	46,80,113	2.31	12 (26%)
15	CLA	B2	817	-	50,58,73	1.44	7 (14%)	58,95,113	1.55	10 (17%)
15	CLA	B2	808	-	65,73,73	1.34	7 (10%)	76,113,113	1.68	14 (18%)
18	BCR	I2	103	-	41,41,41	0.18	0	56,56,56	0.35	0
15	CLA	A1	837	-	50,58,73	1.41	7 (14%)	58,95,113	1.53	12 (20%)
15	CLA	A2	818	-	50,58,73	1.48	7 (14%)	58,95,113	1.54	9 (15%)
15	CLA	J2	1303	-	35,44,73	1.73	9 (25%)	46,78,113	1.78	12 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	B2	833	-	37,45,73	1.73	9 (24%)	44,78,113	1.79	10 (22%)
15	CLA	A2	820	-	36,46,73	1.59	8 (22%)	45,80,113	1.76	10 (22%)
15	CLA	A1	839	-	55,63,73	1.43	7 (12%)	64,101,113	1.39	9 (14%)
15	CLA	L2	1003	-	60,68,73	1.30	6 (10%)	70,107,113	1.40	11 (15%)
15	CLA	A1	813	-	44,52,73	1.47	8 (18%)	55,88,113	1.53	10 (18%)
15	CLA	A1	803	-	63,72,73	1.31	7 (11%)	73,112,113	1.39	9 (12%)
21	DGD	B2	848	-	67,67,67	0.18	0	81,81,81	0.16	0
18	BCR	J3	1306	-	41,41,41	0.20	0	56,56,56	0.54	0
18	BCR	A2	851	-	41,41,41	0.14	0	56,56,56	0.43	0
15	CLA	A1	816	-	41,49,73	1.66	8 (19%)	47,84,113	1.70	9 (19%)
15	CLA	B1	806	-	50,58,73	1.43	7 (14%)	58,95,113	1.46	10 (17%)
18	BCR	L1	1011	-	41,41,41	0.16	0	56,56,56	0.33	0
15	CLA	A1	838	-	55,63,73	1.40	7 (12%)	64,101,113	1.40	9 (14%)
15	CLA	A1	821	-	64,72,73	1.28	7 (10%)	75,112,113	1.33	11 (14%)
15	CLA	A2	822	-	45,53,73	1.52	7 (15%)	52,89,113	1.65	9 (17%)
15	CLA	A2	814	-	33,41,73	1.75	9 (27%)	43,72,113	2.06	15 (34%)
15	CLA	B3	839	-	65,73,73	1.31	7 (10%)	76,113,113	1.27	9 (11%)
15	CLA	B2	802	24	65,73,73	1.35	6 (9%)	76,113,113	1.35	7 (9%)
15	CLA	B3	827	-	65,73,73	1.25	7 (10%)	76,113,113	1.27	8 (10%)
18	BCR	A1	852	-	41,41,41	0.16	0	56,56,56	0.38	0
17	SF4	A3	846	1,2	0,12,12	-	-	-	-	-
18	BCR	A3	849	-	41,41,41	0.13	0	56,56,56	0.29	0
15	CLA	B1	833	-	37,45,73	1.74	9 (24%)	44,78,113	1.80	10 (22%)
18	BCR	I2	102	-	41,41,41	0.19	0	56,56,56	0.45	0
19	LHG	A1	853	-	46,46,48	0.24	0	49,52,54	0.24	0
15	CLA	A2	826	24	55,63,73	1.38	7 (12%)	64,101,113	1.50	9 (14%)
15	CLA	A2	840	-	65,73,73	1.29	7 (10%)	76,113,113	1.44	10 (13%)
15	CLA	A2	838	-	55,63,73	1.40	7 (12%)	64,101,113	1.41	9 (14%)
15	CLA	B1	826	-	45,53,73	1.55	7 (15%)	52,89,113	1.46	8 (15%)
15	CLA	B1	815	-	36,44,73	1.73	7 (19%)	40,76,113	1.83	9 (22%)
15	CLA	A3	842	-	65,73,73	1.30	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	A3	806	-	65,73,73	1.26	7 (10%)	76,113,113	1.29	10 (13%)
15	CLA	A1	832	-	45,53,73	1.58	6 (13%)	52,89,113	1.61	11 (21%)
15	CLA	B3	829	-	35,43,73	1.79	8 (22%)	41,74,113	2.09	13 (31%)
18	BCR	K3	102	-	25,25,41	0.37	0	33,33,56	0.41	0
15	CLA	A2	843	24	65,73,73	1.30	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	A1	823	-	41,49,73	1.68	8 (19%)	47,84,113	1.70	8 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A3	837	-	50,58,73	1.41	7 (14%)	58,95,113	1.53	12 (20%)
15	CLA	A1	810	-	37,46,73	1.92	9 (24%)	42,80,113	2.08	10 (23%)
15	CLA	A2	803	-	63,72,73	1.31	7 (11%)	73,112,113	1.39	9 (12%)
18	BCR	I1	103	-	41,41,41	0.18	0	56,56,56	0.35	0
15	CLA	A2	807	-	43,52,73	1.56	7 (16%)	49,88,113	1.73	10 (20%)
15	CLA	B2	837	-	41,49,73	1.72	8 (19%)	47,84,113	1.67	9 (19%)
15	CLA	A2	809	-	65,73,73	1.27	7 (10%)	76,113,113	1.42	10 (13%)
15	CLA	A3	844	-	45,53,73	1.49	7 (15%)	52,89,113	1.50	9 (17%)
15	CLA	A3	816	-	41,49,73	1.66	8 (19%)	47,84,113	1.71	9 (19%)
15	CLA	A2	812	-	40,48,73	1.69	8 (20%)	46,83,113	1.71	9 (19%)
15	CLA	B3	831	-	41,49,73	1.73	8 (19%)	47,84,113	1.74	12 (25%)
15	CLA	A2	819	-	58,67,73	1.40	7 (12%)	67,106,113	1.64	11 (16%)
15	CLA	B3	836	-	45,53,73	1.55	7 (15%)	52,89,113	1.59	9 (17%)
16	PQN	A3	845	-	34,34,34	0.24	0	42,45,45	0.46	1 (2%)
18	BCR	B3	846	-	41,41,41	0.19	0	56,56,56	0.47	0
15	CLA	A1	811	-	65,73,73	1.29	7 (10%)	76,113,113	1.34	9 (11%)
15	CLA	J1	1303	-	35,44,73	1.72	9 (25%)	46,78,113	1.78	12 (26%)
18	BCR	K1	102	-	25,25,41	0.37	0	33,33,56	0.41	0
18	BCR	A2	849	-	41,41,41	0.12	0	56,56,56	0.29	0
15	CLA	A3	810	-	37,46,73	1.92	9 (24%)	42,80,113	2.07	10 (23%)
15	CLA	A1	820	-	36,46,73	1.59	8 (22%)	45,80,113	1.76	10 (22%)
18	BCR	K2	102	-	25,25,41	0.37	0	33,33,56	0.41	0
15	CLA	A1	844	-	45,53,73	1.49	7 (15%)	52,89,113	1.51	9 (17%)
15	CLA	B2	827	-	65,73,73	1.25	7 (10%)	76,113,113	1.27	8 (10%)
15	CLA	B2	804	-	55,63,73	1.37	7 (12%)	64,101,113	1.38	11 (17%)
18	BCR	B2	841	-	41,41,41	0.19	0	56,56,56	0.35	0
15	CLA	B1	832	-	41,48,73	1.64	6 (14%)	45,82,113	1.97	9 (20%)
18	BCR	A3	852	-	41,41,41	0.15	0	56,56,56	0.38	0
15	CLA	A2	828	-	42,50,73	1.54	7 (16%)	48,85,113	1.72	9 (18%)
15	CLA	B1	823	2	41,49,73	1.71	8 (19%)	47,84,113	1.65	10 (21%)
15	CLA	A3	809	-	65,73,73	1.27	7 (10%)	76,113,113	1.42	10 (13%)
15	CLA	B2	836	-	45,53,73	1.55	7 (15%)	52,89,113	1.59	9 (17%)
15	CLA	A3	832	-	45,53,73	1.58	6 (13%)	52,89,113	1.61	11 (21%)
15	CLA	J2	1301	-	40,46,73	1.71	9 (22%)	48,79,113	1.73	12 (25%)
15	CLA	A3	814	-	33,41,73	1.74	9 (27%)	43,72,113	2.07	14 (32%)
15	CLA	B2	849	-	45,53,73	1.60	6 (13%)	52,89,113	1.47	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	BCR	A1	847	-	41,41,41	0.15	0	56,56,56	0.33	0
15	CLA	A3	823	-	41,49,73	1.67	8 (19%)	47,84,113	1.69	8 (17%)
15	CLA	B2	825	-	65,73,73	1.24	7 (10%)	76,113,113	1.28	11 (14%)
15	CLA	B2	813	-	45,53,73	1.52	7 (15%)	52,89,113	1.64	10 (19%)
15	CLA	X1	102	-	40,48,73	1.72	8 (20%)	46,83,113	1.72	13 (28%)
18	BCR	A3	855	-	30,30,41	0.33	0	39,39,56	0.36	0
15	CLA	K2	101	-	33,42,73	1.73	5 (15%)	35,73,113	2.00	11 (31%)
18	BCR	A1	851	-	41,41,41	0.13	0	56,56,56	0.43	0
15	CLA	B2	839	-	65,73,73	1.30	7 (10%)	76,113,113	1.28	9 (11%)
15	CLA	B2	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.31	9 (11%)
15	CLA	A1	814	-	33,41,73	1.74	9 (27%)	43,72,113	2.06	14 (32%)
18	BCR	B2	844	-	41,41,41	0.13	0	56,56,56	0.28	0
15	CLA	B1	811	-	45,53,73	1.48	6 (13%)	52,89,113	1.49	9 (17%)
15	CLA	A3	818	-	50,58,73	1.48	7 (14%)	58,95,113	1.54	9 (15%)
15	CLA	J1	1301	-	40,46,73	1.71	9 (22%)	48,79,113	1.73	12 (25%)
15	CLA	A1	825	24	60,68,73	1.28	6 (10%)	70,107,113	1.36	12 (17%)
18	BCR	F1	201	-	41,41,41	0.11	0	56,56,56	0.27	0
15	CLA	B2	821	-	38,47,73	1.72	6 (15%)	46,80,113	2.30	12 (26%)
15	CLA	L1	1002	10	65,73,73	1.24	7 (10%)	76,113,113	1.28	10 (13%)
15	CLA	B3	837	-	41,49,73	1.72	8 (19%)	47,84,113	1.68	9 (19%)
15	CLA	B1	813	-	45,53,73	1.52	7 (15%)	52,89,113	1.65	10 (19%)
15	CLA	K2	103	-	32,40,73	1.80	7 (21%)	38,70,113	2.24	13 (34%)
15	CLA	B3	814	-	41,49,73	1.69	8 (19%)	47,84,113	1.62	9 (19%)
15	CLA	X3	102	-	40,48,73	1.72	8 (20%)	46,83,113	1.72	13 (28%)
15	CLA	A3	827	-	60,68,73	1.33	7 (11%)	70,107,113	1.38	6 (8%)
19	LHG	X3	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.10	2 (4%)
19	LHG	X2	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.10	2 (4%)
15	CLA	B3	816	-	38,46,73	1.83	9 (23%)	40,79,113	1.87	10 (25%)
15	CLA	B2	806	-	50,58,73	1.43	7 (14%)	58,95,113	1.46	10 (17%)
15	CLA	A3	808	1	65,73,73	1.29	7 (10%)	76,113,113	1.32	9 (11%)
18	BCR	B2	845	-	41,41,41	0.14	0	56,56,56	0.38	0
15	CLA	L1	1003	-	60,68,73	1.30	6 (10%)	70,107,113	1.40	11 (15%)
15	CLA	A3	839	-	55,63,73	1.43	7 (12%)	64,101,113	1.39	9 (14%)
18	BCR	A3	847	-	41,41,41	0.15	0	56,56,56	0.33	0
15	CLA	A1	833	-	65,73,73	1.31	7 (10%)	76,113,113	1.33	10 (13%)
15	CLA	A1	807	-	43,52,73	1.56	7 (16%)	49,88,113	1.73	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A1	808	1	65,73,73	1.29	7 (10%)	76,113,113	1.31	9 (11%)
16	PQN	B3	840	-	34,34,34	0.23	0	42,45,45	0.52	1 (2%)
18	BCR	B3	841	-	41,41,41	0.19	0	56,56,56	0.35	0
15	CLA	A1	802	24	65,73,73	1.32	7 (10%)	76,113,113	1.36	7 (9%)
18	BCR	I1	102	-	41,41,41	0.19	0	56,56,56	0.45	0
18	BCR	B2	846	-	41,41,41	0.19	0	56,56,56	0.48	0
15	CLA	A1	826	24	55,63,73	1.38	7 (12%)	64,101,113	1.50	9 (14%)
15	CLA	B1	822	-	39,48,73	1.60	7 (17%)	45,82,113	1.66	7 (15%)
15	CLA	B1	803	-	54,62,73	1.45	7 (12%)	62,99,113	1.36	8 (12%)
15	CLA	B1	804	-	55,63,73	1.38	7 (12%)	64,101,113	1.38	11 (17%)
15	CLA	B2	822	-	39,48,73	1.61	7 (17%)	45,82,113	1.67	7 (15%)
15	CLA	B2	807	-	60,68,73	1.41	6 (10%)	70,107,113	1.64	10 (14%)
15	CLA	B2	824	24	45,53,73	1.54	7 (15%)	52,89,113	1.58	8 (15%)
15	CLA	A3	803	-	63,72,73	1.31	7 (11%)	73,112,113	1.38	10 (13%)
18	BCR	A3	851	-	41,41,41	0.13	0	56,56,56	0.43	0
15	CLA	A1	818	-	50,58,73	1.48	7 (14%)	58,95,113	1.54	9 (15%)
18	BCR	F2	201	-	41,41,41	0.11	0	56,56,56	0.28	0
15	CLA	A3	804	-	65,73,73	1.30	7 (10%)	76,113,113	1.38	11 (14%)
15	CLA	B1	838	24	65,73,73	1.27	7 (10%)	76,113,113	1.30	9 (11%)
15	CLA	A3	856	-	65,73,73	1.30	6 (9%)	76,113,113	1.20	8 (10%)
15	CLA	A2	825	24	60,68,73	1.28	6 (10%)	70,107,113	1.36	12 (17%)
15	CLA	A1	819	-	58,67,73	1.40	7 (12%)	67,106,113	1.64	11 (16%)
15	CLA	A2	815	-	37,44,73	1.89	10 (27%)	43,76,113	1.98	9 (20%)
15	CLA	A1	806	-	65,73,73	1.26	7 (10%)	76,113,113	1.28	10 (13%)
15	CLA	B3	813	-	45,53,73	1.53	7 (15%)	52,89,113	1.65	10 (19%)
15	CLA	B3	830	-	41,49,73	1.72	8 (19%)	47,84,113	1.70	8 (17%)
15	CLA	A3	825	24	60,68,73	1.29	7 (11%)	70,107,113	1.36	12 (17%)
15	CLA	A2	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.32	8 (10%)
15	CLA	B2	819	-	45,53,73	1.54	7 (15%)	52,89,113	1.69	9 (17%)
15	CLA	A1	841	24	39,48,73	1.72	8 (20%)	44,83,113	1.66	10 (22%)
15	CLA	B3	808	-	65,73,73	1.35	7 (10%)	76,113,113	1.68	14 (18%)
15	CLA	B3	818	-	50,58,73	1.43	7 (14%)	58,95,113	1.48	9 (15%)
21	DGD	B1	848	-	67,67,67	0.17	0	81,81,81	0.15	0
15	CLA	A1	822	-	45,53,73	1.52	7 (15%)	52,89,113	1.64	9 (17%)
17	SF4	C1	101	3	0,12,12	-	-	-	-	-
17	SF4	C3	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A1	843	24	65,73,73	1.29	7 (10%)	76,113,113	1.29	9 (11%)
15	CLA	B1	824	24	45,53,73	1.54	7 (15%)	52,89,113	1.58	8 (15%)
15	CLA	B3	826	-	45,53,73	1.56	7 (15%)	52,89,113	1.46	8 (15%)
15	CLA	A2	856	-	65,73,73	1.30	6 (9%)	76,113,113	1.20	8 (10%)
17	SF4	C2	102	3	0,12,12	-	-	-		
15	CLA	A2	821	-	64,72,73	1.28	7 (10%)	75,112,113	1.33	11 (14%)
15	CLA	A1	812	-	40,48,73	1.70	8 (20%)	46,83,113	1.72	9 (19%)
15	CLA	B1	828	-	41,50,73	1.65	6 (14%)	49,85,113	1.67	8 (16%)
16	PQN	A1	845	-	34,34,34	0.24	0	42,45,45	0.46	1 (2%)
15	CLA	A2	829	-	55,63,73	1.35	7 (12%)	64,101,113	1.45	10 (15%)
15	CLA	B1	814	-	41,49,73	1.68	8 (19%)	47,84,113	1.62	9 (19%)
15	CLA	B2	828	-	41,50,73	1.66	6 (14%)	49,85,113	1.67	8 (16%)
18	BCR	J2	1305	-	41,41,41	0.17	0	56,56,56	0.29	0
15	CLA	A2	836	1	41,49,73	1.69	7 (17%)	47,84,113	1.67	8 (17%)
15	CLA	B3	835	-	46,54,73	1.48	7 (15%)	53,90,113	1.60	9 (16%)
15	CLA	A3	833	-	65,73,73	1.31	7 (10%)	76,113,113	1.33	10 (13%)
18	BCR	A2	848	-	41,41,41	0.14	0	56,56,56	0.31	0
15	CLA	A3	807	-	43,52,73	1.56	7 (16%)	49,88,113	1.73	10 (20%)
15	CLA	B1	808	-	65,73,73	1.35	7 (10%)	76,113,113	1.68	14 (18%)
15	CLA	B1	818	-	50,58,73	1.43	7 (14%)	58,95,113	1.48	9 (15%)
15	CLA	A3	802	24	65,73,73	1.32	7 (10%)	76,113,113	1.36	7 (9%)
15	CLA	B1	849	-	45,53,73	1.60	6 (13%)	52,89,113	1.47	8 (15%)
15	CLA	A3	815	-	37,44,73	1.90	10 (27%)	43,76,113	1.97	10 (23%)
15	CLA	A2	804	-	65,73,73	1.30	7 (10%)	76,113,113	1.37	10 (13%)
18	BCR	B3	845	-	41,41,41	0.14	0	56,56,56	0.38	0
15	CLA	A2	831	-	50,58,73	1.48	7 (14%)	58,95,113	1.62	9 (15%)
18	BCR	B1	843	-	25,25,41	0.36	0	33,33,56	0.46	0
23	GAK	R3	101	12	0,4,4	-	-	-		
15	CLA	J2	1307	-	34,42,73	1.97	11 (32%)	41,73,113	2.14	12 (29%)
18	BCR	L3	1005	-	41,41,41	0.22	0	56,56,56	0.47	0
15	CLA	A2	810	-	37,46,73	1.92	9 (24%)	42,80,113	2.09	10 (23%)
15	CLA	B3	804	-	55,63,73	1.37	7 (12%)	64,101,113	1.38	11 (17%)
15	CLA	A3	841	24	39,48,73	1.72	8 (20%)	44,83,113	1.65	10 (22%)
15	CLA	B3	824	24	45,53,73	1.54	7 (15%)	52,89,113	1.58	8 (15%)
15	CLA	A1	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.32	8 (10%)
18	BCR	B2	847	-	41,41,41	0.15	0	56,56,56	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A3	831	-	50,58,73	1.48	7 (14%)	58,95,113	1.62	10 (17%)
18	BCR	B3	843	-	25,25,41	0.36	0	33,33,56	0.46	0
15	CLA	B2	816	-	38,46,73	1.84	9 (23%)	40,79,113	1.88	10 (25%)
15	CLA	A2	834	-	65,73,73	1.27	7 (10%)	76,113,113	1.34	11 (14%)
17	SF4	C1	102	3	0,12,12	-	-	-	-	-
16	PQN	A2	845	-	34,34,34	0.25	0	42,45,45	0.46	1 (2%)
18	BCR	M1	101	-	41,41,41	0.16	0	56,56,56	0.30	0
15	CLA	A1	827	-	60,68,73	1.33	7 (11%)	70,107,113	1.38	6 (8%)
15	CLA	A2	811	-	65,73,73	1.29	7 (10%)	76,113,113	1.35	9 (11%)
15	CLA	B3	825	-	65,73,73	1.24	7 (10%)	76,113,113	1.27	11 (14%)
15	CLA	B2	814	-	41,49,73	1.68	8 (19%)	47,84,113	1.62	8 (17%)
15	CLA	B2	812	-	65,73,73	1.29	7 (10%)	76,113,113	1.38	12 (15%)
18	BCR	A2	855	-	30,30,41	0.33	0	39,39,56	0.36	0
18	BCR	J1	1306	-	41,41,41	0.20	0	56,56,56	0.54	0
15	CLA	A2	844	-	45,53,73	1.49	7 (15%)	52,89,113	1.52	9 (17%)
15	CLA	B3	815	-	36,44,73	1.74	7 (19%)	40,76,113	1.83	9 (22%)
18	BCR	B3	844	-	41,41,41	0.13	0	56,56,56	0.28	0
15	CLA	A2	823	-	41,49,73	1.68	8 (19%)	47,84,113	1.69	8 (17%)
15	CLA	A3	812	-	40,48,73	1.70	8 (20%)	46,83,113	1.72	9 (19%)
18	BCR	L1	1005	-	41,41,41	0.23	0	56,56,56	0.47	0
15	CLA	B2	830	-	41,49,73	1.71	8 (19%)	47,84,113	1.71	8 (17%)
19	LHG	A1	854	-	34,34,48	0.22	0	37,40,54	0.31	0
18	BCR	M3	101	-	41,41,41	0.16	0	56,56,56	0.30	0
15	CLA	A3	828	-	42,50,73	1.54	7 (16%)	48,85,113	1.72	9 (18%)
18	BCR	L1	1006	-	41,41,41	0.16	0	56,56,56	0.33	0
18	BCR	A2	847	-	41,41,41	0.15	0	56,56,56	0.33	0
15	CLA	B1	825	-	65,73,73	1.24	7 (10%)	76,113,113	1.27	11 (14%)
15	CLA	B2	810	-	43,52,73	1.55	7 (16%)	49,88,113	1.58	9 (18%)
16	PQN	B2	840	-	34,34,34	0.22	0	42,45,45	0.53	1 (2%)
15	CLA	A2	817	-	39,46,73	1.73	10 (25%)	46,80,113	1.76	11 (23%)
18	BCR	A1	848	-	41,41,41	0.13	0	56,56,56	0.31	0
18	BCR	F3	201	-	41,41,41	0.12	0	56,56,56	0.27	0
17	SF4	A2	846	1,2	0,12,12	-	-	-	-	-
14	CL0	A1	801	-	65,73,73	2.41	7 (10%)	76,113,113	1.19	8 (10%)
15	CLA	A1	830	-	65,73,73	1.29	6 (9%)	76,113,113	1.28	11 (14%)
15	CLA	A3	805	-	65,73,73	1.25	7 (10%)	76,113,113	1.32	8 (10%)
15	CLA	L3	1002	10	65,73,73	1.24	7 (10%)	76,113,113	1.28	11 (14%)
18	BCR	B1	844	-	41,41,41	0.13	0	56,56,56	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A3	811	-	65,73,73	1.29	7 (10%)	76,113,113	1.34	9 (11%)
19	LHG	A3	853	-	46,46,48	0.24	0	49,52,54	0.24	0
15	CLA	B2	834	-	37,47,73	1.65	7 (18%)	42,81,113	1.79	10 (23%)
15	CLA	B1	827	-	65,73,73	1.25	7 (10%)	76,113,113	1.26	8 (10%)
15	CLA	B3	801	-	65,73,73	1.30	6 (9%)	76,113,113	1.27	8 (10%)
19	LHG	A2	854	-	34,34,48	0.23	0	37,40,54	0.31	0
18	BCR	I3	102	-	41,41,41	0.19	0	56,56,56	0.45	0
15	CLA	B1	821	-	38,47,73	1.72	6 (15%)	46,80,113	2.30	12 (26%)
15	CLA	A1	836	1	41,49,73	1.69	7 (17%)	47,84,113	1.67	8 (17%)
18	BCR	J1	1305	-	41,41,41	0.18	0	56,56,56	0.29	0
18	BCR	L2	1005	-	41,41,41	0.22	0	56,56,56	0.47	0
15	CLA	B1	831	-	41,49,73	1.73	8 (19%)	47,84,113	1.74	12 (25%)
15	CLA	B2	820	-	36,44,73	1.76	7 (19%)	40,76,113	1.89	10 (25%)
15	CLA	B1	836	-	45,53,73	1.55	7 (15%)	52,89,113	1.59	9 (17%)
15	CLA	B2	832	-	41,48,73	1.65	6 (14%)	45,82,113	1.98	9 (20%)
18	BCR	J3	1304	-	41,41,41	0.15	0	56,56,56	0.29	0
15	CLA	B1	807	-	60,68,73	1.41	6 (10%)	70,107,113	1.64	10 (14%)
18	BCR	B1	842	-	30,30,41	0.34	0	39,39,56	0.51	0
18	BCR	B1	846	-	41,41,41	0.19	0	56,56,56	0.48	0
15	CLA	A3	824	-	45,53,73	1.51	7 (15%)	52,89,113	1.54	10 (19%)

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
15	CLA	A3	843	24	1/1/15/20	7/37/115/115	-
15	CLA	B1	829	-	1/1/6/20	0/2/69/115	-
15	CLA	L3	1004	24	1/1/15/20	4/37/115/115	-
15	CLA	A1	817	-	1/1/10/20	0/6/82/115	-
18	BCR	B1	845	-	-	2/29/63/63	0/2/2/2
15	CLA	B3	805	-	1/1/15/20	7/37/115/115	-
15	CLA	A2	824	-	1/1/11/20	6/13/91/115	-
15	CLA	A3	838	-	1/1/13/20	8/25/103/115	-
15	CLA	B3	812	-	1/1/15/20	5/37/115/115	-
15	CLA	B1	817	-	1/1/12/20	2/19/97/115	-
18	BCR	M2	101	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A2	808	1	1/1/15/20	3/37/115/115	-
15	CLA	B1	820	-	1/1/7/20	0/2/72/115	-
18	BCR	A2	850	-	-	4/29/63/63	0/2/2/2
18	BCR	B2	843	-	-	2/18/35/63	0/1/1/2
18	BCR	J3	1305	-	-	4/29/63/63	0/2/2/2
15	CLA	A2	802	24	1/1/15/20	1/37/115/115	-
15	CLA	B2	835	-	1/1/11/20	4/15/93/115	-
18	BCR	A3	848	-	-	4/29/63/63	0/2/2/2
15	CLA	B3	832	-	1/1/9/20	2/8/82/115	-
15	CLA	B3	811	-	1/1/11/20	1/13/91/115	-
15	CLA	A3	813	-	1/1/11/20	5/13/89/115	-
15	CLA	B2	829	-	1/1/6/20	0/2/69/115	-
15	CLA	B3	823	2	1/1/10/20	2/8/86/115	-
15	CLA	A1	831	-	1/1/12/20	2/19/97/115	-
15	CLA	B2	815	-	1/1/7/20	0/2/72/115	-
15	CLA	A2	806	-	1/1/15/20	5/37/115/115	-
15	CLA	A3	836	1	1/1/10/20	2/8/86/115	-
18	BCR	I3	103	-	-	5/29/63/63	0/2/2/2
15	CLA	A1	835	-	1/1/11/20	3/13/91/115	-
15	CLA	A2	835	-	1/1/11/20	3/13/91/115	-
15	CLA	B2	818	-	1/1/12/20	2/19/97/115	-
15	CLA	A2	837	-	1/1/12/20	2/19/97/115	-
15	CLA	J3	1302	8	1/1/8/20	-	-
15	CLA	B3	838	24	1/1/15/20	5/37/115/115	-
15	CLA	K3	101	-	1/1/7/20	0/0/70/115	-
15	CLA	B1	809	2	1/1/15/20	4/37/115/115	-
15	CLA	L2	1002	10	1/1/15/20	8/37/115/115	-
15	CLA	B3	834	-	1/1/9/20	0/6/80/115	-
15	CLA	B2	809	2	1/1/15/20	4/37/115/115	-
15	CLA	A3	817	-	1/1/10/20	0/6/82/115	-
15	CLA	A1	829	-	1/1/13/20	3/25/103/115	-
15	CLA	A2	842	-	1/1/15/20	6/37/115/115	-
15	CLA	A2	833	-	1/1/15/20	6/37/115/115	-
18	BCR	B3	842	-	-	1/24/41/63	0/1/1/2
15	CLA	B3	820	-	1/1/7/20	0/2/72/115	-
15	CLA	A3	820	-	1/1/9/20	1/6/78/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B3	803	-	1/1/12/20	3/24/102/115	-
15	CLA	A1	840	-	1/1/15/20	5/37/115/115	-
15	CLA	A1	804	-	1/1/15/20	4/37/115/115	-
18	BCR	A2	852	-	-	4/29/63/63	0/2/2/2
15	CLA	A2	839	-	1/1/13/20	7/25/103/115	-
15	CLA	B2	826	-	1/1/11/20	2/13/91/115	-
18	BCR	L2	1010	-	-	1/29/63/63	0/2/2/2
15	CLA	J1	1302	8	1/1/8/20	-	-
18	BCR	B1	841	-	-	3/29/63/63	0/2/2/2
15	CLA	L2	1004	24	1/1/15/20	4/37/115/115	-
18	BCR	A1	855	-	-	2/24/41/63	0/1/1/2
15	CLA	B1	837	-	1/1/10/20	5/8/86/115	-
15	CLA	B3	809	2	1/1/15/20	4/37/115/115	-
15	CLA	A3	826	24	1/1/13/20	5/25/103/115	-
15	CLA	B1	830	-	1/1/10/20	3/8/86/115	-
15	CLA	A2	816	-	1/1/10/20	0/8/86/115	-
15	CLA	B2	831	-	1/1/10/20	1/8/86/115	-
15	CLA	B1	816	-	1/1/8/20	3/6/76/115	-
15	CLA	A3	822	-	1/1/11/20	2/13/91/115	-
15	CLA	A3	830	-	1/1/15/20	9/37/115/115	-
19	LHG	A2	853	-	-	8/51/51/53	-
15	CLA	K1	101	-	1/1/7/20	0/0/70/115	-
18	BCR	J2	1304	-	-	3/29/63/63	0/2/2/2
17	SF4	A1	846	1,2	-	-	0/6/5/5
18	BCR	A1	849	-	-	0/29/63/63	0/2/2/2
15	CLA	B1	819	-	1/1/11/20	4/13/91/115	-
15	CLA	A1	834	-	1/1/15/20	4/37/115/115	-
15	CLA	A2	827	-	1/1/14/20	9/31/109/115	-
15	CLA	A2	813	-	1/1/11/20	5/13/89/115	-
15	CLA	A1	842	-	1/1/15/20	6/37/115/115	-
15	CLA	I1	101	2	1/1/15/20	4/37/115/115	-
15	CLA	A1	856	-	1/1/15/20	8/37/115/115	-
15	CLA	A3	819	-	1/1/14/20	2/29/107/115	-
15	CLA	B3	806	-	1/1/12/20	2/19/97/115	-
15	CLA	L3	1003	-	1/1/14/20	3/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DGD	B3	848	-	-	8/55/95/95	0/2/2/2
15	CLA	B1	802	24	1/1/15/20	6/37/115/115	-
18	BCR	J1	1304	-	-	3/29/63/63	0/2/2/2
15	CLA	B3	817	-	1/1/12/20	2/19/97/115	-
15	CLA	J1	1307	-	1/1/8/20	0/0/74/115	-
18	BCR	B1	847	-	-	6/29/63/63	0/2/2/2
17	SF4	C3	102	3	-	-	0/6/5/5
15	CLA	B3	822	-	1/1/9/20	0/8/82/115	-
15	CLA	B3	807	-	1/1/14/20	5/31/109/115	-
15	CLA	B2	823	2	1/1/10/20	2/8/86/115	-
15	CLA	B3	802	24	1/1/15/20	6/37/115/115	-
15	CLA	B1	810	-	1/1/11/20	0/11/89/115	-
16	PQN	B1	840	-	-	0/23/43/43	0/2/2/2
15	CLA	A3	821	-	1/1/15/20	0/35/113/115	-
15	CLA	B3	833	-	1/1/8/20	2/4/76/115	-
15	CLA	A1	824	-	1/1/11/20	6/13/91/115	-
15	CLA	K3	103	-	1/1/8/20	-	-
15	CLA	L1	1004	24	1/1/15/20	4/37/115/115	-
15	CLA	J2	1302	8	1/1/8/20	-	-
15	CLA	A2	841	24	1/1/10/20	1/6/84/115	-
14	CL0	A2	801	-	3/3/20/25	4/37/135/135	-
15	CLA	B3	849	-	1/1/11/20	7/13/91/115	-
15	CLA	B1	805	-	1/1/15/20	7/37/115/115	-
15	CLA	J3	1303	-	1/1/9/20	-	-
15	CLA	A2	830	-	1/1/15/20	9/37/115/115	-
15	CLA	A3	834	-	1/1/15/20	4/37/115/115	-
15	CLA	B1	834	-	1/1/9/20	0/6/80/115	-
15	CLA	B1	812	-	1/1/15/20	5/37/115/115	-
15	CLA	A2	832	-	1/1/11/20	6/13/91/115	-
15	CLA	B2	811	-	1/1/11/20	1/13/91/115	-
15	CLA	B3	819	-	1/1/11/20	4/13/91/115	-
18	BCR	J2	1306	-	-	5/29/63/63	0/2/2/2
23	GAK	R2	101	12	-	-	0/1/1/1
19	LHG	X1	101	-	-	20/46/46/53	-
18	BCR	B3	847	-	-	6/29/63/63	0/2/2/2
15	CLA	I3	101	2	1/1/15/20	4/37/115/115	-
15	CLA	J3	1307	-	1/1/8/20	0/0/74/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	B2	842	-	-	1/24/41/63	0/1/1/2
19	LHG	A3	854	-	-	8/38/38/53	-
15	CLA	B2	838	24	1/1/15/20	5/37/115/115	-
15	CLA	I2	101	2	1/1/15/20	4/37/115/115	-
15	CLA	A3	835	-	1/1/11/20	3/13/91/115	-
15	CLA	A1	809	-	1/1/15/20	9/37/115/115	-
15	CLA	B1	801	-	1/1/15/20	8/37/115/115	-
15	CLA	B3	828	-	1/1/10/20	4/7/85/115	-
15	CLA	K1	103	-	1/1/8/20	-	-
15	CLA	B1	839	-	1/1/15/20	7/37/115/115	-
17	SF4	C2	101	3	-	-	0/6/5/5
15	CLA	A3	829	-	1/1/13/20	3/25/103/115	-
18	BCR	A1	850	-	-	4/29/63/63	0/2/2/2
15	CLA	A1	828	-	1/1/10/20	2/10/88/115	-
15	CLA	B3	810	-	1/1/11/20	0/11/89/115	-
15	CLA	B1	835	-	1/1/11/20	4/15/93/115	-
15	CLA	B2	803	-	1/1/12/20	2/24/102/115	-
23	GAK	R1	101	12	-	-	0/1/1/1
14	CL0	A3	801	-	3/3/20/25	4/37/135/135	-
15	CLA	B2	801	-	1/1/15/20	8/37/115/115	-
15	CLA	J3	1301	-	1/1/10/20	1/8/84/115	-
15	CLA	A3	840	-	1/1/15/20	5/37/115/115	-
15	CLA	X2	102	-	1/1/10/20	2/6/84/115	-
18	BCR	A3	850	-	-	4/29/63/63	0/2/2/2
15	CLA	A1	815	-	1/1/10/20	2/6/82/115	-
15	CLA	B3	821	-	1/1/8/20	3/8/79/115	-
15	CLA	B2	817	-	1/1/12/20	2/19/97/115	-
15	CLA	B2	808	-	1/1/15/20	6/37/115/115	-
18	BCR	I2	103	-	-	5/29/63/63	0/2/2/2
15	CLA	A1	837	-	1/1/12/20	2/19/97/115	-
15	CLA	A2	818	-	1/1/12/20	9/19/97/115	-
15	CLA	J2	1303	-	1/1/9/20	-	-
15	CLA	B2	833	-	1/1/8/20	2/4/76/115	-
15	CLA	A2	820	-	1/1/9/20	1/6/78/115	-
15	CLA	A1	839	-	1/1/13/20	7/25/103/115	-
15	CLA	L2	1003	-	1/1/14/20	3/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A1	813	-	1/1/11/20	5/13/89/115	-
15	CLA	A1	803	-	1/1/15/20	3/35/113/115	-
21	DGD	B2	848	-	-	8/55/95/95	0/2/2/2
18	BCR	J3	1306	-	-	5/29/63/63	0/2/2/2
18	BCR	A2	851	-	-	5/29/63/63	0/2/2/2
15	CLA	A1	816	-	1/1/10/20	0/8/86/115	-
15	CLA	B1	806	-	1/1/12/20	2/19/97/115	-
18	BCR	L1	1011	-	-	1/29/63/63	0/2/2/2
15	CLA	A1	838	-	1/1/13/20	8/25/103/115	-
15	CLA	A1	821	-	1/1/15/20	0/35/113/115	-
15	CLA	A2	822	-	1/1/11/20	2/13/91/115	-
15	CLA	A2	814	-	1/1/6/20	-	-
15	CLA	B3	839	-	1/1/15/20	7/37/115/115	-
15	CLA	B2	802	24	1/1/15/20	6/37/115/115	-
15	CLA	B3	827	-	1/1/15/20	12/37/115/115	-
18	BCR	A1	852	-	-	4/29/63/63	0/2/2/2
17	SF4	A3	846	1,2	-	-	0/6/5/5
18	BCR	A3	849	-	-	0/29/63/63	0/2/2/2
15	CLA	B1	833	-	1/1/8/20	2/4/76/115	-
18	BCR	I2	102	-	-	0/29/63/63	0/2/2/2
19	LHG	A1	853	-	-	8/51/51/53	-
15	CLA	A2	826	24	1/1/13/20	5/25/103/115	-
15	CLA	A2	840	-	1/1/15/20	5/37/115/115	-
15	CLA	A2	838	-	1/1/13/20	8/25/103/115	-
15	CLA	B1	826	-	1/1/11/20	2/13/91/115	-
15	CLA	B1	815	-	1/1/7/20	0/2/72/115	-
15	CLA	A3	842	-	1/1/15/20	6/37/115/115	-
15	CLA	A3	806	-	1/1/15/20	5/37/115/115	-
15	CLA	A1	832	-	1/1/11/20	6/13/91/115	-
15	CLA	B3	829	-	1/1/6/20	0/2/69/115	-
18	BCR	K3	102	-	-	2/18/35/63	0/1/1/2
15	CLA	A2	843	24	1/1/15/20	7/37/115/115	-
15	CLA	A1	823	-	1/1/10/20	2/8/86/115	-
15	CLA	A3	837	-	1/1/12/20	2/19/97/115	-
15	CLA	A1	810	-	1/1/10/20	1/4/82/115	-
15	CLA	A2	803	-	1/1/15/20	3/35/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	I1	103	-	-	5/29/63/63	0/2/2/2
15	CLA	A2	807	-	1/1/11/20	7/11/89/115	-
15	CLA	B2	837	-	1/1/10/20	5/8/86/115	-
15	CLA	A2	809	-	1/1/15/20	9/37/115/115	-
15	CLA	A3	844	-	1/1/11/20	3/13/91/115	-
15	CLA	A3	816	-	1/1/10/20	0/8/86/115	-
15	CLA	A2	812	-	1/1/10/20	0/6/84/115	-
15	CLA	B3	831	-	1/1/10/20	1/8/86/115	-
15	CLA	A2	819	-	1/1/14/20	2/29/107/115	-
15	CLA	B3	836	-	1/1/11/20	2/13/91/115	-
16	PQN	A3	845	-	-	0/23/43/43	0/2/2/2
18	BCR	B3	846	-	-	0/29/63/63	0/2/2/2
15	CLA	A1	811	-	1/1/15/20	7/37/115/115	-
15	CLA	J1	1303	-	1/1/9/20	-	-
18	BCR	K1	102	-	-	2/18/35/63	0/1/1/2
18	BCR	A2	849	-	-	0/29/63/63	0/2/2/2
15	CLA	A3	810	-	1/1/10/20	1/4/82/115	-
15	CLA	A1	820	-	1/1/9/20	1/6/78/115	-
18	BCR	K2	102	-	-	2/18/35/63	0/1/1/2
15	CLA	A1	844	-	1/1/11/20	3/13/91/115	-
15	CLA	B2	827	-	1/1/15/20	12/37/115/115	-
15	CLA	B2	804	-	1/1/13/20	2/25/103/115	-
18	BCR	B2	841	-	-	3/29/63/63	0/2/2/2
15	CLA	B1	832	-	1/1/9/20	2/8/82/115	-
18	BCR	A3	852	-	-	4/29/63/63	0/2/2/2
15	CLA	A2	828	-	1/1/10/20	2/10/88/115	-
15	CLA	B1	823	2	1/1/10/20	2/8/86/115	-
15	CLA	A3	809	-	1/1/15/20	9/37/115/115	-
15	CLA	B2	836	-	1/1/11/20	2/13/91/115	-
15	CLA	A3	832	-	1/1/11/20	6/13/91/115	-
15	CLA	J2	1301	-	1/1/10/20	1/8/84/115	-
15	CLA	A3	814	-	1/1/6/20	-	-
15	CLA	B2	849	-	1/1/11/20	7/13/91/115	-
18	BCR	A1	847	-	-	1/29/63/63	0/2/2/2
15	CLA	A3	823	-	1/1/10/20	2/8/86/115	-
15	CLA	B2	825	-	1/1/15/20	1/37/115/115	-
15	CLA	B2	813	-	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	X1	102	-	1/1/10/20	2/6/84/115	-
18	BCR	A3	855	-	-	2/24/41/63	0/1/1/2
15	CLA	K2	101	-	1/1/7/20	0/0/70/115	-
18	BCR	A1	851	-	-	5/29/63/63	0/2/2/2
15	CLA	B2	839	-	1/1/15/20	7/37/115/115	-
15	CLA	B2	805	-	1/1/15/20	7/37/115/115	-
15	CLA	A1	814	-	1/1/6/20	-	-
18	BCR	B2	844	-	-	2/29/63/63	0/2/2/2
15	CLA	B1	811	-	1/1/11/20	1/13/91/115	-
15	CLA	A3	818	-	1/1/12/20	9/19/97/115	-
15	CLA	J1	1301	-	1/1/10/20	1/8/84/115	-
15	CLA	A1	825	24	1/1/14/20	9/31/109/115	-
18	BCR	F1	201	-	-	2/29/63/63	0/2/2/2
15	CLA	B2	821	-	1/1/8/20	3/8/79/115	-
15	CLA	L1	1002	10	1/1/15/20	8/37/115/115	-
15	CLA	B3	837	-	1/1/10/20	5/8/86/115	-
15	CLA	B1	813	-	1/1/11/20	7/13/91/115	-
15	CLA	K2	103	-	1/1/8/20	-	-
15	CLA	B3	814	-	1/1/10/20	3/8/86/115	-
15	CLA	X3	102	-	1/1/10/20	2/6/84/115	-
15	CLA	A3	827	-	1/1/14/20	9/31/109/115	-
19	LHG	X3	101	-	-	20/46/46/53	-
19	LHG	X2	101	-	-	20/46/46/53	-
15	CLA	B3	816	-	1/1/8/20	3/6/76/115	-
15	CLA	B2	806	-	1/1/12/20	2/19/97/115	-
15	CLA	A3	808	1	1/1/15/20	3/37/115/115	-
18	BCR	B2	845	-	-	2/29/63/63	0/2/2/2
15	CLA	L1	1003	-	1/1/14/20	3/31/109/115	-
15	CLA	A3	839	-	1/1/13/20	7/25/103/115	-
18	BCR	A3	847	-	-	1/29/63/63	0/2/2/2
15	CLA	A1	833	-	1/1/15/20	6/37/115/115	-
15	CLA	A1	807	-	1/1/11/20	7/11/89/115	-
15	CLA	A1	808	1	1/1/15/20	3/37/115/115	-
16	PQN	B3	840	-	-	0/23/43/43	0/2/2/2
18	BCR	B3	841	-	-	3/29/63/63	0/2/2/2
15	CLA	A1	802	24	1/1/15/20	1/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	I1	102	-	-	0/29/63/63	0/2/2/2
18	BCR	B2	846	-	-	0/29/63/63	0/2/2/2
15	CLA	A1	826	24	1/1/13/20	5/25/103/115	-
15	CLA	B1	822	-	1/1/9/20	0/8/82/115	-
15	CLA	B1	803	-	1/1/12/20	3/24/102/115	-
15	CLA	B1	804	-	1/1/13/20	2/25/103/115	-
15	CLA	B2	822	-	1/1/9/20	0/8/82/115	-
15	CLA	B2	807	-	1/1/14/20	5/31/109/115	-
15	CLA	B2	824	24	1/1/11/20	2/13/91/115	-
15	CLA	A3	803	-	1/1/15/20	3/35/113/115	-
18	BCR	A3	851	-	-	5/29/63/63	0/2/2/2
15	CLA	A1	818	-	1/1/12/20	9/19/97/115	-
18	BCR	F2	201	-	-	2/29/63/63	0/2/2/2
15	CLA	A3	804	-	1/1/15/20	4/37/115/115	-
15	CLA	B1	838	24	1/1/15/20	5/37/115/115	-
15	CLA	A3	856	-	1/1/15/20	8/37/115/115	-
15	CLA	A2	825	24	1/1/14/20	9/31/109/115	-
15	CLA	A1	819	-	1/1/14/20	2/29/107/115	-
15	CLA	A2	815	-	1/1/10/20	2/6/82/115	-
15	CLA	A1	806	-	1/1/15/20	5/37/115/115	-
15	CLA	B3	813	-	1/1/11/20	7/13/91/115	-
15	CLA	B3	830	-	1/1/10/20	3/8/86/115	-
15	CLA	A3	825	24	1/1/14/20	9/31/109/115	-
15	CLA	A2	805	-	1/1/15/20	4/37/115/115	-
15	CLA	B2	819	-	1/1/11/20	4/13/91/115	-
15	CLA	A1	841	24	1/1/10/20	1/6/84/115	-
15	CLA	B3	808	-	1/1/15/20	6/37/115/115	-
15	CLA	B3	818	-	1/1/12/20	2/19/97/115	-
21	DGD	B1	848	-	-	8/55/95/95	0/2/2/2
15	CLA	A1	822	-	1/1/11/20	2/13/91/115	-
17	SF4	C1	101	3	-	-	0/6/5/5
17	SF4	C3	101	3	-	-	0/6/5/5
15	CLA	A1	843	24	1/1/15/20	7/37/115/115	-
15	CLA	B1	824	24	1/1/11/20	2/13/91/115	-
15	CLA	B3	826	-	1/1/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A2	856	-	1/1/15/20	8/37/115/115	-
17	SF4	C2	102	3	-	-	0/6/5/5
15	CLA	A2	821	-	1/1/15/20	0/35/113/115	-
15	CLA	A1	812	-	1/1/10/20	0/6/84/115	-
15	CLA	B1	828	-	1/1/10/20	4/7/85/115	-
16	PQN	A1	845	-	-	0/23/43/43	0/2/2/2
15	CLA	A2	829	-	1/1/13/20	3/25/103/115	-
15	CLA	B1	814	-	1/1/10/20	3/8/86/115	-
15	CLA	B2	828	-	1/1/10/20	4/7/85/115	-
18	BCR	J2	1305	-	-	4/29/63/63	0/2/2/2
15	CLA	A2	836	1	1/1/10/20	2/8/86/115	-
15	CLA	B3	835	-	1/1/11/20	4/15/93/115	-
15	CLA	A3	833	-	1/1/15/20	6/37/115/115	-
18	BCR	A2	848	-	-	4/29/63/63	0/2/2/2
15	CLA	A3	807	-	1/1/11/20	7/11/89/115	-
15	CLA	B1	808	-	1/1/15/20	6/37/115/115	-
15	CLA	B1	818	-	1/1/12/20	2/19/97/115	-
15	CLA	A3	802	24	1/1/15/20	1/37/115/115	-
15	CLA	B1	849	-	1/1/11/20	7/13/91/115	-
15	CLA	A3	815	-	1/1/10/20	2/6/82/115	-
15	CLA	A2	804	-	1/1/15/20	4/37/115/115	-
18	BCR	B3	845	-	-	2/29/63/63	0/2/2/2
15	CLA	A2	831	-	1/1/12/20	2/19/97/115	-
18	BCR	B1	843	-	-	2/18/35/63	0/1/1/2
23	GAK	R3	101	12	-	-	0/1/1/1
15	CLA	J2	1307	-	1/1/8/20	0/0/74/115	-
18	BCR	L3	1005	-	-	2/29/63/63	0/2/2/2
15	CLA	A2	810	-	1/1/10/20	1/4/82/115	-
15	CLA	B3	804	-	1/1/13/20	2/25/103/115	-
15	CLA	A3	841	24	1/1/10/20	1/6/84/115	-
15	CLA	B3	824	24	1/1/11/20	2/13/91/115	-
15	CLA	A1	805	-	1/1/15/20	4/37/115/115	-
18	BCR	B2	847	-	-	6/29/63/63	0/2/2/2
15	CLA	A3	831	-	1/1/12/20	2/19/97/115	-
18	BCR	B3	843	-	-	2/18/35/63	0/1/1/2
15	CLA	B2	816	-	1/1/8/20	3/6/76/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A2	834	-	1/1/15/20	4/37/115/115	-
17	SF4	C1	102	3	-	-	0/6/5/5
16	PQN	A2	845	-	-	0/23/43/43	0/2/2/2
18	BCR	M1	101	-	-	2/29/63/63	0/2/2/2
15	CLA	A1	827	-	1/1/14/20	9/31/109/115	-
15	CLA	A2	811	-	1/1/15/20	7/37/115/115	-
15	CLA	B3	825	-	1/1/15/20	1/37/115/115	-
15	CLA	B2	814	-	1/1/10/20	3/8/86/115	-
15	CLA	B2	812	-	1/1/15/20	5/37/115/115	-
18	BCR	A2	855	-	-	2/24/41/63	0/1/1/2
18	BCR	J1	1306	-	-	5/29/63/63	0/2/2/2
15	CLA	A2	844	-	1/1/11/20	3/13/91/115	-
15	CLA	B3	815	-	1/1/7/20	0/2/72/115	-
18	BCR	B3	844	-	-	2/29/63/63	0/2/2/2
15	CLA	A2	823	-	1/1/10/20	2/8/86/115	-
15	CLA	A3	812	-	1/1/10/20	0/6/84/115	-
18	BCR	L1	1005	-	-	2/29/63/63	0/2/2/2
15	CLA	B2	830	-	1/1/10/20	3/8/86/115	-
19	LHG	A1	854	-	-	8/38/38/53	-
18	BCR	M3	101	-	-	2/29/63/63	0/2/2/2
15	CLA	A3	828	-	1/1/10/20	2/10/88/115	-
18	BCR	L1	1006	-	-	1/29/63/63	0/2/2/2
18	BCR	A2	847	-	-	1/29/63/63	0/2/2/2
15	CLA	B1	825	-	1/1/15/20	2/37/115/115	-
15	CLA	B2	810	-	1/1/11/20	0/11/89/115	-
16	PQN	B2	840	-	-	0/23/43/43	0/2/2/2
15	CLA	A2	817	-	1/1/10/20	0/6/82/115	-
18	BCR	A1	848	-	-	4/29/63/63	0/2/2/2
18	BCR	F3	201	-	-	2/29/63/63	0/2/2/2
17	SF4	A2	846	1,2	-	-	0/6/5/5
14	CL0	A1	801	-	3/3/20/25	4/37/135/135	-
15	CLA	A1	830	-	1/1/15/20	9/37/115/115	-
15	CLA	A3	805	-	1/1/15/20	4/37/115/115	-
15	CLA	L3	1002	10	1/1/15/20	8/37/115/115	-
18	BCR	B1	844	-	-	2/29/63/63	0/2/2/2
15	CLA	A3	811	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	A3	853	-	-	8/51/51/53	-
15	CLA	B2	834	-	1/1/9/20	0/6/80/115	-
15	CLA	B1	827	-	1/1/15/20	12/37/115/115	-
15	CLA	B3	801	-	1/1/15/20	8/37/115/115	-
19	LHG	A2	854	-	-	8/38/38/53	-
18	BCR	I3	102	-	-	0/29/63/63	0/2/2/2
15	CLA	B1	821	-	1/1/8/20	3/8/79/115	-
15	CLA	A1	836	1	1/1/10/20	2/8/86/115	-
18	BCR	J1	1305	-	-	4/29/63/63	0/2/2/2
18	BCR	L2	1005	-	-	2/29/63/63	0/2/2/2
15	CLA	B1	831	-	1/1/10/20	1/8/86/115	-
15	CLA	B2	820	-	1/1/7/20	0/2/72/115	-
15	CLA	B1	836	-	1/1/11/20	2/13/91/115	-
15	CLA	B2	832	-	1/1/9/20	2/8/82/115	-
18	BCR	J3	1304	-	-	3/29/63/63	0/2/2/2
15	CLA	B1	807	-	1/1/14/20	5/31/109/115	-
18	BCR	B1	842	-	-	1/24/41/63	0/1/1/2
18	BCR	B1	846	-	-	0/29/63/63	0/2/2/2
15	CLA	A3	824	-	1/1/11/20	6/13/91/115	-

All (2082) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A3	801	CL0	C4B-NB	13.40	1.47	1.35
14	A1	801	CL0	C4B-NB	13.40	1.47	1.35
14	A2	801	CL0	C4B-NB	13.40	1.47	1.35
14	A1	801	CL0	C1B-NB	9.41	1.43	1.35
14	A3	801	CL0	C1B-NB	9.41	1.43	1.35
14	A2	801	CL0	C1B-NB	9.40	1.43	1.35
14	A2	801	CL0	MG-ND	-7.21	1.91	2.05
14	A1	801	CL0	MG-ND	-7.19	1.91	2.05
14	A3	801	CL0	MG-ND	-7.18	1.91	2.05
15	B3	849	CLA	MG-ND	-6.13	1.93	2.05
15	B1	849	CLA	MG-ND	-6.11	1.93	2.05
15	B3	809	CLA	MG-ND	-6.11	1.93	2.05
15	A2	832	CLA	MG-ND	-6.11	1.93	2.05
15	B2	828	CLA	MG-ND	-6.10	1.93	2.05
15	B1	809	CLA	MG-ND	-6.10	1.93	2.05
15	B3	828	CLA	MG-ND	-6.09	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B2	849	CLA	MG-ND	-6.09	1.93	2.05
15	B2	809	CLA	MG-ND	-6.09	1.93	2.05
15	B1	828	CLA	MG-ND	-6.09	1.93	2.05
15	A1	832	CLA	MG-ND	-6.08	1.93	2.05
15	A3	832	CLA	MG-ND	-6.03	1.93	2.05
15	B2	826	CLA	MG-ND	-6.01	1.93	2.05
15	A2	830	CLA	MG-ND	-6.00	1.93	2.05
15	A1	830	CLA	MG-ND	-6.00	1.93	2.05
15	B3	807	CLA	MG-ND	-6.00	1.93	2.05
15	B2	807	CLA	MG-ND	-5.99	1.93	2.05
15	A3	830	CLA	MG-ND	-5.99	1.93	2.05
15	B3	826	CLA	MG-ND	-5.99	1.93	2.05
15	B1	826	CLA	MG-ND	-5.98	1.93	2.05
15	B1	807	CLA	MG-ND	-5.98	1.93	2.05
15	B2	820	CLA	MG-ND	-5.92	1.94	2.05
15	B3	820	CLA	MG-ND	-5.92	1.94	2.05
15	B1	820	CLA	MG-ND	-5.92	1.94	2.05
15	A3	833	CLA	MG-ND	-5.82	1.94	2.05
15	A2	833	CLA	MG-ND	-5.82	1.94	2.05
15	B3	815	CLA	MG-ND	-5.82	1.94	2.05
15	B2	803	CLA	MG-ND	-5.82	1.94	2.05
15	A1	833	CLA	MG-ND	-5.81	1.94	2.05
15	B2	802	CLA	MG-ND	-5.81	1.94	2.05
15	B1	803	CLA	MG-ND	-5.81	1.94	2.05
15	B3	812	CLA	MG-ND	-5.80	1.94	2.05
15	B3	803	CLA	MG-ND	-5.80	1.94	2.05
15	B1	812	CLA	MG-ND	-5.80	1.94	2.05
15	B2	814	CLA	MG-ND	-5.80	1.94	2.05
15	B1	815	CLA	MG-ND	-5.79	1.94	2.05
15	B2	815	CLA	MG-ND	-5.79	1.94	2.05
15	B2	812	CLA	MG-ND	-5.79	1.94	2.05
15	B3	814	CLA	MG-ND	-5.79	1.94	2.05
15	B1	802	CLA	MG-ND	-5.78	1.94	2.05
15	B1	814	CLA	MG-ND	-5.78	1.94	2.05
15	B3	802	CLA	MG-ND	-5.78	1.94	2.05
15	X2	102	CLA	MG-ND	-5.77	1.94	2.05
15	A1	856	CLA	MG-ND	-5.76	1.94	2.05
15	A3	856	CLA	MG-ND	-5.75	1.94	2.05
15	B1	839	CLA	MG-ND	-5.75	1.94	2.05
15	B3	839	CLA	MG-ND	-5.75	1.94	2.05
15	B2	839	CLA	MG-ND	-5.75	1.94	2.05
15	A2	856	CLA	MG-ND	-5.75	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A1	818	CLA	MG-ND	-5.74	1.94	2.05
15	B2	801	CLA	MG-ND	-5.74	1.94	2.05
15	A2	839	CLA	MG-ND	-5.74	1.94	2.05
15	A2	818	CLA	MG-ND	-5.73	1.94	2.05
15	A3	839	CLA	MG-ND	-5.73	1.94	2.05
15	X1	102	CLA	MG-ND	-5.73	1.94	2.05
15	A3	836	CLA	MG-ND	-5.73	1.94	2.05
15	A3	818	CLA	MG-ND	-5.72	1.94	2.05
15	A1	839	CLA	MG-ND	-5.72	1.94	2.05
15	B1	830	CLA	MG-ND	-5.72	1.94	2.05
15	A1	836	CLA	MG-ND	-5.71	1.94	2.05
15	B2	830	CLA	MG-ND	-5.71	1.94	2.05
15	B3	801	CLA	MG-ND	-5.71	1.94	2.05
15	B1	801	CLA	MG-ND	-5.71	1.94	2.05
15	B3	830	CLA	MG-ND	-5.71	1.94	2.05
15	X3	102	CLA	MG-ND	-5.70	1.94	2.05
15	B3	816	CLA	MG-ND	-5.70	1.94	2.05
15	A2	836	CLA	MG-ND	-5.70	1.94	2.05
15	B1	816	CLA	MG-ND	-5.70	1.94	2.05
15	B2	816	CLA	MG-ND	-5.69	1.94	2.05
15	B1	817	CLA	MG-ND	-5.69	1.94	2.05
15	A2	838	CLA	MG-ND	-5.69	1.94	2.05
15	B3	821	CLA	MG-ND	-5.68	1.94	2.05
15	A3	824	CLA	MG-ND	-5.68	1.94	2.05
15	A1	838	CLA	MG-ND	-5.68	1.94	2.05
15	B1	804	CLA	MG-ND	-5.68	1.94	2.05
15	A2	804	CLA	MG-ND	-5.68	1.94	2.05
15	A3	838	CLA	MG-ND	-5.68	1.94	2.05
15	A1	804	CLA	MG-ND	-5.67	1.94	2.05
15	A3	843	CLA	MG-ND	-5.67	1.94	2.05
15	A3	819	CLA	MG-ND	-5.67	1.94	2.05
15	A2	819	CLA	MG-ND	-5.67	1.94	2.05
15	A3	804	CLA	MG-ND	-5.67	1.94	2.05
15	B3	836	CLA	MG-ND	-5.67	1.94	2.05
15	A1	824	CLA	MG-ND	-5.66	1.94	2.05
15	A1	843	CLA	MG-ND	-5.66	1.94	2.05
15	B1	836	CLA	MG-ND	-5.66	1.94	2.05
15	B2	804	CLA	MG-ND	-5.66	1.94	2.05
15	B3	804	CLA	MG-ND	-5.66	1.94	2.05
15	B1	821	CLA	MG-ND	-5.66	1.94	2.05
15	A1	819	CLA	MG-ND	-5.66	1.94	2.05
15	A2	835	CLA	MG-ND	-5.66	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	817	CLA	MG-ND	-5.66	1.94	2.05
15	B2	817	CLA	MG-ND	-5.66	1.94	2.05
15	B2	821	CLA	MG-ND	-5.65	1.94	2.05
15	B2	836	CLA	MG-ND	-5.65	1.94	2.05
15	A2	824	CLA	MG-ND	-5.65	1.94	2.05
15	A2	843	CLA	MG-ND	-5.65	1.94	2.05
15	A1	835	CLA	MG-ND	-5.64	1.94	2.05
15	L2	1003	CLA	MG-ND	-5.64	1.94	2.05
15	A3	835	CLA	MG-ND	-5.64	1.94	2.05
15	L1	1003	CLA	MG-ND	-5.63	1.94	2.05
15	L3	1003	CLA	MG-ND	-5.62	1.94	2.05
15	A1	842	CLA	MG-ND	-5.61	1.94	2.05
15	A3	842	CLA	MG-ND	-5.61	1.94	2.05
15	A2	842	CLA	MG-ND	-5.61	1.94	2.05
15	A1	802	CLA	MG-ND	-5.61	1.94	2.05
15	J2	1302	CLA	MG-ND	-5.61	1.94	2.05
15	B2	824	CLA	MG-ND	-5.61	1.94	2.05
15	B3	824	CLA	MG-ND	-5.60	1.94	2.05
15	B3	831	CLA	MG-ND	-5.60	1.94	2.05
15	L1	1002	CLA	MG-ND	-5.60	1.94	2.05
15	L3	1002	CLA	MG-ND	-5.59	1.94	2.05
15	A2	802	CLA	MG-ND	-5.59	1.94	2.05
15	L3	1004	CLA	MG-ND	-5.59	1.94	2.05
15	J3	1302	CLA	MG-ND	-5.59	1.94	2.05
15	B1	824	CLA	MG-ND	-5.59	1.94	2.05
15	L2	1004	CLA	MG-ND	-5.59	1.94	2.05
15	B3	821	CLA	MG-NA	-5.59	1.93	2.06
15	L2	1002	CLA	MG-ND	-5.58	1.94	2.05
15	B3	838	CLA	MG-ND	-5.58	1.94	2.05
15	B1	821	CLA	MG-NA	-5.58	1.93	2.06
15	A3	802	CLA	MG-ND	-5.58	1.94	2.05
15	J1	1302	CLA	MG-ND	-5.58	1.94	2.05
15	L1	1004	CLA	MG-ND	-5.58	1.94	2.05
15	B2	821	CLA	MG-NA	-5.57	1.93	2.06
15	B3	827	CLA	MG-ND	-5.57	1.94	2.05
15	B1	827	CLA	MG-ND	-5.57	1.94	2.05
15	B2	832	CLA	MG-ND	-5.57	1.94	2.05
15	B1	831	CLA	MG-ND	-5.57	1.94	2.05
15	B1	838	CLA	MG-ND	-5.56	1.94	2.05
15	B2	827	CLA	MG-ND	-5.56	1.94	2.05
15	B2	838	CLA	MG-ND	-5.56	1.94	2.05
15	B2	831	CLA	MG-ND	-5.56	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A1	834	CLA	MG-ND	-5.55	1.94	2.05
15	A2	834	CLA	MG-ND	-5.54	1.94	2.05
15	A3	834	CLA	MG-ND	-5.53	1.94	2.05
15	B1	832	CLA	MG-ND	-5.53	1.94	2.05
15	K2	103	CLA	MG-ND	-5.53	1.94	2.05
15	K3	103	CLA	MG-ND	-5.52	1.94	2.05
15	K1	103	CLA	MG-ND	-5.51	1.94	2.05
15	B2	810	CLA	MG-ND	-5.49	1.94	2.05
15	B3	832	CLA	MG-ND	-5.49	1.94	2.05
15	B1	808	CLA	MG-ND	-5.48	1.94	2.05
15	B3	808	CLA	MG-ND	-5.48	1.94	2.05
15	A1	828	CLA	MG-ND	-5.48	1.94	2.05
15	B1	810	CLA	MG-ND	-5.47	1.94	2.05
15	A1	806	CLA	MG-ND	-5.47	1.94	2.05
15	B2	808	CLA	MG-ND	-5.47	1.95	2.05
15	A3	828	CLA	MG-ND	-5.46	1.95	2.05
15	A2	806	CLA	MG-ND	-5.46	1.95	2.05
15	B3	810	CLA	MG-ND	-5.46	1.95	2.05
15	A2	828	CLA	MG-ND	-5.45	1.95	2.05
15	A3	806	CLA	MG-ND	-5.45	1.95	2.05
15	B3	813	CLA	MG-ND	-5.44	1.95	2.05
15	B1	837	CLA	MG-ND	-5.44	1.95	2.05
15	B3	837	CLA	MG-ND	-5.44	1.95	2.05
15	B1	813	CLA	MG-ND	-5.44	1.95	2.05
15	A2	826	CLA	MG-ND	-5.44	1.95	2.05
15	B2	837	CLA	MG-ND	-5.44	1.95	2.05
15	B2	813	CLA	MG-ND	-5.43	1.95	2.05
15	A1	826	CLA	MG-ND	-5.43	1.95	2.05
15	A3	826	CLA	MG-ND	-5.42	1.95	2.05
15	B1	805	CLA	MG-ND	-5.39	1.95	2.05
15	B2	822	CLA	MG-ND	-5.39	1.95	2.05
15	J2	1301	CLA	MG-ND	-5.39	1.95	2.05
15	B3	829	CLA	MG-ND	-5.39	1.95	2.05
15	B3	805	CLA	MG-ND	-5.39	1.95	2.05
15	J3	1301	CLA	MG-ND	-5.39	1.95	2.05
15	J1	1301	CLA	MG-ND	-5.39	1.95	2.05
15	A2	829	CLA	MG-ND	-5.39	1.95	2.05
15	B1	835	CLA	MG-ND	-5.39	1.95	2.05
15	B2	835	CLA	MG-ND	-5.39	1.95	2.05
15	B2	805	CLA	MG-ND	-5.39	1.95	2.05
15	A3	829	CLA	MG-ND	-5.38	1.95	2.05
15	B1	822	CLA	MG-ND	-5.38	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A2	823	CLA	MG-ND	-5.38	1.95	2.05
15	B1	829	CLA	MG-ND	-5.38	1.95	2.05
15	B1	806	CLA	MG-ND	-5.37	1.95	2.05
15	B3	822	CLA	MG-ND	-5.37	1.95	2.05
15	A1	823	CLA	MG-ND	-5.37	1.95	2.05
15	B3	835	CLA	MG-ND	-5.37	1.95	2.05
15	B2	806	CLA	MG-ND	-5.37	1.95	2.05
15	A1	829	CLA	MG-ND	-5.37	1.95	2.05
15	B2	829	CLA	MG-ND	-5.35	1.95	2.05
15	B3	806	CLA	MG-ND	-5.35	1.95	2.05
15	A3	823	CLA	MG-ND	-5.35	1.95	2.05
15	A2	844	CLA	MG-ND	-5.34	1.95	2.05
15	A2	808	CLA	MG-ND	-5.33	1.95	2.05
15	A1	844	CLA	MG-ND	-5.33	1.95	2.05
15	A3	844	CLA	MG-ND	-5.32	1.95	2.05
15	A1	808	CLA	MG-ND	-5.31	1.95	2.05
15	B1	823	CLA	MG-ND	-5.31	1.95	2.05
15	A1	809	CLA	MG-ND	-5.30	1.95	2.05
15	A3	808	CLA	MG-ND	-5.29	1.95	2.05
15	B3	823	CLA	MG-ND	-5.29	1.95	2.05
15	A2	809	CLA	MG-ND	-5.29	1.95	2.05
15	A3	809	CLA	MG-ND	-5.28	1.95	2.05
15	B2	823	CLA	MG-ND	-5.28	1.95	2.05
15	A2	837	CLA	MG-ND	-5.27	1.95	2.05
15	B2	833	CLA	MG-ND	-5.27	1.95	2.05
15	A1	837	CLA	MG-ND	-5.27	1.95	2.05
15	I2	101	CLA	MG-ND	-5.27	1.95	2.05
15	B1	833	CLA	MG-ND	-5.26	1.95	2.05
15	A3	837	CLA	MG-ND	-5.26	1.95	2.05
15	I3	101	CLA	MG-ND	-5.24	1.95	2.05
15	A2	811	CLA	MG-ND	-5.24	1.95	2.05
15	A1	821	CLA	MG-ND	-5.24	1.95	2.05
15	A3	811	CLA	MG-ND	-5.24	1.95	2.05
15	B3	833	CLA	MG-ND	-5.24	1.95	2.05
15	A3	825	CLA	MG-ND	-5.24	1.95	2.05
15	A1	811	CLA	MG-ND	-5.24	1.95	2.05
15	A2	825	CLA	MG-ND	-5.24	1.95	2.05
15	A2	821	CLA	MG-ND	-5.24	1.95	2.05
15	I1	101	CLA	MG-ND	-5.22	1.95	2.05
15	A3	821	CLA	MG-ND	-5.22	1.95	2.05
15	A1	825	CLA	MG-ND	-5.21	1.95	2.05
15	A2	827	CLA	MG-ND	-5.18	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A1	827	CLA	MG-ND	-5.17	1.95	2.05
15	A3	841	CLA	MG-ND	-5.17	1.95	2.05
15	A3	827	CLA	MG-ND	-5.17	1.95	2.05
15	A2	831	CLA	MG-ND	-5.16	1.95	2.05
15	A3	831	CLA	MG-ND	-5.16	1.95	2.05
15	B1	819	CLA	MG-ND	-5.15	1.95	2.05
15	B3	819	CLA	MG-ND	-5.15	1.95	2.05
15	B2	819	CLA	MG-ND	-5.14	1.95	2.05
15	A1	831	CLA	MG-ND	-5.14	1.95	2.05
15	A1	841	CLA	MG-ND	-5.14	1.95	2.05
15	A3	805	CLA	MG-ND	-5.14	1.95	2.05
15	A2	841	CLA	MG-ND	-5.14	1.95	2.05
15	A1	805	CLA	MG-ND	-5.12	1.95	2.05
15	B1	818	CLA	MG-ND	-5.11	1.95	2.05
15	A2	814	CLA	MG-ND	-5.11	1.95	2.05
15	B1	834	CLA	MG-ND	-5.10	1.95	2.05
15	A2	805	CLA	MG-ND	-5.09	1.95	2.05
15	A1	814	CLA	MG-ND	-5.09	1.95	2.05
15	A3	817	CLA	MG-ND	-5.09	1.95	2.05
15	B2	834	CLA	MG-ND	-5.09	1.95	2.05
15	A3	807	CLA	MG-ND	-5.09	1.95	2.05
15	A3	814	CLA	MG-ND	-5.09	1.95	2.05
15	A1	813	CLA	MG-ND	-5.08	1.95	2.05
15	B3	834	CLA	MG-ND	-5.08	1.95	2.05
15	A3	813	CLA	MG-ND	-5.08	1.95	2.05
15	B2	818	CLA	MG-ND	-5.08	1.95	2.05
15	A1	840	CLA	MG-ND	-5.07	1.95	2.05
15	J3	1307	CLA	MG-ND	-5.07	1.95	2.05
15	A3	840	CLA	MG-ND	-5.07	1.95	2.05
15	A2	813	CLA	MG-ND	-5.07	1.95	2.05
15	A2	840	CLA	MG-ND	-5.07	1.95	2.05
15	A2	807	CLA	MG-ND	-5.07	1.95	2.05
15	A3	822	CLA	MG-ND	-5.07	1.95	2.05
15	B3	818	CLA	MG-ND	-5.07	1.95	2.05
15	A1	807	CLA	MG-ND	-5.07	1.95	2.05
15	A1	817	CLA	MG-ND	-5.07	1.95	2.05
15	A2	817	CLA	MG-ND	-5.07	1.95	2.05
15	J2	1307	CLA	MG-ND	-5.06	1.95	2.05
15	A1	822	CLA	MG-ND	-5.06	1.95	2.05
15	J1	1307	CLA	MG-ND	-5.06	1.95	2.05
15	A3	812	CLA	MG-ND	-5.06	1.95	2.05
15	B1	808	CLA	MG-NA	-5.05	1.94	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B2	814	CLA	MG-NA	-5.05	1.94	2.06
15	A1	812	CLA	MG-ND	-5.05	1.95	2.05
15	J2	1307	CLA	C3B-C4B	-5.04	1.41	1.43
15	B2	808	CLA	MG-NA	-5.04	1.94	2.06
15	B3	808	CLA	MG-NA	-5.04	1.94	2.06
15	J1	1303	CLA	MG-ND	-5.03	1.95	2.05
15	J3	1303	CLA	MG-ND	-5.03	1.95	2.05
15	A2	822	CLA	MG-ND	-5.03	1.95	2.05
15	A2	810	CLA	MG-ND	-5.03	1.95	2.05
15	A3	810	CLA	MG-ND	-5.03	1.95	2.05
15	A2	812	CLA	MG-ND	-5.03	1.95	2.05
15	J2	1303	CLA	MG-ND	-5.03	1.95	2.05
15	B1	814	CLA	MG-NA	-5.02	1.94	2.06
15	A1	810	CLA	MG-ND	-5.02	1.95	2.05
15	A3	803	CLA	MG-ND	-5.00	1.95	2.05
15	B3	814	CLA	MG-NA	-5.00	1.94	2.06
15	J1	1307	CLA	C3B-C4B	-5.00	1.41	1.43
15	A1	803	CLA	MG-ND	-4.98	1.95	2.05
15	A2	803	CLA	MG-ND	-4.98	1.95	2.05
15	A3	815	CLA	MG-ND	-4.97	1.95	2.05
15	A3	816	CLA	MG-ND	-4.97	1.95	2.05
15	A2	820	CLA	MG-ND	-4.97	1.95	2.05
15	A1	816	CLA	MG-ND	-4.96	1.96	2.05
15	A2	816	CLA	MG-ND	-4.96	1.96	2.05
15	A1	815	CLA	MG-ND	-4.96	1.96	2.05
15	B2	832	CLA	MG-NA	-4.94	1.94	2.06
15	A1	820	CLA	MG-ND	-4.94	1.96	2.05
15	B1	832	CLA	MG-NA	-4.93	1.94	2.06
15	A2	815	CLA	MG-ND	-4.93	1.96	2.05
15	A3	820	CLA	MG-ND	-4.92	1.96	2.05
15	B3	832	CLA	MG-NA	-4.91	1.94	2.06
15	J3	1307	CLA	C3B-C4B	-4.91	1.41	1.43
15	A3	804	CLA	MG-NA	-4.91	1.94	2.06
15	B2	807	CLA	MG-NA	-4.91	1.94	2.06
15	B1	807	CLA	MG-NA	-4.90	1.94	2.06
15	A1	804	CLA	MG-NA	-4.90	1.94	2.06
15	B3	807	CLA	MG-NA	-4.90	1.94	2.06
15	A1	811	CLA	MG-NA	-4.89	1.94	2.06
15	A3	811	CLA	MG-NA	-4.89	1.94	2.06
15	A2	804	CLA	MG-NA	-4.88	1.94	2.06
15	A2	811	CLA	MG-NA	-4.88	1.94	2.06
15	B3	811	CLA	MG-ND	-4.87	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B1	811	CLA	MG-ND	-4.87	1.96	2.05
15	A2	832	CLA	MG-NA	-4.87	1.94	2.06
15	A3	832	CLA	MG-NA	-4.86	1.94	2.06
15	A1	832	CLA	MG-NA	-4.86	1.94	2.06
15	B1	801	CLA	MG-NA	-4.85	1.94	2.06
15	B2	811	CLA	MG-ND	-4.85	1.96	2.05
15	B3	801	CLA	MG-NA	-4.85	1.94	2.06
15	K3	101	CLA	MG-ND	-4.85	1.96	2.05
15	A2	819	CLA	MG-NA	-4.85	1.94	2.06
15	A3	819	CLA	MG-NA	-4.84	1.94	2.06
15	B3	849	CLA	MG-NA	-4.84	1.94	2.06
15	B2	849	CLA	MG-NA	-4.84	1.94	2.06
15	K1	101	CLA	MG-ND	-4.84	1.96	2.05
15	B2	801	CLA	MG-NA	-4.84	1.94	2.06
15	A1	819	CLA	MG-NA	-4.84	1.94	2.06
15	B1	849	CLA	MG-NA	-4.84	1.94	2.06
15	K2	101	CLA	MG-ND	-4.84	1.96	2.05
15	A1	856	CLA	MG-NA	-4.84	1.94	2.06
15	A2	856	CLA	MG-NA	-4.82	1.94	2.06
15	A3	856	CLA	MG-NA	-4.82	1.94	2.06
15	A3	840	CLA	MG-NA	-4.82	1.94	2.06
15	B3	820	CLA	MG-NA	-4.81	1.94	2.06
15	A1	840	CLA	MG-NA	-4.81	1.94	2.06
15	B2	830	CLA	MG-NA	-4.81	1.94	2.06
15	B1	816	CLA	MG-NA	-4.81	1.94	2.06
15	B1	830	CLA	MG-NA	-4.81	1.94	2.06
15	B2	816	CLA	MG-NA	-4.81	1.94	2.06
15	A3	815	CLA	C2C-C1C	4.81	1.47	1.40
15	A1	815	CLA	C2C-C1C	4.80	1.47	1.40
15	B2	820	CLA	MG-NA	-4.80	1.94	2.06
15	B1	820	CLA	MG-NA	-4.80	1.94	2.06
15	B3	830	CLA	MG-NA	-4.80	1.94	2.06
15	B3	816	CLA	MG-NA	-4.79	1.94	2.06
15	A2	840	CLA	MG-NA	-4.78	1.94	2.06
15	A2	815	CLA	C2C-C1C	4.78	1.47	1.40
15	B3	836	CLA	MG-NA	-4.77	1.94	2.06
15	B1	836	CLA	MG-NA	-4.76	1.95	2.06
15	B2	825	CLA	MG-ND	-4.75	1.96	2.05
15	B2	836	CLA	MG-NA	-4.74	1.95	2.06
15	B1	828	CLA	MG-NA	-4.74	1.95	2.06
15	B2	828	CLA	MG-NA	-4.74	1.95	2.06
15	B3	828	CLA	MG-NA	-4.73	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B1	825	CLA	MG-ND	-4.72	1.96	2.05
15	A2	836	CLA	MG-NA	-4.71	1.95	2.06
15	A3	836	CLA	MG-NA	-4.70	1.95	2.06
15	B3	825	CLA	MG-ND	-4.70	1.96	2.05
15	A1	836	CLA	MG-NA	-4.70	1.95	2.06
15	A1	839	CLA	C3B-C2B	-4.69	1.33	1.40
15	A2	839	CLA	C3B-C2B	-4.68	1.33	1.40
15	A1	826	CLA	MG-NA	-4.68	1.95	2.06
15	B3	837	CLA	MG-NA	-4.67	1.95	2.06
15	A1	828	CLA	MG-NA	-4.67	1.95	2.06
15	B1	831	CLA	C3A-C2A	-4.66	1.50	1.54
15	A3	828	CLA	MG-NA	-4.66	1.95	2.06
15	A2	828	CLA	MG-NA	-4.66	1.95	2.06
15	A3	826	CLA	MG-NA	-4.66	1.95	2.06
15	B1	837	CLA	MG-NA	-4.65	1.95	2.06
15	A2	826	CLA	MG-NA	-4.65	1.95	2.06
15	B2	831	CLA	C3A-C2A	-4.65	1.50	1.54
15	A3	839	CLA	C3B-C2B	-4.65	1.33	1.40
15	B3	831	CLA	C3A-C2A	-4.65	1.50	1.54
15	A1	830	CLA	MG-NA	-4.65	1.95	2.06
15	A3	830	CLA	MG-NA	-4.64	1.95	2.06
15	A2	830	CLA	MG-NA	-4.64	1.95	2.06
15	B2	803	CLA	MG-NA	-4.63	1.95	2.06
15	B3	824	CLA	MG-NA	-4.63	1.95	2.06
15	B1	803	CLA	MG-NA	-4.63	1.95	2.06
15	B2	837	CLA	MG-NA	-4.63	1.95	2.06
15	A1	808	CLA	MG-NA	-4.63	1.95	2.06
15	A1	807	CLA	MG-NA	-4.63	1.95	2.06
15	B1	824	CLA	MG-NA	-4.63	1.95	2.06
15	K3	101	CLA	MG-NA	-4.62	1.95	2.06
15	K1	101	CLA	MG-NA	-4.62	1.95	2.06
15	A2	810	CLA	MG-NA	-4.62	1.95	2.06
15	A3	807	CLA	MG-NA	-4.62	1.95	2.06
15	A2	843	CLA	C3B-C2B	-4.62	1.34	1.40
15	B3	803	CLA	MG-NA	-4.61	1.95	2.06
15	B1	829	CLA	MG-NA	-4.61	1.95	2.06
15	A2	807	CLA	MG-NA	-4.61	1.95	2.06
15	A3	808	CLA	MG-NA	-4.61	1.95	2.06
15	A3	835	CLA	MG-NA	-4.61	1.95	2.06
15	A1	810	CLA	MG-NA	-4.61	1.95	2.06
15	B3	839	CLA	C3B-C2B	-4.61	1.34	1.40
15	B2	824	CLA	MG-NA	-4.61	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B2	829	CLA	MG-NA	-4.60	1.95	2.06
15	A2	808	CLA	MG-NA	-4.60	1.95	2.06
15	A3	810	CLA	MG-NA	-4.60	1.95	2.06
15	B3	829	CLA	MG-NA	-4.60	1.95	2.06
15	K2	101	CLA	MG-NA	-4.59	1.95	2.06
15	A1	809	CLA	MG-NA	-4.59	1.95	2.06
15	A3	843	CLA	C3B-C2B	-4.59	1.34	1.40
15	A1	835	CLA	MG-NA	-4.59	1.95	2.06
15	K3	103	CLA	MG-NA	-4.59	1.95	2.06
15	B1	839	CLA	C3B-C2B	-4.59	1.34	1.40
15	A2	835	CLA	MG-NA	-4.58	1.95	2.06
15	K1	103	CLA	MG-NA	-4.58	1.95	2.06
15	A1	843	CLA	C3B-C2B	-4.57	1.34	1.40
15	K2	103	CLA	MG-NA	-4.57	1.95	2.06
15	A2	809	CLA	MG-NA	-4.57	1.95	2.06
15	A3	809	CLA	MG-NA	-4.57	1.95	2.06
15	B3	813	CLA	MG-NA	-4.56	1.95	2.06
15	J2	1301	CLA	C3A-C2A	-4.55	1.50	1.54
15	B2	839	CLA	C3B-C2B	-4.53	1.34	1.40
15	J3	1301	CLA	C3A-C2A	-4.53	1.50	1.54
15	B1	813	CLA	MG-NA	-4.52	1.95	2.06
15	J1	1301	CLA	C3A-C2A	-4.52	1.50	1.54
15	A2	818	CLA	MG-NA	-4.51	1.95	2.06
15	A1	818	CLA	MG-NA	-4.50	1.95	2.06
15	B3	819	CLA	MG-NA	-4.50	1.95	2.06
15	A3	822	CLA	MG-NA	-4.50	1.95	2.06
15	A2	816	CLA	MG-NA	-4.50	1.95	2.06
15	A1	831	CLA	MG-NA	-4.50	1.95	2.06
15	A2	831	CLA	MG-NA	-4.50	1.95	2.06
15	B2	819	CLA	MG-NA	-4.50	1.95	2.06
15	B2	813	CLA	MG-NA	-4.50	1.95	2.06
15	A3	831	CLA	MG-NA	-4.50	1.95	2.06
15	A3	818	CLA	MG-NA	-4.50	1.95	2.06
15	B1	819	CLA	MG-NA	-4.50	1.95	2.06
15	B2	804	CLA	MG-NA	-4.49	1.95	2.06
15	A1	822	CLA	MG-NA	-4.49	1.95	2.06
15	A3	834	CLA	MG-NA	-4.49	1.95	2.06
15	B3	825	CLA	MG-NA	-4.49	1.95	2.06
15	A2	822	CLA	MG-NA	-4.49	1.95	2.06
15	B1	804	CLA	MG-NA	-4.48	1.95	2.06
15	B3	804	CLA	MG-NA	-4.48	1.95	2.06
15	A1	834	CLA	MG-NA	-4.48	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B2	825	CLA	MG-NA	-4.48	1.95	2.06
15	B1	825	CLA	MG-NA	-4.48	1.95	2.06
15	A3	816	CLA	MG-NA	-4.47	1.95	2.06
15	A1	802	CLA	MG-NA	-4.46	1.95	2.06
15	A1	816	CLA	MG-NA	-4.46	1.95	2.06
15	A3	802	CLA	MG-NA	-4.46	1.95	2.06
15	A2	834	CLA	MG-NA	-4.46	1.95	2.06
15	A3	814	CLA	MG-NA	-4.46	1.95	2.06
15	A2	802	CLA	MG-NA	-4.45	1.95	2.06
15	L2	1003	CLA	MG-NA	-4.45	1.95	2.06
15	A1	814	CLA	MG-NA	-4.45	1.95	2.06
15	A2	810	CLA	C2C-C1C	4.44	1.47	1.40
15	L3	1003	CLA	MG-NA	-4.44	1.95	2.06
15	A2	814	CLA	MG-NA	-4.44	1.95	2.06
15	A2	803	CLA	MG-NA	-4.44	1.95	2.06
15	B2	802	CLA	C3B-C2B	-4.44	1.34	1.40
15	J3	1303	CLA	MG-NA	-4.43	1.95	2.06
15	A1	842	CLA	MG-NA	-4.43	1.95	2.06
15	A1	810	CLA	C2C-C1C	4.42	1.47	1.40
15	A2	815	CLA	MG-NA	-4.42	1.95	2.06
15	B2	809	CLA	MG-NA	-4.42	1.95	2.06
15	A2	842	CLA	MG-NA	-4.42	1.95	2.06
15	L1	1003	CLA	MG-NA	-4.42	1.95	2.06
15	A1	803	CLA	MG-NA	-4.42	1.95	2.06
15	I3	101	CLA	C3B-C2B	-4.42	1.34	1.40
15	B1	809	CLA	MG-NA	-4.42	1.95	2.06
15	A3	842	CLA	MG-NA	-4.41	1.95	2.06
15	I1	101	CLA	C3B-C2B	-4.41	1.34	1.40
15	B3	809	CLA	MG-NA	-4.41	1.95	2.06
15	B1	802	CLA	C3B-C2B	-4.41	1.34	1.40
15	J2	1303	CLA	MG-NA	-4.41	1.95	2.06
15	J1	1303	CLA	MG-NA	-4.41	1.95	2.06
15	A3	810	CLA	C2C-C1C	4.41	1.47	1.40
15	A3	803	CLA	MG-NA	-4.40	1.95	2.06
15	I2	101	CLA	C3B-C2B	-4.40	1.34	1.40
15	A1	805	CLA	MG-NA	-4.40	1.95	2.06
15	A1	838	CLA	C3B-C2B	-4.40	1.34	1.40
15	A2	833	CLA	C3B-C2B	-4.40	1.34	1.40
15	B3	802	CLA	C3B-C2B	-4.40	1.34	1.40
15	A2	838	CLA	C3B-C2B	-4.40	1.34	1.40
15	A2	805	CLA	MG-NA	-4.40	1.95	2.06
15	B2	833	CLA	MG-NA	-4.40	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A3	805	CLA	MG-NA	-4.40	1.95	2.06
15	B1	833	CLA	MG-NA	-4.39	1.95	2.06
15	B3	802	CLA	MG-NA	-4.39	1.95	2.06
15	A3	815	CLA	MG-NA	-4.39	1.95	2.06
15	A1	815	CLA	MG-NA	-4.39	1.95	2.06
15	A3	838	CLA	C3B-C2B	-4.39	1.34	1.40
15	A1	823	CLA	MG-NA	-4.38	1.95	2.06
15	B1	802	CLA	MG-NA	-4.38	1.95	2.06
15	B2	802	CLA	MG-NA	-4.38	1.95	2.06
15	A2	823	CLA	MG-NA	-4.37	1.95	2.06
15	A1	817	CLA	MG-NA	-4.37	1.95	2.06
15	A3	823	CLA	MG-NA	-4.36	1.95	2.06
15	A3	817	CLA	MG-NA	-4.36	1.95	2.06
15	B1	823	CLA	C3A-C2A	-4.36	1.50	1.54
15	B1	834	CLA	MG-NA	-4.36	1.95	2.06
15	A1	833	CLA	C3B-C2B	-4.35	1.34	1.40
15	B3	833	CLA	MG-NA	-4.35	1.95	2.06
15	A2	817	CLA	MG-NA	-4.35	1.95	2.06
15	B2	834	CLA	MG-NA	-4.35	1.95	2.06
15	B3	834	CLA	MG-NA	-4.35	1.95	2.06
15	B2	823	CLA	C3A-C2A	-4.34	1.50	1.54
15	A2	821	CLA	MG-NA	-4.34	1.96	2.06
19	X3	101	LHG	O8-C23	4.33	1.46	1.33
15	B3	837	CLA	C3B-C2B	-4.33	1.34	1.40
15	A2	831	CLA	C3B-C2B	-4.33	1.34	1.40
19	X2	101	LHG	O8-C23	4.33	1.46	1.33
15	A3	821	CLA	MG-NA	-4.33	1.96	2.06
15	X2	102	CLA	MG-NA	-4.33	1.96	2.06
15	X1	102	CLA	MG-NA	-4.33	1.96	2.06
15	X3	102	CLA	MG-NA	-4.33	1.96	2.06
15	B1	837	CLA	C3B-C2B	-4.32	1.34	1.40
19	X1	101	LHG	O8-C23	4.32	1.46	1.33
15	A1	821	CLA	MG-NA	-4.32	1.96	2.06
15	A3	820	CLA	MG-NA	-4.32	1.96	2.06
15	B3	823	CLA	C3A-C2A	-4.32	1.50	1.54
15	A3	833	CLA	C3B-C2B	-4.31	1.34	1.40
15	A1	820	CLA	MG-NA	-4.31	1.96	2.06
15	A2	820	CLA	MG-NA	-4.30	1.96	2.06
15	B2	818	CLA	MG-NA	-4.30	1.96	2.06
15	A1	831	CLA	C3B-C2B	-4.29	1.34	1.40
15	B1	818	CLA	MG-NA	-4.29	1.96	2.06
15	A3	831	CLA	C3B-C2B	-4.29	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	818	CLA	MG-NA	-4.29	1.96	2.06
15	A3	835	CLA	C3B-C2B	-4.29	1.34	1.40
15	B2	837	CLA	C3B-C2B	-4.28	1.34	1.40
15	B1	815	CLA	MG-NA	-4.28	1.96	2.06
15	B2	815	CLA	MG-NA	-4.27	1.96	2.06
15	B3	815	CLA	MG-NA	-4.27	1.96	2.06
15	A2	827	CLA	MG-NA	-4.25	1.96	2.06
15	A2	806	CLA	MG-NA	-4.25	1.96	2.06
15	A1	827	CLA	MG-NA	-4.25	1.96	2.06
15	A3	827	CLA	MG-NA	-4.25	1.96	2.06
15	L3	1004	CLA	MG-NA	-4.25	1.96	2.06
15	A1	806	CLA	MG-NA	-4.24	1.96	2.06
15	L1	1004	CLA	MG-NA	-4.24	1.96	2.06
15	A1	835	CLA	C3B-C2B	-4.24	1.34	1.40
15	A3	806	CLA	MG-NA	-4.24	1.96	2.06
15	A2	812	CLA	MG-NA	-4.24	1.96	2.06
15	L2	1004	CLA	MG-NA	-4.23	1.96	2.06
15	A1	812	CLA	MG-NA	-4.23	1.96	2.06
15	A3	812	CLA	MG-NA	-4.23	1.96	2.06
15	A2	841	CLA	MG-NA	-4.21	1.96	2.06
15	B2	826	CLA	MG-NA	-4.21	1.96	2.06
15	B3	826	CLA	MG-NA	-4.21	1.96	2.06
15	B1	826	CLA	MG-NA	-4.20	1.96	2.06
15	A1	841	CLA	MG-NA	-4.20	1.96	2.06
15	J2	1307	CLA	MG-NA	-4.20	1.96	2.06
15	B3	805	CLA	MG-NA	-4.19	1.96	2.06
15	J1	1307	CLA	MG-NA	-4.18	1.96	2.06
15	B2	806	CLA	MG-NA	-4.18	1.96	2.06
15	B1	805	CLA	MG-NA	-4.18	1.96	2.06
15	B2	805	CLA	MG-NA	-4.18	1.96	2.06
15	B2	823	CLA	MG-NA	-4.18	1.96	2.06
15	B3	823	CLA	MG-NA	-4.18	1.96	2.06
15	J3	1307	CLA	MG-NA	-4.18	1.96	2.06
15	B2	838	CLA	C3B-C2B	-4.17	1.34	1.40
15	B1	823	CLA	MG-NA	-4.17	1.96	2.06
15	A2	835	CLA	C3B-C2B	-4.17	1.34	1.40
15	B1	806	CLA	MG-NA	-4.16	1.96	2.06
15	B2	849	CLA	C3B-C2B	-4.16	1.34	1.40
15	A3	841	CLA	MG-NA	-4.16	1.96	2.06
15	A1	842	CLA	C3B-C2B	-4.16	1.34	1.40
15	A3	842	CLA	C3B-C2B	-4.16	1.34	1.40
15	B3	806	CLA	MG-NA	-4.16	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A2	842	CLA	C3B-C2B	-4.15	1.34	1.40
15	B2	831	CLA	MG-NA	-4.15	1.96	2.06
15	B1	831	CLA	MG-NA	-4.14	1.96	2.06
15	A1	803	CLA	C3B-C2B	-4.14	1.34	1.40
15	A2	803	CLA	C3B-C2B	-4.14	1.34	1.40
15	J2	1301	CLA	MG-NA	-4.14	1.96	2.06
15	J3	1301	CLA	MG-NA	-4.14	1.96	2.06
15	B3	831	CLA	MG-NA	-4.13	1.96	2.06
15	B1	838	CLA	C3B-C2B	-4.13	1.34	1.40
15	A3	803	CLA	C3B-C2B	-4.13	1.34	1.40
15	B1	849	CLA	C3B-C2B	-4.13	1.34	1.40
15	J1	1301	CLA	MG-NA	-4.12	1.96	2.06
15	A3	824	CLA	MG-NA	-4.12	1.96	2.06
15	B3	838	CLA	C3B-C2B	-4.12	1.34	1.40
15	B3	849	CLA	C3B-C2B	-4.12	1.34	1.40
15	A3	818	CLA	C3B-C2B	-4.12	1.34	1.40
15	B2	822	CLA	MG-NA	-4.11	1.96	2.06
15	A1	824	CLA	MG-NA	-4.11	1.96	2.06
15	A2	824	CLA	MG-NA	-4.10	1.96	2.06
15	A1	818	CLA	C3B-C2B	-4.09	1.34	1.40
15	A2	844	CLA	MG-NA	-4.09	1.96	2.06
15	A2	838	CLA	MG-NA	-4.09	1.96	2.06
15	A3	838	CLA	MG-NA	-4.09	1.96	2.06
15	B1	822	CLA	MG-NA	-4.09	1.96	2.06
15	A1	838	CLA	MG-NA	-4.09	1.96	2.06
15	B2	817	CLA	MG-NA	-4.09	1.96	2.06
15	B3	810	CLA	MG-NA	-4.08	1.96	2.06
15	B1	810	CLA	MG-NA	-4.08	1.96	2.06
15	B1	817	CLA	MG-NA	-4.08	1.96	2.06
15	A2	818	CLA	C3B-C2B	-4.08	1.34	1.40
19	X2	101	LHG	O7-C7	4.08	1.45	1.34
15	A1	833	CLA	MG-NA	-4.07	1.96	2.06
15	A3	827	CLA	C3B-C2B	-4.07	1.34	1.40
15	A2	833	CLA	MG-NA	-4.07	1.96	2.06
15	B3	817	CLA	MG-NA	-4.07	1.96	2.06
15	A1	844	CLA	MG-NA	-4.07	1.96	2.06
15	J2	1302	CLA	MG-NA	-4.07	1.96	2.06
15	A1	823	CLA	C3B-C2B	-4.07	1.34	1.40
15	A2	827	CLA	C3B-C2B	-4.07	1.34	1.40
15	A3	833	CLA	MG-NA	-4.07	1.96	2.06
15	J3	1302	CLA	MG-NA	-4.07	1.96	2.06
15	J1	1302	CLA	MG-NA	-4.07	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A1	827	CLA	C3B-C2B	-4.06	1.34	1.40
15	A3	823	CLA	C3B-C2B	-4.06	1.34	1.40
15	B2	810	CLA	MG-NA	-4.06	1.96	2.06
15	A2	823	CLA	C3B-C2B	-4.06	1.34	1.40
15	A1	813	CLA	MG-NA	-4.06	1.96	2.06
15	B3	822	CLA	MG-NA	-4.06	1.96	2.06
15	A3	813	CLA	MG-NA	-4.05	1.96	2.06
19	X1	101	LHG	O7-C7	4.05	1.45	1.34
19	X3	101	LHG	O7-C7	4.05	1.45	1.34
15	A2	841	CLA	C3B-C2B	-4.05	1.34	1.40
15	B3	838	CLA	MG-NA	-4.05	1.96	2.06
15	A2	813	CLA	MG-NA	-4.04	1.96	2.06
15	A3	844	CLA	MG-NA	-4.04	1.96	2.06
15	A2	843	CLA	MG-NA	-4.04	1.96	2.06
15	A3	841	CLA	C3B-C2B	-4.04	1.34	1.40
15	B1	838	CLA	MG-NA	-4.03	1.96	2.06
15	A1	808	CLA	C3B-C2B	-4.03	1.34	1.40
15	A2	802	CLA	C3B-C2B	-4.03	1.34	1.40
15	A3	802	CLA	C3B-C2B	-4.03	1.34	1.40
15	A1	802	CLA	C3B-C2B	-4.03	1.34	1.40
15	A3	808	CLA	C3B-C2B	-4.03	1.34	1.40
15	A1	841	CLA	C3B-C2B	-4.02	1.34	1.40
15	B1	812	CLA	MG-NA	-4.02	1.96	2.06
15	B2	812	CLA	MG-NA	-4.02	1.96	2.06
15	B3	812	CLA	MG-NA	-4.02	1.96	2.06
15	A3	843	CLA	MG-NA	-4.02	1.96	2.06
15	A2	829	CLA	MG-NA	-4.02	1.96	2.06
15	A1	821	CLA	C3B-C2B	-4.02	1.34	1.40
15	A2	808	CLA	C3B-C2B	-4.02	1.34	1.40
15	A1	829	CLA	MG-NA	-4.02	1.96	2.06
15	A3	829	CLA	MG-NA	-4.01	1.96	2.06
15	A1	843	CLA	MG-NA	-4.01	1.96	2.06
15	I3	101	CLA	MG-NA	-4.01	1.96	2.06
15	B2	827	CLA	MG-NA	-4.01	1.96	2.06
15	B3	827	CLA	MG-NA	-4.01	1.96	2.06
15	B2	838	CLA	MG-NA	-4.01	1.96	2.06
15	A3	821	CLA	C3B-C2B	-4.01	1.34	1.40
15	B1	827	CLA	MG-NA	-4.00	1.96	2.06
15	I1	101	CLA	MG-NA	-4.00	1.96	2.06
15	I2	101	CLA	MG-NA	-4.00	1.96	2.06
15	A2	825	CLA	MG-NA	-4.00	1.96	2.06
15	B2	818	CLA	C3B-C2B	-4.00	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A1	812	CLA	C3B-C2B	-4.00	1.34	1.40
15	A2	812	CLA	C3B-C2B	-4.00	1.34	1.40
15	A3	825	CLA	MG-NA	-4.00	1.96	2.06
15	B1	822	CLA	C3B-C2B	-4.00	1.34	1.40
15	A3	812	CLA	C3B-C2B	-3.99	1.34	1.40
15	A2	821	CLA	C3B-C2B	-3.99	1.34	1.40
15	B3	822	CLA	C3B-C2B	-3.99	1.34	1.40
15	B2	822	CLA	C3B-C2B	-3.99	1.34	1.40
15	A1	825	CLA	MG-NA	-3.99	1.96	2.06
15	A3	836	CLA	C3B-C2B	-3.99	1.34	1.40
15	A3	856	CLA	MG-NC	-3.98	1.96	2.06
15	B3	818	CLA	C3B-C2B	-3.98	1.34	1.40
15	A2	810	CLA	C3B-C2B	-3.98	1.34	1.40
15	B3	803	CLA	MG-NC	-3.98	1.96	2.06
15	A1	839	CLA	MG-NA	-3.98	1.96	2.06
15	B2	803	CLA	MG-NC	-3.98	1.96	2.06
15	B1	807	CLA	MG-NC	-3.98	1.96	2.06
15	L1	1002	CLA	MG-NA	-3.98	1.96	2.06
15	B1	803	CLA	MG-NC	-3.98	1.96	2.06
15	B1	818	CLA	C3B-C2B	-3.97	1.34	1.40
15	B3	807	CLA	MG-NC	-3.97	1.96	2.06
15	A1	810	CLA	C3B-C2B	-3.97	1.34	1.40
15	A3	810	CLA	C3B-C2B	-3.97	1.34	1.40
15	B2	807	CLA	MG-NC	-3.97	1.96	2.06
15	A2	839	CLA	MG-NA	-3.97	1.96	2.06
15	A1	836	CLA	C3B-C2B	-3.96	1.34	1.40
15	A2	836	CLA	C3B-C2B	-3.96	1.34	1.40
15	A3	839	CLA	MG-NA	-3.96	1.96	2.06
15	L2	1002	CLA	MG-NA	-3.96	1.96	2.06
15	B2	811	CLA	MG-NA	-3.96	1.96	2.06
15	B2	839	CLA	MG-NA	-3.96	1.96	2.06
15	B2	809	CLA	C3B-C2B	-3.96	1.34	1.40
15	B3	811	CLA	MG-NA	-3.96	1.96	2.06
15	B1	811	CLA	MG-NA	-3.96	1.96	2.06
15	L3	1002	CLA	MG-NA	-3.96	1.96	2.06
15	A1	856	CLA	MG-NC	-3.95	1.96	2.06
15	B3	839	CLA	MG-NA	-3.95	1.96	2.06
15	B1	839	CLA	MG-NA	-3.95	1.96	2.06
15	B1	809	CLA	C3B-C2B	-3.94	1.34	1.40
15	A2	856	CLA	MG-NC	-3.94	1.96	2.06
15	B3	809	CLA	C3B-C2B	-3.93	1.34	1.40
15	X2	102	CLA	C3B-C2B	-3.93	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B1	835	CLA	MG-NA	-3.92	1.97	2.06
15	B1	809	CLA	MG-NC	-3.92	1.97	2.06
15	A3	802	CLA	MG-NC	-3.92	1.97	2.06
15	X1	102	CLA	C3B-C2B	-3.92	1.34	1.40
15	B1	834	CLA	C3B-C2B	-3.92	1.34	1.40
15	A1	802	CLA	MG-NC	-3.91	1.97	2.06
15	A2	802	CLA	MG-NC	-3.91	1.97	2.06
15	K2	101	CLA	MG-NC	-3.91	1.97	2.06
15	B3	808	CLA	C3B-C2B	-3.91	1.34	1.40
15	B2	809	CLA	MG-NC	-3.91	1.97	2.06
15	B3	809	CLA	MG-NC	-3.91	1.97	2.06
15	B2	835	CLA	MG-NA	-3.90	1.97	2.06
15	X3	102	CLA	C3A-C2A	-3.90	1.50	1.54
15	B1	808	CLA	C3B-C2B	-3.90	1.35	1.40
15	A1	816	CLA	C3B-C2B	-3.90	1.35	1.40
15	L2	1002	CLA	C3B-C2B	-3.90	1.35	1.40
15	B1	829	CLA	C3B-C2B	-3.90	1.35	1.40
15	X3	102	CLA	C3B-C2B	-3.90	1.35	1.40
15	B3	829	CLA	C3B-C2B	-3.89	1.35	1.40
15	K1	101	CLA	MG-NC	-3.89	1.97	2.06
15	B2	821	CLA	MG-NC	-3.89	1.97	2.06
15	B2	829	CLA	C3B-C2B	-3.89	1.35	1.40
15	A3	816	CLA	C3B-C2B	-3.89	1.35	1.40
15	B1	821	CLA	MG-NC	-3.89	1.97	2.06
15	B3	808	CLA	MG-NC	-3.89	1.97	2.06
15	B3	834	CLA	C3B-C2B	-3.89	1.35	1.40
15	B2	808	CLA	MG-NC	-3.88	1.97	2.06
15	B3	835	CLA	MG-NA	-3.88	1.97	2.06
15	X1	102	CLA	C3A-C2A	-3.88	1.50	1.54
15	L1	1002	CLA	C3B-C2B	-3.88	1.35	1.40
15	A3	837	CLA	MG-NA	-3.88	1.97	2.06
15	L3	1002	CLA	C3B-C2B	-3.88	1.35	1.40
15	B2	834	CLA	C3B-C2B	-3.88	1.35	1.40
15	K3	101	CLA	MG-NC	-3.88	1.97	2.06
15	A2	816	CLA	C3B-C2B	-3.88	1.35	1.40
15	B1	808	CLA	MG-NC	-3.88	1.97	2.06
15	B3	821	CLA	MG-NC	-3.88	1.97	2.06
15	B3	811	CLA	C3B-C2B	-3.87	1.35	1.40
15	A1	837	CLA	MG-NA	-3.87	1.97	2.06
15	A2	840	CLA	C3B-C2B	-3.86	1.35	1.40
15	A2	837	CLA	MG-NA	-3.86	1.97	2.06
15	B2	811	CLA	C3B-C2B	-3.86	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B1	811	CLA	C3B-C2B	-3.86	1.35	1.40
15	B2	828	CLA	C3B-C2B	-3.86	1.35	1.40
15	A2	840	CLA	MG-NC	-3.85	1.97	2.06
15	A1	840	CLA	MG-NC	-3.84	1.97	2.06
15	A3	840	CLA	MG-NC	-3.84	1.97	2.06
15	K3	103	CLA	MG-NC	-3.84	1.97	2.06
15	B1	828	CLA	C3B-C2B	-3.84	1.35	1.40
15	X2	102	CLA	C3A-C2A	-3.83	1.50	1.54
15	B2	808	CLA	C3B-C2B	-3.83	1.35	1.40
15	B3	828	CLA	C3B-C2B	-3.83	1.35	1.40
15	B2	835	CLA	C3B-C2B	-3.83	1.35	1.40
15	A1	840	CLA	C3B-C2B	-3.83	1.35	1.40
15	B2	802	CLA	MG-NC	-3.82	1.97	2.06
15	A2	811	CLA	MG-NC	-3.82	1.97	2.06
15	K1	103	CLA	MG-NC	-3.82	1.97	2.06
15	K2	103	CLA	MG-NC	-3.82	1.97	2.06
15	B3	835	CLA	C3B-C2B	-3.82	1.35	1.40
15	B3	807	CLA	C3B-C2B	-3.81	1.35	1.40
15	B1	825	CLA	C3B-C2B	-3.81	1.35	1.40
14	A3	801	CL0	MG-NA	-3.81	1.97	2.06
15	A3	840	CLA	C3B-C2B	-3.81	1.35	1.40
15	B1	802	CLA	MG-NC	-3.81	1.97	2.06
14	A1	801	CL0	MG-NA	-3.81	1.97	2.06
15	B3	802	CLA	MG-NC	-3.81	1.97	2.06
15	B3	832	CLA	MG-NC	-3.80	1.97	2.06
15	B2	832	CLA	MG-NC	-3.80	1.97	2.06
15	B1	807	CLA	C3B-C2B	-3.80	1.35	1.40
14	A2	801	CL0	MG-NA	-3.80	1.97	2.06
15	B2	819	CLA	C3B-C2B	-3.80	1.35	1.40
15	B3	825	CLA	C3B-C2B	-3.80	1.35	1.40
15	A1	811	CLA	MG-NC	-3.80	1.97	2.06
15	B2	825	CLA	C3B-C2B	-3.80	1.35	1.40
15	A3	811	CLA	MG-NC	-3.80	1.97	2.06
15	B1	835	CLA	C3B-C2B	-3.80	1.35	1.40
15	B3	819	CLA	C3B-C2B	-3.80	1.35	1.40
15	B1	832	CLA	MG-NC	-3.79	1.97	2.06
15	B1	819	CLA	C3B-C2B	-3.79	1.35	1.40
14	A1	801	CL0	MG-NC	-3.79	1.97	2.06
14	A3	801	CL0	MG-NC	-3.79	1.97	2.06
15	B2	829	CLA	MG-NC	-3.79	1.97	2.06
14	A2	801	CL0	MG-NC	-3.78	1.97	2.06
15	B2	807	CLA	C3B-C2B	-3.78	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A3	811	CLA	C3B-C2B	-3.78	1.35	1.40
15	B2	806	CLA	C3B-C2B	-3.78	1.35	1.40
15	B1	829	CLA	MG-NC	-3.78	1.97	2.06
15	B1	806	CLA	C3B-C2B	-3.78	1.35	1.40
15	B1	832	CLA	C3B-C2B	-3.77	1.35	1.40
15	B2	831	CLA	C3B-C2B	-3.77	1.35	1.40
15	B3	806	CLA	C3B-C2B	-3.77	1.35	1.40
15	A1	822	CLA	C3B-C2B	-3.77	1.35	1.40
15	A2	822	CLA	C3B-C2B	-3.77	1.35	1.40
15	B3	829	CLA	MG-NC	-3.76	1.97	2.06
15	B2	832	CLA	C3B-C2B	-3.76	1.35	1.40
15	A3	844	CLA	C3B-C2B	-3.76	1.35	1.40
15	A1	811	CLA	C3B-C2B	-3.76	1.35	1.40
15	B3	832	CLA	C3B-C2B	-3.76	1.35	1.40
15	A3	822	CLA	C3B-C2B	-3.76	1.35	1.40
15	B3	833	CLA	C2A-C1A	-3.76	1.50	1.53
15	A2	811	CLA	C3B-C2B	-3.75	1.35	1.40
15	B1	831	CLA	C3B-C2B	-3.74	1.35	1.40
15	A1	844	CLA	C3B-C2B	-3.74	1.35	1.40
15	A2	814	CLA	MG-NC	-3.73	1.97	2.06
15	A3	830	CLA	C3B-C2B	-3.73	1.35	1.40
15	B1	833	CLA	C2A-C1A	-3.72	1.50	1.53
15	B1	801	CLA	MG-NC	-3.71	1.97	2.06
15	A3	831	CLA	MG-NC	-3.71	1.97	2.06
15	A1	830	CLA	C3B-C2B	-3.71	1.35	1.40
15	A1	814	CLA	MG-NC	-3.71	1.97	2.06
15	A2	844	CLA	C3B-C2B	-3.71	1.35	1.40
15	B3	831	CLA	C3B-C2B	-3.71	1.35	1.40
15	A1	815	CLA	MG-NC	-3.71	1.97	2.06
15	B3	801	CLA	MG-NC	-3.71	1.97	2.06
15	B2	801	CLA	MG-NC	-3.71	1.97	2.06
15	A2	830	CLA	C3B-C2B	-3.70	1.35	1.40
15	K2	101	CLA	C3B-C2B	-3.70	1.35	1.40
15	A3	814	CLA	MG-NC	-3.70	1.97	2.06
15	K1	101	CLA	C3B-C2B	-3.69	1.35	1.40
15	B3	833	CLA	MG-NC	-3.69	1.97	2.06
15	A1	831	CLA	MG-NC	-3.69	1.97	2.06
15	K3	101	CLA	C3B-C2B	-3.69	1.35	1.40
15	A2	831	CLA	MG-NC	-3.69	1.97	2.06
15	B2	833	CLA	C2A-C1A	-3.68	1.50	1.53
15	L1	1004	CLA	C3B-C2B	-3.68	1.35	1.40
15	L2	1004	CLA	C3B-C2B	-3.68	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B2	830	CLA	MG-NC	-3.68	1.97	2.06
15	A1	812	CLA	C3A-C2A	-3.68	1.51	1.54
15	B3	805	CLA	C3B-C2B	-3.68	1.35	1.40
15	A3	812	CLA	C3A-C2A	-3.68	1.51	1.54
15	A3	819	CLA	MG-NC	-3.68	1.97	2.06
15	B1	830	CLA	MG-NC	-3.67	1.97	2.06
15	B3	830	CLA	MG-NC	-3.67	1.97	2.06
15	A1	819	CLA	MG-NC	-3.67	1.97	2.06
15	A2	819	CLA	MG-NC	-3.67	1.97	2.06
15	B2	805	CLA	C3B-C2B	-3.67	1.35	1.40
15	A2	809	CLA	MG-NC	-3.67	1.97	2.06
15	L3	1004	CLA	C3B-C2B	-3.67	1.35	1.40
15	A2	815	CLA	MG-NC	-3.66	1.97	2.06
15	B1	805	CLA	C3B-C2B	-3.66	1.35	1.40
15	A3	815	CLA	MG-NC	-3.66	1.97	2.06
15	B1	833	CLA	MG-NC	-3.66	1.97	2.06
15	B3	817	CLA	C3B-C2B	-3.66	1.35	1.40
15	B2	817	CLA	C3B-C2B	-3.65	1.35	1.40
15	B3	836	CLA	C3B-C2B	-3.65	1.35	1.40
15	B1	817	CLA	C3B-C2B	-3.65	1.35	1.40
15	A2	829	CLA	C3B-C2B	-3.65	1.35	1.40
15	B3	810	CLA	C3B-C2B	-3.64	1.35	1.40
15	A3	809	CLA	MG-NC	-3.64	1.97	2.06
15	B2	833	CLA	MG-NC	-3.64	1.97	2.06
15	A1	829	CLA	C3B-C2B	-3.64	1.35	1.40
15	A1	809	CLA	MG-NC	-3.64	1.97	2.06
15	A3	829	CLA	C3B-C2B	-3.63	1.35	1.40
15	A1	834	CLA	C3B-C2B	-3.63	1.35	1.40
15	B1	836	CLA	C3B-C2B	-3.63	1.35	1.40
15	A2	834	CLA	C3B-C2B	-3.63	1.35	1.40
15	A2	822	CLA	MG-NC	-3.63	1.97	2.06
15	A2	806	CLA	C3B-C2B	-3.62	1.35	1.40
15	A3	834	CLA	C3B-C2B	-3.62	1.35	1.40
15	A1	822	CLA	MG-NC	-3.62	1.97	2.06
15	A2	817	CLA	MG-NC	-3.61	1.97	2.06
15	A3	817	CLA	MG-NC	-3.61	1.97	2.06
15	A1	817	CLA	MG-NC	-3.61	1.97	2.06
15	B1	810	CLA	C3B-C2B	-3.61	1.35	1.40
15	B2	836	CLA	C3B-C2B	-3.61	1.35	1.40
15	B2	812	CLA	C3B-C2B	-3.61	1.35	1.40
15	A3	822	CLA	MG-NC	-3.61	1.97	2.06
15	A1	806	CLA	C3B-C2B	-3.61	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	803	CLA	C3B-C2B	-3.61	1.35	1.40
15	A3	806	CLA	C3B-C2B	-3.61	1.35	1.40
15	A1	842	CLA	MG-NC	-3.61	1.97	2.06
15	A2	842	CLA	MG-NC	-3.60	1.97	2.06
15	B2	803	CLA	C3B-C2B	-3.60	1.35	1.40
15	A2	812	CLA	C3A-C2A	-3.60	1.51	1.54
15	B2	810	CLA	C3B-C2B	-3.60	1.35	1.40
15	B1	837	CLA	MG-NC	-3.60	1.97	2.06
15	J2	1307	CLA	MG-NC	-3.60	1.97	2.06
15	B1	803	CLA	C3B-C2B	-3.60	1.35	1.40
15	B2	837	CLA	MG-NC	-3.60	1.97	2.06
15	J3	1307	CLA	MG-NC	-3.59	1.97	2.06
15	B1	812	CLA	C3B-C2B	-3.59	1.35	1.40
15	J1	1307	CLA	MG-NC	-3.59	1.97	2.06
15	A3	803	CLA	MG-NC	-3.59	1.97	2.06
15	B2	813	CLA	MG-NC	-3.59	1.97	2.06
15	A2	805	CLA	C3B-C2B	-3.59	1.35	1.40
15	A3	837	CLA	C3B-C2B	-3.59	1.35	1.40
15	A3	842	CLA	MG-NC	-3.59	1.97	2.06
15	B1	813	CLA	MG-NC	-3.58	1.97	2.06
15	A1	824	CLA	C3B-C2B	-3.58	1.35	1.40
15	A2	804	CLA	MG-NC	-3.58	1.97	2.06
15	A2	808	CLA	MG-NC	-3.58	1.97	2.06
15	B3	837	CLA	MG-NC	-3.58	1.97	2.06
15	A3	824	CLA	C3B-C2B	-3.58	1.35	1.40
15	B3	830	CLA	C3A-C2A	-3.57	1.51	1.54
15	A2	820	CLA	MG-NC	-3.57	1.97	2.06
15	B3	801	CLA	C3B-C2B	-3.57	1.35	1.40
15	A1	803	CLA	MG-NC	-3.57	1.97	2.06
15	A1	805	CLA	C3B-C2B	-3.57	1.35	1.40
15	B2	804	CLA	C3B-C2B	-3.57	1.35	1.40
15	A3	805	CLA	C3B-C2B	-3.57	1.35	1.40
15	A3	808	CLA	MG-NC	-3.57	1.97	2.06
15	A3	836	CLA	MG-NC	-3.57	1.97	2.06
15	A1	836	CLA	MG-NC	-3.57	1.97	2.06
15	A1	820	CLA	MG-NC	-3.57	1.97	2.06
15	A3	816	CLA	MG-NC	-3.57	1.97	2.06
15	B1	819	CLA	MG-NC	-3.56	1.97	2.06
15	A2	816	CLA	MG-NC	-3.56	1.97	2.06
15	A1	816	CLA	MG-NC	-3.56	1.97	2.06
15	A2	824	CLA	C3B-C2B	-3.56	1.35	1.40
15	B3	812	CLA	C3B-C2B	-3.56	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	804	CLA	C3B-C2B	-3.56	1.35	1.40
15	A1	804	CLA	MG-NC	-3.56	1.97	2.06
15	A2	841	CLA	C3A-C2A	-3.56	1.51	1.54
15	A1	808	CLA	MG-NC	-3.55	1.97	2.06
15	A1	810	CLA	MG-NC	-3.55	1.97	2.06
15	B2	819	CLA	MG-NC	-3.55	1.97	2.06
15	B3	819	CLA	MG-NC	-3.55	1.97	2.06
15	B1	827	CLA	C3B-C2B	-3.55	1.35	1.40
15	B3	827	CLA	C3B-C2B	-3.55	1.35	1.40
15	B3	813	CLA	MG-NC	-3.55	1.97	2.06
15	A3	820	CLA	MG-NC	-3.55	1.97	2.06
15	B1	804	CLA	C3B-C2B	-3.55	1.35	1.40
15	A2	836	CLA	MG-NC	-3.55	1.97	2.06
15	A3	807	CLA	MG-NC	-3.55	1.97	2.06
15	B2	834	CLA	MG-NC	-3.55	1.97	2.06
15	A3	810	CLA	MG-NC	-3.55	1.97	2.06
15	A1	841	CLA	C3A-C2A	-3.55	1.51	1.54
15	A2	803	CLA	MG-NC	-3.55	1.97	2.06
15	A1	837	CLA	C3B-C2B	-3.55	1.35	1.40
15	A3	804	CLA	MG-NC	-3.54	1.97	2.06
15	B2	820	CLA	MG-NC	-3.54	1.97	2.06
15	B1	834	CLA	MG-NC	-3.54	1.97	2.06
15	A2	807	CLA	MG-NC	-3.54	1.97	2.06
15	B1	820	CLA	MG-NC	-3.54	1.97	2.06
15	A1	807	CLA	MG-NC	-3.54	1.97	2.06
15	A3	833	CLA	MG-NC	-3.54	1.97	2.06
15	B2	827	CLA	C3B-C2B	-3.54	1.35	1.40
15	A2	810	CLA	MG-NC	-3.54	1.97	2.06
15	B3	820	CLA	MG-NC	-3.54	1.97	2.06
15	B1	839	CLA	MG-NC	-3.54	1.97	2.06
15	B1	801	CLA	C3B-C2B	-3.53	1.35	1.40
15	B1	830	CLA	C3A-C2A	-3.53	1.51	1.54
15	J3	1302	CLA	MG-NC	-3.53	1.97	2.06
15	A2	837	CLA	C3B-C2B	-3.53	1.35	1.40
15	A2	839	CLA	MG-NC	-3.53	1.97	2.06
15	A2	833	CLA	MG-NC	-3.53	1.97	2.06
15	B2	839	CLA	MG-NC	-3.53	1.97	2.06
15	A1	833	CLA	MG-NC	-3.53	1.97	2.06
15	J2	1302	CLA	MG-NC	-3.53	1.97	2.06
15	B2	801	CLA	C3B-C2B	-3.53	1.35	1.40
15	A3	841	CLA	C3A-C2A	-3.53	1.51	1.54
15	B3	839	CLA	MG-NC	-3.53	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A2	819	CLA	C3B-C2B	-3.52	1.35	1.40
15	A3	839	CLA	MG-NC	-3.52	1.97	2.06
15	B3	834	CLA	MG-NC	-3.51	1.97	2.06
15	A3	804	CLA	C3B-C2B	-3.51	1.35	1.40
15	J1	1302	CLA	MG-NC	-3.51	1.97	2.06
15	B1	826	CLA	MG-NC	-3.51	1.97	2.06
15	B3	824	CLA	MG-NC	-3.51	1.97	2.06
15	A1	819	CLA	C3B-C2B	-3.51	1.35	1.40
15	A2	804	CLA	C3B-C2B	-3.51	1.35	1.40
15	B1	815	CLA	C3B-C2B	-3.51	1.35	1.40
15	B3	815	CLA	MG-NC	-3.51	1.97	2.06
15	B2	815	CLA	C3B-C2B	-3.51	1.35	1.40
15	B1	815	CLA	MG-NC	-3.51	1.97	2.06
15	A1	839	CLA	MG-NC	-3.50	1.97	2.06
15	B2	816	CLA	C3B-C2B	-3.50	1.35	1.40
15	B3	815	CLA	C3B-C2B	-3.50	1.35	1.40
15	L3	1003	CLA	C3B-C2B	-3.50	1.35	1.40
15	A3	819	CLA	C3B-C2B	-3.50	1.35	1.40
15	B1	823	CLA	MG-NC	-3.50	1.98	2.06
15	A1	804	CLA	C3B-C2B	-3.50	1.35	1.40
15	B3	826	CLA	MG-NC	-3.50	1.98	2.06
15	B2	826	CLA	MG-NC	-3.50	1.98	2.06
15	B2	815	CLA	MG-NC	-3.50	1.98	2.06
15	B2	826	CLA	C3B-C2B	-3.50	1.35	1.40
15	B1	826	CLA	C3B-C2B	-3.49	1.35	1.40
15	B1	836	CLA	MG-NC	-3.49	1.98	2.06
15	B1	816	CLA	C3B-C2B	-3.49	1.35	1.40
15	B3	826	CLA	C3B-C2B	-3.49	1.35	1.40
15	A1	832	CLA	C3B-C2B	-3.49	1.35	1.40
15	A2	827	CLA	MG-NC	-3.49	1.98	2.06
15	B3	816	CLA	MG-NC	-3.49	1.98	2.06
15	A1	827	CLA	MG-NC	-3.49	1.98	2.06
15	B1	817	CLA	MG-NC	-3.49	1.98	2.06
15	B2	836	CLA	MG-NC	-3.49	1.98	2.06
15	A3	832	CLA	C3B-C2B	-3.49	1.35	1.40
15	B2	823	CLA	MG-NC	-3.49	1.98	2.06
15	B3	817	CLA	MG-NC	-3.49	1.98	2.06
15	B2	816	CLA	MG-NC	-3.48	1.98	2.06
15	B2	830	CLA	C3A-C2A	-3.48	1.51	1.54
15	B2	817	CLA	MG-NC	-3.48	1.98	2.06
15	B1	816	CLA	MG-NC	-3.48	1.98	2.06
15	B3	823	CLA	MG-NC	-3.48	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A2	832	CLA	C3B-C2B	-3.48	1.35	1.40
15	B3	816	CLA	C3B-C2B	-3.48	1.35	1.40
15	A3	827	CLA	MG-NC	-3.48	1.98	2.06
15	B1	824	CLA	MG-NC	-3.48	1.98	2.06
15	A3	828	CLA	MG-NC	-3.47	1.98	2.06
15	A3	826	CLA	C3B-C2B	-3.47	1.35	1.40
15	B2	824	CLA	MG-NC	-3.47	1.98	2.06
15	A3	812	CLA	MG-NC	-3.47	1.98	2.06
15	A1	812	CLA	MG-NC	-3.47	1.98	2.06
15	B3	836	CLA	MG-NC	-3.47	1.98	2.06
15	B3	820	CLA	C3B-C2B	-3.47	1.35	1.40
15	A2	828	CLA	MG-NC	-3.46	1.98	2.06
15	A2	812	CLA	MG-NC	-3.46	1.98	2.06
15	L1	1003	CLA	C3B-C2B	-3.46	1.35	1.40
15	A1	828	CLA	MG-NC	-3.46	1.98	2.06
15	B3	813	CLA	C3B-C2B	-3.45	1.35	1.40
15	A3	826	CLA	MG-NC	-3.45	1.98	2.06
15	B1	820	CLA	C3B-C2B	-3.45	1.35	1.40
15	B3	824	CLA	C3B-C2B	-3.44	1.35	1.40
15	A3	823	CLA	MG-NC	-3.44	1.98	2.06
15	A2	823	CLA	MG-NC	-3.44	1.98	2.06
15	A1	823	CLA	MG-NC	-3.44	1.98	2.06
15	A2	826	CLA	C3B-C2B	-3.44	1.35	1.40
15	A1	826	CLA	MG-NC	-3.44	1.98	2.06
15	A1	826	CLA	C3B-C2B	-3.44	1.35	1.40
15	A1	821	CLA	MG-NC	-3.44	1.98	2.06
15	A2	826	CLA	MG-NC	-3.44	1.98	2.06
15	B1	824	CLA	C3B-C2B	-3.43	1.35	1.40
15	B3	828	CLA	MG-NC	-3.43	1.98	2.06
15	B1	813	CLA	C3B-C2B	-3.43	1.35	1.40
15	A3	821	CLA	MG-NC	-3.43	1.98	2.06
15	B1	828	CLA	MG-NC	-3.43	1.98	2.06
15	L2	1003	CLA	C3B-C2B	-3.43	1.35	1.40
15	A2	835	CLA	MG-NC	-3.42	1.98	2.06
15	B2	820	CLA	C3B-C2B	-3.42	1.35	1.40
15	B2	828	CLA	MG-NC	-3.42	1.98	2.06
15	J2	1303	CLA	MG-NC	-3.42	1.98	2.06
15	A1	816	CLA	C3A-C2A	-3.42	1.51	1.54
15	B2	837	CLA	C3A-C2A	-3.42	1.51	1.54
15	A2	821	CLA	MG-NC	-3.42	1.98	2.06
15	B2	824	CLA	C3B-C2B	-3.41	1.35	1.40
15	J1	1303	CLA	MG-NC	-3.41	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	814	CLA	C3B-C2B	-3.41	1.35	1.40
15	B3	822	CLA	MG-NC	-3.41	1.98	2.06
15	A3	805	CLA	MG-NC	-3.41	1.98	2.06
15	A2	805	CLA	MG-NC	-3.41	1.98	2.06
15	B1	849	CLA	MG-NC	-3.41	1.98	2.06
15	A1	805	CLA	MG-NC	-3.41	1.98	2.06
15	B2	813	CLA	C3B-C2B	-3.40	1.35	1.40
15	B2	849	CLA	MG-NC	-3.40	1.98	2.06
15	B3	849	CLA	MG-NC	-3.40	1.98	2.06
15	J3	1303	CLA	MG-NC	-3.40	1.98	2.06
15	A3	816	CLA	C3A-C2A	-3.40	1.51	1.54
15	B2	818	CLA	MG-NC	-3.40	1.98	2.06
15	A2	823	CLA	C3A-C2A	-3.40	1.51	1.54
15	A1	823	CLA	C3A-C2A	-3.39	1.51	1.54
15	B1	818	CLA	MG-NC	-3.39	1.98	2.06
15	A1	835	CLA	MG-NC	-3.39	1.98	2.06
15	B1	814	CLA	C3B-C2B	-3.39	1.35	1.40
15	B1	822	CLA	MG-NC	-3.39	1.98	2.06
15	B3	818	CLA	MG-NC	-3.38	1.98	2.06
15	A1	843	CLA	MG-NC	-3.38	1.98	2.06
15	A3	841	CLA	MG-NC	-3.38	1.98	2.06
15	B2	814	CLA	C3B-C2B	-3.38	1.35	1.40
15	B1	837	CLA	C3A-C2A	-3.38	1.51	1.54
15	B3	811	CLA	MG-NC	-3.38	1.98	2.06
15	B2	830	CLA	C3B-C2B	-3.38	1.35	1.40
15	A3	823	CLA	C3A-C2A	-3.37	1.51	1.54
15	B1	811	CLA	MG-NC	-3.37	1.98	2.06
15	A1	841	CLA	MG-NC	-3.37	1.98	2.06
15	B2	822	CLA	MG-NC	-3.37	1.98	2.06
15	A3	835	CLA	MG-NC	-3.37	1.98	2.06
15	B1	830	CLA	C3B-C2B	-3.36	1.35	1.40
15	I1	101	CLA	MG-NC	-3.36	1.98	2.06
15	I3	101	CLA	MG-NC	-3.36	1.98	2.06
15	B2	810	CLA	MG-NC	-3.36	1.98	2.06
15	B3	814	CLA	MG-NC	-3.36	1.98	2.06
15	I2	101	CLA	MG-NC	-3.36	1.98	2.06
15	A3	843	CLA	MG-NC	-3.36	1.98	2.06
15	B2	811	CLA	MG-NC	-3.36	1.98	2.06
15	B3	830	CLA	C3B-C2B	-3.35	1.35	1.40
15	A1	825	CLA	C3B-C2B	-3.35	1.35	1.40
15	B1	810	CLA	MG-NC	-3.35	1.98	2.06
15	A2	817	CLA	C3A-C2A	-3.35	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B1	814	CLA	MG-NC	-3.35	1.98	2.06
15	A2	841	CLA	MG-NC	-3.35	1.98	2.06
15	B2	823	CLA	C3B-C2B	-3.35	1.35	1.40
15	A1	825	CLA	MG-NC	-3.35	1.98	2.06
15	A2	843	CLA	MG-NC	-3.35	1.98	2.06
15	A1	807	CLA	C3B-C2B	-3.34	1.35	1.40
15	A3	825	CLA	C3B-C2B	-3.34	1.35	1.40
15	B2	812	CLA	MG-NC	-3.34	1.98	2.06
15	A2	825	CLA	MG-NC	-3.34	1.98	2.06
15	L1	1004	CLA	MG-NC	-3.34	1.98	2.06
15	A3	825	CLA	MG-NC	-3.34	1.98	2.06
15	L2	1004	CLA	MG-NC	-3.34	1.98	2.06
15	A2	816	CLA	C3A-C2A	-3.34	1.51	1.54
15	B1	823	CLA	C3B-C2B	-3.34	1.35	1.40
15	B3	823	CLA	C3B-C2B	-3.33	1.35	1.40
15	B3	810	CLA	MG-NC	-3.33	1.98	2.06
15	B2	814	CLA	MG-NC	-3.33	1.98	2.06
15	L3	1004	CLA	MG-NC	-3.33	1.98	2.06
15	A2	825	CLA	C3B-C2B	-3.33	1.35	1.40
15	B1	812	CLA	MG-NC	-3.32	1.98	2.06
15	A2	807	CLA	C3B-C2B	-3.32	1.35	1.40
15	A3	817	CLA	C3A-C2A	-3.32	1.51	1.54
15	A1	832	CLA	MG-NC	-3.32	1.98	2.06
15	B3	812	CLA	MG-NC	-3.32	1.98	2.06
15	B3	837	CLA	C3A-C2A	-3.32	1.51	1.54
15	A2	832	CLA	MG-NC	-3.31	1.98	2.06
15	A3	807	CLA	C3B-C2B	-3.31	1.35	1.40
15	A1	817	CLA	C3A-C2A	-3.31	1.51	1.54
15	A3	832	CLA	MG-NC	-3.30	1.98	2.06
15	B2	827	CLA	MG-NC	-3.30	1.98	2.06
15	A2	834	CLA	MG-NC	-3.29	1.98	2.06
15	A1	834	CLA	MG-NC	-3.29	1.98	2.06
15	B1	827	CLA	MG-NC	-3.29	1.98	2.06
15	A3	834	CLA	MG-NC	-3.29	1.98	2.06
15	A1	806	CLA	MG-NC	-3.28	1.98	2.06
15	A2	806	CLA	MG-NC	-3.28	1.98	2.06
15	B3	827	CLA	MG-NC	-3.28	1.98	2.06
15	B1	805	CLA	MG-NC	-3.28	1.98	2.06
15	A3	806	CLA	MG-NC	-3.28	1.98	2.06
15	B2	805	CLA	MG-NC	-3.27	1.98	2.06
15	B3	805	CLA	MG-NC	-3.27	1.98	2.06
15	B2	831	CLA	MG-NC	-3.27	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B2	835	CLA	MG-NC	-3.26	1.98	2.06
15	A2	829	CLA	MG-NC	-3.26	1.98	2.06
15	J1	1301	CLA	MG-NC	-3.25	1.98	2.06
15	A2	838	CLA	MG-NC	-3.25	1.98	2.06
15	B1	831	CLA	MG-NC	-3.25	1.98	2.06
15	A1	856	CLA	C3B-C2B	-3.25	1.35	1.40
15	B3	821	CLA	C3B-C2B	-3.25	1.35	1.40
15	A2	856	CLA	C3B-C2B	-3.25	1.35	1.40
15	J2	1301	CLA	MG-NC	-3.25	1.98	2.06
15	A3	856	CLA	C3B-C2B	-3.25	1.35	1.40
15	J3	1301	CLA	MG-NC	-3.24	1.98	2.06
15	B1	821	CLA	C3B-C2B	-3.24	1.35	1.40
15	A1	838	CLA	MG-NC	-3.24	1.98	2.06
15	A3	838	CLA	MG-NC	-3.24	1.98	2.06
15	B3	831	CLA	MG-NC	-3.24	1.98	2.06
15	A1	829	CLA	MG-NC	-3.23	1.98	2.06
15	B1	835	CLA	MG-NC	-3.23	1.98	2.06
15	A2	813	CLA	MG-NC	-3.23	1.98	2.06
15	B3	835	CLA	MG-NC	-3.23	1.98	2.06
15	A3	829	CLA	MG-NC	-3.22	1.98	2.06
15	A1	813	CLA	MG-NC	-3.22	1.98	2.06
15	B2	821	CLA	C3B-C2B	-3.22	1.35	1.40
15	A2	809	CLA	C3B-C2B	-3.21	1.35	1.40
15	A3	844	CLA	MG-NC	-3.21	1.98	2.06
15	A3	813	CLA	MG-NC	-3.21	1.98	2.06
15	A2	810	CLA	C3A-C2A	-3.20	1.51	1.54
15	A1	810	CLA	C3A-C2A	-3.20	1.51	1.54
15	A1	844	CLA	MG-NC	-3.19	1.98	2.06
15	A2	824	CLA	MG-NC	-3.19	1.98	2.06
15	A3	824	CLA	MG-NC	-3.19	1.98	2.06
15	A1	809	CLA	C3B-C2B	-3.19	1.35	1.40
15	B2	825	CLA	MG-NC	-3.19	1.98	2.06
15	A3	810	CLA	C3A-C2A	-3.18	1.51	1.54
15	A1	824	CLA	MG-NC	-3.18	1.98	2.06
15	B1	825	CLA	MG-NC	-3.17	1.98	2.06
15	B3	825	CLA	MG-NC	-3.17	1.98	2.06
15	A2	837	CLA	MG-NC	-3.17	1.98	2.06
15	L1	1003	CLA	MG-NC	-3.17	1.98	2.06
15	A3	809	CLA	C3B-C2B	-3.17	1.36	1.40
15	L2	1003	CLA	MG-NC	-3.17	1.98	2.06
15	A2	844	CLA	MG-NC	-3.16	1.98	2.06
15	A1	837	CLA	MG-NC	-3.16	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B1	806	CLA	MG-NC	-3.16	1.98	2.06
15	B3	806	CLA	MG-NC	-3.15	1.98	2.06
15	L3	1003	CLA	MG-NC	-3.15	1.98	2.06
15	B2	806	CLA	MG-NC	-3.15	1.98	2.06
15	B1	838	CLA	MG-NC	-3.14	1.98	2.06
15	A3	837	CLA	MG-NC	-3.14	1.98	2.06
15	B2	838	CLA	MG-NC	-3.14	1.98	2.06
15	J3	1303	CLA	C3A-C2A	-3.14	1.51	1.54
15	B2	825	CLA	C1D-ND	3.13	1.41	1.37
15	B3	838	CLA	MG-NC	-3.13	1.98	2.06
15	B1	825	CLA	C1D-ND	3.10	1.41	1.37
15	A2	818	CLA	MG-NC	-3.09	1.98	2.06
15	A1	818	CLA	MG-NC	-3.08	1.99	2.06
15	J2	1303	CLA	C3A-C2A	-3.08	1.51	1.54
15	A1	815	CLA	C3A-C2A	-3.08	1.51	1.54
15	B3	825	CLA	C1D-ND	3.07	1.41	1.37
15	A3	818	CLA	MG-NC	-3.07	1.99	2.06
15	J1	1303	CLA	C3A-C2A	-3.05	1.51	1.54
15	B1	804	CLA	MG-NC	-3.04	1.99	2.06
15	A3	815	CLA	C3A-C2A	-3.04	1.51	1.54
15	B2	804	CLA	MG-NC	-3.03	1.99	2.06
15	X1	102	CLA	MG-NC	-3.03	1.99	2.06
15	L2	1002	CLA	MG-NC	-3.03	1.99	2.06
15	X2	102	CLA	MG-NC	-3.03	1.99	2.06
15	L3	1002	CLA	MG-NC	-3.02	1.99	2.06
15	X3	102	CLA	MG-NC	-3.02	1.99	2.06
15	A2	815	CLA	C3A-C2A	-3.01	1.51	1.54
15	L1	1002	CLA	MG-NC	-3.01	1.99	2.06
15	B3	804	CLA	MG-NC	-3.01	1.99	2.06
15	B1	816	CLA	C4D-C3D	-2.99	1.39	1.45
15	B3	816	CLA	C4D-C3D	-2.98	1.39	1.45
15	B2	823	CLA	C1D-ND	2.98	1.41	1.37
15	B2	816	CLA	C4D-C3D	-2.97	1.39	1.45
15	B1	823	CLA	C1D-ND	2.97	1.41	1.37
15	B3	823	CLA	C1D-ND	2.97	1.41	1.37
15	A2	830	CLA	MG-NC	-2.97	1.99	2.06
15	B3	814	CLA	C3A-C2A	-2.96	1.51	1.54
15	A1	830	CLA	MG-NC	-2.95	1.99	2.06
15	A1	825	CLA	C1D-ND	2.95	1.41	1.37
15	A3	830	CLA	MG-NC	-2.95	1.99	2.06
15	A2	825	CLA	C1D-ND	2.94	1.41	1.37
15	A3	825	CLA	C1D-ND	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A1	828	CLA	C3B-C2B	-2.92	1.36	1.40
15	A2	828	CLA	C3B-C2B	-2.92	1.36	1.40
15	A3	828	CLA	C3B-C2B	-2.91	1.36	1.40
15	B1	814	CLA	C3A-C2A	-2.90	1.51	1.54
15	B2	816	CLA	CAD-C3D	-2.89	1.45	1.50
15	B1	811	CLA	C1D-ND	2.88	1.41	1.37
15	B3	816	CLA	CAD-C3D	-2.88	1.45	1.50
15	B3	811	CLA	C1D-ND	2.88	1.41	1.37
15	B1	816	CLA	CAD-C3D	-2.87	1.45	1.50
15	A3	813	CLA	C1D-ND	2.86	1.41	1.37
15	A1	813	CLA	C1D-ND	2.86	1.41	1.37
15	A2	813	CLA	C1D-ND	2.86	1.41	1.37
15	B2	811	CLA	C1D-ND	2.85	1.41	1.37
15	B2	814	CLA	C3A-C2A	-2.85	1.51	1.54
15	J1	1307	CLA	C1D-ND	2.84	1.41	1.37
15	J2	1307	CLA	C1D-ND	2.83	1.41	1.37
15	A1	809	CLA	C1D-ND	2.82	1.41	1.37
15	J3	1307	CLA	C1D-ND	2.82	1.41	1.37
15	A2	809	CLA	C1D-ND	2.81	1.41	1.37
15	A2	836	CLA	C3A-C2A	-2.80	1.51	1.54
15	A3	836	CLA	C3A-C2A	-2.80	1.51	1.54
15	A1	836	CLA	C3A-C2A	-2.79	1.51	1.54
15	A3	809	CLA	C1D-ND	2.79	1.41	1.37
15	J3	1307	CLA	C3C-C4C	2.78	1.44	1.40
15	A3	837	CLA	C1D-ND	2.78	1.41	1.37
15	J3	1303	CLA	C1D-ND	2.77	1.41	1.37
15	J1	1307	CLA	C3C-C4C	2.77	1.44	1.40
15	A3	812	CLA	C1D-ND	2.77	1.41	1.37
15	A1	837	CLA	C1D-ND	2.76	1.41	1.37
15	A2	837	CLA	C1D-ND	2.76	1.41	1.37
15	I2	101	CLA	C1D-ND	2.76	1.41	1.37
15	A1	812	CLA	C1D-ND	2.74	1.41	1.37
15	B3	806	CLA	C1D-ND	2.74	1.41	1.37
15	J2	1307	CLA	C3C-C4C	2.74	1.44	1.40
15	I1	101	CLA	C1D-ND	2.73	1.41	1.37
15	J1	1303	CLA	C1D-ND	2.73	1.41	1.37
15	I3	101	CLA	C1D-ND	2.73	1.41	1.37
15	J2	1303	CLA	C1D-ND	2.72	1.41	1.37
15	A3	803	CLA	C1D-ND	2.71	1.41	1.37
15	B1	806	CLA	C1D-ND	2.70	1.41	1.37
15	A3	841	CLA	C1D-ND	2.70	1.41	1.37
15	A2	803	CLA	C1D-ND	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A2	812	CLA	C1D-ND	2.69	1.41	1.37
15	B2	806	CLA	C1D-ND	2.68	1.41	1.37
15	B2	818	CLA	C1D-ND	2.68	1.41	1.37
15	A2	816	CLA	C1D-ND	2.68	1.41	1.37
15	B2	819	CLA	C1D-ND	2.68	1.41	1.37
15	A1	841	CLA	C1D-ND	2.67	1.41	1.37
15	A1	803	CLA	C1D-ND	2.67	1.41	1.37
15	A2	841	CLA	C1D-ND	2.67	1.41	1.37
15	B3	815	CLA	C4D-CHA	-2.66	1.36	1.44
15	B2	815	CLA	C4D-CHA	-2.66	1.36	1.44
15	B1	818	CLA	C1D-ND	2.66	1.41	1.37
15	K2	101	CLA	C4D-CHA	-2.66	1.36	1.44
15	B1	815	CLA	C4D-CHA	-2.66	1.36	1.44
15	K1	101	CLA	C4D-CHA	-2.66	1.36	1.44
15	B3	819	CLA	C1D-ND	2.65	1.41	1.37
15	B1	819	CLA	C1D-ND	2.65	1.41	1.37
15	K3	101	CLA	C4D-CHA	-2.65	1.36	1.44
15	J3	1301	CLA	C1D-ND	2.64	1.41	1.37
15	J2	1301	CLA	C1D-ND	2.64	1.41	1.37
15	A3	815	CLA	C1D-ND	2.64	1.41	1.37
15	J1	1301	CLA	C1D-ND	2.63	1.41	1.37
15	A3	817	CLA	C1D-ND	2.62	1.41	1.37
15	A1	816	CLA	C1D-ND	2.62	1.41	1.37
15	A1	817	CLA	C1D-ND	2.61	1.41	1.37
15	A3	816	CLA	C1D-ND	2.61	1.41	1.37
15	B3	818	CLA	C1D-ND	2.60	1.41	1.37
15	A2	814	CLA	C4D-CHA	-2.59	1.36	1.44
15	A2	817	CLA	C1D-ND	2.58	1.41	1.37
15	A1	815	CLA	C1D-ND	2.58	1.41	1.37
15	B1	812	CLA	C1D-ND	2.57	1.40	1.37
15	B3	812	CLA	C1D-ND	2.57	1.40	1.37
15	B3	829	CLA	C4D-CHA	-2.57	1.36	1.44
15	A2	815	CLA	C1D-ND	2.57	1.40	1.37
15	B2	812	CLA	C1D-ND	2.57	1.40	1.37
15	A2	844	CLA	C1D-ND	2.57	1.40	1.37
15	A1	814	CLA	C4D-CHA	-2.57	1.36	1.44
15	B1	829	CLA	C4D-CHA	-2.56	1.36	1.44
15	A1	844	CLA	C1D-ND	2.55	1.40	1.37
15	A3	810	CLA	C1D-ND	2.55	1.40	1.37
15	B2	829	CLA	C4D-CHA	-2.55	1.36	1.44
15	B2	834	CLA	C1D-ND	2.55	1.40	1.37
15	A3	807	CLA	C1D-ND	2.55	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A3	844	CLA	C1D-ND	2.55	1.40	1.37
15	A2	810	CLA	C1D-ND	2.55	1.40	1.37
15	B2	816	CLA	C3D-C2D	2.55	1.42	1.36
15	A3	814	CLA	C4D-CHA	-2.54	1.36	1.44
15	B3	834	CLA	C1D-ND	2.54	1.40	1.37
15	B3	816	CLA	C3D-C2D	2.54	1.42	1.36
15	B1	834	CLA	C1D-ND	2.54	1.40	1.37
15	B1	816	CLA	C3D-C2D	2.53	1.42	1.36
15	A3	806	CLA	C1D-ND	2.52	1.40	1.37
15	A1	810	CLA	C1D-ND	2.52	1.40	1.37
14	A3	801	CL0	C1D-C2D	-2.52	1.40	1.45
15	A2	806	CLA	C1D-ND	2.52	1.40	1.37
15	A1	806	CLA	C1D-ND	2.52	1.40	1.37
14	A1	801	CL0	C1D-C2D	-2.50	1.40	1.45
15	B1	835	CLA	C1D-ND	2.49	1.40	1.37
15	B2	835	CLA	C1D-ND	2.49	1.40	1.37
15	B3	835	CLA	C1D-ND	2.48	1.40	1.37
15	A3	822	CLA	C1D-ND	2.48	1.40	1.37
15	A1	807	CLA	C1D-ND	2.48	1.40	1.37
14	A2	801	CL0	C1D-C2D	-2.47	1.40	1.45
15	B3	820	CLA	C4D-CHA	-2.46	1.36	1.44
15	A1	822	CLA	C1D-ND	2.46	1.40	1.37
15	B3	810	CLA	C1D-ND	2.46	1.40	1.37
15	B1	820	CLA	C4D-CHA	-2.45	1.36	1.44
15	A2	807	CLA	C1D-ND	2.45	1.40	1.37
15	B2	810	CLA	C1D-ND	2.45	1.40	1.37
15	B3	831	CLA	C1D-ND	2.45	1.40	1.37
15	B2	820	CLA	C4D-CHA	-2.44	1.36	1.44
15	A2	817	CLA	C1B-CHB	-2.43	1.39	1.43
15	A3	817	CLA	C1B-CHB	-2.43	1.39	1.43
15	A1	817	CLA	C1B-CHB	-2.43	1.39	1.43
15	B1	810	CLA	C1D-ND	2.43	1.40	1.37
15	A2	808	CLA	C1D-ND	2.43	1.40	1.37
15	J1	1301	CLA	C4B-CHC	-2.43	1.39	1.43
15	J3	1301	CLA	C4B-CHC	-2.43	1.39	1.43
15	A2	822	CLA	C1D-ND	2.42	1.40	1.37
15	J2	1301	CLA	C4B-CHC	-2.42	1.39	1.43
15	A3	808	CLA	C1D-ND	2.41	1.40	1.37
15	A3	827	CLA	C1D-ND	2.41	1.40	1.37
15	A1	808	CLA	C1D-ND	2.40	1.40	1.37
15	A1	820	CLA	C1D-ND	2.40	1.40	1.37
15	A3	829	CLA	C1D-ND	2.40	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J3	1301	CLA	C1B-CHB	-2.40	1.39	1.43
15	B1	831	CLA	C1D-ND	2.40	1.40	1.37
15	B1	829	CLA	C1D-ND	2.40	1.40	1.37
15	B2	823	CLA	C1D-C2D	-2.39	1.40	1.45
15	B3	829	CLA	C1D-ND	2.39	1.40	1.37
15	J1	1301	CLA	C1B-CHB	-2.39	1.39	1.43
14	A2	801	CL0	C1D-ND	2.39	1.40	1.37
15	B2	829	CLA	C1D-ND	2.39	1.40	1.37
15	A2	823	CLA	C1D-ND	2.39	1.40	1.37
14	A3	801	CL0	C1D-ND	2.39	1.40	1.37
15	B1	823	CLA	C1D-C2D	-2.39	1.40	1.45
14	A1	801	CL0	C1D-ND	2.38	1.40	1.37
15	A1	814	CLA	C1D-ND	2.38	1.40	1.37
15	B2	831	CLA	C1D-ND	2.38	1.40	1.37
15	A2	829	CLA	C1D-ND	2.38	1.40	1.37
15	A1	827	CLA	C1D-ND	2.38	1.40	1.37
15	A3	820	CLA	C1D-ND	2.38	1.40	1.37
15	A1	823	CLA	C1D-ND	2.38	1.40	1.37
15	A2	814	CLA	C1D-ND	2.38	1.40	1.37
15	B3	823	CLA	C1D-C2D	-2.38	1.40	1.45
15	A2	820	CLA	C1D-ND	2.38	1.40	1.37
15	A2	825	CLA	C1D-C2D	-2.37	1.40	1.45
15	A2	827	CLA	C1D-ND	2.37	1.40	1.37
15	A2	831	CLA	C1D-ND	2.37	1.40	1.37
15	A1	825	CLA	C1D-C2D	-2.36	1.40	1.45
15	A1	831	CLA	C1D-ND	2.36	1.40	1.37
15	A3	837	CLA	C1D-C2D	-2.36	1.40	1.45
15	A3	814	CLA	C1D-ND	2.36	1.40	1.37
15	A3	825	CLA	C1D-C2D	-2.36	1.40	1.45
15	B3	803	CLA	C1D-C2D	-2.35	1.40	1.45
15	B1	808	CLA	C1D-ND	2.35	1.40	1.37
15	A2	856	CLA	C1D-C2D	-2.35	1.40	1.45
15	A3	856	CLA	C1D-C2D	-2.35	1.40	1.45
15	J2	1301	CLA	C1B-CHB	-2.35	1.39	1.43
15	B3	826	CLA	C1D-C2D	-2.35	1.40	1.45
15	A3	831	CLA	C1D-ND	2.35	1.40	1.37
15	B3	805	CLA	C1D-ND	2.35	1.40	1.37
15	A1	856	CLA	C1D-C2D	-2.35	1.40	1.45
15	B1	803	CLA	C1D-C2D	-2.34	1.40	1.45
15	B2	805	CLA	C1D-ND	2.34	1.40	1.37
15	A1	837	CLA	C1D-C2D	-2.34	1.40	1.45
15	I2	101	CLA	C1D-C2D	-2.34	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A3	821	CLA	C1D-C2D	-2.34	1.40	1.45
15	A3	805	CLA	C1D-ND	2.34	1.40	1.37
15	B3	827	CLA	C1D-C2D	-2.34	1.40	1.45
15	I3	101	CLA	C1D-C2D	-2.34	1.40	1.45
15	J3	1307	CLA	C2B-C1B	2.33	1.42	1.39
15	A3	823	CLA	C1D-ND	2.33	1.40	1.37
15	A2	821	CLA	C1D-ND	2.33	1.40	1.37
15	A3	821	CLA	C1D-ND	2.33	1.40	1.37
15	X2	102	CLA	C1D-ND	2.33	1.40	1.37
15	A1	821	CLA	C1D-ND	2.33	1.40	1.37
15	A1	806	CLA	C1D-C2D	-2.33	1.40	1.45
15	B1	826	CLA	C1D-C2D	-2.33	1.40	1.45
15	B3	808	CLA	C1D-C2D	-2.33	1.40	1.45
15	B2	803	CLA	C1D-C2D	-2.32	1.40	1.45
15	A1	821	CLA	C1D-C2D	-2.32	1.40	1.45
15	A1	829	CLA	C1D-ND	2.32	1.40	1.37
15	A2	821	CLA	C1D-C2D	-2.32	1.40	1.45
15	B1	805	CLA	C1D-ND	2.32	1.40	1.37
15	A2	837	CLA	C1D-C2D	-2.32	1.40	1.45
15	B2	808	CLA	C1D-ND	2.32	1.40	1.37
15	I1	101	CLA	C1D-C2D	-2.32	1.40	1.45
15	B1	827	CLA	C1D-C2D	-2.32	1.40	1.45
15	B1	833	CLA	C1D-ND	2.32	1.40	1.37
15	B3	808	CLA	C1D-ND	2.32	1.40	1.37
15	A1	844	CLA	C1D-C2D	-2.32	1.40	1.45
15	B1	808	CLA	C1D-C2D	-2.31	1.40	1.45
15	B2	826	CLA	C1D-ND	2.31	1.40	1.37
15	B3	826	CLA	C1D-ND	2.31	1.40	1.37
15	A2	806	CLA	C1D-C2D	-2.31	1.40	1.45
15	A2	802	CLA	C1D-ND	2.31	1.40	1.37
15	A3	844	CLA	C1D-C2D	-2.31	1.40	1.45
15	B1	826	CLA	C1D-ND	2.31	1.40	1.37
15	B2	827	CLA	C1D-C2D	-2.31	1.40	1.45
15	A2	840	CLA	C1D-ND	2.31	1.40	1.37
15	B2	825	CLA	C1D-C2D	-2.31	1.40	1.45
15	A2	844	CLA	C1D-C2D	-2.31	1.40	1.45
15	A2	813	CLA	C1D-C2D	-2.31	1.40	1.45
15	A3	806	CLA	C1D-C2D	-2.31	1.40	1.45
15	J2	1307	CLA	C2B-C1B	2.31	1.42	1.39
15	A1	805	CLA	C1D-ND	2.31	1.40	1.37
15	A2	805	CLA	C1D-ND	2.31	1.40	1.37
15	J1	1307	CLA	C2B-C1B	2.30	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L1	1002	CLA	C1D-C2D	-2.30	1.40	1.45
15	B1	825	CLA	C1D-C2D	-2.30	1.40	1.45
15	A3	840	CLA	C1D-ND	2.30	1.40	1.37
15	X1	102	CLA	C1D-ND	2.30	1.40	1.37
15	L2	1004	CLA	C1D-ND	2.30	1.40	1.37
15	B2	826	CLA	C1D-C2D	-2.29	1.40	1.45
15	B3	817	CLA	C1D-C2D	-2.29	1.40	1.45
15	A1	802	CLA	C1D-ND	2.29	1.40	1.37
15	A2	824	CLA	C1D-ND	2.29	1.40	1.37
15	B2	817	CLA	C1D-C2D	-2.29	1.40	1.45
15	A2	817	CLA	CAB-C3B	-2.29	1.46	1.51
15	L3	1002	CLA	C1D-ND	2.29	1.40	1.37
15	B2	849	CLA	C1D-C2D	-2.28	1.40	1.45
15	L3	1004	CLA	C1D-ND	2.28	1.40	1.37
15	B2	808	CLA	C1D-C2D	-2.28	1.40	1.45
15	B3	825	CLA	C1D-C2D	-2.28	1.40	1.45
15	A1	813	CLA	C1D-C2D	-2.28	1.40	1.45
15	A3	830	CLA	C1D-C2D	-2.28	1.40	1.45
15	B1	817	CLA	C1D-C2D	-2.28	1.40	1.45
15	A1	834	CLA	C1D-ND	2.28	1.40	1.37
15	L3	1002	CLA	C1D-C2D	-2.28	1.40	1.45
15	L1	1002	CLA	C1D-ND	2.28	1.40	1.37
15	A1	817	CLA	CAB-C3B	-2.28	1.46	1.51
15	L2	1002	CLA	C1D-C2D	-2.27	1.40	1.45
15	B1	804	CLA	C1D-ND	2.27	1.40	1.37
15	L2	1003	CLA	C1D-C2D	-2.27	1.40	1.45
15	B3	822	CLA	C1D-C2D	-2.27	1.40	1.45
15	A1	830	CLA	C1D-C2D	-2.27	1.40	1.45
15	A1	838	CLA	C1D-C2D	-2.27	1.40	1.45
15	B1	849	CLA	C1D-C2D	-2.27	1.40	1.45
15	B2	812	CLA	C1D-C2D	-2.27	1.40	1.45
15	A3	834	CLA	C1D-ND	2.27	1.40	1.37
15	B1	812	CLA	C1D-C2D	-2.27	1.40	1.45
15	A3	817	CLA	CAB-C3B	-2.27	1.46	1.51
15	A3	804	CLA	C1D-C2D	-2.27	1.40	1.45
15	B2	837	CLA	C1D-ND	2.27	1.40	1.37
15	B1	838	CLA	C1D-C2D	-2.27	1.40	1.45
15	A2	839	CLA	C1D-C2D	-2.27	1.40	1.45
15	B3	839	CLA	C1D-C2D	-2.27	1.40	1.45
15	A1	839	CLA	C1D-C2D	-2.27	1.40	1.45
15	B2	833	CLA	C1D-ND	2.27	1.40	1.37
15	A2	838	CLA	C1D-C2D	-2.27	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	806	CLA	C1D-C2D	-2.27	1.40	1.45
15	B1	821	CLA	C1D-C2D	-2.26	1.40	1.45
15	B2	801	CLA	C1D-C2D	-2.26	1.40	1.45
15	A3	838	CLA	C1D-C2D	-2.26	1.40	1.45
15	A1	824	CLA	C1D-ND	2.26	1.40	1.37
15	L1	1004	CLA	C1D-ND	2.26	1.40	1.37
15	A1	840	CLA	C1D-ND	2.26	1.40	1.37
15	B3	827	CLA	C1D-ND	2.26	1.40	1.37
15	B2	822	CLA	C1D-C2D	-2.26	1.40	1.45
15	B3	802	CLA	C1D-C2D	-2.26	1.40	1.45
15	A3	813	CLA	C1D-C2D	-2.26	1.40	1.45
15	A3	839	CLA	C1D-C2D	-2.26	1.40	1.45
15	A3	824	CLA	C1D-C2D	-2.26	1.40	1.45
15	B3	833	CLA	C1D-ND	2.26	1.40	1.37
15	B1	801	CLA	C1D-C2D	-2.26	1.40	1.45
15	B3	812	CLA	C1D-C2D	-2.26	1.40	1.45
15	B3	849	CLA	C1D-C2D	-2.26	1.40	1.45
15	B1	837	CLA	C1D-ND	2.26	1.40	1.37
15	A3	824	CLA	C1D-ND	2.26	1.40	1.37
15	L1	1003	CLA	C1D-C2D	-2.26	1.40	1.45
15	B3	837	CLA	C1D-ND	2.26	1.40	1.37
15	B1	802	CLA	C1D-C2D	-2.26	1.40	1.45
15	B1	834	CLA	C1D-C2D	-2.26	1.40	1.45
15	B2	813	CLA	C1D-C2D	-2.26	1.40	1.45
15	B3	838	CLA	C1D-C2D	-2.26	1.40	1.45
15	B2	828	CLA	C1D-C2D	-2.25	1.40	1.45
15	B2	839	CLA	C1D-C2D	-2.25	1.40	1.45
15	K3	103	CLA	C1D-ND	2.25	1.40	1.37
15	B2	834	CLA	C1D-C2D	-2.25	1.40	1.45
15	B3	821	CLA	C1D-C2D	-2.25	1.40	1.45
15	A2	834	CLA	C1D-C2D	-2.25	1.40	1.45
15	B2	822	CLA	C1D-ND	2.25	1.40	1.37
15	A3	802	CLA	C1D-ND	2.25	1.40	1.37
15	B2	821	CLA	C1D-C2D	-2.25	1.40	1.45
15	B3	821	CLA	C3D-C4D	-2.25	1.39	1.44
15	A2	834	CLA	C1D-ND	2.25	1.40	1.37
15	B3	835	CLA	C1D-C2D	-2.25	1.40	1.45
15	A2	824	CLA	C1D-C2D	-2.25	1.40	1.45
15	K2	103	CLA	C1D-ND	2.25	1.40	1.37
15	B2	821	CLA	C3D-C4D	-2.25	1.39	1.44
15	B1	835	CLA	C1D-C2D	-2.25	1.40	1.45
15	B1	839	CLA	C1D-C2D	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	830	CLA	C1D-ND	2.24	1.40	1.37
15	A1	804	CLA	C1D-C2D	-2.24	1.40	1.45
15	B3	824	CLA	C1D-C2D	-2.24	1.40	1.45
15	B2	802	CLA	C1D-C2D	-2.24	1.40	1.45
15	B1	821	CLA	C3D-C4D	-2.24	1.39	1.44
15	B3	804	CLA	C1D-ND	2.24	1.40	1.37
15	A1	803	CLA	C1D-C2D	-2.24	1.40	1.45
15	A1	841	CLA	C1D-C2D	-2.24	1.40	1.45
15	A1	829	CLA	C1D-C2D	-2.24	1.40	1.45
15	J1	1307	CLA	C1C-C2C	2.24	1.46	1.42
15	J2	1302	CLA	C1D-ND	2.24	1.40	1.37
15	B3	812	CLA	C3D-C4D	-2.24	1.39	1.44
15	B1	824	CLA	C1D-C2D	-2.24	1.40	1.45
15	A3	808	CLA	C1D-C2D	-2.24	1.40	1.45
15	L2	1002	CLA	C1D-ND	2.24	1.40	1.37
15	X1	102	CLA	C1D-C2D	-2.24	1.40	1.45
15	A2	829	CLA	C1D-C2D	-2.24	1.40	1.45
15	B2	824	CLA	C1D-C2D	-2.24	1.40	1.45
15	B2	804	CLA	C1D-ND	2.24	1.40	1.37
15	B3	813	CLA	C1D-ND	2.24	1.40	1.37
15	A1	809	CLA	C1D-C2D	-2.24	1.40	1.45
15	B2	811	CLA	C1D-C2D	-2.24	1.40	1.45
15	X3	102	CLA	C1D-ND	2.24	1.40	1.37
15	A3	817	CLA	C2B-C1B	2.24	1.42	1.39
15	B1	829	CLA	C3D-C4D	-2.24	1.39	1.44
15	J2	1307	CLA	C1C-C2C	2.24	1.46	1.42
15	A2	830	CLA	C1D-C2D	-2.24	1.40	1.45
15	A1	834	CLA	C1D-C2D	-2.24	1.40	1.45
15	B3	801	CLA	C1D-C2D	-2.24	1.40	1.45
15	K3	103	CLA	C4B-CHC	-2.24	1.39	1.43
15	B1	811	CLA	C1D-C2D	-2.24	1.40	1.45
15	A3	827	CLA	C1D-C2D	-2.24	1.40	1.45
15	B1	831	CLA	C1D-C2D	-2.24	1.40	1.45
15	A1	817	CLA	C1D-C2D	-2.24	1.40	1.45
15	B1	822	CLA	C1D-C2D	-2.24	1.40	1.45
15	A1	817	CLA	C2B-C1B	2.24	1.42	1.39
15	B1	813	CLA	C1D-C2D	-2.24	1.40	1.45
15	A3	829	CLA	C1D-C2D	-2.24	1.40	1.45
15	X2	102	CLA	C1D-C2D	-2.23	1.40	1.45
15	B3	813	CLA	C1D-C2D	-2.23	1.40	1.45
15	X3	102	CLA	C1D-C2D	-2.23	1.40	1.45
15	A3	814	CLA	CAB-C3B	-2.23	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B2	835	CLA	C1D-C2D	-2.23	1.40	1.45
15	A3	817	CLA	C1D-C2D	-2.23	1.40	1.45
15	B1	827	CLA	C1D-ND	2.23	1.40	1.37
15	B2	838	CLA	C1D-C2D	-2.23	1.40	1.45
15	A1	824	CLA	C1D-C2D	-2.23	1.40	1.45
15	A2	804	CLA	C1D-C2D	-2.23	1.40	1.45
15	A2	815	CLA	C1B-CHB	-2.23	1.39	1.43
15	B3	831	CLA	C1D-C2D	-2.23	1.40	1.45
15	B1	830	CLA	C1D-ND	2.23	1.40	1.37
15	A2	838	CLA	C1D-ND	2.23	1.40	1.37
15	B2	805	CLA	C1D-C2D	-2.23	1.40	1.45
15	A2	817	CLA	C2B-C1B	2.23	1.42	1.39
15	K2	103	CLA	C4B-CHC	-2.23	1.39	1.43
15	A1	808	CLA	C1D-C2D	-2.23	1.40	1.45
15	A1	827	CLA	C1D-C2D	-2.23	1.40	1.45
15	A2	808	CLA	C1D-C2D	-2.23	1.40	1.45
15	B2	827	CLA	C1D-ND	2.23	1.40	1.37
15	B1	828	CLA	C1D-C2D	-2.23	1.40	1.45
15	L3	1003	CLA	C1D-C2D	-2.23	1.40	1.45
15	K1	103	CLA	C1D-ND	2.23	1.40	1.37
15	A3	841	CLA	C1D-C2D	-2.23	1.40	1.45
15	B2	831	CLA	C1D-C2D	-2.23	1.40	1.45
15	A3	815	CLA	C1B-CHB	-2.23	1.39	1.43
15	B3	834	CLA	C1D-C2D	-2.23	1.40	1.45
15	B3	805	CLA	C1D-C2D	-2.23	1.40	1.45
15	B2	830	CLA	C1D-ND	2.23	1.40	1.37
15	A1	815	CLA	C1B-CHB	-2.23	1.39	1.43
15	A1	833	CLA	C1D-C2D	-2.23	1.40	1.45
15	A2	833	CLA	C1D-C2D	-2.23	1.40	1.45
15	A3	840	CLA	C1D-C2D	-2.23	1.40	1.45
15	A2	814	CLA	CAB-C3B	-2.23	1.47	1.51
15	B1	812	CLA	C3D-C4D	-2.22	1.39	1.44
15	B2	829	CLA	C3D-C4D	-2.22	1.39	1.44
15	B1	806	CLA	C1D-C2D	-2.22	1.40	1.45
15	J2	1301	CLA	C1D-C2D	-2.22	1.40	1.45
15	J3	1301	CLA	C1D-C2D	-2.22	1.40	1.45
15	B1	816	CLA	C1D-C2D	-2.22	1.40	1.45
15	A2	841	CLA	C1D-C2D	-2.22	1.40	1.45
15	A2	843	CLA	C1D-C2D	-2.22	1.40	1.45
15	B3	809	CLA	C1D-C2D	-2.22	1.40	1.45
15	A3	820	CLA	CAB-C3B	-2.22	1.47	1.51
15	A3	834	CLA	C1D-C2D	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	811	CLA	C1D-C2D	-2.22	1.40	1.45
15	A1	820	CLA	CAB-C3B	-2.22	1.47	1.51
15	B3	822	CLA	C1D-ND	2.22	1.40	1.37
15	A1	823	CLA	C1D-C2D	-2.22	1.40	1.45
15	A3	833	CLA	C1D-C2D	-2.22	1.40	1.45
15	B3	814	CLA	C1D-C2D	-2.22	1.40	1.45
15	A2	813	CLA	CAB-C3B	-2.22	1.47	1.51
15	A1	840	CLA	C1D-C2D	-2.22	1.40	1.45
15	A1	814	CLA	CAB-C3B	-2.22	1.47	1.51
15	B3	828	CLA	C1D-C2D	-2.22	1.40	1.45
15	B3	829	CLA	C3D-C4D	-2.22	1.39	1.44
15	A1	835	CLA	C1D-C2D	-2.22	1.41	1.45
15	B3	815	CLA	C1D-C2D	-2.22	1.41	1.45
15	B1	814	CLA	C1D-C2D	-2.21	1.41	1.45
15	J1	1301	CLA	C1D-C2D	-2.21	1.41	1.45
15	A2	823	CLA	C1D-C2D	-2.21	1.41	1.45
15	A2	835	CLA	C1D-C2D	-2.21	1.41	1.45
15	A2	840	CLA	C1D-C2D	-2.21	1.41	1.45
15	L2	1004	CLA	C1D-C2D	-2.21	1.41	1.45
15	B1	813	CLA	C1D-ND	2.21	1.40	1.37
15	A2	820	CLA	CAB-C3B	-2.21	1.47	1.51
15	A2	817	CLA	C1D-C2D	-2.21	1.41	1.45
15	J2	1302	CLA	C3B-C2B	-2.21	1.34	1.41
15	K1	103	CLA	C4B-CHC	-2.21	1.39	1.43
15	B2	809	CLA	C1D-C2D	-2.21	1.41	1.45
15	B2	816	CLA	C1D-C2D	-2.21	1.41	1.45
15	L3	1004	CLA	C1D-C2D	-2.21	1.41	1.45
15	B2	812	CLA	C3D-C4D	-2.21	1.39	1.44
15	B2	813	CLA	C1D-ND	2.21	1.40	1.37
15	J3	1302	CLA	CAB-C3B	-2.21	1.47	1.51
15	B2	814	CLA	C1D-C2D	-2.21	1.41	1.45
15	B2	818	CLA	C1D-C2D	-2.21	1.41	1.45
15	B1	805	CLA	C1D-C2D	-2.21	1.41	1.45
15	B3	838	CLA	C1D-ND	2.21	1.40	1.37
15	J2	1307	CLA	C1B-CHB	-2.21	1.39	1.43
15	A3	820	CLA	C3B-C2B	-2.21	1.34	1.41
15	A3	828	CLA	C1D-C2D	-2.21	1.41	1.45
15	A3	803	CLA	C1D-C2D	-2.21	1.41	1.45
15	B1	804	CLA	C1D-C2D	-2.21	1.41	1.45
15	B2	806	CLA	C1D-C2D	-2.21	1.41	1.45
15	A3	809	CLA	C1D-C2D	-2.21	1.41	1.45
15	J1	1302	CLA	C3B-C2B	-2.21	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A3	835	CLA	C1D-C2D	-2.21	1.41	1.45
15	J3	1307	CLA	C1C-C2C	2.20	1.46	1.42
15	B3	833	CLA	CAB-C3B	-2.20	1.47	1.51
15	B3	804	CLA	C1D-C2D	-2.20	1.41	1.45
15	A2	826	CLA	C1D-C2D	-2.20	1.41	1.45
15	A3	819	CLA	C3D-C4D	-2.20	1.39	1.44
15	J1	1307	CLA	C1B-CHB	-2.20	1.39	1.43
15	A1	826	CLA	C1D-C2D	-2.20	1.41	1.45
15	B1	815	CLA	C1D-C2D	-2.20	1.41	1.45
15	L1	1004	CLA	C1D-C2D	-2.20	1.41	1.45
15	A2	803	CLA	C1D-C2D	-2.20	1.41	1.45
15	A2	815	CLA	C1D-C2D	-2.20	1.41	1.45
15	A3	811	CLA	C1D-C2D	-2.20	1.41	1.45
15	A3	813	CLA	C3B-C2B	-2.20	1.34	1.41
15	A3	810	CLA	C1D-C2D	-2.20	1.41	1.45
15	A2	827	CLA	C1D-C2D	-2.20	1.41	1.45
15	A2	811	CLA	C1D-ND	2.20	1.40	1.37
15	A1	828	CLA	C1D-C2D	-2.20	1.41	1.45
15	B2	804	CLA	C1D-C2D	-2.20	1.41	1.45
15	B1	818	CLA	C1D-C2D	-2.20	1.41	1.45
15	A3	823	CLA	C1D-C2D	-2.20	1.41	1.45
15	B2	802	CLA	C3D-C4D	-2.20	1.39	1.44
15	A1	815	CLA	C1D-C2D	-2.20	1.41	1.45
15	J3	1307	CLA	C1B-CHB	-2.20	1.39	1.43
15	J2	1302	CLA	CAB-C3B	-2.20	1.47	1.51
15	A2	805	CLA	C1D-C2D	-2.20	1.41	1.45
15	B3	832	CLA	C1D-C2D	-2.20	1.41	1.45
15	A3	815	CLA	C1D-C2D	-2.20	1.41	1.45
15	A3	820	CLA	C1D-C2D	-2.20	1.41	1.45
15	A2	820	CLA	C3B-C2B	-2.20	1.34	1.41
15	B1	833	CLA	CAB-C3B	-2.19	1.47	1.51
15	B3	817	CLA	C1D-ND	2.19	1.40	1.37
15	A1	813	CLA	C3B-C2B	-2.19	1.34	1.41
15	A1	823	CLA	C3D-C4D	-2.19	1.39	1.44
15	A3	813	CLA	CAB-C3B	-2.19	1.47	1.51
15	A3	826	CLA	C1D-C2D	-2.19	1.41	1.45
15	B3	809	CLA	C3D-C4D	-2.19	1.39	1.44
15	B2	824	CLA	C1D-ND	2.19	1.40	1.37
15	A1	810	CLA	C1D-C2D	-2.19	1.41	1.45
15	A2	809	CLA	C1D-C2D	-2.19	1.41	1.45
15	A3	804	CLA	C1D-ND	2.19	1.40	1.37
15	B3	816	CLA	C1D-C2D	-2.19	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J1	1302	CLA	CAB-C3B	-2.19	1.47	1.51
15	J3	1302	CLA	C3B-C2B	-2.19	1.34	1.41
15	B1	822	CLA	C1D-ND	2.19	1.40	1.37
15	A2	828	CLA	C1D-C2D	-2.19	1.41	1.45
15	B1	809	CLA	C1D-C2D	-2.19	1.41	1.45
15	A3	838	CLA	C1D-ND	2.19	1.40	1.37
15	B1	802	CLA	C3D-C4D	-2.19	1.39	1.44
15	A1	805	CLA	C1D-C2D	-2.19	1.41	1.45
15	A2	818	CLA	C3D-C4D	-2.19	1.39	1.44
15	A1	820	CLA	C3B-C2B	-2.19	1.34	1.41
15	A2	827	CLA	C3D-C4D	-2.19	1.39	1.44
15	B3	833	CLA	C1D-C2D	-2.19	1.41	1.45
15	A1	838	CLA	C1D-ND	2.19	1.40	1.37
15	B2	833	CLA	CAB-C3B	-2.19	1.47	1.51
15	B2	815	CLA	C1D-C2D	-2.19	1.41	1.45
15	A1	820	CLA	C1D-C2D	-2.19	1.41	1.45
15	A1	812	CLA	C1D-C2D	-2.19	1.41	1.45
15	A3	805	CLA	C1D-C2D	-2.19	1.41	1.45
15	A3	812	CLA	C1D-C2D	-2.19	1.41	1.45
15	A2	811	CLA	C1D-C2D	-2.19	1.41	1.45
15	B1	833	CLA	C3B-C2B	-2.18	1.34	1.41
15	B1	833	CLA	C1D-C2D	-2.18	1.41	1.45
15	A2	823	CLA	C3D-C4D	-2.18	1.39	1.44
15	B2	833	CLA	C3B-C2B	-2.18	1.34	1.41
15	B1	836	CLA	C3D-C4D	-2.18	1.39	1.44
15	A1	818	CLA	C1D-C2D	-2.18	1.41	1.45
15	A2	813	CLA	C3B-C2B	-2.18	1.34	1.41
15	A1	818	CLA	C3D-C4D	-2.18	1.39	1.44
15	A1	843	CLA	C1D-C2D	-2.18	1.41	1.45
15	B3	819	CLA	C1D-C2D	-2.18	1.41	1.45
15	A1	842	CLA	C1D-C2D	-2.18	1.41	1.45
15	B1	832	CLA	C1D-C2D	-2.18	1.41	1.45
15	A1	819	CLA	C3D-C4D	-2.18	1.39	1.44
15	B2	819	CLA	C1D-C2D	-2.18	1.41	1.45
15	A2	842	CLA	C1D-C2D	-2.18	1.41	1.45
15	B2	836	CLA	C3D-C4D	-2.18	1.39	1.44
15	A2	810	CLA	C1D-C2D	-2.18	1.41	1.45
15	A3	818	CLA	C1D-C2D	-2.18	1.41	1.45
15	J3	1303	CLA	C1D-C2D	-2.18	1.41	1.45
15	A1	813	CLA	CAB-C3B	-2.18	1.47	1.51
15	A2	819	CLA	C3D-C4D	-2.18	1.39	1.44
15	B1	819	CLA	C1D-C2D	-2.18	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A2	802	CLA	C1D-C2D	-2.18	1.41	1.45
15	B1	817	CLA	C1D-ND	2.18	1.40	1.37
15	A3	843	CLA	C1D-C2D	-2.18	1.41	1.45
15	A2	812	CLA	C1D-C2D	-2.18	1.41	1.45
15	J1	1302	CLA	C1D-ND	2.18	1.40	1.37
15	B3	836	CLA	C3D-C4D	-2.18	1.39	1.44
15	B3	818	CLA	C1D-C2D	-2.18	1.41	1.45
15	A1	811	CLA	C1D-C2D	-2.18	1.41	1.45
15	J1	1303	CLA	C1D-C2D	-2.18	1.41	1.45
15	A2	818	CLA	C1D-C2D	-2.18	1.41	1.45
15	A1	811	CLA	C1D-ND	2.18	1.40	1.37
15	B2	832	CLA	C1D-C2D	-2.18	1.41	1.45
15	B3	833	CLA	C3B-C2B	-2.18	1.34	1.41
15	A3	842	CLA	C1D-C2D	-2.18	1.41	1.45
15	J3	1302	CLA	C1D-ND	2.18	1.40	1.37
15	B1	820	CLA	C3D-C4D	-2.18	1.39	1.44
15	J3	1303	CLA	CAB-C3B	-2.18	1.47	1.51
15	B2	838	CLA	C3D-C4D	-2.17	1.39	1.44
15	L3	1003	CLA	C3D-C4D	-2.17	1.39	1.44
15	A1	819	CLA	C1D-C2D	-2.17	1.41	1.45
15	A3	831	CLA	C1D-C2D	-2.17	1.41	1.45
15	A3	818	CLA	C3D-C4D	-2.17	1.39	1.44
15	J1	1303	CLA	CAB-C3B	-2.17	1.47	1.51
15	A2	804	CLA	C1D-ND	2.17	1.40	1.37
15	J2	1303	CLA	C1D-C2D	-2.17	1.41	1.45
15	A1	831	CLA	C1D-C2D	-2.17	1.41	1.45
15	A1	832	CLA	C1D-C2D	-2.17	1.41	1.45
15	B1	809	CLA	C3D-C4D	-2.17	1.39	1.44
15	A1	836	CLA	C3D-C4D	-2.17	1.39	1.44
15	B3	808	CLA	C3D-C4D	-2.17	1.39	1.44
15	B1	838	CLA	C1D-ND	2.17	1.40	1.37
15	A3	819	CLA	C1D-C2D	-2.17	1.41	1.45
15	A3	832	CLA	C1D-C2D	-2.17	1.41	1.45
15	B2	820	CLA	C3D-C4D	-2.17	1.39	1.44
15	A2	828	CLA	C1D-ND	2.17	1.40	1.37
15	L1	1003	CLA	C3D-C4D	-2.17	1.39	1.44
15	A3	823	CLA	C3D-C4D	-2.17	1.39	1.44
15	A2	822	CLA	C1D-C2D	-2.17	1.41	1.45
15	B3	810	CLA	C1D-C2D	-2.17	1.41	1.45
15	B3	830	CLA	C1D-C2D	-2.17	1.41	1.45
15	A1	828	CLA	C1D-ND	2.17	1.40	1.37
15	A1	832	CLA	C3D-C4D	-2.17	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A1	822	CLA	C1D-C2D	-2.16	1.41	1.45
15	A3	822	CLA	C1D-C2D	-2.16	1.41	1.45
15	B1	838	CLA	C3D-C4D	-2.16	1.39	1.44
15	B2	810	CLA	C1D-C2D	-2.16	1.41	1.45
15	A3	828	CLA	C1D-ND	2.16	1.40	1.37
15	A2	819	CLA	C1D-C2D	-2.16	1.41	1.45
15	B2	820	CLA	C1D-C2D	-2.16	1.41	1.45
15	A2	820	CLA	C1D-C2D	-2.16	1.41	1.45
15	A2	832	CLA	C1D-C2D	-2.16	1.41	1.45
15	J2	1303	CLA	CAB-C3B	-2.16	1.47	1.51
15	J1	1302	CLA	C1D-C2D	-2.16	1.41	1.45
15	B3	838	CLA	C3D-C4D	-2.16	1.39	1.44
15	L2	1003	CLA	C3D-C4D	-2.16	1.39	1.44
15	B1	810	CLA	C1D-C2D	-2.16	1.41	1.45
15	K2	103	CLA	C1D-C2D	-2.16	1.41	1.45
15	J2	1302	CLA	C1D-C2D	-2.16	1.41	1.45
15	A2	816	CLA	C1D-C2D	-2.16	1.41	1.45
15	A1	827	CLA	C3D-C4D	-2.16	1.39	1.44
15	A2	837	CLA	C3D-C4D	-2.16	1.39	1.44
15	B1	830	CLA	C1D-C2D	-2.16	1.41	1.45
15	A2	814	CLA	C3B-C2B	-2.16	1.34	1.41
15	B2	817	CLA	C1D-ND	2.16	1.40	1.37
15	A2	832	CLA	C3D-C4D	-2.16	1.39	1.44
15	B2	833	CLA	C1D-C2D	-2.16	1.41	1.45
15	A1	837	CLA	C3D-C4D	-2.16	1.39	1.44
15	A1	816	CLA	C1D-C2D	-2.16	1.41	1.45
15	J3	1307	CLA	C1D-C2D	-2.16	1.41	1.45
15	A2	836	CLA	C1D-C2D	-2.16	1.41	1.45
15	A3	837	CLA	C3D-C4D	-2.16	1.39	1.44
15	J2	1303	CLA	C3B-C2B	-2.15	1.34	1.41
15	B2	807	CLA	C1D-C2D	-2.15	1.41	1.45
15	B1	828	CLA	C3D-C4D	-2.15	1.39	1.44
15	A2	815	CLA	C4B-CHC	-2.15	1.39	1.43
15	A1	815	CLA	C4B-CHC	-2.15	1.39	1.43
15	B3	820	CLA	C3D-C4D	-2.15	1.39	1.44
15	B1	807	CLA	C1D-C2D	-2.15	1.41	1.45
15	B2	809	CLA	C3D-C4D	-2.15	1.39	1.44
15	A3	828	CLA	C3D-C4D	-2.15	1.39	1.44
15	B2	838	CLA	C1D-ND	2.15	1.40	1.37
15	J1	1303	CLA	C3B-C2B	-2.15	1.34	1.41
15	A3	816	CLA	C1D-C2D	-2.15	1.41	1.45
15	A2	807	CLA	C1D-C2D	-2.15	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B2	830	CLA	C1D-C2D	-2.15	1.41	1.45
15	J3	1302	CLA	C1D-C2D	-2.15	1.41	1.45
15	B3	828	CLA	C3D-C4D	-2.15	1.39	1.44
15	A1	836	CLA	C1D-C2D	-2.15	1.41	1.45
15	B3	820	CLA	C1D-C2D	-2.15	1.41	1.45
15	A2	839	CLA	C1D-ND	2.15	1.40	1.37
15	A3	827	CLA	C3D-C4D	-2.15	1.39	1.44
15	B3	824	CLA	C1D-ND	2.15	1.40	1.37
15	A3	815	CLA	C4B-CHC	-2.15	1.39	1.43
15	B1	820	CLA	C1D-C2D	-2.15	1.41	1.45
15	B3	807	CLA	C1D-C2D	-2.15	1.41	1.45
15	A1	810	CLA	C3D-C4D	-2.15	1.39	1.44
15	A1	814	CLA	C3D-C4D	-2.15	1.39	1.44
15	B3	830	CLA	C3D-C4D	-2.15	1.39	1.44
15	A3	836	CLA	C3D-C4D	-2.14	1.39	1.44
15	A3	840	CLA	C3D-C4D	-2.14	1.39	1.44
15	A1	804	CLA	C1D-ND	2.14	1.40	1.37
15	A1	807	CLA	C1D-C2D	-2.14	1.41	1.45
15	A2	831	CLA	C3D-C4D	-2.14	1.39	1.44
15	A3	810	CLA	C3D-C4D	-2.14	1.39	1.44
15	A3	822	CLA	C3D-C4D	-2.14	1.39	1.44
15	B2	837	CLA	C3D-C4D	-2.14	1.39	1.44
15	A3	826	CLA	C3D-C4D	-2.14	1.39	1.44
15	A3	832	CLA	C3D-C4D	-2.14	1.39	1.44
15	A3	811	CLA	C1D-ND	2.14	1.40	1.37
15	A3	839	CLA	C1D-ND	2.14	1.40	1.37
15	A1	814	CLA	C3B-C2B	-2.14	1.34	1.41
15	A1	802	CLA	C1D-C2D	-2.14	1.41	1.45
15	A3	842	CLA	C3D-C4D	-2.14	1.39	1.44
15	B1	808	CLA	C3D-C4D	-2.14	1.39	1.44
15	A2	812	CLA	C3D-C4D	-2.14	1.39	1.44
15	A3	814	CLA	C3D-C4D	-2.14	1.39	1.44
15	A2	802	CLA	C3D-C4D	-2.14	1.39	1.44
15	A2	842	CLA	C3D-C4D	-2.14	1.39	1.44
15	A3	821	CLA	C3D-C4D	-2.14	1.39	1.44
15	A1	842	CLA	C3D-C4D	-2.14	1.39	1.44
15	A2	805	CLA	C3D-C4D	-2.14	1.39	1.44
15	A1	826	CLA	C3D-C4D	-2.14	1.39	1.44
15	A2	836	CLA	C3D-C4D	-2.14	1.39	1.44
15	B3	836	CLA	C1D-C2D	-2.14	1.41	1.45
15	B1	807	CLA	C3D-C4D	-2.14	1.39	1.44
15	B2	836	CLA	C1D-C2D	-2.14	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A3	836	CLA	C1D-C2D	-2.14	1.41	1.45
15	B3	822	CLA	C3D-C4D	-2.14	1.39	1.44
15	A1	812	CLA	C3D-C4D	-2.14	1.39	1.44
15	B1	837	CLA	C3D-C4D	-2.14	1.39	1.44
15	B3	837	CLA	C3D-C4D	-2.14	1.39	1.44
15	A2	803	CLA	C3D-C4D	-2.14	1.39	1.44
15	A2	817	CLA	C3D-C4D	-2.14	1.39	1.44
15	B3	802	CLA	C3D-C4D	-2.14	1.39	1.44
15	B1	822	CLA	C3D-C4D	-2.14	1.39	1.44
15	A2	820	CLA	C3D-C4D	-2.14	1.39	1.44
15	A2	826	CLA	C3D-C4D	-2.14	1.39	1.44
15	A1	828	CLA	C3D-C4D	-2.14	1.39	1.44
15	B1	830	CLA	C3D-C4D	-2.14	1.39	1.44
15	B2	808	CLA	C3D-C4D	-2.14	1.39	1.44
15	A1	822	CLA	C3D-C4D	-2.13	1.39	1.44
15	B2	828	CLA	C3D-C4D	-2.13	1.39	1.44
15	A3	831	CLA	C3D-C4D	-2.13	1.39	1.44
15	K1	103	CLA	C1D-C2D	-2.13	1.41	1.45
15	B1	824	CLA	C1D-ND	2.13	1.40	1.37
15	A1	831	CLA	C3D-C4D	-2.13	1.39	1.44
15	A1	821	CLA	C3D-C4D	-2.13	1.39	1.44
15	A2	814	CLA	C3D-C4D	-2.13	1.39	1.44
15	B1	836	CLA	C1D-C2D	-2.13	1.41	1.45
15	A3	812	CLA	C3D-C4D	-2.13	1.39	1.44
15	A3	817	CLA	C3D-C4D	-2.13	1.39	1.44
15	B3	824	CLA	C3D-C4D	-2.13	1.39	1.44
15	J3	1303	CLA	C3B-C2B	-2.13	1.34	1.41
15	A3	802	CLA	C1D-C2D	-2.13	1.41	1.45
15	A2	828	CLA	C3D-C4D	-2.13	1.39	1.44
15	B3	807	CLA	C3D-C4D	-2.13	1.39	1.44
15	A2	822	CLA	C3D-C4D	-2.13	1.39	1.44
15	A3	814	CLA	C3B-C2B	-2.13	1.34	1.41
15	A1	805	CLA	C3D-C4D	-2.13	1.39	1.44
15	B2	829	CLA	C1D-C2D	-2.13	1.41	1.45
15	A1	815	CLA	C3D-C4D	-2.13	1.39	1.44
15	B2	824	CLA	C3D-C4D	-2.13	1.39	1.44
15	A2	831	CLA	C1D-C2D	-2.13	1.41	1.45
15	B2	807	CLA	C3D-C4D	-2.12	1.39	1.44
15	A2	810	CLA	C3D-C4D	-2.12	1.39	1.44
15	B2	822	CLA	C3D-C4D	-2.12	1.39	1.44
15	J1	1307	CLA	C1D-C2D	-2.12	1.41	1.45
15	A3	815	CLA	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B1	824	CLA	C3D-C4D	-2.12	1.39	1.44
15	L1	1004	CLA	C3D-C4D	-2.12	1.39	1.44
15	A3	807	CLA	C1D-C2D	-2.12	1.41	1.45
15	B1	813	CLA	C3D-C4D	-2.12	1.39	1.44
15	A3	820	CLA	C3D-C4D	-2.12	1.39	1.44
15	L2	1004	CLA	C3D-C4D	-2.12	1.39	1.44
15	A1	817	CLA	C3D-C4D	-2.12	1.39	1.44
15	K3	103	CLA	C1D-C2D	-2.12	1.41	1.45
15	A1	834	CLA	C3D-C4D	-2.12	1.39	1.44
15	A1	840	CLA	C3D-C4D	-2.12	1.39	1.44
15	B1	829	CLA	C1D-C2D	-2.12	1.41	1.45
15	A2	815	CLA	C3D-C4D	-2.12	1.39	1.44
15	A1	814	CLA	C1D-C2D	-2.12	1.41	1.45
15	A1	835	CLA	C3D-C4D	-2.12	1.39	1.44
15	J2	1303	CLA	C3D-C4D	-2.12	1.39	1.44
15	B3	813	CLA	C3D-C4D	-2.12	1.39	1.44
15	B2	813	CLA	C3D-C4D	-2.12	1.39	1.44
15	L3	1004	CLA	C3D-C4D	-2.12	1.39	1.44
15	A2	834	CLA	C3D-C4D	-2.11	1.39	1.44
15	A3	839	CLA	C3D-C4D	-2.11	1.39	1.44
15	B3	835	CLA	C3D-C4D	-2.11	1.39	1.44
15	A2	821	CLA	C3D-C4D	-2.11	1.39	1.44
15	A1	841	CLA	C3D-C4D	-2.11	1.39	1.44
15	A1	803	CLA	C3D-C4D	-2.11	1.39	1.44
15	A3	808	CLA	C3D-C4D	-2.11	1.39	1.44
15	A3	819	CLA	C1D-ND	2.11	1.40	1.37
15	B2	809	CLA	C1D-ND	2.11	1.40	1.37
15	A3	814	CLA	C1D-C2D	-2.11	1.41	1.45
15	B1	833	CLA	C3D-C4D	-2.11	1.39	1.44
15	A2	841	CLA	C3D-C4D	-2.11	1.39	1.44
15	B3	814	CLA	C3D-C4D	-2.11	1.39	1.44
15	A1	820	CLA	C3D-C4D	-2.11	1.39	1.44
15	A3	807	CLA	C3D-C4D	-2.11	1.39	1.44
15	B1	835	CLA	C3D-C4D	-2.10	1.39	1.44
15	A2	808	CLA	C3D-C4D	-2.10	1.39	1.44
15	A2	839	CLA	C3D-C4D	-2.10	1.39	1.44
15	A1	839	CLA	C3D-C4D	-2.10	1.39	1.44
15	A3	834	CLA	C3D-C4D	-2.10	1.39	1.44
15	A1	829	CLA	C3D-C4D	-2.10	1.39	1.44
15	B2	835	CLA	C3D-C4D	-2.10	1.39	1.44
15	A3	805	CLA	C3D-C4D	-2.10	1.39	1.44
15	A2	809	CLA	C3D-C4D	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A1	819	CLA	C1D-ND	2.10	1.40	1.37
15	B2	827	CLA	C3D-C4D	-2.10	1.39	1.44
15	A3	833	CLA	C1D-ND	2.10	1.40	1.37
15	A1	839	CLA	C1D-ND	2.10	1.40	1.37
15	A2	816	CLA	C3D-C4D	-2.10	1.39	1.44
15	A2	814	CLA	C1D-C2D	-2.10	1.41	1.45
15	A1	802	CLA	C3D-C4D	-2.10	1.39	1.44
15	A2	835	CLA	C3D-C4D	-2.10	1.39	1.44
15	J2	1307	CLA	C1D-C2D	-2.10	1.41	1.45
15	B2	833	CLA	C3D-C4D	-2.10	1.39	1.44
15	A1	816	CLA	C3D-C4D	-2.10	1.39	1.44
15	B3	801	CLA	C3D-C4D	-2.10	1.39	1.44
15	A2	807	CLA	C3D-C4D	-2.10	1.39	1.44
15	B2	814	CLA	C3D-C4D	-2.09	1.39	1.44
15	A1	833	CLA	C3D-C4D	-2.09	1.39	1.44
15	A1	808	CLA	C3D-C4D	-2.09	1.39	1.44
15	B3	827	CLA	C3D-C4D	-2.09	1.39	1.44
15	A1	807	CLA	C3D-C4D	-2.09	1.39	1.44
15	B3	849	CLA	C3D-C4D	-2.09	1.39	1.44
15	B3	829	CLA	C1D-C2D	-2.09	1.41	1.45
15	A3	841	CLA	C3D-C4D	-2.09	1.39	1.44
15	J1	1303	CLA	C3D-C4D	-2.09	1.39	1.44
15	B2	830	CLA	C3D-C4D	-2.09	1.39	1.44
15	A1	838	CLA	C3D-C4D	-2.09	1.39	1.44
15	A3	835	CLA	C3D-C4D	-2.09	1.39	1.44
15	B1	839	CLA	C3D-C4D	-2.09	1.39	1.44
15	A2	829	CLA	C3D-C4D	-2.09	1.39	1.44
15	B2	839	CLA	C3D-C4D	-2.09	1.39	1.44
15	B3	839	CLA	C3D-C4D	-2.09	1.39	1.44
15	J3	1303	CLA	C3D-C4D	-2.09	1.39	1.44
15	A2	840	CLA	C3D-C4D	-2.09	1.39	1.44
15	A2	838	CLA	C3D-C4D	-2.09	1.39	1.44
15	B1	809	CLA	C1D-ND	2.09	1.40	1.37
15	A2	819	CLA	C1D-ND	2.09	1.40	1.37
15	A3	843	CLA	C1D-ND	2.09	1.40	1.37
15	B1	814	CLA	C3D-C4D	-2.09	1.39	1.44
15	A3	803	CLA	C3D-C4D	-2.09	1.39	1.44
15	A3	809	CLA	C3D-C4D	-2.09	1.39	1.44
15	A1	809	CLA	C3D-C4D	-2.08	1.39	1.44
15	B1	801	CLA	C3D-C4D	-2.08	1.39	1.44
15	B2	826	CLA	C3D-C4D	-2.08	1.39	1.44
15	A3	838	CLA	C3D-C4D	-2.08	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	815	CLA	C3D-C4D	-2.08	1.39	1.44
15	B3	833	CLA	C3D-C4D	-2.08	1.39	1.44
15	B1	849	CLA	C3D-C4D	-2.08	1.39	1.44
15	A2	833	CLA	C3D-C4D	-2.08	1.39	1.44
15	A2	806	CLA	C3D-C4D	-2.08	1.39	1.44
15	B2	819	CLA	C3D-C4D	-2.08	1.39	1.44
15	B2	817	CLA	C3D-C4D	-2.08	1.39	1.44
15	A3	842	CLA	C1D-ND	2.08	1.40	1.37
15	A3	816	CLA	C3D-C4D	-2.08	1.39	1.44
15	B1	827	CLA	C3D-C4D	-2.08	1.39	1.44
15	A3	833	CLA	C3D-C4D	-2.08	1.39	1.44
15	B3	837	CLA	C1D-C2D	-2.08	1.41	1.45
15	A2	830	CLA	C3D-C4D	-2.08	1.39	1.44
15	A2	833	CLA	C1D-ND	2.08	1.40	1.37
15	B1	815	CLA	C3D-C4D	-2.08	1.39	1.44
15	B1	819	CLA	C3D-C4D	-2.08	1.39	1.44
15	A1	830	CLA	C3D-C4D	-2.08	1.39	1.44
15	A1	833	CLA	C1D-ND	2.07	1.40	1.37
15	J3	1302	CLA	C3D-C4D	-2.07	1.39	1.44
15	A1	824	CLA	C3D-C4D	-2.07	1.39	1.44
15	A3	802	CLA	C3D-C4D	-2.07	1.39	1.44
15	B3	809	CLA	C1D-ND	2.07	1.40	1.37
15	B2	837	CLA	C1D-C2D	-2.07	1.41	1.45
15	A1	811	CLA	C3D-C4D	-2.07	1.39	1.44
15	B2	831	CLA	C3D-C4D	-2.07	1.39	1.44
15	B1	837	CLA	C1D-C2D	-2.07	1.41	1.45
15	B2	804	CLA	C3D-C4D	-2.07	1.39	1.44
15	B2	815	CLA	C3D-C4D	-2.07	1.39	1.44
15	A3	830	CLA	C3D-C4D	-2.07	1.39	1.44
15	A3	824	CLA	C3D-C4D	-2.07	1.39	1.44
15	B3	806	CLA	C3D-C4D	-2.07	1.39	1.44
15	A3	829	CLA	C3D-C4D	-2.07	1.39	1.44
15	A1	806	CLA	C3D-C4D	-2.07	1.39	1.44
15	A2	811	CLA	C3D-C4D	-2.07	1.39	1.44
15	A1	844	CLA	C3D-C4D	-2.07	1.39	1.44
15	A1	804	CLA	C3D-C4D	-2.07	1.39	1.44
15	A2	824	CLA	C3D-C4D	-2.07	1.39	1.44
15	B3	831	CLA	C3D-C4D	-2.07	1.39	1.44
15	J2	1302	CLA	C3D-C4D	-2.06	1.39	1.44
15	B2	814	CLA	C1D-ND	2.06	1.40	1.37
15	B2	801	CLA	C3D-C4D	-2.06	1.39	1.44
15	A3	806	CLA	C3D-C4D	-2.06	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A3	811	CLA	C3D-C4D	-2.06	1.39	1.44
15	B3	804	CLA	C3D-C4D	-2.06	1.39	1.44
15	A2	844	CLA	C3D-C4D	-2.06	1.39	1.44
15	B3	814	CLA	C1D-ND	2.06	1.40	1.37
15	B3	826	CLA	C3D-C4D	-2.06	1.39	1.44
15	B1	806	CLA	C3D-C4D	-2.06	1.39	1.44
15	B1	814	CLA	C1D-ND	2.06	1.40	1.37
15	A2	843	CLA	C1D-ND	2.06	1.40	1.37
15	B1	804	CLA	C3D-C4D	-2.06	1.39	1.44
15	B1	831	CLA	C3D-C4D	-2.06	1.39	1.44
15	A1	813	CLA	C3D-C4D	-2.06	1.39	1.44
15	B3	810	CLA	C3D-C4D	-2.06	1.39	1.44
15	J1	1302	CLA	C3D-C4D	-2.06	1.39	1.44
15	B1	826	CLA	C3D-C4D	-2.06	1.39	1.44
15	A3	813	CLA	C3D-C4D	-2.06	1.39	1.44
15	J1	1307	CLA	C3D-C4D	-2.05	1.39	1.44
15	B2	806	CLA	C3D-C4D	-2.05	1.39	1.44
15	B2	849	CLA	C3D-C4D	-2.05	1.39	1.44
15	A3	844	CLA	C3D-C4D	-2.05	1.39	1.44
15	B2	803	CLA	C3D-C4D	-2.05	1.39	1.44
15	B3	825	CLA	C3D-C4D	-2.05	1.39	1.44
15	B3	818	CLA	C3D-C4D	-2.05	1.39	1.44
15	A3	804	CLA	C3D-C4D	-2.05	1.39	1.44
15	B1	817	CLA	C3D-C4D	-2.05	1.39	1.44
15	A2	804	CLA	C3D-C4D	-2.05	1.39	1.44
15	A2	856	CLA	C3D-C4D	-2.05	1.39	1.44
15	B3	819	CLA	C3D-C4D	-2.05	1.39	1.44
15	A1	818	CLA	C1D-ND	2.05	1.40	1.37
15	B2	839	CLA	C1D-ND	2.05	1.40	1.37
15	B1	805	CLA	C3D-C4D	-2.05	1.39	1.44
15	B1	810	CLA	C3D-C4D	-2.05	1.39	1.44
15	L2	1002	CLA	C3D-C4D	-2.05	1.39	1.44
15	B3	832	CLA	C3D-C4D	-2.05	1.39	1.44
15	K2	103	CLA	C3D-C4D	-2.05	1.39	1.44
15	A3	843	CLA	C3D-C4D	-2.04	1.39	1.44
15	A1	856	CLA	C3D-C4D	-2.04	1.39	1.44
15	X1	102	CLA	C3D-C4D	-2.04	1.39	1.44
15	A2	813	CLA	C3D-C4D	-2.04	1.39	1.44
15	B1	839	CLA	C1D-ND	2.04	1.40	1.37
15	B2	805	CLA	C3D-C4D	-2.04	1.39	1.44
15	J3	1307	CLA	C3D-C4D	-2.04	1.39	1.44
15	B1	818	CLA	C3D-C4D	-2.04	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B3	839	CLA	C1D-ND	2.04	1.40	1.37
15	K1	103	CLA	C3D-C4D	-2.04	1.39	1.44
15	B2	818	CLA	C3D-C4D	-2.04	1.39	1.44
15	A2	842	CLA	C1D-ND	2.04	1.40	1.37
15	B3	803	CLA	C1D-ND	2.04	1.40	1.37
15	B1	803	CLA	C3D-C4D	-2.04	1.39	1.44
15	K3	103	CLA	C3D-C4D	-2.04	1.39	1.44
15	B3	805	CLA	C3D-C4D	-2.04	1.39	1.44
15	B2	823	CLA	C3D-C4D	-2.04	1.39	1.44
15	J2	1301	CLA	C3D-C4D	-2.04	1.39	1.44
15	J1	1301	CLA	C3D-C4D	-2.04	1.39	1.44
15	A2	818	CLA	C1D-ND	2.04	1.40	1.37
15	B1	832	CLA	C3D-C4D	-2.04	1.39	1.44
15	X2	102	CLA	C3D-C4D	-2.04	1.39	1.44
15	J3	1301	CLA	C3D-C4D	-2.04	1.39	1.44
15	B1	803	CLA	C1D-ND	2.04	1.40	1.37
15	B1	834	CLA	C3D-C4D	-2.04	1.39	1.44
15	B1	816	CLA	CAD-CBD	-2.04	1.51	1.54
15	A3	818	CLA	C1D-ND	2.04	1.40	1.37
15	B3	803	CLA	C3D-C4D	-2.04	1.39	1.44
15	X3	102	CLA	C3D-C4D	-2.04	1.39	1.44
15	B1	823	CLA	C3D-C4D	-2.03	1.39	1.44
15	I3	101	CLA	C3D-C4D	-2.03	1.39	1.44
15	L1	1002	CLA	C3D-C4D	-2.03	1.39	1.44
15	A1	843	CLA	C1D-ND	2.03	1.40	1.37
15	A2	826	CLA	C1D-ND	2.03	1.40	1.37
15	B1	825	CLA	C3D-C4D	-2.03	1.39	1.44
15	A1	843	CLA	C3D-C4D	-2.03	1.39	1.44
15	A1	826	CLA	C1D-ND	2.03	1.40	1.37
15	A3	856	CLA	C3D-C4D	-2.03	1.39	1.44
15	B3	816	CLA	CAD-CBD	-2.03	1.51	1.54
15	B2	803	CLA	C1D-ND	2.03	1.40	1.37
15	J2	1307	CLA	C3D-C4D	-2.03	1.39	1.44
15	A2	843	CLA	C3D-C4D	-2.03	1.39	1.44
15	A1	842	CLA	C1D-ND	2.03	1.40	1.37
15	B3	834	CLA	C3D-C4D	-2.03	1.39	1.44
15	I2	101	CLA	C3D-C4D	-2.03	1.39	1.44
15	B2	832	CLA	C3D-C4D	-2.02	1.39	1.44
15	B3	817	CLA	C3D-C4D	-2.02	1.39	1.44
15	B2	816	CLA	CAD-CBD	-2.02	1.51	1.54
15	B2	825	CLA	C3D-C4D	-2.02	1.39	1.44
15	B2	810	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B2	836	CLA	C1D-ND	2.02	1.40	1.37
15	B3	836	CLA	C1D-ND	2.02	1.40	1.37
15	L3	1002	CLA	C3D-C4D	-2.02	1.39	1.44
15	B3	823	CLA	C3D-C4D	-2.01	1.39	1.44
15	B2	834	CLA	C3D-C4D	-2.01	1.39	1.44
15	A3	825	CLA	C3D-C4D	-2.00	1.39	1.44
15	I1	101	CLA	C3D-C4D	-2.00	1.39	1.44
15	B1	836	CLA	C1D-ND	2.00	1.40	1.37

All (2818) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	821	CLA	C4A-NA-C1A	-8.08	103.07	106.71
15	B1	821	CLA	C4A-NA-C1A	-8.03	103.10	106.71
15	B2	821	CLA	C4A-NA-C1A	-8.02	103.10	106.71
15	B1	808	CLA	C4A-NA-C1A	-7.61	103.28	106.71
15	B2	808	CLA	C4A-NA-C1A	-7.55	103.31	106.71
15	B3	808	CLA	C4A-NA-C1A	-7.52	103.33	106.71
15	B2	807	CLA	C4A-NA-C1A	-7.20	103.47	106.71
15	B1	807	CLA	C4A-NA-C1A	-7.19	103.47	106.71
15	B3	807	CLA	C4A-NA-C1A	-7.17	103.48	106.71
15	K2	103	CLA	C4A-NA-C1A	-6.45	103.80	106.71
15	K3	103	CLA	C4A-NA-C1A	-6.44	103.81	106.71
15	K1	103	CLA	C4A-NA-C1A	-6.39	103.83	106.71
15	B3	832	CLA	C2A-C3A-C4A	-6.31	99.31	106.26
15	A2	819	CLA	C4A-NA-C1A	-6.30	103.87	106.71
15	A3	819	CLA	C4A-NA-C1A	-6.30	103.87	106.71
15	B2	832	CLA	C2A-C3A-C4A	-6.29	99.33	106.26
15	B1	832	CLA	C2A-C3A-C4A	-6.29	99.33	106.26
15	A1	819	CLA	C4A-NA-C1A	-6.24	103.90	106.71
15	B1	819	CLA	C4A-NA-C1A	-6.15	103.94	106.71
15	A1	815	CLA	C1C-NC-C4C	-6.15	103.94	106.71
15	B3	819	CLA	C4A-NA-C1A	-6.13	103.95	106.71
15	A3	815	CLA	C1C-NC-C4C	-6.13	103.95	106.71
15	A2	815	CLA	C1C-NC-C4C	-6.11	103.96	106.71
15	B2	819	CLA	C4A-NA-C1A	-6.10	103.96	106.71
15	K3	103	CLA	C1C-NC-C4C	-6.10	103.96	106.71
15	A2	831	CLA	C4A-NA-C1A	-6.05	103.98	106.71
15	A2	809	CLA	C4A-NA-C1A	-6.05	103.99	106.71
15	A1	831	CLA	C4A-NA-C1A	-6.04	103.99	106.71
15	K2	103	CLA	C1C-NC-C4C	-6.04	103.99	106.71
15	K1	103	CLA	C1C-NC-C4C	-6.04	103.99	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	831	CLA	C4A-NA-C1A	-6.03	104.00	106.71
15	A2	802	CLA	CHD-C1D-ND	-6.02	118.92	124.45
15	A1	810	CLA	C1C-NC-C4C	-6.01	104.00	106.71
15	A3	810	CLA	C1C-NC-C4C	-6.01	104.00	106.71
15	B1	829	CLA	C4A-NA-C1A	-6.00	104.01	106.71
15	A1	809	CLA	C4A-NA-C1A	-5.99	104.01	106.71
15	A2	810	CLA	C1C-NC-C4C	-5.99	104.01	106.71
15	A3	802	CLA	CHD-C1D-ND	-5.99	118.95	124.45
15	A1	802	CLA	CHD-C1D-ND	-5.98	118.96	124.45
15	B3	829	CLA	C4A-NA-C1A	-5.96	104.03	106.71
15	B2	829	CLA	C4A-NA-C1A	-5.95	104.03	106.71
15	A3	807	CLA	C4A-NA-C1A	-5.93	104.04	106.71
15	A3	814	CLA	C4A-NA-C1A	-5.93	104.04	106.71
15	A1	807	CLA	C4A-NA-C1A	-5.92	104.04	106.71
15	A2	807	CLA	C4A-NA-C1A	-5.92	104.05	106.71
15	A3	809	CLA	C4A-NA-C1A	-5.90	104.05	106.71
15	A3	832	CLA	CHD-C1D-ND	-5.90	119.03	124.45
15	A2	832	CLA	CHD-C1D-ND	-5.89	119.04	124.45
15	B2	832	CLA	C4A-NA-C1A	-5.88	104.06	106.71
15	J2	1307	CLA	C1C-NC-C4C	-5.88	104.06	106.71
15	A1	814	CLA	C4A-NA-C1A	-5.87	104.07	106.71
15	A2	814	CLA	C4A-NA-C1A	-5.87	104.07	106.71
15	A1	832	CLA	CHD-C1D-ND	-5.87	119.06	124.45
15	J3	1307	CLA	C1C-NC-C4C	-5.85	104.07	106.71
15	B3	821	CLA	C2A-C3A-C4A	-5.85	96.89	103.59
15	B2	821	CLA	C2A-C3A-C4A	-5.83	96.91	103.59
15	B3	832	CLA	C4A-NA-C1A	-5.83	104.08	106.71
15	B1	832	CLA	C4A-NA-C1A	-5.83	104.08	106.71
15	B1	821	CLA	C2A-C3A-C4A	-5.83	96.91	103.59
15	B1	807	CLA	CHD-C1D-ND	-5.82	119.11	124.45
15	B2	832	CLA	CHD-C1D-ND	-5.81	119.11	124.45
15	B3	832	CLA	CHD-C1D-ND	-5.81	119.12	124.45
15	B1	832	CLA	CHD-C1D-ND	-5.80	119.12	124.45
15	B3	836	CLA	CHD-C1D-ND	-5.80	119.13	124.45
15	J1	1307	CLA	C1C-NC-C4C	-5.79	104.10	106.71
15	B2	807	CLA	CHD-C1D-ND	-5.79	119.13	124.45
15	B1	836	CLA	CHD-C1D-ND	-5.78	119.14	124.45
15	B3	807	CLA	CHD-C1D-ND	-5.78	119.14	124.45
15	B2	836	CLA	CHD-C1D-ND	-5.78	119.14	124.45
15	B2	802	CLA	CHD-C1D-ND	-5.77	119.15	124.45
15	B1	802	CLA	CHD-C1D-ND	-5.75	119.17	124.45
15	B3	802	CLA	CHD-C1D-ND	-5.74	119.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	836	CLA	CHD-C1D-ND	-5.73	119.19	124.45
15	A2	822	CLA	C4A-NA-C1A	-5.73	104.13	106.71
15	A1	836	CLA	CHD-C1D-ND	-5.72	119.20	124.45
15	A3	836	CLA	CHD-C1D-ND	-5.71	119.21	124.45
15	A1	840	CLA	C4A-NA-C1A	-5.71	104.14	106.71
15	A1	822	CLA	C4A-NA-C1A	-5.69	104.15	106.71
15	A2	840	CLA	C4A-NA-C1A	-5.69	104.15	106.71
15	B2	820	CLA	CHD-C1D-ND	-5.68	119.23	124.45
15	A3	840	CLA	C4A-NA-C1A	-5.68	104.15	106.71
15	B1	820	CLA	CHD-C1D-ND	-5.67	119.24	124.45
15	B3	820	CLA	CHD-C1D-ND	-5.67	119.25	124.45
15	K3	101	CLA	C4A-NA-C1A	-5.66	104.16	106.71
15	A3	856	CLA	CHD-C1D-ND	-5.65	119.26	124.45
15	A1	826	CLA	CHD-C1D-ND	-5.65	119.27	124.45
15	K1	101	CLA	C4A-NA-C1A	-5.65	104.17	106.71
15	K2	103	CLA	CHD-C1D-ND	-5.64	119.27	124.45
15	A3	822	CLA	C4A-NA-C1A	-5.64	104.17	106.71
15	K1	103	CLA	CHD-C1D-ND	-5.64	119.27	124.45
15	B3	815	CLA	CHD-C1D-ND	-5.64	119.27	124.45
15	A2	856	CLA	CHD-C1D-ND	-5.63	119.28	124.45
15	K3	103	CLA	CHD-C1D-ND	-5.63	119.28	124.45
15	A1	856	CLA	CHD-C1D-ND	-5.63	119.28	124.45
15	B1	829	CLA	CHD-C1D-ND	-5.63	119.28	124.45
15	B2	813	CLA	CHD-C1D-ND	-5.63	119.28	124.45
15	B2	849	CLA	CHD-C1D-ND	-5.63	119.28	124.45
15	A2	826	CLA	CHD-C1D-ND	-5.63	119.28	124.45
15	A3	826	CLA	CHD-C1D-ND	-5.62	119.28	124.45
15	B3	837	CLA	CHD-C1D-ND	-5.62	119.28	124.45
15	B2	829	CLA	CHD-C1D-ND	-5.62	119.29	124.45
15	A3	811	CLA	CHD-C1D-ND	-5.62	119.29	124.45
15	B1	849	CLA	CHD-C1D-ND	-5.62	119.29	124.45
15	A2	811	CLA	CHD-C1D-ND	-5.62	119.29	124.45
15	B1	815	CLA	CHD-C1D-ND	-5.61	119.30	124.45
15	B3	829	CLA	CHD-C1D-ND	-5.61	119.30	124.45
15	A1	842	CLA	CHD-C1D-ND	-5.61	119.30	124.45
15	K2	101	CLA	C4A-NA-C1A	-5.61	104.18	106.71
15	A1	818	CLA	CHD-C1D-ND	-5.61	119.30	124.45
15	A2	842	CLA	CHD-C1D-ND	-5.61	119.30	124.45
15	A2	818	CLA	CHD-C1D-ND	-5.60	119.30	124.45
15	B3	809	CLA	CHD-C1D-ND	-5.60	119.31	124.45
15	A3	818	CLA	CHD-C1D-ND	-5.60	119.31	124.45
15	B3	813	CLA	CHD-C1D-ND	-5.60	119.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	816	CLA	CHD-C1D-ND	-5.60	119.31	124.45
15	A1	811	CLA	CHD-C1D-ND	-5.59	119.31	124.45
15	B1	813	CLA	CHD-C1D-ND	-5.59	119.31	124.45
15	B1	816	CLA	CHD-C1D-ND	-5.59	119.31	124.45
15	B2	828	CLA	CHD-C1D-ND	-5.59	119.31	124.45
15	A1	834	CLA	CHD-C1D-ND	-5.59	119.32	124.45
15	A3	839	CLA	CHD-C1D-ND	-5.59	119.32	124.45
15	B1	837	CLA	CHD-C1D-ND	-5.59	119.32	124.45
15	B3	849	CLA	CHD-C1D-ND	-5.59	119.32	124.45
15	A2	839	CLA	CHD-C1D-ND	-5.59	119.32	124.45
15	B2	837	CLA	CHD-C1D-ND	-5.59	119.32	124.45
15	A3	819	CLA	CHD-C1D-ND	-5.58	119.32	124.45
15	A3	842	CLA	CHD-C1D-ND	-5.58	119.32	124.45
15	B2	801	CLA	CHD-C1D-ND	-5.58	119.33	124.45
15	B1	828	CLA	CHD-C1D-ND	-5.58	119.33	124.45
15	B1	833	CLA	CHD-C1D-ND	-5.58	119.33	124.45
15	A1	839	CLA	CHD-C1D-ND	-5.58	119.33	124.45
15	A2	819	CLA	CHD-C1D-ND	-5.58	119.33	124.45
15	A1	819	CLA	CHD-C1D-ND	-5.57	119.33	124.45
15	A1	833	CLA	CHD-C1D-ND	-5.57	119.33	124.45
15	B2	816	CLA	CHD-C1D-ND	-5.57	119.33	124.45
15	B3	828	CLA	CHD-C1D-ND	-5.57	119.33	124.45
15	B2	815	CLA	CHD-C1D-ND	-5.57	119.34	124.45
15	B2	833	CLA	CHD-C1D-ND	-5.57	119.34	124.45
15	J2	1302	CLA	CHD-C1D-ND	-5.57	119.34	124.45
15	L2	1003	CLA	CHD-C1D-ND	-5.57	119.34	124.45
15	B2	809	CLA	CHD-C1D-ND	-5.57	119.34	124.45
15	L1	1003	CLA	CHD-C1D-ND	-5.56	119.34	124.45
15	A2	815	CLA	CHD-C1D-ND	-5.56	119.35	124.45
15	B2	835	CLA	CHD-C1D-ND	-5.56	119.35	124.45
15	A2	833	CLA	CHD-C1D-ND	-5.56	119.35	124.45
15	J1	1302	CLA	CHD-C1D-ND	-5.55	119.35	124.45
15	A3	824	CLA	CHD-C1D-ND	-5.55	119.35	124.45
15	A2	834	CLA	CHD-C1D-ND	-5.55	119.35	124.45
15	B3	833	CLA	CHD-C1D-ND	-5.55	119.35	124.45
15	J3	1302	CLA	CHD-C1D-ND	-5.55	119.36	124.45
15	B1	801	CLA	CHD-C1D-ND	-5.55	119.36	124.45
15	A3	830	CLA	CHD-C1D-ND	-5.55	119.36	124.45
15	B3	830	CLA	CHD-C1D-ND	-5.55	119.36	124.45
15	B1	809	CLA	CHD-C1D-ND	-5.55	119.36	124.45
15	A3	833	CLA	CHD-C1D-ND	-5.55	119.36	124.45
15	A3	834	CLA	CHD-C1D-ND	-5.55	119.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	840	CLA	CHD-C1D-ND	-5.54	119.36	124.45
15	A1	815	CLA	CHD-C1D-ND	-5.54	119.36	124.45
15	B3	835	CLA	CHD-C1D-ND	-5.54	119.36	124.45
15	B1	835	CLA	CHD-C1D-ND	-5.54	119.37	124.45
15	B3	801	CLA	CHD-C1D-ND	-5.54	119.37	124.45
15	A3	815	CLA	CHD-C1D-ND	-5.53	119.38	124.45
15	A3	814	CLA	CHD-C1D-ND	-5.53	119.38	124.45
15	B2	830	CLA	C4A-NA-C1A	-5.53	104.22	106.71
15	L3	1003	CLA	CHD-C1D-ND	-5.52	119.38	124.45
15	A1	831	CLA	CHD-C1D-ND	-5.52	119.38	124.45
15	A3	804	CLA	CHD-C1D-ND	-5.52	119.38	124.45
15	A1	804	CLA	CHD-C1D-ND	-5.52	119.38	124.45
15	B3	817	CLA	CHD-C1D-ND	-5.52	119.38	124.45
15	A3	831	CLA	CHD-C1D-ND	-5.52	119.38	124.45
15	B2	822	CLA	CHD-C1D-ND	-5.51	119.39	124.45
15	B3	831	CLA	CHD-C1D-ND	-5.51	119.39	124.45
15	A3	805	CLA	CHD-C1D-ND	-5.51	119.39	124.45
15	A1	830	CLA	CHD-C1D-ND	-5.51	119.39	124.45
15	B1	830	CLA	CHD-C1D-ND	-5.51	119.39	124.45
15	A2	824	CLA	CHD-C1D-ND	-5.51	119.39	124.45
15	A1	824	CLA	CHD-C1D-ND	-5.50	119.39	124.45
15	A1	814	CLA	CHD-C1D-ND	-5.50	119.40	124.45
15	B3	821	CLA	C3A-C2A-C1A	-5.50	97.06	104.74
15	A1	838	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	A2	804	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	B2	830	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	A3	835	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	A1	840	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	L2	1004	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	B1	817	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	A2	830	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	B1	831	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	A2	831	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	B3	839	CLA	CHD-C1D-ND	-5.49	119.41	124.45
15	A3	840	CLA	CHD-C1D-ND	-5.48	119.41	124.45
15	B1	839	CLA	CHD-C1D-ND	-5.48	119.42	124.45
15	A2	805	CLA	CHD-C1D-ND	-5.48	119.42	124.45
15	A3	827	CLA	CHD-C1D-ND	-5.48	119.42	124.45
15	A2	814	CLA	CHD-C1D-ND	-5.48	119.42	124.45
15	B2	839	CLA	CHD-C1D-ND	-5.48	119.42	124.45
15	B1	830	CLA	C4A-NA-C1A	-5.48	104.24	106.71
15	B1	821	CLA	C3A-C2A-C1A	-5.48	97.10	104.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J2	1307	CLA	C4A-NA-C1A	-5.48	104.24	106.71
15	A2	838	CLA	CHD-C1D-ND	-5.48	119.42	124.45
15	B2	821	CLA	C3A-C2A-C1A	-5.48	97.10	104.74
15	A1	835	CLA	CHD-C1D-ND	-5.48	119.42	124.45
15	A3	838	CLA	CHD-C1D-ND	-5.48	119.42	124.45
15	B3	822	CLA	CHD-C1D-ND	-5.47	119.43	124.45
15	A2	835	CLA	CHD-C1D-ND	-5.47	119.43	124.45
15	B3	805	CLA	CHD-C1D-ND	-5.47	119.43	124.45
15	A2	816	CLA	CHD-C1D-ND	-5.47	119.43	124.45
15	B2	831	CLA	CHD-C1D-ND	-5.47	119.43	124.45
15	A2	807	CLA	CHD-C1D-ND	-5.46	119.43	124.45
15	B3	830	CLA	C4A-NA-C1A	-5.46	104.25	106.71
15	B2	817	CLA	CHD-C1D-ND	-5.46	119.43	124.45
15	J1	1307	CLA	C4A-NA-C1A	-5.46	104.25	106.71
15	A1	827	CLA	CHD-C1D-ND	-5.46	119.44	124.45
15	B2	805	CLA	CHD-C1D-ND	-5.46	119.44	124.45
15	B1	838	CLA	CHD-C1D-ND	-5.46	119.44	124.45
15	A2	827	CLA	CHD-C1D-ND	-5.45	119.44	124.45
15	A2	828	CLA	CHD-C1D-ND	-5.45	119.44	124.45
15	A1	805	CLA	CHD-C1D-ND	-5.45	119.44	124.45
15	A3	807	CLA	CHD-C1D-ND	-5.45	119.45	124.45
15	B1	824	CLA	CHD-C1D-ND	-5.45	119.45	124.45
15	J3	1307	CLA	CHD-C1D-ND	-5.44	119.45	124.45
15	A1	807	CLA	CHD-C1D-ND	-5.44	119.45	124.45
15	B3	838	CLA	CHD-C1D-ND	-5.44	119.45	124.45
15	B1	805	CLA	CHD-C1D-ND	-5.44	119.45	124.45
15	A1	816	CLA	CHD-C1D-ND	-5.44	119.46	124.45
15	J3	1307	CLA	C4A-NA-C1A	-5.44	104.26	106.71
15	A1	828	CLA	CHD-C1D-ND	-5.44	119.46	124.45
15	B3	810	CLA	CHD-C1D-ND	-5.44	119.46	124.45
15	B1	810	CLA	CHD-C1D-ND	-5.43	119.46	124.45
15	B2	824	CLA	CHD-C1D-ND	-5.43	119.46	124.45
15	A3	816	CLA	CHD-C1D-ND	-5.43	119.46	124.45
15	B1	822	CLA	CHD-C1D-ND	-5.43	119.47	124.45
15	J2	1307	CLA	CHD-C1D-ND	-5.43	119.47	124.45
15	B3	824	CLA	CHD-C1D-ND	-5.43	119.47	124.45
15	A3	828	CLA	CHD-C1D-ND	-5.42	119.47	124.45
15	B1	814	CLA	CHD-C1D-ND	-5.42	119.47	124.45
15	J1	1307	CLA	CHD-C1D-ND	-5.42	119.47	124.45
15	L1	1004	CLA	CHD-C1D-ND	-5.42	119.47	124.45
15	L3	1004	CLA	CHD-C1D-ND	-5.42	119.47	124.45
15	B3	814	CLA	CHD-C1D-ND	-5.41	119.48	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J2	1301	CLA	CHD-C1D-ND	-5.41	119.48	124.45
15	B2	814	CLA	CHD-C1D-ND	-5.41	119.48	124.45
15	B2	838	CLA	CHD-C1D-ND	-5.41	119.48	124.45
15	B2	810	CLA	CHD-C1D-ND	-5.41	119.48	124.45
15	A1	803	CLA	CHD-C1D-ND	-5.41	119.48	124.45
15	J1	1301	CLA	CHD-C1D-ND	-5.41	119.48	124.45
15	B2	834	CLA	C4A-NA-C1A	-5.40	104.28	106.71
15	J3	1301	CLA	CHD-C1D-ND	-5.39	119.50	124.45
15	J1	1303	CLA	CHD-C1D-ND	-5.39	119.50	124.45
15	A2	822	CLA	CHD-C1D-ND	-5.39	119.50	124.45
15	A2	803	CLA	CHD-C1D-ND	-5.38	119.51	124.45
15	J3	1303	CLA	CHD-C1D-ND	-5.38	119.51	124.45
15	B1	813	CLA	C4A-NA-C1A	-5.38	104.29	106.71
15	A3	803	CLA	CHD-C1D-ND	-5.38	119.51	124.45
15	A3	808	CLA	CHD-C1D-ND	-5.38	119.51	124.45
15	B3	821	CLA	CHD-C1D-ND	-5.38	119.51	124.45
15	A1	822	CLA	CHD-C1D-ND	-5.38	119.51	124.45
15	B3	813	CLA	C4A-NA-C1A	-5.38	104.29	106.71
15	B2	812	CLA	CHD-C1D-ND	-5.37	119.52	124.45
15	B3	812	CLA	CHD-C1D-ND	-5.37	119.52	124.45
15	A2	810	CLA	CHD-C1D-ND	-5.37	119.52	124.45
15	A1	823	CLA	CHD-C1D-ND	-5.37	119.52	124.45
15	J2	1303	CLA	CHD-C1D-ND	-5.37	119.52	124.45
15	B1	812	CLA	CHD-C1D-ND	-5.37	119.52	124.45
15	B1	821	CLA	CHD-C1D-ND	-5.37	119.52	124.45
15	B2	821	CLA	CHD-C1D-ND	-5.36	119.52	124.45
15	A3	822	CLA	CHD-C1D-ND	-5.36	119.52	124.45
15	A2	808	CLA	CHD-C1D-ND	-5.36	119.53	124.45
15	A3	817	CLA	CHD-C1D-ND	-5.36	119.53	124.45
15	A1	826	CLA	C4A-NA-C1A	-5.36	104.30	106.71
15	A3	812	CLA	CHD-C1D-ND	-5.36	119.53	124.45
15	A1	812	CLA	CHD-C1D-ND	-5.35	119.53	124.45
15	A3	810	CLA	CHD-C1D-ND	-5.35	119.53	124.45
15	A3	817	CLA	C4A-NA-C1A	-5.35	104.30	106.71
15	A1	810	CLA	CHD-C1D-ND	-5.35	119.54	124.45
15	A2	843	CLA	CHD-C1D-ND	-5.35	119.54	124.45
15	B1	804	CLA	CHD-C1D-ND	-5.35	119.54	124.45
15	A3	823	CLA	CHD-C1D-ND	-5.35	119.54	124.45
15	B3	808	CLA	CHD-C1D-ND	-5.35	119.54	124.45
15	A1	817	CLA	CHD-C1D-ND	-5.35	119.54	124.45
15	A2	823	CLA	CHD-C1D-ND	-5.35	119.54	124.45
15	B2	818	CLA	CHD-C1D-ND	-5.34	119.54	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A1	808	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	X1	102	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	X2	102	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	B3	803	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	A1	817	CLA	C4A-NA-C1A	-5.34	104.31	106.71
15	A1	820	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	X3	102	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	B1	818	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	B2	804	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	B3	819	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	A2	820	CLA	CHD-C1D-ND	-5.33	119.55	124.45
15	A3	820	CLA	CHD-C1D-ND	-5.33	119.55	124.45
15	A2	812	CLA	CHD-C1D-ND	-5.33	119.56	124.45
15	B1	819	CLA	CHD-C1D-ND	-5.33	119.56	124.45
15	A3	843	CLA	CHD-C1D-ND	-5.32	119.56	124.45
15	A1	843	CLA	CHD-C1D-ND	-5.32	119.56	124.45
15	B1	803	CLA	CHD-C1D-ND	-5.32	119.56	124.45
15	A2	817	CLA	CHD-C1D-ND	-5.32	119.56	124.45
15	K3	101	CLA	CHD-C1D-ND	-5.32	119.38	124.52
15	B1	808	CLA	CHD-C1D-ND	-5.31	119.57	124.45
15	A3	826	CLA	C4A-NA-C1A	-5.31	104.32	106.71
15	B2	813	CLA	C4A-NA-C1A	-5.30	104.32	106.71
15	B2	819	CLA	CHD-C1D-ND	-5.30	119.58	124.45
15	B2	834	CLA	CHD-C1D-ND	-5.30	119.58	124.45
15	B3	804	CLA	CHD-C1D-ND	-5.30	119.58	124.45
15	A1	809	CLA	CHD-C1D-ND	-5.30	119.58	124.45
15	B1	834	CLA	CHD-C1D-ND	-5.30	119.58	124.45
15	K1	101	CLA	CHD-C1D-ND	-5.30	119.40	124.52
15	B3	826	CLA	CHD-C1D-ND	-5.30	119.59	124.45
15	B1	834	CLA	C4A-NA-C1A	-5.30	104.33	106.71
15	A2	817	CLA	C4A-NA-C1A	-5.30	104.33	106.71
15	K2	101	CLA	CHD-C1D-ND	-5.29	119.40	124.52
15	B3	824	CLA	C4A-NA-C1A	-5.29	104.33	106.71
15	B2	803	CLA	CHD-C1D-ND	-5.29	119.60	124.45
15	B3	834	CLA	C4A-NA-C1A	-5.28	104.33	106.71
15	B1	826	CLA	CHD-C1D-ND	-5.28	119.61	124.45
15	B3	818	CLA	CHD-C1D-ND	-5.27	119.61	124.45
15	B2	808	CLA	CHD-C1D-ND	-5.27	119.61	124.45
15	A2	826	CLA	C4A-NA-C1A	-5.27	104.34	106.71
15	B3	834	CLA	CHD-C1D-ND	-5.27	119.61	124.45
15	B3	806	CLA	CHD-C1D-ND	-5.26	119.62	124.45
15	B2	826	CLA	CHD-C1D-ND	-5.26	119.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	809	CLA	CHD-C1D-ND	-5.26	119.62	124.45
15	A2	809	CLA	CHD-C1D-ND	-5.26	119.62	124.45
15	I2	101	CLA	CHD-C1D-ND	-5.26	119.62	124.45
15	I3	101	CLA	CHD-C1D-ND	-5.24	119.64	124.45
15	I1	101	CLA	CHD-C1D-ND	-5.24	119.64	124.45
15	B2	824	CLA	C4A-NA-C1A	-5.23	104.35	106.71
15	A2	810	CLA	C4A-NA-C1A	-5.22	104.36	106.71
15	A3	829	CLA	CHD-C1D-ND	-5.22	119.66	124.45
15	A1	813	CLA	CHD-C1D-ND	-5.22	119.66	124.45
15	B1	824	CLA	C4A-NA-C1A	-5.22	104.36	106.71
15	A2	829	CLA	CHD-C1D-ND	-5.21	119.66	124.45
15	B1	806	CLA	CHD-C1D-ND	-5.21	119.66	124.45
15	A2	813	CLA	CHD-C1D-ND	-5.21	119.66	124.45
15	A3	828	CLA	C4A-NA-C1A	-5.21	104.36	106.71
15	L3	1002	CLA	CHD-C1D-ND	-5.21	119.67	124.45
15	A3	813	CLA	CHD-C1D-ND	-5.21	119.67	124.45
15	A1	828	CLA	C4A-NA-C1A	-5.20	104.37	106.71
15	A2	828	CLA	C4A-NA-C1A	-5.20	104.37	106.71
15	A1	829	CLA	CHD-C1D-ND	-5.19	119.68	124.45
15	A1	810	CLA	C4A-NA-C1A	-5.19	104.37	106.71
15	L1	1002	CLA	CHD-C1D-ND	-5.19	119.69	124.45
15	B2	806	CLA	CHD-C1D-ND	-5.18	119.69	124.45
15	A2	806	CLA	CHD-C1D-ND	-5.18	119.69	124.45
15	B3	811	CLA	CHD-C1D-ND	-5.18	119.69	124.45
15	A1	806	CLA	CHD-C1D-ND	-5.18	119.70	124.45
15	A2	803	CLA	C4A-NA-C1A	-5.17	104.38	106.71
15	B1	811	CLA	CHD-C1D-ND	-5.17	119.71	124.45
15	A3	811	CLA	C4A-NA-C1A	-5.16	104.38	106.71
15	A1	841	CLA	CHD-C1D-ND	-5.16	119.71	124.45
15	L2	1002	CLA	CHD-C1D-ND	-5.16	119.71	124.45
15	A3	806	CLA	CHD-C1D-ND	-5.16	119.71	124.45
15	A1	821	CLA	CHD-C1D-ND	-5.15	119.72	124.45
15	A2	811	CLA	C4A-NA-C1A	-5.15	104.39	106.71
15	A3	841	CLA	CHD-C1D-ND	-5.14	119.73	124.45
15	A3	821	CLA	CHD-C1D-ND	-5.14	119.73	124.45
15	A1	811	CLA	C4A-NA-C1A	-5.14	104.39	106.71
15	A2	821	CLA	CHD-C1D-ND	-5.13	119.74	124.45
15	A1	837	CLA	CHD-C1D-ND	-5.12	119.75	124.45
15	A2	844	CLA	CHD-C1D-ND	-5.12	119.75	124.45
15	A2	841	CLA	CHD-C1D-ND	-5.12	119.75	124.45
15	B2	811	CLA	CHD-C1D-ND	-5.12	119.75	124.45
15	A1	803	CLA	C4A-NA-C1A	-5.11	104.41	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	837	CLA	CHD-C1D-ND	-5.11	119.76	124.45
15	B3	827	CLA	CHD-C1D-ND	-5.11	119.76	124.45
15	B3	820	CLA	C4A-NA-C1A	-5.10	104.41	106.71
15	A3	837	CLA	CHD-C1D-ND	-5.10	119.77	124.45
15	A3	810	CLA	C4A-NA-C1A	-5.09	104.42	106.71
15	B2	827	CLA	CHD-C1D-ND	-5.08	119.78	124.45
15	A3	816	CLA	C4A-NA-C1A	-5.08	104.42	106.71
15	A1	844	CLA	CHD-C1D-ND	-5.08	119.79	124.45
15	A3	844	CLA	CHD-C1D-ND	-5.08	119.79	124.45
15	A2	816	CLA	C4A-NA-C1A	-5.07	104.43	106.71
15	B1	827	CLA	CHD-C1D-ND	-5.07	119.80	124.45
15	B2	825	CLA	CHD-C1D-ND	-5.06	119.81	124.45
15	B1	825	CLA	CHD-C1D-ND	-5.05	119.81	124.45
15	B2	823	CLA	CHD-C1D-ND	-5.04	119.82	124.45
15	B2	820	CLA	C4A-NA-C1A	-5.04	104.44	106.71
15	B3	823	CLA	CHD-C1D-ND	-5.03	119.83	124.45
15	A3	825	CLA	CHD-C1D-ND	-5.03	119.83	124.45
15	B1	802	CLA	C4A-NA-C1A	-5.03	104.45	106.71
15	B1	820	CLA	C4A-NA-C1A	-5.03	104.45	106.71
15	B1	823	CLA	CHD-C1D-ND	-5.03	119.83	124.45
15	B3	802	CLA	C4A-NA-C1A	-5.02	104.45	106.71
15	A3	803	CLA	C4A-NA-C1A	-5.02	104.45	106.71
15	B1	833	CLA	C4A-NA-C1A	-5.01	104.45	106.71
15	B2	802	CLA	C4A-NA-C1A	-5.01	104.45	106.71
15	A2	825	CLA	CHD-C1D-ND	-5.01	119.85	124.45
15	B3	825	CLA	CHD-C1D-ND	-5.01	119.85	124.45
15	A1	825	CLA	CHD-C1D-ND	-4.99	119.87	124.45
15	A1	816	CLA	C4A-NA-C1A	-4.98	104.47	106.71
15	B3	833	CLA	C4A-NA-C1A	-4.96	104.48	106.71
15	B2	833	CLA	C4A-NA-C1A	-4.95	104.48	106.71
15	B3	815	CLA	C4A-NA-C1A	-4.95	104.48	106.71
15	A1	823	CLA	C4A-NA-C1A	-4.91	104.50	106.71
15	B1	815	CLA	C4A-NA-C1A	-4.90	104.50	106.71
15	A1	819	CLA	CAA-C2A-C1A	-4.90	95.92	111.97
15	A2	815	CLA	C4A-NA-C1A	-4.90	104.50	106.71
15	A3	819	CLA	CAA-C2A-C1A	-4.90	95.93	111.97
15	A2	819	CLA	CAA-C2A-C1A	-4.89	95.94	111.97
15	B1	816	CLA	C4A-NA-C1A	-4.89	104.51	106.71
15	B2	816	CLA	C4A-NA-C1A	-4.89	104.51	106.71
15	B2	815	CLA	C4A-NA-C1A	-4.89	104.51	106.71
15	A3	804	CLA	C4A-NA-C1A	-4.89	104.51	106.71
15	A2	823	CLA	C4A-NA-C1A	-4.88	104.51	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	823	CLA	C4A-NA-C1A	-4.88	104.51	106.71
15	A1	804	CLA	C4A-NA-C1A	-4.87	104.52	106.71
15	A2	804	CLA	C4A-NA-C1A	-4.87	104.52	106.71
15	B3	816	CLA	C4A-NA-C1A	-4.87	104.52	106.71
15	A2	812	CLA	C4A-NA-C1A	-4.86	104.52	106.71
15	A1	812	CLA	C4A-NA-C1A	-4.86	104.52	106.71
15	A3	812	CLA	C4A-NA-C1A	-4.86	104.52	106.71
15	A1	815	CLA	C4A-NA-C1A	-4.84	104.53	106.71
15	B3	837	CLA	C4A-NA-C1A	-4.83	104.54	106.71
15	A2	802	CLA	C4A-NA-C1A	-4.82	104.54	106.71
15	A2	827	CLA	C4A-NA-C1A	-4.80	104.55	106.71
15	A3	802	CLA	C4A-NA-C1A	-4.80	104.55	106.71
15	A1	802	CLA	C4A-NA-C1A	-4.79	104.55	106.71
15	A2	820	CLA	C4A-NA-C1A	-4.78	104.56	106.71
15	B2	837	CLA	C4A-NA-C1A	-4.78	104.56	106.71
15	B1	837	CLA	C4A-NA-C1A	-4.78	104.56	106.71
15	A1	827	CLA	C4A-NA-C1A	-4.77	104.56	106.71
15	A3	827	CLA	C4A-NA-C1A	-4.77	104.56	106.71
15	A3	820	CLA	C4A-NA-C1A	-4.75	104.57	106.71
15	A3	815	CLA	C4A-NA-C1A	-4.74	104.58	106.71
15	A1	820	CLA	C4A-NA-C1A	-4.73	104.58	106.71
15	B1	828	CLA	C4A-NA-C1A	-4.68	104.60	106.71
15	J3	1303	CLA	C4A-NA-C1A	-4.65	104.62	106.71
15	B2	828	CLA	C4A-NA-C1A	-4.62	104.63	106.71
15	B3	828	CLA	C4A-NA-C1A	-4.60	104.64	106.71
15	J2	1303	CLA	C4A-NA-C1A	-4.58	104.65	106.71
14	A3	801	CL0	C4A-NA-C1A	-4.56	104.65	106.71
15	J1	1303	CLA	C4A-NA-C1A	-4.56	104.66	106.71
14	A1	801	CL0	C4A-NA-C1A	-4.52	104.67	106.71
15	A2	805	CLA	C4A-NA-C1A	-4.50	104.68	106.71
15	A1	805	CLA	C4A-NA-C1A	-4.50	104.69	106.71
15	A3	805	CLA	C4A-NA-C1A	-4.50	104.69	106.71
15	B2	835	CLA	C4A-NA-C1A	-4.48	104.69	106.71
14	A2	801	CL0	C4A-NA-C1A	-4.47	104.70	106.71
15	B1	835	CLA	C4A-NA-C1A	-4.46	104.70	106.71
15	A2	836	CLA	C4A-NA-C1A	-4.42	104.72	106.71
15	A1	836	CLA	C4A-NA-C1A	-4.41	104.72	106.71
15	A3	836	CLA	C4A-NA-C1A	-4.40	104.73	106.71
15	B3	827	CLA	C4A-NA-C1A	-4.40	104.73	106.71
15	B2	827	CLA	C4A-NA-C1A	-4.40	104.73	106.71
15	B3	835	CLA	C4A-NA-C1A	-4.38	104.74	106.71
15	B1	836	CLA	C4A-NA-C1A	-4.37	104.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	810	CLA	C4A-NA-C1A	-4.37	104.74	106.71
15	A1	808	CLA	C4A-NA-C1A	-4.36	104.75	106.71
15	A3	808	CLA	C4A-NA-C1A	-4.36	104.75	106.71
15	A2	808	CLA	C4A-NA-C1A	-4.35	104.75	106.71
15	B3	801	CLA	C4A-NA-C1A	-4.35	104.75	106.71
15	B3	836	CLA	C4A-NA-C1A	-4.35	104.75	106.71
15	B2	812	CLA	C4A-NA-C1A	-4.35	104.75	106.71
15	B3	808	CLA	C1-C2-C3	-4.35	118.53	126.04
15	B1	808	CLA	C1-C2-C3	-4.34	118.53	126.04
15	B1	801	CLA	C4A-NA-C1A	-4.34	104.76	106.71
15	B1	827	CLA	C4A-NA-C1A	-4.33	104.76	106.71
15	B2	836	CLA	C4A-NA-C1A	-4.33	104.76	106.71
15	B2	808	CLA	C1-C2-C3	-4.33	118.56	126.04
15	B1	810	CLA	C4A-NA-C1A	-4.33	104.76	106.71
15	B1	812	CLA	C4A-NA-C1A	-4.32	104.76	106.71
19	X1	101	LHG	O7-C7-C8	4.30	120.78	111.50
19	X3	101	LHG	O7-C7-C8	4.30	120.77	111.50
15	B1	822	CLA	C4A-NA-C1A	-4.30	104.78	106.71
19	X2	101	LHG	O7-C7-C8	4.29	120.75	111.50
15	B2	822	CLA	C4A-NA-C1A	-4.29	104.78	106.71
15	B2	801	CLA	C4A-NA-C1A	-4.28	104.78	106.71
15	B3	812	CLA	C4A-NA-C1A	-4.28	104.78	106.71
15	B3	822	CLA	C4A-NA-C1A	-4.28	104.78	106.71
15	A3	821	CLA	C4A-NA-C1A	-4.27	104.79	106.71
15	A2	810	CLA	C1C-C2C-C3C	-4.25	104.18	108.89
15	A2	821	CLA	C4A-NA-C1A	-4.24	104.80	106.71
15	B3	808	CLA	C2A-C3A-C4A	-4.23	95.03	101.87
15	B2	810	CLA	C4A-NA-C1A	-4.23	104.80	106.71
15	B2	808	CLA	C2A-C3A-C4A	-4.23	95.04	101.87
15	A1	821	CLA	C4A-NA-C1A	-4.22	104.81	106.71
15	B1	808	CLA	C2A-C3A-C4A	-4.22	95.05	101.87
15	A1	810	CLA	C1C-C2C-C3C	-4.21	104.22	108.89
15	A3	810	CLA	C1C-C2C-C3C	-4.20	104.23	108.89
15	B2	831	CLA	C4A-NA-C1A	-4.20	104.82	106.71
15	B1	831	CLA	C4A-NA-C1A	-4.17	104.83	106.71
15	A3	833	CLA	C4A-NA-C1A	-4.16	104.83	106.71
15	B3	831	CLA	C4A-NA-C1A	-4.16	104.83	106.71
15	B2	817	CLA	C4A-NA-C1A	-4.15	104.84	106.71
15	A2	833	CLA	C4A-NA-C1A	-4.15	104.84	106.71
15	J2	1302	CLA	C4A-NA-C1A	-4.14	104.84	106.71
15	A1	833	CLA	C4A-NA-C1A	-4.12	104.85	106.71
15	L3	1004	CLA	C4A-NA-C1A	-4.11	104.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	817	CLA	C4A-NA-C1A	-4.10	104.86	106.71
15	L1	1004	CLA	C4A-NA-C1A	-4.09	104.87	106.71
15	L2	1004	CLA	C4A-NA-C1A	-4.07	104.88	106.71
15	B1	805	CLA	C4A-NA-C1A	-4.06	104.88	106.71
15	B3	805	CLA	C4A-NA-C1A	-4.06	104.88	106.71
15	J1	1302	CLA	C4A-NA-C1A	-4.05	104.88	106.71
15	B2	814	CLA	C4A-NA-C1A	-4.05	104.89	106.71
15	B3	817	CLA	C4A-NA-C1A	-4.03	104.89	106.71
15	B1	814	CLA	C4A-NA-C1A	-4.03	104.89	106.71
15	B3	814	CLA	C4A-NA-C1A	-4.03	104.89	106.71
15	B2	805	CLA	C4A-NA-C1A	-4.02	104.90	106.71
15	A2	843	CLA	C4A-NA-C1A	-3.99	104.91	106.71
15	A3	806	CLA	C4A-NA-C1A	-3.98	104.92	106.71
15	A3	829	CLA	C4A-NA-C1A	-3.98	104.92	106.71
15	A2	829	CLA	C4A-NA-C1A	-3.97	104.92	106.71
15	J3	1302	CLA	C4A-NA-C1A	-3.97	104.92	106.71
15	B2	823	CLA	C4A-NA-C1A	-3.96	104.93	106.71
15	B2	803	CLA	C4A-NA-C1A	-3.95	104.93	106.71
15	A2	806	CLA	C4A-NA-C1A	-3.95	104.93	106.71
15	A1	829	CLA	C4A-NA-C1A	-3.95	104.93	106.71
15	A3	837	CLA	C4A-NA-C1A	-3.95	104.93	106.71
15	A1	843	CLA	C4A-NA-C1A	-3.94	104.93	106.71
15	A1	806	CLA	C4A-NA-C1A	-3.93	104.94	106.71
15	A1	842	CLA	C4A-NA-C1A	-3.93	104.94	106.71
15	A1	837	CLA	C4A-NA-C1A	-3.93	104.94	106.71
15	A2	837	CLA	C4A-NA-C1A	-3.92	104.94	106.71
15	A3	843	CLA	C4A-NA-C1A	-3.92	104.94	106.71
15	B1	803	CLA	C4A-NA-C1A	-3.92	104.94	106.71
15	B3	823	CLA	C4A-NA-C1A	-3.91	104.95	106.71
15	B1	823	CLA	C4A-NA-C1A	-3.91	104.95	106.71
15	B3	803	CLA	C4A-NA-C1A	-3.90	104.95	106.71
15	B1	829	CLA	C3A-C2A-C1A	-3.89	99.31	104.74
15	B3	811	CLA	C4A-NA-C1A	-3.88	104.96	106.71
15	B2	829	CLA	C3A-C2A-C1A	-3.88	99.33	104.74
15	B1	811	CLA	C4A-NA-C1A	-3.87	104.97	106.71
15	B3	829	CLA	C3A-C2A-C1A	-3.87	99.34	104.74
15	A3	814	CLA	C3A-C2A-C1A	-3.84	99.38	104.74
15	A3	842	CLA	C4A-NA-C1A	-3.84	104.98	106.71
15	A2	842	CLA	C4A-NA-C1A	-3.83	104.98	106.71
15	A1	814	CLA	C3A-C2A-C1A	-3.83	99.40	104.74
15	A3	835	CLA	C4A-NA-C1A	-3.81	104.99	106.71
15	A2	814	CLA	C3A-C2A-C1A	-3.81	99.42	104.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B2	811	CLA	C4A-NA-C1A	-3.81	104.99	106.71
15	B2	818	CLA	C4A-NA-C1A	-3.80	105.00	106.71
15	A2	835	CLA	C4A-NA-C1A	-3.78	105.00	106.71
15	B1	812	CLA	CGD-CBD-CAD	-3.76	98.56	110.73
15	B3	818	CLA	C4A-NA-C1A	-3.75	105.02	106.71
15	B3	812	CLA	CGD-CBD-CAD	-3.75	98.58	110.73
15	B2	812	CLA	CGD-CBD-CAD	-3.75	98.59	110.73
15	B1	818	CLA	C4A-NA-C1A	-3.75	105.02	106.71
15	A1	835	CLA	C4A-NA-C1A	-3.73	105.03	106.71
15	J3	1307	CLA	CHC-C1C-C2C	-3.72	120.93	129.77
15	A2	844	CLA	C4A-NA-C1A	-3.71	105.04	106.71
15	J1	1307	CLA	CHC-C1C-C2C	-3.71	120.95	129.77
15	B1	809	CLA	C4A-NA-C1A	-3.70	105.04	106.71
15	B3	809	CLA	C4A-NA-C1A	-3.70	105.04	106.71
15	J2	1307	CLA	CHC-C1C-C2C	-3.70	120.98	129.77
15	B3	838	CLA	C4A-NA-C1A	-3.69	105.05	106.71
15	B2	809	CLA	C4A-NA-C1A	-3.66	105.06	106.71
15	B2	826	CLA	C4A-NA-C1A	-3.65	105.06	106.71
15	B1	826	CLA	C4A-NA-C1A	-3.65	105.07	106.71
15	B1	807	CLA	C1-C2-C3	-3.64	119.75	126.04
15	B2	807	CLA	C1-C2-C3	-3.63	119.77	126.04
15	B3	826	CLA	C4A-NA-C1A	-3.63	105.08	106.71
15	B3	807	CLA	C1-C2-C3	-3.62	119.78	126.04
15	B1	838	CLA	C4A-NA-C1A	-3.62	105.08	106.71
15	A2	834	CLA	C1-C2-C3	-3.62	119.78	126.04
15	A3	834	CLA	C1-C2-C3	-3.62	119.78	126.04
15	A1	834	CLA	C1-C2-C3	-3.62	119.78	126.04
15	A2	840	CLA	C1-C2-C3	-3.61	119.79	126.04
15	A3	840	CLA	C1-C2-C3	-3.61	119.79	126.04
15	A1	840	CLA	C1-C2-C3	-3.61	119.80	126.04
15	A1	844	CLA	C4A-NA-C1A	-3.60	105.09	106.71
15	A3	844	CLA	C4A-NA-C1A	-3.59	105.09	106.71
15	A2	833	CLA	C1-C2-C3	-3.58	119.84	126.04
15	J2	1301	CLA	C4A-NA-C1A	-3.58	105.10	106.71
15	A3	833	CLA	C1-C2-C3	-3.58	119.85	126.04
15	A1	833	CLA	C1-C2-C3	-3.58	119.85	126.04
15	B2	838	CLA	C4A-NA-C1A	-3.57	105.10	106.71
15	J1	1301	CLA	C4A-NA-C1A	-3.56	105.11	106.71
15	A3	829	CLA	C1-C2-C3	-3.54	119.92	126.04
15	J3	1301	CLA	C4A-NA-C1A	-3.54	105.12	106.71
15	J2	1301	CLA	C4B-CHC-C1C	-3.53	124.19	129.64
15	A1	829	CLA	C1-C2-C3	-3.52	119.95	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J3	1301	CLA	C4B-CHC-C1C	-3.52	124.20	129.64
15	J1	1301	CLA	C4B-CHC-C1C	-3.51	124.22	129.64
15	A2	829	CLA	C1-C2-C3	-3.50	119.99	126.04
15	A1	803	CLA	C1D-ND-C4D	-3.49	103.86	106.33
15	A2	803	CLA	C1D-ND-C4D	-3.49	103.86	106.33
15	A1	818	CLA	C4A-NA-C1A	-3.48	105.14	106.71
15	A2	818	CLA	C4A-NA-C1A	-3.46	105.15	106.71
15	A3	818	CLA	C4A-NA-C1A	-3.46	105.15	106.71
15	A3	803	CLA	C1D-ND-C4D	-3.46	103.88	106.33
15	B2	825	CLA	C1D-ND-C4D	-3.45	103.89	106.33
15	A1	841	CLA	C4A-NA-C1A	-3.44	105.16	106.71
15	A2	832	CLA	C4A-NA-C1A	-3.44	105.16	106.71
15	A2	832	CLA	CHD-C4C-C3C	-3.43	119.80	124.84
15	B2	802	CLA	C1-C2-C3	-3.43	120.11	126.04
15	B1	802	CLA	C1-C2-C3	-3.43	120.11	126.04
15	B3	802	CLA	C1-C2-C3	-3.43	120.11	126.04
15	A1	832	CLA	CHD-C4C-C3C	-3.41	119.82	124.84
15	A3	832	CLA	CHD-C4C-C3C	-3.41	119.83	124.84
15	B1	825	CLA	C1D-ND-C4D	-3.40	103.92	106.33
15	A1	832	CLA	C4A-NA-C1A	-3.40	105.18	106.71
15	A1	815	CLA	C1D-ND-C4D	-3.40	103.92	106.33
15	A3	815	CLA	C1D-ND-C4D	-3.40	103.92	106.33
15	B3	825	CLA	C1D-ND-C4D	-3.40	103.92	106.33
15	A2	841	CLA	C4A-NA-C1A	-3.39	105.18	106.71
15	A1	804	CLA	C1-C2-C3	-3.38	120.19	126.04
15	A2	825	CLA	C4A-NA-C1A	-3.38	105.19	106.71
15	A2	804	CLA	C1-C2-C3	-3.38	120.20	126.04
15	A3	805	CLA	C1D-ND-C4D	-3.38	103.94	106.33
15	J1	1303	CLA	C1D-ND-C4D	-3.37	103.94	106.33
15	A3	804	CLA	C1-C2-C3	-3.37	120.21	126.04
15	A3	832	CLA	C4A-NA-C1A	-3.37	105.19	106.71
15	B3	818	CLA	C1-C2-C3	-3.37	121.31	126.75
15	J3	1303	CLA	C1D-ND-C4D	-3.36	103.94	106.33
15	J3	1307	CLA	C1D-ND-C4D	-3.36	103.94	106.33
15	J2	1303	CLA	C1D-ND-C4D	-3.36	103.95	106.33
15	B1	818	CLA	C1-C2-C3	-3.36	121.31	126.75
15	A1	856	CLA	C4A-NA-C1A	-3.36	105.19	106.71
15	A3	838	CLA	C4A-NA-C1A	-3.36	105.19	106.71
15	A3	825	CLA	C4A-NA-C1A	-3.36	105.20	106.71
15	A2	815	CLA	C1D-ND-C4D	-3.36	103.95	106.33
15	B1	817	CLA	C1-C2-C3	-3.36	121.32	126.75
15	A3	822	CLA	C1D-ND-C4D	-3.35	103.95	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	805	CLA	C1D-ND-C4D	-3.35	103.95	106.33
15	A1	805	CLA	C1D-ND-C4D	-3.35	103.95	106.33
15	A2	816	CLA	C1D-ND-C4D	-3.35	103.95	106.33
15	B2	818	CLA	C1-C2-C3	-3.35	121.33	126.75
15	A2	834	CLA	CHD-C4C-C3C	-3.35	119.92	124.84
15	A1	834	CLA	C4A-NA-C1A	-3.35	105.20	106.71
15	B3	817	CLA	C1-C2-C3	-3.35	121.34	126.75
15	A1	825	CLA	C4A-NA-C1A	-3.34	105.20	106.71
15	A3	834	CLA	C4A-NA-C1A	-3.34	105.20	106.71
15	B2	817	CLA	C1-C2-C3	-3.34	121.34	126.75
15	A2	838	CLA	C4A-NA-C1A	-3.34	105.20	106.71
15	A3	841	CLA	C4A-NA-C1A	-3.34	105.20	106.71
15	A1	817	CLA	C1D-ND-C4D	-3.34	103.96	106.33
15	A2	856	CLA	C4A-NA-C1A	-3.33	105.21	106.71
15	A3	813	CLA	C4A-NA-C1A	-3.33	105.21	106.71
15	A1	813	CLA	C4A-NA-C1A	-3.33	105.21	106.71
15	A3	812	CLA	C1D-ND-C4D	-3.33	103.97	106.33
15	L3	1004	CLA	C1-C2-C3	-3.33	120.28	126.04
15	A3	817	CLA	C1D-ND-C4D	-3.33	103.97	106.33
15	A2	824	CLA	C4A-NA-C1A	-3.33	105.21	106.71
15	A3	856	CLA	C4A-NA-C1A	-3.33	105.21	106.71
15	L2	1004	CLA	C1-C2-C3	-3.33	120.29	126.04
15	A2	817	CLA	C1D-ND-C4D	-3.33	103.97	106.33
15	L2	1003	CLA	C4A-NA-C1A	-3.33	105.21	106.71
15	A3	824	CLA	C4A-NA-C1A	-3.33	105.21	106.71
15	L1	1004	CLA	C1-C2-C3	-3.32	120.29	126.04
15	J1	1307	CLA	C1D-ND-C4D	-3.32	103.97	106.33
15	B3	829	CLA	C2A-C3A-C4A	-3.32	99.79	103.59
15	A2	834	CLA	C4A-NA-C1A	-3.32	105.21	106.71
15	A1	812	CLA	C1D-ND-C4D	-3.32	103.98	106.33
15	A1	816	CLA	C1D-ND-C4D	-3.32	103.98	106.33
15	A1	825	CLA	CHD-C4C-C3C	-3.32	119.97	124.84
15	I1	101	CLA	C4A-NA-C1A	-3.31	105.22	106.71
15	A1	834	CLA	CHD-C4C-C3C	-3.31	119.97	124.84
15	A2	825	CLA	CHD-C4C-C3C	-3.31	119.97	124.84
15	A3	834	CLA	CHD-C4C-C3C	-3.31	119.97	124.84
15	A2	813	CLA	C4A-NA-C1A	-3.31	105.22	106.71
15	L3	1003	CLA	C4A-NA-C1A	-3.31	105.22	106.71
15	B1	829	CLA	C2A-C3A-C4A	-3.31	99.80	103.59
15	A3	825	CLA	CHD-C4C-C3C	-3.30	119.98	124.84
15	A1	822	CLA	C1D-ND-C4D	-3.30	103.99	106.33
15	A2	827	CLA	C1D-ND-C4D	-3.30	103.99	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	822	CLA	C1D-ND-C4D	-3.30	103.99	106.33
15	B2	829	CLA	C2A-C3A-C4A	-3.30	99.81	103.59
15	A1	823	CLA	C1D-ND-C4D	-3.30	103.99	106.33
15	A1	827	CLA	C1D-ND-C4D	-3.29	104.00	106.33
15	A2	823	CLA	C1D-ND-C4D	-3.29	104.00	106.33
15	A3	827	CLA	C1D-ND-C4D	-3.29	104.00	106.33
15	I3	101	CLA	C4A-NA-C1A	-3.29	105.23	106.71
15	A2	812	CLA	C1D-ND-C4D	-3.29	104.00	106.33
15	A1	824	CLA	C4A-NA-C1A	-3.29	105.23	106.71
15	L1	1003	CLA	C4A-NA-C1A	-3.28	105.23	106.71
15	J2	1307	CLA	C1D-ND-C4D	-3.28	104.01	106.33
15	A1	813	CLA	C1D-ND-C4D	-3.27	104.01	106.33
15	A2	820	CLA	C1D-ND-C4D	-3.27	104.01	106.33
15	X2	102	CLA	CHD-C4C-C3C	-3.27	119.87	124.98
15	X3	102	CLA	CHD-C4C-C3C	-3.27	119.87	124.98
15	A3	816	CLA	C1D-ND-C4D	-3.27	104.01	106.33
15	A3	820	CLA	C1D-ND-C4D	-3.26	104.02	106.33
15	A2	813	CLA	C1D-ND-C4D	-3.26	104.02	106.33
15	B3	812	CLA	CHD-C4C-C3C	-3.26	120.05	124.84
15	X1	102	CLA	CHD-C4C-C3C	-3.26	119.89	124.98
15	A2	821	CLA	C1D-ND-C4D	-3.26	104.02	106.33
15	B3	839	CLA	CHD-C4C-C3C	-3.26	120.05	124.84
15	B1	839	CLA	CHD-C4C-C3C	-3.25	120.06	124.84
15	B2	812	CLA	CHD-C4C-C3C	-3.25	120.06	124.84
15	B2	839	CLA	CHD-C4C-C3C	-3.25	120.06	124.84
15	B1	812	CLA	CHD-C4C-C3C	-3.25	120.06	124.84
15	A3	813	CLA	C1D-ND-C4D	-3.25	104.03	106.33
15	L1	1003	CLA	C1-C2-C3	-3.24	120.43	126.04
15	A2	810	CLA	C1D-ND-C4D	-3.24	104.03	106.33
15	L2	1003	CLA	C1-C2-C3	-3.24	120.44	126.04
15	L3	1003	CLA	C1-C2-C3	-3.24	120.44	126.04
15	A1	820	CLA	C1D-ND-C4D	-3.24	104.03	106.33
15	A1	821	CLA	C1D-ND-C4D	-3.24	104.03	106.33
15	A3	807	CLA	C1D-ND-C4D	-3.24	104.03	106.33
15	I2	101	CLA	C4A-NA-C1A	-3.23	105.25	106.71
15	A1	838	CLA	C4A-NA-C1A	-3.23	105.25	106.71
15	A2	807	CLA	C1D-ND-C4D	-3.23	104.04	106.33
15	A1	807	CLA	C1D-ND-C4D	-3.22	104.04	106.33
15	A3	823	CLA	C1D-ND-C4D	-3.22	104.05	106.33
15	A3	809	CLA	C1D-ND-C4D	-3.22	104.05	106.33
15	B2	806	CLA	C4A-NA-C1A	-3.21	105.26	106.71
15	A1	809	CLA	C1D-ND-C4D	-3.21	104.06	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A1	814	CLA	C1D-ND-C4D	-3.21	104.06	106.33
15	A1	810	CLA	C1D-ND-C4D	-3.21	104.06	106.33
15	A3	821	CLA	C1D-ND-C4D	-3.21	104.06	106.33
15	L2	1004	CLA	CAA-C2A-C1A	-3.20	101.47	111.97
15	A3	839	CLA	CHD-C4C-C3C	-3.20	120.13	124.84
15	A3	842	CLA	CHD-C4C-C3C	-3.20	120.13	124.84
15	L1	1004	CLA	CAA-C2A-C1A	-3.20	101.49	111.97
15	A3	814	CLA	C1D-ND-C4D	-3.20	104.06	106.33
15	L3	1004	CLA	CAA-C2A-C1A	-3.19	101.51	111.97
15	A1	831	CLA	C1D-ND-C4D	-3.19	104.07	106.33
15	A2	808	CLA	C1-C2-C3	-3.19	120.52	126.04
15	L1	1003	CLA	CHD-C4C-C3C	-3.19	120.15	124.84
15	A3	808	CLA	C1-C2-C3	-3.19	120.53	126.04
15	B1	829	CLA	C1D-ND-C4D	-3.19	104.07	106.33
15	A2	809	CLA	C1D-ND-C4D	-3.19	104.07	106.33
15	A1	839	CLA	CHD-C4C-C3C	-3.19	120.15	124.84
15	A2	841	CLA	CHD-C4C-C3C	-3.19	120.15	124.84
15	A1	842	CLA	CHD-C4C-C3C	-3.19	120.15	124.84
15	A3	824	CLA	CHD-C4C-C3C	-3.19	120.16	124.84
15	B2	829	CLA	C1D-ND-C4D	-3.19	104.07	106.33
15	L2	1003	CLA	CHD-C4C-C3C	-3.19	120.16	124.84
15	A1	808	CLA	C1-C2-C3	-3.19	120.53	126.04
15	B3	829	CLA	C1D-ND-C4D	-3.18	104.07	106.33
15	A2	842	CLA	CHD-C4C-C3C	-3.18	120.16	124.84
15	A2	814	CLA	C1D-ND-C4D	-3.18	104.07	106.33
15	A2	839	CLA	CHD-C4C-C3C	-3.18	120.17	124.84
15	J3	1301	CLA	CHD-C4C-C3C	-3.18	120.17	124.84
15	J1	1301	CLA	CHD-C4C-C3C	-3.18	120.17	124.84
15	A2	838	CLA	CHD-C4C-C3C	-3.18	120.17	124.84
15	A2	824	CLA	CHD-C4C-C3C	-3.18	120.17	124.84
15	A1	824	CLA	CHD-C4C-C3C	-3.18	120.17	124.84
15	B1	819	CLA	C1D-ND-C4D	-3.18	104.08	106.33
15	B1	806	CLA	C4A-NA-C1A	-3.18	105.28	106.71
15	A3	841	CLA	CHD-C4C-C3C	-3.17	120.17	124.84
15	A3	810	CLA	C1D-ND-C4D	-3.17	104.08	106.33
15	J2	1301	CLA	CHD-C4C-C3C	-3.17	120.17	124.84
15	L3	1003	CLA	CHD-C4C-C3C	-3.17	120.17	124.84
15	A1	841	CLA	CHD-C4C-C3C	-3.17	120.18	124.84
15	A3	831	CLA	C1D-ND-C4D	-3.17	104.08	106.33
15	A2	831	CLA	C1D-ND-C4D	-3.17	104.08	106.33
15	A1	837	CLA	C1D-ND-C4D	-3.17	104.08	106.33
15	B2	819	CLA	C1D-ND-C4D	-3.17	104.08	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	821	CLA	C1D-ND-C4D	-3.17	104.09	106.33
15	A3	813	CLA	CHD-C4C-C3C	-3.17	120.19	124.84
15	A3	831	CLA	C1-C2-C3	-3.16	121.63	126.75
15	A1	838	CLA	CHD-C4C-C3C	-3.16	120.19	124.84
15	B1	833	CLA	C1D-ND-C4D	-3.16	104.09	106.33
15	A2	841	CLA	C1D-ND-C4D	-3.16	104.09	106.33
15	A3	837	CLA	C1D-ND-C4D	-3.16	104.09	106.33
15	B3	806	CLA	C4A-NA-C1A	-3.16	105.29	106.71
15	A3	818	CLA	C1-C2-C3	-3.15	121.65	126.75
15	A1	827	CLA	CHD-C4C-C3C	-3.15	120.20	124.84
15	A1	818	CLA	C1-C2-C3	-3.15	121.65	126.75
15	A1	813	CLA	CHD-C4C-C3C	-3.15	120.21	124.84
15	B3	823	CLA	CAA-C2A-C3A	-3.15	108.74	116.10
15	B2	833	CLA	C1D-ND-C4D	-3.15	104.10	106.33
15	A3	838	CLA	CHD-C4C-C3C	-3.15	120.21	124.84
15	A3	827	CLA	CHD-C4C-C3C	-3.15	120.21	124.84
15	B3	804	CLA	CHD-C4C-C3C	-3.15	120.21	124.84
15	A1	841	CLA	C1D-ND-C4D	-3.15	104.10	106.33
15	A3	841	CLA	C1D-ND-C4D	-3.15	104.10	106.33
15	A2	813	CLA	CHD-C4C-C3C	-3.15	120.21	124.84
15	B1	823	CLA	CAA-C2A-C3A	-3.15	108.75	116.10
15	A2	837	CLA	C1D-ND-C4D	-3.15	104.10	106.33
15	A2	818	CLA	C1-C2-C3	-3.15	121.66	126.75
15	A2	827	CLA	CHD-C4C-C3C	-3.14	120.22	124.84
15	B2	823	CLA	CAA-C2A-C3A	-3.14	108.77	116.10
15	B2	831	CLA	CAA-C2A-C1A	-3.14	104.05	111.81
15	A2	831	CLA	C1-C2-C3	-3.14	121.67	126.75
15	A1	831	CLA	C1-C2-C3	-3.14	121.67	126.75
15	B1	831	CLA	CAA-C2A-C1A	-3.14	104.06	111.81
15	B1	837	CLA	C1D-ND-C4D	-3.14	104.11	106.33
15	B3	819	CLA	C1D-ND-C4D	-3.14	104.11	106.33
15	B3	831	CLA	CAA-C2A-C1A	-3.13	104.07	111.81
15	B3	837	CLA	C1D-ND-C4D	-3.13	104.11	106.33
15	L2	1004	CLA	C1D-ND-C4D	-3.13	104.11	106.33
15	B2	804	CLA	CHD-C4C-C3C	-3.13	120.24	124.84
15	A1	837	CLA	CHD-C4C-C3C	-3.12	120.25	124.84
15	B1	804	CLA	CHD-C4C-C3C	-3.12	120.25	124.84
15	B2	831	CLA	CHD-C4C-C3C	-3.12	120.25	124.84
15	B3	807	CLA	C3A-C2A-C1A	-3.12	96.66	101.34
15	B3	814	CLA	CHD-C4C-C3C	-3.12	120.25	124.84
15	B2	837	CLA	C1D-ND-C4D	-3.12	104.12	106.33
15	B3	833	CLA	C1D-ND-C4D	-3.12	104.12	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	837	CLA	CHD-C4C-C3C	-3.12	120.26	124.84
15	B2	807	CLA	C3A-C2A-C1A	-3.12	96.67	101.34
15	B1	807	CLA	C3A-C2A-C1A	-3.12	96.67	101.34
14	A3	801	CL0	C2C-C1C-NC	3.12	112.89	109.97
15	B2	814	CLA	CHD-C4C-C3C	-3.12	120.26	124.84
15	B1	821	CLA	C1D-ND-C4D	-3.11	104.12	106.33
15	A3	840	CLA	C1D-ND-C4D	-3.11	104.12	106.33
14	A2	801	CL0	C2C-C1C-NC	3.11	112.89	109.97
15	A3	818	CLA	CHD-C4C-C3C	-3.11	120.27	124.84
14	A1	801	CL0	C2C-C1C-NC	3.11	112.89	109.97
15	X1	102	CLA	C4A-NA-C1A	-3.11	105.31	106.71
15	A1	803	CLA	CHD-C4C-C3C	-3.11	120.27	124.84
15	B1	814	CLA	CHD-C4C-C3C	-3.11	120.27	124.84
15	A2	803	CLA	CHD-C4C-C3C	-3.11	120.27	124.84
15	B1	831	CLA	CHD-C4C-C3C	-3.10	120.28	124.84
15	A1	818	CLA	CHD-C4C-C3C	-3.10	120.28	124.84
15	A2	837	CLA	CHD-C4C-C3C	-3.10	120.28	124.84
15	X2	102	CLA	C4A-NA-C1A	-3.10	105.31	106.71
15	J3	1301	CLA	CAA-C2A-C1A	-3.10	104.16	111.81
15	B3	831	CLA	CHD-C4C-C3C	-3.09	120.29	124.84
15	B3	806	CLA	CHD-C4C-C3C	-3.09	120.29	124.84
15	B1	806	CLA	CHD-C4C-C3C	-3.09	120.30	124.84
15	X3	102	CLA	C4A-NA-C1A	-3.09	105.32	106.71
15	B2	821	CLA	C1D-ND-C4D	-3.09	104.14	106.33
15	J1	1301	CLA	CAA-C2A-C1A	-3.09	104.18	111.81
15	A3	803	CLA	CHD-C4C-C3C	-3.09	120.30	124.84
15	A2	818	CLA	CHD-C4C-C3C	-3.09	120.30	124.84
15	B2	804	CLA	C4A-NA-C1A	-3.09	105.32	106.71
15	B2	806	CLA	CHD-C4C-C3C	-3.08	120.31	124.84
15	A2	809	CLA	C1-C2-C3	-3.08	120.71	126.04
15	A2	840	CLA	C1D-ND-C4D	-3.08	104.15	106.33
15	J2	1301	CLA	CAA-C2A-C1A	-3.08	104.21	111.81
15	A1	809	CLA	C1-C2-C3	-3.08	120.72	126.04
15	A1	815	CLA	CHD-C4C-C3C	-3.08	120.32	124.84
15	A3	815	CLA	CHD-C4C-C3C	-3.08	120.32	124.84
15	A3	809	CLA	C1-C2-C3	-3.08	120.72	126.04
15	K3	101	CLA	C4D-ND-C1D	-3.08	104.15	106.33
15	L3	1004	CLA	C1D-ND-C4D	-3.07	104.15	106.33
15	X1	102	CLA	CAA-C2A-C1A	-3.07	104.22	111.81
15	I2	101	CLA	CHD-C4C-C3C	-3.07	120.33	124.84
15	X3	102	CLA	CAA-C2A-C1A	-3.07	104.22	111.81
15	B1	818	CLA	C1D-ND-C4D	-3.07	104.16	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	808	CLA	C1D-ND-C4D	-3.07	104.16	106.33
15	I1	101	CLA	CHD-C4C-C3C	-3.07	120.33	124.84
15	X2	102	CLA	CAA-C2A-C1A	-3.06	104.25	111.81
15	A3	825	CLA	C1D-ND-C4D	-3.06	104.16	106.33
15	I3	101	CLA	CHD-C4C-C3C	-3.06	120.34	124.84
15	A2	825	CLA	C1D-ND-C4D	-3.06	104.16	106.33
15	A2	815	CLA	CHD-C4C-C3C	-3.06	120.35	124.84
15	A1	840	CLA	C1D-ND-C4D	-3.05	104.17	106.33
15	B2	835	CLA	C1D-ND-C4D	-3.05	104.17	106.33
15	A2	802	CLA	C1D-ND-C4D	-3.05	104.17	106.33
15	A2	806	CLA	C1D-ND-C4D	-3.05	104.17	106.33
15	A3	819	CLA	C1D-ND-C4D	-3.05	104.17	106.33
15	A3	808	CLA	C1D-ND-C4D	-3.05	104.17	106.33
14	A3	801	CL0	CHC-C1C-C2C	-3.05	118.29	126.72
15	A2	830	CLA	CHD-C4C-C3C	-3.05	120.36	124.84
15	A2	844	CLA	C1D-ND-C4D	-3.04	104.17	106.33
15	B2	818	CLA	C1D-ND-C4D	-3.04	104.17	106.33
14	A1	801	CL0	CHC-C1C-C2C	-3.04	118.30	126.72
15	L1	1004	CLA	C1D-ND-C4D	-3.04	104.17	106.33
15	A1	830	CLA	CHD-C4C-C3C	-3.04	120.37	124.84
15	B1	804	CLA	C4A-NA-C1A	-3.04	105.34	106.71
14	A2	801	CL0	CHC-C1C-C2C	-3.04	118.32	126.72
15	B2	822	CLA	C1D-ND-C4D	-3.03	104.18	106.33
15	B3	825	CLA	C1-C2-C3	-3.03	120.80	126.04
15	B1	835	CLA	C1D-ND-C4D	-3.03	104.18	106.33
15	A1	836	CLA	CHD-C4C-C3C	-3.03	120.39	124.84
15	A2	836	CLA	CHD-C4C-C3C	-3.03	120.39	124.84
15	A3	836	CLA	CHD-C4C-C3C	-3.03	120.39	124.84
15	A1	808	CLA	C1D-ND-C4D	-3.03	104.19	106.33
15	B3	835	CLA	C1D-ND-C4D	-3.02	104.19	106.33
15	B2	825	CLA	C1-C2-C3	-3.02	120.81	126.04
15	B2	822	CLA	CHD-C4C-C3C	-3.02	120.40	124.84
15	B1	838	CLA	CHD-C4C-C3C	-3.02	120.40	124.84
15	B1	822	CLA	CHD-C4C-C3C	-3.02	120.40	124.84
15	B1	825	CLA	C1-C2-C3	-3.02	120.82	126.04
15	A3	830	CLA	CHD-C4C-C3C	-3.02	120.40	124.84
15	A1	819	CLA	C1D-ND-C4D	-3.02	104.19	106.33
14	A3	801	CL0	CHC-C1C-NC	3.02	128.78	124.20
15	K1	101	CLA	C4D-ND-C1D	-3.02	104.19	106.33
14	A1	801	CL0	CHC-C1C-NC	3.01	128.78	124.20
15	B1	813	CLA	C1D-ND-C4D	-3.01	104.19	106.33
15	B2	838	CLA	CHD-C4C-C3C	-3.01	120.41	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	819	CLA	C1D-ND-C4D	-3.01	104.20	106.33
15	B3	813	CLA	C1D-ND-C4D	-3.01	104.20	106.33
15	B1	811	CLA	C1D-ND-C4D	-3.01	104.20	106.33
15	A1	806	CLA	C1D-ND-C4D	-3.01	104.20	106.33
15	B3	811	CLA	C1D-ND-C4D	-3.01	104.20	106.33
15	A1	844	CLA	C1D-ND-C4D	-3.00	104.20	106.33
15	B2	813	CLA	C1D-ND-C4D	-3.00	104.20	106.33
15	A3	806	CLA	C1D-ND-C4D	-3.00	104.20	106.33
14	A2	801	CL0	CHC-C1C-NC	3.00	128.76	124.20
15	A1	802	CLA	C1D-ND-C4D	-3.00	104.20	106.33
15	A3	806	CLA	CHD-C4C-C3C	-3.00	120.43	124.84
15	A1	826	CLA	C1D-ND-C4D	-3.00	104.20	106.33
15	A1	829	CLA	CHD-C4C-C3C	-3.00	120.44	124.84
15	B3	822	CLA	C1D-ND-C4D	-3.00	104.21	106.33
15	A2	829	CLA	CHD-C4C-C3C	-3.00	120.44	124.84
15	A1	825	CLA	C1D-ND-C4D	-2.99	104.21	106.33
15	B3	818	CLA	C1D-ND-C4D	-2.99	104.21	106.33
15	A1	818	CLA	C1D-ND-C4D	-2.99	104.21	106.33
15	B3	838	CLA	CHD-C4C-C3C	-2.99	120.44	124.84
15	B1	838	CLA	C1D-ND-C4D	-2.99	104.21	106.33
15	K2	101	CLA	C4D-ND-C1D	-2.99	104.21	106.33
15	B2	802	CLA	CHD-C4C-C3C	-2.99	120.45	124.84
15	A3	826	CLA	C1D-ND-C4D	-2.99	104.21	106.33
15	B3	822	CLA	CHD-C4C-C3C	-2.98	120.45	124.84
15	A1	806	CLA	CHD-C4C-C3C	-2.98	120.46	124.84
15	A3	802	CLA	C1-C2-C3	-2.98	120.89	126.04
15	A2	826	CLA	C1D-ND-C4D	-2.98	104.22	106.33
15	A3	844	CLA	C1D-ND-C4D	-2.98	104.22	106.33
15	B3	806	CLA	C1D-ND-C4D	-2.98	104.22	106.33
15	A2	806	CLA	CHD-C4C-C3C	-2.98	120.46	124.84
15	A3	829	CLA	CHD-C4C-C3C	-2.98	120.46	124.84
15	B2	811	CLA	C1D-ND-C4D	-2.98	104.22	106.33
15	B3	838	CLA	C1D-ND-C4D	-2.98	104.22	106.33
15	B3	804	CLA	C4A-NA-C1A	-2.98	105.37	106.71
15	A2	818	CLA	C1D-ND-C4D	-2.98	104.22	106.33
15	B3	811	CLA	CHD-C4C-C3C	-2.98	120.47	124.84
15	B1	805	CLA	CHD-C4C-C3C	-2.98	120.47	124.84
15	B3	818	CLA	CHD-C4C-C3C	-2.97	120.47	124.84
15	B2	821	CLA	CHA-C1A-NA	-2.97	119.72	126.41
15	A3	814	CLA	C2A-C3A-C4A	-2.97	100.18	103.59
15	B1	823	CLA	CHD-C4C-C3C	-2.97	120.47	124.84
15	A1	802	CLA	C1-C2-C3	-2.97	120.90	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L1	1002	CLA	C4A-NA-C1A	-2.97	105.37	106.71
15	L2	1002	CLA	C4A-NA-C1A	-2.97	105.37	106.71
15	L3	1004	CLA	CHD-C4C-C3C	-2.97	120.47	124.84
15	B3	802	CLA	CHD-C4C-C3C	-2.97	120.47	124.84
15	A2	802	CLA	C1-C2-C3	-2.97	120.91	126.04
15	B3	823	CLA	CHD-C4C-C3C	-2.97	120.48	124.84
15	B3	805	CLA	CHD-C4C-C3C	-2.97	120.48	124.84
15	B2	815	CLA	CHD-C4C-C3C	-2.97	120.48	124.84
15	B2	823	CLA	CHD-C4C-C3C	-2.97	120.48	124.84
15	B1	821	CLA	CHA-C1A-NA	-2.97	119.74	126.41
15	B1	802	CLA	CHD-C4C-C3C	-2.97	120.48	124.84
15	L1	1004	CLA	CHD-C4C-C3C	-2.97	120.48	124.84
15	A2	844	CLA	CHD-C4C-C3C	-2.96	120.48	124.84
15	A1	817	CLA	CHD-C4C-C3C	-2.96	120.35	124.98
15	A2	817	CLA	CHD-C4C-C3C	-2.96	120.35	124.98
15	B3	821	CLA	CHA-C1A-NA	-2.96	119.75	126.41
15	B2	805	CLA	CHD-C4C-C3C	-2.96	120.48	124.84
15	A3	818	CLA	C1D-ND-C4D	-2.96	104.23	106.33
15	A1	844	CLA	CHD-C4C-C3C	-2.96	120.48	124.84
15	A1	814	CLA	C2A-C3A-C4A	-2.96	100.19	103.59
15	A3	817	CLA	CHD-C4C-C3C	-2.96	120.35	124.98
15	B1	811	CLA	CHD-C4C-C3C	-2.96	120.49	124.84
15	B2	818	CLA	CHD-C4C-C3C	-2.96	120.49	124.84
15	B3	835	CLA	CHD-C4C-C3C	-2.96	120.49	124.84
15	A3	802	CLA	C1D-ND-C4D	-2.96	104.23	106.33
15	L2	1004	CLA	CHD-C4C-C3C	-2.96	120.49	124.84
15	A3	844	CLA	CHD-C4C-C3C	-2.96	120.49	124.84
15	B2	835	CLA	CHD-C4C-C3C	-2.96	120.50	124.84
15	B3	836	CLA	CHD-C4C-C3C	-2.96	120.50	124.84
15	A2	829	CLA	C1D-ND-C4D	-2.95	104.24	106.33
15	A3	802	CLA	CHD-C4C-C3C	-2.95	120.50	124.84
15	L1	1003	CLA	C1D-ND-C4D	-2.95	104.24	106.33
15	A2	814	CLA	C2A-C3A-C4A	-2.95	100.21	103.59
15	B1	835	CLA	CHD-C4C-C3C	-2.95	120.50	124.84
15	B1	822	CLA	C1D-ND-C4D	-2.95	104.24	106.33
15	B1	818	CLA	CHD-C4C-C3C	-2.95	120.51	124.84
15	A3	826	CLA	CHD-C4C-C3C	-2.95	120.51	124.84
15	A3	839	CLA	C4A-NA-C1A	-2.95	105.38	106.71
15	B3	834	CLA	C1D-ND-C4D	-2.95	104.24	106.33
15	B1	836	CLA	CHD-C4C-C3C	-2.95	120.51	124.84
15	B1	806	CLA	C1D-ND-C4D	-2.94	104.24	106.33
15	L2	1003	CLA	C1D-ND-C4D	-2.94	104.24	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	831	CLA	C1D-ND-C4D	-2.94	104.24	106.33
15	B2	806	CLA	C1D-ND-C4D	-2.94	104.25	106.33
15	B1	815	CLA	CHD-C4C-C3C	-2.94	120.52	124.84
15	B1	820	CLA	CHD-C4C-C3C	-2.94	120.52	124.84
15	B2	836	CLA	CHD-C4C-C3C	-2.94	120.52	124.84
15	A2	811	CLA	C1D-ND-C4D	-2.94	104.25	106.33
15	A1	802	CLA	CHD-C4C-C3C	-2.94	120.52	124.84
15	L3	1002	CLA	C4A-NA-C1A	-2.94	105.39	106.71
15	B2	821	CLA	C2A-C1A-CHA	2.93	127.26	122.71
15	A1	837	CLA	C1-C2-C3	-2.93	122.01	126.75
15	B2	811	CLA	CHD-C4C-C3C	-2.93	120.53	124.84
15	B2	838	CLA	C1D-ND-C4D	-2.93	104.25	106.33
15	B2	820	CLA	CHD-C4C-C3C	-2.93	120.53	124.84
15	B2	825	CLA	CHD-C4C-C3C	-2.93	120.54	124.84
15	B3	810	CLA	CHD-C4C-C3C	-2.93	120.54	124.84
15	B3	825	CLA	CHD-C4C-C3C	-2.93	120.54	124.84
15	A3	816	CLA	CHD-C4C-C3C	-2.93	120.54	124.84
15	A3	829	CLA	C1D-ND-C4D	-2.93	104.26	106.33
15	B3	820	CLA	CHD-C4C-C3C	-2.93	120.54	124.84
15	B1	834	CLA	C1D-ND-C4D	-2.92	104.26	106.33
15	A2	833	CLA	CHD-C4C-C3C	-2.92	120.54	124.84
15	A2	802	CLA	CHD-C4C-C3C	-2.92	120.54	124.84
15	L3	1003	CLA	C1D-ND-C4D	-2.92	104.26	106.33
15	A2	826	CLA	CHD-C4C-C3C	-2.92	120.55	124.84
15	A1	826	CLA	CHD-C4C-C3C	-2.92	120.55	124.84
15	B1	825	CLA	CHD-C4C-C3C	-2.92	120.55	124.84
15	A2	816	CLA	CHD-C4C-C3C	-2.92	120.55	124.84
15	B3	815	CLA	CHD-C4C-C3C	-2.92	120.55	124.84
15	A3	837	CLA	C1-C2-C3	-2.92	122.03	126.75
15	A1	829	CLA	C1D-ND-C4D	-2.92	104.26	106.33
15	J3	1302	CLA	C1D-ND-C4D	-2.92	104.26	106.33
15	L3	1002	CLA	CHD-C4C-C3C	-2.91	120.56	124.84
15	B2	805	CLA	C1D-ND-C4D	-2.91	104.27	106.33
15	L2	1002	CLA	C2C-C1C-NC	2.91	112.70	109.97
15	A2	839	CLA	C4A-NA-C1A	-2.91	105.40	106.71
15	A2	837	CLA	C1-C2-C3	-2.91	122.04	126.75
15	B3	826	CLA	CHD-C4C-C3C	-2.91	120.56	124.84
15	B1	821	CLA	C2A-C1A-CHA	2.91	127.22	122.71
15	A1	812	CLA	CHD-C4C-C3C	-2.91	120.43	124.98
15	L2	1002	CLA	CHD-C4C-C3C	-2.91	120.56	124.84
15	A1	816	CLA	CHD-C4C-C3C	-2.91	120.56	124.84
15	B1	810	CLA	CHD-C4C-C3C	-2.91	120.56	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	831	CLA	C1D-ND-C4D	-2.91	104.27	106.33
15	B2	823	CLA	C1D-ND-C4D	-2.91	104.27	106.33
15	I2	101	CLA	C1D-ND-C4D	-2.91	104.27	106.33
15	A3	812	CLA	CHD-C4C-C3C	-2.91	120.44	124.98
15	L1	1002	CLA	CHD-C4C-C3C	-2.91	120.57	124.84
15	L3	1002	CLA	C2C-C1C-NC	2.90	112.69	109.97
15	A1	833	CLA	CHD-C4C-C3C	-2.90	120.57	124.84
15	B1	826	CLA	CHD-C4C-C3C	-2.90	120.58	124.84
15	B2	810	CLA	C1D-ND-C4D	-2.90	104.27	106.33
15	J3	1302	CLA	CHD-C4C-C3C	-2.90	120.45	124.98
15	A3	833	CLA	CHD-C4C-C3C	-2.90	120.58	124.84
15	B3	810	CLA	C1D-ND-C4D	-2.90	104.28	106.33
15	J2	1302	CLA	CHD-C4C-C3C	-2.90	120.45	124.98
15	B2	810	CLA	CHD-C4C-C3C	-2.90	120.58	124.84
15	B1	810	CLA	C1D-ND-C4D	-2.90	104.28	106.33
15	I3	101	CLA	C1D-ND-C4D	-2.90	104.28	106.33
15	J1	1302	CLA	CHD-C4C-C3C	-2.90	120.46	124.98
15	B3	805	CLA	C1D-ND-C4D	-2.89	104.28	106.33
15	B2	826	CLA	CHD-C4C-C3C	-2.89	120.59	124.84
15	B2	831	CLA	C1D-ND-C4D	-2.89	104.28	106.33
15	A2	812	CLA	CHD-C4C-C3C	-2.89	120.47	124.98
15	B3	821	CLA	C2A-C1A-CHA	2.89	127.19	122.71
14	A1	801	CL0	C1-C2-C3	-2.89	121.05	126.04
15	A1	811	CLA	C1D-ND-C4D	-2.88	104.29	106.33
15	B1	823	CLA	C1D-ND-C4D	-2.88	104.29	106.33
15	B2	834	CLA	C1D-ND-C4D	-2.88	104.29	106.33
15	B3	829	CLA	CHD-C4C-C3C	-2.88	120.60	124.84
15	B2	849	CLA	CHD-C4C-C3C	-2.88	120.60	124.84
14	A3	801	CL0	C1-C2-C3	-2.88	121.06	126.04
15	L1	1002	CLA	C2C-C1C-NC	2.88	112.67	109.97
15	J2	1302	CLA	C1D-ND-C4D	-2.88	104.29	106.33
15	A1	839	CLA	C4A-NA-C1A	-2.88	105.41	106.71
15	J1	1302	CLA	C1D-ND-C4D	-2.88	104.29	106.33
15	A2	836	CLA	C1D-ND-C4D	-2.88	104.29	106.33
15	A3	811	CLA	C1D-ND-C4D	-2.88	104.29	106.33
15	J1	1303	CLA	CHD-C4C-C3C	-2.88	120.48	124.98
15	A3	821	CLA	CHD-C4C-C3C	-2.87	120.49	124.98
15	B3	836	CLA	C1D-ND-C4D	-2.87	104.29	106.33
15	B3	849	CLA	CHD-C4C-C3C	-2.87	120.61	124.84
14	A2	801	CL0	C1-C2-C3	-2.87	121.07	126.04
15	J3	1303	CLA	CHD-C4C-C3C	-2.87	120.49	124.98
15	A3	840	CLA	CHD-C4C-C3C	-2.87	120.62	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	805	CLA	C1D-ND-C4D	-2.87	104.30	106.33
15	B1	849	CLA	CHD-C4C-C3C	-2.87	120.62	124.84
15	B1	829	CLA	CHD-C4C-C3C	-2.87	120.63	124.84
15	A1	836	CLA	C1D-ND-C4D	-2.87	104.30	106.33
15	A3	807	CLA	CHD-C4C-C3C	-2.87	120.63	124.84
15	A2	821	CLA	CHD-C4C-C3C	-2.86	120.50	124.98
15	B2	824	CLA	C1D-ND-C4D	-2.86	104.30	106.33
15	A1	840	CLA	CHD-C4C-C3C	-2.86	120.63	124.84
15	A3	836	CLA	C1D-ND-C4D	-2.86	104.30	106.33
15	J2	1303	CLA	CHD-C4C-C3C	-2.86	120.51	124.98
15	B2	816	CLA	CHD-C4C-C3C	-2.86	120.64	124.84
15	B3	813	CLA	CHD-C4C-C3C	-2.86	120.64	124.84
15	A1	807	CLA	CHD-C4C-C3C	-2.86	120.64	124.84
15	B1	816	CLA	CHD-C4C-C3C	-2.86	120.64	124.84
15	B1	827	CLA	CHD-C4C-C3C	-2.86	120.64	124.84
15	B2	813	CLA	CHD-C4C-C3C	-2.86	120.64	124.84
15	B3	819	CLA	CHD-C4C-C3C	-2.86	120.64	124.84
15	B2	836	CLA	C1D-ND-C4D	-2.85	104.31	106.33
15	B2	808	CLA	CHD-C4C-C3C	-2.85	120.64	124.84
15	K2	103	CLA	C3C-C2C-C1C	-2.85	103.79	107.21
15	B2	839	CLA	C2C-C1C-NC	2.85	112.64	109.97
15	B1	839	CLA	C2C-C1C-NC	2.85	112.64	109.97
15	B3	808	CLA	CHD-C4C-C3C	-2.85	120.65	124.84
15	B3	823	CLA	C1D-ND-C4D	-2.85	104.31	106.33
15	B3	827	CLA	C1D-ND-C4D	-2.85	104.31	106.33
15	A2	840	CLA	CHD-C4C-C3C	-2.85	120.65	124.84
15	A1	821	CLA	CHD-C4C-C3C	-2.85	120.53	124.98
15	B1	836	CLA	C1D-ND-C4D	-2.85	104.31	106.33
15	B2	819	CLA	CHD-C4C-C3C	-2.85	120.66	124.84
15	B2	829	CLA	CHD-C4C-C3C	-2.85	120.66	124.84
15	B1	808	CLA	CHD-C4C-C3C	-2.85	120.66	124.84
15	K2	103	CLA	C1D-ND-C4D	-2.85	104.31	106.33
15	A2	807	CLA	CHD-C4C-C3C	-2.85	120.66	124.84
15	B1	824	CLA	C1D-ND-C4D	-2.84	104.31	106.33
15	B3	817	CLA	CHD-C4C-C3C	-2.84	120.66	124.84
15	K1	103	CLA	C3C-C2C-C1C	-2.84	103.81	107.21
15	I1	101	CLA	C1D-ND-C4D	-2.84	104.32	106.33
15	B3	839	CLA	C2C-C1C-NC	2.84	112.63	109.97
15	B3	816	CLA	CHD-C4C-C3C	-2.84	120.67	124.84
15	B3	827	CLA	CHD-C4C-C3C	-2.84	120.67	124.84
15	K3	103	CLA	C3C-C2C-C1C	-2.84	103.81	107.21
15	B1	834	CLA	CHD-C4C-C3C	-2.84	120.67	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B2	827	CLA	CHD-C4C-C3C	-2.84	120.67	124.84
15	A3	820	CLA	CHD-C4C-C3C	-2.84	120.67	124.84
15	A2	820	CLA	CHD-C4C-C3C	-2.84	120.67	124.84
15	B2	812	CLA	C1D-ND-C4D	-2.84	104.32	106.33
15	B3	824	CLA	C1D-ND-C4D	-2.84	104.32	106.33
15	K3	103	CLA	C1D-ND-C4D	-2.84	104.32	106.33
15	B3	834	CLA	CHD-C4C-C3C	-2.84	120.67	124.84
15	B1	813	CLA	CHD-C4C-C3C	-2.84	120.67	124.84
15	B1	817	CLA	CHD-C4C-C3C	-2.83	120.68	124.84
15	A1	820	CLA	CHD-C4C-C3C	-2.83	120.68	124.84
15	B1	819	CLA	CHD-C4C-C3C	-2.83	120.68	124.84
15	B2	834	CLA	CHD-C4C-C3C	-2.83	120.68	124.84
15	B1	821	CLA	CHD-C4C-C3C	-2.83	120.68	124.84
15	B1	812	CLA	C1D-ND-C4D	-2.83	104.33	106.33
15	K1	103	CLA	C1D-ND-C4D	-2.83	104.33	106.33
15	B3	812	CLA	C1D-ND-C4D	-2.83	104.33	106.33
15	A1	805	CLA	CHD-C4C-C3C	-2.83	120.68	124.84
15	A1	803	CLA	C1-C2-C3	-2.83	121.15	126.04
15	A2	808	CLA	CHD-C4C-C3C	-2.83	120.68	124.84
15	A2	829	CLA	C2C-C1C-NC	2.83	112.62	109.97
15	A2	805	CLA	CHD-C4C-C3C	-2.83	120.69	124.84
15	A3	805	CLA	CHD-C4C-C3C	-2.83	120.69	124.84
15	B3	821	CLA	CHD-C4C-C3C	-2.83	120.69	124.84
15	B1	806	CLA	C1-C2-C3	-2.82	122.18	126.75
15	B2	821	CLA	CHD-C4C-C3C	-2.82	120.69	124.84
15	B3	806	CLA	C1-C2-C3	-2.82	122.18	126.75
15	A2	835	CLA	CHD-C4C-C3C	-2.82	120.69	124.84
15	B2	806	CLA	C1-C2-C3	-2.82	122.19	126.75
15	A1	837	CLA	C2C-C1C-NC	2.82	112.61	109.97
15	A2	837	CLA	C2C-C1C-NC	2.82	112.61	109.97
15	A3	803	CLA	C1-C2-C3	-2.82	121.17	126.04
15	A3	808	CLA	CHD-C4C-C3C	-2.82	120.70	124.84
15	A1	808	CLA	CHD-C4C-C3C	-2.82	120.70	124.84
15	B2	817	CLA	CHD-C4C-C3C	-2.82	120.70	124.84
15	J2	1301	CLA	C1D-ND-C4D	-2.82	104.33	106.33
15	J3	1307	CLA	C3C-C4C-NC	2.82	112.53	109.95
15	A1	835	CLA	CHD-C4C-C3C	-2.81	120.70	124.84
15	J3	1301	CLA	CAA-C2A-C3A	-2.81	109.53	116.10
15	B1	827	CLA	C1D-ND-C4D	-2.81	104.34	106.33
15	B3	815	CLA	C1D-ND-C4D	-2.81	104.34	106.33
15	A3	835	CLA	CHD-C4C-C3C	-2.81	120.71	124.84
15	A2	803	CLA	C1-C2-C3	-2.81	121.18	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J1	1301	CLA	C1D-ND-C4D	-2.81	104.34	106.33
15	A2	828	CLA	CHD-C4C-C3C	-2.81	120.71	124.84
15	A1	828	CLA	CHD-C4C-C3C	-2.81	120.71	124.84
15	A1	830	CLA	C2C-C1C-NC	2.81	112.60	109.97
15	J1	1301	CLA	CAA-C2A-C3A	-2.80	109.56	116.10
15	J2	1307	CLA	C3C-C4C-NC	2.80	112.52	109.95
15	A1	842	CLA	C1D-ND-C4D	-2.80	104.34	106.33
15	A3	837	CLA	C2C-C1C-NC	2.80	112.60	109.97
15	A1	843	CLA	CHD-C4C-C3C	-2.80	120.72	124.84
15	B2	827	CLA	C1D-ND-C4D	-2.80	104.35	106.33
15	B1	830	CLA	CHD-C4C-C3C	-2.80	120.73	124.84
15	A2	844	CLA	C2C-C1C-NC	2.80	112.59	109.97
15	B1	801	CLA	CHD-C4C-C3C	-2.80	120.73	124.84
15	A3	829	CLA	C2C-C1C-NC	2.80	112.59	109.97
15	A3	843	CLA	CHD-C4C-C3C	-2.80	120.73	124.84
15	A3	828	CLA	CHD-C4C-C3C	-2.80	120.73	124.84
15	B2	830	CLA	CHD-C4C-C3C	-2.80	120.73	124.84
15	A2	842	CLA	C1D-ND-C4D	-2.80	104.35	106.33
15	A3	828	CLA	C1D-ND-C4D	-2.80	104.35	106.33
15	B3	801	CLA	CHD-C4C-C3C	-2.80	120.73	124.84
15	A1	828	CLA	C1D-ND-C4D	-2.79	104.35	106.33
15	A1	844	CLA	C2C-C1C-NC	2.79	112.59	109.97
15	A2	830	CLA	C2C-C1C-NC	2.79	112.59	109.97
15	B2	801	CLA	CHD-C4C-C3C	-2.79	120.74	124.84
15	J2	1301	CLA	CAA-C2A-C3A	-2.79	109.58	116.10
15	B2	833	CLA	CHD-C4C-C3C	-2.79	120.74	124.84
15	B1	815	CLA	C1D-ND-C4D	-2.79	104.35	106.33
15	J3	1301	CLA	C1D-ND-C4D	-2.79	104.35	106.33
15	A2	828	CLA	C1D-ND-C4D	-2.79	104.36	106.33
15	B3	808	CLA	C1D-ND-C4D	-2.79	104.36	106.33
15	A1	819	CLA	CHD-C4C-C3C	-2.79	120.75	124.84
15	A3	830	CLA	C2C-C1C-NC	2.78	112.58	109.97
15	A1	834	CLA	C1D-ND-C4D	-2.78	104.36	106.33
15	A2	843	CLA	CHD-C4C-C3C	-2.78	120.75	124.84
15	A3	842	CLA	C1D-ND-C4D	-2.78	104.36	106.33
15	B3	833	CLA	CHD-C4C-C3C	-2.78	120.75	124.84
15	J1	1307	CLA	C3C-C4C-NC	2.78	112.50	109.95
15	B1	833	CLA	CHD-C4C-C3C	-2.78	120.76	124.84
15	B1	820	CLA	C1D-ND-C4D	-2.78	104.36	106.33
15	B2	839	CLA	C4A-NA-C1A	-2.78	105.46	106.71
15	A2	819	CLA	CHD-C4C-C3C	-2.77	120.76	124.84
15	A1	829	CLA	C2C-C1C-NC	2.77	112.57	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	844	CLA	C2C-C1C-NC	2.77	112.57	109.97
15	A2	832	CLA	C1D-ND-C4D	-2.77	104.37	106.33
15	B1	808	CLA	C1D-ND-C4D	-2.77	104.37	106.33
15	L3	1002	CLA	C1D-ND-C4D	-2.77	104.37	106.33
15	A2	824	CLA	C2C-C1C-NC	2.77	112.56	109.97
15	B3	809	CLA	C1-C2-C3	-2.77	121.26	126.04
15	B3	830	CLA	CHD-C4C-C3C	-2.77	120.77	124.84
15	A3	819	CLA	CHD-C4C-C3C	-2.76	120.78	124.84
15	B3	814	CLA	C1D-ND-C4D	-2.76	104.37	106.33
15	B1	817	CLA	C1D-ND-C4D	-2.76	104.37	106.33
15	B2	802	CLA	C1D-ND-C4D	-2.76	104.38	106.33
15	B2	820	CLA	C1D-ND-C4D	-2.76	104.38	106.33
15	A2	810	CLA	CHD-C4C-C3C	-2.76	120.69	124.98
15	X3	102	CLA	C2C-C1C-NC	2.76	112.55	109.97
15	L1	1002	CLA	C1D-ND-C4D	-2.75	104.38	106.33
15	B2	814	CLA	C1D-ND-C4D	-2.75	104.38	106.33
15	B1	830	CLA	C1D-ND-C4D	-2.75	104.38	106.33
15	A2	838	CLA	C1D-ND-C4D	-2.75	104.38	106.33
15	B2	808	CLA	C1D-ND-C4D	-2.75	104.38	106.33
15	A1	824	CLA	C2C-C1C-NC	2.75	112.55	109.97
15	B3	820	CLA	C1D-ND-C4D	-2.75	104.38	106.33
15	B3	830	CLA	C1D-ND-C4D	-2.75	104.38	106.33
15	A1	810	CLA	CHD-C4C-C3C	-2.75	120.71	124.98
15	B2	837	CLA	CHD-C4C-C3C	-2.75	120.80	124.84
15	B1	809	CLA	C1-C2-C3	-2.75	121.29	126.04
15	B1	804	CLA	C1-C2-C3	-2.75	121.29	126.04
15	B3	817	CLA	C1D-ND-C4D	-2.75	104.38	106.33
15	A2	834	CLA	C1D-ND-C4D	-2.74	104.39	106.33
15	B3	804	CLA	C1-C2-C3	-2.74	121.30	126.04
15	B2	803	CLA	CHD-C4C-C3C	-2.74	120.81	124.84
15	A1	838	CLA	C1D-ND-C4D	-2.74	104.39	106.33
15	A3	810	CLA	CHD-C4C-C3C	-2.74	120.72	124.98
15	B2	835	CLA	C2C-C1C-NC	2.74	112.54	109.97
15	A3	820	CLA	CAB-C3B-C4B	-2.74	124.25	128.46
15	L2	1002	CLA	C1D-ND-C4D	-2.74	104.39	106.33
15	B1	803	CLA	CHD-C4C-C3C	-2.74	120.81	124.84
15	B2	815	CLA	C1D-ND-C4D	-2.74	104.39	106.33
15	A2	814	CLA	CHD-C4C-C3C	-2.74	120.70	124.98
15	A3	822	CLA	CHD-C4C-C3C	-2.74	120.82	124.84
15	A1	814	CLA	CHD-C4C-C3C	-2.74	120.70	124.98
15	B3	803	CLA	CHD-C4C-C3C	-2.74	120.82	124.84
15	B2	809	CLA	C1-C2-C3	-2.74	121.31	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B2	804	CLA	C1-C2-C3	-2.74	121.31	126.04
15	B1	802	CLA	C1D-ND-C4D	-2.74	104.39	106.33
15	A2	823	CLA	CHD-C4C-C3C	-2.73	120.82	124.84
15	B1	814	CLA	C1D-ND-C4D	-2.73	104.39	106.33
15	B1	837	CLA	CHD-C4C-C3C	-2.73	120.82	124.84
15	X1	102	CLA	C2C-C1C-NC	2.73	112.53	109.97
15	A3	824	CLA	C2C-C1C-NC	2.73	112.53	109.97
15	A2	835	CLA	C1D-ND-C4D	-2.73	104.40	106.33
15	B2	849	CLA	C4A-NA-C1A	-2.72	105.48	106.71
15	B2	817	CLA	C1D-ND-C4D	-2.72	104.40	106.33
15	B2	825	CLA	C2C-C1C-NC	2.72	112.52	109.97
15	A1	832	CLA	C1D-ND-C4D	-2.72	104.40	106.33
15	A3	834	CLA	C1D-ND-C4D	-2.72	104.40	106.33
15	A3	838	CLA	C1D-ND-C4D	-2.72	104.40	106.33
15	B3	837	CLA	CHD-C4C-C3C	-2.72	120.84	124.84
15	B1	828	CLA	C1D-ND-C4D	-2.72	104.40	106.33
15	A2	820	CLA	CAB-C3B-C4B	-2.72	124.28	128.46
15	A1	823	CLA	CHD-C4C-C3C	-2.72	120.84	124.84
15	A1	835	CLA	C1D-ND-C4D	-2.72	104.40	106.33
15	B2	830	CLA	C1D-ND-C4D	-2.72	104.40	106.33
15	A1	820	CLA	CAB-C3B-C4B	-2.72	124.29	128.46
15	A3	814	CLA	CHD-C4C-C3C	-2.71	120.74	124.98
15	B1	835	CLA	C2C-C1C-NC	2.71	112.52	109.97
15	A3	823	CLA	CHD-C4C-C3C	-2.71	120.85	124.84
15	B3	802	CLA	C1D-ND-C4D	-2.71	104.41	106.33
15	B3	835	CLA	C2C-C1C-NC	2.71	112.51	109.97
15	K3	101	CLA	CHD-C4C-C3C	-2.71	120.74	124.98
15	B2	828	CLA	C1D-ND-C4D	-2.71	104.41	106.33
15	B3	825	CLA	C2C-C1C-NC	2.71	112.51	109.97
15	A1	831	CLA	CHD-C4C-C3C	-2.71	120.86	124.84
15	A2	822	CLA	CHD-C4C-C3C	-2.71	120.86	124.84
15	A3	831	CLA	CHD-C4C-C3C	-2.71	120.86	124.84
15	A3	806	CLA	C1-C2-C3	-2.71	121.36	126.04
15	K1	101	CLA	CHD-C4C-C3C	-2.71	120.75	124.98
15	B3	828	CLA	C1D-ND-C4D	-2.71	104.41	106.33
15	B3	829	CLA	CAD-CBD-CHA	-2.70	102.09	105.14
15	A1	822	CLA	CHD-C4C-C3C	-2.70	120.87	124.84
15	A1	856	CLA	CHD-C4C-C3C	-2.70	120.87	124.84
15	B2	829	CLA	CAD-CBD-CHA	-2.70	102.10	105.14
15	B2	828	CLA	C2C-C1C-NC	2.70	112.50	109.97
15	A2	839	CLA	C2C-C1C-NC	2.70	112.50	109.97
15	A2	856	CLA	CHD-C4C-C3C	-2.69	120.88	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K2	101	CLA	CHD-C4C-C3C	-2.69	120.77	124.98
15	A3	835	CLA	C1D-ND-C4D	-2.69	104.42	106.33
15	X2	102	CLA	C2C-C1C-NC	2.69	112.49	109.97
15	A1	839	CLA	C2C-C1C-NC	2.69	112.49	109.97
15	A2	831	CLA	CHD-C4C-C3C	-2.69	120.89	124.84
15	B1	839	CLA	C4A-NA-C1A	-2.69	105.50	106.71
15	B1	849	CLA	C4A-NA-C1A	-2.69	105.50	106.71
15	A3	809	CLA	CHD-C4C-C3C	-2.69	120.89	124.84
15	B3	806	CLA	C2C-C1C-NC	2.68	112.49	109.97
15	B3	839	CLA	C4A-NA-C1A	-2.68	105.50	106.71
15	B1	829	CLA	CAD-CBD-CHA	-2.68	102.12	105.14
15	A1	806	CLA	C1-C2-C3	-2.68	121.41	126.04
15	B1	828	CLA	C2C-C1C-NC	2.68	112.48	109.97
15	A3	856	CLA	CHD-C4C-C3C	-2.68	120.91	124.84
15	A3	843	CLA	C1D-ND-C4D	-2.67	104.44	106.33
15	B2	828	CLA	CHD-C4C-C3C	-2.67	120.91	124.84
15	A2	806	CLA	C1-C2-C3	-2.67	121.42	126.04
15	B1	825	CLA	C2C-C1C-NC	2.67	112.47	109.97
15	B2	801	CLA	C1D-ND-C4D	-2.67	104.44	106.33
15	A3	839	CLA	C2C-C1C-NC	2.67	112.47	109.97
15	B2	823	CLA	C2C-C1C-NC	2.66	112.47	109.97
15	B3	801	CLA	C1D-ND-C4D	-2.66	104.44	106.33
15	B3	804	CLA	C2C-C1C-NC	2.66	112.47	109.97
15	B1	804	CLA	C2C-C1C-NC	2.66	112.47	109.97
15	B1	823	CLA	C2C-C1C-NC	2.66	112.47	109.97
15	A3	824	CLA	C1D-ND-C4D	-2.66	104.44	106.33
15	A1	843	CLA	C1D-ND-C4D	-2.66	104.44	106.33
15	B1	806	CLA	C2C-C1C-NC	2.66	112.46	109.97
15	A1	809	CLA	CHD-C4C-C3C	-2.66	120.93	124.84
15	A2	804	CLA	CHD-C4C-C3C	-2.66	120.93	124.84
15	B3	803	CLA	C1-C2-C3	-2.66	121.45	126.04
15	A1	825	CLA	C2C-C1C-NC	2.66	112.46	109.97
15	A2	809	CLA	CHD-C4C-C3C	-2.66	120.93	124.84
15	B3	809	CLA	CHD-C4C-C3C	-2.65	120.94	124.84
15	A1	811	CLA	CHD-C4C-C3C	-2.65	120.94	124.84
15	B3	831	CLA	CAA-C2A-C3A	-2.65	109.91	116.10
15	B1	801	CLA	C1D-ND-C4D	-2.65	104.45	106.33
15	J2	1302	CLA	CAB-C3B-C4B	-2.65	124.39	128.46
15	A3	832	CLA	C1D-ND-C4D	-2.65	104.45	106.33
15	A3	811	CLA	CHD-C4C-C3C	-2.65	120.94	124.84
15	B2	831	CLA	C2C-C1C-NC	2.65	112.45	109.97
15	B1	833	CLA	CAB-C3B-C4B	-2.65	124.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	828	CLA	C2C-C1C-NC	2.65	112.45	109.97
15	A2	811	CLA	CHD-C4C-C3C	-2.65	120.95	124.84
15	A3	813	CLA	CAB-C3B-C4B	-2.65	124.39	128.46
15	B1	803	CLA	C1-C2-C3	-2.65	121.46	126.04
15	B3	823	CLA	C2C-C1C-NC	2.65	112.45	109.97
15	A1	824	CLA	C1D-ND-C4D	-2.65	104.45	106.33
15	B2	809	CLA	CHD-C4C-C3C	-2.64	120.95	124.84
15	B2	803	CLA	C1-C2-C3	-2.64	121.47	126.04
15	B1	831	CLA	CAA-C2A-C3A	-2.64	109.93	116.10
15	B2	817	CLA	CAA-C2A-C1A	-2.64	103.32	111.97
15	B2	806	CLA	C2C-C1C-NC	2.64	112.45	109.97
15	A3	815	CLA	C1C-C2C-C3C	-2.64	104.02	107.65
15	B2	824	CLA	CHD-C4C-C3C	-2.64	120.96	124.84
15	B1	809	CLA	CHD-C4C-C3C	-2.64	120.96	124.84
15	A3	804	CLA	CHD-C4C-C3C	-2.64	120.96	124.84
15	A1	813	CLA	CAB-C3B-C4B	-2.64	124.41	128.46
15	B2	831	CLA	CAA-C2A-C3A	-2.64	109.94	116.10
15	B2	833	CLA	CAB-C3B-C4B	-2.64	124.41	128.46
15	J3	1302	CLA	CAB-C3B-C4B	-2.64	124.41	128.46
15	B1	817	CLA	CAA-C2A-C1A	-2.64	103.34	111.97
15	B3	817	CLA	CAA-C2A-C1A	-2.64	103.34	111.97
15	B1	828	CLA	CHD-C4C-C3C	-2.63	120.97	124.84
15	A2	843	CLA	C1D-ND-C4D	-2.63	104.46	106.33
15	B2	804	CLA	C2C-C1C-NC	2.63	112.44	109.97
15	J1	1302	CLA	CAB-C3B-C4B	-2.63	124.42	128.46
15	A2	824	CLA	C1D-ND-C4D	-2.63	104.47	106.33
15	B2	832	CLA	C1D-ND-C4D	-2.63	104.47	106.33
15	J1	1303	CLA	CAB-C3B-C4B	-2.63	124.42	128.46
15	J2	1303	CLA	CAB-C3B-C4B	-2.63	124.42	128.46
15	B3	839	CLA	C1D-ND-C4D	-2.63	104.47	106.33
15	B3	824	CLA	CHD-C4C-C3C	-2.63	120.97	124.84
15	B3	833	CLA	CAB-C3B-C4B	-2.63	124.42	128.46
15	A1	804	CLA	CHD-C4C-C3C	-2.63	120.98	124.84
15	B1	831	CLA	C2C-C1C-NC	2.63	112.43	109.97
15	A3	825	CLA	C2C-C1C-NC	2.63	112.43	109.97
15	B2	839	CLA	C1D-ND-C4D	-2.63	104.47	106.33
15	B3	816	CLA	C1D-ND-C4D	-2.62	104.47	106.33
15	A2	832	CLA	C2C-C1C-NC	2.62	112.43	109.97
15	A1	843	CLA	C1-C2-C3	-2.62	121.51	126.04
15	B1	824	CLA	CHD-C4C-C3C	-2.62	120.98	124.84
15	B3	828	CLA	CHD-C4C-C3C	-2.62	120.99	124.84
15	A2	813	CLA	CAB-C3B-C4B	-2.62	124.44	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A1	815	CLA	C1C-C2C-C3C	-2.62	104.05	107.65
15	A3	843	CLA	C1-C2-C3	-2.62	121.51	126.04
15	B1	839	CLA	C1D-ND-C4D	-2.62	104.47	106.33
15	B3	849	CLA	C4A-NA-C1A	-2.62	105.53	106.71
15	A2	825	CLA	C2C-C1C-NC	2.61	112.42	109.97
15	A2	843	CLA	C1-C2-C3	-2.61	121.52	126.04
15	A1	832	CLA	C2C-C1C-NC	2.61	112.42	109.97
15	B2	810	CLA	C2C-C1C-NC	2.61	112.42	109.97
14	A2	801	CL0	C1B-CHB-C4A	-2.61	124.95	130.12
15	A3	834	CLA	C2C-C1C-NC	2.61	112.42	109.97
14	A3	801	CL0	CHA-C1A-NA	-2.61	120.42	126.40
15	J3	1303	CLA	CAB-C3B-C4B	-2.61	124.46	128.46
15	B3	822	CLA	C2C-C1C-NC	2.61	112.41	109.97
15	A3	821	CLA	C1-C2-C3	-2.61	121.53	126.04
14	A1	801	CL0	CHA-C1A-NA	-2.61	120.43	126.40
15	A2	802	CLA	CHD-C1D-C2D	2.61	130.94	125.48
15	X3	102	CLA	C1C-C2C-C3C	-2.60	104.68	107.07
14	A2	801	CL0	CHA-C1A-NA	-2.60	120.43	126.40
14	A3	801	CL0	C1B-CHB-C4A	-2.60	124.96	130.12
15	A1	821	CLA	C1-C2-C3	-2.60	121.54	126.04
15	X2	102	CLA	CAA-C2A-C3A	-2.60	110.03	116.10
15	X2	102	CLA	C1D-ND-C4D	-2.60	104.49	106.33
14	A1	801	CL0	C1B-CHB-C4A	-2.60	124.97	130.12
15	X3	102	CLA	CAA-C2A-C3A	-2.60	110.03	116.10
15	B1	816	CLA	C1D-ND-C4D	-2.60	104.49	106.33
15	A2	821	CLA	C1-C2-C3	-2.60	121.55	126.04
15	B1	810	CLA	C2C-C1C-NC	2.60	112.41	109.97
15	A3	832	CLA	C2C-C1C-NC	2.60	112.40	109.97
15	B2	816	CLA	C1D-ND-C4D	-2.60	104.49	106.33
15	A1	825	CLA	CHA-C1A-NA	-2.60	120.45	126.40
15	A2	815	CLA	C1C-C2C-C3C	-2.59	104.08	107.65
15	A3	825	CLA	CHA-C1A-NA	-2.59	120.46	126.40
15	A1	823	CLA	C2C-C1C-NC	2.59	112.40	109.97
15	X1	102	CLA	C1C-C2C-C3C	-2.59	104.69	107.07
15	A3	823	CLA	C2C-C1C-NC	2.59	112.40	109.97
15	B2	838	CLA	C2C-C1C-NC	2.59	112.40	109.97
15	A3	802	CLA	CHD-C1D-C2D	2.59	130.91	125.48
15	A1	834	CLA	C2C-C1C-NC	2.59	112.40	109.97
15	A3	830	CLA	C1-C2-C3	-2.59	121.57	126.04
15	B1	832	CLA	C1D-ND-C4D	-2.59	104.50	106.33
15	A1	802	CLA	CHD-C1D-C2D	2.59	130.91	125.48
15	B1	838	CLA	C2C-C1C-NC	2.58	112.39	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K3	103	CLA	C3C-C4C-NC	2.58	112.36	109.97
15	A2	825	CLA	CHA-C1A-NA	-2.58	120.48	126.40
15	X1	102	CLA	CAA-C2A-C3A	-2.58	110.07	116.10
15	A1	830	CLA	C1-C2-C3	-2.58	121.58	126.04
15	B3	831	CLA	C2C-C1C-NC	2.58	112.39	109.97
15	B3	832	CLA	C1D-ND-C4D	-2.58	104.50	106.33
15	A2	823	CLA	C2C-C1C-NC	2.58	112.39	109.97
15	A2	830	CLA	C1-C2-C3	-2.58	121.58	126.04
15	J2	1302	CLA	C1C-C2C-C3C	-2.58	104.70	107.07
15	X2	102	CLA	C1C-C2C-C3C	-2.57	104.71	107.07
15	A3	821	CLA	C1C-C2C-C3C	-2.57	104.71	107.07
15	K1	101	CLA	C2D-C1D-CHD	2.57	130.40	125.00
15	A2	834	CLA	C2C-C1C-NC	2.57	112.38	109.97
15	A2	843	CLA	C2C-C1C-NC	2.57	112.38	109.97
15	B1	822	CLA	C2C-C1C-NC	2.57	112.38	109.97
15	I1	101	CLA	C2C-C1C-NC	2.57	112.38	109.97
15	A1	821	CLA	C1C-C2C-C3C	-2.57	104.72	107.07
15	I3	101	CLA	C2C-C1C-NC	2.57	112.38	109.97
15	K3	101	CLA	C2D-C1D-CHD	2.57	130.39	125.00
15	A2	821	CLA	C1C-C2C-C3C	-2.57	104.72	107.07
15	J1	1302	CLA	C1C-C2C-C3C	-2.57	104.72	107.07
15	K2	101	CLA	C2D-C1D-CHD	2.57	130.38	125.00
15	J3	1302	CLA	C1C-C2C-C3C	-2.56	104.72	107.07
15	A2	819	CLA	C3A-C2A-C1A	-2.56	97.50	101.34
15	B3	807	CLA	CHD-C4C-C3C	-2.56	121.08	124.84
15	K2	103	CLA	C2A-C1A-CHA	2.56	126.68	122.71
15	A2	830	CLA	C4A-NA-C1A	-2.56	105.56	106.71
15	A2	835	CLA	C2C-C1C-NC	2.56	112.37	109.97
15	K2	103	CLA	C3C-C4C-NC	2.56	112.33	109.97
15	B3	849	CLA	C2C-C1C-NC	2.56	112.37	109.97
14	A2	801	CL0	CHD-C1D-ND	-2.56	122.11	124.45
15	B1	828	CLA	CHA-C1A-NA	-2.56	120.55	126.40
15	K1	103	CLA	C3C-C4C-NC	2.56	112.33	109.97
15	A1	814	CLA	CAB-C3B-C4B	-2.55	124.54	128.46
15	B3	816	CLA	C2C-C1C-NC	2.55	112.36	109.97
15	A1	819	CLA	C3A-C2A-C1A	-2.55	97.52	101.34
15	A3	819	CLA	C3A-C2A-C1A	-2.55	97.52	101.34
14	A3	801	CL0	CHD-C1D-ND	-2.55	122.11	124.45
15	B2	816	CLA	C2C-C1C-NC	2.55	112.36	109.97
15	A3	832	CLA	CHD-C1D-C2D	2.55	130.83	125.48
15	B1	849	CLA	C2C-C1C-NC	2.55	112.36	109.97
15	K1	103	CLA	C2A-C1A-CHA	2.55	126.66	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	814	CLA	CAB-C3B-C4B	-2.55	124.55	128.46
15	B3	810	CLA	C2C-C1C-NC	2.55	112.36	109.97
15	B1	807	CLA	CHD-C4C-C3C	-2.55	121.10	124.84
15	K3	103	CLA	C2A-C1A-CHA	2.54	126.66	122.71
15	A1	804	CLA	C1D-ND-C4D	-2.54	104.53	106.33
15	X1	102	CLA	C1D-ND-C4D	-2.54	104.53	106.33
15	A3	814	CLA	CAB-C3B-C4B	-2.54	124.56	128.46
15	B2	804	CLA	C1D-ND-C4D	-2.54	104.53	106.33
15	I2	101	CLA	C2C-C1C-NC	2.54	112.35	109.97
15	B1	827	CLA	C2C-C1C-NC	2.54	112.35	109.97
15	B2	828	CLA	CHA-C1A-NA	-2.54	120.58	126.40
15	B3	828	CLA	CHA-C1A-NA	-2.54	120.58	126.40
15	L1	1003	CLA	C2C-C1C-NC	2.54	112.35	109.97
15	L3	1003	CLA	C2C-C1C-NC	2.54	112.35	109.97
15	A3	804	CLA	C1D-ND-C4D	-2.54	104.53	106.33
15	A2	832	CLA	CHD-C1D-C2D	2.54	130.80	125.48
15	B3	838	CLA	C2C-C1C-NC	2.54	112.35	109.97
15	A1	843	CLA	C2C-C1C-NC	2.54	112.35	109.97
15	A1	832	CLA	CHD-C1D-C2D	2.53	130.80	125.48
15	B3	836	CLA	CHD-C1D-C2D	2.53	130.80	125.48
14	A1	801	CL0	CHD-C1D-ND	-2.53	122.12	124.45
15	L2	1003	CLA	C2C-C1C-NC	2.53	112.35	109.97
15	B1	836	CLA	CHD-C1D-C2D	2.53	130.79	125.48
15	B1	816	CLA	C2C-C1C-NC	2.53	112.34	109.97
15	B2	807	CLA	CHD-C4C-C3C	-2.53	121.12	124.84
15	I1	101	CLA	CHA-C1A-NA	-2.53	120.60	126.40
15	A1	821	CLA	C2C-C1C-NC	2.53	112.34	109.97
15	B2	822	CLA	C2C-C1C-NC	2.53	112.34	109.97
15	A3	843	CLA	C2C-C1C-NC	2.53	112.34	109.97
15	I3	101	CLA	CHA-C1A-NA	-2.53	120.61	126.40
15	B1	804	CLA	C1D-ND-C4D	-2.53	104.54	106.33
15	A3	839	CLA	C1D-ND-C4D	-2.53	104.54	106.33
15	B2	836	CLA	CHD-C1D-C2D	2.53	130.78	125.48
15	A2	804	CLA	C1D-ND-C4D	-2.53	104.54	106.33
15	B3	804	CLA	C1D-ND-C4D	-2.52	104.54	106.33
15	A1	835	CLA	C2C-C1C-NC	2.52	112.34	109.97
15	A1	839	CLA	C1D-ND-C4D	-2.52	104.54	106.33
15	A1	838	CLA	C2C-C1C-NC	2.52	112.33	109.97
15	L1	1004	CLA	C2C-C1C-NC	2.52	112.33	109.97
15	A3	820	CLA	C2C-C1C-NC	2.52	112.33	109.97
15	A3	821	CLA	C2C-C1C-NC	2.52	112.33	109.97
15	I2	101	CLA	CHA-C1A-NA	-2.52	120.62	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	839	CLA	C1D-ND-C4D	-2.52	104.54	106.33
15	B3	827	CLA	C2C-C1C-NC	2.52	112.33	109.97
16	B1	840	PQN	C11-C3-C4	-2.52	115.81	118.50
15	J2	1302	CLA	C2C-C1C-NC	2.52	112.33	109.97
15	B2	823	CLA	CHA-C1A-NA	-2.52	120.64	126.40
15	B2	827	CLA	C2C-C1C-NC	2.52	112.33	109.97
15	B1	823	CLA	CHA-C1A-NA	-2.52	120.64	126.40
15	A1	820	CLA	C2C-C1C-NC	2.51	112.33	109.97
15	B1	807	CLA	C1D-ND-C4D	-2.51	104.55	106.33
15	B1	809	CLA	C2C-C1C-NC	2.51	112.33	109.97
15	B2	807	CLA	C1D-ND-C4D	-2.51	104.55	106.33
15	B3	823	CLA	CHA-C1A-NA	-2.51	120.65	126.40
15	A3	814	CLA	C1C-C2C-C3C	-2.51	104.77	107.07
16	B2	840	PQN	C11-C3-C4	-2.51	115.81	118.50
15	B2	826	CLA	C1D-ND-C4D	-2.51	104.55	106.33
15	L3	1004	CLA	C2C-C1C-NC	2.51	112.32	109.97
15	B1	807	CLA	CHD-C1D-C2D	2.51	130.74	125.48
15	B3	807	CLA	C1D-ND-C4D	-2.51	104.55	106.33
15	A2	821	CLA	C2C-C1C-NC	2.51	112.32	109.97
15	A2	833	CLA	C2C-C1C-NC	2.51	112.32	109.97
15	A2	838	CLA	C2C-C1C-NC	2.51	112.32	109.97
15	B2	849	CLA	C2C-C1C-NC	2.51	112.32	109.97
15	B2	807	CLA	CHD-C1D-C2D	2.50	130.73	125.48
15	A1	806	CLA	C2C-C1C-NC	2.50	112.32	109.97
15	A2	820	CLA	C2C-C1C-NC	2.50	112.32	109.97
15	L2	1004	CLA	C2C-C1C-NC	2.50	112.32	109.97
15	B3	809	CLA	C2C-C1C-NC	2.50	112.32	109.97
15	B3	812	CLA	C2C-C1C-NC	2.50	112.32	109.97
15	B2	809	CLA	C2C-C1C-NC	2.50	112.31	109.97
15	A3	835	CLA	C2C-C1C-NC	2.50	112.31	109.97
15	X3	102	CLA	C1D-ND-C4D	-2.50	104.56	106.33
15	A1	830	CLA	C4A-NA-C1A	-2.50	105.58	106.71
15	B3	807	CLA	CHD-C1D-C2D	2.50	130.72	125.48
15	B2	807	CLA	CHA-C1A-NA	-2.50	120.68	126.40
16	B3	840	PQN	C11-C3-C4	-2.50	115.83	118.50
15	A3	838	CLA	C2C-C1C-NC	2.50	112.31	109.97
15	A3	806	CLA	C2C-C1C-NC	2.49	112.31	109.97
15	J1	1302	CLA	C2C-C1C-NC	2.49	112.31	109.97
15	B1	807	CLA	CHA-C1A-NA	-2.49	120.70	126.40
15	B3	807	CLA	CHA-C1A-NA	-2.49	120.70	126.40
15	B2	835	CLA	CHA-C1A-NA	-2.49	120.70	126.40
15	B1	835	CLA	CHA-C1A-NA	-2.49	120.70	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	817	CLA	CAA-C2A-C1A	-2.49	105.67	111.81
15	A3	817	CLA	CAA-C2A-C1A	-2.49	105.67	111.81
15	B3	835	CLA	CHA-C1A-NA	-2.49	120.71	126.40
15	J3	1303	CLA	C1C-C2C-C3C	-2.49	104.79	107.07
15	B2	832	CLA	CHD-C1D-C2D	2.48	130.69	125.48
15	B3	817	CLA	C2C-C1C-NC	2.48	112.30	109.97
15	J3	1302	CLA	C2C-C1C-NC	2.48	112.30	109.97
15	B1	812	CLA	C2C-C1C-NC	2.48	112.30	109.97
15	B2	805	CLA	C2C-C1C-NC	2.48	112.30	109.97
15	A1	817	CLA	CAA-C2A-C1A	-2.48	105.68	111.81
15	B3	805	CLA	C2C-C1C-NC	2.48	112.30	109.97
15	A1	814	CLA	C1C-C2C-C3C	-2.48	104.80	107.07
15	A2	806	CLA	C2C-C1C-NC	2.48	112.29	109.97
15	A3	833	CLA	C2C-C1C-NC	2.48	112.29	109.97
15	A1	833	CLA	C2C-C1C-NC	2.48	112.29	109.97
15	B1	817	CLA	C2C-C1C-NC	2.48	112.29	109.97
15	B1	826	CLA	C1D-ND-C4D	-2.48	104.58	106.33
15	B3	832	CLA	CHD-C1D-C2D	2.48	130.67	125.48
15	B3	811	CLA	C2C-C1C-NC	2.48	112.29	109.97
15	B2	820	CLA	CHD-C1D-C2D	2.47	130.67	125.48
15	B2	802	CLA	CHD-C1D-C2D	2.47	130.67	125.48
15	B2	817	CLA	C2C-C1C-NC	2.47	112.29	109.97
15	B2	820	CLA	C2C-C1C-NC	2.47	112.29	109.97
15	A3	830	CLA	C4A-NA-C1A	-2.47	105.59	106.71
15	B1	820	CLA	CHD-C1D-C2D	2.47	130.66	125.48
15	B1	805	CLA	C2C-C1C-NC	2.47	112.28	109.97
15	B1	832	CLA	CHD-C1D-C2D	2.47	130.66	125.48
15	B2	820	CLA	CHA-C1A-NA	-2.47	120.86	126.41
15	B3	820	CLA	CHA-C1A-NA	-2.47	120.86	126.41
15	B2	812	CLA	C2C-C1C-NC	2.47	112.28	109.97
15	A2	812	CLA	C1C-C2C-C3C	-2.47	104.81	107.07
15	B1	814	CLA	C2C-C1C-NC	2.46	112.28	109.97
15	A2	813	CLA	C2C-C1C-NC	2.46	112.28	109.97
15	B3	820	CLA	CHD-C1D-C2D	2.46	130.65	125.48
16	A3	845	PQN	C11-C3-C4	-2.46	115.87	118.50
15	B3	826	CLA	C1D-ND-C4D	-2.46	104.59	106.33
15	A1	813	CLA	C2C-C1C-NC	2.46	112.28	109.97
15	K3	103	CLA	CHD-C1D-C2D	2.46	130.64	125.48
15	J2	1303	CLA	C1C-C2C-C3C	-2.46	104.81	107.07
15	A3	804	CLA	C2C-C1C-NC	2.46	112.28	109.97
15	A2	836	CLA	CHD-C1D-C2D	2.46	130.64	125.48
15	A2	832	CLA	C1C-C2C-C3C	-2.46	104.37	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B2	825	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
15	B1	820	CLA	CHA-C1A-NA	-2.46	120.89	126.41
15	B1	802	CLA	CHD-C1D-C2D	2.46	130.63	125.48
15	A3	832	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
15	A1	832	CLA	C1C-C2C-C3C	-2.46	104.38	106.96
15	A3	813	CLA	C2C-C1C-NC	2.46	112.27	109.97
15	B3	825	CLA	CHC-C1C-C2C	-2.45	119.93	126.72
15	A2	814	CLA	C1C-C2C-C3C	-2.45	104.82	107.07
15	B2	814	CLA	C2C-C1C-NC	2.45	112.27	109.97
15	B3	809	CLA	C1D-ND-C4D	-2.45	104.59	106.33
15	A3	836	CLA	CHD-C1D-C2D	2.45	130.63	125.48
15	A1	836	CLA	CHD-C1D-C2D	2.45	130.62	125.48
15	A3	812	CLA	C1C-C2C-C3C	-2.45	104.82	107.07
15	J1	1303	CLA	C1C-C2C-C3C	-2.45	104.82	107.07
15	B1	825	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
15	B1	832	CLA	CHD-C4C-C3C	-2.45	121.24	124.84
15	B1	849	CLA	C1D-ND-C4D	-2.45	104.59	106.33
16	A1	845	PQN	C11-C3-C4	-2.45	115.88	118.50
15	B2	809	CLA	CHD-C1D-C2D	2.45	130.62	125.48
15	B3	814	CLA	C2C-C1C-NC	2.45	112.27	109.97
15	B3	837	CLA	CHD-C1D-C2D	2.45	130.61	125.48
15	J1	1301	CLA	C2C-C1C-NC	2.45	112.26	109.97
15	B3	849	CLA	C1D-ND-C4D	-2.45	104.60	106.33
15	K1	103	CLA	CHD-C1D-C2D	2.45	130.61	125.48
15	A1	812	CLA	C1C-C2C-C3C	-2.44	104.83	107.07
16	A2	845	PQN	C11-C3-C4	-2.44	115.89	118.50
15	B3	802	CLA	CHD-C1D-C2D	2.44	130.61	125.48
15	A1	830	CLA	C1D-ND-C4D	-2.44	104.60	106.33
15	B1	820	CLA	C2C-C1C-NC	2.44	112.26	109.97
15	B1	811	CLA	C2C-C1C-NC	2.44	112.26	109.97
15	J3	1301	CLA	C2C-C1C-NC	2.44	112.26	109.97
15	B2	829	CLA	CHD-C1D-C2D	2.44	130.60	125.48
15	A3	830	CLA	C1D-ND-C4D	-2.44	104.60	106.33
15	B1	829	CLA	CHD-C1D-C2D	2.44	130.60	125.48
15	B2	837	CLA	CHD-C1D-C2D	2.44	130.59	125.48
15	K2	103	CLA	CHD-C1D-C2D	2.44	130.59	125.48
15	A3	826	CLA	C1-C2-C3	-2.44	121.83	126.04
15	A2	804	CLA	C2C-C1C-NC	2.44	112.25	109.97
15	J2	1301	CLA	C2C-C1C-NC	2.44	112.25	109.97
15	B3	809	CLA	CHD-C1D-C2D	2.44	130.59	125.48
15	B1	809	CLA	CHD-C1D-C2D	2.44	130.59	125.48
15	B2	828	CLA	CHD-C1D-C2D	2.43	130.59	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B2	811	CLA	C2C-C1C-NC	2.43	112.25	109.97
15	B2	832	CLA	CHD-C4C-C3C	-2.43	121.27	124.84
15	A1	826	CLA	C1-C2-C3	-2.43	121.84	126.04
15	B3	829	CLA	CHD-C1D-C2D	2.43	130.57	125.48
15	A1	804	CLA	C2C-C1C-NC	2.43	112.25	109.97
15	B3	832	CLA	CHD-C4C-C3C	-2.43	121.27	124.84
15	J2	1302	CLA	CHD-C1D-C2D	2.43	130.57	125.48
15	A3	842	CLA	CHD-C1D-C2D	2.43	130.57	125.48
15	A2	826	CLA	C1-C2-C3	-2.43	121.85	126.04
15	B1	816	CLA	CHD-C1D-C2D	2.43	130.57	125.48
15	B1	837	CLA	CHD-C1D-C2D	2.43	130.57	125.48
15	B3	816	CLA	CHD-C1D-C2D	2.42	130.56	125.48
15	A2	842	CLA	CHD-C1D-C2D	2.42	130.56	125.48
15	A1	834	CLA	CHD-C1D-C2D	2.42	130.56	125.48
15	A2	830	CLA	C1D-ND-C4D	-2.42	104.61	106.33
15	B1	828	CLA	CHD-C1D-C2D	2.42	130.56	125.48
15	B3	815	CLA	CHD-C1D-C2D	2.42	130.56	125.48
15	A1	842	CLA	CHD-C1D-C2D	2.42	130.56	125.48
15	A2	839	CLA	CHD-C1D-C2D	2.42	130.56	125.48
15	A2	818	CLA	C2C-C1C-NC	2.42	112.24	109.97
15	B2	849	CLA	C1D-ND-C4D	-2.42	104.62	106.33
15	A1	818	CLA	C2C-C1C-NC	2.42	112.24	109.97
15	B3	828	CLA	CHD-C1D-C2D	2.42	130.55	125.48
15	B2	816	CLA	CHD-C1D-C2D	2.42	130.55	125.48
15	A3	839	CLA	CHD-C1D-C2D	2.42	130.55	125.48
15	A3	818	CLA	C2C-C1C-NC	2.42	112.23	109.97
15	A3	832	CLA	CAA-C2A-C1A	-2.41	104.06	111.97
19	X1	101	LHG	O8-C23-C24	2.41	119.48	111.91
15	B1	815	CLA	CHD-C1D-C2D	2.41	130.54	125.48
15	A2	832	CLA	CAA-C2A-C1A	-2.41	104.07	111.97
15	B2	813	CLA	CHD-C1D-C2D	2.41	130.54	125.48
19	X2	101	LHG	O8-C23-C24	2.41	119.48	111.91
15	A1	833	CLA	CHD-C1D-C2D	2.41	130.54	125.48
15	J1	1302	CLA	CHD-C1D-C2D	2.41	130.54	125.48
15	A2	809	CLA	CHA-C1A-NA	-2.41	120.88	126.40
19	X3	101	LHG	O8-C23-C24	2.41	119.47	111.91
15	A2	834	CLA	CHD-C1D-C2D	2.41	130.53	125.48
15	B3	813	CLA	C2C-C1C-NC	2.41	112.23	109.97
15	B1	808	CLA	C2A-C1A-CHA	2.41	128.07	123.86
15	A1	832	CLA	CAA-C2A-C1A	-2.41	104.08	111.97
15	B2	849	CLA	CHD-C1D-C2D	2.41	130.53	125.48
15	A3	833	CLA	CHD-C1D-C2D	2.41	130.53	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J3	1302	CLA	CHD-C1D-C2D	2.41	130.53	125.48
15	A3	804	CLA	CHD-C1D-C2D	2.41	130.53	125.48
15	A1	839	CLA	CHD-C1D-C2D	2.41	130.53	125.48
15	B3	820	CLA	C2C-C1C-NC	2.41	112.23	109.97
15	B3	830	CLA	CHD-C1D-C2D	2.41	130.53	125.48
15	B3	808	CLA	C2A-C1A-CHA	2.41	128.06	123.86
15	B3	816	CLA	CHA-C1A-NA	-2.40	121.00	126.41
15	B2	816	CLA	CHA-C1A-NA	-2.40	121.00	126.41
15	B1	808	CLA	C3A-C2A-C1A	-2.40	97.74	101.34
15	A3	809	CLA	CHA-C1A-NA	-2.40	120.89	126.40
15	A3	834	CLA	CHD-C1D-C2D	2.40	130.52	125.48
15	B1	816	CLA	CHA-C1A-NA	-2.40	121.01	126.41
15	A2	824	CLA	CHD-C1D-C2D	2.40	130.52	125.48
15	A3	814	CLA	CHD-C1D-C2D	2.40	130.52	125.48
15	A1	809	CLA	CHA-C1A-NA	-2.40	120.90	126.40
15	B1	813	CLA	C2C-C1C-NC	2.40	112.22	109.97
15	A3	818	CLA	CHD-C1D-C2D	2.40	130.51	125.48
15	A2	809	CLA	C2C-C1C-NC	2.40	112.22	109.97
15	B2	808	CLA	C3A-C2A-C1A	-2.40	97.75	101.34
15	A1	818	CLA	CHD-C1D-C2D	2.40	130.51	125.48
15	A2	838	CLA	CHA-C1A-NA	-2.40	120.91	126.40
15	A2	833	CLA	CHD-C1D-C2D	2.40	130.50	125.48
15	B3	808	CLA	C3A-C2A-C1A	-2.39	97.75	101.34
15	A2	818	CLA	CHD-C1D-C2D	2.39	130.50	125.48
15	A1	837	CLA	CHA-C1A-NA	-2.39	120.92	126.40
15	B3	809	CLA	CHA-C1A-NA	-2.39	120.92	126.40
15	A2	837	CLA	CHA-C1A-NA	-2.39	120.92	126.40
15	A1	804	CLA	CHD-C1D-C2D	2.39	130.50	125.48
15	A1	817	CLA	C1C-C2C-C3C	-2.39	104.88	107.07
15	B1	813	CLA	CHD-C1D-C2D	2.39	130.50	125.48
15	A3	824	CLA	CHD-C1D-C2D	2.39	130.50	125.48
15	B2	808	CLA	C2A-C1A-CHA	2.39	128.04	123.86
15	A2	833	CLA	C1D-ND-C4D	-2.39	104.64	106.33
15	B2	809	CLA	C1D-ND-C4D	-2.39	104.64	106.33
15	K3	101	CLA	CAD-CBD-CHA	-2.39	102.45	105.14
15	A1	826	CLA	CHD-C1D-C2D	2.39	130.49	125.48
15	A3	817	CLA	C1C-C2C-C3C	-2.39	104.88	107.07
15	B3	813	CLA	CHD-C1D-C2D	2.39	130.49	125.48
15	A3	837	CLA	CHA-C1A-NA	-2.39	120.93	126.40
15	B2	815	CLA	CHD-C1D-C2D	2.39	130.49	125.48
15	B1	833	CLA	CHD-C1D-C2D	2.39	130.49	125.48
15	B2	825	CLA	CHA-C1A-NA	-2.39	120.93	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A1	819	CLA	CHD-C1D-C2D	2.39	130.49	125.48
15	A1	824	CLA	CHD-C1D-C2D	2.39	130.48	125.48
15	A2	819	CLA	CHD-C1D-C2D	2.39	130.48	125.48
15	A1	814	CLA	CHD-C1D-C2D	2.39	130.48	125.48
15	B1	849	CLA	CHD-C1D-C2D	2.39	130.48	125.48
15	A3	819	CLA	CHD-C1D-C2D	2.39	130.48	125.48
15	B1	830	CLA	CHD-C1D-C2D	2.38	130.48	125.48
15	A3	812	CLA	C2C-C1C-NC	2.38	112.21	109.97
15	K2	101	CLA	CAD-CBD-CHA	-2.38	102.45	105.14
15	B1	809	CLA	CHA-C1A-NA	-2.38	120.94	126.40
15	B2	805	CLA	CAA-C2A-C1A	-2.38	104.16	111.97
15	A2	817	CLA	C1C-C2C-C3C	-2.38	104.89	107.07
15	B3	836	CLA	C2C-C1C-NC	2.38	112.20	109.97
15	B3	805	CLA	CAA-C2A-C1A	-2.38	104.17	111.97
15	B2	839	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
15	A2	841	CLA	C2C-C1C-NC	2.38	112.20	109.97
15	A2	856	CLA	CHD-C1D-C2D	2.38	130.47	125.48
15	A2	807	CLA	CHD-C1D-C2D	2.38	130.47	125.48
15	A2	826	CLA	CHD-C1D-C2D	2.38	130.47	125.48
15	A2	840	CLA	CHD-C1D-C2D	2.38	130.47	125.48
15	A3	807	CLA	CHD-C1D-C2D	2.38	130.47	125.48
15	L1	1002	CLA	CHA-C1A-NA	-2.38	120.95	126.40
15	B1	805	CLA	CAA-C2A-C1A	-2.38	104.18	111.97
15	B1	809	CLA	C1D-ND-C4D	-2.38	104.65	106.33
15	A2	814	CLA	CHD-C1D-C2D	2.38	130.47	125.48
15	B1	836	CLA	C2C-C1C-NC	2.38	112.20	109.97
15	B3	825	CLA	CHA-C1A-NA	-2.38	120.95	126.40
15	B2	830	CLA	CHD-C1D-C2D	2.38	130.47	125.48
15	B3	838	CLA	CHD-C1D-C2D	2.38	130.47	125.48
15	A2	804	CLA	CHD-C1D-C2D	2.38	130.46	125.48
15	B1	839	CLA	CHD-C1D-C2D	2.37	130.46	125.48
15	B1	825	CLA	CHA-C1A-NA	-2.37	120.96	126.40
15	B1	839	CLA	C1C-C2C-C3C	-2.37	104.46	106.96
15	A3	838	CLA	CHA-C1A-NA	-2.37	120.96	126.40
15	L3	1002	CLA	CHC-C1C-C2C	-2.37	120.16	126.72
15	A2	815	CLA	CHD-C1D-C2D	2.37	130.46	125.48
15	B2	833	CLA	CHD-C1D-C2D	2.37	130.46	125.48
15	A2	835	CLA	CHD-C1D-C2D	2.37	130.46	125.48
15	B1	837	CLA	C2C-C1C-NC	2.37	112.19	109.97
15	B2	836	CLA	C2C-C1C-NC	2.37	112.19	109.97
15	A3	826	CLA	CHD-C1D-C2D	2.37	130.46	125.48
15	A3	856	CLA	CHD-C1D-C2D	2.37	130.46	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	815	CLA	CHD-C1D-C2D	2.37	130.46	125.48
15	L1	1002	CLA	CHC-C1C-C2C	-2.37	120.16	126.72
15	B1	813	CLA	CHA-C1A-NA	-2.37	120.97	126.40
15	B3	813	CLA	CHA-C1A-NA	-2.37	120.97	126.40
15	K2	101	CLA	C1C-C2C-C3C	-2.37	104.90	107.07
15	A1	831	CLA	CHD-C1D-C2D	2.37	130.45	125.48
15	A2	823	CLA	CAA-C2A-C1A	-2.37	105.95	111.81
15	A1	856	CLA	CHD-C1D-C2D	2.37	130.45	125.48
15	B2	839	CLA	CHD-C1D-C2D	2.37	130.45	125.48
15	L3	1003	CLA	CHD-C1D-C2D	2.37	130.45	125.48
15	A1	835	CLA	CHD-C1D-C2D	2.37	130.45	125.48
15	A3	831	CLA	CHD-C1D-C2D	2.37	130.45	125.48
15	A1	838	CLA	CHA-C1A-NA	-2.37	120.98	126.40
15	K1	101	CLA	CAD-CBD-CHA	-2.37	102.47	105.14
15	L2	1002	CLA	CHC-C1C-C2C	-2.37	120.17	126.72
15	A2	812	CLA	C2C-C1C-NC	2.37	112.19	109.97
15	B2	813	CLA	C2C-C1C-NC	2.37	112.19	109.97
15	J3	1307	CLA	C2C-C1C-NC	2.37	112.19	109.97
15	A1	823	CLA	CAA-C2A-C1A	-2.37	105.96	111.81
15	A3	823	CLA	CAA-C2A-C1A	-2.37	105.97	111.81
15	B1	849	CLA	CHA-C1A-NA	-2.37	120.98	126.40
15	L2	1002	CLA	CHA-C1A-NA	-2.37	120.98	126.40
15	A2	811	CLA	CHD-C1D-C2D	2.37	130.44	125.48
15	A1	830	CLA	CHC-C1C-C2C	-2.36	120.18	126.72
15	B3	839	CLA	CHD-C1D-C2D	2.36	130.44	125.48
15	A1	815	CLA	CHD-C1D-C2D	2.36	130.44	125.48
15	B3	817	CLA	CHD-C1D-C2D	2.36	130.44	125.48
15	B3	833	CLA	CHD-C1D-C2D	2.36	130.44	125.48
15	A3	830	CLA	CHC-C1C-C2C	-2.36	120.18	126.72
15	B3	839	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
15	A1	840	CLA	CHD-C1D-C2D	2.36	130.44	125.48
15	L3	1002	CLA	CHA-C1A-NA	-2.36	120.98	126.40
15	A1	833	CLA	C1D-ND-C4D	-2.36	104.66	106.33
15	A3	833	CLA	C1D-ND-C4D	-2.36	104.66	106.33
15	A1	807	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	B2	817	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	A3	840	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	B2	809	CLA	CHA-C1A-NA	-2.36	120.99	126.40
15	B2	835	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	B1	823	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
15	B2	817	CLA	CHA-C1A-NA	-2.36	120.99	126.40
15	B1	838	CLA	CHD-C1D-C2D	2.36	130.43	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	849	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	A3	811	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	A3	830	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	A1	812	CLA	C2C-C1C-NC	2.36	112.18	109.97
15	A2	831	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	A2	838	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	B1	834	CLA	C2C-C1C-NC	2.36	112.18	109.97
15	A3	814	CLA	CAD-CBD-CHA	-2.36	102.48	105.14
15	B2	823	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
15	B2	849	CLA	CHA-C1A-NA	-2.36	121.00	126.40
15	A2	830	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
15	L1	1003	CLA	CHD-C1D-C2D	2.36	130.43	125.48
15	K1	101	CLA	C1C-C2C-C3C	-2.36	104.91	107.07
15	B2	838	CLA	CHD-C1D-C2D	2.36	130.42	125.48
15	A1	838	CLA	CAA-C2A-C1A	-2.36	104.25	111.97
15	A3	838	CLA	CAA-C2A-C1A	-2.36	104.25	111.97
15	B1	817	CLA	CHD-C1D-C2D	2.36	130.42	125.48
15	B2	835	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
15	A3	856	CLA	C1D-ND-C4D	-2.36	104.66	106.33
15	A1	823	CLA	CHD-C1D-C2D	2.36	130.42	125.48
15	B3	831	CLA	CHD-C1D-C2D	2.36	130.42	125.48
15	A1	856	CLA	C1D-ND-C4D	-2.36	104.66	106.33
15	B3	803	CLA	C1D-ND-C4D	-2.36	104.66	106.33
15	B2	813	CLA	CHA-C1A-NA	-2.35	121.00	126.40
15	A1	811	CLA	CHD-C1D-C2D	2.35	130.42	125.48
15	B3	849	CLA	CHA-C1A-NA	-2.35	121.01	126.40
15	A2	823	CLA	CHD-C1D-C2D	2.35	130.42	125.48
15	A1	838	CLA	CHD-C1D-C2D	2.35	130.42	125.48
15	B1	810	CLA	CHD-C1D-C2D	2.35	130.42	125.48
15	A3	809	CLA	C2C-C1C-NC	2.35	112.18	109.97
15	B3	834	CLA	C2C-C1C-NC	2.35	112.18	109.97
15	A2	816	CLA	CHD-C1D-C2D	2.35	130.42	125.48
15	A3	835	CLA	CHD-C1D-C2D	2.35	130.41	125.48
15	B3	810	CLA	CHD-C1D-C2D	2.35	130.41	125.48
15	A3	838	CLA	CHD-C1D-C2D	2.35	130.41	125.48
15	B1	835	CLA	CHD-C1D-C2D	2.35	130.41	125.48
15	A1	805	CLA	C2C-C1C-NC	2.35	112.17	109.97
15	A1	809	CLA	C2C-C1C-NC	2.35	112.17	109.97
15	B2	824	CLA	CHD-C1D-C2D	2.35	130.41	125.48
15	B1	831	CLA	CHD-C1D-C2D	2.35	130.41	125.48
15	B2	822	CLA	CHD-C1D-C2D	2.35	130.41	125.48
15	A2	829	CLA	CHA-C1A-NA	-2.35	121.02	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	830	CLA	C2C-C1C-NC	2.35	112.17	109.97
15	A3	823	CLA	CHD-C1D-C2D	2.35	130.41	125.48
15	B3	835	CLA	CHD-C1D-C2D	2.35	130.41	125.48
15	A1	807	CLA	C2C-C1C-NC	2.35	112.17	109.97
15	B3	823	CLA	CHC-C1C-C2C	-2.35	120.23	126.72
15	A1	807	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
15	B1	817	CLA	CHA-C1A-NA	-2.35	121.02	126.40
15	B2	810	CLA	CHD-C1D-C2D	2.35	130.40	125.48
15	A3	829	CLA	CHA-C1A-NA	-2.35	121.02	126.40
15	K3	101	CLA	C1C-C2C-C3C	-2.35	104.92	107.07
15	B1	835	CLA	CHC-C1C-C2C	-2.35	120.23	126.72
15	A1	829	CLA	CHA-C1A-NA	-2.35	121.03	126.40
15	B1	803	CLA	C1D-ND-C4D	-2.35	104.67	106.33
15	B1	830	CLA	C2C-C1C-NC	2.35	112.17	109.97
15	A1	814	CLA	CAD-CBD-CHA	-2.34	102.50	105.14
15	B1	824	CLA	CHD-C1D-C2D	2.34	130.40	125.48
15	A2	828	CLA	CHD-C1D-C2D	2.34	130.40	125.48
15	A3	805	CLA	CHD-C1D-C2D	2.34	130.40	125.48
15	B2	837	CLA	C2C-C1C-NC	2.34	112.17	109.97
15	B3	824	CLA	CHD-C1D-C2D	2.34	130.40	125.48
15	L2	1003	CLA	CHD-C1D-C2D	2.34	130.40	125.48
15	B3	835	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
15	B2	830	CLA	C2C-C1C-NC	2.34	112.17	109.97
15	A3	816	CLA	CHD-C1D-C2D	2.34	130.39	125.48
15	A1	841	CLA	C2C-C1C-NC	2.34	112.17	109.97
15	A2	807	CLA	C2C-C1C-NC	2.34	112.17	109.97
15	A3	841	CLA	C2C-C1C-NC	2.34	112.17	109.97
15	B2	801	CLA	CHD-C1D-C2D	2.34	130.39	125.48
15	B2	831	CLA	CHD-C1D-C2D	2.34	130.39	125.48
15	L2	1004	CLA	CHD-C1D-C2D	2.34	130.39	125.48
15	A2	807	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
15	A2	838	CLA	CAA-C2A-C1A	-2.34	104.31	111.97
15	A2	814	CLA	CAD-CBD-CHA	-2.34	102.50	105.14
15	A1	830	CLA	CHD-C1D-C2D	2.34	130.39	125.48
15	A2	844	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
15	B3	837	CLA	C2C-C1C-NC	2.34	112.16	109.97
15	B3	817	CLA	CHA-C1A-NA	-2.34	121.04	126.40
15	A1	816	CLA	CHD-C1D-C2D	2.34	130.38	125.48
15	A3	816	CLA	C2C-C1C-NC	2.34	112.16	109.97
15	A1	828	CLA	CHD-C1D-C2D	2.34	130.38	125.48
15	A2	805	CLA	CHD-C1D-C2D	2.34	130.38	125.48
15	J2	1307	CLA	CHD-C1D-C2D	2.34	130.38	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B2	834	CLA	C2C-C1C-NC	2.34	112.16	109.97
15	B2	804	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
15	B1	804	CLA	CHD-C1D-C2D	2.34	130.38	125.48
15	A3	828	CLA	CHD-C1D-C2D	2.33	130.38	125.48
15	A2	842	CLA	C2C-C1C-NC	2.33	112.16	109.97
15	A3	825	CLA	C1-C2-C3	-2.33	122.01	126.04
15	A3	807	CLA	C2C-C1C-NC	2.33	112.16	109.97
15	J1	1307	CLA	CHD-C1D-C2D	2.33	130.37	125.48
15	X1	102	CLA	CHD-C1D-C2D	2.33	130.37	125.48
15	B1	814	CLA	CHD-C1D-C2D	2.33	130.37	125.48
15	X3	102	CLA	CHD-C1D-C2D	2.33	130.37	125.48
15	B3	801	CLA	CHD-C1D-C2D	2.33	130.37	125.48
15	L1	1004	CLA	CHD-C1D-C2D	2.33	130.37	125.48
15	J3	1303	CLA	C2C-C1C-NC	2.33	112.16	109.97
15	A3	844	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
15	A3	810	CLA	CHD-C1D-C2D	2.33	130.37	125.48
15	J3	1307	CLA	CHD-C1D-C2D	2.33	130.37	125.48
15	B2	849	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
15	A3	827	CLA	CHD-C1D-C2D	2.33	130.37	125.48
15	A1	842	CLA	C2C-C1C-NC	2.33	112.15	109.97
15	B1	801	CLA	CHD-C1D-C2D	2.33	130.36	125.48
15	A1	844	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
15	B2	821	CLA	CHD-C1D-C2D	2.33	130.36	125.48
15	B3	822	CLA	CHD-C1D-C2D	2.33	130.36	125.48
15	A1	825	CLA	C1-C2-C3	-2.33	122.02	126.04
15	A3	805	CLA	C1-C2-C3	-2.33	122.02	126.04
15	A1	805	CLA	CHD-C1D-C2D	2.33	130.36	125.48
15	B3	803	CLA	CHD-C1D-C2D	2.33	130.36	125.48
15	X2	102	CLA	CHD-C1D-C2D	2.33	130.36	125.48
15	A1	816	CLA	CAA-C2A-C1A	-2.33	106.06	111.81
15	A2	856	CLA	C1D-ND-C4D	-2.33	104.68	106.33
15	A3	807	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
15	J2	1303	CLA	C2C-C1C-NC	2.33	112.15	109.97
15	A2	810	CLA	CHD-C1D-C2D	2.33	130.36	125.48
15	L3	1004	CLA	CHD-C1D-C2D	2.33	130.36	125.48
15	B1	803	CLA	CHD-C1D-C2D	2.33	130.36	125.48
15	B1	849	CLA	CHC-C1C-C2C	-2.33	120.29	126.72
15	B1	821	CLA	CHD-C1D-C2D	2.32	130.36	125.48
15	B3	805	CLA	CHD-C1D-C2D	2.32	130.36	125.48
15	B3	814	CLA	CHD-C1D-C2D	2.32	130.35	125.48
15	B2	814	CLA	CHD-C1D-C2D	2.32	130.35	125.48
15	B3	804	CLA	C1C-C2C-C3C	-2.32	104.51	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	830	CLA	CHD-C1D-C2D	2.32	130.35	125.48
15	A2	816	CLA	CAA-C2A-C1A	-2.32	106.07	111.81
15	B1	804	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
15	A3	816	CLA	CAA-C2A-C1A	-2.32	106.07	111.81
15	B2	803	CLA	CHD-C1D-C2D	2.32	130.35	125.48
15	B2	826	CLA	C2C-C1C-NC	2.32	112.15	109.97
15	A1	822	CLA	CHD-C1D-C2D	2.32	130.35	125.48
15	B2	803	CLA	C1D-ND-C4D	-2.32	104.69	106.33
15	B1	822	CLA	CHD-C1D-C2D	2.32	130.34	125.48
15	J1	1301	CLA	CHD-C1D-C2D	2.32	130.34	125.48
15	B2	818	CLA	C2C-C1C-NC	2.32	112.14	109.97
15	K2	103	CLA	CHA-C1A-NA	-2.32	121.20	126.41
15	A2	822	CLA	CHD-C1D-C2D	2.32	130.34	125.48
15	B2	804	CLA	CHD-C1D-C2D	2.32	130.34	125.48
15	J3	1301	CLA	CHD-C1D-C2D	2.32	130.34	125.48
15	A1	827	CLA	CHD-C1D-C2D	2.32	130.34	125.48
15	J2	1301	CLA	CHD-C1D-C2D	2.32	130.34	125.48
15	B3	821	CLA	CHD-C1D-C2D	2.32	130.34	125.48
15	A1	810	CLA	CHD-C1D-C2D	2.31	130.34	125.48
15	A1	816	CLA	C2C-C1C-NC	2.31	112.14	109.97
15	B2	839	CLA	CHC-C1C-C2C	-2.31	120.32	126.72
15	A3	805	CLA	C2C-C1C-NC	2.31	112.14	109.97
15	B1	812	CLA	CHA-C1A-NA	-2.31	121.10	126.40
15	B1	839	CLA	CHC-C1C-C2C	-2.31	120.32	126.72
15	I3	101	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
15	B1	805	CLA	CHD-C1D-C2D	2.31	130.33	125.48
15	B2	805	CLA	CHD-C1D-C2D	2.31	130.33	125.48
15	A3	822	CLA	CHD-C1D-C2D	2.31	130.33	125.48
15	B3	849	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
15	B3	839	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
15	A2	825	CLA	C1-C2-C3	-2.31	122.05	126.04
15	J2	1303	CLA	CHD-C1D-C2D	2.31	130.33	125.48
15	A2	808	CLA	CHD-C1D-C2D	2.31	130.32	125.48
15	A1	836	CLA	C2C-C1C-NC	2.31	112.14	109.97
15	J2	1307	CLA	C2C-C1C-NC	2.31	112.14	109.97
15	B3	826	CLA	C2C-C1C-NC	2.31	112.14	109.97
15	J2	1303	CLA	CAA-C2A-C1A	-2.31	106.10	111.81
15	I2	101	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
15	B3	812	CLA	CHA-C1A-NA	-2.31	121.11	126.40
15	A2	827	CLA	CHD-C1D-C2D	2.31	130.32	125.48
15	B2	812	CLA	CHA-C1A-NA	-2.31	121.11	126.40
15	A1	805	CLA	C1-C2-C3	-2.31	122.05	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	842	CLA	C2C-C1C-NC	2.31	112.13	109.97
15	A1	812	CLA	CHD-C1D-C2D	2.31	130.32	125.48
15	A1	837	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
15	J1	1307	CLA	C2C-C1C-NC	2.31	112.13	109.97
15	A2	805	CLA	C2C-C1C-NC	2.31	112.13	109.97
15	I1	101	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
15	A2	824	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
15	A2	837	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
15	A3	843	CLA	CHD-C1D-C2D	2.31	130.32	125.48
15	B1	815	CLA	C2C-C1C-NC	2.31	112.13	109.97
15	J3	1303	CLA	CAA-C2A-C1A	-2.31	106.11	111.81
15	A1	837	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
15	A2	837	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
15	A3	812	CLA	CHD-C1D-C2D	2.30	130.31	125.48
15	B1	826	CLA	C2C-C1C-NC	2.30	112.13	109.97
15	B3	804	CLA	CHD-C1D-C2D	2.30	130.31	125.48
15	A1	828	CLA	CHA-C1A-NA	-2.30	121.12	126.40
15	B3	808	CLA	CHD-C1D-C2D	2.30	130.31	125.48
15	J3	1303	CLA	CHD-C1D-C2D	2.30	130.31	125.48
15	B3	812	CLA	CHD-C1D-C2D	2.30	130.31	125.48
15	A1	839	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
15	A2	828	CLA	CHA-C1A-NA	-2.30	121.13	126.40
15	A3	835	CLA	CHA-C1A-NA	-2.30	121.13	126.40
15	J1	1303	CLA	C2C-C1C-NC	2.30	112.13	109.97
15	A2	843	CLA	CHD-C1D-C2D	2.30	130.31	125.48
15	A1	824	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
15	K1	103	CLA	CHA-C1A-NA	-2.30	121.24	126.41
15	A2	829	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
15	B3	809	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
15	A1	809	CLA	CHD-C1D-C2D	2.30	130.31	125.48
15	J1	1303	CLA	CAA-C2A-C1A	-2.30	106.13	111.81
15	A3	836	CLA	C2C-C1C-NC	2.30	112.13	109.97
15	J1	1303	CLA	CHD-C1D-C2D	2.30	130.30	125.48
15	A3	803	CLA	CHD-C1D-C2D	2.30	130.30	125.48
15	K3	103	CLA	CHA-C1A-NA	-2.30	121.24	126.41
15	A2	812	CLA	CHD-C1D-C2D	2.30	130.30	125.48
15	B1	807	CLA	CAA-C2A-C1A	-2.30	104.44	111.97
15	B3	815	CLA	C2C-C1C-NC	2.30	112.12	109.97
15	A3	837	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
15	B2	812	CLA	CHD-C1D-C2D	2.30	130.30	125.48
15	A3	808	CLA	CHD-C1D-C2D	2.30	130.30	125.48
15	A3	828	CLA	CHA-C1A-NA	-2.30	121.14	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	812	CLA	CHD-C1D-C2D	2.30	130.30	125.48
15	A3	817	CLA	CHD-C1D-C2D	2.30	130.30	125.48
15	A2	805	CLA	C1-C2-C3	-2.30	122.07	126.04
15	B2	807	CLA	CAA-C2A-C1A	-2.30	104.45	111.97
15	A2	803	CLA	CHD-C1D-C2D	2.30	130.29	125.48
15	B2	809	CLA	CHC-C1C-C2C	-2.30	120.37	126.72
15	A1	808	CLA	CHD-C1D-C2D	2.30	130.29	125.48
15	A2	809	CLA	CHD-C1D-C2D	2.30	130.29	125.48
15	A3	829	CLA	CHC-C1C-C2C	-2.30	120.37	126.72
15	A1	810	CLA	CAA-C2A-C1A	-2.29	106.14	111.81
15	B2	834	CLA	CHD-C1D-C2D	2.29	130.29	125.48
15	B1	809	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
15	A3	837	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
15	A3	822	CLA	CHA-C1A-NA	-2.29	121.15	126.40
15	A1	843	CLA	CHD-C1D-C2D	2.29	130.29	125.48
15	B3	807	CLA	CAA-C2A-C1A	-2.29	104.46	111.97
15	A1	829	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
15	A3	810	CLA	CAA-C2A-C1A	-2.29	106.15	111.81
15	B3	821	CLA	C3D-C4D-ND	2.29	113.94	110.24
15	A3	824	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
15	L1	1002	CLA	C1-C2-C3	-2.29	122.08	126.04
15	B3	826	CLA	CHD-C1D-C2D	2.29	130.28	125.48
15	A3	809	CLA	CHD-C1D-C2D	2.29	130.28	125.48
15	B1	808	CLA	CHD-C1D-C2D	2.29	130.28	125.48
15	B2	818	CLA	CHD-C1D-C2D	2.29	130.28	125.48
15	B1	819	CLA	CHD-C1D-C2D	2.29	130.28	125.48
15	B3	819	CLA	CHD-C1D-C2D	2.29	130.28	125.48
15	A1	822	CLA	CHA-C1A-NA	-2.29	121.16	126.40
15	A2	810	CLA	CAA-C2A-C1A	-2.29	106.16	111.81
15	A2	822	CLA	CHA-C1A-NA	-2.29	121.16	126.40
15	A1	803	CLA	CHD-C1D-C2D	2.29	130.28	125.48
15	B2	819	CLA	CHD-C1D-C2D	2.29	130.28	125.48
15	A1	817	CLA	CHD-C1D-C2D	2.29	130.28	125.48
15	B3	828	CLA	CHC-C1C-C2C	-2.29	120.40	126.72
15	A2	839	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
15	L2	1002	CLA	C1-C2-C3	-2.29	122.09	126.04
15	B1	819	CLA	CHA-C1A-NA	-2.29	121.16	126.40
15	L3	1002	CLA	C1-C2-C3	-2.29	122.09	126.04
15	B3	829	CLA	CHA-C1A-NA	-2.29	121.27	126.41
15	A3	823	CLA	CHC-C1C-C2C	-2.29	120.40	126.72
15	B2	832	CLA	CHA-C1A-NA	-2.29	121.16	126.40
15	A1	835	CLA	CHA-C1A-NA	-2.29	121.17	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	828	CLA	CHC-C1C-C2C	-2.28	120.40	126.72
15	B3	819	CLA	CHA-C1A-NA	-2.28	121.17	126.40
15	B3	806	CLA	CHD-C1D-C2D	2.28	130.27	125.48
15	A3	839	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
15	A2	823	CLA	CHC-C1C-C2C	-2.28	120.40	126.72
15	B1	826	CLA	CHD-C1D-C2D	2.28	130.27	125.48
15	B1	832	CLA	CHA-C1A-NA	-2.28	121.17	126.40
15	A1	823	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
15	A2	816	CLA	C2C-C1C-NC	2.28	112.11	109.97
15	B2	828	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
15	A1	819	CLA	C1-C2-C3	-2.28	122.09	126.04
15	A1	820	CLA	CHD-C1D-C2D	2.28	130.27	125.48
15	B2	808	CLA	CHD-C1D-C2D	2.28	130.26	125.48
15	A3	820	CLA	CHD-C1D-C2D	2.28	130.26	125.48
15	B1	834	CLA	CHD-C1D-C2D	2.28	130.26	125.48
15	B3	832	CLA	CHA-C1A-NA	-2.28	121.18	126.40
15	X3	102	CLA	C3C-C4C-NC	2.28	113.06	110.57
15	B1	821	CLA	C3D-C4D-ND	2.28	113.92	110.24
15	A1	826	CLA	CHA-C1A-NA	-2.28	121.18	126.40
15	B1	829	CLA	CHA-C1A-NA	-2.28	121.29	126.41
15	A3	808	CLA	C2C-C1C-NC	2.28	112.11	109.97
15	B3	822	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
15	B2	819	CLA	CHA-C1A-NA	-2.28	121.18	126.40
15	A2	811	CLA	C2C-C1C-NC	2.28	112.11	109.97
15	B2	802	CLA	CHA-C1A-NA	-2.28	121.18	126.40
15	B2	826	CLA	CHD-C1D-C2D	2.28	130.25	125.48
15	A1	820	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
15	J3	1307	CLA	CHA-C1A-NA	-2.27	121.30	126.41
15	B1	818	CLA	C2C-C1C-NC	2.27	112.10	109.97
15	A2	817	CLA	CHD-C1D-C2D	2.27	130.25	125.48
15	A2	820	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
15	A3	820	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
15	B3	806	CLA	CHC-C1C-C2C	-2.27	120.43	126.72
15	A2	835	CLA	CHA-C1A-NA	-2.27	121.19	126.40
15	J2	1307	CLA	CHA-C1A-NA	-2.27	121.30	126.41
15	A3	811	CLA	C2C-C1C-NC	2.27	112.10	109.97
15	X2	102	CLA	C3C-C4C-NC	2.27	113.05	110.57
15	A3	819	CLA	C1-C2-C3	-2.27	122.11	126.04
15	B3	834	CLA	CHD-C1D-C2D	2.27	130.25	125.48
15	A3	826	CLA	CHA-C1A-NA	-2.27	121.19	126.40
15	B1	818	CLA	CHD-C1D-C2D	2.27	130.25	125.48
15	J1	1307	CLA	CHA-C1A-NA	-2.27	121.30	126.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B2	821	CLA	C3D-C4D-ND	2.27	113.91	110.24
15	B2	838	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
15	B2	815	CLA	C2C-C1C-NC	2.27	112.10	109.97
15	B2	829	CLA	CHA-C1A-NA	-2.27	121.31	126.41
15	B1	802	CLA	CHA-C1A-NA	-2.27	121.20	126.40
15	A2	836	CLA	C2C-C1C-NC	2.27	112.10	109.97
15	A2	820	CLA	CHD-C1D-C2D	2.27	130.24	125.48
15	A3	824	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
15	A2	807	CLA	CAA-C2A-C1A	-2.27	104.55	111.97
15	B1	806	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
15	A2	838	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
15	B1	838	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
15	A2	819	CLA	C1-C2-C3	-2.27	122.12	126.04
15	A2	826	CLA	CHA-C1A-NA	-2.26	121.21	126.40
15	A1	824	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
15	B2	806	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
15	B3	802	CLA	CHA-C1A-NA	-2.26	121.22	126.40
15	A1	838	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
15	A2	824	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
15	A3	838	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
15	B1	806	CLA	CHD-C1D-C2D	2.26	130.22	125.48
15	B2	819	CLA	C2C-C1C-NC	2.26	112.09	109.97
15	B1	822	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
15	X1	102	CLA	C3C-C4C-NC	2.26	113.04	110.57
15	A1	807	CLA	CAA-C2A-C1A	-2.26	104.58	111.97
15	A3	807	CLA	CAA-C2A-C1A	-2.26	104.58	111.97
15	B1	819	CLA	C2C-C1C-NC	2.26	112.09	109.97
15	A1	811	CLA	C2C-C1C-NC	2.26	112.08	109.97
15	B3	818	CLA	C2C-C1C-NC	2.26	112.08	109.97
15	A2	808	CLA	C2C-C1C-NC	2.25	112.08	109.97
15	J2	1302	CLA	CHC-C1C-C2C	-2.25	120.49	126.72
15	A1	825	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
15	A3	842	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
15	J1	1302	CLA	CHC-C1C-C2C	-2.25	120.49	126.72
15	A2	839	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
15	A1	839	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
15	A1	835	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
15	A1	842	CLA	CHA-C1A-NA	-2.25	121.25	126.40
15	B3	818	CLA	CHD-C1D-C2D	2.25	130.20	125.48
15	A3	829	CLA	CHD-C1D-C2D	2.25	130.19	125.48
15	B2	805	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
15	A3	839	CLA	CHC-C1C-C2C	-2.25	120.50	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	834	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
15	A2	833	CLA	CHA-C1A-NA	-2.25	121.25	126.40
15	J3	1302	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
15	A1	834	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
15	A1	842	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
15	B3	813	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
15	X3	102	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
15	X1	102	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
15	L1	1004	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
15	B2	822	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
15	X2	102	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
15	B3	838	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
15	B3	829	CLA	C2A-C1A-CHA	2.24	126.19	122.71
15	A2	843	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
15	A3	835	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
15	A2	829	CLA	CHD-C1D-C2D	2.24	130.18	125.48
15	A1	808	CLA	C2C-C1C-NC	2.24	112.07	109.97
15	B3	819	CLA	C2C-C1C-NC	2.24	112.07	109.97
15	B1	838	CLA	CHA-C1A-NA	-2.24	121.27	126.40
15	B2	806	CLA	CHD-C1D-C2D	2.24	130.18	125.48
15	A1	836	CLA	CHA-C1A-NA	-2.24	121.27	126.40
15	A2	836	CLA	CHA-C1A-NA	-2.24	121.27	126.40
15	B2	838	CLA	CHA-C1A-NA	-2.24	121.27	126.40
15	B1	805	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
15	A1	843	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
15	A2	835	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
15	B3	815	CLA	CAD-CBD-CHA	-2.24	102.62	105.14
15	B3	805	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
15	A1	829	CLA	CHD-C1D-C2D	2.24	130.17	125.48
15	B3	838	CLA	CHA-C1A-NA	-2.24	121.27	126.40
15	A3	833	CLA	CHA-C1A-NA	-2.24	121.28	126.40
15	L1	1002	CLA	CHD-C1D-C2D	2.24	130.17	125.48
15	A3	836	CLA	CHA-C1A-NA	-2.24	121.28	126.40
15	A2	834	CLA	C1C-C2C-C3C	-2.24	104.61	106.96
15	A1	833	CLA	CHA-C1A-NA	-2.24	121.28	126.40
15	L3	1002	CLA	CHD-C1D-C2D	2.24	130.17	125.48
15	L3	1004	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
15	A2	832	CLA	CHA-C1A-NA	-2.23	121.28	126.40
15	A3	843	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
15	L2	1004	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
15	A2	842	CLA	CHA-C1A-NA	-2.23	121.28	126.40
15	B1	815	CLA	CAD-CBD-CHA	-2.23	102.62	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	813	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
15	A3	842	CLA	CHA-C1A-NA	-2.23	121.29	126.40
15	B2	816	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
15	B3	806	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
15	B2	831	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
15	B3	816	CLA	C2A-C1A-CHA	2.23	126.17	122.71
15	B2	833	CLA	C2C-C1C-NC	2.23	112.06	109.97
15	B3	826	CLA	CHA-C1A-NA	-2.23	121.30	126.40
15	A2	842	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
15	B3	833	CLA	C2C-C1C-NC	2.23	112.06	109.97
15	B1	838	CLA	C1-C2-C3	-2.23	122.19	126.04
15	B1	826	CLA	CHA-C1A-NA	-2.23	121.30	126.40
15	B3	831	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
15	A2	841	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
15	A3	813	CLA	CHD-C1D-C2D	2.22	130.15	125.48
15	B1	831	CLA	CHC-C1C-C2C	-2.22	120.57	126.72
15	L2	1002	CLA	CHD-C1D-C2D	2.22	130.14	125.48
15	K3	101	CLA	C2A-C3A-C4A	-2.22	99.64	103.59
15	B3	816	CLA	CHC-C1C-C2C	-2.22	120.57	126.72
15	A2	843	CLA	CHA-C1A-NA	-2.22	121.31	126.40
15	A3	825	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
15	A1	832	CLA	CHA-C1A-NA	-2.22	121.31	126.40
15	A3	832	CLA	CHA-C1A-NA	-2.22	121.31	126.40
15	K1	101	CLA	CHA-C1A-NA	-2.22	121.41	126.41
15	A3	814	CLA	CHA-C1A-NA	-2.22	121.42	126.41
15	A3	841	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
15	B2	829	CLA	C2A-C1A-CHA	2.22	126.16	122.71
15	K3	101	CLA	CHA-C1A-NA	-2.22	121.42	126.41
15	A1	843	CLA	CHA-C1A-NA	-2.22	121.31	126.40
15	B2	826	CLA	CHA-C1A-NA	-2.22	121.31	126.40
15	B1	829	CLA	C2A-C1A-CHA	2.22	126.15	122.71
15	A2	814	CLA	CHA-C1A-NA	-2.22	121.42	126.41
15	K1	101	CLA	C2A-C3A-C4A	-2.22	99.64	103.59
15	A2	825	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
15	B1	827	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
15	B3	838	CLA	C1-C2-C3	-2.22	122.20	126.04
15	B1	816	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
15	K2	101	CLA	CHA-C1A-NA	-2.22	121.42	126.41
15	A1	813	CLA	CHD-C1D-C2D	2.22	130.13	125.48
15	A3	839	CLA	CHA-C1A-NA	-2.22	121.32	126.40
15	A3	821	CLA	CHD-C1D-C2D	2.22	130.13	125.48
15	B2	827	CLA	CHC-C1C-C2C	-2.22	120.59	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	833	CLA	C2C-C1C-NC	2.22	112.05	109.97
15	B2	806	CLA	C1C-C2C-C3C	-2.22	104.63	106.96
15	A1	814	CLA	CHA-C1A-NA	-2.22	121.43	126.41
15	A1	805	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
15	A2	813	CLA	CHD-C1D-C2D	2.22	130.13	125.48
15	A2	832	CLA	CHC-C1C-C2C	-2.21	120.59	126.72
15	I2	101	CLA	CHD-C1D-C2D	2.21	130.12	125.48
15	B2	815	CLA	CAD-CBD-CHA	-2.21	102.64	105.14
15	B3	827	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
15	B2	813	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
15	A2	839	CLA	CHA-C1A-NA	-2.21	121.33	126.40
15	A1	821	CLA	CHD-C1D-C2D	2.21	130.12	125.48
15	K2	101	CLA	C2C-C1C-NC	2.21	112.04	109.97
15	B1	806	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
15	B2	810	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
15	K2	101	CLA	C2A-C3A-C4A	-2.21	99.66	103.59
15	A1	832	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
15	A3	806	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
15	A1	815	CLA	CAA-C2A-C1A	-2.21	106.35	111.81
15	B2	816	CLA	C2A-C1A-CHA	2.21	126.14	122.71
15	A1	806	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
15	A1	806	CLA	CHD-C1D-C2D	2.21	130.12	125.48
15	I1	101	CLA	CHD-C1D-C2D	2.21	130.12	125.48
15	B3	827	CLA	CHD-C1D-C2D	2.21	130.12	125.48
15	B1	816	CLA	C2A-C1A-CHA	2.21	126.14	122.71
15	A1	839	CLA	CHA-C1A-NA	-2.21	121.34	126.40
15	B2	830	CLA	CHA-C1A-NA	-2.21	121.34	126.40
15	A3	805	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
15	A2	815	CLA	CAA-C2A-C1A	-2.21	106.35	111.81
15	B1	810	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
15	A2	831	CLA	CHA-C1A-NA	-2.21	121.34	126.40
15	A3	843	CLA	CHA-C1A-NA	-2.21	121.34	126.40
15	B3	819	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
15	B1	811	CLA	CHD-C1D-C2D	2.21	130.11	125.48
15	B3	811	CLA	CHD-C1D-C2D	2.21	130.11	125.48
15	A2	805	CLA	CHC-C1C-C2C	-2.21	120.62	126.72
15	A1	841	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
15	B3	836	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
15	A1	831	CLA	CHA-C1A-NA	-2.21	121.34	126.40
15	A2	824	CLA	CHA-C1A-NA	-2.21	121.35	126.40
15	B2	838	CLA	C1-C2-C3	-2.21	122.23	126.04
15	A3	832	CLA	CHC-C1C-C2C	-2.21	120.62	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	819	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
15	A2	806	CLA	CHC-C1C-C2C	-2.20	120.62	126.72
15	B2	819	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
15	A3	821	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
15	B2	827	CLA	CHD-C1D-C2D	2.20	130.10	125.48
15	A3	806	CLA	CHD-C1D-C2D	2.20	130.10	125.48
15	A3	831	CLA	CHA-C1A-NA	-2.20	121.35	126.40
15	B3	830	CLA	CHA-C1A-NA	-2.20	121.35	126.40
15	A1	821	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
15	B2	804	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
15	B3	804	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
15	B3	830	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
15	L2	1003	CLA	CHA-C1A-NA	-2.20	121.36	126.40
15	B1	830	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
15	I3	101	CLA	CHD-C1D-C2D	2.20	130.09	125.48
15	B1	830	CLA	CHA-C1A-NA	-2.20	121.36	126.40
15	A2	830	CLA	CHA-C1A-NA	-2.20	121.36	126.40
15	A2	821	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
15	B3	810	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
15	B1	804	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
15	A3	813	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
15	A1	841	CLA	CHD-C1D-C2D	2.20	130.09	125.48
15	A2	806	CLA	CHD-C1D-C2D	2.20	130.09	125.48
15	A2	828	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
15	B2	811	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
15	B2	830	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
15	A2	821	CLA	CHD-C1D-C2D	2.20	130.09	125.48
15	A2	844	CLA	CHD-C1D-C2D	2.20	130.09	125.48
15	A3	815	CLA	CAA-C2A-C1A	-2.20	106.38	111.81
15	B1	825	CLA	CHC-C1C-NC	2.20	127.53	124.20
15	A3	818	CLA	CHC-C1C-C2C	-2.20	120.65	126.72
15	A1	831	CLA	CAA-C2A-C1A	-2.19	104.78	111.97
15	A3	831	CLA	CAA-C2A-C1A	-2.19	104.78	111.97
15	A1	813	CLA	CHC-C1C-C2C	-2.19	120.65	126.72
15	A2	841	CLA	CHD-C1D-C2D	2.19	130.08	125.48
15	A1	818	CLA	CHC-C1C-C2C	-2.19	120.65	126.72
15	B1	817	CLA	CHC-C1C-C2C	-2.19	120.65	126.72
15	B3	812	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
15	A2	813	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
15	L3	1003	CLA	C1C-C2C-C3C	-2.19	104.65	106.96
15	A3	824	CLA	CHA-C1A-NA	-2.19	121.38	126.40
15	J3	1301	CLA	CHC-C1C-C2C	-2.19	120.66	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	831	CLA	CAA-C2A-C1A	-2.19	104.79	111.97
15	A1	824	CLA	CHA-C1A-NA	-2.19	121.38	126.40
15	A3	830	CLA	CHA-C1A-NA	-2.19	121.38	126.40
15	J1	1301	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
15	B3	817	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
15	B2	825	CLA	C4A-NA-C1A	-2.19	105.72	106.71
15	B1	827	CLA	CHD-C1D-C2D	2.19	130.07	125.48
15	B1	836	CLA	C1C-C2C-C3C	-2.19	104.65	106.96
15	B2	817	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
15	J2	1301	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
15	B3	814	CLA	CHC-C1C-C2C	-2.19	120.66	126.72
15	B2	836	CLA	C1C-C2C-C3C	-2.19	104.65	106.96
15	A3	830	CLA	CAA-C2A-C1A	-2.19	104.80	111.97
15	B2	811	CLA	CHD-C1D-C2D	2.19	130.07	125.48
15	B3	811	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
15	A1	825	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
15	B1	814	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
15	B1	811	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
15	L1	1003	CLA	CHA-C1A-NA	-2.19	121.39	126.40
15	B3	824	CLA	C2C-C1C-NC	2.19	112.02	109.97
15	L1	1003	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
15	A3	841	CLA	CHD-C1D-C2D	2.19	130.06	125.48
15	A1	830	CLA	CHA-C1A-NA	-2.19	121.39	126.40
15	A2	830	CLA	CAA-C2A-C1A	-2.19	104.81	111.97
15	K1	101	CLA	C2C-C1C-NC	2.19	112.02	109.97
15	A2	818	CLA	CHC-C1C-C2C	-2.18	120.68	126.72
15	A1	844	CLA	CHD-C1D-C2D	2.18	130.06	125.48
15	A3	816	CLA	CHC-C1C-C2C	-2.18	120.68	126.72
15	B1	824	CLA	C2C-C1C-NC	2.18	112.02	109.97
15	B3	825	CLA	CHC-C1C-NC	2.18	127.52	124.20
15	A2	834	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
15	B2	837	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
15	A3	811	CLA	C1C-C2C-C3C	-2.18	104.66	106.96
15	A3	828	CLA	C1C-C2C-C3C	-2.18	104.66	106.96
15	A1	830	CLA	CAA-C2A-C1A	-2.18	104.83	111.97
15	A3	804	CLA	CHA-C1A-NA	-2.18	121.40	126.40
15	B3	839	CLA	CHA-C1A-NA	-2.18	121.40	126.40
15	A3	844	CLA	CHD-C1D-C2D	2.18	130.05	125.48
15	B1	812	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
15	A2	804	CLA	CHA-C1A-NA	-2.18	121.41	126.40
15	A3	812	CLA	CAA-C2A-C1A	-2.18	106.42	111.81
15	A1	816	CLA	CHC-C1C-C2C	-2.18	120.69	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	814	CLA	CHA-C1A-NA	-2.18	121.41	126.40
15	A3	834	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
15	A2	829	CLA	C1C-C2C-C3C	-2.18	104.67	106.96
15	A1	804	CLA	CHA-C1A-NA	-2.18	121.41	126.40
15	A2	811	CLA	C1C-C2C-C3C	-2.18	104.67	106.96
15	B2	839	CLA	CHA-C1A-NA	-2.18	121.41	126.40
15	B1	808	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
15	B2	814	CLA	CHA-C1A-NA	-2.18	121.41	126.40
15	B1	837	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
15	A2	816	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
15	A1	828	CLA	C1C-C2C-C3C	-2.18	104.67	106.96
15	A3	829	CLA	C1C-C2C-C3C	-2.18	104.67	106.96
15	B1	839	CLA	CHA-C1A-NA	-2.18	121.41	126.40
15	A2	812	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
15	B2	825	CLA	CHC-C1C-NC	2.18	127.50	124.20
15	X1	102	CLA	CHA-C1A-NA	-2.18	121.42	126.40
15	B2	823	CLA	CHD-C1D-C2D	2.18	130.04	125.48
15	B3	823	CLA	CHD-C1D-C2D	2.18	130.04	125.48
15	B2	801	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	B2	820	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
15	A2	820	CLA	CHA-C1A-NA	-2.17	121.52	126.41
15	B3	808	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
15	A3	813	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	B2	814	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
15	L3	1003	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	B2	824	CLA	C2C-C1C-NC	2.17	112.01	109.97
15	B1	801	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	B3	837	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
15	B2	831	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	X2	102	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	B3	801	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	A3	825	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
15	A2	828	CLA	C2C-C1C-NC	2.17	112.01	109.97
15	A1	813	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	B2	811	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	B2	833	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	X3	102	CLA	CHA-C1A-NA	-2.17	121.42	126.40
15	B1	820	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	A1	812	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	B3	831	CLA	CHA-C1A-NA	-2.17	121.43	126.40
15	A1	834	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	B1	831	CLA	CHA-C1A-NA	-2.17	121.43	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	833	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	A2	825	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	B3	833	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	A3	812	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	B3	811	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	A2	844	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
15	B1	811	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
15	B2	808	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
15	B3	827	CLA	CHA-C1A-NA	-2.17	121.43	126.40
15	B1	823	CLA	CHD-C1D-C2D	2.17	130.03	125.48
15	B1	836	CLA	CHA-C1A-NA	-2.17	121.44	126.40
15	K3	101	CLA	C2C-C1C-NC	2.17	112.00	109.97
15	A1	820	CLA	CHA-C1A-NA	-2.17	121.54	126.41
15	B1	833	CLA	CHA-C1A-NA	-2.16	121.44	126.40
15	A2	844	CLA	CHA-C1A-NA	-2.16	121.44	126.40
15	A3	820	CLA	CHA-C1A-NA	-2.16	121.54	126.41
15	A1	837	CLA	CHD-C1D-C2D	2.16	130.02	125.48
15	B2	812	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
15	A2	808	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
15	A2	813	CLA	CHA-C1A-NA	-2.16	121.44	126.40
15	B3	833	CLA	CHA-C1A-NA	-2.16	121.44	126.40
15	A2	837	CLA	CHD-C1D-C2D	2.16	130.02	125.48
15	A3	828	CLA	C2C-C1C-NC	2.16	112.00	109.97
15	B3	836	CLA	CHA-C1A-NA	-2.16	121.45	126.40
15	A1	825	CLA	C3C-C4C-NC	2.16	113.00	110.57
15	A1	811	CLA	C1C-C2C-C3C	-2.16	104.68	106.96
15	A3	808	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
15	B3	820	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
15	A1	829	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
15	B2	827	CLA	CHA-C1A-NA	-2.16	121.45	126.40
15	A1	812	CLA	CAA-C2A-C1A	-2.16	106.48	111.81
15	A1	828	CLA	C2C-C1C-NC	2.16	111.99	109.97
15	B3	813	CLA	CMC-C2C-C1C	2.16	128.32	125.04
15	B3	834	CLA	CHC-C1C-C2C	-2.16	120.76	126.72
15	B3	814	CLA	CHA-C1A-NA	-2.16	121.46	126.40
15	B3	825	CLA	C4A-NA-C1A	-2.16	105.74	106.71
15	A2	825	CLA	C3C-C4C-NC	2.16	112.99	110.57
15	A2	812	CLA	CAA-C2A-C1A	-2.15	106.49	111.81
15	A3	817	CLA	CHA-C1A-NA	-2.15	121.46	126.40
15	B2	833	CLA	CHA-C1A-NA	-2.15	121.47	126.40
15	B1	834	CLA	CHC-C1C-C2C	-2.15	120.76	126.72
15	B2	820	CLA	C2A-C1A-CHA	2.15	126.05	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	825	CLA	C4A-NA-C1A	-2.15	105.74	106.71
15	A1	808	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
15	B1	827	CLA	CHA-C1A-NA	-2.15	121.47	126.40
15	J3	1307	CLA	C4C-C3C-C2C	-2.15	106.50	108.89
15	A3	833	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
15	B2	836	CLA	CHA-C1A-NA	-2.15	121.47	126.40
15	A2	808	CLA	CHA-C1A-NA	-2.15	121.47	126.40
15	A3	825	CLA	C3C-C4C-NC	2.15	112.98	110.57
15	A3	837	CLA	CHD-C1D-C2D	2.15	129.99	125.48
15	A1	844	CLA	CHA-C1A-NA	-2.15	121.47	126.40
15	B2	835	CLA	C1C-C2C-C3C	-2.15	104.70	106.96
15	A3	844	CLA	C1C-C2C-C3C	-2.15	104.70	106.96
15	B3	810	CLA	CHA-C1A-NA	-2.15	121.48	126.40
15	B1	820	CLA	C2A-C1A-CHA	2.15	126.04	122.71
15	J1	1303	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
15	A1	833	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
15	A2	856	CLA	CHA-C1A-NA	-2.15	121.48	126.40
15	A3	844	CLA	CHA-C1A-NA	-2.15	121.48	126.40
15	B3	820	CLA	C2A-C1A-CHA	2.15	126.04	122.71
15	A2	833	CLA	CHC-C1C-C2C	-2.15	120.79	126.72
15	A1	804	CLA	CHC-C1C-C2C	-2.15	120.79	126.72
15	A3	809	CLA	CHC-C1C-C2C	-2.15	120.79	126.72
15	B1	820	CLA	CAD-CBD-CHA	-2.14	102.72	105.14
15	A3	826	CLA	C2C-C1C-NC	2.14	111.98	109.97
15	A3	804	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
15	A1	817	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	B2	818	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
15	J2	1303	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
15	A2	827	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	B3	821	CLA	C2C-C1C-NC	2.14	111.98	109.97
15	A2	807	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	A3	807	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	A1	808	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	B1	813	CLA	CMC-C2C-C1C	2.14	128.30	125.04
15	B2	820	CLA	CAD-CBD-CHA	-2.14	102.72	105.14
15	B2	810	CLA	C1C-C2C-C3C	-2.14	104.70	106.96
15	B1	818	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
15	A3	836	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
15	A2	819	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	A1	836	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
15	A2	817	CLA	CHA-C1A-NA	-2.14	121.49	126.40
15	B3	820	CLA	CAD-CBD-CHA	-2.14	102.73	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	819	CLA	CHA-C1A-NA	-2.14	121.50	126.40
15	B3	801	CLA	C2C-C1C-NC	2.14	111.98	109.97
15	A1	827	CLA	CHA-C1A-NA	-2.14	121.50	126.40
15	A1	807	CLA	CHA-C1A-NA	-2.14	121.50	126.40
15	B1	810	CLA	CHA-C1A-NA	-2.14	121.50	126.40
15	L2	1003	CLA	C1C-C2C-C3C	-2.14	104.71	106.96
15	A1	809	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
15	J3	1303	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
15	A1	826	CLA	C2C-C1C-NC	2.14	111.97	109.97
15	A1	844	CLA	C1C-C2C-C3C	-2.14	104.71	106.96
15	A1	856	CLA	CHA-C1A-NA	-2.14	121.50	126.40
15	B1	810	CLA	C1C-C2C-C3C	-2.14	104.71	106.96
15	A2	836	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
15	A3	808	CLA	CHA-C1A-NA	-2.14	121.51	126.40
15	A2	804	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
15	B3	818	CLA	CHC-C1C-C2C	-2.14	120.82	126.72
15	B2	834	CLA	CHC-C1C-C2C	-2.13	120.82	126.72
15	J2	1301	CLA	C3C-C4C-NC	2.13	112.96	110.57
15	A2	840	CLA	C1C-C2C-C3C	-2.13	104.71	106.96
15	A3	827	CLA	CHA-C1A-NA	-2.13	121.51	126.40
15	B1	825	CLA	CHD-C1D-C2D	2.13	129.95	125.48
15	A1	819	CLA	CHA-C1A-NA	-2.13	121.52	126.40
15	K3	103	CLA	C3C-C4C-CHD	-2.13	120.55	125.22
15	B3	810	CLA	C1C-C2C-C3C	-2.13	104.72	106.96
15	B3	824	CLA	CHA-C1A-NA	-2.13	121.52	126.40
15	B1	801	CLA	C2C-C1C-NC	2.13	111.97	109.97
15	B2	825	CLA	CHD-C1D-C2D	2.13	129.95	125.48
15	J3	1301	CLA	C3C-C4C-NC	2.13	112.96	110.57
15	K2	103	CLA	C3C-C4C-CHD	-2.13	120.55	125.22
15	B2	801	CLA	C2C-C1C-NC	2.13	111.97	109.97
15	A3	856	CLA	CHA-C1A-NA	-2.13	121.52	126.40
15	A2	837	CLA	C3C-C4C-NC	2.13	112.96	110.57
15	A2	809	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
15	B2	824	CLA	CHA-C1A-NA	-2.13	121.52	126.40
15	J1	1301	CLA	C3C-C4C-NC	2.13	112.96	110.57
15	A2	826	CLA	C2C-C1C-NC	2.13	111.97	109.97
15	B2	810	CLA	CHA-C1A-NA	-2.13	121.53	126.40
15	B3	813	CLA	CHC-C1C-C2C	-2.13	120.84	126.72
15	B1	821	CLA	C2C-C1C-NC	2.13	111.96	109.97
15	K1	103	CLA	C3C-C4C-CHD	-2.13	120.57	125.22
15	B1	836	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
15	A3	814	CLA	CHC-C1C-C2C	-2.12	120.85	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	841	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
15	J3	1307	CLA	C3C-C4C-CHD	-2.12	120.53	125.23
15	A3	841	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
15	B2	836	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
15	A3	833	CLA	C1C-C2C-C3C	-2.12	104.73	106.96
15	A1	817	CLA	C2C-C1C-NC	2.12	111.96	109.97
15	A2	810	CLA	CHA-C1A-NA	-2.12	121.54	126.40
15	A1	814	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
15	A1	810	CLA	CHA-C1A-NA	-2.12	121.54	126.40
15	B1	813	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
15	A2	817	CLA	C2C-C1C-NC	2.12	111.96	109.97
15	B2	806	CLA	CHA-C1A-NA	-2.12	121.55	126.40
15	B3	836	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
15	B1	824	CLA	CHA-C1A-NA	-2.12	121.55	126.40
15	B1	815	CLA	CHC-C1C-C2C	-2.12	120.86	126.72
15	J1	1307	CLA	C4C-C3C-C2C	-2.12	106.54	108.89
15	B2	813	CLA	CMC-C2C-C1C	2.12	128.26	125.04
15	K2	101	CLA	CHC-C1C-C2C	-2.12	120.87	126.72
15	K3	103	CLA	CBD-CHA-C1A	2.12	130.30	128.06
15	A1	841	CLA	CHC-C1C-C2C	-2.12	120.87	126.72
15	B3	815	CLA	CHC-C1C-C2C	-2.12	120.87	126.72
15	B2	813	CLA	CHC-C1C-C2C	-2.12	120.87	126.72
15	B2	805	CLA	CHA-C1A-NA	-2.11	121.56	126.40
15	B2	815	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
15	B1	834	CLA	CHA-C1A-NA	-2.11	121.66	126.41
15	B2	834	CLA	CHA-C1A-NA	-2.11	121.66	126.41
15	J2	1307	CLA	C4C-C3C-C2C	-2.11	106.55	108.89
15	B3	825	CLA	CHD-C1D-C2D	2.11	129.91	125.48
15	K1	101	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
15	A1	833	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
15	B2	808	CLA	C2C-C1C-NC	2.11	111.95	109.97
15	B3	835	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
15	A2	814	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
15	A2	840	CLA	CHA-C1A-NA	-2.11	121.56	126.40
15	A3	803	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
15	B2	803	CLA	CHA-C1A-NA	-2.11	121.57	126.40
15	A2	802	CLA	CHA-C1A-NA	-2.11	121.57	126.40
15	B3	803	CLA	CHA-C1A-NA	-2.11	121.57	126.40
15	A1	840	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
15	A1	840	CLA	CHA-C1A-NA	-2.11	121.57	126.40
15	A2	803	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
15	B1	803	CLA	CHA-C1A-NA	-2.11	121.57	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	835	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
15	B1	806	CLA	CHA-C1A-NA	-2.11	121.58	126.40
15	B3	805	CLA	CHA-C1A-NA	-2.11	121.58	126.40
15	B1	805	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	B2	804	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	A2	833	CLA	C1C-C2C-C3C	-2.10	104.74	106.96
15	B3	834	CLA	C1C-C2C-C3C	-2.10	104.74	106.96
15	A1	830	CLA	C3C-C4C-NC	2.10	112.93	110.57
15	A1	837	CLA	CMC-C2C-C1C	2.10	128.24	125.04
15	K3	101	CLA	CHC-C1C-C2C	-2.10	120.90	126.72
15	A1	802	CLA	CHA-C1A-NA	-2.10	121.58	126.40
15	L3	1003	CLA	CHC-C1C-C2C	-2.10	120.91	126.72
15	B1	807	CLA	C2A-C1A-CHA	2.10	127.53	123.86
15	A1	803	CLA	CHC-C1C-C2C	-2.10	120.91	126.72
15	A1	837	CLA	C3C-C4C-NC	2.10	112.93	110.57
15	A2	830	CLA	C3C-C4C-NC	2.10	112.93	110.57
15	A3	830	CLA	C3C-C4C-NC	2.10	112.93	110.57
15	B1	804	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	B1	811	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	B3	811	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	B2	812	CLA	CAA-C2A-C1A	-2.10	105.09	111.97
15	A2	815	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	B3	821	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
15	A2	837	CLA	CMC-C2C-C1C	2.10	128.24	125.04
15	B1	829	CLA	C2C-C1C-NC	2.10	111.94	109.97
15	B1	832	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
15	A3	840	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	A3	817	CLA	C2C-C1C-NC	2.10	111.94	109.97
15	A3	802	CLA	CHA-C1A-NA	-2.10	121.59	126.40
15	B1	812	CLA	CAA-C2A-C1A	-2.10	105.11	111.97
15	L1	1003	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
15	A3	837	CLA	CMC-C2C-C1C	2.10	128.23	125.04
15	J1	1307	CLA	C3C-C4C-CHD	-2.10	120.60	125.23
15	A3	811	CLA	CHA-C1A-NA	-2.10	121.60	126.40
15	B1	821	CLA	CHC-C1C-C2C	-2.09	120.93	126.72
15	B2	807	CLA	C2A-C1A-CHA	2.09	127.52	123.86
15	A3	810	CLA	CHA-C1A-NA	-2.09	121.60	126.40
15	B3	812	CLA	CAA-C2A-C1A	-2.09	105.11	111.97
15	B3	806	CLA	CHA-C1A-NA	-2.09	121.60	126.40
15	A3	825	CLA	CHD-C1D-C2D	2.09	129.87	125.48
15	A1	825	CLA	CHD-C1D-C2D	2.09	129.87	125.48
15	A3	842	CLA	CHC-C1C-C2C	-2.09	120.93	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	808	CLA	C2C-C1C-NC	2.09	111.93	109.97
15	B3	807	CLA	C2A-C1A-CHA	2.09	127.52	123.86
15	A1	815	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	B2	811	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	B2	818	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	B1	808	CLA	C2C-C1C-NC	2.09	111.93	109.97
15	B3	818	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	A3	837	CLA	C3C-C4C-NC	2.09	112.92	110.57
15	B2	832	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
15	B3	829	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
15	A2	842	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
15	B3	804	CLA	CHA-C1A-NA	-2.09	121.61	126.40
15	B2	819	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
15	B1	834	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
15	A3	840	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
15	B1	819	CLA	CHC-C1C-C2C	-2.09	120.95	126.72
15	B3	819	CLA	CHC-C1C-C2C	-2.09	120.95	126.72
15	B3	832	CLA	CHC-C1C-C2C	-2.09	120.95	126.72
15	A1	811	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	B2	837	CLA	CHA-C1A-NA	-2.09	121.62	126.40
15	B3	834	CLA	CHA-C1A-NA	-2.09	121.72	126.41
15	B2	821	CLA	CHC-C1C-C2C	-2.09	120.95	126.72
15	B1	818	CLA	CHA-C1A-NA	-2.08	121.62	126.40
15	A1	842	CLA	CHC-C1C-C2C	-2.08	120.95	126.72
15	J2	1307	CLA	C3C-C4C-CHD	-2.08	120.62	125.23
15	B1	829	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
15	A2	811	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	A2	825	CLA	CHD-C1D-C2D	2.08	129.85	125.48
15	B1	833	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
15	B2	812	CLA	C3C-C4C-NC	2.08	112.91	110.57
15	J2	1307	CLA	C2A-C1A-CHA	2.08	125.94	122.71
15	B1	824	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
15	B2	821	CLA	C2C-C1C-NC	2.08	111.92	109.97
15	A3	815	CLA	CHA-C1A-NA	-2.08	121.63	126.40
15	B2	826	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
15	B1	832	CLA	C2C-C1C-NC	2.08	111.92	109.97
15	A2	840	CLA	C2C-C1C-NC	2.08	111.92	109.97
15	B2	829	CLA	C2C-C1C-NC	2.08	111.92	109.97
15	J3	1307	CLA	C2A-C1A-CHA	2.08	125.94	122.71
15	B3	824	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
15	B2	808	CLA	CBA-CAA-C2A	2.08	120.00	113.86
15	L2	1003	CLA	CHC-C1C-C2C	-2.08	120.97	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A2	819	CLA	C2C-C1C-NC	2.08	111.92	109.97
15	A3	807	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
15	B2	824	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
15	A3	811	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
15	K1	103	CLA	CBD-CHA-C1A	2.07	130.25	128.06
15	A2	811	CLA	CHC-C1C-C2C	-2.07	120.98	126.72
15	B2	815	CLA	CHA-C1A-NA	-2.07	121.75	126.41
15	A2	841	CLA	CHA-C1A-NA	-2.07	121.65	126.40
15	A1	807	CLA	CHC-C1C-C2C	-2.07	120.99	126.72
15	B3	815	CLA	CHA-C1A-NA	-2.07	121.75	126.41
15	A2	856	CLA	CHC-C1C-NC	2.07	127.35	124.20
15	A1	811	CLA	CHC-C1C-C2C	-2.07	120.99	126.72
15	A3	803	CLA	C2C-C1C-NC	2.07	111.91	109.97
15	A2	807	CLA	CHC-C1C-C2C	-2.07	120.99	126.72
15	B1	837	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	A3	834	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	B2	834	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
15	B2	832	CLA	C2C-C1C-NC	2.07	111.91	109.97
15	J1	1307	CLA	C2A-C1A-CHA	2.07	125.92	122.71
15	B1	808	CLA	CBA-CAA-C2A	2.07	119.97	113.86
15	A3	806	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	B1	826	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
15	A1	841	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	A3	816	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	A1	831	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
15	A2	822	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
15	B2	829	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
15	B1	815	CLA	CHA-C1A-NA	-2.07	121.76	126.41
15	B3	837	CLA	CHA-C1A-NA	-2.07	121.66	126.40
15	B3	829	CLA	C2C-C1C-NC	2.07	111.91	109.97
15	B2	829	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
15	B3	826	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
15	A1	822	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
15	A2	814	CLA	C2C-C1C-NC	2.07	111.91	109.97
15	A2	806	CLA	CHA-C1A-NA	-2.07	121.67	126.40
15	A1	834	CLA	CHA-C1A-NA	-2.07	121.67	126.40
15	B3	829	CLA	CHC-C1C-C2C	-2.07	121.01	126.72
15	B3	833	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
15	A1	806	CLA	CHA-C1A-NA	-2.06	121.67	126.40
15	B3	808	CLA	CBA-CAA-C2A	2.06	119.96	113.86
15	B2	816	CLA	C1C-C2C-C3C	-2.06	104.79	106.96
15	B1	829	CLA	CHC-C1C-C2C	-2.06	121.01	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	822	CLA	CHC-C1C-C2C	-2.06	121.01	126.72
15	B1	801	CLA	CHC-C1C-C2C	-2.06	121.01	126.72
15	B3	812	CLA	C1C-C2C-C3C	-2.06	104.79	106.96
15	A2	803	CLA	CHA-C1A-NA	-2.06	121.68	126.40
15	A3	821	CLA	CHA-C1A-NA	-2.06	121.68	126.40
15	A2	810	CLA	C2C-C1C-CHC	-2.06	120.69	125.72
15	B1	834	CLA	C2A-C1A-CHA	2.06	125.91	122.71
15	A1	825	CLA	CMC-C2C-C1C	2.06	128.18	125.04
15	A1	826	CLA	CHC-C1C-C2C	-2.06	121.02	126.72
15	B1	812	CLA	C3C-C4C-NC	2.06	112.88	110.57
15	A2	804	CLA	C1C-C2C-C3C	-2.06	104.79	106.96
15	A3	831	CLA	CHC-C1C-C2C	-2.06	121.03	126.72
15	A1	822	CLA	C2C-C1C-NC	2.06	111.90	109.97
15	A3	826	CLA	CHC-C1C-C2C	-2.06	121.03	126.72
15	B3	801	CLA	CHC-C1C-C2C	-2.06	121.03	126.72
15	B2	833	CLA	C1C-C2C-C3C	-2.06	104.79	106.96
15	A1	803	CLA	CHA-C1A-NA	-2.06	121.69	126.40
15	I3	101	CLA	C2A-C1A-CHA	2.06	127.46	123.86
15	B2	801	CLA	CHC-C1C-C2C	-2.06	121.03	126.72
15	A3	804	CLA	C1C-C2C-C3C	-2.06	104.79	106.96
15	A2	831	CLA	CHC-C1C-C2C	-2.06	121.03	126.72
15	B3	812	CLA	C3C-C4C-NC	2.06	112.88	110.57
15	A1	803	CLA	C2C-C1C-NC	2.06	111.90	109.97
15	B3	809	CLA	CHC-C1C-NC	2.06	127.32	124.20
15	A1	804	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
15	A3	841	CLA	CHA-C1A-NA	-2.05	121.69	126.40
15	A1	817	CLA	CHC-C1C-C2C	-2.05	121.04	126.72
15	A2	819	CLA	CHC-C1C-C2C	-2.05	121.04	126.72
15	A2	834	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	A3	809	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
15	A2	816	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	A2	826	CLA	CHC-C1C-C2C	-2.05	121.04	126.72
15	B3	814	CLA	C3C-C4C-NC	2.05	112.87	110.57
15	A1	816	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	A3	814	CLA	C3D-C4D-ND	2.05	113.56	110.24
15	K1	103	CLA	C2C-C1C-CHC	-2.05	120.75	125.67
15	A3	810	CLA	C2C-C1C-CHC	-2.05	120.71	125.72
15	A3	817	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
15	A3	803	CLA	CHA-C1A-NA	-2.05	121.70	126.40
15	K3	103	CLA	C2C-C1C-CHC	-2.05	120.76	125.67
15	A2	817	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
15	I2	101	CLA	CHC-C1C-NC	2.05	127.31	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B3	831	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
15	L1	1004	CLA	CHA-C1A-NA	-2.05	121.71	126.40
15	X3	102	CLA	CMC-C2C-C1C	2.05	128.16	125.04
15	A3	824	CLA	C3C-C4C-NC	2.05	112.87	110.57
15	B2	809	CLA	CHC-C1C-NC	2.05	127.31	124.20
15	L3	1004	CLA	CHA-C1A-NA	-2.05	121.71	126.40
15	A1	819	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
15	L3	1003	CLA	CMC-C2C-C1C	2.05	128.16	125.04
15	A1	821	CLA	CHA-C1A-NA	-2.05	121.71	126.40
15	B3	803	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
15	A1	856	CLA	CHC-C1C-NC	2.05	127.31	124.20
15	A3	819	CLA	C2C-C1C-NC	2.05	111.89	109.97
15	L1	1003	CLA	CMC-C2C-C1C	2.04	128.15	125.04
15	A2	821	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	B2	831	CLA	C1C-C2C-C3C	-2.04	104.81	106.96
15	B3	816	CLA	C1C-C2C-C3C	-2.04	104.81	106.96
15	A3	825	CLA	CMC-C2C-C1C	2.04	128.15	125.04
15	I1	101	CLA	C2A-C1A-CHA	2.04	127.43	123.86
15	K2	103	CLA	C2C-C1C-CHC	-2.04	120.78	125.67
15	B3	834	CLA	C2A-C1A-CHA	2.04	125.88	122.71
15	A1	810	CLA	C2C-C1C-CHC	-2.04	120.73	125.72
15	K2	103	CLA	CBD-CHA-C1A	2.04	130.22	128.06
15	A3	822	CLA	C2C-C1C-NC	2.04	111.89	109.97
15	B1	816	CLA	C1C-C2C-C3C	-2.04	104.81	106.96
15	J2	1301	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	A3	819	CLA	CHC-C1C-C2C	-2.04	121.08	126.72
15	A1	818	CLA	C3C-C4C-NC	2.04	112.86	110.57
15	L2	1004	CLA	CHA-C1A-NA	-2.04	121.72	126.40
15	A2	818	CLA	C3C-C4C-NC	2.04	112.86	110.57
15	A2	828	CLA	CMC-C2C-C1C	2.04	128.15	125.04
15	A1	814	CLA	C3D-C4D-ND	2.04	113.54	110.24
15	A2	825	CLA	CMC-C2C-C1C	2.04	128.14	125.04
15	A2	803	CLA	C2C-C1C-NC	2.04	111.88	109.97
15	B2	837	CLA	C3D-C4D-ND	2.04	113.53	110.24
15	A3	818	CLA	C3C-C4C-NC	2.04	112.86	110.57
15	B1	809	CLA	CHC-C1C-NC	2.04	127.30	124.20
15	I3	101	CLA	CHC-C1C-NC	2.04	127.30	124.20
15	A1	819	CLA	C2C-C1C-NC	2.04	111.88	109.97
15	A3	828	CLA	CMC-C2C-C1C	2.04	128.14	125.04
15	B1	823	CLA	CHC-C1C-NC	2.04	127.29	124.20
15	B3	808	CLA	CHC-C1C-C2C	-2.04	121.09	126.72
15	A1	814	CLA	C2C-C1C-NC	2.04	111.88	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B1	825	CLA	C3C-C4C-NC	2.04	112.86	110.57
15	B1	837	CLA	C3D-C4D-ND	2.04	113.53	110.24
15	A2	832	CLA	CHD-C4C-NC	2.04	127.41	124.20
15	L2	1003	CLA	CMC-C2C-C1C	2.03	128.14	125.04
15	B2	825	CLA	C3C-C4C-NC	2.03	112.85	110.57
15	A3	831	CLA	C2C-C1C-NC	2.03	111.88	109.97
15	B3	832	CLA	C2C-C1C-NC	2.03	111.88	109.97
15	B1	808	CLA	CHC-C1C-C2C	-2.03	121.09	126.72
15	B1	831	CLA	C3C-C4C-NC	2.03	112.85	110.57
15	B3	825	CLA	C3C-C4C-NC	2.03	112.85	110.57
15	L3	1002	CLA	C3C-C4C-NC	2.03	112.85	110.57
15	A1	832	CLA	CHD-C4C-NC	2.03	127.41	124.20
15	B2	823	CLA	CHC-C1C-NC	2.03	127.29	124.20
15	A2	822	CLA	C2C-C1C-NC	2.03	111.88	109.97
15	A3	820	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
15	A1	828	CLA	CMC-C2C-C1C	2.03	128.13	125.04
15	A2	821	CLA	C3D-C4D-ND	2.03	113.52	110.24
15	B3	837	CLA	C3D-C4D-ND	2.03	113.52	110.24
15	B1	803	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
15	A3	814	CLA	C2C-C1C-NC	2.03	111.87	109.97
15	J2	1302	CLA	CHA-C1A-NA	-2.03	121.84	126.41
15	B2	834	CLA	C2A-C1A-CHA	2.03	125.86	122.71
15	B2	808	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
15	B1	831	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
15	A3	813	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
15	A2	841	CLA	C3C-C4C-NC	2.03	112.85	110.57
15	B2	831	CLA	C3C-C4C-NC	2.03	112.85	110.57
15	B3	831	CLA	C3C-C4C-NC	2.03	112.85	110.57
15	A1	820	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
15	B2	803	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
15	J1	1301	CLA	CHA-C1A-NA	-2.03	121.75	126.40
15	A1	821	CLA	C3D-C4D-ND	2.03	113.52	110.24
15	X1	102	CLA	CMC-C2C-C1C	2.03	128.13	125.04
15	A2	817	CLA	C3D-C4D-ND	2.03	113.52	110.24
15	I1	101	CLA	CHC-C1C-NC	2.03	127.28	124.20
15	A3	817	CLA	C3D-C4D-ND	2.03	113.52	110.24
15	A3	841	CLA	C3C-C4C-NC	2.03	112.84	110.57
15	A3	822	CLA	CAA-C2A-C1A	-2.03	105.34	111.97
15	A3	815	CLA	C3D-C4D-ND	2.03	113.51	110.24
15	I2	101	CLA	C2A-C1A-CHA	2.03	127.40	123.86
15	A1	831	CLA	C2C-C1C-NC	2.02	111.87	109.97
15	A1	817	CLA	C3D-C4D-ND	2.02	113.51	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A1	822	CLA	CAA-C2A-C1A	-2.02	105.34	111.97
15	X2	102	CLA	CMC-C2C-C1C	2.02	128.12	125.04
15	A3	856	CLA	CHC-C1C-NC	2.02	127.27	124.20
15	A3	832	CLA	CHD-C4C-NC	2.02	127.39	124.20
15	A2	856	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
15	B3	823	CLA	CHC-C1C-NC	2.02	127.27	124.20
15	A2	809	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
15	B1	814	CLA	C3C-C4C-NC	2.02	112.84	110.57
15	J3	1301	CLA	CHA-C1A-NA	-2.02	121.77	126.40
15	A2	814	CLA	C3D-C4D-ND	2.02	113.51	110.24
15	A1	840	CLA	C2C-C1C-NC	2.02	111.87	109.97
15	A1	809	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
15	B1	812	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
15	A1	815	CLA	C3D-C4D-ND	2.02	113.51	110.24
15	A2	840	CLA	CMC-C2C-C1C	2.02	128.12	125.04
15	J1	1302	CLA	CHA-C1A-NA	-2.02	121.87	126.41
15	A2	822	CLA	CAA-C2A-C1A	-2.02	105.36	111.97
15	A1	856	CLA	CHC-C1C-C2C	-2.02	121.14	126.72
15	B1	804	CLA	CMC-C2C-C1C	2.02	128.11	125.04
15	A3	856	CLA	CHC-C1C-C2C	-2.02	121.14	126.72
15	A1	841	CLA	C3C-C4C-NC	2.02	112.83	110.57
15	J3	1303	CLA	CHA-C1A-NA	-2.02	121.78	126.40
15	A1	813	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
15	A2	832	CLA	CMC-C2C-C1C	2.02	128.11	125.04
15	B3	804	CLA	CMC-C2C-C1C	2.02	128.11	125.04
15	A3	813	CLA	C3C-C4C-NC	2.02	112.83	110.57
15	J2	1303	CLA	C3D-C4D-ND	2.02	113.50	110.24
15	K2	103	CLA	C2A-C3A-C4A	-2.02	100.01	103.59
15	A2	813	CLA	C1C-C2C-C3C	-2.02	104.84	106.96
15	A2	820	CLA	C1C-C2C-C3C	-2.01	104.84	106.96
15	A3	804	CLA	CMC-C2C-C1C	2.01	128.11	125.04
15	A2	814	CLA	C2A-C1A-CHA	2.01	125.83	122.71
15	A2	841	CLA	CMC-C2C-C1C	2.01	128.10	125.04
15	B3	806	CLA	CMC-C2C-C1C	2.01	128.10	125.04
15	A3	806	CLA	C1C-C2C-C3C	-2.01	104.84	106.96
15	B1	808	CLA	CAA-C2A-C1A	-2.01	105.38	111.97
15	A1	824	CLA	C3C-C4C-NC	2.01	112.83	110.57
15	L1	1002	CLA	C3C-C4C-NC	2.01	112.83	110.57
15	B2	804	CLA	CMC-C2C-C1C	2.01	128.10	125.04
15	L3	1002	CLA	C1C-C2C-C3C	-2.01	104.84	106.96
15	A2	813	CLA	C3C-C4C-NC	2.01	112.82	110.57
15	A3	803	CLA	C3D-C4D-ND	2.01	113.49	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A3	821	CLA	C3D-C4D-ND	2.01	113.49	110.24
15	B3	808	CLA	CAA-C2A-C1A	-2.01	105.39	111.97
15	A3	840	CLA	C2C-C1C-NC	2.01	111.85	109.97
15	K1	103	CLA	C2A-C3A-C4A	-2.01	100.02	103.59
15	K3	103	CLA	C2A-C3A-C4A	-2.01	100.02	103.59
15	B2	808	CLA	CAA-C2A-C1A	-2.01	105.40	111.97
15	A2	834	CLA	C3C-C4C-NC	2.01	112.82	110.57
15	A1	806	CLA	C1C-C2C-C3C	-2.00	104.85	106.96
15	J1	1303	CLA	C3D-C4D-ND	2.00	113.48	110.24
15	J1	1303	CLA	CHA-C1A-NA	-2.00	121.81	126.40
15	J2	1303	CLA	CHA-C1A-NA	-2.00	121.81	126.40
15	I2	101	CLA	C3C-C4C-NC	2.00	112.82	110.57
15	L2	1002	CLA	C3C-C4C-NC	2.00	112.82	110.57
15	B2	812	CLA	C1C-C2C-C3C	-2.00	104.85	106.96
15	B2	835	CLA	CMC-C2C-C1C	2.00	128.09	125.04
15	I1	101	CLA	C1C-C2C-C3C	-2.00	104.85	106.96

All (294) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A1	801	CL0	NA
14	A1	801	CL0	NC
14	A1	801	CL0	ND
14	A2	801	CL0	NA
14	A2	801	CL0	NC
14	A2	801	CL0	ND
14	A3	801	CL0	NA
14	A3	801	CL0	NC
14	A3	801	CL0	ND
15	A1	802	CLA	ND
15	A1	803	CLA	ND
15	A1	804	CLA	ND
15	A1	805	CLA	ND
15	A1	806	CLA	ND
15	A1	807	CLA	ND
15	A1	808	CLA	ND
15	A1	809	CLA	ND
15	A1	810	CLA	ND
15	A1	811	CLA	ND
15	A1	812	CLA	ND
15	A1	813	CLA	ND
15	A1	814	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A1	815	CLA	ND
15	A1	816	CLA	ND
15	A1	817	CLA	ND
15	A1	818	CLA	ND
15	A1	819	CLA	ND
15	A1	820	CLA	ND
15	A1	821	CLA	ND
15	A1	822	CLA	ND
15	A1	823	CLA	ND
15	A1	824	CLA	ND
15	A1	825	CLA	ND
15	A1	826	CLA	ND
15	A1	827	CLA	ND
15	A1	828	CLA	ND
15	A1	829	CLA	ND
15	A1	830	CLA	ND
15	A1	831	CLA	ND
15	A1	832	CLA	ND
15	A1	833	CLA	ND
15	A1	834	CLA	ND
15	A1	835	CLA	ND
15	A1	836	CLA	ND
15	A1	837	CLA	ND
15	A1	838	CLA	ND
15	A1	839	CLA	ND
15	A1	840	CLA	ND
15	A1	841	CLA	ND
15	A1	842	CLA	ND
15	A1	843	CLA	ND
15	A1	844	CLA	ND
15	A1	856	CLA	ND
15	B1	801	CLA	ND
15	B1	802	CLA	ND
15	B1	803	CLA	ND
15	B1	804	CLA	ND
15	B1	805	CLA	ND
15	B1	806	CLA	ND
15	B1	807	CLA	ND
15	B1	808	CLA	ND
15	B1	809	CLA	ND
15	B1	810	CLA	ND
15	B1	811	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B1	812	CLA	ND
15	B1	813	CLA	ND
15	B1	814	CLA	ND
15	B1	815	CLA	ND
15	B1	816	CLA	ND
15	B1	817	CLA	ND
15	B1	818	CLA	ND
15	B1	819	CLA	ND
15	B1	820	CLA	ND
15	B1	821	CLA	ND
15	B1	822	CLA	ND
15	B1	823	CLA	ND
15	B1	824	CLA	ND
15	B1	825	CLA	ND
15	B1	826	CLA	ND
15	B1	827	CLA	ND
15	B1	828	CLA	ND
15	B1	829	CLA	ND
15	B1	830	CLA	ND
15	B1	831	CLA	ND
15	B1	832	CLA	ND
15	B1	833	CLA	ND
15	B1	834	CLA	ND
15	B1	835	CLA	ND
15	B1	836	CLA	ND
15	B1	837	CLA	ND
15	B1	838	CLA	ND
15	B1	839	CLA	ND
15	B1	849	CLA	ND
15	I1	101	CLA	ND
15	J1	1301	CLA	ND
15	J1	1302	CLA	ND
15	J1	1303	CLA	ND
15	J1	1307	CLA	ND
15	K1	101	CLA	ND
15	K1	103	CLA	ND
15	L1	1002	CLA	ND
15	L1	1003	CLA	ND
15	L1	1004	CLA	ND
15	X1	102	CLA	ND
15	A2	802	CLA	ND
15	A2	803	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A2	804	CLA	ND
15	A2	805	CLA	ND
15	A2	806	CLA	ND
15	A2	807	CLA	ND
15	A2	808	CLA	ND
15	A2	809	CLA	ND
15	A2	810	CLA	ND
15	A2	811	CLA	ND
15	A2	812	CLA	ND
15	A2	813	CLA	ND
15	A2	814	CLA	ND
15	A2	815	CLA	ND
15	A2	816	CLA	ND
15	A2	817	CLA	ND
15	A2	818	CLA	ND
15	A2	819	CLA	ND
15	A2	820	CLA	ND
15	A2	821	CLA	ND
15	A2	822	CLA	ND
15	A2	823	CLA	ND
15	A2	824	CLA	ND
15	A2	825	CLA	ND
15	A2	826	CLA	ND
15	A2	827	CLA	ND
15	A2	828	CLA	ND
15	A2	829	CLA	ND
15	A2	830	CLA	ND
15	A2	831	CLA	ND
15	A2	832	CLA	ND
15	A2	833	CLA	ND
15	A2	834	CLA	ND
15	A2	835	CLA	ND
15	A2	836	CLA	ND
15	A2	837	CLA	ND
15	A2	838	CLA	ND
15	A2	839	CLA	ND
15	A2	840	CLA	ND
15	A2	841	CLA	ND
15	A2	842	CLA	ND
15	A2	843	CLA	ND
15	A2	844	CLA	ND
15	A2	856	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B2	801	CLA	ND
15	B2	802	CLA	ND
15	B2	803	CLA	ND
15	B2	804	CLA	ND
15	B2	805	CLA	ND
15	B2	806	CLA	ND
15	B2	807	CLA	ND
15	B2	808	CLA	ND
15	B2	809	CLA	ND
15	B2	810	CLA	ND
15	B2	811	CLA	ND
15	B2	812	CLA	ND
15	B2	813	CLA	ND
15	B2	814	CLA	ND
15	B2	815	CLA	ND
15	B2	816	CLA	ND
15	B2	817	CLA	ND
15	B2	818	CLA	ND
15	B2	819	CLA	ND
15	B2	820	CLA	ND
15	B2	821	CLA	ND
15	B2	822	CLA	ND
15	B2	823	CLA	ND
15	B2	824	CLA	ND
15	B2	825	CLA	ND
15	B2	826	CLA	ND
15	B2	827	CLA	ND
15	B2	828	CLA	ND
15	B2	829	CLA	ND
15	B2	830	CLA	ND
15	B2	831	CLA	ND
15	B2	832	CLA	ND
15	B2	833	CLA	ND
15	B2	834	CLA	ND
15	B2	835	CLA	ND
15	B2	836	CLA	ND
15	B2	837	CLA	ND
15	B2	838	CLA	ND
15	B2	839	CLA	ND
15	B2	849	CLA	ND
15	I2	101	CLA	ND
15	J2	1301	CLA	ND

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Mol	Chain	Res	Type	Atom
15	J2	1302	CLA	ND
15	J2	1303	CLA	ND
15	J2	1307	CLA	ND
15	K2	101	CLA	ND
15	K2	103	CLA	ND
15	L2	1002	CLA	ND
15	L2	1003	CLA	ND
15	L2	1004	CLA	ND
15	X2	102	CLA	ND
15	A3	802	CLA	ND
15	A3	803	CLA	ND
15	A3	804	CLA	ND
15	A3	805	CLA	ND
15	A3	806	CLA	ND
15	A3	807	CLA	ND
15	A3	808	CLA	ND
15	A3	809	CLA	ND
15	A3	810	CLA	ND
15	A3	811	CLA	ND
15	A3	812	CLA	ND
15	A3	813	CLA	ND
15	A3	814	CLA	ND
15	A3	815	CLA	ND
15	A3	816	CLA	ND
15	A3	817	CLA	ND
15	A3	818	CLA	ND
15	A3	819	CLA	ND
15	A3	820	CLA	ND
15	A3	821	CLA	ND
15	A3	822	CLA	ND
15	A3	823	CLA	ND
15	A3	824	CLA	ND
15	A3	825	CLA	ND
15	A3	826	CLA	ND
15	A3	827	CLA	ND
15	A3	828	CLA	ND
15	A3	829	CLA	ND
15	A3	830	CLA	ND
15	A3	831	CLA	ND
15	A3	832	CLA	ND
15	A3	833	CLA	ND
15	A3	834	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A3	835	CLA	ND
15	A3	836	CLA	ND
15	A3	837	CLA	ND
15	A3	838	CLA	ND
15	A3	839	CLA	ND
15	A3	840	CLA	ND
15	A3	841	CLA	ND
15	A3	842	CLA	ND
15	A3	843	CLA	ND
15	A3	844	CLA	ND
15	A3	856	CLA	ND
15	B3	801	CLA	ND
15	B3	802	CLA	ND
15	B3	803	CLA	ND
15	B3	804	CLA	ND
15	B3	805	CLA	ND
15	B3	806	CLA	ND
15	B3	807	CLA	ND
15	B3	808	CLA	ND
15	B3	809	CLA	ND
15	B3	810	CLA	ND
15	B3	811	CLA	ND
15	B3	812	CLA	ND
15	B3	813	CLA	ND
15	B3	814	CLA	ND
15	B3	815	CLA	ND
15	B3	816	CLA	ND
15	B3	817	CLA	ND
15	B3	818	CLA	ND
15	B3	819	CLA	ND
15	B3	820	CLA	ND
15	B3	821	CLA	ND
15	B3	822	CLA	ND
15	B3	823	CLA	ND
15	B3	824	CLA	ND
15	B3	825	CLA	ND
15	B3	826	CLA	ND
15	B3	827	CLA	ND
15	B3	828	CLA	ND
15	B3	829	CLA	ND
15	B3	830	CLA	ND
15	B3	831	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B3	832	CLA	ND
15	B3	833	CLA	ND
15	B3	834	CLA	ND
15	B3	835	CLA	ND
15	B3	836	CLA	ND
15	B3	837	CLA	ND
15	B3	838	CLA	ND
15	B3	839	CLA	ND
15	B3	849	CLA	ND
15	I3	101	CLA	ND
15	J3	1301	CLA	ND
15	J3	1302	CLA	ND
15	J3	1303	CLA	ND
15	J3	1307	CLA	ND
15	K3	101	CLA	ND
15	K3	103	CLA	ND
15	L3	1002	CLA	ND
15	L3	1003	CLA	ND
15	L3	1004	CLA	ND
15	X3	102	CLA	ND

All (1338) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A1	804	CLA	CHA-CBD-CGD-O1D
15	A1	804	CLA	CHA-CBD-CGD-O2D
15	A1	805	CLA	CHA-CBD-CGD-O1D
15	A1	805	CLA	CHA-CBD-CGD-O2D
15	A1	805	CLA	CAD-CBD-CGD-O1D
15	A1	807	CLA	C1A-C2A-CAA-CBA
15	A1	808	CLA	CHA-CBD-CGD-O2D
15	A1	811	CLA	C1A-C2A-CAA-CBA
15	A1	811	CLA	C4-C3-C5-C6
15	A1	818	CLA	C3A-C2A-CAA-CBA
15	A1	823	CLA	CHA-CBD-CGD-O1D
15	A1	824	CLA	C1A-C2A-CAA-CBA
15	A1	828	CLA	C1A-C2A-CAA-CBA
15	A1	829	CLA	C2A-CAA-CBA-CGA
15	A1	830	CLA	CHA-CBD-CGD-O1D
15	A1	830	CLA	CHA-CBD-CGD-O2D
15	A1	832	CLA	C1A-C2A-CAA-CBA
15	A1	832	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A1	834	CLA	CHA-CBD-CGD-O1D
15	A1	834	CLA	CHA-CBD-CGD-O2D
15	A1	836	CLA	CHA-CBD-CGD-O1D
15	A1	839	CLA	CHA-CBD-CGD-O1D
15	A1	839	CLA	CHA-CBD-CGD-O2D
15	A1	840	CLA	CHA-CBD-CGD-O1D
15	B1	802	CLA	C1A-C2A-CAA-CBA
15	B1	802	CLA	C3A-C2A-CAA-CBA
15	B1	807	CLA	C1A-C2A-CAA-CBA
15	B1	808	CLA	CHA-CBD-CGD-O1D
15	B1	808	CLA	CHA-CBD-CGD-O2D
15	B1	809	CLA	C1A-C2A-CAA-CBA
15	B1	812	CLA	CAD-CBD-CGD-O2D
15	B1	817	CLA	C1A-C2A-CAA-CBA
15	B1	817	CLA	C3A-C2A-CAA-CBA
15	B1	819	CLA	C1A-C2A-CAA-CBA
15	B1	827	CLA	C1A-C2A-CAA-CBA
15	B1	827	CLA	C3A-C2A-CAA-CBA
15	B1	833	CLA	C1A-C2A-CAA-CBA
15	B1	833	CLA	C3A-C2A-CAA-CBA
15	B1	835	CLA	C1A-C2A-CAA-CBA
15	B1	838	CLA	C2A-CAA-CBA-CGA
15	B1	849	CLA	C1A-C2A-CAA-CBA
15	A2	804	CLA	CHA-CBD-CGD-O1D
15	A2	804	CLA	CHA-CBD-CGD-O2D
15	A2	805	CLA	CHA-CBD-CGD-O1D
15	A2	805	CLA	CHA-CBD-CGD-O2D
15	A2	805	CLA	CAD-CBD-CGD-O1D
15	A2	807	CLA	C1A-C2A-CAA-CBA
15	A2	808	CLA	CHA-CBD-CGD-O2D
15	A2	811	CLA	C1A-C2A-CAA-CBA
15	A2	811	CLA	C4-C3-C5-C6
15	A2	818	CLA	C3A-C2A-CAA-CBA
15	A2	823	CLA	CHA-CBD-CGD-O1D
15	A2	824	CLA	C1A-C2A-CAA-CBA
15	A2	828	CLA	C1A-C2A-CAA-CBA
15	A2	829	CLA	C2A-CAA-CBA-CGA
15	A2	830	CLA	CHA-CBD-CGD-O1D
15	A2	830	CLA	CHA-CBD-CGD-O2D
15	A2	832	CLA	C1A-C2A-CAA-CBA
15	A2	832	CLA	C3A-C2A-CAA-CBA
15	A2	834	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	A2	834	CLA	CHA-CBD-CGD-O2D
15	A2	836	CLA	CHA-CBD-CGD-O1D
15	A2	839	CLA	CHA-CBD-CGD-O1D
15	A2	839	CLA	CHA-CBD-CGD-O2D
15	A2	840	CLA	CHA-CBD-CGD-O1D
15	A2	840	CLA	CHA-CBD-CGD-O2D
15	B2	802	CLA	C1A-C2A-CAA-CBA
15	B2	802	CLA	C3A-C2A-CAA-CBA
15	B2	807	CLA	C1A-C2A-CAA-CBA
15	B2	808	CLA	CHA-CBD-CGD-O1D
15	B2	808	CLA	CHA-CBD-CGD-O2D
15	B2	809	CLA	C1A-C2A-CAA-CBA
15	B2	812	CLA	CAD-CBD-CGD-O2D
15	B2	817	CLA	C1A-C2A-CAA-CBA
15	B2	817	CLA	C3A-C2A-CAA-CBA
15	B2	819	CLA	C1A-C2A-CAA-CBA
15	B2	827	CLA	C1A-C2A-CAA-CBA
15	B2	827	CLA	C3A-C2A-CAA-CBA
15	B2	833	CLA	C1A-C2A-CAA-CBA
15	B2	833	CLA	C3A-C2A-CAA-CBA
15	B2	835	CLA	C1A-C2A-CAA-CBA
15	B2	838	CLA	C2A-CAA-CBA-CGA
15	B2	849	CLA	C1A-C2A-CAA-CBA
15	A3	804	CLA	CHA-CBD-CGD-O1D
15	A3	804	CLA	CHA-CBD-CGD-O2D
15	A3	805	CLA	CHA-CBD-CGD-O1D
15	A3	805	CLA	CHA-CBD-CGD-O2D
15	A3	805	CLA	CAD-CBD-CGD-O1D
15	A3	807	CLA	C1A-C2A-CAA-CBA
15	A3	808	CLA	CHA-CBD-CGD-O2D
15	A3	811	CLA	C1A-C2A-CAA-CBA
15	A3	811	CLA	C4-C3-C5-C6
15	A3	818	CLA	C3A-C2A-CAA-CBA
15	A3	823	CLA	CHA-CBD-CGD-O1D
15	A3	824	CLA	C1A-C2A-CAA-CBA
15	A3	828	CLA	C1A-C2A-CAA-CBA
15	A3	829	CLA	C2A-CAA-CBA-CGA
15	A3	830	CLA	CHA-CBD-CGD-O1D
15	A3	830	CLA	CHA-CBD-CGD-O2D
15	A3	832	CLA	C1A-C2A-CAA-CBA
15	A3	832	CLA	C3A-C2A-CAA-CBA
15	A3	834	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	A3	834	CLA	CHA-CBD-CGD-O2D
15	A3	836	CLA	CHA-CBD-CGD-O1D
15	A3	839	CLA	CHA-CBD-CGD-O1D
15	A3	839	CLA	CHA-CBD-CGD-O2D
15	A3	840	CLA	CHA-CBD-CGD-O1D
15	B3	802	CLA	C1A-C2A-CAA-CBA
15	B3	802	CLA	C3A-C2A-CAA-CBA
15	B3	807	CLA	C1A-C2A-CAA-CBA
15	B3	808	CLA	CHA-CBD-CGD-O1D
15	B3	808	CLA	CHA-CBD-CGD-O2D
15	B3	809	CLA	C1A-C2A-CAA-CBA
15	B3	812	CLA	CAD-CBD-CGD-O2D
15	B3	817	CLA	C1A-C2A-CAA-CBA
15	B3	817	CLA	C3A-C2A-CAA-CBA
15	B3	819	CLA	C1A-C2A-CAA-CBA
15	B3	827	CLA	C1A-C2A-CAA-CBA
15	B3	827	CLA	C3A-C2A-CAA-CBA
15	B3	833	CLA	C1A-C2A-CAA-CBA
15	B3	833	CLA	C3A-C2A-CAA-CBA
15	B3	835	CLA	C1A-C2A-CAA-CBA
15	B3	838	CLA	C2A-CAA-CBA-CGA
15	B3	849	CLA	C1A-C2A-CAA-CBA
18	A1	848	BCR	C23-C24-C25-C26
18	A1	848	BCR	C23-C24-C25-C30
18	A1	851	BCR	C7-C8-C9-C10
18	A1	851	BCR	C7-C8-C9-C34
18	B1	841	BCR	C1-C6-C7-C8
18	B1	841	BCR	C5-C6-C7-C8
18	B1	845	BCR	C23-C24-C25-C30
18	B1	847	BCR	C21-C22-C23-C24
18	B1	847	BCR	C37-C22-C23-C24
18	B1	847	BCR	C23-C24-C25-C26
18	J1	1304	BCR	C5-C6-C7-C8
18	J1	1305	BCR	C23-C24-C25-C26
18	J1	1305	BCR	C23-C24-C25-C30
18	J1	1306	BCR	C7-C8-C9-C10
18	J1	1306	BCR	C7-C8-C9-C34
18	M1	101	BCR	C1-C6-C7-C8
18	M1	101	BCR	C5-C6-C7-C8
18	A2	848	BCR	C23-C24-C25-C26
18	A2	848	BCR	C23-C24-C25-C30
18	A2	851	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
18	A2	851	BCR	C7-C8-C9-C34
18	B2	841	BCR	C1-C6-C7-C8
18	B2	841	BCR	C5-C6-C7-C8
18	B2	845	BCR	C23-C24-C25-C30
18	B2	847	BCR	C21-C22-C23-C24
18	B2	847	BCR	C37-C22-C23-C24
18	B2	847	BCR	C23-C24-C25-C26
18	J2	1304	BCR	C5-C6-C7-C8
18	J2	1305	BCR	C23-C24-C25-C26
18	J2	1305	BCR	C23-C24-C25-C30
18	J2	1306	BCR	C7-C8-C9-C10
18	J2	1306	BCR	C7-C8-C9-C34
18	M2	101	BCR	C1-C6-C7-C8
18	M2	101	BCR	C5-C6-C7-C8
18	A3	848	BCR	C23-C24-C25-C26
18	A3	848	BCR	C23-C24-C25-C30
18	A3	851	BCR	C7-C8-C9-C10
18	A3	851	BCR	C7-C8-C9-C34
18	B3	841	BCR	C1-C6-C7-C8
18	B3	841	BCR	C5-C6-C7-C8
18	B3	845	BCR	C23-C24-C25-C30
18	B3	847	BCR	C21-C22-C23-C24
18	B3	847	BCR	C37-C22-C23-C24
18	B3	847	BCR	C23-C24-C25-C26
18	J3	1304	BCR	C5-C6-C7-C8
18	J3	1305	BCR	C23-C24-C25-C26
18	J3	1305	BCR	C23-C24-C25-C30
18	J3	1306	BCR	C7-C8-C9-C10
18	J3	1306	BCR	C7-C8-C9-C34
18	M3	101	BCR	C1-C6-C7-C8
18	M3	101	BCR	C5-C6-C7-C8
19	A1	854	LHG	O9-C7-O7-C5
19	A1	854	LHG	C8-C7-O7-C5
19	X1	101	LHG	C3-O3-P-O5
19	X1	101	LHG	C4-O6-P-O4
19	A2	854	LHG	O9-C7-O7-C5
19	A2	854	LHG	C8-C7-O7-C5
19	X2	101	LHG	C3-O3-P-O5
19	X2	101	LHG	C4-O6-P-O4
19	A3	854	LHG	O9-C7-O7-C5
19	A3	854	LHG	C8-C7-O7-C5
19	X3	101	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
19	X3	101	LHG	C4-O6-P-O4
21	B1	848	DGD	O6D-C1D-O3G-C3G
21	B2	848	DGD	O6D-C1D-O3G-C3G
21	B3	848	DGD	O6D-C1D-O3G-C3G
15	A1	818	CLA	O1D-CGD-O2D-CED
15	A2	818	CLA	O1D-CGD-O2D-CED
15	A3	818	CLA	O1D-CGD-O2D-CED
15	A1	818	CLA	CBD-CGD-O2D-CED
15	A1	842	CLA	CBD-CGD-O2D-CED
15	B1	801	CLA	CBD-CGD-O2D-CED
15	A2	818	CLA	CBD-CGD-O2D-CED
15	A2	842	CLA	CBD-CGD-O2D-CED
15	B2	801	CLA	CBD-CGD-O2D-CED
15	A3	818	CLA	CBD-CGD-O2D-CED
15	A3	842	CLA	CBD-CGD-O2D-CED
15	B3	801	CLA	CBD-CGD-O2D-CED
15	B1	801	CLA	O1D-CGD-O2D-CED
15	B2	801	CLA	O1D-CGD-O2D-CED
15	B3	801	CLA	O1D-CGD-O2D-CED
15	A1	824	CLA	CBD-CGD-O2D-CED
15	A1	834	CLA	CBD-CGD-O2D-CED
15	A1	839	CLA	CBD-CGD-O2D-CED
15	B1	804	CLA	CBD-CGD-O2D-CED
15	B1	830	CLA	CBD-CGD-O2D-CED
15	B1	837	CLA	CBD-CGD-O2D-CED
15	B1	849	CLA	CBD-CGD-O2D-CED
15	X1	102	CLA	CBD-CGD-O2D-CED
15	A2	824	CLA	CBD-CGD-O2D-CED
15	A2	834	CLA	CBD-CGD-O2D-CED
15	A2	839	CLA	CBD-CGD-O2D-CED
15	B2	804	CLA	CBD-CGD-O2D-CED
15	B2	830	CLA	CBD-CGD-O2D-CED
15	B2	837	CLA	CBD-CGD-O2D-CED
15	B2	849	CLA	CBD-CGD-O2D-CED
15	X2	102	CLA	CBD-CGD-O2D-CED
15	A3	824	CLA	CBD-CGD-O2D-CED
15	A3	834	CLA	CBD-CGD-O2D-CED
15	A3	839	CLA	CBD-CGD-O2D-CED
15	B3	804	CLA	CBD-CGD-O2D-CED
15	B3	830	CLA	CBD-CGD-O2D-CED
15	B3	837	CLA	CBD-CGD-O2D-CED
15	B3	849	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	X3	102	CLA	CBD-CGD-O2D-CED
15	B1	839	CLA	CBD-CGD-O2D-CED
15	B2	839	CLA	CBD-CGD-O2D-CED
15	B3	839	CLA	CBD-CGD-O2D-CED
15	A1	825	CLA	C3-C5-C6-C7
15	A2	825	CLA	C3-C5-C6-C7
15	A3	825	CLA	C3-C5-C6-C7
15	B1	803	CLA	CBD-CGD-O2D-CED
15	B2	803	CLA	CBD-CGD-O2D-CED
15	B3	803	CLA	CBD-CGD-O2D-CED
15	A1	811	CLA	C2-C3-C5-C6
15	A2	811	CLA	C2-C3-C5-C6
15	A3	811	CLA	C2-C3-C5-C6
15	B2	805	CLA	CBD-CGD-O2D-CED
15	A1	832	CLA	CBD-CGD-O2D-CED
15	B1	805	CLA	CBD-CGD-O2D-CED
15	A2	832	CLA	CBD-CGD-O2D-CED
15	A3	832	CLA	CBD-CGD-O2D-CED
15	B3	805	CLA	CBD-CGD-O2D-CED
15	A1	830	CLA	CBD-CGD-O2D-CED
15	B1	814	CLA	CBD-CGD-O2D-CED
15	B1	821	CLA	CBD-CGD-O2D-CED
15	B1	824	CLA	CBD-CGD-O2D-CED
15	A2	830	CLA	CBD-CGD-O2D-CED
15	A2	838	CLA	CBD-CGD-O2D-CED
15	B2	814	CLA	CBD-CGD-O2D-CED
15	B2	821	CLA	CBD-CGD-O2D-CED
15	B2	824	CLA	CBD-CGD-O2D-CED
15	A3	830	CLA	CBD-CGD-O2D-CED
15	A3	838	CLA	CBD-CGD-O2D-CED
15	B3	814	CLA	CBD-CGD-O2D-CED
15	B3	821	CLA	CBD-CGD-O2D-CED
15	B3	824	CLA	CBD-CGD-O2D-CED
19	X1	101	LHG	O2-C2-C3-O3
19	X2	101	LHG	O2-C2-C3-O3
19	X3	101	LHG	O2-C2-C3-O3
15	A1	838	CLA	CBD-CGD-O2D-CED
15	A1	842	CLA	O1D-CGD-O2D-CED
15	A2	842	CLA	O1D-CGD-O2D-CED
15	A3	842	CLA	O1D-CGD-O2D-CED
15	A1	834	CLA	O1D-CGD-O2D-CED
15	X1	102	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	A2	834	CLA	O1D-CGD-O2D-CED
15	X2	102	CLA	O1D-CGD-O2D-CED
15	A3	834	CLA	O1D-CGD-O2D-CED
15	X3	102	CLA	O1D-CGD-O2D-CED
19	X1	101	LHG	C1-C2-C3-O3
19	X2	101	LHG	C1-C2-C3-O3
19	X3	101	LHG	C1-C2-C3-O3
15	B1	830	CLA	O1D-CGD-O2D-CED
15	B2	830	CLA	O1D-CGD-O2D-CED
15	B3	830	CLA	O1D-CGD-O2D-CED
15	B1	813	CLA	CBD-CGD-O2D-CED
15	B2	813	CLA	CBD-CGD-O2D-CED
15	B3	813	CLA	CBD-CGD-O2D-CED
18	A1	855	BCR	C19-C20-C21-C22
18	A2	855	BCR	C19-C20-C21-C22
18	A3	855	BCR	C19-C20-C21-C22
15	A1	856	CLA	C11-C10-C8-C9
15	A2	856	CLA	C11-C10-C8-C9
15	A3	856	CLA	C11-C10-C8-C9
15	A1	839	CLA	O1D-CGD-O2D-CED
15	A2	839	CLA	O1D-CGD-O2D-CED
15	A3	839	CLA	O1D-CGD-O2D-CED
15	B1	804	CLA	O1D-CGD-O2D-CED
15	B1	837	CLA	O1D-CGD-O2D-CED
15	B2	804	CLA	O1D-CGD-O2D-CED
15	B2	837	CLA	O1D-CGD-O2D-CED
15	B3	837	CLA	O1D-CGD-O2D-CED
15	A1	830	CLA	C10-C11-C12-C13
15	A2	830	CLA	C10-C11-C12-C13
15	A3	830	CLA	C10-C11-C12-C13
15	B3	804	CLA	O1D-CGD-O2D-CED
15	A1	838	CLA	CBA-CGA-O2A-C1
15	A2	838	CLA	CBA-CGA-O2A-C1
15	A3	838	CLA	CBA-CGA-O2A-C1
15	B1	849	CLA	O1D-CGD-O2D-CED
15	B2	849	CLA	O1D-CGD-O2D-CED
15	B3	849	CLA	O1D-CGD-O2D-CED
15	A1	824	CLA	O1D-CGD-O2D-CED
15	A2	824	CLA	O1D-CGD-O2D-CED
15	B1	808	CLA	C6-C7-C8-C10
15	B2	808	CLA	C6-C7-C8-C10
15	B3	808	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	B1	844	BCR	C19-C20-C21-C22
18	B2	844	BCR	C19-C20-C21-C22
18	B3	844	BCR	C19-C20-C21-C22
15	B1	826	CLA	CBD-CGD-O2D-CED
15	B1	803	CLA	O1D-CGD-O2D-CED
15	B1	839	CLA	O1D-CGD-O2D-CED
15	B2	803	CLA	O1D-CGD-O2D-CED
15	B2	839	CLA	O1D-CGD-O2D-CED
15	A3	824	CLA	O1D-CGD-O2D-CED
15	B3	803	CLA	O1D-CGD-O2D-CED
15	B3	839	CLA	O1D-CGD-O2D-CED
15	B2	826	CLA	CBD-CGD-O2D-CED
15	B3	826	CLA	CBD-CGD-O2D-CED
15	A1	843	CLA	C5-C6-C7-C8
15	B1	802	CLA	C10-C11-C12-C13
15	A2	843	CLA	C5-C6-C7-C8
15	B2	802	CLA	C10-C11-C12-C13
15	A3	843	CLA	C5-C6-C7-C8
15	B3	802	CLA	C10-C11-C12-C13
19	A1	853	LHG	C4-O6-P-O3
19	A1	854	LHG	C3-O3-P-O6
19	X1	101	LHG	C3-O3-P-O6
19	X1	101	LHG	C4-O6-P-O3
19	A2	853	LHG	C4-O6-P-O3
19	A2	854	LHG	C3-O3-P-O6
19	X2	101	LHG	C3-O3-P-O6
19	X2	101	LHG	C4-O6-P-O3
19	A3	853	LHG	C4-O6-P-O3
19	A3	854	LHG	C3-O3-P-O6
19	X3	101	LHG	C3-O3-P-O6
19	X3	101	LHG	C4-O6-P-O3
15	A1	843	CLA	CBA-CGA-O2A-C1
15	A2	843	CLA	CBA-CGA-O2A-C1
15	A3	843	CLA	CBA-CGA-O2A-C1
15	B1	808	CLA	C4-C3-C5-C6
15	B2	808	CLA	C4-C3-C5-C6
15	B3	808	CLA	C4-C3-C5-C6
15	A1	807	CLA	C2C-C3C-CAC-CBC
15	A2	807	CLA	C2C-C3C-CAC-CBC
15	A3	807	CLA	C2C-C3C-CAC-CBC
19	X2	101	LHG	C11-C10-C9-C8
19	X3	101	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	X1	101	LHG	C11-C10-C9-C8
15	B1	824	CLA	O1D-CGD-O2D-CED
15	B2	824	CLA	O1D-CGD-O2D-CED
15	B3	824	CLA	O1D-CGD-O2D-CED
15	A1	832	CLA	O1D-CGD-O2D-CED
15	B1	805	CLA	O1D-CGD-O2D-CED
15	A2	832	CLA	O1D-CGD-O2D-CED
15	B2	805	CLA	O1D-CGD-O2D-CED
15	A3	832	CLA	O1D-CGD-O2D-CED
15	B3	805	CLA	O1D-CGD-O2D-CED
19	X1	101	LHG	C9-C10-C11-C12
19	X2	101	LHG	C9-C10-C11-C12
19	X3	101	LHG	C9-C10-C11-C12
15	A1	838	CLA	O1A-CGA-O2A-C1
15	A2	838	CLA	O1A-CGA-O2A-C1
15	A3	838	CLA	O1A-CGA-O2A-C1
15	A1	833	CLA	C4-C3-C5-C6
15	A2	833	CLA	C4-C3-C5-C6
15	A3	833	CLA	C4-C3-C5-C6
15	A1	825	CLA	C11-C10-C8-C9
15	B1	802	CLA	C6-C7-C8-C9
15	A2	825	CLA	C11-C10-C8-C9
15	B2	802	CLA	C6-C7-C8-C9
15	A3	825	CLA	C11-C10-C8-C9
15	B3	802	CLA	C6-C7-C8-C9
15	A1	838	CLA	O1D-CGD-O2D-CED
15	A2	838	CLA	O1D-CGD-O2D-CED
15	A3	838	CLA	O1D-CGD-O2D-CED
21	B1	848	DGD	C4B-C5B-C6B-C7B
21	B2	848	DGD	C4B-C5B-C6B-C7B
21	B3	848	DGD	C4B-C5B-C6B-C7B
15	A1	830	CLA	O1D-CGD-O2D-CED
15	B1	814	CLA	O1D-CGD-O2D-CED
15	A2	830	CLA	O1D-CGD-O2D-CED
15	A3	856	CLA	C3-C5-C6-C7
15	A3	830	CLA	O1D-CGD-O2D-CED
15	B3	814	CLA	O1D-CGD-O2D-CED
15	A1	804	CLA	C3A-C2A-CAA-CBA
15	A1	811	CLA	C3A-C2A-CAA-CBA
15	A1	824	CLA	C3A-C2A-CAA-CBA
15	A1	827	CLA	C3A-C2A-CAA-CBA
15	B1	809	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	B1	812	CLA	C3A-C2A-CAA-CBA
15	B1	835	CLA	C3A-C2A-CAA-CBA
15	A2	804	CLA	C3A-C2A-CAA-CBA
15	A2	811	CLA	C3A-C2A-CAA-CBA
15	A2	824	CLA	C3A-C2A-CAA-CBA
15	A2	827	CLA	C3A-C2A-CAA-CBA
15	B2	809	CLA	C3A-C2A-CAA-CBA
15	B2	812	CLA	C3A-C2A-CAA-CBA
15	B2	835	CLA	C3A-C2A-CAA-CBA
15	A3	804	CLA	C3A-C2A-CAA-CBA
15	A3	811	CLA	C3A-C2A-CAA-CBA
15	A3	824	CLA	C3A-C2A-CAA-CBA
15	A3	827	CLA	C3A-C2A-CAA-CBA
15	B3	809	CLA	C3A-C2A-CAA-CBA
15	B3	812	CLA	C3A-C2A-CAA-CBA
15	B3	835	CLA	C3A-C2A-CAA-CBA
15	B2	814	CLA	O1D-CGD-O2D-CED
15	A1	856	CLA	C3-C5-C6-C7
15	A2	856	CLA	C3-C5-C6-C7
15	B1	808	CLA	C2-C3-C5-C6
15	B2	808	CLA	C2-C3-C5-C6
15	B3	808	CLA	C2-C3-C5-C6
15	A1	842	CLA	C3-C5-C6-C7
15	A2	842	CLA	C3-C5-C6-C7
15	A3	842	CLA	C3-C5-C6-C7
15	B2	821	CLA	O1D-CGD-O2D-CED
15	B1	821	CLA	O1D-CGD-O2D-CED
15	B3	821	CLA	O1D-CGD-O2D-CED
15	A1	843	CLA	O1A-CGA-O2A-C1
15	A2	843	CLA	O1A-CGA-O2A-C1
15	A3	843	CLA	O1A-CGA-O2A-C1
19	A2	853	LHG	C24-C25-C26-C27
18	B1	845	BCR	C23-C24-C25-C26
18	B1	847	BCR	C23-C24-C25-C30
18	I1	103	BCR	C23-C24-C25-C26
18	I1	103	BCR	C23-C24-C25-C30
18	J1	1304	BCR	C1-C6-C7-C8
18	J1	1305	BCR	C1-C6-C7-C8
18	J1	1305	BCR	C5-C6-C7-C8
18	J1	1306	BCR	C1-C6-C7-C8
18	J1	1306	BCR	C5-C6-C7-C8
18	K1	102	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	K1	102	BCR	C5-C6-C7-C8
18	B2	845	BCR	C23-C24-C25-C26
18	B2	847	BCR	C23-C24-C25-C30
18	I2	103	BCR	C23-C24-C25-C26
18	I2	103	BCR	C23-C24-C25-C30
18	J2	1304	BCR	C1-C6-C7-C8
18	J2	1305	BCR	C1-C6-C7-C8
18	J2	1305	BCR	C5-C6-C7-C8
18	J2	1306	BCR	C1-C6-C7-C8
18	J2	1306	BCR	C5-C6-C7-C8
18	K2	102	BCR	C1-C6-C7-C8
18	K2	102	BCR	C5-C6-C7-C8
18	B3	845	BCR	C23-C24-C25-C26
18	B3	847	BCR	C23-C24-C25-C30
18	I3	103	BCR	C23-C24-C25-C26
18	I3	103	BCR	C23-C24-C25-C30
18	J3	1304	BCR	C1-C6-C7-C8
18	J3	1305	BCR	C1-C6-C7-C8
18	J3	1305	BCR	C5-C6-C7-C8
18	J3	1306	BCR	C1-C6-C7-C8
18	J3	1306	BCR	C5-C6-C7-C8
18	K3	102	BCR	C1-C6-C7-C8
18	K3	102	BCR	C5-C6-C7-C8
19	A1	853	LHG	C24-C25-C26-C27
19	A3	853	LHG	C24-C25-C26-C27
19	A1	853	LHG	C9-C10-C11-C12
19	A2	853	LHG	C9-C10-C11-C12
19	A3	853	LHG	C9-C10-C11-C12
15	B1	807	CLA	C4-C3-C5-C6
15	A2	830	CLA	C4-C3-C5-C6
15	B2	807	CLA	C4-C3-C5-C6
15	A3	830	CLA	C4-C3-C5-C6
15	B3	807	CLA	C4-C3-C5-C6
15	B1	802	CLA	C6-C7-C8-C10
15	B2	802	CLA	C6-C7-C8-C10
15	B3	802	CLA	C6-C7-C8-C10
15	B1	813	CLA	O1D-CGD-O2D-CED
15	B2	813	CLA	O1D-CGD-O2D-CED
15	B3	813	CLA	O1D-CGD-O2D-CED
15	A1	830	CLA	C4-C3-C5-C6
15	B1	827	CLA	C4-C3-C5-C6
15	B2	827	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	B3	827	CLA	C4-C3-C5-C6
15	A1	833	CLA	C2-C3-C5-C6
15	B1	807	CLA	C2-C3-C5-C6
15	A2	833	CLA	C2-C3-C5-C6
15	B2	807	CLA	C2-C3-C5-C6
15	A3	833	CLA	C2-C3-C5-C6
15	B3	807	CLA	C2-C3-C5-C6
15	A1	808	CLA	C11-C10-C8-C9
15	B1	808	CLA	C6-C7-C8-C9
15	A2	808	CLA	C11-C10-C8-C9
15	B2	808	CLA	C6-C7-C8-C9
15	A3	808	CLA	C11-C10-C8-C9
15	B3	808	CLA	C6-C7-C8-C9
15	A1	838	CLA	C2A-CAA-CBA-CGA
15	A2	838	CLA	C2A-CAA-CBA-CGA
15	A3	838	CLA	C2A-CAA-CBA-CGA
15	A3	818	CLA	CBA-CGA-O2A-C1
15	A1	804	CLA	C1A-C2A-CAA-CBA
15	A1	818	CLA	C1A-C2A-CAA-CBA
15	A1	827	CLA	C1A-C2A-CAA-CBA
15	A2	804	CLA	C1A-C2A-CAA-CBA
15	A2	818	CLA	C1A-C2A-CAA-CBA
15	A2	827	CLA	C1A-C2A-CAA-CBA
15	A3	804	CLA	C1A-C2A-CAA-CBA
15	A3	818	CLA	C1A-C2A-CAA-CBA
15	A3	827	CLA	C1A-C2A-CAA-CBA
21	B3	848	DGD	C5A-C6A-C7A-C8A
21	B1	848	DGD	C5A-C6A-C7A-C8A
21	B2	848	DGD	C5A-C6A-C7A-C8A
15	A1	818	CLA	CBA-CGA-O2A-C1
15	A2	818	CLA	CBA-CGA-O2A-C1
15	B1	809	CLA	CBD-CGD-O2D-CED
15	B3	809	CLA	CBD-CGD-O2D-CED
15	A1	828	CLA	C3A-C2A-CAA-CBA
15	A2	828	CLA	C3A-C2A-CAA-CBA
15	A3	828	CLA	C3A-C2A-CAA-CBA
15	B2	809	CLA	CBD-CGD-O2D-CED
15	A1	818	CLA	O1A-CGA-O2A-C1
15	A2	818	CLA	O1A-CGA-O2A-C1
15	A3	818	CLA	O1A-CGA-O2A-C1
15	B1	838	CLA	C3-C5-C6-C7
15	B2	838	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	B3	838	CLA	C3-C5-C6-C7
21	B1	848	DGD	O1G-C1G-C2G-C3G
21	B2	848	DGD	O1G-C1G-C2G-C3G
21	B3	848	DGD	O1G-C1G-C2G-C3G
15	A1	807	CLA	C4C-C3C-CAC-CBC
15	A2	807	CLA	C4C-C3C-CAC-CBC
15	A3	807	CLA	C4C-C3C-CAC-CBC
14	A1	801	CL0	CAA-CBA-CGA-O2A
14	A2	801	CL0	CAA-CBA-CGA-O2A
14	A3	801	CL0	CAA-CBA-CGA-O2A
15	A1	827	CLA	C4-C3-C5-C6
15	A2	827	CLA	C4-C3-C5-C6
15	A3	827	CLA	C4-C3-C5-C6
15	A1	827	CLA	C2-C3-C5-C6
15	A2	827	CLA	C2-C3-C5-C6
15	A3	827	CLA	C2-C3-C5-C6
15	A1	818	CLA	CAA-CBA-CGA-O2A
15	A2	818	CLA	CAA-CBA-CGA-O2A
15	A3	818	CLA	CAA-CBA-CGA-O2A
15	B1	839	CLA	C16-C17-C18-C20
15	B2	839	CLA	C16-C17-C18-C20
15	B3	839	CLA	C16-C17-C18-C20
15	A1	809	CLA	C11-C10-C8-C9
15	A2	809	CLA	C11-C10-C8-C9
15	A3	809	CLA	C11-C10-C8-C9
15	B1	827	CLA	CBA-CGA-O2A-C1
15	B2	827	CLA	CBA-CGA-O2A-C1
15	B3	827	CLA	CBA-CGA-O2A-C1
19	X1	101	LHG	C24-C23-O8-C6
19	X3	101	LHG	C24-C23-O8-C6
19	X2	101	LHG	C24-C23-O8-C6
15	B2	827	CLA	C2-C3-C5-C6
15	A1	807	CLA	C3A-C2A-CAA-CBA
15	A1	830	CLA	C3A-C2A-CAA-CBA
15	B1	849	CLA	C3A-C2A-CAA-CBA
15	A2	807	CLA	C3A-C2A-CAA-CBA
15	A2	830	CLA	C3A-C2A-CAA-CBA
15	A2	844	CLA	C3A-C2A-CAA-CBA
15	B2	849	CLA	C3A-C2A-CAA-CBA
15	A3	807	CLA	C3A-C2A-CAA-CBA
15	A3	830	CLA	C3A-C2A-CAA-CBA
15	B3	849	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	L1	1002	CLA	CBA-CGA-O2A-C1
15	L2	1002	CLA	CBA-CGA-O2A-C1
15	L3	1002	CLA	CBA-CGA-O2A-C1
21	B1	848	DGD	O6D-C5D-C6D-O5D
15	B1	801	CLA	C4-C3-C5-C6
15	B2	801	CLA	C4-C3-C5-C6
15	B3	801	CLA	C4-C3-C5-C6
15	B1	827	CLA	C2-C3-C5-C6
15	B3	827	CLA	C2-C3-C5-C6
21	B2	848	DGD	O6D-C5D-C6D-O5D
21	B3	848	DGD	O6D-C5D-C6D-O5D
19	A1	853	LHG	O7-C5-C6-O8
19	A2	853	LHG	O7-C5-C6-O8
19	A3	853	LHG	O7-C5-C6-O8
15	A1	806	CLA	C16-C17-C18-C20
15	A2	806	CLA	C16-C17-C18-C20
15	A3	806	CLA	C16-C17-C18-C20
15	A3	830	CLA	C2-C3-C5-C6
19	X1	101	LHG	C2-C3-O3-P
19	X2	101	LHG	C2-C3-O3-P
19	X3	101	LHG	C2-C3-O3-P
15	A1	843	CLA	C2A-CAA-CBA-CGA
15	A2	843	CLA	C2A-CAA-CBA-CGA
15	A3	843	CLA	C2A-CAA-CBA-CGA
15	B1	839	CLA	C16-C17-C18-C19
15	B2	839	CLA	C16-C17-C18-C19
15	B3	839	CLA	C16-C17-C18-C19
18	A1	851	BCR	C1-C6-C7-C8
18	A1	851	BCR	C5-C6-C7-C8
18	B1	847	BCR	C1-C6-C7-C8
18	A2	851	BCR	C1-C6-C7-C8
18	A2	851	BCR	C5-C6-C7-C8
18	B2	847	BCR	C1-C6-C7-C8
18	A3	851	BCR	C1-C6-C7-C8
18	A3	851	BCR	C5-C6-C7-C8
18	B3	847	BCR	C1-C6-C7-C8
15	B3	809	CLA	O1D-CGD-O2D-CED
15	B1	809	CLA	O1D-CGD-O2D-CED
19	A1	853	LHG	C8-C7-O7-C5
19	A2	853	LHG	C8-C7-O7-C5
19	A3	853	LHG	C8-C7-O7-C5
15	B2	809	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B2	826	CLA	O1D-CGD-O2D-CED
15	B3	826	CLA	O1D-CGD-O2D-CED
15	B1	826	CLA	O1D-CGD-O2D-CED
15	A1	830	CLA	C2-C3-C5-C6
15	A2	830	CLA	C2-C3-C5-C6
18	A1	851	BCR	C19-C20-C21-C22
18	A2	851	BCR	C19-C20-C21-C22
18	A3	851	BCR	C19-C20-C21-C22
19	X1	101	LHG	O10-C23-O8-C6
19	X2	101	LHG	O10-C23-O8-C6
19	X3	101	LHG	O10-C23-O8-C6
15	A1	826	CLA	C2A-CAA-CBA-CGA
15	A2	826	CLA	C2A-CAA-CBA-CGA
15	A3	826	CLA	C2A-CAA-CBA-CGA
15	B2	839	CLA	CBA-CGA-O2A-C1
15	A1	809	CLA	CAD-CBD-CGD-O2D
15	A1	825	CLA	CAD-CBD-CGD-O2D
15	A1	826	CLA	CAD-CBD-CGD-O2D
15	A1	831	CLA	CAD-CBD-CGD-O2D
15	B1	813	CLA	CAD-CBD-CGD-O2D
15	B1	821	CLA	CAD-CBD-CGD-O2D
15	B1	831	CLA	CAD-CBD-CGD-O2D
15	B1	849	CLA	CAD-CBD-CGD-O2D
15	I1	101	CLA	CAD-CBD-CGD-O2D
15	A2	809	CLA	CAD-CBD-CGD-O2D
15	A2	825	CLA	CAD-CBD-CGD-O2D
15	A2	826	CLA	CAD-CBD-CGD-O2D
15	A2	831	CLA	CAD-CBD-CGD-O2D
15	B2	813	CLA	CAD-CBD-CGD-O2D
15	B2	821	CLA	CAD-CBD-CGD-O2D
15	B2	831	CLA	CAD-CBD-CGD-O2D
15	B2	849	CLA	CAD-CBD-CGD-O2D
15	I2	101	CLA	CAD-CBD-CGD-O2D
15	A3	809	CLA	CAD-CBD-CGD-O2D
15	A3	825	CLA	CAD-CBD-CGD-O2D
15	A3	826	CLA	CAD-CBD-CGD-O2D
15	A3	831	CLA	CAD-CBD-CGD-O2D
15	B3	813	CLA	CAD-CBD-CGD-O2D
15	B3	821	CLA	CAD-CBD-CGD-O2D
15	B3	831	CLA	CAD-CBD-CGD-O2D
15	B3	849	CLA	CAD-CBD-CGD-O2D
15	I3	101	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	A1	856	CLA	C5-C6-C7-C8
15	A2	856	CLA	C5-C6-C7-C8
15	B1	839	CLA	CBA-CGA-O2A-C1
15	B3	839	CLA	CBA-CGA-O2A-C1
15	B1	827	CLA	O1A-CGA-O2A-C1
15	B2	827	CLA	O1A-CGA-O2A-C1
15	B3	827	CLA	O1A-CGA-O2A-C1
19	A1	854	LHG	O6-C4-C5-O7
19	A2	854	LHG	O6-C4-C5-O7
19	A3	854	LHG	O6-C4-C5-O7
15	A3	856	CLA	C5-C6-C7-C8
15	A1	802	CLA	C2A-CAA-CBA-CGA
15	A2	802	CLA	C2A-CAA-CBA-CGA
15	A3	802	CLA	C2A-CAA-CBA-CGA
19	A1	853	LHG	O9-C7-O7-C5
19	A2	853	LHG	O9-C7-O7-C5
19	A3	853	LHG	O9-C7-O7-C5
15	A1	808	CLA	CHA-CBD-CGD-O1D
15	A1	840	CLA	CHA-CBD-CGD-O2D
15	A1	856	CLA	CHA-CBD-CGD-O1D
15	B1	823	CLA	CHA-CBD-CGD-O1D
15	B1	823	CLA	CHA-CBD-CGD-O2D
15	B1	836	CLA	CHA-CBD-CGD-O1D
15	B1	836	CLA	CHA-CBD-CGD-O2D
15	B1	837	CLA	CHA-CBD-CGD-O1D
15	A2	808	CLA	CHA-CBD-CGD-O1D
15	A2	856	CLA	CHA-CBD-CGD-O1D
15	B2	823	CLA	CHA-CBD-CGD-O1D
15	B2	823	CLA	CHA-CBD-CGD-O2D
15	B2	836	CLA	CHA-CBD-CGD-O1D
15	B2	836	CLA	CHA-CBD-CGD-O2D
15	B2	837	CLA	CHA-CBD-CGD-O1D
15	A3	808	CLA	CHA-CBD-CGD-O1D
15	A3	840	CLA	CHA-CBD-CGD-O2D
15	A3	856	CLA	CHA-CBD-CGD-O1D
15	B3	823	CLA	CHA-CBD-CGD-O1D
15	B3	823	CLA	CHA-CBD-CGD-O2D
15	B3	836	CLA	CHA-CBD-CGD-O1D
15	B3	836	CLA	CHA-CBD-CGD-O2D
15	B3	837	CLA	CHA-CBD-CGD-O1D
15	L1	1002	CLA	O1A-CGA-O2A-C1
15	L2	1002	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	L3	1002	CLA	O1A-CGA-O2A-C1
19	X1	101	LHG	O7-C5-C6-O8
19	X2	101	LHG	O7-C5-C6-O8
19	X3	101	LHG	O7-C5-C6-O8
21	B1	848	DGD	O1G-C1G-C2G-O2G
21	B2	848	DGD	O1G-C1G-C2G-O2G
21	B3	848	DGD	O1G-C1G-C2G-O2G
15	B1	805	CLA	C1A-C2A-CAA-CBA
15	B1	812	CLA	C1A-C2A-CAA-CBA
15	L1	1003	CLA	C1A-C2A-CAA-CBA
15	B2	805	CLA	C1A-C2A-CAA-CBA
15	B2	812	CLA	C1A-C2A-CAA-CBA
15	L2	1003	CLA	C1A-C2A-CAA-CBA
15	B3	805	CLA	C1A-C2A-CAA-CBA
15	B3	812	CLA	C1A-C2A-CAA-CBA
15	L3	1003	CLA	C1A-C2A-CAA-CBA
21	B1	848	DGD	C4A-C5A-C6A-C7A
21	B2	848	DGD	C4A-C5A-C6A-C7A
21	B3	848	DGD	C4A-C5A-C6A-C7A
15	B1	839	CLA	O1A-CGA-O2A-C1
15	B2	839	CLA	O1A-CGA-O2A-C1
15	B3	839	CLA	O1A-CGA-O2A-C1
15	B1	816	CLA	CAD-CBD-CGD-O1D
15	B1	816	CLA	CAD-CBD-CGD-O2D
15	B2	816	CLA	CAD-CBD-CGD-O1D
15	B2	816	CLA	CAD-CBD-CGD-O2D
15	B3	816	CLA	CAD-CBD-CGD-O1D
15	B3	816	CLA	CAD-CBD-CGD-O2D
19	A1	854	LHG	C3-O3-P-O5
19	X1	101	LHG	C3-O3-P-O4
19	A2	854	LHG	C3-O3-P-O5
19	X2	101	LHG	C3-O3-P-O4
19	A3	854	LHG	C3-O3-P-O5
19	X3	101	LHG	C3-O3-P-O4
19	A1	854	LHG	O6-C4-C5-C6
19	X1	101	LHG	O6-C4-C5-C6
19	A2	854	LHG	O6-C4-C5-C6
19	X2	101	LHG	O6-C4-C5-C6
19	A3	854	LHG	O6-C4-C5-C6
19	X3	101	LHG	O6-C4-C5-C6
19	X1	101	LHG	C25-C26-C27-C28
19	X2	101	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	X3	101	LHG	C25-C26-C27-C28
15	A1	818	CLA	C2A-CAA-CBA-CGA
15	A2	818	CLA	C2A-CAA-CBA-CGA
15	A3	818	CLA	C2A-CAA-CBA-CGA
15	B1	830	CLA	CAD-CBD-CGD-O1D
15	B1	837	CLA	CAD-CBD-CGD-O1D
15	B2	830	CLA	CAD-CBD-CGD-O1D
15	B2	837	CLA	CAD-CBD-CGD-O1D
15	B3	830	CLA	CAD-CBD-CGD-O1D
15	B3	837	CLA	CAD-CBD-CGD-O1D
15	A1	806	CLA	C16-C17-C18-C19
15	A2	806	CLA	C16-C17-C18-C19
15	A3	806	CLA	C16-C17-C18-C19
15	A1	815	CLA	CAD-CBD-CGD-O2D
15	A1	840	CLA	C3A-C2A-CAA-CBA
15	A1	844	CLA	C3A-C2A-CAA-CBA
15	B1	827	CLA	C6-C7-C8-C10
15	A2	815	CLA	CAD-CBD-CGD-O2D
15	A2	840	CLA	C3A-C2A-CAA-CBA
15	B2	827	CLA	C6-C7-C8-C10
15	A3	815	CLA	CAD-CBD-CGD-O2D
15	A3	840	CLA	C3A-C2A-CAA-CBA
15	A3	844	CLA	C3A-C2A-CAA-CBA
15	B3	827	CLA	C6-C7-C8-C10
19	X1	101	LHG	O6-C4-C5-O7
19	X2	101	LHG	O6-C4-C5-O7
19	X3	101	LHG	O6-C4-C5-O7
15	A1	826	CLA	C6-C7-C8-C9
15	A1	843	CLA	C16-C17-C18-C20
15	A2	826	CLA	C6-C7-C8-C9
15	A2	843	CLA	C16-C17-C18-C20
15	A3	826	CLA	C6-C7-C8-C9
15	A3	843	CLA	C16-C17-C18-C20
19	X1	101	LHG	C15-C16-C17-C18
19	X2	101	LHG	C15-C16-C17-C18
19	X3	101	LHG	C15-C16-C17-C18
15	B1	827	CLA	C6-C7-C8-C9
15	B2	827	CLA	C6-C7-C8-C9
15	B3	827	CLA	C6-C7-C8-C9
15	B1	839	CLA	C15-C16-C17-C18
15	B3	839	CLA	C15-C16-C17-C18
15	B2	839	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	A1	801	CL0	C5-C6-C7-C8
14	A2	801	CL0	C5-C6-C7-C8
14	A3	801	CL0	C5-C6-C7-C8
19	X1	101	LHG	C24-C25-C26-C27
19	X2	101	LHG	C24-C25-C26-C27
19	X3	101	LHG	C24-C25-C26-C27
14	A1	801	CL0	C4-C3-C5-C6
14	A3	801	CL0	C4-C3-C5-C6
18	L1	1005	BCR	C23-C24-C25-C26
18	L1	1005	BCR	C23-C24-C25-C30
18	L2	1005	BCR	C23-C24-C25-C26
18	L2	1005	BCR	C23-C24-C25-C30
18	L3	1005	BCR	C23-C24-C25-C26
19	A1	853	LHG	C3-O3-P-O6
19	A2	853	LHG	C3-O3-P-O6
19	A3	853	LHG	C3-O3-P-O6
15	B1	812	CLA	C8-C10-C11-C12
15	B2	812	CLA	C8-C10-C11-C12
15	B3	812	CLA	C8-C10-C11-C12
19	X1	101	LHG	C4-C5-C6-O8
19	X2	101	LHG	C4-C5-C6-O8
19	X3	101	LHG	C4-C5-C6-O8
14	A2	801	CL0	C4-C3-C5-C6
15	A1	825	CLA	C11-C10-C8-C7
15	A2	825	CLA	C11-C10-C8-C7
15	A3	825	CLA	C11-C10-C8-C7
18	J1	1306	BCR	C19-C20-C21-C22
18	J2	1306	BCR	C19-C20-C21-C22
18	J3	1306	BCR	C19-C20-C21-C22
19	A1	854	LHG	O2-C2-C3-O3
19	A2	854	LHG	O2-C2-C3-O3
19	A3	854	LHG	O2-C2-C3-O3
15	B1	827	CLA	C5-C6-C7-C8
15	B2	827	CLA	C5-C6-C7-C8
15	B3	827	CLA	C5-C6-C7-C8
15	A3	842	CLA	C5-C6-C7-C8
15	A1	842	CLA	C5-C6-C7-C8
15	A2	842	CLA	C5-C6-C7-C8
18	B1	842	BCR	C19-C20-C21-C22
18	B2	842	BCR	C19-C20-C21-C22
18	B3	842	BCR	C19-C20-C21-C22
15	I1	101	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	I2	101	CLA	C3-C5-C6-C7
15	I3	101	CLA	C3-C5-C6-C7
15	A1	806	CLA	C10-C11-C12-C13
15	A2	806	CLA	C10-C11-C12-C13
15	A3	806	CLA	C10-C11-C12-C13
15	A1	840	CLA	C2A-CAA-CBA-CGA
15	B1	801	CLA	C2A-CAA-CBA-CGA
15	A2	840	CLA	C2A-CAA-CBA-CGA
15	B2	801	CLA	C2A-CAA-CBA-CGA
15	A3	840	CLA	C2A-CAA-CBA-CGA
15	B3	801	CLA	C2A-CAA-CBA-CGA
14	A1	801	CL0	CAA-CBA-CGA-O1A
14	A2	801	CL0	CAA-CBA-CGA-O1A
14	A3	801	CL0	CAA-CBA-CGA-O1A
15	A1	809	CLA	C3A-C2A-CAA-CBA
15	B1	805	CLA	C3A-C2A-CAA-CBA
15	A2	809	CLA	C3A-C2A-CAA-CBA
15	B2	805	CLA	C3A-C2A-CAA-CBA
15	A3	809	CLA	C3A-C2A-CAA-CBA
15	B3	805	CLA	C3A-C2A-CAA-CBA
15	A1	835	CLA	CAA-CBA-CGA-O2A
15	B1	849	CLA	CAA-CBA-CGA-O2A
15	A2	835	CLA	CAA-CBA-CGA-O2A
15	B2	849	CLA	CAA-CBA-CGA-O2A
15	A3	835	CLA	CAA-CBA-CGA-O2A
15	B3	849	CLA	CAA-CBA-CGA-O2A
15	A1	825	CLA	C6-C7-C8-C9
15	A1	843	CLA	C11-C10-C8-C9
15	A2	825	CLA	C6-C7-C8-C9
15	A2	843	CLA	C11-C10-C8-C9
15	A3	825	CLA	C6-C7-C8-C9
15	A3	843	CLA	C11-C10-C8-C9
15	A1	835	CLA	CAA-CBA-CGA-O1A
15	A3	835	CLA	CAA-CBA-CGA-O1A
18	A1	850	BCR	C20-C21-C22-C37
18	A1	852	BCR	C11-C10-C9-C34
18	A1	852	BCR	C16-C17-C18-C36
18	B1	843	BCR	C11-C10-C9-C34
18	F1	201	BCR	C35-C13-C14-C15
18	I1	103	BCR	C20-C21-C22-C37
18	A2	850	BCR	C20-C21-C22-C37
18	A2	852	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
18	A2	852	BCR	C16-C17-C18-C36
18	B2	843	BCR	C11-C10-C9-C34
18	F2	201	BCR	C35-C13-C14-C15
18	I2	103	BCR	C20-C21-C22-C37
18	A3	850	BCR	C20-C21-C22-C37
18	A3	852	BCR	C11-C10-C9-C34
18	A3	852	BCR	C16-C17-C18-C36
18	B3	843	BCR	C11-C10-C9-C34
18	F3	201	BCR	C35-C13-C14-C15
18	I3	103	BCR	C20-C21-C22-C37
15	A1	807	CLA	CAA-CBA-CGA-O1A
15	B1	849	CLA	CAA-CBA-CGA-O1A
15	A2	807	CLA	CAA-CBA-CGA-O1A
15	A2	835	CLA	CAA-CBA-CGA-O1A
15	B2	849	CLA	CAA-CBA-CGA-O1A
15	A3	807	CLA	CAA-CBA-CGA-O1A
15	B3	849	CLA	CAA-CBA-CGA-O1A
15	B3	827	CLA	C2A-CAA-CBA-CGA
15	B1	813	CLA	CAA-CBA-CGA-O2A
15	B1	828	CLA	CAA-CBA-CGA-O1A
15	B2	813	CLA	CAA-CBA-CGA-O2A
15	B2	828	CLA	CAA-CBA-CGA-O1A
15	B3	813	CLA	CAA-CBA-CGA-O2A
15	B3	828	CLA	CAA-CBA-CGA-O1A
15	A1	813	CLA	CAA-CBA-CGA-O1A
15	B1	813	CLA	CAA-CBA-CGA-O1A
15	A2	813	CLA	CAA-CBA-CGA-O1A
15	B2	813	CLA	CAA-CBA-CGA-O1A
15	A3	813	CLA	CAA-CBA-CGA-O1A
15	B3	813	CLA	CAA-CBA-CGA-O1A
15	A1	813	CLA	C1A-C2A-CAA-CBA
15	A1	835	CLA	C1A-C2A-CAA-CBA
15	A1	844	CLA	C1A-C2A-CAA-CBA
15	A2	813	CLA	C1A-C2A-CAA-CBA
15	A2	835	CLA	C1A-C2A-CAA-CBA
15	A2	844	CLA	C1A-C2A-CAA-CBA
15	A3	813	CLA	C1A-C2A-CAA-CBA
15	A3	835	CLA	C1A-C2A-CAA-CBA
15	A3	844	CLA	C1A-C2A-CAA-CBA
15	A1	856	CLA	C11-C10-C8-C7
15	A2	856	CLA	C11-C10-C8-C7
15	A3	856	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
15	A1	813	CLA	CAA-CBA-CGA-O2A
15	A2	813	CLA	CAA-CBA-CGA-O2A
15	A3	813	CLA	CAA-CBA-CGA-O2A
15	A1	807	CLA	CAA-CBA-CGA-O2A
15	A2	807	CLA	CAA-CBA-CGA-O2A
15	B1	827	CLA	C2A-CAA-CBA-CGA
15	B2	827	CLA	C2A-CAA-CBA-CGA
15	A3	807	CLA	CAA-CBA-CGA-O2A
15	A1	833	CLA	CBA-CGA-O2A-C1
15	A2	833	CLA	CBA-CGA-O2A-C1
15	A3	833	CLA	CBA-CGA-O2A-C1
15	L1	1004	CLA	C13-C15-C16-C17
15	L2	1004	CLA	C13-C15-C16-C17
15	L3	1004	CLA	C13-C15-C16-C17
18	A1	850	BCR	C20-C21-C22-C23
18	A1	852	BCR	C11-C10-C9-C8
18	A1	852	BCR	C16-C17-C18-C19
18	B1	843	BCR	C11-C10-C9-C8
18	F1	201	BCR	C12-C13-C14-C15
18	I1	103	BCR	C20-C21-C22-C23
18	A2	850	BCR	C20-C21-C22-C23
18	A2	852	BCR	C11-C10-C9-C8
18	A2	852	BCR	C16-C17-C18-C19
18	B2	843	BCR	C11-C10-C9-C8
18	F2	201	BCR	C12-C13-C14-C15
18	I2	103	BCR	C20-C21-C22-C23
18	A3	850	BCR	C20-C21-C22-C23
18	A3	852	BCR	C11-C10-C9-C8
18	A3	852	BCR	C16-C17-C18-C19
18	B3	843	BCR	C11-C10-C9-C8
18	F3	201	BCR	C12-C13-C14-C15
18	I3	103	BCR	C20-C21-C22-C23
18	B1	841	BCR	C19-C20-C21-C22
18	J1	1304	BCR	C19-C20-C21-C22
18	L1	1006	BCR	C19-C20-C21-C22
18	L1	1011	BCR	C19-C20-C21-C22
18	B2	841	BCR	C19-C20-C21-C22
18	J2	1304	BCR	C19-C20-C21-C22
18	L2	1010	BCR	C19-C20-C21-C22
18	B3	841	BCR	C19-C20-C21-C22
18	J3	1304	BCR	C19-C20-C21-C22
15	B1	838	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B2	838	CLA	O1D-CGD-O2D-CED
15	B3	838	CLA	O1D-CGD-O2D-CED
15	A2	833	CLA	O1A-CGA-O2A-C1
15	A1	809	CLA	C4-C3-C5-C6
15	A2	809	CLA	C4-C3-C5-C6
15	A3	809	CLA	C4-C3-C5-C6
15	A1	833	CLA	O1A-CGA-O2A-C1
15	A3	833	CLA	O1A-CGA-O2A-C1
15	A1	832	CLA	CAA-CBA-CGA-O2A
15	A3	832	CLA	CAA-CBA-CGA-O2A
15	A1	840	CLA	C11-C10-C8-C9
15	A2	840	CLA	C11-C10-C8-C9
15	A3	840	CLA	C11-C10-C8-C9
15	B1	828	CLA	CAA-CBA-CGA-O2A
15	A2	832	CLA	CAA-CBA-CGA-O2A
15	B2	828	CLA	CAA-CBA-CGA-O2A
15	B3	828	CLA	CAA-CBA-CGA-O2A
18	A1	848	BCR	C1-C6-C7-C8
18	A1	850	BCR	C23-C24-C25-C30
18	A1	855	BCR	C23-C24-C25-C30
18	B1	844	BCR	C1-C6-C7-C8
18	B1	847	BCR	C5-C6-C7-C8
18	A2	848	BCR	C1-C6-C7-C8
18	A2	850	BCR	C23-C24-C25-C30
18	A2	855	BCR	C23-C24-C25-C30
18	B2	844	BCR	C1-C6-C7-C8
18	B2	847	BCR	C5-C6-C7-C8
18	A3	848	BCR	C1-C6-C7-C8
18	A3	850	BCR	C23-C24-C25-C30
18	A3	855	BCR	C23-C24-C25-C30
18	B3	844	BCR	C1-C6-C7-C8
18	B3	847	BCR	C5-C6-C7-C8
18	L3	1005	BCR	C23-C24-C25-C30
15	A1	829	CLA	C4-C3-C5-C6
15	A1	842	CLA	C4-C3-C5-C6
15	I1	101	CLA	C4-C3-C5-C6
15	A2	829	CLA	C4-C3-C5-C6
15	A2	842	CLA	C4-C3-C5-C6
15	I2	101	CLA	C4-C3-C5-C6
15	A3	829	CLA	C4-C3-C5-C6
15	A3	842	CLA	C4-C3-C5-C6
15	I3	101	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	B1	802	CLA	C5-C6-C7-C8
15	B3	802	CLA	C5-C6-C7-C8
15	B2	802	CLA	C5-C6-C7-C8
15	A1	809	CLA	C2-C3-C5-C6
15	A1	829	CLA	C2-C3-C5-C6
15	A2	809	CLA	C2-C3-C5-C6
15	A2	829	CLA	C2-C3-C5-C6
15	A3	809	CLA	C2-C3-C5-C6
15	A3	829	CLA	C2-C3-C5-C6
15	A3	803	CLA	C13-C15-C16-C17
15	A1	803	CLA	C13-C15-C16-C17
15	A2	803	CLA	C13-C15-C16-C17
15	A1	805	CLA	C2A-CAA-CBA-CGA
15	B2	832	CLA	O1D-CGD-O2D-CED
15	A1	811	CLA	C10-C11-C12-C13
15	A2	811	CLA	C10-C11-C12-C13
15	A1	822	CLA	CAA-CBA-CGA-O2A
15	A3	822	CLA	CAA-CBA-CGA-O2A
15	A3	811	CLA	C10-C11-C12-C13
15	A1	806	CLA	CAA-CBA-CGA-O2A
15	A2	806	CLA	CAA-CBA-CGA-O2A
15	A3	806	CLA	CAA-CBA-CGA-O2A
15	A1	819	CLA	C4-C3-C5-C6
15	L1	1004	CLA	C4-C3-C5-C6
15	A2	819	CLA	C4-C3-C5-C6
15	L2	1004	CLA	C4-C3-C5-C6
15	A3	819	CLA	C4-C3-C5-C6
15	L3	1004	CLA	C4-C3-C5-C6
15	A1	822	CLA	CAA-CBA-CGA-O1A
15	A2	822	CLA	CAA-CBA-CGA-O1A
15	A2	822	CLA	CAA-CBA-CGA-O2A
15	A3	822	CLA	CAA-CBA-CGA-O1A
15	B1	807	CLA	C11-C10-C8-C9
15	B1	838	CLA	C14-C13-C15-C16
15	B2	807	CLA	C11-C10-C8-C9
15	B2	838	CLA	C14-C13-C15-C16
15	B3	807	CLA	C11-C10-C8-C9
15	B3	838	CLA	C14-C13-C15-C16
15	B1	832	CLA	O1D-CGD-O2D-CED
15	A1	813	CLA	C3A-C2A-CAA-CBA
15	A1	825	CLA	C3A-C2A-CAA-CBA
15	A1	838	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	B1	818	CLA	C3A-C2A-CAA-CBA
15	A2	813	CLA	C3A-C2A-CAA-CBA
15	A2	825	CLA	C3A-C2A-CAA-CBA
15	A2	838	CLA	C3A-C2A-CAA-CBA
15	B2	818	CLA	C3A-C2A-CAA-CBA
15	A3	813	CLA	C3A-C2A-CAA-CBA
15	A3	825	CLA	C3A-C2A-CAA-CBA
15	A3	838	CLA	C3A-C2A-CAA-CBA
15	B3	818	CLA	C3A-C2A-CAA-CBA
15	A1	803	CLA	CAA-CBA-CGA-O2A
15	A2	803	CLA	CAA-CBA-CGA-O2A
15	A3	803	CLA	CAA-CBA-CGA-O2A
15	A1	833	CLA	CAD-CBD-CGD-O2D
15	A1	837	CLA	CAD-CBD-CGD-O2D
15	B1	811	CLA	CAD-CBD-CGD-O2D
15	B1	814	CLA	CAD-CBD-CGD-O2D
15	B1	819	CLA	CAD-CBD-CGD-O2D
15	J1	1301	CLA	CAD-CBD-CGD-O2D
15	L1	1002	CLA	CAD-CBD-CGD-O2D
15	L1	1004	CLA	CAD-CBD-CGD-O2D
15	A2	833	CLA	CAD-CBD-CGD-O2D
15	A2	837	CLA	CAD-CBD-CGD-O2D
15	B2	811	CLA	CAD-CBD-CGD-O2D
15	B2	814	CLA	CAD-CBD-CGD-O2D
15	B2	819	CLA	CAD-CBD-CGD-O2D
15	J2	1301	CLA	CAD-CBD-CGD-O2D
15	L2	1002	CLA	CAD-CBD-CGD-O2D
15	L2	1004	CLA	CAD-CBD-CGD-O2D
15	A3	833	CLA	CAD-CBD-CGD-O2D
15	A3	837	CLA	CAD-CBD-CGD-O2D
15	B3	811	CLA	CAD-CBD-CGD-O2D
15	B3	814	CLA	CAD-CBD-CGD-O2D
15	B3	819	CLA	CAD-CBD-CGD-O2D
15	J3	1301	CLA	CAD-CBD-CGD-O2D
15	L3	1002	CLA	CAD-CBD-CGD-O2D
15	L3	1004	CLA	CAD-CBD-CGD-O2D
15	L1	1002	CLA	C5-C6-C7-C8
15	L2	1002	CLA	C5-C6-C7-C8
15	L3	1002	CLA	C5-C6-C7-C8
15	A2	805	CLA	C2A-CAA-CBA-CGA
15	A3	805	CLA	C2A-CAA-CBA-CGA
19	X1	101	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	X2	101	LHG	C14-C15-C16-C17
19	X3	101	LHG	C14-C15-C16-C17
15	A1	818	CLA	CAA-CBA-CGA-O1A
15	A2	818	CLA	CAA-CBA-CGA-O1A
15	A3	818	CLA	CAA-CBA-CGA-O1A
15	A1	832	CLA	CAA-CBA-CGA-O1A
15	A2	832	CLA	CAA-CBA-CGA-O1A
15	I1	101	CLA	C2-C3-C5-C6
15	I2	101	CLA	C2-C3-C5-C6
15	I3	101	CLA	C2-C3-C5-C6
15	B1	805	CLA	CAA-CBA-CGA-O2A
15	B3	805	CLA	CAA-CBA-CGA-O2A
15	B1	819	CLA	CAA-CBA-CGA-O1A
15	B2	819	CLA	CAA-CBA-CGA-O1A
15	A3	832	CLA	CAA-CBA-CGA-O1A
15	B3	819	CLA	CAA-CBA-CGA-O1A
15	B3	832	CLA	O1D-CGD-O2D-CED
15	B2	805	CLA	CAA-CBA-CGA-O2A
15	A1	825	CLA	O2A-C1-C2-C3
15	A1	826	CLA	O2A-C1-C2-C3
15	A1	827	CLA	O2A-C1-C2-C3
15	A1	843	CLA	O2A-C1-C2-C3
15	B1	801	CLA	O2A-C1-C2-C3
15	A2	825	CLA	O2A-C1-C2-C3
15	A2	826	CLA	O2A-C1-C2-C3
15	A2	827	CLA	O2A-C1-C2-C3
15	A2	843	CLA	O2A-C1-C2-C3
15	B2	801	CLA	O2A-C1-C2-C3
15	A3	825	CLA	O2A-C1-C2-C3
15	A3	826	CLA	O2A-C1-C2-C3
15	A3	827	CLA	O2A-C1-C2-C3
15	A3	843	CLA	O2A-C1-C2-C3
15	B3	801	CLA	O2A-C1-C2-C3
21	B3	848	DGD	CCA-CDA-CEA-CFA
15	A1	809	CLA	C2A-CAA-CBA-CGA
15	A2	809	CLA	C2A-CAA-CBA-CGA
15	A3	809	CLA	C2A-CAA-CBA-CGA
21	B2	848	DGD	CCA-CDA-CEA-CFA
15	B1	807	CLA	C11-C12-C13-C15
15	B2	807	CLA	C11-C12-C13-C15
15	B3	807	CLA	C11-C12-C13-C15
21	B1	848	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
15	A1	823	CLA	CHA-CBD-CGD-O2D
15	A1	824	CLA	CHA-CBD-CGD-O1D
15	A1	824	CLA	CHA-CBD-CGD-O2D
15	A1	827	CLA	CHA-CBD-CGD-O1D
15	A1	827	CLA	CHA-CBD-CGD-O2D
15	A1	836	CLA	CHA-CBD-CGD-O2D
15	A1	838	CLA	CHA-CBD-CGD-O1D
15	A1	838	CLA	CHA-CBD-CGD-O2D
15	A1	856	CLA	CHA-CBD-CGD-O2D
15	B1	805	CLA	CHA-CBD-CGD-O1D
15	B1	818	CLA	CHA-CBD-CGD-O2D
15	B1	825	CLA	CHA-CBD-CGD-O1D
15	B1	827	CLA	CHA-CBD-CGD-O1D
15	B1	827	CLA	CHA-CBD-CGD-O2D
15	B1	835	CLA	CHA-CBD-CGD-O1D
15	B1	835	CLA	CHA-CBD-CGD-O2D
15	B1	837	CLA	CHA-CBD-CGD-O2D
15	L1	1003	CLA	CHA-CBD-CGD-O1D
15	L1	1003	CLA	CHA-CBD-CGD-O2D
15	A2	823	CLA	CHA-CBD-CGD-O2D
15	A2	824	CLA	CHA-CBD-CGD-O1D
15	A2	824	CLA	CHA-CBD-CGD-O2D
15	A2	827	CLA	CHA-CBD-CGD-O1D
15	A2	827	CLA	CHA-CBD-CGD-O2D
15	A2	836	CLA	CHA-CBD-CGD-O2D
15	A2	838	CLA	CHA-CBD-CGD-O1D
15	A2	838	CLA	CHA-CBD-CGD-O2D
15	A2	856	CLA	CHA-CBD-CGD-O2D
15	B2	805	CLA	CHA-CBD-CGD-O1D
15	B2	818	CLA	CHA-CBD-CGD-O2D
15	B2	827	CLA	CHA-CBD-CGD-O1D
15	B2	827	CLA	CHA-CBD-CGD-O2D
15	B2	835	CLA	CHA-CBD-CGD-O1D
15	B2	835	CLA	CHA-CBD-CGD-O2D
15	B2	837	CLA	CHA-CBD-CGD-O2D
15	L2	1003	CLA	CHA-CBD-CGD-O1D
15	L2	1003	CLA	CHA-CBD-CGD-O2D
15	A3	823	CLA	CHA-CBD-CGD-O2D
15	A3	824	CLA	CHA-CBD-CGD-O1D
15	A3	824	CLA	CHA-CBD-CGD-O2D
15	A3	827	CLA	CHA-CBD-CGD-O1D
15	A3	827	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	A3	836	CLA	CHA-CBD-CGD-O2D
15	A3	838	CLA	CHA-CBD-CGD-O1D
15	A3	838	CLA	CHA-CBD-CGD-O2D
15	A3	856	CLA	CHA-CBD-CGD-O2D
15	B3	805	CLA	CHA-CBD-CGD-O1D
15	B3	818	CLA	CHA-CBD-CGD-O2D
15	B3	827	CLA	CHA-CBD-CGD-O1D
15	B3	827	CLA	CHA-CBD-CGD-O2D
15	B3	835	CLA	CHA-CBD-CGD-O1D
15	B3	835	CLA	CHA-CBD-CGD-O2D
15	B3	837	CLA	CHA-CBD-CGD-O2D
15	L3	1003	CLA	CHA-CBD-CGD-O1D
15	L3	1003	CLA	CHA-CBD-CGD-O2D
15	A1	839	CLA	CAA-CBA-CGA-O2A
15	B1	819	CLA	CAA-CBA-CGA-O2A
15	B2	819	CLA	CAA-CBA-CGA-O2A
15	B3	819	CLA	CAA-CBA-CGA-O2A
15	B1	806	CLA	CAA-CBA-CGA-O2A
15	B2	806	CLA	CAA-CBA-CGA-O2A
15	B3	806	CLA	CAA-CBA-CGA-O2A
15	A1	811	CLA	C15-C16-C17-C18
15	A2	811	CLA	C15-C16-C17-C18
15	A3	811	CLA	C15-C16-C17-C18
15	A2	839	CLA	CAA-CBA-CGA-O2A
15	A3	839	CLA	CAA-CBA-CGA-O2A
15	A1	803	CLA	CAA-CBA-CGA-O1A
15	A2	803	CLA	CAA-CBA-CGA-O1A
15	A3	803	CLA	CAA-CBA-CGA-O1A
15	L1	1004	CLA	C2-C3-C5-C6
15	L2	1004	CLA	C2-C3-C5-C6
15	L3	1004	CLA	C2-C3-C5-C6
15	A1	809	CLA	C14-C13-C15-C16
15	A2	809	CLA	C14-C13-C15-C16
15	A3	809	CLA	C14-C13-C15-C16
18	A1	847	BCR	C19-C20-C21-C22
18	A2	847	BCR	C19-C20-C21-C22
18	A3	847	BCR	C19-C20-C21-C22
15	B1	801	CLA	CAA-CBA-CGA-O2A
15	B3	801	CLA	CAA-CBA-CGA-O2A
15	A1	806	CLA	CAA-CBA-CGA-O1A
15	A2	806	CLA	CAA-CBA-CGA-O1A
15	A3	806	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	B2	801	CLA	CAA-CBA-CGA-O2A
15	A1	842	CLA	C2-C3-C5-C6
15	A2	842	CLA	C2-C3-C5-C6
15	A3	842	CLA	C2-C3-C5-C6
15	A1	807	CLA	CHA-CBD-CGD-O2D
15	A1	820	CLA	CHA-CBD-CGD-O2D
15	A1	825	CLA	C1A-C2A-CAA-CBA
15	A1	830	CLA	C1A-C2A-CAA-CBA
15	A1	837	CLA	C1A-C2A-CAA-CBA
15	B1	813	CLA	C1A-C2A-CAA-CBA
15	B1	828	CLA	C1A-C2A-CAA-CBA
15	L1	1002	CLA	C1A-C2A-CAA-CBA
15	A2	807	CLA	CHA-CBD-CGD-O2D
15	A2	820	CLA	CHA-CBD-CGD-O2D
15	A2	825	CLA	C1A-C2A-CAA-CBA
15	A2	830	CLA	C1A-C2A-CAA-CBA
15	A2	837	CLA	C1A-C2A-CAA-CBA
15	B2	813	CLA	C1A-C2A-CAA-CBA
15	B2	828	CLA	C1A-C2A-CAA-CBA
15	L2	1002	CLA	C1A-C2A-CAA-CBA
15	A3	807	CLA	CHA-CBD-CGD-O2D
15	A3	820	CLA	CHA-CBD-CGD-O2D
15	A3	825	CLA	C1A-C2A-CAA-CBA
15	A3	830	CLA	C1A-C2A-CAA-CBA
15	A3	837	CLA	C1A-C2A-CAA-CBA
15	B3	813	CLA	C1A-C2A-CAA-CBA
15	B3	828	CLA	C1A-C2A-CAA-CBA
15	L3	1002	CLA	C1A-C2A-CAA-CBA
15	A1	839	CLA	C6-C7-C8-C10
15	A2	839	CLA	C6-C7-C8-C10
15	A3	839	CLA	C6-C7-C8-C10
15	A1	811	CLA	C2-C1-O2A-CGA
15	A1	827	CLA	C2-C1-O2A-CGA
15	A2	811	CLA	C2-C1-O2A-CGA
15	A2	827	CLA	C2-C1-O2A-CGA
15	A3	811	CLA	C2-C1-O2A-CGA
15	A3	827	CLA	C2-C1-O2A-CGA
15	B1	806	CLA	CAA-CBA-CGA-O1A
15	B2	806	CLA	CAA-CBA-CGA-O1A
15	B3	806	CLA	CAA-CBA-CGA-O1A
15	B1	816	CLA	CHA-CBD-CGD-O2D
15	B2	816	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	B3	816	CLA	CHA-CBD-CGD-O2D
18	A1	848	BCR	C5-C6-C7-C8
18	A1	850	BCR	C23-C24-C25-C26
18	A2	848	BCR	C5-C6-C7-C8
18	A2	850	BCR	C23-C24-C25-C26
18	A3	848	BCR	C5-C6-C7-C8
18	A3	850	BCR	C23-C24-C25-C26
15	A1	833	CLA	O1D-CGD-O2D-CED
15	A3	827	CLA	C2A-CAA-CBA-CGA
15	B2	838	CLA	CBD-CGD-O2D-CED
15	A2	833	CLA	O1D-CGD-O2D-CED
15	A3	833	CLA	O1D-CGD-O2D-CED
15	A1	819	CLA	C2-C3-C5-C6
15	B1	801	CLA	C2-C3-C5-C6
15	A2	819	CLA	C2-C3-C5-C6
15	A3	819	CLA	C2-C3-C5-C6
15	B3	801	CLA	C2-C3-C5-C6
15	A1	813	CLA	CAD-CBD-CGD-O1D
15	A1	844	CLA	CAD-CBD-CGD-O1D
15	B1	805	CLA	CAD-CBD-CGD-O1D
15	B1	812	CLA	CAD-CBD-CGD-O1D
15	B1	825	CLA	CAD-CBD-CGD-O1D
15	B1	832	CLA	CAD-CBD-CGD-O1D
15	A2	813	CLA	CAD-CBD-CGD-O1D
15	A2	844	CLA	CAD-CBD-CGD-O1D
15	B2	805	CLA	CAD-CBD-CGD-O1D
15	B2	812	CLA	CAD-CBD-CGD-O1D
15	B2	825	CLA	CAD-CBD-CGD-O1D
15	B2	832	CLA	CAD-CBD-CGD-O1D
15	A3	813	CLA	CAD-CBD-CGD-O1D
15	A3	844	CLA	CAD-CBD-CGD-O1D
15	B3	805	CLA	CAD-CBD-CGD-O1D
15	B3	812	CLA	CAD-CBD-CGD-O1D
15	B3	825	CLA	CAD-CBD-CGD-O1D
15	B3	832	CLA	CAD-CBD-CGD-O1D
15	B3	838	CLA	CBD-CGD-O2D-CED
15	B1	838	CLA	CBD-CGD-O2D-CED
15	L1	1002	CLA	CAA-CBA-CGA-O2A
15	L2	1002	CLA	CAA-CBA-CGA-O2A
15	L3	1002	CLA	CAA-CBA-CGA-O2A
15	A1	827	CLA	C2A-CAA-CBA-CGA
15	A2	827	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	A1	831	CLA	CAA-CBA-CGA-O2A
15	A2	831	CLA	CAA-CBA-CGA-O2A
15	A3	831	CLA	CAA-CBA-CGA-O2A
19	A1	853	LHG	C1-C2-C3-O3
19	A1	854	LHG	C1-C2-C3-O3
19	A2	853	LHG	C1-C2-C3-O3
19	A2	854	LHG	C1-C2-C3-O3
19	A3	853	LHG	C1-C2-C3-O3
19	A3	854	LHG	C1-C2-C3-O3
15	A1	810	CLA	CAD-CBD-CGD-O2D
15	A1	815	CLA	CHA-CBD-CGD-O1D
15	A1	825	CLA	C6-C7-C8-C10
15	A1	841	CLA	CAD-CBD-CGD-O2D
15	B1	813	CLA	C3A-C2A-CAA-CBA
15	B1	828	CLA	C3A-C2A-CAA-CBA
15	L1	1002	CLA	C11-C10-C8-C7
15	A2	810	CLA	CAD-CBD-CGD-O2D
15	A2	815	CLA	CHA-CBD-CGD-O1D
15	A2	825	CLA	C6-C7-C8-C10
15	A2	841	CLA	CAD-CBD-CGD-O2D
15	B2	801	CLA	C2-C3-C5-C6
15	B2	813	CLA	C3A-C2A-CAA-CBA
15	B2	828	CLA	C3A-C2A-CAA-CBA
15	L2	1002	CLA	C11-C10-C8-C7
15	A3	810	CLA	CAD-CBD-CGD-O2D
15	A3	815	CLA	CHA-CBD-CGD-O1D
15	A3	825	CLA	C6-C7-C8-C10
15	A3	841	CLA	CAD-CBD-CGD-O2D
15	B3	813	CLA	C3A-C2A-CAA-CBA
15	B3	828	CLA	C3A-C2A-CAA-CBA
15	L3	1002	CLA	C11-C10-C8-C7
15	A1	839	CLA	CAA-CBA-CGA-O1A
15	B1	801	CLA	CAA-CBA-CGA-O1A
15	A2	839	CLA	CAA-CBA-CGA-O1A
15	B2	801	CLA	CAA-CBA-CGA-O1A
15	A3	839	CLA	CAA-CBA-CGA-O1A
15	B3	801	CLA	CAA-CBA-CGA-O1A
15	A1	856	CLA	CAA-CBA-CGA-O2A
15	A2	856	CLA	CAA-CBA-CGA-O2A
15	A3	856	CLA	CAA-CBA-CGA-O2A
15	A1	826	CLA	C3-C5-C6-C7
15	A2	826	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	A3	826	CLA	C3-C5-C6-C7
18	I1	103	BCR	C19-C20-C21-C22
18	I2	103	BCR	C19-C20-C21-C22
18	I3	103	BCR	C19-C20-C21-C22
15	L2	1002	CLA	CAA-CBA-CGA-O1A
15	A2	809	CLA	C5-C6-C7-C8
15	A2	809	CLA	C13-C15-C16-C17
15	A3	809	CLA	C13-C15-C16-C17
15	A1	809	CLA	C5-C6-C7-C8
15	A3	809	CLA	C5-C6-C7-C8
15	L1	1002	CLA	CAA-CBA-CGA-O1A
15	A1	809	CLA	C13-C15-C16-C17
15	A1	856	CLA	CAA-CBA-CGA-O1A
15	A2	856	CLA	CAA-CBA-CGA-O1A
15	A3	856	CLA	CAA-CBA-CGA-O1A
15	L3	1002	CLA	CAA-CBA-CGA-O1A
15	B1	803	CLA	CAA-CBA-CGA-O2A
15	B3	803	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

276 monomers are involved in 522 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A3	843	CLA	1	0
15	L3	1004	CLA	1	0
18	B1	845	BCR	3	0
15	B3	805	CLA	2	0
15	A3	838	CLA	2	0
15	B3	812	CLA	4	0
15	B1	817	CLA	1	0
18	M2	101	BCR	2	0
15	A2	808	CLA	2	0
15	B1	820	CLA	1	0
18	A2	850	BCR	3	0
18	B2	843	BCR	2	0
18	J3	1305	BCR	5	0
15	A2	802	CLA	5	0
15	B2	835	CLA	1	0
18	A3	848	BCR	5	0
15	B3	832	CLA	1	0
15	A3	813	CLA	4	0
15	B3	823	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A1	831	CLA	2	0
15	B2	815	CLA	1	0
15	A2	806	CLA	1	0
15	A3	836	CLA	1	0
18	I3	103	BCR	2	0
15	A1	835	CLA	1	0
15	A2	835	CLA	1	0
15	A2	837	CLA	1	0
15	B3	838	CLA	3	0
15	B1	809	CLA	1	0
15	L2	1002	CLA	3	0
15	B2	809	CLA	2	0
15	A1	829	CLA	4	0
15	A2	842	CLA	4	0
15	A2	833	CLA	3	0
18	B3	842	BCR	3	0
15	B3	820	CLA	1	0
15	A3	820	CLA	1	0
15	B3	803	CLA	2	0
15	A1	840	CLA	1	0
15	A1	804	CLA	2	0
18	A2	852	BCR	3	0
15	A2	839	CLA	2	0
15	B2	826	CLA	1	0
18	L2	1010	BCR	2	0
18	B1	841	BCR	4	0
15	L2	1004	CLA	1	0
18	A1	855	BCR	1	0
15	B3	809	CLA	1	0
15	A3	826	CLA	1	0
15	B2	831	CLA	1	0
15	B1	816	CLA	1	0
15	A3	830	CLA	2	0
18	J2	1304	BCR	2	0
18	A1	849	BCR	3	0
15	A1	834	CLA	1	0
15	A2	827	CLA	1	0
15	A2	813	CLA	4	0
15	A1	842	CLA	4	0
15	I1	101	CLA	3	0
15	A1	856	CLA	4	0
15	A3	819	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	L3	1003	CLA	4	0
15	B1	802	CLA	5	0
18	J1	1304	BCR	2	0
15	B3	822	CLA	1	0
15	B3	807	CLA	2	0
15	B2	823	CLA	2	0
15	B3	802	CLA	5	0
15	B1	810	CLA	1	0
16	B1	840	PQN	4	0
15	A3	821	CLA	3	0
15	A1	824	CLA	1	0
15	K3	103	CLA	2	0
15	L1	1004	CLA	1	0
14	A2	801	CL0	2	0
15	B3	849	CLA	2	0
15	B1	805	CLA	1	0
15	J3	1303	CLA	1	0
15	A2	830	CLA	2	0
15	A3	834	CLA	1	0
15	B1	812	CLA	4	0
18	J2	1306	BCR	2	0
19	X1	101	LHG	5	0
18	B3	847	BCR	1	0
15	I3	101	CLA	3	0
18	B2	842	BCR	2	0
15	B2	838	CLA	3	0
15	I2	101	CLA	3	0
15	A3	835	CLA	1	0
15	A1	809	CLA	1	0
15	B1	801	CLA	4	0
15	K1	103	CLA	2	0
15	B1	839	CLA	3	0
15	A3	829	CLA	3	0
18	A1	850	BCR	3	0
15	A1	828	CLA	4	0
15	B3	810	CLA	1	0
15	B1	835	CLA	1	0
15	B2	803	CLA	2	0
14	A3	801	CL0	2	0
15	B2	801	CLA	4	0
15	A3	840	CLA	1	0
15	X2	102	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A3	850	BCR	3	0
15	A1	815	CLA	1	0
15	B3	821	CLA	1	0
15	B2	808	CLA	5	0
18	I2	103	BCR	1	0
15	A1	837	CLA	1	0
15	A2	818	CLA	3	0
15	J2	1303	CLA	1	0
15	A2	820	CLA	1	0
15	A1	839	CLA	2	0
15	L2	1003	CLA	4	0
15	A1	813	CLA	4	0
15	A1	803	CLA	2	0
18	J3	1306	BCR	4	0
18	A2	851	BCR	5	0
18	L1	1011	BCR	2	0
15	A1	838	CLA	2	0
15	A1	821	CLA	3	0
15	A2	814	CLA	1	0
15	B3	839	CLA	3	0
15	B2	802	CLA	5	0
15	B3	827	CLA	6	0
18	A1	852	BCR	4	0
18	A3	849	BCR	3	0
18	I2	102	BCR	1	0
15	A2	826	CLA	1	0
15	A2	840	CLA	1	0
15	A2	838	CLA	2	0
15	B1	826	CLA	1	0
15	A3	842	CLA	4	0
15	A3	806	CLA	1	0
15	A2	843	CLA	1	0
15	A3	837	CLA	1	0
15	A2	803	CLA	2	0
18	I1	103	BCR	1	0
15	A2	807	CLA	2	0
15	B2	837	CLA	1	0
15	A2	809	CLA	1	0
15	B3	831	CLA	1	0
15	A2	819	CLA	6	0
15	B3	836	CLA	2	0
18	B3	846	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A1	811	CLA	4	0
18	A2	849	BCR	1	0
15	A1	820	CLA	1	0
15	B2	827	CLA	5	0
15	B2	804	CLA	1	0
18	B2	841	BCR	4	0
15	B1	832	CLA	1	0
18	A3	852	BCR	3	0
15	A2	828	CLA	4	0
15	B1	823	CLA	2	0
15	A3	809	CLA	1	0
15	B2	836	CLA	2	0
15	B2	849	CLA	2	0
18	A1	847	BCR	2	0
15	X1	102	CLA	1	0
18	A3	855	BCR	1	0
18	A1	851	BCR	5	0
15	B2	839	CLA	3	0
15	B2	805	CLA	2	0
15	A1	814	CLA	1	0
15	A3	818	CLA	3	0
15	A1	825	CLA	5	0
18	F1	201	BCR	3	0
15	B2	821	CLA	1	0
15	L1	1002	CLA	5	0
15	B3	837	CLA	1	0
15	K2	103	CLA	2	0
15	X3	102	CLA	1	0
15	A3	827	CLA	1	0
19	X3	101	LHG	4	0
19	X2	101	LHG	5	0
15	B3	816	CLA	1	0
15	A3	808	CLA	2	0
18	B2	845	BCR	1	0
15	L1	1003	CLA	4	0
15	A3	839	CLA	2	0
18	A3	847	BCR	1	0
15	A1	833	CLA	3	0
15	A1	807	CLA	2	0
15	A1	808	CLA	2	0
16	B3	840	PQN	5	0
18	B3	841	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A1	802	CLA	4	0
18	I1	102	BCR	1	0
18	B2	846	BCR	3	0
15	A1	826	CLA	1	0
15	B1	822	CLA	1	0
15	B1	803	CLA	2	0
15	B1	804	CLA	1	0
15	B2	822	CLA	1	0
15	B2	807	CLA	2	0
15	B2	824	CLA	1	0
15	A3	803	CLA	2	0
18	A3	851	BCR	4	0
15	A1	818	CLA	2	0
18	F2	201	BCR	4	0
15	A3	804	CLA	2	0
15	B1	838	CLA	3	0
15	A3	856	CLA	4	0
15	A2	825	CLA	5	0
15	A1	819	CLA	6	0
15	A2	815	CLA	1	0
15	A1	806	CLA	1	0
15	A3	825	CLA	5	0
15	A2	805	CLA	4	0
15	B3	808	CLA	5	0
15	A1	843	CLA	1	0
15	B3	826	CLA	1	0
15	A2	856	CLA	4	0
15	A2	821	CLA	3	0
15	A2	829	CLA	4	0
18	J2	1305	BCR	4	0
15	A2	836	CLA	1	0
15	B3	835	CLA	1	0
15	A3	833	CLA	3	0
18	A2	848	BCR	5	0
15	A3	807	CLA	2	0
15	B1	808	CLA	4	0
15	A3	802	CLA	5	0
15	B1	849	CLA	2	0
15	A3	815	CLA	1	0
15	A2	804	CLA	2	0
18	B3	845	BCR	1	0
15	A2	831	CLA	2	0

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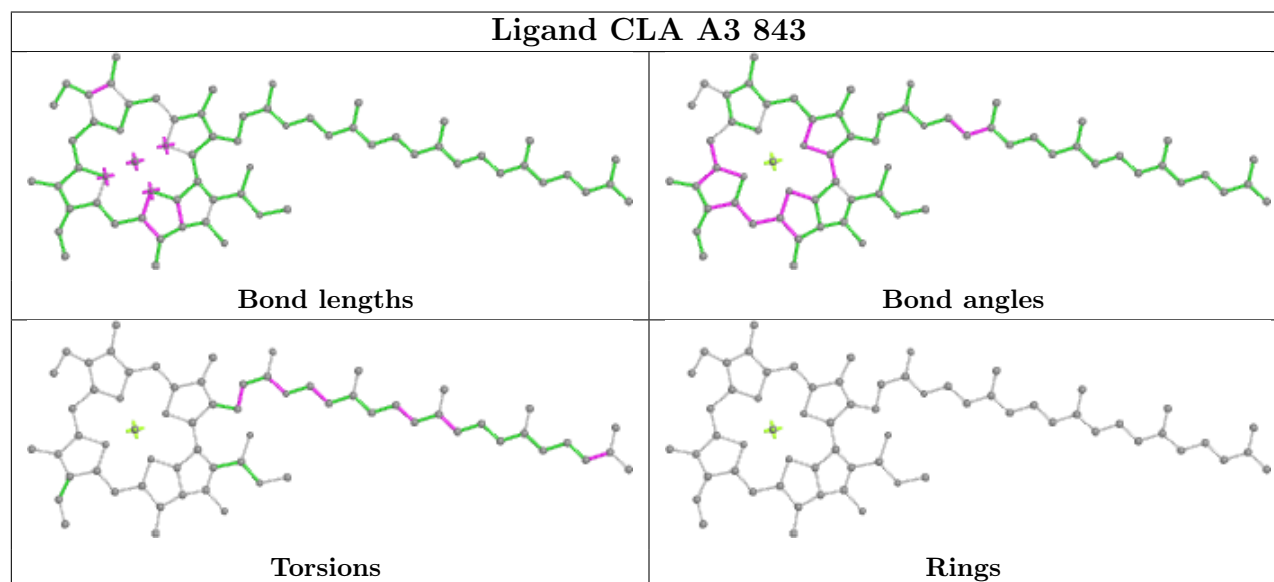
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B1	843	BCR	2	0
18	L3	1005	BCR	4	0
15	B3	804	CLA	1	0
15	B3	824	CLA	1	0
15	A1	805	CLA	4	0
15	A3	831	CLA	2	0
18	B3	843	BCR	2	0
15	B2	816	CLA	1	0
15	A2	834	CLA	1	0
18	M1	101	BCR	2	0
15	A1	827	CLA	1	0
15	A2	811	CLA	4	0
15	B2	812	CLA	4	0
18	A2	855	BCR	1	0
18	J1	1306	BCR	3	0
15	B3	815	CLA	1	0
18	B3	844	BCR	1	0
18	L1	1005	BCR	4	0
18	M3	101	BCR	3	0
15	A3	828	CLA	4	0
18	L1	1006	BCR	2	0
18	A2	847	BCR	1	0
15	B2	810	CLA	1	0
16	B2	840	PQN	4	0
18	A1	848	BCR	5	0
18	F3	201	BCR	3	0
14	A1	801	CL0	4	0
15	A1	830	CLA	2	0
15	A3	805	CLA	4	0
15	L3	1002	CLA	4	0
18	B1	844	BCR	1	0
15	A3	811	CLA	4	0
15	B1	827	CLA	4	0
15	B3	801	CLA	4	0
18	I3	102	BCR	2	0
15	B1	821	CLA	1	0
15	A1	836	CLA	1	0
18	J1	1305	BCR	6	0
18	L2	1005	BCR	3	0
15	B1	831	CLA	1	0
15	B2	820	CLA	2	0
15	B1	836	CLA	2	0

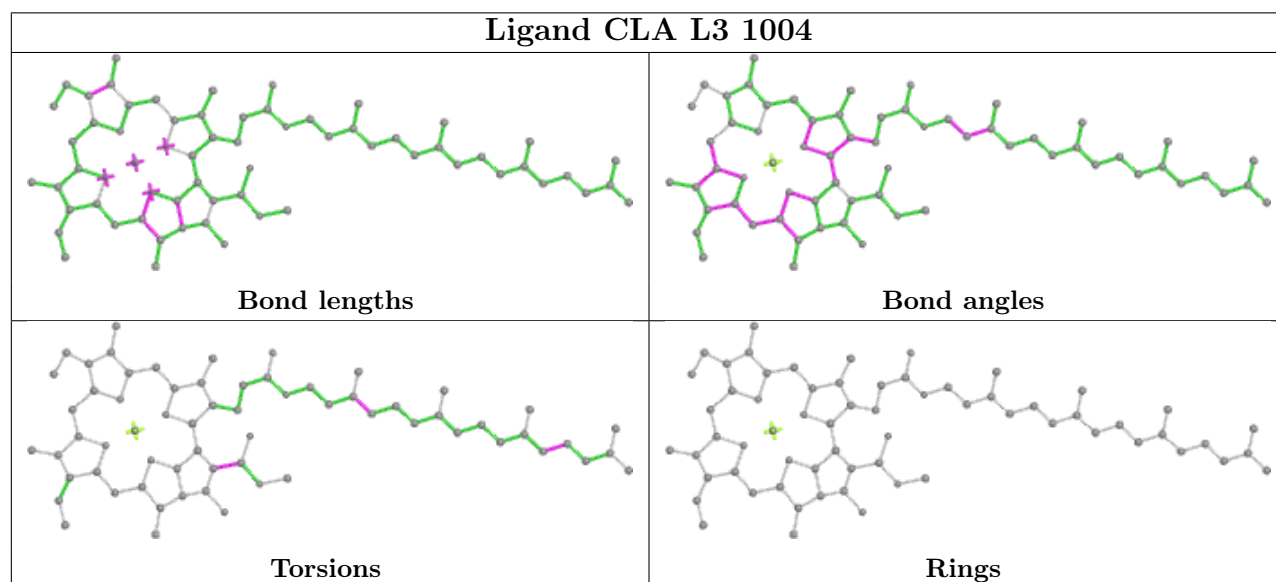
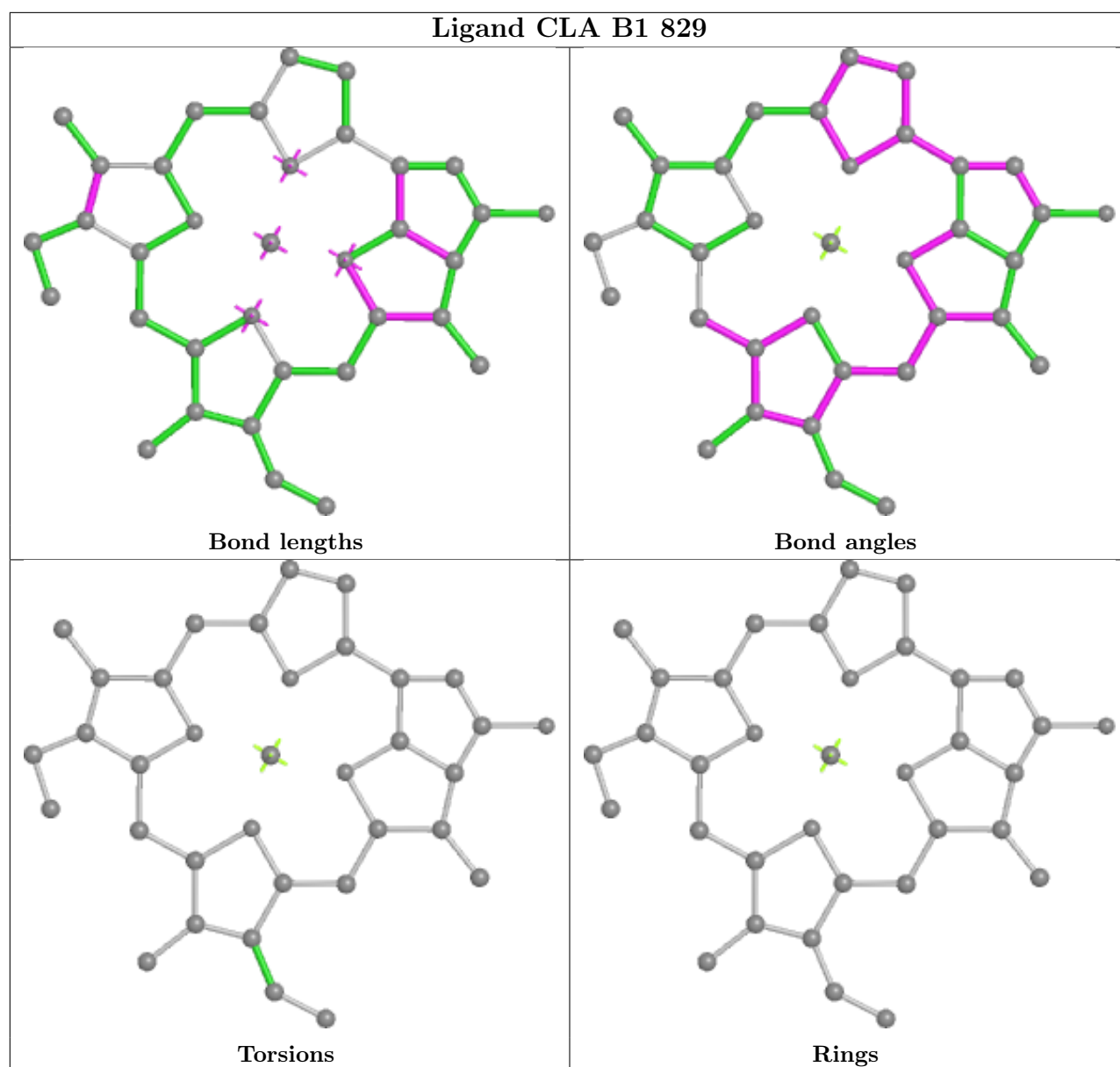
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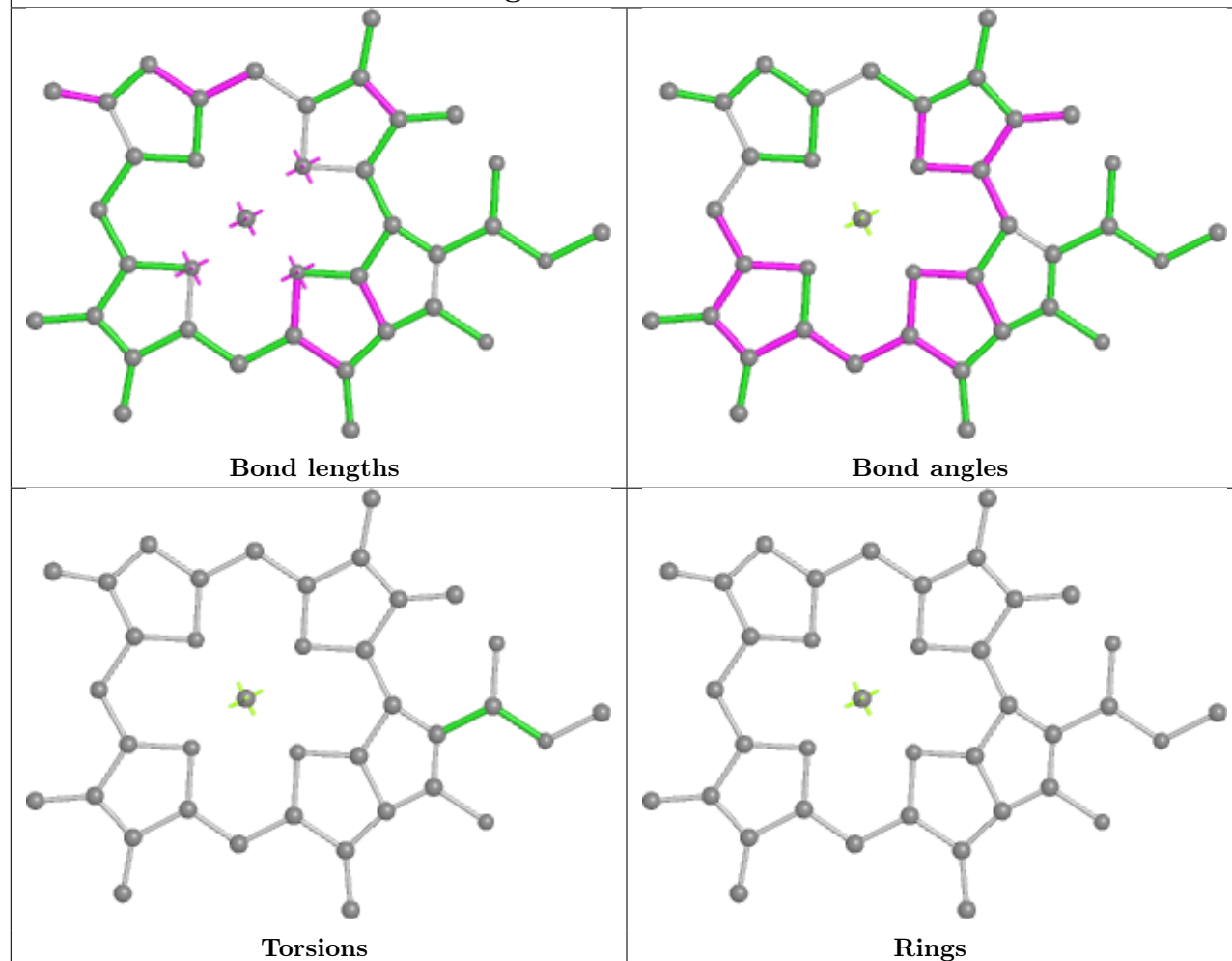
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B2	832	CLA	1	0
18	J3	1304	BCR	2	0
15	B1	807	CLA	2	0
18	B1	842	BCR	3	0
18	B1	846	BCR	2	0

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.

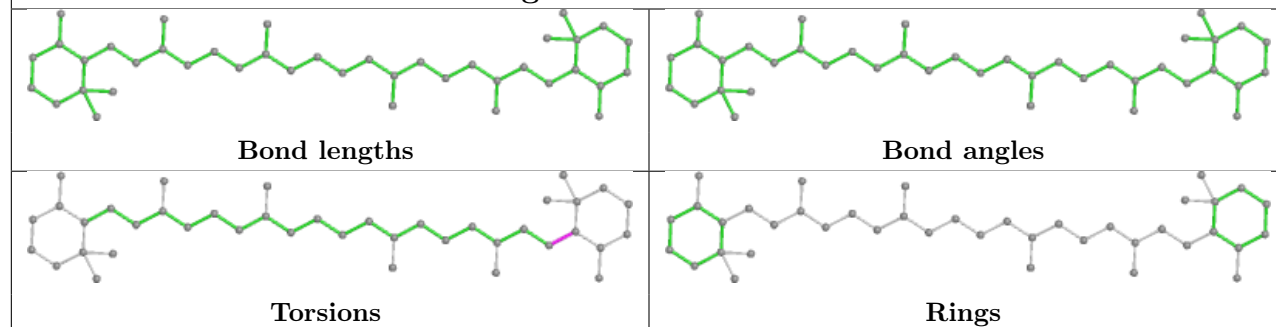




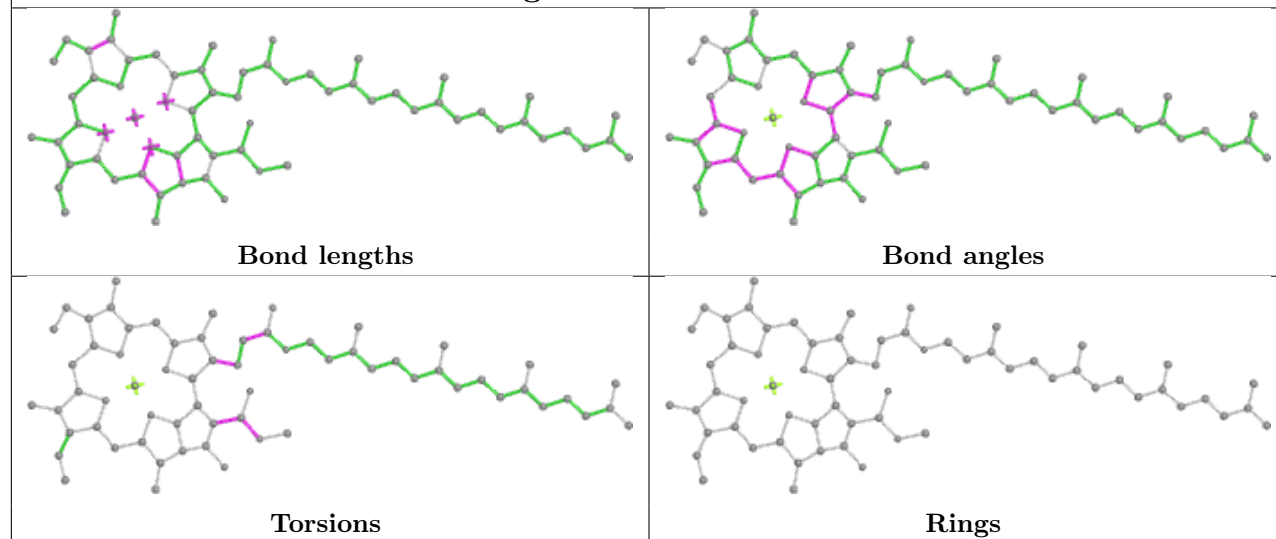
## Ligand CLA A1 817



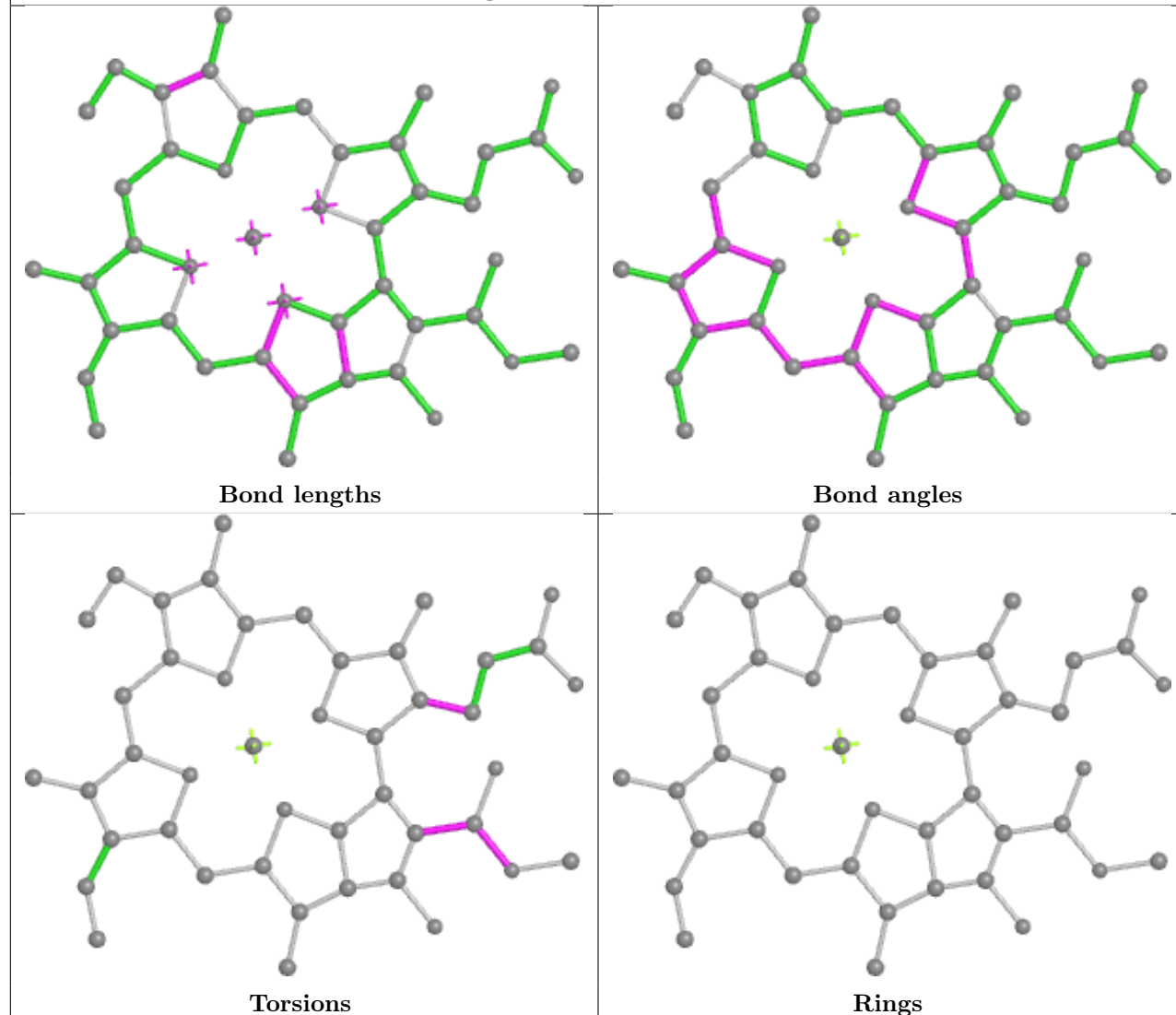
## Ligand BCR B1 845

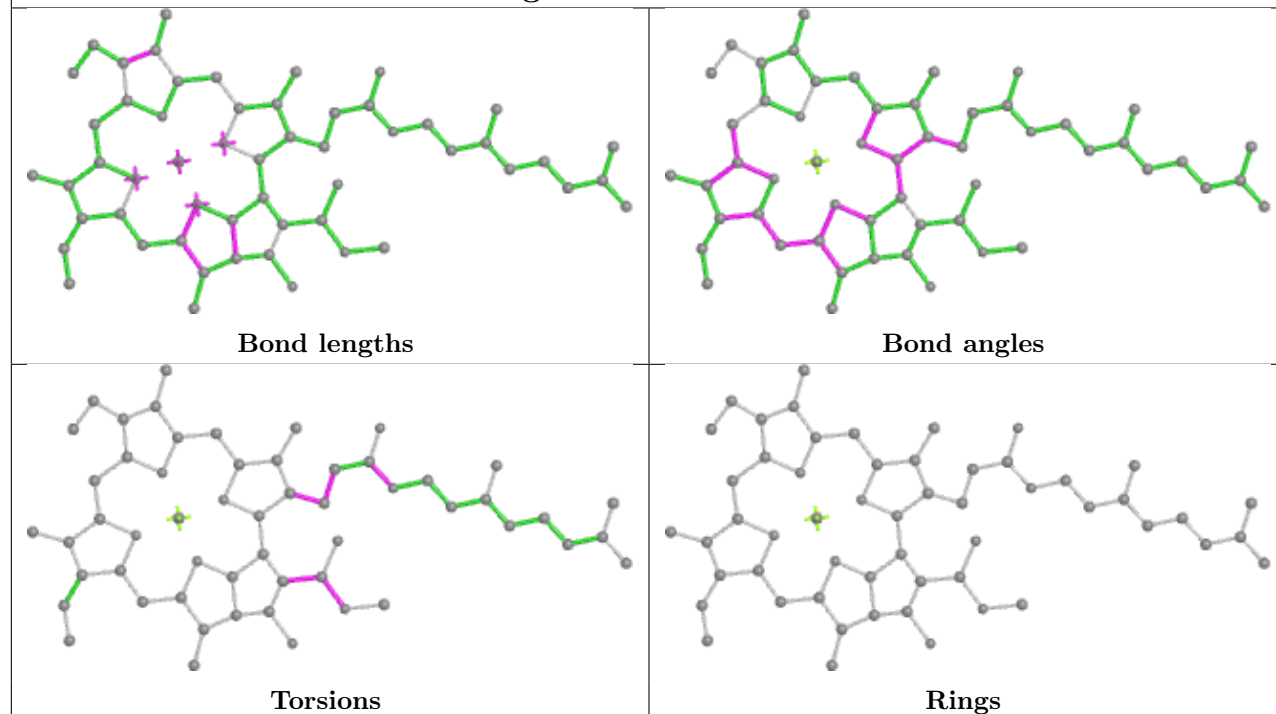
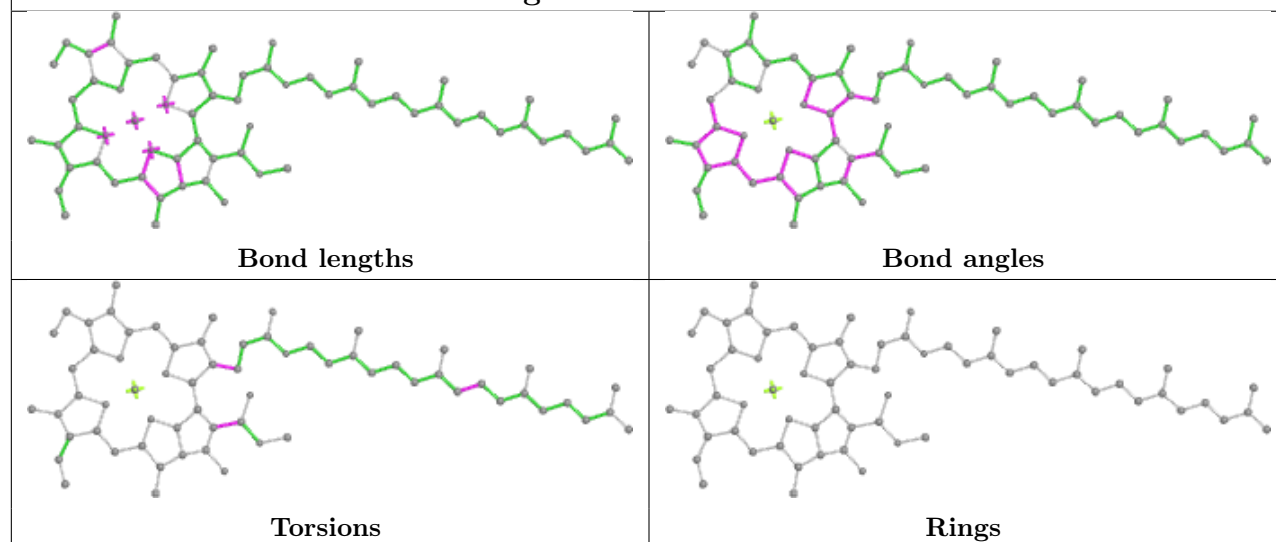


## Ligand CLA B3 805

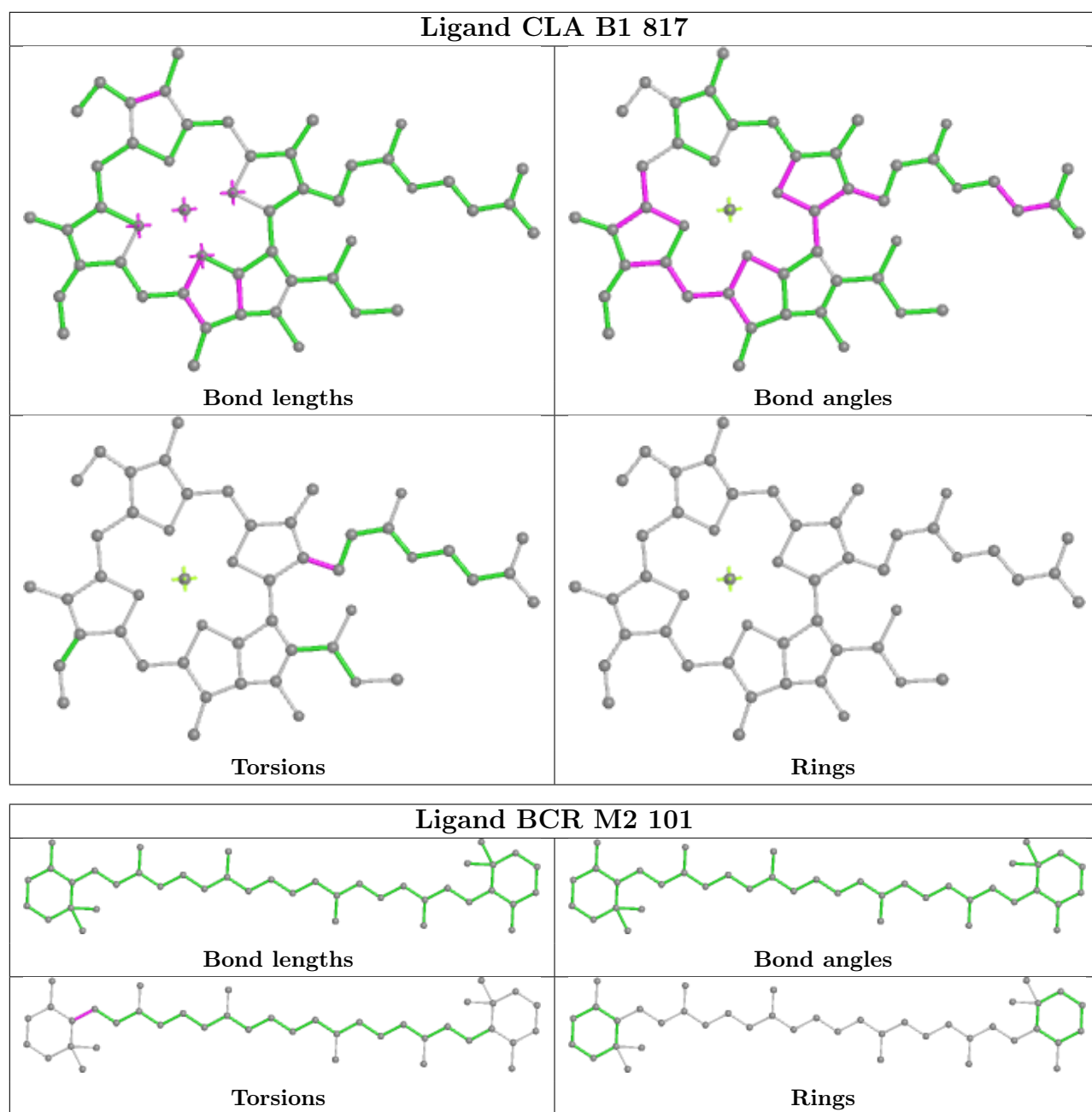


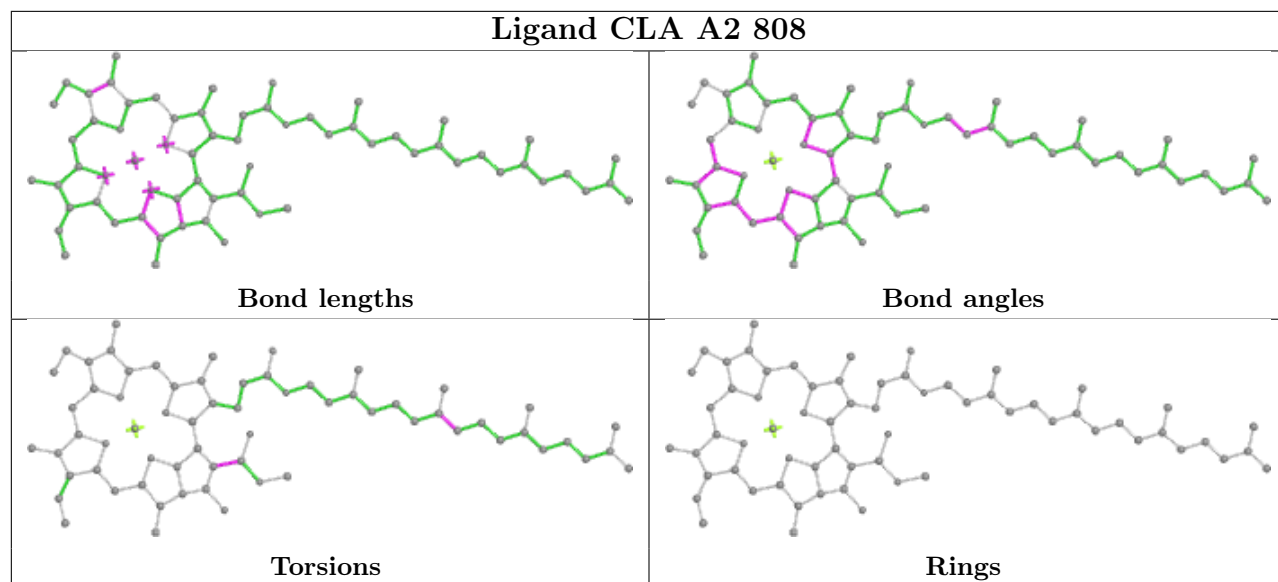
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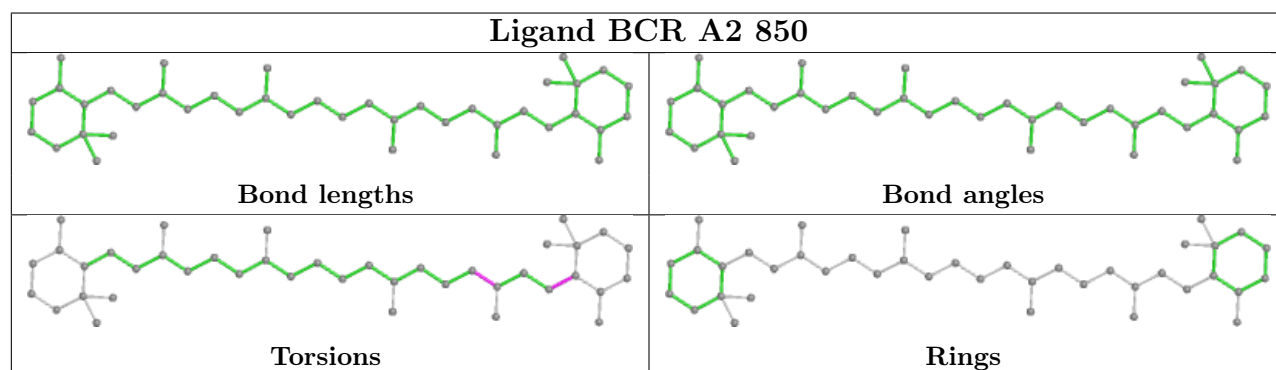
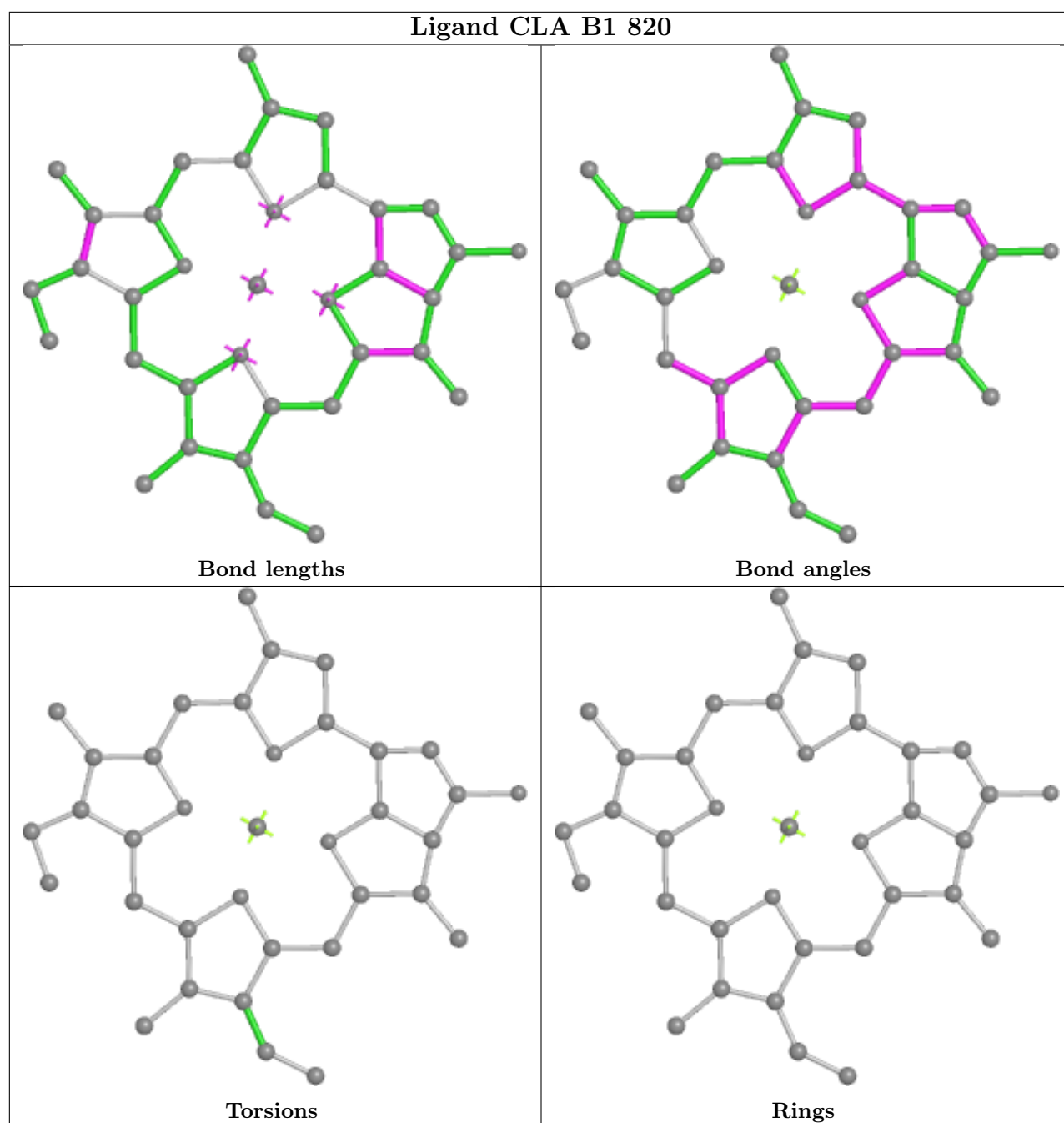


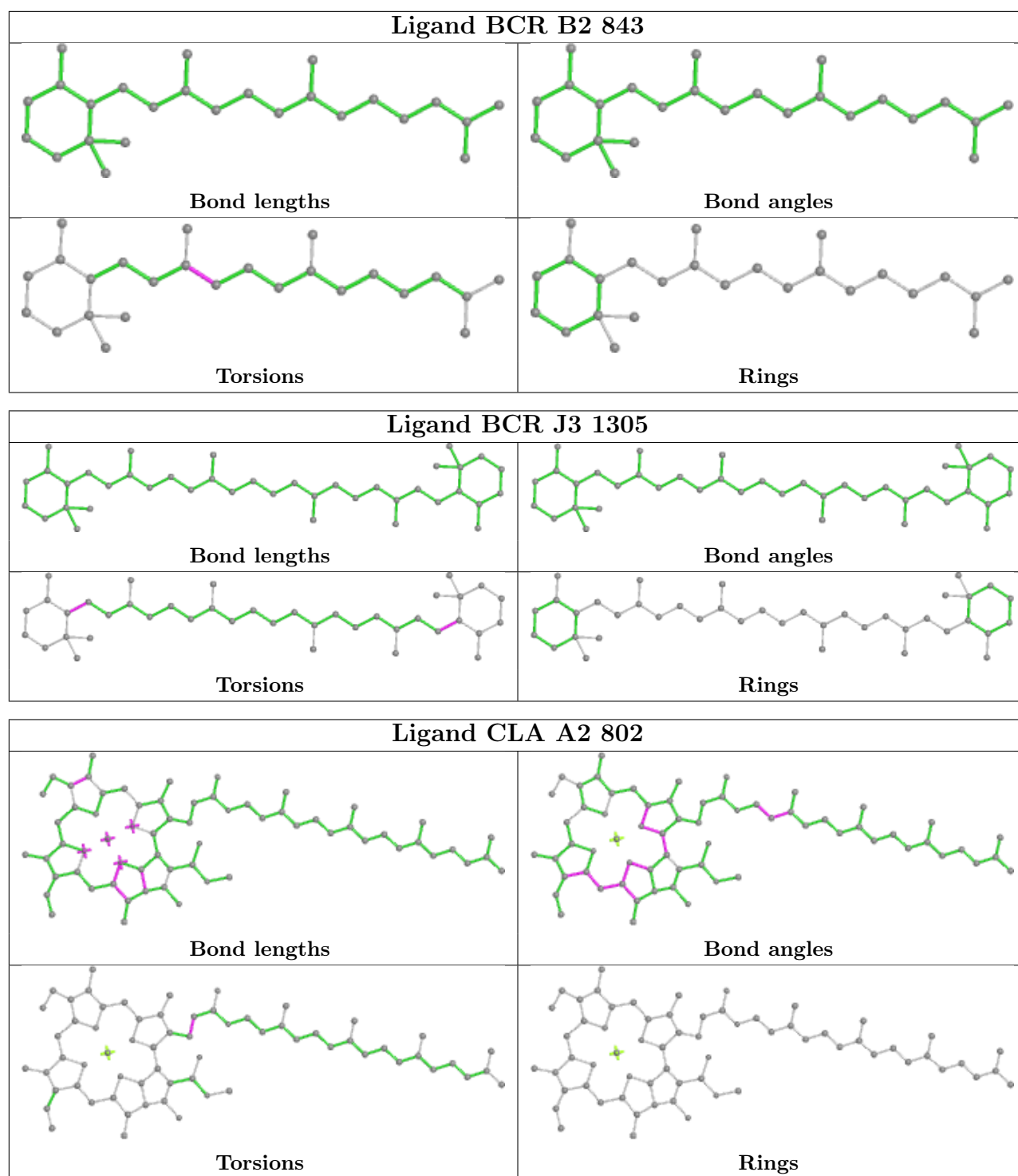
**Ligand CLA A3 838****Ligand CLA B3 812**



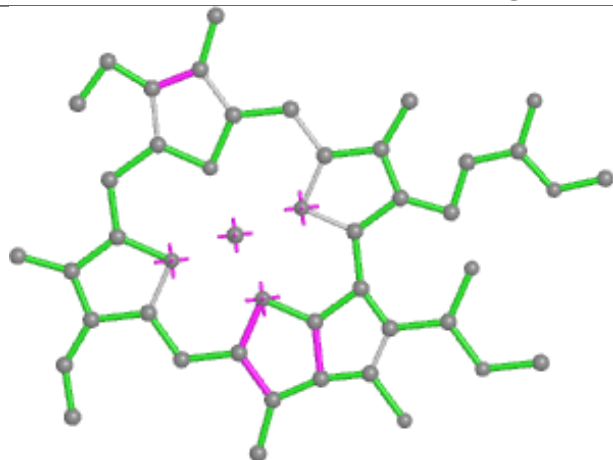




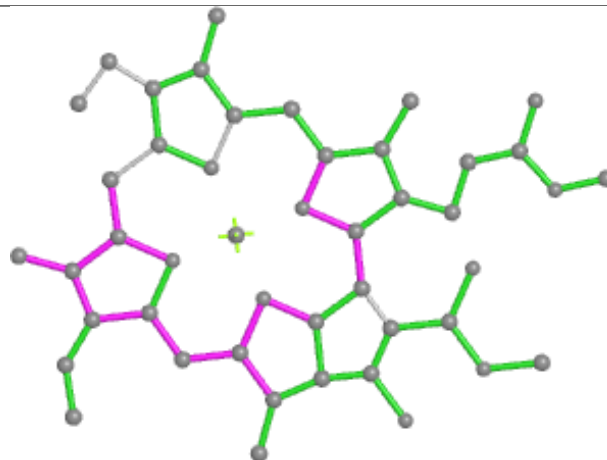




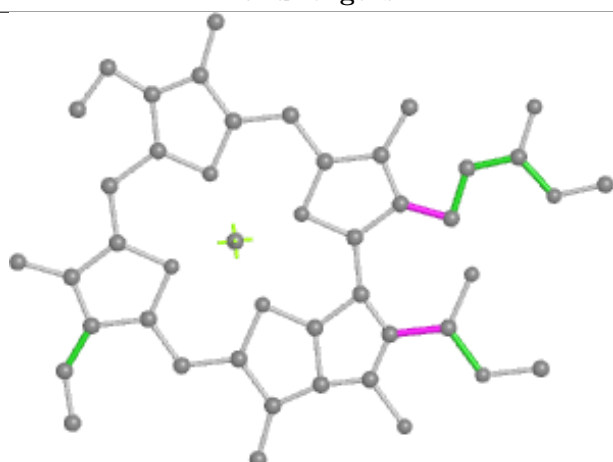
## Ligand CLA B2 835



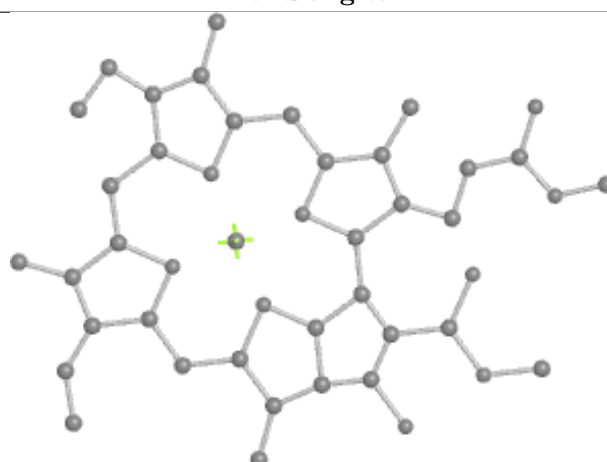
Bond lengths



Bond angles

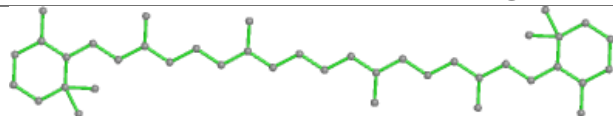


Torsions

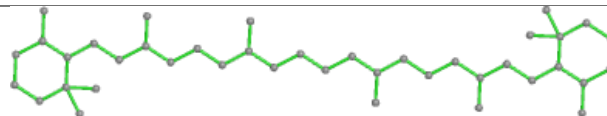


Rings

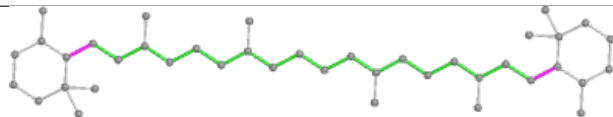
## Ligand BCR A3 848



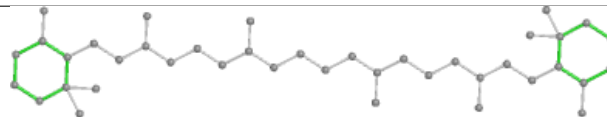
Bond lengths



Bond angles

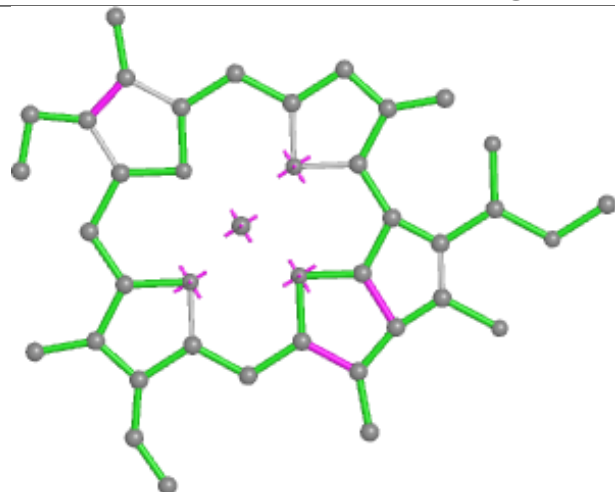


Torsions

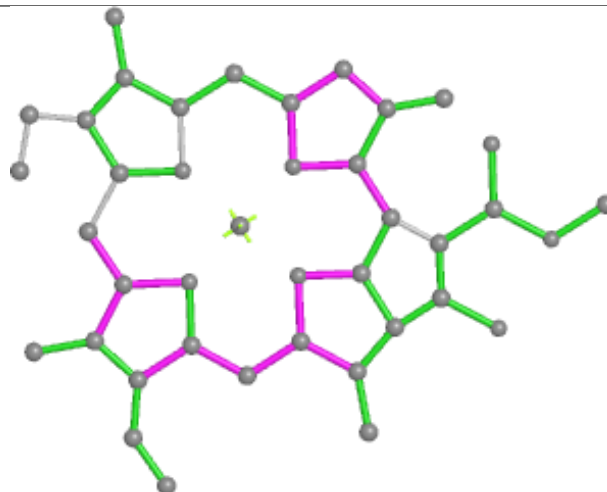


Rings

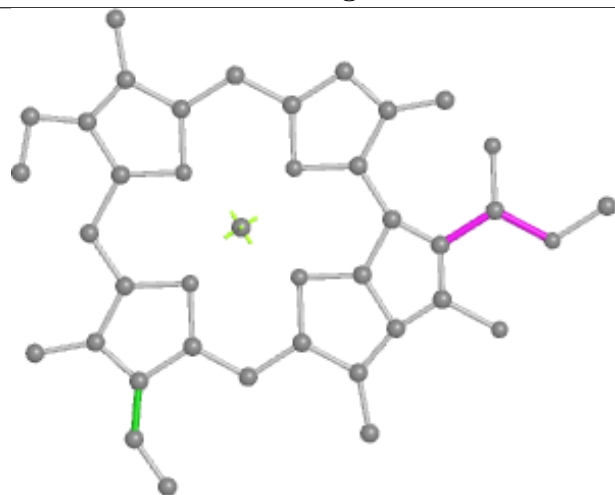
## Ligand CLA B3 832



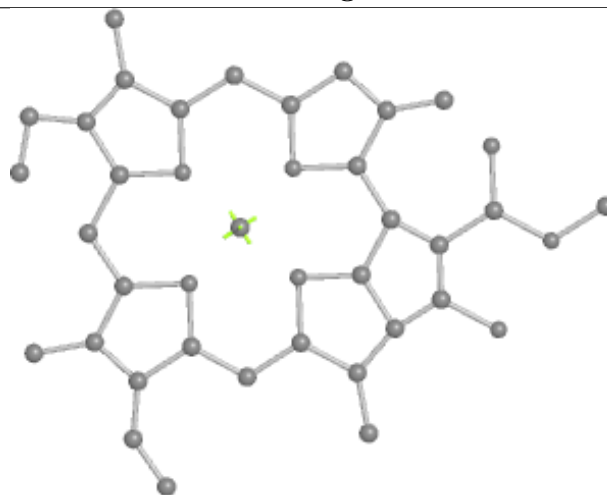
Bond lengths



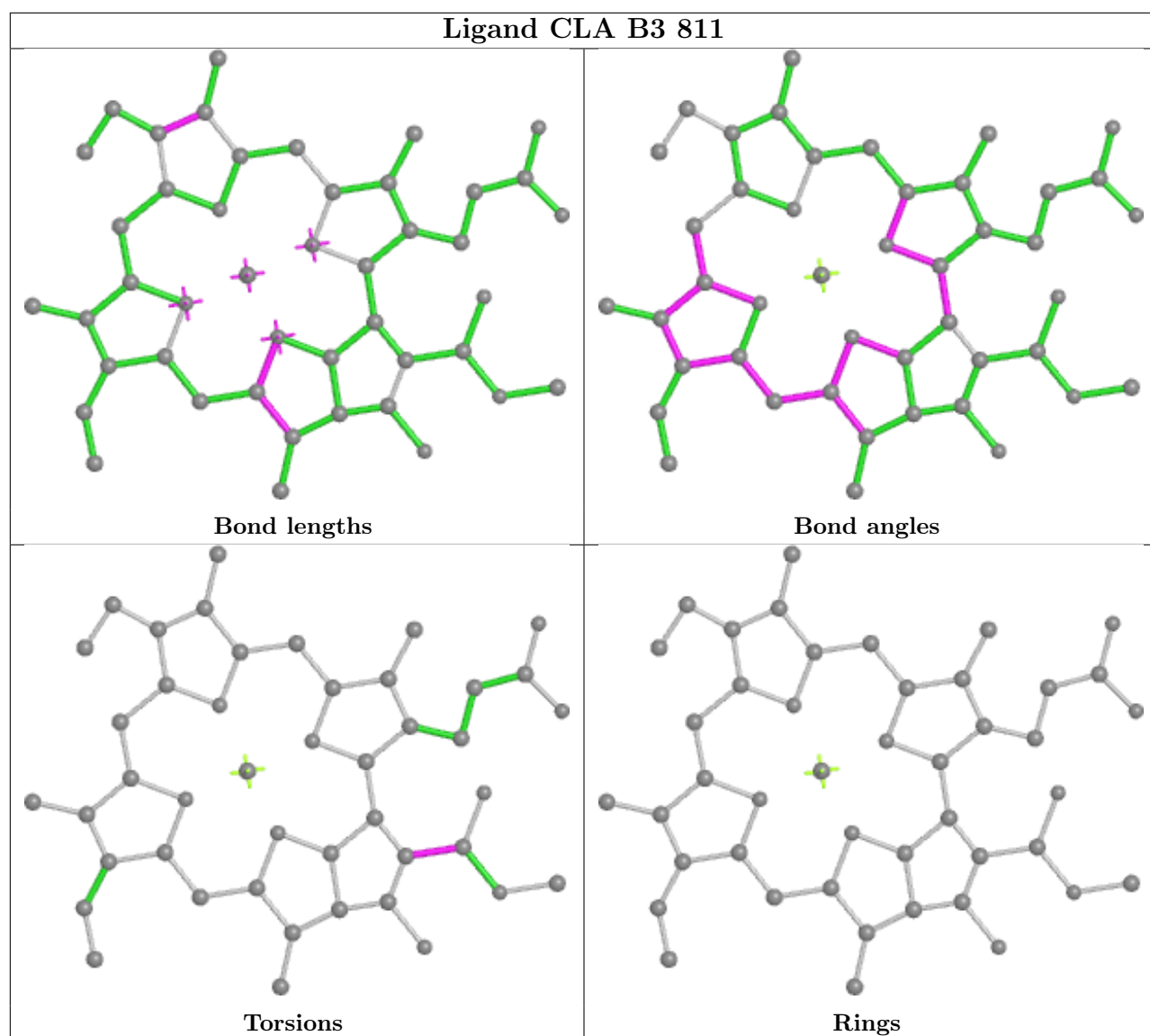
Bond angles

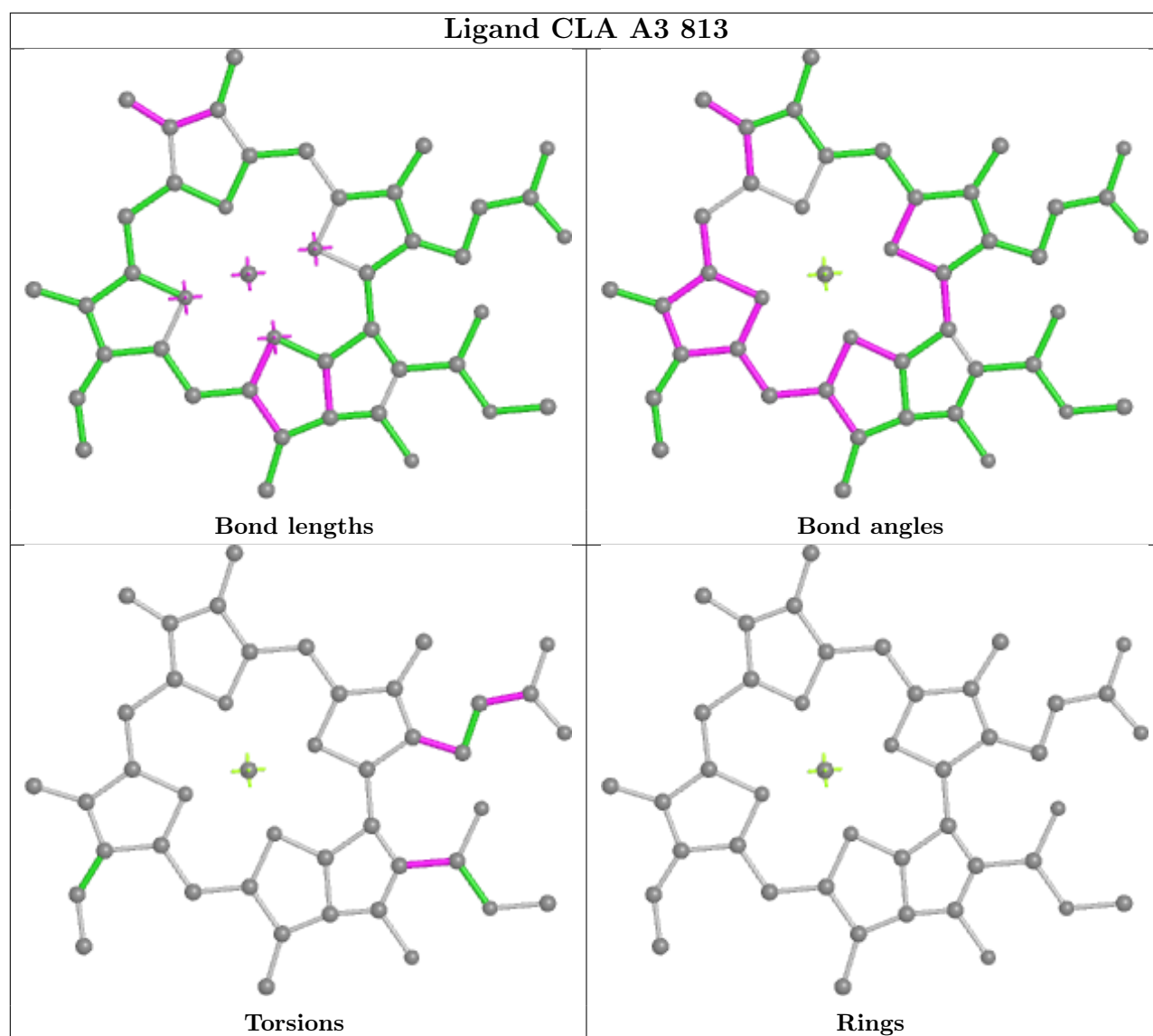


Torsions

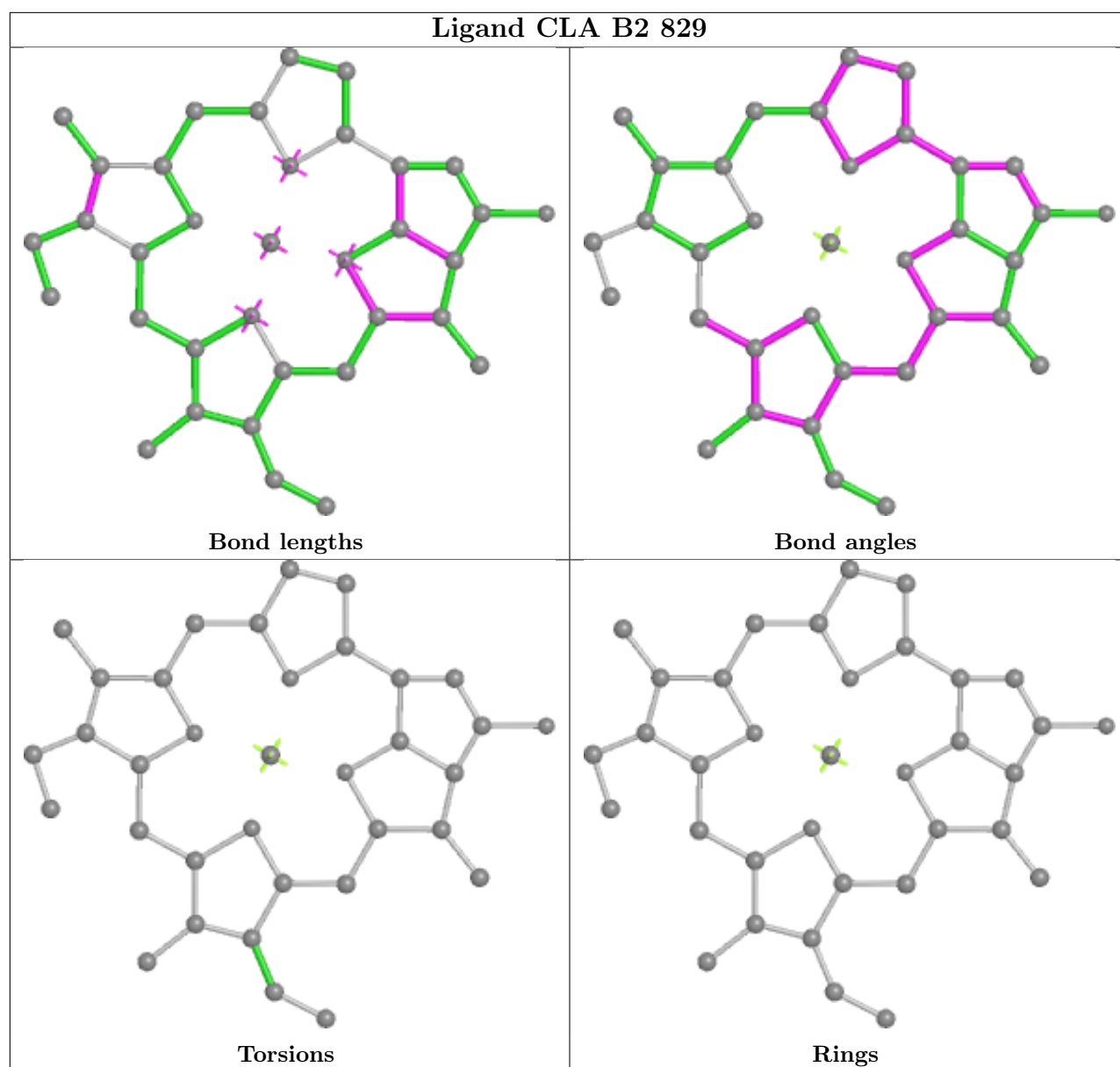


Rings

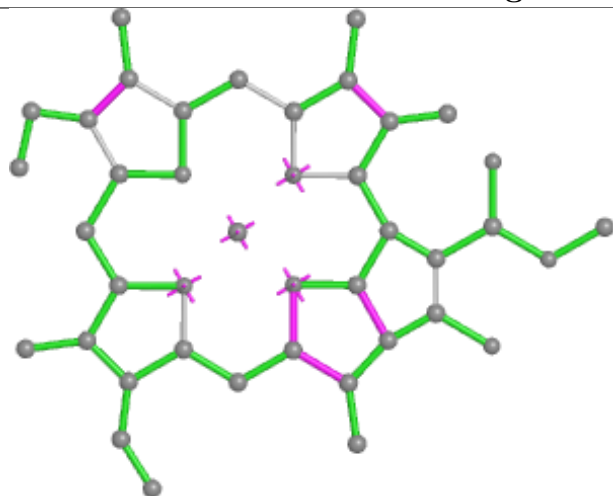




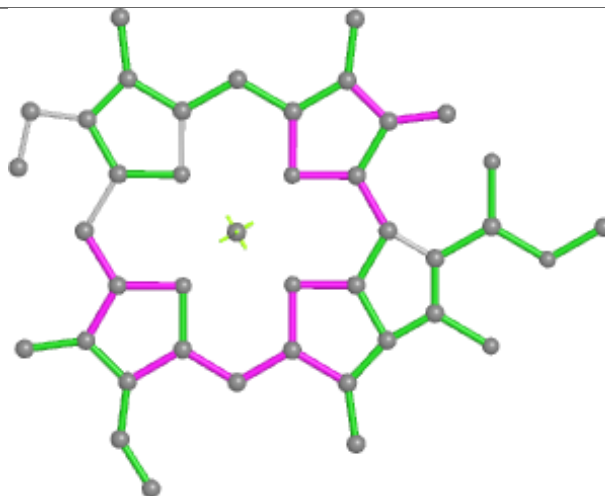




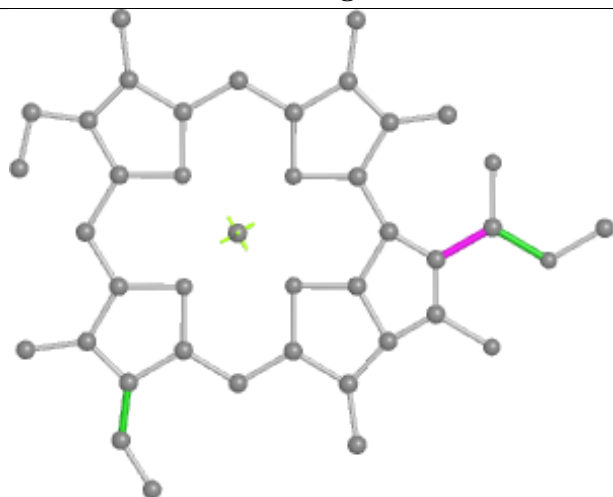
## Ligand CLA B3 823



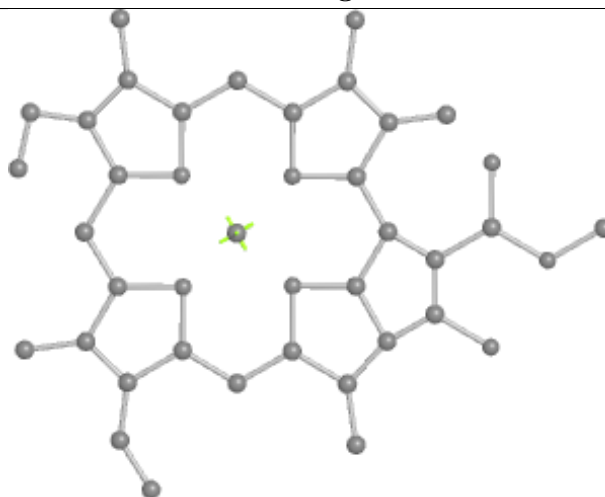
Bond lengths



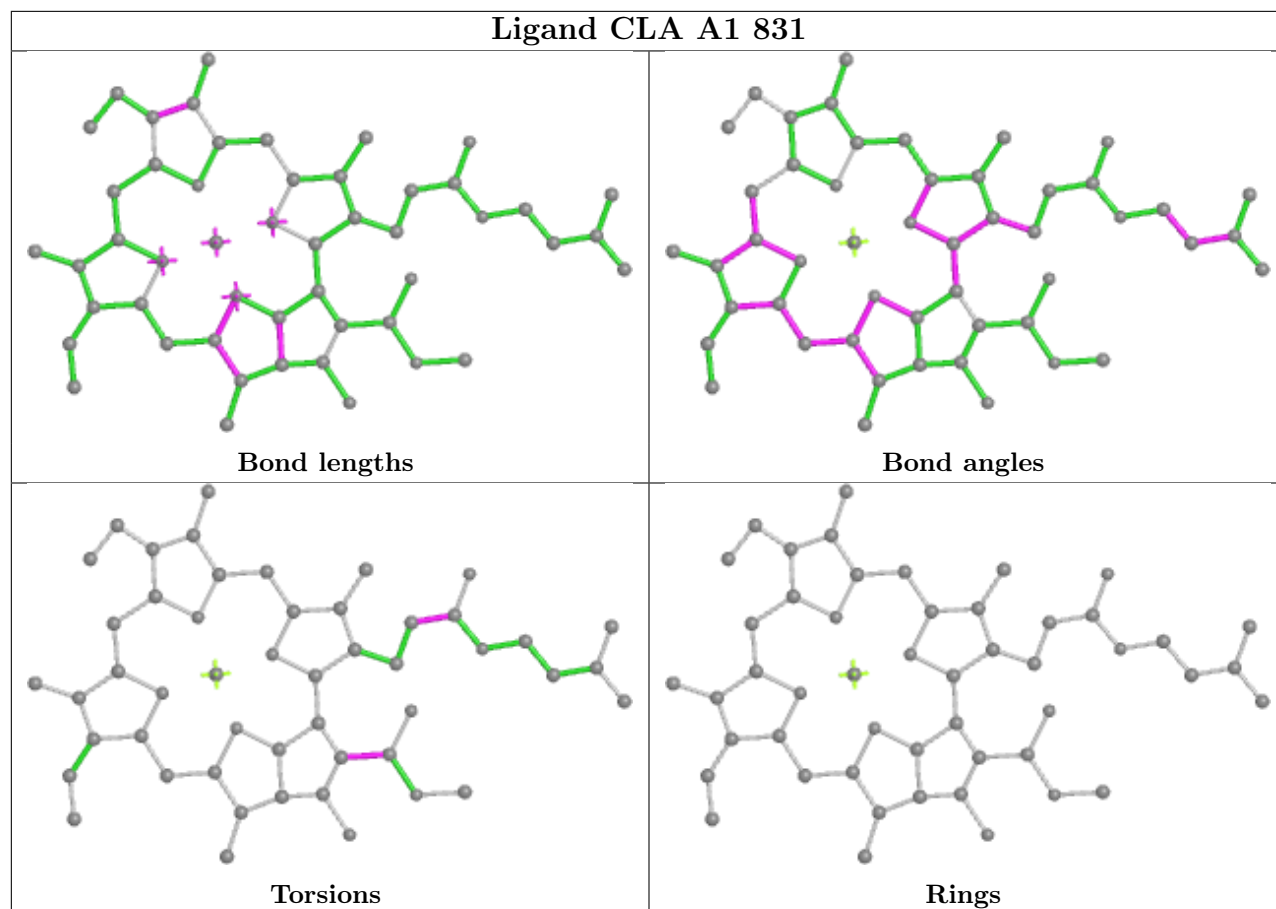
Bond angles

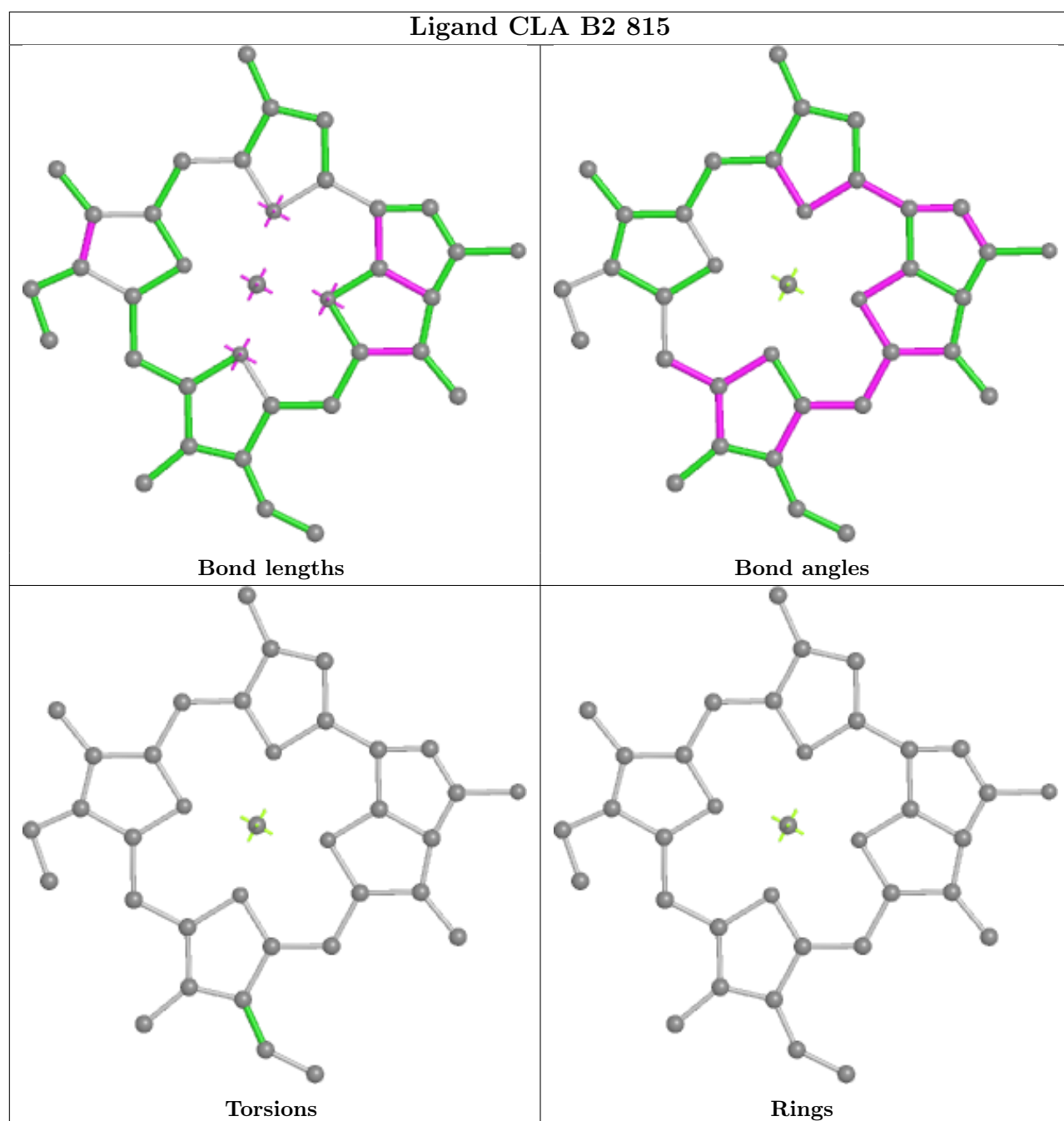


Torsions

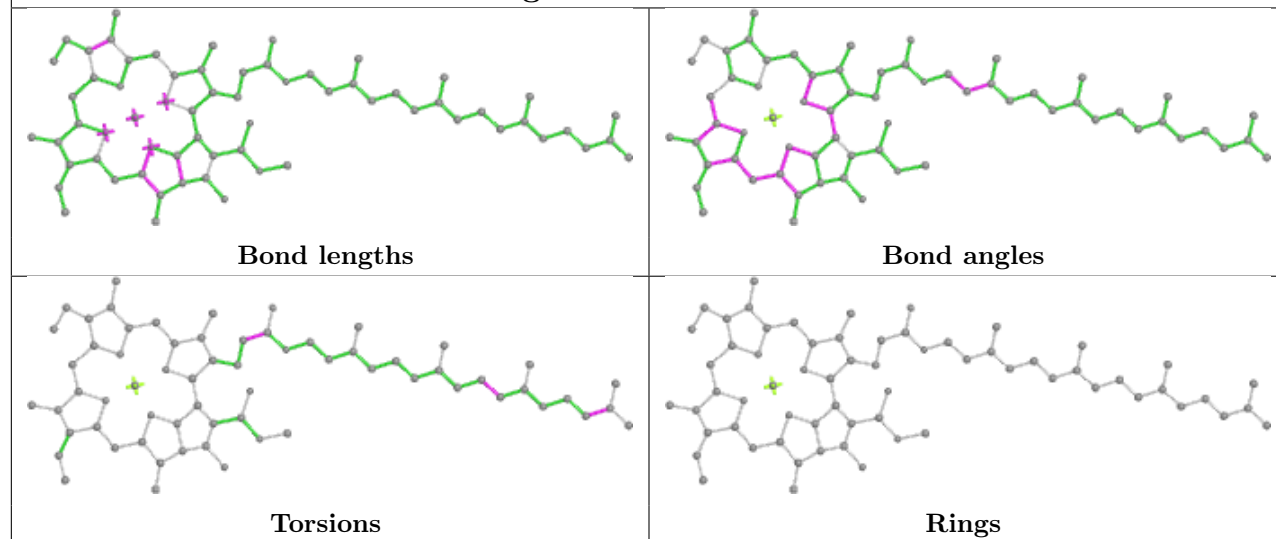


Rings

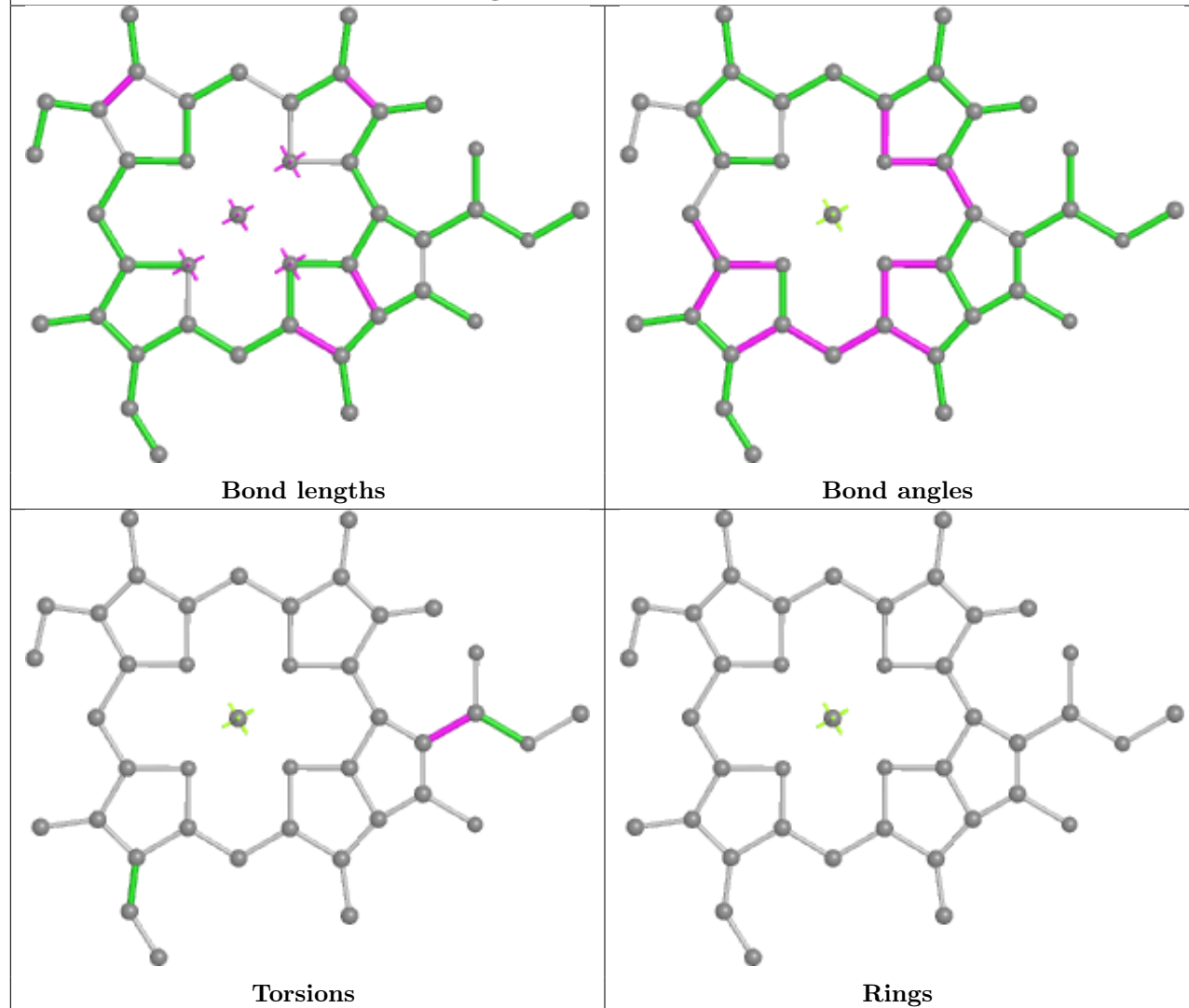


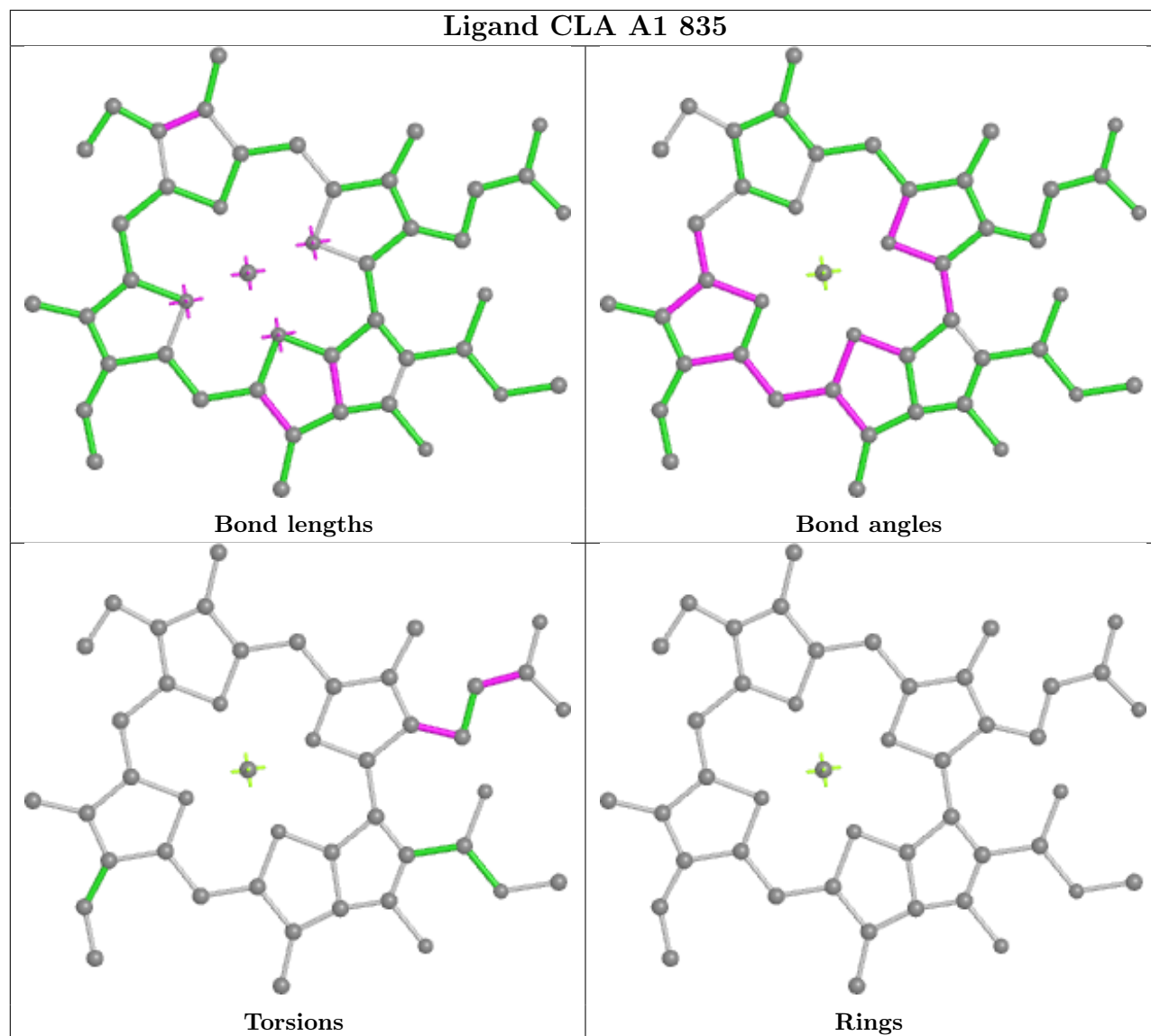
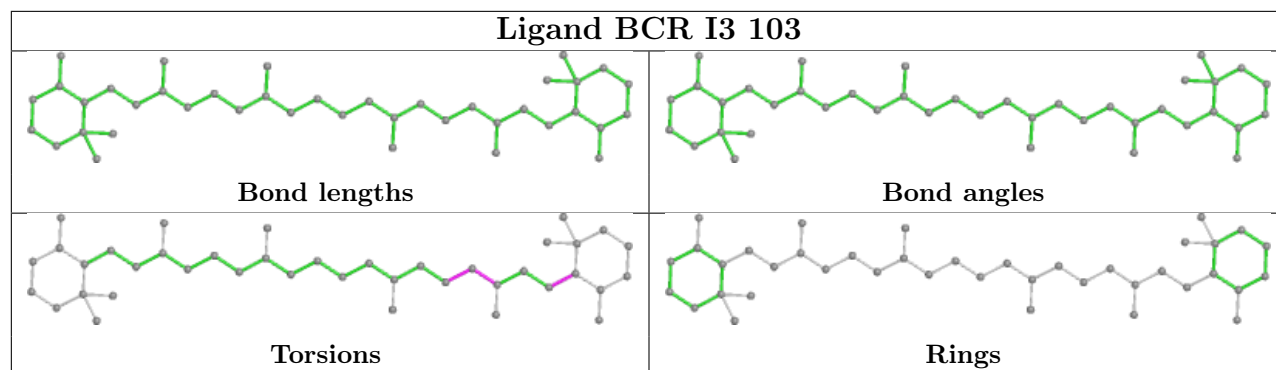


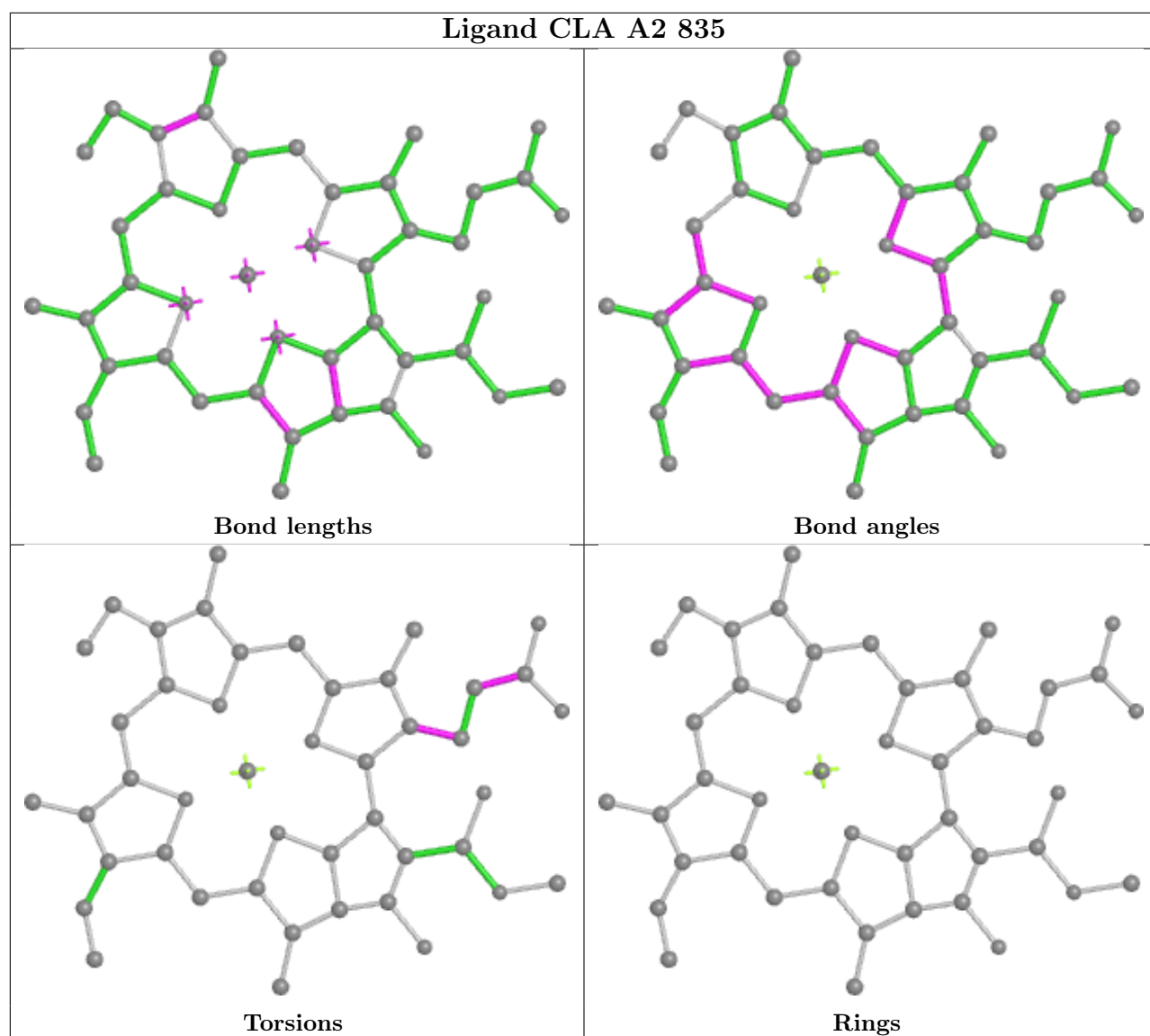
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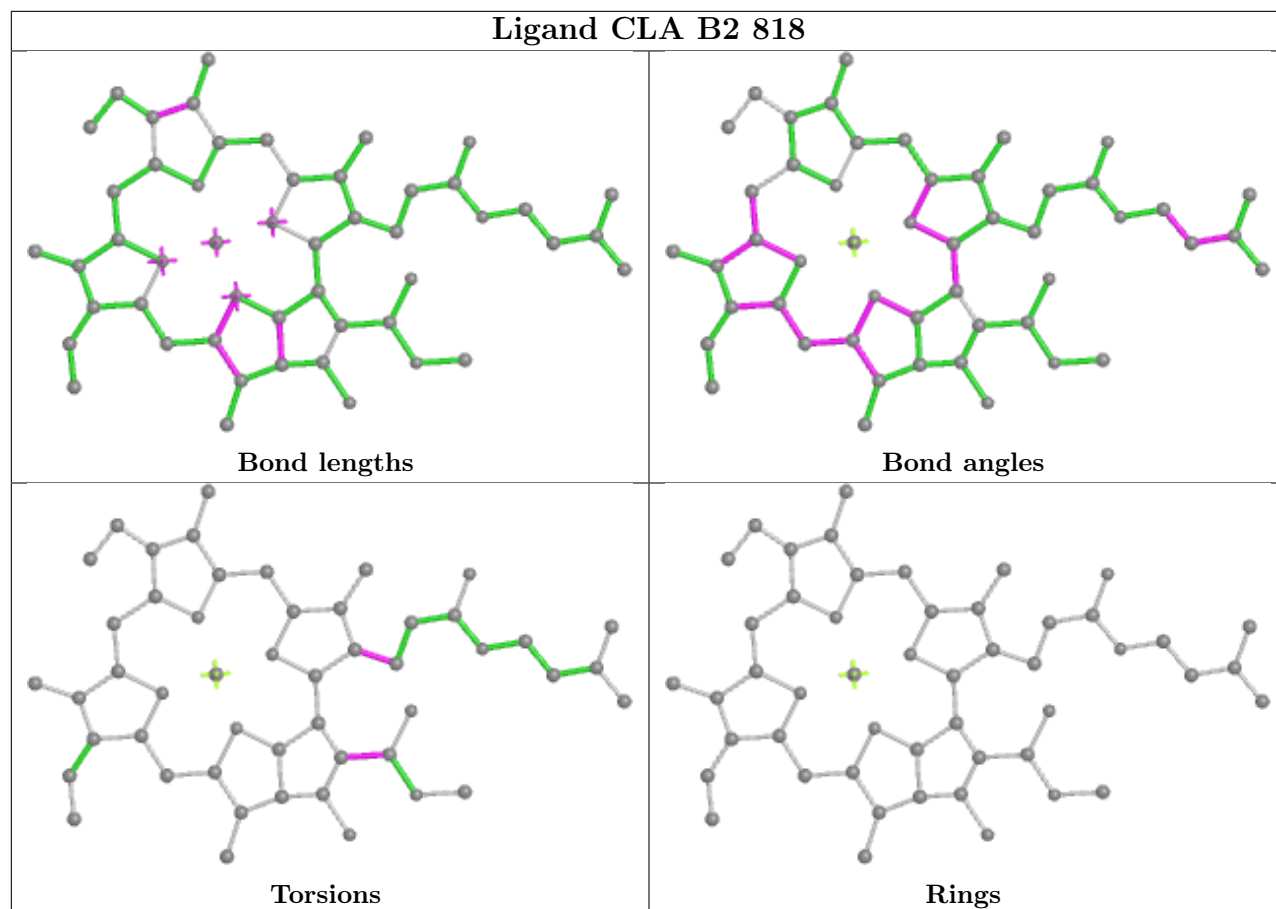


## Ligand CLA A3 836

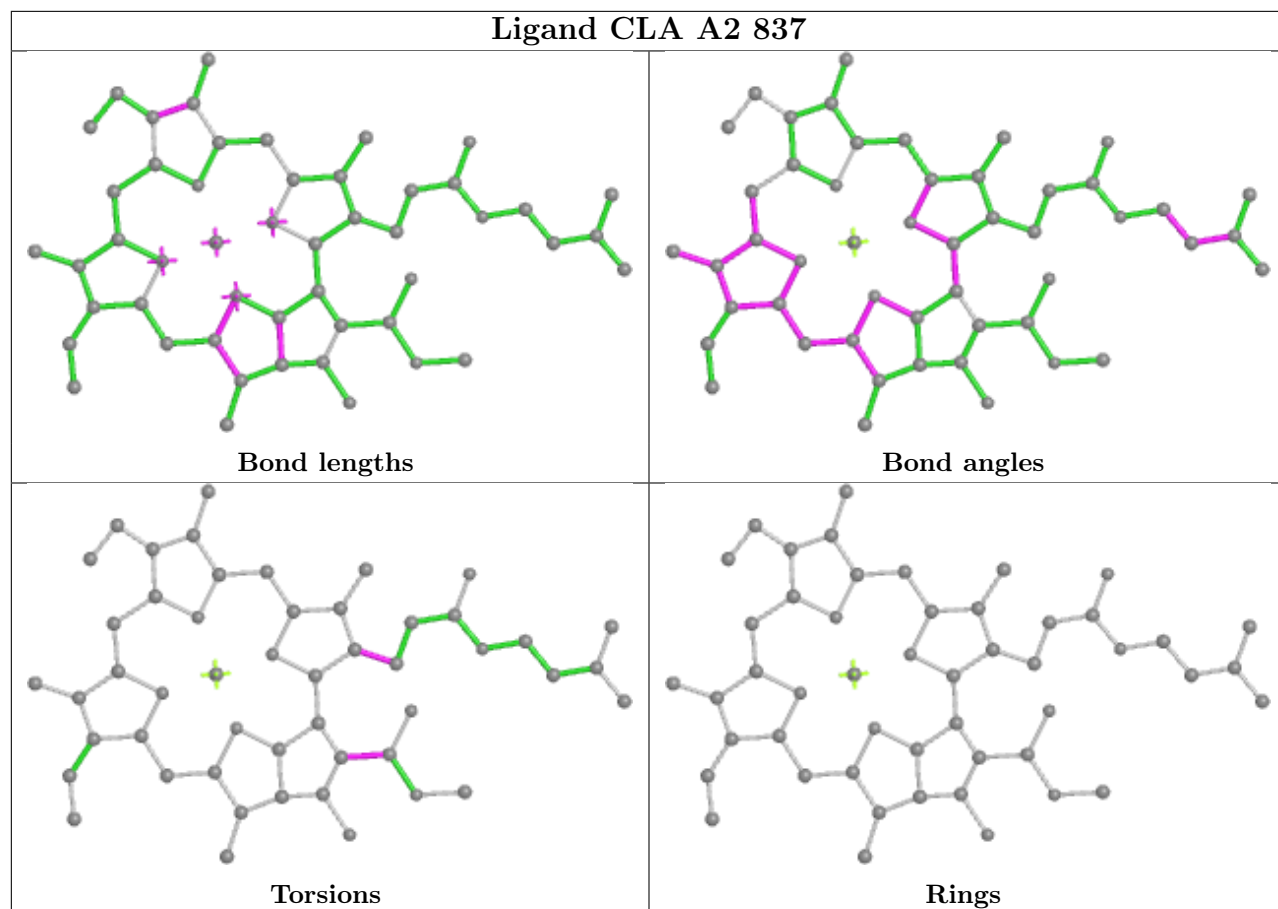




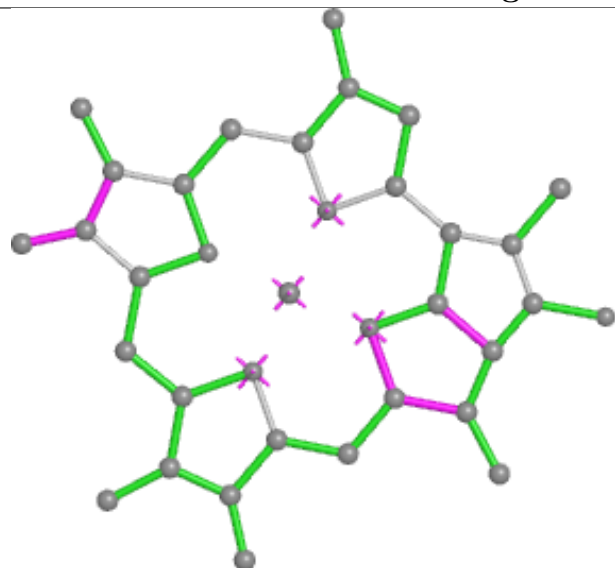




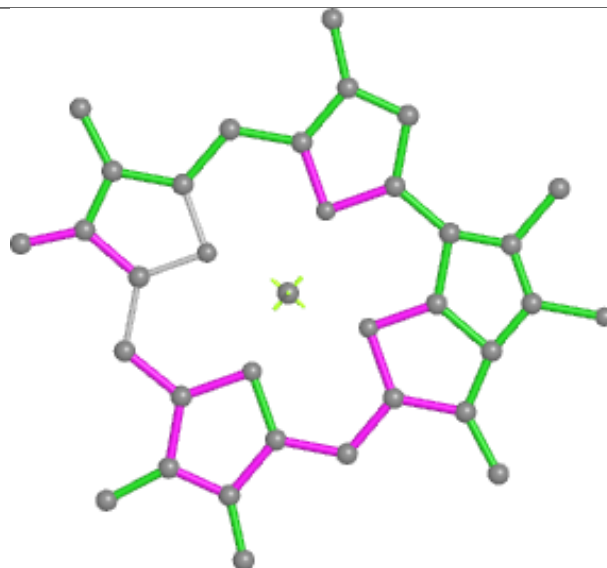




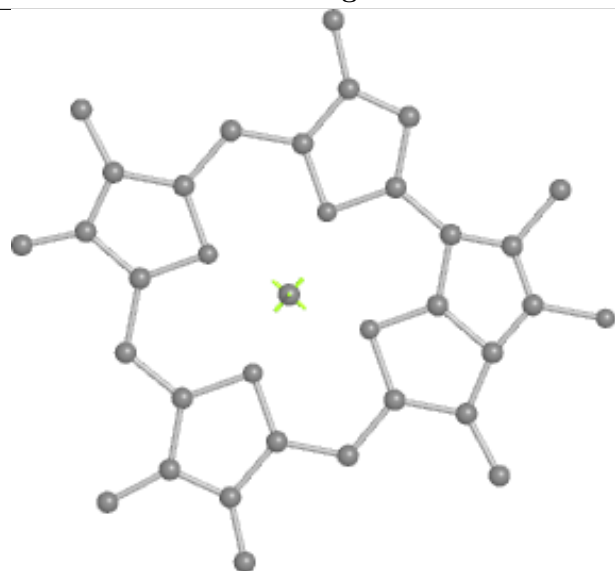
## Ligand CLA J3 1302



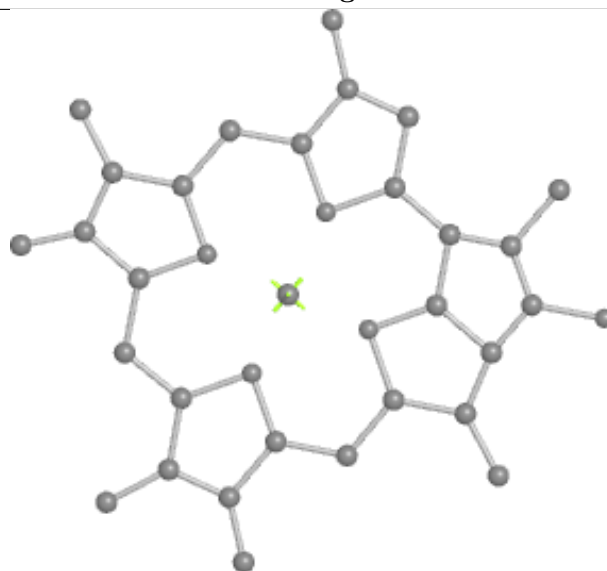
Bond lengths



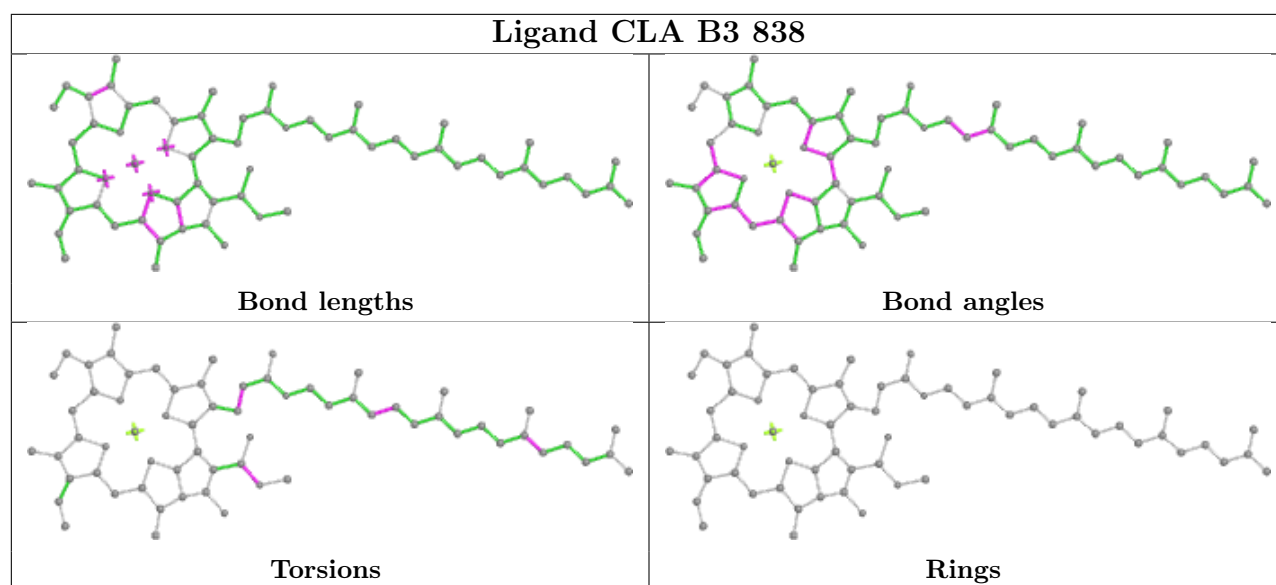
Bond angles



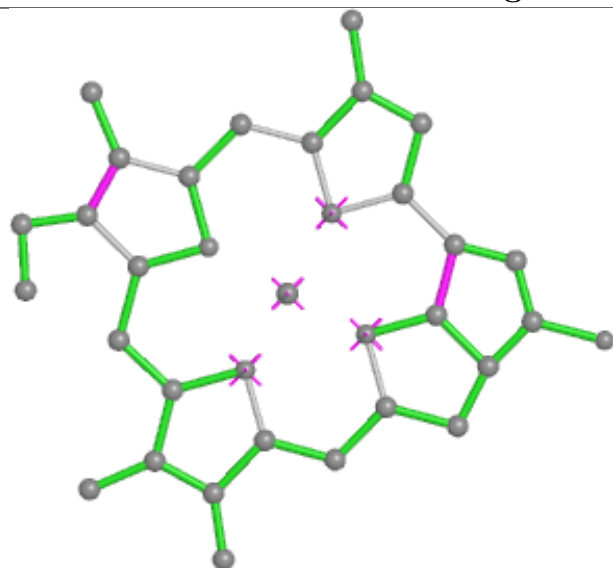
Torsions



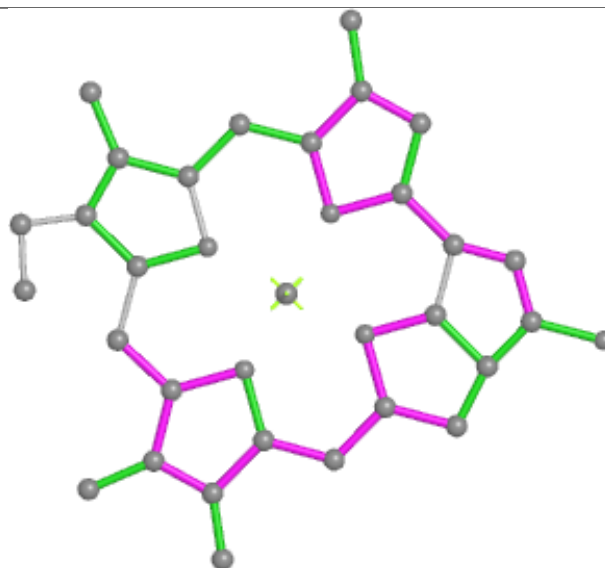
Rings



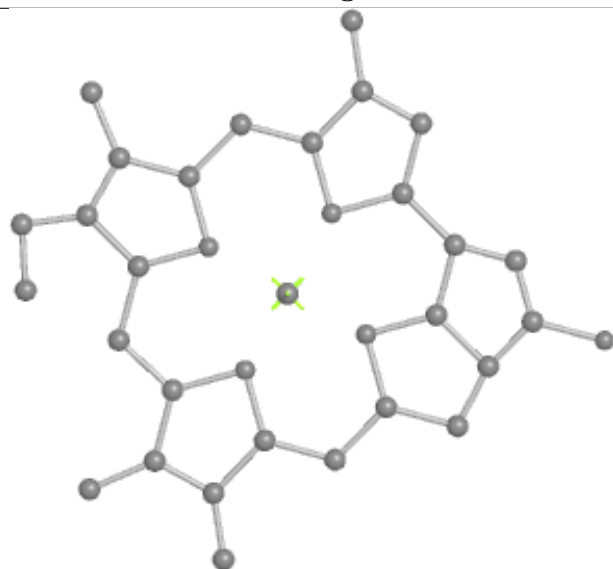
## Ligand CLA K3 101



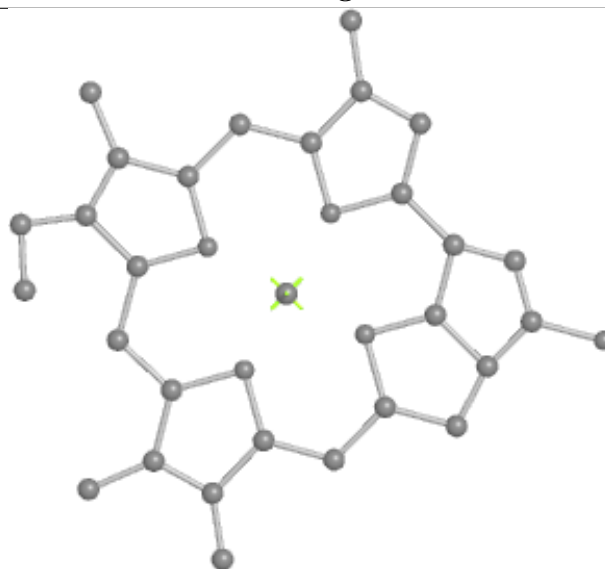
Bond lengths



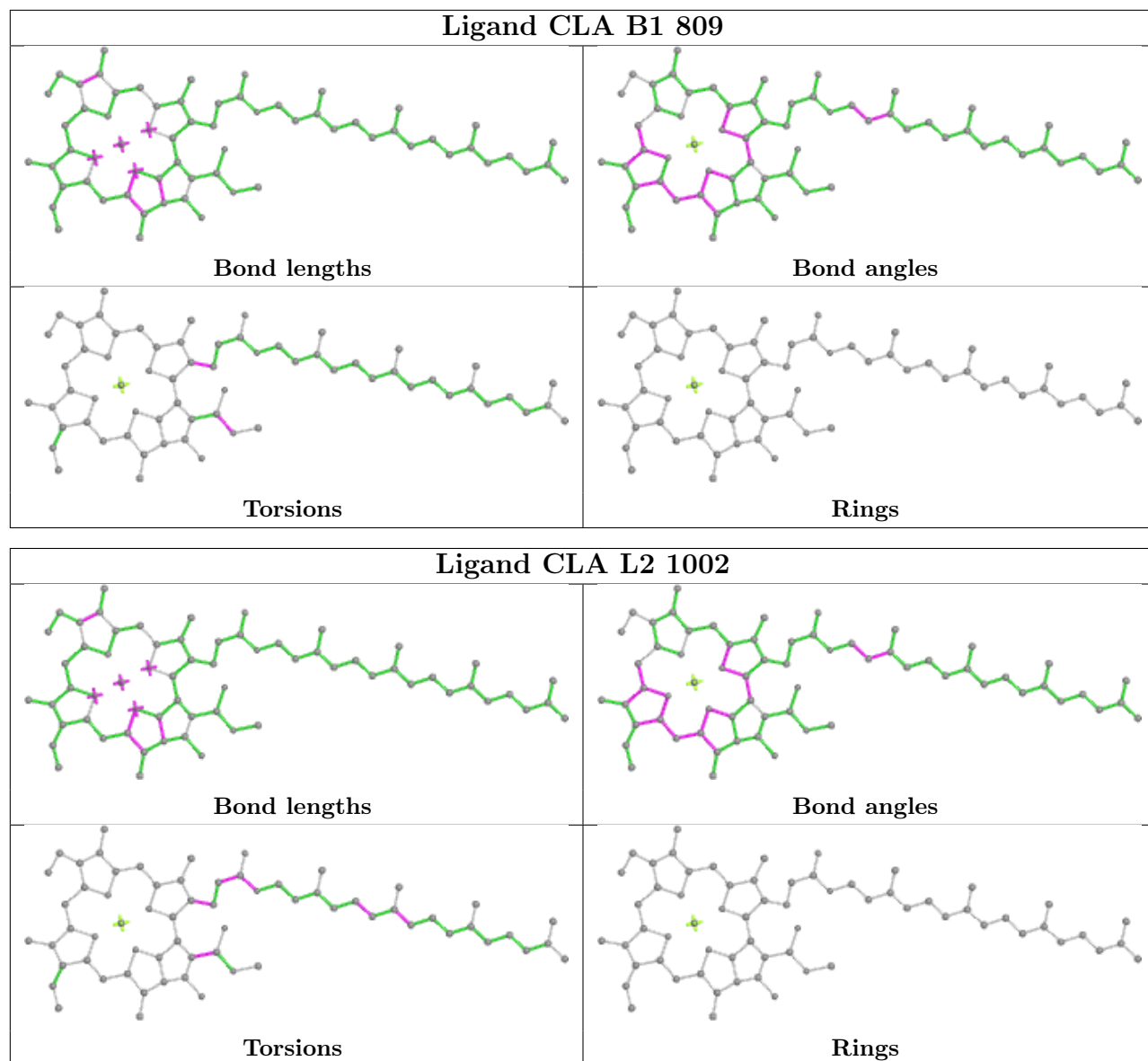
Bond angles

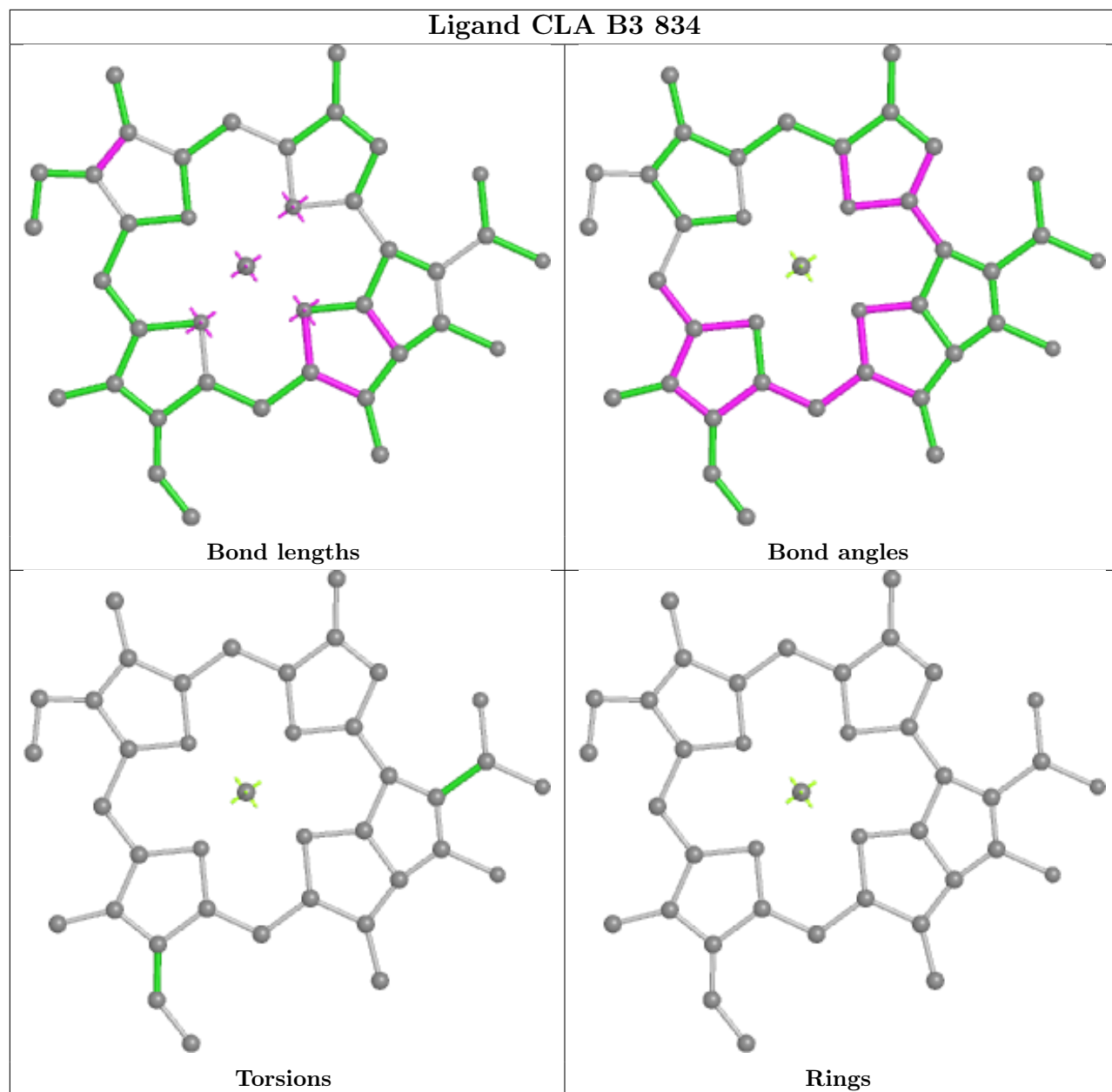


Torsions

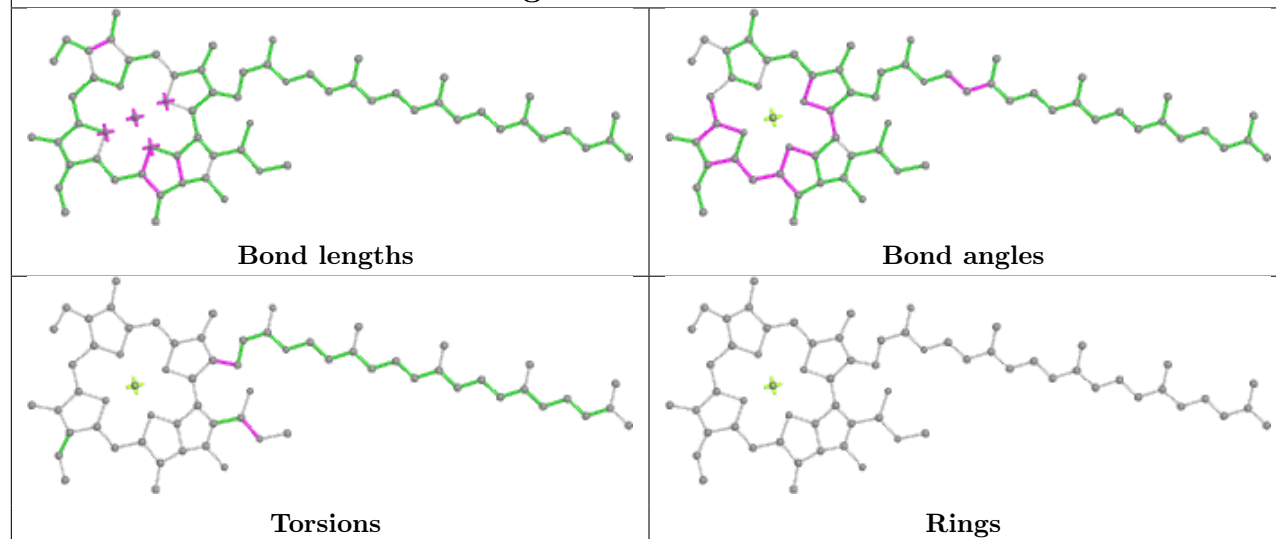


Rings

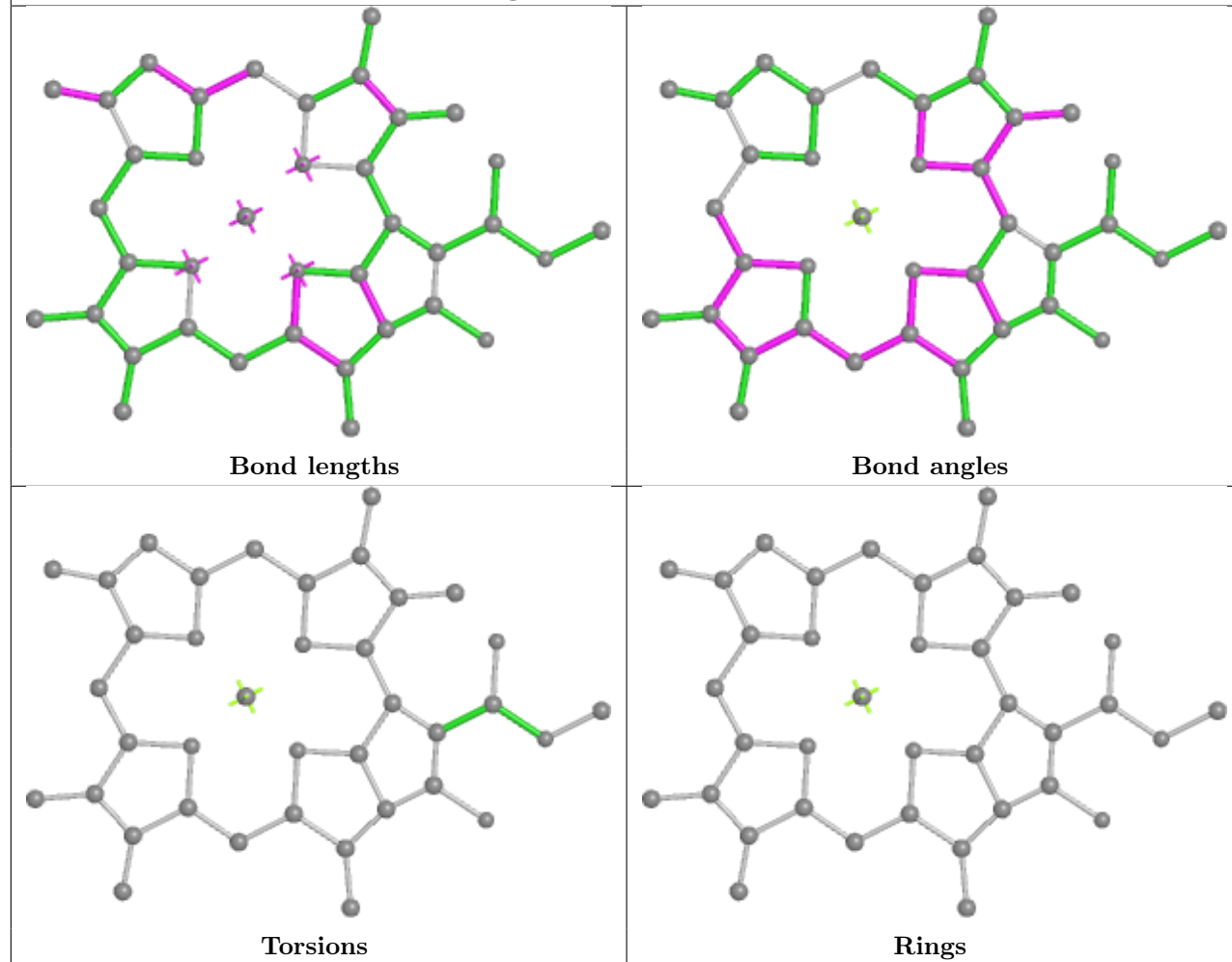




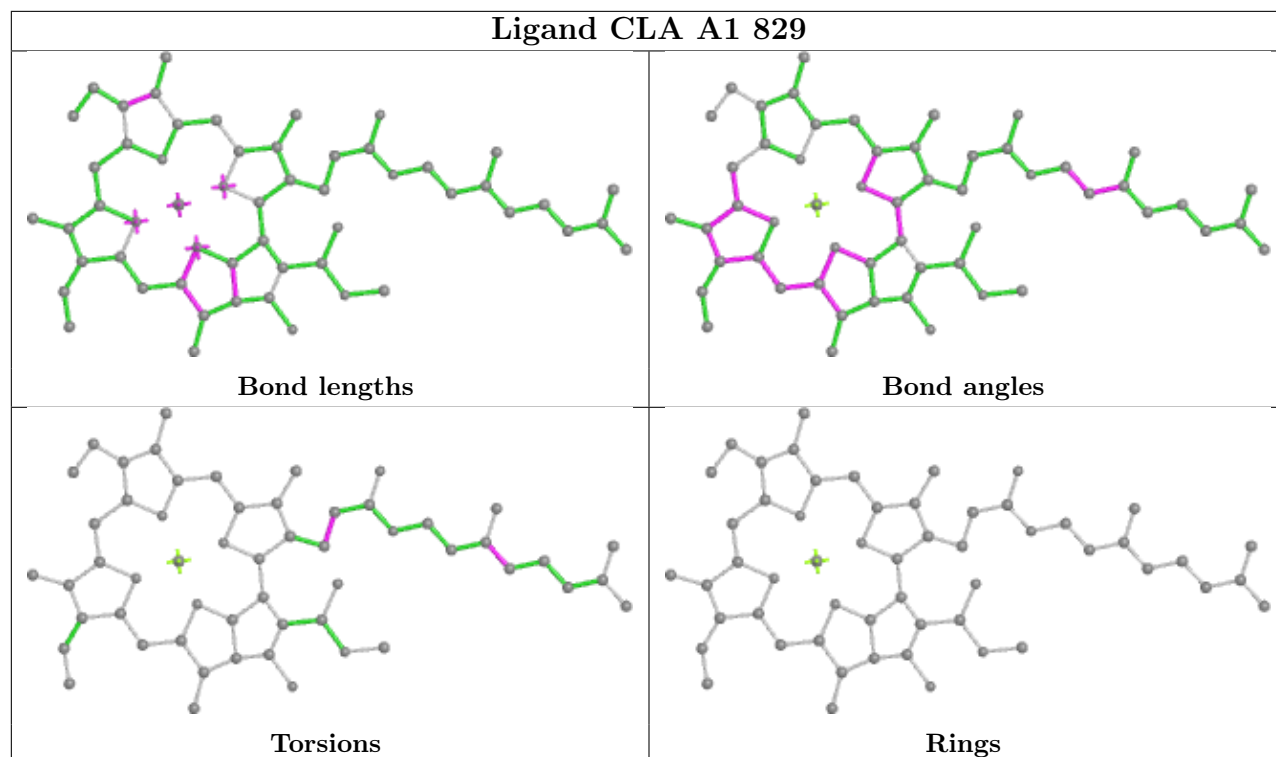
## Ligand CLA B2 809



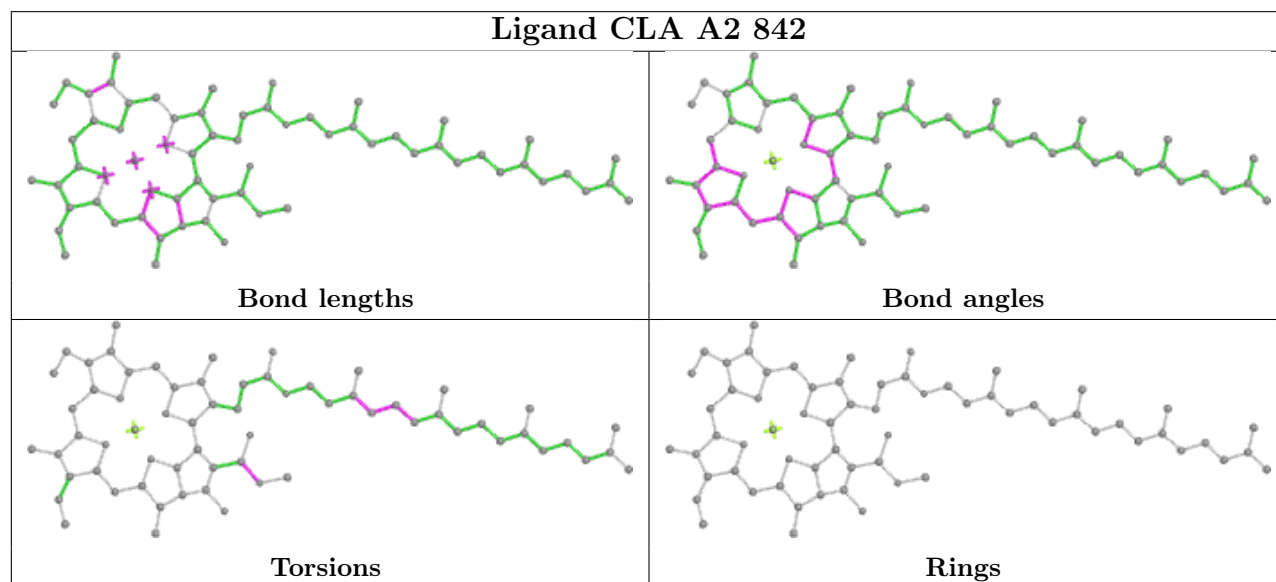
## Ligand CLA A3 817



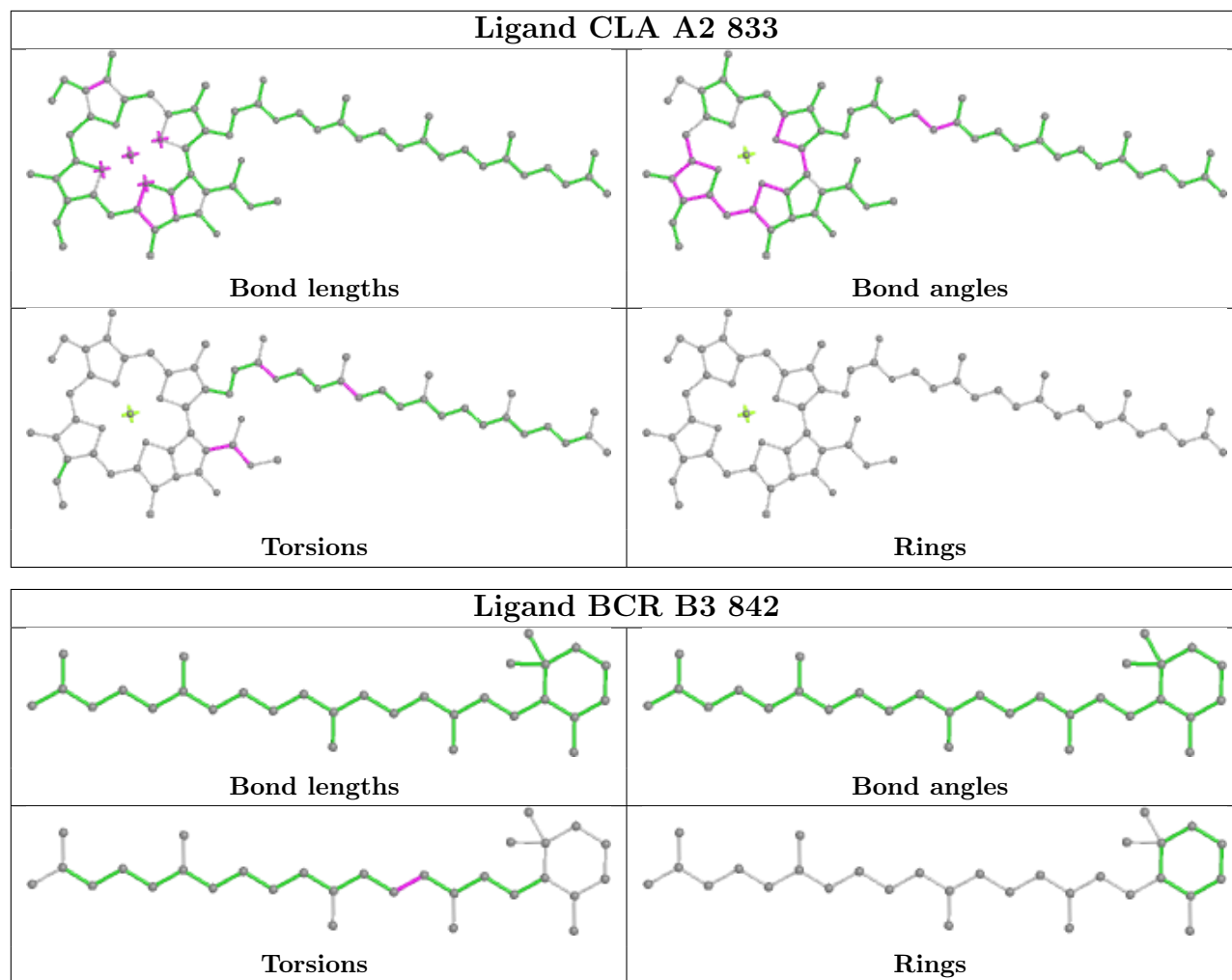
## Ligand CLA A1 829

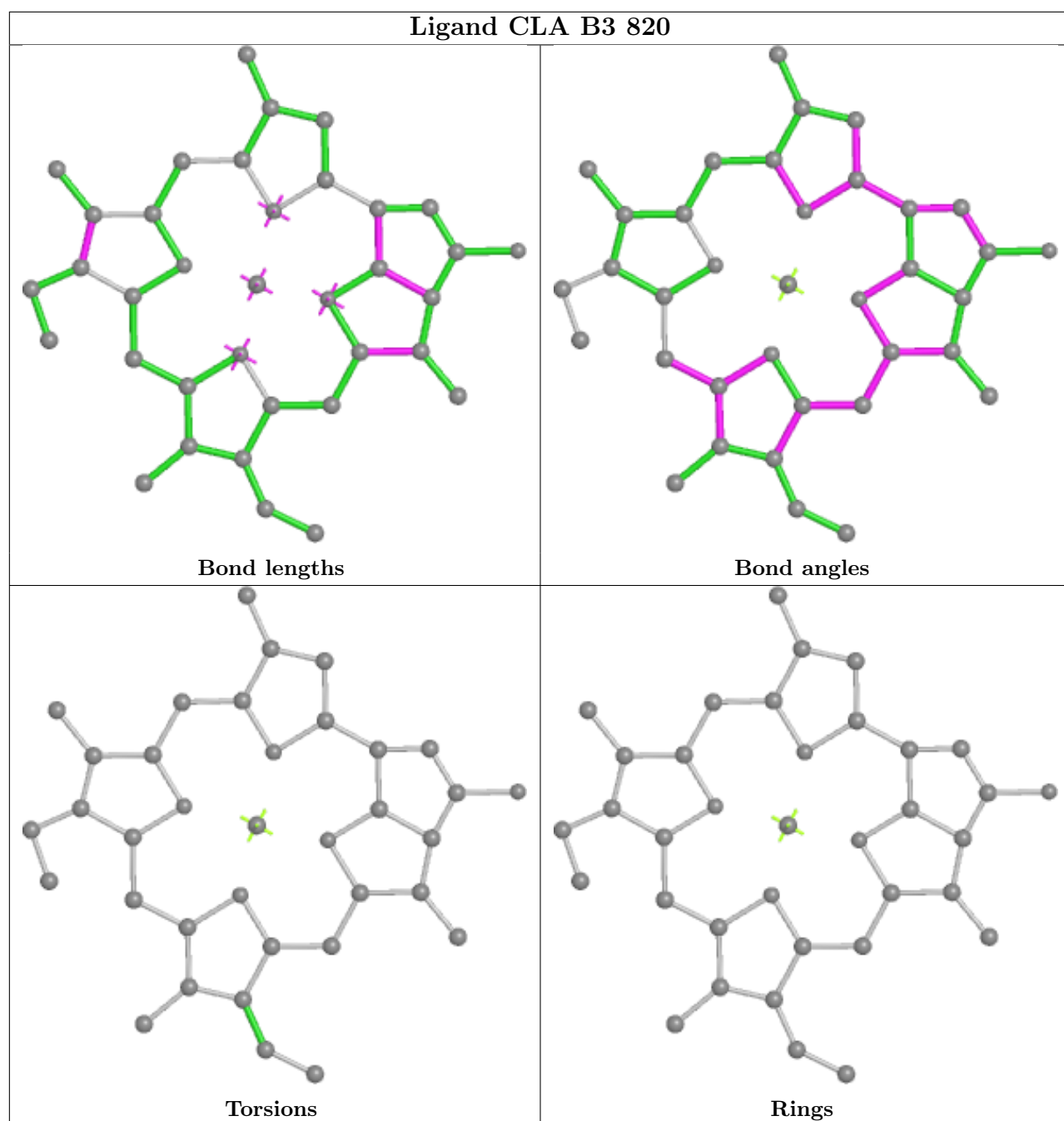


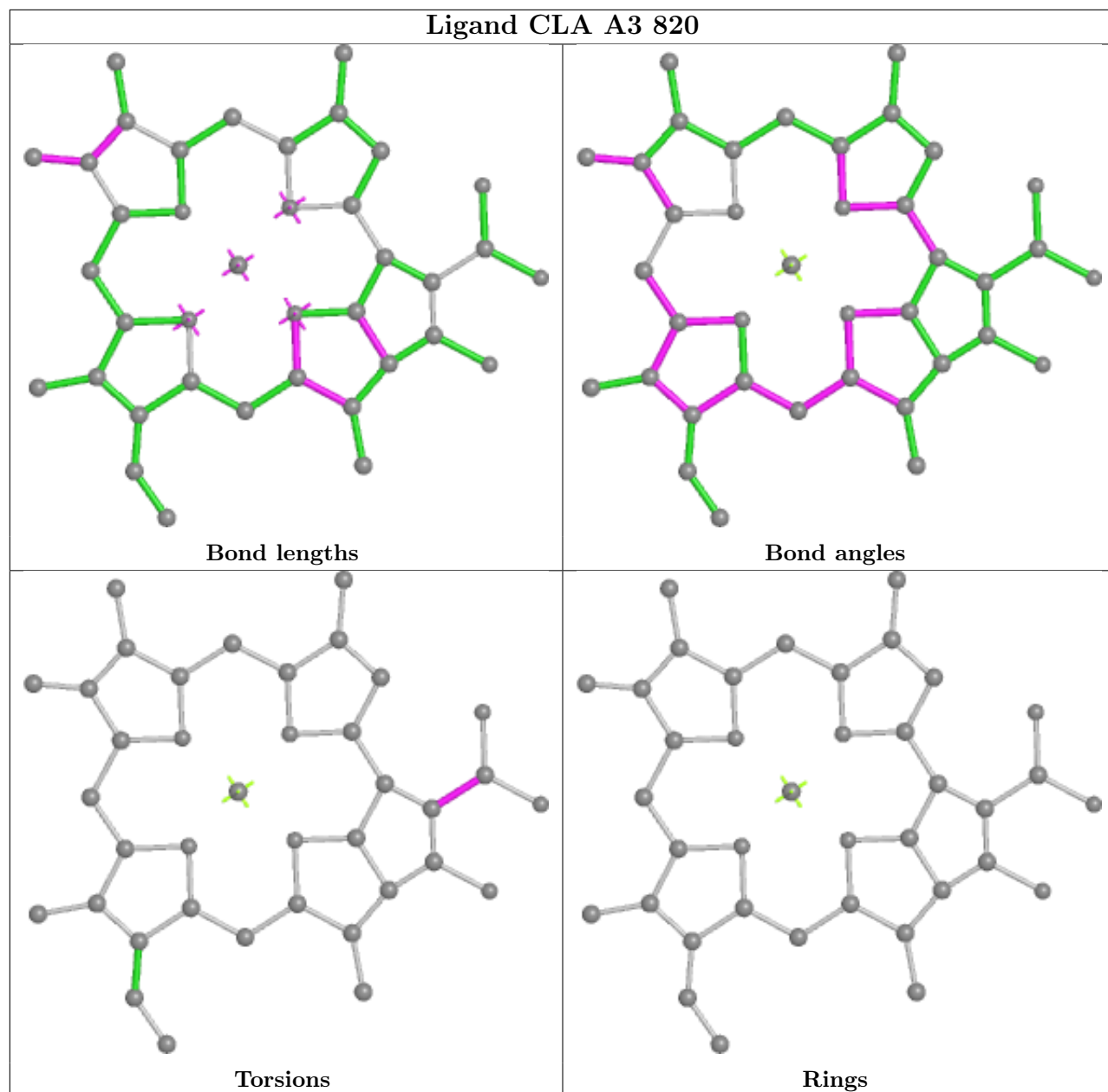
## Ligand CLA A2 842

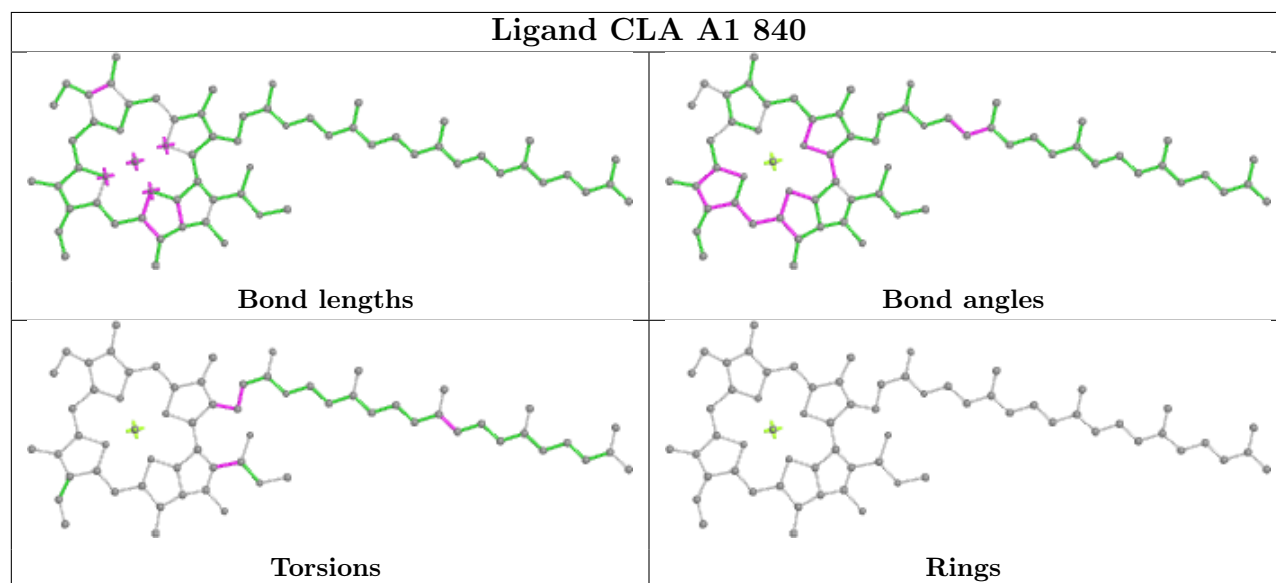
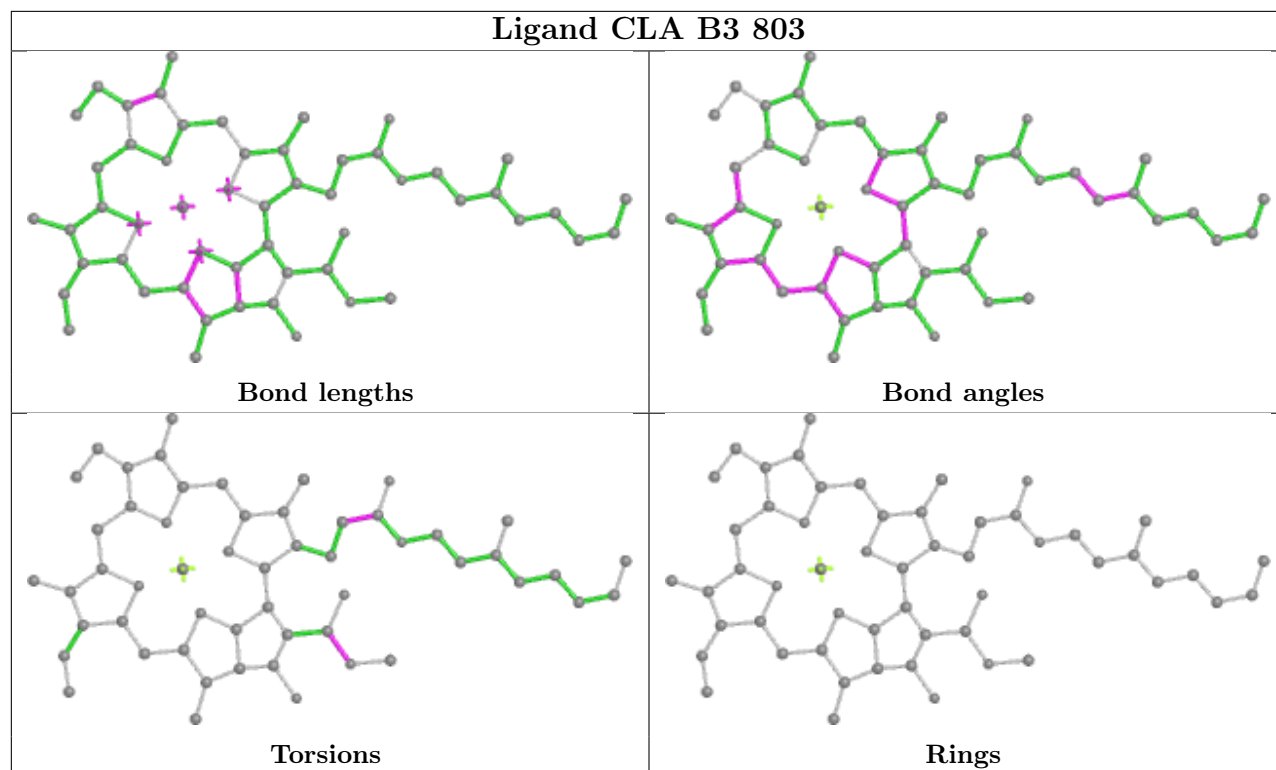




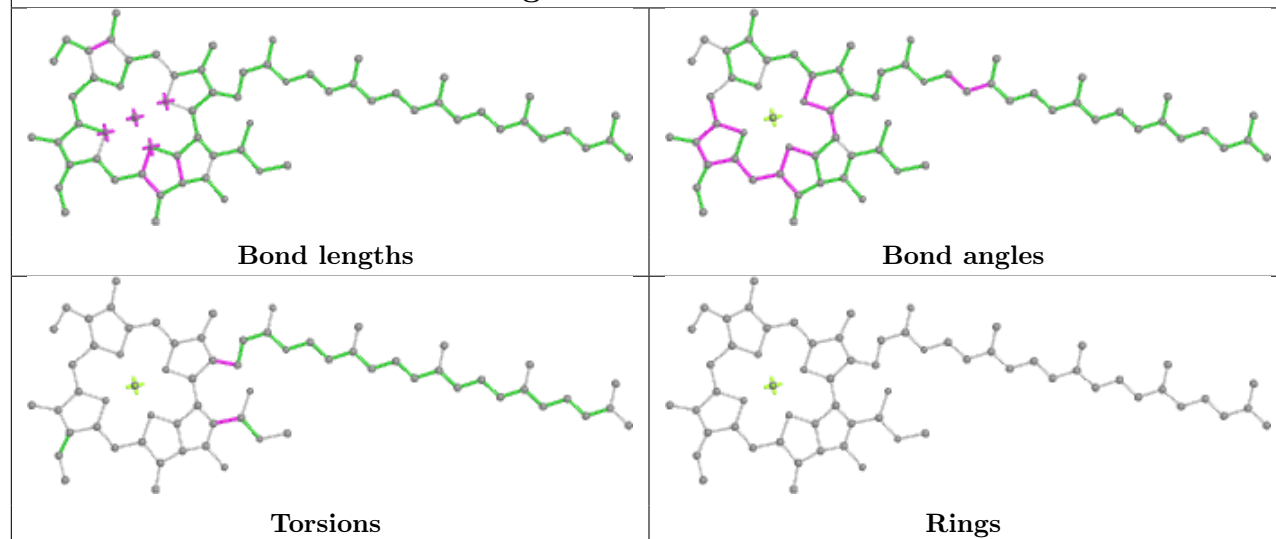




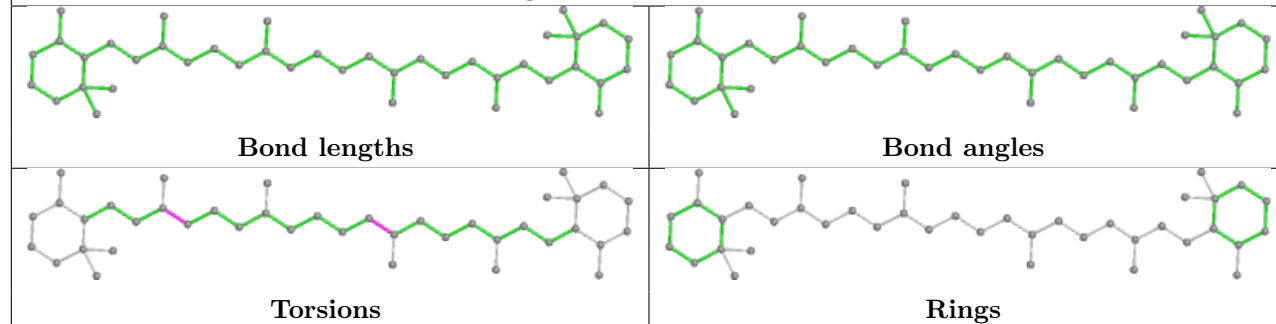




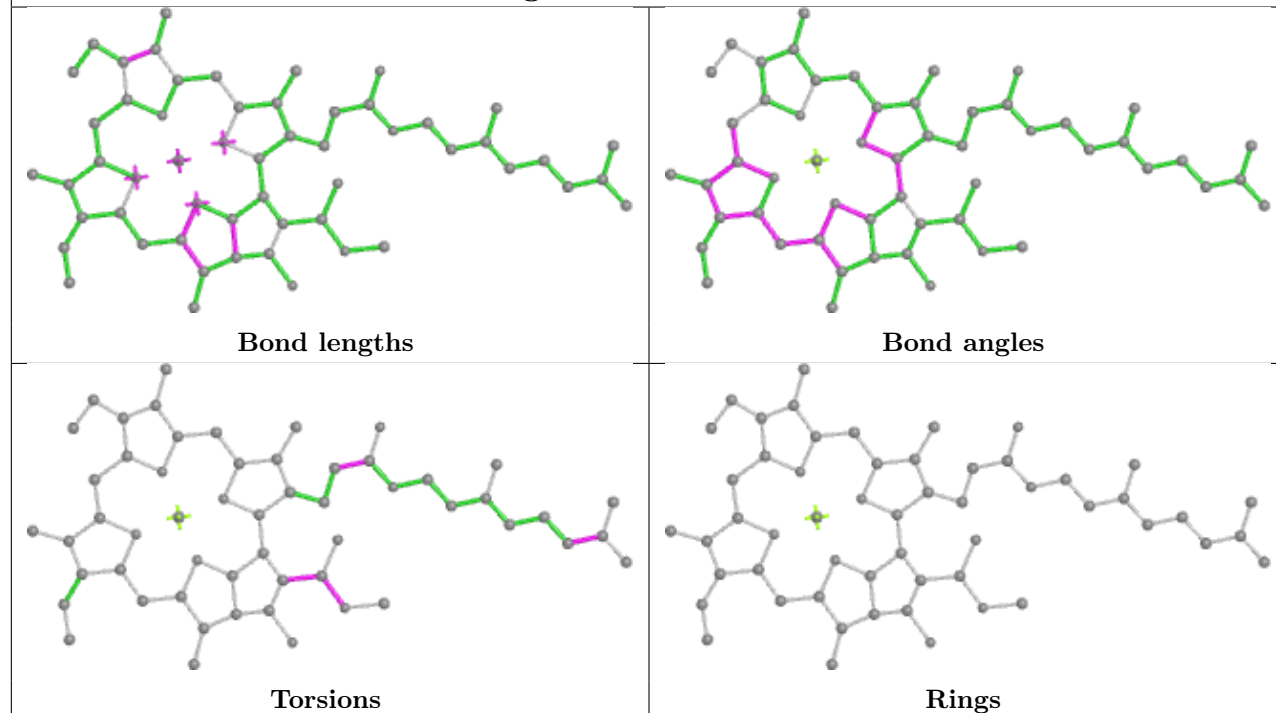
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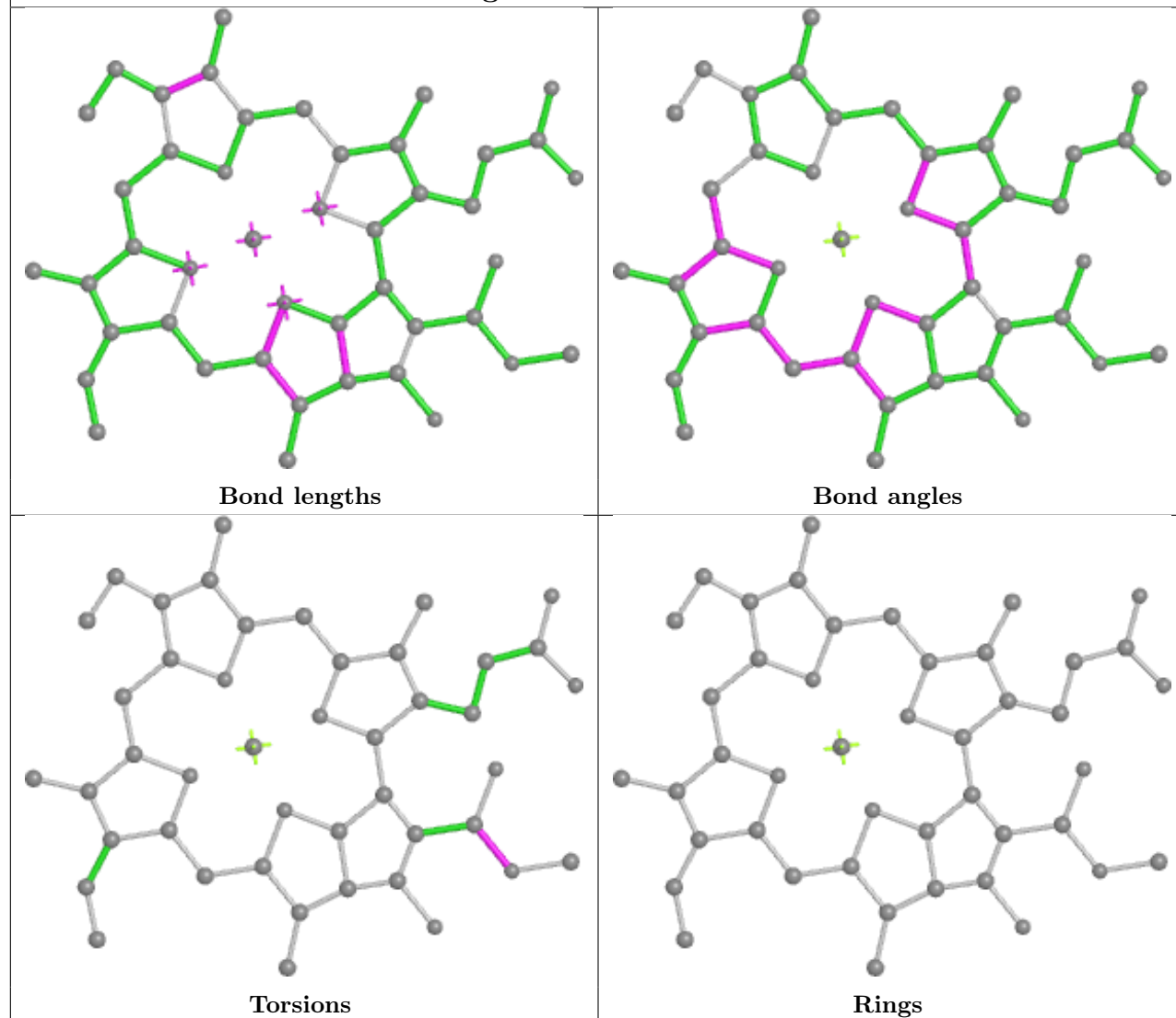
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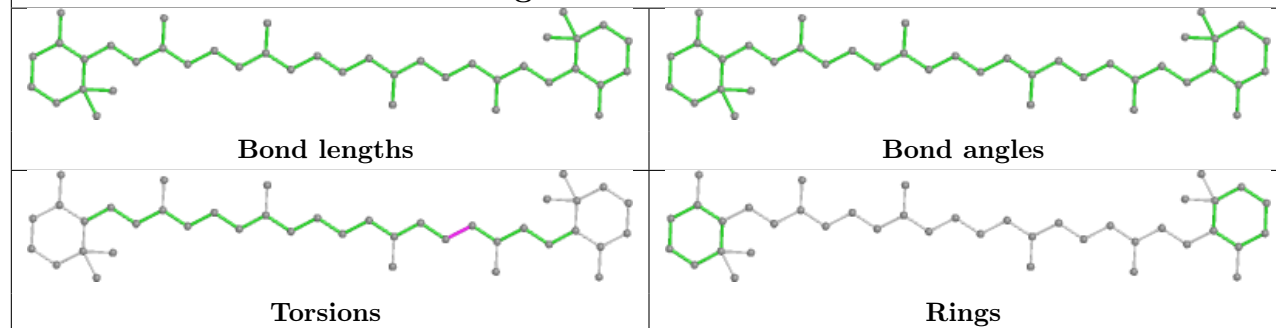
## Ligand CLA A2 839



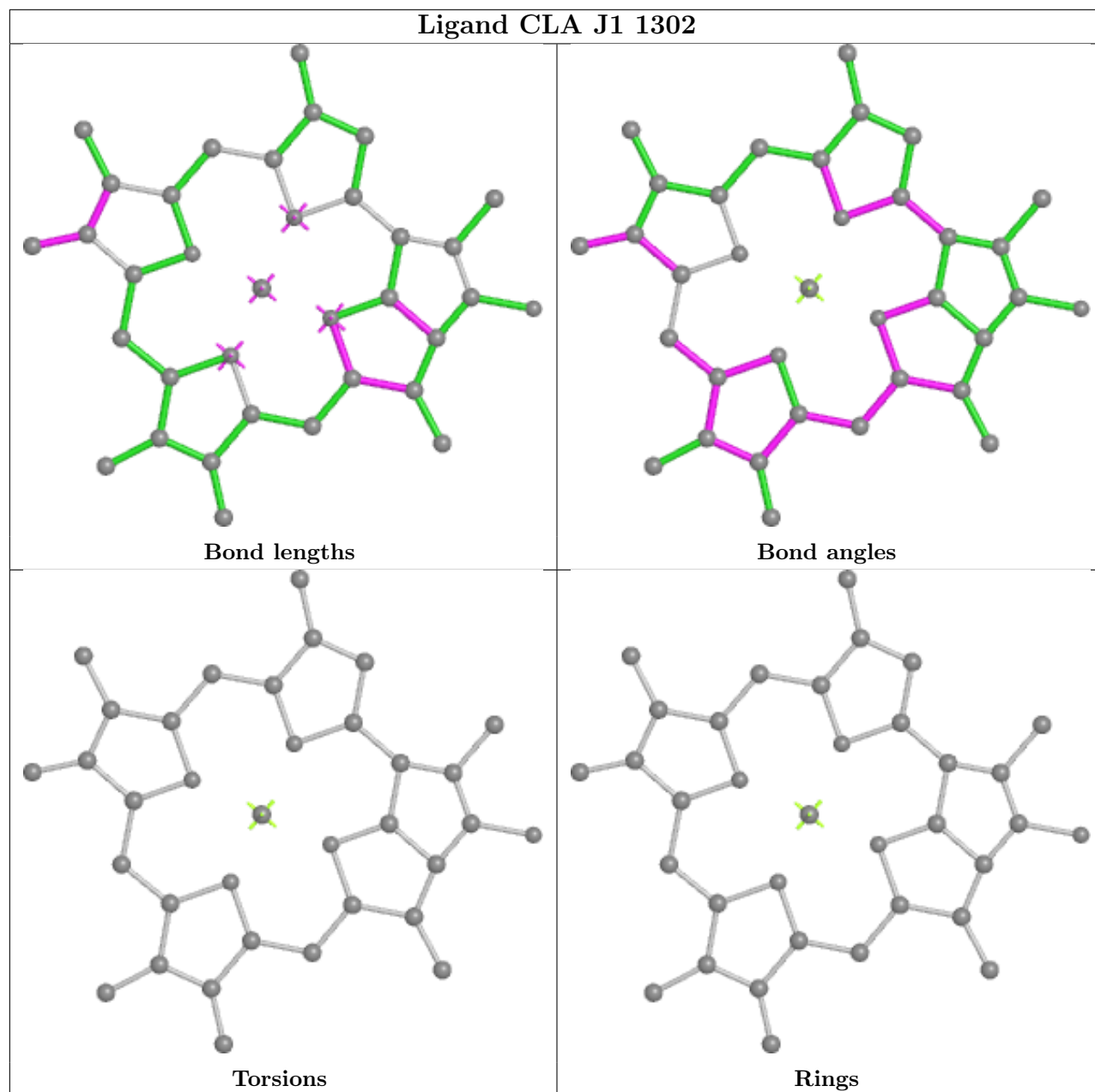
## Ligand CLA B2 826



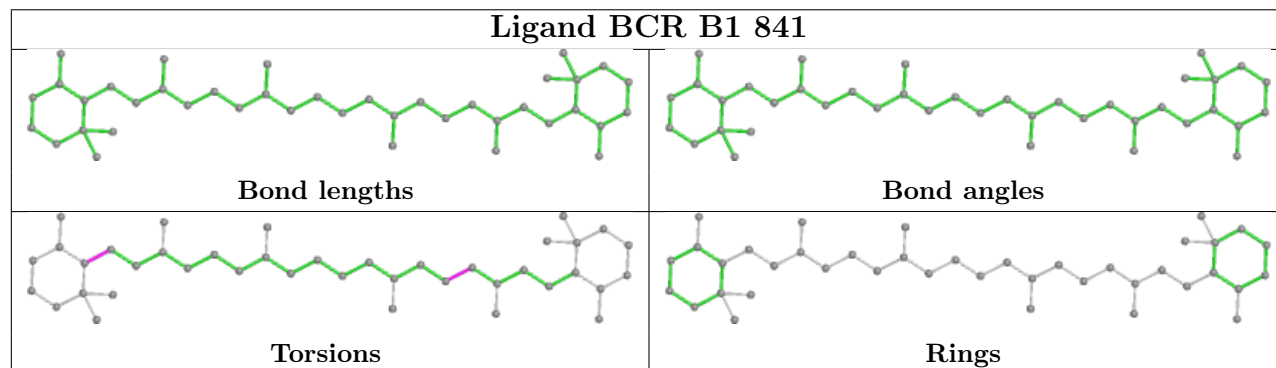
## Ligand BCR L2 1010

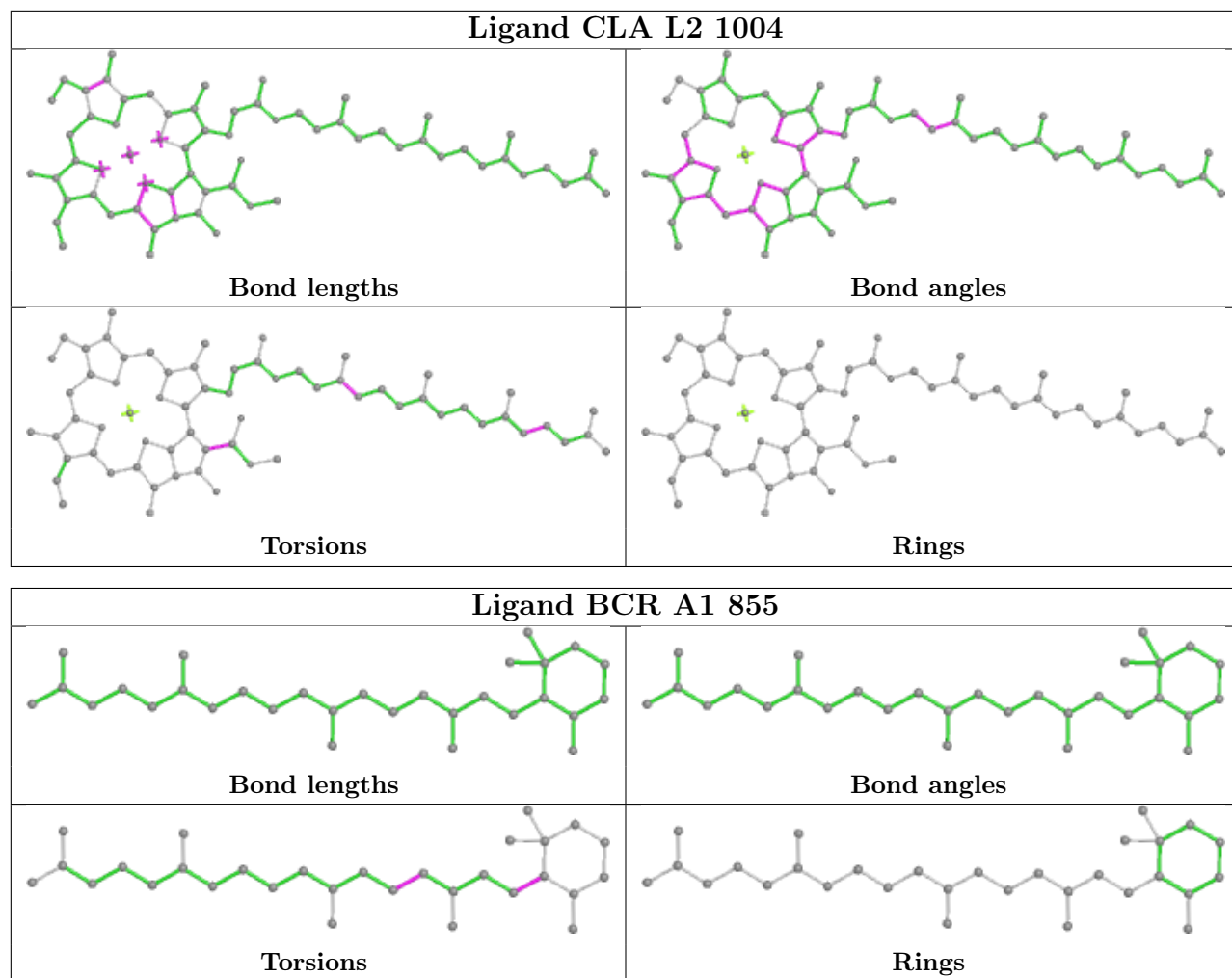


## Ligand CLA J1 1302

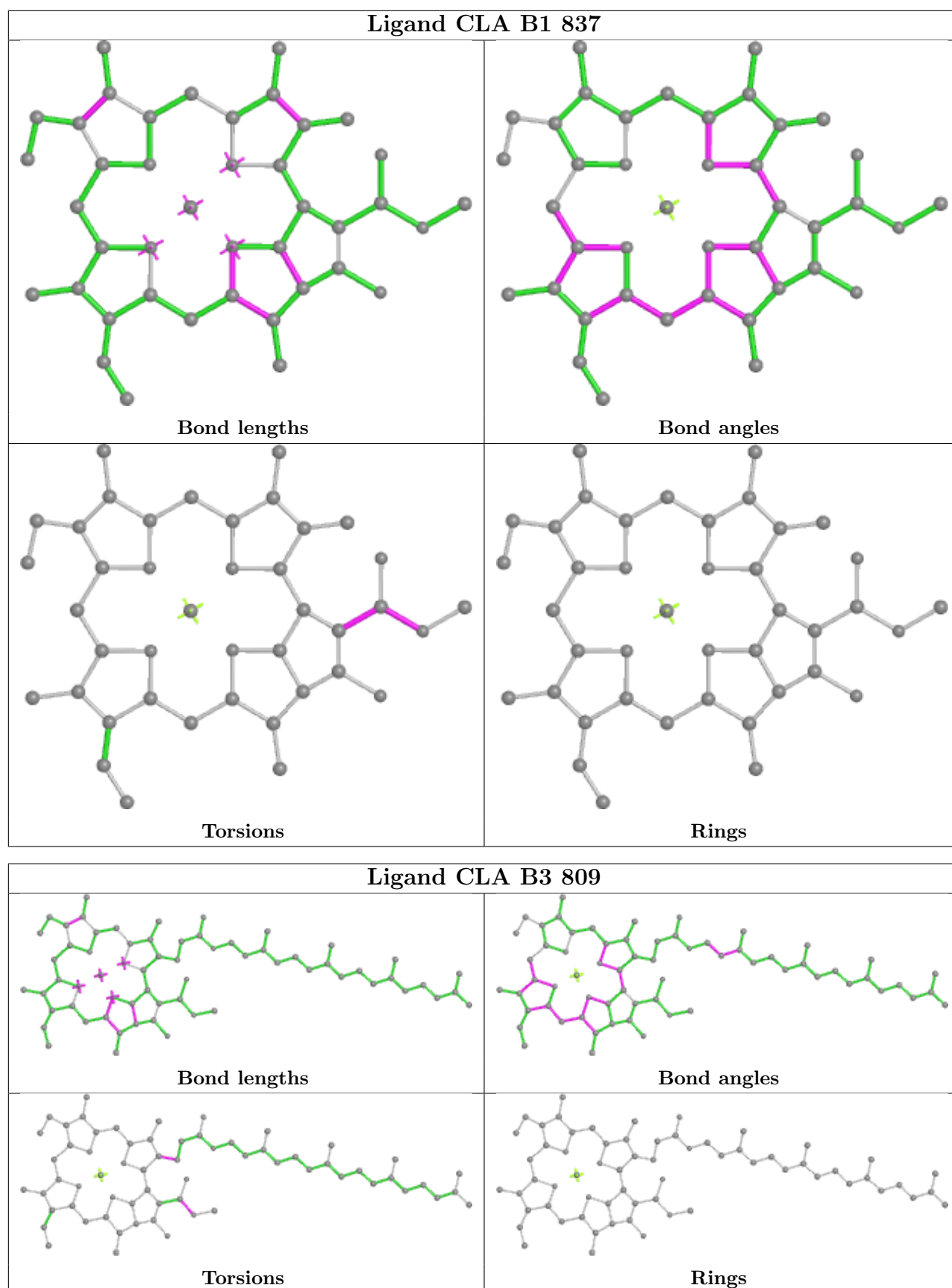


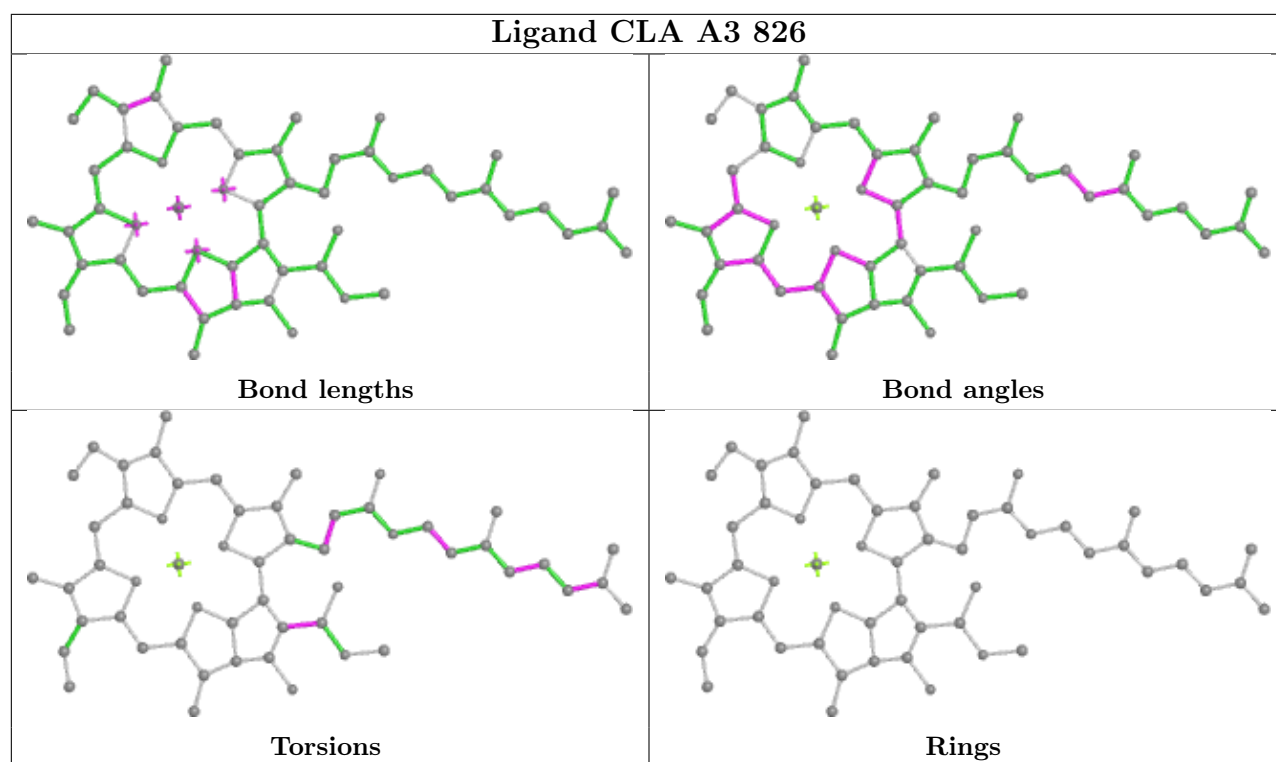
## Ligand BCR B1 841

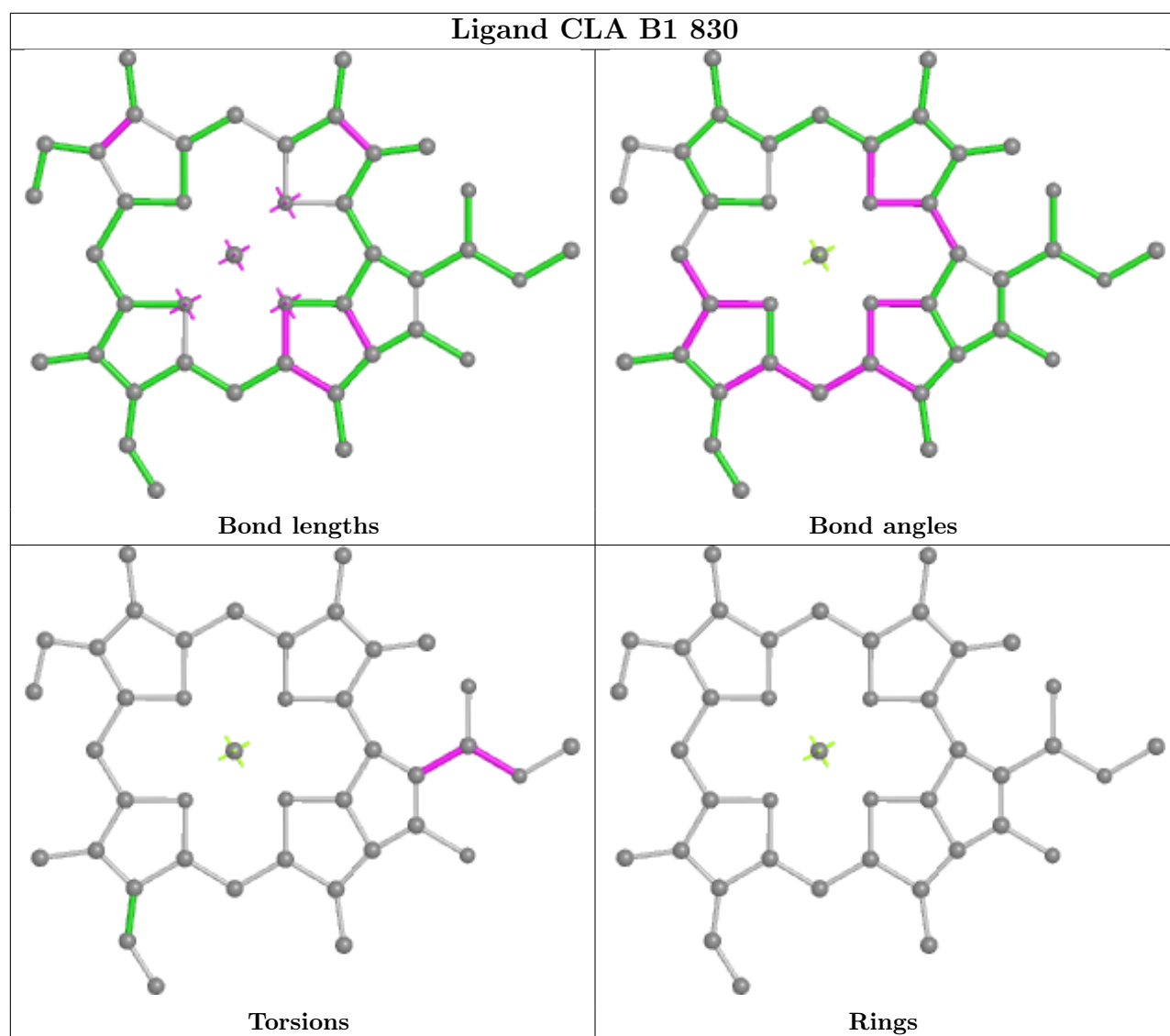


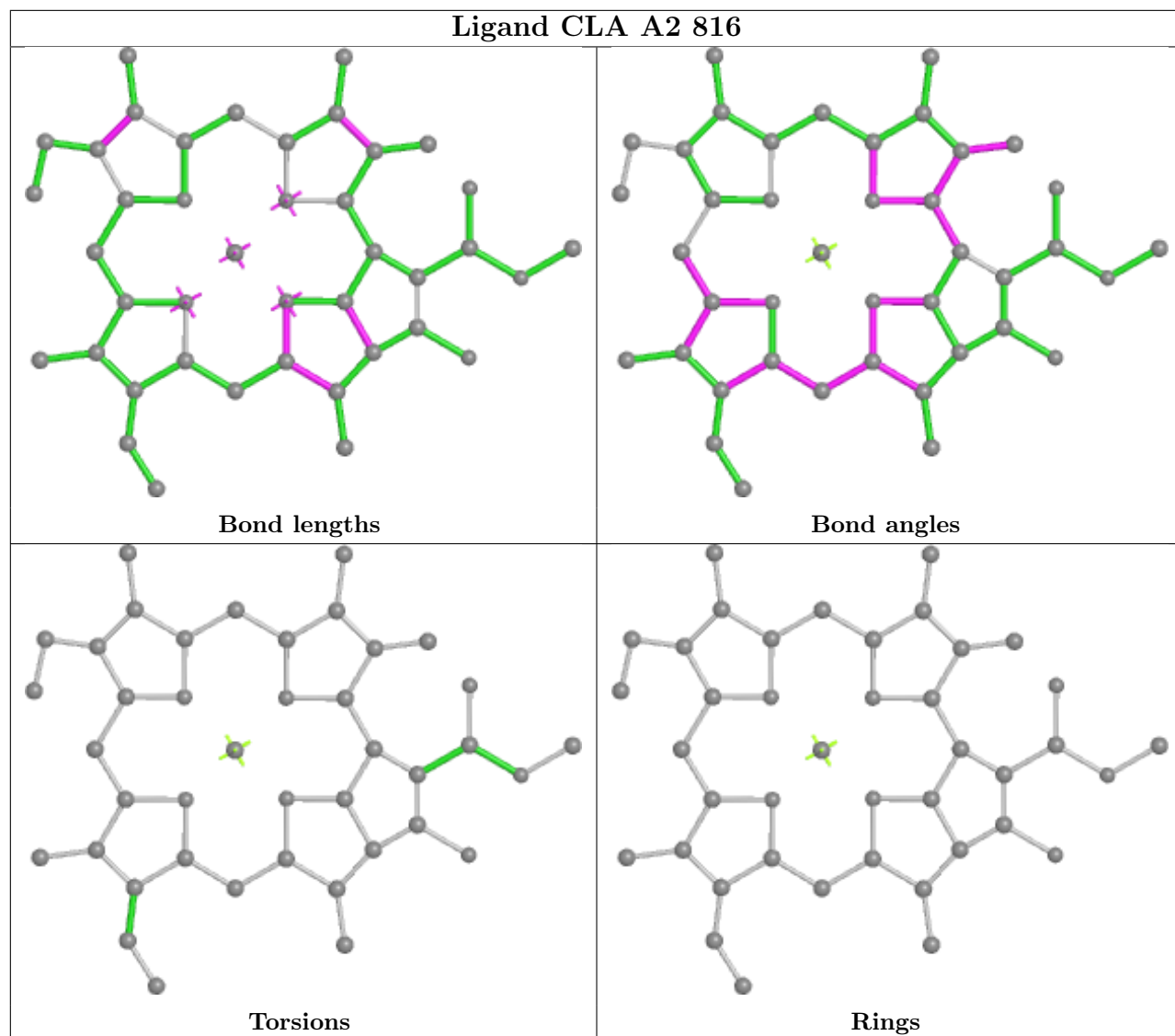


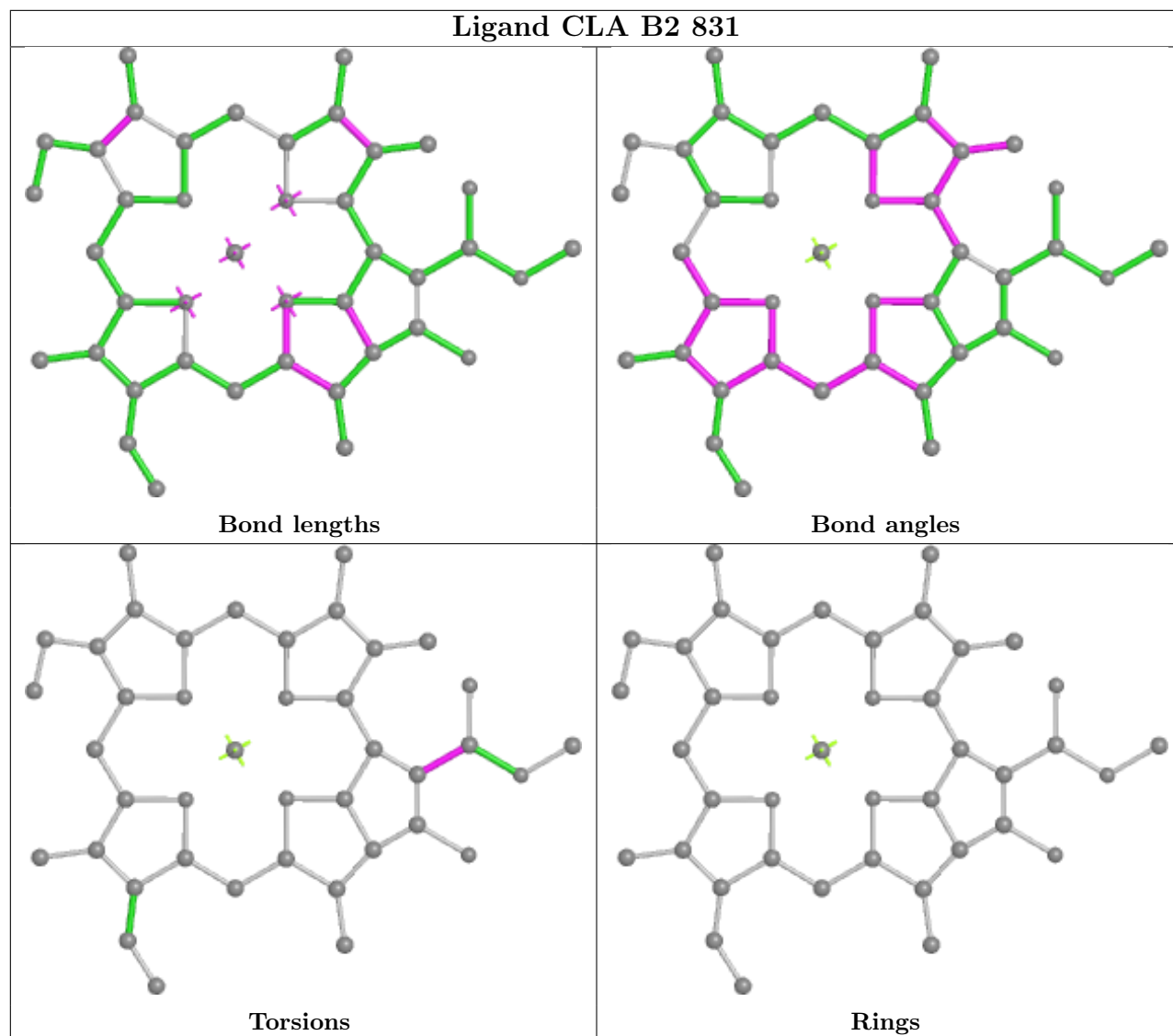


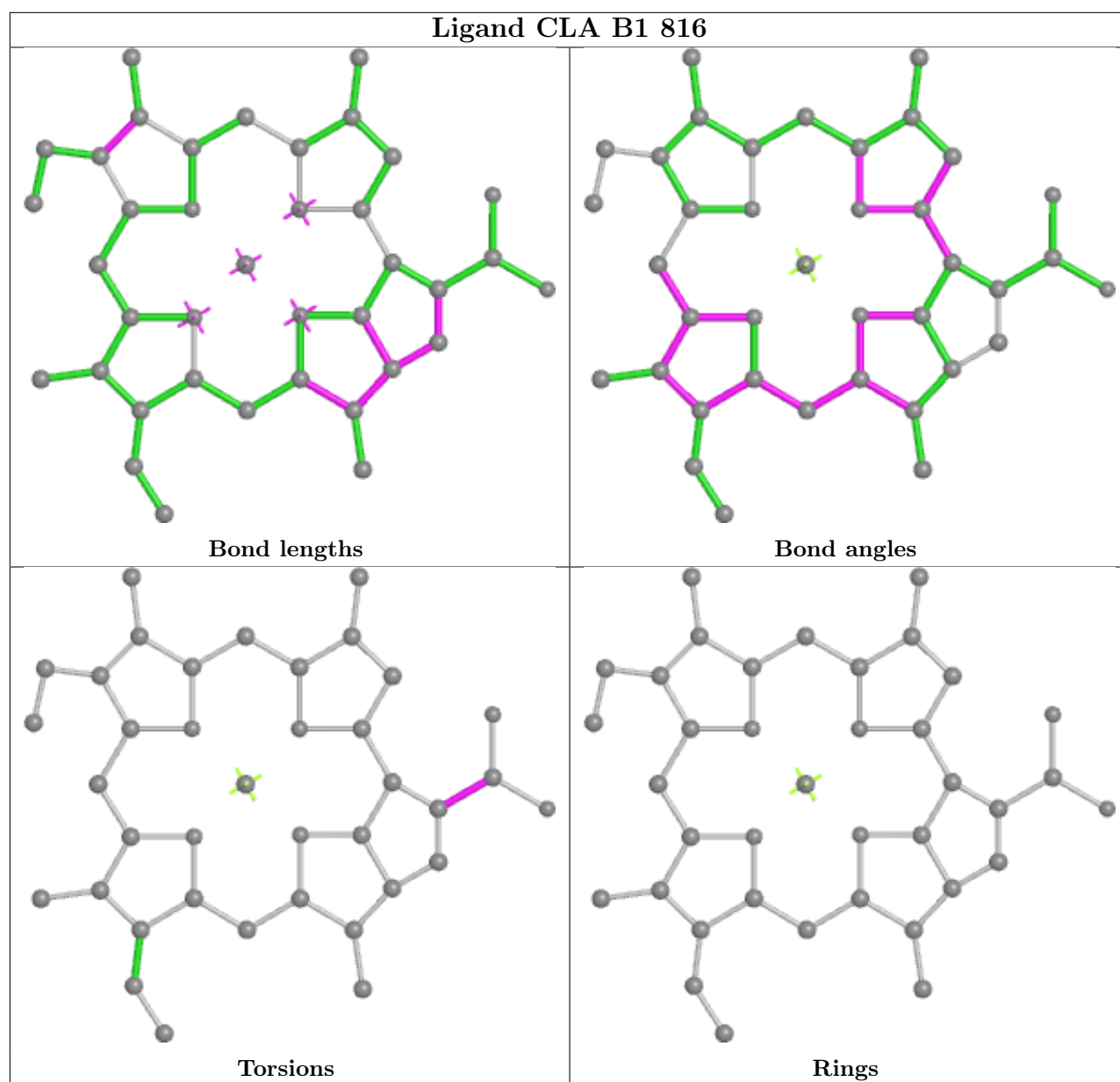




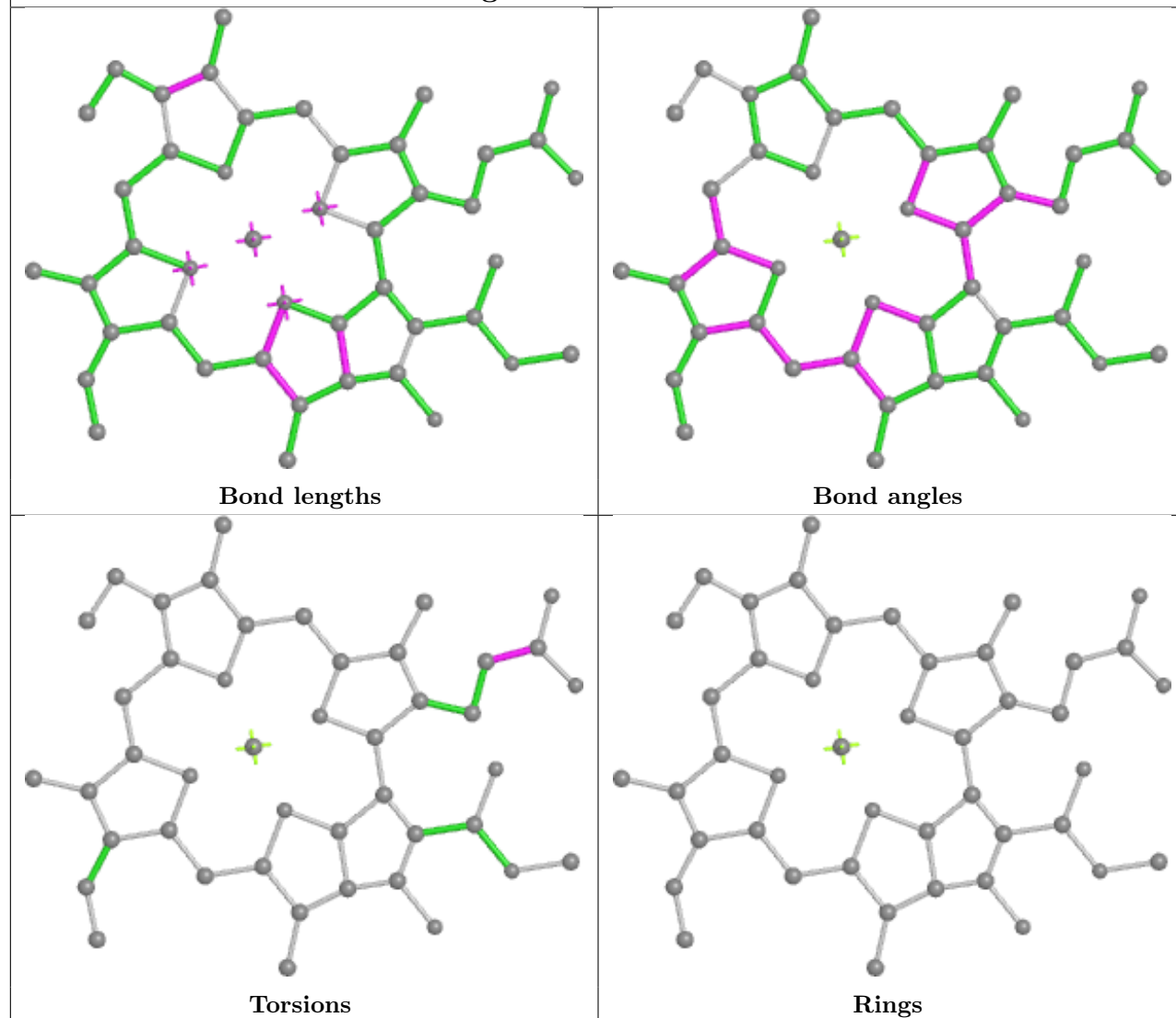




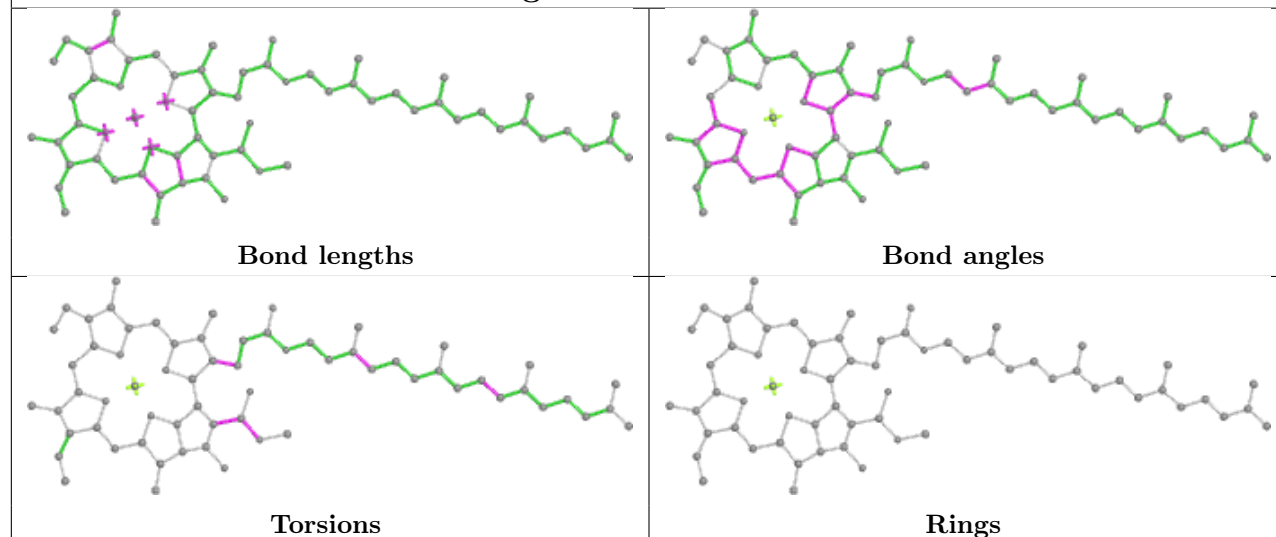


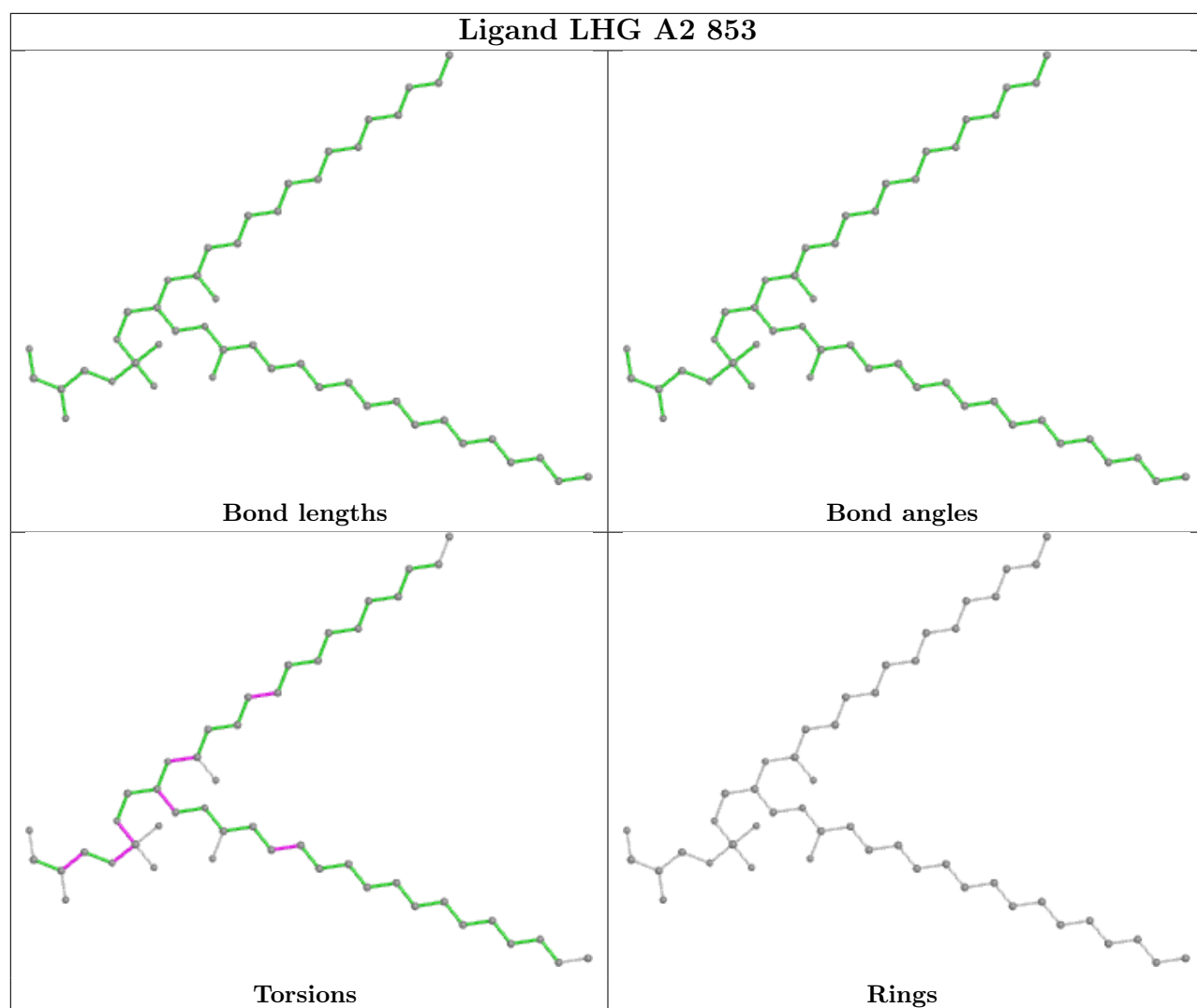


## Ligand CLA A3 822



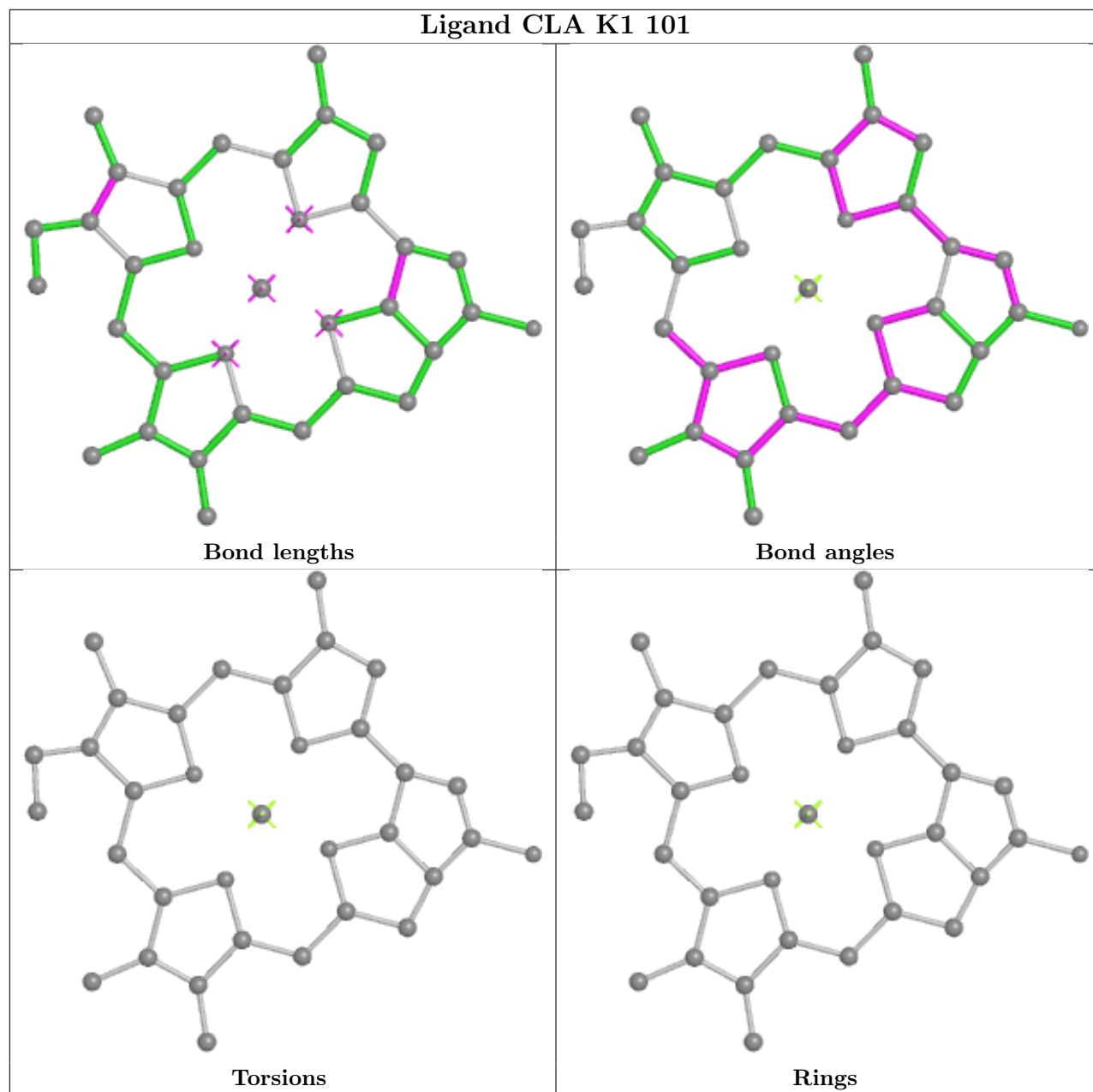
## Ligand CLA A3 830



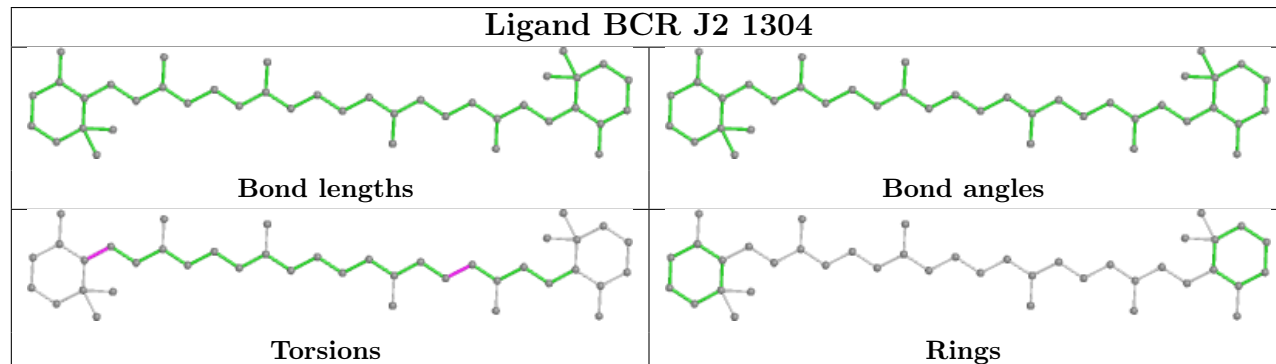


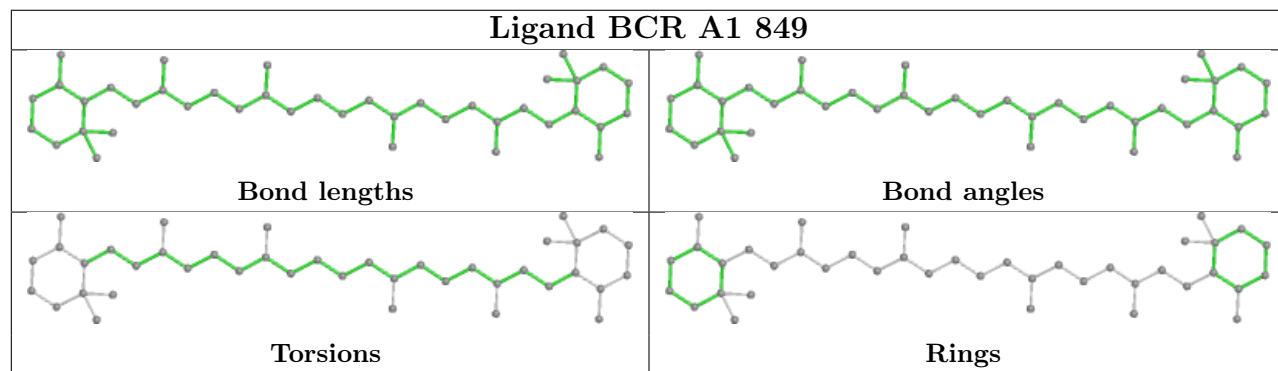
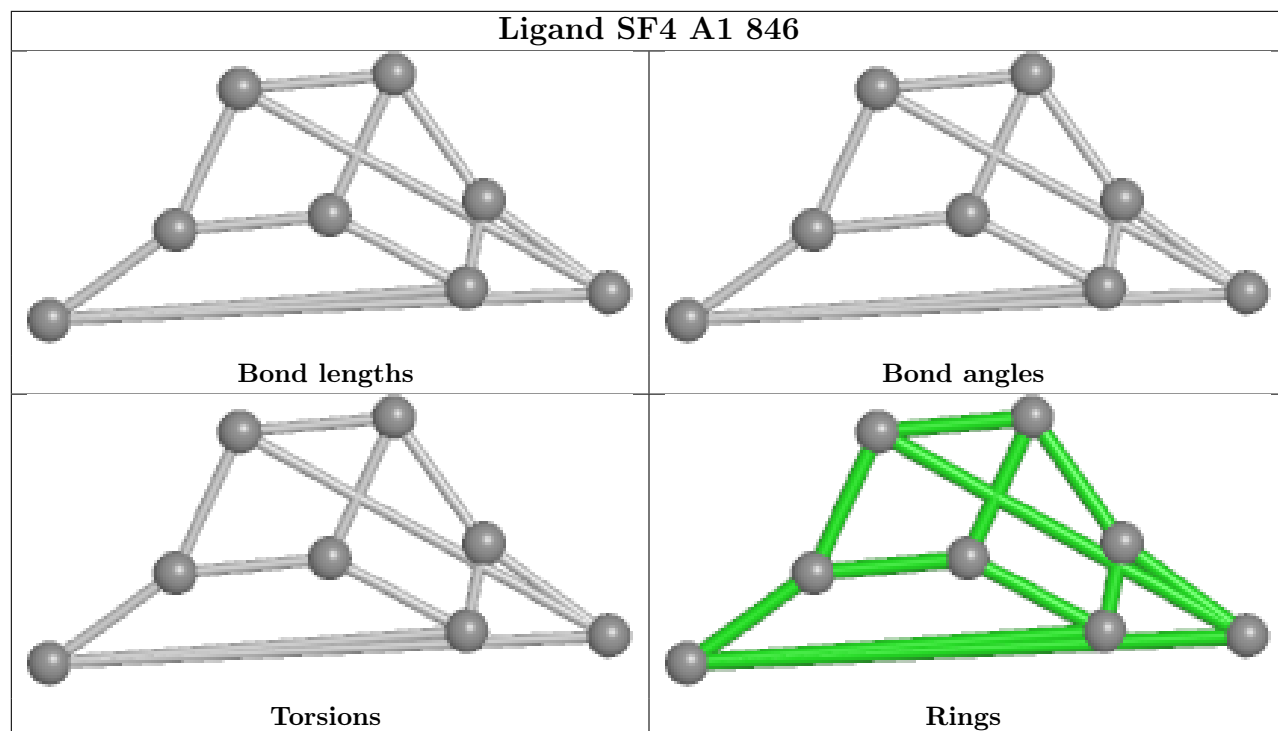


## Ligand CLA K1 101

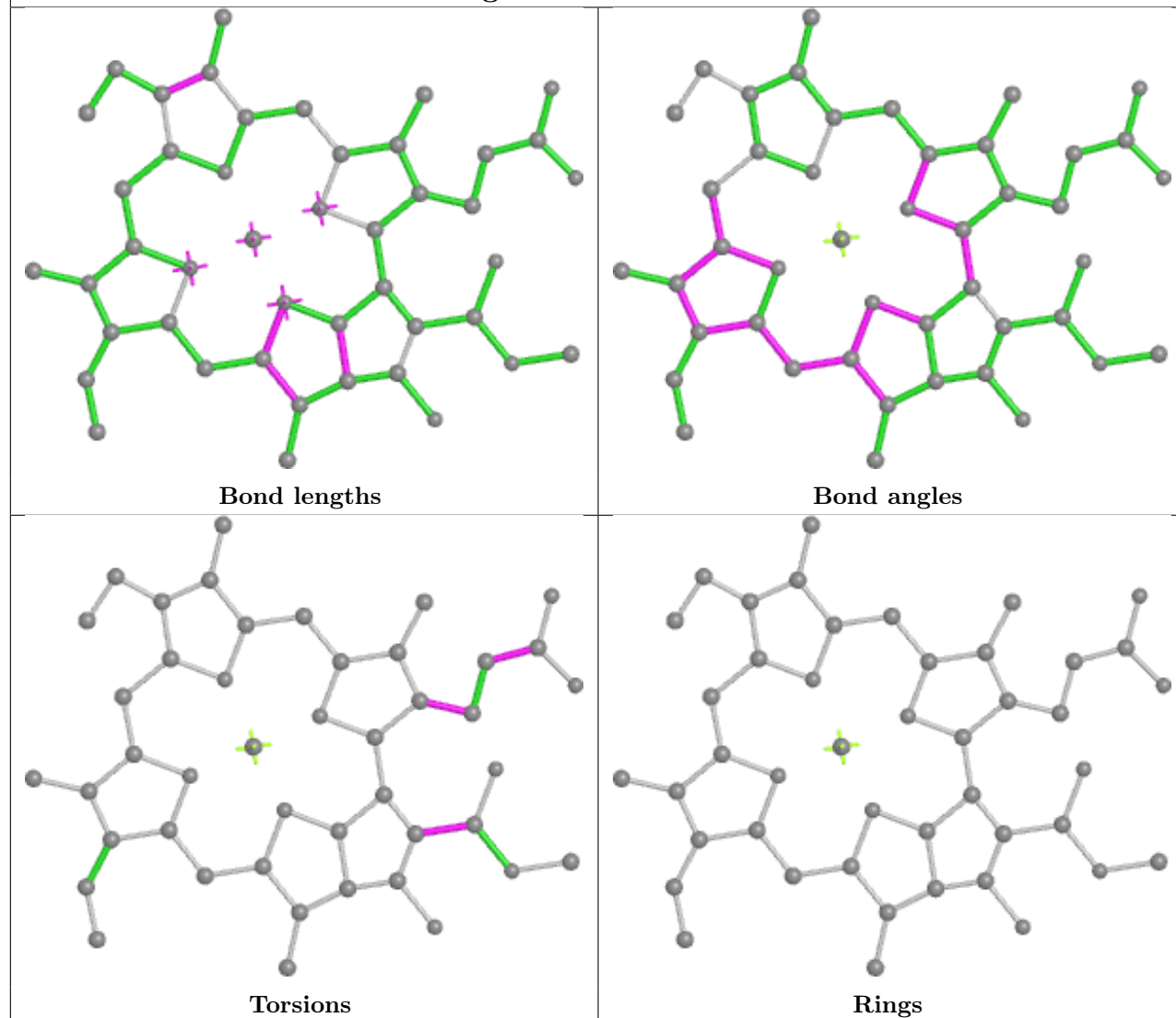


## Ligand BCR J2 1304

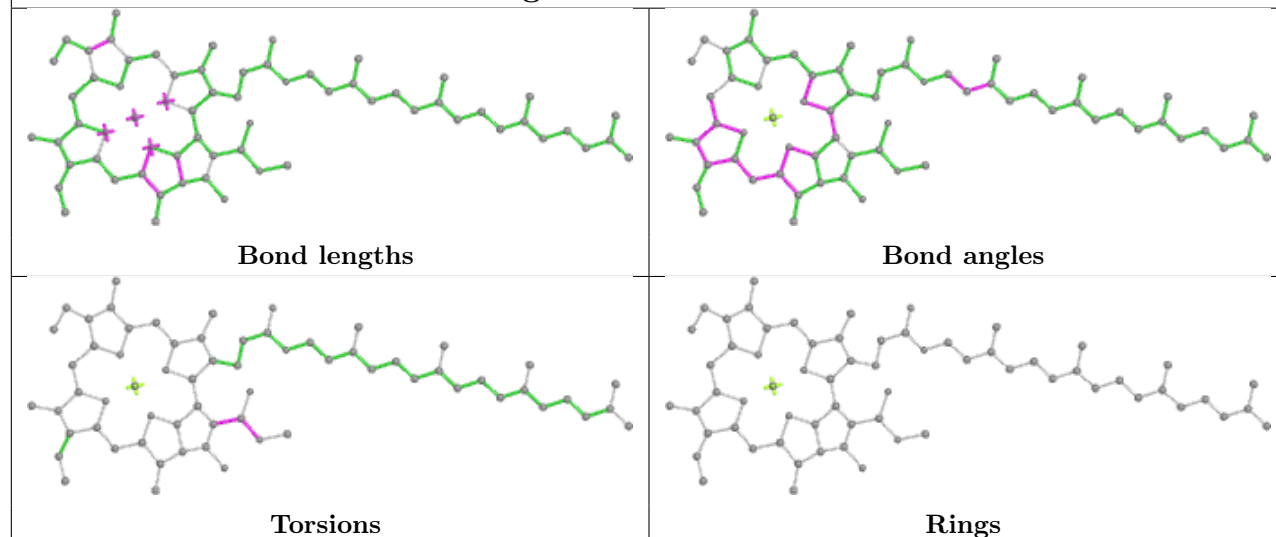




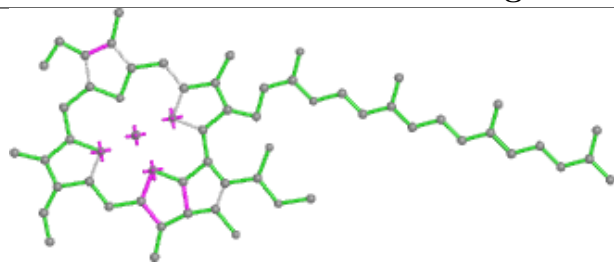
## Ligand CLA B1 819



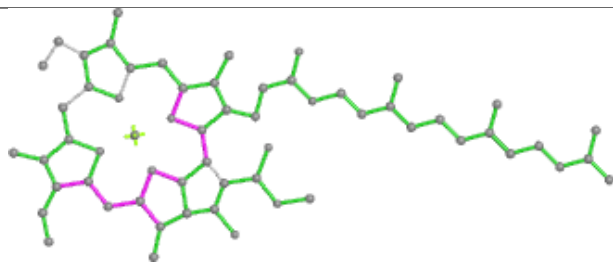
## Ligand CLA A1 834



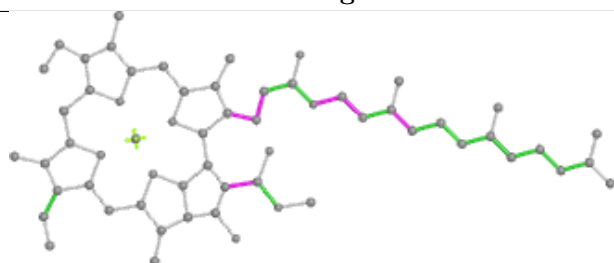
## Ligand CLA A2 827



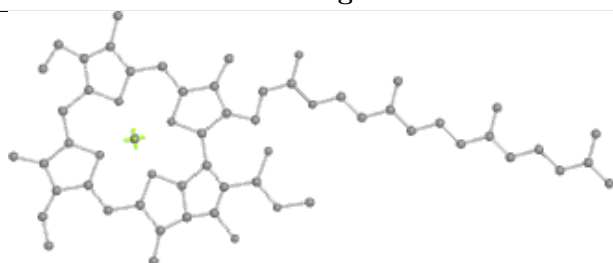
Bond lengths



Bond angles

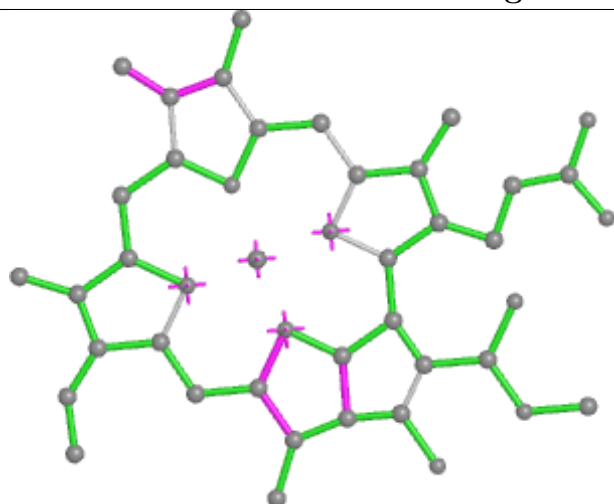


Torsions

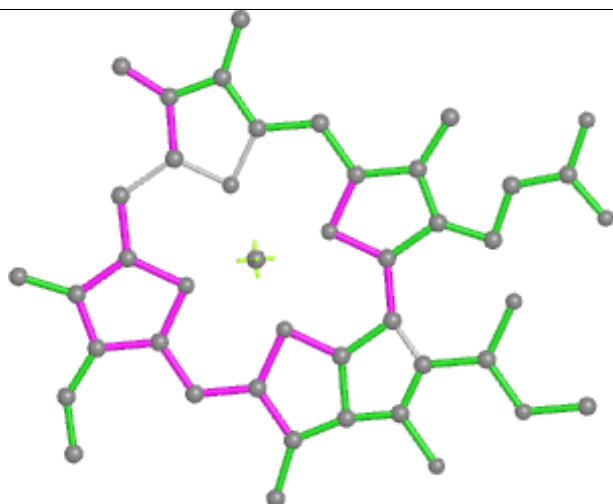


Rings

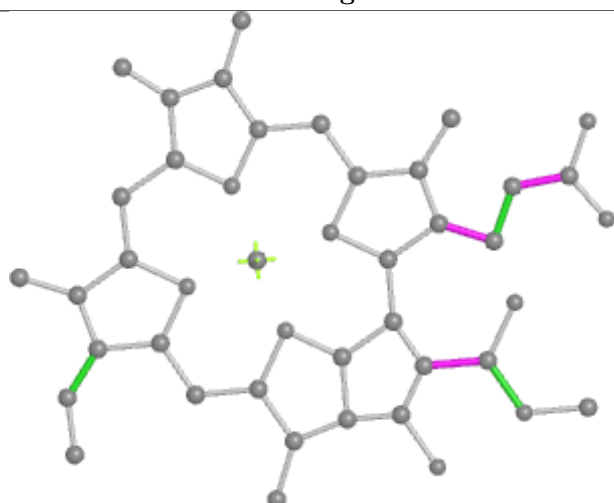
## Ligand CLA A2 813



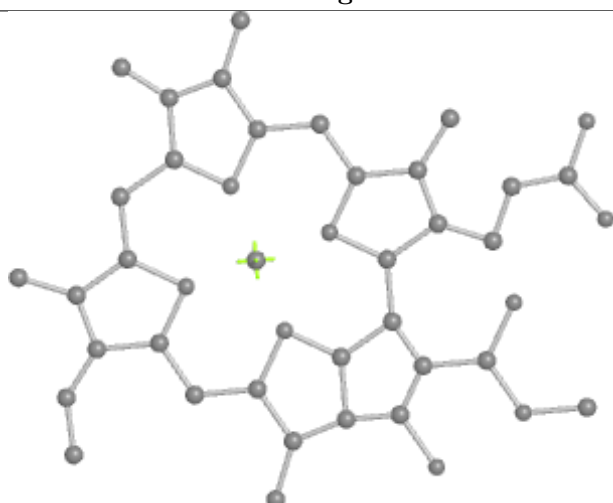
Bond lengths



Bond angles

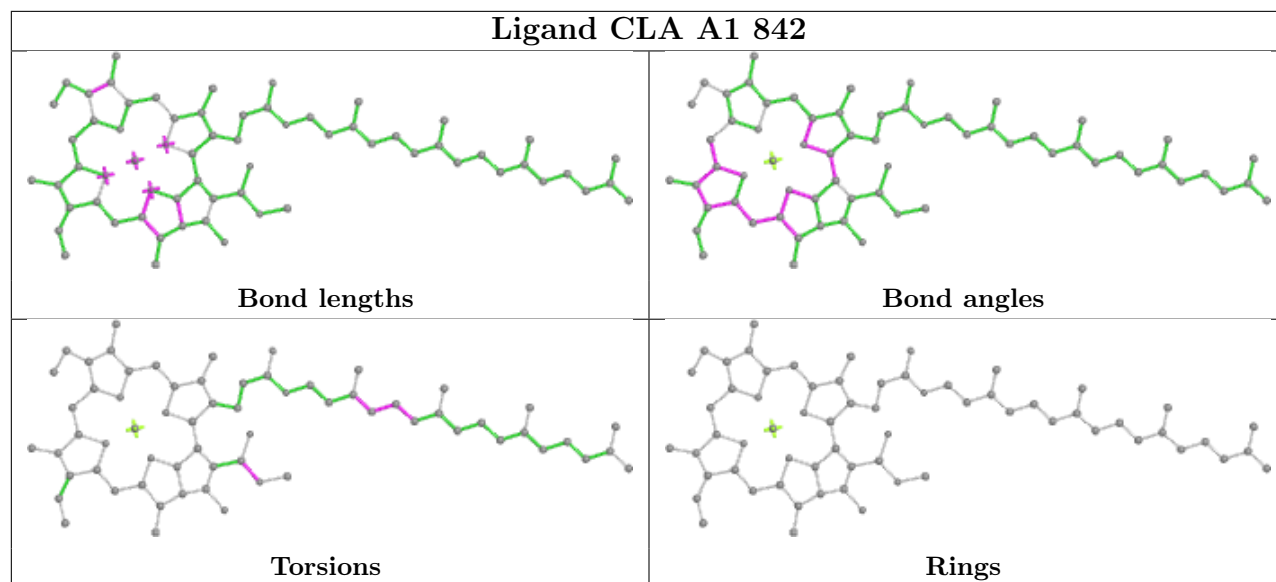


Torsions

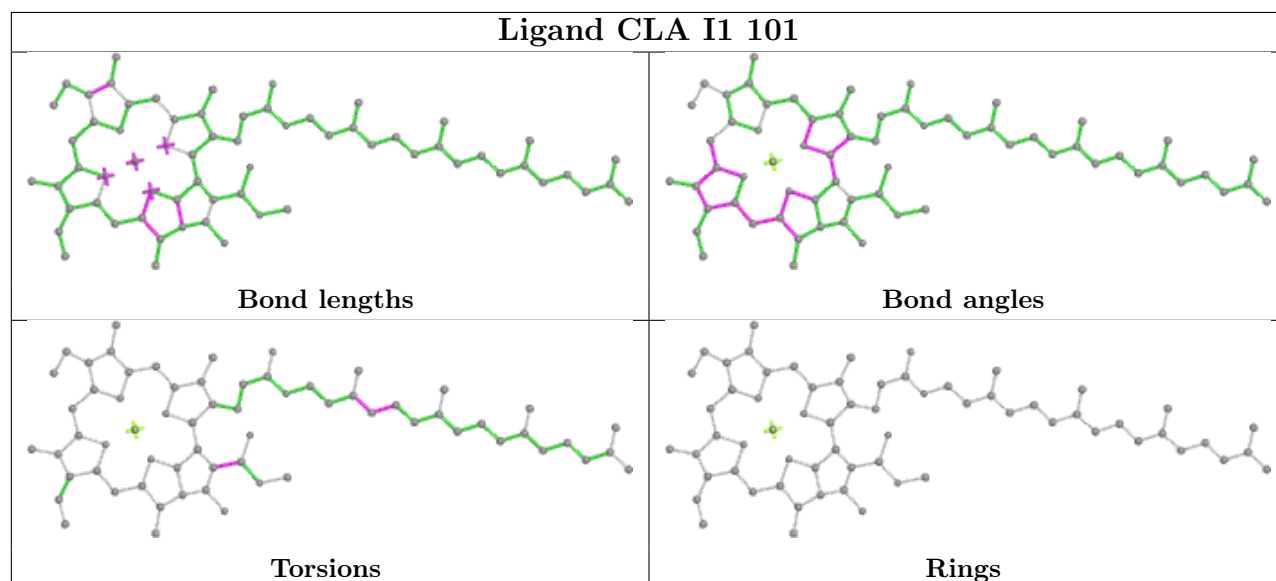


Rings

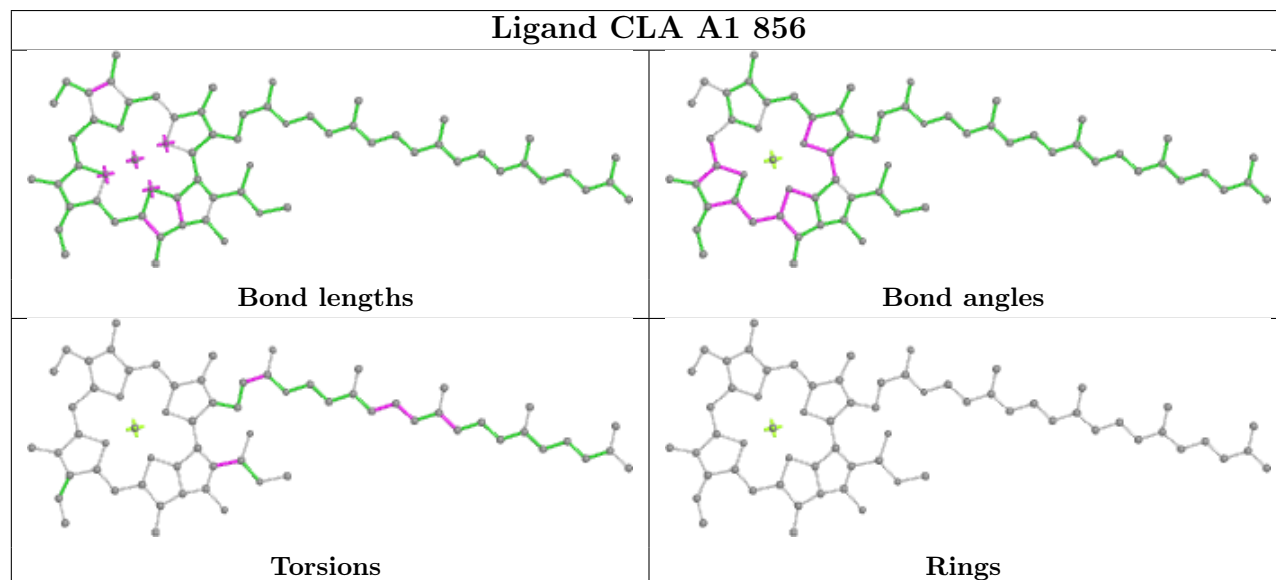
## Ligand CLA A1 842



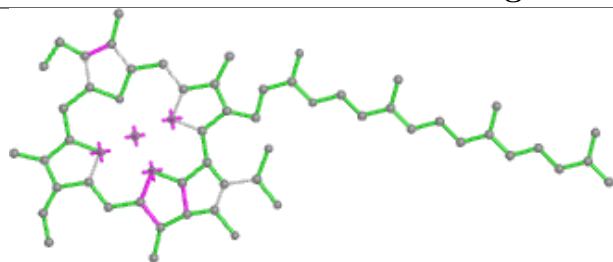
## Ligand CLA I1 101



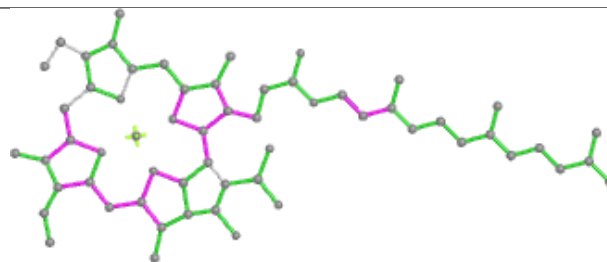
## Ligand CLA A1 856



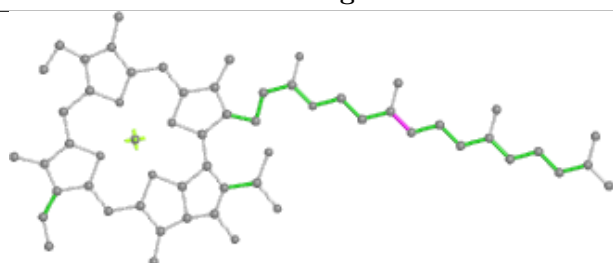
## Ligand CLA A3 819



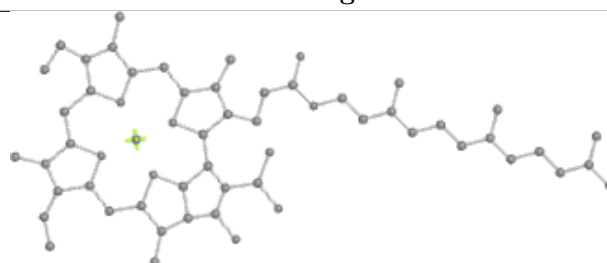
Bond lengths



Bond angles

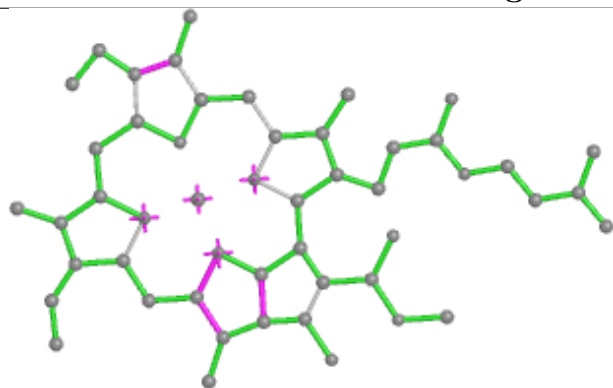


Torsions

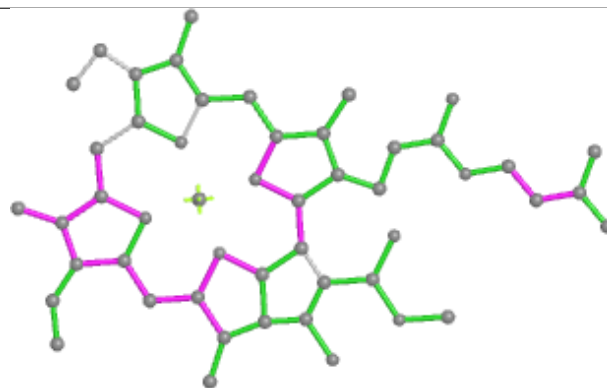


Rings

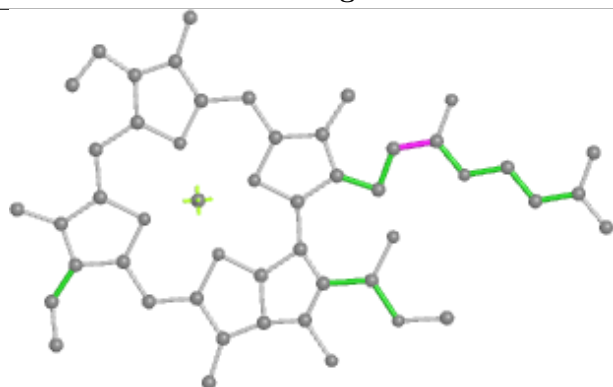
## Ligand CLA B3 806



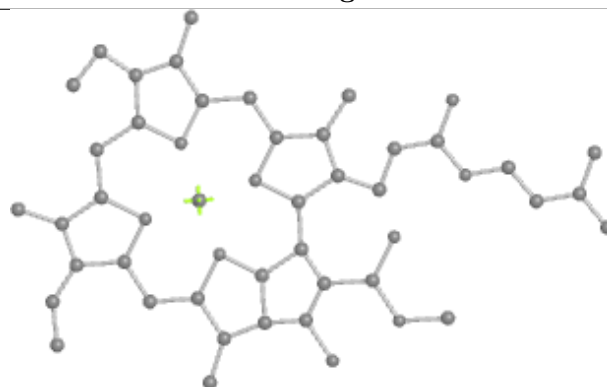
Bond lengths



Bond angles

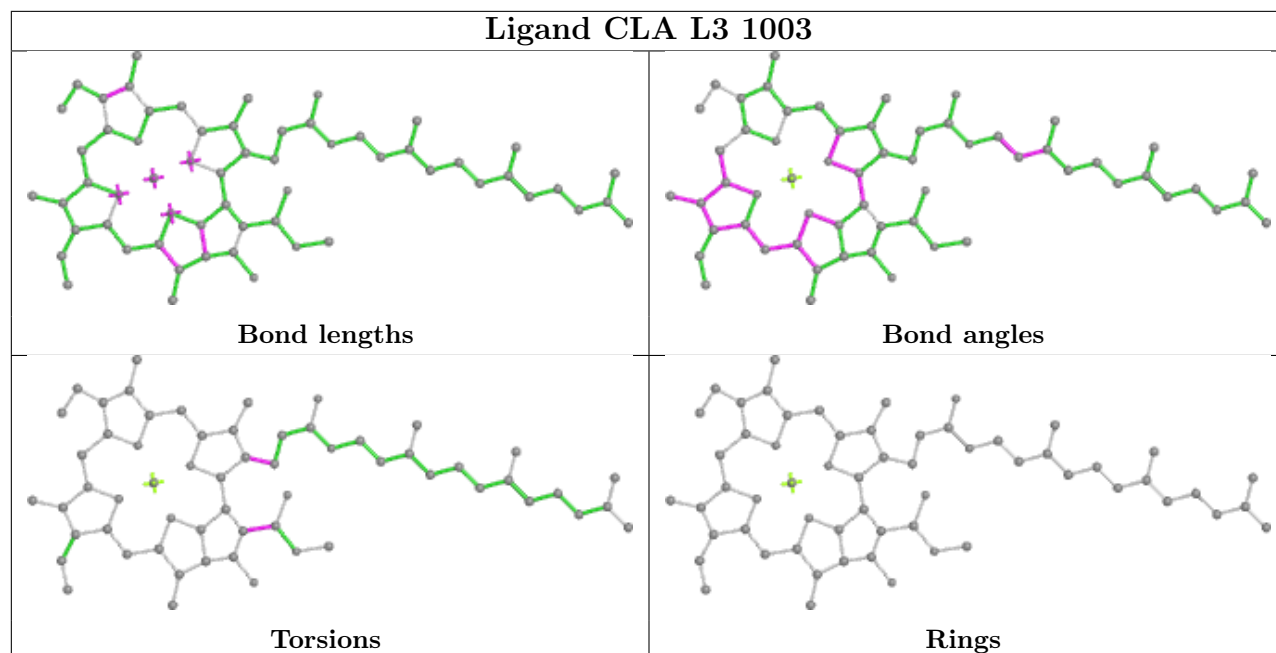


Torsions

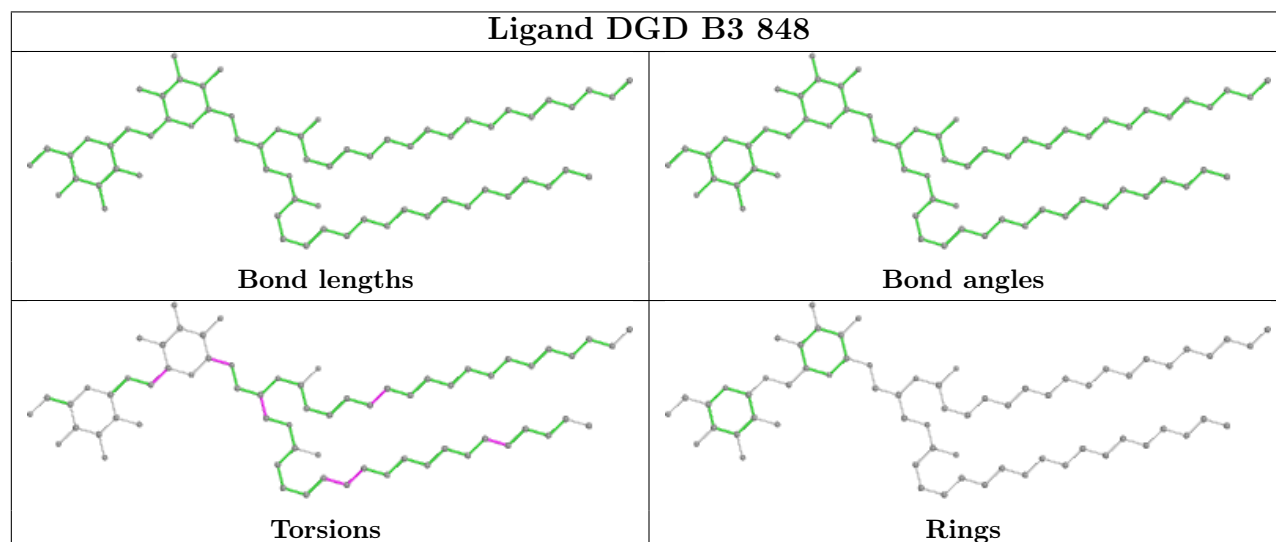


Rings

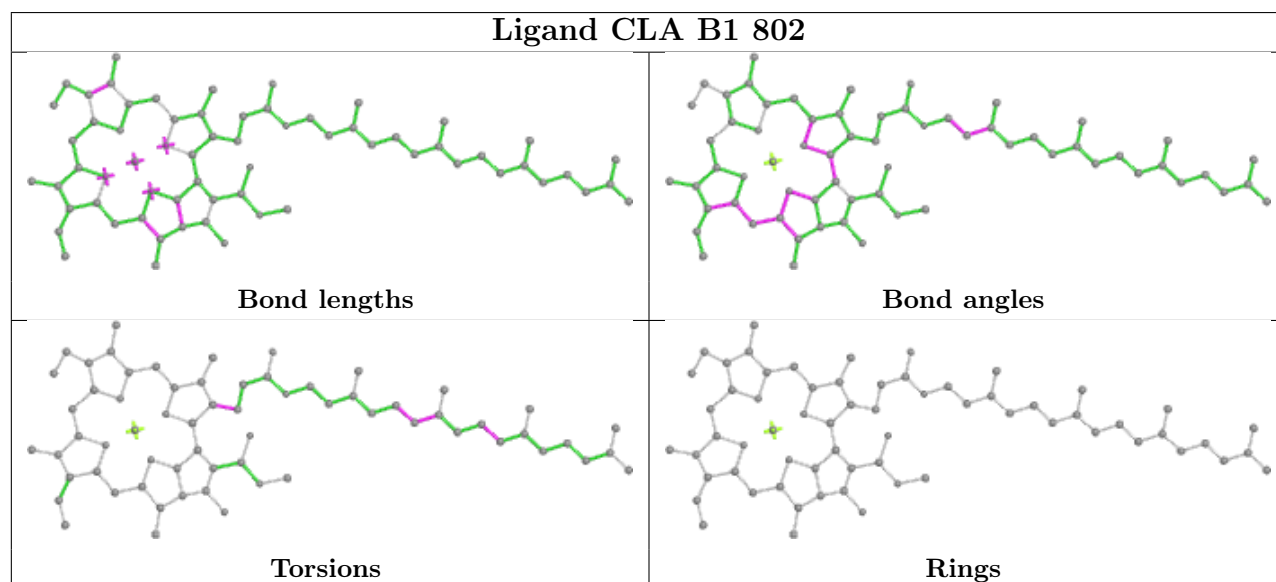
## Ligand CLA L3 1003

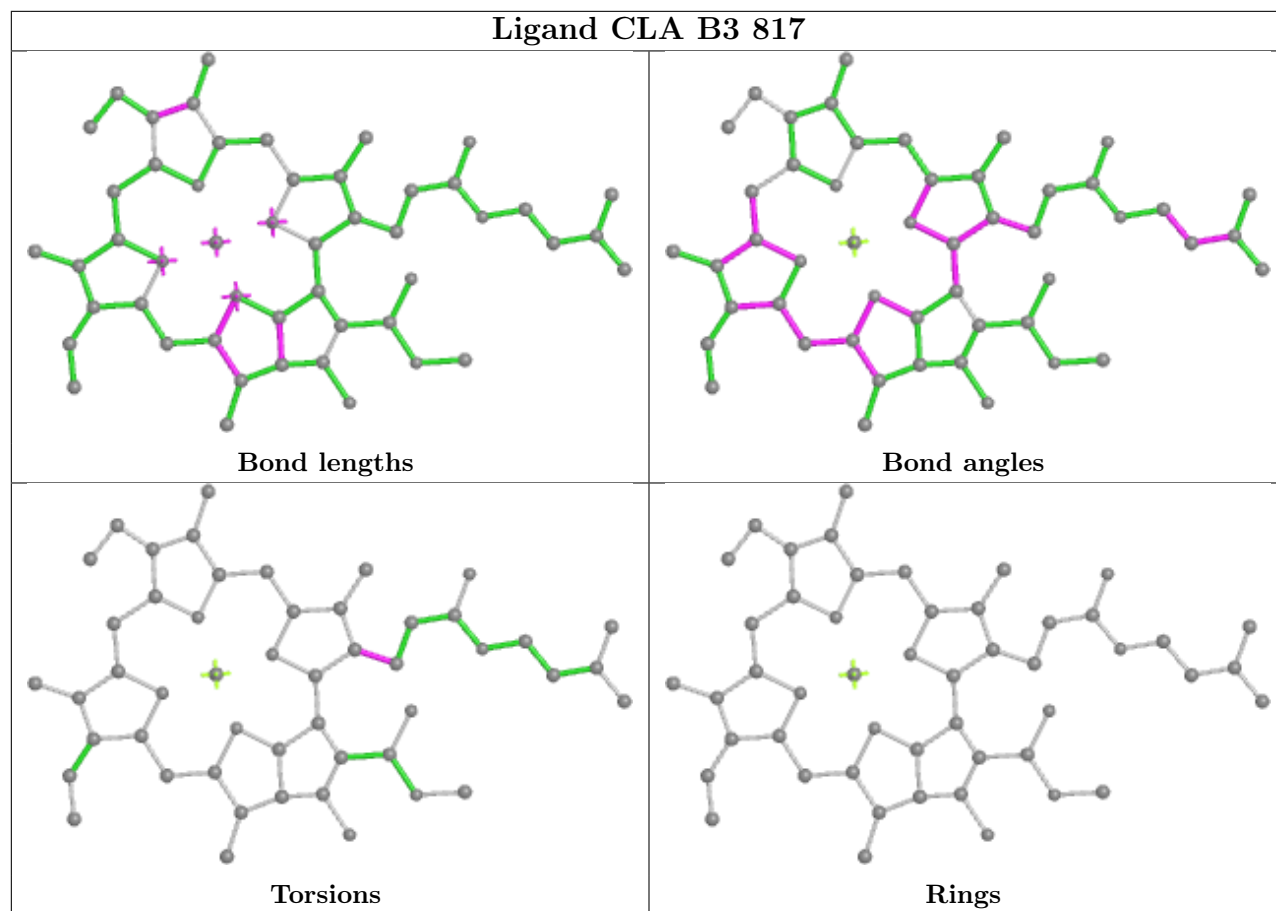
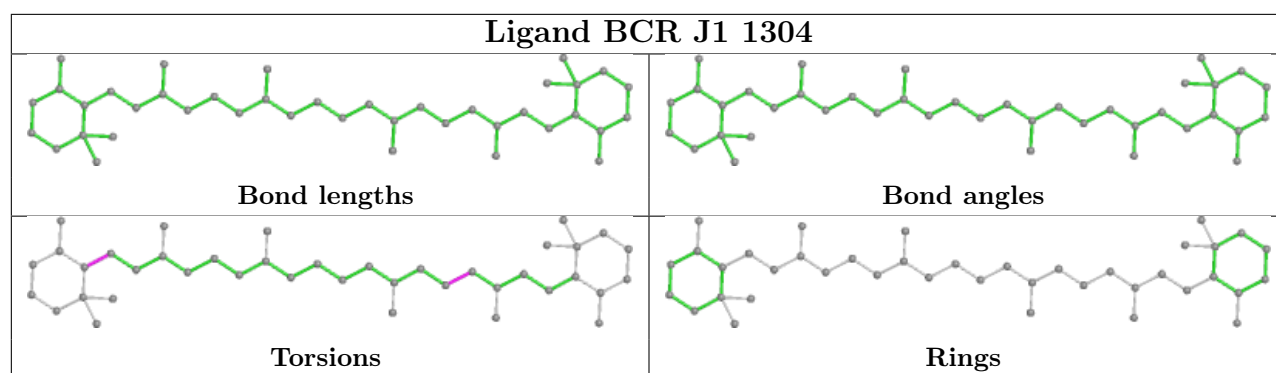


## Ligand DGD B3 848



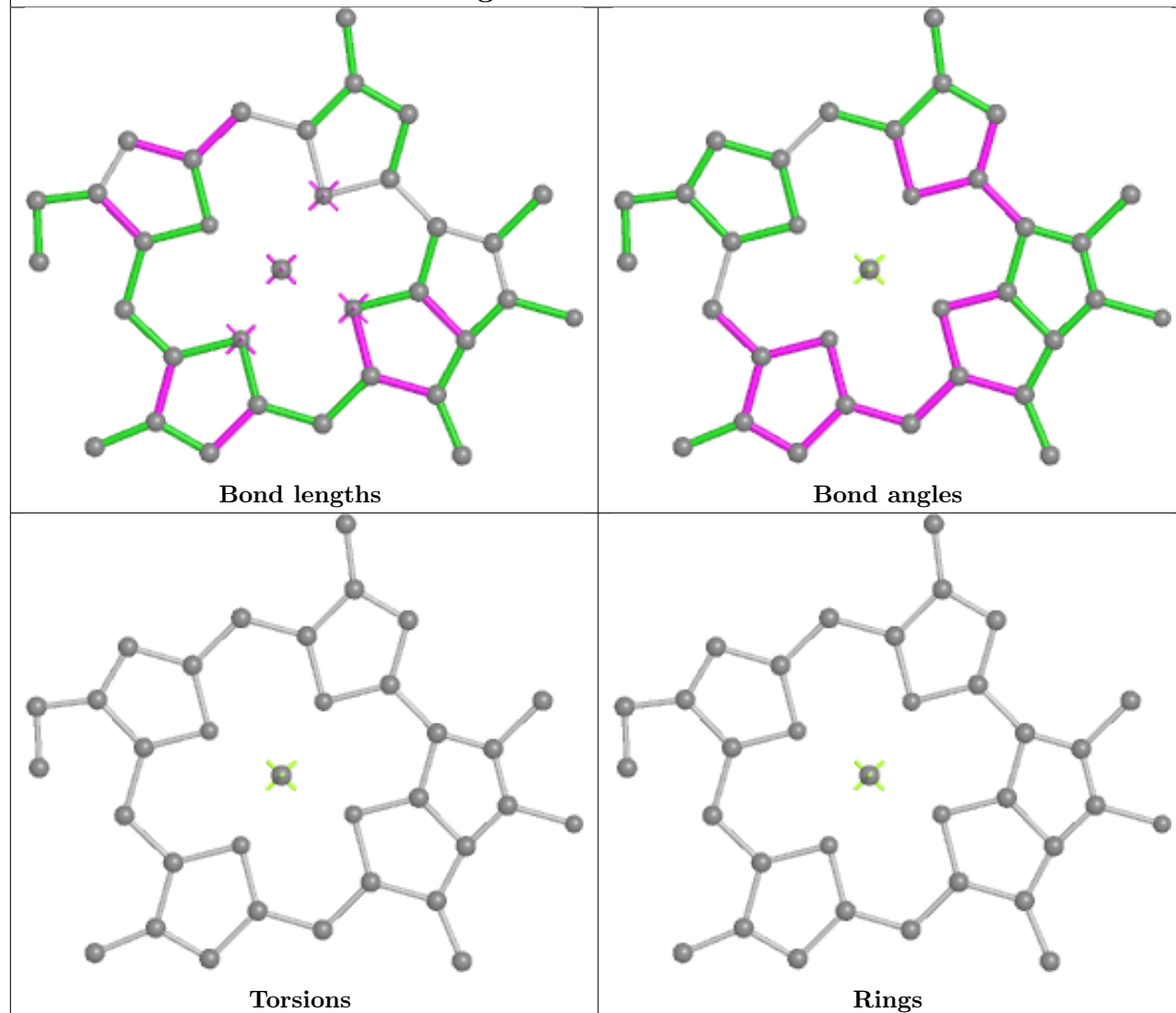
## Ligand CLA B1 802



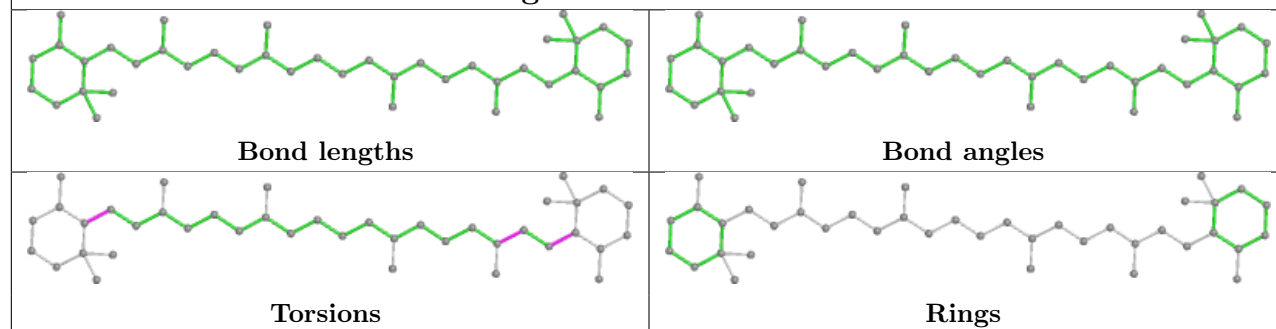


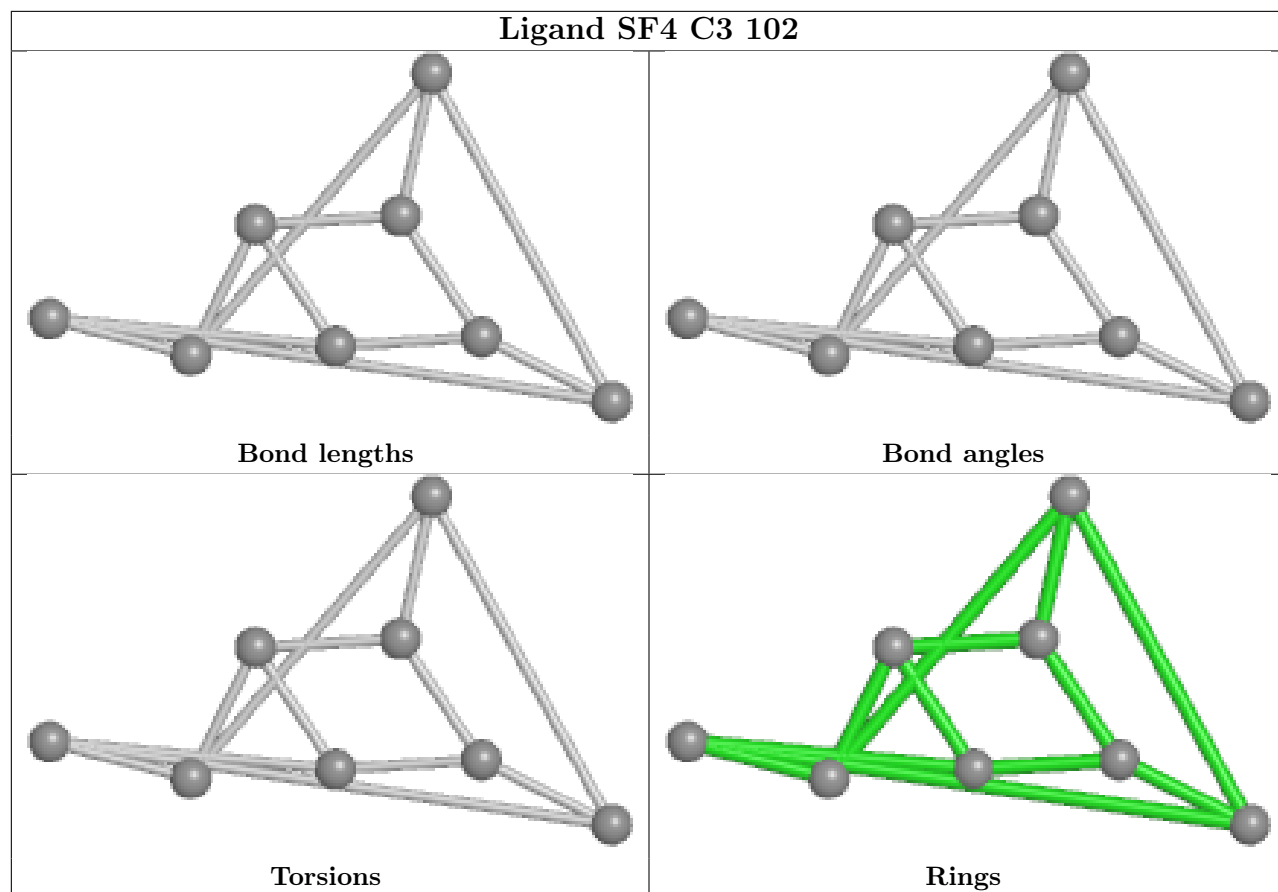


## Ligand CLA J1 1307

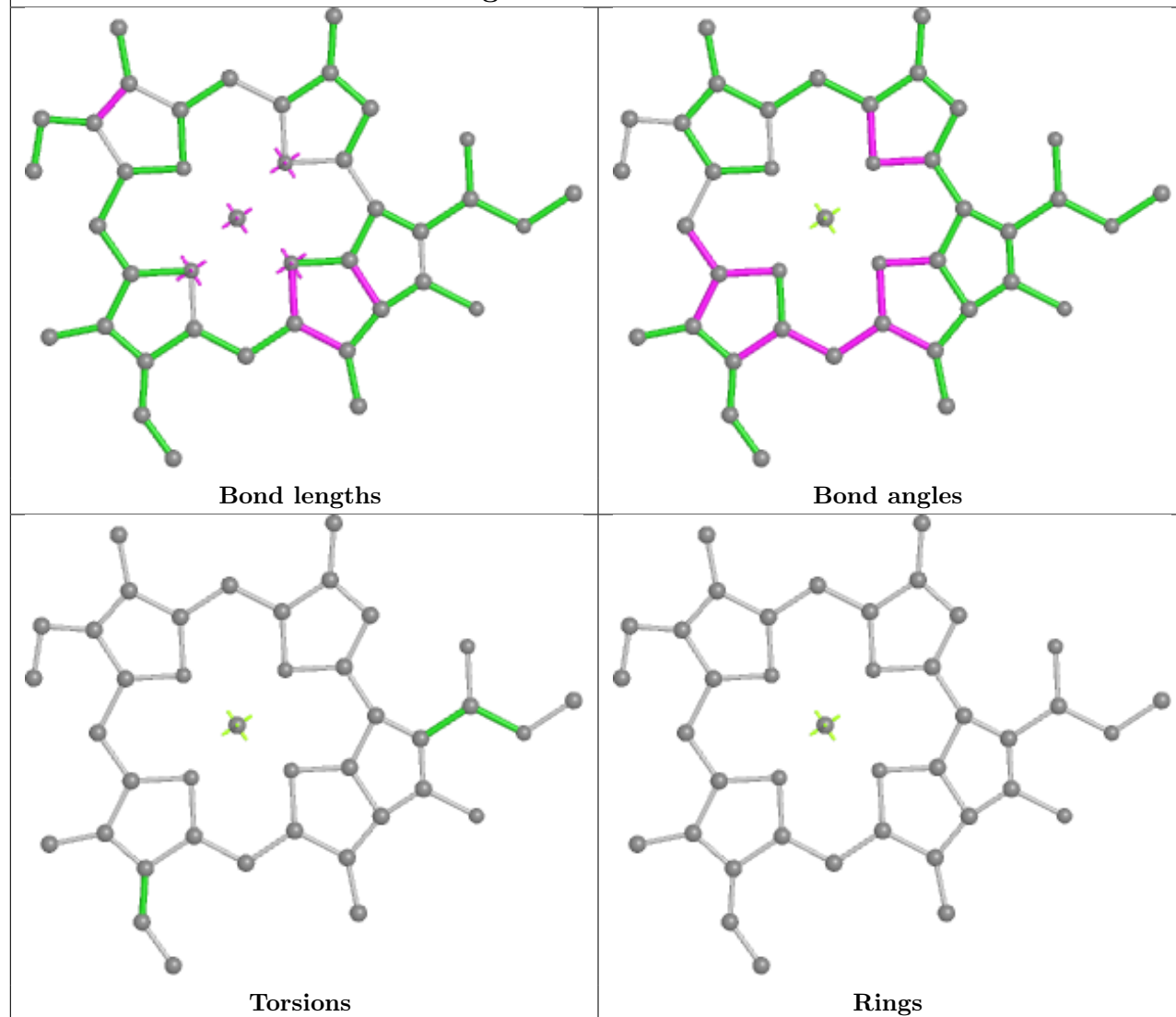


## Ligand BCR B1 847

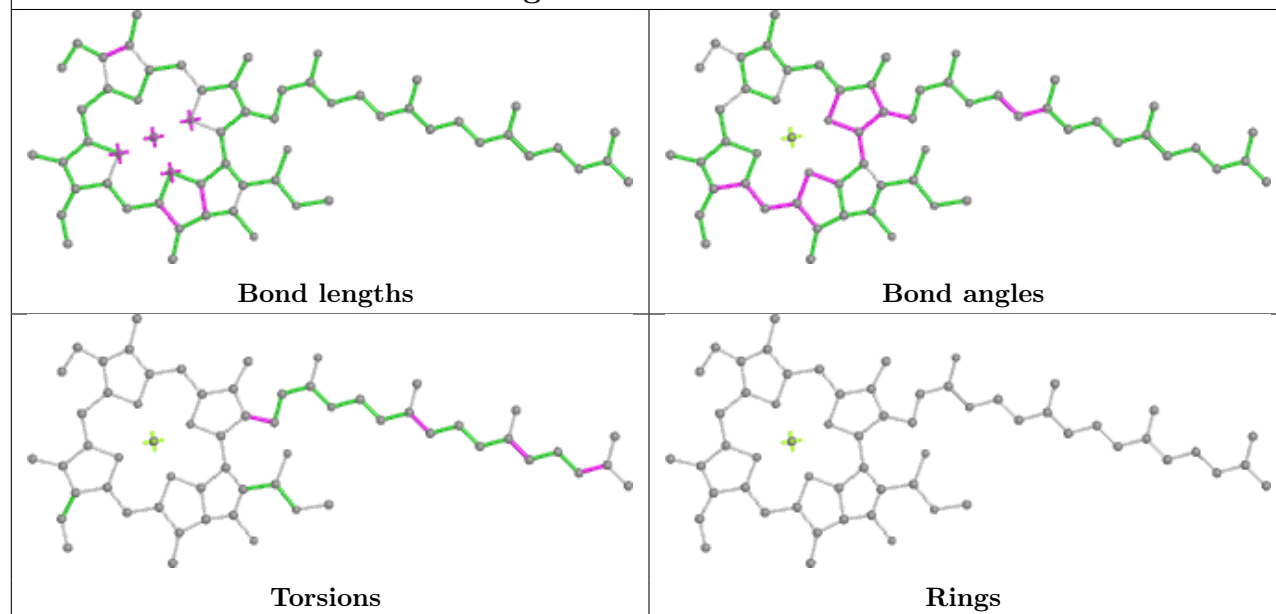


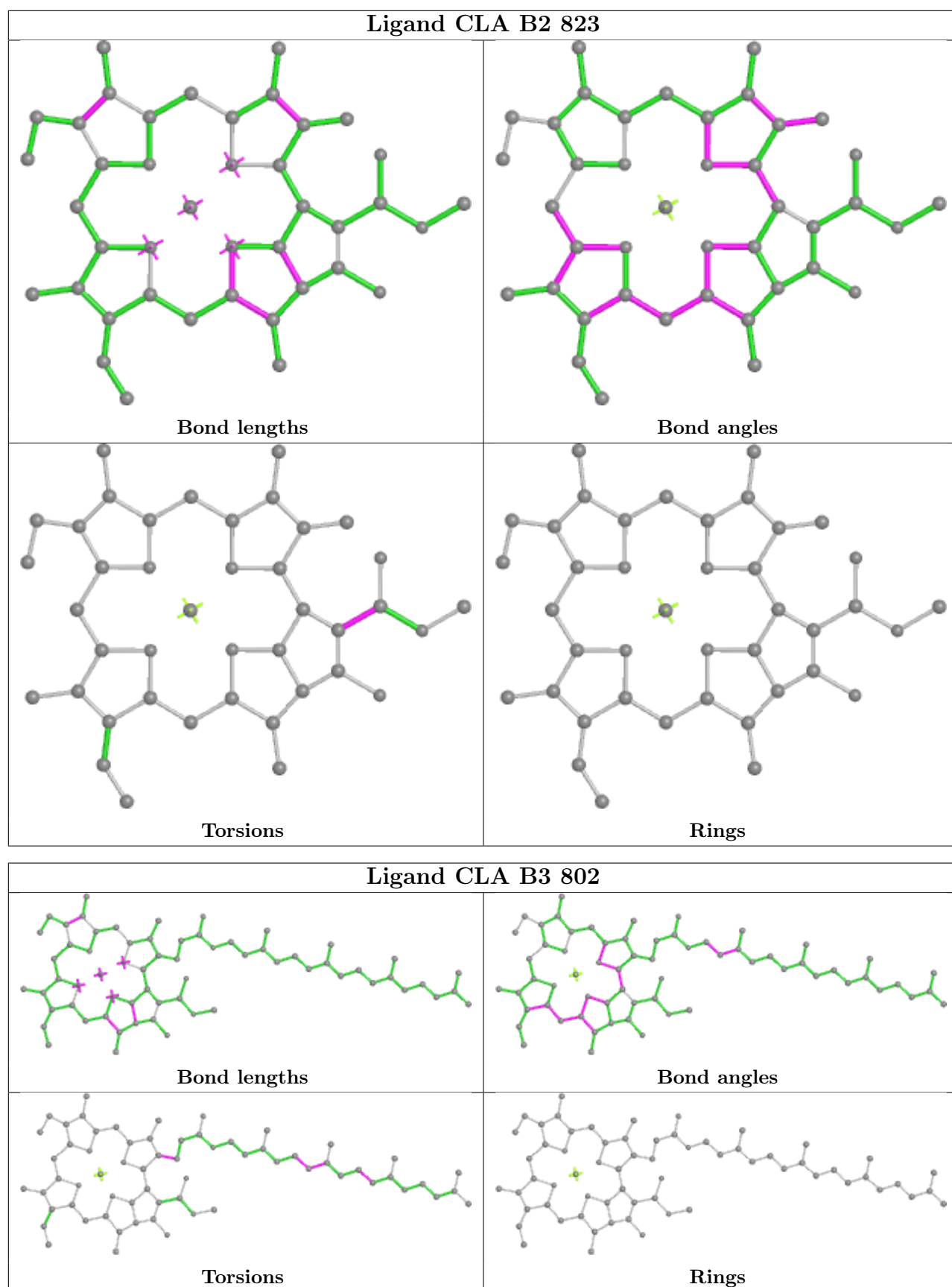


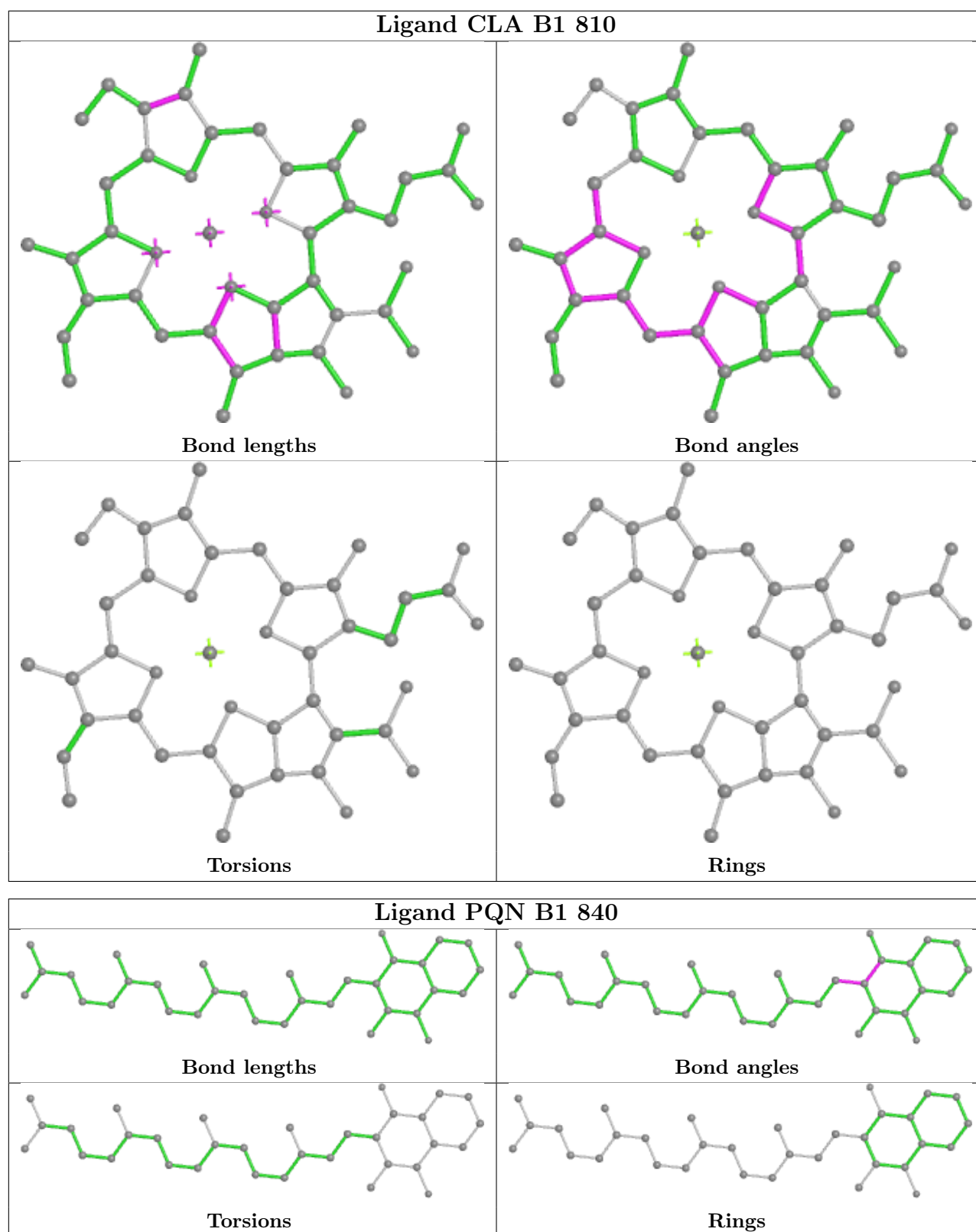
## Ligand CLA B3 822

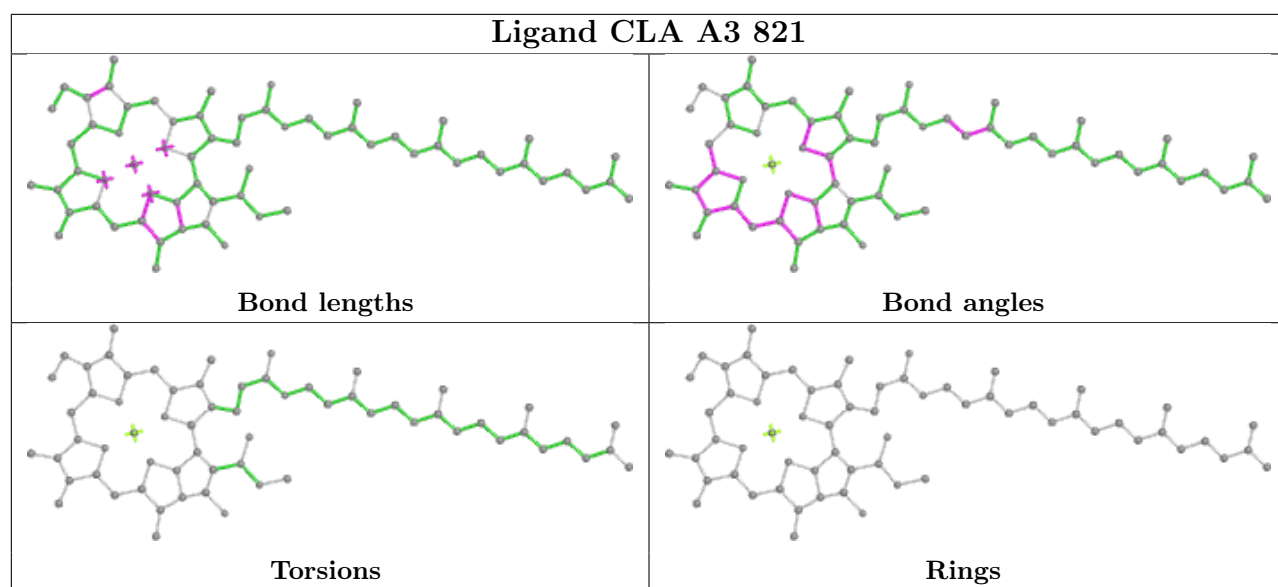


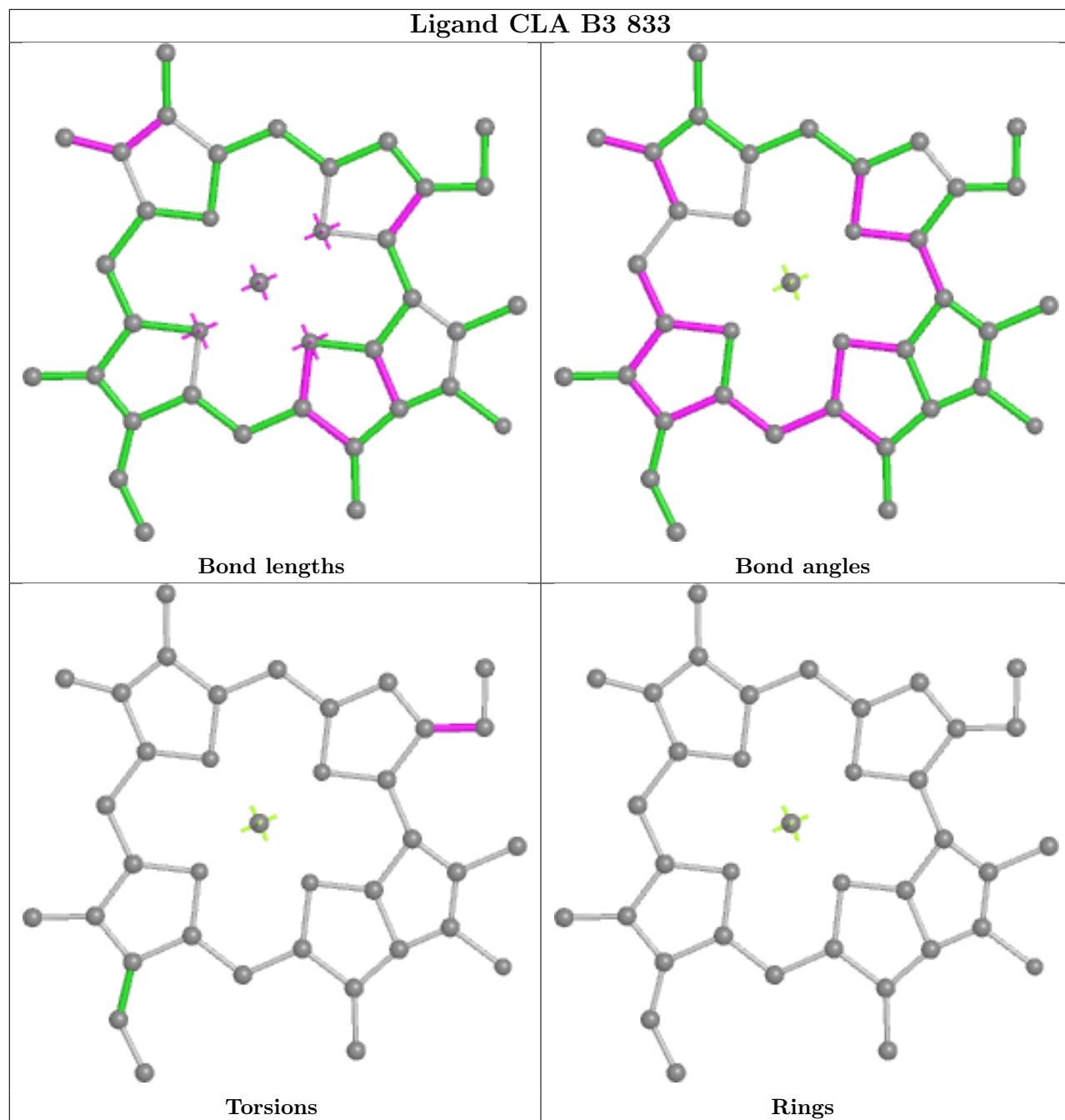
## Ligand CLA B3 807

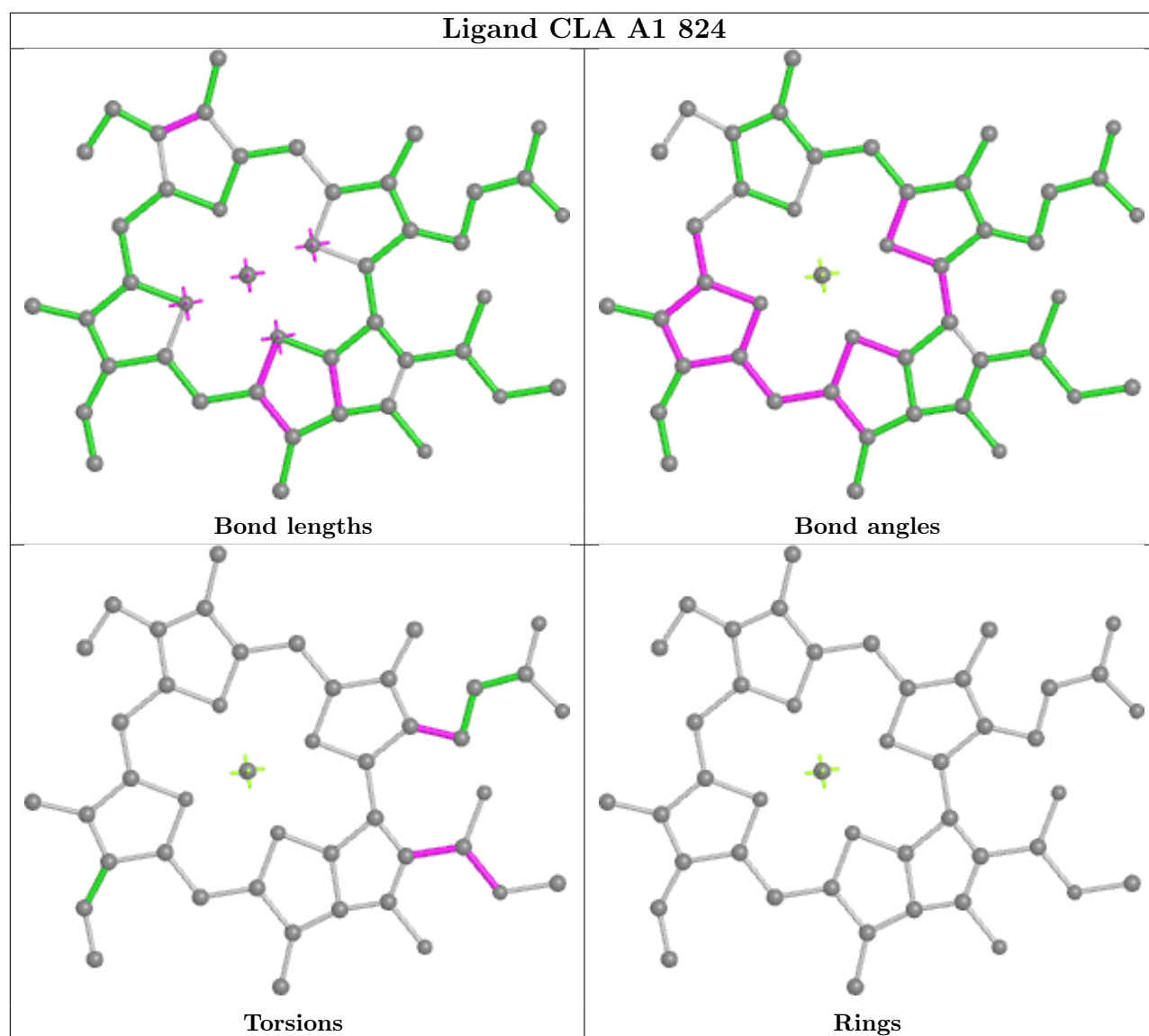






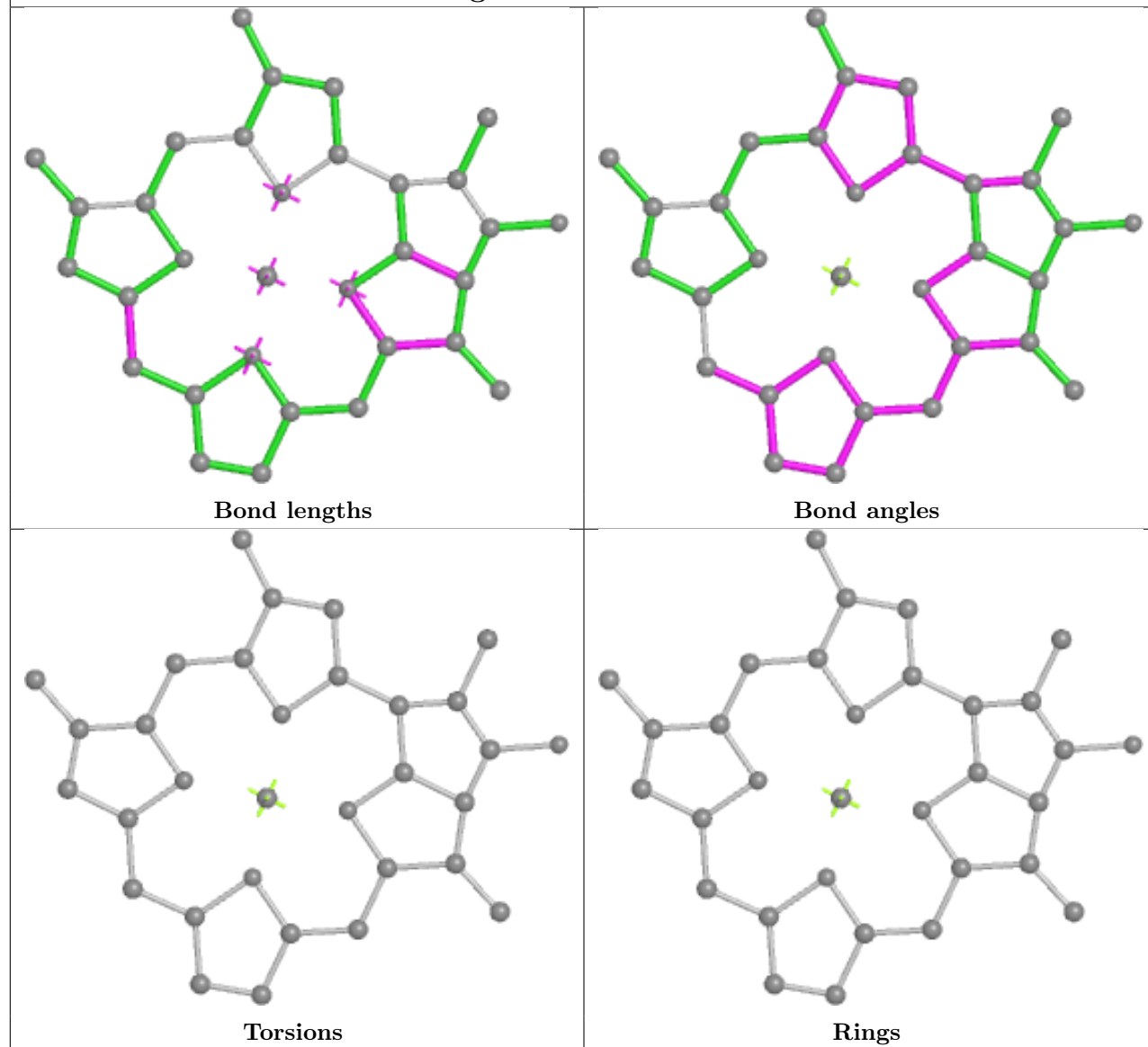




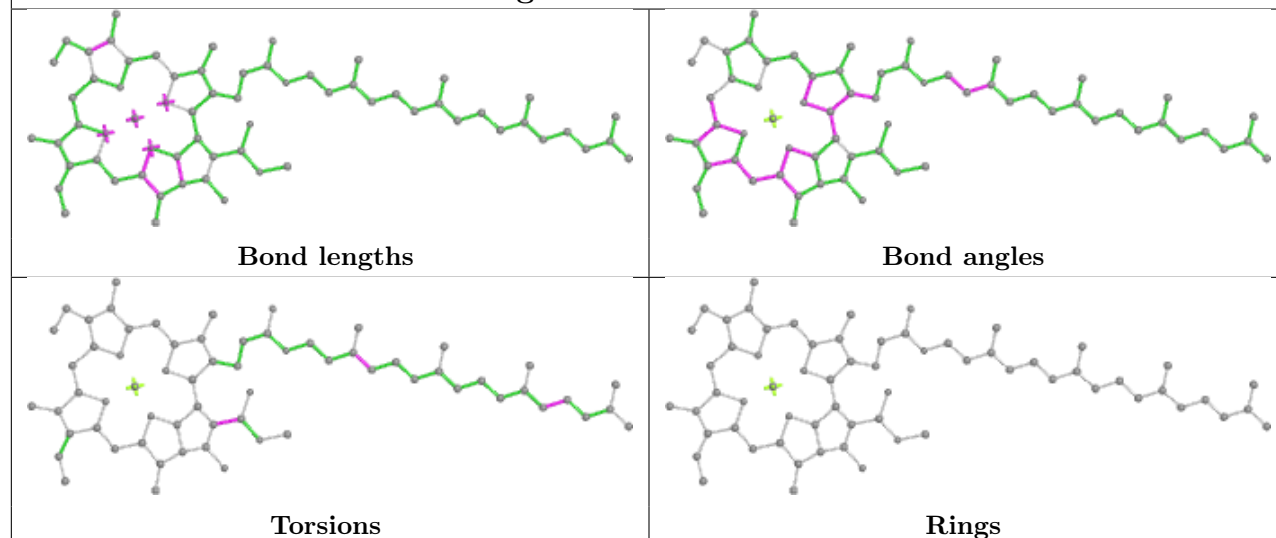




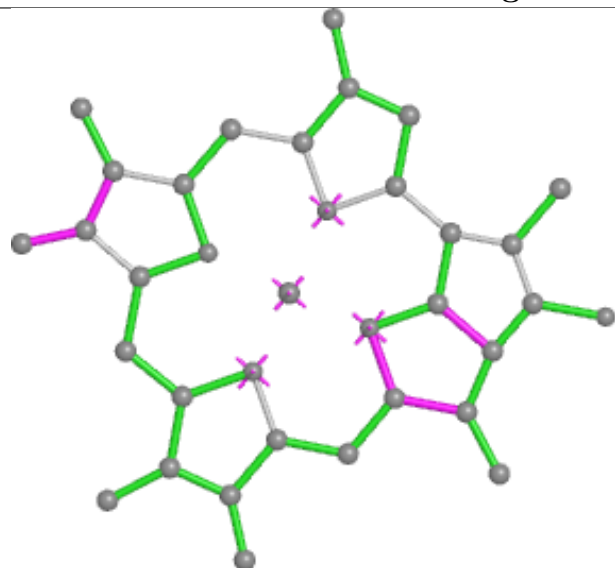
## Ligand CLA K3 103



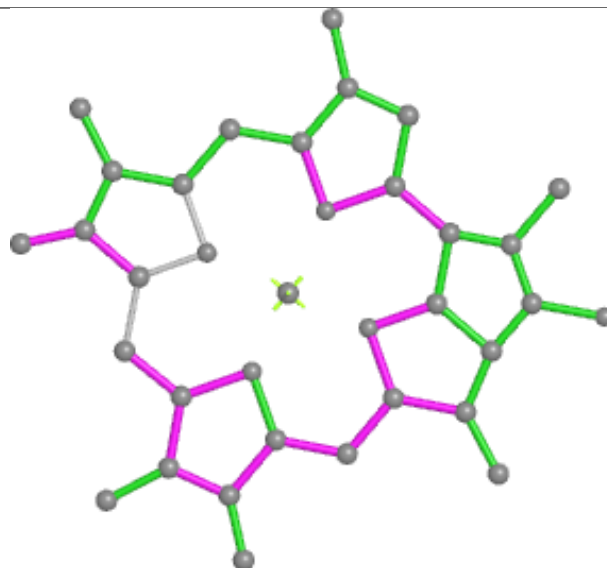
## Ligand CLA L1 1004



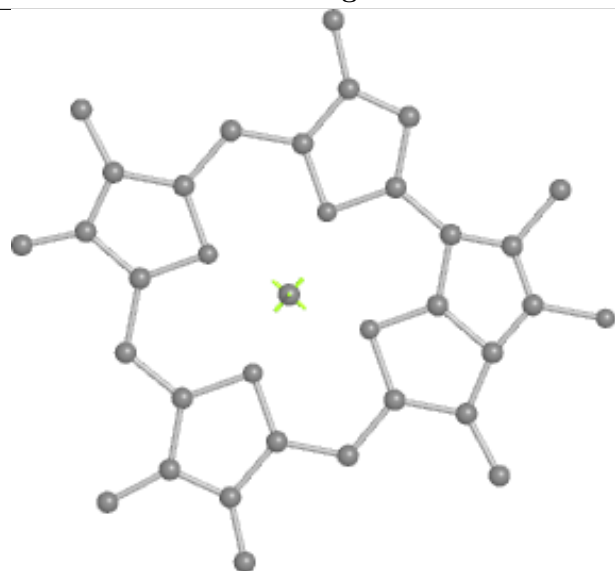
## Ligand CLA J2 1302



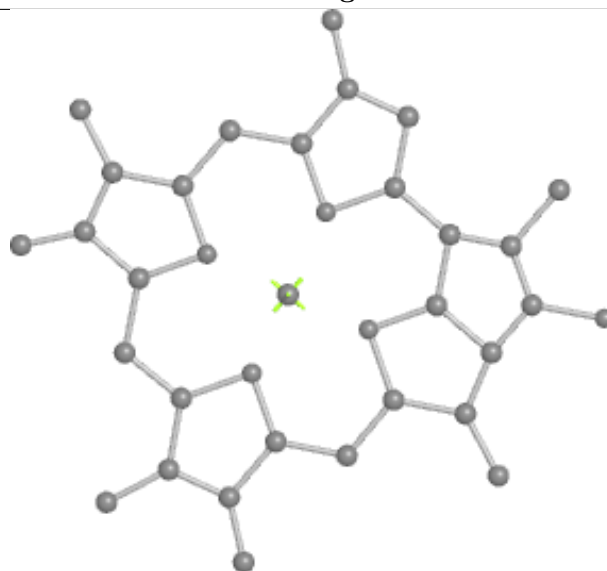
Bond lengths



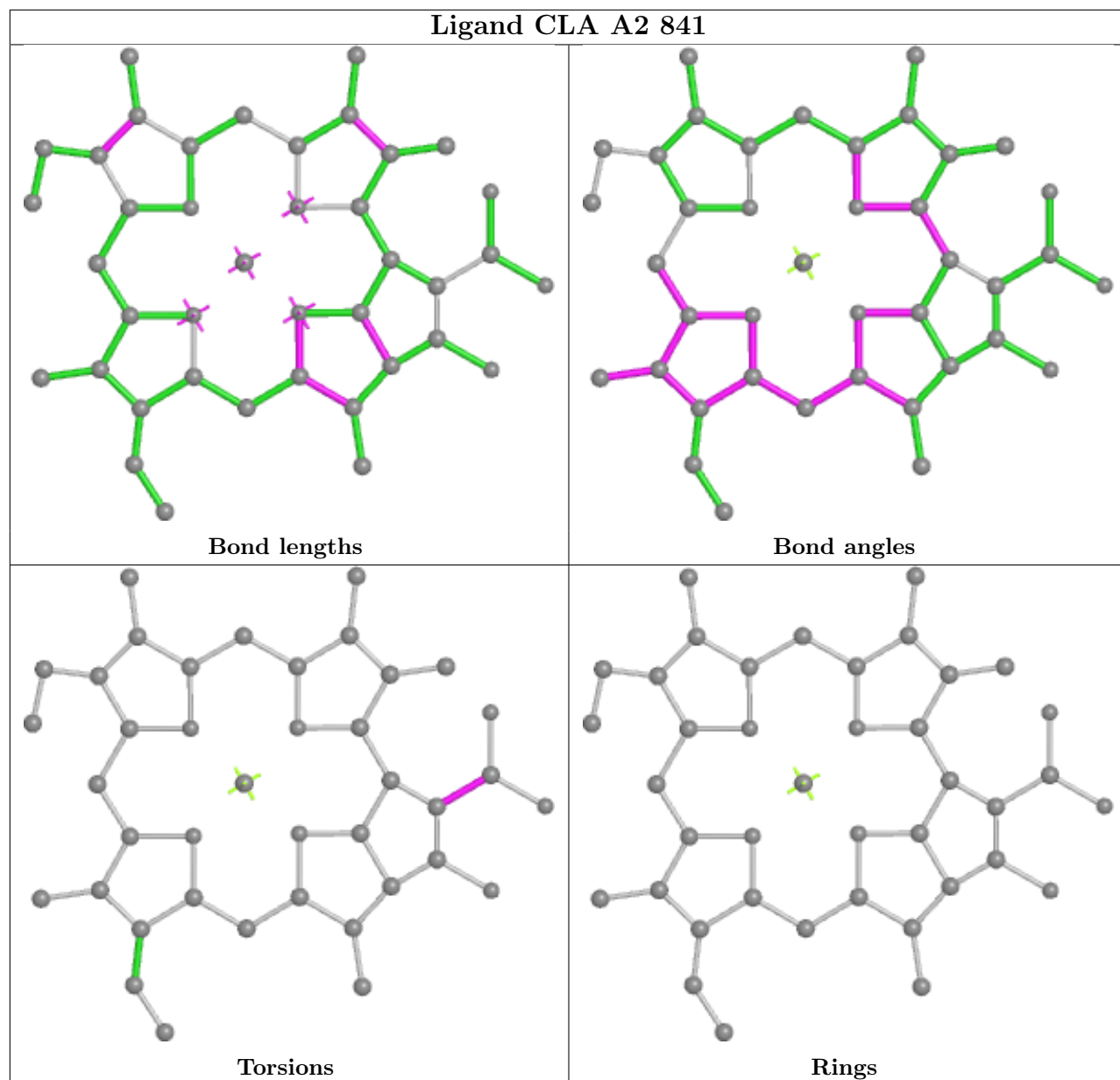
Bond angles

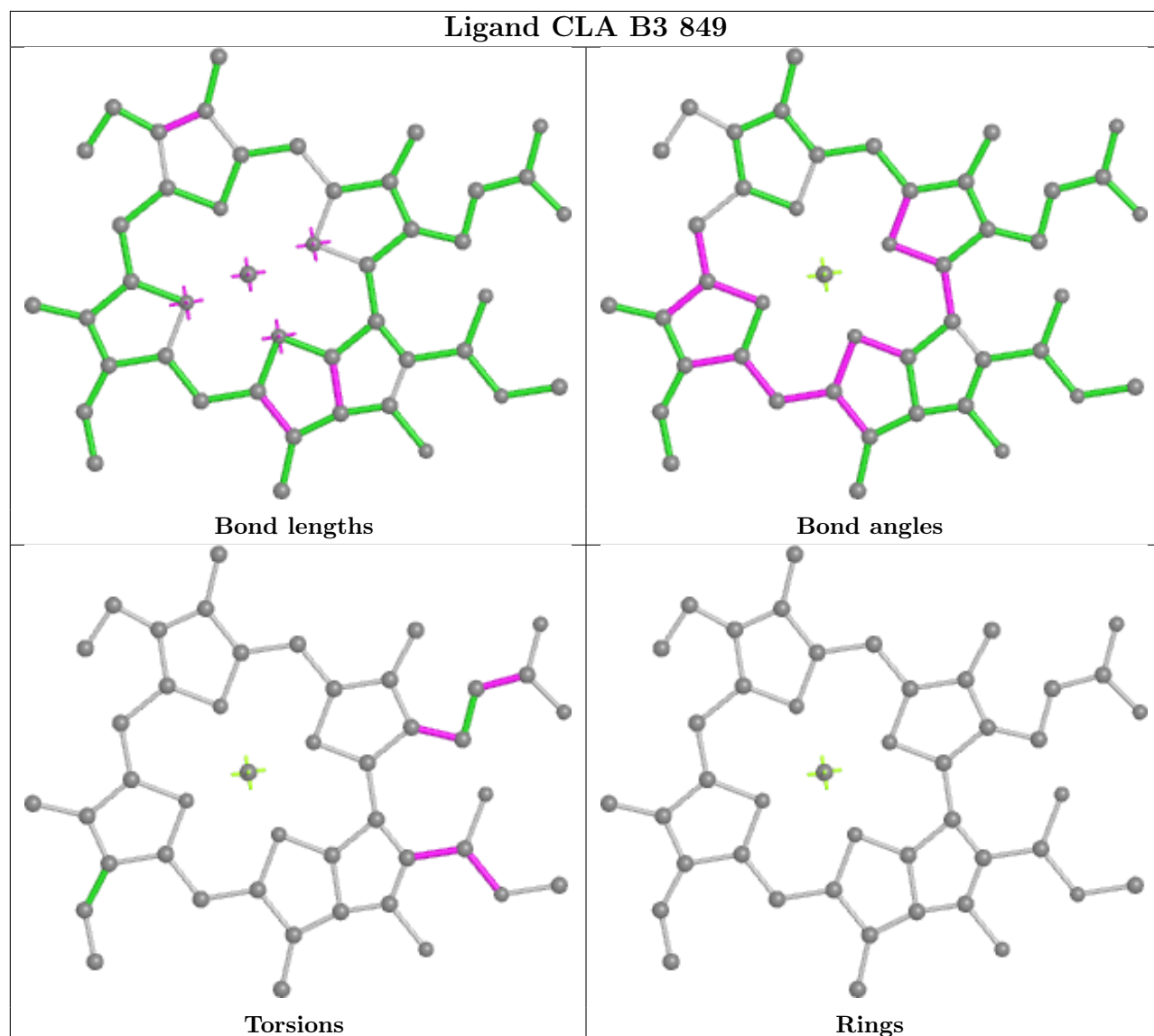
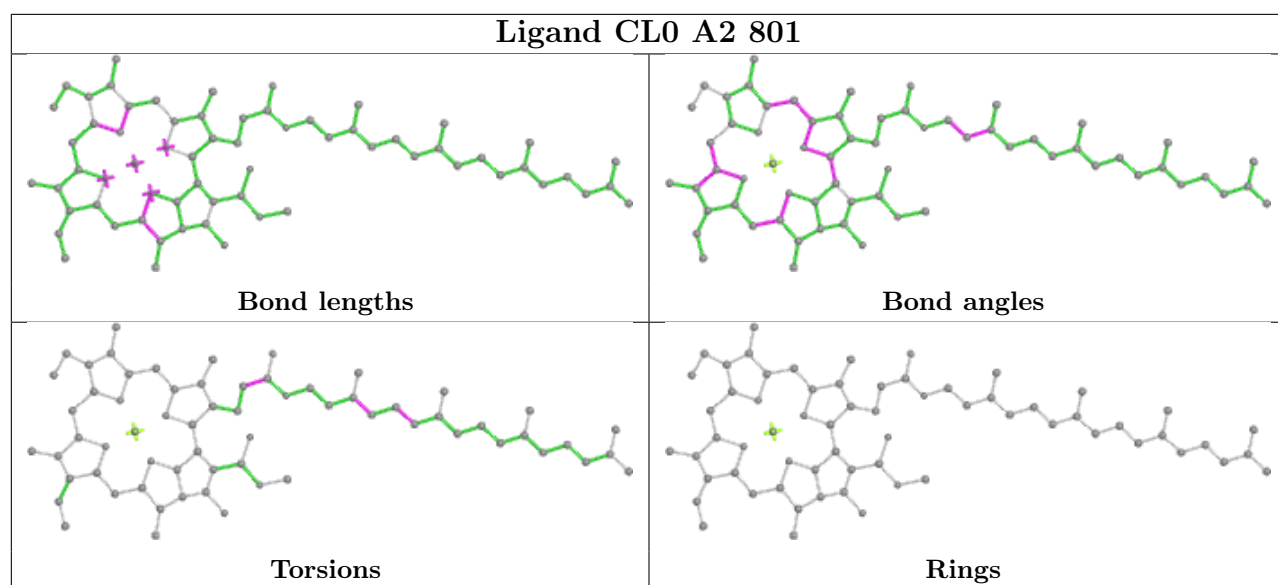


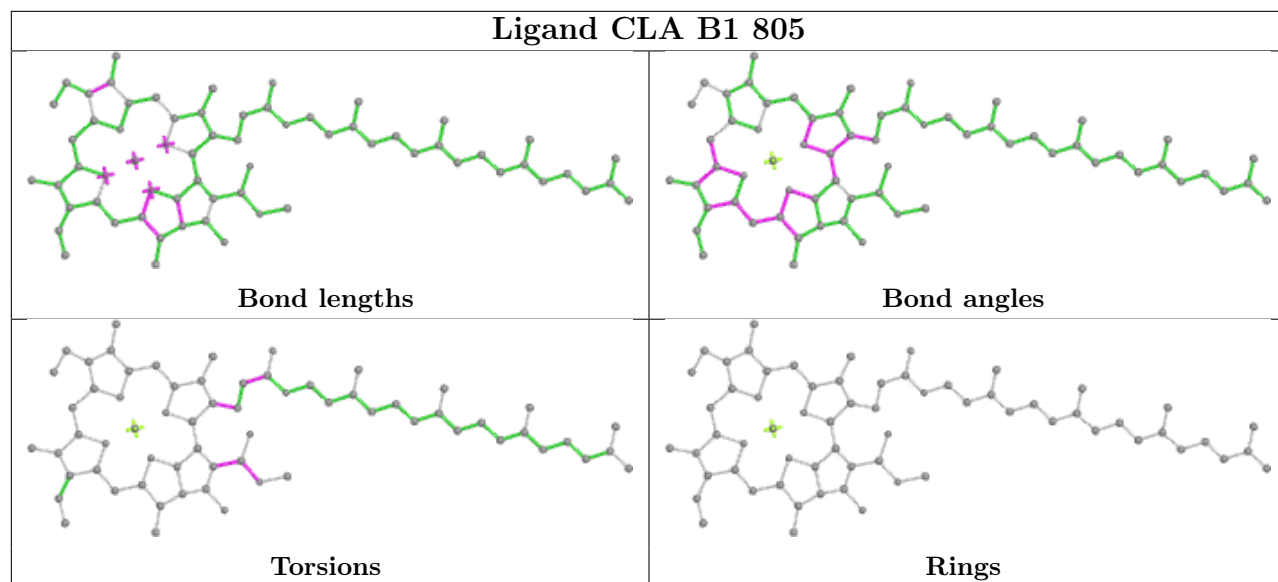
Torsions



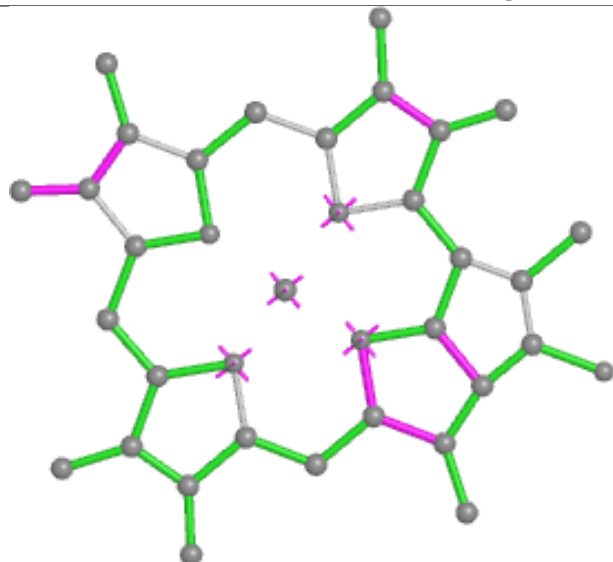
Rings



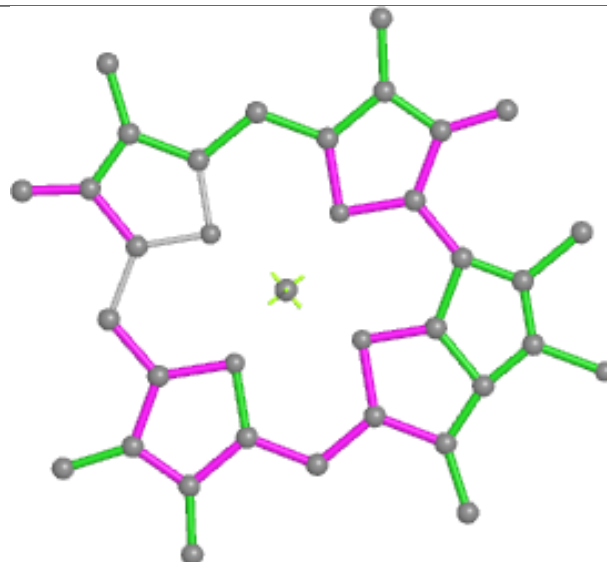




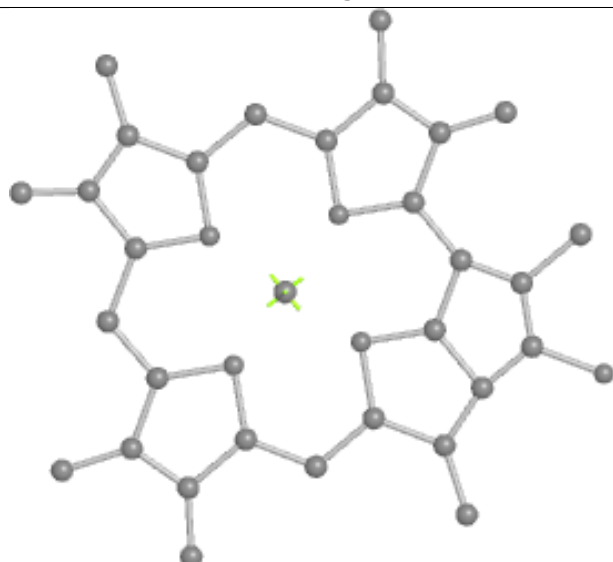
## Ligand CLA J3 1303



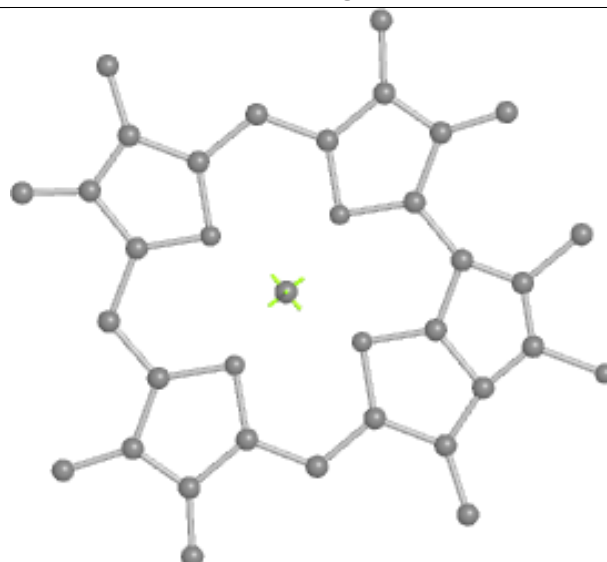
Bond lengths



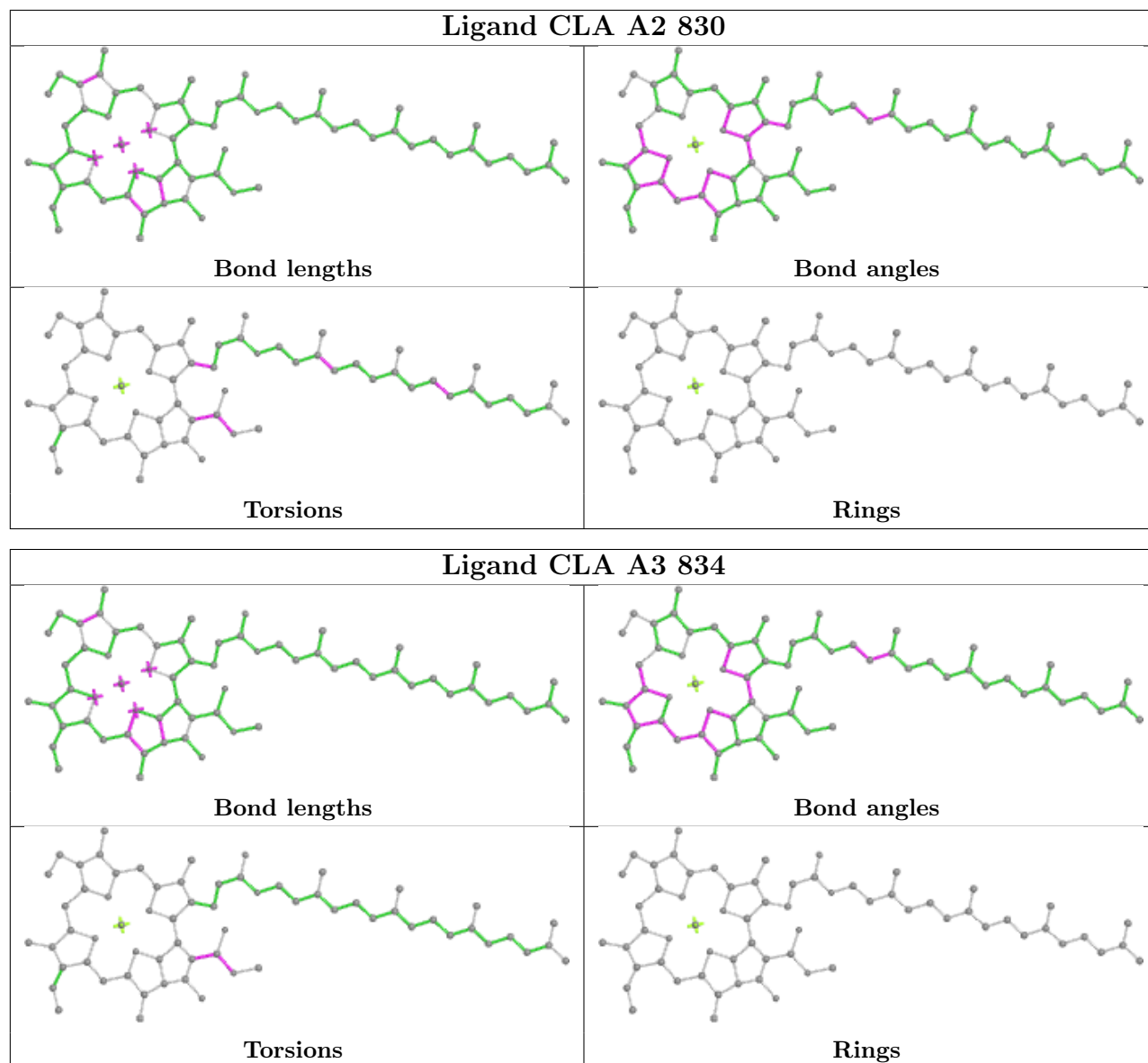
Bond angles

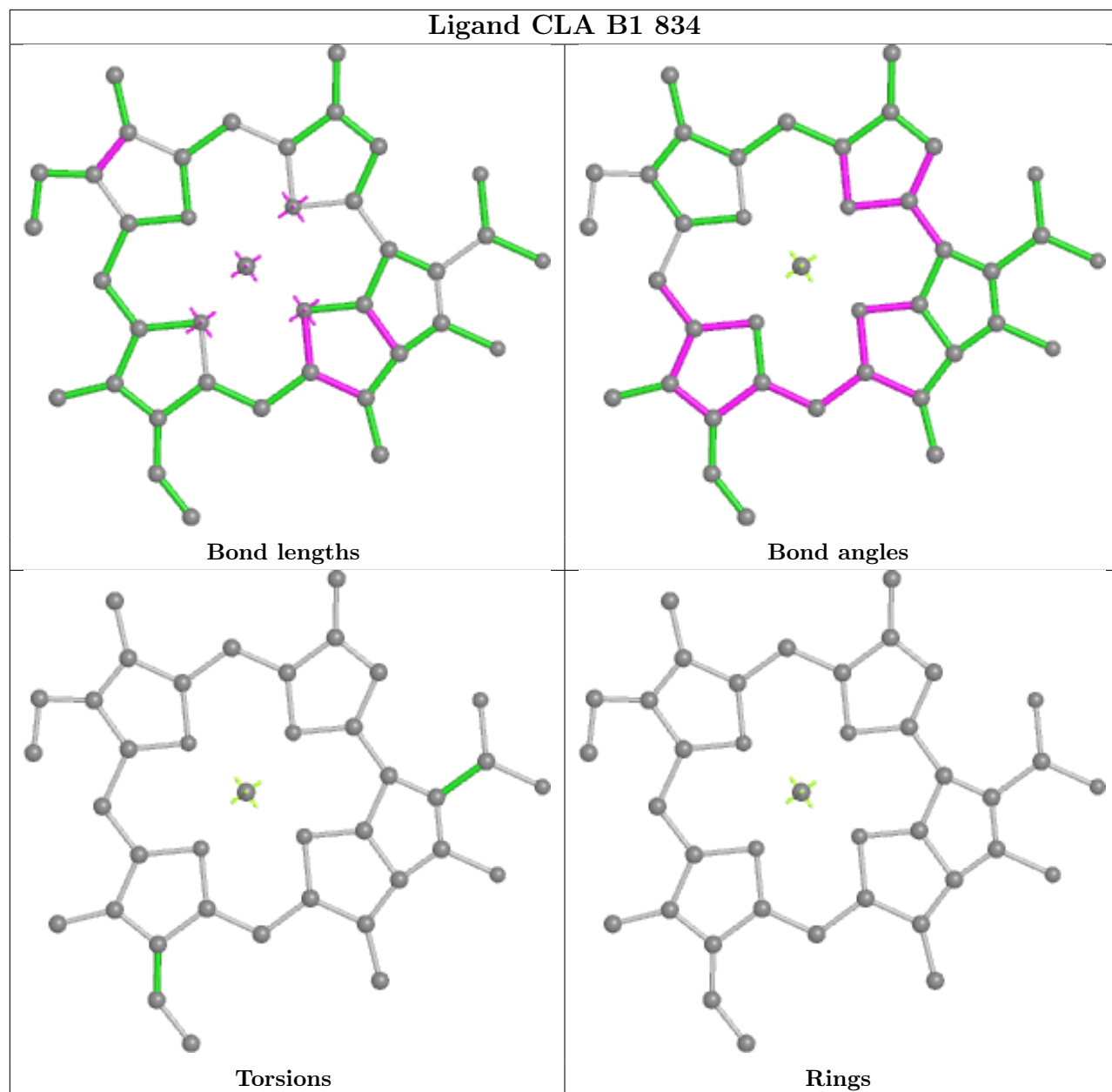


Torsions



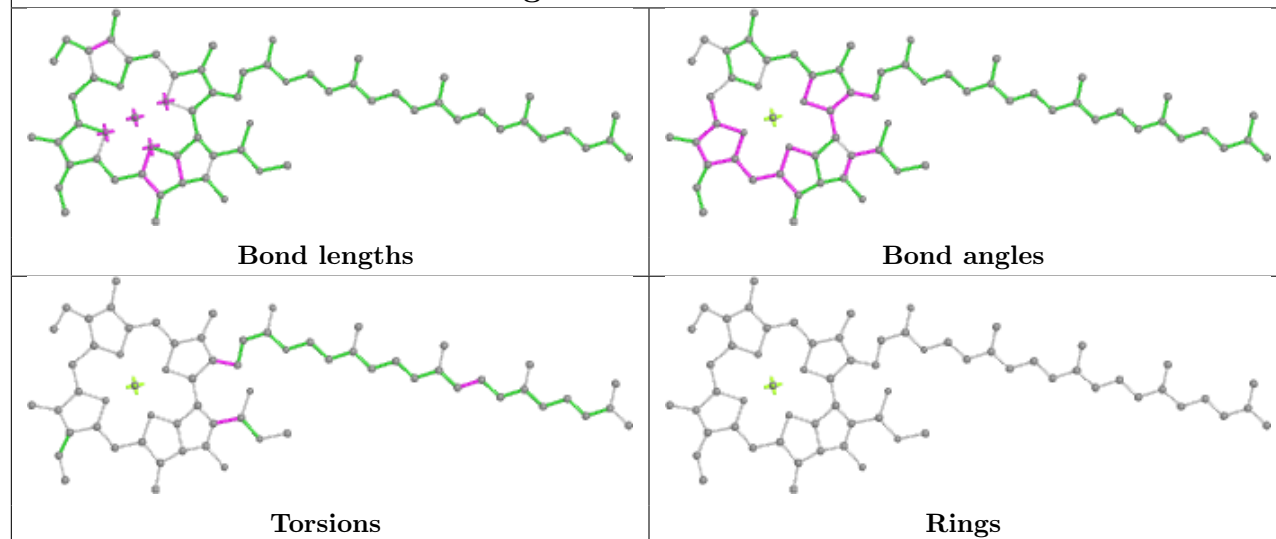
Rings



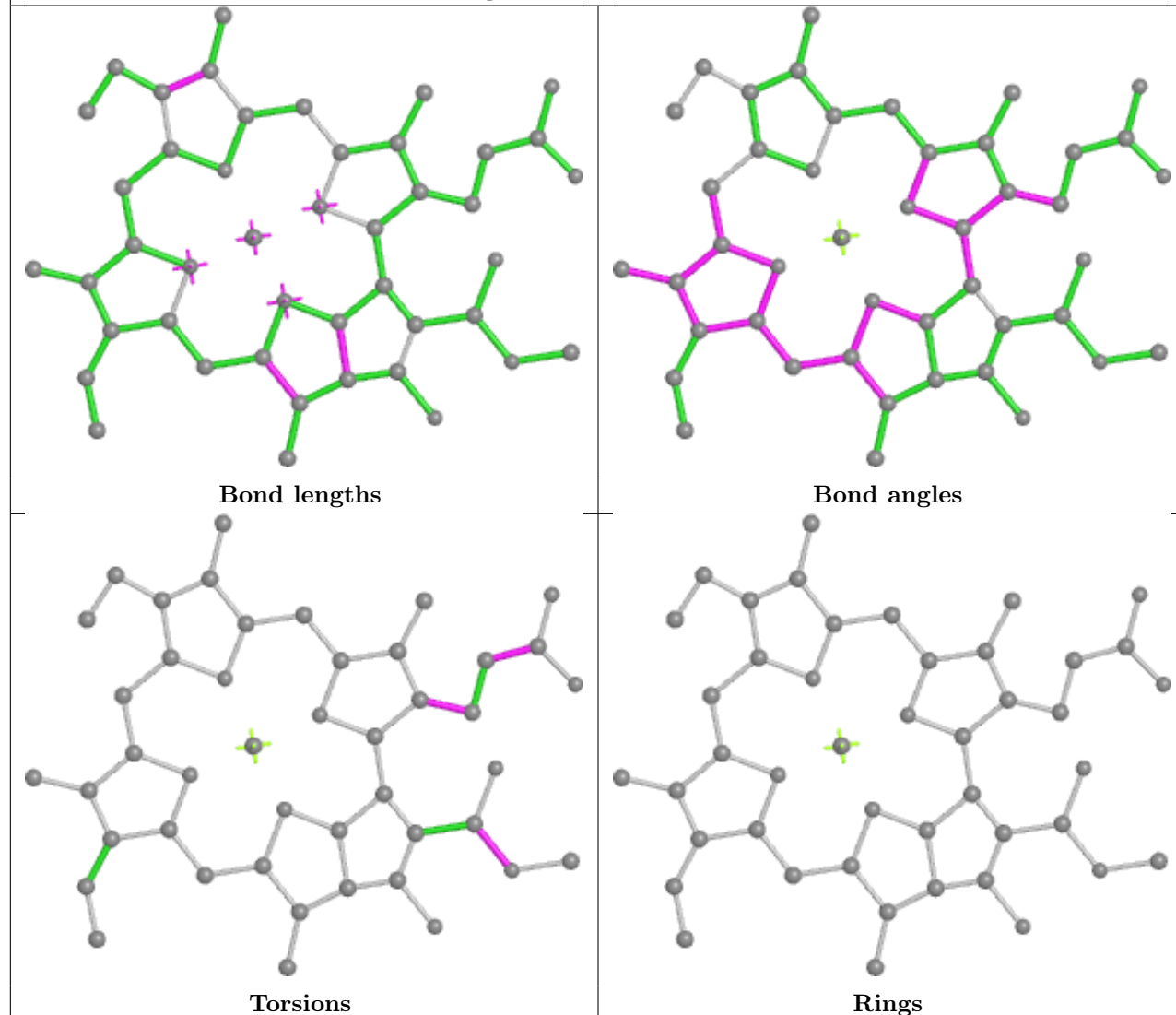


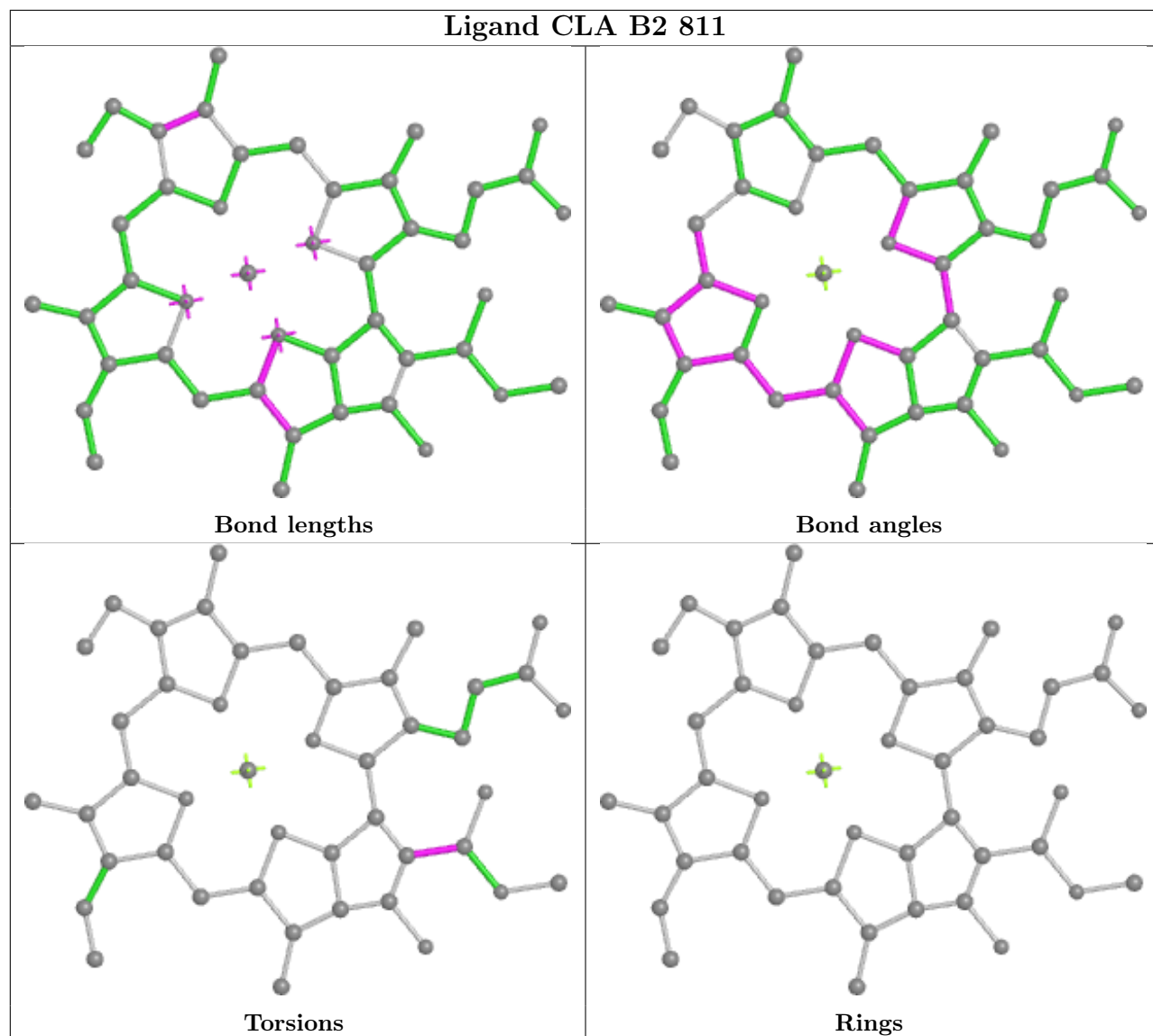


## Ligand CLA B1 812

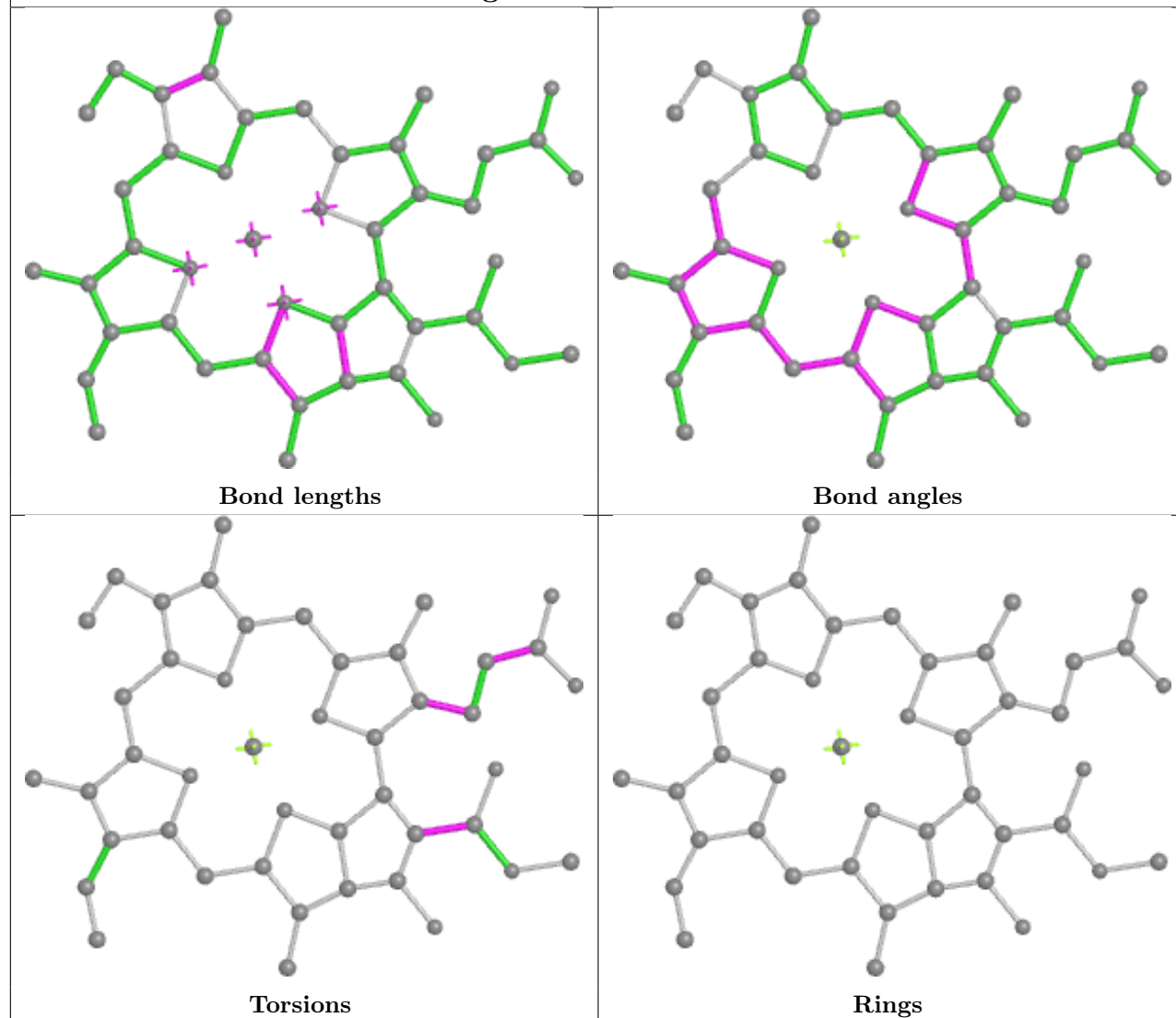


## Ligand CLA A2 832

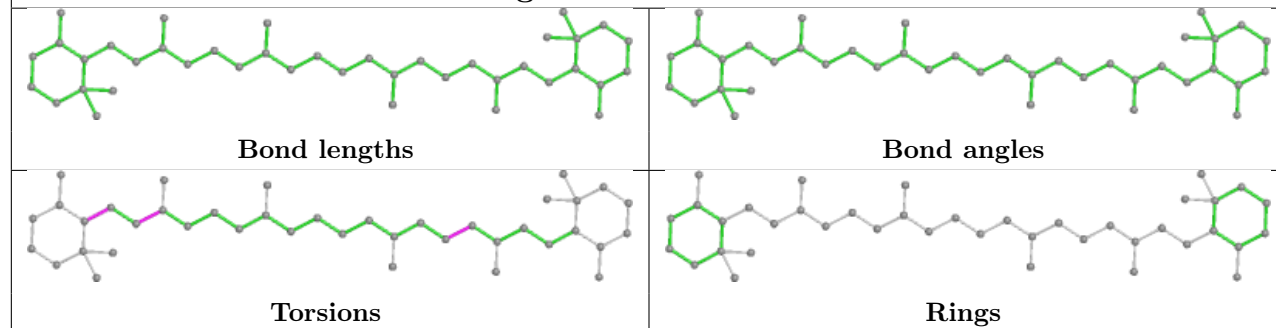


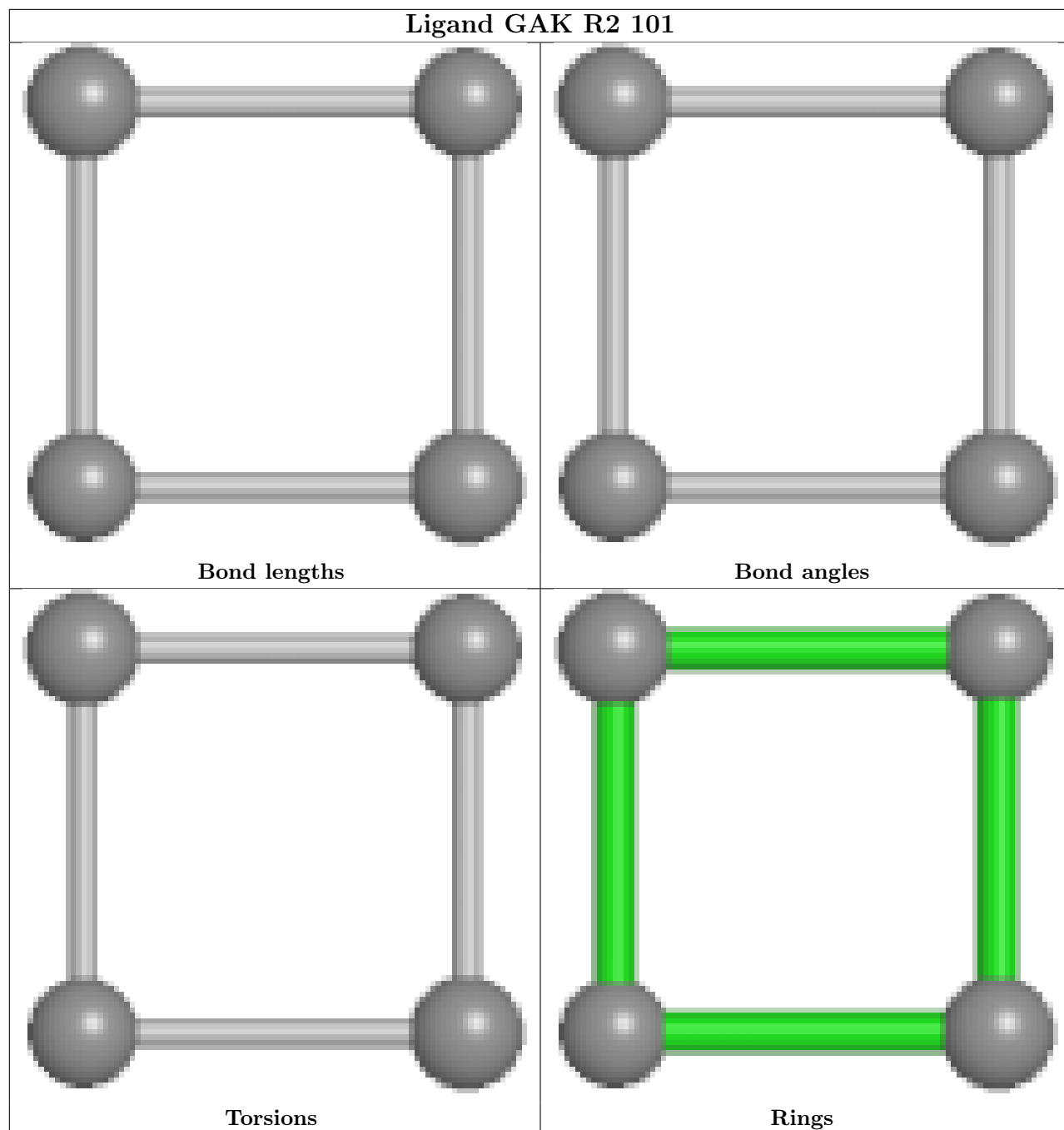


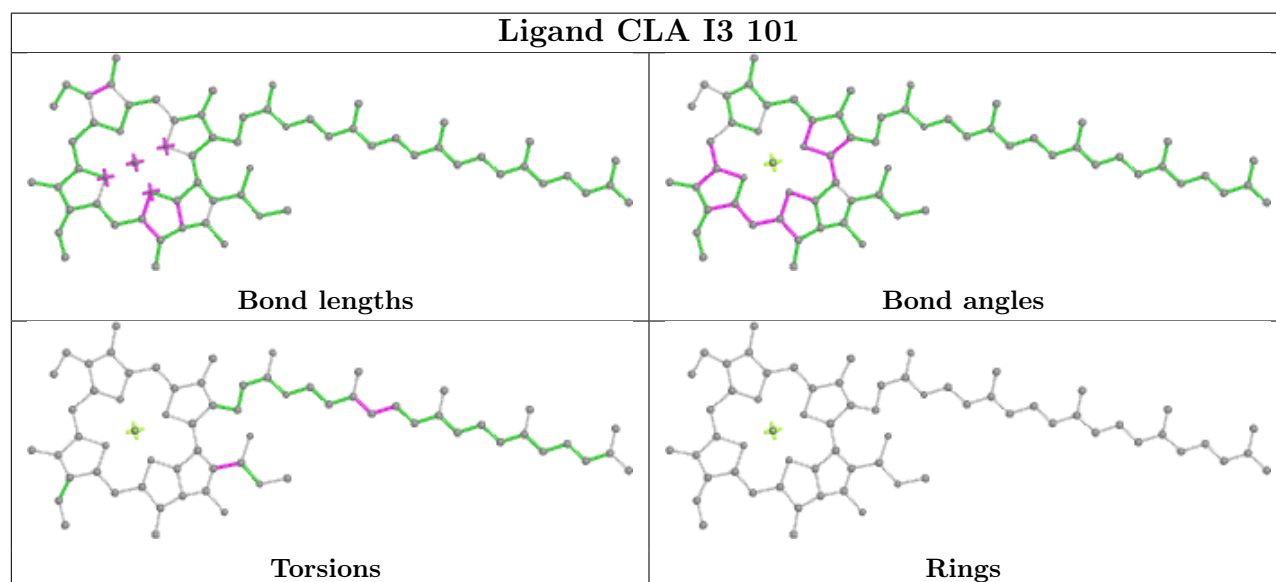
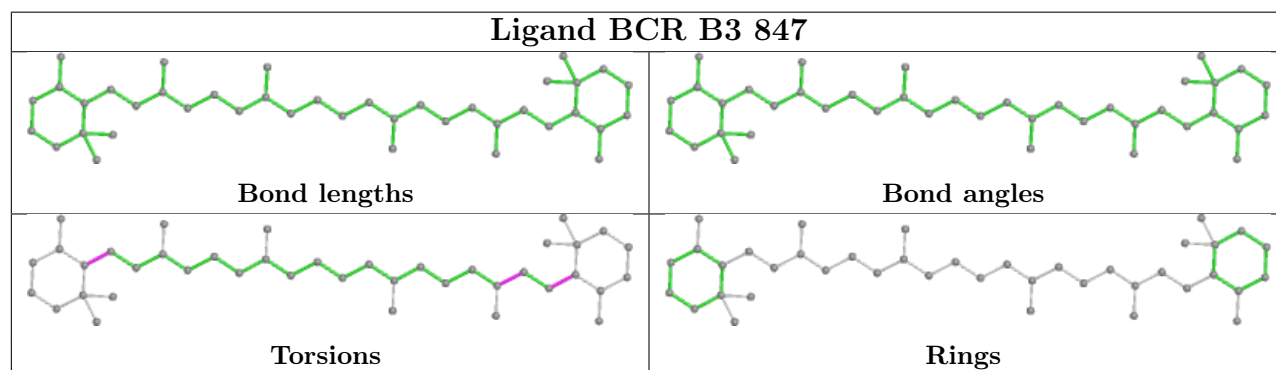
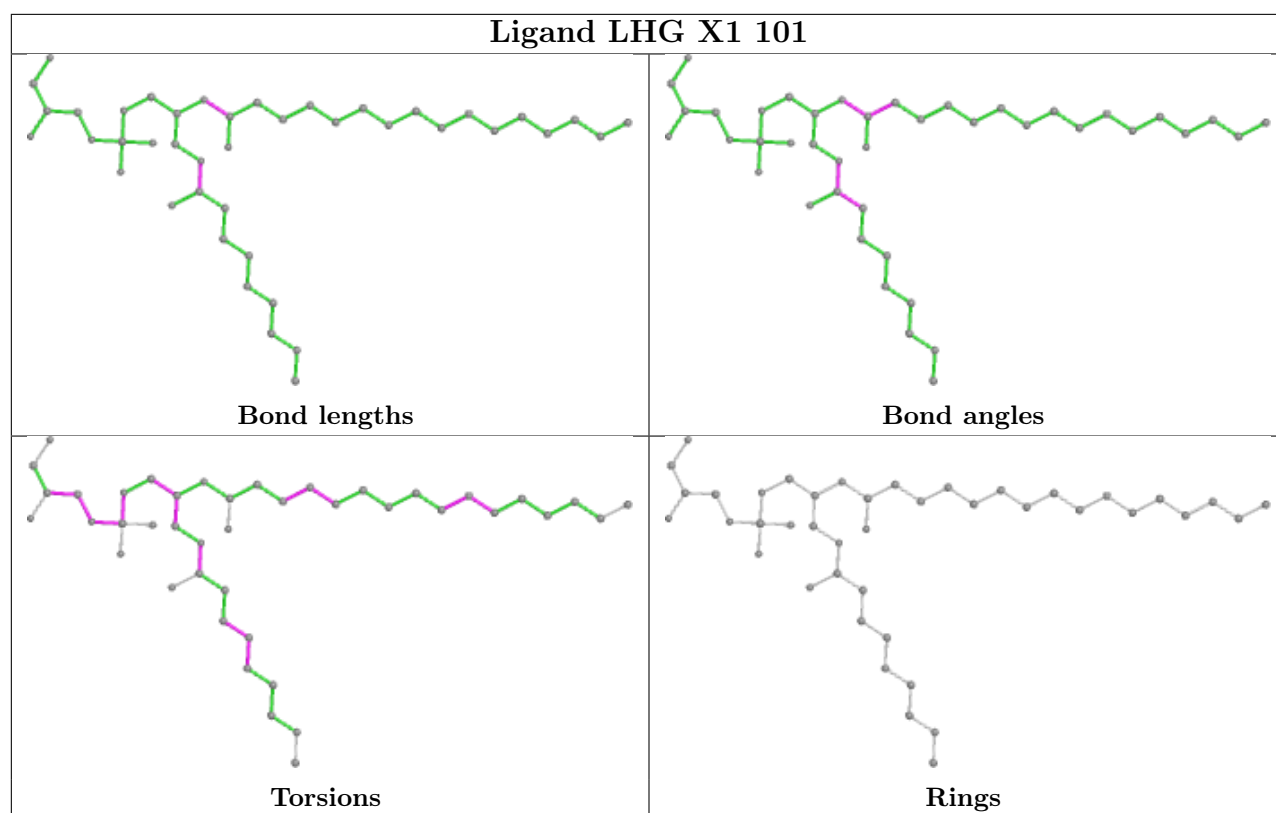
## Ligand CLA B3 819



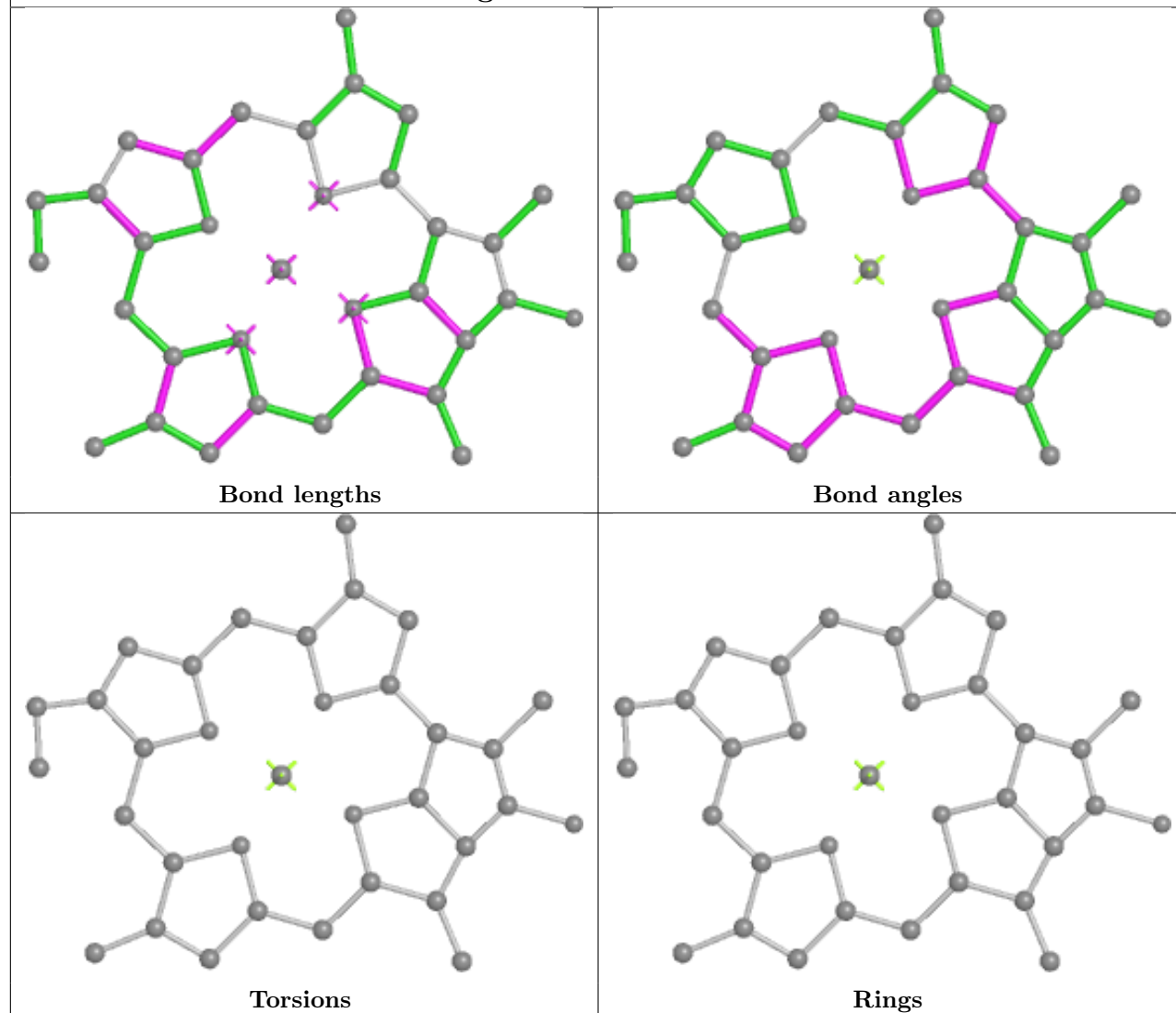
## Ligand BCR J2 1306



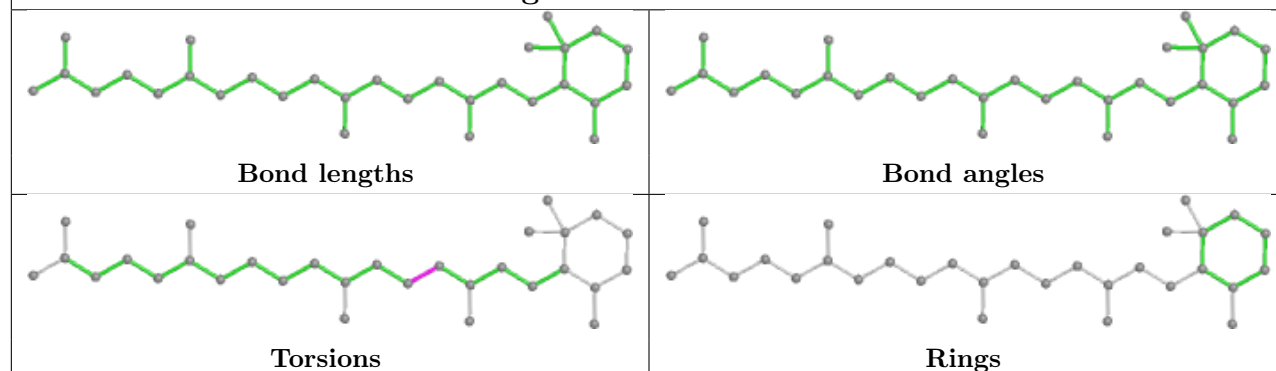


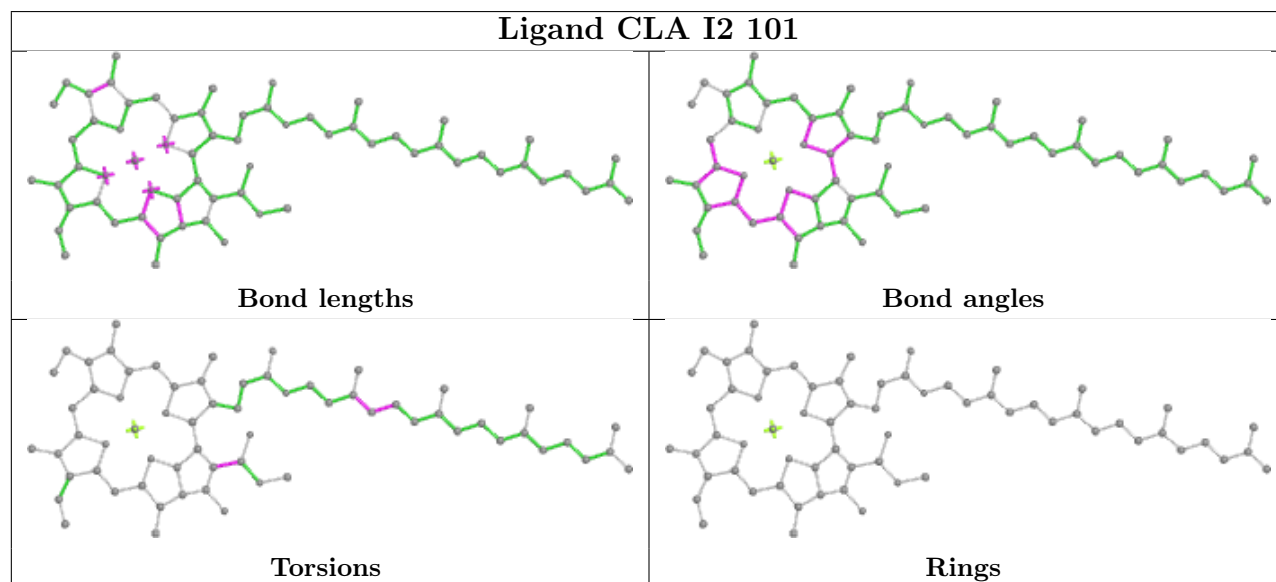
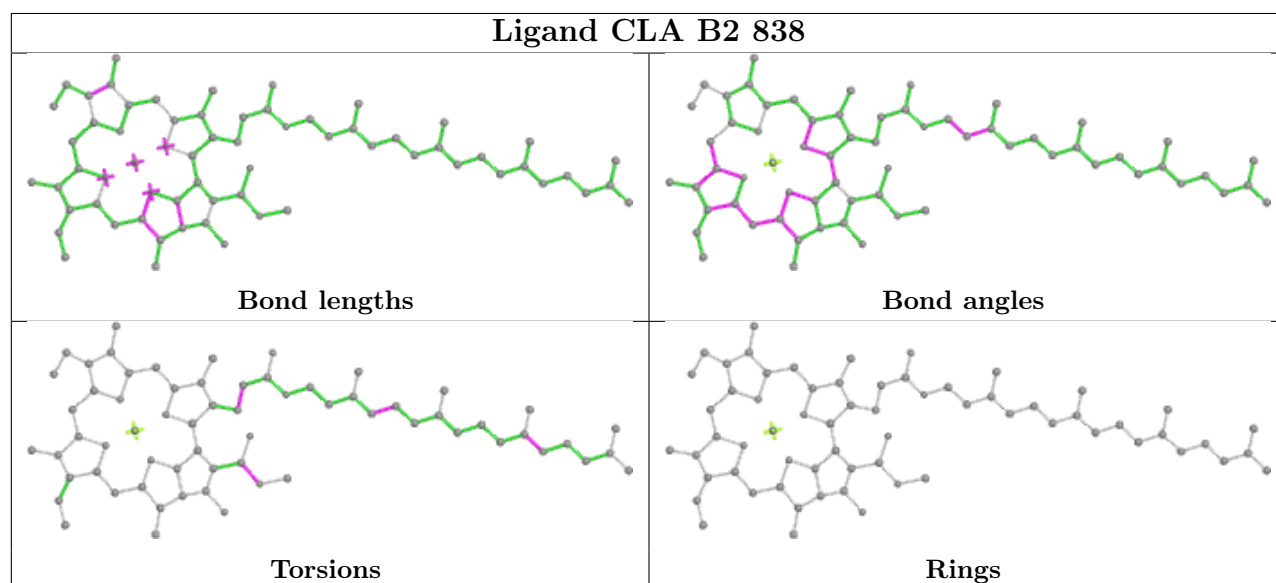
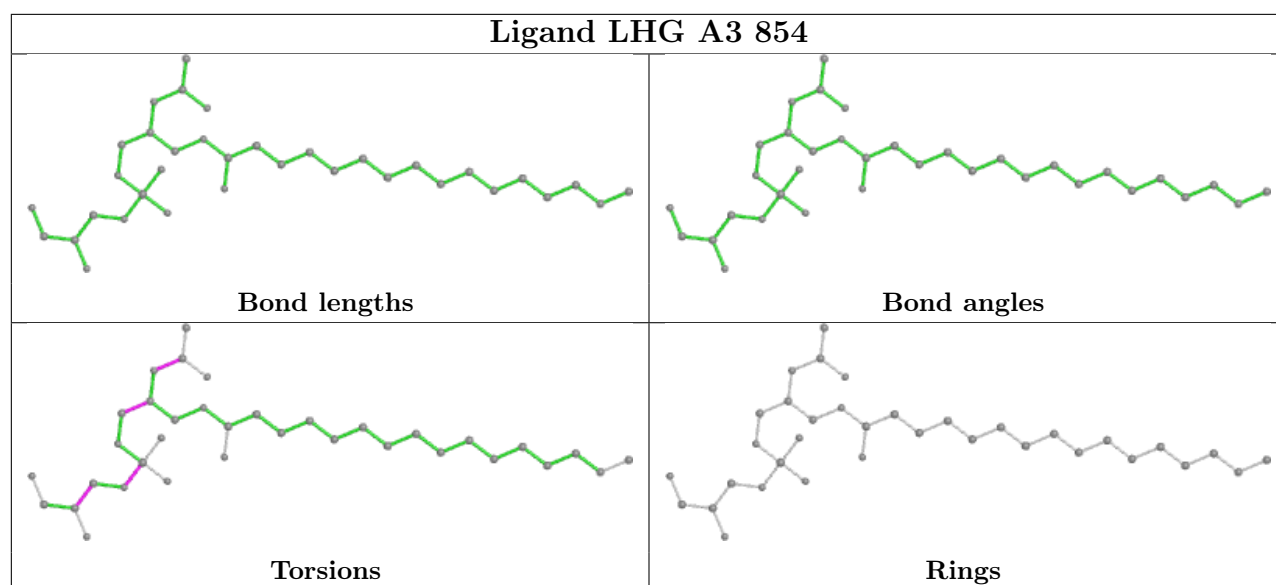


## Ligand CLA J3 1307

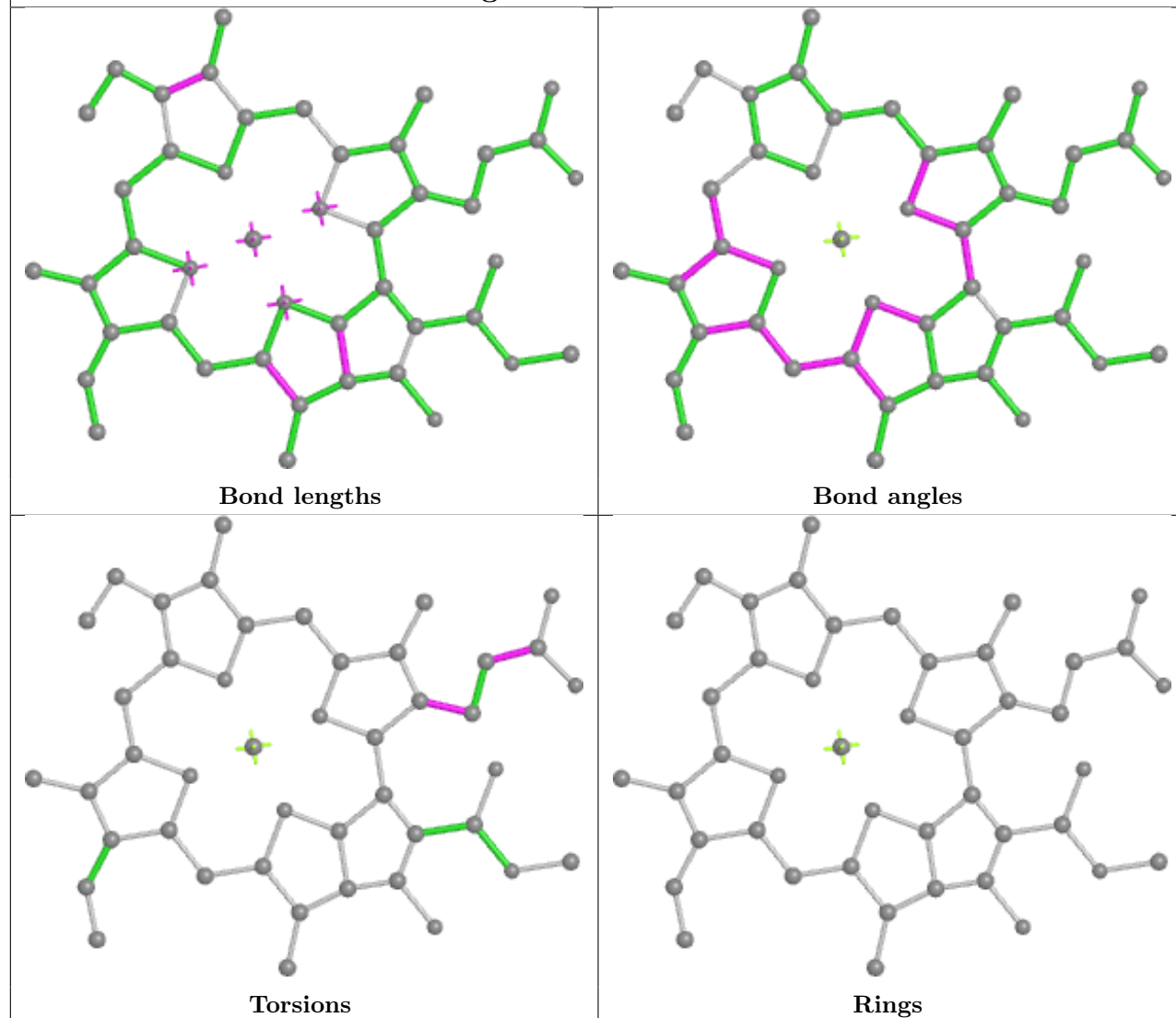


## Ligand BCR B2 842

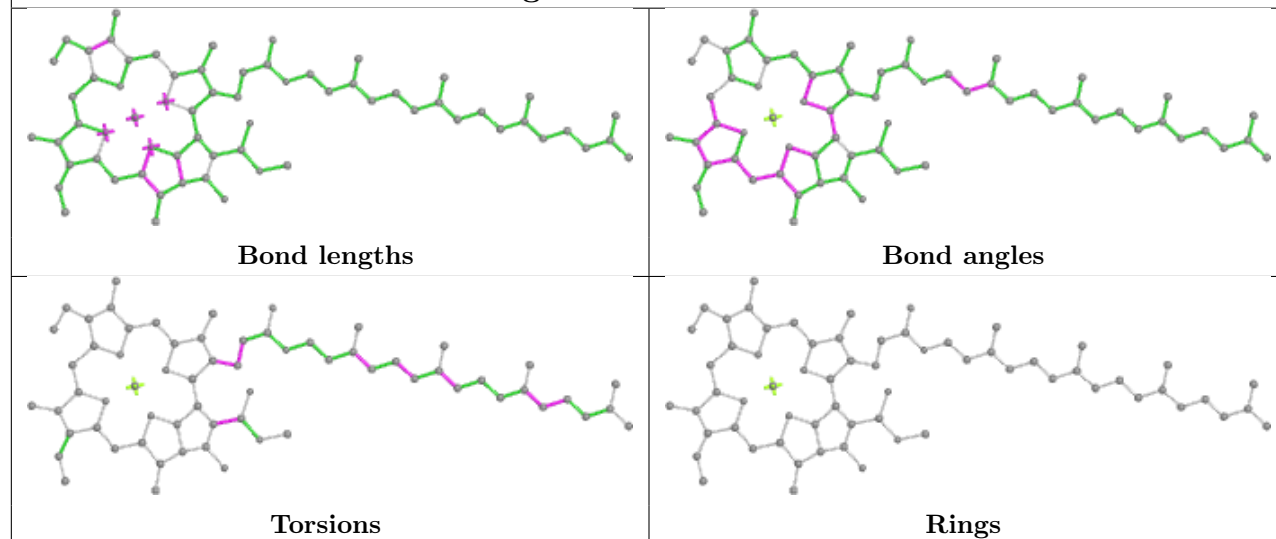




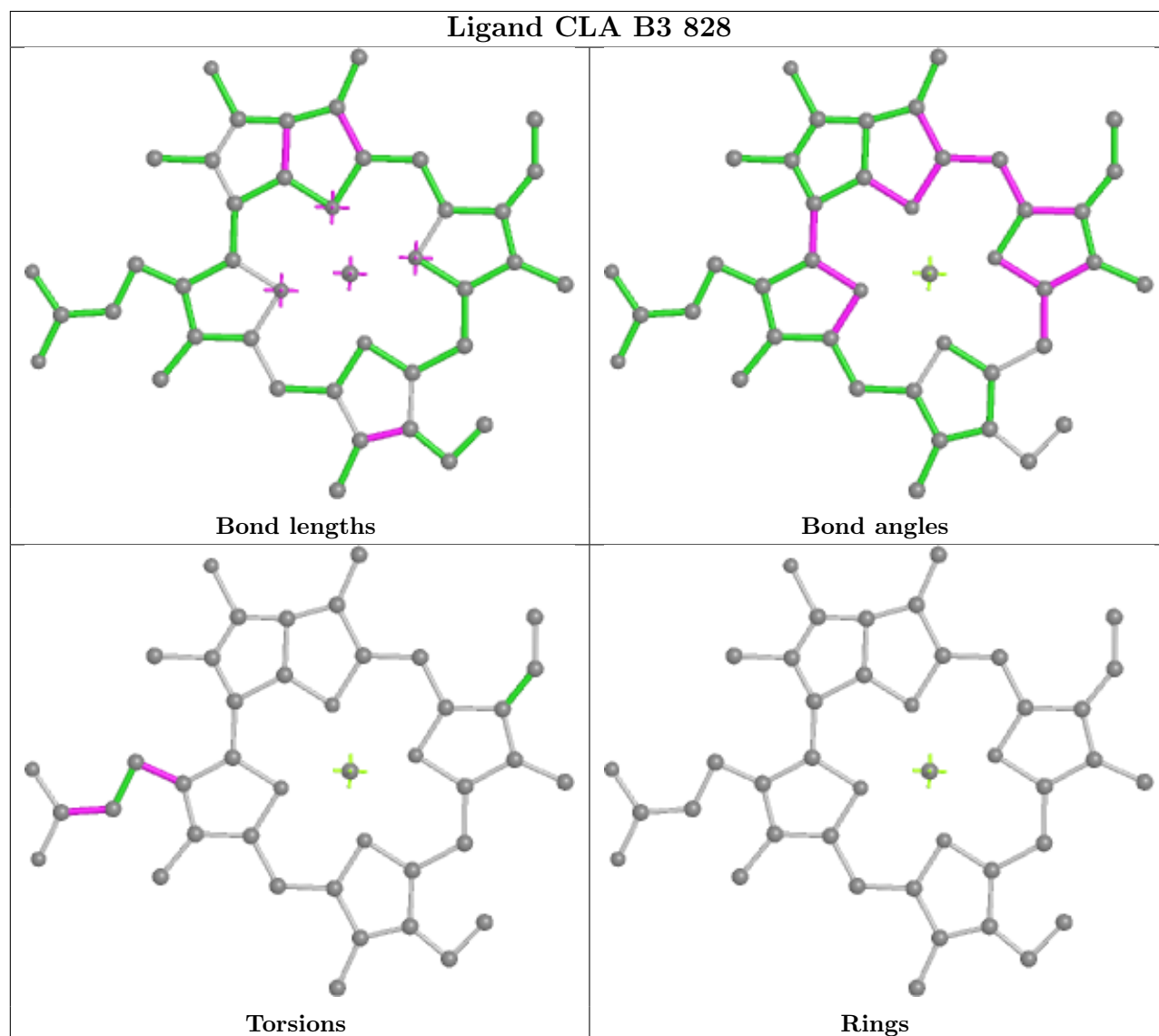
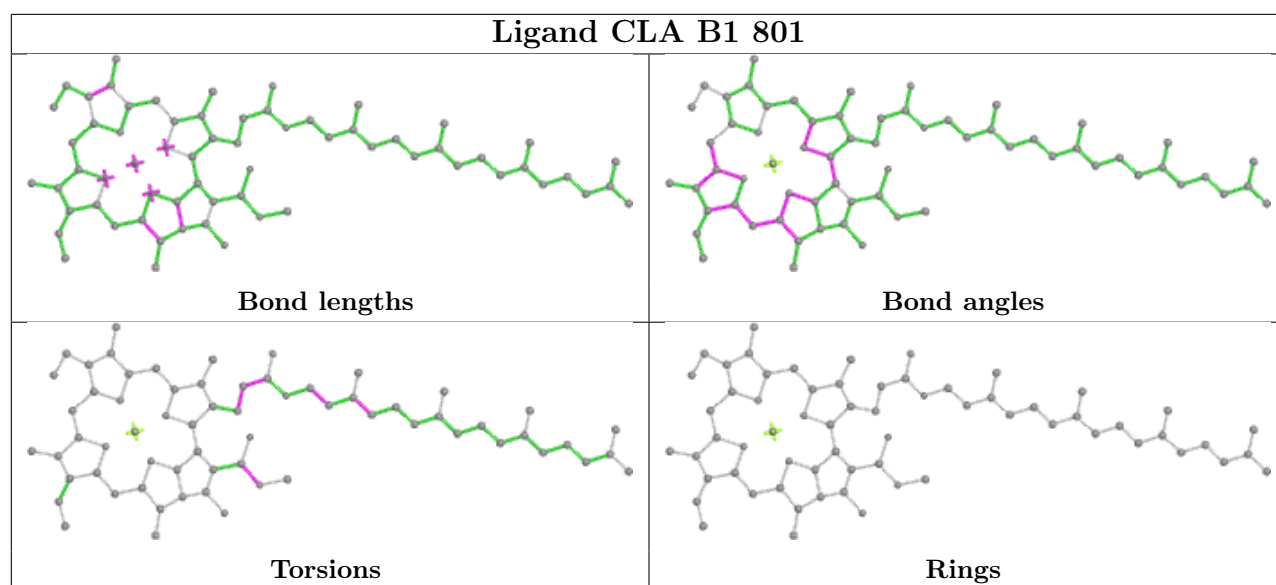
## Ligand CLA A3 835



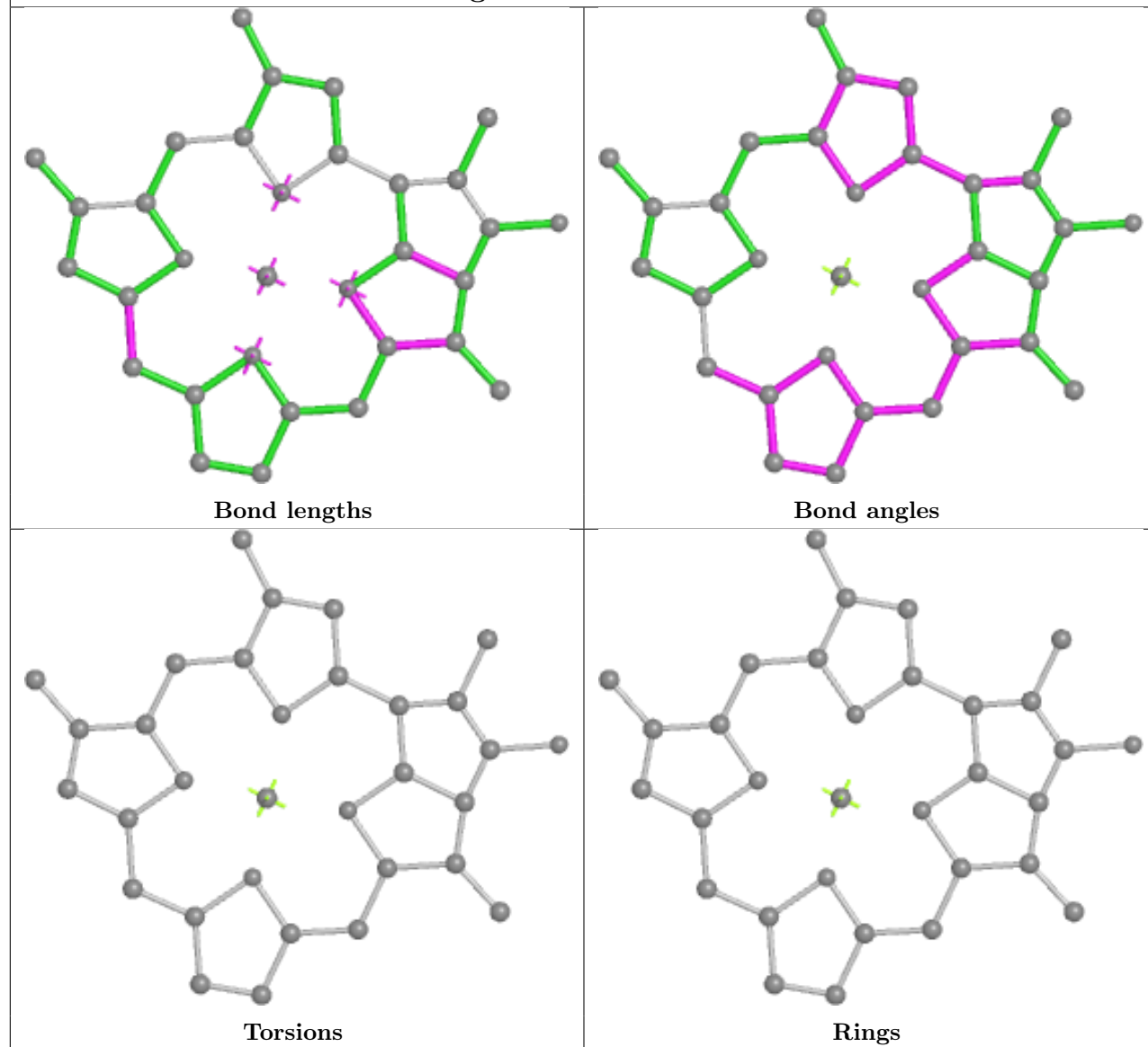
## Ligand CLA A1 809



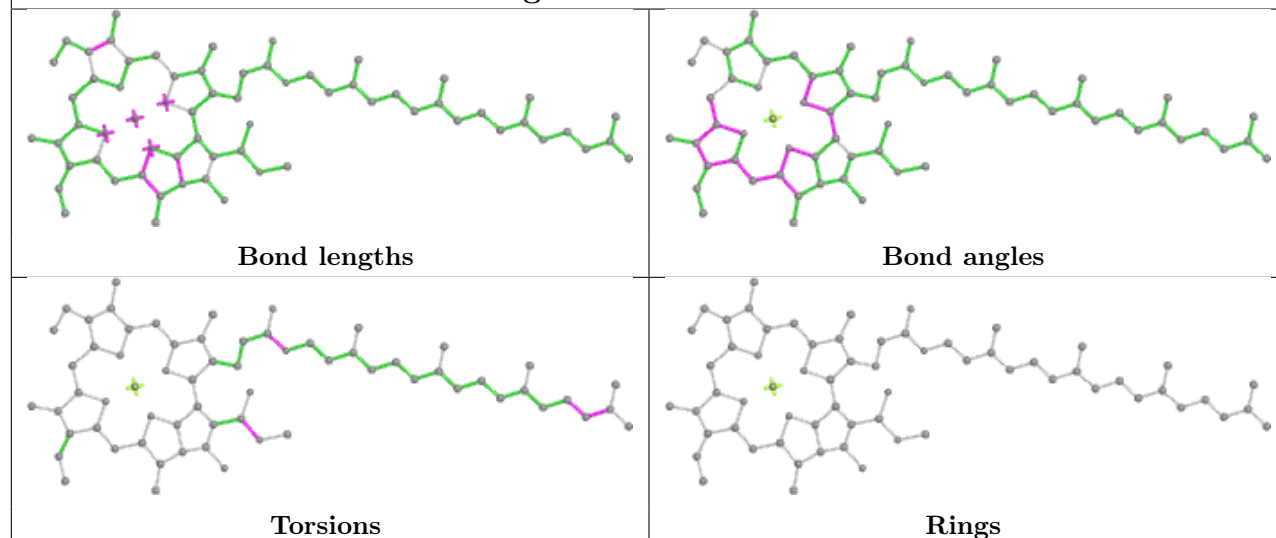


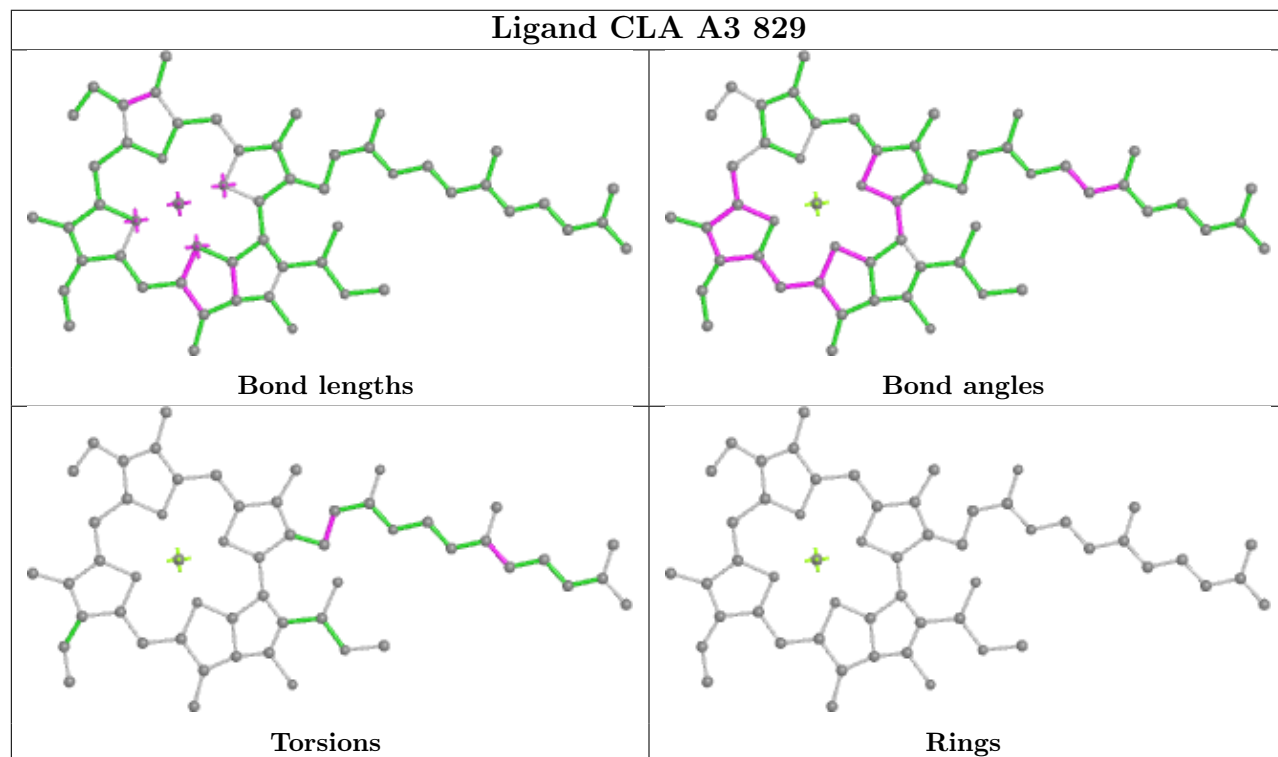
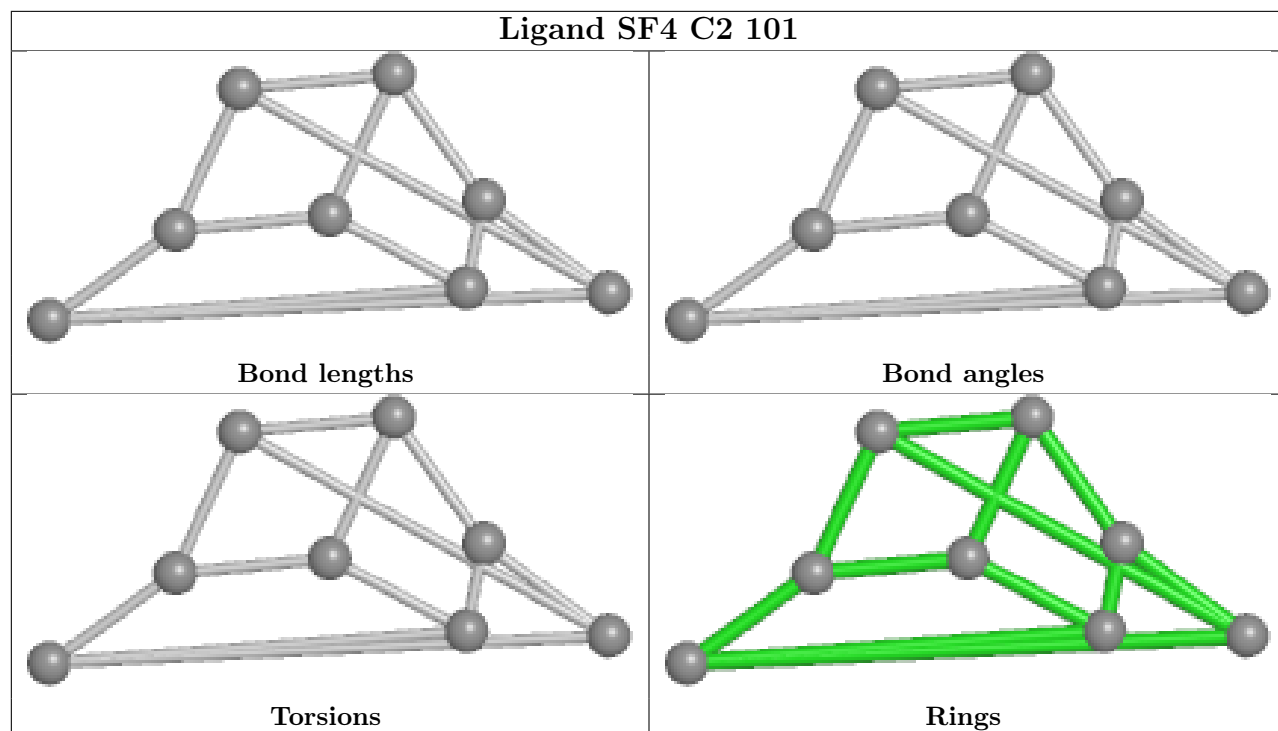


## Ligand CLA K1 103

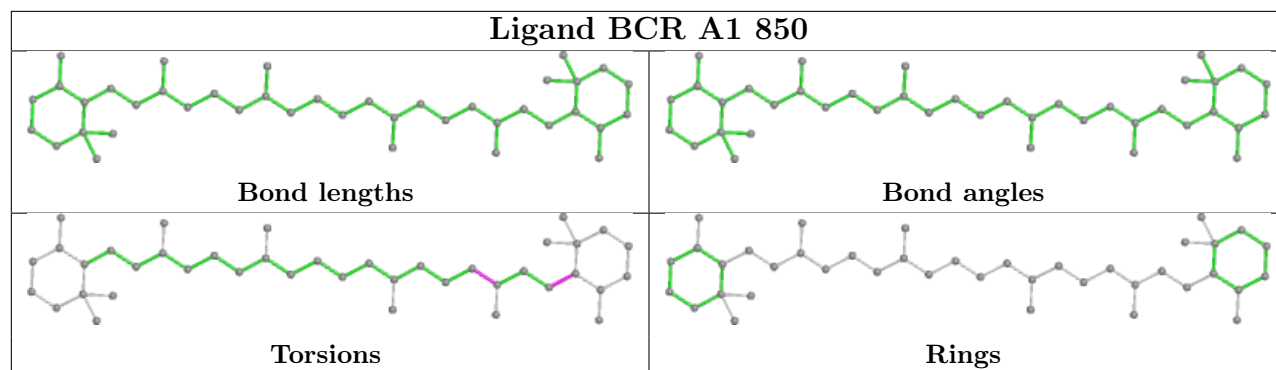


## Ligand CLA B1 839

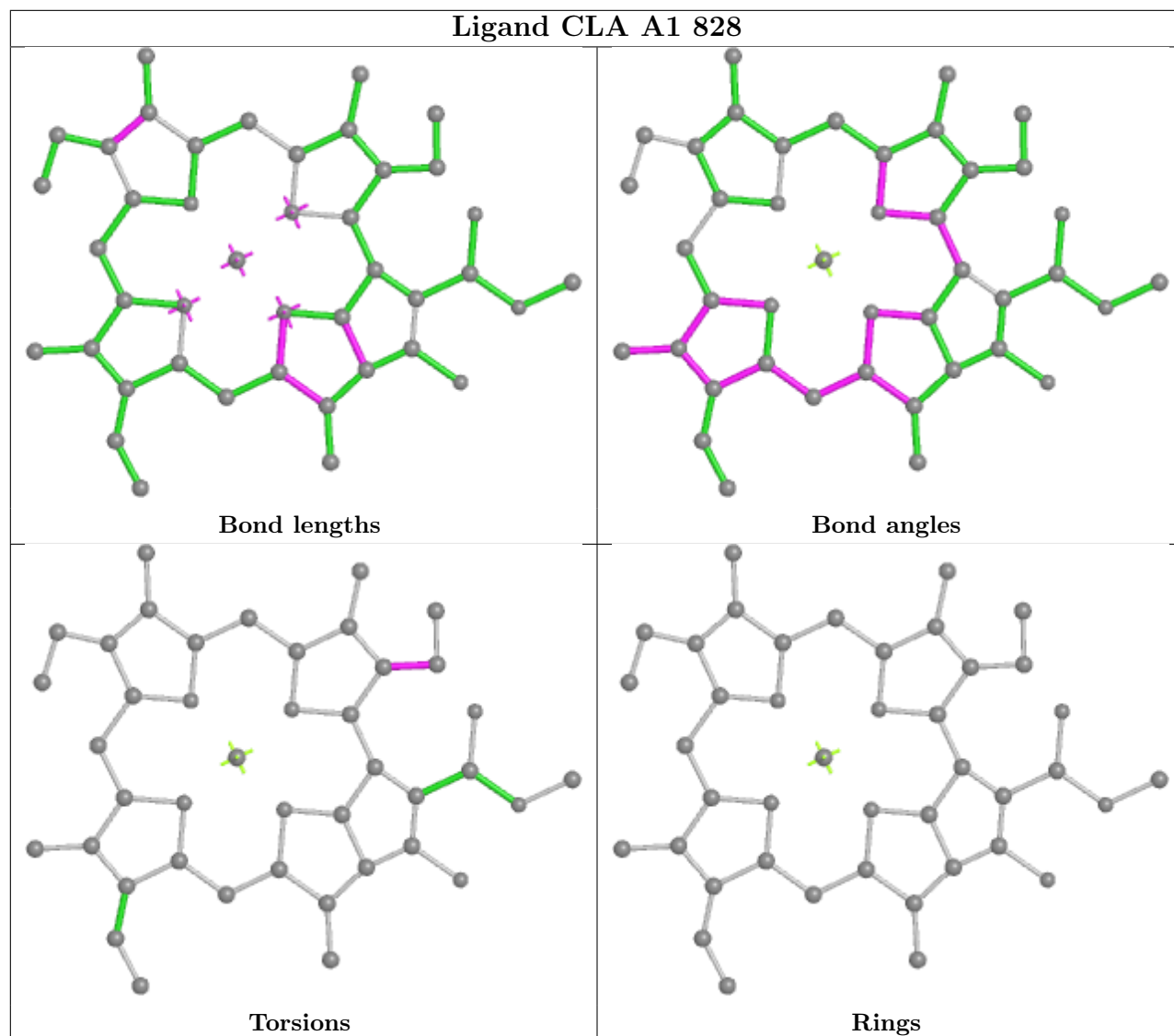


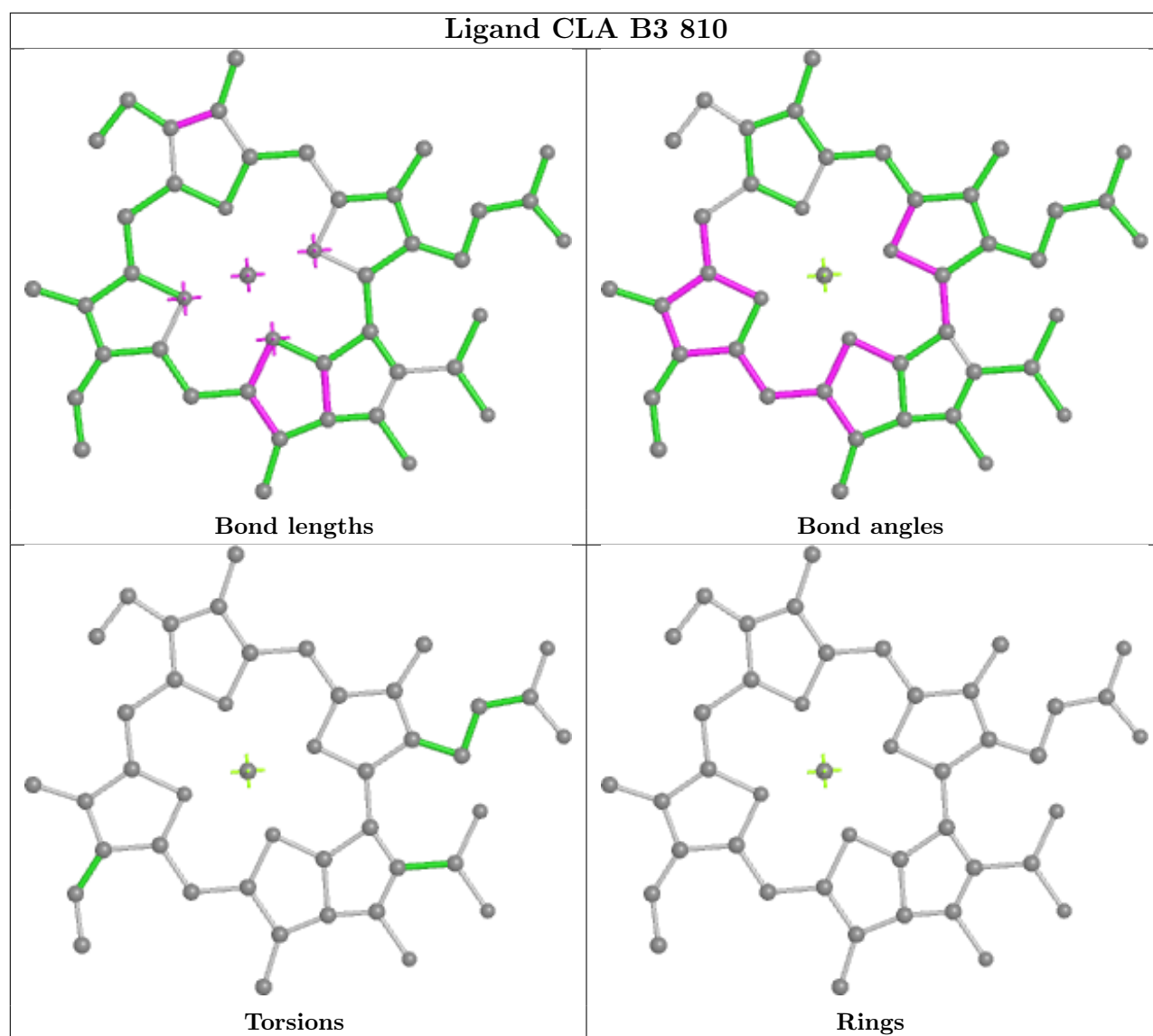


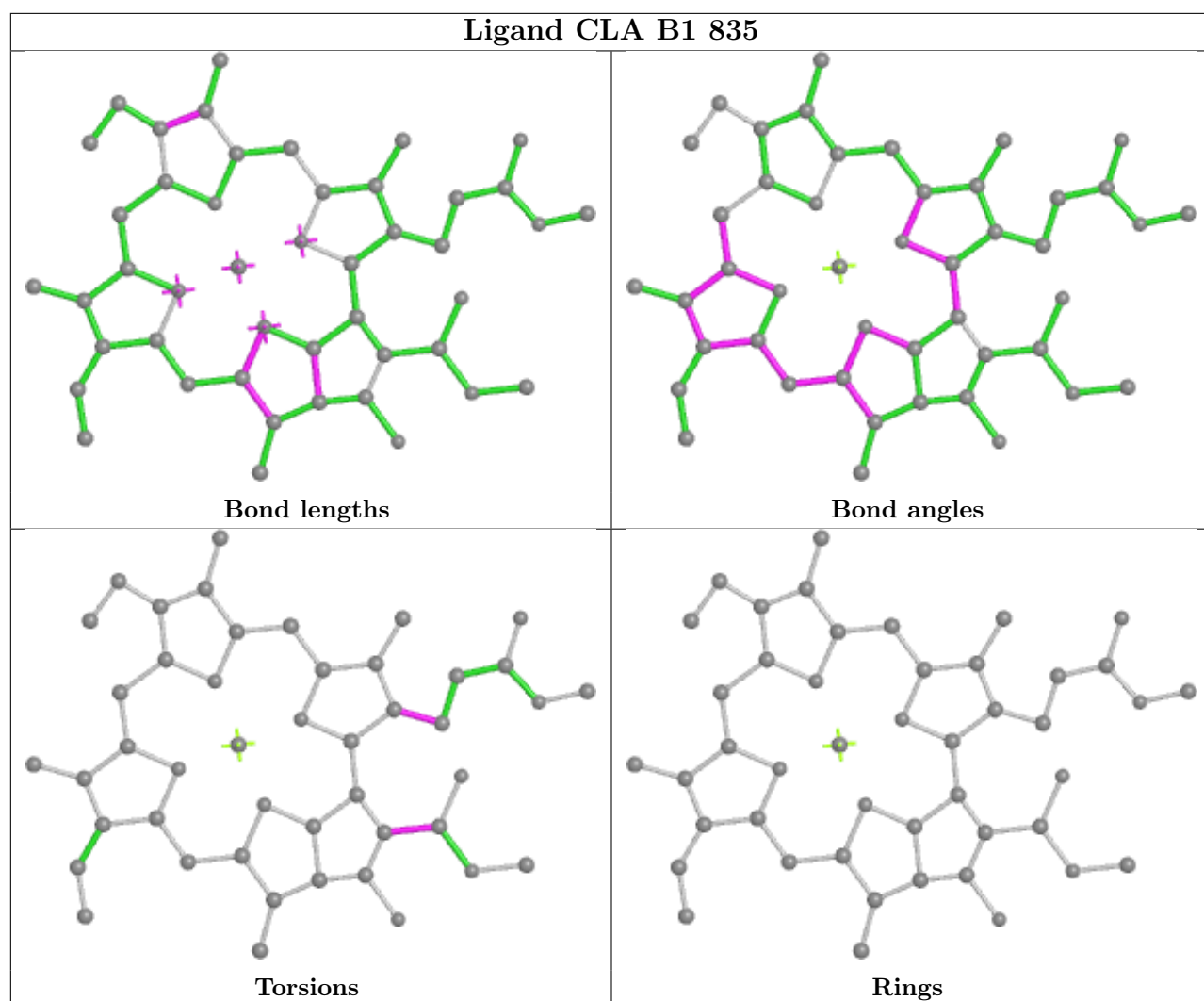
## Ligand BCR A1 850

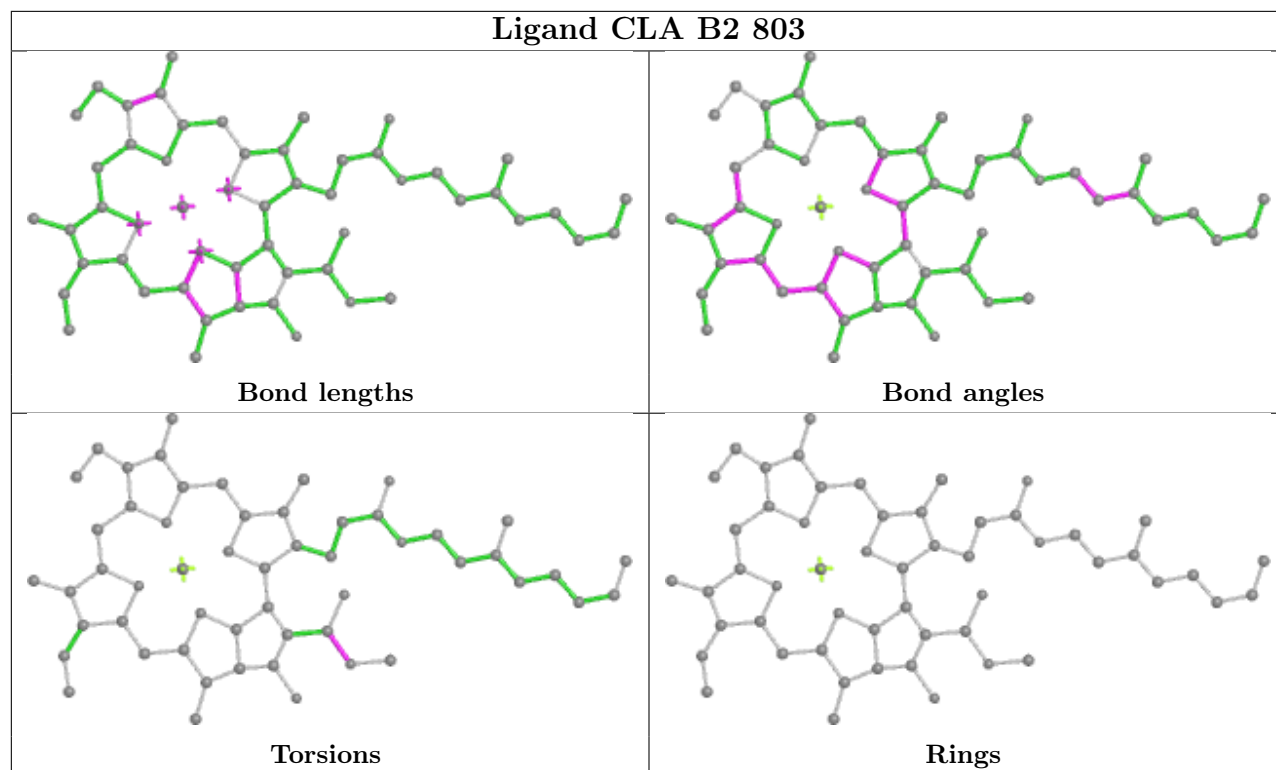


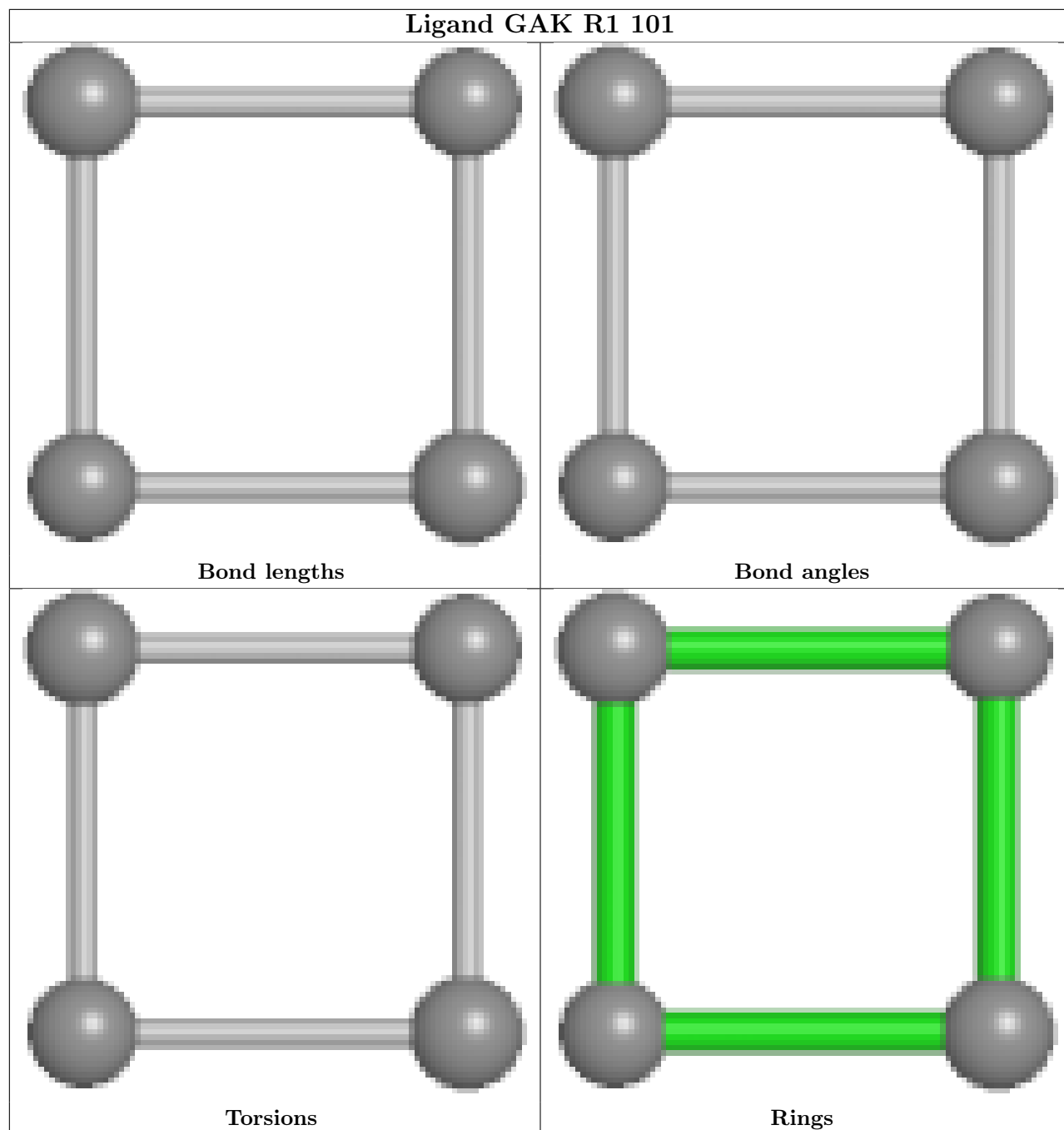
## Ligand CLA A1 828



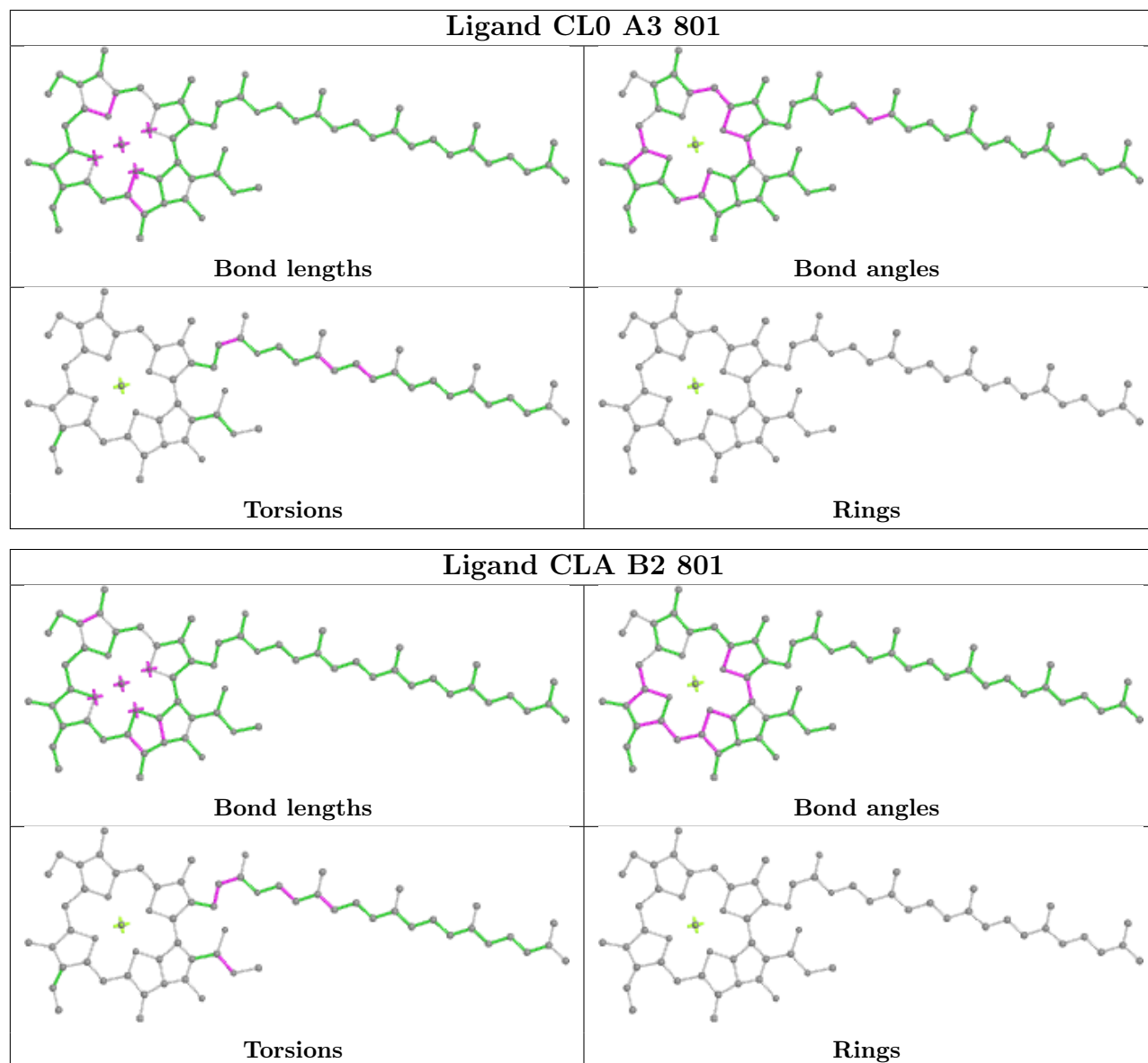




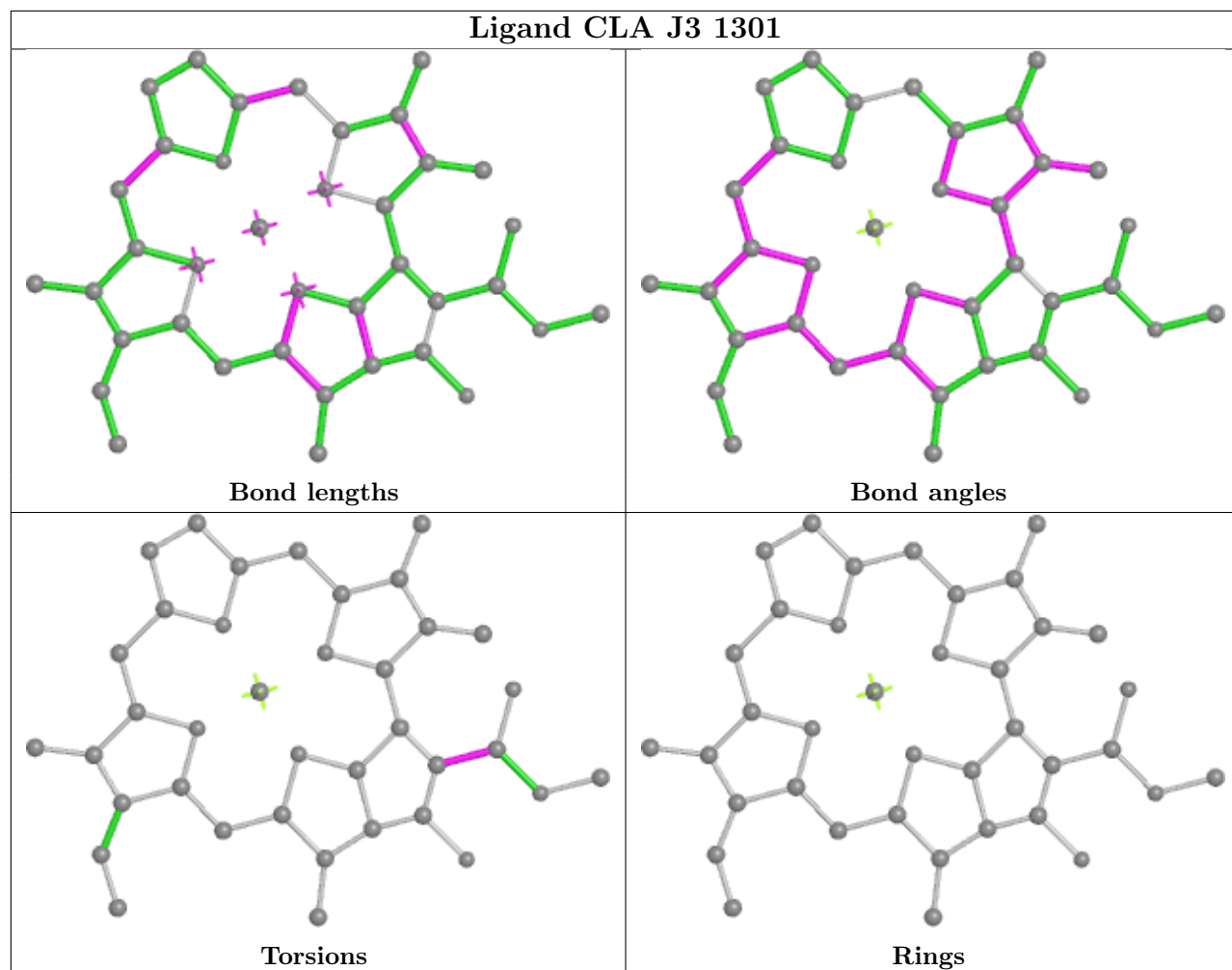




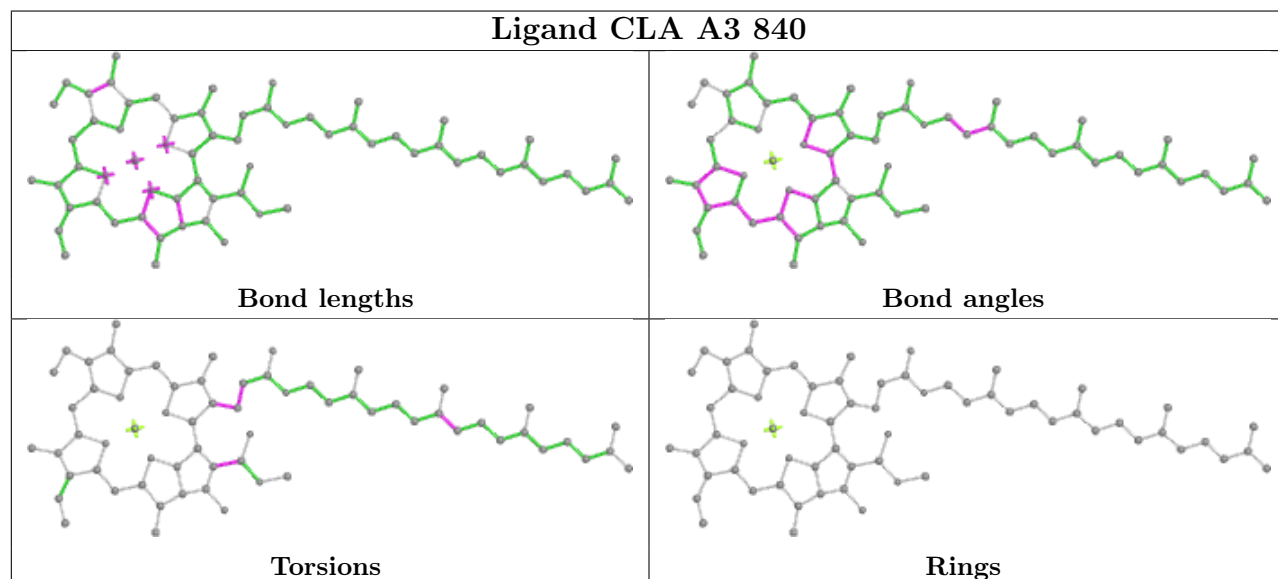


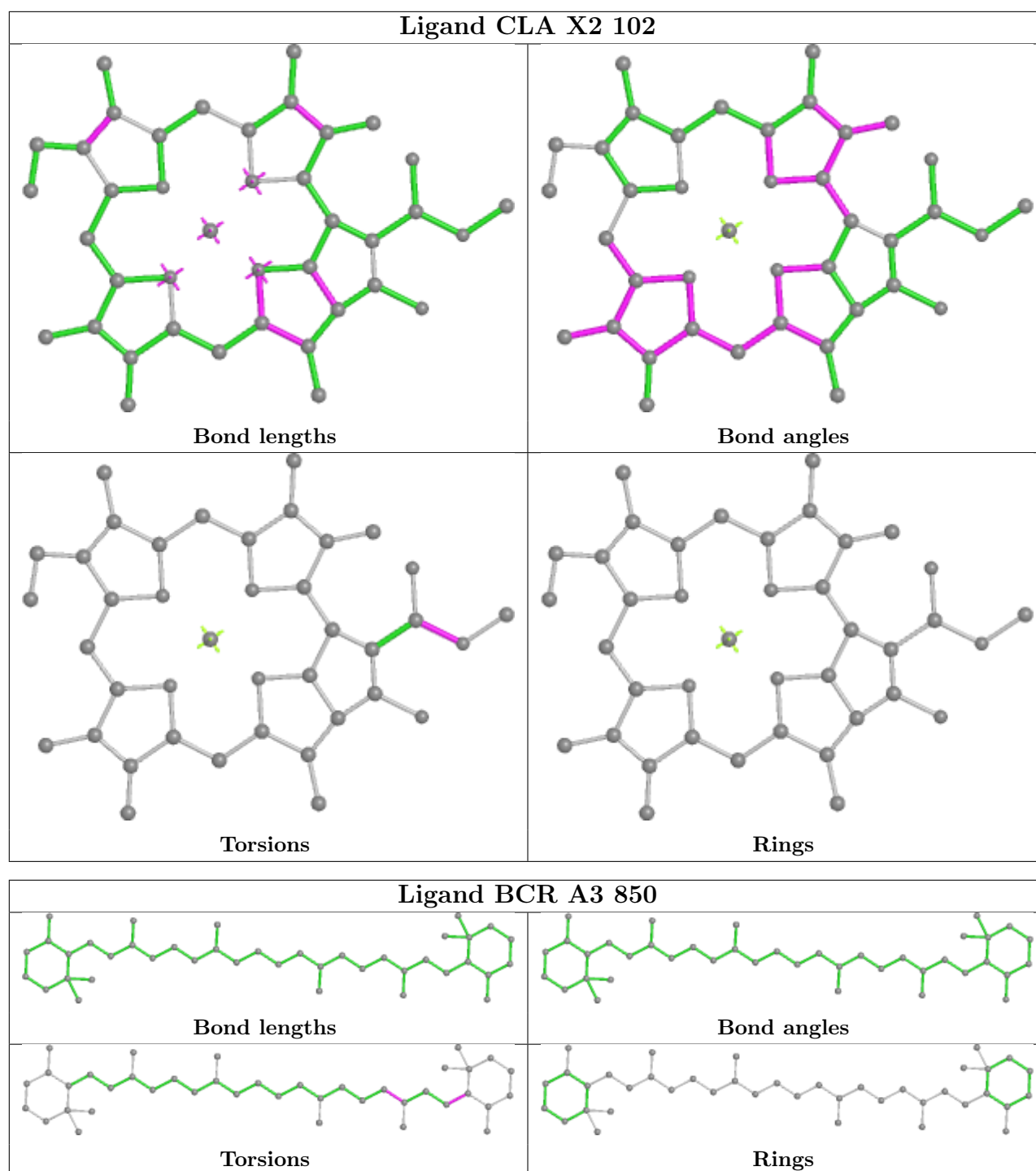


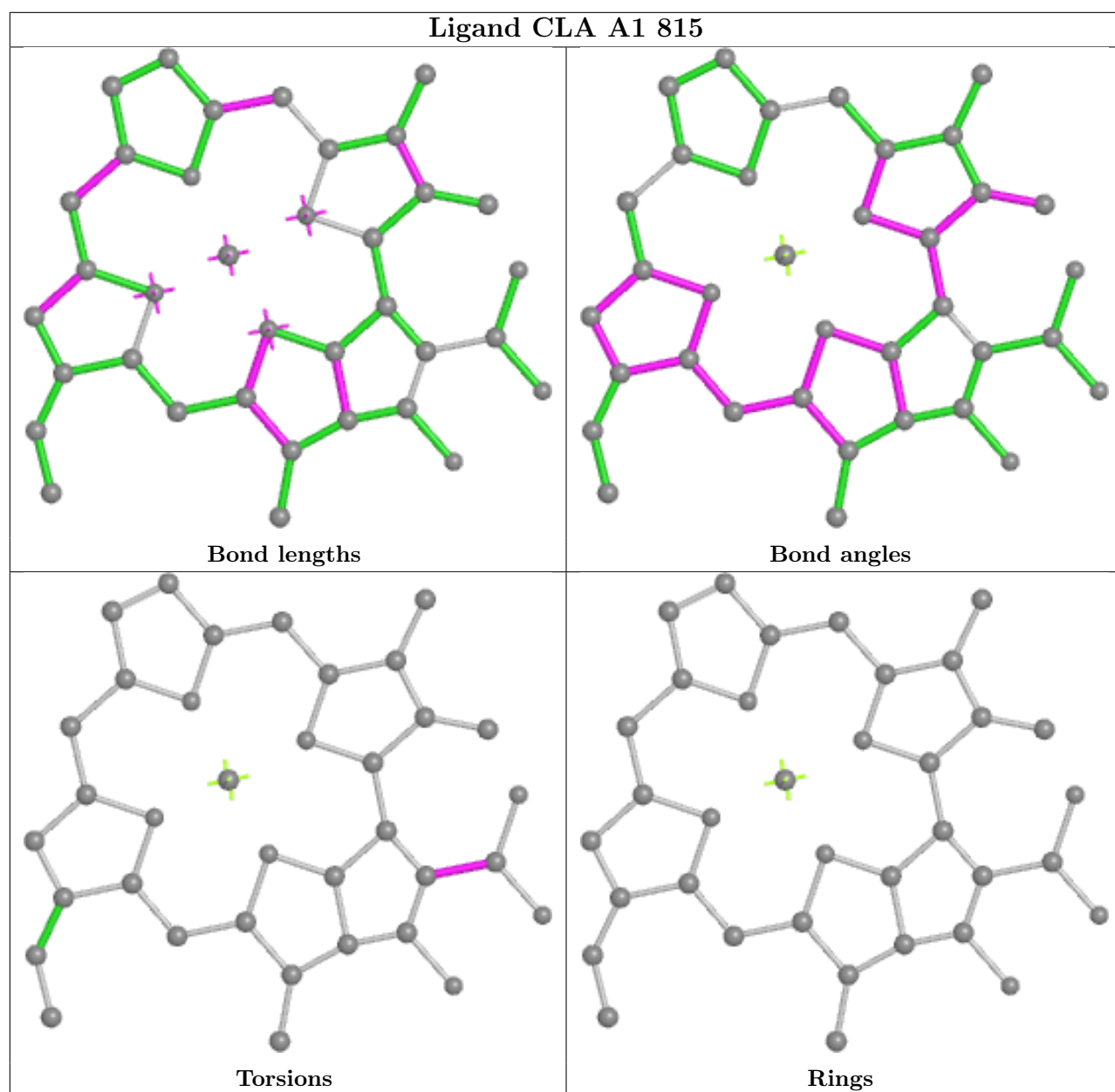
## Ligand CLA J3 1301



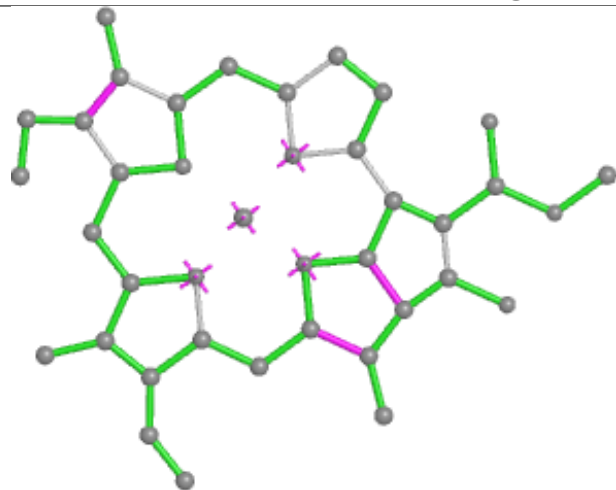
## Ligand CLA A3 840



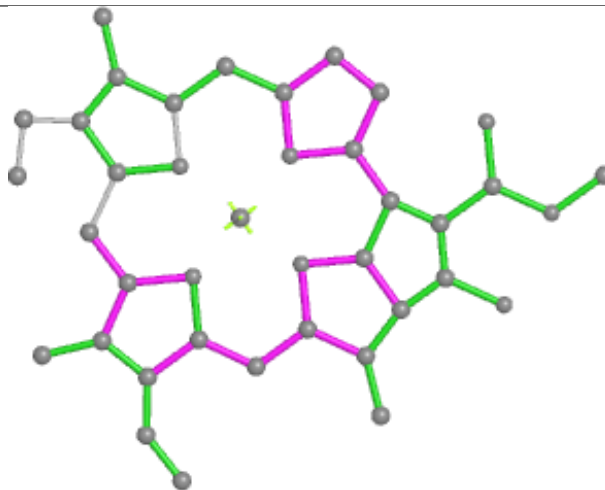




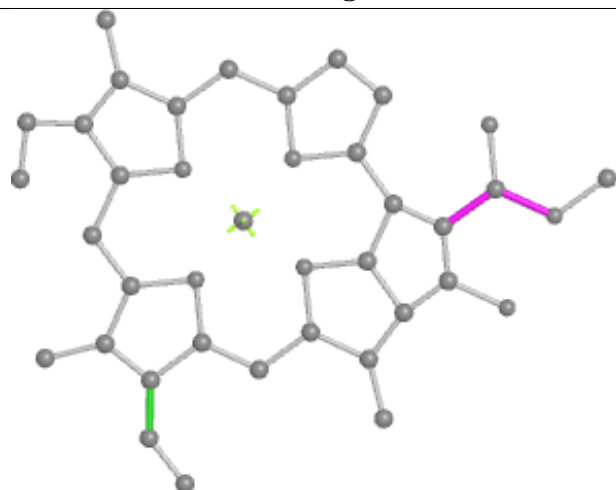
## Ligand CLA B3 821



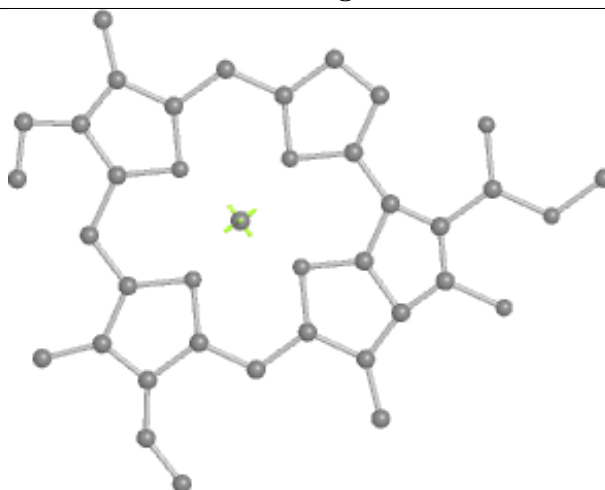
Bond lengths



Bond angles

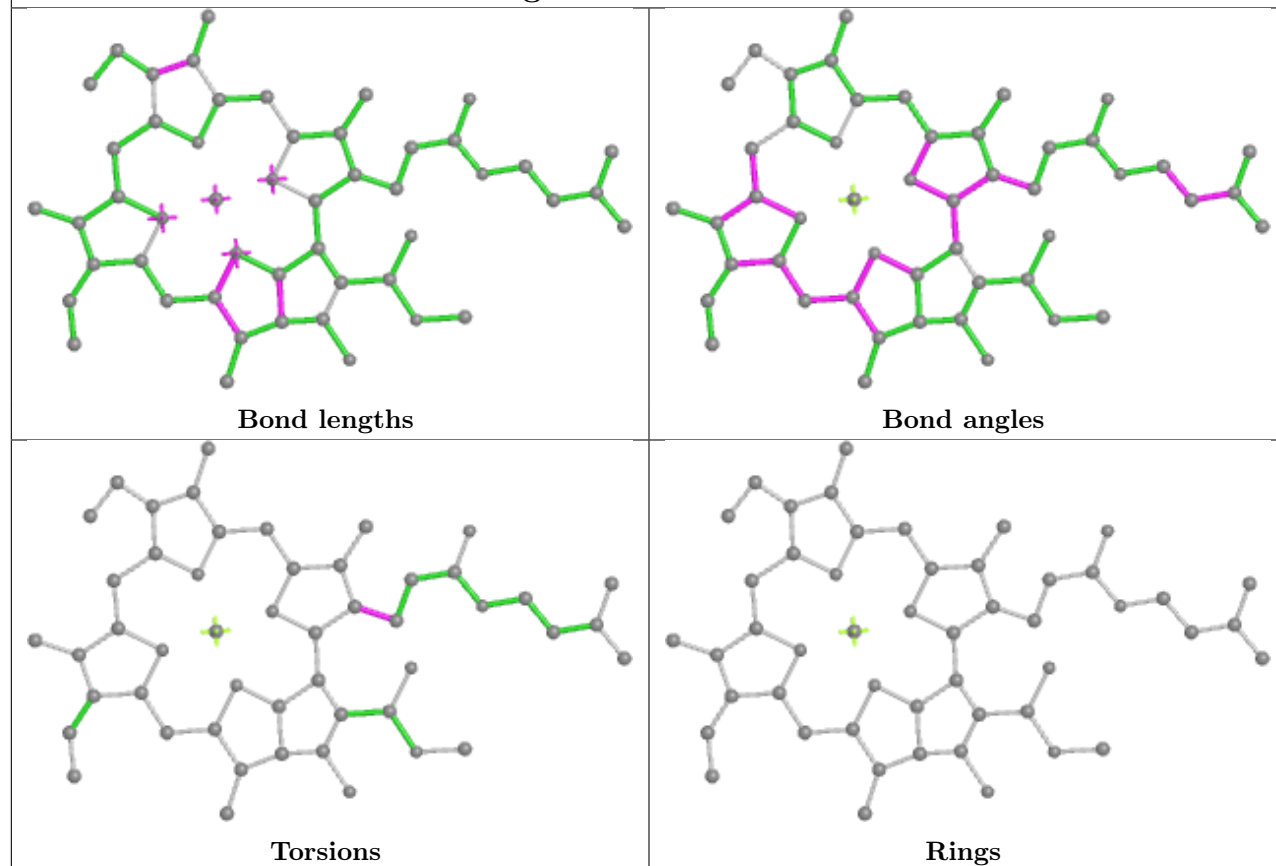


Torsions

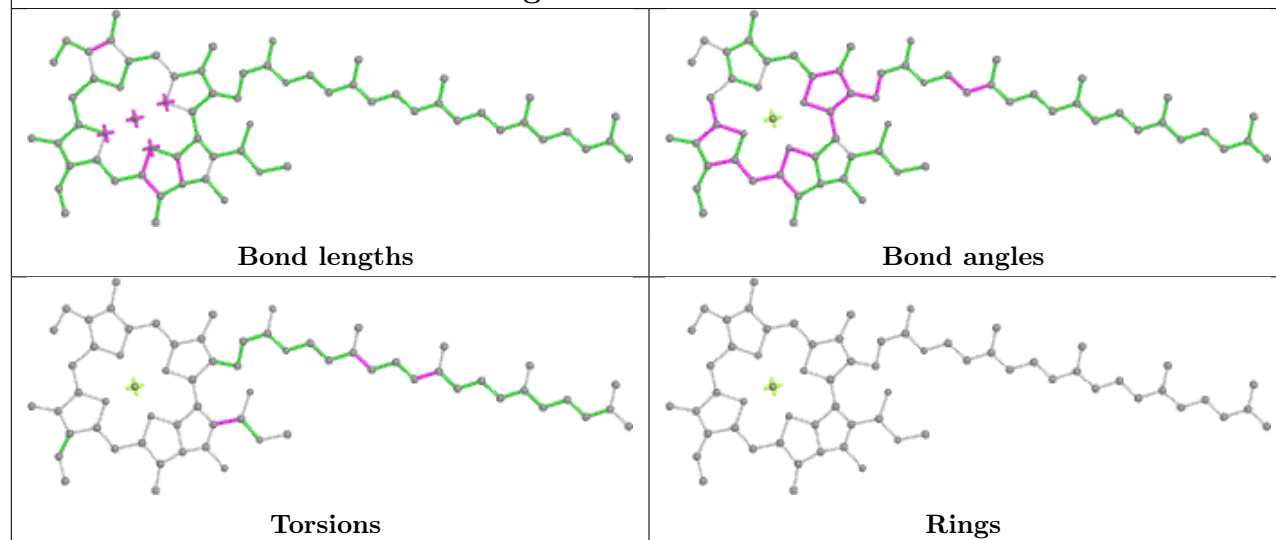


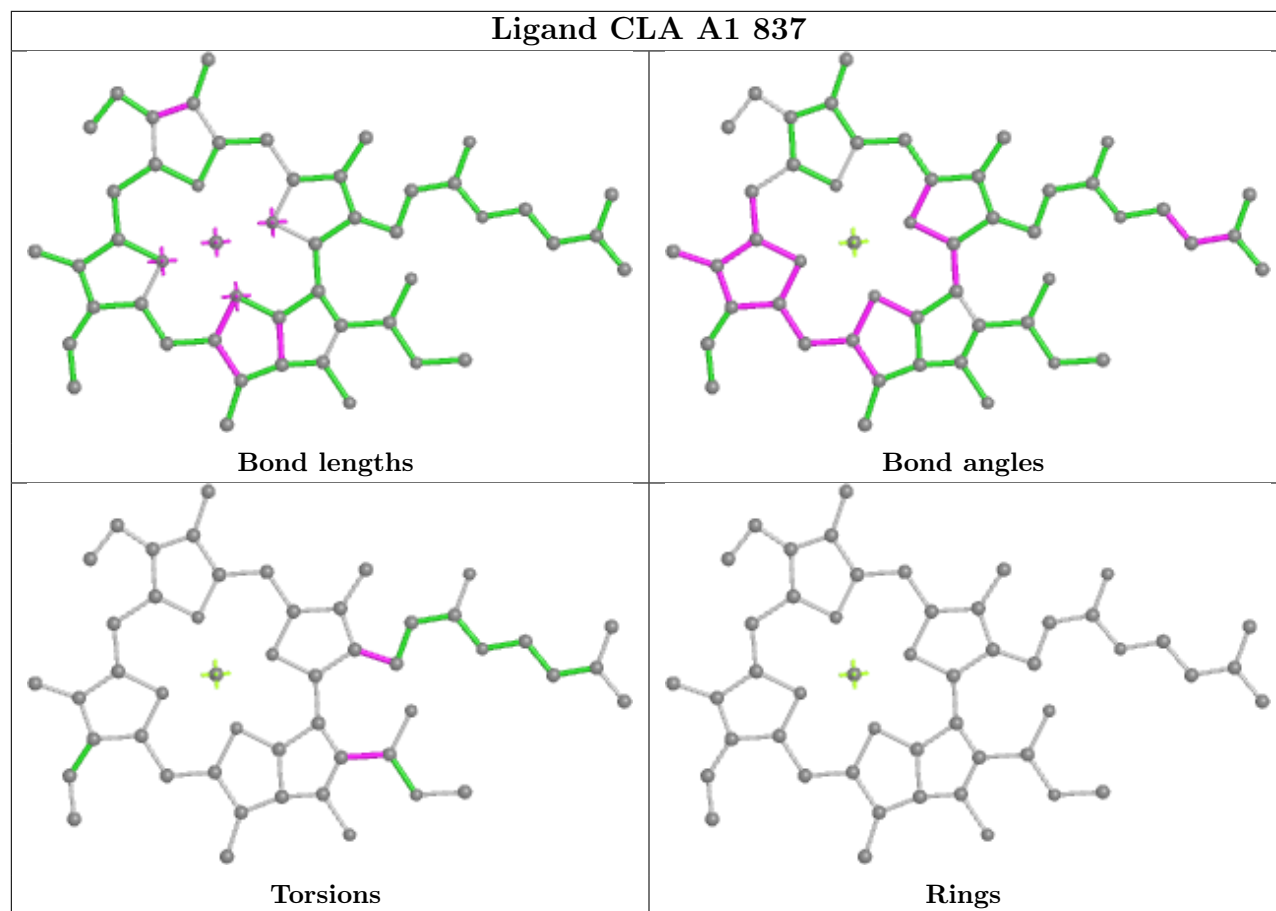
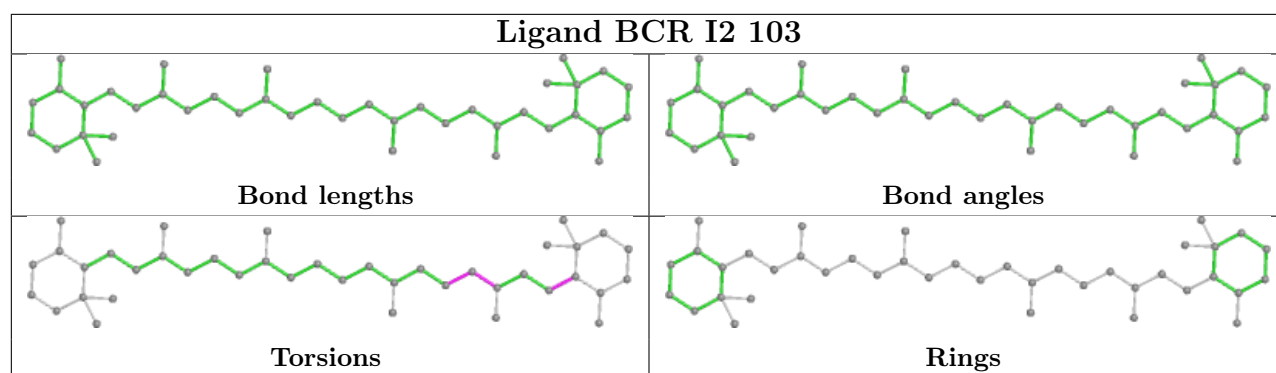
Rings

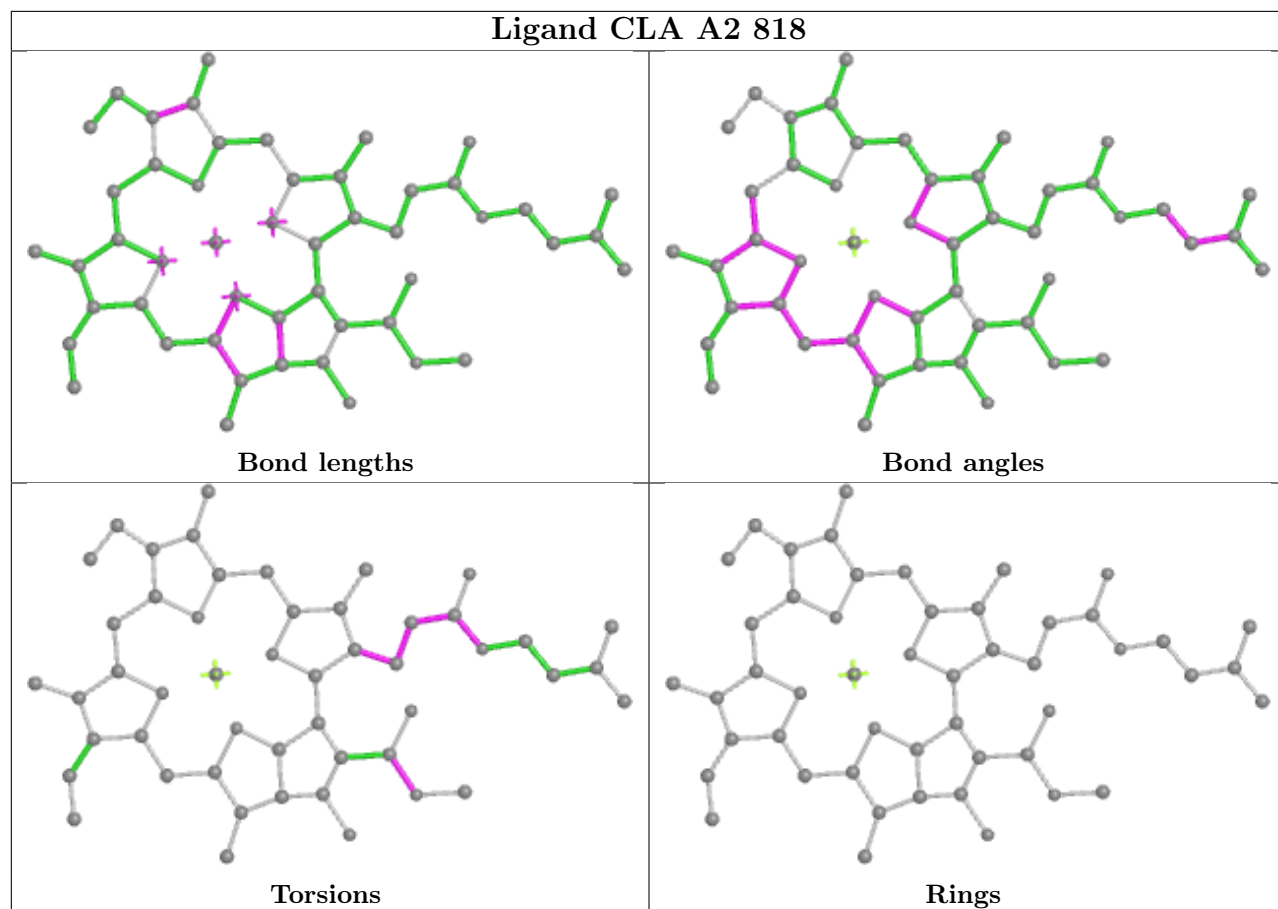
## Ligand CLA B2 817



## Ligand CLA B2 808

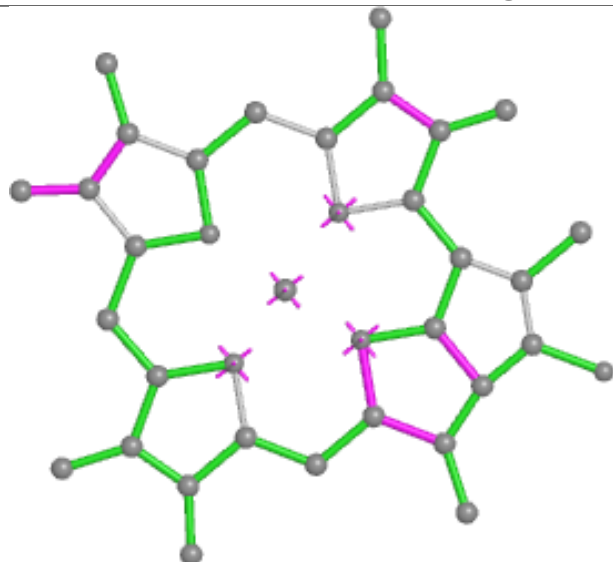




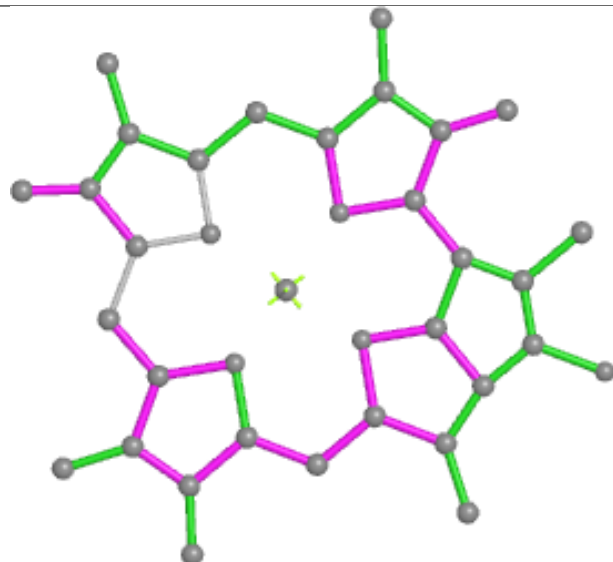




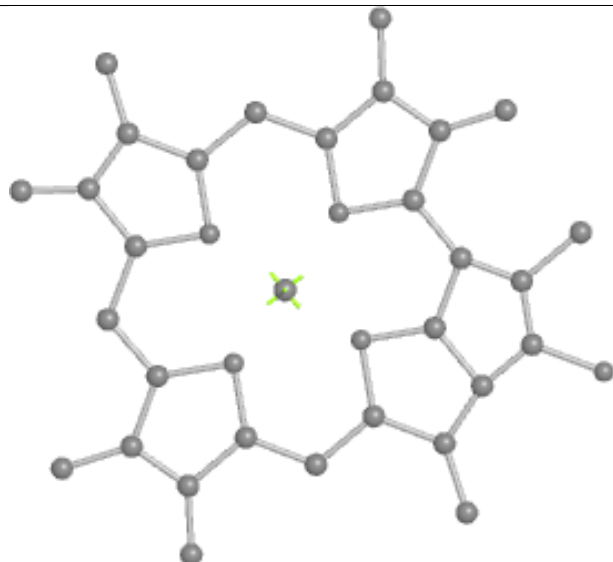
## Ligand CLA J2 1303



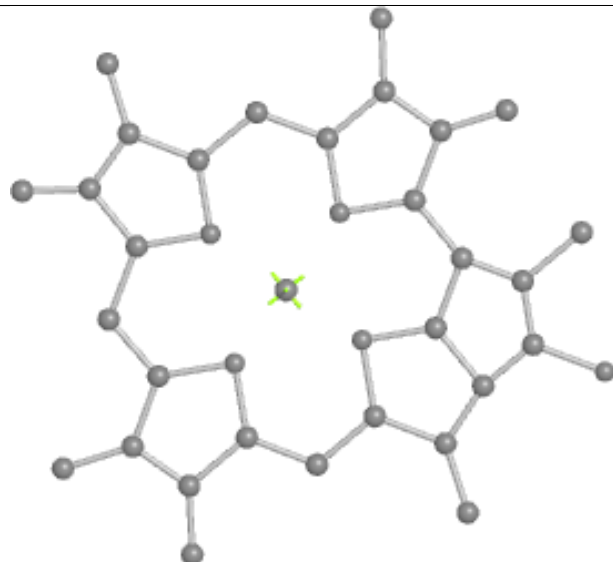
Bond lengths



Bond angles

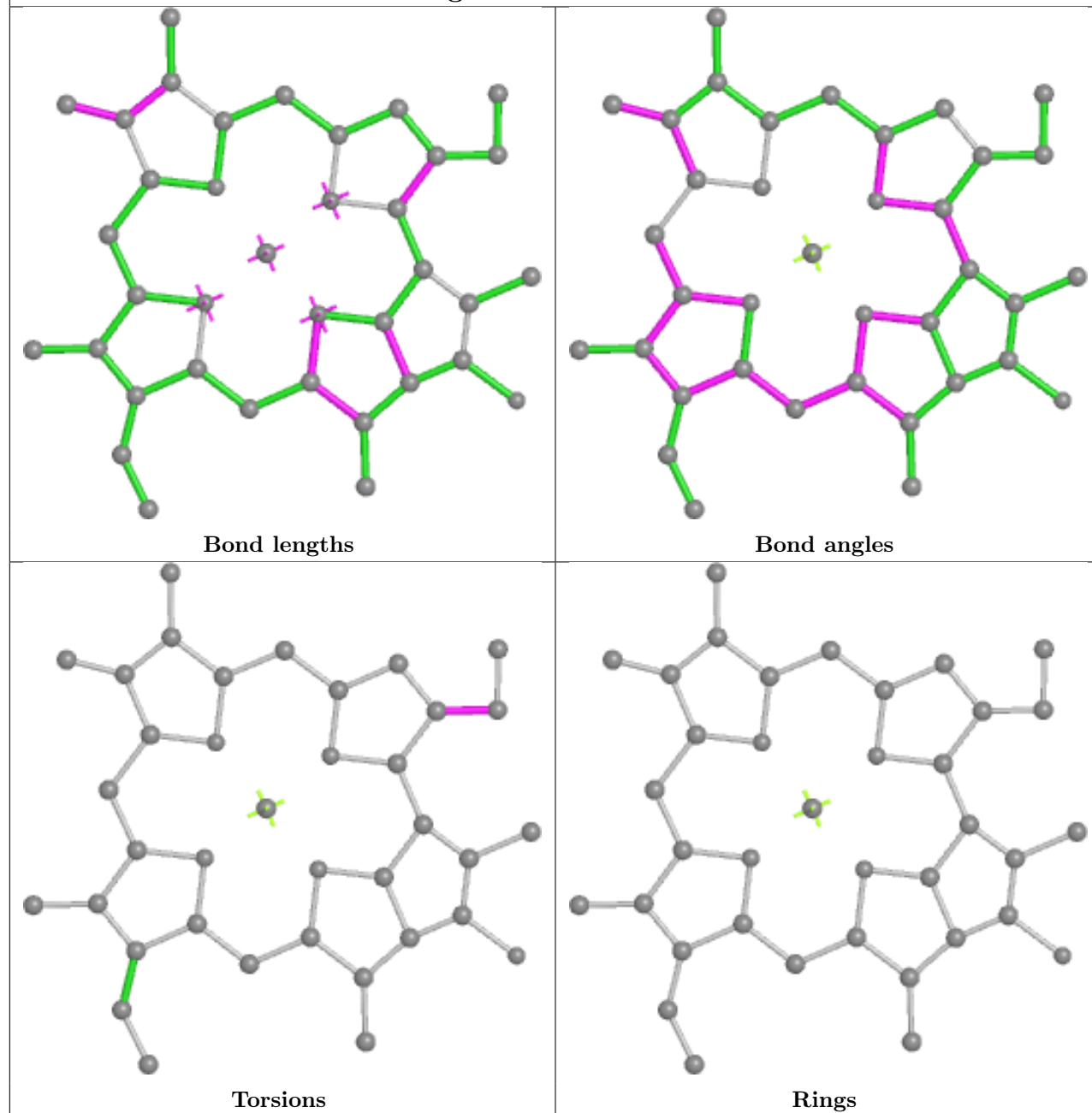


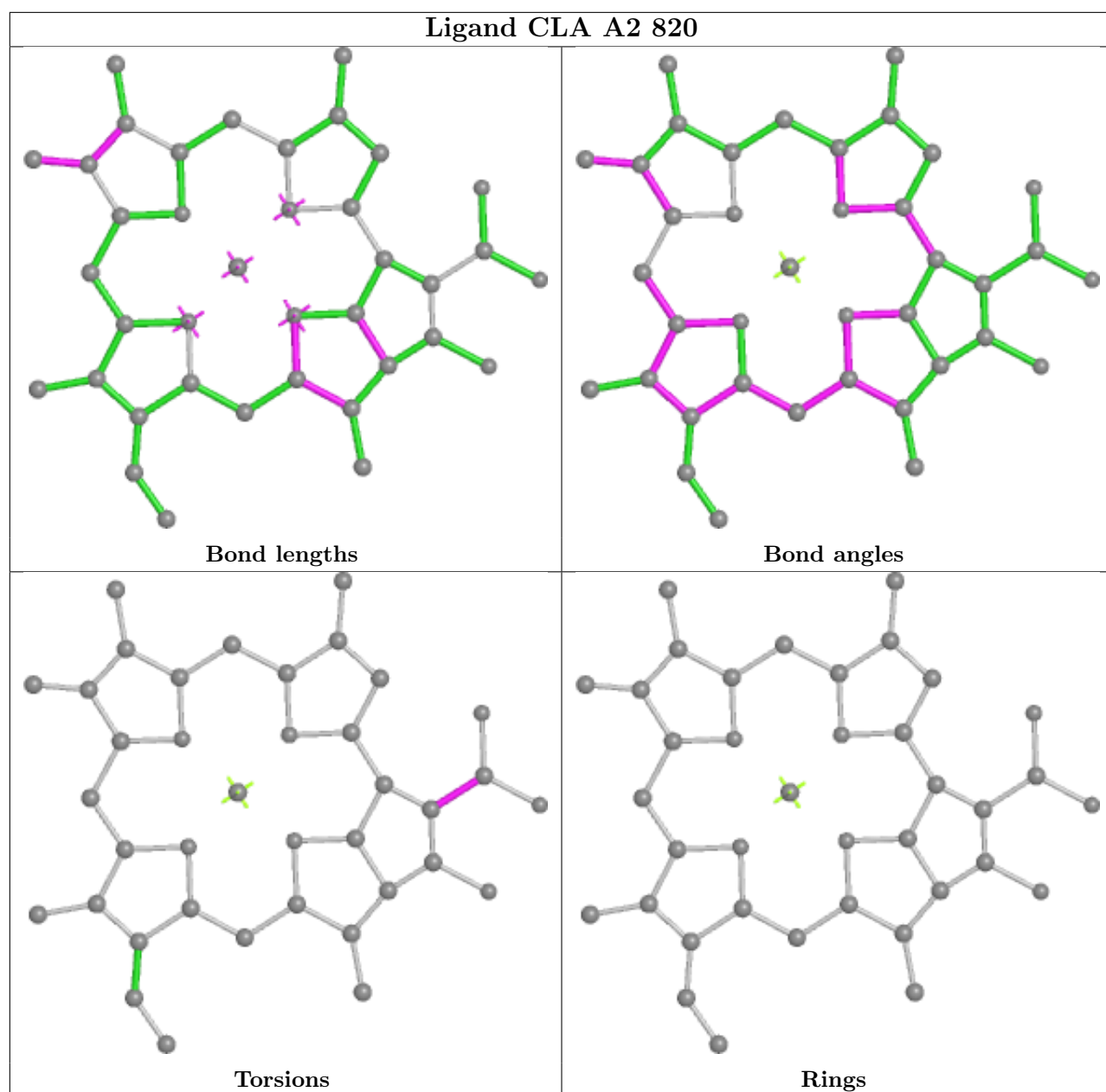
Torsions



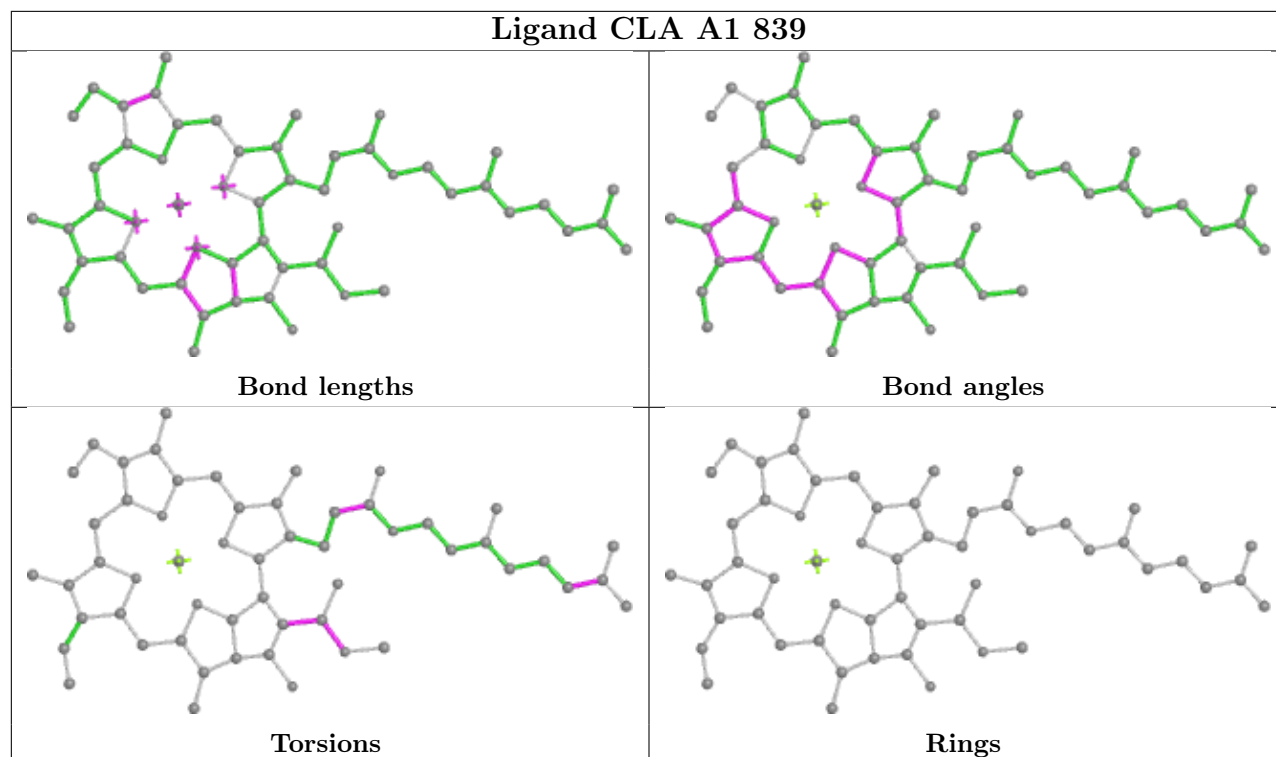
Rings

## Ligand CLA B2 833

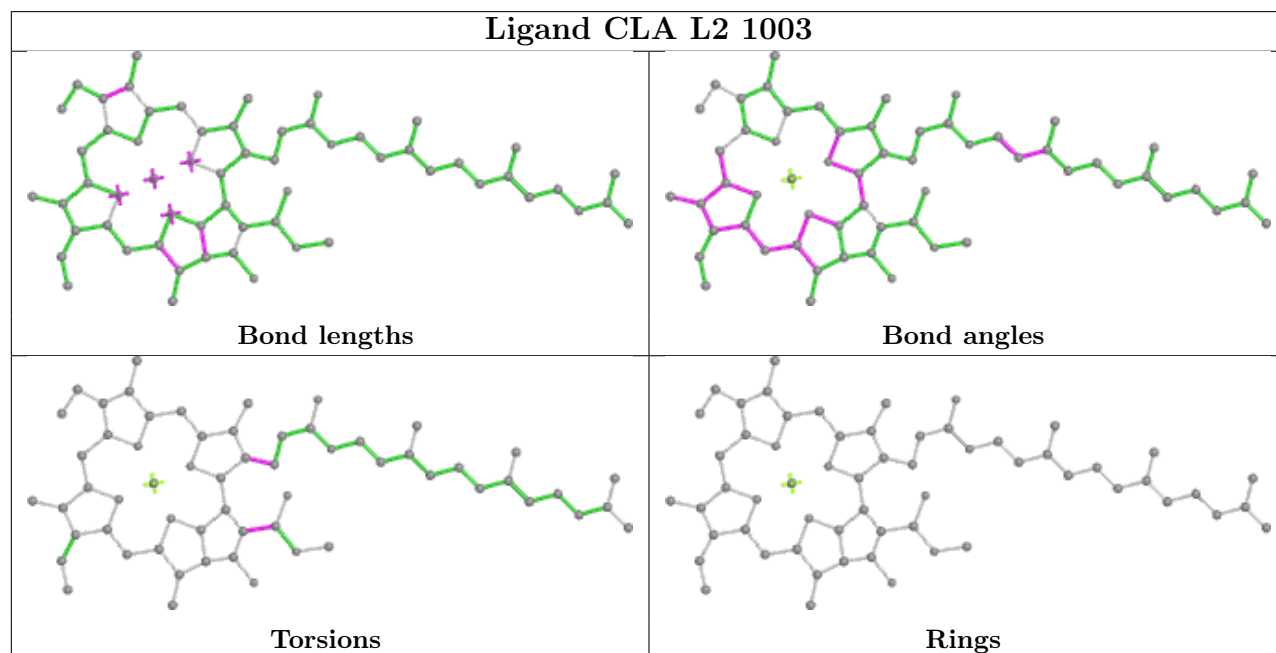




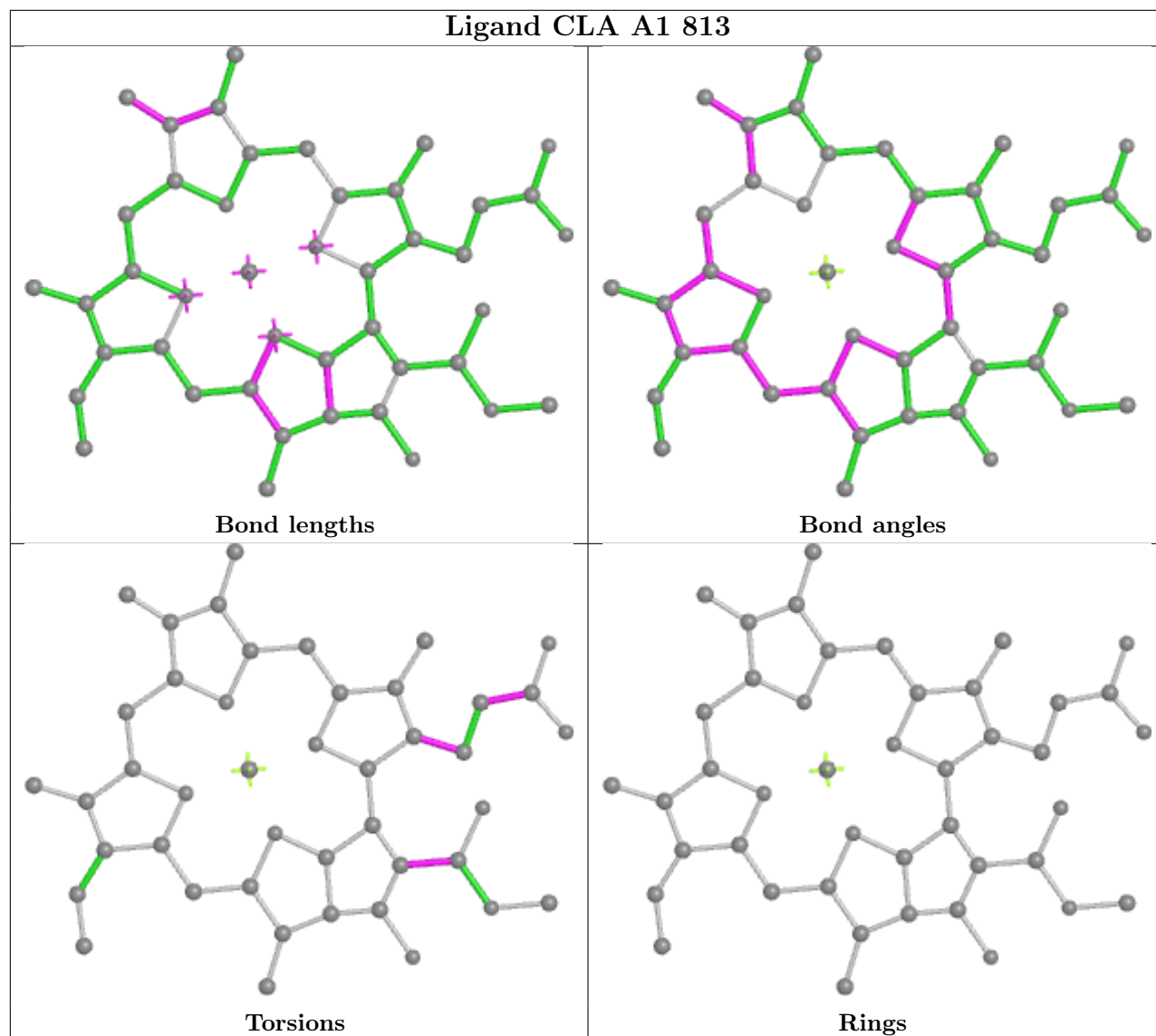
## Ligand CLA A1 839



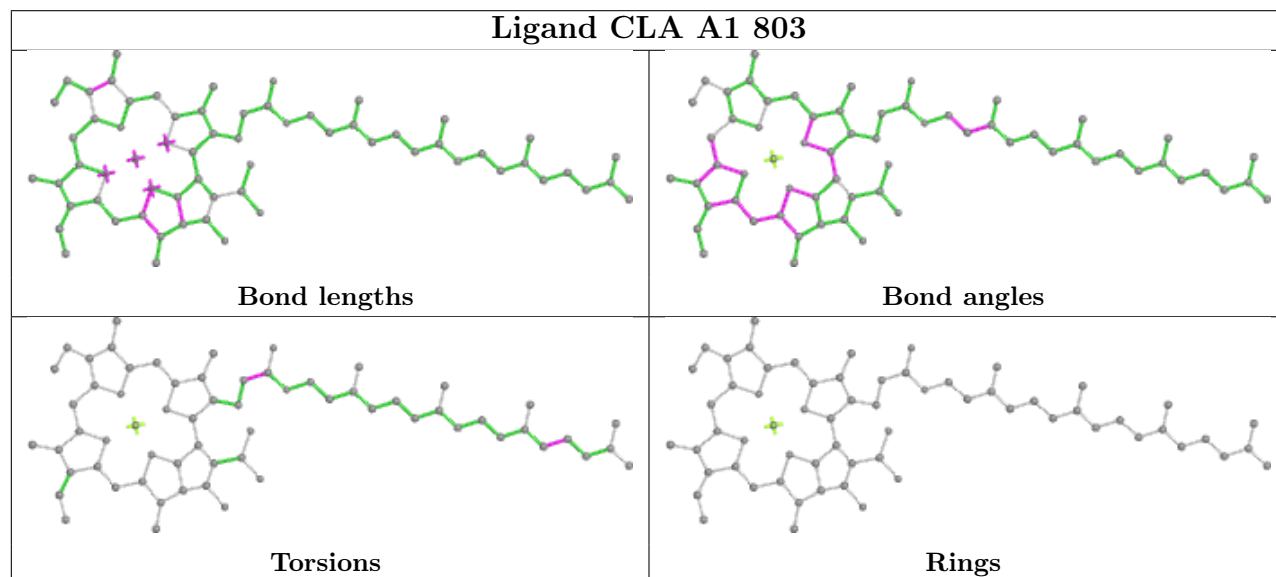
## Ligand CLA L2 1003

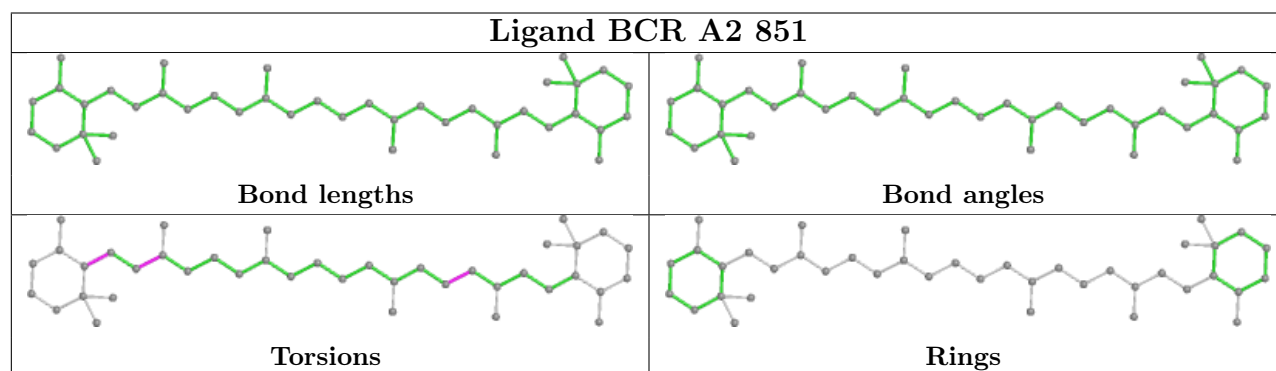
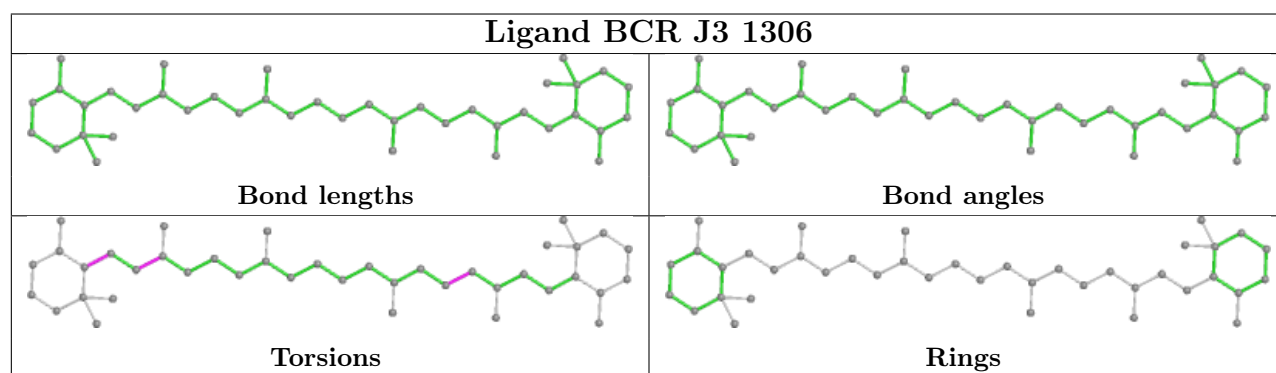
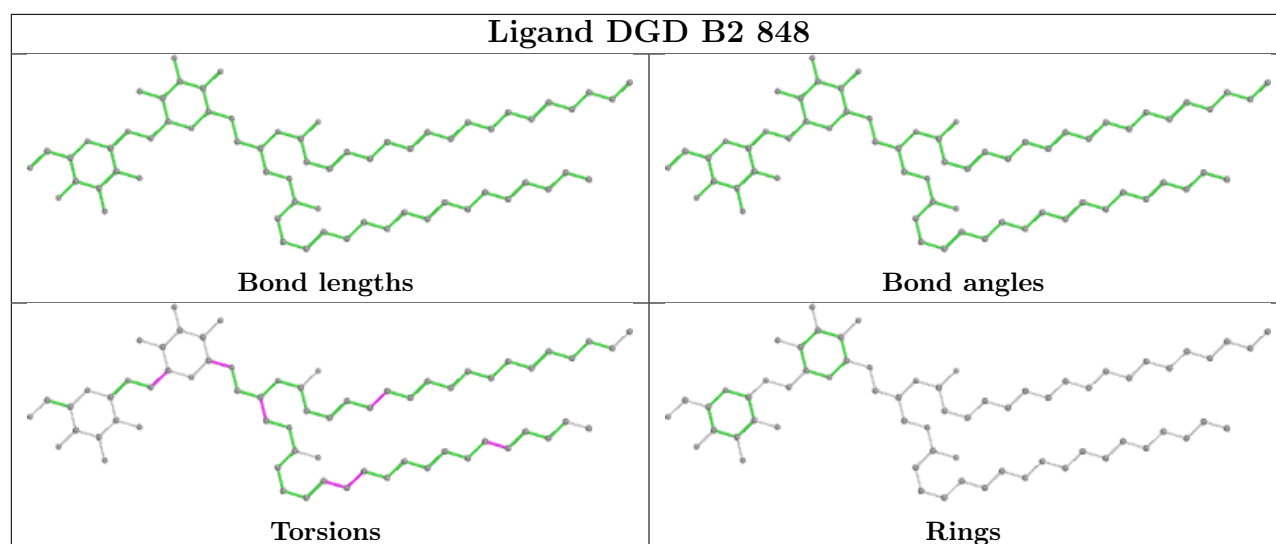


## Ligand CLA A1 813

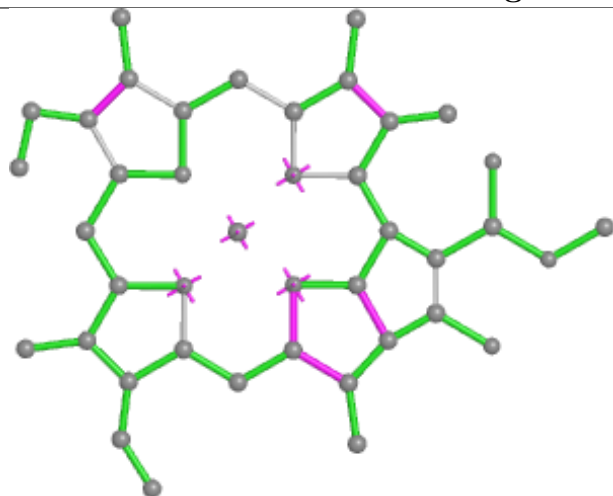


## Ligand CLA A1 803

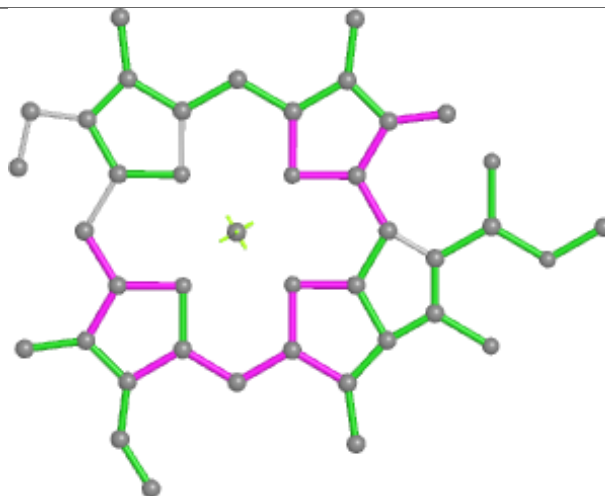




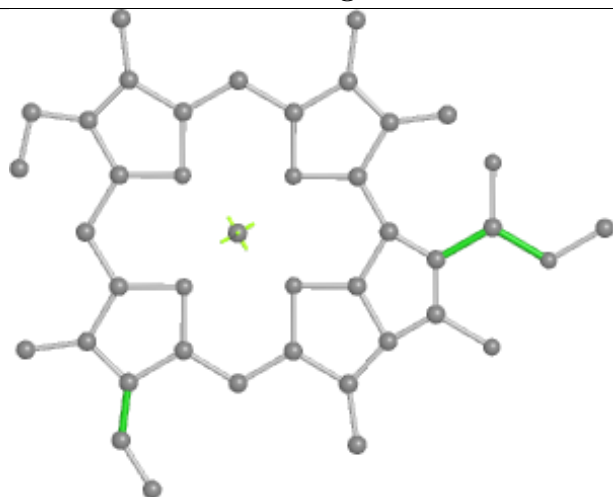
## Ligand CLA A1 816



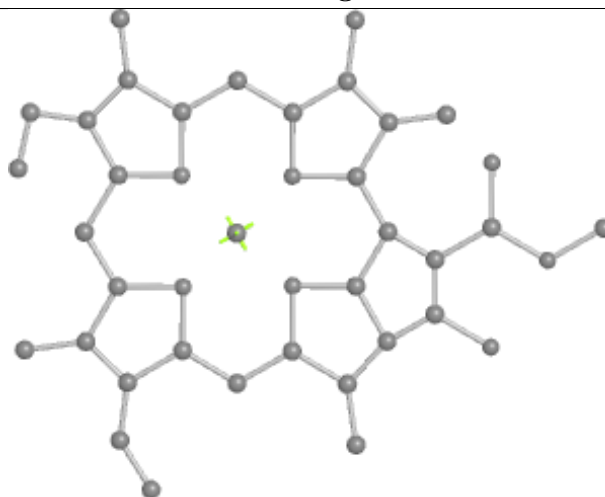
Bond lengths



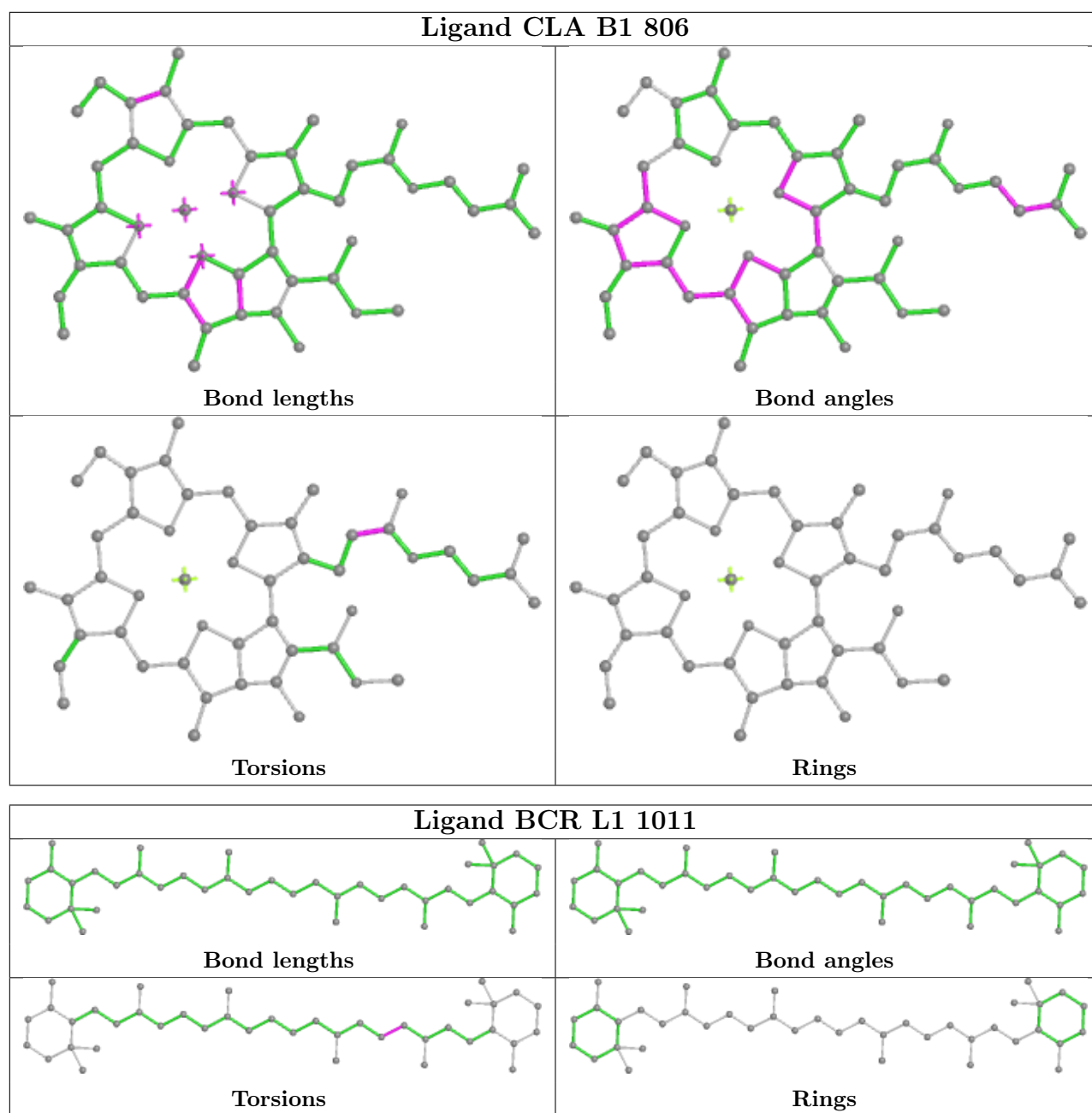
Bond angles



Torsions

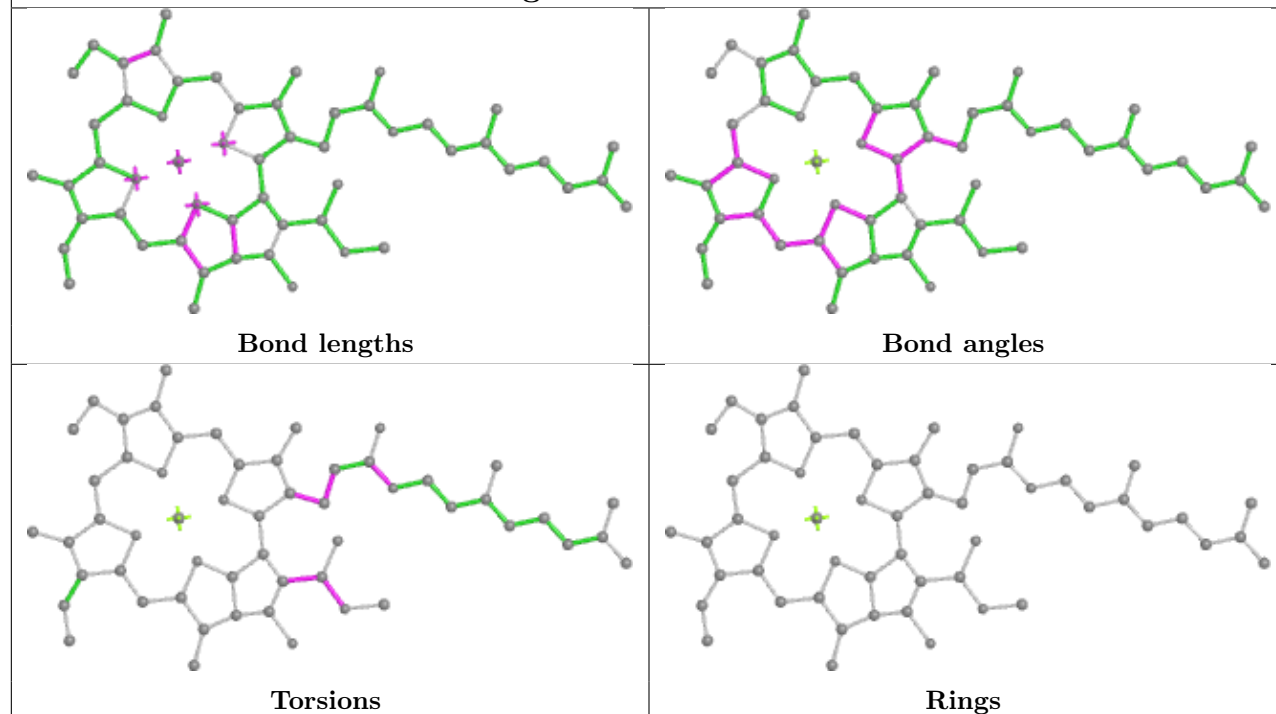


Rings

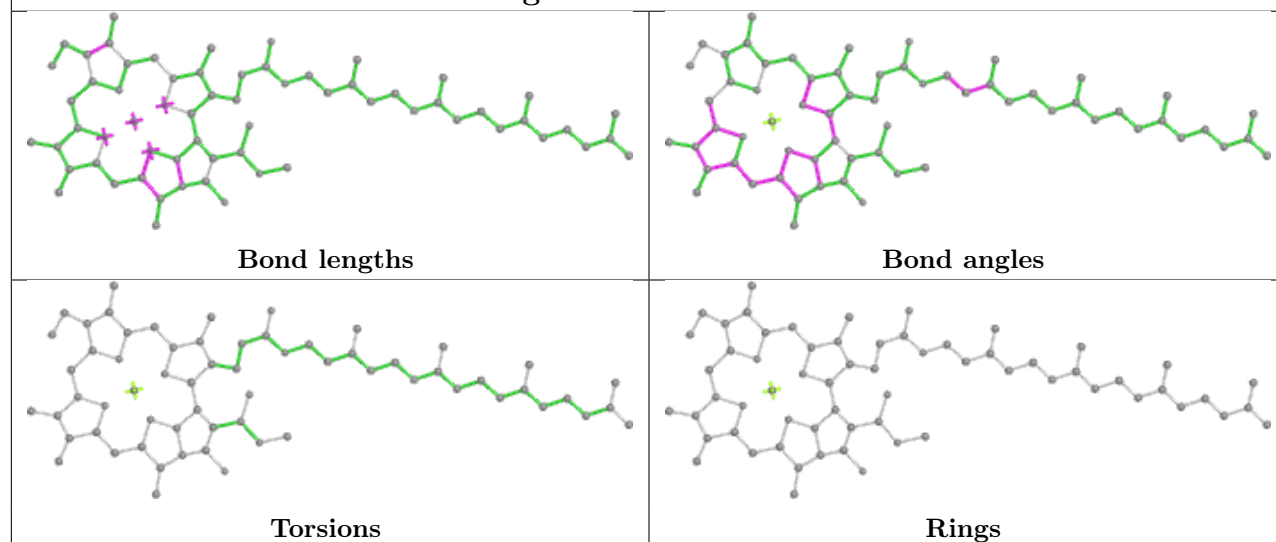




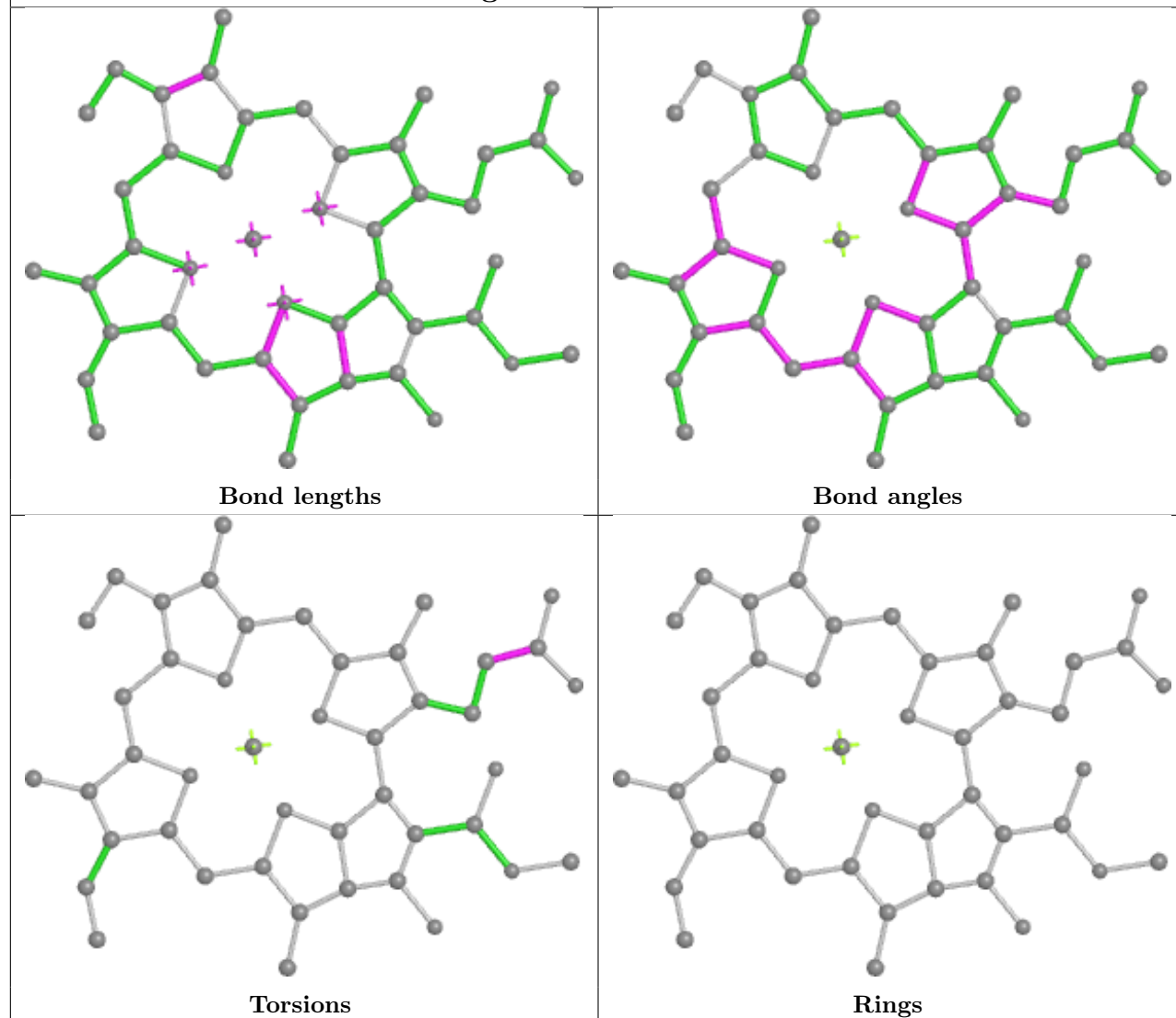
## Ligand CLA A1 838



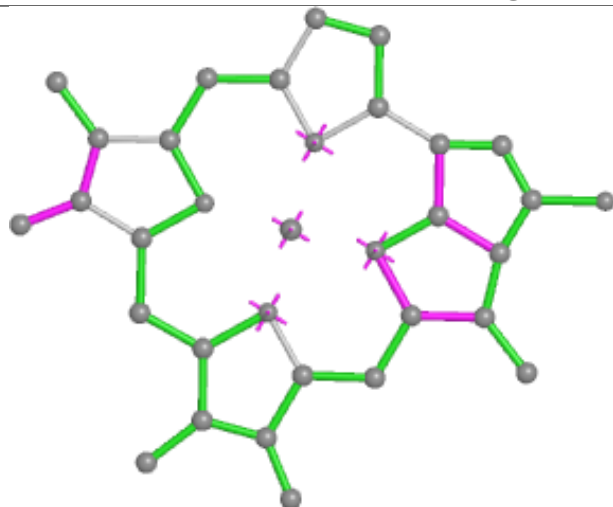
## Ligand CLA A1 821



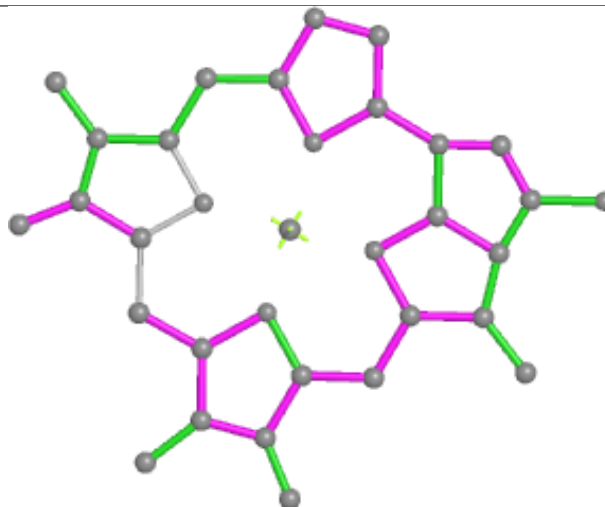
## Ligand CLA A2 822



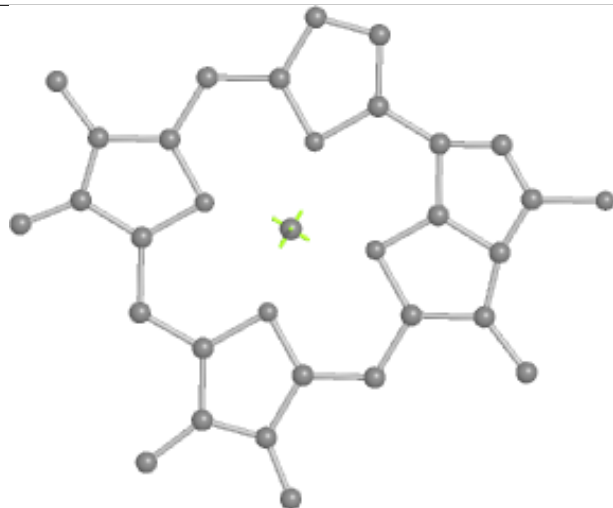
## Ligand CLA A2 814



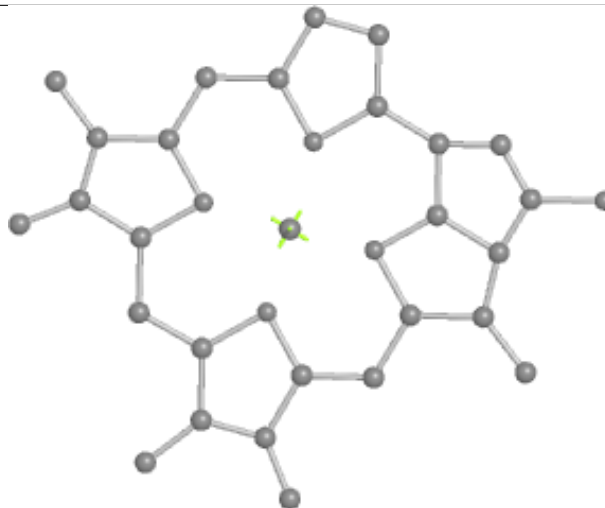
Bond lengths



Bond angles

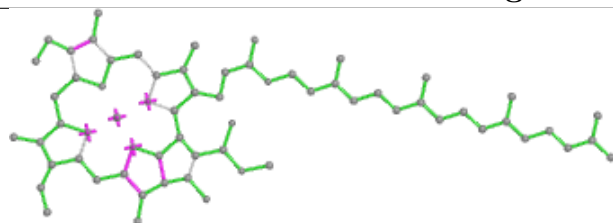


Torsions

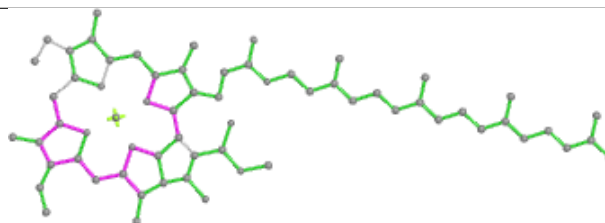


Rings

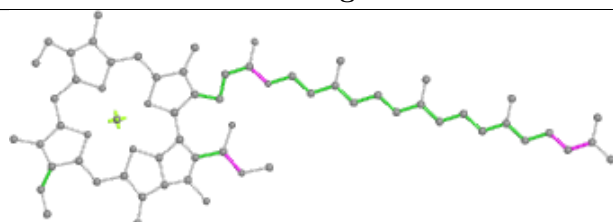
## Ligand CLA B3 839



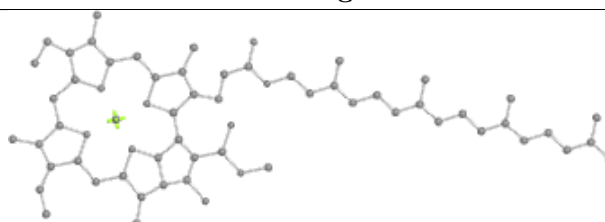
Bond lengths



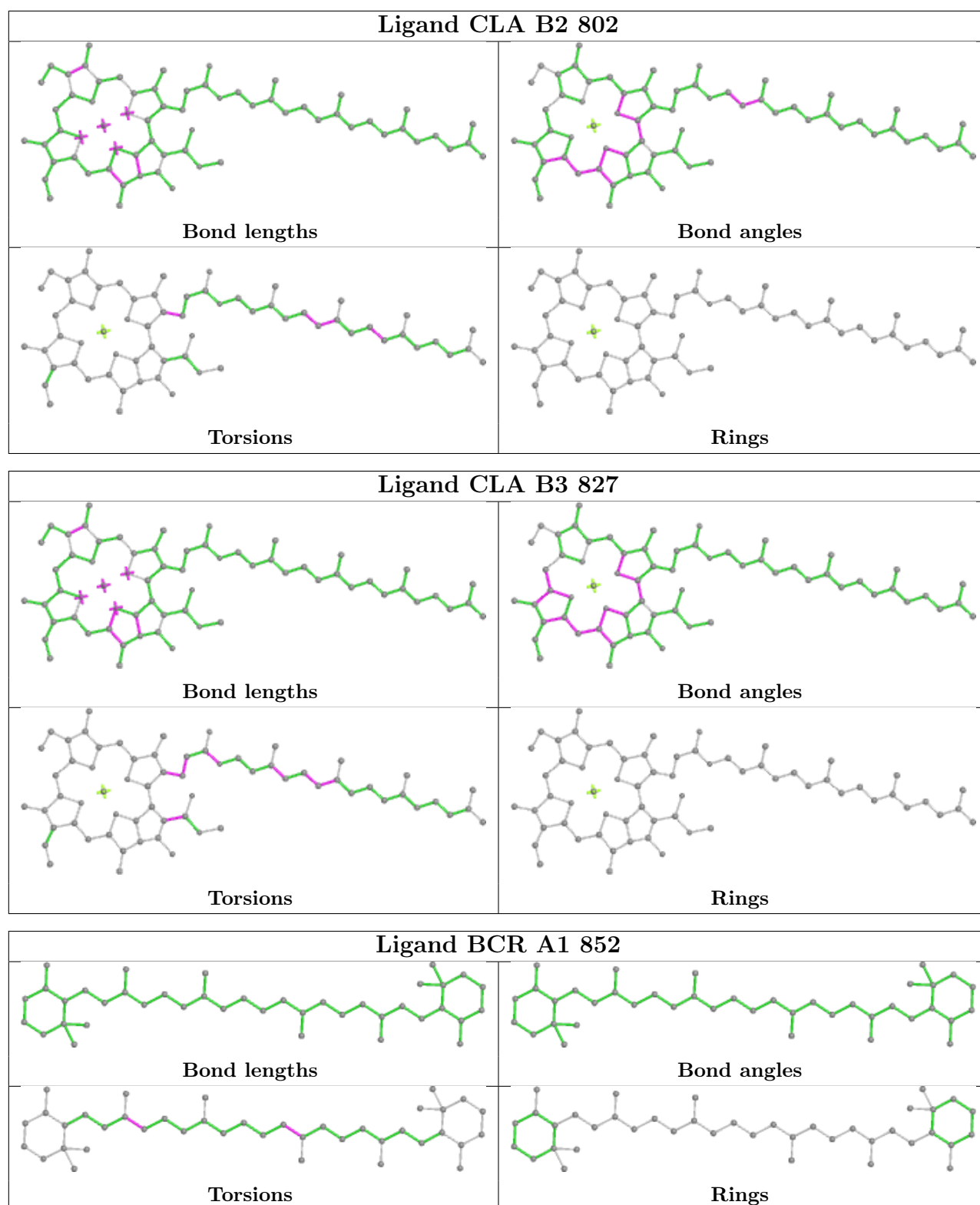
Bond angles

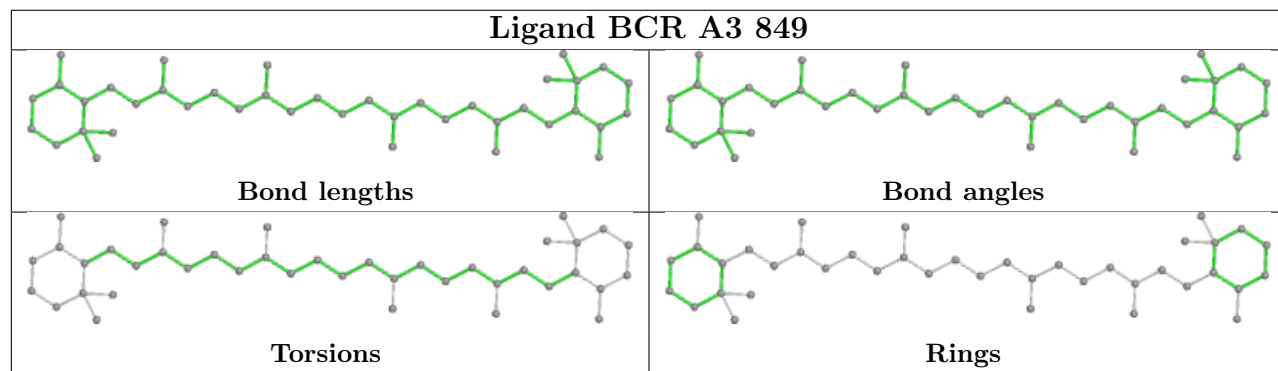
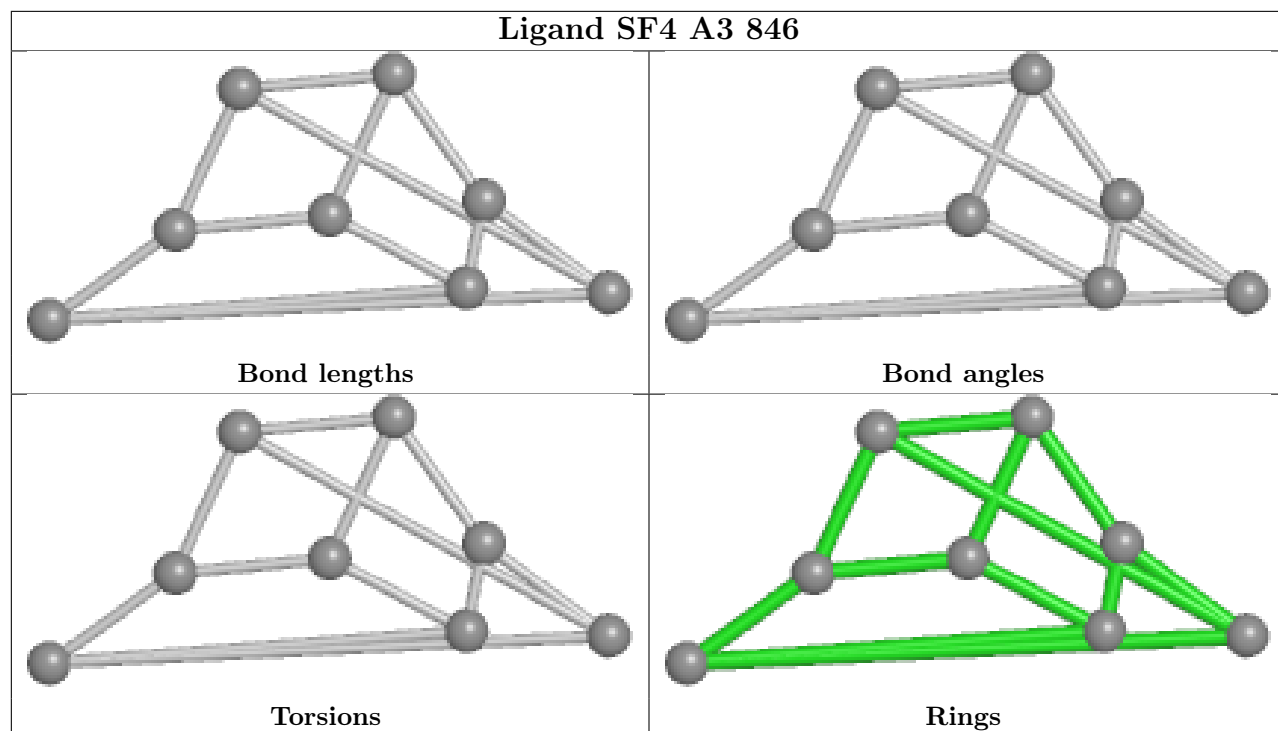


Torsions

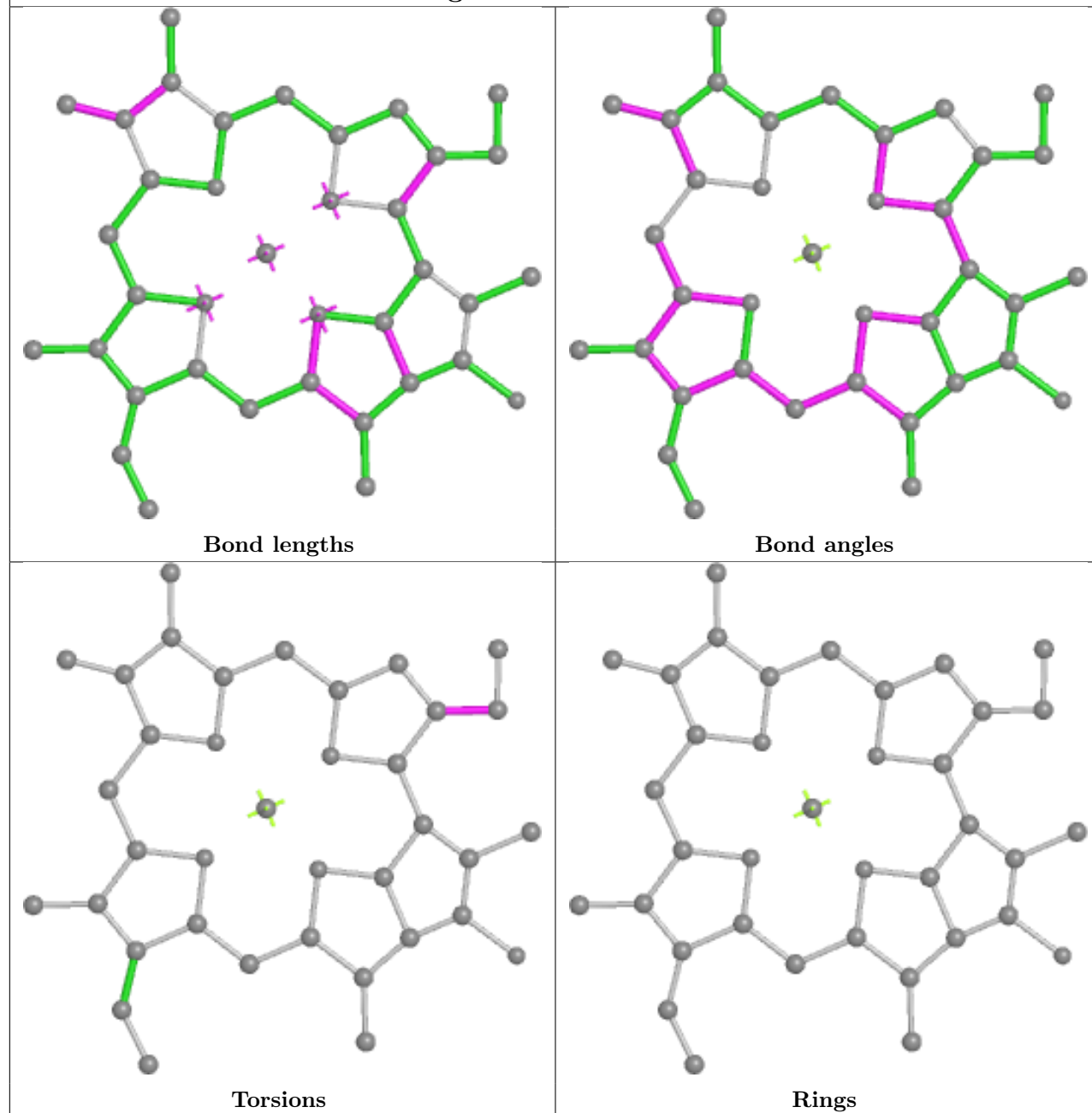


Rings

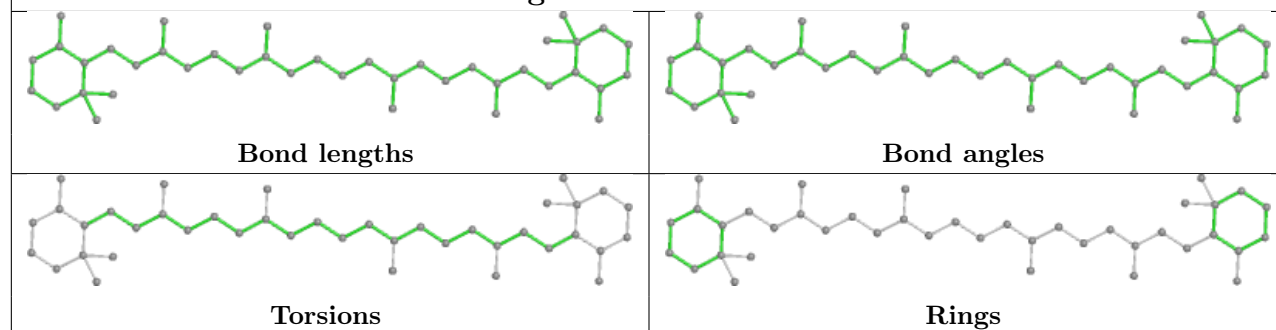


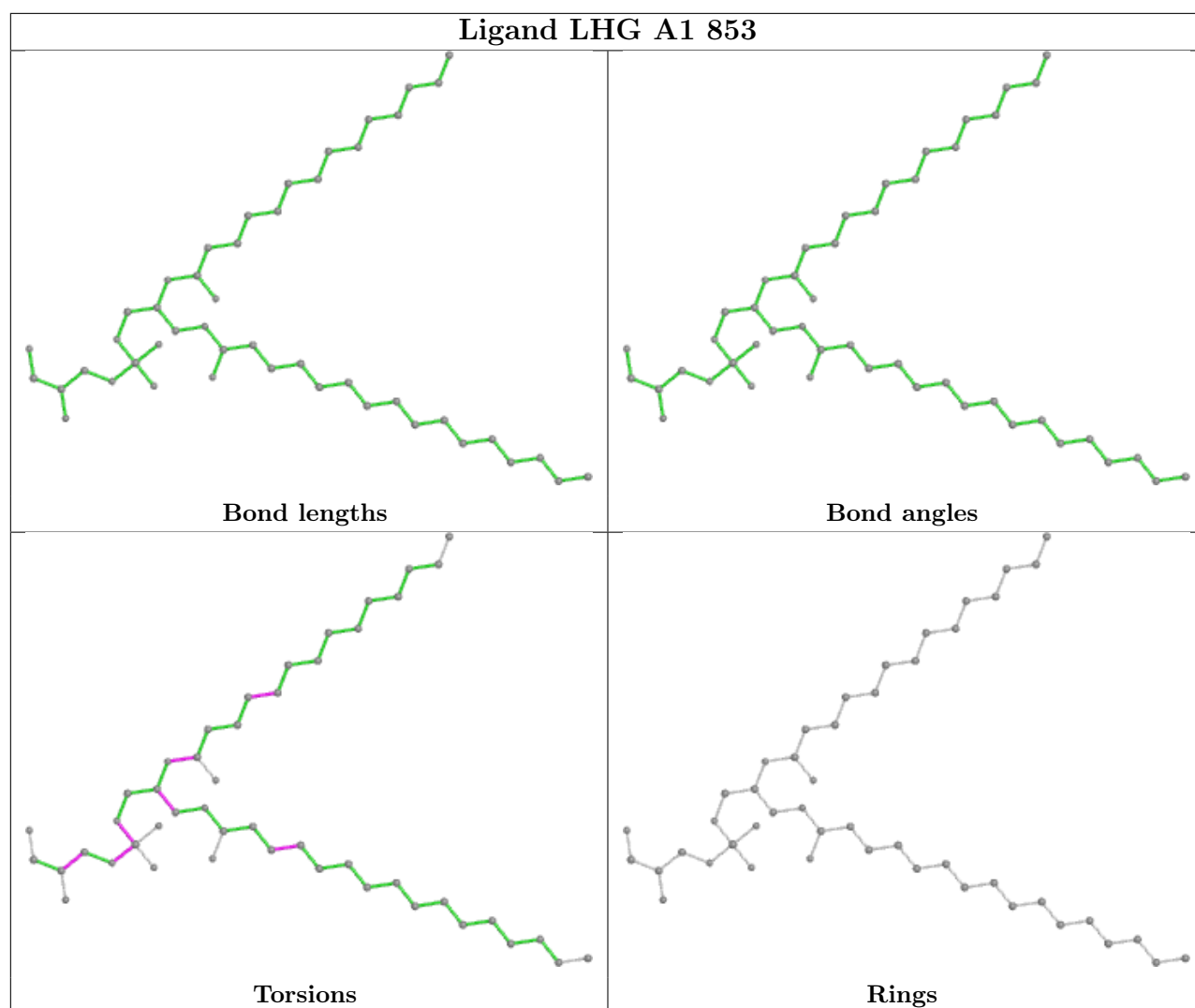


## Ligand CLA B1 833

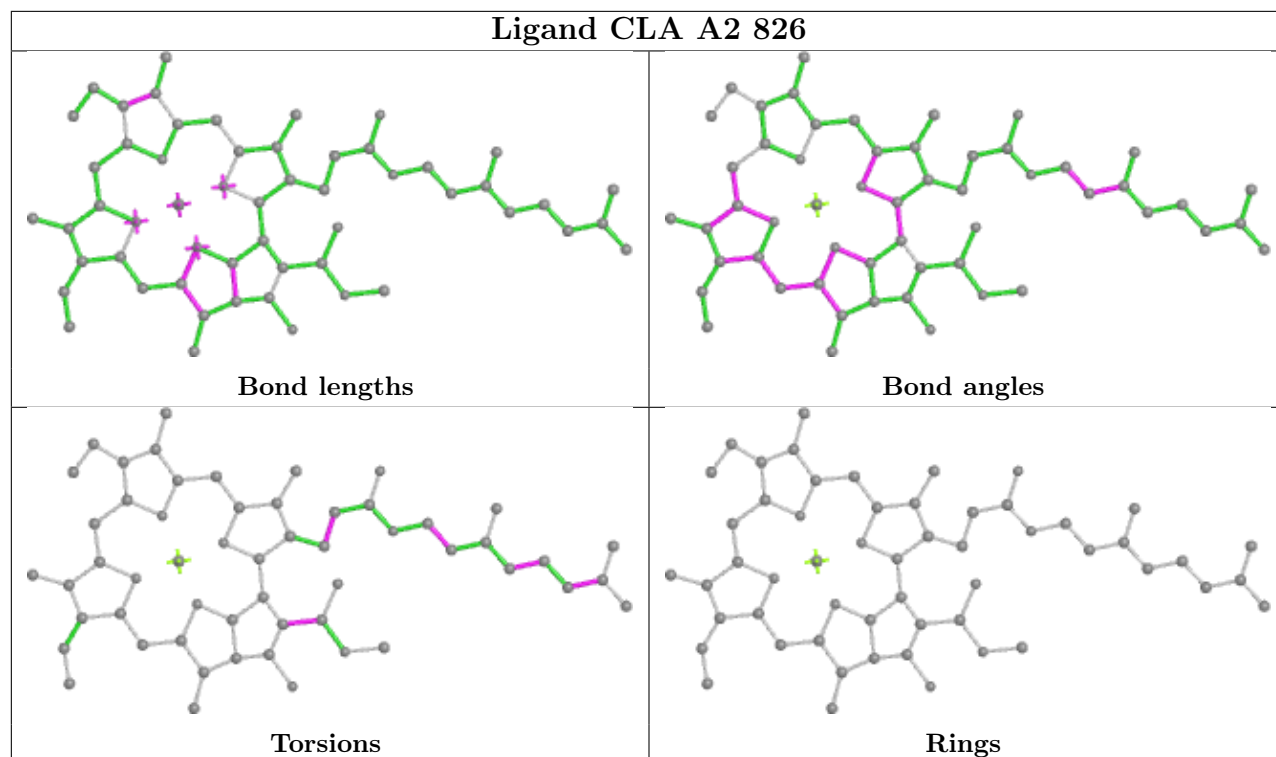


## Ligand BCR I2 102

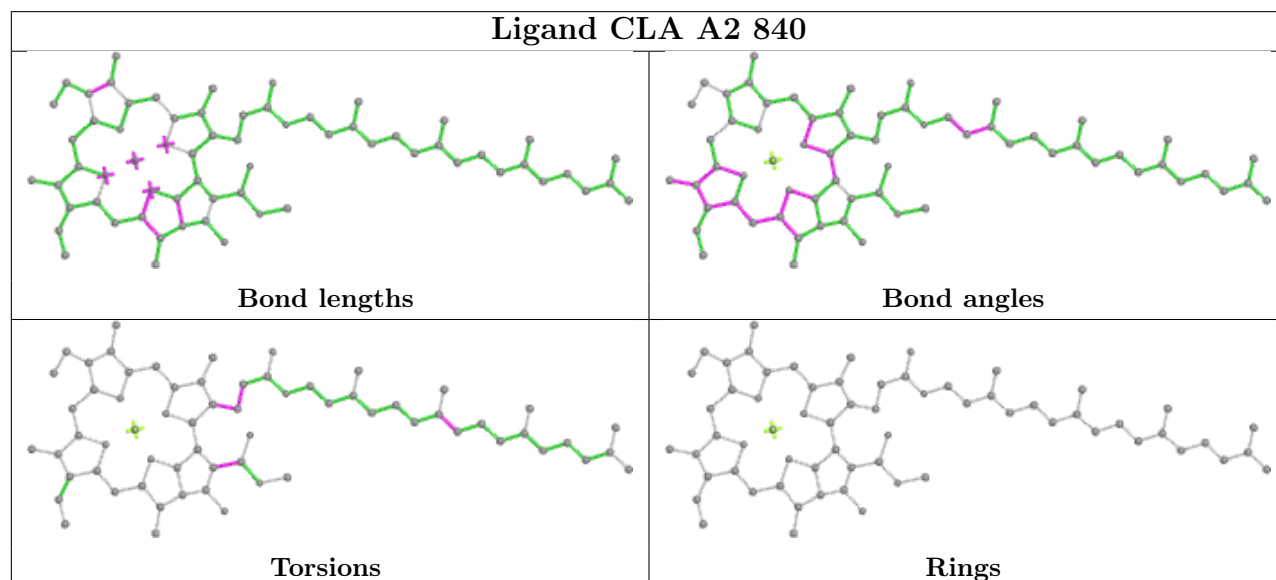




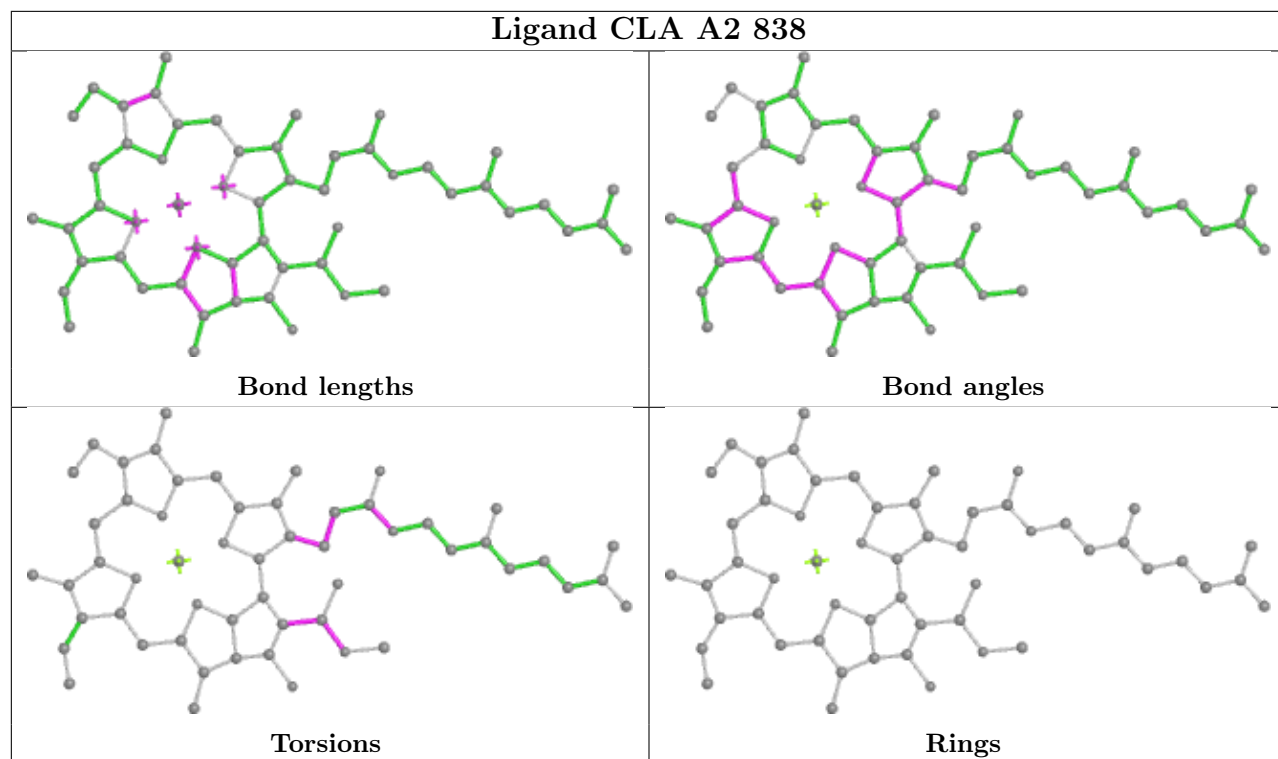
## Ligand CLA A2 826

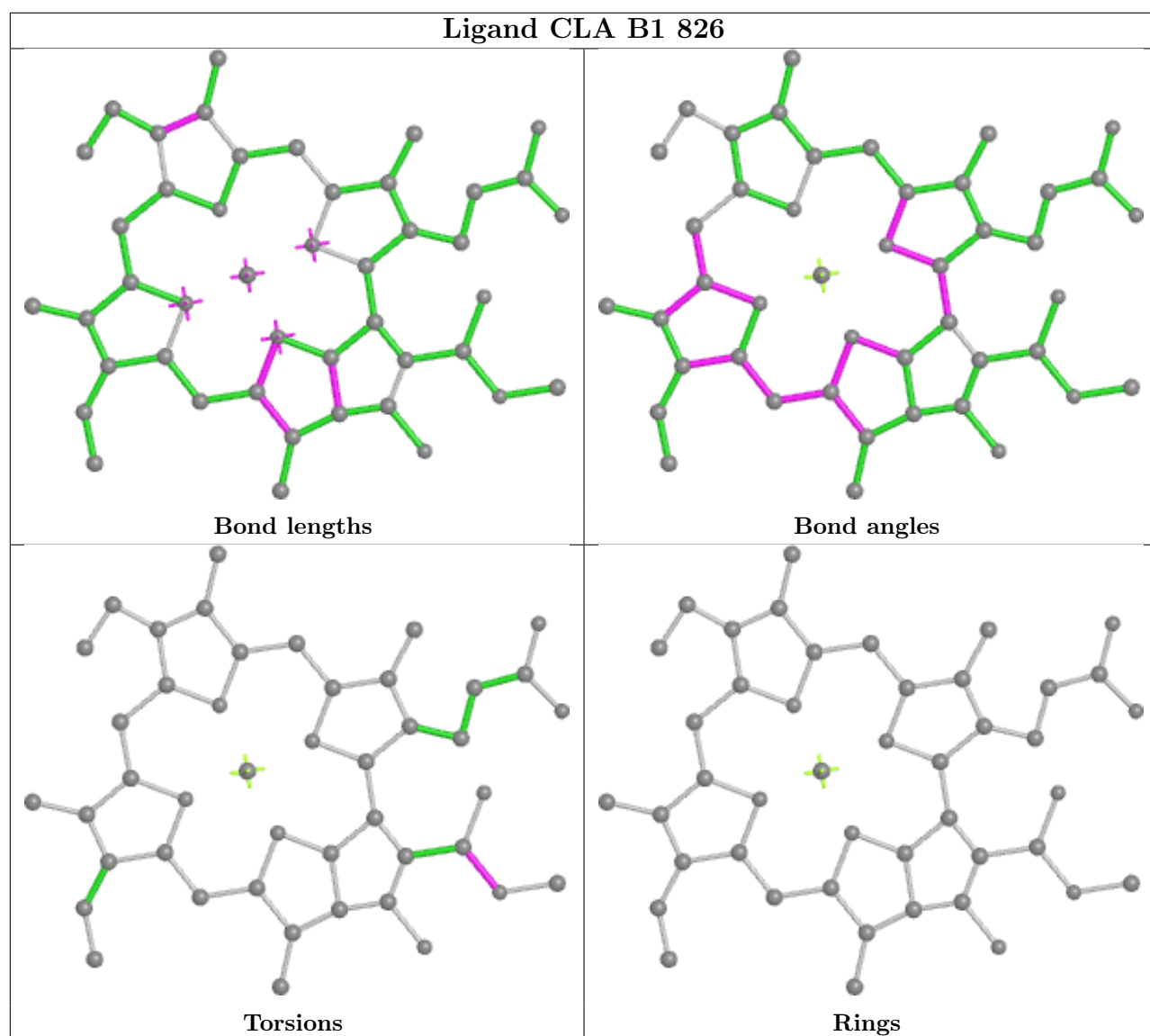


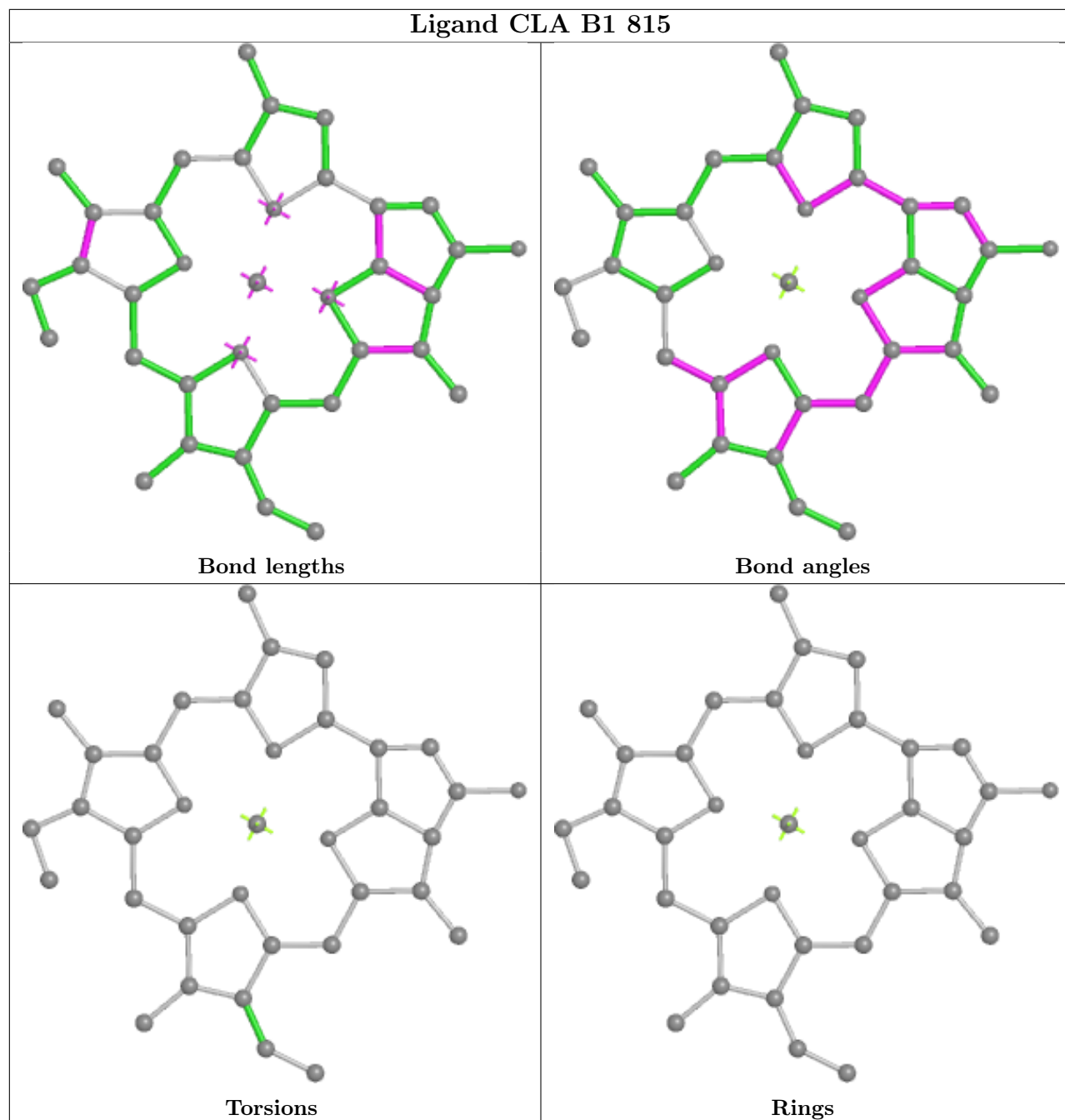
## Ligand CLA A2 840

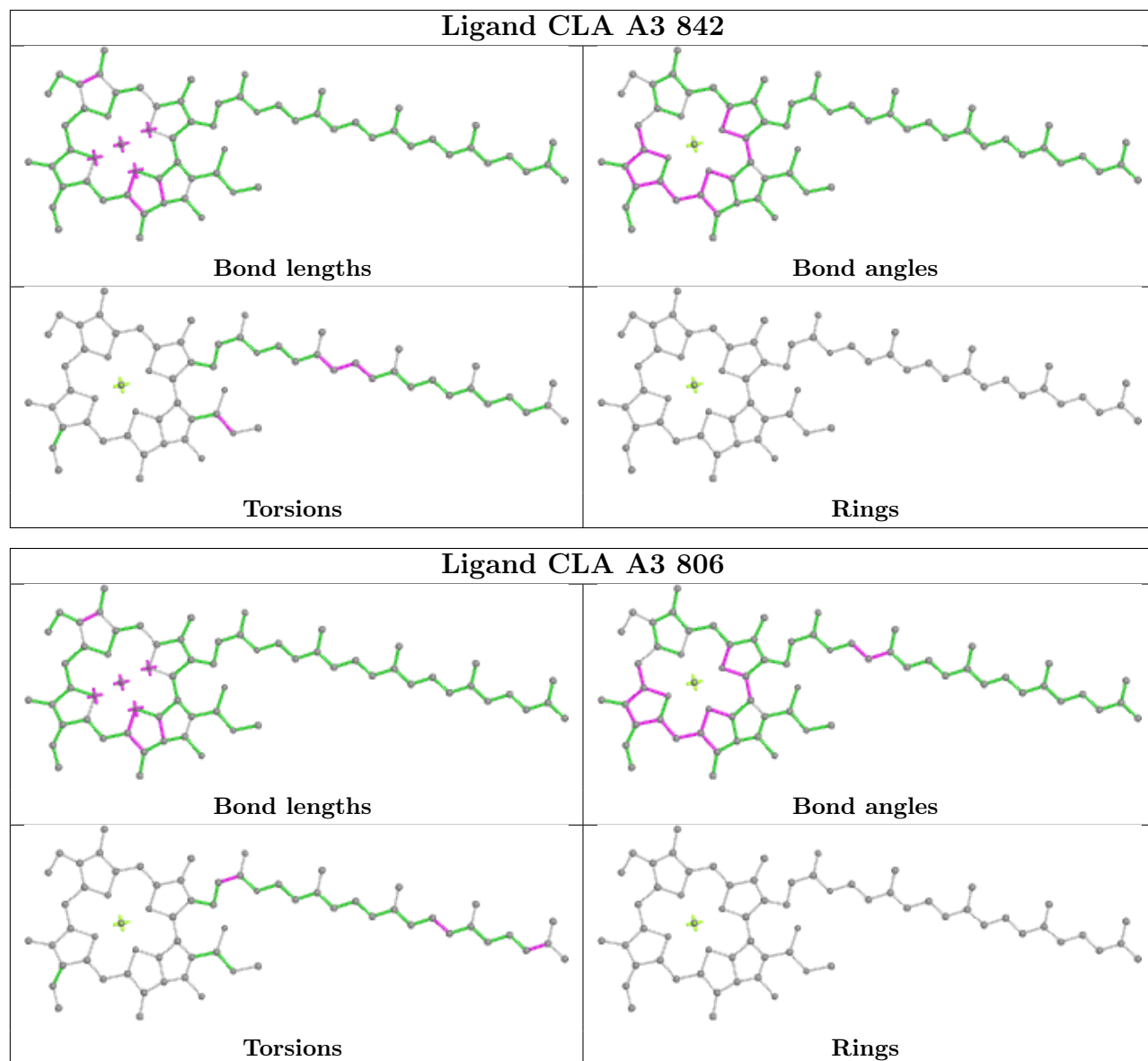


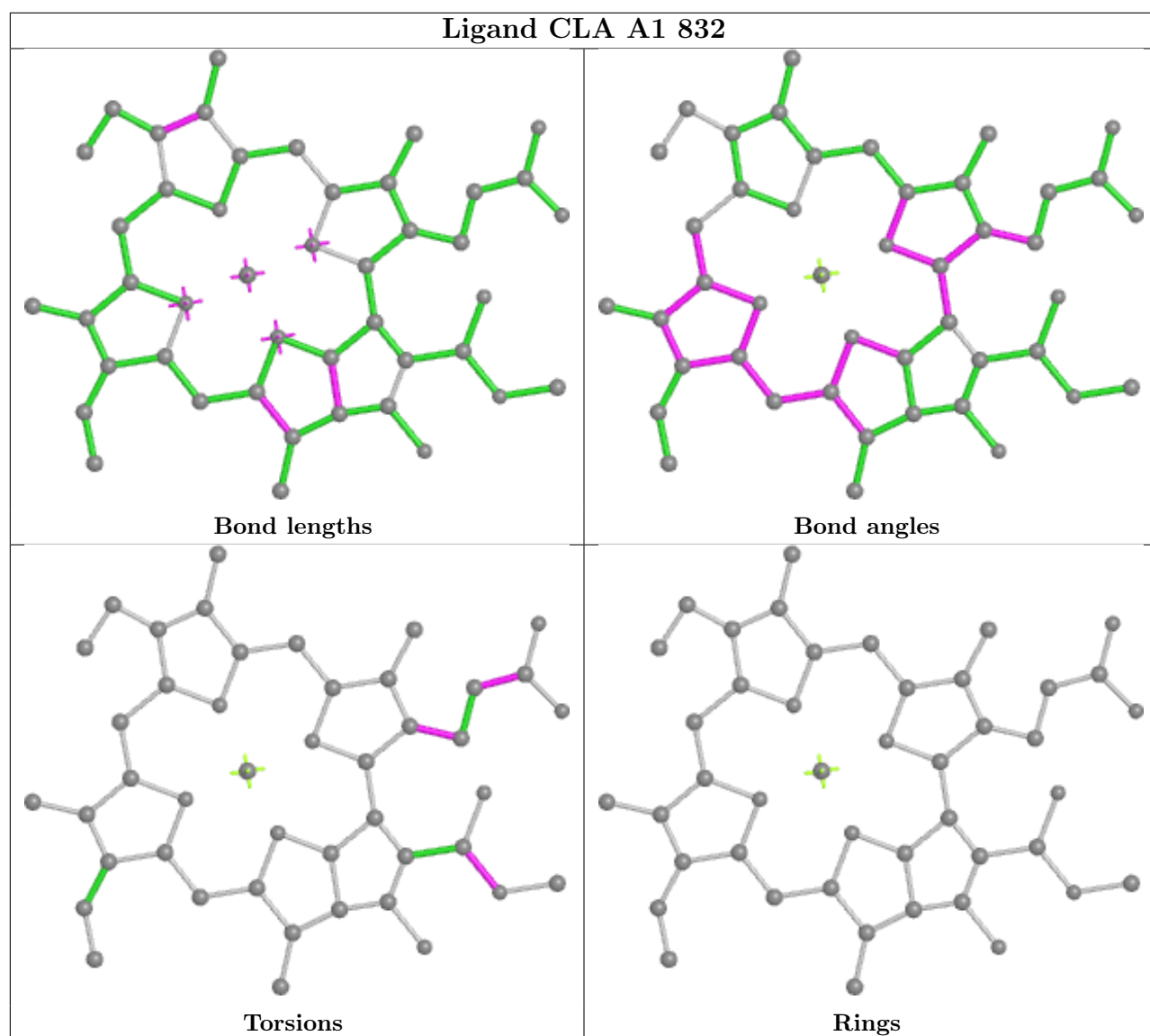


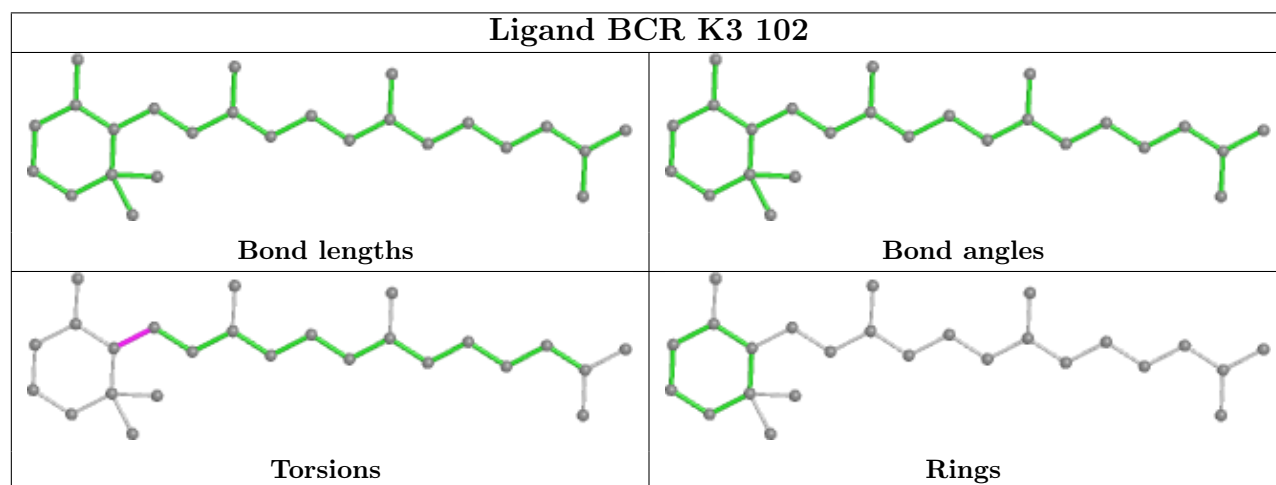
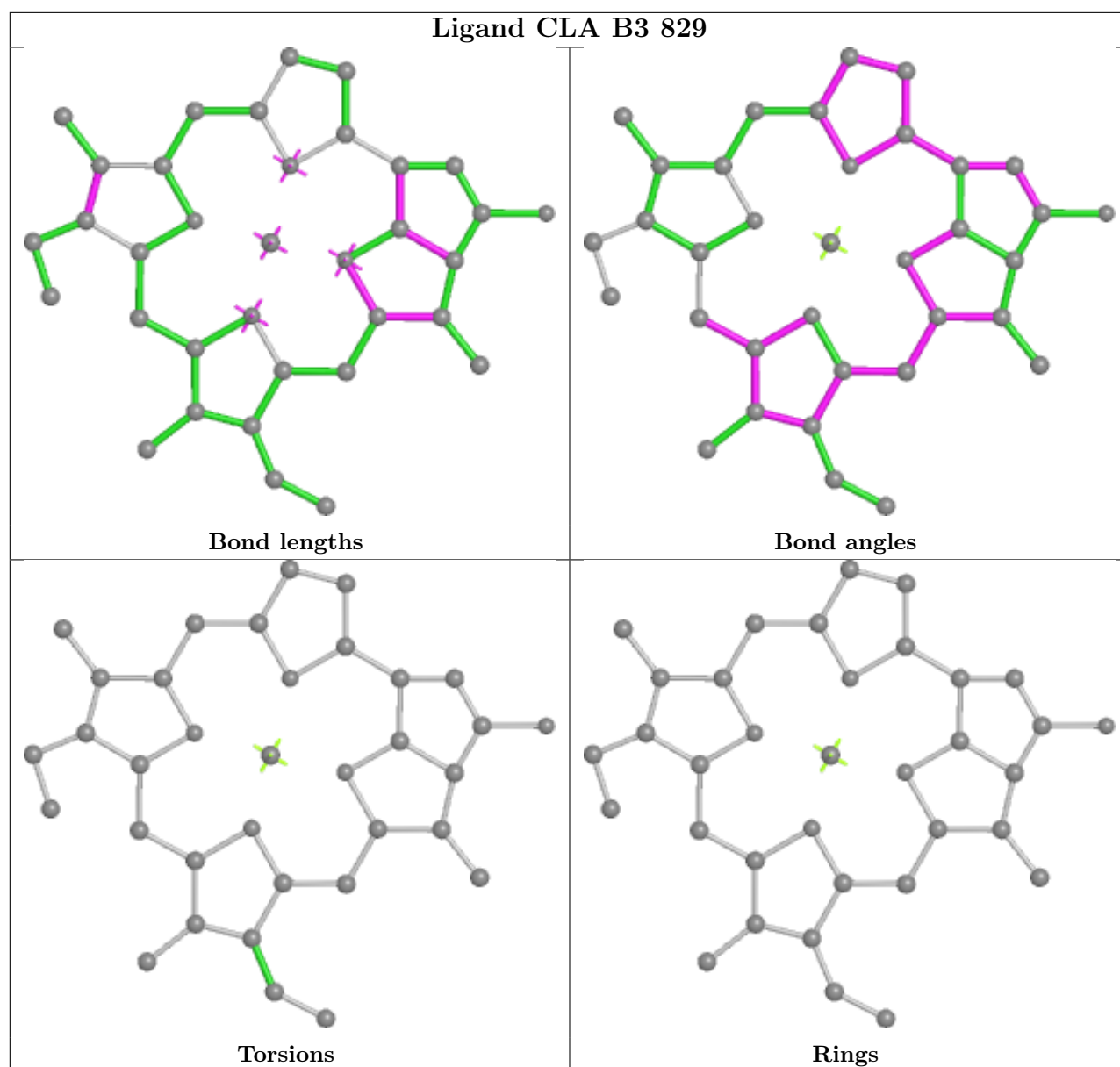




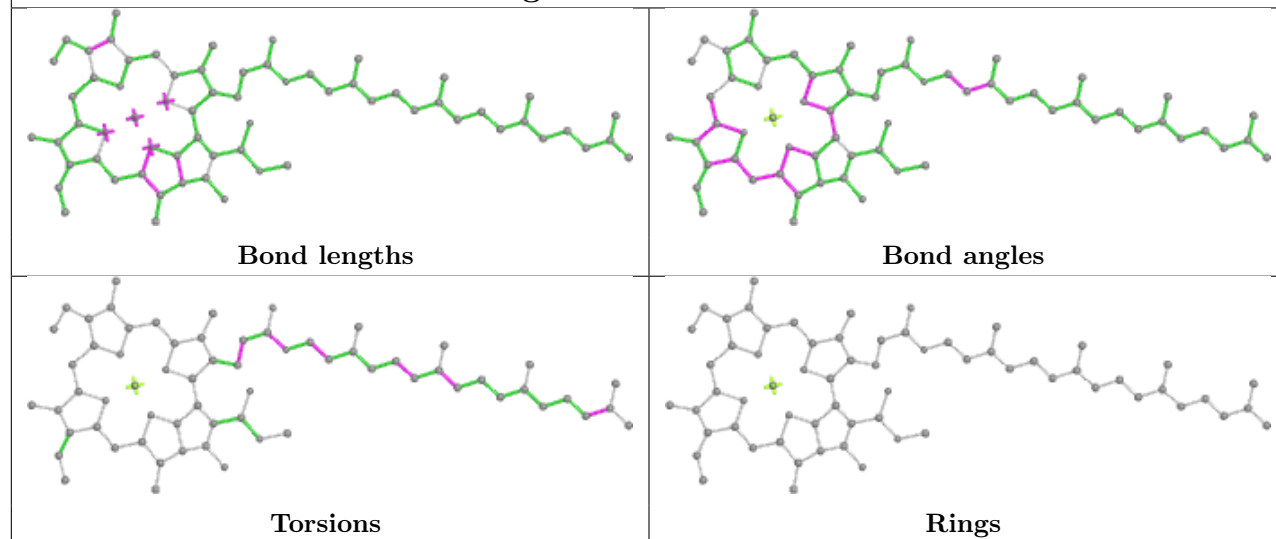




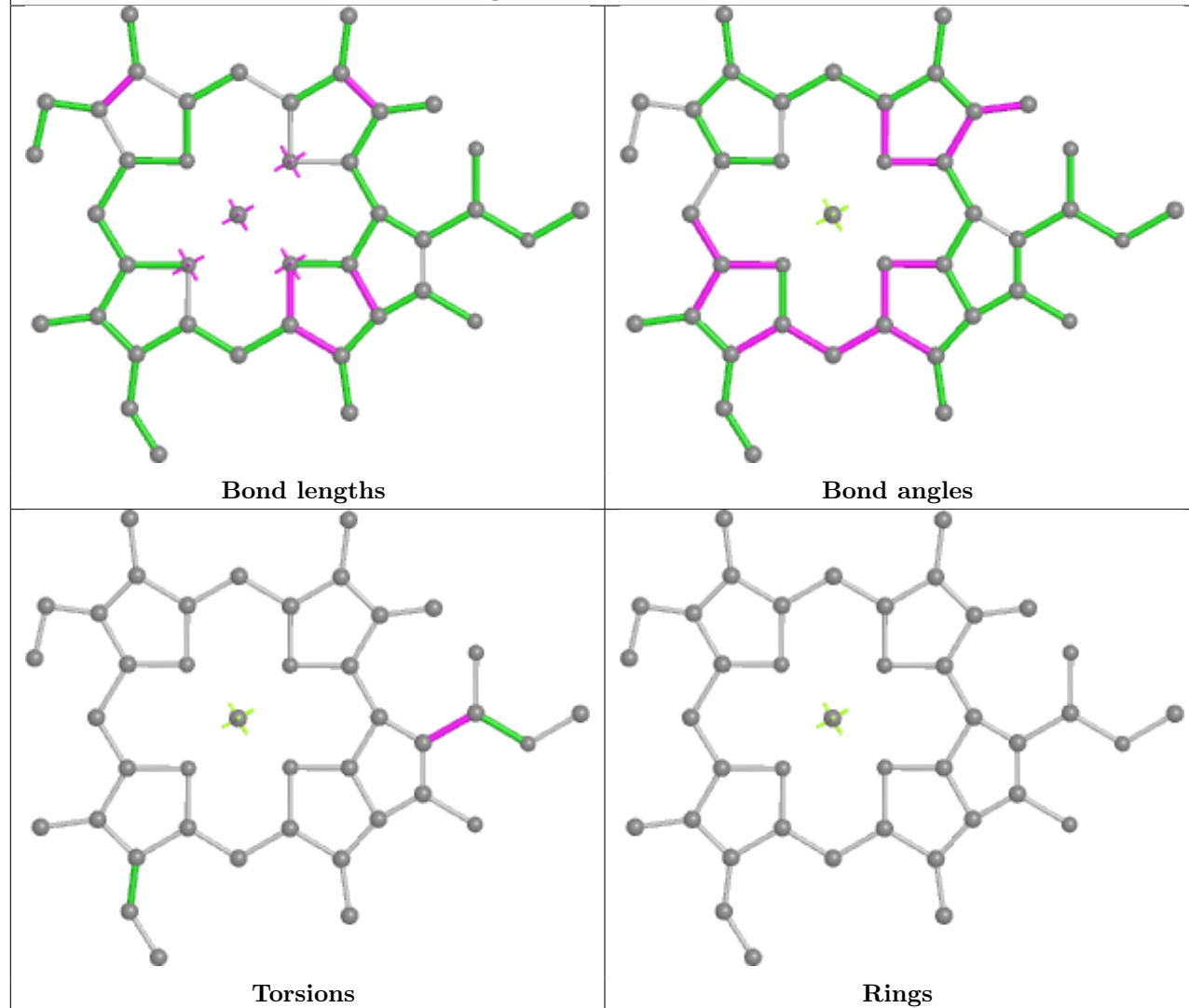


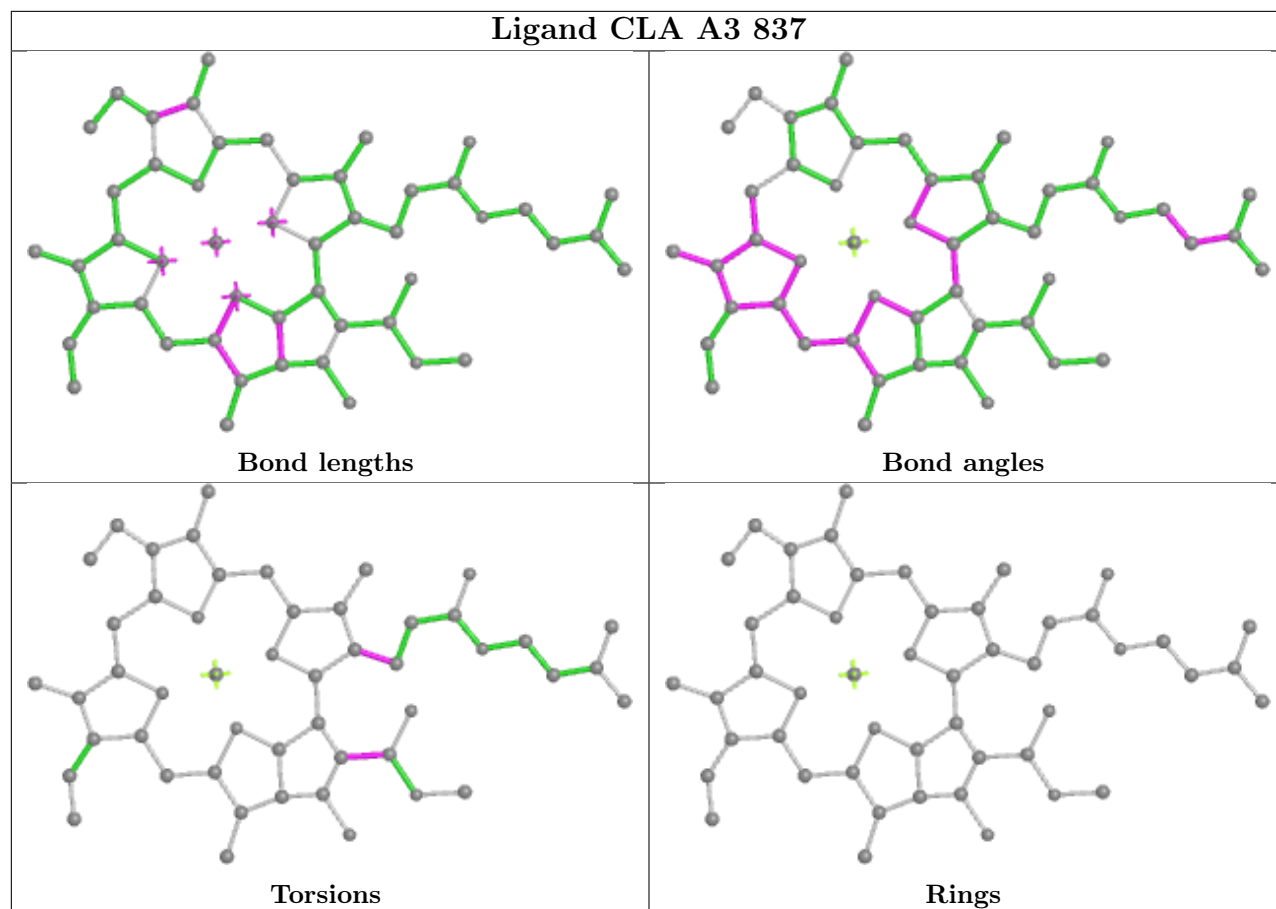


## Ligand CLA A2 843

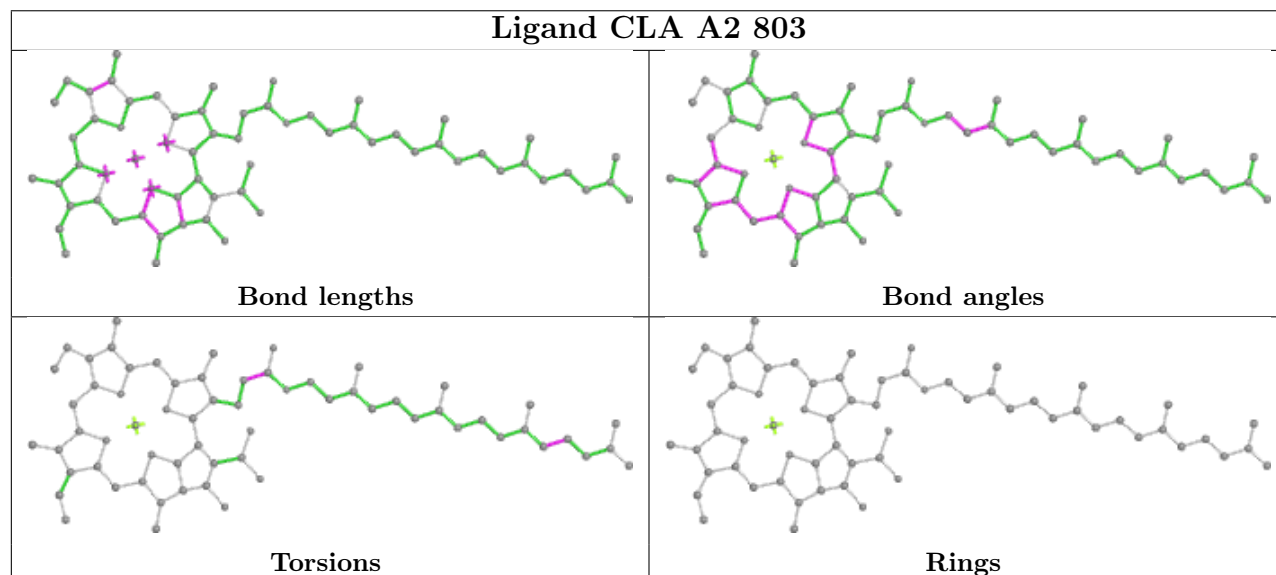
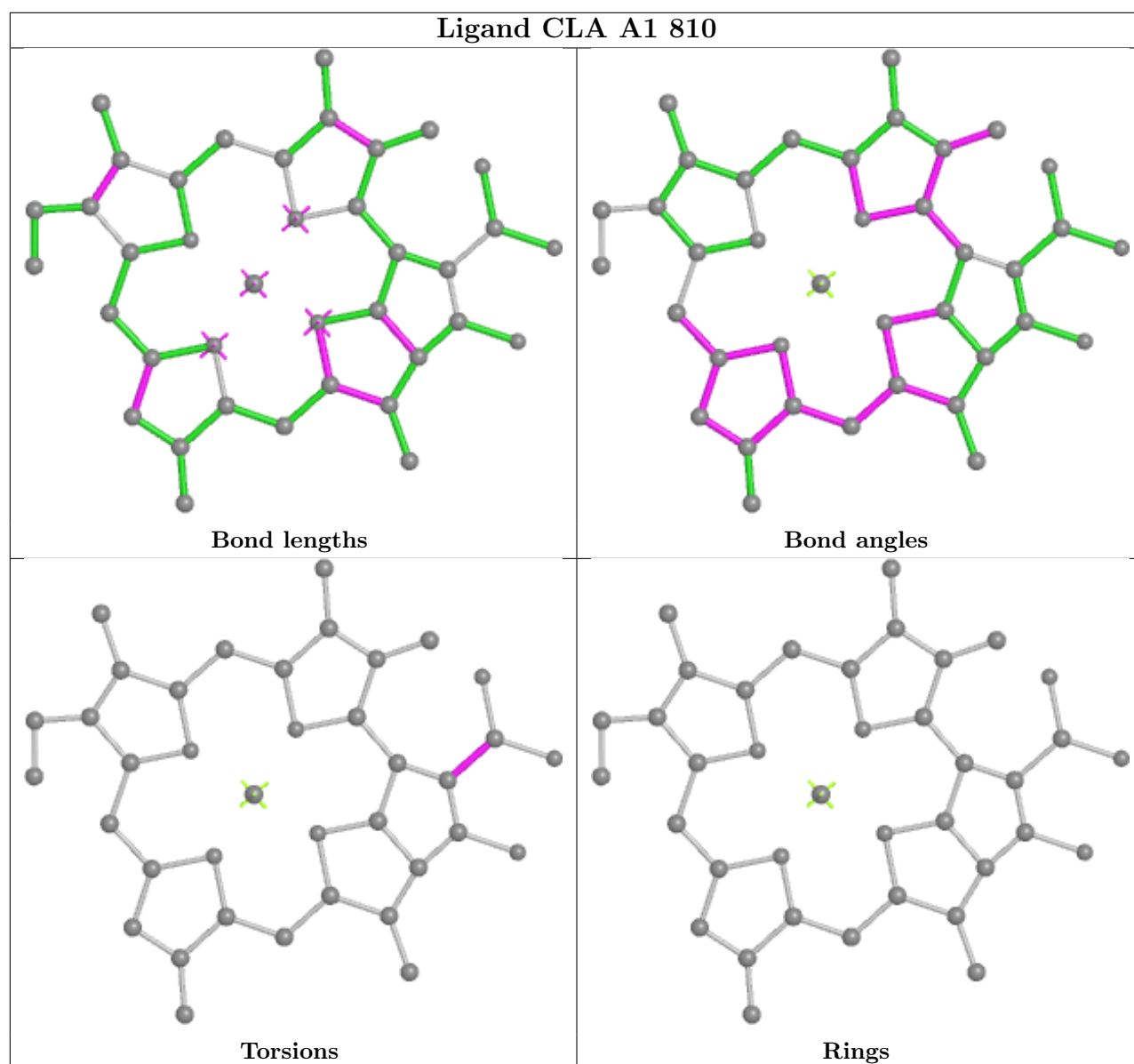


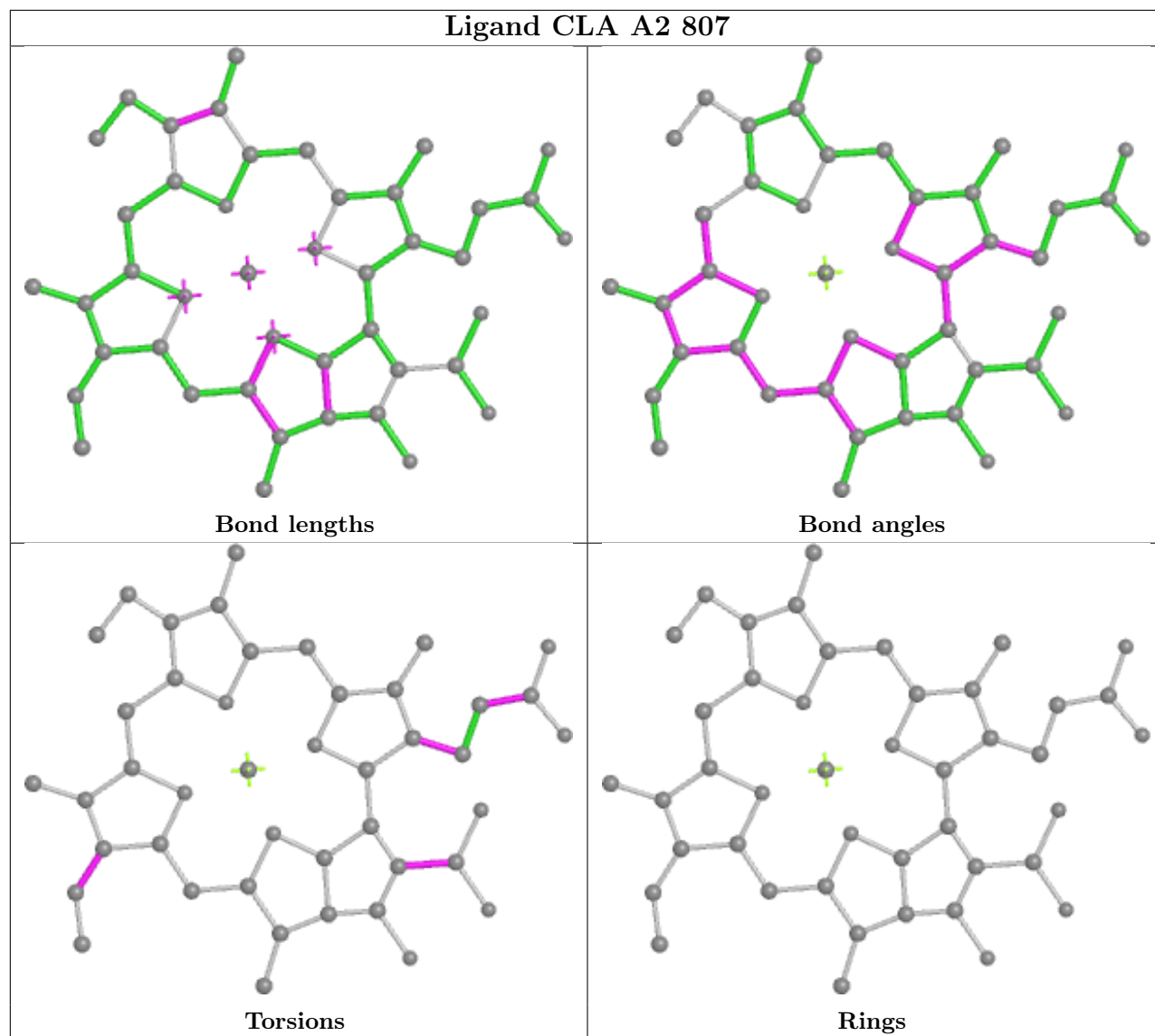
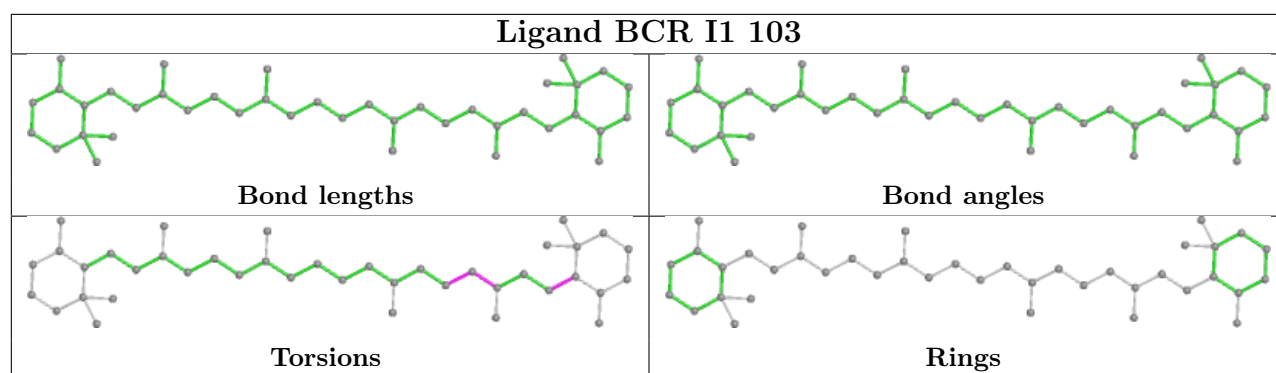
## Ligand CLA A1 823



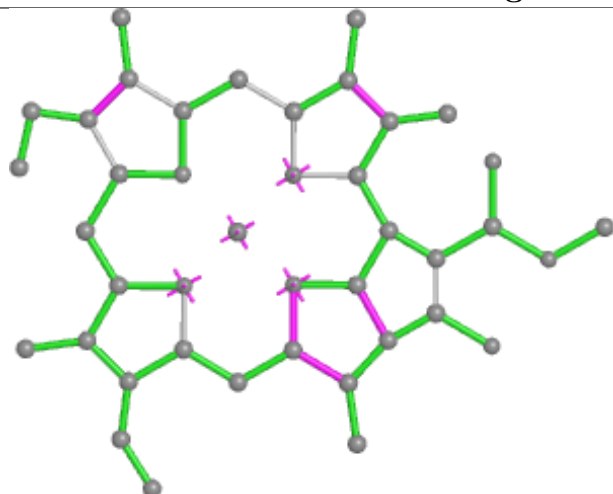




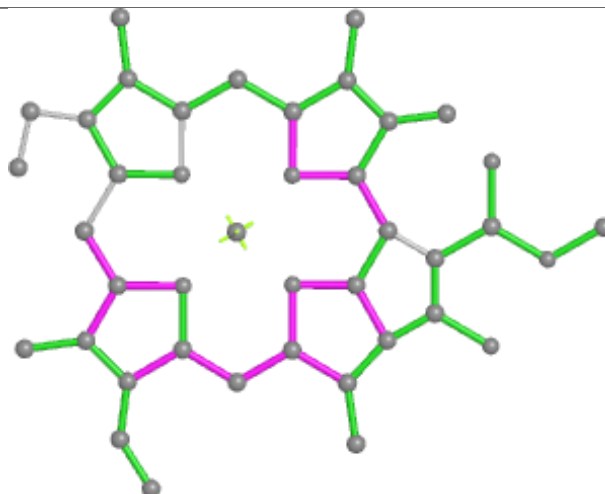




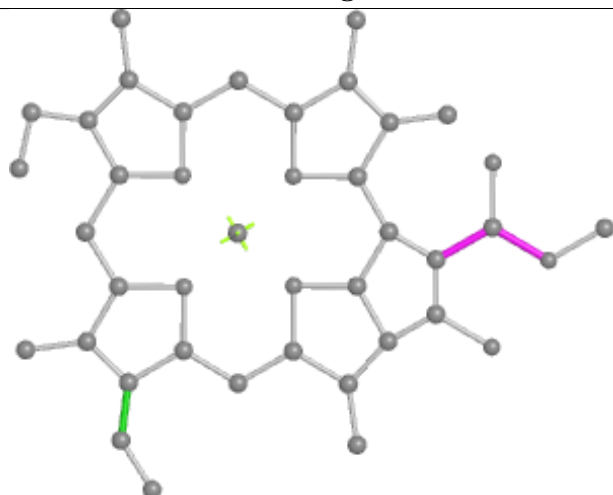
## Ligand CLA B2 837



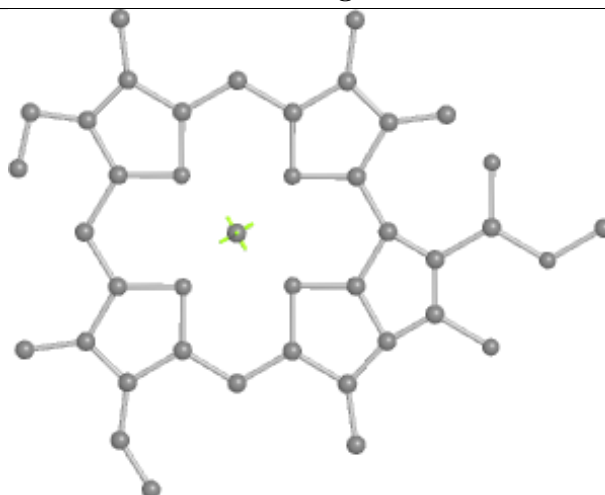
Bond lengths



Bond angles

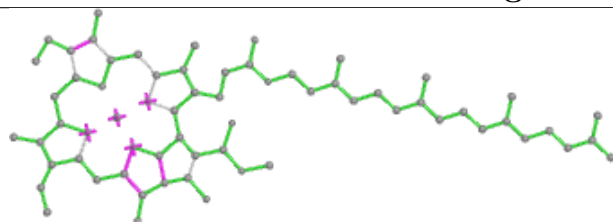


Torsions

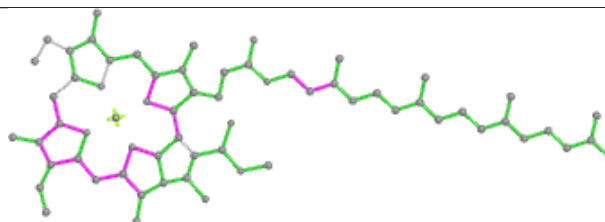


Rings

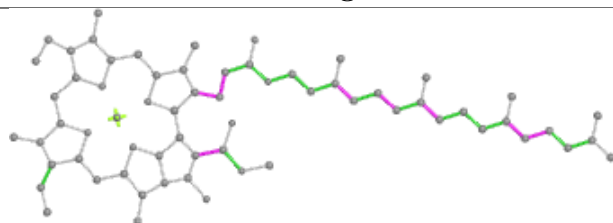
## Ligand CLA A2 809



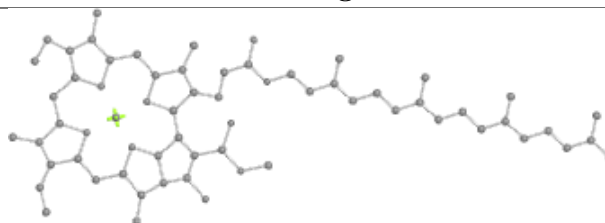
Bond lengths



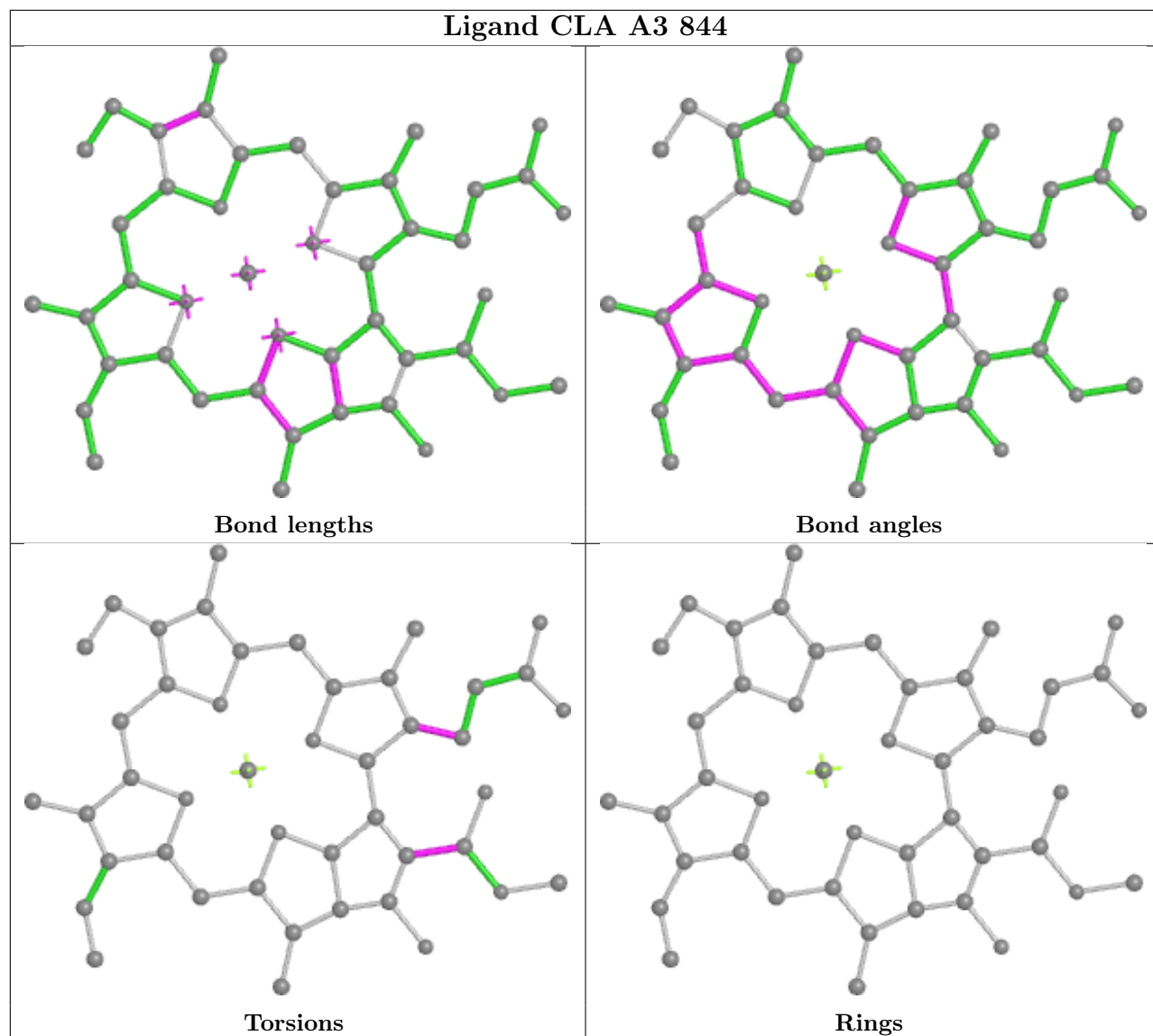
Bond angles



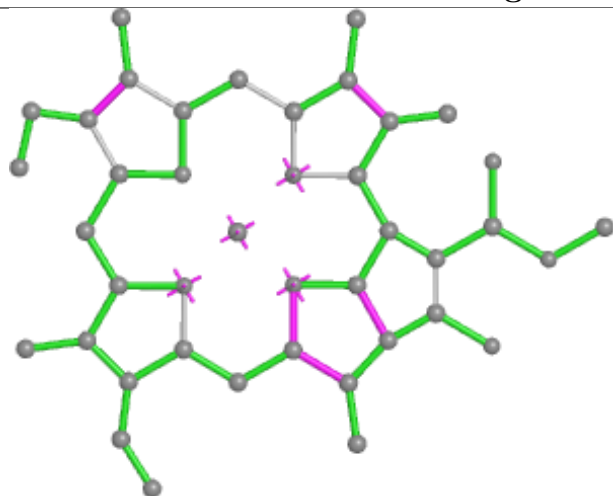
Torsions



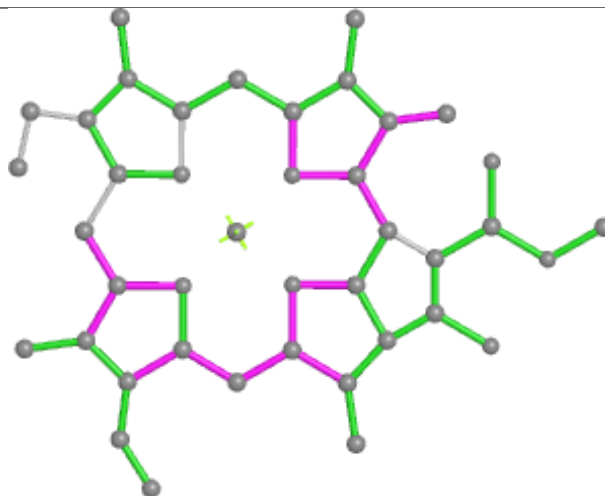
Rings



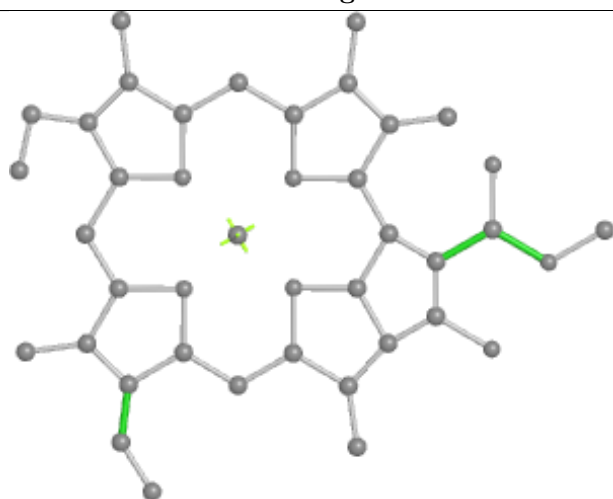
## Ligand CLA A3 816



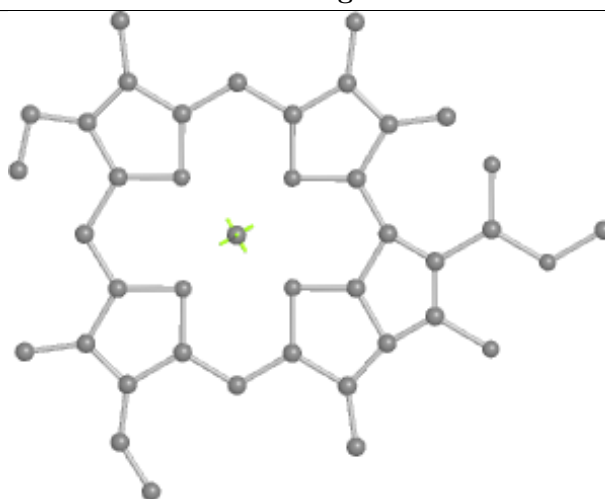
Bond lengths



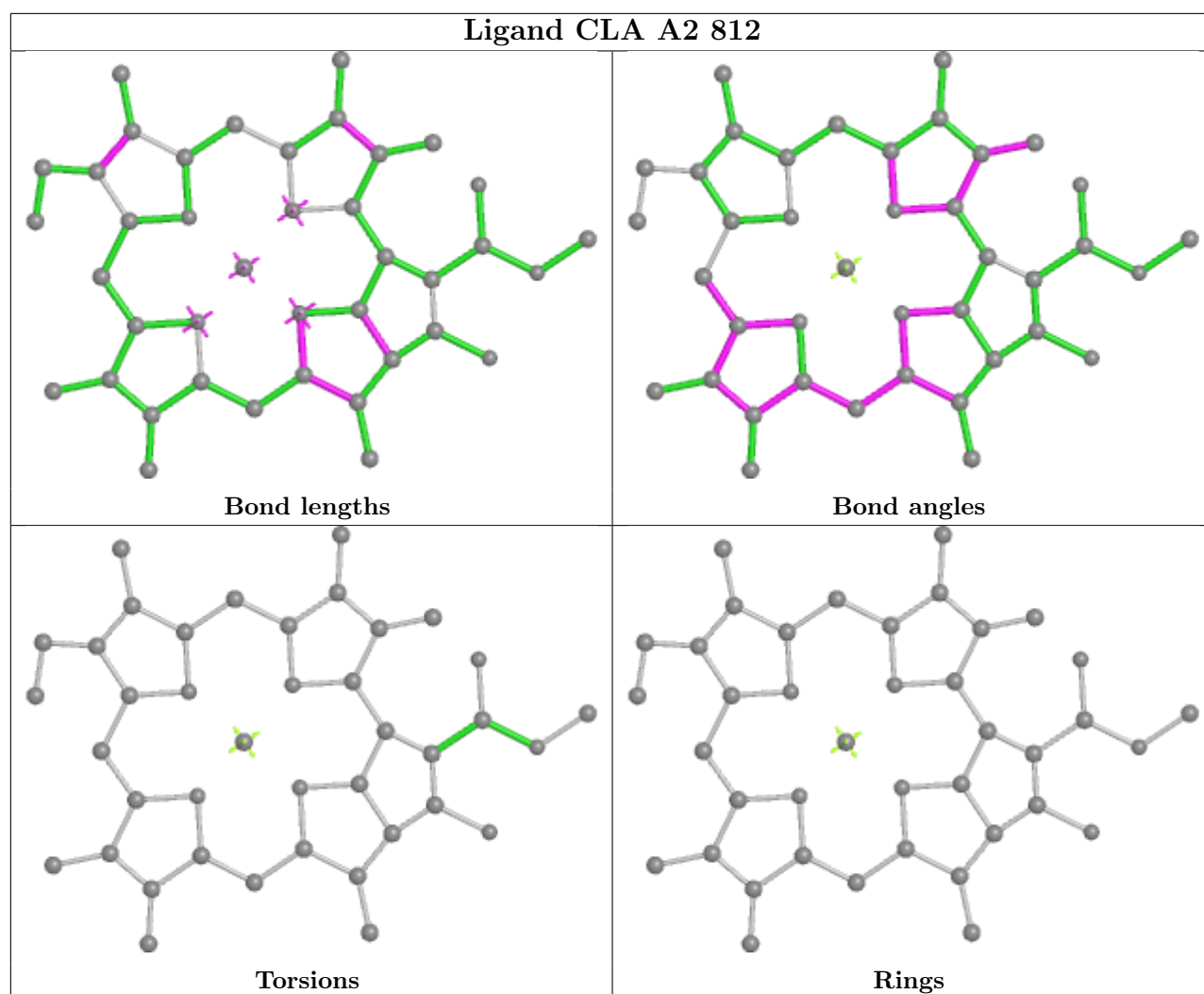
Bond angles



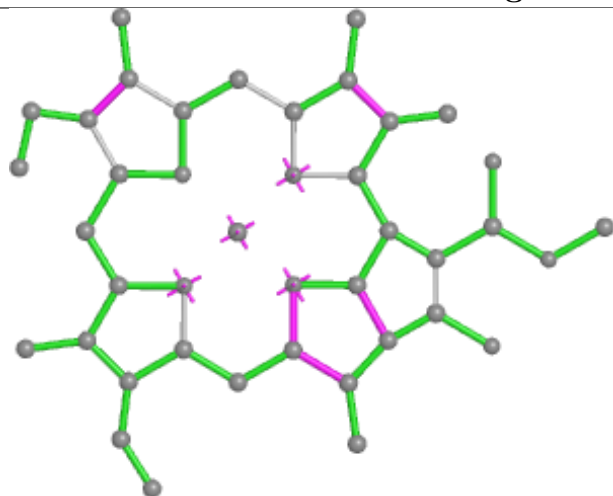
Torsions



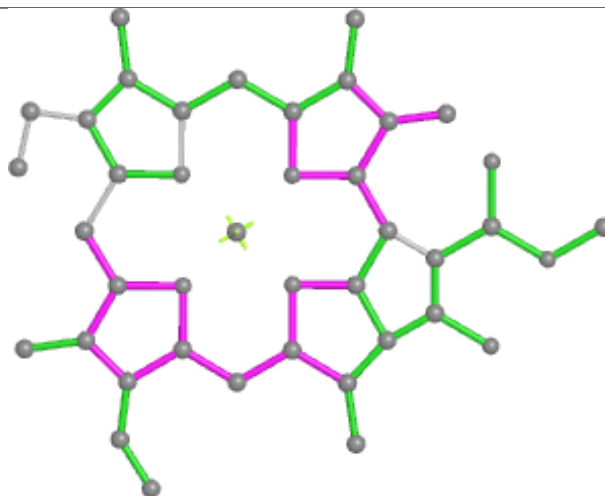
Rings



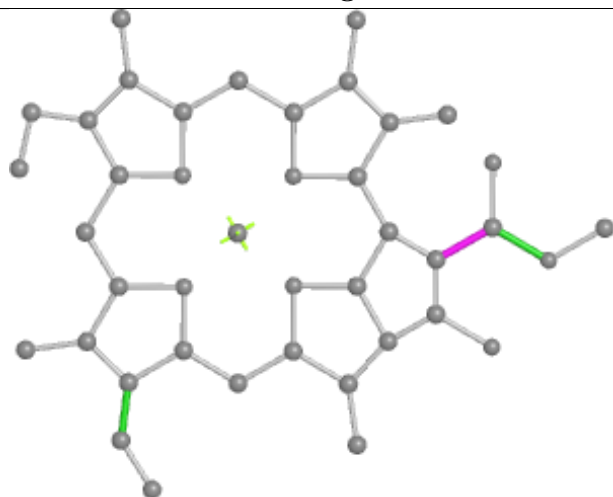
## Ligand CLA B3 831



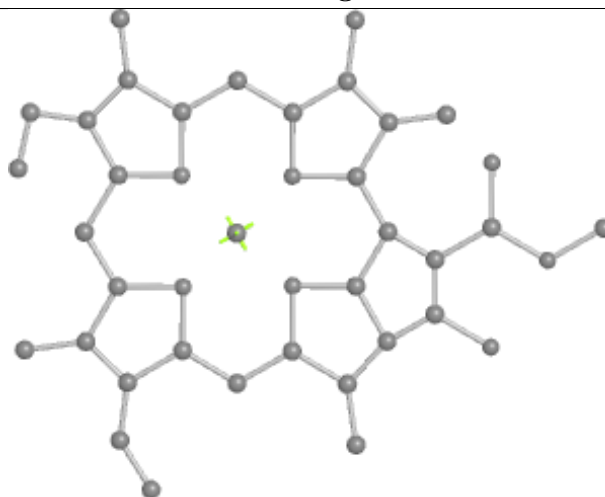
Bond lengths



Bond angles

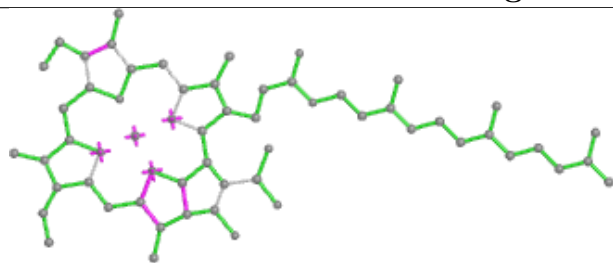


Torsions

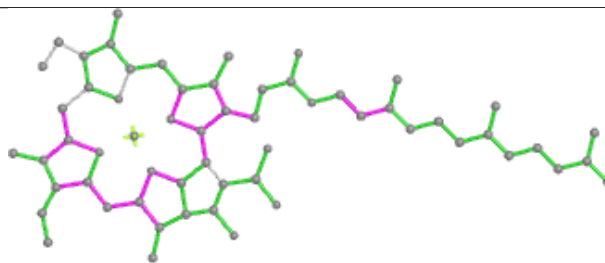


Rings

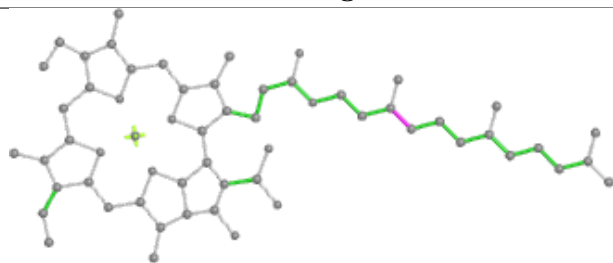
## Ligand CLA A2 819



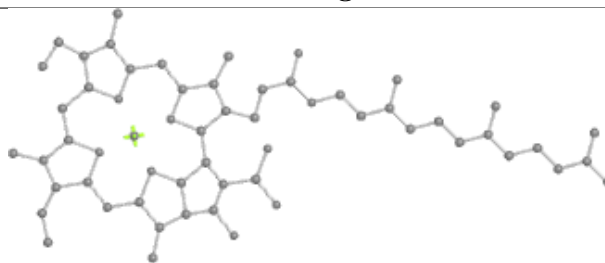
Bond lengths



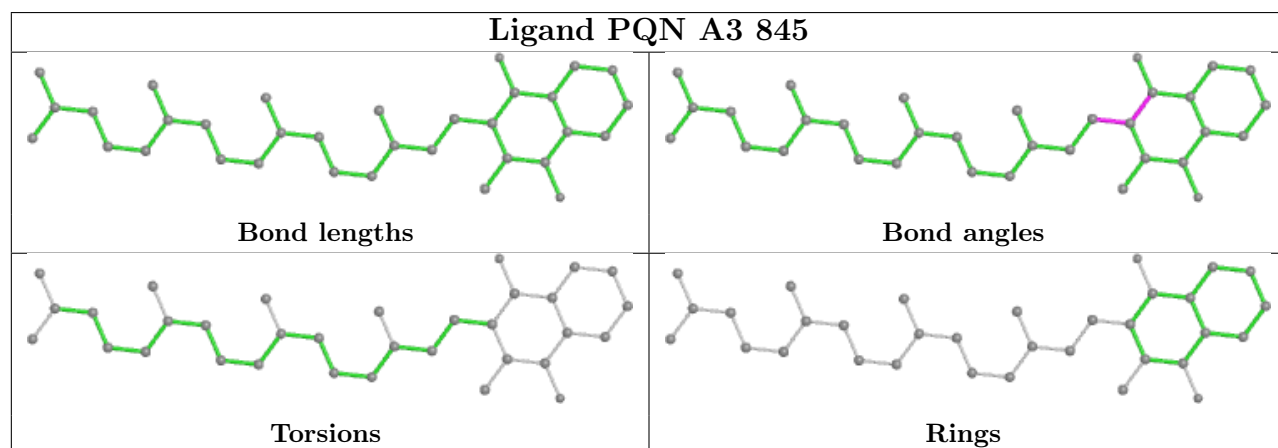
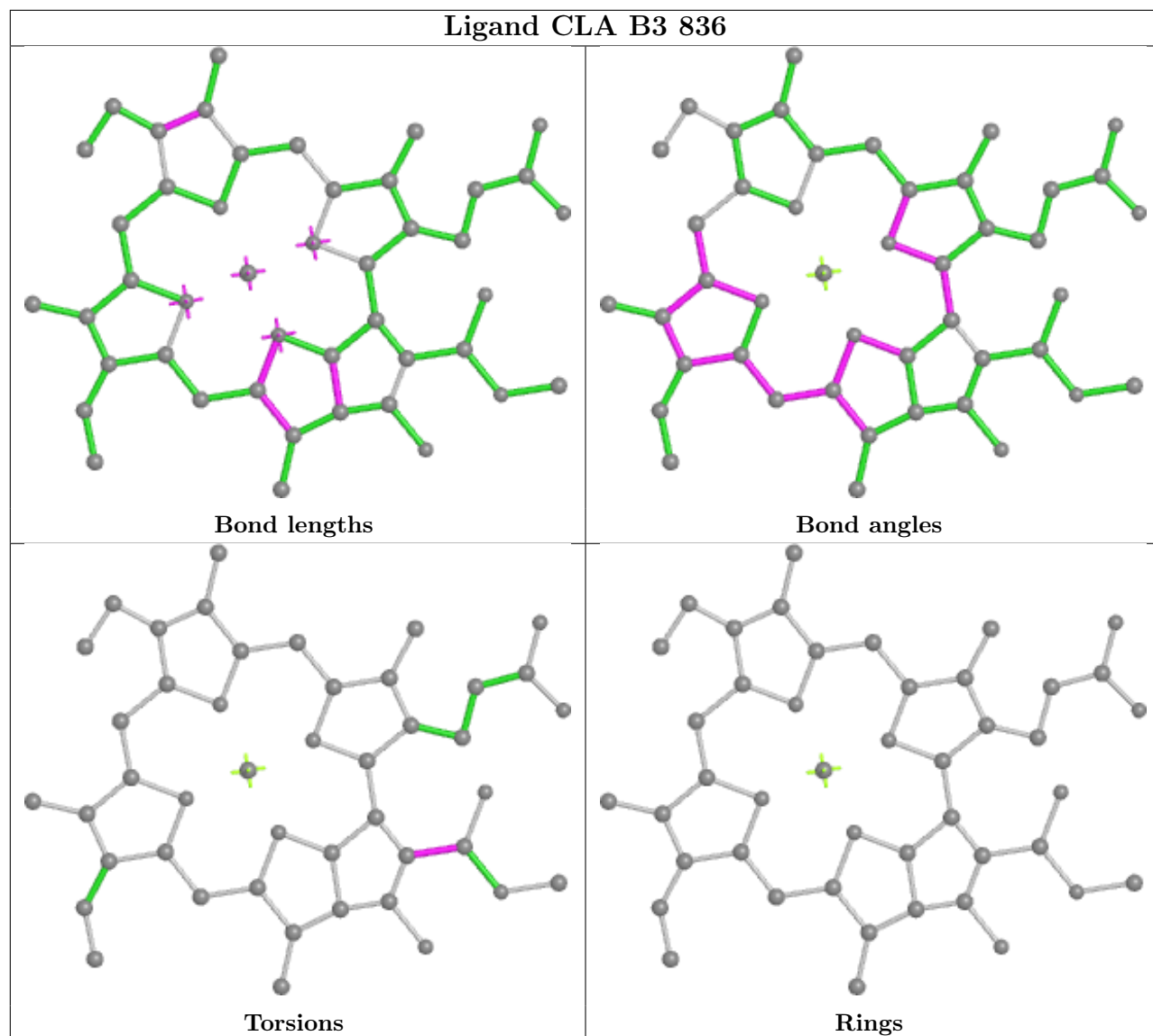
Bond angles



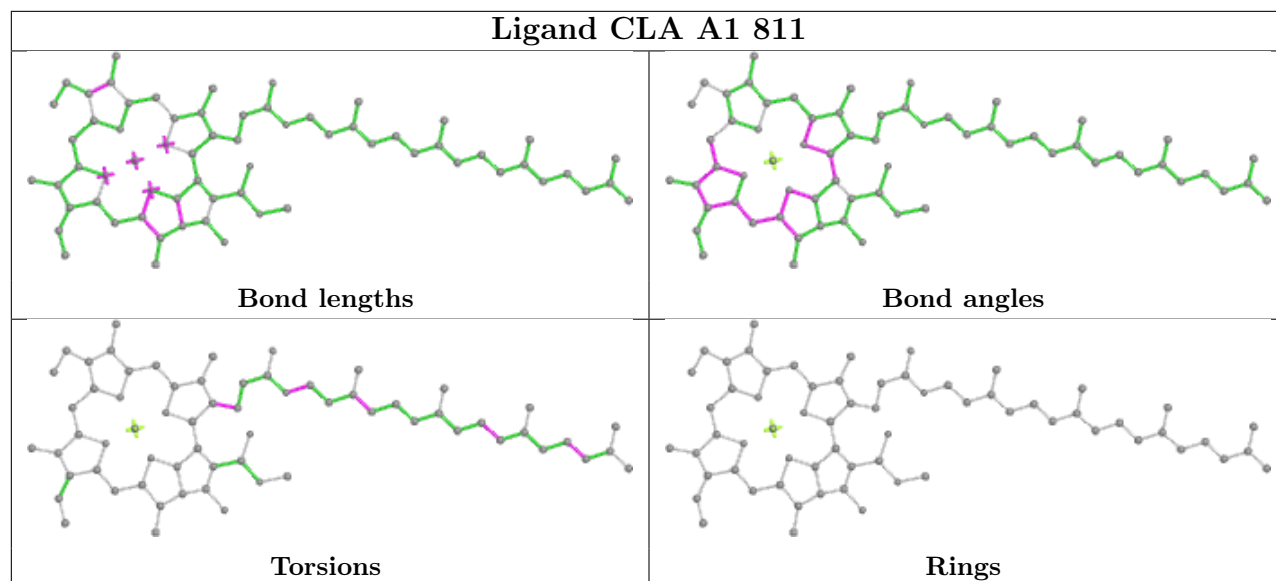
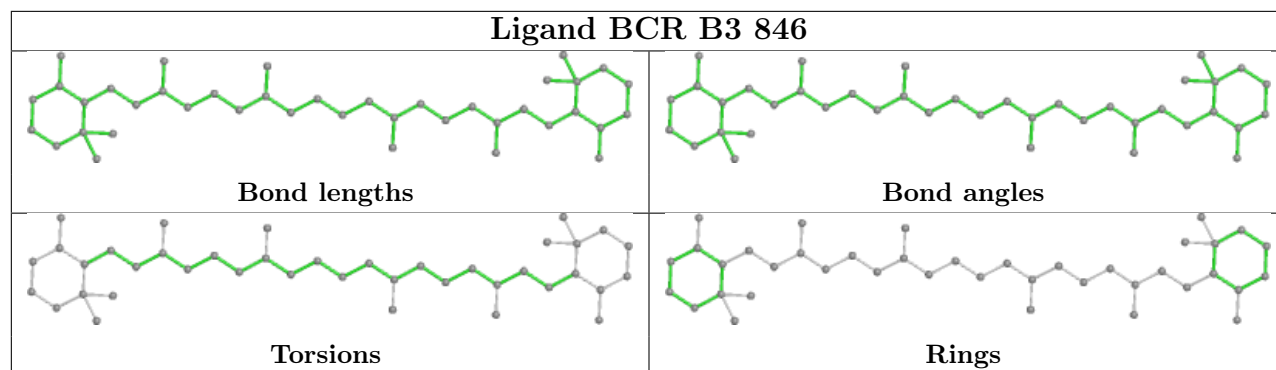
Torsions



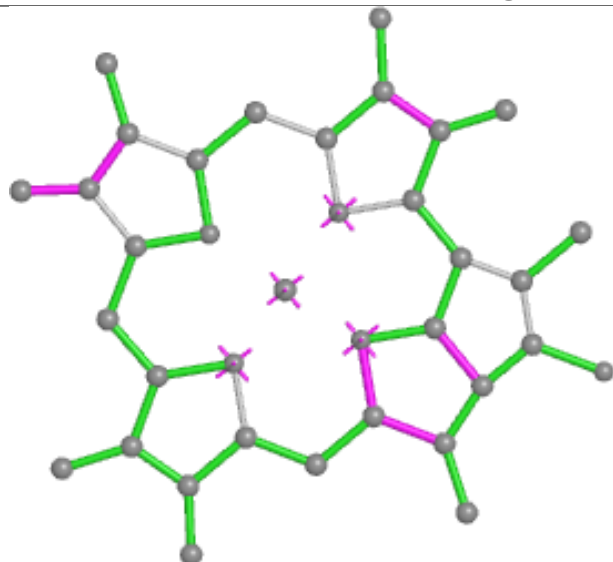
Rings



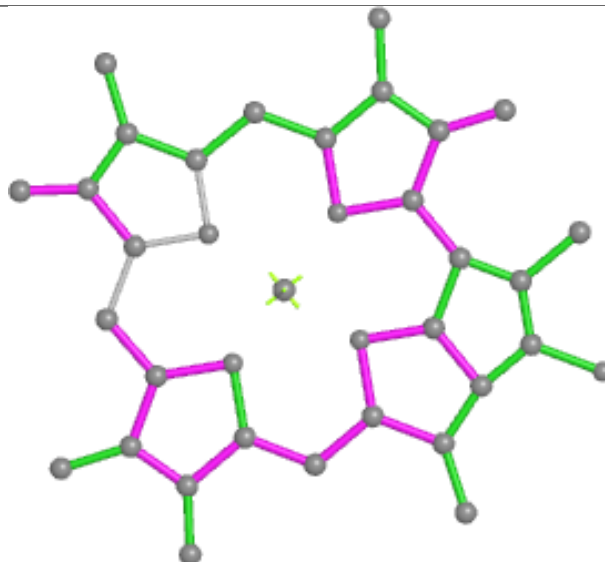




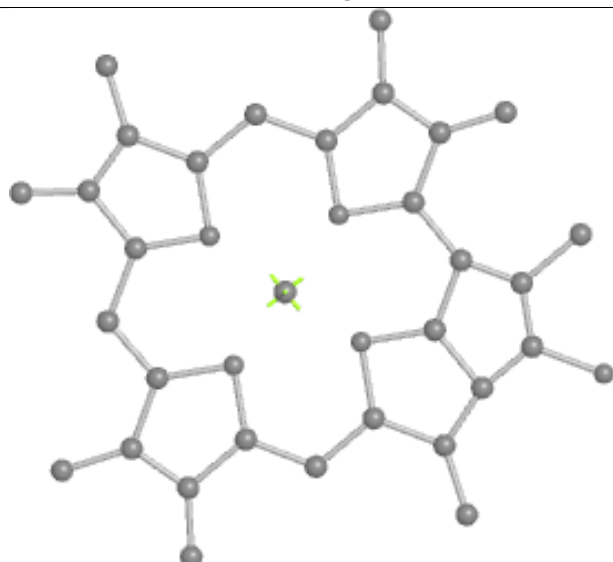
## Ligand CLA J1 1303



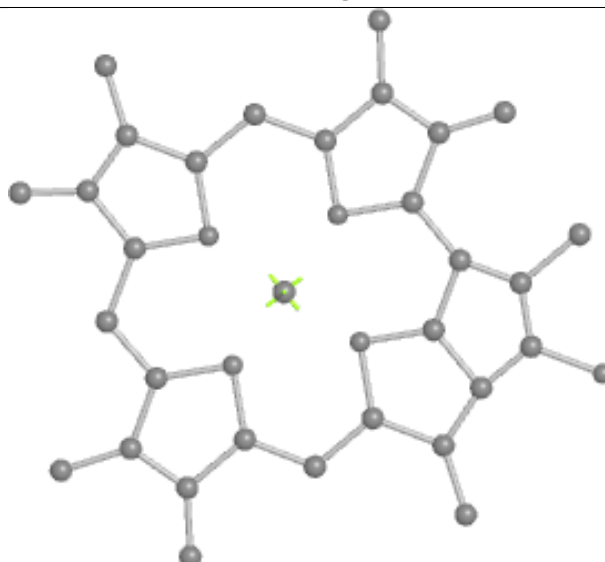
Bond lengths



Bond angles

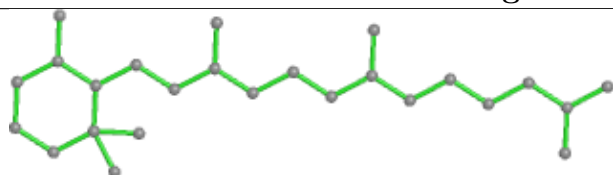


Torsions

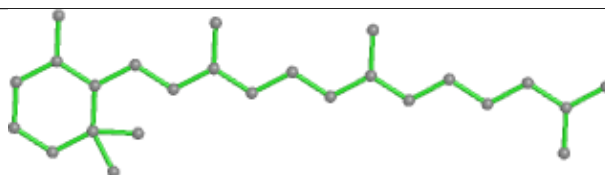


Rings

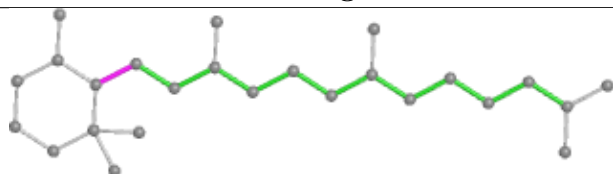
## Ligand BCR K1 102



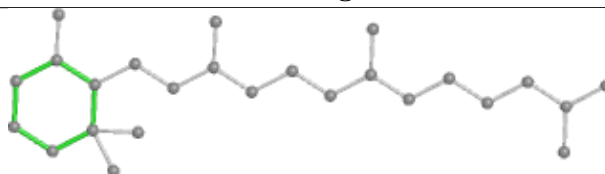
Bond lengths



Bond angles

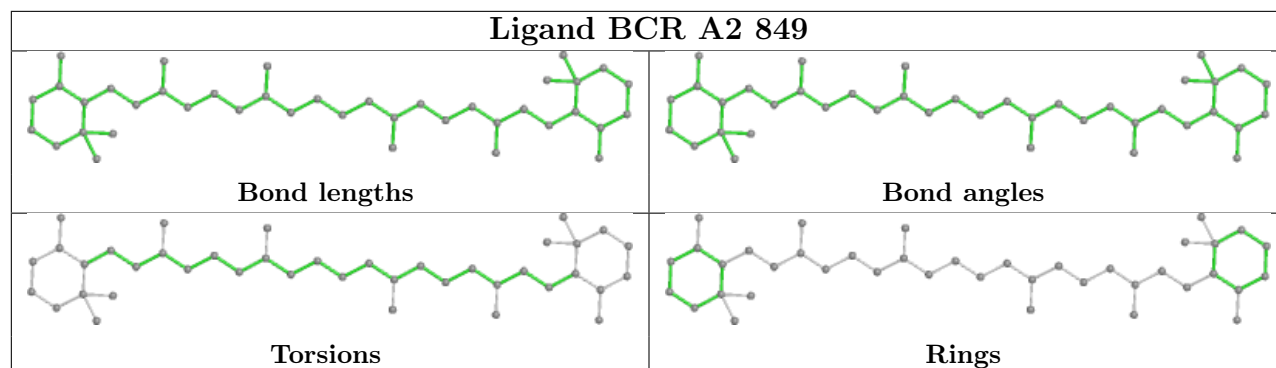


Torsions

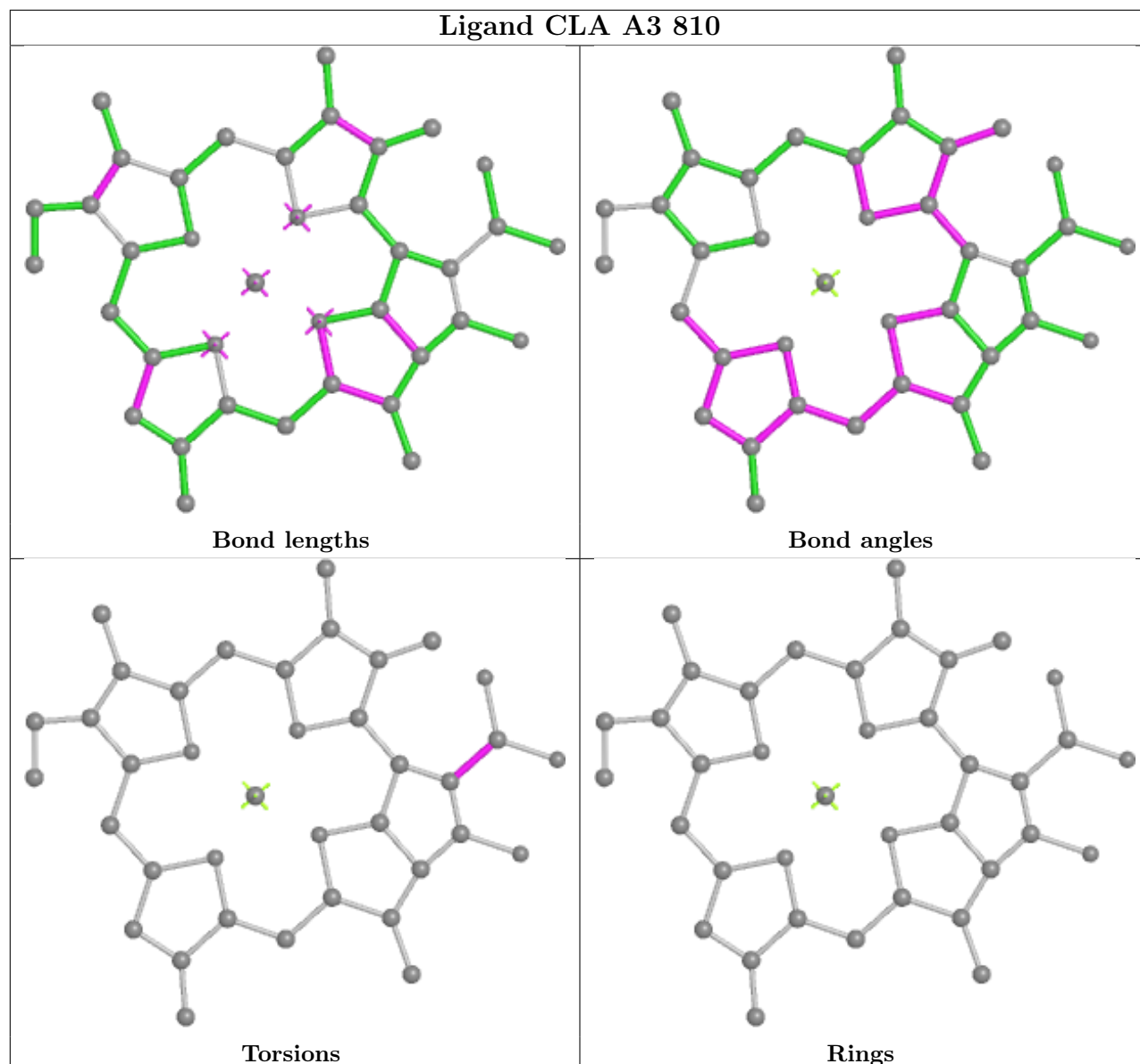


Rings

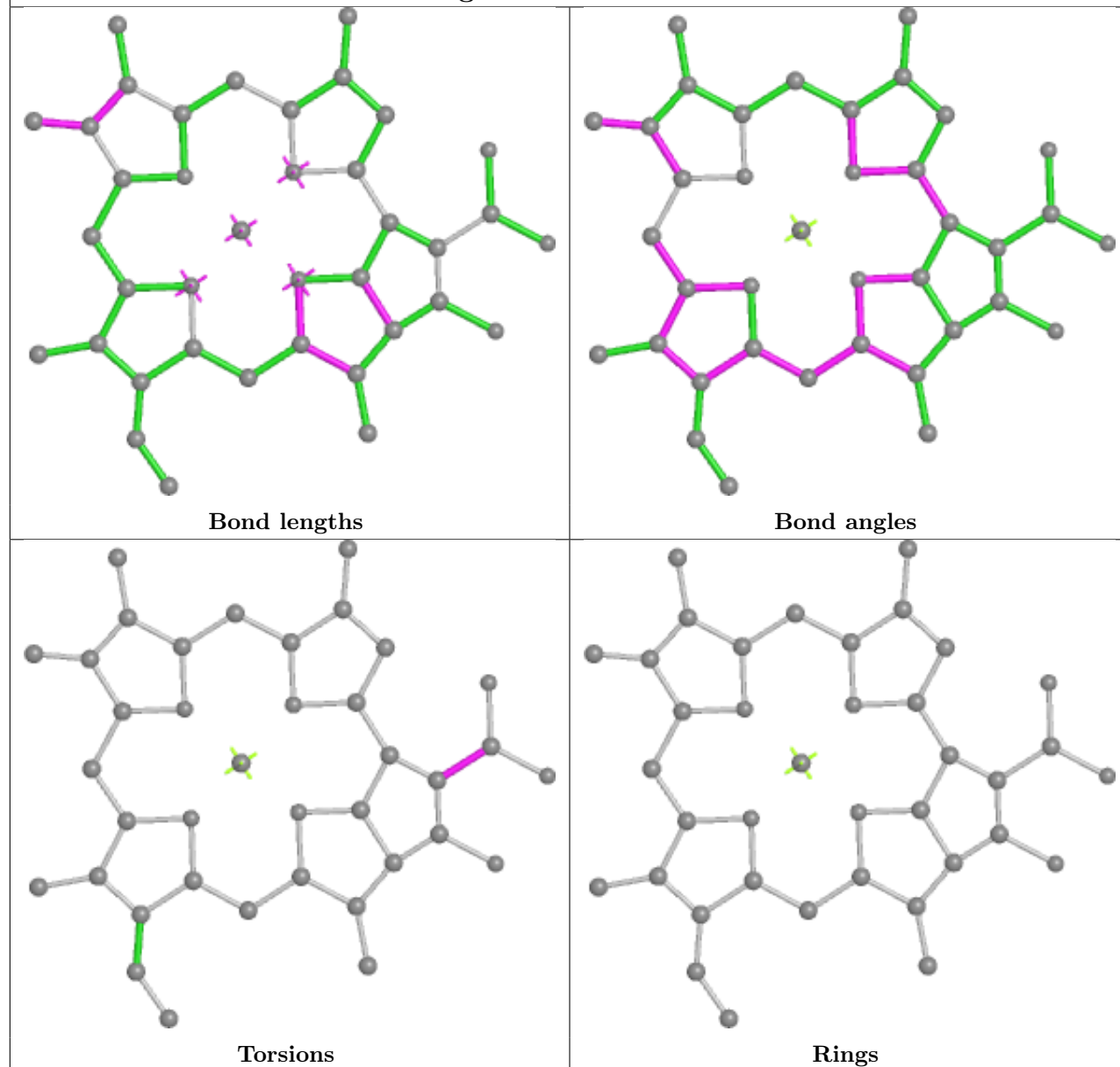
## Ligand BCR A2 849



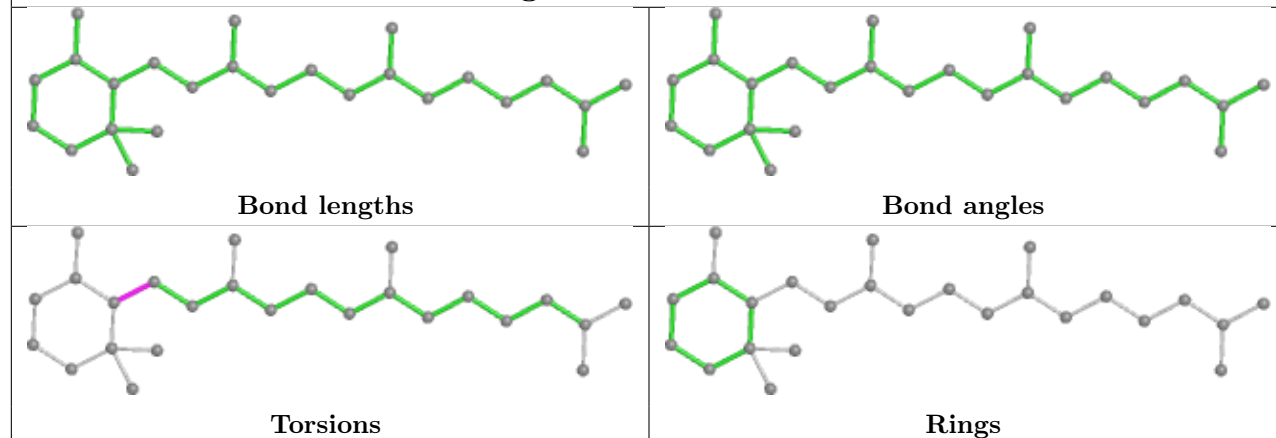
## Ligand CLA A3 810



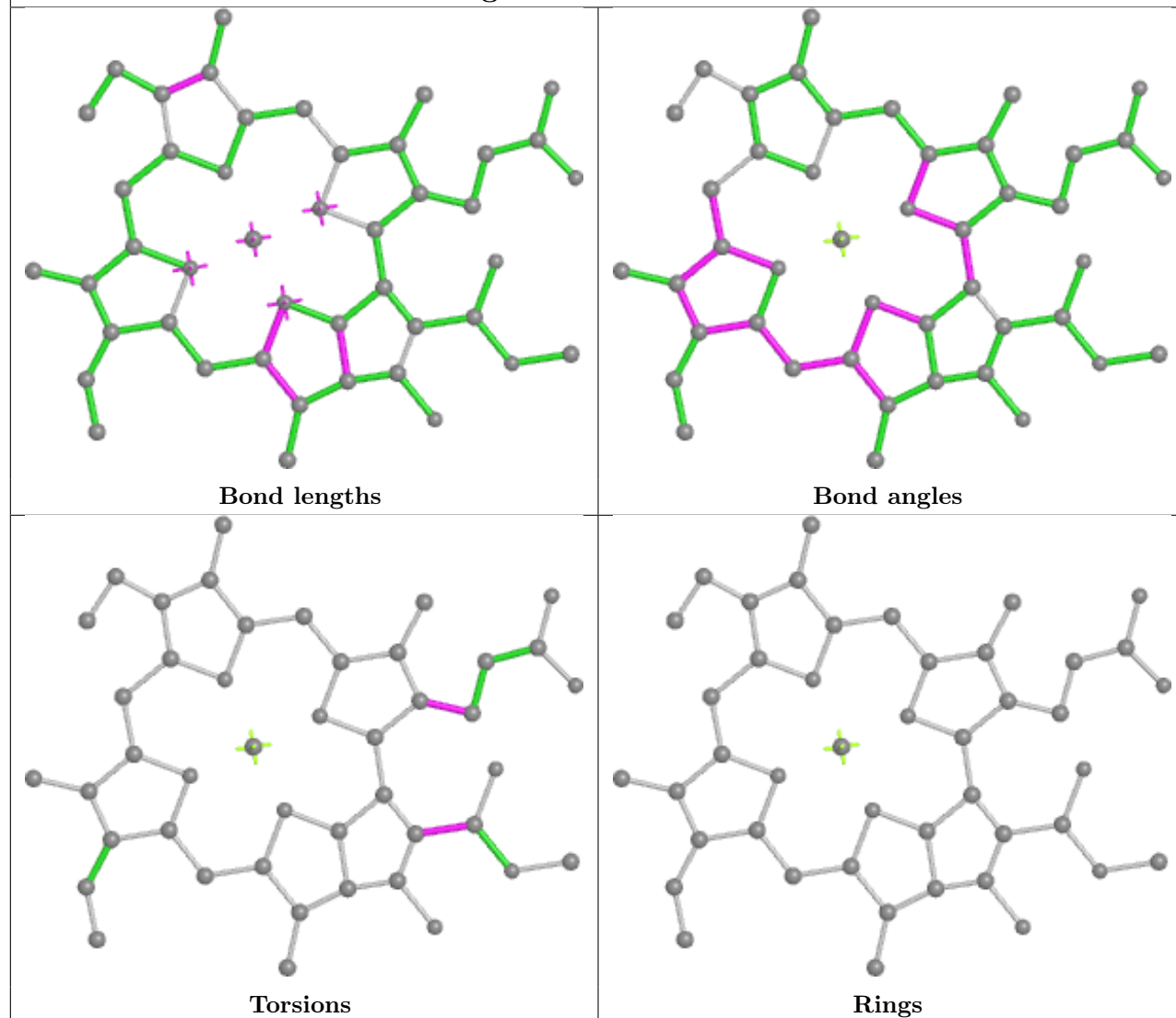
## Ligand CLA A1 820



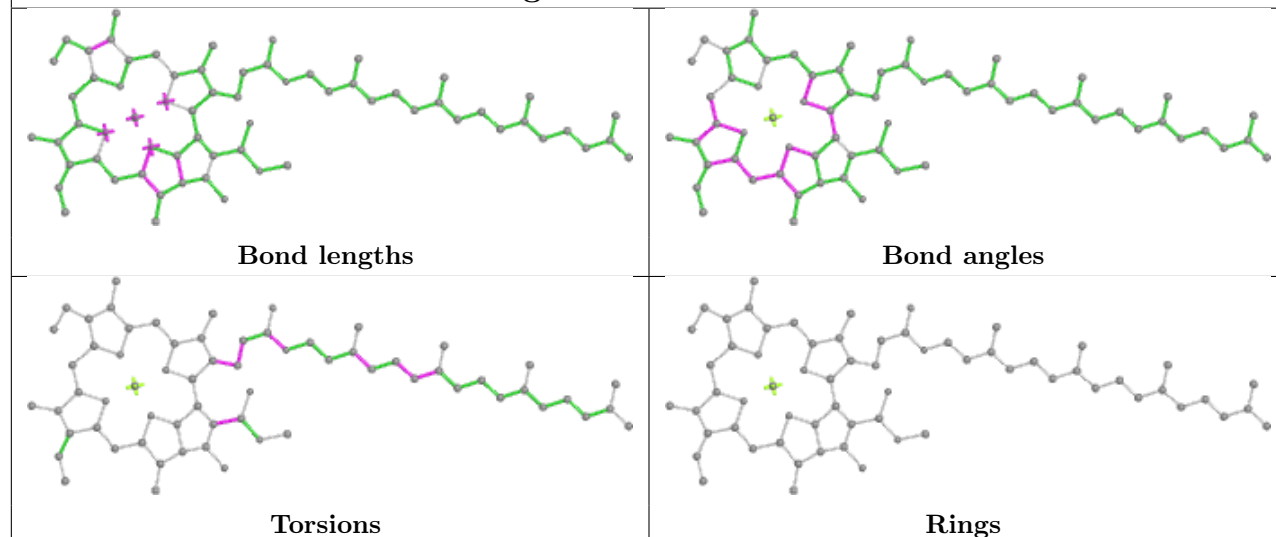
## Ligand BCR K2 102

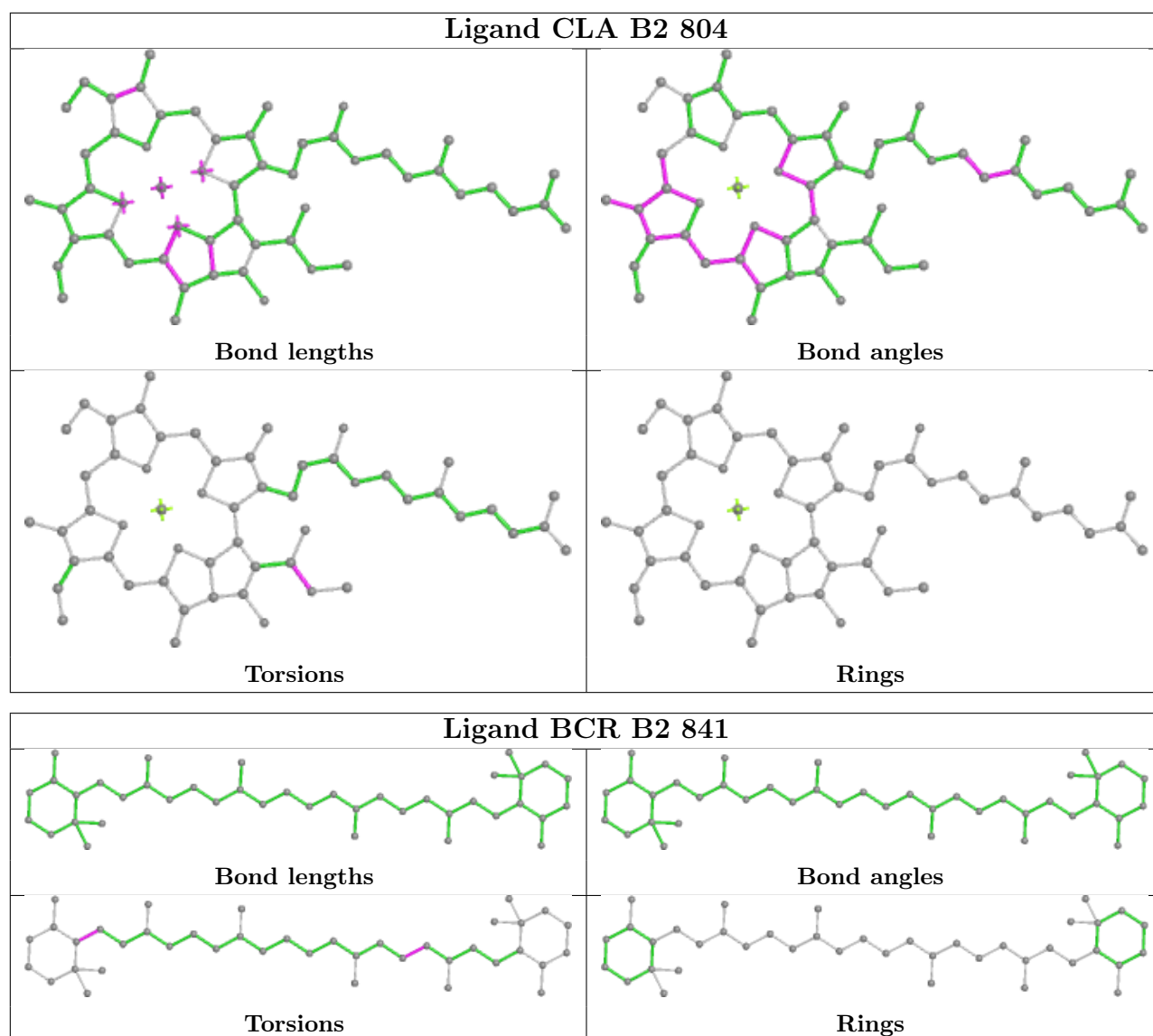


## Ligand CLA A1 844

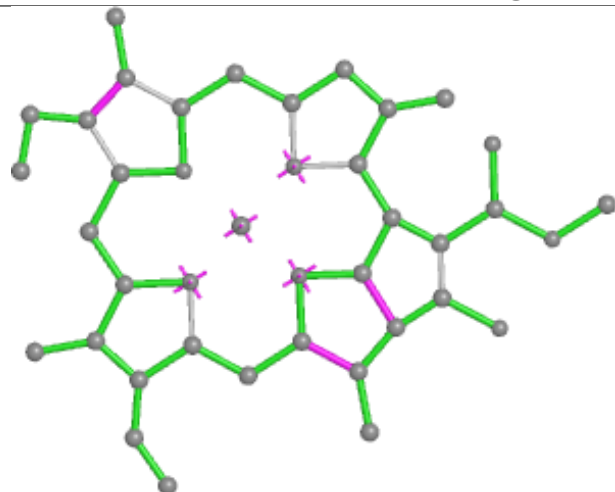


## Ligand CLA B2 827

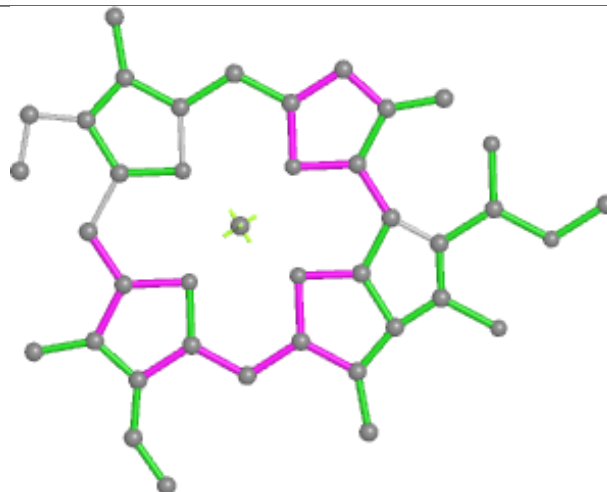




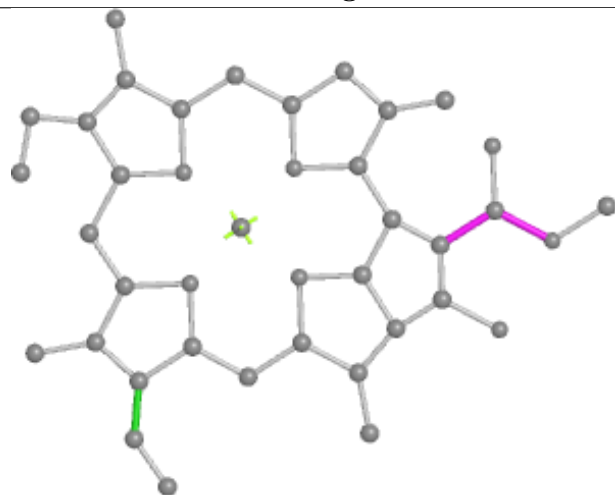
## Ligand CLA B1 832



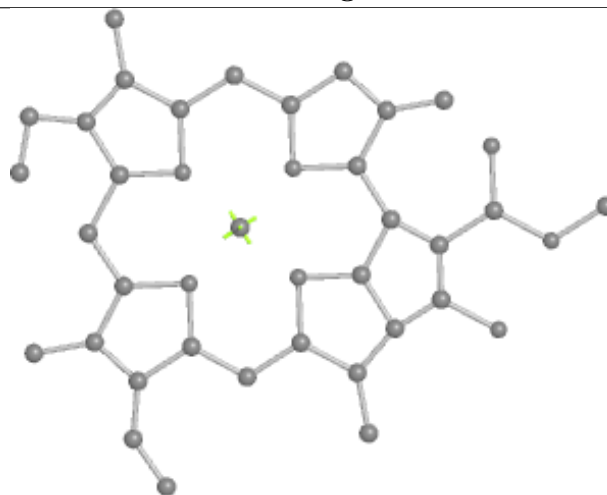
Bond lengths



Bond angles

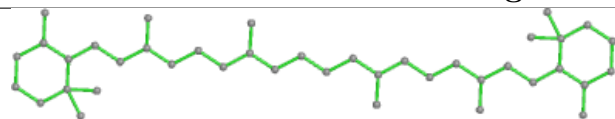


Torsions

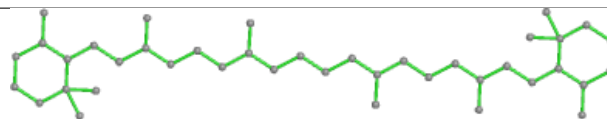


Rings

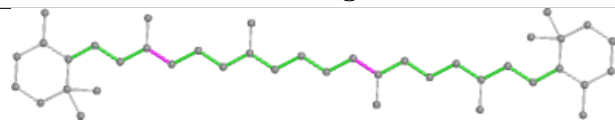
## Ligand BCR A3 852



Bond lengths



Bond angles

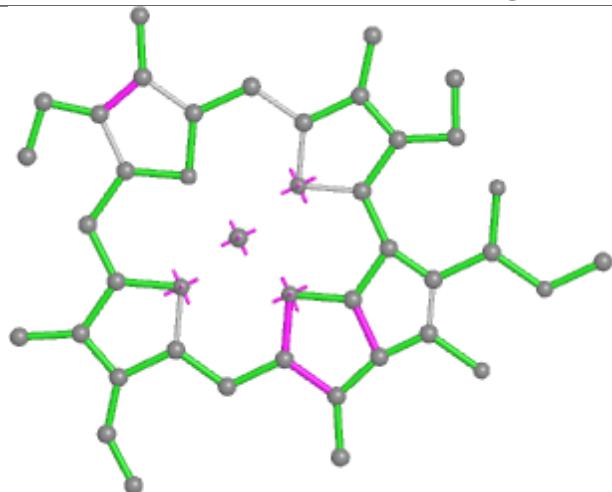


Torsions

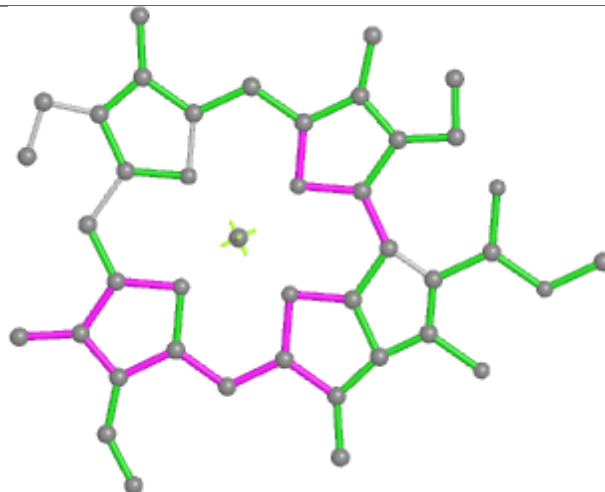


Rings

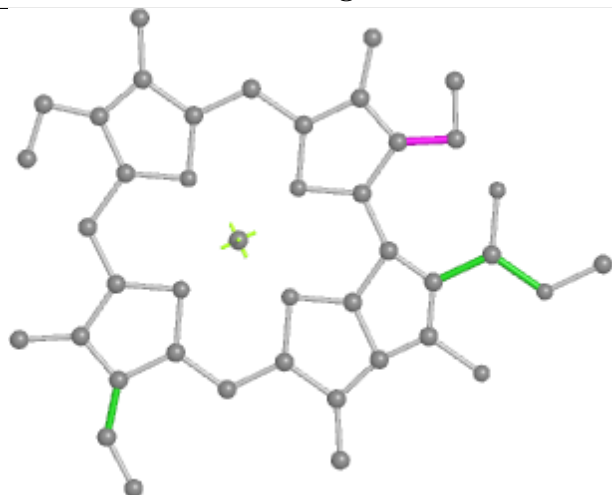
## Ligand CLA A2 828



Bond lengths



Bond angles



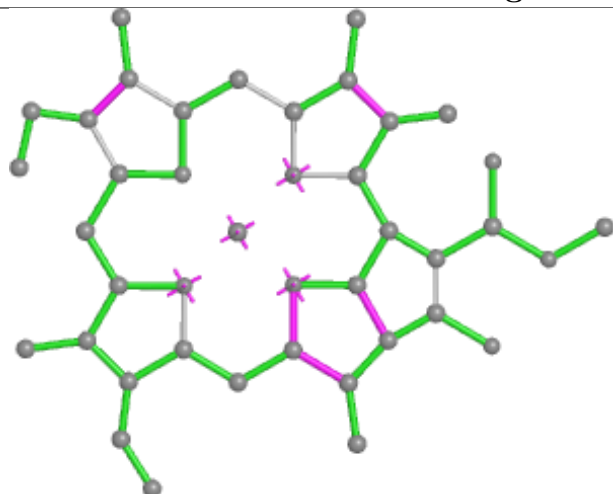
Torsions



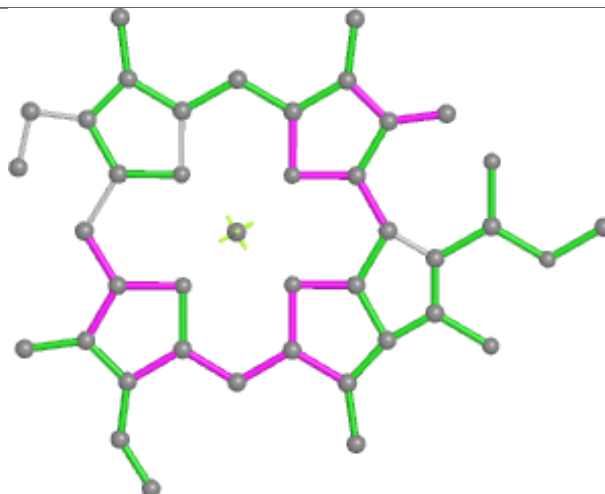
Rings



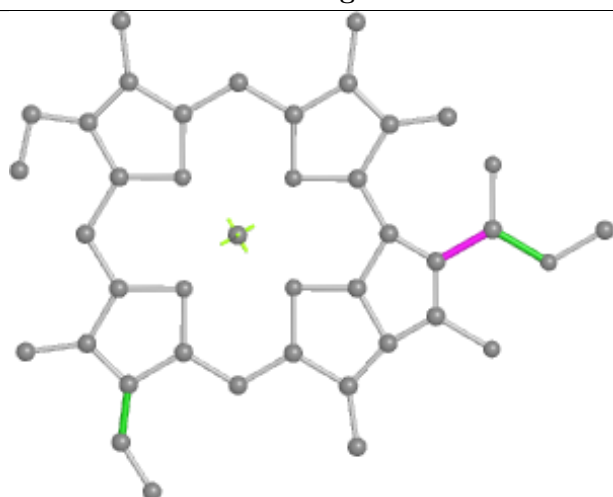
## Ligand CLA B1 823



Bond lengths



Bond angles

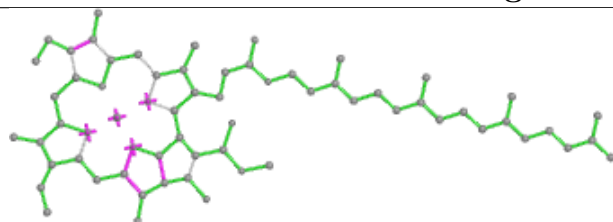


Torsions

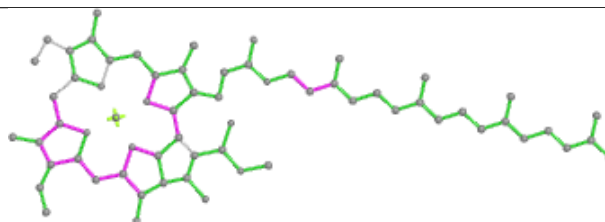


Rings

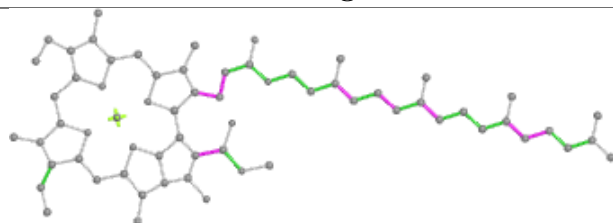
## Ligand CLA A3 809



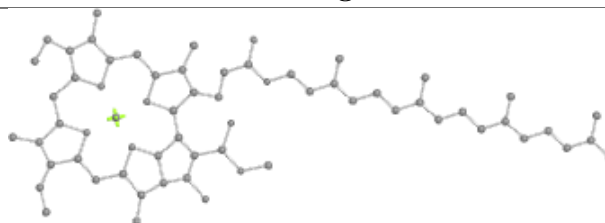
Bond lengths



Bond angles

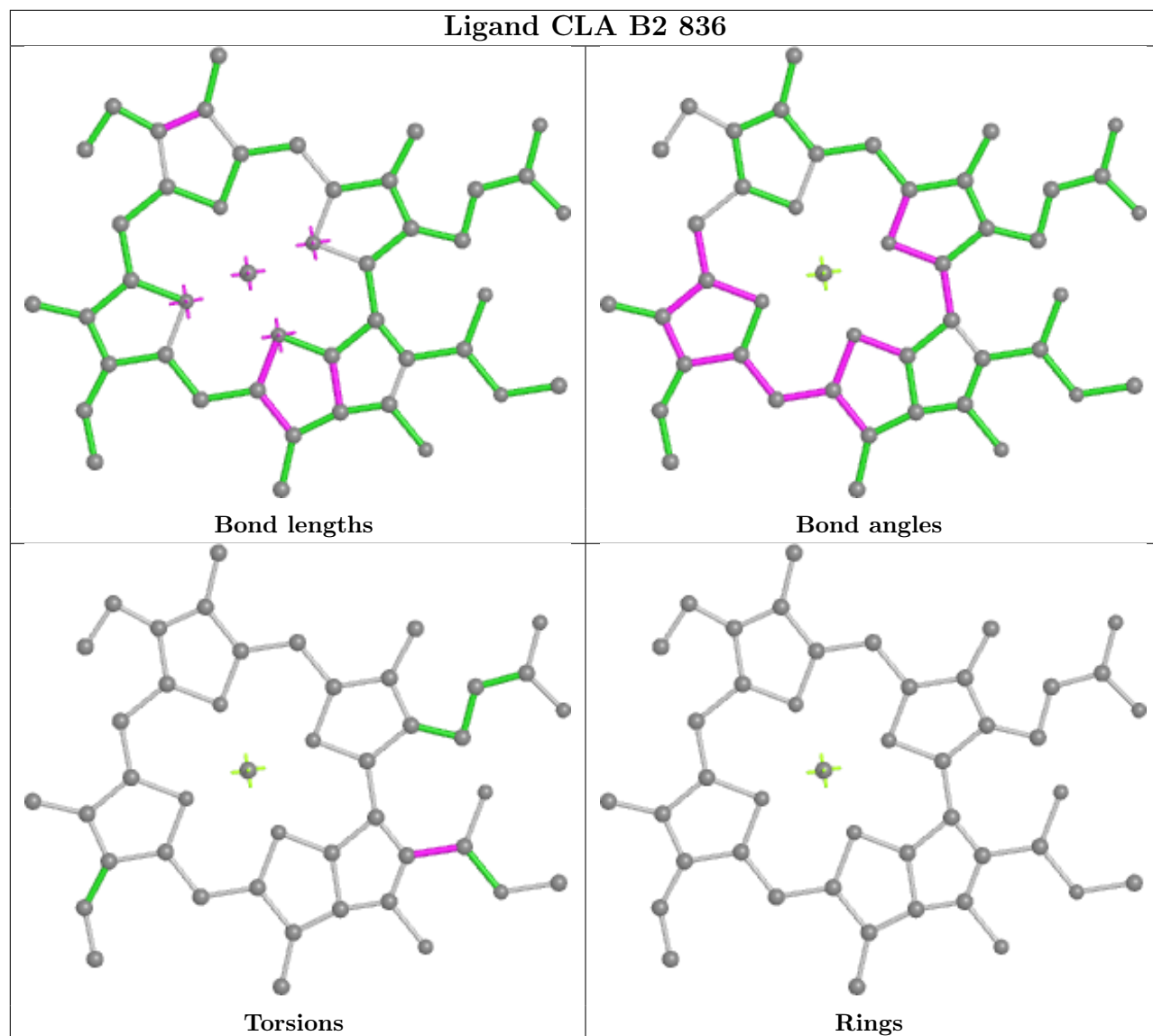


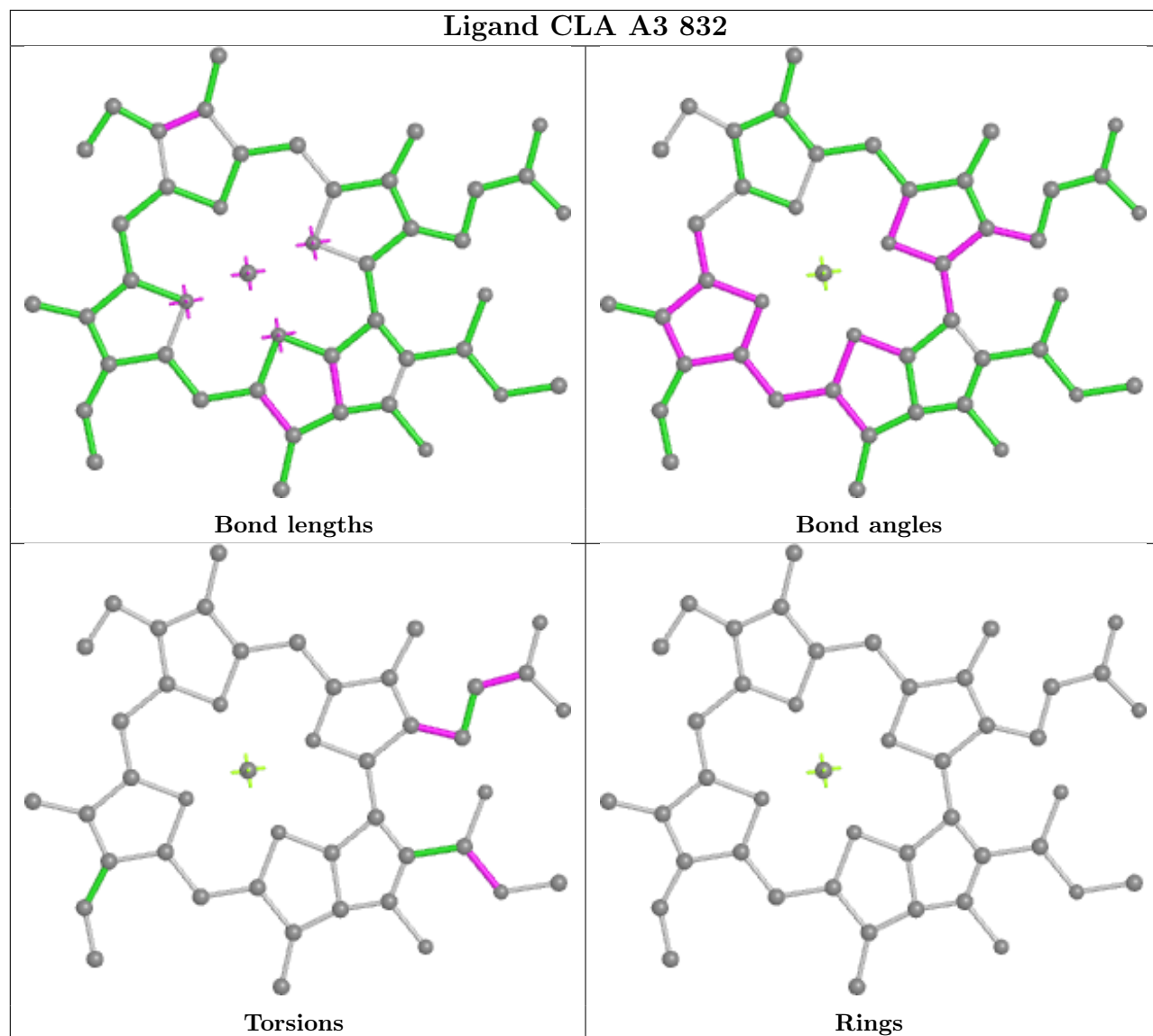
Torsions

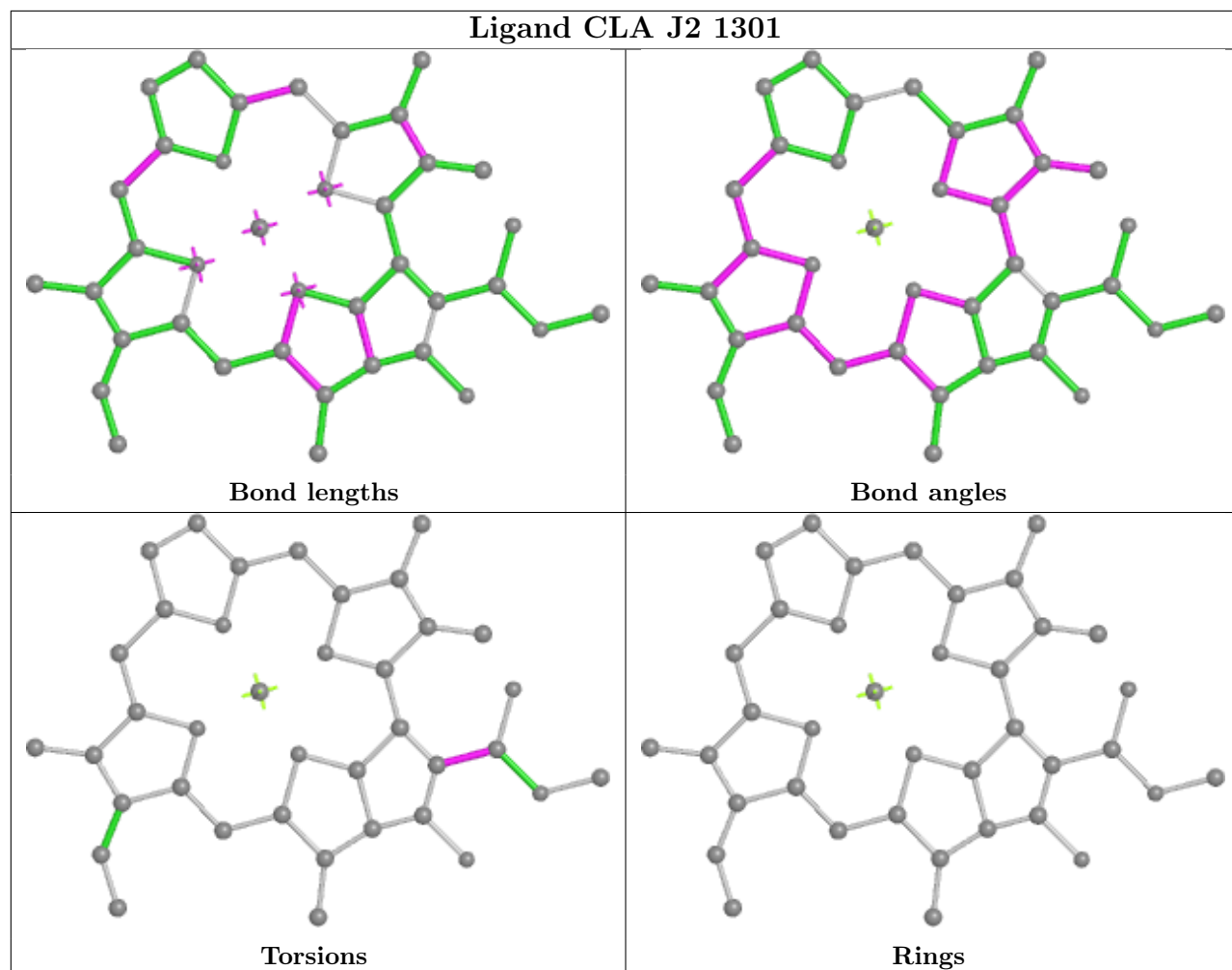


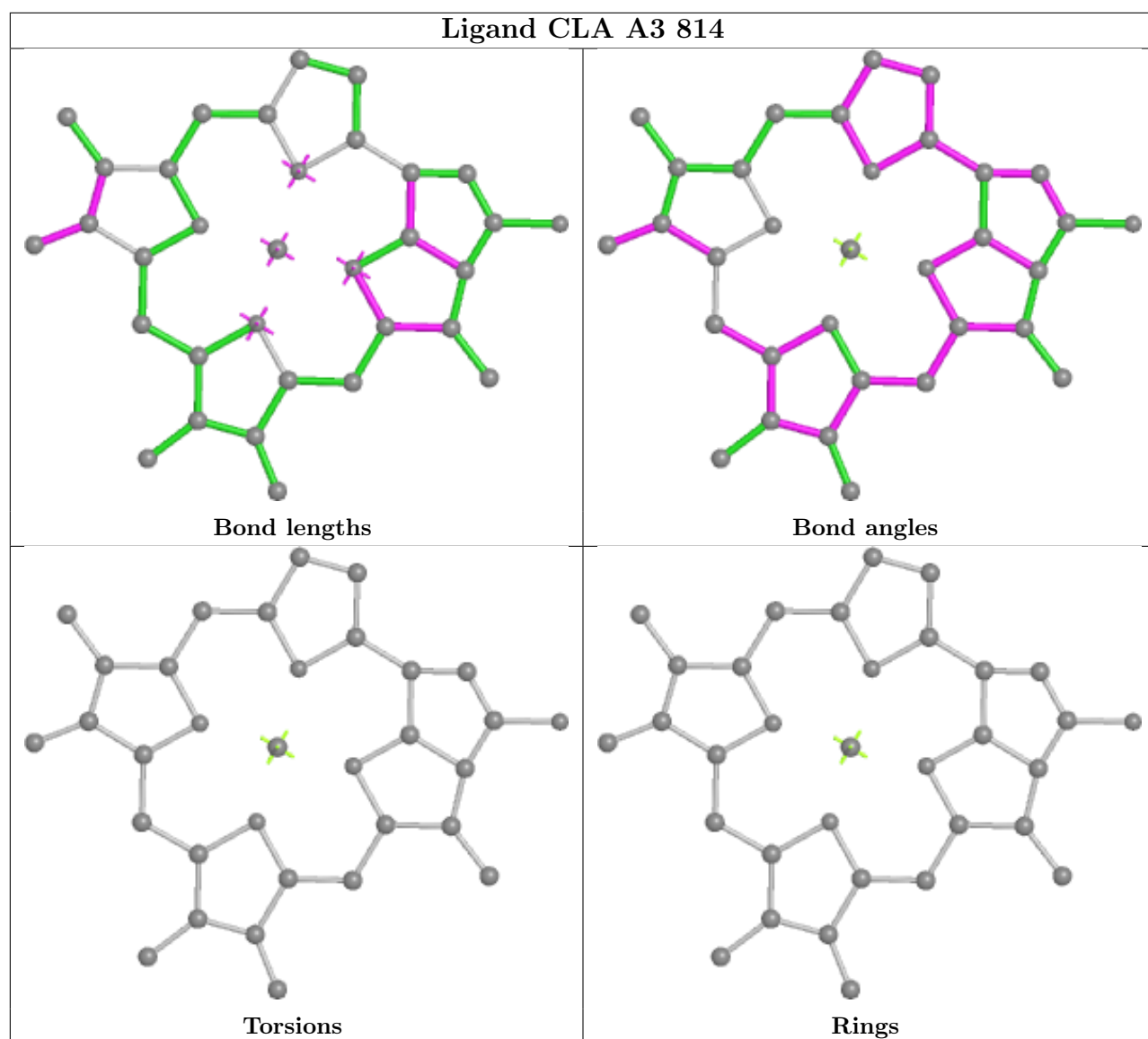
Rings

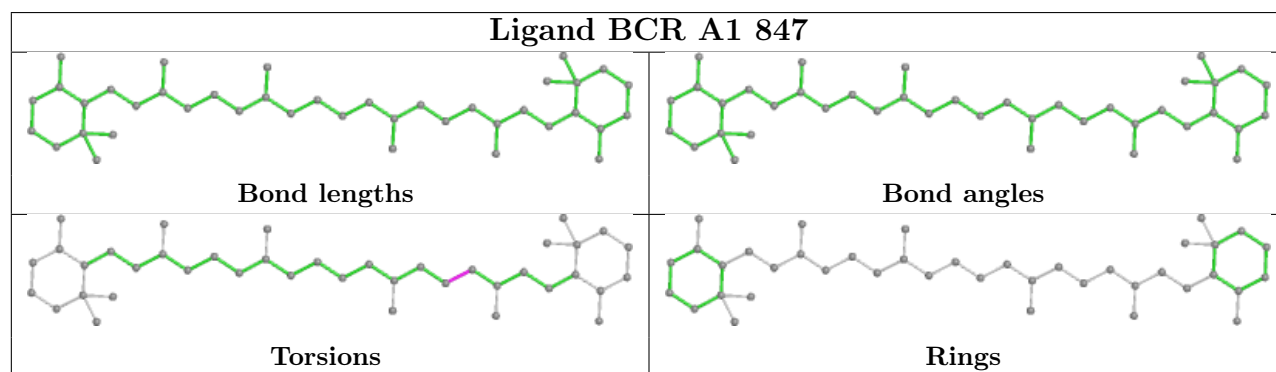
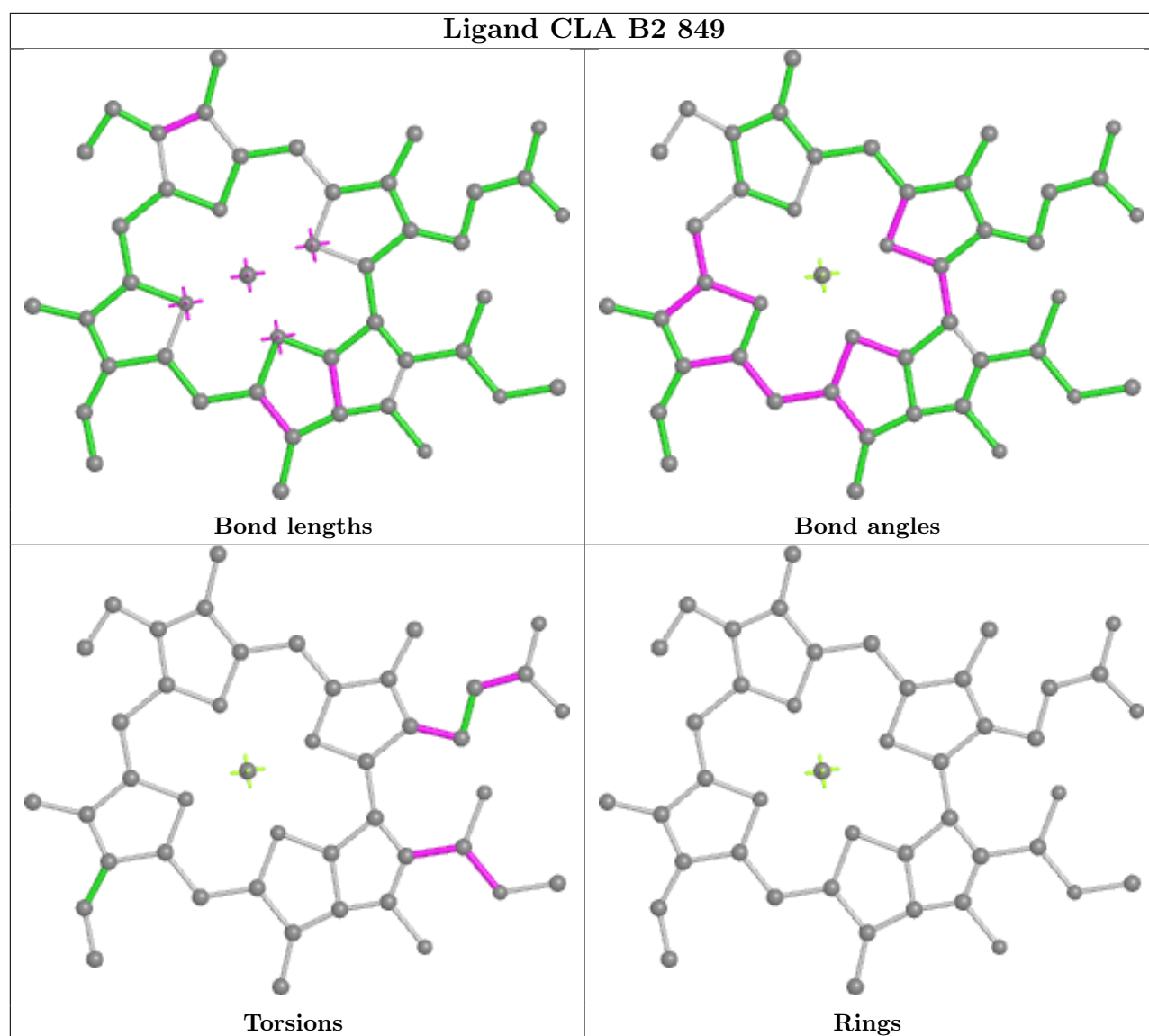
## Ligand CLA B2 836



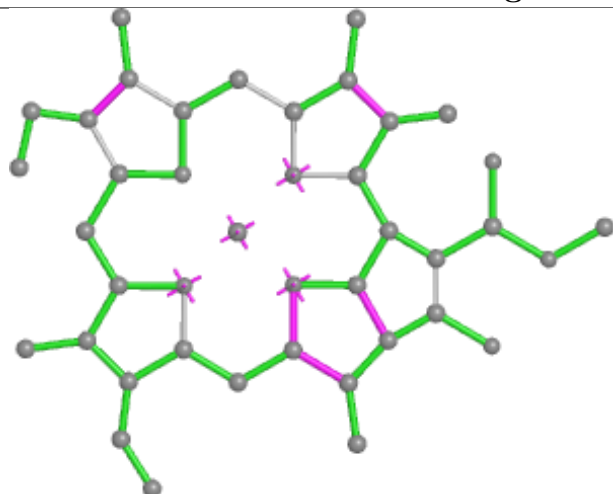




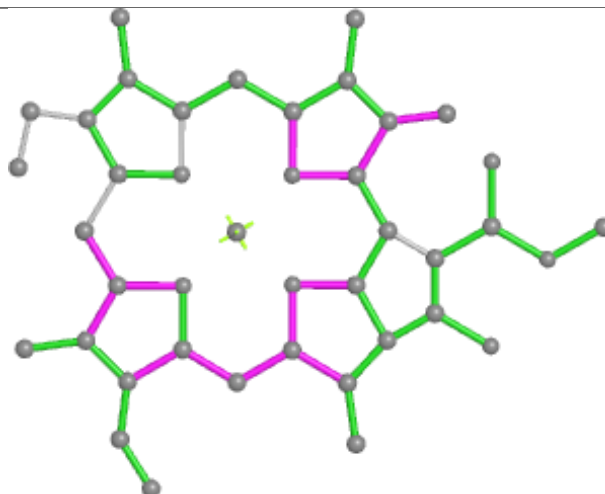




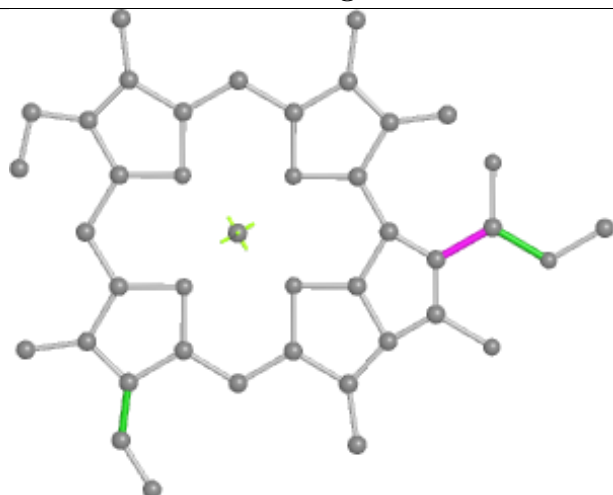
## Ligand CLA A3 823



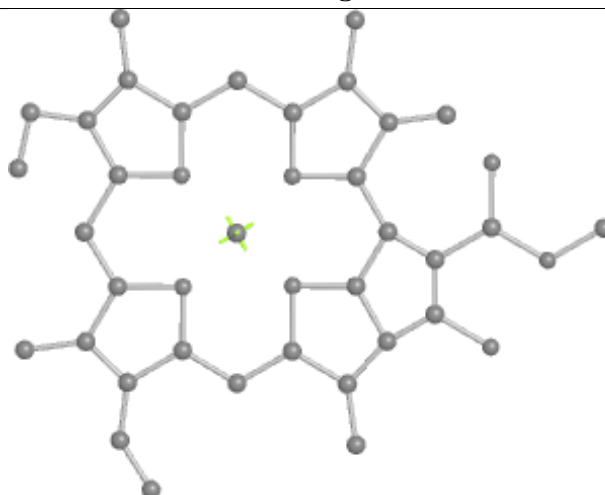
Bond lengths



Bond angles

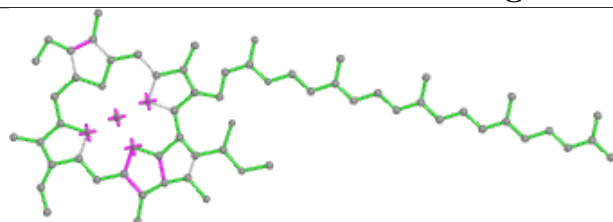


Torsions

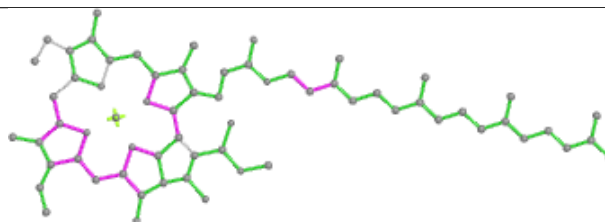


Rings

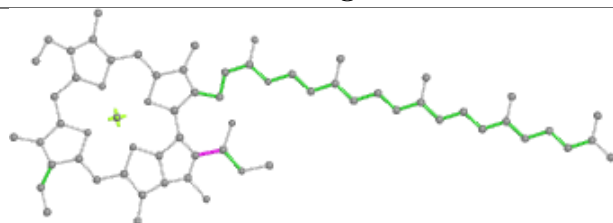
## Ligand CLA B2 825



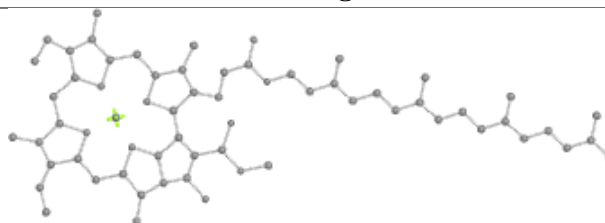
Bond lengths



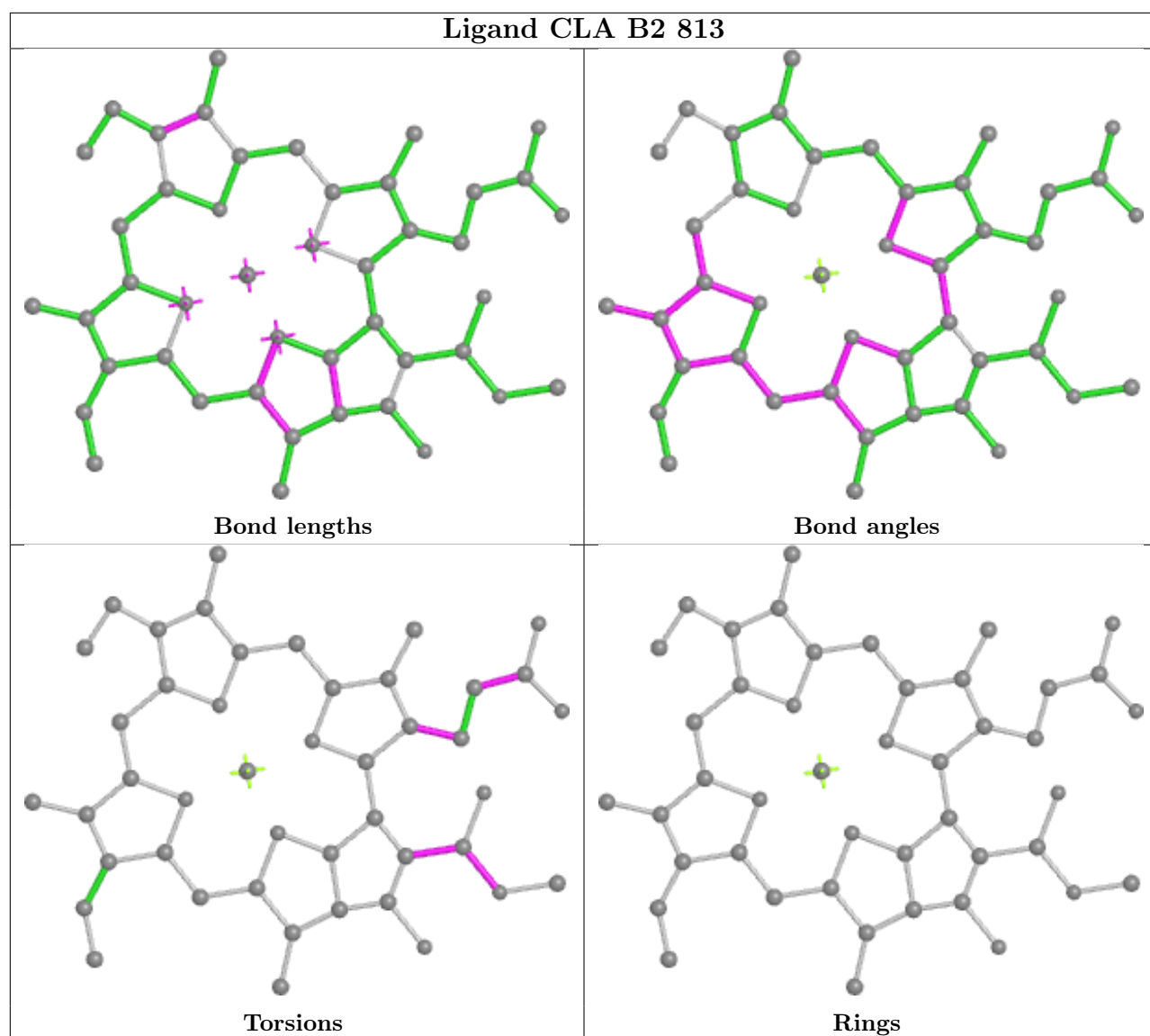
Bond angles



Torsions

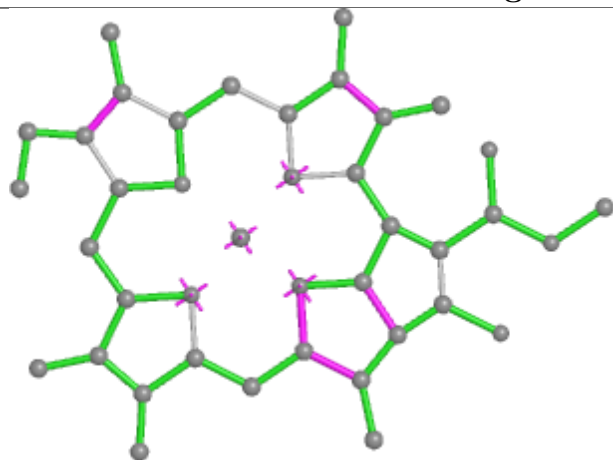


Rings

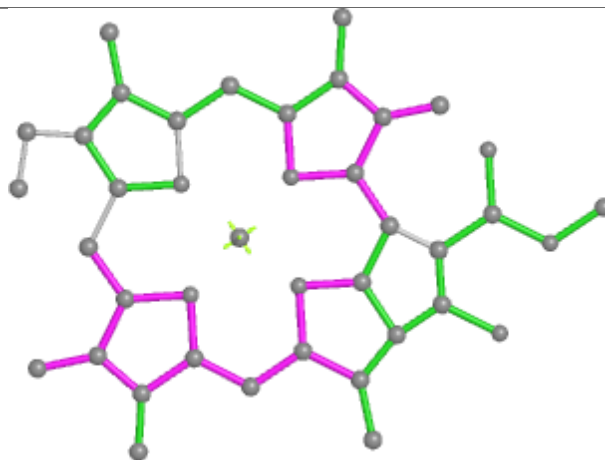




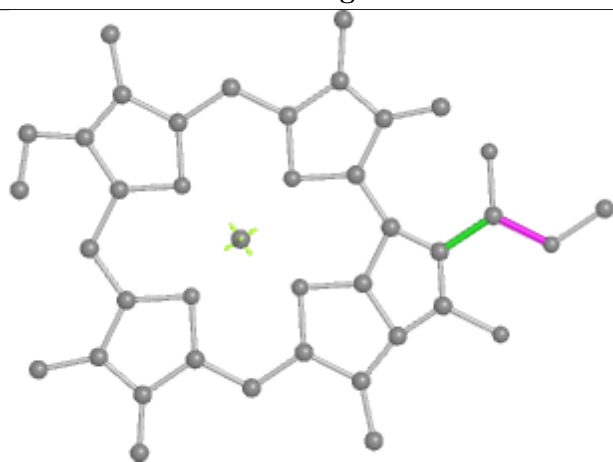
## Ligand CLA X1 102



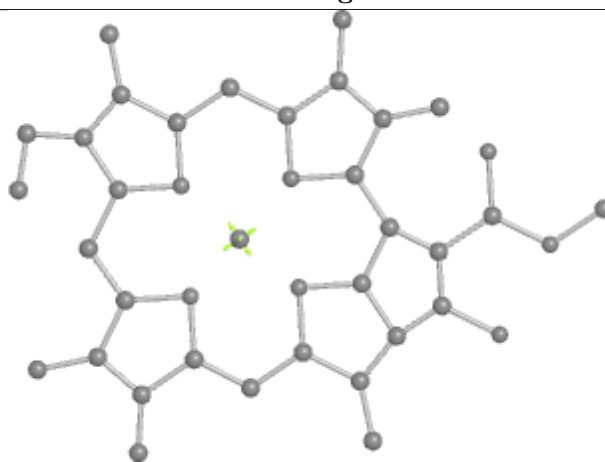
Bond lengths



Bond angles

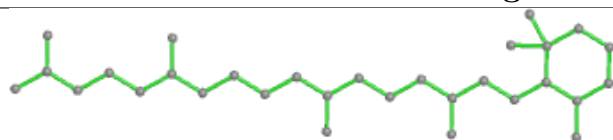


Torsions

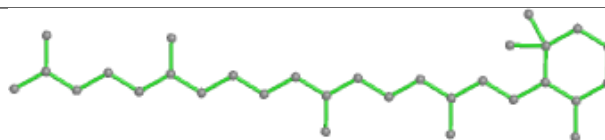


Rings

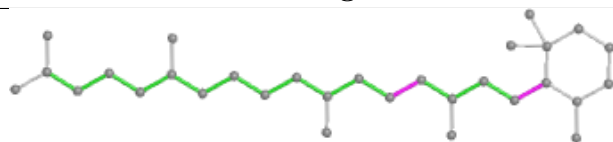
## Ligand BCR A3 855



Bond lengths



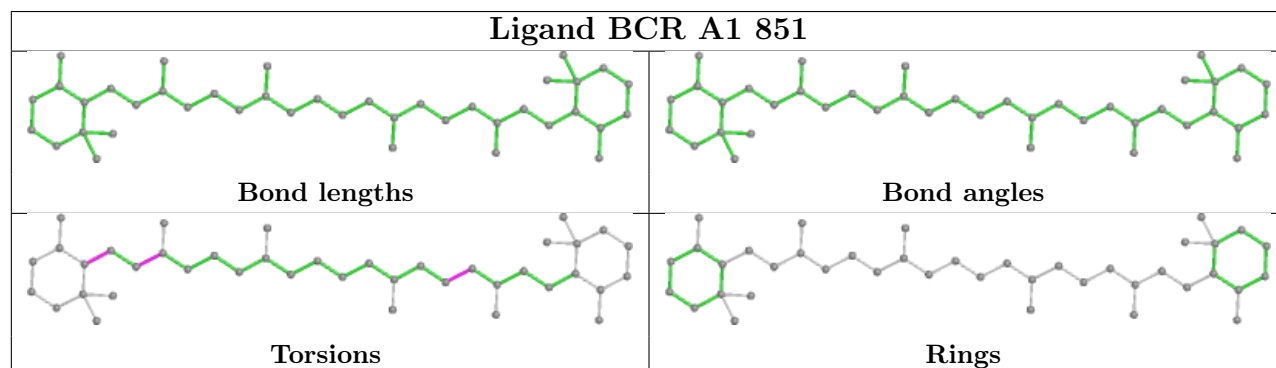
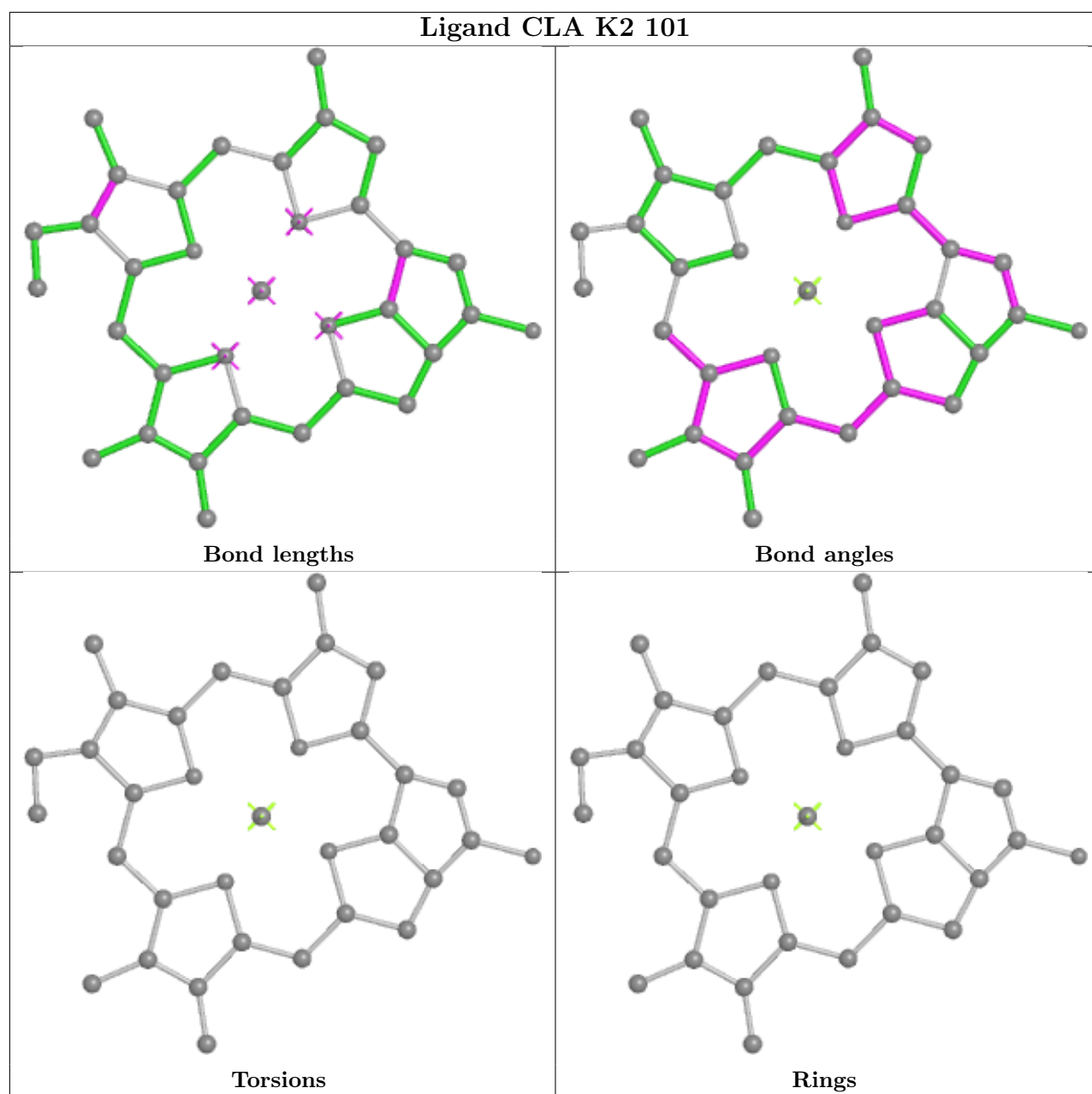
Bond angles

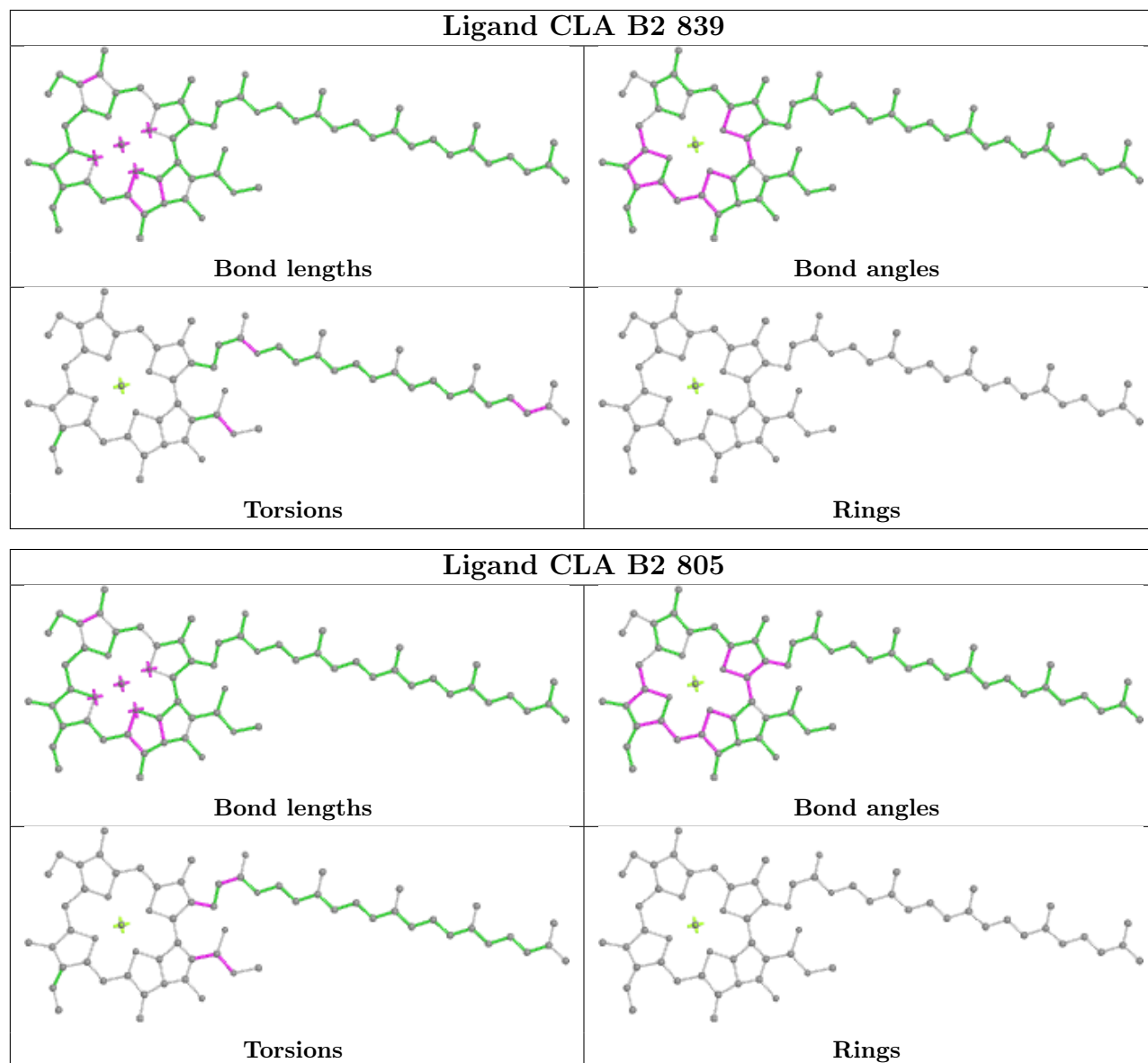


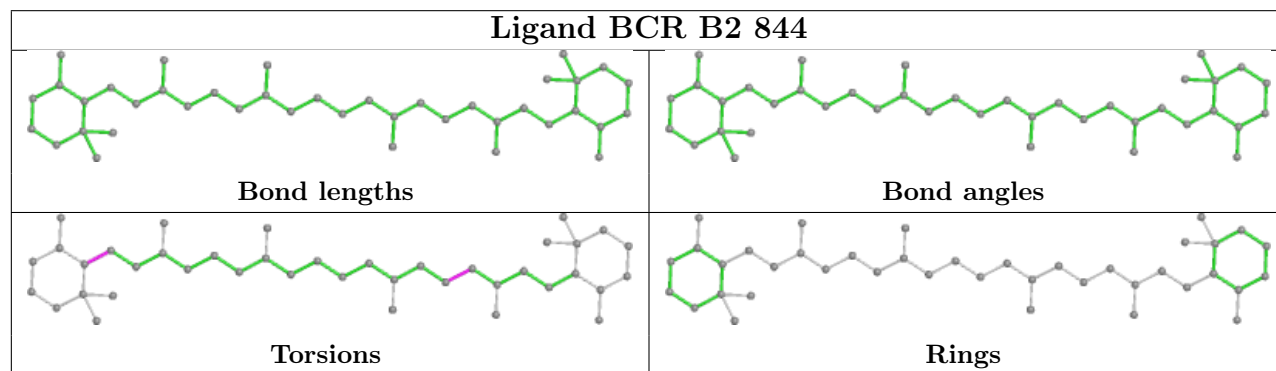
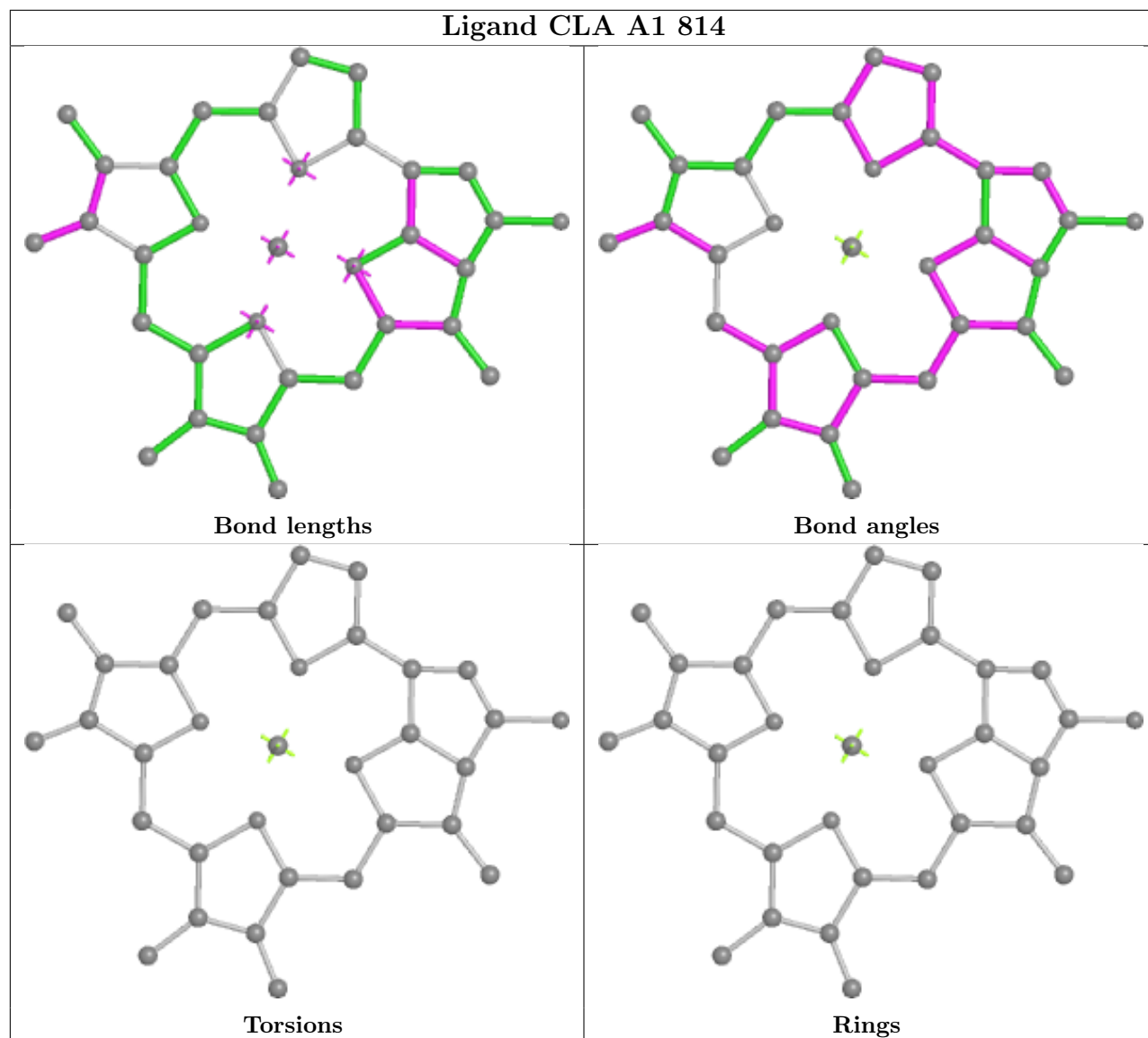
Torsions

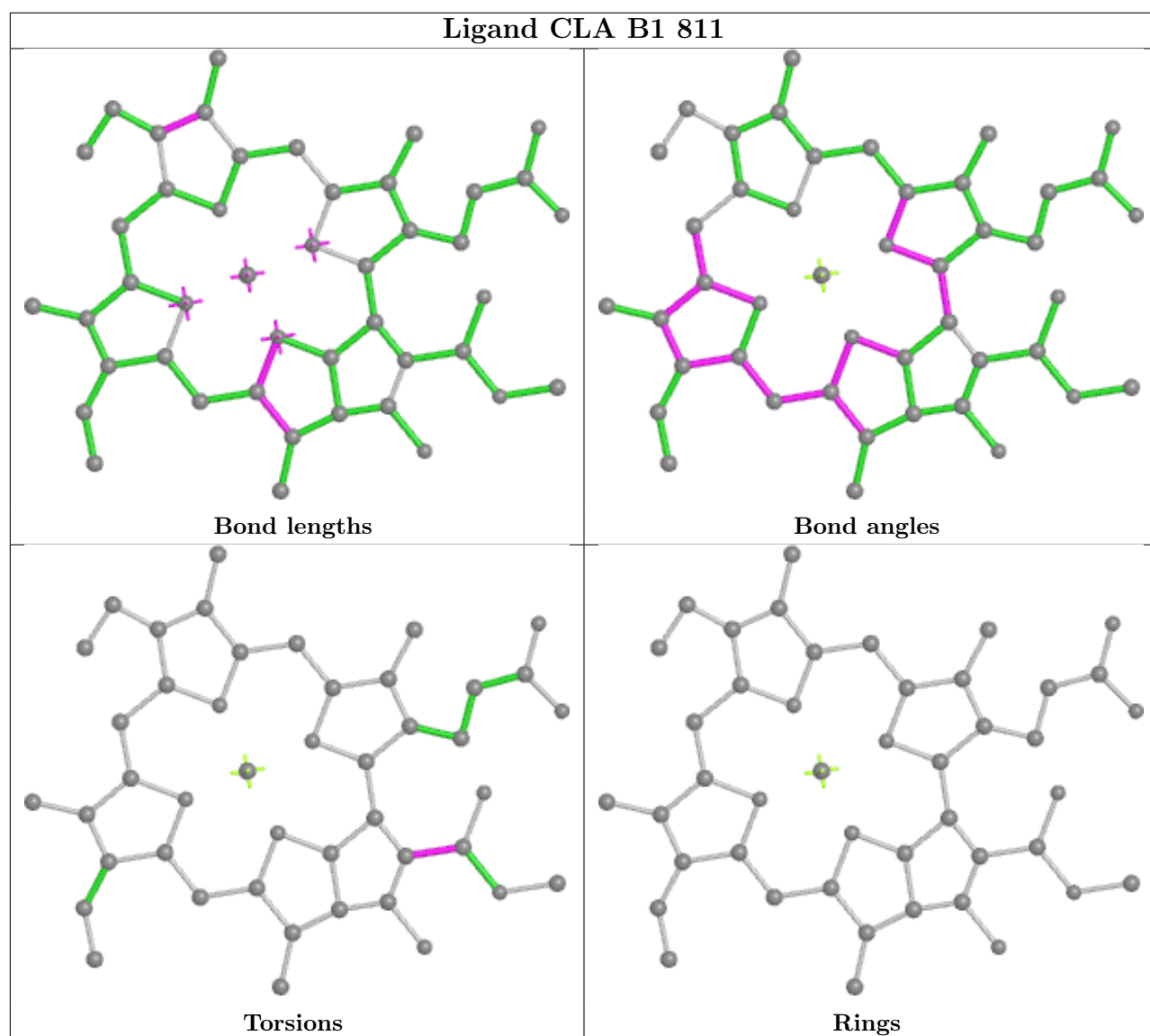


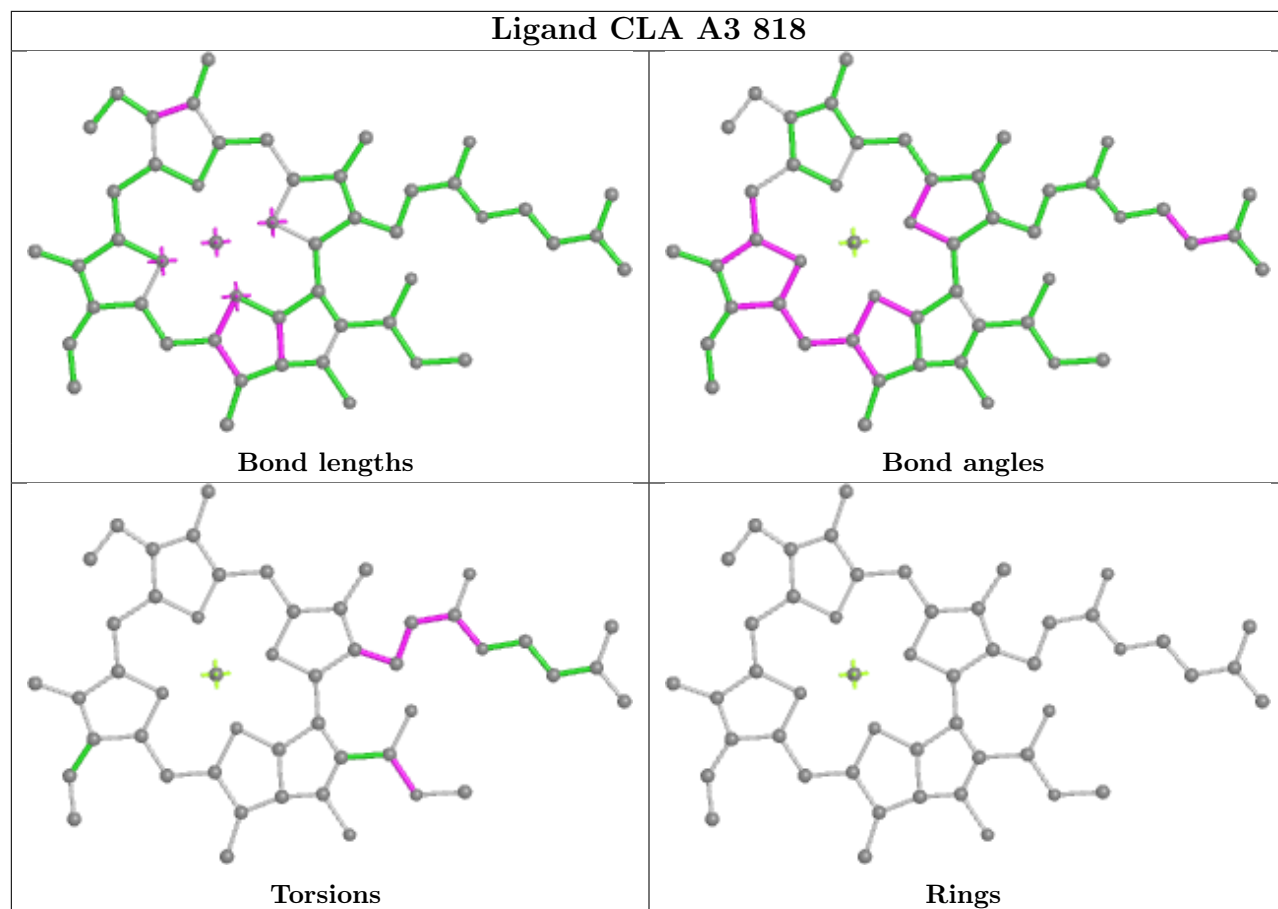
Rings



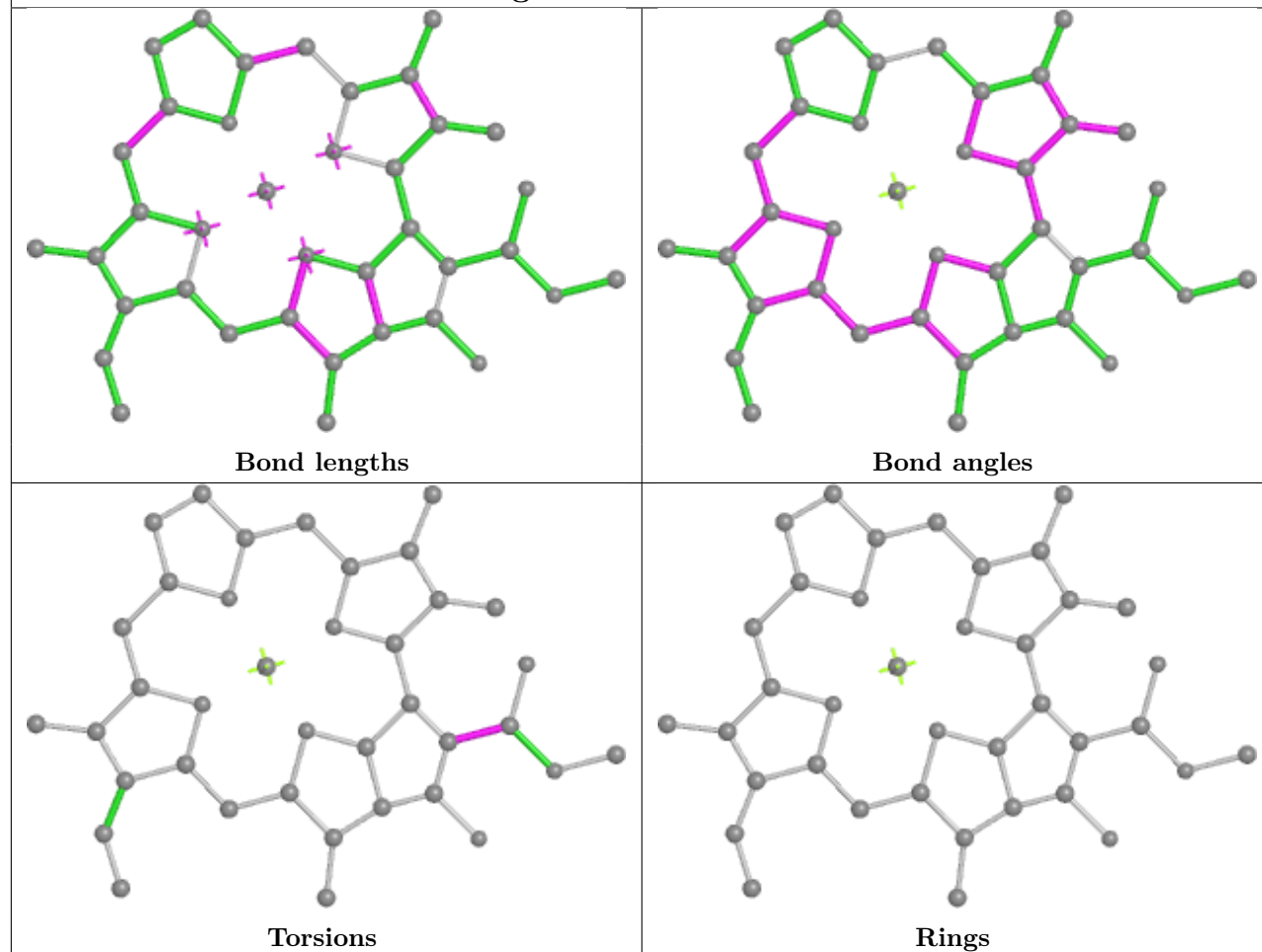




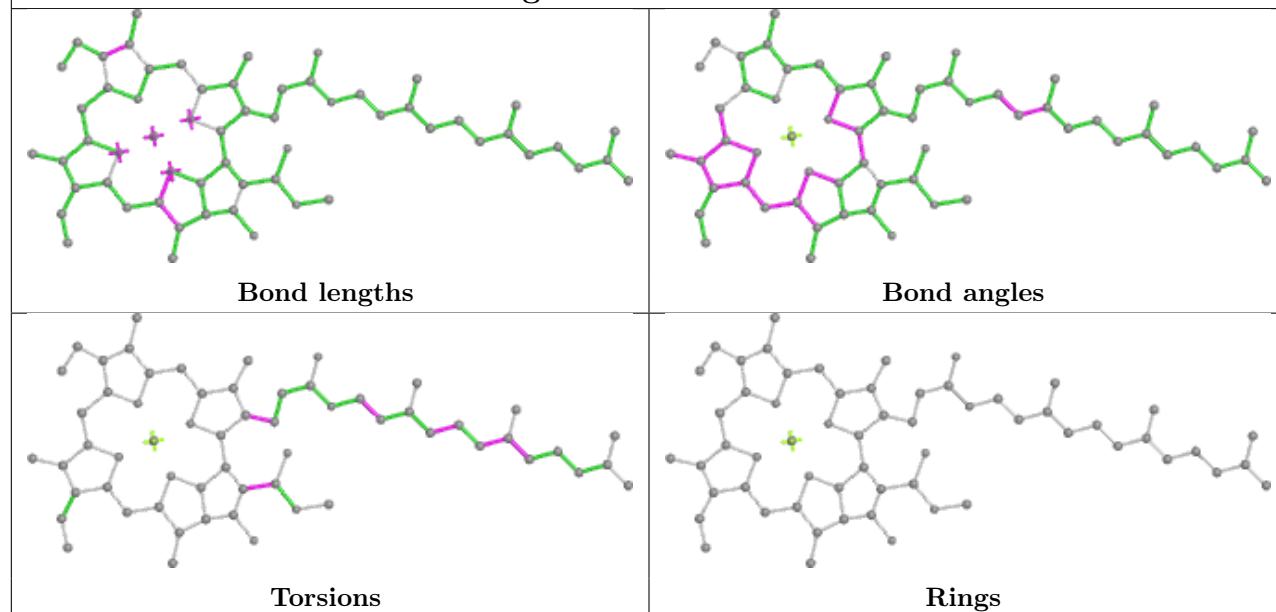


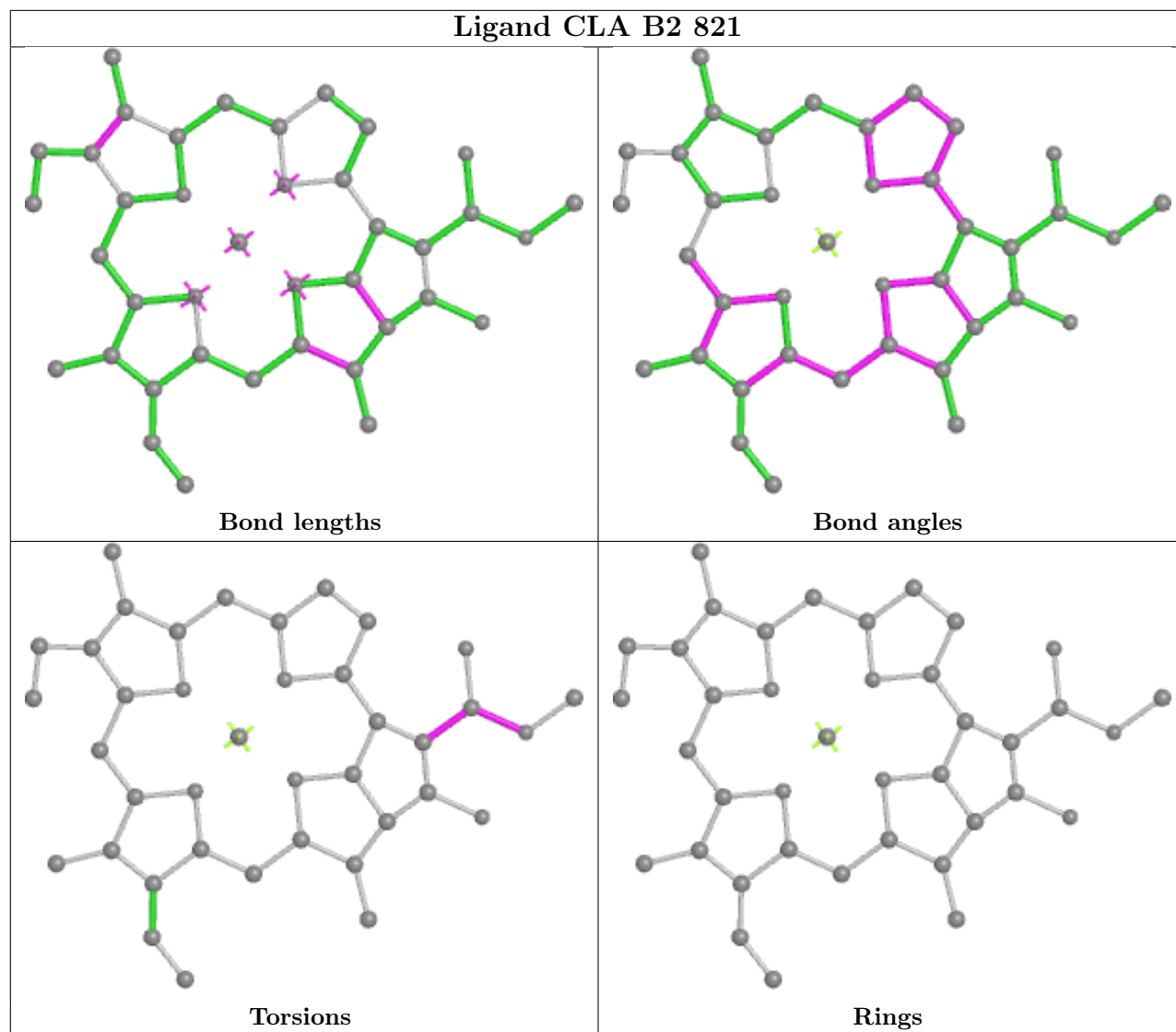
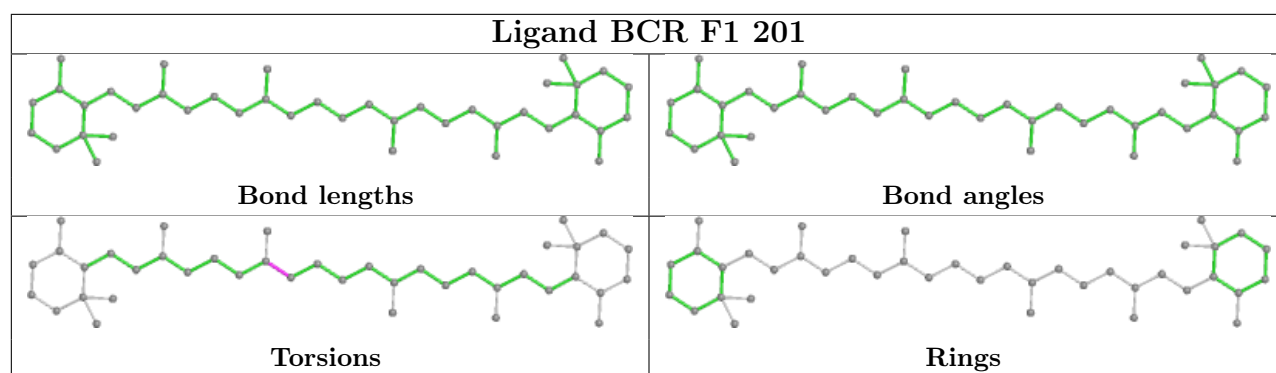


## Ligand CLA J1 1301



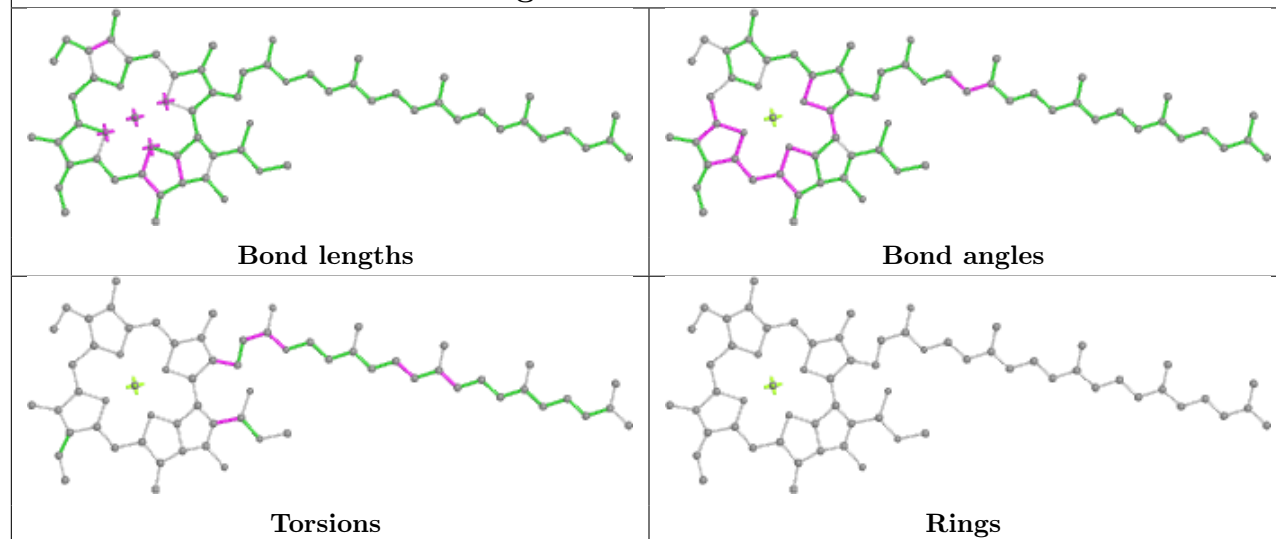
## Ligand CLA A1 825



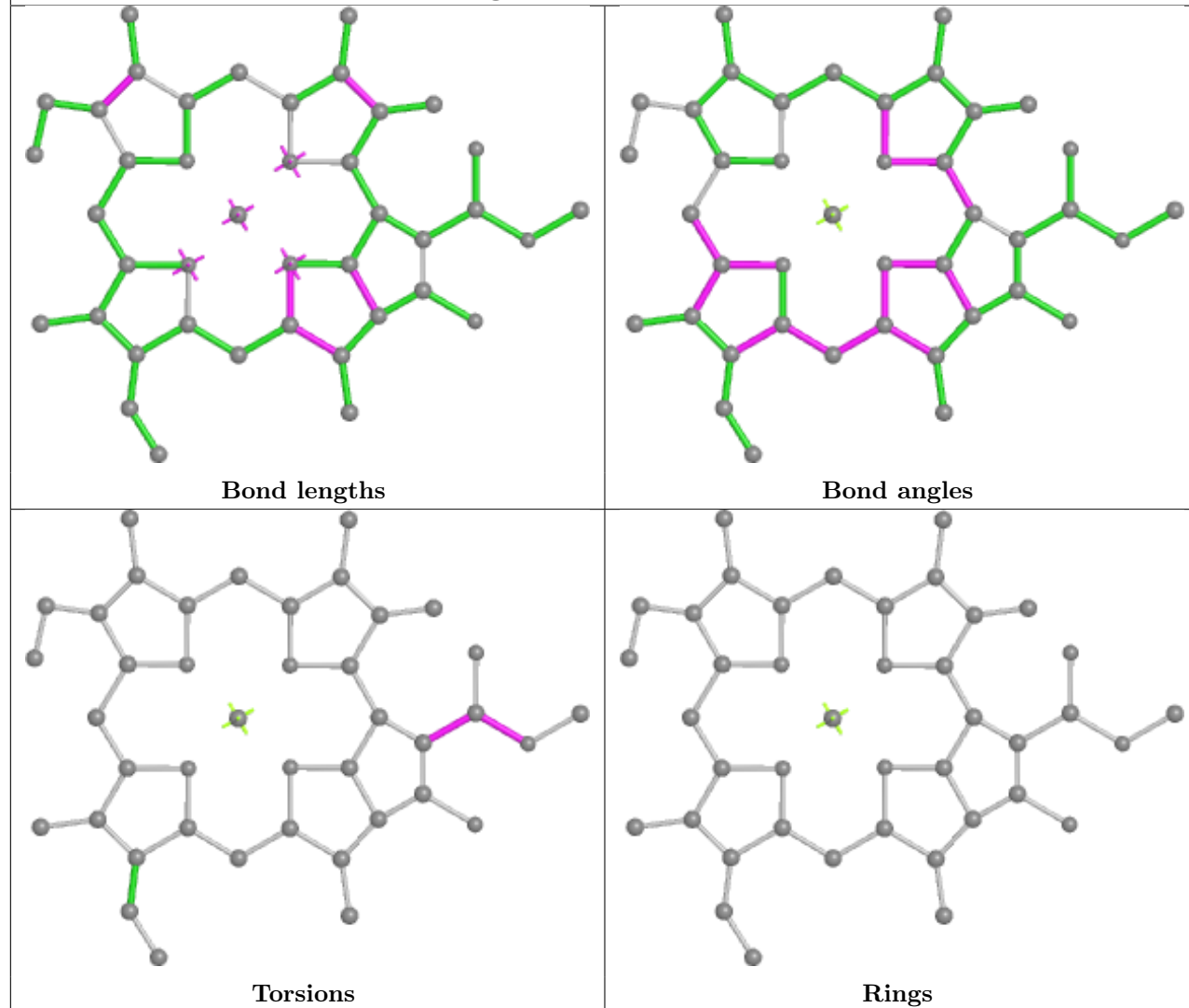


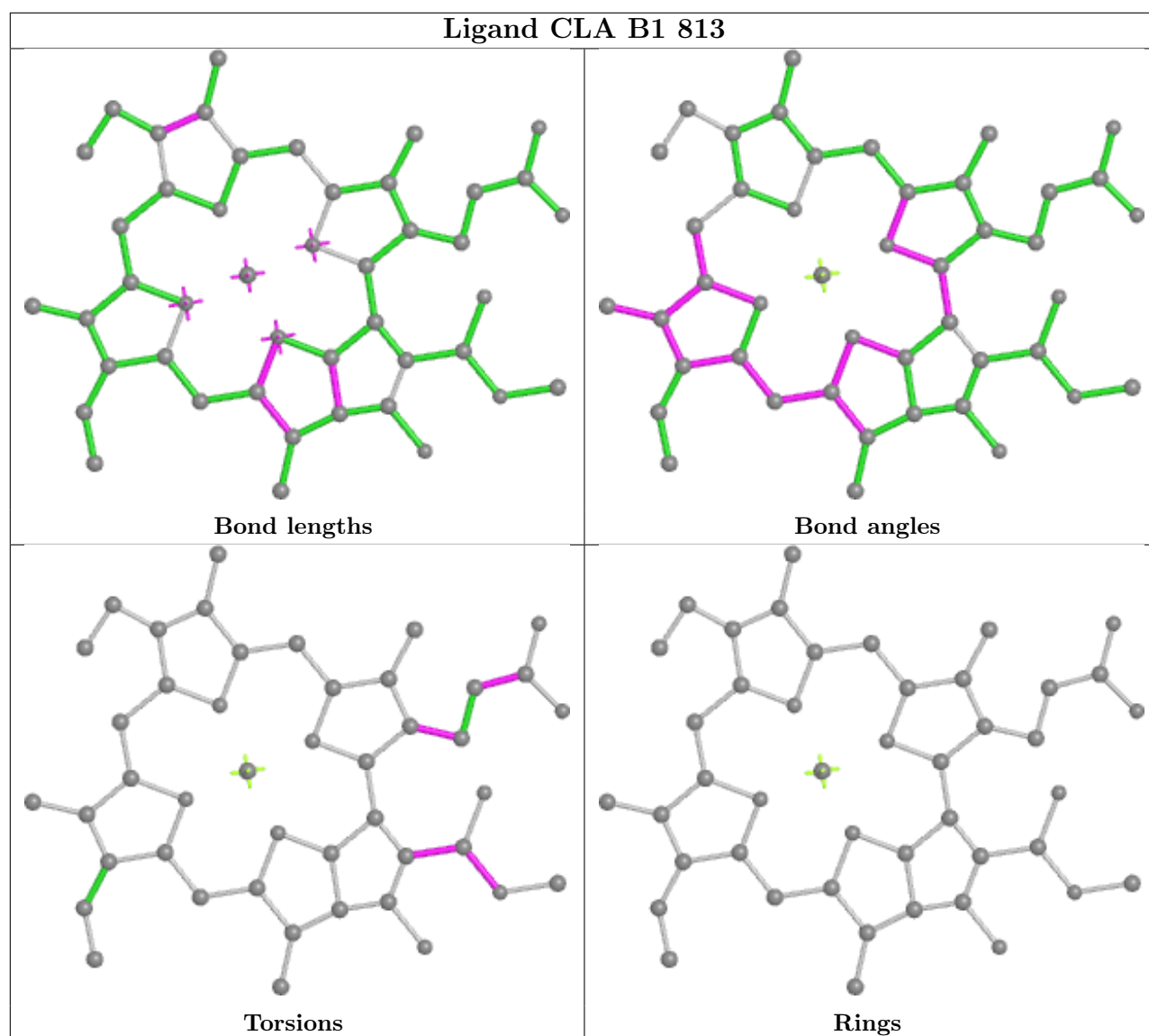


## Ligand CLA L1 1002

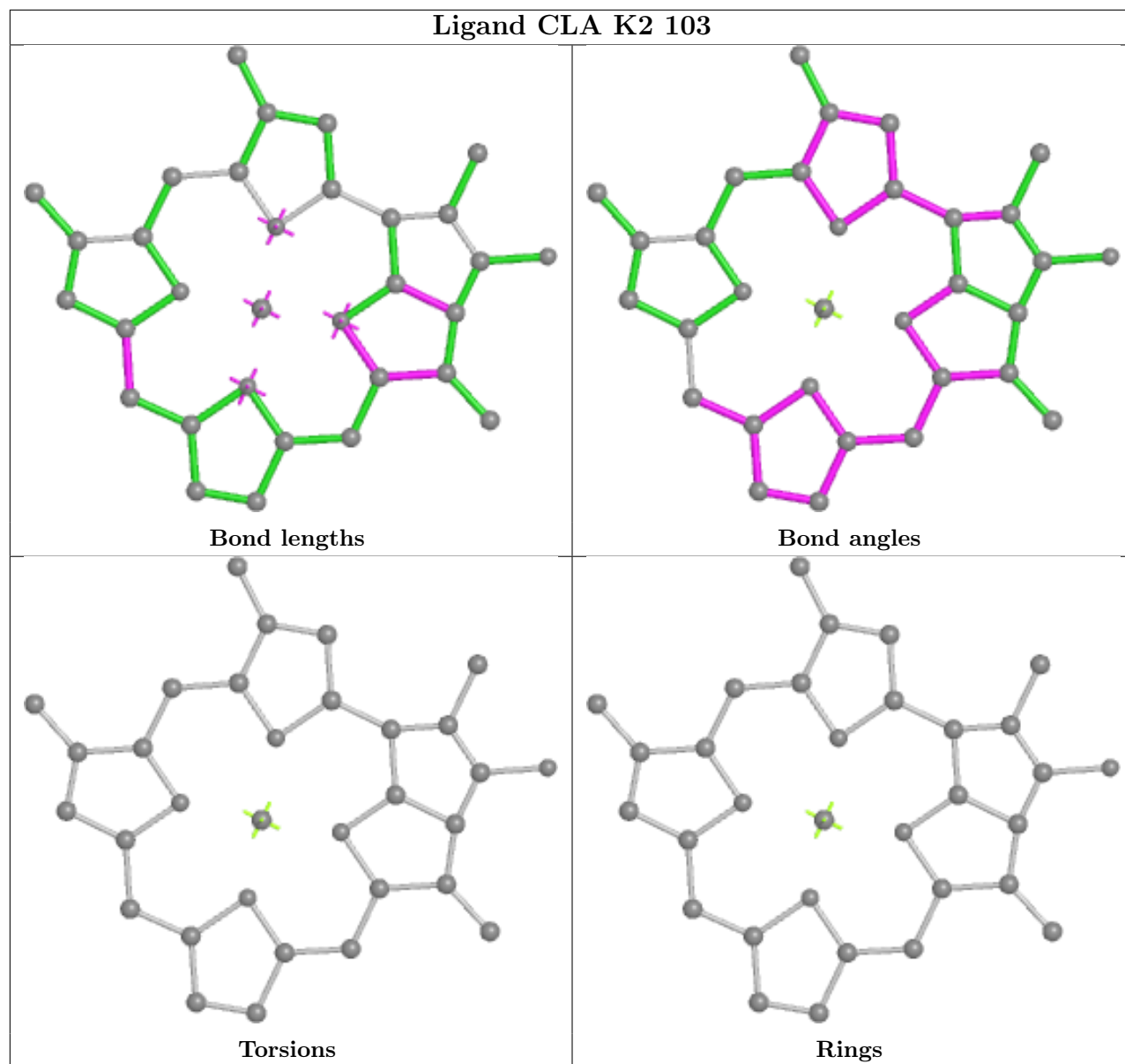


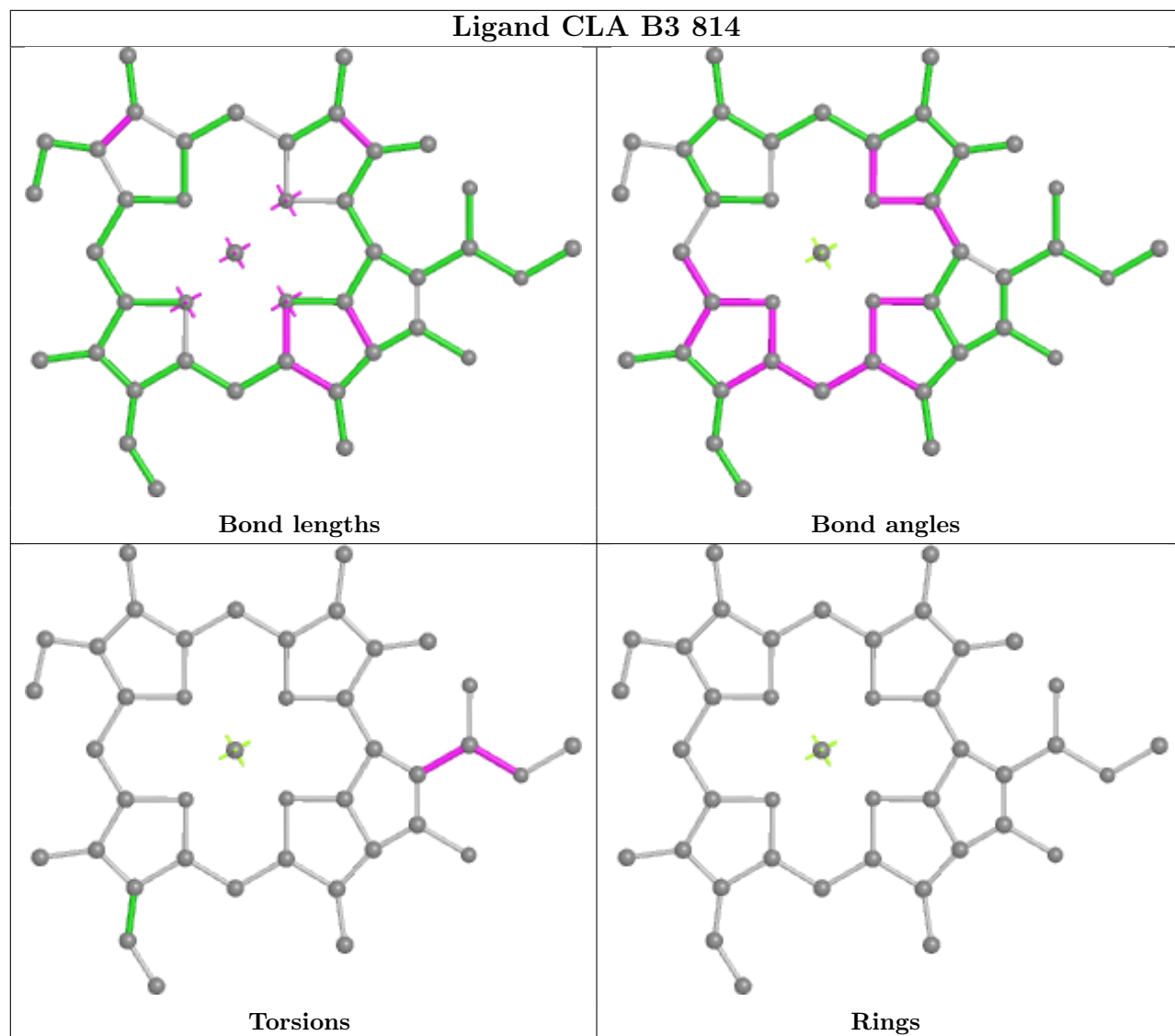
## Ligand CLA B3 837



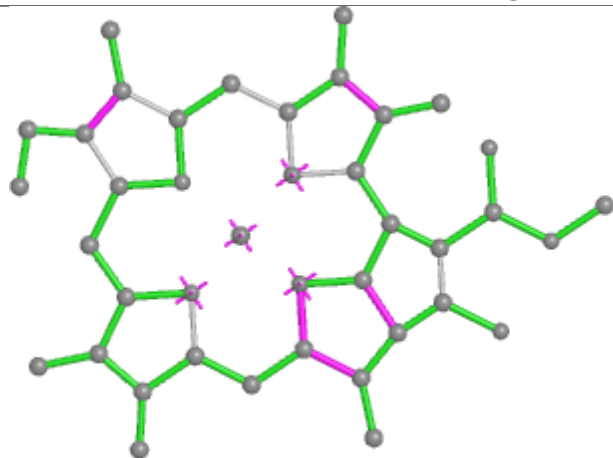


## Ligand CLA K2 103

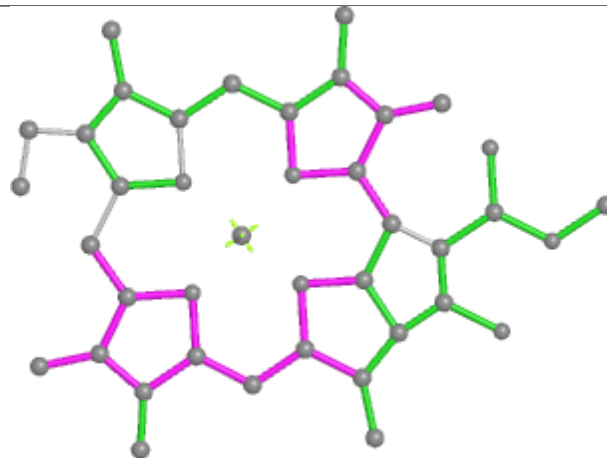




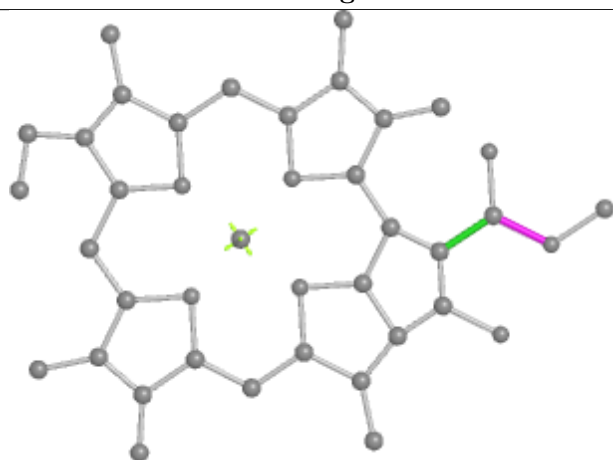
## Ligand CLA X3 102



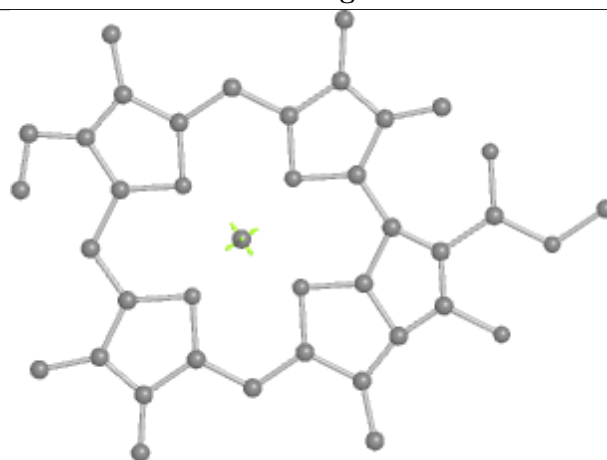
Bond lengths



Bond angles

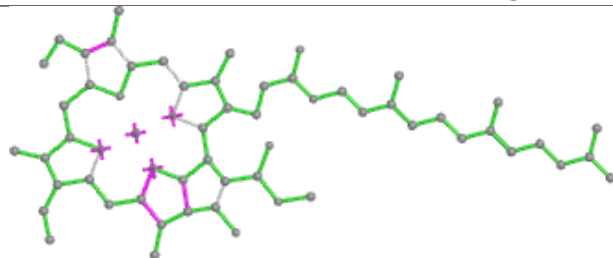


Torsions

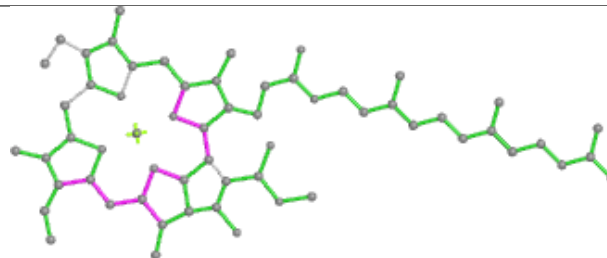


Rings

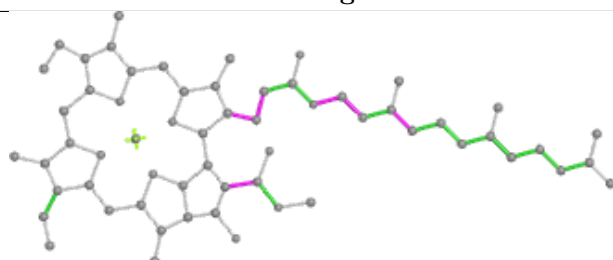
## Ligand CLA A3 827



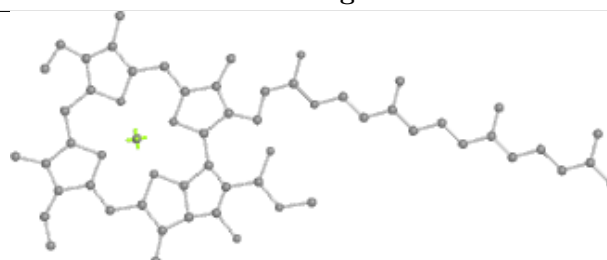
Bond lengths



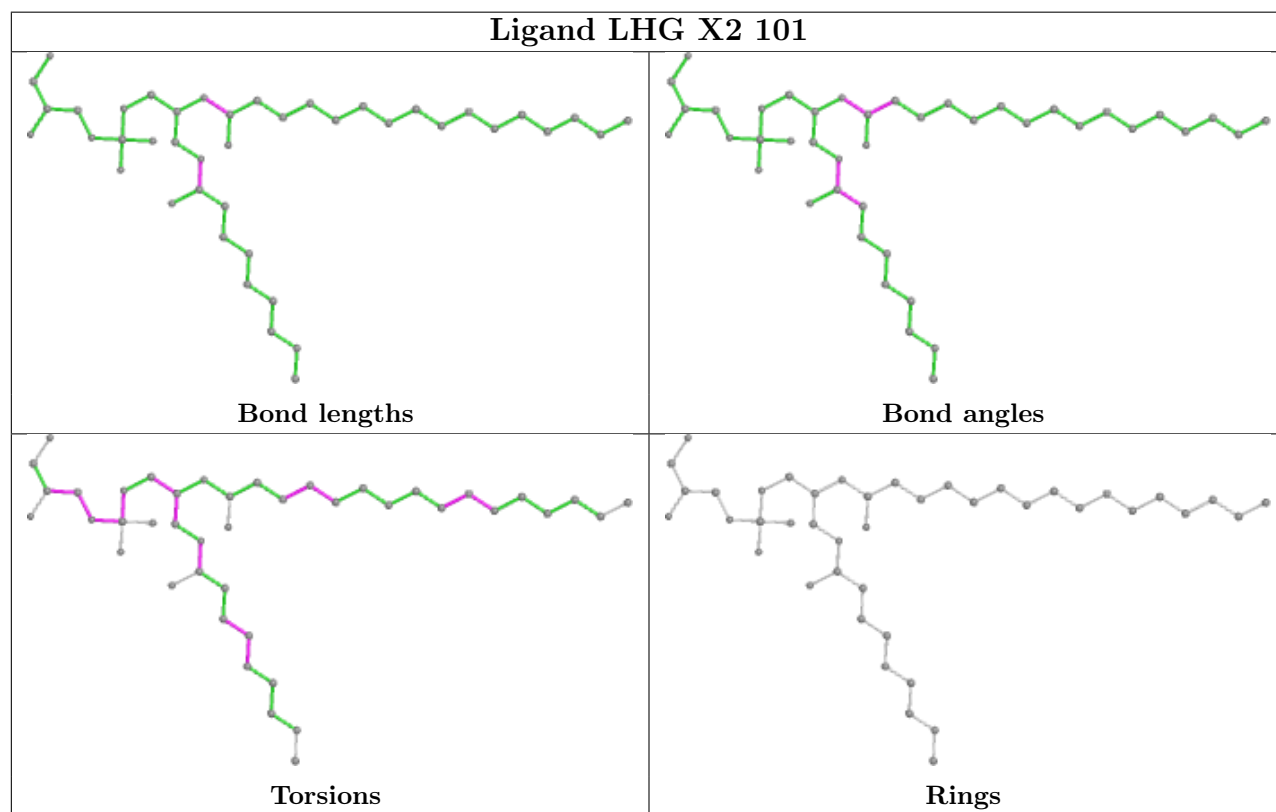
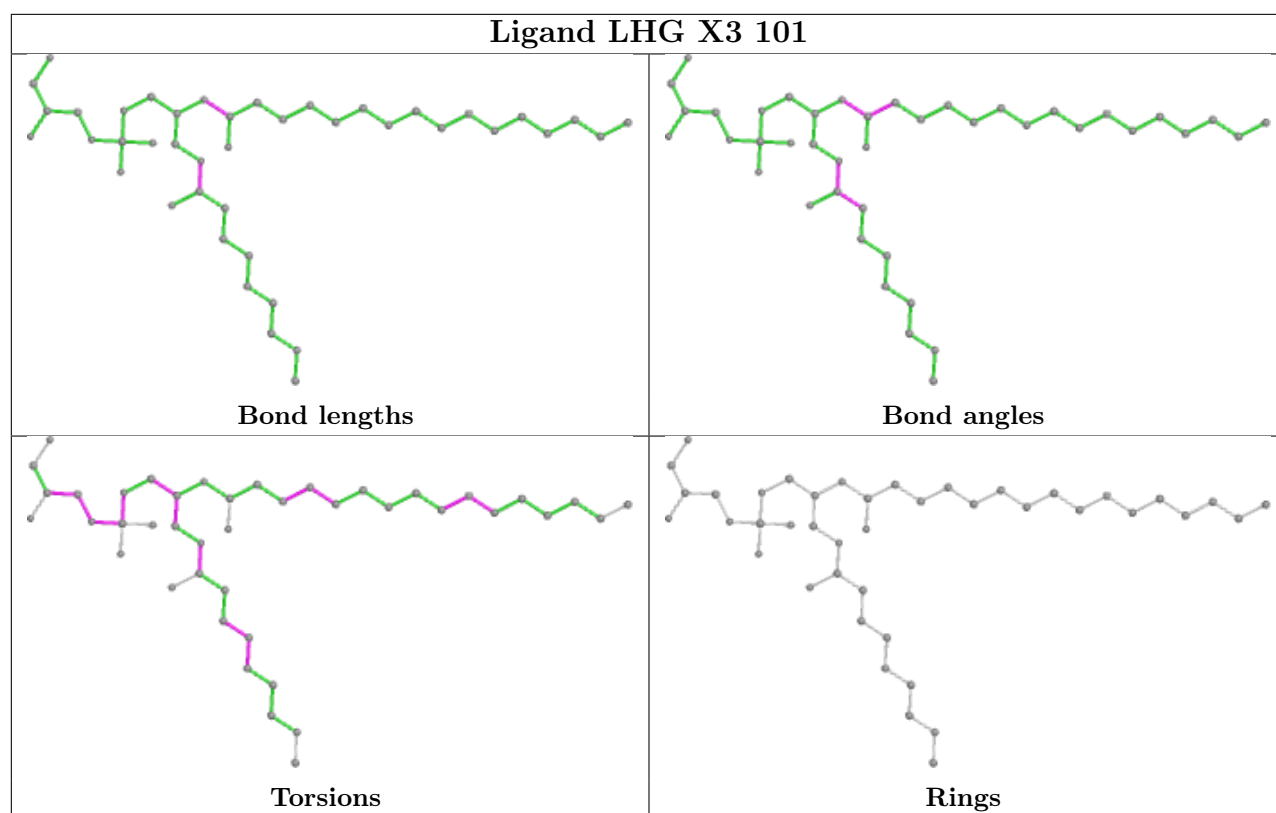
Bond angles

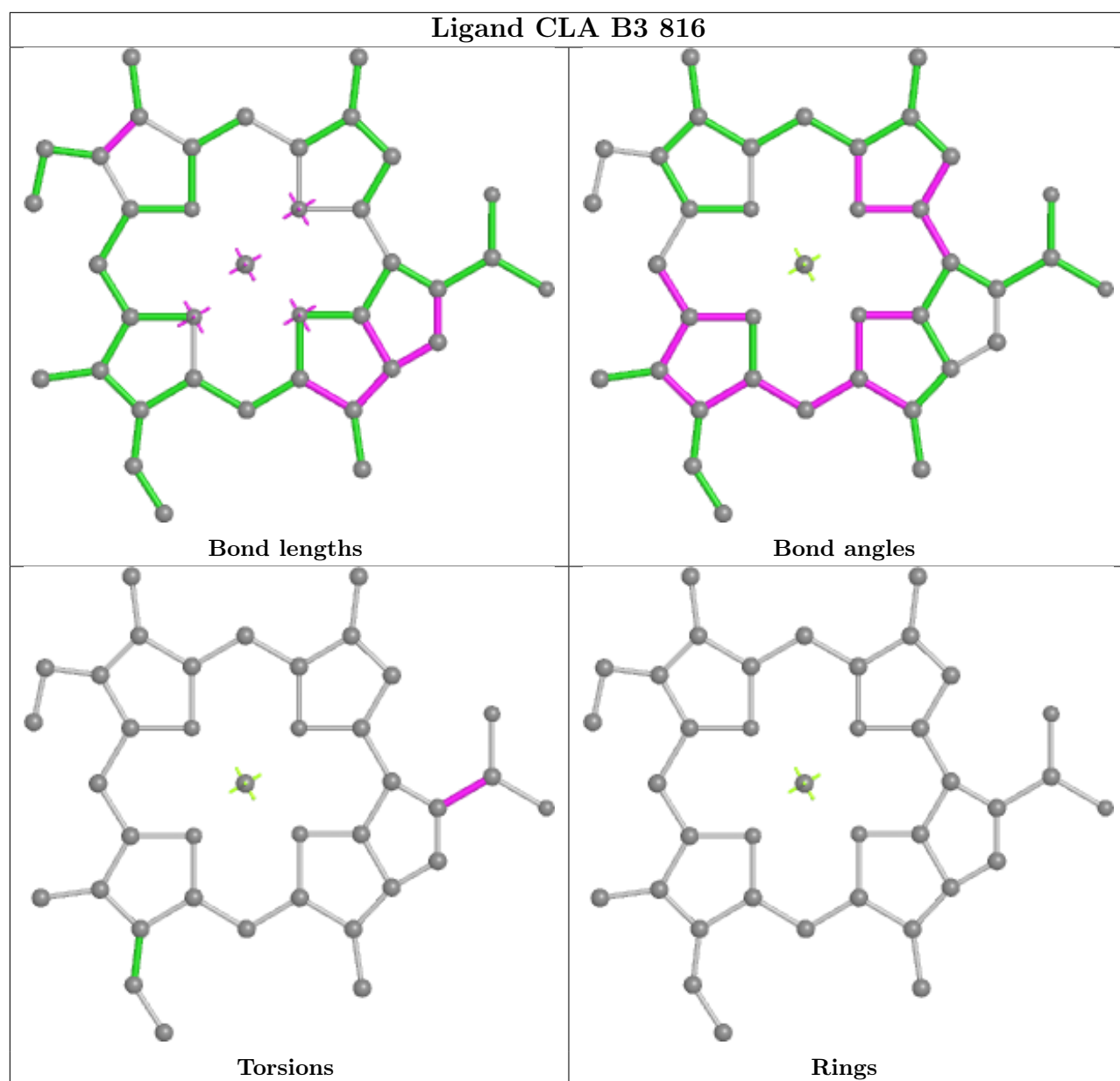


Torsions

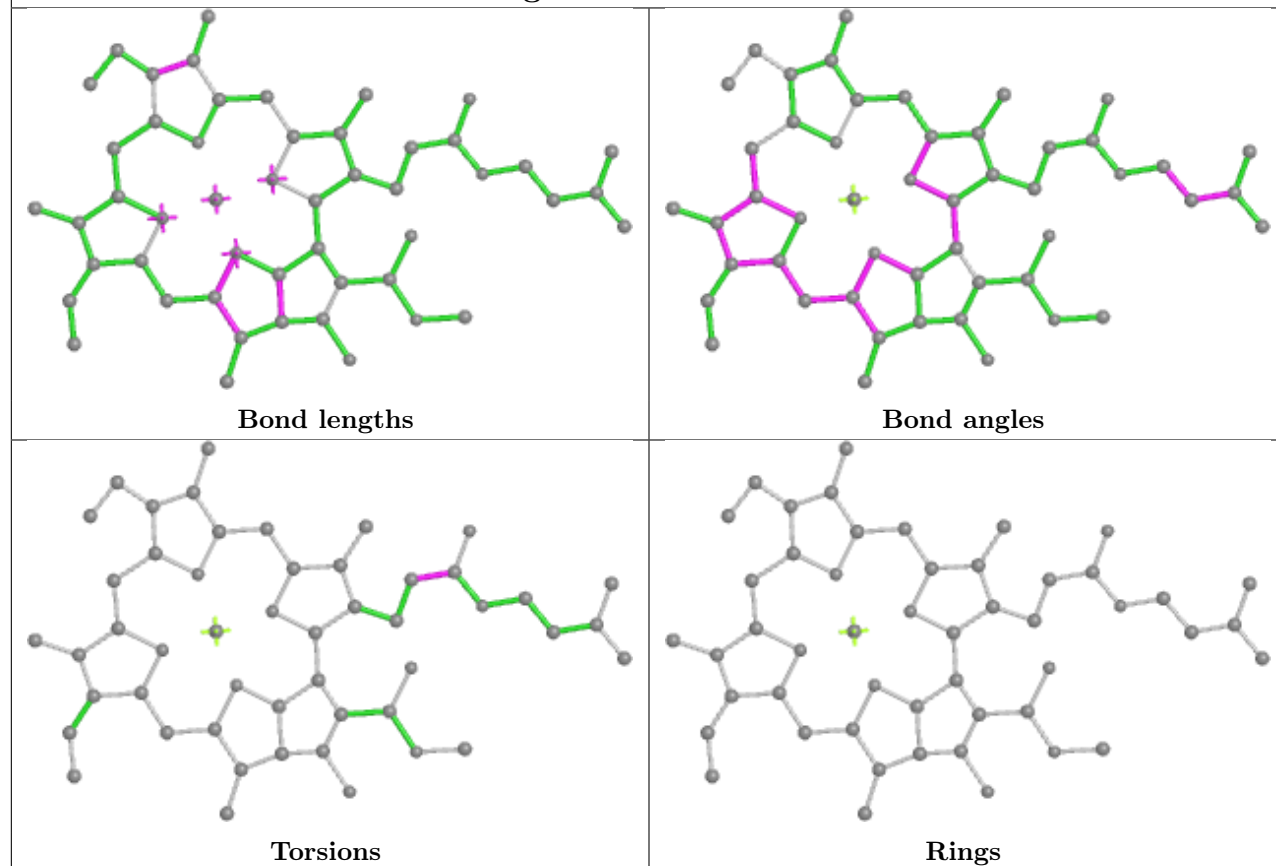


Rings

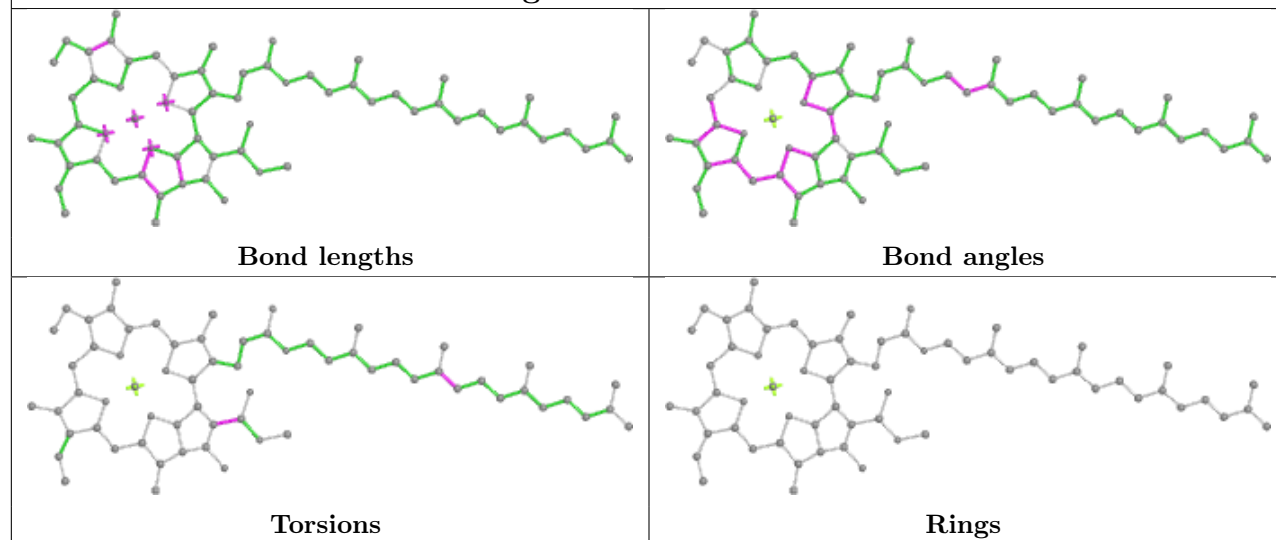




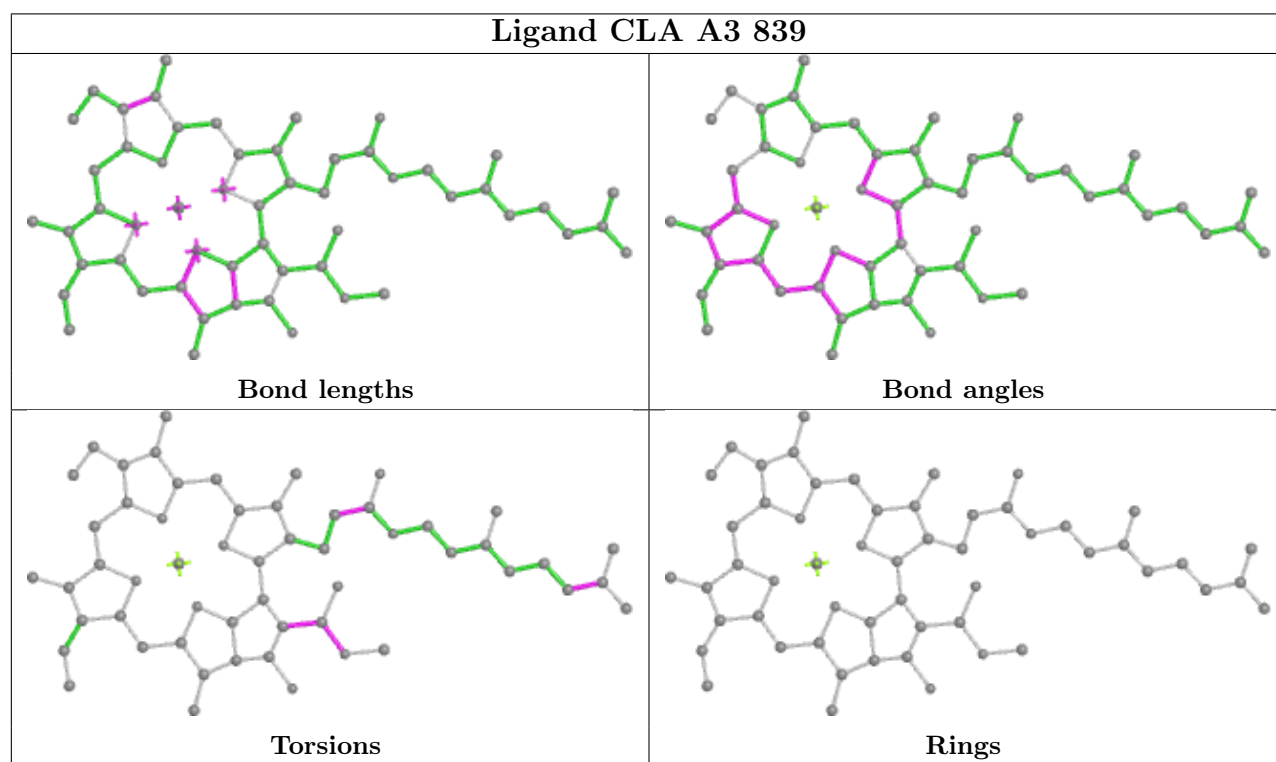
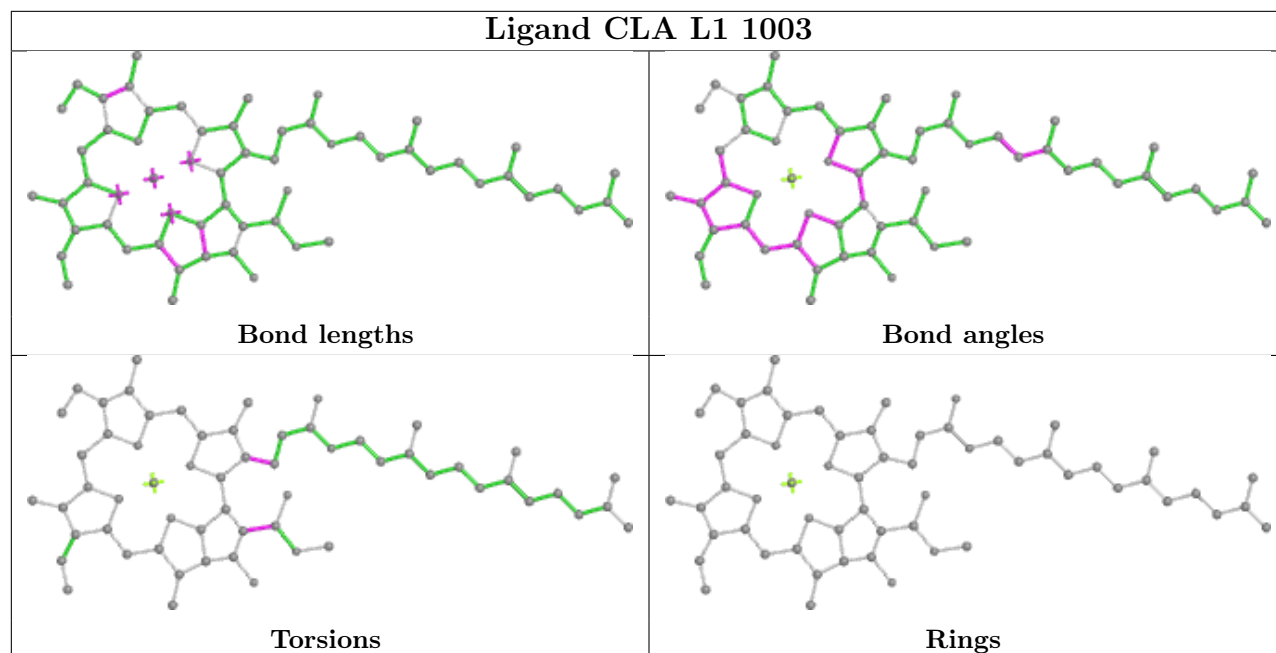
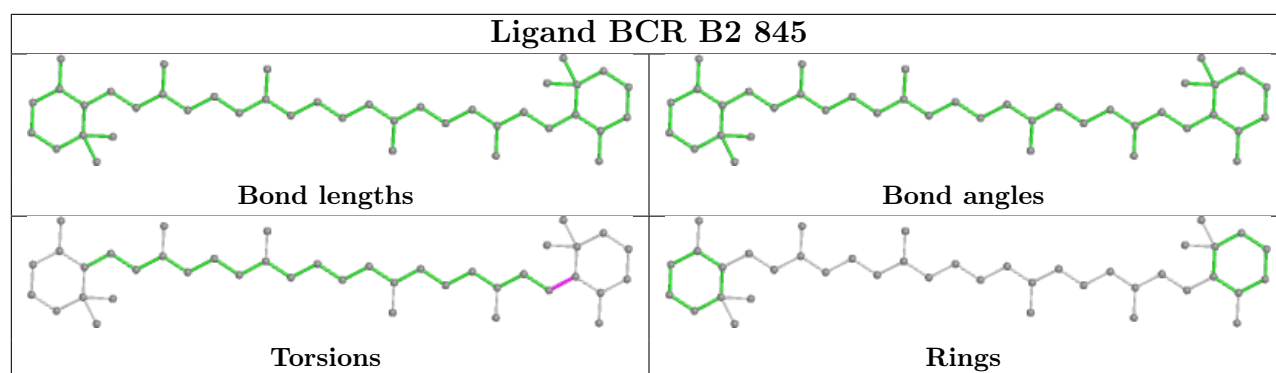
## Ligand CLA B2 806

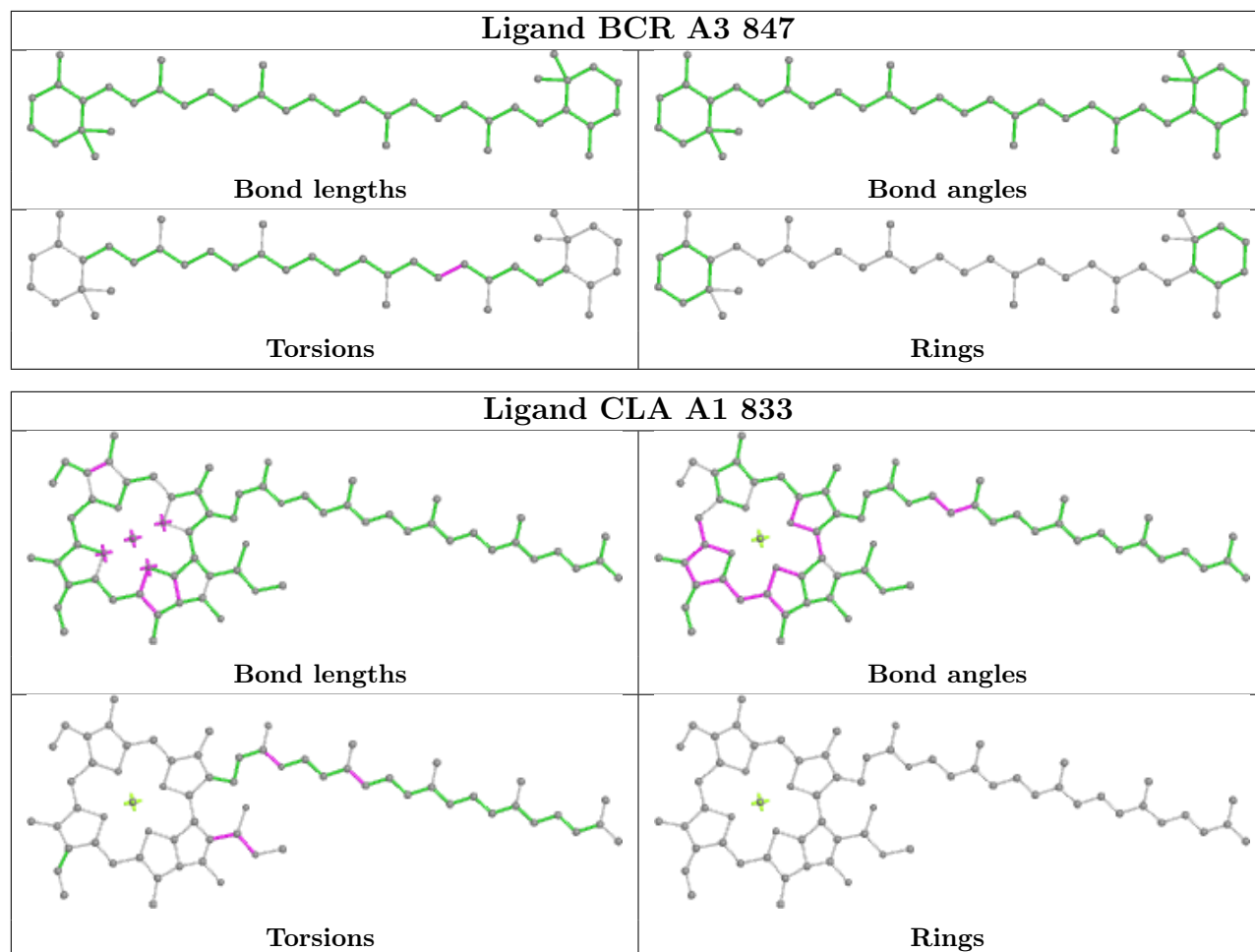


## Ligand CLA A3 808

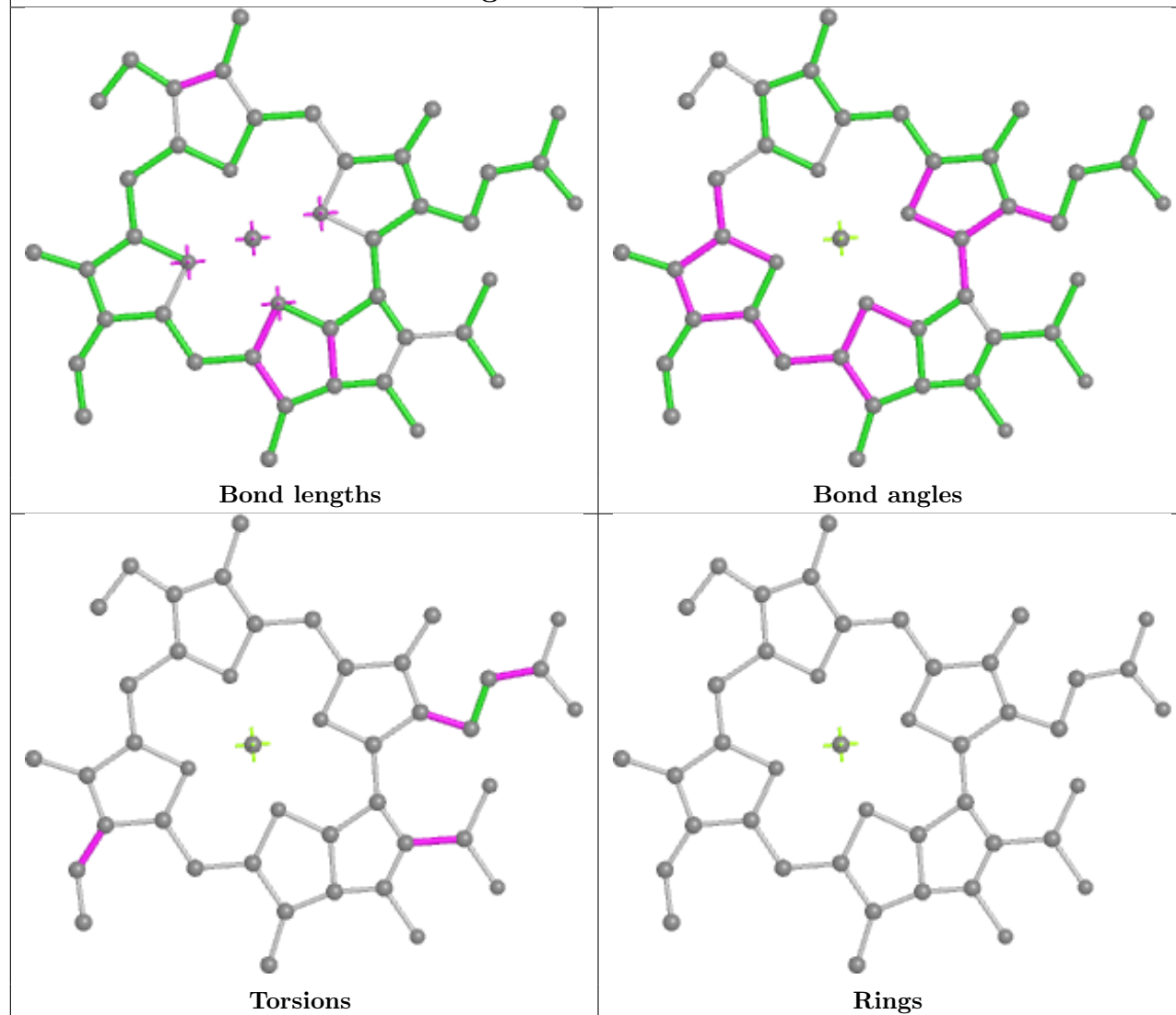




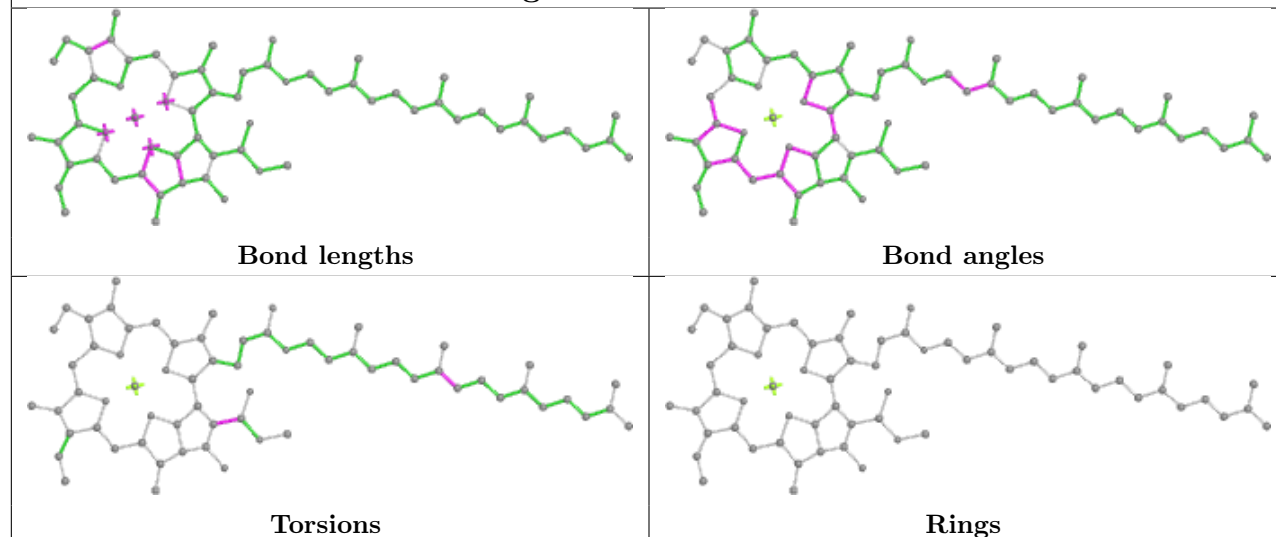


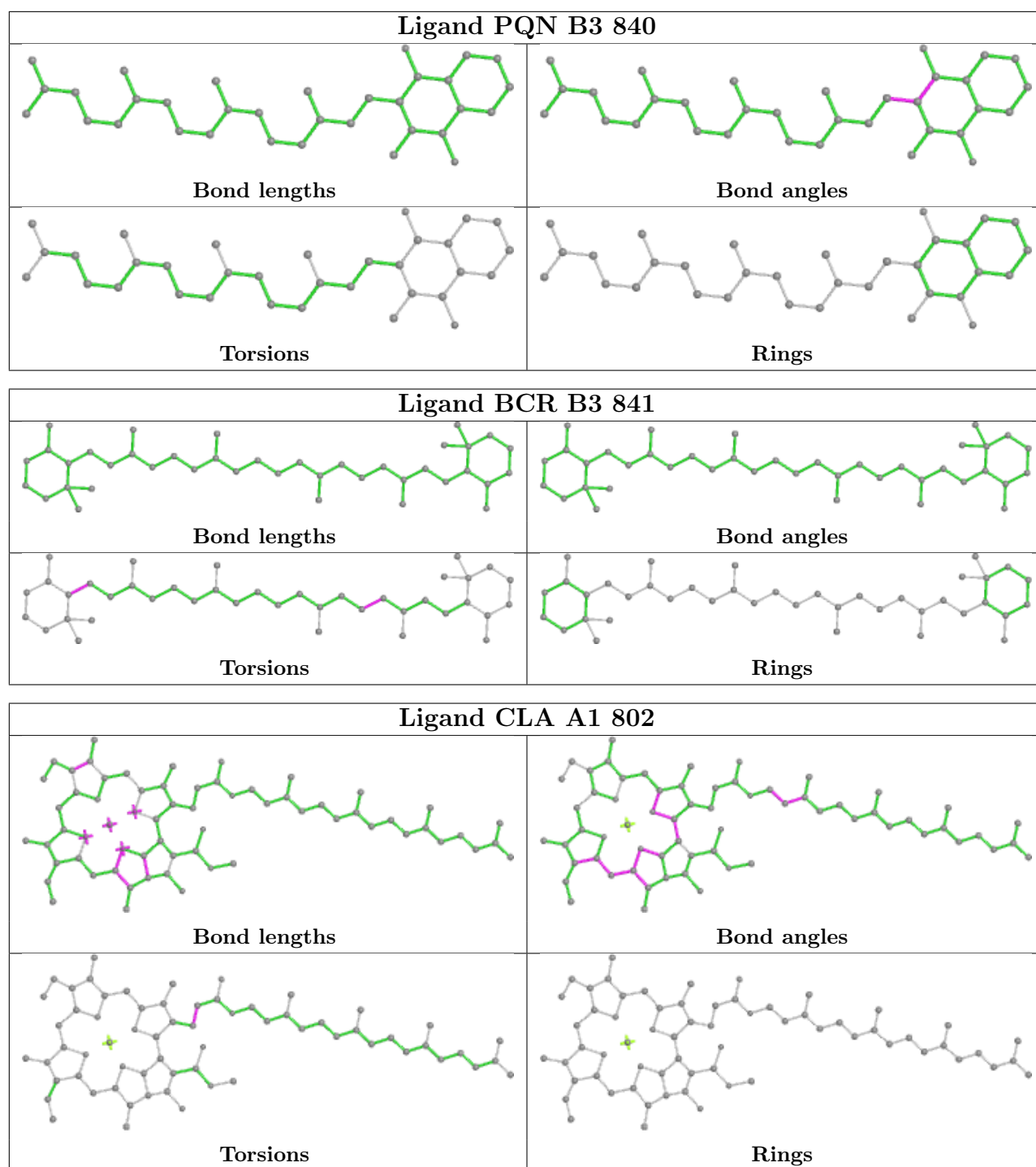


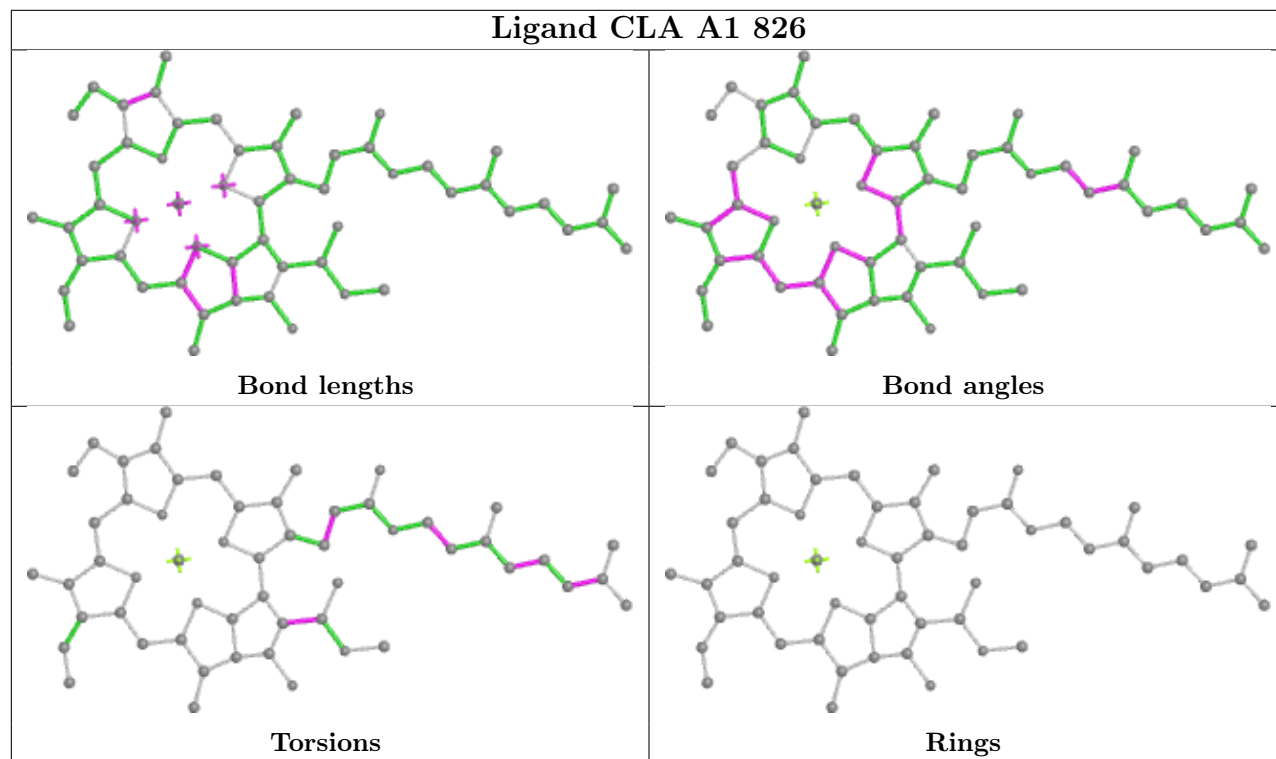
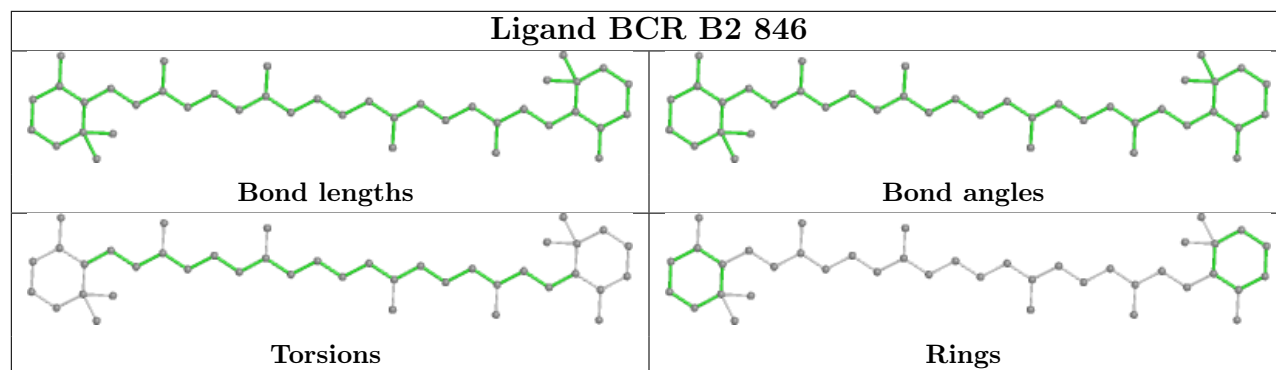
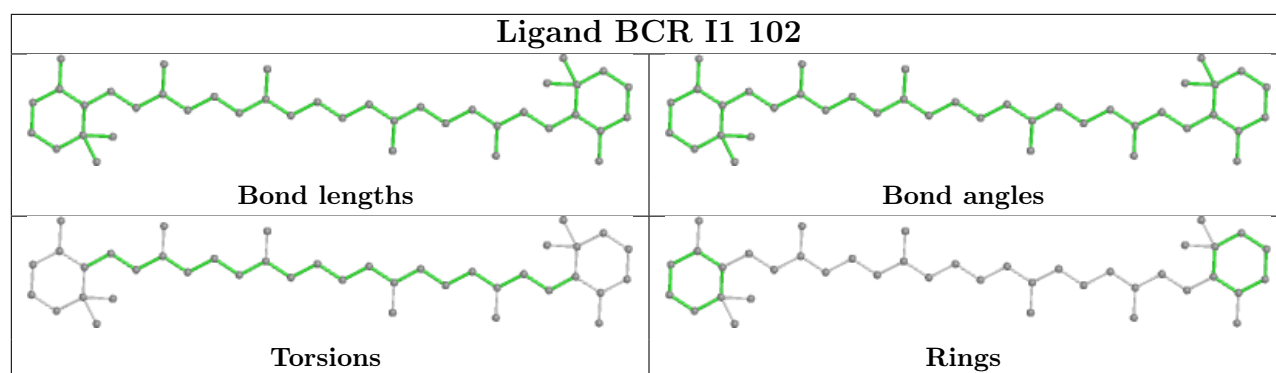
## Ligand CLA A1 807

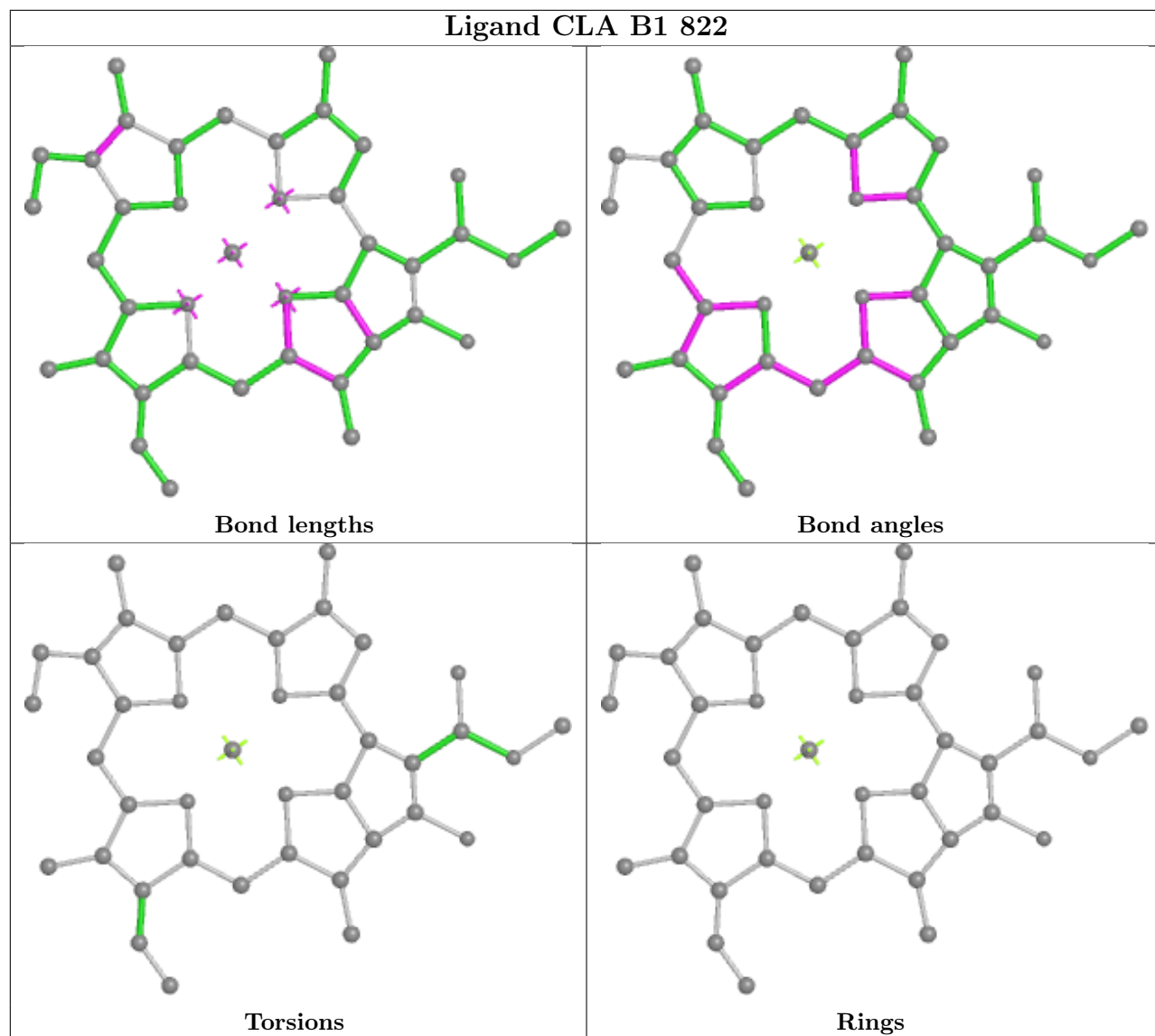


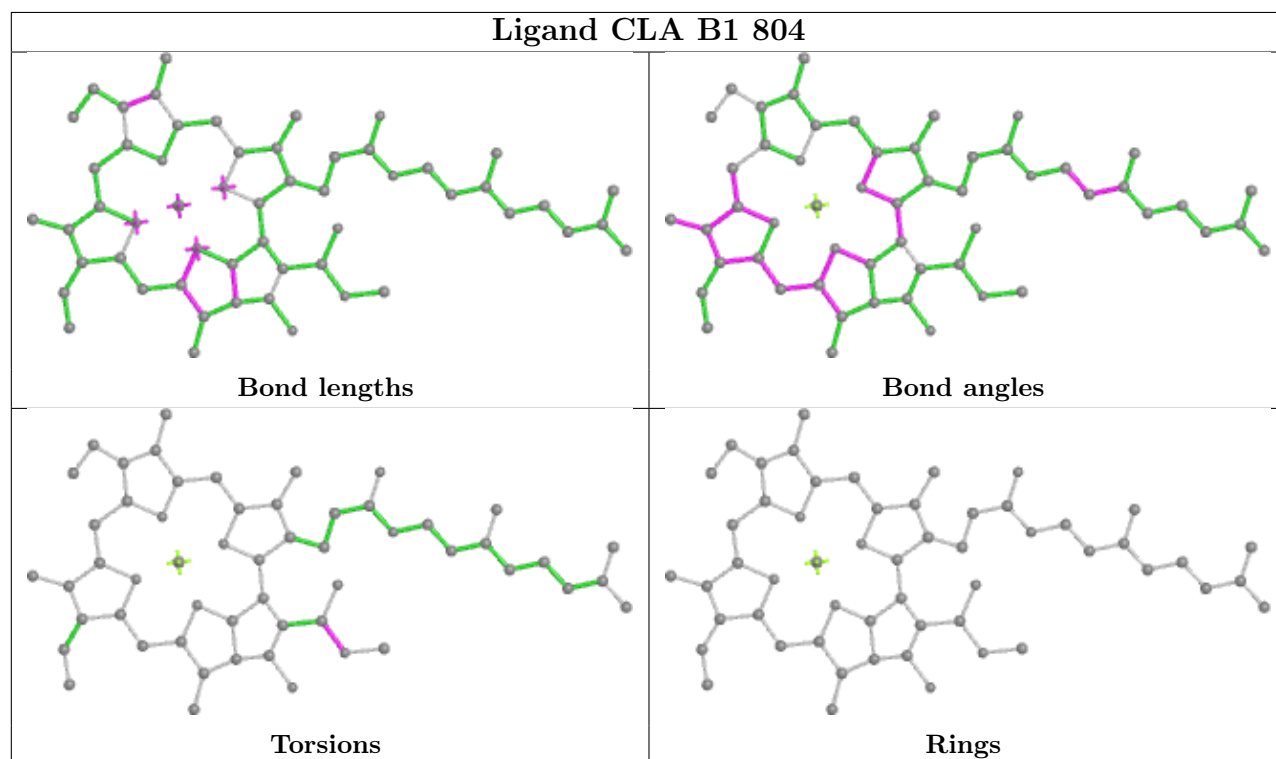
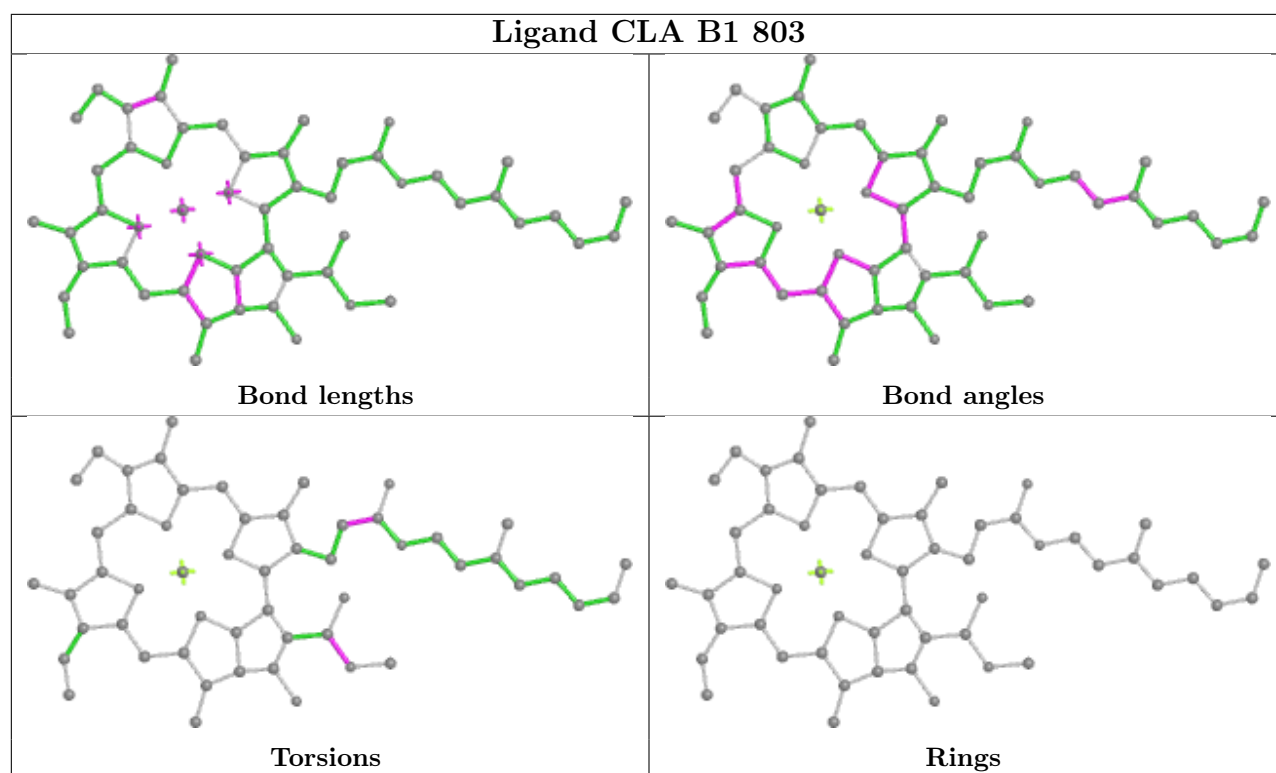
## Ligand CLA A1 808

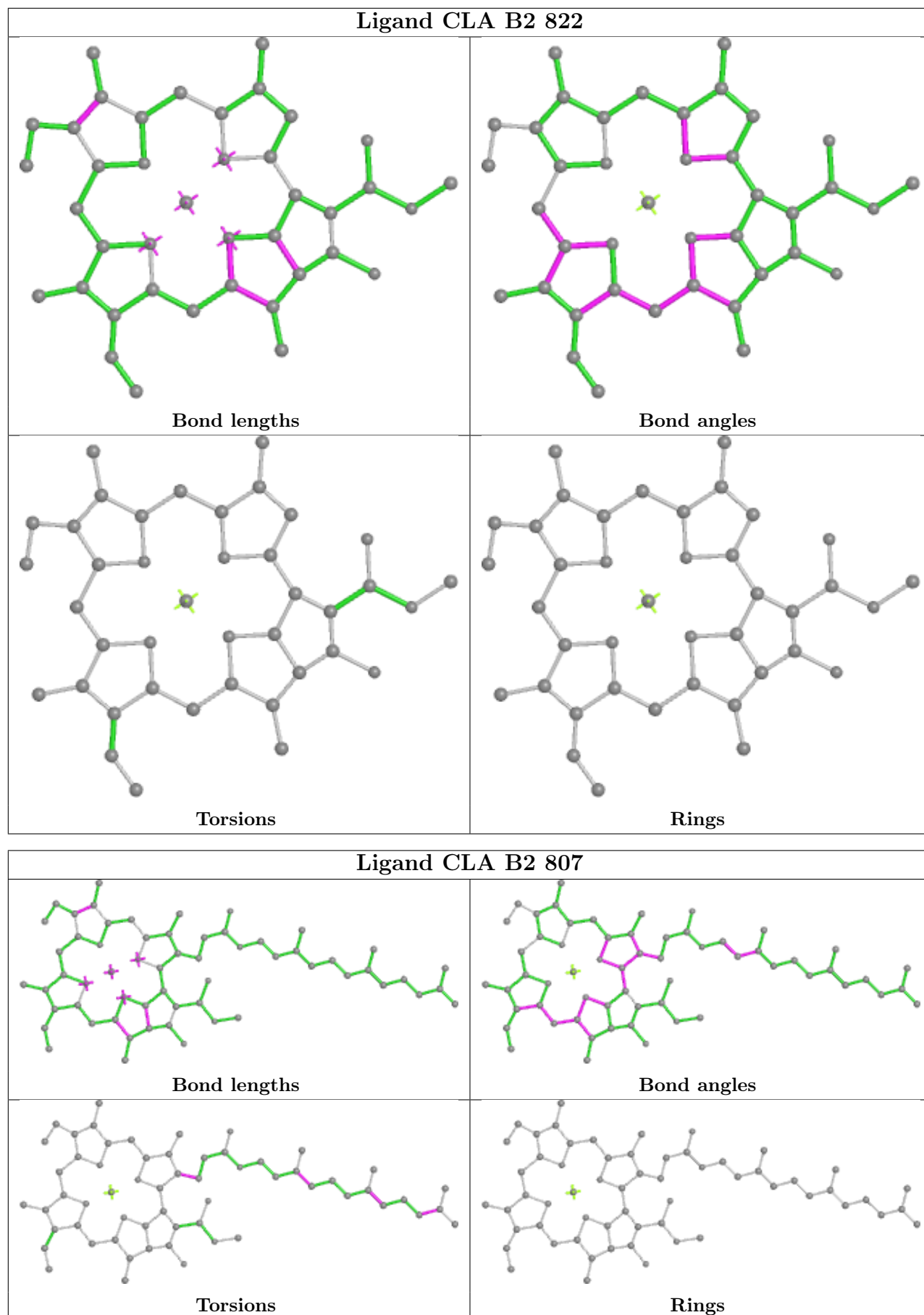






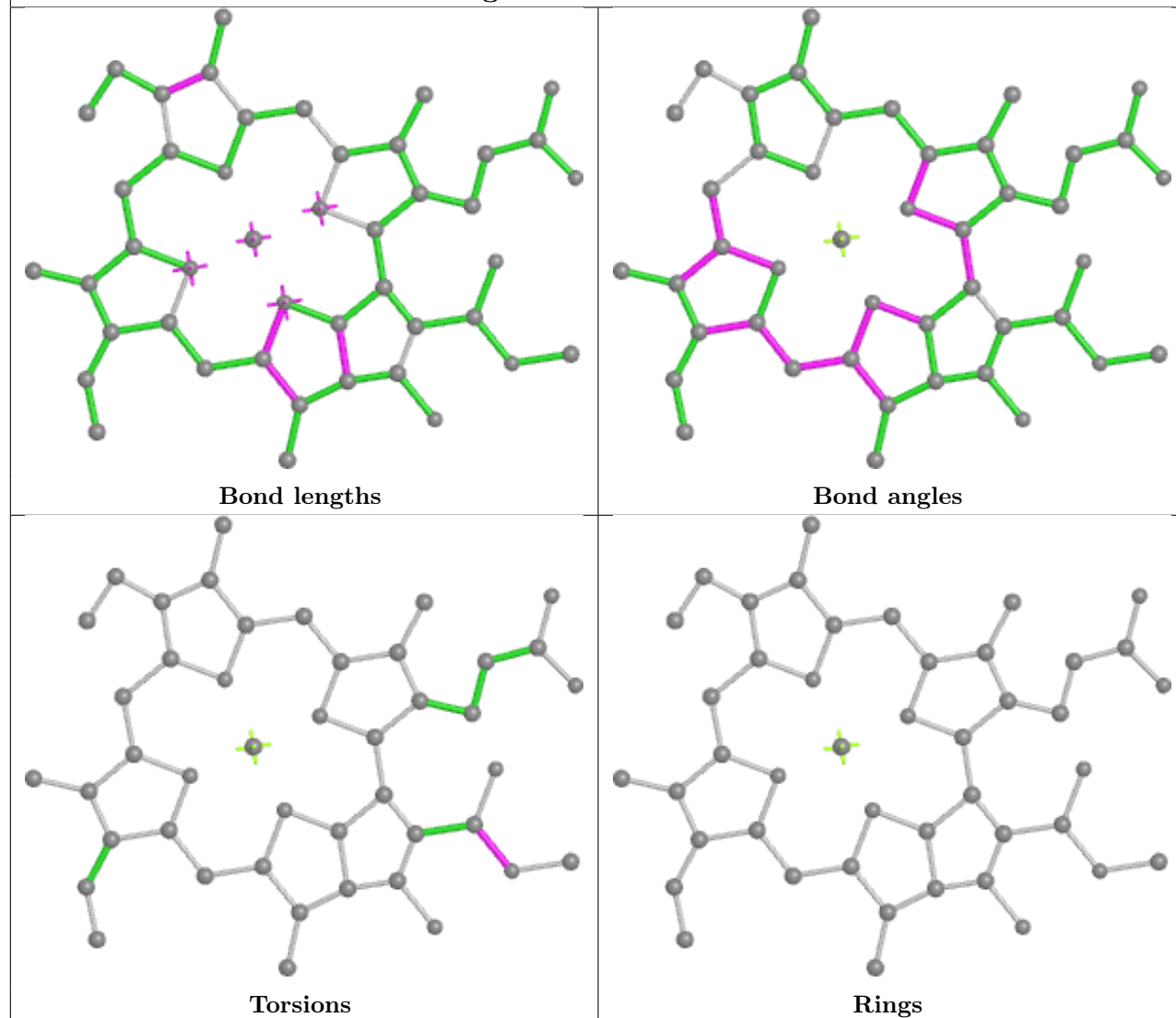




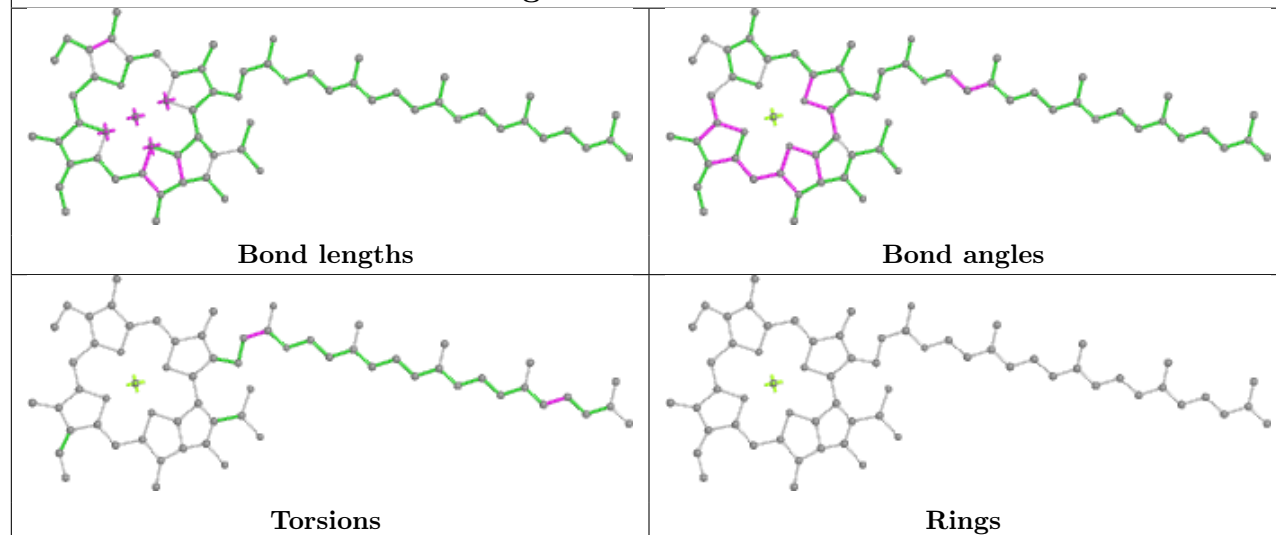


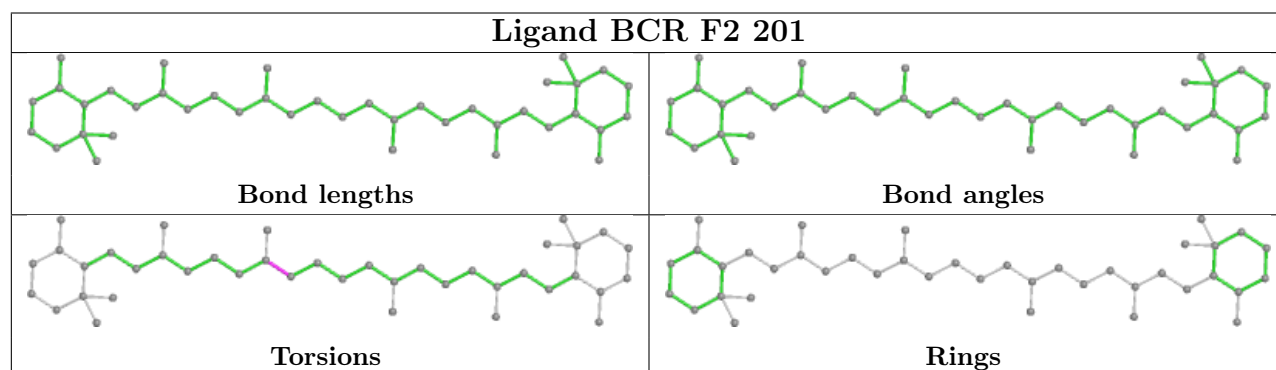
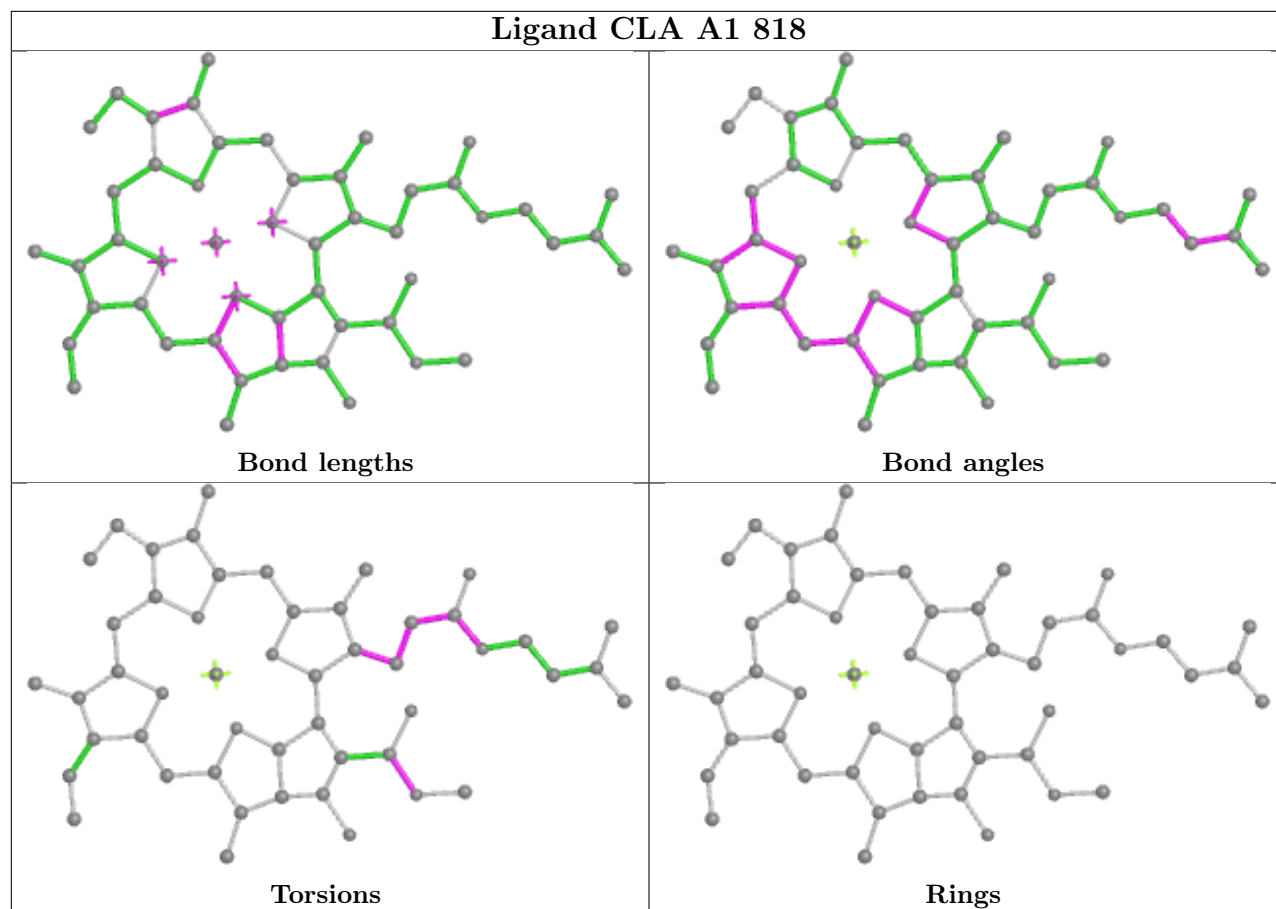
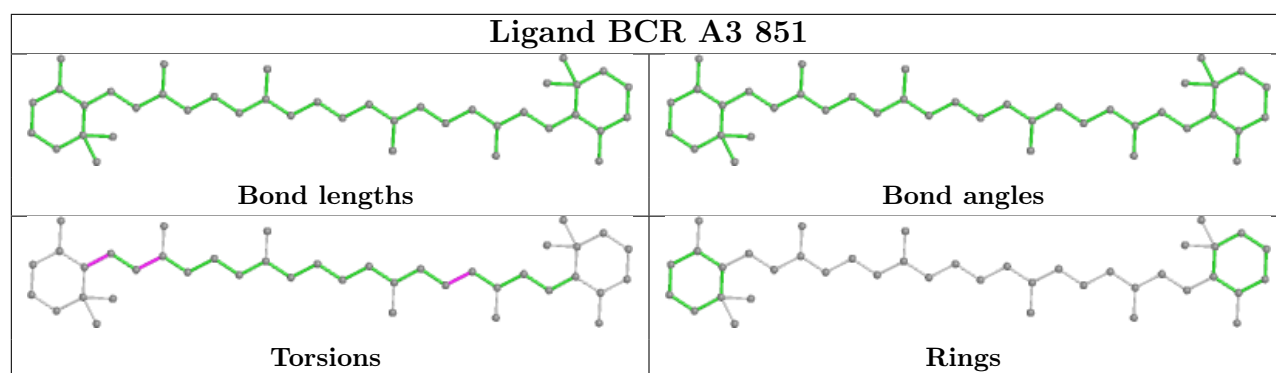


## Ligand CLA B2 824

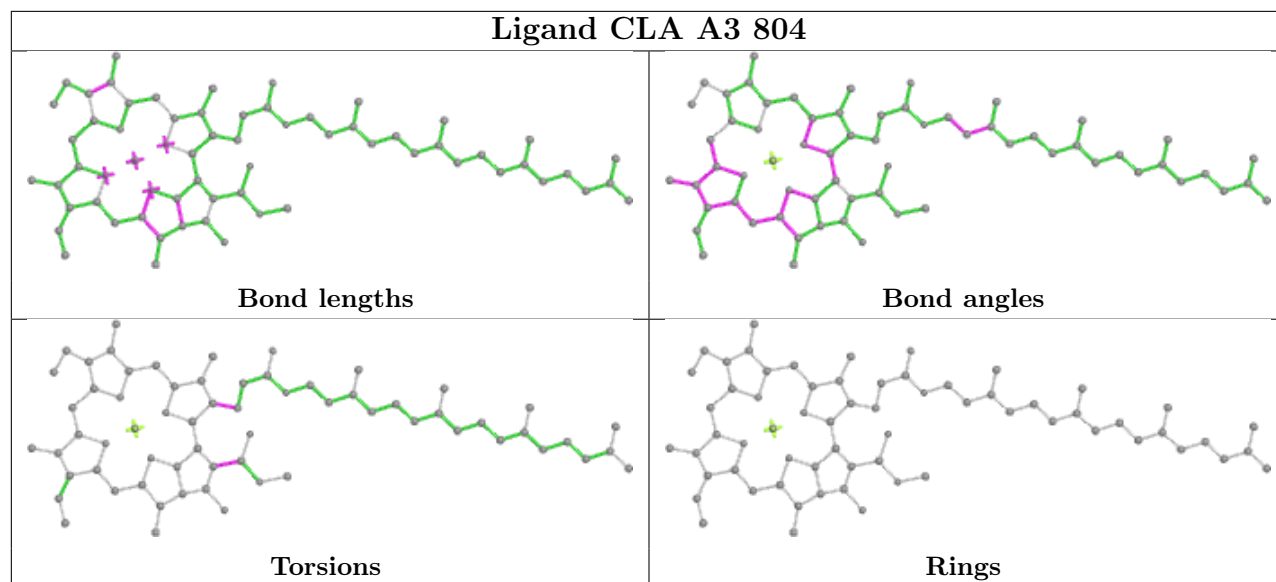


## Ligand CLA A3 803

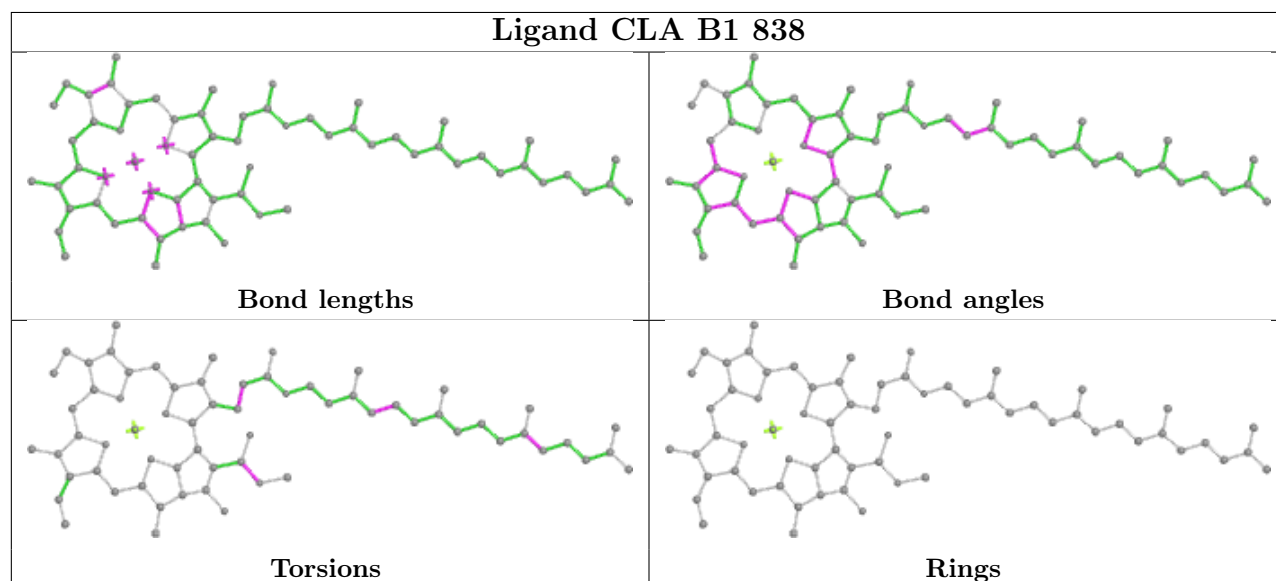




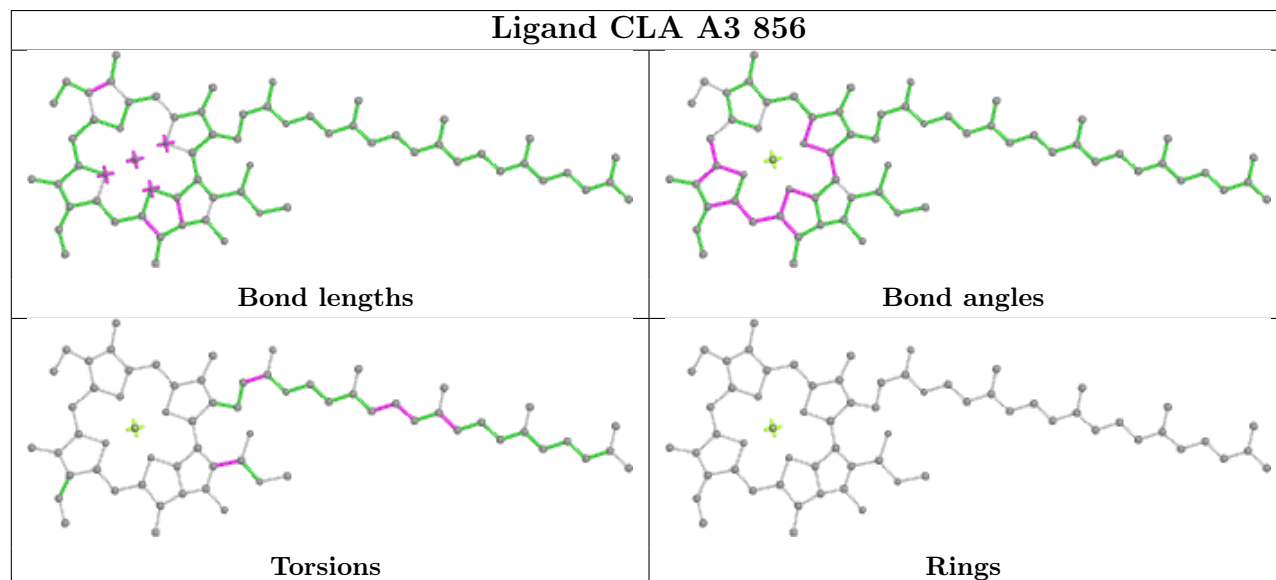
## Ligand CLA A3 804

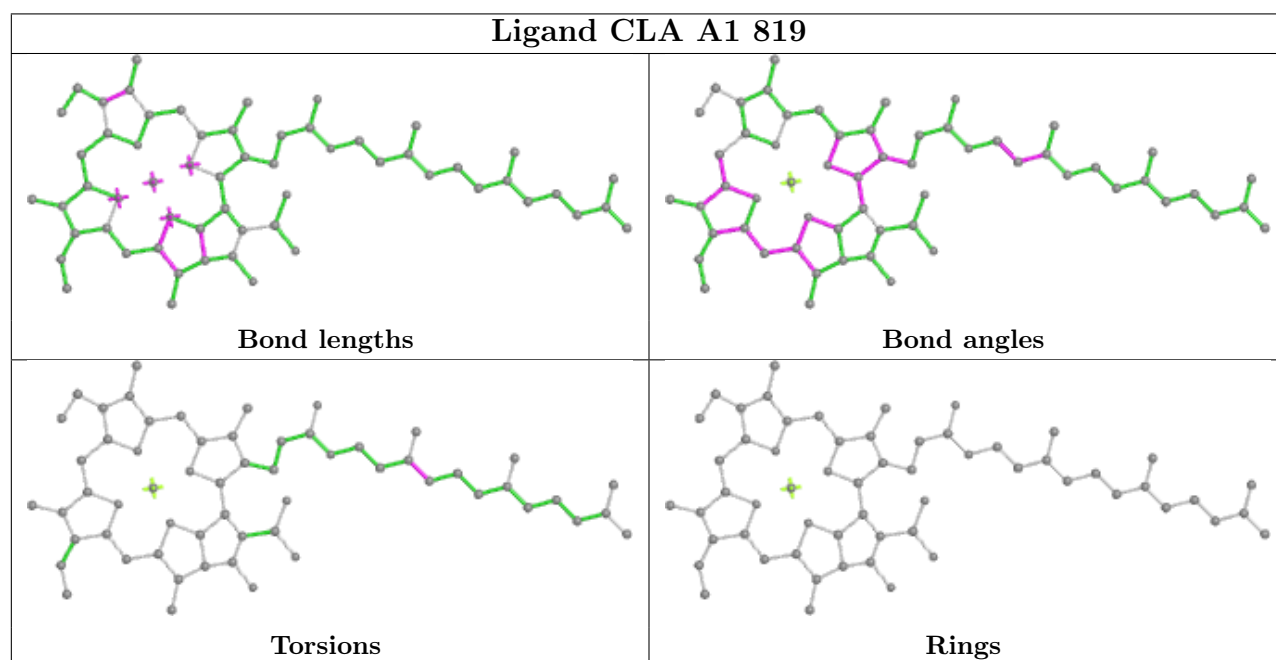
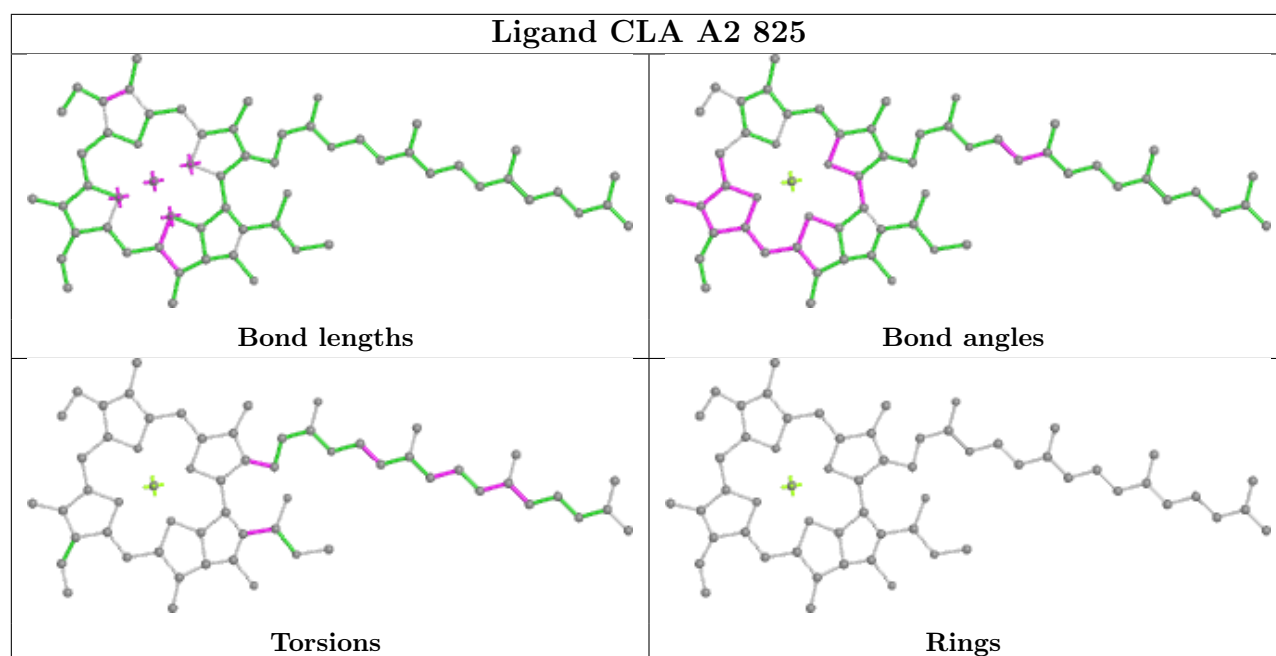


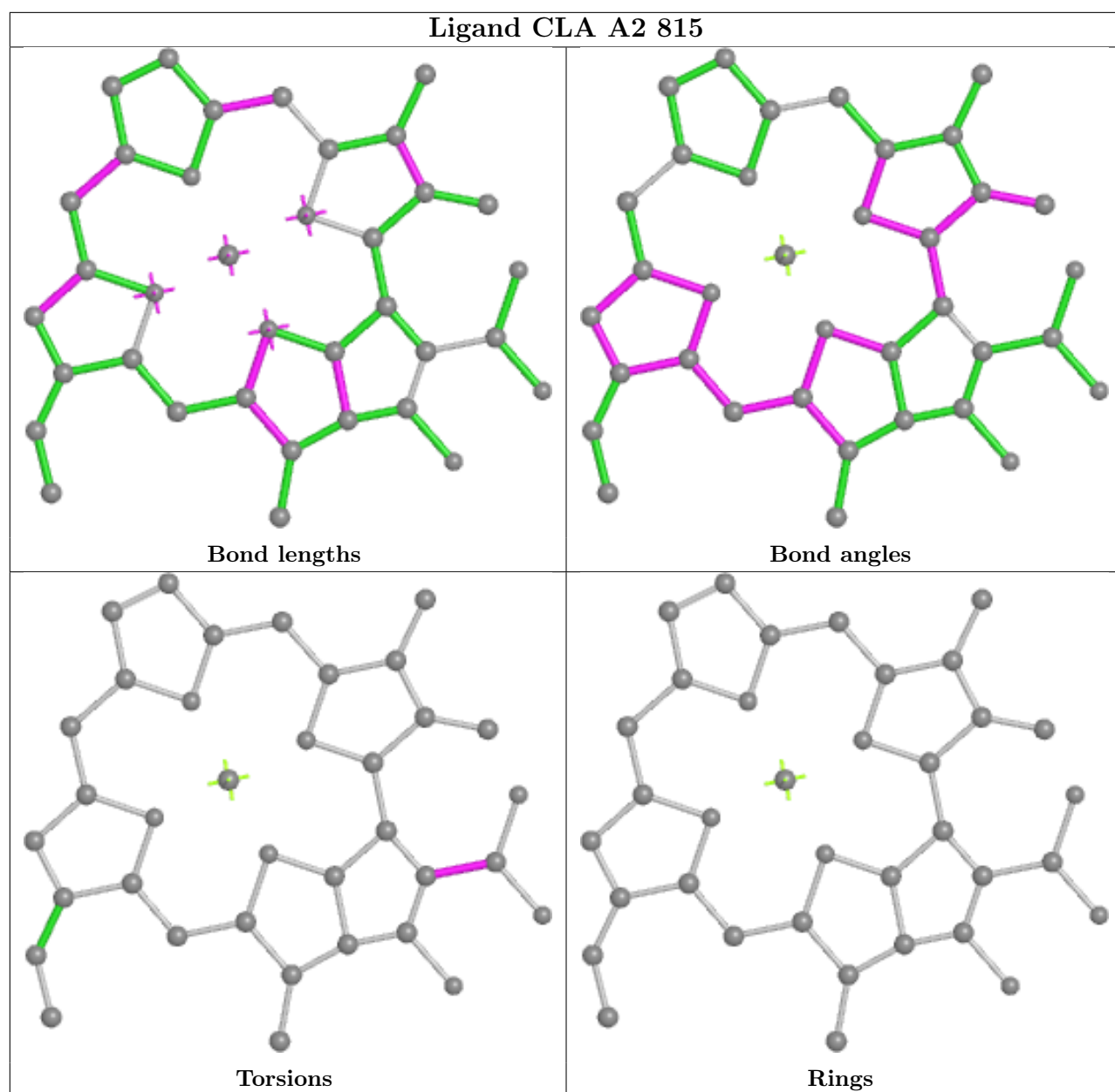
## Ligand CLA B1 838



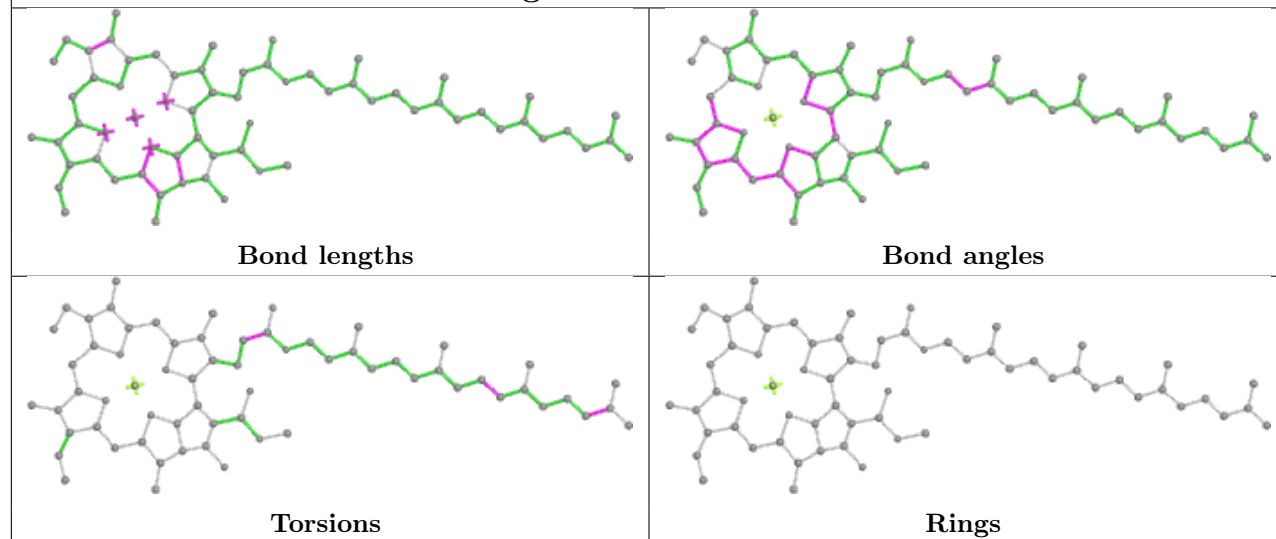
## Ligand CLA A3 856



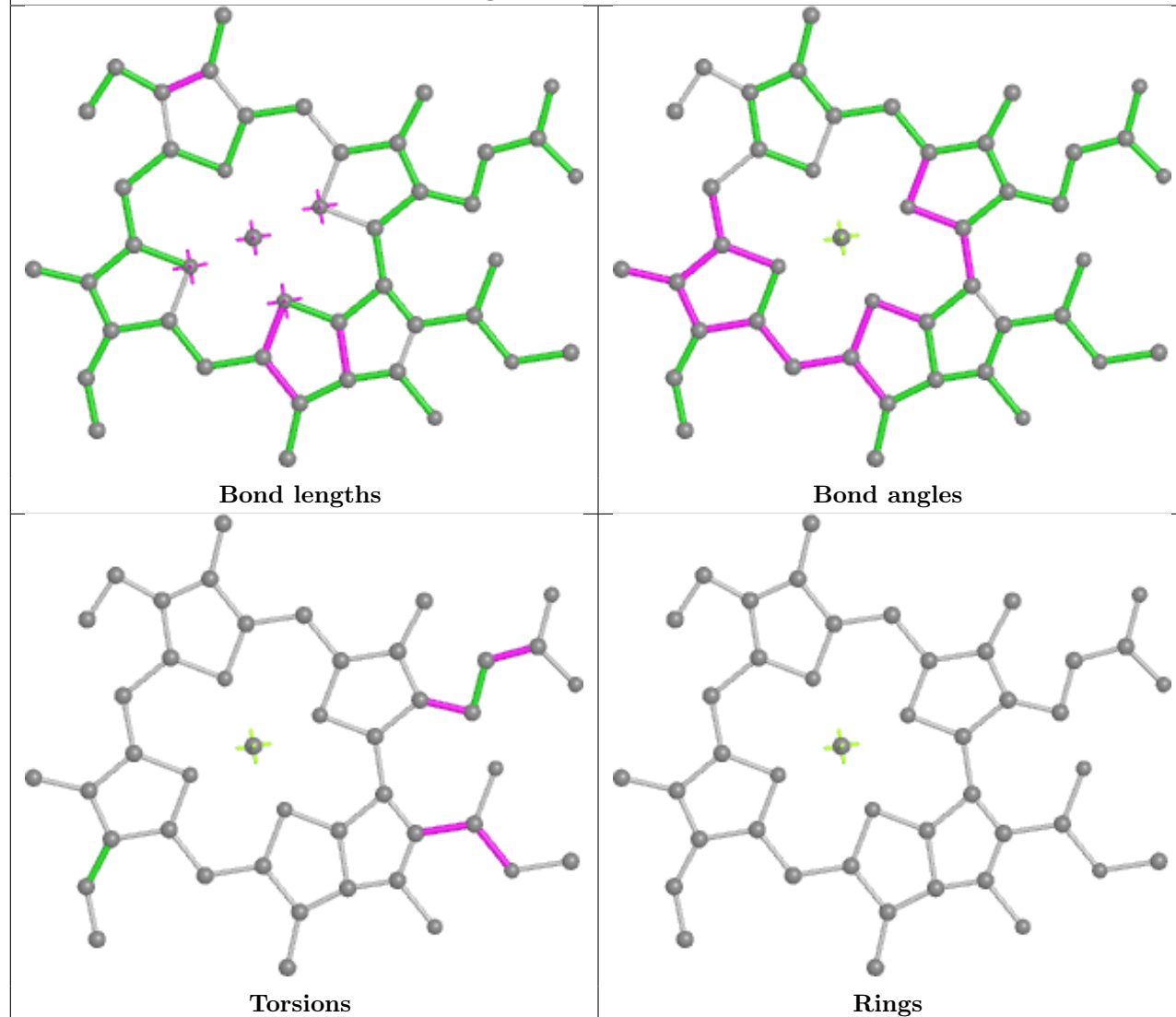




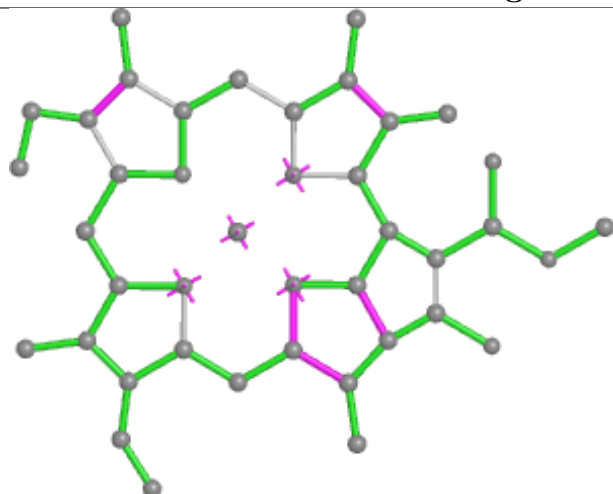
## Ligand CLA A1 806



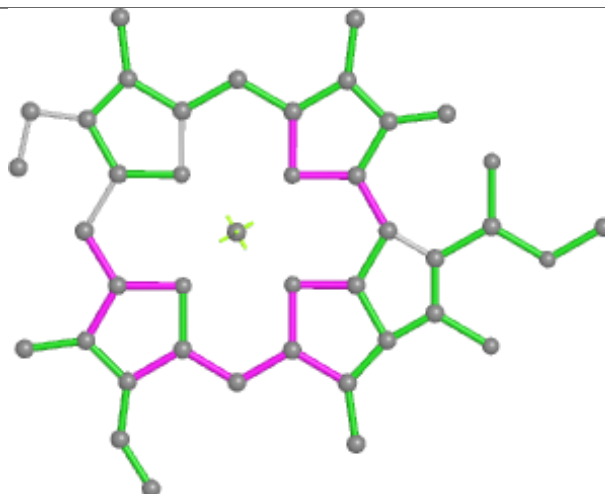
## Ligand CLA B3 813



## Ligand CLA B3 830



Bond lengths



Bond angles

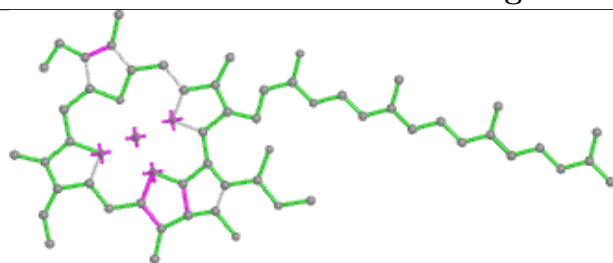


Torsions

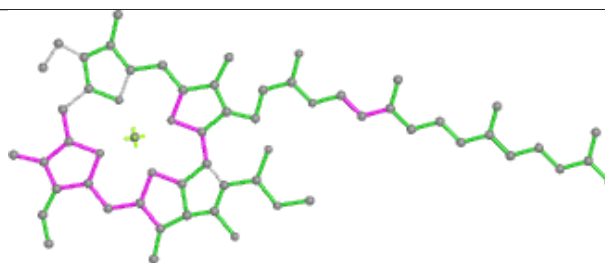


Rings

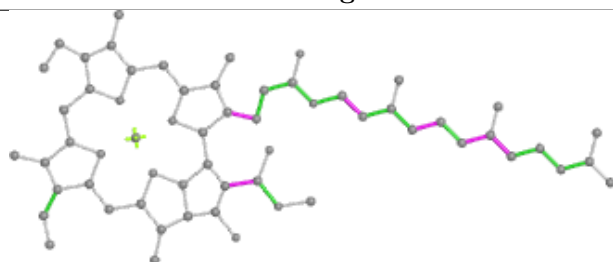
## Ligand CLA A3 825



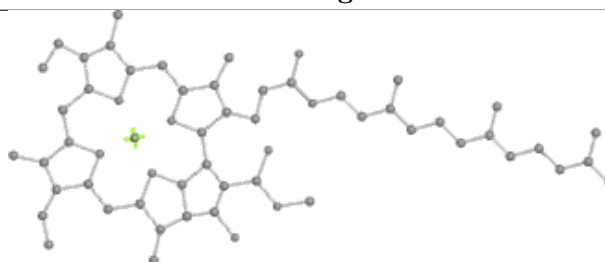
Bond lengths



Bond angles

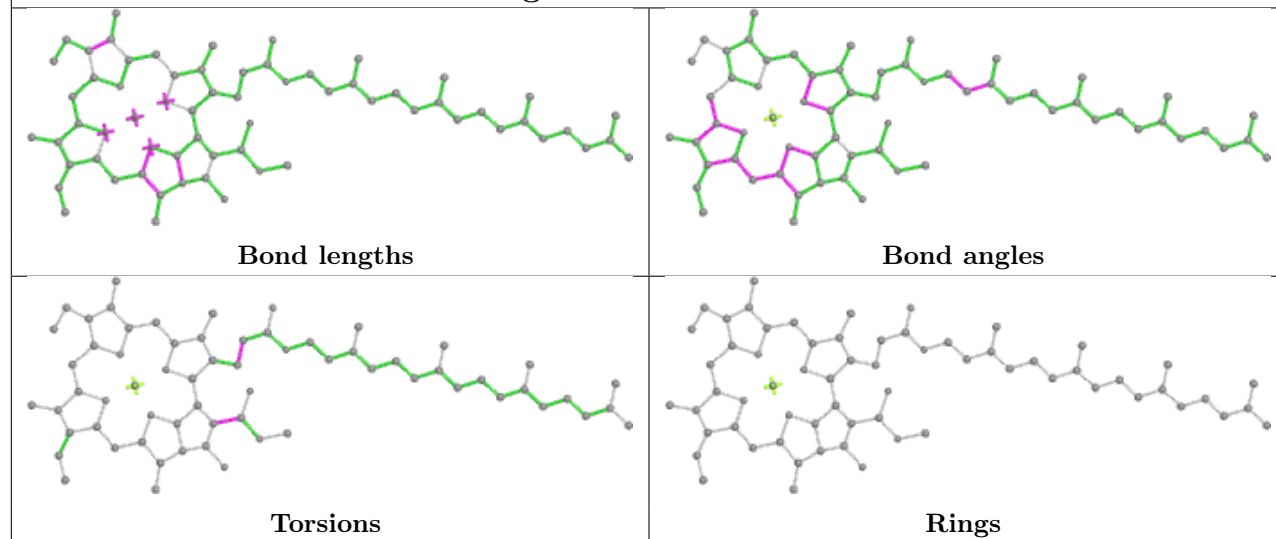


Torsions

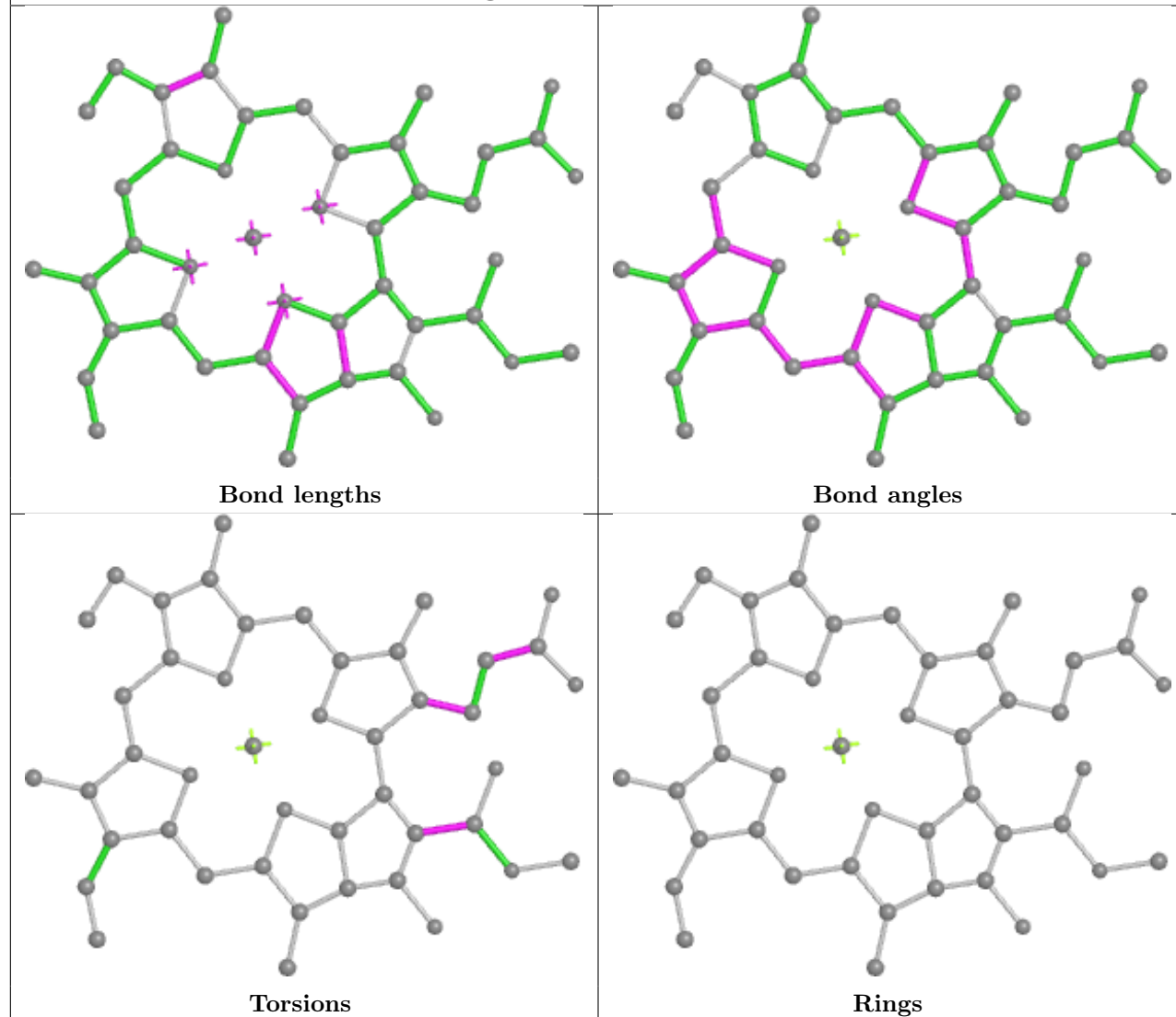


Rings

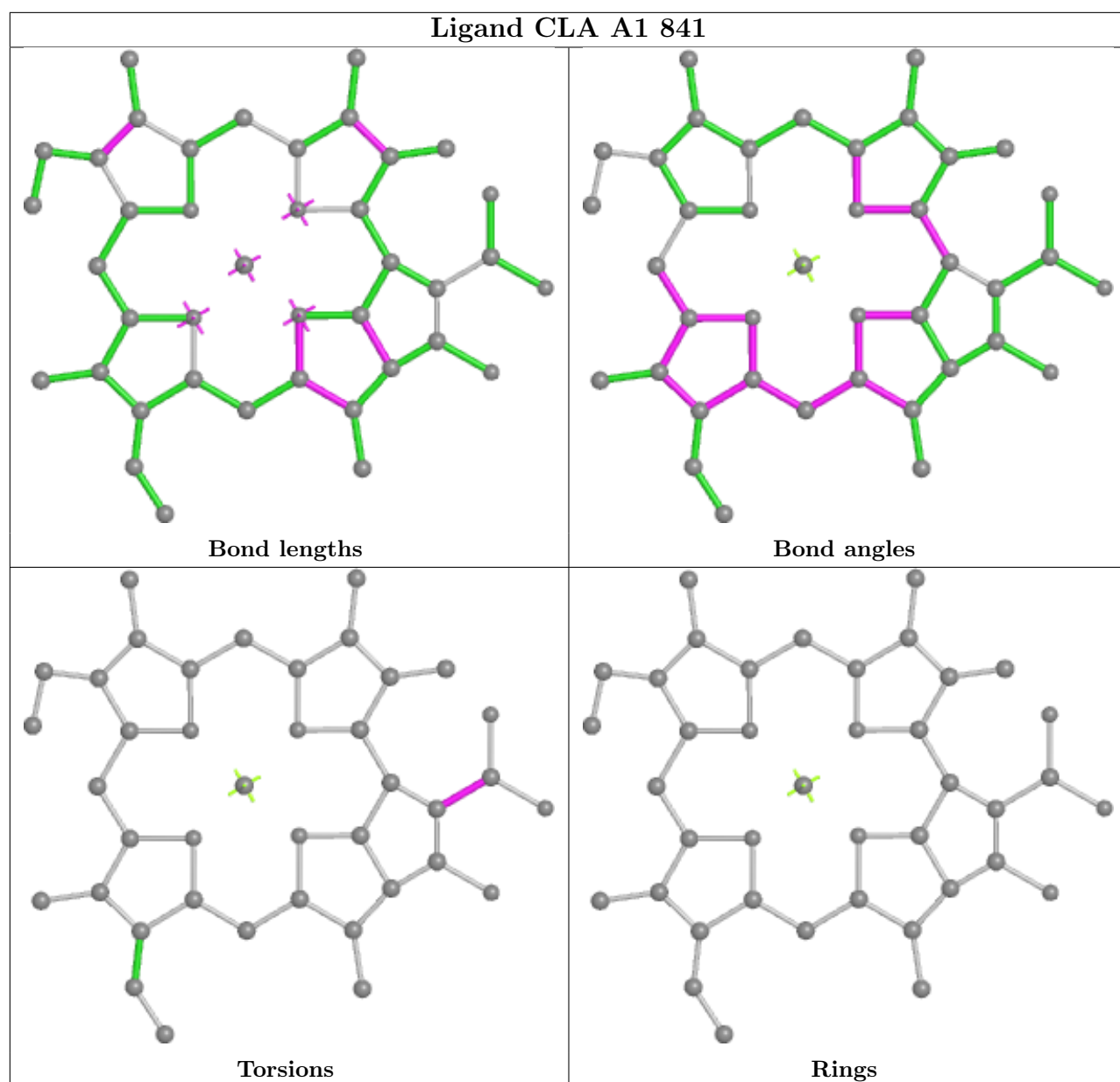
## Ligand CLA A2 805

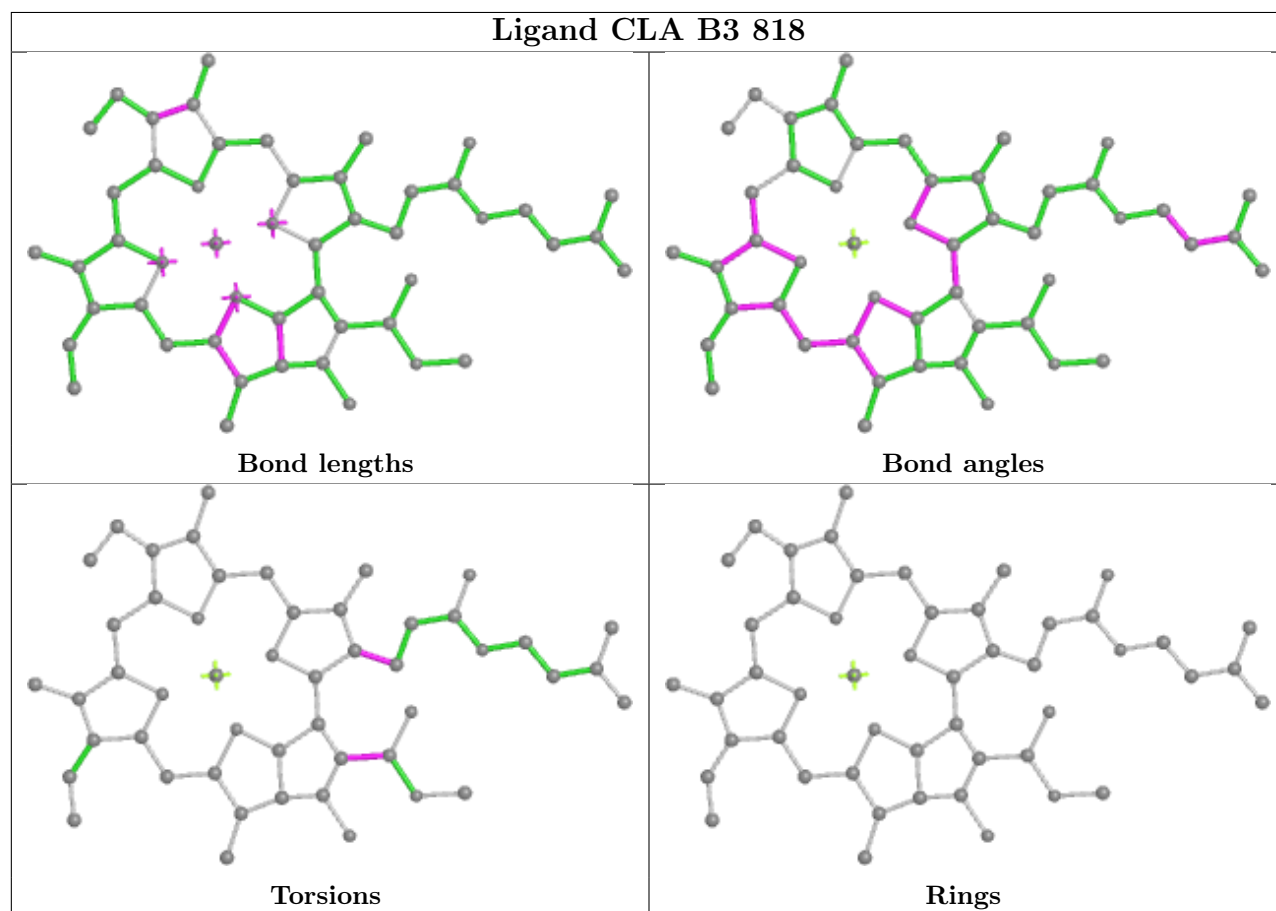
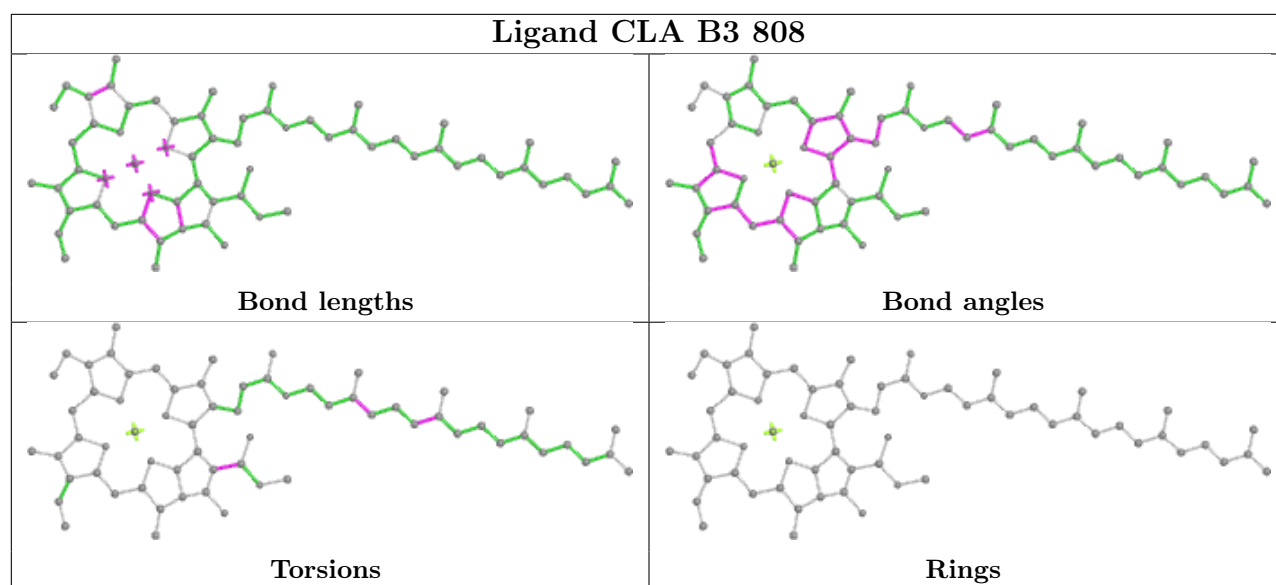


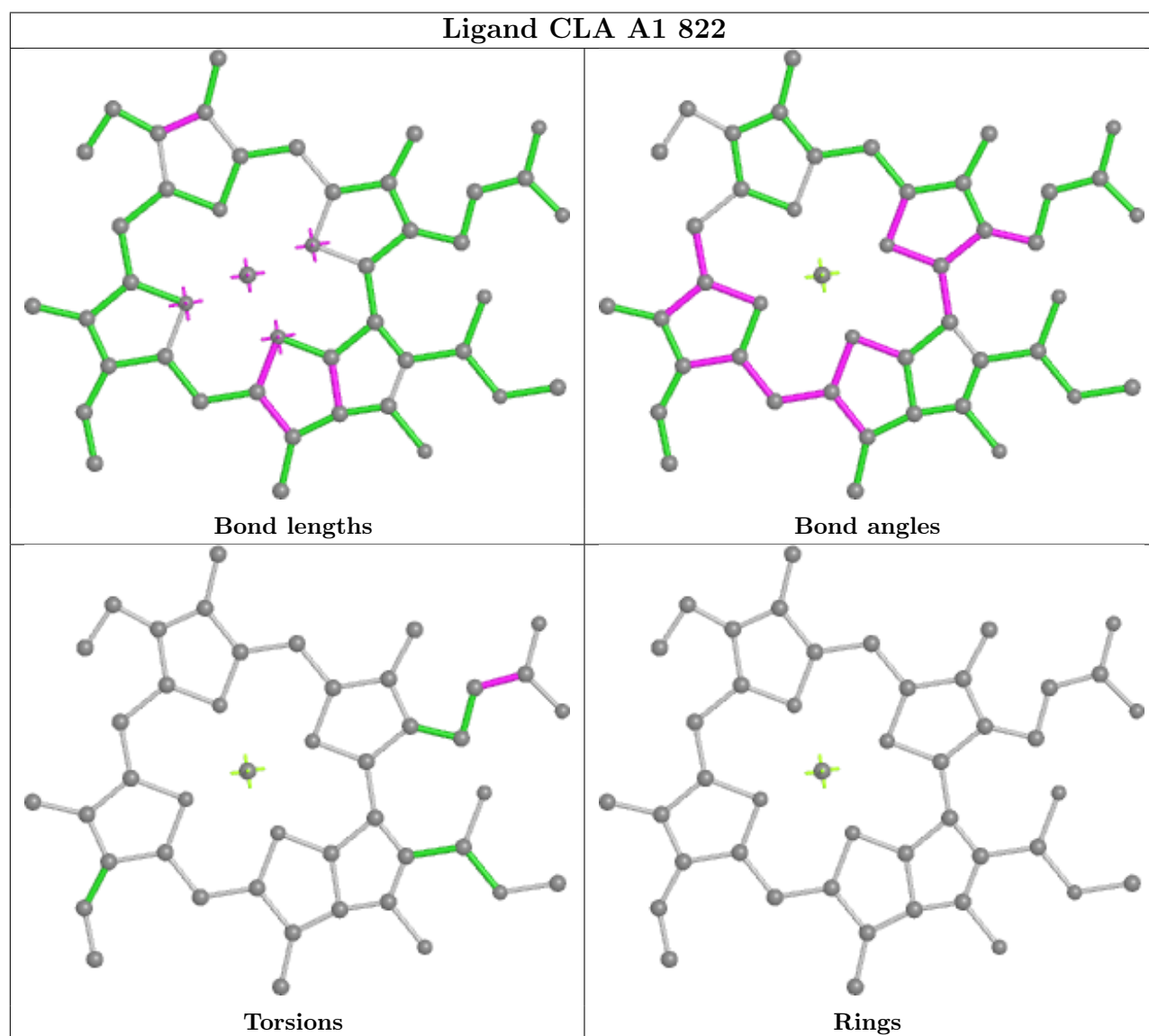
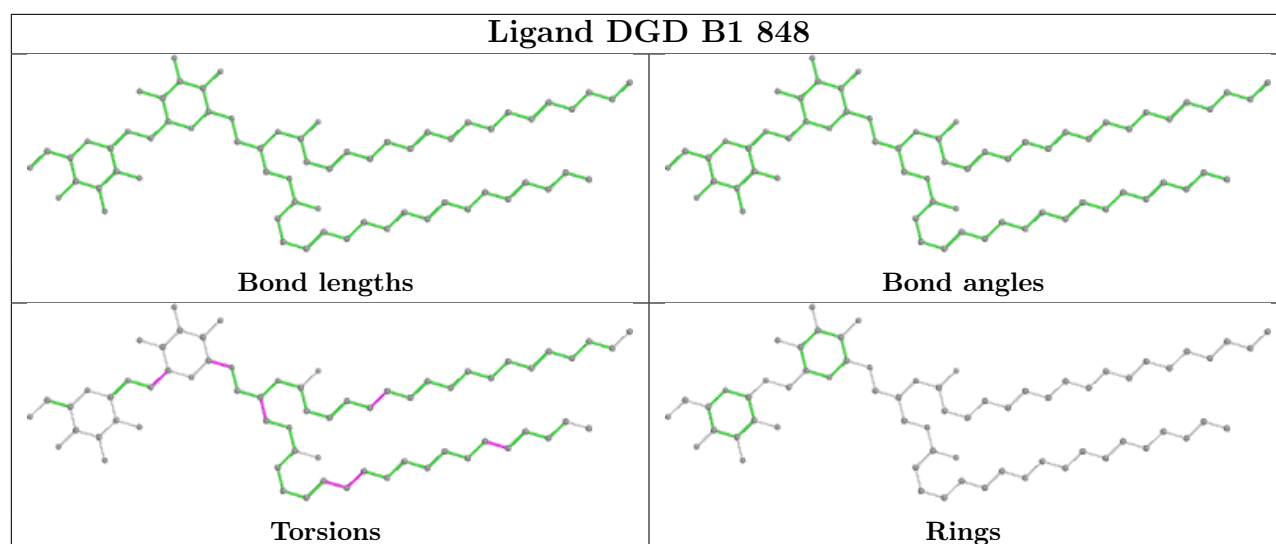
## Ligand CLA B2 819

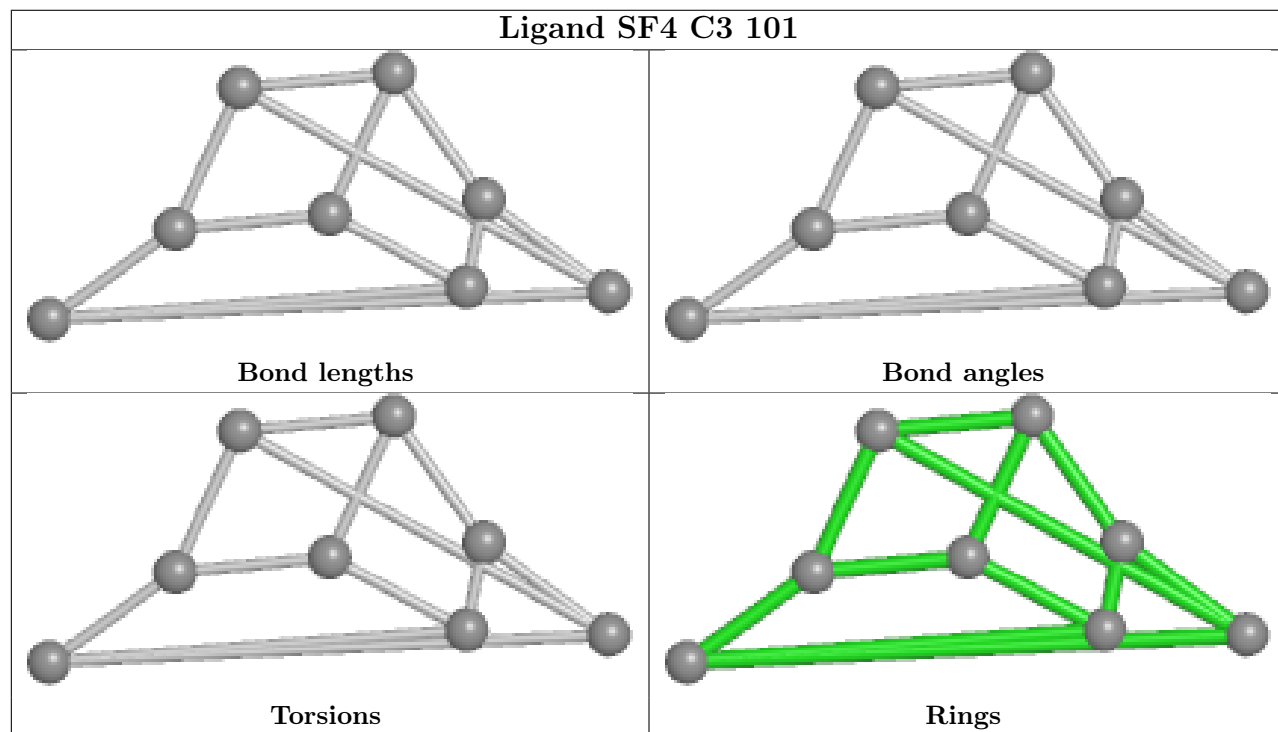
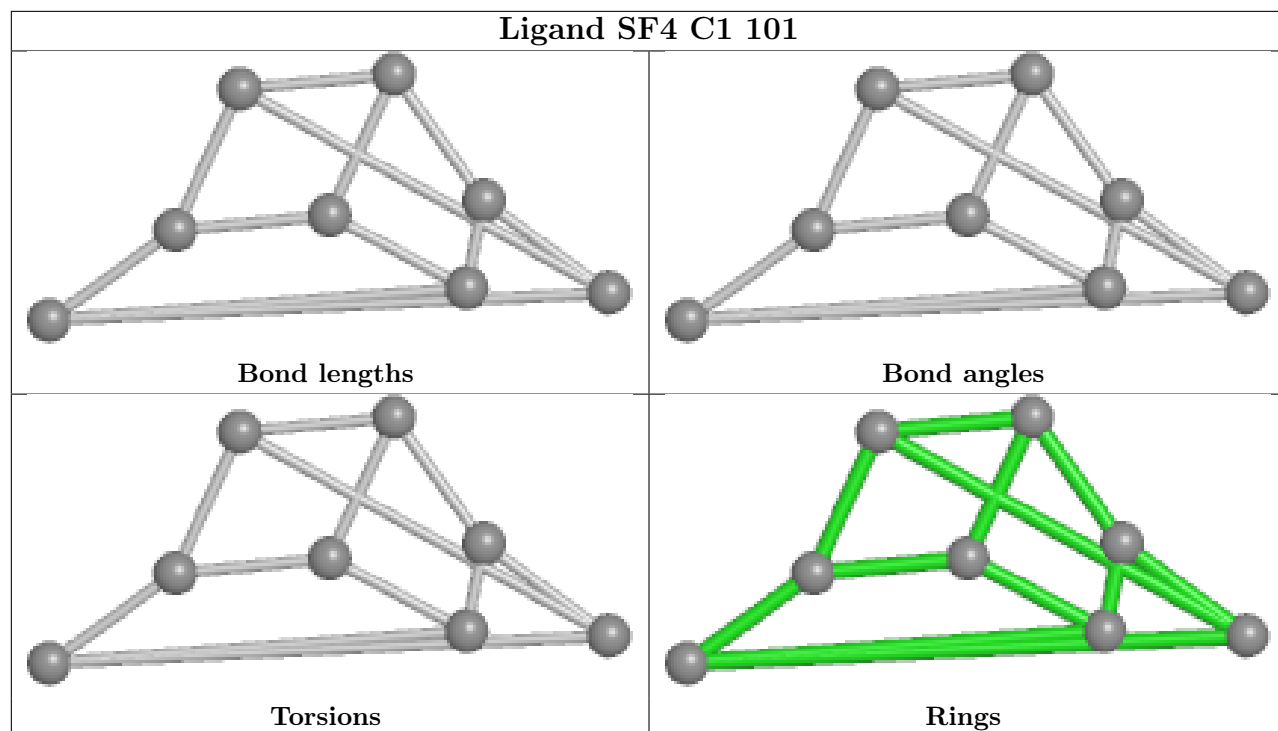




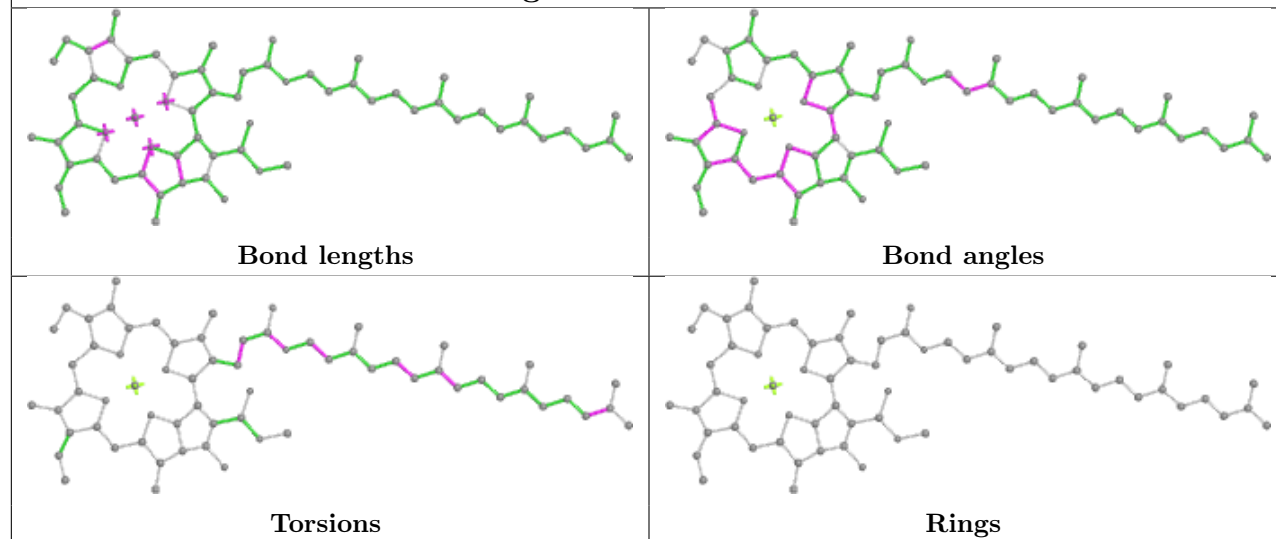




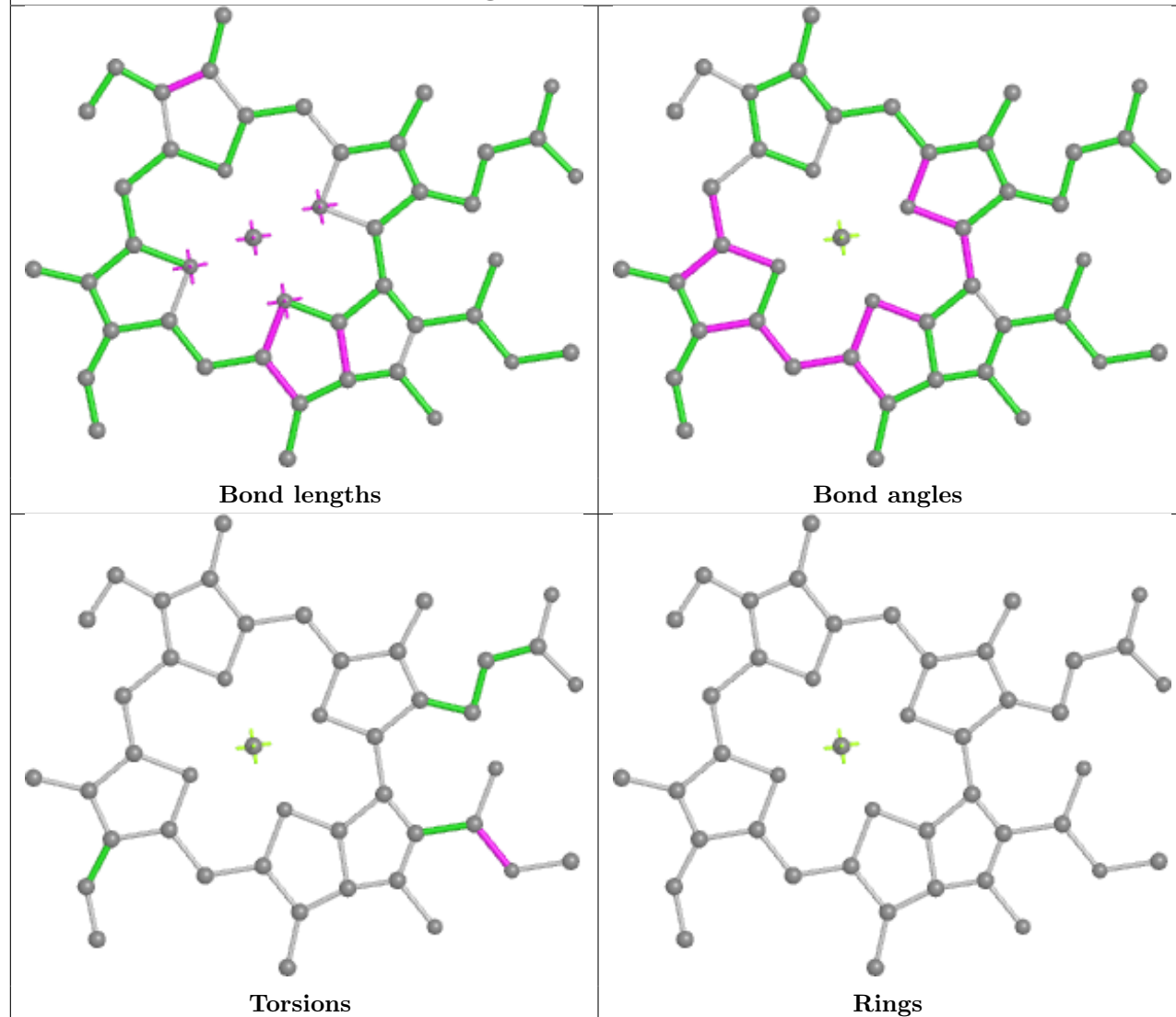




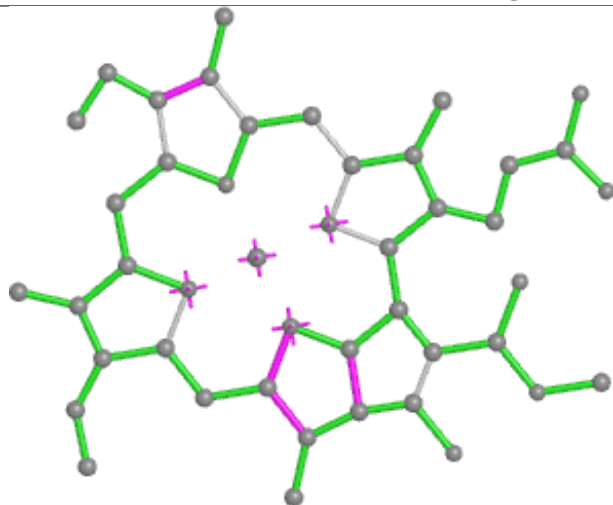
## Ligand CLA A1 843



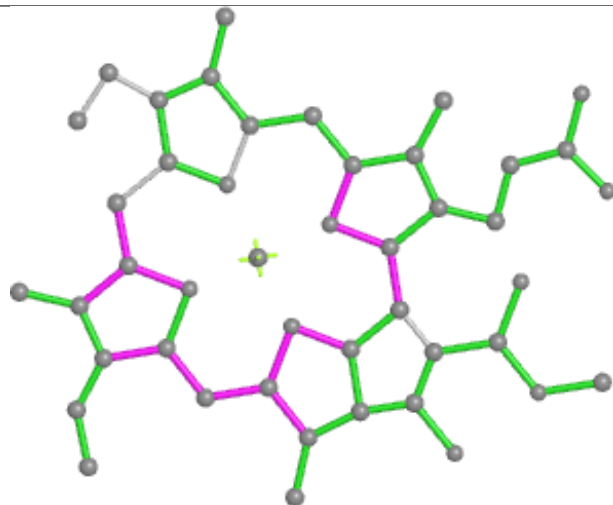
## Ligand CLA B1 824



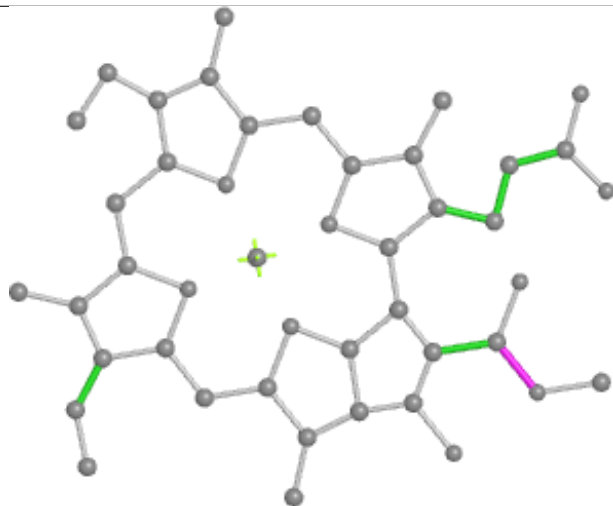
## Ligand CLA B3 826



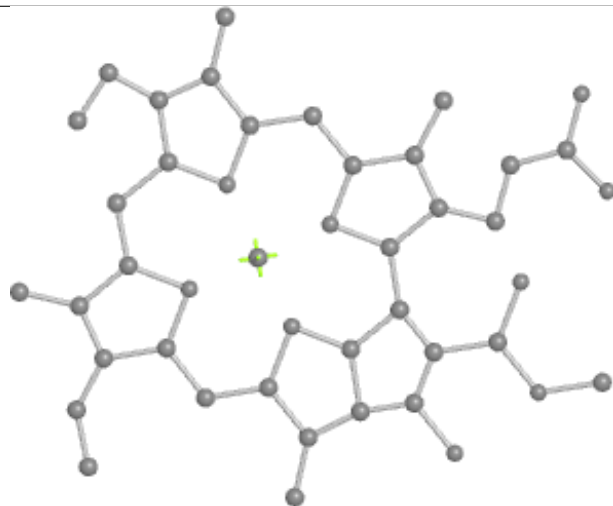
Bond lengths



Bond angles

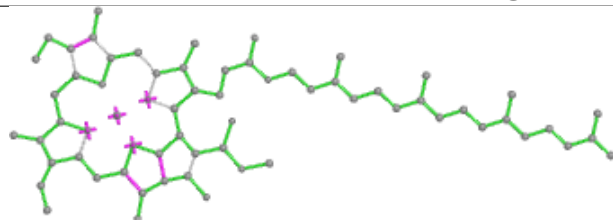


Torsions

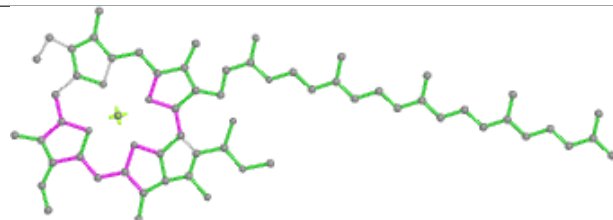


Rings

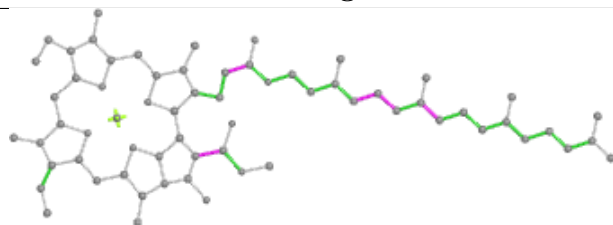
## Ligand CLA A2 856



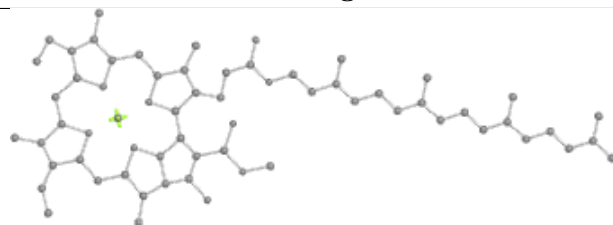
Bond lengths



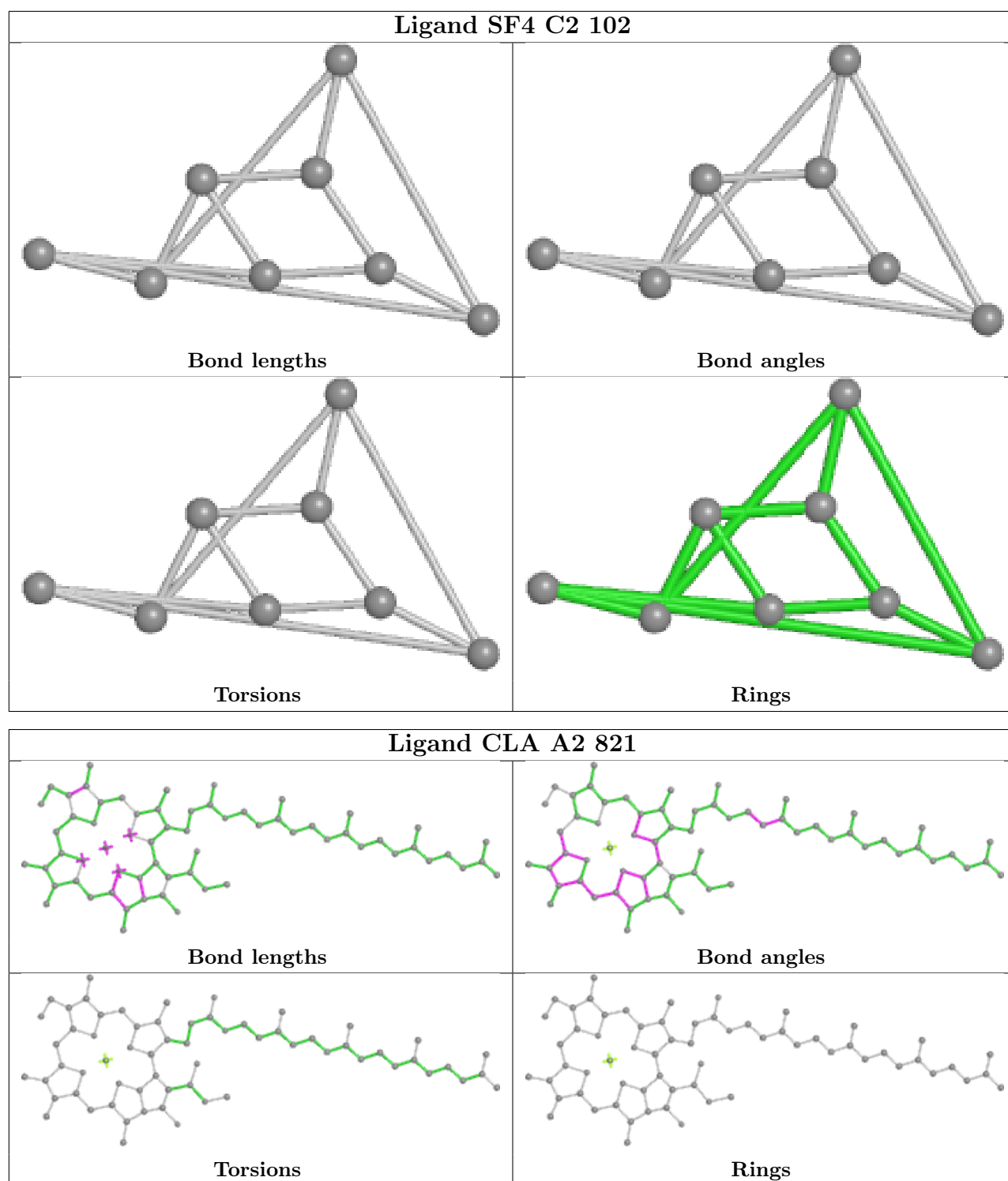
Bond angles



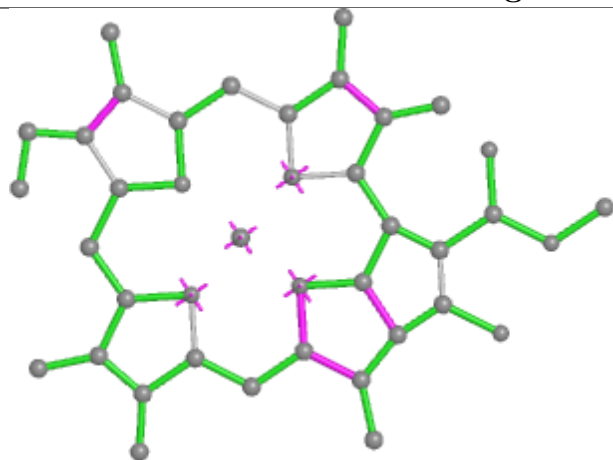
Torsions



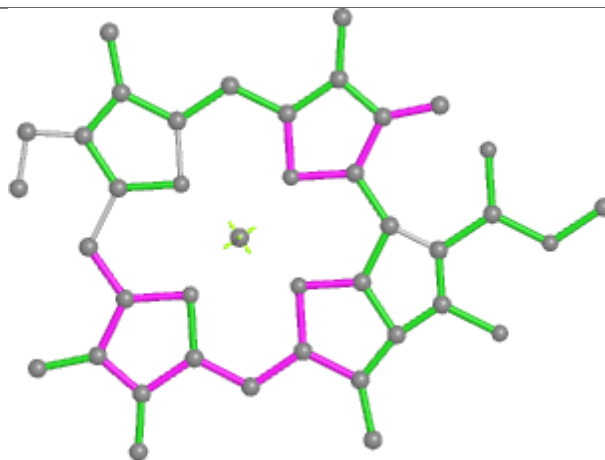
Rings



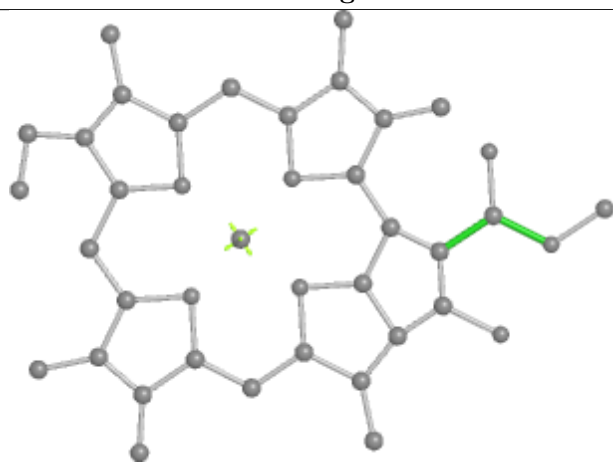
## Ligand CLA A1 812



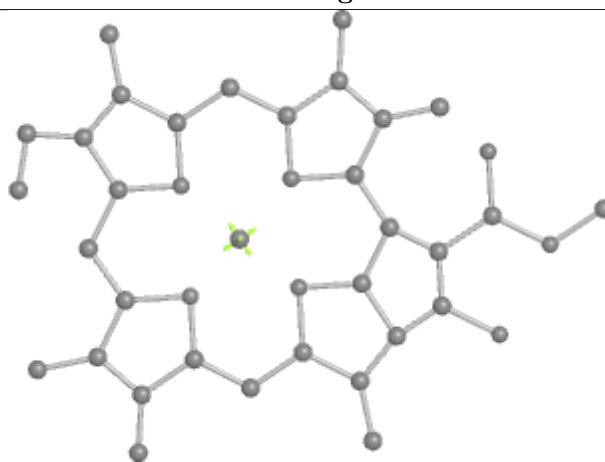
Bond lengths



Bond angles

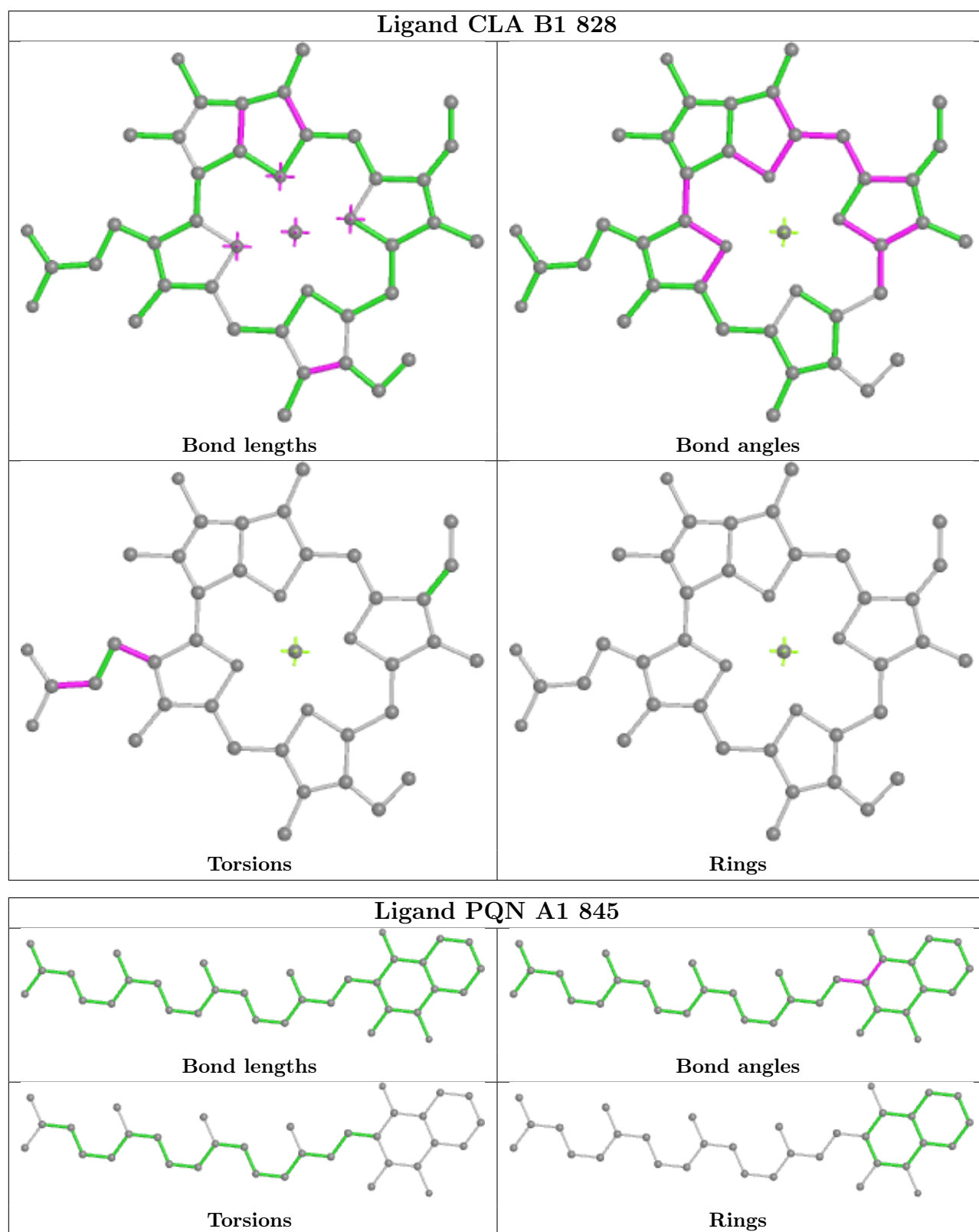


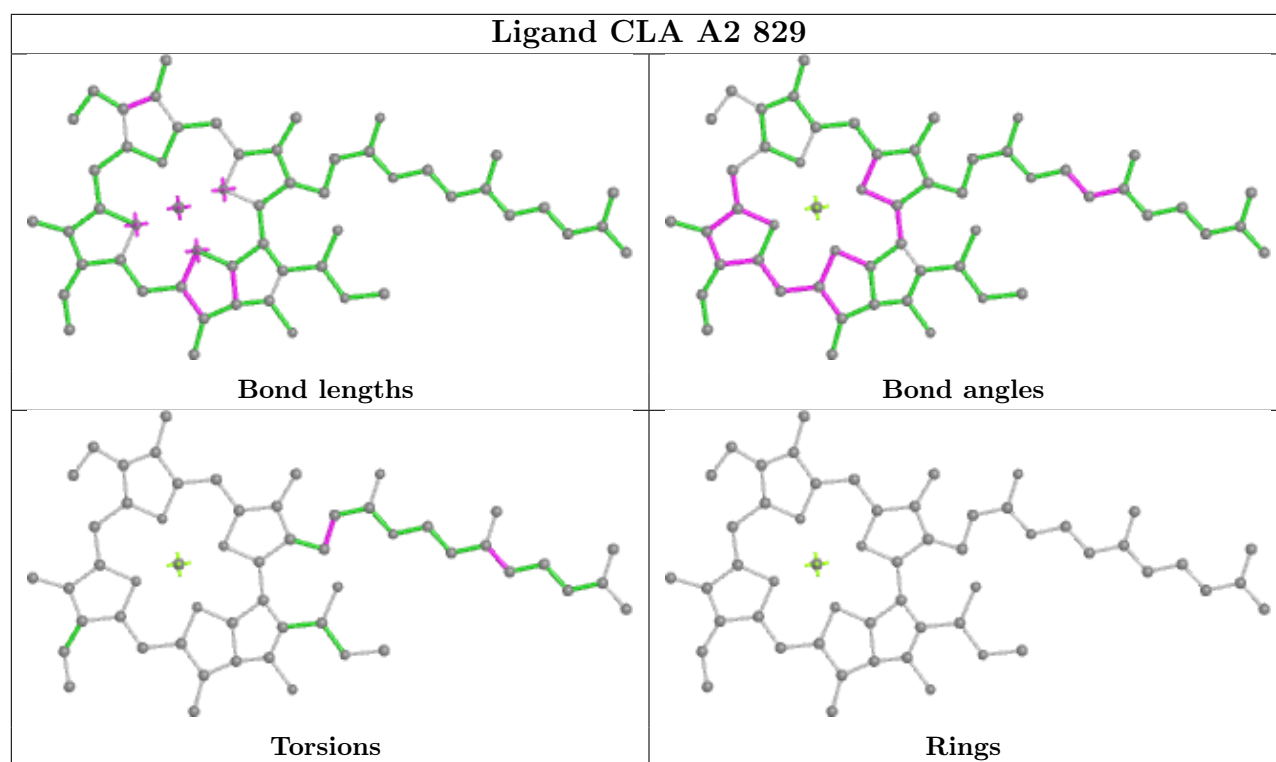
Torsions

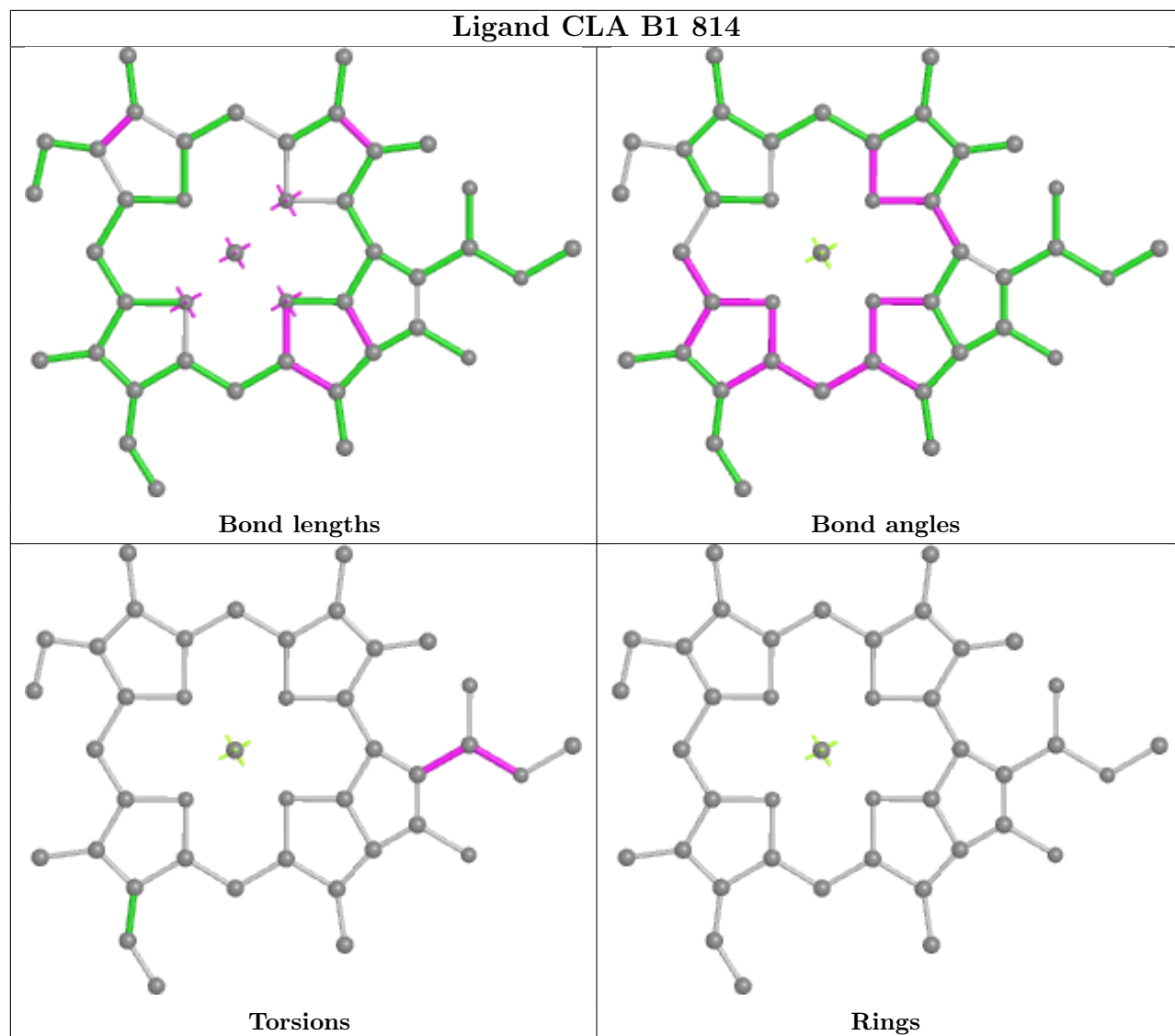


Rings

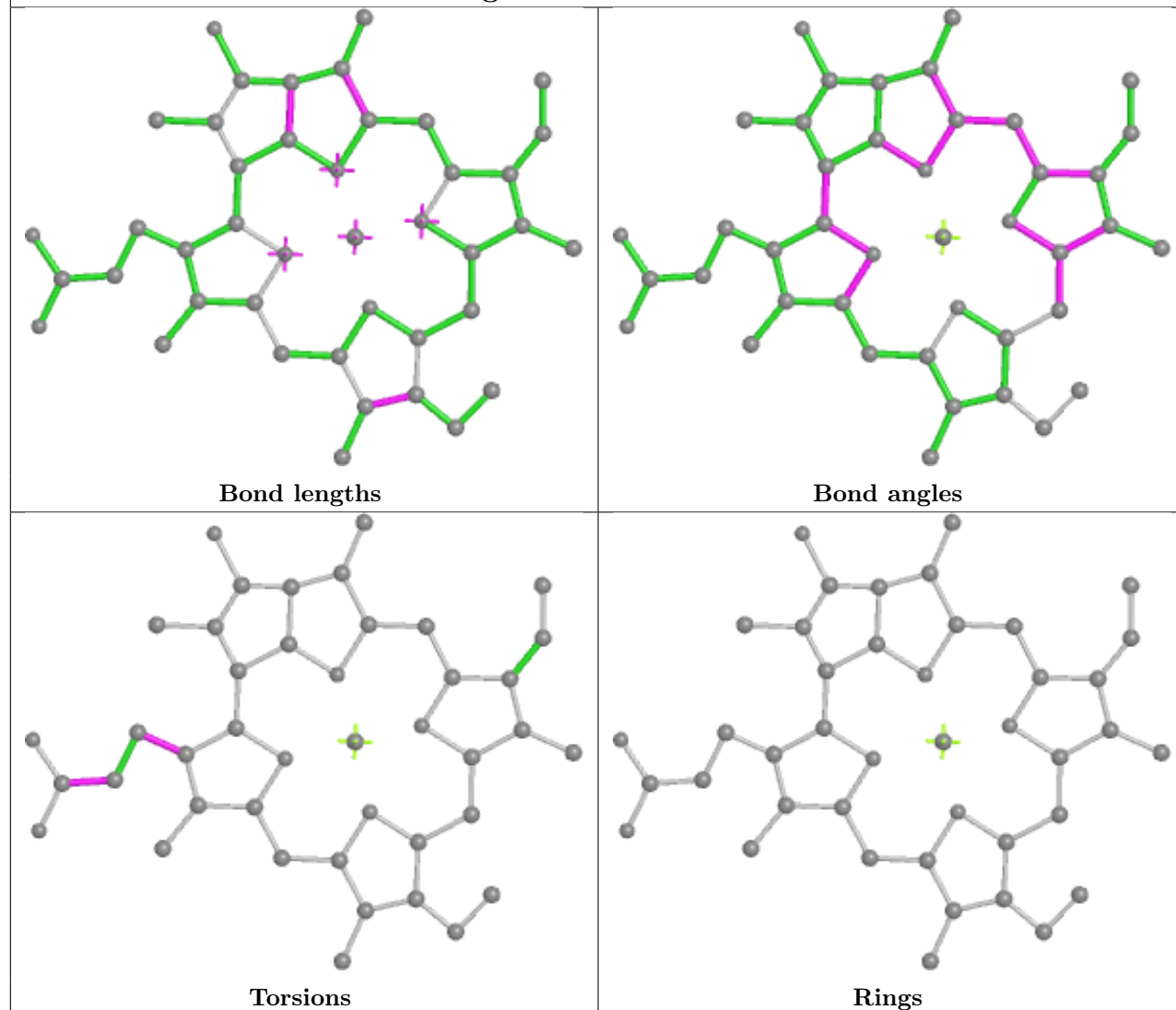




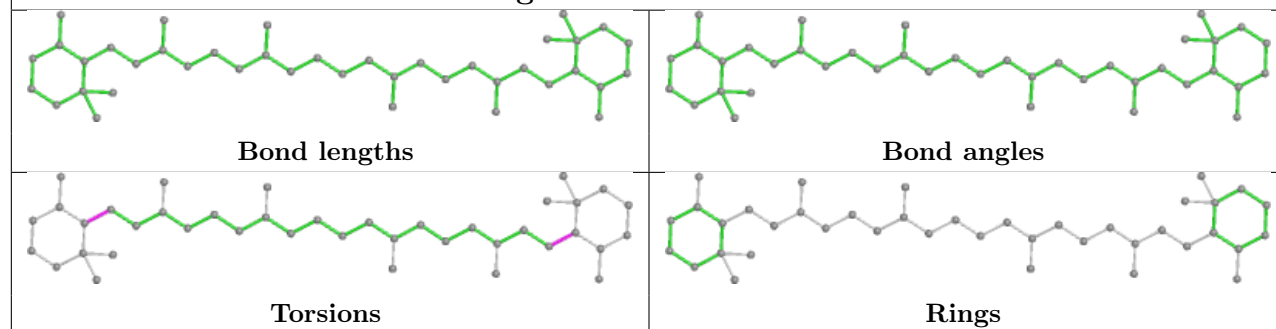




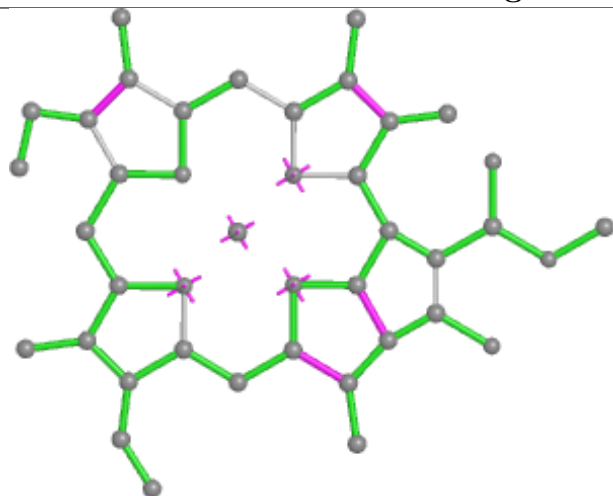
## Ligand CLA B2 828



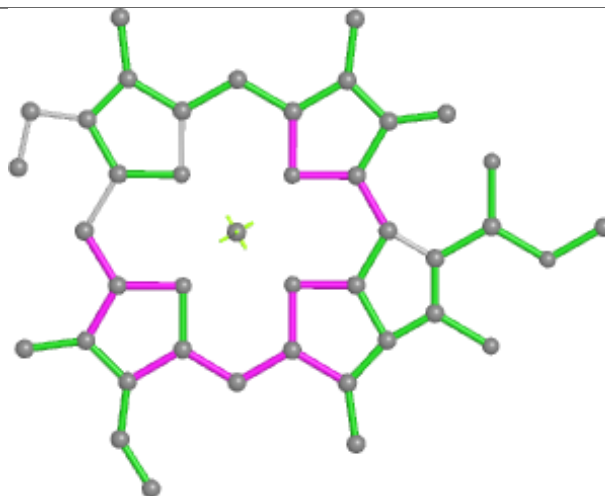
## Ligand BCR J2 1305



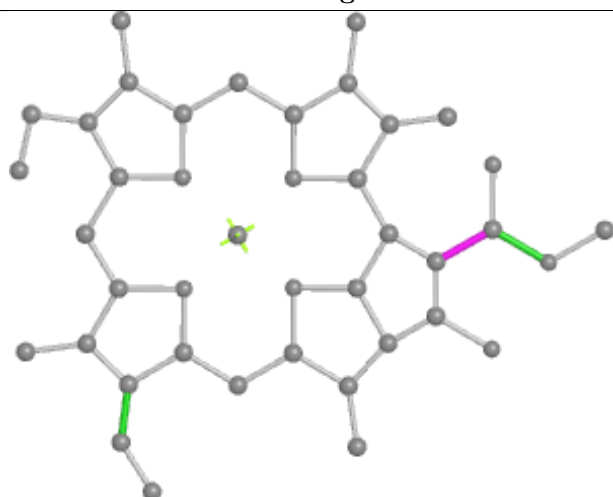
## Ligand CLA A2 836



Bond lengths



Bond angles

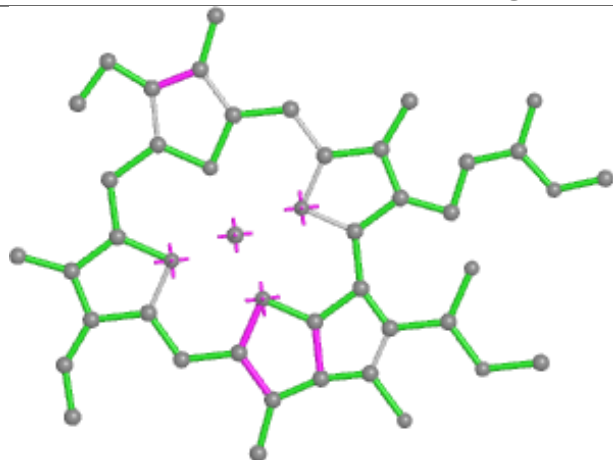


Torsions

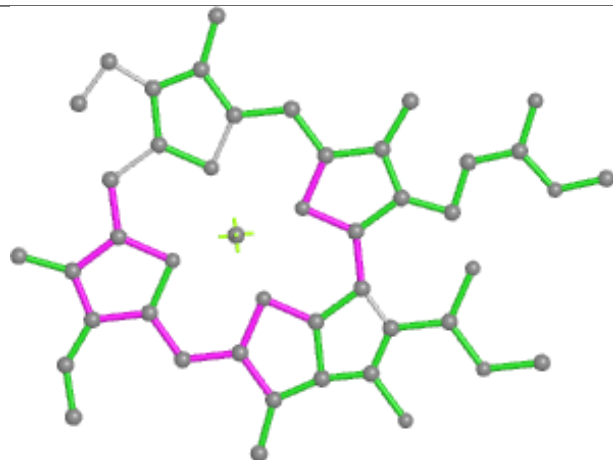


Rings

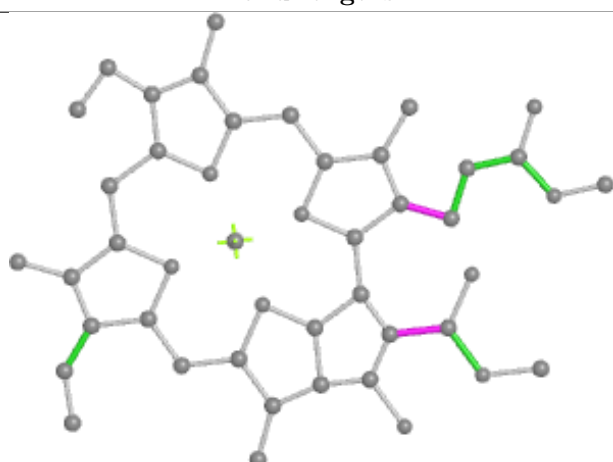
## Ligand CLA B3 835



Bond lengths



Bond angles

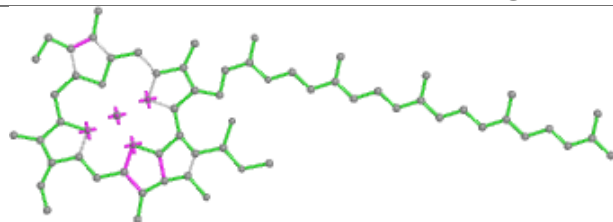


Torsions

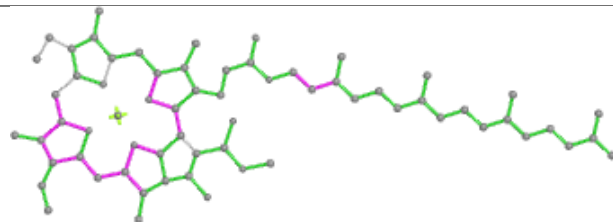


Rings

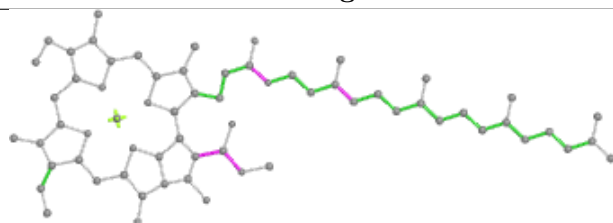
## Ligand CLA A3 833



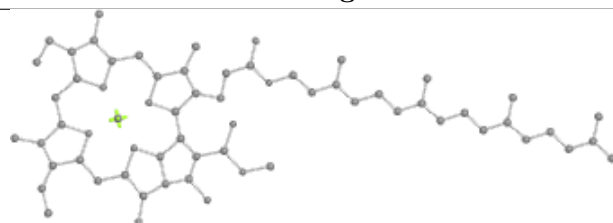
Bond lengths



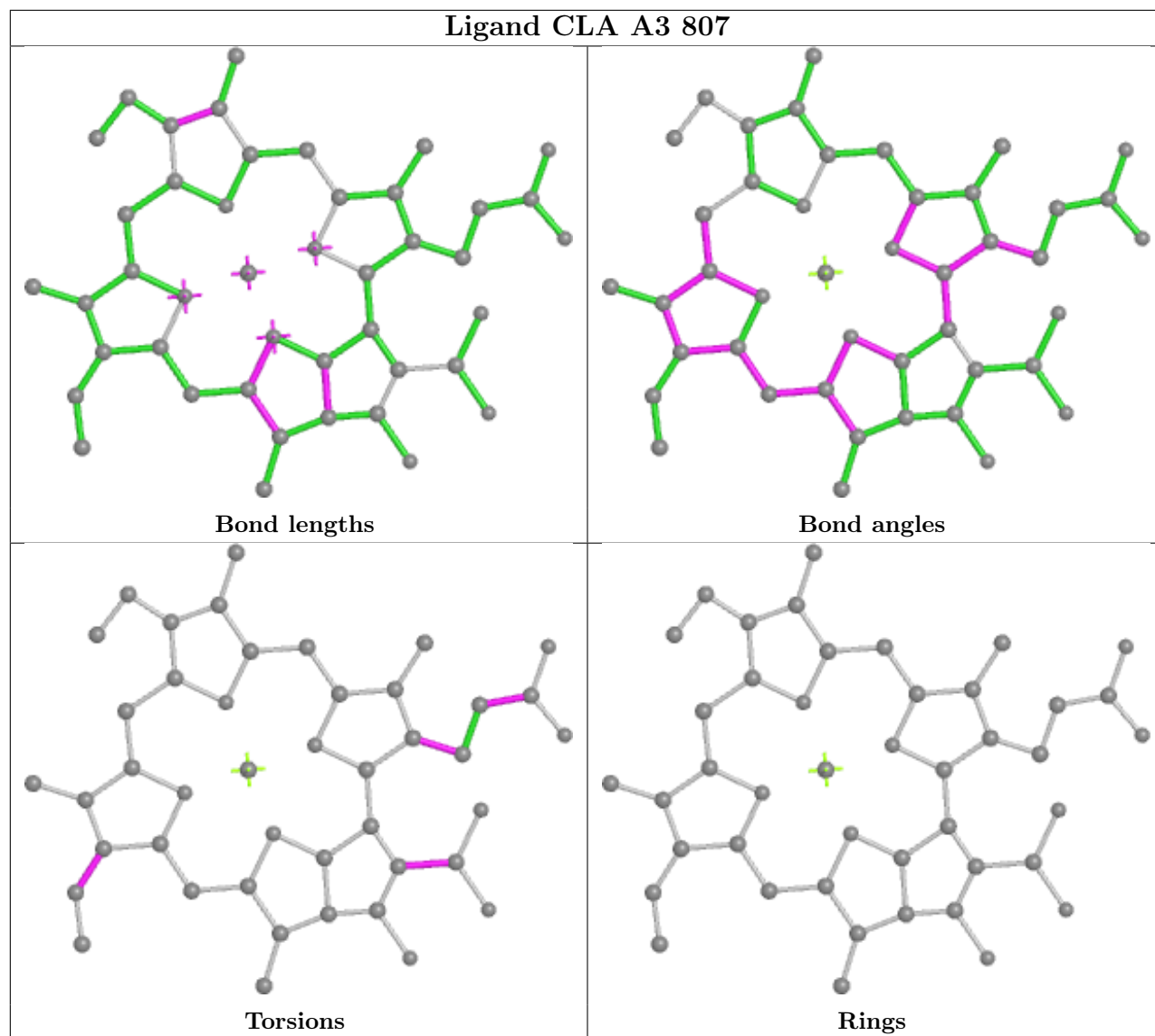
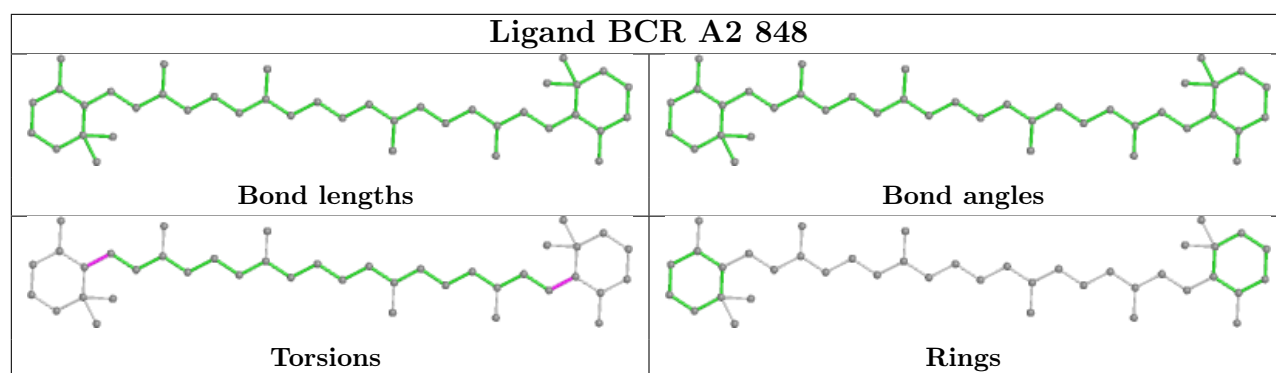
Bond angles

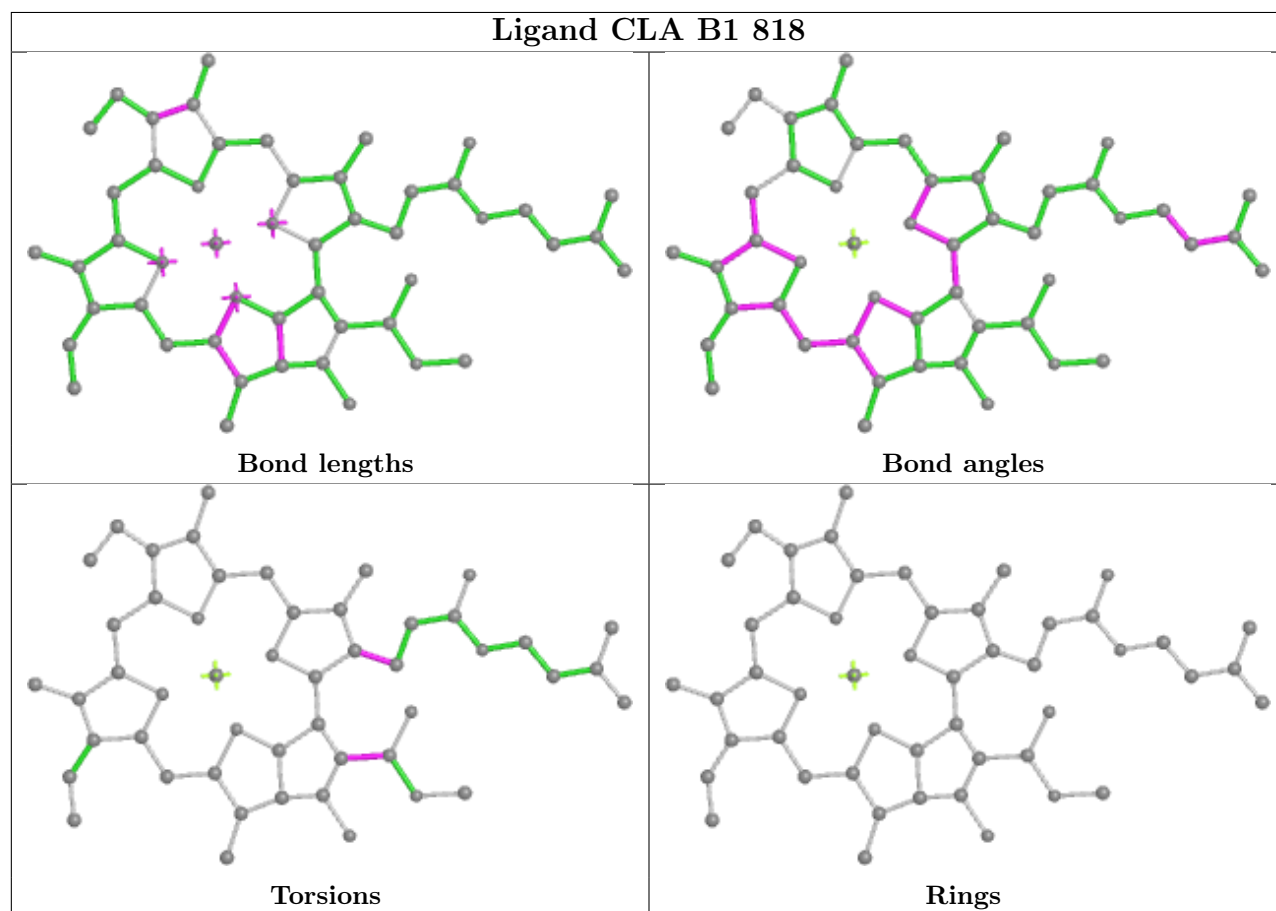
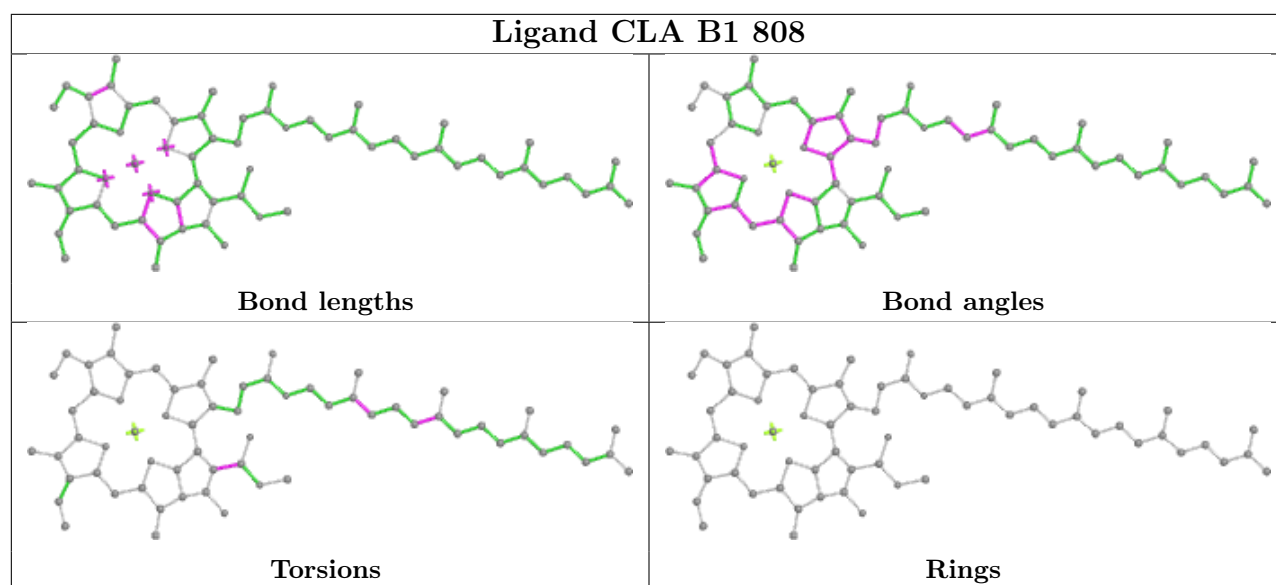


Torsions



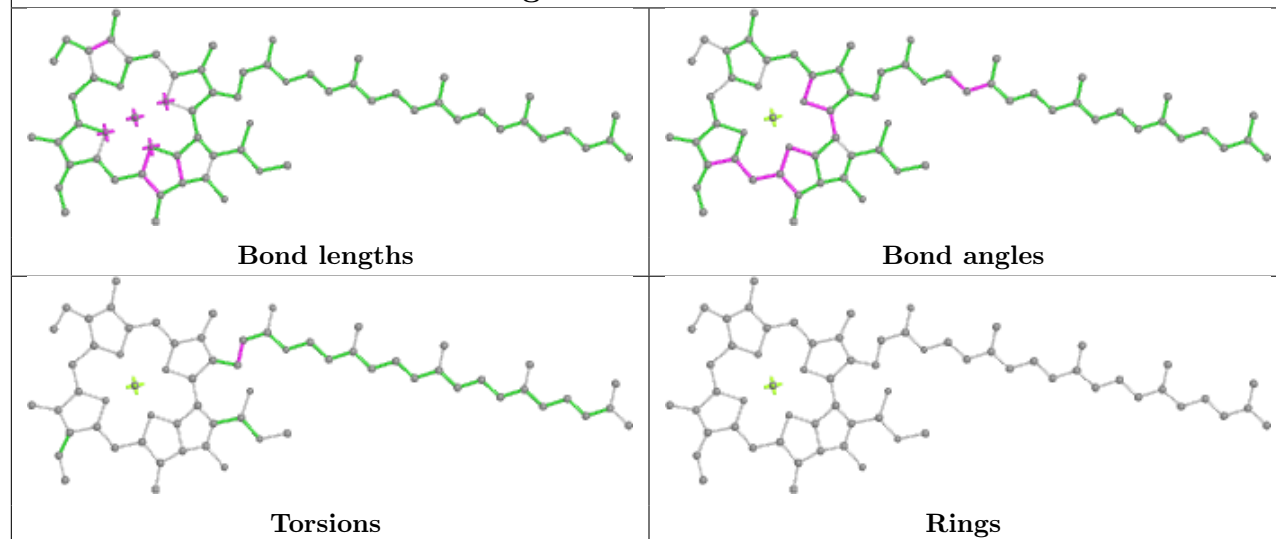
Rings



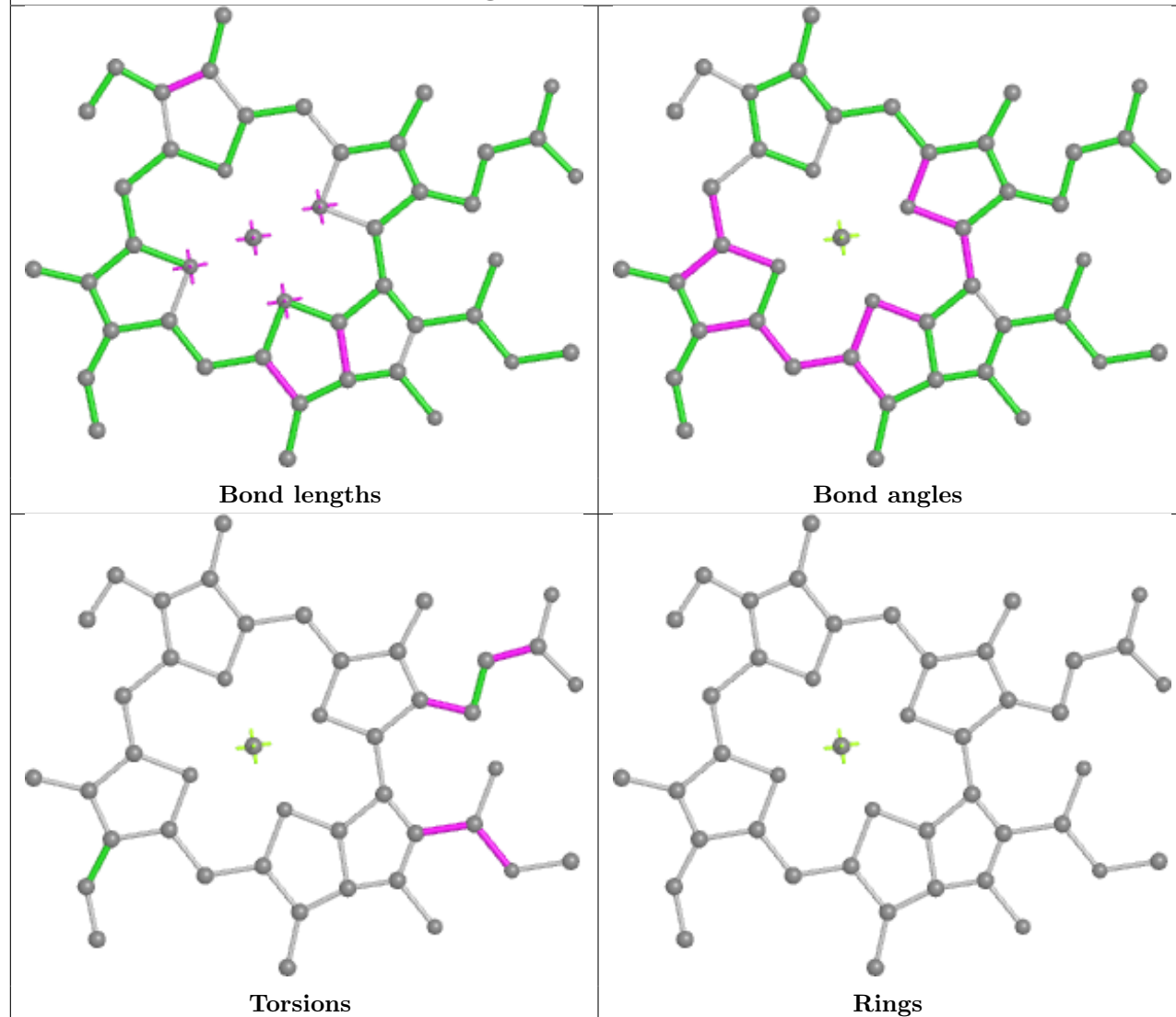




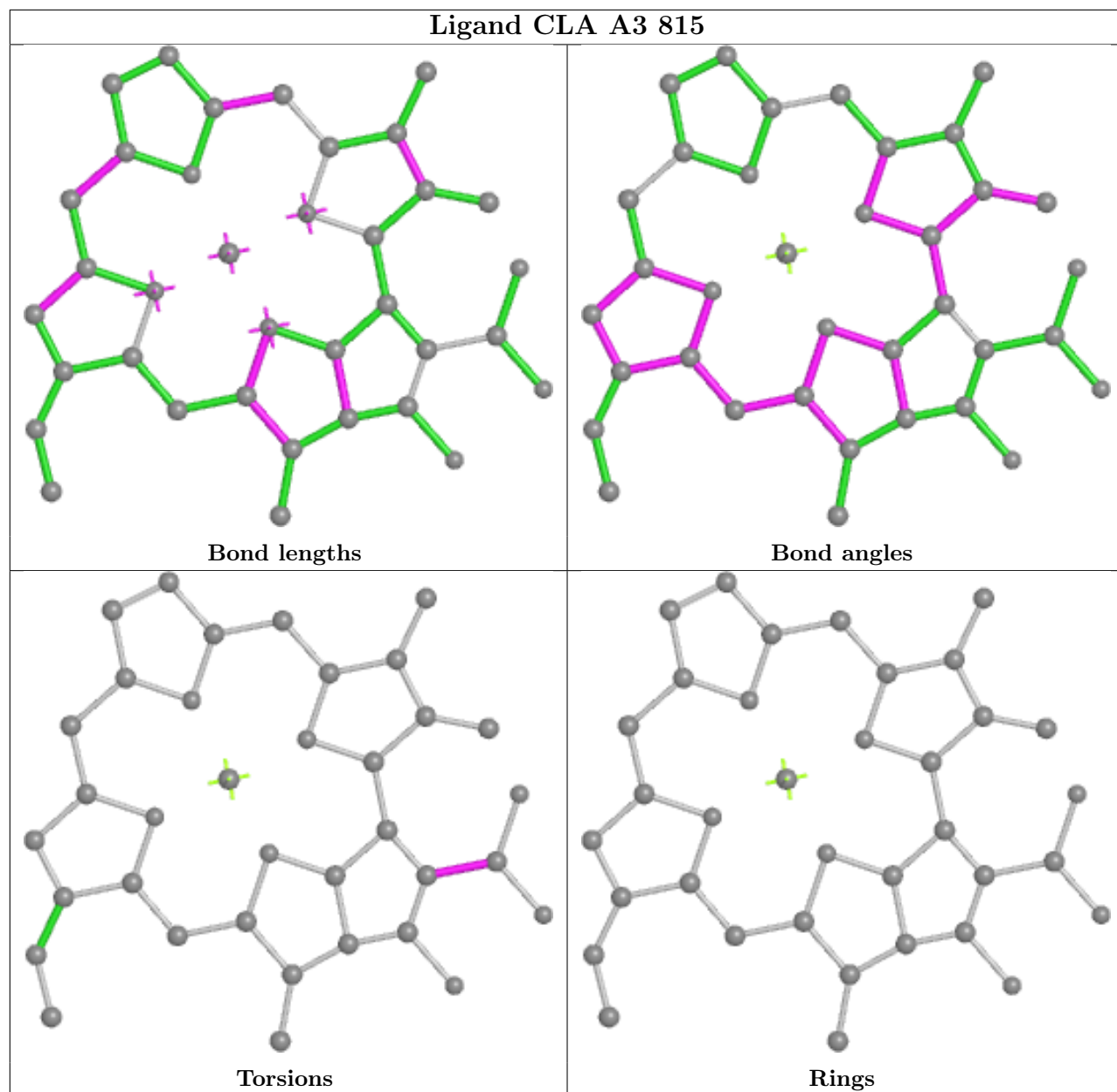
## Ligand CLA A3 802

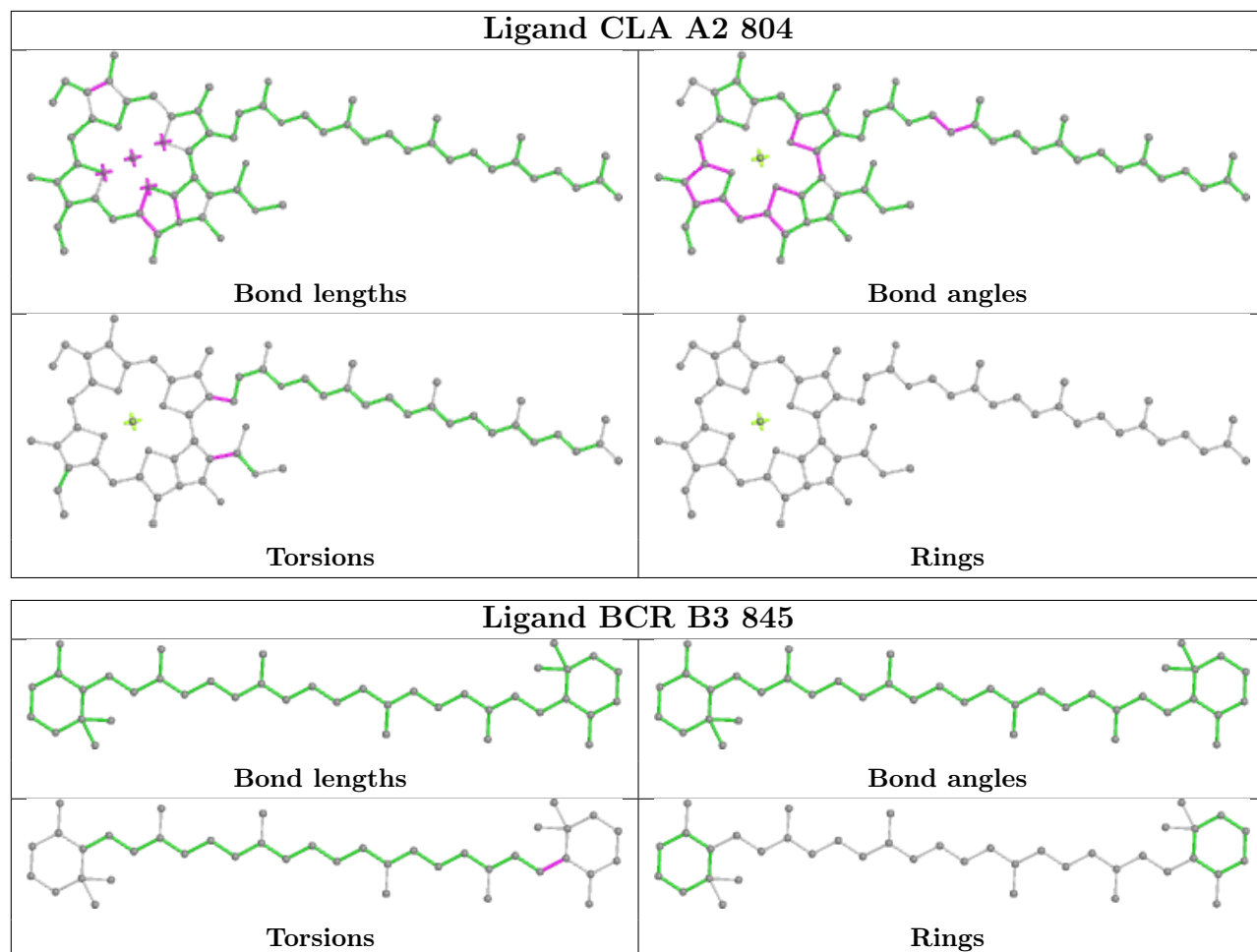


## Ligand CLA B1 849

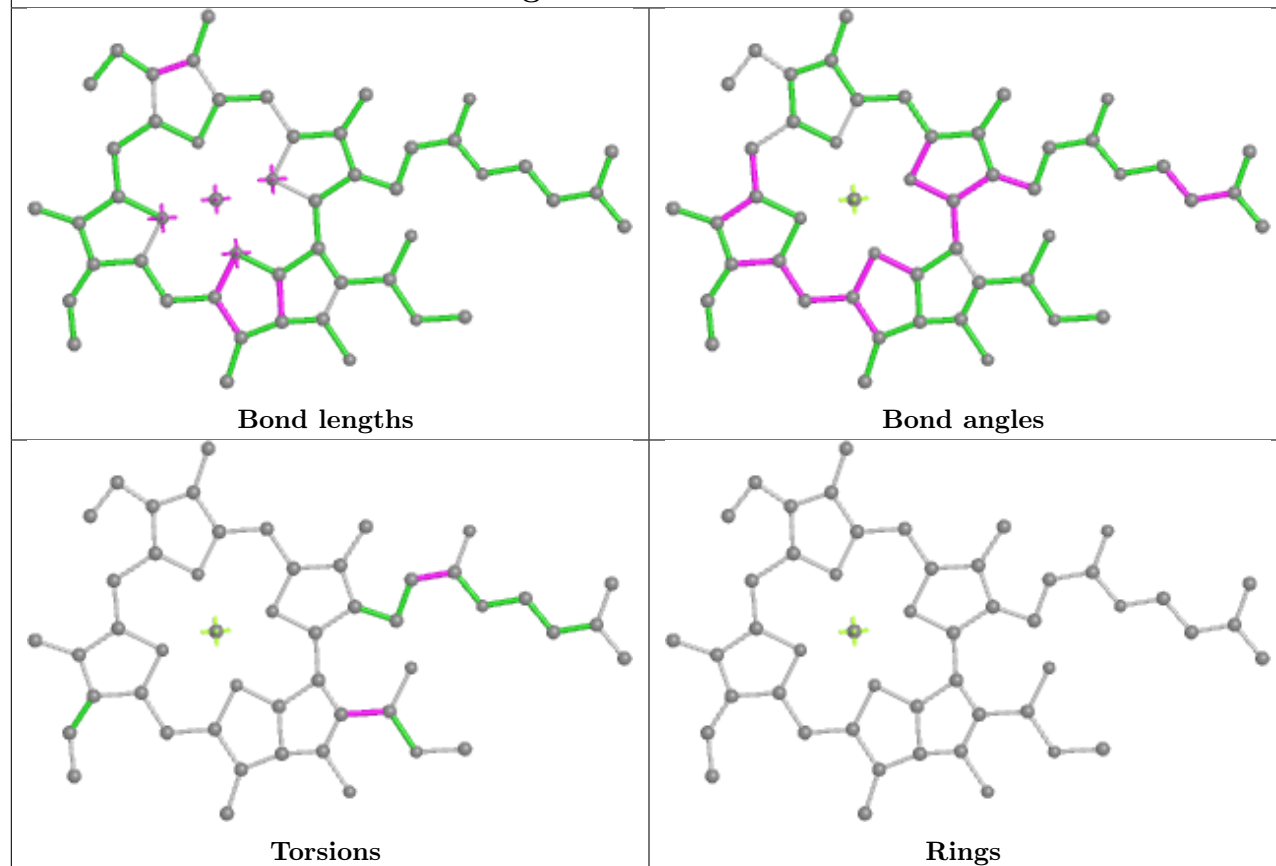


## Ligand CLA A3 815

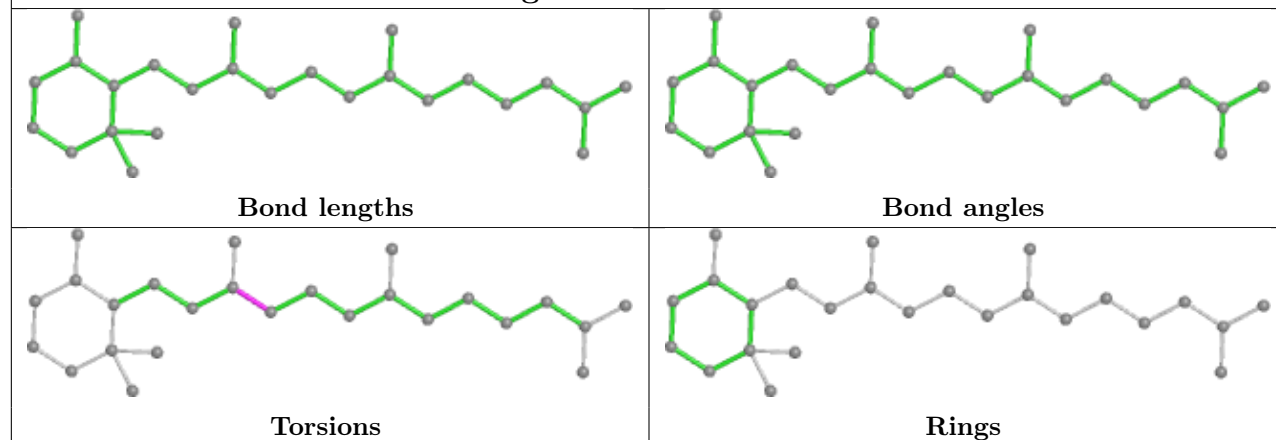


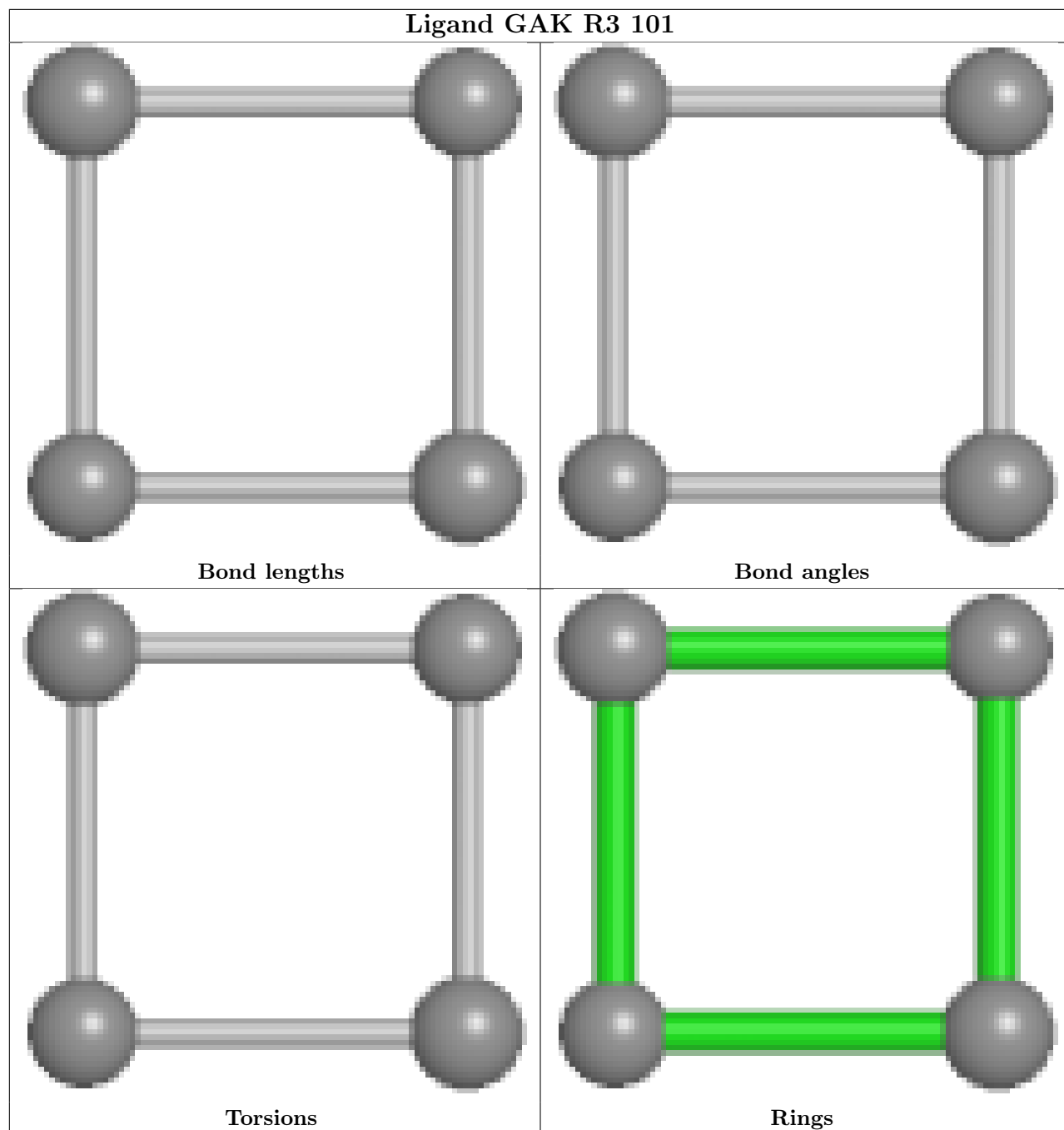


## Ligand CLA A2 831

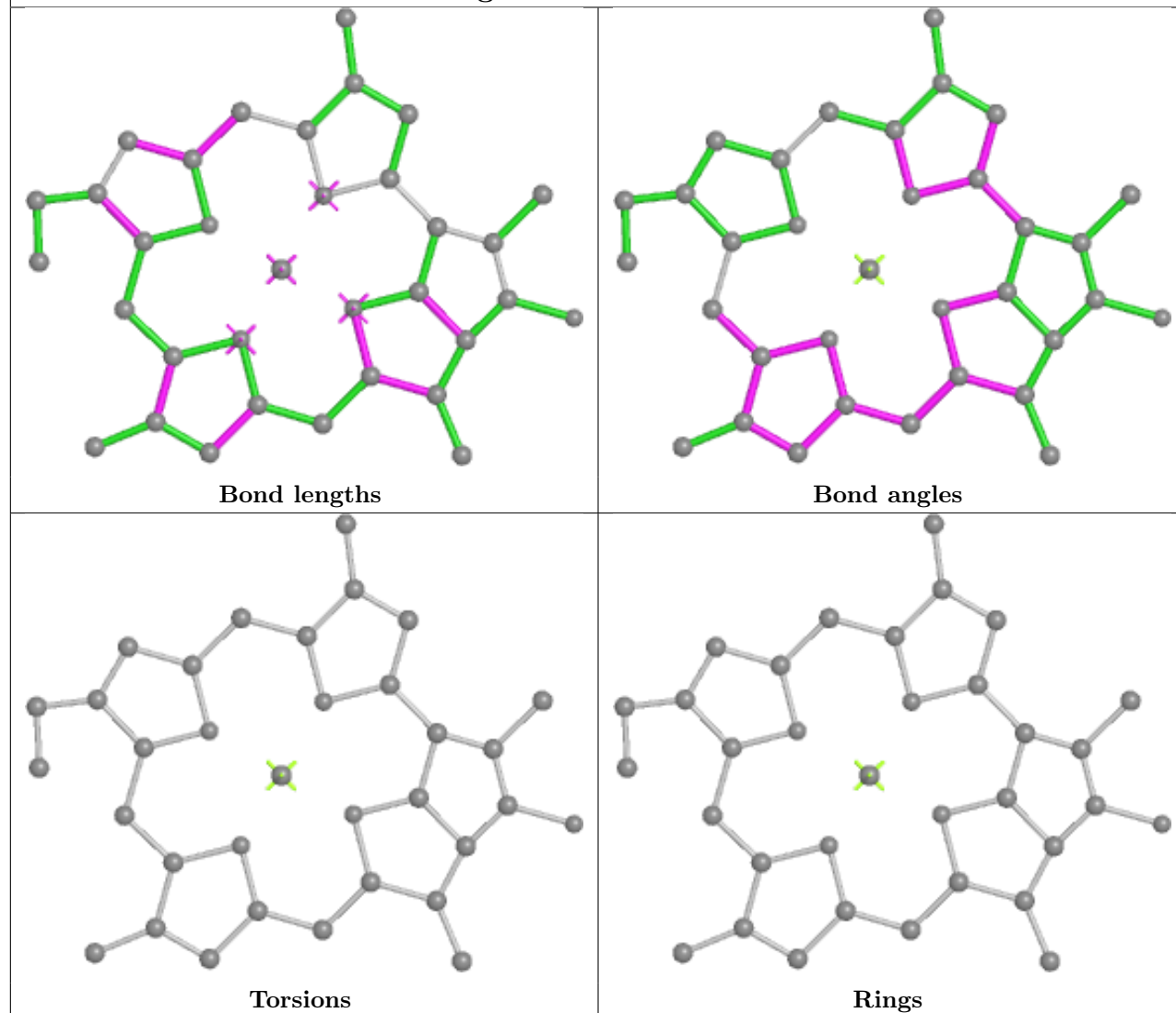


## Ligand BCR B1 843

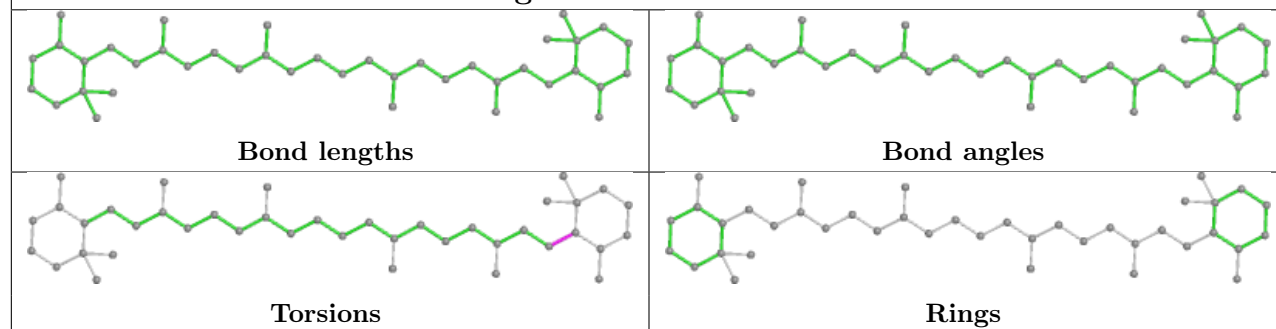


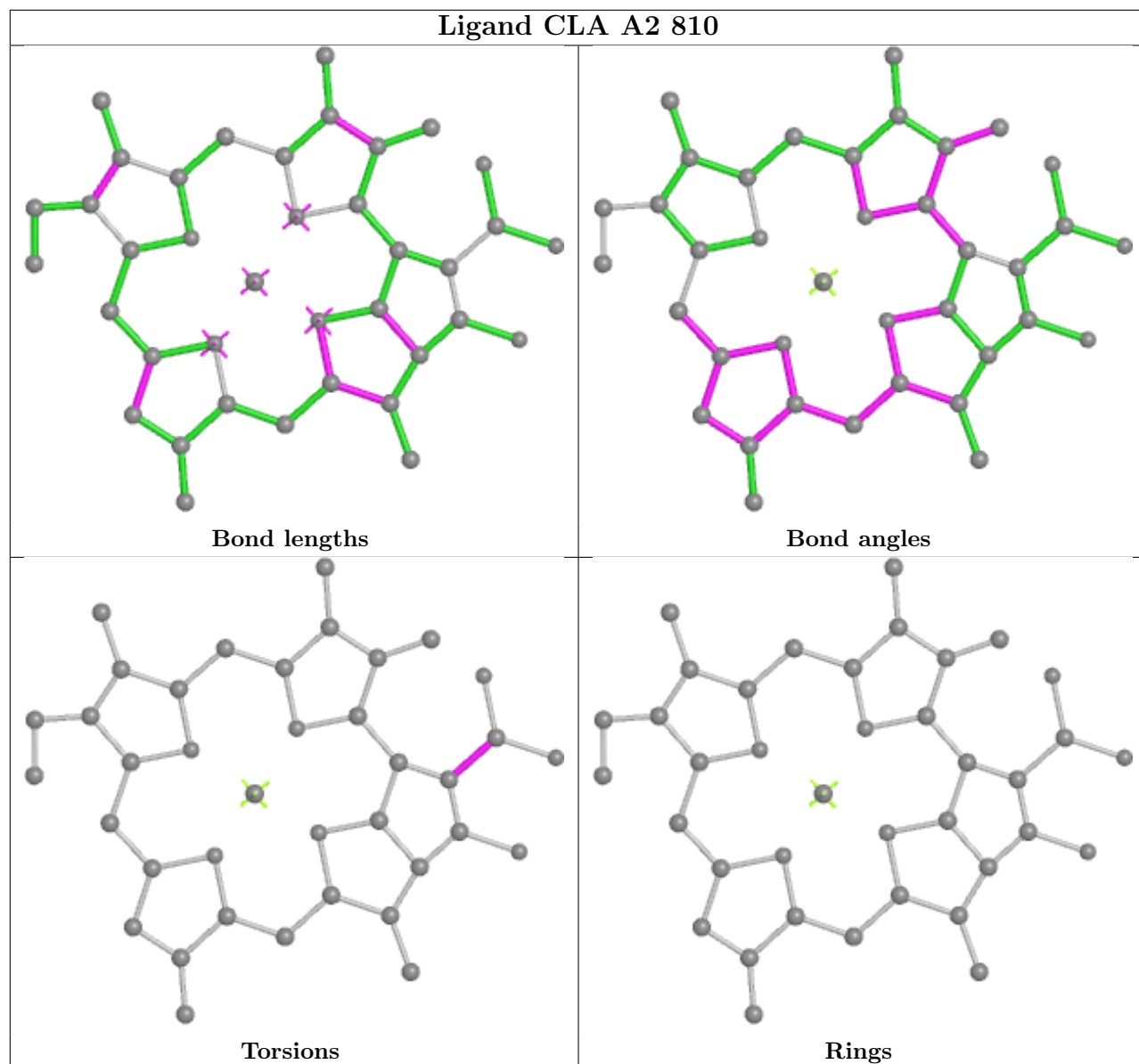


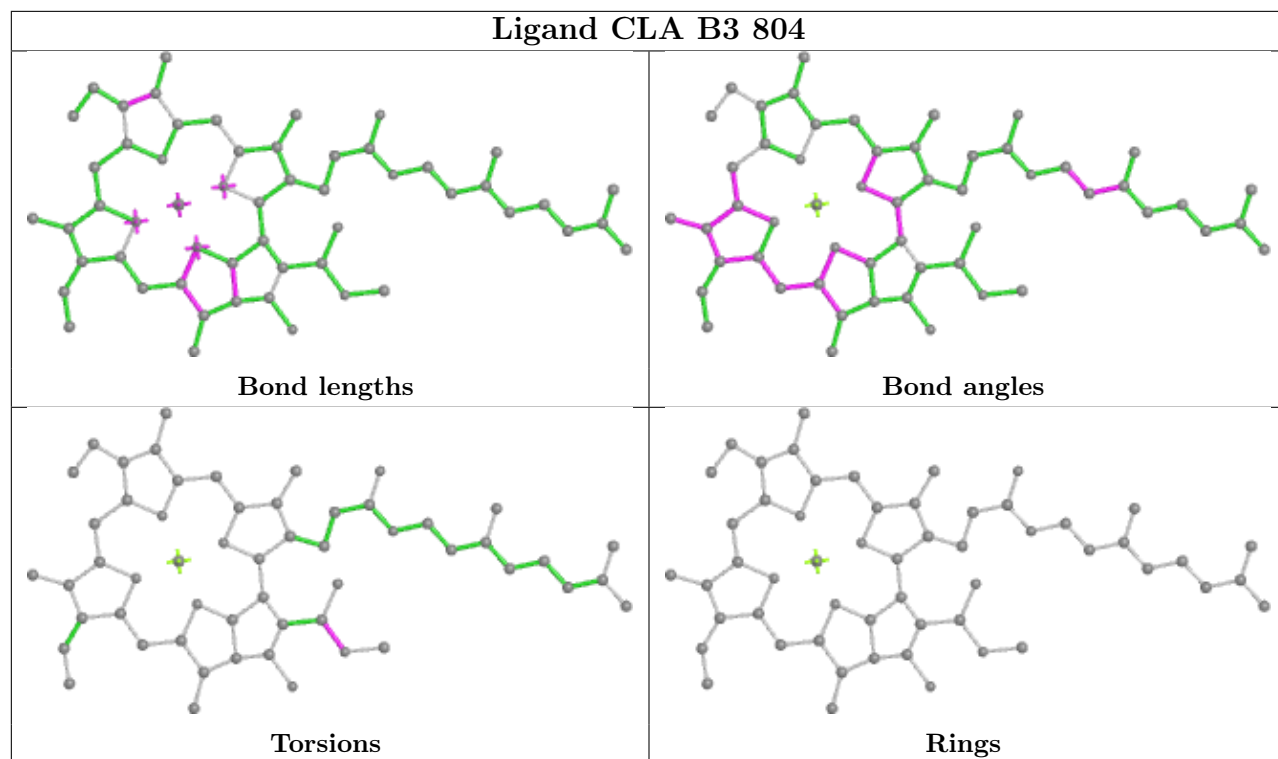
## Ligand CLA J2 1307



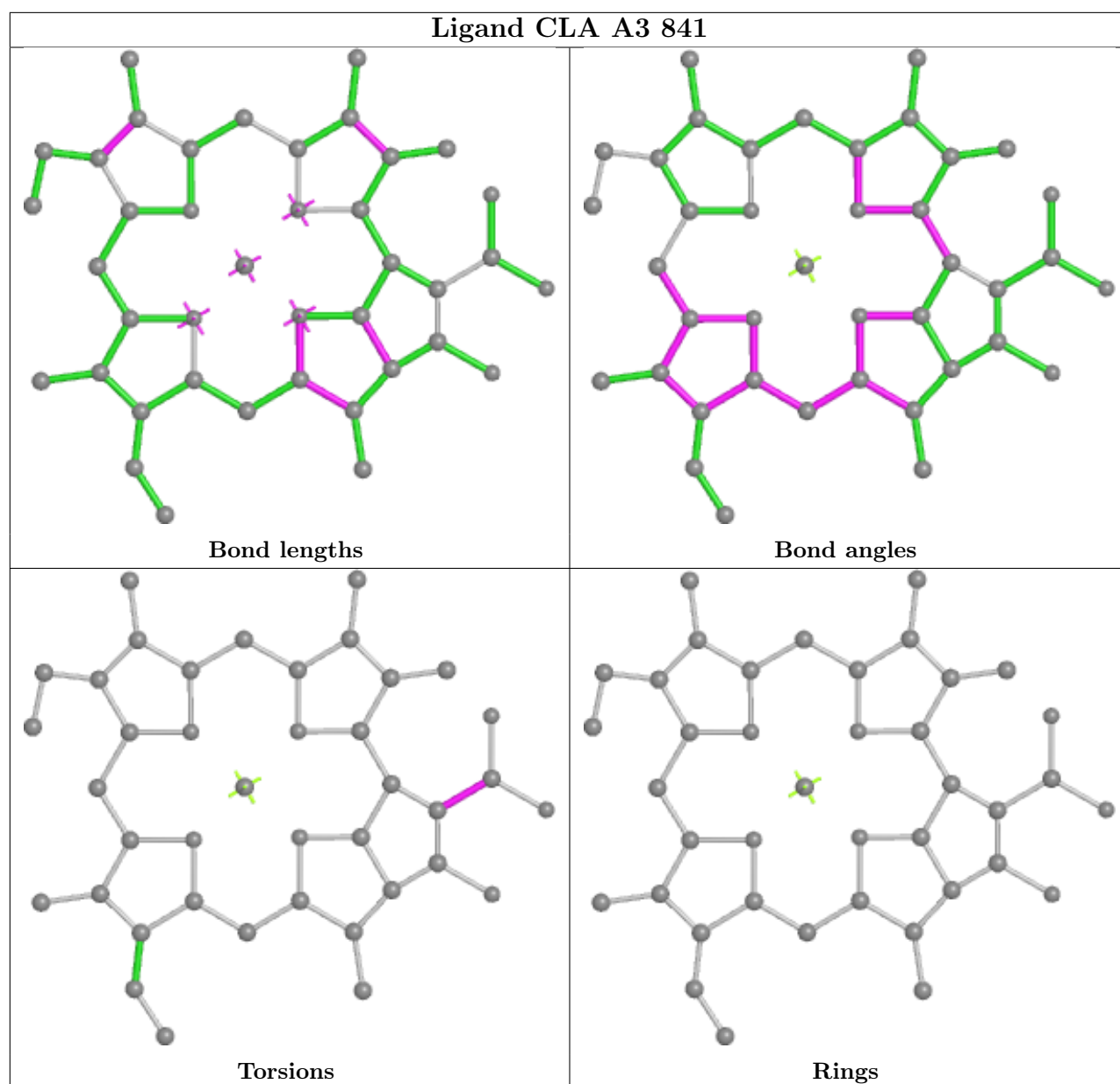
## Ligand BCR L3 1005



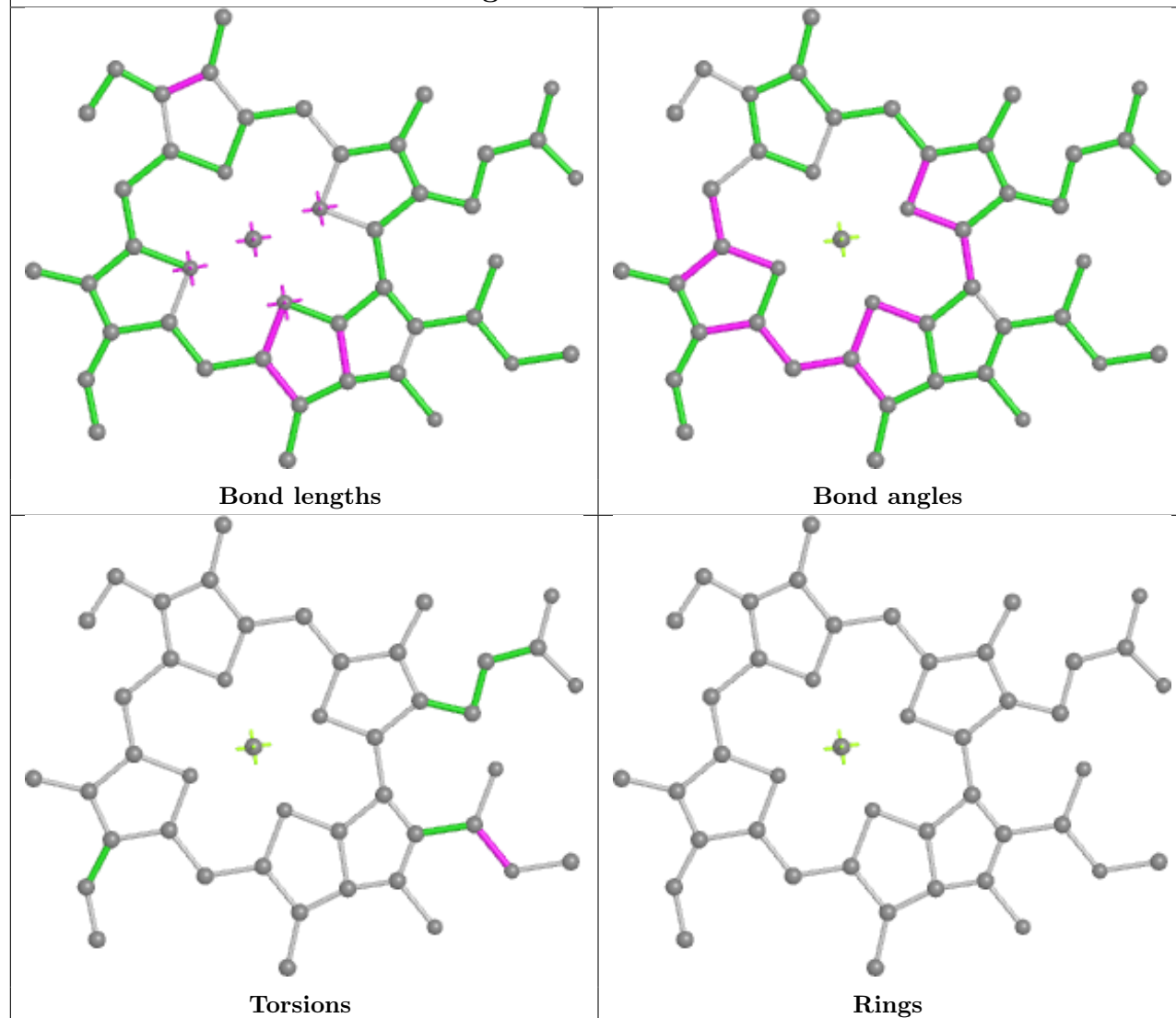




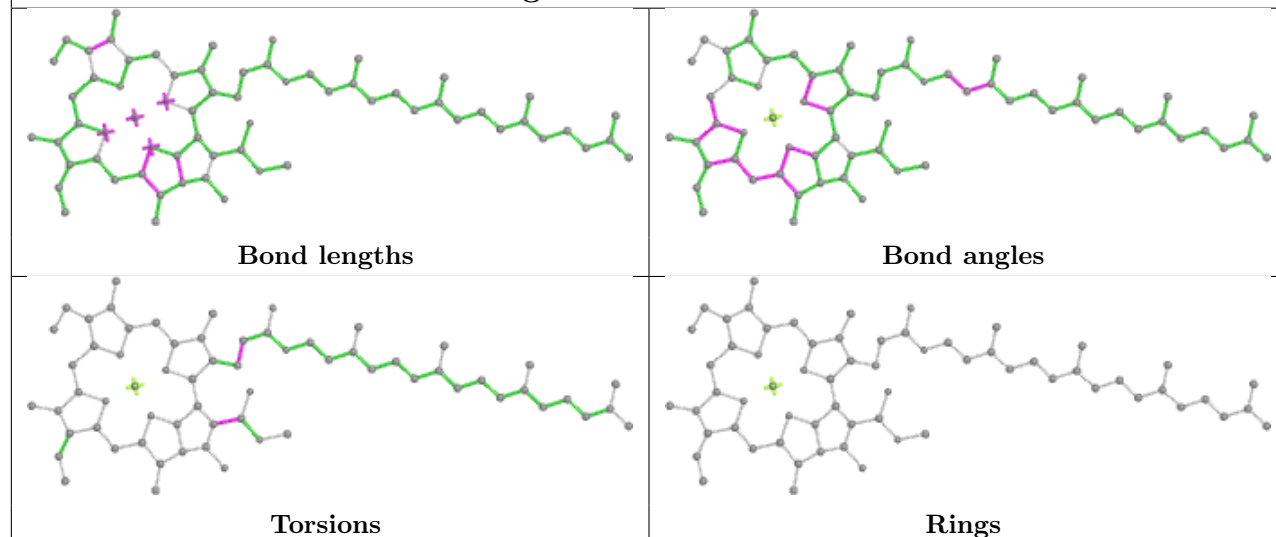


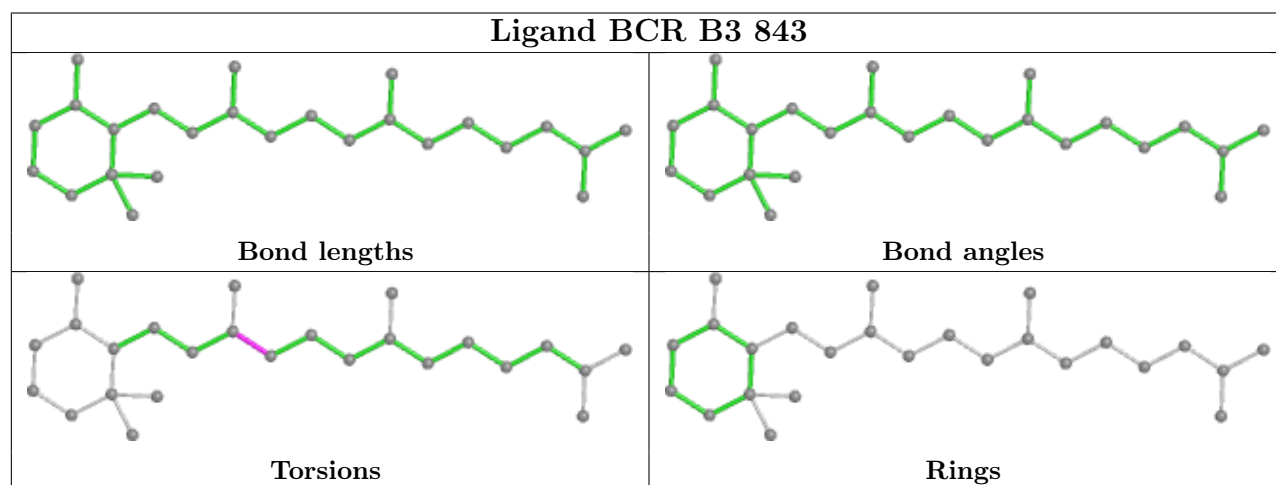
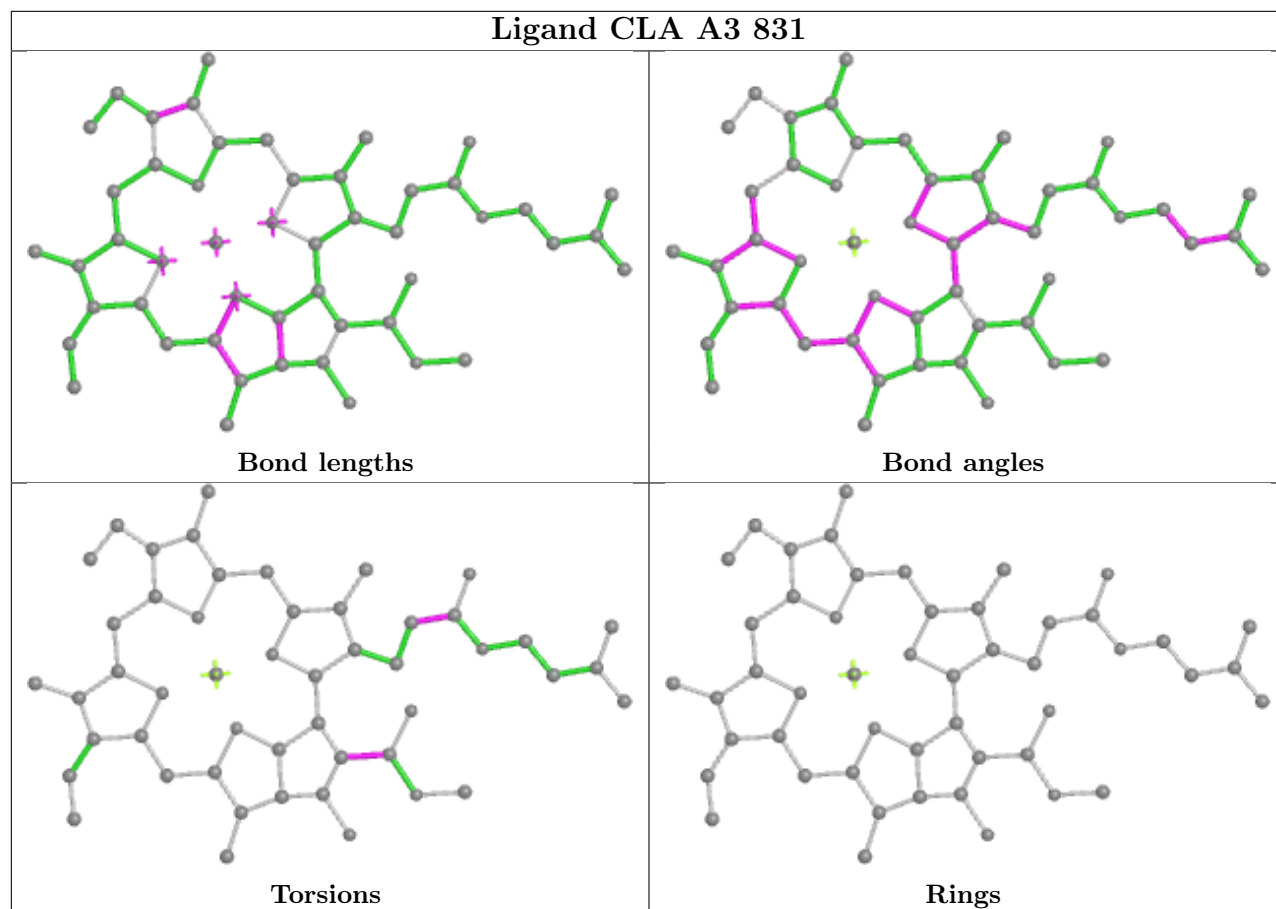
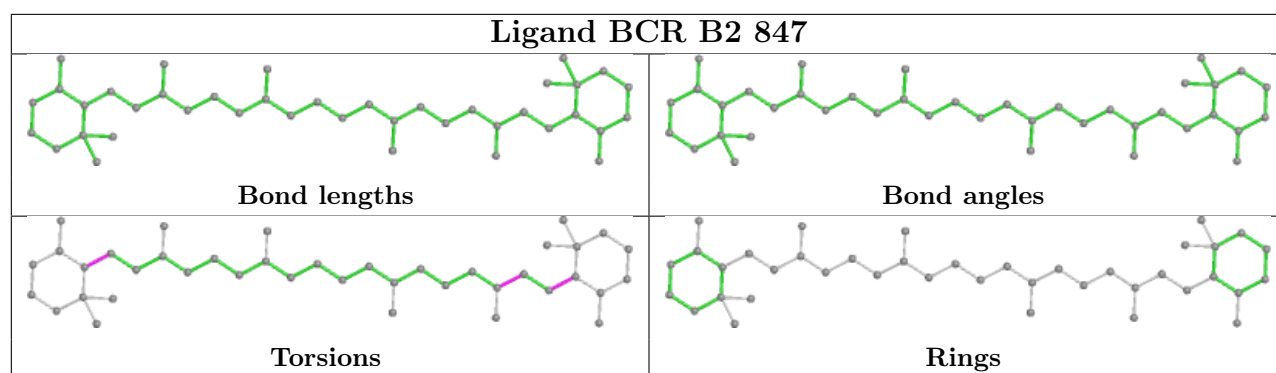


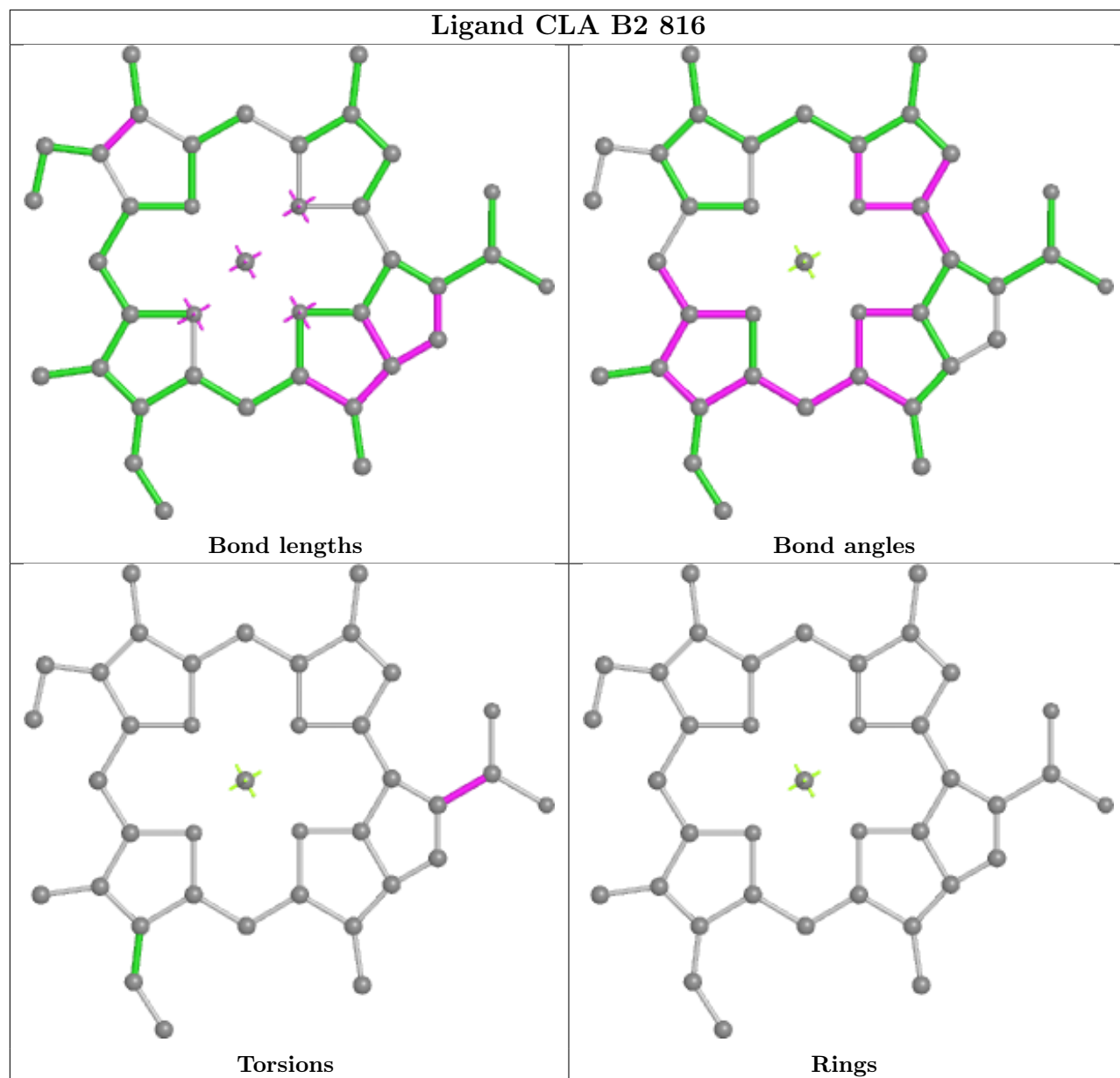
## Ligand CLA B3 824

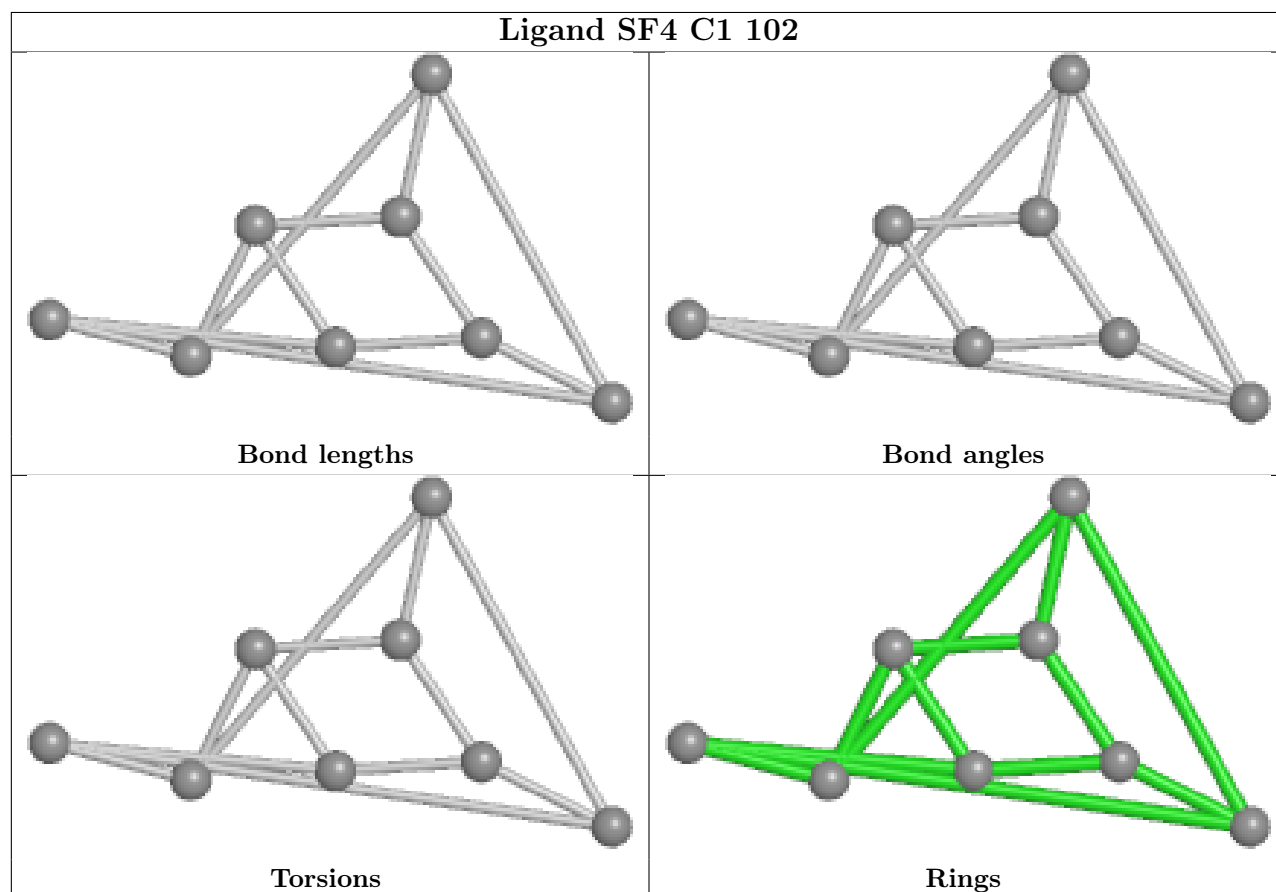
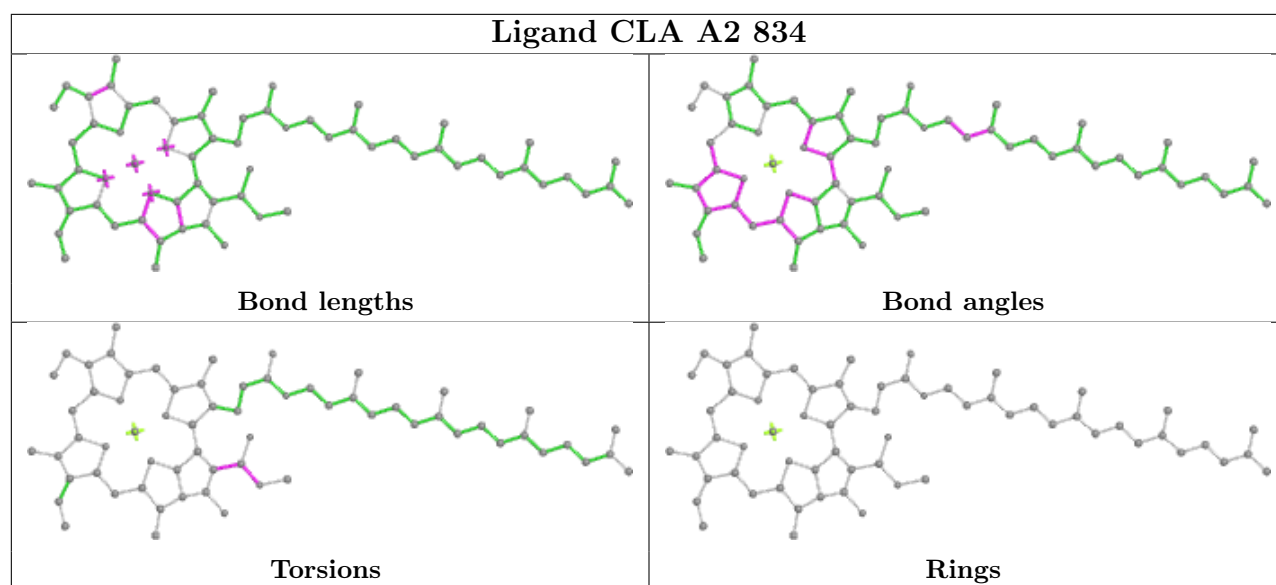


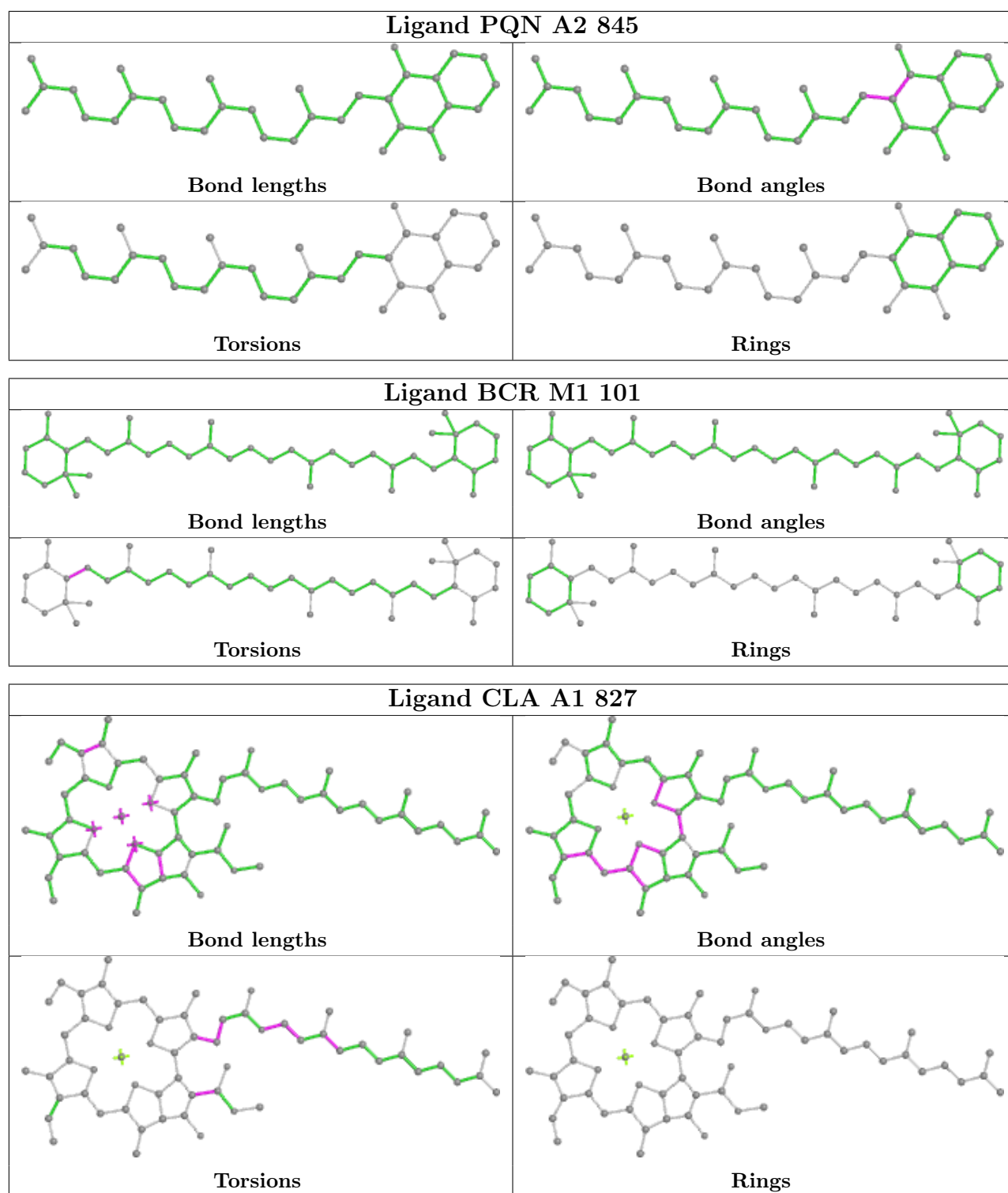
## Ligand CLA A1 805

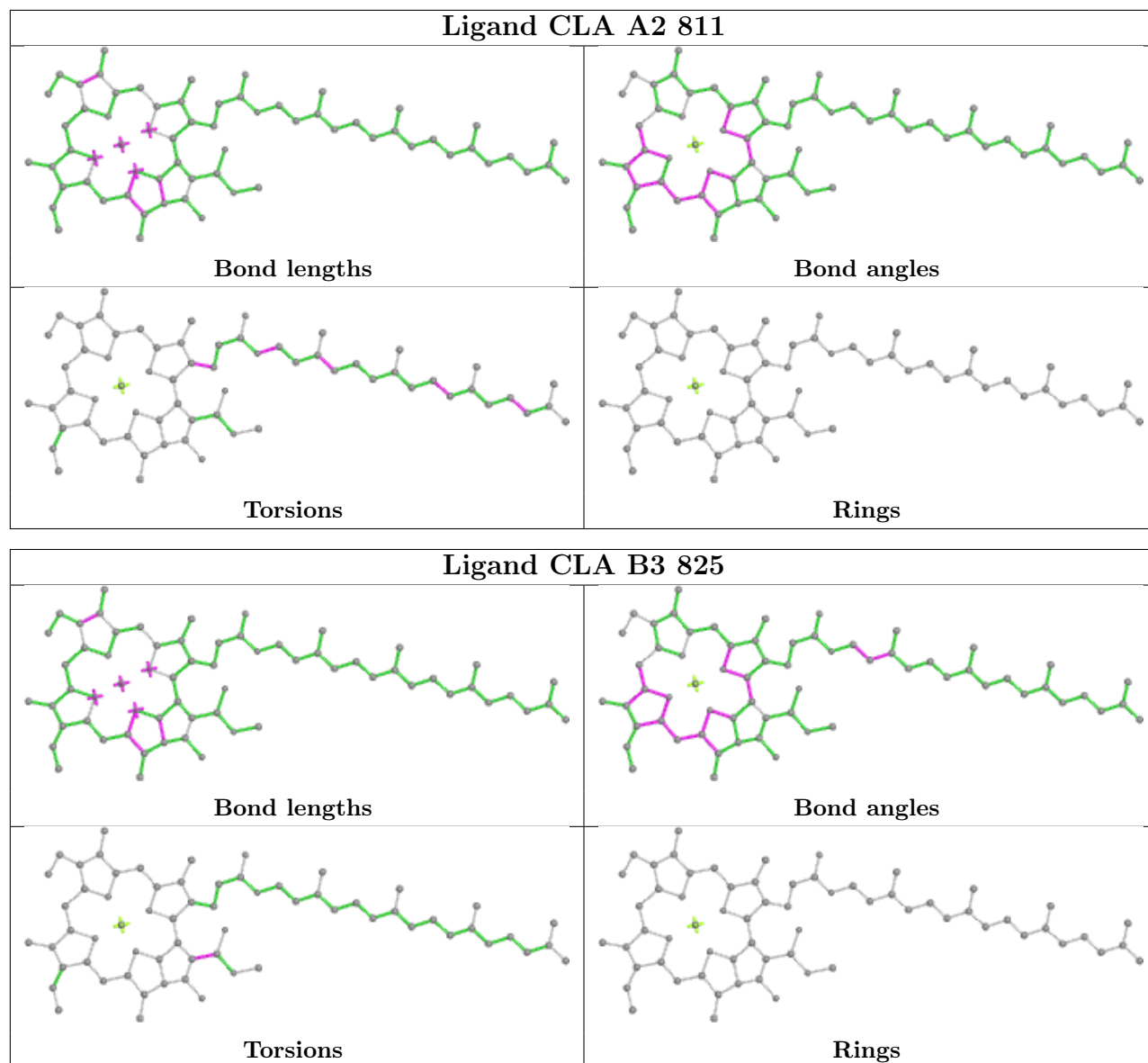


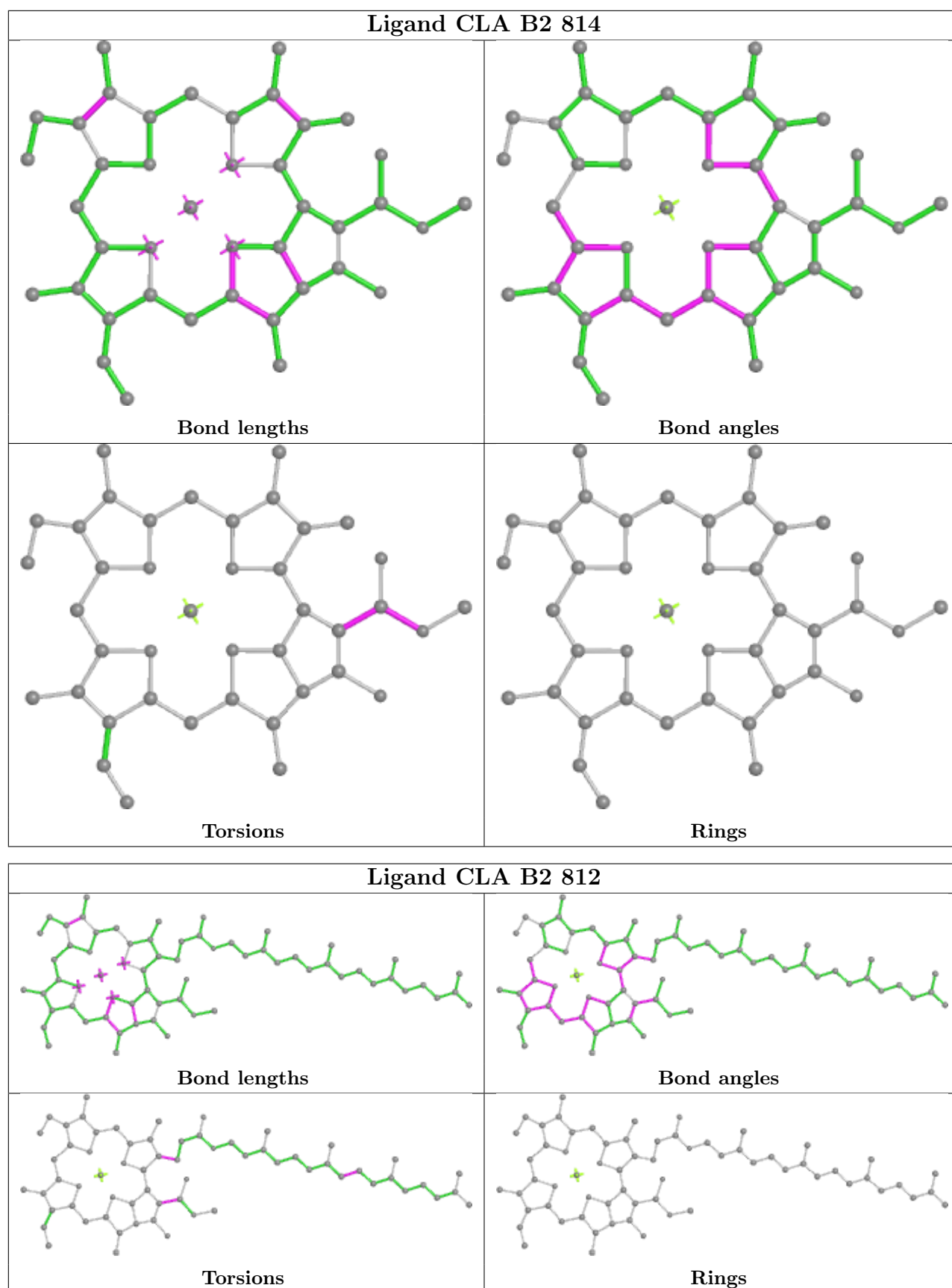




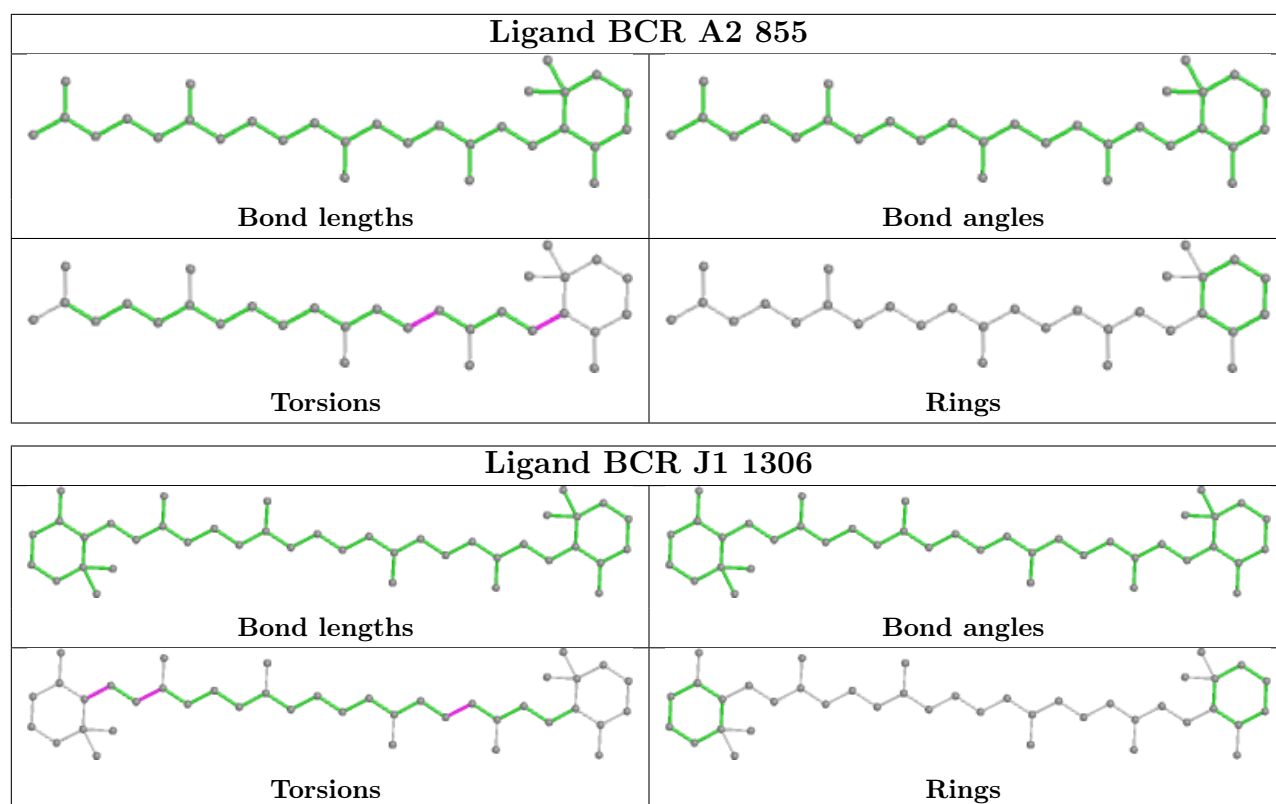


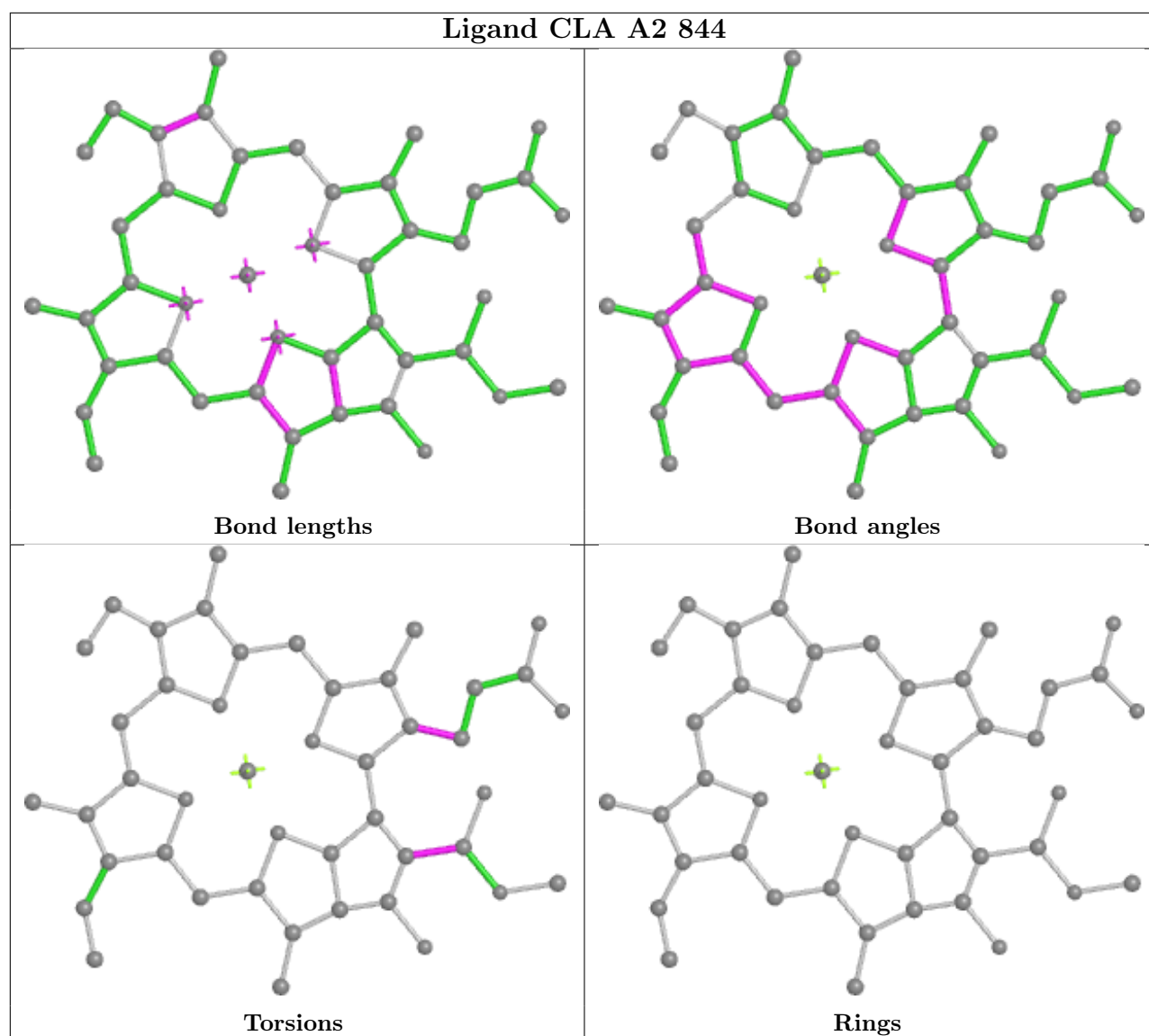


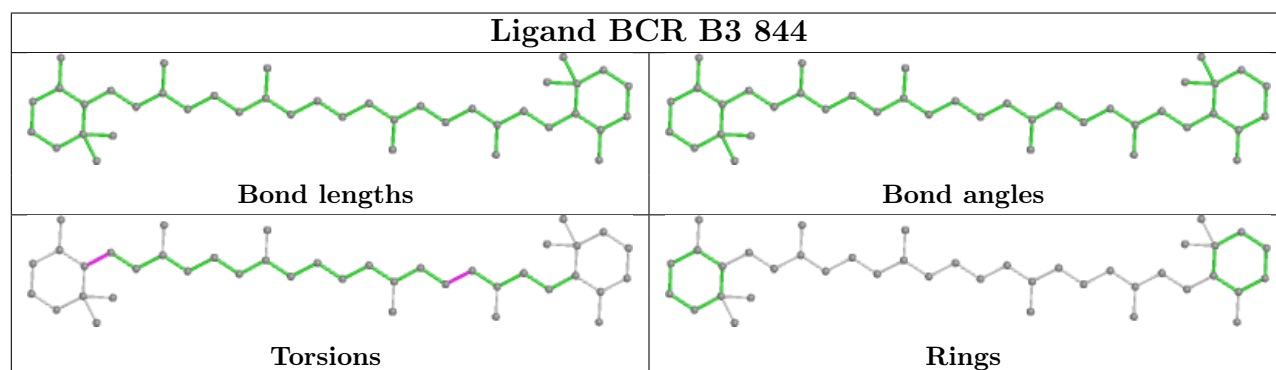
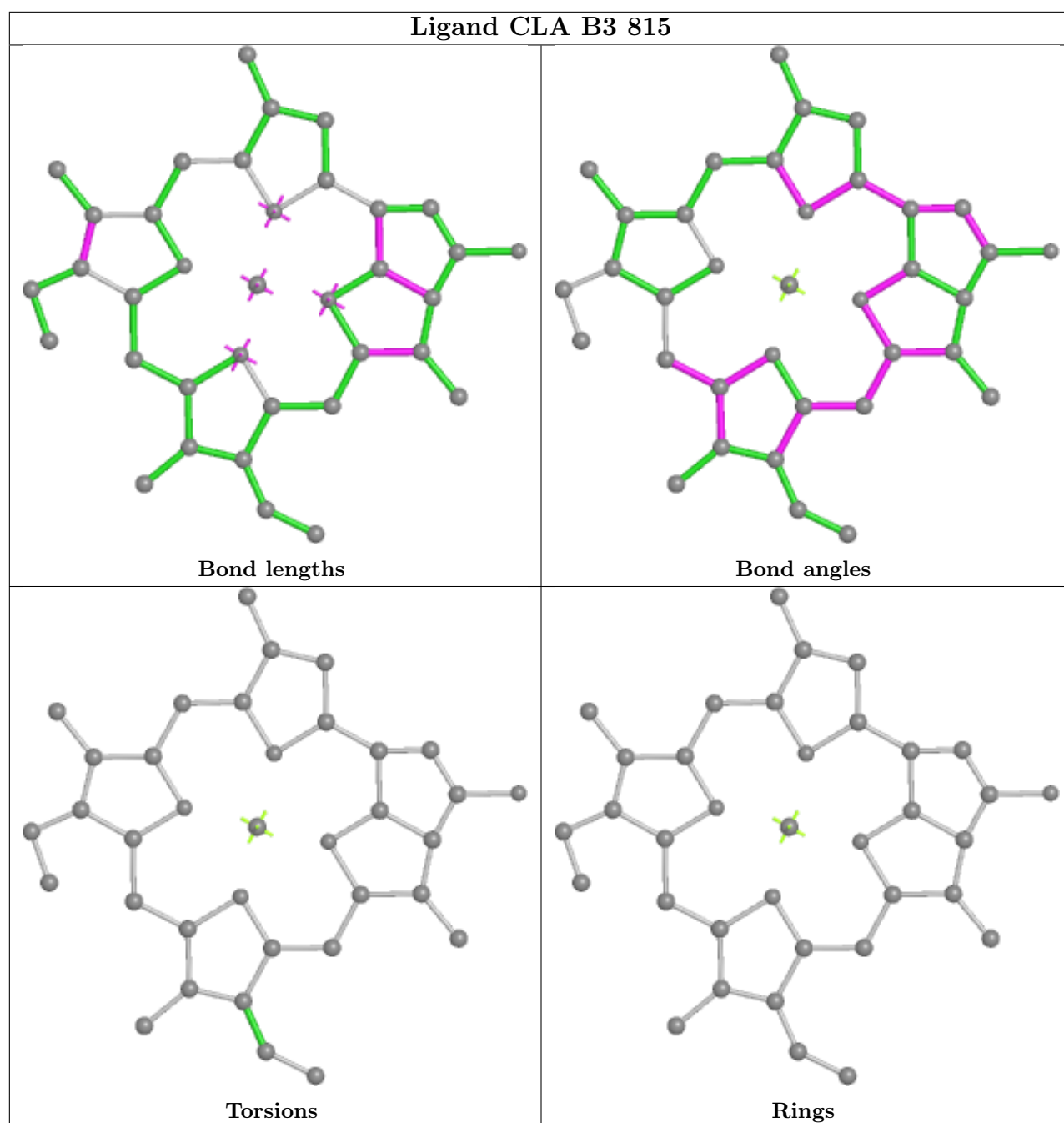


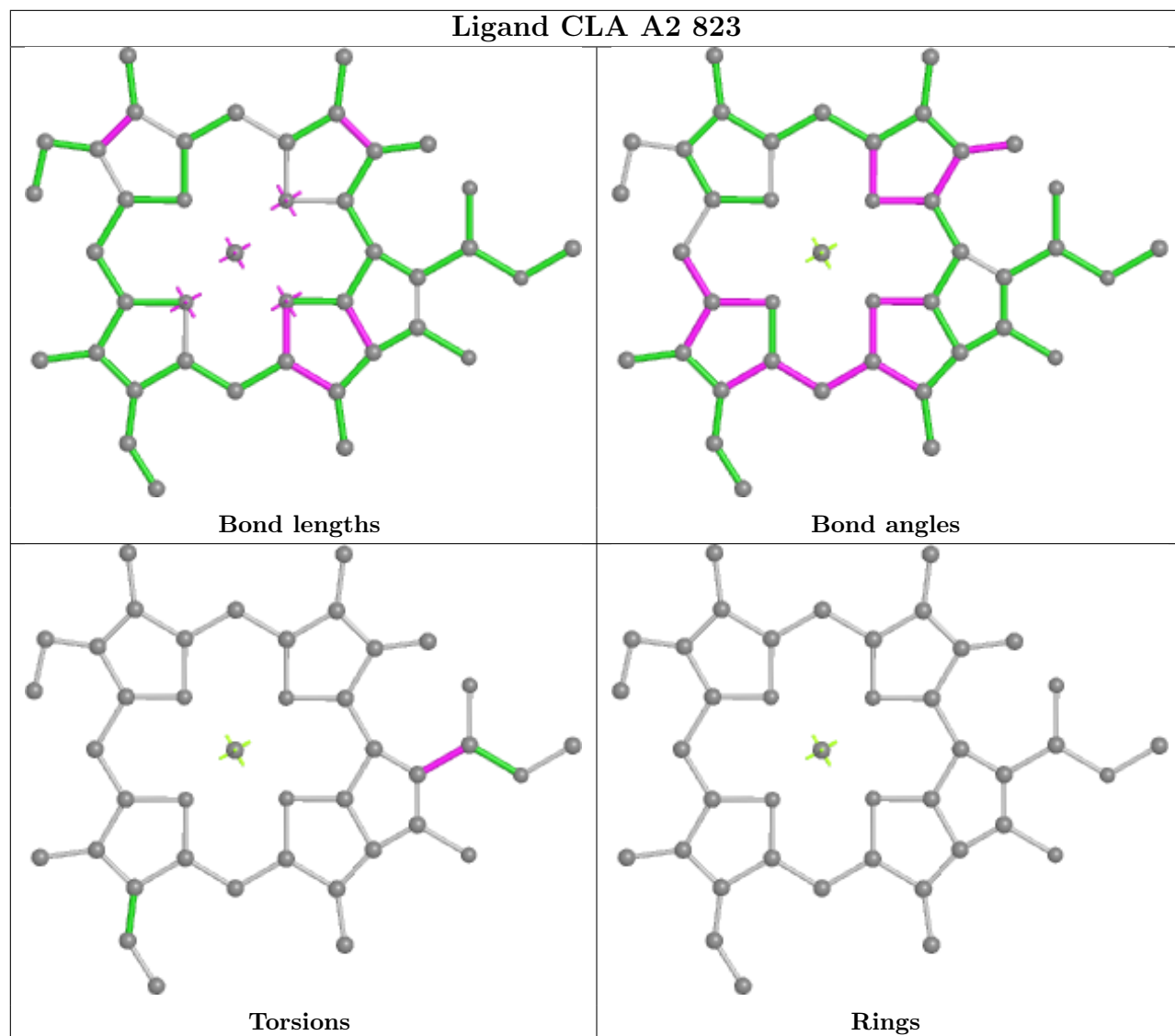


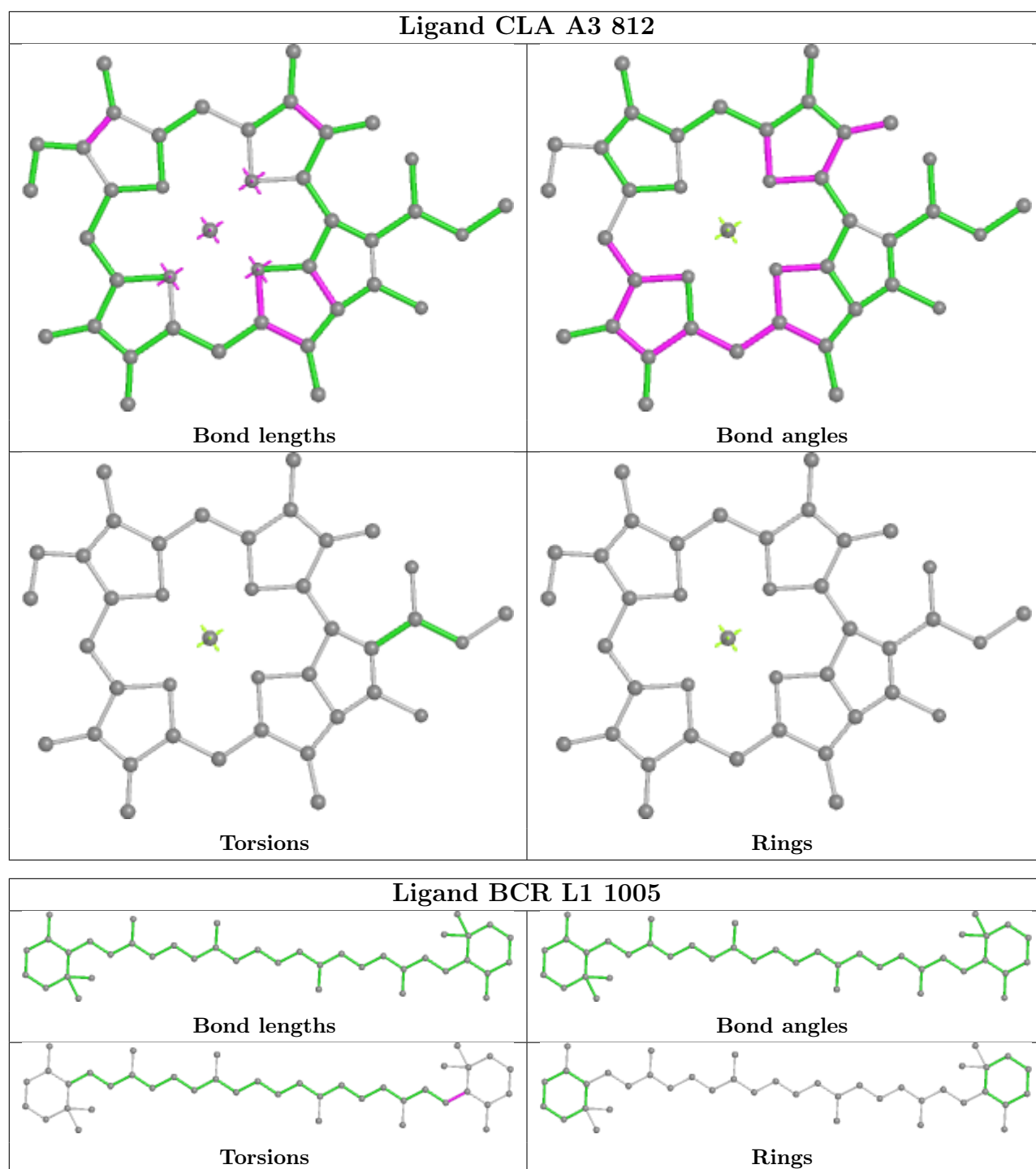




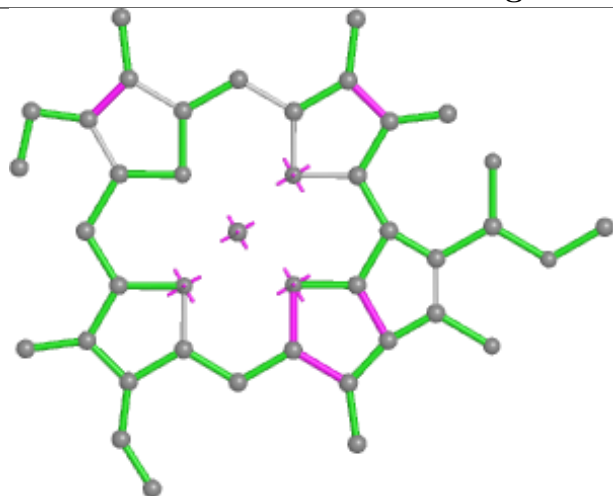




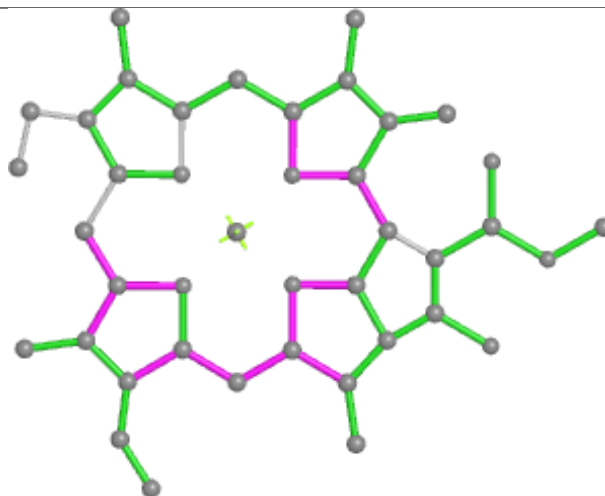




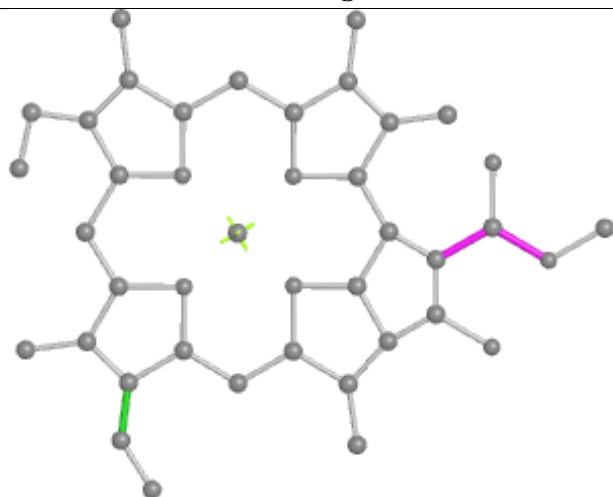
## Ligand CLA B2 830



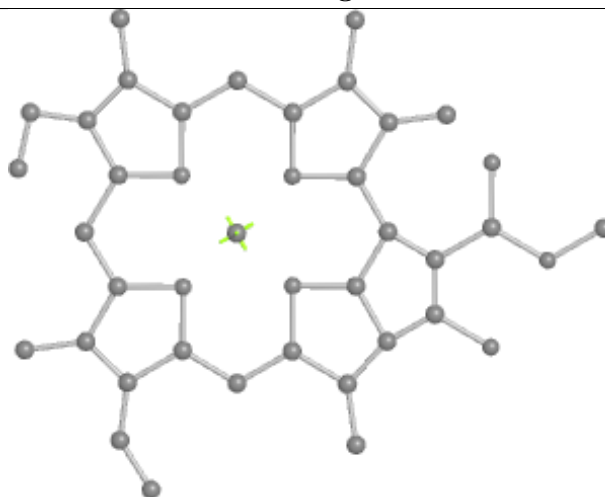
Bond lengths



Bond angles

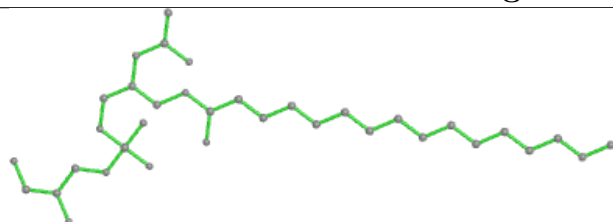


Torsions

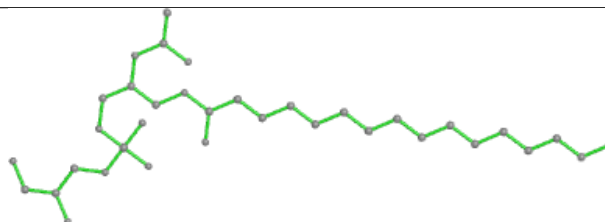


Rings

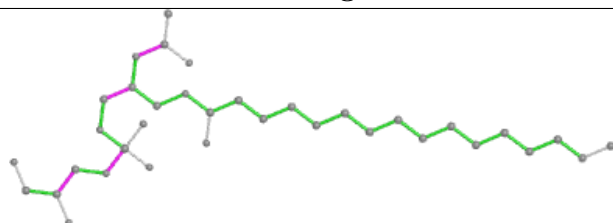
## Ligand LHG A1 854



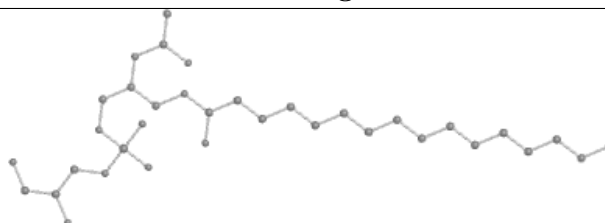
Bond lengths



Bond angles

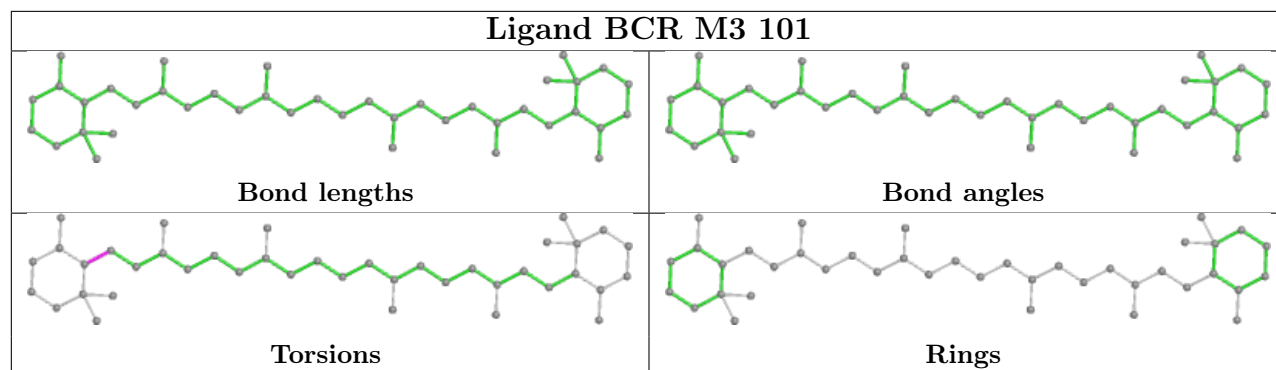


Torsions

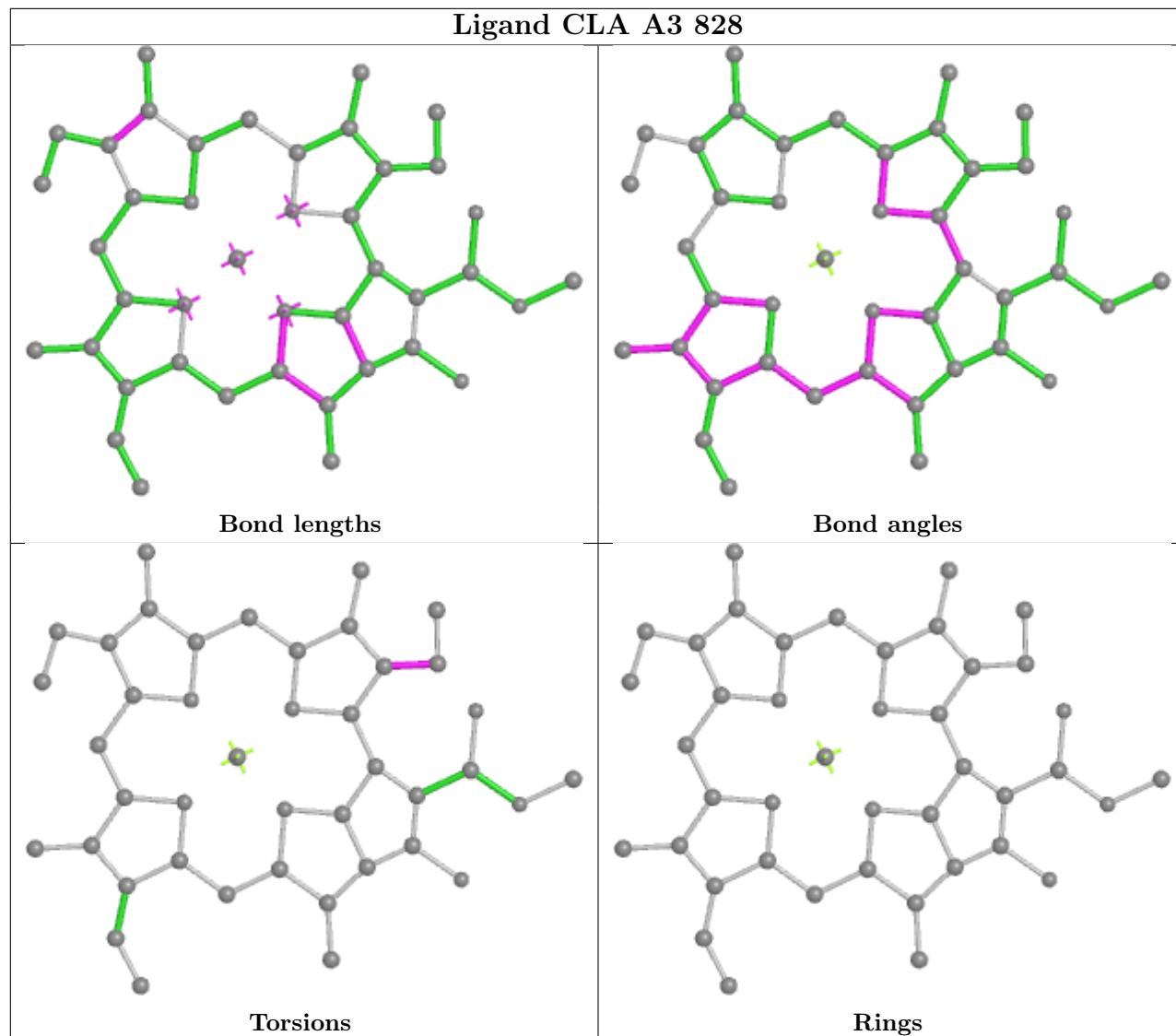


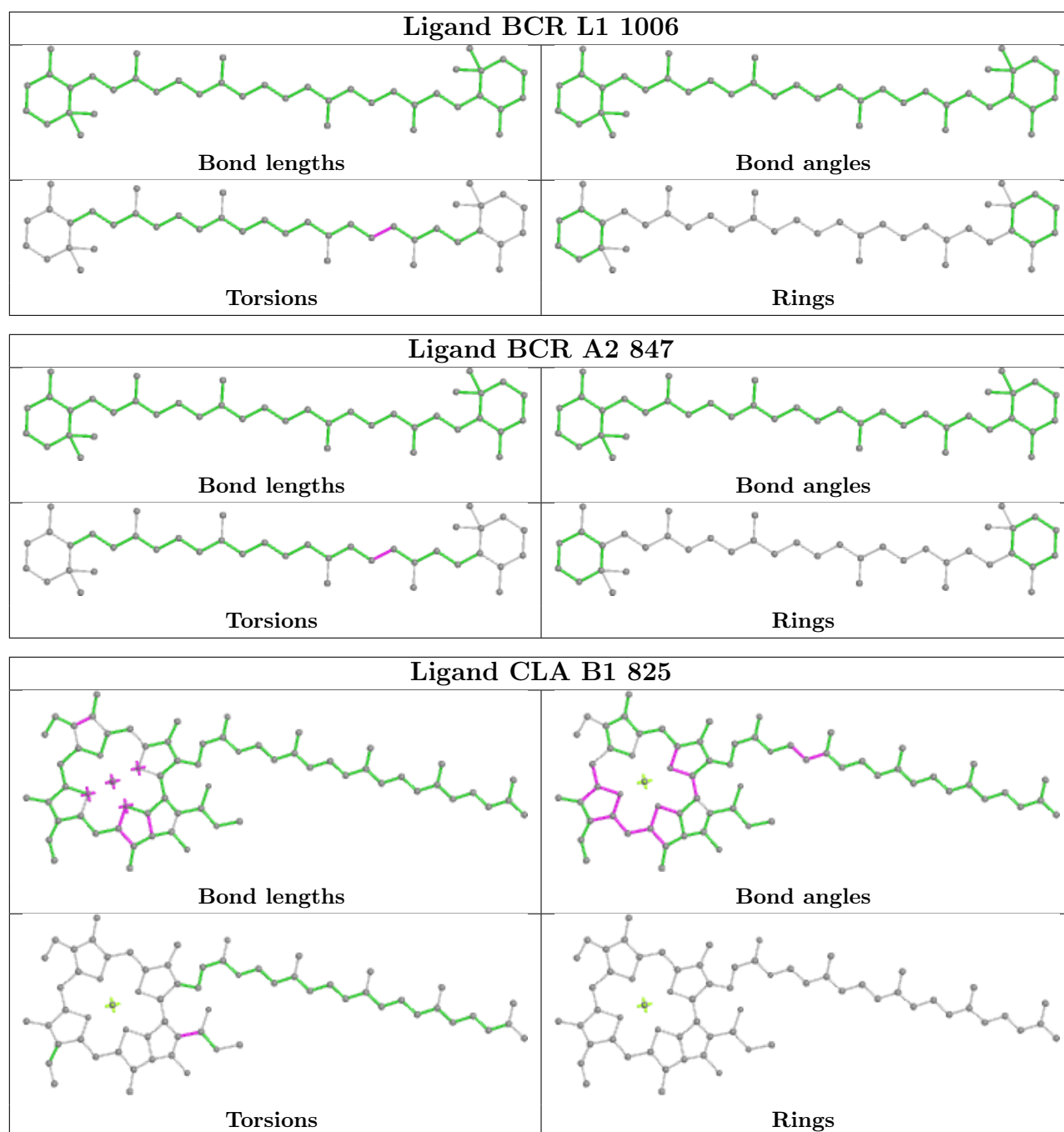
Rings

## Ligand BCR M3 101

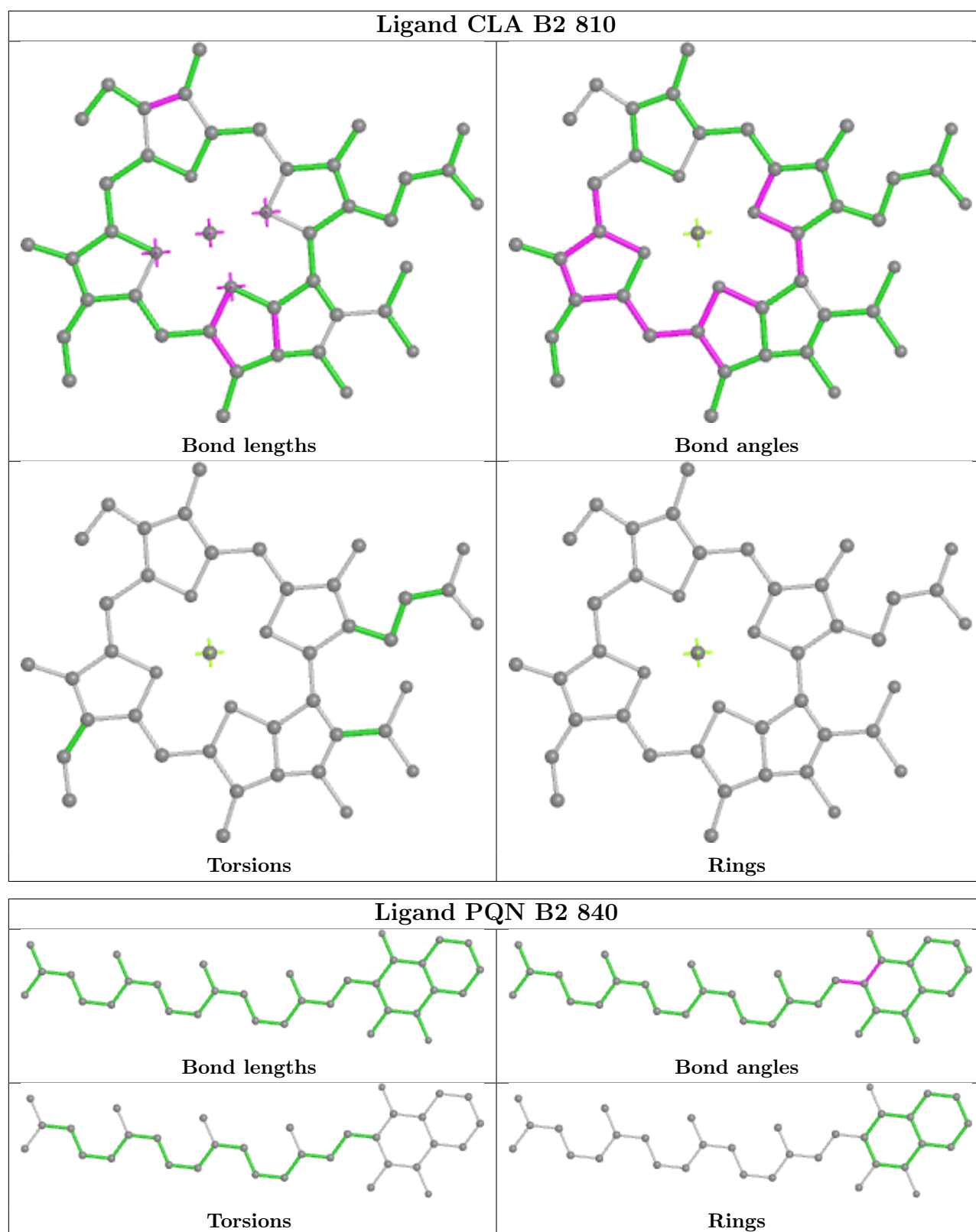


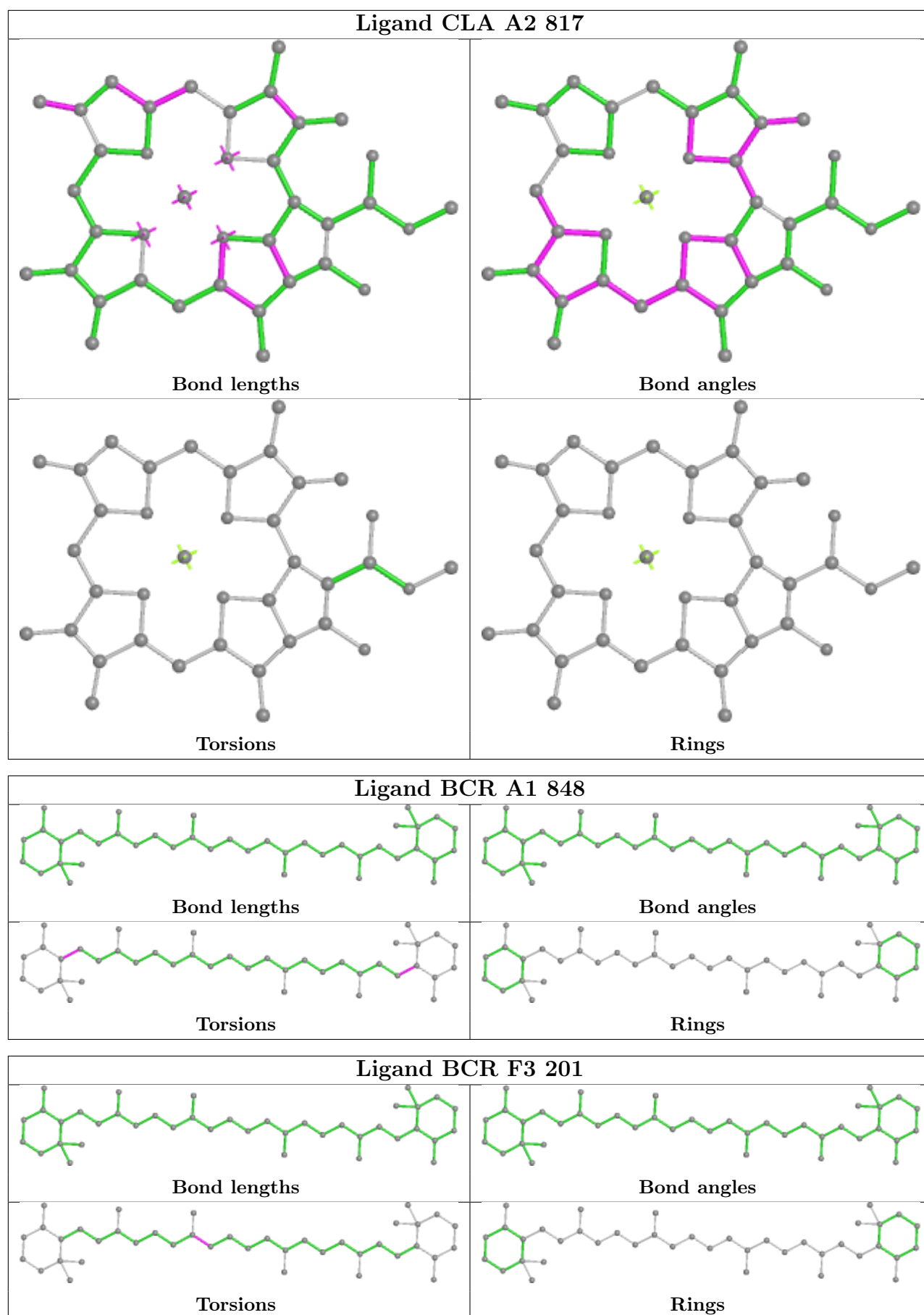
## Ligand CLA A3 828

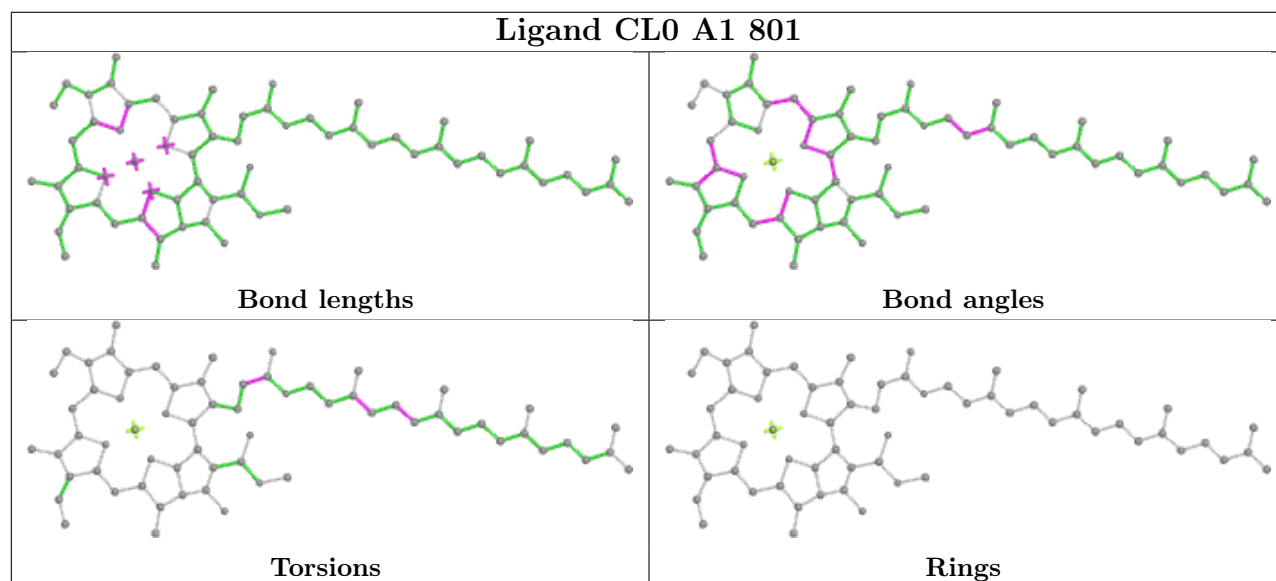
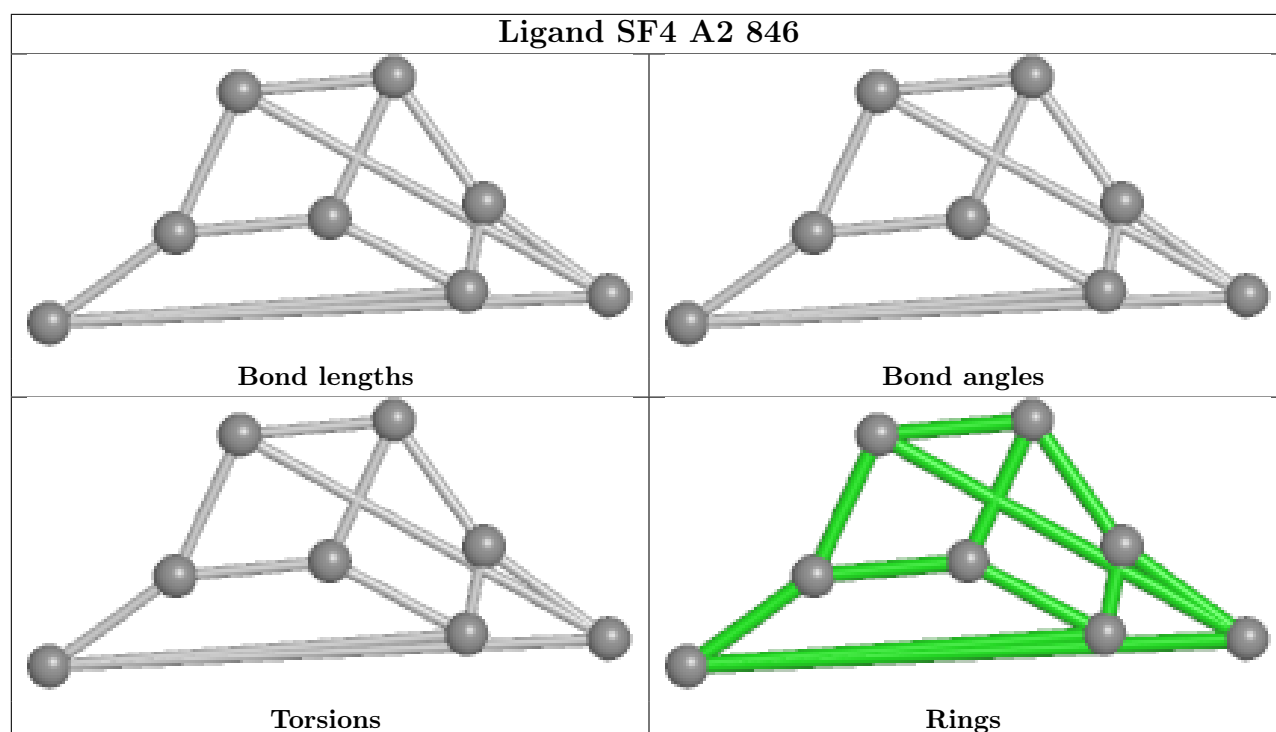


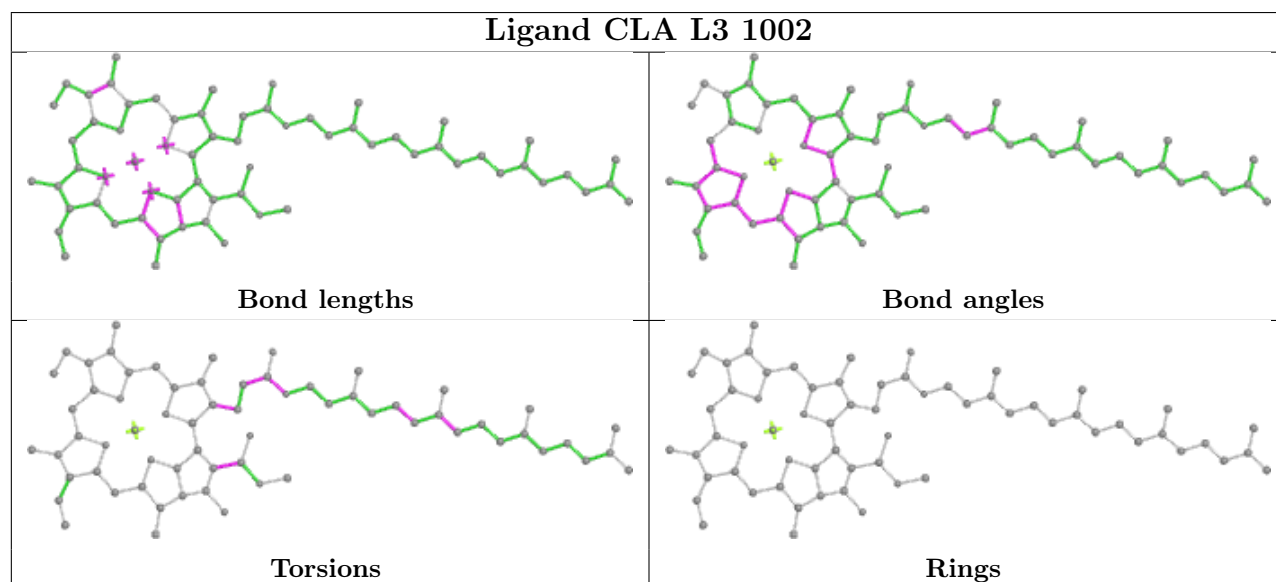
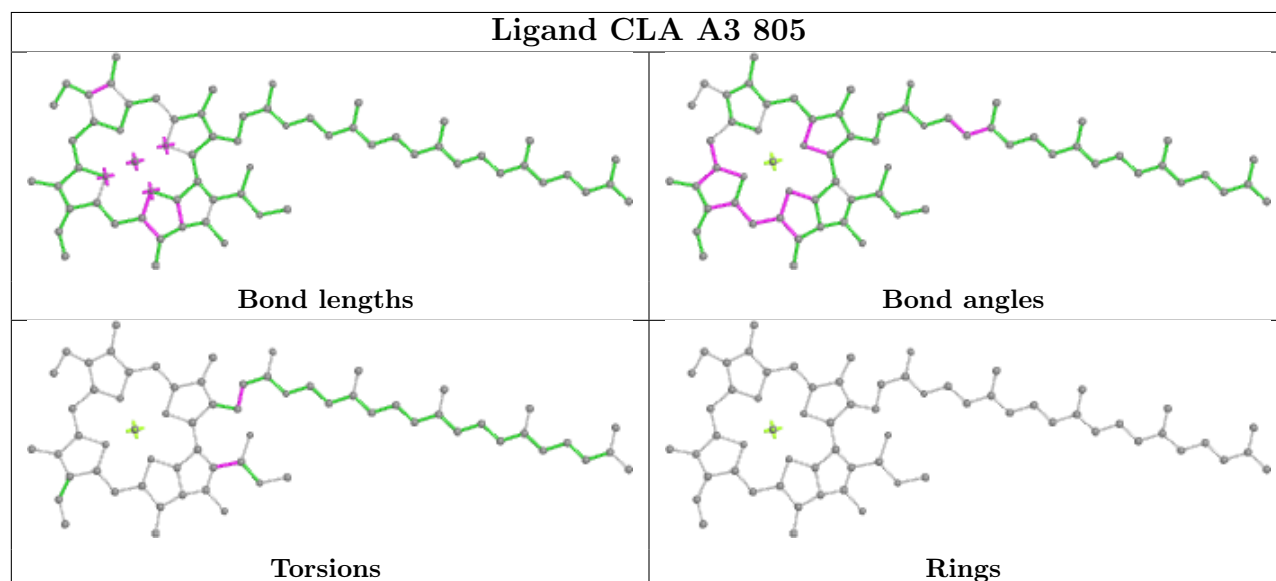
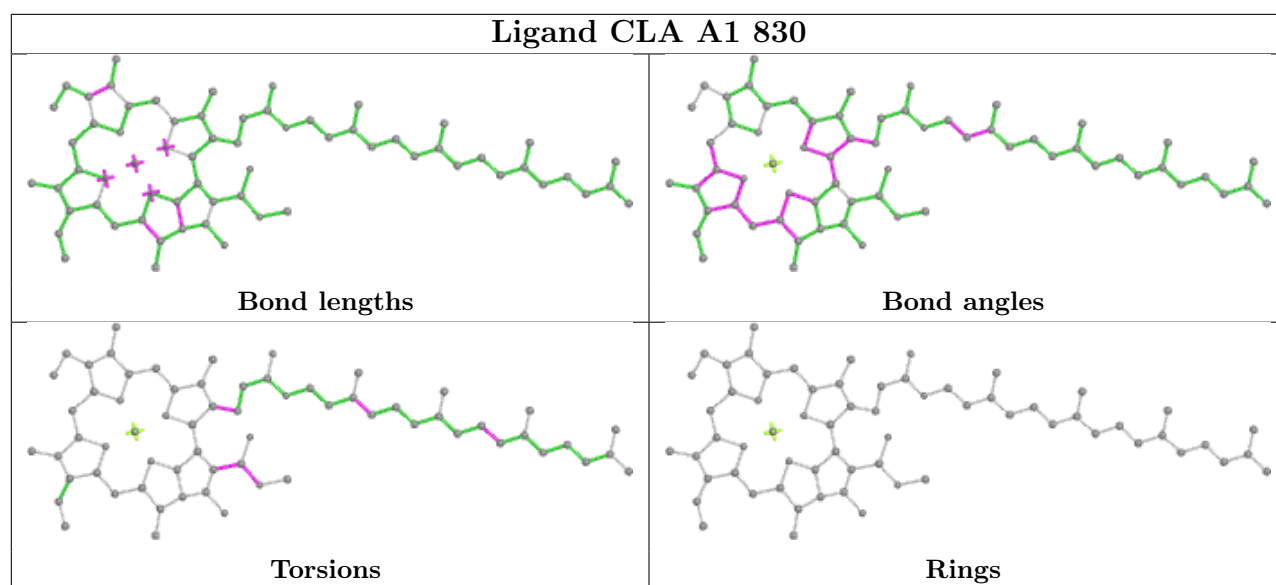


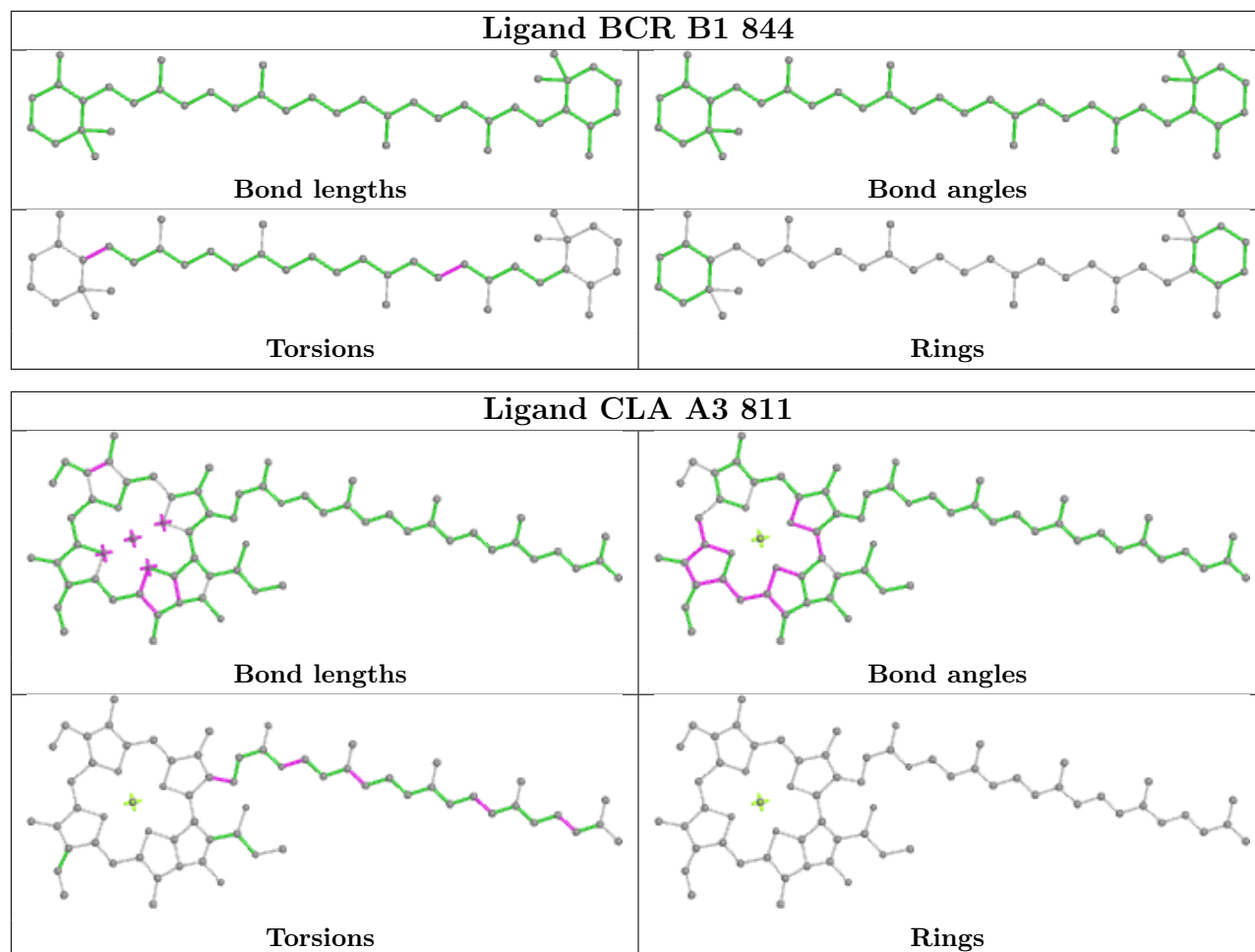


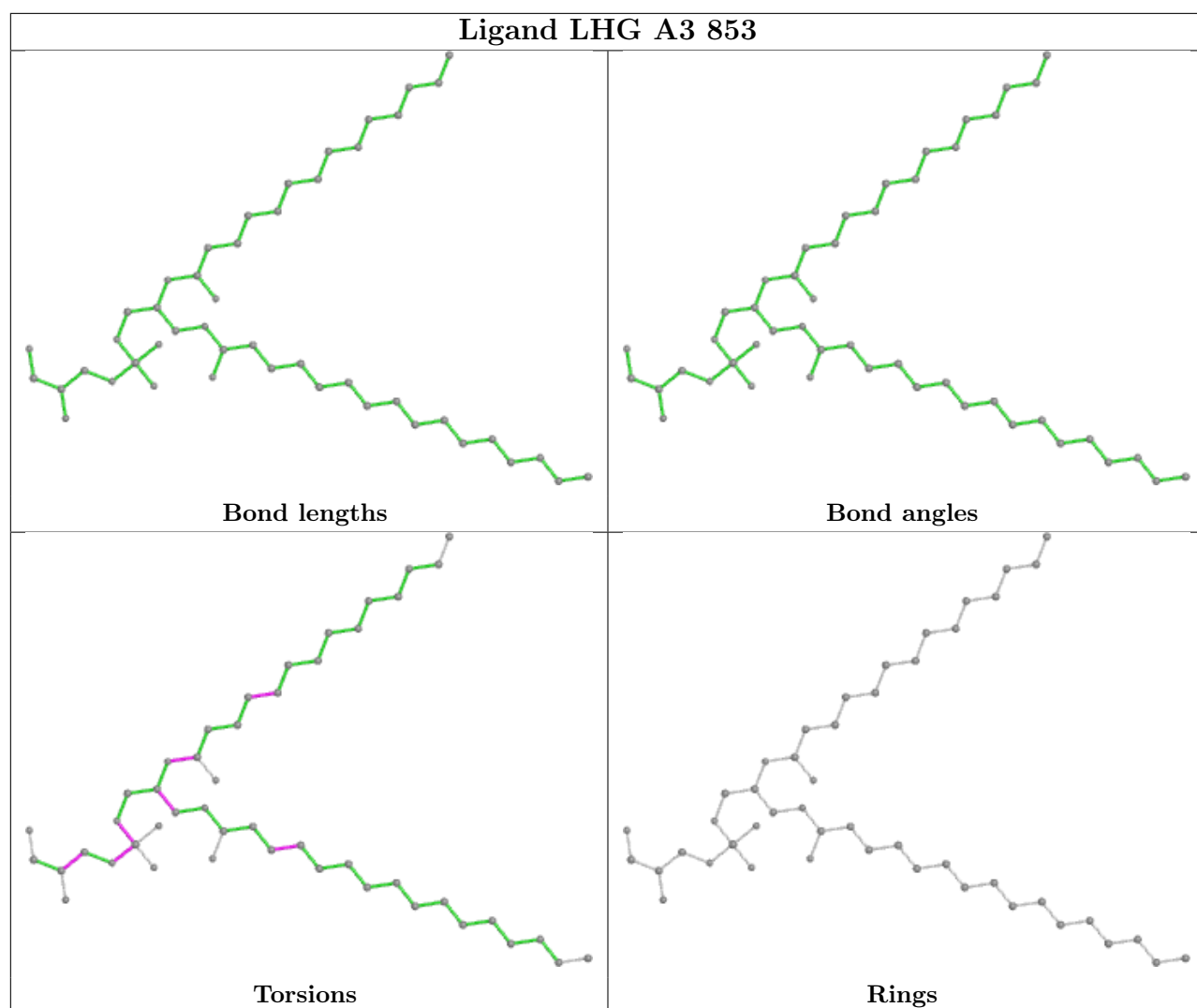


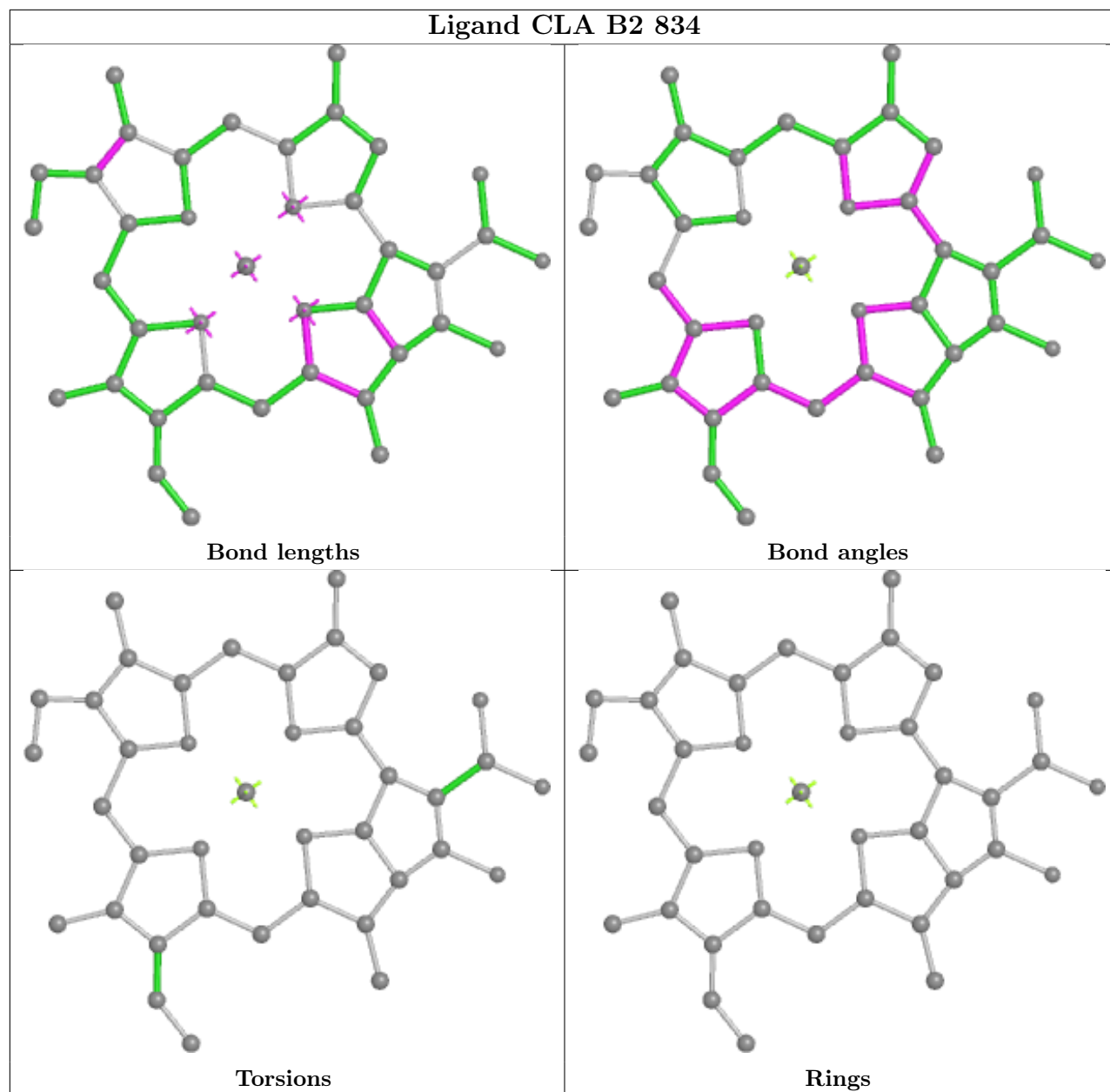


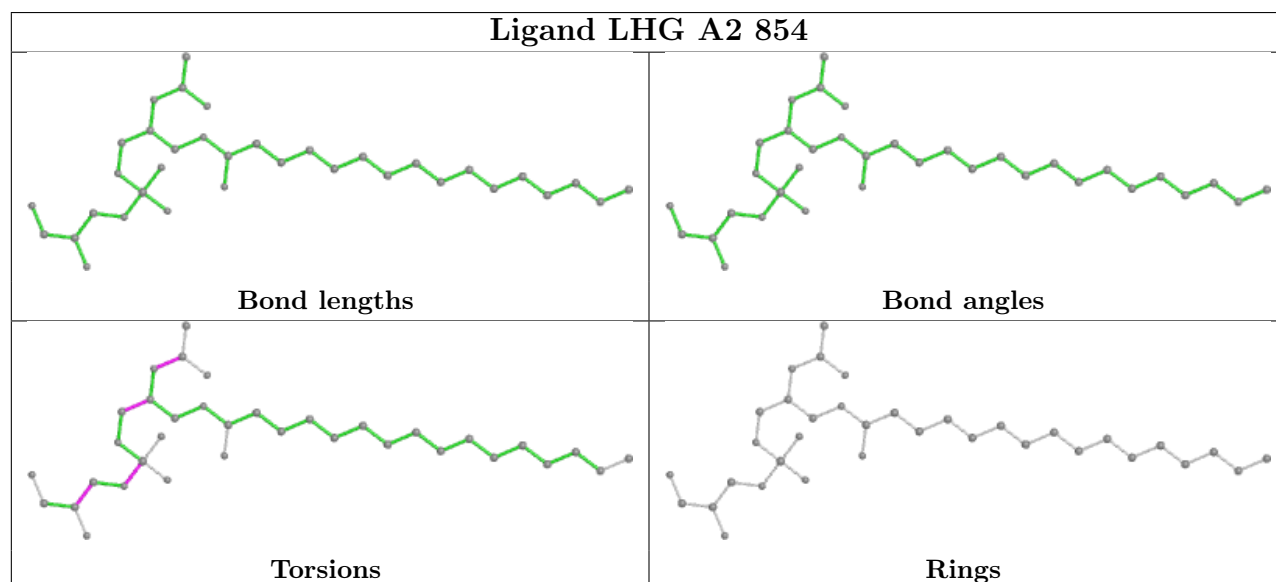
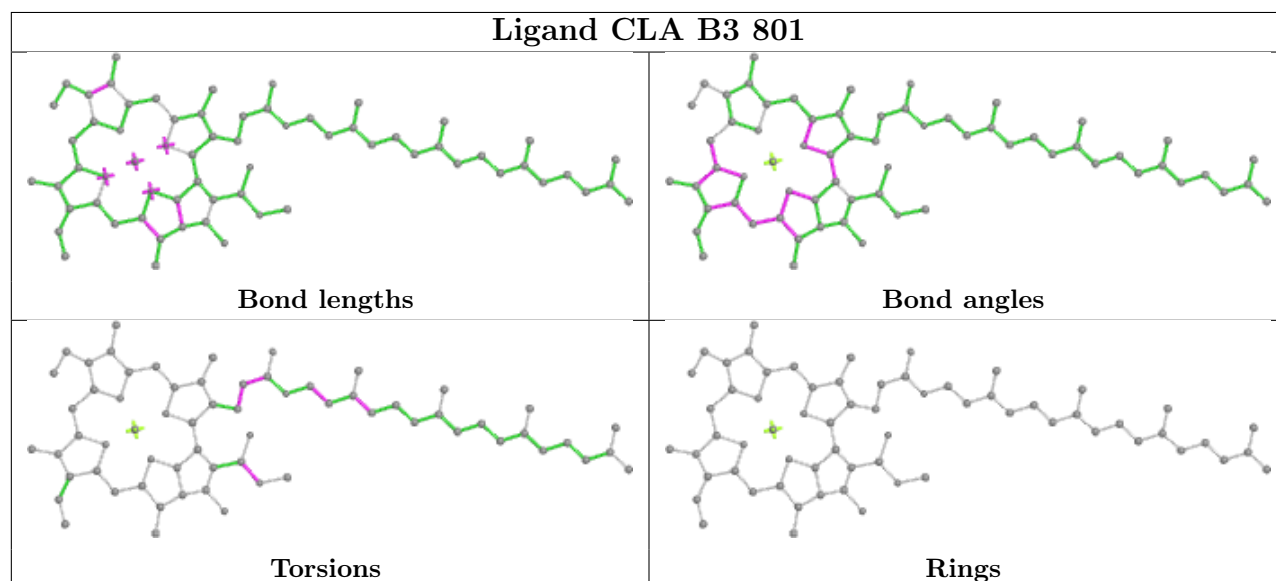
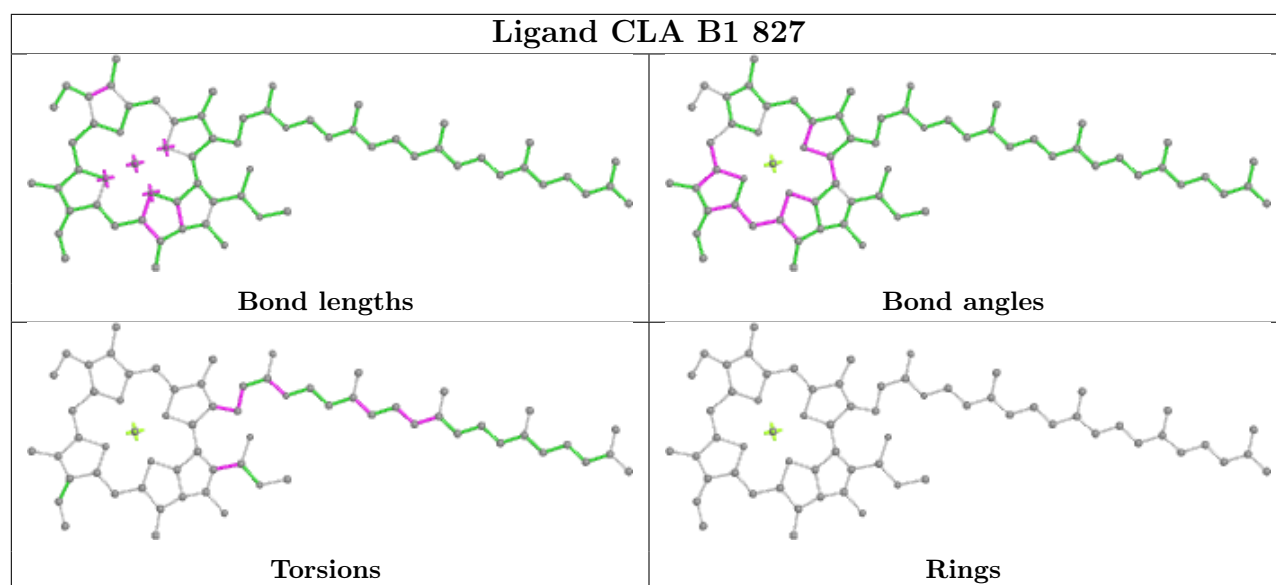




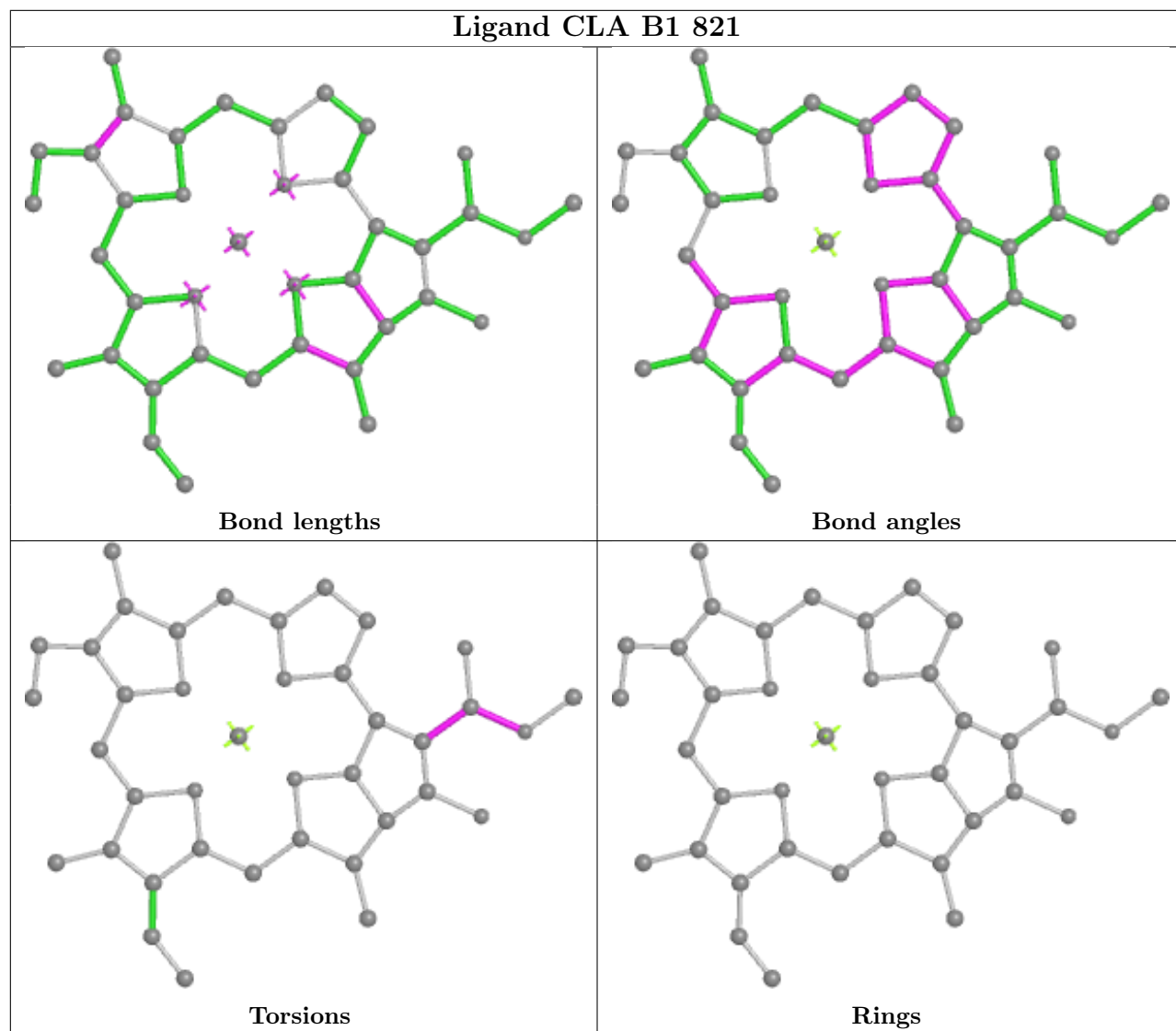
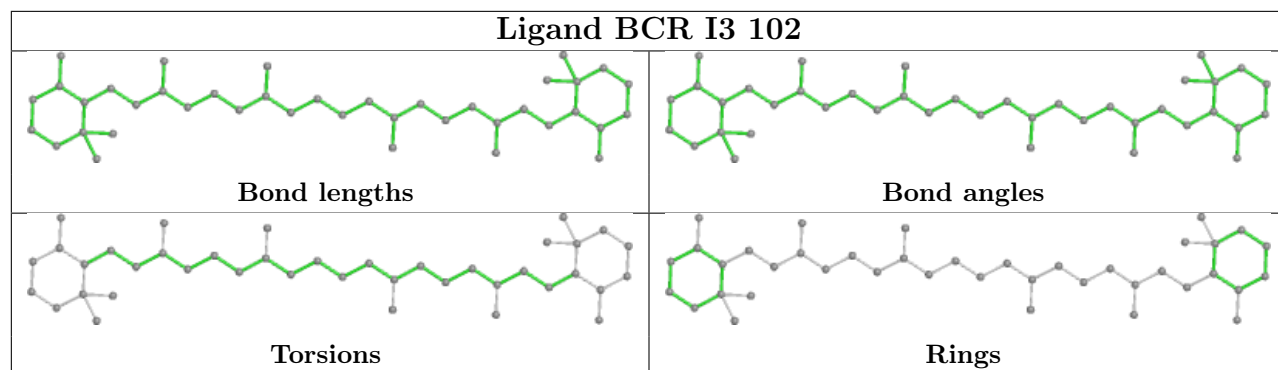




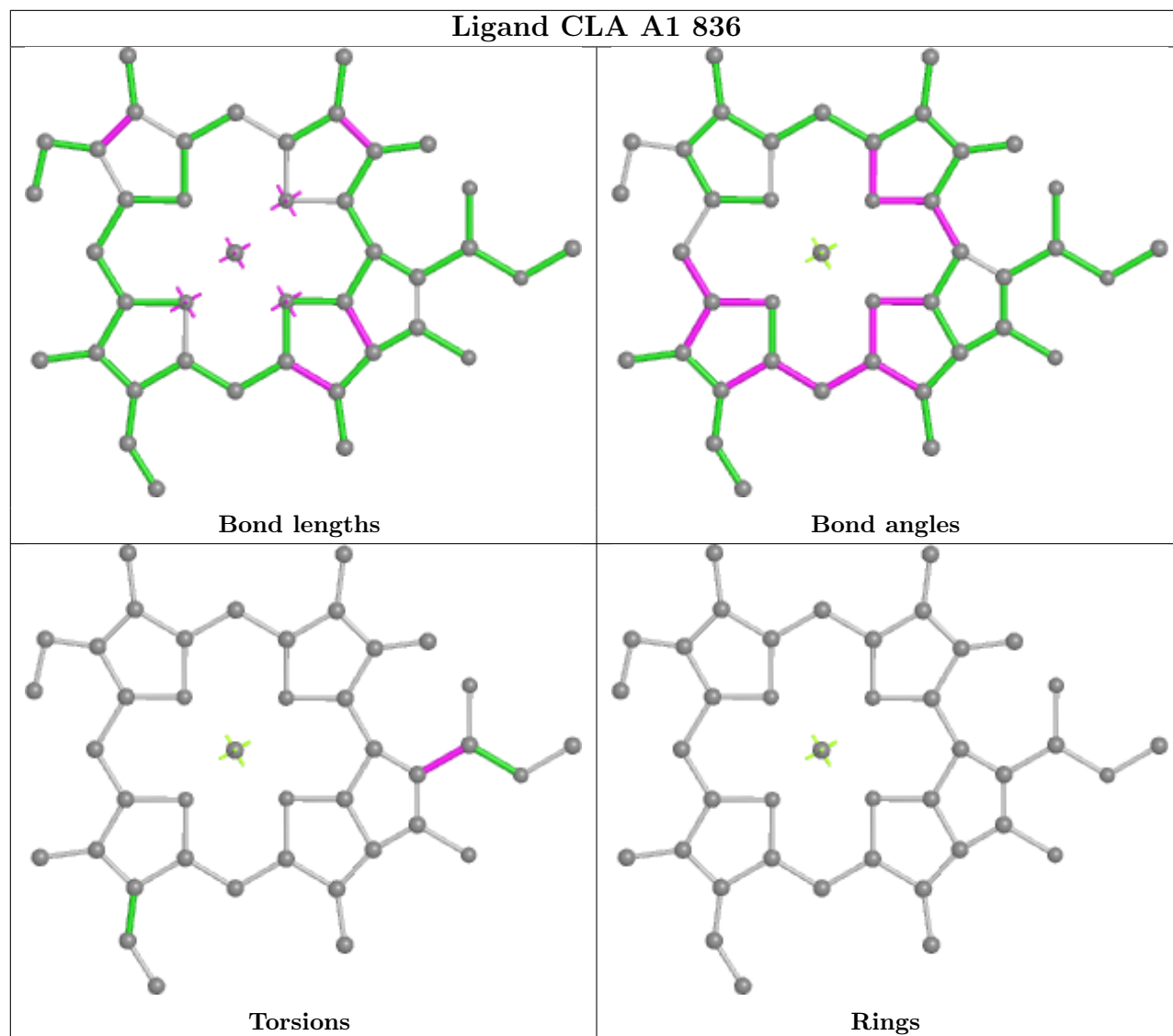




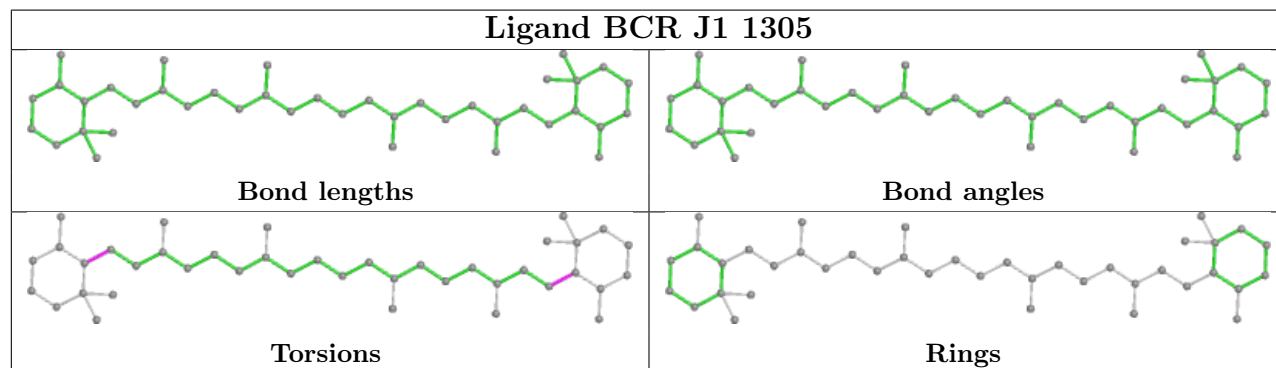




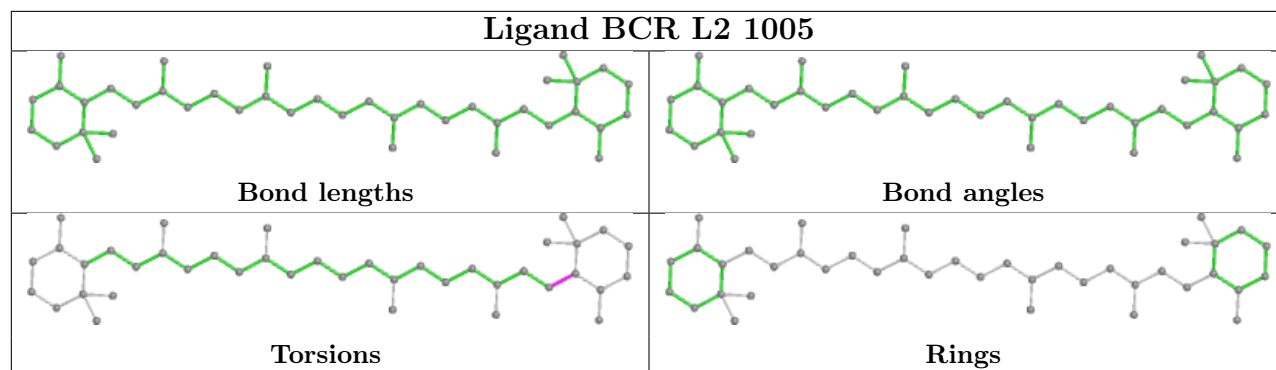
## Ligand CLA A1 836



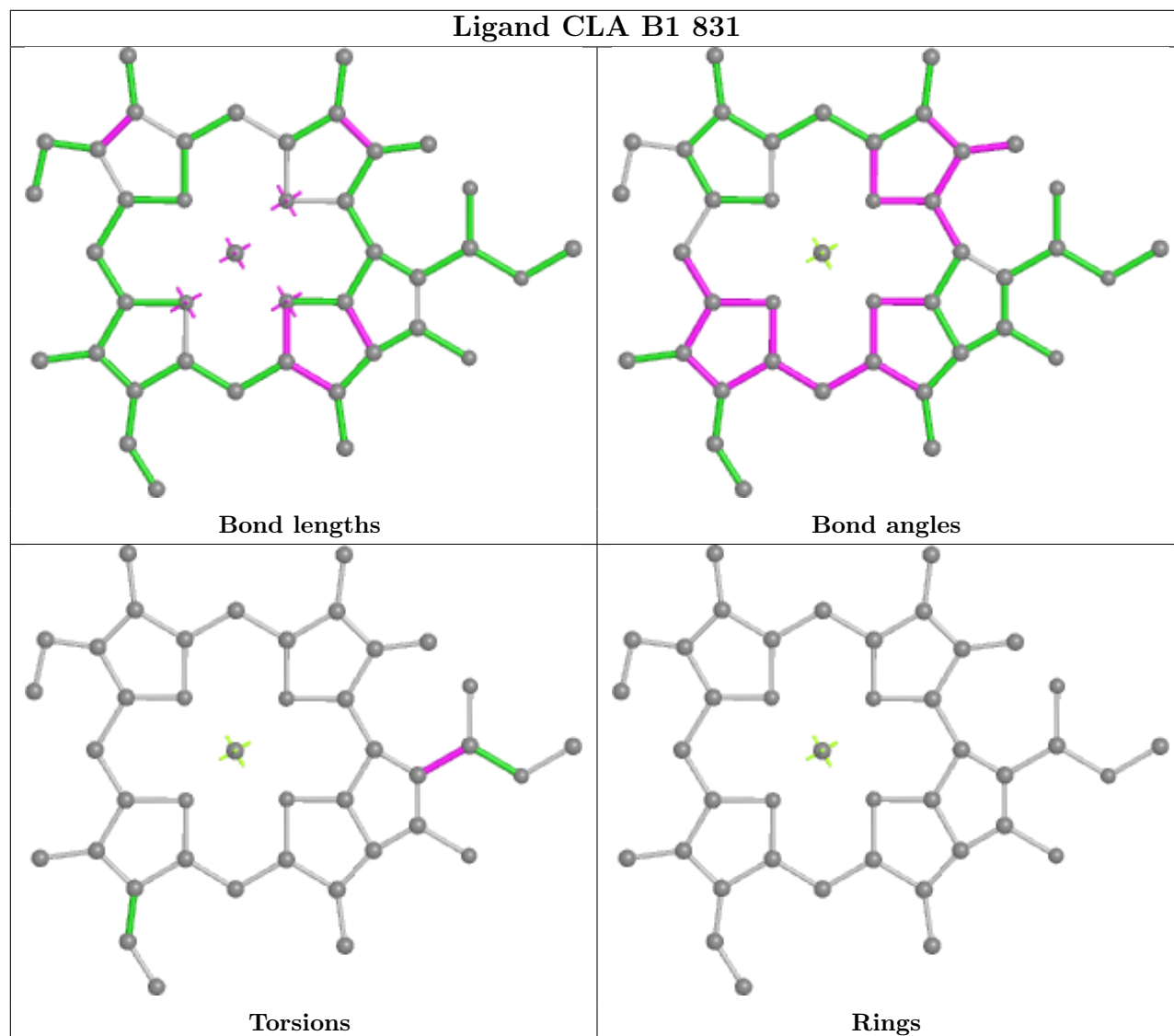
## Ligand BCR J1 1305

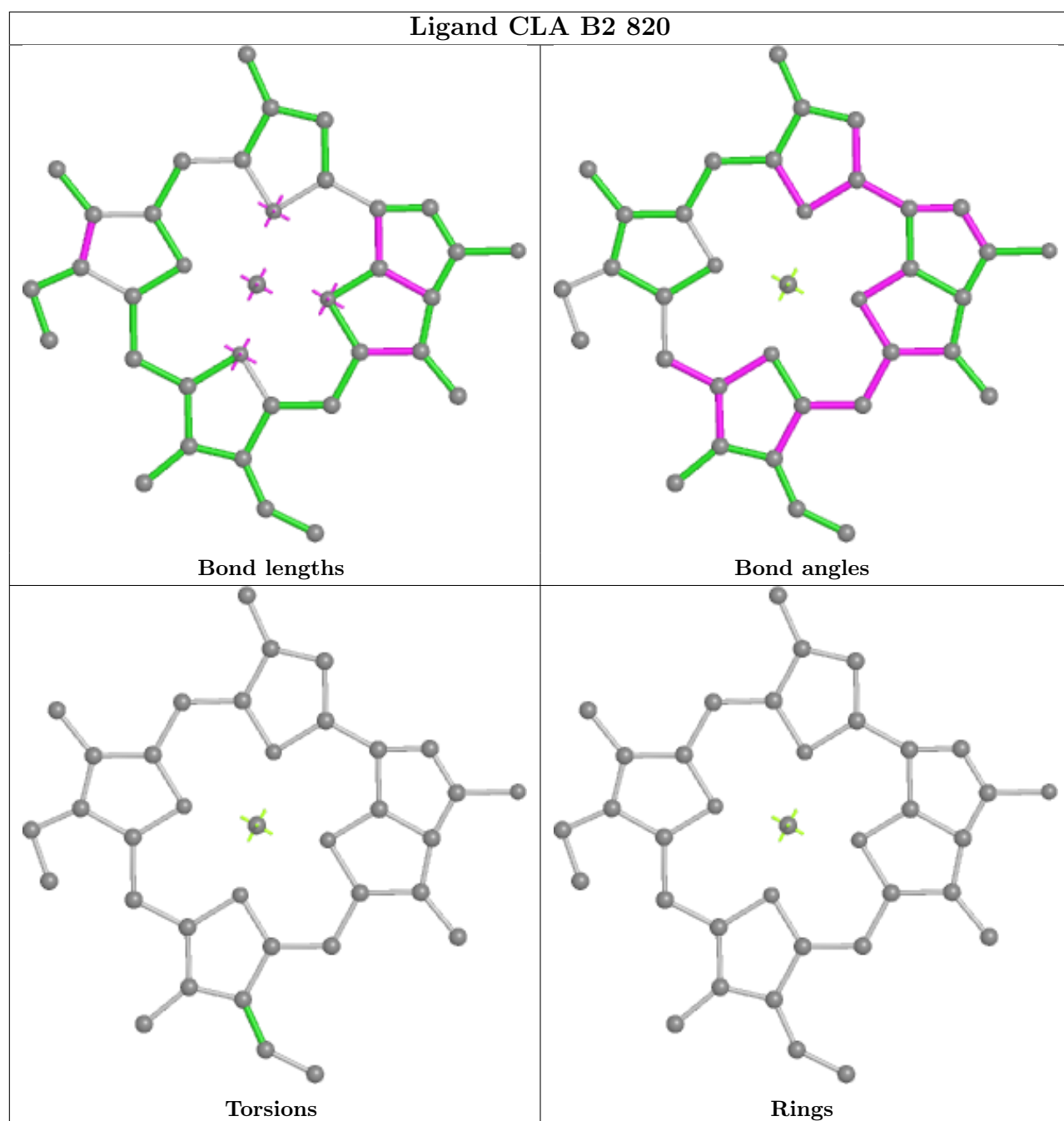


## Ligand BCR L2 1005

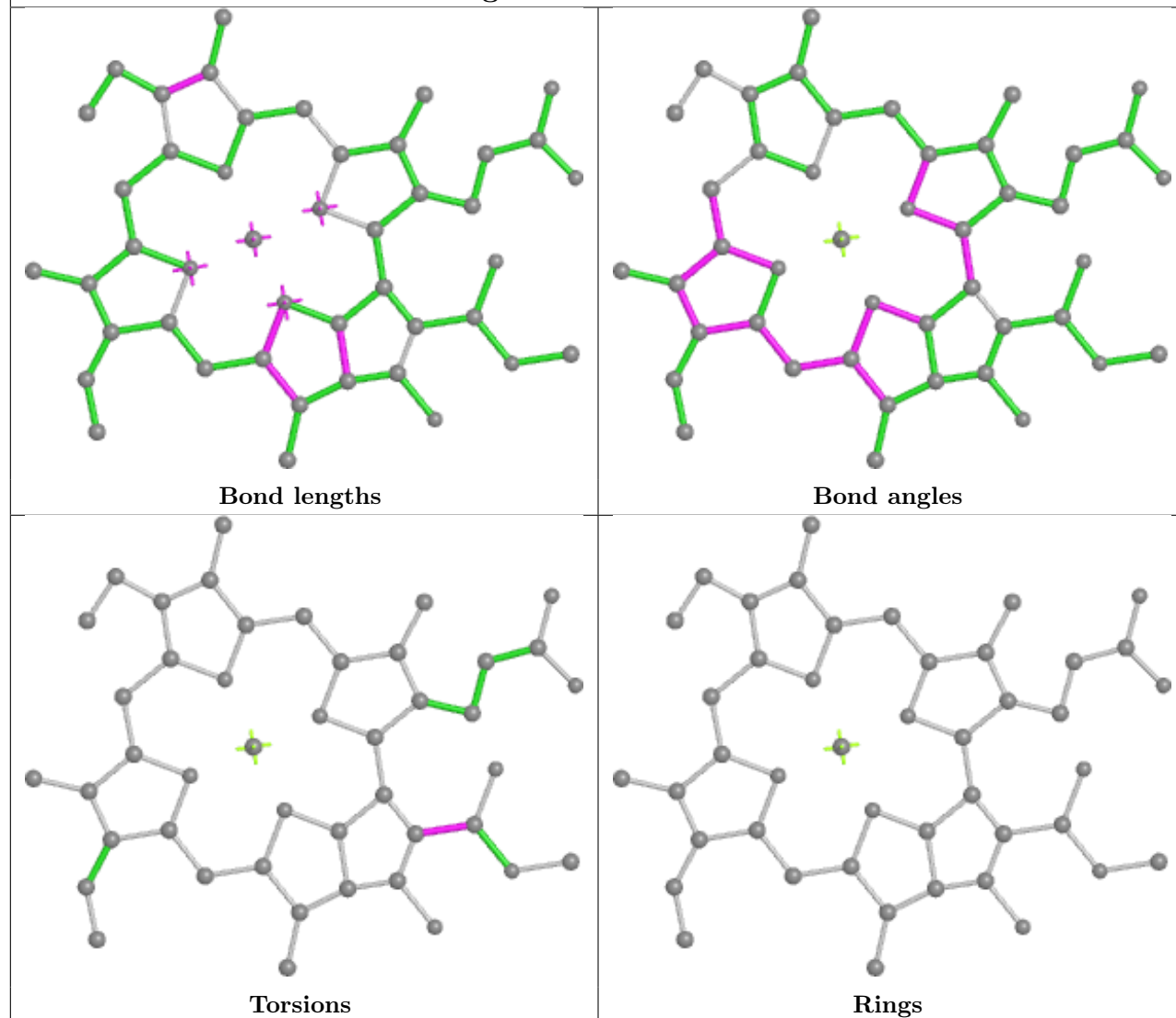


## Ligand CLA B1 831

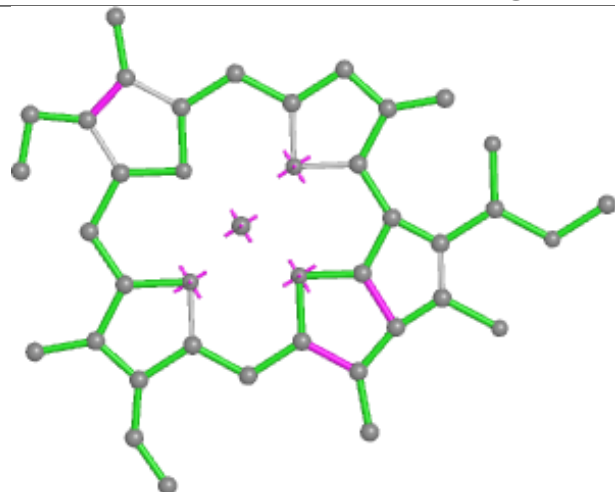




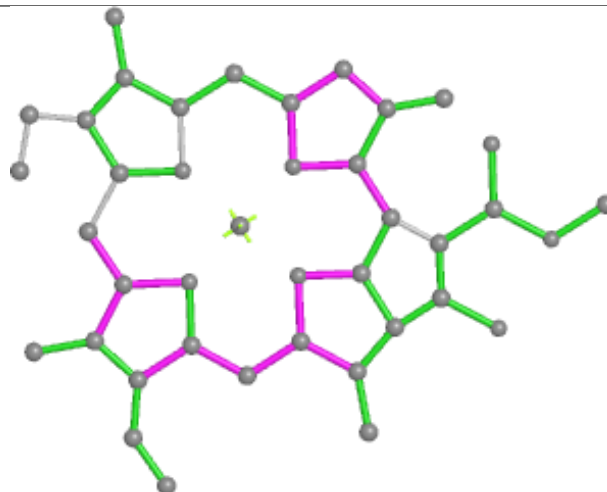
## Ligand CLA B1 836



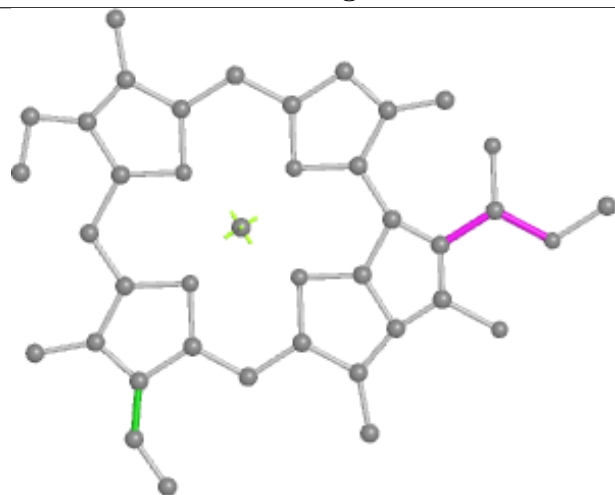
## Ligand CLA B2 832



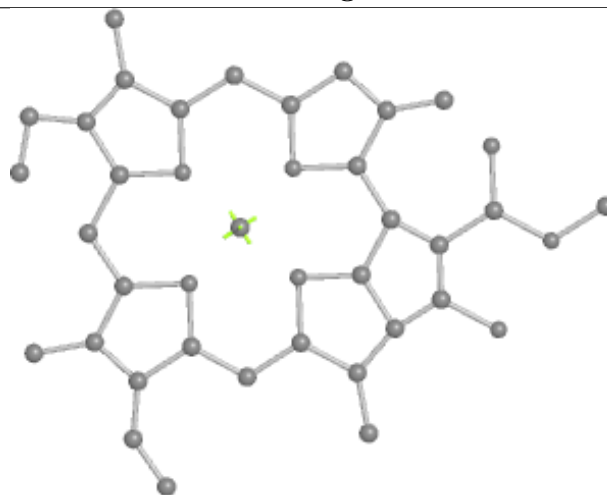
Bond lengths



Bond angles

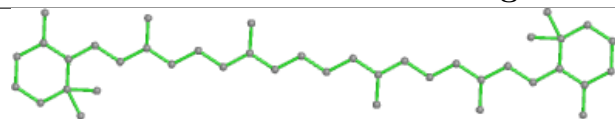


Torsions

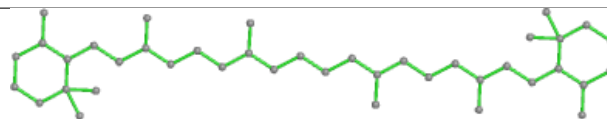


Rings

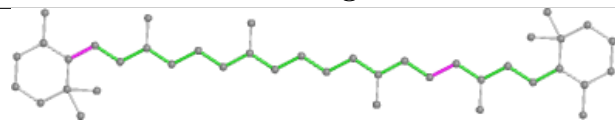
## Ligand BCR J3 1304



Bond lengths



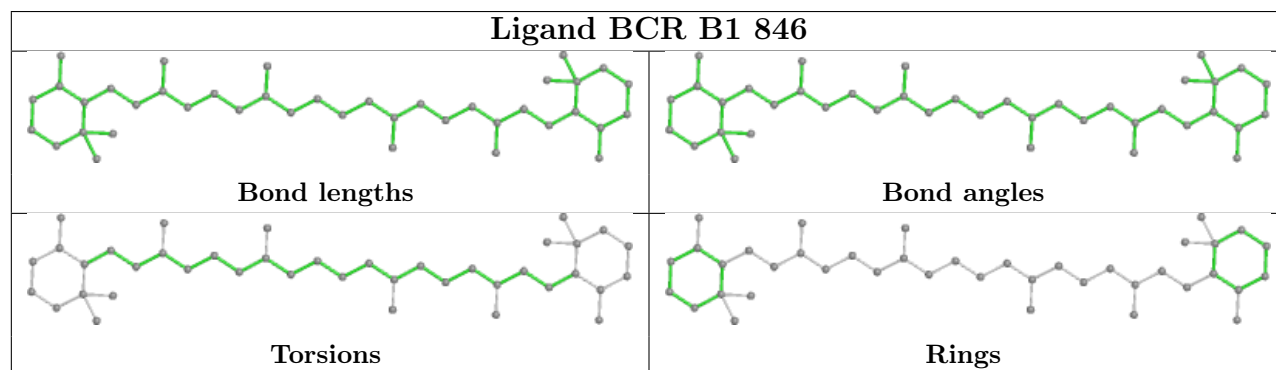
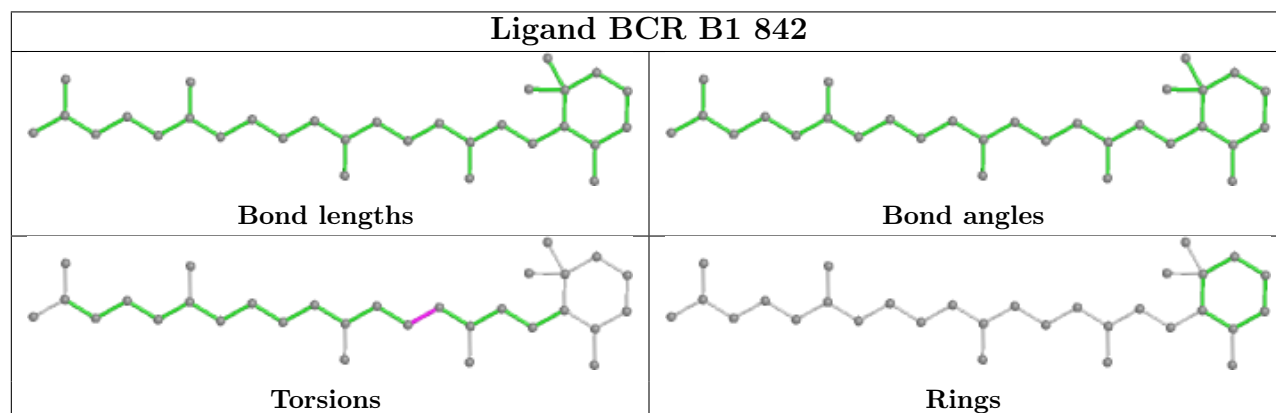
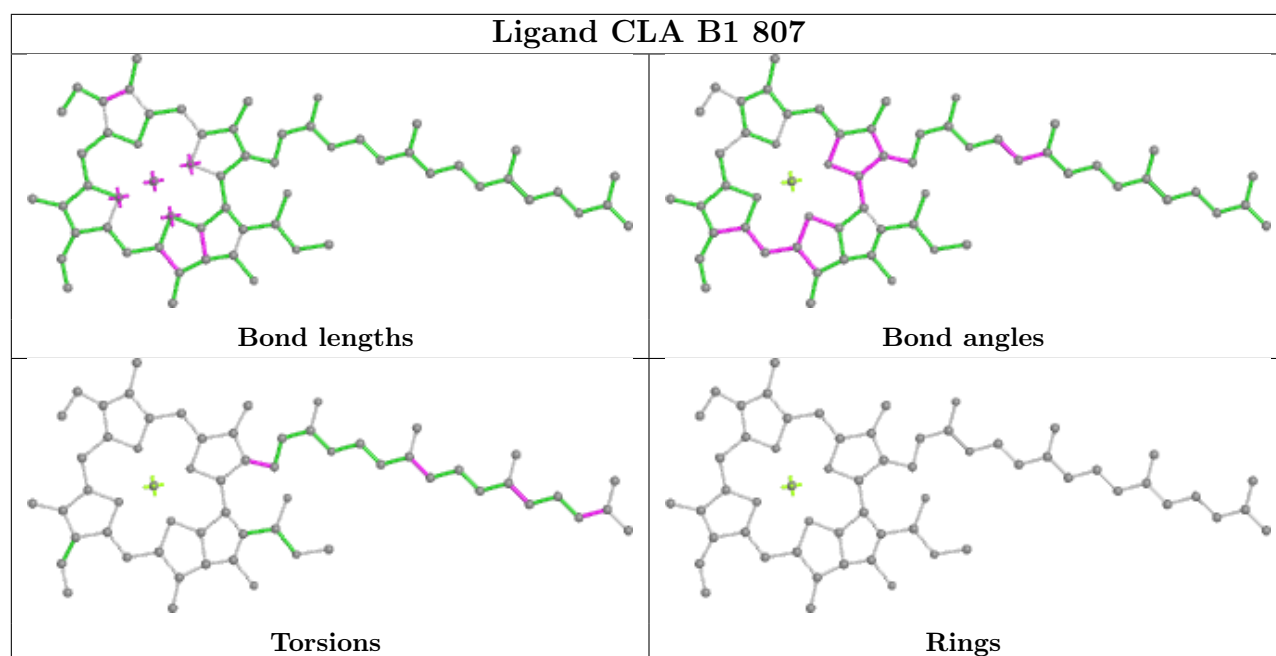
Bond angles

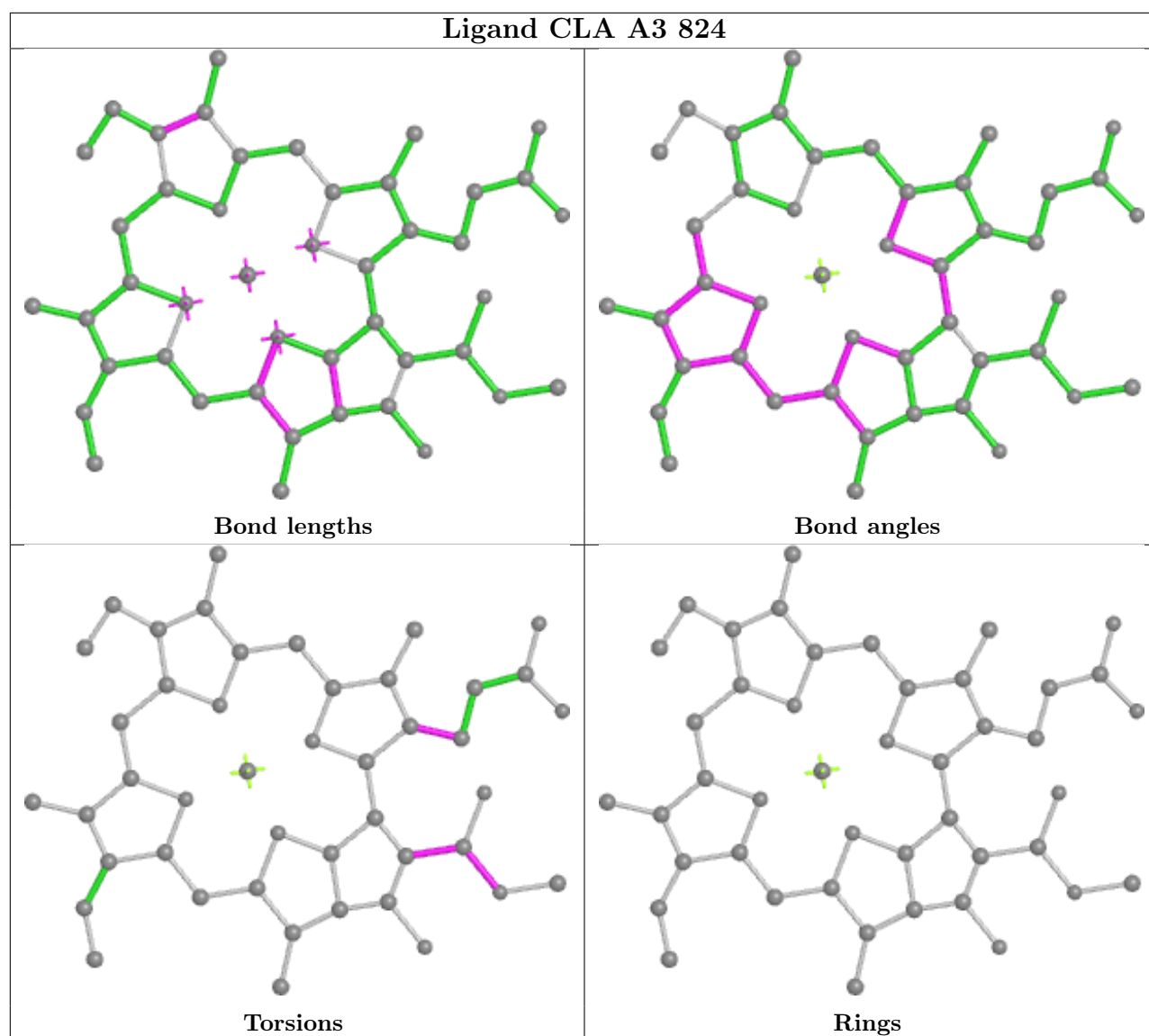


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



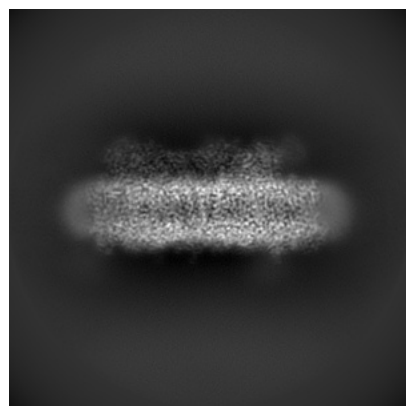
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31605. These allow visual inspection of the internal detail of the map and identification of artifacts.

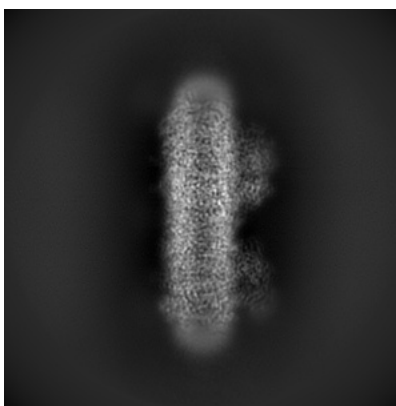
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

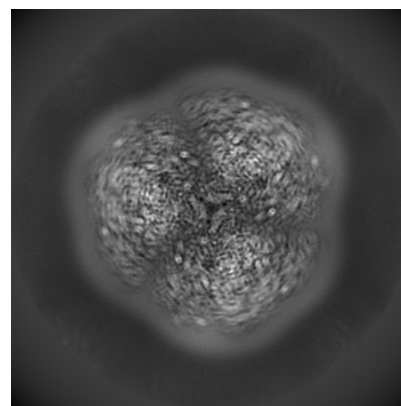
#### 6.1.1 Primary map



X

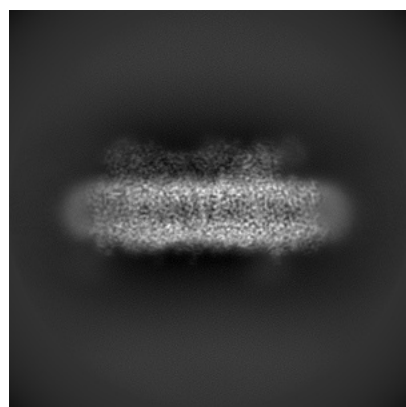


Y

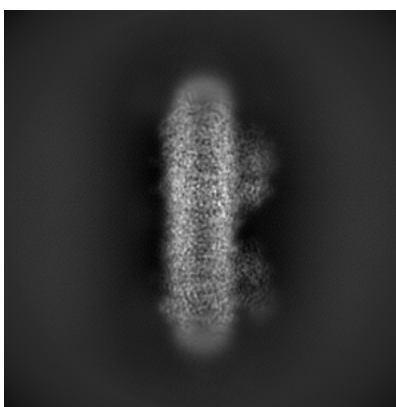


Z

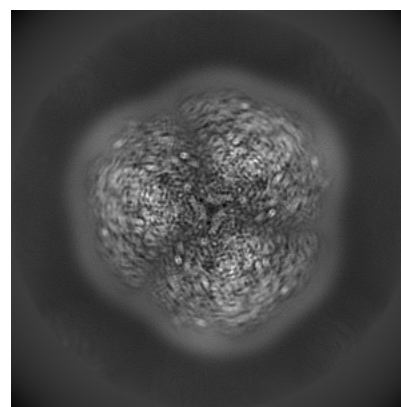
#### 6.1.2 Raw map



X



Y

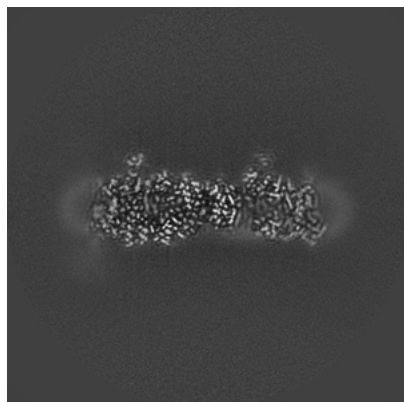


Z

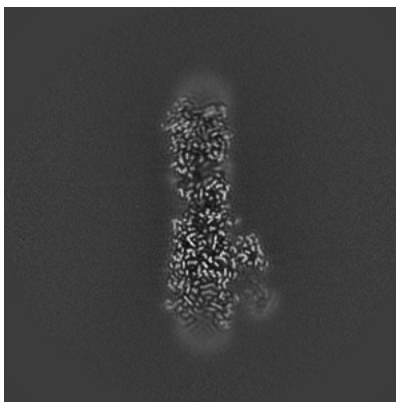
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

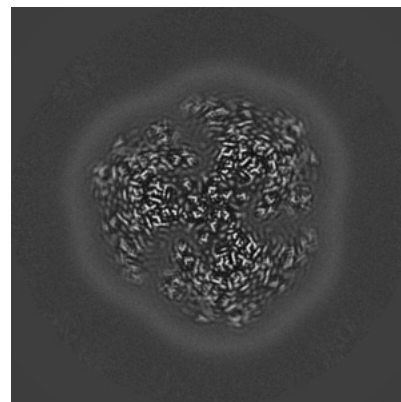
### 6.2.1 Primary map



X Index: 200

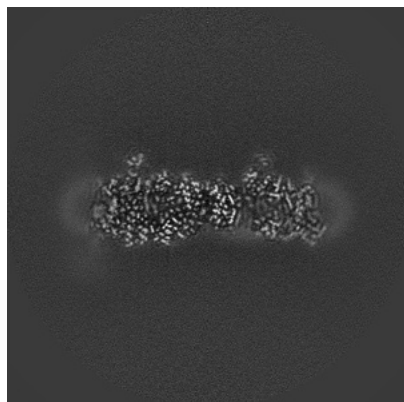


Y Index: 200

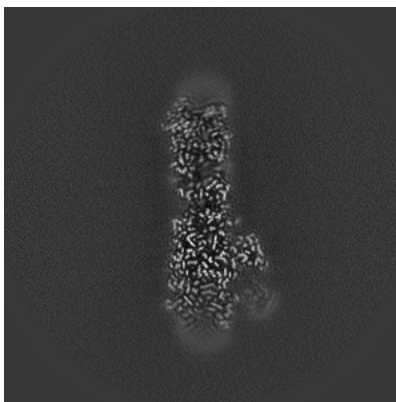


Z Index: 200

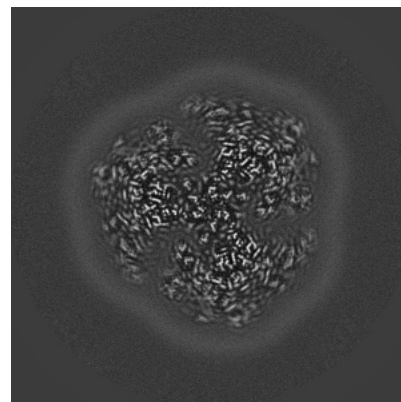
### 6.2.2 Raw map



X Index: 200



Y Index: 200

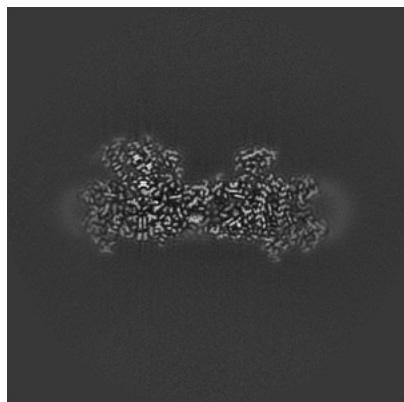


Z Index: 200

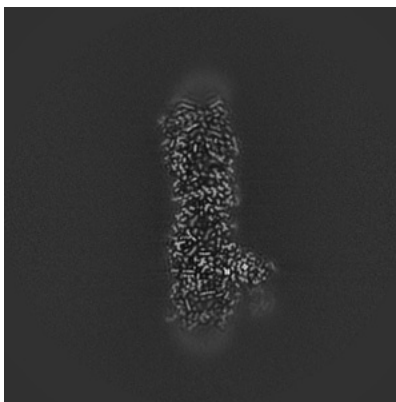
The images above show central slices of the map in three orthogonal directions.

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

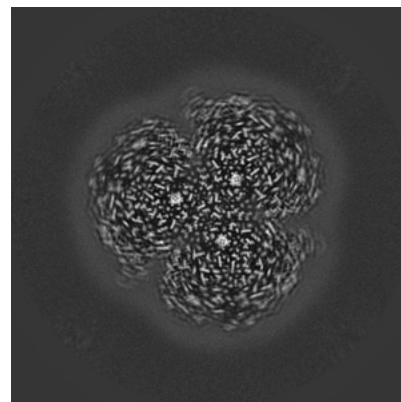
### 6.3.1 Primary map



X Index: 221

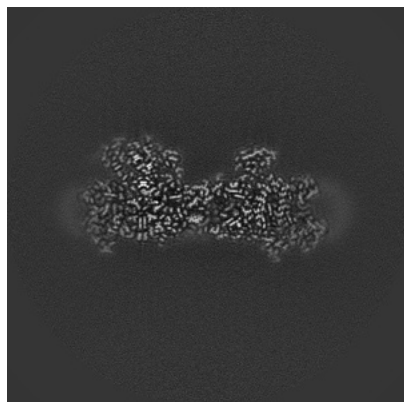


Y Index: 213

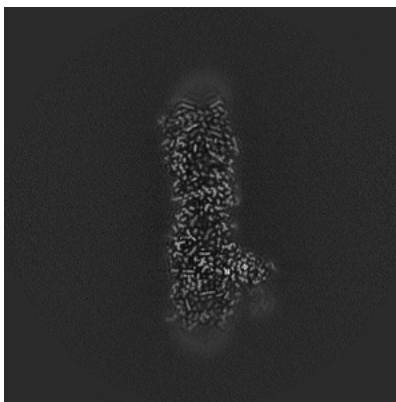


Z Index: 215

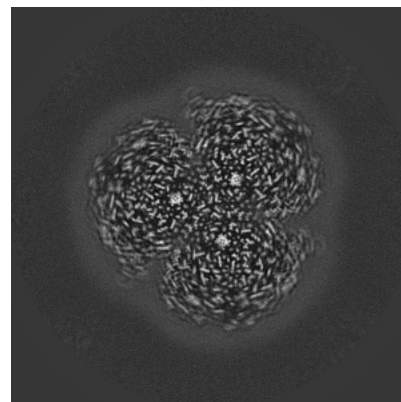
### 6.3.2 Raw map



X Index: 221



Y Index: 213

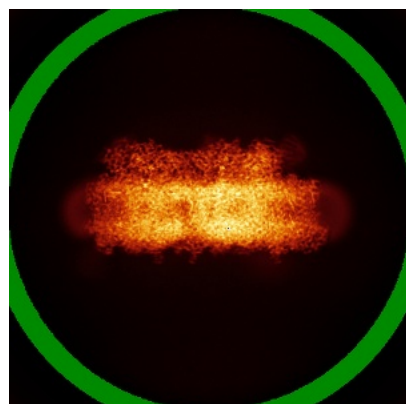


Z Index: 215

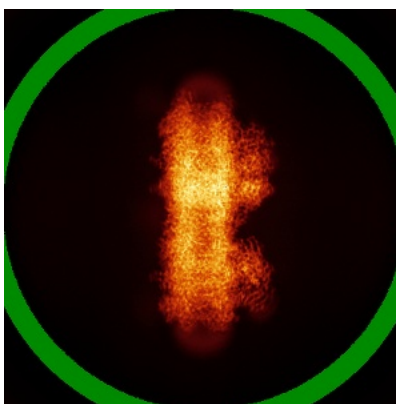
The images above show the largest variance slices of the map in three orthogonal directions.

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

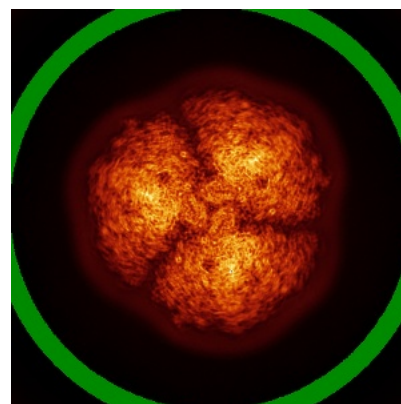
### 6.4.1 Primary map



X

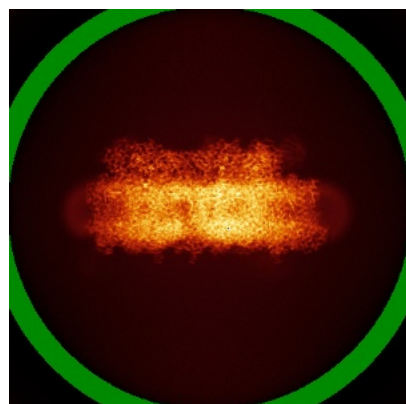


Y

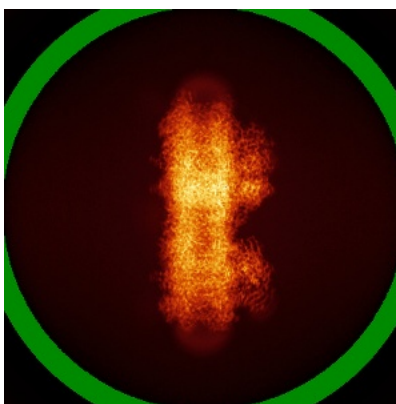


Z

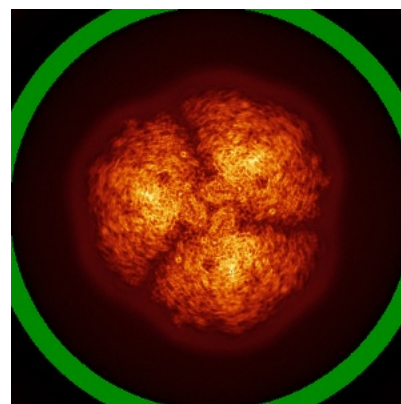
### 6.4.2 Raw map



X



Y

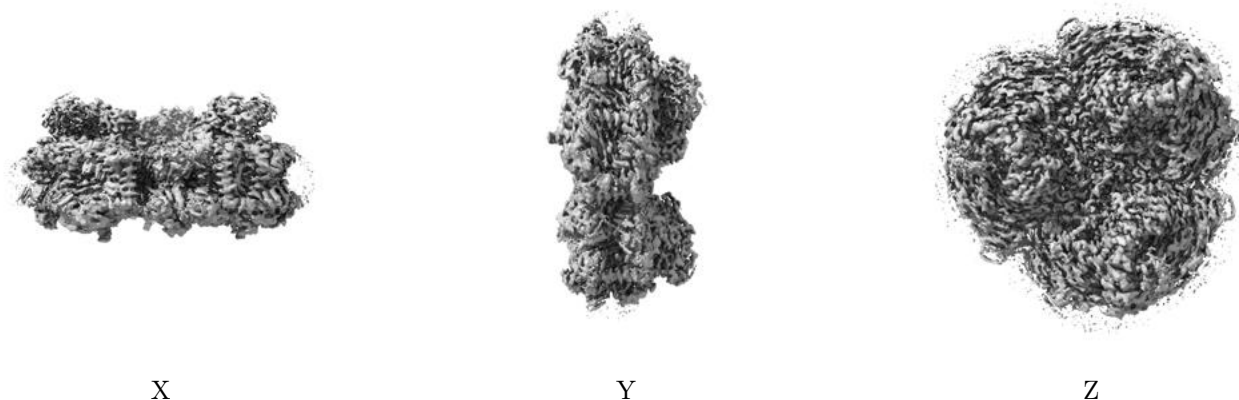


Z

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

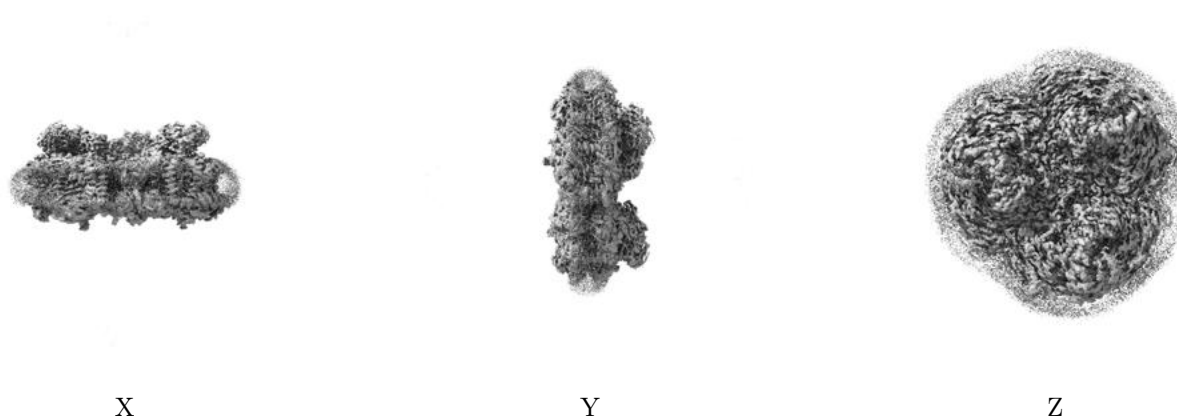
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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



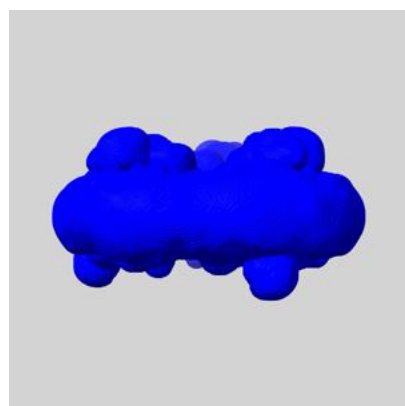
## 6.6 Mask visualisation [i](#)

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

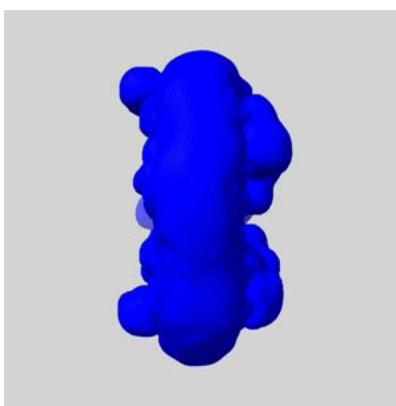
A mask typically either:

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

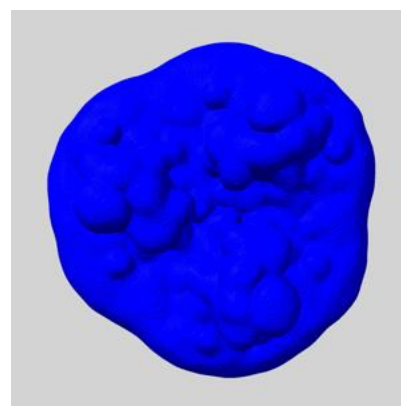
### 6.6.1 emd\_31605\_msk\_1.map [i](#)



X



Y

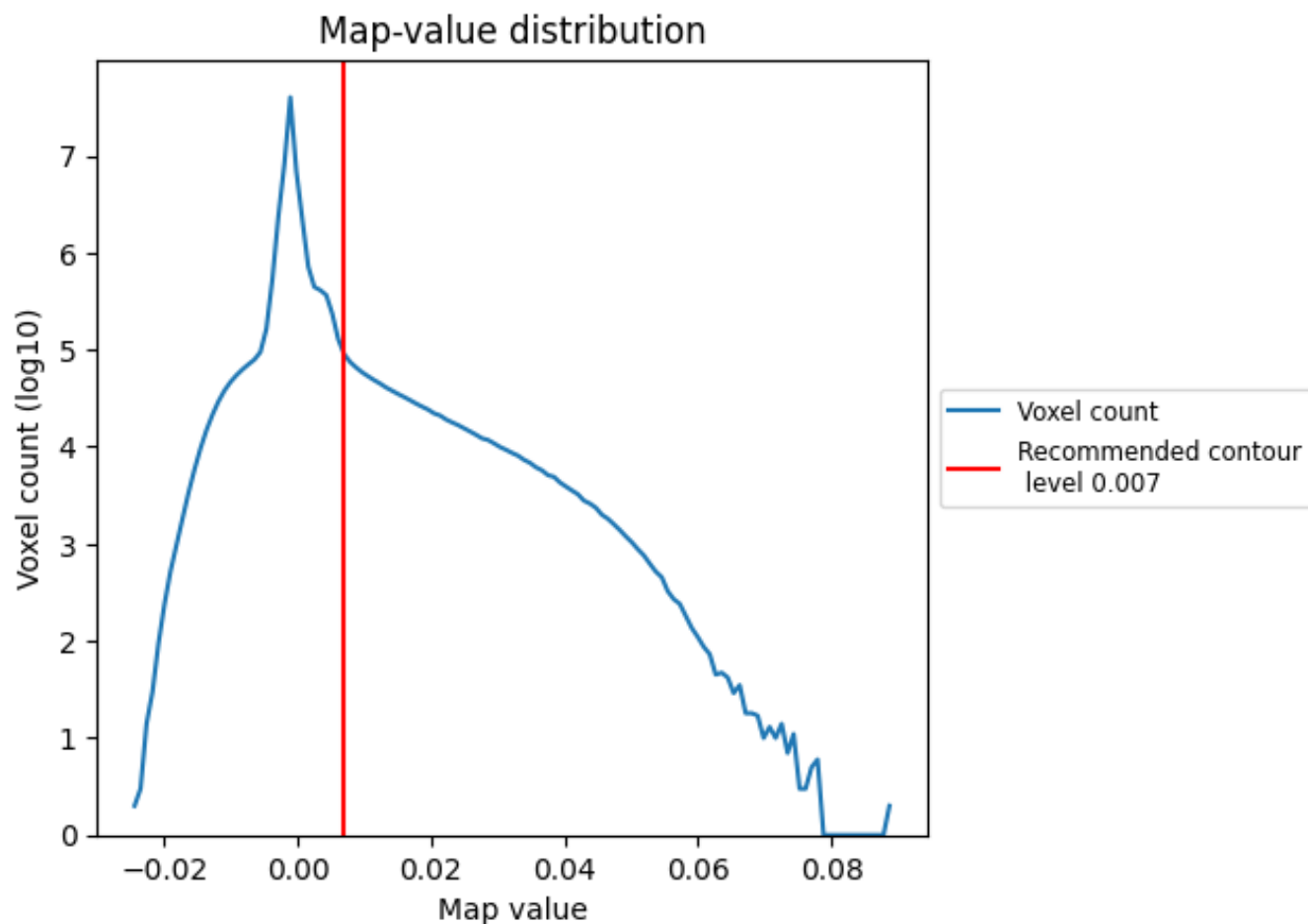


Z

## 7 Map analysis [i](#)

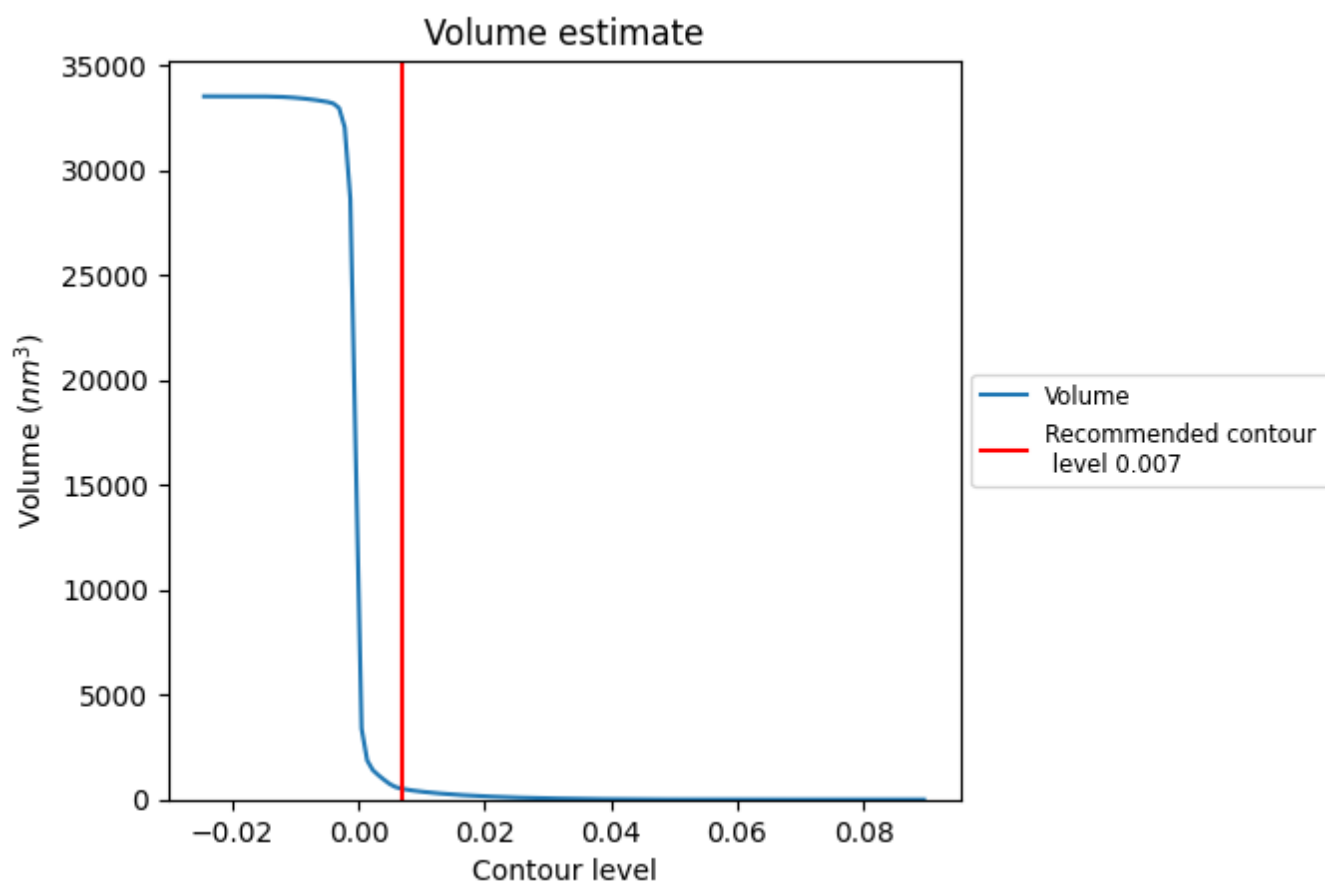
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

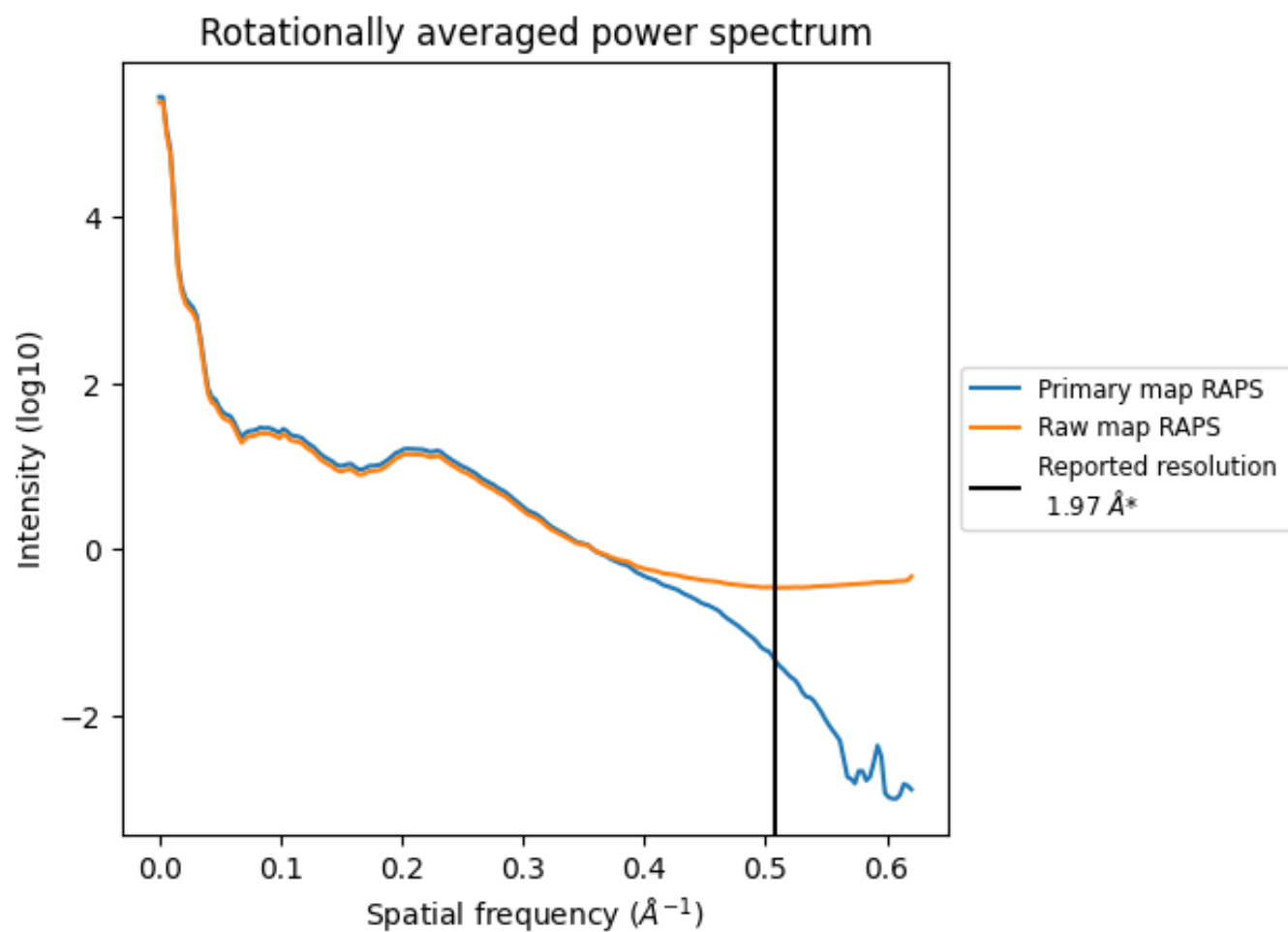


The volume at the recommended contour level is 511 nm<sup>3</sup>; this corresponds to an approximate mass of 461 kDa.

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 ⓘ

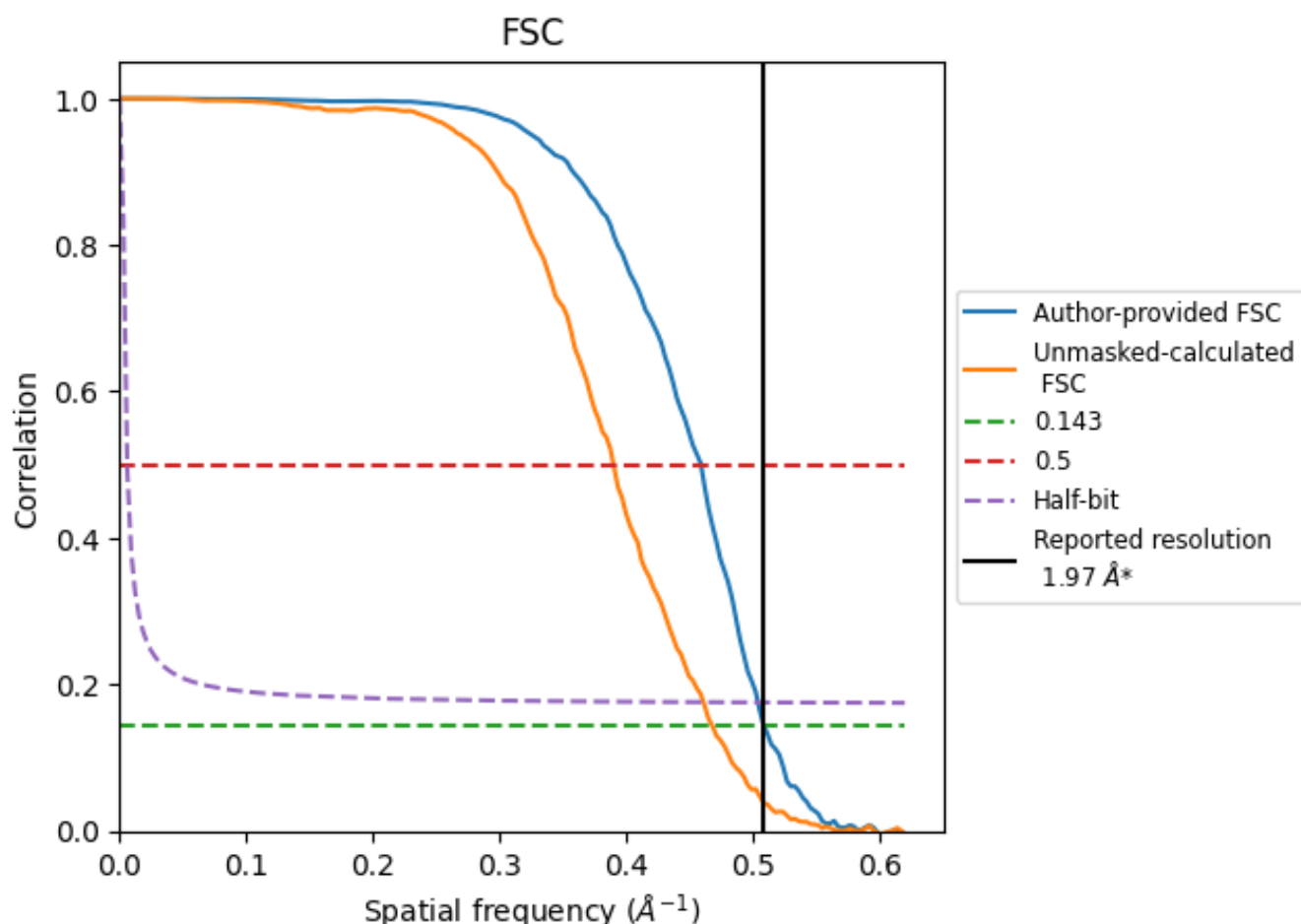


\*Reported resolution corresponds to spatial frequency of 0.508 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.508 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

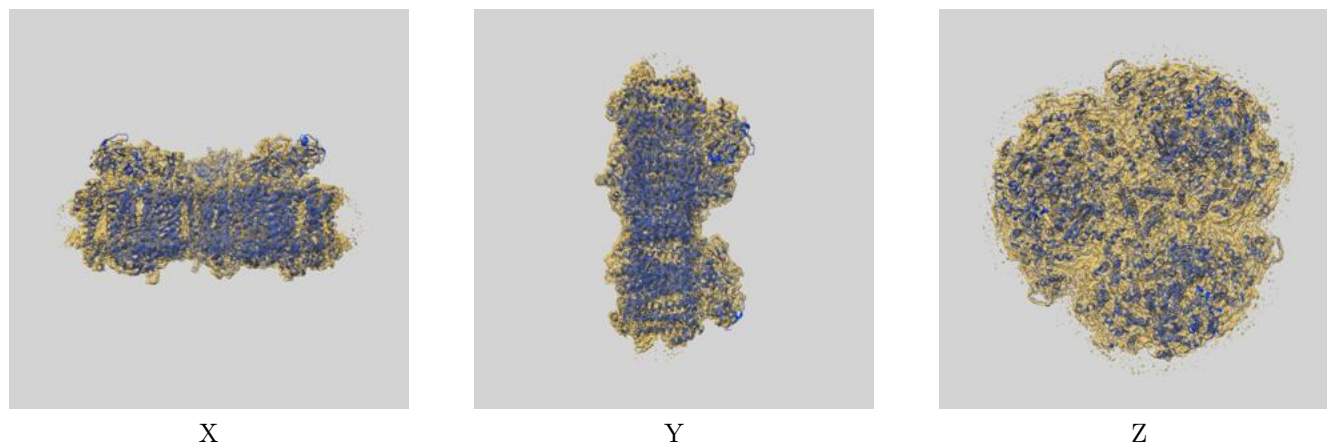
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.97	-	-
Author-provided FSC curve	1.96	2.18	1.98
Unmasked-calculated*	2.14	2.56	2.17

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

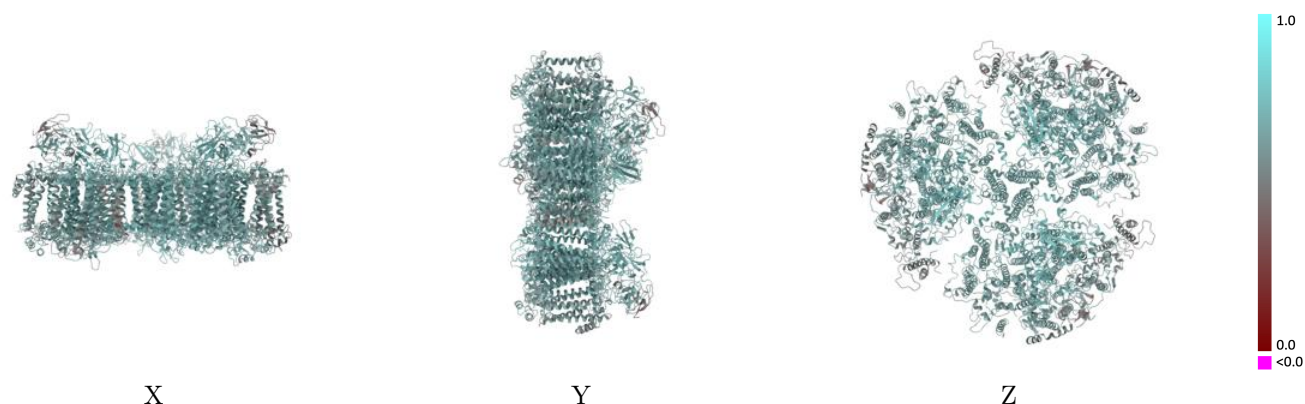
This section contains information regarding the fit between EMDB map EMD-31605 and PDB model 7FIX. Per-residue inclusion information can be found in [section 3](#) on [page 42](#).

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



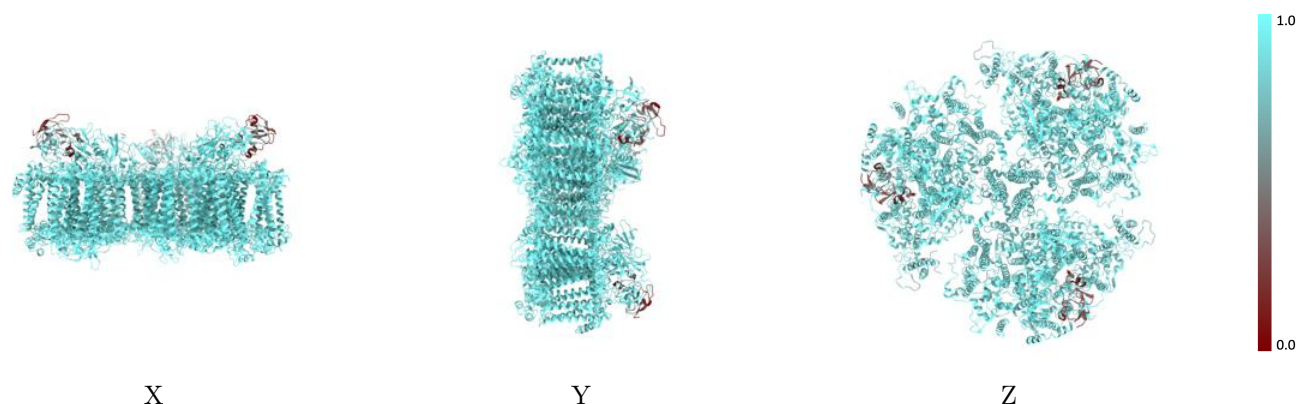
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



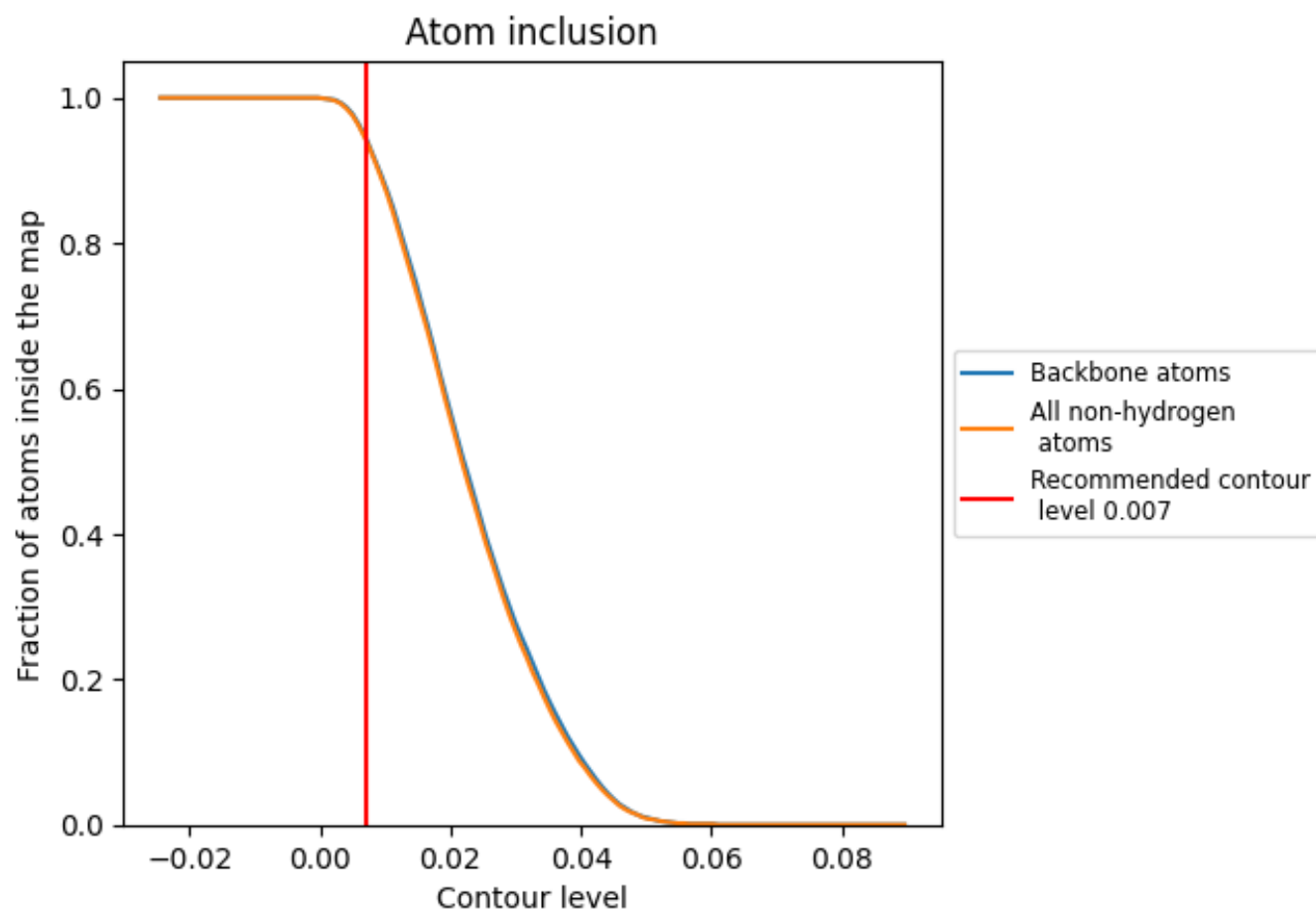
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.6510
A1	 0.9630	 0.6500
A2	 0.9630	 0.6500
A3	 0.9630	 0.6480
B1	 0.9770	 0.6710
B2	 0.9770	 0.6700
B3	 0.9760	 0.6690
C1	 0.9880	 0.7040
C2	 0.9870	 0.7030
C3	 0.9870	 0.7030
D1	 0.9550	 0.6810
D2	 0.9530	 0.6810
D3	 0.9530	 0.6800
E1	 0.9520	 0.6450
E2	 0.9560	 0.6500
E3	 0.9600	 0.6450
F1	 0.9010	 0.5810
F2	 0.8930	 0.5760
F3	 0.9010	 0.5770
I1	 0.9820	 0.7090
I2	 0.9880	 0.7080
I3	 0.9880	 0.7050
J1	 0.9120	 0.5770
J2	 0.9190	 0.5750
J3	 0.9100	 0.5750
K1	 0.8390	 0.4810
K2	 0.8400	 0.4870
K3	 0.8320	 0.4860
L1	 0.9770	 0.7110
L2	 0.9780	 0.7100
L3	 0.9800	 0.7100
M1	 0.9680	 0.6650
M2	 0.9680	 0.6660
M3	 0.9680	 0.6620
R1	 0.3870	 0.5300



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Chain	Atom inclusion	Q-score
R2	 0.4020	 0.5250
R3	 0.4020	 0.5250
X1	 0.9260	 0.5940
X2	 0.9120	 0.5900
X3	 0.9290	 0.5910