



Full wwPDB EM Model Validation Report ⓘ

Mar 9, 2020 – 11:26 PM EDT

PDB ID : 6QWJ
EMDB ID : EMD-4659
Title : The structure of tetrameric cyanobacterial Photosystem I of *Chroococcidiopsis* sp. TS-821
Authors : Semchonok, D.A.; Ramirez-Aportela, E.; Sorzano, C.O.S.; Boekema, E.J.; Bruce, B.D.; Guskov, A.
Deposited on : 2019-03-05
Resolution : 4.50 Å (reported)
Based on initial model : 1JB0

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

We welcome your comments at 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

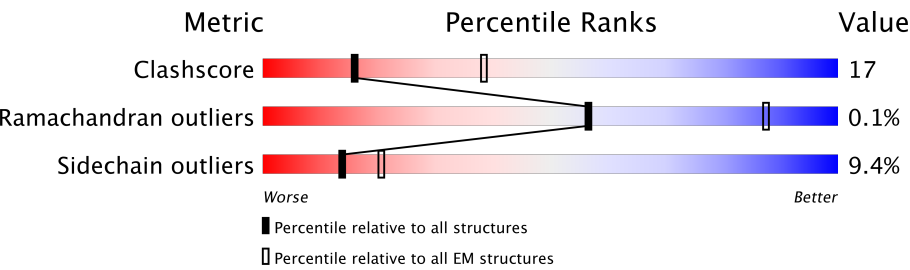
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.














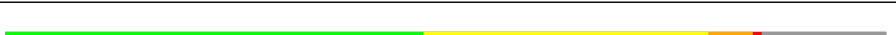

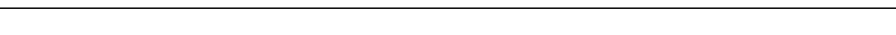
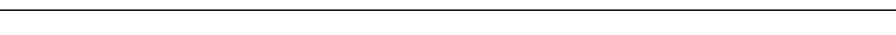
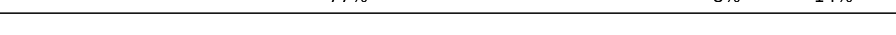

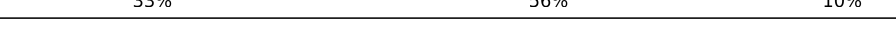







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	752	43% 50% . .
1	E	752	44% 49% . .
1	a	752	91% 5% .
1	e	752	91% 5% .
2	B	737	45% 50% .
2	G	737	44% 51% .
2	b	737	92% 7%
2	g	737	92% 7%
3	C	82	40% 50% 7% . .







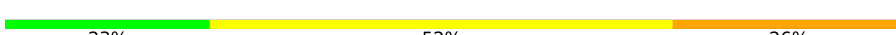
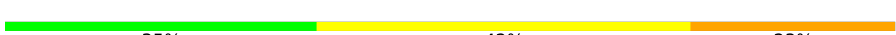


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Mol	Chain	Length	Quality of chain
3	H	82	
3	c	82	
3	h	82	
4	D	168	
4	N	168	
4	d	168	
4	n	168	
5	V	126	
5	W	126	
5	v	126	
5	w	126	
6	F	164	
6	O	164	
6	f	164	
6	o	164	
7	I	39	
7	P	39	
7	i	39	
7	p	39	
8	J	49	
8	Q	49	
8	j	49	
8	q	49	
9	K	93	
9	R	93	

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	801	X	-	-	-
12	CLA	A	802	X	-	-	-
12	CLA	A	803	X	-	-	-
12	CLA	A	804	X	-	-	-
12	CLA	A	805	X	-	-	-
12	CLA	A	806	X	-	-	-
12	CLA	A	807	X	-	-	-
12	CLA	A	808	X	-	-	-
12	CLA	A	809	X	-	-	-
12	CLA	A	810	X	-	-	-
12	CLA	A	811	X	-	-	-
12	CLA	A	812	X	-	-	-
12	CLA	A	813	X	-	-	-
12	CLA	A	814	X	-	-	-
12	CLA	A	815	X	-	-	-
12	CLA	A	816	X	-	-	-
12	CLA	A	817	X	-	-	-
12	CLA	A	818	X	-	-	-
12	CLA	A	819	X	-	-	-
12	CLA	A	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	821	X	-	-	-
12	CLA	A	822	X	-	-	-
12	CLA	A	823	X	-	-	-
12	CLA	A	824	X	-	-	-
12	CLA	A	825	X	-	-	-
12	CLA	A	826	X	-	-	-
12	CLA	A	827	X	-	-	-
12	CLA	A	828	X	-	-	-
12	CLA	A	829	X	-	-	-
12	CLA	A	830	X	-	-	-
12	CLA	A	831	X	-	-	-
12	CLA	A	832	X	-	-	-
12	CLA	A	833	X	-	-	-
12	CLA	A	834	X	-	-	-
12	CLA	A	835	X	-	-	-
12	CLA	A	836	X	-	-	-
12	CLA	A	837	X	-	-	-
12	CLA	A	838	X	-	-	-
12	CLA	A	839	X	-	-	-
12	CLA	A	840	X	-	-	-
12	CLA	A	841	X	-	-	-
12	CLA	B	801	X	-	-	-
12	CLA	B	802	X	-	-	-
12	CLA	B	803	X	-	-	-
12	CLA	B	805	X	-	-	-
12	CLA	B	806	X	-	-	-
12	CLA	B	807	X	-	-	-
12	CLA	B	808	X	-	-	-
12	CLA	B	809	X	-	-	-
12	CLA	B	810	X	-	-	-
12	CLA	B	811	X	-	-	-
12	CLA	B	812	X	-	-	-
12	CLA	B	813	X	-	-	-
12	CLA	B	814	X	-	-	-
12	CLA	B	815	X	-	-	-
12	CLA	B	816	X	-	-	-
12	CLA	B	817	X	-	-	-
12	CLA	B	818	X	-	-	-
12	CLA	B	819	X	-	-	-
12	CLA	B	820	X	-	-	-
12	CLA	B	821	X	-	-	-
12	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	B	823	X	-	-	-
12	CLA	B	824	X	-	-	-
12	CLA	B	825	X	-	-	-
12	CLA	B	826	X	-	-	-
12	CLA	B	827	X	-	-	-
12	CLA	B	828	X	-	-	-
12	CLA	B	829	X	-	-	-
12	CLA	B	830	X	-	-	-
12	CLA	B	831	X	-	-	-
12	CLA	B	832	X	-	-	-
12	CLA	B	833	X	-	-	-
12	CLA	B	834	X	-	-	-
12	CLA	B	835	X	-	-	-
12	CLA	B	836	X	-	-	-
12	CLA	B	837	X	-	-	-
12	CLA	B	838	X	-	-	-
12	CLA	B	839	X	-	-	-
12	CLA	B	840	X	-	-	-
12	CLA	B	841	X	-	-	-
12	CLA	B	842	X	-	-	-
12	CLA	B	843	X	-	-	-
12	CLA	E	801	X	-	-	-
12	CLA	E	802	X	-	-	-
12	CLA	E	803	X	-	-	-
12	CLA	E	804	X	-	-	-
12	CLA	E	805	X	-	-	-
12	CLA	E	806	X	-	-	-
12	CLA	E	807	X	-	-	-
12	CLA	E	808	X	-	-	-
12	CLA	E	809	X	-	-	-
12	CLA	E	810	X	-	-	-
12	CLA	E	811	X	-	-	-
12	CLA	E	812	X	-	-	-
12	CLA	E	813	X	-	-	-
12	CLA	E	814	X	-	-	-
12	CLA	E	815	X	-	-	-
12	CLA	E	816	X	-	-	-
12	CLA	E	817	X	-	-	-
12	CLA	E	818	X	-	-	-
12	CLA	E	819	X	-	-	-
12	CLA	E	820	X	-	-	-
12	CLA	E	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	E	822	X	-	-	-
12	CLA	E	823	X	-	-	-
12	CLA	E	824	X	-	-	-
12	CLA	E	825	X	-	-	-
12	CLA	E	826	X	-	-	-
12	CLA	E	827	X	-	-	-
12	CLA	E	828	X	-	-	-
12	CLA	E	829	X	-	-	-
12	CLA	E	830	X	-	-	-
12	CLA	E	831	X	-	-	-
12	CLA	E	832	X	-	-	-
12	CLA	E	833	X	-	-	-
12	CLA	E	834	X	-	-	-
12	CLA	E	835	X	-	-	-
12	CLA	E	836	X	-	-	-
12	CLA	E	837	X	-	-	-
12	CLA	E	838	X	-	-	-
12	CLA	E	839	X	-	-	-
12	CLA	E	840	X	-	-	-
12	CLA	E	841	X	-	-	-
12	CLA	E	842	X	-	-	-
12	CLA	E	843	X	-	-	-
12	CLA	E	844	X	-	-	-
12	CLA	F	1301	X	-	-	-
12	CLA	G	801	X	-	-	-
12	CLA	G	802	X	-	-	-
12	CLA	G	803	X	-	-	-
12	CLA	G	804	X	-	-	-
12	CLA	G	805	X	-	-	-
12	CLA	G	806	X	-	-	-
12	CLA	G	807	X	-	-	-
12	CLA	G	808	X	-	-	-
12	CLA	G	809	X	-	-	-
12	CLA	G	810	X	-	-	-
12	CLA	G	811	X	-	-	-
12	CLA	G	812	X	-	-	-
12	CLA	G	813	X	-	-	-
12	CLA	G	814	X	-	-	-
12	CLA	G	815	X	-	-	-
12	CLA	G	816	X	-	-	-
12	CLA	G	817	X	-	-	-
12	CLA	G	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	G	819	X	-	-	-
12	CLA	G	820	X	-	-	-
12	CLA	G	821	X	-	-	-
12	CLA	G	822	X	-	-	-
12	CLA	G	823	X	-	-	-
12	CLA	G	824	X	-	-	-
12	CLA	G	825	X	-	-	-
12	CLA	G	826	X	-	-	-
12	CLA	G	827	X	-	-	-
12	CLA	G	828	X	-	-	-
12	CLA	G	829	X	-	-	-
12	CLA	G	830	X	-	-	-
12	CLA	G	831	X	-	-	-
12	CLA	G	832	X	-	-	-
12	CLA	G	833	X	-	-	-
12	CLA	G	834	X	-	-	-
12	CLA	G	835	X	-	-	-
12	CLA	G	836	X	-	-	-
12	CLA	G	837	X	-	-	-
12	CLA	G	838	X	-	-	-
12	CLA	G	839	X	-	-	-
12	CLA	G	840	X	-	-	-
12	CLA	G	841	X	-	-	-
12	CLA	G	843	X	-	-	-
12	CLA	J	1101	X	-	-	-
12	CLA	J	1102	X	-	-	-
12	CLA	K	1401	X	-	-	-
12	CLA	L	201	X	-	-	-
12	CLA	L	202	X	-	-	-
12	CLA	L	203	X	-	-	-
12	CLA	L	204	X	-	-	-
12	CLA	O	1301	X	-	-	-
12	CLA	R	1401	X	-	-	-
12	CLA	S	1501	X	-	-	-
12	CLA	S	1502	X	-	-	-
12	CLA	a	801	X	-	-	-
12	CLA	a	802	X	-	-	-
12	CLA	a	803	X	-	-	-
12	CLA	a	804	X	-	-	-
12	CLA	a	805	X	-	-	-
12	CLA	a	806	X	-	-	-
12	CLA	a	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	a	808	X	-	-	-
12	CLA	a	809	X	-	-	-
12	CLA	a	810	X	-	-	-
12	CLA	a	811	X	-	-	-
12	CLA	a	812	X	-	-	-
12	CLA	a	813	X	-	-	-
12	CLA	a	814	X	-	-	-
12	CLA	a	815	X	-	-	-
12	CLA	a	816	X	-	-	-
12	CLA	a	817	X	-	-	-
12	CLA	a	818	X	-	-	-
12	CLA	a	819	X	-	-	-
12	CLA	a	820	X	-	-	-
12	CLA	a	821	X	-	-	-
12	CLA	a	822	X	-	-	-
12	CLA	a	823	X	-	-	-
12	CLA	a	824	X	-	-	-
12	CLA	a	825	X	-	-	-
12	CLA	a	826	X	-	-	-
12	CLA	a	827	X	-	-	-
12	CLA	a	828	X	-	-	-
12	CLA	a	829	X	-	-	-
12	CLA	a	830	X	-	-	-
12	CLA	a	831	X	-	-	-
12	CLA	a	832	X	-	-	-
12	CLA	a	833	X	-	-	-
12	CLA	a	834	X	-	-	-
12	CLA	a	835	X	-	-	-
12	CLA	a	836	X	-	-	-
12	CLA	a	837	X	-	-	-
12	CLA	a	838	X	-	-	-
12	CLA	a	839	X	-	-	-
12	CLA	a	840	X	-	-	-
12	CLA	a	841	X	-	-	-
12	CLA	a	842	X	-	-	-
12	CLA	b	801	X	-	-	-
12	CLA	b	802	X	-	-	-
12	CLA	b	803	X	-	-	-
12	CLA	b	804	X	-	-	-
12	CLA	b	805	X	-	-	-
12	CLA	b	806	X	-	-	-
12	CLA	b	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	b	808	X	-	-	-
12	CLA	b	809	X	-	-	-
12	CLA	b	810	X	-	-	-
12	CLA	b	811	X	-	-	-
12	CLA	b	812	X	-	-	-
12	CLA	b	813	X	-	-	-
12	CLA	b	814	X	-	-	-
12	CLA	b	815	X	-	-	-
12	CLA	b	816	X	-	-	-
12	CLA	b	817	X	-	-	-
12	CLA	b	818	X	-	-	-
12	CLA	b	819	X	-	-	-
12	CLA	b	820	X	-	-	-
12	CLA	b	821	X	-	-	-
12	CLA	b	822	X	-	-	-
12	CLA	b	823	X	-	-	-
12	CLA	b	824	X	-	-	-
12	CLA	b	825	X	-	-	-
12	CLA	b	826	X	-	-	-
12	CLA	b	827	X	-	-	-
12	CLA	b	828	X	-	-	-
12	CLA	b	829	X	-	-	-
12	CLA	b	830	X	-	-	-
12	CLA	b	831	X	-	-	-
12	CLA	b	832	X	-	-	-
12	CLA	b	833	X	-	-	-
12	CLA	b	834	X	-	-	-
12	CLA	b	835	X	-	-	-
12	CLA	b	836	X	-	-	-
12	CLA	b	837	X	-	-	-
12	CLA	b	838	X	-	-	-
12	CLA	b	839	X	-	-	-
12	CLA	b	840	X	-	-	-
12	CLA	b	841	X	-	-	-
12	CLA	b	842	X	-	-	-
12	CLA	e	801	X	-	-	-
12	CLA	e	802	X	-	-	-
12	CLA	e	803	X	-	-	-
12	CLA	e	804	X	-	-	-
12	CLA	e	805	X	-	-	-
12	CLA	e	806	X	-	-	-
12	CLA	e	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	e	808	X	-	-	-
12	CLA	e	809	X	-	-	-
12	CLA	e	810	X	-	-	-
12	CLA	e	811	X	-	-	-
12	CLA	e	812	X	-	-	-
12	CLA	e	813	X	-	-	-
12	CLA	e	814	X	-	-	-
12	CLA	e	815	X	-	-	-
12	CLA	e	816	X	-	-	-
12	CLA	e	817	X	-	-	-
12	CLA	e	818	X	-	-	-
12	CLA	e	819	X	-	-	-
12	CLA	e	820	X	-	-	-
12	CLA	e	821	X	-	-	-
12	CLA	e	822	X	-	-	-
12	CLA	e	823	X	-	-	-
12	CLA	e	824	X	-	-	-
12	CLA	e	825	X	-	-	-
12	CLA	e	826	X	-	-	-
12	CLA	e	827	X	-	-	-
12	CLA	e	828	X	-	-	-
12	CLA	e	829	X	-	-	-
12	CLA	e	830	X	-	-	-
12	CLA	e	831	X	-	-	-
12	CLA	e	832	X	-	-	-
12	CLA	e	833	X	-	-	-
12	CLA	e	834	X	-	-	-
12	CLA	e	835	X	-	-	-
12	CLA	e	836	X	-	-	-
12	CLA	e	837	X	-	-	-
12	CLA	e	838	X	-	-	-
12	CLA	e	839	X	-	-	-
12	CLA	e	840	X	-	-	-
12	CLA	e	841	X	-	-	-
12	CLA	e	842	X	-	-	-
12	CLA	e	844	X	-	-	-
12	CLA	e	845	X	-	-	-
12	CLA	f	1301	X	-	-	-
12	CLA	g	801	X	-	-	-
12	CLA	g	802	X	-	-	-
12	CLA	g	803	X	-	-	-
12	CLA	g	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	g	806	X	-	-	-
12	CLA	g	807	X	-	-	-
12	CLA	g	808	X	-	-	-
12	CLA	g	809	X	-	-	-
12	CLA	g	810	X	-	-	-
12	CLA	g	811	X	-	-	-
12	CLA	g	812	X	-	-	-
12	CLA	g	813	X	-	-	-
12	CLA	g	814	X	-	-	-
12	CLA	g	815	X	-	-	-
12	CLA	g	816	X	-	-	-
12	CLA	g	817	X	-	-	-
12	CLA	g	818	X	-	-	-
12	CLA	g	819	X	-	-	-
12	CLA	g	820	X	-	-	-
12	CLA	g	821	X	-	-	-
12	CLA	g	822	X	-	-	-
12	CLA	g	823	X	-	-	-
12	CLA	g	824	X	-	-	-
12	CLA	g	825	X	-	-	-
12	CLA	g	826	X	-	-	-
12	CLA	g	827	X	-	-	-
12	CLA	g	828	X	-	-	-
12	CLA	g	829	X	-	-	-
12	CLA	g	830	X	-	-	-
12	CLA	g	831	X	-	-	-
12	CLA	g	832	X	-	-	-
12	CLA	g	833	X	-	-	-
12	CLA	g	834	X	-	-	-
12	CLA	g	835	X	-	-	-
12	CLA	g	836	X	-	-	-
12	CLA	g	837	X	-	-	-
12	CLA	g	838	X	-	-	-
12	CLA	g	839	X	-	-	-
12	CLA	g	840	X	-	-	-
12	CLA	g	841	X	-	-	-
12	CLA	g	842	X	-	-	-
12	CLA	k	1401	X	-	-	-
12	CLA	l	201	X	-	-	-
12	CLA	l	202	X	-	-	-
12	CLA	l	203	X	-	-	-
12	CLA	l	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	o	1301	X	-	-	-
12	CLA	r	1401	X	-	-	-
12	CLA	s	201	X	-	-	-
12	CLA	s	202	X	-	-	-
12	CLA	s	203	X	-	-	-
12	CLA	s	204	X	-	-	-
13	PQN	A	842	X	-	-	-
13	PQN	B	844	X	-	-	-
13	PQN	E	846	X	-	-	-
13	PQN	G	842	X	-	-	-
13	PQN	a	844	X	-	-	-
13	PQN	b	843	X	-	-	-
13	PQN	e	843	X	-	-	-
13	PQN	g	843	X	-	-	-
14	SF4	C	102	-	-	X	-
14	SF4	H	102	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 87228 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	E	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	e	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	a	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	O	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	o	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	f	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		

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

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

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

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

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

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

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

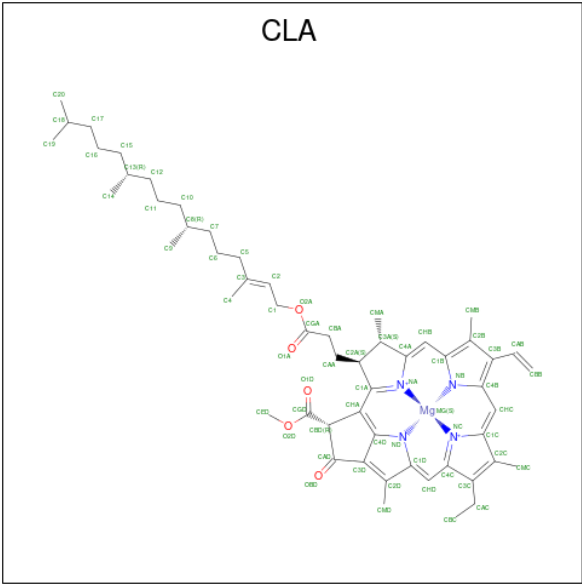
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

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

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

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

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	J	1	Total 100	C 80	Mg 2	N 8	O 10	0
12	J	1	Total 100	C 80	Mg 2	N 8	O 10	0
12	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	L	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	L	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	L	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	L	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	E	1	Total 2166	C 1728	Mg 44	N 176	O 218	0

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Mol	Chain	Residues	Atoms					AltConf
12	E	1	Total	C	Mg	N	O	0
			2166	1728	44	176	218	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	
12	G	1	Total	C	Mg	N	O	0
			2049	1629	42	168	210	

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Mol	Chain	Residues	Atoms					AltConf
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	S	1	Total 100	C 80	Mg 2	N 8	O 10	0
12	S	1	Total 100	C 80	Mg 2	N 8	O 10	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0

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Mol	Chain	Residues	Atoms					AltConf
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	

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Mol	Chain	Residues	Atoms					AltConf
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
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12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
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12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
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12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	s	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	s	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	s	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	s	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0

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Mol	Chain	Residues	Atoms					AltConf
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
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12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
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Mol	Chain	Residues	Atoms					AltConf
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12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
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12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
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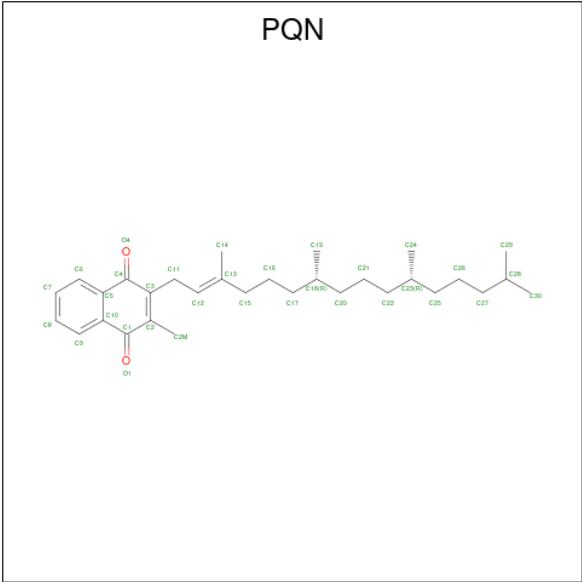
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12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
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12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
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12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
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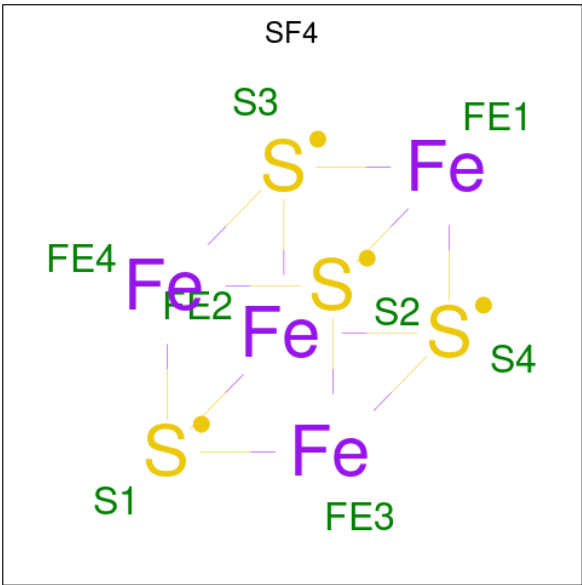
Mol	Chain	Residues	Atoms					AltConf
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12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	l	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	l	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	l	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	l	1	Total 200	C 160	Mg 4	N 16	O 20	0

- Molecule 13 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

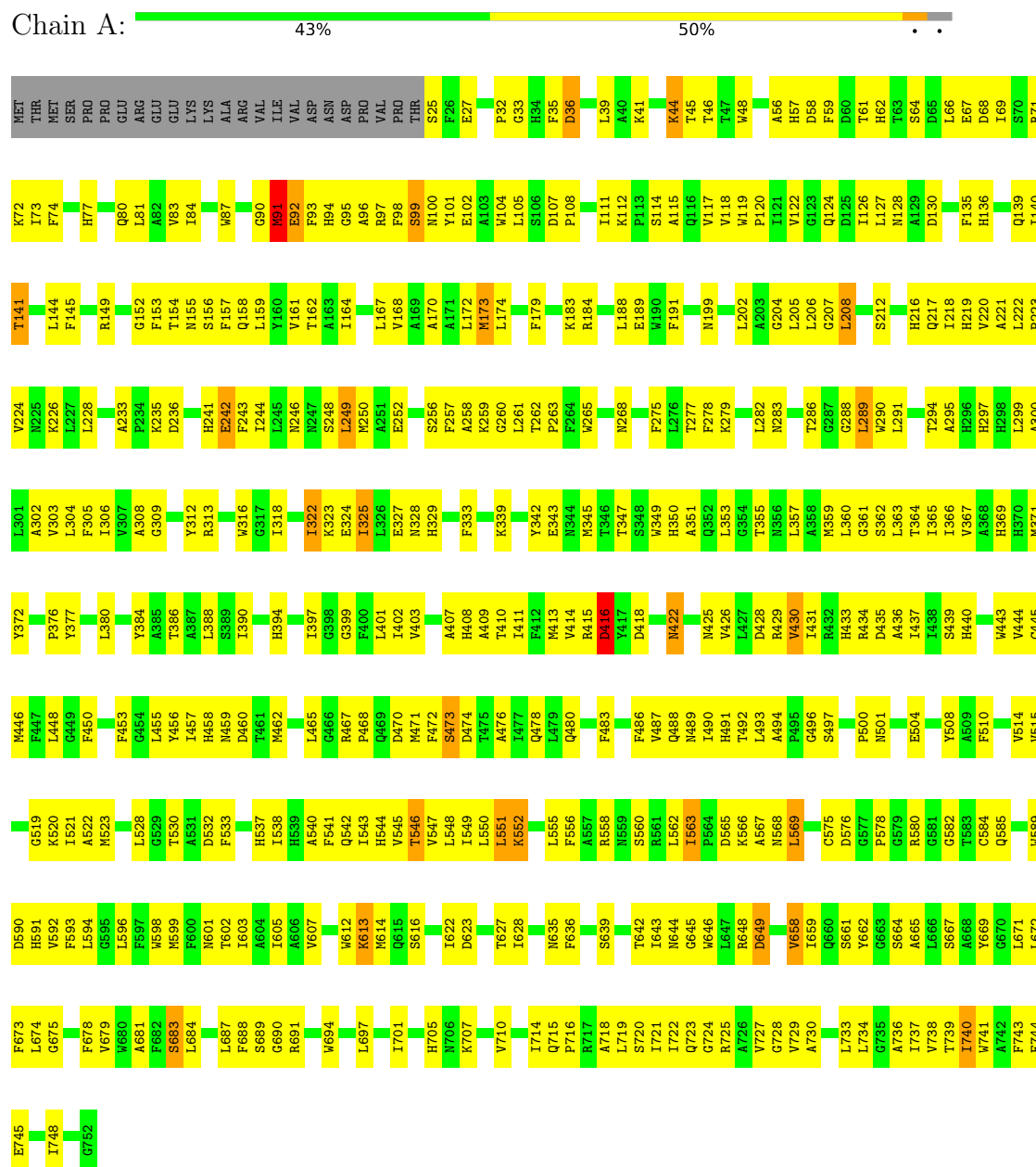


Mol	Chain	Residues	Atoms			AltConf
14	B	1	Total	Fe	S	0
			8	4	4	
14	C	1	Total	Fe	S	0
			16	8	8	
14	C	1	Total	Fe	S	0
			16	8	8	
14	E	1	Total	Fe	S	0
			8	4	4	
14	H	1	Total	Fe	S	0
			16	8	8	
14	H	1	Total	Fe	S	0
			16	8	8	
14	g	1	Total	Fe	S	0
			8	4	4	
14	h	1	Total	Fe	S	0
			16	8	8	
14	h	1	Total	Fe	S	0
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

3 Residue-property plots

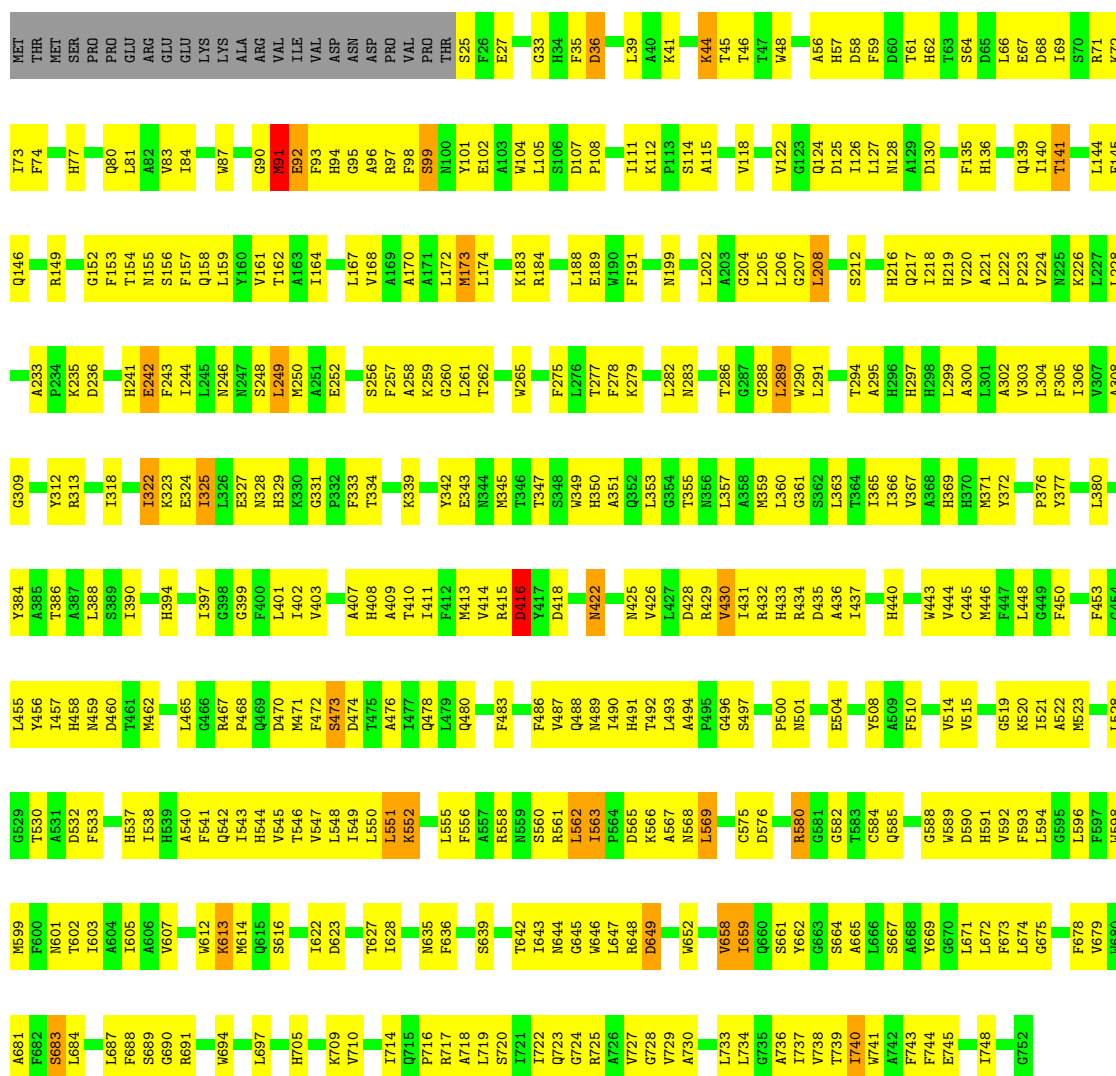
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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

Chain E:  44% 49%



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain e:  91% 5%



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

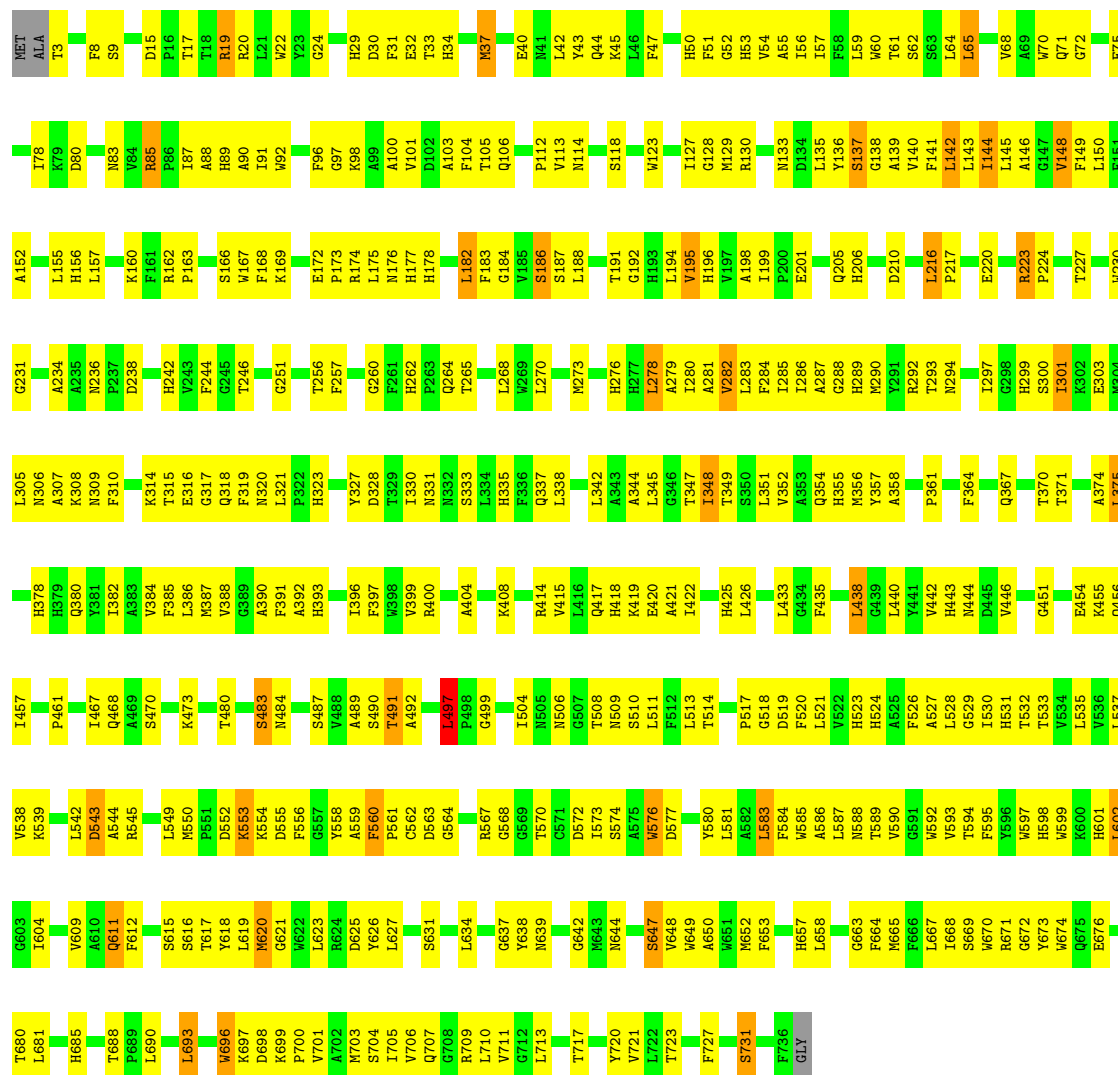
Chain a:  91% 5%





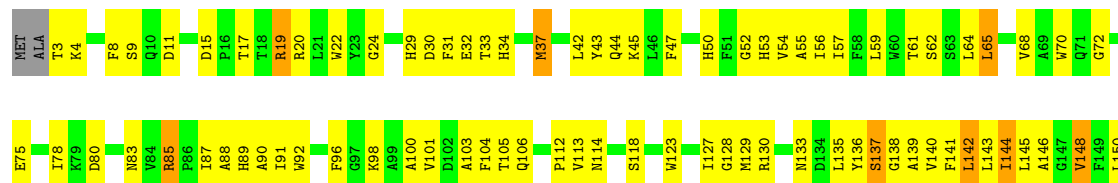
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

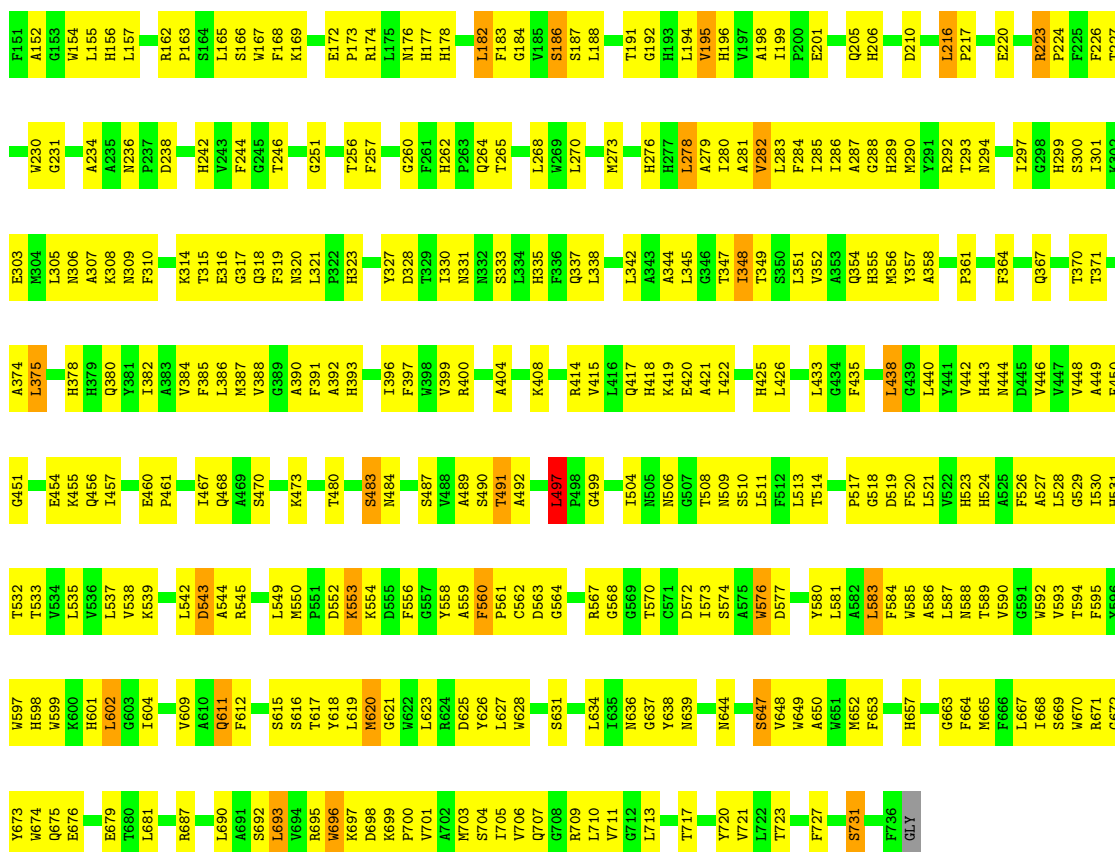
Chain B: 45% 50%



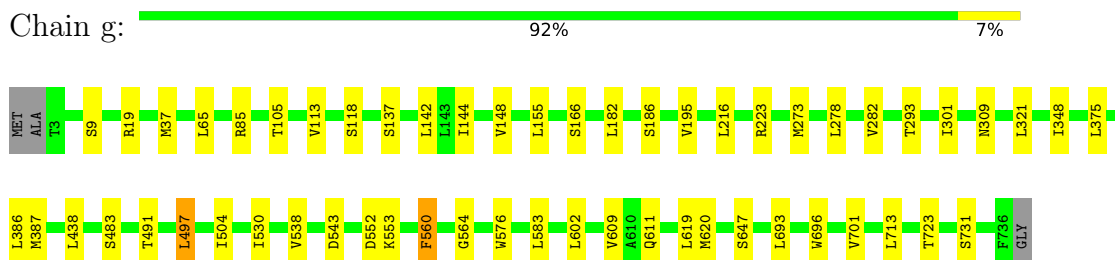
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain G: 44% 51%

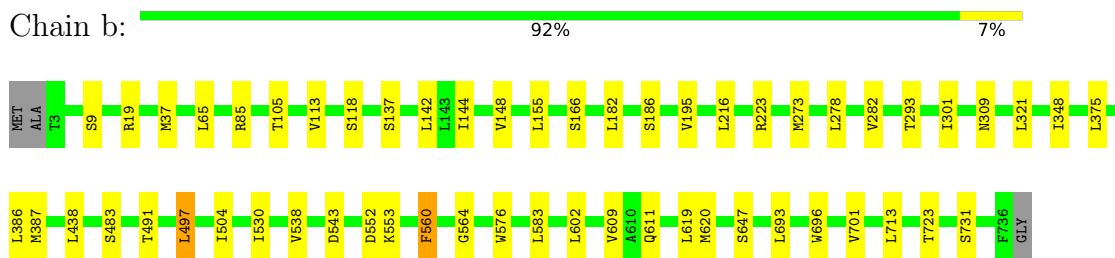




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

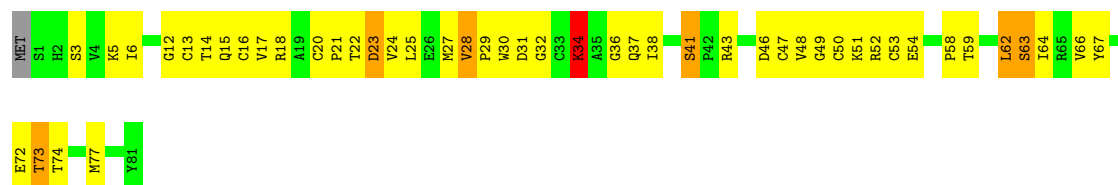


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



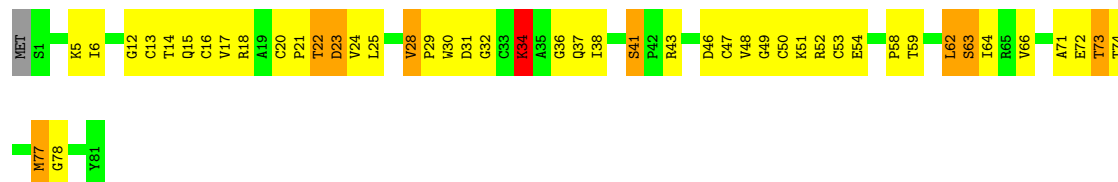
- Molecule 3: Photosystem I iron-sulfur center





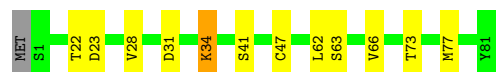
- Molecule 3: Photosystem I iron-sulfur center

Chain H: 41% 46% 10% ..



- Molecule 3: Photosystem I iron-sulfur center

Chain h: 84% 13% ..



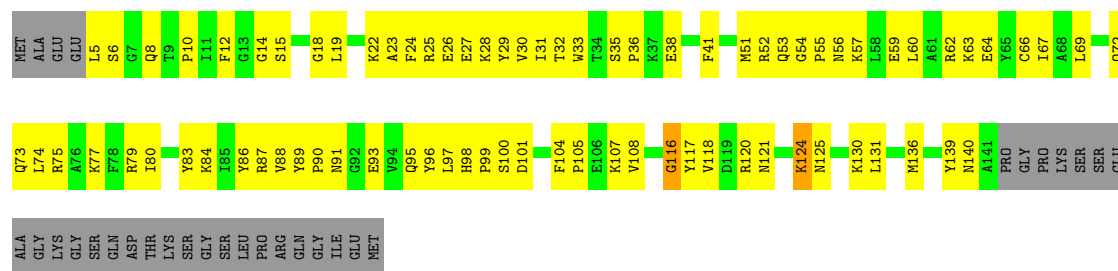
- Molecule 3: Photosystem I iron-sulfur center

Chain c: 84% 13% ..



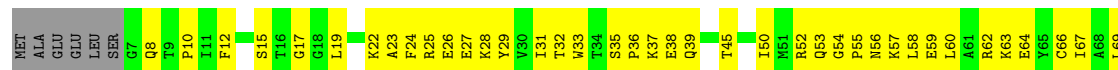
- Molecule 4: Photosystem I reaction center subunit II

Chain D: 35% 46% 18%

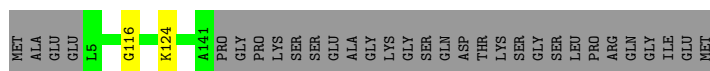
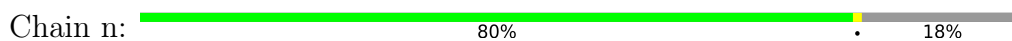


- Molecule 4: Photosystem I reaction center subunit II

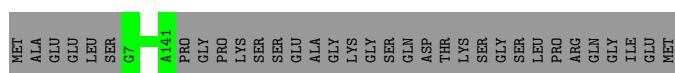
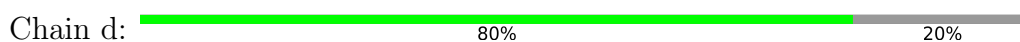
Chain N: 32% 48% 20%



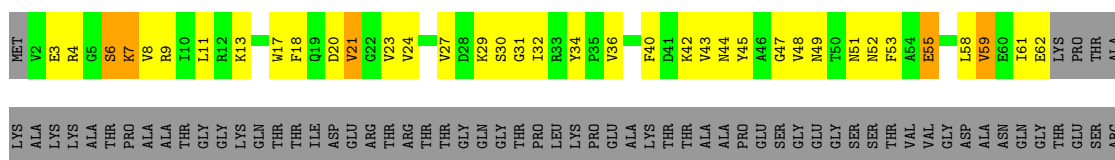
- Molecule 4: Photosystem I reaction center subunit II



- Molecule 4: Photosystem I reaction center subunit II



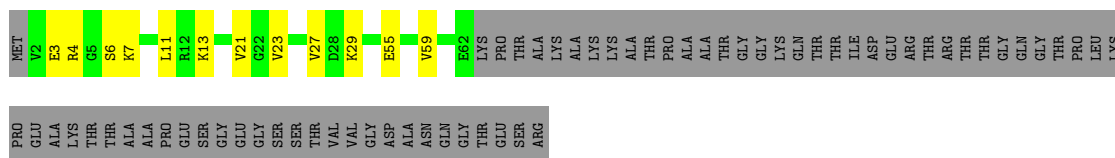
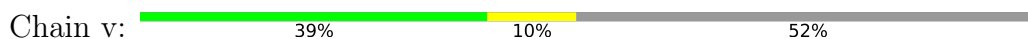
- Molecule 5: Photosystem I reaction center subunit IV



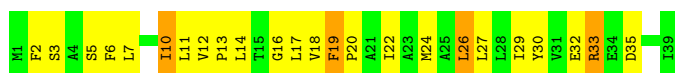
- Molecule 5: Photosystem I reaction center subunit IV



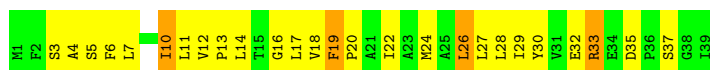
- Molecule 5: Photosystem I reaction center subunit IV



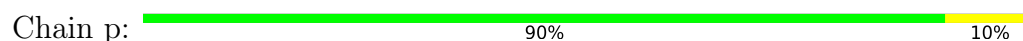
- Molecule 5: Photosystem I reaction center subunit IV



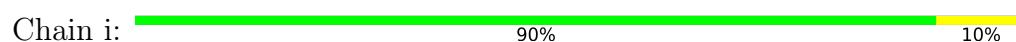
- Molecule 7: Photosystem I reaction center subunit VIII



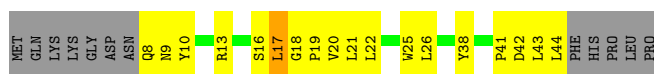
- Molecule 7: Photosystem I reaction center subunit VIII



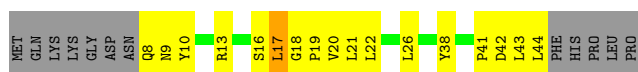
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX

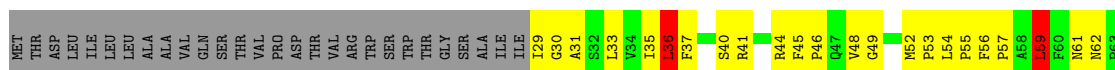


- Molecule 8: Photosystem I reaction center subunit IX

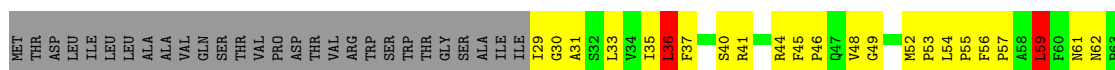




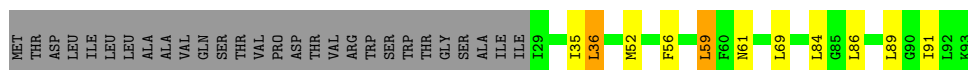
• Molecule 9: Photosystem I reaction center subunit PsaK



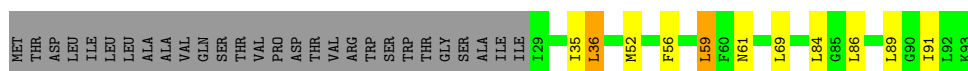
• Molecule 9: Photosystem I reaction center subunit PsaK



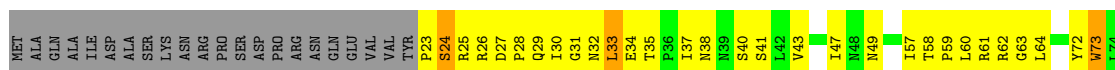
• Molecule 9: Photosystem I reaction center subunit PsaK



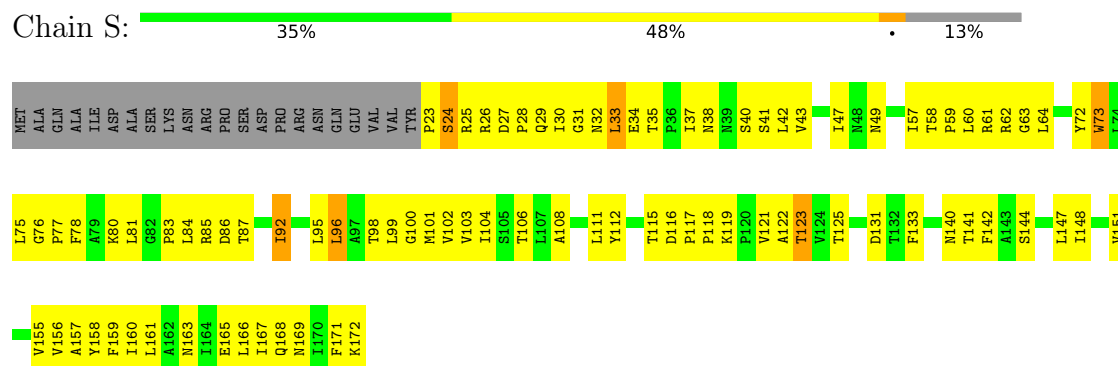
• Molecule 9: Photosystem I reaction center subunit PsaK



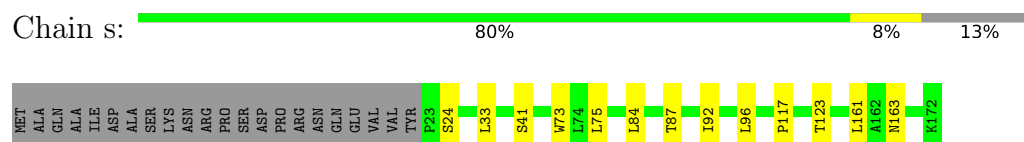
• Molecule 10: Photosystem I reaction center subunit XI



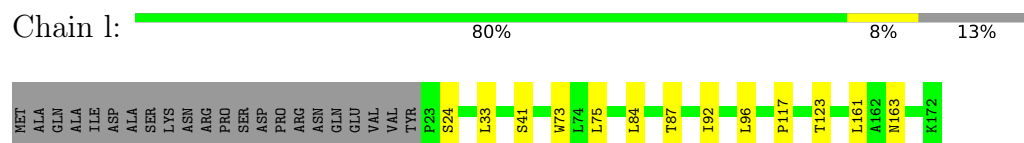
- Molecule 10: Photosystem I reaction center subunit XI



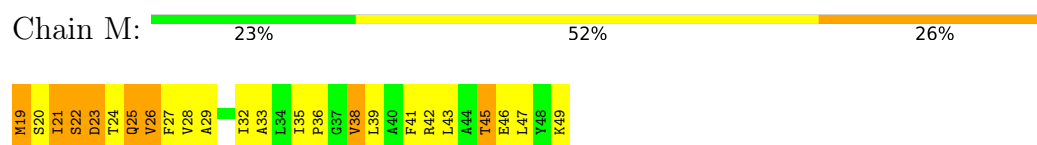
- Molecule 10: Photosystem I reaction center subunit XI



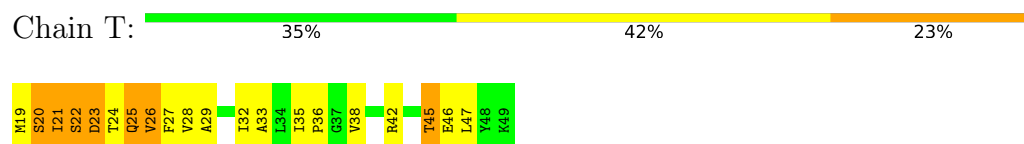
- Molecule 10: Photosystem I reaction center subunit XI



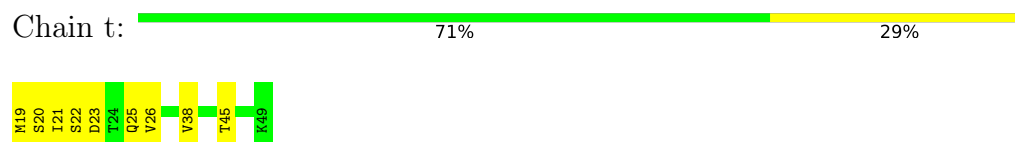
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	60561	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.3	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	0/5908	0.50	2/8056 (0.0%)
1	E	0.30	0/5908	0.50	2/8056 (0.0%)
1	a	0.30	0/5908	0.50	2/8056 (0.0%)
1	e	0.30	0/5908	0.50	2/8056 (0.0%)
2	B	0.30	0/6072	0.50	2/8301 (0.0%)
2	G	0.30	0/6072	0.50	2/8301 (0.0%)
2	b	0.30	0/6072	0.50	2/8301 (0.0%)
2	g	0.30	0/6072	0.50	2/8301 (0.0%)
3	C	0.32	0/615	0.53	0/833
3	H	0.32	0/615	0.53	0/833
3	c	0.32	0/615	0.53	0/833
3	h	0.32	0/615	0.52	0/833
4	D	0.28	0/1105	0.49	0/1489
4	N	0.27	0/1091	0.51	0/1470
4	d	0.30	0/1091	0.53	0/1470
4	n	0.28	0/1105	0.50	0/1489
5	V	0.33	0/502	0.57	0/678
5	W	0.33	0/502	0.57	0/678
5	v	0.33	0/502	0.57	0/678
5	w	0.33	0/502	0.57	0/678
6	F	0.27	0/1119	0.54	2/1522 (0.1%)
6	O	0.28	0/1119	0.54	2/1522 (0.1%)
6	f	0.27	0/1119	0.55	2/1522 (0.1%)
6	o	0.27	0/1119	0.54	2/1522 (0.1%)
7	I	0.30	0/302	0.60	0/411
7	P	0.30	0/302	0.60	0/411
7	i	0.29	0/302	0.60	0/411
7	p	0.30	0/302	0.60	0/411
8	J	0.27	0/321	0.49	0/441
8	Q	0.27	0/321	0.49	0/441
8	j	0.26	0/321	0.49	0/441
8	q	0.27	0/321	0.49	0/441

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	K	0.30	0/484	0.74	3/659 (0.5%)
9	R	0.30	0/484	0.74	3/659 (0.5%)
9	k	0.30	0/484	0.74	3/659 (0.5%)
9	r	0.30	0/484	0.74	3/659 (0.5%)
10	L	0.37	1/1165 (0.1%)	0.51	0/1597
10	S	0.37	1/1165 (0.1%)	0.51	0/1597
10	l	0.37	1/1165 (0.1%)	0.51	0/1597
10	s	0.37	1/1165 (0.1%)	0.51	0/1597
11	M	0.31	0/241	0.55	0/326
11	T	0.32	0/241	0.55	0/326
11	m	0.32	0/241	0.55	0/326
11	t	0.32	0/241	0.55	0/326
All	All	0.31	4/71308 (0.0%)	0.52	36/97214 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	E	0	3
1	a	0	3
1	e	0	3
2	B	0	3
2	G	0	3
2	b	0	3
2	g	0	3
3	C	0	1
3	H	0	1
3	c	0	1
3	h	0	1
4	D	0	1
4	n	0	1
7	I	0	1
7	P	0	1
7	i	0	1
7	p	0	1
9	K	0	1
9	R	0	1
9	k	0	1
9	r	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	L	0	1
10	S	0	1
10	l	0	1
10	s	0	1
All	All	0	42

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	s	73	TRP	C-N	7.98	1.52	1.34
10	S	73	TRP	C-N	7.96	1.52	1.34
10	L	73	TRP	C-N	7.96	1.52	1.34
10	l	73	TRP	C-N	7.95	1.52	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	r	36	LEU	CA-CB-CG	8.39	134.59	115.30
9	R	36	LEU	CA-CB-CG	8.39	134.59	115.30
9	K	36	LEU	CA-CB-CG	8.38	134.58	115.30
9	k	36	LEU	CA-CB-CG	8.38	134.57	115.30
2	G	497	LEU	CA-CB-CG	7.71	133.03	115.30
2	b	497	LEU	CA-CB-CG	7.71	133.02	115.30
2	B	497	LEU	CA-CB-CG	7.70	133.01	115.30
2	g	497	LEU	CA-CB-CG	7.69	132.99	115.30
6	O	141	LEU	CA-CB-CG	6.76	130.86	115.30
6	F	141	LEU	CA-CB-CG	6.75	130.83	115.30
6	o	141	LEU	CA-CB-CG	6.74	130.80	115.30
6	f	141	LEU	CA-CB-CG	6.74	130.80	115.30
6	O	152	LEU	CA-CB-CG	6.26	129.69	115.30
6	F	152	LEU	CA-CB-CG	6.25	129.67	115.30
6	o	152	LEU	CA-CB-CG	6.24	129.65	115.30
6	f	152	LEU	CA-CB-CG	6.24	129.65	115.30
9	k	86	LEU	CA-CB-CG	5.71	128.44	115.30
9	K	86	LEU	CA-CB-CG	5.71	128.43	115.30
9	R	86	LEU	CA-CB-CG	5.69	128.39	115.30
9	r	86	LEU	CA-CB-CG	5.69	128.39	115.30
1	a	91	MET	CB-CG-SD	5.58	129.15	112.40
1	A	91	MET	CB-CG-SD	5.58	129.12	112.40
1	e	91	MET	CB-CG-SD	5.57	129.10	112.40
1	E	91	MET	CB-CG-SD	5.56	129.09	112.40
1	e	569	LEU	CA-CB-CG	5.48	127.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	LEU	CA-CB-CG	5.48	127.90	115.30
1	a	569	LEU	CA-CB-CG	5.48	127.90	115.30
1	E	569	LEU	CA-CB-CG	5.47	127.88	115.30
2	b	497	LEU	CB-CG-CD2	5.21	119.85	111.00
2	g	497	LEU	CB-CG-CD2	5.20	119.85	111.00
2	B	497	LEU	CB-CG-CD2	5.20	119.83	111.00
2	G	497	LEU	CB-CG-CD2	5.19	119.83	111.00
9	k	59	LEU	CA-CB-CG	5.15	127.14	115.30
9	R	59	LEU	CA-CB-CG	5.12	127.08	115.30
9	K	59	LEU	CA-CB-CG	5.11	127.05	115.30
9	r	59	LEU	CA-CB-CG	5.10	127.04	115.30

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	ALA	Peptide
1	A	416	ASP	Peptide
1	A	669	TYR	Peptide
2	B	560	PHE	Peptide
2	B	576	TRP	Peptide
2	B	696	TRP	Peptide
3	C	34	LYS	Peptide
4	D	116	GLY	Peptide
1	E	258	ALA	Peptide
1	E	416	ASP	Peptide
1	E	669	TYR	Peptide
2	G	560	PHE	Peptide
2	G	576	TRP	Peptide
2	G	696	TRP	Peptide
3	H	34	LYS	Peptide
7	I	10	ILE	Peptide
9	K	61	ASN	Peptide
10	L	117	PRO	Peptide
7	P	10	ILE	Peptide
9	R	61	ASN	Peptide
10	S	117	PRO	Peptide
1	a	258	ALA	Peptide
1	a	416	ASP	Peptide
1	a	669	TYR	Peptide
2	b	560	PHE	Peptide
2	b	576	TRP	Peptide

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Mol	Chain	Res	Type	Group
2	b	696	TRP	Peptide
3	c	34	LYS	Peptide
1	e	258	ALA	Peptide
1	e	416	ASP	Peptide
1	e	669	TYR	Peptide
2	g	560	PHE	Peptide
2	g	576	TRP	Peptide
2	g	696	TRP	Peptide
3	h	34	LYS	Peptide
7	i	10	ILE	Peptide
9	k	61	ASN	Peptide
10	l	117	PRO	Peptide
4	n	116	GLY	Peptide
7	p	10	ILE	Peptide
9	r	61	ASN	Peptide
10	s	117	PRO	Peptide

5.2 Too-close contacts [i](#)

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	A	5713	0	5565	431	0
1	E	5713	0	5565	440	0
1	a	5713	0	5565	0	0
1	e	5713	0	5565	0	0
2	B	5857	0	5642	426	0
2	G	5857	0	5642	449	0
2	b	5857	0	5642	0	0
2	g	5857	0	5642	0	0
3	C	605	0	590	61	0
3	H	605	0	590	52	0
3	c	605	0	590	0	0
3	h	605	0	590	0	0
4	D	1080	0	1083	92	0
4	N	1066	0	1067	84	0
4	d	1066	0	1067	0	0
4	n	1080	0	1083	0	0
5	V	494	0	493	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	W	494	0	493	30	0
5	v	494	0	493	0	0
5	w	494	0	493	0	0
6	F	1093	0	1095	53	0
6	O	1093	0	1095	58	0
6	f	1093	0	1095	0	0
6	o	1093	0	1095	0	0
7	I	295	0	314	18	0
7	P	295	0	314	23	0
7	i	295	0	314	0	0
7	p	295	0	314	0	0
8	J	311	0	323	24	0
8	Q	311	0	323	18	0
8	j	311	0	323	0	0
8	q	311	0	323	0	0
9	K	474	0	521	30	0
9	R	474	0	521	33	0
9	k	474	0	521	0	0
9	r	474	0	521	0	0
10	L	1134	0	1151	75	0
10	S	1134	0	1151	85	0
10	l	1134	0	1151	0	0
10	s	1134	0	1151	0	0
11	M	238	0	257	29	0
11	T	238	0	257	19	0
11	m	238	0	257	0	0
11	t	238	0	257	0	0
12	A	2016	0	1561	231	0
12	B	2049	0	1576	241	0
12	E	2166	0	1678	250	0
12	F	45	0	33	4	0
12	G	2049	0	1576	250	0
12	J	100	0	78	13	0
12	K	45	0	33	2	0
12	L	200	0	156	14	0
12	O	45	0	33	1	0
12	R	45	0	33	3	0
12	S	100	0	78	6	0
12	a	2066	0	1600	0	0
12	b	2049	0	1576	0	0
12	e	2165	0	1678	0	0
12	f	45	0	33	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	g	2000	0	1537	0	0
12	k	45	0	33	0	0
12	l	200	0	156	0	0
12	o	45	0	33	0	0
12	r	45	0	33	0	0
12	s	200	0	156	0	0
13	A	33	0	46	7	0
13	B	33	0	46	4	0
13	E	33	0	46	9	0
13	G	33	0	46	4	0
13	a	33	0	46	0	0
13	b	33	0	46	0	0
13	e	33	0	46	0	0
13	g	33	0	46	0	0
14	B	8	0	0	0	0
14	C	16	0	0	7	0
14	E	8	0	0	0	0
14	H	16	0	0	7	0
14	a	8	0	0	0	0
14	c	16	0	0	0	0
14	g	8	0	0	0	0
14	h	16	0	0	0	0
All	All	87228	0	82142	2889	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 17.

All (2889) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:GLN:HA	6:F:164:ARG:HH22	1.65	0.93
4:D:29:TYR:HB2	4:D:60:LEU:O	1.94	0.92
6:O:60:ARG:HH12	8:Q:43:LEU:HA	1.34	0.91
2:G:690:LEU:HD21	10:S:47:ILE:HD11	2.39	0.88
1:A:448:LEU:HD22	1:A:541:PHE:HB2	1.58	0.85
1:E:448:LEU:HD22	1:E:541:PHE:HB2	1.58	0.85
2:B:262:HIS:HD2	2:B:265:THR:H	1.25	0.84
2:G:262:HIS:HD2	2:G:265:THR:H	1.26	0.84
4:N:35:SER:OG	4:N:56:ASN:ND2	2.10	0.84
4:D:35:SER:OG	4:D:56:ASN:ND2	2.22	0.84
2:G:83:ASN:O	2:G:85:ARG:NH1	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ASN:O	2:B:85:ARG:NH1	2.11	0.83
10:L:80:LYS:HE3	12:L:204:CLA:HHB	1.61	0.82
1:E:339:LYS:O	1:E:425:ASN:ND2	2.12	0.82
10:S:80:LYS:HE3	12:S:1502:CLA:HHB	1.61	0.82
4:D:59:GLU:N	10:L:29:GLN:OE1	2.73	0.82
2:B:690:LEU:HD21	10:L:47:ILE:HD11	1.62	0.82
1:A:339:LYS:O	1:A:425:ASN:ND2	2.12	0.81
2:G:103:ALA:O	2:G:106:GLN:NE2	2.14	0.81
2:B:103:ALA:O	2:B:106:GLN:NE2	2.14	0.81
1:E:343:GLU:O	1:E:347:THR:OG1	1.99	0.81
1:A:328:ASN:HD21	12:A:821:CLA:H2A	1.46	0.80
1:A:343:GLU:O	1:A:347:THR:OG1	1.99	0.80
1:A:328:ASN:HD21	12:A:823:CLA:H2A	24.67	0.80
3:C:54:GLU:HB2	3:C:62:LEU:HD22	1.64	0.79
1:A:575:CYS:SG	1:A:576:ASP:N	2.56	0.79
1:E:575:CYS:SG	1:E:576:ASP:N	2.56	0.79
1:E:328:ASN:HD21	12:E:824:CLA:H2A	1.46	0.79
4:N:29:TYR:HB2	4:N:60:LEU:O	1.83	0.79
2:G:549:LEU:HD21	2:G:567:ARG:HH21	1.48	0.78
1:E:328:ASN:HD21	12:E:822:CLA:H2A	15.25	0.78
3:H:54:GLU:HB2	3:H:62:LEU:HD22	1.64	0.78
2:B:549:LEU:HD21	2:B:567:ARG:HH21	1.49	0.78
10:L:61:ARG:NH2	10:S:140:ASN:O	2.15	0.78
12:B:830:CLA:HED1	12:B:837:CLA:HAB	1.67	0.77
5:W:55:GLU:CD	5:W:55:GLU:H	1.88	0.77
2:G:419:LYS:HD2	2:G:542:LEU:HD13	1.66	0.77
3:H:14:THR:OG1	3:H:18:ARG:NH2	2.18	0.77
2:B:399:VAL:HG11	2:B:544:ALA:HB3	1.67	0.77
2:G:399:VAL:HG11	2:G:544:ALA:HB3	1.67	0.77
12:G:829:CLA:HED1	12:G:836:CLA:HAB	33.35	0.77
12:E:801:CLA:HHC	12:E:801:CLA:HBB1	1.68	0.77
12:G:827:CLA:HED1	12:G:835:CLA:HAB	1.67	0.77
4:N:74:LEU:HB3	4:N:80:ILE:HB	1.66	0.77
5:V:55:GLU:CD	5:V:55:GLU:H	1.88	0.77
12:A:801:CLA:HHC	12:A:801:CLA:HBB1	1.68	0.76
1:A:476:ALA:O	1:A:478:GLN:NE2	2.19	0.76
3:C:14:THR:OG1	3:C:18:ARG:NH2	2.18	0.76
10:S:49:ASN:HB2	12:S:1501:CLA:HAC1	1.68	0.76
2:B:419:LYS:HD2	2:B:542:LEU:HD13	1.66	0.76
12:B:828:CLA:HED1	12:B:836:CLA:HAB	51.10	0.76
4:D:74:LEU:HB3	4:D:80:ILE:HB	1.89	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:49:ASN:HB2	12:L:202:CLA:HAC1	1.68	0.76
12:E:835:CLA:H2	10:S:78:PHE:HB3	1.66	0.76
10:L:81:LEU:O	10:L:85:ARG:NH1	2.19	0.76
12:G:837:CLA:HBA2	12:G:838:CLA:HAA2	1.68	0.75
1:E:476:ALA:O	1:E:478:GLN:NE2	2.18	0.75
12:B:839:CLA:HBA2	12:B:840:CLA:HAA2	1.68	0.75
1:E:722:ILE:HG13	1:E:723:GLN:H	1.52	0.75
2:B:480:THR:H	2:B:483:SER:HB3	1.52	0.75
5:W:32:ILE:HG22	5:W:34:TYR:H	1.51	0.75
4:D:28:LYS:HB2	4:D:88:VAL:HB	1.67	0.75
5:V:32:ILE:HG22	5:V:34:TYR:H	1.51	0.75
12:B:838:CLA:HBA2	12:B:839:CLA:HAA2	19.73	0.75
2:G:19:ARG:NH2	3:H:72:GLU:OE1	2.59	0.75
2:G:480:THR:H	2:G:483:SER:HB3	1.51	0.75
3:C:34:LYS:NZ	5:W:30:SER:HB2	128.84	0.74
10:S:33:LEU:O	10:S:38:ASN:ND2	2.20	0.74
10:L:33:LEU:O	10:L:38:ASN:ND2	2.20	0.74
9:R:57:PRO:HA	9:R:65:VAL:HB	1.69	0.74
9:K:57:PRO:HA	9:K:65:VAL:HB	1.69	0.74
10:S:81:LEU:O	10:S:85:ARG:NH1	2.19	0.74
12:G:838:CLA:HBA2	12:G:839:CLA:HAA2	10.29	0.74
1:A:722:ILE:HG13	1:A:723:GLN:H	1.52	0.74
2:G:70:TRP:HD1	11:T:21:ILE:HD11	1.50	0.74
10:L:34:GLU:OE1	10:L:34:GLU:N	2.21	0.73
9:R:53:PRO:HD2	9:R:54:LEU:HD12	1.70	0.73
1:E:697:LEU:HD11	2:G:539:LYS:HE3	2.17	0.73
12:A:841:CLA:H2	12:A:841:CLA:HMB2	1.69	0.73
9:K:53:PRO:HD2	9:K:54:LEU:HD12	1.70	0.73
12:E:842:CLA:HMB2	12:E:842:CLA:H2	12.79	0.72
10:S:34:GLU:OE1	10:S:34:GLU:N	2.21	0.72
1:E:217:GLN:HA	1:E:221:ALA:HB3	1.72	0.72
4:N:72:GLN:O	4:N:77:LYS:NZ	2.24	0.72
2:B:518:GLY:HA2	2:B:521:LEU:HD12	1.72	0.72
12:A:803:CLA:H2	12:A:811:CLA:H2	1.72	0.72
1:E:353:LEU:HB2	12:E:806:CLA:HMD3	1.72	0.72
3:C:34:LYS:NZ	5:V:30:SER:HB2	2.04	0.72
2:G:518:GLY:HA2	2:G:521:LEU:HD12	1.72	0.72
1:A:217:GLN:HA	1:A:221:ALA:HB3	1.72	0.72
4:D:84:LYS:HD3	4:D:99:PRO:HD3	3.55	0.72
1:E:353:LEU:HB2	12:E:804:CLA:HMD3	28.60	0.72
1:E:643:ILE:HA	1:E:646:TRP:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:841:CLA:HMD2	13:G:842:PQN:H171	1.72	0.71
10:L:140:ASN:O	10:S:61:ARG:NH2	20.31	0.71
1:A:67:GLU:OE2	1:A:71:ARG:NH2	2.23	0.71
12:E:804:CLA:H2	12:E:812:CLA:H2	19.61	0.71
6:F:157:ASP:OD2	6:F:157:ASP:N	2.21	0.71
1:A:643:ILE:HA	1:A:646:TRP:HB3	1.72	0.71
1:E:377:TYR:HB2	1:E:380:LEU:HD11	1.73	0.71
1:E:67:GLU:OE2	1:E:71:ARG:NH2	2.23	0.71
1:E:73:ILE:HG22	1:E:77:HIS:CE1	2.26	0.70
1:A:73:ILE:HG22	1:A:77:HIS:CE1	2.26	0.70
1:E:349:TRP:HE1	12:E:804:CLA:HHD	24.17	0.70
1:A:433:HIS:HD2	1:A:437:ILE:HD11	1.57	0.70
1:A:353:LEU:HB2	12:A:805:CLA:HMD3	38.51	0.70
4:D:72:GLN:O	4:D:77:LYS:NZ	2.24	0.70
1:A:349:TRP:HE1	12:A:803:CLA:HHD	1.56	0.70
1:A:377:TYR:HB2	1:A:380:LEU:HD11	1.73	0.70
1:A:66:LEU:HA	1:A:69:ILE:HD12	1.74	0.70
1:E:433:HIS:HD2	1:E:437:ILE:HD11	1.57	0.70
2:G:692:SER:OG	10:S:123:THR:O	3.19	0.70
1:E:66:LEU:HA	1:E:69:ILE:HD12	1.74	0.70
2:G:695:ARG:NH2	10:S:118:PRO:O	3.74	0.70
6:F:152:LEU:H	6:F:152:LEU:HD12	1.57	0.70
6:O:152:LEU:HD12	6:O:152:LEU:H	1.57	0.70
1:A:353:LEU:HB2	12:A:803:CLA:HMD3	1.72	0.70
12:B:843:CLA:HMD2	13:B:844:PQN:H171	1.73	0.70
1:E:467:ARG:HH22	2:G:98:LYS:HB2	2.31	0.70
3:H:63:SER:OG	14:H:102:SF4:S2	2.50	0.70
4:N:28:LYS:HB2	4:N:88:VAL:HB	1.73	0.70
2:B:157:LEU:O	2:B:162:ARG:NH2	2.25	0.70
2:B:673:TYR:OH	12:B:805:CLA:OBD	27.16	0.70
1:E:349:TRP:HE1	12:E:806:CLA:HHD	1.56	0.70
2:G:157:LEU:O	2:G:162:ARG:NH2	2.25	0.70
1:E:652:TRP:HZ3	2:G:628:TRP:CE3	2.42	0.70
4:N:84:LYS:HD3	4:N:99:PRO:HD3	1.73	0.70
3:C:63:SER:OG	14:C:102:SF4:S2	2.50	0.69
12:E:806:CLA:H2	12:E:814:CLA:H2	1.72	0.69
12:A:838:CLA:HBA1	12:A:838:CLA:HED2	1.74	0.69
1:A:183:LYS:O	1:A:184:ARG:NH1	2.26	0.69
1:E:183:LYS:O	1:E:184:ARG:NH1	2.26	0.69
5:V:34:TYR:HB2	5:V:52:ASN:HD22	1.58	0.69
5:W:34:TYR:HB2	5:W:52:ASN:HD22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:687:ARG:NH1	10:S:32:ASN:OD1	3.37	0.69
1:A:468:PRO:HA	1:A:471:MET:HG2	1.75	0.69
1:E:468:PRO:HA	1:E:471:MET:HG2	1.75	0.69
7:I:3:SER:OG	11:M:21:ILE:O	2.67	0.69
2:B:143:LEU:HD22	11:M:32:ILE:CD1	3.37	0.69
12:E:842:CLA:HED2	12:E:842:CLA:HBA1	1.74	0.69
1:E:199:ASN:ND2	1:E:309:GLY:O	2.25	0.69
1:E:690:GLY:HA3	2:G:572:ASP:HB2	2.12	0.69
12:E:839:CLA:HED2	12:E:839:CLA:HBA1	6.90	0.69
1:A:349:TRP:HE1	12:A:805:CLA:HHH	35.14	0.68
1:A:460:ASP:OD1	1:A:642:THR:HG23	1.93	0.68
2:G:70:TRP:CD1	11:T:21:ILE:HD11	2.27	0.68
2:G:342:LEU:HB2	2:G:390:ALA:HB2	1.76	0.68
1:E:460:ASP:OD1	1:E:642:THR:HG23	1.93	0.68
1:E:687:LEU:HD11	2:G:668:ILE:HG12	1.98	0.68
4:N:87:ARG:HB2	4:N:97:LEU:HD11	1.76	0.68
4:N:59:GLU:N	10:S:29:GLN:OE1	2.23	0.68
2:B:342:LEU:HB2	2:B:390:ALA:HB2	1.76	0.68
1:E:648:ARG:HH12	2:G:639:ASN:HD22	1.86	0.68
3:H:13:CYS:O	3:H:15:GLN:NE2	2.26	0.68
1:A:429:ARG:NE	12:A:831:CLA:OBD	49.58	0.68
3:C:34:LYS:HZ1	5:W:30:SER:HB2	129.69	0.68
1:A:207:GLY:HA3	1:A:306:ILE:HD11	1.76	0.68
2:B:96:PHE:HD2	2:B:101:VAL:HG21	1.59	0.68
3:C:13:CYS:O	3:C:15:GLN:NE2	2.26	0.68
4:D:73:GLN:HA	4:D:77:LYS:HZ3	1.59	0.68
1:E:207:GLY:HA3	1:E:306:ILE:HD11	1.76	0.68
2:B:157:LEU:HG	2:B:162:ARG:HH12	1.59	0.67
4:D:87:ARG:HB2	4:D:97:LEU:HD11	1.99	0.67
2:G:553:LYS:NZ	2:G:573:ILE:O	2.28	0.67
2:G:70:TRP:HE1	7:P:4:ALA:HB2	1.59	0.67
12:G:840:CLA:HHB	13:G:842:PQN:H252	1.76	0.67
2:B:553:LYS:NZ	2:B:573:ILE:O	2.28	0.67
10:L:96:LEU:HA	10:L:99:LEU:HD12	1.77	0.67
1:E:359:MET:HE1	12:E:824:CLA:HMA1	24.55	0.67
2:G:96:PHE:HD2	2:G:101:VAL:HG21	1.59	0.67
10:S:165:GLU:O	10:S:169:ASN:ND2	2.28	0.67
1:A:359:MET:HE3	12:A:825:CLA:HHB	14.15	0.67
2:B:580:TYR:HE2	2:B:709:ARG:HE	1.43	0.67
1:E:68:ASP:HA	1:E:71:ARG:HD2	1.76	0.67
1:E:388:LEU:HD11	1:E:748:ILE:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:157:LEU:HG	2:G:162:ARG:HH12	1.60	0.67
1:A:233:ALA:O	1:A:236:ASP:N	2.28	0.67
12:E:824:CLA:HED2	12:E:824:CLA:H2A	4.39	0.67
10:L:165:GLU:O	10:L:169:ASN:ND2	2.28	0.67
2:B:70:TRP:HD1	11:M:21:ILE:HD11	2.15	0.67
3:C:27:MET:HB2	4:D:107:LYS:NZ	2.09	0.67
2:G:539:LYS:O	2:G:543:ASP:HB2	1.95	0.67
2:G:580:TYR:HE2	2:G:709:ARG:HE	1.43	0.67
6:O:157:ASP:N	6:O:157:ASP:OD2	2.21	0.67
1:A:388:LEU:HD11	1:A:748:ILE:HG21	1.76	0.66
1:A:68:ASP:HA	1:A:71:ARG:HD2	1.76	0.66
12:A:823:CLA:HED2	12:A:823:CLA:H2A	1.77	0.66
4:D:89:TYR:HD2	4:D:93:GLU:HB2	1.61	0.66
1:E:233:ALA:O	1:E:236:ASP:N	2.28	0.66
12:E:826:CLA:H2A	12:E:826:CLA:HED2	1.77	0.66
3:C:27:MET:HB2	4:D:107:LYS:HZ3	1.59	0.66
2:B:183:PHE:HB2	12:B:822:CLA:HMC1	1.78	0.66
12:E:821:CLA:HBD	9:R:48:VAL:HG12	14.32	0.66
2:G:433:LEU:HD22	2:G:528:LEU:HB2	1.78	0.66
9:K:46:PRO:HB2	9:K:48:VAL:HG13	1.76	0.66
2:B:539:LYS:O	2:B:543:ASP:HB2	1.95	0.66
2:B:597:TRP:O	2:B:601:HIS:ND1	2.29	0.66
2:G:191:THR:HA	2:G:194:LEU:HD12	1.77	0.66
10:S:96:LEU:HA	10:S:99:LEU:HD12	1.77	0.66
2:B:183:PHE:HB2	12:B:820:CLA:HMC1	15.29	0.66
2:G:183:PHE:HB2	12:G:821:CLA:HMC1	11.92	0.66
6:O:60:ARG:NH2	8:Q:42:ASP:O	2.29	0.66
12:B:842:CLA:HHB	13:B:844:PQN:H252	1.76	0.66
1:E:612:TRP:O	1:E:616:SER:HB2	1.97	0.65
1:E:652:TRP:HZ3	2:G:628:TRP:HE3	1.90	0.65
1:E:429:ARG:NE	12:E:830:CLA:OBD	43.39	0.65
9:R:46:PRO:HB2	9:R:48:VAL:HG13	1.76	0.65
5:W:9:ARG:HG3	5:W:61:ILE:HD11	1.78	0.65
3:C:34:LYS:HZ1	5:V:30:SER:HB2	1.61	0.65
4:D:28:LYS:O	4:D:88:VAL:N	2.44	0.65
12:A:840:CLA:OBD	6:F:108:LEU:HD21	88.50	0.65
2:B:191:THR:HA	2:B:194:LEU:HD12	1.78	0.65
5:V:9:ARG:HG3	5:V:61:ILE:HD11	1.78	0.65
1:A:199:ASN:ND2	1:A:309:GLY:O	2.25	0.65
1:E:582:GLY:H	2:G:671:ARG:HD3	2.22	0.65
9:R:55:PRO:HD2	9:R:66:GLY:HA3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:17:TRP:HB3	5:V:20:ASP:HB2	1.79	0.65
1:A:612:TRP:O	1:A:616:SER:HB2	1.97	0.65
2:B:433:LEU:HD22	2:B:528:LEU:HB2	1.78	0.65
12:G:808:CLA:HBD	7:P:11:LEU:HD11	1.78	0.65
2:B:92:TRP:CZ2	10:S:172:LYS:HD3	53.30	0.65
1:A:721:ILE:HA	13:A:842:PQN:H7	1.78	0.65
1:A:497:SER:HA	2:B:227:THR:O	119.63	0.65
12:E:802:CLA:H3A	12:E:802:CLA:CGA	2.27	0.65
2:G:358:ALA:HB2	12:G:829:CLA:HBC3	18.47	0.65
1:A:540:ALA:O	1:A:544:HIS:ND1	2.30	0.65
12:A:802:CLA:CGA	12:A:802:CLA:H3A	3.72	0.65
12:B:801:CLA:CGA	12:B:801:CLA:H3A	2.27	0.65
2:G:183:PHE:HB2	12:G:819:CLA:HMC1	1.78	0.65
9:K:55:PRO:HD2	9:K:66:GLY:HA3	1.79	0.65
5:W:17:TRP:HB3	5:W:20:ASP:HB2	1.79	0.65
8:J:19:PRO:HG3	12:J:1101:CLA:C1D	2.27	0.65
10:L:62:ARG:NH1	10:L:131:ASP:OD2	2.30	0.65
1:E:429:ARG:NE	12:E:832:CLA:OBD	2.23	0.64
10:S:62:ARG:NH1	10:S:131:ASP:OD2	2.30	0.64
1:E:644:ASN:OD1	1:E:645:GLY:N	2.29	0.64
2:G:597:TRP:O	2:G:601:HIS:ND1	2.28	0.64
12:G:801:CLA:H3A	12:G:801:CLA:CGA	4.23	0.64
2:B:358:ALA:HB2	12:B:828:CLA:HBC3	35.02	0.64
1:E:297:HIS:HB2	12:E:817:CLA:C1B	26.83	0.64
1:A:648:ARG:NH2	2:B:638:TYR:O	2.31	0.64
1:E:540:ALA:O	1:E:544:HIS:ND1	2.30	0.64
1:E:720:SER:O	1:E:724:GLY:N	2.28	0.64
4:N:89:TYR:HD2	4:N:93:GLU:HB2	1.69	0.64
1:E:297:HIS:HB2	12:E:819:CLA:C1B	2.28	0.64
2:G:577:ASP:OD1	2:G:577:ASP:N	2.30	0.64
2:B:399:VAL:HG12	2:B:545:ARG:HG2	1.80	0.64
1:A:297:HIS:HB2	12:A:816:CLA:C1B	2.27	0.64
2:B:577:ASP:N	2:B:577:ASP:OD1	2.30	0.64
1:E:202:LEU:HD12	1:E:305:PHE:HB2	1.80	0.64
1:E:585:GLN:OE1	2:G:670:TRP:N	3.05	0.64
2:G:358:ALA:HB2	12:G:827:CLA:HBC3	1.79	0.64
1:E:359:MET:HE3	12:E:826:CLA:HHB	1.80	0.64
2:G:673:TYR:OH	12:G:806:CLA:OBD	46.49	0.64
2:G:671:ARG:NH2	2:G:703:MET:O	2.31	0.64
4:N:120:ARG:NH1	4:N:121:ASN:O	2.35	0.64
1:A:720:SER:O	1:A:724:GLY:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:806:CLA:O2A	12:A:806:CLA:H2A	5.38	0.64
12:A:825:CLA:H2A	12:A:825:CLA:HED2	3.41	0.64
2:B:419:LYS:HA	2:B:422:ILE:HD12	1.80	0.64
1:E:644:ASN:O	1:E:648:ARG:N	2.21	0.64
2:G:419:LYS:HA	2:G:422:ILE:HD12	1.80	0.64
8:J:16:SER:HA	8:J:21:LEU:HD21	1.80	0.64
2:B:673:TYR:OH	12:B:807:CLA:OBD	2.07	0.63
1:A:297:HIS:HB2	12:A:818:CLA:C1B	24.18	0.63
1:A:429:ARG:NE	12:A:829:CLA:OBD	2.23	0.63
2:G:17:THR:HG21	3:H:77:MET:HG2	2.54	0.63
11:M:35:ILE:HB	11:M:36:PRO:HD3	1.81	0.63
1:A:446:MET:HG2	1:A:450:PHE:HE1	1.63	0.63
2:G:15:ASP:OD2	2:G:17:THR:OG1	2.13	0.63
1:E:662:TYR:OH	2:G:451:GLY:N	2.36	0.63
4:N:28:LYS:O	4:N:88:VAL:N	2.30	0.63
1:A:202:LEU:HD12	1:A:305:PHE:HB2	1.80	0.63
1:A:741:TRP:HA	1:A:744:PHE:CE1	2.34	0.63
2:B:671:ARG:NH2	2:B:703:MET:O	2.31	0.63
2:B:358:ALA:HB2	12:B:830:CLA:HBC3	1.79	0.63
2:G:399:VAL:HG12	2:G:545:ARG:HG2	1.80	0.63
12:F:1301:CLA:HBC3	8:J:25:TRP:CD1	2.34	0.63
1:A:313:ARG:HH22	9:K:49:GLY:HA3	1.62	0.63
1:A:32:PRO:HG3	8:J:17:LEU:HD11	1.81	0.63
2:B:205:GLN:NE2	2:B:206:HIS:O	2.32	0.63
2:B:231:GLY:N	12:B:818:CLA:O1A	30.85	0.63
2:G:205:GLN:NE2	2:G:206:HIS:O	2.32	0.63
2:G:231:GLY:N	12:G:817:CLA:O1A	2.32	0.63
2:G:673:TYR:OH	12:G:804:CLA:OBD	2.07	0.63
10:L:78:PHE:HZ	10:L:98:THR:HB	1.64	0.63
1:A:328:ASN:ND2	12:A:823:CLA:H2A	24.25	0.63
3:C:48:VAL:HG23	3:C:50:CYS:H	1.64	0.63
1:E:302:ALA:O	1:E:306:ILE:HG12	1.99	0.63
2:G:231:GLY:N	12:G:819:CLA:O1A	27.78	0.63
12:G:803:CLA:HED2	12:G:803:CLA:HBA1	1.80	0.63
4:N:75:ARG:O	4:N:79:ARG:NH1	2.32	0.63
8:Q:16:SER:HA	8:Q:21:LEU:HD21	1.80	0.63
1:A:302:ALA:O	1:A:306:ILE:HG12	1.99	0.63
1:A:508:TYR:HB2	1:A:523:MET:HG3	1.81	0.63
2:B:231:GLY:N	12:B:820:CLA:O1A	2.32	0.63
1:A:644:ASN:O	1:A:648:ARG:N	2.21	0.62
1:E:582:GLY:H	2:G:671:ARG:CD	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:741:TRP:HA	1:E:744:PHE:CE1	2.34	0.62
11:T:35:ILE:HB	11:T:36:PRO:HD3	1.80	0.62
2:B:150:LEU:HB3	11:M:43:LEU:HD11	2.59	0.62
2:B:337:GLN:N	2:B:337:GLN:OE1	2.32	0.62
12:B:806:CLA:HBA1	12:B:806:CLA:HED2	1.80	0.62
1:E:446:MET:HG2	1:E:450:PHE:HE1	1.63	0.62
1:E:590:ASP:OD1	1:E:591:HIS:N	2.32	0.62
2:G:178:HIS:O	2:G:182:LEU:N	2.30	0.62
12:A:804:CLA:H2A	12:A:804:CLA:O2A	1.99	0.62
2:B:242:HIS:NE2	2:B:246:THR:O	2.29	0.62
1:E:328:ASN:ND2	12:E:822:CLA:H2A	14.82	0.62
1:E:508:TYR:HB2	1:E:523:MET:HG3	1.81	0.62
12:G:806:CLA:HBB1	12:G:806:CLA:HMB1	4.19	0.62
2:B:15:ASP:OD2	2:B:17:THR:OG1	2.13	0.62
2:B:707:GLN:O	2:B:711:VAL:HG23	2.00	0.62
2:G:337:GLN:N	2:G:337:GLN:OE1	2.32	0.62
12:G:804:CLA:CGA	12:G:804:CLA:H3A	2.30	0.62
1:A:91:MET:HE3	1:A:91:MET:HA	1.82	0.62
2:B:676:GLU:N	2:B:676:GLU:OE1	2.32	0.62
12:B:805:CLA:HMB1	12:B:805:CLA:HBB1	1.85	0.62
1:E:27:GLU:OE2	8:Q:8:GLN:NE2	3.39	0.62
1:E:313:ARG:HH22	9:R:49:GLY:HA3	3.00	0.62
6:F:60:ARG:NH2	8:J:42:ASP:O	3.32	0.62
7:P:19:PHE:HB3	7:P:20:PRO:HD3	1.82	0.62
10:S:78:PHE:HZ	10:S:98:THR:HB	1.64	0.62
1:A:590:ASP:OD1	1:A:591:HIS:N	2.32	0.62
1:A:44:LYS:N	1:A:44:LYS:HD3	2.15	0.62
2:B:587:LEU:HB3	2:B:720:TYR:CE2	2.35	0.62
12:B:807:CLA:CGA	12:B:807:CLA:H3A	2.30	0.62
1:E:246:ASN:HD21	1:E:249:LEU:HB2	1.65	0.62
1:E:328:ASN:ND2	12:E:824:CLA:H2A	2.14	0.62
2:G:242:HIS:NE2	2:G:246:THR:O	2.29	0.62
3:H:48:VAL:HG23	3:H:50:CYS:H	1.64	0.62
1:A:644:ASN:OD1	1:A:645:GLY:N	2.29	0.62
2:G:707:GLN:O	2:G:711:VAL:HG23	2.00	0.62
12:G:805:CLA:HED2	12:G:805:CLA:HBA1	8.65	0.62
7:I:19:PHE:HB3	7:I:20:PRO:HD3	1.81	0.62
1:A:697:LEU:HD11	2:B:539:LYS:HE3	1.82	0.62
12:G:804:CLA:HMB1	12:G:804:CLA:HBB1	1.82	0.62
6:O:46:ASN:OD1	6:O:55:GLN:NE2	2.33	0.62
2:G:172:GLU:OE1	2:G:172:GLU:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:TRP:O	1:A:745:GLU:HG2	2.00	0.61
1:E:349:TRP:HE1	12:E:806:CLA:CHD	2.13	0.61
12:E:831:CLA:HMB1	12:E:831:CLA:HBB1	1.82	0.61
6:F:46:ASN:OD1	6:F:55:GLN:NE2	2.33	0.61
2:G:727:PHE:O	2:G:731:SER:OG	2.18	0.61
1:A:246:ASN:HD21	1:A:249:LEU:HB2	1.64	0.61
1:A:349:TRP:HE1	12:A:803:CLA:CHD	2.13	0.61
1:E:161:VAL:HA	1:E:164:ILE:HD12	1.82	0.61
1:E:69:ILE:O	1:E:73:ILE:HG13	2.00	0.61
1:E:741:TRP:O	1:E:745:GLU:HG2	2.00	0.61
12:E:805:CLA:H2A	12:E:805:CLA:O2A	5.12	0.61
6:F:66:CYS:HB3	6:F:70:GLY:HA2	1.83	0.61
2:G:426:LEU:HD21	2:G:535:LEU:HA	1.82	0.61
2:G:676:GLU:N	2:G:676:GLU:OE1	2.32	0.61
2:B:426:LEU:HD21	2:B:535:LEU:HA	1.82	0.61
12:B:807:CLA:HBB1	12:B:807:CLA:HMB1	1.82	0.61
12:E:801:CLA:HBA1	12:G:805:CLA:HMB1	40.89	0.61
13:A:842:PQN:H241	12:J:1101:CLA:H42	1.81	0.61
6:F:30:PRO:HA	6:F:65:LEU:HA	1.83	0.61
2:G:595:PHE:HA	2:G:598:HIS:CD2	2.35	0.61
2:B:595:PHE:HA	2:B:598:HIS:CD2	2.35	0.61
2:B:697:LYS:HB3	12:B:841:CLA:CGD	55.11	0.61
2:B:422:ILE:HG23	12:B:841:CLA:HBB2	1.83	0.61
12:G:806:CLA:H3A	12:G:806:CLA:CGA	3.58	0.61
6:O:30:PRO:HA	6:O:65:LEU:HA	1.83	0.61
5:W:40:PHE:N	5:W:49:ASN:O	2.34	0.61
1:E:349:TRP:HE1	12:E:804:CLA:CHD	24.10	0.61
12:E:829:CLA:HMB1	12:E:829:CLA:HBB1	1.87	0.61
1:A:324:GLU:HA	1:A:327:GLU:HG3	1.83	0.61
1:E:44:LYS:N	1:E:44:LYS:HD3	2.15	0.61
12:A:820:CLA:HBD	9:K:48:VAL:HG12	1.81	0.61
6:O:66:CYS:HB3	6:O:70:GLY:HA2	1.83	0.61
1:A:161:VAL:HA	1:A:164:ILE:HD12	1.82	0.61
1:A:289:LEU:HD22	1:A:376:PRO:HA	1.83	0.61
1:A:445:CYS:HB3	1:A:545:VAL:HG12	1.83	0.61
1:A:69:ILE:O	1:A:73:ILE:HG13	2.00	0.61
12:E:843:CLA:HHD	13:E:846:PQN:H212	1.83	0.61
6:F:120:ARG:HH21	6:F:125:ASP:HB2	1.66	0.61
2:G:399:VAL:HA	2:G:545:ARG:HD3	1.83	0.61
4:N:73:GLN:HA	4:N:77:LYS:HZ3	1.71	0.61
6:O:120:ARG:HH21	6:O:125:ASP:HB2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:O	1:A:149:ARG:NH2	2.34	0.61
1:A:328:ASN:ND2	12:A:821:CLA:H2A	2.14	0.61
1:E:324:GLU:HA	1:E:327:GLU:HG3	1.83	0.61
1:E:445:CYS:HB3	1:E:545:VAL:HG12	1.83	0.61
6:F:124:ILE:HD13	8:J:21:LEU:HD12	1.81	0.61
2:G:587:LEU:HB3	2:G:720:TYR:CE2	2.35	0.61
2:G:690:LEU:HD12	12:G:843:CLA:C3D	2.31	0.61
2:G:354:GLN:HE22	12:G:826:CLA:CGD	2.14	0.61
1:A:359:MET:HE1	12:A:823:CLA:HMA1	1.83	0.61
2:B:727:PHE:O	2:B:731:SER:OG	2.18	0.61
2:G:693:LEU:HA	10:S:122:ALA:CB	3.70	0.61
1:A:690:GLY:HA3	2:B:572:ASP:HB2	1.83	0.60
1:A:349:TRP:HE1	12:A:805:CLA:CHD	34.67	0.60
12:B:834:CLA:HMC3	12:B:841:CLA:HBB1	1.82	0.60
2:B:697:LYS:HB3	12:B:842:CLA:CGD	2.31	0.60
12:E:807:CLA:H2A	12:E:807:CLA:O2A	1.99	0.60
2:G:563:ASP:O	2:G:570:THR:OG1	2.13	0.60
1:E:561:ARG:HG2	2:G:679:GLU:HG2	2.53	0.60
1:A:57:HIS:ND1	12:A:803:CLA:HBB2	2.17	0.60
1:A:91:MET:HA	1:A:91:MET:CE	2.31	0.60
2:G:444:ASN:OD1	2:G:456:GLN:NE2	2.33	0.60
2:B:419:LYS:NZ	2:B:420:GLU:OE2	2.34	0.60
1:E:105:LEU:O	1:E:149:ARG:NH2	2.34	0.60
2:G:422:ILE:HG23	12:G:839:CLA:HBB2	1.83	0.60
2:B:192:GLY:O	2:B:196:HIS:ND1	2.34	0.60
12:B:805:CLA:CGA	12:B:805:CLA:H3A	3.01	0.60
12:B:821:CLA:HBA1	12:B:826:CLA:HAB	35.62	0.60
4:D:120:ARG:NH1	4:D:121:ASN:O	2.35	0.60
2:G:455:LYS:HD3	6:O:57:ARG:CZ	2.31	0.60
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.83	0.60
2:G:194:LEU:HA	2:G:198:ALA:HB3	1.83	0.60
2:G:697:LYS:HB3	12:G:841:CLA:CGD	20.00	0.60
2:B:279:ALA:O	2:B:283:LEU:HG	2.02	0.60
2:B:32:GLU:N	2:B:32:GLU:OE1	2.35	0.60
12:E:844:CLA:HAC2	12:G:801:CLA:HMC2	77.03	0.60
12:G:808:CLA:OBD	7:P:11:LEU:HD21	2.00	0.60
9:R:30:GLY:HA2	9:R:33:LEU:HD13	1.84	0.60
1:A:128:ASN:O	1:A:136:HIS:ND1	2.32	0.60
2:B:650:ALA:HA	2:B:653:PHE:HD2	1.67	0.60
2:B:354:GLN:HE22	12:B:827:CLA:CGD	26.32	0.60
1:E:91:MET:HA	1:E:91:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:621:GLY:O	2:G:625:ASP:HB2	2.02	0.60
1:E:582:GLY:H	2:G:671:ARG:NE	2.32	0.60
1:A:300:ALA:HB1	12:A:815:CLA:HBC2	1.84	0.60
12:E:834:CLA:HMB2	12:E:835:CLA:H42	1.84	0.60
12:A:828:CLA:HBB1	12:A:828:CLA:HMB1	1.82	0.60
2:B:621:GLY:O	2:B:625:ASP:HB2	2.02	0.60
12:B:806:CLA:C2A	11:M:47:LEU:HD21	40.64	0.60
2:B:354:GLN:HE22	12:B:829:CLA:CGD	2.14	0.60
12:B:832:CLA:HMC3	12:B:840:CLA:HBB1	28.66	0.60
1:E:289:LEU:HD22	1:E:376:PRO:HA	1.82	0.60
2:G:354:GLN:HE22	12:G:828:CLA:CGD	22.19	0.60
12:G:820:CLA:HBA1	12:G:825:CLA:HAB	1.84	0.60
12:G:831:CLA:HMC3	12:G:839:CLA:HBB1	1.83	0.60
12:G:833:CLA:HMC3	12:G:840:CLA:HBB1	57.10	0.60
8:J:18:GLY:O	8:J:22:LEU:N	2.27	0.60
12:F:1301:CLA:HBC3	8:J:25:TRP:NE1	2.16	0.60
9:K:30:GLY:HA2	9:K:33:LEU:HD13	1.84	0.60
9:K:83:ILE:O	9:K:86:LEU:HB3	2.02	0.60
1:A:359:MET:HE3	12:A:823:CLA:HHB	1.83	0.60
12:A:830:CLA:HBB1	12:A:830:CLA:HMB1	4.25	0.60
2:B:484:ASN:O	2:B:490:SER:OG	2.20	0.60
2:B:422:ILE:HG23	12:B:840:CLA:HBB2	13.00	0.60
2:B:88:ALA:HB3	2:B:114:ASN:HB3	1.84	0.60
2:G:32:GLU:N	2:G:32:GLU:OE1	2.35	0.60
10:L:57:ILE:HD11	10:L:61:ARG:HD2	1.84	0.60
10:S:133:PHE:HZ	10:S:142:PHE:HB2	1.67	0.60
1:A:262:THR:HB	1:A:265:TRP:CD1	2.37	0.59
2:B:19:ARG:NH2	3:C:72:GLU:OE1	2.35	0.59
12:B:809:CLA:H2A	12:B:809:CLA:HED2	1.84	0.59
1:E:408:HIS:HA	1:E:411:ILE:HG22	1.84	0.59
2:G:697:LYS:HB3	12:G:840:CLA:CGD	2.31	0.59
12:E:834:CLA:C2	12:G:843:CLA:HBB2	2.32	0.59
10:S:57:ILE:HD11	10:S:61:ARG:HD2	1.84	0.59
1:A:233:ALA:HB3	1:A:236:ASP:HB2	1.84	0.59
2:B:520:PHE:O	2:B:524:HIS:ND1	2.30	0.59
2:B:681:LEU:HD21	12:B:802:CLA:HMD3	26.57	0.59
1:E:57:HIS:ND1	12:E:804:CLA:HBB2	9.83	0.59
1:E:57:HIS:ND1	12:E:806:CLA:HBB2	2.17	0.59
2:G:279:ALA:O	2:G:283:LEU:HG	2.02	0.59
2:G:650:ALA:HA	2:G:653:PHE:HD2	1.67	0.59
2:G:88:ALA:HB3	2:G:114:ASN:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:83:ILE:O	9:R:86:LEU:HB3	2.02	0.59
5:V:40:PHE:N	5:V:49:ASN:O	2.34	0.59
1:A:589:TRP:HH2	1:A:722:ILE:HB	1.68	0.59
12:A:822:CLA:O2D	12:A:822:CLA:H2A	3.66	0.59
12:A:830:CLA:HMB2	12:A:831:CLA:H42	1.84	0.59
2:G:419:LYS:NZ	2:G:420:GLU:OE2	2.34	0.59
2:G:422:ILE:HG23	12:G:840:CLA:HBB2	43.46	0.59
2:G:3:THR:HG22	7:P:35:ASP:HB2	1.83	0.59
12:G:805:CLA:H2A	11:T:47:LEU:HD21	1.83	0.59
1:A:164:ILE:O	1:A:167:LEU:HG	2.02	0.59
1:A:300:ALA:HB1	12:A:817:CLA:HBC2	15.32	0.59
1:A:57:HIS:ND1	12:A:805:CLA:HBB2	18.54	0.59
1:E:262:THR:HB	1:E:265:TRP:CD1	2.37	0.59
1:E:612:TRP:O	1:E:616:SER:CB	2.51	0.59
12:E:823:CLA:H2A	12:E:823:CLA:O2D	2.03	0.59
1:E:681:ALA:HB3	12:G:801:CLA:HBB2	44.14	0.59
3:C:34:LYS:HZ1	5:V:31:GLY:N	2.00	0.59
2:B:305:LEU:HD22	2:B:327:TYR:CD1	2.38	0.59
2:B:611:GLN:H	2:B:611:GLN:CD	2.06	0.59
1:E:430:VAL:HA	1:E:433:HIS:CE1	2.38	0.59
12:E:831:CLA:HMB2	12:E:832:CLA:H42	39.17	0.59
1:E:533:PHE:HA	12:E:839:CLA:HED1	1.85	0.59
10:L:133:PHE:HZ	10:L:142:PHE:HB2	1.67	0.59
7:P:32:GLU:HG2	10:S:115:THR:HG22	1.84	0.59
1:E:533:PHE:HA	12:E:836:CLA:HED1	22.64	0.59
8:J:10:TYR:O	8:J:13:ARG:HG2	2.03	0.59
1:A:430:VAL:HA	1:A:433:HIS:CE1	2.38	0.59
1:A:612:TRP:O	1:A:616:SER:CB	2.51	0.59
2:B:178:HIS:O	2:B:182:LEU:N	2.30	0.59
2:B:399:VAL:HA	2:B:545:ARG:HD3	1.83	0.59
12:B:807:CLA:H2A	12:B:807:CLA:HED2	3.68	0.59
4:D:38:GLU:HG2	4:D:52:ARG:HA	1.83	0.59
1:E:164:ILE:O	1:E:167:LEU:HG	2.02	0.59
12:G:808:CLA:H2A	12:G:808:CLA:HED2	3.50	0.59
1:A:681:ALA:HB3	12:A:802:CLA:HBB2	30.80	0.59
2:B:649:TRP:HA	2:B:652:MET:HG2	1.85	0.59
12:B:823:CLA:HBA1	12:B:828:CLA:HAB	1.84	0.59
4:D:31:ILE:HA	4:D:84:LYS:O	2.21	0.59
1:E:473:SER:OG	1:E:474:ASP:N	2.36	0.59
1:E:96:ALA:HB1	1:E:156:SER:HB2	1.85	0.59
2:G:216:LEU:HB3	12:G:818:CLA:OBD	31.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:484:ASN:O	2:G:490:SER:OG	2.20	0.59
11:M:24:THR:HA	11:M:27:PHE:HD2	1.68	0.59
11:T:24:THR:HA	11:T:27:PHE:HD2	1.68	0.59
12:A:820:CLA:O2D	12:A:820:CLA:H2A	2.03	0.59
2:G:305:LEU:HD22	2:G:327:TYR:CD1	2.38	0.59
2:G:695:ARG:CZ	10:S:119:LYS:O	4.13	0.59
1:A:349:TRP:CD1	12:A:805:CLA:HAC1	34.36	0.58
1:A:399:GLY:HA2	1:A:402:ILE:HG22	1.85	0.58
2:B:152:ALA:HB2	12:B:813:CLA:HBC2	45.41	0.58
2:B:421:ALA:O	2:B:425:HIS:ND1	2.35	0.58
1:E:399:GLY:HA2	1:E:402:ILE:HG22	1.85	0.58
1:E:709:LYS:HD2	6:O:152:LEU:O	2.86	0.58
12:E:836:CLA:HMB2	12:E:837:CLA:C3D	18.64	0.58
2:G:146:ALA:O	2:G:150:LEU:HG	2.03	0.58
2:G:563:ASP:HA	3:H:51:LYS:NZ	2.34	0.58
1:A:681:ALA:HB3	12:B:801:CLA:HBB2	1.85	0.58
1:A:691:ARG:HA	1:A:694:TRP:HD1	1.68	0.58
2:B:146:ALA:O	2:B:150:LEU:HG	2.03	0.58
2:B:444:ASN:OD1	2:B:456:GLN:NE2	2.33	0.58
1:E:473:SER:OG	1:E:474:ASP:OD2	2.22	0.58
1:E:300:ALA:HB1	12:E:816:CLA:HBC2	13.31	0.58
2:G:30:ASP:O	2:G:33:THR:OG1	2.22	0.58
2:G:649:TRP:HA	2:G:652:MET:HG2	1.85	0.58
8:J:18:GLY:H	8:J:21:LEU:HG	1.68	0.58
6:F:60:ARG:HH12	8:J:43:LEU:HA	3.08	0.58
8:Q:10:TYR:O	8:Q:13:ARG:HG2	2.03	0.58
2:B:152:ALA:HB2	12:B:815:CLA:HBC2	1.85	0.58
1:E:589:TRP:O	1:E:592:VAL:HG22	2.04	0.58
1:E:691:ARG:HA	1:E:694:TRP:HD1	1.68	0.58
1:E:589:TRP:HH2	1:E:722:ILE:HB	1.68	0.58
12:E:801:CLA:C1A	12:G:805:CLA:HAB	39.22	0.58
12:E:844:CLA:HMB1	12:E:844:CLA:HBB1	2.76	0.58
2:G:440:LEU:O	2:G:444:ASN:ND2	2.37	0.58
1:A:408:HIS:HA	1:A:411:ILE:HG22	1.84	0.58
1:A:473:SER:OG	1:A:474:ASP:OD2	2.22	0.58
1:A:648:ARG:HH12	2:B:639:ASN:HD22	1.51	0.58
12:A:801:CLA:HBD	12:A:801:CLA:HBA2	1.85	0.58
1:A:533:PHE:HA	12:A:835:CLA:HED1	1.85	0.58
12:A:837:CLA:HMB2	12:A:838:CLA:C3D	6.45	0.58
2:B:440:LEU:O	2:B:444:ASN:ND2	2.37	0.58
12:B:806:CLA:CAA	11:M:47:LEU:HD21	40.95	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ALA:HB3	1:E:236:ASP:HB2	1.85	0.58
1:E:300:ALA:HB1	12:E:818:CLA:HBC2	1.84	0.58
1:E:681:ALA:HB3	12:E:802:CLA:HBB2	1.85	0.58
12:A:835:CLA:HMB2	12:A:836:CLA:C3D	2.33	0.58
2:B:216:LEU:HB3	12:B:819:CLA:OBD	2.03	0.58
1:E:384:TYR:OH	1:E:521:ILE:N	2.37	0.58
1:E:349:TRP:CD1	12:E:806:CLA:HAC1	2.38	0.58
12:E:821:CLA:O2D	12:E:821:CLA:H2A	3.41	0.58
2:G:611:GLN:H	2:G:611:GLN:CD	2.06	0.58
8:Q:18:GLY:H	8:Q:21:LEU:HG	1.68	0.58
1:A:473:SER:OG	1:A:474:ASP:N	2.36	0.58
2:B:348:ILE:O	2:B:352:VAL:HG23	2.04	0.58
12:B:803:CLA:HMB1	12:B:803:CLA:HBB1	4.30	0.58
12:E:839:CLA:HMB2	12:E:840:CLA:C3D	2.33	0.58
2:G:192:GLY:O	2:G:196:HIS:ND1	2.34	0.58
2:G:520:PHE:O	2:G:524:HIS:ND1	2.30	0.58
1:A:349:TRP:CD1	12:A:803:CLA:HAC1	2.38	0.58
12:E:801:CLA:HBD	12:E:801:CLA:HBA2	1.85	0.58
12:F:1301:CLA:HBD	12:F:1301:CLA:HBA2	1.85	0.58
12:O:1301:CLA:HBA2	12:O:1301:CLA:HBD	1.85	0.58
8:Q:18:GLY:O	8:Q:22:LEU:N	2.27	0.58
1:A:96:ALA:HB1	1:A:156:SER:HB2	1.85	0.58
12:E:801:CLA:CHA	12:G:805:CLA:HAB	40.08	0.58
2:G:216:LEU:HB3	12:G:816:CLA:OBD	2.03	0.58
2:G:348:ILE:O	2:G:352:VAL:HG23	2.04	0.58
1:A:648:ARG:HD2	1:A:649:ASP:OD1	2.04	0.58
2:B:581:LEU:HA	2:B:584:PHE:HD2	1.69	0.58
4:D:75:ARG:NH2	4:D:83:TYR:OH	2.37	0.58
1:E:243:PHE:HA	1:E:246:ASN:HB3	1.86	0.58
1:E:473:SER:HA	1:E:530:THR:HG21	1.86	0.58
1:E:558:ARG:HA	1:E:567:ALA:HB2	1.86	0.58
1:E:349:TRP:CD1	12:E:804:CLA:HAC1	23.13	0.58
12:G:806:CLA:H2A	12:G:806:CLA:HED2	1.84	0.58
1:A:243:PHE:HA	1:A:246:ASN:HB3	1.86	0.58
2:B:137:SER:HA	2:B:140:VAL:HG22	1.86	0.58
3:C:17:VAL:HG12	3:C:25:LEU:HD23	1.86	0.58
1:E:128:ASN:O	1:E:136:HIS:ND1	2.32	0.58
2:G:4:LYS:HD3	7:P:37:SER:HA	1.86	0.58
12:A:837:CLA:HBC3	13:A:842:PQN:H261	1.86	0.57
2:B:563:ASP:O	2:B:570:THR:OG1	2.13	0.57
2:B:216:LEU:HB3	12:B:817:CLA:OBD	39.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:648:ARG:HD2	1:E:649:ASP:OD1	2.04	0.57
2:G:581:LEU:HA	2:G:584:PHE:HD2	1.69	0.57
2:G:693:LEU:HA	10:S:122:ALA:HB1	3.32	0.57
1:A:384:TYR:OH	1:A:521:ILE:N	2.37	0.57
1:A:558:ARG:HA	1:A:567:ALA:HB2	1.86	0.57
1:A:589:TRP:O	1:A:592:VAL:HG22	2.04	0.57
2:B:129:MET:O	2:B:130:ARG:NH1	2.34	0.57
1:E:691:ARG:HD3	2:G:568:GLY:O	2.04	0.57
12:G:822:CLA:HBA1	12:G:827:CLA:HAB	31.90	0.57
1:A:128:ASN:HB3	1:A:136:HIS:HB3	1.87	0.57
1:A:598:TRP:O	1:A:602:THR:HG23	2.04	0.57
1:E:363:LEU:O	1:E:367:VAL:HG23	2.05	0.57
1:E:598:TRP:O	1:E:602:THR:HG23	2.04	0.57
12:E:811:CLA:HBB1	12:E:811:CLA:HMB1	4.26	0.57
2:G:11:ASP:OD1	3:H:71:ALA:HA	2.65	0.57
12:G:802:CLA:HMB1	12:G:802:CLA:HBB1	1.85	0.57
2:G:152:ALA:HB2	12:G:812:CLA:HBC2	1.85	0.57
4:N:58:LEU:HD13	10:S:29:GLN:HE22	1.69	0.57
1:A:533:PHE:HA	12:A:837:CLA:HED1	63.58	0.57
12:A:812:CLA:HBB1	12:A:812:CLA:HMB1	4.12	0.57
2:B:357:TYR:O	2:B:510:SER:OG	2.22	0.57
12:B:801:CLA:HMB1	12:B:801:CLA:HBB1	1.93	0.57
2:G:559:ALA:O	2:G:574:SER:OG	2.14	0.57
12:G:833:CLA:HMB1	12:G:834:CLA:HHC	1.86	0.57
12:G:834:CLA:HMB1	12:G:835:CLA:HHC	34.81	0.57
10:S:119:LYS:O	10:S:121:VAL:N	2.37	0.57
1:A:363:LEU:O	1:A:367:VAL:HG23	2.05	0.57
2:B:611:GLN:O	2:B:615:SER:OG	2.23	0.57
12:B:836:CLA:HMB1	12:J:1102:CLA:HHC	1.86	0.57
3:H:17:VAL:HG12	3:H:25:LEU:HD23	1.86	0.57
4:D:136:MET:HE1	4:D:139:TYR:HB2	1.87	0.57
1:E:738:VAL:HG12	1:E:741:TRP:CZ2	2.40	0.57
12:E:827:CLA:HBB1	12:E:827:CLA:HMB1	4.25	0.57
1:A:473:SER:HA	1:A:530:THR:HG21	1.86	0.57
1:A:738:VAL:HG12	1:A:741:TRP:CZ2	2.40	0.57
2:B:172:GLU:N	2:B:172:GLU:OE1	2.30	0.57
2:B:176:ASN:ND2	2:B:288:GLY:O	2.32	0.57
1:E:500:PRO:HD2	12:E:837:CLA:CGD	2.35	0.57
12:E:803:CLA:HBB1	12:E:803:CLA:HMB1	1.86	0.57
2:G:421:ALA:O	2:G:425:HIS:ND1	2.35	0.57
4:N:62:ARG:NH2	4:N:64:GLU:OE1	6.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:455:LYS:HD3	6:O:57:ARG:NH1	2.19	0.57
12:A:826:CLA:HMB1	12:A:826:CLA:HBB1	1.87	0.57
1:E:542:GLN:HA	1:E:545:VAL:HG22	1.86	0.57
2:G:527:ALA:O	2:G:531:HIS:ND1	2.36	0.57
1:A:101:TYR:O	1:A:105:LEU:N	2.37	0.57
2:B:380:GLN:O	2:B:384:VAL:HG23	2.05	0.57
1:A:687:LEU:HD11	2:B:668:ILE:HG12	1.87	0.57
1:E:687:LEU:HD21	2:G:668:ILE:HG12	1.87	0.57
7:I:12:VAL:O	7:I:16:GLY:N	2.38	0.57
4:N:12:PHE:HZ	4:N:15:SER:HG	3.31	0.57
1:A:217:GLN:O	1:A:222:LEU:N	2.37	0.57
1:A:542:GLN:HA	1:A:545:VAL:HG22	1.86	0.57
6:F:130:LEU:HA	6:F:133:MET:HE2	1.87	0.57
1:A:435:ASP:OD1	1:A:436:ALA:N	2.38	0.56
1:A:500:PRO:HD2	12:A:833:CLA:CGD	2.35	0.56
1:A:278:PHE:HD1	12:A:816:CLA:HMB2	1.70	0.56
2:B:30:ASP:O	2:B:33:THR:OG1	2.22	0.56
2:B:562:CYS:O	2:B:570:THR:OG1	2.23	0.56
12:B:834:CLA:HMB1	12:B:835:CLA:HHC	7.88	0.56
3:C:13:CYS:N	14:C:102:SF4:S1	2.78	0.56
1:E:435:ASP:OD1	1:E:436:ALA:N	2.38	0.56
1:E:278:PHE:HD1	12:E:817:CLA:HMB2	29.98	0.56
1:E:500:PRO:HD2	12:E:834:CLA:CGD	46.87	0.56
2:G:562:CYS:O	2:G:570:THR:OG1	2.23	0.56
2:G:152:ALA:HB2	12:G:814:CLA:HBC2	16.58	0.56
3:H:5:LYS:NZ	3:H:6:ILE:O	2.37	0.56
1:A:159:LEU:O	1:A:162:THR:OG1	2.18	0.56
1:A:457:ILE:HA	1:A:460:ASP:OD2	2.05	0.56
1:A:488:GLN:HG2	1:A:510:PHE:CG	2.40	0.56
1:A:736:ALA:O	1:A:740:ILE:HG12	2.05	0.56
1:E:457:ILE:HA	1:E:460:ASP:OD2	2.05	0.56
1:E:465:LEU:HD23	1:E:467:ARG:HG3	1.88	0.56
1:E:736:ALA:O	1:E:740:ILE:HG12	2.05	0.56
12:B:806:CLA:HAA2	11:M:47:LEU:HD21	41.59	0.56
3:C:34:LYS:NZ	5:V:31:GLY:N	2.53	0.56
1:E:489:ASN:O	1:E:492:THR:OG1	2.20	0.56
1:E:488:GLN:HG2	1:E:510:PHE:CG	2.40	0.56
12:E:838:CLA:HED2	12:E:838:CLA:H2A	1.88	0.56
2:G:184:GLY:O	2:G:187:SER:OG	2.21	0.56
2:G:380:GLN:O	2:G:384:VAL:HG23	2.05	0.56
4:N:136:MET:HE1	4:N:139:TYR:HB2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:58:THR:HG23	10:S:61:ARG:H	1.70	0.56
1:A:478:GLN:OE1	1:A:480:GLN:NE2	2.39	0.56
1:A:500:PRO:HD2	12:A:835:CLA:CGD	28.70	0.56
3:C:30:TRP:N	3:C:36:GLY:O	2.38	0.56
1:E:478:GLN:OE1	1:E:480:GLN:NE2	2.39	0.56
1:E:519:GLY:HA2	1:E:622:ILE:HB	1.88	0.56
1:E:278:PHE:HD1	12:E:819:CLA:HMB2	1.70	0.56
10:L:58:THR:HG23	10:L:61:ARG:H	1.70	0.56
4:N:31:ILE:HA	4:N:84:LYS:O	2.06	0.56
1:A:84:ILE:HA	1:A:87:TRP:CD1	2.40	0.56
2:B:554:LYS:NZ	4:D:125:ASN:HB2	2.20	0.56
4:D:69:LEU:HD12	4:D:73:GLN:HB2	1.86	0.56
1:E:257:PHE:HB2	1:E:275:PHE:HE1	1.70	0.56
12:G:835:CLA:H2A	12:G:835:CLA:O2A	2.05	0.56
3:H:13:CYS:N	14:H:102:SF4:S1	2.79	0.56
2:B:276:HIS:O	2:B:280:ILE:HG12	2.06	0.56
12:B:802:CLA:HMB1	12:B:802:CLA:HBB1	1.85	0.56
1:E:159:LEU:O	1:E:162:THR:OG1	2.18	0.56
12:E:835:CLA:H2A	12:E:835:CLA:HED2	5.49	0.56
1:E:84:ILE:HA	1:E:87:TRP:CD1	2.40	0.56
2:G:129:MET:O	2:G:130:ARG:NH1	2.34	0.56
2:G:137:SER:HA	2:G:140:VAL:HG22	1.86	0.56
2:G:276:HIS:O	2:G:280:ILE:HG12	2.06	0.56
1:A:519:GLY:HA2	1:A:622:ILE:HB	1.88	0.56
1:A:71:ARG:HA	1:A:74:PHE:CD2	2.41	0.56
1:A:740:ILE:HA	1:A:743:PHE:HD2	1.71	0.56
12:A:810:CLA:HBB1	12:A:810:CLA:HMB1	1.87	0.56
12:B:806:CLA:H2A	11:M:47:LEU:HD21	39.74	0.56
1:E:538:ILE:HA	1:E:541:PHE:HB3	1.88	0.56
1:A:465:LEU:O	1:A:467:ARG:NH1	2.39	0.56
2:B:244:PHE:N	2:B:264:GLN:OE1	2.39	0.56
3:C:21:PRO:HD3	3:C:52:ARG:HD2	1.88	0.56
3:C:27:MET:HB2	4:D:107:LYS:CE	2.35	0.56
1:E:128:ASN:HB3	1:E:136:HIS:HB3	1.86	0.56
12:E:802:CLA:H2A	12:E:802:CLA:O2D	2.06	0.56
2:G:344:ALA:O	2:G:347:THR:OG1	2.21	0.56
10:L:119:LYS:O	10:L:121:VAL:N	2.37	0.56
2:B:497:LEU:H	2:B:497:LEU:CD2	2.19	0.56
1:A:707:LYS:NZ	12:B:835:CLA:HAA2	2.21	0.56
1:E:202:LEU:HA	1:E:206:LEU:HD12	1.88	0.56
1:E:359:MET:HE3	12:E:824:CLA:HHB	22.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:740:ILE:HA	1:E:743:PHE:HD2	1.71	0.56
12:E:813:CLA:HBB1	12:E:813:CLA:HMB1	1.87	0.56
2:G:244:PHE:N	2:G:264:GLN:OE1	2.39	0.56
4:N:69:LEU:HD13	4:N:73:GLN:HG3	1.99	0.56
1:A:257:PHE:HB2	1:A:275:PHE:HE1	1.71	0.56
1:A:538:ILE:HA	1:A:541:PHE:HB3	1.88	0.56
2:B:527:ALA:O	2:B:531:HIS:ND1	2.36	0.56
12:B:837:CLA:H2A	12:B:837:CLA:O2A	2.05	0.56
1:E:295:ALA:O	1:E:299:LEU:HG	2.06	0.56
2:G:310:PHE:H	2:G:314:LYS:HA	1.71	0.56
2:G:611:GLN:O	2:G:615:SER:OG	2.23	0.56
3:H:16:CYS:N	14:H:102:SF4:S4	2.70	0.56
3:H:21:PRO:HD3	3:H:52:ARG:HD2	1.88	0.56
1:A:278:PHE:HD1	12:A:818:CLA:HMB2	27.01	0.56
1:A:687:LEU:HD21	2:B:668:ILE:HG12	2.19	0.56
1:E:101:TYR:O	1:E:105:LEU:N	2.38	0.56
1:E:359:MET:HE1	12:E:826:CLA:HMA1	1.88	0.56
1:E:71:ARG:HA	1:E:74:PHE:CD2	2.41	0.56
5:V:7:LYS:N	5:V:62:GLU:OE2	2.33	0.56
2:B:587:LEU:HD22	2:B:720:TYR:HD2	1.71	0.55
12:B:809:CLA:HMA1	12:B:810:CLA:HMB3	5.36	0.55
12:B:814:CLA:H3A	12:B:814:CLA:CGA	2.36	0.55
12:B:836:CLA:O2A	12:B:836:CLA:H2A	4.90	0.55
4:D:74:LEU:O	4:D:79:ARG:N	2.39	0.55
1:E:722:ILE:HG13	1:E:723:GLN:N	2.21	0.55
3:H:30:TRP:N	3:H:36:GLY:O	2.38	0.55
1:A:465:LEU:HD23	1:A:467:ARG:HG3	1.87	0.55
1:A:533:PHE:O	1:A:537:HIS:ND1	2.39	0.55
2:B:167:TRP:CH2	12:B:813:CLA:HMA1	44.81	0.55
2:B:199:ILE:HA	2:B:270:LEU:HD11	1.89	0.55
2:B:310:PHE:H	2:B:314:LYS:HA	1.71	0.55
3:C:5:LYS:NZ	3:C:6:ILE:O	2.37	0.55
1:E:433:HIS:CD2	1:E:437:ILE:HD11	2.41	0.55
2:G:210:ASP:OD1	2:G:210:ASP:N	2.39	0.55
2:G:497:LEU:H	2:G:497:LEU:HD22	1.71	0.55
2:G:497:LEU:H	2:G:497:LEU:CD2	2.19	0.55
4:D:18:GLY:HA3	10:L:31:GLY:H	2.16	0.55
12:A:834:CLA:HED2	12:A:834:CLA:H2A	1.88	0.55
3:C:16:CYS:N	14:C:102:SF4:S4	2.69	0.55
1:E:635:ASN:O	1:E:639:SER:OG	2.25	0.55
2:G:587:LEU:HD22	2:G:720:TYR:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:12:VAL:O	7:P:16:GLY:N	2.38	0.55
1:A:168:VAL:O	1:A:172:LEU:HG	2.07	0.55
2:B:210:ASP:OD1	2:B:210:ASP:N	2.39	0.55
2:B:338:LEU:O	2:B:342:LEU:HG	2.07	0.55
1:E:440:HIS:O	1:E:444:VAL:HG23	2.07	0.55
1:E:465:LEU:O	1:E:467:ARG:NH1	2.39	0.55
1:E:95:GLY:O	1:E:99:SER:HB3	2.07	0.55
2:G:338:LEU:O	2:G:342:LEU:HG	2.07	0.55
12:G:836:CLA:H2A	12:G:836:CLA:O2A	4.83	0.55
1:E:467:ARG:NH2	2:G:98:LYS:HB2	2.99	0.55
2:B:688:THR:HG22	12:L:201:CLA:HHB	1.88	0.55
4:N:38:GLU:HG2	4:N:52:ARG:HA	1.96	0.55
6:O:108:LEU:O	6:O:112:LYS:HD3	2.07	0.55
10:S:24:SER:OG	10:S:25:ARG:N	2.38	0.55
1:A:474:ASP:O	1:A:478:GLN:NE2	2.39	0.55
1:A:722:ILE:HG13	1:A:723:GLN:N	2.21	0.55
12:A:836:CLA:H2A	12:A:836:CLA:HED2	3.43	0.55
2:B:653:PHE:O	2:B:657:HIS:ND1	2.28	0.55
1:E:303:VAL:HG11	12:E:816:CLA:HMC3	13.76	0.55
1:E:303:VAL:HG11	12:E:818:CLA:HMC3	1.89	0.55
2:G:199:ILE:HA	2:G:270:LEU:HD11	1.89	0.55
12:G:811:CLA:CGA	12:G:811:CLA:H3A	2.36	0.55
1:A:95:GLY:O	1:A:99:SER:HB3	2.07	0.55
2:B:497:LEU:HD22	2:B:497:LEU:H	1.71	0.55
6:F:108:LEU:O	6:F:112:LYS:HD3	2.07	0.55
1:E:648:ARG:HD3	2:G:636:ASN:ND2	2.82	0.55
12:G:801:CLA:H2A	12:G:801:CLA:O2D	3.47	0.55
10:L:24:SER:OG	10:L:25:ARG:N	2.38	0.55
1:A:202:LEU:HA	1:A:206:LEU:HD12	1.88	0.55
1:A:303:VAL:HG11	12:A:817:CLA:HMC3	11.75	0.55
1:A:440:HIS:O	1:A:444:VAL:HG23	2.07	0.55
1:A:635:ASN:O	1:A:639:SER:OG	2.25	0.55
12:B:801:CLA:O2D	12:B:801:CLA:H2A	2.06	0.55
2:B:276:HIS:HB2	12:B:821:CLA:C1B	2.37	0.55
12:B:825:CLA:H2A	12:B:825:CLA:HED3	3.56	0.55
1:E:114:SER:OG	1:E:139:GLN:OE1	2.25	0.55
2:G:156:HIS:CE1	2:G:163:PRO:HG3	2.42	0.55
2:G:290:MET:HG2	2:G:299:HIS:HD1	1.72	0.55
2:G:167:TRP:CH2	12:G:814:CLA:HMA1	11.11	0.55
12:G:824:CLA:H2A	12:G:824:CLA:HED3	1.89	0.55
3:H:28:VAL:O	3:H:37:GLN:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:10:ILE:HD12	7:I:13:PRO:HD2	1.89	0.55
1:A:114:SER:OG	1:A:139:GLN:OE1	2.25	0.55
1:A:92:GLU:OE1	1:A:93:PHE:N	2.40	0.55
2:B:290:MET:HG2	2:B:299:HIS:HD1	1.72	0.55
2:B:667:LEU:O	2:B:670:TRP:NE1	2.32	0.55
12:B:811:CLA:HMA1	12:B:812:CLA:HMB3	1.88	0.55
3:C:28:VAL:O	3:C:37:GLN:HA	2.07	0.55
1:E:217:GLN:O	1:E:222:LEU:N	2.37	0.55
2:G:143:LEU:HD22	11:T:32:ILE:CD1	2.37	0.55
1:A:33:GLY:HA2	1:A:39:LEU:HD22	1.89	0.55
2:B:665:MET:HG3	12:B:807:CLA:NC	2.22	0.55
2:B:276:HIS:HB2	12:B:819:CLA:C1B	19.34	0.55
1:E:33:GLY:HA2	1:E:39:LEU:HD22	1.89	0.55
2:G:276:HIS:HB2	12:G:818:CLA:C1B	2.37	0.55
12:G:826:CLA:HED3	12:G:826:CLA:H2A	3.07	0.55
4:N:96:TYR:OH	4:N:99:PRO:HD2	2.07	0.55
2:B:156:HIS:CE1	2:B:163:PRO:HG3	2.42	0.55
12:B:812:CLA:H3A	12:B:812:CLA:CGA	3.58	0.55
3:C:24:VAL:HG22	3:C:46:ASP:HB2	1.89	0.55
2:G:440:LEU:HA	2:G:443:HIS:HD2	1.72	0.55
12:G:813:CLA:CGA	12:G:813:CLA:H3A	3.25	0.55
2:G:276:HIS:HB2	12:G:820:CLA:C1B	20.32	0.55
10:L:72:TYR:HD1	10:L:157:ALA:HB2	1.72	0.55
1:A:403:VAL:HG11	1:A:599:MET:HG2	1.90	0.54
2:B:316:GLU:N	2:B:320:ASN:OD1	2.40	0.54
2:B:328:ASP:N	2:B:328:ASP:OD1	2.40	0.54
12:B:827:CLA:HED3	12:B:827:CLA:H2A	1.89	0.54
1:E:164:ILE:O	1:E:168:VAL:HG23	2.07	0.54
2:G:53:HIS:CE1	12:G:808:CLA:HMA1	19.22	0.54
2:G:585:TRP:HZ2	12:G:801:CLA:ND	41.79	0.54
9:K:82:ILE:HG12	12:K:1401:CLA:HAB	1.90	0.54
1:A:118:VAL:H	1:A:128:ASN:HD21	1.56	0.54
1:A:164:ILE:O	1:A:168:VAL:HG23	2.07	0.54
1:A:295:ALA:O	1:A:299:LEU:HG	2.06	0.54
12:A:826:CLA:H2	12:A:836:CLA:H3A	33.82	0.54
2:B:440:LEU:HA	2:B:443:HIS:HD2	1.73	0.54
2:B:96:PHE:CD2	2:B:101:VAL:HG21	2.42	0.54
1:E:168:VAL:O	1:E:172:LEU:HG	2.07	0.54
1:E:533:PHE:O	1:E:537:HIS:ND1	2.39	0.54
1:E:92:GLU:OE1	1:E:93:PHE:N	2.40	0.54
2:G:328:ASP:N	2:G:328:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:24:VAL:HG22	3:H:46:ASP:HB2	1.89	0.54
1:A:158:GLN:O	1:A:162:THR:HG23	2.08	0.54
12:A:802:CLA:O2D	12:A:802:CLA:H2A	4.18	0.54
1:A:458:HIS:HB2	12:A:831:CLA:C1C	2.38	0.54
1:A:90:GLY:O	1:A:94:HIS:ND1	2.40	0.54
2:B:559:ALA:O	2:B:574:SER:OG	2.14	0.54
3:C:27:MET:HB2	4:D:107:LYS:HE2	1.90	0.54
1:A:345:MET:HB3	12:A:825:CLA:HBC3	33.32	0.54
2:B:306:ASN:HA	2:B:308:LYS:HZ2	1.75	0.54
2:B:335:HIS:CB	2:B:397:PHE:HB2	2.38	0.54
2:B:665:MET:HG3	12:B:805:CLA:NC	21.22	0.54
2:B:167:TRP:CH2	12:B:815:CLA:HMA1	2.42	0.54
1:E:474:ASP:O	1:E:478:GLN:NE2	2.39	0.54
12:E:825:CLA:H2	12:E:835:CLA:H3A	40.68	0.54
2:G:167:TRP:CH2	12:G:812:CLA:HMA1	2.42	0.54
3:H:15:GLN:HA	3:H:18:ARG:HE	1.73	0.54
2:B:444:ASN:HA	2:B:456:GLN:HG3	1.90	0.54
2:B:53:HIS:CE1	12:B:807:CLA:HMA1	33.54	0.54
3:C:15:GLN:HA	3:C:18:ARG:HE	1.73	0.54
1:E:458:HIS:HB2	12:E:835:CLA:C1C	2.38	0.54
2:G:316:GLU:N	2:G:320:ASN:OD1	2.40	0.54
2:G:335:HIS:CB	2:G:397:PHE:HB2	2.38	0.54
2:G:357:TYR:O	2:G:510:SER:OG	2.22	0.54
2:G:696:TRP:HZ3	12:G:841:CLA:HAC2	15.52	0.54
1:E:158:GLN:O	1:E:162:THR:HG23	2.08	0.54
2:G:444:ASN:HA	2:G:456:GLN:HG3	1.90	0.54
2:G:53:HIS:CE1	12:G:806:CLA:HMA1	2.43	0.54
2:G:665:MET:HG3	12:G:806:CLA:NC	35.47	0.54
2:G:96:PHE:CD2	2:G:101:VAL:HG21	2.42	0.54
10:S:72:TYR:HD1	10:S:157:ALA:HB2	1.72	0.54
5:V:44:ASN:HD21	5:V:48:VAL:HB	1.73	0.54
1:A:222:LEU:C	1:A:226:LYS:HZ2	2.11	0.54
12:A:831:CLA:HMB1	12:A:831:CLA:HBB1	1.90	0.54
2:B:344:ALA:O	2:B:347:THR:OG1	2.21	0.54
2:B:696:TRP:HZ3	12:B:842:CLA:HAC2	1.72	0.54
3:C:34:LYS:NZ	5:V:31:GLY:H	2.05	0.54
1:E:90:GLY:O	1:E:94:HIS:ND1	2.40	0.54
6:F:138:THR:O	6:F:138:THR:OG1	2.25	0.54
12:G:810:CLA:HMA1	12:G:811:CLA:HMB3	4.36	0.54
7:P:10:ILE:HD12	7:P:13:PRO:HD2	1.89	0.54
1:A:459:ASN:OD1	1:A:471:MET:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:LEU:N	4:D:57:LYS:HZ1	2.06	0.54
4:D:97:LEU:O	4:D:100:SER:OG	2.21	0.54
1:E:118:VAL:H	1:E:128:ASN:HD21	1.56	0.54
1:E:345:MET:HB3	12:E:826:CLA:HBC3	1.89	0.54
2:G:665:MET:HG3	12:G:804:CLA:NC	2.22	0.54
12:G:808:CLA:HMA1	12:G:809:CLA:HMB3	1.88	0.54
2:B:3:THR:HG22	7:I:35:ASP:HB2	1.90	0.54
4:N:22:LYS:HG2	4:N:26:GLU:HB2	2.16	0.54
12:E:839:CLA:H12	8:Q:22:LEU:HD13	60.95	0.54
1:A:458:HIS:HB2	12:A:833:CLA:C1C	44.25	0.54
1:E:459:ASN:OD1	1:E:471:MET:HA	2.08	0.54
12:E:822:CLA:HMA1	12:E:842:CLA:HBC1	57.67	0.54
2:G:281:ALA:O	2:G:285:ILE:HG12	2.08	0.54
2:G:653:PHE:O	2:G:657:HIS:ND1	2.28	0.54
3:C:21:PRO:HB2	4:D:64:GLU:OE2	6.91	0.54
4:D:107:LYS:O	4:D:108:VAL:HG13	4.44	0.54
3:C:5:LYS:HE2	4:D:118:VAL:HG21	1.88	0.54
3:H:37:GLN:OE1	4:N:107:LYS:HE3	2.45	0.54
3:C:15:GLN:N	14:C:102:SF4:S4	2.81	0.53
12:E:827:CLA:H2	12:E:838:CLA:H3A	1.90	0.53
4:N:86:TYR:HB3	4:N:95:GLN:O	2.08	0.53
9:R:82:ILE:HG12	12:R:1401:CLA:HAB	1.89	0.53
1:A:303:VAL:HG11	12:A:815:CLA:HMC3	1.89	0.53
1:A:345:MET:HB3	12:A:823:CLA:HBC3	1.89	0.53
4:D:131:LEU:HD11	4:D:140:ASN:HD21	3.57	0.53
1:E:282:LEU:HD23	1:E:515:VAL:HG11	1.90	0.53
2:G:54:VAL:HA	2:G:57:ILE:HD12	1.91	0.53
1:E:648:ARG:CZ	2:G:636:ASN:HA	2.90	0.53
3:H:15:GLN:N	14:H:102:SF4:S4	2.81	0.53
4:N:113:GLN:C	4:N:114:LYS:HD2	6.09	0.53
10:S:112:TYR:O	10:S:116:ASP:N	2.42	0.53
10:S:86:ASP:OD1	10:S:86:ASP:N	2.42	0.53
1:A:80:GLN:O	1:A:84:ILE:HG12	2.09	0.53
2:B:281:ALA:O	2:B:285:ILE:HG12	2.08	0.53
9:R:68:VAL:HG23	9:R:69:LEU:H	1.73	0.53
1:A:282:LEU:HD23	1:A:515:VAL:HG11	1.90	0.53
1:A:363:LEU:O	1:A:366:ILE:HG22	2.08	0.53
1:A:489:ASN:O	1:A:492:THR:OG1	2.20	0.53
12:A:821:CLA:HMA1	12:A:841:CLA:HBC1	1.91	0.53
2:B:173:PRO:O	2:B:177:HIS:ND1	2.38	0.53
2:B:456:GLN:NE2	2:B:457:ILE:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:HIS:CE1	12:B:809:CLA:HMA1	2.43	0.53
2:B:54:VAL:HA	2:B:57:ILE:HD12	1.91	0.53
2:B:696:TRP:HZ3	12:B:841:CLA:HAC2	59.26	0.53
3:C:37:GLN:OE1	4:D:107:LYS:HE3	2.07	0.53
1:E:345:MET:HB3	12:E:824:CLA:HBC3	15.64	0.53
1:E:363:LEU:O	1:E:366:ILE:HG22	2.08	0.53
1:E:446:MET:HG2	1:E:450:PHE:CE1	2.43	0.53
2:G:173:PRO:O	2:G:177:HIS:ND1	2.38	0.53
4:N:97:LEU:O	4:N:100:SER:OG	4.80	0.53
5:W:44:ASN:HD21	5:W:48:VAL:HB	1.73	0.53
1:A:418:ASP:O	1:A:422:ASN:HB2	2.09	0.53
1:A:35:PHE:HZ	1:A:56:ALA:HA	1.73	0.53
4:D:86:TYR:HB3	4:D:95:GLN:O	2.20	0.53
1:E:222:LEU:C	1:E:226:LYS:HZ2	2.12	0.53
6:F:105:ARG:O	6:F:109:GLN:HG3	2.09	0.53
10:L:86:ASP:OD1	10:L:86:ASP:N	2.42	0.53
1:A:446:MET:HG2	1:A:450:PHE:CE1	2.43	0.53
3:C:51:LYS:HB2	3:C:54:GLU:OE2	2.09	0.53
1:E:286:THR:HG23	1:E:288:GLY:H	1.74	0.53
1:E:349:TRP:NE1	12:E:806:CLA:HHD	2.23	0.53
2:G:696:TRP:HZ3	12:G:840:CLA:HAC2	1.72	0.53
9:K:68:VAL:HG23	9:K:69:LEU:H	1.73	0.53
10:L:112:TYR:O	10:L:116:ASP:N	2.42	0.53
10:L:147:LEU:O	10:L:151:VAL:HG13	2.09	0.53
1:A:584:CYS:O	2:B:672:GLY:HA3	2.25	0.53
12:A:833:CLA:HBB1	12:A:833:CLA:HMB1	4.35	0.53
12:A:839:CLA:HHD	13:A:842:PQN:H212	1.89	0.53
2:B:577:ASP:O	2:B:581:LEU:HD12	2.08	0.53
3:C:41:SER:O	3:C:41:SER:OG	2.27	0.53
1:E:416:ASP:OD1	1:E:416:ASP:N	2.42	0.53
1:E:80:GLN:O	1:E:84:ILE:HG12	2.09	0.53
1:E:458:HIS:HB2	12:E:832:CLA:C1C	32.77	0.53
12:E:832:CLA:HBB1	12:E:832:CLA:HMB1	4.18	0.53
2:G:577:ASP:O	2:G:581:LEU:HD12	2.08	0.53
3:H:41:SER:OG	3:H:41:SER:O	2.27	0.53
12:E:835:CLA:O2D	10:S:83:PRO:HB3	2.09	0.53
1:A:433:HIS:CD2	1:A:437:ILE:HD11	2.41	0.53
1:A:691:ARG:HD3	2:B:568:GLY:O	2.22	0.53
2:B:637:GLY:HA2	2:B:644:ASN:HD21	1.74	0.53
1:E:35:PHE:HZ	1:E:56:ALA:HA	1.74	0.53
3:H:13:CYS:SG	3:H:15:GLN:HG2	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:LYS:HB2	3:H:54:GLU:OE2	2.09	0.53
12:F:1301:CLA:HBC3	8:J:25:TRP:HE1	1.74	0.53
7:P:18:VAL:O	7:P:22:ILE:HG22	2.09	0.53
3:C:16:CYS:SG	3:C:17:VAL:N	2.82	0.53
1:E:91:MET:HE3	1:E:91:MET:HA	1.91	0.53
2:G:637:GLY:HA2	2:G:644:ASN:HD21	1.74	0.53
12:B:809:CLA:HBC1	11:M:29:ALA:HA	36.29	0.53
4:N:75:ARG:NH2	4:N:83:TYR:OH	8.39	0.53
1:A:101:TYR:HB2	1:A:145:PHE:HE1	1.74	0.53
12:A:824:CLA:H2	12:A:834:CLA:H3A	1.90	0.53
2:B:361:PRO:HB2	12:B:822:CLA:HAA2	1.91	0.53
1:E:349:TRP:NE1	12:E:804:CLA:HHD	24.76	0.53
2:G:361:PRO:HB2	12:G:821:CLA:HAA2	36.73	0.53
2:G:456:GLN:NE2	2:G:457:ILE:O	2.42	0.53
2:G:612:PHE:O	2:G:616:SER:OG	2.26	0.53
4:D:14:GLY:HA3	10:L:23:PRO:N	2.71	0.53
10:S:147:LEU:O	10:S:151:VAL:HG13	2.09	0.53
10:S:167:ILE:O	10:S:171:PHE:N	2.43	0.53
10:S:59:PRO:HB3	10:S:133:PHE:CE1	2.44	0.53
2:B:361:PRO:HB2	12:B:820:CLA:HAA2	23.86	0.52
7:I:18:VAL:O	7:I:22:ILE:HG22	2.09	0.52
10:L:167:ILE:O	10:L:171:PHE:N	2.43	0.52
10:L:59:PRO:HB3	10:L:133:PHE:CE1	2.44	0.52
1:A:491:HIS:HD1	1:A:510:PHE:HE2	1.57	0.52
1:E:403:VAL:HG11	1:E:599:MET:HG2	1.90	0.52
2:G:667:LEU:O	2:G:670:TRP:NE1	2.32	0.52
6:O:105:ARG:O	6:O:109:GLN:HG3	2.09	0.52
11:T:46:GLU:OE2	11:T:47:LEU:HD23	2.09	0.52
1:A:349:TRP:NE1	12:A:805:CLA:HHD	35.93	0.52
2:B:223:ARG:NH1	2:B:223:ARG:HA	2.25	0.52
2:B:385:PHE:HA	2:B:388:VAL:HG12	1.91	0.52
6:F:107:TYR:O	6:F:111:ILE:HG13	2.10	0.52
2:B:574:SER:O	2:B:576:TRP:N	2.43	0.52
12:B:827:CLA:HAA2	12:B:828:CLA:OBD	16.11	0.52
1:E:491:HIS:HD1	1:E:510:PHE:HE2	1.57	0.52
3:H:16:CYS:SG	3:H:17:VAL:N	2.82	0.52
9:K:86:LEU:HG	9:K:90:GLY:HA3	1.92	0.52
1:A:349:TRP:NE1	12:A:803:CLA:HHD	2.24	0.52
2:B:150:LEU:HB2	11:M:39:LEU:HD12	3.47	0.52
4:D:99:PRO:HG3	4:D:104:PHE:CE1	2.44	0.52
1:E:101:TYR:HB2	1:E:145:PHE:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:585:GLN:CD	2:G:670:TRP:H	2.82	0.52
12:G:826:CLA:HAA2	12:G:827:CLA:OBD	2.10	0.52
6:O:130:LEU:HA	6:O:133:MET:HE2	1.92	0.52
5:V:55:GLU:N	5:V:55:GLU:CD	2.62	0.52
2:G:182:LEU:O	2:G:186:SER:OG	2.27	0.52
4:N:27:GLU:OE2	4:N:87:ARG:HG3	2.11	0.52
7:P:5:SER:OG	7:P:6:PHE:N	2.43	0.52
12:A:801:CLA:O2D	12:A:801:CLA:H2A	2.10	0.52
3:C:13:CYS:SG	3:C:15:GLN:HG2	2.49	0.52
12:E:801:CLA:H2A	12:E:801:CLA:O2D	2.10	0.52
2:G:123:TRP:O	2:G:127:ILE:HG12	2.10	0.52
7:I:5:SER:OG	7:I:6:PHE:N	2.43	0.52
1:A:286:THR:HG23	1:A:288:GLY:H	1.74	0.52
2:B:182:LEU:O	2:B:186:SER:OG	2.27	0.52
2:B:333:SER:O	2:B:337:GLN:NE2	2.41	0.52
2:G:223:ARG:HA	2:G:223:ARG:NH1	2.25	0.52
2:G:278:LEU:O	2:G:282:VAL:HG12	2.10	0.52
2:G:176:ASN:ND2	2:G:288:GLY:O	2.32	0.52
10:L:25:ARG:NH2	10:L:125:THR:O	2.33	0.52
4:N:74:LEU:O	4:N:79:ARG:N	2.43	0.52
1:A:416:ASP:N	1:A:416:ASP:OD1	2.42	0.52
1:A:45:THR:OG1	1:A:46:THR:N	2.43	0.52
2:B:278:LEU:O	2:B:282:VAL:HG12	2.10	0.52
2:B:318:GLN:HG2	12:B:826:CLA:HMA3	1.92	0.52
1:E:418:ASP:O	1:E:422:ASN:HB2	2.09	0.52
1:E:582:GLY:N	2:G:671:ARG:HD3	2.81	0.52
1:E:739:THR:HG22	1:E:743:PHE:CE2	2.45	0.52
12:E:804:CLA:H42	13:E:846:PQN:H241	1.92	0.52
12:G:828:CLA:HAA2	12:G:829:CLA:OBD	14.54	0.52
10:L:156:VAL:O	10:L:160:ILE:HG12	2.10	0.52
4:N:87:ARG:HG2	4:N:95:GLN:NE2	2.25	0.52
6:O:107:TYR:O	6:O:111:ILE:HG13	2.10	0.52
6:O:88:ILE:O	6:O:92:LEU:HG	2.10	0.52
10:S:148:ILE:O	10:S:151:VAL:HG22	2.10	0.52
10:S:35:THR:HG22	10:S:38:ASN:ND2	2.25	0.52
1:A:104:TRP:HA	1:A:111:ILE:HD12	1.92	0.52
1:A:433:HIS:O	1:A:437:ILE:HG12	2.10	0.52
1:A:532:ASP:OD1	1:A:532:ASP:N	2.43	0.52
3:C:3:SER:OG	4:D:139:TYR:OH	2.14	0.52
1:E:504:GLU:OE1	1:E:508:TYR:OH	2.29	0.52
10:L:148:ILE:O	10:L:151:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:46:GLU:OE2	11:M:47:LEU:HD23	2.09	0.52
6:O:155:LYS:HB3	6:O:158:GLU:H	1.75	0.52
2:B:123:TRP:O	2:B:127:ILE:HG12	2.10	0.51
2:B:392:ALA:O	2:B:396:ILE:HG23	2.11	0.51
1:E:386:THR:O	1:E:390:ILE:HG13	2.10	0.51
12:E:835:CLA:HBB1	12:E:835:CLA:HMB1	1.90	0.51
2:G:574:SER:O	2:G:576:TRP:N	2.43	0.51
9:K:41:ARG:NH2	9:K:67:THR:OG1	2.42	0.51
9:R:86:LEU:HG	9:R:90:GLY:HA3	1.92	0.51
1:A:739:THR:HG22	1:A:743:PHE:CE2	2.45	0.51
2:B:260:GLY:HA3	2:B:499:GLY:HA3	1.92	0.51
1:E:514:VAL:HG21	1:E:628:ILE:HD11	1.92	0.51
1:E:333:PHE:HE2	12:E:823:CLA:HBB1	18.17	0.51
9:R:41:ARG:NH2	9:R:67:THR:OG1	2.42	0.51
9:R:45:PHE:CZ	9:R:53:PRO:HG3	2.45	0.51
1:A:386:THR:O	1:A:390:ILE:HG13	2.10	0.51
1:E:532:ASP:N	1:E:532:ASP:OD1	2.43	0.51
6:F:155:LYS:HB3	6:F:158:GLU:H	1.75	0.51
2:G:392:ALA:O	2:G:396:ILE:HG23	2.11	0.51
9:K:45:PHE:CZ	9:K:53:PRO:HG3	2.46	0.51
10:L:35:THR:HG22	10:L:38:ASN:ND2	2.25	0.51
5:V:20:ASP:OD1	6:O:160:PRO:HB2	145.62	0.51
10:S:156:VAL:O	10:S:160:ILE:HG12	2.10	0.51
5:V:6:SER:O	5:V:24:VAL:HG23	2.10	0.51
5:W:6:SER:O	5:W:24:VAL:HG23	2.10	0.51
1:A:504:GLU:OE1	1:A:508:TYR:OH	2.29	0.51
2:B:378:HIS:CE1	2:B:382:ILE:HD11	2.46	0.51
2:B:467:ILE:HA	2:B:470:SER:HB3	1.92	0.51
12:B:829:CLA:HAA2	12:B:830:CLA:OBD	2.10	0.51
4:D:96:TYR:OH	4:D:99:PRO:HD2	2.31	0.51
1:E:433:HIS:O	1:E:437:ILE:HG12	2.10	0.51
1:E:333:PHE:HE2	12:E:825:CLA:HBB1	1.76	0.51
2:G:19:ARG:HH11	2:G:20:ARG:N	2.08	0.51
2:G:385:PHE:HA	2:G:388:VAL:HG12	1.91	0.51
2:G:260:GLY:HA3	2:G:499:GLY:HA3	1.92	0.51
2:G:621:GLY:O	2:G:625:ASP:CB	2.59	0.51
2:G:663:GLY:O	2:G:667:LEU:HG	2.11	0.51
5:V:8:VAL:HG11	5:V:58:LEU:HD13	1.93	0.51
1:A:514:VAL:HG21	1:A:628:ILE:HD11	1.92	0.51
12:A:801:CLA:CHA	12:B:806:CLA:HAB	2.40	0.51
1:A:333:PHE:HE2	12:A:824:CLA:HBB1	16.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:588:ASN:OD1	2:B:589:THR:N	2.44	0.51
2:B:663:GLY:O	2:B:667:LEU:HG	2.11	0.51
6:F:130:LEU:O	6:F:134:LEU:HG	2.11	0.51
2:G:443:HIS:HE1	12:G:834:CLA:CHC	2.24	0.51
4:N:24:PHE:HA	4:N:28:LYS:HD2	1.93	0.51
1:A:80:GLN:HE22	12:A:804:CLA:C4C	2.24	0.51
2:B:184:GLY:O	2:B:187:SER:OG	2.21	0.51
12:E:802:CLA:HMB1	12:E:802:CLA:HBB1	1.93	0.51
2:G:43:TYR:HB3	2:G:168:PHE:CE2	2.46	0.51
2:G:91:ILE:HB	2:G:112:PRO:HB2	1.93	0.51
2:B:19:ARG:HH11	2:B:20:ARG:N	2.08	0.51
2:B:262:HIS:CD2	2:B:265:THR:H	2.17	0.51
2:B:621:GLY:O	2:B:625:ASP:CB	2.59	0.51
2:B:70:TRP:CD1	11:M:21:ILE:HD11	2.70	0.51
12:B:808:CLA:HBD	11:M:49:LYS:HD2	1.92	0.51
12:B:832:CLA:H2A	12:B:832:CLA:HED2	3.40	0.51
4:D:25:ARG:O	4:D:90:PRO:HB3	2.13	0.51
6:F:88:ILE:O	6:F:92:LEU:HG	2.10	0.51
12:G:801:CLA:HBB1	12:G:801:CLA:HMB1	4.30	0.51
12:G:805:CLA:C2A	11:T:47:LEU:HD21	2.41	0.51
12:G:833:CLA:H2A	12:G:833:CLA:HED2	5.54	0.51
4:N:99:PRO:HG3	4:N:104:PHE:CE1	2.46	0.51
5:W:8:VAL:HG11	5:W:58:LEU:HD13	1.93	0.51
1:A:36:ASP:H	1:A:39:LEU:HD21	1.76	0.51
12:A:801:CLA:C1A	12:B:806:CLA:HAB	2.40	0.51
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.93	0.51
3:C:59:THR:OG1	14:C:102:SF4:S2	2.60	0.51
4:D:87:ARG:HG2	4:D:95:GLN:NE2	2.30	0.51
1:E:36:ASP:H	1:E:39:LEU:HD21	1.76	0.51
1:E:45:THR:OG1	1:E:46:THR:N	2.43	0.51
2:G:318:GLN:HG2	12:G:823:CLA:HMA3	1.92	0.51
2:G:361:PRO:HB2	12:G:819:CLA:HAA2	1.91	0.51
2:G:378:HIS:CE1	2:G:382:ILE:HD11	2.46	0.51
12:G:835:CLA:O2A	12:G:835:CLA:H3A	4.18	0.51
12:J:1102:CLA:O2A	12:J:1102:CLA:H3A	2.11	0.51
6:O:138:THR:OG1	6:O:138:THR:O	2.25	0.51
1:A:36:ASP:HB2	1:A:39:LEU:HD23	1.93	0.51
1:A:411:ILE:HA	1:A:414:VAL:HG12	1.93	0.51
1:A:58:ASP:O	1:A:61:THR:OG1	2.24	0.51
1:E:58:ASP:O	1:E:61:THR:OG1	2.24	0.51
2:G:318:GLN:HG2	12:G:825:CLA:HMA3	18.60	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:443:HIS:HE1	12:G:835:CLA:CHC	33.98	0.51
2:G:467:ILE:HA	2:G:470:SER:HB3	1.92	0.51
2:G:484:ASN:HB3	2:G:487:SER:HB3	1.93	0.51
3:H:51:LYS:HE3	3:H:54:GLU:OE2	2.11	0.51
6:O:130:LEU:O	6:O:134:LEU:HG	2.11	0.51
6:O:60:ARG:NH1	8:Q:43:LEU:HA	2.14	0.51
1:A:145:PHE:O	1:A:149:ARG:N	2.44	0.51
1:A:77:HIS:O	1:A:81:LEU:HG	2.11	0.51
12:A:801:CLA:HBA1	12:B:806:CLA:HMB1	1.93	0.51
2:B:443:HIS:HE1	12:B:835:CLA:CHC	22.71	0.51
12:B:811:CLA:H2	12:B:811:CLA:ND	2.26	0.51
1:E:145:PHE:O	1:E:149:ARG:N	2.44	0.51
1:E:80:GLN:HE22	12:E:807:CLA:C4C	2.24	0.51
2:G:443:HIS:HE1	12:G:834:CLA:C1C	2.24	0.51
2:G:588:ASN:OD1	2:G:589:THR:N	2.44	0.51
1:E:582:GLY:H	2:G:671:ARG:HE	1.66	0.51
12:G:834:CLA:H3A	12:G:834:CLA:O2A	2.11	0.51
2:B:443:HIS:HE1	12:J:1102:CLA:C1C	2.24	0.51
2:B:443:HIS:HE1	12:J:1102:CLA:CHC	2.24	0.51
10:L:101:MET:O	10:L:104:ILE:HG12	2.11	0.51
12:A:832:CLA:HMC2	12:L:204:CLA:HBB2	27.80	0.51
4:N:25:ARG:O	4:N:90:PRO:HB3	2.11	0.51
2:G:455:LYS:HD3	6:O:57:ARG:NE	2.55	0.51
1:A:212:SER:OG	12:A:814:CLA:HHC	10.19	0.50
1:A:723:GLN:O	1:A:727:VAL:HG23	2.11	0.50
12:A:802:CLA:HBB1	12:A:802:CLA:HMB1	2.13	0.50
2:B:31:PHE:O	2:B:34:HIS:ND1	2.39	0.50
3:C:20:CYS:SG	3:C:24:VAL:N	2.78	0.50
4:D:98:HIS:CG	4:D:99:PRO:HA	2.46	0.50
1:E:723:GLN:O	1:E:727:VAL:HG23	2.11	0.50
1:E:216:HIS:HE1	12:E:813:CLA:HMA3	30.37	0.50
12:E:839:CLA:H42	8:Q:22:LEU:HD12	63.28	0.50
8:J:38:TYR:HA	8:J:41:PRO:HG3	1.93	0.50
8:Q:38:TYR:HA	8:Q:41:PRO:HG3	1.93	0.50
10:S:25:ARG:NH2	10:S:125:THR:O	2.33	0.50
1:A:565:ASP:HB3	1:A:568:ASN:HB2	1.93	0.50
12:A:817:CLA:C4D	12:A:817:CLA:H11	6.55	0.50
12:A:810:CLA:HHC	12:A:818:CLA:HBC2	1.93	0.50
2:B:43:TYR:HB3	2:B:168:PHE:CE2	2.46	0.50
1:A:439:SER:HB3	2:B:680:THR:OG1	2.11	0.50
12:A:837:CLA:H3A	12:B:836:CLA:C5	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:TRP:HA	1:E:111:ILE:HD12	1.92	0.50
1:E:80:GLN:HE22	12:E:805:CLA:C4C	12.86	0.50
1:E:212:SER:OG	12:E:813:CLA:HHC	15.04	0.50
2:G:256:THR:OG1	2:G:257:PHE:N	2.45	0.50
2:G:634:LEU:HD11	2:G:653:PHE:CZ	2.46	0.50
12:G:808:CLA:ND	12:G:808:CLA:H2	2.26	0.50
10:L:170:ILE:HG12	12:G:811:CLA:C3	2.42	0.50
10:S:101:MET:O	10:S:104:ILE:HG12	2.11	0.50
1:A:130:ASP:HB2	1:A:136:HIS:CE1	2.46	0.50
2:B:634:LEU:HD11	2:B:653:PHE:CZ	2.47	0.50
1:E:130:ASP:HB2	1:E:136:HIS:CE1	2.46	0.50
1:E:260:GLY:C	1:E:262:THR:H	2.15	0.50
1:E:77:HIS:O	1:E:81:LEU:HG	2.11	0.50
12:E:805:CLA:H12	12:E:812:CLA:H43	1.94	0.50
3:H:53:CYS:HB3	3:H:64:ILE:HD11	1.94	0.50
11:T:22:SER:O	11:T:24:THR:N	2.45	0.50
1:A:260:GLY:C	1:A:262:THR:H	2.15	0.50
1:A:613:LYS:HG3	1:A:614:MET:N	2.27	0.50
1:A:689:SER:HB2	1:A:694:TRP:HE1	1.77	0.50
1:A:212:SER:OG	12:A:812:CLA:HHC	2.11	0.50
2:B:318:GLN:HG2	12:B:824:CLA:HMA3	23.99	0.50
2:B:65:LEU:HA	2:B:68:VAL:HG12	1.94	0.50
12:B:834:CLA:H2A	12:B:834:CLA:HED2	1.93	0.50
12:E:813:CLA:HHC	12:E:821:CLA:HBC2	1.93	0.50
6:F:118:GLU:OE2	6:F:118:GLU:N	2.45	0.50
2:G:634:LEU:HD21	2:G:653:PHE:CE2	2.47	0.50
12:G:810:CLA:ND	12:G:810:CLA:H2	10.14	0.50
5:W:7:LYS:N	5:W:62:GLU:OE2	2.33	0.50
1:A:216:HIS:HE1	12:A:814:CLA:HMA3	10.37	0.50
1:A:333:PHE:HE2	12:A:822:CLA:HBB1	1.76	0.50
1:A:684:LEU:HD12	1:A:688:PHE:HE2	1.77	0.50
12:B:809:CLA:H2	12:B:809:CLA:ND	9.60	0.50
12:B:835:CLA:O2A	12:B:835:CLA:H3A	4.39	0.50
4:D:98:HIS:HA	4:D:100:SER:N	2.26	0.50
12:E:818:CLA:H11	12:E:818:CLA:C4D	2.42	0.50
2:G:443:HIS:HE1	12:G:835:CLA:C1C	34.24	0.50
2:G:65:LEU:HA	2:G:68:VAL:HG12	1.94	0.50
10:L:25:ARG:HB2	10:L:26:ARG:CZ	2.42	0.50
11:M:22:SER:O	11:M:24:THR:N	2.45	0.50
11:M:32:ILE:HG22	11:M:33:ALA:H	1.77	0.50
11:T:32:ILE:HG22	11:T:33:ALA:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:802:CLA:H12	12:A:809:CLA:H43	1.93	0.50
2:B:138:GLY:HA2	2:B:141:PHE:CE1	2.47	0.50
2:B:319:PHE:H	12:B:824:CLA:C2B	31.19	0.50
3:C:51:LYS:HE3	3:C:54:GLU:OE2	2.11	0.50
3:C:53:CYS:HB3	3:C:64:ILE:HD11	1.94	0.50
1:E:216:HIS:HE1	12:E:815:CLA:HMA3	1.76	0.50
1:E:659:ILE:HD12	2:G:628:TRP:CE2	2.95	0.50
1:E:212:SER:OG	12:E:815:CLA:HHC	2.11	0.50
2:G:138:GLY:HA2	2:G:141:PHE:CE1	2.47	0.50
6:O:88:ILE:HA	6:O:91:ILE:HD12	1.93	0.50
1:A:80:GLN:HE22	12:A:806:CLA:C4C	21.18	0.50
2:B:133:ASN:HA	2:B:136:TYR:HB3	1.94	0.50
2:B:319:PHE:H	12:B:826:CLA:C2B	2.25	0.50
1:A:467:ARG:HH12	2:B:97:GLY:HA2	1.77	0.50
1:E:188:LEU:HA	1:E:191:PHE:CD2	2.47	0.50
2:G:333:SER:O	2:G:337:GLN:NE2	2.41	0.50
2:G:351:LEU:HG	2:G:355:HIS:CD2	2.47	0.50
2:G:681:LEU:HD11	12:G:801:CLA:C2D	2.42	0.50
10:L:99:LEU:O	10:L:103:VAL:HG23	2.12	0.50
10:L:24:SER:HA	10:L:32:ASN:HB2	1.94	0.50
1:E:122:VAL:HG22	6:O:47:THR:OG1	3.47	0.50
2:B:139:ALA:O	2:B:143:LEU:HD12	2.12	0.50
2:B:351:LEU:HG	2:B:355:HIS:CD2	2.47	0.50
4:D:27:GLU:OE2	4:D:87:ARG:HG3	2.12	0.50
4:D:31:ILE:HD12	4:D:66:CYS:HB2	3.67	0.50
6:F:88:ILE:HA	6:F:91:ILE:HD12	1.93	0.50
4:N:127:ASP:HB2	4:N:130:LYS:NZ	7.26	0.50
4:N:37:LYS:HG3	4:N:39:GLN:OE1	5.06	0.50
6:O:40:ARG:NH2	6:O:69:GLU:O	2.45	0.50
2:B:634:LEU:HD21	2:B:653:PHE:CE2	2.47	0.50
4:D:121:ASN:ND2	4:D:124:LYS:H	3.10	0.50
4:D:30:VAL:HG12	4:D:59:GLU:HG2	1.94	0.50
1:E:36:ASP:HB2	1:E:39:LEU:HD23	1.93	0.50
1:E:684:LEU:HD12	1:E:688:PHE:HE2	1.77	0.50
12:E:811:CLA:HHC	12:E:819:CLA:HBC2	27.37	0.50
2:G:224:PRO:HA	2:G:227:THR:HG22	1.93	0.50
2:G:319:PHE:H	12:G:823:CLA:C2B	2.25	0.50
12:G:831:CLA:H2A	12:G:831:CLA:HED2	1.93	0.50
10:S:24:SER:HB3	10:S:30:ILE:HG13	1.94	0.50
1:A:188:LEU:HA	1:A:191:PHE:CD2	2.47	0.49
1:A:35:PHE:CZ	1:A:56:ALA:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:599:TRP:CZ3	2:B:626:TYR:HB2	2.47	0.49
4:D:121:ASN:HD21	4:D:124:LYS:H	2.82	0.49
4:D:24:PHE:HA	4:D:28:LYS:HD2	1.93	0.49
1:E:453:PHE:HA	1:E:456:TYR:HB2	1.94	0.49
1:E:35:PHE:CZ	1:E:56:ALA:HA	2.47	0.49
1:E:648:ARG:NH2	2:G:636:ASN:HA	2.74	0.49
2:G:133:ASN:HA	2:G:136:TYR:HB3	1.94	0.49
10:S:25:ARG:HB2	10:S:26:ARG:CZ	2.42	0.49
2:B:139:ALA:O	2:B:142:LEU:HD23	2.12	0.49
2:B:484:ASN:HB3	2:B:487:SER:HB3	1.93	0.49
12:B:814:CLA:HMC3	12:B:822:CLA:HBC1	41.75	0.49
1:E:613:LYS:HG3	1:E:614:MET:N	2.27	0.49
1:E:689:SER:HB2	1:E:694:TRP:HE1	1.77	0.49
6:F:40:ARG:NH2	6:F:69:GLU:O	2.45	0.49
3:H:20:CYS:SG	3:H:24:VAL:N	2.78	0.49
10:S:25:ARG:HB2	10:S:26:ARG:NH2	2.27	0.49
10:S:24:SER:HA	10:S:32:ASN:HB2	1.94	0.49
1:A:27:GLU:OE2	8:J:8:GLN:NE2	2.45	0.49
1:A:455:LEU:HD11	1:A:472:PHE:CZ	2.48	0.49
12:A:815:CLA:H11	12:A:815:CLA:C4D	2.42	0.49
2:B:224:PRO:HA	2:B:227:THR:HG22	1.94	0.49
2:B:70:TRP:NE1	7:I:2:PHE:HE2	2.10	0.49
1:E:248:SER:O	1:E:252:GLU:HG3	2.13	0.49
1:E:411:ILE:HA	1:E:414:VAL:HG12	1.93	0.49
1:E:593:PHE:O	1:E:596:LEU:HG	2.13	0.49
1:E:59:PHE:CD1	1:E:72:LYS:HE3	2.48	0.49
12:E:803:CLA:H12	12:E:810:CLA:H43	42.97	0.49
2:G:139:ALA:O	2:G:143:LEU:HD12	2.12	0.49
2:G:435:PHE:CE1	12:G:801:CLA:H2	50.70	0.49
10:L:24:SER:HB3	10:L:30:ILE:HG13	1.94	0.49
9:R:33:LEU:HD23	9:R:76:HIS:HA	1.94	0.49
1:A:216:HIS:HE1	12:A:812:CLA:HMA3	1.77	0.49
1:A:578:PRO:HD2	3:C:51:LYS:HD3	2.01	0.49
1:A:59:PHE:CD1	1:A:72:LYS:HE3	2.48	0.49
12:A:812:CLA:HHC	12:A:820:CLA:HBC2	26.67	0.49
2:B:44:GLN:CD	2:B:162:ARG:HD2	2.33	0.49
1:A:497:SER:CB	2:B:227:THR:HA	118.55	0.49
2:B:335:HIS:HB3	2:B:397:PHE:HB2	1.95	0.49
3:C:27:MET:O	4:D:107:LYS:NZ	2.45	0.49
2:G:139:ALA:O	2:G:142:LEU:HD23	2.12	0.49
1:E:652:TRP:CZ3	2:G:628:TRP:HE3	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:813:CLA:HMC3	12:G:821:CLA:HBC1	1.94	0.49
12:G:822:CLA:HMB2	12:G:827:CLA:HMA3	23.12	0.49
12:G:820:CLA:HMB2	12:G:825:CLA:HMA3	1.94	0.49
10:L:25:ARG:HB2	10:L:26:ARG:NH2	2.28	0.49
6:O:95:TYR:HA	6:O:139:TRP:CZ2	2.48	0.49
1:A:384:TYR:HE1	1:A:520:LYS:HB3	1.78	0.49
1:A:542:GLN:HG3	1:A:602:THR:HG22	1.95	0.49
2:B:443:HIS:HE1	12:B:835:CLA:C1C	23.62	0.49
2:B:580:TYR:HD2	2:B:709:ARG:HH21	1.60	0.49
12:B:825:CLA:H3A	12:B:825:CLA:O1A	4.75	0.49
1:E:114:SER:HG	1:E:139:GLN:HA	1.77	0.49
1:E:455:LEU:HD11	1:E:472:PHE:CZ	2.48	0.49
1:E:565:ASP:HB3	1:E:568:ASN:HB2	1.93	0.49
2:G:319:PHE:H	12:G:825:CLA:C2B	16.24	0.49
12:G:813:CLA:HHC	12:G:821:CLA:HBC2	1.95	0.49
12:G:826:CLA:O1A	12:G:826:CLA:H3A	4.41	0.49
2:G:563:ASP:HA	3:H:51:LYS:HZ1	1.93	0.49
9:K:33:LEU:HD23	9:K:76:HIS:HA	1.95	0.49
9:K:79:GLY:HA2	9:K:82:ILE:HD12	1.95	0.49
10:S:40:SER:O	10:S:43:VAL:HG22	2.13	0.49
1:A:491:HIS:HB3	12:A:834:CLA:HED3	8.58	0.49
12:A:833:CLA:HBD	12:A:833:CLA:O1A	2.12	0.49
12:A:835:CLA:O1A	12:A:835:CLA:HBD	3.13	0.49
1:A:678:PHE:HE2	12:A:839:CLA:HBB2	1.78	0.49
2:B:590:VAL:O	2:B:594:THR:HG22	2.12	0.49
12:B:823:CLA:HMB2	12:B:828:CLA:HMA3	1.93	0.49
12:B:821:CLA:HMB2	12:B:826:CLA:HMA3	36.31	0.49
4:D:12:PHE:HZ	4:D:15:SER:HG	1.60	0.49
6:F:117:THR:O	6:F:121:GLU:HB3	2.13	0.49
2:G:590:VAL:O	2:G:594:THR:HG22	2.12	0.49
2:G:599:TRP:CZ3	2:G:626:TYR:HB2	2.47	0.49
12:G:815:CLA:HMC3	12:G:823:CLA:HBC1	32.55	0.49
6:O:118:GLU:OE2	6:O:118:GLU:N	2.45	0.49
6:O:117:THR:O	6:O:121:GLU:HB3	2.13	0.49
9:R:79:GLY:HA2	9:R:82:ILE:HD12	1.95	0.49
1:A:323:LYS:O	1:A:327:GLU:HG3	2.13	0.49
1:A:453:PHE:HA	1:A:456:TYR:HB2	1.94	0.49
12:B:827:CLA:H3A	12:B:827:CLA:O1A	2.13	0.49
1:E:46:THR:HA	1:E:714:ILE:HD11	1.95	0.49
2:G:306:ASN:HA	2:G:308:LYS:HZ2	1.77	0.49
7:I:17:LEU:C	7:I:20:PRO:HD2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:106:THR:HG21	10:L:147:LEU:HD22	1.95	0.49
12:G:808:CLA:HBC1	11:T:29:ALA:HA	1.94	0.49
1:A:715:GLN:HE22	5:V:43:VAL:HG23	1.78	0.49
12:A:810:CLA:H2	12:A:810:CLA:C1D	2.43	0.49
12:A:804:CLA:H12	12:A:811:CLA:H43	22.35	0.49
1:A:491:HIS:HB3	12:A:832:CLA:HED3	1.95	0.49
2:B:583:LEU:HD23	2:B:587:LEU:HD11	1.95	0.49
12:B:816:CLA:HMC3	12:B:824:CLA:HBC1	1.94	0.49
4:D:26:GLU:HA	4:D:90:PRO:HG3	1.96	0.49
4:D:98:HIS:CD2	4:D:99:PRO:HA	2.48	0.49
1:E:323:LYS:O	1:E:327:GLU:HG3	2.13	0.49
1:E:91:MET:HE1	12:E:807:CLA:HMA2	22.65	0.49
2:G:172:GLU:HG2	2:G:173:PRO:HD3	1.95	0.49
2:G:308:LYS:O	2:G:314:LYS:HB3	2.13	0.49
2:G:34:HIS:HB2	2:G:37:MET:SD	2.53	0.49
1:E:584:CYS:O	2:G:672:GLY:HA3	2.13	0.49
12:G:824:CLA:H3A	12:G:824:CLA:O1A	2.13	0.49
7:P:17:LEU:C	7:P:20:PRO:HD2	2.33	0.49
1:A:545:VAL:O	1:A:548:LEU:HB3	2.13	0.49
2:B:141:PHE:O	2:B:145:LEU:HG	2.13	0.49
2:B:305:LEU:HD13	2:B:327:TYR:CE2	2.48	0.49
2:B:34:HIS:HB2	2:B:37:MET:SD	2.53	0.49
4:D:36:PRO:O	4:D:53:GLN:NE2	2.46	0.49
1:E:359:MET:CE	12:E:824:CLA:HMA1	24.27	0.49
1:E:359:MET:CE	12:E:826:CLA:HMA1	2.43	0.49
12:E:837:CLA:HBD	12:E:837:CLA:O1A	2.12	0.49
12:E:841:CLA:HBC3	13:E:846:PQN:H261	1.95	0.49
6:F:95:TYR:HA	6:F:139:TRP:CZ2	2.48	0.49
2:G:31:PHE:O	2:G:34:HIS:ND1	2.39	0.49
12:L:202:CLA:H3A	12:L:202:CLA:HBA2	1.56	0.49
3:C:34:LYS:HZ2	5:V:30:SER:HB2	1.77	0.49
1:A:623:ASP:HB2	1:A:627:THR:HB	1.95	0.49
2:B:172:GLU:HG2	2:B:173:PRO:HD3	1.95	0.49
2:B:308:LYS:O	2:B:314:LYS:HB3	2.13	0.49
2:B:567:ARG:HB3	5:W:45:TYR:CE2	117.17	0.49
12:B:842:CLA:HBB1	13:B:844:PQN:H211	1.94	0.49
1:E:545:VAL:O	1:E:548:LEU:HB3	2.13	0.49
1:E:623:ASP:HB2	1:E:627:THR:HB	1.95	0.49
1:E:612:TRP:CD2	1:E:636:PHE:HE1	2.31	0.49
2:G:44:GLN:CD	2:G:162:ARG:HD2	2.33	0.49
12:G:818:CLA:H3A	12:G:818:CLA:HBA2	1.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:99:LEU:O	10:S:103:VAL:HG23	2.12	0.49
10:S:106:THR:HG21	10:S:147:LEU:HD22	1.95	0.49
1:A:114:SER:HA	1:A:140:ILE:HG12	1.95	0.48
1:A:361:GLY:HA2	1:A:401:LEU:HD21	1.95	0.48
1:A:46:THR:HA	1:A:714:ILE:HD11	1.95	0.48
1:A:593:PHE:O	1:A:596:LEU:HG	2.13	0.48
1:A:612:TRP:CD2	1:A:636:PHE:HE1	2.31	0.48
1:A:59:PHE:HA	1:A:62:HIS:ND1	2.28	0.48
12:A:836:CLA:HBA2	12:A:836:CLA:H3A	1.58	0.48
2:B:256:THR:OG1	2:B:257:PHE:N	2.45	0.48
2:B:306:ASN:HA	2:B:308:LYS:NZ	2.29	0.48
2:B:327:TYR:O	2:B:331:ASN:ND2	2.46	0.48
1:E:599:MET:O	1:E:602:THR:OG1	2.24	0.48
1:E:205:LEU:HD12	12:E:812:CLA:HHB	29.22	0.48
2:G:306:ASN:HA	2:G:308:LYS:NZ	2.28	0.48
2:G:327:TYR:O	2:G:331:ASN:ND2	2.46	0.48
2:G:580:TYR:HD2	2:G:709:ARG:HH21	1.60	0.48
3:H:12:GLY:N	14:H:102:SF4:S1	2.86	0.48
10:L:40:SER:O	10:L:43:VAL:HG22	2.13	0.48
10:S:165:GLU:HA	10:S:168:GLN:OE1	2.13	0.48
1:A:59:PHE:HA	1:A:62:HIS:CG	2.49	0.48
2:B:143:LEU:HD22	11:M:32:ILE:HD11	3.01	0.48
1:E:114:SER:HA	1:E:140:ILE:HG12	1.95	0.48
1:E:206:LEU:HD22	12:E:820:CLA:HMC1	1.95	0.48
1:E:384:TYR:HE1	1:E:520:LYS:HB3	1.78	0.48
1:E:59:PHE:HA	1:E:62:HIS:CG	2.48	0.48
1:E:678:PHE:HE2	12:E:840:CLA:HBB2	42.91	0.48
2:G:141:PHE:O	2:G:145:LEU:HG	2.13	0.48
7:I:7:LEU:HB3	7:I:11:LEU:HD23	1.96	0.48
4:N:76:ALA:C	4:N:79:ARG:HH12	2.16	0.48
1:A:248:SER:O	1:A:252:GLU:HG3	2.13	0.48
2:B:20:ARG:O	2:B:24:GLY:N	2.43	0.48
2:B:519:ASP:O	2:B:523:HIS:ND1	2.46	0.48
1:E:205:LEU:HD12	12:E:814:CLA:HHB	1.95	0.48
1:E:705:HIS:CG	12:E:839:CLA:HBC1	68.67	0.48
2:G:114:ASN:HD21	12:G:811:CLA:C4C	19.84	0.48
2:G:648:VAL:O	2:G:652:MET:HG2	2.14	0.48
2:G:294:ASN:HD21	12:G:815:CLA:HAA2	34.76	0.48
10:L:60:LEU:HA	10:L:60:LEU:HD23	1.72	0.48
4:N:10:PRO:HA	4:N:52:ARG:HD3	2.18	0.48
9:R:68:VAL:O	9:R:72:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:3:SER:OG	11:T:20:SER:HB3	2.39	0.48
2:B:585:TRP:CH2	12:B:803:CLA:HAB	46.98	0.48
2:B:648:VAL:O	2:B:652:MET:HG2	2.14	0.48
12:B:814:CLA:HHC	12:B:822:CLA:HBC2	40.86	0.48
3:C:12:GLY:N	14:C:102:SF4:S1	2.86	0.48
1:E:59:PHE:HA	1:E:62:HIS:ND1	2.28	0.48
12:E:834:CLA:HBD	12:E:834:CLA:O1A	5.91	0.48
12:E:837:CLA:HBA2	12:E:837:CLA:H3A	3.75	0.48
2:G:52:GLY:O	2:G:56:ILE:HG23	2.14	0.48
12:G:815:CLA:HHC	12:G:823:CLA:HBC2	33.77	0.48
8:Q:17:LEU:O	8:Q:19:PRO:HD2	2.14	0.48
2:B:91:ILE:N	2:B:112:PRO:O	2.41	0.48
2:B:585:TRP:CH2	12:B:805:CLA:HAB	2.48	0.48
2:B:418:HIS:HB3	12:B:834:CLA:HED1	1.96	0.48
2:B:554:LYS:HZ1	4:D:125:ASN:HB2	1.77	0.48
12:E:813:CLA:C1D	12:E:813:CLA:H2	2.43	0.48
2:G:585:TRP:CH2	12:G:802:CLA:HAB	2.49	0.48
12:G:823:CLA:HBA2	12:G:823:CLA:H3A	2.00	0.48
12:G:840:CLA:HBB1	13:G:842:PQN:H211	1.94	0.48
7:I:24:MET:HA	7:I:27:LEU:HD12	1.96	0.48
8:J:22:LEU:O	8:J:26:LEU:HG	2.14	0.48
10:L:165:GLU:HA	10:L:168:GLN:OE1	2.13	0.48
12:S:1501:CLA:H3A	12:S:1501:CLA:HBA2	1.56	0.48
1:A:590:ASP:HA	1:A:593:PHE:CD2	2.49	0.48
1:A:206:LEU:HD22	12:A:817:CLA:HMC1	1.95	0.48
1:A:705:HIS:CG	12:A:840:CLA:HBC1	84.20	0.48
1:A:678:PHE:HE2	12:A:841:CLA:HBB2	54.22	0.48
2:B:658:LEU:HB2	12:B:802:CLA:HBA2	1.95	0.48
12:B:803:CLA:H2A	12:B:803:CLA:HED2	5.35	0.48
1:E:542:GLN:HG3	1:E:602:THR:HG22	1.95	0.48
2:G:318:GLN:HA	12:G:825:CLA:CHB	17.86	0.48
2:G:305:LEU:HD13	2:G:327:TYR:CE2	2.48	0.48
2:G:335:HIS:HB3	2:G:397:PHE:HB2	1.95	0.48
2:G:450:PHE:O	6:O:45:ARG:NH2	2.42	0.48
9:R:29:ILE:HG23	9:R:31:ALA:H	1.79	0.48
12:A:817:CLA:H3A	12:A:817:CLA:HBA2	1.56	0.48
2:B:418:HIS:HB3	12:B:832:CLA:HED1	47.53	0.48
12:B:816:CLA:HHC	12:B:824:CLA:HBC2	1.95	0.48
2:B:349:THR:HG22	12:B:832:CLA:HAC1	1.96	0.48
1:E:259:LYS:O	12:E:814:CLA:HAA2	34.85	0.48
1:E:361:GLY:HA2	1:E:401:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:590:ASP:HA	1:E:593:PHE:CD2	2.49	0.48
1:E:491:HIS:HB3	12:E:833:CLA:HED3	41.86	0.48
1:E:491:HIS:HB3	12:E:836:CLA:HED3	1.95	0.48
1:E:678:PHE:HE2	12:E:843:CLA:HBB2	1.78	0.48
12:E:844:CLA:HAB	2:G:585:TRP:CH2	77.22	0.48
13:E:846:PQN:H202	13:E:846:PQN:H23	1.57	0.48
2:G:114:ASN:HD21	12:G:809:CLA:C4C	2.27	0.48
2:G:20:ARG:O	2:G:24:GLY:N	2.43	0.48
2:G:418:HIS:HB3	12:G:833:CLA:HED1	20.70	0.48
6:O:83:ALA:HA	6:O:86:PHE:CZ	2.49	0.48
1:A:359:MET:CE	12:A:825:CLA:HMA1	13.23	0.48
12:A:830:CLA:C3B	12:A:831:CLA:HMB2	2.44	0.48
12:A:832:CLA:C3B	12:A:833:CLA:HMB2	9.97	0.48
2:B:50:HIS:O	2:B:54:VAL:HG22	2.14	0.48
2:B:553:LYS:HB3	2:B:553:LYS:HE2	1.53	0.48
2:B:52:GLY:O	2:B:56:ILE:HG23	2.14	0.48
2:B:601:HIS:HA	2:B:604:ILE:HD12	1.96	0.48
2:B:294:ASN:HD21	12:B:816:CLA:HAA2	1.78	0.48
2:B:349:THR:HG22	12:B:830:CLA:HAC1	17.74	0.48
1:E:552:LYS:O	1:E:556:PHE:HB2	2.14	0.48
1:E:671:LEU:O	1:E:673:PHE:N	2.41	0.48
2:G:705:ILE:H	2:G:705:ILE:HD12	1.79	0.48
12:G:838:CLA:HBA1	12:G:838:CLA:H3A	3.10	0.48
9:K:29:ILE:HG23	9:K:31:ALA:H	1.79	0.48
1:A:425:ASN:O	1:A:429:ARG:N	2.42	0.48
1:A:552:LYS:O	1:A:556:PHE:HB2	2.14	0.48
1:A:205:LEU:HD12	12:A:811:CLA:HHB	1.95	0.48
12:A:816:CLA:HBA2	12:A:816:CLA:H3A	1.66	0.48
2:B:294:ASN:HD21	12:B:814:CLA:HAA2	66.33	0.48
12:B:805:CLA:HED2	12:B:805:CLA:H2A	1.96	0.48
12:B:812:CLA:HMC3	12:B:813:CLA:CAD	2.44	0.48
2:B:318:GLN:HA	12:B:826:CLA:CHB	2.44	0.48
2:G:50:HIS:O	2:G:54:VAL:HG22	2.14	0.48
2:G:53:HIS:O	2:G:57:ILE:HG13	2.14	0.48
12:G:811:CLA:HMC3	12:G:812:CLA:CAD	46.84	0.48
2:G:318:GLN:HA	12:G:823:CLA:CHB	2.44	0.48
12:G:830:CLA:H3A	12:G:830:CLA:HBA2	1.48	0.48
8:J:17:LEU:O	8:J:19:PRO:HD2	2.14	0.48
1:A:91:MET:HE1	12:A:808:CLA:HMA2	35.30	0.48
2:B:114:ASN:HD21	12:B:812:CLA:C4C	2.27	0.48
2:B:300:SER:HG	2:B:303:GLU:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:83:ALA:HA	6:F:86:PHE:CZ	2.49	0.48
2:G:480:THR:N	2:G:483:SER:HB3	2.26	0.48
8:Q:22:LEU:O	8:Q:26:LEU:HG	2.14	0.48
5:W:55:GLU:CD	5:W:55:GLU:N	2.62	0.48
1:A:684:LEU:HD13	2:B:664:PHE:HE2	1.82	0.47
1:A:205:LEU:HD12	12:A:813:CLA:HHB	24.00	0.47
12:A:818:CLA:HBB1	12:A:818:CLA:HMB1	4.38	0.47
12:A:827:CLA:HBA1	12:A:827:CLA:H3A	3.98	0.47
12:B:810:CLA:HMC3	12:B:811:CLA:CAD	21.45	0.47
1:E:256:SER:HA	1:E:261:LEU:HD12	1.96	0.47
2:G:323:HIS:HB3	2:G:327:TYR:OH	2.14	0.47
2:G:442:VAL:O	2:G:446:VAL:HG22	2.14	0.47
2:G:519:ASP:O	2:G:523:HIS:ND1	2.46	0.47
12:G:819:CLA:H3A	12:G:819:CLA:HBA2	1.62	0.47
3:H:24:VAL:HB	3:H:25:LEU:HD12	1.96	0.47
10:L:35:THR:C	10:L:37:ILE:H	2.17	0.47
7:P:14:LEU:HD23	7:P:14:LEU:H	1.79	0.47
9:R:59:LEU:HG	9:R:59:LEU:O	2.14	0.47
1:A:104:TRP:CH2	1:A:145:PHE:HB3	2.49	0.47
12:A:825:CLA:HBA1	12:A:825:CLA:H3A	1.42	0.47
2:B:183:PHE:HE2	2:B:284:PHE:CG	2.32	0.47
2:B:53:HIS:O	2:B:57:ILE:HG13	2.14	0.47
2:B:705:ILE:H	2:B:705:ILE:HD12	1.79	0.47
2:B:318:GLN:HA	12:B:824:CLA:CHB	28.85	0.47
2:B:80:ASP:OD2	2:B:83:ASN:HB2	2.14	0.47
3:C:24:VAL:HB	3:C:25:LEU:HD12	1.96	0.47
4:D:19:LEU:HD13	4:D:23:ALA:HB1	2.56	0.47
1:E:206:LEU:HD22	12:E:818:CLA:HMC1	15.54	0.47
1:E:259:LYS:O	12:E:816:CLA:HAA2	2.14	0.47
1:E:141:THR:N	12:E:809:CLA:OBD	2.38	0.47
12:E:828:CLA:H3A	12:E:828:CLA:HBA1	1.42	0.47
2:G:183:PHE:O	2:G:187:SER:N	2.43	0.47
12:G:807:CLA:H3A	12:G:807:CLA:HBA2	3.49	0.47
2:G:80:ASP:OD2	2:G:83:ASN:HB2	2.14	0.47
2:B:223:ARG:HA	2:B:223:ARG:HH11	1.79	0.47
2:B:231:GLY:HA2	2:B:234:ALA:HB3	1.96	0.47
12:B:834:CLA:HAB	12:B:835:CLA:C3B	10.56	0.47
6:F:80:LEU:HA	6:F:83:ALA:HB3	1.96	0.47
2:G:183:PHE:HE2	2:G:284:PHE:CG	2.32	0.47
12:G:802:CLA:H2A	12:G:802:CLA:HED2	1.96	0.47
9:K:59:LEU:HG	9:K:59:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:101:ASP:HB3	4:N:105:PRO:HD2	1.96	0.47
7:P:24:MET:HA	7:P:27:LEU:HD12	1.96	0.47
5:W:42:LYS:HG2	5:W:43:VAL:H	1.80	0.47
1:A:585:GLN:OE1	2:B:670:TRP:N	2.47	0.47
1:A:705:HIS:CG	12:A:838:CLA:HBC1	2.49	0.47
12:A:818:CLA:HBA2	12:A:818:CLA:H3A	4.10	0.47
2:B:556:PHE:HB3	2:B:561:PRO:HG2	1.96	0.47
2:B:706:VAL:O	2:B:710:LEU:HG	2.15	0.47
1:E:217:GLN:HB3	1:E:222:LEU:HD23	1.97	0.47
2:G:223:ARG:HA	2:G:223:ARG:HH11	1.79	0.47
2:G:556:PHE:HB3	2:G:561:PRO:HG2	1.96	0.47
2:G:583:LEU:HD23	2:G:587:LEU:HD11	1.95	0.47
2:G:601:HIS:HA	2:G:604:ILE:HD12	1.95	0.47
9:K:68:VAL:O	9:K:72:VAL:HG23	2.14	0.47
4:N:31:ILE:HD12	4:N:66:CYS:HB2	1.96	0.47
6:O:49:ALA:HB3	8:Q:38:TYR:OH	2.13	0.47
6:O:80:LEU:HA	6:O:83:ALA:HB3	1.96	0.47
5:V:42:LYS:HG2	5:V:43:VAL:H	1.80	0.47
1:A:259:LYS:HG3	1:A:260:GLY:H	1.80	0.47
1:A:66:LEU:H	1:A:66:LEU:HD23	1.80	0.47
1:A:259:LYS:O	12:A:813:CLA:HAA2	2.14	0.47
1:A:426:VAL:HG22	12:A:824:CLA:HMC3	18.52	0.47
2:B:135:LEU:HD23	2:B:135:LEU:H	1.80	0.47
2:B:529:GLY:O	2:B:533:THR:HG23	2.14	0.47
1:E:705:HIS:CG	12:E:842:CLA:HBC1	2.48	0.47
6:F:57:ARG:HH12	8:J:42:ASP:HA	1.79	0.47
2:G:349:THR:HG22	12:G:829:CLA:HAC1	1.96	0.47
2:G:669:SER:HG	2:G:674:TRP:HZ2	1.63	0.47
12:G:834:CLA:HAB	12:G:835:CLA:C3B	36.83	0.47
1:A:217:GLN:HB3	1:A:222:LEU:HD23	1.97	0.47
1:A:241:HIS:HA	1:A:244:ILE:HG13	1.95	0.47
1:A:599:MET:O	1:A:602:THR:OG1	2.24	0.47
1:A:359:MET:HE1	12:A:825:CLA:HMA1	13.01	0.47
2:B:506:ASN:ND2	2:B:508:THR:OG1	2.48	0.47
1:E:104:TRP:CH2	1:E:145:PHE:HB3	2.49	0.47
1:E:205:LEU:HB2	12:E:812:CLA:HMB2	31.95	0.47
1:E:590:ASP:O	1:E:594:LEU:HG	2.15	0.47
12:E:834:CLA:C3B	12:E:835:CLA:HMB2	2.44	0.47
2:G:135:LEU:H	2:G:135:LEU:HD23	1.80	0.47
2:G:349:THR:HG22	12:G:831:CLA:HAC1	24.20	0.47
2:G:529:GLY:O	2:G:533:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:598:HIS:O	2:G:602:LEU:HB2	2.15	0.47
12:G:809:CLA:HMC3	12:G:810:CLA:CAD	2.44	0.47
12:G:833:CLA:HAB	12:G:834:CLA:C3B	2.44	0.47
12:B:836:CLA:HAB	12:J:1102:CLA:C3B	2.44	0.47
9:K:53:PRO:C	9:K:55:PRO:HD3	2.35	0.47
10:L:92:ILE:HG13	10:L:92:ILE:H	1.25	0.47
4:N:26:GLU:HA	4:N:90:PRO:HG3	1.95	0.47
3:H:21:PRO:HB2	4:N:64:GLU:OE2	2.15	0.47
1:A:440:HIS:O	1:A:443:TRP:HB3	2.15	0.47
12:A:816:CLA:HBB1	12:A:816:CLA:HMB1	1.96	0.47
1:A:206:LEU:HD22	12:A:819:CLA:HMC1	10.75	0.47
2:B:323:HIS:HB3	2:B:327:TYR:OH	2.14	0.47
4:D:8:GLN:HE22	4:D:52:ARG:NH1	2.44	0.47
4:D:69:LEU:HD13	4:D:73:GLN:HG3	2.92	0.47
1:E:118:VAL:H	1:E:128:ASN:ND2	2.13	0.47
1:E:425:ASN:N	1:E:428:ASP:HB3	2.30	0.47
12:E:831:CLA:C3B	12:E:832:CLA:HMB2	34.70	0.47
2:G:231:GLY:HA2	2:G:234:ALA:HB3	1.96	0.47
2:B:150:LEU:HB3	11:M:43:LEU:CD1	3.11	0.47
4:N:36:PRO:O	4:N:53:GLN:NE2	2.48	0.47
7:P:7:LEU:HB3	7:P:11:LEU:HD23	1.96	0.47
1:A:170:ALA:O	1:A:174:LEU:HG	2.15	0.47
1:A:246:ASN:ND2	1:A:249:LEU:HB2	2.30	0.47
1:A:359:MET:CE	12:A:823:CLA:HMA1	2.43	0.47
1:A:590:ASP:O	1:A:594:LEU:HG	2.15	0.47
12:A:814:CLA:HBA2	12:A:814:CLA:H3A	1.52	0.47
1:A:426:VAL:HG22	12:A:822:CLA:HMC3	1.96	0.47
2:B:345:LEU:O	2:B:349:THR:HG23	2.15	0.47
2:B:685:HIS:CD2	12:B:803:CLA:HMA3	2.50	0.47
1:E:241:HIS:HA	1:E:244:ILE:HG13	1.95	0.47
2:G:294:ASN:HD21	12:G:813:CLA:HAA2	1.78	0.47
10:S:35:THR:C	10:S:37:ILE:H	2.17	0.47
5:W:9:ARG:HB2	5:W:59:VAL:HG23	1.97	0.47
1:A:118:VAL:H	1:A:128:ASN:ND2	2.13	0.47
1:A:425:ASN:N	1:A:428:ASP:HB3	2.30	0.47
2:B:178:HIS:HA	2:B:182:LEU:HD23	1.97	0.47
2:B:612:PHE:O	2:B:616:SER:OG	2.26	0.47
2:B:414:ARG:NE	12:B:832:CLA:OBD	42.60	0.47
4:D:87:ARG:HB3	4:D:95:GLN:HB2	1.96	0.47
12:E:827:CLA:O1D	12:E:827:CLA:H2A	2.45	0.47
2:G:178:HIS:HA	2:G:182:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:14:LEU:HD23	7:I:14:LEU:H	1.79	0.47
4:N:121:ASN:ND2	4:N:124:LYS:H	2.12	0.47
6:O:28:LEU:HD22	6:O:67:GLY:HA2	1.97	0.47
5:V:9:ARG:HB2	5:V:59:VAL:HG23	1.97	0.47
1:A:710:VAL:HG11	12:A:839:CLA:HMA3	29.34	0.47
1:A:719:LEU:HD11	1:A:723:GLN:HB2	1.97	0.47
1:A:259:LYS:O	12:A:815:CLA:HAA2	17.65	0.47
1:A:716:PRO:HB3	12:A:840:CLA:HHC	74.60	0.47
1:E:407:ALA:O	1:E:410:THR:OG1	2.27	0.47
1:E:66:LEU:HD23	1:E:66:LEU:H	1.80	0.47
12:E:801:CLA:HAB	12:G:805:CLA:HAA2	41.99	0.47
12:E:815:CLA:HBA2	12:E:815:CLA:H3A	1.60	0.47
13:E:846:PQN:H2M1	13:E:846:PQN:H111	1.75	0.47
2:G:345:LEU:O	2:G:349:THR:HG23	2.15	0.47
1:E:697:LEU:CD1	2:G:539:LYS:HE3	2.98	0.47
2:G:438:LEU:HD13	12:G:801:CLA:H43	51.67	0.47
12:G:806:CLA:HBD	12:G:806:CLA:HED2	4.01	0.47
11:M:32:ILE:HG22	11:M:33:ALA:N	2.30	0.47
4:N:98:HIS:HA	4:N:100:SER:N	2.74	0.47
4:N:33:TRP:HB3	4:N:83:TYR:HA	2.07	0.47
4:N:84:LYS:CD	4:N:99:PRO:HD3	2.42	0.47
1:A:740:ILE:O	1:A:743:PHE:HB2	2.15	0.47
2:B:307:ALA:O	2:B:315:THR:OG1	2.31	0.47
2:B:370:THR:OG1	2:B:371:THR:N	2.48	0.47
2:B:388:VAL:HG23	2:B:537:LEU:HD11	1.97	0.47
2:B:627:LEU:O	2:B:631:SER:OG	2.33	0.47
2:B:114:ASN:HD21	12:B:810:CLA:C4C	18.63	0.47
1:E:170:ALA:O	1:E:174:LEU:HG	2.15	0.47
1:E:350:HIS:ND1	1:E:353:LEU:HD23	2.30	0.47
6:F:99:TRP:O	6:F:103:VAL:HG23	2.15	0.47
2:G:388:VAL:HG23	2:G:537:LEU:HD11	1.97	0.47
2:G:391:PHE:CG	2:G:537:LEU:HD13	2.51	0.47
2:G:585:TRP:HE1	12:G:801:CLA:C1D	38.86	0.47
10:L:95:LEU:HD13	10:L:158:TYR:HB2	1.97	0.47
12:L:204:CLA:H3A	12:L:204:CLA:HBA2	1.35	0.47
1:A:710:VAL:HG11	12:A:837:CLA:HMA3	1.97	0.46
1:A:205:LEU:HB2	12:A:813:CLA:HMB2	22.74	0.46
12:A:826:CLA:O1D	12:A:826:CLA:H2A	2.15	0.46
1:A:716:PRO:HB3	12:A:838:CLA:HHC	1.97	0.46
2:B:442:VAL:O	2:B:446:VAL:HG22	2.14	0.46
2:B:535:LEU:HG	2:B:539:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:598:HIS:O	2:B:602:LEU:HB2	2.15	0.46
1:E:259:LYS:HG3	1:E:260:GLY:H	1.80	0.46
1:E:312:TYR:HD1	1:E:322:ILE:HD11	1.80	0.46
1:E:41:LYS:HB2	1:E:44:LYS:NZ	2.31	0.46
1:E:562:LEU:HD13	2:G:675:GLN:HG2	2.66	0.46
1:E:563:ILE:HA	1:E:563:ILE:HD12	1.76	0.46
2:G:513:LEU:HG	2:G:514:THR:N	2.31	0.46
2:B:443:HIS:CE1	12:J:1102:CLA:C1C	2.98	0.46
6:O:99:TRP:O	6:O:103:VAL:HG23	2.15	0.46
9:R:53:PRO:C	9:R:55:PRO:HD3	2.35	0.46
2:B:262:HIS:CD2	2:B:264:GLN:HB3	2.51	0.46
2:B:480:THR:N	2:B:483:SER:HB3	2.26	0.46
2:B:669:SER:HG	2:B:674:TRP:HZ2	1.62	0.46
4:D:22:LYS:HG2	4:D:26:GLU:HB2	1.96	0.46
1:E:350:HIS:CE1	1:E:353:LEU:HD23	2.51	0.46
1:E:474:ASP:OD2	1:E:474:ASP:N	2.48	0.46
1:E:719:LEU:HD11	1:E:723:GLN:HB2	1.97	0.46
12:E:829:CLA:H2A	12:E:829:CLA:O1D	2.15	0.46
6:F:147:LEU:HB3	6:F:148:LEU:HD23	1.98	0.46
12:E:802:CLA:HAC1	2:G:581:LEU:HD23	1.95	0.46
2:G:681:LEU:HD21	12:G:801:CLA:HMD3	1.97	0.46
2:G:706:VAL:O	2:G:710:LEU:HG	2.15	0.46
12:G:837:CLA:CBA	12:G:838:CLA:HAA2	2.43	0.46
3:H:54:GLU:N	3:H:54:GLU:OE1	2.37	0.46
6:O:95:TYR:HA	6:O:139:TRP:HZ2	1.81	0.46
10:S:95:LEU:HD13	10:S:158:TYR:HB2	1.97	0.46
1:A:124:GLN:O	1:A:124:GLN:HG2	2.16	0.46
1:A:291:LEU:HD12	1:A:294:THR:OG1	2.15	0.46
1:A:318:ILE:HG22	12:A:820:CLA:HMD1	1.97	0.46
1:A:318:ILE:HG22	12:A:822:CLA:HMD1	22.37	0.46
1:A:126:ILE:HG12	1:A:665:ALA:HA	1.97	0.46
12:A:828:CLA:H2A	12:A:828:CLA:O1D	2.47	0.46
1:E:426:VAL:HG22	12:E:823:CLA:HMC3	23.54	0.46
1:E:426:VAL:HG22	12:E:825:CLA:HMC3	1.96	0.46
1:E:740:ILE:O	1:E:743:PHE:HB2	2.15	0.46
12:E:813:CLA:ND	12:E:813:CLA:H2	2.31	0.46
12:E:835:CLA:HBA2	12:E:835:CLA:H3A	1.40	0.46
6:F:28:LEU:HD22	6:F:67:GLY:HA2	1.97	0.46
2:G:506:ASN:ND2	2:G:508:THR:OG1	2.48	0.46
2:G:693:LEU:HA	10:S:122:ALA:HB2	3.18	0.46
12:G:804:CLA:H3A	12:G:804:CLA:O2A	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:832:CLA:H3A	12:G:832:CLA:HBA2	1.92	0.46
12:A:832:CLA:C2	12:L:203:CLA:HBB2	37.70	0.46
6:O:140:PRO:O	6:O:144:VAL:HG23	2.16	0.46
5:V:45:TYR:O	5:V:48:VAL:HG23	2.16	0.46
1:A:46:THR:HG23	12:A:840:CLA:HMB1	68.41	0.46
12:A:810:CLA:H2	12:A:810:CLA:ND	2.31	0.46
12:A:819:CLA:HBA2	12:A:819:CLA:H3A	1.90	0.46
2:B:174:ARG:HB2	12:B:815:CLA:HBC2	18.86	0.46
1:E:46:THR:HG23	12:E:839:CLA:HMB1	47.79	0.46
1:E:648:ARG:NH1	2:G:636:ASN:HD22	2.52	0.46
12:E:819:CLA:HMB1	12:E:819:CLA:HBB1	1.96	0.46
1:E:648:ARG:NH2	2:G:638:TYR:O	2.54	0.46
2:G:414:ARG:NE	12:G:833:CLA:OBD	28.54	0.46
7:P:33:ARG:HA	7:P:33:ARG:HD3	1.35	0.46
1:A:256:SER:HA	1:A:261:LEU:HD12	1.96	0.46
2:B:443:HIS:CE1	12:B:835:CLA:C1C	23.59	0.46
2:B:513:LEU:HG	2:B:514:THR:N	2.31	0.46
3:C:54:GLU:N	3:C:54:GLU:OE1	2.37	0.46
4:D:91:ASN:HB3	4:D:93:GLU:OE1	2.16	0.46
1:E:124:GLN:O	1:E:124:GLN:HG2	2.16	0.46
1:E:486:PHE:O	1:E:490:ILE:HG23	2.16	0.46
1:E:716:PRO:HB3	12:E:842:CLA:HHC	1.97	0.46
6:F:95:TYR:HA	6:F:139:TRP:HZ2	1.81	0.46
2:G:262:HIS:CD2	2:G:265:THR:H	2.17	0.46
2:G:303:GLU:N	2:G:303:GLU:OE1	2.49	0.46
1:E:125:ASP:H	2:G:450:PHE:HE1	1.75	0.46
2:G:414:ARG:NE	12:G:831:CLA:OBD	2.48	0.46
10:L:58:THR:HG21	10:S:141:THR:HG22	1.97	0.46
11:T:32:ILE:HG22	11:T:33:ALA:N	2.30	0.46
1:A:350:HIS:ND1	1:A:353:LEU:HD23	2.30	0.46
1:A:501:ASN:ND2	12:A:815:CLA:O2D	2.49	0.46
1:A:59:PHE:CG	1:A:72:LYS:HE3	2.51	0.46
2:B:454:GLU:HA	6:F:71:LEU:HD22	1.97	0.46
2:B:42:LEU:HA	2:B:45:LYS:HE2	1.97	0.46
4:D:32:THR:HA	4:D:56:ASN:O	2.24	0.46
1:E:549:ILE:HG13	1:E:550:LEU:HD22	1.98	0.46
12:E:836:CLA:O2D	12:E:836:CLA:H2A	2.16	0.46
2:G:262:HIS:CD2	2:G:264:GLN:HB3	2.51	0.46
2:G:370:THR:OG1	2:G:371:THR:N	2.48	0.46
1:E:647:LEU:HD11	12:G:805:CLA:HMC3	35.81	0.46
12:G:814:CLA:H3A	12:G:814:CLA:HBA1	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:443:HIS:CE1	12:G:834:CLA:C1C	2.98	0.46
12:G:834:CLA:HBD	12:G:834:CLA:HED2	1.75	0.46
12:G:841:CLA:HBA2	12:G:841:CLA:H43	1.98	0.46
1:A:671:LEU:O	1:A:673:PHE:N	2.41	0.46
12:A:837:CLA:C1A	12:A:837:CLA:CGA	3.09	0.46
2:B:364:PHE:HB3	2:B:367:GLN:HE21	1.81	0.46
12:B:805:CLA:O2A	12:B:805:CLA:H3A	4.25	0.46
12:B:822:CLA:HBA2	12:B:822:CLA:H3A	1.62	0.46
2:B:414:ARG:NE	12:B:834:CLA:OBD	2.48	0.46
1:E:46:THR:HG23	12:E:842:CLA:HMB1	1.98	0.46
1:E:599:MET:O	1:E:603:ILE:HG12	2.16	0.46
1:E:205:LEU:HB2	12:E:814:CLA:HMB2	1.97	0.46
1:E:318:ILE:HG22	12:E:823:CLA:HMD1	1.97	0.46
12:E:836:CLA:C1A	12:E:836:CLA:CGA	3.13	0.46
6:F:83:ALA:HA	6:F:86:PHE:CE1	2.51	0.46
2:G:697:LYS:HG3	2:G:698:ASP:N	2.31	0.46
12:E:844:CLA:CAC	12:G:801:CLA:HMC2	76.41	0.46
12:G:804:CLA:HED2	12:G:804:CLA:HBD	1.76	0.46
2:G:443:HIS:CE1	12:G:835:CLA:C1C	33.61	0.46
3:H:34:LYS:HE3	5:W:32:ILE:CG1	2.45	0.46
4:N:17:GLY:O	4:N:45:THR:OG1	2.25	0.46
6:O:83:ALA:HA	6:O:86:PHE:CE1	2.51	0.46
1:A:350:HIS:CE1	1:A:353:LEU:HD23	2.50	0.46
1:A:41:LYS:HB2	1:A:44:LYS:NZ	2.31	0.46
1:A:501:ASN:ND2	12:A:817:CLA:O2D	22.23	0.46
1:A:681:ALA:HA	1:A:684:LEU:HD21	1.98	0.46
12:A:834:CLA:H2A	12:A:834:CLA:O2D	2.83	0.46
2:B:303:GLU:OE1	2:B:303:GLU:N	2.49	0.46
1:E:291:LEU:HD12	1:E:294:THR:OG1	2.15	0.46
2:G:300:SER:HG	2:G:303:GLU:HB2	1.94	0.46
2:G:44:GLN:O	2:G:47:PHE:HB3	2.16	0.46
2:G:42:LEU:HA	2:G:45:LYS:HE2	1.97	0.46
2:B:133:ASN:HB3	10:L:172:LYS:HG3	78.51	0.46
10:L:73:TRP:HB3	12:L:204:CLA:HBC3	1.97	0.46
12:S:1502:CLA:H3A	12:S:1502:CLA:HBA2	1.35	0.46
5:W:45:TYR:O	5:W:48:VAL:HG23	2.16	0.46
1:A:407:ALA:O	1:A:410:THR:OG1	2.27	0.46
1:A:691:ARG:NE	1:A:719:LEU:O	2.36	0.46
13:A:842:PQN:H23	13:A:842:PQN:H202	1.60	0.46
2:B:532:THR:O	2:B:535:LEU:HB3	2.16	0.46
2:B:391:PHE:CG	2:B:537:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:ASP:HA	3:C:51:LYS:NZ	2.30	0.46
2:B:697:LYS:HG3	2:B:698:ASP:N	2.31	0.46
12:B:811:CLA:H3A	12:B:811:CLA:HBA1	3.10	0.46
1:E:681:ALA:HA	1:E:684:LEU:HD21	1.98	0.46
12:E:817:CLA:HBB1	12:E:817:CLA:HMB1	2.47	0.46
1:E:501:ASN:ND2	12:E:818:CLA:O2D	2.49	0.46
12:E:819:CLA:CGA	12:E:819:CLA:H3A	2.42	0.46
12:E:844:CLA:HAB	2:G:585:TRP:HH2	76.73	0.46
6:F:140:PRO:O	6:F:144:VAL:HG23	2.16	0.46
2:G:418:HIS:HB3	12:G:831:CLA:HED1	1.96	0.46
2:G:627:LEU:O	2:G:631:SER:OG	2.33	0.46
2:G:697:LYS:HD3	12:G:841:CLA:C2A	18.54	0.46
3:H:59:THR:OG1	14:H:102:SF4:S2	2.60	0.46
3:H:29:PRO:HA	3:H:37:GLN:HG2	1.98	0.46
11:M:23:ASP:HA	11:M:26:VAL:HG13	1.98	0.46
12:G:808:CLA:CBD	7:P:11:LEU:HD11	2.44	0.46
1:A:490:ILE:HG13	1:A:491:HIS:CD2	2.52	0.46
1:A:205:LEU:HB2	12:A:811:CLA:HMB2	1.97	0.46
12:A:832:CLA:H2A	12:A:832:CLA:O2D	2.16	0.46
12:A:841:CLA:HBD	12:A:841:CLA:HED2	4.05	0.46
13:A:842:PQN:H111	13:A:842:PQN:H2M1	1.77	0.46
2:B:307:ALA:HB3	12:B:824:CLA:HMA2	23.81	0.46
2:B:585:TRP:HH2	12:B:805:CLA:HAB	1.81	0.46
12:B:802:CLA:HMC3	12:B:841:CLA:ND	42.40	0.46
12:B:831:CLA:HBA2	12:B:831:CLA:H3A	3.93	0.46
12:B:842:CLA:H43	12:B:842:CLA:HBA2	4.83	0.46
3:C:29:PRO:HA	3:C:37:GLN:HG2	1.98	0.46
2:G:535:LEU:HG	2:G:539:LYS:HE2	1.97	0.46
2:G:585:TRP:HH2	12:G:802:CLA:HAB	1.81	0.46
2:G:697:LYS:HD3	12:G:840:CLA:C2A	2.46	0.46
12:E:801:CLA:HAB	12:G:805:CLA:CAA	41.09	0.46
4:N:116:GLY:O	4:N:117:TYR:CG	2.71	0.46
1:A:218:ILE:HA	1:A:222:LEU:HB2	1.98	0.45
1:A:474:ASP:OD2	1:A:474:ASP:N	2.48	0.45
1:A:486:PHE:O	1:A:490:ILE:HG23	2.16	0.45
1:A:560:SER:HB2	1:A:566:LYS:HD3	1.98	0.45
12:B:819:CLA:H3A	12:B:819:CLA:HBA2	1.60	0.45
3:C:73:THR:OG1	3:C:74:THR:N	2.49	0.45
1:E:218:ILE:HA	1:E:222:LEU:HB2	1.98	0.45
1:E:691:ARG:NE	1:E:719:LEU:O	2.36	0.45
1:E:501:ASN:ND2	12:E:816:CLA:O2D	19.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:174:ARG:HB2	12:G:814:CLA:HBC2	1.98	0.45
2:G:307:ALA:O	2:G:315:THR:OG1	2.31	0.45
2:G:364:PHE:HB3	2:G:367:GLN:HE21	1.81	0.45
12:G:835:CLA:HBA2	12:G:835:CLA:HBD	1.98	0.45
10:L:172:LYS:HG2	2:G:96:PHE:CZ	2.51	0.45
10:L:166:LEU:HG	10:L:167:ILE:HG12	1.98	0.45
4:N:15:SER:O	10:S:31:GLY:HA3	2.33	0.45
6:O:147:LEU:HB3	6:O:148:LEU:HD23	1.98	0.45
1:A:312:TYR:HD1	1:A:322:ILE:HD11	1.81	0.45
1:A:599:MET:O	1:A:603:ILE:HG12	2.16	0.45
12:A:816:CLA:CGA	12:A:816:CLA:H3A	2.42	0.45
2:B:335:HIS:HB2	2:B:397:PHE:HB2	1.98	0.45
12:B:801:CLA:HMC2	12:B:805:CLA:HAC2	1.98	0.45
12:B:839:CLA:CGA	12:B:839:CLA:C1A	4.65	0.45
4:D:32:THR:O	4:D:83:TYR:HA	2.26	0.45
1:E:467:ARG:HB3	1:E:470:ASP:OD1	2.17	0.45
12:E:817:CLA:H3A	12:E:817:CLA:HBA2	1.53	0.45
2:G:91:ILE:N	2:G:112:PRO:O	2.41	0.45
2:G:638:TYR:CD1	2:G:647:SER:HB3	2.52	0.45
12:G:801:CLA:H12	12:G:801:CLA:HBA2	1.82	0.45
10:L:98:THR:O	10:L:102:VAL:HG23	2.16	0.45
8:Q:17:LEU:C	8:Q:19:PRO:HD2	2.37	0.45
10:S:166:LEU:HG	10:S:167:ILE:HG12	1.98	0.45
10:S:98:THR:O	10:S:102:VAL:HG23	2.16	0.45
12:B:838:CLA:CBA	12:B:839:CLA:HAA2	20.58	0.45
12:B:840:CLA:CGA	12:B:840:CLA:C1A	2.94	0.45
1:E:490:ILE:HG13	1:E:491:HIS:CD2	2.52	0.45
1:E:560:SER:HB2	1:E:566:LYS:HD3	1.98	0.45
1:E:716:PRO:HB3	12:E:839:CLA:HHC	55.47	0.45
1:E:710:VAL:HG11	12:E:838:CLA:HMA3	64.09	0.45
1:A:122:VAL:HG22	6:F:47:THR:OG1	2.17	0.45
2:G:292:ARG:HH21	2:G:297:ILE:HA	1.82	0.45
2:G:307:ALA:HB3	12:G:825:CLA:HMA2	22.68	0.45
2:G:620:MET:O	2:G:623:LEU:HD23	2.16	0.45
2:G:355:HIS:HE1	12:G:827:CLA:NC	2.15	0.45
2:G:98:LYS:HA	2:G:98:LYS:HD2	1.82	0.45
3:H:23:ASP:O	3:H:43:ARG:NE	2.48	0.45
8:J:17:LEU:C	8:J:19:PRO:HD2	2.37	0.45
12:A:833:CLA:O2D	10:L:83:PRO:HB3	55.41	0.45
10:S:73:TRP:HB3	12:S:1502:CLA:HBC3	1.97	0.45
1:A:104:TRP:CH2	1:A:149:ARG:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ILE:HG22	1:A:566:LYS:HG3	1.99	0.45
12:A:812:CLA:HBA2	12:A:812:CLA:H3A	1.60	0.45
12:A:820:CLA:HBA2	12:A:820:CLA:H3A	1.68	0.45
12:A:820:CLA:HAA1	9:K:48:VAL:HG12	1.97	0.45
2:B:290:MET:O	2:B:299:HIS:ND1	2.50	0.45
2:B:491:THR:OG1	2:B:491:THR:O	2.33	0.45
2:B:537:LEU:HD23	2:B:537:LEU:HA	1.54	0.45
2:B:638:TYR:CD1	2:B:647:SER:HB3	2.52	0.45
4:D:87:ARG:NH1	4:D:95:GLN:HE21	2.22	0.45
1:E:104:TRP:CH2	1:E:149:ARG:HD2	2.52	0.45
12:E:801:CLA:HHC	12:E:801:CLA:CBB	2.43	0.45
12:E:806:CLA:H3A	12:E:806:CLA:HBA1	3.99	0.45
12:E:814:CLA:H3A	12:E:814:CLA:O1A	2.17	0.45
2:G:223:ARG:HA	2:G:223:ARG:HD2	1.50	0.45
12:G:808:CLA:HBA2	12:G:808:CLA:H3A	1.65	0.45
8:J:19:PRO:HG3	12:J:1101:CLA:CHD	2.47	0.45
4:N:32:THR:HA	4:N:56:ASN:O	2.21	0.45
4:N:36:PRO:HA	4:N:54:GLY:H	1.82	0.45
11:T:23:ASP:HA	11:T:26:VAL:HG13	1.98	0.45
1:A:715:GLN:NE2	5:W:42:LYS:HD3	137.64	0.45
1:A:467:ARG:HB3	1:A:470:ASP:OD1	2.17	0.45
12:A:838:CLA:H3A	12:A:838:CLA:HBA2	3.65	0.45
1:A:46:THR:HG23	12:A:838:CLA:HMB1	1.98	0.45
12:A:839:CLA:C4D	12:A:839:CLA:H11	2.62	0.45
2:B:141:PHE:CE2	2:B:145:LEU:HD11	2.52	0.45
2:B:338:LEU:HG	12:B:809:CLA:HMD3	1.99	0.45
2:B:570:THR:HB	2:B:573:ILE:HD11	1.98	0.45
2:B:438:LEU:HD13	12:B:801:CLA:H43	1.97	0.45
12:B:814:CLA:H3A	12:B:814:CLA:HBA2	3.34	0.45
12:B:821:CLA:HBA2	12:B:821:CLA:H3A	1.40	0.45
12:B:837:CLA:HBA2	12:B:837:CLA:HBD	1.98	0.45
1:E:59:PHE:CG	1:E:72:LYS:HE3	2.51	0.45
12:E:804:CLA:O1A	12:E:804:CLA:H3A	2.92	0.45
12:E:833:CLA:H2A	12:E:833:CLA:O2D	3.64	0.45
6:F:146:GLU:HA	6:F:149:SER:OG	2.17	0.45
2:G:169:LYS:HD3	2:G:169:LYS:HA	1.76	0.45
2:G:532:THR:O	2:G:535:LEU:HB3	2.16	0.45
12:G:836:CLA:HBD	12:G:836:CLA:HBA2	4.99	0.45
12:G:838:CLA:CGA	12:G:838:CLA:C1A	2.94	0.45
4:N:39:GLN:C	4:N:50:ILE:HG13	2.71	0.45
4:N:91:ASN:HB3	4:N:93:GLU:OE1	6.06	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:146:GLU:HA	6:O:149:SER:OG	2.17	0.45
1:A:487:VAL:HG12	1:A:491:HIS:CE1	2.52	0.45
12:A:801:CLA:HHC	12:A:801:CLA:CBB	2.43	0.45
1:A:141:THR:N	12:A:808:CLA:OBD	44.33	0.45
12:A:835:CLA:C1A	12:A:835:CLA:CGA	2.94	0.45
2:B:162:ARG:HA	2:B:162:ARG:HD3	1.71	0.45
2:B:40:GLU:N	2:B:40:GLU:OE1	2.38	0.45
2:B:44:GLN:O	2:B:47:PHE:HB3	2.16	0.45
2:B:620:MET:O	2:B:623:LEU:HD23	2.16	0.45
12:B:811:CLA:H3A	12:B:811:CLA:HBA2	1.65	0.45
12:B:824:CLA:H3A	12:B:824:CLA:HBA2	1.53	0.45
1:E:440:HIS:O	1:E:443:TRP:HB3	2.15	0.45
1:E:126:ILE:HG12	1:E:665:ALA:HA	1.97	0.45
12:E:806:CLA:H3A	12:E:806:CLA:O1A	2.17	0.45
12:E:805:CLA:HHB	12:E:829:CLA:CBB	26.37	0.45
2:G:141:PHE:CE2	2:G:145:LEU:HD11	2.52	0.45
2:G:144:ILE:H	2:G:144:ILE:HG13	1.45	0.45
2:G:509:ASN:HD21	2:G:511:LEU:HD12	1.82	0.45
12:G:806:CLA:H3A	12:G:806:CLA:O2A	3.80	0.45
3:H:30:TRP:CZ3	3:H:38:ILE:HD12	2.52	0.45
4:D:19:LEU:HB2	10:L:30:ILE:HG22	2.55	0.45
4:N:98:HIS:CD2	4:N:100:SER:H	5.03	0.45
10:S:96:LEU:HG	10:S:96:LEU:H	1.62	0.45
1:A:153:PHE:CG	1:A:159:LEU:HD21	2.52	0.45
1:A:458:HIS:O	1:A:462:MET:HG2	2.17	0.45
1:A:549:ILE:HG13	1:A:550:LEU:HD22	1.98	0.45
2:B:292:ARG:HH21	2:B:297:ILE:HA	1.82	0.45
4:D:33:TRP:CD1	4:D:80:ILE:HD13	2.55	0.45
1:E:458:HIS:O	1:E:462:MET:HG2	2.17	0.45
12:E:833:CLA:HBA2	12:E:833:CLA:H3A	1.81	0.45
2:G:156:HIS:NE2	12:G:812:CLA:HMA3	2.32	0.45
2:G:174:ARG:HB2	12:G:816:CLA:HBC2	30.70	0.45
2:G:290:MET:O	2:G:299:HIS:ND1	2.50	0.45
2:G:335:HIS:HB2	2:G:397:PHE:HB2	1.98	0.45
2:G:468:GLN:HE21	2:G:473:LYS:HB2	1.82	0.45
2:G:553:LYS:HB3	2:G:553:LYS:HE2	1.53	0.45
2:G:570:THR:HB	2:G:573:ILE:HD11	1.98	0.45
6:O:152:LEU:CD1	6:O:152:LEU:H	2.29	0.45
1:A:107:ASP:HB3	1:A:111:ILE:HG13	1.99	0.45
1:A:155:ASN:HB3	1:A:235:LYS:HE3	1.99	0.45
1:A:658:VAL:HA	1:A:661:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:813:CLA:H3A	12:A:813:CLA:O1A	2.70	0.45
1:A:483:PHE:HB3	12:A:834:CLA:C2	2.47	0.45
12:A:837:CLA:C4D	12:A:837:CLA:H11	2.47	0.45
2:B:697:LYS:HD3	12:B:841:CLA:C2A	50.93	0.45
2:B:697:LYS:HD3	12:B:842:CLA:C2A	2.46	0.45
12:B:836:CLA:HBD	12:B:836:CLA:HBA2	2.87	0.45
4:D:98:HIS:CE1	4:D:104:PHE:HD1	2.34	0.45
1:E:487:VAL:HG12	1:E:491:HIS:CE1	2.52	0.45
12:E:807:CLA:HHB	12:E:831:CLA:CBB	2.47	0.45
12:E:802:CLA:H2	2:G:435:PHE:CE1	2.52	0.45
2:G:491:THR:O	2:G:491:THR:OG1	2.33	0.45
12:G:841:CLA:H12	12:G:841:CLA:HBA2	3.44	0.45
3:H:73:THR:OG1	3:H:74:THR:N	2.49	0.45
1:A:114:SER:HG	1:A:139:GLN:HA	1.82	0.45
12:A:803:CLA:O1A	12:A:803:CLA:H3A	2.17	0.45
1:E:118:VAL:HG21	1:E:127:LEU:HB2	1.99	0.45
1:E:153:PHE:CG	1:E:159:LEU:HD21	2.52	0.45
12:E:812:CLA:O1A	12:E:812:CLA:H3A	4.62	0.45
1:E:216:HIS:HB2	12:E:813:CLA:C1C	20.32	0.45
1:E:216:HIS:HB2	12:E:815:CLA:C1C	2.47	0.45
1:E:483:PHE:HB3	12:E:838:CLA:C2	2.47	0.45
1:E:497:SER:HA	2:G:227:THR:O	119.89	0.45
2:G:526:PHE:CZ	2:G:593:VAL:HA	2.52	0.45
2:G:611:GLN:N	2:G:611:GLN:CD	2.71	0.45
12:G:832:CLA:HBD	12:G:832:CLA:HED2	1.86	0.45
5:V:32:ILE:CG1	3:H:34:LYS:HE3	127.91	0.45
7:I:30:TYR:O	7:I:33:ARG:HB2	2.17	0.45
6:O:141:LEU:H	6:O:141:LEU:HD23	1.82	0.45
7:P:26:LEU:HA	7:P:29:ILE:HG22	1.99	0.45
1:A:202:LEU:O	1:A:206:LEU:HB2	2.18	0.45
1:A:521:ILE:H	1:A:521:ILE:HD12	1.82	0.45
1:A:394:HIS:HE1	12:A:829:CLA:HMA3	43.15	0.45
2:B:169:LYS:HD3	2:B:169:LYS:HA	1.76	0.45
2:B:230:TRP:HB3	12:B:818:CLA:H3A	27.15	0.45
2:B:468:GLN:HE21	2:B:473:LYS:HB2	1.82	0.45
2:B:331:ASN:OD1	12:B:826:CLA:HBC3	18.31	0.45
2:B:355:HIS:HE1	12:B:830:CLA:NC	2.15	0.45
2:B:72:GLY:HA2	2:B:87:ILE:HB	1.99	0.45
4:D:62:ARG:NH2	4:D:64:GLU:OE1	2.50	0.45
1:E:202:LEU:O	1:E:206:LEU:HB2	2.17	0.45
1:E:246:ASN:ND2	1:E:249:LEU:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:LYS:HB3	1:E:552:LYS:HE3	1.65	0.45
1:E:658:VAL:HA	1:E:661:SER:HB3	1.99	0.45
1:E:710:VAL:HG11	12:E:841:CLA:HMA3	1.97	0.45
12:E:839:CLA:C1A	12:E:839:CLA:CGA	2.94	0.45
6:F:141:LEU:H	6:F:141:LEU:HD23	1.82	0.45
2:G:338:LEU:HG	12:G:808:CLA:HMD3	36.79	0.45
2:G:550:MET:HG3	2:G:553:LYS:HG2	1.99	0.45
2:G:627:LEU:HA	2:G:627:LEU:HD12	1.71	0.45
12:G:805:CLA:H3A	12:G:805:CLA:HBA2	1.48	0.45
12:G:821:CLA:HBA2	12:G:821:CLA:H3A	1.53	0.45
4:N:108:VAL:O	4:N:109:ASN:ND2	3.11	0.45
4:N:8:GLN:HE22	4:N:52:ARG:NH1	2.15	0.45
4:N:89:TYR:CD2	4:N:93:GLU:HB2	2.54	0.45
2:B:567:ARG:NH1	5:V:45:TYR:HA	2.32	0.45
1:A:220:VAL:O	1:A:224:VAL:HG12	2.17	0.44
1:A:305:PHE:HA	1:A:308:ALA:HB3	1.99	0.44
1:A:483:PHE:HB3	12:A:836:CLA:C2	18.31	0.44
1:A:552:LYS:HE3	1:A:552:LYS:HB3	1.66	0.44
1:A:648:ARG:HH22	2:B:639:ASN:HB3	1.83	0.44
12:A:805:CLA:H3A	12:A:805:CLA:O1A	4.52	0.44
2:B:156:HIS:NE2	12:B:813:CLA:HMA3	43.04	0.44
2:B:276:HIS:CE1	2:B:280:ILE:HD11	2.52	0.44
2:B:489:ALA:HA	2:B:492:ALA:HB3	1.99	0.44
12:B:807:CLA:O2A	12:B:807:CLA:H3A	2.16	0.44
2:B:338:LEU:HG	12:B:807:CLA:HMD3	39.78	0.44
3:C:30:TRP:CZ3	3:C:38:ILE:HD12	2.52	0.44
1:E:107:ASP:HB3	1:E:111:ILE:HG13	1.99	0.44
1:E:220:VAL:O	1:E:224:VAL:HG12	2.17	0.44
1:E:425:ASN:O	1:E:429:ARG:N	2.42	0.44
1:E:483:PHE:HB3	12:E:835:CLA:C3	27.21	0.44
12:E:802:CLA:CED	12:E:802:CLA:H2A	2.47	0.44
1:E:318:ILE:HG22	12:E:821:CLA:HMD1	12.18	0.44
12:E:844:CLA:HMC2	12:G:801:CLA:C1C	72.07	0.44
1:E:497:SER:HB3	2:G:227:THR:OG1	118.88	0.44
12:G:801:CLA:H2A	12:G:801:CLA:CED	4.84	0.44
12:G:839:CLA:C1A	12:G:839:CLA:CGA	4.00	0.44
3:H:34:LYS:HE3	5:W:32:ILE:HG12	1.99	0.44
10:L:72:TYR:CD1	10:L:157:ALA:HB2	2.52	0.44
1:E:432:ARG:HH21	4:N:12:PHE:HE1	1.71	0.44
1:A:483:PHE:HB3	12:A:834:CLA:C3	2.47	0.44
1:A:519:GLY:O	1:A:622:ILE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:ILE:HG12	1:A:740:ILE:H	1.38	0.44
12:A:804:CLA:HHB	12:A:828:CLA:CBB	2.47	0.44
12:A:821:CLA:HHB	12:A:841:CLA:HBC3	1.99	0.44
2:B:487:SER:N	2:B:490:SER:OG	2.50	0.44
2:B:526:PHE:CZ	2:B:593:VAL:HA	2.52	0.44
2:B:690:LEU:HG	12:L:203:CLA:O1A	3.14	0.44
12:B:827:CLA:H3A	12:B:827:CLA:HBA1	3.47	0.44
4:D:116:GLY:O	4:D:117:TYR:CG	2.71	0.44
4:D:27:GLU:C	4:D:28:LYS:HD3	2.38	0.44
1:E:360:LEU:HG	1:E:401:LEU:HD11	2.00	0.44
1:E:547:VAL:O	1:E:551:LEU:HB3	2.18	0.44
12:E:821:CLA:HBD	9:R:48:VAL:CG1	14.34	0.44
12:E:823:CLA:HBA2	12:E:823:CLA:H3A	1.68	0.44
1:E:483:PHE:HB3	12:E:835:CLA:C2	27.26	0.44
2:G:162:ARG:HA	2:G:162:ARG:HD3	1.71	0.44
2:G:331:ASN:OD1	12:G:827:CLA:HBC3	35.33	0.44
1:A:547:VAL:O	1:A:551:LEU:HB3	2.18	0.44
12:A:805:CLA:H2A	12:A:805:CLA:HED2	3.80	0.44
2:B:156:HIS:NE2	12:B:815:CLA:HMA3	2.32	0.44
2:B:286:ILE:HG13	2:B:287:ALA:N	2.32	0.44
2:B:307:ALA:HB3	12:B:826:CLA:HMA2	1.98	0.44
2:B:378:HIS:HB2	12:B:831:CLA:C1B	2.48	0.44
2:B:558:TYR:OH	2:B:576:TRP:HB3	2.17	0.44
12:B:818:CLA:HBA2	12:B:818:CLA:H3A	1.63	0.44
1:E:305:PHE:HA	1:E:308:ALA:HB3	1.99	0.44
1:E:488:GLN:O	1:E:492:THR:HG23	2.17	0.44
1:E:394:HIS:HE1	12:E:830:CLA:HMA3	1.82	0.44
2:G:352:VAL:O	2:G:356:MET:HG2	2.18	0.44
2:G:687:ARG:NH1	10:S:31:GLY:O	4.04	0.44
9:K:40:SER:HA	9:K:44:ARG:CZ	2.48	0.44
11:M:42:ARG:HA	11:M:45:THR:HG23	1.99	0.44
6:O:141:LEU:O	6:O:145:LYS:HG2	2.18	0.44
2:B:223:ARG:HD2	2:B:223:ARG:HA	1.50	0.44
2:B:284:PHE:HA	2:B:287:ALA:HB3	2.00	0.44
2:B:393:HIS:HA	2:B:396:ILE:HG12	2.00	0.44
2:B:550:MET:HG3	2:B:553:LYS:HG2	1.99	0.44
2:B:55:ALA:O	2:B:59:LEU:HG	2.18	0.44
12:B:801:CLA:CED	12:B:801:CLA:H2A	2.47	0.44
2:B:355:HIS:HE1	12:B:828:CLA:NC	25.51	0.44
1:E:519:GLY:O	1:E:622:ILE:N	2.51	0.44
1:E:521:ILE:HD12	1:E:521:ILE:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:563:ILE:HG22	1:E:566:LYS:HG3	1.99	0.44
1:E:662:TYR:CE2	2:G:449:ALA:HA	2.52	0.44
1:E:394:HIS:HE1	12:E:828:CLA:HMA3	21.50	0.44
1:E:483:PHE:HB3	12:E:838:CLA:C3	2.47	0.44
6:F:107:TYR:CZ	6:F:111:ILE:HD11	2.53	0.44
2:G:307:ALA:HB3	12:G:823:CLA:HMA2	1.98	0.44
7:I:26:LEU:HA	7:I:29:ILE:HG22	1.99	0.44
12:B:806:CLA:H2	11:M:49:LYS:HD3	43.17	0.44
4:N:87:ARG:NH1	4:N:95:GLN:HE21	2.15	0.44
11:T:42:ARG:HA	11:T:45:THR:HG23	1.99	0.44
3:C:34:LYS:HZ2	5:W:30:SER:HB2	128.60	0.44
1:A:428:ASP:O	1:A:431:ILE:HG12	2.18	0.44
1:A:681:ALA:HA	1:A:684:LEU:CD2	2.48	0.44
1:A:589:TRP:CH2	1:A:722:ILE:HB	2.52	0.44
1:A:734:LEU:O	1:A:738:VAL:HG22	2.18	0.44
12:A:801:CLA:HAB	12:B:806:CLA:CAA	2.47	0.44
12:A:811:CLA:H3A	12:A:811:CLA:O1A	2.17	0.44
2:B:174:ARG:HB2	12:B:817:CLA:HBC2	1.98	0.44
2:B:371:THR:O	2:B:375:LEU:HG	2.18	0.44
4:D:101:ASP:HB3	4:D:105:PRO:HD2	1.99	0.44
12:E:804:CLA:HED2	12:E:804:CLA:H2A	4.29	0.44
12:E:826:CLA:O2D	12:E:826:CLA:H2A	2.77	0.44
12:E:838:CLA:C4D	12:E:838:CLA:H11	8.51	0.44
12:E:843:CLA:HED2	12:E:843:CLA:HBD	1.69	0.44
6:F:152:LEU:H	6:F:152:LEU:CD1	2.28	0.44
2:G:276:HIS:CE1	2:G:280:ILE:HD11	2.52	0.44
2:G:378:HIS:HB2	12:G:828:CLA:C1B	2.48	0.44
2:G:338:LEU:HG	12:G:806:CLA:HMD3	1.99	0.44
2:G:217:PRO:HD2	12:G:816:CLA:C3D	2.48	0.44
2:G:183:PHE:CB	12:G:821:CLA:HMC1	11.68	0.44
2:G:355:HIS:HE1	12:G:829:CLA:NC	15.98	0.44
7:I:33:ARG:HA	7:I:33:ARG:HD3	1.35	0.44
7:P:30:TYR:O	7:P:33:ARG:HB2	2.17	0.44
1:A:216:HIS:HB2	12:A:814:CLA:C1C	10.89	0.44
1:A:603:ILE:O	1:A:607:VAL:HG13	2.18	0.44
1:A:684:LEU:HD23	1:A:684:LEU:H	1.83	0.44
1:A:394:HIS:HE1	12:A:827:CLA:HMA3	1.82	0.44
2:B:136:TYR:O	2:B:140:VAL:HG13	2.18	0.44
2:B:352:VAL:O	2:B:356:MET:HG2	2.18	0.44
2:B:378:HIS:HB2	12:B:829:CLA:C1B	21.66	0.44
2:B:509:ASN:HD21	2:B:511:LEU:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:ALA:O	2:B:589:THR:OG1	2.25	0.44
2:B:217:PRO:HD2	12:B:819:CLA:C3D	2.48	0.44
2:B:331:ASN:OD1	12:B:828:CLA:HBC3	2.18	0.44
12:B:835:CLA:HBD	12:B:835:CLA:HED2	1.86	0.44
4:D:73:GLN:HA	4:D:77:LYS:NZ	2.31	0.44
1:E:155:ASN:HB3	1:E:235:LYS:HE3	1.99	0.44
1:E:725:ARG:HD2	1:E:725:ARG:HA	1.76	0.44
12:E:821:CLA:H3A	12:E:821:CLA:HBA2	4.11	0.44
12:E:843:CLA:HHD	13:E:846:PQN:H192	2.00	0.44
2:G:156:HIS:NE2	12:G:814:CLA:HMA3	10.86	0.44
2:G:217:PRO:HD2	12:G:818:CLA:C3D	26.39	0.44
4:N:98:HIS:HA	4:N:99:PRO:C	2.62	0.44
9:R:40:SER:HA	9:R:44:ARG:CZ	2.47	0.44
10:S:63:GLY:HA2	10:S:142:PHE:CE1	2.53	0.44
2:G:143:LEU:HD22	11:T:32:ILE:HD11	2.00	0.44
5:V:8:VAL:O	5:V:21:VAL:HA	2.18	0.44
1:A:204:GLY:O	1:A:208:LEU:HB2	2.18	0.44
1:A:494:ALA:O	1:A:497:SER:OG	2.33	0.44
2:B:19:ARG:HA	2:B:22:TRP:CD1	2.53	0.44
2:B:585:TRP:HH2	12:B:803:CLA:HAB	47.57	0.44
2:B:627:LEU:HA	2:B:627:LEU:HD12	1.71	0.44
2:B:673:TYR:CZ	12:B:807:CLA:HMD1	2.53	0.44
12:B:843:CLA:H43	12:B:843:CLA:HBA2	1.98	0.44
4:D:136:MET:CE	4:D:139:TYR:HB2	2.49	0.44
4:D:84:LYS:CD	4:D:99:PRO:HD3	3.60	0.44
1:E:204:GLY:O	1:E:208:LEU:HB2	2.18	0.44
1:E:603:ILE:O	1:E:607:VAL:HG13	2.18	0.44
1:E:675:GLY:HA2	12:G:802:CLA:H12	1.99	0.44
12:E:818:CLA:H3A	12:E:818:CLA:HBA2	1.99	0.44
2:G:19:ARG:HA	2:G:22:TRP:CD1	2.53	0.44
1:E:684:LEU:HD13	2:G:664:PHE:HE2	1.87	0.44
2:G:673:TYR:CZ	12:G:806:CLA:HMD1	44.81	0.44
12:G:816:CLA:H3A	12:G:816:CLA:HBA1	3.07	0.44
1:A:360:LEU:HG	1:A:401:LEU:HD11	2.00	0.44
1:A:488:GLN:O	1:A:492:THR:HG23	2.17	0.44
1:A:543:ILE:HD11	12:A:834:CLA:CBB	2.48	0.44
12:A:806:CLA:HHB	12:A:830:CLA:CBB	56.94	0.44
12:A:827:CLA:O2D	12:A:827:CLA:H2A	2.40	0.44
2:B:681:LEU:HD21	12:B:803:CLA:HMD3	1.99	0.44
2:B:183:PHE:CB	12:B:820:CLA:HMC1	15.98	0.44
12:B:833:CLA:HED2	12:B:833:CLA:HBD	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:LYS:HD3	1:E:112:LYS:HA	1.83	0.44
1:E:681:ALA:HA	1:E:684:LEU:CD2	2.47	0.44
12:E:809:CLA:HBA2	12:E:809:CLA:H3A	1.40	0.44
2:G:284:PHE:HA	2:G:287:ALA:HB3	2.00	0.44
2:G:587:LEU:HB3	2:G:720:TYR:HE2	1.82	0.44
12:G:813:CLA:HBA2	12:G:813:CLA:H3A	1.67	0.44
12:G:837:CLA:H3A	12:G:837:CLA:HBA1	1.35	0.44
10:L:63:GLY:HA2	10:L:142:PHE:CE1	2.53	0.44
10:L:23:PRO:HA	10:L:28:PRO:HA	2.00	0.44
4:N:73:GLN:HA	4:N:77:LYS:NZ	2.38	0.44
6:O:107:TYR:CZ	6:O:111:ILE:HD11	2.53	0.44
9:R:37:PHE:O	9:R:40:SER:OG	2.30	0.44
12:B:809:CLA:H43	12:B:817:CLA:H42	2.00	0.44
2:B:174:ARG:HH11	12:B:817:CLA:HBC2	1.83	0.44
4:D:107:LYS:HD2	4:D:107:LYS:HA	1.43	0.44
4:D:10:PRO:HA	4:D:52:ARG:HD3	2.00	0.44
1:E:453:PHE:O	1:E:457:ILE:HG23	2.18	0.44
1:E:734:LEU:O	1:E:738:VAL:HG22	2.18	0.44
12:E:834:CLA:HED3	12:E:834:CLA:HBD	1.84	0.44
12:E:841:CLA:C4D	12:E:841:CLA:H11	2.47	0.44
2:G:286:ILE:HG13	2:G:287:ALA:N	2.32	0.44
2:G:558:TYR:OH	2:G:576:TRP:HB3	2.18	0.44
2:G:61:THR:O	2:G:64:LEU:HG	2.18	0.44
10:L:172:LYS:HD3	2:G:92:TRP:CZ2	2.53	0.44
4:N:33:TRP:CD1	4:N:80:ILE:HD13	2.53	0.44
4:N:63:LYS:O	4:N:67:ILE:HG12	2.17	0.44
4:N:84:LYS:HD3	4:N:86:TYR:OH	3.81	0.44
10:S:72:TYR:CE1	12:S:1502:CLA:HED2	2.53	0.44
5:W:8:VAL:O	5:W:21:VAL:HA	2.18	0.44
1:A:100:ASN:N	1:A:100:ASN:OD1	2.48	0.43
1:A:216:HIS:HB2	12:A:812:CLA:C1C	2.47	0.43
12:A:821:CLA:H3A	12:A:821:CLA:HBA2	1.70	0.43
12:A:825:CLA:H2A	12:A:825:CLA:O2D	2.18	0.43
1:A:678:PHE:CE2	12:A:839:CLA:HBB2	2.53	0.43
2:B:236:ASN:OD1	2:B:236:ASN:N	2.51	0.43
4:D:38:GLU:HG3	4:D:53:GLN:OE1	2.18	0.43
1:E:242:GLU:OE1	1:E:242:GLU:HA	2.18	0.43
1:E:331:GLY:H	1:E:334:THR:HG1	1.64	0.43
1:E:684:LEU:HD23	1:E:684:LEU:H	1.83	0.43
1:E:589:TRP:CH2	1:E:722:ILE:HB	2.52	0.43
12:E:817:CLA:H3A	12:E:817:CLA:CGA	3.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:836:CLA:HAC2	2:G:226:PHE:CE2	111.68	0.43
2:G:378:HIS:HB2	12:G:830:CLA:C1B	21.37	0.43
2:G:537:LEU:HD23	2:G:537:LEU:HA	1.54	0.43
2:G:690:LEU:HG	12:G:843:CLA:O1A	2.18	0.43
2:G:72:GLY:HA2	2:G:87:ILE:HB	2.00	0.43
9:K:54:LEU:HG	9:K:64:SER:OG	2.18	0.43
1:A:118:VAL:HG21	1:A:127:LEU:HB2	1.99	0.43
1:A:679:VAL:O	1:A:683:SER:OG	2.35	0.43
1:A:725:ARG:HA	1:A:725:ARG:HD2	1.76	0.43
12:A:803:CLA:HED1	12:A:803:CLA:C2	8.40	0.43
12:A:806:CLA:HBA2	12:A:806:CLA:H3A	1.40	0.43
1:A:81:LEU:HB2	1:A:173:MET:HE1	1.99	0.43
2:B:673:TYR:CZ	12:B:805:CLA:HMD1	24.87	0.43
2:B:98:LYS:HA	2:B:98:LYS:HD2	1.82	0.43
1:E:399:GLY:O	1:E:403:VAL:HG22	2.18	0.43
1:E:543:ILE:HD11	12:E:838:CLA:CBB	2.48	0.43
1:E:679:VAL:O	1:E:683:SER:OG	2.35	0.43
1:E:740:ILE:H	1:E:740:ILE:HG12	1.38	0.43
12:E:822:CLA:HBB	12:E:842:CLA:HBC3	56.92	0.43
1:E:93:PHE:CE1	1:E:97:ARG:HB2	2.53	0.43
6:F:146:GLU:HA	6:F:149:SER:HG	1.83	0.43
2:G:681:LEU:HD11	12:G:801:CLA:C3D	2.48	0.43
12:G:817:CLA:HBA2	12:G:817:CLA:H3A	3.54	0.43
2:G:183:PHE:CB	12:G:819:CLA:HMC1	2.47	0.43
2:G:331:ASN:OD1	12:G:825:CLA:HBC3	2.17	0.43
12:G:826:CLA:HBA1	12:G:826:CLA:H3A	1.52	0.43
12:G:834:CLA:HBB1	12:G:834:CLA:HMB1	2.01	0.43
4:N:87:ARG:HB3	4:N:95:GLN:HB2	2.00	0.43
1:A:596:LEU:HA	1:A:599:MET:HG3	2.00	0.43
12:B:841:CLA:H2A	12:B:841:CLA:O2D	2.19	0.43
3:C:16:CYS:HB2	3:C:53:CYS:HB3	2.00	0.43
1:E:184:ARG:HA	1:E:184:ARG:HD3	1.85	0.43
1:E:428:ASP:O	1:E:431:ILE:HG12	2.18	0.43
1:E:496:GLY:HA2	1:E:500:PRO:HA	2.01	0.43
2:G:489:ALA:HA	2:G:492:ALA:HB3	1.99	0.43
2:G:55:ALA:O	2:G:59:LEU:HG	2.18	0.43
2:G:703:MET:HG2	2:G:704:SER:H	1.83	0.43
2:G:174:ARG:HH11	12:G:814:CLA:HBC2	1.83	0.43
12:G:820:CLA:H3A	12:G:820:CLA:HBA2	2.01	0.43
9:K:69:LEU:HG	9:K:70:GLY:N	2.34	0.43
10:L:25:ARG:HD2	10:L:26:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:25:GLN:O	11:M:28:VAL:HG22	2.18	0.43
9:R:54:LEU:HG	9:R:64:SER:OG	2.19	0.43
10:S:25:ARG:HD2	10:S:26:ARG:HH22	1.84	0.43
10:S:60:LEU:HA	10:S:60:LEU:HD23	1.72	0.43
5:V:8:VAL:HB	5:V:58:LEU:HB2	2.00	0.43
1:A:119:TRP:HA	1:A:120:PRO:HD3	1.88	0.43
1:A:399:GLY:O	1:A:403:VAL:HG22	2.18	0.43
2:B:576:TRP:CD1	2:B:580:TYR:CZ	3.07	0.43
1:E:409:ALA:O	1:E:413:MET:HG3	2.19	0.43
1:E:543:ILE:HD11	12:E:835:CLA:CBB	21.10	0.43
12:E:822:CLA:H3A	12:E:822:CLA:HBA2	1.91	0.43
12:E:837:CLA:HBA1	12:E:837:CLA:HED2	2.00	0.43
12:E:842:CLA:OBD	6:O:108:LEU:HD21	2.18	0.43
2:G:165:LEU:O	2:G:169:LYS:NZ	2.40	0.43
2:G:487:SER:N	2:G:490:SER:OG	2.50	0.43
10:L:57:ILE:HA	10:L:57:ILE:HD12	1.88	0.43
1:E:313:ARG:HH22	9:R:49:GLY:CA	3.22	0.43
10:S:92:ILE:H	10:S:92:ILE:HG13	1.25	0.43
5:V:9:ARG:HA	5:V:20:ASP:O	2.19	0.43
1:A:104:TRP:CD1	1:A:108:PRO:HA	2.54	0.43
1:A:691:ARG:HH21	1:A:718:ALA:C	2.22	0.43
1:A:93:PHE:CE1	1:A:97:ARG:HB2	2.53	0.43
2:B:315:THR:HB	2:B:317:GLY:H	1.84	0.43
12:B:813:CLA:HBA1	12:B:813:CLA:H3A	1.72	0.43
2:B:174:ARG:HH11	12:B:815:CLA:HBC2	18.38	0.43
12:B:816:CLA:HBA2	12:B:816:CLA:H3A	1.67	0.43
12:B:839:CLA:CBA	12:B:840:CLA:HAA2	2.43	0.43
3:C:14:THR:HB	3:C:17:VAL:HG22	2.01	0.43
1:E:104:TRP:CD1	1:E:108:PRO:HA	2.54	0.43
12:E:820:CLA:HBA2	12:E:820:CLA:H3A	1.57	0.43
6:F:141:LEU:O	6:F:145:LYS:HG2	2.18	0.43
2:G:230:TRP:HB3	12:G:817:CLA:H3A	1.99	0.43
2:G:230:TRP:HB3	12:G:819:CLA:H3A	21.94	0.43
2:G:371:THR:O	2:G:375:LEU:HG	2.18	0.43
2:G:393:HIS:HA	2:G:396:ILE:HG12	2.00	0.43
2:G:396:ILE:O	2:G:400:ARG:HB2	2.19	0.43
2:G:589:THR:O	2:G:592:TRP:HB2	2.19	0.43
12:G:835:CLA:HED2	12:G:835:CLA:HBD	1.91	0.43
12:J:1102:CLA:HMB1	12:J:1102:CLA:HBB1	2.00	0.43
6:O:69:GLU:N	6:O:69:GLU:OE1	2.51	0.43
1:A:112:LYS:HD3	1:A:112:LYS:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HB2	1:A:44:LYS:HZ2	1.84	0.43
1:A:453:PHE:O	1:A:457:ILE:HG23	2.18	0.43
1:A:563:ILE:HD12	1:A:563:ILE:HA	1.76	0.43
1:A:672:LEU:HB3	1:A:675:GLY:HA3	2.01	0.43
2:B:61:THR:O	2:B:64:LEU:HG	2.18	0.43
2:B:703:MET:HG2	2:B:704:SER:H	1.83	0.43
2:B:92:TRP:NE1	10:S:172:LYS:O	52.84	0.43
4:D:31:ILE:HD13	4:D:69:LEU:HD23	2.00	0.43
1:E:322:ILE:HD12	1:E:322:ILE:HA	1.82	0.43
1:E:672:LEU:HB3	1:E:675:GLY:HA3	2.01	0.43
12:E:830:CLA:HBA1	12:E:830:CLA:CHA	2.49	0.43
12:E:834:CLA:HED2	12:E:834:CLA:HBA1	4.48	0.43
2:G:315:THR:HB	2:G:317:GLY:H	1.84	0.43
2:G:586:ALA:O	2:G:589:THR:OG1	2.25	0.43
1:E:561:ARG:HB3	2:G:679:GLU:HG2	2.86	0.43
2:G:673:TYR:CZ	12:G:804:CLA:HMD1	2.53	0.43
12:G:816:CLA:H3A	12:G:816:CLA:HBA2	1.60	0.43
13:G:842:PQN:H292	13:G:842:PQN:H261	1.66	0.43
10:S:23:PRO:HA	10:S:28:PRO:HA	2.00	0.43
1:A:242:GLU:HA	1:A:242:GLU:OE1	2.18	0.43
1:A:359:MET:O	1:A:362:SER:OG	2.33	0.43
1:A:542:GLN:O	1:A:546:THR:OG1	2.36	0.43
1:A:664:SER:N	1:A:667:SER:OG	2.50	0.43
12:A:802:CLA:CED	12:A:802:CLA:H2A	4.56	0.43
12:A:813:CLA:H3A	12:A:813:CLA:HBA1	1.82	0.43
1:A:497:SER:HB3	2:B:227:THR:OG1	118.61	0.43
2:B:230:TRP:HB3	12:B:820:CLA:H3A	1.99	0.43
2:B:338:LEU:HD23	2:B:338:LEU:HA	1.89	0.43
2:B:611:GLN:N	2:B:611:GLN:CD	2.70	0.43
2:B:617:THR:OG1	2:B:618:TYR:N	2.52	0.43
12:B:806:CLA:HBA2	12:B:806:CLA:H3A	3.24	0.43
2:B:217:PRO:HD2	12:B:817:CLA:C3D	35.68	0.43
4:D:98:HIS:HA	4:D:99:PRO:C	2.39	0.43
1:E:350:HIS:HB3	1:E:415:ARG:NH1	2.34	0.43
1:E:580:ARG:CG	3:H:78:GLY:HA3	2.49	0.43
2:G:511:LEU:HD23	2:G:511:LEU:HA	1.81	0.43
2:G:576:TRP:CD1	2:G:580:TYR:CZ	3.07	0.43
12:G:829:CLA:HBA2	12:G:829:CLA:H12	5.03	0.43
12:G:839:CLA:H2A	12:G:839:CLA:O2D	2.18	0.43
10:L:72:TYR:CE1	12:L:204:CLA:HED2	2.53	0.43
11:M:32:ILE:HD12	11:M:36:PRO:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:33:TRP:CD1	4:N:80:ILE:HG21	2.56	0.43
2:G:454:GLU:HA	6:O:71:LEU:HD22	2.47	0.43
5:W:8:VAL:HB	5:W:58:LEU:HB2	2.01	0.43
5:W:9:ARG:HA	5:W:20:ASP:O	2.19	0.43
1:A:437:ILE:HG23	12:A:836:CLA:HBB2	2.01	0.43
1:A:91:MET:CE	12:A:806:CLA:HMA2	2.49	0.43
2:B:364:PHE:HB3	2:B:367:GLN:NE2	2.34	0.43
2:B:599:TRP:HE1	2:B:612:PHE:HB2	1.84	0.43
12:B:802:CLA:HMB2	12:B:807:CLA:HMB2	2.00	0.43
12:B:840:CLA:H2A	12:B:840:CLA:O2D	2.19	0.43
1:E:664:SER:N	1:E:667:SER:OG	2.50	0.43
1:E:671:LEU:HD23	1:E:671:LEU:H	1.84	0.43
12:E:826:CLA:H3A	12:E:826:CLA:HBA1	4.09	0.43
12:E:828:CLA:O2D	12:E:828:CLA:H2A	2.18	0.43
12:E:838:CLA:HAC2	12:E:839:CLA:HMC2	22.41	0.43
6:F:155:LYS:O	6:F:159:ILE:HG12	2.19	0.43
6:F:69:GLU:OE1	6:F:69:GLU:N	2.51	0.43
2:G:100:ALA:O	2:G:104:PHE:N	2.52	0.43
2:G:136:TYR:O	2:G:140:VAL:HG13	2.18	0.43
2:G:393:HIS:ND1	2:G:396:ILE:HD11	2.34	0.43
2:G:374:ALA:HB1	12:G:828:CLA:HMA1	2.01	0.43
12:J:1101:CLA:HED1	12:J:1101:CLA:C2	2.48	0.43
9:K:62:ASN:N	9:K:62:ASN:OD1	2.52	0.43
6:O:155:LYS:O	6:O:159:ILE:HG12	2.19	0.43
9:R:69:LEU:HG	9:R:70:GLY:N	2.34	0.43
10:S:155:VAL:O	10:S:159:PHE:HD1	2.02	0.43
1:A:543:ILE:HD11	12:A:836:CLA:CBB	15.42	0.43
1:A:590:ASP:O	1:A:593:PHE:HB2	2.19	0.43
1:A:725:ARG:NH1	1:A:728:GLY:HA3	2.34	0.43
12:A:803:CLA:H2A	12:A:803:CLA:HED2	1.99	0.43
12:A:833:CLA:HED2	12:A:833:CLA:HBA1	2.00	0.43
12:B:827:CLA:O1A	12:B:838:CLA:HHB	20.34	0.43
2:B:374:ALA:HB1	12:B:829:CLA:HMA1	25.59	0.43
2:B:374:ALA:HB1	12:B:831:CLA:HMA1	2.01	0.43
12:B:835:CLA:HMB1	12:B:835:CLA:HBB1	4.15	0.43
4:D:35:SER:O	4:D:54:GLY:N	2.78	0.43
4:D:89:TYR:CD2	4:D:93:GLU:HB2	2.48	0.43
1:E:426:VAL:O	1:E:430:VAL:HG22	2.19	0.43
1:E:437:ILE:HG23	12:E:840:CLA:HBB2	2.01	0.43
1:E:678:PHE:CE2	12:E:843:CLA:HBB2	2.53	0.43
12:E:802:CLA:HED1	12:E:802:CLA:C2	6.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:364:PHE:HB3	2:G:367:GLN:NE2	2.34	0.43
2:G:617:THR:OG1	2:G:618:TYR:N	2.52	0.43
2:G:174:ARG:HH11	12:G:816:CLA:HBC2	32.55	0.43
12:G:831:CLA:HBA2	12:G:831:CLA:H3A	2.37	0.43
1:A:496:GLY:HA2	1:A:500:PRO:HA	2.01	0.43
1:A:602:THR:OG1	1:A:603:ILE:N	2.52	0.43
12:A:802:CLA:HBA2	12:A:802:CLA:H3A	1.83	0.43
12:A:832:CLA:C2B	12:A:833:CLA:HMB2	9.59	0.43
2:B:100:ALA:O	2:B:104:PHE:N	2.52	0.43
2:B:268:LEU:HD13	12:B:821:CLA:HMA2	2.01	0.43
2:B:314:LYS:O	2:B:315:THR:HG23	2.19	0.43
2:B:396:ILE:O	2:B:400:ARG:HB2	2.19	0.43
2:B:517:PRO:O	2:B:520:PHE:HB3	2.19	0.43
1:E:91:MET:CE	12:E:807:CLA:HMA2	22.61	0.43
1:E:91:MET:CE	12:E:809:CLA:HMA2	2.49	0.43
2:G:128:GLY:HA3	2:G:201:GLU:HG3	2.01	0.43
2:G:268:LEU:HD13	12:G:820:CLA:HMA2	29.63	0.43
3:H:16:CYS:HB2	3:H:53:CYS:HB3	2.00	0.43
10:L:155:VAL:O	10:L:159:PHE:HD1	2.02	0.43
12:L:201:CLA:H3A	12:L:201:CLA:HBA2	1.81	0.43
10:S:59:PRO:O	10:S:62:ARG:HB3	2.19	0.43
1:A:152:GLY:HA3	1:A:224:VAL:HG11	2.01	0.42
1:A:671:LEU:H	1:A:671:LEU:HD23	1.84	0.42
12:A:829:CLA:CHA	12:A:829:CLA:HBA1	2.59	0.42
12:A:834:CLA:HBB1	12:A:834:CLA:HMB1	2.01	0.42
12:A:835:CLA:HED2	12:A:835:CLA:HBA1	6.90	0.42
1:A:437:ILE:HG23	12:A:838:CLA:HBB2	44.65	0.42
2:B:160:LYS:HD3	2:B:160:LYS:HA	1.75	0.42
2:B:128:GLY:HA3	2:B:201:GLU:HG3	2.01	0.42
1:E:152:GLY:HA3	1:E:224:VAL:HG11	2.01	0.42
1:E:325:ILE:HG13	1:E:329:HIS:HE1	1.84	0.42
13:E:846:PQN:H262	13:E:846:PQN:H241	1.90	0.42
12:G:806:CLA:H43	12:G:814:CLA:H42	2.00	0.42
12:G:836:CLA:H3A	12:G:836:CLA:HBA2	1.77	0.42
2:G:89:HIS:ND1	2:G:90:ALA:O	2.46	0.42
10:L:78:PHE:CZ	10:L:98:THR:HB	2.50	0.42
6:O:87:LEU:HD23	6:O:91:ILE:HD11	2.01	0.42
8:Q:22:LEU:HA	8:Q:22:LEU:HD12	1.87	0.42
9:R:37:PHE:HE1	9:R:71:SER:OG	2.02	0.42
10:S:108:ALA:O	10:S:111:LEU:HG	2.19	0.42
1:A:184:ARG:HA	1:A:184:ARG:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ALA:O	1:A:413:MET:HG3	2.19	0.42
12:A:839:CLA:HAC2	12:A:840:CLA:HMC2	67.85	0.42
2:B:195:VAL:HA	2:B:199:ILE:HD12	2.01	0.42
2:B:230:TRP:CB	12:B:818:CLA:H3A	28.05	0.42
13:B:844:PQN:H292	13:B:844:PQN:H261	1.66	0.42
1:E:678:PHE:CE2	12:E:840:CLA:HBB2	42.82	0.42
1:E:691:ARG:HH21	1:E:718:ALA:C	2.22	0.42
1:E:705:HIS:HD2	1:E:710:VAL:HG13	1.84	0.42
12:E:832:CLA:HBA2	12:E:832:CLA:H3A	4.08	0.42
2:G:717:THR:O	2:G:721:VAL:HG23	2.19	0.42
12:E:801:CLA:CHD	12:G:805:CLA:HMC2	37.77	0.42
12:G:810:CLA:H3A	12:G:810:CLA:HBA2	2.11	0.42
2:G:289:HIS:CD2	12:G:821:CLA:HED2	2.55	0.42
3:H:14:THR:HB	3:H:17:VAL:HG22	2.01	0.42
3:H:13:CYS:SG	3:H:58:PRO:HG2	2.60	0.42
4:N:29:TYR:OH	4:N:63:LYS:HE3	3.90	0.42
4:N:93:GLU:OE1	4:N:93:GLU:N	4.30	0.42
1:A:350:HIS:HB3	1:A:415:ARG:NH1	2.34	0.42
1:A:488:GLN:HG2	1:A:510:PHE:CD1	2.55	0.42
1:A:730:ALA:O	1:A:734:LEU:HB2	2.19	0.42
2:B:393:HIS:ND1	2:B:396:ILE:HD11	2.34	0.42
2:B:585:TRP:HZ2	12:B:801:CLA:ND	2.17	0.42
2:B:589:THR:O	2:B:592:TRP:HB2	2.19	0.42
4:D:84:LYS:HD3	4:D:86:TYR:OH	2.18	0.42
1:E:590:ASP:O	1:E:593:PHE:HB2	2.19	0.42
12:E:805:CLA:H2	12:E:812:CLA:NB	2.35	0.42
12:E:834:CLA:C2B	12:E:835:CLA:HMB2	2.49	0.42
12:E:841:CLA:HAC2	12:E:842:CLA:HMC2	2.01	0.42
2:G:59:LEU:O	2:G:62:SER:OG	2.29	0.42
12:G:840:CLA:H12	12:G:840:CLA:HBA2	1.79	0.42
5:V:31:GLY:N	3:H:34:LYS:HZ1	129.25	0.42
10:L:166:LEU:HA	10:L:169:ASN:HD21	1.84	0.42
10:L:59:PRO:O	10:L:62:ARG:HB3	2.19	0.42
4:N:19:LEU:HD13	4:N:23:ALA:HB1	2.01	0.42
11:T:32:ILE:HD12	11:T:36:PRO:HG2	2.01	0.42
1:A:325:ILE:HG13	1:A:329:HIS:HE1	1.84	0.42
1:A:359:MET:HB2	1:A:359:MET:HE2	2.03	0.42
12:A:836:CLA:HMB1	12:A:836:CLA:HBB1	2.64	0.42
1:A:91:MET:CE	12:A:808:CLA:HMA2	34.82	0.42
2:B:223:ARG:C	2:B:227:THR:HG22	2.40	0.42
2:B:597:TRP:CE2	2:B:601:HIS:CE1	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:THR:O	2:B:721:VAL:HG23	2.19	0.42
1:E:437:ILE:HG23	12:E:837:CLA:HBB2	30.38	0.42
1:E:488:GLN:HG2	1:E:510:PHE:CD1	2.54	0.42
1:E:596:LEU:HA	1:E:599:MET:HG3	2.00	0.42
1:E:730:ALA:O	1:E:734:LEU:HB2	2.19	0.42
1:E:81:LEU:HB2	1:E:173:MET:HE1	2.00	0.42
1:E:94:HIS:HA	1:E:98:PHE:CD2	2.55	0.42
2:G:338:LEU:HA	2:G:338:LEU:HD23	1.88	0.42
2:G:517:PRO:O	2:G:520:PHE:HB3	2.19	0.42
4:N:38:GLU:HG3	4:N:53:GLN:OE1	2.24	0.42
10:S:72:TYR:CD1	10:S:157:ALA:HB2	2.52	0.42
5:V:7:LYS:HE2	5:V:21:VAL:HB	2.01	0.42
1:A:283:ASN:HA	1:A:290:TRP:CZ2	2.54	0.42
1:A:601:ASN:O	1:A:605:ILE:HG12	2.20	0.42
12:A:816:CLA:HBD	12:A:816:CLA:HED2	4.20	0.42
12:A:827:CLA:HBA1	12:A:827:CLA:CHA	2.49	0.42
12:A:831:CLA:H3A	12:A:831:CLA:HBA2	1.40	0.42
2:B:144:ILE:O	2:B:148:VAL:HG12	2.20	0.42
2:B:230:TRP:CB	12:B:820:CLA:H3A	2.50	0.42
12:B:802:CLA:HBA1	12:B:802:CLA:H3A	1.77	0.42
12:B:817:CLA:H3A	12:B:817:CLA:HBA2	3.03	0.42
2:B:268:LEU:HD13	12:B:819:CLA:HMA2	27.34	0.42
2:B:461:PRO:HB3	12:B:839:CLA:O1D	10.41	0.42
3:C:30:TRP:CZ2	3:C:32:GLY:HA3	2.54	0.42
3:C:13:CYS:SG	3:C:58:PRO:HG2	2.60	0.42
4:D:22:LYS:HA	4:D:26:GLU:OE1	2.35	0.42
1:E:146:GLN:H	1:E:146:GLN:HG2	1.67	0.42
1:E:283:ASN:HA	1:E:290:TRP:CZ2	2.55	0.42
12:E:803:CLA:H2	12:E:810:CLA:NB	43.78	0.42
12:E:806:CLA:H2A	12:E:806:CLA:HED2	1.99	0.42
2:G:188:LEU:O	2:G:191:THR:OG1	2.33	0.42
2:G:223:ARG:C	2:G:227:THR:HG22	2.40	0.42
2:G:314:LYS:O	2:G:315:THR:HG23	2.19	0.42
12:G:840:CLA:O2D	12:G:840:CLA:H2A	4.27	0.42
10:S:166:LEU:HA	10:S:169:ASN:HD21	1.84	0.42
11:T:25:GLN:O	11:T:28:VAL:HG22	2.19	0.42
1:A:99:SER:HB2	1:A:114:SER:O	2.20	0.42
1:A:350:HIS:NE2	1:A:411:ILE:HG23	2.35	0.42
1:A:515:VAL:O	1:A:522:ALA:HB3	2.20	0.42
1:A:141:THR:N	12:A:806:CLA:OBD	2.38	0.42
12:A:810:CLA:HMC3	12:A:818:CLA:HBC1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:842:PQN:H193	13:A:842:PQN:H162	1.68	0.42
4:D:55:PRO:HB2	4:D:57:LYS:NZ	7.49	0.42
1:E:99:SER:HB2	1:E:114:SER:O	2.20	0.42
1:E:277:THR:OG1	1:E:279:LYS:HE3	2.20	0.42
1:E:602:THR:OG1	1:E:603:ILE:N	2.52	0.42
1:E:91:MET:HE1	12:E:809:CLA:HMA2	2.01	0.42
2:G:144:ILE:O	2:G:148:VAL:HG12	2.20	0.42
12:G:812:CLA:H3A	12:G:812:CLA:HBA1	1.84	0.42
12:G:828:CLA:O1A	12:G:838:CLA:HHB	32.91	0.42
9:K:37:PHE:HE1	9:K:71:SER:OG	2.03	0.42
4:N:27:GLU:C	4:N:28:LYS:HD3	2.41	0.42
5:W:51:ASN:HB3	5:W:53:PHE:CZ	2.55	0.42
1:A:312:TYR:CD1	1:A:322:ILE:HD11	2.54	0.42
1:A:99:SER:HA	1:A:135:PHE:CZ	2.55	0.42
2:B:289:HIS:CD2	12:B:822:CLA:HED2	27.65	0.42
12:B:829:CLA:H3A	12:B:829:CLA:HBA1	1.52	0.42
12:B:829:CLA:O1A	12:B:839:CLA:HHB	2.19	0.42
4:D:105:PRO:C	4:D:107:LYS:H	2.22	0.42
1:E:528:LEU:HB3	1:E:532:ASP:OD2	2.20	0.42
1:E:601:ASN:O	1:E:605:ILE:HG12	2.20	0.42
12:E:804:CLA:HED1	12:E:804:CLA:C2	2.48	0.42
12:E:805:CLA:H3A	12:E:805:CLA:HBA2	1.83	0.42
12:E:811:CLA:HMC3	12:E:819:CLA:HBC1	28.96	0.42
12:E:831:CLA:C2B	12:E:832:CLA:HMB2	35.32	0.42
1:E:99:SER:HA	1:E:135:PHE:CZ	2.55	0.42
2:G:195:VAL:HA	2:G:199:ILE:HD12	2.01	0.42
2:G:50:HIS:HE1	12:G:808:CLA:NA	27.23	0.42
12:G:801:CLA:C4C	12:G:840:CLA:HBC3	2.50	0.42
12:G:815:CLA:H3A	12:G:815:CLA:HBA2	1.63	0.42
12:G:820:CLA:H11	12:G:824:CLA:HAA1	2.02	0.42
7:I:32:GLU:HG2	10:L:115:THR:HG22	2.78	0.42
10:L:61:ARG:HH12	10:S:141:THR:HA	1.84	0.42
1:A:224:VAL:O	1:A:228:LEU:HG	2.20	0.42
1:A:279:LYS:HD2	1:A:290:TRP:CG	2.55	0.42
1:A:426:VAL:O	1:A:430:VAL:HG22	2.19	0.42
1:A:596:LEU:HA	1:A:599:MET:CG	2.50	0.42
1:A:671:LEU:C	1:A:673:PHE:H	2.23	0.42
12:A:820:CLA:HBD	9:K:48:VAL:CG1	2.49	0.42
12:A:830:CLA:C2B	12:A:831:CLA:HMB2	2.49	0.42
12:A:834:CLA:CED	12:A:834:CLA:H2A	2.67	0.42
2:B:183:PHE:O	2:B:187:SER:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:HIS:HE1	12:B:809:CLA:NA	2.18	0.42
12:B:821:CLA:H11	12:B:825:CLA:HAA1	34.53	0.42
3:C:49:GLY:N	14:C:101:SF4:S2	2.93	0.42
1:E:279:LYS:HD2	1:E:290:TRP:CG	2.55	0.42
1:E:725:ARG:O	1:E:729:VAL:HG12	2.20	0.42
12:E:819:CLA:HBA2	12:E:819:CLA:H3A	1.66	0.42
2:G:141:PHE:HZ	12:G:817:CLA:H11	35.64	0.42
2:G:554:LYS:HZ3	4:N:125:ASN:HB2	3.31	0.42
2:G:597:TRP:CE2	2:G:601:HIS:CE1	3.08	0.42
12:G:814:CLA:H2A	12:G:814:CLA:O1D	2.45	0.42
2:G:289:HIS:CD2	12:G:823:CLA:HED2	18.89	0.42
2:G:461:PRO:HB3	12:G:839:CLA:O1D	12.87	0.42
3:H:22:THR:HG22	4:N:63:LYS:HZ3	1.85	0.42
3:H:30:TRP:CZ2	3:H:32:GLY:HA3	2.54	0.42
3:H:49:GLY:N	14:H:101:SF4:S2	2.93	0.42
10:L:108:ALA:O	10:L:111:LEU:HG	2.19	0.42
2:B:688:THR:HG22	12:L:201:CLA:H3A	2.02	0.42
4:N:36:PRO:HB2	4:N:37:LYS:HZ3	1.85	0.42
6:O:146:GLU:HA	6:O:149:SER:HG	1.85	0.42
9:R:62:ASN:N	9:R:62:ASN:OD1	2.52	0.42
10:S:78:PHE:CZ	10:S:98:THR:HB	2.50	0.42
5:W:7:LYS:HE2	5:W:21:VAL:HB	2.01	0.42
1:A:725:ARG:O	1:A:729:VAL:HG12	2.20	0.42
12:A:823:CLA:HBA2	12:A:823:CLA:H3A	3.76	0.42
1:A:94:HIS:HA	1:A:98:PHE:CD2	2.55	0.42
12:B:802:CLA:C3C	12:B:807:CLA:HMC2	2.49	0.42
12:B:805:CLA:H3A	12:B:805:CLA:C1	4.61	0.42
12:B:833:CLA:HBA2	12:B:833:CLA:H3A	1.48	0.42
12:B:838:CLA:H3A	12:B:838:CLA:HBA1	3.19	0.42
3:C:23:ASP:O	3:C:43:ARG:NE	2.48	0.42
2:B:556:PHE:HE1	3:C:67:TYR:CE2	2.65	0.42
1:E:312:TYR:CD1	1:E:322:ILE:HD11	2.54	0.42
1:E:350:HIS:NE2	1:E:411:ILE:HG23	2.34	0.42
1:E:515:VAL:O	1:E:522:ALA:HB3	2.20	0.42
1:E:596:LEU:HA	1:E:599:MET:CG	2.50	0.42
1:E:716:PRO:O	1:E:717:ARG:NE	2.50	0.42
2:G:220:GLU:OE1	2:G:220:GLU:N	2.53	0.42
2:G:230:TRP:CB	12:G:817:CLA:H3A	2.50	0.42
2:G:230:TRP:CB	12:G:819:CLA:H3A	22.83	0.42
2:G:289:HIS:O	12:G:822:CLA:HHD	2.20	0.42
5:V:30:SER:HB2	3:H:34:LYS:NZ	127.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:60:ARG:NH1	8:J:43:LEU:HA	3.61	0.42
7:P:11:LEU:HA	7:P:14:LEU:HD21	2.02	0.42
9:R:33:LEU:O	9:R:36:LEU:HD12	2.20	0.42
10:S:57:ILE:HA	10:S:57:ILE:HD12	1.88	0.42
5:V:18:PHE:HB3	6:F:162:SER:OG	2.20	0.42
1:A:528:LEU:HB3	1:A:532:ASP:OD2	2.20	0.42
1:A:434:ARG:HD2	1:A:555:LEU:HD13	2.02	0.42
12:A:812:CLA:HMC3	12:A:820:CLA:HBC1	24.49	0.42
2:B:262:HIS:NE2	2:B:264:GLN:HB3	2.35	0.42
2:B:289:HIS:O	12:B:823:CLA:HHD	9.61	0.42
2:B:289:HIS:O	12:B:825:CLA:HHD	2.20	0.42
2:B:305:LEU:HD22	2:B:327:TYR:CE1	2.55	0.42
2:B:511:LEU:HA	2:B:511:LEU:HD23	1.81	0.42
2:B:693:LEU:HD13	2:B:693:LEU:N	2.35	0.42
12:B:814:CLA:HMB3	12:B:822:CLA:C3D	41.01	0.42
2:B:183:PHE:CB	12:B:822:CLA:HMC1	2.47	0.42
1:E:257:PHE:HB2	1:E:275:PHE:CE1	2.53	0.42
1:E:725:ARG:NH1	1:E:728:GLY:HA3	2.34	0.42
12:E:813:CLA:HMC3	12:E:821:CLA:HBC1	2.02	0.42
6:F:88:ILE:HB	6:F:89:PRO:HD3	2.02	0.42
2:G:450:PHE:O	6:O:45:ARG:NH1	3.21	0.42
2:G:289:HIS:O	12:G:824:CLA:HHD	22.75	0.42
10:L:61:ARG:NH2	10:S:144:SER:HB3	2.35	0.42
5:V:43:VAL:HB	5:V:47:GLY:HA2	2.02	0.42
1:A:141:THR:O	1:A:141:THR:HG22	2.19	0.41
1:A:705:HIS:HD2	1:A:710:VAL:HG13	1.85	0.41
12:A:801:CLA:CHD	12:B:806:CLA:HMC2	2.50	0.41
1:E:141:THR:HG22	1:E:141:THR:O	2.19	0.41
1:E:434:ARG:HD2	1:E:555:LEU:HD13	2.02	0.41
12:E:838:CLA:HBB1	12:E:838:CLA:HMB1	2.01	0.41
2:G:305:LEU:HD22	2:G:327:TYR:CE1	2.55	0.41
7:I:11:LEU:HA	7:I:14:LEU:HD21	2.02	0.41
4:N:136:MET:CE	4:N:139:TYR:HB2	2.50	0.41
6:O:111:ILE:HG22	6:O:117:THR:HG22	2.02	0.41
9:R:68:VAL:HG23	9:R:69:LEU:N	2.35	0.41
5:W:43:VAL:HB	5:W:47:GLY:HA2	2.02	0.41
1:A:115:ALA:HB3	1:A:140:ILE:HD13	2.02	0.41
1:A:157:PHE:O	1:A:161:VAL:HG23	2.21	0.41
1:A:205:LEU:HD12	12:A:811:CLA:CHB	2.50	0.41
1:A:277:THR:OG1	1:A:279:LYS:HE3	2.20	0.41
12:A:804:CLA:H2	12:A:811:CLA:NB	24.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:832:CLA:H2A	12:A:832:CLA:CED	2.50	0.41
2:B:461:PRO:HB3	12:B:840:CLA:O1D	2.20	0.41
1:A:648:ARG:NH2	2:B:639:ASN:HB3	2.35	0.41
2:B:50:HIS:HE1	12:B:807:CLA:NA	40.28	0.41
12:B:815:CLA:H2A	12:B:815:CLA:O1D	2.20	0.41
12:B:816:CLA:HMB3	12:B:824:CLA:C3D	2.50	0.41
2:B:289:HIS:CD2	12:B:824:CLA:HED2	2.55	0.41
12:B:839:CLA:O2D	12:B:839:CLA:H2A	3.95	0.41
4:D:63:LYS:O	4:D:67:ILE:HG12	2.40	0.41
12:E:833:CLA:CED	12:E:833:CLA:H2A	4.31	0.41
13:E:846:PQN:H162	13:E:846:PQN:H193	1.68	0.41
2:G:238:ASP:OD1	2:G:251:GLY:N	2.43	0.41
2:G:262:HIS:NE2	2:G:264:GLN:HB3	2.35	0.41
2:G:599:TRP:HE1	2:G:612:PHE:HB2	1.84	0.41
12:G:808:CLA:CAD	7:P:11:LEU:HD11	2.50	0.41
2:G:461:PRO:HB3	12:G:838:CLA:O1D	2.20	0.41
1:A:343:GLU:OE1	1:A:343:GLU:N	2.36	0.41
1:A:369:HIS:HD2	1:A:372:TYR:CE1	2.39	0.41
1:A:377:TYR:HB2	1:A:380:LEU:CD1	2.48	0.41
12:A:808:CLA:H3A	12:A:808:CLA:HBA2	4.09	0.41
1:A:678:PHE:CE2	12:A:841:CLA:HBB2	54.32	0.41
2:B:220:GLU:N	2:B:220:GLU:OE1	2.53	0.41
12:B:820:CLA:H3A	12:B:820:CLA:HBA2	3.54	0.41
4:D:105:PRO:CB	4:D:108:VAL:HG22	6.04	0.41
4:D:93:GLU:N	4:D:93:GLU:OE1	2.50	0.41
1:E:543:ILE:O	1:E:547:VAL:HG23	2.20	0.41
1:E:545:VAL:HG23	1:E:598:TRP:CE3	2.56	0.41
12:E:809:CLA:O1A	12:E:829:CLA:H12	2.21	0.41
1:E:678:PHE:HB2	12:E:844:CLA:HAA1	75.29	0.41
6:F:87:LEU:HD23	6:F:91:ILE:HD11	2.01	0.41
2:G:236:ASN:OD1	2:G:236:ASN:N	2.51	0.41
2:G:693:LEU:N	2:G:693:LEU:HD13	2.35	0.41
2:G:699:LYS:HA	2:G:700:PRO:HD3	1.93	0.41
2:G:268:LEU:HD13	12:G:818:CLA:HMA2	2.01	0.41
1:E:580:ARG:HG2	3:H:78:GLY:HA3	2.01	0.41
2:B:690:LEU:HD12	12:L:203:CLA:C3D	3.44	0.41
10:L:92:ILE:O	10:L:96:LEU:HG	2.20	0.41
4:N:22:LYS:HA	4:N:26:GLU:OE1	2.20	0.41
4:N:55:PRO:HB2	4:N:57:LYS:NZ	2.35	0.41
10:S:92:ILE:HA	10:S:95:LEU:HB3	2.02	0.41
5:V:51:ASN:HB3	5:V:53:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:36:VAL:HG13	5:V:53:PHE:O	2.21	0.41
5:W:28:ASP:OD1	5:W:30:SER:OG	2.25	0.41
1:A:351:ALA:O	1:A:355:THR:HG23	2.21	0.41
1:A:545:VAL:HG23	1:A:598:TRP:CE3	2.56	0.41
12:A:806:CLA:O1A	12:A:826:CLA:H12	2.21	0.41
12:A:837:CLA:HAC2	12:A:838:CLA:HMC2	2.01	0.41
2:B:143:LEU:HD22	11:M:32:ILE:HD12	3.30	0.41
2:B:238:ASP:OD1	2:B:251:GLY:N	2.43	0.41
12:B:815:CLA:H3A	12:B:815:CLA:HBA1	1.83	0.41
1:E:115:ALA:HB3	1:E:140:ILE:HD13	2.02	0.41
1:E:282:LEU:HD12	1:E:283:ASN:H	1.86	0.41
12:E:828:CLA:HBA1	12:E:828:CLA:CHA	4.82	0.41
2:G:50:HIS:HE1	12:G:806:CLA:NA	2.18	0.41
12:G:812:CLA:O1D	12:G:812:CLA:H2A	2.20	0.41
9:R:85:GLY:HA3	12:R:1401:CLA:C2B	2.50	0.41
1:A:179:PHE:CZ	1:A:184:ARG:HB2	2.56	0.41
1:A:543:ILE:O	1:A:547:VAL:HG23	2.20	0.41
1:A:582:GLY:H	2:B:671:ARG:HE	1.79	0.41
12:A:802:CLA:H2	12:A:809:CLA:NB	2.35	0.41
1:A:705:HIS:ND1	12:A:838:CLA:HBC1	2.35	0.41
2:B:51:PHE:CD1	2:B:149:PHE:CE2	3.09	0.41
12:B:808:CLA:HBA2	12:B:808:CLA:H3A	1.48	0.41
2:B:47:PHE:CE1	12:B:817:CLA:HED1	2.56	0.41
1:E:157:PHE:O	1:E:161:VAL:HG23	2.21	0.41
1:E:224:VAL:O	1:E:228:LEU:HG	2.20	0.41
1:E:494:ALA:O	1:E:497:SER:OG	2.33	0.41
6:F:111:ILE:HG22	6:F:117:THR:HG22	2.02	0.41
2:G:178:HIS:HB3	2:G:182:LEU:HG	2.03	0.41
2:G:415:VAL:HA	2:G:418:HIS:CE1	2.56	0.41
2:G:75:GLU:HA	2:G:78:ILE:HD12	2.03	0.41
12:G:826:CLA:O1A	12:G:837:CLA:HHB	2.19	0.41
12:G:835:CLA:HMB1	12:G:835:CLA:HBB1	3.95	0.41
10:L:92:ILE:HA	10:L:95:LEU:HB3	2.02	0.41
6:O:119:LEU:HB3	6:O:123:ILE:HD12	2.02	0.41
12:G:840:CLA:HAA2	7:P:28:LEU:HD11	2.03	0.41
10:S:64:LEU:HD21	10:S:148:ILE:HD11	2.02	0.41
10:S:92:ILE:O	10:S:96:LEU:HG	2.20	0.41
1:A:342:TYR:CE2	12:A:823:CLA:HAC1	2.56	0.41
1:A:435:ASP:O	2:B:680:THR:OG1	2.31	0.41
1:A:705:HIS:ND1	12:A:840:CLA:HBC1	83.97	0.41
2:B:178:HIS:HB3	2:B:182:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:ILE:HA	2:B:301:ILE:HD12	1.83	0.41
2:B:89:HIS:ND1	2:B:90:ALA:O	2.46	0.41
3:C:12:GLY:O	3:C:14:THR:HG23	2.20	0.41
4:D:36:PRO:HA	4:D:54:GLY:H	1.90	0.41
1:E:39:LEU:HA	1:E:48:TRP:HE1	1.86	0.41
2:G:417:GLN:HA	6:O:164:ARG:HH22	1.85	0.41
12:G:806:CLA:H3A	12:G:806:CLA:C1	4.81	0.41
2:G:141:PHE:HZ	12:G:815:CLA:H11	1.85	0.41
12:G:838:CLA:O2D	12:G:838:CLA:H2A	2.19	0.41
2:G:89:HIS:O	2:G:114:ASN:N	2.49	0.41
2:B:455:LYS:HG2	8:J:44:LEU:HD21	3.49	0.41
9:K:41:ARG:NH1	9:K:67:THR:OG1	2.54	0.41
4:N:104:PHE:N	4:N:105:PRO:HD3	2.38	0.41
6:O:88:ILE:HB	6:O:89:PRO:HD3	2.02	0.41
6:O:60:ARG:NH1	8:Q:43:LEU:HD12	2.35	0.41
10:S:33:LEU:HD13	10:S:33:LEU:HA	1.76	0.41
10:S:98:THR:HA	10:S:101:MET:HB2	2.03	0.41
1:A:126:ILE:HD12	6:F:45:ARG:NH1	3.34	0.41
1:A:205:LEU:HD12	12:A:813:CLA:CHB	23.47	0.41
12:A:827:CLA:H2A	12:A:827:CLA:HED3	2.03	0.41
12:A:832:CLA:H3A	12:A:832:CLA:HBA2	4.01	0.41
12:A:839:CLA:HED2	12:A:839:CLA:HBD	1.68	0.41
2:B:417:GLN:HA	6:F:164:ARG:HH12	1.86	0.41
2:B:415:VAL:HA	2:B:418:HIS:CE1	2.56	0.41
2:B:29:HIS:CE1	12:B:808:CLA:HED1	9.09	0.41
1:E:369:HIS:HD2	1:E:372:TYR:CE1	2.39	0.41
12:E:807:CLA:HBA2	12:E:807:CLA:H3A	4.35	0.41
2:G:374:ALA:HB1	12:G:830:CLA:HMA1	30.24	0.41
12:G:837:CLA:HBA2	12:G:837:CLA:H3A	2.86	0.41
12:G:838:CLA:CBA	12:G:839:CLA:HAA2	11.05	0.41
2:G:15:ASP:HB2	3:H:72:GLU:O	2.76	0.41
9:K:85:GLY:HA3	12:K:1401:CLA:C2B	2.50	0.41
9:K:33:LEU:O	9:K:36:LEU:HD12	2.20	0.41
11:M:19:MET:HE3	11:M:19:MET:HB3	1.83	0.41
6:O:60:ARG:NH2	8:Q:44:LEU:HD12	2.35	0.41
1:A:282:LEU:HD12	1:A:283:ASN:H	1.86	0.41
1:A:613:LYS:HD3	12:A:834:CLA:CAC	2.51	0.41
1:A:701:ILE:HD13	1:A:701:ILE:HA	1.90	0.41
2:B:141:PHE:HZ	12:B:818:CLA:H11	1.85	0.41
2:B:188:LEU:O	2:B:191:THR:OG1	2.33	0.41
2:B:574:SER:O	2:B:574:SER:OG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:813:CLA:H2A	12:B:813:CLA:O1D	2.22	0.41
3:C:37:GLN:OE1	4:D:107:LYS:CE	2.69	0.41
1:E:102:GLU:HA	1:E:105:LEU:HD12	2.03	0.41
1:E:250:MET:HB3	1:E:257:PHE:HE2	1.86	0.41
1:E:705:HIS:ND1	12:E:842:CLA:HBC1	2.35	0.41
12:E:836:CLA:CED	12:E:836:CLA:H2A	2.50	0.41
6:F:107:TYR:CE2	6:F:111:ILE:HD11	2.56	0.41
2:G:460:GLU:HA	2:G:461:PRO:HD3	1.94	0.41
2:G:644:ASN:O	2:G:647:SER:OG	2.39	0.41
2:G:29:HIS:CE1	12:G:809:CLA:HED1	26.24	0.41
12:G:813:CLA:HMB3	12:G:821:CLA:C3D	2.50	0.41
2:G:47:PHE:CE1	12:G:814:CLA:HED1	2.56	0.41
12:G:815:CLA:HMB3	12:G:823:CLA:C3D	36.44	0.41
10:L:77:PRO:O	10:L:81:LEU:HB2	2.21	0.41
5:W:9:ARG:O	5:W:58:LEU:HA	2.21	0.41
1:A:102:GLU:HA	1:A:105:LEU:HD12	2.03	0.41
1:A:127:LEU:HD12	1:A:127:LEU:H	1.86	0.41
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.95	0.41
1:A:250:MET:HB3	1:A:257:PHE:HE2	1.86	0.41
1:A:483:PHE:O	1:A:487:VAL:HG23	2.21	0.41
12:A:808:CLA:O1A	12:A:828:CLA:H12	31.07	0.41
1:A:662:TYR:OH	2:B:451:GLY:N	2.53	0.41
2:B:59:LEU:O	2:B:62:SER:OG	2.29	0.41
12:B:823:CLA:H11	12:B:827:CLA:HAA1	2.02	0.41
4:D:98:HIS:ND1	4:D:99:PRO:HA	2.81	0.41
1:E:205:LEU:HD12	12:E:812:CLA:CHB	28.26	0.41
12:E:816:CLA:HBA1	12:E:816:CLA:H3A	1.82	0.41
12:E:832:CLA:HMC3	12:E:840:CLA:HBB1	2.03	0.41
2:G:574:SER:OG	2:G:574:SER:O	2.39	0.41
2:G:29:HIS:CE1	12:G:807:CLA:HED1	2.56	0.41
4:N:24:PHE:CE2	4:N:25:ARG:HG2	2.56	0.41
12:E:821:CLA:HAA1	9:R:48:VAL:HG12	12.75	0.41
1:A:220:VAL:C	1:A:223:PRO:HD2	2.42	0.41
1:A:733:LEU:O	1:A:737:ILE:HG23	2.21	0.41
3:C:34:LYS:HZ1	5:V:30:SER:CB	2.32	0.41
4:D:6:SER:O	4:D:57:LYS:HG2	2.21	0.41
1:E:342:TYR:CE2	12:E:826:CLA:HAC1	2.56	0.41
1:E:588:GLY:O	1:E:591:HIS:HB2	2.21	0.41
12:E:807:CLA:HBA2	12:E:807:CLA:CGD	2.51	0.41
12:E:830:CLA:HED3	12:E:830:CLA:H2A	2.03	0.41
2:G:587:LEU:HD22	2:G:720:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:68:VAL:HG23	9:K:69:LEU:N	2.35	0.41
5:W:36:VAL:HG13	5:W:53:PHE:O	2.21	0.41
1:A:183:LYS:HD3	1:A:183:LYS:HA	1.84	0.41
12:A:829:CLA:CGA	12:A:829:CLA:C1A	3.00	0.41
2:B:699:LYS:HA	2:B:700:PRO:HD3	1.93	0.41
12:B:801:CLA:H3A	12:B:801:CLA:O2A	2.21	0.41
2:B:175:LEU:HD22	12:B:826:CLA:HMD3	15.61	0.41
12:E:818:CLA:H43	12:R:1401:CLA:O2D	2.20	0.41
12:E:828:CLA:H2A	12:E:828:CLA:CED	3.14	0.41
2:G:154:TRP:CZ2	11:T:42:ARG:HD3	2.83	0.41
2:G:354:GLN:HA	2:G:357:TYR:CE1	2.57	0.41
12:G:804:CLA:C1	12:G:804:CLA:H3A	2.50	0.41
2:G:47:PHE:CE1	12:G:816:CLA:HED1	34.41	0.41
8:J:43:LEU:O	12:J:1102:CLA:CGA	2.68	0.41
10:L:64:LEU:HD21	10:L:148:ILE:HD11	2.02	0.41
10:L:24:SER:N	10:L:27:ASP:O	2.50	0.41
4:N:136:MET:CE	4:N:137:THR:H	2.34	0.41
9:R:33:LEU:HG	9:R:79:GLY:HA3	2.03	0.41
10:S:100:GLY:O	10:S:104:ILE:HG23	2.21	0.41
10:S:76:GLY:N	10:S:77:PRO:HD2	2.36	0.41
5:V:9:ARG:O	5:V:58:LEU:HA	2.21	0.41
1:A:257:PHE:HB2	1:A:275:PHE:CE1	2.53	0.40
1:A:542:GLN:CG	1:A:602:THR:HG22	2.51	0.40
12:A:806:CLA:HBA2	12:A:806:CLA:CGD	5.73	0.40
2:B:75:GLU:HA	2:B:78:ILE:HD12	2.03	0.40
12:B:807:CLA:C1	12:B:807:CLA:H3A	2.50	0.40
12:B:810:CLA:HED3	12:B:810:CLA:HBD	1.86	0.40
2:B:8:PHE:CB	2:B:34:HIS:HD2	2.34	0.40
2:B:71:GLN:OE1	2:B:90:ALA:N	2.54	0.40
4:D:41:PHE:CD1	4:D:51:MET:HE2	2.56	0.40
1:E:104:TRP:CZ3	1:E:145:PHE:HB3	2.57	0.40
1:E:220:VAL:C	1:E:223:PRO:HD2	2.42	0.40
1:E:342:TYR:CE2	12:E:824:CLA:HAC1	14.79	0.40
1:E:377:TYR:HB2	1:E:380:LEU:CD1	2.48	0.40
1:E:422:ASN:HA	1:E:422:ASN:HD22	1.60	0.40
12:E:843:CLA:HAC1	13:E:846:PQN:H201	2.03	0.40
12:G:801:CLA:H3A	12:G:801:CLA:O2A	4.70	0.40
3:H:12:GLY:O	3:H:14:THR:HG23	2.20	0.40
10:L:100:GLY:O	10:L:104:ILE:HG23	2.21	0.40
11:M:25:GLN:HA	11:M:28:VAL:HG22	2.03	0.40
6:O:107:TYR:CE2	6:O:111:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:41:ARG:NH1	9:R:67:THR:OG1	2.54	0.40
1:A:39:LEU:HA	1:A:48:TRP:HE1	1.86	0.40
1:A:598:TRP:HZ2	12:B:807:CLA:C1D	2.34	0.40
12:A:829:CLA:CED	12:A:829:CLA:H2A	2.85	0.40
2:B:29:HIS:CE1	12:B:810:CLA:HED1	2.56	0.40
2:B:31:PHE:HA	2:B:34:HIS:CE1	2.56	0.40
2:B:330:ILE:HG13	2:B:331:ASN:OD1	2.21	0.40
2:B:644:ASN:O	2:B:647:SER:OG	2.39	0.40
12:B:809:CLA:H3A	12:B:809:CLA:HBA2	3.67	0.40
12:B:817:CLA:H2A	12:B:817:CLA:HED2	4.25	0.40
2:B:319:PHE:HE2	12:B:824:CLA:HMC3	30.92	0.40
1:E:127:LEU:HD12	1:E:127:LEU:H	1.86	0.40
1:E:219:HIS:O	1:E:223:PRO:HG2	2.21	0.40
1:E:207:GLY:N	1:E:305:PHE:HE2	2.19	0.40
12:E:805:CLA:CGD	12:E:805:CLA:HBA2	5.71	0.40
12:E:830:CLA:H2A	12:E:830:CLA:CED	2.51	0.40
2:G:130:ARG:HA	2:G:130:ARG:HD3	1.85	0.40
2:G:330:ILE:HG13	2:G:331:ASN:OD1	2.21	0.40
2:G:31:PHE:HA	2:G:34:HIS:CE1	2.56	0.40
7:I:17:LEU:O	7:I:20:PRO:HD2	2.21	0.40
11:M:38:VAL:HA	11:M:41:PHE:HB3	2.03	0.40
6:O:75:ILE:HD11	6:O:82:HIS:CD2	2.57	0.40
1:A:219:HIS:O	1:A:223:PRO:HG2	2.21	0.40
1:A:316:TRP:HZ3	12:A:810:CLA:HMA1	1.87	0.40
12:A:818:CLA:H3A	12:A:818:CLA:CGA	3.04	0.40
12:A:833:CLA:H3A	12:A:833:CLA:HBA2	3.75	0.40
2:B:130:ARG:HD3	2:B:130:ARG:HA	1.85	0.40
2:B:420:GLU:OE1	2:B:420:GLU:N	2.51	0.40
12:B:805:CLA:HED2	12:B:805:CLA:HBD	4.10	0.40
12:B:808:CLA:HMB1	12:B:808:CLA:HBB1	2.08	0.40
12:B:817:CLA:H3A	12:B:817:CLA:HBA1	1.55	0.40
12:B:819:CLA:HED2	12:B:819:CLA:H2A	2.03	0.40
4:D:105:PRO:HB2	4:D:108:VAL:HG22	5.56	0.40
1:E:154:THR:HG23	1:E:155:ASN:H	1.86	0.40
1:E:353:LEU:HD13	12:E:806:CLA:C1D	2.52	0.40
12:E:832:CLA:C1A	12:E:832:CLA:CGA	3.00	0.40
1:E:705:HIS:ND1	12:E:839:CLA:HBC1	67.64	0.40
6:F:119:LEU:HB3	6:F:123:ILE:HD12	2.02	0.40
2:G:29:HIS:N	2:G:29:HIS:CD2	2.90	0.40
2:G:404:ALA:O	2:G:408:LYS:N	2.55	0.40
2:G:230:TRP:CE3	12:G:817:CLA:HMB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:818:CLA:H2A	12:G:818:CLA:HED2	4.45	0.40
10:L:98:THR:HA	10:L:101:MET:HB2	2.03	0.40
10:L:24:SER:HB3	10:L:27:ASP:O	2.21	0.40
4:N:8:GLN:OE1	4:N:52:ARG:HG3	2.22	0.40
10:S:77:PRO:O	10:S:81:LEU:HB2	2.21	0.40
1:A:249:LEU:HD12	1:A:252:GLU:OE1	2.22	0.40
1:A:263:PRO:HB2	1:A:268:ASN:HB3	2.03	0.40
12:A:814:CLA:HBD	12:A:814:CLA:HED2	1.85	0.40
12:A:829:CLA:HMC3	12:A:836:CLA:HBB1	2.03	0.40
1:A:98:PHE:HB3	1:A:117:VAL:CG1	2.52	0.40
2:B:144:ILE:H	2:B:144:ILE:HG13	1.45	0.40
2:B:554:LYS:HG2	2:B:555:ASP:N	2.37	0.40
2:B:681:LEU:HD11	12:B:802:CLA:C3D	26.28	0.40
12:B:810:CLA:HBA2	12:B:810:CLA:H3A	3.49	0.40
12:B:810:CLA:HBB1	12:B:810:CLA:HMB1	2.03	0.40
1:E:249:LEU:HD12	1:E:252:GLU:OE1	2.22	0.40
1:E:648:ARG:HH22	2:G:639:ASN:HB3	1.87	0.40
12:E:808:CLA:H3A	12:E:808:CLA:HBA1	1.87	0.40
12:E:817:CLA:HED2	12:E:817:CLA:HBD	1.85	0.40
8:J:19:PRO:HB3	12:J:1101:CLA:C4D	2.51	0.40
4:N:98:HIS:CD2	4:N:99:PRO:HA	3.38	0.40
10:S:47:ILE:HA	10:S:47:ILE:HD12	1.98	0.40
1:A:154:THR:HG23	1:A:155:ASN:H	1.86	0.40
1:A:207:GLY:N	1:A:305:PHE:HE2	2.19	0.40
1:A:364:THR:HG22	12:A:827:CLA:HAC1	2.04	0.40
2:B:404:ALA:O	2:B:408:LYS:N	2.55	0.40
2:B:419:LYS:HZ1	6:F:164:ARG:HG3	2.45	0.40
2:B:576:TRP:HD1	2:B:580:TYR:CZ	2.40	0.40
2:B:639:ASN:OD1	2:B:642:GLY:N	2.40	0.40
2:B:703:MET:HG2	2:B:704:SER:N	2.37	0.40
2:B:435:PHE:CE1	12:B:801:CLA:H2	2.56	0.40
2:B:60:TRP:HZ2	12:B:831:CLA:OBD	2.05	0.40
3:C:12:GLY:HA2	3:C:27:MET:HE1	2.09	0.40
4:D:130:LYS:HE3	4:D:130:LYS:HA	4.53	0.40
1:E:351:ALA:O	1:E:355:THR:HG23	2.21	0.40
1:E:542:GLN:CG	1:E:602:THR:HG22	2.51	0.40
1:E:733:LEU:O	1:E:737:ILE:HG23	2.21	0.40
1:E:681:ALA:CB	12:E:802:CLA:HBB2	2.51	0.40
2:G:319:PHE:HE2	12:G:823:CLA:HMC3	1.87	0.40
2:G:8:PHE:CB	2:G:34:HIS:HD2	2.34	0.40
1:E:662:TYR:CZ	2:G:448:VAL:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:576:TRP:HD1	2:G:580:TYR:CZ	2.40	0.40
2:G:697:LYS:HB3	12:G:841:CLA:O1D	21.12	0.40
8:J:22:LEU:HA	8:J:22:LEU:HD12	1.87	0.40
2:B:688:THR:CG2	12:L:201:CLA:HHB	2.51	0.40
4:N:130:LYS:HD2	4:N:130:LYS:N	2.36	0.40
4:N:32:THR:O	4:N:83:TYR:HA	2.20	0.40
10:S:24:SER:N	10:S:27:ASP:O	2.50	0.40
12:G:814:CLA:OBD	10:S:42:LEU:HB2	75.80	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	A	726/752 (96%)	636 (88%)	90 (12%)	0	100	100
1	E	726/752 (96%)	636 (88%)	90 (12%)	0	100	100
1	a	726/752 (96%)	636 (88%)	90 (12%)	0	100	100
1	e	726/752 (96%)	636 (88%)	90 (12%)	0	100	100
2	B	732/737 (99%)	653 (89%)	78 (11%)	1 (0%)	53	88
2	G	732/737 (99%)	654 (89%)	77 (10%)	1 (0%)	53	88
2	b	732/737 (99%)	653 (89%)	78 (11%)	1 (0%)	53	88
2	g	732/737 (99%)	654 (89%)	77 (10%)	1 (0%)	53	88
3	C	79/82 (96%)	69 (87%)	9 (11%)	1 (1%)	13	53
3	H	79/82 (96%)	68 (86%)	10 (13%)	1 (1%)	13	53
3	c	79/82 (96%)	69 (87%)	9 (11%)	1 (1%)	13	53
3	h	79/82 (96%)	68 (86%)	10 (13%)	1 (1%)	13	53
4	D	135/168 (80%)	118 (87%)	17 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N	133/168 (79%)	116 (87%)	17 (13%)	0	100	100
4	d	133/168 (79%)	116 (87%)	17 (13%)	0	100	100
4	n	135/168 (80%)	118 (87%)	17 (13%)	0	100	100
5	V	59/126 (47%)	49 (83%)	10 (17%)	0	100	100
5	W	59/126 (47%)	49 (83%)	10 (17%)	0	100	100
5	v	59/126 (47%)	49 (83%)	10 (17%)	0	100	100
5	w	59/126 (47%)	49 (83%)	10 (17%)	0	100	100
6	F	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
6	O	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
6	f	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
6	o	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
7	I	37/39 (95%)	31 (84%)	6 (16%)	0	100	100
7	P	37/39 (95%)	31 (84%)	6 (16%)	0	100	100
7	i	37/39 (95%)	31 (84%)	6 (16%)	0	100	100
7	p	37/39 (95%)	31 (84%)	6 (16%)	0	100	100
8	J	35/49 (71%)	29 (83%)	6 (17%)	0	100	100
8	Q	35/49 (71%)	29 (83%)	6 (17%)	0	100	100
8	j	35/49 (71%)	29 (83%)	6 (17%)	0	100	100
8	q	35/49 (71%)	29 (83%)	6 (17%)	0	100	100
9	K	63/93 (68%)	46 (73%)	17 (27%)	0	100	100
9	R	63/93 (68%)	46 (73%)	17 (27%)	0	100	100
9	k	63/93 (68%)	46 (73%)	17 (27%)	0	100	100
9	r	63/93 (68%)	46 (73%)	17 (27%)	0	100	100
10	L	148/172 (86%)	124 (84%)	24 (16%)	0	100	100
10	S	148/172 (86%)	125 (84%)	23 (16%)	0	100	100
10	l	148/172 (86%)	125 (84%)	23 (16%)	0	100	100
10	s	148/172 (86%)	125 (84%)	23 (16%)	0	100	100
11	M	29/31 (94%)	22 (76%)	6 (21%)	1 (3%)	4	34
11	T	29/31 (94%)	22 (76%)	6 (21%)	1 (3%)	4	34
11	m	29/31 (94%)	22 (76%)	6 (21%)	1 (3%)	4	34
11	t	29/31 (94%)	22 (76%)	6 (21%)	1 (3%)	4	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8724/9652 (90%)	7619 (87%)	1093 (12%)	12 (0%)	56	88

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	LEU
11	M	23	ASP
3	H	62	LEU
11	T	23	ASP
3	h	62	LEU
11	t	23	ASP
3	c	62	LEU
11	m	23	ASP
2	G	564	GLY
2	b	564	GLY
2	B	564	GLY
2	g	564	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	578/601 (96%)	536 (93%)	42 (7%)	15	47
1	E	578/601 (96%)	536 (93%)	42 (7%)	15	47
1	a	578/601 (96%)	536 (93%)	42 (7%)	15	47
1	e	578/601 (96%)	536 (93%)	42 (7%)	15	47
2	B	594/595 (100%)	541 (91%)	53 (9%)	11	38
2	G	594/595 (100%)	541 (91%)	53 (9%)	11	38
2	b	594/595 (100%)	541 (91%)	53 (9%)	11	38
2	g	594/595 (100%)	541 (91%)	53 (9%)	11	38
3	C	68/70 (97%)	57 (84%)	11 (16%)	2	17
3	H	68/70 (97%)	57 (84%)	11 (16%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	68/70 (97%)	57 (84%)	11 (16%)	2	17
3	h	68/70 (97%)	57 (84%)	11 (16%)	2	17
4	D	113/137 (82%)	112 (99%)	1 (1%)	81	90
4	N	111/137 (81%)	111 (100%)	0	100	100
4	d	111/137 (81%)	111 (100%)	0	100	100
4	n	113/137 (82%)	112 (99%)	1 (1%)	81	90
5	V	54/102 (53%)	42 (78%)	12 (22%)	1	7
5	W	54/102 (53%)	42 (78%)	12 (22%)	1	7
5	v	54/102 (53%)	42 (78%)	12 (22%)	1	7
5	w	54/102 (53%)	42 (78%)	12 (22%)	1	7
6	F	116/135 (86%)	101 (87%)	15 (13%)	5	24
6	O	116/135 (86%)	101 (87%)	15 (13%)	5	24
6	f	116/135 (86%)	101 (87%)	15 (13%)	5	24
6	o	116/135 (86%)	101 (87%)	15 (13%)	5	24
7	I	33/33 (100%)	30 (91%)	3 (9%)	10	37
7	P	33/33 (100%)	30 (91%)	3 (9%)	10	37
7	i	33/33 (100%)	30 (91%)	3 (9%)	10	37
7	p	33/33 (100%)	30 (91%)	3 (9%)	10	37
8	J	34/45 (76%)	31 (91%)	3 (9%)	11	39
8	Q	34/45 (76%)	31 (91%)	3 (9%)	11	39
8	j	34/45 (76%)	31 (91%)	3 (9%)	11	39
8	q	34/45 (76%)	31 (91%)	3 (9%)	11	39
9	K	53/77 (69%)	44 (83%)	9 (17%)	2	15
9	R	53/77 (69%)	44 (83%)	9 (17%)	2	15
9	k	53/77 (69%)	44 (83%)	9 (17%)	2	15
9	r	53/77 (69%)	44 (83%)	9 (17%)	2	15
10	L	121/140 (86%)	110 (91%)	11 (9%)	10	37
10	S	121/140 (86%)	110 (91%)	11 (9%)	10	37
10	l	121/140 (86%)	110 (91%)	11 (9%)	10	37
10	s	121/140 (86%)	110 (91%)	11 (9%)	10	37
11	M	26/26 (100%)	18 (69%)	8 (31%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	T	26/26 (100%)	18 (69%)	8 (31%)	0	2
11	m	26/26 (100%)	18 (69%)	8 (31%)	0	2
11	t	26/26 (100%)	18 (69%)	8 (31%)	0	2
All	All	7156/7844 (91%)	6486 (91%)	670 (9%)	14	35

All (670) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	36	ASP
1	A	44	LYS
1	A	64	SER
1	A	83	VAL
1	A	91	MET
1	A	92	GLU
1	A	99	SER
1	A	141	THR
1	A	144	LEU
1	A	173	MET
1	A	189	GLU
1	A	208	LEU
1	A	242	GLU
1	A	249	LEU
1	A	289	LEU
1	A	304	LEU
1	A	322	ILE
1	A	325	ILE
1	A	357	LEU
1	A	365	ILE
1	A	371	MET
1	A	397	ILE
1	A	416	ASP
1	A	422	ASN
1	A	430	VAL
1	A	473	SER
1	A	493	LEU
1	A	546	THR
1	A	551	LEU
1	A	552	LYS
1	A	562	LEU
1	A	563	ILE

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Mol	Chain	Res	Type
1	A	569	LEU
1	A	580	ARG
1	A	613	LYS
1	A	649	ASP
1	A	658	VAL
1	A	659	ILE
1	A	674	LEU
1	A	683	SER
1	A	740	ILE
2	B	9	SER
2	B	19	ARG
2	B	37	MET
2	B	65	LEU
2	B	85	ARG
2	B	105	THR
2	B	113	VAL
2	B	118	SER
2	B	137	SER
2	B	142	LEU
2	B	144	ILE
2	B	148	VAL
2	B	155	LEU
2	B	166	SER
2	B	182	LEU
2	B	186	SER
2	B	195	VAL
2	B	216	LEU
2	B	223	ARG
2	B	273	MET
2	B	278	LEU
2	B	282	VAL
2	B	293	THR
2	B	301	ILE
2	B	309	ASN
2	B	321	LEU
2	B	348	ILE
2	B	375	LEU
2	B	386	LEU
2	B	387	MET
2	B	438	LEU
2	B	483	SER
2	B	491	THR

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Mol	Chain	Res	Type
2	B	497	LEU
2	B	504	ILE
2	B	530	ILE
2	B	538	VAL
2	B	543	ASP
2	B	552	ASP
2	B	553	LYS
2	B	560	PHE
2	B	583	LEU
2	B	602	LEU
2	B	609	VAL
2	B	611	GLN
2	B	619	LEU
2	B	620	MET
2	B	647	SER
2	B	693	LEU
2	B	701	VAL
2	B	713	LEU
2	B	723	THR
2	B	731	SER
3	C	22	THR
3	C	23	ASP
3	C	28	VAL
3	C	31	ASP
3	C	34	LYS
3	C	41	SER
3	C	47	CYS
3	C	63	SER
3	C	66	VAL
3	C	73	THR
3	C	77	MET
4	D	124	LYS
5	V	3	GLU
5	V	4	ARG
5	V	6	SER
5	V	7	LYS
5	V	11	LEU
5	V	13	LYS
5	V	21	VAL
5	V	23	VAL
5	V	27	VAL
5	V	29	LYS

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Mol	Chain	Res	Type
5	V	55	GLU
5	V	59	VAL
6	F	24	VAL
6	F	47	THR
6	F	48	THR
6	F	50	ASP
6	F	87	LEU
6	F	108	LEU
6	F	115	ASP
6	F	121	GLU
6	F	138	THR
6	F	141	LEU
6	F	147	LEU
6	F	148	LEU
6	F	152	LEU
6	F	155	LYS
6	F	157	ASP
7	I	19	PHE
7	I	26	LEU
7	I	33	ARG
8	J	9	ASN
8	J	17	LEU
8	J	20	VAL
9	K	35	ILE
9	K	36	LEU
9	K	52	MET
9	K	56	PHE
9	K	59	LEU
9	K	69	LEU
9	K	84	LEU
9	K	89	LEU
9	K	91	ILE
10	L	24	SER
10	L	33	LEU
10	L	41	SER
10	L	75	LEU
10	L	84	LEU
10	L	87	THR
10	L	92	ILE
10	L	96	LEU
10	L	123	THR
10	L	161	LEU

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Mol	Chain	Res	Type
10	L	163	ASN
11	M	19	MET
11	M	20	SER
11	M	21	ILE
11	M	22	SER
11	M	25	GLN
11	M	26	VAL
11	M	38	VAL
11	M	45	THR
1	E	25	SER
1	E	36	ASP
1	E	44	LYS
1	E	64	SER
1	E	83	VAL
1	E	91	MET
1	E	92	GLU
1	E	99	SER
1	E	141	THR
1	E	144	LEU
1	E	173	MET
1	E	189	GLU
1	E	208	LEU
1	E	242	GLU
1	E	249	LEU
1	E	289	LEU
1	E	304	LEU
1	E	322	ILE
1	E	325	ILE
1	E	357	LEU
1	E	365	ILE
1	E	371	MET
1	E	397	ILE
1	E	416	ASP
1	E	422	ASN
1	E	430	VAL
1	E	473	SER
1	E	493	LEU
1	E	546	THR
1	E	551	LEU
1	E	552	LYS
1	E	562	LEU
1	E	563	ILE

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Mol	Chain	Res	Type
1	E	569	LEU
1	E	580	ARG
1	E	613	LYS
1	E	649	ASP
1	E	658	VAL
1	E	659	ILE
1	E	674	LEU
1	E	683	SER
1	E	740	ILE
2	G	9	SER
2	G	19	ARG
2	G	37	MET
2	G	65	LEU
2	G	85	ARG
2	G	105	THR
2	G	113	VAL
2	G	118	SER
2	G	137	SER
2	G	142	LEU
2	G	144	ILE
2	G	148	VAL
2	G	155	LEU
2	G	166	SER
2	G	182	LEU
2	G	186	SER
2	G	195	VAL
2	G	216	LEU
2	G	223	ARG
2	G	273	MET
2	G	278	LEU
2	G	282	VAL
2	G	293	THR
2	G	301	ILE
2	G	309	ASN
2	G	321	LEU
2	G	348	ILE
2	G	375	LEU
2	G	386	LEU
2	G	387	MET
2	G	438	LEU
2	G	483	SER
2	G	491	THR

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Mol	Chain	Res	Type
2	G	497	LEU
2	G	504	ILE
2	G	530	ILE
2	G	538	VAL
2	G	543	ASP
2	G	552	ASP
2	G	553	LYS
2	G	560	PHE
2	G	583	LEU
2	G	602	LEU
2	G	609	VAL
2	G	611	GLN
2	G	619	LEU
2	G	620	MET
2	G	647	SER
2	G	693	LEU
2	G	701	VAL
2	G	713	LEU
2	G	723	THR
2	G	731	SER
3	H	22	THR
3	H	23	ASP
3	H	28	VAL
3	H	31	ASP
3	H	34	LYS
3	H	41	SER
3	H	47	CYS
3	H	63	SER
3	H	66	VAL
3	H	73	THR
3	H	77	MET
5	W	3	GLU
5	W	4	ARG
5	W	6	SER
5	W	7	LYS
5	W	11	LEU
5	W	13	LYS
5	W	21	VAL
5	W	23	VAL
5	W	27	VAL
5	W	29	LYS
5	W	55	GLU

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Mol	Chain	Res	Type
5	W	59	VAL
6	O	24	VAL
6	O	47	THR
6	O	48	THR
6	O	50	ASP
6	O	87	LEU
6	O	108	LEU
6	O	115	ASP
6	O	121	GLU
6	O	138	THR
6	O	141	LEU
6	O	147	LEU
6	O	148	LEU
6	O	152	LEU
6	O	155	LYS
6	O	157	ASP
7	P	19	PHE
7	P	26	LEU
7	P	33	ARG
8	Q	9	ASN
8	Q	17	LEU
8	Q	20	VAL
9	R	35	ILE
9	R	36	LEU
9	R	52	MET
9	R	56	PHE
9	R	59	LEU
9	R	69	LEU
9	R	84	LEU
9	R	89	LEU
9	R	91	ILE
10	S	24	SER
10	S	33	LEU
10	S	41	SER
10	S	75	LEU
10	S	84	LEU
10	S	87	THR
10	S	92	ILE
10	S	96	LEU
10	S	123	THR
10	S	161	LEU
10	S	163	ASN

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Mol	Chain	Res	Type
11	T	19	MET
11	T	20	SER
11	T	21	ILE
11	T	22	SER
11	T	25	GLN
11	T	26	VAL
11	T	38	VAL
11	T	45	THR
1	e	25	SER
1	e	36	ASP
1	e	44	LYS
1	e	64	SER
1	e	83	VAL
1	e	91	MET
1	e	92	GLU
1	e	99	SER
1	e	141	THR
1	e	144	LEU
1	e	173	MET
1	e	189	GLU
1	e	208	LEU
1	e	242	GLU
1	e	249	LEU
1	e	289	LEU
1	e	304	LEU
1	e	322	ILE
1	e	325	ILE
1	e	357	LEU
1	e	365	ILE
1	e	371	MET
1	e	397	ILE
1	e	416	ASP
1	e	422	ASN
1	e	430	VAL
1	e	473	SER
1	e	493	LEU
1	e	546	THR
1	e	551	LEU
1	e	552	LYS
1	e	562	LEU
1	e	563	ILE
1	e	569	LEU

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Mol	Chain	Res	Type
1	e	580	ARG
1	e	613	LYS
1	e	649	ASP
1	e	658	VAL
1	e	659	ILE
1	e	674	LEU
1	e	683	SER
1	e	740	ILE
2	g	9	SER
2	g	19	ARG
2	g	37	MET
2	g	65	LEU
2	g	85	ARG
2	g	105	THR
2	g	113	VAL
2	g	118	SER
2	g	137	SER
2	g	142	LEU
2	g	144	ILE
2	g	148	VAL
2	g	155	LEU
2	g	166	SER
2	g	182	LEU
2	g	186	SER
2	g	195	VAL
2	g	216	LEU
2	g	223	ARG
2	g	273	MET
2	g	278	LEU
2	g	282	VAL
2	g	293	THR
2	g	301	ILE
2	g	309	ASN
2	g	321	LEU
2	g	348	ILE
2	g	375	LEU
2	g	386	LEU
2	g	387	MET
2	g	438	LEU
2	g	483	SER
2	g	491	THR
2	g	497	LEU

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Mol	Chain	Res	Type
2	g	504	ILE
2	g	530	ILE
2	g	538	VAL
2	g	543	ASP
2	g	552	ASP
2	g	553	LYS
2	g	560	PHE
2	g	583	LEU
2	g	602	LEU
2	g	609	VAL
2	g	611	GLN
2	g	619	LEU
2	g	620	MET
2	g	647	SER
2	g	693	LEU
2	g	701	VAL
2	g	713	LEU
2	g	723	THR
2	g	731	SER
3	h	22	THR
3	h	23	ASP
3	h	28	VAL
3	h	31	ASP
3	h	34	LYS
3	h	41	SER
3	h	47	CYS
3	h	63	SER
3	h	66	VAL
3	h	73	THR
3	h	77	MET
4	n	124	LYS
5	v	3	GLU
5	v	4	ARG
5	v	6	SER
5	v	7	LYS
5	v	11	LEU
5	v	13	LYS
5	v	21	VAL
5	v	23	VAL
5	v	27	VAL
5	v	29	LYS
5	v	55	GLU

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Mol	Chain	Res	Type
5	v	59	VAL
6	o	24	VAL
6	o	47	THR
6	o	48	THR
6	o	50	ASP
6	o	87	LEU
6	o	108	LEU
6	o	115	ASP
6	o	121	GLU
6	o	138	THR
6	o	141	LEU
6	o	147	LEU
6	o	148	LEU
6	o	152	LEU
6	o	155	LYS
6	o	157	ASP
7	p	19	PHE
7	p	26	LEU
7	p	33	ARG
8	q	9	ASN
8	q	17	LEU
8	q	20	VAL
9	r	35	ILE
9	r	36	LEU
9	r	52	MET
9	r	56	PHE
9	r	59	LEU
9	r	69	LEU
9	r	84	LEU
9	r	89	LEU
9	r	91	ILE
10	s	24	SER
10	s	33	LEU
10	s	41	SER
10	s	75	LEU
10	s	84	LEU
10	s	87	THR
10	s	92	ILE
10	s	96	LEU
10	s	123	THR
10	s	161	LEU
10	s	163	ASN

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Mol	Chain	Res	Type
11	t	19	MET
11	t	20	SER
11	t	21	ILE
11	t	22	SER
11	t	25	GLN
11	t	26	VAL
11	t	38	VAL
11	t	45	THR
1	a	25	SER
1	a	36	ASP
1	a	44	LYS
1	a	64	SER
1	a	83	VAL
1	a	91	MET
1	a	92	GLU
1	a	99	SER
1	a	141	THR
1	a	144	LEU
1	a	173	MET
1	a	189	GLU
1	a	208	LEU
1	a	242	GLU
1	a	249	LEU
1	a	289	LEU
1	a	304	LEU
1	a	322	ILE
1	a	325	ILE
1	a	357	LEU
1	a	365	ILE
1	a	371	MET
1	a	397	ILE
1	a	416	ASP
1	a	422	ASN
1	a	430	VAL
1	a	473	SER
1	a	493	LEU
1	a	546	THR
1	a	551	LEU
1	a	552	LYS
1	a	562	LEU
1	a	563	ILE
1	a	569	LEU

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Mol	Chain	Res	Type
1	a	580	ARG
1	a	613	LYS
1	a	649	ASP
1	a	658	VAL
1	a	659	ILE
1	a	674	LEU
1	a	683	SER
1	a	740	ILE
2	b	9	SER
2	b	19	ARG
2	b	37	MET
2	b	65	LEU
2	b	85	ARG
2	b	105	THR
2	b	113	VAL
2	b	118	SER
2	b	137	SER
2	b	142	LEU
2	b	144	ILE
2	b	148	VAL
2	b	155	LEU
2	b	166	SER
2	b	182	LEU
2	b	186	SER
2	b	195	VAL
2	b	216	LEU
2	b	223	ARG
2	b	273	MET
2	b	278	LEU
2	b	282	VAL
2	b	293	THR
2	b	301	ILE
2	b	309	ASN
2	b	321	LEU
2	b	348	ILE
2	b	375	LEU
2	b	386	LEU
2	b	387	MET
2	b	438	LEU
2	b	483	SER
2	b	491	THR
2	b	497	LEU

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Mol	Chain	Res	Type
2	b	504	ILE
2	b	530	ILE
2	b	538	VAL
2	b	543	ASP
2	b	552	ASP
2	b	553	LYS
2	b	560	PHE
2	b	583	LEU
2	b	602	LEU
2	b	609	VAL
2	b	611	GLN
2	b	619	LEU
2	b	620	MET
2	b	647	SER
2	b	693	LEU
2	b	701	VAL
2	b	713	LEU
2	b	723	THR
2	b	731	SER
3	c	22	THR
3	c	23	ASP
3	c	28	VAL
3	c	31	ASP
3	c	34	LYS
3	c	41	SER
3	c	47	CYS
3	c	63	SER
3	c	66	VAL
3	c	73	THR
3	c	77	MET
5	w	3	GLU
5	w	4	ARG
5	w	6	SER
5	w	7	LYS
5	w	11	LEU
5	w	13	LYS
5	w	21	VAL
5	w	23	VAL
5	w	27	VAL
5	w	29	LYS
5	w	55	GLU
5	w	59	VAL

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Mol	Chain	Res	Type
6	f	24	VAL
6	f	47	THR
6	f	48	THR
6	f	50	ASP
6	f	87	LEU
6	f	108	LEU
6	f	115	ASP
6	f	121	GLU
6	f	138	THR
6	f	141	LEU
6	f	147	LEU
6	f	148	LEU
6	f	152	LEU
6	f	155	LYS
6	f	157	ASP
7	i	19	PHE
7	i	26	LEU
7	i	33	ARG
8	j	9	ASN
8	j	17	LEU
8	j	20	VAL
9	k	35	ILE
9	k	36	LEU
9	k	52	MET
9	k	56	PHE
9	k	59	LEU
9	k	69	LEU
9	k	84	LEU
9	k	89	LEU
9	k	91	ILE
10	l	24	SER
10	l	33	LEU
10	l	41	SER
10	l	75	LEU
10	l	84	LEU
10	l	87	THR
10	l	92	ILE
10	l	96	LEU
10	l	123	THR
10	l	161	LEU
10	l	163	ASN
11	m	19	MET

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Mol	Chain	Res	Type
11	m	20	SER
11	m	21	ILE
11	m	22	SER
11	m	25	GLN
11	m	26	VAL
11	m	38	VAL
11	m	45	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	77	HIS
1	A	80	GLN
1	A	116	GLN
1	A	128	ASN
1	A	216	HIS
1	A	219	HIS
1	A	369	HIS
1	A	422	ASN
1	A	433	HIS
1	A	463	GLN
1	A	615	GLN
1	A	654	GLN
2	B	53	HIS
2	B	106	GLN
2	B	133	ASN
2	B	193	HIS
2	B	262	HIS
2	B	275	HIS
2	B	354	GLN
2	B	355	HIS
2	B	367	GLN
2	B	407	ASN
2	B	443	HIS
2	B	505	ASN
2	B	506	ASN
2	B	611	GLN
2	B	636	ASN
4	D	56	ASN
4	D	98	HIS
4	D	109	ASN

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Mol	Chain	Res	Type
4	D	140	ASN
5	V	52	ASN
6	F	46	ASN
6	F	55	GLN
6	F	82	HIS
8	J	8	GLN
9	K	76	HIS
10	L	48	ASN
1	E	53	HIS
1	E	77	HIS
1	E	80	GLN
1	E	116	GLN
1	E	128	ASN
1	E	216	HIS
1	E	219	HIS
1	E	369	HIS
1	E	422	ASN
1	E	433	HIS
1	E	463	GLN
1	E	615	GLN
1	E	654	GLN
2	G	53	HIS
2	G	106	GLN
2	G	133	ASN
2	G	193	HIS
2	G	262	HIS
2	G	275	HIS
2	G	354	GLN
2	G	355	HIS
2	G	367	GLN
2	G	407	ASN
2	G	443	HIS
2	G	505	ASN
2	G	506	ASN
2	G	611	GLN
2	G	636	ASN
4	N	56	ASN
4	N	109	ASN
4	N	121	ASN
5	W	52	ASN
6	O	46	ASN
6	O	55	GLN

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Mol	Chain	Res	Type
6	O	82	HIS
8	Q	8	GLN
9	R	76	HIS
10	S	48	ASN
1	e	53	HIS
1	e	77	HIS
1	e	80	GLN
1	e	116	GLN
1	e	128	ASN
1	e	216	HIS
1	e	219	HIS
1	e	369	HIS
1	e	422	ASN
1	e	433	HIS
1	e	463	GLN
1	e	615	GLN
1	e	654	GLN
2	g	53	HIS
2	g	106	GLN
2	g	133	ASN
2	g	193	HIS
2	g	262	HIS
2	g	275	HIS
2	g	354	GLN
2	g	355	HIS
2	g	367	GLN
2	g	407	ASN
2	g	443	HIS
2	g	465	GLN
2	g	505	ASN
2	g	506	ASN
2	g	611	GLN
2	g	636	ASN
4	n	98	HIS
4	n	109	ASN
4	n	140	ASN
5	v	52	ASN
6	o	46	ASN
6	o	55	GLN
6	o	82	HIS
8	q	8	GLN
9	r	76	HIS

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Mol	Chain	Res	Type
10	s	48	ASN
1	a	53	HIS
1	a	77	HIS
1	a	80	GLN
1	a	116	GLN
1	a	128	ASN
1	a	216	HIS
1	a	219	HIS
1	a	369	HIS
1	a	422	ASN
1	a	433	HIS
1	a	463	GLN
1	a	615	GLN
1	a	654	GLN
2	b	53	HIS
2	b	106	GLN
2	b	133	ASN
2	b	193	HIS
2	b	262	HIS
2	b	275	HIS
2	b	354	GLN
2	b	355	HIS
2	b	367	GLN
2	b	407	ASN
2	b	443	HIS
2	b	505	ASN
2	b	506	ASN
2	b	611	GLN
2	b	636	ASN
4	d	56	ASN
4	d	121	ASN
5	w	52	ASN
6	f	46	ASN
6	f	55	GLN
6	f	82	HIS
9	k	76	HIS
10	l	48	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

382 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	CLA	A	801	-	42,58,73	1.14	4 (9%)	48,95,113	1.70	10 (20%)
12	CLA	A	802	-	42,58,73	1.17	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	A	803	-	42,58,73	1.19	5 (11%)	48,95,113	1.75	11 (22%)
12	CLA	A	804	1	42,58,73	1.18	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	A	805	1	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	A	806	1	42,58,73	1.19	4 (9%)	48,95,113	1.81	10 (20%)
12	CLA	A	807	1	42,58,73	1.16	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	A	808	-	34,53,73	1.27	4 (11%)	37,89,113	1.72	7 (18%)
12	CLA	A	809	-	42,58,73	1.18	5 (11%)	48,95,113	1.66	9 (18%)
12	CLA	A	810	1	42,58,73	1.14	4 (9%)	48,95,113	1.71	9 (18%)
12	CLA	A	811	1	42,58,73	1.18	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	A	812	-	34,53,73	1.29	5 (14%)	37,89,113	1.78	6 (16%)
12	CLA	A	813	-	34,53,73	1.26	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	A	814	1	41,57,73	1.18	4 (9%)	46,93,113	1.65	7 (15%)
12	CLA	A	815	1	42,58,73	1.17	5 (11%)	48,95,113	1.71	9 (18%)
12	CLA	A	816	1	42,58,73	1.14	4 (9%)	48,95,113	1.76	9 (18%)
12	CLA	A	817	-	42,58,73	1.18	4 (9%)	48,95,113	1.61	9 (18%)
12	CLA	A	818	-	42,58,73	1.19	5 (11%)	48,95,113	1.63	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	819	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	8 (16%)
12	CLA	A	820	1	41,57,73	1.16	4 (9%)	46,93,113	1.80	10 (21%)
12	CLA	A	821	1	42,58,73	1.18	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	A	822	1	42,58,73	1.18	4 (9%)	48,95,113	1.61	9 (18%)
12	CLA	A	823	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	A	824	-	42,58,73	1.20	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	A	825	-	42,58,73	1.15	4 (9%)	48,95,113	1.71	8 (16%)
12	CLA	A	826	1	42,58,73	1.16	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	A	827	-	42,58,73	1.19	5 (11%)	48,95,113	1.63	9 (18%)
12	CLA	A	828	1	42,58,73	1.16	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	A	829	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	9 (18%)
12	CLA	A	830	-	42,58,73	1.19	5 (11%)	48,95,113	1.62	8 (16%)
12	CLA	A	831	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	7 (14%)
12	CLA	A	832	1	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	A	833	-	34,53,73	1.28	5 (14%)	37,89,113	1.84	8 (21%)
12	CLA	A	834	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	A	835	-	42,58,73	1.21	6 (14%)	48,95,113	1.66	9 (18%)
12	CLA	A	836	-	39,55,73	1.22	5 (12%)	44,91,113	1.77	8 (18%)
12	CLA	A	837	-	42,58,73	1.18	4 (9%)	48,95,113	1.64	10 (20%)
12	CLA	A	838	-	42,58,73	1.17	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	A	839	-	42,58,73	1.21	5 (11%)	48,95,113	1.68	8 (16%)
12	CLA	A	840	-	30,49,73	1.31	4 (13%)	31,83,113	1.89	7 (22%)
12	CLA	A	841	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
13	PQN	A	842	-	34,34,34	1.73	5 (14%)	42,45,45	1.29	6 (14%)
12	CLA	B	801	-	42,58,73	1.16	5 (11%)	48,95,113	1.80	10 (20%)
12	CLA	B	802	-	42,58,73	1.18	5 (11%)	48,95,113	1.72	9 (18%)
12	CLA	B	803	-	42,58,73	1.20	6 (14%)	48,95,113	1.67	9 (18%)
14	SF4	B	804	-	0,12,12	0.00	-	-	-	-
12	CLA	B	805	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	B	806	-	42,58,73	1.20	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	B	807	-	42,58,73	1.17	5 (11%)	48,95,113	1.78	11 (22%)
12	CLA	B	808	2	42,58,73	1.16	4 (9%)	48,95,113	1.77	10 (20%)
12	CLA	B	809	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	B	810	-	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	B	811	-	42,58,73	1.18	4 (9%)	48,95,113	1.67	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	812	-	42,58,73	1.16	5 (11%)	48,95,113	1.72	9 (18%)
12	CLA	B	813	2	42,58,73	1.18	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	B	814	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	B	815	-	34,53,73	1.28	4 (11%)	37,89,113	1.70	7 (18%)
12	CLA	B	816	-	34,53,73	1.26	4 (11%)	37,89,113	1.78	7 (18%)
12	CLA	B	817	2	42,58,73	1.17	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	B	818	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	B	819	2	34,53,73	1.27	5 (14%)	37,89,113	1.75	7 (18%)
12	CLA	B	820	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	B	821	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	8 (16%)
12	CLA	B	822	-	42,58,73	1.18	5 (11%)	48,95,113	1.71	8 (16%)
12	CLA	B	823	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	B	824	2	39,55,73	1.22	5 (12%)	44,91,113	1.73	7 (15%)
12	CLA	B	825	-	34,53,73	1.27	4 (11%)	37,89,113	1.83	8 (21%)
12	CLA	B	826	2	42,58,73	1.19	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	B	827	-	34,53,73	1.28	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	B	828	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	B	829	-	38,54,73	1.21	4 (10%)	43,90,113	1.75	7 (16%)
12	CLA	B	830	-	42,58,73	1.18	5 (11%)	48,95,113	1.60	8 (16%)
12	CLA	B	831	2	42,58,73	1.18	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	B	832	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	B	833	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	B	834	-	34,53,73	1.26	4 (11%)	37,89,113	1.69	7 (18%)
12	CLA	B	835	-	41,57,73	1.19	5 (12%)	46,93,113	1.61	8 (17%)
12	CLA	B	836	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	B	837	2	34,53,73	1.30	5 (14%)	37,89,113	1.76	8 (21%)
12	CLA	B	838	-	34,53,73	1.27	4 (11%)	37,89,113	1.82	7 (18%)
12	CLA	B	839	-	42,58,73	1.20	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	B	840	-	42,58,73	1.17	4 (9%)	48,95,113	1.75	9 (18%)
12	CLA	B	841	-	39,55,73	1.21	5 (12%)	44,91,113	1.81	7 (15%)
12	CLA	B	842	-	42,58,73	1.20	5 (11%)	48,95,113	1.77	9 (18%)
12	CLA	B	843	-	42,58,73	1.21	5 (11%)	48,95,113	1.60	8 (16%)
13	PQN	B	844	-	34,34,34	1.70	5 (14%)	42,45,45	1.19	2 (4%)
14	SF4	C	101	-	0,12,12	0.00	-	-	-	-
14	SF4	C	102	3	0,12,12	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	E	801	-	42,58,73	1.14	4 (9%)	48,95,113	1.71	10 (20%)
12	CLA	E	802	-	42,58,73	1.16	5 (11%)	48,95,113	1.80	10 (20%)
12	CLA	E	803	-	42,58,73	1.18	5 (11%)	48,95,113	1.73	10 (20%)
12	CLA	E	804	-	42,58,73	1.20	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	E	805	-	42,58,73	1.17	5 (11%)	48,95,113	1.69	8 (16%)
12	CLA	E	806	-	42,58,73	1.18	5 (11%)	48,95,113	1.75	11 (22%)
12	CLA	E	807	1	42,58,73	1.18	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	E	808	1	42,58,73	1.16	4 (9%)	48,95,113	1.71	8 (16%)
12	CLA	E	809	1	42,58,73	1.19	4 (9%)	48,95,113	1.80	10 (20%)
12	CLA	E	810	1	42,58,73	1.16	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	E	811	-	34,53,73	1.27	4 (11%)	37,89,113	1.71	7 (18%)
12	CLA	E	812	-	42,58,73	1.18	5 (11%)	48,95,113	1.66	8 (16%)
12	CLA	E	813	1	42,58,73	1.14	4 (9%)	48,95,113	1.72	9 (18%)
12	CLA	E	814	1	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	E	815	-	34,53,73	1.29	5 (14%)	37,89,113	1.77	7 (18%)
12	CLA	E	816	-	34,53,73	1.26	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	E	817	1	41,57,73	1.18	4 (9%)	46,93,113	1.63	7 (15%)
12	CLA	E	818	1	42,58,73	1.18	5 (11%)	48,95,113	1.72	9 (18%)
12	CLA	E	819	1	42,58,73	1.15	4 (9%)	48,95,113	1.75	9 (18%)
12	CLA	E	820	-	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	E	821	-	42,58,73	1.18	5 (11%)	48,95,113	1.62	8 (16%)
12	CLA	E	822	-	42,58,73	1.20	5 (11%)	48,95,113	1.64	8 (16%)
12	CLA	E	823	1	41,57,73	1.16	4 (9%)	46,93,113	1.80	10 (21%)
12	CLA	E	824	1	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	E	825	1	42,58,73	1.18	4 (9%)	48,95,113	1.60	9 (18%)
12	CLA	E	826	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	E	827	-	42,58,73	1.20	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	E	828	-	42,58,73	1.15	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	E	829	1	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	E	830	-	42,58,73	1.20	5 (11%)	48,95,113	1.63	9 (18%)
12	CLA	E	831	1	42,58,73	1.16	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	E	832	-	42,58,73	1.19	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	E	833	-	42,58,73	1.17	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	E	834	-	42,58,73	1.19	5 (11%)	48,95,113	1.63	8 (16%)
12	CLA	E	835	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	E	836	1	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	E	837	-	34,53,73	1.28	5 (14%)	37,89,113	1.82	8 (21%)
12	CLA	E	838	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	E	839	-	42,58,73	1.21	6 (14%)	48,95,113	1.66	9 (18%)
12	CLA	E	840	-	39,55,73	1.21	6 (15%)	44,91,113	1.76	8 (18%)
12	CLA	E	841	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	10 (20%)
12	CLA	E	842	-	42,58,73	1.17	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	E	843	-	42,58,73	1.20	5 (11%)	48,95,113	1.67	8 (16%)
12	CLA	E	844	-	30,49,73	1.31	4 (13%)	31,83,113	1.89	7 (22%)
14	SF4	E	845	-	0,12,12	0.00	-	-	-	-
13	PQN	E	846	-	34,34,34	1.69	5 (14%)	42,45,45	1.32	7 (16%)
12	CLA	F	1301	-	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	G	801	-	42,58,73	1.20	5 (11%)	48,95,113	1.67	9 (18%)
12	CLA	G	802	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	G	803	-	42,58,73	1.20	4 (9%)	48,95,113	1.61	9 (18%)
12	CLA	G	804	-	42,58,73	1.17	5 (11%)	48,95,113	1.77	11 (22%)
12	CLA	G	805	2	42,58,73	1.15	4 (9%)	48,95,113	1.77	10 (20%)
12	CLA	G	806	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	G	807	-	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	G	808	-	42,58,73	1.18	4 (9%)	48,95,113	1.67	9 (18%)
12	CLA	G	809	-	42,58,73	1.17	5 (11%)	48,95,113	1.73	9 (18%)
12	CLA	G	810	2	42,58,73	1.18	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	G	811	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	G	812	-	34,53,73	1.28	4 (11%)	37,89,113	1.69	7 (18%)
12	CLA	G	813	-	34,53,73	1.26	4 (11%)	37,89,113	1.78	7 (18%)
12	CLA	G	814	2	42,58,73	1.16	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	G	815	2	42,58,73	1.17	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	G	816	2	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	G	817	-	42,58,73	1.19	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	G	818	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	G	819	-	42,58,73	1.19	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	G	820	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	G	821	2	39,55,73	1.22	5 (12%)	44,91,113	1.74	7 (15%)
12	CLA	G	822	-	34,53,73	1.26	4 (11%)	37,89,113	1.82	8 (21%)
12	CLA	G	823	2	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	G	824	-	34,53,73	1.27	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	G	825	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	G	826	-	38,54,73	1.21	4 (10%)	43,90,113	1.76	7 (16%)
12	CLA	G	827	-	42,58,73	1.17	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	G	828	2	42,58,73	1.18	5 (11%)	48,95,113	1.62	8 (16%)
12	CLA	G	829	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	G	830	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	G	831	-	34,53,73	1.26	4 (11%)	37,89,113	1.68	7 (18%)
12	CLA	G	832	-	41,57,73	1.19	5 (12%)	46,93,113	1.61	8 (17%)
12	CLA	G	833	-	42,58,73	1.19	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	G	834	-	42,58,73	1.16	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	G	835	2	34,53,73	1.30	5 (14%)	37,89,113	1.76	8 (21%)
12	CLA	G	836	-	34,53,73	1.27	4 (11%)	37,89,113	1.83	7 (18%)
12	CLA	G	837	-	42,58,73	1.19	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	G	838	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	G	839	-	39,55,73	1.21	4 (10%)	44,91,113	1.80	8 (18%)
12	CLA	G	840	-	42,58,73	1.19	4 (9%)	48,95,113	1.76	9 (18%)
12	CLA	G	841	-	42,58,73	1.20	5 (11%)	48,95,113	1.62	8 (16%)
13	PQN	G	842	-	34,34,34	1.71	5 (14%)	42,45,45	1.19	2 (4%)
12	CLA	G	843	10	42,58,73	1.18	4 (9%)	48,95,113	1.73	8 (16%)
14	SF4	H	101	-	0,12,12	0.00	-	-		
14	SF4	H	102	3	0,12,12	0.00	-	-		
12	CLA	J	1101	-	42,58,73	1.19	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	J	1102	-	42,58,73	1.15	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	K	1401	-	34,53,73	1.24	4 (11%)	37,89,113	1.86	8 (21%)
12	CLA	L	201	-	42,58,73	1.17	5 (11%)	48,95,113	1.68	9 (18%)
12	CLA	L	202	-	42,58,73	1.17	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	L	203	10	42,58,73	1.18	4 (9%)	48,95,113	1.73	8 (16%)
12	CLA	L	204	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	O	1301	-	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	R	1401	-	34,53,73	1.25	4 (11%)	37,89,113	1.86	8 (21%)
12	CLA	S	1501	-	42,58,73	1.17	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	S	1502	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	a	801	-	42,58,73	1.14	4 (9%)	48,95,113	1.70	10 (20%)
12	CLA	a	802	-	42,58,73	1.16	5 (11%)	48,95,113	1.80	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	803	-	42,58,73	1.19	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	a	804	-	42,58,73	1.17	5 (11%)	48,95,113	1.68	8 (16%)
12	CLA	a	805	-	42,58,73	1.18	5 (11%)	48,95,113	1.75	11 (22%)
12	CLA	a	806	1	42,58,73	1.18	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	a	807	1	42,58,73	1.16	4 (9%)	48,95,113	1.70	8 (16%)
12	CLA	a	808	1	42,58,73	1.18	4 (9%)	48,95,113	1.79	10 (20%)
12	CLA	a	809	1	42,58,73	1.17	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	a	810	-	34,53,73	1.27	4 (11%)	37,89,113	1.71	7 (18%)
12	CLA	a	811	-	42,58,73	1.18	5 (11%)	48,95,113	1.66	8 (16%)
12	CLA	a	812	1	42,58,73	1.13	4 (9%)	48,95,113	1.71	9 (18%)
12	CLA	a	813	1	42,58,73	1.18	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	a	814	-	34,53,73	1.29	5 (14%)	37,89,113	1.78	6 (16%)
12	CLA	a	815	-	34,53,73	1.26	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	a	816	1	41,57,73	1.18	4 (9%)	46,93,113	1.63	7 (15%)
12	CLA	a	817	1	42,58,73	1.18	5 (11%)	48,95,113	1.71	9 (18%)
12	CLA	a	818	1	42,58,73	1.14	4 (9%)	48,95,113	1.76	9 (18%)
12	CLA	a	819	-	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	a	820	-	42,58,73	1.18	5 (11%)	48,95,113	1.63	8 (16%)
12	CLA	a	821	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	8 (16%)
12	CLA	a	822	1	41,57,73	1.16	4 (9%)	46,93,113	1.80	10 (21%)
12	CLA	a	823	1	42,58,73	1.17	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	a	824	1	42,58,73	1.18	4 (9%)	48,95,113	1.61	9 (18%)
12	CLA	a	825	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	a	826	-	42,58,73	1.20	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	a	827	-	42,58,73	1.15	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	a	828	1	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	a	829	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	9 (18%)
12	CLA	a	830	1	42,58,73	1.16	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	a	831	-	42,58,73	1.19	5 (11%)	48,95,113	1.66	9 (18%)
12	CLA	a	832	-	42,58,73	1.20	5 (11%)	48,95,113	1.63	8 (16%)
12	CLA	a	833	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	7 (14%)
12	CLA	a	834	1	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	a	835	-	34,53,73	1.28	5 (14%)	37,89,113	1.83	8 (21%)
12	CLA	a	836	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	a	837	-	42,58,73	1.21	6 (14%)	48,95,113	1.65	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	838	-	39,55,73	1.21	5 (12%)	44,91,113	1.76	8 (18%)
12	CLA	a	839	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	10 (20%)
12	CLA	a	840	-	42,58,73	1.17	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	a	841	-	42,58,73	1.21	5 (11%)	48,95,113	1.69	8 (16%)
12	CLA	a	842	-	30,49,73	1.31	4 (13%)	31,83,113	1.92	7 (22%)
14	SF4	a	843	-	0,12,12	0.00	-	-		
13	PQN	a	844	-	34,34,34	1.68	5 (14%)	42,45,45	1.33	8 (19%)
12	CLA	b	801	-	42,58,73	1.17	5 (11%)	48,95,113	1.72	10 (20%)
12	CLA	b	802	-	42,58,73	1.20	6 (14%)	48,95,113	1.67	9 (18%)
12	CLA	b	803	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	b	804	-	42,58,73	1.20	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	b	805	-	42,58,73	1.18	5 (11%)	48,95,113	1.79	11 (22%)
12	CLA	b	806	2	42,58,73	1.16	4 (9%)	48,95,113	1.78	10 (20%)
12	CLA	b	807	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	b	808	-	42,58,73	1.17	4 (9%)	48,95,113	1.71	8 (16%)
12	CLA	b	809	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	b	810	-	42,58,73	1.17	5 (11%)	48,95,113	1.73	9 (18%)
12	CLA	b	811	2	42,58,73	1.18	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	b	812	-	42,58,73	1.18	4 (9%)	48,95,113	1.64	9 (18%)
12	CLA	b	813	-	34,53,73	1.28	4 (11%)	37,89,113	1.69	6 (16%)
12	CLA	b	814	-	34,53,73	1.26	4 (11%)	37,89,113	1.78	7 (18%)
12	CLA	b	815	2	42,58,73	1.17	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	b	816	2	42,58,73	1.17	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	b	817	2	34,53,73	1.26	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	b	818	-	42,58,73	1.19	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	b	819	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	b	820	-	42,58,73	1.18	5 (11%)	48,95,113	1.72	8 (16%)
12	CLA	b	821	-	42,58,73	1.18	4 (9%)	48,95,113	1.67	9 (18%)
12	CLA	b	822	2	39,55,73	1.22	5 (12%)	44,91,113	1.75	7 (15%)
12	CLA	b	823	-	34,53,73	1.27	4 (11%)	37,89,113	1.82	7 (18%)
12	CLA	b	824	2	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	b	825	-	34,53,73	1.27	4 (11%)	37,89,113	1.79	7 (18%)
12	CLA	b	826	-	42,58,73	1.19	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	b	827	-	38,54,73	1.22	4 (10%)	43,90,113	1.75	7 (16%)
12	CLA	b	828	-	42,58,73	1.17	4 (9%)	48,95,113	1.60	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	b	829	2	42,58,73	1.18	5 (11%)	48,95,113	1.61	8 (16%)
12	CLA	b	830	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	b	831	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	9 (18%)
12	CLA	b	832	-	34,53,73	1.26	4 (11%)	37,89,113	1.70	7 (18%)
12	CLA	b	833	-	41,57,73	1.19	5 (12%)	46,93,113	1.60	8 (17%)
12	CLA	b	834	-	42,58,73	1.19	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	b	835	-	42,58,73	1.16	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	b	836	2	34,53,73	1.30	5 (14%)	37,89,113	1.77	8 (21%)
12	CLA	b	837	-	34,53,73	1.28	4 (11%)	37,89,113	1.82	7 (18%)
12	CLA	b	838	-	42,58,73	1.19	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	b	839	-	42,58,73	1.17	4 (9%)	48,95,113	1.75	9 (18%)
12	CLA	b	840	-	39,55,73	1.21	5 (12%)	44,91,113	1.81	8 (18%)
12	CLA	b	841	-	42,58,73	1.20	4 (9%)	48,95,113	1.77	10 (20%)
12	CLA	b	842	-	42,58,73	1.20	6 (14%)	48,95,113	1.61	8 (16%)
13	PQN	b	843	-	34,34,34	1.71	5 (14%)	42,45,45	1.20	2 (4%)
14	SF4	c	101	-	0,12,12	0.00	-	-	-	-
14	SF4	c	102	3	0,12,12	0.00	-	-	-	-
12	CLA	e	801	-	42,58,73	1.14	4 (9%)	48,95,113	1.71	10 (20%)
12	CLA	e	802	-	42,58,73	1.19	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	e	803	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	8 (16%)
12	CLA	e	804	-	42,58,73	1.18	5 (11%)	48,95,113	1.75	11 (22%)
12	CLA	e	805	1	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	e	806	1	42,58,73	1.16	4 (9%)	48,95,113	1.71	8 (16%)
12	CLA	e	807	1	42,58,73	1.18	4 (9%)	48,95,113	1.80	10 (20%)
12	CLA	e	808	1	42,58,73	1.17	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	e	809	-	34,53,73	1.27	4 (11%)	37,89,113	1.72	7 (18%)
12	CLA	e	810	-	42,58,73	1.19	5 (11%)	48,95,113	1.67	8 (16%)
12	CLA	e	811	1	42,58,73	1.14	4 (9%)	48,95,113	1.72	9 (18%)
12	CLA	e	812	1	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	e	813	-	34,53,73	1.29	5 (14%)	37,89,113	1.77	7 (18%)
12	CLA	e	814	-	34,53,73	1.26	4 (11%)	37,89,113	1.79	7 (18%)
12	CLA	e	815	1	41,57,73	1.18	4 (9%)	46,93,113	1.65	7 (15%)
12	CLA	e	816	1	42,58,73	1.17	5 (11%)	48,95,113	1.70	9 (18%)
12	CLA	e	817	1	42,58,73	1.15	4 (9%)	48,95,113	1.76	9 (18%)
12	CLA	e	818	-	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	e	819	-	42,58,73	1.19	5 (11%)	48,95,113	1.63	8 (16%)
12	CLA	e	820	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	8 (16%)
12	CLA	e	821	1	41,57,73	1.16	4 (9%)	46,93,113	1.81	10 (21%)
12	CLA	e	822	1	42,58,73	1.17	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	e	823	1	42,58,73	1.18	4 (9%)	48,95,113	1.60	9 (18%)
12	CLA	e	824	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	e	825	-	42,58,73	1.20	5 (11%)	48,95,113	1.68	8 (16%)
12	CLA	e	826	-	42,58,73	1.15	4 (9%)	48,95,113	1.69	8 (16%)
12	CLA	e	827	1	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	e	828	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	9 (18%)
12	CLA	e	829	1	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	e	830	-	42,58,73	1.19	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	e	831	-	42,58,73	1.19	5 (11%)	48,95,113	1.62	8 (16%)
12	CLA	e	832	-	42,58,73	1.16	4 (9%)	48,95,113	1.66	7 (14%)
12	CLA	e	833	1	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	e	834	-	34,53,73	1.28	5 (14%)	37,89,113	1.83	8 (21%)
12	CLA	e	835	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	e	836	-	42,58,73	1.21	6 (14%)	48,95,113	1.66	9 (18%)
12	CLA	e	837	-	39,55,73	1.22	5 (12%)	44,91,113	1.77	8 (18%)
12	CLA	e	838	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	10 (20%)
12	CLA	e	839	-	42,58,73	1.17	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	e	840	-	42,58,73	1.21	5 (11%)	48,95,113	1.67	8 (16%)
12	CLA	e	841	-	30,49,73	1.31	4 (13%)	31,83,113	1.88	7 (22%)
12	CLA	e	842	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	9 (18%)
13	PQN	e	843	-	34,34,34	1.73	5 (14%)	42,45,45	1.28	5 (11%)
12	CLA	e	844	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	e	845	-	41,57,73	1.19	5 (12%)	46,93,113	1.60	8 (17%)
12	CLA	f	1301	-	34,53,73	1.28	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	g	801	-	42,58,73	1.16	5 (11%)	48,95,113	1.80	10 (20%)
12	CLA	g	802	-	42,58,73	1.17	5 (11%)	48,95,113	1.72	9 (18%)
12	CLA	g	803	-	42,58,73	1.20	6 (14%)	48,95,113	1.67	9 (18%)
14	SF4	g	804	-	0,12,12	0.00	-	-	-	-
12	CLA	g	805	-	42,58,73	1.20	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	g	806	-	42,58,73	1.17	5 (11%)	48,95,113	1.79	11 (22%)
12	CLA	g	807	2	42,58,73	1.15	4 (9%)	48,95,113	1.77	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	g	808	-	42,58,73	1.19	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	g	809	-	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	g	810	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	g	811	-	42,58,73	1.17	5 (11%)	48,95,113	1.72	9 (18%)
12	CLA	g	812	2	42,58,73	1.18	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	g	813	-	42,58,73	1.19	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	g	814	-	34,53,73	1.28	4 (11%)	37,89,113	1.69	6 (16%)
12	CLA	g	815	-	34,53,73	1.26	4 (11%)	37,89,113	1.78	7 (18%)
12	CLA	g	816	2	42,58,73	1.17	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	g	817	2	42,58,73	1.17	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	g	818	2	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	g	819	-	42,58,73	1.19	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	g	820	-	42,58,73	1.19	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	g	821	-	42,58,73	1.18	5 (11%)	48,95,113	1.72	8 (16%)
12	CLA	g	822	-	42,58,73	1.18	4 (9%)	48,95,113	1.67	9 (18%)
12	CLA	g	823	2	39,55,73	1.22	5 (12%)	44,91,113	1.73	7 (15%)
12	CLA	g	824	-	34,53,73	1.27	4 (11%)	37,89,113	1.82	8 (21%)
12	CLA	g	825	2	42,58,73	1.18	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	g	826	-	34,53,73	1.27	5 (14%)	37,89,113	1.80	7 (18%)
12	CLA	g	827	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	g	828	-	38,54,73	1.22	4 (10%)	43,90,113	1.76	7 (16%)
12	CLA	g	829	-	42,58,73	1.17	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	g	830	2	42,58,73	1.17	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	g	831	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	g	832	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	g	833	-	34,53,73	1.26	4 (11%)	37,89,113	1.69	7 (18%)
12	CLA	g	834	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	g	835	-	42,58,73	1.16	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	g	836	2	34,53,73	1.30	5 (14%)	37,89,113	1.76	8 (21%)
12	CLA	g	837	-	34,53,73	1.27	4 (11%)	37,89,113	1.82	7 (18%)
12	CLA	g	838	-	42,58,73	1.20	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	g	839	-	42,58,73	1.17	4 (9%)	48,95,113	1.75	9 (18%)
12	CLA	g	840	-	39,55,73	1.21	4 (10%)	44,91,113	1.80	8 (18%)
12	CLA	g	841	-	42,58,73	1.20	4 (9%)	48,95,113	1.76	10 (20%)
12	CLA	g	842	-	42,58,73	1.20	5 (11%)	48,95,113	1.60	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PQN	g	843	-	34,34,34	1.71	5 (14%)	42,45,45	1.19	2 (4%)
14	SF4	h	101	-	0,12,12	0.00	-	-		
14	SF4	h	102	3	0,12,12	0.00	-	-		
12	CLA	k	1401	-	34,53,73	1.25	4 (11%)	37,89,113	1.85	8 (21%)
12	CLA	l	201	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	l	202	-	42,58,73	1.18	5 (11%)	48,95,113	1.66	9 (18%)
12	CLA	l	203	10	42,58,73	1.18	4 (9%)	48,95,113	1.73	8 (16%)
12	CLA	l	204	-	42,58,73	1.17	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	o	1301	-	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	r	1401	-	34,53,73	1.25	4 (11%)	37,89,113	1.84	7 (18%)
12	CLA	s	201	-	42,58,73	1.17	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	s	202	-	42,58,73	1.18	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	s	203	10	42,58,73	1.17	4 (9%)	48,95,113	1.73	8 (16%)
12	CLA	s	204	-	42,58,73	1.17	4 (9%)	48,95,113	1.65	9 (18%)

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
12	CLA	A	801	-	3/3/17/25	8/19/117/135	-
12	CLA	A	802	-	3/3/17/25	5/19/117/135	-
12	CLA	A	803	-	3/3/17/25	8/19/117/135	-
12	CLA	A	804	1	3/3/17/25	2/19/117/135	-
12	CLA	A	805	1	2/2/17/25	10/19/117/135	-
12	CLA	A	806	1	3/3/17/25	8/19/117/135	-
12	CLA	A	807	1	3/3/17/25	8/19/117/135	-
12	CLA	A	808	-	3/3/16/25	5/11/111/135	-
12	CLA	A	809	-	3/3/17/25	6/19/117/135	-
12	CLA	A	810	1	3/3/17/25	3/19/117/135	-
12	CLA	A	811	1	3/3/17/25	4/19/117/135	-
12	CLA	A	812	-	3/3/16/25	9/11/111/135	-
12	CLA	A	813	-	3/3/16/25	6/11/111/135	-
12	CLA	A	814	1	3/3/16/25	8/18/116/135	-
12	CLA	A	815	1	3/3/17/25	5/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	816	1	3/3/17/25	6/19/117/135	-
12	CLA	A	817	-	3/3/17/25	9/19/117/135	-
12	CLA	A	818	-	3/3/17/25	7/19/117/135	-
12	CLA	A	819	-	3/3/17/25	6/19/117/135	-
12	CLA	A	820	1	3/3/16/25	7/18/116/135	-
12	CLA	A	821	1	3/3/17/25	8/19/117/135	-
12	CLA	A	822	1	3/3/17/25	8/19/117/135	-
12	CLA	A	823	-	3/3/17/25	9/19/117/135	-
12	CLA	A	824	-	3/3/17/25	7/19/117/135	-
12	CLA	A	825	-	3/3/17/25	9/19/117/135	-
12	CLA	A	826	1	3/3/17/25	8/19/117/135	-
12	CLA	A	827	-	3/3/17/25	8/19/117/135	-
12	CLA	A	828	1	3/3/17/25	8/19/117/135	-
12	CLA	A	829	-	2/2/17/25	9/19/117/135	-
12	CLA	A	830	-	3/3/17/25	8/19/117/135	-
12	CLA	A	831	-	3/3/17/25	7/19/117/135	-
12	CLA	A	832	1	3/3/17/25	6/19/117/135	-
12	CLA	A	833	-	3/3/16/25	7/11/111/135	-
12	CLA	A	834	-	3/3/17/25	6/19/117/135	-
12	CLA	A	835	-	3/3/17/25	3/19/117/135	-
12	CLA	A	836	-	3/3/16/25	6/16/114/135	-
12	CLA	A	837	-	2/2/17/25	4/19/117/135	-
12	CLA	A	838	-	3/3/17/25	8/19/117/135	-
12	CLA	A	839	-	3/3/17/25	3/19/117/135	-
12	CLA	A	840	-	3/3/14/25	1/5/101/135	-
12	CLA	A	841	-	3/3/17/25	8/19/117/135	-
13	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
12	CLA	B	801	-	3/3/17/25	8/19/117/135	-
12	CLA	B	802	-	3/3/17/25	2/19/117/135	-
12	CLA	B	803	-	3/3/17/25	5/19/117/135	-
14	SF4	B	804	-	-	-	0/6/5/5
12	CLA	B	805	-	3/3/17/25	9/19/117/135	-
12	CLA	B	806	-	3/3/17/25	6/19/117/135	-
12	CLA	B	807	-	3/3/17/25	9/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	808	2	3/3/17/25	9/19/117/135	-
12	CLA	B	809	-	3/3/17/25	7/19/117/135	-
12	CLA	B	810	-	3/3/17/25	4/19/117/135	-
12	CLA	B	811	-	3/3/17/25	6/19/117/135	-
12	CLA	B	812	-	3/3/17/25	6/19/117/135	-
12	CLA	B	813	2	3/3/17/25	7/19/117/135	-
12	CLA	B	814	-	3/3/17/25	10/19/117/135	-
12	CLA	B	815	-	3/3/16/25	6/11/111/135	-
12	CLA	B	816	-	3/3/16/25	4/11/111/135	-
12	CLA	B	817	2	3/3/17/25	10/19/117/135	-
12	CLA	B	818	2	3/3/17/25	7/19/117/135	-
12	CLA	B	819	2	3/3/16/25	4/11/111/135	-
12	CLA	B	820	-	3/3/17/25	6/19/117/135	-
12	CLA	B	821	-	3/3/17/25	13/19/117/135	-
12	CLA	B	822	-	3/3/17/25	8/19/117/135	-
12	CLA	B	823	-	3/3/17/25	6/19/117/135	-
12	CLA	B	824	2	3/3/16/25	7/16/114/135	-
12	CLA	B	825	-	3/3/16/25	3/11/111/135	-
12	CLA	B	826	2	3/3/17/25	3/19/117/135	-
12	CLA	B	827	-	3/3/16/25	5/11/111/135	-
12	CLA	B	828	-	3/3/17/25	5/19/117/135	-
12	CLA	B	829	-	3/3/16/25	7/15/113/135	-
12	CLA	B	830	-	3/3/17/25	6/19/117/135	-
12	CLA	B	831	2	3/3/17/25	9/19/117/135	-
12	CLA	B	832	-	3/3/17/25	8/19/117/135	-
12	CLA	B	833	2	3/3/17/25	7/19/117/135	-
12	CLA	B	834	-	3/3/16/25	4/11/111/135	-
12	CLA	B	835	-	3/3/16/25	11/18/116/135	-
12	CLA	B	836	-	3/3/17/25	7/19/117/135	-
12	CLA	B	837	2	3/3/16/25	4/11/111/135	-
12	CLA	B	838	-	3/3/16/25	7/11/111/135	-
12	CLA	B	839	-	3/3/17/25	9/19/117/135	-
12	CLA	B	840	-	3/3/17/25	5/19/117/135	-
12	CLA	B	841	-	2/2/16/25	8/16/114/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	842	-	3/3/17/25	8/19/117/135	-
12	CLA	B	843	-	3/3/17/25	9/19/117/135	-
13	PQN	B	844	-	1/1/8/9	11/23/43/43	0/2/2/2
14	SF4	C	101	-	-	-	0/6/5/5
14	SF4	C	102	3	-	-	0/6/5/5
12	CLA	E	801	-	3/3/17/25	8/19/117/135	-
12	CLA	E	802	-	3/3/17/25	8/19/117/135	-
12	CLA	E	803	-	3/3/17/25	2/19/117/135	-
12	CLA	E	804	-	3/3/17/25	8/19/117/135	-
12	CLA	E	805	-	3/3/17/25	5/19/117/135	-
12	CLA	E	806	-	3/3/17/25	8/19/117/135	-
12	CLA	E	807	1	3/3/17/25	2/19/117/135	-
12	CLA	E	808	1	2/2/17/25	10/19/117/135	-
12	CLA	E	809	1	3/3/17/25	8/19/117/135	-
12	CLA	E	810	1	3/3/17/25	8/19/117/135	-
12	CLA	E	811	-	3/3/16/25	5/11/111/135	-
12	CLA	E	812	-	3/3/17/25	6/19/117/135	-
12	CLA	E	813	1	3/3/17/25	3/19/117/135	-
12	CLA	E	814	1	3/3/17/25	4/19/117/135	-
12	CLA	E	815	-	3/3/16/25	9/11/111/135	-
12	CLA	E	816	-	3/3/16/25	6/11/111/135	-
12	CLA	E	817	1	3/3/16/25	8/18/116/135	-
12	CLA	E	818	1	3/3/17/25	5/19/117/135	-
12	CLA	E	819	1	3/3/17/25	6/19/117/135	-
12	CLA	E	820	-	3/3/17/25	9/19/117/135	-
12	CLA	E	821	-	3/3/17/25	7/19/117/135	-
12	CLA	E	822	-	3/3/17/25	6/19/117/135	-
12	CLA	E	823	1	3/3/16/25	7/18/116/135	-
12	CLA	E	824	1	3/3/17/25	8/19/117/135	-
12	CLA	E	825	1	3/3/17/25	8/19/117/135	-
12	CLA	E	826	-	3/3/17/25	9/19/117/135	-
12	CLA	E	827	-	3/3/17/25	7/19/117/135	-
12	CLA	E	828	-	3/3/17/25	9/19/117/135	-
12	CLA	E	829	1	3/3/17/25	8/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	E	830	-	3/3/17/25	8/19/117/135	-
12	CLA	E	831	1	3/3/17/25	8/19/117/135	-
12	CLA	E	832	-	2/2/17/25	9/19/117/135	-
12	CLA	E	833	-	3/3/17/25	10/19/117/135	-
12	CLA	E	834	-	3/3/17/25	9/19/117/135	-
12	CLA	E	835	-	3/3/17/25	7/19/117/135	-
12	CLA	E	836	1	3/3/17/25	6/19/117/135	-
12	CLA	E	837	-	3/3/16/25	7/11/111/135	-
12	CLA	E	838	-	3/3/17/25	6/19/117/135	-
12	CLA	E	839	-	3/3/17/25	3/19/117/135	-
12	CLA	E	840	-	3/3/16/25	6/16/114/135	-
12	CLA	E	841	-	2/2/17/25	4/19/117/135	-
12	CLA	E	842	-	3/3/17/25	8/19/117/135	-
12	CLA	E	843	-	3/3/17/25	3/19/117/135	-
12	CLA	E	844	-	3/3/14/25	1/5/101/135	-
14	SF4	E	845	-	-	-	0/6/5/5
13	PQN	E	846	-	1/1/8/9	12/23/43/43	0/2/2/2
12	CLA	F	1301	-	3/3/16/25	7/11/111/135	-
12	CLA	G	801	-	3/3/17/25	5/19/117/135	-
12	CLA	G	802	-	3/3/17/25	9/19/117/135	-
12	CLA	G	803	-	3/3/17/25	6/19/117/135	-
12	CLA	G	804	-	3/3/17/25	9/19/117/135	-
12	CLA	G	805	2	3/3/17/25	9/19/117/135	-
12	CLA	G	806	-	3/3/17/25	7/19/117/135	-
12	CLA	G	807	-	3/3/17/25	4/19/117/135	-
12	CLA	G	808	-	3/3/17/25	6/19/117/135	-
12	CLA	G	809	-	3/3/17/25	6/19/117/135	-
12	CLA	G	810	2	3/3/17/25	7/19/117/135	-
12	CLA	G	811	-	3/3/17/25	10/19/117/135	-
12	CLA	G	812	-	3/3/16/25	6/11/111/135	-
12	CLA	G	813	-	3/3/16/25	4/11/111/135	-
12	CLA	G	814	2	3/3/17/25	10/19/117/135	-
12	CLA	G	815	2	3/3/17/25	7/19/117/135	-
12	CLA	G	816	2	3/3/16/25	4/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	817	-	3/3/17/25	6/19/117/135	-
12	CLA	G	818	-	3/3/17/25	13/19/117/135	-
12	CLA	G	819	-	3/3/17/25	8/19/117/135	-
12	CLA	G	820	-	3/3/17/25	6/19/117/135	-
12	CLA	G	821	2	3/3/16/25	7/16/114/135	-
12	CLA	G	822	-	3/3/16/25	3/11/111/135	-
12	CLA	G	823	2	3/3/17/25	3/19/117/135	-
12	CLA	G	824	-	3/3/16/25	5/11/111/135	-
12	CLA	G	825	-	3/3/17/25	5/19/117/135	-
12	CLA	G	826	-	3/3/16/25	7/15/113/135	-
12	CLA	G	827	-	3/3/17/25	6/19/117/135	-
12	CLA	G	828	2	3/3/17/25	9/19/117/135	-
12	CLA	G	829	-	3/3/17/25	8/19/117/135	-
12	CLA	G	830	2	3/3/17/25	7/19/117/135	-
12	CLA	G	831	-	3/3/16/25	4/11/111/135	-
12	CLA	G	832	-	3/3/16/25	11/18/116/135	-
12	CLA	G	833	-	3/3/17/25	7/19/117/135	-
12	CLA	G	834	-	3/3/17/25	12/19/117/135	-
12	CLA	G	835	2	3/3/16/25	4/11/111/135	-
12	CLA	G	836	-	3/3/16/25	7/11/111/135	-
12	CLA	G	837	-	3/3/17/25	9/19/117/135	-
12	CLA	G	838	-	3/3/17/25	5/19/117/135	-
12	CLA	G	839	-	2/2/16/25	8/16/114/135	-
12	CLA	G	840	-	3/3/17/25	8/19/117/135	-
12	CLA	G	841	-	3/3/17/25	9/19/117/135	-
13	PQN	G	842	-	1/1/8/9	11/23/43/43	0/2/2/2
12	CLA	G	843	10	3/3/17/25	4/19/117/135	-
14	SF4	H	101	-	-	-	0/6/5/5
14	SF4	H	102	3	-	-	0/6/5/5
12	CLA	J	1101	-	3/3/17/25	8/19/117/135	-
12	CLA	J	1102	-	3/3/17/25	12/19/117/135	-
12	CLA	K	1401	-	3/3/16/25	4/11/111/135	-
12	CLA	L	201	-	3/3/17/25	10/19/117/135	-
12	CLA	L	202	-	3/3/17/25	7/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	L	203	10	3/3/17/25	4/19/117/135	-
12	CLA	L	204	-	3/3/17/25	11/19/117/135	-
12	CLA	O	1301	-	3/3/16/25	7/11/111/135	-
12	CLA	R	1401	-	3/3/16/25	4/11/111/135	-
12	CLA	S	1501	-	3/3/17/25	7/19/117/135	-
12	CLA	S	1502	-	3/3/17/25	11/19/117/135	-
12	CLA	a	801	-	3/3/17/25	8/19/117/135	-
12	CLA	a	802	-	3/3/17/25	8/19/117/135	-
12	CLA	a	803	-	3/3/17/25	8/19/117/135	-
12	CLA	a	804	-	3/3/17/25	5/19/117/135	-
12	CLA	a	805	-	3/3/17/25	8/19/117/135	-
12	CLA	a	806	1	3/3/17/25	2/19/117/135	-
12	CLA	a	807	1	2/2/17/25	9/19/117/135	-
12	CLA	a	808	1	3/3/17/25	8/19/117/135	-
12	CLA	a	809	1	3/3/17/25	8/19/117/135	-
12	CLA	a	810	-	3/3/16/25	5/11/111/135	-
12	CLA	a	811	-	3/3/17/25	6/19/117/135	-
12	CLA	a	812	1	3/3/17/25	3/19/117/135	-
12	CLA	a	813	1	3/3/17/25	4/19/117/135	-
12	CLA	a	814	-	3/3/16/25	9/11/111/135	-
12	CLA	a	815	-	3/3/16/25	6/11/111/135	-
12	CLA	a	816	1	3/3/16/25	8/18/116/135	-
12	CLA	a	817	1	3/3/17/25	5/19/117/135	-
12	CLA	a	818	1	3/3/17/25	6/19/117/135	-
12	CLA	a	819	-	3/3/17/25	9/19/117/135	-
12	CLA	a	820	-	3/3/17/25	7/19/117/135	-
12	CLA	a	821	-	3/3/17/25	6/19/117/135	-
12	CLA	a	822	1	3/3/16/25	7/18/116/135	-
12	CLA	a	823	1	3/3/17/25	8/19/117/135	-
12	CLA	a	824	1	3/3/17/25	8/19/117/135	-
12	CLA	a	825	-	3/3/17/25	9/19/117/135	-
12	CLA	a	826	-	3/3/17/25	7/19/117/135	-
12	CLA	a	827	-	3/3/17/25	9/19/117/135	-
12	CLA	a	828	1	3/3/17/25	8/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	a	829	-	3/3/17/25	8/19/117/135	-
12	CLA	a	830	1	3/3/17/25	8/19/117/135	-
12	CLA	a	831	-	2/2/17/25	9/19/117/135	-
12	CLA	a	832	-	3/3/17/25	8/19/117/135	-
12	CLA	a	833	-	3/3/17/25	7/19/117/135	-
12	CLA	a	834	1	3/3/17/25	6/19/117/135	-
12	CLA	a	835	-	3/3/16/25	7/11/111/135	-
12	CLA	a	836	-	3/3/17/25	6/19/117/135	-
12	CLA	a	837	-	3/3/17/25	3/19/117/135	-
12	CLA	a	838	-	3/3/16/25	6/16/114/135	-
12	CLA	a	839	-	2/2/17/25	4/19/117/135	-
12	CLA	a	840	-	3/3/17/25	8/19/117/135	-
12	CLA	a	841	-	3/3/17/25	3/19/117/135	-
12	CLA	a	842	-	3/3/14/25	1/5/101/135	-
14	SF4	a	843	-	-	-	0/6/5/5
13	PQN	a	844	-	1/1/8/9	12/23/43/43	0/2/2/2
12	CLA	b	801	-	3/3/17/25	2/19/117/135	-
12	CLA	b	802	-	3/3/17/25	5/19/117/135	-
12	CLA	b	803	-	3/3/17/25	9/19/117/135	-
12	CLA	b	804	-	3/3/17/25	6/19/117/135	-
12	CLA	b	805	-	3/3/17/25	9/19/117/135	-
12	CLA	b	806	2	3/3/17/25	9/19/117/135	-
12	CLA	b	807	-	3/3/17/25	7/19/117/135	-
12	CLA	b	808	-	3/3/17/25	4/19/117/135	-
12	CLA	b	809	-	3/3/17/25	6/19/117/135	-
12	CLA	b	810	-	3/3/17/25	6/19/117/135	-
12	CLA	b	811	2	3/3/17/25	7/19/117/135	-
12	CLA	b	812	-	3/3/17/25	10/19/117/135	-
12	CLA	b	813	-	3/3/16/25	6/11/111/135	-
12	CLA	b	814	-	3/3/16/25	4/11/111/135	-
12	CLA	b	815	2	3/3/17/25	10/19/117/135	-
12	CLA	b	816	2	3/3/17/25	7/19/117/135	-
12	CLA	b	817	2	3/3/16/25	4/11/111/135	-
12	CLA	b	818	-	3/3/17/25	6/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	819	-	3/3/17/25	13/19/117/135	-
12	CLA	b	820	-	3/3/17/25	8/19/117/135	-
12	CLA	b	821	-	3/3/17/25	6/19/117/135	-
12	CLA	b	822	2	3/3/16/25	7/16/114/135	-
12	CLA	b	823	-	3/3/16/25	3/11/111/135	-
12	CLA	b	824	2	3/3/17/25	3/19/117/135	-
12	CLA	b	825	-	3/3/16/25	5/11/111/135	-
12	CLA	b	826	-	3/3/17/25	5/19/117/135	-
12	CLA	b	827	-	3/3/16/25	7/15/113/135	-
12	CLA	b	828	-	3/3/17/25	6/19/117/135	-
12	CLA	b	829	2	3/3/17/25	9/19/117/135	-
12	CLA	b	830	-	3/3/17/25	8/19/117/135	-
12	CLA	b	831	2	3/3/17/25	7/19/117/135	-
12	CLA	b	832	-	3/3/16/25	4/11/111/135	-
12	CLA	b	833	-	3/3/16/25	11/18/116/135	-
12	CLA	b	834	-	3/3/17/25	7/19/117/135	-
12	CLA	b	835	-	3/3/17/25	12/19/117/135	-
12	CLA	b	836	2	3/3/16/25	4/11/111/135	-
12	CLA	b	837	-	3/3/16/25	7/11/111/135	-
12	CLA	b	838	-	3/3/17/25	9/19/117/135	-
12	CLA	b	839	-	3/3/17/25	5/19/117/135	-
12	CLA	b	840	-	2/2/16/25	8/16/114/135	-
12	CLA	b	841	-	3/3/17/25	8/19/117/135	-
12	CLA	b	842	-	3/3/17/25	9/19/117/135	-
13	PQN	b	843	-	1/1/8/9	11/23/43/43	0/2/2/2
14	SF4	c	101	-	-	-	0/6/5/5
14	SF4	c	102	3	-	-	0/6/5/5
12	CLA	e	801	-	3/3/17/25	8/19/117/135	-
12	CLA	e	802	-	3/3/17/25	8/19/117/135	-
12	CLA	e	803	-	3/3/17/25	5/19/117/135	-
12	CLA	e	804	-	3/3/17/25	8/19/117/135	-
12	CLA	e	805	1	3/3/17/25	2/19/117/135	-
12	CLA	e	806	1	2/2/17/25	10/19/117/135	-
12	CLA	e	807	1	3/3/17/25	8/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	e	808	1	3/3/17/25	8/19/117/135	-
12	CLA	e	809	-	3/3/16/25	5/11/111/135	-
12	CLA	e	810	-	3/3/17/25	6/19/117/135	-
12	CLA	e	811	1	3/3/17/25	3/19/117/135	-
12	CLA	e	812	1	3/3/17/25	4/19/117/135	-
12	CLA	e	813	-	3/3/16/25	9/11/111/135	-
12	CLA	e	814	-	3/3/16/25	6/11/111/135	-
12	CLA	e	815	1	3/3/16/25	8/18/116/135	-
12	CLA	e	816	1	3/3/17/25	5/19/117/135	-
12	CLA	e	817	1	3/3/17/25	6/19/117/135	-
12	CLA	e	818	-	3/3/17/25	9/19/117/135	-
12	CLA	e	819	-	3/3/17/25	7/19/117/135	-
12	CLA	e	820	-	3/3/17/25	6/19/117/135	-
12	CLA	e	821	1	3/3/16/25	7/18/116/135	-
12	CLA	e	822	1	3/3/17/25	8/19/117/135	-
12	CLA	e	823	1	3/3/17/25	8/19/117/135	-
12	CLA	e	824	-	3/3/17/25	9/19/117/135	-
12	CLA	e	825	-	3/3/17/25	7/19/117/135	-
12	CLA	e	826	-	3/3/17/25	9/19/117/135	-
12	CLA	e	827	1	3/3/17/25	8/19/117/135	-
12	CLA	e	828	-	3/3/17/25	8/19/117/135	-
12	CLA	e	829	1	3/3/17/25	8/19/117/135	-
12	CLA	e	830	-	2/2/17/25	9/19/117/135	-
12	CLA	e	831	-	3/3/17/25	8/19/117/135	-
12	CLA	e	832	-	3/3/17/25	8/19/117/135	-
12	CLA	e	833	1	3/3/17/25	6/19/117/135	-
12	CLA	e	834	-	3/3/16/25	7/11/111/135	-
12	CLA	e	835	-	3/3/17/25	6/19/117/135	-
12	CLA	e	836	-	3/3/17/25	3/19/117/135	-
12	CLA	e	837	-	3/3/16/25	6/16/114/135	-
12	CLA	e	838	-	2/2/17/25	4/19/117/135	-
12	CLA	e	839	-	3/3/17/25	8/19/117/135	-
12	CLA	e	840	-	3/3/17/25	3/19/117/135	-
12	CLA	e	841	-	3/3/14/25	1/5/101/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	e	842	-	3/3/17/25	9/19/117/135	-
13	PQN	e	843	-	1/1/8/9	12/23/43/43	0/2/2/2
12	CLA	e	844	-	3/3/17/25	9/19/117/135	-
12	CLA	e	845	-	3/3/16/25	11/18/116/135	-
12	CLA	f	1301	-	3/3/16/25	7/11/111/135	-
12	CLA	g	801	-	3/3/17/25	8/19/117/135	-
12	CLA	g	802	-	3/3/17/25	2/19/117/135	-
12	CLA	g	803	-	3/3/17/25	5/19/117/135	-
14	SF4	g	804	-	-	-	0/6/5/5
12	CLA	g	805	-	3/3/17/25	6/19/117/135	-
12	CLA	g	806	-	3/3/17/25	9/19/117/135	-
12	CLA	g	807	2	3/3/17/25	9/19/117/135	-
12	CLA	g	808	-	3/3/17/25	7/19/117/135	-
12	CLA	g	809	-	3/3/17/25	4/19/117/135	-
12	CLA	g	810	-	3/3/17/25	6/19/117/135	-
12	CLA	g	811	-	3/3/17/25	6/19/117/135	-
12	CLA	g	812	2	3/3/17/25	7/19/117/135	-
12	CLA	g	813	-	3/3/17/25	10/19/117/135	-
12	CLA	g	814	-	3/3/16/25	6/11/111/135	-
12	CLA	g	815	-	3/3/16/25	4/11/111/135	-
12	CLA	g	816	2	3/3/17/25	10/19/117/135	-
12	CLA	g	817	2	3/3/17/25	7/19/117/135	-
12	CLA	g	818	2	3/3/16/25	4/11/111/135	-
12	CLA	g	819	-	3/3/17/25	6/19/117/135	-
12	CLA	g	820	-	3/3/17/25	13/19/117/135	-
12	CLA	g	821	-	3/3/17/25	8/19/117/135	-
12	CLA	g	822	-	3/3/17/25	6/19/117/135	-
12	CLA	g	823	2	3/3/16/25	7/16/114/135	-
12	CLA	g	824	-	3/3/16/25	3/11/111/135	-
12	CLA	g	825	2	3/3/17/25	3/19/117/135	-
12	CLA	g	826	-	3/3/16/25	5/11/111/135	-
12	CLA	g	827	-	3/3/17/25	5/19/117/135	-
12	CLA	g	828	-	3/3/16/25	7/15/113/135	-
12	CLA	g	829	-	3/3/17/25	6/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	g	830	2	3/3/17/25	9/19/117/135	-
12	CLA	g	831	-	3/3/17/25	8/19/117/135	-
12	CLA	g	832	2	3/3/17/25	7/19/117/135	-
12	CLA	g	833	-	3/3/16/25	4/11/111/135	-
12	CLA	g	834	-	3/3/17/25	7/19/117/135	-
12	CLA	g	835	-	3/3/17/25	12/19/117/135	-
12	CLA	g	836	2	3/3/16/25	4/11/111/135	-
12	CLA	g	837	-	3/3/16/25	7/11/111/135	-
12	CLA	g	838	-	3/3/17/25	9/19/117/135	-
12	CLA	g	839	-	3/3/17/25	5/19/117/135	-
12	CLA	g	840	-	2/2/16/25	9/16/114/135	-
12	CLA	g	841	-	3/3/17/25	8/19/117/135	-
12	CLA	g	842	-	3/3/17/25	9/19/117/135	-
13	PQN	g	843	-	1/1/8/9	11/23/43/43	0/2/2/2
14	SF4	h	101	-	-	-	0/6/5/5
14	SF4	h	102	3	-	-	0/6/5/5
12	CLA	k	1401	-	3/3/16/25	4/11/111/135	-
12	CLA	l	201	-	3/3/17/25	10/19/117/135	-
12	CLA	l	202	-	3/3/17/25	7/19/117/135	-
12	CLA	l	203	10	3/3/17/25	4/19/117/135	-
12	CLA	l	204	-	3/3/17/25	11/19/117/135	-
12	CLA	o	1301	-	3/3/16/25	7/11/111/135	-
12	CLA	r	1401	-	3/3/16/25	4/11/111/135	-
12	CLA	s	201	-	3/3/17/25	10/19/117/135	-
12	CLA	s	202	-	3/3/17/25	7/19/117/135	-
12	CLA	s	203	10	3/3/17/25	4/19/117/135	-
12	CLA	s	204	-	3/3/17/25	11/19/117/135	-

All (1612) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	842	PQN	C3-C2	6.28	1.48	1.35
13	b	843	PQN	C3-C2	6.24	1.48	1.35
13	e	843	PQN	C3-C2	6.23	1.48	1.35
13	g	843	PQN	C3-C2	6.20	1.48	1.35
13	G	842	PQN	C3-C2	6.19	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	844	PQN	C3-C2	6.16	1.48	1.35
13	a	844	PQN	C3-C2	6.11	1.48	1.35
13	E	846	PQN	C3-C2	6.10	1.48	1.35
13	e	843	PQN	C10-C1	4.51	1.56	1.48
13	A	842	PQN	C10-C1	4.51	1.56	1.48
13	e	843	PQN	C5-C4	4.49	1.56	1.48
13	G	842	PQN	C10-C1	4.46	1.56	1.48
13	G	842	PQN	C5-C4	4.45	1.56	1.48
13	A	842	PQN	C5-C4	4.44	1.56	1.48
13	B	844	PQN	C5-C4	4.44	1.56	1.48
13	b	843	PQN	C5-C4	4.44	1.56	1.48
13	g	843	PQN	C10-C1	4.43	1.56	1.48
13	b	843	PQN	C10-C1	4.43	1.56	1.48
13	B	844	PQN	C10-C1	4.42	1.56	1.48
13	g	843	PQN	C5-C4	4.40	1.56	1.48
13	E	846	PQN	C5-C4	4.39	1.56	1.48
13	E	846	PQN	C10-C1	4.36	1.56	1.48
13	a	844	PQN	C5-C4	4.31	1.56	1.48
13	a	844	PQN	C10-C1	4.28	1.56	1.48
12	G	834	CLA	CHC-C1C	3.14	1.43	1.35
12	b	835	CLA	CHC-C1C	3.12	1.43	1.35
12	g	835	CLA	CHC-C1C	3.10	1.43	1.35
12	J	1102	CLA	CHC-C1C	3.10	1.43	1.35
12	A	822	CLA	CHC-C1C	3.05	1.43	1.35
12	e	823	CLA	CHC-C1C	3.05	1.43	1.35
12	a	824	CLA	CHC-C1C	3.04	1.43	1.35
12	E	831	CLA	CHC-C1C	3.04	1.43	1.35
12	a	830	CLA	CHC-C1C	3.03	1.43	1.35
12	E	825	CLA	CHC-C1C	3.02	1.43	1.35
12	A	828	CLA	CHC-C1C	3.02	1.43	1.35
12	e	829	CLA	CHC-C1C	3.01	1.43	1.35
12	b	831	CLA	CHC-C1C	3.00	1.43	1.35
12	G	830	CLA	CHC-C1C	3.00	1.43	1.35
12	B	821	CLA	CHC-C1C	2.99	1.43	1.35
12	g	820	CLA	CHC-C1C	2.98	1.43	1.35
12	G	818	CLA	CHC-C1C	2.98	1.43	1.35
12	g	832	CLA	CHC-C1C	2.97	1.43	1.35
12	b	811	CLA	CHC-C1C	2.97	1.43	1.35
12	b	819	CLA	CHC-C1C	2.97	1.43	1.35
12	B	833	CLA	CHC-C1C	2.96	1.43	1.35
12	a	816	CLA	CHC-C1C	2.96	1.43	1.35
12	g	812	CLA	CHC-C1C	2.95	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	816	CLA	CHC-C1C	2.94	1.43	1.35
12	b	817	CLA	CHC-C1C	2.94	1.43	1.35
12	B	813	CLA	CHC-C1C	2.94	1.43	1.35
12	G	810	CLA	CHC-C1C	2.94	1.43	1.35
12	g	818	CLA	CHC-C1C	2.94	1.43	1.35
12	E	817	CLA	CHC-C1C	2.94	1.43	1.35
12	e	815	CLA	CHC-C1C	2.94	1.43	1.35
12	B	842	CLA	CHC-C1C	2.94	1.43	1.35
12	E	836	CLA	CHC-C1C	2.93	1.43	1.35
12	G	820	CLA	CHC-C1C	2.93	1.42	1.35
12	B	808	CLA	CHC-C1C	2.93	1.42	1.35
12	E	814	CLA	CHC-C1C	2.93	1.42	1.35
12	B	823	CLA	CHC-C1C	2.93	1.42	1.35
12	B	819	CLA	CHC-C1C	2.93	1.42	1.35
12	A	832	CLA	CHC-C1C	2.93	1.42	1.35
12	g	822	CLA	CHC-C1C	2.92	1.42	1.35
12	G	815	CLA	CHC-C1C	2.92	1.42	1.35
12	g	841	CLA	CHC-C1C	2.92	1.42	1.35
12	E	819	CLA	CHC-C1C	2.92	1.42	1.35
12	g	807	CLA	CHC-C1C	2.92	1.42	1.35
12	a	813	CLA	CHC-C1C	2.92	1.42	1.35
12	g	817	CLA	CHC-C1C	2.92	1.42	1.35
12	B	839	CLA	CHC-C1C	2.92	1.42	1.35
12	g	833	CLA	CHC-C1C	2.92	1.42	1.35
12	g	839	CLA	CHC-C1C	2.92	1.42	1.35
12	a	834	CLA	CHC-C1C	2.91	1.42	1.35
12	A	816	CLA	CHC-C1C	2.91	1.42	1.35
12	e	817	CLA	CHC-C1C	2.91	1.42	1.35
12	A	811	CLA	CHC-C1C	2.91	1.42	1.35
12	b	821	CLA	CHC-C1C	2.91	1.42	1.35
12	E	827	CLA	CHC-C1C	2.91	1.42	1.35
12	b	806	CLA	CHC-C1C	2.91	1.42	1.35
12	B	827	CLA	CHC-C1C	2.91	1.42	1.35
12	G	824	CLA	CHC-C1C	2.91	1.42	1.35
12	a	809	CLA	CHC-C1C	2.91	1.42	1.35
12	g	814	CLA	CHC-C1C	2.90	1.42	1.35
12	b	816	CLA	CHC-C1C	2.90	1.42	1.35
12	e	820	CLA	CHC-C1C	2.90	1.42	1.35
12	G	831	CLA	CHC-C1C	2.90	1.42	1.35
12	a	818	CLA	CHC-C1C	2.90	1.42	1.35
12	G	812	CLA	CHC-C1C	2.90	1.42	1.35
12	E	822	CLA	CHC-C1C	2.90	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	815	CLA	CHC-C1C	2.90	1.42	1.35
12	A	814	CLA	CHC-C1C	2.90	1.42	1.35
12	G	813	CLA	CHC-C1C	2.90	1.42	1.35
12	E	810	CLA	CHC-C1C	2.90	1.42	1.35
12	e	833	CLA	CHC-C1C	2.90	1.42	1.35
12	B	818	CLA	CHC-C1C	2.90	1.42	1.35
12	g	838	CLA	CHC-C1C	2.90	1.42	1.35
12	A	815	CLA	CHC-C1C	2.90	1.42	1.35
12	G	840	CLA	CHC-C1C	2.90	1.42	1.35
12	b	839	CLA	CHC-C1C	2.90	1.42	1.35
12	b	813	CLA	CHC-C1C	2.90	1.42	1.35
12	e	808	CLA	CHC-C1C	2.90	1.42	1.35
12	g	815	CLA	CHC-C1C	2.90	1.42	1.35
12	B	802	CLA	CHC-C1C	2.90	1.42	1.35
12	b	814	CLA	CHC-C1C	2.89	1.42	1.35
12	e	832	CLA	CHC-C1C	2.89	1.42	1.35
12	b	827	CLA	CHC-C1C	2.89	1.42	1.35
12	A	807	CLA	CHC-C1C	2.89	1.42	1.35
12	G	805	CLA	CHC-C1C	2.89	1.42	1.35
12	A	838	CLA	CHC-C1C	2.89	1.42	1.35
12	g	826	CLA	CHC-C1C	2.89	1.42	1.35
12	e	822	CLA	CHC-C1C	2.89	1.42	1.35
12	a	826	CLA	CHC-C1C	2.89	1.42	1.35
12	b	825	CLA	CHC-C1C	2.89	1.42	1.35
12	b	841	CLA	CHC-C1C	2.89	1.42	1.35
12	A	821	CLA	CHC-C1C	2.89	1.42	1.35
12	l	203	CLA	CHC-C1C	2.89	1.42	1.35
12	E	842	CLA	CHC-C1C	2.89	1.42	1.35
12	a	821	CLA	CHC-C1C	2.89	1.42	1.35
12	B	829	CLA	CHC-C1C	2.89	1.42	1.35
12	A	810	CLA	CHC-C1C	2.89	1.42	1.35
12	E	813	CLA	CHC-C1C	2.89	1.42	1.35
12	B	834	CLA	CHC-C1C	2.89	1.42	1.35
12	b	801	CLA	CHC-C1C	2.89	1.42	1.35
12	e	812	CLA	CHC-C1C	2.89	1.42	1.35
12	e	811	CLA	CHC-C1C	2.89	1.42	1.35
12	G	838	CLA	CHC-C1C	2.89	1.42	1.35
12	g	824	CLA	CHC-C1C	2.88	1.42	1.35
12	B	840	CLA	CHC-C1C	2.88	1.42	1.35
12	b	838	CLA	CHC-C1C	2.88	1.42	1.35
12	b	823	CLA	CHC-C1C	2.88	1.42	1.35
12	G	822	CLA	CHC-C1C	2.88	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	826	CLA	CHC-C1C	2.88	1.42	1.35
12	e	825	CLA	CHC-C1C	2.88	1.42	1.35
12	g	828	CLA	CHC-C1C	2.88	1.42	1.35
12	g	806	CLA	CHC-C1C	2.88	1.42	1.35
12	A	819	CLA	CHC-C1C	2.88	1.42	1.35
12	A	835	CLA	CHC-C1C	2.88	1.42	1.35
12	a	812	CLA	CHC-C1C	2.88	1.42	1.35
12	E	803	CLA	CHC-C1C	2.88	1.42	1.35
12	E	818	CLA	CHC-C1C	2.88	1.42	1.35
12	b	832	CLA	CHC-C1C	2.88	1.42	1.35
12	A	824	CLA	CHC-C1C	2.88	1.42	1.35
12	s	203	CLA	CHC-C1C	2.88	1.42	1.35
12	G	837	CLA	CHC-C1C	2.88	1.42	1.35
12	g	811	CLA	CHC-C1C	2.88	1.42	1.35
12	B	816	CLA	CHC-C1C	2.87	1.42	1.35
12	e	816	CLA	CHC-C1C	2.87	1.42	1.35
12	B	825	CLA	CHC-C1C	2.87	1.42	1.35
12	G	801	CLA	CHC-C1C	2.87	1.42	1.35
12	b	805	CLA	CHC-C1C	2.87	1.42	1.35
12	L	203	CLA	CHC-C1C	2.87	1.42	1.35
12	a	823	CLA	CHC-C1C	2.87	1.42	1.35
12	e	839	CLA	CHC-C1C	2.87	1.42	1.35
12	E	804	CLA	CHC-C1C	2.87	1.42	1.35
12	e	802	CLA	CHC-C1C	2.87	1.42	1.35
12	E	837	CLA	CHC-C1C	2.87	1.42	1.35
12	A	806	CLA	CHC-C1C	2.87	1.42	1.35
12	b	803	CLA	CHC-C1C	2.87	1.42	1.35
12	e	836	CLA	CHC-C1C	2.87	1.42	1.35
12	a	803	CLA	CHC-C1C	2.87	1.42	1.35
12	A	831	CLA	CHC-C1C	2.87	1.42	1.35
12	e	844	CLA	CHC-C1C	2.86	1.42	1.35
12	b	826	CLA	CHC-C1C	2.86	1.42	1.35
12	G	843	CLA	CHC-C1C	2.86	1.42	1.35
12	B	812	CLA	CHC-C1C	2.86	1.42	1.35
12	E	835	CLA	CHC-C1C	2.86	1.42	1.35
12	B	828	CLA	CHC-C1C	2.86	1.42	1.35
12	a	817	CLA	CHC-C1C	2.86	1.42	1.35
12	a	835	CLA	CHC-C1C	2.86	1.42	1.35
12	E	824	CLA	CHC-C1C	2.86	1.42	1.35
12	a	840	CLA	CHC-C1C	2.86	1.42	1.35
12	b	807	CLA	CHC-C1C	2.86	1.42	1.35
12	G	827	CLA	CHC-C1C	2.86	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	g	808	CLA	CHC-C1C	2.86	1.42	1.35
12	e	807	CLA	CHC-C1C	2.86	1.42	1.35
12	g	802	CLA	CHC-C1C	2.86	1.42	1.35
12	B	826	CLA	CHC-C1C	2.86	1.42	1.35
12	a	837	CLA	CHC-C1C	2.86	1.42	1.35
12	b	810	CLA	CHC-C1C	2.86	1.42	1.35
12	A	833	CLA	CHC-C1C	2.85	1.42	1.35
12	B	838	CLA	CHC-C1C	2.85	1.42	1.35
12	g	803	CLA	CHC-C1C	2.85	1.42	1.35
12	G	802	CLA	CHC-C1C	2.85	1.42	1.35
12	B	837	CLA	CHC-C1C	2.85	1.42	1.35
12	A	820	CLA	CHC-C1C	2.85	1.42	1.35
12	B	805	CLA	CHC-C1C	2.85	1.42	1.35
12	G	832	CLA	CHC-C1C	2.85	1.42	1.35
12	B	803	CLA	CHC-C1C	2.85	1.42	1.35
12	G	804	CLA	CHC-C1C	2.85	1.42	1.35
12	b	828	CLA	CHC-C1C	2.85	1.42	1.35
12	b	824	CLA	CHC-C1C	2.85	1.42	1.35
12	G	823	CLA	CHC-C1C	2.85	1.42	1.35
12	E	834	CLA	CHC-C1C	2.85	1.42	1.35
12	E	839	CLA	CHC-C1C	2.85	1.42	1.35
12	G	836	CLA	CHC-C1C	2.85	1.42	1.35
12	E	823	CLA	CHC-C1C	2.84	1.42	1.35
12	b	836	CLA	CHC-C1C	2.84	1.42	1.35
12	G	829	CLA	CHC-C1C	2.84	1.42	1.35
12	B	830	CLA	CHC-C1C	2.84	1.42	1.35
12	J	1101	CLA	CHC-C1C	2.84	1.42	1.35
12	E	809	CLA	CHC-C1C	2.84	1.42	1.35
12	g	813	CLA	CHC-C1C	2.84	1.42	1.35
12	B	814	CLA	CHC-C1C	2.84	1.42	1.35
12	a	808	CLA	CHC-C1C	2.84	1.42	1.35
12	B	807	CLA	CHC-C1C	2.84	1.42	1.35
12	a	833	CLA	CHC-C1C	2.84	1.42	1.35
12	B	835	CLA	CHC-C1C	2.84	1.42	1.35
12	g	836	CLA	CHC-C1C	2.84	1.42	1.35
12	b	802	CLA	CHC-C1C	2.84	1.42	1.35
12	B	832	CLA	CHC-C1C	2.84	1.42	1.35
12	G	821	CLA	CHC-C1C	2.84	1.42	1.35
12	e	834	CLA	CHC-C1C	2.84	1.42	1.35
12	G	825	CLA	CHC-C1C	2.84	1.42	1.35
12	E	828	CLA	CHC-C1C	2.84	1.42	1.35
12	f	1301	CLA	CHC-C1C	2.84	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	e	845	CLA	CHC-C1C	2.84	1.42	1.35
12	O	1301	CLA	CHC-C1C	2.84	1.42	1.35
12	a	810	CLA	CHC-C1C	2.83	1.42	1.35
12	G	811	CLA	CHC-C1C	2.83	1.42	1.35
12	E	816	CLA	CHC-C1C	2.83	1.42	1.35
12	e	809	CLA	CHC-C1C	2.83	1.42	1.35
12	b	809	CLA	CHC-C1C	2.83	1.42	1.35
12	g	827	CLA	CHC-C1C	2.83	1.42	1.35
12	e	826	CLA	CHC-C1C	2.83	1.42	1.35
12	G	806	CLA	CHC-C1C	2.83	1.42	1.35
12	g	831	CLA	CHC-C1C	2.83	1.42	1.35
12	A	813	CLA	CHC-C1C	2.83	1.42	1.35
12	G	835	CLA	CHC-C1C	2.83	1.42	1.35
12	A	805	CLA	CHC-C1C	2.83	1.42	1.35
12	g	810	CLA	CHC-C1C	2.83	1.42	1.35
12	g	825	CLA	CHC-C1C	2.83	1.42	1.35
12	A	825	CLA	CHC-C1C	2.83	1.42	1.35
12	B	809	CLA	CHC-C1C	2.83	1.42	1.35
12	e	814	CLA	CHC-C1C	2.83	1.42	1.35
12	G	809	CLA	CHC-C1C	2.83	1.42	1.35
12	g	837	CLA	CHC-C1C	2.83	1.42	1.35
12	a	827	CLA	CHC-C1C	2.83	1.42	1.35
12	b	837	CLA	CHC-C1C	2.82	1.42	1.35
12	E	812	CLA	CHC-C1C	2.82	1.42	1.35
12	a	822	CLA	CHC-C1C	2.82	1.42	1.35
12	B	824	CLA	CHC-C1C	2.82	1.42	1.35
12	A	804	CLA	CHC-C1C	2.82	1.42	1.35
12	G	808	CLA	CHC-C1C	2.82	1.42	1.35
12	g	829	CLA	CHC-C1C	2.82	1.42	1.35
12	b	830	CLA	CHC-C1C	2.82	1.42	1.35
12	b	822	CLA	CHC-C1C	2.82	1.42	1.35
12	b	812	CLA	CHC-C1C	2.82	1.42	1.35
12	A	823	CLA	CHC-C1C	2.82	1.42	1.35
12	e	831	CLA	CHC-C1C	2.82	1.42	1.35
12	L	204	CLA	CHC-C1C	2.82	1.42	1.35
12	a	815	CLA	CHC-C1C	2.82	1.42	1.35
12	E	811	CLA	CHC-C1C	2.82	1.42	1.35
12	R	1401	CLA	CHC-C1C	2.82	1.42	1.35
12	o	1301	CLA	CHC-C1C	2.82	1.42	1.35
12	E	808	CLA	CHC-C1C	2.82	1.42	1.35
12	A	802	CLA	CHC-C1C	2.82	1.42	1.35
12	b	833	CLA	CHC-C1C	2.81	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	832	CLA	CHC-C1C	2.81	1.42	1.35
12	e	821	CLA	CHC-C1C	2.81	1.42	1.35
12	a	806	CLA	CHC-C1C	2.81	1.42	1.35
12	G	833	CLA	CHC-C1C	2.81	1.42	1.35
12	e	819	CLA	CHC-C1C	2.81	1.42	1.35
12	b	834	CLA	CHC-C1C	2.81	1.42	1.35
12	A	808	CLA	CHC-C1C	2.81	1.42	1.35
12	g	816	CLA	CHC-C1C	2.81	1.42	1.35
12	S	1502	CLA	CHC-C1C	2.81	1.42	1.35
12	B	831	CLA	CHC-C1C	2.81	1.42	1.35
12	g	823	CLA	CHC-C1C	2.81	1.42	1.35
12	A	818	CLA	CHC-C1C	2.81	1.42	1.35
12	A	826	CLA	CHC-C1C	2.81	1.42	1.35
12	E	830	CLA	CHC-C1C	2.81	1.42	1.35
12	a	811	CLA	CHC-C1C	2.81	1.42	1.35
12	F	1301	CLA	CHC-C1C	2.81	1.42	1.35
12	a	828	CLA	CHC-C1C	2.81	1.42	1.35
12	e	805	CLA	CHC-C1C	2.81	1.42	1.35
12	e	824	CLA	CHC-C1C	2.80	1.42	1.35
12	g	834	CLA	CHC-C1C	2.80	1.42	1.35
12	A	809	CLA	CHC-C1C	2.80	1.42	1.35
12	a	807	CLA	CHC-C1C	2.80	1.42	1.35
12	s	204	CLA	CHC-C1C	2.80	1.42	1.35
12	a	839	CLA	CHC-C1C	2.80	1.42	1.35
12	a	829	CLA	CHC-C1C	2.80	1.42	1.35
12	A	830	CLA	CHC-C1C	2.80	1.42	1.35
12	A	837	CLA	CHC-C1C	2.80	1.42	1.35
12	E	844	CLA	CHC-C1C	2.80	1.42	1.35
12	G	814	CLA	CHC-C1C	2.80	1.42	1.35
12	A	817	CLA	CHC-C1C	2.80	1.42	1.35
12	a	825	CLA	CHC-C1C	2.80	1.42	1.35
12	E	807	CLA	CHC-C1C	2.80	1.42	1.35
12	r	1401	CLA	CHC-C1C	2.80	1.42	1.35
12	B	811	CLA	CHC-C1C	2.80	1.42	1.35
12	l	204	CLA	CHC-C1C	2.80	1.42	1.35
12	e	810	CLA	CHC-C1C	2.79	1.42	1.35
12	k	1401	CLA	CHC-C1C	2.79	1.42	1.35
12	B	836	CLA	CHC-C1C	2.79	1.42	1.35
12	e	842	CLA	CHC-C1C	2.79	1.42	1.35
12	e	806	CLA	CHC-C1C	2.79	1.42	1.35
12	E	841	CLA	CHC-C1C	2.79	1.42	1.35
12	b	818	CLA	CHC-C1C	2.79	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	829	CLA	CHC-C1C	2.79	1.42	1.35
12	B	820	CLA	CHC-C1C	2.79	1.42	1.35
12	B	817	CLA	CHC-C1C	2.79	1.42	1.35
12	e	830	CLA	CHC-C1C	2.79	1.42	1.35
12	a	842	CLA	CHC-C1C	2.79	1.42	1.35
12	e	838	CLA	CHC-C1C	2.79	1.42	1.35
12	e	837	CLA	CHC-C1C	2.79	1.42	1.35
12	e	828	CLA	CHC-C1C	2.79	1.42	1.35
12	b	815	CLA	CHC-C1C	2.79	1.42	1.35
12	a	802	CLA	CHC-C1C	2.79	1.42	1.35
12	E	832	CLA	CHC-C1C	2.79	1.42	1.35
12	E	805	CLA	CHC-C1C	2.79	1.42	1.35
12	a	804	CLA	CHC-C1C	2.79	1.42	1.35
12	E	839	CLA	CMB-C2B	-2.79	1.45	1.51
12	G	828	CLA	CHC-C1C	2.79	1.42	1.35
12	A	841	CLA	CHC-C1C	2.79	1.42	1.35
12	e	803	CLA	CHC-C1C	2.79	1.42	1.35
12	g	805	CLA	CHC-C1C	2.78	1.42	1.35
12	A	840	CLA	CHC-C1C	2.78	1.42	1.35
12	l	201	CLA	CHC-C1C	2.78	1.42	1.35
12	E	826	CLA	CHC-C1C	2.78	1.42	1.35
12	L	201	CLA	CHC-C1C	2.78	1.42	1.35
12	K	1401	CLA	CHC-C1C	2.78	1.42	1.35
12	g	830	CLA	CHC-C1C	2.78	1.42	1.35
12	a	837	CLA	CMB-C2B	-2.78	1.45	1.51
12	b	829	CLA	CHC-C1C	2.78	1.42	1.35
12	A	836	CLA	CHC-C1C	2.78	1.42	1.35
12	E	829	CLA	CHC-C1C	2.78	1.42	1.35
12	e	841	CLA	CHC-C1C	2.78	1.42	1.35
12	e	827	CLA	CHC-C1C	2.77	1.42	1.35
12	a	820	CLA	CHC-C1C	2.77	1.42	1.35
12	G	817	CLA	CHC-C1C	2.77	1.42	1.35
12	B	843	CLA	CHC-C1C	2.77	1.42	1.35
12	B	810	CLA	CHC-C1C	2.77	1.42	1.35
12	E	833	CLA	CHC-C1C	2.77	1.42	1.35
12	a	814	CLA	CHC-C1C	2.77	1.42	1.35
12	b	804	CLA	CHC-C1C	2.77	1.42	1.35
12	B	806	CLA	CHC-C1C	2.77	1.42	1.35
12	a	819	CLA	CHC-C1C	2.77	1.42	1.35
12	A	812	CLA	CHC-C1C	2.77	1.42	1.35
12	G	839	CLA	CHC-C1C	2.77	1.42	1.35
12	G	841	CLA	CHC-C1C	2.77	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	807	CLA	CHC-C1C	2.77	1.42	1.35
12	a	831	CLA	CHC-C1C	2.77	1.42	1.35
12	E	840	CLA	CHC-C1C	2.76	1.42	1.35
12	e	818	CLA	CHC-C1C	2.76	1.42	1.35
12	E	821	CLA	CHC-C1C	2.76	1.42	1.35
12	E	820	CLA	CHC-C1C	2.76	1.42	1.35
12	G	803	CLA	CHC-C1C	2.76	1.42	1.35
12	e	813	CLA	CHC-C1C	2.76	1.42	1.35
12	g	801	CLA	CHC-C1C	2.76	1.42	1.35
12	b	808	CLA	CHC-C1C	2.76	1.42	1.35
12	s	201	CLA	CHC-C1C	2.76	1.42	1.35
12	g	809	CLA	CHC-C1C	2.75	1.42	1.35
12	A	819	CLA	CMB-C2B	-2.75	1.45	1.51
12	A	827	CLA	CHC-C1C	2.75	1.42	1.35
12	B	801	CLA	CHC-C1C	2.75	1.42	1.35
12	a	841	CLA	CHC-C1C	2.75	1.42	1.35
12	g	840	CLA	CHC-C1C	2.75	1.42	1.35
12	g	819	CLA	CHC-C1C	2.75	1.42	1.35
12	E	802	CLA	CHC-C1C	2.75	1.42	1.35
12	E	815	CLA	CHC-C1C	2.75	1.42	1.35
12	a	838	CLA	CHC-C1C	2.74	1.42	1.35
12	L	202	CLA	CHC-C1C	2.74	1.42	1.35
12	b	842	CLA	CHC-C1C	2.74	1.42	1.35
12	e	836	CLA	CMB-C2B	-2.74	1.45	1.51
12	E	843	CLA	CHC-C1C	2.74	1.42	1.35
12	A	835	CLA	CMB-C2B	-2.74	1.45	1.51
12	b	840	CLA	CHC-C1C	2.74	1.42	1.35
12	s	202	CLA	CHC-C1C	2.74	1.42	1.35
12	l	202	CLA	CHC-C1C	2.74	1.42	1.35
12	A	839	CLA	CHC-C1C	2.74	1.42	1.35
12	B	841	CLA	CHC-C1C	2.73	1.42	1.35
12	e	840	CLA	CHC-C1C	2.73	1.42	1.35
12	g	842	CLA	CHC-C1C	2.73	1.42	1.35
12	A	803	CLA	CHC-C1C	2.72	1.42	1.35
12	S	1501	CLA	CHC-C1C	2.72	1.42	1.35
12	E	822	CLA	CMB-C2B	-2.72	1.46	1.51
12	G	819	CLA	CHC-C1C	2.71	1.42	1.35
12	E	806	CLA	CHC-C1C	2.71	1.42	1.35
12	e	820	CLA	CMB-C2B	-2.71	1.46	1.51
12	B	822	CLA	CHC-C1C	2.71	1.42	1.35
12	a	821	CLA	CMB-C2B	-2.70	1.46	1.51
12	b	820	CLA	CHC-C1C	2.70	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	834	CLA	C1D-C2D	2.69	1.48	1.42
12	e	804	CLA	CHC-C1C	2.69	1.42	1.35
12	A	827	CLA	C1D-C2D	2.69	1.48	1.42
12	a	829	CLA	C1D-C2D	2.69	1.48	1.42
12	e	833	CLA	C1D-C2D	2.68	1.48	1.42
12	g	824	CLA	C1D-C2D	2.68	1.48	1.42
12	g	821	CLA	CHC-C1C	2.68	1.42	1.35
12	a	805	CLA	CHC-C1C	2.68	1.42	1.35
12	g	841	CLA	CMB-C2B	-2.68	1.46	1.51
12	b	823	CLA	C1D-C2D	2.68	1.48	1.42
12	E	836	CLA	C1D-C2D	2.67	1.48	1.42
12	E	830	CLA	C1D-C2D	2.67	1.48	1.42
12	B	825	CLA	C1D-C2D	2.67	1.48	1.42
12	A	832	CLA	C1D-C2D	2.67	1.48	1.42
12	e	828	CLA	C1D-C2D	2.66	1.48	1.42
12	E	821	CLA	CMB-C2B	-2.66	1.46	1.51
12	A	818	CLA	CMB-C2B	-2.66	1.46	1.51
12	G	840	CLA	CMB-C2B	-2.66	1.46	1.51
12	e	835	CLA	C1D-C2D	2.65	1.48	1.42
12	g	825	CLA	C1D-C2D	2.65	1.48	1.42
12	b	812	CLA	C1D-C2D	2.65	1.48	1.42
12	b	841	CLA	CMB-C2B	-2.65	1.46	1.51
12	a	820	CLA	CMB-C2B	-2.65	1.46	1.51
12	e	819	CLA	CMB-C2B	-2.64	1.46	1.51
12	a	836	CLA	C1D-C2D	2.64	1.48	1.42
12	A	834	CLA	C1D-C2D	2.64	1.48	1.42
12	B	819	CLA	C1D-C2D	2.64	1.48	1.42
12	B	814	CLA	C1D-C2D	2.64	1.48	1.42
12	g	813	CLA	C1D-C2D	2.63	1.48	1.42
12	b	818	CLA	CMB-C2B	-2.63	1.46	1.51
12	G	811	CLA	C1D-C2D	2.63	1.48	1.42
12	B	842	CLA	CMB-C2B	-2.63	1.46	1.51
12	B	820	CLA	CMB-C2B	-2.62	1.46	1.51
12	E	838	CLA	C1D-C2D	2.62	1.48	1.42
12	B	826	CLA	C1D-C2D	2.62	1.48	1.42
12	B	818	CLA	C1D-C2D	2.62	1.48	1.42
12	g	818	CLA	C1D-C2D	2.62	1.48	1.42
12	G	822	CLA	C1D-C2D	2.62	1.48	1.42
12	b	824	CLA	C1D-C2D	2.62	1.48	1.42
12	b	816	CLA	C1D-C2D	2.62	1.48	1.42
12	g	819	CLA	CMB-C2B	-2.62	1.46	1.51
12	G	817	CLA	CMB-C2B	-2.61	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	801	CLA	CMB-C2B	-2.61	1.46	1.51
12	f	1301	CLA	C1D-C2D	2.61	1.48	1.42
12	G	816	CLA	C1D-C2D	2.61	1.48	1.42
12	b	837	CLA	C1D-C2D	2.61	1.48	1.42
12	E	824	CLA	C1D-C2D	2.60	1.48	1.42
12	A	821	CLA	C1D-C2D	2.60	1.48	1.42
12	a	822	CLA	C1D-C2D	2.60	1.48	1.42
12	b	817	CLA	C1D-C2D	2.60	1.48	1.42
12	G	823	CLA	C1D-C2D	2.60	1.48	1.42
12	g	817	CLA	C1D-C2D	2.60	1.48	1.42
12	a	801	CLA	CHC-C1C	2.60	1.42	1.35
12	A	801	CLA	CHC-C1C	2.60	1.42	1.35
12	O	1301	CLA	C1D-C2D	2.60	1.48	1.42
12	G	815	CLA	C1D-C2D	2.60	1.48	1.42
12	A	802	CLA	C1D-C2D	2.60	1.48	1.42
12	e	801	CLA	CHC-C1C	2.59	1.42	1.35
12	B	803	CLA	CMB-C2B	-2.59	1.46	1.51
12	e	822	CLA	C1D-C2D	2.59	1.48	1.42
12	k	1401	CLA	C1D-C2D	2.59	1.48	1.42
12	e	803	CLA	C1D-C2D	2.59	1.48	1.42
12	A	806	CLA	C1D-C2D	2.59	1.48	1.42
12	K	1401	CLA	C1D-C2D	2.59	1.48	1.42
12	E	835	CLA	C1D-C2D	2.59	1.48	1.42
12	e	841	CLA	C1D-C2D	2.59	1.48	1.42
12	g	840	CLA	CMB-C2B	-2.58	1.46	1.51
12	E	801	CLA	CHC-C1C	2.58	1.42	1.35
12	a	836	CLA	CHC-C1C	2.58	1.42	1.35
12	a	841	CLA	C1D-C2D	2.58	1.48	1.42
12	a	810	CLA	C1D-C2D	2.58	1.48	1.42
12	A	840	CLA	C1D-C2D	2.58	1.48	1.42
12	a	826	CLA	CMB-C2B	-2.58	1.46	1.51
12	e	802	CLA	C1D-C2D	2.58	1.48	1.42
12	E	804	CLA	C1D-C2D	2.58	1.48	1.42
12	E	816	CLA	C1D-C2D	2.58	1.48	1.42
12	E	807	CLA	CMB-C2B	-2.58	1.46	1.51
12	A	813	CLA	C1D-C2D	2.58	1.48	1.42
12	g	837	CLA	C1D-C2D	2.58	1.48	1.42
12	a	808	CLA	C1D-C2D	2.58	1.48	1.42
12	G	836	CLA	C1D-C2D	2.58	1.48	1.42
12	E	805	CLA	C1D-C2D	2.58	1.48	1.42
12	A	841	CLA	C1D-C2D	2.57	1.48	1.42
12	R	1401	CLA	C1D-C2D	2.57	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	802	CLA	CMB-C2B	-2.57	1.46	1.51
12	r	1401	CLA	C1D-C2D	2.57	1.48	1.42
12	b	839	CLA	C1D-C2D	2.57	1.48	1.42
12	a	803	CLA	C1D-C2D	2.57	1.48	1.42
12	s	201	CLA	CMB-C2B	-2.57	1.46	1.51
12	o	1301	CLA	C1D-C2D	2.57	1.48	1.42
12	B	840	CLA	C1D-C2D	2.57	1.48	1.42
12	E	811	CLA	C1D-C2D	2.57	1.48	1.42
12	e	821	CLA	C1D-C2D	2.57	1.48	1.42
12	e	831	CLA	CMB-C2B	-2.57	1.46	1.51
12	e	828	CLA	CMB-C2B	-2.57	1.46	1.51
12	E	809	CLA	C1D-C2D	2.57	1.48	1.42
12	E	823	CLA	C1D-C2D	2.57	1.48	1.42
12	a	823	CLA	C1D-C2D	2.57	1.48	1.42
12	G	808	CLA	CMB-C2B	-2.57	1.46	1.51
12	b	840	CLA	CMB-C2B	-2.57	1.46	1.51
12	B	838	CLA	C1D-C2D	2.57	1.48	1.42
12	E	844	CLA	C1D-C2D	2.56	1.48	1.42
12	b	810	CLA	C1D-C2D	2.56	1.48	1.42
12	a	833	CLA	C1D-C2D	2.56	1.48	1.42
12	E	833	CLA	CMB-C2B	-2.56	1.46	1.51
12	E	843	CLA	C1D-C2D	2.56	1.48	1.42
12	e	825	CLA	CMB-C2B	-2.56	1.46	1.51
12	g	834	CLA	CMB-C2B	-2.56	1.46	1.51
12	e	840	CLA	C1D-C2D	2.56	1.48	1.42
12	L	203	CLA	C1D-C2D	2.56	1.48	1.42
12	E	827	CLA	CMB-C2B	-2.56	1.46	1.51
12	g	831	CLA	C1D-C2D	2.56	1.48	1.42
12	e	832	CLA	C1D-C2D	2.56	1.48	1.42
12	a	804	CLA	C1D-C2D	2.56	1.48	1.42
12	g	839	CLA	C1D-C2D	2.56	1.48	1.42
12	a	842	CLA	C1D-C2D	2.56	1.48	1.42
12	B	832	CLA	C1D-C2D	2.56	1.48	1.42
12	g	832	CLA	C1D-C2D	2.56	1.48	1.42
12	B	806	CLA	C1D-C2D	2.56	1.48	1.42
12	A	834	CLA	CHC-C1C	2.56	1.41	1.35
12	J	1101	CLA	C1D-C2D	2.56	1.48	1.42
12	G	831	CLA	C1D-C2D	2.56	1.48	1.42
12	E	840	CLA	CMB-C2B	-2.56	1.46	1.51
12	E	838	CLA	CHC-C1C	2.55	1.41	1.35
12	B	811	CLA	C1D-C2D	2.55	1.48	1.42
12	F	1301	CLA	C1D-C2D	2.55	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	e	837	CLA	CMB-C2B	-2.55	1.46	1.51
12	A	836	CLA	CMB-C2B	-2.55	1.46	1.51
12	G	810	CLA	CMB-C2B	-2.55	1.46	1.51
12	g	842	CLA	CMB-C2B	-2.55	1.46	1.51
12	g	803	CLA	C1D-C2D	2.55	1.48	1.42
12	a	805	CLA	CMB-C2B	-2.55	1.46	1.51
12	e	835	CLA	CHC-C1C	2.55	1.41	1.35
12	G	809	CLA	C1D-C2D	2.55	1.48	1.42
12	B	834	CLA	C1D-C2D	2.55	1.48	1.42
12	B	805	CLA	C1D-C2D	2.55	1.48	1.42
12	G	843	CLA	C1D-C2D	2.55	1.48	1.42
12	G	838	CLA	C1D-C2D	2.55	1.48	1.42
12	g	838	CLA	C1D-C2D	2.55	1.48	1.42
12	e	807	CLA	C1D-C2D	2.55	1.48	1.42
12	A	839	CLA	C1D-C2D	2.55	1.48	1.42
12	L	201	CLA	CMB-C2B	-2.55	1.46	1.51
12	G	801	CLA	C1D-C2D	2.55	1.48	1.42
12	e	808	CLA	C1D-C2D	2.55	1.48	1.42
12	g	811	CLA	C1D-C2D	2.55	1.48	1.42
12	b	831	CLA	C1D-C2D	2.55	1.48	1.42
12	g	822	CLA	CMB-C2B	-2.55	1.46	1.51
12	b	813	CLA	C1D-C2D	2.55	1.48	1.42
12	l	201	CLA	CMB-C2B	-2.54	1.46	1.51
12	B	811	CLA	CMB-C2B	-2.54	1.46	1.51
12	A	824	CLA	CMB-C2B	-2.54	1.46	1.51
12	g	812	CLA	CMB-C2B	-2.54	1.46	1.51
12	E	834	CLA	CMB-C2B	-2.54	1.46	1.51
12	A	831	CLA	C1D-C2D	2.54	1.48	1.42
12	G	841	CLA	CMB-C2B	-2.54	1.46	1.51
12	a	809	CLA	C1D-C2D	2.54	1.48	1.42
12	a	811	CLA	C1D-C2D	2.54	1.48	1.42
12	B	824	CLA	C1D-C2D	2.54	1.48	1.42
12	e	805	CLA	CMB-C2B	-2.54	1.46	1.51
12	g	805	CLA	C1D-C2D	2.54	1.48	1.42
12	e	809	CLA	C1D-C2D	2.54	1.48	1.42
12	G	839	CLA	CMB-C2B	-2.54	1.46	1.51
12	G	803	CLA	C1D-C2D	2.54	1.48	1.42
12	b	802	CLA	C1D-C2D	2.54	1.48	1.42
12	a	832	CLA	CMB-C2B	-2.54	1.46	1.51
12	g	841	CLA	C1D-C2D	2.54	1.48	1.42
12	b	842	CLA	CMB-C2B	-2.54	1.46	1.51
12	b	832	CLA	C1D-C2D	2.54	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	203	CLA	C1D-C2D	2.54	1.48	1.42
12	B	843	CLA	CMB-C2B	-2.54	1.46	1.51
12	b	838	CLA	C1D-C2D	2.54	1.48	1.42
12	G	812	CLA	C1D-C2D	2.54	1.48	1.42
12	g	805	CLA	CMB-C2B	-2.54	1.46	1.51
12	s	203	CLA	C1D-C2D	2.54	1.48	1.42
12	g	827	CLA	CMB-C2B	-2.54	1.46	1.51
12	B	836	CLA	CMB-C2B	-2.54	1.46	1.51
12	E	806	CLA	CMB-C2B	-2.54	1.46	1.51
12	A	820	CLA	C1D-C2D	2.54	1.48	1.42
12	A	809	CLA	C1D-C2D	2.53	1.48	1.42
12	B	809	CLA	CMB-C2B	-2.53	1.46	1.51
12	B	803	CLA	C1D-C2D	2.53	1.48	1.42
12	b	834	CLA	CMB-C2B	-2.53	1.46	1.51
12	G	829	CLA	C1D-C2D	2.53	1.48	1.42
12	e	810	CLA	C1D-C2D	2.53	1.48	1.42
12	G	806	CLA	CMB-C2B	-2.53	1.46	1.51
12	b	830	CLA	C1D-C2D	2.53	1.48	1.42
12	g	803	CLA	CMB-C2B	-2.53	1.46	1.51
12	g	833	CLA	C1D-C2D	2.53	1.48	1.42
12	G	803	CLA	CMB-C2B	-2.53	1.46	1.51
12	E	810	CLA	C1D-C2D	2.53	1.48	1.42
12	a	815	CLA	C1D-C2D	2.53	1.48	1.42
12	G	833	CLA	CMB-C2B	-2.53	1.46	1.51
12	b	807	CLA	CMB-C2B	-2.53	1.46	1.51
12	G	804	CLA	CMB-C2B	-2.53	1.46	1.51
12	A	830	CLA	CMB-C2B	-2.53	1.46	1.51
12	E	812	CLA	C1D-C2D	2.53	1.48	1.42
12	B	841	CLA	CMB-C2B	-2.53	1.46	1.51
12	G	820	CLA	CMB-C2B	-2.53	1.46	1.51
12	G	808	CLA	C1D-C2D	2.53	1.48	1.42
12	a	838	CLA	CMB-C2B	-2.53	1.46	1.51
12	A	804	CLA	CMB-C2B	-2.53	1.46	1.51
12	B	813	CLA	CMB-C2B	-2.53	1.46	1.51
12	G	804	CLA	C1D-C2D	2.52	1.48	1.42
12	g	814	CLA	C1D-C2D	2.52	1.48	1.42
12	E	815	CLA	C1D-C2D	2.52	1.48	1.42
12	b	809	CLA	CMB-C2B	-2.52	1.46	1.51
12	e	804	CLA	CMB-C2B	-2.52	1.46	1.51
12	G	802	CLA	C1D-C2D	2.52	1.48	1.42
12	B	812	CLA	C1D-C2D	2.52	1.48	1.42
12	A	812	CLA	C1D-C2D	2.52	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	818	CLA	CMB-C2B	-2.52	1.46	1.51
12	B	822	CLA	C1D-C2D	2.52	1.48	1.42
12	A	807	CLA	C1D-C2D	2.52	1.48	1.42
12	a	814	CLA	C1D-C2D	2.52	1.48	1.42
12	B	813	CLA	C1D-C2D	2.52	1.48	1.42
12	b	811	CLA	CMB-C2B	-2.52	1.46	1.51
12	B	839	CLA	C1D-C2D	2.52	1.48	1.42
12	e	814	CLA	C1D-C2D	2.52	1.48	1.42
12	b	805	CLA	C1D-C2D	2.52	1.48	1.42
12	b	804	CLA	CMB-C2B	-2.52	1.46	1.51
12	B	824	CLA	CMB-C2B	-2.52	1.46	1.51
12	G	810	CLA	C1D-C2D	2.52	1.48	1.42
12	e	840	CLA	CMB-C2B	-2.52	1.46	1.51
12	g	823	CLA	CMB-C2B	-2.52	1.46	1.51
12	e	842	CLA	C1D-C2D	2.52	1.48	1.42
12	g	801	CLA	CMB-C2B	-2.52	1.46	1.51
12	E	841	CLA	C1D-C2D	2.52	1.48	1.42
12	B	815	CLA	C1D-C2D	2.52	1.48	1.42
12	e	820	CLA	C1D-C2D	2.52	1.48	1.42
12	a	806	CLA	CMB-C2B	-2.52	1.46	1.51
12	a	829	CLA	CMB-C2B	-2.52	1.46	1.51
12	g	808	CLA	CMB-C2B	-2.52	1.46	1.51
12	A	808	CLA	C1D-C2D	2.51	1.48	1.42
12	e	813	CLA	C1D-C2D	2.51	1.48	1.42
12	G	840	CLA	C1D-C2D	2.51	1.48	1.42
12	B	842	CLA	C1D-C2D	2.51	1.48	1.42
12	g	823	CLA	C1D-C2D	2.51	1.48	1.42
12	b	804	CLA	C1D-C2D	2.51	1.48	1.42
12	g	812	CLA	C1D-C2D	2.51	1.48	1.42
12	e	839	CLA	CMB-C2B	-2.51	1.46	1.51
12	B	828	CLA	CMB-C2B	-2.51	1.46	1.51
12	B	833	CLA	C1D-C2D	2.51	1.48	1.42
12	g	829	CLA	CMB-C2B	-2.51	1.46	1.51
12	b	821	CLA	CMB-C2B	-2.51	1.46	1.51
12	g	810	CLA	C1D-C2D	2.51	1.48	1.42
12	g	838	CLA	CMB-C2B	-2.51	1.46	1.51
12	B	816	CLA	C1D-C2D	2.51	1.48	1.42
12	G	828	CLA	CMB-C2B	-2.51	1.46	1.51
12	b	828	CLA	CMB-C2B	-2.51	1.46	1.51
12	G	830	CLA	C1D-C2D	2.51	1.48	1.42
12	b	811	CLA	C1D-C2D	2.51	1.48	1.42
12	b	824	CLA	CMB-C2B	-2.51	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	837	CLA	CMB-C2B	-2.51	1.46	1.51
12	e	813	CLA	CMB-C2B	-2.51	1.46	1.51
12	A	833	CLA	CMB-C2B	-2.51	1.46	1.51
12	A	803	CLA	CMB-C2B	-2.51	1.46	1.51
12	A	837	CLA	C1D-C2D	2.51	1.48	1.42
12	b	830	CLA	CMB-C2B	-2.51	1.46	1.51
12	G	825	CLA	CMB-C2B	-2.51	1.46	1.51
12	e	823	CLA	CMB-C2B	-2.51	1.46	1.51
12	a	835	CLA	CMB-C2B	-2.51	1.46	1.51
12	B	832	CLA	CMB-C2B	-2.51	1.46	1.51
12	G	837	CLA	C1D-C2D	2.51	1.48	1.42
12	a	831	CLA	CMB-C2B	-2.51	1.46	1.51
12	E	825	CLA	CMB-C2B	-2.50	1.46	1.51
12	E	830	CLA	CMB-C2B	-2.50	1.46	1.51
12	e	845	CLA	CMB-C2B	-2.50	1.46	1.51
12	b	841	CLA	C1D-C2D	2.50	1.48	1.42
12	A	822	CLA	CMB-C2B	-2.50	1.46	1.51
12	g	819	CLA	C1D-C2D	2.50	1.48	1.42
12	B	817	CLA	C1D-C2D	2.50	1.48	1.42
12	S	1501	CLA	CMB-C2B	-2.50	1.46	1.51
12	b	803	CLA	C1D-C2D	2.50	1.48	1.42
12	A	841	CLA	CMB-C2B	-2.50	1.46	1.51
12	a	816	CLA	C1D-C2D	2.50	1.48	1.42
12	G	820	CLA	C1D-C2D	2.50	1.48	1.42
12	a	839	CLA	C1D-C2D	2.50	1.48	1.42
12	A	815	CLA	CMB-C2B	-2.50	1.46	1.51
12	G	827	CLA	CMB-C2B	-2.50	1.46	1.51
12	g	835	CLA	C1D-C2D	2.50	1.48	1.42
12	A	814	CLA	C1D-C2D	2.50	1.48	1.42
12	B	823	CLA	CMB-C2B	-2.50	1.46	1.51
12	a	817	CLA	CMB-C2B	-2.50	1.46	1.51
12	e	842	CLA	CMB-C2B	-2.50	1.46	1.51
12	B	801	CLA	CMB-C2B	-2.50	1.46	1.51
12	b	814	CLA	CMB-C2B	-2.50	1.46	1.51
12	g	821	CLA	C1D-C2D	2.50	1.48	1.42
12	g	806	CLA	CMB-C2B	-2.50	1.46	1.51
12	e	830	CLA	CMB-C2B	-2.50	1.46	1.51
12	G	826	CLA	C1D-C2D	2.50	1.48	1.42
12	b	820	CLA	C1D-C2D	2.50	1.48	1.42
12	B	806	CLA	CMB-C2B	-2.50	1.46	1.51
12	G	813	CLA	CMB-C2B	-2.50	1.46	1.51
12	A	835	CLA	C1D-C2D	2.50	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	826	CLA	C1D-C2D	2.50	1.48	1.42
12	G	818	CLA	C1D-C2D	2.50	1.48	1.42
12	g	820	CLA	CMB-C2B	-2.50	1.46	1.51
12	E	818	CLA	C1D-C2D	2.50	1.48	1.42
12	G	835	CLA	CMB-C2B	-2.50	1.46	1.51
12	e	844	CLA	C1D-C2D	2.50	1.48	1.42
12	e	834	CLA	CMB-C2B	-2.50	1.46	1.51
12	A	811	CLA	CMB-C2B	-2.50	1.46	1.51
12	A	812	CLA	CMB-C2B	-2.50	1.46	1.51
12	b	822	CLA	C1D-C2D	2.50	1.48	1.42
12	A	817	CLA	CMB-C2B	-2.50	1.46	1.51
12	s	202	CLA	CMB-C2B	-2.50	1.46	1.51
12	a	837	CLA	C1D-C2D	2.49	1.48	1.42
12	E	802	CLA	CMB-C2B	-2.49	1.46	1.51
12	A	839	CLA	CMB-C2B	-2.49	1.46	1.51
12	b	833	CLA	CMB-C2B	-2.49	1.46	1.51
12	b	809	CLA	C1D-C2D	2.49	1.48	1.42
12	g	831	CLA	CMB-C2B	-2.49	1.46	1.51
12	a	802	CLA	CMB-C2B	-2.49	1.46	1.51
12	E	815	CLA	CMB-C2B	-2.49	1.46	1.51
12	G	829	CLA	CMB-C2B	-2.49	1.46	1.51
12	g	836	CLA	CMB-C2B	-2.49	1.46	1.51
12	E	820	CLA	CMB-C2B	-2.49	1.46	1.51
12	b	827	CLA	CMB-C2B	-2.49	1.46	1.51
12	g	807	CLA	CMB-C2B	-2.49	1.46	1.51
12	E	839	CLA	C1D-C2D	2.49	1.48	1.42
12	a	801	CLA	CMB-C2B	-2.49	1.46	1.51
12	B	837	CLA	CMB-C2B	-2.49	1.46	1.51
12	B	835	CLA	CMB-C2B	-2.49	1.46	1.51
12	b	827	CLA	C1D-C2D	2.49	1.48	1.42
12	g	822	CLA	C1D-C2D	2.49	1.48	1.42
12	a	823	CLA	CMB-C2B	-2.49	1.46	1.51
12	s	204	CLA	C1D-C2D	2.49	1.48	1.42
12	A	827	CLA	CMB-C2B	-2.49	1.46	1.51
12	b	826	CLA	CMB-C2B	-2.49	1.46	1.51
12	g	830	CLA	CMB-C2B	-2.49	1.46	1.51
12	b	814	CLA	C1D-C2D	2.49	1.48	1.42
12	E	842	CLA	CMB-C2B	-2.49	1.46	1.51
12	B	807	CLA	CMB-C2B	-2.49	1.46	1.51
12	E	817	CLA	C1D-C2D	2.49	1.48	1.42
12	g	815	CLA	C1D-C2D	2.49	1.48	1.42
12	A	834	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	202	CLA	CMB-C2B	-2.49	1.46	1.51
12	g	820	CLA	C1D-C2D	2.49	1.48	1.42
12	e	838	CLA	C1D-C2D	2.49	1.48	1.42
12	G	806	CLA	C1D-C2D	2.49	1.48	1.42
12	a	817	CLA	C1D-C2D	2.49	1.48	1.42
12	B	815	CLA	CMB-C2B	-2.49	1.46	1.51
12	b	806	CLA	CMB-C2B	-2.49	1.46	1.51
12	A	801	CLA	C1D-C2D	2.49	1.48	1.42
12	e	827	CLA	C1D-C2D	2.49	1.48	1.42
12	G	832	CLA	C1D-C2D	2.49	1.48	1.42
12	g	828	CLA	C1D-C2D	2.49	1.48	1.42
12	b	829	CLA	CMB-C2B	-2.49	1.46	1.51
12	a	811	CLA	CMB-C2B	-2.49	1.46	1.51
12	e	829	CLA	C1D-C2D	2.49	1.48	1.42
12	B	826	CLA	CMB-C2B	-2.49	1.46	1.51
12	e	815	CLA	C1D-C2D	2.48	1.48	1.42
12	G	821	CLA	C1D-C2D	2.48	1.48	1.42
12	g	815	CLA	CMB-C2B	-2.48	1.46	1.51
12	e	841	CLA	CMB-C2B	-2.48	1.46	1.51
12	g	806	CLA	C1D-C2D	2.48	1.48	1.42
12	L	203	CLA	CMB-C2B	-2.48	1.46	1.51
12	a	841	CLA	CMB-C2B	-2.48	1.46	1.51
12	E	838	CLA	CMB-C2B	-2.48	1.46	1.51
12	E	843	CLA	CMB-C2B	-2.48	1.46	1.51
12	b	806	CLA	C1D-C2D	2.48	1.48	1.42
12	b	805	CLA	CMB-C2B	-2.48	1.46	1.51
12	A	815	CLA	C1D-C2D	2.48	1.48	1.42
12	A	833	CLA	C1D-C2D	2.48	1.48	1.42
12	A	805	CLA	C1D-C2D	2.48	1.48	1.42
12	g	814	CLA	CMB-C2B	-2.48	1.46	1.51
12	B	816	CLA	CMB-C2B	-2.48	1.46	1.51
12	e	834	CLA	C1D-C2D	2.48	1.48	1.42
12	B	823	CLA	C1D-C2D	2.48	1.48	1.42
12	l	202	CLA	CMB-C2B	-2.48	1.46	1.51
12	e	835	CLA	CMB-C2B	-2.48	1.46	1.51
12	e	816	CLA	CMB-C2B	-2.48	1.46	1.51
12	a	825	CLA	CMB-C2B	-2.48	1.46	1.51
12	e	801	CLA	CMB-C2B	-2.48	1.46	1.51
12	G	817	CLA	C1D-C2D	2.48	1.48	1.42
12	b	835	CLA	C1D-C2D	2.48	1.48	1.42
12	b	822	CLA	CMB-C2B	-2.48	1.46	1.51
12	g	813	CLA	CMB-C2B	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	e	806	CLA	C1D-C2D	2.48	1.48	1.42
12	G	843	CLA	CMB-C2B	-2.48	1.46	1.51
12	E	829	CLA	CMB-C2B	-2.48	1.46	1.51
12	g	808	CLA	C1D-C2D	2.48	1.48	1.42
12	B	829	CLA	C1D-C2D	2.48	1.48	1.42
12	B	807	CLA	C1D-C2D	2.48	1.48	1.42
12	G	823	CLA	CMB-C2B	-2.48	1.46	1.51
12	G	832	CLA	CMB-C2B	-2.48	1.46	1.51
12	a	813	CLA	CMB-C2B	-2.48	1.46	1.51
12	E	844	CLA	CMB-C2B	-2.48	1.46	1.51
12	a	813	CLA	C1D-C2D	2.48	1.48	1.42
12	E	804	CLA	CMB-C2B	-2.48	1.46	1.51
12	a	807	CLA	C1D-C2D	2.48	1.48	1.42
12	B	821	CLA	C1D-C2D	2.48	1.48	1.42
12	e	823	CLA	C1D-C2D	2.48	1.48	1.42
12	b	836	CLA	CMB-C2B	-2.48	1.46	1.51
12	E	822	CLA	C1D-C2D	2.48	1.48	1.42
12	B	839	CLA	CMB-C2B	-2.48	1.46	1.51
12	E	824	CLA	CMB-C2B	-2.48	1.46	1.51
12	G	819	CLA	C1D-C2D	2.48	1.48	1.42
12	e	802	CLA	CMB-C2B	-2.48	1.46	1.51
12	E	820	CLA	C1D-C2D	2.48	1.48	1.42
12	e	836	CLA	C1D-C2D	2.48	1.48	1.42
12	g	816	CLA	C1D-C2D	2.48	1.48	1.42
12	G	805	CLA	CMB-C2B	-2.48	1.46	1.51
12	b	821	CLA	C1D-C2D	2.48	1.48	1.42
12	B	830	CLA	C1D-C2D	2.48	1.48	1.42
12	B	830	CLA	CMB-C2B	-2.48	1.46	1.51
12	a	828	CLA	C1D-C2D	2.47	1.48	1.42
12	e	810	CLA	CMB-C2B	-2.47	1.46	1.51
12	A	821	CLA	CMB-C2B	-2.47	1.46	1.51
12	B	835	CLA	C1D-C2D	2.47	1.48	1.42
12	B	829	CLA	CMB-C2B	-2.47	1.46	1.51
12	b	819	CLA	CMB-C2B	-2.47	1.46	1.51
12	E	829	CLA	C1D-C2D	2.47	1.48	1.42
12	B	838	CLA	CMB-C2B	-2.47	1.46	1.51
12	e	818	CLA	CMB-C2B	-2.47	1.46	1.51
12	G	825	CLA	C1D-C2D	2.47	1.48	1.42
12	b	815	CLA	C1D-C2D	2.47	1.48	1.42
12	A	822	CLA	C1D-C2D	2.47	1.48	1.42
12	E	801	CLA	C1D-C2D	2.47	1.48	1.42
12	a	819	CLA	C1D-C2D	2.47	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	814	CLA	CMB-C2B	-2.47	1.46	1.51
12	a	842	CLA	CMB-C2B	-2.47	1.46	1.51
12	G	812	CLA	CMB-C2B	-2.47	1.46	1.51
12	b	819	CLA	C1D-C2D	2.47	1.48	1.42
12	a	840	CLA	CMB-C2B	-2.47	1.46	1.51
12	A	817	CLA	C1D-C2D	2.47	1.48	1.42
12	b	825	CLA	CMB-C2B	-2.47	1.46	1.51
12	E	832	CLA	CMB-C2B	-2.47	1.46	1.51
12	B	831	CLA	CMB-C2B	-2.47	1.46	1.51
12	A	819	CLA	C1D-C2D	2.47	1.48	1.42
12	J	1101	CLA	CMB-C2B	-2.47	1.46	1.51
12	G	821	CLA	CMB-C2B	-2.47	1.46	1.51
12	a	824	CLA	CMB-C2B	-2.47	1.46	1.51
12	b	808	CLA	CMB-C2B	-2.47	1.46	1.51
12	a	808	CLA	CMB-C2B	-2.47	1.46	1.51
12	g	810	CLA	CMB-C2B	-2.47	1.46	1.51
12	s	202	CLA	C1D-C2D	2.47	1.48	1.42
12	L	202	CLA	C1D-C2D	2.47	1.48	1.42
12	A	801	CLA	CMB-C2B	-2.47	1.46	1.51
12	s	203	CLA	CMB-C2B	-2.47	1.46	1.51
12	b	813	CLA	CMB-C2B	-2.47	1.46	1.51
12	l	204	CLA	C1D-C2D	2.47	1.48	1.42
12	G	818	CLA	CMB-C2B	-2.47	1.46	1.51
12	E	809	CLA	CMB-C2B	-2.46	1.46	1.51
12	S	1501	CLA	C1D-C2D	2.46	1.48	1.42
12	A	810	CLA	C1D-C2D	2.46	1.48	1.42
12	S	1502	CLA	CMB-C2B	-2.46	1.46	1.51
12	b	810	CLA	CMB-C2B	-2.46	1.46	1.51
12	e	807	CLA	CMB-C2B	-2.46	1.46	1.51
12	a	819	CLA	CMB-C2B	-2.46	1.46	1.51
12	e	822	CLA	CMB-C2B	-2.46	1.46	1.51
12	e	811	CLA	C1D-C2D	2.46	1.48	1.42
12	E	825	CLA	C1D-C2D	2.46	1.48	1.42
12	G	805	CLA	C1D-C2D	2.46	1.48	1.42
12	g	828	CLA	CMB-C2B	-2.46	1.46	1.51
12	E	826	CLA	CMB-C2B	-2.46	1.46	1.51
12	G	813	CLA	C1D-C2D	2.46	1.48	1.42
12	a	836	CLA	CMB-C2B	-2.46	1.46	1.51
12	b	828	CLA	C1D-C2D	2.46	1.48	1.42
12	A	806	CLA	CMB-C2B	-2.46	1.46	1.51
12	B	821	CLA	CMB-C2B	-2.46	1.46	1.51
12	e	817	CLA	C1D-C2D	2.46	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	g	824	CLA	CMB-C2B	-2.46	1.46	1.51
12	a	803	CLA	CMB-C2B	-2.46	1.46	1.51
12	E	819	CLA	C1D-C2D	2.46	1.48	1.42
12	A	826	CLA	C1D-C2D	2.46	1.48	1.42
12	a	821	CLA	C1D-C2D	2.46	1.48	1.42
12	l	202	CLA	C1D-C2D	2.46	1.48	1.42
12	B	809	CLA	C1D-C2D	2.46	1.48	1.42
12	G	824	CLA	C1D-C2D	2.46	1.48	1.42
12	B	808	CLA	CMB-C2B	-2.46	1.46	1.51
12	B	840	CLA	CMB-C2B	-2.46	1.46	1.51
12	b	825	CLA	C1D-C2D	2.46	1.48	1.42
12	A	826	CLA	CMB-C2B	-2.46	1.46	1.51
12	s	204	CLA	CMB-C2B	-2.46	1.46	1.51
12	a	801	CLA	C1D-C2D	2.46	1.48	1.42
12	e	812	CLA	C1D-C2D	2.46	1.48	1.42
12	g	825	CLA	CMB-C2B	-2.46	1.46	1.51
12	A	829	CLA	CMB-C2B	-2.46	1.46	1.51
12	A	838	CLA	CMB-C2B	-2.46	1.46	1.51
12	E	828	CLA	CMB-C2B	-2.46	1.46	1.51
12	A	823	CLA	C1D-C2D	2.46	1.48	1.42
12	A	831	CLA	CMB-C2B	-2.46	1.46	1.51
12	E	808	CLA	C1D-C2D	2.46	1.48	1.42
12	b	837	CLA	CMB-C2B	-2.46	1.46	1.51
12	g	818	CLA	CMB-C2B	-2.46	1.46	1.51
12	l	203	CLA	CMB-C2B	-2.46	1.46	1.51
12	L	204	CLA	CMB-C2B	-2.46	1.46	1.51
12	A	802	CLA	CMB-C2B	-2.46	1.46	1.51
12	e	801	CLA	C1D-C2D	2.46	1.48	1.42
12	B	818	CLA	CMB-C2B	-2.46	1.46	1.51
12	B	802	CLA	CMB-C2B	-2.45	1.46	1.51
12	e	814	CLA	CMB-C2B	-2.45	1.46	1.51
12	b	818	CLA	C1D-C2D	2.45	1.48	1.42
12	g	826	CLA	C1D-C2D	2.45	1.48	1.42
12	b	832	CLA	CMB-C2B	-2.45	1.46	1.51
12	g	827	CLA	C1D-C2D	2.45	1.48	1.42
12	J	1102	CLA	C1D-C2D	2.45	1.48	1.42
12	A	840	CLA	CMB-C2B	-2.45	1.46	1.51
12	e	827	CLA	CMB-C2B	-2.45	1.46	1.51
12	g	829	CLA	C1D-C2D	2.45	1.48	1.42
12	E	813	CLA	C1D-C2D	2.45	1.48	1.42
12	g	817	CLA	CMB-C2B	-2.45	1.46	1.51
12	a	812	CLA	C1D-C2D	2.45	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	811	CLA	C1D-C2D	2.45	1.48	1.42
12	b	838	CLA	CMB-C2B	-2.45	1.46	1.51
12	G	827	CLA	C1D-C2D	2.45	1.48	1.42
12	B	820	CLA	C1D-C2D	2.45	1.48	1.42
12	B	802	CLA	C1D-C2D	2.45	1.48	1.42
12	B	827	CLA	C1D-C2D	2.45	1.48	1.42
12	a	827	CLA	C1D-C2D	2.45	1.48	1.42
12	a	825	CLA	C1D-C2D	2.45	1.48	1.42
12	A	825	CLA	C1D-C2D	2.45	1.48	1.42
12	G	836	CLA	CMB-C2B	-2.45	1.46	1.51
12	e	824	CLA	CMB-C2B	-2.45	1.46	1.51
12	e	815	CLA	CMB-C2B	-2.45	1.46	1.51
12	B	843	CLA	C1D-C2D	2.45	1.48	1.42
12	G	834	CLA	C1D-C2D	2.45	1.48	1.42
12	e	824	CLA	C1D-C2D	2.45	1.48	1.42
12	a	810	CLA	CMB-C2B	-2.45	1.46	1.51
12	a	824	CLA	C1D-C2D	2.45	1.48	1.42
12	e	812	CLA	CMB-C2B	-2.45	1.46	1.51
12	a	804	CLA	CMB-C2B	-2.45	1.46	1.51
12	G	814	CLA	C1D-C2D	2.45	1.48	1.42
12	E	817	CLA	CMB-C2B	-2.45	1.46	1.51
12	b	812	CLA	CMB-C2B	-2.45	1.46	1.51
12	G	819	CLA	CMB-C2B	-2.45	1.46	1.51
12	b	816	CLA	CMB-C2B	-2.45	1.46	1.51
12	E	805	CLA	CMB-C2B	-2.45	1.46	1.51
12	G	816	CLA	CMB-C2B	-2.45	1.46	1.51
12	A	808	CLA	CMB-C2B	-2.45	1.46	1.51
12	A	807	CLA	CMB-C2B	-2.45	1.46	1.51
12	A	825	CLA	CMB-C2B	-2.45	1.46	1.51
12	e	809	CLA	CMB-C2B	-2.44	1.46	1.51
12	G	807	CLA	CMB-C2B	-2.44	1.46	1.51
12	A	809	CLA	CMB-C2B	-2.44	1.46	1.51
12	g	802	CLA	CMB-C2B	-2.44	1.46	1.51
12	G	837	CLA	CMB-C2B	-2.44	1.46	1.51
12	g	811	CLA	CMB-C2B	-2.44	1.46	1.51
12	a	814	CLA	CMB-C2B	-2.44	1.46	1.51
12	A	810	CLA	CMB-C2B	-2.44	1.46	1.51
12	A	816	CLA	C1D-C2D	2.44	1.48	1.42
12	g	807	CLA	C1D-C2D	2.44	1.48	1.42
12	A	823	CLA	CMB-C2B	-2.44	1.46	1.51
12	a	835	CLA	C1D-C2D	2.44	1.48	1.42
12	E	837	CLA	C1D-C2D	2.44	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	e	838	CLA	CMB-C2B	-2.44	1.46	1.51
12	b	817	CLA	CMB-C2B	-2.44	1.46	1.51
12	O	1301	CLA	CMB-C2B	-2.44	1.46	1.51
12	G	838	CLA	CMB-C2B	-2.44	1.46	1.51
12	e	826	CLA	CMB-C2B	-2.44	1.46	1.51
12	E	827	CLA	C1D-C2D	2.44	1.48	1.42
12	A	832	CLA	CMB-C2B	-2.44	1.46	1.51
12	B	805	CLA	CMB-C2B	-2.44	1.46	1.51
12	e	818	CLA	C1D-C2D	2.44	1.48	1.42
12	e	845	CLA	C1D-C2D	2.44	1.48	1.42
12	E	803	CLA	CMB-C2B	-2.44	1.46	1.51
12	S	1502	CLA	C1D-C2D	2.44	1.48	1.42
12	L	204	CLA	C1D-C2D	2.44	1.48	1.42
12	E	826	CLA	C1D-C2D	2.44	1.48	1.42
12	B	808	CLA	C1D-C2D	2.44	1.48	1.42
12	b	833	CLA	C1D-C2D	2.44	1.48	1.42
12	E	811	CLA	CMB-C2B	-2.44	1.46	1.51
12	g	837	CLA	CMB-C2B	-2.44	1.46	1.51
12	A	838	CLA	C1D-C2D	2.44	1.48	1.42
12	a	840	CLA	C1D-C2D	2.44	1.48	1.42
12	G	824	CLA	CMB-C2B	-2.44	1.46	1.51
12	B	833	CLA	CMB-C2B	-2.44	1.46	1.51
12	A	824	CLA	C1D-C2D	2.44	1.48	1.42
12	G	826	CLA	CMB-C2B	-2.43	1.46	1.51
12	B	810	CLA	CMB-C2B	-2.43	1.46	1.51
12	l	204	CLA	CMB-C2B	-2.43	1.46	1.51
12	B	825	CLA	CMB-C2B	-2.43	1.46	1.51
12	B	837	CLA	C1D-C2D	2.43	1.48	1.42
12	B	827	CLA	CMB-C2B	-2.43	1.46	1.51
12	g	839	CLA	CMB-C2B	-2.43	1.46	1.51
12	e	811	CLA	CMB-C2B	-2.43	1.46	1.51
12	e	826	CLA	C1D-C2D	2.43	1.48	1.42
12	E	842	CLA	C1D-C2D	2.43	1.48	1.42
12	a	826	CLA	C1D-C2D	2.43	1.48	1.42
12	a	820	CLA	C1D-C2D	2.43	1.48	1.42
12	b	831	CLA	CMB-C2B	-2.43	1.46	1.51
12	e	804	CLA	C1D-C2D	2.43	1.48	1.42
12	E	828	CLA	C1D-C2D	2.43	1.48	1.42
12	E	835	CLA	CMB-C2B	-2.43	1.46	1.51
12	E	840	CLA	C1D-C2D	2.43	1.48	1.42
12	E	831	CLA	C1D-C2D	2.43	1.48	1.42
12	g	832	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	828	CLA	C1D-C2D	2.43	1.48	1.42
12	G	831	CLA	CMB-C2B	-2.43	1.46	1.51
12	g	802	CLA	C1D-C2D	2.43	1.48	1.42
12	e	819	CLA	C1D-C2D	2.43	1.48	1.42
12	f	1301	CLA	CMB-C2B	-2.43	1.46	1.51
12	a	818	CLA	C1D-C2D	2.43	1.48	1.42
12	a	815	CLA	CMB-C2B	-2.43	1.46	1.51
12	G	809	CLA	CMB-C2B	-2.43	1.46	1.51
12	A	814	CLA	CMB-C2B	-2.43	1.46	1.51
12	A	828	CLA	C1D-C2D	2.43	1.48	1.42
12	e	816	CLA	C1D-C2D	2.43	1.48	1.42
12	b	801	CLA	CMB-C2B	-2.43	1.46	1.51
12	e	833	CLA	CMB-C2B	-2.43	1.46	1.51
12	E	814	CLA	C1D-C2D	2.43	1.48	1.42
12	g	809	CLA	CMB-C2B	-2.43	1.46	1.51
12	a	832	CLA	C1D-C2D	2.43	1.48	1.42
12	E	841	CLA	CMB-C2B	-2.43	1.46	1.51
12	b	807	CLA	C1D-C2D	2.43	1.48	1.42
12	G	815	CLA	CMB-C2B	-2.43	1.46	1.51
12	b	801	CLA	C1D-C2D	2.43	1.48	1.42
12	b	820	CLA	CMB-C2B	-2.43	1.46	1.51
12	a	816	CLA	CMB-C2B	-2.42	1.46	1.51
12	g	826	CLA	CMB-C2B	-2.42	1.46	1.51
12	E	801	CLA	CMB-C2B	-2.42	1.46	1.51
12	a	805	CLA	C1D-C2D	2.42	1.48	1.42
12	E	812	CLA	CMB-C2B	-2.42	1.46	1.51
12	F	1301	CLA	CMB-C2B	-2.42	1.46	1.51
12	e	831	CLA	C1D-C2D	2.42	1.48	1.42
12	a	806	CLA	C1D-C2D	2.42	1.48	1.42
12	G	802	CLA	CMB-C2B	-2.42	1.46	1.51
12	a	831	CLA	C1D-C2D	2.42	1.48	1.42
12	a	834	CLA	CMB-C2B	-2.42	1.46	1.51
12	a	833	CLA	CMB-C2B	-2.42	1.46	1.51
12	A	837	CLA	CMB-C2B	-2.42	1.46	1.51
12	E	823	CLA	CMB-C2B	-2.42	1.46	1.51
12	a	839	CLA	CMB-C2B	-2.42	1.46	1.51
12	E	806	CLA	C1D-C2D	2.42	1.48	1.42
12	G	830	CLA	CMB-C2B	-2.42	1.46	1.51
12	e	806	CLA	CMB-C2B	-2.42	1.46	1.51
12	b	842	CLA	C1D-C2D	2.42	1.48	1.42
12	g	836	CLA	C1D-C2D	2.42	1.48	1.42
12	B	819	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	818	CLA	C1D-C2D	2.42	1.48	1.42
12	G	841	CLA	C1D-C2D	2.42	1.48	1.42
12	e	832	CLA	CMB-C2B	-2.42	1.46	1.51
12	B	822	CLA	CMB-C2B	-2.42	1.46	1.51
12	A	813	CLA	CMB-C2B	-2.42	1.46	1.51
12	o	1301	CLA	CMB-C2B	-2.42	1.46	1.51
12	E	807	CLA	C1D-C2D	2.42	1.48	1.42
12	a	830	CLA	C1D-C2D	2.42	1.48	1.42
12	e	839	CLA	C1D-C2D	2.42	1.48	1.42
12	e	803	CLA	CMB-C2B	-2.42	1.46	1.51
12	a	828	CLA	CMB-C2B	-2.42	1.46	1.51
12	A	805	CLA	CMB-C2B	-2.42	1.46	1.51
12	B	836	CLA	C1D-C2D	2.42	1.48	1.42
12	E	810	CLA	CMB-C2B	-2.42	1.46	1.51
12	A	804	CLA	C1D-C2D	2.41	1.48	1.42
12	B	834	CLA	CMB-C2B	-2.41	1.46	1.51
12	E	816	CLA	CMB-C2B	-2.41	1.46	1.51
12	G	811	CLA	CMB-C2B	-2.41	1.46	1.51
12	B	814	CLA	CMB-C2B	-2.41	1.46	1.51
12	A	828	CLA	CMB-C2B	-2.41	1.46	1.51
12	E	808	CLA	CMB-C2B	-2.41	1.46	1.51
12	a	827	CLA	CMB-C2B	-2.41	1.46	1.51
12	E	836	CLA	CMB-C2B	-2.41	1.46	1.51
12	E	813	CLA	CMB-C2B	-2.41	1.46	1.51
12	G	833	CLA	C1D-C2D	2.41	1.48	1.42
12	e	805	CLA	C1D-C2D	2.41	1.48	1.42
12	B	810	CLA	C1D-C2D	2.41	1.48	1.42
12	A	803	CLA	C1D-C2D	2.41	1.48	1.42
12	b	836	CLA	C1D-C2D	2.41	1.48	1.42
12	b	839	CLA	CMB-C2B	-2.41	1.46	1.51
12	G	822	CLA	CMB-C2B	-2.41	1.46	1.51
12	e	837	CLA	C1D-C2D	2.41	1.48	1.42
12	A	836	CLA	C1D-C2D	2.41	1.48	1.42
12	E	834	CLA	C1D-C2D	2.41	1.48	1.42
12	B	812	CLA	CMB-C2B	-2.41	1.46	1.51
12	g	842	CLA	C1D-C2D	2.41	1.48	1.42
12	b	823	CLA	CMB-C2B	-2.40	1.46	1.51
12	E	821	CLA	C1D-C2D	2.40	1.48	1.42
12	g	833	CLA	CMB-C2B	-2.40	1.46	1.51
12	r	1401	CLA	CMB-C2B	-2.40	1.46	1.51
12	G	807	CLA	C1D-C2D	2.40	1.48	1.42
12	E	803	CLA	C1D-C2D	2.40	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	g	821	CLA	CMB-C2B	-2.40	1.46	1.51
12	e	830	CLA	C1D-C2D	2.40	1.48	1.42
12	a	807	CLA	CMB-C2B	-2.40	1.46	1.51
12	e	821	CLA	CMB-C2B	-2.40	1.46	1.51
12	e	829	CLA	CMB-C2B	-2.40	1.46	1.51
12	l	201	CLA	C1D-C2D	2.39	1.48	1.42
12	G	835	CLA	C1D-C2D	2.39	1.48	1.42
12	a	809	CLA	CMB-C2B	-2.39	1.46	1.51
12	E	832	CLA	C1D-C2D	2.39	1.48	1.42
12	a	838	CLA	C1D-C2D	2.39	1.48	1.42
12	e	817	CLA	CMB-C2B	-2.39	1.46	1.51
12	g	809	CLA	C1D-C2D	2.39	1.48	1.42
12	A	830	CLA	C1D-C2D	2.39	1.48	1.42
12	e	825	CLA	C1D-C2D	2.39	1.48	1.42
12	e	844	CLA	CMB-C2B	-2.39	1.46	1.51
12	g	816	CLA	CMB-C2B	-2.39	1.46	1.51
12	k	1401	CLA	CMB-C2B	-2.39	1.46	1.51
12	A	829	CLA	C1D-C2D	2.39	1.48	1.42
12	A	820	CLA	CMB-C2B	-2.39	1.46	1.51
12	b	834	CLA	C1D-C2D	2.39	1.48	1.42
12	E	831	CLA	CMB-C2B	-2.38	1.46	1.51
12	e	808	CLA	CMB-C2B	-2.38	1.46	1.51
12	b	808	CLA	C1D-C2D	2.38	1.48	1.42
12	g	834	CLA	C1D-C2D	2.38	1.48	1.42
12	a	822	CLA	CMB-C2B	-2.38	1.46	1.51
12	a	802	CLA	C1D-C2D	2.38	1.48	1.42
12	K	1401	CLA	CMB-C2B	-2.38	1.46	1.51
12	B	831	CLA	C1D-C2D	2.38	1.48	1.42
12	E	819	CLA	CMB-C2B	-2.38	1.46	1.51
12	b	803	CLA	CMB-C2B	-2.38	1.46	1.51
12	A	816	CLA	CMB-C2B	-2.38	1.46	1.51
12	a	830	CLA	CMB-C2B	-2.38	1.46	1.51
12	R	1401	CLA	CMB-C2B	-2.37	1.46	1.51
12	b	815	CLA	CMB-C2B	-2.37	1.46	1.51
12	G	828	CLA	C1D-C2D	2.37	1.47	1.42
12	B	817	CLA	CMB-C2B	-2.37	1.46	1.51
12	L	201	CLA	C1D-C2D	2.37	1.47	1.42
12	g	830	CLA	C1D-C2D	2.37	1.47	1.42
12	b	829	CLA	C1D-C2D	2.36	1.47	1.42
12	a	818	CLA	CMB-C2B	-2.36	1.46	1.51
12	a	812	CLA	CMB-C2B	-2.35	1.46	1.51
12	s	201	CLA	C1D-C2D	2.35	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	802	CLA	C1D-C2D	2.35	1.47	1.42
12	g	801	CLA	C1D-C2D	2.35	1.47	1.42
12	G	814	CLA	CMB-C2B	-2.35	1.46	1.51
12	E	833	CLA	C1D-C2D	2.35	1.47	1.42
12	G	841	CLA	CMD-C2D	-2.34	1.45	1.51
12	g	835	CLA	CMB-C2B	-2.32	1.46	1.51
12	G	839	CLA	C1D-C2D	2.32	1.47	1.42
12	B	843	CLA	CMD-C2D	-2.32	1.46	1.51
12	g	842	CLA	CMD-C2D	-2.32	1.46	1.51
12	a	802	CLA	CMD-C2D	-2.32	1.46	1.51
12	E	802	CLA	CMD-C2D	-2.32	1.46	1.51
12	G	834	CLA	CMB-C2B	-2.31	1.46	1.51
12	a	831	CLA	CMD-C2D	-2.31	1.46	1.51
12	g	801	CLA	CMD-C2D	-2.31	1.46	1.51
12	b	835	CLA	CMB-C2B	-2.31	1.46	1.51
12	b	842	CLA	CMD-C2D	-2.31	1.46	1.51
12	B	801	CLA	C1D-C2D	2.30	1.47	1.42
12	J	1102	CLA	CMB-C2B	-2.30	1.46	1.51
12	B	801	CLA	CMD-C2D	-2.30	1.46	1.51
12	g	840	CLA	C1D-C2D	2.29	1.47	1.42
12	E	832	CLA	CMD-C2D	-2.29	1.46	1.51
12	b	840	CLA	C1D-C2D	2.29	1.47	1.42
12	A	827	CLA	C3B-C2B	-2.28	1.37	1.40
12	E	830	CLA	C3B-C2B	-2.28	1.37	1.40
12	B	841	CLA	C1D-C2D	2.27	1.47	1.42
13	a	844	PQN	O1-C1	-2.27	1.18	1.23
12	A	829	CLA	CMD-C2D	-2.27	1.46	1.51
12	B	837	CLA	CMD-C2D	-2.26	1.46	1.51
12	b	836	CLA	CMD-C2D	-2.25	1.46	1.51
12	g	806	CLA	CMD-C2D	-2.24	1.46	1.51
12	E	806	CLA	CMD-C2D	-2.24	1.46	1.51
12	E	815	CLA	CMD-C2D	-2.24	1.46	1.51
12	e	830	CLA	CMD-C2D	-2.24	1.46	1.51
12	a	841	CLA	CMD-C2D	-2.24	1.46	1.51
12	G	835	CLA	CMD-C2D	-2.24	1.46	1.51
12	A	803	CLA	CMD-C2D	-2.23	1.46	1.51
12	g	836	CLA	CMD-C2D	-2.23	1.46	1.51
12	A	839	CLA	C3B-C2B	-2.23	1.37	1.40
12	a	805	CLA	CMD-C2D	-2.23	1.46	1.51
12	b	805	CLA	CMD-C2D	-2.23	1.46	1.51
12	B	807	CLA	CMD-C2D	-2.22	1.46	1.51
13	E	846	PQN	O1-C1	-2.22	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	e	843	PQN	O1-C1	-2.22	1.18	1.23
12	G	804	CLA	CMD-C2D	-2.22	1.46	1.51
12	a	814	CLA	C3B-C2B	-2.22	1.37	1.40
12	A	812	CLA	CMD-C2D	-2.22	1.46	1.51
12	e	804	CLA	CMD-C2D	-2.22	1.46	1.51
12	e	813	CLA	CMD-C2D	-2.22	1.46	1.51
12	a	806	CLA	CMD-C2D	-2.21	1.46	1.51
13	G	842	PQN	O1-C1	-2.21	1.18	1.23
12	E	807	CLA	CMD-C2D	-2.21	1.46	1.51
12	e	840	CLA	CMD-C2D	-2.21	1.46	1.51
12	a	829	CLA	C3B-C2B	-2.21	1.37	1.40
12	g	827	CLA	CMD-C2D	-2.21	1.46	1.51
12	B	808	CLA	CMD-C2D	-2.21	1.46	1.51
12	a	825	CLA	CMD-C2D	-2.21	1.46	1.51
12	b	826	CLA	CMD-C2D	-2.21	1.46	1.51
12	l	201	CLA	CMD-C2D	-2.21	1.46	1.51
12	A	804	CLA	CMD-C2D	-2.21	1.46	1.51
12	E	843	CLA	CMD-C2D	-2.20	1.46	1.51
12	G	807	CLA	CMD-C2D	-2.20	1.46	1.51
12	a	817	CLA	CMD-C2D	-2.20	1.46	1.51
12	E	826	CLA	CMD-C2D	-2.20	1.46	1.51
12	a	837	CLA	C3B-C2B	-2.20	1.37	1.40
12	b	806	CLA	CMD-C2D	-2.20	1.46	1.51
12	A	812	CLA	C3B-C2B	-2.19	1.37	1.40
12	b	808	CLA	CMD-C2D	-2.19	1.46	1.51
12	A	839	CLA	CMD-C2D	-2.19	1.46	1.51
12	e	824	CLA	CMD-C2D	-2.19	1.46	1.51
12	G	824	CLA	CMD-C2D	-2.19	1.46	1.51
12	A	835	CLA	C3B-C2B	-2.19	1.37	1.40
12	g	809	CLA	CMD-C2D	-2.19	1.46	1.51
12	B	828	CLA	CMD-C2D	-2.19	1.46	1.51
12	b	801	CLA	CMC-C2C	-2.19	1.46	1.50
12	B	803	CLA	CMD-C2D	-2.19	1.46	1.51
12	G	825	CLA	CMD-C2D	-2.19	1.46	1.51
12	g	803	CLA	CMD-C2D	-2.19	1.46	1.51
12	g	807	CLA	CMD-C2D	-2.19	1.46	1.51
12	a	814	CLA	CMD-C2D	-2.19	1.46	1.51
12	B	805	CLA	CMD-C2D	-2.19	1.46	1.51
12	G	802	CLA	CMD-C2D	-2.18	1.46	1.51
12	e	836	CLA	C3B-C2B	-2.18	1.37	1.40
12	G	805	CLA	CMD-C2D	-2.18	1.46	1.51
12	b	802	CLA	CMD-C2D	-2.18	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	841	CLA	C3B-C2B	-2.18	1.37	1.40
12	A	829	CLA	C3B-C2B	-2.18	1.37	1.40
12	E	820	CLA	CMD-C2D	-2.18	1.46	1.51
12	B	827	CLA	CMD-C2D	-2.18	1.46	1.51
12	E	843	CLA	C3B-C2B	-2.18	1.37	1.40
12	E	839	CLA	C3B-C2B	-2.18	1.37	1.40
12	E	827	CLA	CMD-C2D	-2.18	1.46	1.51
12	e	831	CLA	CMD-C2D	-2.18	1.46	1.51
12	E	818	CLA	CMD-C2D	-2.18	1.46	1.51
12	a	833	CLA	CMD-C2D	-2.18	1.46	1.51
12	e	829	CLA	CMD-C2D	-2.18	1.46	1.51
12	E	803	CLA	CMD-C2D	-2.18	1.46	1.51
12	A	828	CLA	CMD-C2D	-2.17	1.46	1.51
12	b	829	CLA	CMD-C2D	-2.17	1.46	1.51
12	A	823	CLA	CMD-C2D	-2.17	1.46	1.51
12	E	834	CLA	CMD-C2D	-2.17	1.46	1.51
12	G	832	CLA	CMD-C2D	-2.17	1.46	1.51
12	A	841	CLA	CMD-C2D	-2.17	1.46	1.51
12	B	802	CLA	CMC-C2C	-2.17	1.46	1.50
12	a	811	CLA	CMD-C2D	-2.17	1.46	1.51
12	E	803	CLA	CMC-C2C	-2.17	1.46	1.50
12	e	816	CLA	CMC-C2C	-2.17	1.46	1.50
12	E	840	CLA	CMD-C2D	-2.17	1.46	1.51
12	G	801	CLA	CMD-C2D	-2.17	1.46	1.51
12	E	833	CLA	CMD-C2D	-2.17	1.46	1.51
12	e	816	CLA	CMD-C2D	-2.17	1.46	1.51
12	e	844	CLA	CMD-C2D	-2.17	1.46	1.51
12	E	816	CLA	CMD-C2D	-2.17	1.46	1.51
12	L	203	CLA	CMD-C2D	-2.17	1.46	1.51
12	b	827	CLA	CMD-C2D	-2.17	1.46	1.51
12	b	825	CLA	CMD-C2D	-2.17	1.46	1.51
12	E	809	CLA	CMD-C2D	-2.17	1.46	1.51
12	A	815	CLA	CMD-C2D	-2.17	1.46	1.51
12	g	824	CLA	CMD-C2D	-2.17	1.46	1.51
13	g	843	PQN	O1-C1	-2.17	1.18	1.23
12	e	818	CLA	CMD-C2D	-2.17	1.46	1.51
12	a	826	CLA	CMD-C2D	-2.17	1.46	1.51
12	e	805	CLA	CMD-C2D	-2.17	1.46	1.51
12	G	818	CLA	CMD-C2D	-2.16	1.46	1.51
12	B	822	CLA	CMC-C2C	-2.16	1.46	1.50
12	l	203	CLA	CMD-C2D	-2.16	1.46	1.51
12	b	801	CLA	CMD-C2D	-2.16	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	831	CLA	CMD-C2D	-2.16	1.46	1.51
12	E	835	CLA	CMD-C2D	-2.16	1.46	1.51
12	g	820	CLA	CMD-C2D	-2.16	1.46	1.51
12	A	806	CLA	CMD-C2D	-2.16	1.46	1.51
12	e	813	CLA	C3B-C2B	-2.16	1.37	1.40
12	e	825	CLA	CMD-C2D	-2.16	1.46	1.51
12	A	831	CLA	CMD-C2D	-2.16	1.46	1.51
12	s	201	CLA	CMD-C2D	-2.16	1.46	1.51
12	g	828	CLA	CMD-C2D	-2.16	1.46	1.51
12	L	201	CLA	CMD-C2D	-2.16	1.46	1.51
12	B	810	CLA	CMD-C2D	-2.16	1.46	1.51
12	e	810	CLA	CMD-C2D	-2.16	1.46	1.51
12	a	810	CLA	CMD-C2D	-2.16	1.46	1.51
12	E	831	CLA	CMD-C2D	-2.16	1.46	1.51
12	b	833	CLA	CMD-C2D	-2.16	1.46	1.51
12	E	818	CLA	CMC-C2C	-2.16	1.46	1.50
12	A	837	CLA	CMD-C2D	-2.16	1.46	1.51
13	B	844	PQN	O1-C1	-2.16	1.18	1.23
12	A	824	CLA	CMD-C2D	-2.16	1.46	1.51
12	b	803	CLA	CMD-C2D	-2.16	1.46	1.51
12	G	806	CLA	CMD-C2D	-2.16	1.46	1.51
12	a	839	CLA	CMD-C2D	-2.16	1.46	1.51
12	G	801	CLA	CMC-C2C	-2.16	1.46	1.50
12	g	821	CLA	CMC-C2C	-2.16	1.46	1.50
12	G	833	CLA	CMD-C2D	-2.16	1.46	1.51
13	b	843	PQN	O1-C1	-2.16	1.18	1.23
12	G	819	CLA	CMC-C2C	-2.16	1.46	1.50
12	B	809	CLA	CMD-C2D	-2.16	1.46	1.51
12	B	833	CLA	CMD-C2D	-2.16	1.46	1.51
12	b	819	CLA	CMD-C2D	-2.15	1.46	1.51
12	A	817	CLA	CMD-C2D	-2.15	1.46	1.51
12	A	810	CLA	CMD-C2D	-2.15	1.46	1.51
12	b	820	CLA	CMD-C2D	-2.15	1.46	1.51
12	a	834	CLA	CMD-C2D	-2.15	1.46	1.51
12	G	821	CLA	CMD-C2D	-2.15	1.46	1.51
12	g	830	CLA	CMD-C2D	-2.15	1.46	1.51
12	B	836	CLA	CMD-C2D	-2.15	1.46	1.51
12	B	820	CLA	CMD-C2D	-2.15	1.46	1.51
12	G	826	CLA	CMD-C2D	-2.15	1.46	1.51
12	E	815	CLA	C3B-C2B	-2.15	1.37	1.40
12	E	841	CLA	CMD-C2D	-2.15	1.46	1.51
12	B	824	CLA	CMD-C2D	-2.15	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	808	CLA	CMD-C2D	-2.15	1.46	1.51
12	A	807	CLA	CMD-C2D	-2.15	1.46	1.51
12	a	830	CLA	CMD-C2D	-2.15	1.46	1.51
12	g	823	CLA	CMD-C2D	-2.15	1.46	1.51
12	a	817	CLA	CMC-C2C	-2.15	1.46	1.50
12	b	815	CLA	CMD-C2D	-2.15	1.46	1.51
12	e	837	CLA	CMD-C2D	-2.15	1.46	1.51
12	g	826	CLA	CMD-C2D	-2.15	1.46	1.51
12	G	831	CLA	CMD-C2D	-2.15	1.46	1.51
12	e	832	CLA	CMD-C2D	-2.15	1.46	1.51
12	E	825	CLA	CMD-C2D	-2.15	1.46	1.51
12	e	808	CLA	CMD-C2D	-2.15	1.46	1.51
12	b	822	CLA	CMD-C2D	-2.15	1.46	1.51
12	B	832	CLA	CMD-C2D	-2.15	1.46	1.51
12	B	835	CLA	CMD-C2D	-2.15	1.46	1.51
12	a	821	CLA	CMD-C2D	-2.15	1.46	1.51
12	e	845	CLA	CMD-C2D	-2.15	1.46	1.51
13	A	842	PQN	O1-C1	-2.15	1.18	1.23
12	g	802	CLA	CMC-C2C	-2.15	1.46	1.50
12	g	816	CLA	CMD-C2D	-2.15	1.46	1.51
13	B	844	PQN	O4-C4	-2.14	1.18	1.23
12	e	828	CLA	C3B-C2B	-2.14	1.37	1.40
12	b	832	CLA	CMD-C2D	-2.14	1.46	1.51
12	A	821	CLA	CMD-C2D	-2.14	1.46	1.51
12	G	814	CLA	CMD-C2D	-2.14	1.46	1.51
12	b	834	CLA	CMD-C2D	-2.14	1.46	1.51
12	g	802	CLA	CMD-C2D	-2.14	1.46	1.51
12	L	202	CLA	CMD-C2D	-2.14	1.46	1.51
12	e	834	CLA	C3B-C2B	-2.14	1.37	1.40
12	B	802	CLA	CMD-C2D	-2.14	1.46	1.51
12	A	830	CLA	C3B-C2B	-2.14	1.37	1.40
12	b	831	CLA	CMD-C2D	-2.14	1.46	1.51
12	E	812	CLA	CMD-C2D	-2.14	1.46	1.51
12	A	836	CLA	CMD-C2D	-2.14	1.46	1.51
12	e	809	CLA	CMD-C2D	-2.14	1.46	1.51
12	A	815	CLA	CMC-C2C	-2.14	1.46	1.50
12	B	811	CLA	CMD-C2D	-2.14	1.46	1.51
12	g	832	CLA	CMD-C2D	-2.14	1.46	1.51
12	G	819	CLA	CMD-C2D	-2.14	1.46	1.51
12	e	823	CLA	CMD-C2D	-2.14	1.46	1.51
12	a	809	CLA	CMD-C2D	-2.14	1.46	1.51
12	a	832	CLA	CMD-C2D	-2.14	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	812	CLA	CMD-C2D	-2.14	1.46	1.51
12	e	838	CLA	CMD-C2D	-2.14	1.46	1.51
12	b	804	CLA	CMD-C2D	-2.14	1.46	1.51
12	a	835	CLA	C3B-C2B	-2.14	1.37	1.40
12	a	838	CLA	CMD-C2D	-2.14	1.46	1.51
12	E	823	CLA	CMD-C2D	-2.14	1.46	1.51
12	A	840	CLA	CMD-C2D	-2.14	1.46	1.51
12	g	819	CLA	CMD-C2D	-2.14	1.46	1.51
12	A	835	CLA	CMD-C2D	-2.14	1.46	1.51
12	a	832	CLA	C3B-C2B	-2.14	1.37	1.40
12	G	843	CLA	CMD-C2D	-2.14	1.46	1.51
12	a	815	CLA	CMD-C2D	-2.14	1.46	1.51
12	a	819	CLA	CMD-C2D	-2.14	1.46	1.51
12	a	813	CLA	CMD-C2D	-2.14	1.46	1.51
12	s	203	CLA	CMD-C2D	-2.14	1.46	1.51
12	g	805	CLA	CMD-C2D	-2.14	1.46	1.51
12	E	832	CLA	C3B-C2B	-2.13	1.37	1.40
12	a	822	CLA	CMD-C2D	-2.13	1.46	1.51
12	g	821	CLA	CMD-C2D	-2.13	1.46	1.51
12	a	831	CLA	C3B-C2B	-2.13	1.37	1.40
12	a	837	CLA	CMD-C2D	-2.13	1.46	1.51
12	b	818	CLA	CMD-C2D	-2.13	1.46	1.51
12	E	844	CLA	CMD-C2D	-2.13	1.46	1.51
12	A	808	CLA	CMD-C2D	-2.13	1.46	1.51
12	a	828	CLA	CMD-C2D	-2.13	1.46	1.51
12	a	824	CLA	CMD-C2D	-2.13	1.46	1.51
12	e	820	CLA	CMD-C2D	-2.13	1.46	1.51
13	b	843	PQN	O4-C4	-2.13	1.18	1.23
12	g	835	CLA	CMD-C2D	-2.13	1.46	1.51
12	e	841	CLA	CMD-C2D	-2.13	1.46	1.51
12	A	822	CLA	CMD-C2D	-2.13	1.46	1.51
12	E	811	CLA	CMD-C2D	-2.13	1.46	1.51
12	f	1301	CLA	CMD-C2D	-2.13	1.46	1.51
12	G	828	CLA	CMD-C2D	-2.13	1.46	1.51
12	g	831	CLA	CMD-C2D	-2.13	1.46	1.51
12	B	825	CLA	CMD-C2D	-2.13	1.46	1.51
12	E	813	CLA	CMD-C2D	-2.13	1.46	1.51
12	A	809	CLA	CMD-C2D	-2.13	1.46	1.51
12	E	836	CLA	CMD-C2D	-2.13	1.46	1.51
12	G	817	CLA	CMD-C2D	-2.13	1.46	1.51
12	G	812	CLA	CMD-C2D	-2.13	1.46	1.51
12	G	810	CLA	CMD-C2D	-2.13	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	e	833	CLA	CMD-C2D	-2.13	1.46	1.51
12	E	817	CLA	CMD-C2D	-2.13	1.46	1.51
12	k	1401	CLA	CMD-C2D	-2.13	1.46	1.51
12	B	806	CLA	CMD-C2D	-2.13	1.46	1.51
12	b	816	CLA	CMD-C2D	-2.13	1.46	1.51
12	A	833	CLA	C3B-C2B	-2.13	1.37	1.40
12	g	808	CLA	CMD-C2D	-2.13	1.46	1.51
12	E	838	CLA	CMD-C2D	-2.13	1.46	1.51
12	B	839	CLA	CMD-C2D	-2.13	1.46	1.51
12	B	840	CLA	CMD-C2D	-2.13	1.46	1.51
12	A	819	CLA	CMD-C2D	-2.13	1.46	1.51
12	A	832	CLA	CMD-C2D	-2.13	1.46	1.51
12	a	803	CLA	CMD-C2D	-2.13	1.46	1.51
12	B	834	CLA	CMD-C2D	-2.13	1.46	1.51
12	B	817	CLA	CMD-C2D	-2.13	1.46	1.51
12	e	830	CLA	C3B-C2B	-2.12	1.37	1.40
12	b	830	CLA	CMD-C2D	-2.12	1.46	1.51
12	A	830	CLA	CMD-C2D	-2.12	1.46	1.51
12	e	840	CLA	C3B-C2B	-2.12	1.37	1.40
12	E	822	CLA	CMD-C2D	-2.12	1.46	1.51
12	B	830	CLA	CMD-C2D	-2.12	1.46	1.51
12	A	834	CLA	CMD-C2D	-2.12	1.46	1.51
12	E	839	CLA	CMD-C2D	-2.12	1.46	1.51
12	b	802	CLA	CMC-C2C	-2.12	1.46	1.50
12	g	839	CLA	CMD-C2D	-2.12	1.46	1.51
13	g	843	PQN	O4-C4	-2.12	1.18	1.23
12	b	813	CLA	CMD-C2D	-2.12	1.46	1.51
12	e	802	CLA	CMD-C2D	-2.12	1.46	1.51
12	g	833	CLA	CMD-C2D	-2.12	1.46	1.51
12	G	820	CLA	CMD-C2D	-2.12	1.46	1.51
12	e	821	CLA	CMD-C2D	-2.12	1.46	1.51
12	e	811	CLA	CMD-C2D	-2.12	1.46	1.51
12	A	811	CLA	CMD-C2D	-2.12	1.46	1.51
12	E	810	CLA	CMD-C2D	-2.12	1.46	1.51
12	G	808	CLA	CMD-C2D	-2.12	1.46	1.51
12	g	814	CLA	CMD-C2D	-2.12	1.46	1.51
12	b	810	CLA	CMD-C2D	-2.12	1.46	1.51
12	b	823	CLA	CMD-C2D	-2.12	1.46	1.51
12	l	204	CLA	CMD-C2D	-2.12	1.46	1.51
12	b	835	CLA	CMD-C2D	-2.12	1.46	1.51
12	G	829	CLA	CMD-C2D	-2.12	1.46	1.51
12	S	1501	CLA	CMD-C2D	-2.12	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	833	CLA	CMD-C2D	-2.12	1.46	1.51
12	G	821	CLA	C3B-C2B	-2.12	1.37	1.40
12	b	809	CLA	CMD-C2D	-2.12	1.46	1.51
12	e	836	CLA	CMD-C2D	-2.12	1.46	1.51
12	A	813	CLA	CMD-C2D	-2.12	1.46	1.51
12	g	834	CLA	CMD-C2D	-2.12	1.46	1.51
12	A	818	CLA	C3B-C2B	-2.12	1.37	1.40
12	e	827	CLA	CMD-C2D	-2.12	1.46	1.51
12	e	807	CLA	CMD-C2D	-2.12	1.46	1.51
12	G	803	CLA	CMD-C2D	-2.12	1.46	1.51
12	e	835	CLA	CMD-C2D	-2.12	1.46	1.51
12	b	807	CLA	CMD-C2D	-2.12	1.46	1.51
12	s	202	CLA	CMD-C2D	-2.12	1.46	1.51
12	b	811	CLA	CMD-C2D	-2.11	1.46	1.51
12	G	813	CLA	CMD-C2D	-2.11	1.46	1.51
12	e	810	CLA	C3B-C2B	-2.11	1.37	1.40
12	b	814	CLA	CMD-C2D	-2.11	1.46	1.51
12	a	816	CLA	CMD-C2D	-2.11	1.46	1.51
12	a	836	CLA	CMD-C2D	-2.11	1.46	1.51
12	B	829	CLA	CMD-C2D	-2.11	1.46	1.51
12	b	840	CLA	CMD-C2D	-2.11	1.46	1.51
12	A	814	CLA	CMD-C2D	-2.11	1.46	1.51
12	g	812	CLA	CMD-C2D	-2.11	1.46	1.51
12	B	813	CLA	CMD-C2D	-2.11	1.46	1.51
12	e	822	CLA	CMD-C2D	-2.11	1.46	1.51
12	e	834	CLA	CMD-C2D	-2.11	1.46	1.51
12	B	815	CLA	CMD-C2D	-2.11	1.46	1.51
12	b	821	CLA	CMD-C2D	-2.11	1.46	1.51
12	E	837	CLA	CMD-C2D	-2.11	1.46	1.51
12	E	829	CLA	CMD-C2D	-2.11	1.46	1.51
12	g	822	CLA	CMD-C2D	-2.11	1.46	1.51
12	B	821	CLA	CMD-C2D	-2.11	1.46	1.51
12	l	202	CLA	CMD-C2D	-2.11	1.46	1.51
12	K	1401	CLA	CMD-C2D	-2.11	1.46	1.51
12	e	826	CLA	CMD-C2D	-2.11	1.46	1.51
12	B	822	CLA	CMD-C2D	-2.11	1.46	1.51
12	E	828	CLA	CMD-C2D	-2.11	1.46	1.51
12	R	1401	CLA	CMD-C2D	-2.11	1.46	1.51
12	e	842	CLA	CMD-C2D	-2.11	1.46	1.51
12	B	812	CLA	CMD-C2D	-2.11	1.46	1.51
12	L	204	CLA	CMD-C2D	-2.11	1.46	1.51
12	g	838	CLA	CMD-C2D	-2.11	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	g	803	CLA	CMC-C2C	-2.11	1.46	1.50
12	B	807	CLA	CMC-C2C	-2.11	1.46	1.50
12	e	819	CLA	CMD-C2D	-2.11	1.46	1.51
12	A	825	CLA	CMD-C2D	-2.11	1.46	1.51
12	e	812	CLA	CMD-C2D	-2.11	1.46	1.51
12	g	840	CLA	CMD-C2D	-2.11	1.46	1.51
12	G	822	CLA	CMD-C2D	-2.11	1.46	1.51
12	F	1301	CLA	CMD-C2D	-2.11	1.46	1.51
12	g	810	CLA	CMD-C2D	-2.11	1.46	1.51
12	b	837	CLA	CMD-C2D	-2.11	1.46	1.51
12	G	830	CLA	CMD-C2D	-2.11	1.46	1.51
13	G	842	PQN	O4-C4	-2.10	1.18	1.23
12	G	839	CLA	CMD-C2D	-2.10	1.46	1.51
12	a	820	CLA	CMD-C2D	-2.10	1.46	1.51
12	b	824	CLA	CMD-C2D	-2.10	1.46	1.51
12	e	815	CLA	CMD-C2D	-2.10	1.46	1.51
12	B	803	CLA	CMC-C2C	-2.10	1.46	1.50
12	e	814	CLA	CMD-C2D	-2.10	1.46	1.51
12	a	842	CLA	CMD-C2D	-2.10	1.46	1.51
12	A	818	CLA	CMD-C2D	-2.10	1.46	1.51
12	E	804	CLA	CMD-C2D	-2.10	1.46	1.51
12	g	815	CLA	CMD-C2D	-2.10	1.46	1.51
12	B	823	CLA	CMD-C2D	-2.10	1.46	1.51
12	e	804	CLA	CMC-C2C	-2.10	1.46	1.50
12	J	1102	CLA	CMD-C2D	-2.10	1.46	1.51
12	b	836	CLA	C3B-C2B	-2.10	1.37	1.40
12	A	820	CLA	CMD-C2D	-2.10	1.46	1.51
12	G	827	CLA	CMD-C2D	-2.10	1.46	1.51
12	G	834	CLA	CMD-C2D	-2.10	1.46	1.51
12	E	824	CLA	CMD-C2D	-2.10	1.46	1.51
12	E	805	CLA	CMD-C2D	-2.10	1.46	1.51
12	A	803	CLA	CMC-C2C	-2.10	1.46	1.50
12	J	1101	CLA	CMD-C2D	-2.09	1.46	1.51
12	G	809	CLA	CMD-C2D	-2.09	1.46	1.51
12	e	806	CLA	CMD-C2D	-2.09	1.46	1.51
12	g	817	CLA	CMD-C2D	-2.09	1.46	1.51
12	E	814	CLA	CMD-C2D	-2.09	1.46	1.51
12	E	822	CLA	C3B-C2B	-2.09	1.37	1.40
12	a	807	CLA	CMD-C2D	-2.09	1.46	1.51
12	a	804	CLA	CMD-C2D	-2.09	1.46	1.51
12	b	820	CLA	CMC-C2C	-2.09	1.46	1.50
12	A	826	CLA	CMD-C2D	-2.09	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	805	CLA	CMD-C2D	-2.09	1.46	1.51
12	G	815	CLA	CMD-C2D	-2.09	1.46	1.51
12	B	841	CLA	CMD-C2D	-2.09	1.46	1.51
13	E	846	PQN	O4-C4	-2.09	1.18	1.23
12	s	204	CLA	CMD-C2D	-2.09	1.46	1.51
12	b	839	CLA	CMD-C2D	-2.09	1.46	1.51
12	B	835	CLA	C3B-C2B	-2.09	1.37	1.40
12	E	819	CLA	CMD-C2D	-2.09	1.46	1.51
12	B	838	CLA	CMD-C2D	-2.09	1.46	1.51
12	e	831	CLA	C3B-C2B	-2.09	1.37	1.40
12	b	838	CLA	CMD-C2D	-2.09	1.46	1.51
12	r	1401	CLA	CMD-C2D	-2.09	1.46	1.51
12	G	838	CLA	CMD-C2D	-2.09	1.46	1.51
12	B	816	CLA	CMD-C2D	-2.09	1.46	1.51
12	E	802	CLA	CMC-C2C	-2.09	1.46	1.50
12	g	811	CLA	CMD-C2D	-2.09	1.46	1.51
12	B	824	CLA	C3B-C2B	-2.08	1.37	1.40
12	O	1301	CLA	CMD-C2D	-2.08	1.46	1.51
12	S	1502	CLA	CMD-C2D	-2.08	1.46	1.51
13	A	842	PQN	O4-C4	-2.08	1.18	1.23
12	E	834	CLA	C3B-C2B	-2.08	1.37	1.40
12	E	808	CLA	CMD-C2D	-2.08	1.46	1.51
12	A	816	CLA	CMD-C2D	-2.08	1.46	1.51
12	a	823	CLA	CMD-C2D	-2.08	1.46	1.51
12	g	829	CLA	CMD-C2D	-2.08	1.46	1.51
12	b	822	CLA	C3B-C2B	-2.08	1.37	1.40
12	b	810	CLA	CMC-C2C	-2.08	1.46	1.50
12	e	828	CLA	CMD-C2D	-2.08	1.46	1.51
12	b	828	CLA	CMD-C2D	-2.08	1.46	1.51
12	B	818	CLA	CMD-C2D	-2.08	1.46	1.51
12	e	819	CLA	C3B-C2B	-2.08	1.37	1.40
12	E	821	CLA	CMD-C2D	-2.08	1.46	1.51
12	A	802	CLA	CMD-C2D	-2.08	1.46	1.51
12	b	805	CLA	CMC-C2C	-2.08	1.46	1.50
12	g	825	CLA	CMD-C2D	-2.08	1.46	1.51
12	a	835	CLA	CMD-C2D	-2.08	1.46	1.51
12	g	801	CLA	CMC-C2C	-2.08	1.46	1.50
12	a	811	CLA	C3B-C2B	-2.08	1.37	1.40
12	B	826	CLA	CMD-C2D	-2.07	1.46	1.51
12	g	823	CLA	C3B-C2B	-2.07	1.37	1.40
12	G	804	CLA	CMC-C2C	-2.07	1.46	1.50
12	g	813	CLA	CMD-C2D	-2.07	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	o	1301	CLA	CMD-C2D	-2.07	1.46	1.51
12	e	845	CLA	C3B-C2B	-2.07	1.37	1.40
12	g	836	CLA	C3B-C2B	-2.07	1.37	1.40
12	e	817	CLA	CMD-C2D	-2.07	1.46	1.51
12	B	801	CLA	CMC-C2C	-2.07	1.46	1.50
12	E	837	CLA	C3B-C2B	-2.07	1.37	1.40
12	E	830	CLA	CMD-C2D	-2.07	1.46	1.51
12	g	837	CLA	CMD-C2D	-2.07	1.46	1.51
12	a	827	CLA	CMD-C2D	-2.07	1.46	1.51
12	A	809	CLA	C3B-C2B	-2.07	1.37	1.40
12	B	814	CLA	CMD-C2D	-2.07	1.46	1.51
12	A	835	CLA	C3B-CAB	-2.07	1.43	1.47
12	G	816	CLA	CMD-C2D	-2.07	1.46	1.51
12	g	803	CLA	C3B-C2B	-2.07	1.37	1.40
12	G	809	CLA	CMC-C2C	-2.07	1.46	1.50
12	G	823	CLA	CMD-C2D	-2.06	1.46	1.51
12	G	832	CLA	C3B-C2B	-2.06	1.37	1.40
12	G	836	CLA	CMD-C2D	-2.06	1.46	1.51
12	g	818	CLA	CMD-C2D	-2.06	1.46	1.51
12	G	837	CLA	CMD-C2D	-2.06	1.46	1.51
12	E	812	CLA	C3B-C2B	-2.06	1.37	1.40
12	B	819	CLA	CMD-C2D	-2.06	1.46	1.51
12	E	842	CLA	CMD-C2D	-2.06	1.46	1.51
12	g	841	CLA	CMD-C2D	-2.06	1.46	1.51
13	e	843	PQN	O4-C4	-2.06	1.18	1.23
12	e	836	CLA	C3B-CAB	-2.06	1.43	1.47
12	l	202	CLA	CMC-C2C	-2.06	1.46	1.50
12	A	824	CLA	C3B-C2B	-2.06	1.37	1.40
13	a	844	PQN	O4-C4	-2.05	1.18	1.23
12	B	837	CLA	C3B-C2B	-2.05	1.37	1.40
12	B	812	CLA	CMC-C2C	-2.05	1.46	1.50
12	a	838	CLA	C3B-CAB	-2.05	1.43	1.47
12	E	821	CLA	C3B-C2B	-2.05	1.37	1.40
12	E	806	CLA	CMC-C2C	-2.05	1.46	1.50
12	G	840	CLA	CMD-C2D	-2.05	1.46	1.51
12	S	1501	CLA	CMC-C2C	-2.05	1.46	1.50
12	a	818	CLA	CMD-C2D	-2.05	1.46	1.51
12	e	837	CLA	C3B-CAB	-2.05	1.43	1.47
12	b	841	CLA	CMD-C2D	-2.05	1.46	1.51
12	E	839	CLA	C3B-CAB	-2.05	1.43	1.47
12	b	812	CLA	CMD-C2D	-2.05	1.46	1.51
12	a	805	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	821	CLA	C3B-C2B	-2.05	1.37	1.40
12	A	827	CLA	CMD-C2D	-2.05	1.46	1.51
12	G	835	CLA	C3B-C2B	-2.05	1.37	1.40
12	e	803	CLA	CMD-C2D	-2.05	1.46	1.51
12	E	801	CLA	CMD-C2D	-2.05	1.46	1.51
12	a	820	CLA	C3B-C2B	-2.04	1.37	1.40
12	A	838	CLA	CMD-C2D	-2.04	1.46	1.51
12	b	833	CLA	C3B-C2B	-2.04	1.37	1.40
12	a	802	CLA	CMC-C2C	-2.04	1.46	1.50
12	a	827	CLA	CMC-C2C	-2.04	1.46	1.50
12	a	829	CLA	CMD-C2D	-2.04	1.46	1.51
12	g	806	CLA	CMC-C2C	-2.04	1.46	1.50
12	E	828	CLA	CMC-C2C	-2.04	1.46	1.50
12	g	811	CLA	CMC-C2C	-2.04	1.46	1.50
12	b	802	CLA	C3B-C2B	-2.03	1.37	1.40
12	b	817	CLA	CMD-C2D	-2.03	1.46	1.51
12	s	202	CLA	CMC-C2C	-2.03	1.46	1.50
12	e	825	CLA	C3B-C2B	-2.03	1.37	1.40
12	E	840	CLA	C3B-CAB	-2.03	1.43	1.47
12	E	827	CLA	C3B-C2B	-2.03	1.37	1.40
12	B	841	CLA	C3B-C2B	-2.03	1.37	1.40
12	e	801	CLA	CMD-C2D	-2.03	1.46	1.51
12	B	843	CLA	C3B-C2B	-2.03	1.37	1.40
12	e	820	CLA	C3B-C2B	-2.03	1.37	1.40
12	G	811	CLA	CMD-C2D	-2.03	1.46	1.51
12	L	202	CLA	CMC-C2C	-2.03	1.46	1.50
12	e	839	CLA	CMD-C2D	-2.03	1.46	1.51
12	A	819	CLA	C3B-C2B	-2.03	1.37	1.40
12	B	803	CLA	C3B-C2B	-2.02	1.37	1.40
12	a	801	CLA	CMD-C2D	-2.02	1.46	1.51
12	g	842	CLA	C3B-C2B	-2.02	1.37	1.40
12	a	840	CLA	CMD-C2D	-2.02	1.46	1.51
12	L	201	CLA	C3B-C2B	-2.02	1.37	1.40
12	g	826	CLA	CMC-C2C	-2.02	1.46	1.50
12	G	841	CLA	C3B-C2B	-2.02	1.37	1.40
12	B	842	CLA	C3B-C2B	-2.02	1.37	1.40
12	b	842	CLA	CMC-C2C	-2.02	1.46	1.50
12	a	837	CLA	C3B-CAB	-2.02	1.43	1.47
12	A	801	CLA	CMD-C2D	-2.01	1.46	1.51
12	b	829	CLA	CMC-C2C	-2.01	1.46	1.50
12	B	842	CLA	CMD-C2D	-2.01	1.46	1.51
12	E	805	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	840	CLA	C3B-C2B	-2.01	1.37	1.40
12	b	842	CLA	C3B-C2B	-2.01	1.37	1.40
12	A	836	CLA	C3B-CAB	-2.01	1.43	1.47
12	a	826	CLA	C3B-C2B	-2.01	1.37	1.40
12	G	828	CLA	CMC-C2C	-2.01	1.46	1.50
12	E	840	CLA	C3B-C2B	-2.01	1.37	1.40
12	B	819	CLA	CMC-C2C	-2.01	1.46	1.50
12	a	804	CLA	CMC-C2C	-2.00	1.46	1.50
12	B	830	CLA	CMC-C2C	-2.00	1.46	1.50
12	b	838	CLA	C3B-C2B	-2.00	1.37	1.40
12	B	839	CLA	C3B-C2B	-2.00	1.37	1.40

All (3068) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	806	CLA	C4A-NA-C1A	7.42	110.04	106.71
12	e	807	CLA	C4A-NA-C1A	7.33	110.00	106.71
12	e	837	CLA	C4A-NA-C1A	7.30	109.99	106.71
12	E	809	CLA	C4A-NA-C1A	7.27	109.98	106.71
12	b	840	CLA	C4A-NA-C1A	7.24	109.96	106.71
12	B	841	CLA	C4A-NA-C1A	7.24	109.96	106.71
12	a	838	CLA	C4A-NA-C1A	7.22	109.95	106.71
12	A	836	CLA	C4A-NA-C1A	7.21	109.95	106.71
12	a	808	CLA	C4A-NA-C1A	7.16	109.93	106.71
12	E	840	CLA	C4A-NA-C1A	7.14	109.92	106.71
12	g	840	CLA	C4A-NA-C1A	7.14	109.92	106.71
12	G	839	CLA	C4A-NA-C1A	7.11	109.90	106.71
12	b	822	CLA	C4A-NA-C1A	7.06	109.88	106.71
12	e	835	CLA	C4A-NA-C1A	7.02	109.86	106.71
12	a	822	CLA	C4A-NA-C1A	7.00	109.86	106.71
12	e	821	CLA	C4A-NA-C1A	7.00	109.85	106.71
12	E	823	CLA	C4A-NA-C1A	6.99	109.85	106.71
12	A	820	CLA	C4A-NA-C1A	6.99	109.85	106.71
12	G	821	CLA	C4A-NA-C1A	6.97	109.84	106.71
12	a	836	CLA	C4A-NA-C1A	6.96	109.83	106.71
12	A	834	CLA	C4A-NA-C1A	6.96	109.83	106.71
12	A	816	CLA	C4A-NA-C1A	6.93	109.82	106.71
12	B	820	CLA	C4A-NA-C1A	6.92	109.82	106.71
12	b	820	CLA	C4A-NA-C1A	6.92	109.81	106.71
12	b	830	CLA	C4A-NA-C1A	6.91	109.81	106.71
12	b	818	CLA	C4A-NA-C1A	6.90	109.81	106.71
12	g	819	CLA	C4A-NA-C1A	6.89	109.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	823	CLA	C4A-NA-C1A	6.89	109.81	106.71
12	b	809	CLA	C4A-NA-C1A	6.89	109.80	106.71
12	E	838	CLA	C4A-NA-C1A	6.89	109.80	106.71
12	g	810	CLA	C4A-NA-C1A	6.89	109.80	106.71
12	G	815	CLA	C4A-NA-C1A	6.88	109.80	106.71
12	B	824	CLA	C4A-NA-C1A	6.88	109.80	106.71
12	b	839	CLA	C4A-NA-C1A	6.88	109.80	106.71
12	g	821	CLA	C4A-NA-C1A	6.88	109.80	106.71
12	a	818	CLA	C4A-NA-C1A	6.87	109.80	106.71
12	b	802	CLA	C4A-NA-C1A	6.87	109.79	106.71
12	e	817	CLA	C4A-NA-C1A	6.86	109.79	106.71
12	b	806	CLA	C4A-NA-C1A	6.85	109.78	106.71
12	G	813	CLA	C4A-NA-C1A	6.85	109.78	106.71
12	G	809	CLA	C4A-NA-C1A	6.84	109.78	106.71
12	G	808	CLA	C4A-NA-C1A	6.84	109.78	106.71
12	E	819	CLA	C4A-NA-C1A	6.84	109.78	106.71
12	g	839	CLA	C4A-NA-C1A	6.83	109.78	106.71
12	G	817	CLA	C4A-NA-C1A	6.83	109.78	106.71
12	B	811	CLA	C4A-NA-C1A	6.82	109.77	106.71
12	g	807	CLA	C4A-NA-C1A	6.82	109.77	106.71
12	b	814	CLA	C4A-NA-C1A	6.81	109.77	106.71
12	b	810	CLA	C4A-NA-C1A	6.80	109.76	106.71
12	B	840	CLA	C4A-NA-C1A	6.80	109.76	106.71
12	g	817	CLA	C4A-NA-C1A	6.80	109.76	106.71
12	G	805	CLA	C4A-NA-C1A	6.80	109.76	106.71
12	b	816	CLA	C4A-NA-C1A	6.80	109.76	106.71
12	e	806	CLA	C4A-NA-C1A	6.80	109.76	106.71
12	a	825	CLA	C4A-NA-C1A	6.79	109.76	106.71
12	g	815	CLA	C4A-NA-C1A	6.79	109.76	106.71
12	G	836	CLA	C4A-NA-C1A	6.79	109.76	106.71
12	e	836	CLA	C4A-NA-C1A	6.79	109.76	106.71
12	E	813	CLA	C4A-NA-C1A	6.79	109.76	106.71
12	G	838	CLA	C4A-NA-C1A	6.79	109.76	106.71
12	G	801	CLA	C4A-NA-C1A	6.78	109.76	106.71
12	A	805	CLA	C4A-NA-C1A	6.78	109.76	106.71
12	B	822	CLA	C4A-NA-C1A	6.78	109.75	106.71
12	E	839	CLA	C4A-NA-C1A	6.78	109.75	106.71
12	g	837	CLA	C4A-NA-C1A	6.76	109.75	106.71
12	A	823	CLA	C4A-NA-C1A	6.76	109.75	106.71
12	B	803	CLA	C4A-NA-C1A	6.76	109.74	106.71
12	E	808	CLA	C4A-NA-C1A	6.76	109.74	106.71
12	B	816	CLA	C4A-NA-C1A	6.75	109.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	812	CLA	C4A-NA-C1A	6.75	109.74	106.71
12	B	812	CLA	C4A-NA-C1A	6.75	109.74	106.71
12	B	838	CLA	C4A-NA-C1A	6.75	109.74	106.71
12	g	803	CLA	C4A-NA-C1A	6.75	109.74	106.71
12	B	832	CLA	C4A-NA-C1A	6.74	109.74	106.71
12	G	819	CLA	C4A-NA-C1A	6.74	109.74	106.71
12	a	831	CLA	C4A-NA-C1A	6.74	109.74	106.71
12	B	808	CLA	C4A-NA-C1A	6.74	109.74	106.71
12	e	811	CLA	C4A-NA-C1A	6.73	109.73	106.71
12	e	824	CLA	C4A-NA-C1A	6.73	109.73	106.71
12	B	818	CLA	C4A-NA-C1A	6.73	109.73	106.71
12	G	829	CLA	C4A-NA-C1A	6.73	109.73	106.71
12	E	832	CLA	C4A-NA-C1A	6.72	109.73	106.71
12	A	835	CLA	C4A-NA-C1A	6.72	109.73	106.71
12	B	825	CLA	C4A-NA-C1A	6.72	109.73	106.71
12	g	811	CLA	C4A-NA-C1A	6.72	109.73	106.71
12	E	826	CLA	C4A-NA-C1A	6.71	109.72	106.71
12	g	831	CLA	C4A-NA-C1A	6.70	109.72	106.71
12	e	830	CLA	C4A-NA-C1A	6.70	109.72	106.71
12	E	818	CLA	C4A-NA-C1A	6.69	109.72	106.71
12	a	837	CLA	C4A-NA-C1A	6.68	109.71	106.71
12	e	834	CLA	C4A-NA-C1A	6.67	109.71	106.71
12	A	810	CLA	C4A-NA-C1A	6.67	109.71	106.71
12	a	823	CLA	C4A-NA-C1A	6.67	109.70	106.71
12	A	833	CLA	C4A-NA-C1A	6.67	109.70	106.71
12	b	837	CLA	C4A-NA-C1A	6.66	109.70	106.71
12	a	807	CLA	C4A-NA-C1A	6.66	109.70	106.71
12	E	824	CLA	C4A-NA-C1A	6.66	109.70	106.71
12	g	826	CLA	C4A-NA-C1A	6.66	109.70	106.71
12	G	824	CLA	C4A-NA-C1A	6.65	109.70	106.71
12	b	823	CLA	C4A-NA-C1A	6.64	109.69	106.71
12	G	822	CLA	C4A-NA-C1A	6.63	109.69	106.71
12	g	838	CLA	C4A-NA-C1A	6.62	109.68	106.71
12	A	829	CLA	C4A-NA-C1A	6.62	109.68	106.71
12	G	837	CLA	C4A-NA-C1A	6.62	109.68	106.71
12	e	828	CLA	C4A-NA-C1A	6.61	109.68	106.71
12	l	201	CLA	C4A-NA-C1A	6.61	109.68	106.71
12	g	825	CLA	C4A-NA-C1A	6.61	109.68	106.71
12	b	838	CLA	C4A-NA-C1A	6.61	109.68	106.71
12	e	822	CLA	C4A-NA-C1A	6.61	109.68	106.71
12	a	835	CLA	C4A-NA-C1A	6.61	109.68	106.71
12	g	824	CLA	C4A-NA-C1A	6.60	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	825	CLA	C4A-NA-C1A	6.60	109.67	106.71
12	B	827	CLA	C4A-NA-C1A	6.60	109.67	106.71
12	A	841	CLA	C4A-NA-C1A	6.59	109.67	106.71
12	a	829	CLA	C4A-NA-C1A	6.58	109.66	106.71
12	B	836	CLA	C4A-NA-C1A	6.58	109.66	106.71
12	B	826	CLA	C4A-NA-C1A	6.57	109.66	106.71
12	a	817	CLA	C4A-NA-C1A	6.57	109.66	106.71
12	a	842	CLA	C4A-NA-C1A	6.57	109.66	106.71
12	s	203	CLA	C4A-NA-C1A	6.56	109.66	106.71
12	A	815	CLA	C4A-NA-C1A	6.56	109.66	106.71
12	G	833	CLA	C4A-NA-C1A	6.56	109.66	106.71
12	A	821	CLA	C4A-NA-C1A	6.56	109.65	106.71
12	G	823	CLA	C4A-NA-C1A	6.56	109.65	106.71
12	l	203	CLA	C4A-NA-C1A	6.55	109.65	106.71
12	B	839	CLA	C4A-NA-C1A	6.55	109.65	106.71
12	b	824	CLA	C4A-NA-C1A	6.55	109.65	106.71
12	g	841	CLA	C4A-NA-C1A	6.54	109.65	106.71
12	E	837	CLA	C4A-NA-C1A	6.54	109.65	106.71
12	g	834	CLA	C4A-NA-C1A	6.54	109.65	106.71
12	L	203	CLA	C4A-NA-C1A	6.54	109.65	106.71
12	G	843	CLA	C4A-NA-C1A	6.54	109.65	106.71
12	E	830	CLA	C4A-NA-C1A	6.53	109.64	106.71
12	b	815	CLA	C4A-NA-C1A	6.53	109.64	106.71
12	L	201	CLA	C4A-NA-C1A	6.53	109.64	106.71
12	b	834	CLA	C4A-NA-C1A	6.52	109.64	106.71
12	B	817	CLA	C4A-NA-C1A	6.52	109.64	106.71
12	b	826	CLA	C4A-NA-C1A	6.52	109.64	106.71
12	s	201	CLA	C4A-NA-C1A	6.51	109.63	106.71
12	E	833	CLA	C4A-NA-C1A	6.50	109.63	106.71
12	B	842	CLA	C4A-NA-C1A	6.50	109.63	106.71
12	G	814	CLA	C4A-NA-C1A	6.50	109.63	106.71
12	G	828	CLA	C4A-NA-C1A	6.50	109.63	106.71
12	e	803	CLA	C4A-NA-C1A	6.49	109.63	106.71
12	A	827	CLA	C4A-NA-C1A	6.49	109.63	106.71
12	e	816	CLA	C4A-NA-C1A	6.49	109.62	106.71
12	E	807	CLA	C4A-NA-C1A	6.49	109.62	106.71
12	E	805	CLA	C4A-NA-C1A	6.49	109.62	106.71
12	A	831	CLA	C4A-NA-C1A	6.48	109.62	106.71
12	g	816	CLA	C4A-NA-C1A	6.48	109.62	106.71
12	A	807	CLA	C4A-NA-C1A	6.48	109.62	106.71
12	e	832	CLA	C4A-NA-C1A	6.48	109.62	106.71
12	A	838	CLA	C4A-NA-C1A	6.48	109.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	842	CLA	C4A-NA-C1A	6.48	109.62	106.71
12	G	826	CLA	C4A-NA-C1A	6.47	109.62	106.71
12	A	832	CLA	C4A-NA-C1A	6.47	109.62	106.71
12	b	841	CLA	C4A-NA-C1A	6.47	109.61	106.71
12	a	826	CLA	C4A-NA-C1A	6.47	109.61	106.71
12	e	815	CLA	C4A-NA-C1A	6.47	109.61	106.71
12	E	810	CLA	C4A-NA-C1A	6.47	109.61	106.71
12	G	825	CLA	C4A-NA-C1A	6.46	109.61	106.71
12	e	839	CLA	C4A-NA-C1A	6.46	109.61	106.71
12	G	840	CLA	C4A-NA-C1A	6.45	109.61	106.71
12	e	842	CLA	C4A-NA-C1A	6.45	109.61	106.71
12	a	809	CLA	C4A-NA-C1A	6.45	109.61	106.71
12	e	808	CLA	C4A-NA-C1A	6.45	109.61	106.71
12	B	831	CLA	C4A-NA-C1A	6.45	109.61	106.71
12	E	831	CLA	C4A-NA-C1A	6.45	109.60	106.71
12	B	810	CLA	C4A-NA-C1A	6.44	109.60	106.71
12	a	833	CLA	C4A-NA-C1A	6.44	109.60	106.71
12	a	827	CLA	C4A-NA-C1A	6.44	109.60	106.71
12	A	814	CLA	C4A-NA-C1A	6.44	109.60	106.71
12	g	830	CLA	C4A-NA-C1A	6.44	109.60	106.71
12	e	820	CLA	C4A-NA-C1A	6.44	109.60	106.71
12	a	830	CLA	C4A-NA-C1A	6.43	109.60	106.71
12	S	1502	CLA	C4A-NA-C1A	6.43	109.60	106.71
12	E	827	CLA	C4A-NA-C1A	6.43	109.60	106.71
12	g	828	CLA	C4A-NA-C1A	6.43	109.60	106.71
12	a	834	CLA	C4A-NA-C1A	6.43	109.60	106.71
12	a	840	CLA	C4A-NA-C1A	6.43	109.60	106.71
12	B	828	CLA	C4A-NA-C1A	6.43	109.59	106.71
12	g	827	CLA	C4A-NA-C1A	6.42	109.59	106.71
12	E	836	CLA	C4A-NA-C1A	6.42	109.59	106.71
12	A	804	CLA	C4A-NA-C1A	6.42	109.59	106.71
12	A	819	CLA	C4A-NA-C1A	6.41	109.59	106.71
12	b	827	CLA	C4A-NA-C1A	6.41	109.59	106.71
12	b	821	CLA	C4A-NA-C1A	6.41	109.59	106.71
12	e	805	CLA	C4A-NA-C1A	6.41	109.59	106.71
12	E	802	CLA	C4A-NA-C1A	6.41	109.59	106.71
12	E	835	CLA	C4A-NA-C1A	6.41	109.59	106.71
12	a	821	CLA	C4A-NA-C1A	6.41	109.59	106.71
12	e	829	CLA	C4A-NA-C1A	6.41	109.59	106.71
12	b	811	CLA	C4A-NA-C1A	6.41	109.59	106.71
12	R	1401	CLA	C4A-NA-C1A	6.40	109.58	106.71
12	K	1401	CLA	C4A-NA-C1A	6.40	109.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	840	CLA	C4A-NA-C1A	6.40	109.58	106.71
12	a	806	CLA	C4A-NA-C1A	6.40	109.58	106.71
12	A	824	CLA	C4A-NA-C1A	6.40	109.58	106.71
12	G	807	CLA	C4A-NA-C1A	6.40	109.58	106.71
12	g	822	CLA	C4A-NA-C1A	6.39	109.58	106.71
12	a	805	CLA	C4A-NA-C1A	6.39	109.58	106.71
12	A	828	CLA	C4A-NA-C1A	6.39	109.58	106.71
12	e	809	CLA	C4A-NA-C1A	6.39	109.58	106.71
12	E	828	CLA	C4A-NA-C1A	6.39	109.58	106.71
12	a	841	CLA	C4A-NA-C1A	6.39	109.58	106.71
12	A	839	CLA	C4A-NA-C1A	6.39	109.58	106.71
12	b	829	CLA	C4A-NA-C1A	6.38	109.58	106.71
12	B	813	CLA	C4A-NA-C1A	6.38	109.58	106.71
12	L	204	CLA	C4A-NA-C1A	6.38	109.58	106.71
12	A	825	CLA	C4A-NA-C1A	6.38	109.58	106.71
12	B	801	CLA	C4A-NA-C1A	6.38	109.57	106.71
12	e	804	CLA	C4A-NA-C1A	6.37	109.57	106.71
12	B	829	CLA	C4A-NA-C1A	6.37	109.57	106.71
12	e	833	CLA	C4A-NA-C1A	6.37	109.57	106.71
12	a	814	CLA	C4A-NA-C1A	6.37	109.57	106.71
12	l	204	CLA	C4A-NA-C1A	6.37	109.57	106.71
12	E	822	CLA	C4A-NA-C1A	6.37	109.57	106.71
12	b	836	CLA	C4A-NA-C1A	6.37	109.57	106.71
12	g	809	CLA	C4A-NA-C1A	6.36	109.57	106.71
12	E	844	CLA	C4A-NA-C1A	6.36	109.57	106.71
12	g	801	CLA	C4A-NA-C1A	6.35	109.56	106.71
12	G	835	CLA	C4A-NA-C1A	6.35	109.56	106.71
12	g	808	CLA	C4A-NA-C1A	6.34	109.56	106.71
12	E	815	CLA	C4A-NA-C1A	6.34	109.56	106.71
12	E	806	CLA	C4A-NA-C1A	6.34	109.56	106.71
12	k	1401	CLA	C4A-NA-C1A	6.34	109.56	106.71
12	r	1401	CLA	C4A-NA-C1A	6.34	109.56	106.71
12	A	803	CLA	C4A-NA-C1A	6.34	109.56	106.71
12	E	817	CLA	C4A-NA-C1A	6.33	109.55	106.71
12	s	204	CLA	C4A-NA-C1A	6.33	109.55	106.71
12	B	823	CLA	C4A-NA-C1A	6.33	109.55	106.71
12	E	811	CLA	C4A-NA-C1A	6.33	109.55	106.71
12	G	810	CLA	C4A-NA-C1A	6.33	109.55	106.71
12	G	820	CLA	C4A-NA-C1A	6.33	109.55	106.71
12	A	808	CLA	C4A-NA-C1A	6.31	109.55	106.71
12	A	802	CLA	C4A-NA-C1A	6.31	109.55	106.71
12	b	805	CLA	C4A-NA-C1A	6.31	109.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	813	CLA	C4A-NA-C1A	6.31	109.54	106.71
12	B	837	CLA	C4A-NA-C1A	6.31	109.54	106.71
12	e	841	CLA	C4A-NA-C1A	6.31	109.54	106.71
12	E	841	CLA	C4A-NA-C1A	6.31	109.54	106.71
12	a	802	CLA	C4A-NA-C1A	6.31	109.54	106.71
12	g	806	CLA	C4A-NA-C1A	6.30	109.54	106.71
12	B	809	CLA	C4A-NA-C1A	6.30	109.54	106.71
12	E	816	CLA	C4A-NA-C1A	6.29	109.54	106.71
12	A	812	CLA	C4A-NA-C1A	6.29	109.53	106.71
12	b	808	CLA	C4A-NA-C1A	6.29	109.53	106.71
12	e	813	CLA	C4A-NA-C1A	6.29	109.53	106.71
12	a	804	CLA	C4A-NA-C1A	6.29	109.53	106.71
12	L	202	CLA	C4A-NA-C1A	6.28	109.53	106.71
12	e	825	CLA	C4A-NA-C1A	6.28	109.53	106.71
12	a	828	CLA	C4A-NA-C1A	6.28	109.53	106.71
12	g	812	CLA	C4A-NA-C1A	6.28	109.53	106.71
12	g	836	CLA	C4A-NA-C1A	6.27	109.53	106.71
12	e	826	CLA	C4A-NA-C1A	6.27	109.53	106.71
12	A	826	CLA	C4A-NA-C1A	6.27	109.53	106.71
12	a	810	CLA	C4A-NA-C1A	6.27	109.53	106.71
12	l	202	CLA	C4A-NA-C1A	6.27	109.52	106.71
12	e	810	CLA	C4A-NA-C1A	6.27	109.52	106.71
12	e	827	CLA	C4A-NA-C1A	6.27	109.52	106.71
12	s	202	CLA	C4A-NA-C1A	6.27	109.52	106.71
12	a	816	CLA	C4A-NA-C1A	6.26	109.52	106.71
12	G	827	CLA	C4A-NA-C1A	6.26	109.52	106.71
12	E	834	CLA	C4A-NA-C1A	6.26	109.52	106.71
12	a	815	CLA	C4A-NA-C1A	6.26	109.52	106.71
12	B	807	CLA	C4A-NA-C1A	6.26	109.52	106.71
12	b	828	CLA	C4A-NA-C1A	6.26	109.52	106.71
12	e	840	CLA	C4A-NA-C1A	6.25	109.52	106.71
12	e	814	CLA	C4A-NA-C1A	6.25	109.52	106.71
12	E	843	CLA	C4A-NA-C1A	6.25	109.52	106.71
12	G	818	CLA	C4A-NA-C1A	6.24	109.51	106.71
12	B	830	CLA	C4A-NA-C1A	6.23	109.51	106.71
12	E	829	CLA	C4A-NA-C1A	6.21	109.50	106.71
12	E	812	CLA	C4A-NA-C1A	6.21	109.50	106.71
12	b	807	CLA	C4A-NA-C1A	6.21	109.50	106.71
12	e	838	CLA	C4A-NA-C1A	6.21	109.50	106.71
12	O	1301	CLA	C4A-NA-C1A	6.21	109.50	106.71
12	a	839	CLA	C4A-NA-C1A	6.20	109.50	106.71
12	A	809	CLA	C4A-NA-C1A	6.20	109.49	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	806	CLA	C4A-NA-C1A	6.19	109.49	106.71
12	F	1301	CLA	C4A-NA-C1A	6.19	109.49	106.71
12	g	829	CLA	C4A-NA-C1A	6.19	109.49	106.71
12	o	1301	CLA	C4A-NA-C1A	6.19	109.49	106.71
12	a	832	CLA	C4A-NA-C1A	6.18	109.48	106.71
12	S	1501	CLA	C4A-NA-C1A	6.17	109.48	106.71
12	a	811	CLA	C4A-NA-C1A	6.17	109.48	106.71
12	A	837	CLA	C4A-NA-C1A	6.17	109.48	106.71
12	E	820	CLA	C4A-NA-C1A	6.17	109.48	106.71
12	G	830	CLA	C4A-NA-C1A	6.15	109.47	106.71
12	G	804	CLA	C4A-NA-C1A	6.15	109.47	106.71
12	B	833	CLA	C4A-NA-C1A	6.15	109.47	106.71
12	g	818	CLA	C4A-NA-C1A	6.14	109.47	106.71
12	b	831	CLA	C4A-NA-C1A	6.14	109.47	106.71
12	A	830	CLA	C4A-NA-C1A	6.14	109.47	106.71
12	e	831	CLA	C4A-NA-C1A	6.13	109.46	106.71
12	b	819	CLA	C4A-NA-C1A	6.13	109.46	106.71
12	g	820	CLA	C4A-NA-C1A	6.13	109.46	106.71
12	f	1301	CLA	C4A-NA-C1A	6.13	109.46	106.71
12	g	832	CLA	C4A-NA-C1A	6.13	109.46	106.71
12	a	803	CLA	C4A-NA-C1A	6.12	109.46	106.71
12	e	819	CLA	C4A-NA-C1A	6.12	109.46	106.71
12	B	821	CLA	C4A-NA-C1A	6.11	109.45	106.71
12	J	1101	CLA	C4A-NA-C1A	6.10	109.45	106.71
12	b	817	CLA	C4A-NA-C1A	6.09	109.45	106.71
12	e	845	CLA	C4A-NA-C1A	6.09	109.44	106.71
12	e	802	CLA	C4A-NA-C1A	6.09	109.44	106.71
12	B	835	CLA	C4A-NA-C1A	6.09	109.44	106.71
12	E	814	CLA	C4A-NA-C1A	6.09	109.44	106.71
12	e	844	CLA	C4A-NA-C1A	6.09	109.44	106.71
12	A	822	CLA	C4A-NA-C1A	6.08	109.44	106.71
12	b	812	CLA	C4A-NA-C1A	6.08	109.44	106.71
12	b	832	CLA	C4A-NA-C1A	6.07	109.44	106.71
12	G	816	CLA	C4A-NA-C1A	6.07	109.44	106.71
12	b	833	CLA	C4A-NA-C1A	6.07	109.44	106.71
12	e	812	CLA	C4A-NA-C1A	6.07	109.44	106.71
12	a	820	CLA	C4A-NA-C1A	6.07	109.44	106.71
12	g	833	CLA	C4A-NA-C1A	6.07	109.43	106.71
12	e	801	CLA	C4A-NA-C1A	6.07	109.43	106.71
12	a	819	CLA	C4A-NA-C1A	6.06	109.43	106.71
12	A	811	CLA	C4A-NA-C1A	6.06	109.43	106.71
12	B	834	CLA	C4A-NA-C1A	6.06	109.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	818	CLA	C4A-NA-C1A	6.06	109.43	106.71
12	e	823	CLA	C4A-NA-C1A	6.06	109.43	106.71
12	E	804	CLA	C4A-NA-C1A	6.06	109.43	106.71
12	G	832	CLA	C4A-NA-C1A	6.05	109.43	106.71
12	G	841	CLA	C4A-NA-C1A	6.05	109.43	106.71
12	B	819	CLA	C4A-NA-C1A	6.05	109.43	106.71
12	E	801	CLA	C4A-NA-C1A	6.05	109.42	106.71
12	a	813	CLA	C4A-NA-C1A	6.04	109.42	106.71
12	a	824	CLA	C4A-NA-C1A	6.04	109.42	106.71
12	G	802	CLA	C4A-NA-C1A	6.03	109.42	106.71
12	A	818	CLA	C4A-NA-C1A	6.02	109.41	106.71
12	A	817	CLA	C4A-NA-C1A	6.01	109.41	106.71
12	E	825	CLA	C4A-NA-C1A	6.01	109.41	106.71
12	G	811	CLA	C4A-NA-C1A	6.01	109.41	106.71
12	E	821	CLA	C4A-NA-C1A	6.01	109.41	106.71
12	B	805	CLA	C4A-NA-C1A	6.01	109.41	106.71
12	E	803	CLA	C4A-NA-C1A	6.00	109.41	106.71
12	b	801	CLA	C4A-NA-C1A	5.99	109.40	106.71
12	G	831	CLA	C4A-NA-C1A	5.98	109.40	106.71
12	b	803	CLA	C4A-NA-C1A	5.98	109.40	106.71
12	g	805	CLA	C4A-NA-C1A	5.97	109.39	106.71
12	A	801	CLA	C4A-NA-C1A	5.97	109.39	106.71
12	b	842	CLA	C4A-NA-C1A	5.97	109.39	106.71
12	B	815	CLA	C4A-NA-C1A	5.96	109.39	106.71
12	B	814	CLA	C4A-NA-C1A	5.94	109.38	106.71
12	g	842	CLA	C4A-NA-C1A	5.93	109.37	106.71
12	B	843	CLA	C4A-NA-C1A	5.93	109.37	106.71
12	g	813	CLA	C4A-NA-C1A	5.93	109.37	106.71
12	a	801	CLA	C4A-NA-C1A	5.92	109.37	106.71
12	g	802	CLA	C4A-NA-C1A	5.92	109.37	106.71
12	B	806	CLA	C4A-NA-C1A	5.92	109.37	106.71
12	B	802	CLA	C4A-NA-C1A	5.92	109.37	106.71
12	b	804	CLA	C4A-NA-C1A	5.91	109.36	106.71
12	g	814	CLA	C4A-NA-C1A	5.85	109.33	106.71
12	G	812	CLA	C4A-NA-C1A	5.84	109.33	106.71
12	b	813	CLA	C4A-NA-C1A	5.82	109.32	106.71
12	G	803	CLA	C4A-NA-C1A	5.80	109.31	106.71
12	G	834	CLA	C4A-NA-C1A	5.76	109.30	106.71
12	J	1102	CLA	C4A-NA-C1A	5.76	109.30	106.71
12	g	835	CLA	C4A-NA-C1A	5.69	109.27	106.71
12	b	835	CLA	C4A-NA-C1A	5.69	109.26	106.71
12	g	806	CLA	CMB-C2B-C1B	-4.59	121.41	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	804	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
12	b	805	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
12	B	801	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
12	a	802	CLA	CMB-C2B-C1B	-4.55	121.46	128.46
12	B	807	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
12	E	802	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
12	g	801	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
12	g	802	CLA	CMB-C2B-C1B	-4.51	121.54	128.46
12	B	802	CLA	CMB-C2B-C1B	-4.51	121.54	128.46
12	b	801	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
12	E	803	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
12	G	802	CLA	CMB-C2B-C1B	-4.29	121.88	128.46
12	A	828	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
12	B	805	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
12	a	830	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
12	e	844	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
12	a	812	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
12	e	829	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
12	b	803	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
12	E	813	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
12	A	810	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
12	a	828	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
12	e	811	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
12	A	826	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
12	E	829	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
12	l	203	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
12	e	827	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
12	L	203	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
12	E	831	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
12	b	806	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
12	G	843	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
12	G	805	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
12	g	807	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
12	B	808	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
12	s	203	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
12	J	1102	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
12	g	835	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
12	b	835	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
12	G	834	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
12	G	807	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
12	B	810	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
12	A	816	CLA	CMB-C2B-C1B	-4.11	122.15	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	818	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
12	e	817	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
12	g	809	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
12	e	832	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
12	b	808	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
12	b	831	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
12	B	833	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
12	G	830	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
12	a	833	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
12	E	819	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
12	g	832	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
12	A	825	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
12	E	835	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
12	A	831	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
12	e	803	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
12	A	802	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
12	a	804	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
12	a	822	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
12	a	827	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
12	e	826	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
12	E	805	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
12	A	820	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
12	e	821	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
12	E	828	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
12	E	823	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
12	g	828	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
12	G	826	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
12	B	829	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
12	b	827	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
12	a	805	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
12	R	1401	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
12	A	804	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
12	a	806	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
12	e	805	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
12	e	804	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
12	A	803	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
12	E	807	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
12	k	1401	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
12	K	1401	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
12	E	806	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
12	r	1401	CLA	CMB-C2B-C1B	-3.86	122.52	128.46
12	B	801	CLA	CMB-C2B-C3B	3.86	132.03	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	844	PQN	C11-C12-C13	-3.85	120.39	126.79
12	a	802	CLA	CMB-C2B-C3B	3.84	132.00	124.80
12	g	818	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
13	g	843	PQN	C11-C12-C13	-3.84	120.40	126.79
12	E	802	CLA	CMB-C2B-C3B	3.83	131.99	124.80
12	A	814	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
12	E	817	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
13	b	843	PQN	C11-C12-C13	-3.82	120.42	126.79
12	G	816	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
12	g	801	CLA	CMB-C2B-C3B	3.82	131.96	124.80
13	G	842	PQN	C11-C12-C13	-3.82	120.44	126.79
12	B	819	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
12	A	823	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
12	e	824	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
12	a	816	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
12	g	839	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
12	b	839	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
12	E	826	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
13	B	844	PQN	C11-C12-C13	-3.81	120.45	126.79
12	b	817	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
12	e	815	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
12	G	815	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
12	a	825	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
12	B	818	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
12	g	817	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
12	A	805	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
12	B	840	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
12	E	808	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
12	e	835	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
12	e	806	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
12	G	811	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
12	G	838	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
12	b	816	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
12	B	842	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
12	a	807	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
12	g	813	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
12	E	838	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
12	g	806	CLA	CMB-C2B-C3B	3.77	131.86	124.80
12	b	812	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
12	a	836	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
12	B	814	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
12	b	841	CLA	CMB-C2B-C1B	-3.74	122.71	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	804	CLA	CMB-C2B-C3B	3.74	131.82	124.80
12	A	834	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
12	G	840	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
12	b	801	CLA	CMB-C2B-C3B	3.73	131.79	124.80
12	g	802	CLA	CMB-C2B-C3B	3.73	131.79	124.80
12	B	807	CLA	CMB-C2B-C3B	3.73	131.79	124.80
12	B	802	CLA	CMB-C2B-C3B	3.72	131.78	124.80
12	b	805	CLA	CMB-C2B-C3B	3.72	131.78	124.80
12	E	803	CLA	CMB-C2B-C3B	3.72	131.77	124.80
12	a	811	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
12	g	841	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
12	e	810	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
12	l	204	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
12	B	813	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
12	E	825	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
12	A	822	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
12	a	824	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
12	L	204	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
12	g	812	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
12	S	1502	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
12	E	812	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
12	s	204	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
12	e	823	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
12	A	809	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
12	B	841	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
13	E	846	PQN	C11-C12-C13	-3.66	120.69	126.79
12	g	831	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
12	b	830	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
12	b	811	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
12	G	839	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
12	b	840	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
12	G	810	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
12	G	829	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
12	g	840	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
12	e	812	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
12	A	807	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
12	a	813	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
12	B	832	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
12	G	841	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
12	E	822	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
12	e	808	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
12	B	843	CLA	CMB-C2B-C1B	-3.62	122.90	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	837	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
12	a	821	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
12	E	810	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
12	a	809	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
12	G	836	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
12	B	838	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
12	b	821	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
12	E	814	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
12	A	828	CLA	CMB-C2B-C3B	3.61	131.56	124.80
12	G	818	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
12	A	811	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
12	a	817	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
12	s	203	CLA	CMB-C2B-C3B	3.59	131.54	124.80
12	B	821	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
12	e	820	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
12	A	819	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
12	a	830	CLA	CMB-C2B-C3B	3.58	131.52	124.80
12	g	842	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
12	b	819	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
12	g	837	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
12	G	809	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
12	e	816	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
12	J	1102	CLA	CMB-C2B-C3B	3.58	131.52	124.80
12	b	823	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
12	l	203	CLA	CMB-C2B-C3B	3.58	131.51	124.80
12	b	842	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
12	B	823	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
12	G	802	CLA	CMB-C2B-C3B	3.57	131.50	124.80
12	G	843	CLA	CMB-C2B-C3B	3.57	131.50	124.80
12	G	820	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
12	A	815	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
12	L	203	CLA	CMB-C2B-C3B	3.57	131.49	124.80
12	g	820	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
12	g	835	CLA	CMB-C2B-C3B	3.57	131.49	124.80
12	b	806	CLA	CMB-C2B-C3B	3.57	131.49	124.80
12	E	840	CLA	CMB-C2B-C1B	-3.56	122.98	128.46
12	B	805	CLA	CMB-C2B-C3B	3.56	131.48	124.80
12	g	822	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
12	e	829	CLA	CMB-C2B-C3B	3.56	131.48	124.80
12	B	812	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
12	E	818	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
12	G	805	CLA	CMB-C2B-C3B	3.56	131.48	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	831	CLA	CMB-C2B-C3B	3.56	131.48	124.80
12	G	822	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
13	A	842	PQN	C11-C12-C13	-3.56	120.87	126.79
12	g	811	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
12	B	808	CLA	CMB-C2B-C3B	3.56	131.47	124.80
12	b	803	CLA	CMB-C2B-C3B	3.56	131.47	124.80
12	A	836	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
12	e	844	CLA	CMB-C2B-C3B	3.55	131.46	124.80
12	b	835	CLA	CMB-C2B-C3B	3.55	131.46	124.80
12	g	824	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
12	a	819	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
12	G	834	CLA	CMB-C2B-C3B	3.55	131.45	124.80
12	e	837	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
12	B	825	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
12	b	810	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
12	A	817	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
12	g	807	CLA	CMB-C2B-C3B	3.54	131.44	124.80
12	a	838	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
12	e	818	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
12	E	820	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
12	B	827	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
12	E	829	CLA	CMB-C2B-C3B	3.50	131.37	124.80
12	l	202	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
12	g	826	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
12	S	1501	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
12	A	826	CLA	CMB-C2B-C3B	3.49	131.35	124.80
12	G	824	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
12	a	828	CLA	CMB-C2B-C3B	3.49	131.34	124.80
12	s	202	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
12	L	202	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
12	a	842	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
12	A	813	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
12	E	836	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
12	e	827	CLA	CMB-C2B-C3B	3.47	131.31	124.80
12	e	841	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
12	A	840	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
12	b	825	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
12	E	844	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
12	L	201	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
12	E	816	CLA	CMB-C2B-C1B	-3.45	123.15	128.46
12	b	841	CLA	O2D-CGD-O1D	-3.45	117.01	123.83
12	a	834	CLA	CMB-C2B-C1B	-3.45	123.16	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	825	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
12	G	840	CLA	O2D-CGD-O1D	-3.45	117.02	123.83
12	B	842	CLA	O2D-CGD-O1D	-3.45	117.03	123.83
12	E	833	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
12	G	821	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
12	l	201	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
12	e	833	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
12	e	811	CLA	CMB-C2B-C3B	3.44	131.26	124.80
12	A	830	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
12	s	201	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
12	E	813	CLA	CMB-C2B-C3B	3.43	131.24	124.80
12	g	841	CLA	O2D-CGD-O1D	-3.43	117.05	123.83
12	A	810	CLA	CMB-C2B-C3B	3.43	131.24	124.80
12	a	815	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
12	A	824	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
12	E	827	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
12	a	832	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
12	e	814	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
12	A	832	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
12	g	810	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
12	g	823	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
12	B	811	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
12	B	824	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
12	b	822	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
12	a	812	CLA	CMB-C2B-C3B	3.42	131.21	124.80
12	b	809	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
12	E	801	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
12	a	826	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
12	a	801	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
12	e	813	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
12	G	808	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
12	e	838	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
12	e	822	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
12	g	809	CLA	CMB-C2B-C3B	3.40	131.17	124.80
12	g	803	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
12	B	830	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
12	b	826	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
12	A	812	CLA	C1B-CHB-C4A	-3.39	123.39	130.12
12	e	831	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
12	a	823	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
12	G	825	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
12	A	837	CLA	CMB-C2B-C1B	-3.39	123.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	815	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
12	a	839	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
12	E	841	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
12	G	807	CLA	CMB-C2B-C3B	3.39	131.15	124.80
12	E	824	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
12	e	817	CLA	C1-C2-C3	-3.39	121.27	126.75
12	A	801	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
12	E	834	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
12	a	814	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
12	b	835	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
12	A	816	CLA	CMB-C2B-C3B	3.38	131.15	124.80
12	G	834	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
12	G	827	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
12	a	818	CLA	C1-C2-C3	-3.38	121.28	126.75
12	g	835	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
12	A	816	CLA	C1-C2-C3	-3.38	121.28	126.75
12	B	810	CLA	CMB-C2B-C3B	3.38	131.13	124.80
12	e	801	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
12	e	817	CLA	CMB-C2B-C3B	3.37	131.13	124.80
12	A	821	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
12	b	808	CLA	CMB-C2B-C3B	3.37	131.13	124.80
12	e	832	CLA	CMB-C2B-C3B	3.37	131.13	124.80
12	a	818	CLA	CMB-C2B-C3B	3.37	131.12	124.80
12	J	1102	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
12	B	835	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
12	g	827	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
12	e	845	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
12	G	801	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
12	E	821	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
12	B	833	CLA	CMB-C2B-C3B	3.37	131.12	124.80
12	g	829	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
12	b	831	CLA	CMB-C2B-C3B	3.37	131.12	124.80
12	E	819	CLA	C1-C2-C3	-3.37	121.30	126.75
12	G	832	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
12	E	819	CLA	CMB-C2B-C3B	3.36	131.11	124.80
12	G	830	CLA	CMB-C2B-C3B	3.36	131.11	124.80
12	A	818	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
12	g	836	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
12	e	839	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
12	e	819	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
12	b	836	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
12	A	838	CLA	CMB-C2B-C1B	-3.36	123.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	828	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
12	a	840	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
12	b	802	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
12	a	820	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
12	E	842	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
12	B	803	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
12	B	831	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
12	b	827	CLA	CMB-C2B-C3B	3.35	131.09	124.80
12	a	833	CLA	CMB-C2B-C3B	3.35	131.08	124.80
12	b	829	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
12	b	804	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
12	g	832	CLA	CMB-C2B-C3B	3.35	131.08	124.80
12	A	831	CLA	CMB-C2B-C3B	3.35	131.08	124.80
12	B	828	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
12	b	833	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
12	g	828	CLA	CMB-C2B-C3B	3.34	131.06	124.80
12	a	804	CLA	CMB-C2B-C3B	3.34	131.06	124.80
12	g	830	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
12	G	826	CLA	CMB-C2B-C3B	3.34	131.06	124.80
12	G	828	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
12	B	829	CLA	CMB-C2B-C3B	3.34	131.06	124.80
12	E	835	CLA	CMB-C2B-C3B	3.34	131.06	124.80
12	A	802	CLA	CMB-C2B-C3B	3.33	131.05	124.80
12	a	822	CLA	CMB-C2B-C3B	3.33	131.05	124.80
12	E	805	CLA	CMB-C2B-C3B	3.33	131.05	124.80
12	A	806	CLA	CHB-C4A-NA	3.33	129.12	124.51
12	e	803	CLA	CMB-C2B-C3B	3.33	131.04	124.80
12	E	804	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
12	G	835	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
12	e	802	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
12	g	805	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
12	e	821	CLA	CMB-C2B-C3B	3.31	131.01	124.80
12	J	1101	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
12	A	835	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
12	B	816	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
12	g	815	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
12	B	806	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
12	G	823	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
12	B	837	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
12	G	806	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
12	g	808	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
12	A	820	CLA	CMB-C2B-C3B	3.30	130.99	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	809	CLA	CHB-C4A-NA	3.30	129.08	124.51
12	E	839	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
12	a	837	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
12	E	823	CLA	CMB-C2B-C3B	3.30	130.99	124.80
12	g	833	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
12	e	807	CLA	CHB-C4A-NA	3.30	129.07	124.51
12	B	809	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
12	b	814	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
12	G	803	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
12	g	825	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
12	e	836	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
12	a	808	CLA	CHB-C4A-NA	3.29	129.06	124.51
12	a	803	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
12	A	812	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
12	b	824	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
12	b	807	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
12	B	834	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
12	g	813	CLA	CMB-C2B-C3B	3.28	130.94	124.80
12	A	825	CLA	CMB-C2B-C3B	3.27	130.94	124.80
12	G	813	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
12	a	814	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
12	G	811	CLA	CMB-C2B-C3B	3.27	130.93	124.80
12	B	835	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
12	b	832	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
12	b	812	CLA	CMB-C2B-C3B	3.26	130.92	124.80
12	B	826	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
12	a	810	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
12	e	842	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
12	A	808	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
12	E	809	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
12	B	814	CLA	CMB-C2B-C3B	3.25	130.89	124.80
12	G	831	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
12	a	808	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
12	E	828	CLA	CMB-C2B-C3B	3.24	130.88	124.80
12	e	809	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
12	e	813	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
12	E	815	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
12	E	837	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
12	A	833	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
12	a	835	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
12	G	832	CLA	C1B-CHB-C4A	-3.23	123.71	130.12
12	e	807	CLA	CMB-C2B-C1B	-3.23	123.50	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	806	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
12	e	834	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
12	R	1401	CLA	CMB-C2B-C3B	3.23	130.86	124.80
12	e	821	CLA	O2D-CGD-O1D	-3.23	117.45	123.83
12	g	816	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
12	a	827	CLA	CMB-C2B-C3B	3.23	130.85	124.80
12	k	1401	CLA	CMB-C2B-C3B	3.23	130.85	124.80
12	e	830	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
12	B	817	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
12	e	826	CLA	CMB-C2B-C3B	3.22	130.85	124.80
12	b	833	CLA	C1B-CHB-C4A	-3.22	123.73	130.12
12	b	813	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
12	E	832	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
12	K	1401	CLA	CMB-C2B-C3B	3.22	130.84	124.80
12	r	1401	CLA	CMB-C2B-C3B	3.22	130.84	124.80
12	G	814	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
12	A	829	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
12	a	841	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
12	E	811	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
12	a	822	CLA	O2D-CGD-O1D	-3.21	117.49	123.83
12	A	839	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
12	G	817	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
12	b	815	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
12	b	838	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
12	e	845	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
12	B	839	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
12	G	833	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
12	E	823	CLA	O2D-CGD-O1D	-3.20	117.50	123.83
12	A	820	CLA	O2D-CGD-O1D	-3.20	117.51	123.83
12	A	841	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
12	B	840	CLA	CMB-C2B-C3B	3.20	130.80	124.80
12	b	834	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
12	E	843	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
12	g	819	CLA	CMB-C2B-C1B	-3.19	123.55	128.46
12	a	831	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
12	G	837	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
12	g	839	CLA	CMB-C2B-C3B	3.19	130.78	124.80
12	G	812	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
12	G	838	CLA	CMB-C2B-C3B	3.19	130.78	124.80
12	A	833	CLA	O2D-CGD-O1D	-3.19	117.53	123.83
12	b	818	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
12	B	815	CLA	CMB-C2B-C1B	-3.18	123.57	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	836	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
12	E	837	CLA	O2D-CGD-O1D	-3.18	117.54	123.83
12	g	834	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
12	g	838	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
12	g	814	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
12	G	819	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
12	a	835	CLA	O2D-CGD-O1D	-3.17	117.56	123.83
12	E	838	CLA	CMB-C2B-C3B	3.17	130.75	124.80
12	e	840	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
12	G	816	CLA	CMB-C2B-C3B	3.17	130.75	124.80
12	b	839	CLA	CMB-C2B-C3B	3.17	130.75	124.80
12	e	835	CLA	CMB-C2B-C3B	3.16	130.73	124.80
12	B	820	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
12	g	821	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
12	g	818	CLA	CMB-C2B-C3B	3.15	130.72	124.80
12	e	804	CLA	CMB-C2B-C3B	3.15	130.71	124.80
12	b	820	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
12	e	810	CLA	CMB-C2B-C3B	3.15	130.71	124.80
12	a	836	CLA	CMB-C2B-C3B	3.15	130.71	124.80
12	B	822	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
12	b	817	CLA	CMB-C2B-C3B	3.14	130.69	124.80
12	e	834	CLA	O2D-CGD-O1D	-3.14	117.63	123.83
12	a	811	CLA	CMB-C2B-C3B	3.14	130.69	124.80
12	e	805	CLA	CMB-C2B-C3B	3.13	130.68	124.80
12	B	806	CLA	C1-C2-C3	-3.13	121.69	126.75
12	a	805	CLA	CMB-C2B-C3B	3.13	130.67	124.80
12	A	803	CLA	CMB-C2B-C3B	3.13	130.67	124.80
12	A	834	CLA	CMB-C2B-C3B	3.13	130.66	124.80
12	E	806	CLA	CMB-C2B-C3B	3.13	130.66	124.80
12	E	807	CLA	CMB-C2B-C3B	3.12	130.66	124.80
12	e	823	CLA	CMB-C2B-C3B	3.12	130.65	124.80
12	B	818	CLA	CMB-C2B-C3B	3.12	130.65	124.80
12	b	804	CLA	C1-C2-C3	-3.12	121.71	126.75
12	E	830	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
12	b	816	CLA	CMB-C2B-C3B	3.12	130.64	124.80
12	B	819	CLA	CMB-C2B-C3B	3.11	130.64	124.80
12	G	815	CLA	CMB-C2B-C3B	3.11	130.64	124.80
12	G	803	CLA	C1-C2-C3	-3.11	121.72	126.75
12	a	824	CLA	CMB-C2B-C3B	3.11	130.63	124.80
12	g	817	CLA	CMB-C2B-C3B	3.11	130.63	124.80
12	B	838	CLA	CMB-C2B-C3B	3.11	130.63	124.80
12	A	804	CLA	CMB-C2B-C3B	3.11	130.63	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	812	CLA	CMB-C2B-C3B	3.11	130.63	124.80
12	g	805	CLA	C1-C2-C3	-3.11	121.72	126.75
12	G	836	CLA	CMB-C2B-C3B	3.11	130.62	124.80
12	F	1301	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
12	A	822	CLA	CMB-C2B-C3B	3.10	130.62	124.80
12	a	825	CLA	CMB-C2B-C3B	3.10	130.62	124.80
12	E	825	CLA	CMB-C2B-C3B	3.10	130.62	124.80
12	G	841	CLA	CMB-C2B-C3B	3.10	130.61	124.80
12	A	823	CLA	CMB-C2B-C3B	3.10	130.61	124.80
12	a	829	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
12	E	826	CLA	CMB-C2B-C3B	3.10	130.61	124.80
12	f	1301	CLA	CMB-C2B-C1B	-3.10	123.71	128.46
12	O	1301	CLA	CMB-C2B-C1B	-3.10	123.71	128.46
12	a	806	CLA	CMB-C2B-C3B	3.10	130.60	124.80
12	S	1502	CLA	CMB-C2B-C3B	3.09	130.60	124.80
12	G	840	CLA	CMB-C2B-C3B	3.09	130.60	124.80
12	b	837	CLA	CMB-C2B-C3B	3.09	130.60	124.80
12	A	805	CLA	CMB-C2B-C3B	3.09	130.60	124.80
12	B	815	CLA	O2D-CGD-O1D	-3.09	117.73	123.83
12	A	809	CLA	CMB-C2B-C3B	3.09	130.59	124.80
12	A	827	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
12	o	1301	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
12	A	814	CLA	CMB-C2B-C3B	3.08	130.58	124.80
12	s	204	CLA	CMB-C2B-C3B	3.08	130.57	124.80
12	e	824	CLA	CMB-C2B-C3B	3.08	130.57	124.80
12	E	817	CLA	CMB-C2B-C3B	3.07	130.57	124.80
12	E	808	CLA	CMB-C2B-C3B	3.07	130.56	124.80
12	B	842	CLA	CMB-C2B-C3B	3.07	130.56	124.80
12	e	806	CLA	CMB-C2B-C3B	3.07	130.56	124.80
12	l	204	CLA	CMB-C2B-C3B	3.07	130.56	124.80
12	g	842	CLA	CMB-C2B-C3B	3.07	130.56	124.80
12	b	842	CLA	CMB-C2B-C3B	3.07	130.56	124.80
12	e	831	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
12	G	809	CLA	CMB-C2B-C3B	3.07	130.55	124.80
12	a	807	CLA	CMB-C2B-C3B	3.07	130.55	124.80
12	G	839	CLA	CMB-C2B-C3B	3.07	130.55	124.80
12	g	837	CLA	CMB-C2B-C3B	3.07	130.55	124.80
12	B	812	CLA	CMB-C2B-C3B	3.07	130.55	124.80
12	b	840	CLA	CMB-C2B-C3B	3.07	130.55	124.80
12	A	830	CLA	C1B-CHB-C4A	-3.07	124.05	130.12
12	g	814	CLA	O2D-CGD-O1D	-3.06	117.78	123.83
12	G	812	CLA	O2D-CGD-O1D	-3.06	117.78	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	810	CLA	CMB-C2B-C3B	3.06	130.54	124.80
12	g	811	CLA	CMB-C2B-C3B	3.06	130.54	124.80
12	a	816	CLA	CMB-C2B-C3B	3.06	130.54	124.80
12	a	832	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
12	e	828	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
12	g	840	CLA	CMB-C2B-C3B	3.06	130.54	124.80
12	e	815	CLA	CMB-C2B-C3B	3.06	130.53	124.80
12	B	843	CLA	CMB-C2B-C3B	3.06	130.53	124.80
12	L	204	CLA	CMB-C2B-C3B	3.06	130.53	124.80
12	B	841	CLA	CMB-C2B-C3B	3.05	130.53	124.80
12	b	841	CLA	CMB-C2B-C3B	3.05	130.52	124.80
12	E	834	CLA	C1B-CHB-C4A	-3.05	124.09	130.12
12	g	841	CLA	CMB-C2B-C3B	3.05	130.51	124.80
12	G	822	CLA	O2D-CGD-O1D	-3.04	117.82	123.83
12	g	801	CLA	O2D-CGD-O1D	-3.04	117.83	123.83
12	b	813	CLA	O2D-CGD-O1D	-3.04	117.83	123.83
12	a	802	CLA	O2D-CGD-O1D	-3.03	117.84	123.83
12	A	807	CLA	CMB-C2B-C3B	3.03	130.49	124.80
12	b	823	CLA	O2D-CGD-O1D	-3.03	117.84	123.83
12	g	824	CLA	O2D-CGD-O1D	-3.03	117.85	123.83
12	e	812	CLA	CMB-C2B-C3B	3.03	130.48	124.80
12	B	825	CLA	O2D-CGD-O1D	-3.03	117.85	123.83
12	a	813	CLA	CMB-C2B-C3B	3.02	130.47	124.80
12	b	819	CLA	CMB-C2B-C3B	3.02	130.46	124.80
12	B	801	CLA	O2D-CGD-O1D	-3.02	117.87	123.83
12	E	814	CLA	CMB-C2B-C3B	3.02	130.46	124.80
12	E	802	CLA	O2D-CGD-O1D	-3.02	117.87	123.83
12	B	813	CLA	CMB-C2B-C3B	3.01	130.45	124.80
12	b	812	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
12	b	830	CLA	CMB-C2B-C3B	3.01	130.44	124.80
12	A	811	CLA	CMB-C2B-C3B	3.01	130.44	124.80
12	g	812	CLA	CMB-C2B-C3B	3.01	130.44	124.80
12	G	818	CLA	CMB-C2B-C3B	3.01	130.44	124.80
12	g	831	CLA	CMB-C2B-C3B	3.00	130.44	124.80
12	g	813	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
12	a	809	CLA	CMB-C2B-C3B	3.00	130.42	124.80
12	B	814	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
12	b	811	CLA	CMB-C2B-C3B	3.00	130.42	124.80
12	G	829	CLA	CMB-C2B-C3B	2.99	130.41	124.80
12	E	829	CLA	O2D-CGD-O1D	-2.99	117.92	123.83
12	E	816	CLA	O2D-CGD-O1D	-2.99	117.93	123.83
12	g	820	CLA	CMB-C2B-C3B	2.99	130.41	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	832	CLA	CMB-C2B-C3B	2.99	130.41	124.80
12	E	840	CLA	CMB-C2B-C3B	2.99	130.40	124.80
12	a	828	CLA	O2D-CGD-O1D	-2.99	117.93	123.83
12	G	810	CLA	CMB-C2B-C3B	2.98	130.40	124.80
12	G	811	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
12	B	821	CLA	CMB-C2B-C3B	2.98	130.39	124.80
12	E	810	CLA	CMB-C2B-C3B	2.98	130.39	124.80
12	e	808	CLA	CMB-C2B-C3B	2.98	130.39	124.80
12	e	827	CLA	O2D-CGD-O1D	-2.98	117.95	123.83
12	A	826	CLA	O2D-CGD-O1D	-2.98	117.95	123.83
12	A	836	CLA	CMB-C2B-C3B	2.97	130.38	124.80
12	A	803	CLA	C1-C2-C3	-2.97	121.95	126.75
12	a	815	CLA	O2D-CGD-O1D	-2.97	117.97	123.83
12	G	809	CLA	C1-C2-C3	-2.97	121.95	126.75
12	e	833	CLA	CMB-C2B-C3B	2.96	130.35	124.80
12	g	811	CLA	C1-C2-C3	-2.96	121.96	126.75
12	e	837	CLA	CMB-C2B-C3B	2.96	130.35	124.80
12	a	838	CLA	CMB-C2B-C3B	2.96	130.35	124.80
12	A	813	CLA	O2D-CGD-O1D	-2.96	117.99	123.83
12	a	842	CLA	CMB-C2B-C3B	2.96	130.34	124.80
12	b	810	CLA	C1-C2-C3	-2.96	121.97	126.75
12	B	812	CLA	C1-C2-C3	-2.96	121.97	126.75
12	e	804	CLA	C1-C2-C3	-2.95	121.97	126.75
12	E	806	CLA	C1-C2-C3	-2.95	121.97	126.75
12	E	829	CLA	C1-C2-C3	-2.95	121.98	126.75
12	E	836	CLA	CMB-C2B-C3B	2.95	130.32	124.80
12	a	834	CLA	CMB-C2B-C3B	2.94	130.32	124.80
12	A	826	CLA	C1-C2-C3	-2.94	121.99	126.75
12	e	814	CLA	CMB-C2B-C3B	2.94	130.32	124.80
12	e	827	CLA	C1-C2-C3	-2.94	121.99	126.75
12	a	805	CLA	C1-C2-C3	-2.94	121.99	126.75
12	g	824	CLA	CMB-C2B-C3B	2.94	130.31	124.80
12	e	814	CLA	O2D-CGD-O1D	-2.94	118.03	123.83
12	G	835	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
12	E	844	CLA	CMB-C2B-C3B	2.94	130.31	124.80
12	a	834	CLA	O2D-CGD-O1D	-2.94	118.03	123.83
12	G	841	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
12	a	828	CLA	C1-C2-C3	-2.94	122.00	126.75
12	e	841	CLA	CMB-C2B-C3B	2.93	130.30	124.80
12	A	832	CLA	O2D-CGD-O1D	-2.93	118.03	123.83
12	A	813	CLA	CMB-C2B-C3B	2.93	130.30	124.80
12	e	833	CLA	O2D-CGD-O1D	-2.93	118.04	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	811	CLA	O2D-CGD-O1D	-2.93	118.04	123.83
12	b	821	CLA	CMB-C2B-C3B	2.93	130.30	124.80
12	g	807	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
13	e	843	PQN	C11-C12-C13	-2.93	121.91	126.79
12	B	825	CLA	CMB-C2B-C3B	2.93	130.29	124.80
12	E	836	CLA	O2D-CGD-O1D	-2.93	118.05	123.83
12	B	838	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
12	B	813	CLA	O2D-CGD-O1D	-2.93	118.05	123.83
12	e	820	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
12	E	816	CLA	CMB-C2B-C3B	2.93	130.29	124.80
12	b	836	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
12	b	806	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
12	A	832	CLA	CMB-C2B-C3B	2.93	130.29	124.80
12	G	810	CLA	O2D-CGD-O1D	-2.93	118.05	123.83
12	A	840	CLA	CMB-C2B-C3B	2.92	130.28	124.80
12	E	801	CLA	O2D-CGD-O1D	-2.92	118.06	123.83
12	G	822	CLA	CMB-C2B-C3B	2.92	130.28	124.80
12	b	837	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
12	E	822	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
12	g	812	CLA	O2D-CGD-O1D	-2.92	118.07	123.83
12	B	835	CLA	CMB-C2B-C3B	2.92	130.27	124.80
12	G	805	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
12	a	815	CLA	CMB-C2B-C3B	2.92	130.27	124.80
12	b	823	CLA	CMB-C2B-C3B	2.92	130.27	124.80
12	B	837	CLA	C1B-CHB-C4A	-2.91	124.34	130.12
12	b	842	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
12	e	801	CLA	O2D-CGD-O1D	-2.91	118.08	123.83
12	a	815	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
13	e	843	PQN	C14-C13-C15	2.91	120.30	115.29
12	g	837	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
12	B	808	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
12	A	819	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
12	E	816	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
12	E	809	CLA	O2D-CGD-O1D	-2.91	118.09	123.83
12	a	821	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
12	g	836	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
12	G	836	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
12	A	806	CLA	O2D-CGD-O1D	-2.90	118.10	123.83
12	E	833	CLA	O2D-CGD-O1D	-2.90	118.10	123.83
12	e	814	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
12	A	801	CLA	O2D-CGD-O1D	-2.90	118.11	123.83
12	a	801	CLA	O2D-CGD-O1D	-2.90	118.11	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	832	CLA	CMB-C2B-C3B	2.90	130.23	124.80
12	A	830	CLA	CMB-C2B-C3B	2.90	130.23	124.80
12	e	807	CLA	O2D-CGD-O1D	-2.90	118.11	123.83
12	e	845	CLA	CMB-C2B-C3B	2.90	130.23	124.80
12	a	832	CLA	CMB-C2B-C3B	2.89	130.23	124.80
12	E	803	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
12	b	801	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
12	g	822	CLA	CMB-C2B-C3B	2.89	130.22	124.80
12	A	813	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
12	B	802	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
12	e	834	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
12	g	802	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
12	E	812	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
12	B	839	CLA	C1-C2-C3	-2.88	122.09	126.75
12	B	824	CLA	CMB-C2B-C3B	2.88	130.20	124.80
12	G	820	CLA	CMB-C2B-C3B	2.88	130.20	124.80
12	b	833	CLA	CMB-C2B-C3B	2.88	130.20	124.80
12	a	808	CLA	O2D-CGD-O1D	-2.88	118.14	123.83
12	a	811	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
12	e	831	CLA	CMB-C2B-C3B	2.88	130.19	124.80
12	l	201	CLA	O2D-CGD-O1D	-2.88	118.15	123.83
12	A	833	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
12	B	823	CLA	CMB-C2B-C3B	2.87	130.19	124.80
12	s	201	CLA	O2D-CGD-O1D	-2.87	118.16	123.83
12	G	836	CLA	O2D-CGD-O1D	-2.87	118.16	123.83
12	G	809	CLA	O2D-CGD-O1D	-2.87	118.16	123.83
12	E	837	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
12	a	817	CLA	CMB-C2B-C3B	2.87	130.19	124.80
12	a	821	CLA	CMB-C2B-C3B	2.87	130.19	124.80
12	E	834	CLA	CMB-C2B-C3B	2.87	130.18	124.80
12	e	810	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
12	g	842	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
12	B	812	CLA	O2D-CGD-O1D	-2.87	118.17	123.83
12	E	818	CLA	CMB-C2B-C3B	2.87	130.18	124.80
12	E	841	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
12	g	838	CLA	C1-C2-C3	-2.87	122.12	126.75
12	B	843	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
12	g	823	CLA	CMB-C2B-C3B	2.86	130.17	124.80
12	a	835	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
12	E	822	CLA	CMB-C2B-C3B	2.86	130.17	124.80
12	g	806	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
12	B	837	CLA	O2D-CGD-O1D	-2.86	118.19	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	201	CLA	O2D-CGD-O1D	-2.86	118.19	123.83
12	b	822	CLA	CMB-C2B-C3B	2.86	130.16	124.80
12	b	838	CLA	C1-C2-C3	-2.86	122.13	126.75
12	B	807	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
12	B	838	CLA	O2D-CGD-O1D	-2.85	118.19	123.83
12	e	838	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
12	b	837	CLA	O2D-CGD-O1D	-2.85	118.20	123.83
12	g	836	CLA	O2D-CGD-O1D	-2.85	118.20	123.83
12	b	836	CLA	O2D-CGD-O1D	-2.85	118.20	123.83
12	B	812	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
12	g	811	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
12	G	821	CLA	CMB-C2B-C3B	2.85	130.15	124.80
12	A	819	CLA	CMB-C2B-C3B	2.85	130.14	124.80
12	A	815	CLA	CMB-C2B-C3B	2.85	130.14	124.80
12	g	837	CLA	O2D-CGD-O1D	-2.85	118.20	123.83
12	a	805	CLA	CHB-C4A-NA	2.85	128.45	124.51
12	G	804	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
12	e	816	CLA	CMB-C2B-C3B	2.84	130.13	124.80
12	A	837	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
12	G	837	CLA	C1-C2-C3	-2.84	122.16	126.75
12	b	810	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
12	A	809	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
12	B	808	CLA	O2D-CGD-O1D	-2.84	118.23	123.83
12	G	809	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
12	G	835	CLA	O2D-CGD-O1D	-2.83	118.23	123.83
12	e	840	CLA	O2D-CGD-O1D	-2.83	118.23	123.83
12	a	839	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
12	b	805	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
12	A	803	CLA	CHB-C4A-NA	2.83	128.43	124.51
12	B	811	CLA	C1-C2-C3	-2.83	122.17	126.75
12	k	1401	CLA	O2D-CGD-O1D	-2.83	118.24	123.83
12	e	820	CLA	CMB-C2B-C3B	2.83	130.10	124.80
12	E	804	CLA	O2D-CGD-O1D	-2.83	118.25	123.83
12	g	811	CLA	O2D-CGD-O1D	-2.83	118.25	123.83
12	G	820	CLA	O2D-CGD-O1D	-2.83	118.25	123.83
12	E	843	CLA	O2D-CGD-O1D	-2.83	118.25	123.83
12	E	828	CLA	O2D-CGD-O1D	-2.83	118.25	123.83
12	b	821	CLA	O2D-CGD-O1D	-2.82	118.25	123.83
12	E	806	CLA	CHB-C4A-NA	2.82	128.42	124.51
12	b	810	CLA	O2D-CGD-O1D	-2.82	118.26	123.83
12	e	804	CLA	CHB-C4A-NA	2.82	128.41	124.51
12	A	812	CLA	CMB-C2B-C3B	2.82	130.09	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	810	CLA	C1-C2-C3	-2.82	122.19	126.75
12	K	1401	CLA	O2D-CGD-O1D	-2.82	118.27	123.83
12	a	841	CLA	O2D-CGD-O1D	-2.82	118.27	123.83
12	a	827	CLA	O2D-CGD-O1D	-2.82	118.27	123.83
12	A	839	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
12	B	827	CLA	CMB-C2B-C3B	2.81	130.07	124.80
12	A	825	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
12	b	806	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
12	a	831	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
12	g	826	CLA	CMB-C2B-C3B	2.81	130.07	124.80
12	l	201	CLA	C1-C2-C3	-2.81	122.21	126.75
12	B	823	CLA	O2D-CGD-O1D	-2.81	118.29	123.83
12	e	802	CLA	O2D-CGD-O1D	-2.81	118.29	123.83
12	b	825	CLA	CMB-C2B-C3B	2.81	130.06	124.80
12	S	1501	CLA	CMB-C2B-C3B	2.81	130.06	124.80
12	a	814	CLA	CMB-C2B-C3B	2.81	130.06	124.80
12	l	202	CLA	CMB-C2B-C3B	2.81	130.06	124.80
12	e	813	CLA	CMB-C2B-C3B	2.80	130.06	124.80
12	G	805	CLA	O2D-CGD-O1D	-2.80	118.29	123.83
12	e	830	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
12	G	817	CLA	O2D-CGD-O1D	-2.80	118.30	123.83
12	g	839	CLA	O2D-CGD-O1D	-2.80	118.30	123.83
12	G	824	CLA	CMB-C2B-C3B	2.80	130.05	124.80
12	J	1101	CLA	O2D-CGD-O1D	-2.80	118.30	123.83
12	E	815	CLA	CMB-C2B-C3B	2.80	130.05	124.80
12	E	818	CLA	O2D-CGD-O1D	-2.80	118.30	123.83
13	a	844	PQN	C14-C13-C15	2.80	120.11	115.29
12	R	1401	CLA	O2D-CGD-O1D	-2.80	118.31	123.83
12	e	838	CLA	CMB-C2B-C3B	2.80	130.05	124.80
12	L	201	CLA	C1-C2-C3	-2.80	122.23	126.75
12	A	818	CLA	O2D-CGD-O1D	-2.80	118.31	123.83
12	g	819	CLA	O2D-CGD-O1D	-2.79	118.31	123.83
13	E	846	PQN	C14-C13-C15	2.79	120.10	115.29
12	G	823	CLA	CMB-C2B-C3B	2.79	130.04	124.80
12	b	809	CLA	C1-C2-C3	-2.79	122.23	126.75
12	r	1401	CLA	O2D-CGD-O1D	-2.79	118.32	123.83
12	A	815	CLA	O2D-CGD-O1D	-2.79	118.32	123.83
12	A	809	CLA	O2D-CGD-O1D	-2.79	118.32	123.83
12	a	803	CLA	O2D-CGD-O1D	-2.79	118.33	123.83
12	g	822	CLA	O2D-CGD-O1D	-2.79	118.33	123.83
12	g	807	CLA	O2D-CGD-O1D	-2.79	118.33	123.83
12	G	808	CLA	C1-C2-C3	-2.79	122.24	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	836	CLA	CHB-C4A-NA	2.79	128.36	124.51
12	E	816	CLA	CHB-C4A-NA	2.79	128.36	124.51
12	A	837	CLA	CMB-C2B-C3B	2.79	130.02	124.80
12	g	825	CLA	CMB-C2B-C3B	2.78	130.02	124.80
12	a	838	CLA	CHB-C4A-NA	2.78	128.36	124.51
12	a	811	CLA	O2D-CGD-O1D	-2.78	118.33	123.83
12	e	826	CLA	O2D-CGD-O1D	-2.78	118.33	123.83
12	L	202	CLA	CMB-C2B-C3B	2.78	130.02	124.80
12	B	840	CLA	O2D-CGD-O1D	-2.78	118.34	123.83
12	a	815	CLA	CHB-C4A-NA	2.78	128.36	124.51
12	e	837	CLA	CHB-C4A-NA	2.78	128.36	124.51
12	b	818	CLA	O2D-CGD-O1D	-2.78	118.34	123.83
12	E	832	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
12	e	816	CLA	O2D-CGD-O1D	-2.78	118.34	123.83
12	e	838	CLA	O2D-CGD-O1D	-2.78	118.35	123.83
12	b	824	CLA	CMB-C2B-C3B	2.78	130.01	124.80
12	s	201	CLA	C1-C2-C3	-2.78	122.26	126.75
12	E	841	CLA	CMB-C2B-C3B	2.78	130.01	124.80
12	B	820	CLA	O2D-CGD-O1D	-2.78	118.35	123.83
12	A	829	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
12	B	821	CLA	O2D-CGD-O1D	-2.78	118.35	123.83
12	s	202	CLA	CMB-C2B-C3B	2.77	130.00	124.80
12	E	833	CLA	C1-C2-C3	-2.77	122.26	126.75
12	a	839	CLA	CMB-C2B-C3B	2.77	130.00	124.80
12	A	834	CLA	O2D-CGD-O1D	-2.77	118.35	123.83
12	E	840	CLA	CHB-C4A-NA	2.77	128.34	124.51
12	a	826	CLA	CMB-C2B-C3B	2.77	130.00	124.80
12	E	821	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
12	a	839	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
12	e	825	CLA	CMB-C2B-C3B	2.77	129.99	124.80
12	b	839	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
12	g	836	CLA	CMB-C2B-C3B	2.77	129.99	124.80
12	L	201	CLA	CMB-C2B-C3B	2.77	129.99	124.80
12	g	825	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
12	B	826	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
12	g	807	CLA	CHB-C4A-NA	2.77	128.34	124.51
12	E	827	CLA	CMB-C2B-C3B	2.77	129.99	124.80
12	E	812	CLA	O2D-CGD-O1D	-2.76	118.37	123.83
12	g	820	CLA	O2D-CGD-O1D	-2.76	118.37	123.83
12	e	819	CLA	O2D-CGD-O1D	-2.76	118.37	123.83
12	E	841	CLA	O2D-CGD-O1D	-2.76	118.37	123.83
12	b	819	CLA	O2D-CGD-O1D	-2.76	118.37	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	811	CLA	CMB-C2B-C3B	2.76	129.98	124.80
12	G	823	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
12	e	810	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
12	a	836	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
12	G	808	CLA	CMB-C2B-C3B	2.76	129.98	124.80
12	b	836	CLA	CMB-C2B-C3B	2.76	129.98	124.80
12	s	201	CLA	CMB-C2B-C3B	2.76	129.97	124.80
12	g	810	CLA	CMB-C2B-C3B	2.76	129.97	124.80
12	A	824	CLA	CMB-C2B-C3B	2.76	129.97	124.80
12	l	201	CLA	CMB-C2B-C3B	2.76	129.97	124.80
12	a	817	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
12	G	838	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
12	B	824	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
12	A	813	CLA	CHB-C4A-NA	2.76	128.32	124.51
12	A	822	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
12	b	822	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
12	G	843	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
12	E	833	CLA	CMB-C2B-C3B	2.75	129.97	124.80
12	A	821	CLA	O2D-CGD-O1D	-2.75	118.39	123.83
12	e	814	CLA	CHB-C4A-NA	2.75	128.32	124.51
12	a	840	CLA	CMB-C2B-C3B	2.75	129.96	124.80
12	a	823	CLA	CMB-C2B-C3B	2.75	129.96	124.80
12	e	839	CLA	CMB-C2B-C3B	2.75	129.96	124.80
12	a	824	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
12	G	821	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
12	e	822	CLA	O2D-CGD-O1D	-2.75	118.40	123.83
12	a	820	CLA	O2D-CGD-O1D	-2.75	118.40	123.83
12	b	824	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
12	G	802	CLA	O2D-CGD-O1D	-2.75	118.40	123.83
12	B	826	CLA	CMB-C2B-C3B	2.75	129.95	124.80
12	b	807	CLA	O2D-CGD-O1D	-2.75	118.41	123.83
12	E	824	CLA	O2D-CGD-O1D	-2.75	118.41	123.83
12	B	837	CLA	CMB-C2B-C3B	2.75	129.95	124.80
12	l	203	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
12	b	806	CLA	CHB-C4A-NA	2.75	128.31	124.51
12	a	819	CLA	CMB-C2B-C3B	2.74	129.95	124.80
12	L	203	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
12	e	811	CLA	O2D-CGD-O1D	-2.74	118.41	123.83
12	A	818	CLA	C1-C2-C3	-2.74	122.31	126.75
12	G	835	CLA	CMB-C2B-C3B	2.74	129.94	124.80
12	A	837	CLA	O2D-CGD-O1D	-2.74	118.41	123.83
12	e	844	CLA	O2D-CGD-O1D	-2.74	118.41	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	809	CLA	CMB-C2B-C3B	2.74	129.94	124.80
12	E	842	CLA	CMB-C2B-C3B	2.74	129.94	124.80
12	A	806	CLA	CMA-C3A-C4A	-2.74	104.40	111.77
12	A	821	CLA	CMB-C2B-C3B	2.74	129.94	124.80
12	B	805	CLA	O2D-CGD-O1D	-2.74	118.42	123.83
12	g	823	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
12	G	805	CLA	CHB-C4A-NA	2.74	128.30	124.51
12	G	812	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
12	g	808	CLA	O2D-CGD-O1D	-2.74	118.42	123.83
12	b	803	CLA	O2D-CGD-O1D	-2.74	118.42	123.83
12	E	820	CLA	CMB-C2B-C3B	2.74	129.93	124.80
12	e	822	CLA	CMB-C2B-C3B	2.74	129.93	124.80
12	s	203	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
12	g	805	CLA	CMB-C2B-C3B	2.73	129.93	124.80
12	G	818	CLA	O2D-CGD-O1D	-2.73	118.43	123.83
12	A	817	CLA	CMB-C2B-C3B	2.73	129.93	124.80
12	A	810	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
12	b	804	CLA	CMB-C2B-C3B	2.73	129.92	124.80
12	a	823	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
12	b	820	CLA	CHB-C4A-NA	2.73	128.29	124.51
12	E	825	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
12	B	806	CLA	CMB-C2B-C3B	2.73	129.92	124.80
12	G	823	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
12	E	838	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
12	a	802	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
12	E	813	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
12	G	831	CLA	O2D-CGD-O1D	-2.73	118.45	123.83
12	E	809	CLA	CMA-C3A-C4A	-2.73	104.45	111.77
12	g	825	CLA	O2D-CGD-O1D	-2.73	118.45	123.83
12	E	824	CLA	CMB-C2B-C3B	2.73	129.91	124.80
12	e	842	CLA	CMB-C2B-C3B	2.72	129.91	124.80
12	e	807	CLA	CMA-C3A-C4A	-2.72	104.45	111.77
12	e	818	CLA	CMB-C2B-C3B	2.72	129.91	124.80
12	e	835	CLA	O2D-CGD-O1D	-2.72	118.45	123.83
12	b	829	CLA	CMB-C2B-C3B	2.72	129.91	124.80
12	A	838	CLA	CMB-C2B-C3B	2.72	129.90	124.80
12	B	815	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
12	G	806	CLA	O2D-CGD-O1D	-2.72	118.46	123.83
12	b	824	CLA	O2D-CGD-O1D	-2.72	118.46	123.83
12	a	807	CLA	O2D-CGD-O1D	-2.72	118.46	123.83
13	E	846	PQN	C21-C22-C23	-2.72	107.28	115.77
12	E	821	CLA	C1-C2-C3	-2.72	122.35	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	821	CLA	CHB-C4A-NA	2.72	128.27	124.51
12	a	829	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
12	e	819	CLA	C1-C2-C3	-2.72	122.35	126.75
12	B	809	CLA	O2D-CGD-O1D	-2.72	118.46	123.83
12	a	808	CLA	CMA-C3A-C4A	-2.72	104.47	111.77
12	e	823	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
13	A	842	PQN	C14-C13-C15	2.72	119.97	115.29
12	g	833	CLA	O2D-CGD-O1D	-2.72	118.47	123.83
12	a	812	CLA	O2D-CGD-O1D	-2.71	118.47	123.83
12	E	815	CLA	CMD-C2D-C3D	2.71	129.89	124.80
12	B	801	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
12	g	805	CLA	O2D-CGD-O1D	-2.71	118.47	123.83
12	A	812	CLA	O2D-CGD-O1D	-2.71	118.47	123.83
12	B	808	CLA	CHB-C4A-NA	2.71	128.26	124.51
12	E	830	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
12	G	803	CLA	CMB-C2B-C3B	2.71	129.89	124.80
12	g	801	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
12	g	830	CLA	CMB-C2B-C3B	2.71	129.88	124.80
12	G	828	CLA	CMB-C2B-C3B	2.71	129.88	124.80
12	F	1301	CLA	O2D-CGD-O1D	-2.71	118.48	123.83
12	A	827	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
12	b	828	CLA	O2D-CGD-O1D	-2.71	118.48	123.83
12	a	814	CLA	CMD-C2D-C3D	2.71	129.88	124.80
12	e	813	CLA	O2D-CGD-O1D	-2.71	118.49	123.83
12	A	805	CLA	O2D-CGD-O1D	-2.71	118.49	123.83
12	a	824	CLA	O2D-CGD-O1D	-2.71	118.49	123.83
12	A	812	CLA	CMD-C2D-C3D	2.70	129.87	124.80
12	b	813	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
12	g	828	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
12	B	830	CLA	O2D-CGD-O1D	-2.70	118.49	123.83
12	a	820	CLA	C1-C2-C3	-2.70	122.38	126.75
12	B	822	CLA	CHB-C4A-NA	2.70	128.25	124.51
12	e	813	CLA	CMD-C2D-C3D	2.70	129.87	124.80
12	e	825	CLA	O2D-CGD-O1D	-2.70	118.49	123.83
12	B	834	CLA	O2D-CGD-O1D	-2.70	118.49	123.83
12	g	801	CLA	CHB-C4A-NA	2.70	128.25	124.51
12	e	818	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
12	e	809	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
12	A	822	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
12	e	821	CLA	CHB-C4A-NA	2.70	128.25	124.51
12	e	806	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
12	g	839	CLA	CHB-C4A-NA	2.70	128.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	814	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
12	B	826	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
12	B	831	CLA	CMB-C2B-C3B	2.70	129.86	124.80
12	b	832	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
12	A	841	CLA	CMB-C2B-C3B	2.70	129.86	124.80
12	a	814	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
12	B	806	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
12	E	802	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
12	G	827	CLA	O2D-CGD-O1D	-2.70	118.51	123.83
12	o	1301	CLA	O2D-CGD-O1D	-2.70	118.51	123.83
12	E	808	CLA	O2D-CGD-O1D	-2.70	118.51	123.83
12	A	808	CLA	O2D-CGD-O1D	-2.70	118.51	123.83
12	a	808	CLA	CMB-C2B-C3B	2.69	129.85	124.80
12	a	801	CLA	CMB-C2B-C3B	2.69	129.85	124.80
12	b	817	CLA	O2D-CGD-O1D	-2.69	118.51	123.83
12	B	809	CLA	CMB-C2B-C3B	2.69	129.85	124.80
12	G	806	CLA	CMB-C2B-C3B	2.69	129.85	124.80
12	a	818	CLA	O2D-CGD-O1D	-2.69	118.51	123.83
12	B	840	CLA	CHB-C4A-NA	2.69	128.24	124.51
12	a	802	CLA	CHB-C4A-NA	2.69	128.24	124.51
12	b	839	CLA	CHB-C4A-NA	2.69	128.24	124.51
12	J	1101	CLA	CMB-C2B-C3B	2.69	129.85	124.80
12	E	815	CLA	O2D-CGD-O1D	-2.69	118.51	123.83
12	g	828	CLA	O2D-CGD-O1D	-2.69	118.51	123.83
12	E	804	CLA	CMB-C2B-C3B	2.69	129.85	124.80
12	B	829	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
12	E	832	CLA	CMB-C2B-C3B	2.69	129.85	124.80
12	e	830	CLA	CMB-C2B-C3B	2.69	129.84	124.80
12	f	1301	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
12	a	830	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
12	E	820	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
12	O	1301	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
12	e	828	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
12	a	810	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
12	b	804	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
12	E	819	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
12	e	823	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
12	A	833	CLA	CMB-C2B-C3B	2.69	129.84	124.80
12	G	838	CLA	CHB-C4A-NA	2.69	128.23	124.51
12	G	826	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
12	A	824	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
12	g	829	CLA	O2D-CGD-O1D	-2.69	118.53	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	816	CLA	O2D-CGD-O1D	-2.69	118.53	123.83
12	E	831	CLA	CHB-C4A-NA	2.69	128.23	124.51
12	E	843	CLA	C1-C2-C3	-2.69	122.41	126.75
12	e	840	CLA	C1-C2-C3	-2.68	122.41	126.75
12	B	841	CLA	CHB-C4A-NA	2.68	128.22	124.51
12	b	814	CLA	CHB-C4A-NA	2.68	128.22	124.51
12	a	841	CLA	C1-C2-C3	-2.68	122.41	126.75
12	G	803	CLA	O2D-CGD-O1D	-2.68	118.53	123.83
12	B	829	CLA	O2D-CGD-O1D	-2.68	118.53	123.83
12	e	829	CLA	CHB-C4A-NA	2.68	128.22	124.51
12	e	807	CLA	CMB-C2B-C3B	2.68	129.83	124.80
12	B	817	CLA	CMB-C2B-C3B	2.68	129.83	124.80
12	B	801	CLA	CHB-C4A-NA	2.68	128.22	124.51
13	a	844	PQN	C21-C22-C23	-2.68	107.40	115.77
12	E	811	CLA	O2D-CGD-O1D	-2.68	118.53	123.83
12	E	837	CLA	CMB-C2B-C3B	2.68	129.83	124.80
12	a	826	CLA	O2D-CGD-O1D	-2.68	118.54	123.83
12	l	203	CLA	CHB-C4A-NA	2.68	128.22	124.51
12	E	809	CLA	C1-C2-C3	-2.68	122.42	126.75
12	E	827	CLA	O2D-CGD-O1D	-2.68	118.54	123.83
12	E	802	CLA	CHB-C4A-NA	2.68	128.22	124.51
12	g	808	CLA	CMB-C2B-C3B	2.68	129.82	124.80
12	G	828	CLA	O2D-CGD-O1D	-2.68	118.54	123.83
12	b	807	CLA	CMB-C2B-C3B	2.68	129.82	124.80
12	E	825	CLA	O2D-CGD-O1D	-2.68	118.54	123.83
12	E	801	CLA	CMB-C2B-C3B	2.68	129.82	124.80
12	A	815	CLA	C1B-CHB-C4A	-2.68	124.82	130.12
12	G	838	CLA	C1B-CHB-C4A	-2.68	124.82	130.12
12	g	818	CLA	O2D-CGD-O1D	-2.68	118.55	123.83
12	G	813	CLA	CHB-C4A-NA	2.68	128.21	124.51
12	S	1501	CLA	C1-C2-C3	-2.68	122.42	126.75
12	a	835	CLA	CMB-C2B-C3B	2.68	129.82	124.80
12	E	823	CLA	CHB-C4A-NA	2.67	128.21	124.51
12	A	835	CLA	O2D-CGD-O1D	-2.67	118.55	123.83
12	E	831	CLA	O2D-CGD-O1D	-2.67	118.55	123.83
12	A	829	CLA	CMB-C2B-C3B	2.67	129.81	124.80
12	e	817	CLA	O2D-CGD-O1D	-2.67	118.55	123.83
12	b	841	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
12	a	819	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
12	A	801	CLA	CMB-C2B-C3B	2.67	129.81	124.80
12	G	826	CLA	O2D-CGD-O1D	-2.67	118.55	123.83
12	a	822	CLA	CHB-C4A-NA	2.67	128.21	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	817	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
12	e	829	CLA	O2D-CGD-O1D	-2.67	118.55	123.83
12	e	802	CLA	CMB-C2B-C3B	2.67	129.81	124.80
12	A	820	CLA	CHB-C4A-NA	2.67	128.20	124.51
12	e	818	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
12	b	808	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
12	A	828	CLA	CHB-C4A-NA	2.67	128.20	124.51
12	A	824	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
12	B	831	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
12	G	843	CLA	CHB-C4A-NA	2.67	128.20	124.51
12	g	809	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
12	G	834	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
12	b	840	CLA	CHB-C4A-NA	2.67	128.20	124.51
12	G	819	CLA	CHB-C4A-NA	2.67	128.20	124.51
12	B	816	CLA	CHB-C4A-NA	2.67	128.20	124.51
12	b	825	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
12	e	834	CLA	CMB-C2B-C3B	2.67	129.80	124.80
12	a	841	CLA	CMB-C2B-C3B	2.66	129.80	124.80
12	G	814	CLA	CMB-C2B-C3B	2.66	129.80	124.80
12	A	839	CLA	C1-C2-C3	-2.66	122.44	126.75
12	b	840	CLA	O2D-CGD-O1D	-2.66	118.57	123.83
12	g	830	CLA	O2D-CGD-O1D	-2.66	118.57	123.83
12	g	816	CLA	CMB-C2B-C3B	2.66	129.79	124.80
12	e	801	CLA	CMB-C2B-C3B	2.66	129.79	124.80
12	a	842	CLA	CHB-C4A-NA	2.66	128.19	124.51
12	G	840	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
12	G	801	CLA	CMB-C2B-C3B	2.66	129.79	124.80
12	a	831	CLA	CMB-C2B-C3B	2.66	129.79	124.80
12	e	836	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
12	A	828	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
12	a	836	CLA	C1-C2-C3	-2.66	122.45	126.75
12	B	824	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
12	g	841	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
12	G	816	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
12	g	827	CLA	CMB-C2B-C3B	2.66	129.79	124.80
12	B	822	CLA	C1-C2-C3	-2.66	122.45	126.75
12	g	813	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
12	b	812	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
12	E	839	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
12	A	806	CLA	CMB-C2B-C3B	2.66	129.79	124.80
12	b	805	CLA	CMD-C2D-C3D	2.66	129.79	124.80
12	a	837	CLA	O2D-CGD-O1D	-2.66	118.58	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	840	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
12	L	203	CLA	CHB-C4A-NA	2.66	128.19	124.51
12	a	808	CLA	C1-C2-C3	-2.66	122.45	126.75
12	a	830	CLA	CHB-C4A-NA	2.66	128.18	124.51
12	g	815	CLA	CHB-C4A-NA	2.66	128.18	124.51
12	E	809	CLA	CMB-C2B-C3B	2.66	129.78	124.80
12	G	807	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
12	b	827	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
12	b	829	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
12	b	827	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
12	A	806	CLA	C1-C2-C3	-2.65	122.46	126.75
12	B	819	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
12	a	819	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
12	J	1102	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
12	B	810	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
12	b	822	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
12	G	839	CLA	CHB-C4A-NA	2.65	128.18	124.51
12	a	817	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
12	a	826	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
12	B	814	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
12	O	1301	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
12	g	826	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
12	B	840	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
12	g	839	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
12	L	202	CLA	C1-C2-C3	-2.65	122.46	126.75
12	A	817	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
12	A	805	CLA	C1-C2-C3	-2.65	122.47	126.75
12	e	806	CLA	C1-C2-C3	-2.65	122.47	126.75
12	G	804	CLA	CMD-C2D-C3D	2.65	129.77	124.80
12	G	824	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
12	b	839	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
12	g	835	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
12	B	827	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
12	b	816	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
12	E	838	CLA	C1-C2-C3	-2.65	122.47	126.75
12	E	818	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
12	B	803	CLA	CMB-C2B-C3B	2.65	129.77	124.80
12	B	830	CLA	CMB-C2B-C3B	2.65	129.76	124.80
12	e	825	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
12	o	1301	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
12	B	842	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
12	g	815	CLA	CMB-C2B-C3B	2.65	129.76	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	839	CLA	O2D-CGD-O1D	-2.65	118.61	123.83
12	B	841	CLA	O2D-CGD-O1D	-2.65	118.61	123.83
12	l	202	CLA	C1-C2-C3	-2.65	122.47	126.75
12	g	821	CLA	C1-C2-C3	-2.65	122.47	126.75
12	l	203	CLA	O2D-CGD-O1D	-2.65	118.61	123.83
12	s	203	CLA	CHB-C4A-NA	2.65	128.17	124.51
12	b	834	CLA	CMB-C2B-C3B	2.65	129.76	124.80
12	b	815	CLA	CMB-C2B-C3B	2.64	129.76	124.80
12	L	203	CLA	O2D-CGD-O1D	-2.64	118.61	123.83
12	B	818	CLA	O2D-CGD-O1D	-2.64	118.61	123.83
12	E	827	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
12	g	834	CLA	CMB-C2B-C3B	2.64	129.76	124.80
12	s	202	CLA	C1-C2-C3	-2.64	122.47	126.75
12	E	843	CLA	CMB-C2B-C3B	2.64	129.76	124.80
12	b	835	CLA	O2D-CGD-O1D	-2.64	118.61	123.83
12	A	839	CLA	CMB-C2B-C3B	2.64	129.76	124.80
12	A	834	CLA	C1-C2-C3	-2.64	122.48	126.75
12	a	807	CLA	C1-C2-C3	-2.64	122.48	126.75
12	g	806	CLA	CMD-C2D-C3D	2.64	129.75	124.80
12	g	803	CLA	CMB-C2B-C3B	2.64	129.75	124.80
12	B	836	CLA	CMB-C2B-C3B	2.64	129.75	124.80
12	E	844	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
12	a	803	CLA	CMB-C2B-C3B	2.64	129.75	124.80
12	g	823	CLA	O2D-CGD-O1D	-2.64	118.61	123.83
12	g	832	CLA	O2D-CGD-O1D	-2.64	118.62	123.83
12	G	840	CLA	CMD-C2D-C3D	2.64	129.75	124.80
12	e	835	CLA	C1-C2-C3	-2.64	122.48	126.75
12	a	841	CLA	CHB-C4A-NA	2.64	128.16	124.51
12	b	841	CLA	CMD-C2D-C3D	2.64	129.75	124.80
12	G	827	CLA	CMB-C2B-C3B	2.64	129.75	124.80
12	E	808	CLA	C1-C2-C3	-2.64	122.48	126.75
12	g	841	CLA	CMD-C2D-C3D	2.64	129.75	124.80
12	G	825	CLA	CMB-C2B-C3B	2.64	129.75	124.80
12	E	844	CLA	CHB-C4A-NA	2.64	128.16	124.51
12	G	821	CLA	O2D-CGD-O1D	-2.64	118.62	123.83
12	b	825	CLA	CHB-C4A-NA	2.64	128.16	124.51
12	B	842	CLA	CMD-C2D-C3D	2.64	129.74	124.80
12	L	204	CLA	C1-C2-C3	-2.64	122.49	126.75
12	E	836	CLA	CHB-C4A-NA	2.64	128.16	124.51
12	e	816	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
12	e	840	CLA	CMB-C2B-C3B	2.64	129.74	124.80
12	E	820	CLA	O2D-CGD-O1D	-2.63	118.63	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	829	CLA	CMB-C2B-C3B	2.63	129.74	124.80
12	B	816	CLA	CMB-C2B-C3B	2.63	129.74	124.80
12	e	807	CLA	C1-C2-C3	-2.63	122.49	126.75
12	B	843	CLA	O2D-CGD-O1D	-2.63	118.63	123.83
12	G	833	CLA	CMB-C2B-C3B	2.63	129.74	124.80
12	E	822	CLA	O2D-CGD-O1D	-2.63	118.63	123.83
12	A	840	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
12	b	803	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
12	a	842	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
12	g	840	CLA	CHB-C4A-NA	2.63	128.15	124.51
12	a	834	CLA	CHB-C4A-NA	2.63	128.15	124.51
12	b	832	CLA	CMB-C2B-C3B	2.63	129.73	124.80
12	b	802	CLA	CMB-C2B-C3B	2.63	129.73	124.80
12	b	813	CLA	CMB-C2B-C3B	2.63	129.73	124.80
12	G	819	CLA	C1-C2-C3	-2.63	122.50	126.75
12	e	836	CLA	CHB-C4A-NA	2.63	128.15	124.51
12	G	833	CLA	CHB-C4A-NA	2.63	128.15	124.51
12	G	830	CLA	O2D-CGD-O1D	-2.63	118.64	123.83
12	g	817	CLA	O2D-CGD-O1D	-2.63	118.64	123.83
12	g	826	CLA	CHB-C4A-NA	2.63	128.15	124.51
12	A	827	CLA	O2D-CGD-O1D	-2.63	118.64	123.83
12	G	815	CLA	O2D-CGD-O1D	-2.63	118.64	123.83
12	A	840	CLA	CHB-C4A-NA	2.63	128.15	124.51
12	E	839	CLA	CHB-C4A-NA	2.63	128.15	124.51
12	g	842	CLA	O2D-CGD-O1D	-2.63	118.64	123.83
12	s	203	CLA	O2D-CGD-O1D	-2.63	118.65	123.83
12	G	811	CLA	O2D-CGD-O1D	-2.63	118.65	123.83
12	b	828	CLA	CMB-C2B-C3B	2.62	129.72	124.80
12	b	814	CLA	CMB-C2B-C3B	2.62	129.72	124.80
12	B	807	CLA	CMD-C2D-C3D	2.62	129.72	124.80
12	B	807	CLA	C1-C2-C3	-2.62	122.51	126.75
12	f	1301	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
12	b	826	CLA	CMB-C2B-C3B	2.62	129.72	124.80
12	B	813	CLA	CHB-C4A-NA	2.62	128.14	124.51
12	B	805	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
12	S	1502	CLA	C1-C2-C3	-2.62	122.51	126.75
12	a	840	CLA	O2D-CGD-O1D	-2.62	118.65	123.83
12	G	802	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
12	b	820	CLA	C1-C2-C3	-2.62	122.51	126.75
12	a	831	CLA	CHB-C4A-NA	2.62	128.14	124.51
12	g	831	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
12	G	824	CLA	CHB-C4A-NA	2.62	128.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	833	CLA	O2D-CGD-O1D	-2.62	118.66	123.83
12	A	832	CLA	CHB-C4A-NA	2.62	128.13	124.51
12	l	204	CLA	C1-C2-C3	-2.62	122.52	126.75
12	B	815	CLA	CMB-C2B-C3B	2.62	129.71	124.80
12	G	839	CLA	CMD-C2D-C3D	2.62	129.71	124.80
12	B	827	CLA	CHB-C4A-NA	2.62	128.13	124.51
12	b	811	CLA	CHB-C4A-NA	2.62	128.13	124.51
12	A	819	CLA	O2D-CGD-O1D	-2.62	118.66	123.83
12	L	204	CLA	O2D-CGD-O1D	-2.62	118.66	123.83
12	B	832	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
12	e	833	CLA	CHB-C4A-NA	2.62	128.13	124.51
12	e	836	CLA	CMB-C2B-C3B	2.62	129.71	124.80
12	g	831	CLA	O2D-CGD-O1D	-2.62	118.67	123.83
12	e	844	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
12	g	833	CLA	CMB-C2B-C3B	2.62	129.71	124.80
12	g	814	CLA	CMB-C2B-C3B	2.62	129.71	124.80
12	E	830	CLA	O2D-CGD-O1D	-2.62	118.67	123.83
12	g	815	CLA	O2D-CGD-O1D	-2.62	118.67	123.83
12	A	841	CLA	O2D-CGD-O1D	-2.62	118.67	123.83
12	a	801	CLA	CMD-C2D-C3D	2.61	129.70	124.80
12	E	839	CLA	CMB-C2B-C3B	2.61	129.70	124.80
12	S	1502	CLA	O2D-CGD-O1D	-2.61	118.67	123.83
12	a	837	CLA	CMB-C2B-C3B	2.61	129.70	124.80
12	G	812	CLA	CMB-C2B-C3B	2.61	129.70	124.80
12	A	839	CLA	CHB-C4A-NA	2.61	128.13	124.51
12	a	837	CLA	CHB-C4A-NA	2.61	128.13	124.51
12	B	839	CLA	CMB-C2B-C3B	2.61	129.70	124.80
12	b	842	CLA	O2D-CGD-O1D	-2.61	118.67	123.83
12	b	805	CLA	C1-C2-C3	-2.61	122.52	126.75
12	b	831	CLA	O2D-CGD-O1D	-2.61	118.67	123.83
12	a	821	CLA	O2D-CGD-O1D	-2.61	118.67	123.83
12	g	806	CLA	C1-C2-C3	-2.61	122.53	126.75
12	A	835	CLA	CHB-C4A-NA	2.61	128.12	124.51
12	E	801	CLA	CMD-C2D-C3D	2.61	129.70	124.80
12	A	835	CLA	CMB-C2B-C3B	2.61	129.70	124.80
12	G	813	CLA	CMB-C2B-C3B	2.61	129.70	124.80
12	B	828	CLA	CMB-C2B-C3B	2.61	129.70	124.80
12	s	204	CLA	O2D-CGD-O1D	-2.61	118.68	123.83
12	E	818	CLA	CMD-C2D-C3D	2.61	129.69	124.80
12	A	801	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
12	b	809	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
12	a	829	CLA	O2D-CGD-O1D	-2.61	118.68	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	830	CLA	CHB-C4A-NA	2.61	128.12	124.51
12	F	1301	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
12	G	843	CLA	O2D-CGD-O1D	-2.61	118.68	123.83
12	B	822	CLA	CMB-C2B-C3B	2.61	129.69	124.80
12	e	828	CLA	CMB-C2B-C3B	2.61	129.69	124.80
12	g	840	CLA	CMD-C2D-C3D	2.61	129.69	124.80
12	b	802	CLA	CHB-C4A-NA	2.61	128.12	124.51
12	L	202	CLA	O2D-CGD-O1D	-2.61	118.68	123.83
12	a	841	CLA	C1B-CHB-C4A	-2.61	124.96	130.12
12	b	840	CLA	CMD-C2D-C3D	2.61	129.69	124.80
12	b	830	CLA	C1B-CHB-C4A	-2.61	124.96	130.12
12	l	204	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
12	B	828	CLA	CHB-C4A-NA	2.60	128.11	124.51
12	G	829	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
12	E	830	CLA	CMB-C2B-C3B	2.60	129.69	124.80
12	g	838	CLA	CMB-C2B-C3B	2.60	129.69	124.80
12	A	838	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
12	b	838	CLA	CMB-C2B-C3B	2.60	129.68	124.80
12	B	842	CLA	C1-C2-C3	-2.60	122.54	126.75
12	E	832	CLA	CHB-C4A-NA	2.60	128.11	124.51
12	A	831	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
12	s	202	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
12	E	801	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
12	a	829	CLA	CMB-C2B-C3B	2.60	129.68	124.80
12	E	834	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
12	e	828	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
12	G	810	CLA	C1-C2-C3	-2.60	122.54	126.75
12	G	819	CLA	CMB-C2B-C3B	2.60	129.68	124.80
12	g	812	CLA	C1-C2-C3	-2.60	122.54	126.75
12	E	842	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
12	B	813	CLA	C1-C2-C3	-2.60	122.55	126.75
12	b	811	CLA	C1-C2-C3	-2.60	122.55	126.75
12	G	841	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
12	a	832	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
12	G	829	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
12	e	841	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
12	b	822	CLA	CHB-C4A-NA	2.60	128.10	124.51
12	e	801	CLA	CMD-C2D-C3D	2.60	129.67	124.80
12	s	204	CLA	C1-C2-C3	-2.60	122.55	126.75
12	e	842	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
12	e	839	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
12	b	834	CLA	O2D-CGD-O1D	-2.60	118.70	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	812	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
12	e	840	CLA	CHB-C4A-NA	2.60	128.10	124.51
12	l	202	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
12	e	820	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
12	B	834	CLA	CMB-C2B-C3B	2.60	129.67	124.80
12	G	832	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
12	G	831	CLA	CMB-C2B-C3B	2.60	129.67	124.80
12	g	838	CLA	CHB-C4A-NA	2.59	128.10	124.51
12	a	839	CLA	CMD-C2D-C3D	2.59	129.67	124.80
12	A	827	CLA	CMB-C2B-C3B	2.59	129.66	124.80
12	E	842	CLA	CMD-C2D-C3D	2.59	129.66	124.80
12	g	827	CLA	CHB-C4A-NA	2.59	128.10	124.51
12	g	819	CLA	CHB-C4A-NA	2.59	128.10	124.51
12	B	835	CLA	O2D-CGD-O1D	-2.59	118.71	123.83
12	S	1501	CLA	O2D-CGD-O1D	-2.59	118.71	123.83
12	b	826	CLA	O2D-CGD-O1D	-2.59	118.71	123.83
12	b	826	CLA	CHB-C4A-NA	2.59	128.10	124.51
12	a	840	CLA	CMD-C2D-C3D	2.59	129.66	124.80
12	G	813	CLA	O2D-CGD-O1D	-2.59	118.71	123.83
12	E	843	CLA	CHB-C4A-NA	2.59	128.10	124.51
12	e	803	CLA	O2D-CGD-O1D	-2.59	118.71	123.83
12	b	833	CLA	O2D-CGD-O1D	-2.59	118.71	123.83
12	b	834	CLA	CHB-C4A-NA	2.59	128.09	124.51
12	A	801	CLA	CMD-C2D-C3D	2.59	129.66	124.80
12	b	830	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
12	E	802	CLA	CMD-C2D-C3D	2.59	129.66	124.80
12	G	825	CLA	CHB-C4A-NA	2.59	128.09	124.51
12	G	804	CLA	C1-C2-C3	-2.59	122.56	126.75
12	a	833	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
12	g	810	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
12	g	834	CLA	CHB-C4A-NA	2.59	128.09	124.51
12	B	841	CLA	CMD-C2D-C3D	2.59	129.65	124.80
12	A	815	CLA	CMD-C2D-C3D	2.59	129.65	124.80
12	G	837	CLA	CMB-C2B-C3B	2.59	129.65	124.80
12	e	801	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
12	a	817	CLA	CMD-C2D-C3D	2.59	129.65	124.80
12	A	802	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
12	B	839	CLA	CHB-C4A-NA	2.59	128.09	124.51
12	B	816	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
12	a	804	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
12	b	814	CLA	O2D-CGD-O1D	-2.58	118.73	123.83
12	e	832	CLA	O2D-CGD-O1D	-2.58	118.73	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	810	CLA	CMB-C2B-C3B	2.58	129.65	124.80
12	B	811	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
12	A	839	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
12	A	808	CLA	CMB-C2B-C3B	2.58	129.65	124.80
12	E	805	CLA	O2D-CGD-O1D	-2.58	118.73	123.83
12	B	820	CLA	CHB-C4A-NA	2.58	128.08	124.51
13	A	842	PQN	C21-C22-C23	-2.58	107.71	115.77
12	e	837	CLA	O2D-CGD-O1D	-2.58	118.73	123.83
12	a	801	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
12	E	843	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
12	G	801	CLA	CHB-C4A-NA	2.58	128.08	124.51
12	a	813	CLA	O2D-CGD-O1D	-2.58	118.73	123.83
12	e	841	CLA	CHB-C4A-NA	2.58	128.08	124.51
12	g	834	CLA	O2D-CGD-O1D	-2.58	118.74	123.83
12	E	833	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
12	L	201	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
12	a	839	CLA	C1-C2-C3	-2.58	122.58	126.75
12	e	831	CLA	O2D-CGD-O1D	-2.58	118.74	123.83
12	a	802	CLA	CMD-C2D-C3D	2.58	129.63	124.80
12	g	821	CLA	O2D-CGD-O1D	-2.58	118.74	123.83
12	G	810	CLA	CHB-C4A-NA	2.58	128.07	124.51
12	b	818	CLA	CHB-C4A-NA	2.58	128.07	124.51
12	b	838	CLA	CHB-C4A-NA	2.58	128.07	124.51
12	l	201	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
12	G	825	CLA	O2D-CGD-O1D	-2.58	118.74	123.83
12	A	838	CLA	CMD-C2D-C3D	2.57	129.63	124.80
12	G	833	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
12	B	832	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
12	e	839	CLA	CMD-C2D-C3D	2.57	129.63	124.80
12	b	820	CLA	CMB-C2B-C3B	2.57	129.63	124.80
12	g	803	CLA	CHB-C4A-NA	2.57	128.07	124.51
12	b	841	CLA	C1-C2-C3	-2.57	122.59	126.75
12	G	808	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
12	G	819	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
12	e	809	CLA	CMB-C2B-C3B	2.57	129.62	124.80
12	G	821	CLA	CHB-C4A-NA	2.57	128.07	124.51
12	B	803	CLA	CHB-C4A-NA	2.57	128.07	124.51
12	a	809	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
12	A	841	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
12	B	822	CLA	O2D-CGD-O1D	-2.57	118.76	123.83
12	G	808	CLA	O2D-CGD-O1D	-2.57	118.76	123.83
12	e	838	CLA	C1-C2-C3	-2.57	122.59	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	s	201	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
12	A	837	CLA	C1-C2-C3	-2.57	122.60	126.75
12	g	821	CLA	CMB-C2B-C3B	2.57	129.62	124.80
12	G	809	CLA	CHB-C4A-NA	2.57	128.06	124.51
12	E	841	CLA	CMD-C2D-C3D	2.57	129.61	124.80
12	E	835	CLA	O2D-CGD-O1D	-2.57	118.76	123.83
12	B	836	CLA	O2D-CGD-O1D	-2.57	118.76	123.83
12	B	836	CLA	CHB-C4A-NA	2.57	128.06	124.51
12	a	823	CLA	CHB-C4A-NA	2.57	128.06	124.51
12	e	816	CLA	CMD-C2D-C3D	2.56	129.61	124.80
12	A	837	CLA	CMD-C2D-C3D	2.56	129.61	124.80
12	G	837	CLA	CHB-C4A-NA	2.56	128.06	124.51
12	e	840	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
12	B	810	CLA	O2D-CGD-O1D	-2.56	118.77	123.83
12	e	808	CLA	O2D-CGD-O1D	-2.56	118.77	123.83
12	e	808	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
12	A	807	CLA	O2D-CGD-O1D	-2.56	118.77	123.83
12	g	822	CLA	CHB-C4A-NA	2.56	128.05	124.51
12	g	803	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
12	b	821	CLA	CHB-C4A-NA	2.56	128.05	124.51
12	E	810	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
12	B	824	CLA	CHB-C4A-NA	2.56	128.05	124.51
12	g	812	CLA	CHB-C4A-NA	2.56	128.05	124.51
13	e	843	PQN	C21-C22-C23	-2.56	107.79	115.77
12	E	811	CLA	CMB-C2B-C3B	2.56	129.60	124.80
12	A	811	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
12	A	807	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
12	b	802	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
12	B	820	CLA	C1-C2-C3	-2.56	122.61	126.75
12	B	828	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
12	E	824	CLA	CHB-C4A-NA	2.56	128.05	124.51
12	g	827	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
12	e	845	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
12	E	814	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
12	A	836	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
12	G	801	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
12	A	816	CLA	CMD-C2D-C3D	2.56	129.59	124.80
12	e	833	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
12	B	801	CLA	CMD-C2D-C3D	2.55	129.59	124.80
12	a	813	CLA	CMD-C2D-C3D	2.55	129.59	124.80
12	b	810	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	A	806	CLA	C1B-CHB-C4A	-2.55	125.06	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	801	CLA	CMD-C2D-C3D	2.55	129.59	124.80
12	E	841	CLA	C1-C2-C3	-2.55	122.62	126.75
12	A	830	CLA	O2D-CGD-O1D	-2.55	118.79	123.83
12	B	826	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	A	822	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	G	817	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	B	803	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
12	A	829	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	a	837	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
12	a	834	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
12	b	818	CLA	C1-C2-C3	-2.55	122.63	126.75
12	B	812	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	a	838	CLA	O2D-CGD-O1D	-2.55	118.80	123.83
12	G	815	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	B	811	CLA	O2D-CGD-O1D	-2.55	118.80	123.83
12	a	808	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
12	E	809	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
12	E	836	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
12	b	808	CLA	O2D-CGD-O1D	-2.55	118.80	123.83
12	g	825	CLA	CHB-C4A-NA	2.55	128.03	124.51
12	a	809	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
12	E	840	CLA	O2D-CGD-O1D	-2.55	118.80	123.83
12	g	810	CLA	O2D-CGD-O1D	-2.55	118.80	123.83
12	e	836	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
12	E	805	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
12	F	1301	CLA	CMB-C2B-C3B	2.55	129.57	124.80
12	b	809	CLA	O2D-CGD-O1D	-2.55	118.80	123.83
12	b	820	CLA	O2D-CGD-O1D	-2.55	118.80	123.83
12	A	832	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
12	G	807	CLA	O2D-CGD-O1D	-2.54	118.81	123.83
12	O	1301	CLA	CMB-C2B-C3B	2.54	129.57	124.80
12	G	837	CLA	O2D-CGD-O1D	-2.54	118.81	123.83
12	g	841	CLA	C1-C2-C3	-2.54	122.64	126.75
12	G	840	CLA	C1-C2-C3	-2.54	122.64	126.75
12	g	817	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
12	g	811	CLA	CHB-C4A-NA	2.54	128.03	124.51
12	e	817	CLA	CMD-C2D-C3D	2.54	129.57	124.80
12	a	824	CLA	CHB-C4A-NA	2.54	128.03	124.51
12	g	819	CLA	C1-C2-C3	-2.54	122.64	126.75
12	E	824	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
12	g	817	CLA	CHB-C4A-NA	2.54	128.02	124.51
12	E	839	CLA	C1B-CHB-C4A	-2.54	125.09	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	803	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
12	e	838	CLA	CMD-C2D-C3D	2.54	129.56	124.80
12	e	812	CLA	CMD-C2D-C3D	2.54	129.56	124.80
12	g	809	CLA	O2D-CGD-O1D	-2.54	118.82	123.83
12	a	818	CLA	CMD-C2D-C3D	2.54	129.56	124.80
12	g	823	CLA	CHB-C4A-NA	2.54	128.02	124.51
12	E	819	CLA	CMD-C2D-C3D	2.54	129.56	124.80
12	A	811	CLA	CMD-C2D-C3D	2.54	129.56	124.80
12	G	815	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
12	a	823	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
12	b	817	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
12	e	842	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
12	E	807	CLA	CHB-C4A-NA	2.53	128.02	124.51
12	b	805	CLA	O2D-CGD-O1D	-2.53	118.83	123.83
12	a	804	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
12	G	818	CLA	CHB-C4A-NA	2.53	128.01	124.51
12	E	810	CLA	O2D-CGD-O1D	-2.53	118.83	123.83
12	B	823	CLA	CHB-C4A-NA	2.53	128.01	124.51
12	G	823	CLA	CHB-C4A-NA	2.53	128.01	124.51
12	f	1301	CLA	CMB-C2B-C3B	2.53	129.54	124.80
12	g	832	CLA	CHB-C4A-NA	2.53	128.01	124.51
12	A	835	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
12	e	804	CLA	O2D-CGD-O1D	-2.53	118.84	123.83
12	E	814	CLA	CMD-C2D-C3D	2.53	129.54	124.80
12	a	801	CLA	C1-C2-C3	-2.53	122.66	126.75
12	g	838	CLA	O2D-CGD-O1D	-2.53	118.84	123.83
12	b	824	CLA	CHB-C4A-NA	2.53	128.01	124.51
12	G	820	CLA	CHB-C4A-NA	2.53	128.01	124.51
12	A	803	CLA	O2D-CGD-O1D	-2.53	118.84	123.83
12	B	818	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
12	a	805	CLA	CMD-C2D-C3D	2.52	129.53	124.80
12	A	802	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
12	e	823	CLA	CHB-C4A-NA	2.52	128.00	124.51
12	o	1301	CLA	CHB-C4A-NA	2.52	128.00	124.51
12	e	807	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
12	O	1301	CLA	CHB-C4A-NA	2.52	128.00	124.51
12	e	824	CLA	O2D-CGD-O1D	-2.52	118.85	123.83
12	o	1301	CLA	CMB-C2B-C3B	2.52	129.53	124.80
12	G	817	CLA	C1-C2-C3	-2.52	122.67	126.75
12	g	818	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
12	g	820	CLA	CHB-C4A-NA	2.52	128.00	124.51
12	E	825	CLA	CHB-C4A-NA	2.52	127.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	1301	CLA	CHB-C4A-NA	2.52	127.99	124.51
12	E	806	CLA	CMD-C2D-C3D	2.52	129.52	124.80
12	B	811	CLA	CMD-C2D-C3D	2.52	129.52	124.80
12	e	804	CLA	CMD-C2D-C3D	2.52	129.52	124.80
12	A	823	CLA	O2D-CGD-O1D	-2.52	118.86	123.83
12	a	805	CLA	O2D-CGD-O1D	-2.52	118.86	123.83
12	e	805	CLA	CHB-C4A-NA	2.52	127.99	124.51
12	A	821	CLA	CHB-C4A-NA	2.52	127.99	124.51
12	g	812	CLA	CMD-C2D-C3D	2.51	129.51	124.80
12	A	816	CLA	CHB-C4A-NA	2.51	127.99	124.51
12	B	821	CLA	CHB-C4A-NA	2.51	127.99	124.51
12	G	816	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
12	E	835	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
12	l	202	CLA	CHB-C4A-NA	2.51	127.99	124.51
12	A	821	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
12	G	804	CLA	O2D-CGD-O1D	-2.51	118.87	123.83
12	e	817	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	L	202	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	e	822	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
12	e	837	CLA	CMD-C2D-C3D	2.51	129.51	124.80
12	a	820	CLA	CMB-C2B-C3B	2.51	129.51	124.80
12	B	803	CLA	C1-C2-C3	-2.51	122.69	126.75
12	A	818	CLA	CMB-C2B-C3B	2.51	129.50	124.80
12	e	819	CLA	CMB-C2B-C3B	2.51	129.50	124.80
12	G	801	CLA	C1-C2-C3	-2.51	122.69	126.75
12	b	811	CLA	CMD-C2D-C3D	2.51	129.50	124.80
12	e	830	CLA	O2D-CGD-O1D	-2.51	118.88	123.83
12	e	822	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	g	828	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	E	806	CLA	O2D-CGD-O1D	-2.51	118.88	123.83
12	b	816	CLA	CHB-C4A-NA	2.50	127.97	124.51
12	G	822	CLA	CHB-C4A-NA	2.50	127.97	124.51
12	A	804	CLA	CHB-C4A-NA	2.50	127.97	124.51
12	E	828	CLA	CHB-C4A-NA	2.50	127.97	124.51
12	e	832	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
12	g	806	CLA	O2D-CGD-O1D	-2.50	118.89	123.83
12	a	833	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
12	B	818	CLA	CHB-C4A-NA	2.50	127.97	124.51
12	B	807	CLA	O2D-CGD-O1D	-2.50	118.89	123.83
12	G	808	CLA	CMD-C2D-C3D	2.50	129.49	124.80
12	E	805	CLA	C1-C2-C3	-2.50	122.70	126.75
12	b	831	CLA	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	816	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
12	E	821	CLA	CMB-C2B-C3B	2.50	129.49	124.80
12	E	840	CLA	CMD-C2D-C3D	2.50	129.49	124.80
12	A	831	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
12	E	840	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
12	A	836	CLA	CMD-C2D-C3D	2.50	129.48	124.80
12	B	839	CLA	O2D-CGD-O1D	-2.50	118.90	123.83
12	a	828	CLA	CMD-C2D-C3D	2.50	129.48	124.80
12	s	202	CLA	CHB-C4A-NA	2.50	127.96	124.51
12	a	806	CLA	CHB-C4A-NA	2.50	127.96	124.51
12	g	822	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
12	G	810	CLA	CMD-C2D-C3D	2.49	129.48	124.80
12	b	809	CLA	CMD-C2D-C3D	2.49	129.48	124.80
12	B	819	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
12	a	802	CLA	O2D-CGD-CBD	2.49	115.62	111.25
12	E	802	CLA	O2D-CGD-CBD	2.49	115.62	111.25
12	g	803	CLA	C1-C2-C3	-2.49	122.72	126.75
12	b	838	CLA	O2D-CGD-O1D	-2.49	118.91	123.83
12	B	825	CLA	CHB-C4A-NA	2.49	127.96	124.51
12	f	1301	CLA	CHB-C4A-NA	2.49	127.96	124.51
12	L	201	CLA	CMD-C2D-C3D	2.49	129.47	124.80
12	B	801	CLA	O2D-CGD-CBD	2.49	115.61	111.25
12	b	802	CLA	C1-C2-C3	-2.49	122.72	126.75
12	a	825	CLA	O2D-CGD-O1D	-2.49	118.91	123.83
12	E	833	CLA	CMD-C2D-C3D	2.49	129.47	124.80
12	e	819	CLA	CMD-C2D-C3D	2.49	129.47	124.80
12	a	838	CLA	CMD-C2D-C3D	2.49	129.47	124.80
12	G	830	CLA	CHB-C4A-NA	2.49	127.95	124.51
12	S	1502	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
12	b	819	CLA	CHB-C4A-NA	2.49	127.95	124.51
12	G	839	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
12	E	826	CLA	O2D-CGD-O1D	-2.49	118.92	123.83
12	B	810	CLA	CHB-C4A-NA	2.49	127.95	124.51
12	g	810	CLA	CMD-C2D-C3D	2.49	129.46	124.80
12	A	825	CLA	CHB-C4A-NA	2.49	127.95	124.51
12	E	826	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
12	B	813	CLA	CMD-C2D-C3D	2.49	129.46	124.80
12	E	801	CLA	C1-C2-C3	-2.49	122.73	126.75
12	g	801	CLA	O2D-CGD-CBD	2.49	115.60	111.25
12	E	819	CLA	CHB-C4A-NA	2.48	127.95	124.51
12	E	831	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
12	A	823	CLA	C1B-CHB-C4A	-2.48	125.20	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	826	CLA	CHB-C4A-NA	2.48	127.95	124.51
12	A	803	CLA	CMD-C2D-C3D	2.48	129.46	124.80
12	A	819	CLA	C1-C2-C3	-2.48	122.73	126.75
12	a	804	CLA	C1-C2-C3	-2.48	122.73	126.75
12	A	824	CLA	CHB-C4A-NA	2.48	127.94	124.51
12	a	830	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
12	a	827	CLA	CHB-C4A-NA	2.48	127.94	124.51
12	g	809	CLA	CHB-C4A-NA	2.48	127.94	124.51
12	a	838	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
12	e	817	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
12	b	821	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
12	A	801	CLA	C1-C2-C3	-2.48	122.74	126.75
12	e	829	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
12	a	818	CLA	CHB-C4A-NA	2.48	127.94	124.51
12	B	829	CLA	CHB-C4A-NA	2.48	127.94	124.51
12	a	826	CLA	CHB-C4A-NA	2.48	127.94	124.51
12	S	1501	CLA	CHB-C4A-NA	2.48	127.94	124.51
12	g	806	CLA	CHB-C4A-NA	2.48	127.94	124.51
12	E	832	CLA	O2D-CGD-O1D	-2.48	118.94	123.83
12	B	841	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
12	g	826	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
12	l	201	CLA	CMD-C2D-C3D	2.48	129.44	124.80
12	E	829	CLA	CMD-C2D-C3D	2.48	129.44	124.80
12	a	821	CLA	C1-C2-C3	-2.47	122.75	126.75
12	e	819	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
12	A	841	CLA	CHB-C4A-NA	2.47	127.93	124.51
12	g	802	CLA	C1-C2-C3	-2.47	122.75	126.75
12	A	829	CLA	O2D-CGD-O1D	-2.47	118.95	123.83
12	g	824	CLA	CHB-C4A-NA	2.47	127.93	124.51
12	A	828	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
12	A	818	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
12	b	825	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
12	B	827	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
12	E	821	CLA	CMD-C2D-C3D	2.47	129.43	124.80
12	a	820	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
12	s	204	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
12	A	816	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
12	a	825	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
12	e	837	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
12	e	824	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
12	e	827	CLA	CMD-C2D-C3D	2.47	129.43	124.80
12	A	818	CLA	CMD-C2D-C3D	2.47	129.43	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	820	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
12	B	833	CLA	CHB-C4A-NA	2.47	127.92	124.51
13	b	843	PQN	C14-C13-C15	2.47	119.54	115.29
12	G	807	CLA	CHB-C4A-NA	2.47	127.92	124.51
12	B	823	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
12	E	827	CLA	CHB-C4A-NA	2.47	127.92	124.51
12	A	826	CLA	CMD-C2D-C3D	2.46	129.42	124.80
12	G	820	CLA	CMD-C2D-C3D	2.46	129.42	124.80
12	A	838	CLA	CHB-C4A-NA	2.46	127.92	124.51
12	g	819	CLA	CMB-C2B-C3B	2.46	129.42	124.80
12	a	820	CLA	CMD-C2D-C3D	2.46	129.42	124.80
12	e	821	CLA	O2D-CGD-CBD	2.46	115.56	111.25
12	A	805	CLA	CMD-C2D-C3D	2.46	129.42	124.80
12	E	819	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
12	A	836	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
12	B	836	CLA	CMD-C2D-C3D	2.46	129.42	124.80
12	A	824	CLA	CMD-C2D-C3D	2.46	129.42	124.80
12	b	815	CLA	CHB-C4A-NA	2.46	127.92	124.51
12	l	204	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
12	G	806	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
12	B	803	CLA	O2D-CGD-O1D	-2.46	118.97	123.83
12	e	801	CLA	C1-C2-C3	-2.46	122.77	126.75
12	b	840	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
13	g	843	PQN	C14-C13-C15	2.46	119.52	115.29
12	e	820	CLA	C1-C2-C3	-2.46	122.77	126.75
12	A	802	CLA	C1-C2-C3	-2.46	122.77	126.75
12	E	822	CLA	C1-C2-C3	-2.46	122.77	126.75
12	B	813	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
13	B	844	PQN	C14-C13-C15	2.46	119.52	115.29
12	g	822	CLA	CMD-C2D-C3D	2.46	129.41	124.80
12	B	823	CLA	CMD-C2D-C3D	2.46	129.41	124.80
12	b	801	CLA	C1-C2-C3	-2.46	122.78	126.75
12	b	811	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
12	a	831	CLA	O2D-CGD-O1D	-2.46	118.98	123.83
12	L	204	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
12	b	807	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
12	E	821	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
12	e	811	CLA	CMD-C2D-C3D	2.45	129.40	124.80
12	A	833	CLA	O2D-CGD-CBD	2.45	115.55	111.25
12	E	827	CLA	CMD-C2D-C3D	2.45	129.40	124.80
12	B	805	CLA	CMD-C2D-C3D	2.45	129.40	124.80
12	e	839	CLA	CHB-C4A-NA	2.45	127.91	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	827	CLA	CHB-C4A-NA	2.45	127.90	124.51
12	g	808	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
12	e	806	CLA	CMD-C2D-C3D	2.45	129.40	124.80
12	a	807	CLA	CMD-C2D-C3D	2.45	129.40	124.80
12	G	824	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
12	B	832	CLA	C1-C2-C3	-2.45	122.79	126.75
12	b	808	CLA	CHB-C4A-NA	2.45	127.90	124.51
12	l	201	CLA	CHB-C4A-NA	2.45	127.90	124.51
12	a	812	CLA	CMD-C2D-C3D	2.45	129.39	124.80
12	l	204	CLA	CMD-C2D-C3D	2.45	129.39	124.80
12	E	842	CLA	CHB-C4A-NA	2.45	127.90	124.51
12	s	201	CLA	CMD-C2D-C3D	2.45	129.39	124.80
12	b	834	CLA	CMD-C2D-C3D	2.45	129.39	124.80
12	e	803	CLA	CHB-C4A-NA	2.45	127.89	124.51
12	e	825	CLA	CHB-C4A-NA	2.45	127.89	124.51
12	B	807	CLA	CHB-C4A-NA	2.45	127.89	124.51
12	b	818	CLA	CMB-C2B-C3B	2.45	129.39	124.80
12	g	840	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
12	E	837	CLA	O2D-CGD-CBD	2.45	115.53	111.25
12	e	826	CLA	CHB-C4A-NA	2.45	127.89	124.51
12	a	835	CLA	O2D-CGD-CBD	2.45	115.53	111.25
12	G	833	CLA	CMD-C2D-C3D	2.45	129.39	124.80
12	E	813	CLA	CMD-C2D-C3D	2.44	129.38	124.80
12	B	802	CLA	C1-C2-C3	-2.44	122.80	126.75
12	E	823	CLA	O2D-CGD-CBD	2.44	115.53	111.25
12	G	817	CLA	CMB-C2B-C3B	2.44	129.38	124.80
12	G	827	CLA	CHB-C4A-NA	2.44	127.89	124.51
12	a	840	CLA	CHB-C4A-NA	2.44	127.89	124.51
12	B	820	CLA	CMB-C2B-C3B	2.44	129.38	124.80
12	B	809	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
12	b	828	CLA	CHB-C4A-NA	2.44	127.89	124.51
12	a	822	CLA	O2D-CGD-CBD	2.44	115.53	111.25
12	E	813	CLA	CHB-C4A-NA	2.44	127.89	124.51
12	e	834	CLA	O2D-CGD-CBD	2.44	115.53	111.25
12	G	801	CLA	O2D-CGD-O1D	-2.44	119.01	123.83
12	E	808	CLA	CMD-C2D-C3D	2.44	129.38	124.80
12	R	1401	CLA	CHB-C4A-NA	2.44	127.89	124.51
12	b	804	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
12	E	804	CLA	CHB-C4A-NA	2.44	127.89	124.51
13	G	842	PQN	C14-C13-C15	2.44	119.49	115.29
12	a	818	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
12	b	814	CLA	C1B-CHB-C4A	-2.44	125.29	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	825	CLA	C1-C2-C3	-2.44	122.81	126.75
12	s	204	CLA	CMD-C2D-C3D	2.44	129.37	124.80
12	B	837	CLA	CMD-C2D-C3D	2.44	129.37	124.80
12	b	809	CLA	CHB-C4A-NA	2.44	127.88	124.51
12	g	829	CLA	CHB-C4A-NA	2.44	127.88	124.51
12	S	1502	CLA	CMD-C2D-C3D	2.44	129.37	124.80
12	a	826	CLA	CMD-C2D-C3D	2.44	129.37	124.80
12	b	815	CLA	CMD-C2D-C3D	2.44	129.37	124.80
12	g	831	CLA	CHB-C4A-NA	2.43	127.88	124.51
12	E	803	CLA	C1-C2-C3	-2.43	122.81	126.75
12	A	803	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
12	G	804	CLA	CHB-C4A-NA	2.43	127.88	124.51
12	G	811	CLA	C1-C2-C3	-2.43	122.82	126.75
12	G	810	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
12	B	832	CLA	CHB-C4A-NA	2.43	127.88	124.51
12	b	821	CLA	CMD-C2D-C3D	2.43	129.36	124.80
12	L	204	CLA	CMD-C2D-C3D	2.43	129.36	124.80
12	E	805	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	b	805	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	g	803	CLA	O2D-CGD-O1D	-2.43	119.03	123.83
12	g	820	CLA	CMD-C2D-C3D	2.43	129.36	124.80
12	g	832	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
12	E	806	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
12	g	818	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	b	817	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	B	807	CLA	OBD-CAD-CBD	-2.43	122.34	125.91
12	b	802	CLA	O2D-CGD-O1D	-2.43	119.03	123.83
12	L	201	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	g	834	CLA	CMD-C2D-C3D	2.43	129.36	124.80
12	A	801	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	G	833	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
12	b	805	CLA	OBD-CAD-CBD	-2.43	122.34	125.91
12	g	831	CLA	C1-C2-C3	-2.43	122.82	126.75
12	B	817	CLA	CMD-C2D-C3D	2.43	129.35	124.80
12	g	812	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
12	E	833	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	b	823	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	g	836	CLA	CMD-C2D-C3D	2.43	129.35	124.80
12	b	815	CLA	O2D-CGD-O1D	-2.43	119.04	123.83
12	e	802	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	a	829	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	B	817	CLA	CHB-C4A-NA	2.43	127.87	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	829	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	e	844	CLA	CMD-C2D-C3D	2.43	129.35	124.80
12	A	820	CLA	O2D-CGD-CBD	2.43	115.50	111.25
12	b	830	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	G	828	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
12	e	825	CLA	CMD-C2D-C3D	2.43	129.35	124.80
12	A	810	CLA	CMD-C2D-C3D	2.43	129.35	124.80
12	e	804	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
12	b	831	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
12	g	816	CLA	CMD-C2D-C3D	2.42	129.35	124.80
12	e	841	CLA	CMD-C2D-C3D	2.42	129.35	124.80
12	a	827	CLA	C1-C2-C3	-2.42	122.83	126.75
12	A	808	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
12	B	806	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
12	A	832	CLA	OBD-CAD-CBD	-2.42	122.35	125.91
12	G	802	CLA	CMD-C2D-C3D	2.42	129.35	124.80
12	G	818	CLA	CMD-C2D-C3D	2.42	129.35	124.80
12	a	805	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
12	A	817	CLA	CMD-C2D-C3D	2.42	129.34	124.80
12	b	841	CLA	CHB-C4A-NA	2.42	127.86	124.51
12	g	830	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
12	E	813	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
12	G	818	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
12	a	832	CLA	CMD-C2D-C3D	2.42	129.34	124.80
12	B	814	CLA	C1-C2-C3	-2.42	122.83	126.75
12	a	819	CLA	CMD-C2D-C3D	2.42	129.34	124.80
12	A	826	CLA	CHB-C4A-NA	2.42	127.86	124.51
12	K	1401	CLA	CHB-C4A-NA	2.42	127.86	124.51
12	b	834	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
12	B	830	CLA	CHB-C4A-NA	2.42	127.86	124.51
12	e	831	CLA	CMD-C2D-C3D	2.42	129.34	124.80
12	E	820	CLA	CMD-C2D-C3D	2.42	129.34	124.80
12	B	830	CLA	CMD-C2D-C3D	2.42	129.34	124.80
12	G	816	CLA	CHB-C4A-NA	2.42	127.86	124.51
12	B	843	CLA	CMD-C2D-C3D	2.42	129.34	124.80
12	e	811	CLA	CHB-C4A-NA	2.42	127.86	124.51
12	G	803	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
12	G	814	CLA	O2D-CGD-O1D	-2.42	119.06	123.83
12	s	202	CLA	CMD-C2D-C3D	2.42	129.33	124.80
12	G	829	CLA	CHB-C4A-NA	2.42	127.85	124.51
12	G	814	CLA	CHB-C4A-NA	2.42	127.85	124.51
12	e	803	CLA	C1-C2-C3	-2.42	122.84	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	829	CLA	C1-C2-C3	-2.42	122.84	126.75
12	A	840	CLA	CMD-C2D-C3D	2.42	129.33	124.80
12	B	821	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
12	r	1401	CLA	CHB-C4A-NA	2.42	127.85	124.51
12	B	816	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
12	b	819	CLA	CMD-C2D-C3D	2.42	129.33	124.80
12	g	805	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
12	J	1101	CLA	CHB-C4A-NA	2.41	127.85	124.51
12	e	801	CLA	CHB-C4A-NA	2.41	127.85	124.51
12	E	844	CLA	CMD-C2D-C3D	2.41	129.33	124.80
12	E	828	CLA	C1-C2-C3	-2.41	122.85	126.75
12	a	812	CLA	CHB-C4A-NA	2.41	127.85	124.51
12	A	834	CLA	CHB-C4A-NA	2.41	127.85	124.51
12	e	811	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
12	e	826	CLA	CMD-C2D-C3D	2.41	129.32	124.80
12	g	806	CLA	OBD-CAD-CBD	-2.41	122.37	125.91
12	A	815	CLA	CHB-C4A-NA	2.41	127.85	124.51
12	b	830	CLA	C1-C2-C3	-2.41	122.85	126.75
12	b	836	CLA	CMD-C2D-C3D	2.41	129.32	124.80
12	A	830	CLA	CMD-C2D-C3D	2.41	129.32	124.80
12	G	812	CLA	CMD-C2D-C3D	2.41	129.32	124.80
12	G	804	CLA	OBD-CAD-CBD	-2.41	122.37	125.91
12	a	827	CLA	CMD-C2D-C3D	2.41	129.32	124.80
12	G	814	CLA	CMD-C2D-C3D	2.41	129.32	124.80
12	b	803	CLA	CMD-C2D-C3D	2.41	129.32	124.80
12	a	842	CLA	CMD-C2D-C3D	2.41	129.32	124.80
12	e	828	CLA	CHB-C4A-NA	2.41	127.84	124.51
12	b	829	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
12	g	815	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
12	B	817	CLA	O2D-CGD-O1D	-2.41	119.07	123.83
12	G	813	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
12	E	818	CLA	CHB-C4A-NA	2.41	127.84	124.51
12	B	842	CLA	CHB-C4A-NA	2.41	127.84	124.51
12	A	810	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
12	A	827	CLA	CHB-C4A-NA	2.41	127.84	124.51
12	G	835	CLA	CMD-C2D-C3D	2.41	129.31	124.80
12	B	831	CLA	CMD-C2D-C3D	2.41	129.31	124.80
12	b	832	CLA	CHB-C4A-NA	2.41	127.84	124.51
12	E	830	CLA	CHB-C4A-NA	2.41	127.84	124.51
12	E	835	CLA	CHB-C4A-NA	2.41	127.84	124.51
12	g	819	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
12	s	202	CLA	C1B-CHB-C4A	-2.40	125.35	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	g	814	CLA	CMD-C2D-C3D	2.40	129.31	124.80
12	G	841	CLA	CMD-C2D-C3D	2.40	129.31	124.80
12	A	825	CLA	CMD-C2D-C3D	2.40	129.31	124.80
12	b	812	CLA	C1-C2-C3	-2.40	122.86	126.75
12	s	201	CLA	CHB-C4A-NA	2.40	127.84	124.51
12	a	806	CLA	CMD-C2D-C3D	2.40	129.31	124.80
12	e	826	CLA	C1-C2-C3	-2.40	122.86	126.75
12	e	820	CLA	CMD-C2D-C3D	2.40	129.31	124.80
12	g	816	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	a	801	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	b	832	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
12	a	817	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	e	835	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	S	1501	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
12	g	813	CLA	C1-C2-C3	-2.40	122.87	126.75
12	B	827	CLA	CMD-C2D-C3D	2.40	129.30	124.80
12	g	841	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	g	820	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
12	b	820	CLA	CMD-C2D-C3D	2.40	129.30	124.80
12	g	830	CLA	C1-C2-C3	-2.40	122.87	126.75
12	a	833	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	E	801	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	E	807	CLA	CMD-C2D-C3D	2.40	129.30	124.80
12	B	836	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
12	e	827	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	a	803	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	a	812	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
12	b	819	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
12	E	828	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
12	l	202	CLA	CMD-C2D-C3D	2.40	129.30	124.80
12	A	825	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
12	e	815	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	a	804	CLA	CHB-C4A-NA	2.40	127.83	124.51
12	S	1501	CLA	CMD-C2D-C3D	2.40	129.30	124.80
12	l	202	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
12	R	1401	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
12	e	833	CLA	OBD-CAD-CBD	-2.40	122.39	125.91
12	e	822	CLA	C1-C2-C3	-2.40	122.87	126.75
12	b	842	CLA	CMD-C2D-C3D	2.40	129.29	124.80
12	g	816	CLA	O2D-CGD-O1D	-2.40	119.10	123.83
12	E	836	CLA	OBD-CAD-CBD	-2.40	122.39	125.91
12	g	838	CLA	CMD-C2D-C3D	2.40	129.29	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	830	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
12	e	821	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
12	E	834	CLA	CMD-C2D-C3D	2.40	129.29	124.80
12	b	813	CLA	CMD-C2D-C3D	2.40	129.29	124.80
12	A	831	CLA	CHB-C4A-NA	2.40	127.82	124.51
12	a	834	CLA	OBD-CAD-CBD	-2.39	122.39	125.91
12	B	820	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
12	g	834	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
12	B	833	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
12	B	831	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
12	b	825	CLA	CMD-C2D-C3D	2.39	129.29	124.80
12	E	828	CLA	CMD-C2D-C3D	2.39	129.29	124.80
12	B	821	CLA	CMD-C2D-C3D	2.39	129.29	124.80
12	b	838	CLA	CMD-C2D-C3D	2.39	129.29	124.80
12	L	202	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
12	g	810	CLA	CHB-C4A-NA	2.39	127.82	124.51
12	E	804	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
12	g	826	CLA	CMD-C2D-C3D	2.39	129.29	124.80
12	J	1101	CLA	C1-C2-C3	-2.39	122.88	126.75
12	A	810	CLA	CHB-C4A-NA	2.39	127.82	124.51
12	E	811	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
12	g	829	CLA	CMD-C2D-C3D	2.39	129.28	124.80
12	B	811	CLA	CHB-C4A-NA	2.39	127.82	124.51
12	A	819	CLA	CMD-C2D-C3D	2.39	129.28	124.80
12	A	804	CLA	CMD-C2D-C3D	2.39	129.28	124.80
12	g	808	CLA	CHB-C4A-NA	2.39	127.82	124.51
12	G	827	CLA	CMD-C2D-C3D	2.39	129.28	124.80
12	a	816	CLA	CMD-C2D-C3D	2.39	129.28	124.80
12	e	842	CLA	CHB-C4A-NA	2.39	127.81	124.51
12	a	828	CLA	CHB-C4A-NA	2.39	127.81	124.51
12	e	832	CLA	CHB-C4A-NA	2.39	127.81	124.51
12	g	809	CLA	CMD-C2D-C3D	2.39	129.28	124.80
12	g	821	CLA	CMD-C2D-C3D	2.39	129.28	124.80
12	b	828	CLA	CMD-C2D-C3D	2.39	129.28	124.80
12	k	1401	CLA	CHB-C4A-NA	2.39	127.81	124.51
12	a	803	CLA	C1-C2-C3	-2.39	122.89	126.75
12	e	818	CLA	CMD-C2D-C3D	2.39	129.28	124.80
12	B	822	CLA	CMD-C2D-C3D	2.39	129.27	124.80
12	g	830	CLA	CMD-C2D-C3D	2.39	129.27	124.80
12	a	823	CLA	C1-C2-C3	-2.38	122.89	126.75
12	G	824	CLA	CMD-C2D-C3D	2.38	129.27	124.80
12	e	826	CLA	C1B-CHB-C4A	-2.38	125.39	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	810	CLA	CMD-C2D-C3D	2.38	129.27	124.80
12	b	810	CLA	CMD-C2D-C3D	2.38	129.27	124.80
12	G	828	CLA	CHB-C4A-NA	2.38	127.81	124.51
12	r	1401	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
12	B	834	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
12	b	818	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
12	b	838	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
12	a	810	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
12	g	842	CLA	CMD-C2D-C3D	2.38	129.27	124.80
12	a	836	CLA	CHB-C4A-NA	2.38	127.81	124.51
12	E	838	CLA	CHB-C4A-NA	2.38	127.81	124.51
12	b	807	CLA	CHB-C4A-NA	2.38	127.81	124.51
12	L	202	CLA	CMD-C2D-C3D	2.38	129.27	124.80
12	g	838	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
12	A	841	CLA	CMD-C2D-C3D	2.38	129.26	124.80
12	E	822	CLA	CMD-C2D-C3D	2.38	129.26	124.80
12	e	802	CLA	C1-C2-C3	-2.38	122.90	126.75
12	b	829	CLA	CMD-C2D-C3D	2.38	129.26	124.80
12	b	829	CLA	C1-C2-C3	-2.38	122.90	126.75
12	G	806	CLA	CHB-C4A-NA	2.38	127.80	124.51
12	A	802	CLA	CHB-C4A-NA	2.38	127.80	124.51
12	G	831	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
12	G	807	CLA	CMD-C2D-C3D	2.38	129.26	124.80
12	E	808	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
12	g	830	CLA	CHB-C4A-NA	2.38	127.80	124.51
12	G	840	CLA	CHB-C4A-NA	2.38	127.80	124.51
12	G	806	CLA	C1-C2-C3	-2.38	122.91	126.75
12	b	837	CLA	CMD-C2D-C3D	2.38	129.26	124.80
12	E	817	CLA	CMD-C2D-C3D	2.38	129.26	124.80
12	B	816	CLA	CMD-C2D-C3D	2.38	129.26	124.80
12	a	827	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
12	b	808	CLA	CMD-C2D-C3D	2.38	129.26	124.80
12	e	805	CLA	CMD-C2D-C3D	2.38	129.26	124.80
12	G	831	CLA	CHB-C4A-NA	2.38	127.80	124.51
12	G	822	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
12	g	819	CLA	CMD-C2D-C3D	2.38	129.25	124.80
12	A	814	CLA	CMD-C2D-C3D	2.37	129.25	124.80
12	G	828	CLA	C1-C2-C3	-2.37	122.91	126.75
12	A	814	CLA	CHB-C4A-NA	2.37	127.79	124.51
12	e	809	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
12	K	1401	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
12	e	802	CLA	C1B-CHB-C4A	-2.37	125.42	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	819	CLA	CHB-C4A-NA	2.37	127.79	124.51
12	K	1401	CLA	CMD-C2D-C3D	2.37	129.25	124.80
12	g	815	CLA	CMD-C2D-C3D	2.37	129.25	124.80
12	B	834	CLA	CHB-C4A-NA	2.37	127.79	124.51
12	B	815	CLA	CMD-C2D-C3D	2.37	129.25	124.80
12	k	1401	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
12	B	809	CLA	CHB-C4A-NA	2.37	127.79	124.51
12	B	831	CLA	CHB-C4A-NA	2.37	127.79	124.51
12	e	815	CLA	CMD-C2D-C3D	2.37	129.24	124.80
12	b	831	CLA	CMD-C2D-C3D	2.37	129.24	124.80
12	g	827	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
12	A	820	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
12	a	807	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
12	G	817	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
12	B	839	CLA	CMD-C2D-C3D	2.37	129.24	124.80
12	E	810	CLA	CMD-C2D-C3D	2.37	129.24	124.80
12	B	831	CLA	C1-C2-C3	-2.37	122.92	126.75
12	B	828	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
12	G	806	CLA	CMD-C2D-C3D	2.37	129.24	124.80
12	g	824	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
12	A	821	CLA	C1-C2-C3	-2.37	122.92	126.75
12	g	832	CLA	CMD-C2D-C3D	2.37	129.24	124.80
12	R	1401	CLA	CMD-C2D-C3D	2.37	129.24	124.80
12	G	808	CLA	CHB-C4A-NA	2.37	127.78	124.51
12	e	808	CLA	CMD-C2D-C3D	2.36	129.24	124.80
12	g	818	CLA	CMD-C2D-C3D	2.36	129.24	124.80
12	a	822	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
12	b	801	CLA	CMD-C2D-C3D	2.36	129.23	124.80
12	g	808	CLA	CMD-C2D-C3D	2.36	129.23	124.80
12	e	806	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
12	G	828	CLA	CMD-C2D-C3D	2.36	129.23	124.80
12	A	813	CLA	CMD-C2D-C3D	2.36	129.23	124.80
12	G	816	CLA	CMD-C2D-C3D	2.36	129.23	124.80
12	E	804	CLA	C1-C2-C3	-2.36	122.93	126.75
12	e	842	CLA	CMD-C2D-C3D	2.36	129.23	124.80
12	r	1401	CLA	CMD-C2D-C3D	2.36	129.23	124.80
12	e	819	CLA	CHB-C4A-NA	2.36	127.78	124.51
12	e	812	CLA	CHB-C4A-NA	2.36	127.78	124.51
12	E	824	CLA	C1-C2-C3	-2.36	122.93	126.75
12	E	817	CLA	CHB-C4A-NA	2.36	127.78	124.51
12	g	802	CLA	CMD-C2D-C3D	2.36	129.23	124.80
12	b	818	CLA	CMD-C2D-C3D	2.36	129.23	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	809	CLA	CMD-C2D-C3D	2.36	129.23	124.80
12	g	822	CLA	C1-C2-C3	-2.36	122.93	126.75
12	B	838	CLA	CMD-C2D-C3D	2.36	129.22	124.80
12	G	825	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
12	A	807	CLA	CMD-C2D-C3D	2.36	129.22	124.80
12	B	825	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
12	a	821	CLA	CMD-C2D-C3D	2.36	129.22	124.80
12	a	813	CLA	CHB-C4A-NA	2.36	127.77	124.51
12	E	814	CLA	CHB-C4A-NA	2.36	127.77	124.51
12	a	803	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
12	B	822	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
12	g	821	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
12	k	1401	CLA	CMD-C2D-C3D	2.35	129.22	124.80
12	b	807	CLA	C1-C2-C3	-2.35	122.94	126.75
12	B	839	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
12	b	820	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
12	g	808	CLA	C1-C2-C3	-2.35	122.94	126.75
12	e	816	CLA	CHB-C4A-NA	2.35	127.77	124.51
12	g	833	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
12	g	825	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	G	837	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
12	b	829	CLA	CHB-C4A-NA	2.35	127.76	124.51
12	B	819	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	b	824	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	G	832	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	G	819	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	b	814	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	B	809	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	G	836	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	J	1101	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
12	g	837	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	A	811	CLA	CHB-C4A-NA	2.35	127.76	124.51
12	G	817	CLA	CMD-C2D-C3D	2.35	129.21	124.80
12	E	803	CLA	CMD-C2D-C3D	2.35	129.20	124.80
12	g	833	CLA	CHB-C4A-NA	2.35	127.76	124.51
12	e	829	CLA	CMD-C2D-C3D	2.35	129.20	124.80
12	g	823	CLA	CMD-C2D-C3D	2.35	129.20	124.80
12	A	805	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
12	B	812	CLA	CMD-C2D-C3D	2.35	129.20	124.80
12	B	833	CLA	CMD-C2D-C3D	2.35	129.20	124.80
12	B	824	CLA	CMD-C2D-C3D	2.35	129.20	124.80
12	E	816	CLA	CMD-C2D-C3D	2.35	129.20	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	813	CLA	CMD-C2D-C3D	2.34	129.20	124.80
12	G	837	CLA	CMD-C2D-C3D	2.34	129.20	124.80
12	B	820	CLA	CMD-C2D-C3D	2.34	129.20	124.80
12	E	803	CLA	O2D-CGD-O1D	-2.34	119.20	123.83
12	b	826	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
12	B	802	CLA	CMD-C2D-C3D	2.34	129.19	124.80
12	B	835	CLA	CMD-C2D-C3D	2.34	129.19	124.80
12	E	810	CLA	CHB-C4A-NA	2.34	127.75	124.51
12	G	819	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
12	b	815	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
12	e	810	CLA	CHB-C4A-NA	2.34	127.75	124.51
12	A	807	CLA	CHB-C4A-NA	2.34	127.75	124.51
12	b	817	CLA	CMD-C2D-C3D	2.34	129.19	124.80
12	g	811	CLA	CMD-C2D-C3D	2.34	129.18	124.80
12	e	842	CLA	C1-C2-C3	-2.34	122.97	126.75
12	E	823	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
12	A	828	CLA	CMD-C2D-C3D	2.34	129.18	124.80
12	G	809	CLA	CMD-C2D-C3D	2.34	129.18	124.80
12	G	821	CLA	CMD-C2D-C3D	2.34	129.18	124.80
12	A	818	CLA	CHB-C4A-NA	2.33	127.74	124.51
12	b	830	CLA	O2A-CGA-O1A	-2.33	117.60	123.56
12	b	806	CLA	O2A-CGA-O1A	-2.33	117.60	123.56
12	a	830	CLA	CMD-C2D-C3D	2.33	129.18	124.80
12	E	831	CLA	CMD-C2D-C3D	2.33	129.18	124.80
12	B	808	CLA	O2A-CGA-O1A	-2.33	117.60	123.56
12	G	829	CLA	O2A-CGA-O1A	-2.33	117.60	123.56
12	b	833	CLA	CMD-C2D-C3D	2.33	129.18	124.80
12	B	809	CLA	C1-C2-C3	-2.33	122.98	126.75
12	e	845	CLA	CMD-C2D-C3D	2.33	129.17	124.80
12	b	821	CLA	C1-C2-C3	-2.33	122.98	126.75
12	a	810	CLA	CMD-C2D-C3D	2.33	129.17	124.80
12	a	816	CLA	CHB-C4A-NA	2.33	127.73	124.51
12	E	821	CLA	CHB-C4A-NA	2.33	127.73	124.51
12	b	801	CLA	O2D-CGD-O1D	-2.33	119.23	123.83
12	B	832	CLA	O2A-CGA-O1A	-2.33	117.61	123.56
13	A	842	PQN	C26-C25-C23	-2.33	108.51	115.77
12	g	807	CLA	O2A-CGA-O1A	-2.33	117.61	123.56
12	B	823	CLA	C1-C2-C3	-2.33	122.99	126.75
12	b	807	CLA	CMD-C2D-C3D	2.33	129.16	124.80
12	E	812	CLA	CHB-C4A-NA	2.33	127.73	124.51
12	e	834	CLA	CMD-C2D-C3D	2.33	129.16	124.80
12	G	830	CLA	CMD-C2D-C3D	2.33	129.16	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	820	CLA	C1-C2-C3	-2.33	122.99	126.75
12	G	814	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
12	A	833	CLA	CMD-C2D-C3D	2.32	129.16	124.80
12	E	811	CLA	CMD-C2D-C3D	2.32	129.16	124.80
12	b	812	CLA	CMD-C2D-C3D	2.32	129.16	124.80
12	g	802	CLA	O2D-CGD-O1D	-2.32	119.24	123.83
12	e	808	CLA	CHB-C4A-NA	2.32	127.72	124.51
12	a	811	CLA	CHB-C4A-NA	2.32	127.72	124.51
12	a	820	CLA	CHB-C4A-NA	2.32	127.72	124.51
12	A	822	CLA	CMD-C2D-C3D	2.32	129.15	124.80
12	G	814	CLA	C1-C2-C3	-2.32	123.00	126.75
12	G	803	CLA	CMD-C2D-C3D	2.32	129.15	124.80
12	B	814	CLA	CMD-C2D-C3D	2.32	129.15	124.80
12	e	815	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
12	G	843	CLA	CMD-C2D-C3D	2.32	129.15	124.80
12	b	815	CLA	C1-C2-C3	-2.32	123.00	126.75
12	a	831	CLA	C1-C2-C3	-2.32	123.00	126.75
12	b	822	CLA	CMD-C2D-C3D	2.32	129.15	124.80
12	G	805	CLA	O2A-CGA-O1A	-2.32	117.64	123.56
12	E	834	CLA	O2D-CGD-CBD	2.32	115.31	111.25
12	a	815	CLA	CMD-C2D-C3D	2.32	129.15	124.80
12	B	826	CLA	CMD-C2D-C3D	2.32	129.15	124.80
12	a	809	CLA	CHB-C4A-NA	2.32	127.72	124.51
12	g	831	CLA	O2A-CGA-O1A	-2.32	117.64	123.56
12	G	823	CLA	CMD-C2D-C3D	2.32	129.15	124.80
12	B	817	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
12	B	802	CLA	O2D-CGD-O1D	-2.32	119.26	123.83
12	e	805	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
12	g	801	CLA	C1-C2-C3	-2.32	123.00	126.75
12	g	813	CLA	CMD-C2D-C3D	2.32	129.14	124.80
12	A	814	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
12	A	835	CLA	CMD-C2D-C3D	2.31	129.14	124.80
12	e	823	CLA	CMD-C2D-C3D	2.31	129.14	124.80
12	e	830	CLA	C1-C2-C3	-2.31	123.01	126.75
12	A	829	CLA	C1-C2-C3	-2.31	123.01	126.75
12	B	817	CLA	C1-C2-C3	-2.31	123.01	126.75
12	L	203	CLA	CMD-C2D-C3D	2.31	129.13	124.80
12	g	811	CLA	O2A-CGA-O1A	-2.31	117.66	123.56
12	B	840	CLA	CMD-C2D-C3D	2.31	129.13	124.80
12	E	829	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
12	B	806	CLA	CMD-C2D-C3D	2.31	129.13	124.80
12	g	816	CLA	C1-C2-C3	-2.31	123.02	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	823	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
12	E	839	CLA	CMD-C2D-C3D	2.31	129.13	124.80
12	A	821	CLA	CMD-C2D-C3D	2.31	129.13	124.80
12	e	831	CLA	O2D-CGD-CBD	2.31	115.29	111.25
12	E	817	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
12	g	805	CLA	CMD-C2D-C3D	2.31	129.13	124.80
12	a	837	CLA	CMD-C2D-C3D	2.31	129.13	124.80
12	E	807	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
12	A	826	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
12	g	839	CLA	CMD-C2D-C3D	2.31	129.12	124.80
12	a	835	CLA	CMD-C2D-C3D	2.30	129.12	124.80
12	G	805	CLA	CMD-C2D-C3D	2.30	129.12	124.80
12	G	811	CLA	CMD-C2D-C3D	2.30	129.12	124.80
12	E	810	CLA	C1-C2-C3	-2.30	123.03	126.75
12	a	816	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
12	E	808	CLA	CHB-C4A-NA	2.30	127.70	124.51
12	a	806	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
12	E	827	CLA	CAA-C2A-C1A	-2.30	104.43	111.97
12	A	802	CLA	CMD-C2D-C3D	2.30	129.12	124.80
12	e	836	CLA	CMD-C2D-C3D	2.30	129.12	124.80
12	a	823	CLA	CMD-C2D-C3D	2.30	129.12	124.80
12	e	808	CLA	C1-C2-C3	-2.30	123.03	126.75
12	g	816	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
12	G	826	CLA	CMD-C2D-C3D	2.30	129.11	124.80
12	a	824	CLA	CMD-C2D-C3D	2.30	129.11	124.80
12	G	827	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
12	G	838	CLA	CMD-C2D-C3D	2.30	129.11	124.80
12	e	806	CLA	CHB-C4A-NA	2.30	127.69	124.51
12	A	814	CLA	O2D-CGD-O1D	-2.30	119.29	123.83
12	e	827	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
12	b	839	CLA	CMD-C2D-C3D	2.30	129.11	124.80
12	E	805	CLA	CMD-C2D-C3D	2.30	129.11	124.80
12	E	832	CLA	C1-C2-C3	-2.30	123.03	126.75
12	S	1502	CLA	CHB-C4A-NA	2.30	127.69	124.51
12	a	802	CLA	C1-C2-C3	-2.30	123.04	126.75
12	A	824	CLA	CAA-C2A-C1A	-2.30	104.45	111.97
12	e	815	CLA	O2D-CGD-O1D	-2.30	119.30	123.83
12	G	836	CLA	CHB-C4A-NA	2.30	127.69	124.51
12	A	804	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
12	e	814	CLA	CMD-C2D-C3D	2.29	129.10	124.80
12	E	824	CLA	CMD-C2D-C3D	2.29	129.10	124.80
12	b	806	CLA	CMD-C2D-C3D	2.29	129.10	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	831	CLA	CMD-C2D-C3D	2.29	129.10	124.80
12	B	808	CLA	C1-C2-C3	-2.29	123.04	126.75
12	E	807	CLA	O2D-CGD-O1D	-2.29	119.30	123.83
12	a	828	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
12	G	805	CLA	C1-C2-C3	-2.29	123.04	126.75
12	E	837	CLA	CMD-C2D-C3D	2.29	129.10	124.80
12	e	822	CLA	CMD-C2D-C3D	2.29	129.10	124.80
12	B	838	CLA	CHB-C4A-NA	2.29	127.68	124.51
12	A	807	CLA	C1-C2-C3	-2.29	123.04	126.75
12	B	805	CLA	C1-C2-C3	-2.29	123.04	126.75
12	e	803	CLA	CMD-C2D-C3D	2.29	129.10	124.80
12	l	203	CLA	CMD-C2D-C3D	2.29	129.10	124.80
12	E	825	CLA	CMD-C2D-C3D	2.29	129.10	124.80
12	a	832	CLA	O2D-CGD-CBD	2.29	115.26	111.25
12	g	831	CLA	CMD-C2D-C3D	2.29	129.09	124.80
12	E	802	CLA	C1-C2-C3	-2.29	123.05	126.75
12	b	810	CLA	O2A-CGA-O1A	-2.29	117.71	123.56
12	a	809	CLA	C1-C2-C3	-2.29	123.05	126.75
12	s	204	CLA	CHB-C4A-NA	2.29	127.68	124.51
12	a	807	CLA	CHB-C4A-NA	2.29	127.68	124.51
12	l	204	CLA	CHB-C4A-NA	2.29	127.67	124.51
13	a	844	PQN	C26-C25-C23	-2.29	108.63	115.77
12	b	816	CLA	CMD-C2D-C3D	2.29	129.09	124.80
12	B	832	CLA	CMD-C2D-C3D	2.29	129.09	124.80
12	a	804	CLA	CMD-C2D-C3D	2.29	129.09	124.80
12	G	807	CLA	C1-C2-C3	-2.28	123.06	126.75
12	A	805	CLA	CHB-C4A-NA	2.28	127.67	124.51
12	g	807	CLA	C1-C2-C3	-2.28	123.06	126.75
12	e	836	CLA	C1-C2-C3	-2.28	123.06	126.75
12	A	809	CLA	CHB-C4A-NA	2.28	127.67	124.51
12	B	812	CLA	O2A-CGA-O1A	-2.28	117.73	123.56
12	B	834	CLA	CMD-C2D-C3D	2.28	129.08	124.80
12	L	204	CLA	CHB-C4A-NA	2.28	127.67	124.51
12	b	804	CLA	CMD-C2D-C3D	2.28	129.08	124.80
13	E	846	PQN	C26-C25-C23	-2.28	108.66	115.77
12	a	806	CLA	O2D-CGD-O1D	-2.28	119.33	123.83
12	g	837	CLA	CHB-C4A-NA	2.28	127.66	124.51
12	A	830	CLA	O2D-CGD-CBD	2.28	115.24	111.25
12	a	826	CLA	CAA-C2A-C1A	-2.28	104.51	111.97
12	a	816	CLA	O2D-CGD-O1D	-2.28	119.33	123.83
12	A	808	CLA	CHB-C4A-NA	2.28	127.66	124.51
12	B	810	CLA	C1-C2-C3	-2.28	123.07	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	1301	CLA	CMD-C2D-C3D	2.28	129.07	124.80
12	e	809	CLA	CMD-C2D-C3D	2.28	129.07	124.80
12	E	817	CLA	O2D-CGD-O1D	-2.27	119.34	123.83
12	e	825	CLA	CAA-C2A-C1A	-2.27	104.52	111.97
12	f	1301	CLA	CMD-C2D-C3D	2.27	129.06	124.80
12	E	835	CLA	CMD-C2D-C3D	2.27	129.06	124.80
12	e	805	CLA	O2D-CGD-O1D	-2.27	119.34	123.83
12	B	801	CLA	C1-C2-C3	-2.27	123.07	126.75
12	b	803	CLA	C1-C2-C3	-2.27	123.08	126.75
12	g	829	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
12	A	808	CLA	CMD-C2D-C3D	2.27	129.06	124.80
12	b	804	CLA	CHB-C4A-NA	2.27	127.65	124.51
12	b	837	CLA	CHB-C4A-NA	2.27	127.65	124.51
12	e	820	CLA	CHB-C4A-NA	2.27	127.65	124.51
12	A	835	CLA	C1-C2-C3	-2.27	123.08	126.75
12	b	830	CLA	CMD-C2D-C3D	2.27	129.06	124.80
12	B	808	CLA	CMD-C2D-C3D	2.27	129.06	124.80
12	a	833	CLA	CMD-C2D-C3D	2.27	129.06	124.80
12	b	828	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
12	b	832	CLA	CMD-C2D-C3D	2.27	129.05	124.80
12	e	818	CLA	CHB-C4A-NA	2.27	127.65	124.51
12	B	830	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
12	b	806	CLA	C1-C2-C3	-2.27	123.09	126.75
12	G	809	CLA	O2A-CGA-O1A	-2.27	117.77	123.56
12	g	807	CLA	CMD-C2D-C3D	2.26	129.05	124.80
12	b	808	CLA	C1-C2-C3	-2.26	123.09	126.75
12	A	809	CLA	CMD-C2D-C3D	2.26	129.05	124.80
12	E	820	CLA	CHB-C4A-NA	2.26	127.64	124.51
12	B	835	CLA	CHB-C4A-NA	2.26	127.64	124.51
12	g	828	CLA	CMD-C2D-C3D	2.26	129.04	124.80
12	e	805	CLA	O2A-CGA-O1A	-2.26	117.78	123.56
12	A	838	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
12	s	203	CLA	CMD-C2D-C3D	2.26	129.04	124.80
12	G	829	CLA	CMD-C2D-C3D	2.26	129.04	124.80
12	e	809	CLA	CHB-C4A-NA	2.26	127.64	124.51
12	B	829	CLA	CMD-C2D-C3D	2.26	129.04	124.80
12	B	818	CLA	CMD-C2D-C3D	2.26	129.04	124.80
12	a	836	CLA	CMD-C2D-C3D	2.26	129.04	124.80
12	e	839	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
12	g	809	CLA	C1-C2-C3	-2.26	123.10	126.75
12	b	827	CLA	CMD-C2D-C3D	2.26	129.03	124.80
12	G	802	CLA	C1-C2-C3	-2.26	123.10	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	832	CLA	CMD-C2D-C3D	2.26	129.03	124.80
12	a	811	CLA	CMD-C2D-C3D	2.26	129.03	124.80
12	E	818	CLA	C1-C2-C3	-2.26	123.10	126.75
12	A	804	CLA	O2D-CGD-O1D	-2.26	119.38	123.83
12	E	820	CLA	C1-C2-C3	-2.26	123.10	126.75
12	a	821	CLA	CHB-C4A-NA	2.25	127.63	124.51
12	E	812	CLA	CMD-C2D-C3D	2.25	129.03	124.80
12	F	1301	CLA	CMD-C2D-C3D	2.25	129.03	124.80
12	B	806	CLA	CHB-C4A-NA	2.25	127.63	124.51
12	a	810	CLA	CHB-C4A-NA	2.25	127.63	124.51
12	e	844	CLA	C1-C2-C3	-2.25	123.11	126.75
12	g	803	CLA	CMD-C2D-C3D	2.25	129.02	124.80
12	g	805	CLA	CHB-C4A-NA	2.25	127.62	124.51
12	B	840	CLA	C1-C2-C3	-2.25	123.11	126.75
12	a	837	CLA	C1-C2-C3	-2.25	123.11	126.75
12	g	833	CLA	CMD-C2D-C3D	2.25	129.02	124.80
12	e	810	CLA	CMD-C2D-C3D	2.25	129.01	124.80
12	g	817	CLA	CMD-C2D-C3D	2.25	129.01	124.80
12	E	807	CLA	O2A-CGA-O1A	-2.25	117.82	123.56
12	E	811	CLA	CHB-C4A-NA	2.25	127.62	124.51
12	A	841	CLA	C1-C2-C3	-2.25	123.12	126.75
12	A	834	CLA	CMD-C2D-C3D	2.24	129.01	124.80
12	G	815	CLA	CMD-C2D-C3D	2.24	129.01	124.80
12	E	838	CLA	CMD-C2D-C3D	2.24	129.01	124.80
12	o	1301	CLA	CMD-C2D-C3D	2.24	129.01	124.80
12	A	817	CLA	CHB-C4A-NA	2.24	127.61	124.51
12	a	840	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
12	e	835	CLA	CMD-C2D-C3D	2.24	129.00	124.80
12	a	806	CLA	O2A-CGA-O1A	-2.24	117.83	123.56
12	a	819	CLA	CHB-C4A-NA	2.24	127.61	124.51
12	A	819	CLA	CHB-C4A-NA	2.24	127.61	124.51
12	G	832	CLA	CHB-C4A-NA	2.24	127.61	124.51
12	E	842	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
12	g	839	CLA	C1-C2-C3	-2.24	123.13	126.75
12	A	831	CLA	CMD-C2D-C3D	2.24	129.00	124.80
12	A	806	CLA	CMD-C2D-C3D	2.24	129.00	124.80
12	A	804	CLA	O2A-CGA-O1A	-2.24	117.84	123.56
12	E	834	CLA	CHB-C4A-NA	2.24	127.61	124.51
12	A	834	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
12	a	817	CLA	C1-C2-C3	-2.24	123.14	126.75
12	B	826	CLA	C1-C2-C3	-2.24	123.14	126.75
12	e	831	CLA	CHB-C4A-NA	2.24	127.60	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	839	CLA	C1-C2-C3	-2.23	123.14	126.75
12	a	808	CLA	CMD-C2D-C3D	2.23	128.99	124.80
12	e	816	CLA	C1-C2-C3	-2.23	123.14	126.75
12	E	809	CLA	CMD-C2D-C3D	2.23	128.99	124.80
12	b	802	CLA	CMD-C2D-C3D	2.23	128.98	124.80
12	e	807	CLA	CMD-C2D-C3D	2.23	128.98	124.80
12	a	831	CLA	CMD-C2D-C3D	2.23	128.98	124.80
12	a	803	CLA	CMD-C2D-C3D	2.23	128.98	124.80
12	G	838	CLA	C1-C2-C3	-2.23	123.15	126.75
12	G	801	CLA	CMD-C2D-C3D	2.23	128.97	124.80
12	E	804	CLA	CMD-C2D-C3D	2.22	128.97	124.80
12	E	822	CLA	CHB-C4A-NA	2.22	127.59	124.51
12	a	832	CLA	CHB-C4A-NA	2.22	127.59	124.51
12	A	817	CLA	C1-C2-C3	-2.22	123.16	126.75
12	b	839	CLA	C1-C2-C3	-2.22	123.16	126.75
12	E	832	CLA	CMD-C2D-C3D	2.22	128.97	124.80
12	b	812	CLA	CHB-C4A-NA	2.22	127.58	124.51
12	A	830	CLA	CHB-C4A-NA	2.22	127.58	124.51
12	J	1101	CLA	CMD-C2D-C3D	2.22	128.97	124.80
12	e	818	CLA	C1-C2-C3	-2.22	123.16	126.75
12	b	842	CLA	C1-C2-C3	-2.22	123.16	126.75
12	E	838	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
12	E	844	CLA	OBD-CAD-C3D	2.22	129.43	127.11
12	a	819	CLA	C1-C2-C3	-2.22	123.16	126.75
12	A	829	CLA	CMD-C2D-C3D	2.22	128.96	124.80
12	b	833	CLA	CHB-C4A-NA	2.22	127.58	124.51
12	G	803	CLA	CHB-C4A-NA	2.22	127.58	124.51
12	a	842	CLA	OBD-CAD-C3D	2.22	129.43	127.11
12	b	835	CLA	CMD-C2D-C3D	2.22	128.96	124.80
12	b	824	CLA	C1-C2-C3	-2.21	123.17	126.75
12	e	830	CLA	CMD-C2D-C3D	2.21	128.95	124.80
12	e	845	CLA	CHB-C4A-NA	2.21	127.57	124.51
12	G	841	CLA	C1-C2-C3	-2.21	123.18	126.75
12	g	825	CLA	C1-C2-C3	-2.21	123.18	126.75
12	a	836	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
12	a	829	CLA	CMD-C2D-C3D	2.21	128.94	124.80
12	g	835	CLA	CMD-C2D-C3D	2.21	128.94	124.80
12	e	835	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
12	e	802	CLA	CMD-C2D-C3D	2.20	128.93	124.80
12	A	815	CLA	C1-C2-C3	-2.20	123.19	126.75
13	e	843	PQN	C26-C25-C23	-2.20	108.90	115.77
12	G	841	CLA	CHB-C4A-NA	2.20	127.56	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	824	CLA	CMD-C2D-C3D	2.20	128.93	124.80
12	B	803	CLA	CMD-C2D-C3D	2.20	128.93	124.80
12	g	813	CLA	CHB-C4A-NA	2.20	127.55	124.51
12	a	819	CLA	O2A-CGA-O1A	-2.20	117.94	123.56
12	A	811	CLA	C1-C2-C3	-2.20	123.19	126.75
12	a	825	CLA	CMD-C2D-C3D	2.20	128.92	124.80
12	g	842	CLA	C1-C2-C3	-2.20	123.20	126.75
12	G	834	CLA	CMD-C2D-C3D	2.20	128.92	124.80
12	A	827	CLA	CMD-C2D-C3D	2.20	128.92	124.80
12	a	812	CLA	C1-C2-C3	-2.19	123.20	126.75
12	e	834	CLA	CHB-C4A-NA	2.19	127.55	124.51
12	A	817	CLA	O2A-CGA-O1A	-2.19	117.95	123.56
12	a	836	CLA	O2A-CGA-O1A	-2.19	117.96	123.56
12	G	811	CLA	CHB-C4A-NA	2.19	127.54	124.51
12	A	810	CLA	C1-C2-C3	-2.19	123.21	126.75
12	e	812	CLA	C1-C2-C3	-2.19	123.21	126.75
12	e	841	CLA	OBD-CAD-C3D	2.19	129.40	127.11
12	B	843	CLA	C1-C2-C3	-2.19	123.21	126.75
12	E	813	CLA	C1-C2-C3	-2.19	123.21	126.75
12	A	833	CLA	CHB-C4A-NA	2.19	127.54	124.51
12	a	813	CLA	C1-C2-C3	-2.19	123.21	126.75
12	A	823	CLA	CMD-C2D-C3D	2.19	128.90	124.80
12	B	814	CLA	CHB-C4A-NA	2.19	127.54	124.51
12	e	818	CLA	O2A-CGA-O1A	-2.19	117.97	123.56
12	B	801	CLA	O2A-CGA-O1A	-2.19	117.97	123.56
12	e	811	CLA	C1-C2-C3	-2.19	123.22	126.75
12	E	802	CLA	O2A-CGA-O1A	-2.19	117.98	123.56
12	a	802	CLA	O2A-CGA-O1A	-2.18	117.98	123.56
12	b	826	CLA	CMD-C2D-C3D	2.18	128.89	124.80
13	E	846	PQN	C2M-C2-C1	2.18	119.95	116.29
12	J	1102	CLA	CMD-C2D-C3D	2.18	128.89	124.80
12	E	833	CLA	O2A-CGA-O1A	-2.18	117.99	123.56
12	G	823	CLA	C1-C2-C3	-2.18	123.23	126.75
12	e	828	CLA	CMD-C2D-C3D	2.18	128.89	124.80
12	e	828	CLA	O2A-CGA-O1A	-2.18	118.00	123.56
12	a	835	CLA	CHB-C4A-NA	2.18	127.52	124.51
12	A	840	CLA	OBD-CAD-C3D	2.18	129.38	127.11
12	E	837	CLA	CHB-C4A-NA	2.18	127.52	124.51
12	E	826	CLA	CMD-C2D-C3D	2.18	128.88	124.80
12	L	201	CLA	O2A-CGA-O1A	-2.18	118.00	123.56
12	E	836	CLA	CMD-C2D-C3D	2.18	128.88	124.80
12	E	830	CLA	O2A-CGA-O1A	-2.17	118.00	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	827	CLA	O2A-CGA-O1A	-2.17	118.00	123.56
12	b	828	CLA	O2A-CGA-O1A	-2.17	118.01	123.56
12	a	829	CLA	O2A-CGA-O1A	-2.17	118.01	123.56
12	E	830	CLA	CMD-C2D-C3D	2.17	128.87	124.80
12	g	829	CLA	O2A-CGA-O1A	-2.17	118.01	123.56
12	e	824	CLA	C1-C2-C3	-2.17	123.24	126.75
12	g	801	CLA	O2A-CGA-O1A	-2.17	118.02	123.56
12	g	827	CLA	CMD-C2D-C3D	2.17	128.87	124.80
12	e	833	CLA	CMD-C2D-C3D	2.17	128.87	124.80
12	b	816	CLA	O2A-CGA-O1A	-2.17	118.02	123.56
12	B	830	CLA	O2A-CGA-O1A	-2.17	118.02	123.56
12	A	834	CLA	O2A-CGA-O1A	-2.17	118.02	123.56
13	E	846	PQN	C21-C20-C18	-2.17	109.00	115.77
12	E	820	CLA	O2A-CGA-O1A	-2.17	118.02	123.56
12	a	801	CLA	O2A-CGA-O1A	-2.17	118.02	123.56
12	A	832	CLA	CMD-C2D-C3D	2.17	128.86	124.80
12	a	834	CLA	CMD-C2D-C3D	2.17	128.86	124.80
12	l	201	CLA	O2A-CGA-O1A	-2.16	118.03	123.56
12	e	844	CLA	CHB-C4A-NA	2.16	127.50	124.51
12	E	838	CLA	O2A-CGA-O1A	-2.16	118.03	123.56
12	G	815	CLA	O2A-CGA-O1A	-2.16	118.04	123.56
12	s	201	CLA	O2A-CGA-O1A	-2.16	118.04	123.56
13	a	844	PQN	C2M-C2-C1	2.16	119.91	116.29
12	E	801	CLA	O2A-CGA-O1A	-2.16	118.05	123.56
12	e	838	CLA	O2A-CGA-O1A	-2.16	118.05	123.56
12	A	801	CLA	C2A-C1A-CHA	2.15	127.62	123.86
12	a	813	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
12	B	805	CLA	CHB-C4A-NA	2.15	127.49	124.51
12	G	825	CLA	CMD-C2D-C3D	2.15	128.84	124.80
12	e	801	CLA	O2A-CGA-O1A	-2.15	118.06	123.56
12	b	842	CLA	CHB-C4A-NA	2.15	127.49	124.51
12	E	814	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
12	G	827	CLA	O2A-CGA-O1A	-2.15	118.07	123.56
12	a	822	CLA	O2A-CGA-O1A	-2.15	118.07	123.56
12	g	817	CLA	O2A-CGA-O1A	-2.15	118.07	123.56
12	E	831	CLA	C1-C2-C3	-2.15	123.28	126.75
12	E	823	CLA	O2A-CGA-O1A	-2.15	118.07	123.56
12	a	822	CLA	CMD-C2D-C3D	2.15	128.83	124.80
12	e	835	CLA	O2A-CGA-O1A	-2.15	118.08	123.56
12	B	820	CLA	O2A-CGA-O1A	-2.15	118.08	123.56
12	B	818	CLA	O2A-CGA-O1A	-2.15	118.08	123.56
12	a	830	CLA	C1-C2-C3	-2.15	123.28	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	801	CLA	O2A-CGA-O1A	-2.15	118.08	123.56
12	G	804	CLA	O2A-CGA-O1A	-2.15	118.08	123.56
12	G	822	CLA	O2D-CGD-CBD	2.14	115.01	111.25
12	g	819	CLA	O2A-CGA-O1A	-2.14	118.09	123.56
12	E	814	CLA	C1-C2-C3	-2.14	123.29	126.75
12	e	829	CLA	C1-C2-C3	-2.14	123.29	126.75
12	b	803	CLA	CHB-C4A-NA	2.14	127.47	124.51
12	a	801	CLA	C2A-C1A-CHA	2.14	127.60	123.86
12	e	801	CLA	C2A-C1A-CHA	2.14	127.60	123.86
12	E	826	CLA	C1-C2-C3	-2.14	123.29	126.75
12	e	812	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
12	a	808	CLA	O2A-CGA-O1A	-2.14	118.09	123.56
12	b	805	CLA	O2A-CGA-O1A	-2.14	118.09	123.56
12	b	818	CLA	O2A-CGA-O1A	-2.14	118.10	123.56
13	a	844	PQN	C11-C3-C4	2.14	120.82	118.50
12	e	821	CLA	CMD-C2D-C3D	2.14	128.81	124.80
12	G	817	CLA	O2A-CGA-O1A	-2.14	118.10	123.56
12	G	802	CLA	CHB-C4A-NA	2.14	127.47	124.51
12	a	839	CLA	C1D-CHD-C4C	2.14	125.41	122.48
12	B	828	CLA	CMD-C2D-C3D	2.14	128.81	124.80
12	B	807	CLA	O2A-CGA-O1A	-2.14	118.10	123.56
12	g	802	CLA	CAA-CBA-CGA	-2.14	106.97	113.26
12	g	806	CLA	C1D-CHD-C4C	2.13	125.40	122.48
12	a	839	CLA	O2A-CGA-O1A	-2.13	118.11	123.56
12	E	823	CLA	CMD-C2D-C3D	2.13	128.80	124.80
12	g	824	CLA	O2D-CGD-CBD	2.13	114.99	111.25
12	e	838	CLA	C1D-CHD-C4C	2.13	125.40	122.48
12	A	828	CLA	C1-C2-C3	-2.13	123.30	126.75
12	B	825	CLA	O2D-CGD-CBD	2.13	114.99	111.25
12	b	823	CLA	O2D-CGD-CBD	2.13	114.99	111.25
12	A	837	CLA	O2A-CGA-O1A	-2.13	118.12	123.56
12	e	821	CLA	O2A-CGA-O1A	-2.13	118.12	123.56
12	A	811	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
12	A	806	CLA	O2A-CGA-O1A	-2.13	118.13	123.56
12	B	802	CLA	CAA-CBA-CGA	-2.13	106.99	113.26
12	A	820	CLA	CMD-C2D-C3D	2.13	128.79	124.80
12	e	838	CLA	CHB-C4A-NA	2.13	127.45	124.51
12	E	841	CLA	CHB-C4A-NA	2.13	127.45	124.51
12	A	823	CLA	CHB-C4A-NA	2.13	127.45	124.51
12	A	837	CLA	C1D-CHD-C4C	2.13	125.39	122.48
12	a	825	CLA	C1-C2-C3	-2.13	123.31	126.75
12	A	809	CLA	O2A-CGA-O1A	-2.13	118.13	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	820	CLA	O2A-CGA-O1A	-2.12	118.13	123.56
12	E	841	CLA	O2A-CGA-O1A	-2.12	118.14	123.56
12	b	836	CLA	CHB-C4A-NA	2.12	127.45	124.51
12	B	837	CLA	O2D-CGD-CBD	2.12	114.97	111.25
13	e	843	PQN	C16-C17-C18	-2.12	109.15	115.77
12	A	823	CLA	C1-C2-C3	-2.12	123.32	126.75
12	E	806	CLA	O2A-CGA-O1A	-2.12	118.14	123.56
12	E	801	CLA	C2A-C1A-CHA	2.12	127.57	123.86
12	G	835	CLA	O2D-CGD-CBD	2.12	114.97	111.25
12	e	824	CLA	CHB-C4A-NA	2.12	127.44	124.51
12	b	801	CLA	CAA-CBA-CGA	-2.12	107.01	113.26
12	G	818	CLA	O2A-CGA-O1A	-2.12	118.14	123.56
12	e	807	CLA	O2A-CGA-O1A	-2.12	118.15	123.56
12	b	806	CLA	CAA-C2A-C1A	-2.12	105.03	111.97
12	g	836	CLA	O2D-CGD-CBD	2.12	114.96	111.25
12	g	806	CLA	O2A-CGA-O1A	-2.12	118.15	123.56
12	A	837	CLA	CHB-C4A-NA	2.12	127.44	124.51
12	B	839	CLA	O2A-CGA-O1A	-2.12	118.15	123.56
12	g	842	CLA	CHB-C4A-NA	2.12	127.44	124.51
12	g	834	CLA	C1-C2-C3	-2.11	123.33	126.75
12	a	825	CLA	CHB-C4A-NA	2.11	127.44	124.51
12	A	803	CLA	O2A-CGA-O1A	-2.11	118.16	123.56
12	E	826	CLA	CHB-C4A-NA	2.11	127.43	124.51
12	B	808	CLA	CAA-C2A-C1A	-2.11	105.05	111.97
12	B	836	CLA	C1-C2-C3	-2.11	123.33	126.75
12	g	841	CLA	O2D-CGD-CBD	2.11	114.95	111.25
12	G	833	CLA	C1-C2-C3	-2.11	123.34	126.75
12	b	841	CLA	O2D-CGD-CBD	2.11	114.94	111.25
12	a	839	CLA	CHB-C4A-NA	2.11	127.43	124.51
12	b	804	CLA	O2A-CGA-O1A	-2.11	118.17	123.56
12	B	806	CLA	O2A-CGA-O1A	-2.11	118.17	123.56
12	B	807	CLA	C1D-CHD-C4C	2.11	125.37	122.48
12	E	803	CLA	CAA-CBA-CGA	-2.11	107.05	113.26
12	G	835	CLA	CHB-C4A-NA	2.11	127.42	124.51
12	G	803	CLA	O2A-CGA-O1A	-2.11	118.18	123.56
12	B	821	CLA	O2A-CGA-O1A	-2.11	118.18	123.56
12	G	804	CLA	C1D-CHD-C4C	2.11	125.36	122.48
12	B	837	CLA	CHB-C4A-NA	2.11	127.42	124.51
12	g	807	CLA	CAA-C2A-C1A	-2.11	105.08	111.97
12	e	804	CLA	O2A-CGA-O1A	-2.11	118.18	123.56
12	E	809	CLA	O2A-CGA-O1A	-2.10	118.18	123.56
12	a	805	CLA	O2A-CGA-O1A	-2.10	118.19	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	834	CLA	C1-C2-C3	-2.10	123.35	126.75
12	b	836	CLA	O2D-CGD-CBD	2.10	114.94	111.25
12	G	805	CLA	CAA-C2A-C1A	-2.10	105.09	111.97
12	b	819	CLA	O2A-CGA-O1A	-2.10	118.19	123.56
12	G	837	CLA	O2A-CGA-O1A	-2.10	118.19	123.56
12	b	838	CLA	O2A-CGA-O1A	-2.10	118.20	123.56
12	B	833	CLA	O2A-CGA-O1A	-2.10	118.20	123.56
12	e	810	CLA	O2A-CGA-O1A	-2.10	118.20	123.56
12	a	822	CLA	C3A-C2A-C1A	2.10	104.48	101.34
12	g	820	CLA	O2A-CGA-O1A	-2.10	118.20	123.56
12	B	843	CLA	CHB-C4A-NA	2.10	127.41	124.51
12	a	824	CLA	C1-C2-C3	-2.10	123.36	126.75
12	E	841	CLA	C1D-CHD-C4C	2.10	125.35	122.48
12	G	834	CLA	CHB-C4A-NA	2.09	127.41	124.51
12	s	203	CLA	O2A-CGA-O1A	-2.09	118.21	123.56
12	e	821	CLA	C3A-C2A-C1A	2.09	104.47	101.34
12	g	832	CLA	O2A-CGA-O1A	-2.09	118.22	123.56
13	E	846	PQN	C2M-C2-C3	-2.09	120.04	124.21
12	g	835	CLA	CHB-C4A-NA	2.09	127.40	124.51
13	a	844	PQN	C21-C20-C18	-2.09	109.25	115.77
12	A	821	CLA	O2A-CGA-O1A	-2.09	118.22	123.56
12	g	805	CLA	O2A-CGA-O1A	-2.09	118.22	123.56
12	E	812	CLA	O2A-CGA-O1A	-2.09	118.22	123.56
13	A	842	PQN	C21-C20-C18	-2.09	109.26	115.77
12	g	838	CLA	O2A-CGA-O1A	-2.09	118.23	123.56
12	a	811	CLA	O2A-CGA-O1A	-2.08	118.24	123.56
12	A	822	CLA	C1-C2-C3	-2.08	123.38	126.75
12	a	805	CLA	OBD-CAD-CBD	-2.08	122.85	125.91
12	G	830	CLA	O2A-CGA-O1A	-2.08	118.24	123.56
12	g	827	CLA	C1D-CHD-C4C	2.08	125.33	122.48
12	G	843	CLA	O2A-CGA-O1A	-2.08	118.24	123.56
12	a	824	CLA	O2A-CGA-O1A	-2.08	118.25	123.56
12	g	822	CLA	O2A-CGA-O1A	-2.08	118.25	123.56
12	L	203	CLA	O2A-CGA-O1A	-2.08	118.25	123.56
12	E	825	CLA	C1-C2-C3	-2.08	123.39	126.75
12	B	842	CLA	O2D-CGD-CBD	2.08	114.89	111.25
12	E	823	CLA	C3A-C2A-C1A	2.08	104.45	101.34
12	g	836	CLA	CHB-C4A-NA	2.08	127.39	124.51
12	e	823	CLA	C1-C2-C3	-2.08	123.39	126.75
12	b	821	CLA	O2A-CGA-O1A	-2.07	118.26	123.56
12	a	823	CLA	O2A-CGA-O1A	-2.07	118.26	123.56
12	E	824	CLA	O2A-CGA-O1A	-2.07	118.26	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	806	CLA	OBD-CAD-CBD	-2.07	122.86	125.91
12	E	803	CLA	CHB-C4A-NA	2.07	127.38	124.51
12	l	203	CLA	O2A-CGA-O1A	-2.07	118.26	123.56
12	E	830	CLA	C1-C2-C3	-2.07	123.40	126.75
12	J	1102	CLA	CHB-C4A-NA	2.07	127.38	124.51
12	G	820	CLA	O2A-CGA-O1A	-2.07	118.27	123.56
12	G	802	CLA	OBD-CAD-CBD	-2.07	122.87	125.91
12	A	803	CLA	OBD-CAD-CBD	-2.07	122.87	125.91
12	G	811	CLA	O2A-CGA-O1A	-2.07	118.27	123.56
12	b	805	CLA	C1D-CHD-C4C	2.07	125.31	122.48
12	a	837	CLA	O2A-CGA-O1A	-2.07	118.27	123.56
12	G	801	CLA	O2A-CGA-O1A	-2.07	118.27	123.56
12	e	804	CLA	C1D-CHD-C4C	2.07	125.31	122.48
12	G	840	CLA	O2D-CGD-CBD	2.07	114.87	111.25
12	E	840	CLA	O2A-CGA-O1A	-2.07	118.28	123.56
13	a	844	PQN	C2M-C2-C3	-2.07	120.09	124.21
12	g	813	CLA	O2A-CGA-O1A	-2.07	118.28	123.56
12	b	831	CLA	O2A-CGA-O1A	-2.07	118.28	123.56
12	B	835	CLA	O2A-CGA-O1A	-2.06	118.28	123.56
12	e	823	CLA	O2A-CGA-O1A	-2.06	118.28	123.56
12	E	836	CLA	O2A-CGA-O1A	-2.06	118.29	123.56
12	A	820	CLA	C3A-C2A-C1A	2.06	104.43	101.34
12	a	825	CLA	O2A-CGA-O1A	-2.06	118.29	123.56
12	B	814	CLA	O2A-CGA-O1A	-2.06	118.29	123.56
12	A	822	CLA	O2A-CGA-O1A	-2.06	118.29	123.56
12	b	803	CLA	OBD-CAD-CBD	-2.06	122.88	125.91
12	b	809	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
12	e	812	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
12	A	803	CLA	C1D-CHD-C4C	2.06	125.30	122.48
12	A	827	CLA	C1-C2-C3	-2.06	123.42	126.75
12	b	801	CLA	CHB-C4A-NA	2.06	127.36	124.51
12	b	835	CLA	CHB-C4A-NA	2.06	127.36	124.51
12	S	1502	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
12	E	813	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
12	e	837	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
12	A	810	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
12	b	835	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
12	e	822	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
12	a	829	CLA	C1-C2-C3	-2.06	123.42	126.75
12	A	832	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
12	E	806	CLA	C1D-CHD-C4C	2.06	125.30	122.48
12	g	803	CLA	O2A-CGA-O1A	-2.06	118.31	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	811	CLA	O2A-CGA-O1A	-2.06	118.31	123.56
12	a	805	CLA	C1D-CHD-C4C	2.05	125.29	122.48
12	b	839	CLA	CAA-C2A-C1A	-2.05	105.24	111.97
12	E	825	CLA	O2A-CGA-O1A	-2.05	118.31	123.56
12	a	838	CLA	O2A-CGA-O1A	-2.05	118.31	123.56
12	E	826	CLA	O2A-CGA-O1A	-2.05	118.31	123.56
12	a	841	CLA	C1D-CHD-C4C	2.05	125.29	122.48
12	B	823	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
12	G	825	CLA	C1D-CHD-C4C	2.05	125.29	122.48
12	A	836	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
12	A	811	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
12	e	836	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
12	e	833	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
12	a	812	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
12	B	802	CLA	CHB-C4A-NA	2.05	127.35	124.51
12	B	803	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
12	A	823	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
12	g	835	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
12	B	805	CLA	OBD-CAD-CBD	-2.05	122.90	125.91
12	G	834	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
12	g	839	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
12	e	804	CLA	OBD-CAD-CBD	-2.05	122.91	125.91
12	A	838	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
12	b	833	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
12	E	814	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
12	b	826	CLA	C1D-CHD-C4C	2.05	125.28	122.48
12	J	1102	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
12	g	810	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
12	a	834	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
12	s	204	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
12	a	813	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
12	e	824	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
12	e	828	CLA	C1-C2-C3	-2.04	123.45	126.75
12	b	802	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
12	G	832	CLA	O2A-CGA-O1A	-2.04	118.35	123.56
12	A	839	CLA	C1D-CHD-C4C	2.04	125.27	122.48
12	a	817	CLA	O2A-CGA-O1A	-2.04	118.35	123.56
12	G	822	CLA	C1D-CHD-C4C	2.04	125.27	122.48
12	A	835	CLA	O2A-CGA-O1A	-2.04	118.35	123.56
12	e	816	CLA	O2A-CGA-O1A	-2.04	118.35	123.56
12	e	844	CLA	OBD-CAD-CBD	-2.04	122.92	125.91
12	E	843	CLA	C1D-CHD-C4C	2.04	125.27	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	845	CLA	O2A-CGA-O1A	-2.04	118.35	123.56
12	E	818	CLA	O2A-CGA-O1A	-2.04	118.36	123.56
12	b	812	CLA	O2A-CGA-O1A	-2.04	118.36	123.56
12	B	825	CLA	C1D-CHD-C4C	2.04	125.27	122.48
12	E	829	CLA	C1D-CHD-C4C	2.04	125.27	122.48
12	E	839	CLA	O2A-CGA-O1A	-2.04	118.36	123.56
12	e	839	CLA	O2A-CGA-O1A	-2.04	118.36	123.56
12	g	824	CLA	C1D-CHD-C4C	2.04	125.27	122.48
12	l	204	CLA	O2A-CGA-O1A	-2.03	118.36	123.56
12	a	828	CLA	C1D-CHD-C4C	2.03	125.27	122.48
12	a	840	CLA	O2A-CGA-O1A	-2.03	118.37	123.56
12	g	802	CLA	CHB-C4A-NA	2.03	127.32	124.51
12	G	838	CLA	CAA-C2A-C1A	-2.03	105.31	111.97
12	B	815	CLA	CHB-C4A-NA	2.03	127.32	124.51
12	B	840	CLA	CAA-C2A-C1A	-2.03	105.32	111.97
12	e	817	CLA	O2A-CGA-O1A	-2.03	118.37	123.56
12	A	816	CLA	O2A-CGA-O1A	-2.03	118.37	123.56
12	B	828	CLA	C1D-CHD-C4C	2.03	125.26	122.48
12	B	811	CLA	O2A-CGA-O1A	-2.03	118.37	123.56
12	g	840	CLA	O2A-CGA-O1A	-2.03	118.37	123.56
12	e	827	CLA	C1D-CHD-C4C	2.03	125.26	122.48
12	A	841	CLA	O2A-CGA-O1A	-2.03	118.37	123.56
12	A	829	CLA	O2A-CGA-O1A	-2.03	118.38	123.56
12	G	808	CLA	O2A-CGA-O1A	-2.03	118.38	123.56
12	A	826	CLA	C1D-CHD-C4C	2.03	125.26	122.48
12	a	818	CLA	O2A-CGA-O1A	-2.03	118.38	123.56
12	A	815	CLA	O2A-CGA-O1A	-2.02	118.39	123.56
12	L	204	CLA	O2A-CGA-O1A	-2.02	118.39	123.56
12	e	808	CLA	O2A-CGA-O1A	-2.02	118.39	123.56
12	e	840	CLA	C1D-CHD-C4C	2.02	125.25	122.48
12	e	842	CLA	O2A-CGA-O1A	-2.02	118.40	123.56
12	E	842	CLA	O2A-CGA-O1A	-2.02	118.40	123.56
12	E	819	CLA	O2A-CGA-O1A	-2.02	118.41	123.56
12	E	832	CLA	O2A-CGA-O1A	-2.02	118.41	123.56
12	s	202	CLA	O2A-CGA-O1A	-2.02	118.41	123.56
12	S	1501	CLA	O2A-CGA-O1A	-2.01	118.41	123.56
12	b	801	CLA	C1D-CHD-C4C	2.01	125.24	122.48
12	R	1401	CLA	O1D-CGD-CBD	2.01	128.65	124.48
12	b	840	CLA	O2A-CGA-O1A	-2.01	118.42	123.56
12	b	831	CLA	C1D-CHD-C4C	2.01	125.24	122.48
12	G	839	CLA	O2A-CGA-O1A	-2.01	118.42	123.56
13	A	842	PQN	C2M-C2-C3	-2.01	120.20	124.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	202	CLA	O2A-CGA-O1A	-2.01	118.42	123.56
12	b	819	CLA	C1-C2-C3	-2.01	123.50	126.75
12	G	812	CLA	CHB-C4A-NA	2.01	127.29	124.51
12	K	1401	CLA	O1D-CGD-CBD	2.01	128.65	124.48
12	g	841	CLA	C2A-C1A-CHA	2.01	127.37	123.86
12	g	808	CLA	O2A-CGA-O1A	-2.01	118.43	123.56
12	E	803	CLA	C1D-CHD-C4C	2.01	125.23	122.48
12	b	841	CLA	C2A-C1A-CHA	2.01	127.36	123.86
12	e	830	CLA	O2A-CGA-O1A	-2.00	118.44	123.56
12	A	809	CLA	C1D-CHD-C4C	2.00	125.22	122.48
12	E	815	CLA	CHB-C4A-NA	2.00	127.28	124.51
12	L	202	CLA	O2A-CGA-O1A	-2.00	118.44	123.56
12	k	1401	CLA	O1D-CGD-CBD	2.00	128.63	124.48
12	g	820	CLA	C1-C2-C3	-2.00	123.51	126.75
12	a	831	CLA	O2A-CGA-O1A	-2.00	118.45	123.56
12	G	818	CLA	C1-C2-C3	-2.00	123.52	126.75
12	e	813	CLA	CHB-C4A-NA	2.00	127.28	124.51

All (1078) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	E	817	CLA	NC
12	E	817	CLA	ND
12	E	817	CLA	NA
12	a	812	CLA	NC
12	a	812	CLA	ND
12	a	812	CLA	NA
13	g	843	PQN	C18
12	E	840	CLA	NC
12	E	840	CLA	ND
12	E	840	CLA	NA
12	e	815	CLA	NC
12	e	815	CLA	ND
12	e	815	CLA	NA
12	b	837	CLA	NC
12	b	837	CLA	ND
12	b	837	CLA	NA
12	A	801	CLA	NC
12	A	801	CLA	ND
12	A	801	CLA	NA
13	B	844	PQN	C18
12	A	834	CLA	NC

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Mol	Chain	Res	Type	Atom
12	A	834	CLA	ND
12	A	834	CLA	NA
12	e	803	CLA	NC
12	e	803	CLA	ND
12	e	803	CLA	NA
12	b	830	CLA	NC
12	b	830	CLA	ND
12	b	830	CLA	NA
12	B	819	CLA	NC
12	B	819	CLA	ND
12	B	819	CLA	NA
12	A	828	CLA	NC
12	A	828	CLA	ND
12	A	828	CLA	NA
12	e	802	CLA	NC
12	e	802	CLA	ND
12	e	802	CLA	NA
12	E	833	CLA	NC
12	E	833	CLA	NA
12	E	833	CLA	ND
12	b	824	CLA	NC
12	b	824	CLA	ND
12	b	824	CLA	NA
12	J	1101	CLA	NC
12	J	1101	CLA	ND
12	J	1101	CLA	NA
12	E	834	CLA	NC
12	E	834	CLA	ND
12	E	834	CLA	NA
13	G	842	PQN	C18
12	B	838	CLA	NC
12	B	838	CLA	ND
12	B	838	CLA	NA
12	e	810	CLA	NC
12	e	810	CLA	NA
12	e	810	CLA	ND
12	a	817	CLA	NC
12	a	817	CLA	ND
12	a	817	CLA	NA
12	r	1401	CLA	NC
12	r	1401	CLA	ND
12	r	1401	CLA	NA

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Mol	Chain	Res	Type	Atom
12	e	807	CLA	NC
12	e	807	CLA	ND
12	e	807	CLA	NA
12	e	840	CLA	NC
12	e	840	CLA	ND
12	e	840	CLA	NA
12	s	204	CLA	NC
12	s	204	CLA	ND
12	s	204	CLA	NA
12	E	820	CLA	NC
12	E	820	CLA	ND
12	E	820	CLA	NA
12	g	820	CLA	NC
12	g	820	CLA	ND
12	g	820	CLA	NA
12	e	808	CLA	NC
12	e	808	CLA	ND
12	e	808	CLA	NA
12	e	825	CLA	NC
12	e	825	CLA	ND
12	e	825	CLA	NA
12	G	809	CLA	NC
12	G	809	CLA	ND
12	G	809	CLA	NA
12	G	802	CLA	NC
12	G	802	CLA	ND
12	G	802	CLA	NA
12	e	838	CLA	NC
12	e	838	CLA	NA
12	B	810	CLA	NC
12	B	810	CLA	NA
12	B	810	CLA	ND
12	A	803	CLA	NC
12	A	803	CLA	ND
12	A	803	CLA	NA
12	g	833	CLA	NC
12	g	833	CLA	ND
12	g	833	CLA	NA
12	l	204	CLA	NC
12	l	204	CLA	ND
12	l	204	CLA	NA
12	B	834	CLA	NC

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Mol	Chain	Res	Type	Atom
12	B	834	CLA	ND
12	B	834	CLA	NA
12	g	825	CLA	NC
12	g	825	CLA	ND
12	g	825	CLA	NA
12	b	829	CLA	NC
12	b	829	CLA	ND
12	b	829	CLA	NA
12	b	831	CLA	NC
12	b	831	CLA	ND
12	b	831	CLA	NA
13	b	843	PQN	C18
12	G	810	CLA	NC
12	G	810	CLA	ND
12	G	810	CLA	NA
12	E	809	CLA	NC
12	E	809	CLA	ND
12	E	809	CLA	NA
12	e	816	CLA	NC
12	e	816	CLA	ND
12	e	816	CLA	NA
12	b	801	CLA	NC
12	b	801	CLA	NA
12	b	801	CLA	ND
12	a	829	CLA	NC
12	a	829	CLA	ND
12	a	829	CLA	NA
12	E	822	CLA	NC
12	E	822	CLA	ND
12	E	822	CLA	NA
12	a	827	CLA	NC
12	a	827	CLA	ND
12	a	827	CLA	NA
12	a	835	CLA	NC
12	a	835	CLA	ND
12	a	835	CLA	NA
12	b	832	CLA	NC
12	b	832	CLA	ND
12	b	832	CLA	NA
12	G	834	CLA	NC
12	G	834	CLA	ND
12	G	834	CLA	NA

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Mol	Chain	Res	Type	Atom
12	A	815	CLA	NC
12	A	815	CLA	ND
12	A	815	CLA	NA
12	g	842	CLA	NC
12	g	842	CLA	ND
12	g	842	CLA	NA
12	b	808	CLA	NC
12	b	808	CLA	NA
12	b	808	CLA	ND
12	a	814	CLA	NC
12	a	814	CLA	ND
12	a	814	CLA	NA
12	B	820	CLA	NC
12	B	820	CLA	ND
12	B	820	CLA	NA
12	a	832	CLA	NC
12	a	832	CLA	ND
12	a	832	CLA	NA
12	A	819	CLA	NC
12	A	819	CLA	ND
12	A	819	CLA	NA
12	e	827	CLA	NC
12	e	827	CLA	ND
12	e	827	CLA	NA
12	a	830	CLA	NC
12	a	830	CLA	ND
12	a	830	CLA	NA
12	g	834	CLA	NC
12	g	834	CLA	ND
12	g	834	CLA	NA
12	g	814	CLA	NC
12	g	814	CLA	ND
12	g	814	CLA	NA
12	B	811	CLA	NC
12	B	811	CLA	ND
12	B	811	CLA	NA
12	G	804	CLA	NC
12	G	804	CLA	ND
12	G	804	CLA	NA
12	g	835	CLA	NC
12	g	835	CLA	ND
12	g	835	CLA	NA

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Mol	Chain	Res	Type	Atom
12	g	827	CLA	NC
12	g	827	CLA	ND
12	g	827	CLA	NA
12	b	809	CLA	NC
12	b	809	CLA	ND
12	b	809	CLA	NA
12	A	806	CLA	NC
12	A	806	CLA	ND
12	A	806	CLA	NA
12	b	804	CLA	NC
12	b	804	CLA	ND
12	b	804	CLA	NA
12	g	808	CLA	NC
12	g	808	CLA	ND
12	g	808	CLA	NA
12	S	1502	CLA	NC
12	S	1502	CLA	ND
12	S	1502	CLA	NA
12	E	825	CLA	NC
12	E	825	CLA	ND
12	E	825	CLA	NA
12	e	817	CLA	NC
12	e	817	CLA	ND
12	e	817	CLA	NA
12	A	827	CLA	NC
12	A	827	CLA	ND
12	A	827	CLA	NA
12	b	827	CLA	NC
12	b	827	CLA	ND
12	b	827	CLA	NA
12	E	819	CLA	NC
12	E	819	CLA	ND
12	E	819	CLA	NA
12	B	843	CLA	NC
12	B	843	CLA	ND
12	B	843	CLA	NA
12	B	808	CLA	NC
12	B	808	CLA	ND
12	B	808	CLA	NA
12	B	802	CLA	NC
12	B	802	CLA	NA
12	B	802	CLA	ND

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Mol	Chain	Res	Type	Atom
12	G	838	CLA	NC
12	G	838	CLA	ND
12	G	838	CLA	NA
12	e	809	CLA	NC
12	e	809	CLA	ND
12	e	809	CLA	NA
12	s	203	CLA	NC
12	s	203	CLA	ND
12	s	203	CLA	NA
12	b	841	CLA	NC
12	b	841	CLA	ND
12	b	841	CLA	NA
12	g	819	CLA	NC
12	g	819	CLA	ND
12	g	819	CLA	NA
12	E	830	CLA	NC
12	E	830	CLA	ND
12	E	830	CLA	NA
12	G	839	CLA	NC
12	G	839	CLA	NA
12	b	818	CLA	NC
12	b	818	CLA	ND
12	b	818	CLA	NA
12	E	811	CLA	NC
12	E	811	CLA	ND
12	E	811	CLA	NA
12	B	822	CLA	NC
12	B	822	CLA	ND
12	B	822	CLA	NA
12	b	810	CLA	NC
12	b	810	CLA	ND
12	b	810	CLA	NA
12	e	836	CLA	NC
12	e	836	CLA	ND
12	e	836	CLA	NA
12	a	819	CLA	NC
12	a	819	CLA	ND
12	a	819	CLA	NA
12	E	812	CLA	NC
12	E	812	CLA	NA
12	E	812	CLA	ND
12	G	831	CLA	NC

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Mol	Chain	Res	Type	Atom
12	G	831	CLA	ND
12	G	831	CLA	NA
12	a	841	CLA	NC
12	a	841	CLA	ND
12	a	841	CLA	NA
12	G	821	CLA	NC
12	G	821	CLA	ND
12	G	821	CLA	NA
12	e	818	CLA	NC
12	e	818	CLA	ND
12	e	818	CLA	NA
12	a	807	CLA	NC
12	a	807	CLA	NA
12	g	822	CLA	NC
12	g	822	CLA	ND
12	g	822	CLA	NA
12	A	826	CLA	NC
12	A	826	CLA	ND
12	A	826	CLA	NA
12	g	813	CLA	NC
12	g	813	CLA	ND
12	g	813	CLA	NA
12	E	832	CLA	NC
12	E	832	CLA	NA
12	A	831	CLA	NC
12	A	831	CLA	ND
12	A	831	CLA	NA
12	g	807	CLA	NC
12	g	807	CLA	ND
12	g	807	CLA	NA
12	E	814	CLA	NC
12	E	814	CLA	ND
12	E	814	CLA	NA
12	G	833	CLA	NC
12	G	833	CLA	ND
12	G	833	CLA	NA
12	a	826	CLA	NC
12	a	826	CLA	ND
12	a	826	CLA	NA
12	l	202	CLA	NC
12	l	202	CLA	ND
12	l	202	CLA	NA

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Mol	Chain	Res	Type	Atom
12	G	815	CLA	NC
12	G	815	CLA	ND
12	G	815	CLA	NA
12	G	803	CLA	NC
12	G	803	CLA	ND
12	G	803	CLA	NA
12	g	809	CLA	NC
12	g	809	CLA	NA
12	g	809	CLA	ND
12	e	835	CLA	NC
12	e	835	CLA	ND
12	e	835	CLA	NA
12	a	811	CLA	NC
12	a	811	CLA	NA
12	a	811	CLA	ND
12	e	830	CLA	NC
12	e	830	CLA	NA
12	g	824	CLA	NC
12	g	824	CLA	ND
12	g	824	CLA	NA
12	a	825	CLA	NC
12	a	825	CLA	ND
12	a	825	CLA	NA
12	A	824	CLA	NC
12	A	824	CLA	ND
12	A	824	CLA	NA
12	A	829	CLA	NC
12	A	829	CLA	NA
12	B	825	CLA	NC
12	B	825	CLA	ND
12	B	825	CLA	NA
12	E	841	CLA	NC
12	E	841	CLA	NA
12	A	835	CLA	NC
12	A	835	CLA	ND
12	A	835	CLA	NA
12	b	838	CLA	NC
12	b	838	CLA	ND
12	b	838	CLA	NA
12	G	826	CLA	NC
12	G	826	CLA	ND
12	G	826	CLA	NA

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Mol	Chain	Res	Type	Atom
12	a	822	CLA	NC
12	a	822	CLA	ND
12	a	822	CLA	NA
12	G	823	CLA	NC
12	G	823	CLA	ND
12	G	823	CLA	NA
12	l	203	CLA	NC
12	l	203	CLA	ND
12	l	203	CLA	NA
12	A	839	CLA	NC
12	A	839	CLA	ND
12	A	839	CLA	NA
12	A	818	CLA	NC
12	A	818	CLA	ND
12	A	818	CLA	NA
12	e	837	CLA	NC
12	e	837	CLA	ND
12	e	837	CLA	NA
12	A	817	CLA	NC
12	A	817	CLA	ND
12	A	817	CLA	NA
12	g	805	CLA	NC
12	g	805	CLA	ND
12	g	805	CLA	NA
12	B	816	CLA	NC
12	B	816	CLA	ND
12	B	816	CLA	NA
12	B	809	CLA	NC
12	B	809	CLA	ND
12	B	809	CLA	NA
12	a	815	CLA	NC
12	a	815	CLA	ND
12	a	815	CLA	NA
12	a	838	CLA	NC
12	a	838	CLA	ND
12	a	838	CLA	NA
12	G	822	CLA	NC
12	G	822	CLA	ND
12	G	822	CLA	NA
13	a	844	PQN	C18
12	a	816	CLA	NC
12	a	816	CLA	ND

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Mol	Chain	Res	Type	Atom
12	a	816	CLA	NA
12	f	1301	CLA	NC
12	f	1301	CLA	ND
12	f	1301	CLA	NA
12	e	842	CLA	NC
12	e	842	CLA	ND
12	e	842	CLA	NA
12	A	804	CLA	NC
12	A	804	CLA	NA
12	A	804	CLA	ND
12	a	836	CLA	NC
12	a	836	CLA	ND
12	a	836	CLA	NA
12	g	816	CLA	NC
12	g	816	CLA	ND
12	g	816	CLA	NA
12	B	813	CLA	NC
12	B	813	CLA	ND
12	B	813	CLA	NA
12	B	833	CLA	NC
12	B	833	CLA	ND
12	B	833	CLA	NA
12	a	833	CLA	NC
12	a	833	CLA	ND
12	a	833	CLA	NA
12	E	838	CLA	NC
12	E	838	CLA	ND
12	E	838	CLA	NA
12	A	837	CLA	NC
12	A	837	CLA	NA
12	G	832	CLA	NC
12	G	832	CLA	ND
12	G	832	CLA	NA
12	B	812	CLA	NC
12	B	812	CLA	ND
12	B	812	CLA	NA
12	G	805	CLA	NC
12	G	805	CLA	ND
12	G	805	CLA	NA
12	s	201	CLA	NC
12	s	201	CLA	NA
12	s	201	CLA	ND

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Mol	Chain	Res	Type	Atom
12	a	808	CLA	NC
12	a	808	CLA	ND
12	a	808	CLA	NA
12	A	809	CLA	NC
12	A	809	CLA	NA
12	A	809	CLA	ND
12	e	804	CLA	NC
12	e	804	CLA	ND
12	e	804	CLA	NA
12	K	1401	CLA	NC
12	K	1401	CLA	ND
12	K	1401	CLA	NA
12	G	828	CLA	NC
12	G	828	CLA	ND
12	G	828	CLA	NA
12	e	822	CLA	NC
12	e	822	CLA	ND
12	e	822	CLA	NA
12	g	815	CLA	NC
12	g	815	CLA	ND
12	g	815	CLA	NA
12	A	807	CLA	NC
12	A	807	CLA	ND
12	A	807	CLA	NA
12	B	829	CLA	NC
12	B	829	CLA	ND
12	B	829	CLA	NA
12	b	836	CLA	NC
12	b	836	CLA	ND
12	b	836	CLA	NA
12	G	836	CLA	NC
12	G	836	CLA	ND
12	G	836	CLA	NA
12	B	839	CLA	NC
12	B	839	CLA	ND
12	B	839	CLA	NA
12	b	825	CLA	NC
12	b	825	CLA	ND
12	b	825	CLA	NA
12	A	832	CLA	NC
12	A	832	CLA	ND
12	A	832	CLA	NA

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Mol	Chain	Res	Type	Atom
12	b	823	CLA	NC
12	b	823	CLA	ND
12	b	823	CLA	NA
12	B	840	CLA	NC
12	B	840	CLA	ND
12	B	840	CLA	NA
12	A	838	CLA	NC
12	A	838	CLA	ND
12	A	838	CLA	NA
12	g	832	CLA	NC
12	g	832	CLA	ND
12	g	832	CLA	NA
12	S	1501	CLA	NC
12	S	1501	CLA	ND
12	S	1501	CLA	NA
12	A	816	CLA	NC
12	A	816	CLA	ND
12	A	816	CLA	NA
12	B	831	CLA	NC
12	B	831	CLA	ND
12	B	831	CLA	NA
12	a	828	CLA	NC
12	a	828	CLA	ND
12	a	828	CLA	NA
12	G	801	CLA	NC
12	G	801	CLA	ND
12	G	801	CLA	NA
12	b	821	CLA	NC
12	b	821	CLA	ND
12	b	821	CLA	NA
12	b	834	CLA	NC
12	b	834	CLA	ND
12	b	834	CLA	NA
12	b	826	CLA	NC
12	b	826	CLA	ND
12	b	826	CLA	NA
12	B	803	CLA	NC
12	B	803	CLA	ND
12	B	803	CLA	NA
12	E	808	CLA	NC
12	E	808	CLA	NA
12	e	813	CLA	NC

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Mol	Chain	Res	Type	Atom
12	e	813	CLA	ND
12	e	813	CLA	NA
12	A	805	CLA	NC
12	A	805	CLA	NA
12	g	831	CLA	NC
12	g	831	CLA	ND
12	g	831	CLA	NA
12	g	806	CLA	NC
12	g	806	CLA	ND
12	g	806	CLA	NA
12	E	824	CLA	NC
12	E	824	CLA	ND
12	E	824	CLA	NA
12	B	817	CLA	NC
12	B	817	CLA	ND
12	B	817	CLA	NA
12	B	824	CLA	NC
12	B	824	CLA	ND
12	B	824	CLA	NA
12	b	839	CLA	NC
12	b	839	CLA	ND
12	b	839	CLA	NA
12	E	823	CLA	NC
12	E	823	CLA	ND
12	E	823	CLA	NA
12	E	831	CLA	NC
12	E	831	CLA	ND
12	E	831	CLA	NA
12	b	813	CLA	NC
12	b	813	CLA	ND
12	b	813	CLA	NA
12	G	824	CLA	NC
12	G	824	CLA	ND
12	G	824	CLA	NA
12	G	830	CLA	NC
12	G	830	CLA	ND
12	G	830	CLA	NA
12	F	1301	CLA	NC
12	F	1301	CLA	ND
12	F	1301	CLA	NA
12	E	810	CLA	NC
12	E	810	CLA	ND

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Mol	Chain	Res	Type	Atom
12	E	810	CLA	NA
12	A	813	CLA	NC
12	A	813	CLA	ND
12	A	813	CLA	NA
12	E	836	CLA	NC
12	E	836	CLA	ND
12	E	836	CLA	NA
12	e	826	CLA	NC
12	e	826	CLA	ND
12	e	826	CLA	NA
12	L	203	CLA	NC
12	L	203	CLA	ND
12	L	203	CLA	NA
12	b	840	CLA	NC
12	b	840	CLA	NA
12	g	830	CLA	NC
12	g	830	CLA	ND
12	g	830	CLA	NA
12	E	842	CLA	NC
12	E	842	CLA	ND
12	E	842	CLA	NA
12	g	803	CLA	NC
12	g	803	CLA	ND
12	g	803	CLA	NA
12	L	204	CLA	NC
12	L	204	CLA	ND
12	L	204	CLA	NA
12	B	801	CLA	NC
12	B	801	CLA	ND
12	B	801	CLA	NA
12	G	811	CLA	NC
12	G	811	CLA	ND
12	G	811	CLA	NA
12	s	202	CLA	NC
12	s	202	CLA	ND
12	s	202	CLA	NA
12	B	814	CLA	NC
12	B	814	CLA	ND
12	B	814	CLA	NA
12	B	841	CLA	NC
12	B	841	CLA	NA
12	A	822	CLA	NC

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Mol	Chain	Res	Type	Atom
12	A	822	CLA	ND
12	A	822	CLA	NA
12	b	822	CLA	NC
12	b	822	CLA	ND
12	b	822	CLA	NA
12	g	821	CLA	NC
12	g	821	CLA	ND
12	g	821	CLA	NA
12	a	801	CLA	NC
12	a	801	CLA	ND
12	a	801	CLA	NA
12	e	824	CLA	NC
12	e	824	CLA	ND
12	e	824	CLA	NA
12	l	201	CLA	NC
12	l	201	CLA	NA
12	l	201	CLA	ND
12	g	838	CLA	NC
12	g	838	CLA	ND
12	g	838	CLA	NA
12	e	828	CLA	NC
12	e	828	CLA	ND
12	e	828	CLA	NA
12	B	826	CLA	NC
12	B	826	CLA	ND
12	B	826	CLA	NA
12	a	813	CLA	NC
12	a	813	CLA	ND
12	a	813	CLA	NA
12	G	813	CLA	NC
12	G	813	CLA	ND
12	G	813	CLA	NA
12	B	827	CLA	NC
12	B	827	CLA	ND
12	B	827	CLA	NA
12	b	816	CLA	NC
12	b	816	CLA	ND
12	b	816	CLA	NA
12	g	801	CLA	NC
12	g	801	CLA	ND
12	g	801	CLA	NA
12	G	820	CLA	NC

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Mol	Chain	Res	Type	Atom
12	G	820	CLA	ND
12	G	820	CLA	NA
12	G	841	CLA	NC
12	G	841	CLA	ND
12	G	841	CLA	NA
12	A	820	CLA	NC
12	A	820	CLA	ND
12	A	820	CLA	NA
12	g	837	CLA	NC
12	g	837	CLA	ND
12	g	837	CLA	NA
12	e	821	CLA	NC
12	e	821	CLA	ND
12	e	821	CLA	NA
12	b	828	CLA	NC
12	b	828	CLA	ND
12	b	828	CLA	NA
12	e	844	CLA	NC
12	e	844	CLA	ND
12	e	844	CLA	NA
12	a	802	CLA	NC
12	a	802	CLA	ND
12	a	802	CLA	NA
12	B	832	CLA	NC
12	B	832	CLA	ND
12	B	832	CLA	NA
12	a	820	CLA	NC
12	a	820	CLA	ND
12	a	820	CLA	NA
12	b	842	CLA	NC
12	b	842	CLA	ND
12	b	842	CLA	NA
12	b	803	CLA	NC
12	b	803	CLA	ND
12	b	803	CLA	NA
12	b	814	CLA	NC
12	b	814	CLA	ND
12	b	814	CLA	NA
12	A	814	CLA	NC
12	A	814	CLA	ND
12	A	814	CLA	NA
12	G	817	CLA	NC

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Mol	Chain	Res	Type	Atom
12	G	817	CLA	ND
12	G	817	CLA	NA
12	B	818	CLA	NC
12	B	818	CLA	ND
12	B	818	CLA	NA
12	E	827	CLA	NC
12	E	827	CLA	ND
12	E	827	CLA	NA
12	A	830	CLA	NC
12	A	830	CLA	ND
12	A	830	CLA	NA
12	g	812	CLA	NC
12	g	812	CLA	ND
12	g	812	CLA	NA
12	e	829	CLA	NC
12	e	829	CLA	ND
12	e	829	CLA	NA
12	g	818	CLA	NC
12	g	818	CLA	ND
12	g	818	CLA	NA
12	a	837	CLA	NC
12	a	837	CLA	ND
12	a	837	CLA	NA
12	G	843	CLA	NC
12	G	843	CLA	ND
12	G	843	CLA	NA
12	A	840	CLA	NC
12	A	840	CLA	ND
12	A	840	CLA	NA
12	G	827	CLA	NC
12	G	827	CLA	ND
12	G	827	CLA	NA
12	E	815	CLA	NC
12	E	815	CLA	ND
12	E	815	CLA	NA
12	J	1102	CLA	NC
12	J	1102	CLA	ND
12	J	1102	CLA	NA
12	B	837	CLA	NC
12	B	837	CLA	ND
12	B	837	CLA	NA
12	E	821	CLA	NC

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Mol	Chain	Res	Type	Atom
12	E	821	CLA	ND
12	E	821	CLA	NA
12	g	828	CLA	NC
12	g	828	CLA	ND
12	g	828	CLA	NA
12	e	834	CLA	NC
12	e	834	CLA	ND
12	e	834	CLA	NA
12	b	812	CLA	NC
12	b	812	CLA	ND
12	b	812	CLA	NA
12	G	806	CLA	NC
12	G	806	CLA	ND
12	G	806	CLA	NA
13	E	846	PQN	C18
12	A	810	CLA	NC
12	A	810	CLA	ND
12	A	810	CLA	NA
12	B	815	CLA	NC
12	B	815	CLA	ND
12	B	815	CLA	NA
12	A	823	CLA	NC
12	A	823	CLA	ND
12	A	823	CLA	NA
12	B	823	CLA	NC
12	B	823	CLA	ND
12	B	823	CLA	NA
12	a	824	CLA	NC
12	a	824	CLA	ND
12	a	824	CLA	NA
12	g	841	CLA	NC
12	g	841	CLA	ND
12	g	841	CLA	NA
12	E	839	CLA	NC
12	E	839	CLA	ND
12	E	839	CLA	NA
12	E	805	CLA	NC
12	E	805	CLA	ND
12	E	805	CLA	NA
12	E	826	CLA	NC
12	E	826	CLA	ND
12	E	826	CLA	NA

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Mol	Chain	Res	Type	Atom
12	g	840	CLA	NC
12	g	840	CLA	NA
12	a	805	CLA	NC
12	a	805	CLA	ND
12	a	805	CLA	NA
12	E	835	CLA	NC
12	E	835	CLA	ND
12	E	835	CLA	NA
12	e	841	CLA	NC
12	e	841	CLA	ND
12	e	841	CLA	NA
12	e	806	CLA	NC
12	e	806	CLA	NA
12	G	825	CLA	NC
12	G	825	CLA	ND
12	G	825	CLA	NA
12	e	814	CLA	NC
12	e	814	CLA	ND
12	e	814	CLA	NA
12	e	805	CLA	NC
12	e	805	CLA	NA
12	e	805	CLA	ND
12	G	835	CLA	NC
12	G	835	CLA	ND
12	G	835	CLA	NA
12	e	831	CLA	NC
12	e	831	CLA	ND
12	e	831	CLA	NA
12	a	818	CLA	NC
12	a	818	CLA	ND
12	a	818	CLA	NA
12	g	802	CLA	NC
12	g	802	CLA	NA
12	g	802	CLA	ND
12	E	818	CLA	NC
12	E	818	CLA	ND
12	E	818	CLA	NA
12	a	803	CLA	NC
12	a	803	CLA	ND
12	a	803	CLA	NA
12	G	808	CLA	NC
12	G	808	CLA	ND

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Mol	Chain	Res	Type	Atom
12	G	808	CLA	NA
12	a	809	CLA	NC
12	a	809	CLA	ND
12	a	809	CLA	NA
12	A	836	CLA	NC
12	A	836	CLA	ND
12	A	836	CLA	NA
12	B	828	CLA	NC
12	B	828	CLA	ND
12	B	828	CLA	NA
12	G	816	CLA	NC
12	G	816	CLA	ND
12	G	816	CLA	NA
12	B	835	CLA	NC
12	B	835	CLA	ND
12	B	835	CLA	NA
12	g	829	CLA	NC
12	g	829	CLA	ND
12	g	829	CLA	NA
12	G	819	CLA	NC
12	G	819	CLA	ND
12	G	819	CLA	NA
12	E	806	CLA	NC
12	E	806	CLA	ND
12	E	806	CLA	NA
12	k	1401	CLA	NC
12	k	1401	CLA	ND
12	k	1401	CLA	NA
12	E	837	CLA	NC
12	E	837	CLA	ND
12	E	837	CLA	NA
12	b	815	CLA	NC
12	b	815	CLA	ND
12	b	815	CLA	NA
12	a	804	CLA	NC
12	a	804	CLA	ND
12	a	804	CLA	NA
12	a	823	CLA	NC
12	a	823	CLA	ND
12	a	823	CLA	NA
12	e	820	CLA	NC
12	e	820	CLA	ND

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Mol	Chain	Res	Type	Atom
12	e	820	CLA	NA
12	b	833	CLA	NC
12	b	833	CLA	ND
12	b	833	CLA	NA
12	A	825	CLA	NC
12	A	825	CLA	ND
12	A	825	CLA	NA
12	B	821	CLA	NC
12	B	821	CLA	ND
12	B	821	CLA	NA
12	g	826	CLA	NC
12	g	826	CLA	ND
12	g	826	CLA	NA
12	e	823	CLA	NC
12	e	823	CLA	ND
12	e	823	CLA	NA
12	g	839	CLA	NC
12	g	839	CLA	ND
12	g	839	CLA	NA
12	e	833	CLA	NC
12	e	833	CLA	ND
12	e	833	CLA	NA
12	b	819	CLA	NC
12	b	819	CLA	ND
12	b	819	CLA	NA
12	b	806	CLA	NC
12	b	806	CLA	ND
12	b	806	CLA	NA
12	G	829	CLA	NC
12	G	829	CLA	ND
12	G	829	CLA	NA
12	E	844	CLA	NC
12	E	844	CLA	ND
12	E	844	CLA	NA
12	e	811	CLA	NC
12	e	811	CLA	ND
12	e	811	CLA	NA
12	G	807	CLA	NC
12	G	807	CLA	NA
12	G	807	CLA	ND
12	A	833	CLA	NC
12	A	833	CLA	ND

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Mol	Chain	Res	Type	Atom
12	A	833	CLA	NA
12	b	811	CLA	NC
12	b	811	CLA	ND
12	b	811	CLA	NA
12	a	821	CLA	NC
12	a	821	CLA	ND
12	a	821	CLA	NA
12	B	830	CLA	NC
12	B	830	CLA	ND
12	B	830	CLA	NA
12	G	840	CLA	NC
12	G	840	CLA	ND
12	G	840	CLA	NA
12	b	835	CLA	NC
12	b	835	CLA	ND
12	b	835	CLA	NA
12	e	845	CLA	NC
12	e	845	CLA	ND
12	e	845	CLA	NA
12	a	806	CLA	NC
12	a	806	CLA	NA
12	a	806	CLA	ND
12	g	810	CLA	NC
12	g	810	CLA	ND
12	g	810	CLA	NA
12	A	808	CLA	NC
12	A	808	CLA	ND
12	A	808	CLA	NA
12	g	836	CLA	NC
12	g	836	CLA	ND
12	g	836	CLA	NA
12	E	804	CLA	NC
12	E	804	CLA	ND
12	E	804	CLA	NA
12	E	801	CLA	NC
12	E	801	CLA	ND
12	E	801	CLA	NA
12	a	831	CLA	NC
12	a	831	CLA	NA
12	A	811	CLA	NC
12	A	811	CLA	ND
12	A	811	CLA	NA

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Mol	Chain	Res	Type	Atom
12	a	834	CLA	NC
12	a	834	CLA	ND
12	a	834	CLA	NA
12	g	817	CLA	NC
12	g	817	CLA	ND
12	g	817	CLA	NA
12	B	806	CLA	NC
12	B	806	CLA	ND
12	B	806	CLA	NA
12	o	1301	CLA	NC
12	o	1301	CLA	ND
12	o	1301	CLA	NA
12	A	812	CLA	NC
12	A	812	CLA	ND
12	A	812	CLA	NA
12	e	819	CLA	NC
12	e	819	CLA	ND
12	e	819	CLA	NA
12	e	801	CLA	NC
12	e	801	CLA	ND
12	e	801	CLA	NA
12	L	202	CLA	NC
12	L	202	CLA	ND
12	L	202	CLA	NA
12	a	839	CLA	NC
12	a	839	CLA	NA
12	B	836	CLA	NC
12	B	836	CLA	ND
12	B	836	CLA	NA
12	G	837	CLA	NC
12	G	837	CLA	ND
12	G	837	CLA	NA
12	E	807	CLA	NC
12	E	807	CLA	NA
12	E	807	CLA	ND
12	L	201	CLA	NC
12	L	201	CLA	NA
12	L	201	CLA	ND
12	A	821	CLA	NC
12	A	821	CLA	ND
12	A	821	CLA	NA
12	b	820	CLA	NC

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Mol	Chain	Res	Type	Atom
12	b	820	CLA	ND
12	b	820	CLA	NA
12	O	1301	CLA	NC
12	O	1301	CLA	ND
12	O	1301	CLA	NA
12	E	816	CLA	NC
12	E	816	CLA	ND
12	E	816	CLA	NA
12	A	802	CLA	NC
12	A	802	CLA	ND
12	A	802	CLA	NA
12	e	812	CLA	NC
12	e	812	CLA	ND
12	e	812	CLA	NA
12	E	803	CLA	NC
12	E	803	CLA	NA
12	E	803	CLA	ND
12	B	805	CLA	NC
12	B	805	CLA	ND
12	B	805	CLA	NA
12	E	829	CLA	NC
12	E	829	CLA	ND
12	E	829	CLA	NA
12	g	811	CLA	NC
12	g	811	CLA	ND
12	g	811	CLA	NA
12	B	842	CLA	NC
12	B	842	CLA	ND
12	B	842	CLA	NA
12	a	810	CLA	NC
12	a	810	CLA	ND
12	a	810	CLA	NA
12	e	832	CLA	NC
12	e	832	CLA	ND
12	e	832	CLA	NA
12	E	828	CLA	NC
12	E	828	CLA	ND
12	E	828	CLA	NA
12	b	805	CLA	NC
12	b	805	CLA	ND
12	b	805	CLA	NA
12	G	814	CLA	NC

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Mol	Chain	Res	Type	Atom
12	G	814	CLA	ND
12	G	814	CLA	NA
12	e	839	CLA	NC
12	e	839	CLA	ND
12	e	839	CLA	NA
12	b	817	CLA	NC
12	b	817	CLA	ND
12	b	817	CLA	NA
13	A	842	PQN	C18
12	g	823	CLA	NC
12	g	823	CLA	ND
12	g	823	CLA	NA
12	b	807	CLA	NC
12	b	807	CLA	ND
12	b	807	CLA	NA
12	E	813	CLA	NC
12	E	813	CLA	ND
12	E	813	CLA	NA
12	a	840	CLA	NC
12	a	840	CLA	ND
12	a	840	CLA	NA
12	a	842	CLA	NC
12	a	842	CLA	ND
12	a	842	CLA	NA
12	E	843	CLA	NC
12	E	843	CLA	ND
12	E	843	CLA	NA
12	G	812	CLA	NC
12	G	812	CLA	ND
12	G	812	CLA	NA
12	G	818	CLA	NC
12	G	818	CLA	ND
12	G	818	CLA	NA
12	E	802	CLA	NC
12	E	802	CLA	ND
12	E	802	CLA	NA
12	b	802	CLA	NC
12	b	802	CLA	ND
12	b	802	CLA	NA
12	B	807	CLA	NC
12	B	807	CLA	ND
12	B	807	CLA	NA

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Mol	Chain	Res	Type	Atom
13	e	843	PQN	C18
12	A	841	CLA	NC
12	A	841	CLA	ND
12	A	841	CLA	NA
12	R	1401	CLA	NC
12	R	1401	CLA	ND
12	R	1401	CLA	NA

All (2550) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	E	817	CLA	C1A-C2A-CAA-CBA
12	E	817	CLA	CHA-CBD-CGD-O1D
12	E	817	CLA	CHA-CBD-CGD-O2D
12	E	817	CLA	CBD-CGD-O2D-CED
12	E	840	CLA	C1A-C2A-CAA-CBA
12	E	840	CLA	C3A-C2A-CAA-CBA
12	E	840	CLA	CHA-CBD-CGD-O1D
12	E	840	CLA	CHA-CBD-CGD-O2D
12	e	815	CLA	C1A-C2A-CAA-CBA
12	e	815	CLA	CHA-CBD-CGD-O1D
12	e	815	CLA	CHA-CBD-CGD-O2D
12	e	815	CLA	CBD-CGD-O2D-CED
12	b	837	CLA	C1A-C2A-CAA-CBA
12	A	801	CLA	CBD-CGD-O2D-CED
12	e	803	CLA	CBD-CGD-O2D-CED
12	b	830	CLA	C1A-C2A-CAA-CBA
12	b	830	CLA	C3A-C2A-CAA-CBA
12	b	830	CLA	CHA-CBD-CGD-O1D
12	b	830	CLA	CHA-CBD-CGD-O2D
12	b	830	CLA	CBD-CGD-O2D-CED
12	b	830	CLA	O1D-CGD-O2D-CED
12	B	819	CLA	C1A-C2A-CAA-CBA
12	B	819	CLA	C3A-C2A-CAA-CBA
12	B	819	CLA	CBD-CGD-O2D-CED
12	A	828	CLA	CBD-CGD-O2D-CED
12	e	802	CLA	CHA-CBD-CGD-O1D
12	e	802	CLA	CHA-CBD-CGD-O2D
12	E	833	CLA	CHA-CBD-CGD-O1D
12	E	833	CLA	CHA-CBD-CGD-O2D
12	b	824	CLA	CBD-CGD-O2D-CED
12	J	1101	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	J	1101	CLA	CHA-CBD-CGD-O2D
12	E	834	CLA	C1A-C2A-CAA-CBA
12	E	834	CLA	C3A-C2A-CAA-CBA
12	E	834	CLA	CBD-CGD-O2D-CED
12	E	834	CLA	O1D-CGD-O2D-CED
12	B	838	CLA	C1A-C2A-CAA-CBA
12	r	1401	CLA	CBD-CGD-O2D-CED
12	e	807	CLA	C1A-C2A-CAA-CBA
12	e	807	CLA	C3A-C2A-CAA-CBA
12	e	840	CLA	CBD-CGD-O2D-CED
12	s	204	CLA	C3A-C2A-CAA-CBA
12	s	204	CLA	CBD-CGD-O2D-CED
12	E	820	CLA	C1A-C2A-CAA-CBA
12	E	820	CLA	C3A-C2A-CAA-CBA
12	E	820	CLA	CHA-CBD-CGD-O1D
12	E	820	CLA	CHA-CBD-CGD-O2D
12	g	820	CLA	C1A-C2A-CAA-CBA
12	g	820	CLA	C3A-C2A-CAA-CBA
12	e	808	CLA	C1A-C2A-CAA-CBA
12	e	808	CLA	CBD-CGD-O2D-CED
12	e	825	CLA	C1A-C2A-CAA-CBA
12	G	809	CLA	CHA-CBD-CGD-O1D
12	G	809	CLA	CHA-CBD-CGD-O2D
12	G	802	CLA	C1A-C2A-CAA-CBA
12	B	810	CLA	CBD-CGD-O2D-CED
12	l	204	CLA	C3A-C2A-CAA-CBA
12	l	204	CLA	CBD-CGD-O2D-CED
12	g	825	CLA	CBD-CGD-O2D-CED
12	b	829	CLA	CAD-CBD-CGD-O1D
12	b	829	CLA	CAD-CBD-CGD-O2D
12	b	831	CLA	C1A-C2A-CAA-CBA
12	b	831	CLA	C3A-C2A-CAA-CBA
12	b	831	CLA	CBD-CGD-O2D-CED
12	G	810	CLA	C1A-C2A-CAA-CBA
12	G	810	CLA	C3A-C2A-CAA-CBA
12	E	809	CLA	C1A-C2A-CAA-CBA
12	E	809	CLA	C3A-C2A-CAA-CBA
12	a	829	CLA	C1A-C2A-CAA-CBA
12	a	829	CLA	CHA-CBD-CGD-O1D
12	a	829	CLA	CHA-CBD-CGD-O2D
12	E	822	CLA	CBD-CGD-O2D-CED
12	a	827	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	a	827	CLA	C3A-C2A-CAA-CBA
12	a	827	CLA	CBD-CGD-O2D-CED
12	G	834	CLA	C1A-C2A-CAA-CBA
12	G	834	CLA	C3A-C2A-CAA-CBA
12	G	834	CLA	CBD-CGD-O2D-CED
12	b	808	CLA	CBD-CGD-O2D-CED
12	a	814	CLA	C1A-C2A-CAA-CBA
12	a	814	CLA	C3A-C2A-CAA-CBA
12	a	814	CLA	CHA-CBD-CGD-O1D
12	a	814	CLA	CHA-CBD-CGD-O2D
12	a	814	CLA	CAD-CBD-CGD-O1D
12	a	814	CLA	CBD-CGD-O2D-CED
12	a	832	CLA	C1A-C2A-CAA-CBA
12	a	832	CLA	C3A-C2A-CAA-CBA
12	a	832	CLA	CBD-CGD-O2D-CED
12	a	832	CLA	O1D-CGD-O2D-CED
12	A	819	CLA	CBD-CGD-O2D-CED
12	e	827	CLA	CBD-CGD-O2D-CED
12	a	830	CLA	CBD-CGD-O2D-CED
12	g	814	CLA	CHA-CBD-CGD-O1D
12	g	814	CLA	CHA-CBD-CGD-O2D
12	g	814	CLA	CAD-CBD-CGD-O1D
12	B	811	CLA	C1A-C2A-CAA-CBA
12	B	811	CLA	C3A-C2A-CAA-CBA
12	B	811	CLA	CBD-CGD-O2D-CED
12	G	804	CLA	CHA-CBD-CGD-O1D
12	G	804	CLA	CHA-CBD-CGD-O2D
12	G	804	CLA	CBD-CGD-O2D-CED
12	g	835	CLA	C1A-C2A-CAA-CBA
12	g	835	CLA	C3A-C2A-CAA-CBA
12	g	835	CLA	CBD-CGD-O2D-CED
12	g	827	CLA	CBD-CGD-O2D-CED
12	b	809	CLA	C1A-C2A-CAA-CBA
12	b	809	CLA	C3A-C2A-CAA-CBA
12	b	809	CLA	CBD-CGD-O2D-CED
12	A	806	CLA	C1A-C2A-CAA-CBA
12	A	806	CLA	C3A-C2A-CAA-CBA
12	b	804	CLA	C1A-C2A-CAA-CBA
12	b	804	CLA	C3A-C2A-CAA-CBA
12	b	804	CLA	CBD-CGD-O2D-CED
12	S	1502	CLA	C3A-C2A-CAA-CBA
12	S	1502	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	e	817	CLA	C3A-C2A-CAA-CBA
12	A	827	CLA	C1A-C2A-CAA-CBA
12	A	827	CLA	CHA-CBD-CGD-O1D
12	A	827	CLA	CHA-CBD-CGD-O2D
12	b	827	CLA	C3A-C2A-CAA-CBA
12	b	827	CLA	CBD-CGD-O2D-CED
12	E	819	CLA	C3A-C2A-CAA-CBA
12	B	808	CLA	C1A-C2A-CAA-CBA
12	B	808	CLA	C3A-C2A-CAA-CBA
12	B	808	CLA	CBD-CGD-O2D-CED
12	G	838	CLA	CBD-CGD-O2D-CED
12	b	841	CLA	CAD-CBD-CGD-O1D
12	b	841	CLA	CAD-CBD-CGD-O2D
12	E	830	CLA	C1A-C2A-CAA-CBA
12	E	830	CLA	CHA-CBD-CGD-O1D
12	E	830	CLA	CHA-CBD-CGD-O2D
12	G	839	CLA	O1A-CGA-O2A-C1
12	b	810	CLA	CHA-CBD-CGD-O1D
12	b	810	CLA	CHA-CBD-CGD-O2D
12	a	819	CLA	C1A-C2A-CAA-CBA
12	a	819	CLA	C3A-C2A-CAA-CBA
12	a	819	CLA	CHA-CBD-CGD-O1D
12	a	819	CLA	CHA-CBD-CGD-O2D
12	a	841	CLA	CBD-CGD-O2D-CED
12	G	821	CLA	C1A-C2A-CAA-CBA
12	G	821	CLA	C3A-C2A-CAA-CBA
12	G	821	CLA	CHA-CBD-CGD-O1D
12	G	821	CLA	CHA-CBD-CGD-O2D
12	e	818	CLA	C1A-C2A-CAA-CBA
12	e	818	CLA	C3A-C2A-CAA-CBA
12	e	818	CLA	CHA-CBD-CGD-O1D
12	e	818	CLA	CHA-CBD-CGD-O2D
12	a	807	CLA	C1A-C2A-CAA-CBA
12	a	807	CLA	C3A-C2A-CAA-CBA
12	A	826	CLA	CBD-CGD-O2D-CED
12	g	813	CLA	C1A-C2A-CAA-CBA
12	g	813	CLA	C3A-C2A-CAA-CBA
12	g	813	CLA	CBD-CGD-O2D-CED
12	E	832	CLA	C1A-C2A-CAA-CBA
12	E	832	CLA	CBD-CGD-O2D-CED
12	E	832	CLA	O1D-CGD-O2D-CED
12	A	831	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	831	CLA	C3A-C2A-CAA-CBA
12	g	807	CLA	C1A-C2A-CAA-CBA
12	g	807	CLA	C3A-C2A-CAA-CBA
12	g	807	CLA	CBD-CGD-O2D-CED
12	a	826	CLA	C1A-C2A-CAA-CBA
12	l	202	CLA	C1A-C2A-CAA-CBA
12	l	202	CLA	CHA-CBD-CGD-O1D
12	l	202	CLA	CHA-CBD-CGD-O2D
12	G	815	CLA	C1A-C2A-CAA-CBA
12	G	815	CLA	CBD-CGD-O2D-CED
12	G	815	CLA	O1D-CGD-O2D-CED
12	G	803	CLA	C1A-C2A-CAA-CBA
12	G	803	CLA	C3A-C2A-CAA-CBA
12	G	803	CLA	CBD-CGD-O2D-CED
12	g	809	CLA	CBD-CGD-O2D-CED
12	e	830	CLA	C1A-C2A-CAA-CBA
12	e	830	CLA	CBD-CGD-O2D-CED
12	e	830	CLA	O1D-CGD-O2D-CED
12	g	824	CLA	CBD-CGD-O2D-CED
12	A	824	CLA	C1A-C2A-CAA-CBA
12	A	829	CLA	C1A-C2A-CAA-CBA
12	A	829	CLA	CBD-CGD-O2D-CED
12	A	829	CLA	O1D-CGD-O2D-CED
12	B	825	CLA	CBD-CGD-O2D-CED
12	b	838	CLA	C3A-C2A-CAA-CBA
12	b	838	CLA	CHA-CBD-CGD-O1D
12	b	838	CLA	CHA-CBD-CGD-O2D
12	b	838	CLA	CBD-CGD-O2D-CED
12	G	826	CLA	C3A-C2A-CAA-CBA
12	G	826	CLA	CBD-CGD-O2D-CED
12	a	822	CLA	C1A-C2A-CAA-CBA
12	G	823	CLA	CBD-CGD-O2D-CED
12	A	839	CLA	CBD-CGD-O2D-CED
12	e	837	CLA	C1A-C2A-CAA-CBA
12	e	837	CLA	C3A-C2A-CAA-CBA
12	e	837	CLA	CHA-CBD-CGD-O1D
12	e	837	CLA	CHA-CBD-CGD-O2D
12	A	817	CLA	C1A-C2A-CAA-CBA
12	A	817	CLA	C3A-C2A-CAA-CBA
12	A	817	CLA	CHA-CBD-CGD-O1D
12	A	817	CLA	CHA-CBD-CGD-O2D
12	g	805	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	g	805	CLA	C3A-C2A-CAA-CBA
12	g	805	CLA	CBD-CGD-O2D-CED
12	B	816	CLA	C1A-C2A-CAA-CBA
12	B	816	CLA	CBD-CGD-O2D-CED
12	a	838	CLA	C1A-C2A-CAA-CBA
12	a	838	CLA	C3A-C2A-CAA-CBA
12	a	838	CLA	CHA-CBD-CGD-O1D
12	a	838	CLA	CHA-CBD-CGD-O2D
12	G	822	CLA	CBD-CGD-O2D-CED
12	a	816	CLA	C1A-C2A-CAA-CBA
12	a	816	CLA	CHA-CBD-CGD-O1D
12	a	816	CLA	CHA-CBD-CGD-O2D
12	a	816	CLA	CBD-CGD-O2D-CED
12	f	1301	CLA	C1A-C2A-CAA-CBA
12	f	1301	CLA	CBD-CGD-O2D-CED
12	g	816	CLA	C1A-C2A-CAA-CBA
12	g	816	CLA	C3A-C2A-CAA-CBA
12	g	816	CLA	CHA-CBD-CGD-O1D
12	g	816	CLA	CHA-CBD-CGD-O2D
12	g	816	CLA	CAD-CBD-CGD-O1D
12	g	816	CLA	CBD-CGD-O2D-CED
12	B	813	CLA	C1A-C2A-CAA-CBA
12	B	813	CLA	C3A-C2A-CAA-CBA
12	B	833	CLA	C1A-C2A-CAA-CBA
12	B	833	CLA	C3A-C2A-CAA-CBA
12	B	833	CLA	CBD-CGD-O2D-CED
12	a	833	CLA	C1A-C2A-CAA-CBA
12	a	833	CLA	C3A-C2A-CAA-CBA
12	G	832	CLA	C1A-C2A-CAA-CBA
12	G	832	CLA	CHA-CBD-CGD-O1D
12	G	832	CLA	CHA-CBD-CGD-O2D
12	G	832	CLA	CBD-CGD-O2D-CED
12	B	812	CLA	CHA-CBD-CGD-O1D
12	B	812	CLA	CHA-CBD-CGD-O2D
12	G	805	CLA	C1A-C2A-CAA-CBA
12	G	805	CLA	C3A-C2A-CAA-CBA
12	G	805	CLA	CBD-CGD-O2D-CED
12	s	201	CLA	CHA-CBD-CGD-O1D
12	s	201	CLA	CHA-CBD-CGD-O2D
12	a	808	CLA	C1A-C2A-CAA-CBA
12	a	808	CLA	C3A-C2A-CAA-CBA
12	K	1401	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	G	828	CLA	CAD-CBD-CGD-O1D
12	G	828	CLA	CAD-CBD-CGD-O2D
12	e	822	CLA	CHA-CBD-CGD-O1D
12	e	822	CLA	CHA-CBD-CGD-O2D
12	e	822	CLA	CBD-CGD-O2D-CED
12	g	815	CLA	C1A-C2A-CAA-CBA
12	g	815	CLA	CBD-CGD-O2D-CED
12	A	807	CLA	C1A-C2A-CAA-CBA
12	A	807	CLA	CBD-CGD-O2D-CED
12	B	829	CLA	C3A-C2A-CAA-CBA
12	B	829	CLA	CBD-CGD-O2D-CED
12	b	836	CLA	C1A-C2A-CAA-CBA
12	b	836	CLA	CBD-CGD-O2D-CED
12	G	836	CLA	C1A-C2A-CAA-CBA
12	B	839	CLA	C3A-C2A-CAA-CBA
12	B	839	CLA	CHA-CBD-CGD-O1D
12	B	839	CLA	CHA-CBD-CGD-O2D
12	B	839	CLA	CBD-CGD-O2D-CED
12	b	825	CLA	C2A-CAA-CBA-CGA
12	b	825	CLA	CHA-CBD-CGD-O1D
12	b	825	CLA	CHA-CBD-CGD-O2D
12	A	832	CLA	C1A-C2A-CAA-CBA
12	b	823	CLA	CBD-CGD-O2D-CED
12	B	840	CLA	CBD-CGD-O2D-CED
12	A	838	CLA	CBD-CGD-O2D-CED
12	g	832	CLA	C1A-C2A-CAA-CBA
12	g	832	CLA	C3A-C2A-CAA-CBA
12	g	832	CLA	CBD-CGD-O2D-CED
12	S	1501	CLA	C1A-C2A-CAA-CBA
12	S	1501	CLA	CHA-CBD-CGD-O1D
12	S	1501	CLA	CHA-CBD-CGD-O2D
12	A	816	CLA	C3A-C2A-CAA-CBA
12	B	831	CLA	CAD-CBD-CGD-O1D
12	B	831	CLA	CAD-CBD-CGD-O2D
12	a	828	CLA	CBD-CGD-O2D-CED
12	b	826	CLA	CBD-CGD-O2D-CED
12	E	808	CLA	C1A-C2A-CAA-CBA
12	E	808	CLA	C3A-C2A-CAA-CBA
12	e	813	CLA	C1A-C2A-CAA-CBA
12	e	813	CLA	C3A-C2A-CAA-CBA
12	e	813	CLA	CHA-CBD-CGD-O1D
12	e	813	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	e	813	CLA	CAD-CBD-CGD-O1D
12	e	813	CLA	CBD-CGD-O2D-CED
12	A	805	CLA	C1A-C2A-CAA-CBA
12	A	805	CLA	C3A-C2A-CAA-CBA
12	g	831	CLA	C1A-C2A-CAA-CBA
12	g	831	CLA	C3A-C2A-CAA-CBA
12	g	831	CLA	CHA-CBD-CGD-O1D
12	g	831	CLA	CHA-CBD-CGD-O2D
12	g	831	CLA	CBD-CGD-O2D-CED
12	g	831	CLA	O1D-CGD-O2D-CED
12	g	806	CLA	CHA-CBD-CGD-O1D
12	g	806	CLA	CHA-CBD-CGD-O2D
12	g	806	CLA	CBD-CGD-O2D-CED
12	E	824	CLA	CHA-CBD-CGD-O1D
12	E	824	CLA	CHA-CBD-CGD-O2D
12	E	824	CLA	CBD-CGD-O2D-CED
12	B	817	CLA	C1A-C2A-CAA-CBA
12	B	817	CLA	C3A-C2A-CAA-CBA
12	B	817	CLA	CHA-CBD-CGD-O1D
12	B	817	CLA	CHA-CBD-CGD-O2D
12	B	817	CLA	CAD-CBD-CGD-O1D
12	B	817	CLA	CBD-CGD-O2D-CED
12	B	824	CLA	C1A-C2A-CAA-CBA
12	B	824	CLA	C3A-C2A-CAA-CBA
12	B	824	CLA	CHA-CBD-CGD-O1D
12	B	824	CLA	CHA-CBD-CGD-O2D
12	b	839	CLA	CBD-CGD-O2D-CED
12	E	823	CLA	C1A-C2A-CAA-CBA
12	E	831	CLA	CBD-CGD-O2D-CED
12	b	813	CLA	CHA-CBD-CGD-O1D
12	b	813	CLA	CHA-CBD-CGD-O2D
12	b	813	CLA	CAD-CBD-CGD-O1D
12	G	824	CLA	C2A-CAA-CBA-CGA
12	G	824	CLA	CHA-CBD-CGD-O1D
12	G	824	CLA	CHA-CBD-CGD-O2D
12	G	830	CLA	C1A-C2A-CAA-CBA
12	G	830	CLA	C3A-C2A-CAA-CBA
12	G	830	CLA	CBD-CGD-O2D-CED
12	F	1301	CLA	C1A-C2A-CAA-CBA
12	F	1301	CLA	CBD-CGD-O2D-CED
12	E	810	CLA	C1A-C2A-CAA-CBA
12	E	810	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	E	836	CLA	C1A-C2A-CAA-CBA
12	e	826	CLA	C1A-C2A-CAA-CBA
12	e	826	CLA	C3A-C2A-CAA-CBA
12	e	826	CLA	CBD-CGD-O2D-CED
12	b	840	CLA	O1A-CGA-O2A-C1
12	g	830	CLA	CAD-CBD-CGD-O1D
12	g	830	CLA	CAD-CBD-CGD-O2D
12	E	842	CLA	CBD-CGD-O2D-CED
12	L	204	CLA	C3A-C2A-CAA-CBA
12	L	204	CLA	CBD-CGD-O2D-CED
12	G	811	CLA	C1A-C2A-CAA-CBA
12	G	811	CLA	C3A-C2A-CAA-CBA
12	G	811	CLA	CBD-CGD-O2D-CED
12	s	202	CLA	C1A-C2A-CAA-CBA
12	s	202	CLA	CHA-CBD-CGD-O1D
12	s	202	CLA	CHA-CBD-CGD-O2D
12	B	814	CLA	C1A-C2A-CAA-CBA
12	B	814	CLA	C3A-C2A-CAA-CBA
12	B	814	CLA	CBD-CGD-O2D-CED
12	B	841	CLA	O1A-CGA-O2A-C1
12	b	822	CLA	C1A-C2A-CAA-CBA
12	b	822	CLA	C3A-C2A-CAA-CBA
12	b	822	CLA	CHA-CBD-CGD-O1D
12	b	822	CLA	CHA-CBD-CGD-O2D
12	a	801	CLA	CBD-CGD-O2D-CED
12	l	201	CLA	CHA-CBD-CGD-O1D
12	l	201	CLA	CHA-CBD-CGD-O2D
12	g	838	CLA	C3A-C2A-CAA-CBA
12	g	838	CLA	CHA-CBD-CGD-O1D
12	g	838	CLA	CHA-CBD-CGD-O2D
12	g	838	CLA	CBD-CGD-O2D-CED
12	e	828	CLA	C1A-C2A-CAA-CBA
12	e	828	CLA	CHA-CBD-CGD-O1D
12	e	828	CLA	CHA-CBD-CGD-O2D
12	B	826	CLA	CBD-CGD-O2D-CED
12	G	813	CLA	C1A-C2A-CAA-CBA
12	G	813	CLA	CBD-CGD-O2D-CED
12	B	827	CLA	C2A-CAA-CBA-CGA
12	B	827	CLA	CHA-CBD-CGD-O1D
12	B	827	CLA	CHA-CBD-CGD-O2D
12	b	816	CLA	C1A-C2A-CAA-CBA
12	b	816	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	b	816	CLA	O1D-CGD-O2D-CED
12	A	820	CLA	C1A-C2A-CAA-CBA
12	g	837	CLA	C1A-C2A-CAA-CBA
12	e	821	CLA	C1A-C2A-CAA-CBA
12	b	828	CLA	CBD-CGD-O2D-CED
12	e	844	CLA	C1A-C2A-CAA-CBA
12	B	832	CLA	C1A-C2A-CAA-CBA
12	B	832	CLA	C3A-C2A-CAA-CBA
12	B	832	CLA	CHA-CBD-CGD-O1D
12	B	832	CLA	CHA-CBD-CGD-O2D
12	B	832	CLA	CBD-CGD-O2D-CED
12	B	832	CLA	O1D-CGD-O2D-CED
12	b	803	CLA	C1A-C2A-CAA-CBA
12	b	814	CLA	C1A-C2A-CAA-CBA
12	b	814	CLA	CBD-CGD-O2D-CED
12	A	814	CLA	C1A-C2A-CAA-CBA
12	A	814	CLA	CHA-CBD-CGD-O1D
12	A	814	CLA	CHA-CBD-CGD-O2D
12	A	814	CLA	CBD-CGD-O2D-CED
12	B	818	CLA	C1A-C2A-CAA-CBA
12	B	818	CLA	CBD-CGD-O2D-CED
12	B	818	CLA	O1D-CGD-O2D-CED
12	E	827	CLA	C1A-C2A-CAA-CBA
12	A	830	CLA	C1A-C2A-CAA-CBA
12	A	830	CLA	C3A-C2A-CAA-CBA
12	A	830	CLA	CBD-CGD-O2D-CED
12	A	830	CLA	O1D-CGD-O2D-CED
12	g	812	CLA	C1A-C2A-CAA-CBA
12	g	812	CLA	C3A-C2A-CAA-CBA
12	e	829	CLA	CBD-CGD-O2D-CED
12	g	818	CLA	C1A-C2A-CAA-CBA
12	g	818	CLA	C3A-C2A-CAA-CBA
12	g	818	CLA	CBD-CGD-O2D-CED
12	G	827	CLA	CBD-CGD-O2D-CED
12	E	815	CLA	C1A-C2A-CAA-CBA
12	E	815	CLA	C3A-C2A-CAA-CBA
12	E	815	CLA	CHA-CBD-CGD-O1D
12	E	815	CLA	CHA-CBD-CGD-O2D
12	E	815	CLA	CAD-CBD-CGD-O1D
12	E	815	CLA	CBD-CGD-O2D-CED
12	J	1102	CLA	C1A-C2A-CAA-CBA
12	J	1102	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	J	1102	CLA	CBD-CGD-O2D-CED
12	B	837	CLA	C1A-C2A-CAA-CBA
12	B	837	CLA	CBD-CGD-O2D-CED
12	g	828	CLA	C1A-C2A-CAA-CBA
12	g	828	CLA	C3A-C2A-CAA-CBA
12	g	828	CLA	CBD-CGD-O2D-CED
12	b	812	CLA	C1A-C2A-CAA-CBA
12	b	812	CLA	C3A-C2A-CAA-CBA
12	b	812	CLA	CBD-CGD-O2D-CED
12	B	815	CLA	CHA-CBD-CGD-O1D
12	B	815	CLA	CHA-CBD-CGD-O2D
12	B	815	CLA	CAD-CBD-CGD-O1D
12	g	841	CLA	CAD-CBD-CGD-O1D
12	g	841	CLA	CAD-CBD-CGD-O2D
12	E	805	CLA	CBD-CGD-O2D-CED
12	g	840	CLA	O1A-CGA-O2A-C1
12	E	835	CLA	C1A-C2A-CAA-CBA
12	E	835	CLA	C3A-C2A-CAA-CBA
12	e	806	CLA	C1A-C2A-CAA-CBA
12	e	806	CLA	C3A-C2A-CAA-CBA
12	G	825	CLA	CBD-CGD-O2D-CED
12	G	835	CLA	C1A-C2A-CAA-CBA
12	G	835	CLA	CBD-CGD-O2D-CED
12	e	831	CLA	C1A-C2A-CAA-CBA
12	e	831	CLA	C3A-C2A-CAA-CBA
12	e	831	CLA	CBD-CGD-O2D-CED
12	e	831	CLA	O1D-CGD-O2D-CED
12	a	818	CLA	C3A-C2A-CAA-CBA
12	a	803	CLA	CHA-CBD-CGD-O1D
12	a	803	CLA	CHA-CBD-CGD-O2D
12	G	808	CLA	C1A-C2A-CAA-CBA
12	G	808	CLA	C3A-C2A-CAA-CBA
12	G	808	CLA	CBD-CGD-O2D-CED
12	a	809	CLA	C1A-C2A-CAA-CBA
12	a	809	CLA	CBD-CGD-O2D-CED
12	A	836	CLA	C1A-C2A-CAA-CBA
12	A	836	CLA	C3A-C2A-CAA-CBA
12	A	836	CLA	CHA-CBD-CGD-O1D
12	A	836	CLA	CHA-CBD-CGD-O2D
12	B	828	CLA	CBD-CGD-O2D-CED
12	G	816	CLA	C1A-C2A-CAA-CBA
12	G	816	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	G	816	CLA	CBD-CGD-O2D-CED
12	B	835	CLA	C1A-C2A-CAA-CBA
12	B	835	CLA	CHA-CBD-CGD-O1D
12	B	835	CLA	CHA-CBD-CGD-O2D
12	B	835	CLA	CBD-CGD-O2D-CED
12	g	829	CLA	CBD-CGD-O2D-CED
12	k	1401	CLA	CBD-CGD-O2D-CED
12	b	815	CLA	C1A-C2A-CAA-CBA
12	b	815	CLA	C3A-C2A-CAA-CBA
12	b	815	CLA	CHA-CBD-CGD-O1D
12	b	815	CLA	CHA-CBD-CGD-O2D
12	b	815	CLA	CAD-CBD-CGD-O1D
12	b	815	CLA	CBD-CGD-O2D-CED
12	a	804	CLA	CBD-CGD-O2D-CED
12	a	823	CLA	CHA-CBD-CGD-O1D
12	a	823	CLA	CHA-CBD-CGD-O2D
12	a	823	CLA	CBD-CGD-O2D-CED
12	e	820	CLA	CBD-CGD-O2D-CED
12	b	833	CLA	C1A-C2A-CAA-CBA
12	b	833	CLA	CHA-CBD-CGD-O1D
12	b	833	CLA	CHA-CBD-CGD-O2D
12	b	833	CLA	CBD-CGD-O2D-CED
12	A	825	CLA	C1A-C2A-CAA-CBA
12	A	825	CLA	C3A-C2A-CAA-CBA
12	A	825	CLA	CBD-CGD-O2D-CED
12	B	821	CLA	C1A-C2A-CAA-CBA
12	B	821	CLA	C3A-C2A-CAA-CBA
12	g	826	CLA	C2A-CAA-CBA-CGA
12	g	826	CLA	CHA-CBD-CGD-O1D
12	g	826	CLA	CHA-CBD-CGD-O2D
12	g	839	CLA	CBD-CGD-O2D-CED
12	e	833	CLA	C1A-C2A-CAA-CBA
12	b	819	CLA	C1A-C2A-CAA-CBA
12	b	819	CLA	C3A-C2A-CAA-CBA
12	b	806	CLA	C1A-C2A-CAA-CBA
12	b	806	CLA	C3A-C2A-CAA-CBA
12	b	806	CLA	CBD-CGD-O2D-CED
12	G	829	CLA	C1A-C2A-CAA-CBA
12	G	829	CLA	C3A-C2A-CAA-CBA
12	G	829	CLA	CHA-CBD-CGD-O1D
12	G	829	CLA	CHA-CBD-CGD-O2D
12	G	829	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	G	829	CLA	O1D-CGD-O2D-CED
12	G	807	CLA	CBD-CGD-O2D-CED
12	b	811	CLA	C1A-C2A-CAA-CBA
12	b	811	CLA	C3A-C2A-CAA-CBA
12	a	821	CLA	CBD-CGD-O2D-CED
12	B	830	CLA	CBD-CGD-O2D-CED
12	G	840	CLA	CAD-CBD-CGD-O1D
12	G	840	CLA	CAD-CBD-CGD-O2D
12	b	835	CLA	C1A-C2A-CAA-CBA
12	b	835	CLA	C3A-C2A-CAA-CBA
12	b	835	CLA	CBD-CGD-O2D-CED
12	e	845	CLA	C1A-C2A-CAA-CBA
12	e	845	CLA	CHA-CBD-CGD-O1D
12	e	845	CLA	CHA-CBD-CGD-O2D
12	e	845	CLA	CBD-CGD-O2D-CED
12	g	810	CLA	C1A-C2A-CAA-CBA
12	g	810	CLA	C3A-C2A-CAA-CBA
12	g	810	CLA	CBD-CGD-O2D-CED
12	g	836	CLA	C1A-C2A-CAA-CBA
12	g	836	CLA	CBD-CGD-O2D-CED
12	E	804	CLA	CHA-CBD-CGD-O1D
12	E	804	CLA	CHA-CBD-CGD-O2D
12	E	801	CLA	CBD-CGD-O2D-CED
12	a	831	CLA	C1A-C2A-CAA-CBA
12	a	831	CLA	CBD-CGD-O2D-CED
12	a	831	CLA	O1D-CGD-O2D-CED
12	a	834	CLA	C1A-C2A-CAA-CBA
12	g	817	CLA	C1A-C2A-CAA-CBA
12	g	817	CLA	CBD-CGD-O2D-CED
12	g	817	CLA	O1D-CGD-O2D-CED
12	B	806	CLA	C1A-C2A-CAA-CBA
12	B	806	CLA	C3A-C2A-CAA-CBA
12	B	806	CLA	CBD-CGD-O2D-CED
12	o	1301	CLA	C1A-C2A-CAA-CBA
12	o	1301	CLA	CBD-CGD-O2D-CED
12	A	812	CLA	C1A-C2A-CAA-CBA
12	A	812	CLA	C3A-C2A-CAA-CBA
12	A	812	CLA	CHA-CBD-CGD-O1D
12	A	812	CLA	CHA-CBD-CGD-O2D
12	A	812	CLA	CAD-CBD-CGD-O1D
12	A	812	CLA	CBD-CGD-O2D-CED
12	e	801	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	L	202	CLA	C1A-C2A-CAA-CBA
12	L	202	CLA	CHA-CBD-CGD-O1D
12	L	202	CLA	CHA-CBD-CGD-O2D
12	G	837	CLA	C3A-C2A-CAA-CBA
12	G	837	CLA	CHA-CBD-CGD-O1D
12	G	837	CLA	CHA-CBD-CGD-O2D
12	G	837	CLA	CBD-CGD-O2D-CED
12	L	201	CLA	CHA-CBD-CGD-O1D
12	L	201	CLA	CHA-CBD-CGD-O2D
12	A	821	CLA	CHA-CBD-CGD-O1D
12	A	821	CLA	CHA-CBD-CGD-O2D
12	A	821	CLA	CBD-CGD-O2D-CED
12	O	1301	CLA	C1A-C2A-CAA-CBA
12	O	1301	CLA	CBD-CGD-O2D-CED
12	A	802	CLA	CBD-CGD-O2D-CED
12	B	805	CLA	C1A-C2A-CAA-CBA
12	E	829	CLA	CBD-CGD-O2D-CED
12	g	811	CLA	CHA-CBD-CGD-O1D
12	g	811	CLA	CHA-CBD-CGD-O2D
12	B	842	CLA	CAD-CBD-CGD-O1D
12	B	842	CLA	CAD-CBD-CGD-O2D
12	e	832	CLA	C1A-C2A-CAA-CBA
12	e	832	CLA	C3A-C2A-CAA-CBA
12	E	828	CLA	C1A-C2A-CAA-CBA
12	E	828	CLA	C3A-C2A-CAA-CBA
12	E	828	CLA	CBD-CGD-O2D-CED
12	b	805	CLA	CHA-CBD-CGD-O1D
12	b	805	CLA	CHA-CBD-CGD-O2D
12	b	805	CLA	CBD-CGD-O2D-CED
12	G	814	CLA	C1A-C2A-CAA-CBA
12	G	814	CLA	C3A-C2A-CAA-CBA
12	G	814	CLA	CHA-CBD-CGD-O1D
12	G	814	CLA	CHA-CBD-CGD-O2D
12	G	814	CLA	CAD-CBD-CGD-O1D
12	G	814	CLA	CBD-CGD-O2D-CED
12	e	839	CLA	CBD-CGD-O2D-CED
12	b	817	CLA	C1A-C2A-CAA-CBA
12	b	817	CLA	C3A-C2A-CAA-CBA
12	b	817	CLA	CBD-CGD-O2D-CED
12	g	823	CLA	C1A-C2A-CAA-CBA
12	g	823	CLA	C3A-C2A-CAA-CBA
12	g	823	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	g	823	CLA	CHA-CBD-CGD-O2D
12	a	840	CLA	CBD-CGD-O2D-CED
12	E	843	CLA	CBD-CGD-O2D-CED
12	G	812	CLA	CHA-CBD-CGD-O1D
12	G	812	CLA	CHA-CBD-CGD-O2D
12	G	812	CLA	CAD-CBD-CGD-O1D
12	G	818	CLA	C1A-C2A-CAA-CBA
12	G	818	CLA	C3A-C2A-CAA-CBA
12	B	807	CLA	CHA-CBD-CGD-O1D
12	B	807	CLA	CHA-CBD-CGD-O2D
12	B	807	CLA	CBD-CGD-O2D-CED
12	R	1401	CLA	CBD-CGD-O2D-CED
12	E	817	CLA	O1D-CGD-O2D-CED
12	e	815	CLA	O1D-CGD-O2D-CED
12	b	824	CLA	O1D-CGD-O2D-CED
12	e	808	CLA	O1D-CGD-O2D-CED
12	g	825	CLA	O1D-CGD-O2D-CED
12	G	810	CLA	O1D-CGD-O2D-CED
12	B	811	CLA	O1D-CGD-O2D-CED
12	G	804	CLA	O1D-CGD-O2D-CED
12	b	809	CLA	O1D-CGD-O2D-CED
12	E	825	CLA	O1D-CGD-O2D-CED
12	G	821	CLA	O1D-CGD-O2D-CED
12	G	823	CLA	O1D-CGD-O2D-CED
12	B	816	CLA	O1D-CGD-O2D-CED
12	a	816	CLA	O1D-CGD-O2D-CED
12	B	813	CLA	O1D-CGD-O2D-CED
12	G	832	CLA	O1D-CGD-O2D-CED
12	g	815	CLA	O1D-CGD-O2D-CED
12	A	807	CLA	O1D-CGD-O2D-CED
12	g	806	CLA	O1D-CGD-O2D-CED
12	B	824	CLA	O1D-CGD-O2D-CED
12	E	810	CLA	O1D-CGD-O2D-CED
12	A	822	CLA	O1D-CGD-O2D-CED
12	b	822	CLA	O1D-CGD-O2D-CED
12	B	826	CLA	O1D-CGD-O2D-CED
12	G	813	CLA	O1D-CGD-O2D-CED
12	b	814	CLA	O1D-CGD-O2D-CED
12	A	814	CLA	O1D-CGD-O2D-CED
12	g	812	CLA	O1D-CGD-O2D-CED
12	a	824	CLA	O1D-CGD-O2D-CED
12	G	808	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	a	809	CLA	O1D-CGD-O2D-CED
12	B	835	CLA	O1D-CGD-O2D-CED
12	b	833	CLA	O1D-CGD-O2D-CED
12	e	823	CLA	O1D-CGD-O2D-CED
12	b	811	CLA	O1D-CGD-O2D-CED
12	e	845	CLA	O1D-CGD-O2D-CED
12	g	810	CLA	O1D-CGD-O2D-CED
12	b	805	CLA	O1D-CGD-O2D-CED
12	g	823	CLA	O1D-CGD-O2D-CED
12	B	807	CLA	O1D-CGD-O2D-CED
12	A	801	CLA	O1D-CGD-O2D-CED
12	e	803	CLA	O1D-CGD-O2D-CED
12	s	204	CLA	O1D-CGD-O2D-CED
12	B	810	CLA	O1D-CGD-O2D-CED
12	l	204	CLA	O1D-CGD-O2D-CED
12	b	831	CLA	O1D-CGD-O2D-CED
12	G	834	CLA	O1D-CGD-O2D-CED
12	b	808	CLA	O1D-CGD-O2D-CED
12	g	835	CLA	O1D-CGD-O2D-CED
12	g	827	CLA	O1D-CGD-O2D-CED
12	S	1502	CLA	O1D-CGD-O2D-CED
12	G	838	CLA	O1D-CGD-O2D-CED
12	G	839	CLA	O1D-CGD-O2D-CED
12	g	813	CLA	O1D-CGD-O2D-CED
12	E	814	CLA	O1D-CGD-O2D-CED
12	g	809	CLA	O1D-CGD-O2D-CED
12	b	838	CLA	O1D-CGD-O2D-CED
12	g	816	CLA	O1D-CGD-O2D-CED
12	B	833	CLA	O1D-CGD-O2D-CED
12	B	839	CLA	O1D-CGD-O2D-CED
12	B	840	CLA	O1D-CGD-O2D-CED
12	g	832	CLA	O1D-CGD-O2D-CED
12	b	826	CLA	O1D-CGD-O2D-CED
12	B	817	CLA	O1D-CGD-O2D-CED
12	b	839	CLA	O1D-CGD-O2D-CED
12	G	830	CLA	O1D-CGD-O2D-CED
12	b	840	CLA	O1D-CGD-O2D-CED
12	L	204	CLA	O1D-CGD-O2D-CED
12	G	811	CLA	O1D-CGD-O2D-CED
12	B	814	CLA	O1D-CGD-O2D-CED
12	B	841	CLA	O1D-CGD-O2D-CED
12	a	801	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	g	838	CLA	O1D-CGD-O2D-CED
12	a	813	CLA	O1D-CGD-O2D-CED
12	b	828	CLA	O1D-CGD-O2D-CED
12	G	827	CLA	O1D-CGD-O2D-CED
12	J	1102	CLA	O1D-CGD-O2D-CED
12	b	812	CLA	O1D-CGD-O2D-CED
12	E	805	CLA	O1D-CGD-O2D-CED
12	g	840	CLA	O1D-CGD-O2D-CED
12	G	825	CLA	O1D-CGD-O2D-CED
12	B	828	CLA	O1D-CGD-O2D-CED
12	g	829	CLA	O1D-CGD-O2D-CED
12	b	815	CLA	O1D-CGD-O2D-CED
12	a	804	CLA	O1D-CGD-O2D-CED
12	g	839	CLA	O1D-CGD-O2D-CED
12	G	807	CLA	O1D-CGD-O2D-CED
12	B	830	CLA	O1D-CGD-O2D-CED
12	b	835	CLA	O1D-CGD-O2D-CED
12	E	801	CLA	O1D-CGD-O2D-CED
12	A	811	CLA	O1D-CGD-O2D-CED
12	e	801	CLA	O1D-CGD-O2D-CED
12	G	837	CLA	O1D-CGD-O2D-CED
12	A	802	CLA	O1D-CGD-O2D-CED
12	e	812	CLA	O1D-CGD-O2D-CED
12	G	814	CLA	O1D-CGD-O2D-CED
12	a	812	CLA	CBD-CGD-O2D-CED
12	A	834	CLA	CBD-CGD-O2D-CED
12	e	802	CLA	CBD-CGD-O2D-CED
12	J	1101	CLA	CBD-CGD-O2D-CED
12	e	807	CLA	CBD-CGD-O2D-CED
12	e	825	CLA	CBD-CGD-O2D-CED
12	b	829	CLA	CBD-CGD-O2D-CED
12	G	810	CLA	CBD-CGD-O2D-CED
12	E	809	CLA	CBD-CGD-O2D-CED
12	g	842	CLA	CBD-CGD-O2D-CED
12	A	806	CLA	CBD-CGD-O2D-CED
12	g	808	CLA	CBD-CGD-O2D-CED
12	E	825	CLA	CBD-CGD-O2D-CED
12	B	843	CLA	CBD-CGD-O2D-CED
12	G	839	CLA	CBD-CGD-O2D-CED
12	B	822	CLA	CBD-CGD-O2D-CED
12	G	821	CLA	CBD-CGD-O2D-CED
12	g	822	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	A	831	CLA	CBD-CGD-O2D-CED
12	E	814	CLA	CBD-CGD-O2D-CED
12	a	826	CLA	CBD-CGD-O2D-CED
12	l	202	CLA	CBD-CGD-O2D-CED
12	e	835	CLA	CBD-CGD-O2D-CED
12	a	825	CLA	CBD-CGD-O2D-CED
12	A	824	CLA	CBD-CGD-O2D-CED
12	B	809	CLA	CBD-CGD-O2D-CED
12	a	836	CLA	CBD-CGD-O2D-CED
12	B	813	CLA	CBD-CGD-O2D-CED
12	a	833	CLA	CBD-CGD-O2D-CED
12	E	838	CLA	CBD-CGD-O2D-CED
12	a	808	CLA	CBD-CGD-O2D-CED
12	G	828	CLA	CBD-CGD-O2D-CED
12	S	1501	CLA	CBD-CGD-O2D-CED
12	B	831	CLA	CBD-CGD-O2D-CED
12	G	801	CLA	CBD-CGD-O2D-CED
12	b	821	CLA	CBD-CGD-O2D-CED
12	B	803	CLA	CBD-CGD-O2D-CED
12	B	824	CLA	CBD-CGD-O2D-CED
12	b	840	CLA	CBD-CGD-O2D-CED
12	g	830	CLA	CBD-CGD-O2D-CED
12	g	803	CLA	CBD-CGD-O2D-CED
12	s	202	CLA	CBD-CGD-O2D-CED
12	B	841	CLA	CBD-CGD-O2D-CED
12	A	822	CLA	CBD-CGD-O2D-CED
12	b	822	CLA	CBD-CGD-O2D-CED
12	g	821	CLA	CBD-CGD-O2D-CED
12	e	824	CLA	CBD-CGD-O2D-CED
12	a	813	CLA	CBD-CGD-O2D-CED
12	G	820	CLA	CBD-CGD-O2D-CED
12	G	841	CLA	CBD-CGD-O2D-CED
12	b	842	CLA	CBD-CGD-O2D-CED
12	E	827	CLA	CBD-CGD-O2D-CED
12	g	812	CLA	CBD-CGD-O2D-CED
12	G	806	CLA	CBD-CGD-O2D-CED
12	A	810	CLA	CBD-CGD-O2D-CED
12	A	823	CLA	CBD-CGD-O2D-CED
12	B	823	CLA	CBD-CGD-O2D-CED
12	a	824	CLA	CBD-CGD-O2D-CED
12	E	826	CLA	CBD-CGD-O2D-CED
12	g	840	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	E	835	CLA	CBD-CGD-O2D-CED
12	a	803	CLA	CBD-CGD-O2D-CED
12	G	819	CLA	CBD-CGD-O2D-CED
12	e	823	CLA	CBD-CGD-O2D-CED
12	e	811	CLA	CBD-CGD-O2D-CED
12	b	811	CLA	CBD-CGD-O2D-CED
12	E	804	CLA	CBD-CGD-O2D-CED
12	A	811	CLA	CBD-CGD-O2D-CED
12	L	202	CLA	CBD-CGD-O2D-CED
12	b	820	CLA	CBD-CGD-O2D-CED
12	e	812	CLA	CBD-CGD-O2D-CED
12	e	832	CLA	CBD-CGD-O2D-CED
12	g	823	CLA	CBD-CGD-O2D-CED
12	b	807	CLA	CBD-CGD-O2D-CED
12	E	813	CLA	CBD-CGD-O2D-CED
12	b	802	CLA	CBD-CGD-O2D-CED
12	E	833	CLA	O1A-CGA-O2A-C1
12	e	807	CLA	O1A-CGA-O2A-C1
12	E	809	CLA	O1A-CGA-O2A-C1
12	b	801	CLA	O1A-CGA-O2A-C1
12	a	827	CLA	O1A-CGA-O2A-C1
12	A	806	CLA	O1A-CGA-O2A-C1
12	g	808	CLA	O1A-CGA-O2A-C1
12	B	802	CLA	O1A-CGA-O2A-C1
12	b	841	CLA	O1A-CGA-O2A-C1
12	B	809	CLA	O1A-CGA-O2A-C1
12	s	201	CLA	O1A-CGA-O2A-C1
12	a	808	CLA	O1A-CGA-O2A-C1
12	G	801	CLA	O1A-CGA-O2A-C1
12	B	803	CLA	O1A-CGA-O2A-C1
12	e	826	CLA	O1A-CGA-O2A-C1
12	g	803	CLA	O1A-CGA-O2A-C1
12	l	201	CLA	O1A-CGA-O2A-C1
12	b	828	CLA	O1A-CGA-O2A-C1
12	G	827	CLA	O1A-CGA-O2A-C1
12	G	806	CLA	O1A-CGA-O2A-C1
12	g	841	CLA	O1A-CGA-O2A-C1
12	g	802	CLA	O1A-CGA-O2A-C1
12	g	829	CLA	O1A-CGA-O2A-C1
12	A	825	CLA	O1A-CGA-O2A-C1
12	B	830	CLA	O1A-CGA-O2A-C1
12	G	840	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	L	201	CLA	O1A-CGA-O2A-C1
12	E	803	CLA	O1A-CGA-O2A-C1
12	B	842	CLA	O1A-CGA-O2A-C1
12	E	828	CLA	O1A-CGA-O2A-C1
12	b	807	CLA	O1A-CGA-O2A-C1
12	b	802	CLA	O1A-CGA-O2A-C1
12	a	827	CLA	O1D-CGD-O2D-CED
12	g	842	CLA	O1D-CGD-O2D-CED
12	b	804	CLA	O1D-CGD-O2D-CED
12	B	843	CLA	O1D-CGD-O2D-CED
12	A	831	CLA	O1D-CGD-O2D-CED
12	G	803	CLA	O1D-CGD-O2D-CED
12	g	805	CLA	O1D-CGD-O2D-CED
12	a	833	CLA	O1D-CGD-O2D-CED
12	b	836	CLA	O1D-CGD-O2D-CED
12	A	838	CLA	O1D-CGD-O2D-CED
12	G	801	CLA	O1D-CGD-O2D-CED
12	B	803	CLA	O1D-CGD-O2D-CED
12	e	826	CLA	O1D-CGD-O2D-CED
12	E	842	CLA	O1D-CGD-O2D-CED
12	g	803	CLA	O1D-CGD-O2D-CED
12	G	841	CLA	O1D-CGD-O2D-CED
12	b	842	CLA	O1D-CGD-O2D-CED
12	B	837	CLA	O1D-CGD-O2D-CED
12	E	835	CLA	O1D-CGD-O2D-CED
12	G	835	CLA	O1D-CGD-O2D-CED
12	A	825	CLA	O1D-CGD-O2D-CED
12	g	836	CLA	O1D-CGD-O2D-CED
12	B	806	CLA	O1D-CGD-O2D-CED
12	e	832	CLA	O1D-CGD-O2D-CED
12	E	828	CLA	O1D-CGD-O2D-CED
12	e	839	CLA	O1D-CGD-O2D-CED
12	a	840	CLA	O1D-CGD-O2D-CED
12	b	802	CLA	O1D-CGD-O2D-CED
12	a	812	CLA	O1D-CGD-O2D-CED
12	A	828	CLA	O1D-CGD-O2D-CED
12	e	802	CLA	O1D-CGD-O2D-CED
12	J	1101	CLA	O1D-CGD-O2D-CED
12	e	840	CLA	O1D-CGD-O2D-CED
12	e	825	CLA	O1D-CGD-O2D-CED
12	E	822	CLA	O1D-CGD-O2D-CED
12	a	814	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	A	819	CLA	O1D-CGD-O2D-CED
12	a	830	CLA	O1D-CGD-O2D-CED
12	b	827	CLA	O1D-CGD-O2D-CED
12	a	841	CLA	O1D-CGD-O2D-CED
12	a	826	CLA	O1D-CGD-O2D-CED
12	g	824	CLA	O1D-CGD-O2D-CED
12	A	824	CLA	O1D-CGD-O2D-CED
12	B	825	CLA	O1D-CGD-O2D-CED
12	G	826	CLA	O1D-CGD-O2D-CED
12	A	839	CLA	O1D-CGD-O2D-CED
12	G	822	CLA	O1D-CGD-O2D-CED
12	f	1301	CLA	O1D-CGD-O2D-CED
12	e	822	CLA	O1D-CGD-O2D-CED
12	B	829	CLA	O1D-CGD-O2D-CED
12	b	823	CLA	O1D-CGD-O2D-CED
12	e	813	CLA	O1D-CGD-O2D-CED
12	E	824	CLA	O1D-CGD-O2D-CED
12	E	831	CLA	O1D-CGD-O2D-CED
12	F	1301	CLA	O1D-CGD-O2D-CED
12	E	827	CLA	O1D-CGD-O2D-CED
12	E	815	CLA	O1D-CGD-O2D-CED
12	g	828	CLA	O1D-CGD-O2D-CED
12	A	810	CLA	O1D-CGD-O2D-CED
12	a	803	CLA	O1D-CGD-O2D-CED
12	a	823	CLA	O1D-CGD-O2D-CED
12	e	820	CLA	O1D-CGD-O2D-CED
12	e	811	CLA	O1D-CGD-O2D-CED
12	a	821	CLA	O1D-CGD-O2D-CED
12	E	804	CLA	O1D-CGD-O2D-CED
12	o	1301	CLA	O1D-CGD-O2D-CED
12	A	812	CLA	O1D-CGD-O2D-CED
12	A	821	CLA	O1D-CGD-O2D-CED
12	O	1301	CLA	O1D-CGD-O2D-CED
12	E	813	CLA	O1D-CGD-O2D-CED
12	E	843	CLA	O1D-CGD-O2D-CED
12	e	807	CLA	CBA-CGA-O2A-C1
12	E	809	CLA	CBA-CGA-O2A-C1
12	b	801	CLA	CBA-CGA-O2A-C1
12	a	827	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	CBA-CGA-O2A-C1
12	E	825	CLA	CBA-CGA-O2A-C1
12	B	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	b	841	CLA	CBA-CGA-O2A-C1
12	a	808	CLA	CBA-CGA-O2A-C1
12	G	801	CLA	CBA-CGA-O2A-C1
12	B	803	CLA	CBA-CGA-O2A-C1
12	e	826	CLA	CBA-CGA-O2A-C1
12	g	803	CLA	CBA-CGA-O2A-C1
12	A	822	CLA	CBA-CGA-O2A-C1
12	b	828	CLA	CBA-CGA-O2A-C1
12	G	827	CLA	CBA-CGA-O2A-C1
12	a	824	CLA	CBA-CGA-O2A-C1
12	g	841	CLA	CBA-CGA-O2A-C1
12	g	802	CLA	CBA-CGA-O2A-C1
12	g	829	CLA	CBA-CGA-O2A-C1
12	A	825	CLA	CBA-CGA-O2A-C1
12	e	823	CLA	CBA-CGA-O2A-C1
12	B	830	CLA	CBA-CGA-O2A-C1
12	G	840	CLA	CBA-CGA-O2A-C1
12	E	803	CLA	CBA-CGA-O2A-C1
12	B	842	CLA	CBA-CGA-O2A-C1
12	E	828	CLA	CBA-CGA-O2A-C1
12	b	802	CLA	CBA-CGA-O2A-C1
12	e	810	CLA	CBD-CGD-O2D-CED
12	a	817	CLA	CBD-CGD-O2D-CED
12	g	820	CLA	CBD-CGD-O2D-CED
12	G	802	CLA	CBD-CGD-O2D-CED
12	A	803	CLA	CBD-CGD-O2D-CED
12	e	816	CLA	CBD-CGD-O2D-CED
12	a	829	CLA	CBD-CGD-O2D-CED
12	A	815	CLA	CBD-CGD-O2D-CED
12	g	834	CLA	CBD-CGD-O2D-CED
12	A	827	CLA	CBD-CGD-O2D-CED
12	E	830	CLA	CBD-CGD-O2D-CED
12	E	812	CLA	CBD-CGD-O2D-CED
12	a	807	CLA	CBD-CGD-O2D-CED
12	G	833	CLA	CBD-CGD-O2D-CED
12	a	811	CLA	CBD-CGD-O2D-CED
12	a	822	CLA	CBD-CGD-O2D-CED
12	a	815	CLA	CBD-CGD-O2D-CED
12	e	842	CLA	CBD-CGD-O2D-CED
12	A	809	CLA	CBD-CGD-O2D-CED
12	e	804	CLA	CBD-CGD-O2D-CED
12	b	825	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	b	834	CLA	CBD-CGD-O2D-CED
12	E	808	CLA	CBD-CGD-O2D-CED
12	A	805	CLA	CBD-CGD-O2D-CED
12	E	823	CLA	CBD-CGD-O2D-CED
12	G	824	CLA	CBD-CGD-O2D-CED
12	A	813	CLA	CBD-CGD-O2D-CED
12	B	801	CLA	CBD-CGD-O2D-CED
12	e	828	CLA	CBD-CGD-O2D-CED
12	B	827	CLA	CBD-CGD-O2D-CED
12	g	801	CLA	CBD-CGD-O2D-CED
12	A	820	CLA	CBD-CGD-O2D-CED
12	e	821	CLA	CBD-CGD-O2D-CED
12	e	844	CLA	CBD-CGD-O2D-CED
12	a	802	CLA	CBD-CGD-O2D-CED
12	b	803	CLA	CBD-CGD-O2D-CED
12	a	805	CLA	CBD-CGD-O2D-CED
12	e	806	CLA	CBD-CGD-O2D-CED
12	e	814	CLA	CBD-CGD-O2D-CED
12	E	818	CLA	CBD-CGD-O2D-CED
12	E	806	CLA	CBD-CGD-O2D-CED
12	B	821	CLA	CBD-CGD-O2D-CED
12	g	826	CLA	CBD-CGD-O2D-CED
12	b	819	CLA	CBD-CGD-O2D-CED
12	B	836	CLA	CBD-CGD-O2D-CED
12	E	816	CLA	CBD-CGD-O2D-CED
12	B	805	CLA	CBD-CGD-O2D-CED
12	G	818	CLA	CBD-CGD-O2D-CED
12	E	802	CLA	CBD-CGD-O2D-CED
12	A	801	CLA	O1A-CGA-O2A-C1
12	A	834	CLA	O1A-CGA-O2A-C1
12	e	802	CLA	O1A-CGA-O2A-C1
12	J	1101	CLA	O1A-CGA-O2A-C1
12	A	803	CLA	O1A-CGA-O2A-C1
12	b	829	CLA	O1A-CGA-O2A-C1
12	a	829	CLA	O1A-CGA-O2A-C1
12	E	825	CLA	O1A-CGA-O2A-C1
12	A	827	CLA	O1A-CGA-O2A-C1
12	E	830	CLA	O1A-CGA-O2A-C1
12	B	822	CLA	O1A-CGA-O2A-C1
12	a	807	CLA	O1A-CGA-O2A-C1
12	g	822	CLA	O1A-CGA-O2A-C1
12	G	815	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	e	835	CLA	O1A-CGA-O2A-C1
12	a	822	CLA	O1A-CGA-O2A-C1
12	A	818	CLA	O1A-CGA-O2A-C1
12	a	836	CLA	O1A-CGA-O2A-C1
12	g	816	CLA	O1A-CGA-O2A-C1
12	E	838	CLA	O1A-CGA-O2A-C1
12	G	832	CLA	O1A-CGA-O2A-C1
12	e	804	CLA	O1A-CGA-O2A-C1
12	G	828	CLA	O1A-CGA-O2A-C1
12	B	831	CLA	O1A-CGA-O2A-C1
12	b	821	CLA	O1A-CGA-O2A-C1
12	E	808	CLA	O1A-CGA-O2A-C1
12	A	805	CLA	O1A-CGA-O2A-C1
12	B	817	CLA	O1A-CGA-O2A-C1
12	E	823	CLA	O1A-CGA-O2A-C1
12	g	830	CLA	O1A-CGA-O2A-C1
12	A	822	CLA	O1A-CGA-O2A-C1
12	g	821	CLA	O1A-CGA-O2A-C1
12	a	801	CLA	O1A-CGA-O2A-C1
12	e	828	CLA	O1A-CGA-O2A-C1
12	b	816	CLA	O1A-CGA-O2A-C1
12	G	820	CLA	O1A-CGA-O2A-C1
12	A	820	CLA	O1A-CGA-O2A-C1
12	e	821	CLA	O1A-CGA-O2A-C1
12	a	820	CLA	O1A-CGA-O2A-C1
12	B	818	CLA	O1A-CGA-O2A-C1
12	E	821	CLA	O1A-CGA-O2A-C1
12	B	823	CLA	O1A-CGA-O2A-C1
12	a	824	CLA	O1A-CGA-O2A-C1
12	a	805	CLA	O1A-CGA-O2A-C1
12	e	806	CLA	O1A-CGA-O2A-C1
12	a	803	CLA	O1A-CGA-O2A-C1
12	B	835	CLA	O1A-CGA-O2A-C1
12	G	819	CLA	O1A-CGA-O2A-C1
12	E	806	CLA	O1A-CGA-O2A-C1
12	b	815	CLA	O1A-CGA-O2A-C1
12	b	833	CLA	O1A-CGA-O2A-C1
12	e	823	CLA	O1A-CGA-O2A-C1
12	e	845	CLA	O1A-CGA-O2A-C1
12	E	804	CLA	O1A-CGA-O2A-C1
12	E	801	CLA	O1A-CGA-O2A-C1
12	g	817	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	e	819	CLA	O1A-CGA-O2A-C1
12	e	801	CLA	O1A-CGA-O2A-C1
12	b	820	CLA	O1A-CGA-O2A-C1
12	G	814	CLA	O1A-CGA-O2A-C1
12	B	819	CLA	O1D-CGD-O2D-CED
12	e	827	CLA	O1D-CGD-O2D-CED
12	B	808	CLA	O1D-CGD-O2D-CED
12	A	826	CLA	O1D-CGD-O2D-CED
12	g	807	CLA	O1D-CGD-O2D-CED
12	G	805	CLA	O1D-CGD-O2D-CED
12	a	828	CLA	O1D-CGD-O2D-CED
12	e	829	CLA	O1D-CGD-O2D-CED
12	g	818	CLA	O1D-CGD-O2D-CED
12	G	816	CLA	O1D-CGD-O2D-CED
12	b	806	CLA	O1D-CGD-O2D-CED
12	E	829	CLA	O1D-CGD-O2D-CED
12	b	817	CLA	O1D-CGD-O2D-CED
12	r	1401	CLA	O1D-CGD-O2D-CED
12	K	1401	CLA	O1D-CGD-O2D-CED
12	k	1401	CLA	O1D-CGD-O2D-CED
12	R	1401	CLA	O1D-CGD-O2D-CED
12	g	833	CLA	CBD-CGD-O2D-CED
12	B	834	CLA	CBD-CGD-O2D-CED
12	b	832	CLA	CBD-CGD-O2D-CED
12	G	831	CLA	CBD-CGD-O2D-CED
12	A	834	CLA	CBA-CGA-O2A-C1
12	E	833	CLA	CBA-CGA-O2A-C1
12	A	803	CLA	CBA-CGA-O2A-C1
12	g	808	CLA	CBA-CGA-O2A-C1
12	G	839	CLA	CBA-CGA-O2A-C1
12	B	822	CLA	CBA-CGA-O2A-C1
12	g	822	CLA	CBA-CGA-O2A-C1
12	G	815	CLA	CBA-CGA-O2A-C1
12	e	835	CLA	CBA-CGA-O2A-C1
12	A	818	CLA	CBA-CGA-O2A-C1
12	B	809	CLA	CBA-CGA-O2A-C1
12	a	836	CLA	CBA-CGA-O2A-C1
12	g	816	CLA	CBA-CGA-O2A-C1
12	E	838	CLA	CBA-CGA-O2A-C1
12	s	201	CLA	CBA-CGA-O2A-C1
12	e	804	CLA	CBA-CGA-O2A-C1
12	b	821	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	B	817	CLA	CBA-CGA-O2A-C1
12	b	840	CLA	CBA-CGA-O2A-C1
12	B	841	CLA	CBA-CGA-O2A-C1
12	g	821	CLA	CBA-CGA-O2A-C1
12	l	201	CLA	CBA-CGA-O2A-C1
12	b	816	CLA	CBA-CGA-O2A-C1
12	G	820	CLA	CBA-CGA-O2A-C1
12	a	820	CLA	CBA-CGA-O2A-C1
12	B	818	CLA	CBA-CGA-O2A-C1
12	E	821	CLA	CBA-CGA-O2A-C1
12	G	806	CLA	CBA-CGA-O2A-C1
12	B	823	CLA	CBA-CGA-O2A-C1
12	g	840	CLA	CBA-CGA-O2A-C1
12	a	805	CLA	CBA-CGA-O2A-C1
12	G	819	CLA	CBA-CGA-O2A-C1
12	E	806	CLA	CBA-CGA-O2A-C1
12	b	815	CLA	CBA-CGA-O2A-C1
12	g	817	CLA	CBA-CGA-O2A-C1
12	e	819	CLA	CBA-CGA-O2A-C1
12	L	201	CLA	CBA-CGA-O2A-C1
12	b	820	CLA	CBA-CGA-O2A-C1
12	G	814	CLA	CBA-CGA-O2A-C1
12	b	807	CLA	CBA-CGA-O2A-C1
12	A	841	CLA	CBD-CGD-O2D-CED
12	E	820	CLA	O1A-CGA-O2A-C1
12	a	819	CLA	O1A-CGA-O2A-C1
12	e	818	CLA	O1A-CGA-O2A-C1
12	A	817	CLA	O1A-CGA-O2A-C1
12	g	827	CLA	C2A-CAA-CBA-CGA
12	b	826	CLA	C2A-CAA-CBA-CGA
12	G	825	CLA	C2A-CAA-CBA-CGA
12	B	828	CLA	C2A-CAA-CBA-CGA
12	G	809	CLA	CBD-CGD-O2D-CED
12	b	810	CLA	CBD-CGD-O2D-CED
12	B	812	CLA	CBD-CGD-O2D-CED
12	A	832	CLA	CBD-CGD-O2D-CED
12	E	836	CLA	CBD-CGD-O2D-CED
12	e	833	CLA	CBD-CGD-O2D-CED
12	a	834	CLA	CBD-CGD-O2D-CED
12	g	811	CLA	CBD-CGD-O2D-CED
12	A	801	CLA	CBA-CGA-O2A-C1
12	e	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	J	1101	CLA	CBA-CGA-O2A-C1
12	b	829	CLA	CBA-CGA-O2A-C1
12	a	829	CLA	CBA-CGA-O2A-C1
12	G	834	CLA	CBA-CGA-O2A-C1
12	g	835	CLA	CBA-CGA-O2A-C1
12	A	827	CLA	CBA-CGA-O2A-C1
12	E	830	CLA	CBA-CGA-O2A-C1
12	a	807	CLA	CBA-CGA-O2A-C1
12	a	822	CLA	CBA-CGA-O2A-C1
12	G	832	CLA	CBA-CGA-O2A-C1
12	G	828	CLA	CBA-CGA-O2A-C1
12	B	831	CLA	CBA-CGA-O2A-C1
12	E	808	CLA	CBA-CGA-O2A-C1
12	A	805	CLA	CBA-CGA-O2A-C1
12	E	823	CLA	CBA-CGA-O2A-C1
12	g	830	CLA	CBA-CGA-O2A-C1
12	a	801	CLA	CBA-CGA-O2A-C1
12	e	828	CLA	CBA-CGA-O2A-C1
12	A	820	CLA	CBA-CGA-O2A-C1
12	e	821	CLA	CBA-CGA-O2A-C1
12	J	1102	CLA	CBA-CGA-O2A-C1
12	e	806	CLA	CBA-CGA-O2A-C1
12	a	803	CLA	CBA-CGA-O2A-C1
12	B	835	CLA	CBA-CGA-O2A-C1
12	b	833	CLA	CBA-CGA-O2A-C1
12	b	835	CLA	CBA-CGA-O2A-C1
12	e	845	CLA	CBA-CGA-O2A-C1
12	E	804	CLA	CBA-CGA-O2A-C1
12	E	801	CLA	CBA-CGA-O2A-C1
12	e	801	CLA	CBA-CGA-O2A-C1
12	b	829	CLA	O1D-CGD-O2D-CED
12	G	828	CLA	O1D-CGD-O2D-CED
12	B	831	CLA	O1D-CGD-O2D-CED
12	g	830	CLA	O1D-CGD-O2D-CED
12	E	840	CLA	CBD-CGD-O2D-CED
12	a	835	CLA	CBD-CGD-O2D-CED
12	e	837	CLA	CBD-CGD-O2D-CED
12	a	838	CLA	CBD-CGD-O2D-CED
12	e	834	CLA	CBD-CGD-O2D-CED
12	A	836	CLA	CBD-CGD-O2D-CED
12	E	837	CLA	CBD-CGD-O2D-CED
12	A	833	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	e	810	CLA	O1A-CGA-O2A-C1
12	G	834	CLA	O1A-CGA-O2A-C1
12	g	835	CLA	O1A-CGA-O2A-C1
12	E	812	CLA	O1A-CGA-O2A-C1
12	a	811	CLA	O1A-CGA-O2A-C1
12	A	809	CLA	O1A-CGA-O2A-C1
12	J	1102	CLA	O1A-CGA-O2A-C1
12	b	835	CLA	O1A-CGA-O2A-C1
12	e	809	CLA	CBD-CGD-O2D-CED
12	E	811	CLA	CBD-CGD-O2D-CED
12	A	808	CLA	CBD-CGD-O2D-CED
12	a	810	CLA	CBD-CGD-O2D-CED
12	A	834	CLA	O1D-CGD-O2D-CED
12	g	822	CLA	O1D-CGD-O2D-CED
12	e	835	CLA	O1D-CGD-O2D-CED
12	a	836	CLA	O1D-CGD-O2D-CED
12	E	838	CLA	O1D-CGD-O2D-CED
12	b	821	CLA	O1D-CGD-O2D-CED
12	G	820	CLA	O1D-CGD-O2D-CED
12	B	823	CLA	O1D-CGD-O2D-CED
12	e	803	CLA	CBA-CGA-O2A-C1
12	E	820	CLA	CBA-CGA-O2A-C1
12	a	819	CLA	CBA-CGA-O2A-C1
12	e	818	CLA	CBA-CGA-O2A-C1
12	A	817	CLA	CBA-CGA-O2A-C1
12	E	805	CLA	CBA-CGA-O2A-C1
12	a	804	CLA	CBA-CGA-O2A-C1
12	A	802	CLA	CBA-CGA-O2A-C1
12	e	807	CLA	O1D-CGD-O2D-CED
12	E	809	CLA	O1D-CGD-O2D-CED
12	A	806	CLA	O1D-CGD-O2D-CED
12	a	808	CLA	O1D-CGD-O2D-CED
12	a	825	CLA	O1D-CGD-O2D-CED
12	e	824	CLA	O1D-CGD-O2D-CED
12	A	823	CLA	O1D-CGD-O2D-CED
12	E	826	CLA	O1D-CGD-O2D-CED
12	g	808	CLA	O1D-CGD-O2D-CED
12	B	809	CLA	O1D-CGD-O2D-CED
12	G	806	CLA	O1D-CGD-O2D-CED
12	b	807	CLA	O1D-CGD-O2D-CED
12	B	822	CLA	O1D-CGD-O2D-CED
12	l	202	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	S	1501	CLA	O1D-CGD-O2D-CED
12	s	202	CLA	O1D-CGD-O2D-CED
12	g	821	CLA	O1D-CGD-O2D-CED
12	G	819	CLA	O1D-CGD-O2D-CED
12	L	202	CLA	O1D-CGD-O2D-CED
12	b	820	CLA	O1D-CGD-O2D-CED
12	e	810	CLA	CBA-CGA-O2A-C1
12	E	812	CLA	CBA-CGA-O2A-C1
12	a	811	CLA	CBA-CGA-O2A-C1
12	A	809	CLA	CBA-CGA-O2A-C1
12	e	803	CLA	O1A-CGA-O2A-C1
12	E	805	CLA	O1A-CGA-O2A-C1
12	a	804	CLA	O1A-CGA-O2A-C1
12	A	802	CLA	O1A-CGA-O2A-C1
12	g	820	CLA	C2A-CAA-CBA-CGA
12	B	821	CLA	C2A-CAA-CBA-CGA
12	b	819	CLA	C2A-CAA-CBA-CGA
12	G	818	CLA	C2A-CAA-CBA-CGA
12	e	810	CLA	O1D-CGD-O2D-CED
12	E	812	CLA	O1D-CGD-O2D-CED
12	a	811	CLA	O1D-CGD-O2D-CED
12	a	822	CLA	O1D-CGD-O2D-CED
12	a	815	CLA	O1D-CGD-O2D-CED
12	A	809	CLA	O1D-CGD-O2D-CED
12	E	823	CLA	O1D-CGD-O2D-CED
12	A	813	CLA	O1D-CGD-O2D-CED
12	A	820	CLA	O1D-CGD-O2D-CED
12	e	821	CLA	O1D-CGD-O2D-CED
12	e	814	CLA	O1D-CGD-O2D-CED
12	E	816	CLA	O1D-CGD-O2D-CED
12	E	832	CLA	CBA-CGA-O2A-C1
12	e	830	CLA	CBA-CGA-O2A-C1
12	A	829	CLA	CBA-CGA-O2A-C1
12	a	831	CLA	CBA-CGA-O2A-C1
13	g	843	PQN	C25-C26-C27-C28
13	B	844	PQN	C25-C26-C27-C28
13	G	842	PQN	C25-C26-C27-C28
13	b	843	PQN	C25-C26-C27-C28
12	a	807	CLA	O1D-CGD-O2D-CED
12	E	808	CLA	O1D-CGD-O2D-CED
12	A	805	CLA	O1D-CGD-O2D-CED
12	g	801	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	e	806	CLA	O1D-CGD-O2D-CED
12	e	836	CLA	CBD-CGD-O2D-CED
12	A	835	CLA	CBD-CGD-O2D-CED
12	a	837	CLA	CBD-CGD-O2D-CED
12	E	839	CLA	CBD-CGD-O2D-CED
12	g	834	CLA	O1D-CGD-O2D-CED
12	G	833	CLA	O1D-CGD-O2D-CED
12	b	834	CLA	O1D-CGD-O2D-CED
12	B	801	CLA	O1D-CGD-O2D-CED
12	a	802	CLA	O1D-CGD-O2D-CED
12	B	836	CLA	O1D-CGD-O2D-CED
12	E	802	CLA	O1D-CGD-O2D-CED
12	b	827	CLA	CBA-CGA-O2A-C1
12	G	826	CLA	CBA-CGA-O2A-C1
12	B	829	CLA	CBA-CGA-O2A-C1
12	g	828	CLA	CBA-CGA-O2A-C1
12	a	835	CLA	C2A-CAA-CBA-CGA
12	e	834	CLA	C2A-CAA-CBA-CGA
12	E	837	CLA	C2A-CAA-CBA-CGA
12	A	833	CLA	C2A-CAA-CBA-CGA
12	e	838	CLA	CBA-CGA-O2A-C1
12	b	831	CLA	CBA-CGA-O2A-C1
12	G	810	CLA	CBA-CGA-O2A-C1
12	g	842	CLA	CBA-CGA-O2A-C1
12	B	820	CLA	CBA-CGA-O2A-C1
12	e	827	CLA	CBA-CGA-O2A-C1
12	g	834	CLA	CBA-CGA-O2A-C1
12	B	843	CLA	CBA-CGA-O2A-C1
12	B	808	CLA	CBA-CGA-O2A-C1
12	g	819	CLA	CBA-CGA-O2A-C1
12	b	818	CLA	CBA-CGA-O2A-C1
12	A	826	CLA	CBA-CGA-O2A-C1
12	g	807	CLA	CBA-CGA-O2A-C1
12	G	833	CLA	CBA-CGA-O2A-C1
12	E	841	CLA	CBA-CGA-O2A-C1
12	B	813	CLA	CBA-CGA-O2A-C1
12	B	833	CLA	CBA-CGA-O2A-C1
12	A	837	CLA	CBA-CGA-O2A-C1
12	G	805	CLA	CBA-CGA-O2A-C1
12	e	822	CLA	CBA-CGA-O2A-C1
12	g	832	CLA	CBA-CGA-O2A-C1
12	a	828	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	b	834	CLA	CBA-CGA-O2A-C1
12	E	824	CLA	CBA-CGA-O2A-C1
12	G	830	CLA	CBA-CGA-O2A-C1
12	G	841	CLA	CBA-CGA-O2A-C1
12	b	842	CLA	CBA-CGA-O2A-C1
12	G	817	CLA	CBA-CGA-O2A-C1
12	g	812	CLA	CBA-CGA-O2A-C1
12	a	823	CLA	CBA-CGA-O2A-C1
12	b	806	CLA	CBA-CGA-O2A-C1
12	b	811	CLA	CBA-CGA-O2A-C1
12	a	839	CLA	CBA-CGA-O2A-C1
12	B	836	CLA	CBA-CGA-O2A-C1
12	A	821	CLA	CBA-CGA-O2A-C1
12	E	829	CLA	CBA-CGA-O2A-C1
12	A	803	CLA	O1D-CGD-O2D-CED
12	e	842	CLA	O1D-CGD-O2D-CED
12	e	804	CLA	O1D-CGD-O2D-CED
12	a	805	CLA	O1D-CGD-O2D-CED
12	E	806	CLA	O1D-CGD-O2D-CED
13	a	844	PQN	C16-C17-C18-C19
13	E	846	PQN	C16-C17-C18-C19
13	A	842	PQN	C16-C17-C18-C19
13	g	843	PQN	C18-C20-C21-C22
13	B	844	PQN	C18-C20-C21-C22
13	G	842	PQN	C18-C20-C21-C22
13	b	843	PQN	C18-C20-C21-C22
12	A	838	CLA	C2A-CAA-CBA-CGA
12	E	842	CLA	C2A-CAA-CBA-CGA
12	e	839	CLA	C2A-CAA-CBA-CGA
12	a	840	CLA	C2A-CAA-CBA-CGA
12	b	825	CLA	O1D-CGD-O2D-CED
12	G	824	CLA	O1D-CGD-O2D-CED
12	B	827	CLA	O1D-CGD-O2D-CED
12	g	826	CLA	O1D-CGD-O2D-CED
12	a	817	CLA	O1D-CGD-O2D-CED
12	G	802	CLA	O1D-CGD-O2D-CED
12	e	816	CLA	O1D-CGD-O2D-CED
12	A	815	CLA	O1D-CGD-O2D-CED
12	E	818	CLA	O1D-CGD-O2D-CED
12	B	805	CLA	O1D-CGD-O2D-CED
12	B	820	CLA	O1A-CGA-O2A-C1
12	g	834	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	g	819	CLA	O1A-CGA-O2A-C1
12	b	818	CLA	O1A-CGA-O2A-C1
12	G	833	CLA	O1A-CGA-O2A-C1
12	b	834	CLA	O1A-CGA-O2A-C1
12	G	817	CLA	O1A-CGA-O2A-C1
12	B	836	CLA	O1A-CGA-O2A-C1
12	e	844	CLA	O1D-CGD-O2D-CED
12	b	803	CLA	O1D-CGD-O2D-CED
12	a	829	CLA	O1D-CGD-O2D-CED
12	A	827	CLA	O1D-CGD-O2D-CED
12	E	830	CLA	O1D-CGD-O2D-CED
12	e	828	CLA	O1D-CGD-O2D-CED
12	G	810	CLA	O1A-CGA-O2A-C1
12	e	827	CLA	O1A-CGA-O2A-C1
12	A	826	CLA	O1A-CGA-O2A-C1
12	B	813	CLA	O1A-CGA-O2A-C1
12	a	828	CLA	O1A-CGA-O2A-C1
12	g	812	CLA	O1A-CGA-O2A-C1
12	b	811	CLA	O1A-CGA-O2A-C1
12	E	829	CLA	O1A-CGA-O2A-C1
13	e	843	PQN	C13-C15-C16-C17
12	s	203	CLA	CBD-CGD-O2D-CED
12	l	203	CLA	CBD-CGD-O2D-CED
12	L	203	CLA	CBD-CGD-O2D-CED
12	g	820	CLA	O1D-CGD-O2D-CED
12	B	821	CLA	O1D-CGD-O2D-CED
12	b	819	CLA	O1D-CGD-O2D-CED
12	G	818	CLA	O1D-CGD-O2D-CED
12	b	841	CLA	C2A-CAA-CBA-CGA
12	g	841	CLA	C2A-CAA-CBA-CGA
12	G	840	CLA	C2A-CAA-CBA-CGA
12	B	842	CLA	C2A-CAA-CBA-CGA
12	A	841	CLA	C2A-CAA-CBA-CGA
12	e	838	CLA	O1A-CGA-O2A-C1
12	b	831	CLA	O1A-CGA-O2A-C1
12	E	841	CLA	O1A-CGA-O2A-C1
12	B	833	CLA	O1A-CGA-O2A-C1
12	A	837	CLA	O1A-CGA-O2A-C1
12	g	832	CLA	O1A-CGA-O2A-C1
12	G	830	CLA	O1A-CGA-O2A-C1
12	a	839	CLA	O1A-CGA-O2A-C1
12	G	843	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	E	846	PQN	C15-C16-C17-C18
12	g	842	CLA	O1A-CGA-O2A-C1
12	B	843	CLA	O1A-CGA-O2A-C1
12	B	808	CLA	O1A-CGA-O2A-C1
12	e	822	CLA	O1A-CGA-O2A-C1
12	E	824	CLA	O1A-CGA-O2A-C1
12	G	841	CLA	O1A-CGA-O2A-C1
12	b	842	CLA	O1A-CGA-O2A-C1
12	a	823	CLA	O1A-CGA-O2A-C1
12	b	806	CLA	O1A-CGA-O2A-C1
12	A	821	CLA	O1A-CGA-O2A-C1
12	A	841	CLA	O1D-CGD-O2D-CED
12	g	833	CLA	O1D-CGD-O2D-CED
12	B	834	CLA	O1D-CGD-O2D-CED
12	b	832	CLA	O1D-CGD-O2D-CED
12	G	831	CLA	O1D-CGD-O2D-CED
12	E	832	CLA	O1A-CGA-O2A-C1
12	g	807	CLA	O1A-CGA-O2A-C1
12	e	830	CLA	O1A-CGA-O2A-C1
12	A	829	CLA	O1A-CGA-O2A-C1
12	G	805	CLA	O1A-CGA-O2A-C1
12	a	831	CLA	O1A-CGA-O2A-C1
13	a	844	PQN	C15-C16-C17-C18
13	A	842	PQN	C15-C16-C17-C18
12	G	802	CLA	CBA-CGA-O2A-C1
12	A	831	CLA	CBA-CGA-O2A-C1
12	a	833	CLA	CBA-CGA-O2A-C1
12	e	844	CLA	CBA-CGA-O2A-C1
12	b	803	CLA	CBA-CGA-O2A-C1
12	E	835	CLA	CBA-CGA-O2A-C1
12	B	805	CLA	CBA-CGA-O2A-C1
12	e	832	CLA	CBA-CGA-O2A-C1
12	G	834	CLA	C2A-CAA-CBA-CGA
12	e	827	CLA	C2A-CAA-CBA-CGA
12	g	835	CLA	C2A-CAA-CBA-CGA
12	g	822	CLA	C2A-CAA-CBA-CGA
12	A	826	CLA	C2A-CAA-CBA-CGA
12	e	842	CLA	C2A-CAA-CBA-CGA
12	a	828	CLA	C2A-CAA-CBA-CGA
12	b	821	CLA	C2A-CAA-CBA-CGA
12	G	820	CLA	C2A-CAA-CBA-CGA
12	J	1102	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	B	823	CLA	C2A-CAA-CBA-CGA
12	b	835	CLA	C2A-CAA-CBA-CGA
12	E	829	CLA	C2A-CAA-CBA-CGA
12	b	841	CLA	CBD-CGD-O2D-CED
12	g	841	CLA	CBD-CGD-O2D-CED
12	G	840	CLA	CBD-CGD-O2D-CED
12	B	842	CLA	CBD-CGD-O2D-CED
12	g	824	CLA	C2A-CAA-CBA-CGA
12	B	825	CLA	C2A-CAA-CBA-CGA
12	G	822	CLA	C2A-CAA-CBA-CGA
12	b	823	CLA	C2A-CAA-CBA-CGA
12	g	820	CLA	CBA-CGA-O2A-C1
12	B	821	CLA	CBA-CGA-O2A-C1
12	b	819	CLA	CBA-CGA-O2A-C1
12	G	818	CLA	CBA-CGA-O2A-C1
12	a	835	CLA	O1D-CGD-O2D-CED
12	A	832	CLA	O1D-CGD-O2D-CED
12	E	836	CLA	O1D-CGD-O2D-CED
12	e	833	CLA	O1D-CGD-O2D-CED
12	A	833	CLA	O1D-CGD-O2D-CED
12	a	834	CLA	O1D-CGD-O2D-CED
12	G	809	CLA	O1D-CGD-O2D-CED
12	b	810	CLA	O1D-CGD-O2D-CED
12	B	812	CLA	O1D-CGD-O2D-CED
12	e	834	CLA	O1D-CGD-O2D-CED
12	E	837	CLA	O1D-CGD-O2D-CED
12	g	811	CLA	O1D-CGD-O2D-CED
13	a	844	PQN	C26-C27-C28-C30
13	E	846	PQN	C26-C27-C28-C30
12	s	204	CLA	CBA-CGA-O2A-C1
12	l	204	CLA	CBA-CGA-O2A-C1
12	S	1502	CLA	CBA-CGA-O2A-C1
12	L	204	CLA	CBA-CGA-O2A-C1
13	A	842	PQN	C26-C27-C28-C30
12	e	844	CLA	O1A-CGA-O2A-C1
12	B	805	CLA	O1A-CGA-O2A-C1
12	g	814	CLA	CBD-CGD-O2D-CED
12	b	813	CLA	CBD-CGD-O2D-CED
12	B	815	CLA	CBD-CGD-O2D-CED
12	G	812	CLA	CBD-CGD-O2D-CED
12	G	802	CLA	O1A-CGA-O2A-C1
12	A	831	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	a	833	CLA	O1A-CGA-O2A-C1
12	b	803	CLA	O1A-CGA-O2A-C1
12	E	835	CLA	O1A-CGA-O2A-C1
12	e	832	CLA	O1A-CGA-O2A-C1
12	E	840	CLA	O1D-CGD-O2D-CED
12	e	837	CLA	O1D-CGD-O2D-CED
12	a	838	CLA	O1D-CGD-O2D-CED
12	A	836	CLA	O1D-CGD-O2D-CED
12	E	834	CLA	CBA-CGA-O2A-C1
12	a	832	CLA	CBA-CGA-O2A-C1
12	A	830	CLA	CBA-CGA-O2A-C1
12	e	831	CLA	CBA-CGA-O2A-C1
13	a	844	PQN	C26-C27-C28-C29
13	E	846	PQN	C26-C27-C28-C29
13	A	842	PQN	C26-C27-C28-C29
13	e	843	PQN	C26-C27-C28-C29
13	e	843	PQN	C26-C27-C28-C30
12	g	833	CLA	C2A-CAA-CBA-CGA
12	B	834	CLA	C2A-CAA-CBA-CGA
12	b	832	CLA	C2A-CAA-CBA-CGA
12	G	831	CLA	C2A-CAA-CBA-CGA
12	b	837	CLA	C3A-C2A-CAA-CBA
12	A	801	CLA	C3A-C2A-CAA-CBA
12	e	802	CLA	C3A-C2A-CAA-CBA
12	J	1101	CLA	C3A-C2A-CAA-CBA
12	B	838	CLA	C3A-C2A-CAA-CBA
12	e	825	CLA	C3A-C2A-CAA-CBA
12	G	802	CLA	C3A-C2A-CAA-CBA
12	a	835	CLA	C3A-C2A-CAA-CBA
12	e	809	CLA	C3A-C2A-CAA-CBA
12	E	811	CLA	C3A-C2A-CAA-CBA
12	E	832	CLA	C3A-C2A-CAA-CBA
12	a	826	CLA	C3A-C2A-CAA-CBA
12	e	830	CLA	C3A-C2A-CAA-CBA
12	a	825	CLA	C3A-C2A-CAA-CBA
12	A	824	CLA	C3A-C2A-CAA-CBA
12	A	829	CLA	C3A-C2A-CAA-CBA
12	B	816	CLA	C3A-C2A-CAA-CBA
12	A	804	CLA	C3A-C2A-CAA-CBA
12	g	815	CLA	C3A-C2A-CAA-CBA
12	b	836	CLA	C3A-C2A-CAA-CBA
12	G	836	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	838	CLA	C3A-C2A-CAA-CBA
12	E	842	CLA	C3A-C2A-CAA-CBA
12	a	801	CLA	C3A-C2A-CAA-CBA
12	e	824	CLA	C3A-C2A-CAA-CBA
12	G	813	CLA	C3A-C2A-CAA-CBA
12	e	844	CLA	C3A-C2A-CAA-CBA
12	b	803	CLA	C3A-C2A-CAA-CBA
12	b	814	CLA	C3A-C2A-CAA-CBA
12	E	827	CLA	C3A-C2A-CAA-CBA
12	B	837	CLA	C3A-C2A-CAA-CBA
12	e	834	CLA	C3A-C2A-CAA-CBA
12	A	823	CLA	C3A-C2A-CAA-CBA
12	E	826	CLA	C3A-C2A-CAA-CBA
12	e	805	CLA	C3A-C2A-CAA-CBA
12	G	835	CLA	C3A-C2A-CAA-CBA
12	a	803	CLA	C3A-C2A-CAA-CBA
12	E	837	CLA	C3A-C2A-CAA-CBA
12	A	833	CLA	C3A-C2A-CAA-CBA
12	a	806	CLA	C3A-C2A-CAA-CBA
12	A	808	CLA	C3A-C2A-CAA-CBA
12	g	836	CLA	C3A-C2A-CAA-CBA
12	E	804	CLA	C3A-C2A-CAA-CBA
12	E	801	CLA	C3A-C2A-CAA-CBA
12	a	831	CLA	C3A-C2A-CAA-CBA
12	e	801	CLA	C3A-C2A-CAA-CBA
12	E	807	CLA	C3A-C2A-CAA-CBA
12	B	805	CLA	C3A-C2A-CAA-CBA
12	a	810	CLA	C3A-C2A-CAA-CBA
12	e	839	CLA	C3A-C2A-CAA-CBA
12	a	840	CLA	C3A-C2A-CAA-CBA
12	b	837	CLA	CBD-CGD-O2D-CED
12	s	204	CLA	C2A-CAA-CBA-CGA
12	l	204	CLA	C2A-CAA-CBA-CGA
12	S	1502	CLA	C2A-CAA-CBA-CGA
12	L	204	CLA	C2A-CAA-CBA-CGA
12	g	820	CLA	O1A-CGA-O2A-C1
12	b	819	CLA	O1A-CGA-O2A-C1
12	G	818	CLA	O1A-CGA-O2A-C1
12	B	838	CLA	CBD-CGD-O2D-CED
12	G	836	CLA	CBD-CGD-O2D-CED
12	g	837	CLA	CBD-CGD-O2D-CED
12	B	821	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	b	827	CLA	O1A-CGA-O2A-C1
12	G	826	CLA	O1A-CGA-O2A-C1
12	B	829	CLA	O1A-CGA-O2A-C1
12	g	828	CLA	O1A-CGA-O2A-C1
12	g	813	CLA	CBA-CGA-O2A-C1
12	G	811	CLA	CBA-CGA-O2A-C1
12	B	814	CLA	CBA-CGA-O2A-C1
12	b	812	CLA	CBA-CGA-O2A-C1
12	e	827	CLA	C2-C1-O2A-CGA
12	A	826	CLA	C2-C1-O2A-CGA
12	a	828	CLA	C2-C1-O2A-CGA
12	E	829	CLA	C2-C1-O2A-CGA
12	E	834	CLA	O1A-CGA-O2A-C1
12	s	204	CLA	O1A-CGA-O2A-C1
12	l	204	CLA	O1A-CGA-O2A-C1
12	a	832	CLA	O1A-CGA-O2A-C1
12	S	1502	CLA	O1A-CGA-O2A-C1
12	L	204	CLA	O1A-CGA-O2A-C1
12	A	830	CLA	O1A-CGA-O2A-C1
12	e	831	CLA	O1A-CGA-O2A-C1
12	a	825	CLA	C2A-CAA-CBA-CGA
12	e	824	CLA	C2A-CAA-CBA-CGA
12	A	823	CLA	C2A-CAA-CBA-CGA
12	E	826	CLA	C2A-CAA-CBA-CGA
12	A	808	CLA	O1D-CGD-O2D-CED
12	a	810	CLA	O1D-CGD-O2D-CED
12	e	809	CLA	O1D-CGD-O2D-CED
12	E	811	CLA	O1D-CGD-O2D-CED
12	g	813	CLA	O1A-CGA-O2A-C1
12	b	812	CLA	O1A-CGA-O2A-C1
13	g	843	PQN	C21-C22-C23-C24
13	g	843	PQN	C24-C23-C25-C26
13	B	844	PQN	C21-C22-C23-C24
13	B	844	PQN	C24-C23-C25-C26
13	G	842	PQN	C21-C22-C23-C24
13	G	842	PQN	C24-C23-C25-C26
13	b	843	PQN	C21-C22-C23-C24
13	b	843	PQN	C24-C23-C25-C26
12	A	801	CLA	C1A-C2A-CAA-CBA
12	e	802	CLA	C1A-C2A-CAA-CBA
12	J	1101	CLA	C1A-C2A-CAA-CBA
12	r	1401	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	s	204	CLA	C1A-C2A-CAA-CBA
12	l	204	CLA	C1A-C2A-CAA-CBA
12	b	829	CLA	C1A-C2A-CAA-CBA
12	a	835	CLA	C1A-C2A-CAA-CBA
12	g	842	CLA	C1A-C2A-CAA-CBA
12	S	1502	CLA	C1A-C2A-CAA-CBA
12	E	825	CLA	C1A-C2A-CAA-CBA
12	e	817	CLA	C1A-C2A-CAA-CBA
12	b	827	CLA	C1A-C2A-CAA-CBA
12	E	819	CLA	C1A-C2A-CAA-CBA
12	B	843	CLA	C1A-C2A-CAA-CBA
12	e	809	CLA	C1A-C2A-CAA-CBA
12	G	839	CLA	C1A-C2A-CAA-CBA
12	E	811	CLA	C1A-C2A-CAA-CBA
12	B	822	CLA	C1A-C2A-CAA-CBA
12	a	825	CLA	C1A-C2A-CAA-CBA
12	b	838	CLA	C1A-C2A-CAA-CBA
12	G	826	CLA	C1A-C2A-CAA-CBA
12	A	818	CLA	C1A-C2A-CAA-CBA
12	A	804	CLA	C1A-C2A-CAA-CBA
12	K	1401	CLA	C1A-C2A-CAA-CBA
12	G	828	CLA	C1A-C2A-CAA-CBA
12	B	829	CLA	C1A-C2A-CAA-CBA
12	B	839	CLA	C1A-C2A-CAA-CBA
12	A	838	CLA	C1A-C2A-CAA-CBA
12	A	816	CLA	C1A-C2A-CAA-CBA
12	B	831	CLA	C1A-C2A-CAA-CBA
12	b	840	CLA	C1A-C2A-CAA-CBA
12	g	830	CLA	C1A-C2A-CAA-CBA
12	E	842	CLA	C1A-C2A-CAA-CBA
12	L	204	CLA	C1A-C2A-CAA-CBA
12	B	841	CLA	C1A-C2A-CAA-CBA
12	A	822	CLA	C1A-C2A-CAA-CBA
12	g	821	CLA	C1A-C2A-CAA-CBA
12	a	801	CLA	C1A-C2A-CAA-CBA
12	e	824	CLA	C1A-C2A-CAA-CBA
12	g	838	CLA	C1A-C2A-CAA-CBA
12	G	841	CLA	C1A-C2A-CAA-CBA
12	a	820	CLA	C1A-C2A-CAA-CBA
12	b	842	CLA	C1A-C2A-CAA-CBA
12	E	821	CLA	C1A-C2A-CAA-CBA
12	e	834	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	823	CLA	C1A-C2A-CAA-CBA
12	a	824	CLA	C1A-C2A-CAA-CBA
12	E	826	CLA	C1A-C2A-CAA-CBA
12	g	840	CLA	C1A-C2A-CAA-CBA
12	e	805	CLA	C1A-C2A-CAA-CBA
12	a	818	CLA	C1A-C2A-CAA-CBA
12	a	803	CLA	C1A-C2A-CAA-CBA
12	k	1401	CLA	C1A-C2A-CAA-CBA
12	E	837	CLA	C1A-C2A-CAA-CBA
12	e	823	CLA	C1A-C2A-CAA-CBA
12	A	833	CLA	C1A-C2A-CAA-CBA
12	a	806	CLA	C1A-C2A-CAA-CBA
12	A	808	CLA	C1A-C2A-CAA-CBA
12	E	804	CLA	C1A-C2A-CAA-CBA
12	E	801	CLA	C1A-C2A-CAA-CBA
12	e	819	CLA	C1A-C2A-CAA-CBA
12	e	801	CLA	C1A-C2A-CAA-CBA
12	G	837	CLA	C1A-C2A-CAA-CBA
12	E	807	CLA	C1A-C2A-CAA-CBA
12	b	820	CLA	C1A-C2A-CAA-CBA
12	a	810	CLA	C1A-C2A-CAA-CBA
12	e	839	CLA	C1A-C2A-CAA-CBA
12	a	840	CLA	C1A-C2A-CAA-CBA
12	R	1401	CLA	C1A-C2A-CAA-CBA
12	A	818	CLA	C2A-CAA-CBA-CGA
12	G	801	CLA	C2A-CAA-CBA-CGA
12	B	803	CLA	C2A-CAA-CBA-CGA
12	g	803	CLA	C2A-CAA-CBA-CGA
12	a	820	CLA	C2A-CAA-CBA-CGA
12	E	821	CLA	C2A-CAA-CBA-CGA
12	e	819	CLA	C2A-CAA-CBA-CGA
12	b	802	CLA	C2A-CAA-CBA-CGA
12	G	811	CLA	O1A-CGA-O2A-C1
12	B	814	CLA	O1A-CGA-O2A-C1
12	e	836	CLA	O1D-CGD-O2D-CED
12	A	835	CLA	O1D-CGD-O2D-CED
12	a	837	CLA	O1D-CGD-O2D-CED
12	E	839	CLA	O1D-CGD-O2D-CED
12	s	203	CLA	CBA-CGA-O2A-C1
12	l	203	CLA	CBA-CGA-O2A-C1
12	L	203	CLA	CBA-CGA-O2A-C1
12	G	843	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	a	821	CLA	CBA-CGA-O2A-C1
12	G	839	CLA	C2A-CAA-CBA-CGA
12	b	840	CLA	C2A-CAA-CBA-CGA
12	B	841	CLA	C2A-CAA-CBA-CGA
12	g	840	CLA	C2A-CAA-CBA-CGA
12	L	203	CLA	O1D-CGD-O2D-CED
12	E	822	CLA	CBA-CGA-O2A-C1
12	A	819	CLA	CBA-CGA-O2A-C1
12	e	820	CLA	CBA-CGA-O2A-C1
12	g	827	CLA	C2-C1-O2A-CGA
12	e	842	CLA	C2-C1-O2A-CGA
12	b	826	CLA	C2-C1-O2A-CGA
12	G	825	CLA	C2-C1-O2A-CGA
12	B	828	CLA	C2-C1-O2A-CGA
12	e	817	CLA	CAA-CBA-CGA-O2A
12	E	819	CLA	CAA-CBA-CGA-O2A
12	A	816	CLA	CAA-CBA-CGA-O2A
12	a	818	CLA	CAA-CBA-CGA-O2A
12	s	203	CLA	O1D-CGD-O2D-CED
13	g	843	PQN	C17-C18-C20-C21
13	g	843	PQN	C21-C22-C23-C25
13	g	843	PQN	C22-C23-C25-C26
13	B	844	PQN	C17-C18-C20-C21
13	B	844	PQN	C21-C22-C23-C25
13	B	844	PQN	C22-C23-C25-C26
13	G	842	PQN	C17-C18-C20-C21
13	G	842	PQN	C21-C22-C23-C25
13	G	842	PQN	C22-C23-C25-C26
13	b	843	PQN	C17-C18-C20-C21
13	b	843	PQN	C21-C22-C23-C25
13	b	843	PQN	C22-C23-C25-C26
13	a	844	PQN	C16-C17-C18-C20
13	E	846	PQN	C16-C17-C18-C20
13	e	843	PQN	C21-C22-C23-C25
12	G	843	CLA	O1D-CGD-O2D-CED
12	l	203	CLA	O1D-CGD-O2D-CED
13	e	843	PQN	C16-C17-C18-C19
13	A	842	PQN	C12-C11-C3-C4
12	e	825	CLA	C2A-CAA-CBA-CGA
12	a	826	CLA	C2A-CAA-CBA-CGA
12	A	824	CLA	C2A-CAA-CBA-CGA
12	E	827	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	e	809	CLA	C2A-CAA-CBA-CGA
12	E	811	CLA	C2A-CAA-CBA-CGA
12	E	817	CLA	C3A-C2A-CAA-CBA
12	e	815	CLA	C3A-C2A-CAA-CBA
12	E	833	CLA	C3A-C2A-CAA-CBA
12	a	829	CLA	C3A-C2A-CAA-CBA
12	E	822	CLA	C3A-C2A-CAA-CBA
12	A	819	CLA	C3A-C2A-CAA-CBA
12	E	830	CLA	C3A-C2A-CAA-CBA
12	B	822	CLA	C3A-C2A-CAA-CBA
12	l	202	CLA	C3A-C2A-CAA-CBA
12	G	815	CLA	C3A-C2A-CAA-CBA
12	a	822	CLA	C3A-C2A-CAA-CBA
12	a	816	CLA	C3A-C2A-CAA-CBA
12	G	832	CLA	C3A-C2A-CAA-CBA
12	s	201	CLA	C3A-C2A-CAA-CBA
12	e	822	CLA	C3A-C2A-CAA-CBA
12	S	1501	CLA	C3A-C2A-CAA-CBA
12	E	824	CLA	C3A-C2A-CAA-CBA
12	E	823	CLA	C3A-C2A-CAA-CBA
12	s	202	CLA	C3A-C2A-CAA-CBA
12	g	821	CLA	C3A-C2A-CAA-CBA
12	l	201	CLA	C3A-C2A-CAA-CBA
12	e	828	CLA	C3A-C2A-CAA-CBA
12	b	816	CLA	C3A-C2A-CAA-CBA
12	A	820	CLA	C3A-C2A-CAA-CBA
12	g	837	CLA	C3A-C2A-CAA-CBA
12	e	821	CLA	C3A-C2A-CAA-CBA
12	A	814	CLA	C3A-C2A-CAA-CBA
12	B	818	CLA	C3A-C2A-CAA-CBA
12	B	835	CLA	C3A-C2A-CAA-CBA
12	G	819	CLA	C3A-C2A-CAA-CBA
12	a	823	CLA	C3A-C2A-CAA-CBA
12	e	820	CLA	C3A-C2A-CAA-CBA
12	b	833	CLA	C3A-C2A-CAA-CBA
12	a	821	CLA	C3A-C2A-CAA-CBA
12	e	845	CLA	C3A-C2A-CAA-CBA
12	g	817	CLA	C3A-C2A-CAA-CBA
12	L	202	CLA	C3A-C2A-CAA-CBA
12	A	821	CLA	C3A-C2A-CAA-CBA
12	b	820	CLA	C3A-C2A-CAA-CBA
12	A	828	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	a	830	CLA	CBA-CGA-O2A-C1
12	E	831	CLA	CBA-CGA-O2A-C1
12	e	829	CLA	CBA-CGA-O2A-C1
12	b	841	CLA	O1D-CGD-O2D-CED
12	G	840	CLA	O1D-CGD-O2D-CED
12	B	842	CLA	O1D-CGD-O2D-CED
12	a	821	CLA	O1A-CGA-O2A-C1
12	g	841	CLA	O1D-CGD-O2D-CED
12	E	822	CLA	O1A-CGA-O2A-C1
12	A	819	CLA	O1A-CGA-O2A-C1
12	s	203	CLA	O1A-CGA-O2A-C1
12	l	203	CLA	O1A-CGA-O2A-C1
12	L	203	CLA	O1A-CGA-O2A-C1
12	G	843	CLA	O1A-CGA-O2A-C1
12	e	820	CLA	O1A-CGA-O2A-C1
12	A	808	CLA	C2A-CAA-CBA-CGA
12	a	810	CLA	C2A-CAA-CBA-CGA
12	B	838	CLA	O1D-CGD-O2D-CED
12	G	836	CLA	O1D-CGD-O2D-CED
12	g	837	CLA	O1D-CGD-O2D-CED
12	F	1301	CLA	C2C-C3C-CAC-CBC
12	b	837	CLA	O1D-CGD-O2D-CED
12	o	1301	CLA	C2C-C3C-CAC-CBC
12	O	1301	CLA	C2C-C3C-CAC-CBC
12	B	815	CLA	O1D-CGD-O2D-CED
12	f	1301	CLA	C2C-C3C-CAC-CBC
12	A	841	CLA	C2-C1-O2A-CGA
12	g	814	CLA	O1D-CGD-O2D-CED
12	b	813	CLA	O1D-CGD-O2D-CED
12	G	812	CLA	O1D-CGD-O2D-CED
13	A	842	PQN	C21-C22-C23-C25
13	e	843	PQN	C16-C17-C18-C20
12	a	818	CLA	CBD-CGD-O2D-CED
12	e	817	CLA	CBD-CGD-O2D-CED
12	E	819	CLA	CBD-CGD-O2D-CED
12	A	816	CLA	CBD-CGD-O2D-CED
12	G	804	CLA	CBA-CGA-O2A-C1
12	A	838	CLA	CBA-CGA-O2A-C1
12	E	842	CLA	CBA-CGA-O2A-C1
13	g	843	PQN	C23-C25-C26-C27
13	B	844	PQN	C23-C25-C26-C27
13	G	842	PQN	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
13	b	843	PQN	C23-C25-C26-C27
12	a	817	CLA	CAD-CBD-CGD-O2D
12	e	816	CLA	CAD-CBD-CGD-O2D
12	A	815	CLA	CAD-CBD-CGD-O2D
12	a	814	CLA	CAD-CBD-CGD-O2D
12	g	814	CLA	CAD-CBD-CGD-O2D
12	b	827	CLA	CAD-CBD-CGD-O2D
12	G	839	CLA	CAD-CBD-CGD-O2D
12	a	807	CLA	CAD-CBD-CGD-O2D
12	g	822	CLA	CAD-CBD-CGD-O2D
12	G	826	CLA	CAD-CBD-CGD-O2D
12	A	838	CLA	CAD-CBD-CGD-O2D
12	b	821	CLA	CAD-CBD-CGD-O2D
12	E	808	CLA	CAD-CBD-CGD-O2D
12	e	813	CLA	CAD-CBD-CGD-O2D
12	A	805	CLA	CAD-CBD-CGD-O2D
12	b	813	CLA	CAD-CBD-CGD-O2D
12	b	840	CLA	CAD-CBD-CGD-O2D
12	E	842	CLA	CAD-CBD-CGD-O2D
12	B	841	CLA	CAD-CBD-CGD-O2D
12	G	820	CLA	CAD-CBD-CGD-O2D
12	E	815	CLA	CAD-CBD-CGD-O2D
12	B	815	CLA	CAD-CBD-CGD-O2D
12	B	823	CLA	CAD-CBD-CGD-O2D
12	g	840	CLA	CAD-CBD-CGD-O2D
12	e	806	CLA	CAD-CBD-CGD-O2D
12	E	818	CLA	CAD-CBD-CGD-O2D
12	A	812	CLA	CAD-CBD-CGD-O2D
12	e	839	CLA	CAD-CBD-CGD-O2D
12	a	840	CLA	CAD-CBD-CGD-O2D
12	G	812	CLA	CAD-CBD-CGD-O2D
12	g	806	CLA	CBA-CGA-O2A-C1
12	b	805	CLA	CBA-CGA-O2A-C1
12	e	839	CLA	CBA-CGA-O2A-C1
12	a	840	CLA	CBA-CGA-O2A-C1
12	B	807	CLA	CBA-CGA-O2A-C1
13	e	843	PQN	C15-C16-C17-C18
12	A	828	CLA	O1A-CGA-O2A-C1
12	a	830	CLA	O1A-CGA-O2A-C1
12	E	831	CLA	O1A-CGA-O2A-C1
12	e	829	CLA	O1A-CGA-O2A-C1
12	b	837	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	b	837	CLA	CHA-CBD-CGD-O2D
12	A	801	CLA	CHA-CBD-CGD-O1D
12	B	838	CLA	CHA-CBD-CGD-O1D
12	B	838	CLA	CHA-CBD-CGD-O2D
12	g	820	CLA	CHA-CBD-CGD-O1D
12	g	820	CLA	CHA-CBD-CGD-O2D
12	a	827	CLA	CHA-CBD-CGD-O1D
12	a	827	CLA	CHA-CBD-CGD-O2D
12	a	835	CLA	CHA-CBD-CGD-O1D
12	a	835	CLA	CHA-CBD-CGD-O2D
12	B	820	CLA	CHA-CBD-CGD-O1D
12	B	820	CLA	CHA-CBD-CGD-O2D
12	E	825	CLA	CHA-CBD-CGD-O1D
12	G	838	CLA	CHA-CBD-CGD-O1D
12	g	819	CLA	CHA-CBD-CGD-O1D
12	g	819	CLA	CHA-CBD-CGD-O2D
12	b	818	CLA	CHA-CBD-CGD-O1D
12	b	818	CLA	CHA-CBD-CGD-O2D
12	E	832	CLA	CHA-CBD-CGD-O1D
12	E	832	CLA	CHA-CBD-CGD-O2D
12	e	830	CLA	CHA-CBD-CGD-O1D
12	e	830	CLA	CHA-CBD-CGD-O2D
12	A	829	CLA	CHA-CBD-CGD-O1D
12	A	829	CLA	CHA-CBD-CGD-O2D
12	G	836	CLA	CHA-CBD-CGD-O1D
12	G	836	CLA	CHA-CBD-CGD-O2D
12	A	832	CLA	CHA-CBD-CGD-O1D
12	A	832	CLA	CHA-CBD-CGD-O2D
12	B	840	CLA	CHA-CBD-CGD-O1D
12	b	839	CLA	CHA-CBD-CGD-O1D
12	E	836	CLA	CHA-CBD-CGD-O1D
12	E	836	CLA	CHA-CBD-CGD-O2D
12	e	826	CLA	CHA-CBD-CGD-O1D
12	e	826	CLA	CHA-CBD-CGD-O2D
12	A	822	CLA	CHA-CBD-CGD-O1D
12	a	801	CLA	CHA-CBD-CGD-O1D
12	g	837	CLA	CHA-CBD-CGD-O1D
12	g	837	CLA	CHA-CBD-CGD-O2D
12	G	817	CLA	CHA-CBD-CGD-O1D
12	G	817	CLA	CHA-CBD-CGD-O2D
12	e	834	CLA	CHA-CBD-CGD-O1D
12	e	834	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	a	824	CLA	CHA-CBD-CGD-O1D
12	E	837	CLA	CHA-CBD-CGD-O1D
12	E	837	CLA	CHA-CBD-CGD-O2D
12	A	825	CLA	CHA-CBD-CGD-O1D
12	A	825	CLA	CHA-CBD-CGD-O2D
12	B	821	CLA	CHA-CBD-CGD-O1D
12	B	821	CLA	CHA-CBD-CGD-O2D
12	e	823	CLA	CHA-CBD-CGD-O1D
12	g	839	CLA	CHA-CBD-CGD-O1D
12	e	833	CLA	CHA-CBD-CGD-O1D
12	e	833	CLA	CHA-CBD-CGD-O2D
12	b	819	CLA	CHA-CBD-CGD-O1D
12	b	819	CLA	CHA-CBD-CGD-O2D
12	A	833	CLA	CHA-CBD-CGD-O1D
12	A	833	CLA	CHA-CBD-CGD-O2D
12	E	801	CLA	CHA-CBD-CGD-O1D
12	a	831	CLA	CHA-CBD-CGD-O1D
12	a	831	CLA	CHA-CBD-CGD-O2D
12	a	834	CLA	CHA-CBD-CGD-O1D
12	a	834	CLA	CHA-CBD-CGD-O2D
12	e	801	CLA	CHA-CBD-CGD-O1D
12	E	828	CLA	CHA-CBD-CGD-O1D
12	E	828	CLA	CHA-CBD-CGD-O2D
12	G	818	CLA	CHA-CBD-CGD-O1D
12	G	818	CLA	CHA-CBD-CGD-O2D
12	G	819	CLA	C1A-C2A-CAA-CBA
12	g	813	CLA	C2A-CAA-CBA-CGA
12	G	811	CLA	C2A-CAA-CBA-CGA
12	b	812	CLA	C2A-CAA-CBA-CGA
12	e	842	CLA	CBA-CGA-O2A-C1
12	b	837	CLA	CAD-CBD-CGD-O1D
12	E	833	CLA	CAD-CBD-CGD-O1D
12	B	838	CLA	CAD-CBD-CGD-O1D
12	g	820	CLA	CAD-CBD-CGD-O1D
12	e	825	CLA	CAD-CBD-CGD-O1D
12	G	810	CLA	CAD-CBD-CGD-O1D
12	E	825	CLA	CAD-CBD-CGD-O1D
12	B	808	CLA	CAD-CBD-CGD-O1D
12	G	821	CLA	CAD-CBD-CGD-O1D
12	g	807	CLA	CAD-CBD-CGD-O1D
12	a	826	CLA	CAD-CBD-CGD-O1D
12	l	202	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	A	824	CLA	CAD-CBD-CGD-O1D
12	b	838	CLA	CAD-CBD-CGD-O1D
12	B	813	CLA	CAD-CBD-CGD-O1D
12	G	805	CLA	CAD-CBD-CGD-O1D
12	s	201	CLA	CAD-CBD-CGD-O1D
12	G	836	CLA	CAD-CBD-CGD-O1D
12	B	839	CLA	CAD-CBD-CGD-O1D
12	S	1501	CLA	CAD-CBD-CGD-O1D
12	B	824	CLA	CAD-CBD-CGD-O1D
12	s	202	CLA	CAD-CBD-CGD-O1D
12	A	822	CLA	CAD-CBD-CGD-O1D
12	b	822	CLA	CAD-CBD-CGD-O1D
12	l	201	CLA	CAD-CBD-CGD-O1D
12	g	838	CLA	CAD-CBD-CGD-O1D
12	a	813	CLA	CAD-CBD-CGD-O1D
12	g	837	CLA	CAD-CBD-CGD-O1D
12	E	827	CLA	CAD-CBD-CGD-O1D
12	g	812	CLA	CAD-CBD-CGD-O1D
12	a	824	CLA	CAD-CBD-CGD-O1D
12	B	821	CLA	CAD-CBD-CGD-O1D
12	e	823	CLA	CAD-CBD-CGD-O1D
12	b	819	CLA	CAD-CBD-CGD-O1D
12	b	806	CLA	CAD-CBD-CGD-O1D
12	b	811	CLA	CAD-CBD-CGD-O1D
12	L	202	CLA	CAD-CBD-CGD-O1D
12	G	837	CLA	CAD-CBD-CGD-O1D
12	L	201	CLA	CAD-CBD-CGD-O1D
12	e	812	CLA	CAD-CBD-CGD-O1D
12	g	823	CLA	CAD-CBD-CGD-O1D
12	G	818	CLA	CAD-CBD-CGD-O1D
12	B	814	CLA	CAA-CBA-CGA-O2A
12	g	813	CLA	CAA-CBA-CGA-O2A
12	G	811	CLA	CAA-CBA-CGA-O2A
12	b	812	CLA	CAA-CBA-CGA-O2A
12	E	834	CLA	C2A-CAA-CBA-CGA
12	A	803	CLA	C2A-CAA-CBA-CGA
12	a	832	CLA	C2A-CAA-CBA-CGA
12	e	804	CLA	C2A-CAA-CBA-CGA
12	B	814	CLA	C2A-CAA-CBA-CGA
12	A	830	CLA	C2A-CAA-CBA-CGA
12	a	805	CLA	C2A-CAA-CBA-CGA
12	e	831	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	E	806	CLA	C2A-CAA-CBA-CGA
12	G	802	CLA	C2-C1-O2A-CGA
12	a	827	CLA	C2-C1-O2A-CGA
12	G	834	CLA	C2-C1-O2A-CGA
12	g	835	CLA	C2-C1-O2A-CGA
12	e	826	CLA	C2-C1-O2A-CGA
12	e	844	CLA	C2-C1-O2A-CGA
12	b	803	CLA	C2-C1-O2A-CGA
12	J	1102	CLA	C2-C1-O2A-CGA
12	A	825	CLA	C2-C1-O2A-CGA
12	b	835	CLA	C2-C1-O2A-CGA
12	B	805	CLA	C2-C1-O2A-CGA
12	E	828	CLA	C2-C1-O2A-CGA
13	a	844	PQN	C21-C22-C23-C25
13	E	846	PQN	C21-C22-C23-C25
13	A	842	PQN	C16-C17-C18-C20
12	A	827	CLA	C3A-C2A-CAA-CBA
12	f	1301	CLA	C3A-C2A-CAA-CBA
12	F	1301	CLA	C3A-C2A-CAA-CBA
12	o	1301	CLA	C3A-C2A-CAA-CBA
12	L	201	CLA	C3A-C2A-CAA-CBA
12	O	1301	CLA	C3A-C2A-CAA-CBA
12	b	819	CLA	C4C-C3C-CAC-CBC
12	A	838	CLA	O1A-CGA-O2A-C1
12	E	842	CLA	O1A-CGA-O2A-C1
12	a	840	CLA	O1A-CGA-O2A-C1
12	e	816	CLA	C2C-C3C-CAC-CBC
12	b	819	CLA	C2C-C3C-CAC-CBC
12	a	817	CLA	C2C-C3C-CAC-CBC
12	A	815	CLA	C2C-C3C-CAC-CBC
12	E	818	CLA	C2C-C3C-CAC-CBC
12	g	820	CLA	C2C-C3C-CAC-CBC
12	g	820	CLA	C4C-C3C-CAC-CBC
12	B	821	CLA	C2C-C3C-CAC-CBC
12	B	821	CLA	C4C-C3C-CAC-CBC
12	G	818	CLA	C2C-C3C-CAC-CBC
12	G	818	CLA	C4C-C3C-CAC-CBC
12	e	839	CLA	O1A-CGA-O2A-C1
12	B	807	CLA	O1A-CGA-O2A-C1
12	g	808	CLA	C2A-CAA-CBA-CGA
12	B	809	CLA	C2A-CAA-CBA-CGA
12	G	806	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	b	807	CLA	C2A-CAA-CBA-CGA
12	G	804	CLA	O1A-CGA-O2A-C1
12	e	842	CLA	O1A-CGA-O2A-C1
12	g	806	CLA	O1A-CGA-O2A-C1
12	b	805	CLA	O1A-CGA-O2A-C1
12	E	834	CLA	CAA-CBA-CGA-O2A
12	a	832	CLA	CAA-CBA-CGA-O2A
12	A	830	CLA	CAA-CBA-CGA-O2A
12	e	831	CLA	CAA-CBA-CGA-O2A
13	g	843	PQN	C19-C18-C20-C21
13	B	844	PQN	C19-C18-C20-C21
13	G	842	PQN	C19-C18-C20-C21
13	b	843	PQN	C19-C18-C20-C21
13	A	842	PQN	C21-C22-C23-C24
13	e	843	PQN	C21-C22-C23-C24
12	A	841	CLA	CBA-CGA-O2A-C1
12	A	841	CLA	O1A-CGA-O2A-C1
12	a	818	CLA	O1D-CGD-O2D-CED
12	E	819	CLA	O1D-CGD-O2D-CED
12	A	816	CLA	O1D-CGD-O2D-CED
13	a	844	PQN	C12-C11-C3-C2
13	A	842	PQN	C12-C11-C3-C2
12	e	817	CLA	O1D-CGD-O2D-CED
13	B	844	PQN	C20-C21-C22-C23
13	G	842	PQN	C20-C21-C22-C23
12	a	822	CLA	C1-C2-C3-C4
12	G	832	CLA	C1-C2-C3-C4
12	E	823	CLA	C1-C2-C3-C4
12	A	820	CLA	C1-C2-C3-C4
12	e	821	CLA	C1-C2-C3-C4
12	B	835	CLA	C1-C2-C3-C4
12	b	833	CLA	C1-C2-C3-C4
12	e	845	CLA	C1-C2-C3-C4
13	g	843	PQN	C20-C21-C22-C23
13	b	843	PQN	C20-C21-C22-C23
12	O	1301	CLA	C4C-C3C-CAC-CBC
12	F	1301	CLA	C4C-C3C-CAC-CBC
12	o	1301	CLA	C4C-C3C-CAC-CBC
12	f	1301	CLA	C4C-C3C-CAC-CBC
12	G	803	CLA	O1A-CGA-O2A-C1
12	g	805	CLA	O1A-CGA-O2A-C1
12	B	806	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	844	PQN	C21-C22-C23-C24
13	E	846	PQN	C21-C22-C23-C24
13	a	844	PQN	C12-C11-C3-C4
13	E	846	PQN	C12-C11-C3-C4
12	b	804	CLA	O1A-CGA-O2A-C1
12	a	825	CLA	CAA-CBA-CGA-O2A
12	e	824	CLA	CAA-CBA-CGA-O2A
12	A	823	CLA	CAA-CBA-CGA-O2A
12	E	826	CLA	CAA-CBA-CGA-O2A
12	A	840	CLA	C2A-CAA-CBA-CGA
12	e	841	CLA	C2A-CAA-CBA-CGA
12	E	844	CLA	C2A-CAA-CBA-CGA
12	a	842	CLA	C2A-CAA-CBA-CGA
12	G	803	CLA	CBA-CGA-O2A-C1
12	b	804	CLA	CBA-CGA-O2A-C1
12	g	805	CLA	CBA-CGA-O2A-C1
12	B	806	CLA	CBA-CGA-O2A-C1
12	a	812	CLA	C2A-CAA-CBA-CGA
12	e	840	CLA	C2A-CAA-CBA-CGA
12	G	802	CLA	C2A-CAA-CBA-CGA
12	e	838	CLA	C2A-CAA-CBA-CGA
12	a	841	CLA	C2A-CAA-CBA-CGA
12	E	841	CLA	C2A-CAA-CBA-CGA
12	A	839	CLA	C2A-CAA-CBA-CGA
12	A	837	CLA	C2A-CAA-CBA-CGA
12	e	844	CLA	C2A-CAA-CBA-CGA
12	b	803	CLA	C2A-CAA-CBA-CGA
12	A	810	CLA	C2A-CAA-CBA-CGA
12	e	811	CLA	C2A-CAA-CBA-CGA
12	a	839	CLA	C2A-CAA-CBA-CGA
12	B	805	CLA	C2A-CAA-CBA-CGA
12	E	813	CLA	C2A-CAA-CBA-CGA
12	E	843	CLA	C2A-CAA-CBA-CGA
13	e	843	PQN	C23-C25-C26-C27
12	G	809	CLA	C3A-C2A-CAA-CBA
12	b	810	CLA	C3A-C2A-CAA-CBA
12	a	815	CLA	C3A-C2A-CAA-CBA
12	B	812	CLA	C3A-C2A-CAA-CBA
12	A	813	CLA	C3A-C2A-CAA-CBA
12	e	814	CLA	C3A-C2A-CAA-CBA
12	E	816	CLA	C3A-C2A-CAA-CBA
12	g	811	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	B	801	CLA	CBA-CGA-O2A-C1
12	E	802	CLA	CBA-CGA-O2A-C1
12	e	817	CLA	CAA-CBA-CGA-O1A
12	E	819	CLA	CAA-CBA-CGA-O1A
12	A	816	CLA	CAA-CBA-CGA-O1A
12	a	818	CLA	CAA-CBA-CGA-O1A
12	g	801	CLA	CBA-CGA-O2A-C1
12	a	802	CLA	CBA-CGA-O2A-C1
12	e	810	CLA	C2-C1-O2A-CGA
12	e	808	CLA	C2-C1-O2A-CGA
12	e	838	CLA	C2-C1-O2A-CGA
12	b	831	CLA	C2-C1-O2A-CGA
12	B	808	CLA	C2-C1-O2A-CGA
12	E	812	CLA	C2-C1-O2A-CGA
12	E	832	CLA	C2-C1-O2A-CGA
12	g	807	CLA	C2-C1-O2A-CGA
12	a	811	CLA	C2-C1-O2A-CGA
12	e	830	CLA	C2-C1-O2A-CGA
12	A	829	CLA	C2-C1-O2A-CGA
12	E	841	CLA	C2-C1-O2A-CGA
12	B	833	CLA	C2-C1-O2A-CGA
12	A	837	CLA	C2-C1-O2A-CGA
12	G	832	CLA	C2-C1-O2A-CGA
12	G	805	CLA	C2-C1-O2A-CGA
12	A	807	CLA	C2-C1-O2A-CGA
12	g	832	CLA	C2-C1-O2A-CGA
12	G	830	CLA	C2-C1-O2A-CGA
12	E	810	CLA	C2-C1-O2A-CGA
12	a	809	CLA	C2-C1-O2A-CGA
12	B	835	CLA	C2-C1-O2A-CGA
12	b	833	CLA	C2-C1-O2A-CGA
12	b	806	CLA	C2-C1-O2A-CGA
12	e	845	CLA	C2-C1-O2A-CGA
12	a	831	CLA	C2-C1-O2A-CGA
12	a	839	CLA	C2-C1-O2A-CGA
12	E	833	CLA	C1A-C2A-CAA-CBA
12	E	822	CLA	C1A-C2A-CAA-CBA
12	A	819	CLA	C1A-C2A-CAA-CBA
12	a	815	CLA	C1A-C2A-CAA-CBA
12	s	201	CLA	C1A-C2A-CAA-CBA
12	e	822	CLA	C1A-C2A-CAA-CBA
12	E	824	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	813	CLA	C1A-C2A-CAA-CBA
12	l	201	CLA	C1A-C2A-CAA-CBA
12	e	814	CLA	C1A-C2A-CAA-CBA
12	a	823	CLA	C1A-C2A-CAA-CBA
12	e	820	CLA	C1A-C2A-CAA-CBA
12	a	821	CLA	C1A-C2A-CAA-CBA
12	L	201	CLA	C1A-C2A-CAA-CBA
12	A	821	CLA	C1A-C2A-CAA-CBA
12	E	816	CLA	C1A-C2A-CAA-CBA
12	G	804	CLA	C2A-CAA-CBA-CGA
12	g	806	CLA	C2A-CAA-CBA-CGA
12	b	805	CLA	C2A-CAA-CBA-CGA
12	B	807	CLA	C2A-CAA-CBA-CGA
12	g	831	CLA	CBA-CGA-O2A-C1
12	G	829	CLA	CBA-CGA-O2A-C1
12	b	830	CLA	CBA-CGA-O2A-C1
12	B	832	CLA	CBA-CGA-O2A-C1
13	a	844	PQN	C23-C25-C26-C27
12	B	801	CLA	O1A-CGA-O2A-C1
12	g	801	CLA	O1A-CGA-O2A-C1
12	a	802	CLA	O1A-CGA-O2A-C1
12	E	802	CLA	O1A-CGA-O2A-C1
12	E	833	CLA	CBD-CGD-O2D-CED
12	r	1401	CLA	C2A-CAA-CBA-CGA
12	K	1401	CLA	C2A-CAA-CBA-CGA
12	k	1401	CLA	C2A-CAA-CBA-CGA
12	R	1401	CLA	C2A-CAA-CBA-CGA
12	b	830	CLA	O1A-CGA-O2A-C1
12	g	831	CLA	O1A-CGA-O2A-C1
12	B	832	CLA	O1A-CGA-O2A-C1
12	G	829	CLA	O1A-CGA-O2A-C1
12	s	201	CLA	CBD-CGD-O2D-CED
12	L	201	CLA	CBD-CGD-O2D-CED
12	E	820	CLA	C2A-CAA-CBA-CGA
12	a	819	CLA	C2A-CAA-CBA-CGA
12	A	817	CLA	C2A-CAA-CBA-CGA
12	b	809	CLA	CAA-CBA-CGA-O2A
12	G	808	CLA	CAA-CBA-CGA-O2A
13	g	843	PQN	C26-C27-C28-C29
12	B	811	CLA	CAA-CBA-CGA-O2A
12	g	810	CLA	CAA-CBA-CGA-O2A
12	l	201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	B	844	PQN	C26-C27-C28-C29
13	G	842	PQN	C26-C27-C28-C29
13	b	843	PQN	C26-C27-C28-C29
12	G	834	CLA	CAA-CBA-CGA-O2A
12	g	842	CLA	CAA-CBA-CGA-O2A
12	g	835	CLA	CAA-CBA-CGA-O2A
12	B	843	CLA	CAA-CBA-CGA-O2A
12	e	842	CLA	CAA-CBA-CGA-O2A
12	G	841	CLA	CAA-CBA-CGA-O2A
12	b	842	CLA	CAA-CBA-CGA-O2A
12	J	1102	CLA	CAA-CBA-CGA-O2A
12	b	835	CLA	CAA-CBA-CGA-O2A
12	G	832	CLA	O2A-C1-C2-C3
12	B	835	CLA	O2A-C1-C2-C3
12	b	833	CLA	O2A-C1-C2-C3
12	e	845	CLA	O2A-C1-C2-C3
13	a	844	PQN	C14-C13-C15-C16
13	E	846	PQN	C14-C13-C15-C16
12	e	818	CLA	C2A-CAA-CBA-CGA
12	a	814	CLA	C2A-CAA-CBA-CGA
12	e	813	CLA	C2A-CAA-CBA-CGA
12	E	815	CLA	C2A-CAA-CBA-CGA
12	A	812	CLA	C2A-CAA-CBA-CGA
12	a	830	CLA	CAA-CBA-CGA-O2A
12	g	834	CLA	CAA-CBA-CGA-O2A
12	G	833	CLA	CAA-CBA-CGA-O2A
12	b	834	CLA	CAA-CBA-CGA-O2A
12	E	831	CLA	CAA-CBA-CGA-O2A
12	e	829	CLA	CAA-CBA-CGA-O2A
12	B	836	CLA	CAA-CBA-CGA-O2A
12	e	808	CLA	C3A-C2A-CAA-CBA
12	A	807	CLA	C3A-C2A-CAA-CBA
12	A	832	CLA	C3A-C2A-CAA-CBA
12	E	810	CLA	C3A-C2A-CAA-CBA
12	E	836	CLA	C3A-C2A-CAA-CBA
12	a	809	CLA	C3A-C2A-CAA-CBA
12	e	833	CLA	C3A-C2A-CAA-CBA
12	a	834	CLA	C3A-C2A-CAA-CBA
12	A	828	CLA	CAA-CBA-CGA-O2A
12	A	841	CLA	CAA-CBA-CGA-O2A
12	A	828	CLA	CAD-CBD-CGD-O2D
12	b	824	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	e	810	CLA	CAD-CBD-CGD-O2D
12	e	807	CLA	CAD-CBD-CGD-O2D
12	e	808	CLA	CAD-CBD-CGD-O2D
12	B	810	CLA	CAD-CBD-CGD-O2D
12	g	825	CLA	CAD-CBD-CGD-O2D
12	E	809	CLA	CAD-CBD-CGD-O2D
12	g	842	CLA	CAD-CBD-CGD-O2D
12	b	808	CLA	CAD-CBD-CGD-O2D
12	a	830	CLA	CAD-CBD-CGD-O2D
12	B	811	CLA	CAD-CBD-CGD-O2D
12	b	809	CLA	CAD-CBD-CGD-O2D
12	A	806	CLA	CAD-CBD-CGD-O2D
12	B	843	CLA	CAD-CBD-CGD-O2D
12	G	838	CLA	CAD-CBD-CGD-O2D
12	B	822	CLA	CAD-CBD-CGD-O2D
12	e	836	CLA	CAD-CBD-CGD-O2D
12	E	812	CLA	CAD-CBD-CGD-O2D
12	g	809	CLA	CAD-CBD-CGD-O2D
12	a	811	CLA	CAD-CBD-CGD-O2D
12	A	835	CLA	CAD-CBD-CGD-O2D
12	G	823	CLA	CAD-CBD-CGD-O2D
12	f	1301	CLA	CAD-CBD-CGD-O2D
12	a	808	CLA	CAD-CBD-CGD-O2D
12	A	809	CLA	CAD-CBD-CGD-O2D
12	A	807	CLA	CAD-CBD-CGD-O2D
12	B	829	CLA	CAD-CBD-CGD-O2D
12	B	840	CLA	CAD-CBD-CGD-O2D
12	b	839	CLA	CAD-CBD-CGD-O2D
12	E	831	CLA	CAD-CBD-CGD-O2D
12	F	1301	CLA	CAD-CBD-CGD-O2D
12	E	810	CLA	CAD-CBD-CGD-O2D
12	B	801	CLA	CAD-CBD-CGD-O2D
12	g	821	CLA	CAD-CBD-CGD-O2D
12	B	826	CLA	CAD-CBD-CGD-O2D
12	g	801	CLA	CAD-CBD-CGD-O2D
12	G	841	CLA	CAD-CBD-CGD-O2D
12	a	802	CLA	CAD-CBD-CGD-O2D
12	b	842	CLA	CAD-CBD-CGD-O2D
12	e	829	CLA	CAD-CBD-CGD-O2D
12	a	837	CLA	CAD-CBD-CGD-O2D
12	g	828	CLA	CAD-CBD-CGD-O2D
12	E	839	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	G	808	CLA	CAD-CBD-CGD-O2D
12	a	809	CLA	CAD-CBD-CGD-O2D
12	G	819	CLA	CAD-CBD-CGD-O2D
12	g	839	CLA	CAD-CBD-CGD-O2D
12	G	807	CLA	CAD-CBD-CGD-O2D
12	g	810	CLA	CAD-CBD-CGD-O2D
12	o	1301	CLA	CAD-CBD-CGD-O2D
12	b	820	CLA	CAD-CBD-CGD-O2D
12	O	1301	CLA	CAD-CBD-CGD-O2D
12	E	802	CLA	CAD-CBD-CGD-O2D
13	A	842	PQN	C14-C13-C15-C16
12	A	828	CLA	O2A-C1-C2-C3
12	E	834	CLA	O2A-C1-C2-C3
12	g	820	CLA	O2A-C1-C2-C3
12	e	825	CLA	O2A-C1-C2-C3
12	g	842	CLA	O2A-C1-C2-C3
12	a	830	CLA	O2A-C1-C2-C3
12	g	834	CLA	O2A-C1-C2-C3
12	B	843	CLA	O2A-C1-C2-C3
12	G	833	CLA	O2A-C1-C2-C3
12	a	826	CLA	O2A-C1-C2-C3
12	G	815	CLA	O2A-C1-C2-C3
12	A	824	CLA	O2A-C1-C2-C3
12	e	842	CLA	O2A-C1-C2-C3
12	g	816	CLA	O2A-C1-C2-C3
12	b	834	CLA	O2A-C1-C2-C3
12	B	817	CLA	O2A-C1-C2-C3
12	E	831	CLA	O2A-C1-C2-C3
12	b	816	CLA	O2A-C1-C2-C3
12	G	841	CLA	O2A-C1-C2-C3
12	b	842	CLA	O2A-C1-C2-C3
12	B	818	CLA	O2A-C1-C2-C3
12	E	827	CLA	O2A-C1-C2-C3
12	e	829	CLA	O2A-C1-C2-C3
12	b	815	CLA	O2A-C1-C2-C3
12	B	821	CLA	O2A-C1-C2-C3
12	b	819	CLA	O2A-C1-C2-C3
12	g	817	CLA	O2A-C1-C2-C3
12	B	836	CLA	O2A-C1-C2-C3
12	G	814	CLA	O2A-C1-C2-C3
12	G	818	CLA	O2A-C1-C2-C3
12	e	807	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	E	809	CLA	C2A-CAA-CBA-CGA
12	A	806	CLA	C2A-CAA-CBA-CGA
12	a	808	CLA	C2A-CAA-CBA-CGA
12	b	806	CLA	C2A-CAA-CBA-CGA
13	a	844	PQN	C12-C13-C15-C16
13	E	846	PQN	C12-C13-C15-C16
13	E	846	PQN	C12-C11-C3-C2
13	e	843	PQN	C12-C11-C3-C2
13	E	846	PQN	C23-C25-C26-C27
12	B	808	CLA	C2A-CAA-CBA-CGA
12	g	807	CLA	C2A-CAA-CBA-CGA
12	b	838	CLA	C2A-CAA-CBA-CGA
12	G	805	CLA	C2A-CAA-CBA-CGA
12	B	839	CLA	C2A-CAA-CBA-CGA
12	g	838	CLA	C2A-CAA-CBA-CGA
12	G	837	CLA	C2A-CAA-CBA-CGA
13	A	842	PQN	C12-C13-C15-C16
12	A	809	CLA	C2-C1-O2A-CGA
12	a	825	CLA	CBA-CGA-O2A-C1
12	e	824	CLA	CBA-CGA-O2A-C1
12	A	823	CLA	CBA-CGA-O2A-C1
12	E	826	CLA	CBA-CGA-O2A-C1
12	b	841	CLA	CAA-CBA-CGA-O2A
12	g	841	CLA	CAA-CBA-CGA-O2A
12	G	840	CLA	CAA-CBA-CGA-O2A
12	B	842	CLA	CAA-CBA-CGA-O2A
12	B	820	CLA	CBD-CGD-O2D-CED
12	g	842	CLA	CAA-CBA-CGA-O1A
12	A	801	CLA	CHA-CBD-CGD-O2D
12	A	834	CLA	CHA-CBD-CGD-O1D
12	A	834	CLA	CHA-CBD-CGD-O2D
12	s	204	CLA	CHA-CBD-CGD-O1D
12	s	204	CLA	CHA-CBD-CGD-O2D
12	G	802	CLA	CHA-CBD-CGD-O2D
12	A	803	CLA	CHA-CBD-CGD-O1D
12	A	803	CLA	CHA-CBD-CGD-O2D
12	g	833	CLA	CHA-CBD-CGD-O2D
12	l	204	CLA	CHA-CBD-CGD-O1D
12	l	204	CLA	CHA-CBD-CGD-O2D
12	B	834	CLA	CHA-CBD-CGD-O2D
12	b	829	CLA	CHA-CBD-CGD-O1D
12	b	829	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	b	832	CLA	CHA-CBD-CGD-O2D
12	G	834	CLA	CHA-CBD-CGD-O1D
12	G	834	CLA	CHA-CBD-CGD-O2D
12	g	835	CLA	CHA-CBD-CGD-O1D
12	g	835	CLA	CHA-CBD-CGD-O2D
12	g	827	CLA	CHA-CBD-CGD-O1D
12	g	808	CLA	CHA-CBD-CGD-O1D
12	g	808	CLA	CHA-CBD-CGD-O2D
12	S	1502	CLA	CHA-CBD-CGD-O1D
12	S	1502	CLA	CHA-CBD-CGD-O2D
12	E	825	CLA	CHA-CBD-CGD-O2D
12	G	838	CLA	CHA-CBD-CGD-O2D
12	G	831	CLA	CHA-CBD-CGD-O2D
12	g	813	CLA	CHA-CBD-CGD-O1D
12	g	813	CLA	CHA-CBD-CGD-O2D
12	E	814	CLA	CHA-CBD-CGD-O1D
12	e	835	CLA	CHA-CBD-CGD-O1D
12	e	835	CLA	CHA-CBD-CGD-O2D
12	a	825	CLA	CHA-CBD-CGD-O2D
12	A	818	CLA	CHA-CBD-CGD-O1D
12	B	809	CLA	CHA-CBD-CGD-O1D
12	B	809	CLA	CHA-CBD-CGD-O2D
12	a	836	CLA	CHA-CBD-CGD-O1D
12	a	836	CLA	CHA-CBD-CGD-O2D
12	E	838	CLA	CHA-CBD-CGD-O1D
12	E	838	CLA	CHA-CBD-CGD-O2D
12	e	804	CLA	CHA-CBD-CGD-O1D
12	e	804	CLA	CHA-CBD-CGD-O2D
12	G	828	CLA	CHA-CBD-CGD-O1D
12	G	828	CLA	CHA-CBD-CGD-O2D
12	B	840	CLA	CHA-CBD-CGD-O2D
12	B	831	CLA	CHA-CBD-CGD-O1D
12	B	831	CLA	CHA-CBD-CGD-O2D
12	b	826	CLA	CHA-CBD-CGD-O1D
12	b	839	CLA	CHA-CBD-CGD-O2D
12	g	830	CLA	CHA-CBD-CGD-O1D
12	g	830	CLA	CHA-CBD-CGD-O2D
12	L	204	CLA	CHA-CBD-CGD-O1D
12	L	204	CLA	CHA-CBD-CGD-O2D
12	B	801	CLA	CHA-CBD-CGD-O1D
12	G	811	CLA	CHA-CBD-CGD-O1D
12	G	811	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	B	814	CLA	CHA-CBD-CGD-O1D
12	B	814	CLA	CHA-CBD-CGD-O2D
12	A	822	CLA	CHA-CBD-CGD-O2D
12	a	801	CLA	CHA-CBD-CGD-O2D
12	e	824	CLA	CHA-CBD-CGD-O2D
12	a	813	CLA	CHA-CBD-CGD-O1D
12	g	801	CLA	CHA-CBD-CGD-O1D
12	b	828	CLA	CHA-CBD-CGD-O1D
12	e	844	CLA	CHA-CBD-CGD-O2D
12	a	802	CLA	CHA-CBD-CGD-O1D
12	a	820	CLA	CHA-CBD-CGD-O1D
12	b	803	CLA	CHA-CBD-CGD-O2D
12	G	827	CLA	CHA-CBD-CGD-O1D
12	J	1102	CLA	CHA-CBD-CGD-O1D
12	J	1102	CLA	CHA-CBD-CGD-O2D
12	E	821	CLA	CHA-CBD-CGD-O1D
12	b	812	CLA	CHA-CBD-CGD-O1D
12	b	812	CLA	CHA-CBD-CGD-O2D
12	G	806	CLA	CHA-CBD-CGD-O1D
12	G	806	CLA	CHA-CBD-CGD-O2D
12	A	823	CLA	CHA-CBD-CGD-O2D
12	a	824	CLA	CHA-CBD-CGD-O2D
12	E	826	CLA	CHA-CBD-CGD-O2D
12	a	805	CLA	CHA-CBD-CGD-O1D
12	a	805	CLA	CHA-CBD-CGD-O2D
12	G	825	CLA	CHA-CBD-CGD-O1D
12	B	828	CLA	CHA-CBD-CGD-O1D
12	g	829	CLA	CHA-CBD-CGD-O1D
12	E	806	CLA	CHA-CBD-CGD-O1D
12	E	806	CLA	CHA-CBD-CGD-O2D
12	e	823	CLA	CHA-CBD-CGD-O2D
12	g	839	CLA	CHA-CBD-CGD-O2D
12	B	830	CLA	CHA-CBD-CGD-O1D
12	b	835	CLA	CHA-CBD-CGD-O1D
12	b	835	CLA	CHA-CBD-CGD-O2D
12	E	801	CLA	CHA-CBD-CGD-O2D
12	A	811	CLA	CHA-CBD-CGD-O1D
12	e	819	CLA	CHA-CBD-CGD-O1D
12	e	801	CLA	CHA-CBD-CGD-O2D
12	e	812	CLA	CHA-CBD-CGD-O1D
12	B	805	CLA	CHA-CBD-CGD-O2D
12	b	807	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	b	807	CLA	CHA-CBD-CGD-O2D
12	E	802	CLA	CHA-CBD-CGD-O1D
12	B	843	CLA	CAA-CBA-CGA-O1A
12	G	841	CLA	CAA-CBA-CGA-O1A
12	b	842	CLA	CAA-CBA-CGA-O1A
12	b	838	CLA	CAA-CBA-CGA-O2A
12	B	839	CLA	CAA-CBA-CGA-O2A
12	g	838	CLA	CAA-CBA-CGA-O2A
12	G	837	CLA	CAA-CBA-CGA-O2A
12	G	817	CLA	CBD-CGD-O2D-CED
12	E	820	CLA	CAA-CBA-CGA-O2A
12	a	819	CLA	CAA-CBA-CGA-O2A
12	e	818	CLA	CAA-CBA-CGA-O2A
12	A	817	CLA	CAA-CBA-CGA-O2A
12	b	818	CLA	O1D-CGD-O2D-CED
12	A	823	CLA	O1A-CGA-O2A-C1
12	E	826	CLA	O1A-CGA-O2A-C1
12	G	817	CLA	O1D-CGD-O2D-CED
12	g	819	CLA	CBD-CGD-O2D-CED
12	G	809	CLA	C1A-C2A-CAA-CBA
12	A	803	CLA	C1A-C2A-CAA-CBA
12	e	827	CLA	C1A-C2A-CAA-CBA
12	b	810	CLA	C1A-C2A-CAA-CBA
12	A	826	CLA	C1A-C2A-CAA-CBA
12	B	812	CLA	C1A-C2A-CAA-CBA
12	e	804	CLA	C1A-C2A-CAA-CBA
12	a	828	CLA	C1A-C2A-CAA-CBA
12	a	805	CLA	C1A-C2A-CAA-CBA
12	E	806	CLA	C1A-C2A-CAA-CBA
12	E	829	CLA	C1A-C2A-CAA-CBA
12	g	811	CLA	C1A-C2A-CAA-CBA
13	e	843	PQN	C12-C11-C3-C4
12	e	808	CLA	CBA-CGA-O2A-C1
12	E	810	CLA	CBA-CGA-O2A-C1
12	a	825	CLA	O1A-CGA-O2A-C1
12	e	824	CLA	O1A-CGA-O2A-C1
12	a	817	CLA	C2A-CAA-CBA-CGA
12	e	816	CLA	C2A-CAA-CBA-CGA
12	A	815	CLA	C2A-CAA-CBA-CGA
12	E	818	CLA	C2A-CAA-CBA-CGA
12	A	807	CLA	CBA-CGA-O2A-C1
12	a	809	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	B	820	CLA	O1D-CGD-O2D-CED
12	E	817	CLA	CAA-CBA-CGA-O2A
12	e	815	CLA	CAA-CBA-CGA-O2A
12	b	818	CLA	CBD-CGD-O2D-CED
12	G	834	CLA	CAA-CBA-CGA-O1A
12	g	835	CLA	CAA-CBA-CGA-O1A
12	J	1102	CLA	CAA-CBA-CGA-O1A
12	b	835	CLA	CAA-CBA-CGA-O1A
12	g	834	CLA	CAA-CBA-CGA-O1A
12	E	831	CLA	CAA-CBA-CGA-O1A
12	e	829	CLA	CAA-CBA-CGA-O1A
12	B	836	CLA	CAA-CBA-CGA-O1A
12	L	201	CLA	O1D-CGD-O2D-CED
12	a	820	CLA	CAA-CBA-CGA-O2A
12	A	828	CLA	CAA-CBA-CGA-O1A
12	a	830	CLA	CAA-CBA-CGA-O1A
12	G	833	CLA	CAA-CBA-CGA-O1A
12	b	834	CLA	CAA-CBA-CGA-O1A
12	g	819	CLA	O1D-CGD-O2D-CED
13	e	843	PQN	C20-C21-C22-C23
12	s	204	CLA	CAA-CBA-CGA-O2A
12	S	1502	CLA	CAA-CBA-CGA-O2A
12	A	818	CLA	CAA-CBA-CGA-O2A
12	E	821	CLA	CAA-CBA-CGA-O2A
12	e	819	CLA	CAA-CBA-CGA-O2A
12	e	842	CLA	CAA-CBA-CGA-O1A
12	e	803	CLA	CAD-CBD-CGD-O1D
12	e	827	CLA	CAD-CBD-CGD-O1D
12	a	807	CLA	CAD-CBD-CGD-O1D
12	A	826	CLA	CAD-CBD-CGD-O1D
12	A	831	CLA	CAD-CBD-CGD-O1D
12	E	814	CLA	CAD-CBD-CGD-O1D
12	A	818	CLA	CAD-CBD-CGD-O1D
12	a	815	CLA	CAD-CBD-CGD-O1D
12	a	833	CLA	CAD-CBD-CGD-O1D
12	a	828	CLA	CAD-CBD-CGD-O1D
12	E	808	CLA	CAD-CBD-CGD-O1D
12	A	805	CLA	CAD-CBD-CGD-O1D
12	A	813	CLA	CAD-CBD-CGD-O1D
12	a	820	CLA	CAD-CBD-CGD-O1D
12	E	821	CLA	CAD-CBD-CGD-O1D
12	E	805	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	E	835	CLA	CAD-CBD-CGD-O1D
12	e	806	CLA	CAD-CBD-CGD-O1D
12	e	814	CLA	CAD-CBD-CGD-O1D
12	a	804	CLA	CAD-CBD-CGD-O1D
12	A	811	CLA	CAD-CBD-CGD-O1D
12	e	819	CLA	CAD-CBD-CGD-O1D
12	E	816	CLA	CAD-CBD-CGD-O1D
12	A	802	CLA	CAD-CBD-CGD-O1D
12	E	829	CLA	CAD-CBD-CGD-O1D
12	e	832	CLA	CAD-CBD-CGD-O1D
12	l	204	CLA	CAA-CBA-CGA-O2A
12	a	816	CLA	CAA-CBA-CGA-O2A
12	L	204	CLA	CAA-CBA-CGA-O2A
12	A	814	CLA	CAA-CBA-CGA-O2A
12	e	808	CLA	O1A-CGA-O2A-C1
12	E	810	CLA	O1A-CGA-O2A-C1
12	A	807	CLA	O1A-CGA-O2A-C1
12	a	809	CLA	O1A-CGA-O2A-C1
12	s	201	CLA	O1D-CGD-O2D-CED
12	A	841	CLA	CAA-CBA-CGA-O1A
12	A	805	CLA	CAA-CBA-CGA-O2A
12	e	806	CLA	CAA-CBA-CGA-O2A
12	B	810	CLA	C2A-CAA-CBA-CGA
12	b	808	CLA	C2A-CAA-CBA-CGA
12	g	809	CLA	C2A-CAA-CBA-CGA
12	G	807	CLA	C2A-CAA-CBA-CGA
12	a	816	CLA	CAA-CBA-CGA-O1A
12	L	204	CLA	CAA-CBA-CGA-O1A
12	E	833	CLA	O1D-CGD-O2D-CED
12	l	201	CLA	O1D-CGD-O2D-CED
12	E	833	CLA	CAA-CBA-CGA-O2A
12	s	201	CLA	CAA-CBA-CGA-O2A
12	E	808	CLA	CAA-CBA-CGA-O2A
12	l	201	CLA	CAA-CBA-CGA-O2A
12	a	802	CLA	CAA-CBA-CGA-O2A
12	L	201	CLA	CAA-CBA-CGA-O2A
12	E	802	CLA	CAA-CBA-CGA-O2A
12	e	815	CLA	CAA-CBA-CGA-O1A
12	E	820	CLA	CAA-CBA-CGA-O1A
12	a	819	CLA	CAA-CBA-CGA-O1A
12	e	818	CLA	CAA-CBA-CGA-O1A
12	A	817	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	G	804	CLA	CAA-CBA-CGA-O2A
12	a	807	CLA	CAA-CBA-CGA-O2A
12	B	801	CLA	CAA-CBA-CGA-O2A
12	g	821	CLA	CAA-CBA-CGA-O2A
12	g	801	CLA	CAA-CBA-CGA-O2A
12	G	819	CLA	CAA-CBA-CGA-O2A
12	a	815	CLA	C2A-CAA-CBA-CGA
12	A	813	CLA	C2A-CAA-CBA-CGA
12	e	814	CLA	C2A-CAA-CBA-CGA
12	E	816	CLA	C2A-CAA-CBA-CGA
12	E	817	CLA	CAA-CBA-CGA-O1A
12	s	204	CLA	CAA-CBA-CGA-O1A
12	S	1502	CLA	CAA-CBA-CGA-O1A
12	B	801	CLA	CAA-CBA-CGA-O1A
12	g	801	CLA	CAA-CBA-CGA-O1A
12	a	802	CLA	CAA-CBA-CGA-O1A
12	A	814	CLA	CAA-CBA-CGA-O1A
12	E	802	CLA	CAA-CBA-CGA-O1A
12	G	839	CLA	CAA-CBA-CGA-O2A
12	B	822	CLA	CAA-CBA-CGA-O2A
12	g	806	CLA	CAA-CBA-CGA-O2A
12	b	840	CLA	CAA-CBA-CGA-O2A
12	B	841	CLA	CAA-CBA-CGA-O2A
12	g	840	CLA	CAA-CBA-CGA-O2A
12	b	820	CLA	CAA-CBA-CGA-O2A
12	b	805	CLA	CAA-CBA-CGA-O2A
12	B	807	CLA	CAA-CBA-CGA-O2A
12	l	204	CLA	CAA-CBA-CGA-O1A
12	e	832	CLA	C2A-CAA-CBA-CGA
12	b	828	CLA	CAA-CBA-CGA-O2A
12	G	827	CLA	CAA-CBA-CGA-O2A
12	g	829	CLA	CAA-CBA-CGA-O2A
12	B	830	CLA	CAA-CBA-CGA-O2A
12	G	804	CLA	CAA-CBA-CGA-O1A
12	E	808	CLA	CAA-CBA-CGA-O1A
12	A	805	CLA	CAA-CBA-CGA-O1A
12	g	806	CLA	CAA-CBA-CGA-O1A
12	g	840	CLA	CAA-CBA-CGA-O1A
12	e	806	CLA	CAA-CBA-CGA-O1A
12	b	805	CLA	CAA-CBA-CGA-O1A
12	B	807	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

188 monomers are involved in 1018 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	801	CLA	9	0
12	A	802	CLA	8	0
12	A	803	CLA	10	0
12	A	804	CLA	5	0
12	A	805	CLA	8	0
12	A	806	CLA	8	0
12	A	808	CLA	5	0
12	A	809	CLA	2	0
12	A	810	CLA	6	0
12	A	811	CLA	7	0
12	A	812	CLA	7	0
12	A	813	CLA	6	0
12	A	814	CLA	5	0
12	A	815	CLA	5	0
12	A	816	CLA	6	0
12	A	817	CLA	6	0
12	A	818	CLA	7	0
12	A	819	CLA	2	0
12	A	820	CLA	8	0
12	A	821	CLA	5	0
12	A	822	CLA	4	0
12	A	823	CLA	9	0
12	A	824	CLA	3	0
12	A	825	CLA	7	0
12	A	826	CLA	4	0
12	A	827	CLA	6	0
12	A	828	CLA	4	0
12	A	829	CLA	6	0
12	A	830	CLA	5	0
12	A	831	CLA	7	0
12	A	832	CLA	8	0
12	A	833	CLA	9	0
12	A	834	CLA	10	0
12	A	835	CLA	6	0
12	A	836	CLA	9	0
12	A	837	CLA	8	0
12	A	838	CLA	9	0
12	A	839	CLA	7	0
12	A	840	CLA	6	0
12	A	841	CLA	6	0
13	A	842	PQN	7	0
12	B	801	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	802	CLA	8	0
12	B	803	CLA	6	0
12	B	805	CLA	12	0
12	B	806	CLA	12	0
12	B	807	CLA	14	0
12	B	808	CLA	4	0
12	B	809	CLA	9	0
12	B	810	CLA	7	0
12	B	811	CLA	5	0
12	B	812	CLA	4	0
12	B	813	CLA	6	0
12	B	814	CLA	6	0
12	B	815	CLA	7	0
12	B	816	CLA	5	0
12	B	817	CLA	9	0
12	B	818	CLA	5	0
12	B	819	CLA	6	0
12	B	820	CLA	7	0
12	B	821	CLA	6	0
12	B	822	CLA	8	0
12	B	823	CLA	4	0
12	B	824	CLA	10	0
12	B	825	CLA	4	0
12	B	826	CLA	8	0
12	B	827	CLA	7	0
12	B	828	CLA	7	0
12	B	829	CLA	6	0
12	B	830	CLA	5	0
12	B	831	CLA	4	0
12	B	832	CLA	5	0
12	B	833	CLA	2	0
12	B	834	CLA	6	0
12	B	835	CLA	9	0
12	B	836	CLA	6	0
12	B	837	CLA	3	0
12	B	838	CLA	4	0
12	B	839	CLA	8	0
12	B	840	CLA	7	0
12	B	841	CLA	7	0
12	B	842	CLA	6	0
12	B	843	CLA	2	0
13	B	844	PQN	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	101	SF4	1	0
14	C	102	SF4	6	0
12	E	801	CLA	10	0
12	E	802	CLA	9	0
12	E	803	CLA	3	0
12	E	804	CLA	11	0
12	E	805	CLA	7	0
12	E	806	CLA	11	0
12	E	807	CLA	7	0
12	E	808	CLA	1	0
12	E	809	CLA	5	0
12	E	810	CLA	2	0
12	E	811	CLA	3	0
12	E	812	CLA	7	0
12	E	813	CLA	8	0
12	E	814	CLA	5	0
12	E	815	CLA	4	0
12	E	816	CLA	5	0
12	E	817	CLA	6	0
12	E	818	CLA	7	0
12	E	819	CLA	7	0
12	E	820	CLA	2	0
12	E	821	CLA	8	0
12	E	822	CLA	5	0
12	E	823	CLA	5	0
12	E	824	CLA	8	0
12	E	825	CLA	3	0
12	E	826	CLA	8	0
12	E	827	CLA	3	0
12	E	828	CLA	5	0
12	E	829	CLA	4	0
12	E	830	CLA	5	0
12	E	831	CLA	5	0
12	E	832	CLA	9	0
12	E	833	CLA	4	0
12	E	834	CLA	8	0
12	E	835	CLA	13	0
12	E	836	CLA	7	0
12	E	837	CLA	6	0
12	E	838	CLA	9	0
12	E	839	CLA	11	0
12	E	840	CLA	5	0

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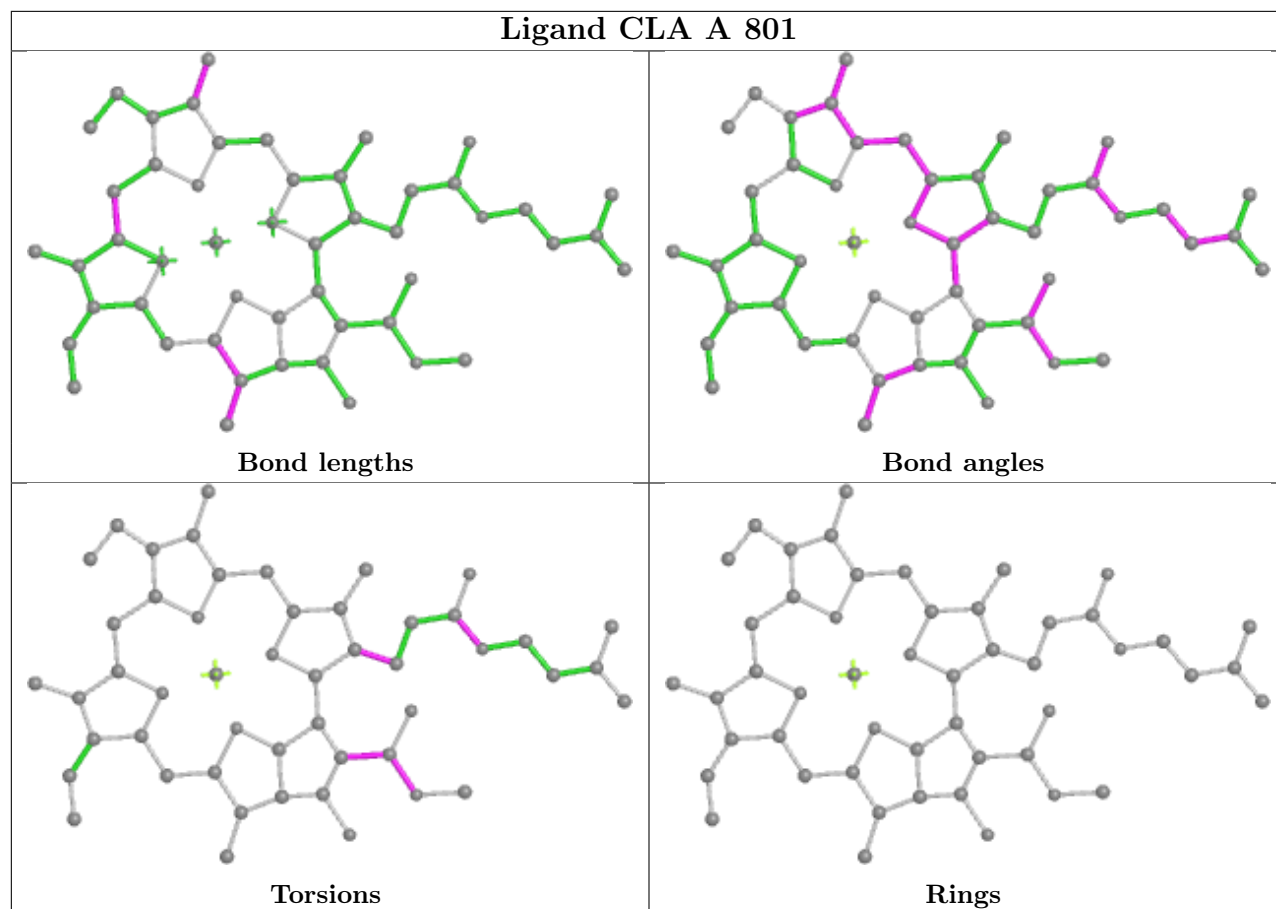
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	841	CLA	4	0
12	E	842	CLA	10	0
12	E	843	CLA	6	0
12	E	844	CLA	7	0
13	E	846	PQN	9	0
12	F	1301	CLA	4	0
12	G	801	CLA	18	0
12	G	802	CLA	5	0
12	G	803	CLA	1	0
12	G	804	CLA	8	0
12	G	805	CLA	11	0
12	G	806	CLA	13	0
12	G	807	CLA	2	0
12	G	808	CLA	12	0
12	G	809	CLA	4	0
12	G	810	CLA	4	0
12	G	811	CLA	5	0
12	G	812	CLA	6	0
12	G	813	CLA	6	0
12	G	814	CLA	10	0
12	G	815	CLA	6	0
12	G	816	CLA	7	0
12	G	817	CLA	6	0
12	G	818	CLA	6	0
12	G	819	CLA	7	0
12	G	820	CLA	6	0
12	G	821	CLA	8	0
12	G	822	CLA	3	0
12	G	823	CLA	10	0
12	G	824	CLA	4	0
12	G	825	CLA	7	0
12	G	826	CLA	6	0
12	G	827	CLA	7	0
12	G	828	CLA	5	0
12	G	829	CLA	6	0
12	G	830	CLA	3	0
12	G	831	CLA	6	0
12	G	832	CLA	2	0
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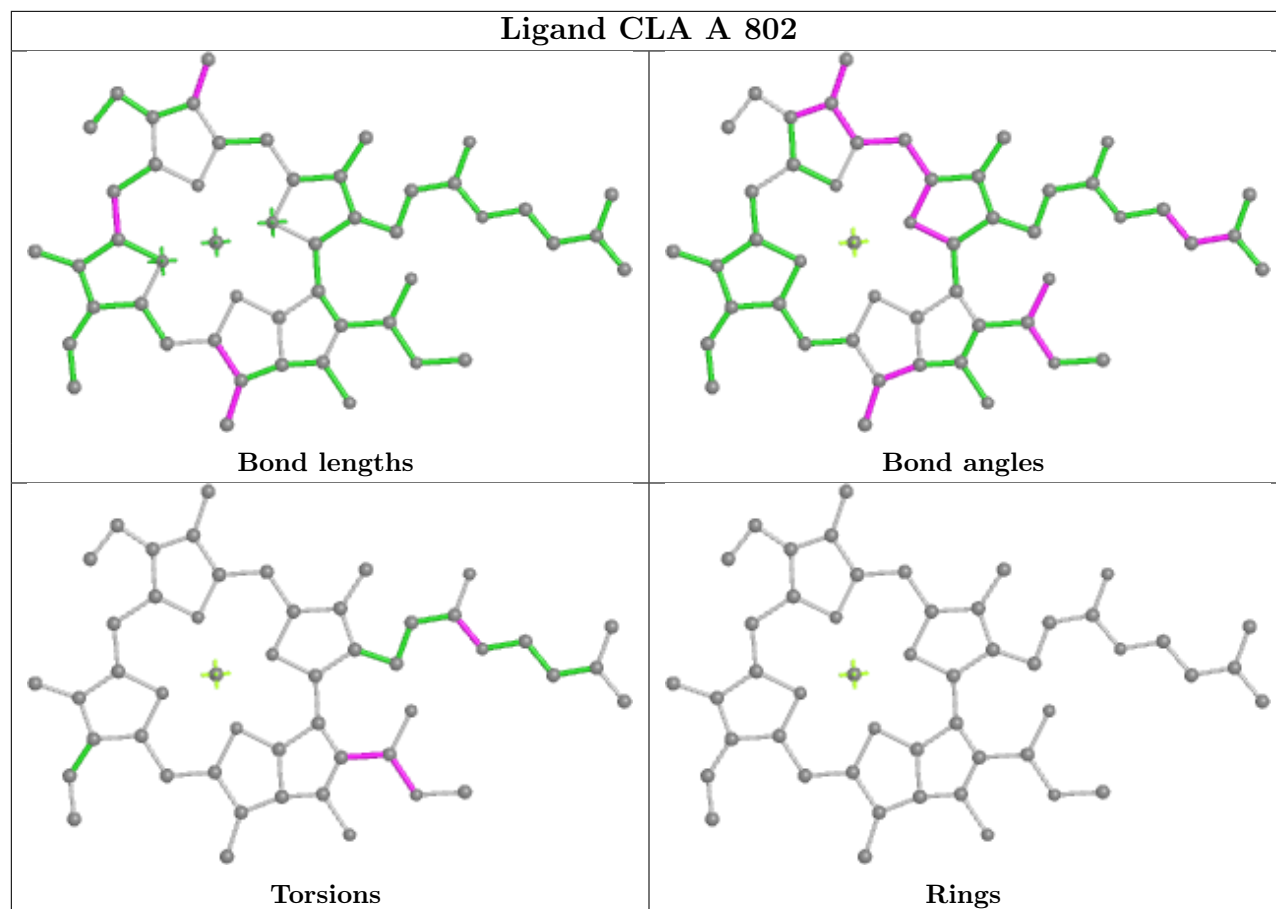
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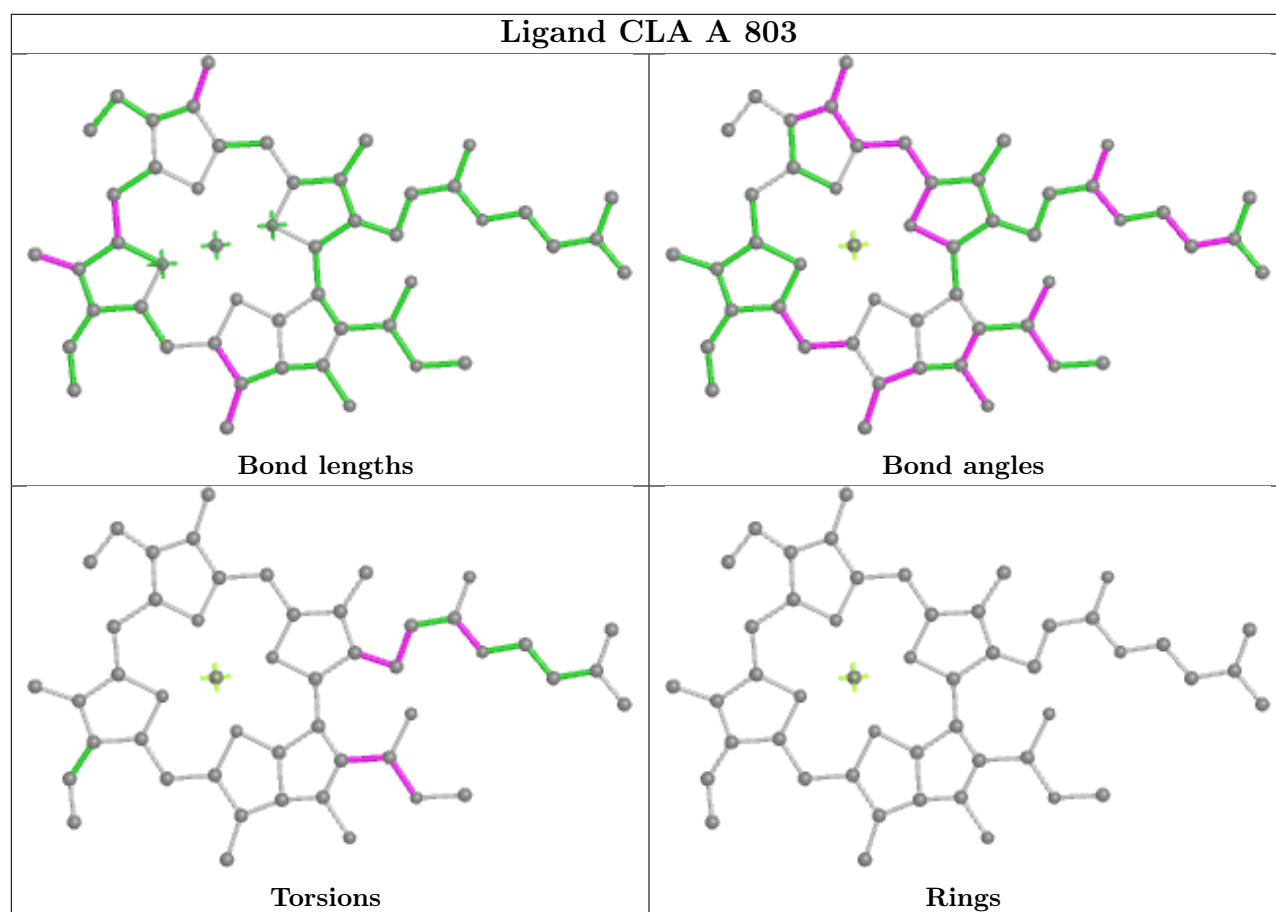
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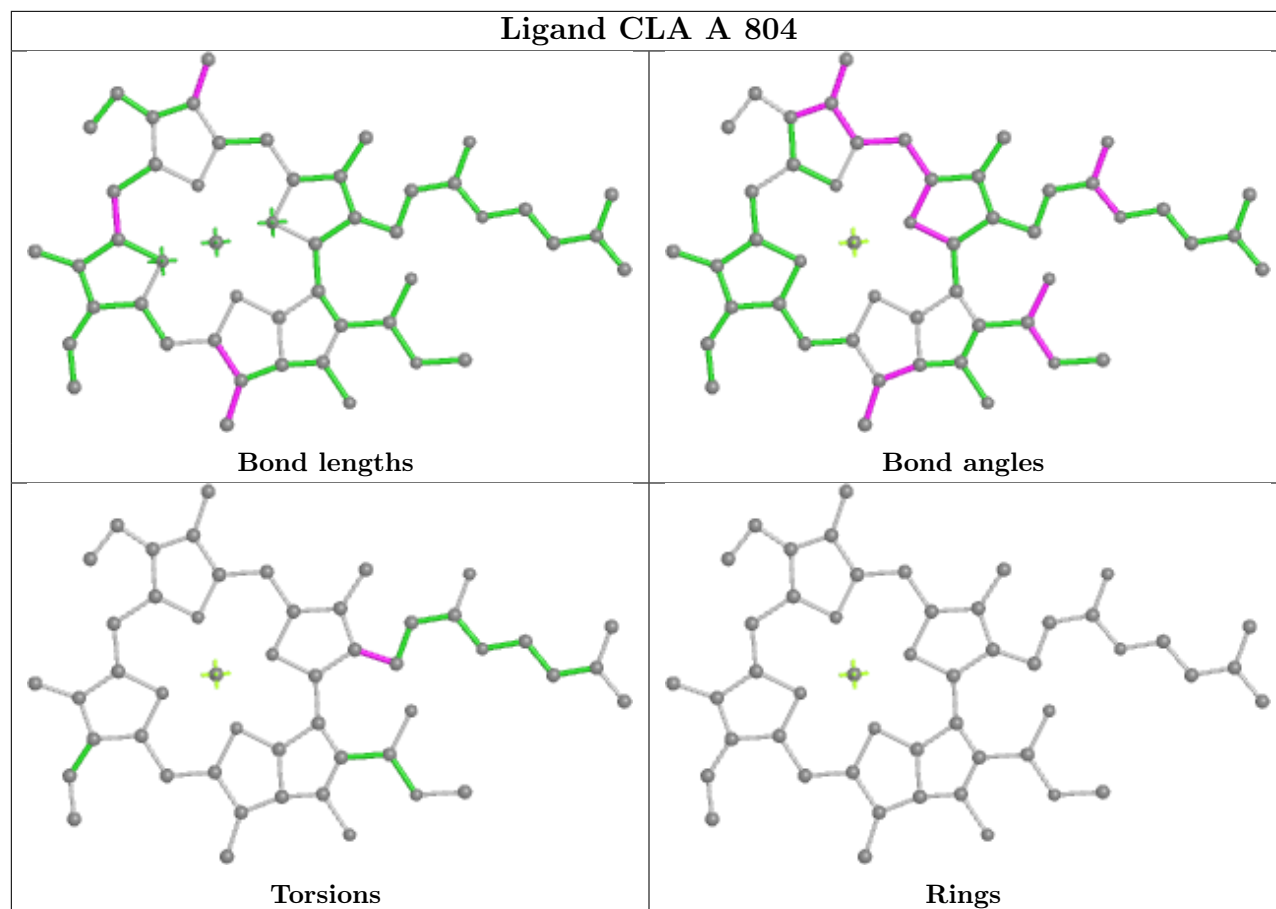
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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12	G	838	CLA	9	0
12	G	839	CLA	7	0
12	G	840	CLA	11	0
12	G	841	CLA	7	0
13	G	842	PQN	4	0
12	G	843	CLA	3	0
14	H	101	SF4	1	0
14	H	102	SF4	6	0
12	J	1101	CLA	5	0
12	J	1102	CLA	8	0
12	K	1401	CLA	2	0
12	L	201	CLA	4	0
12	L	202	CLA	2	0
12	L	203	CLA	3	0
12	L	204	CLA	5	0
12	O	1301	CLA	1	0
12	R	1401	CLA	3	0
12	S	1501	CLA	2	0
12	S	1502	CLA	4	0

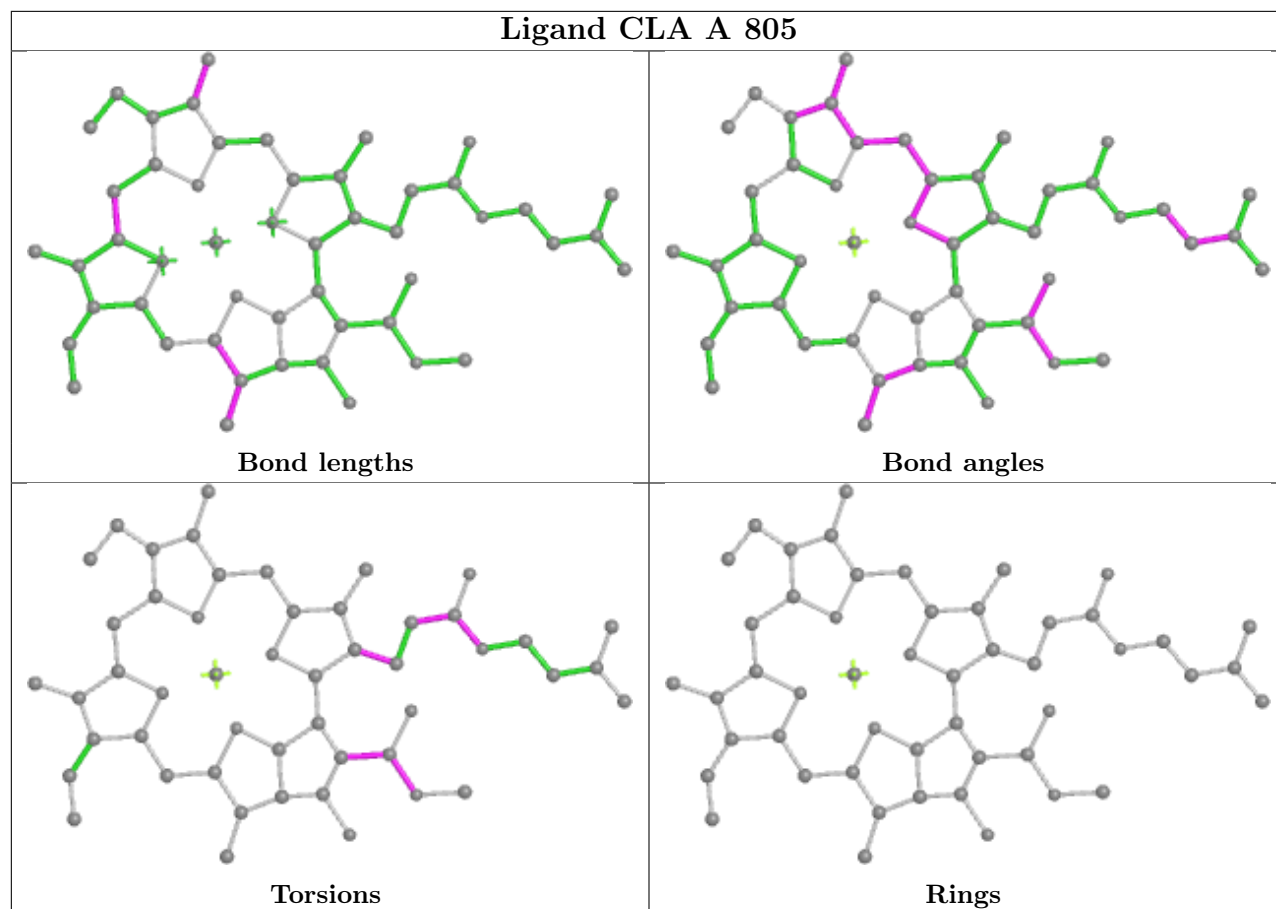
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

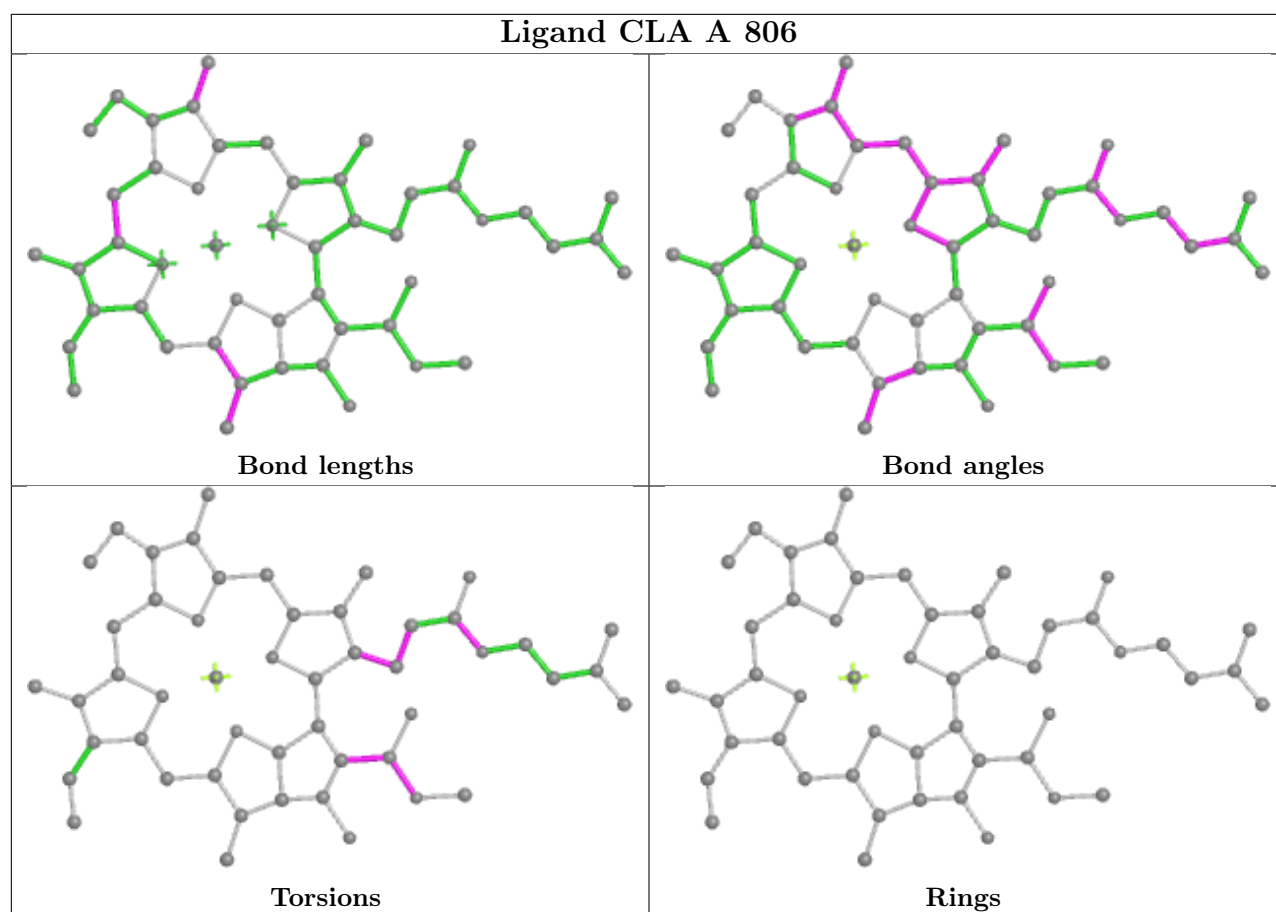


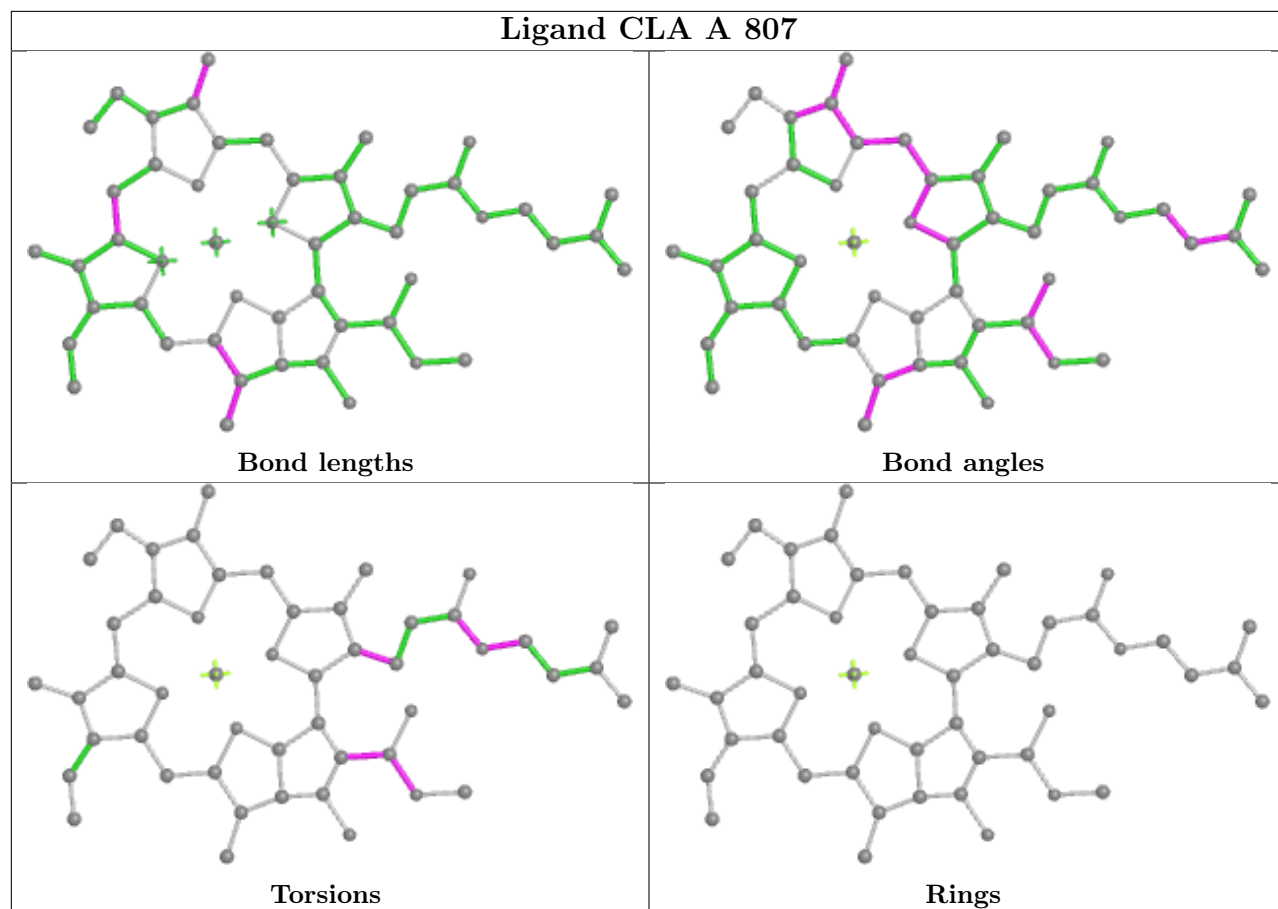




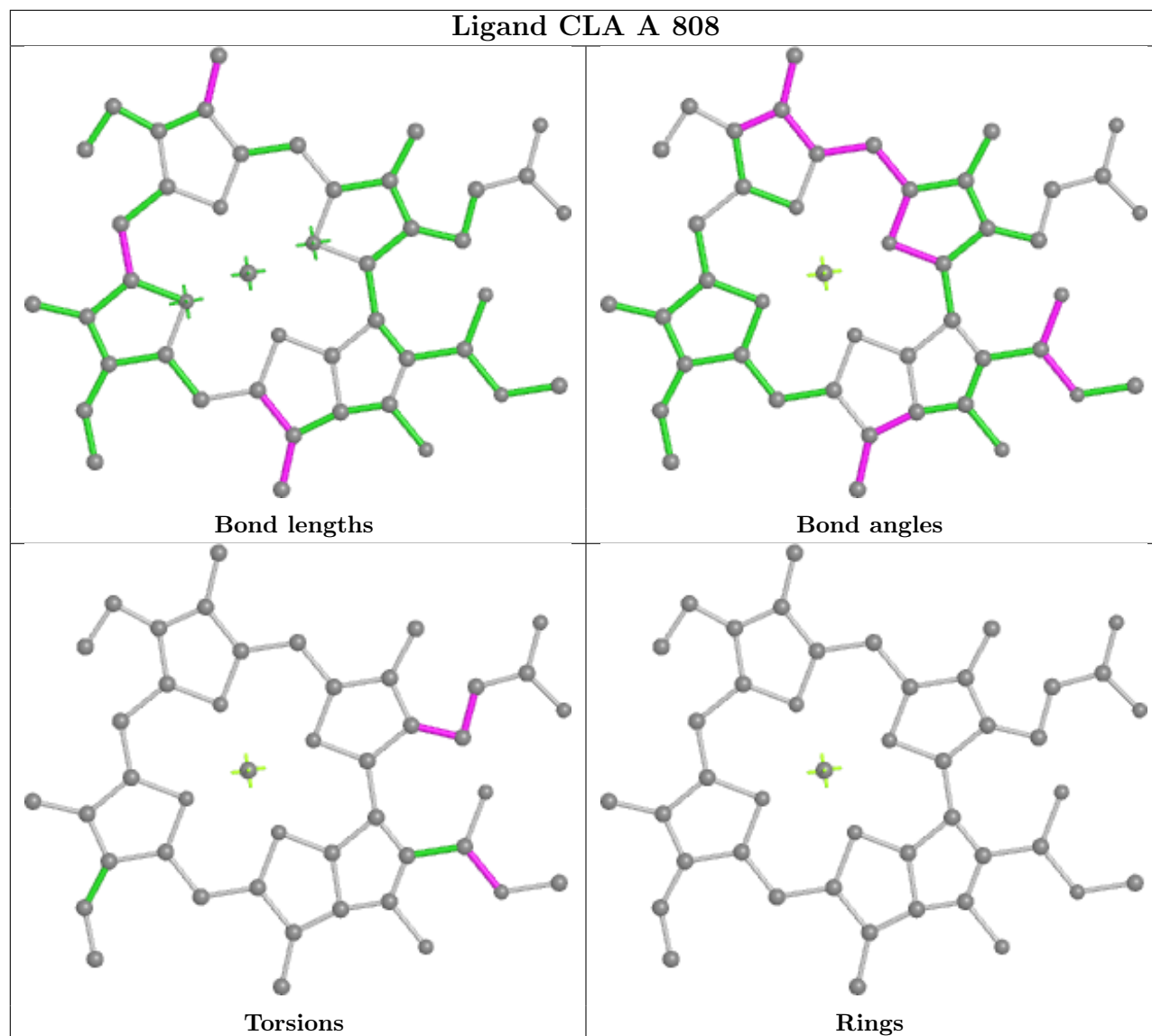


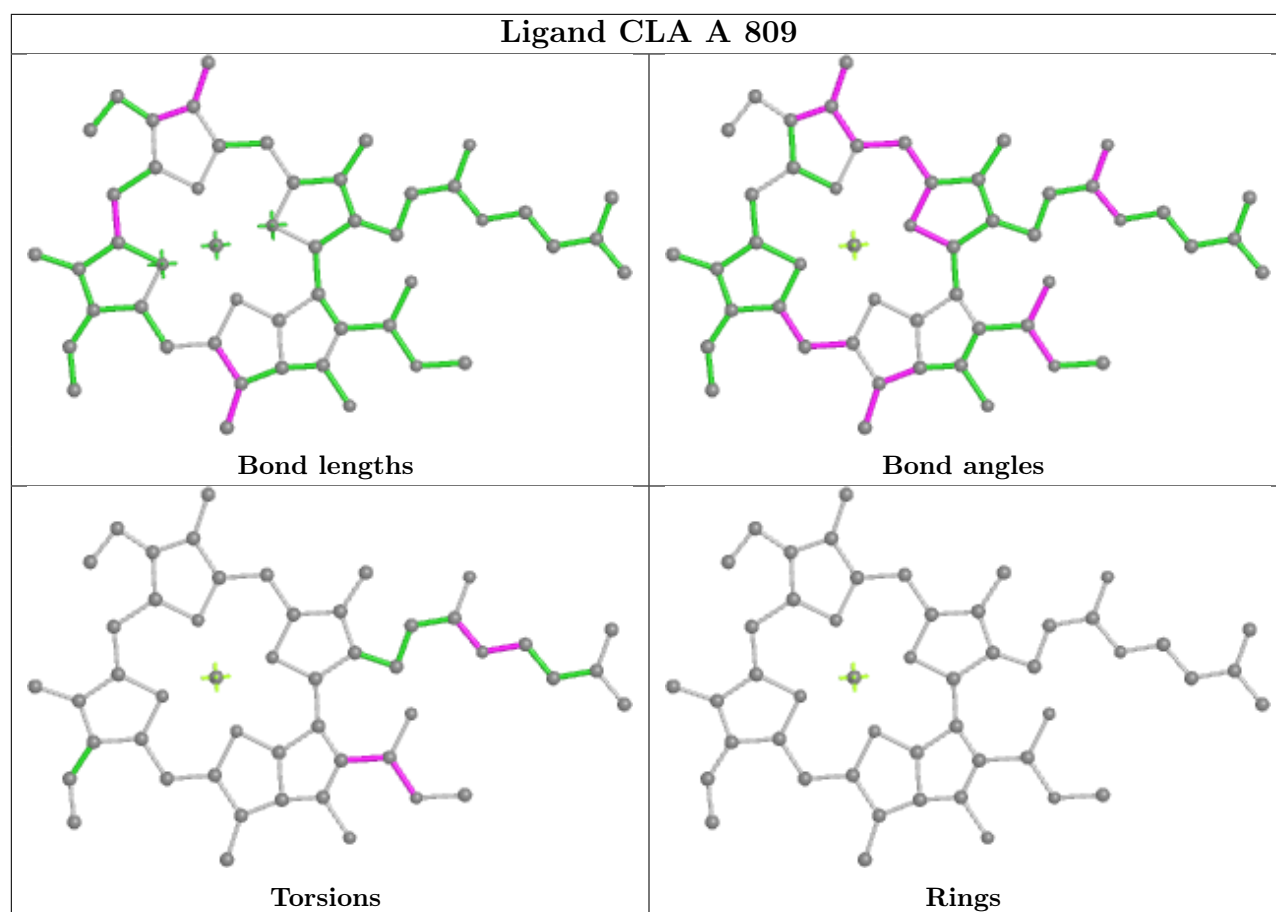


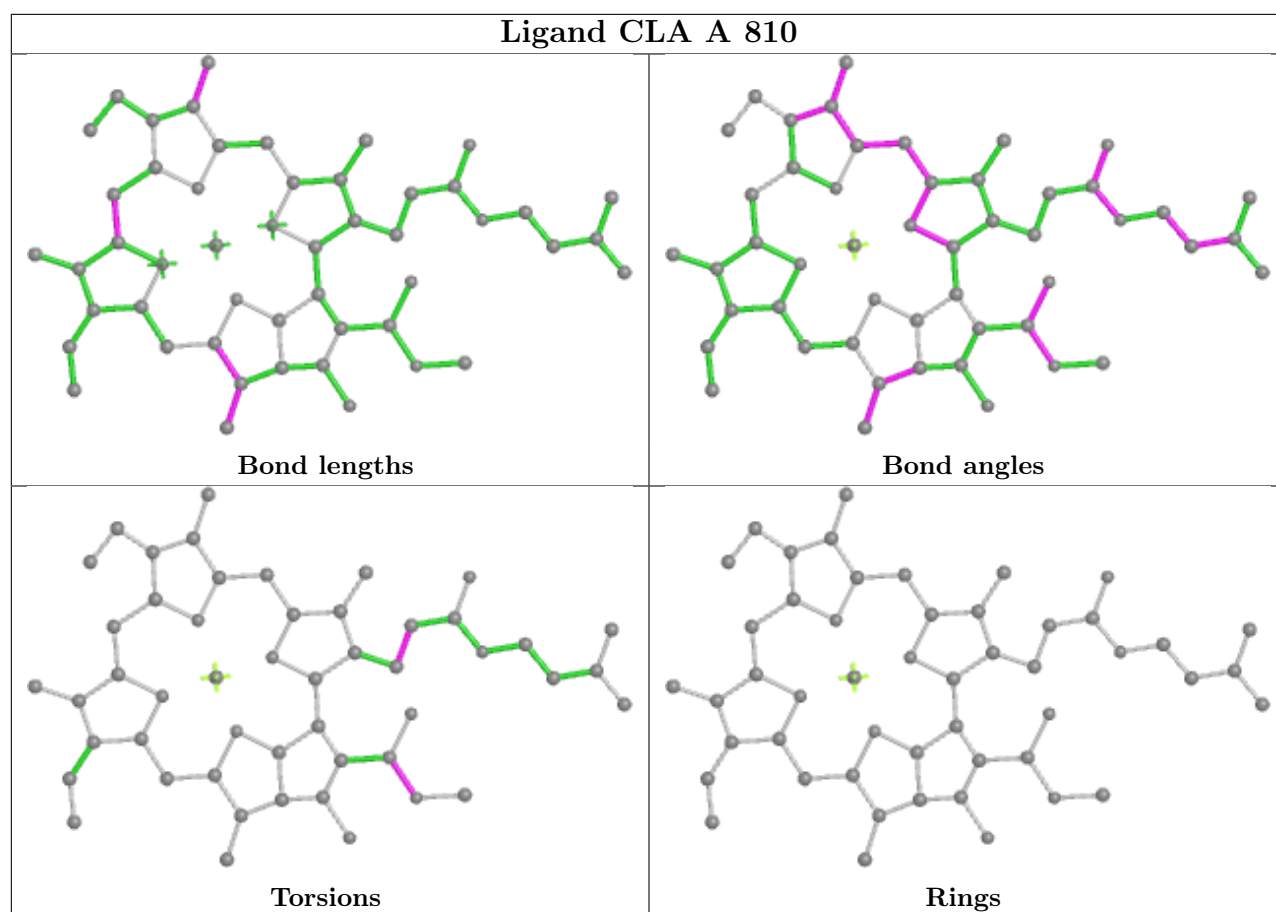




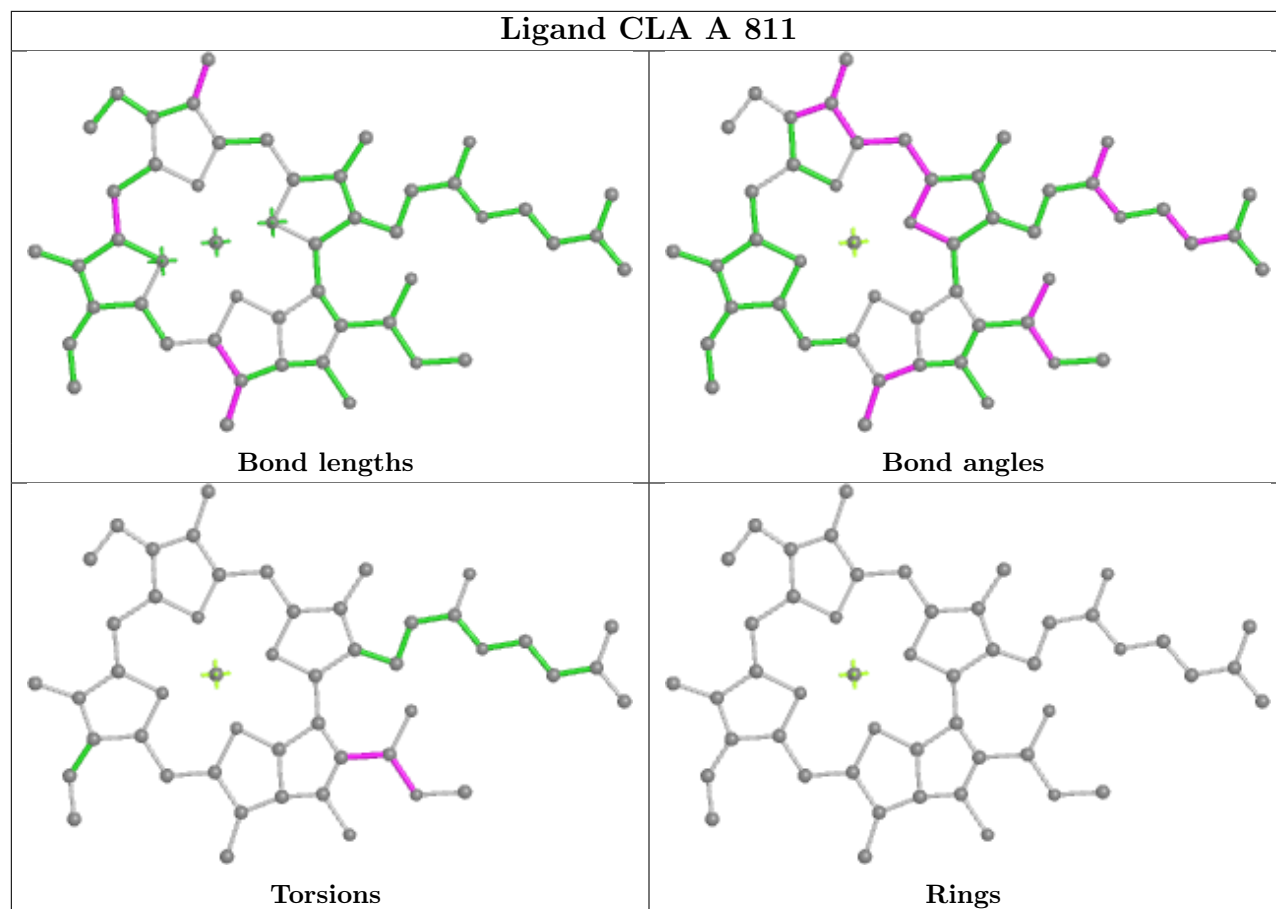
Ligand CLA A 808



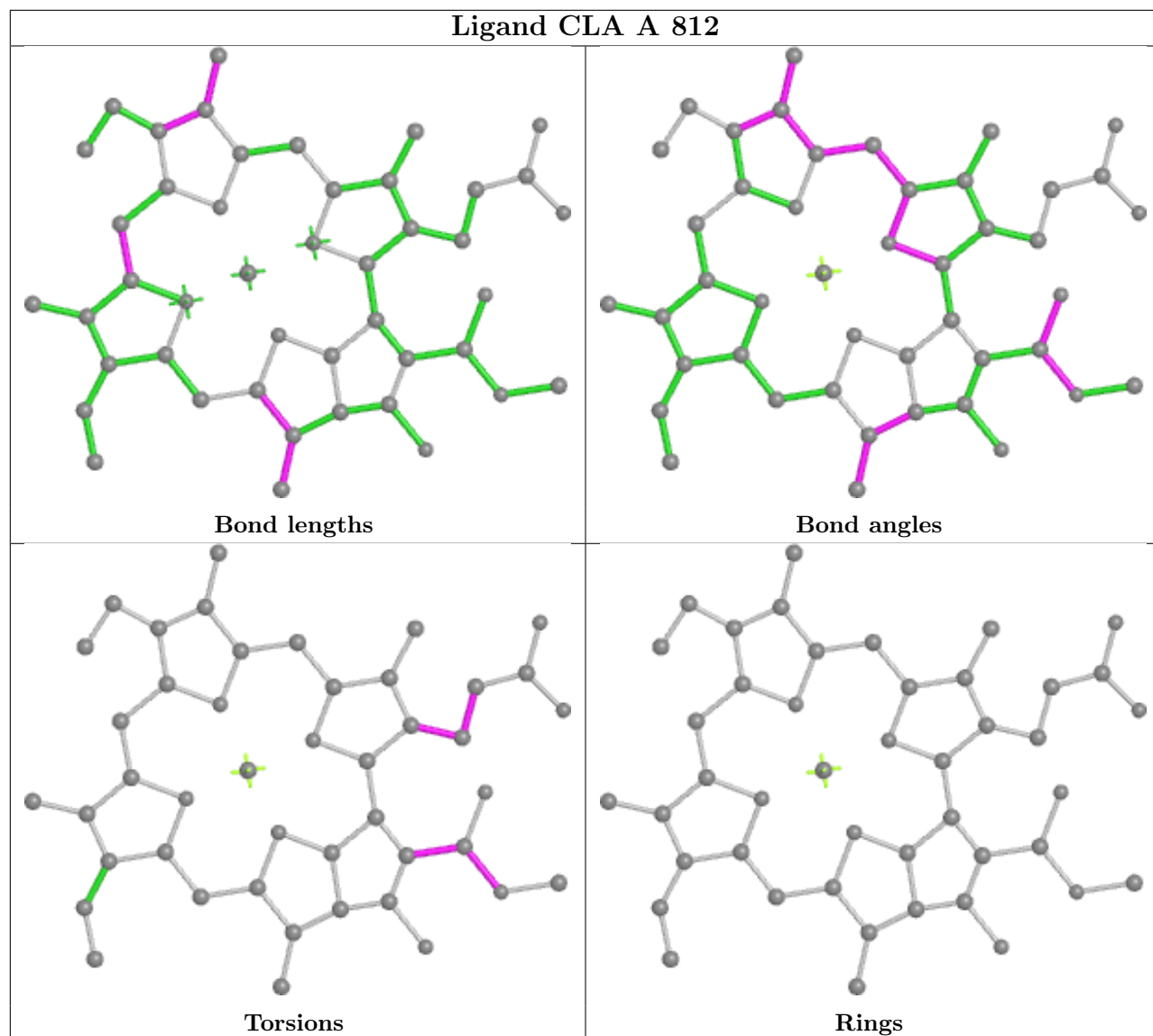




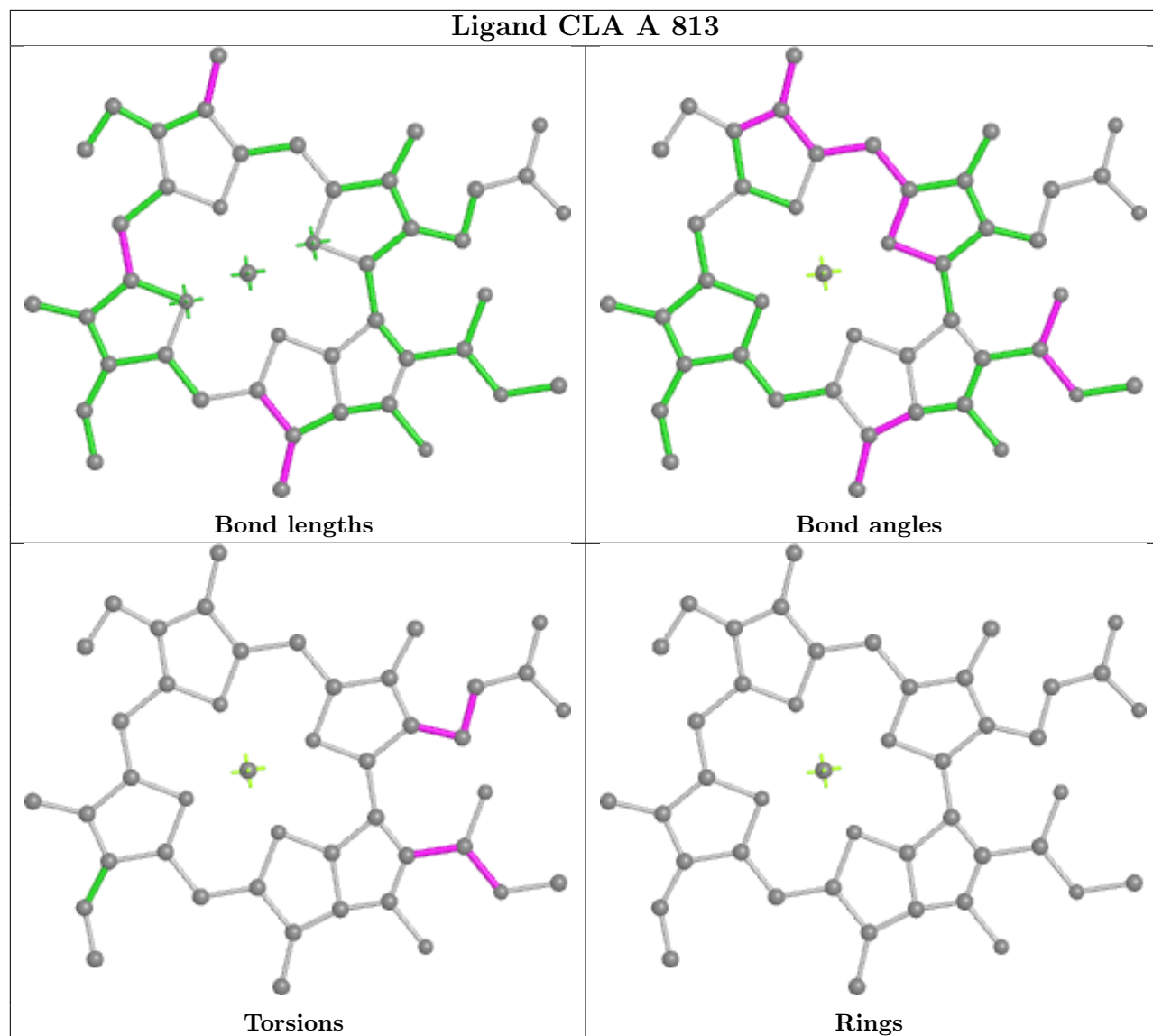
Ligand CLA A 811



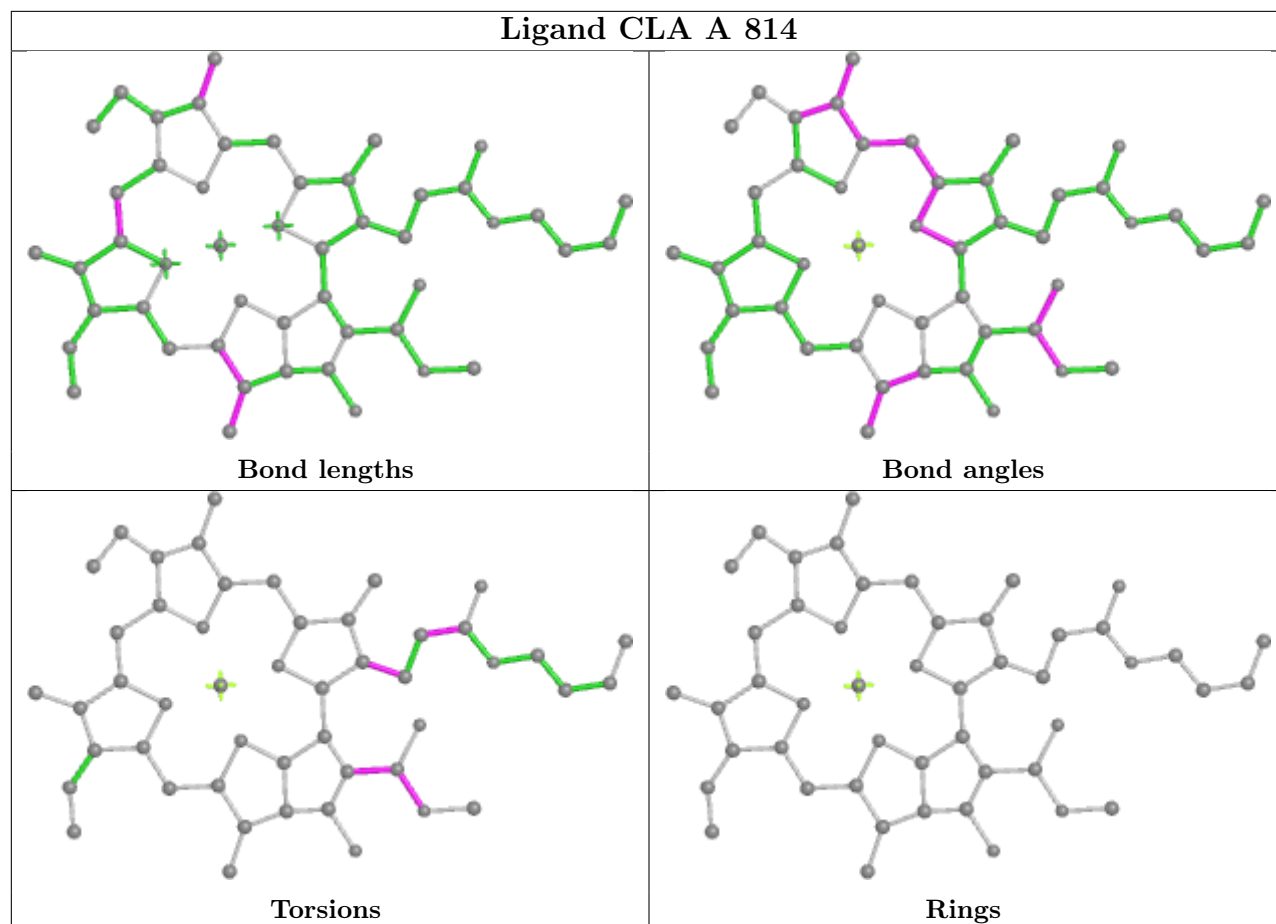
Ligand CLA A 812

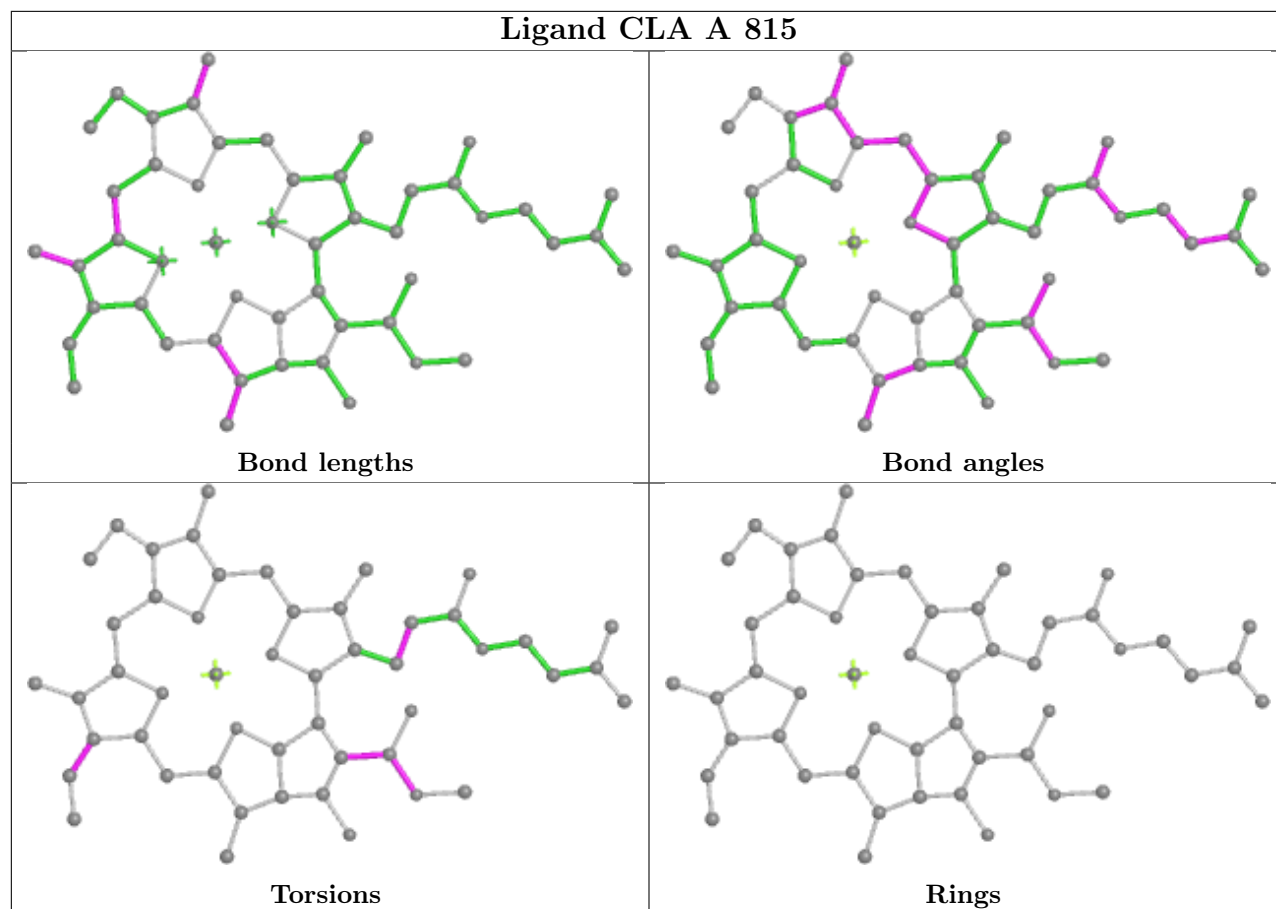


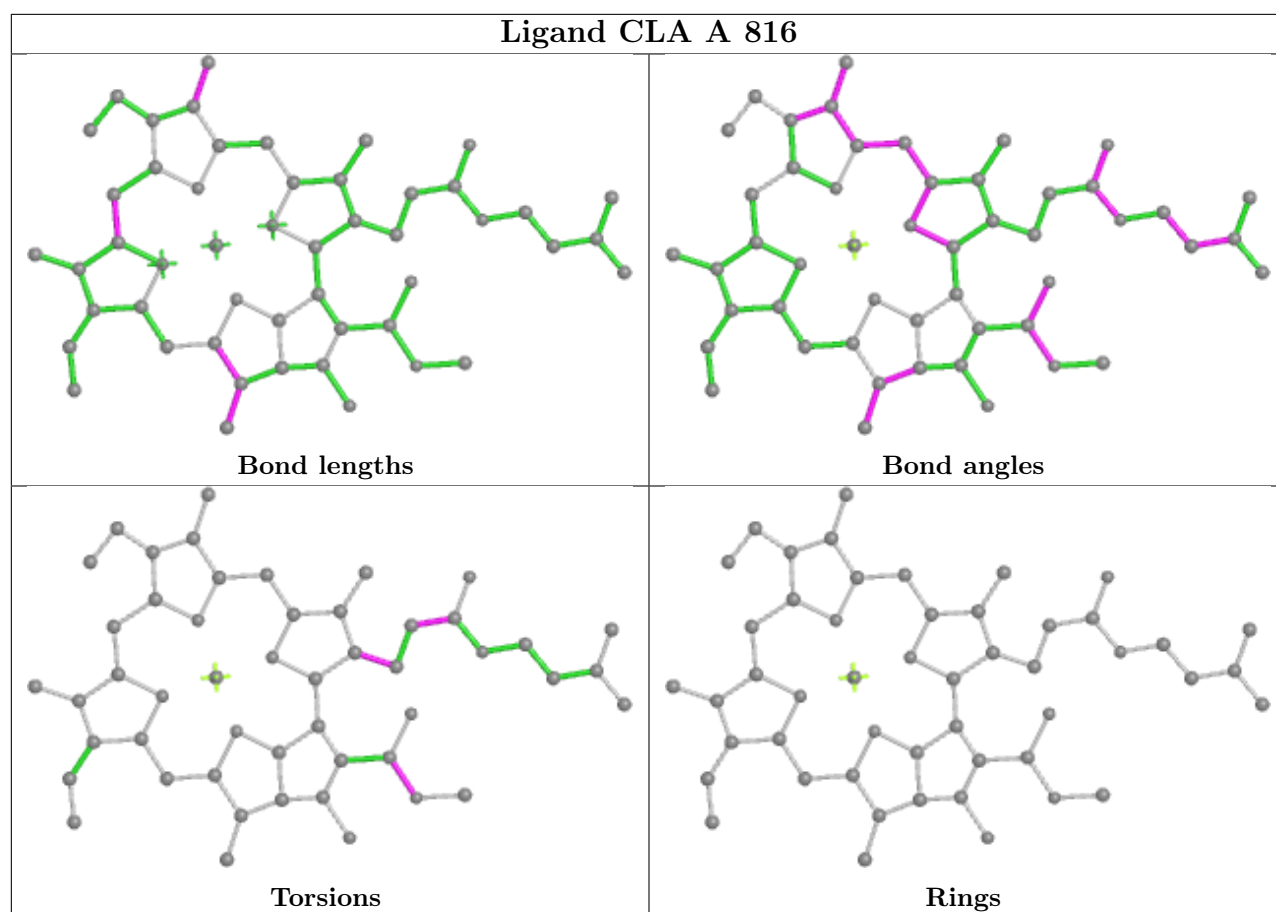
Ligand CLA A 813

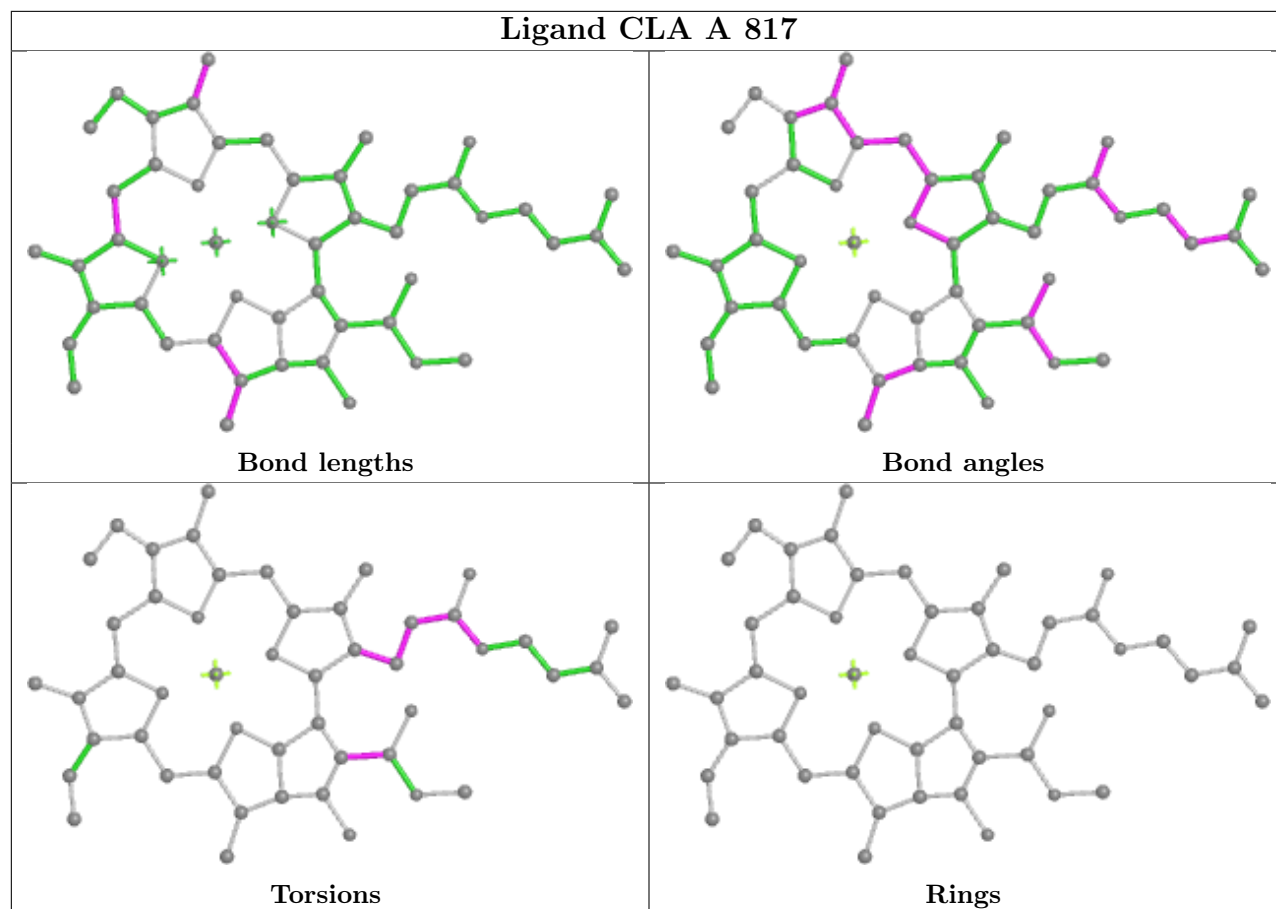


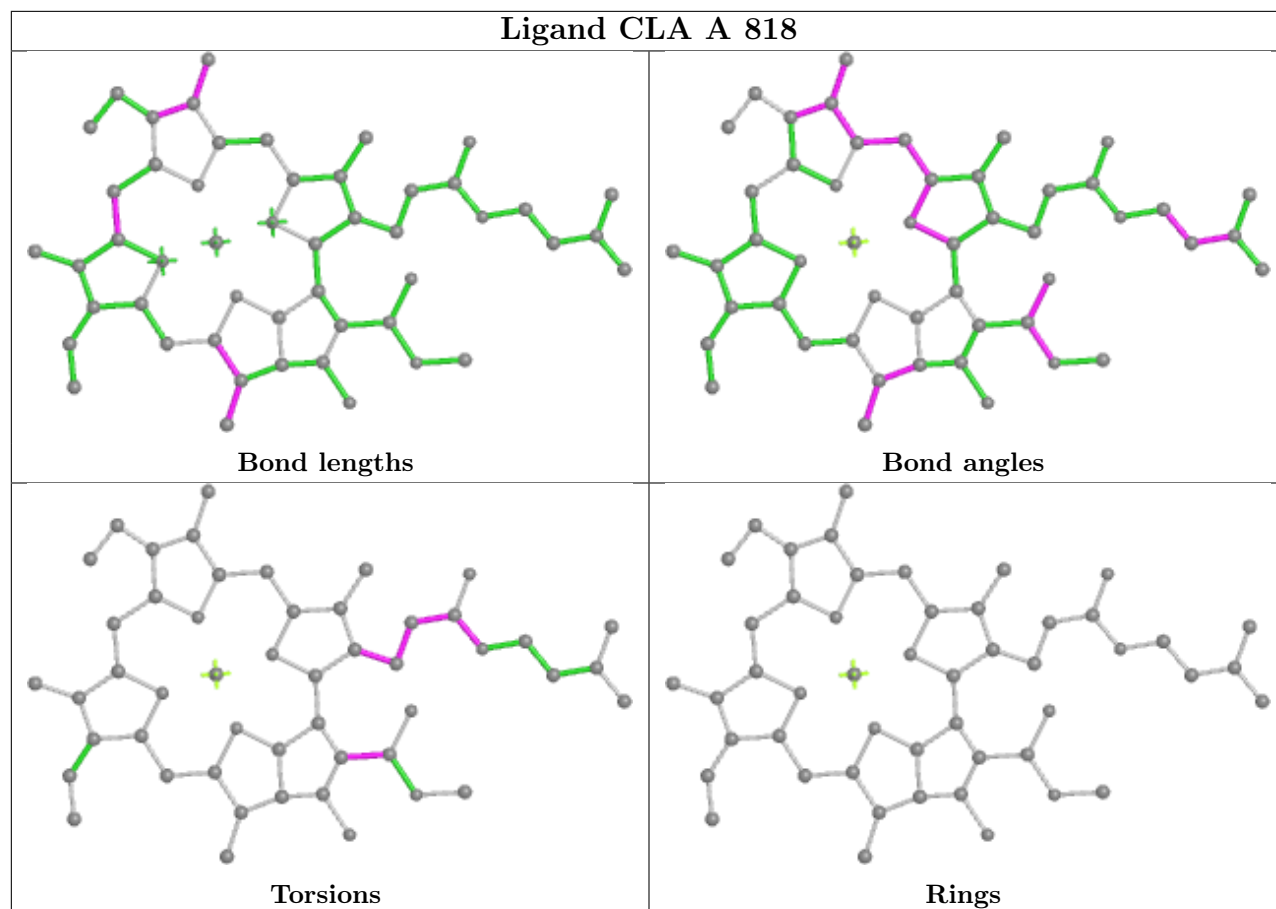
Ligand CLA A 814

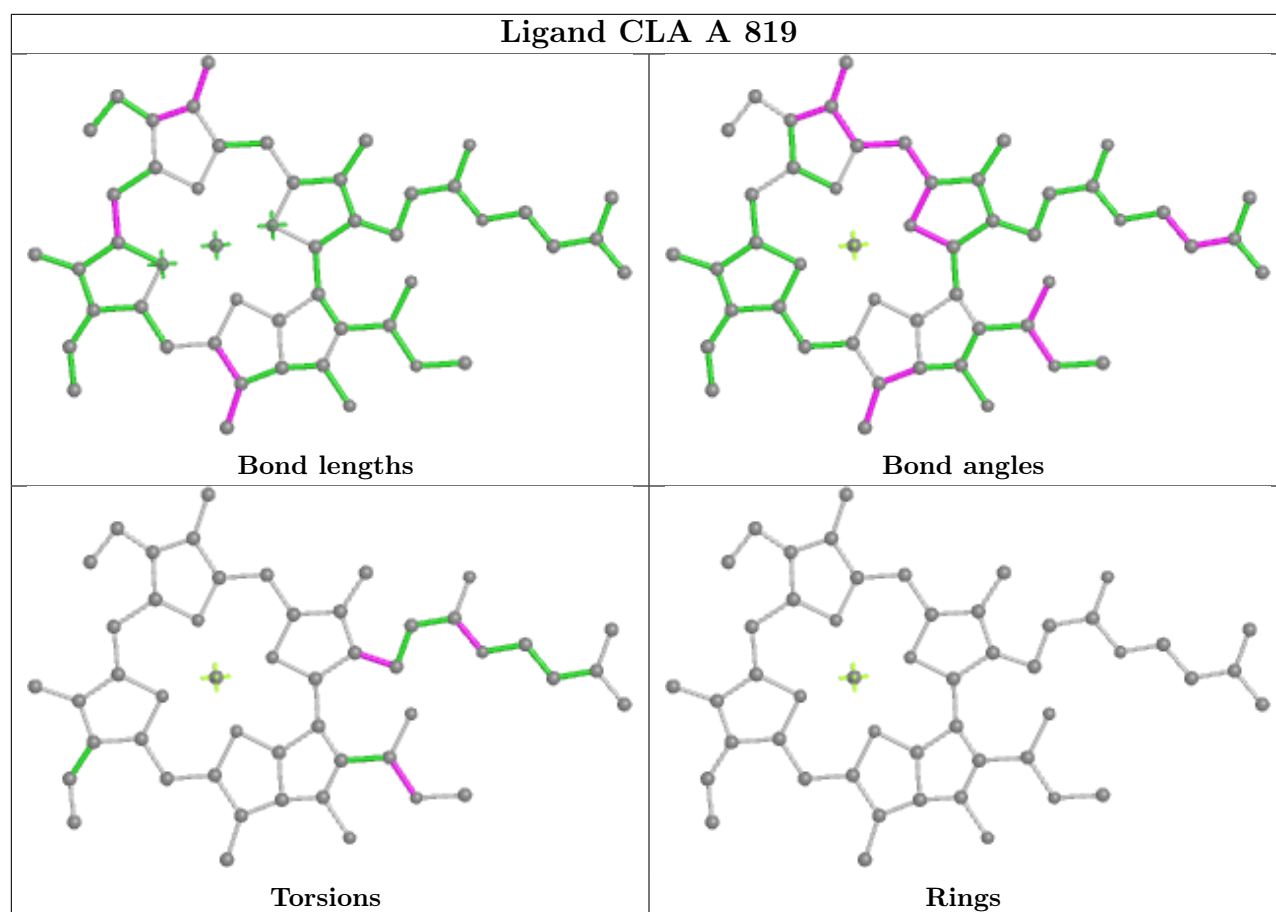


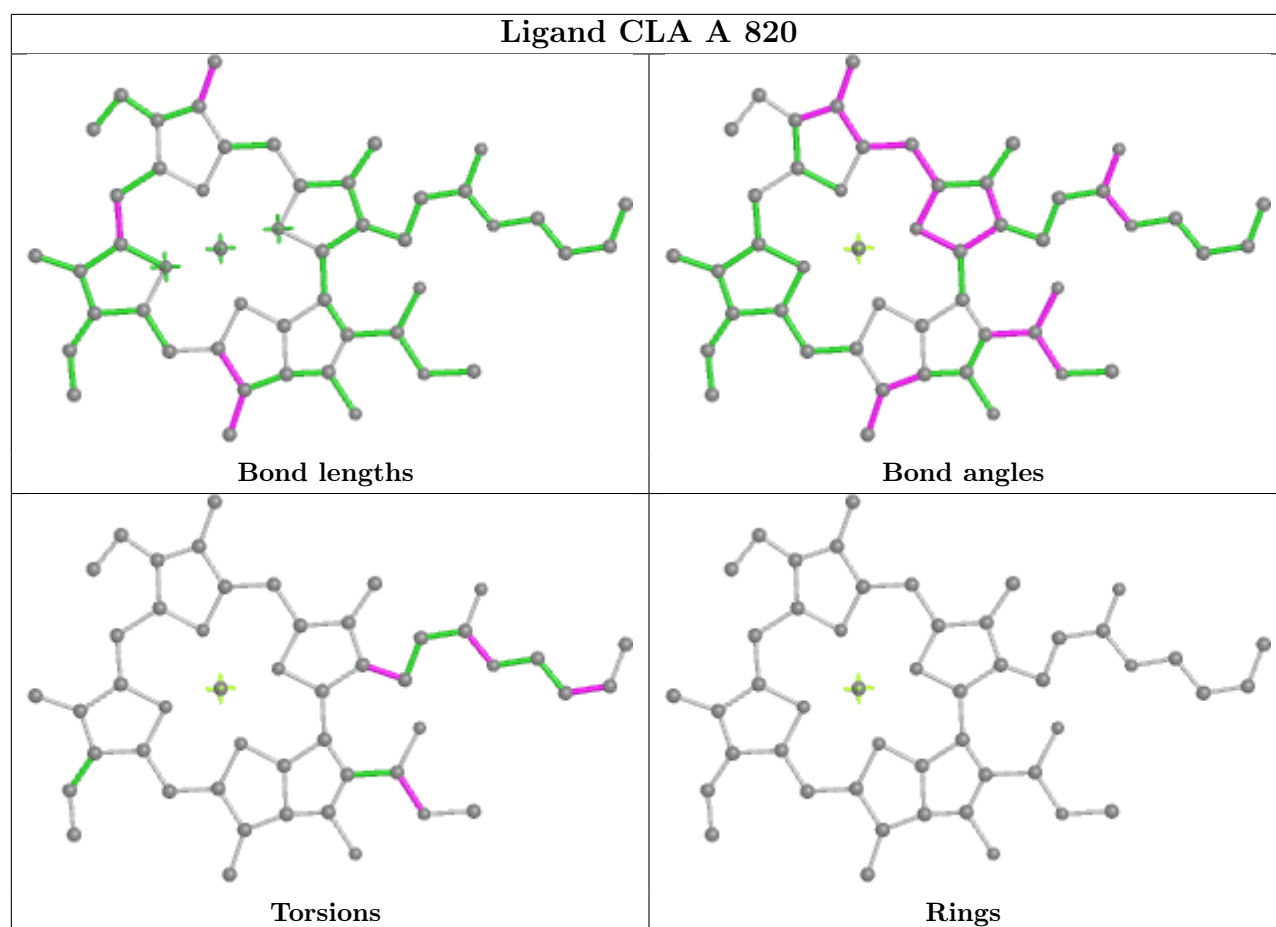


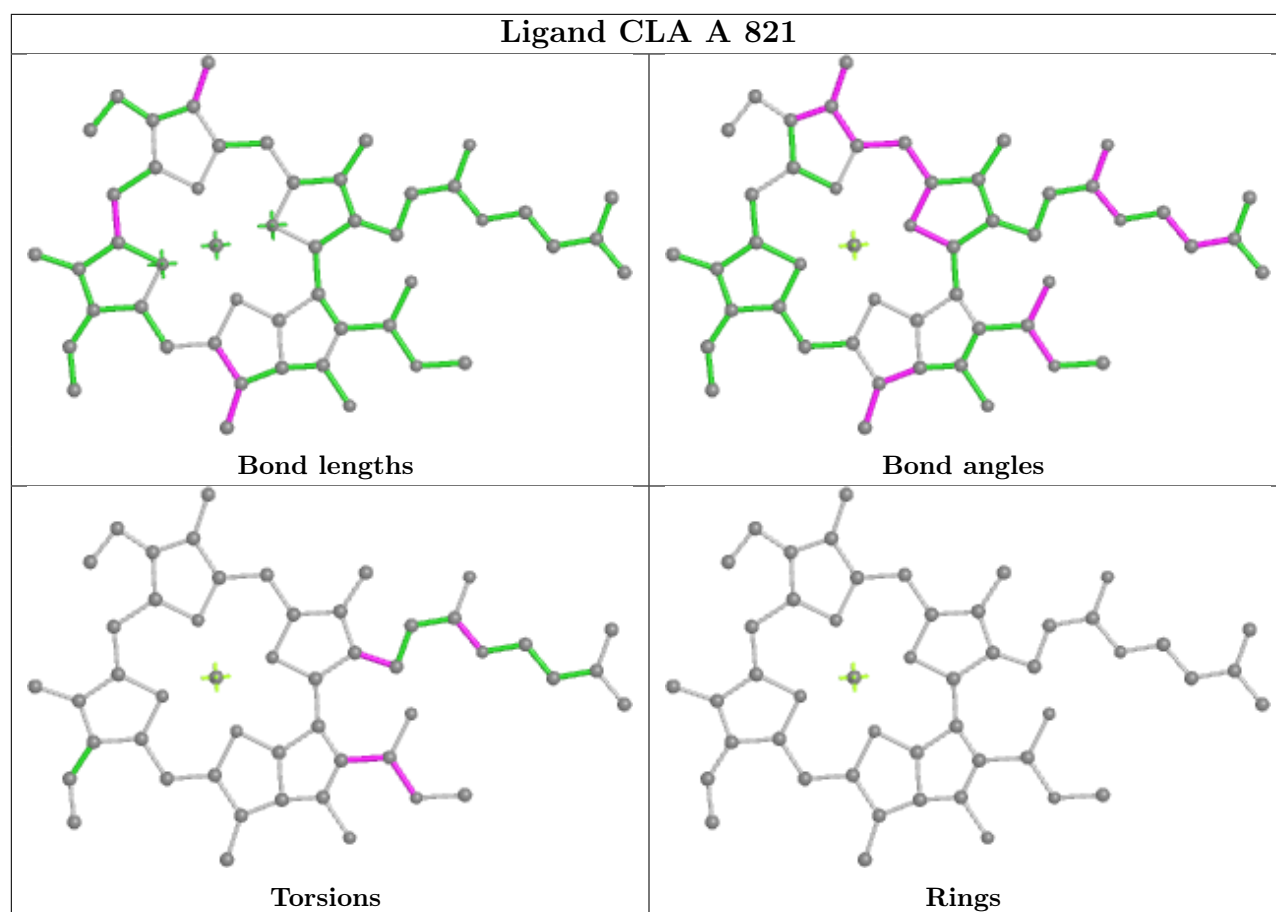


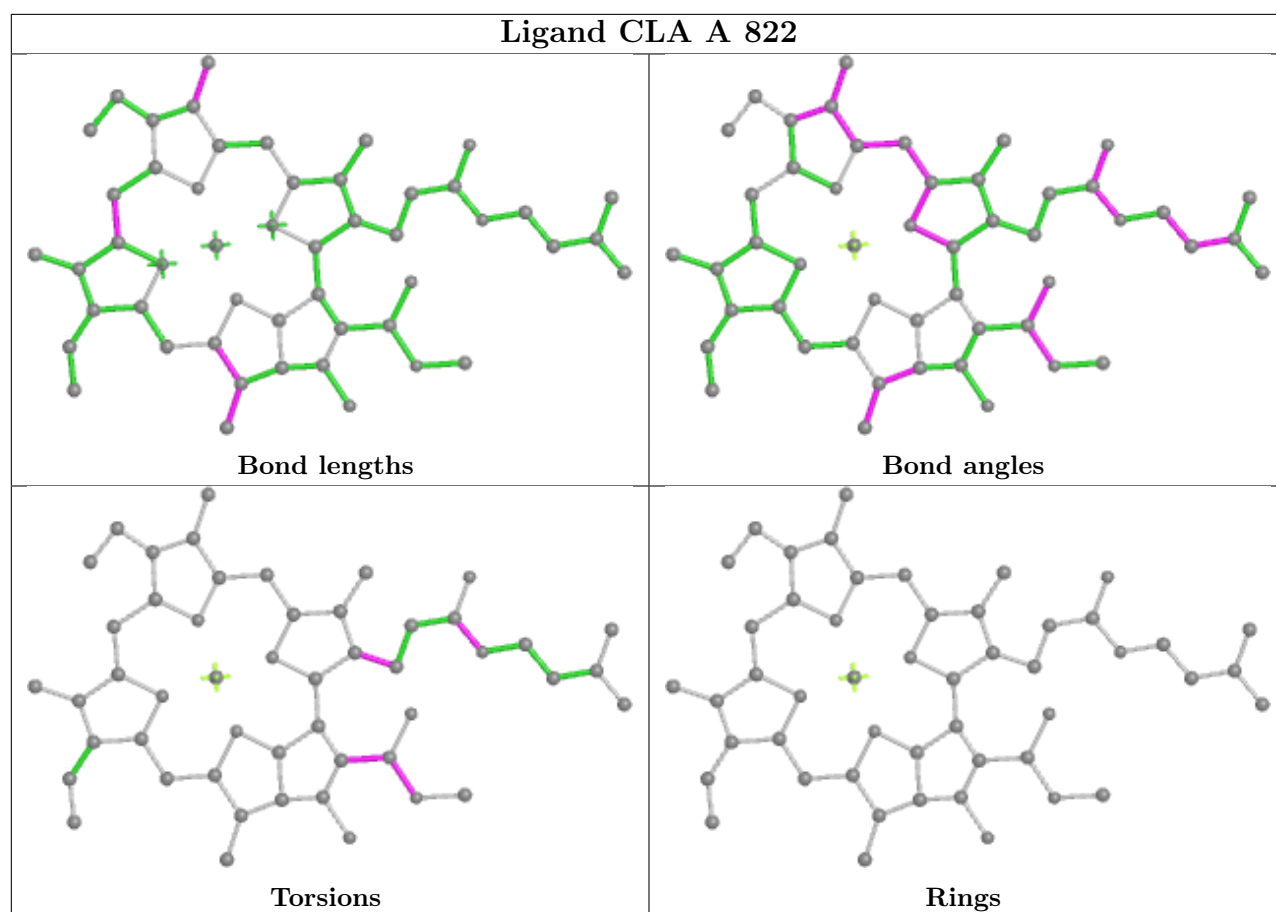


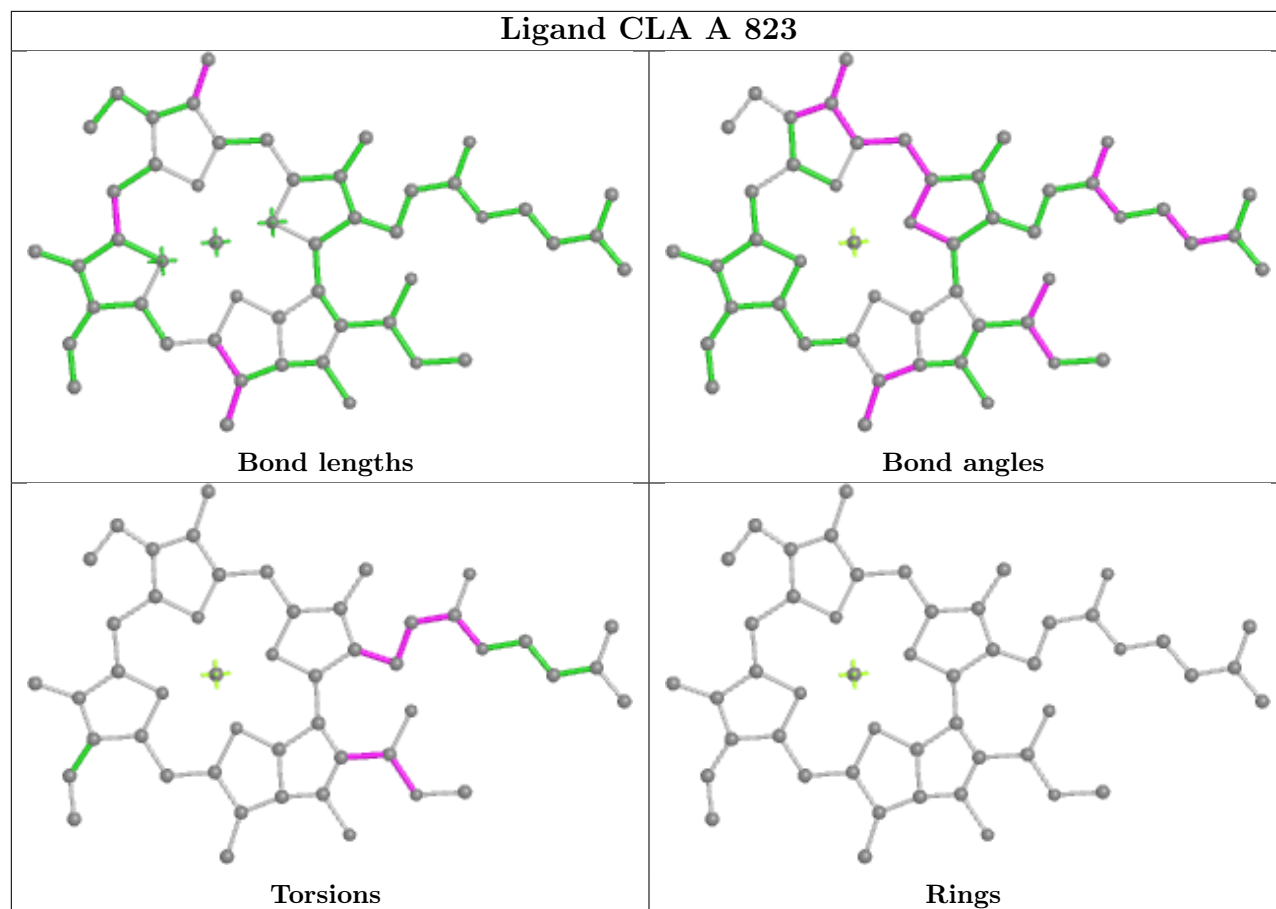


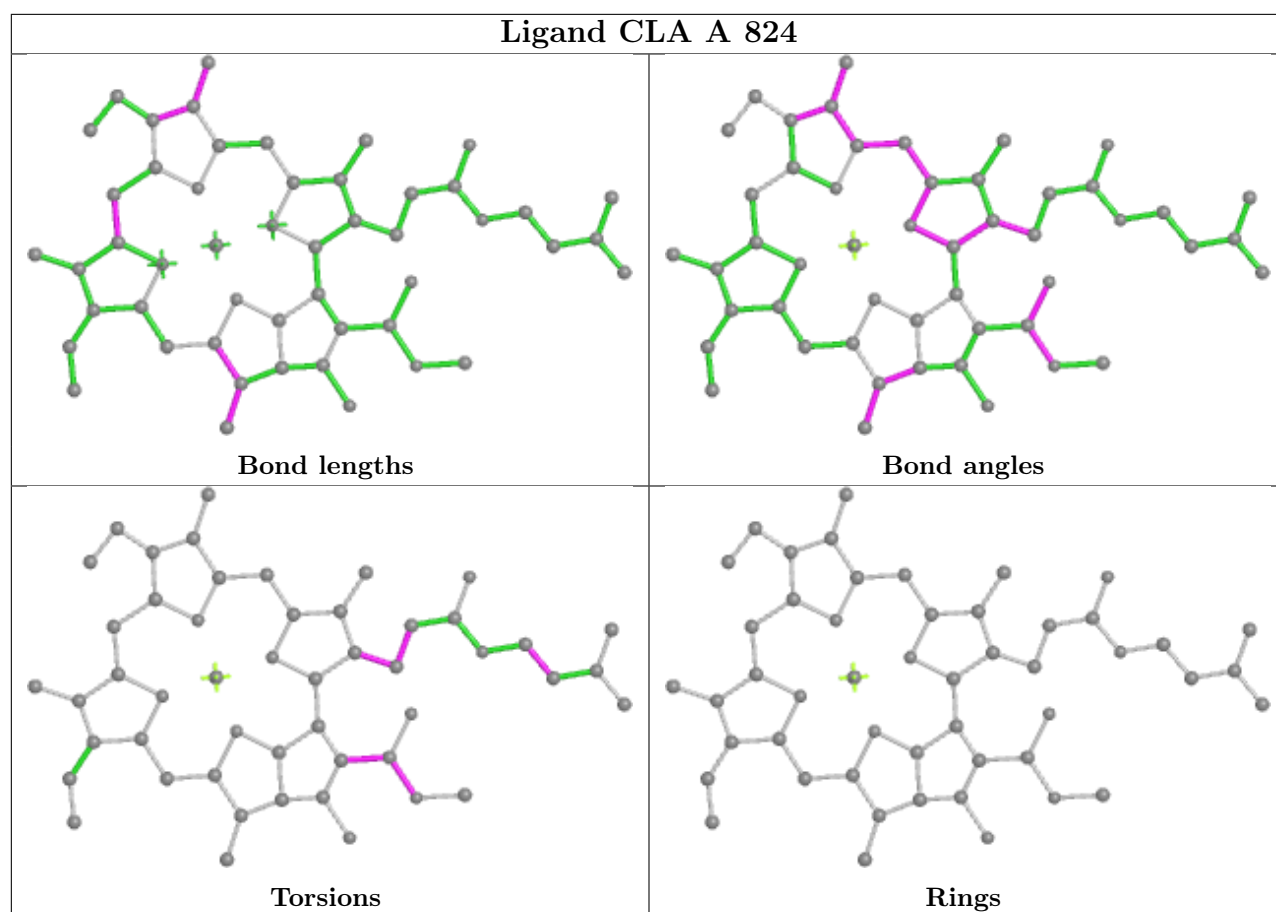


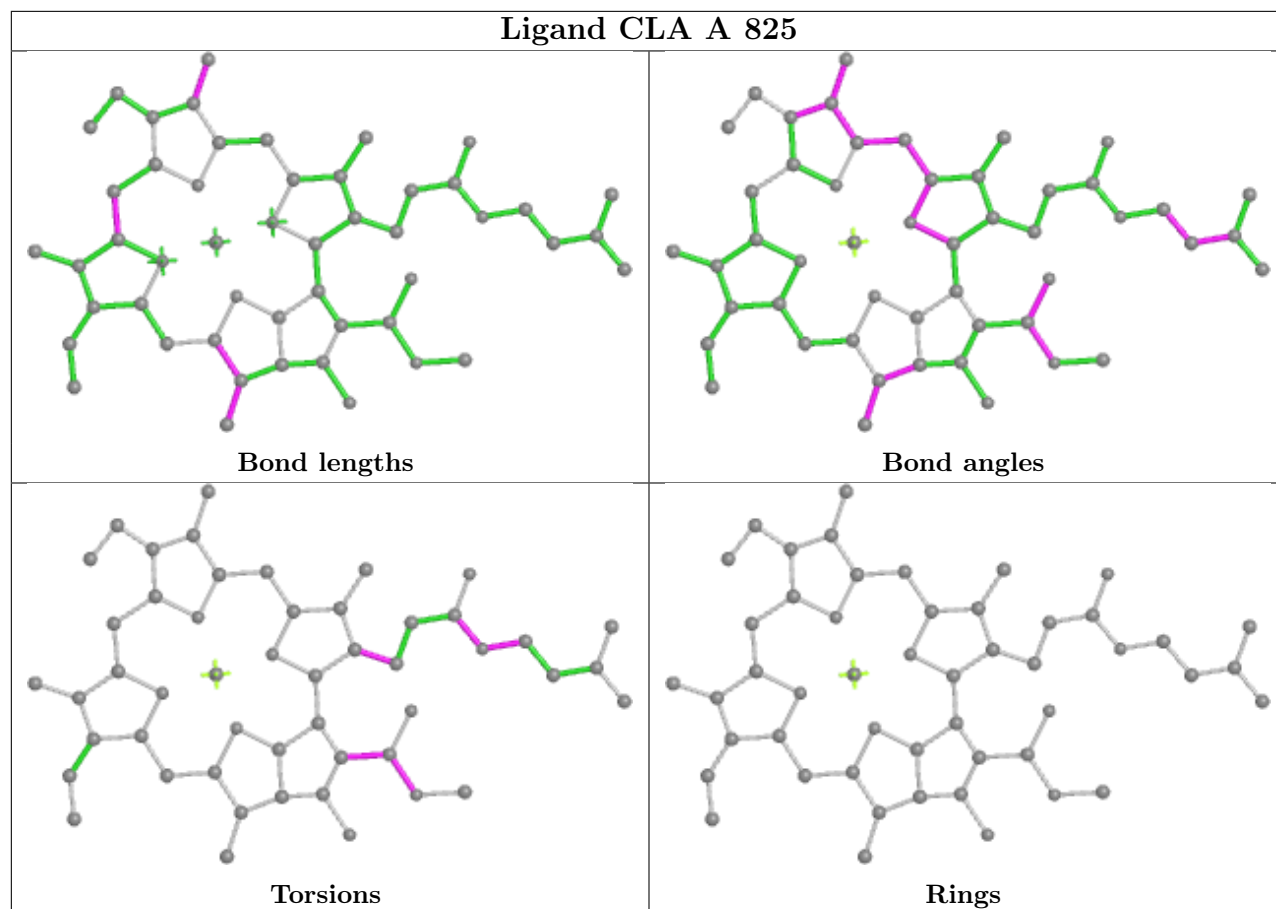


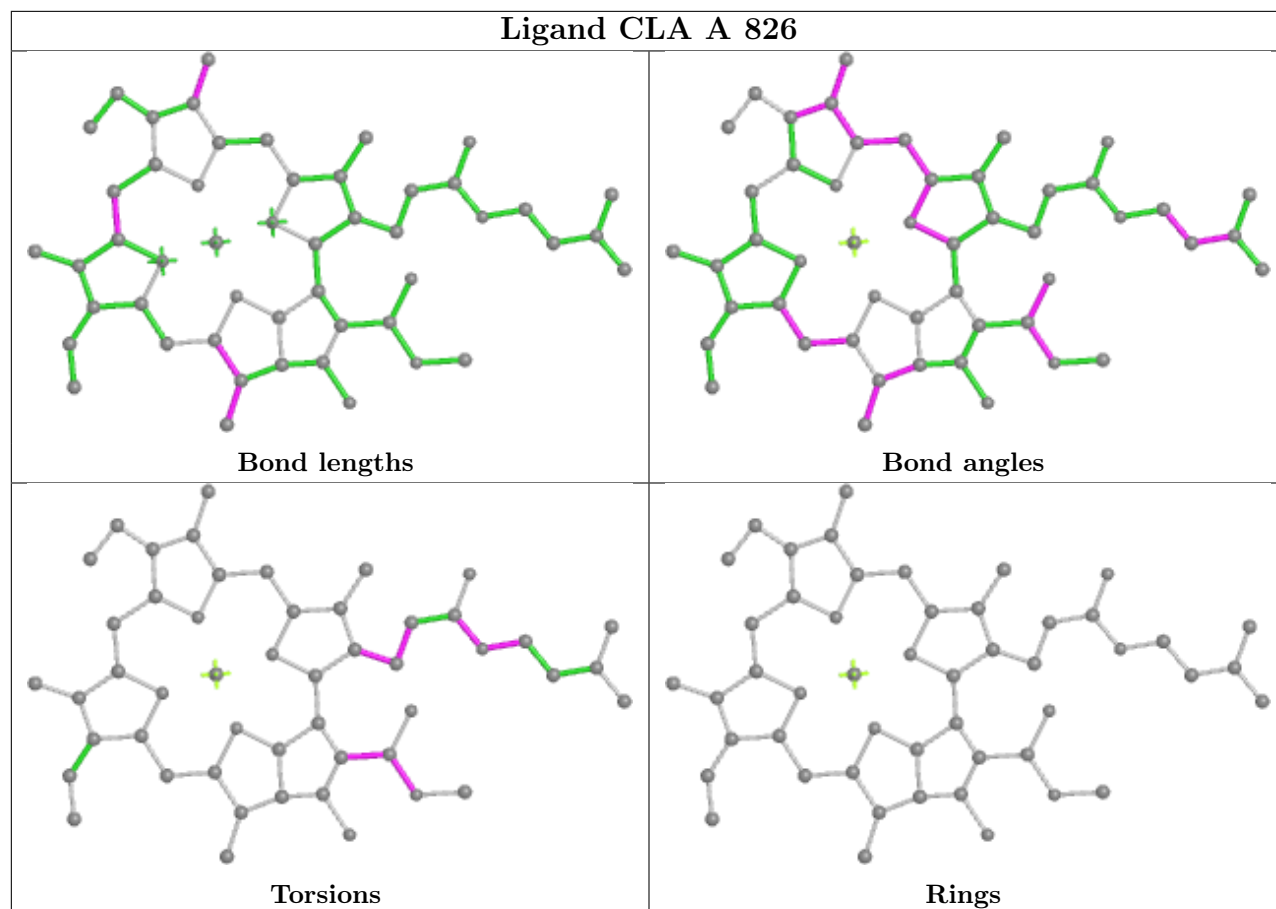


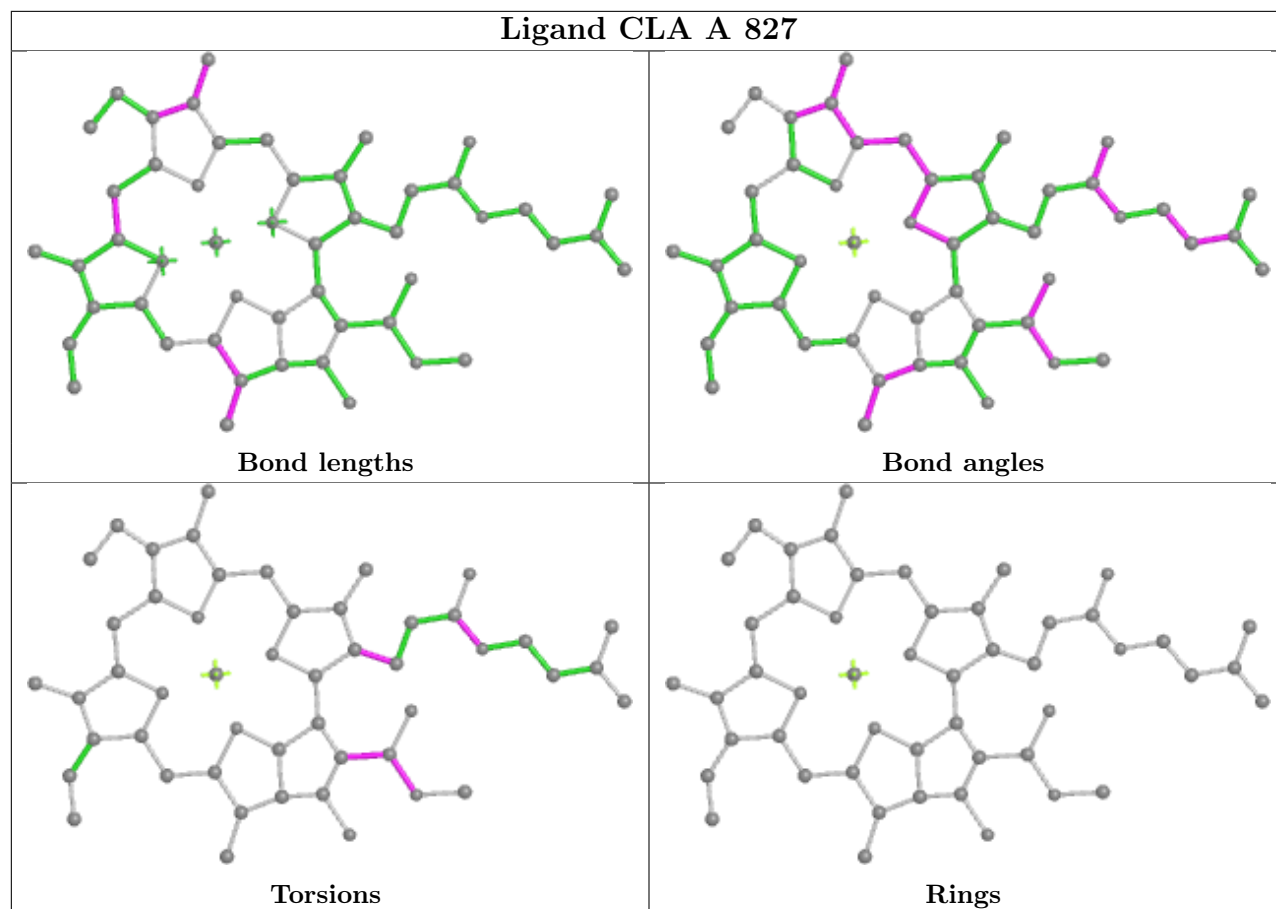


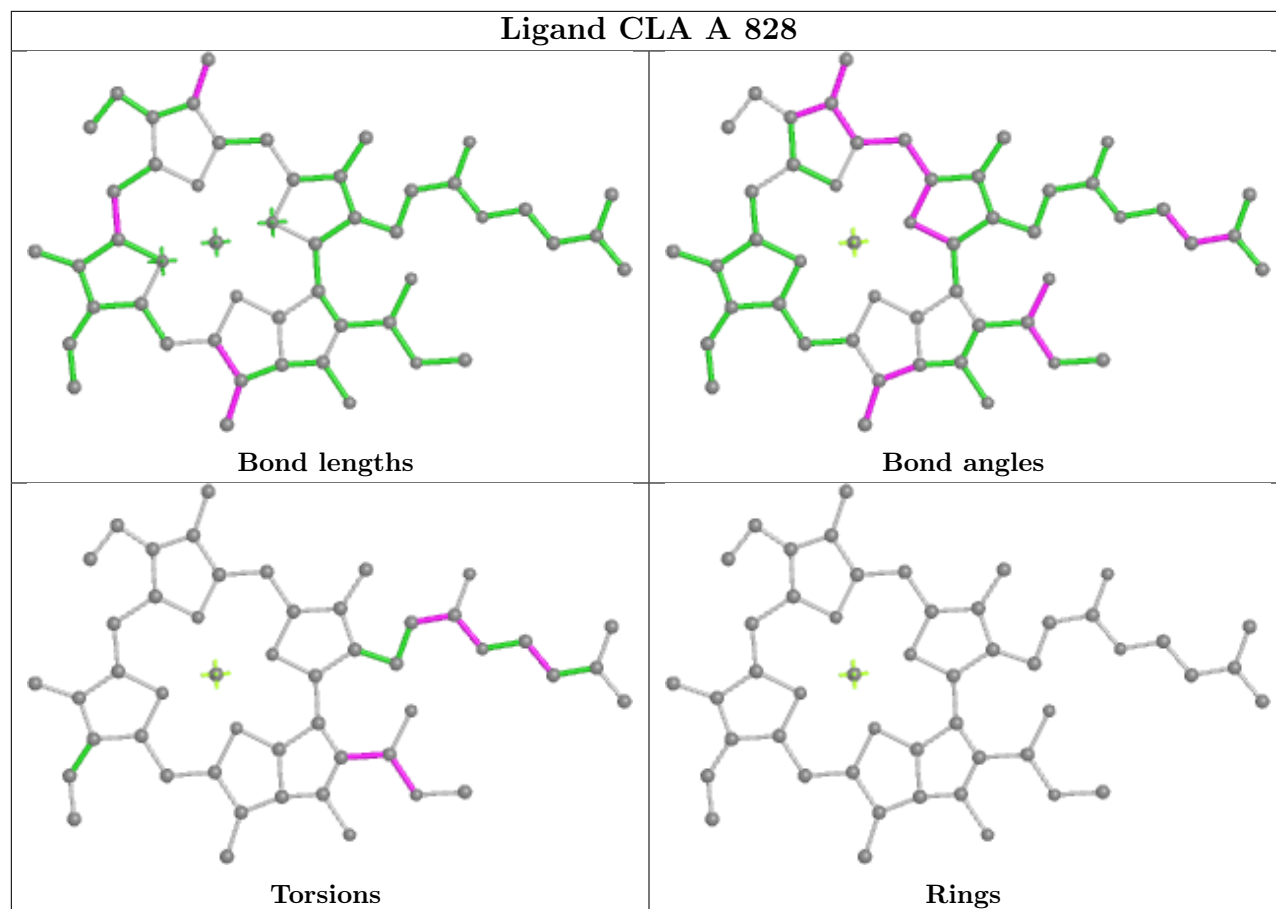


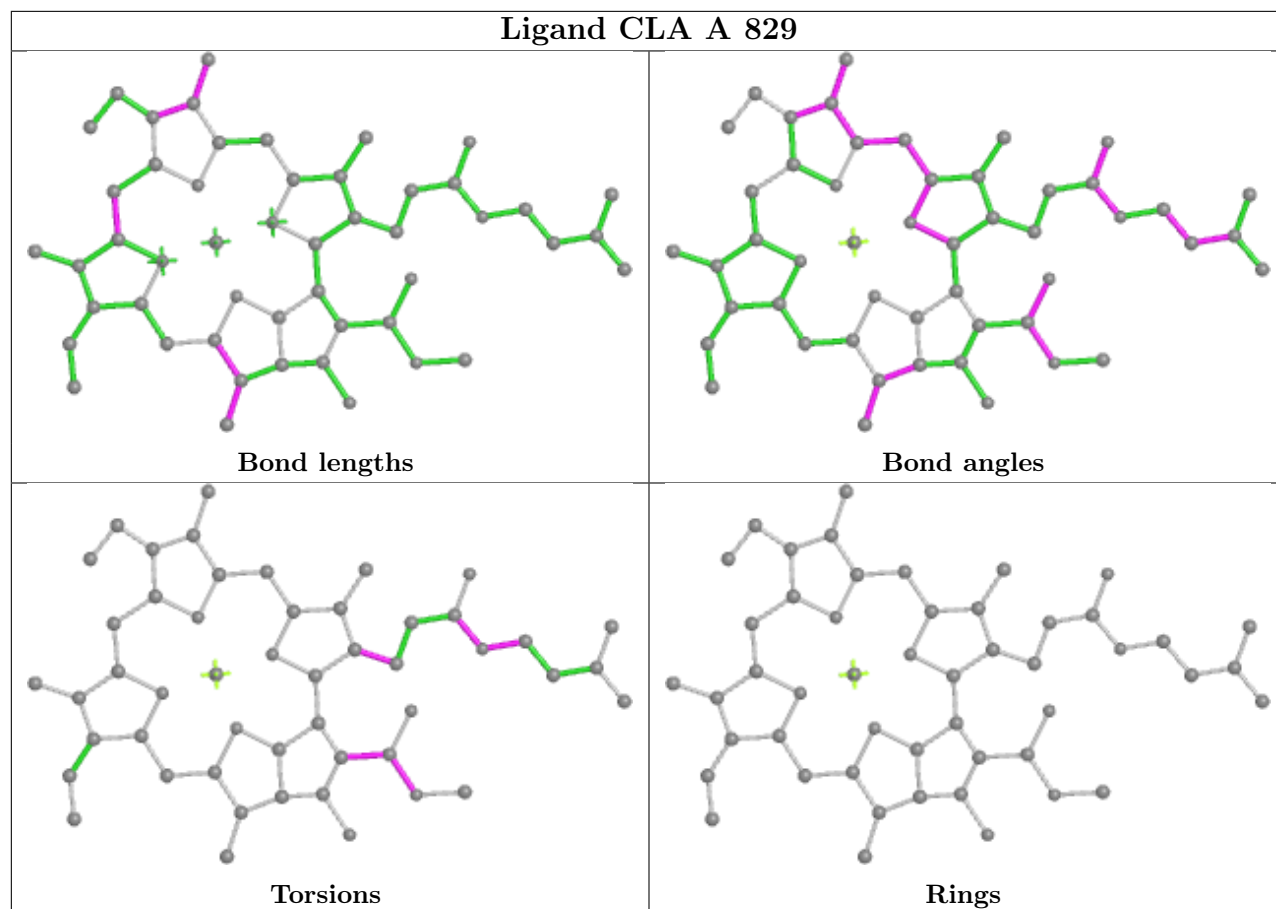


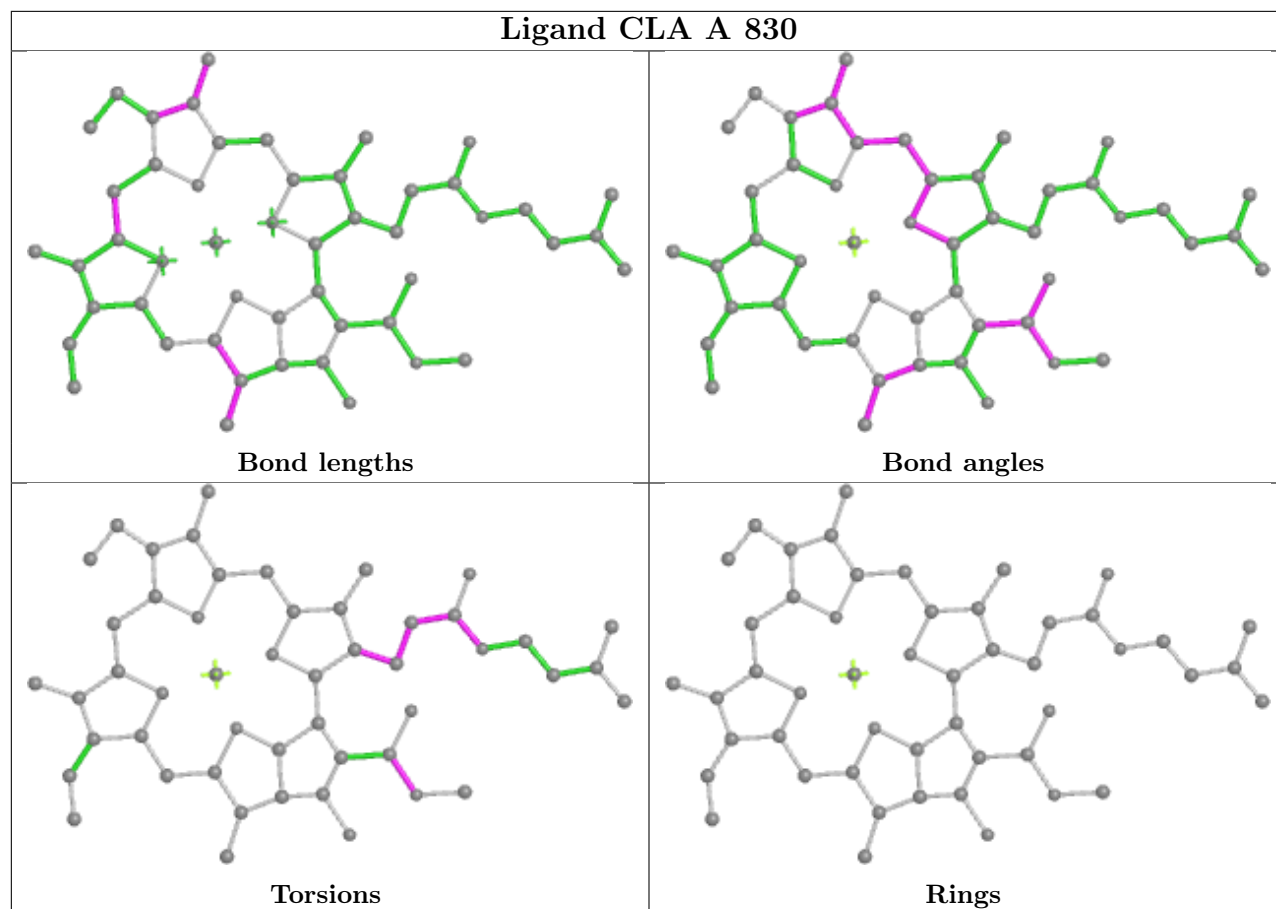


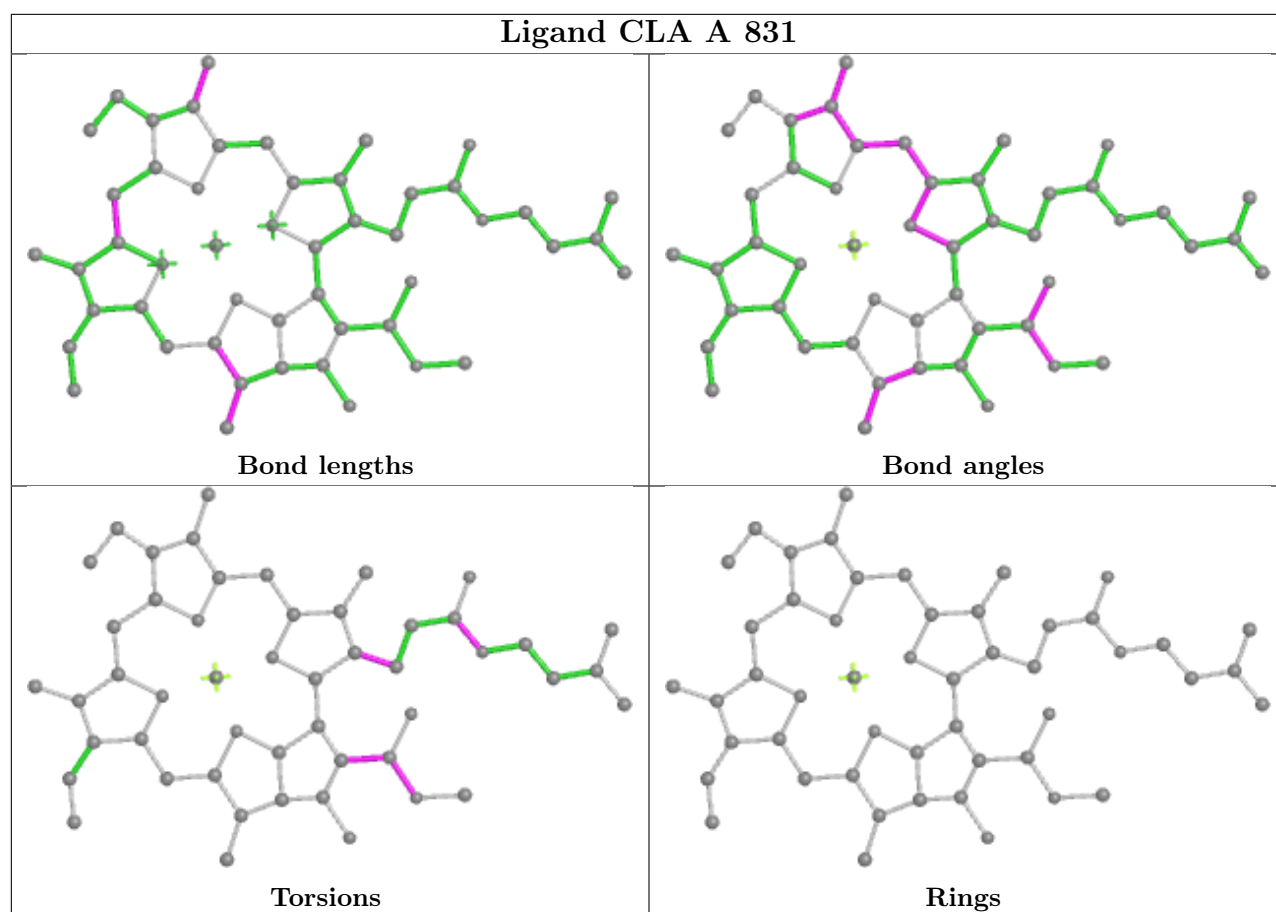


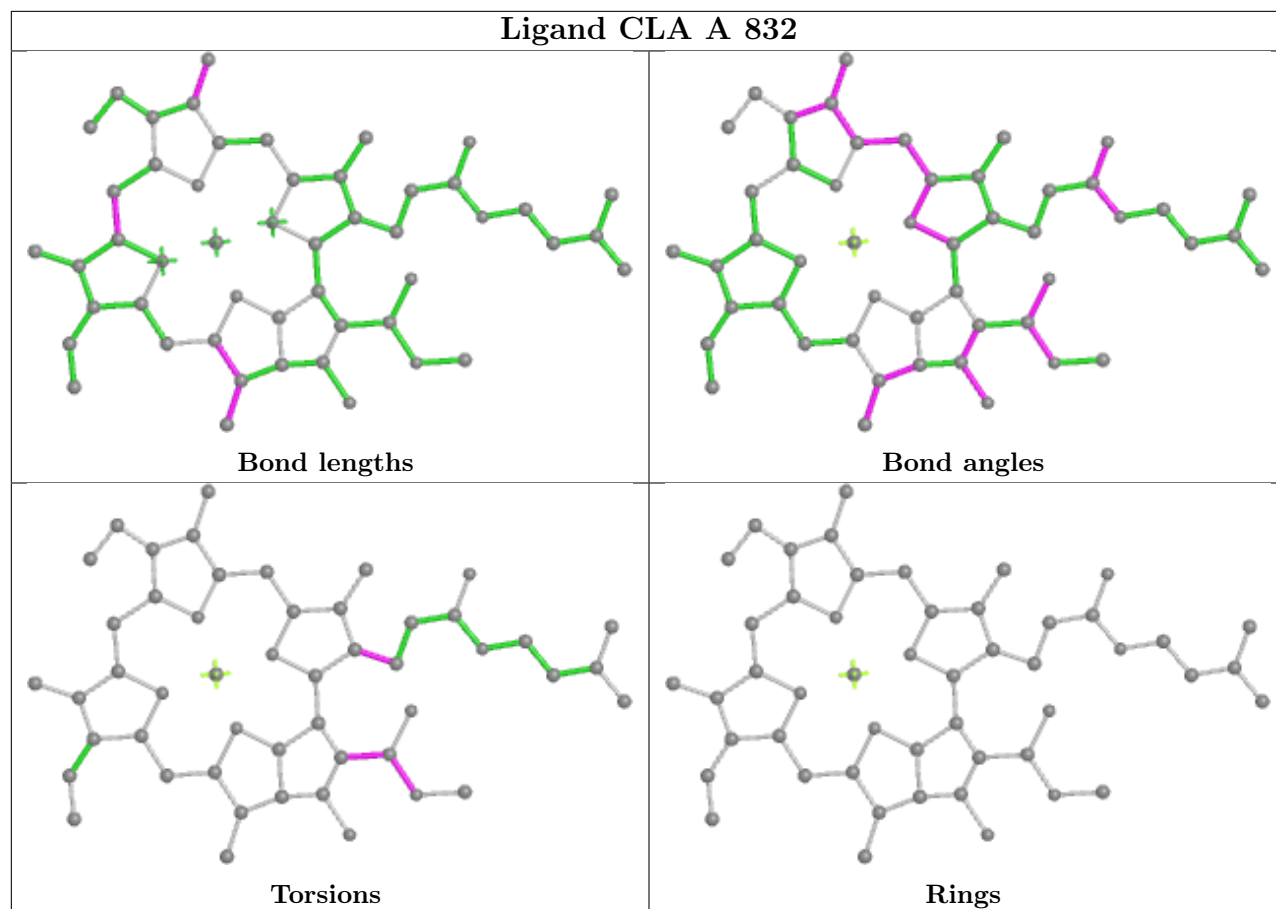




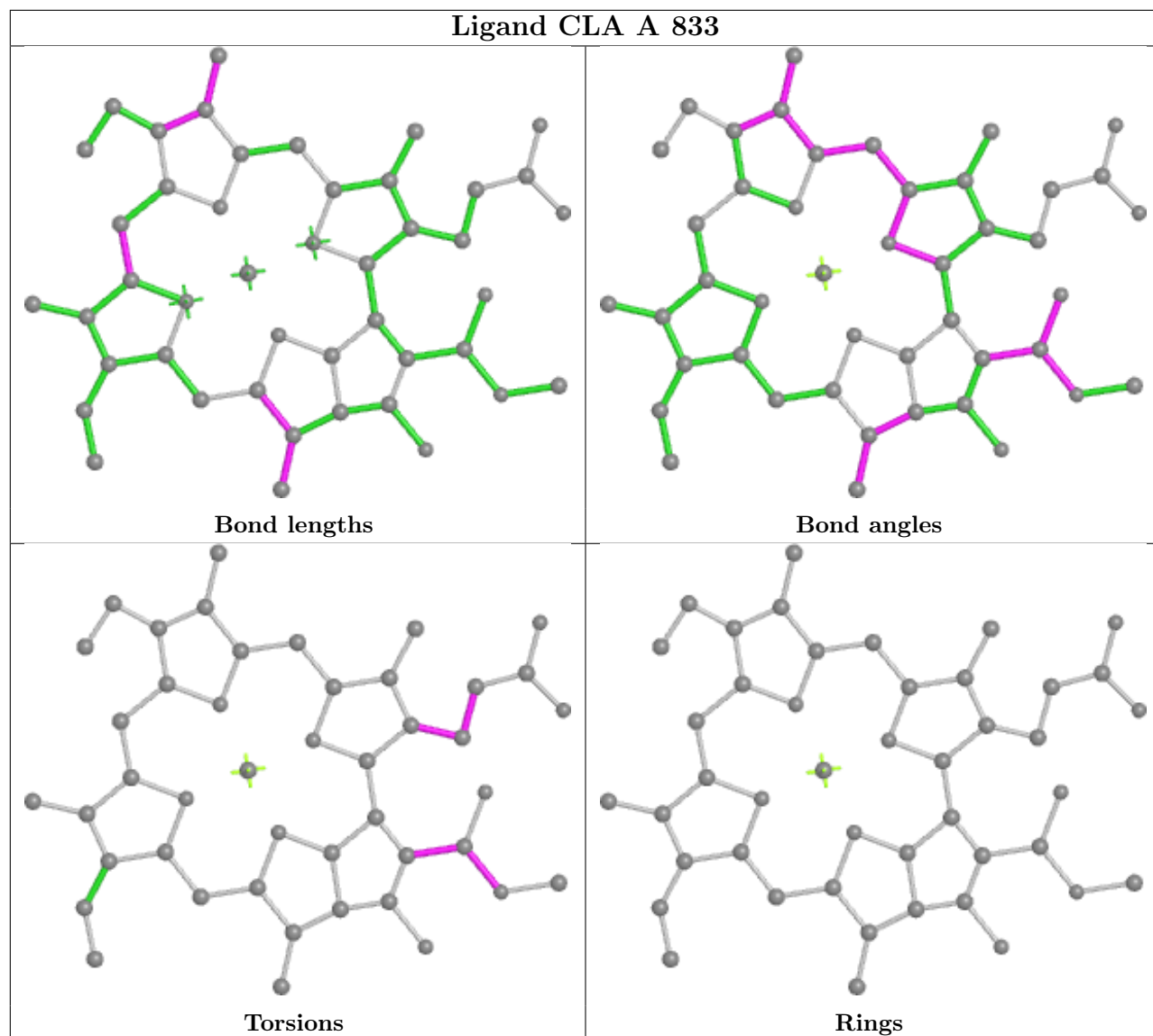


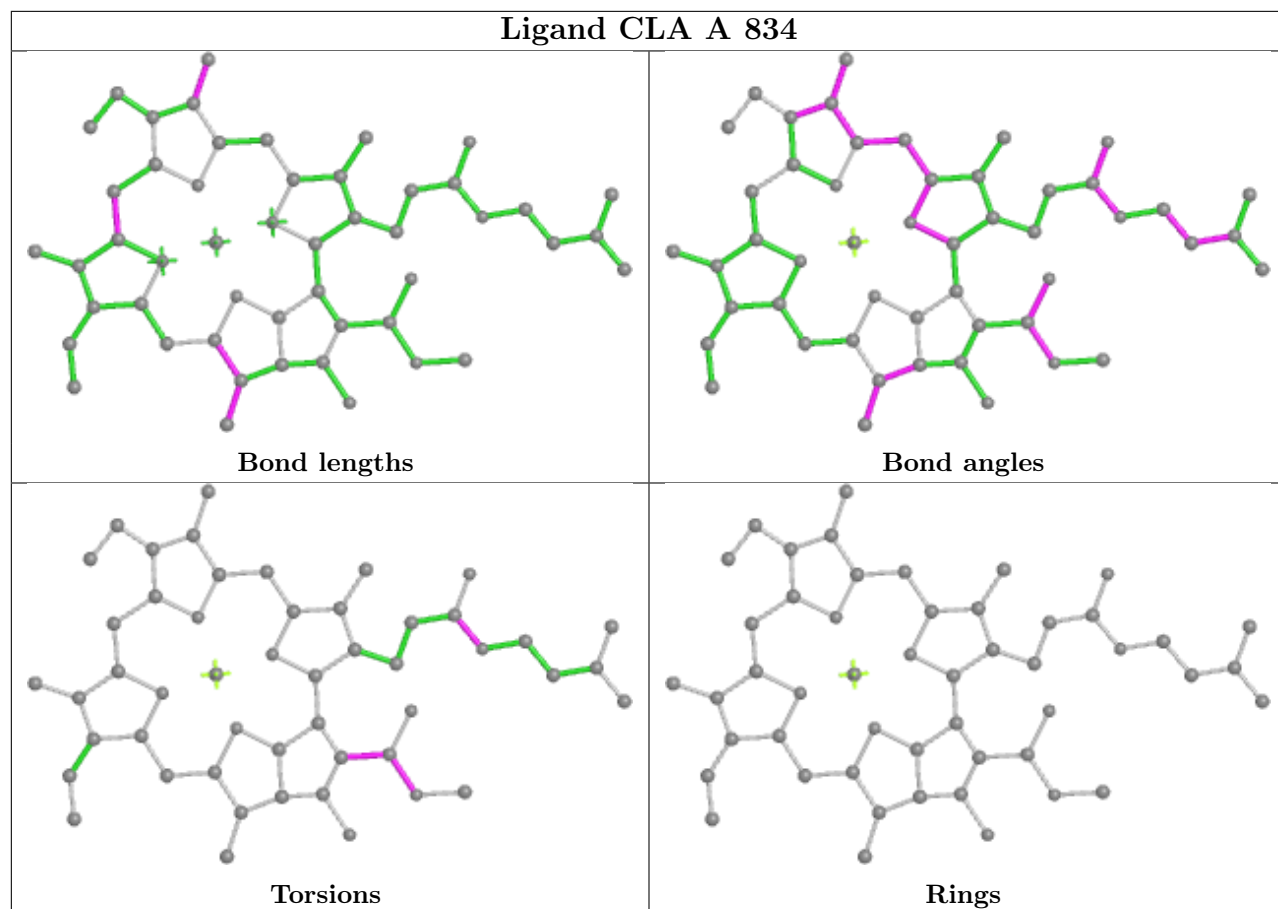


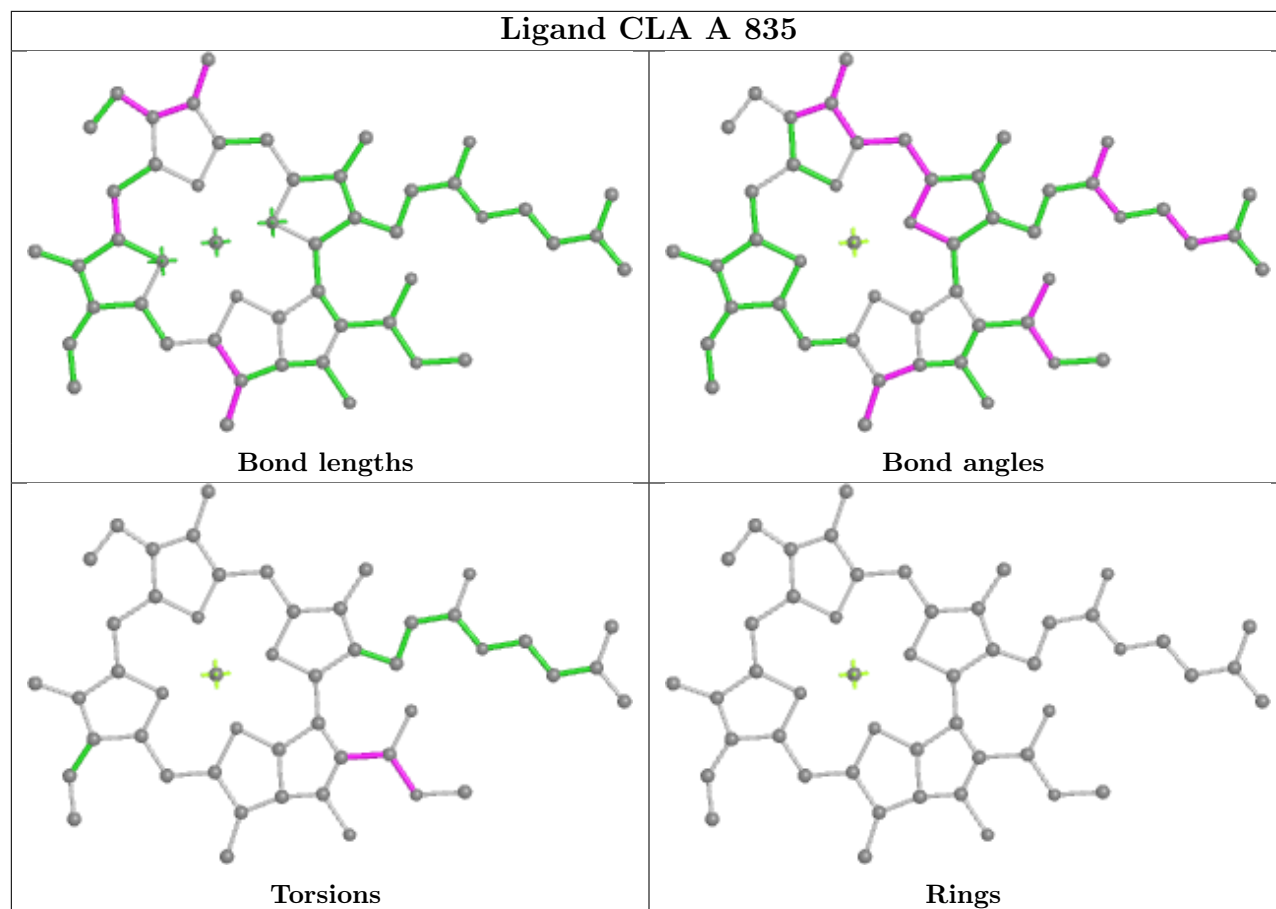




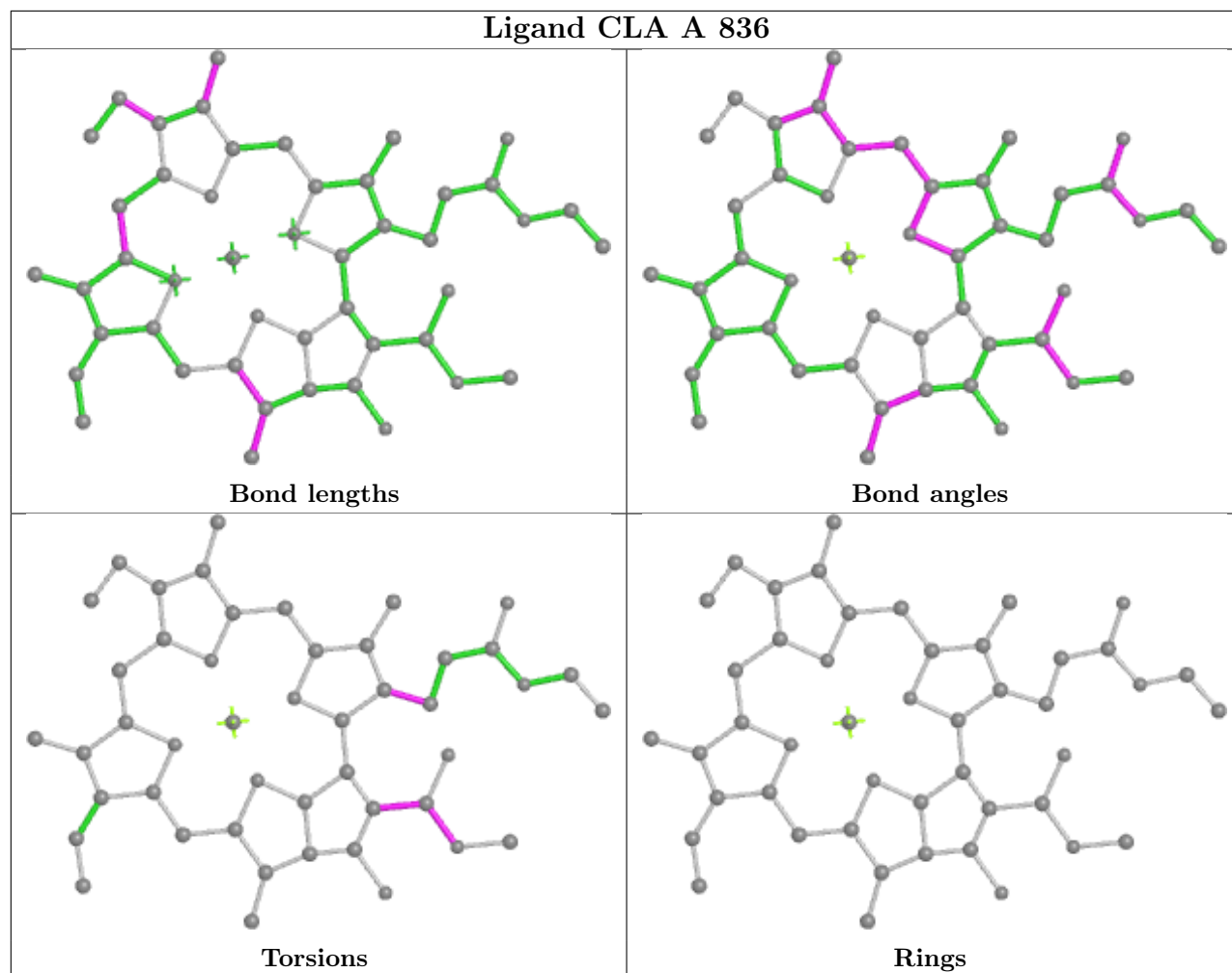
Ligand CLA A 833

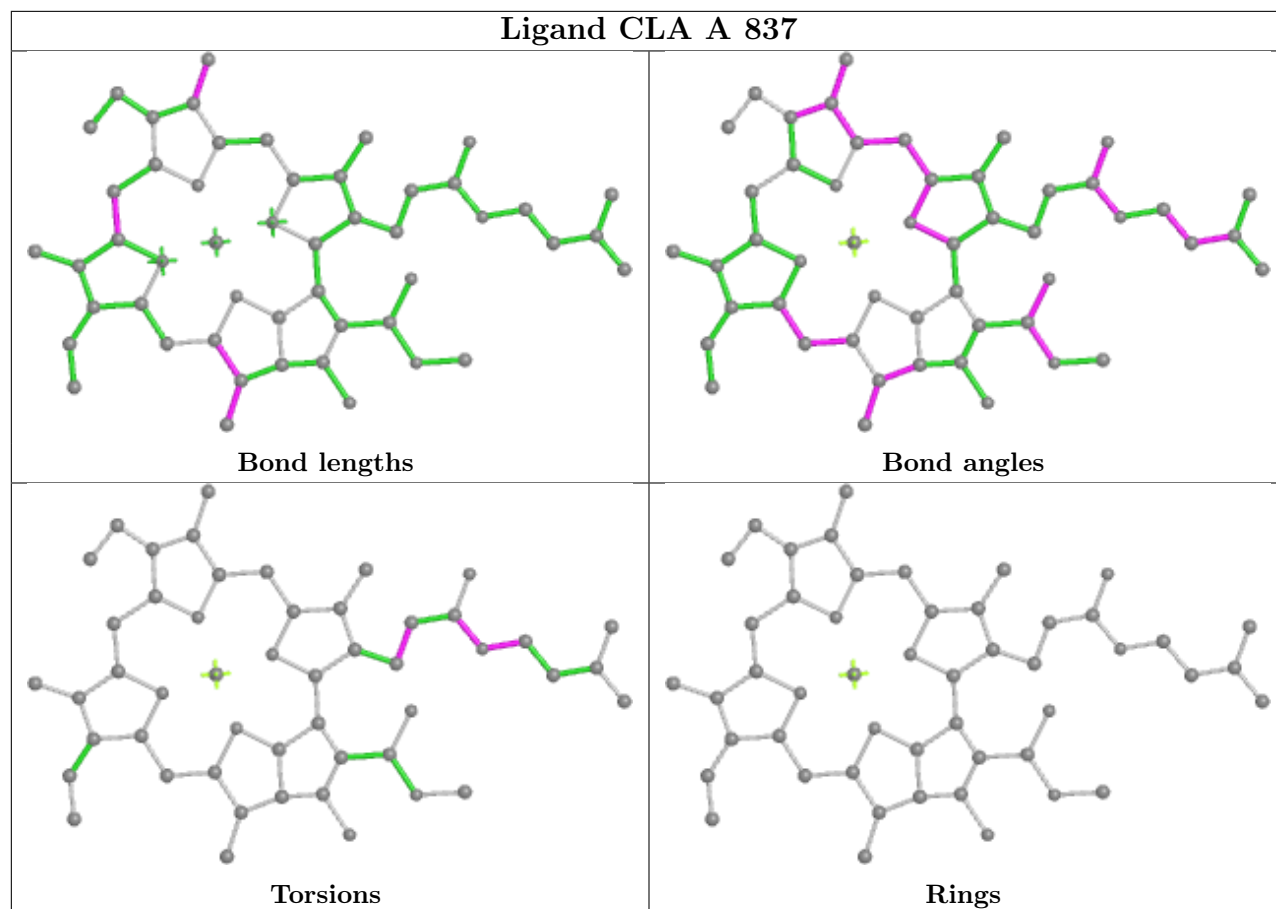


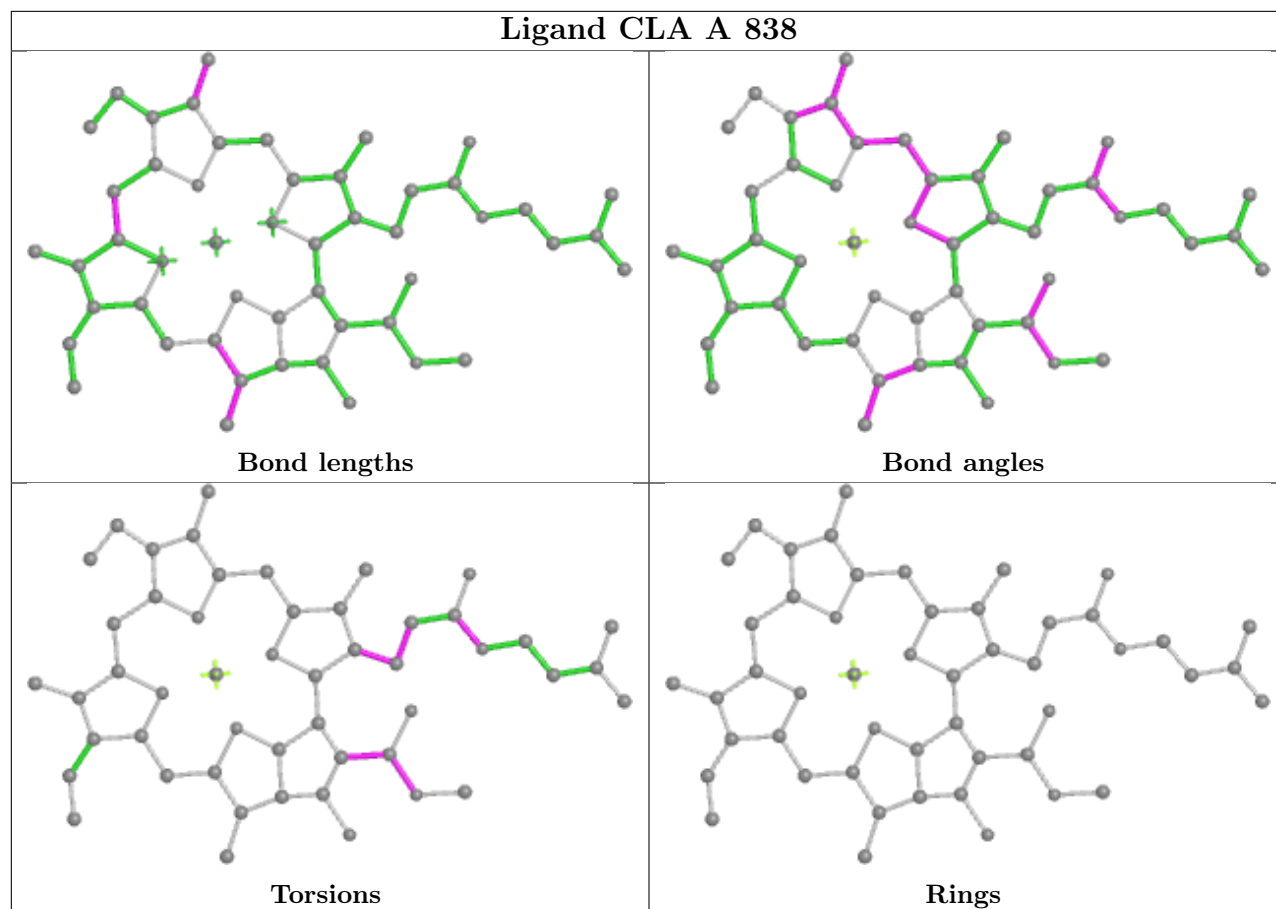


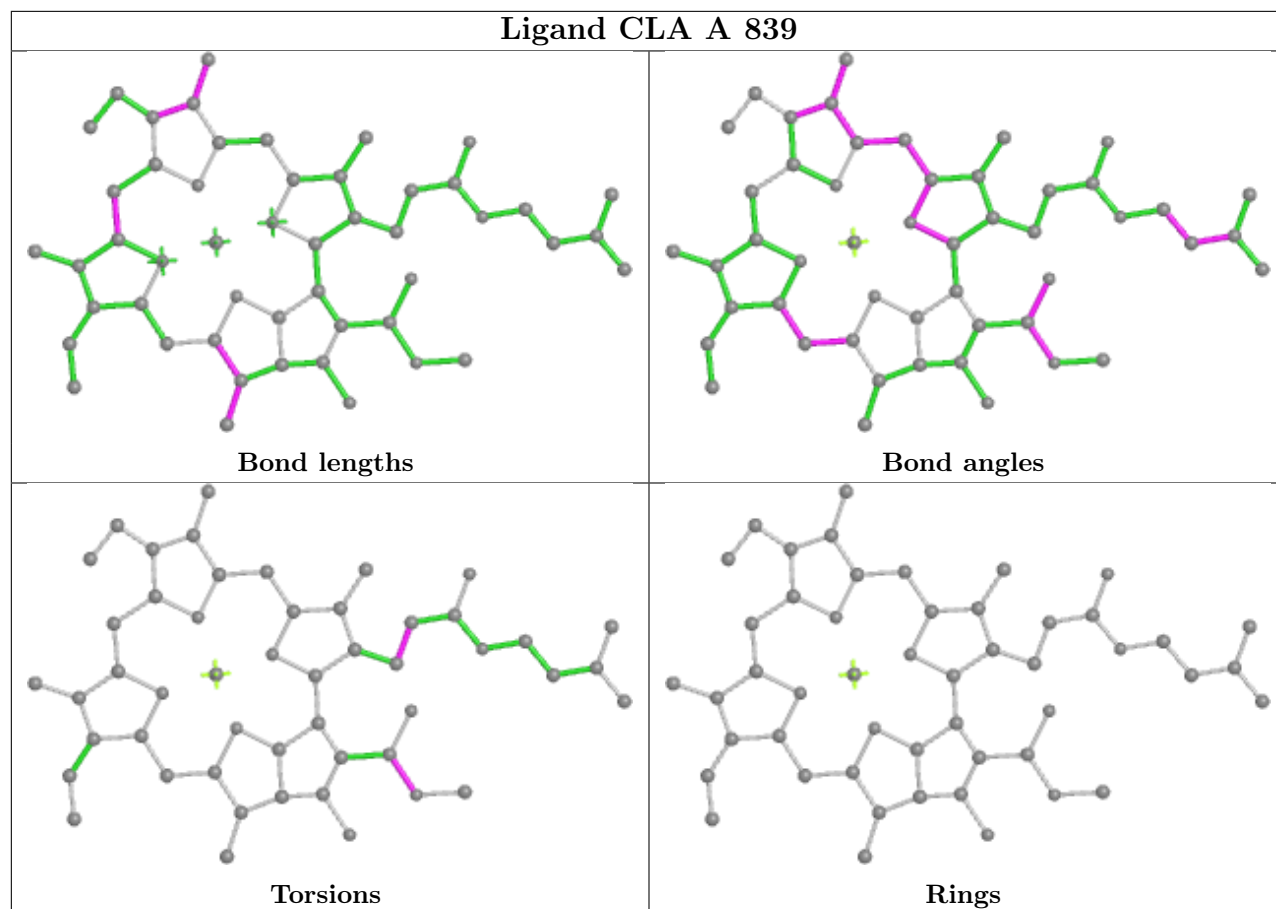


Ligand CLA A 836

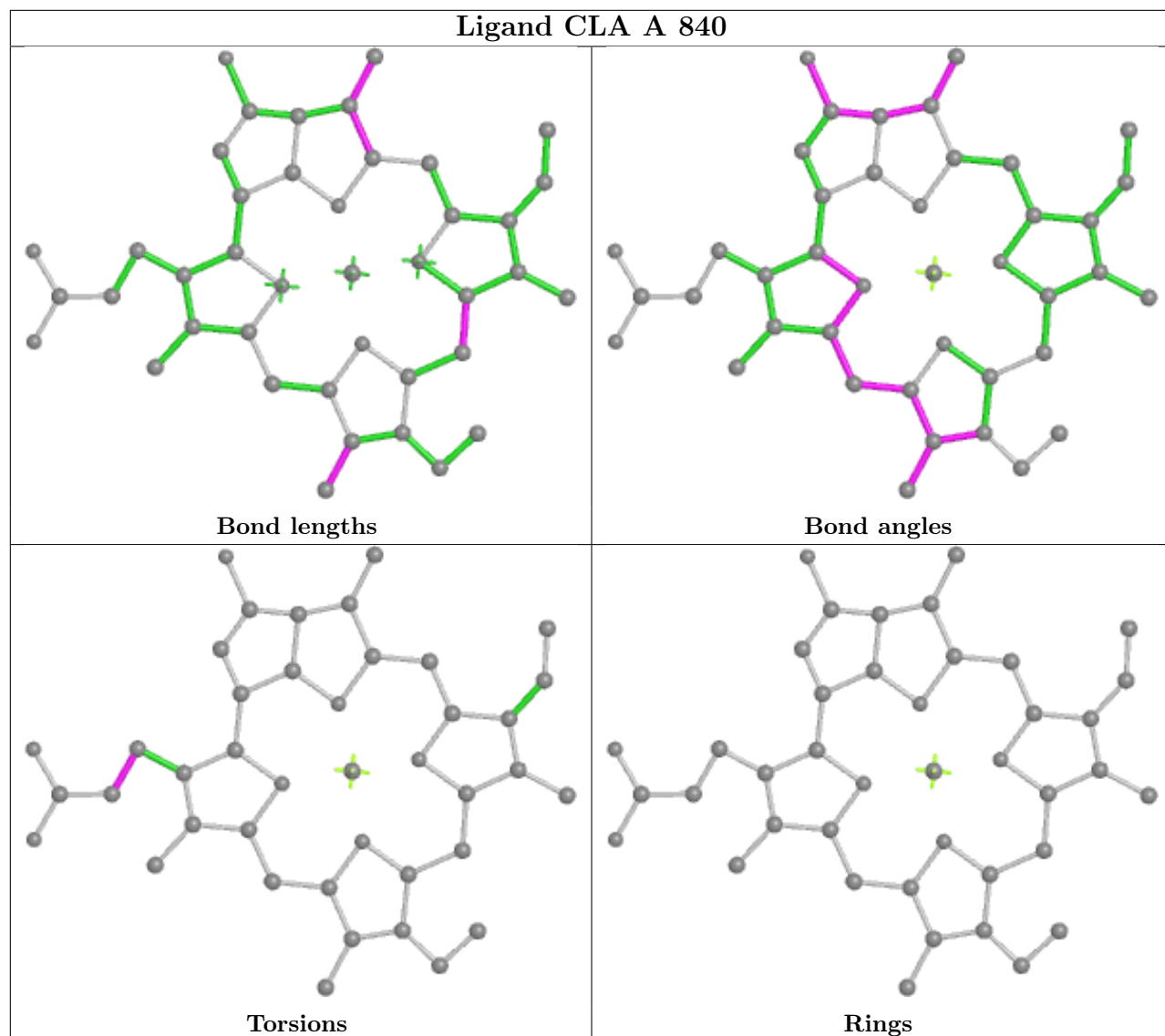


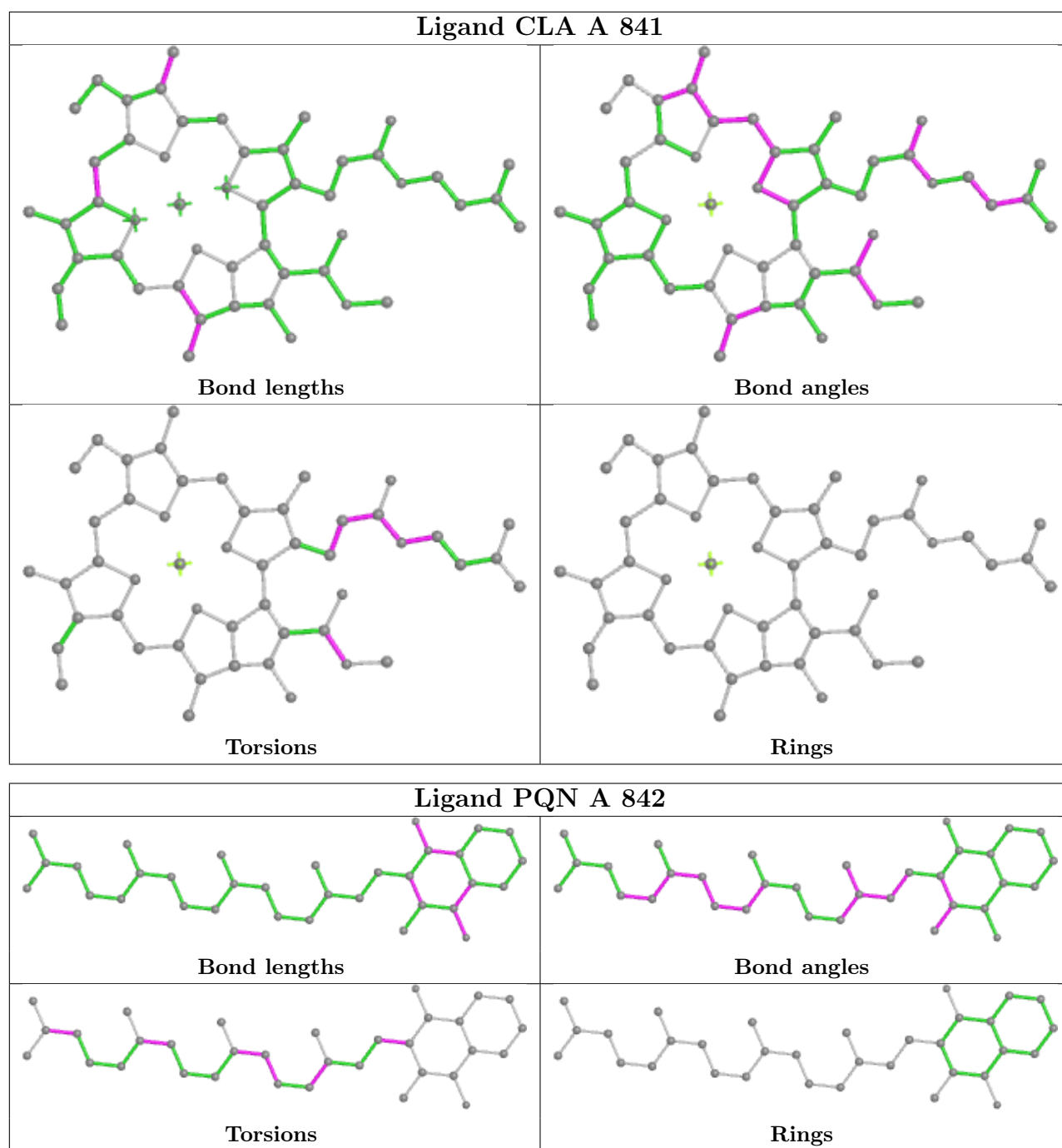


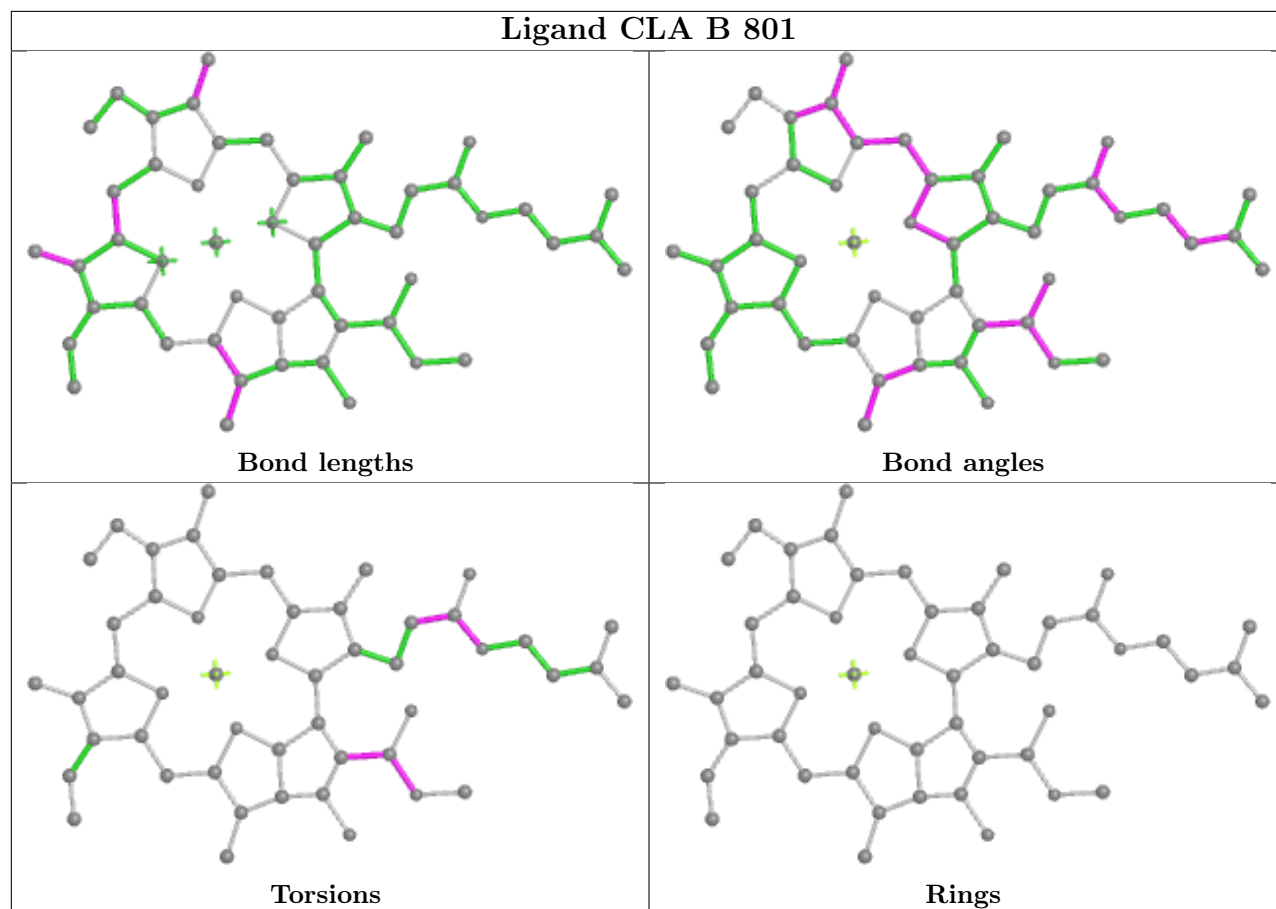


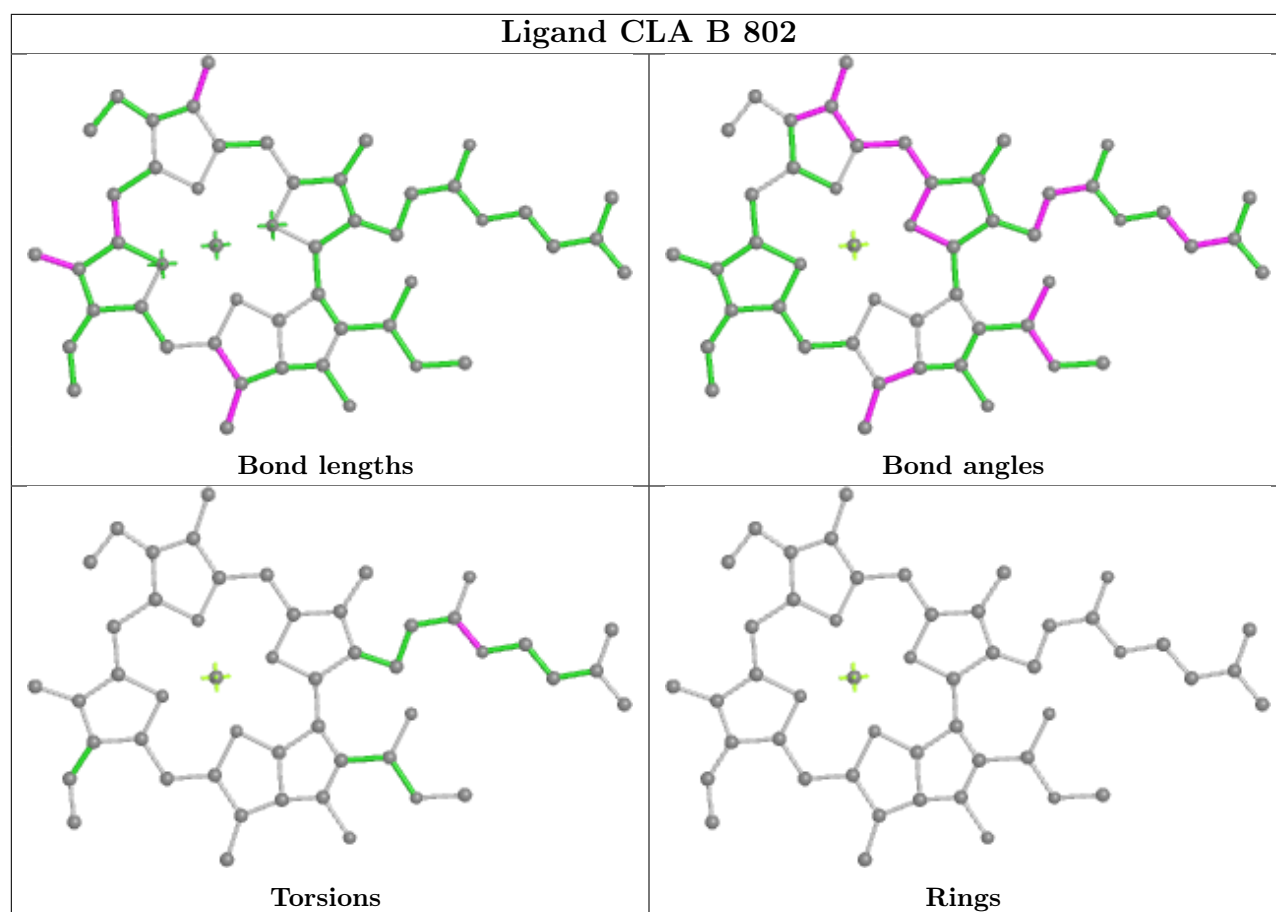


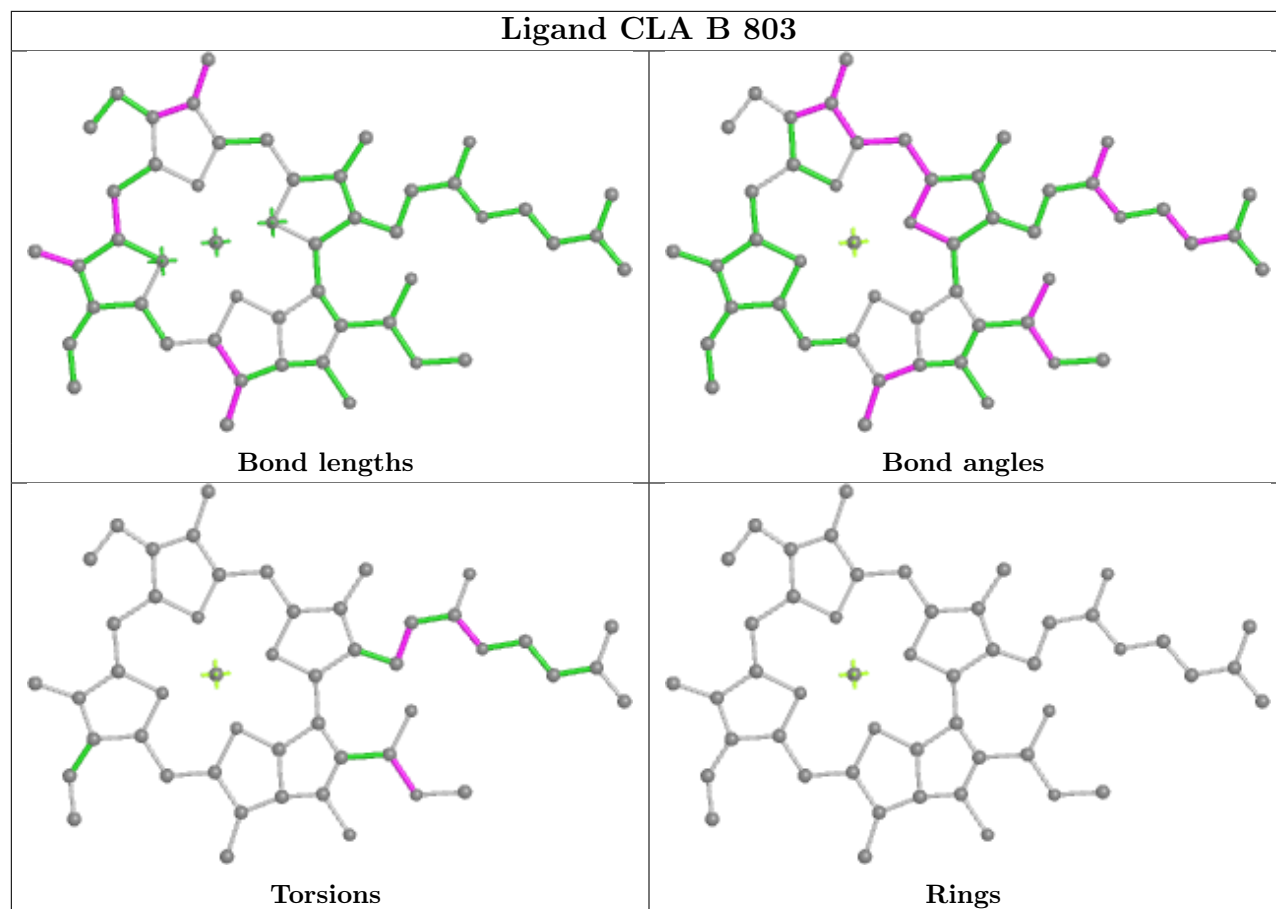
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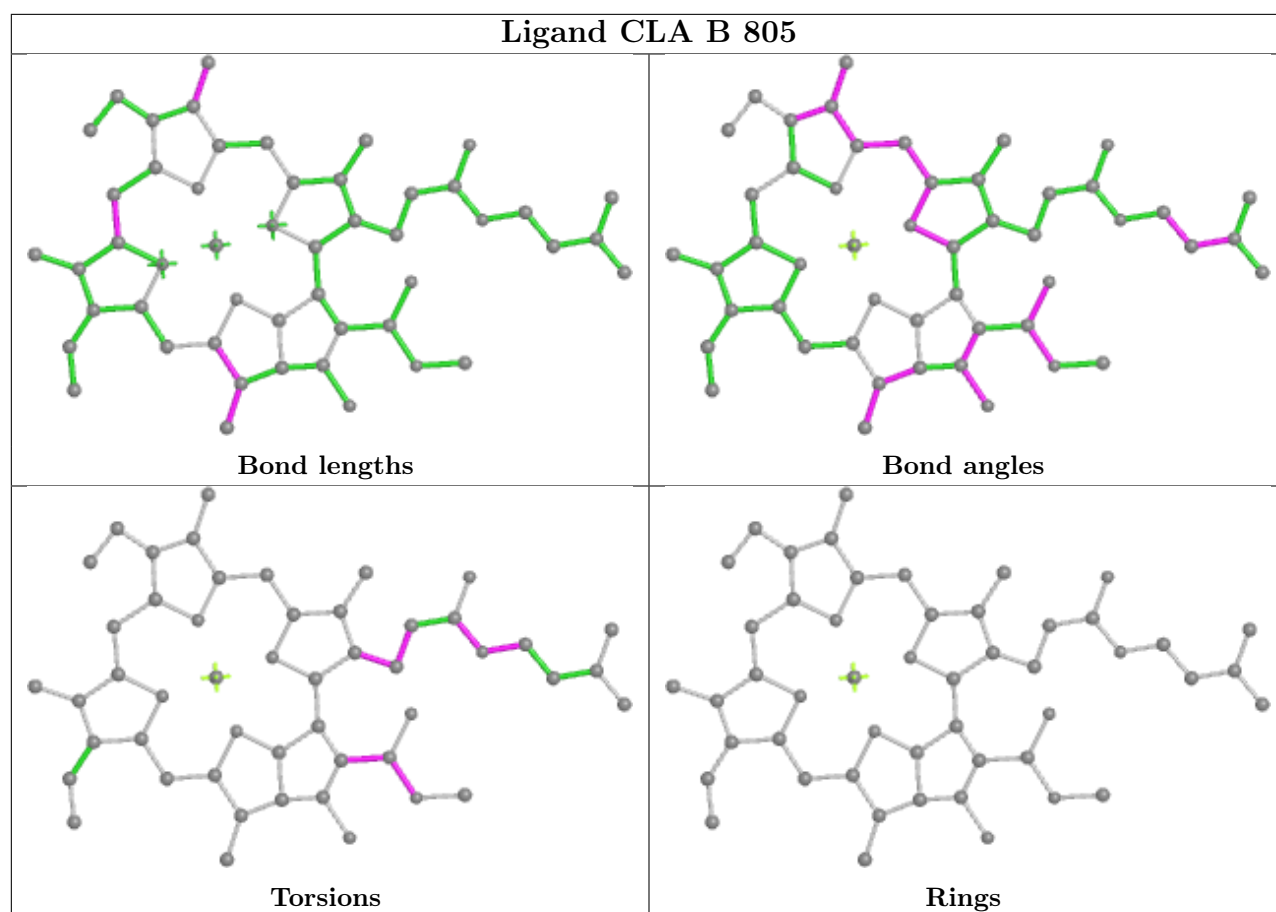


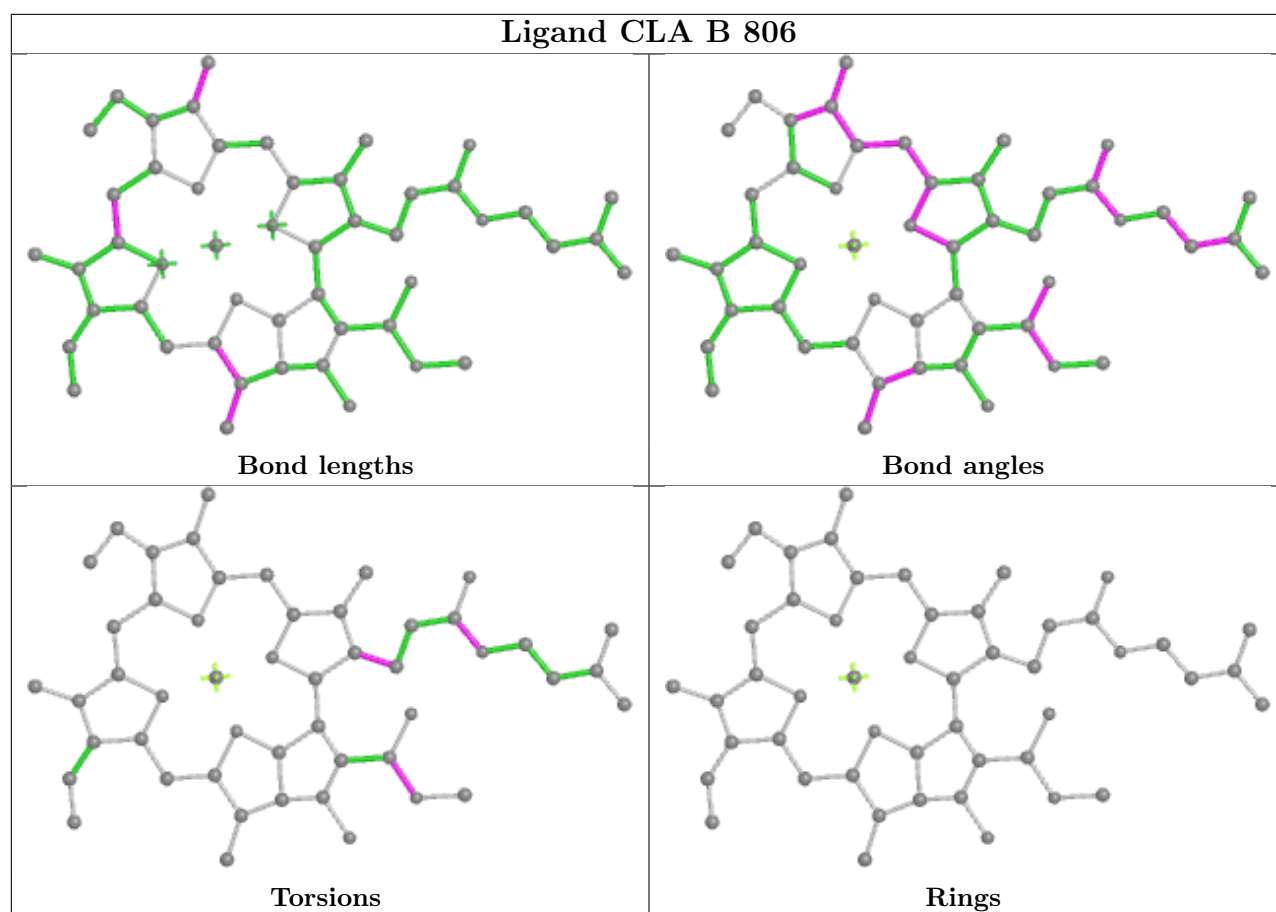


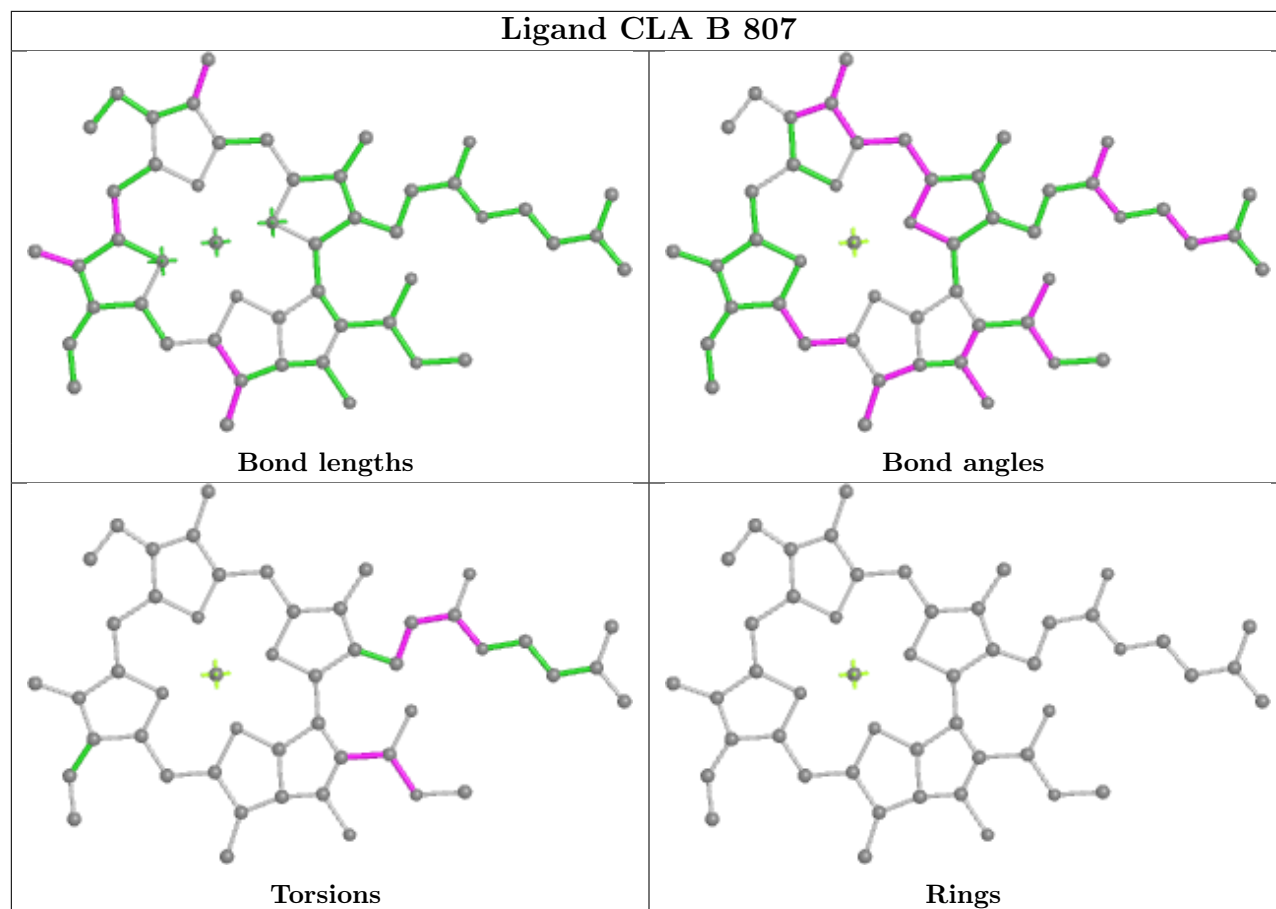


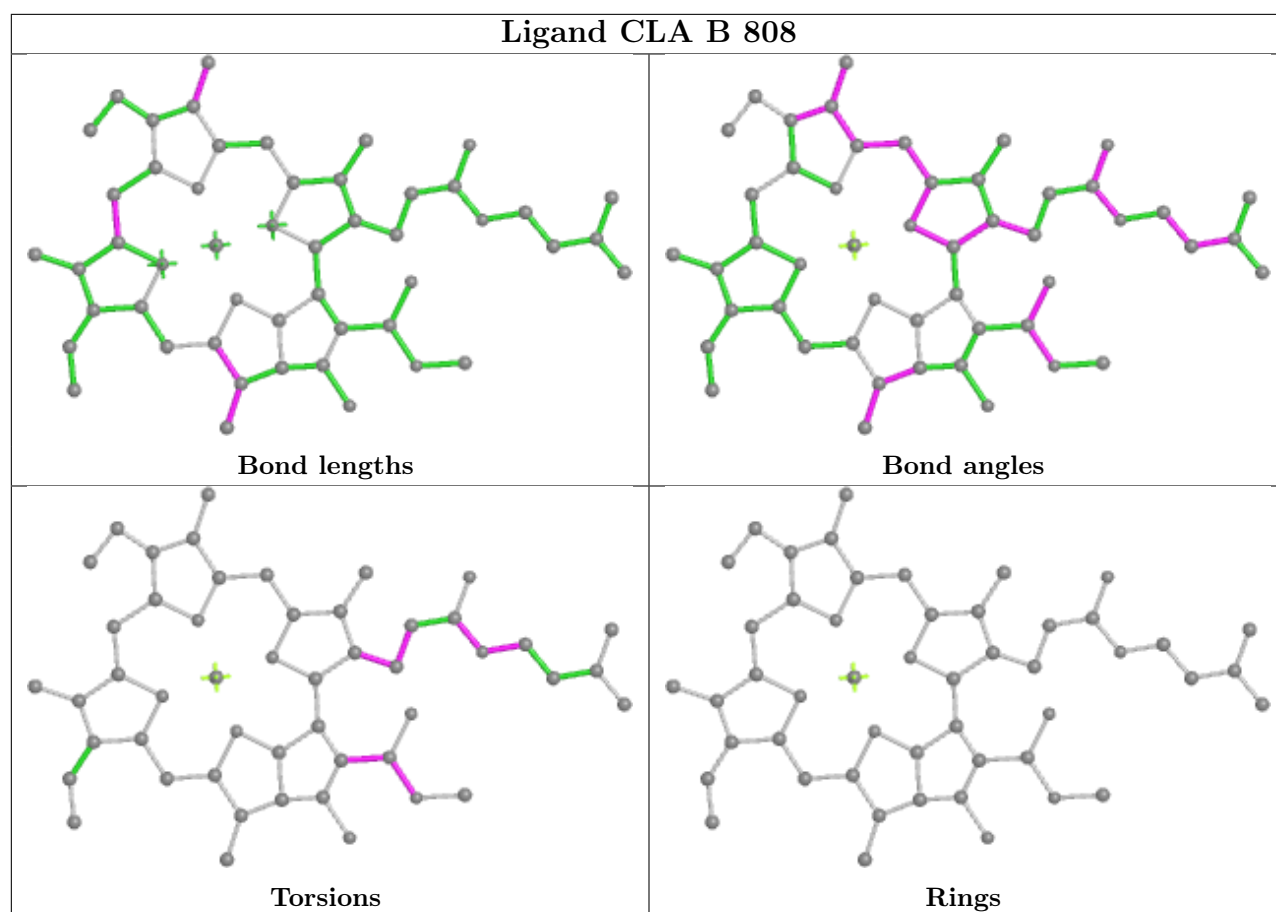


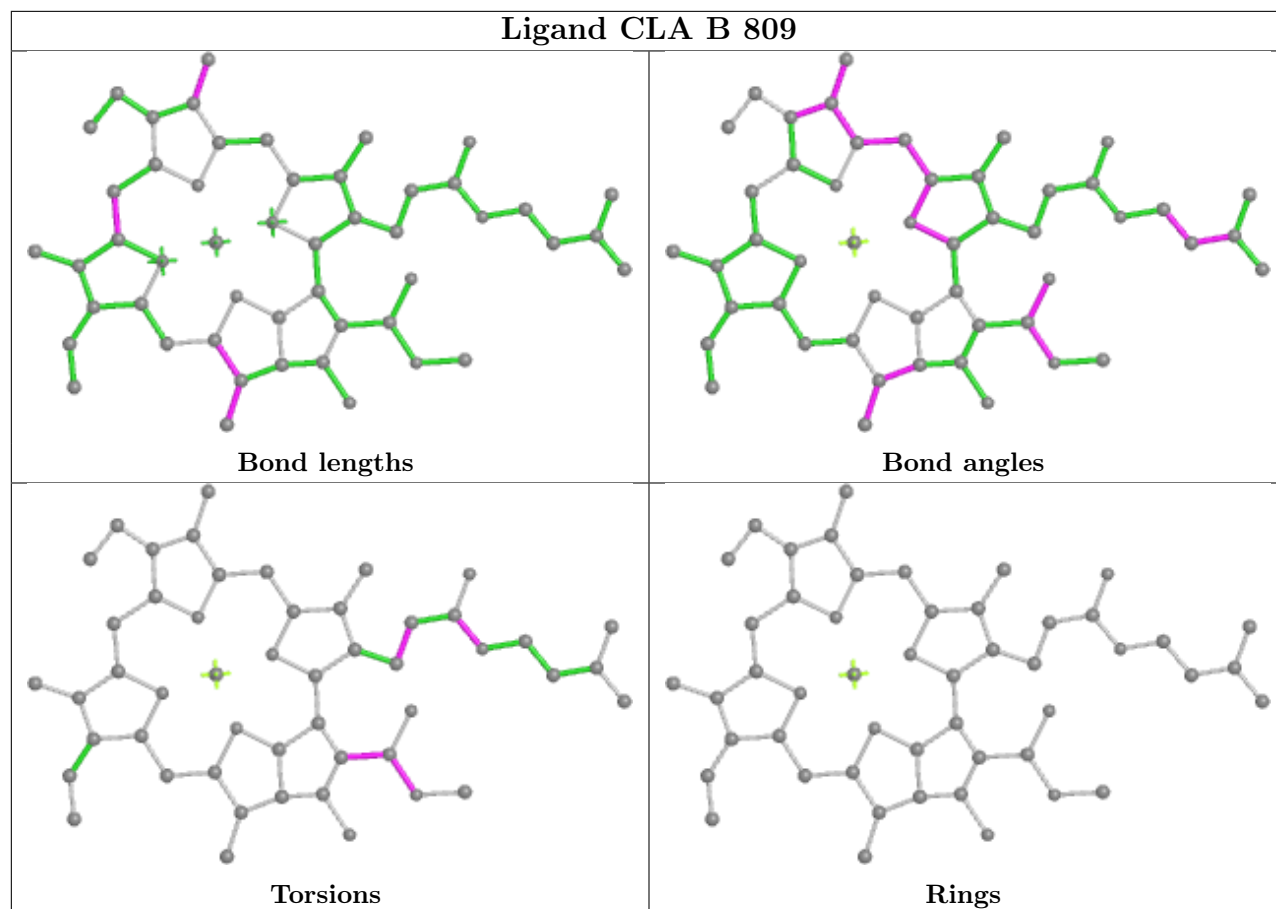


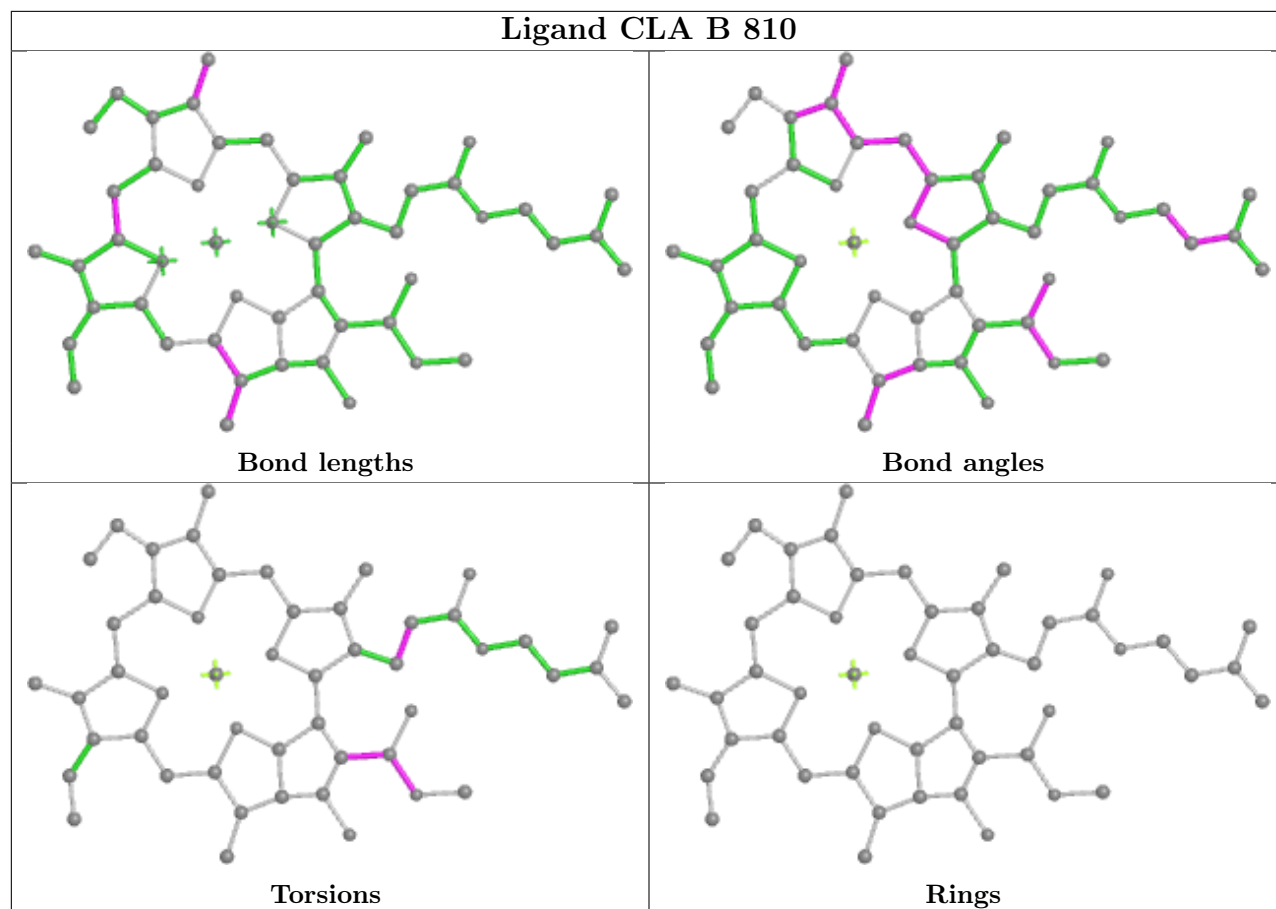


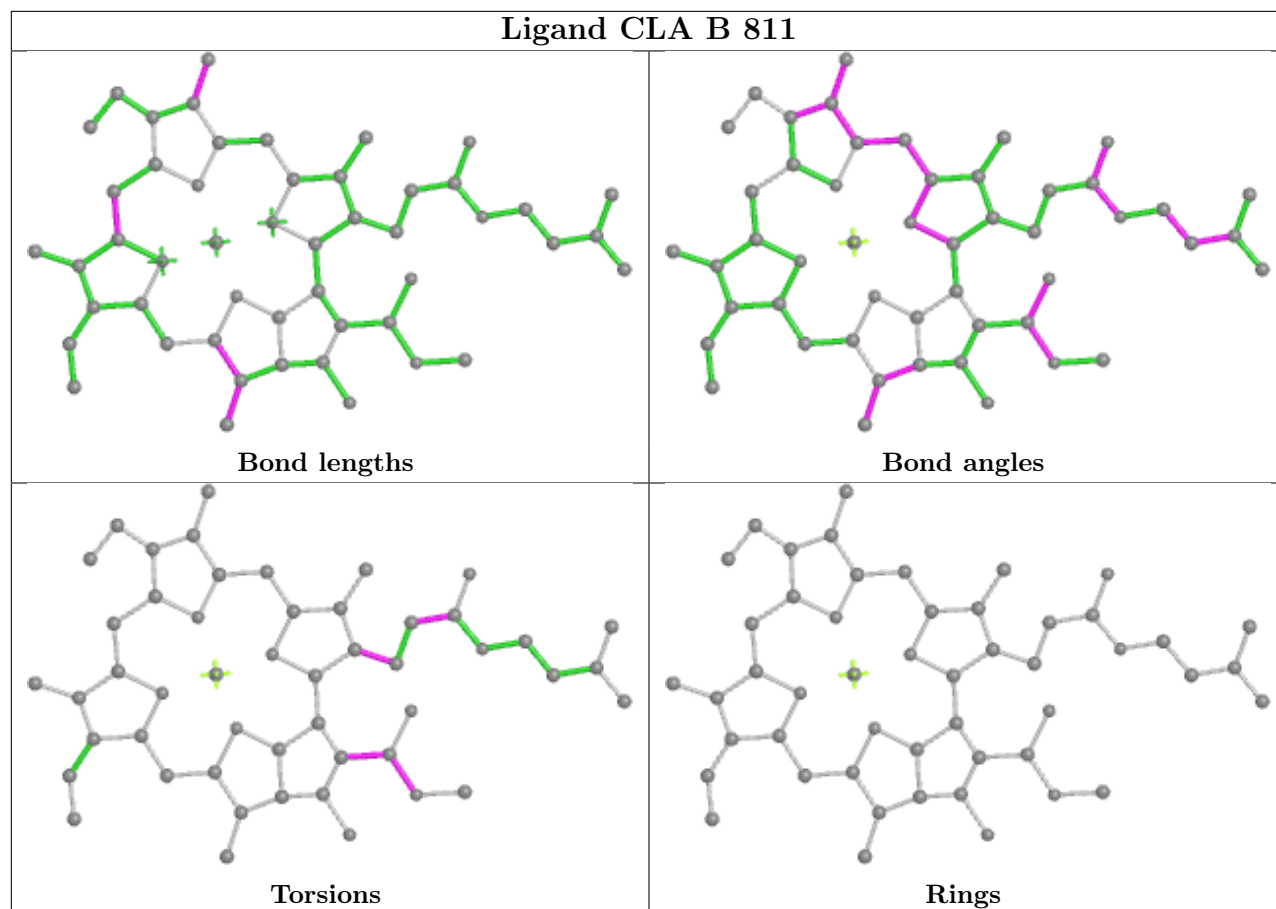


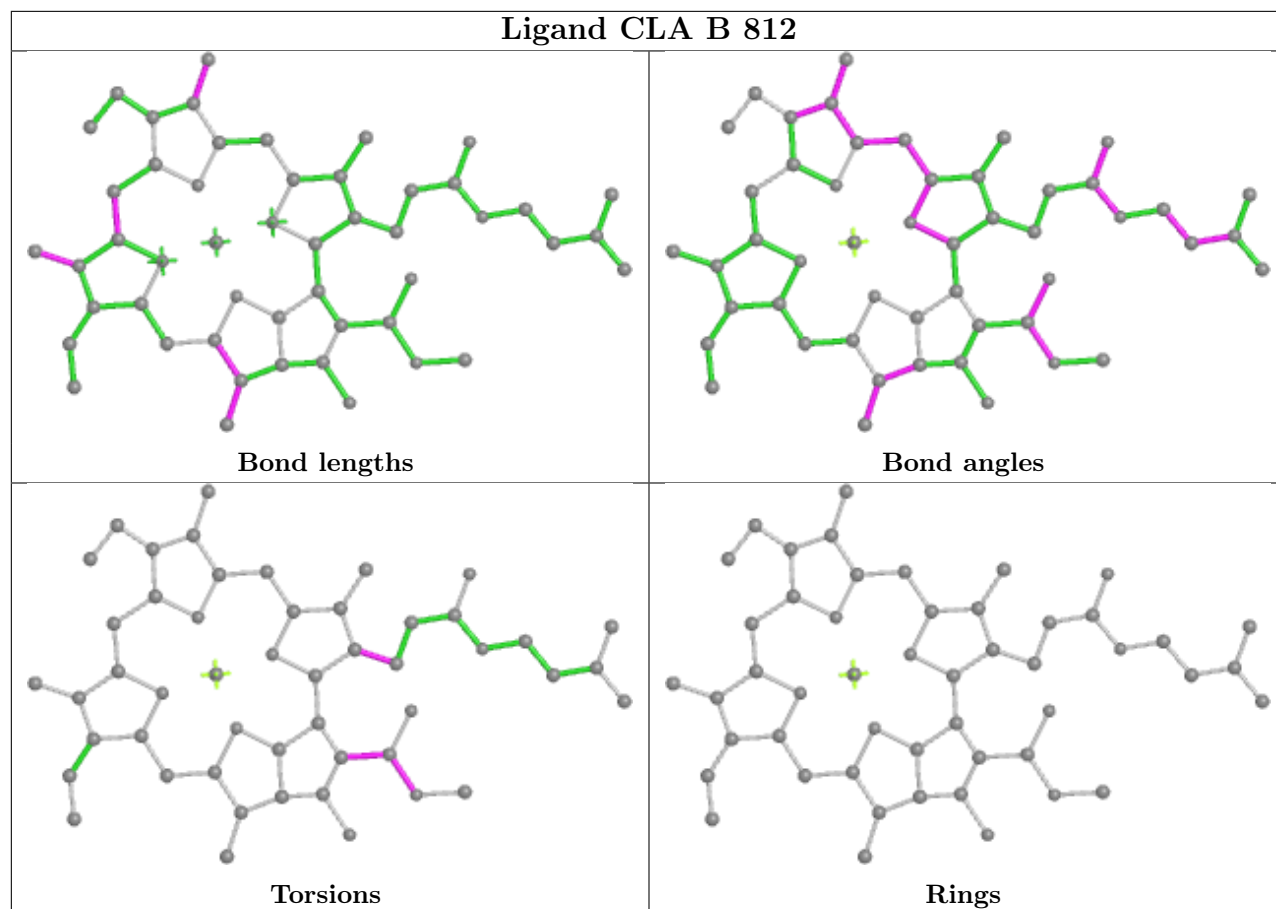


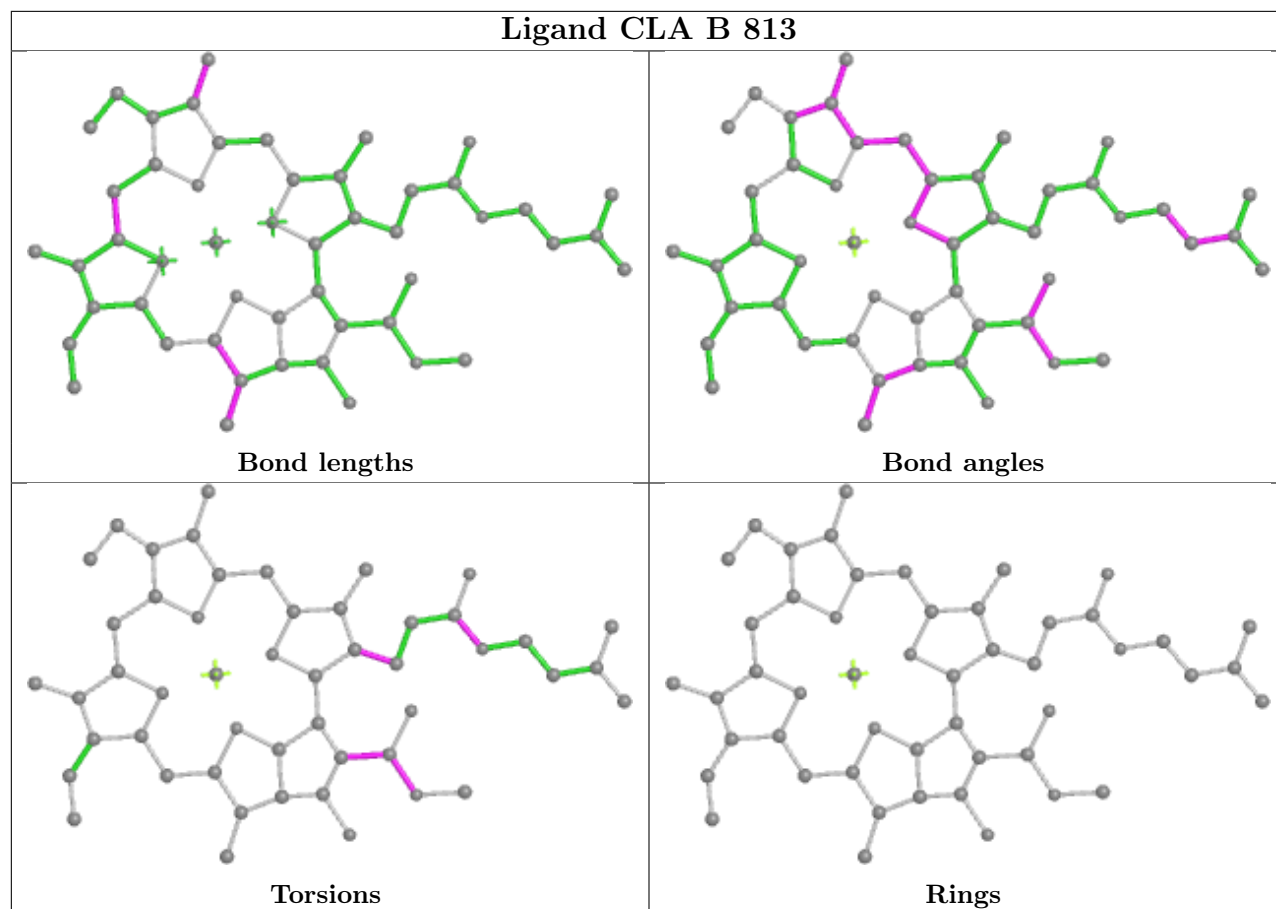


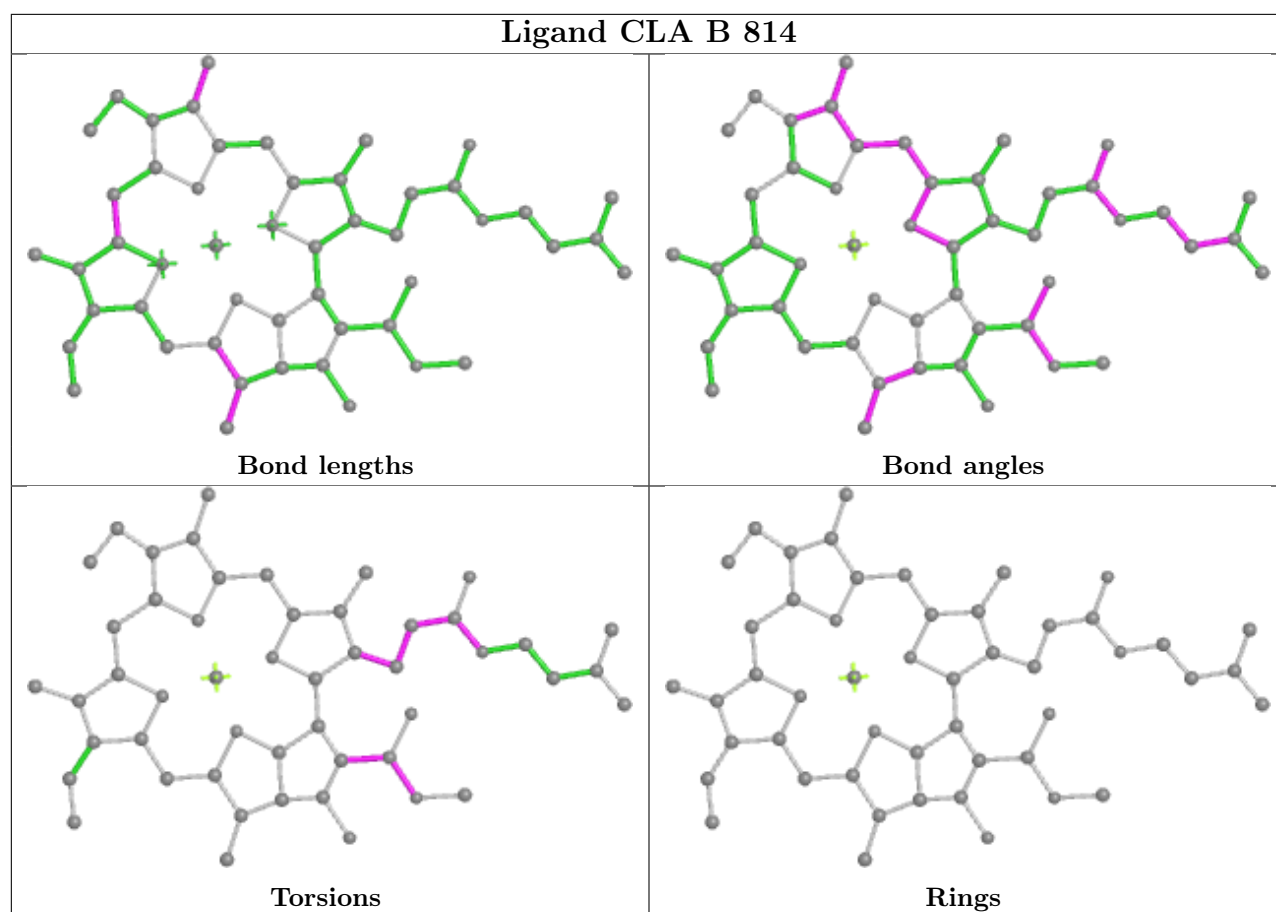




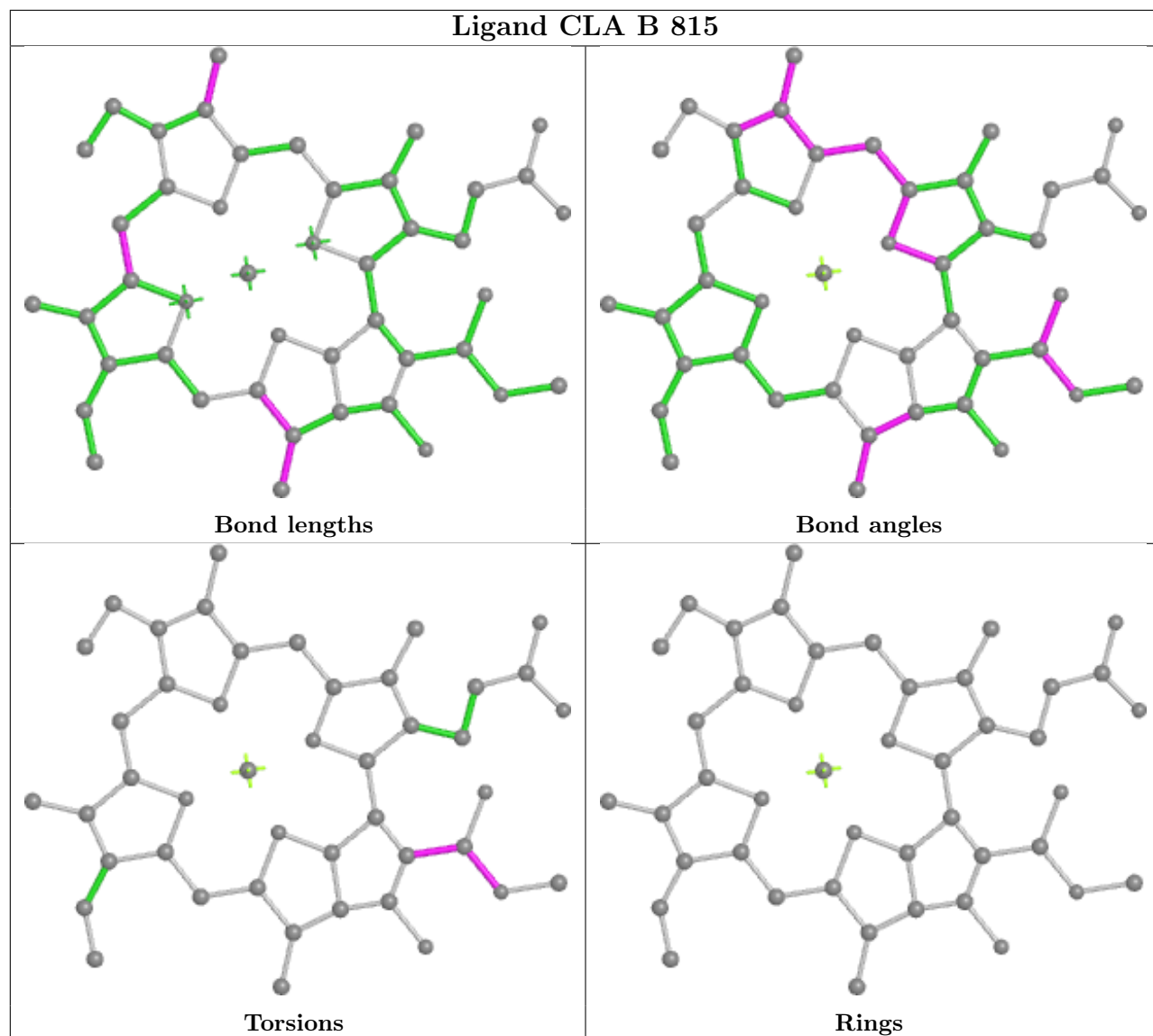




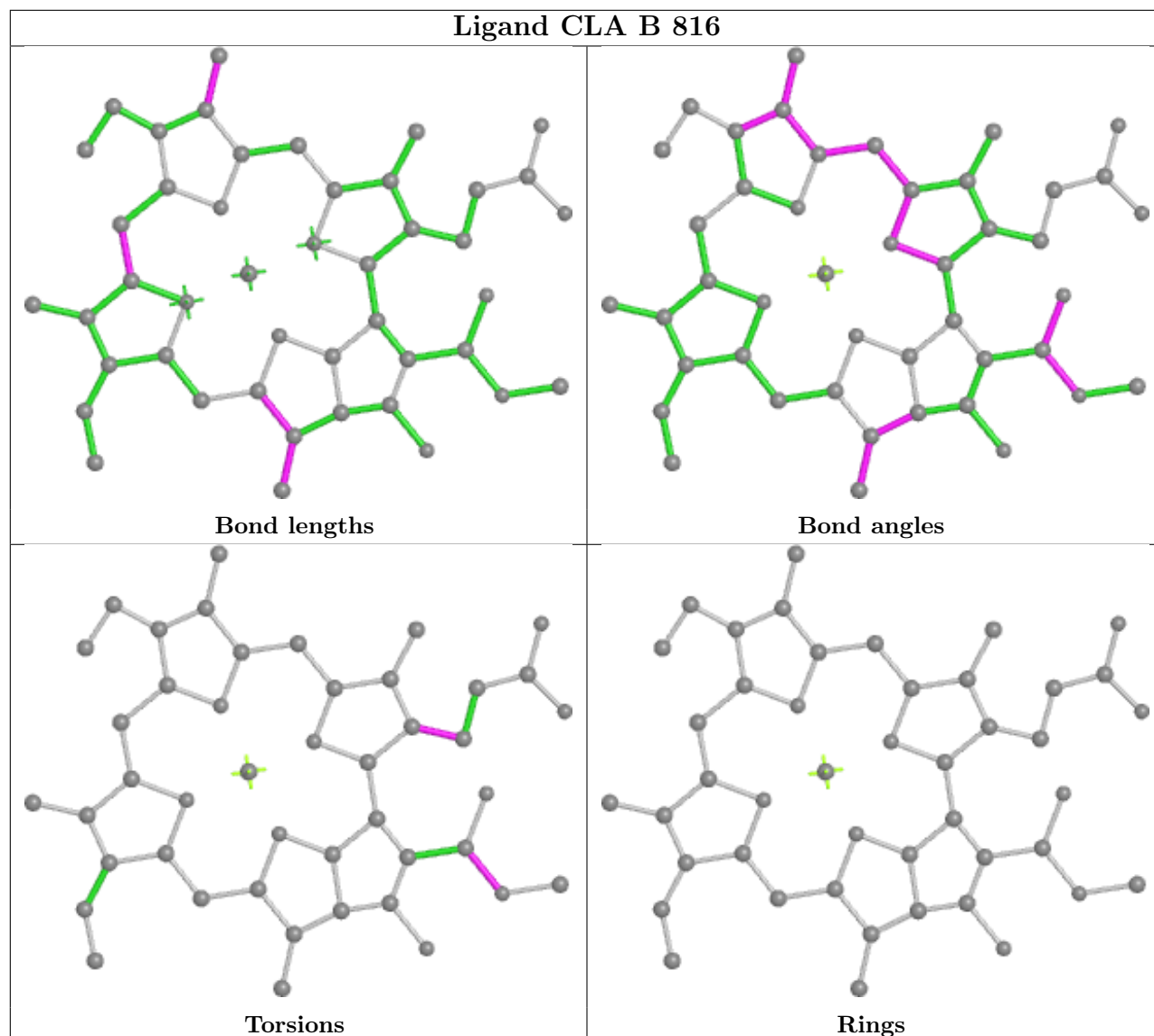


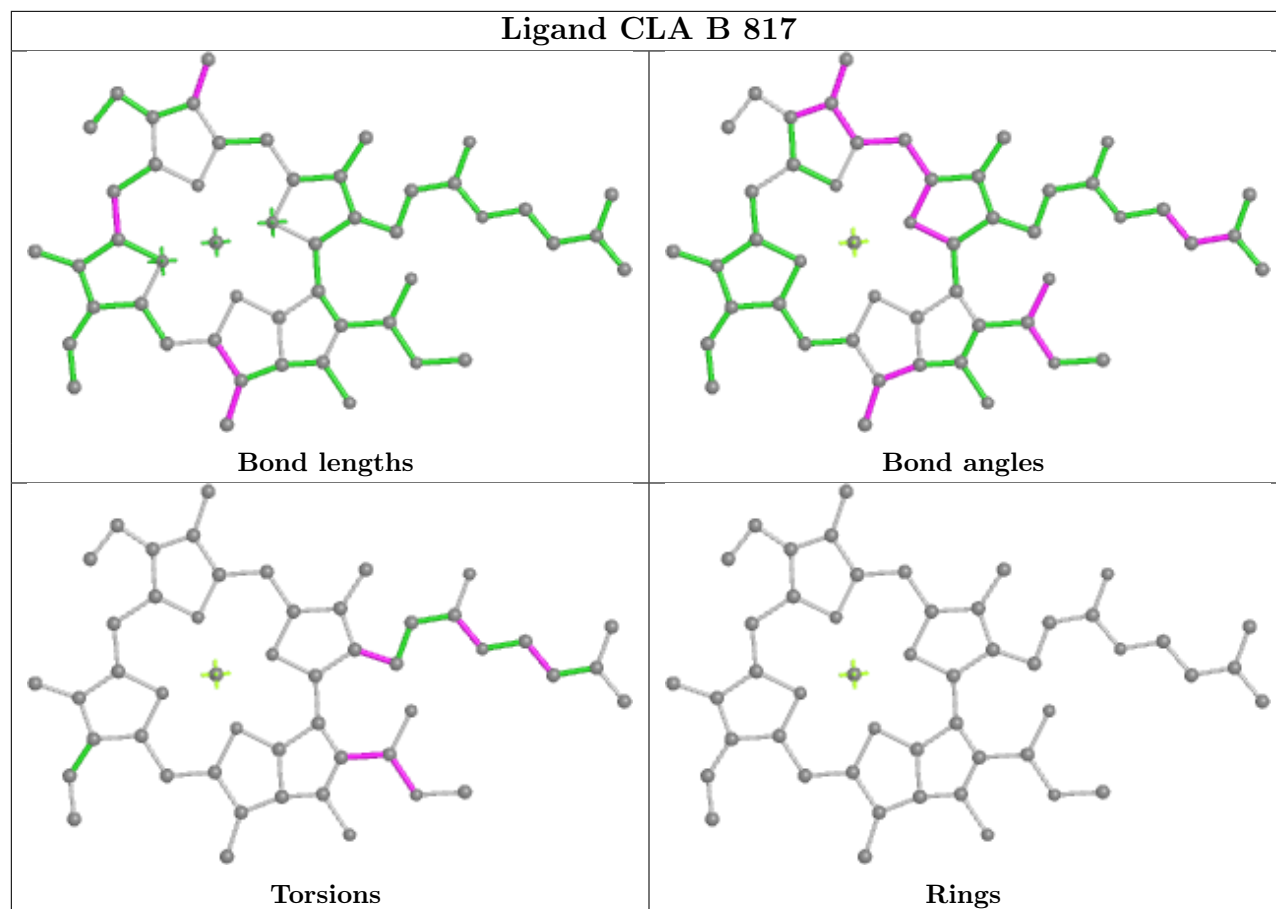


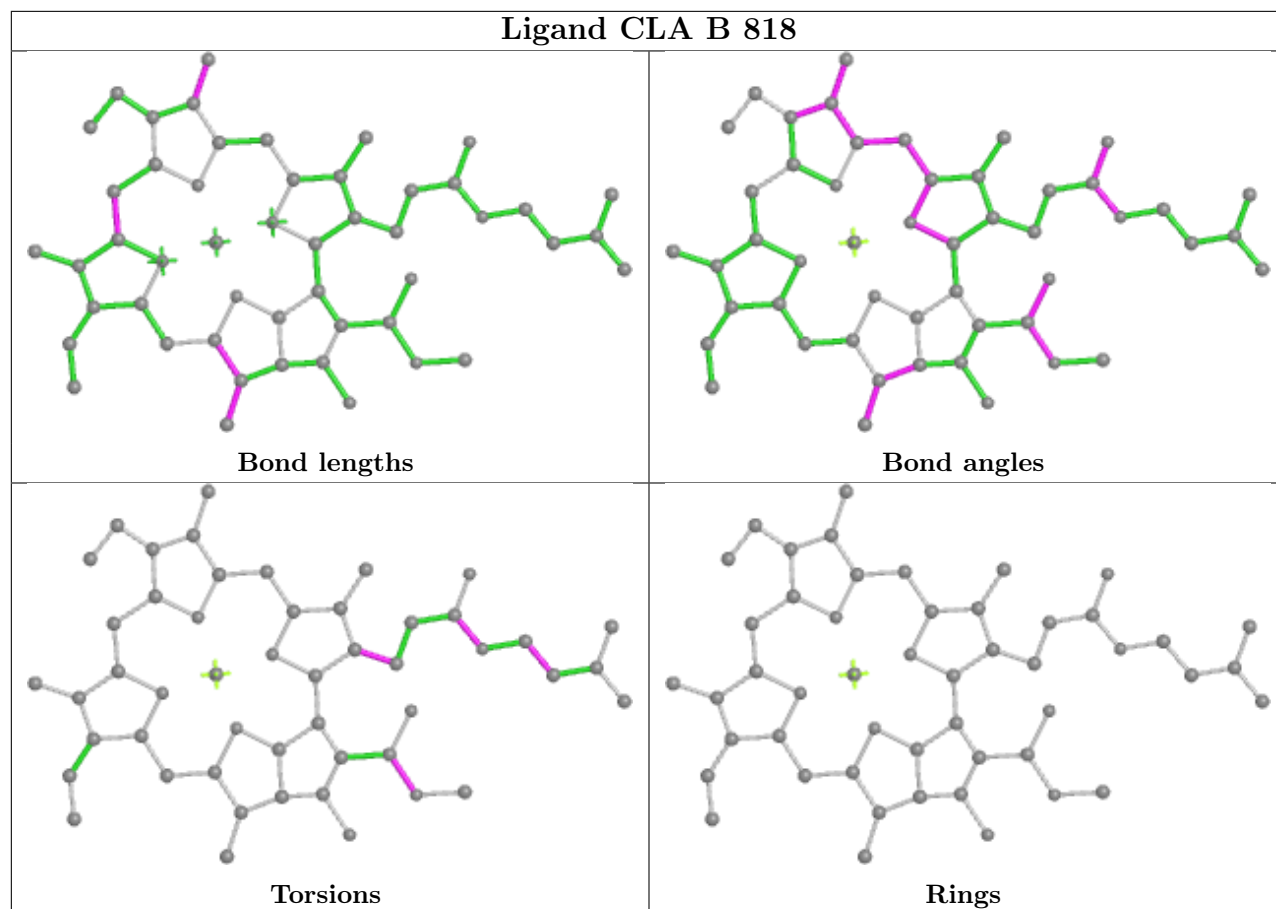
Ligand CLA B 815



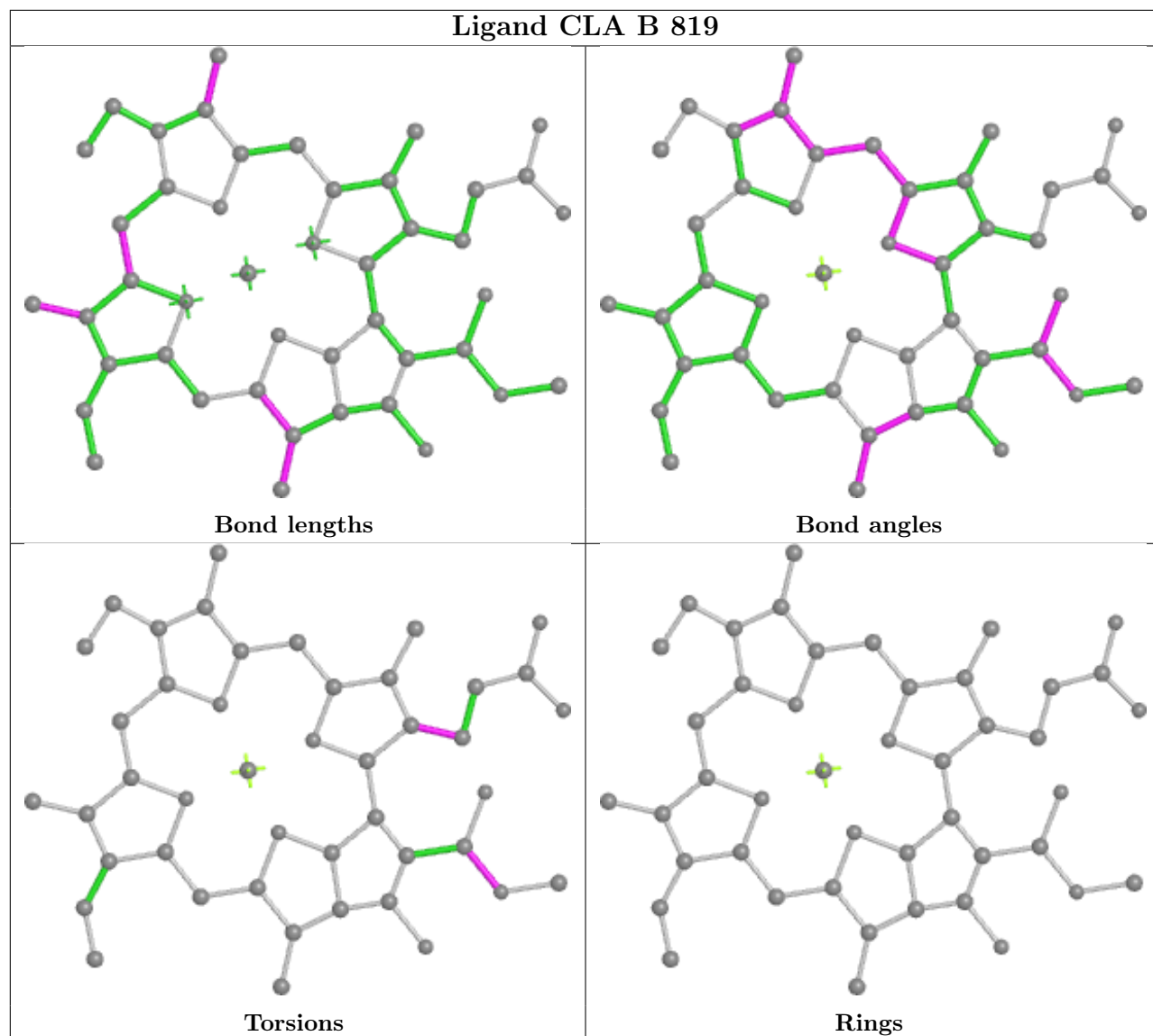
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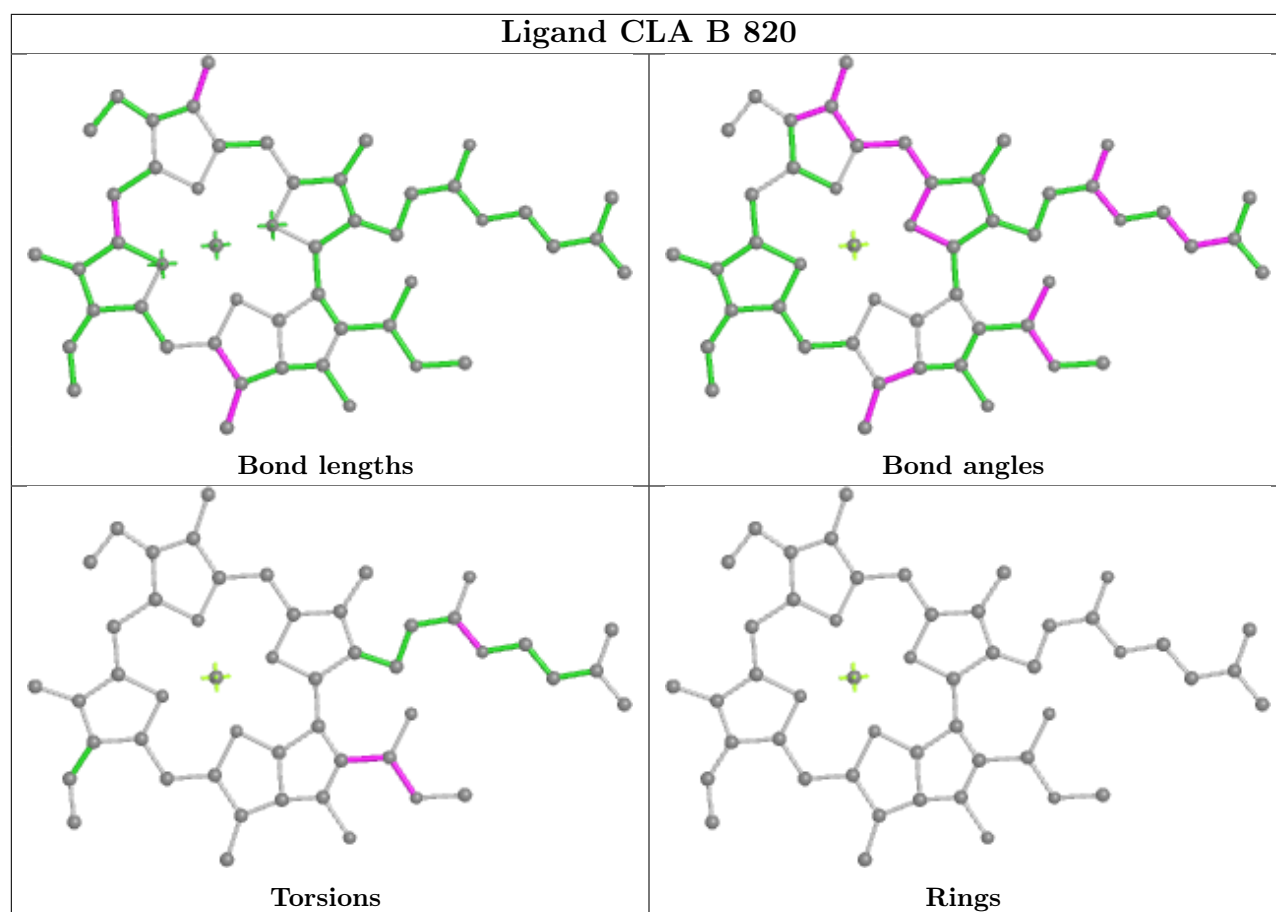




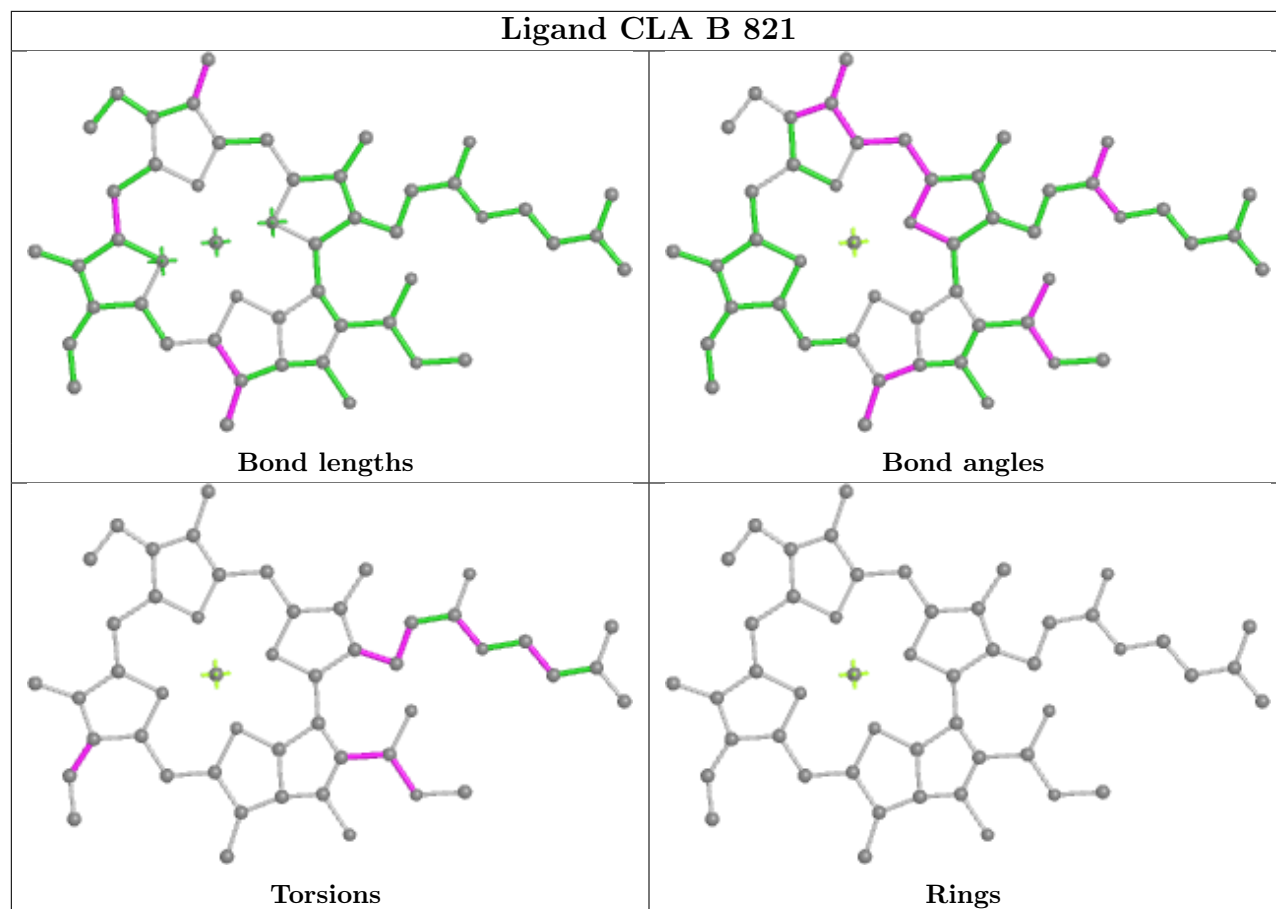


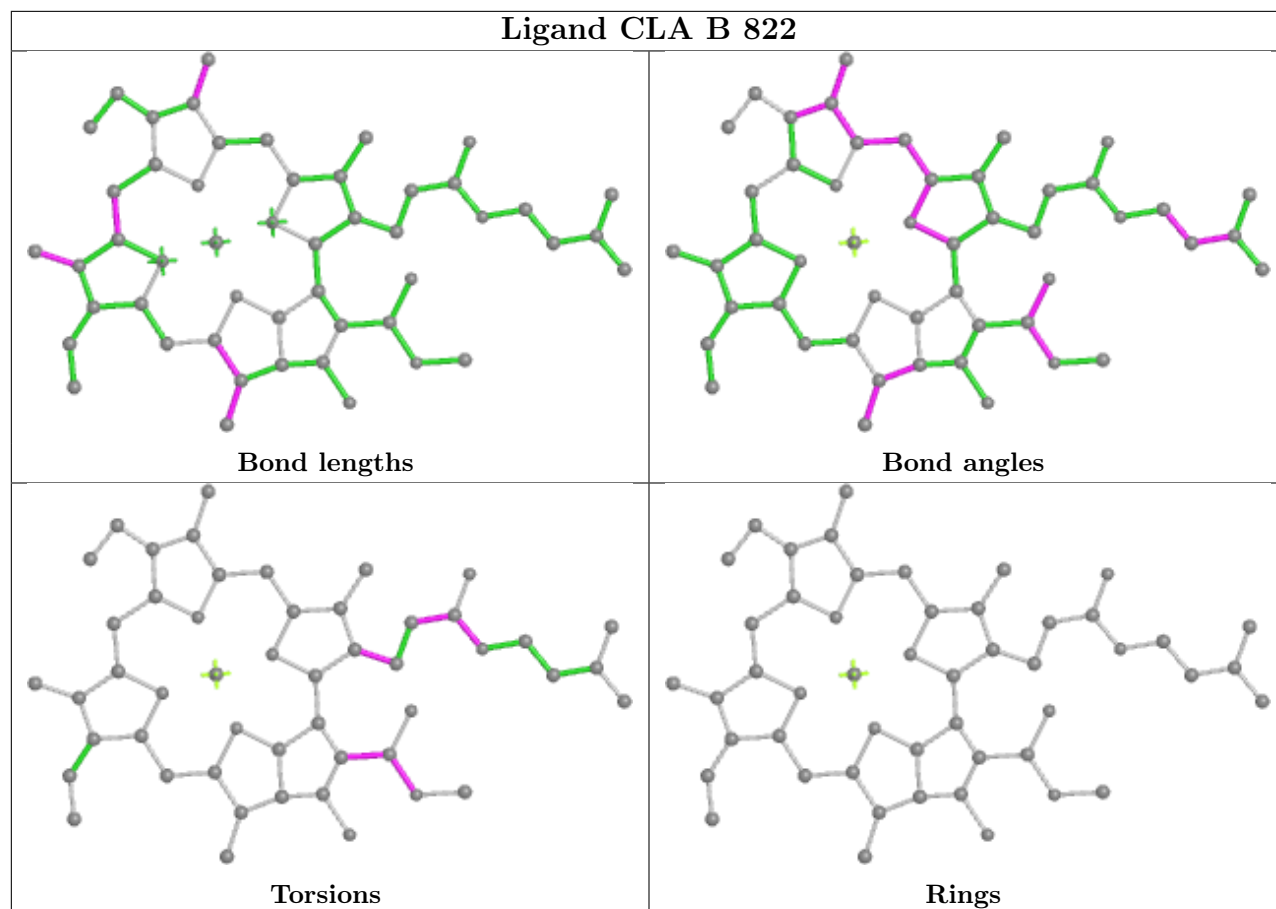
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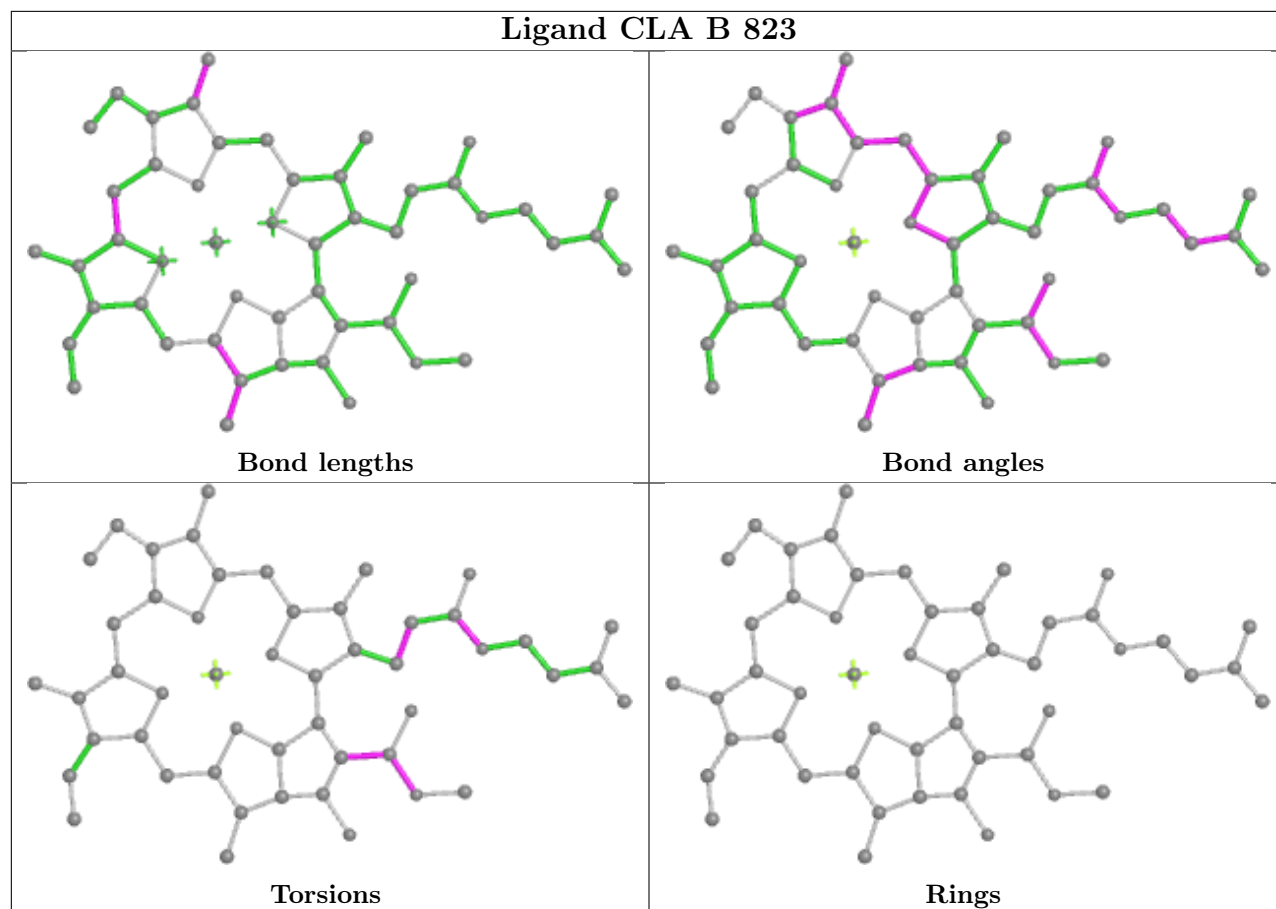




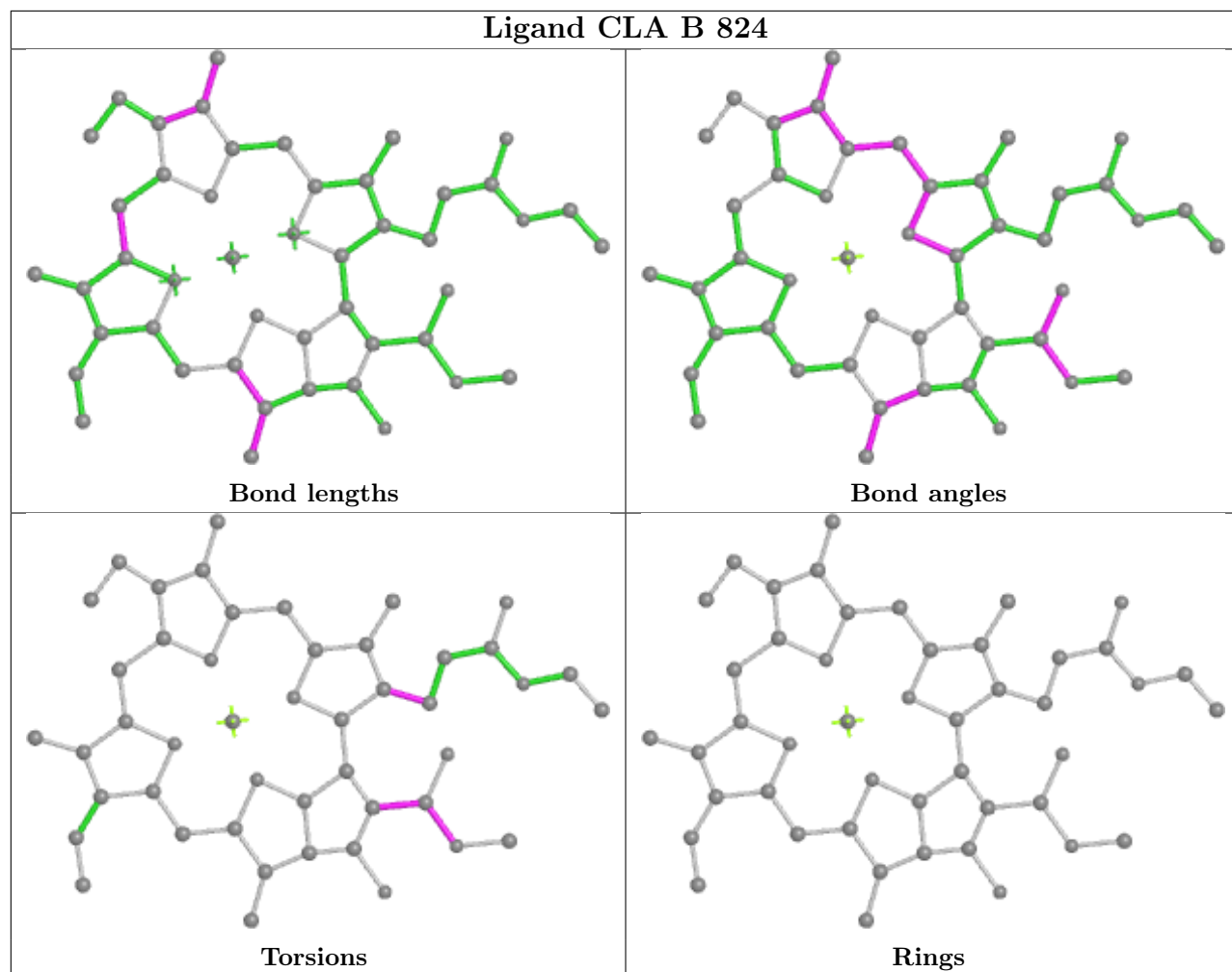
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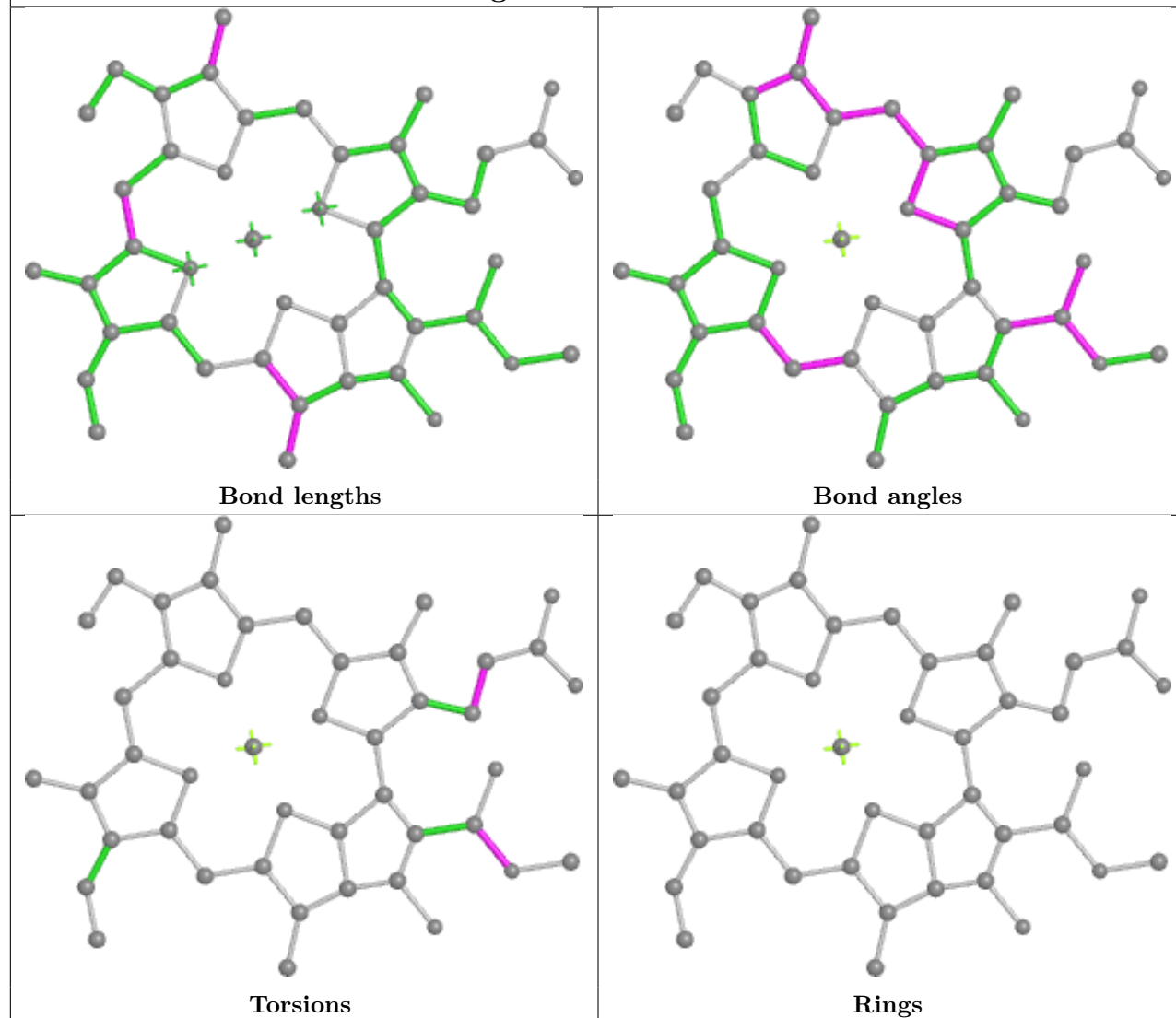


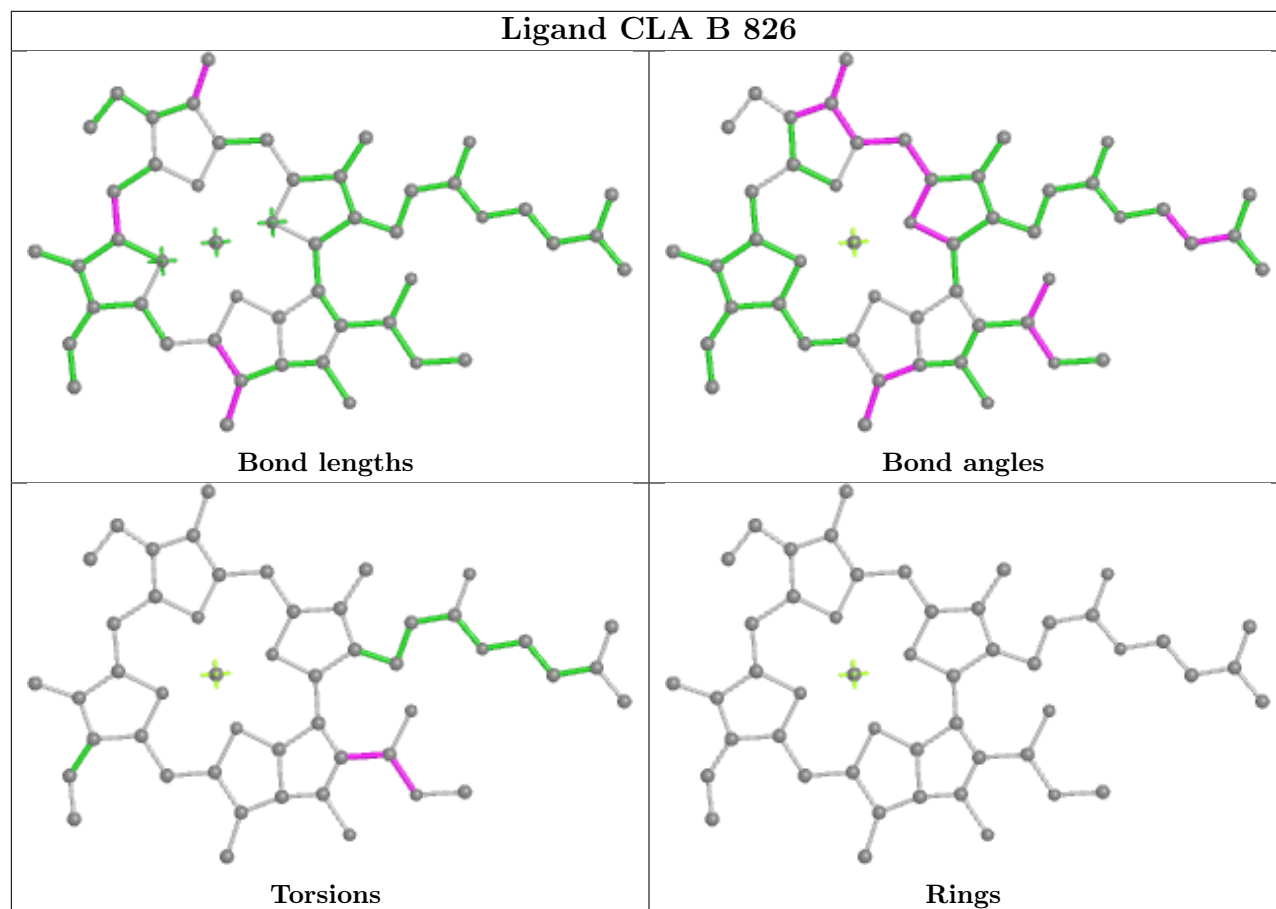


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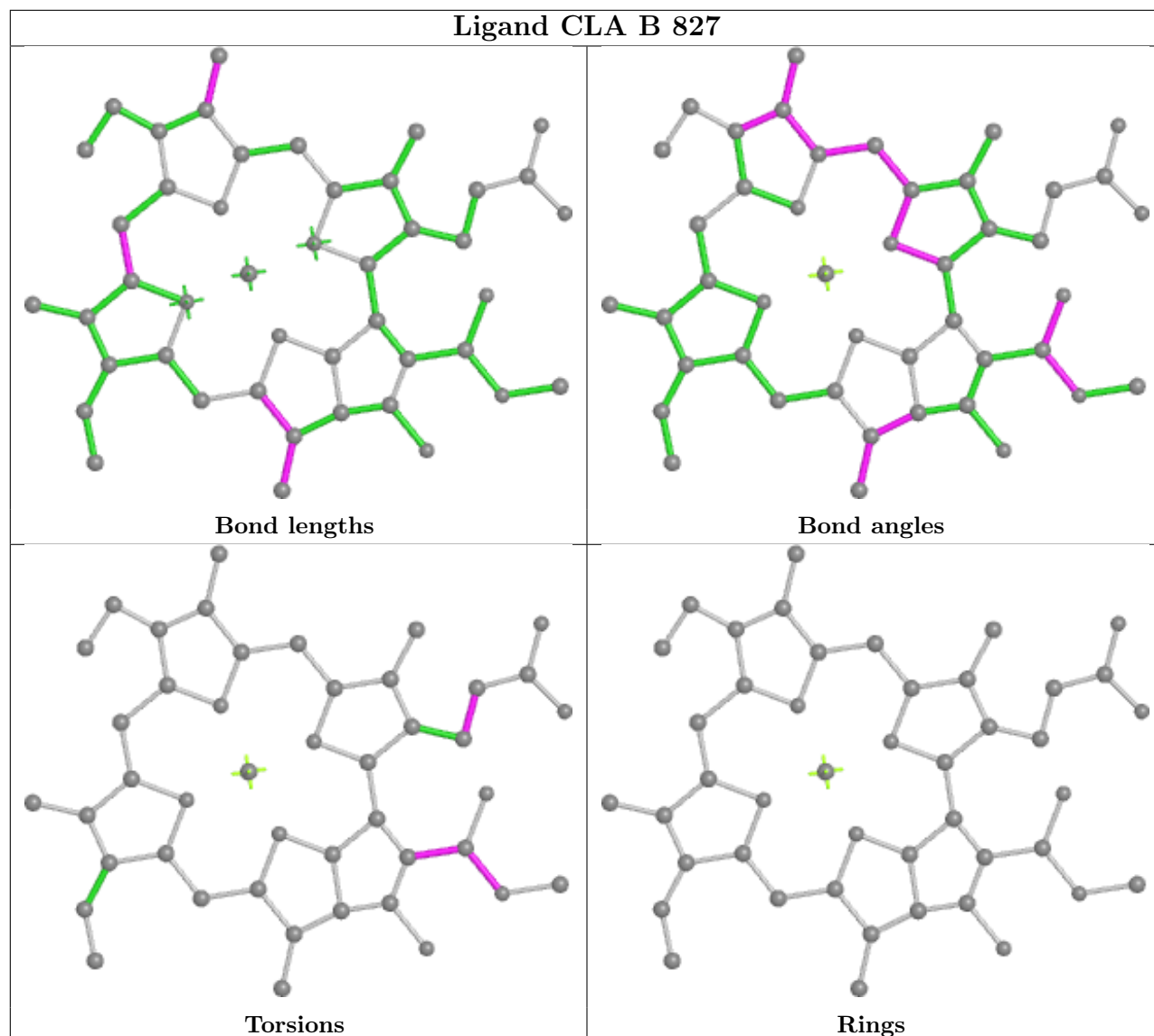


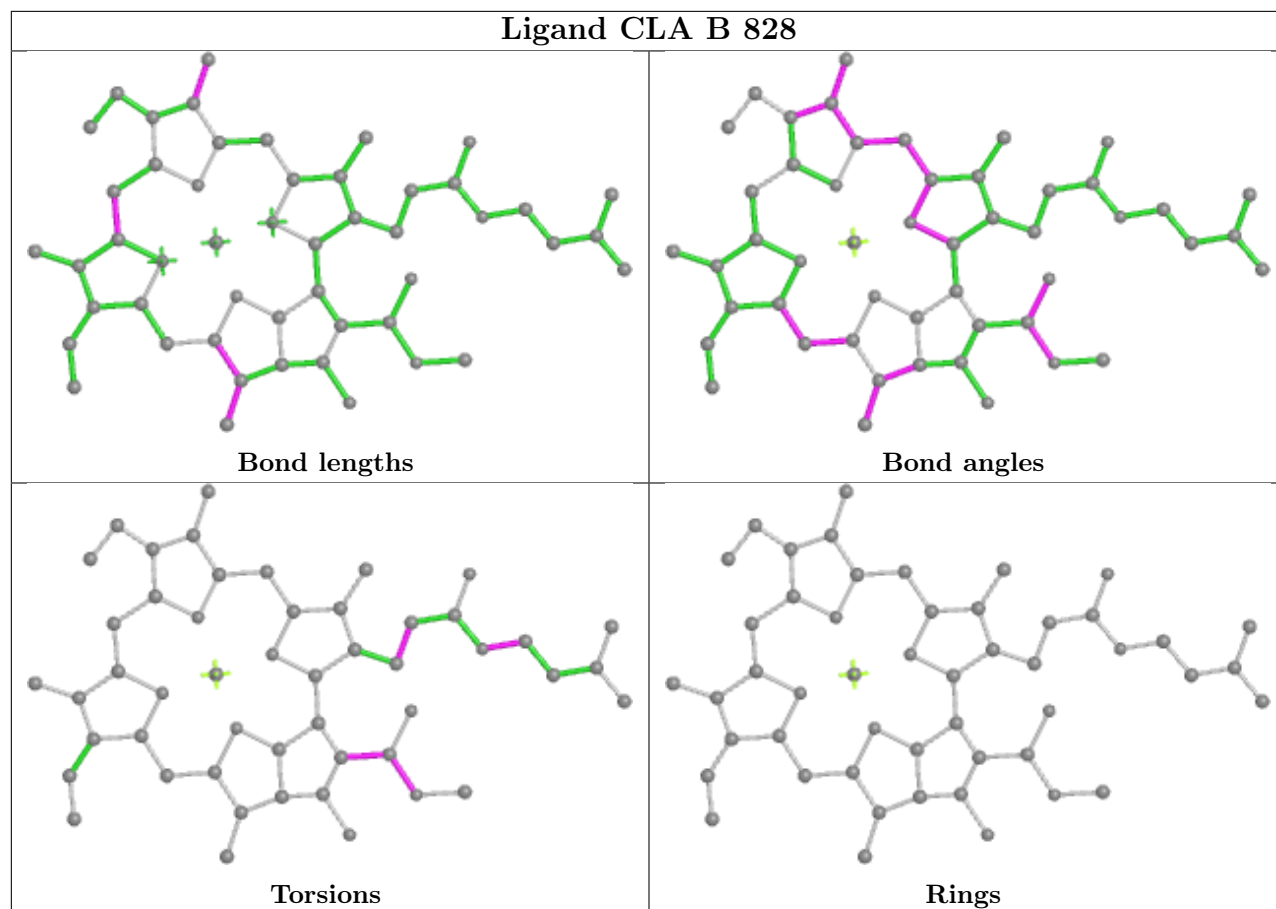
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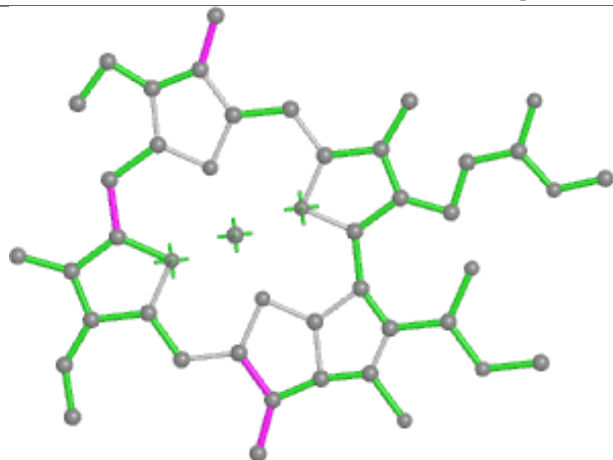


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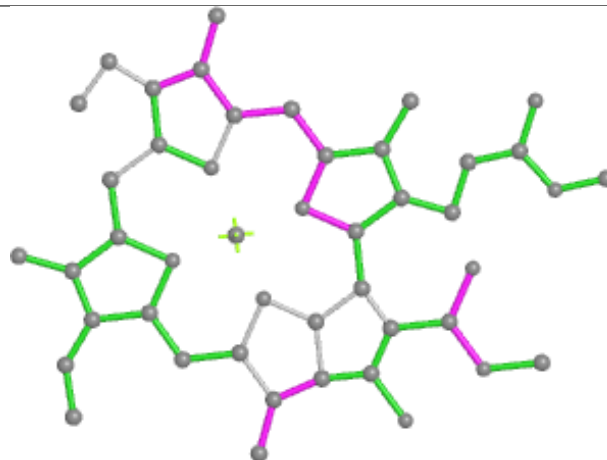




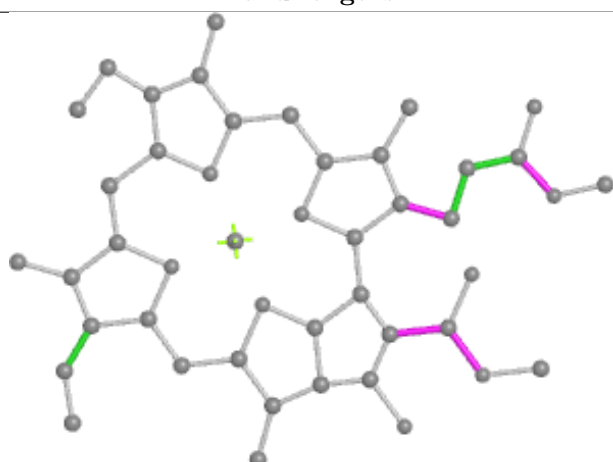
Ligand CLA B 829



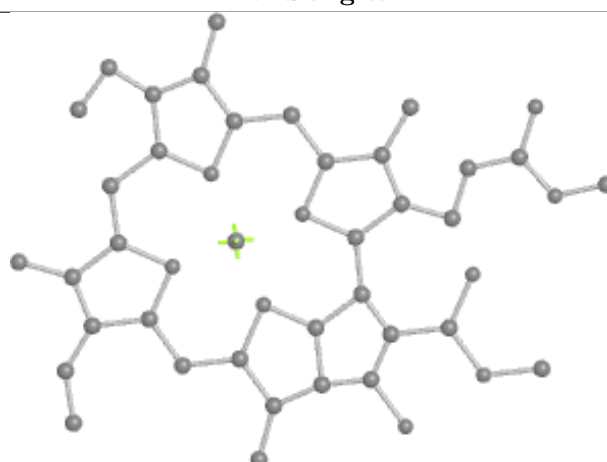
Bond lengths



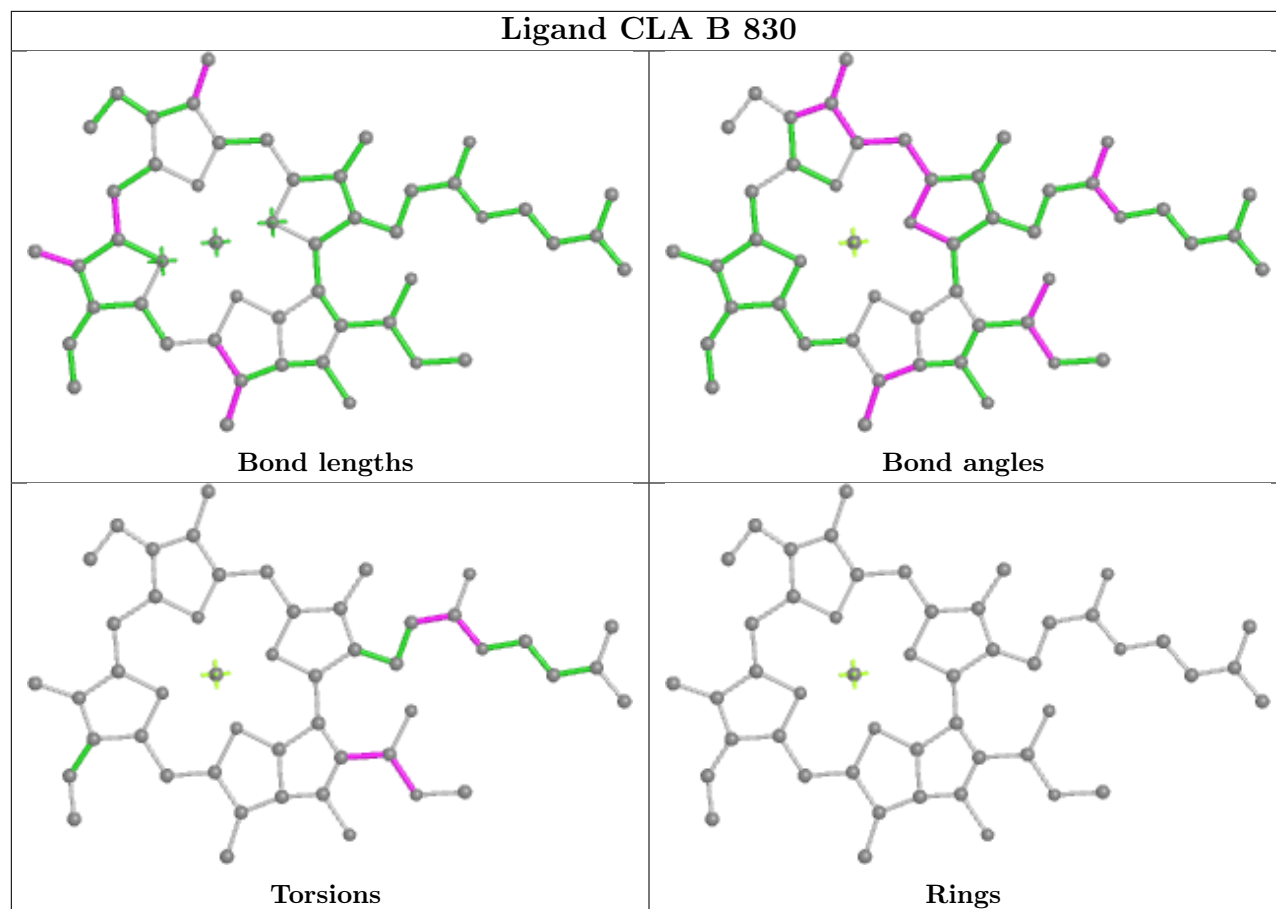
Bond angles

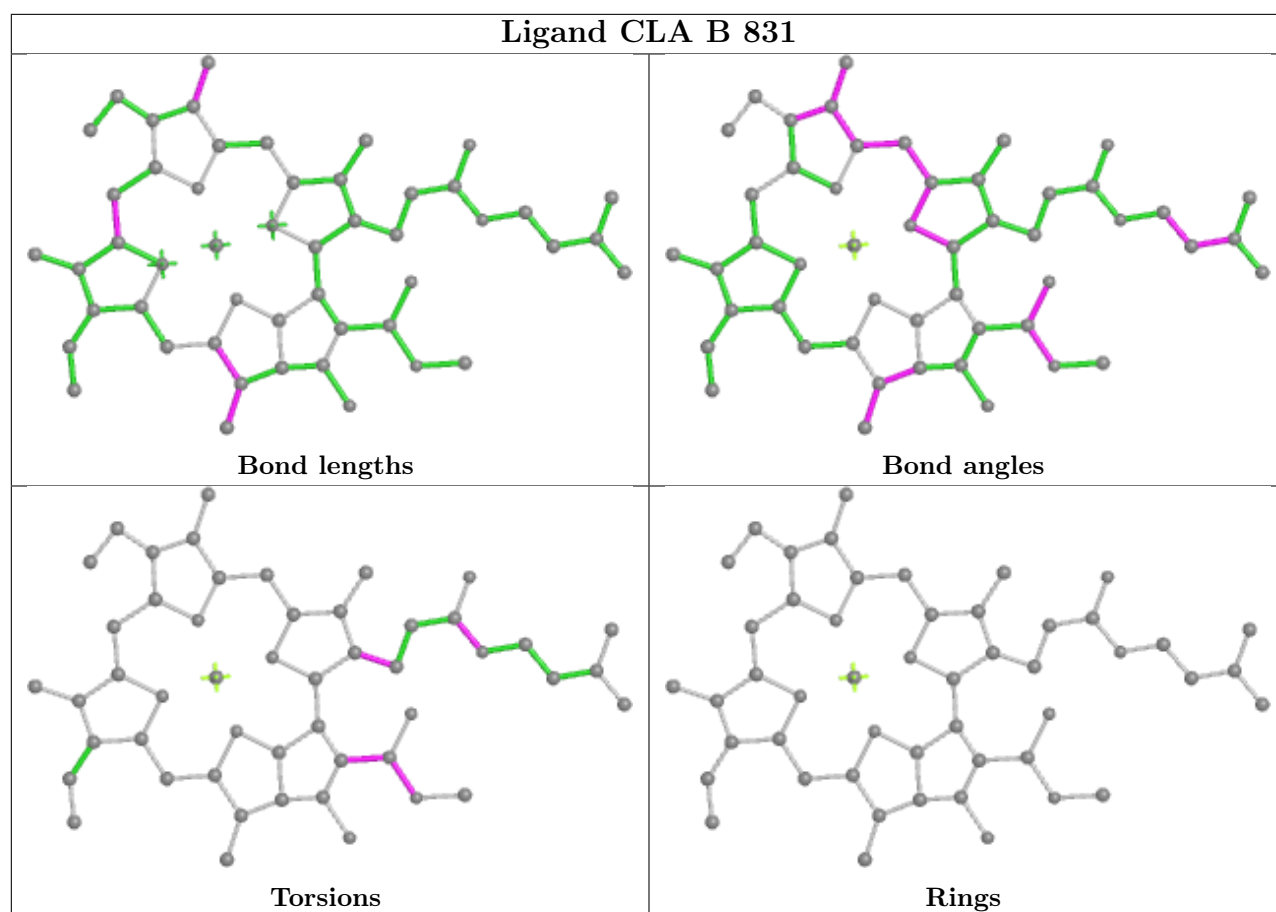


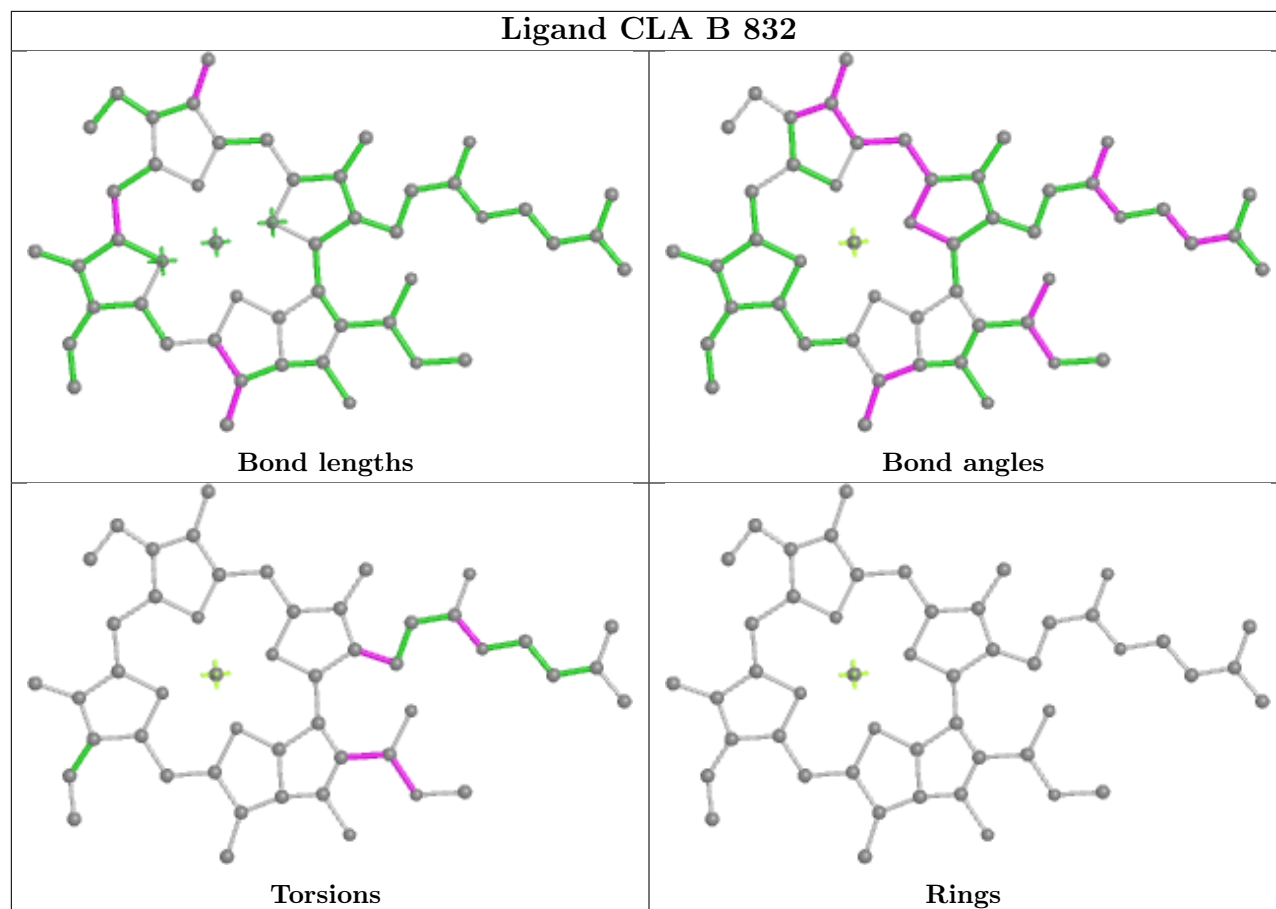
Torsions

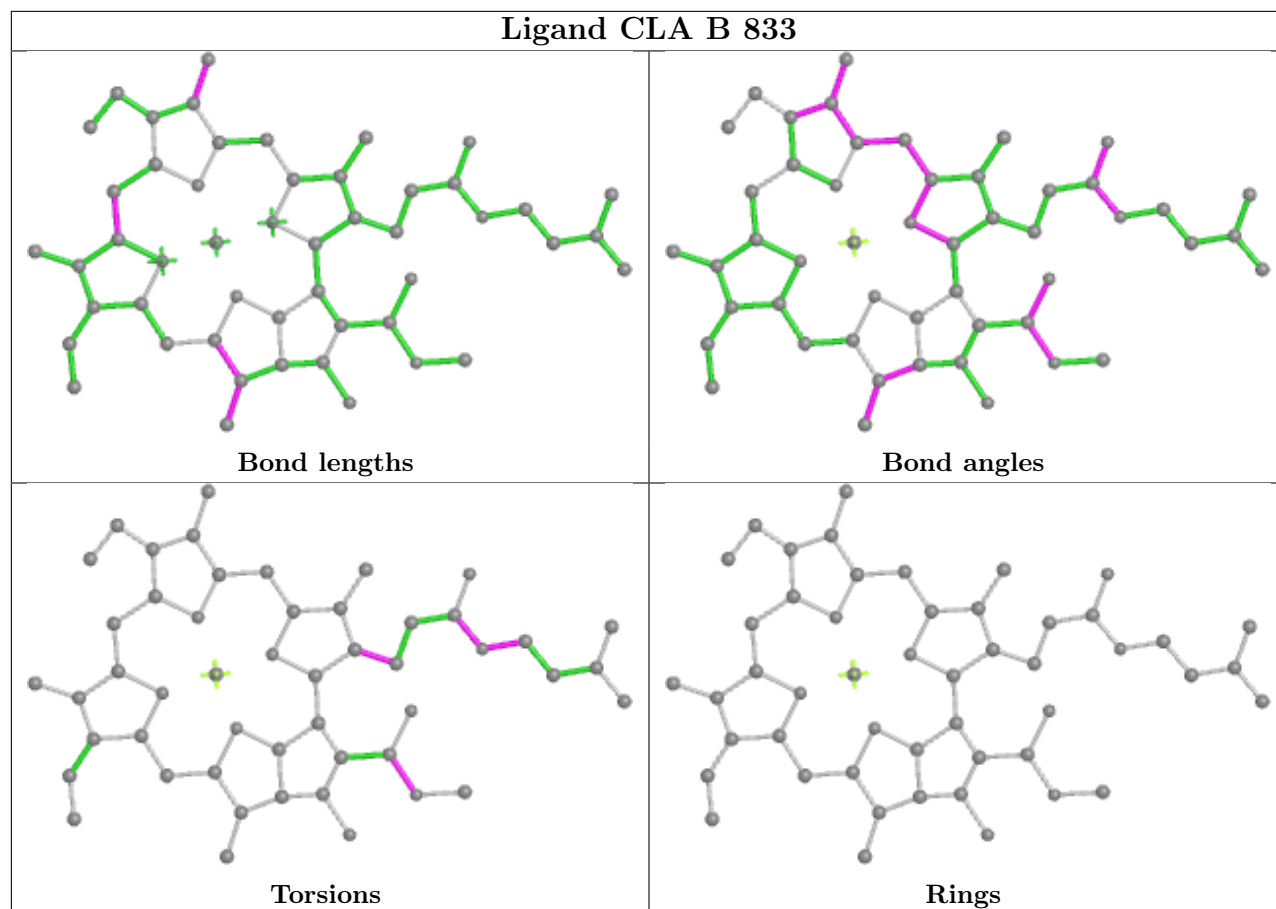


Rings

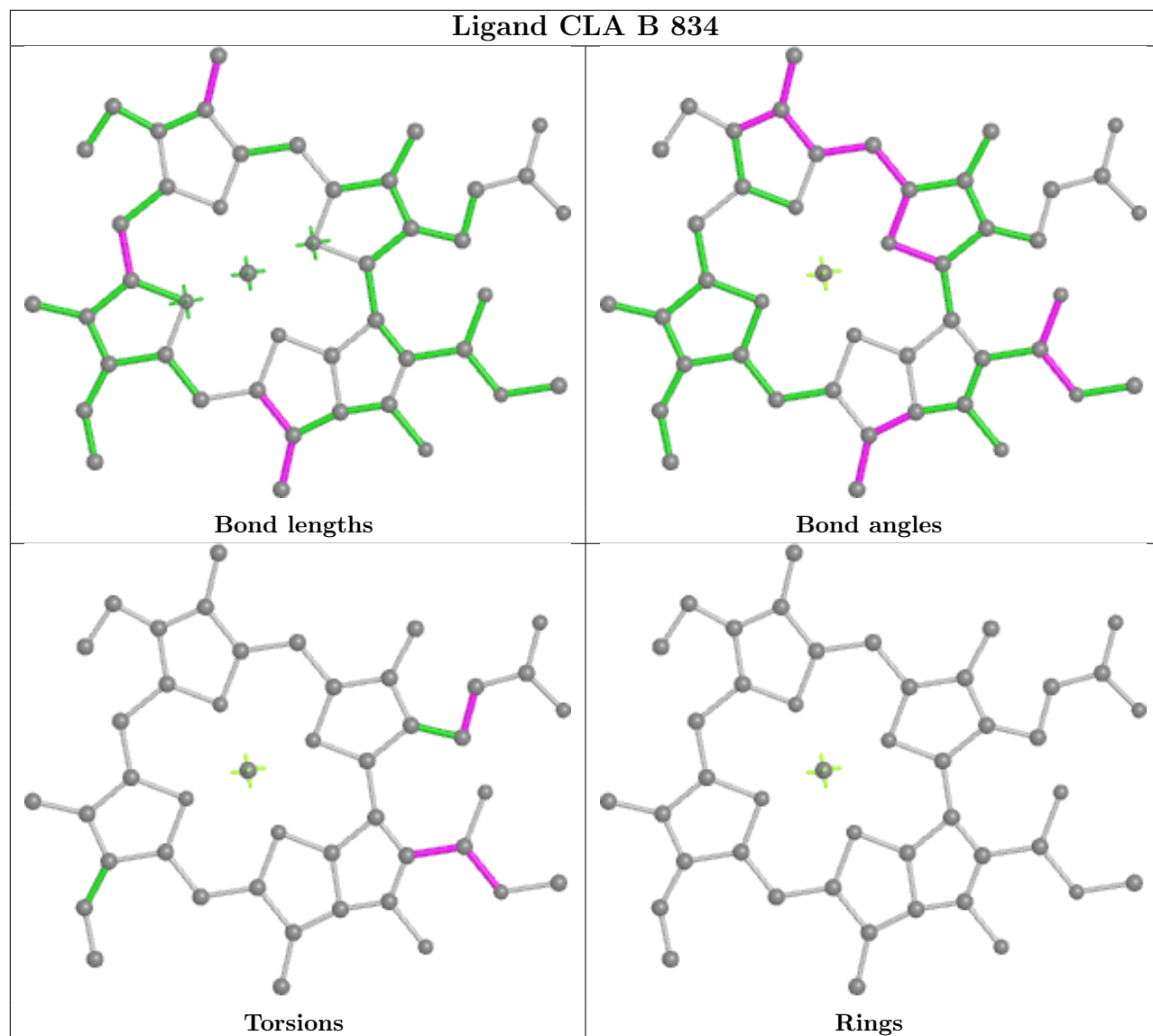


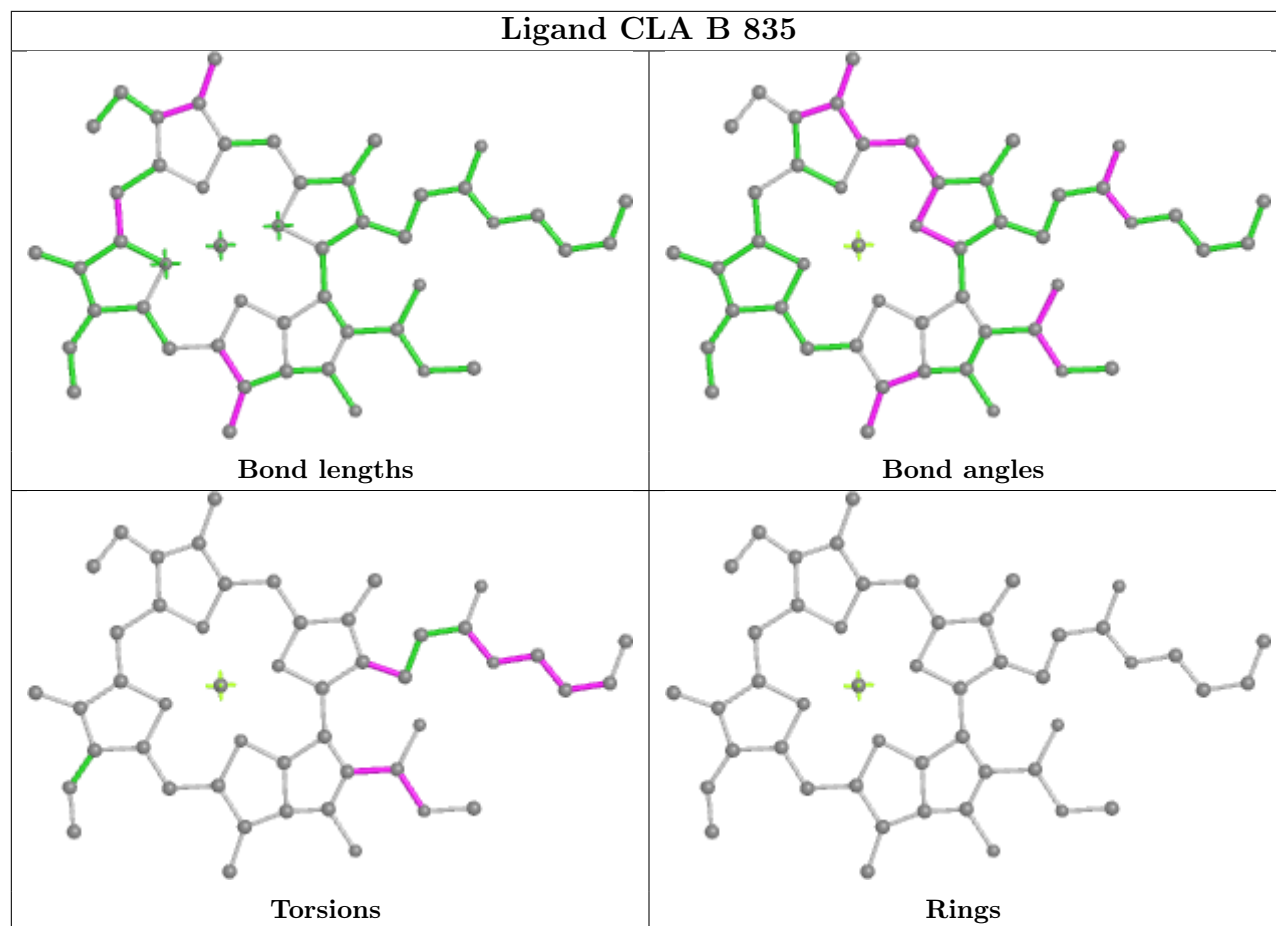


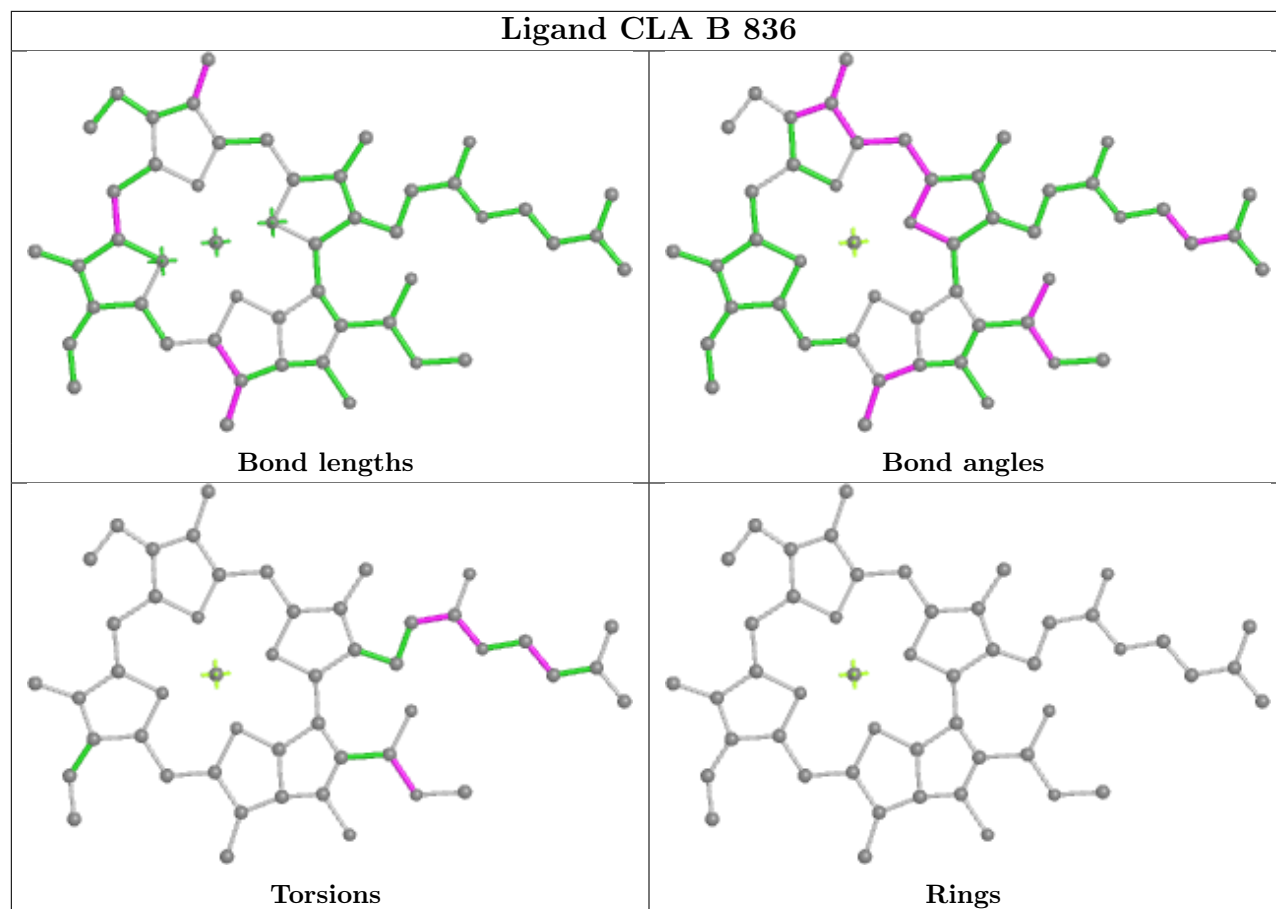




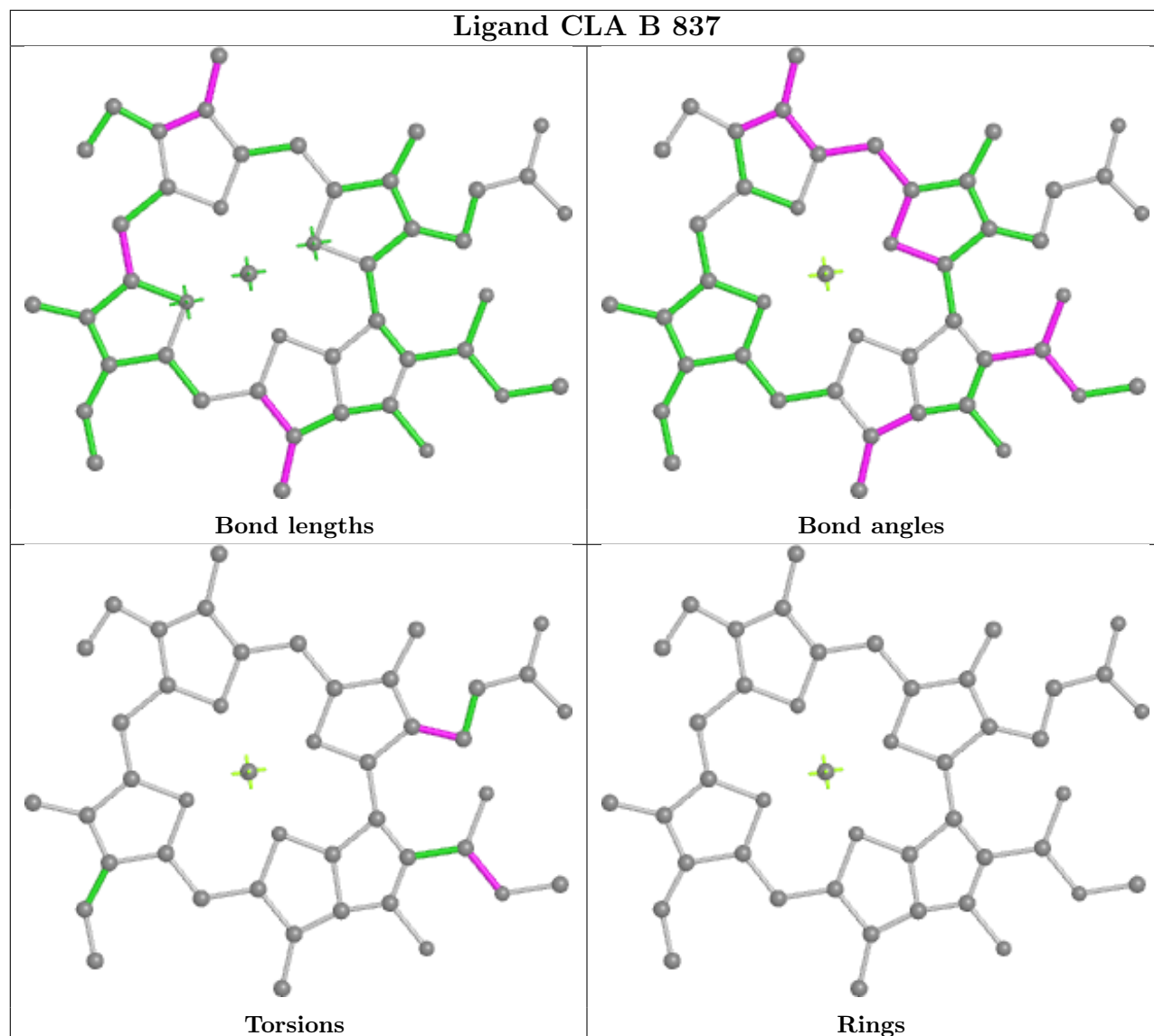
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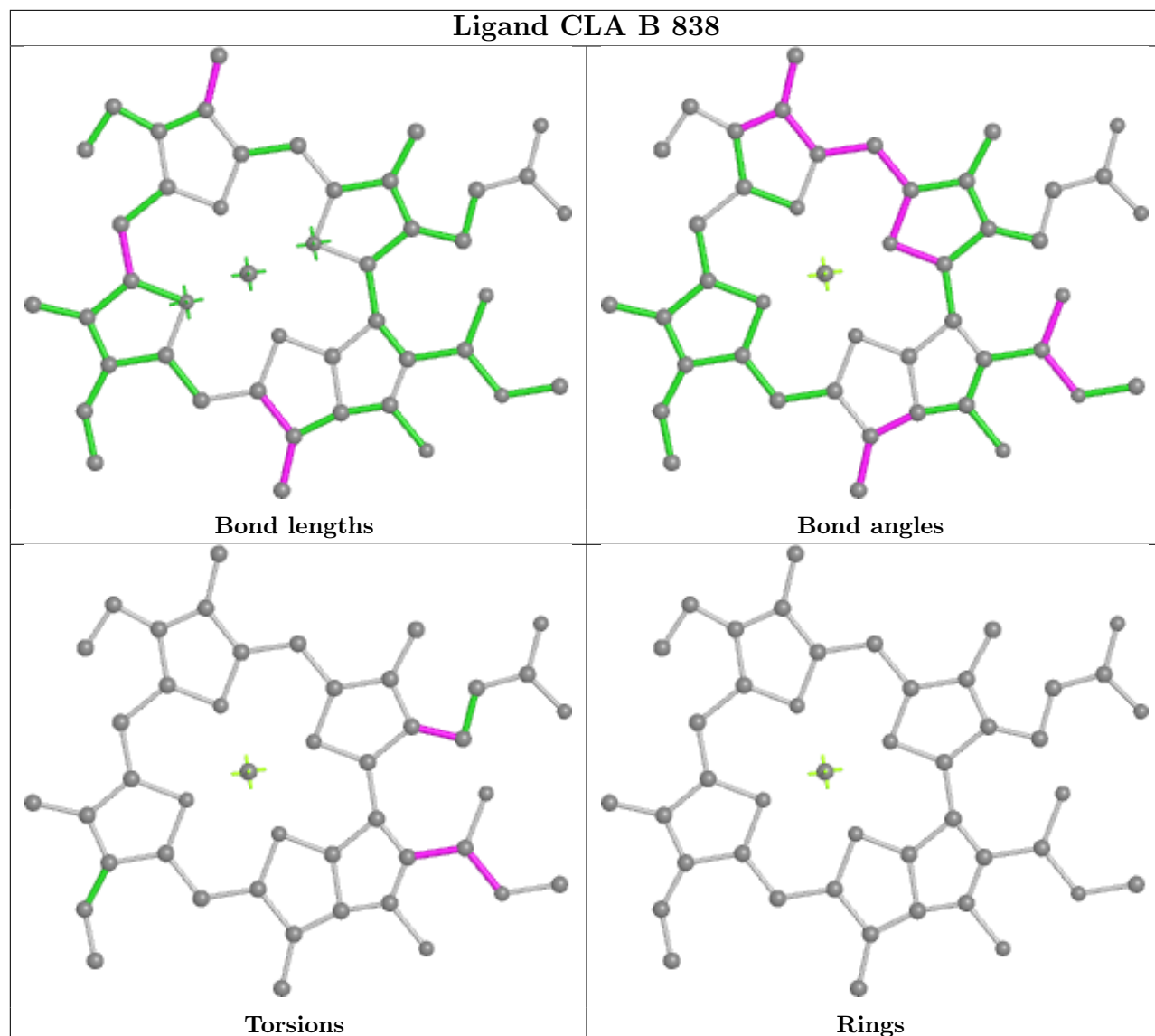


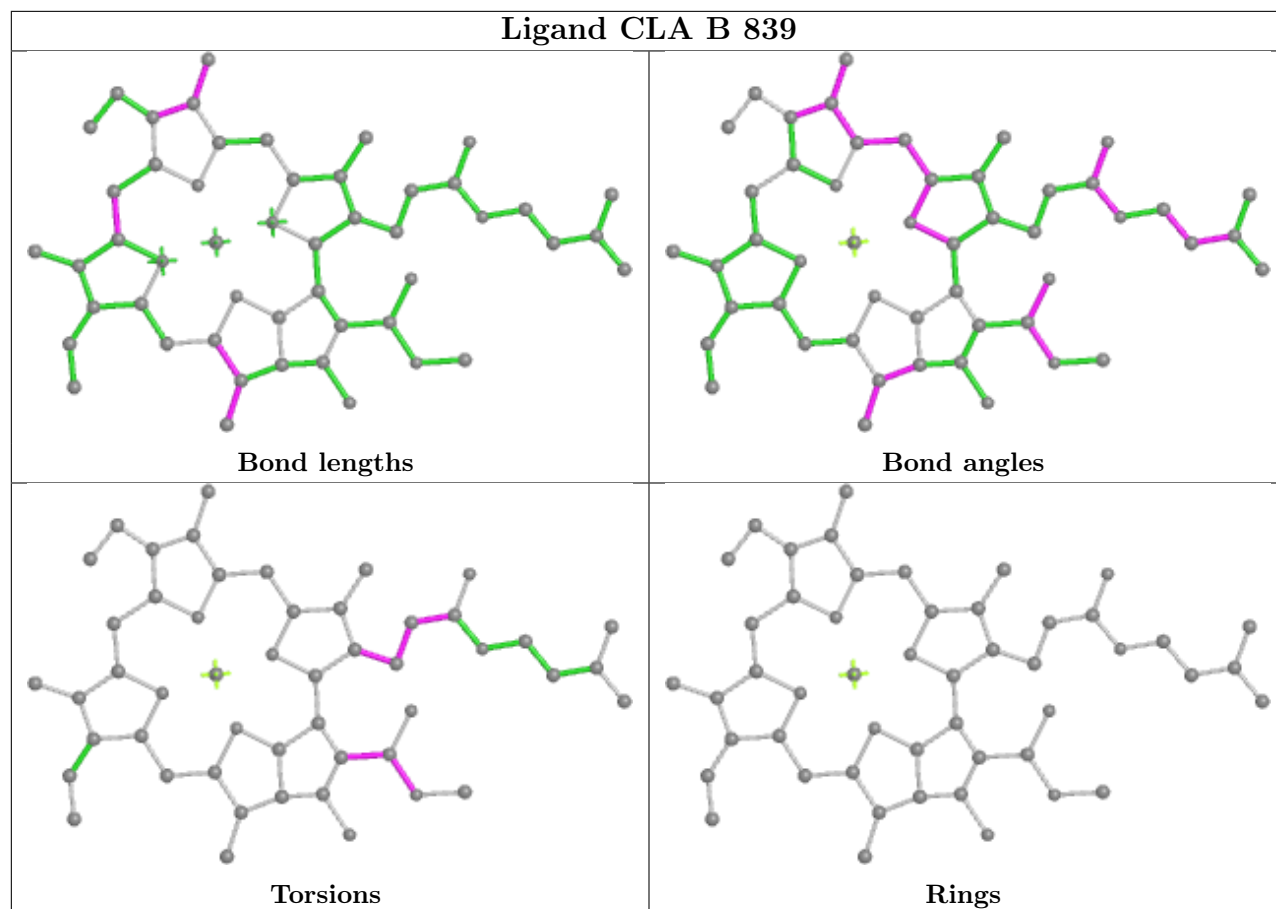


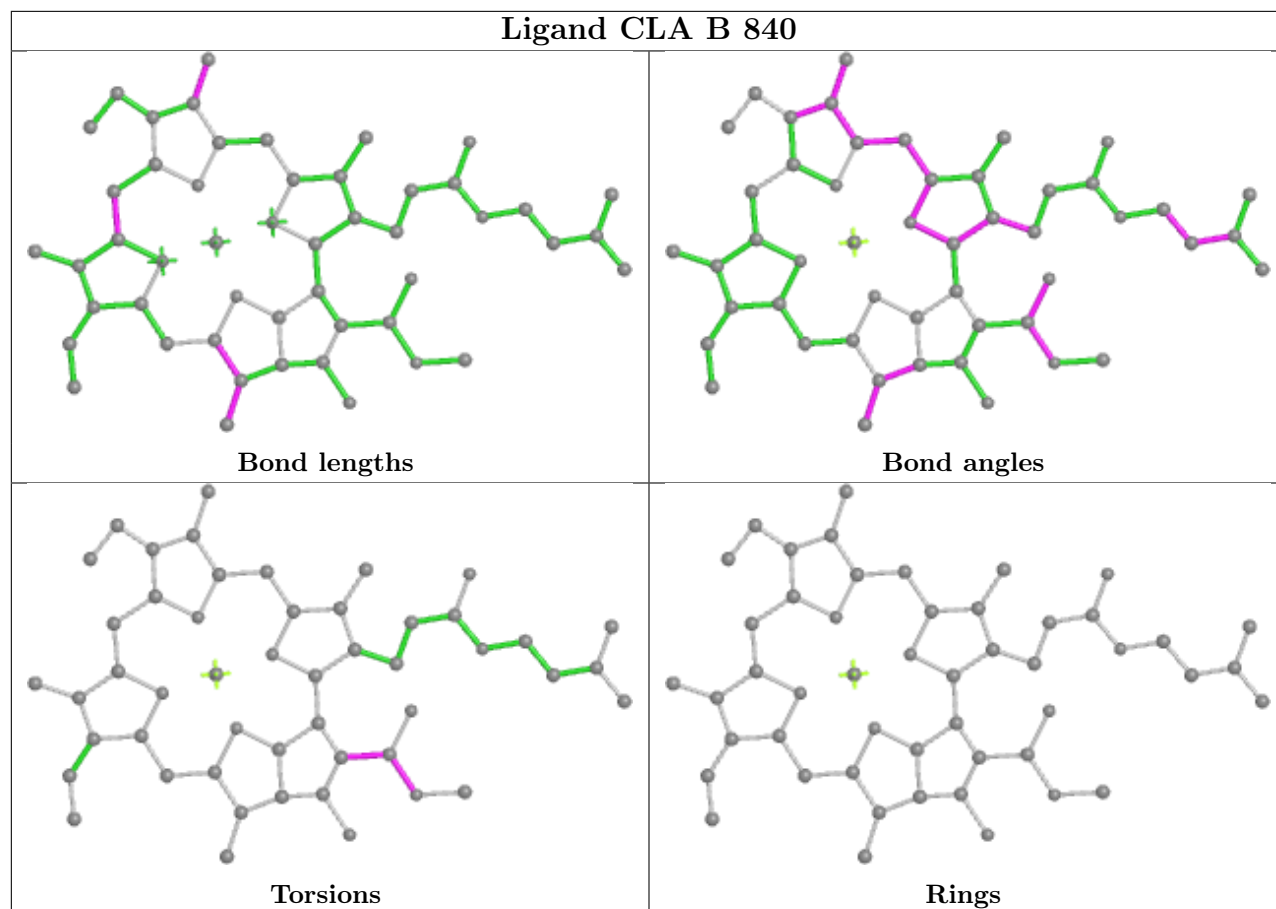
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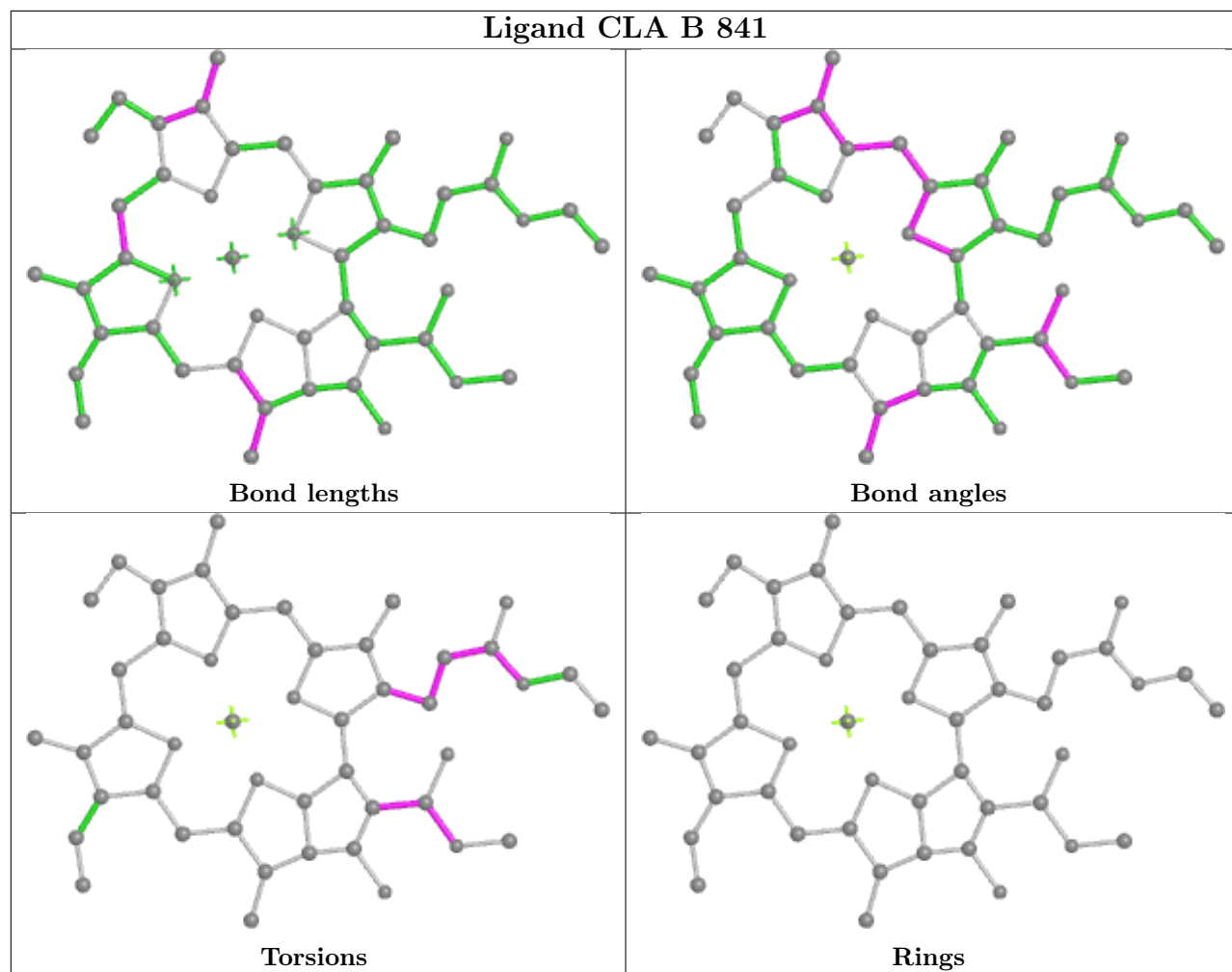
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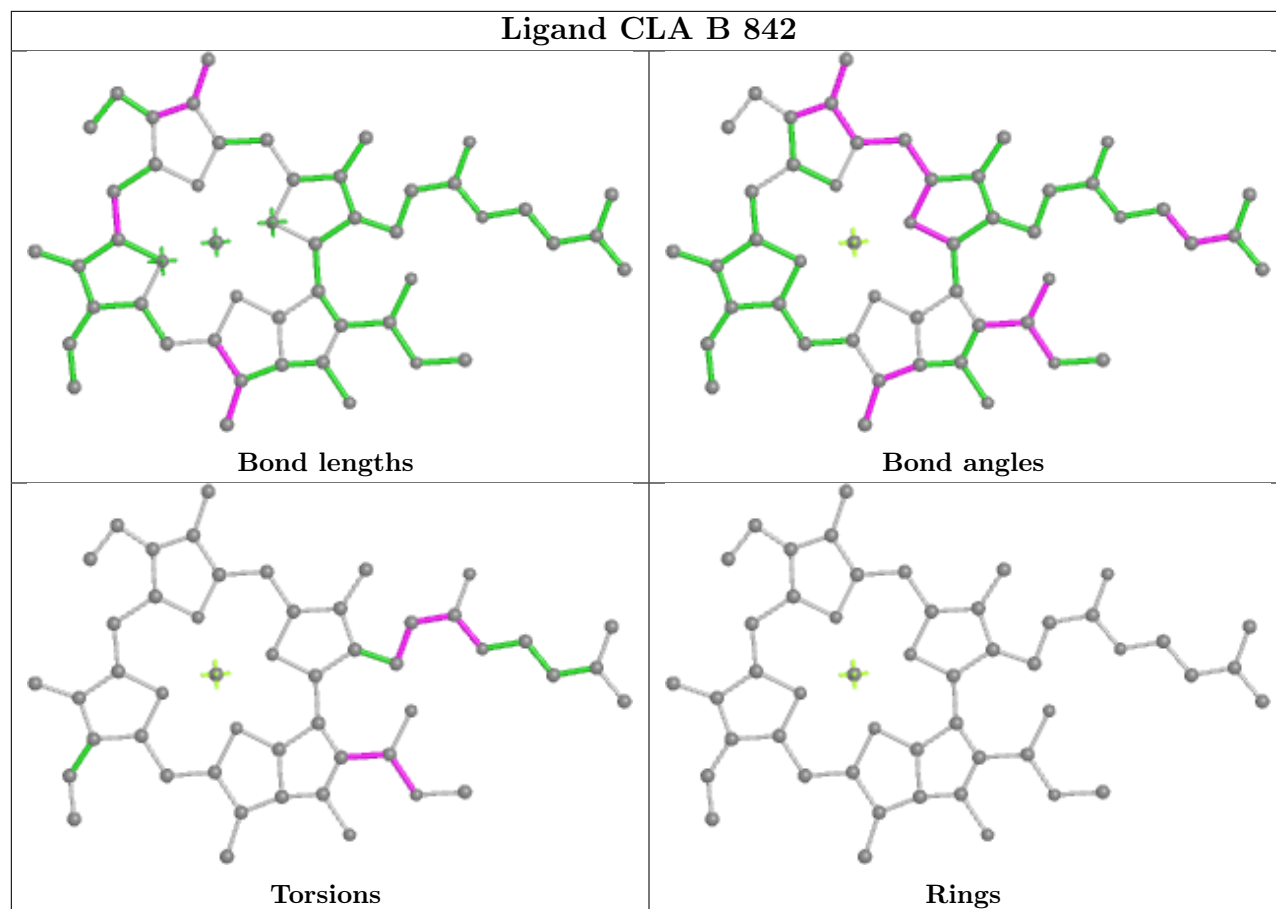


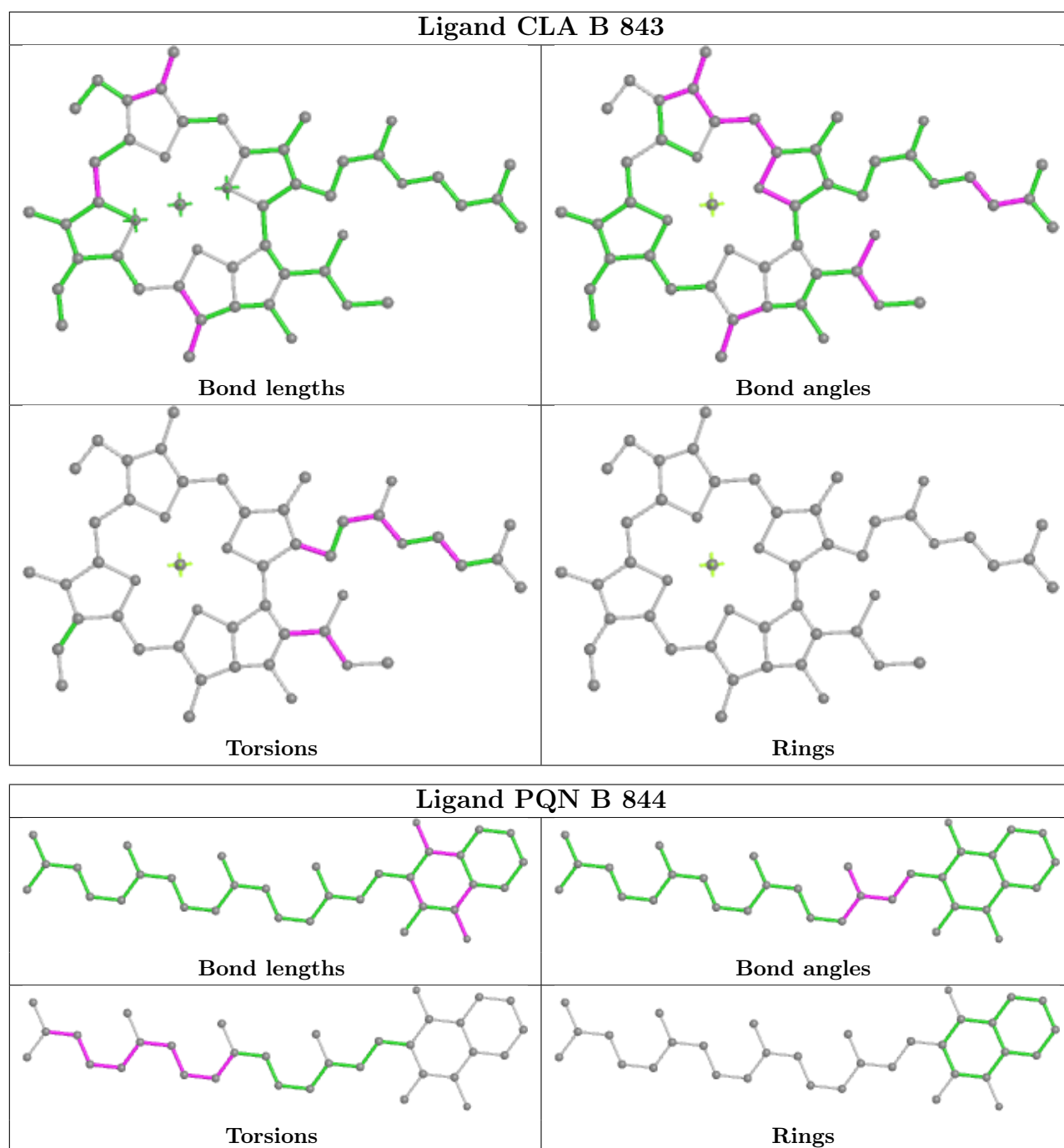




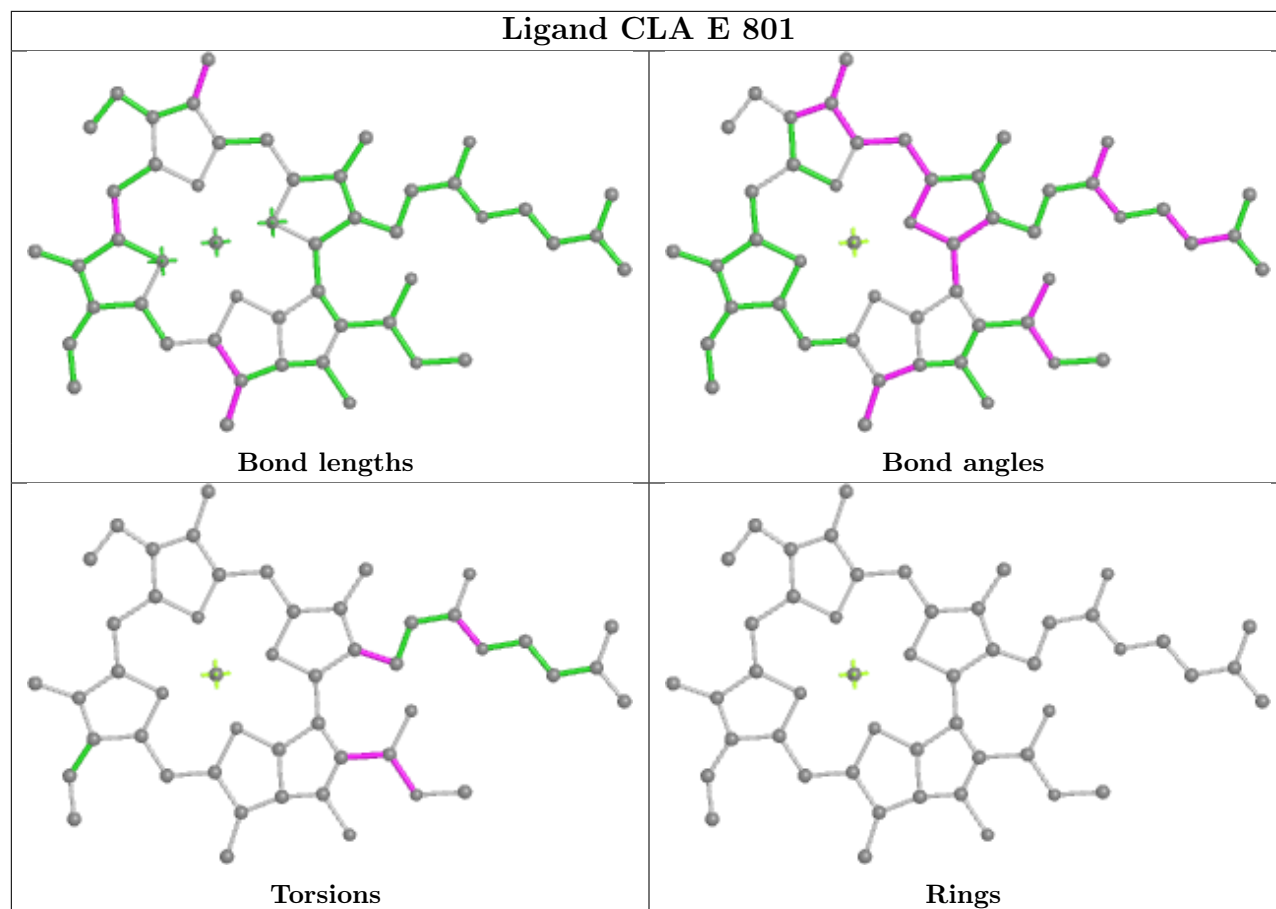
Ligand CLA B 841



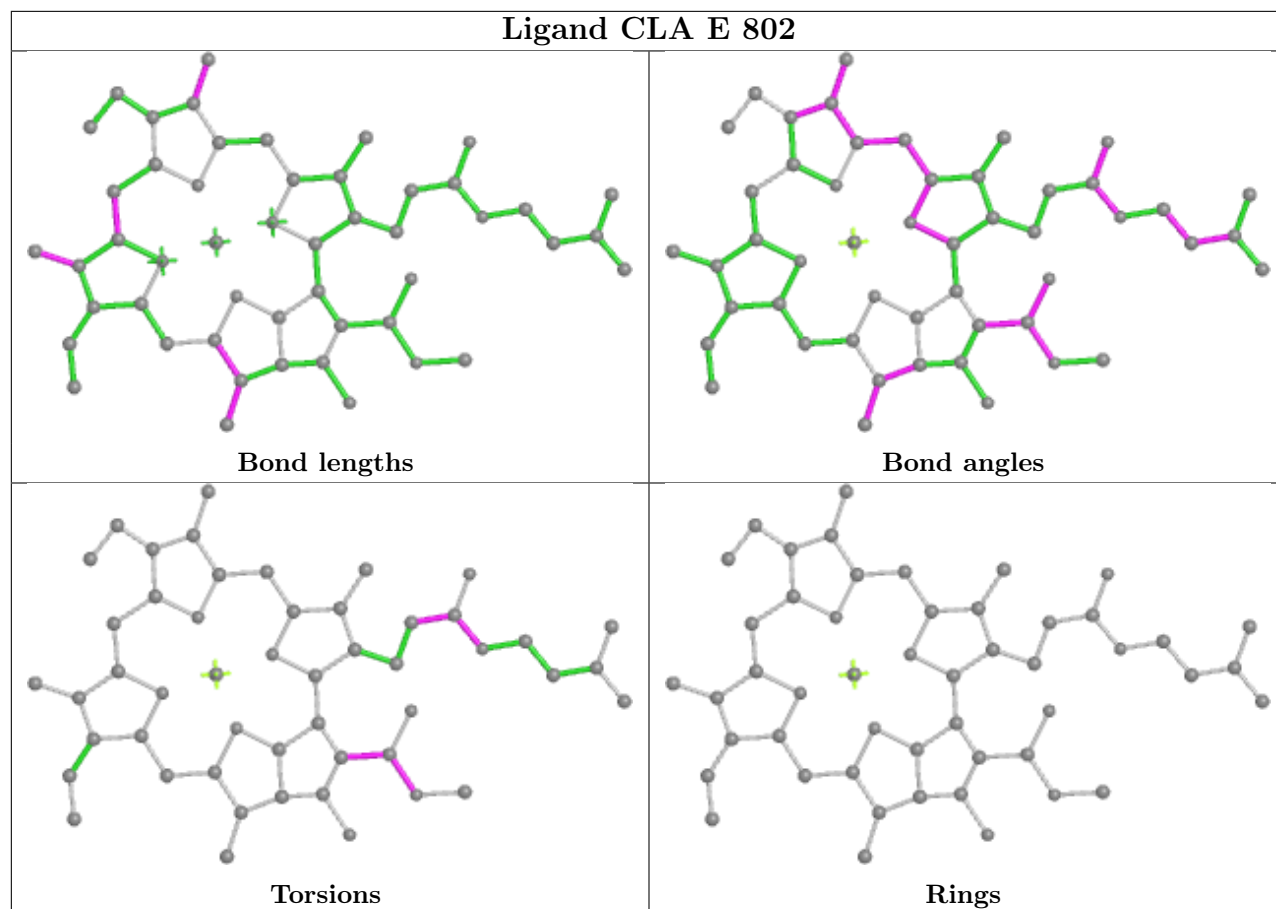


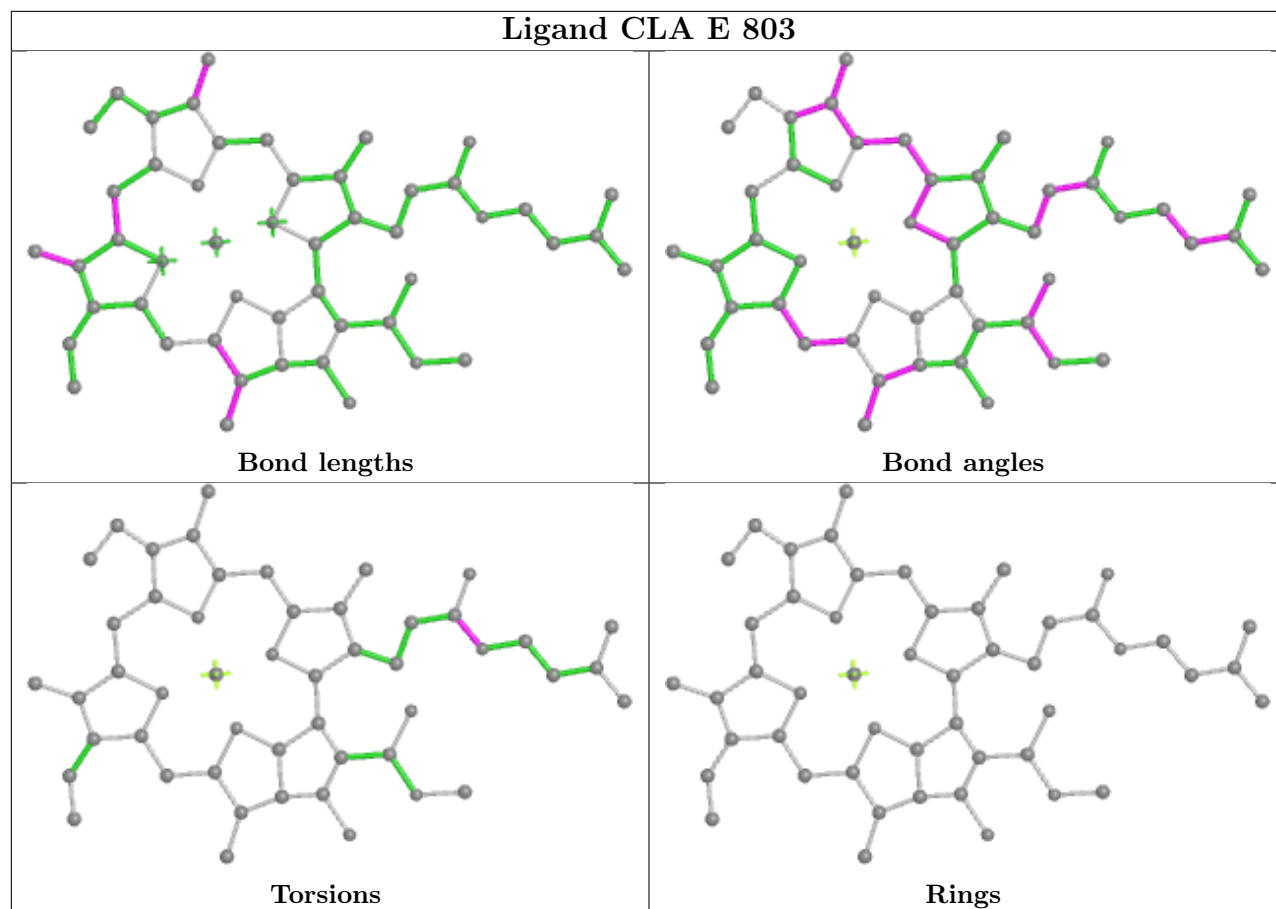


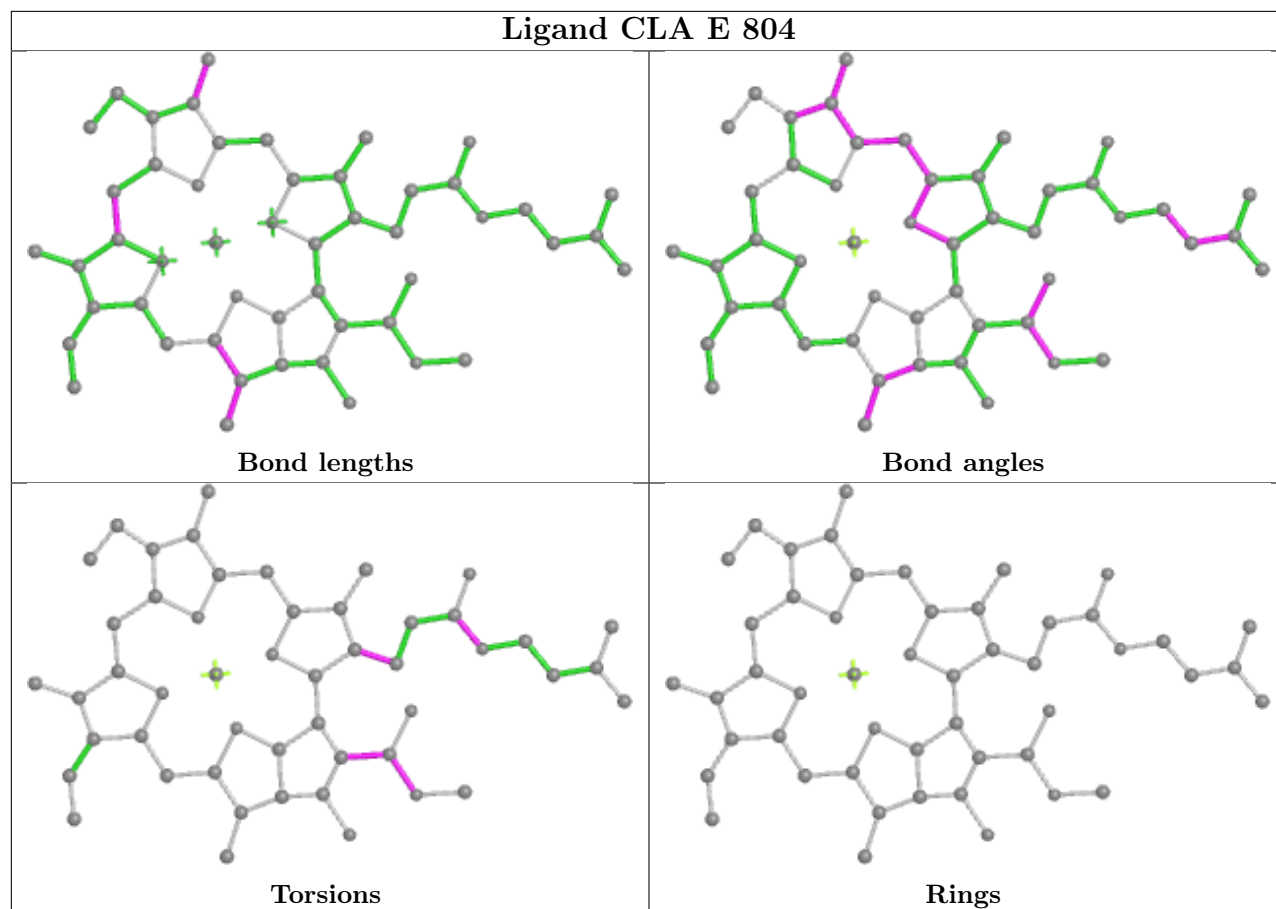
Ligand CLA E 801

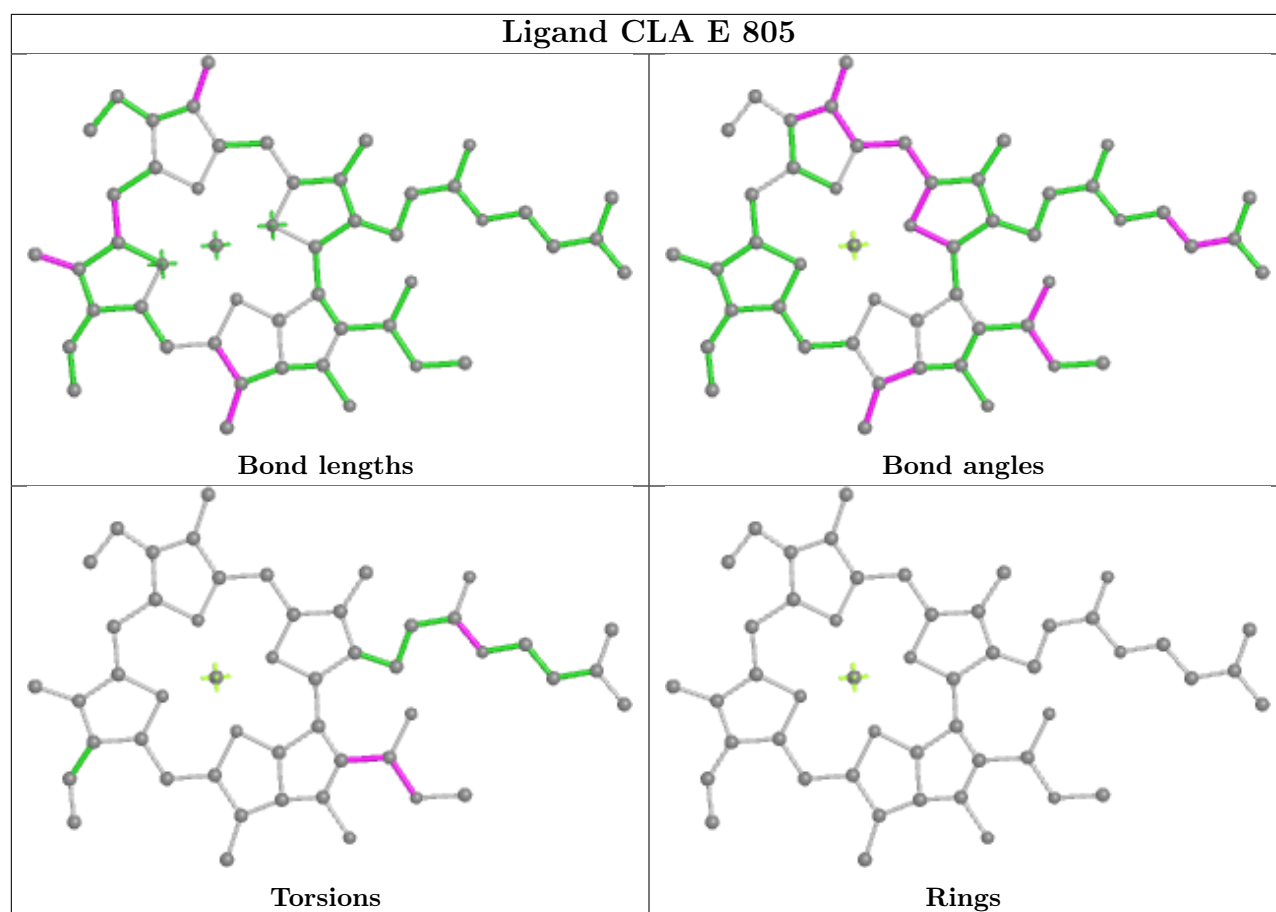


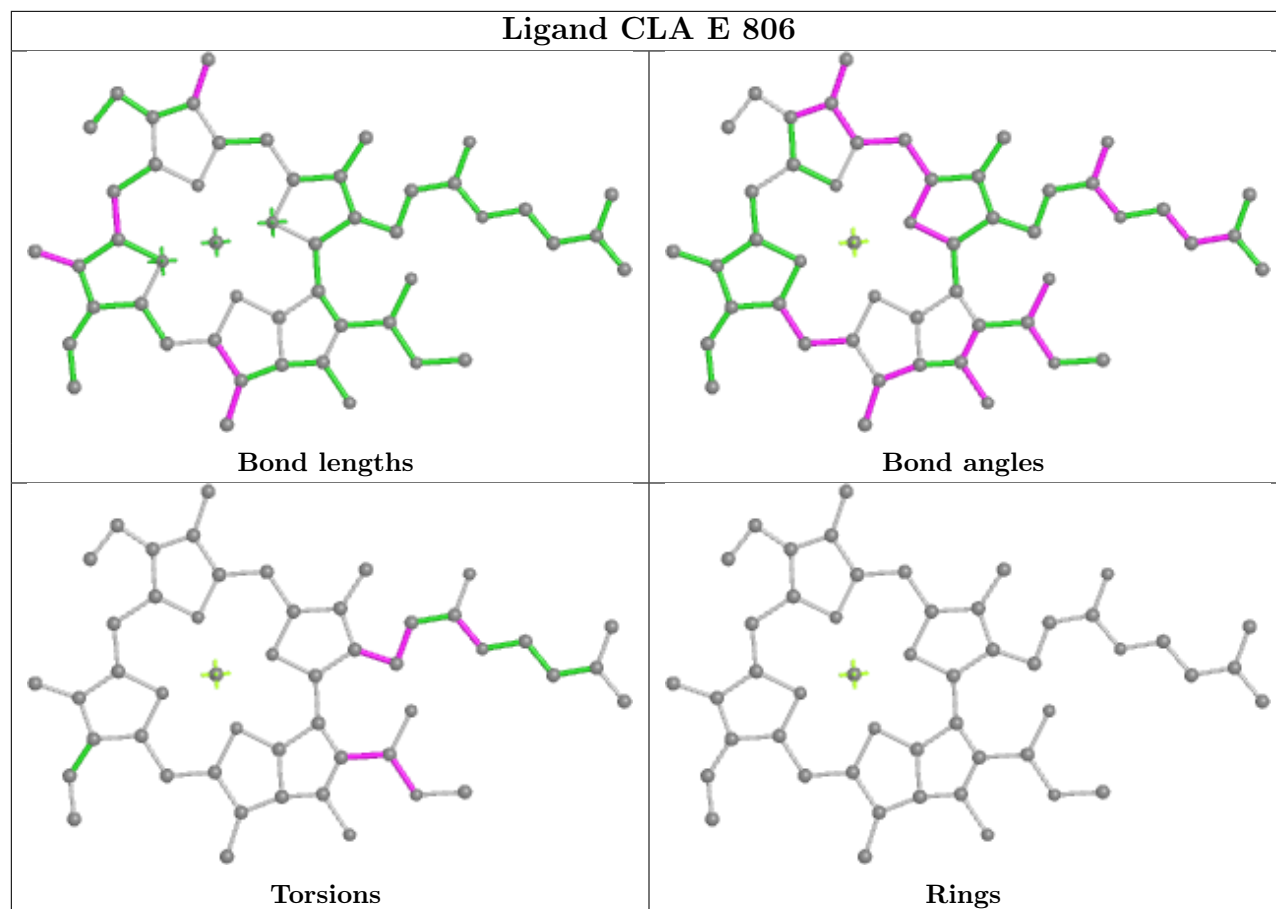
Ligand CLA E 802



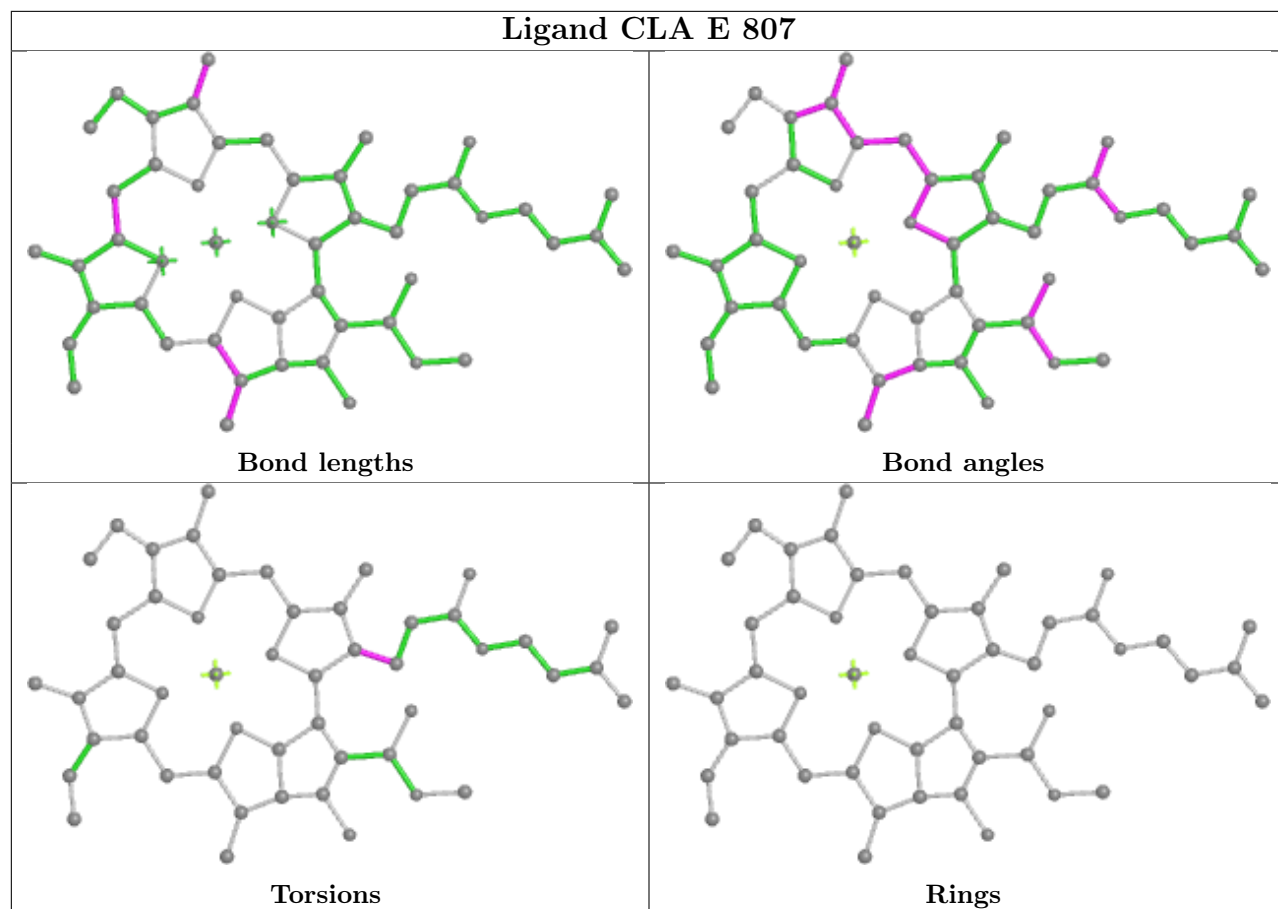


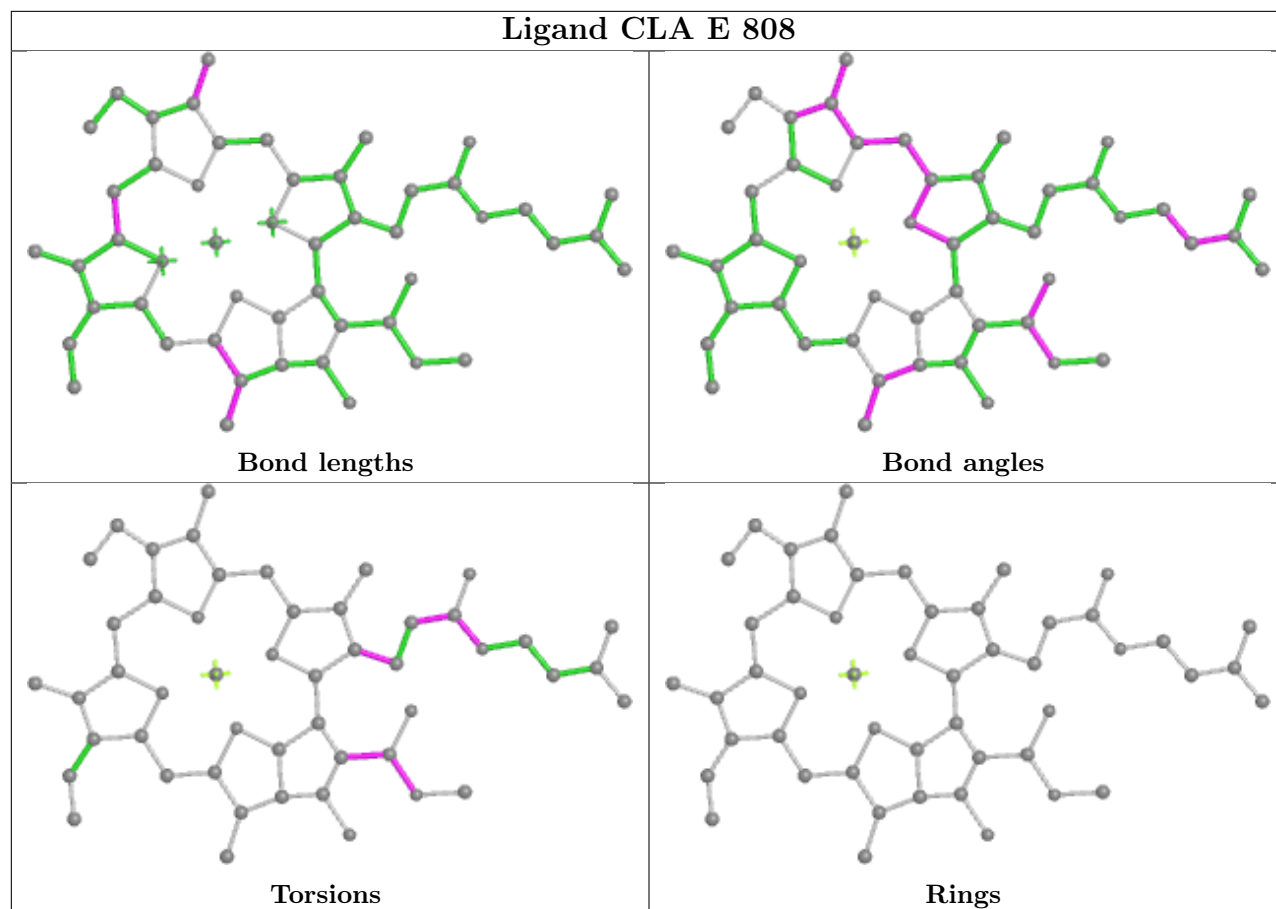


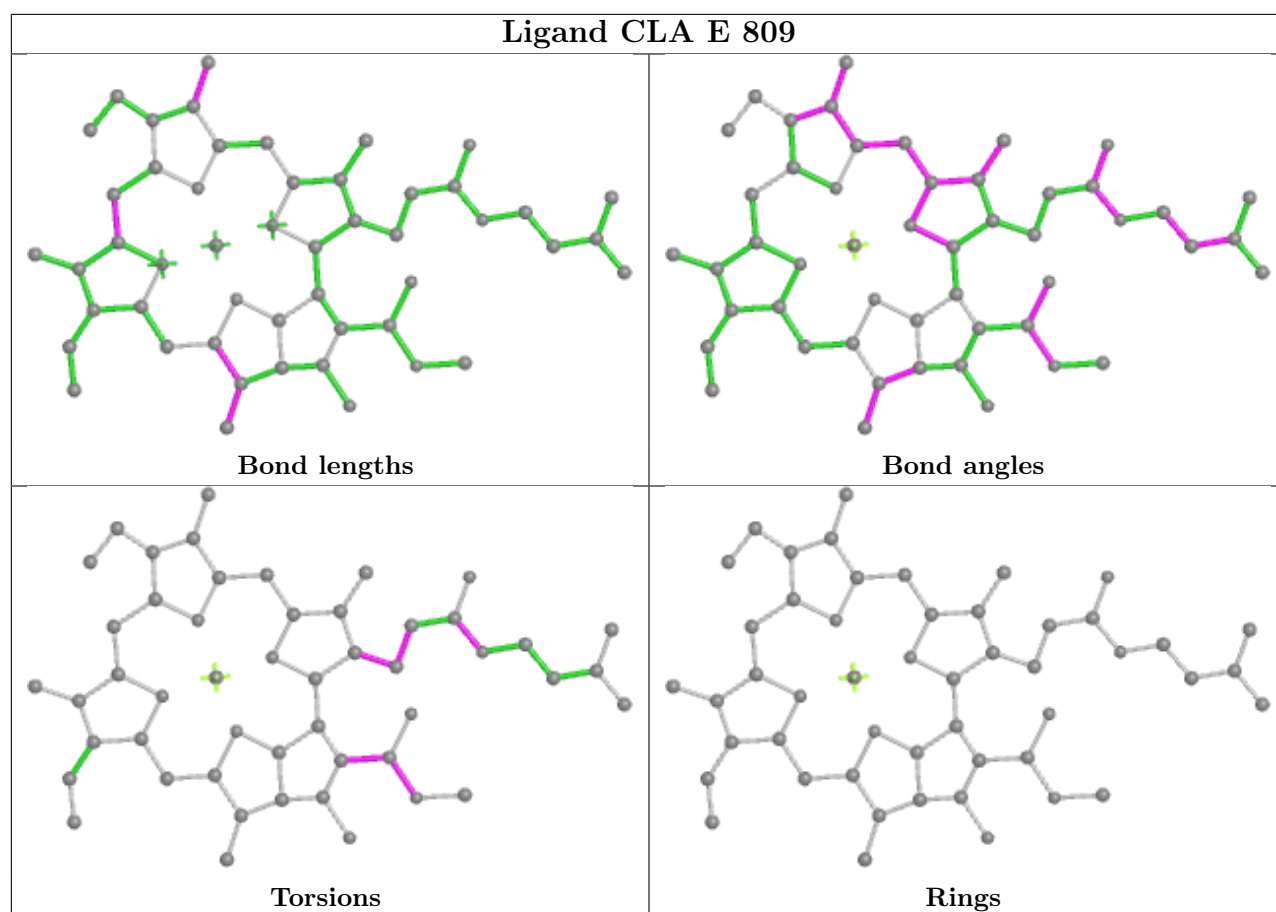


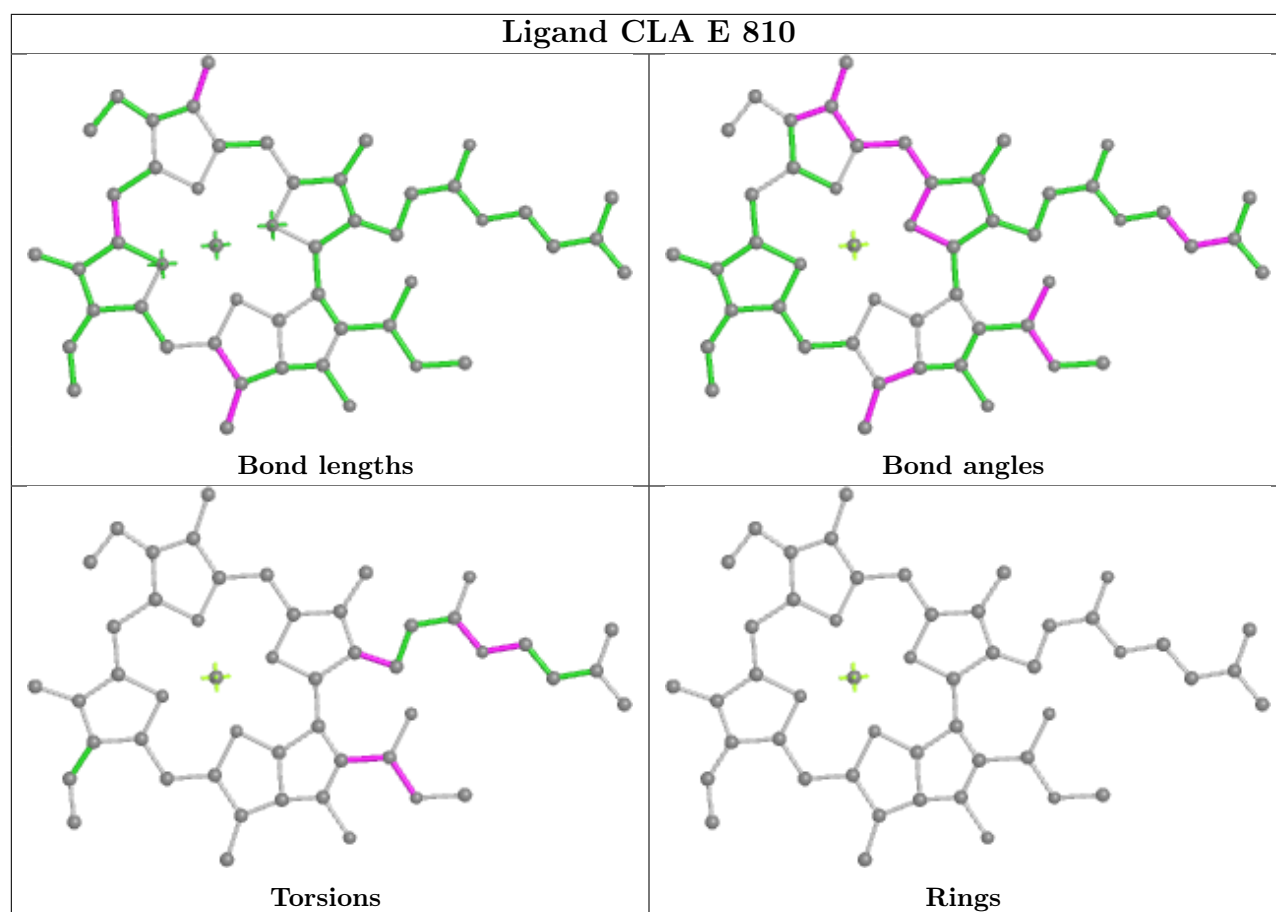


Ligand CLA E 807

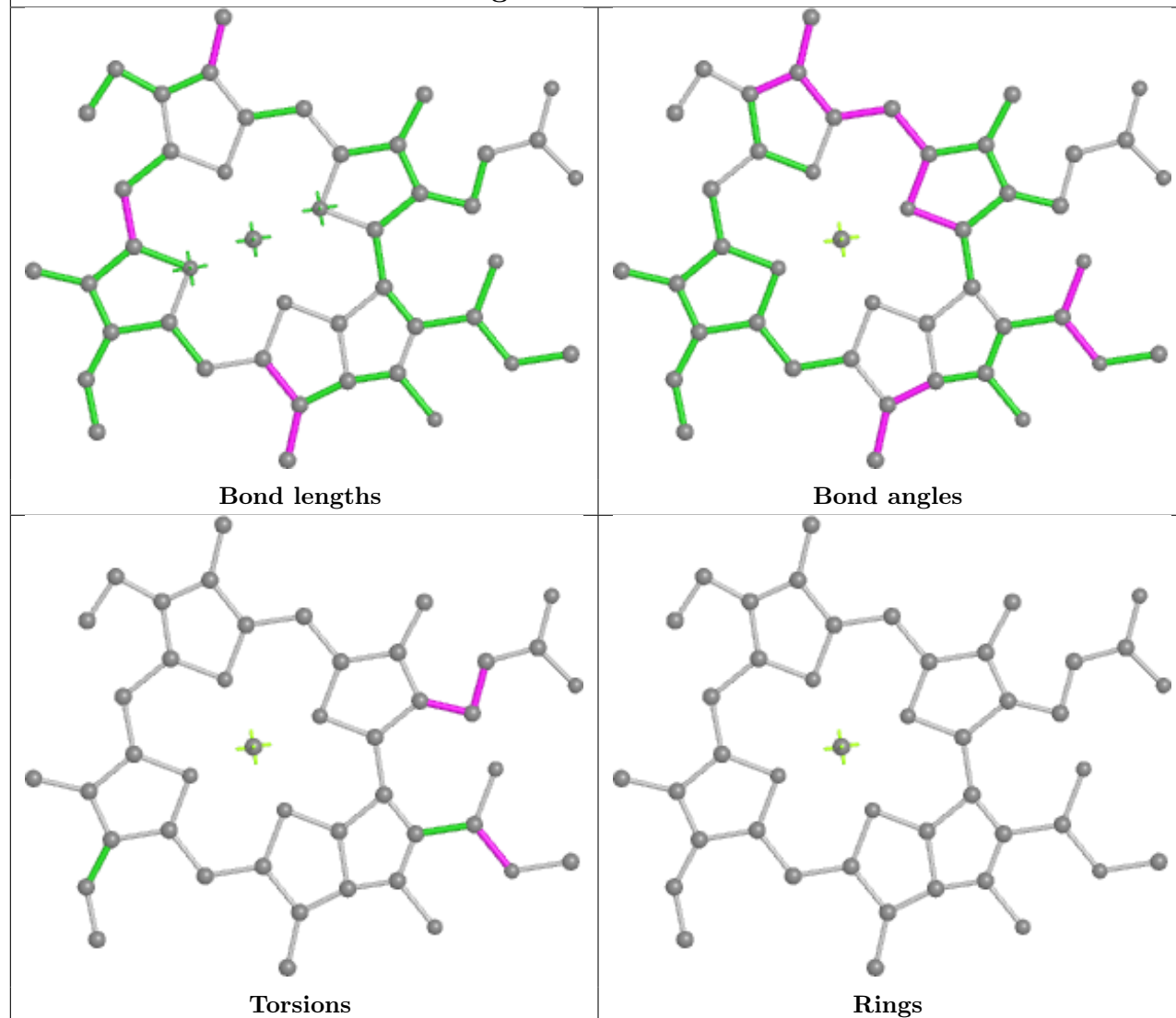


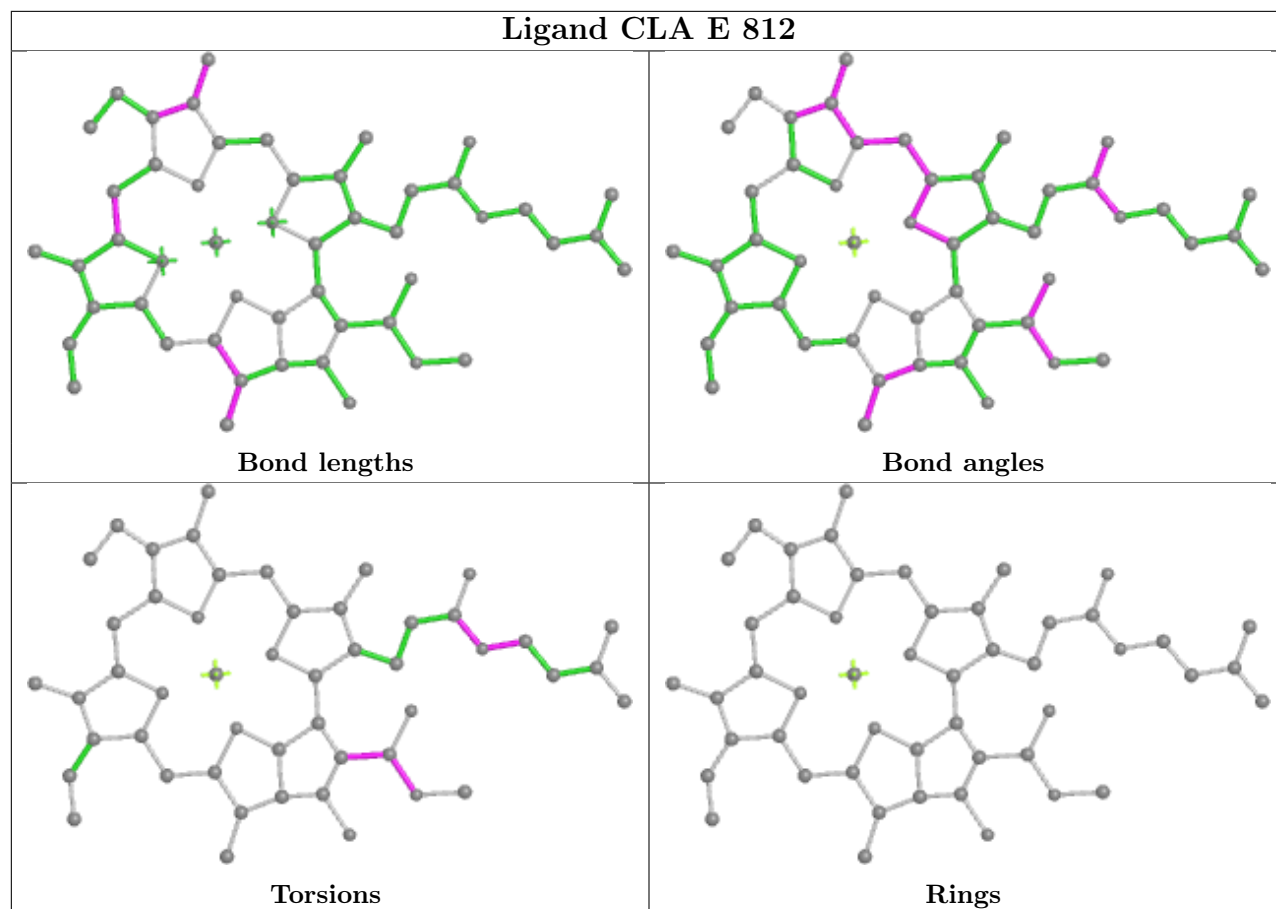


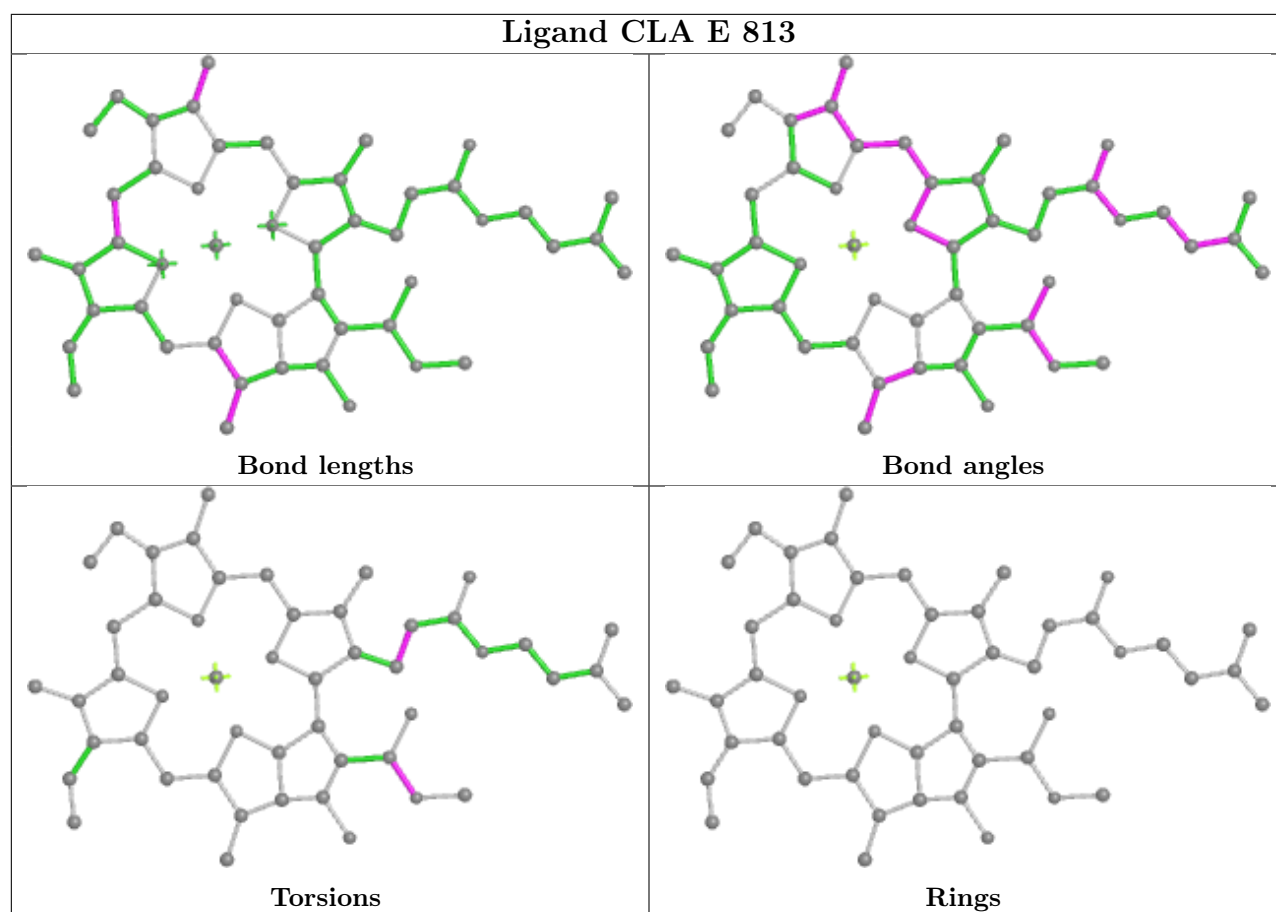


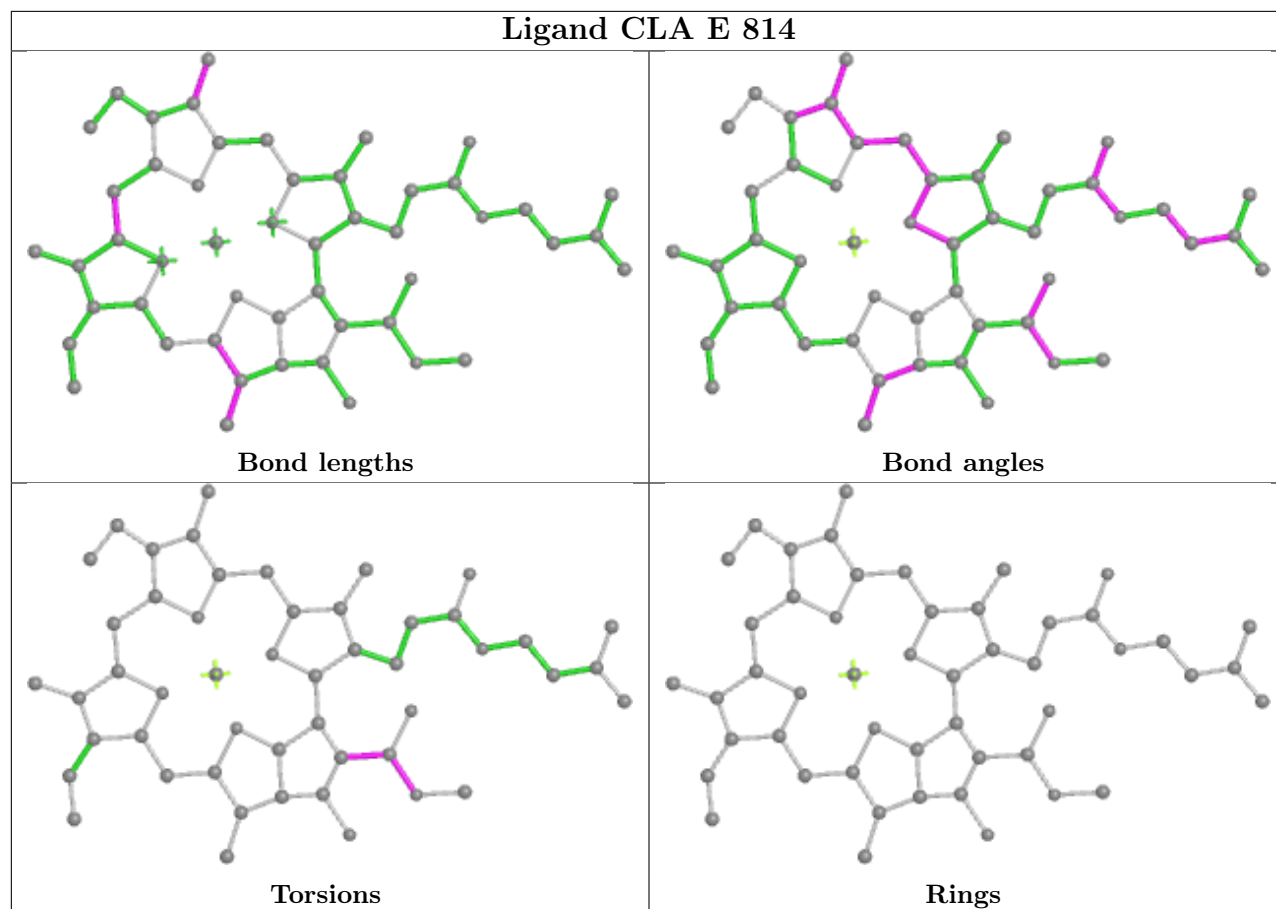


Ligand CLA E 811

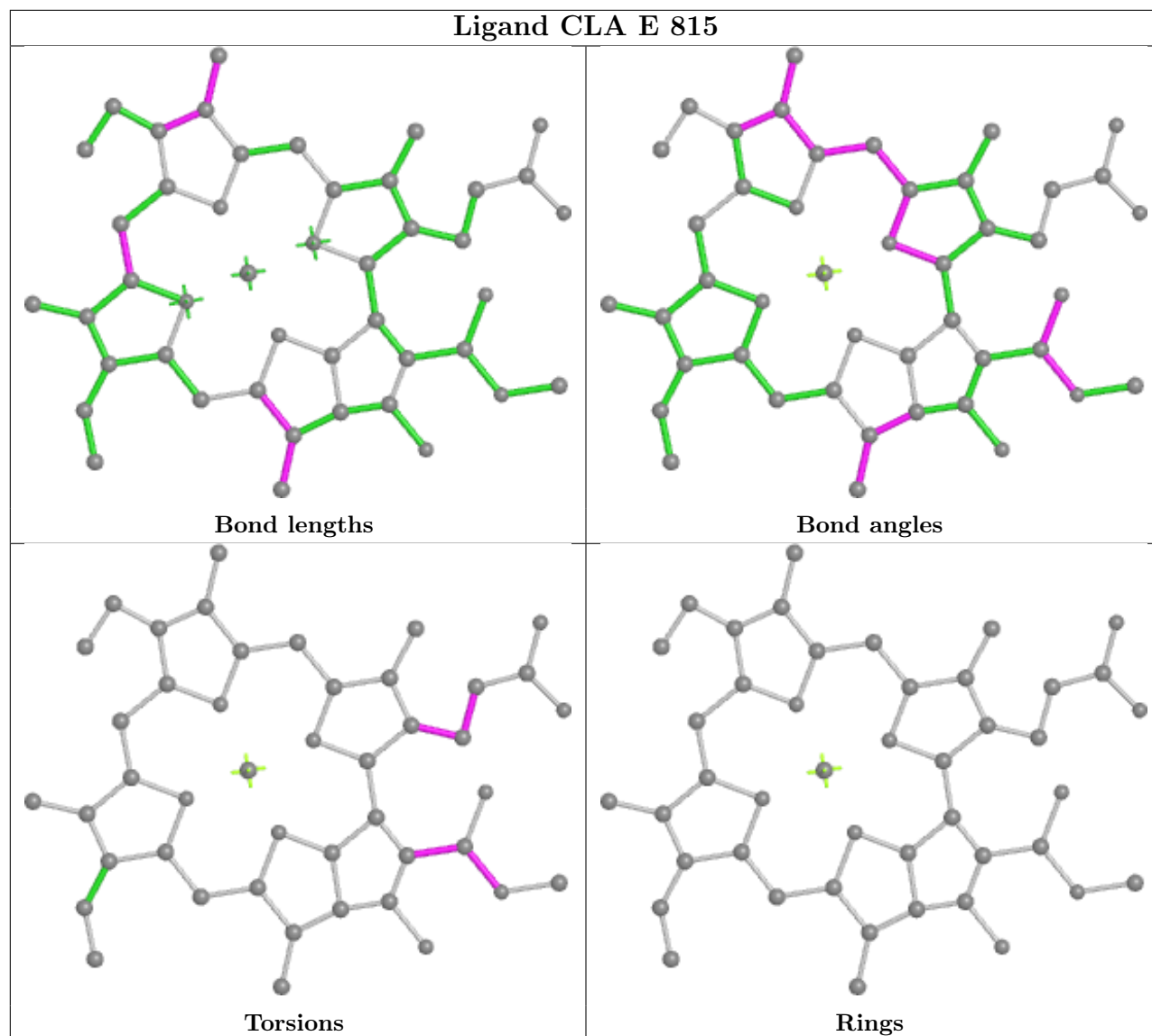




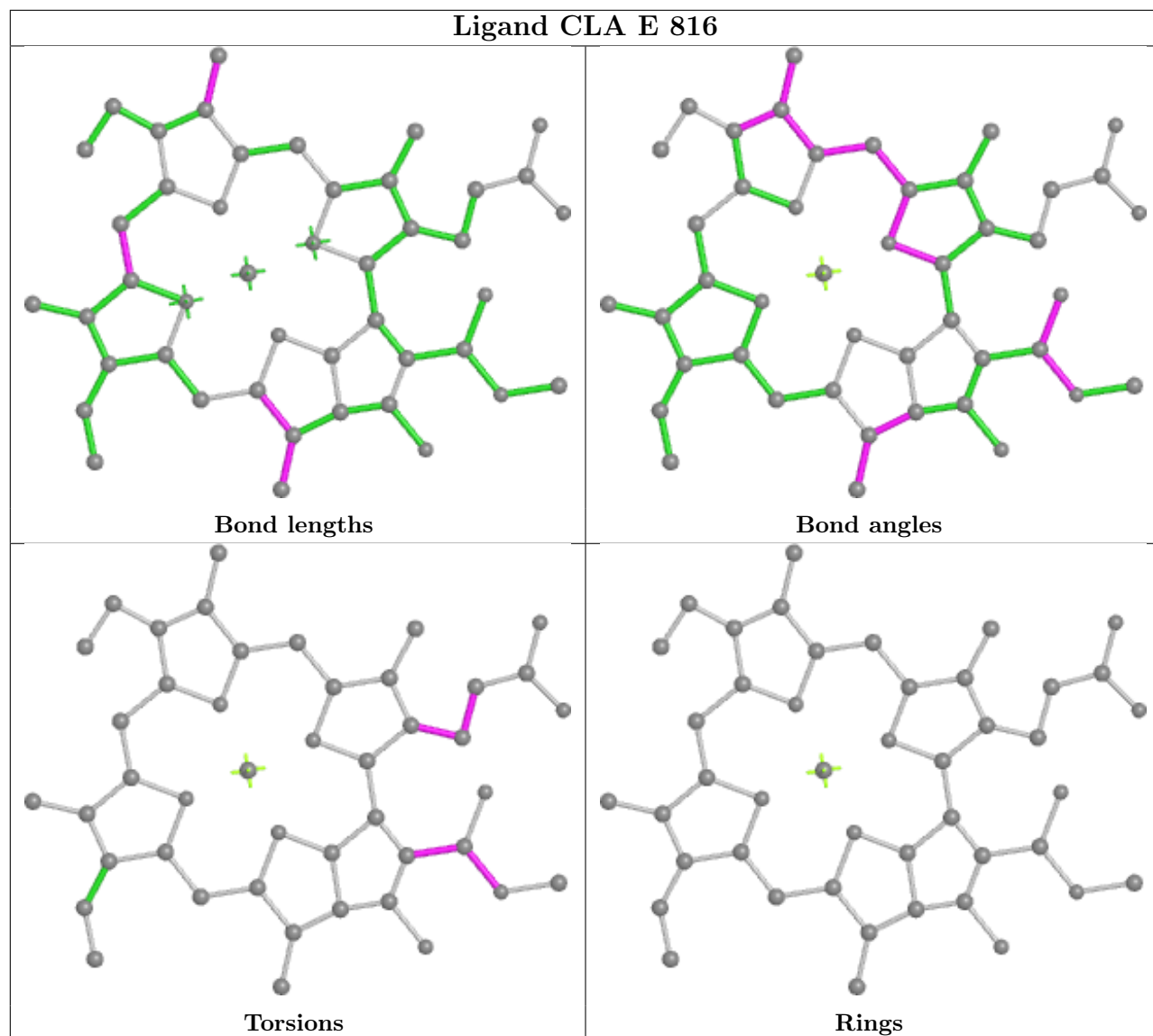


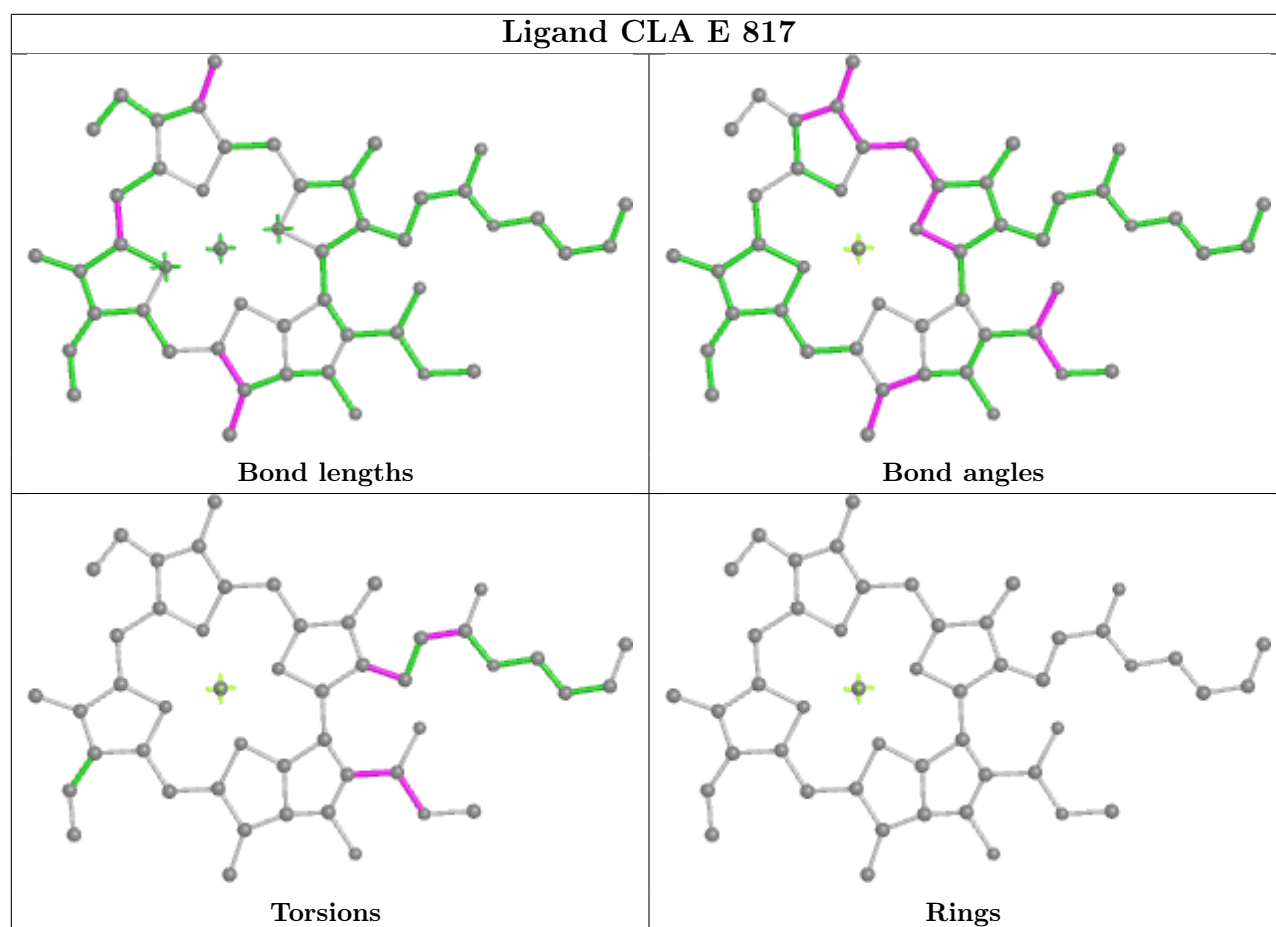


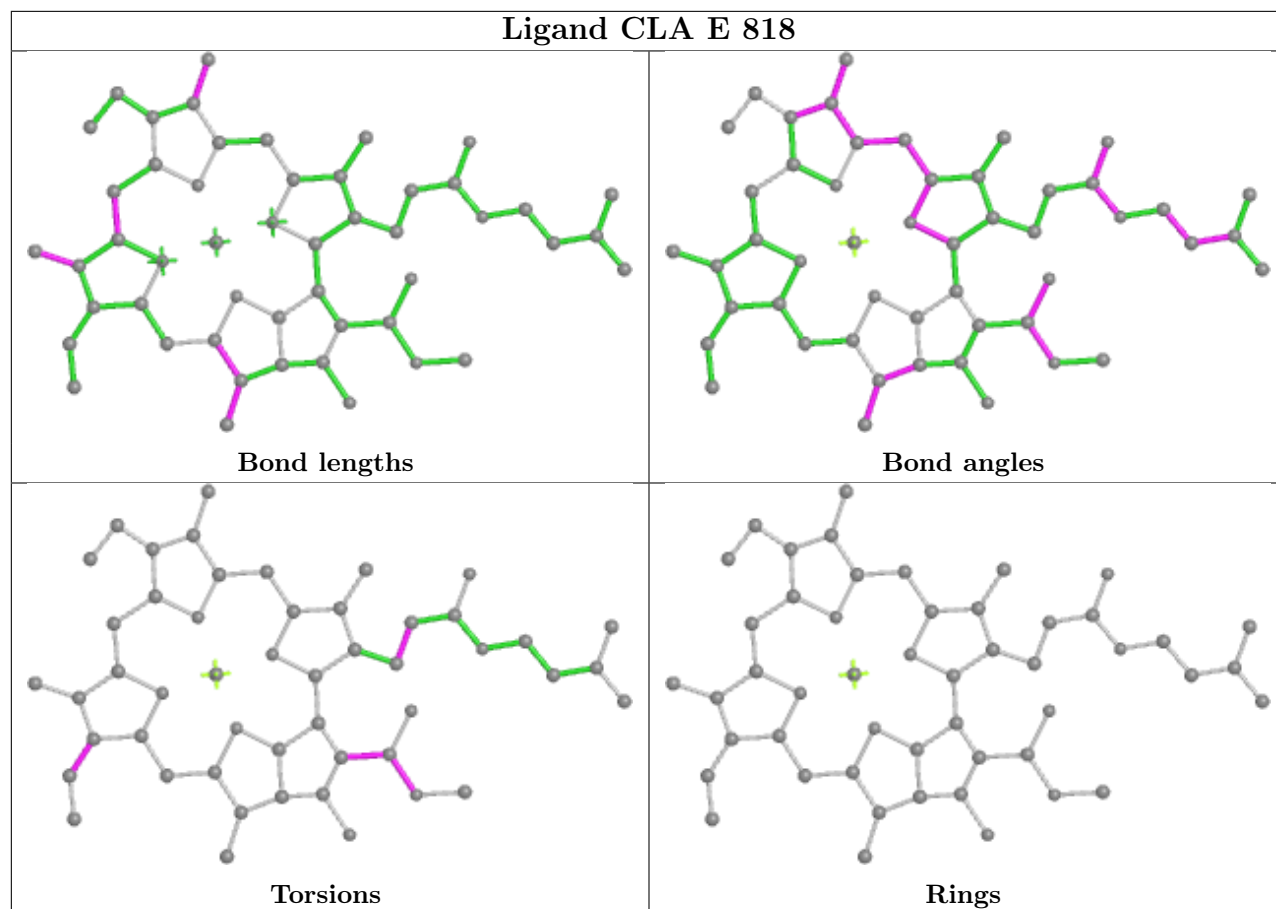
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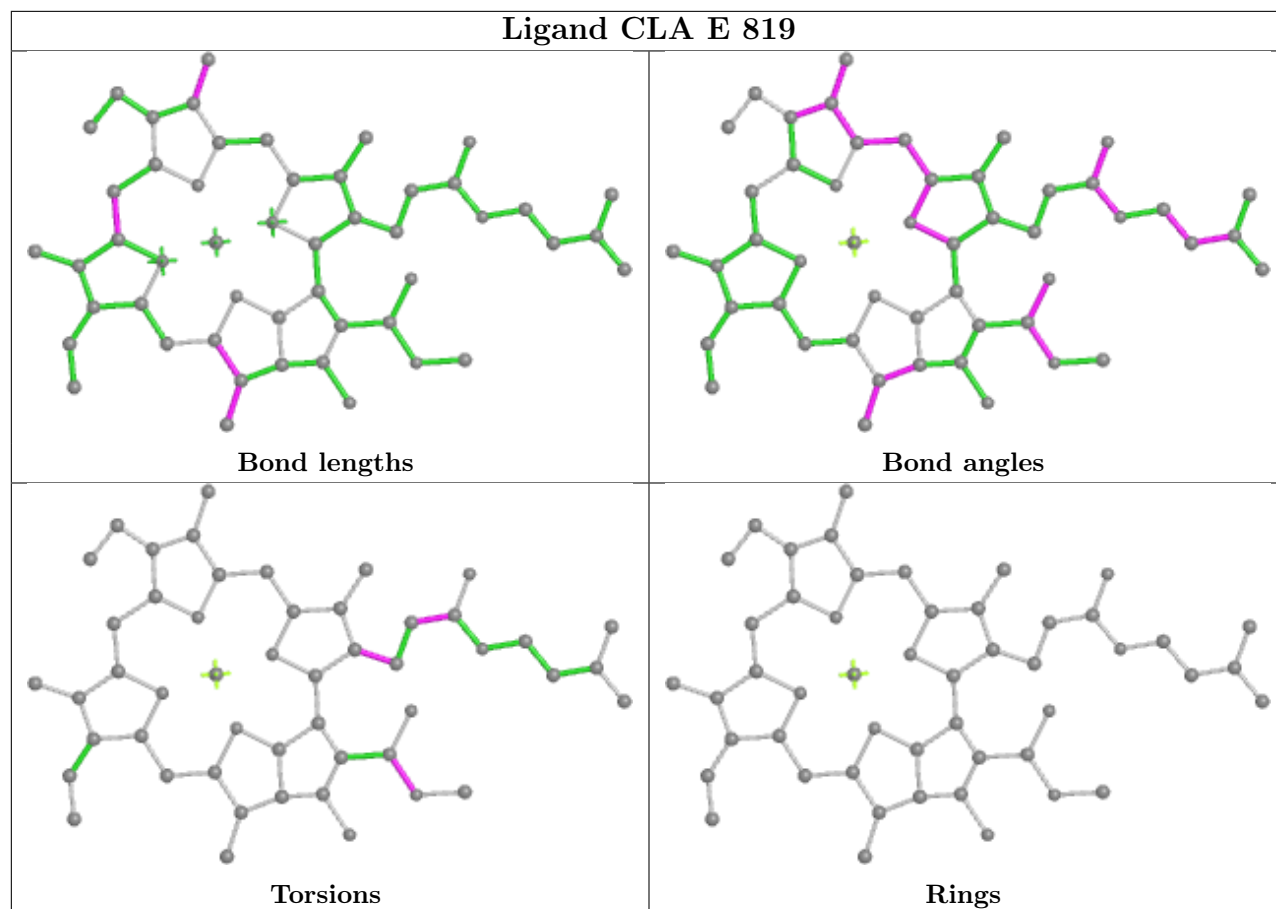


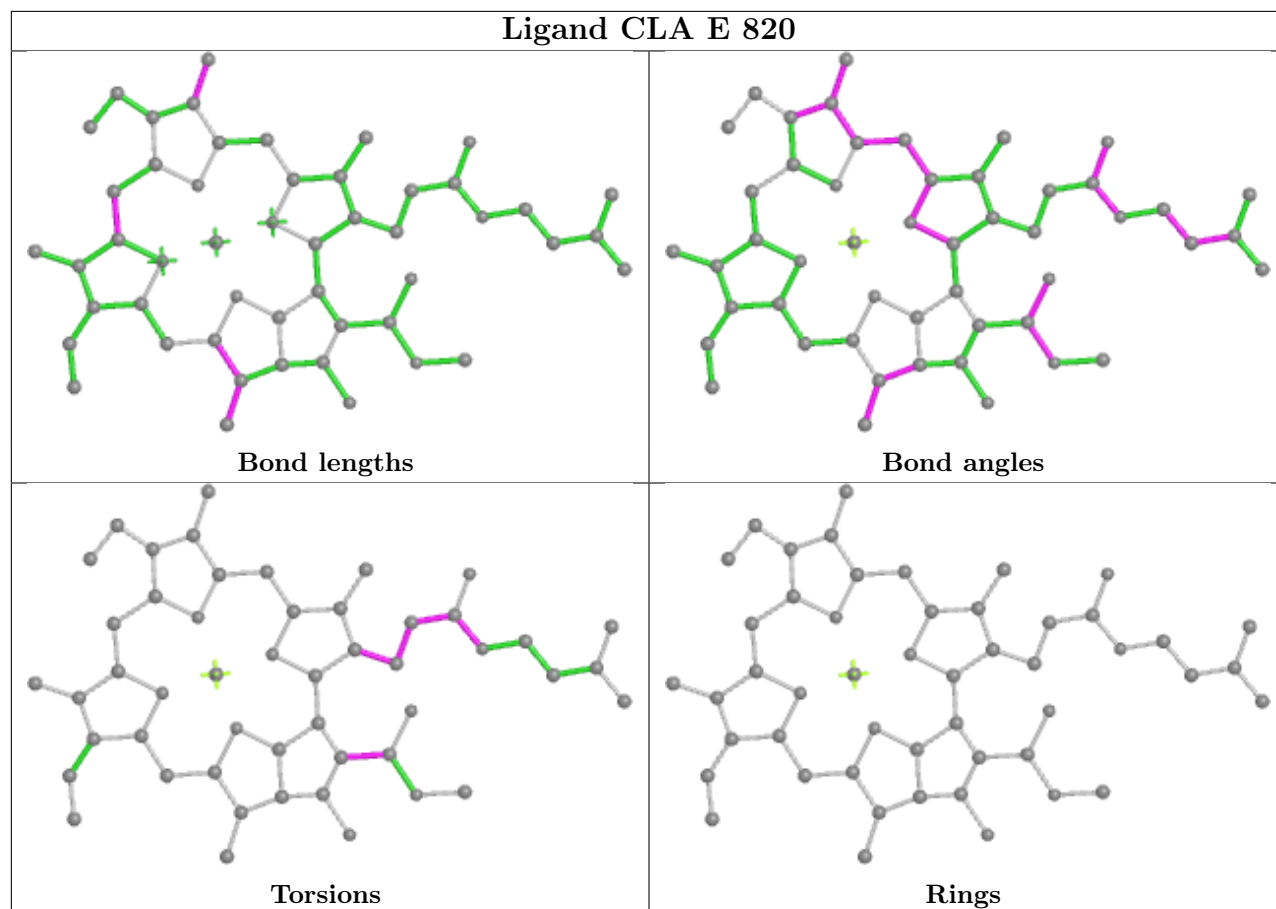
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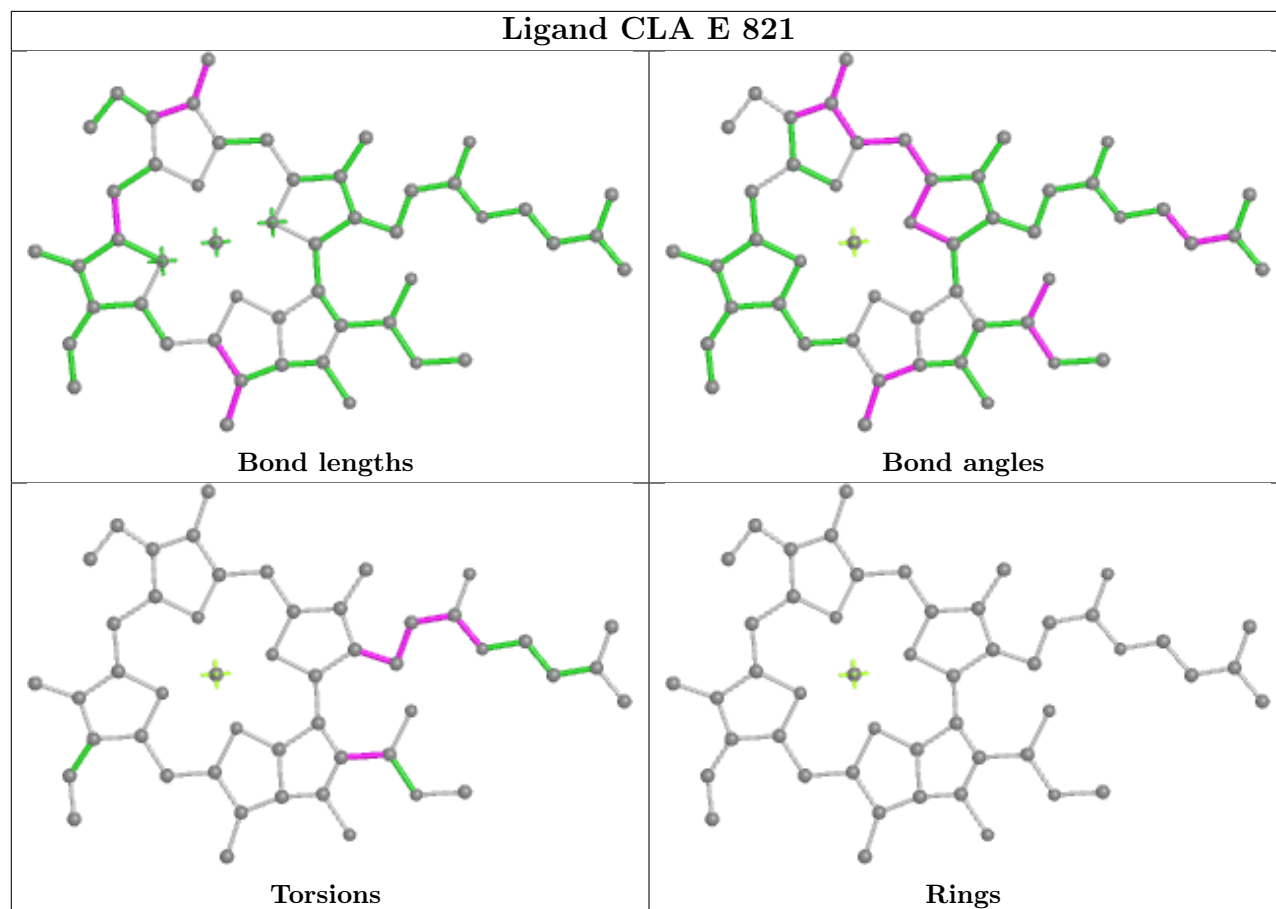


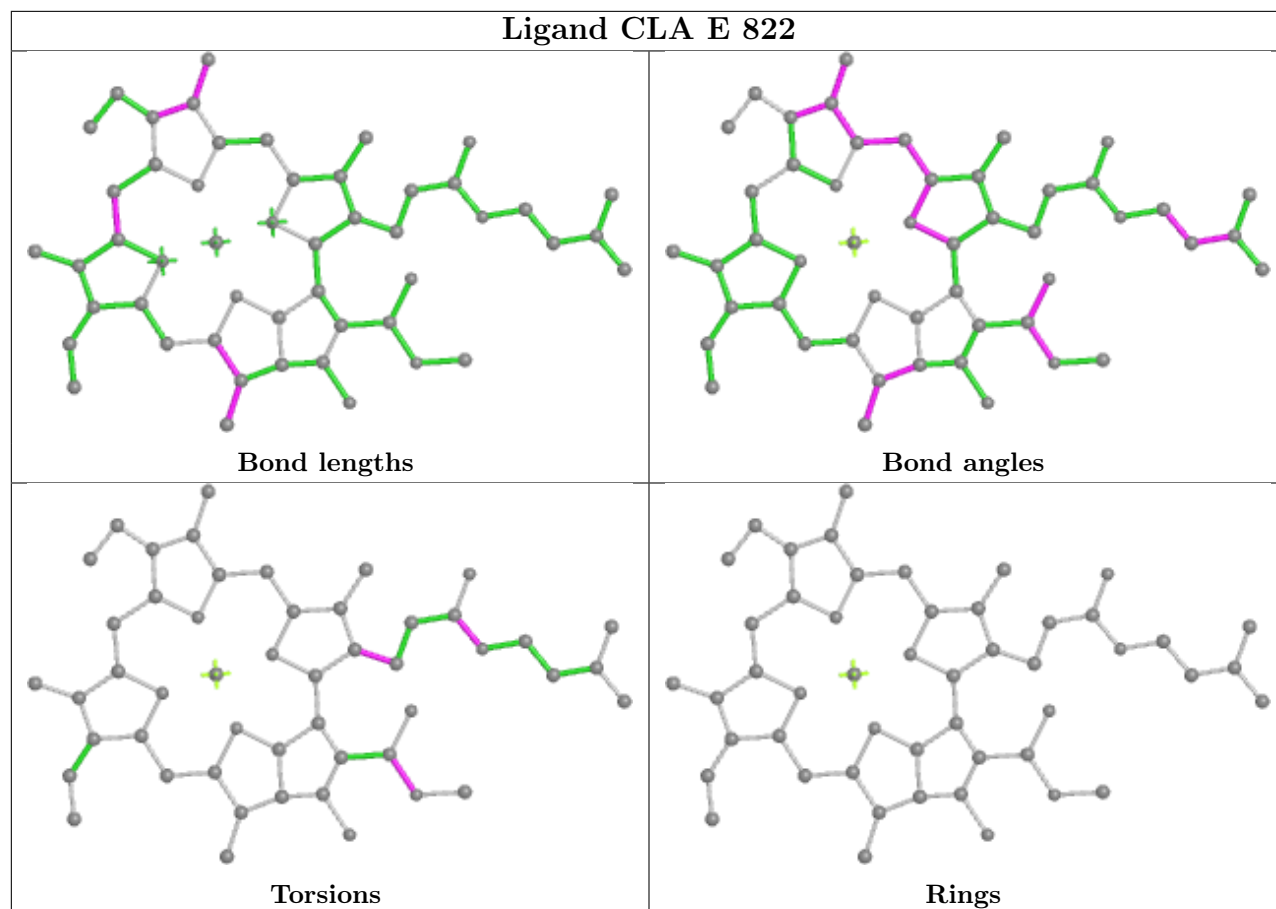


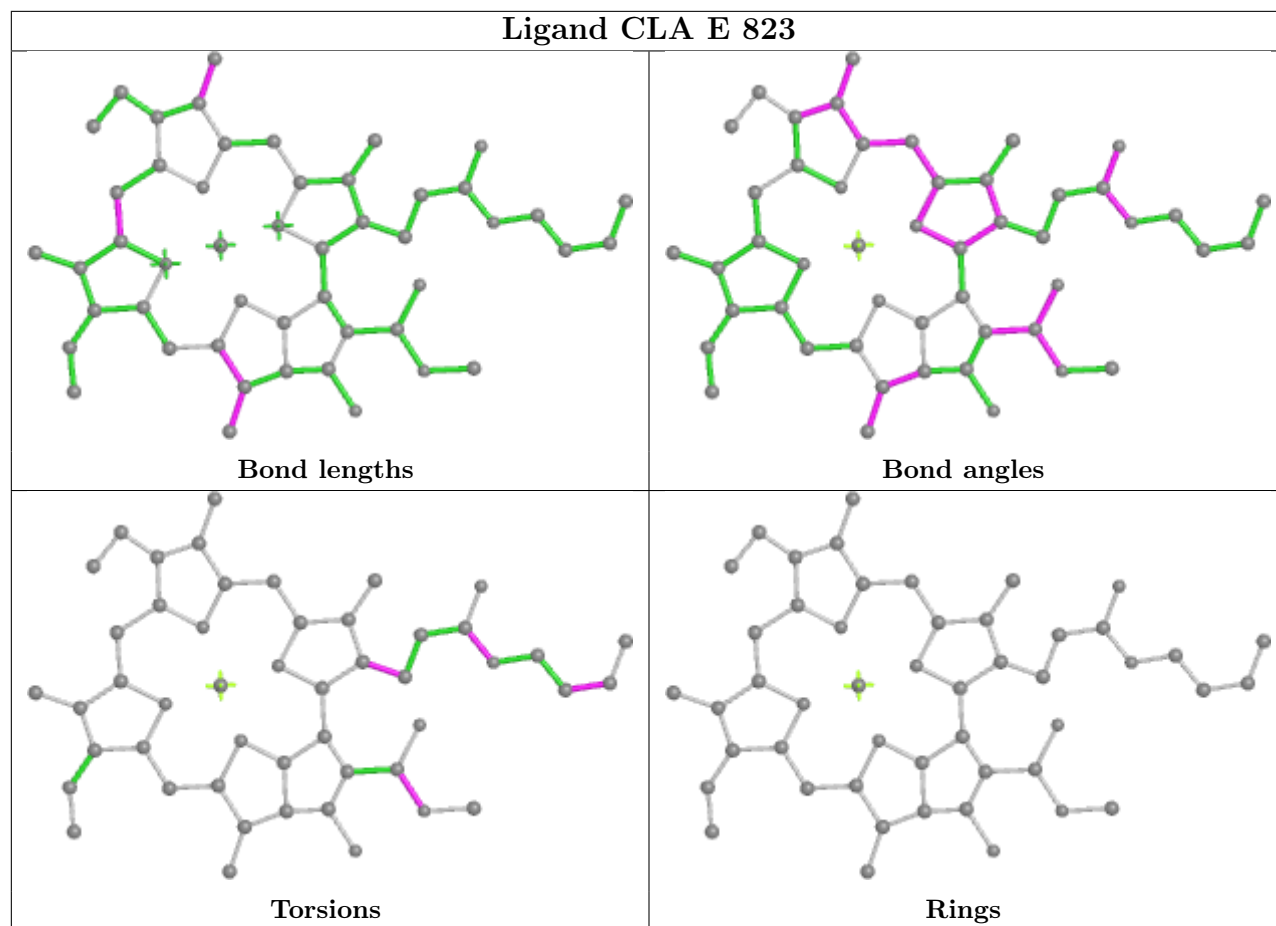


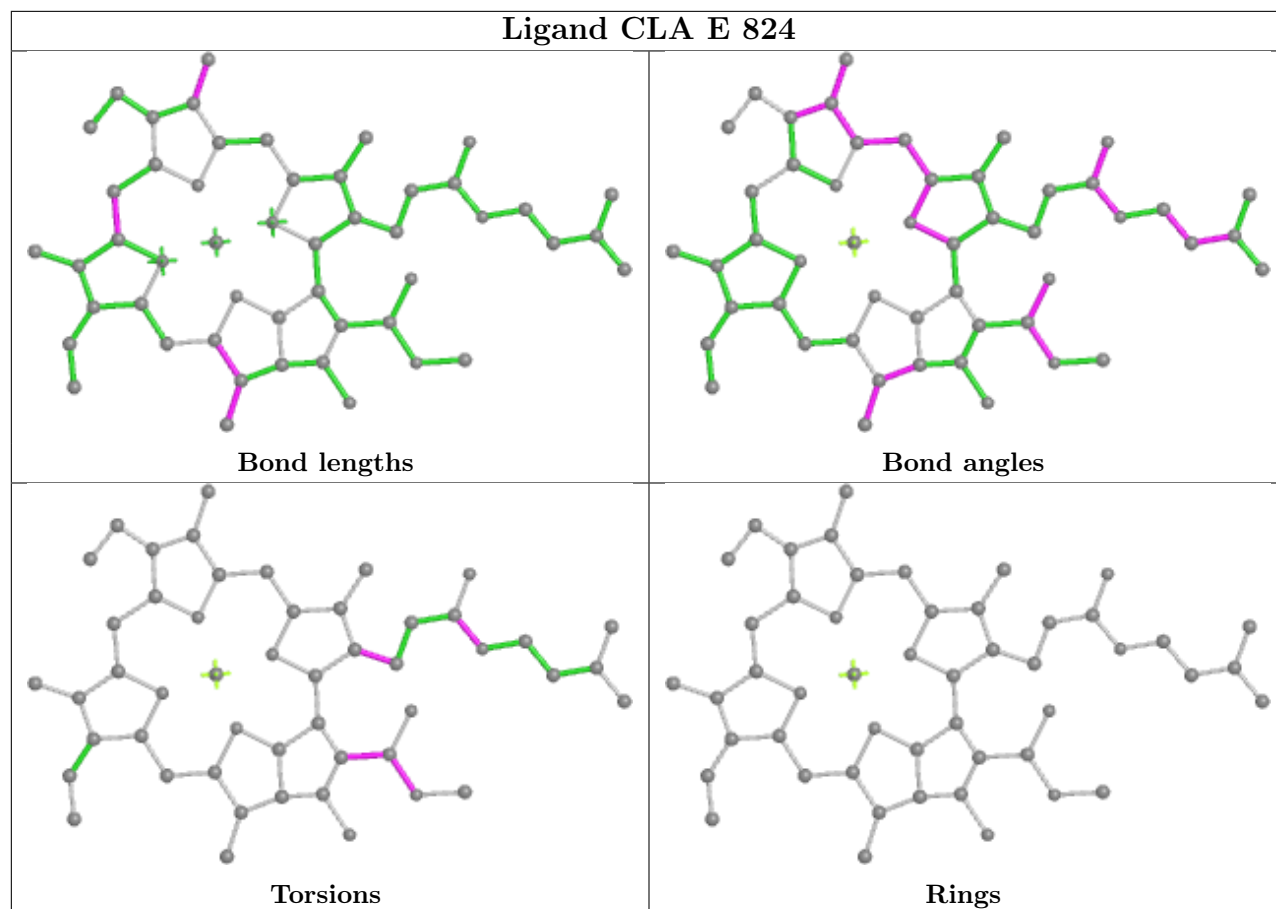


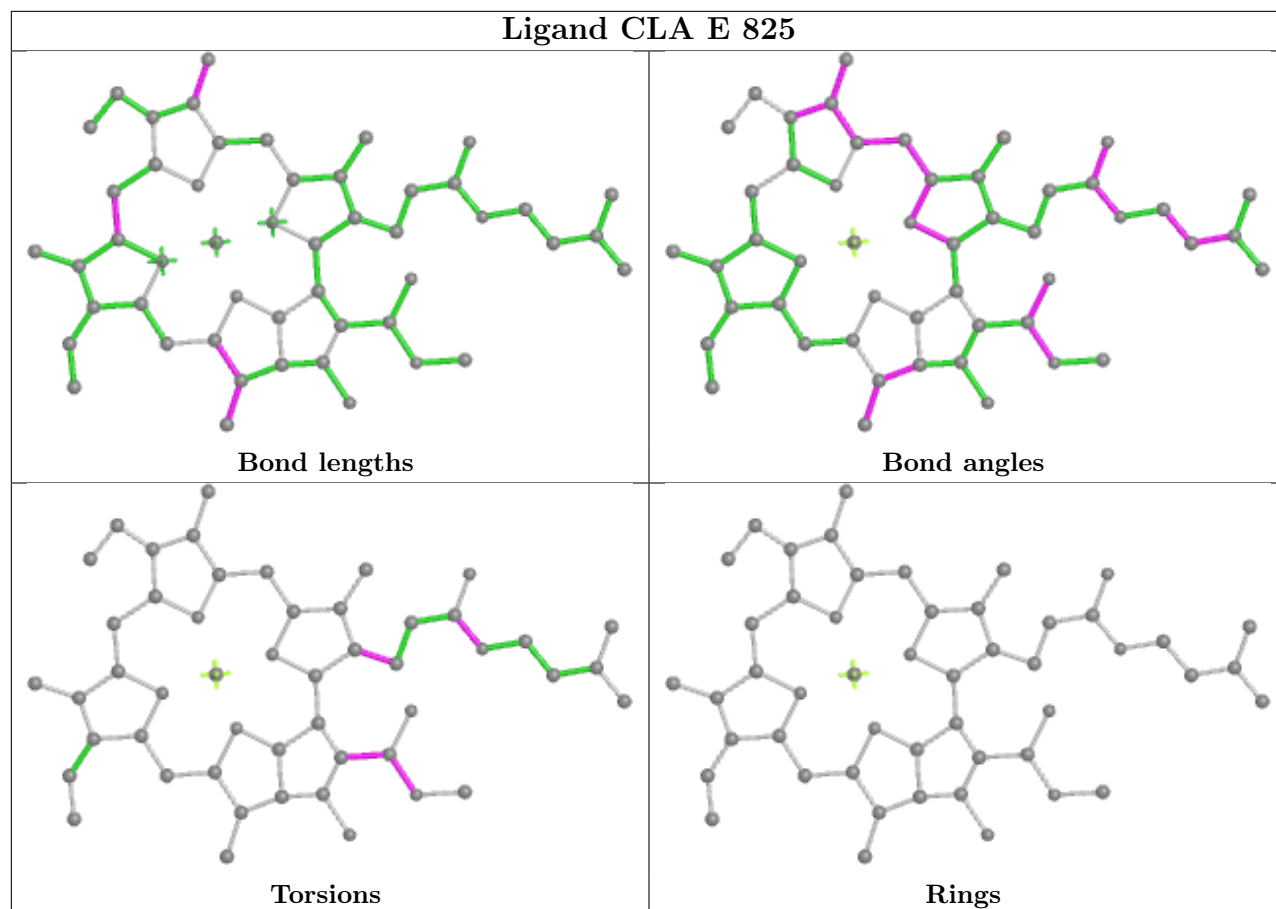




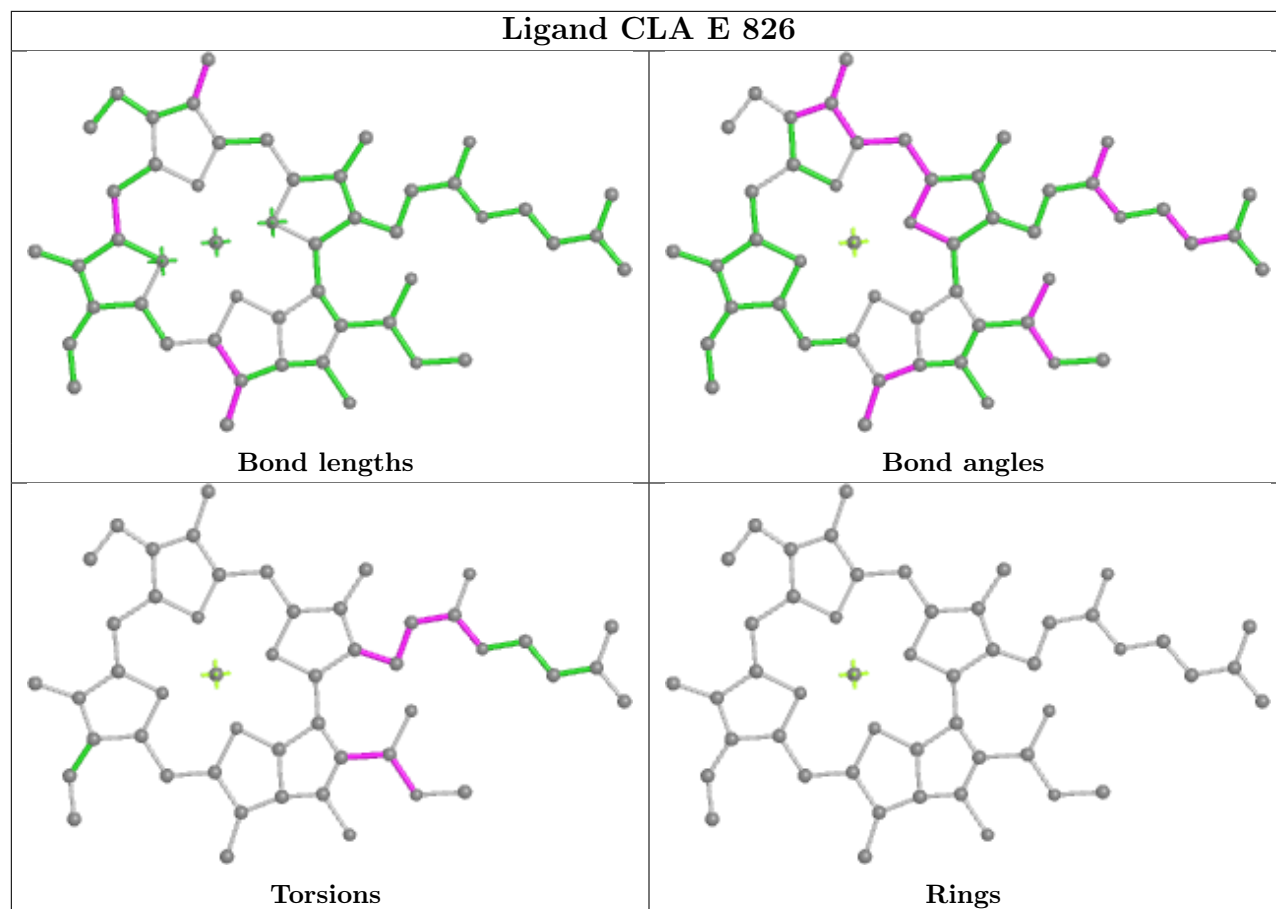




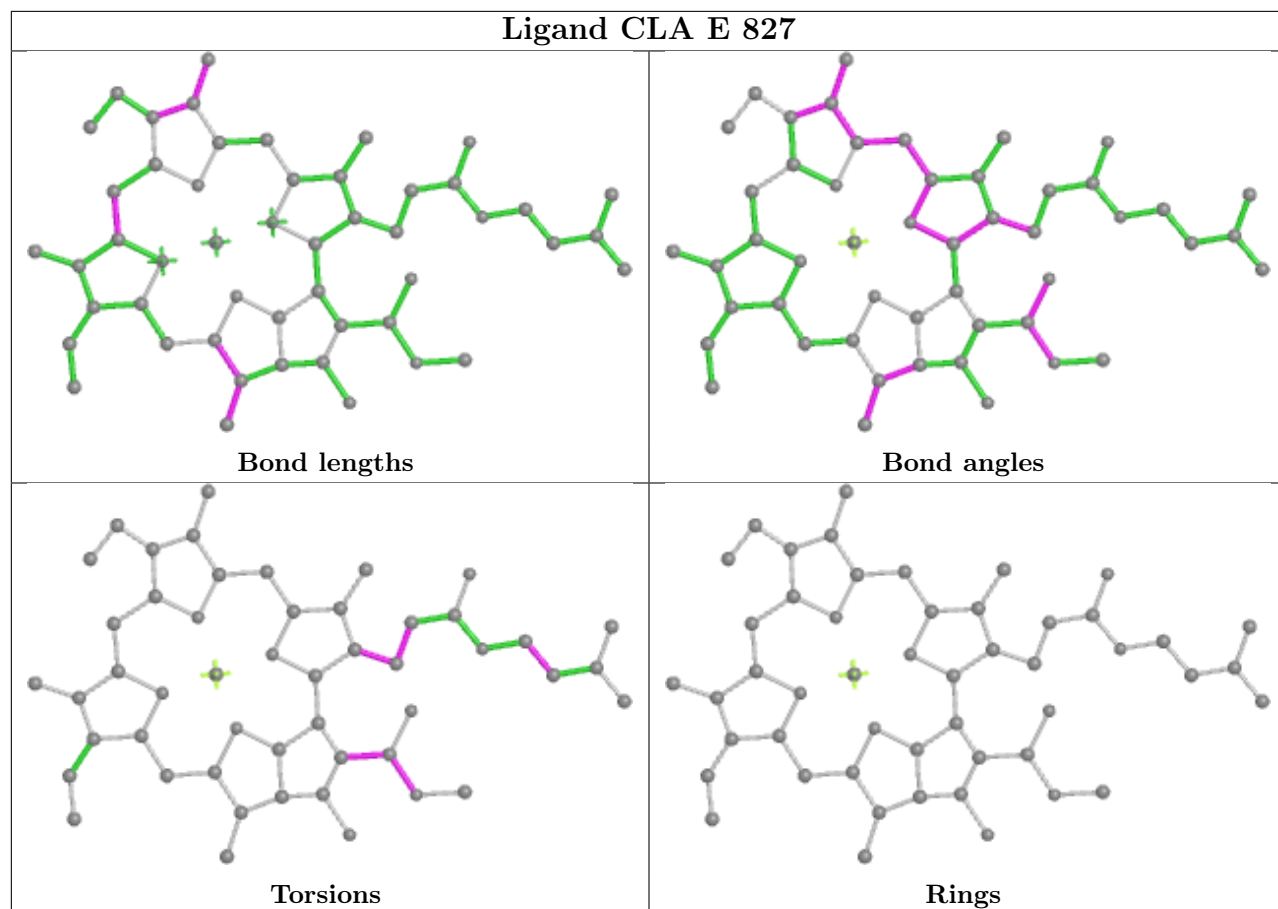


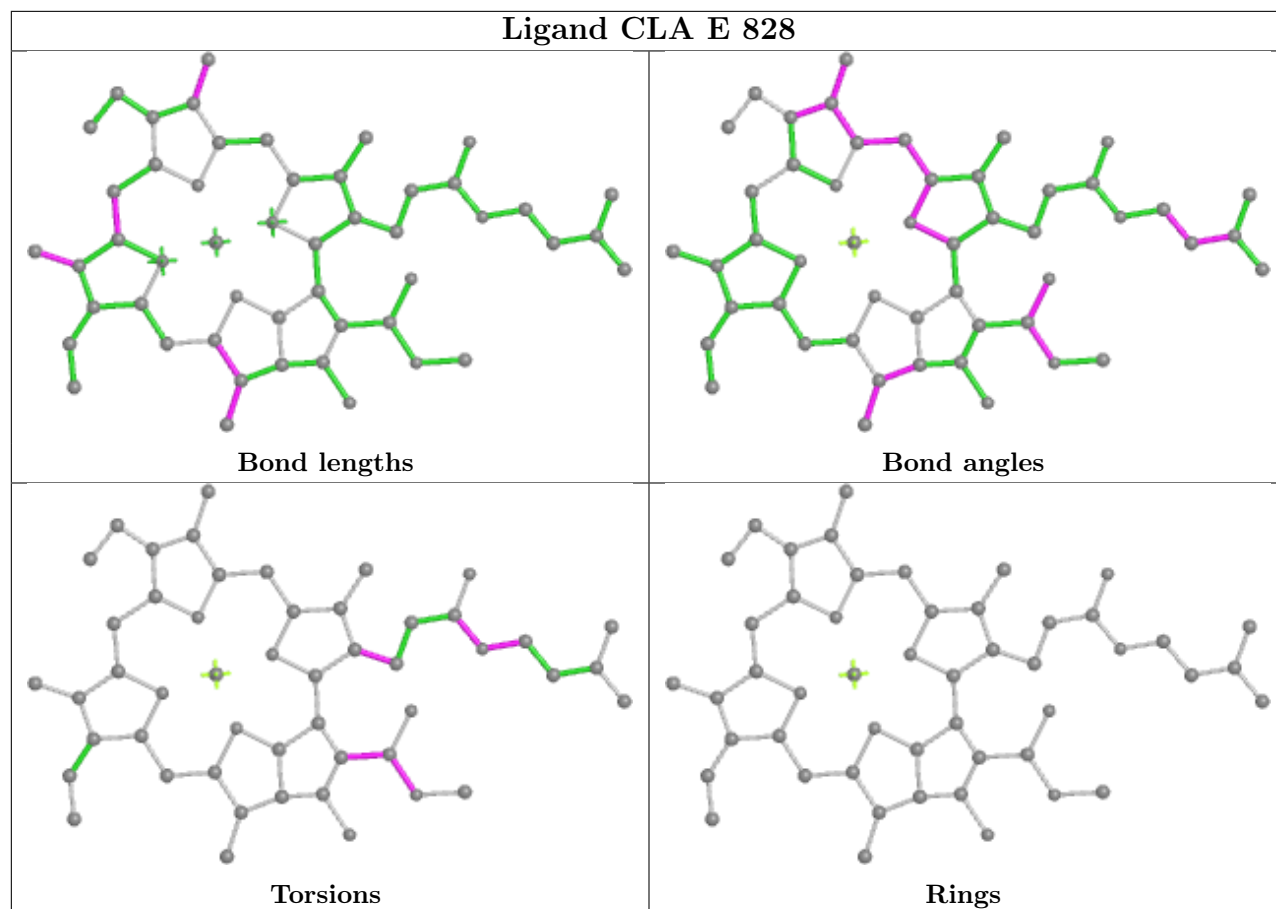


Ligand CLA E 826

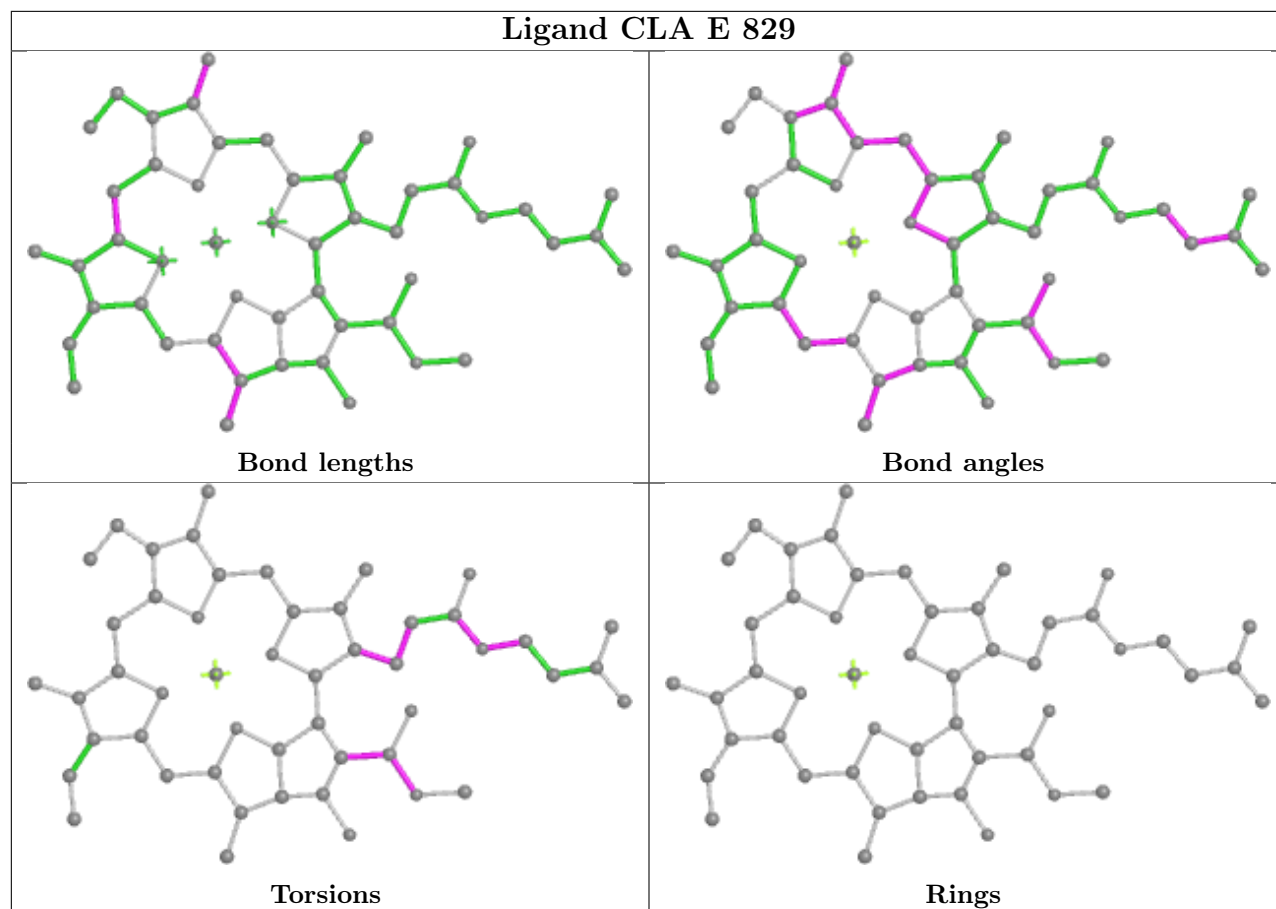


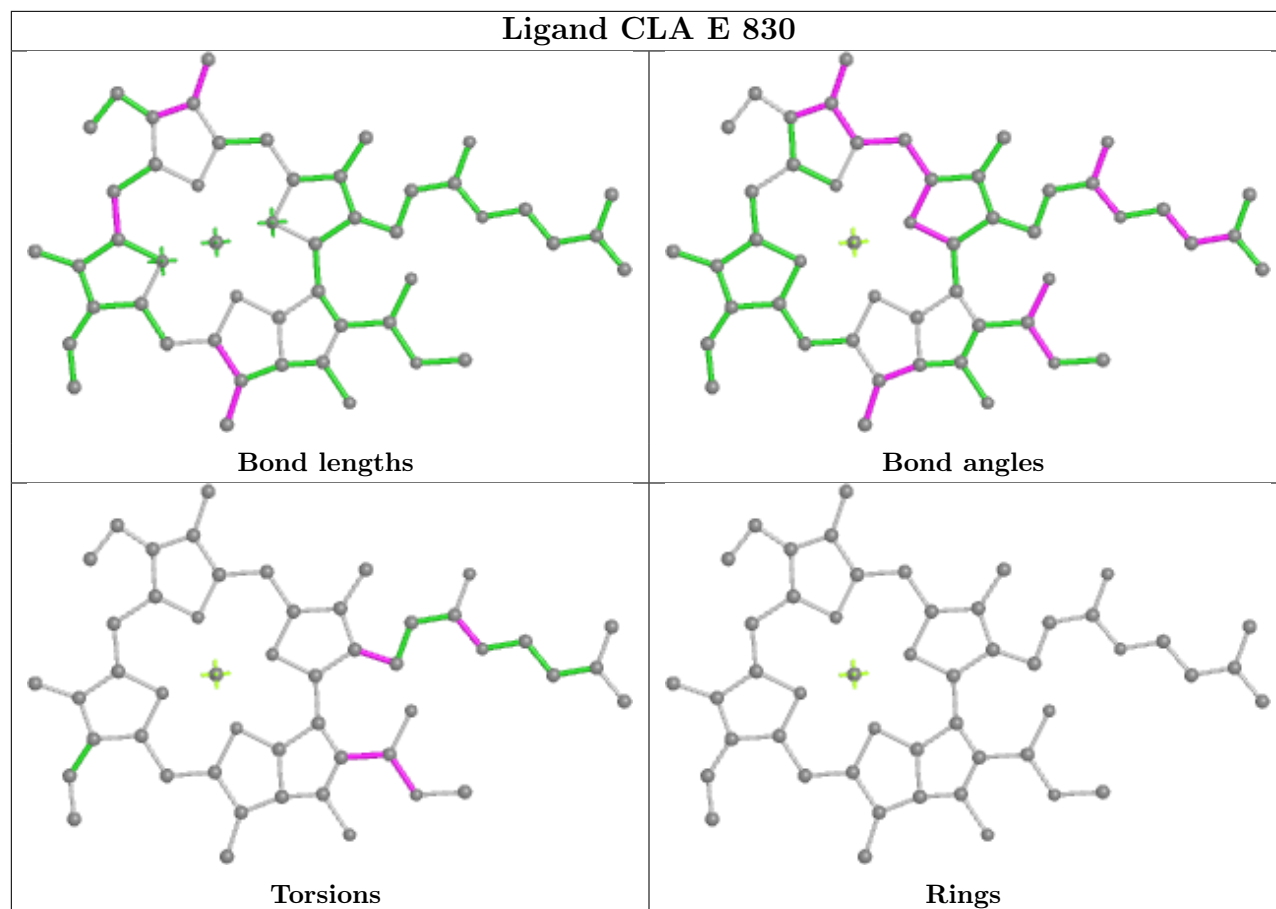
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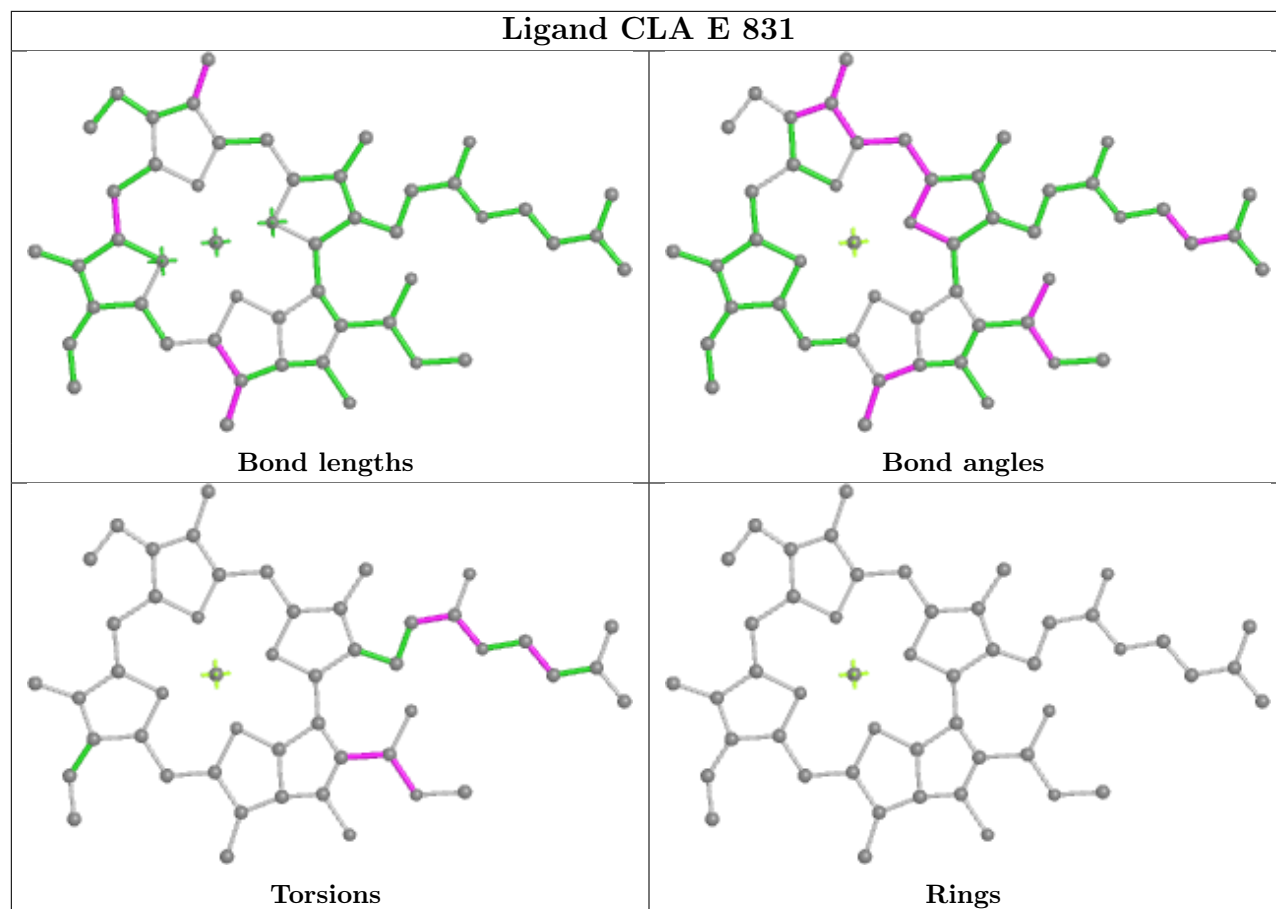


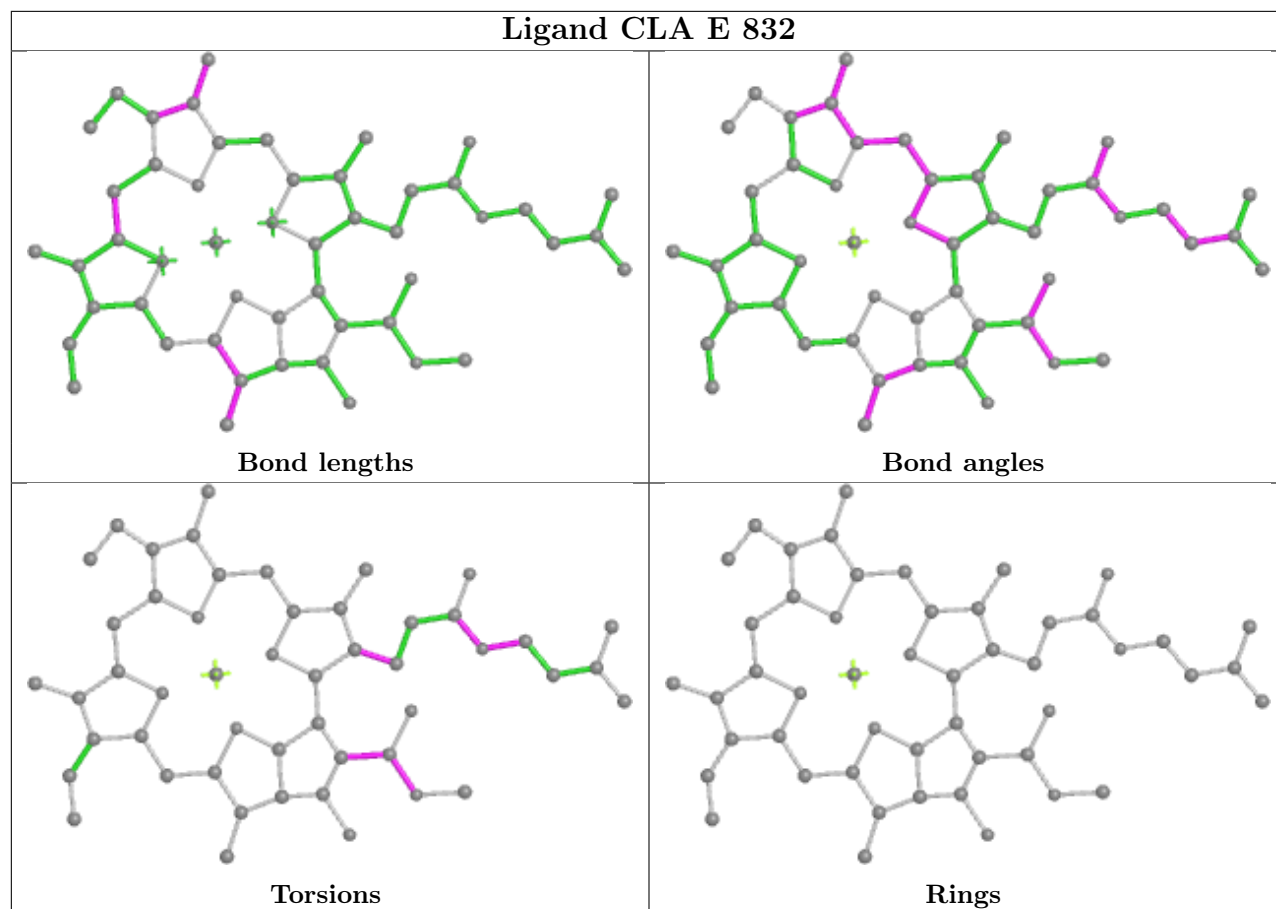


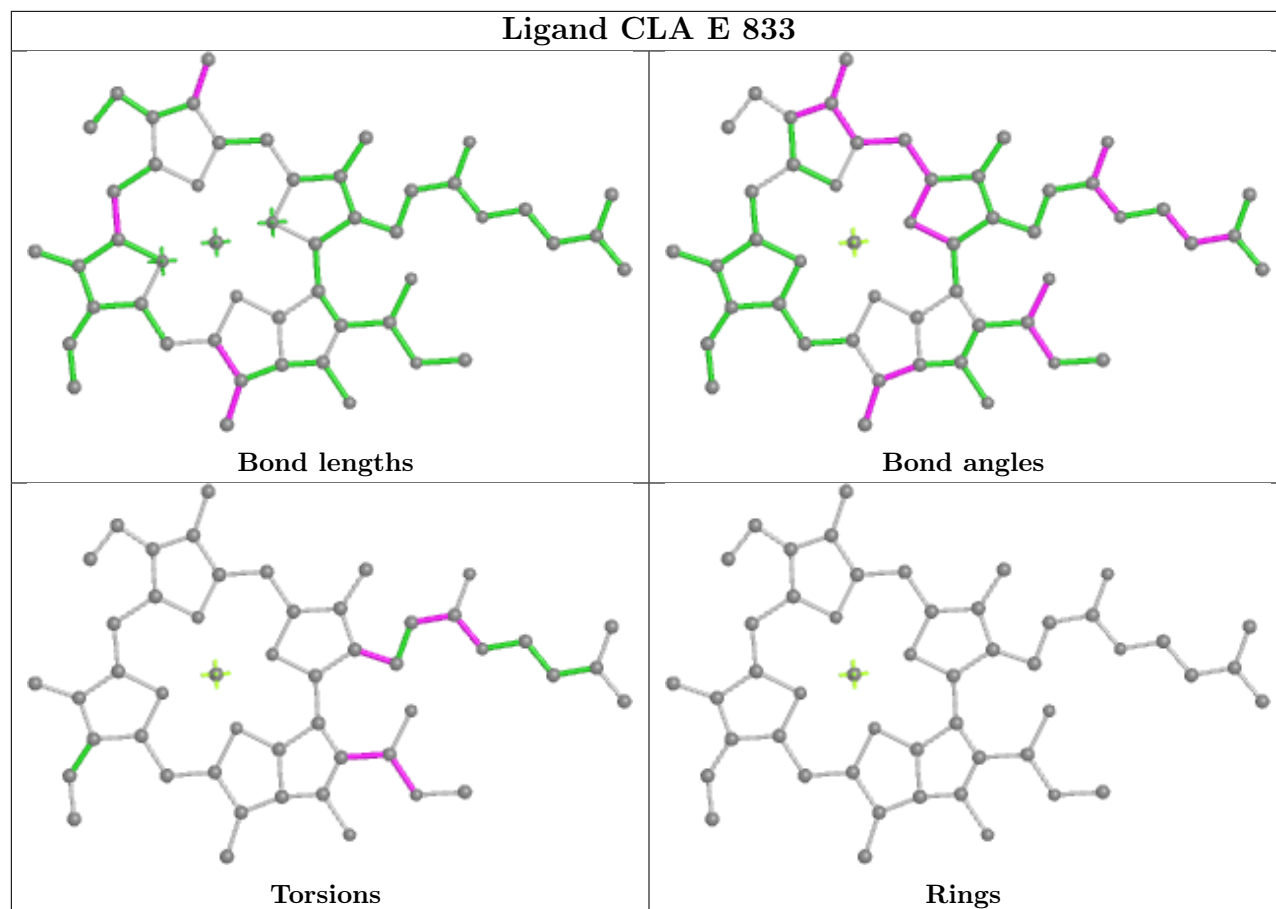
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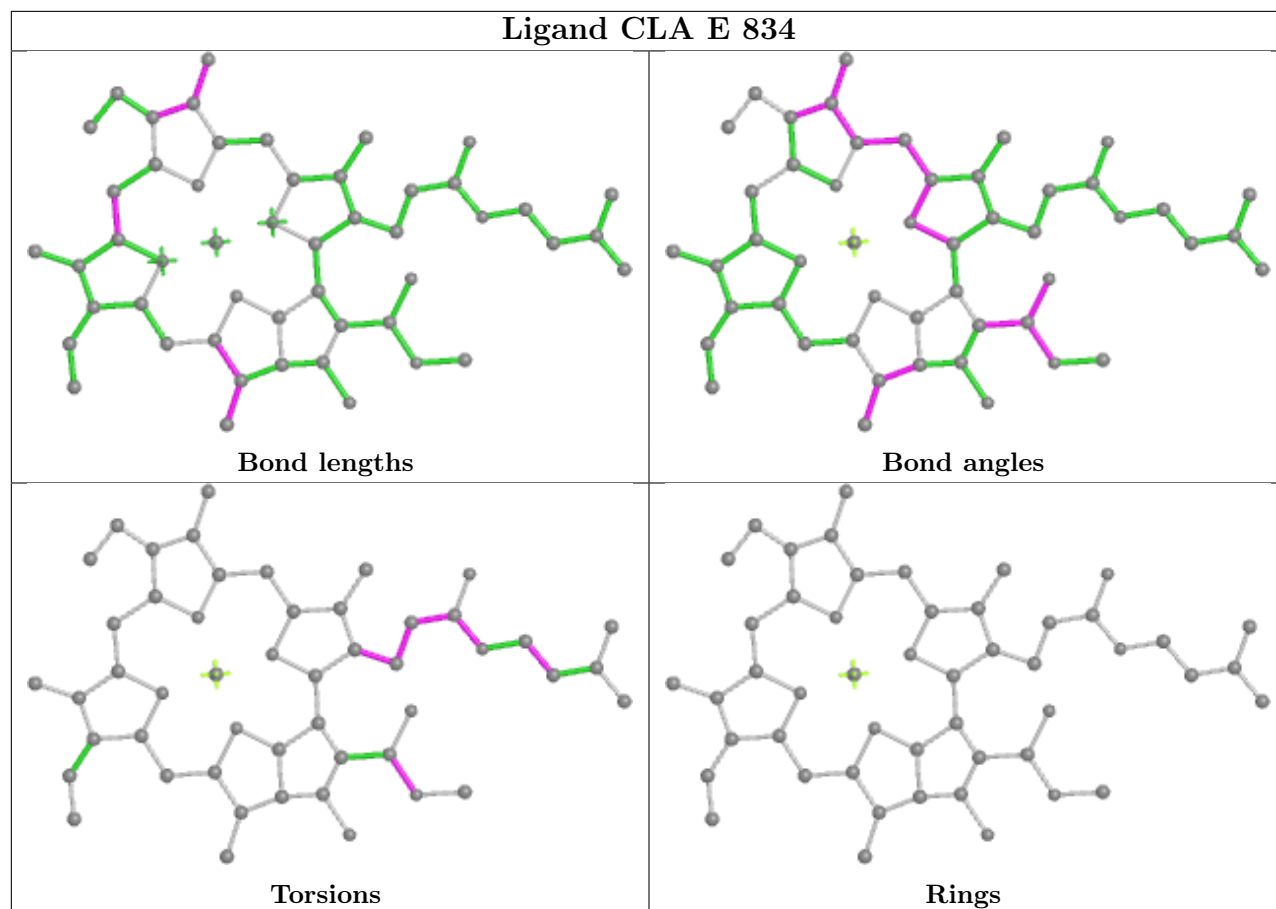




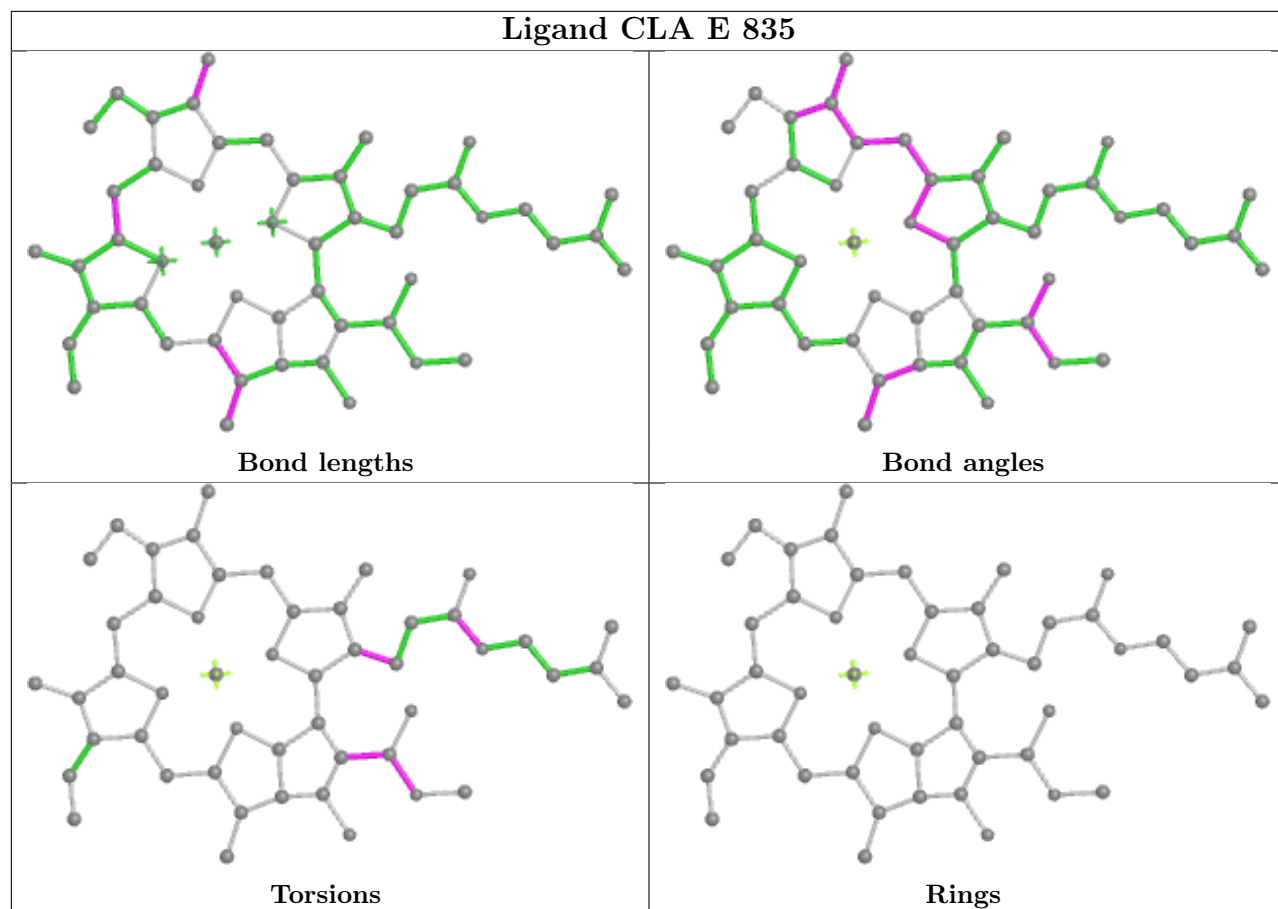




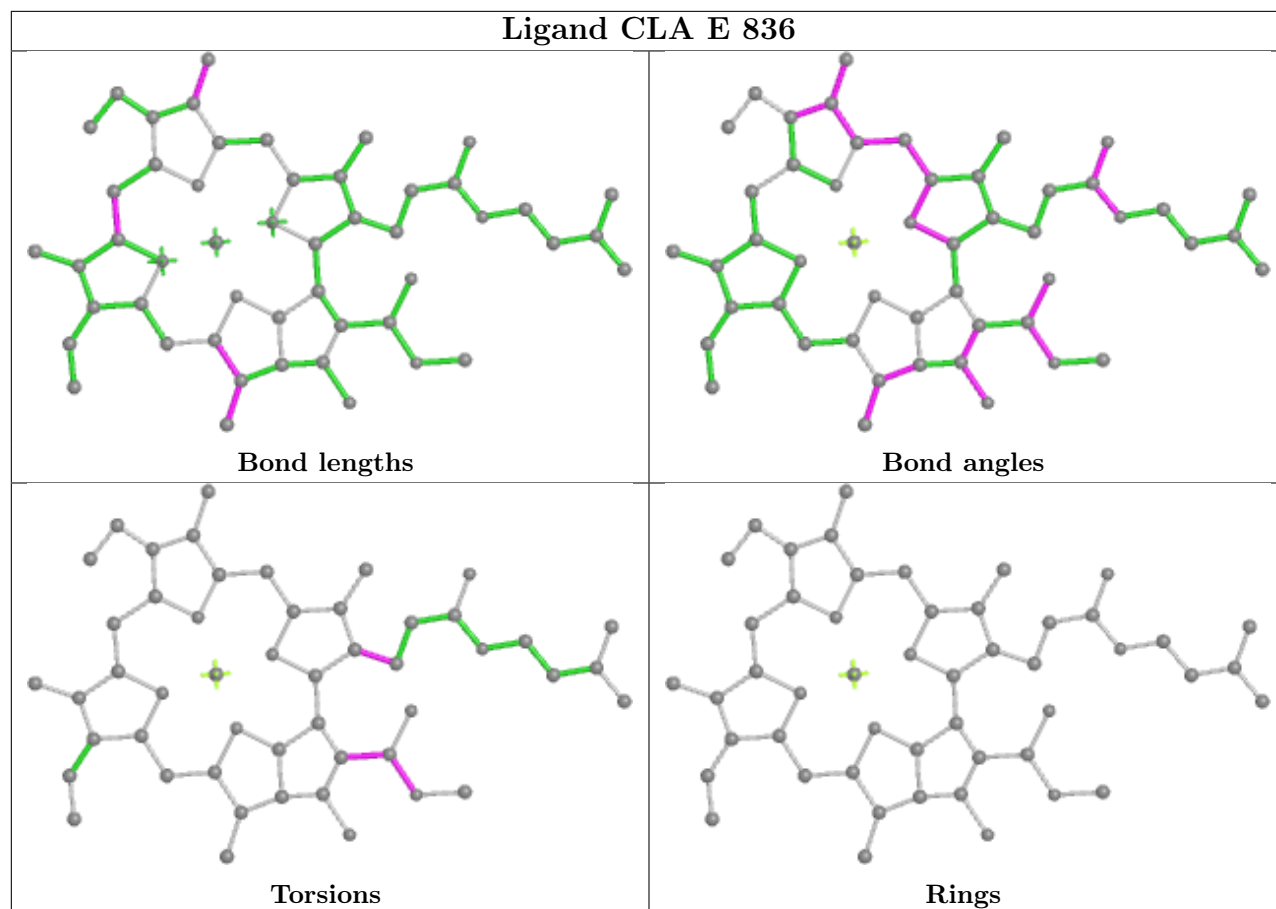
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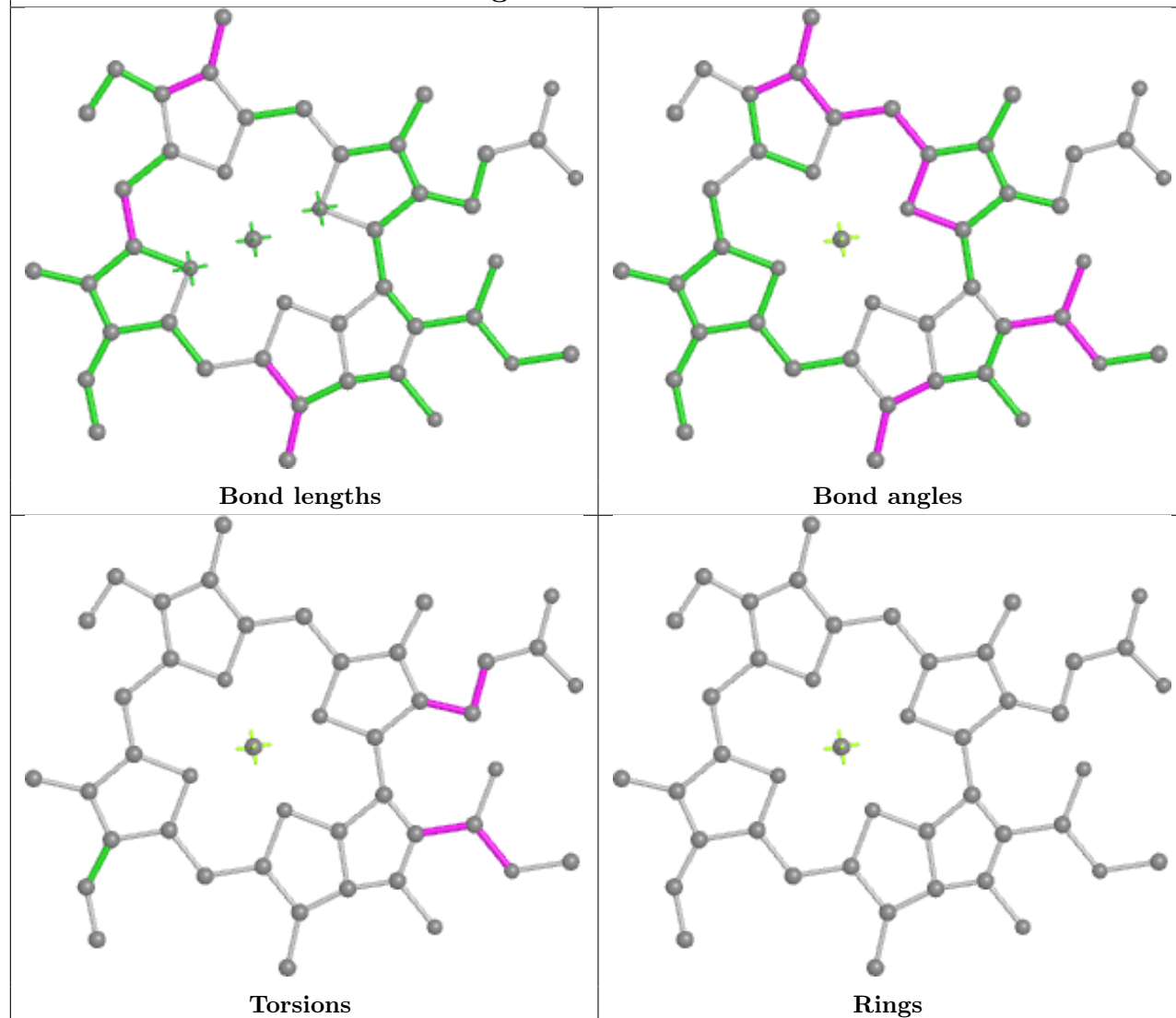
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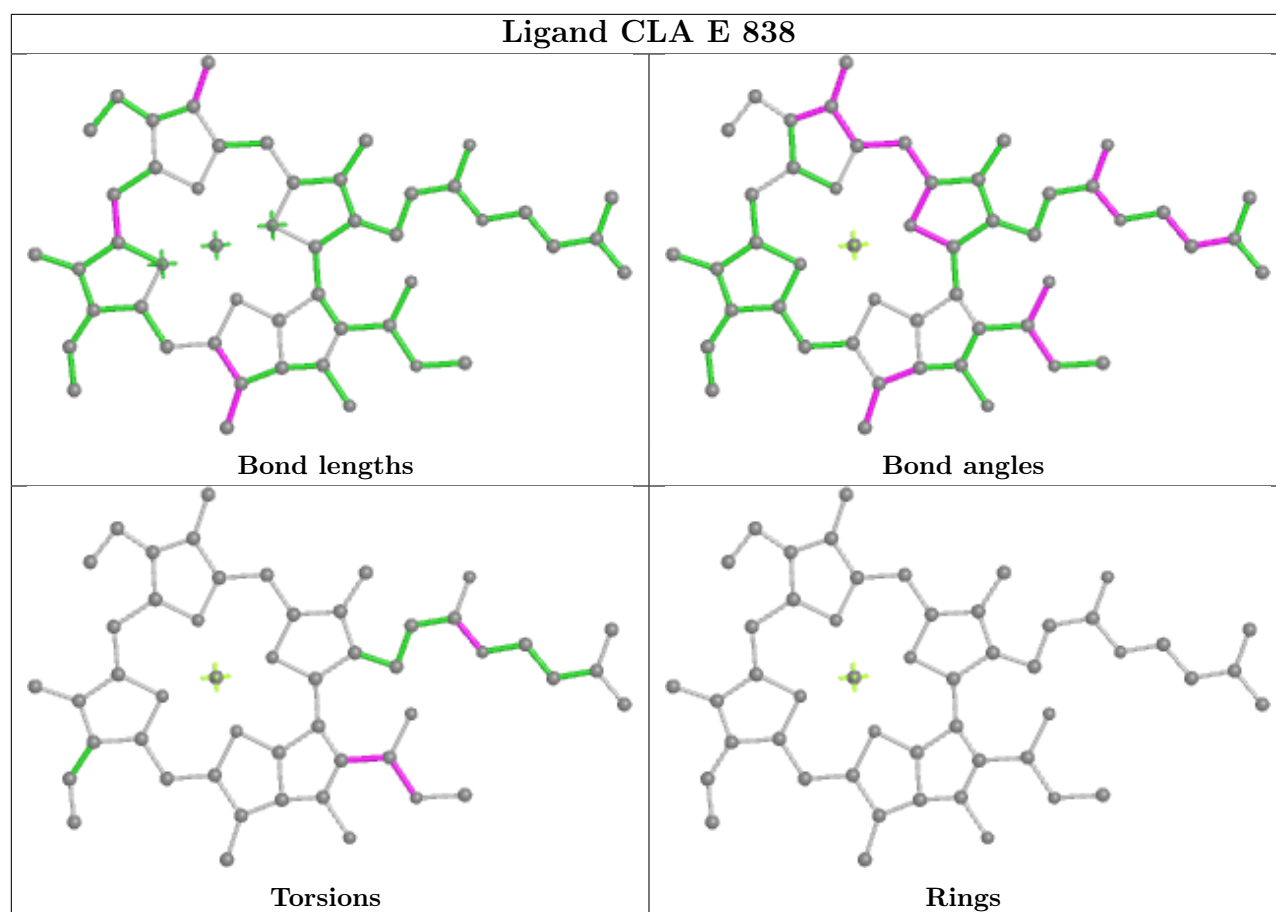


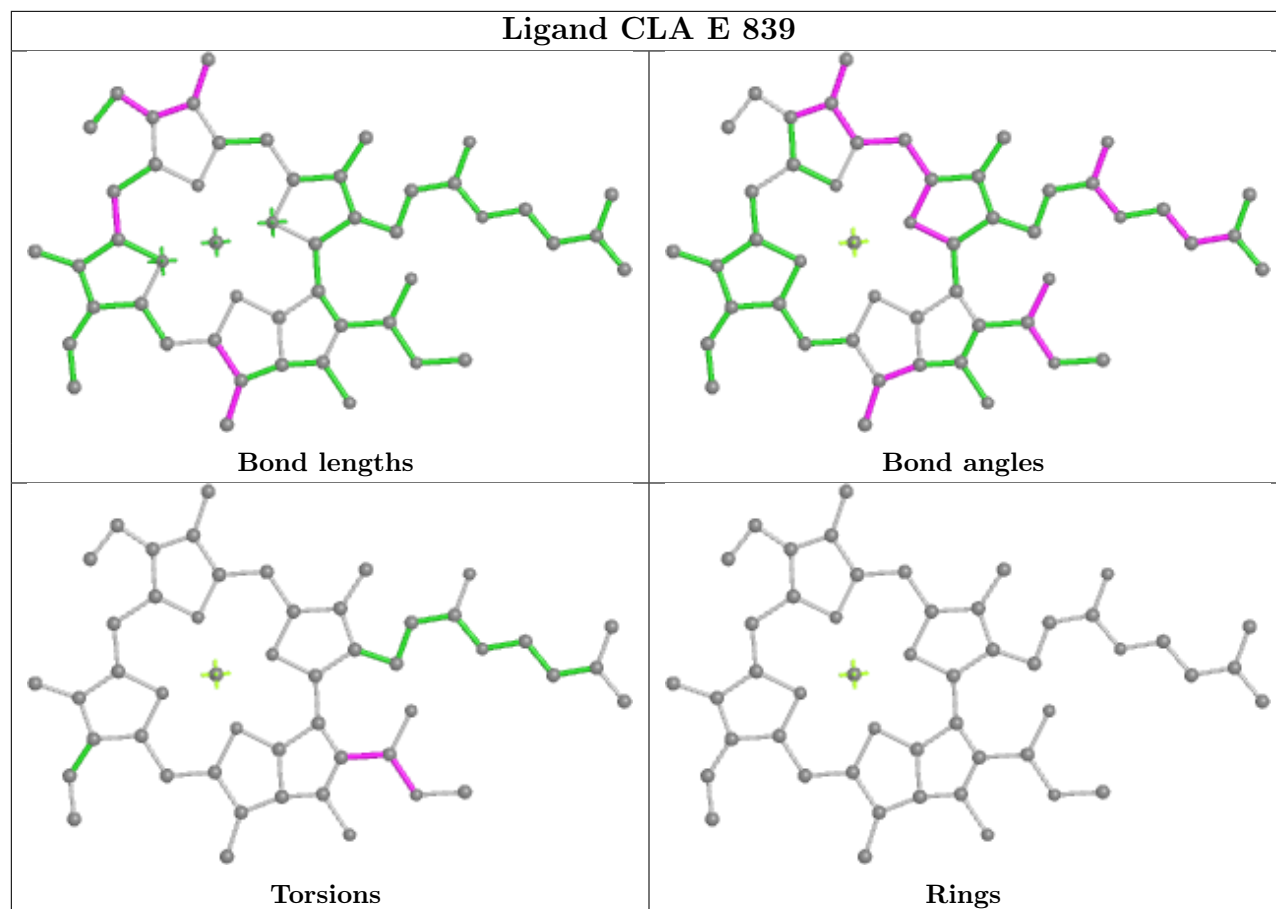
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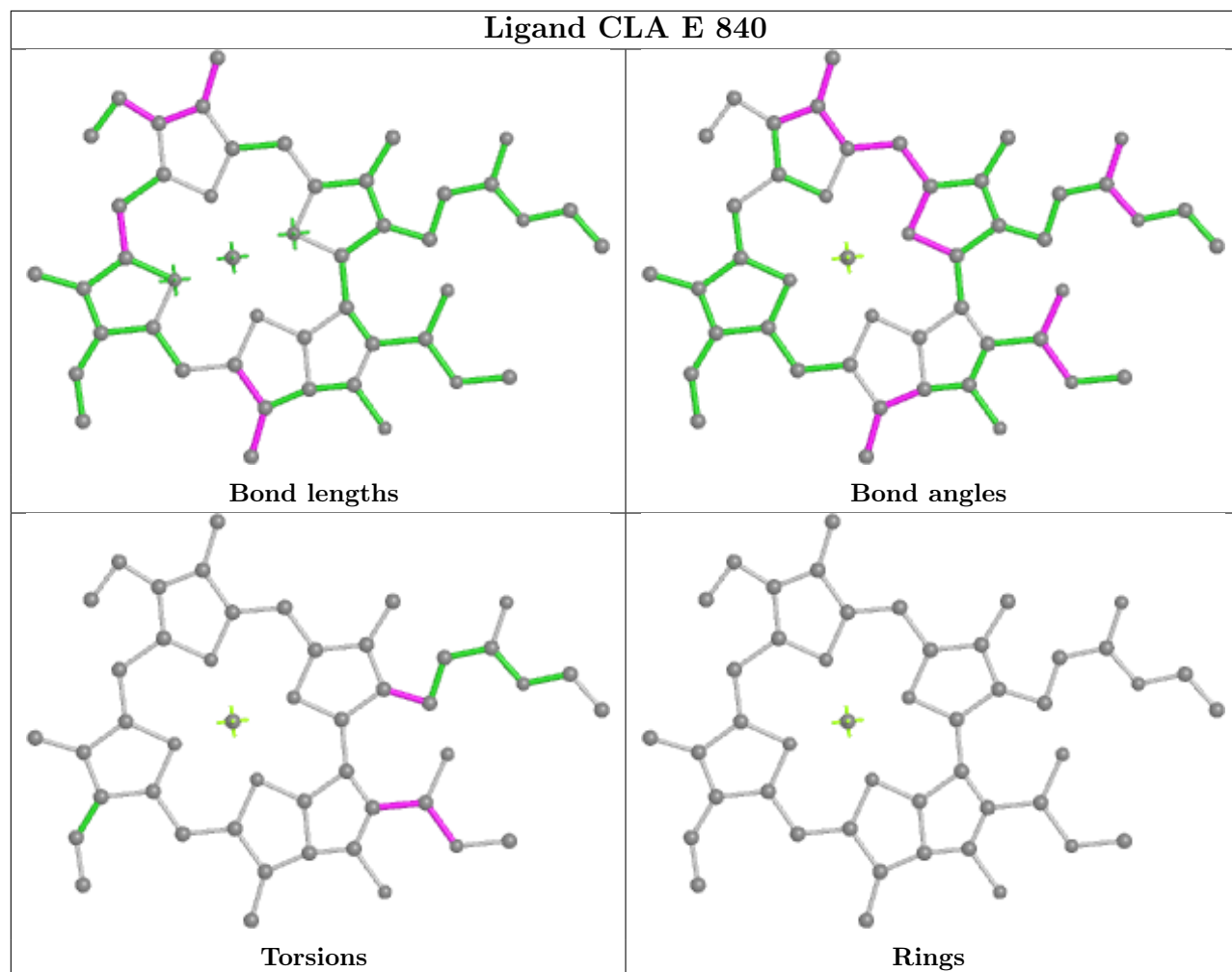
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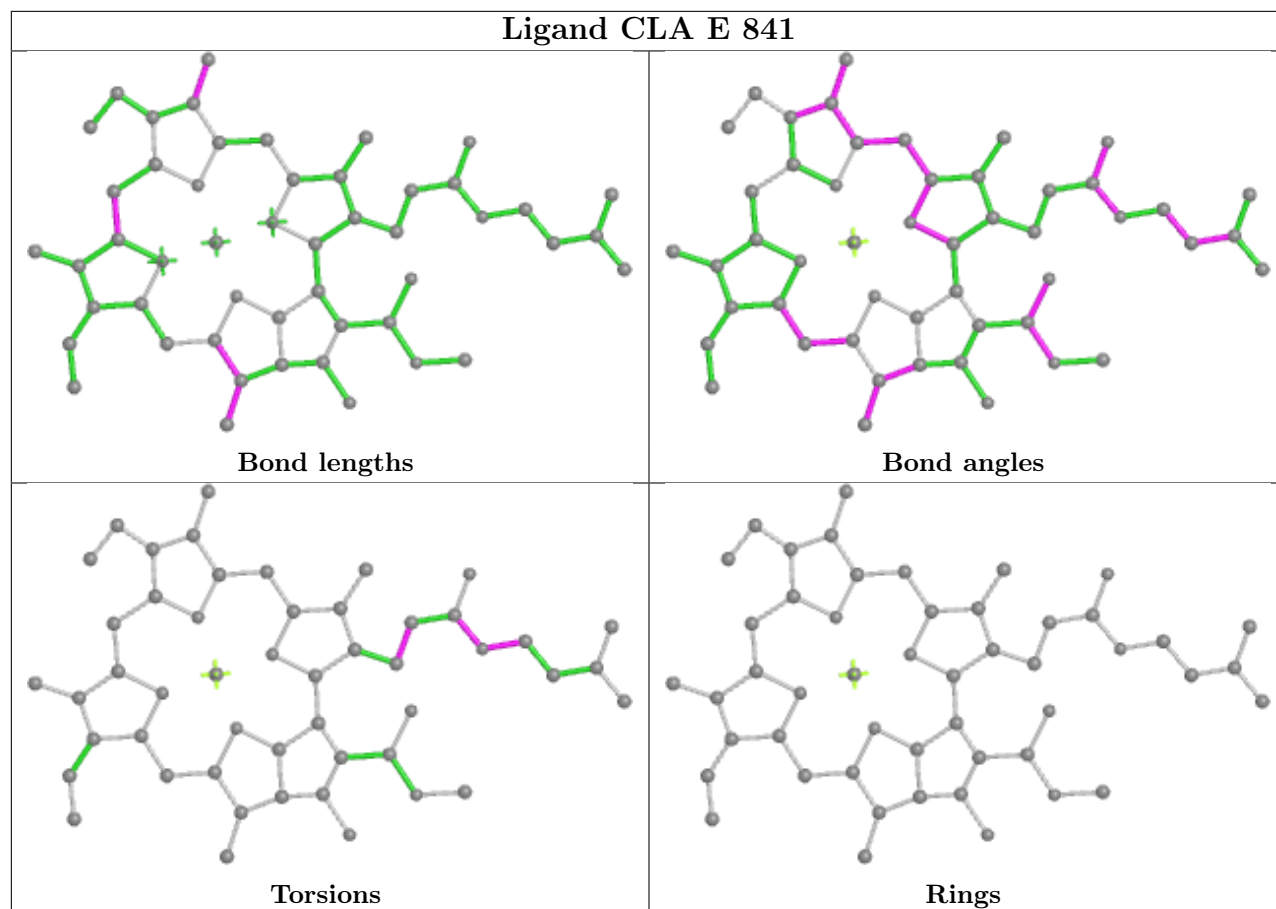


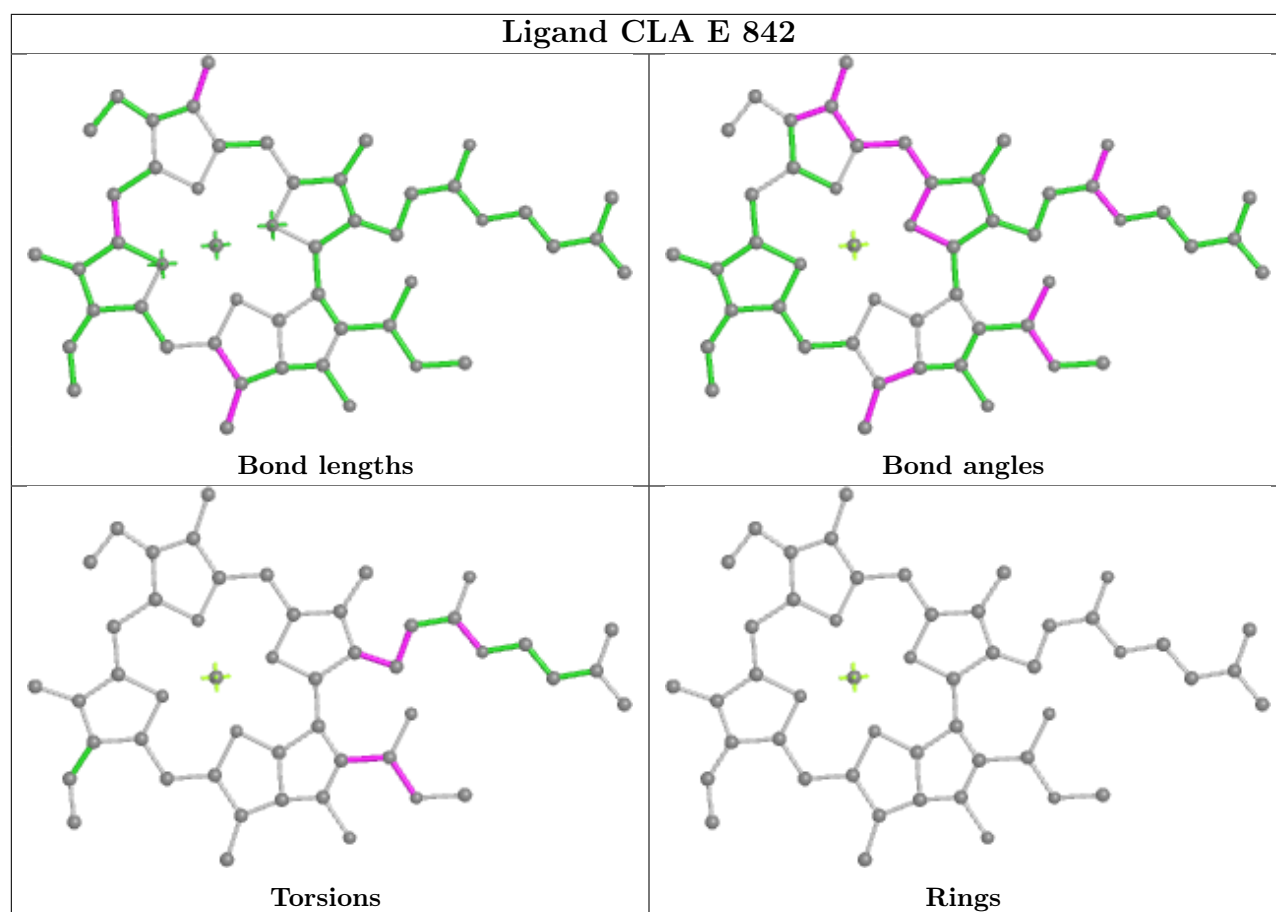


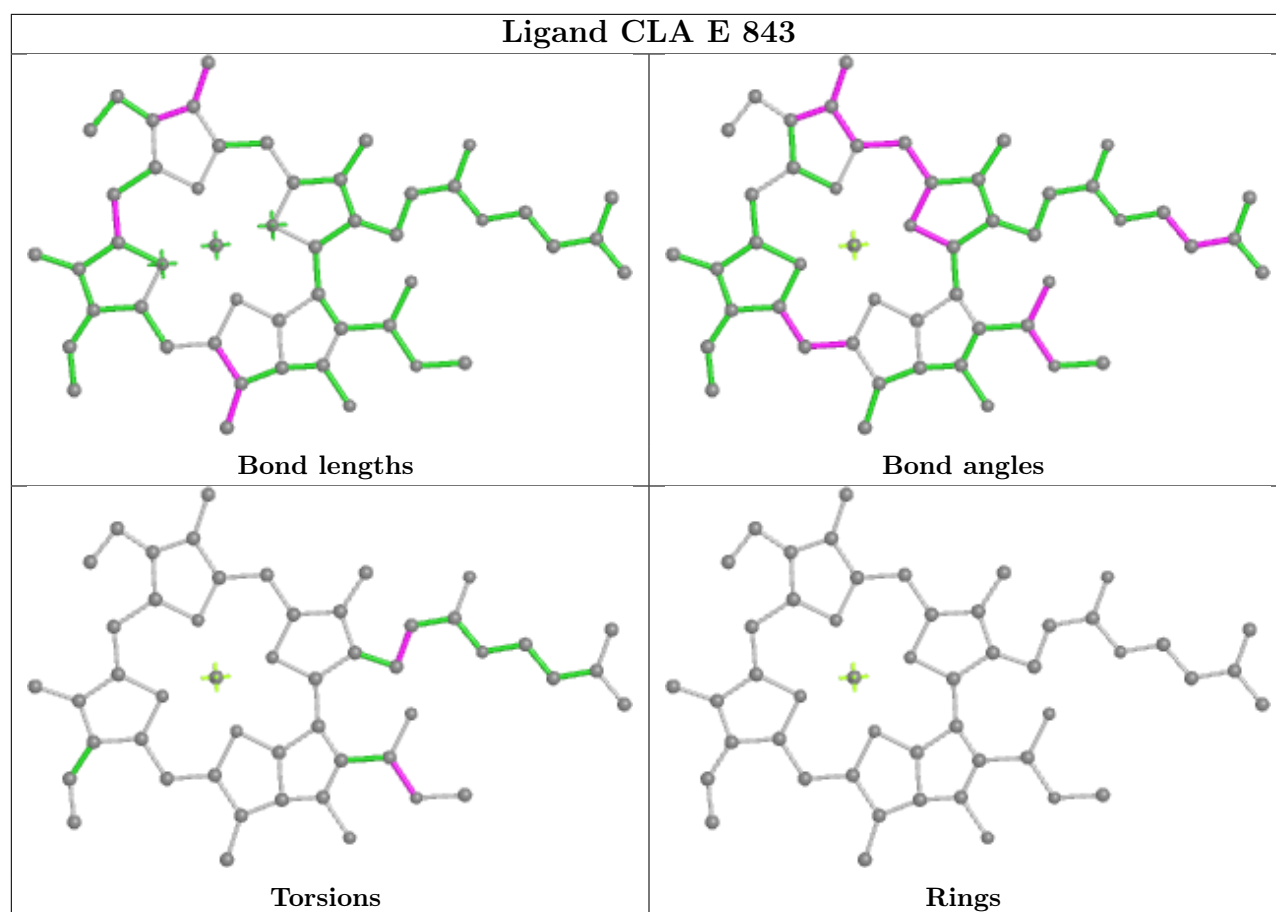
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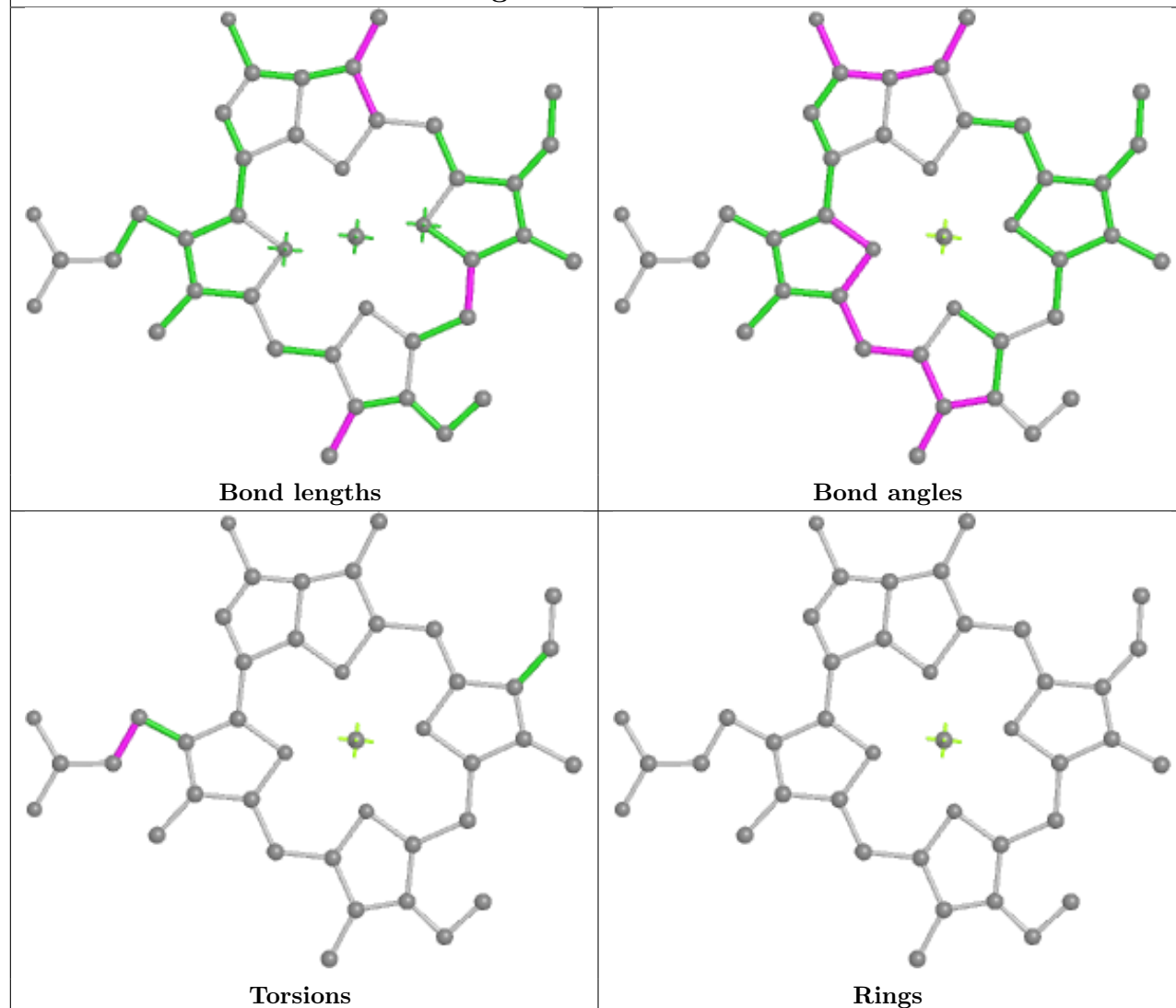
Ligand CLA E 841



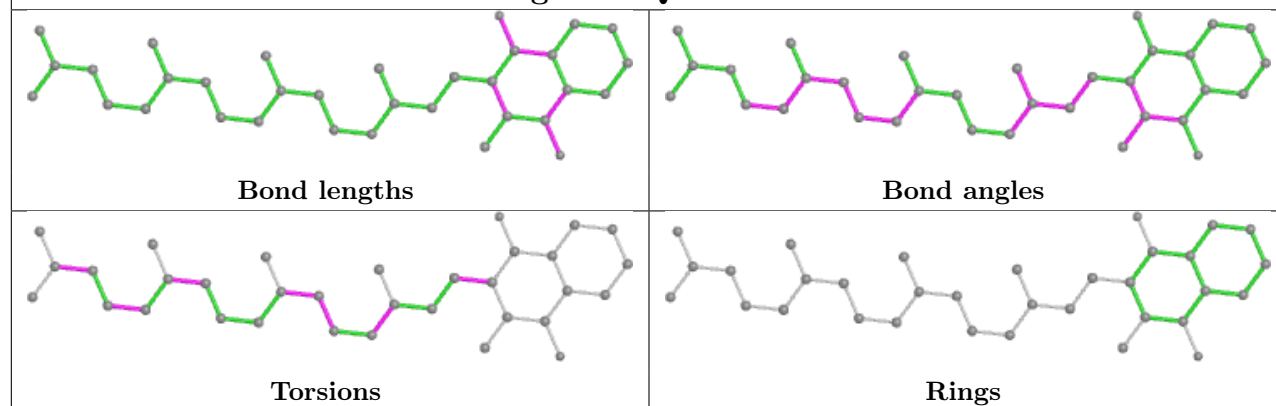


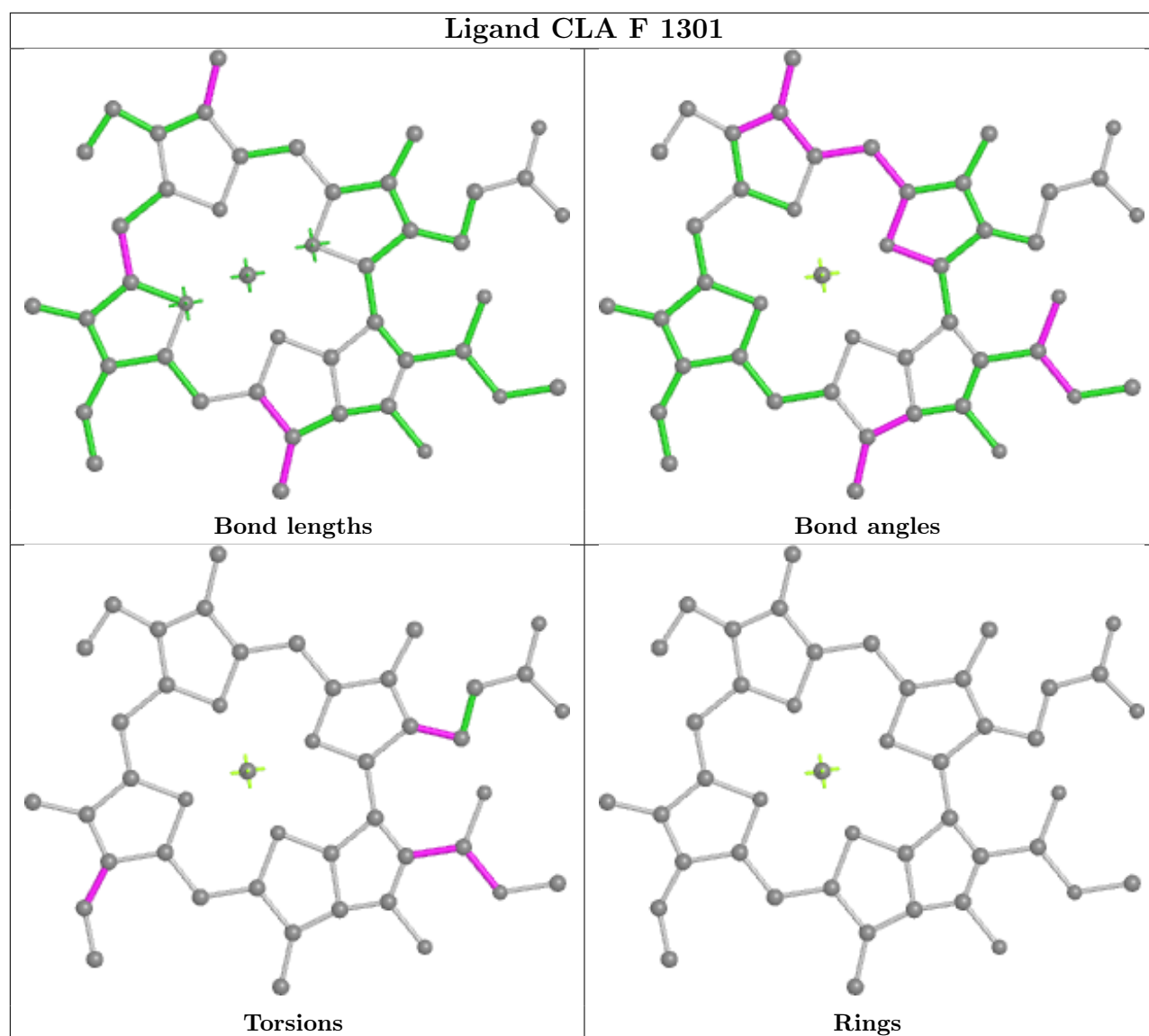


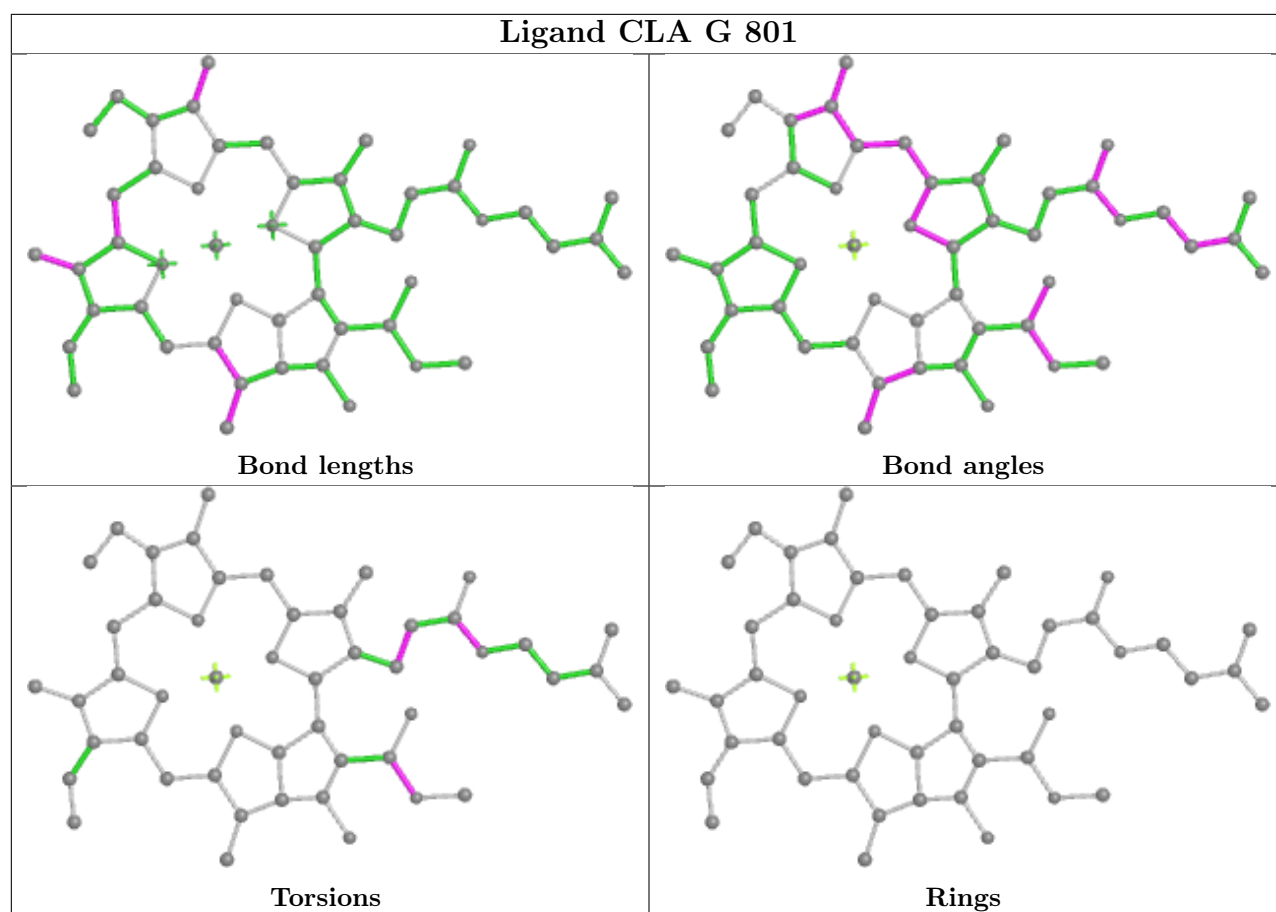
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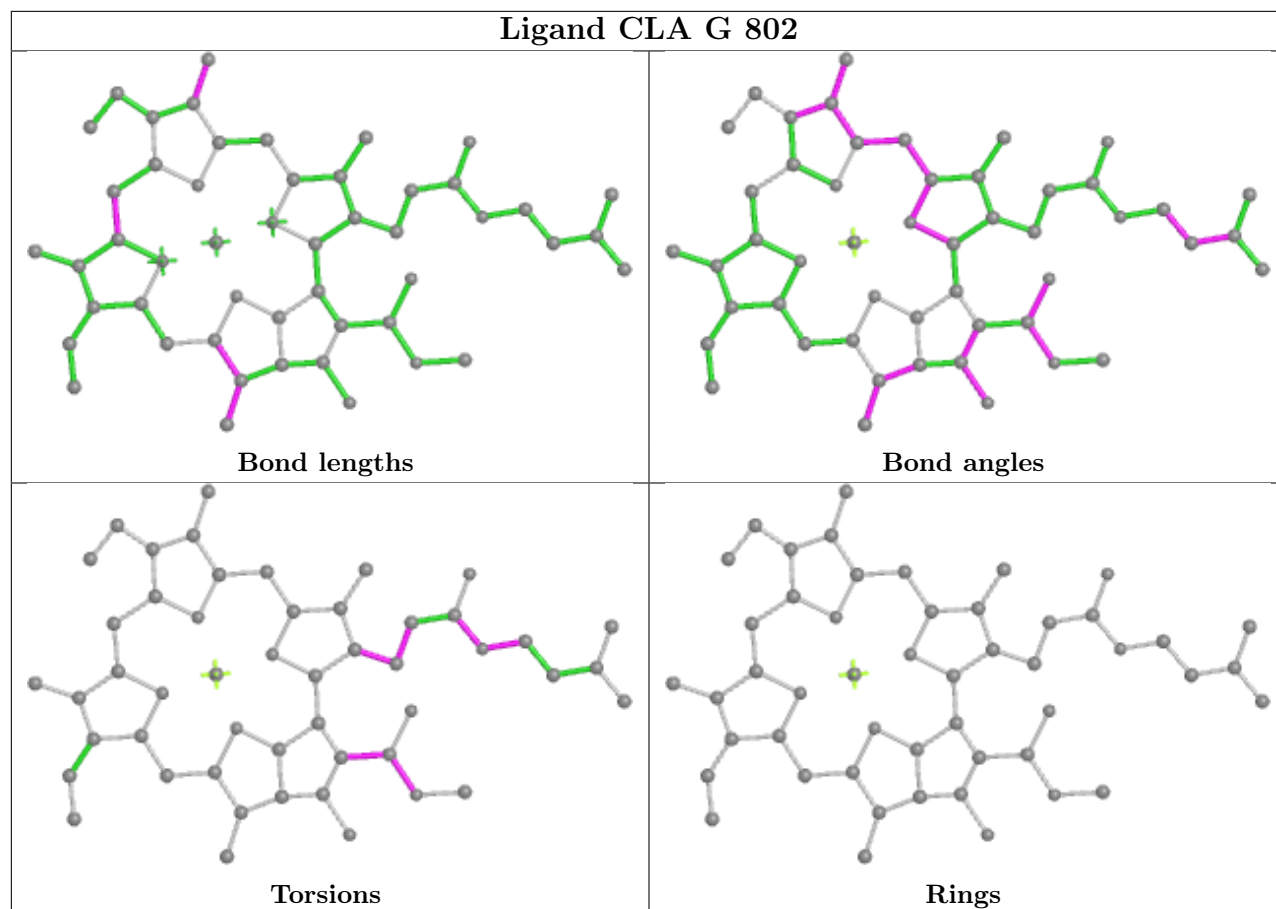


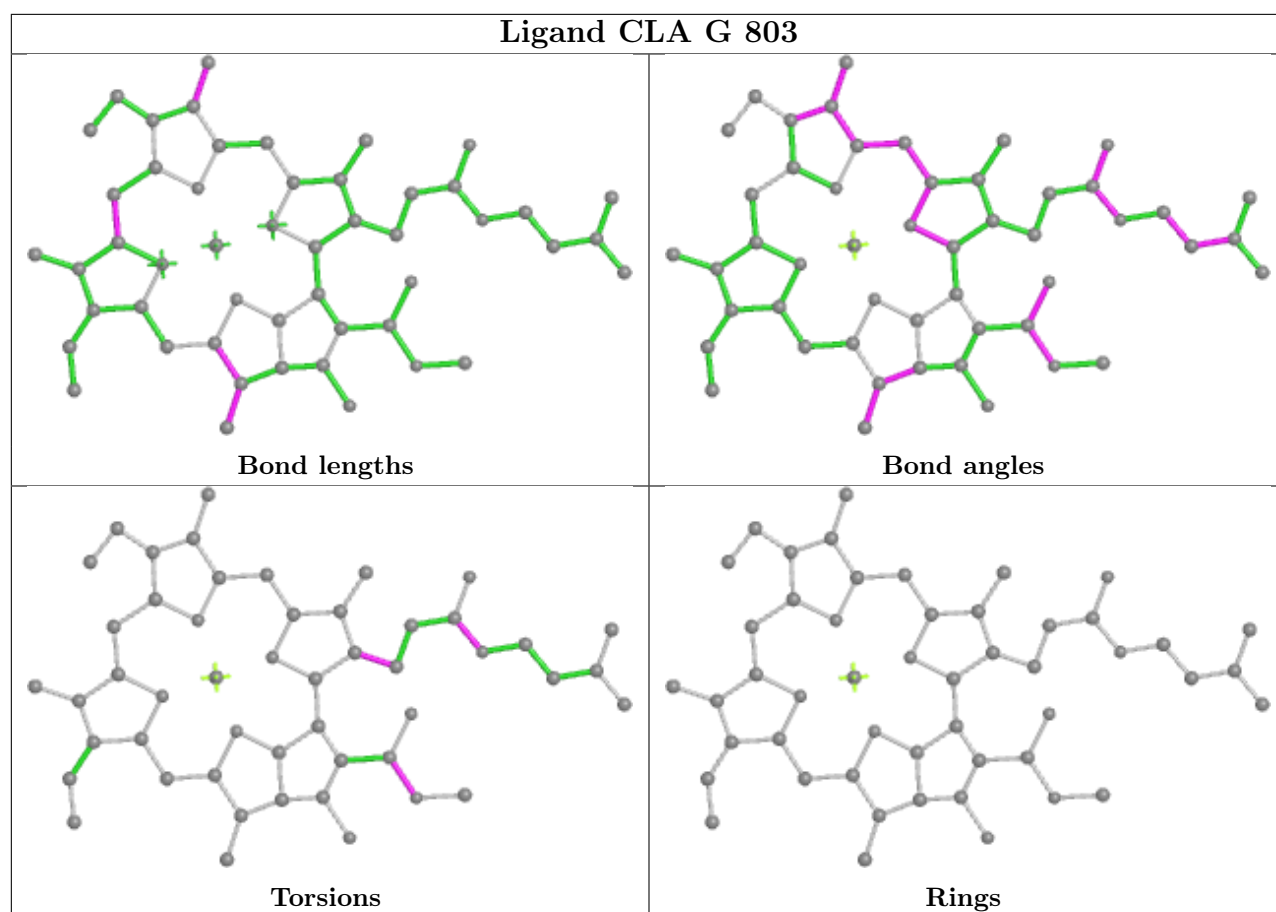
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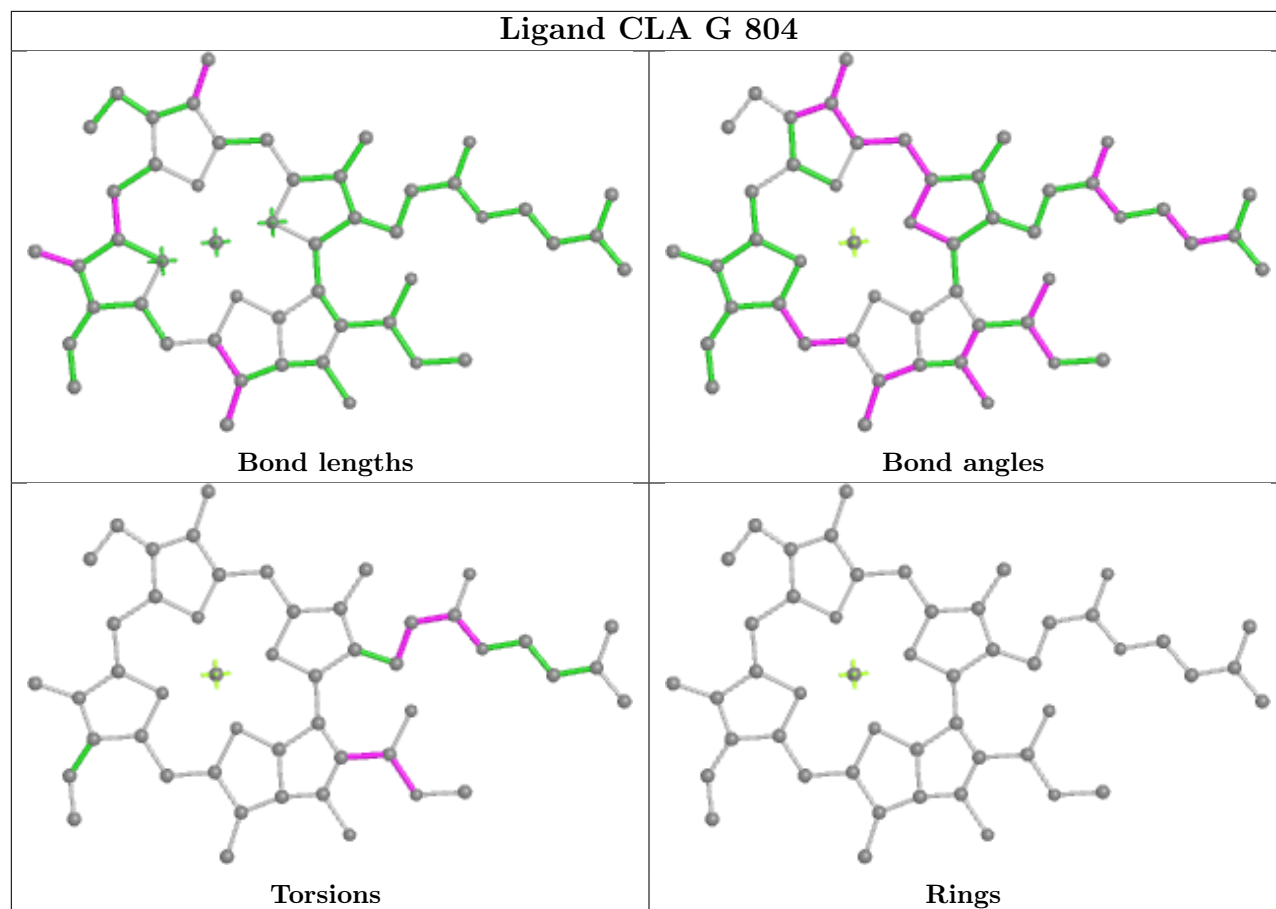


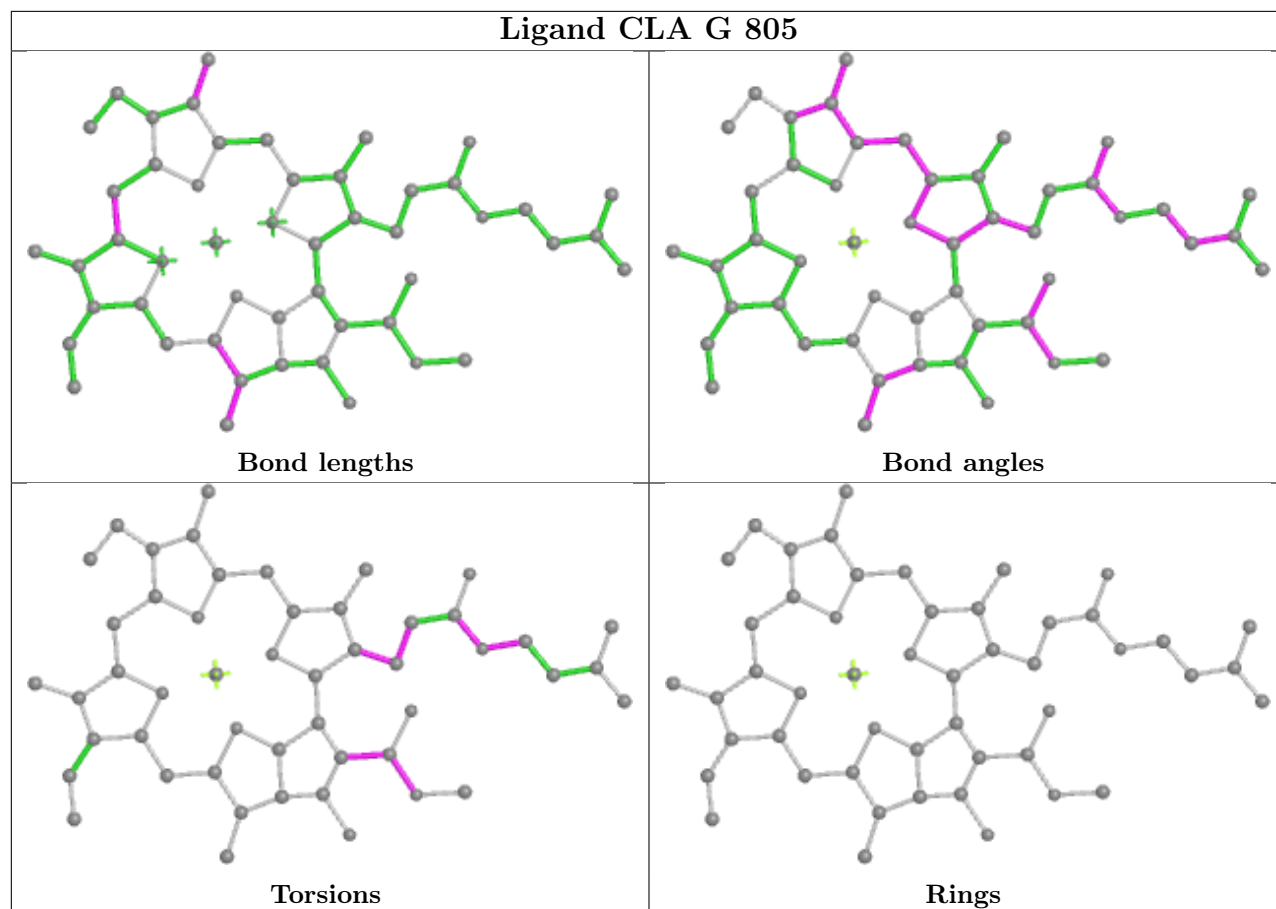


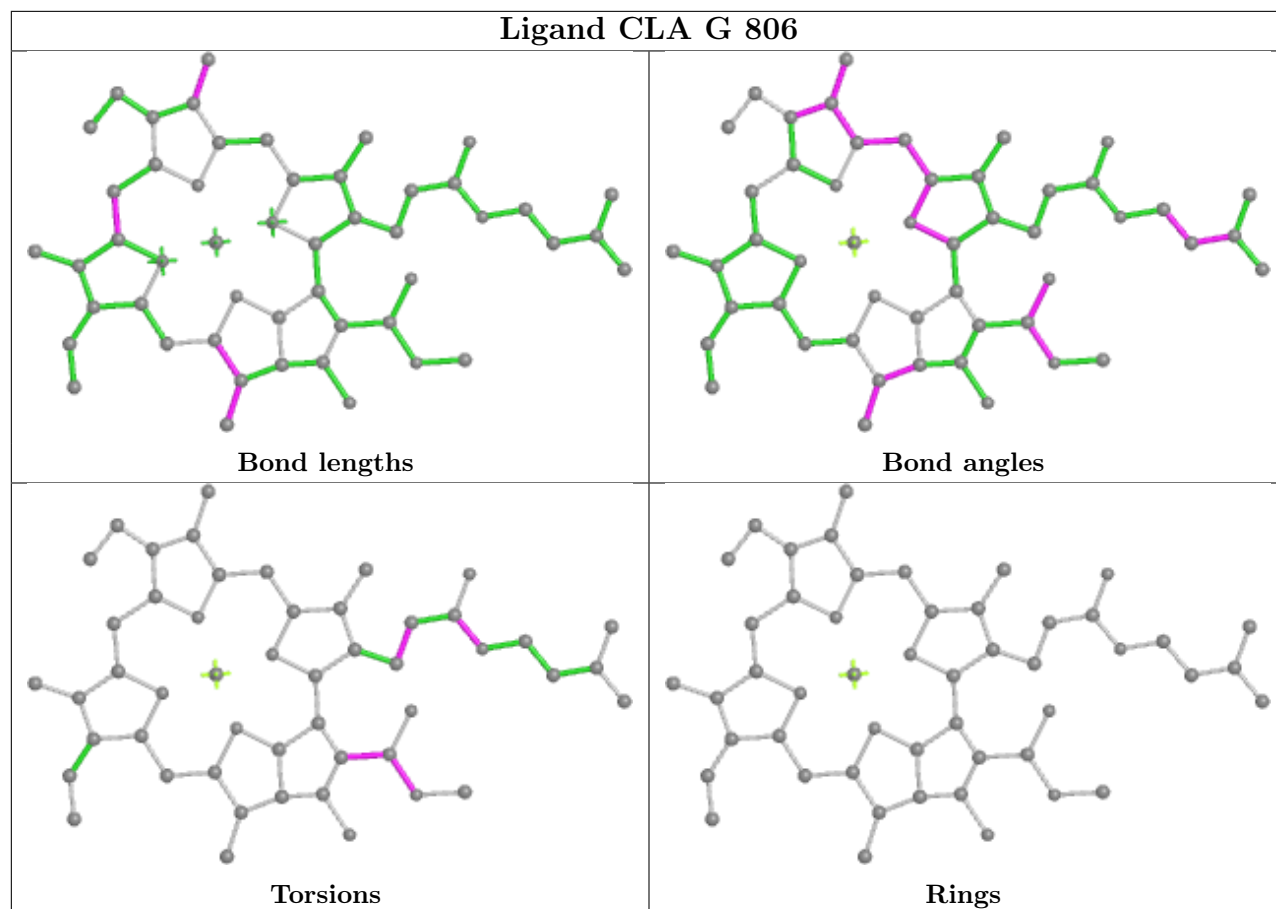


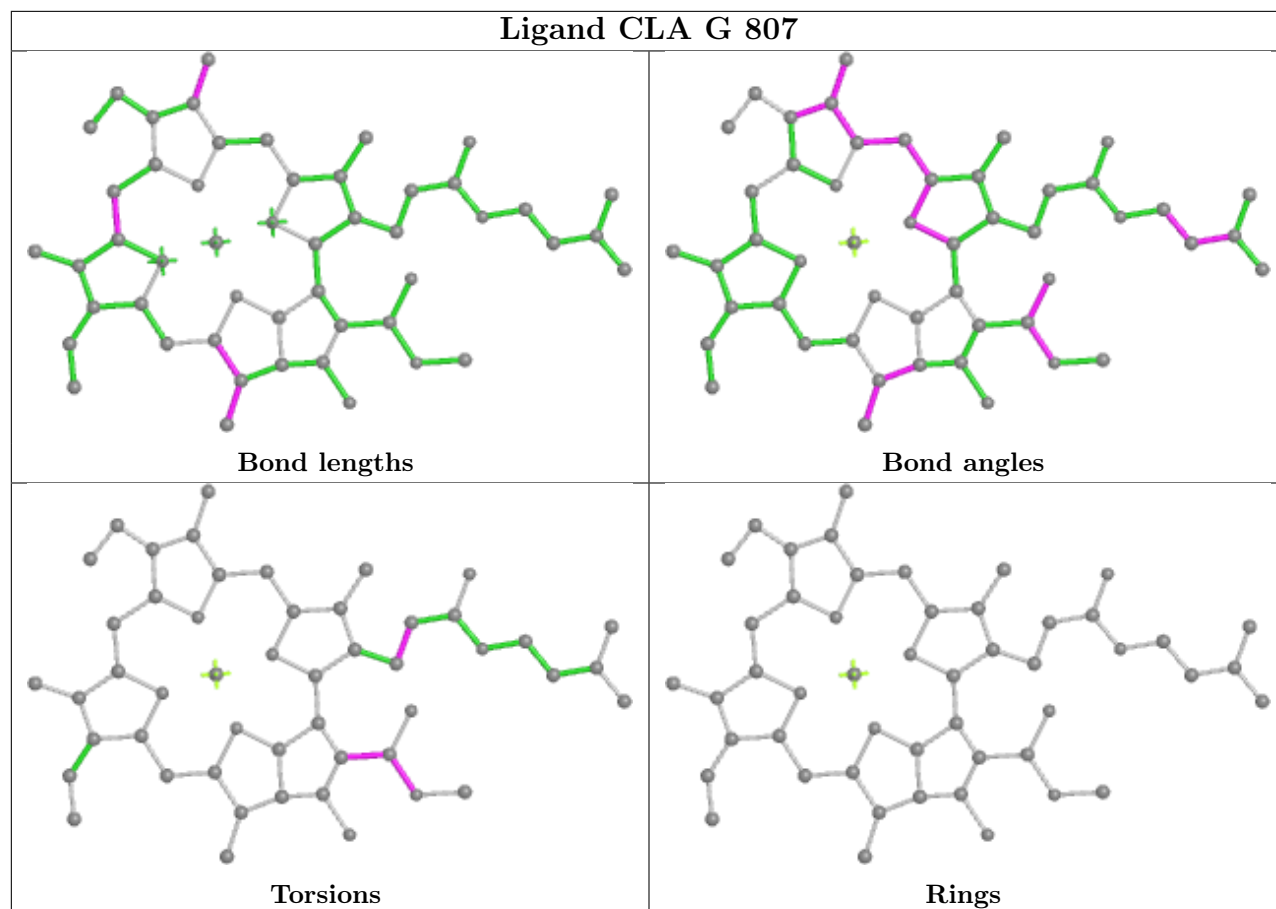


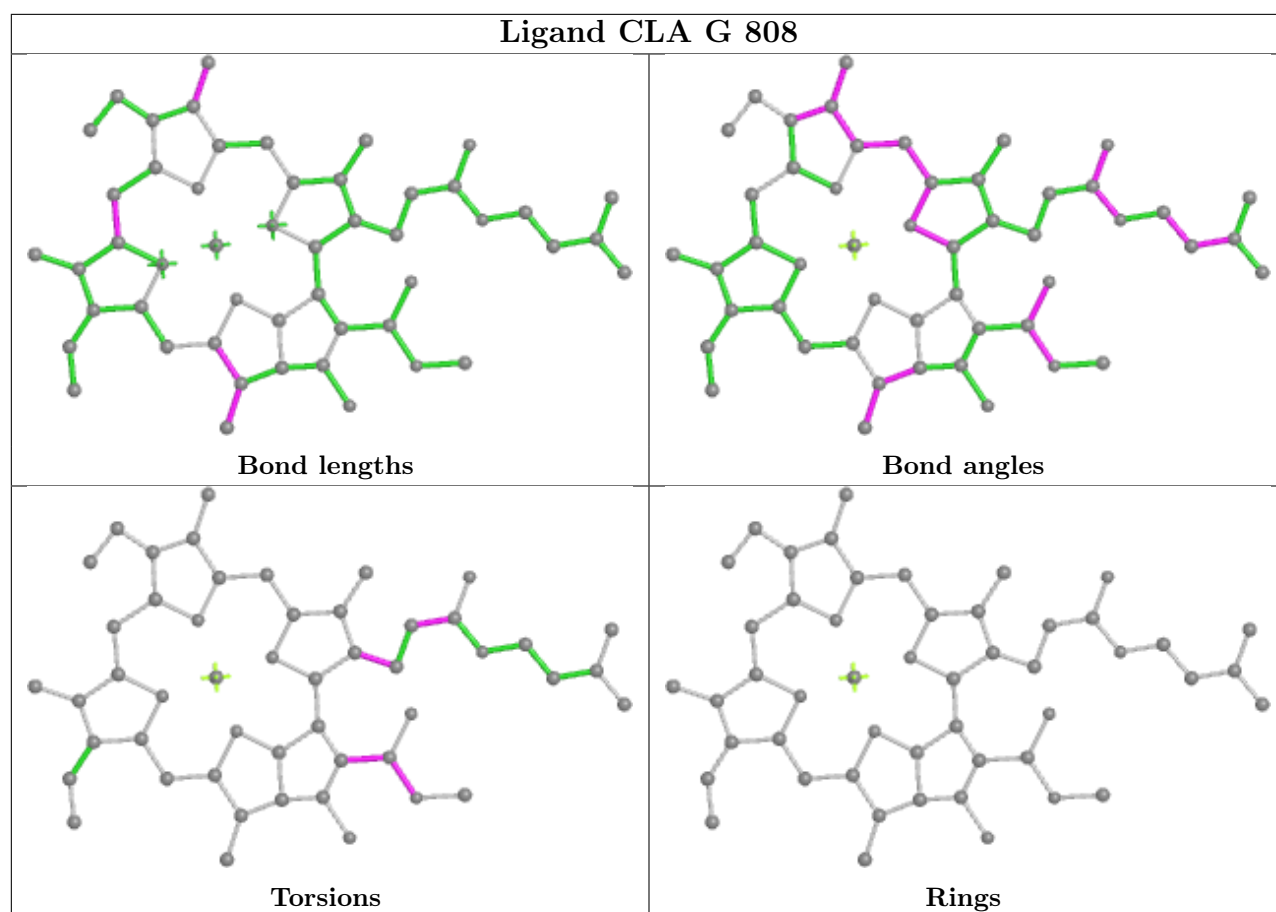


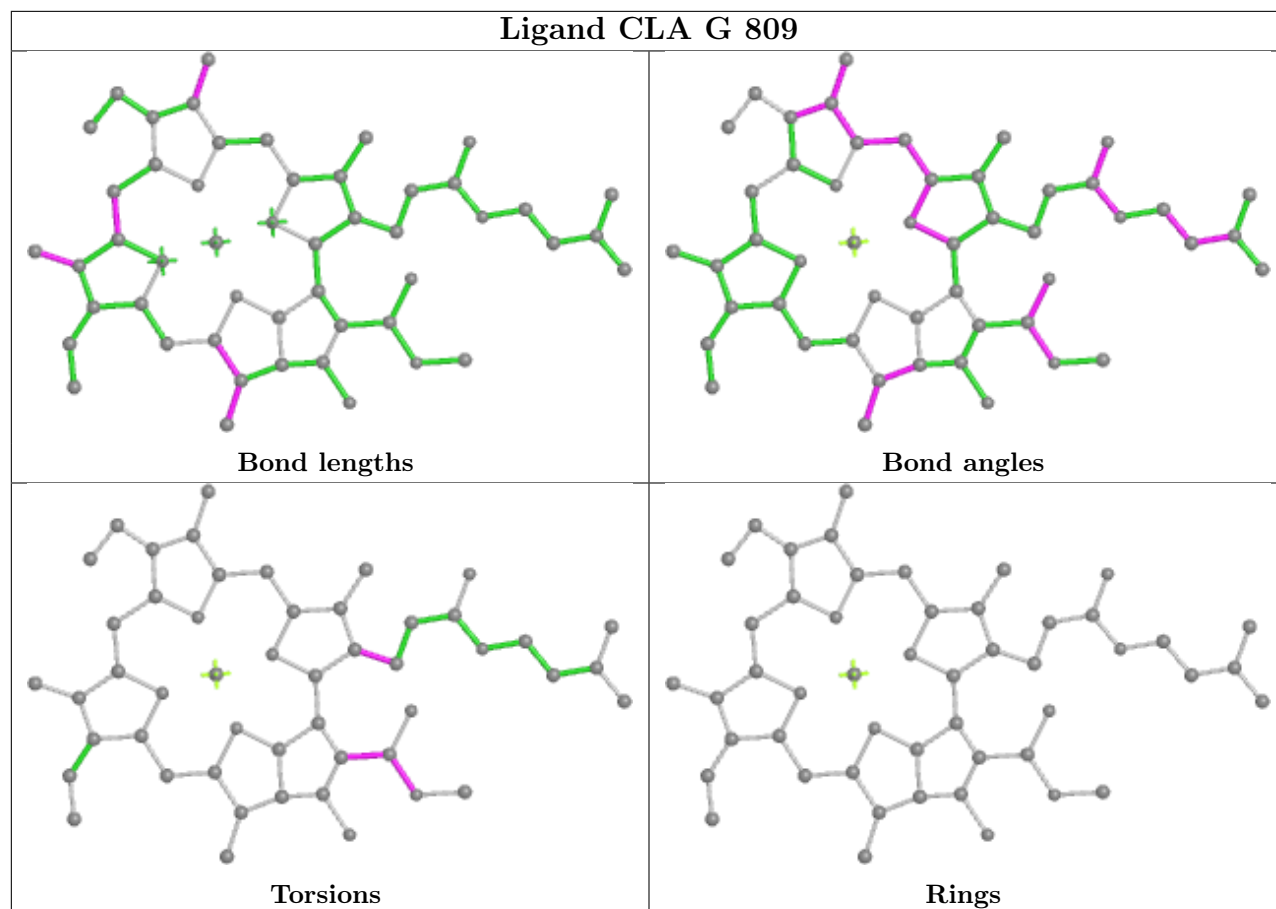


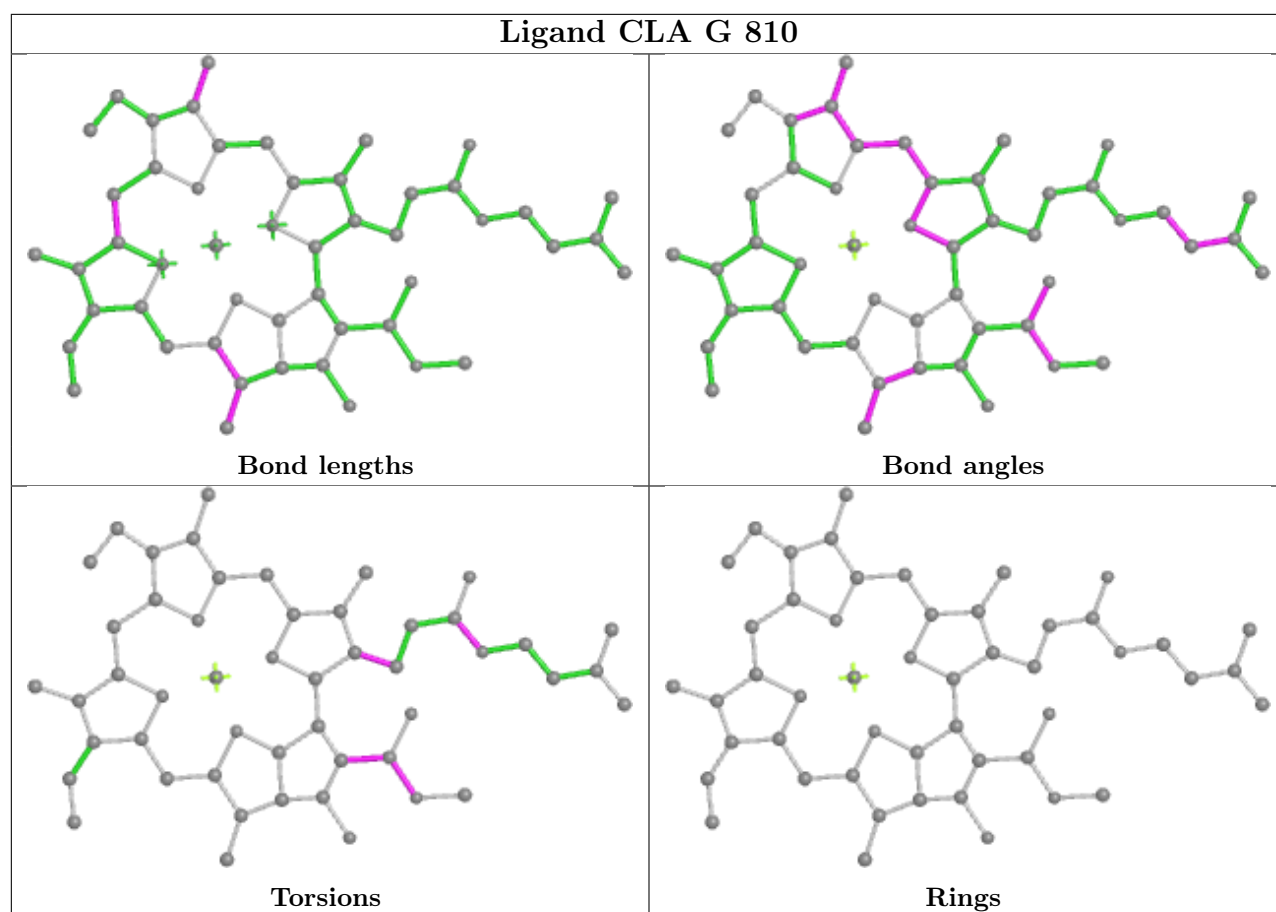


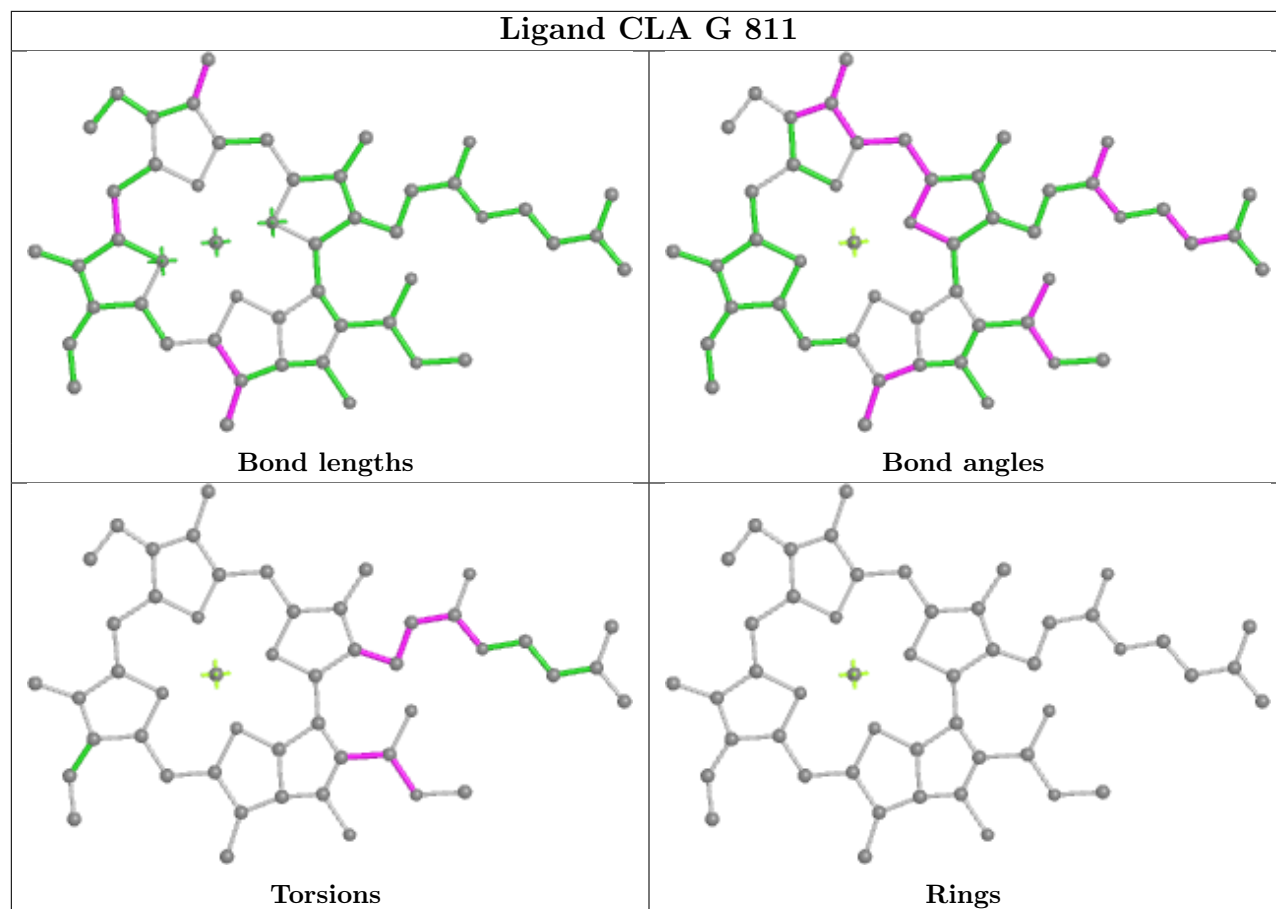




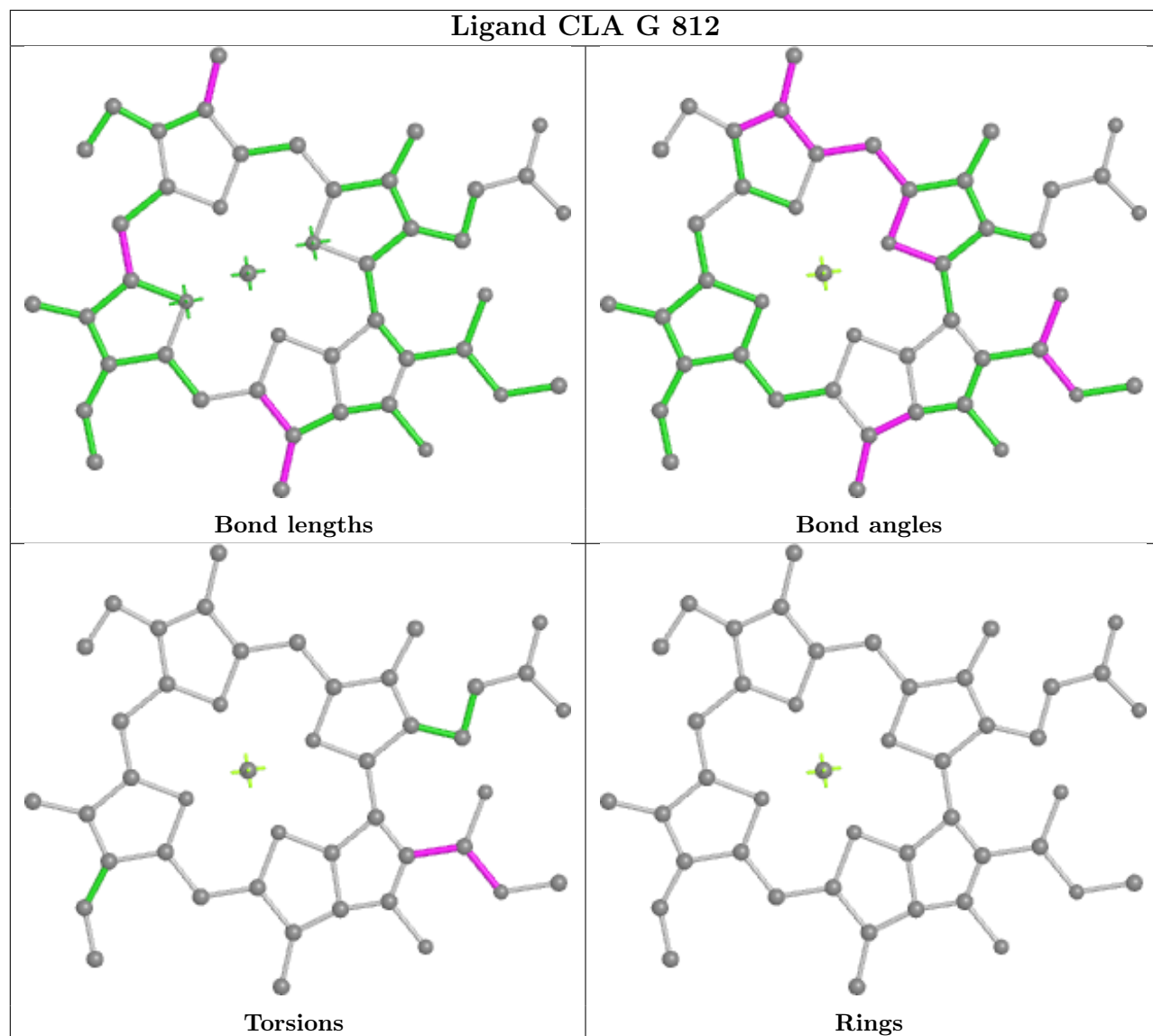




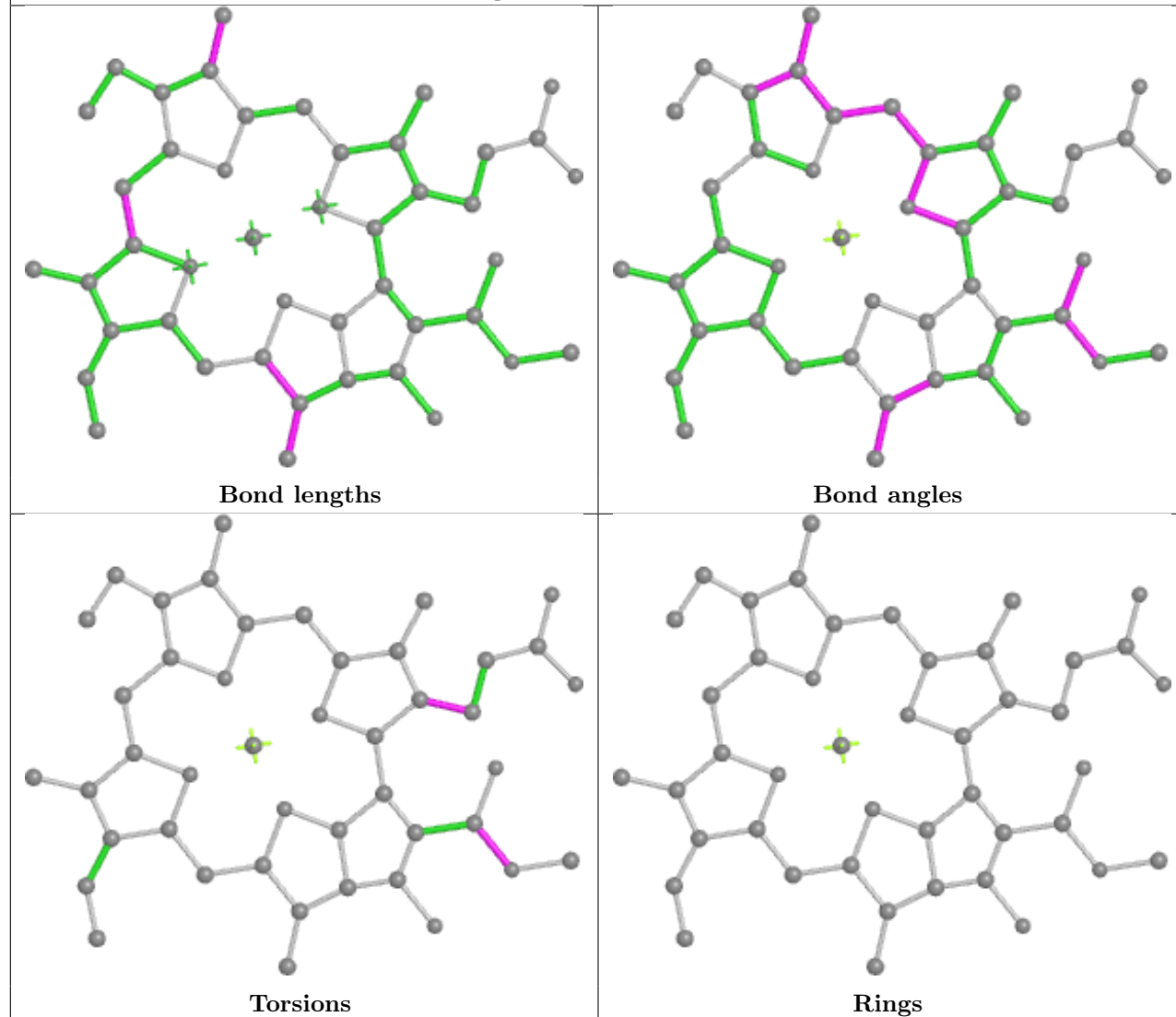


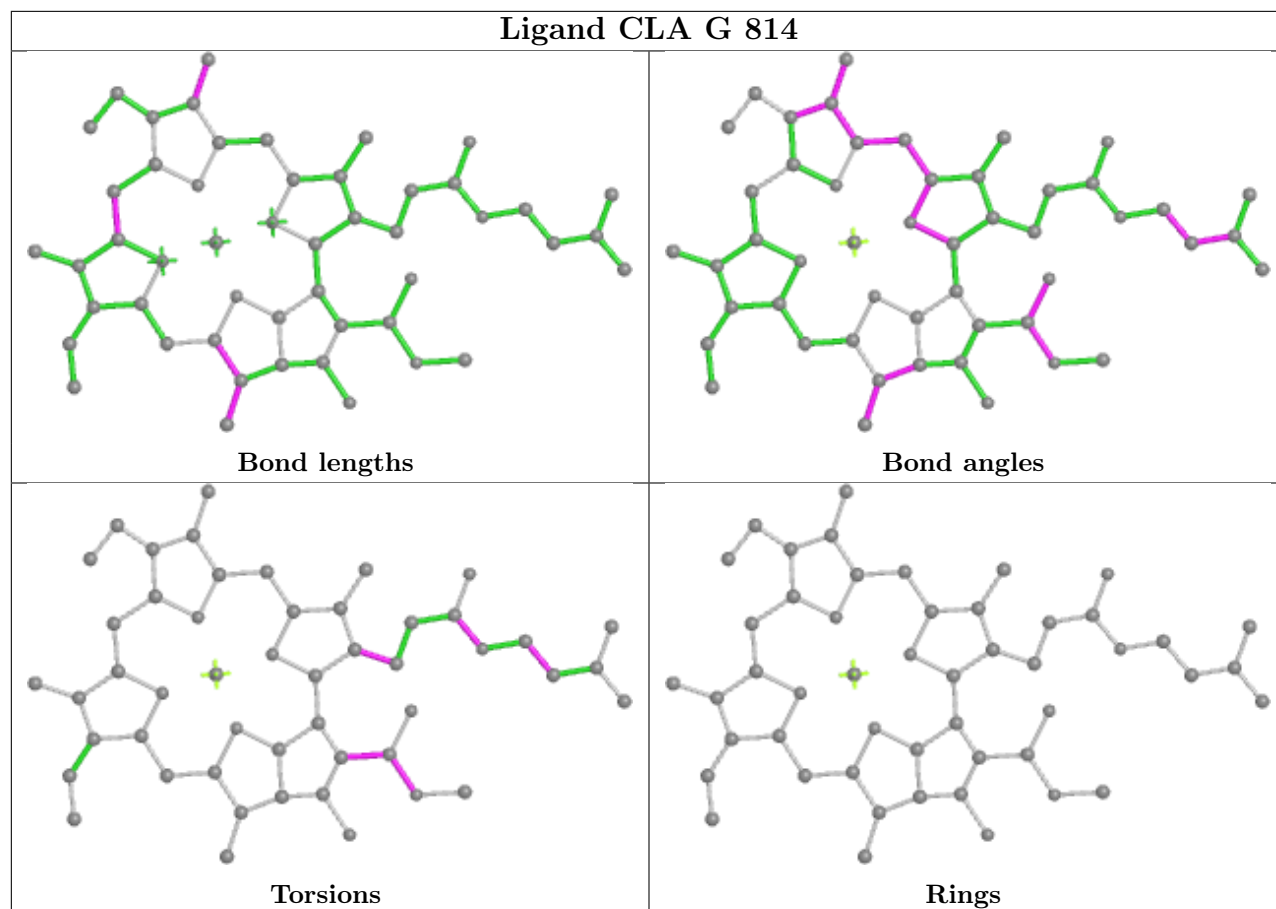


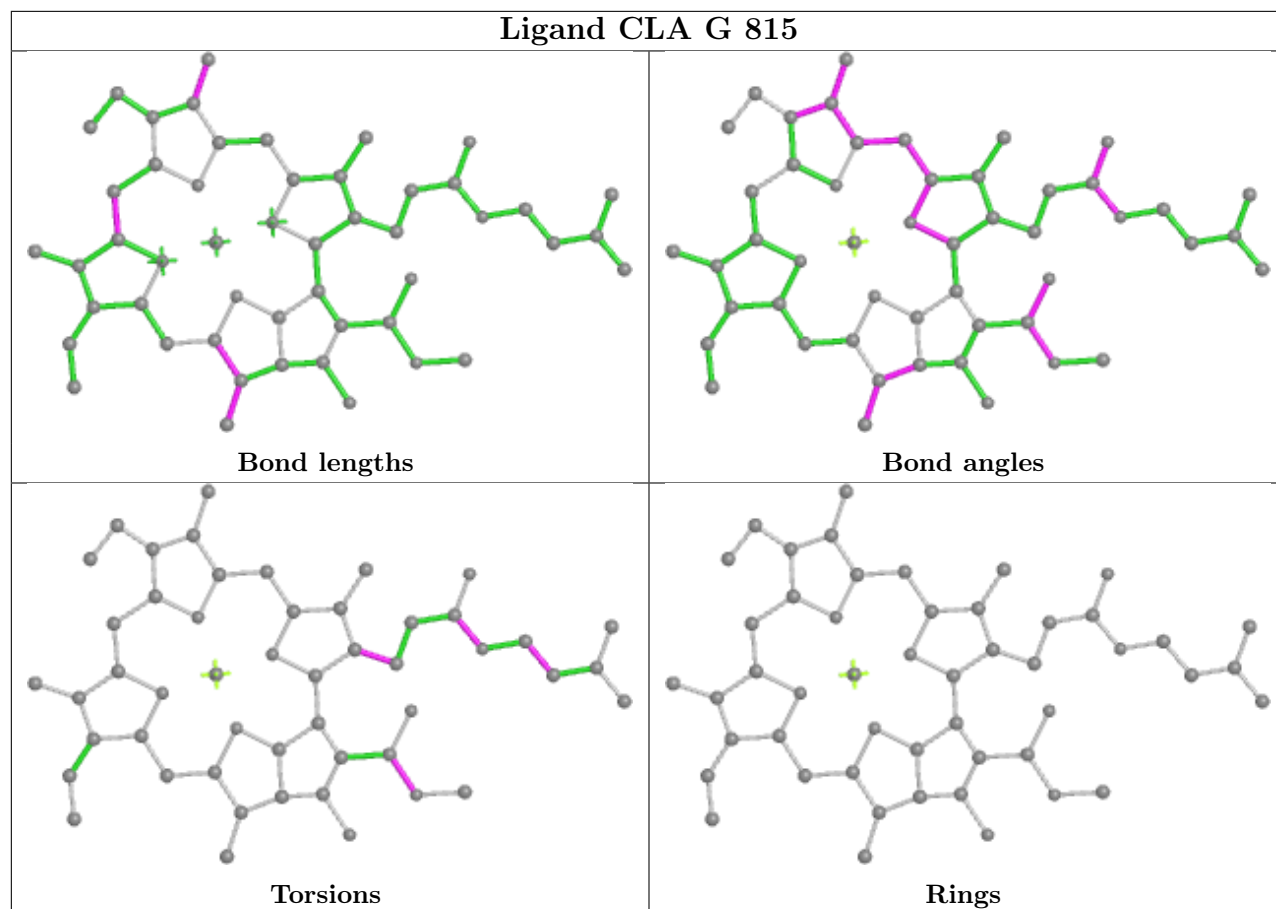
Ligand CLA G 812



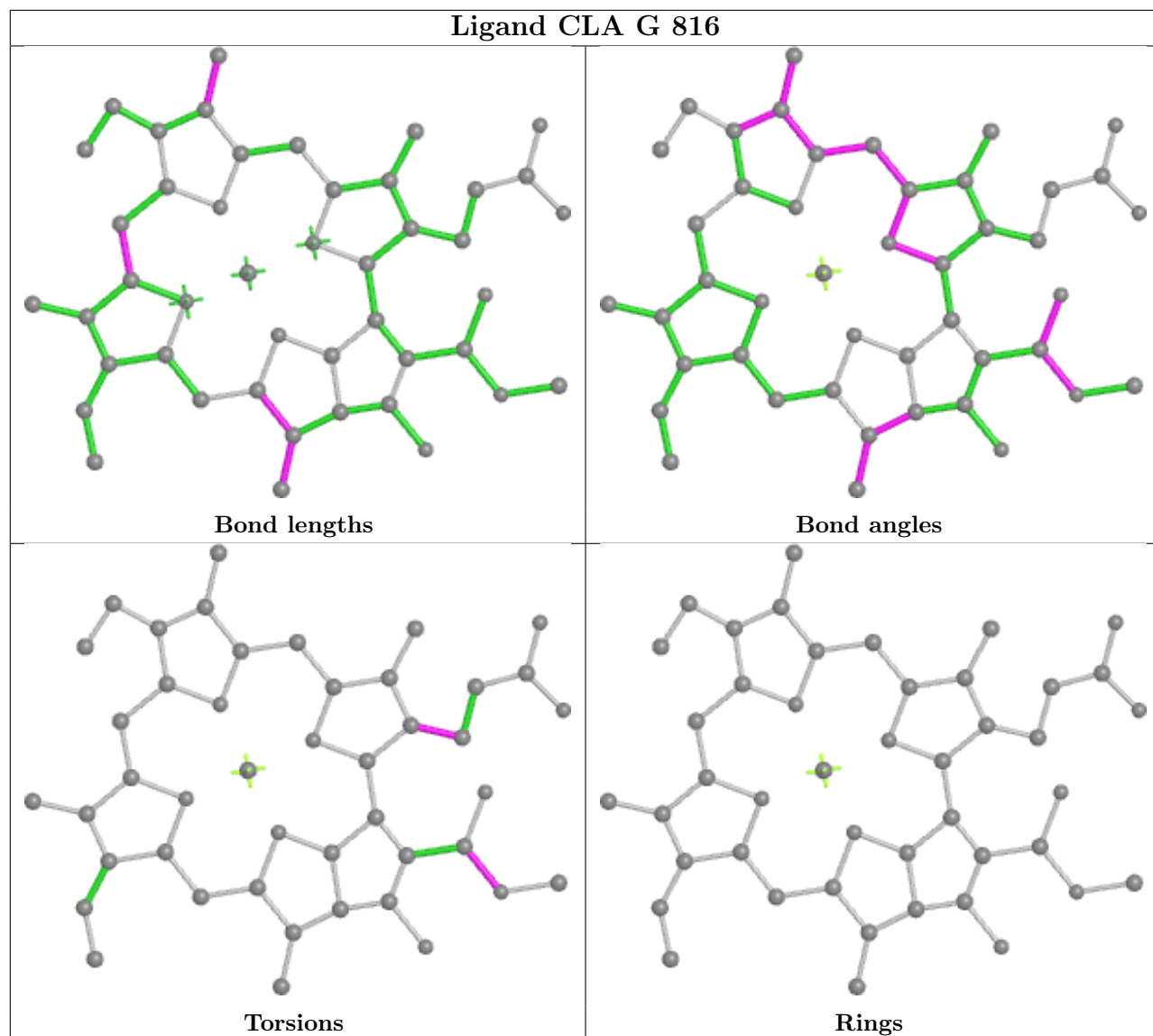
Ligand CLA G 813

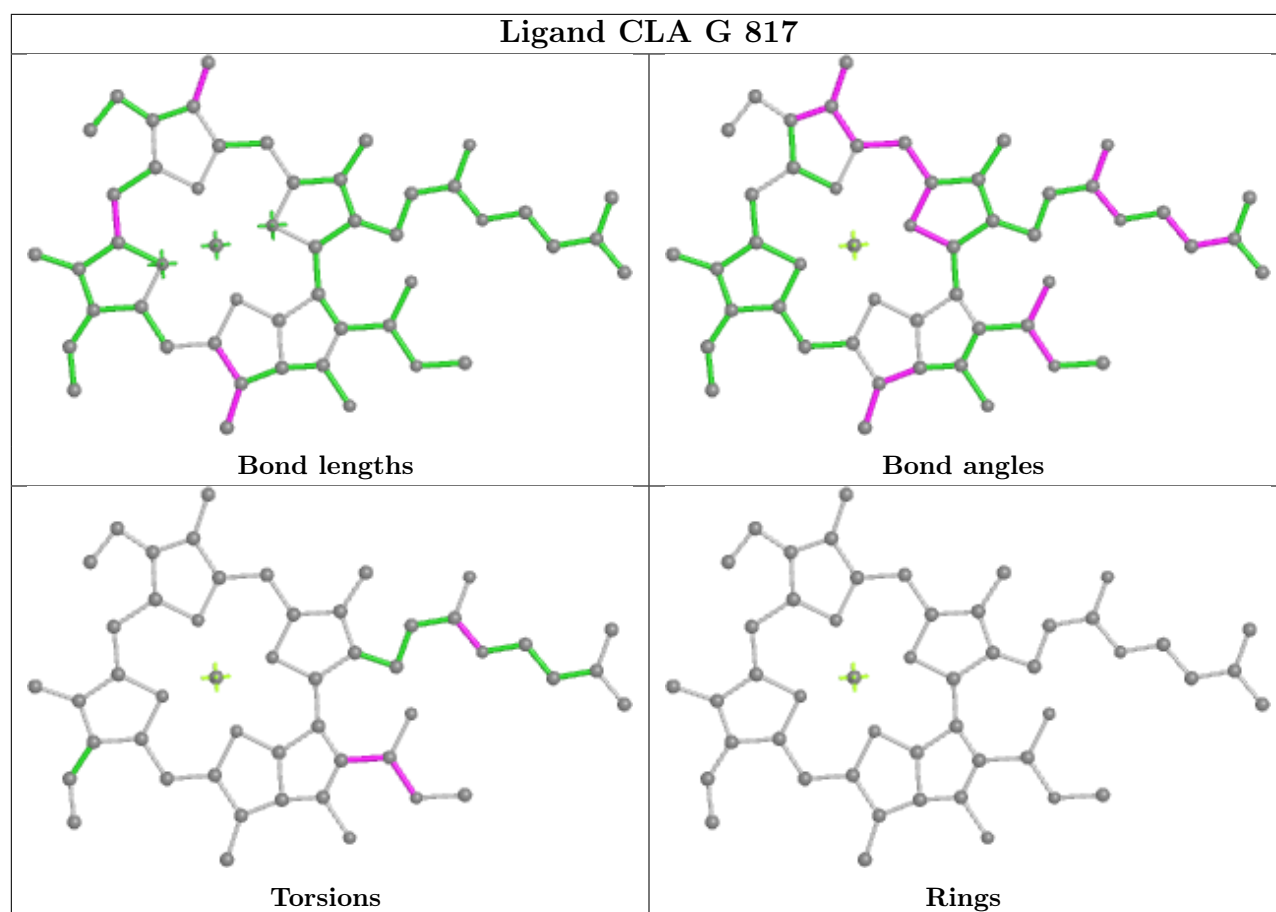


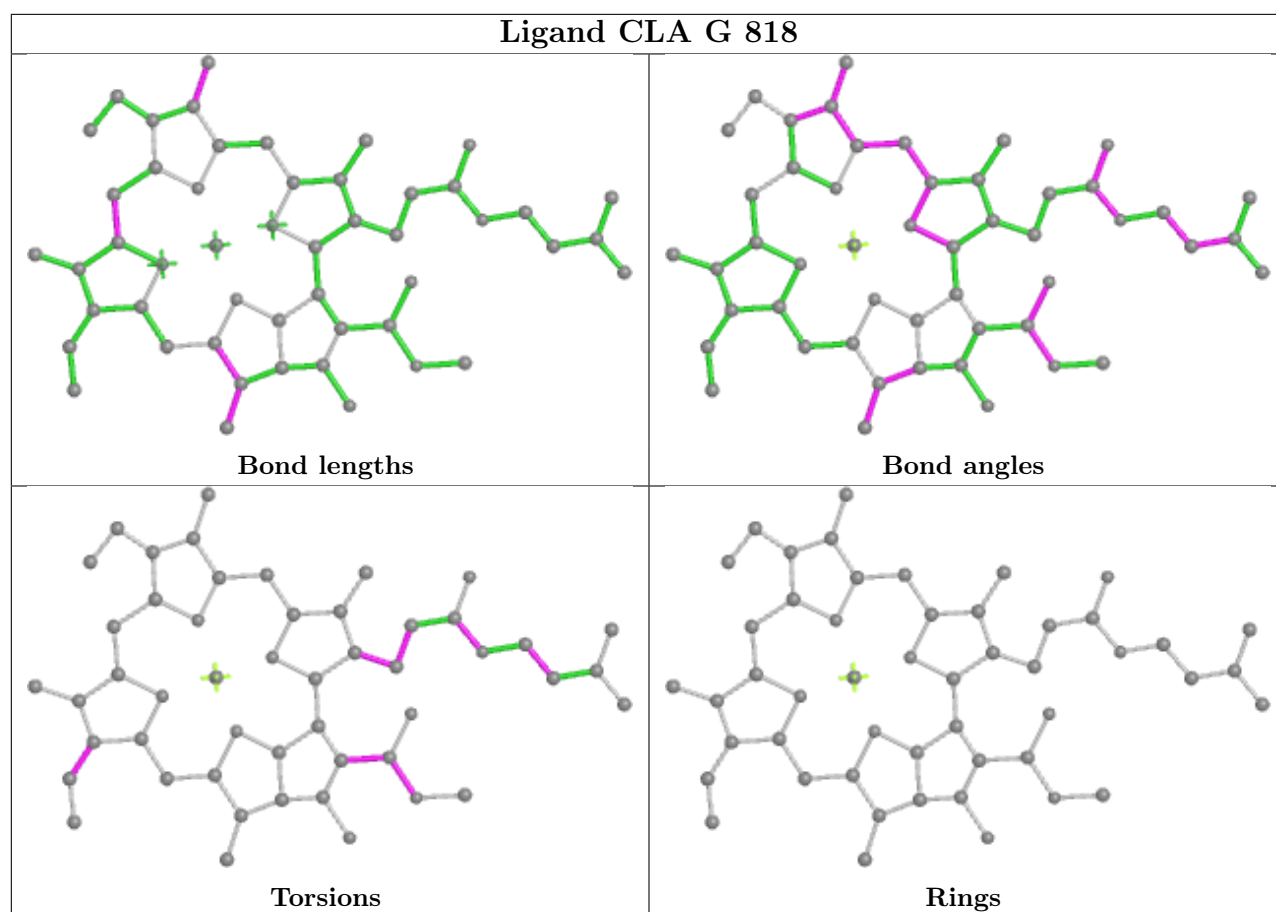


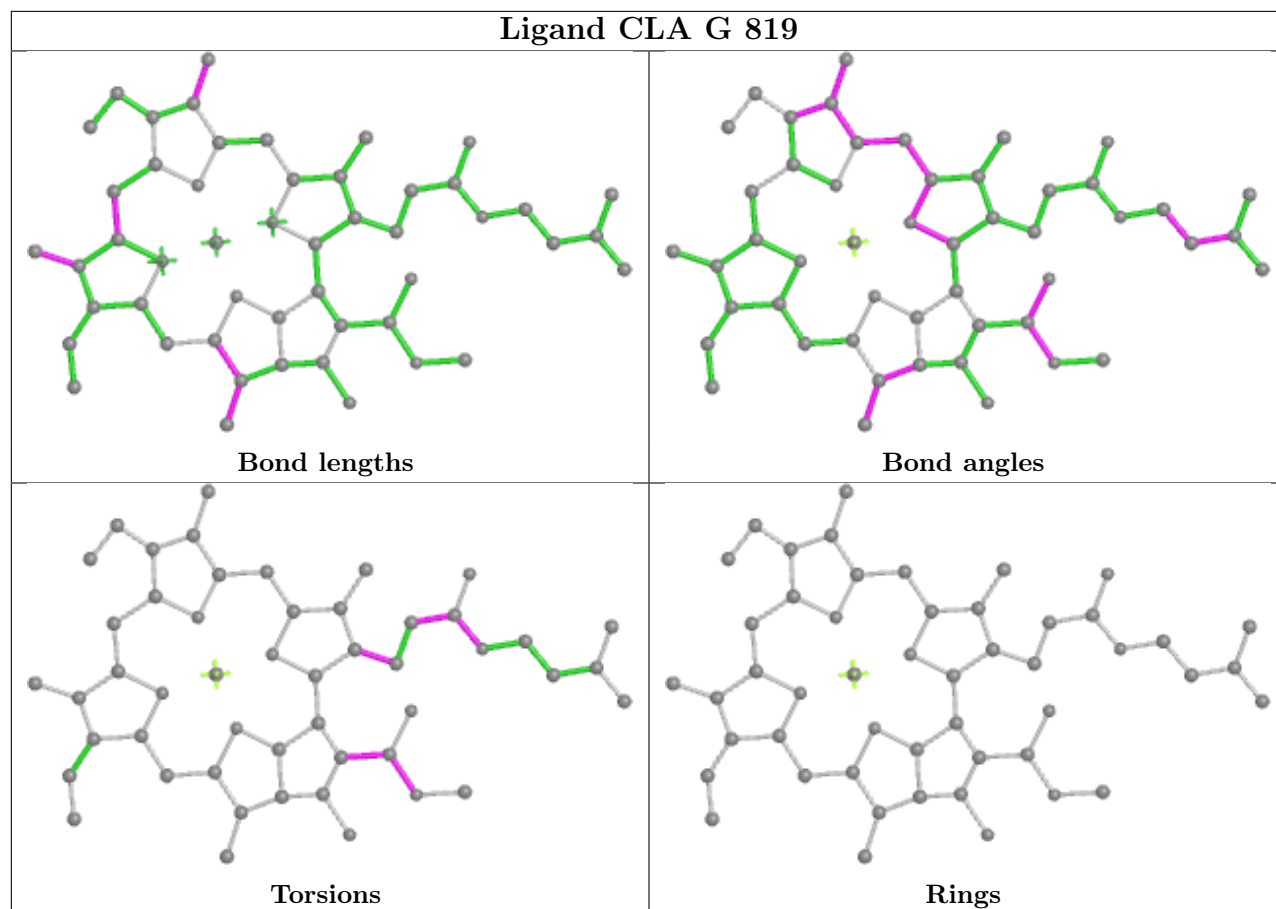


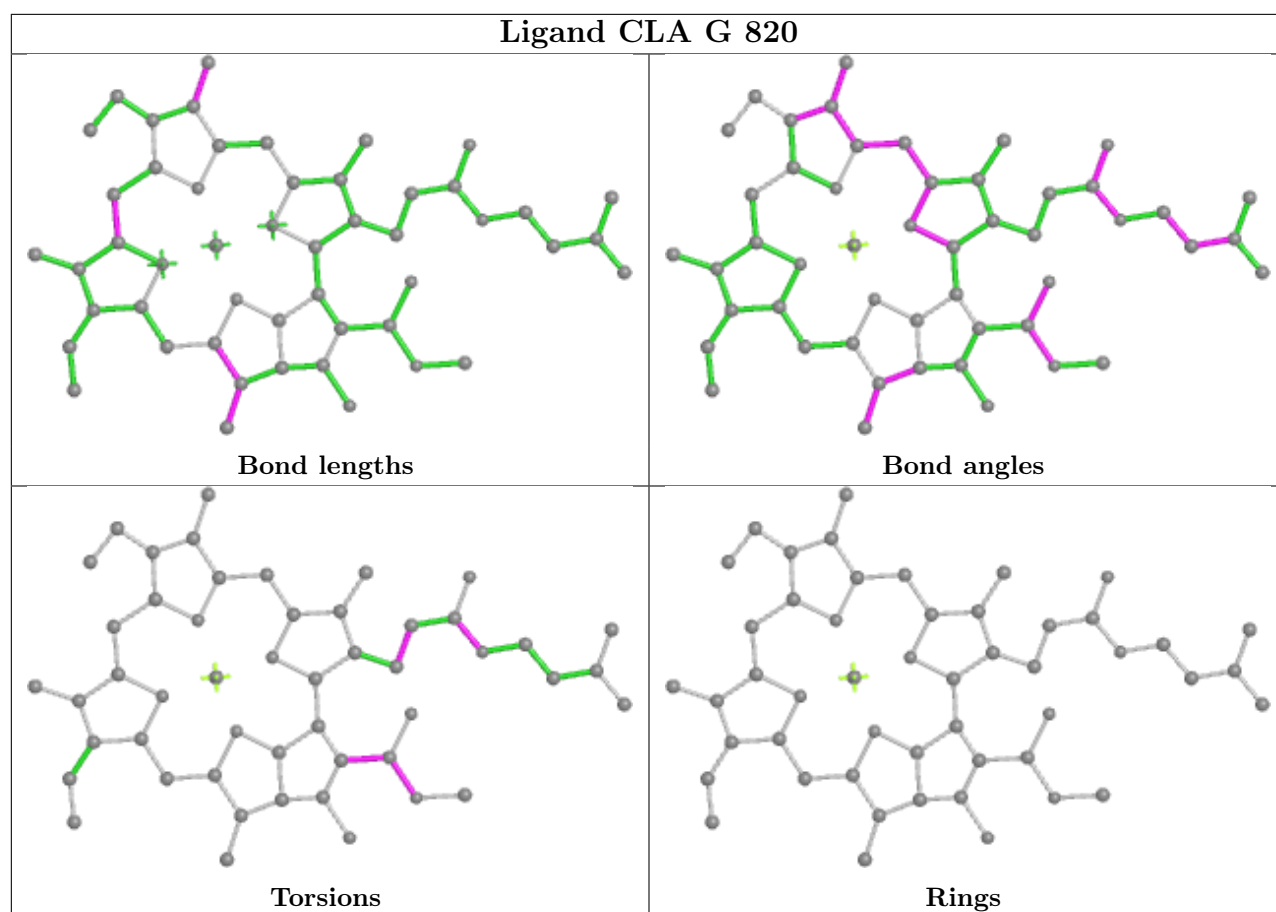
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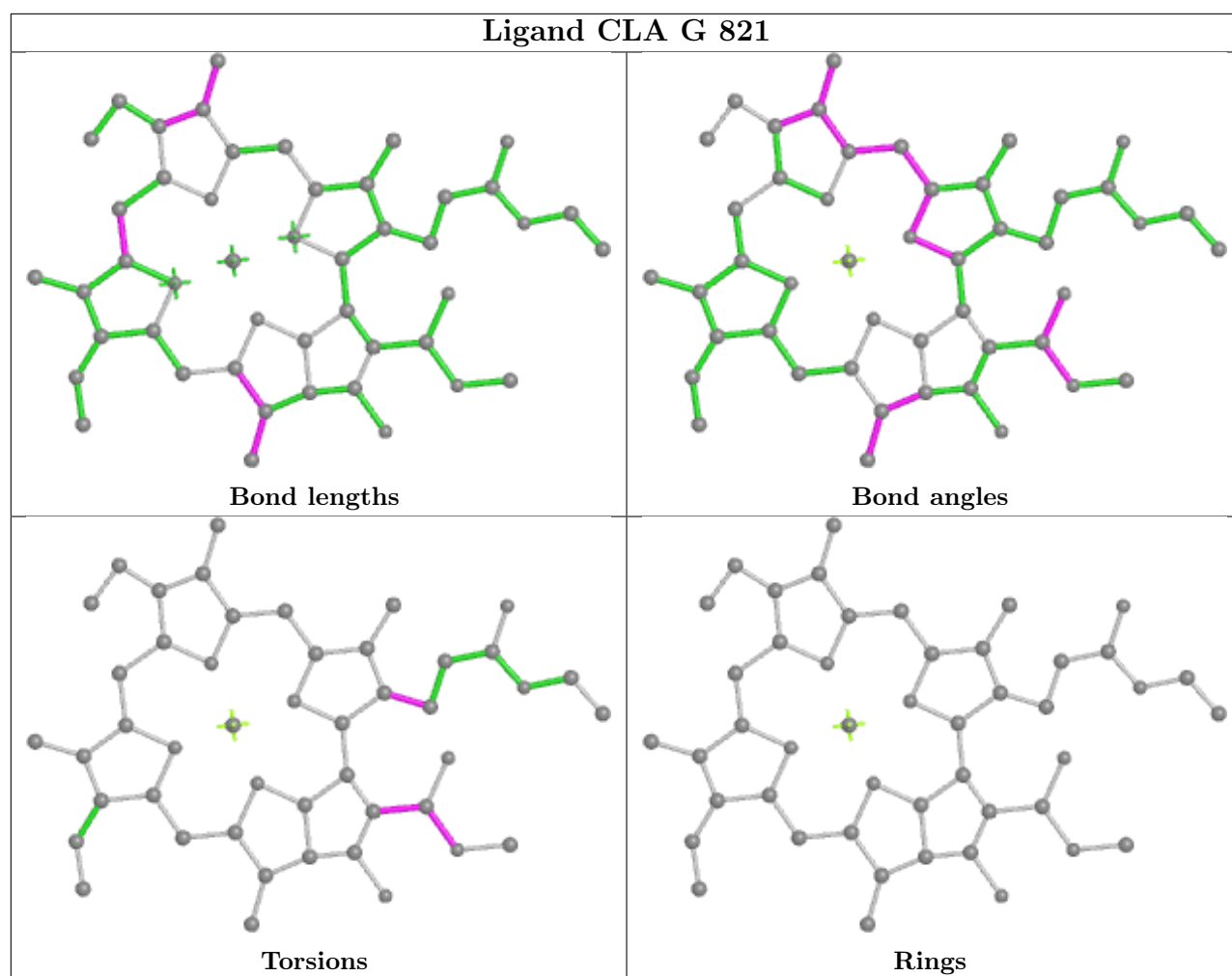




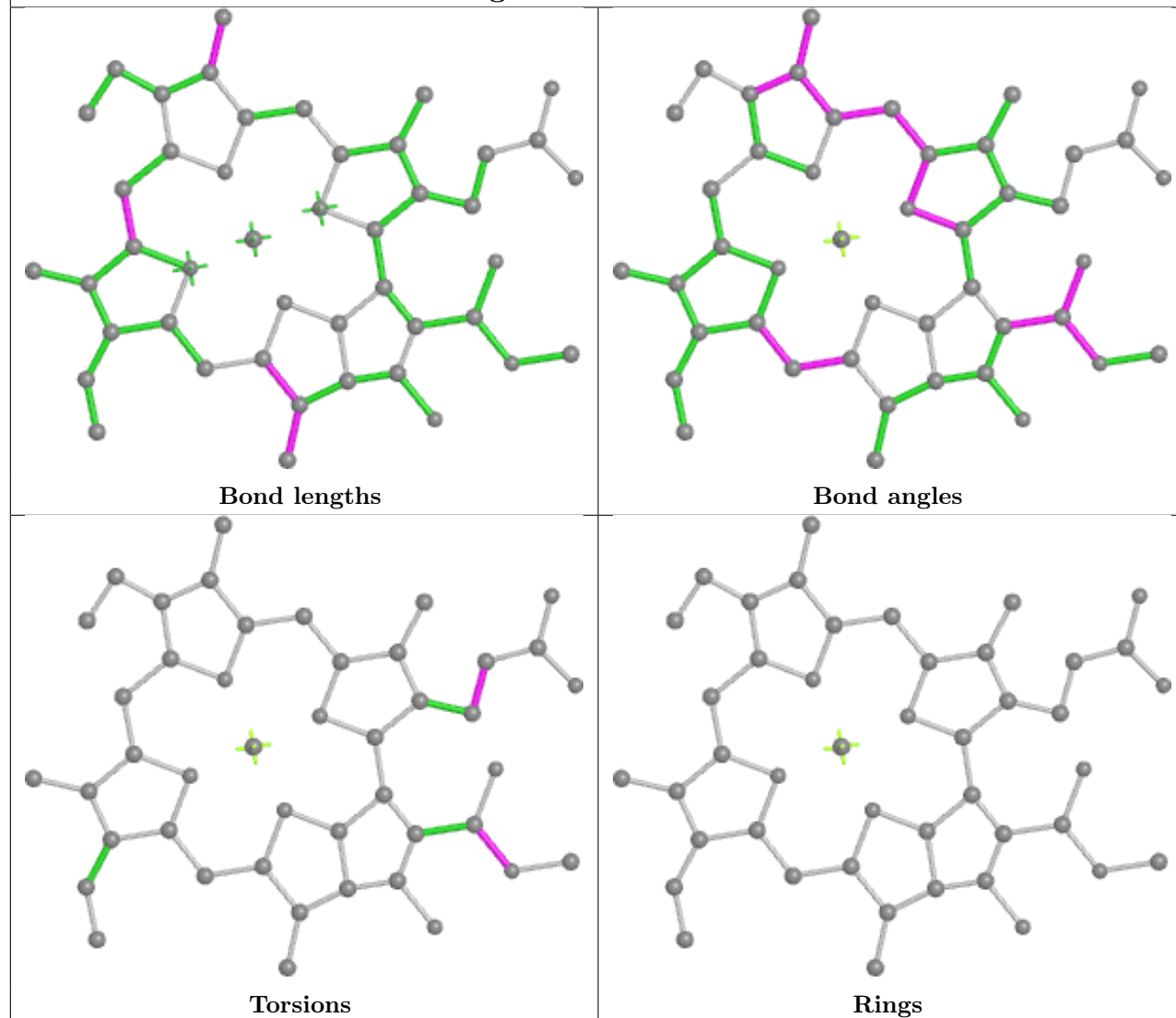


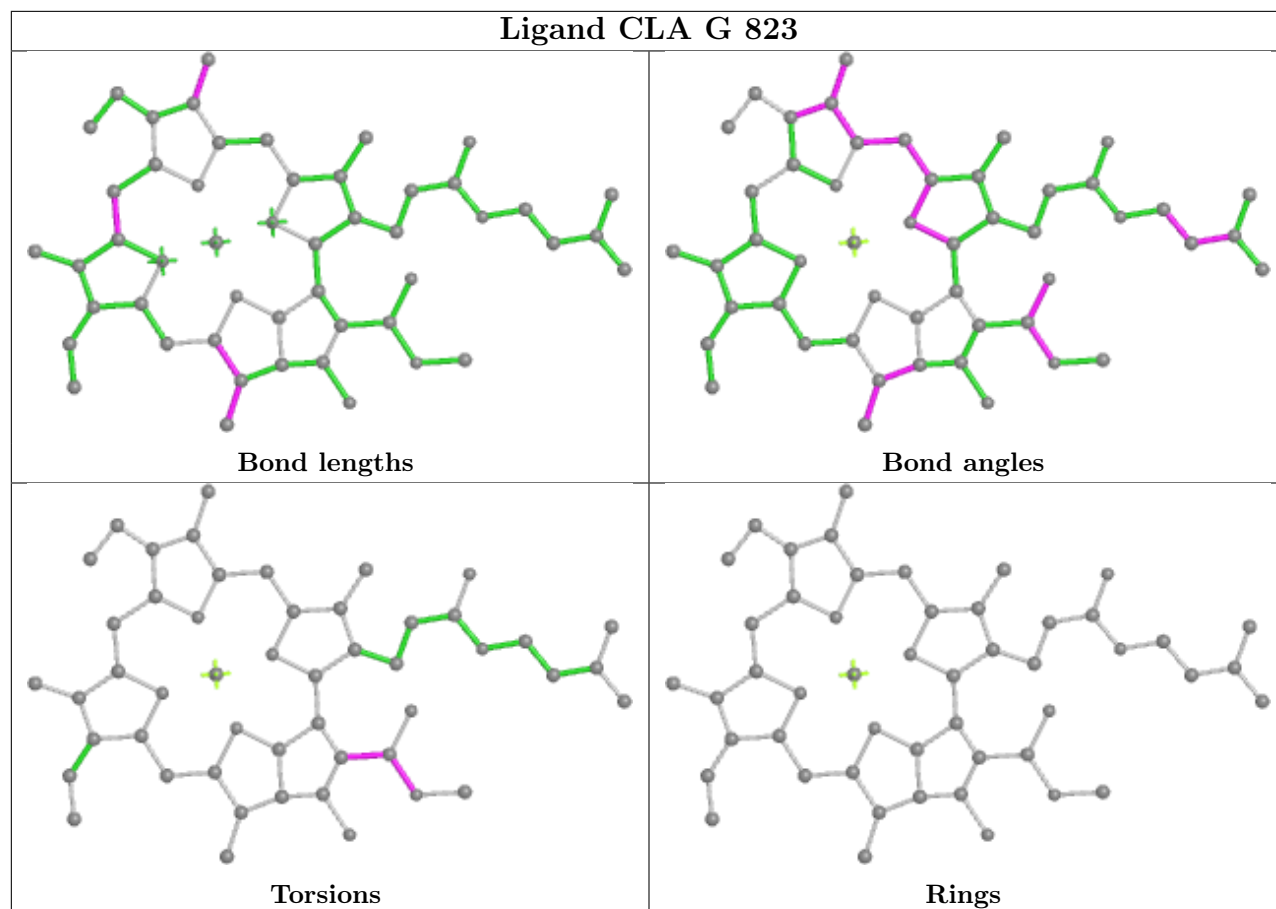




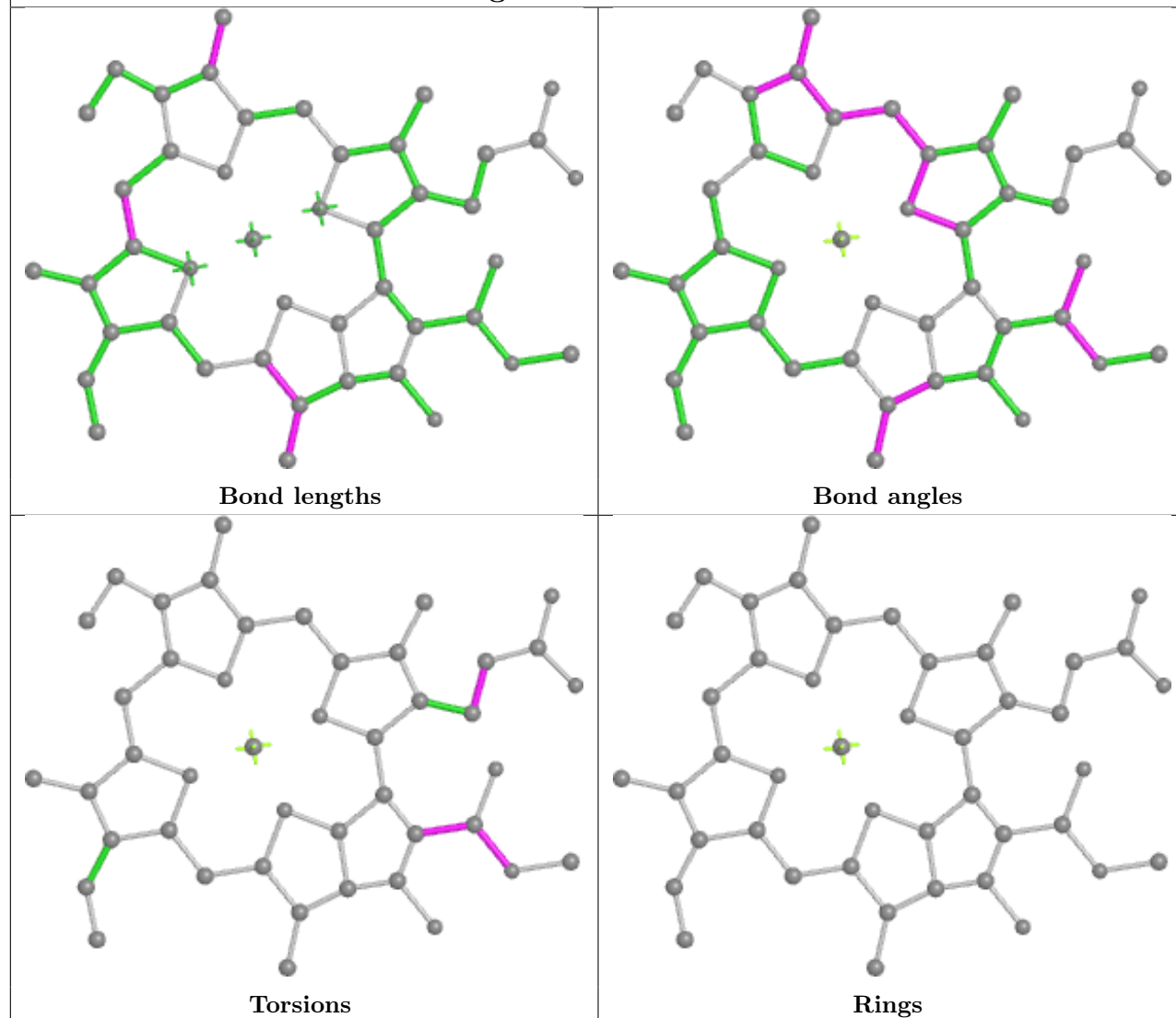


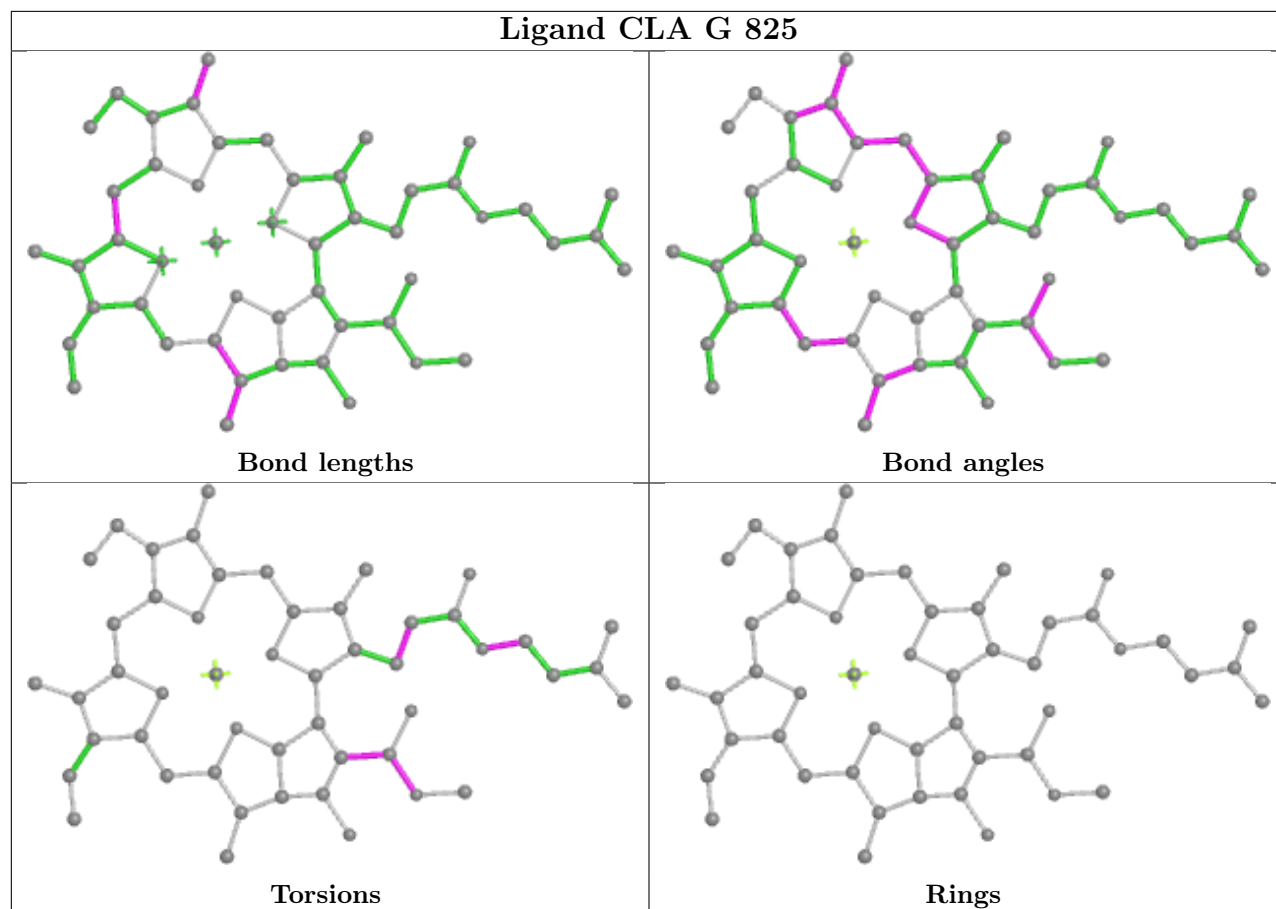
Ligand CLA G 822



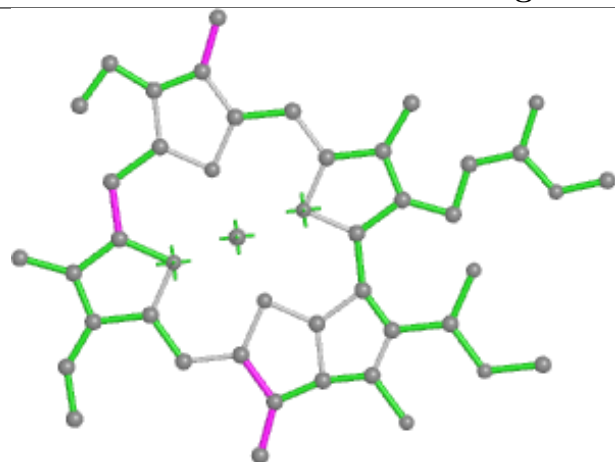


Ligand CLA G 824

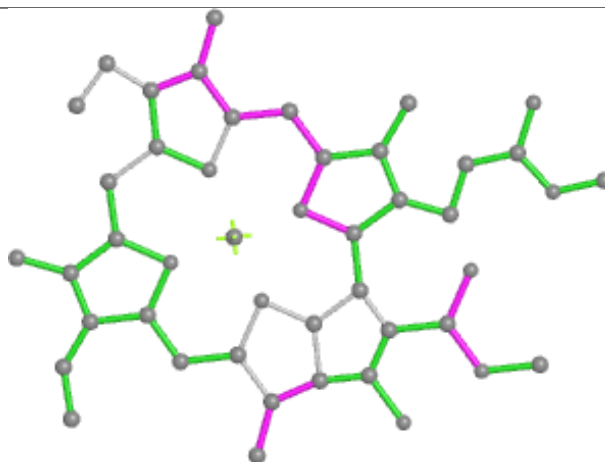




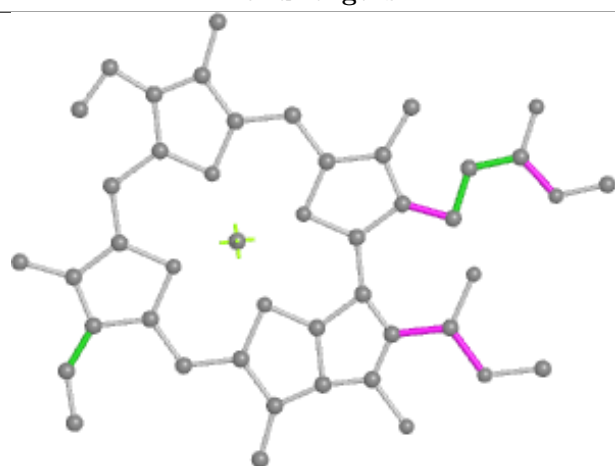
Ligand CLA G 826



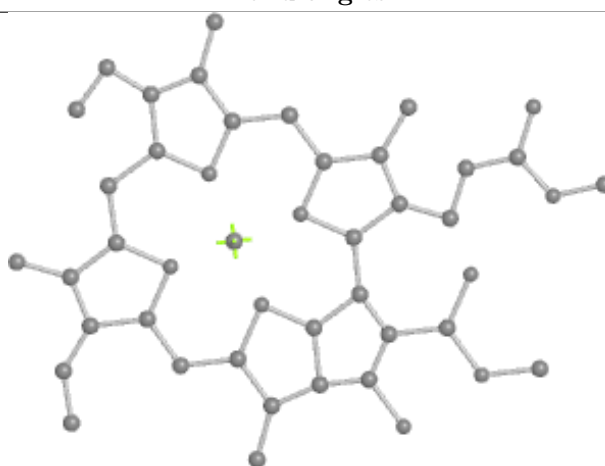
Bond lengths



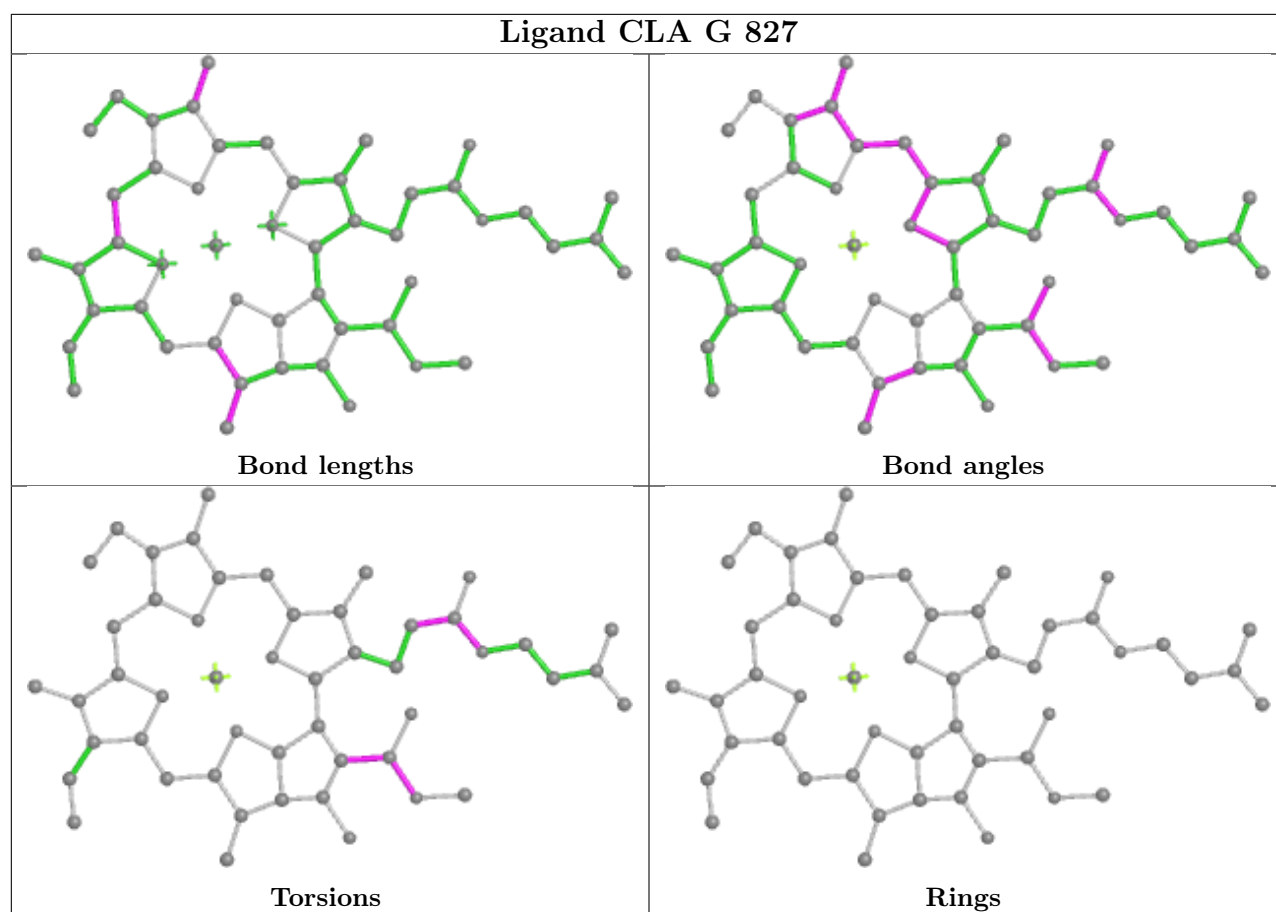
Bond angles

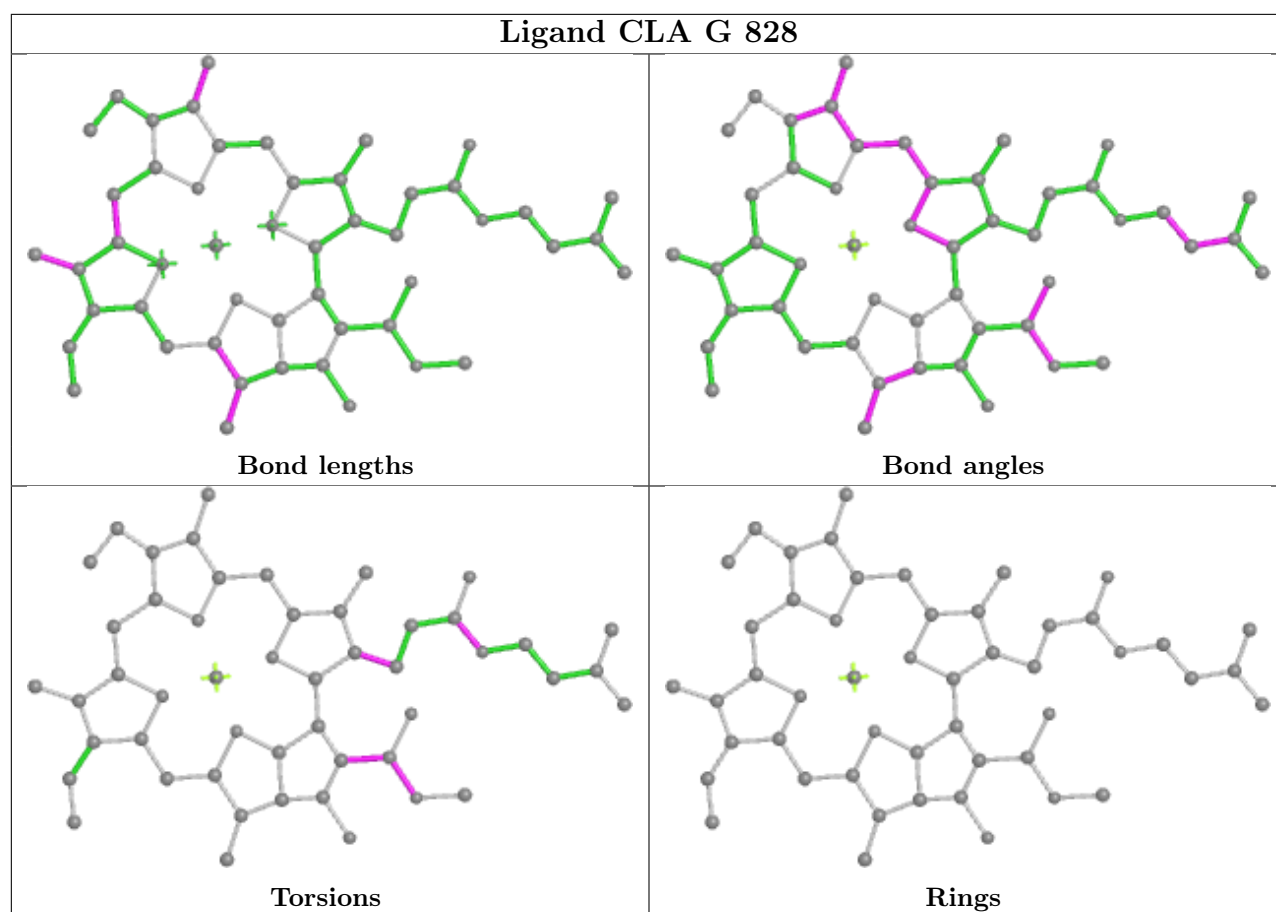


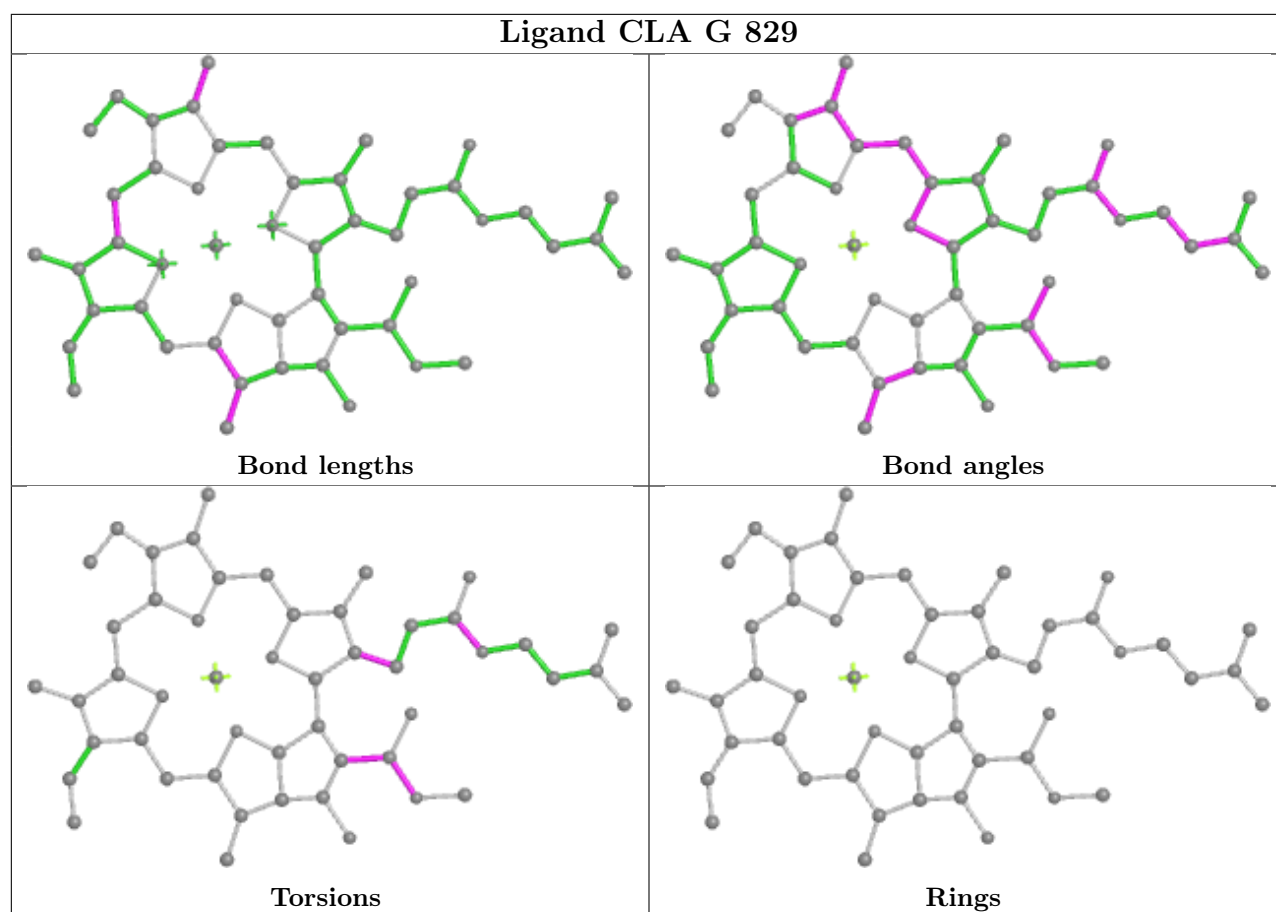
Torsions

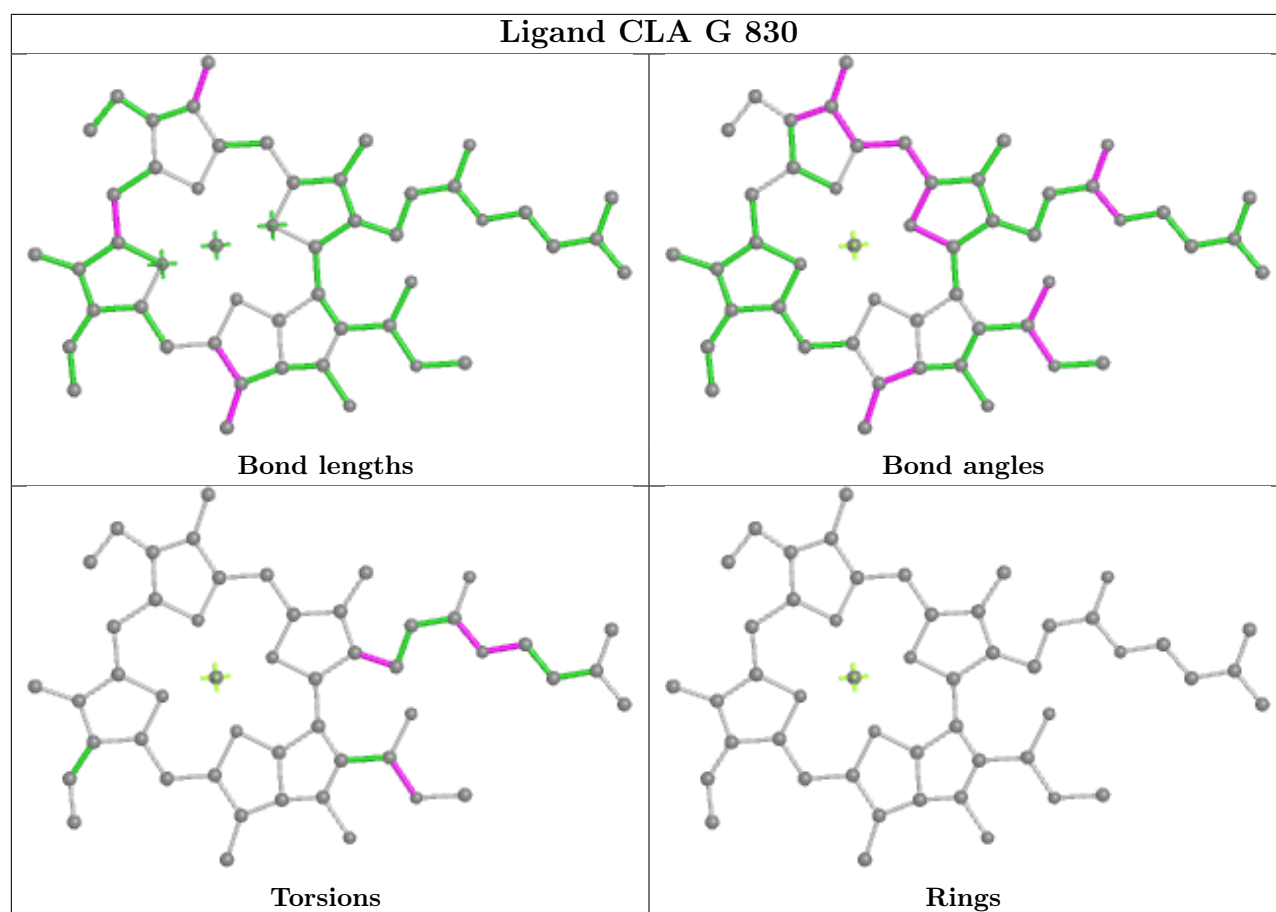


Rings

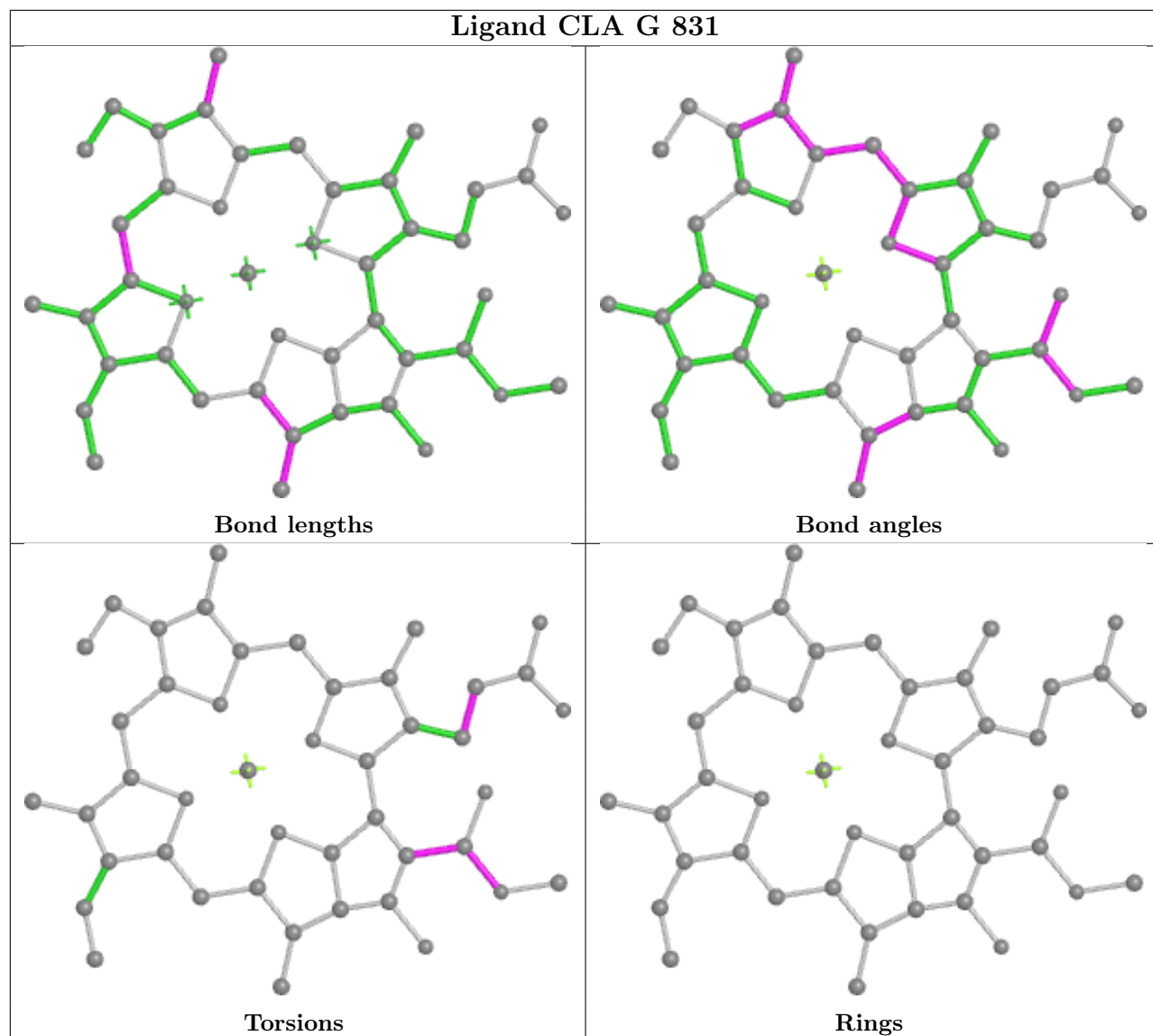


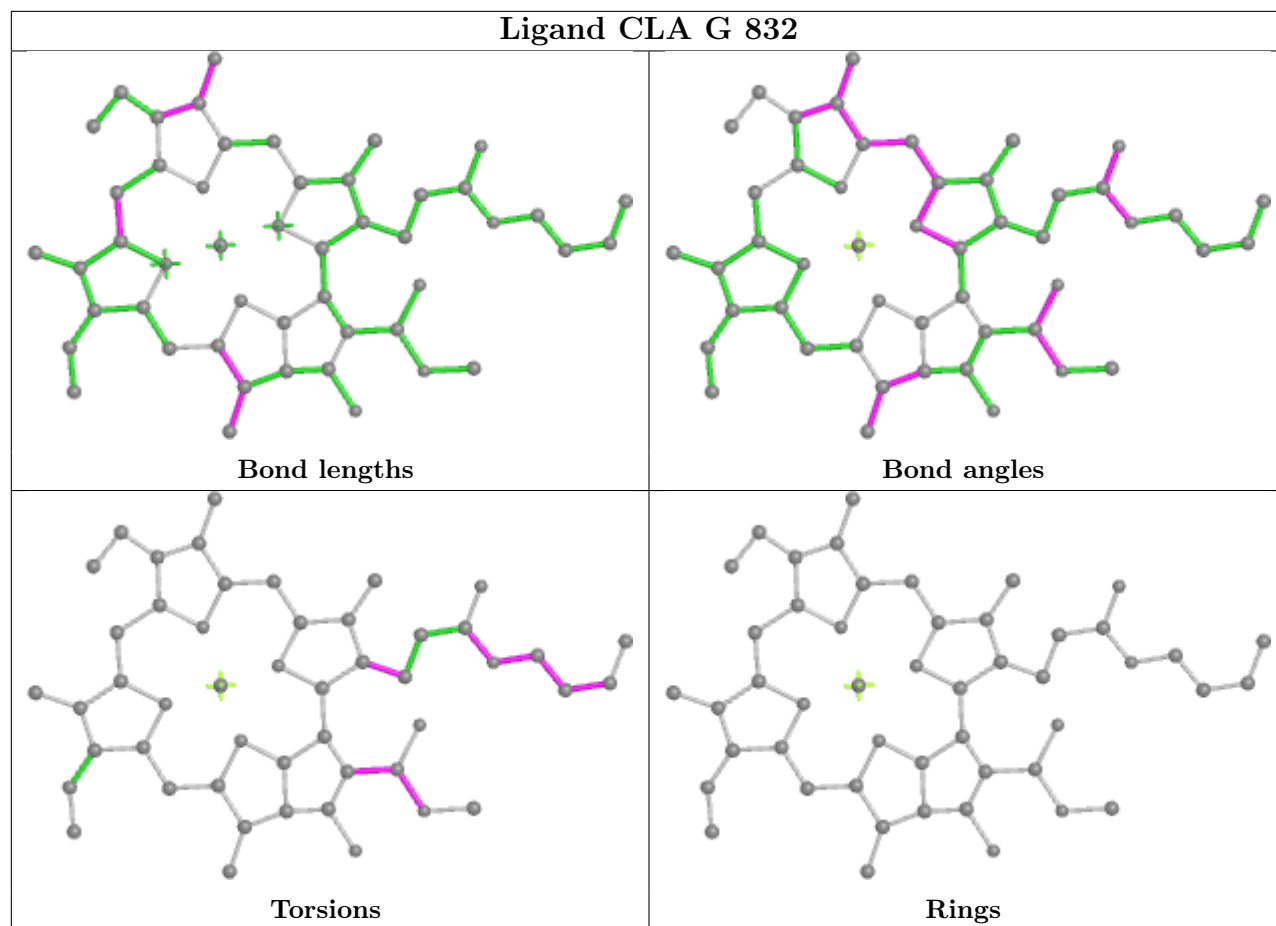


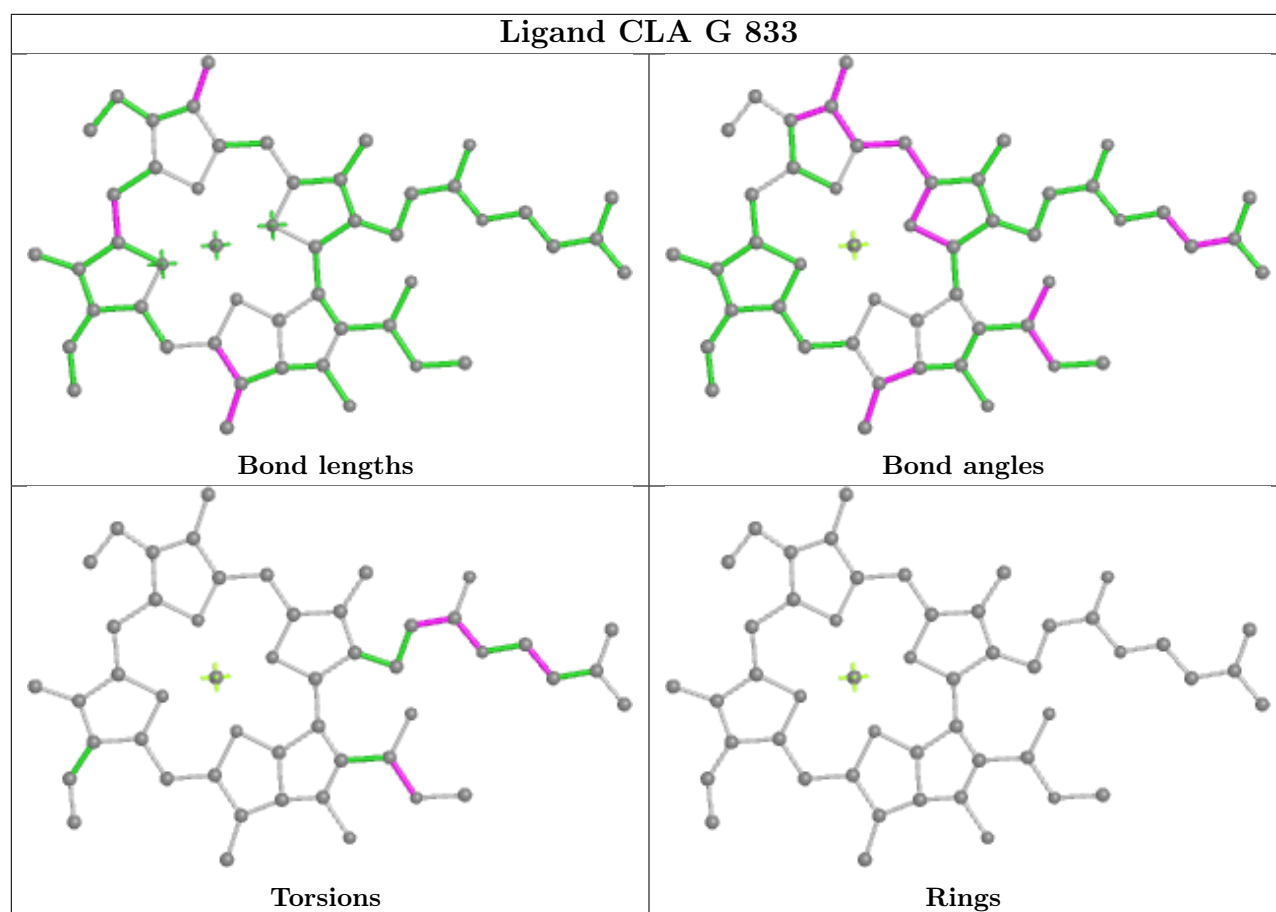


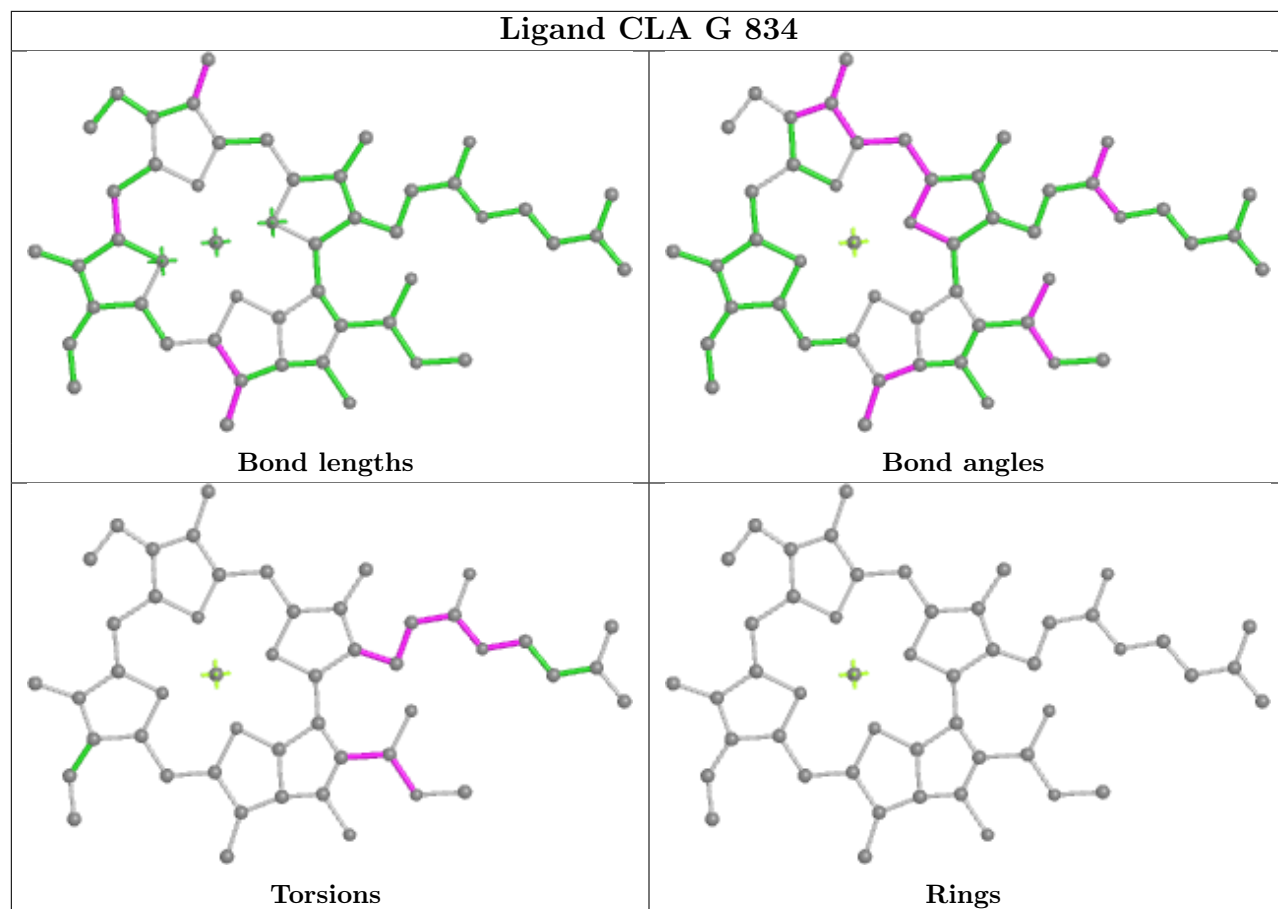


Ligand CLA G 831

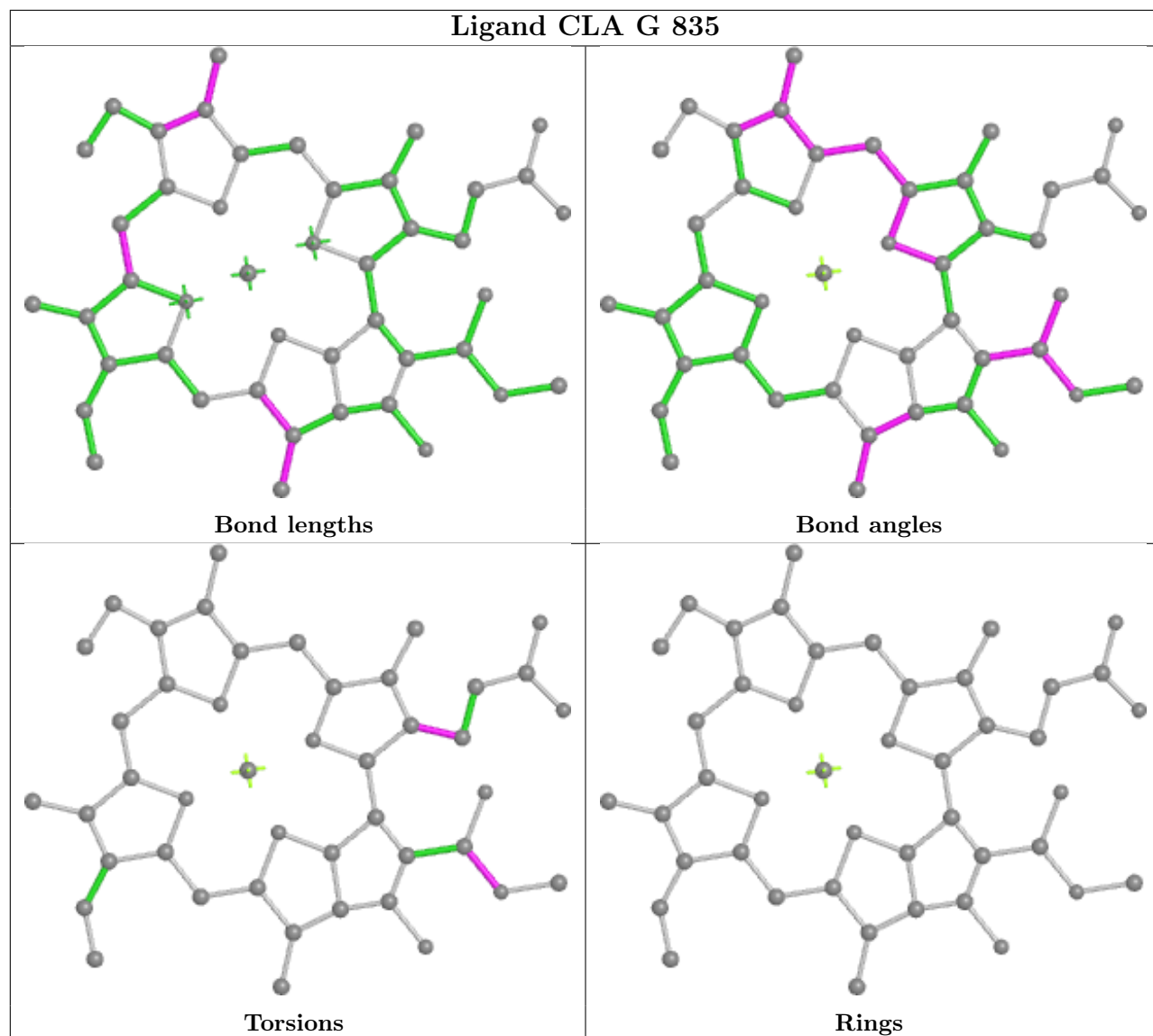




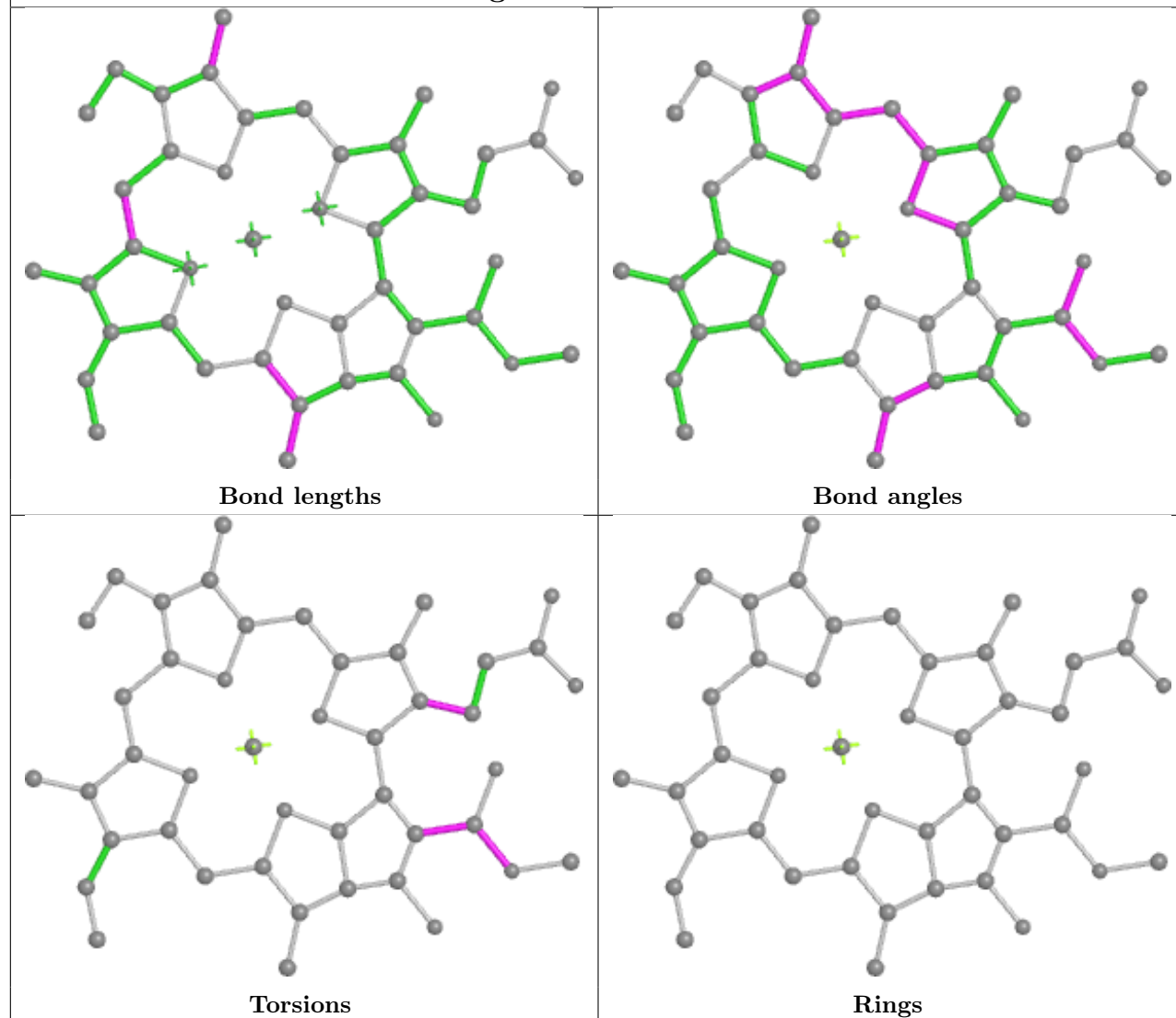


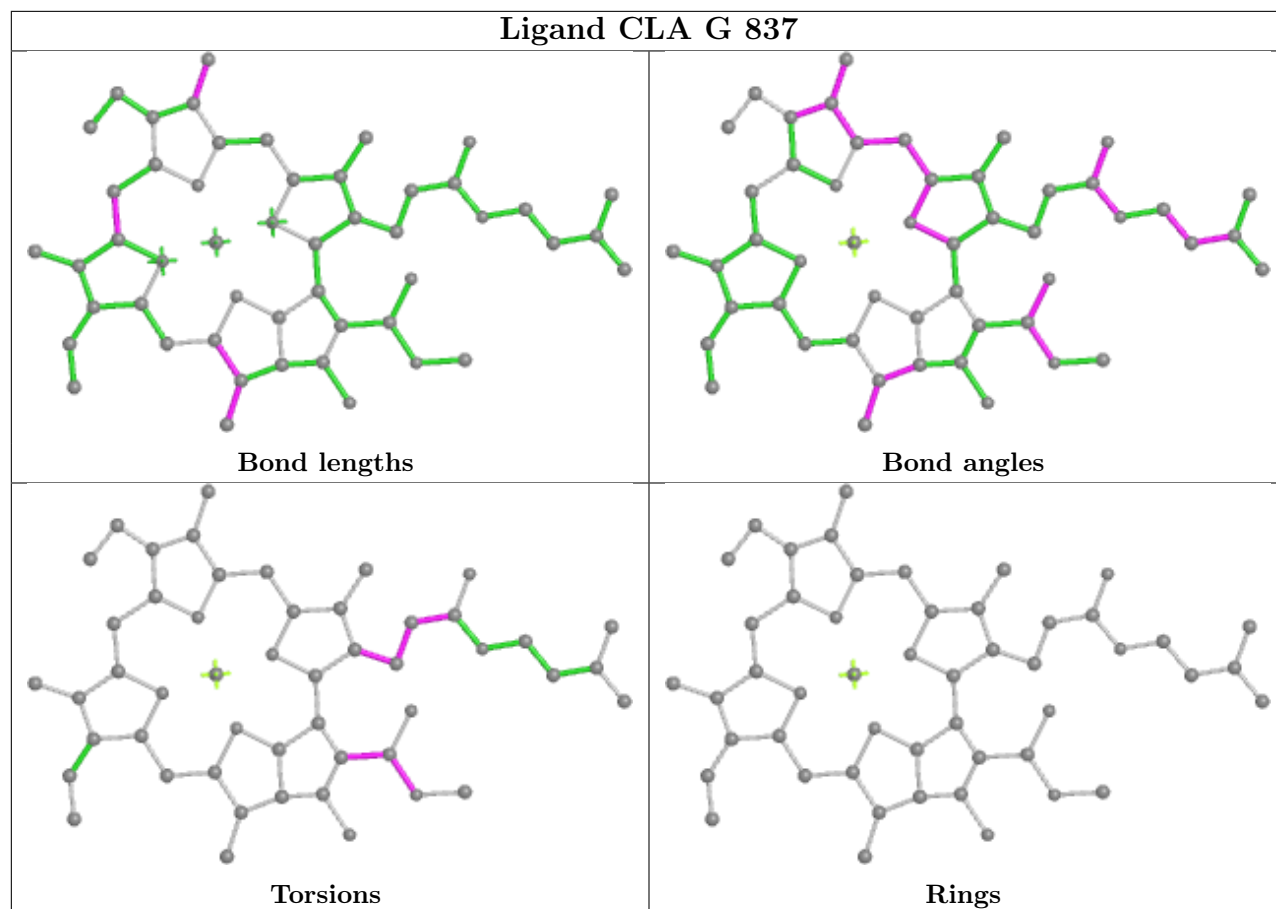


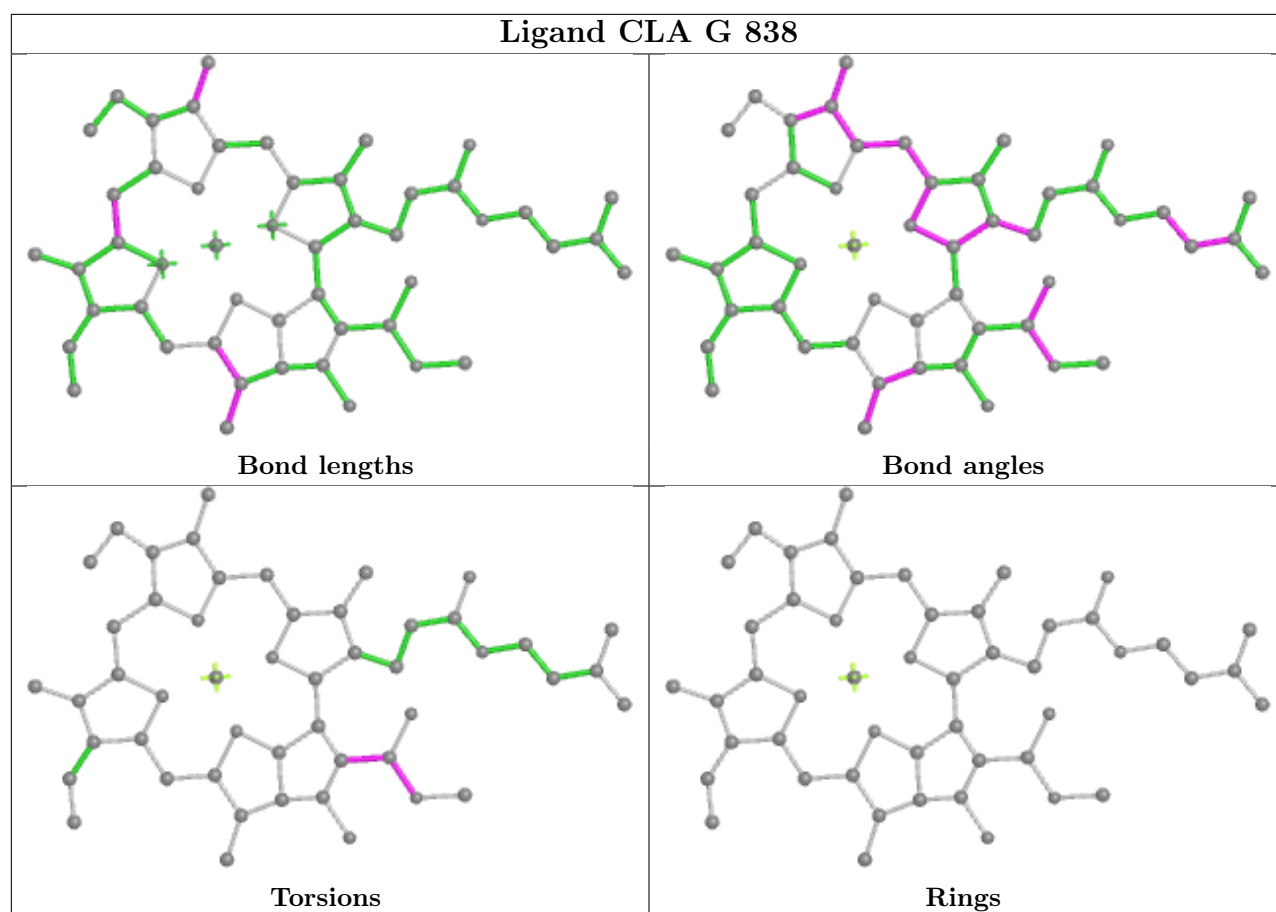
Ligand CLA G 835



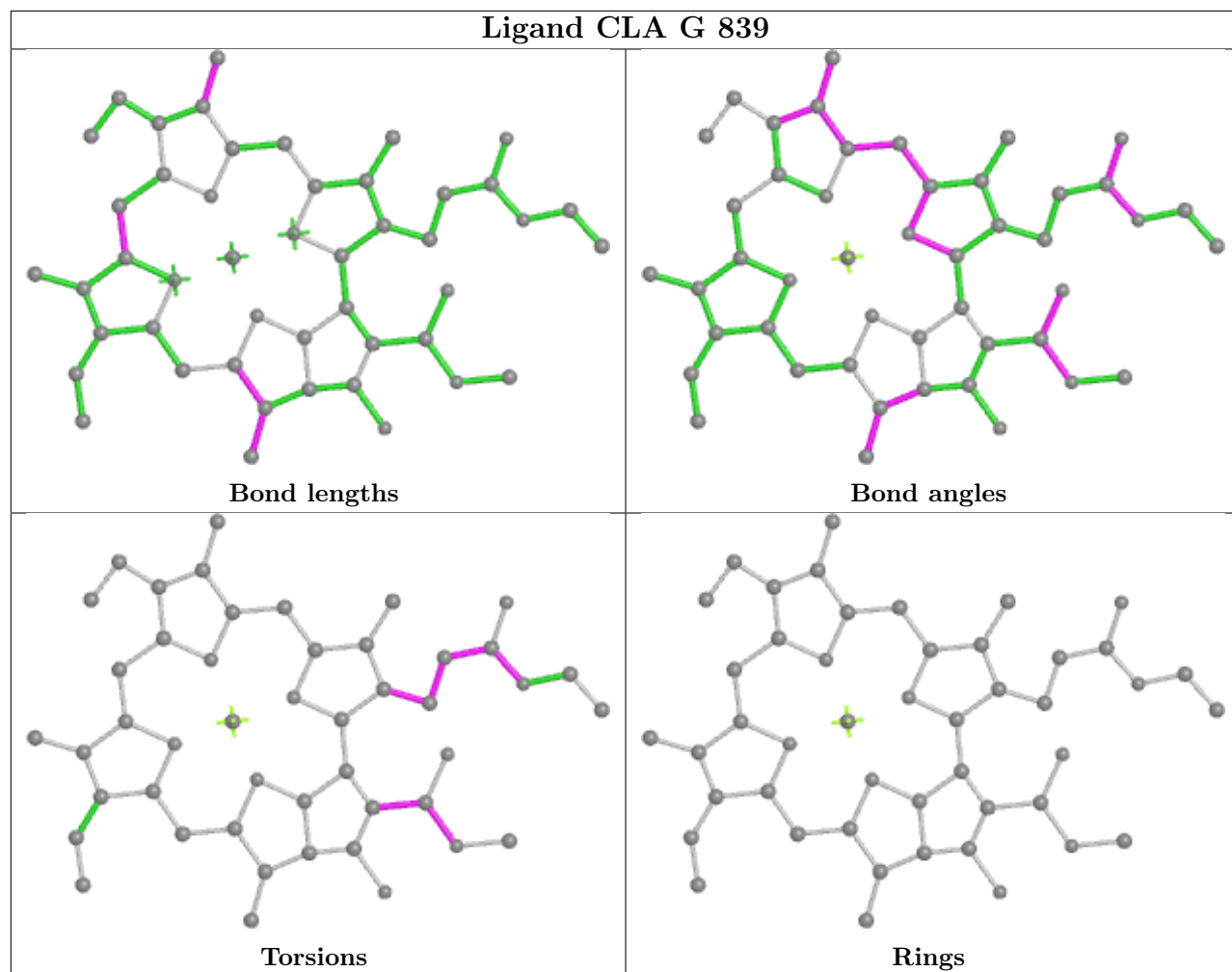
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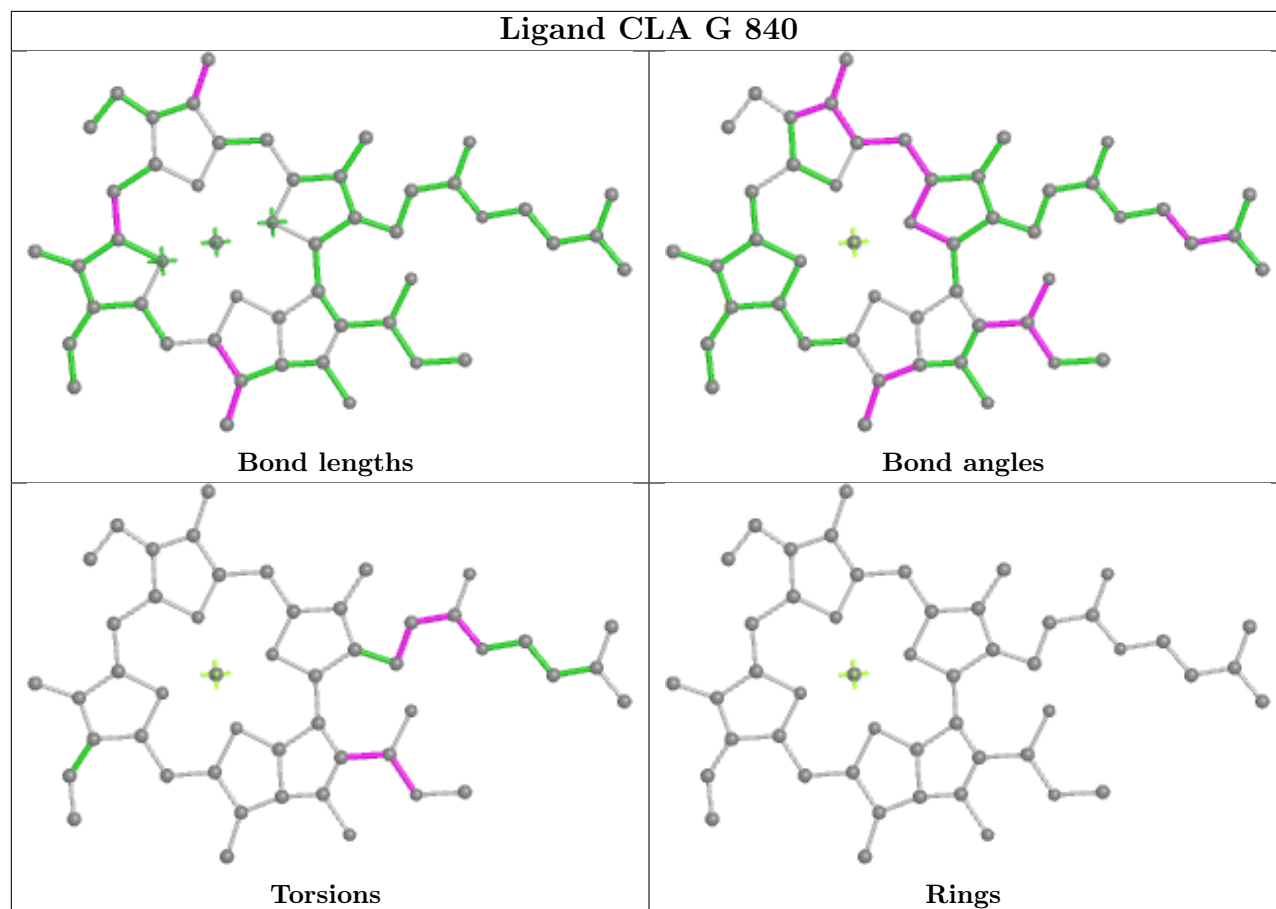


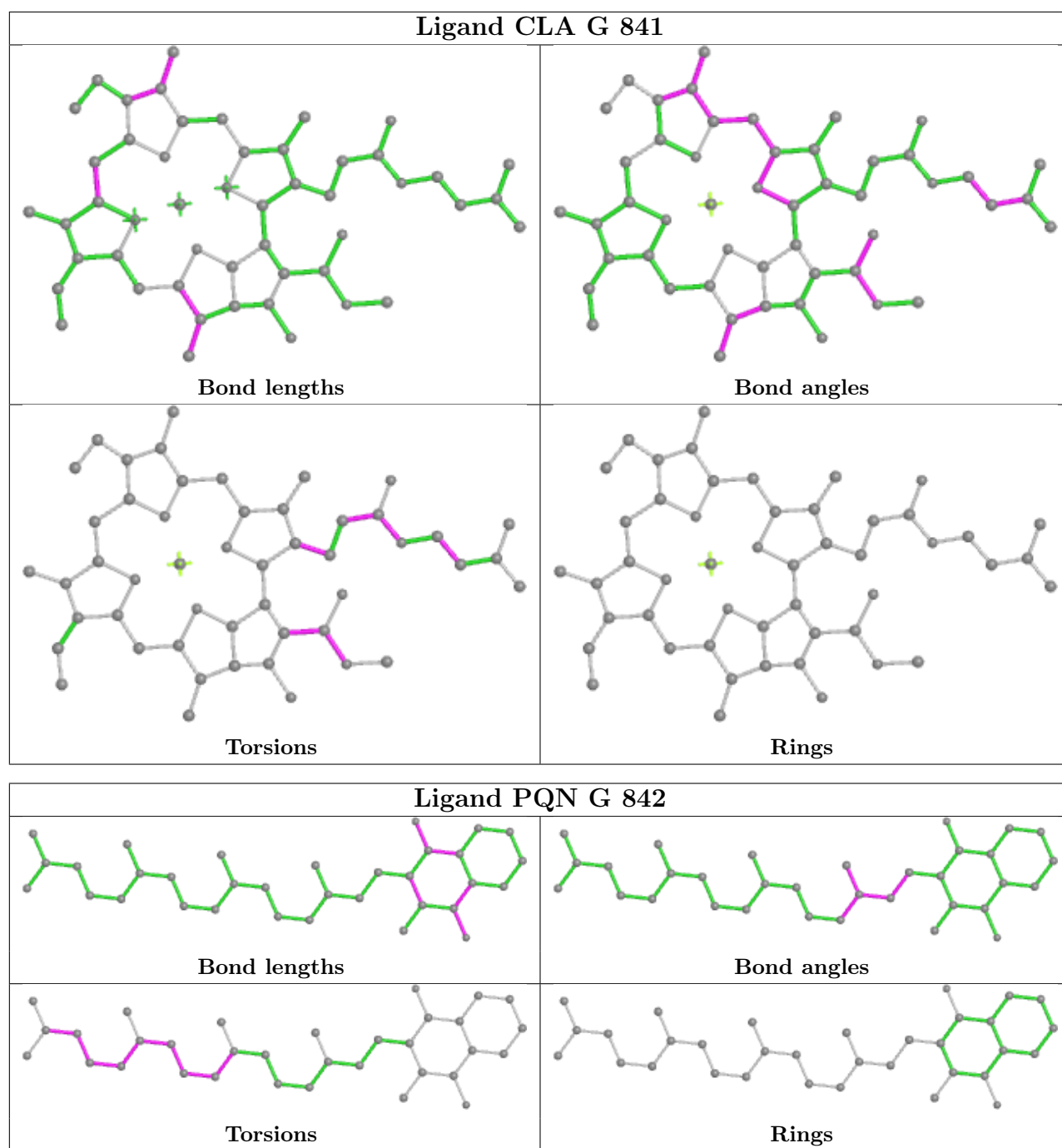


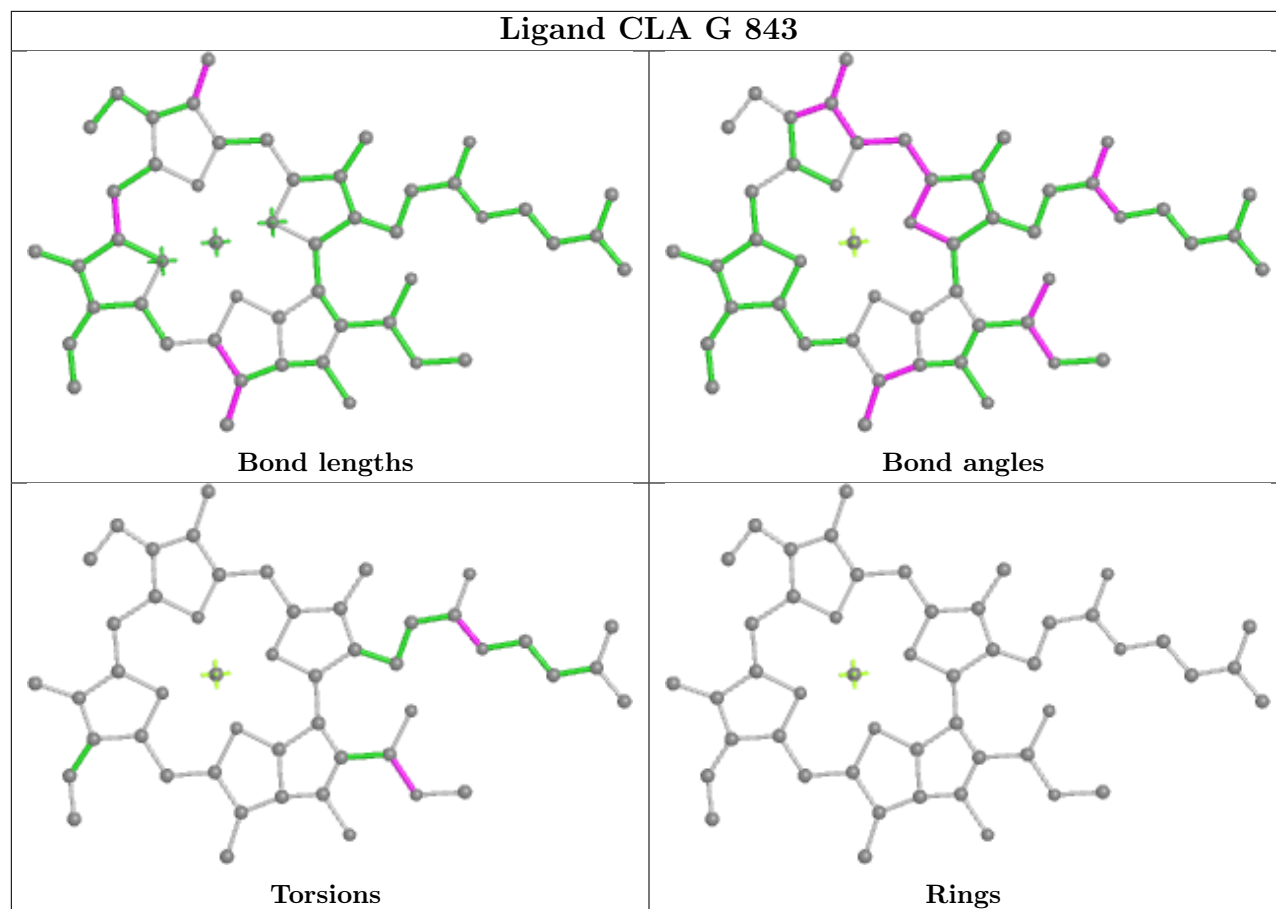


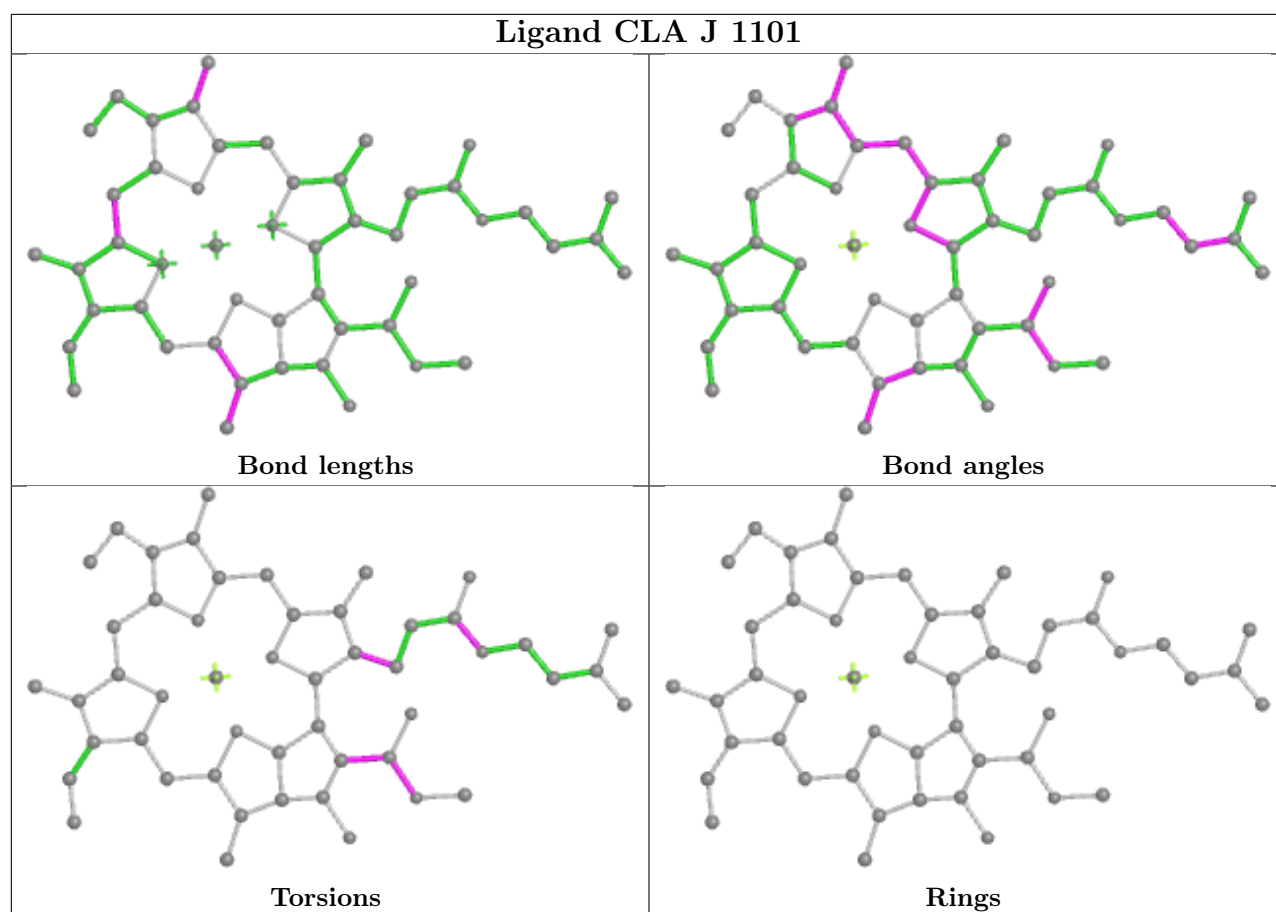
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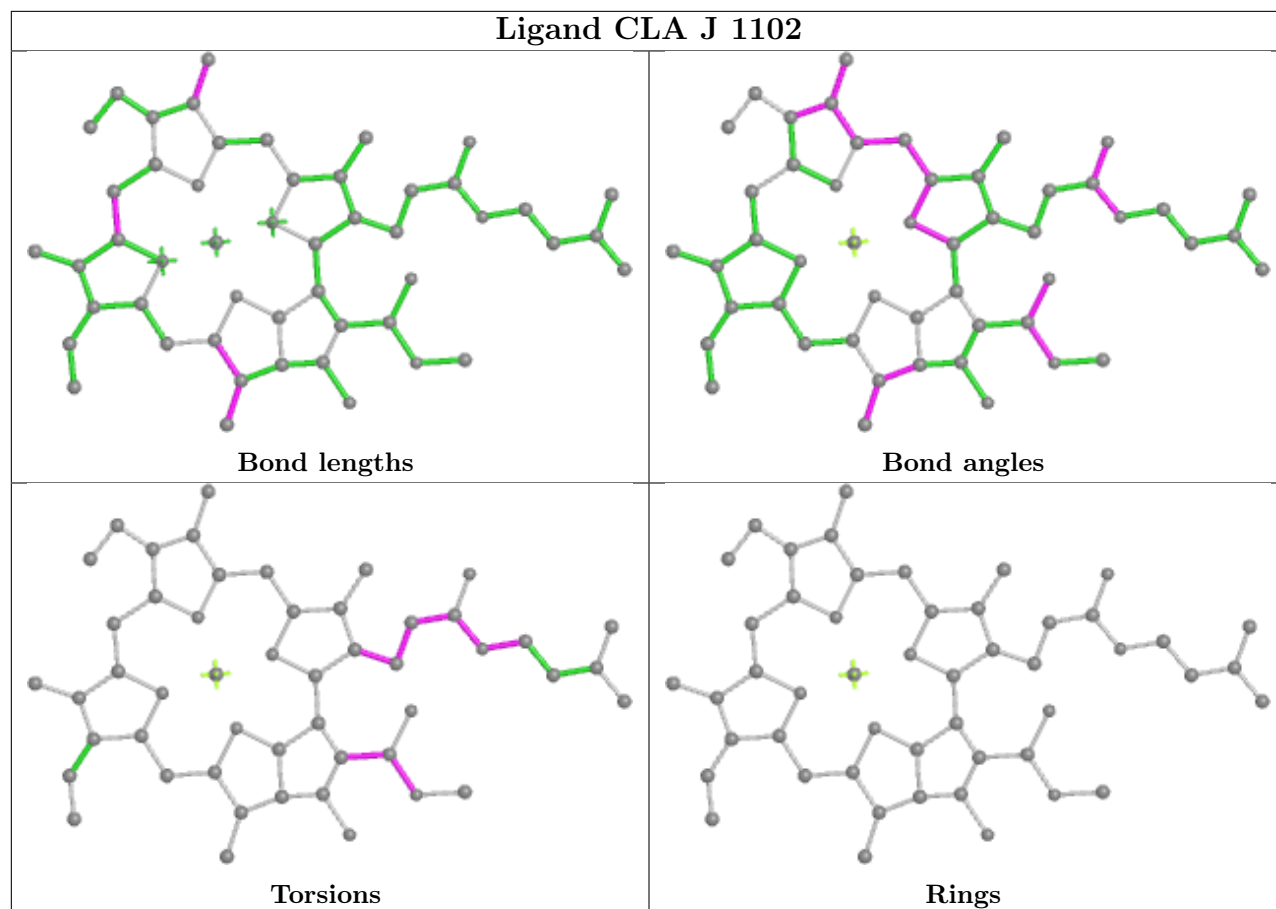




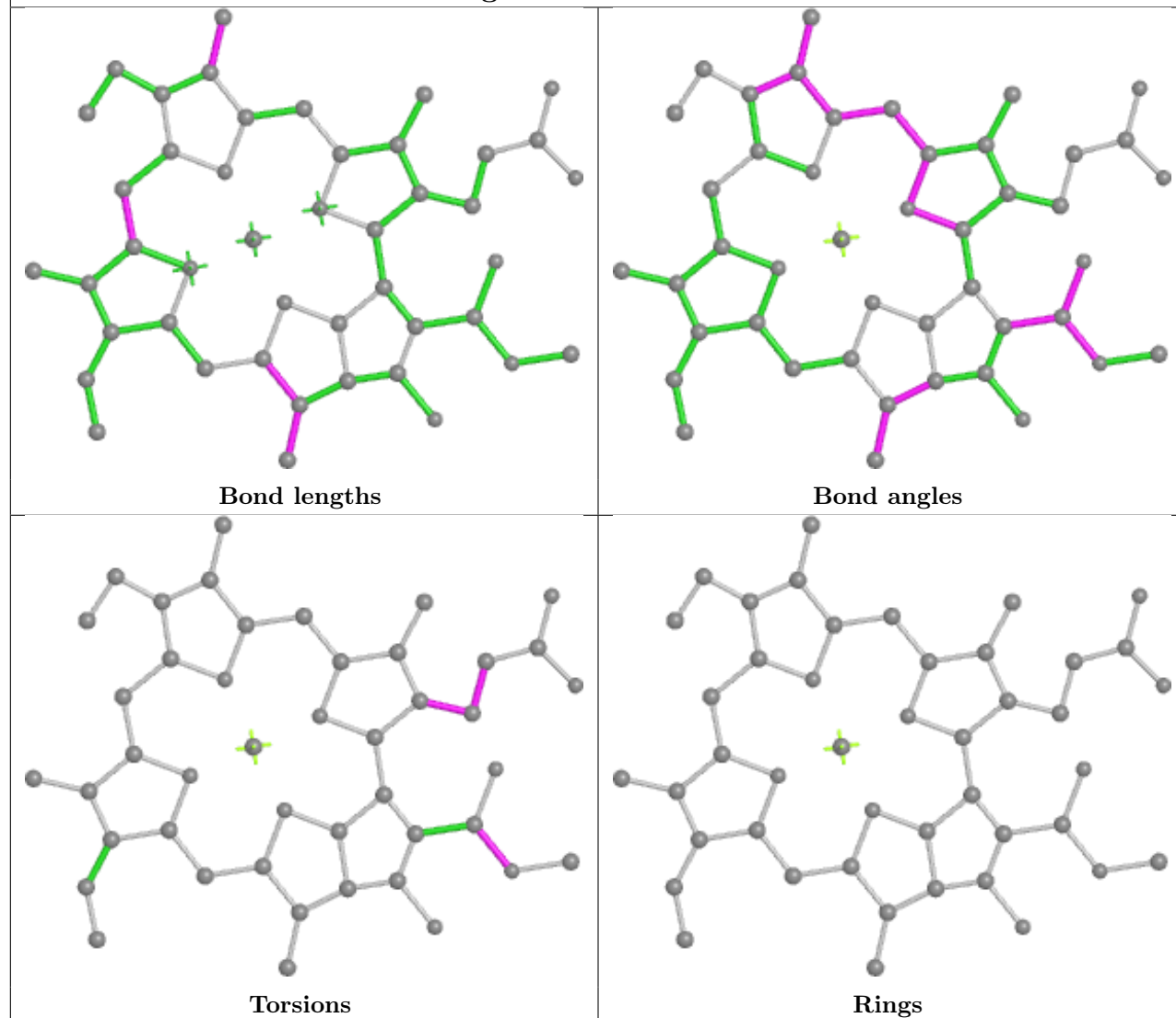




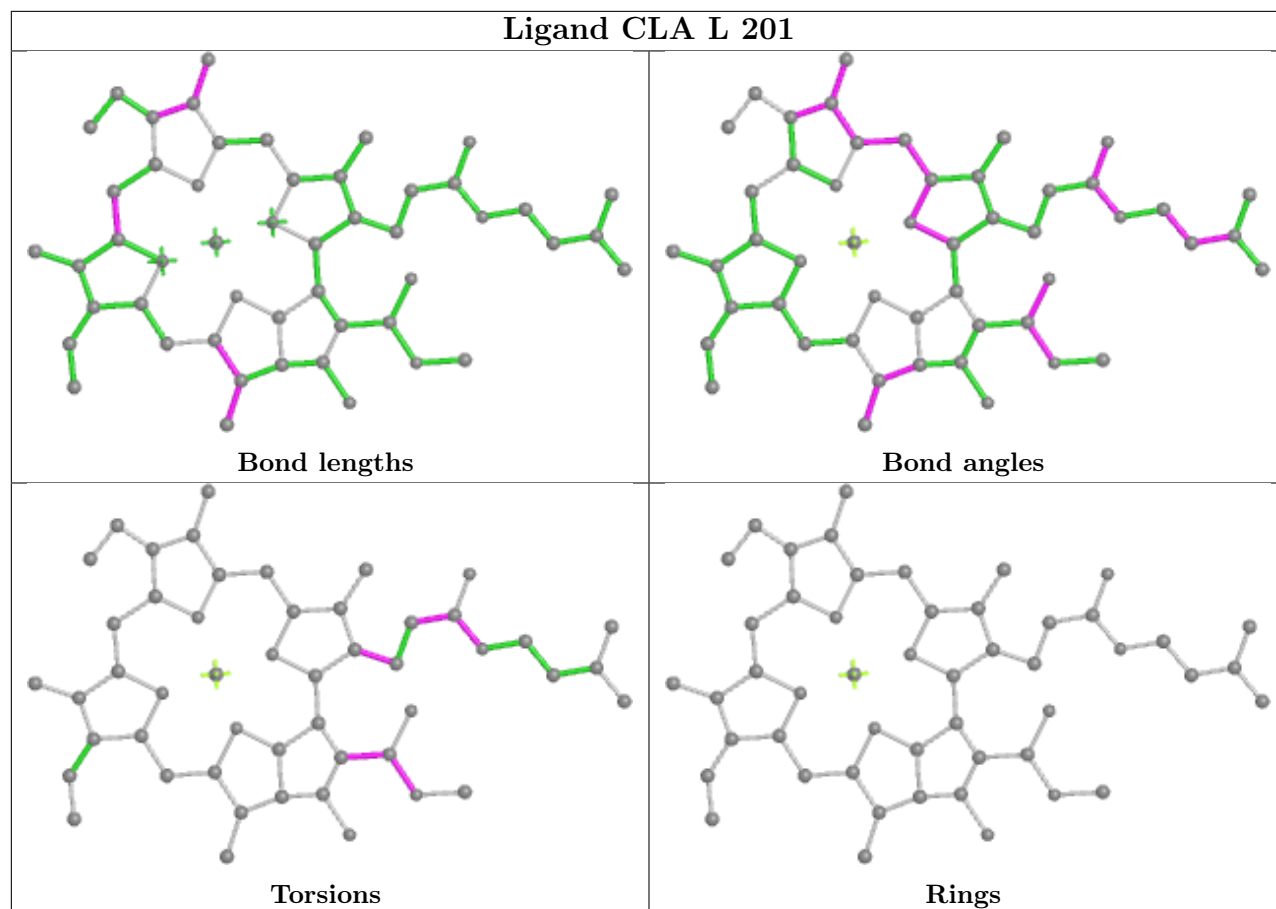


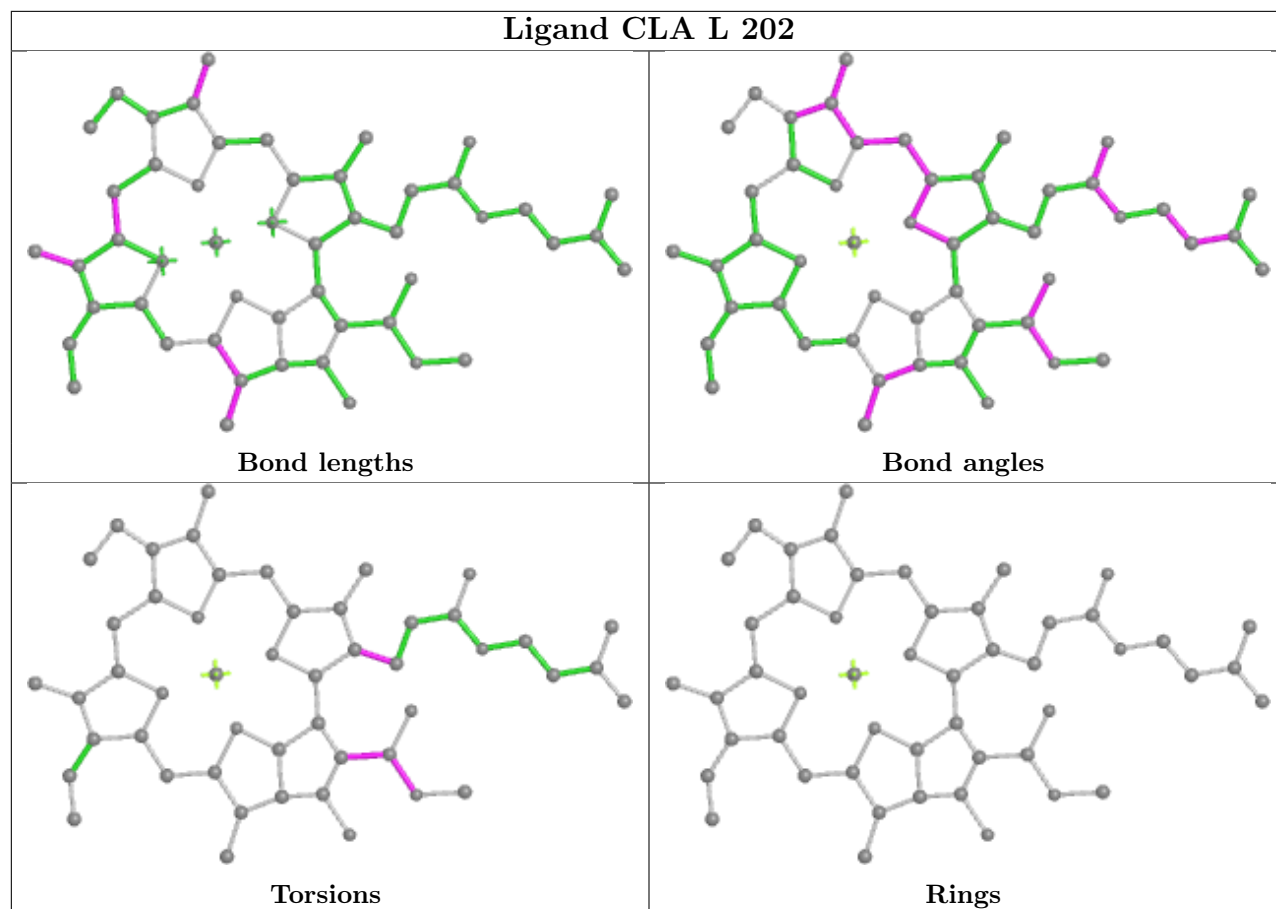


Ligand CLA K 1401

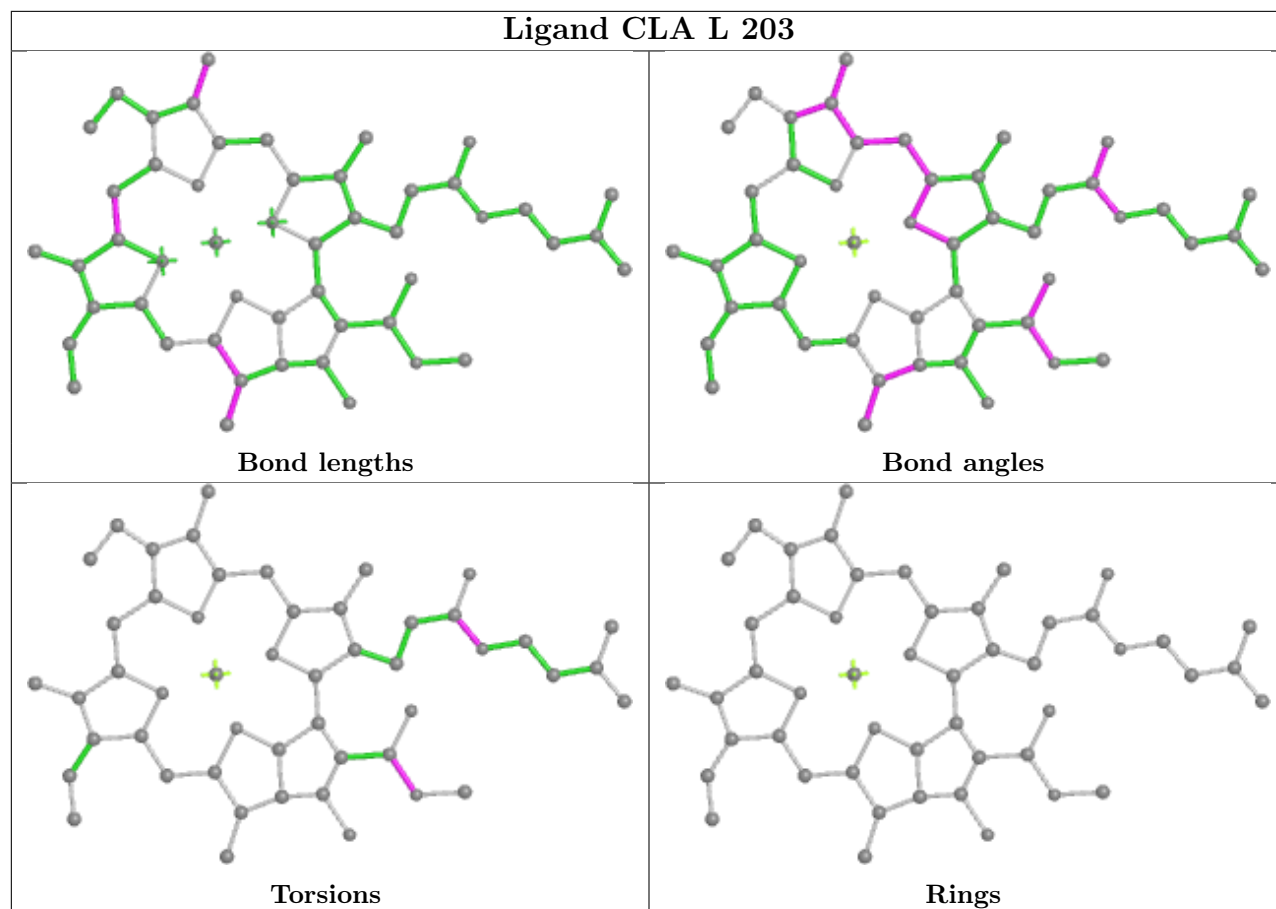


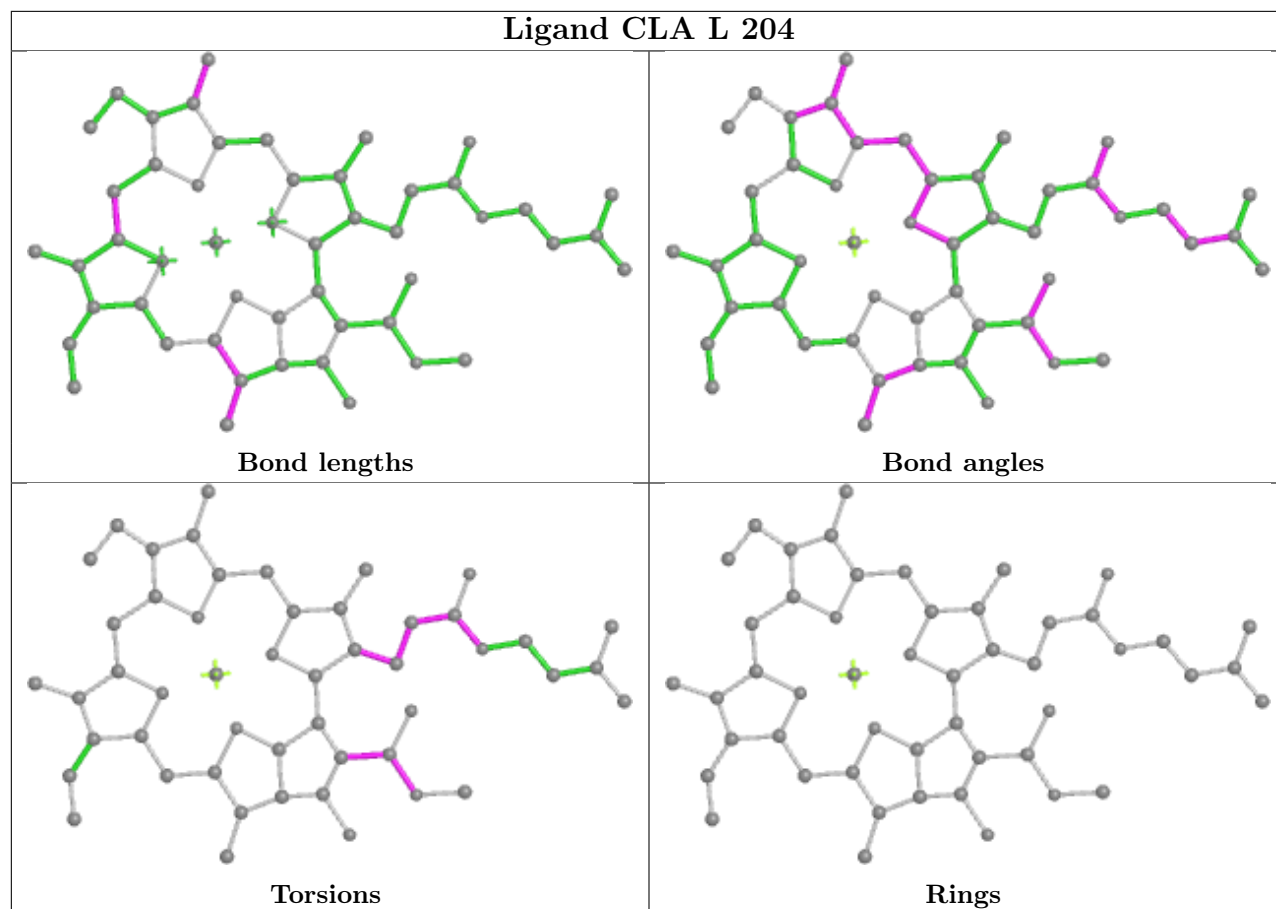
Ligand CLA L 201

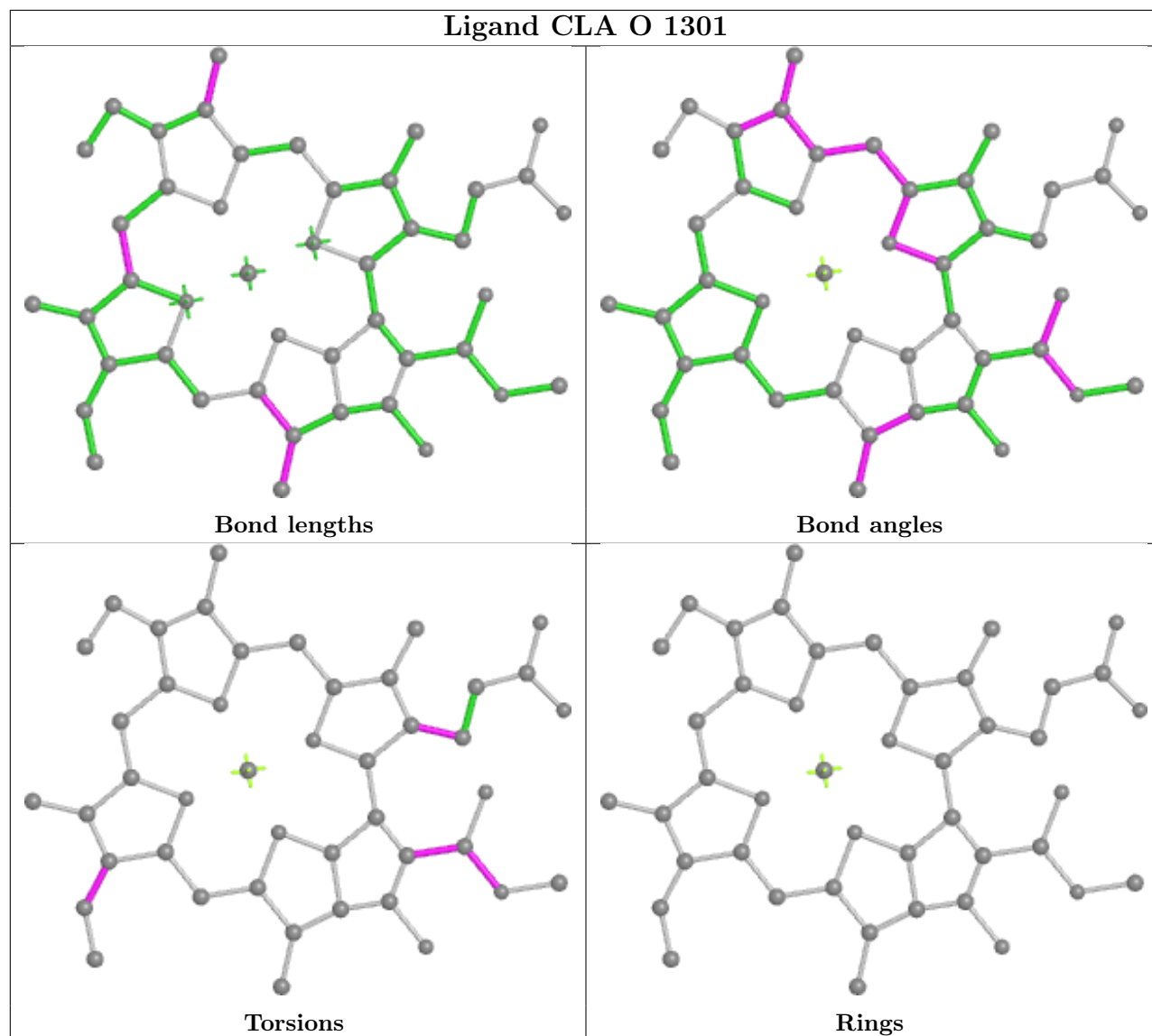


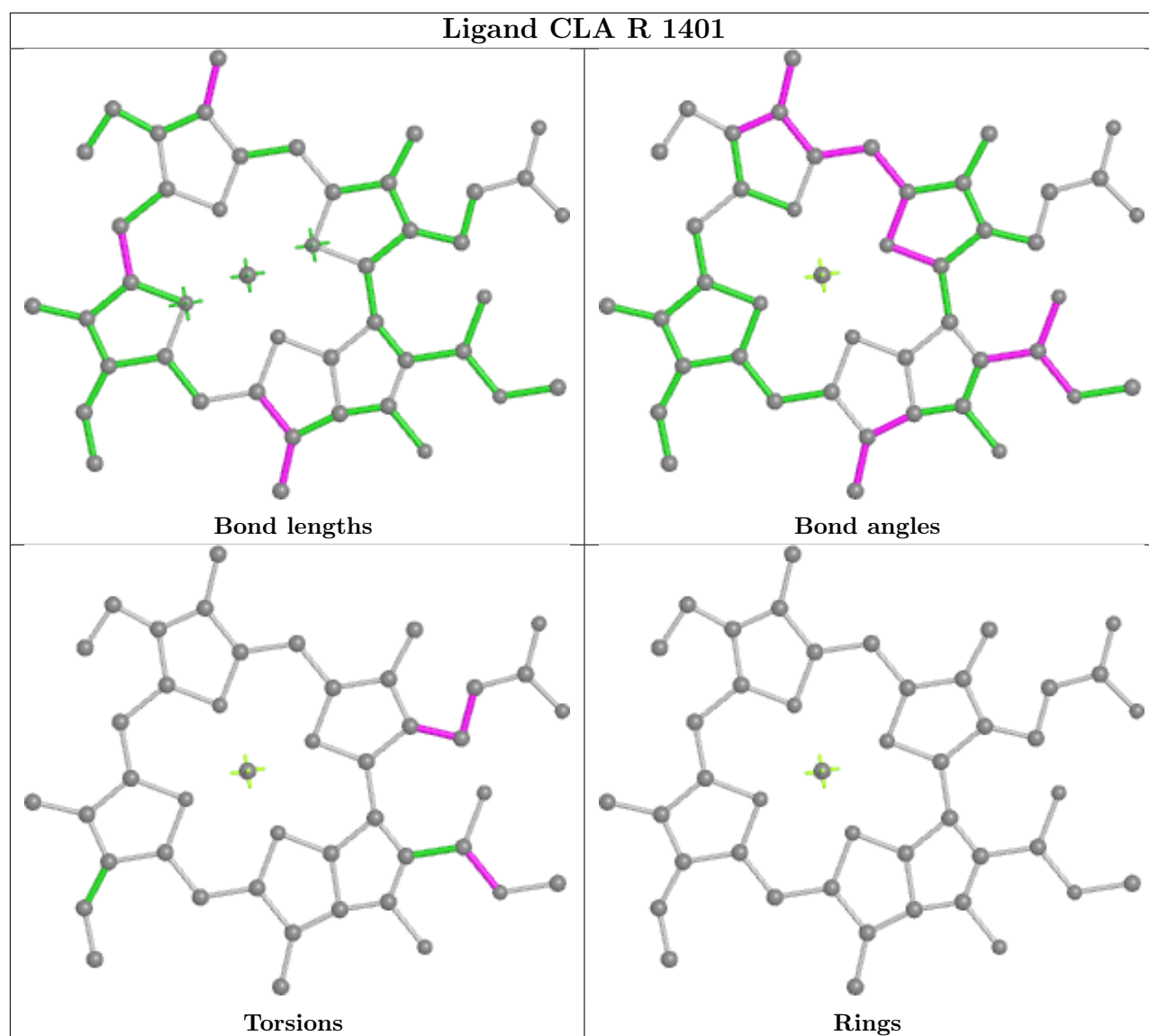


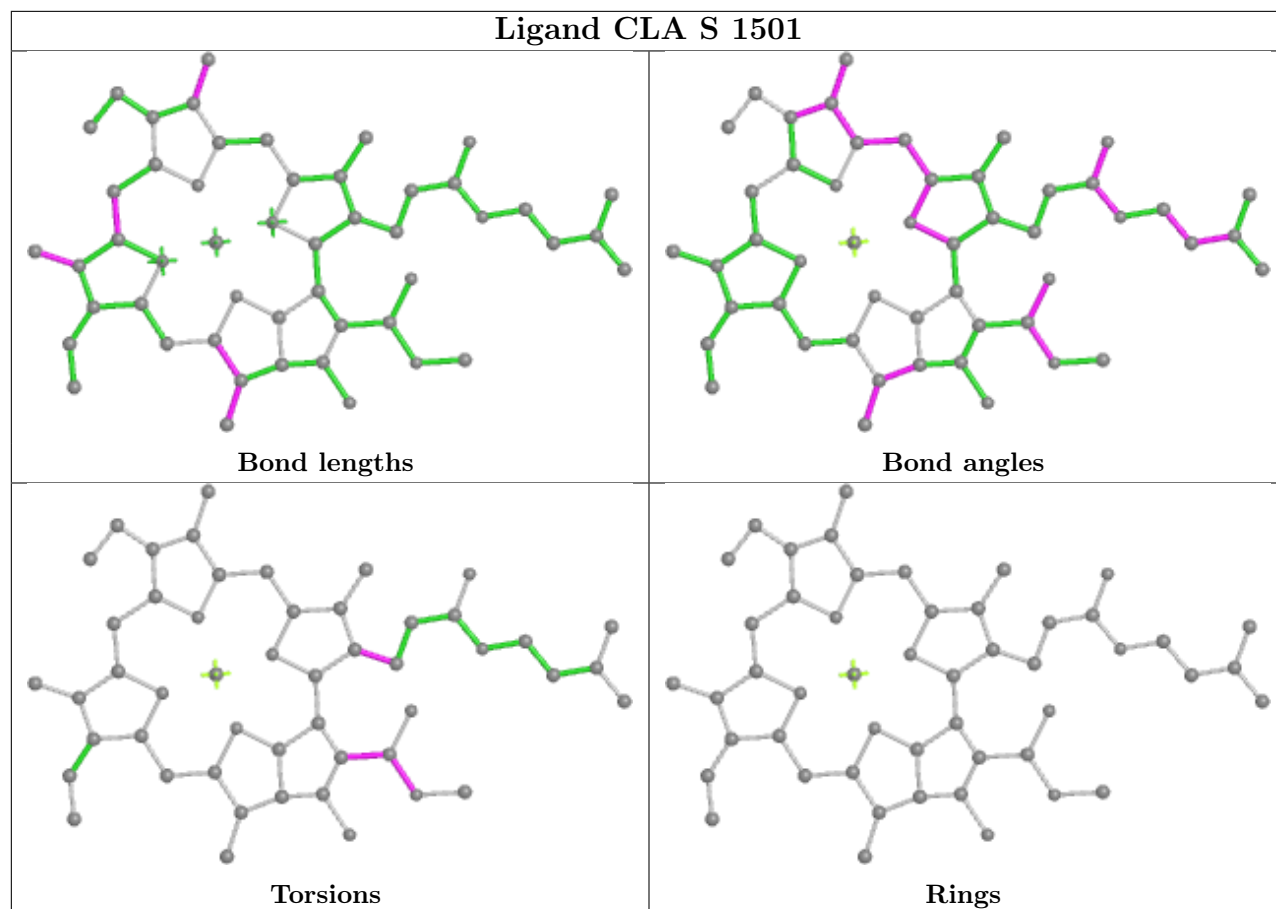
Ligand CLA L 203

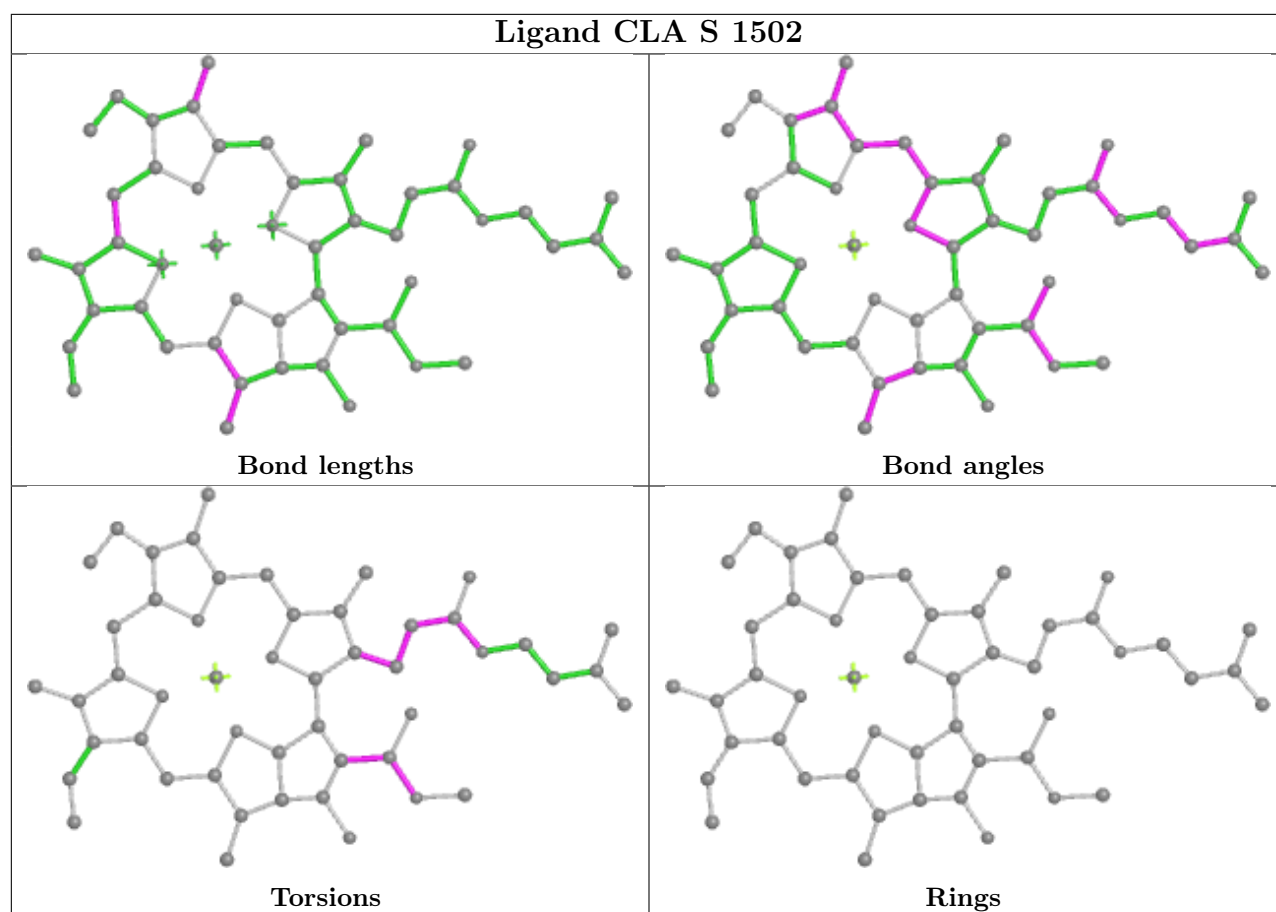




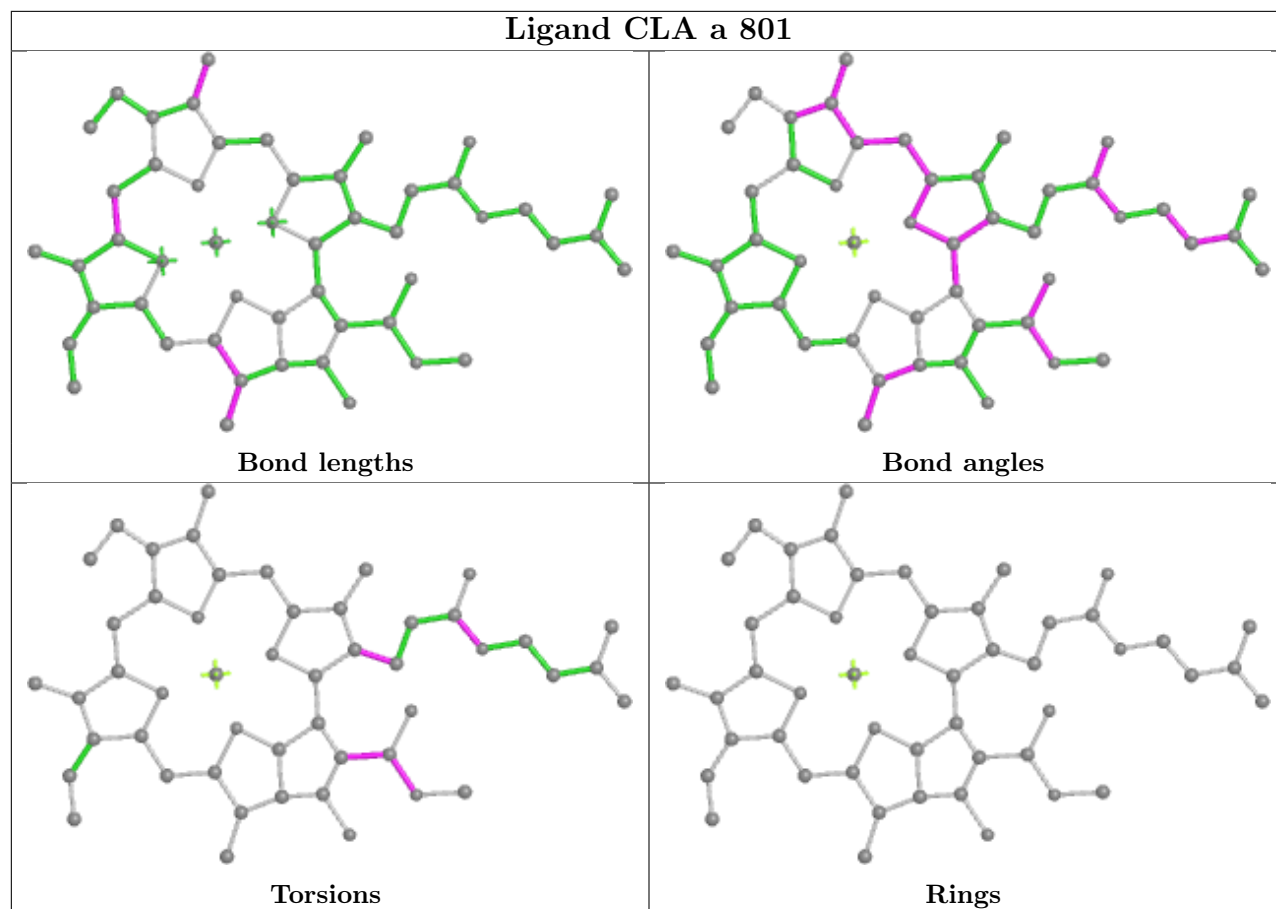




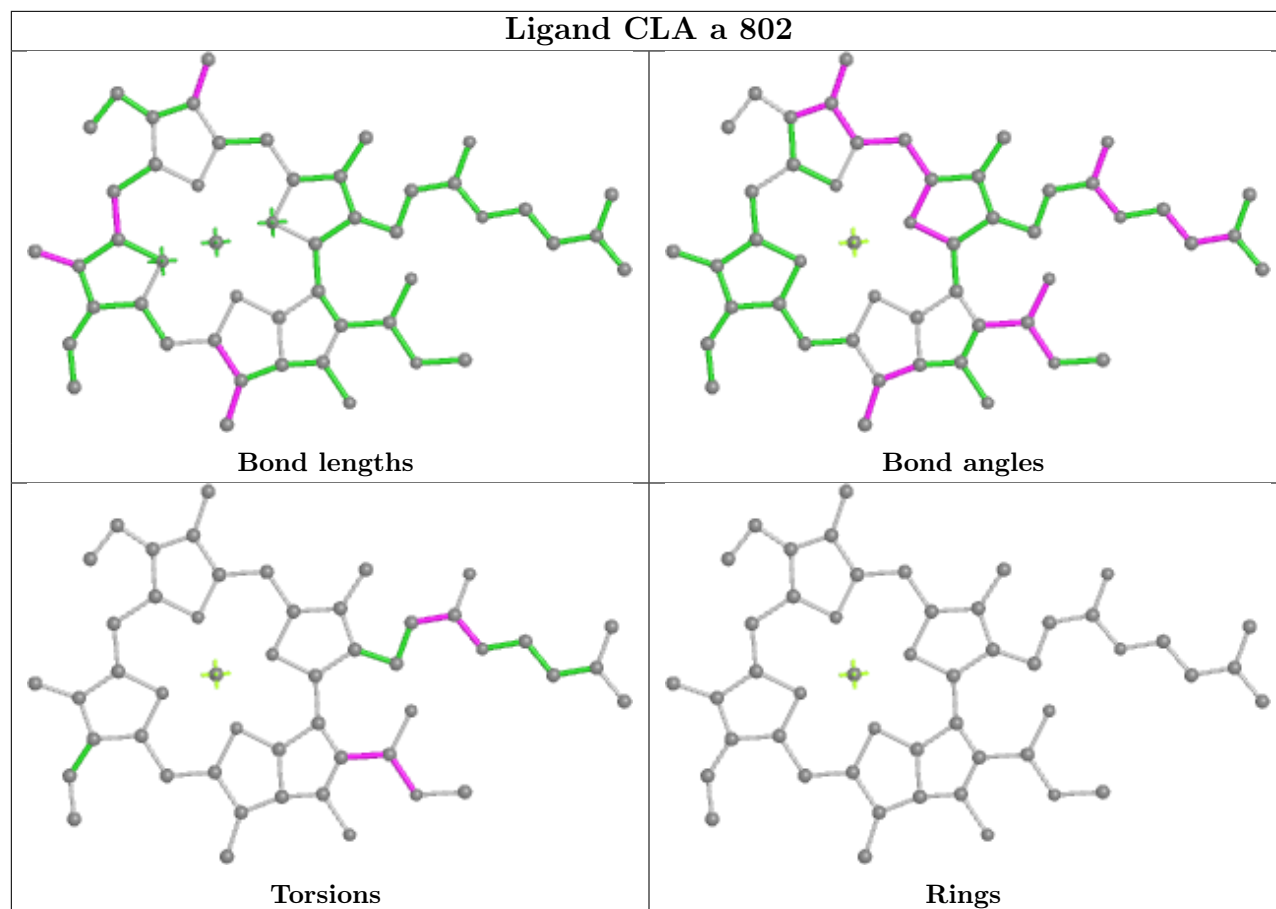




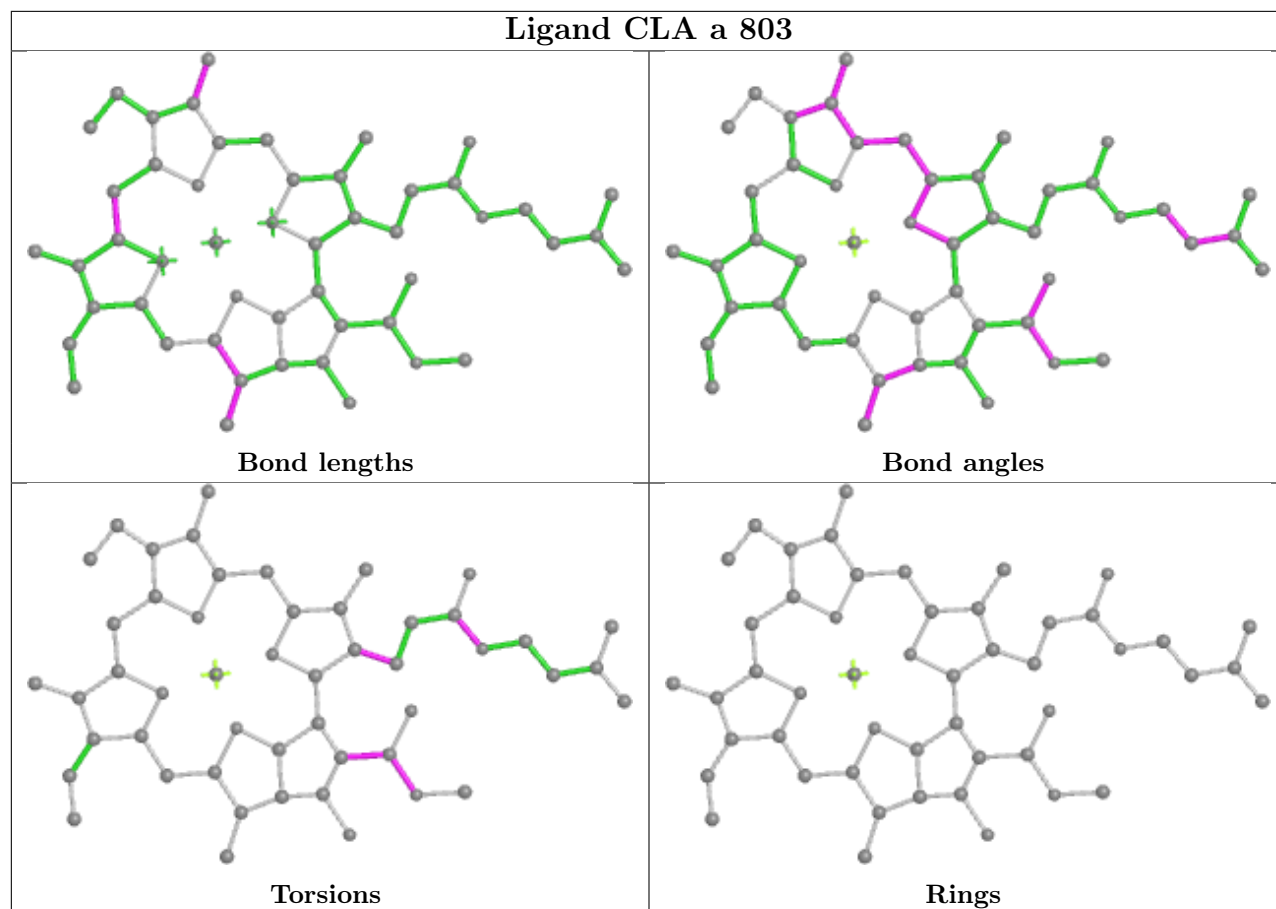
Ligand CLA a 801

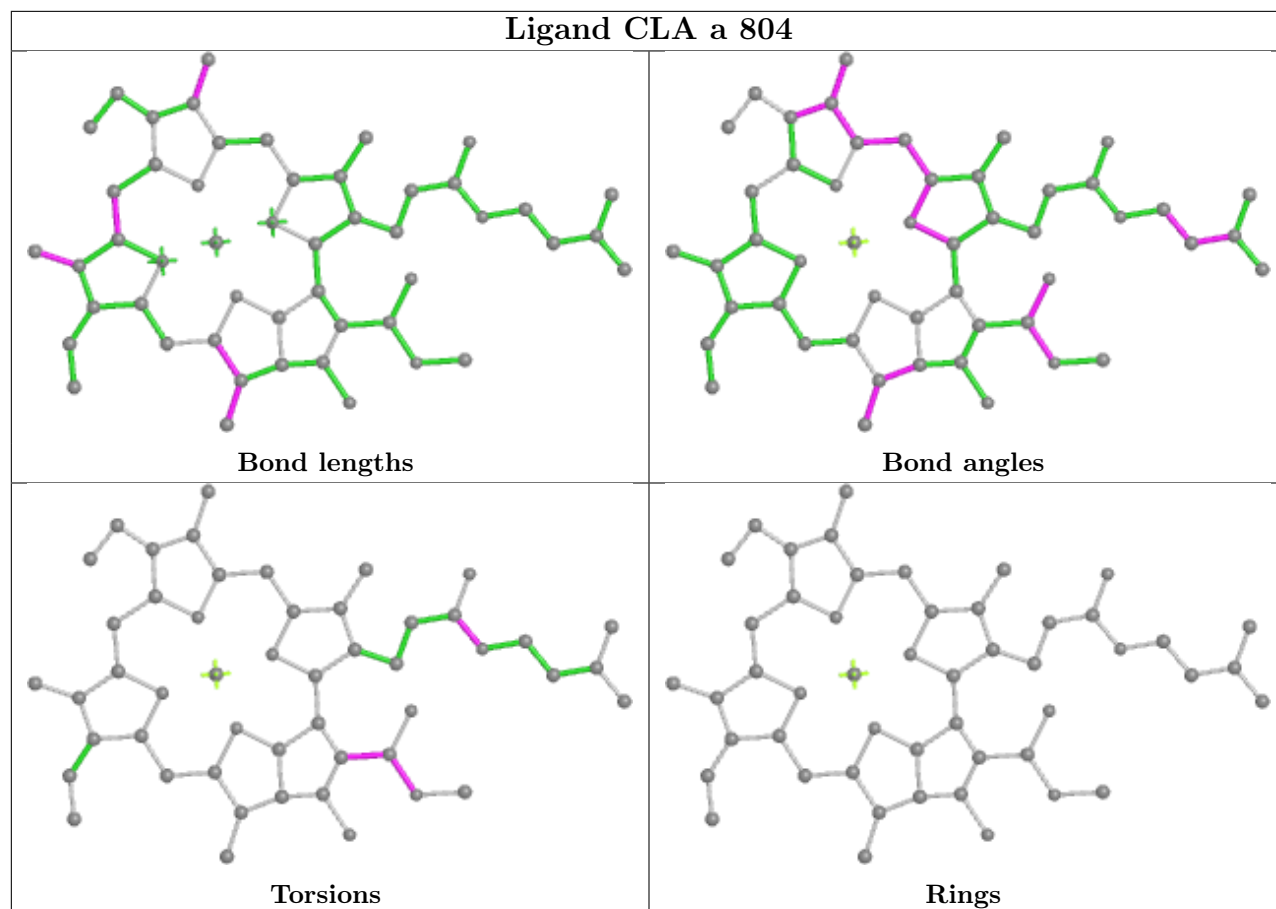


Ligand CLA a 802

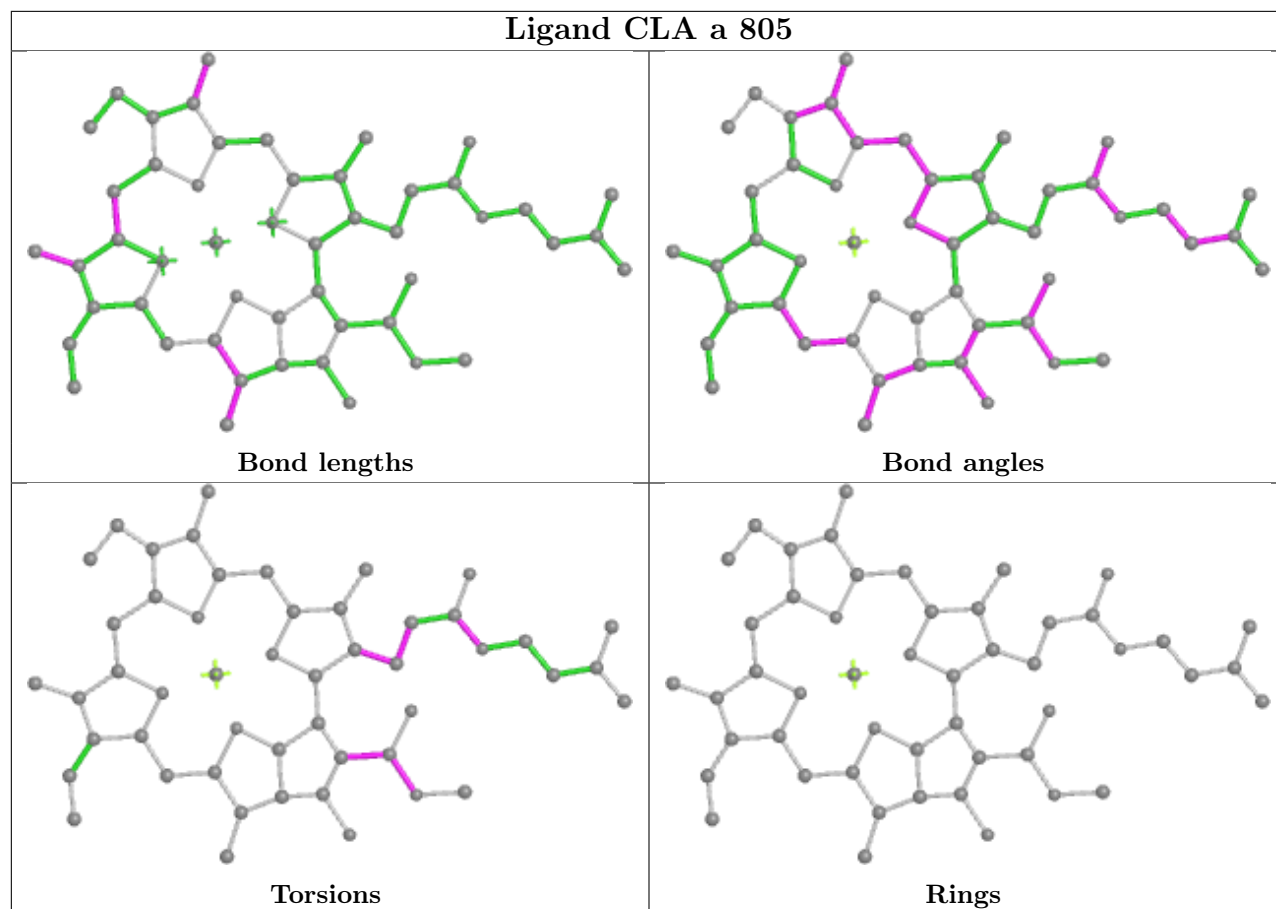


Ligand CLA a 803

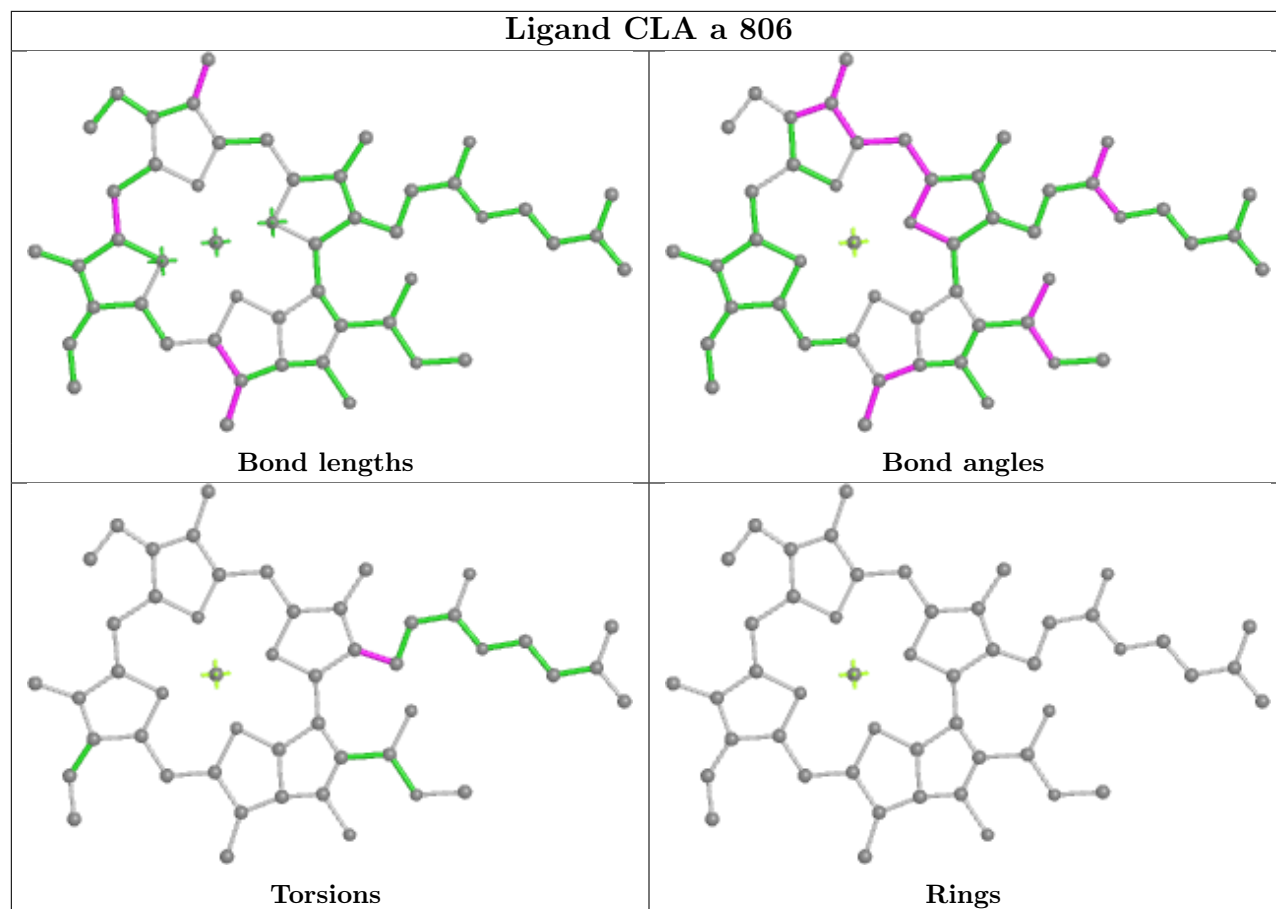




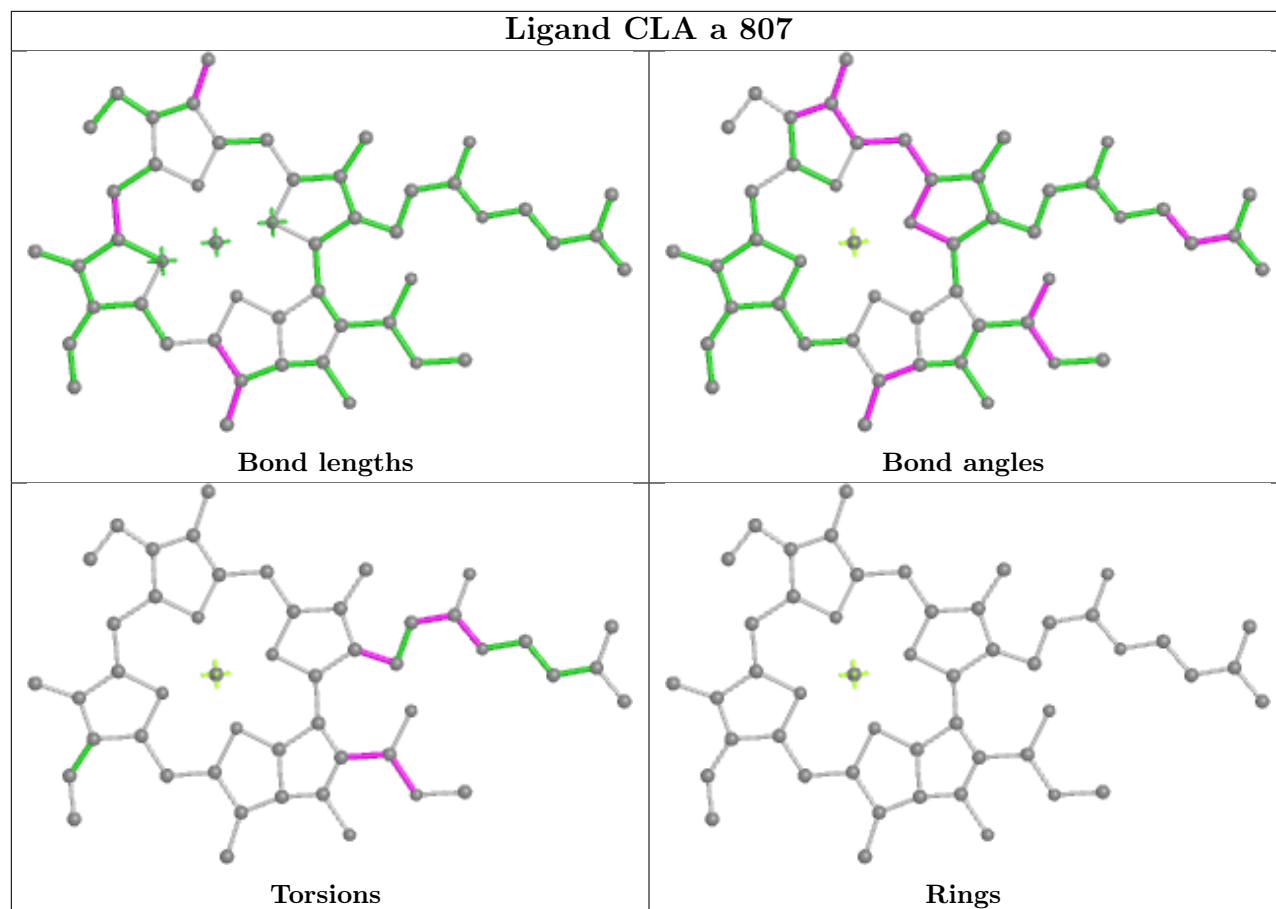
Ligand CLA a 805



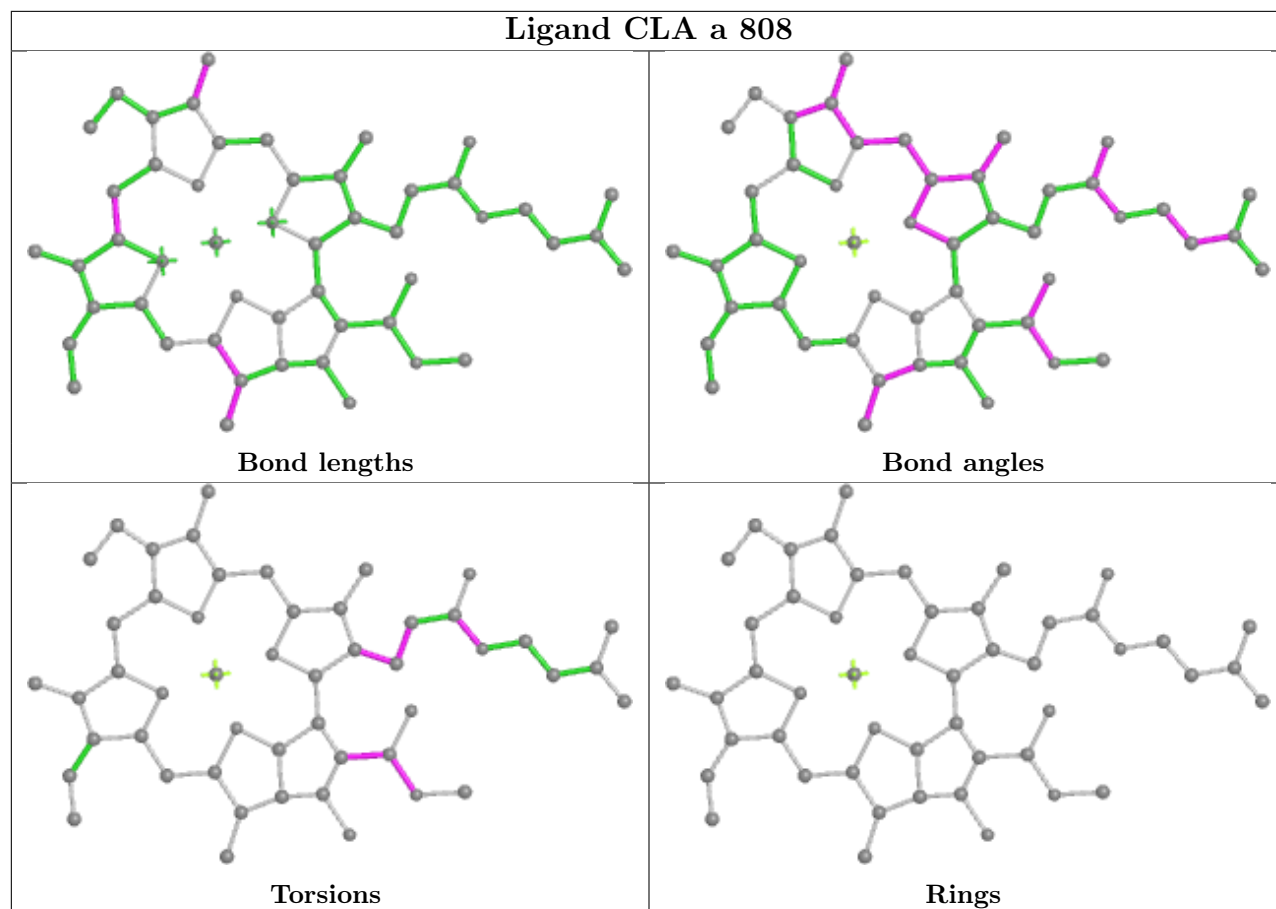
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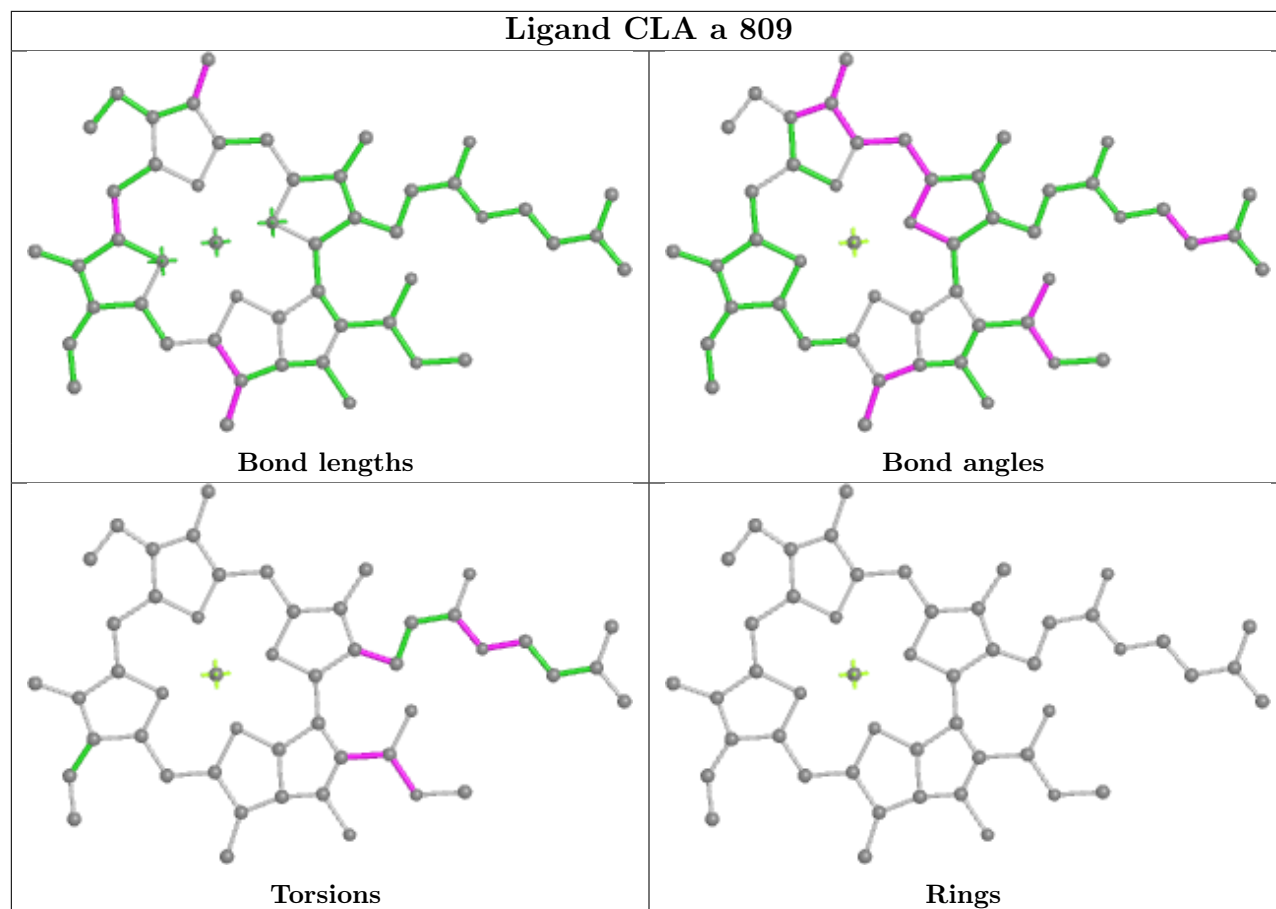
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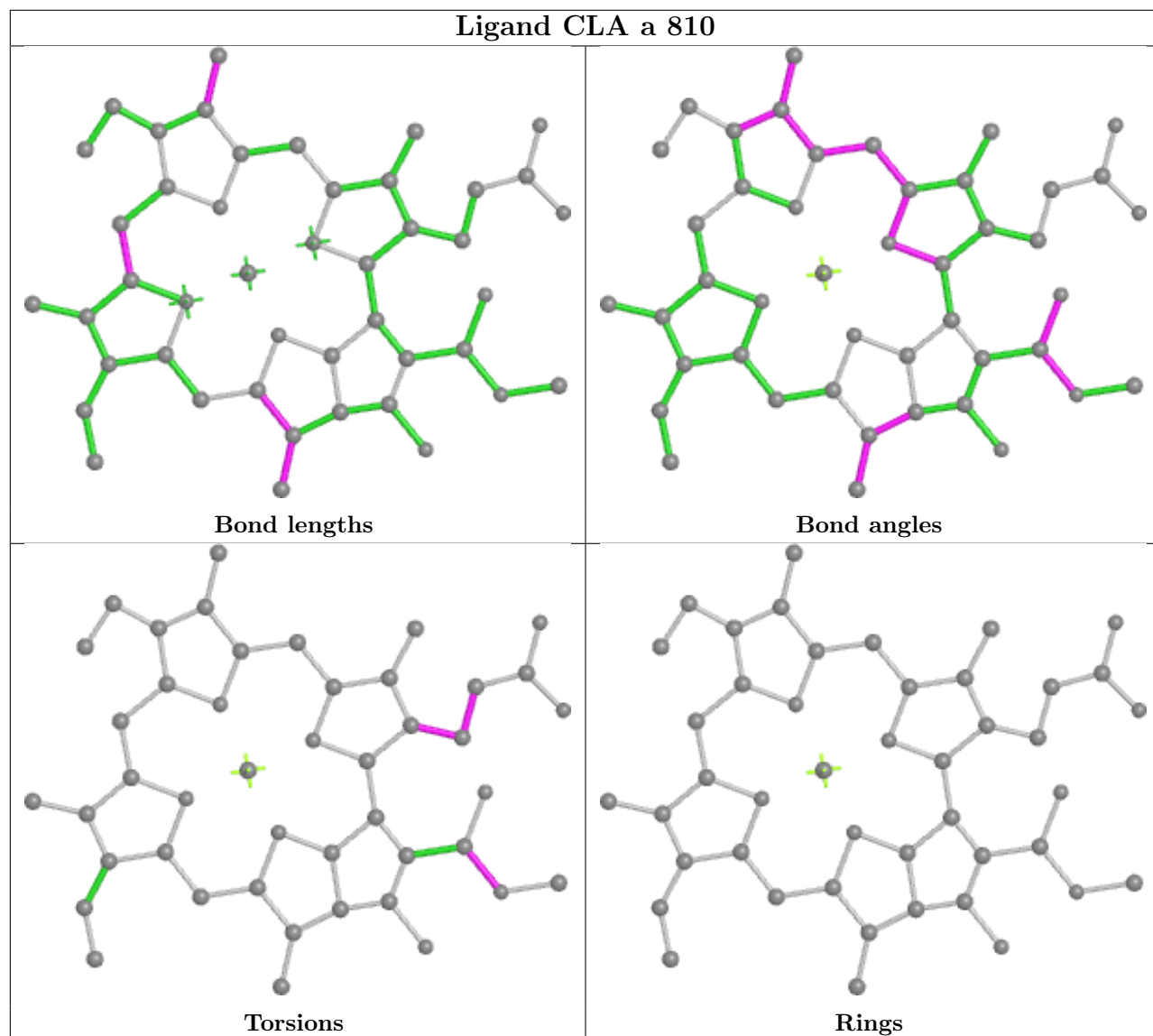
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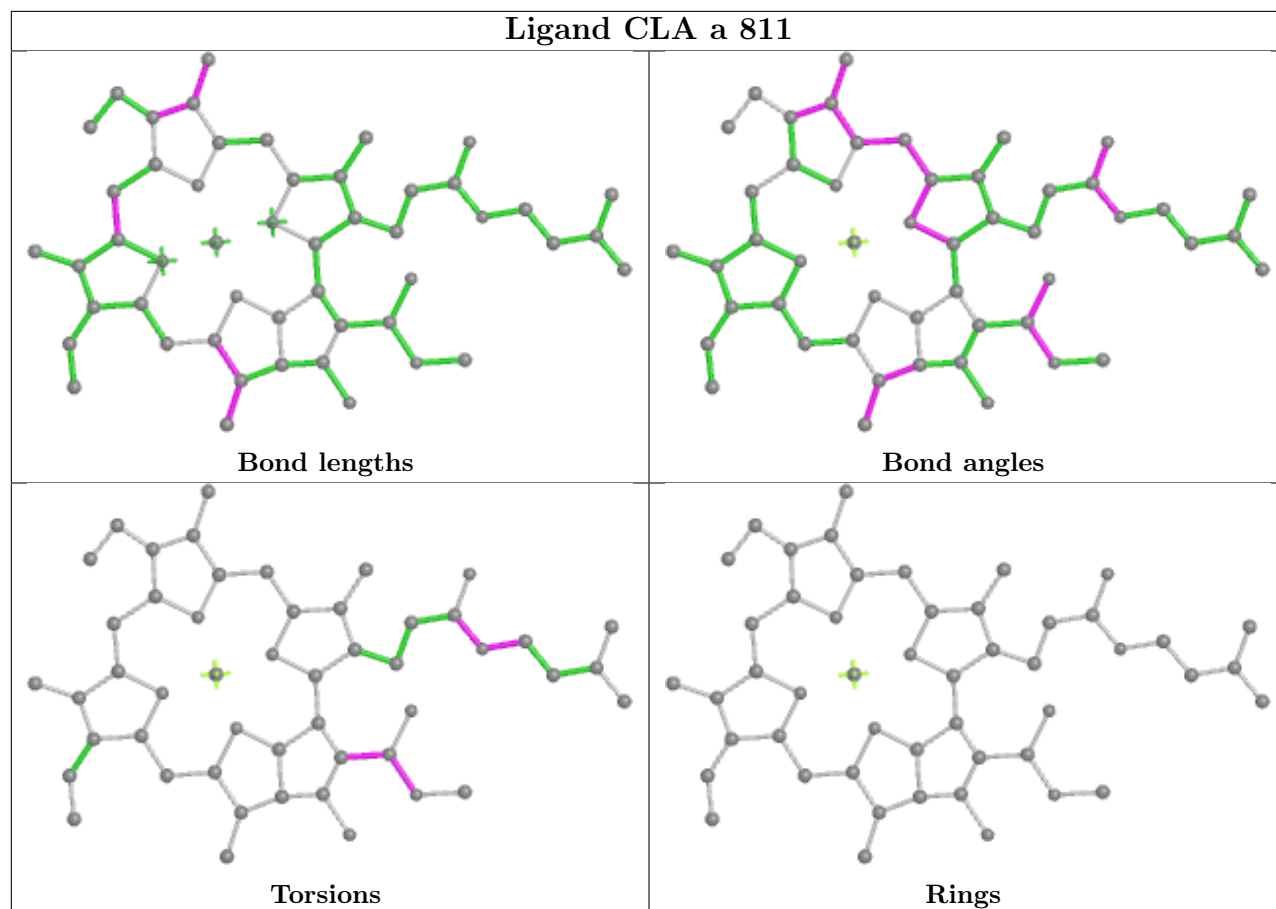
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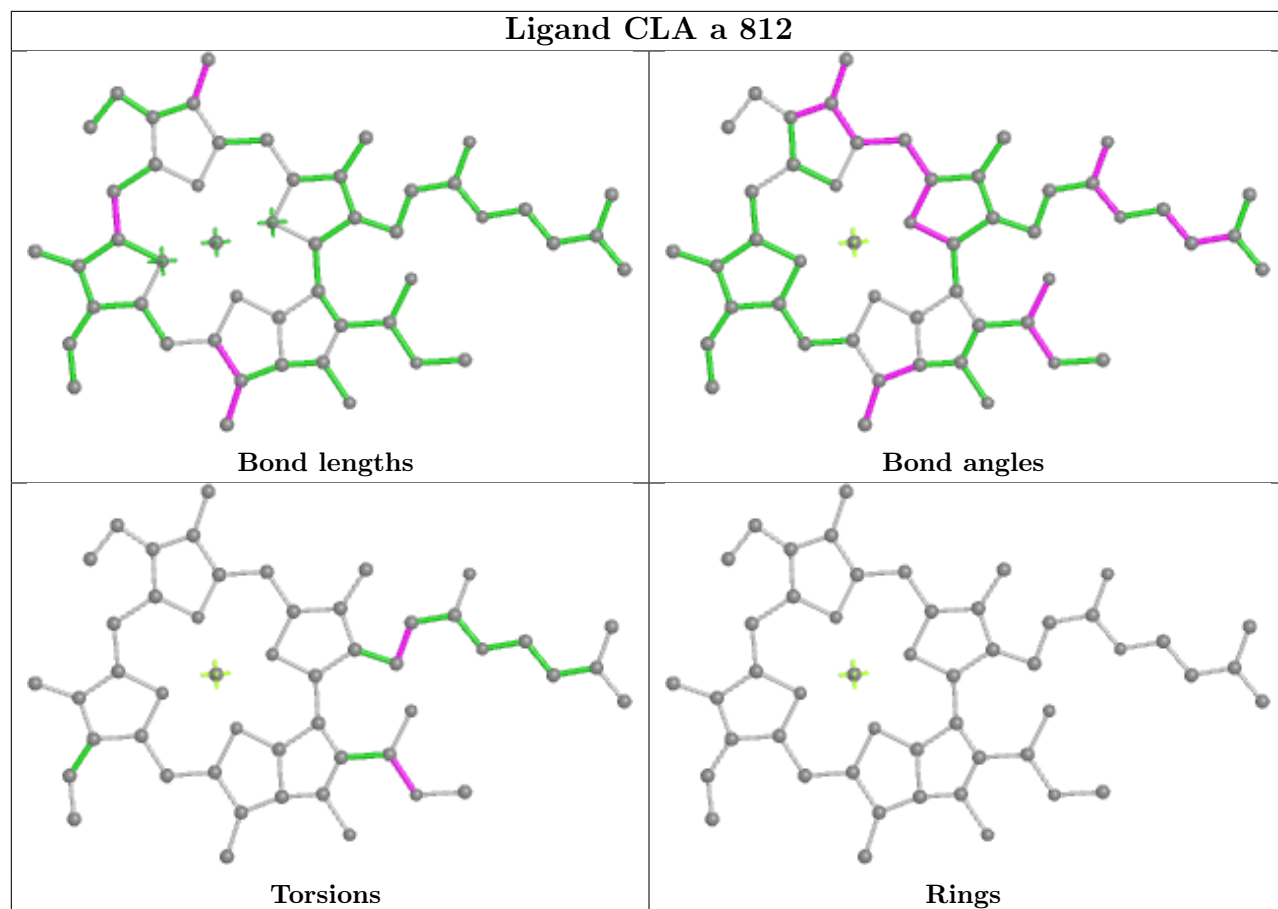
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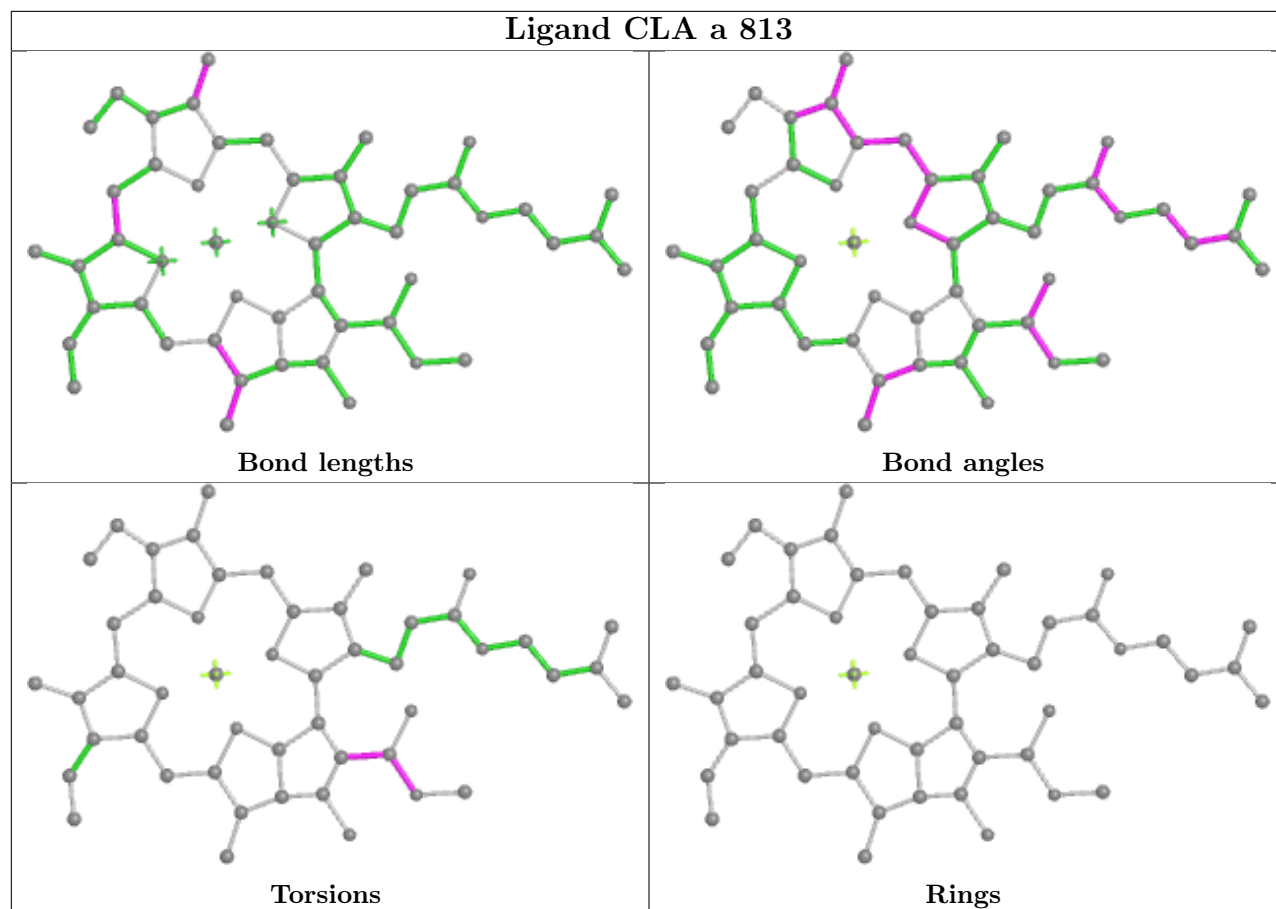
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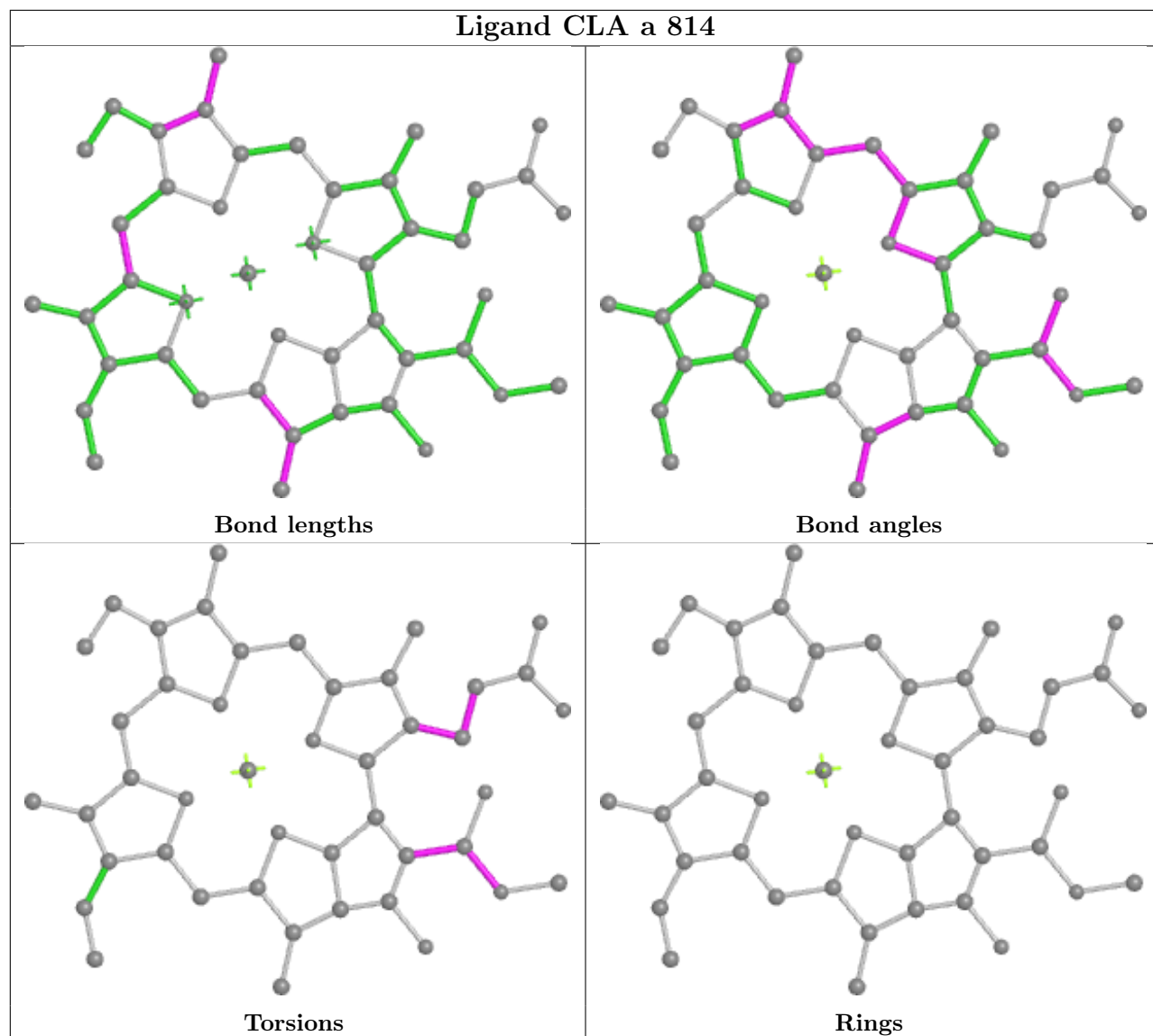
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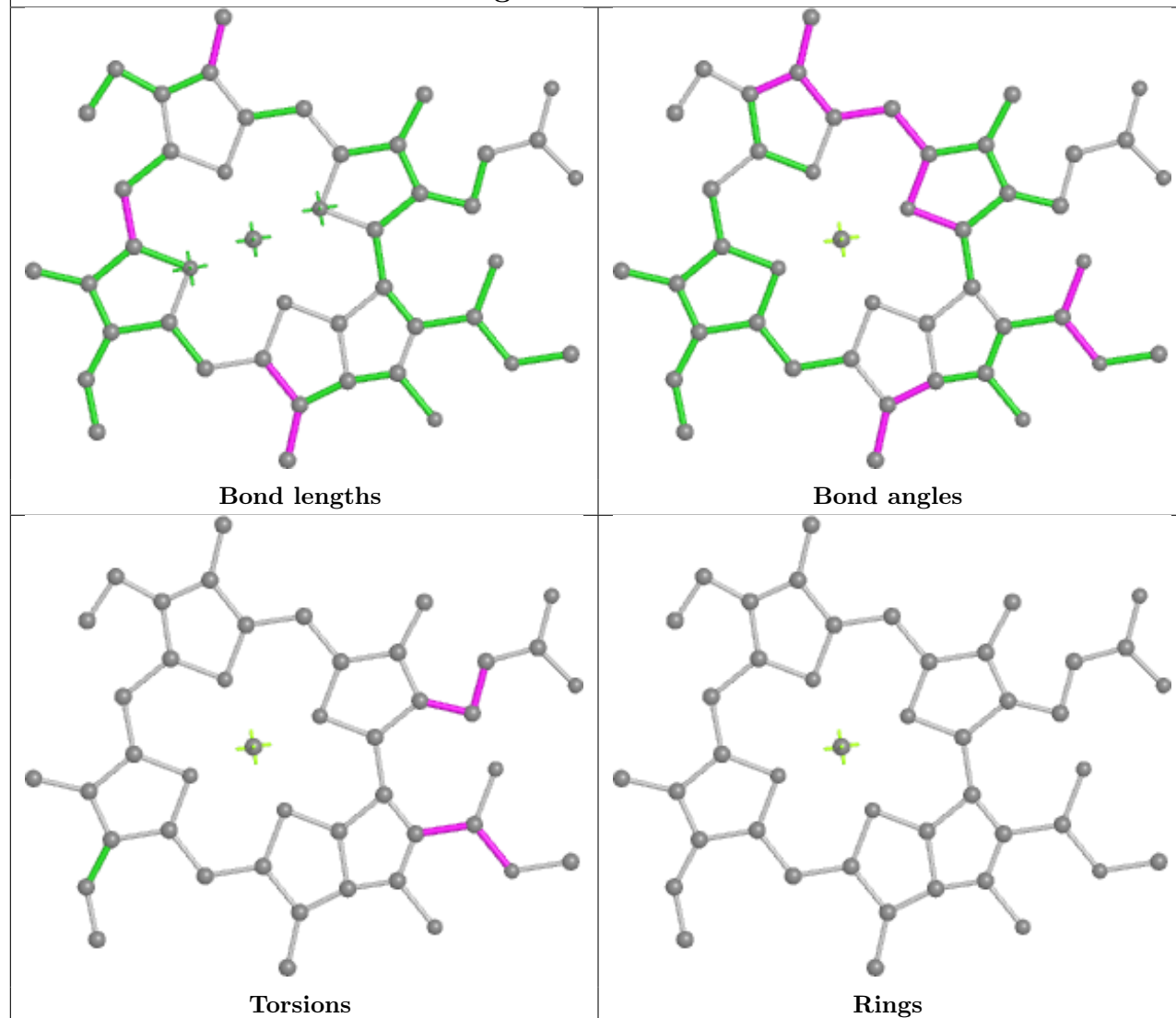
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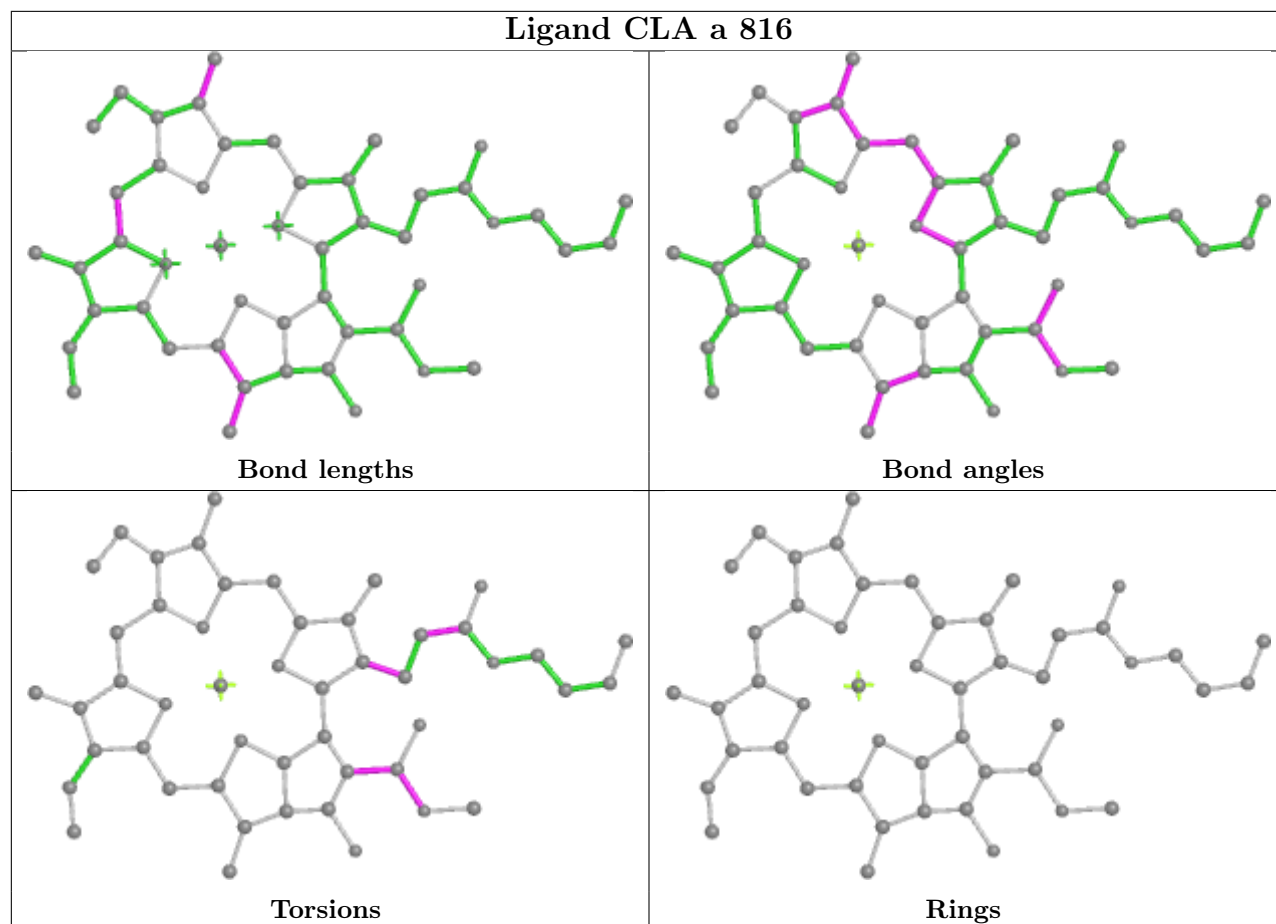
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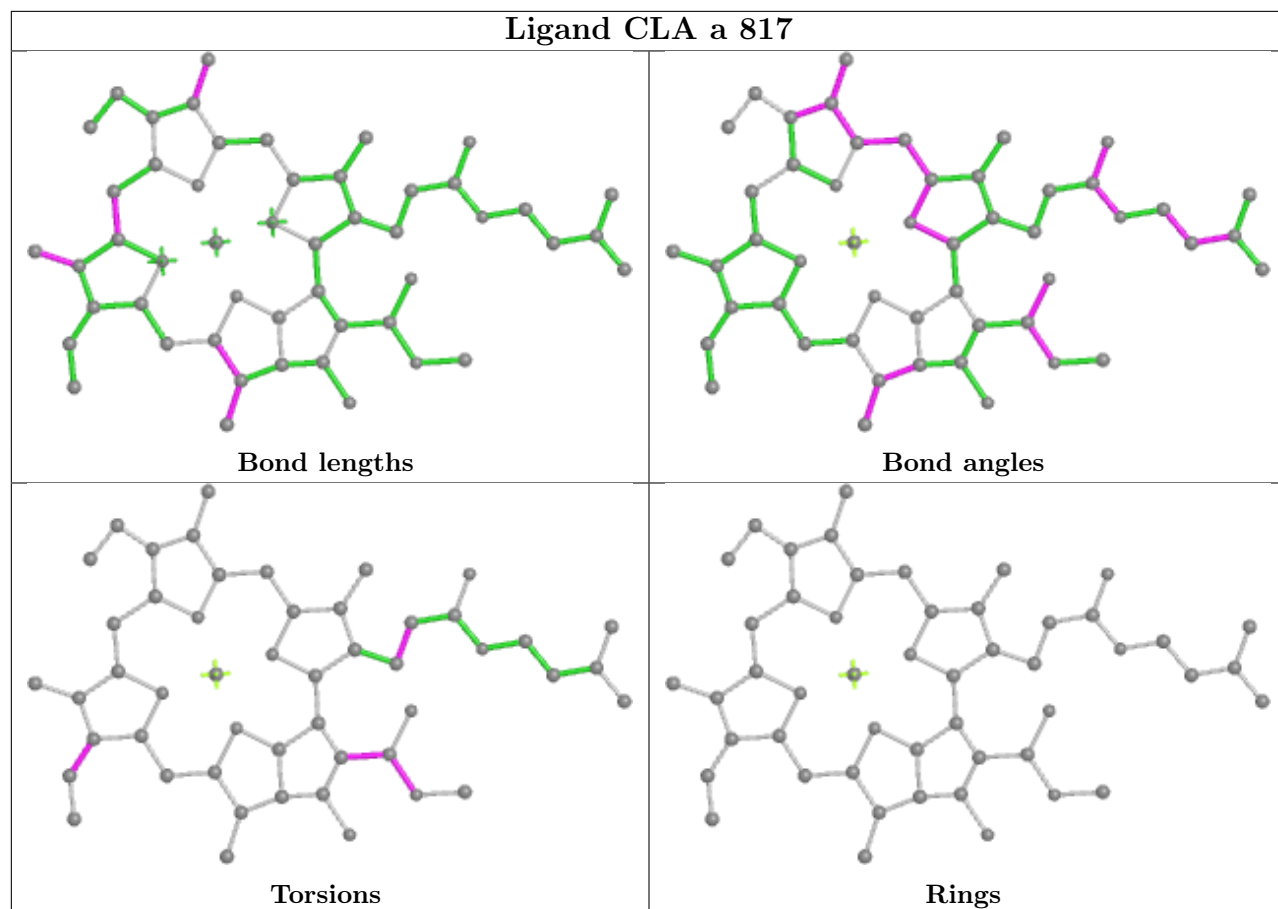
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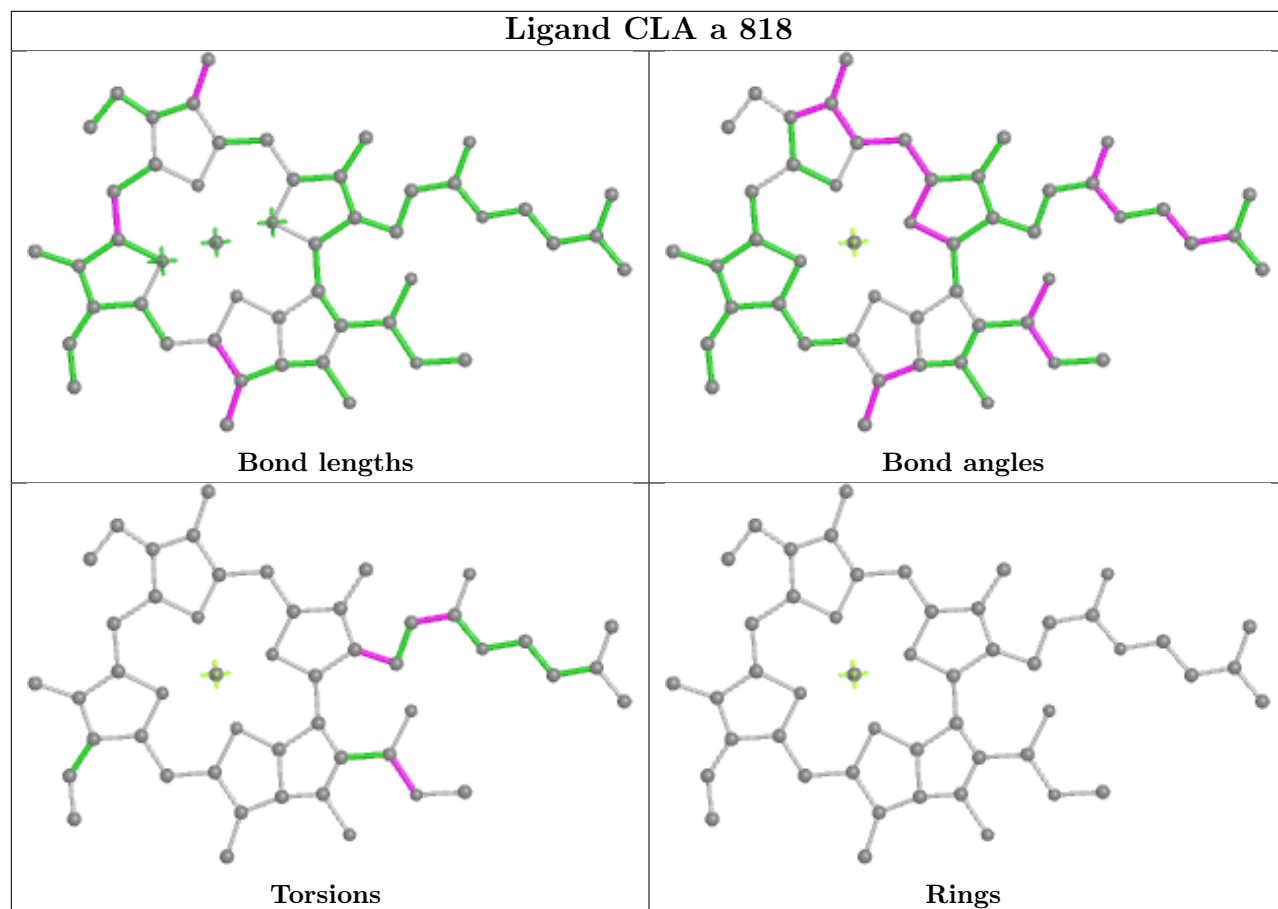
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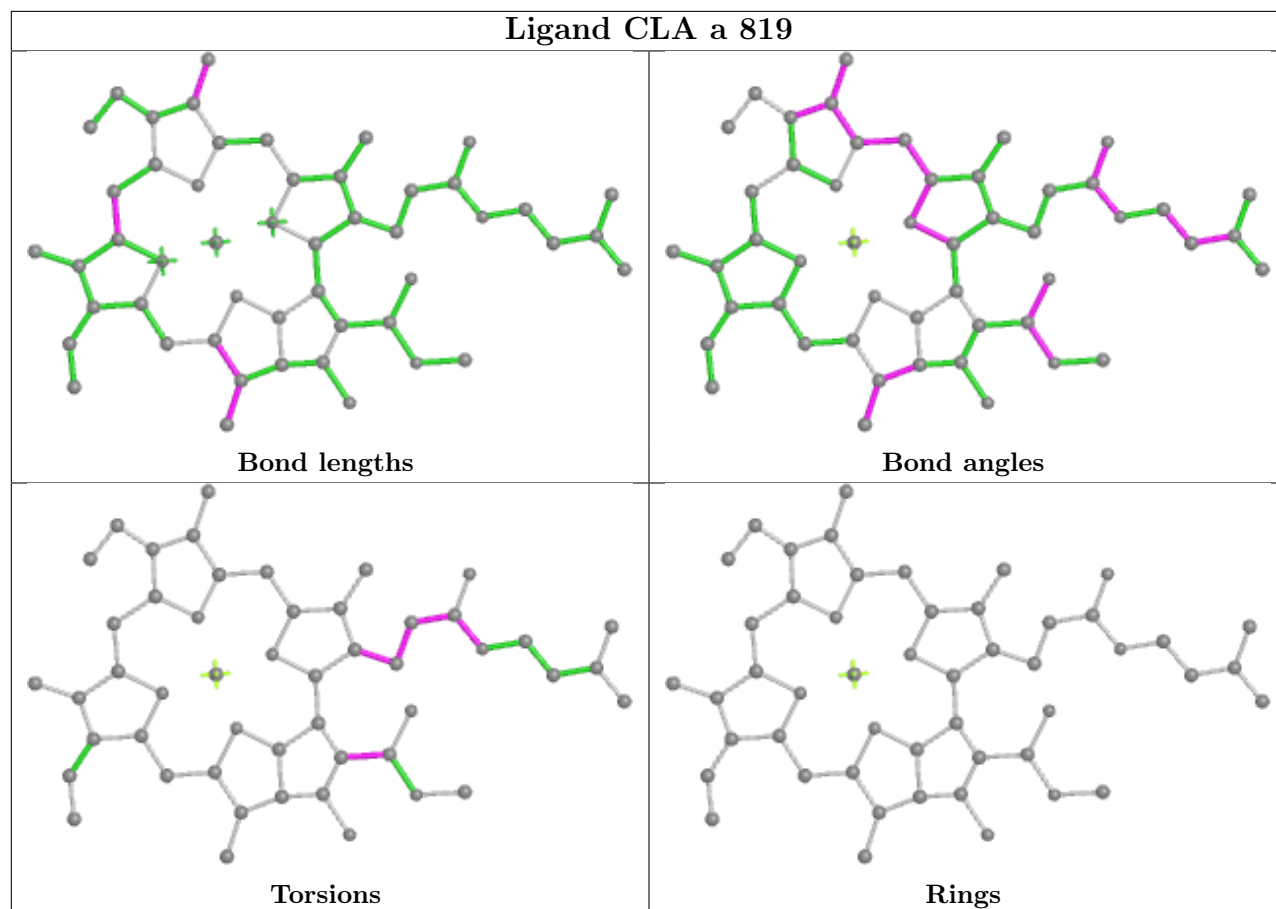
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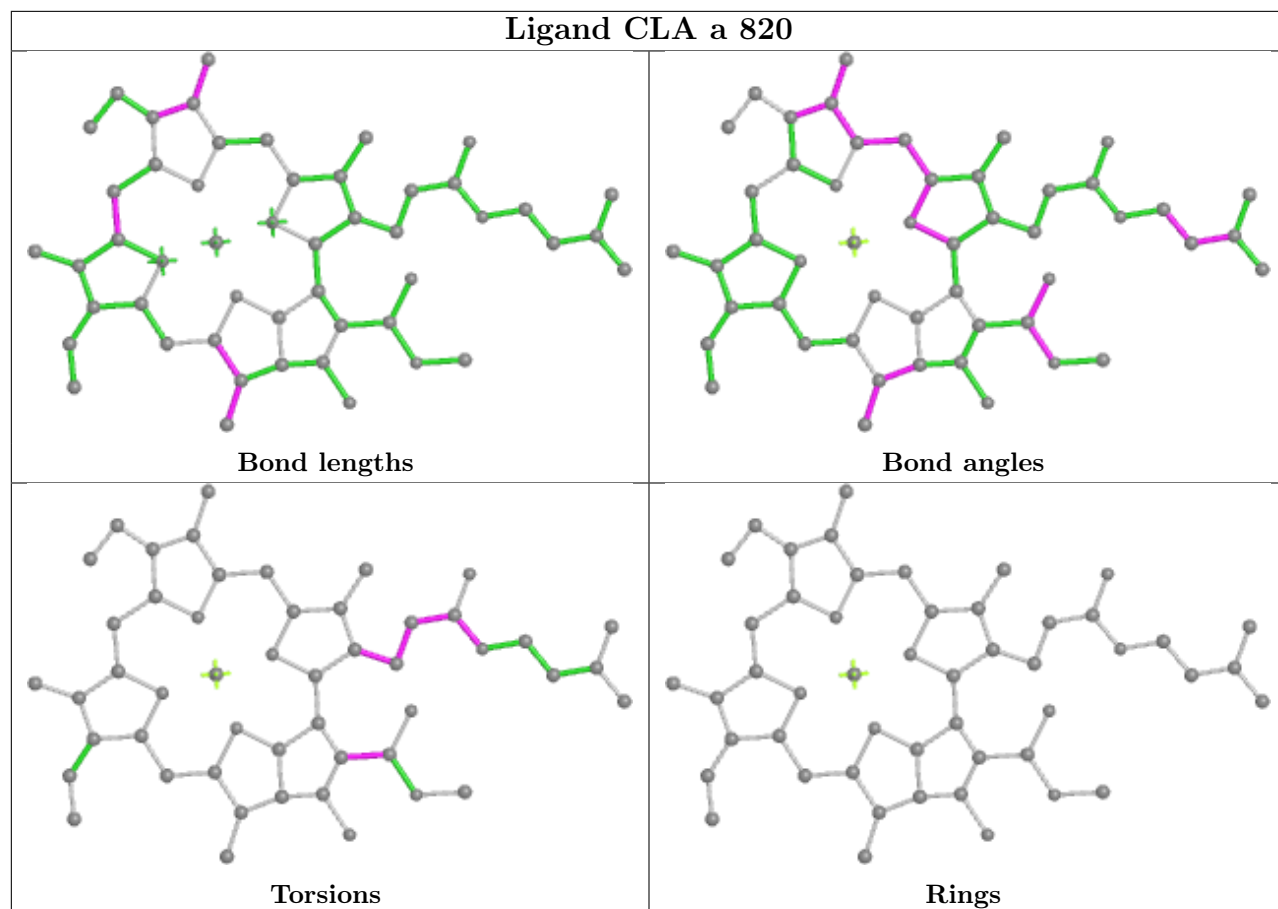
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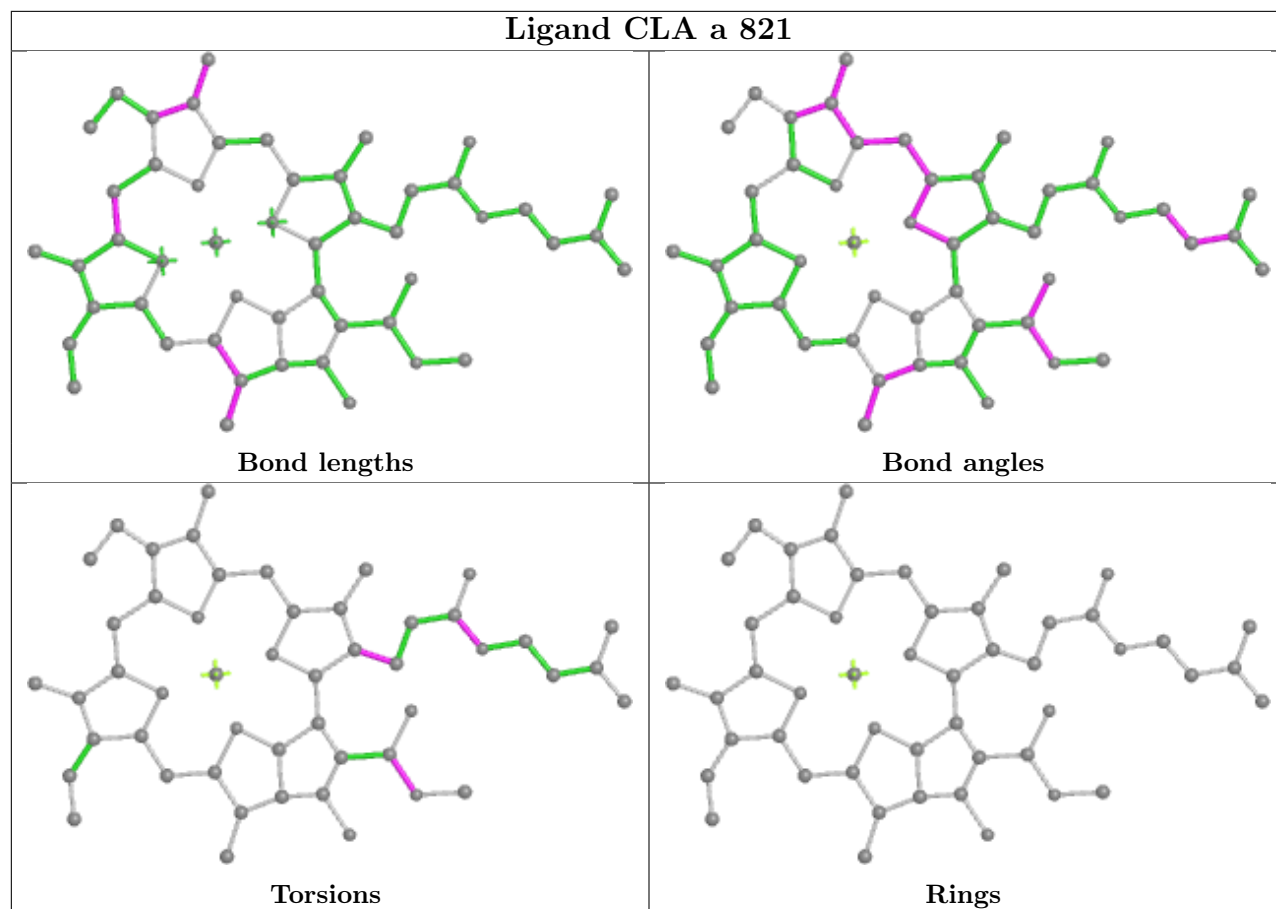
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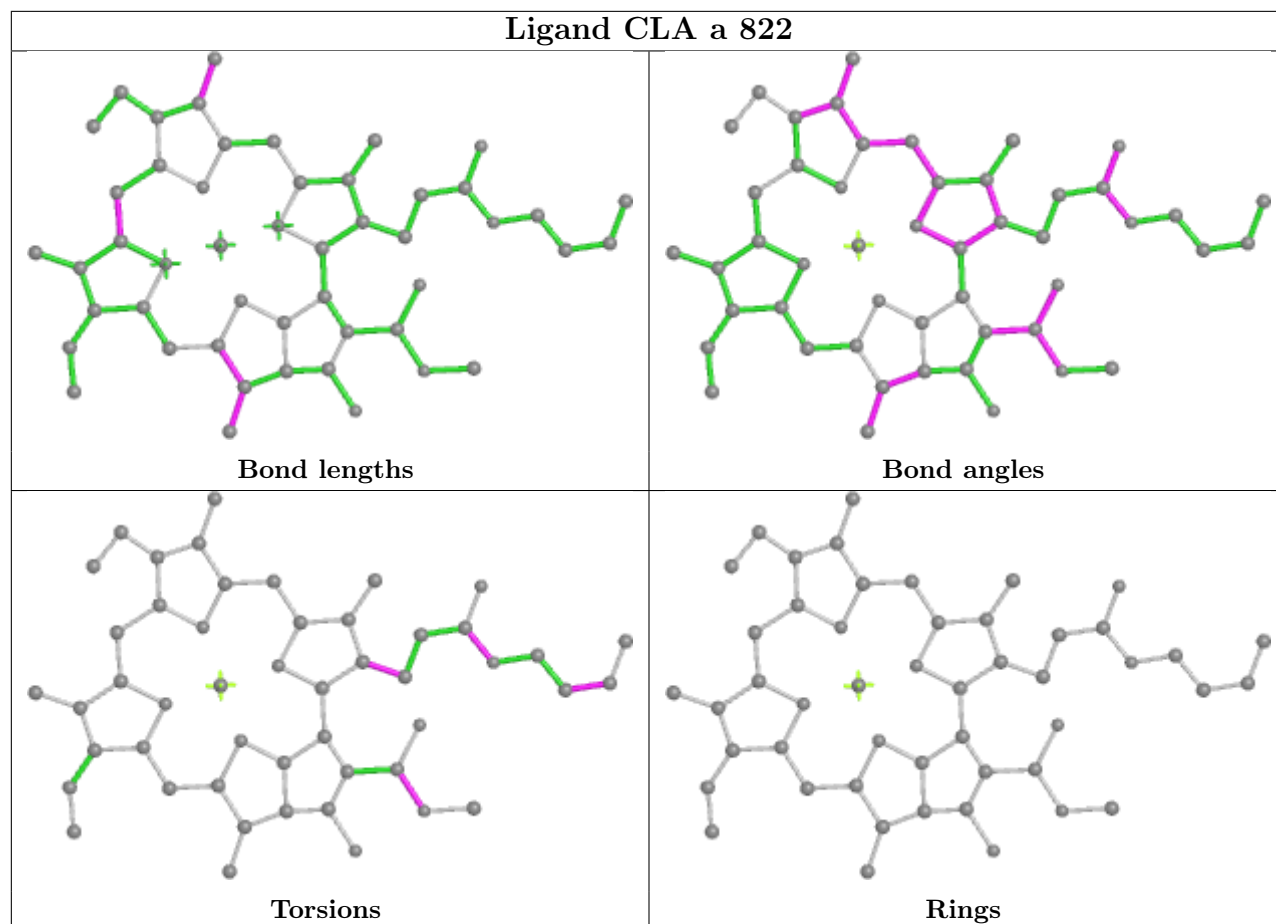
Ligand CLA a 820



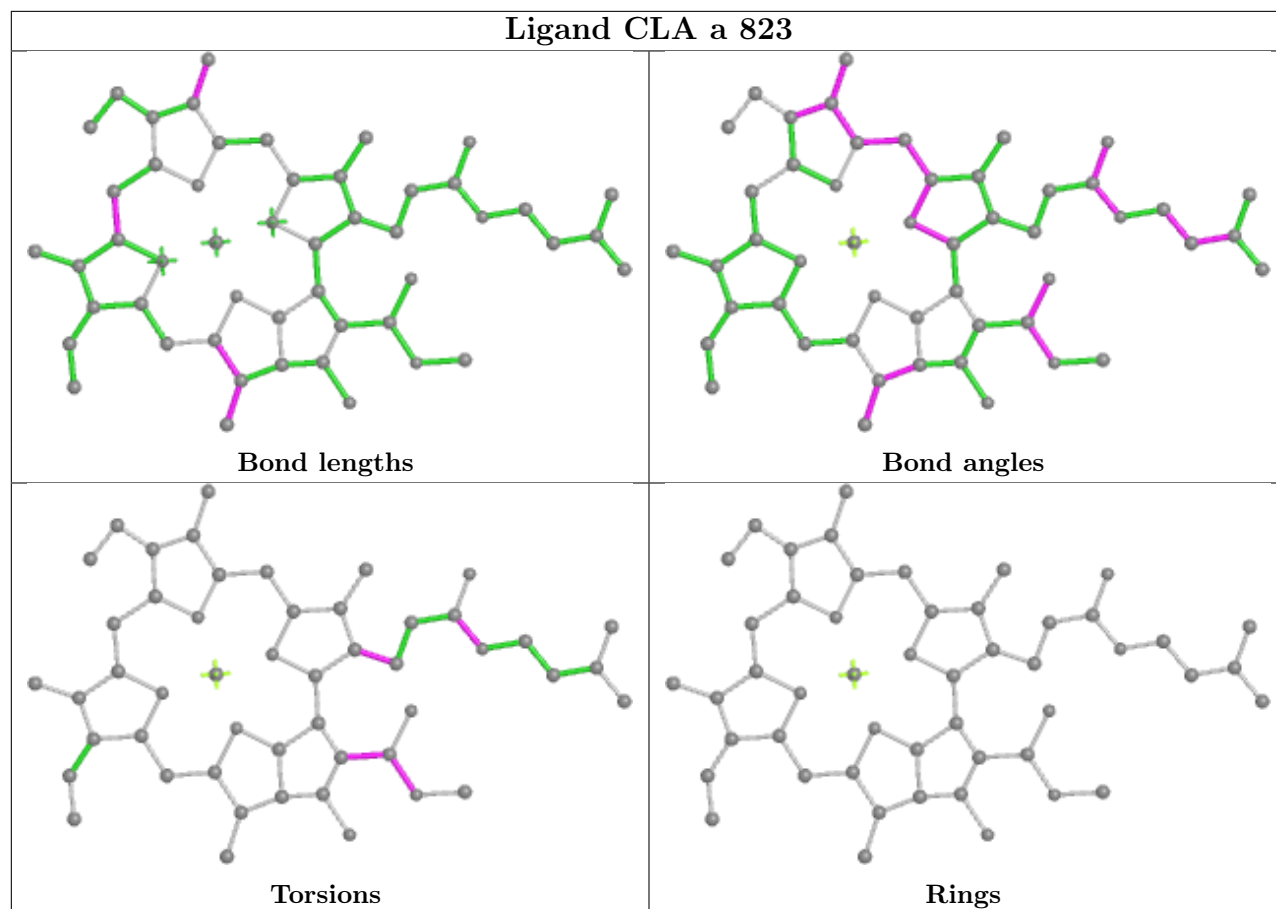
Ligand CLA a 821



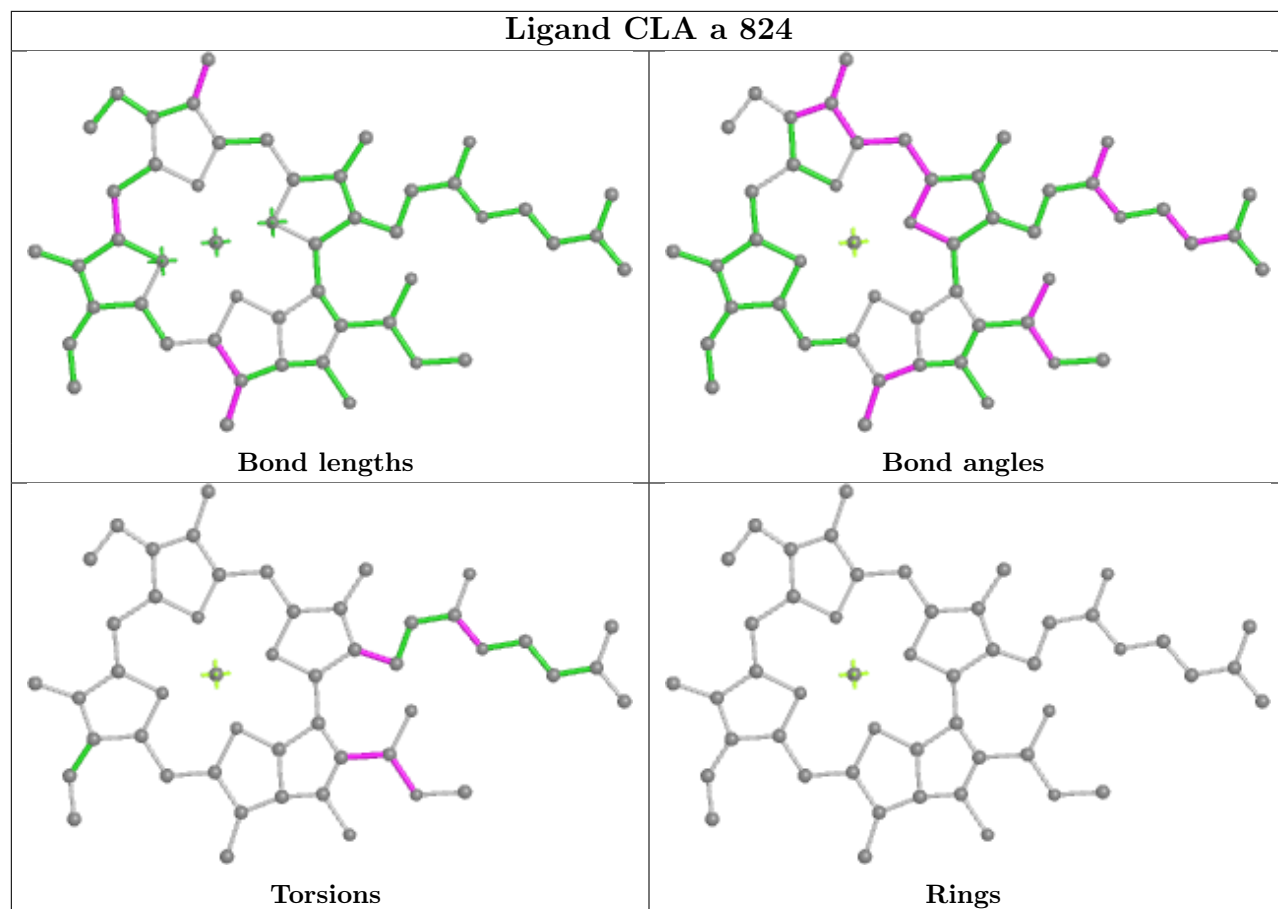
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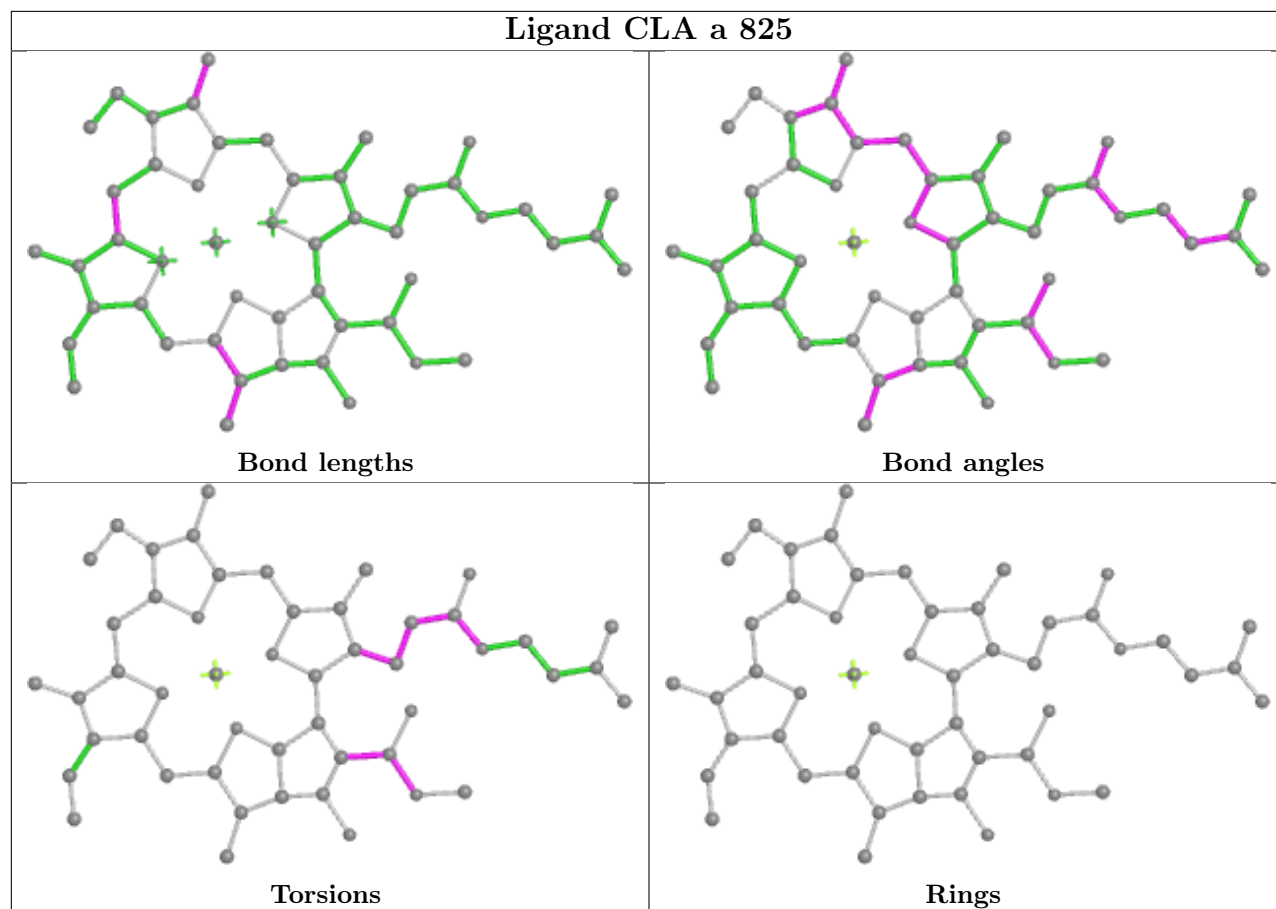
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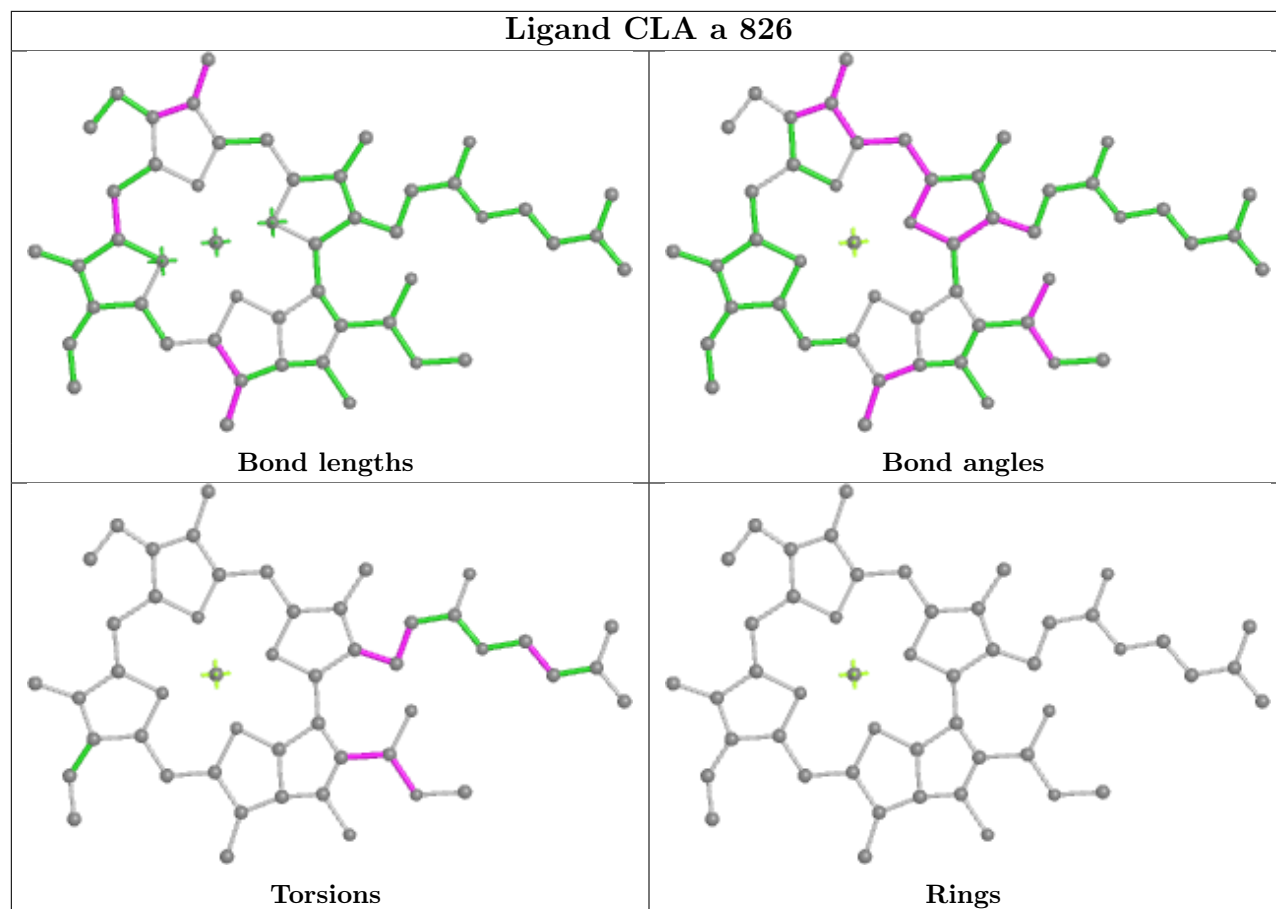
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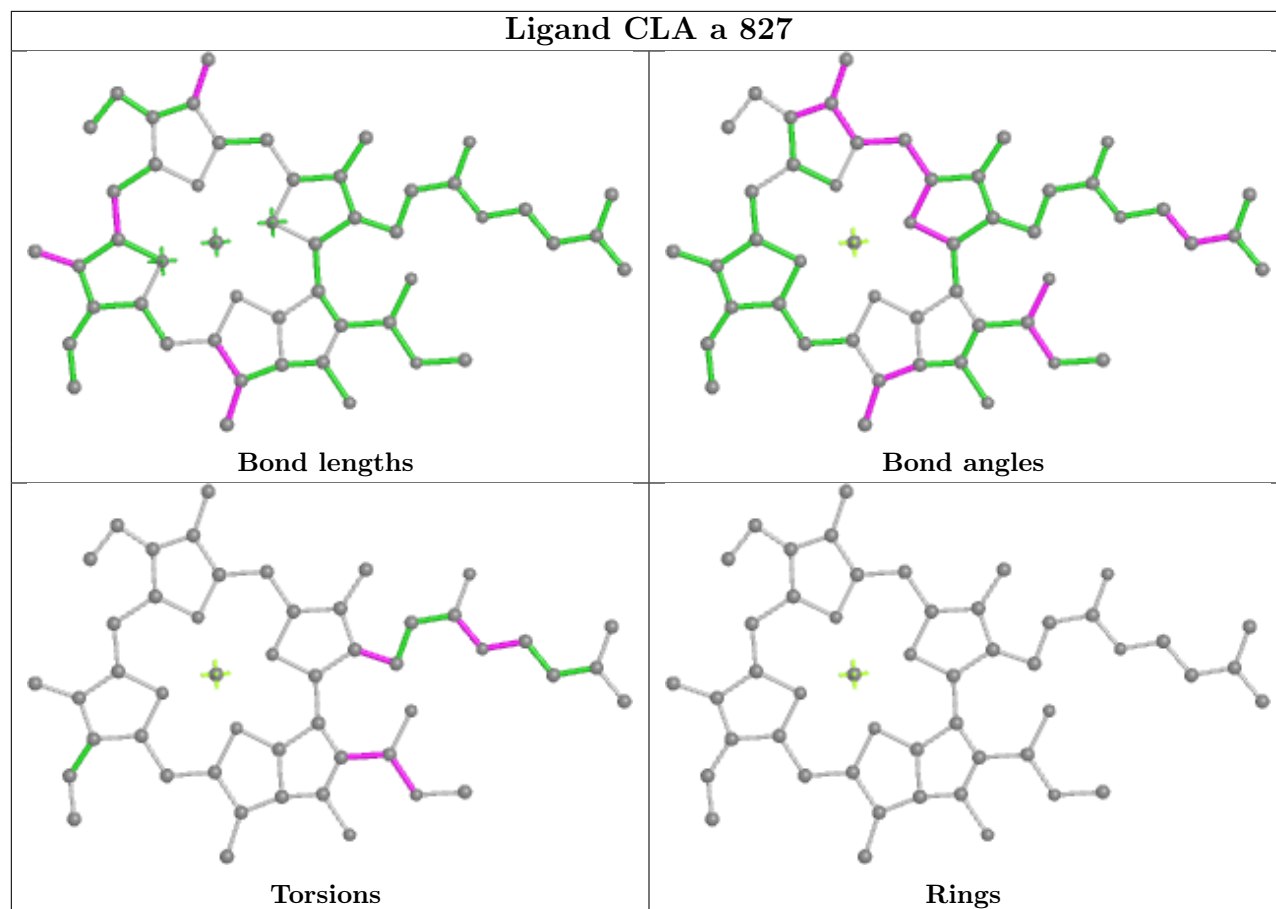
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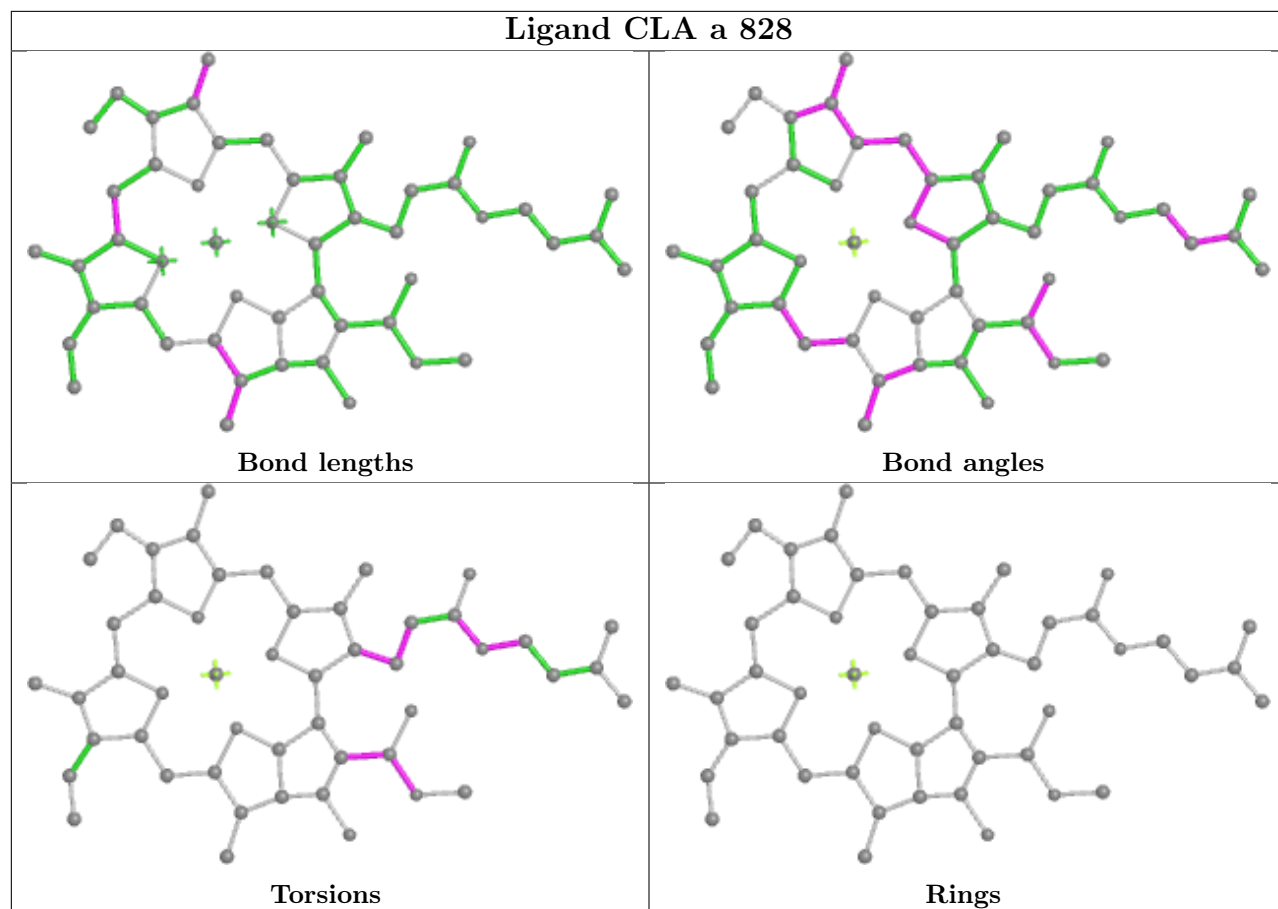
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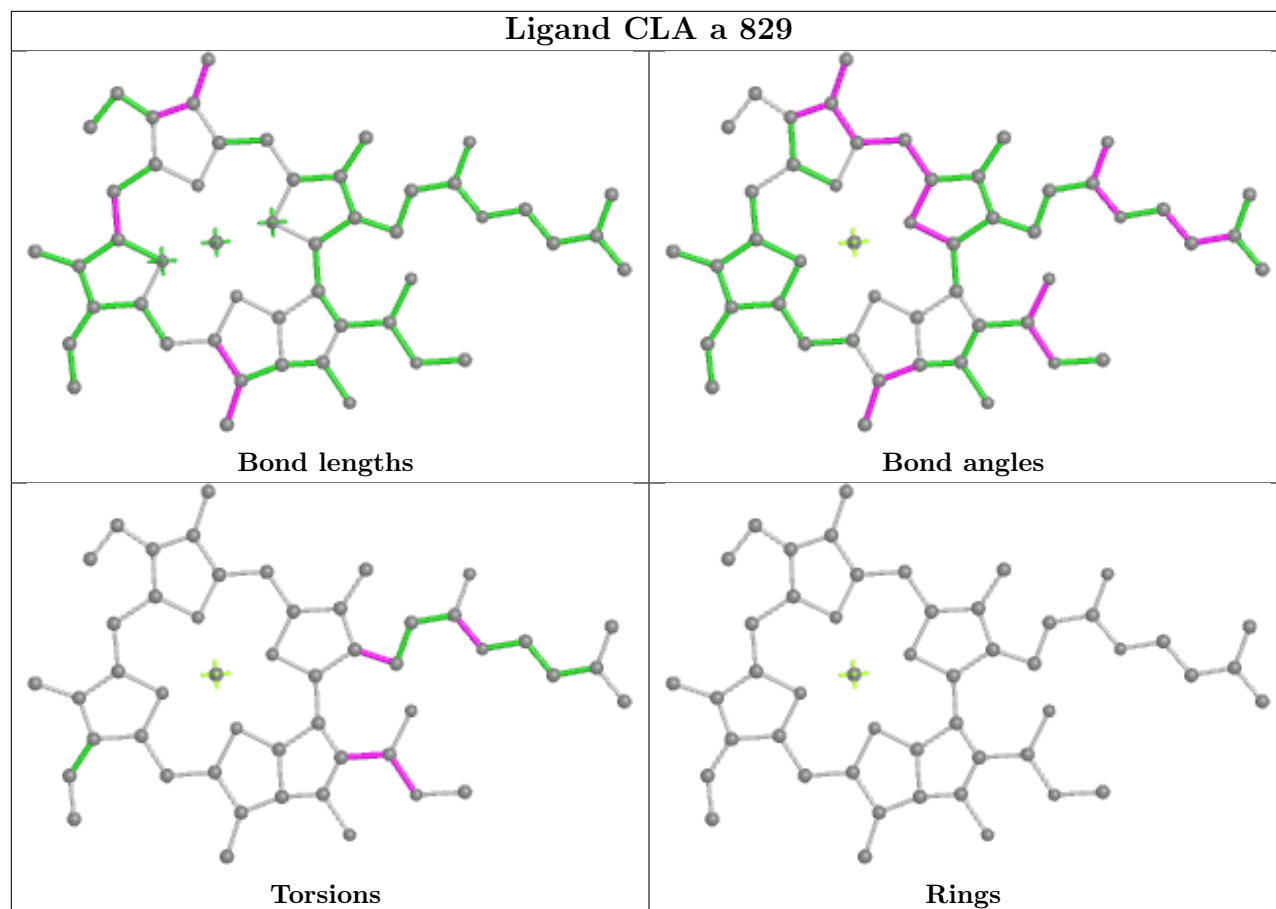
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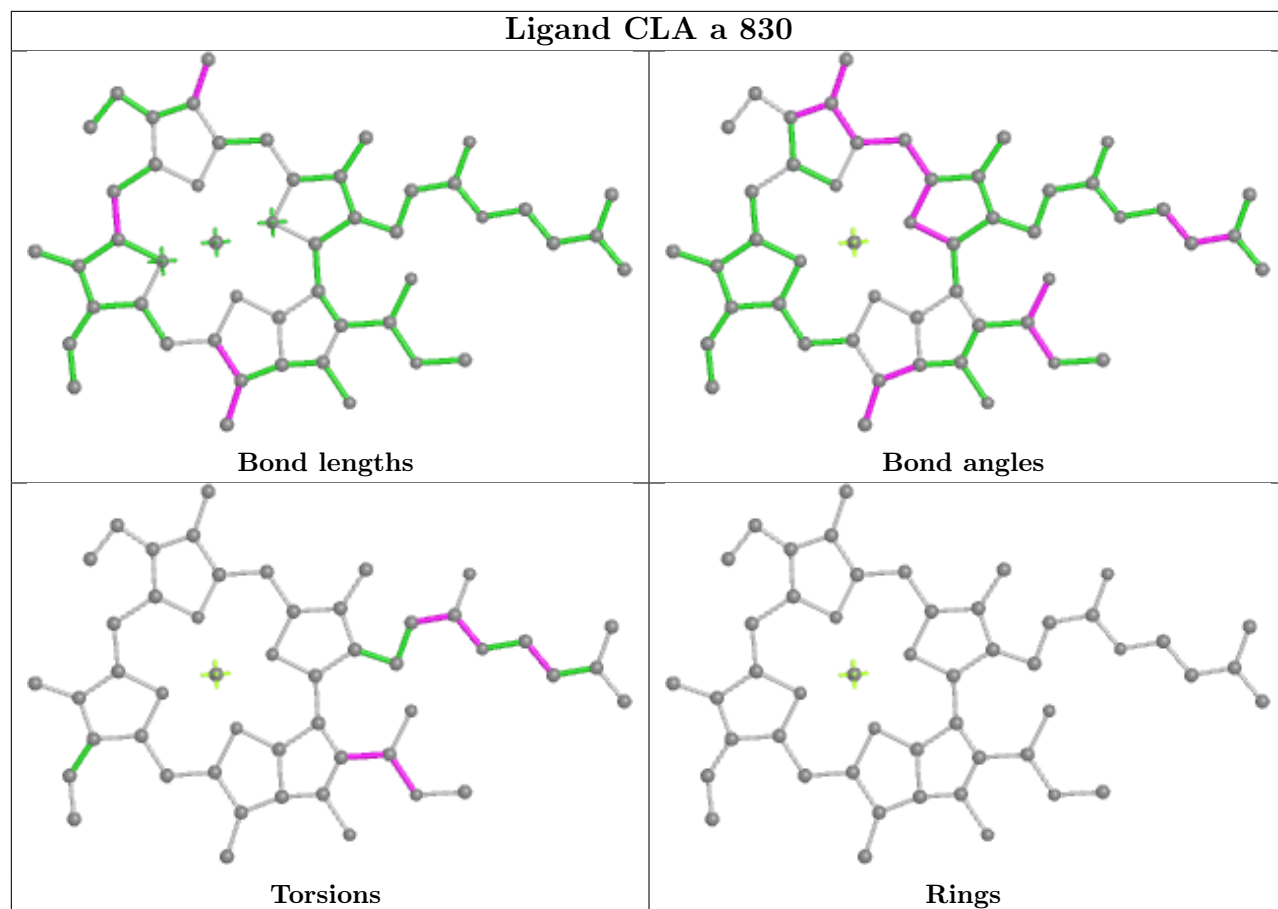
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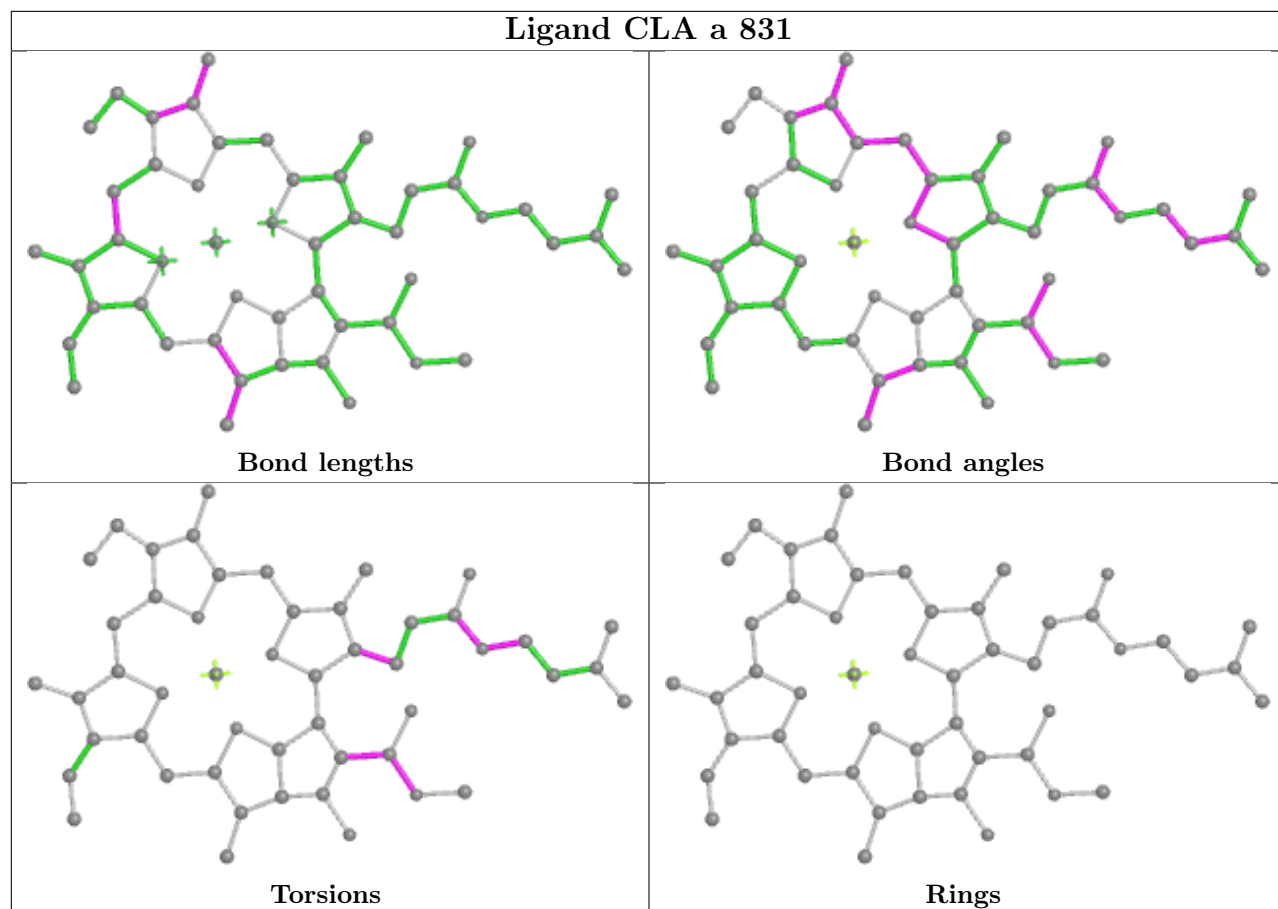
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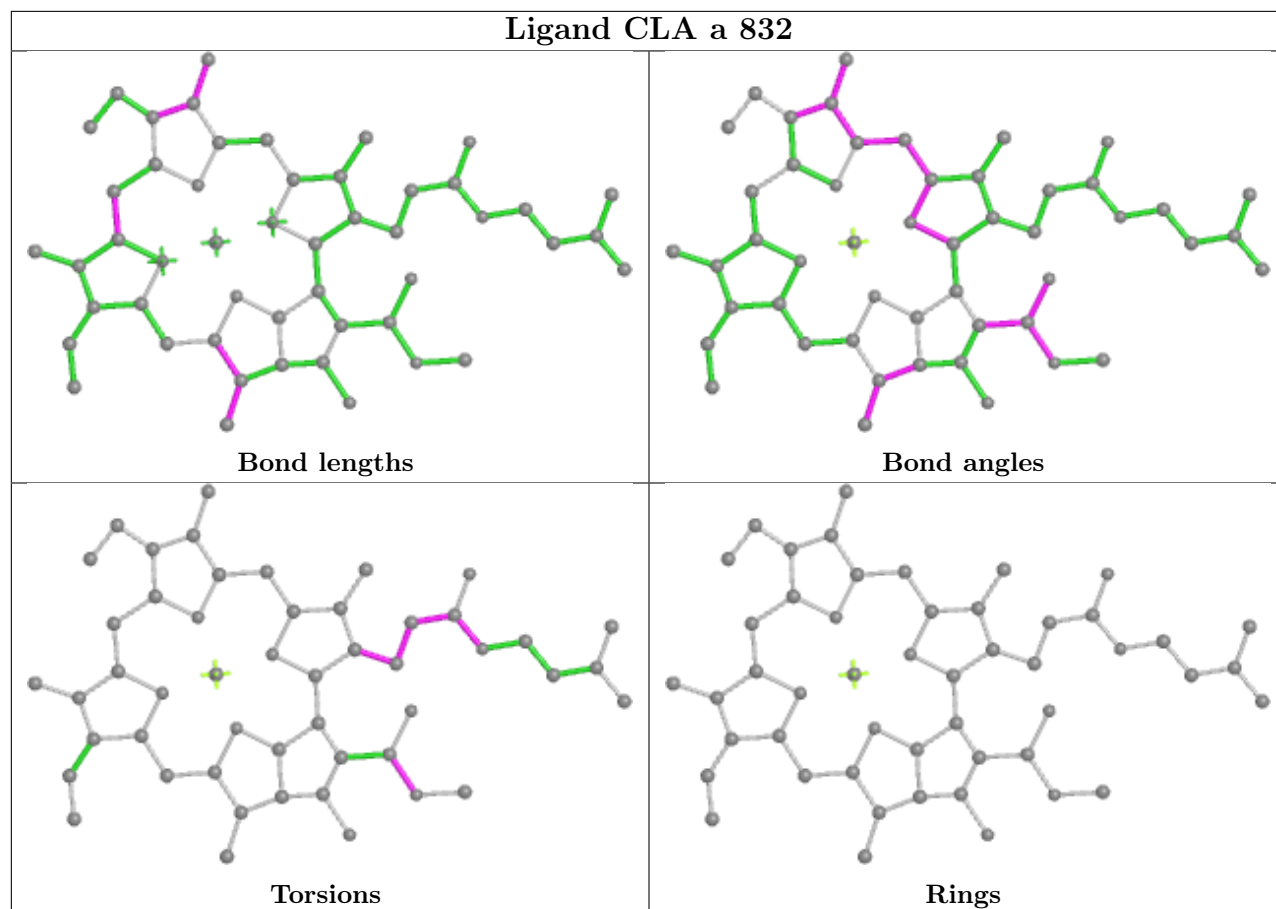
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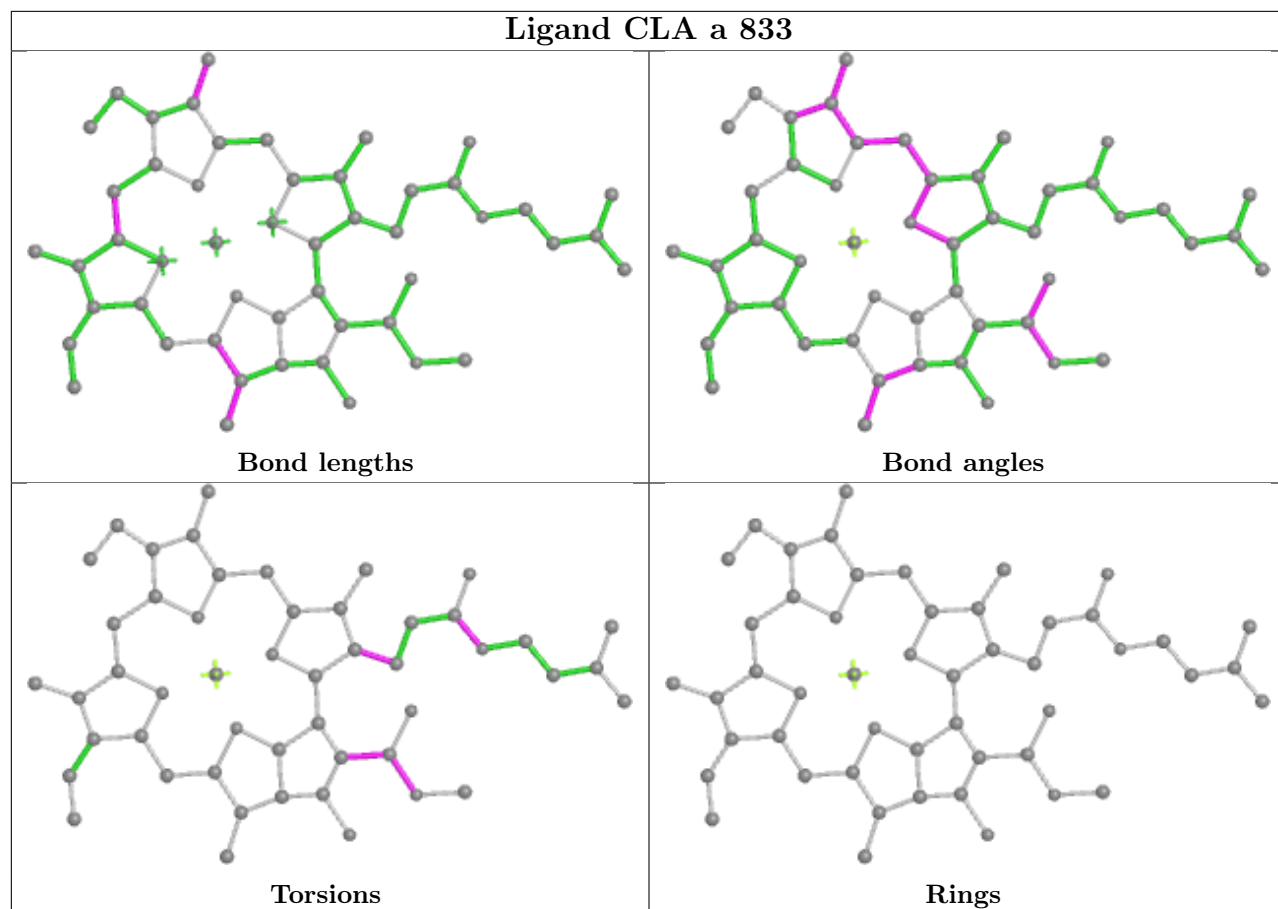
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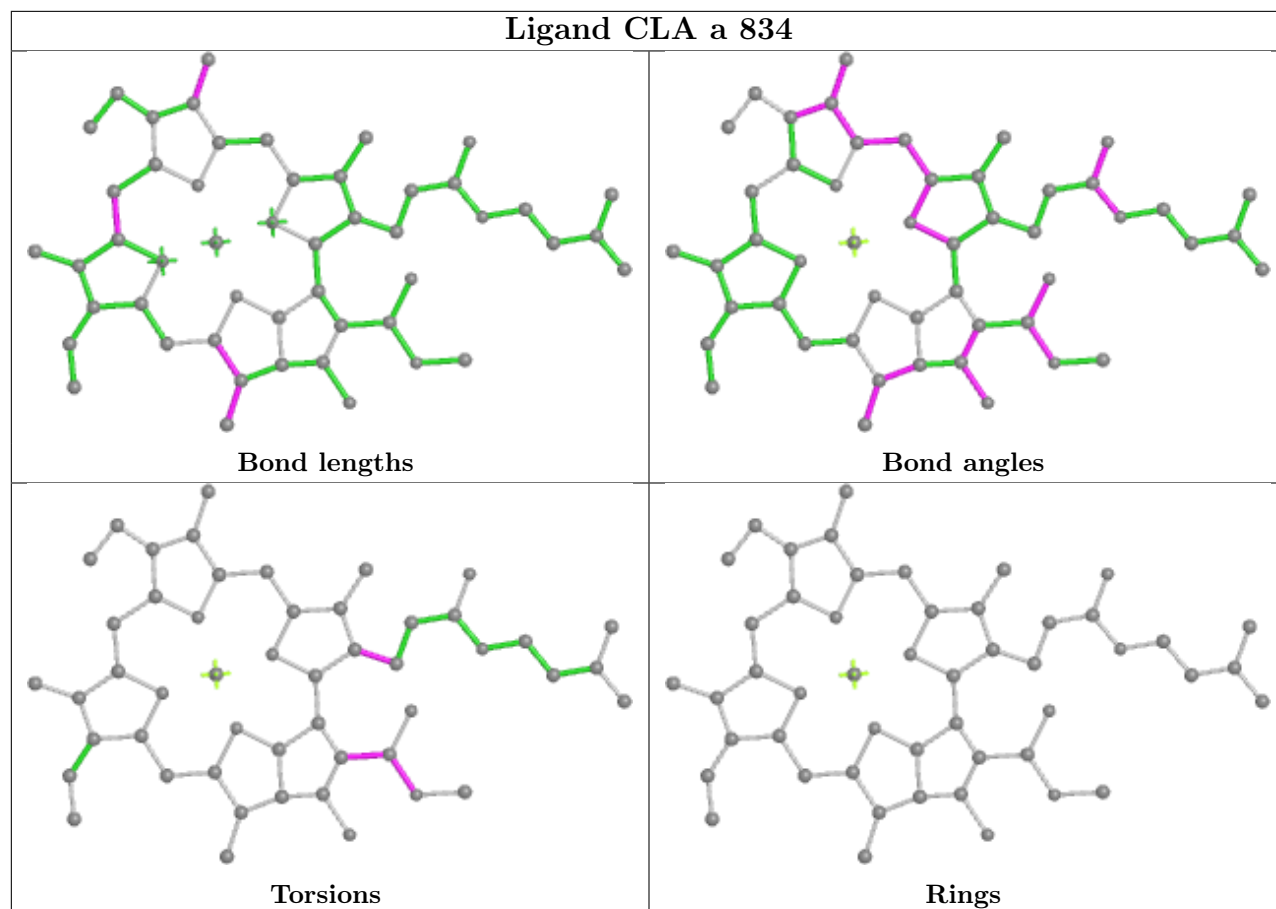
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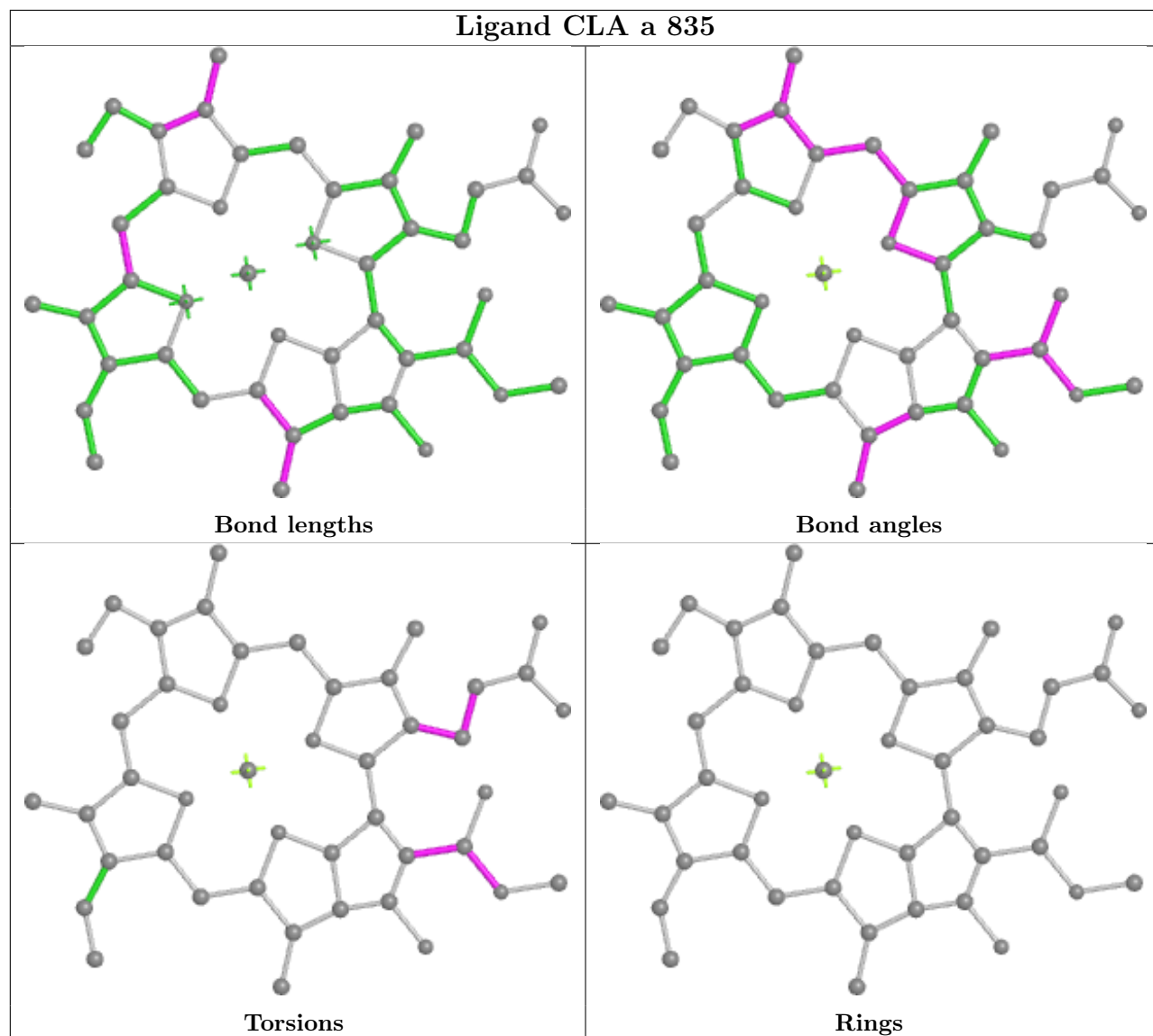
Ligand CLA a 833



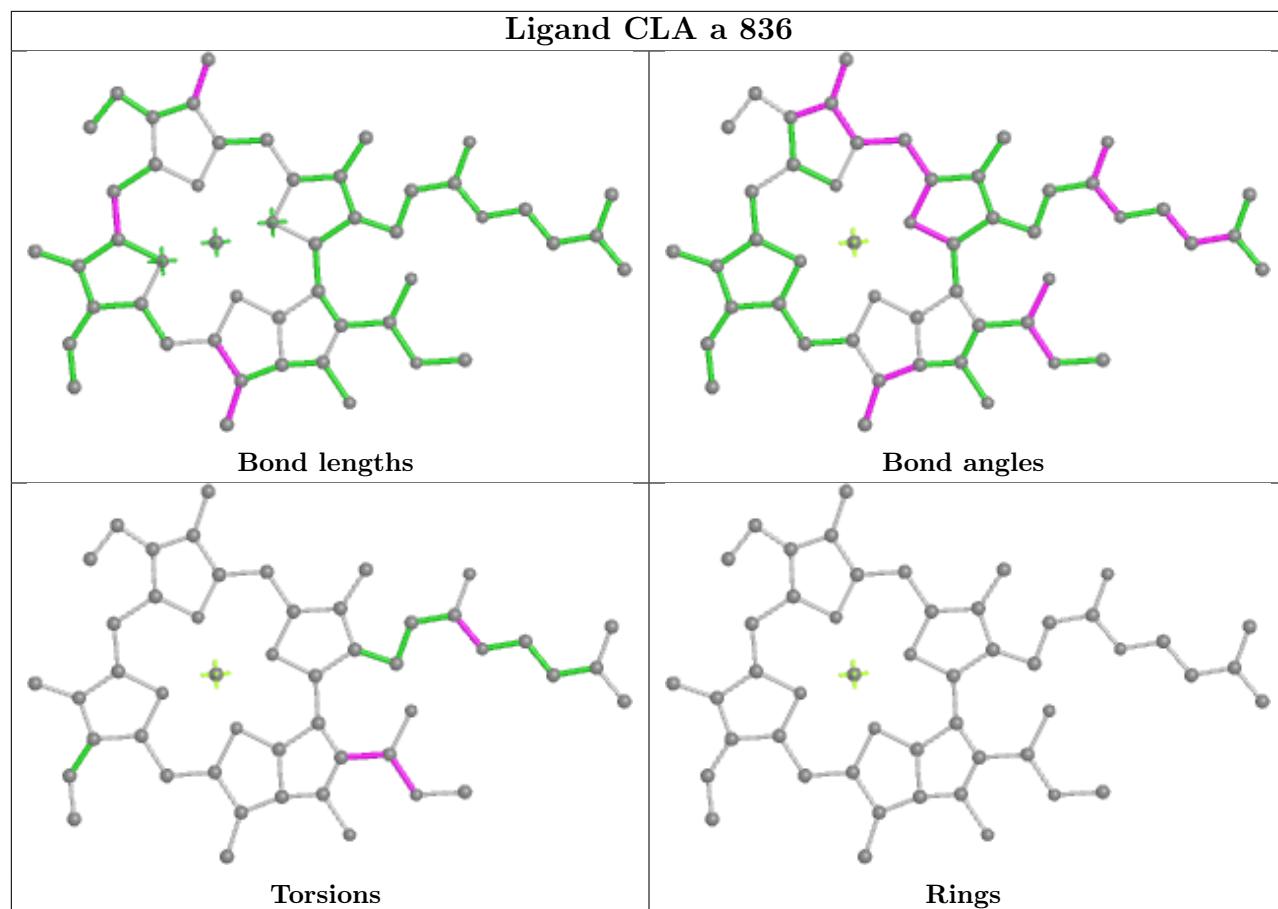
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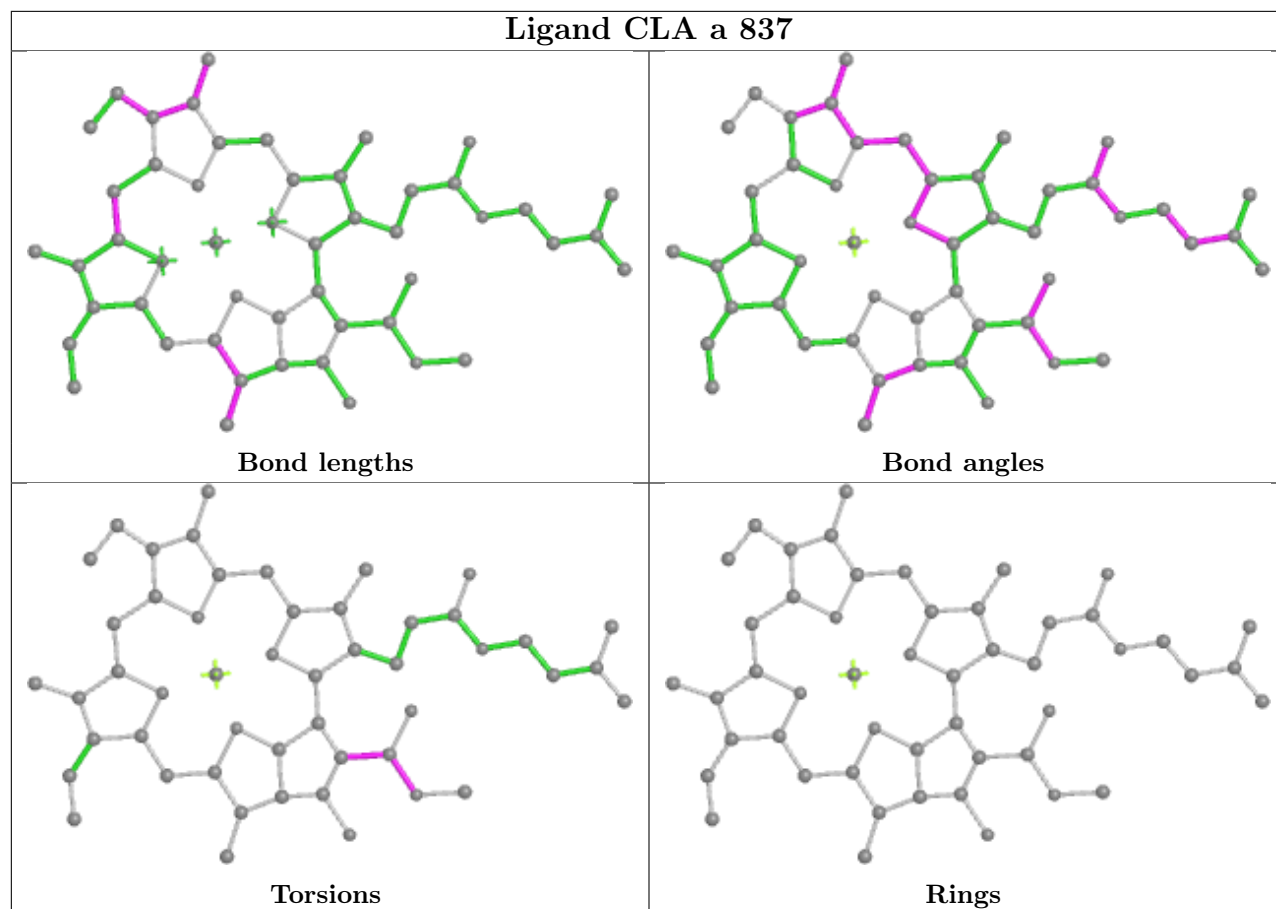
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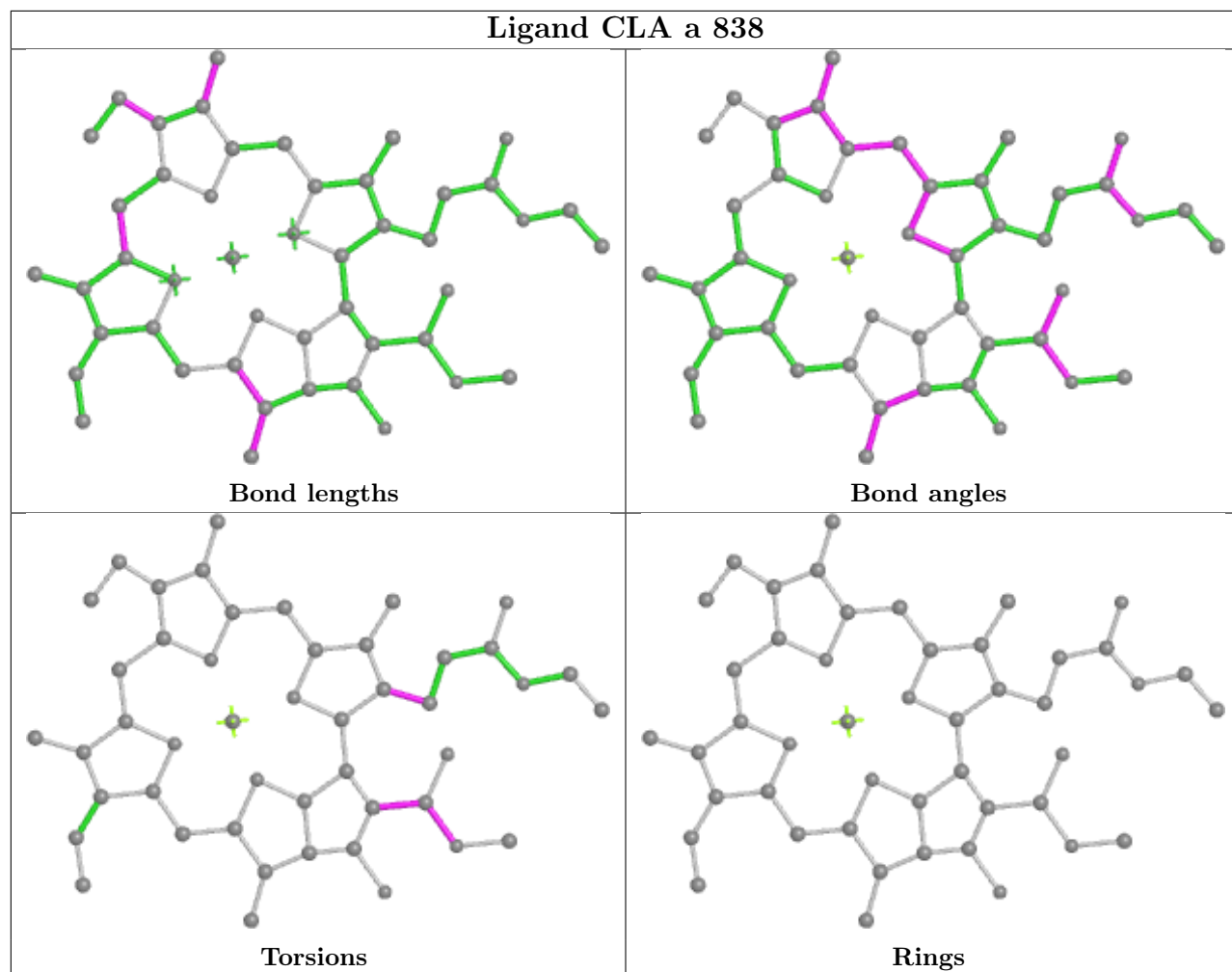
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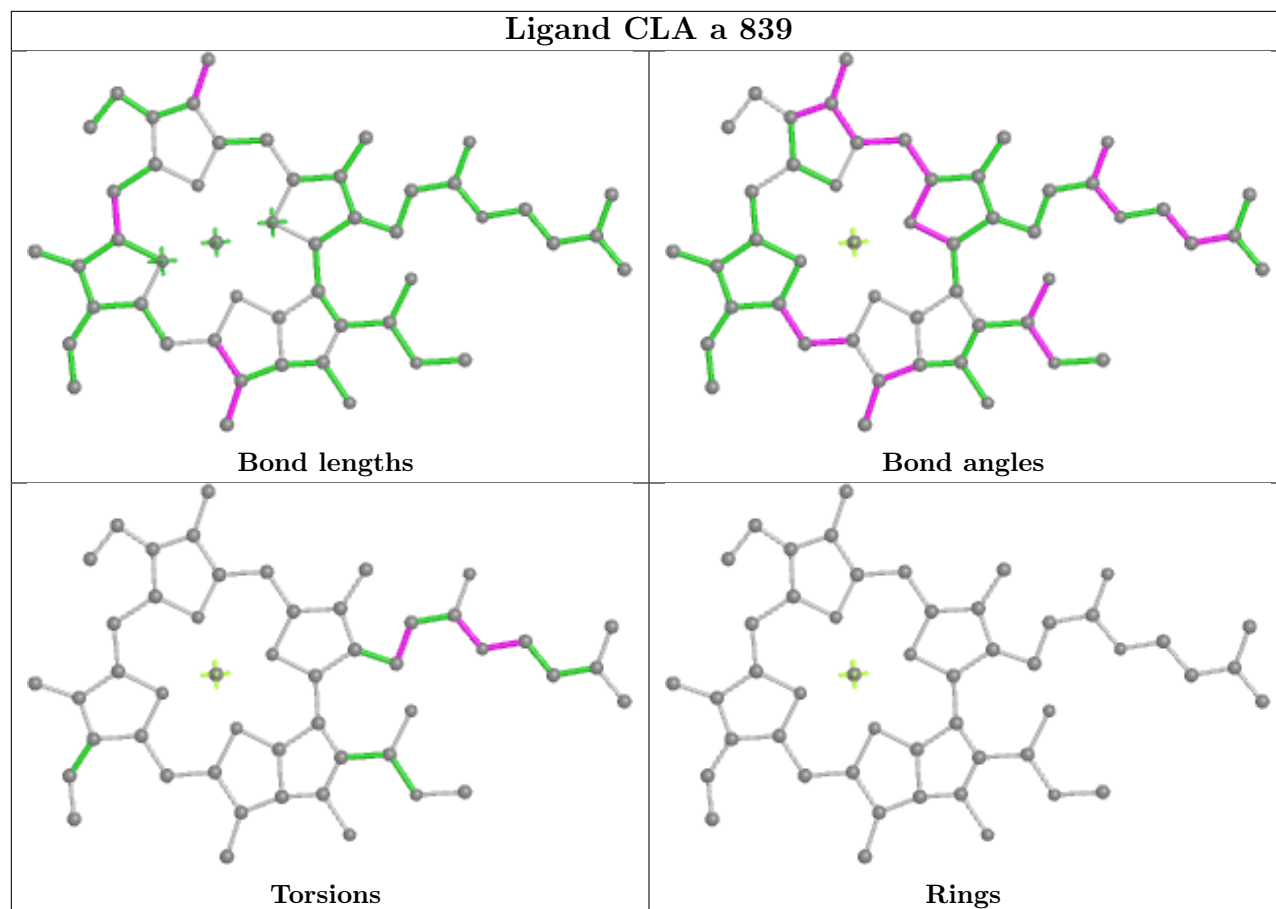
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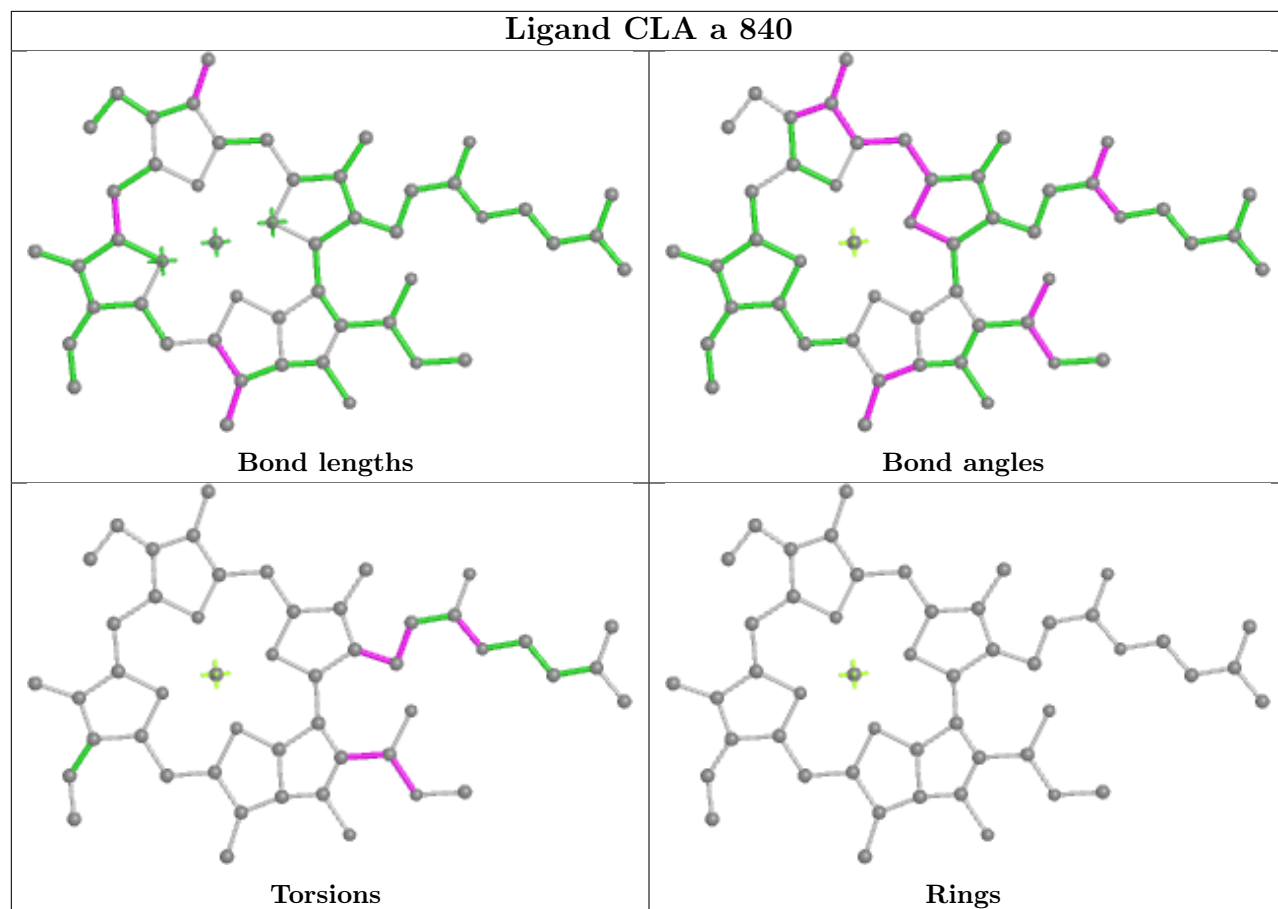
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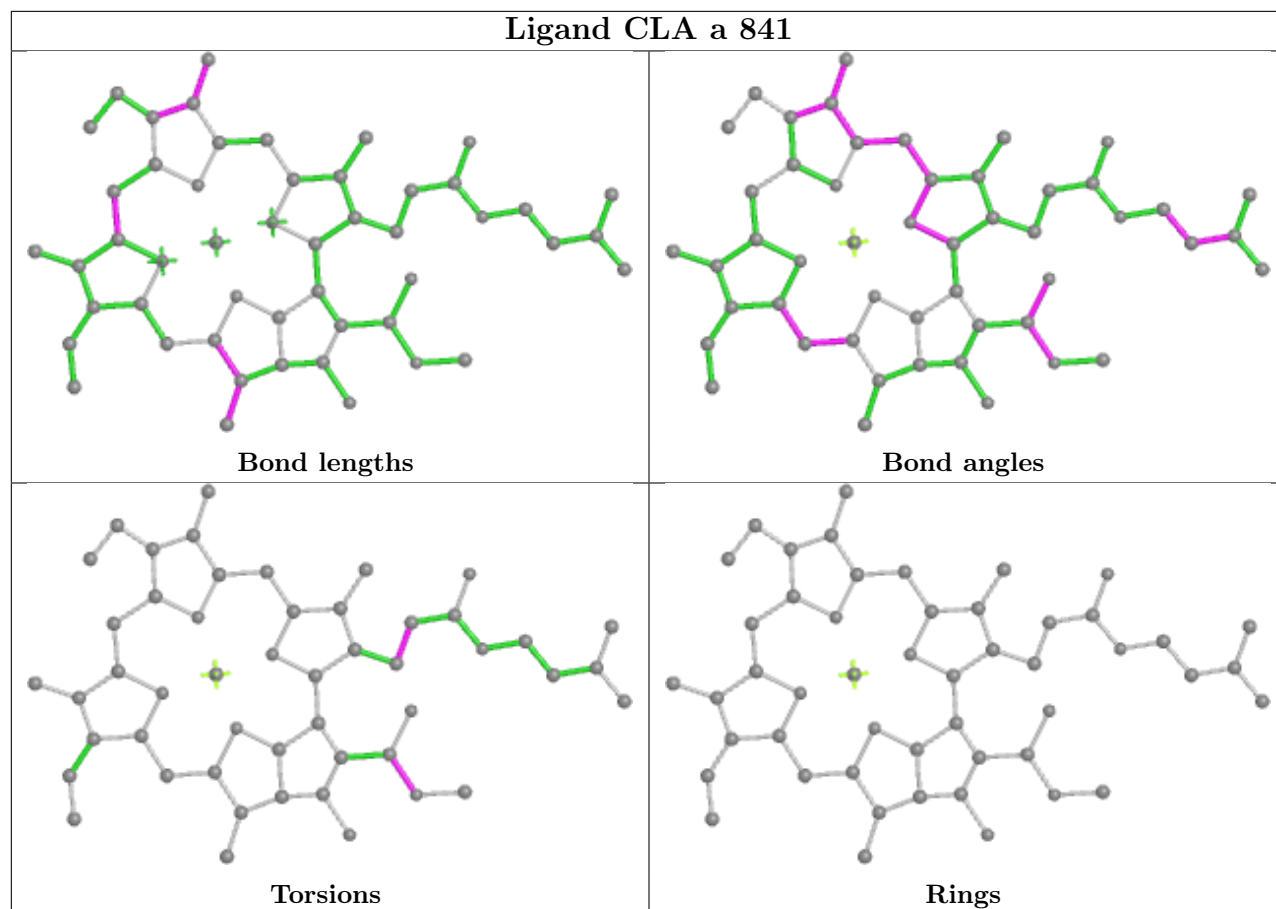
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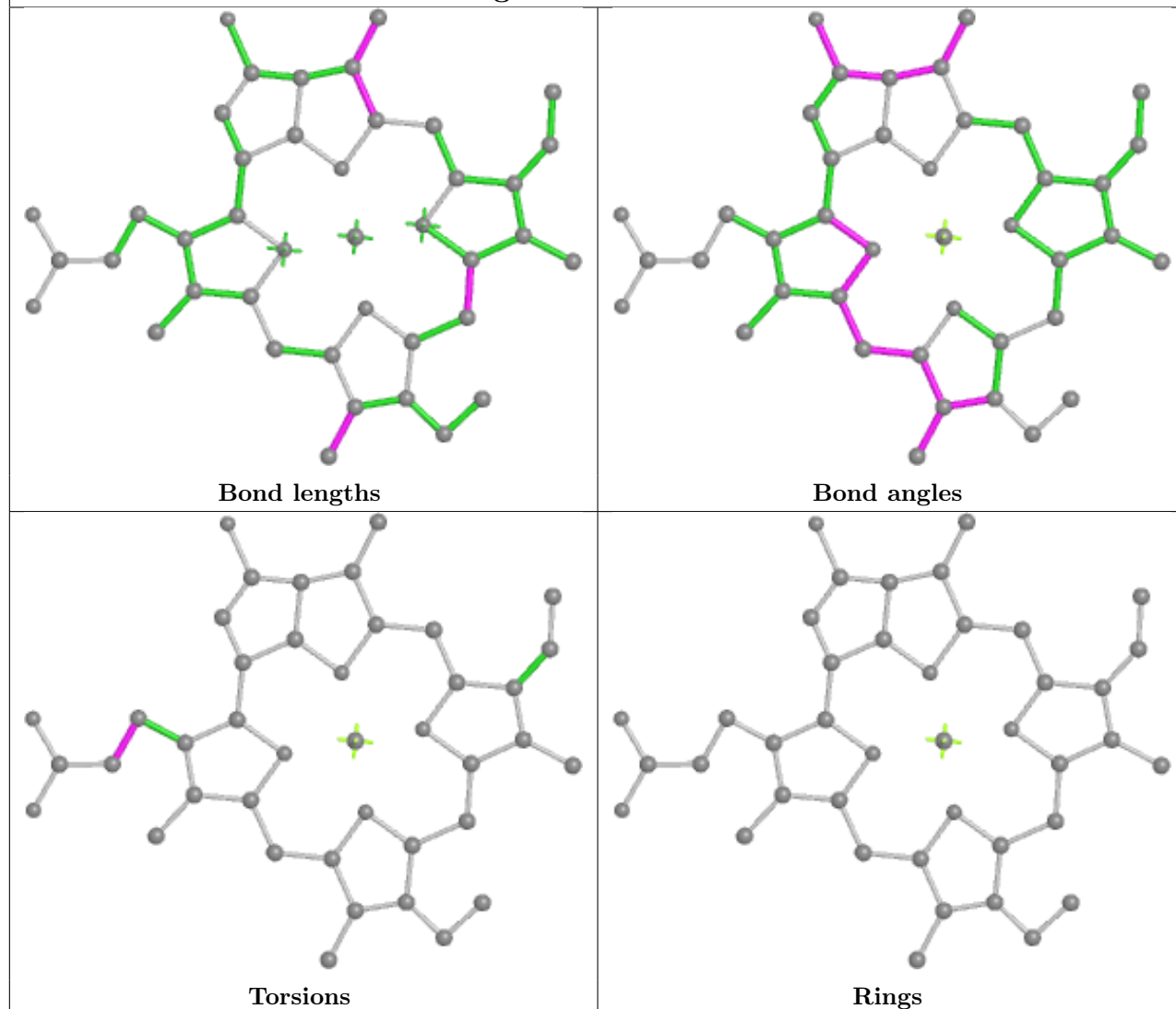
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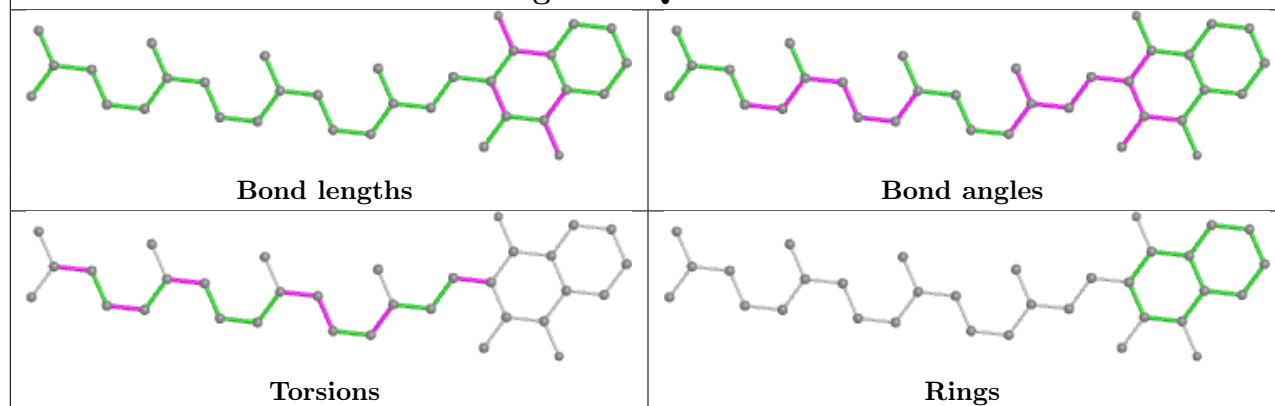
Ligand CLA a 841



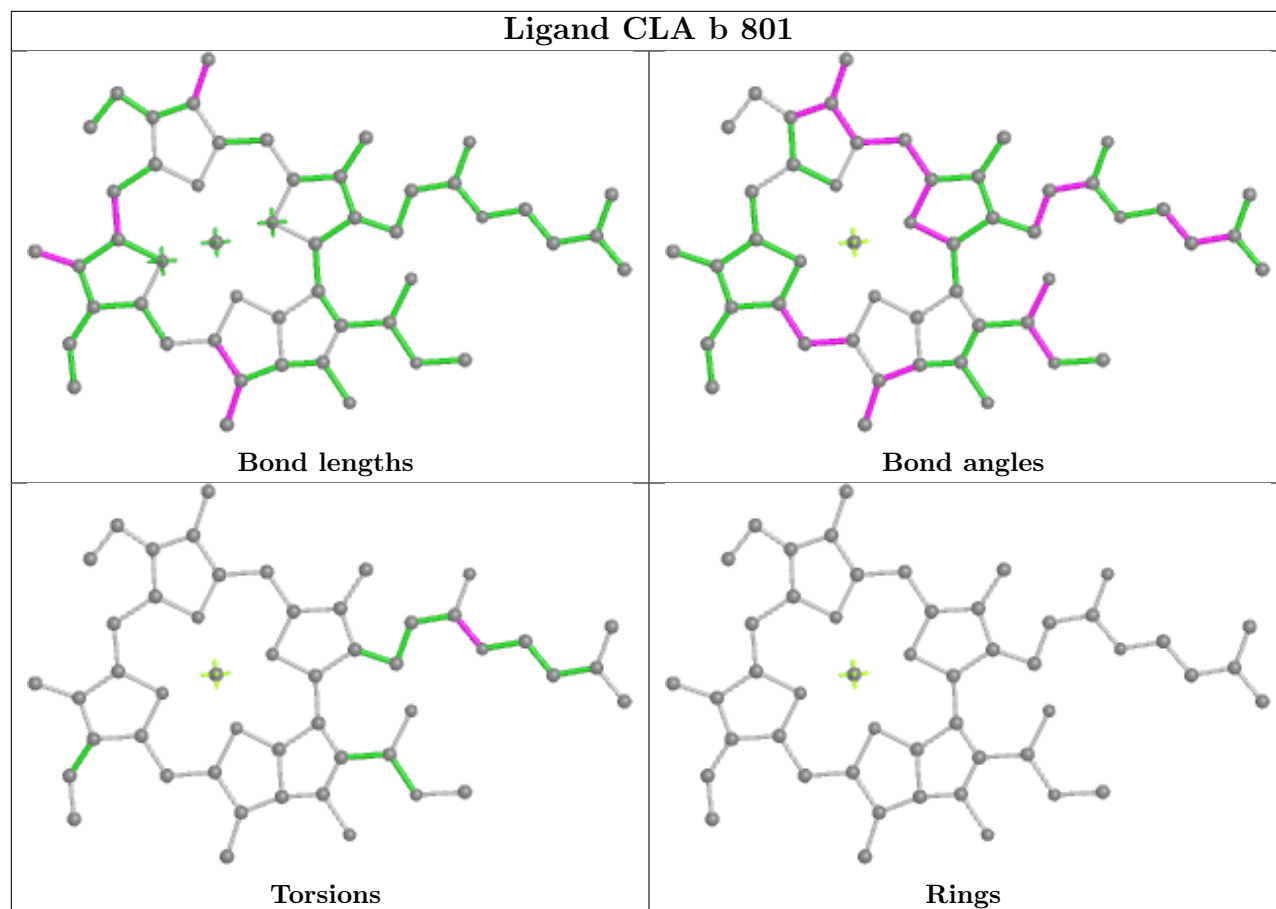
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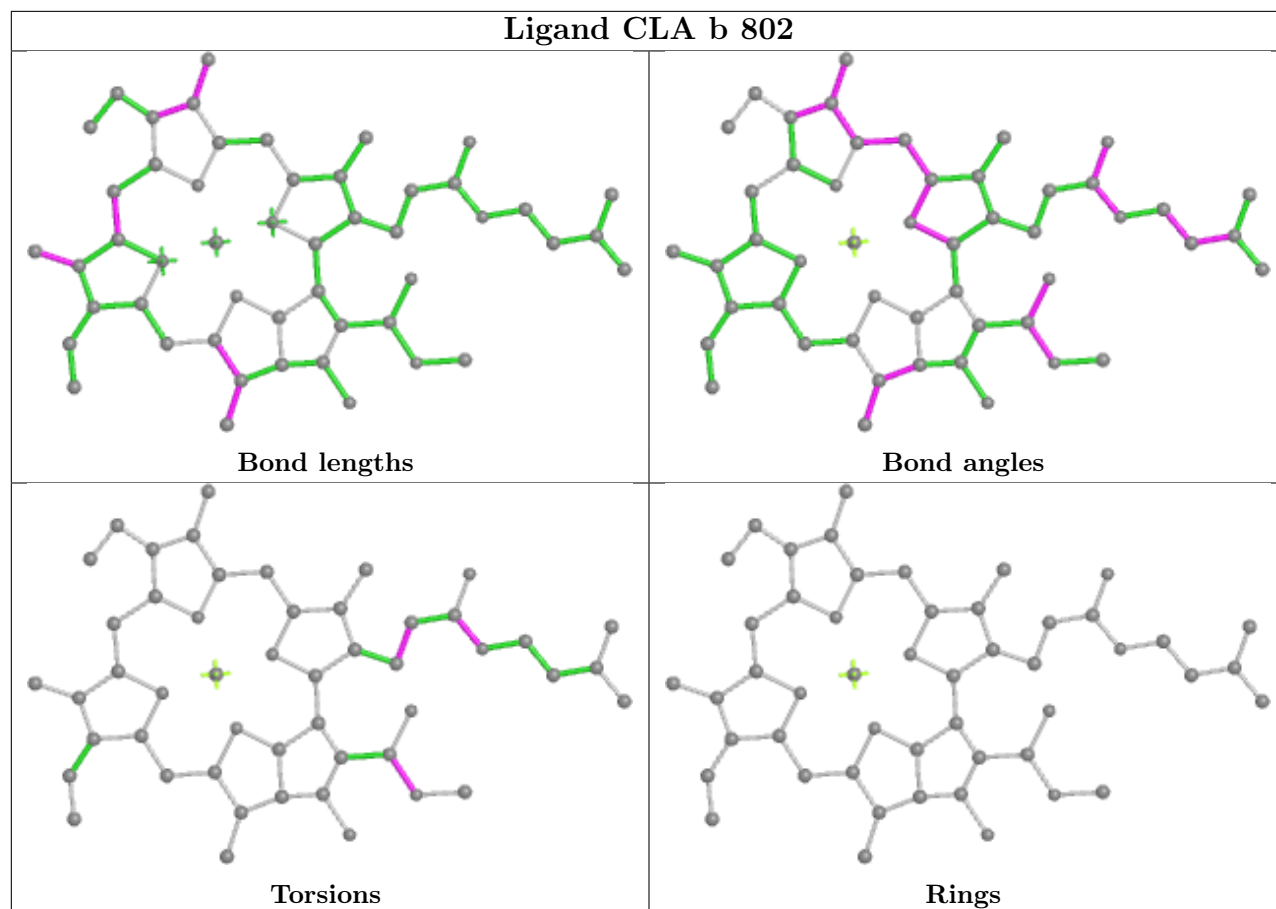
Ligand PQN a 844



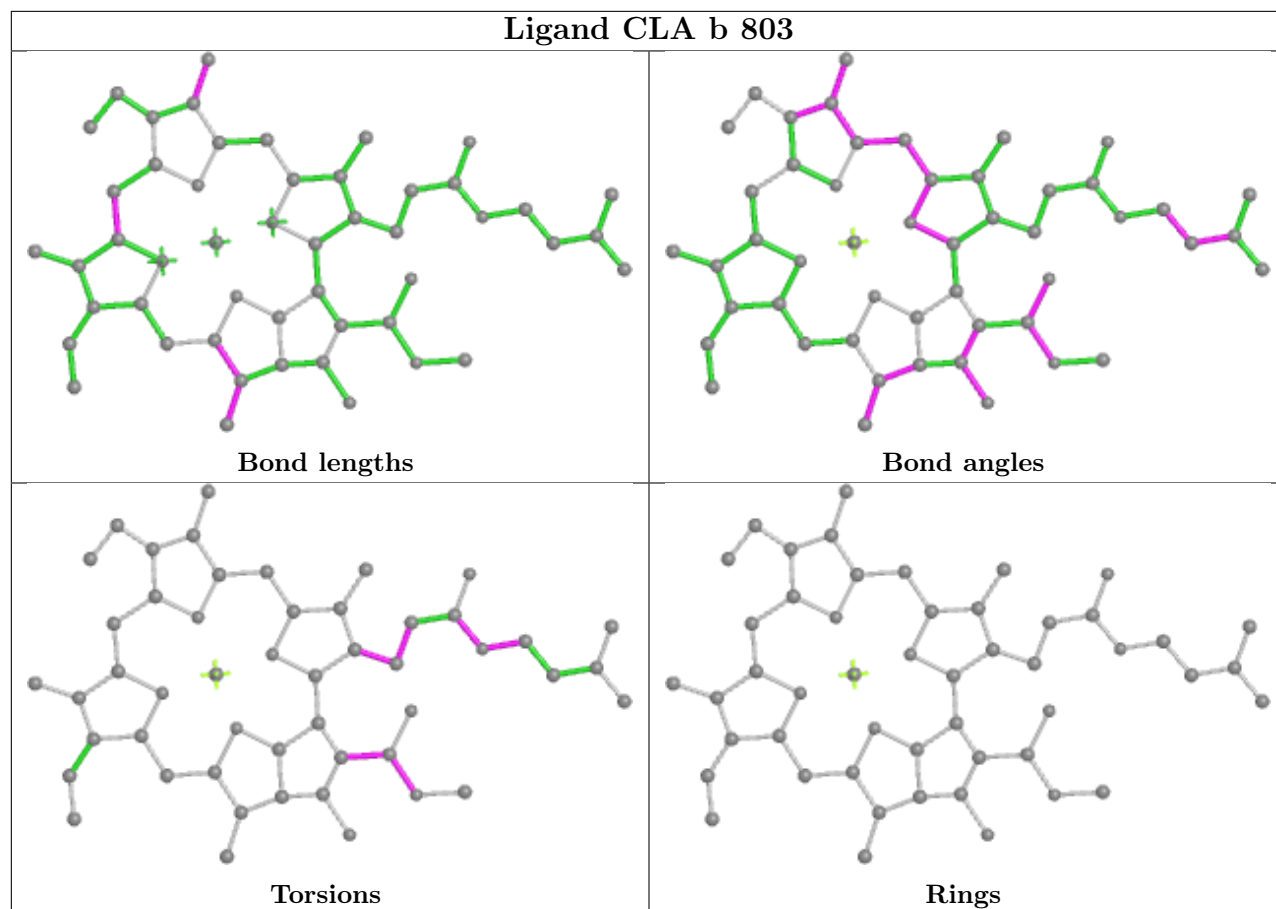
Ligand CLA b 801



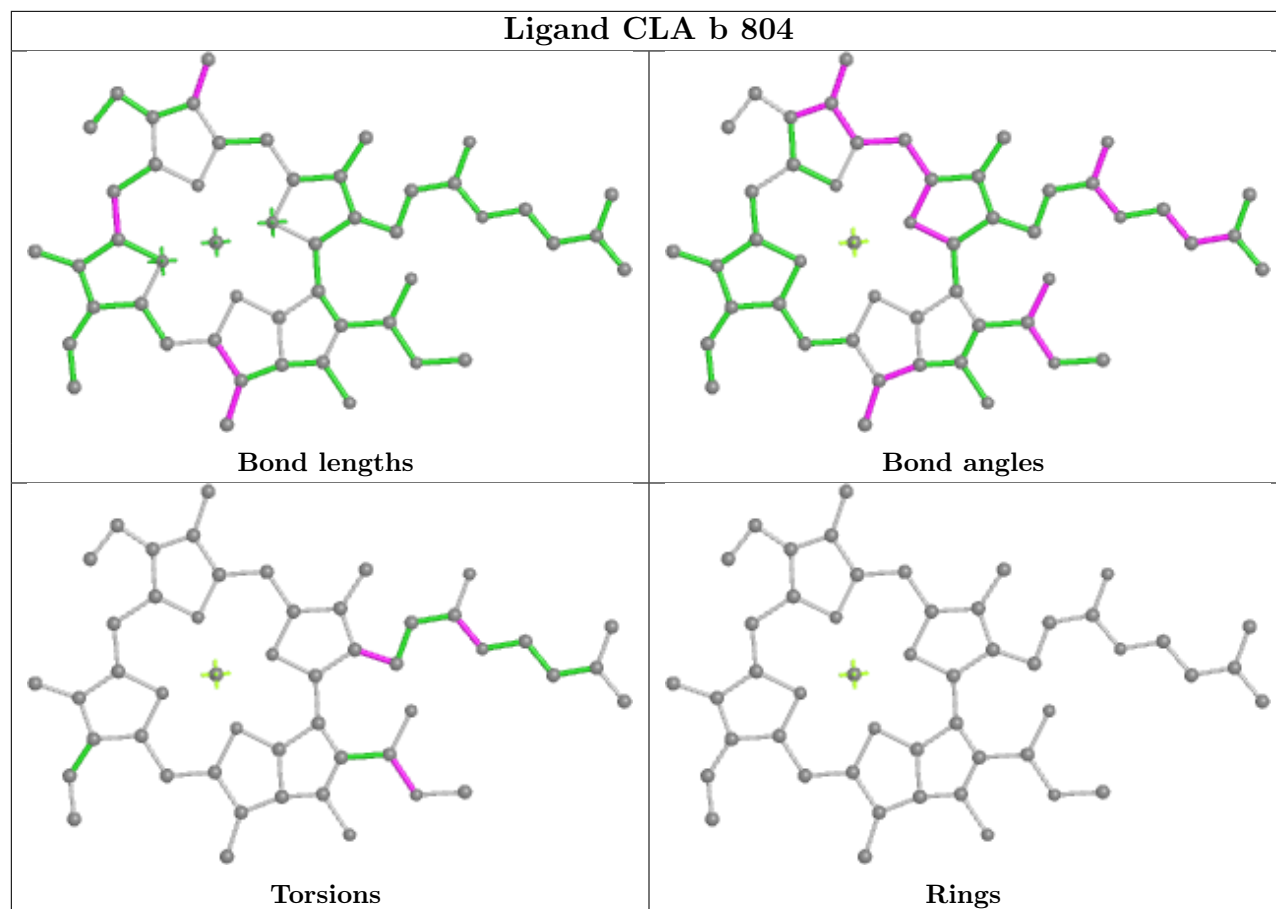
Ligand CLA b 802



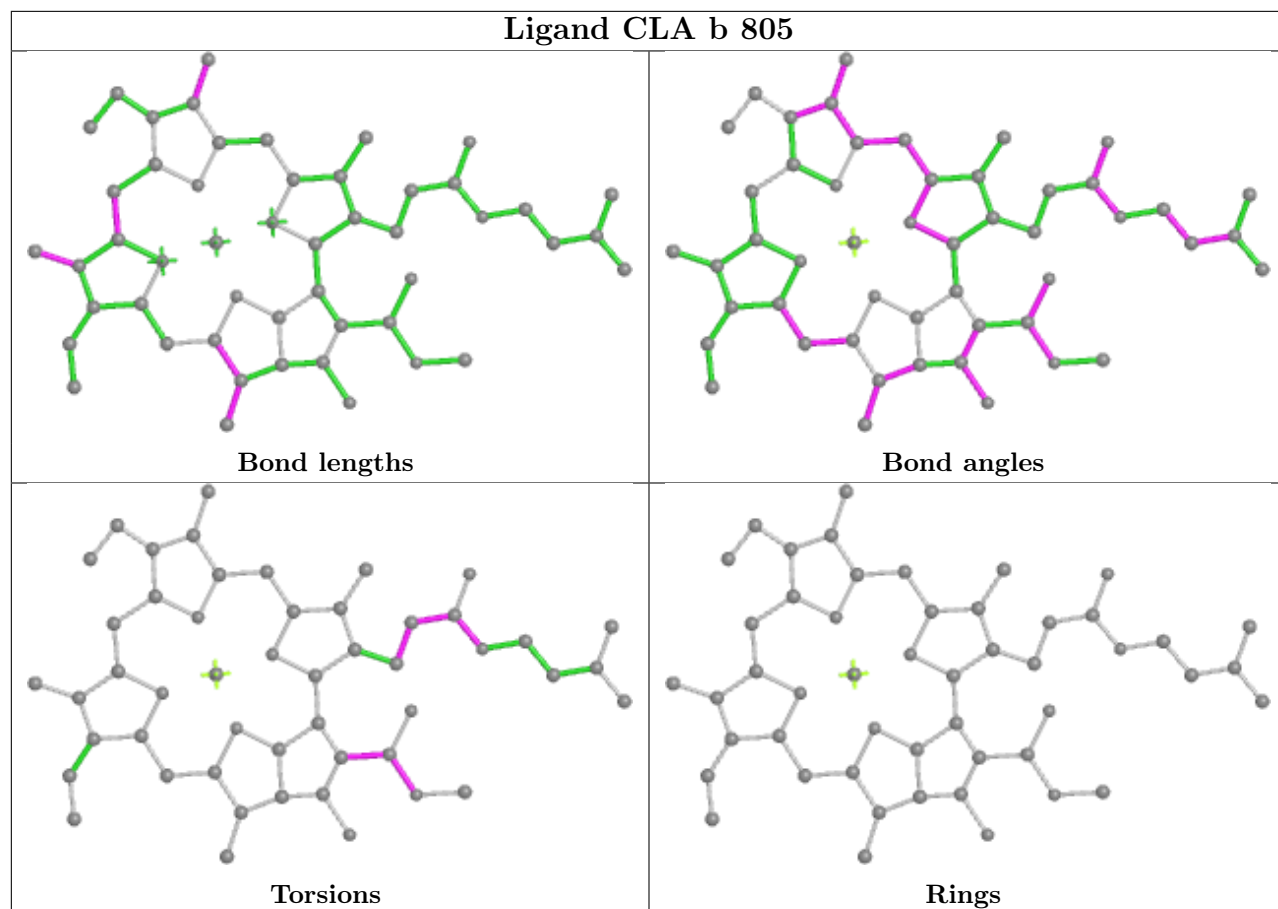
Ligand CLA b 803



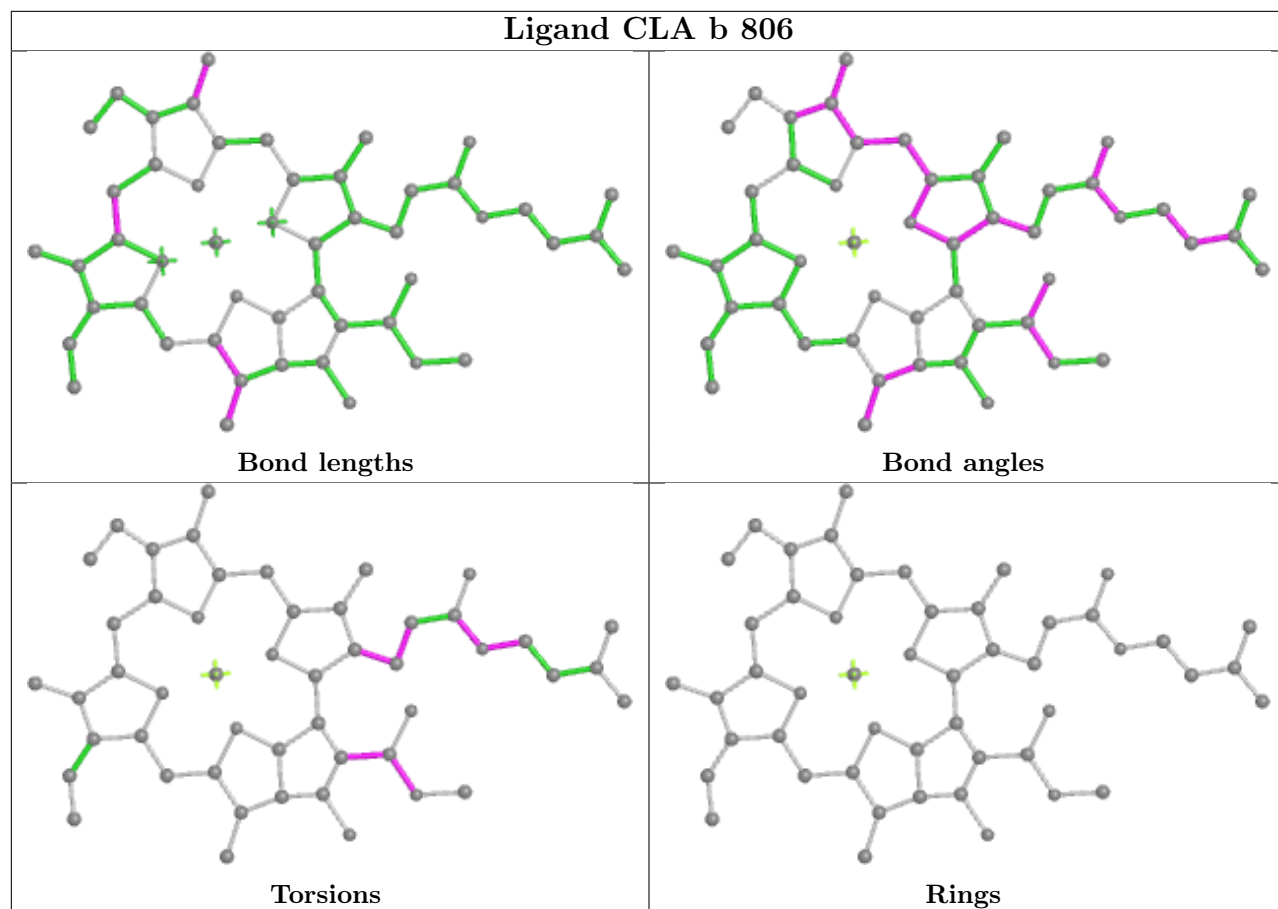
Ligand CLA b 804



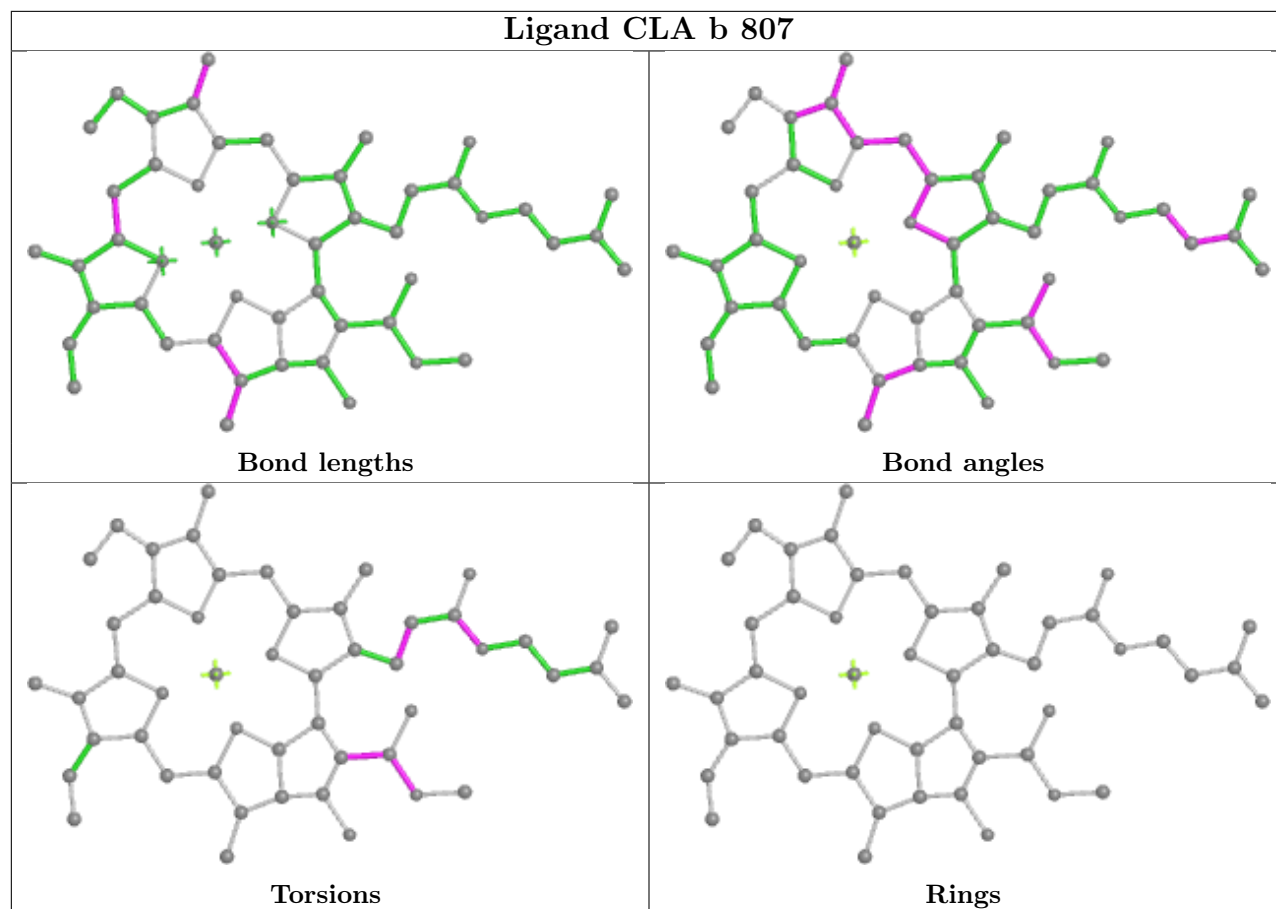
Ligand CLA b 805



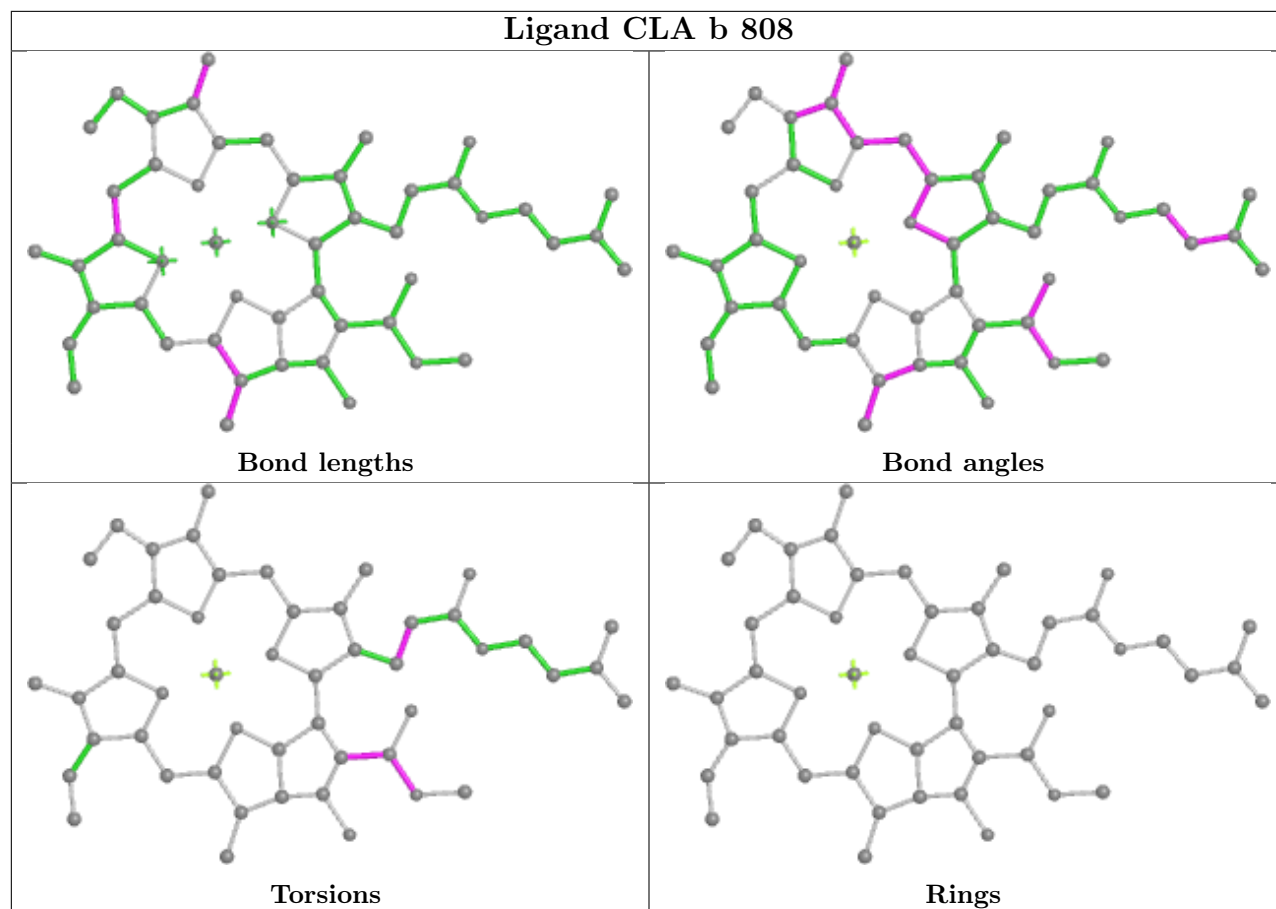
Ligand CLA b 806

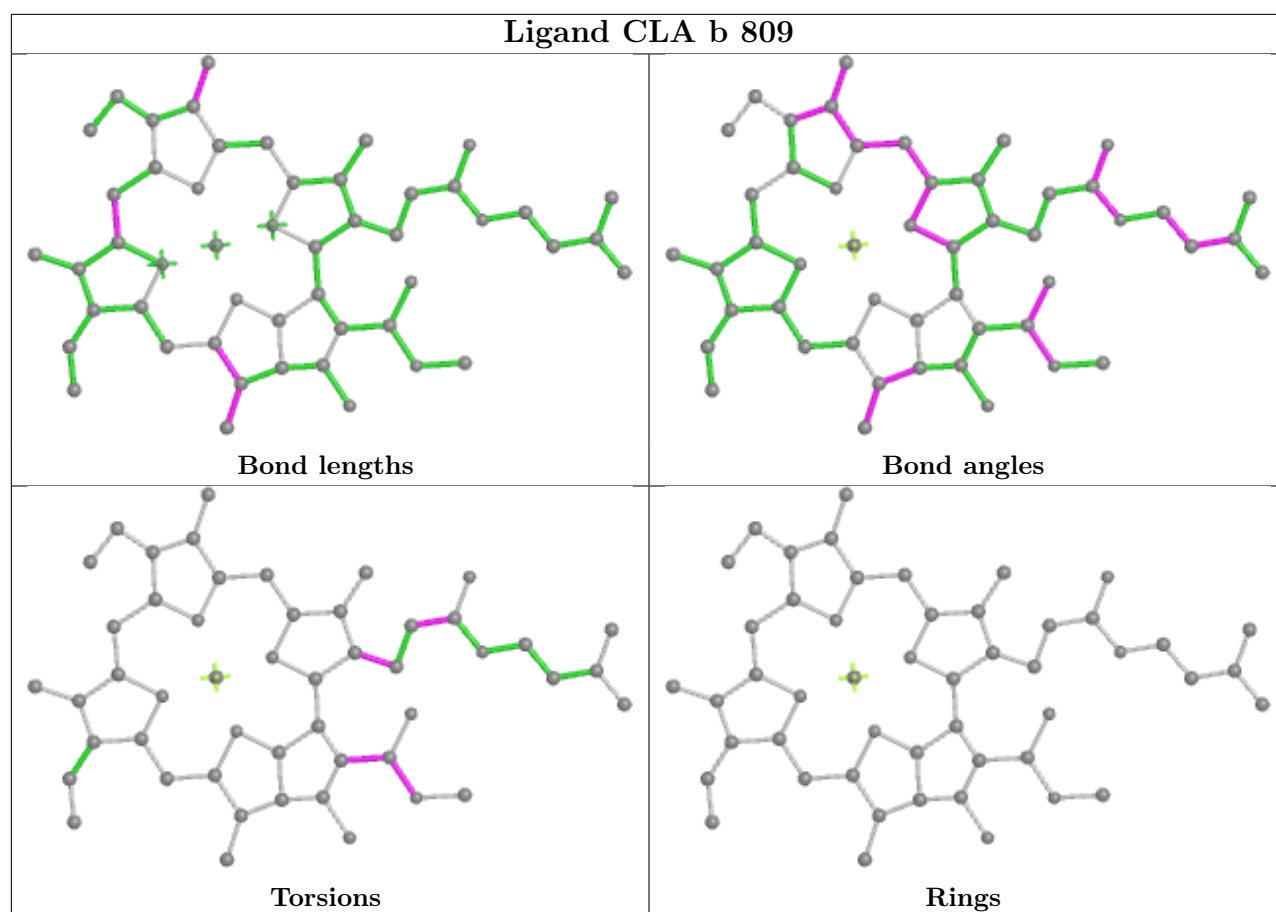


Ligand CLA b 807

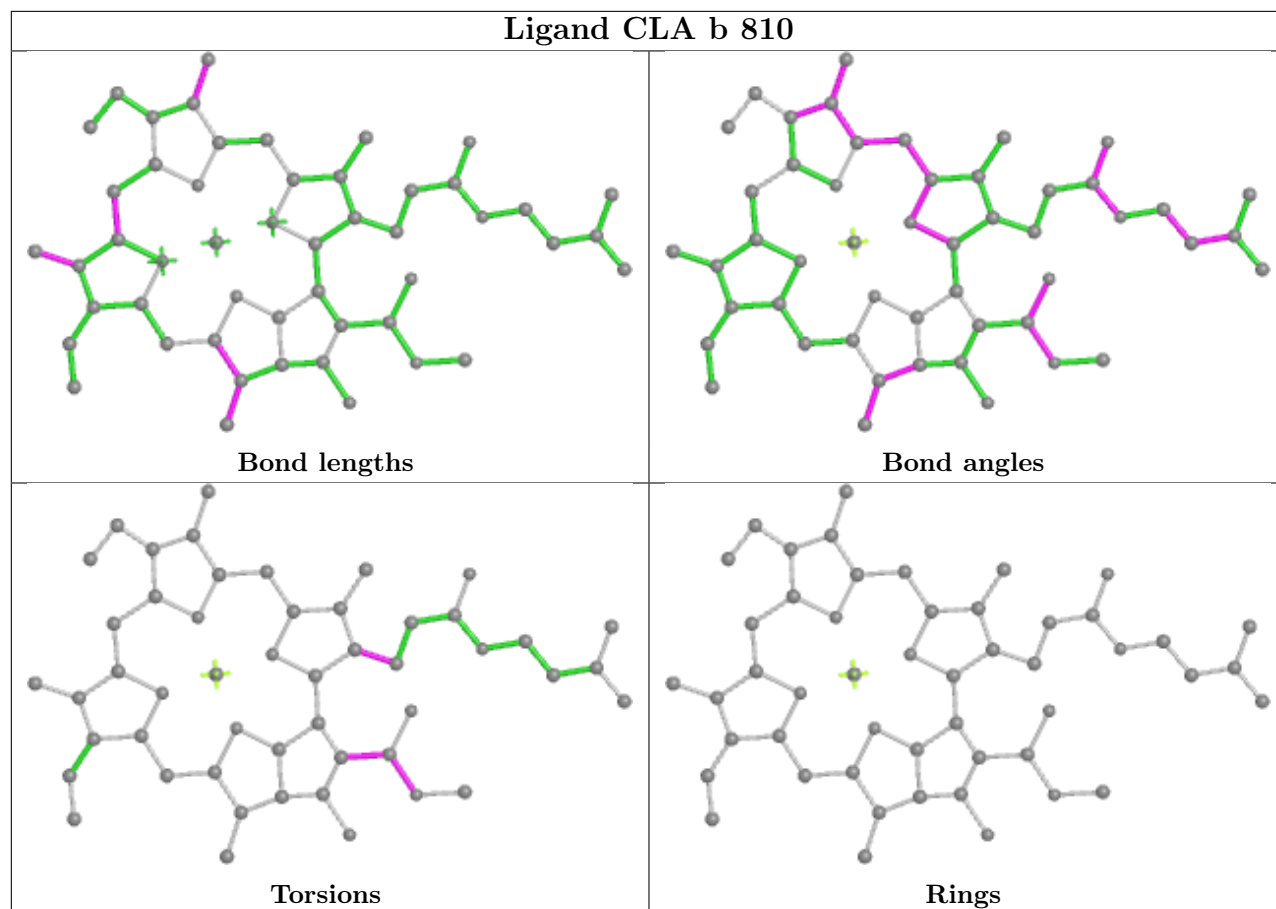


Ligand CLA b 808

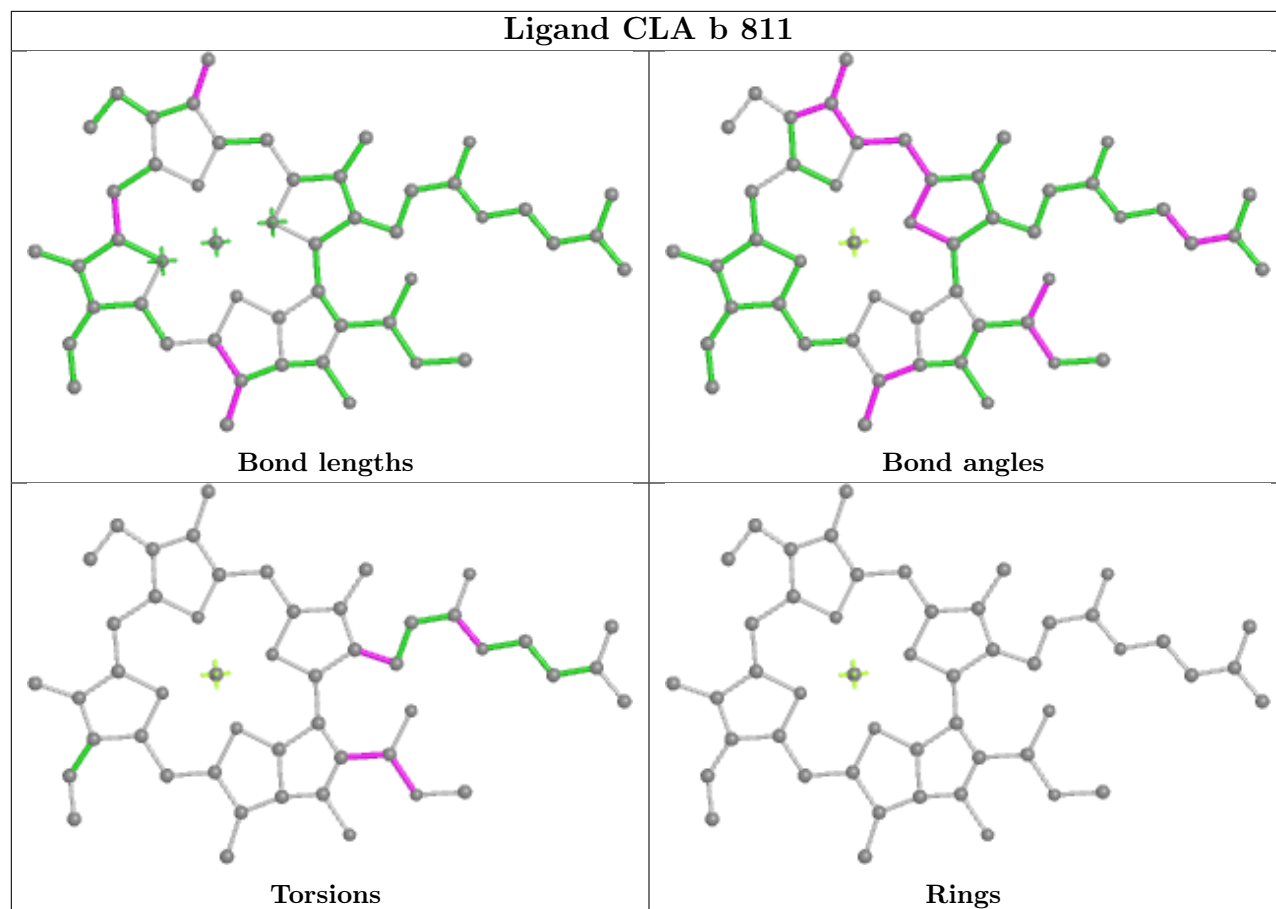




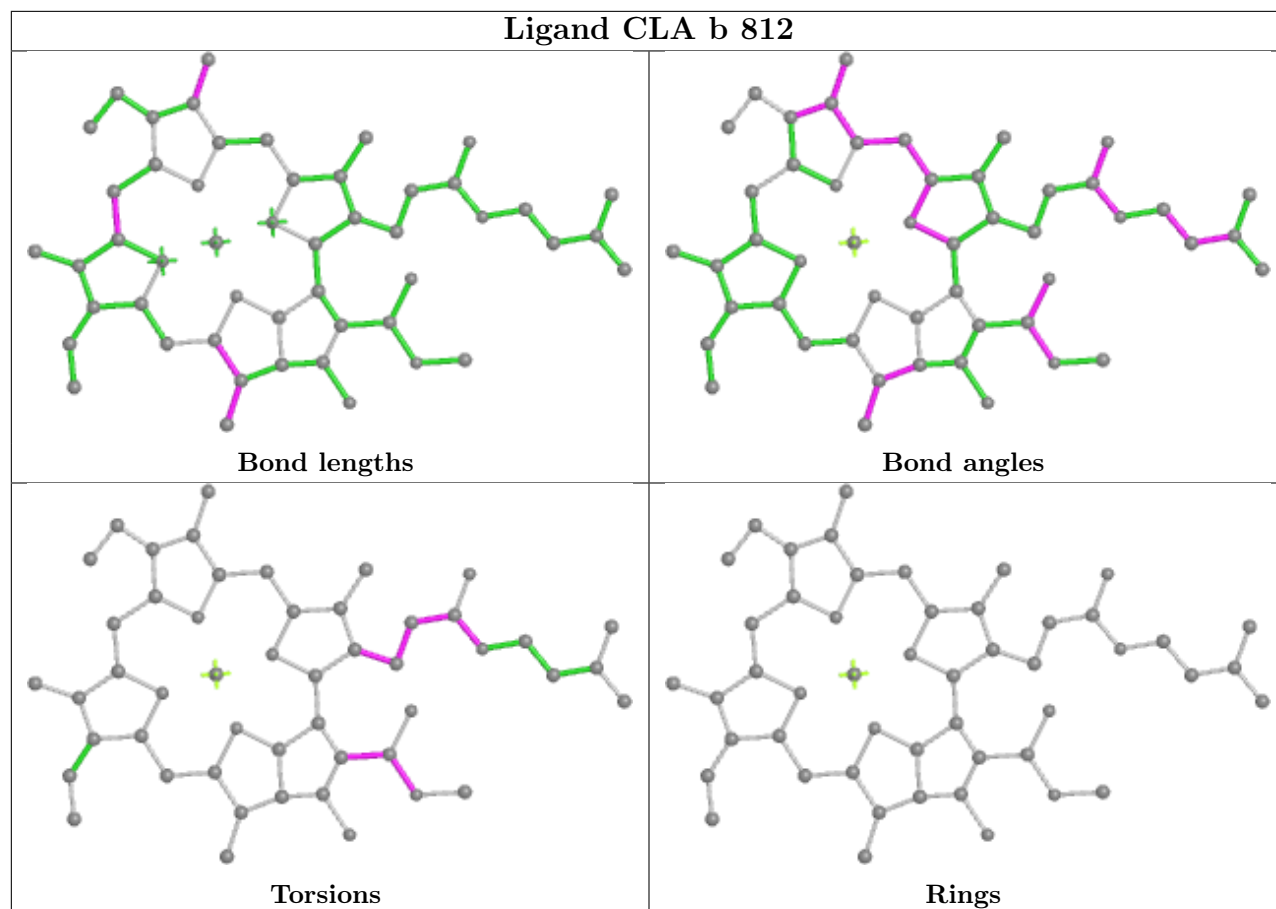
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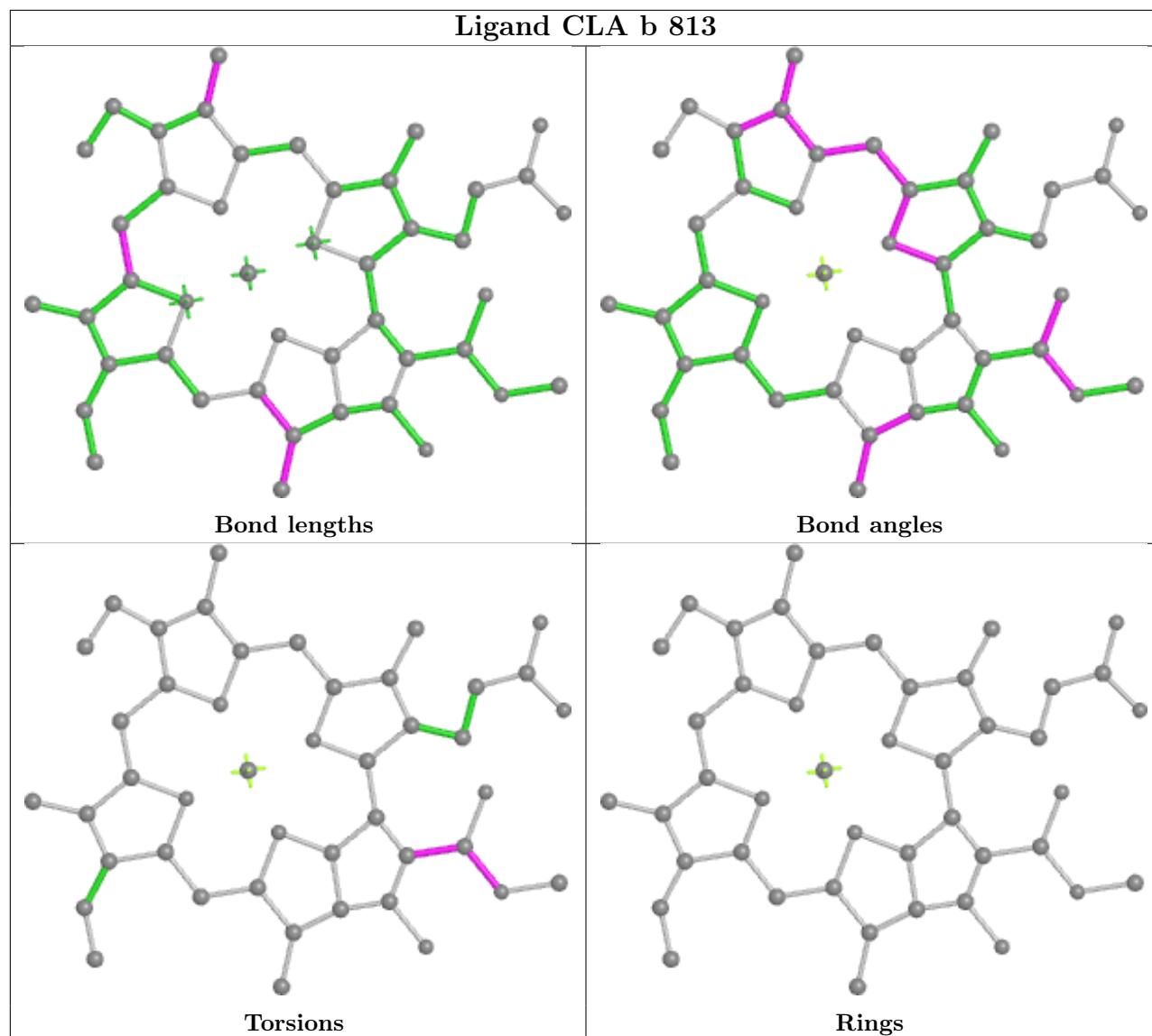
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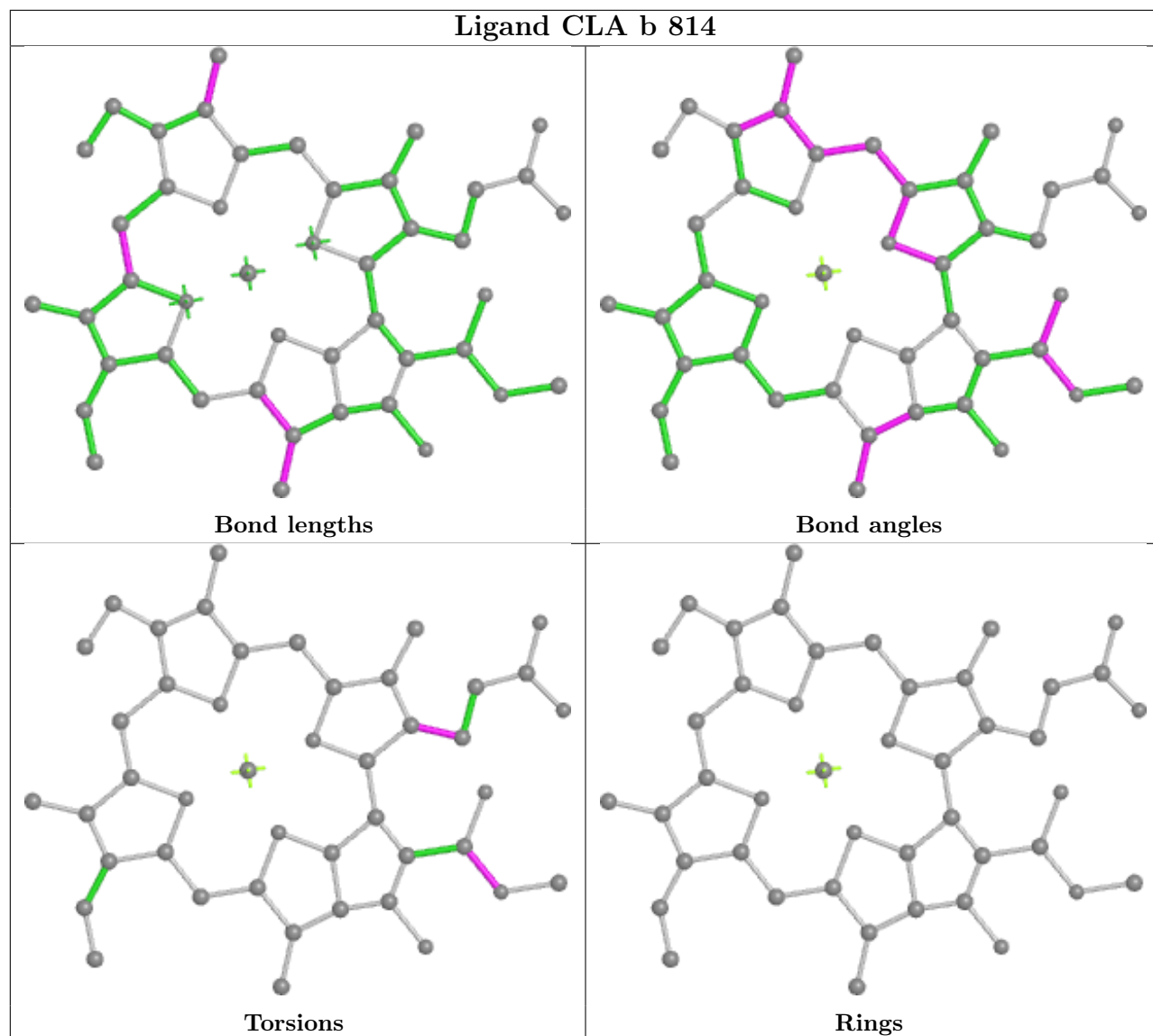
Ligand CLA b 812



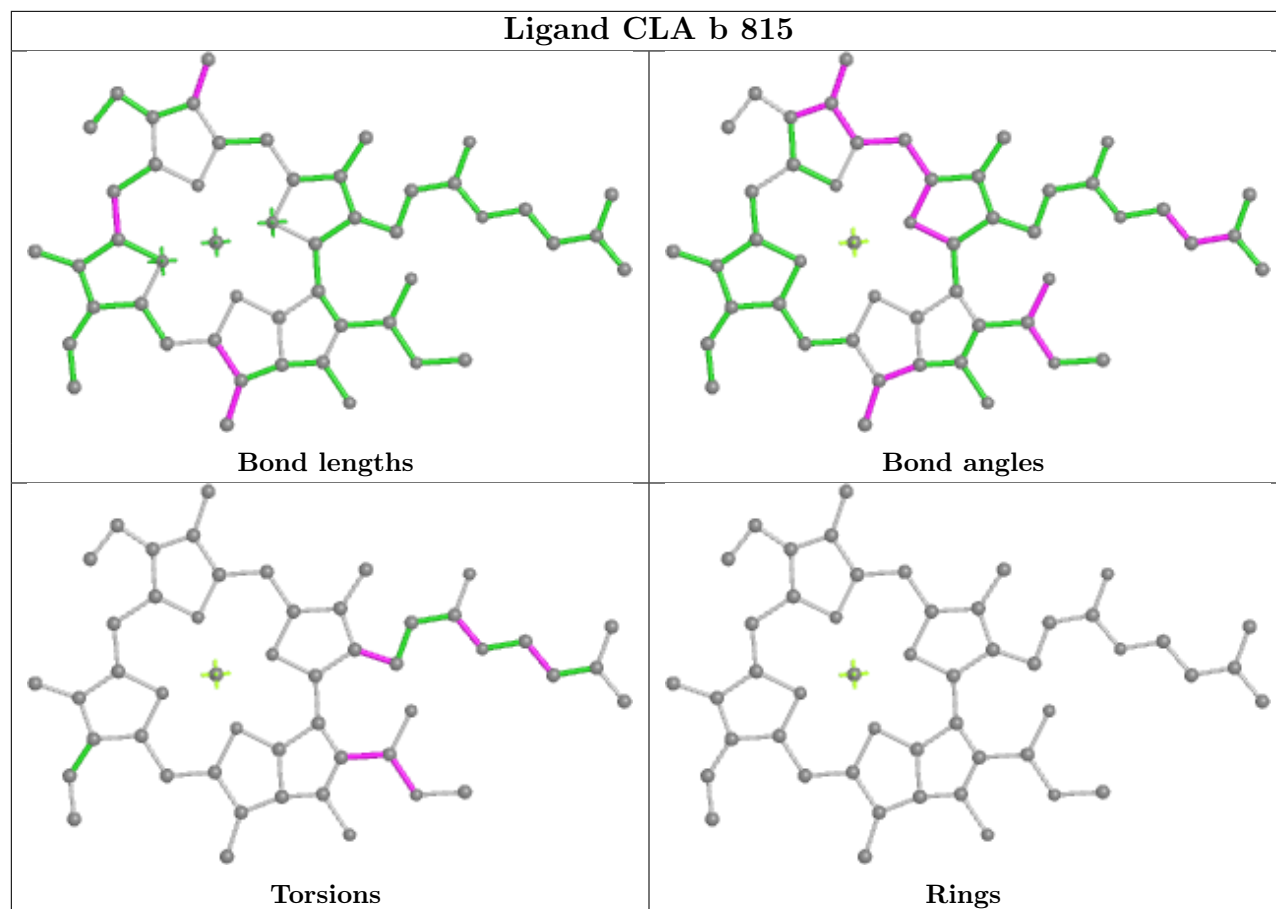
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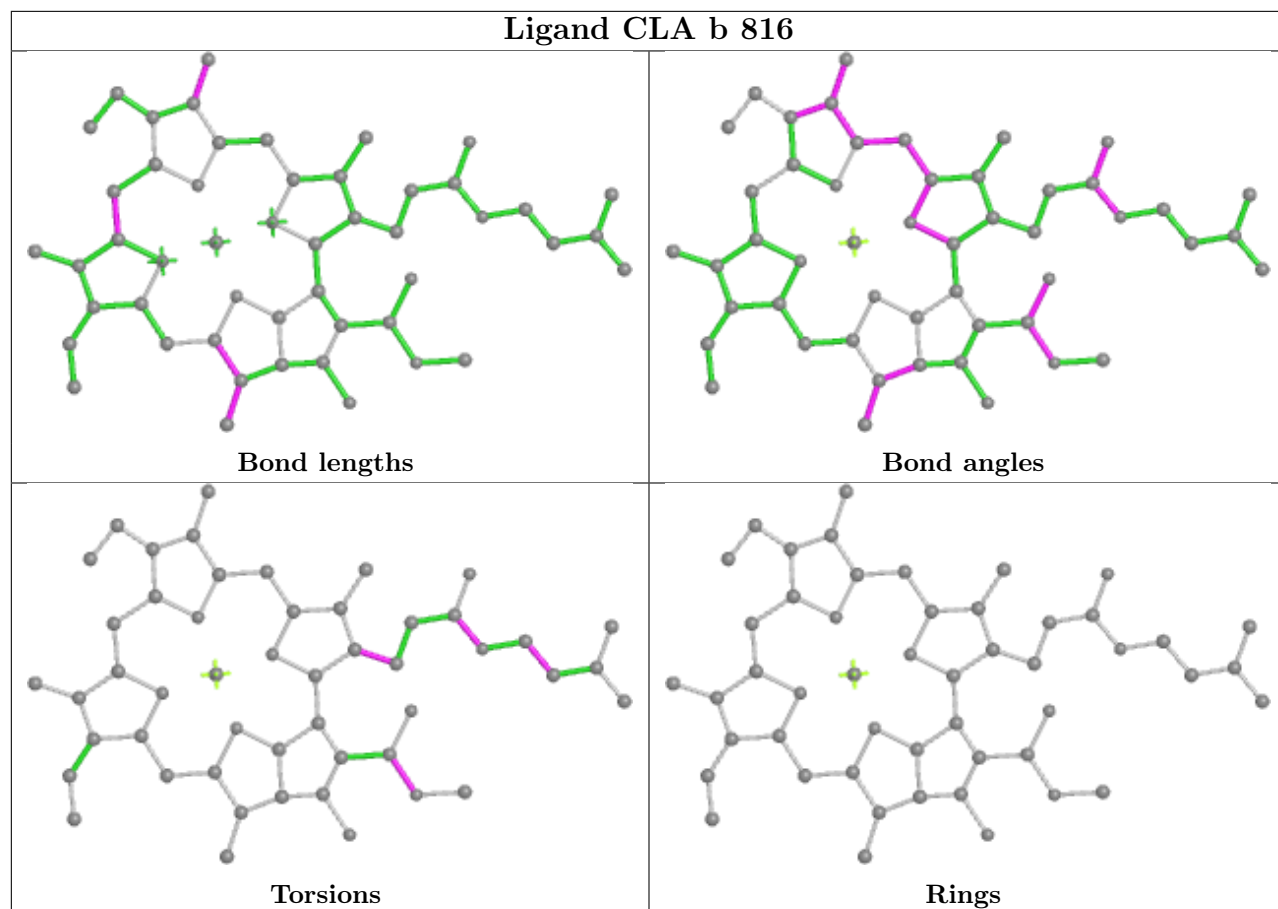
Ligand CLA b 814



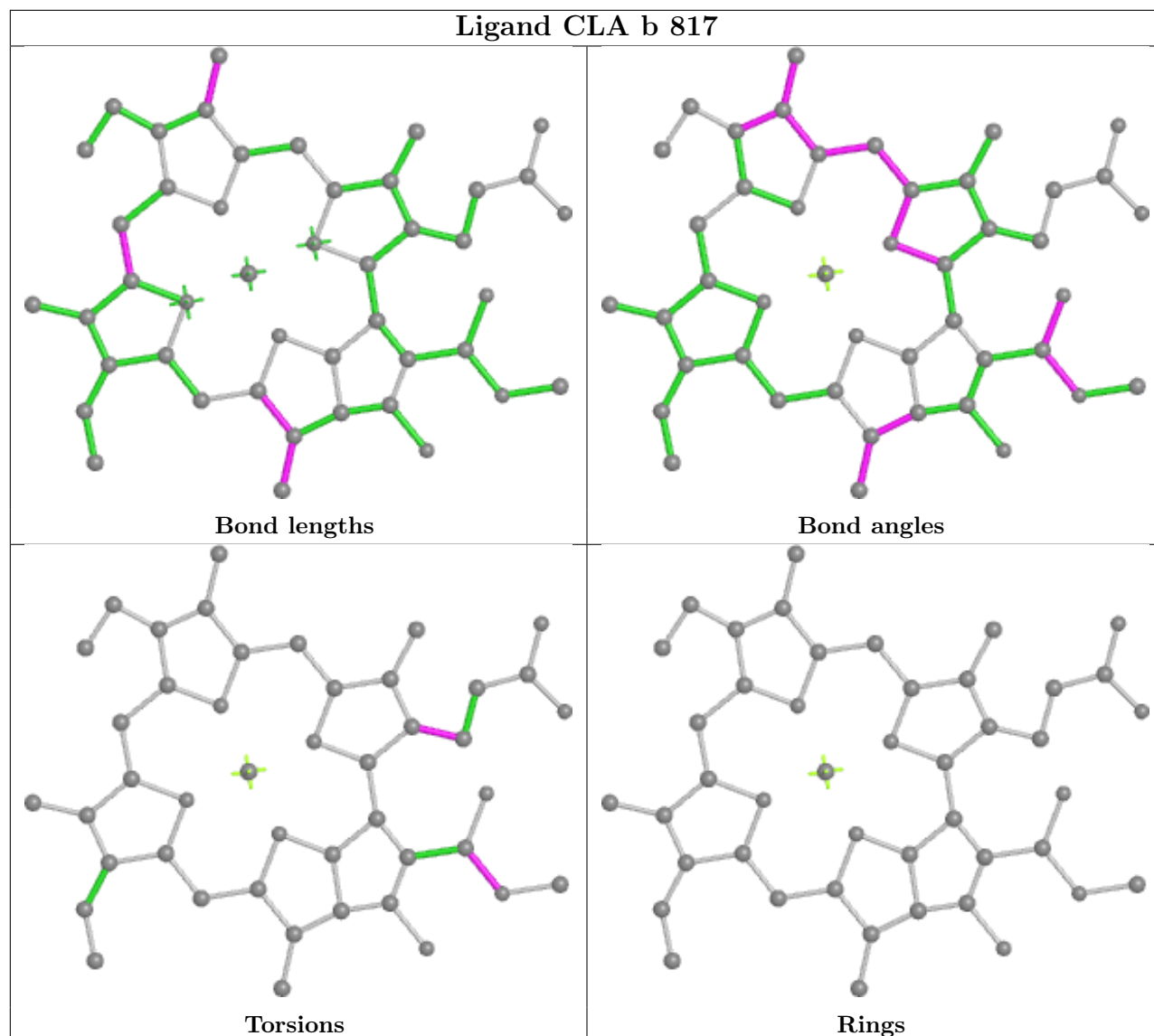
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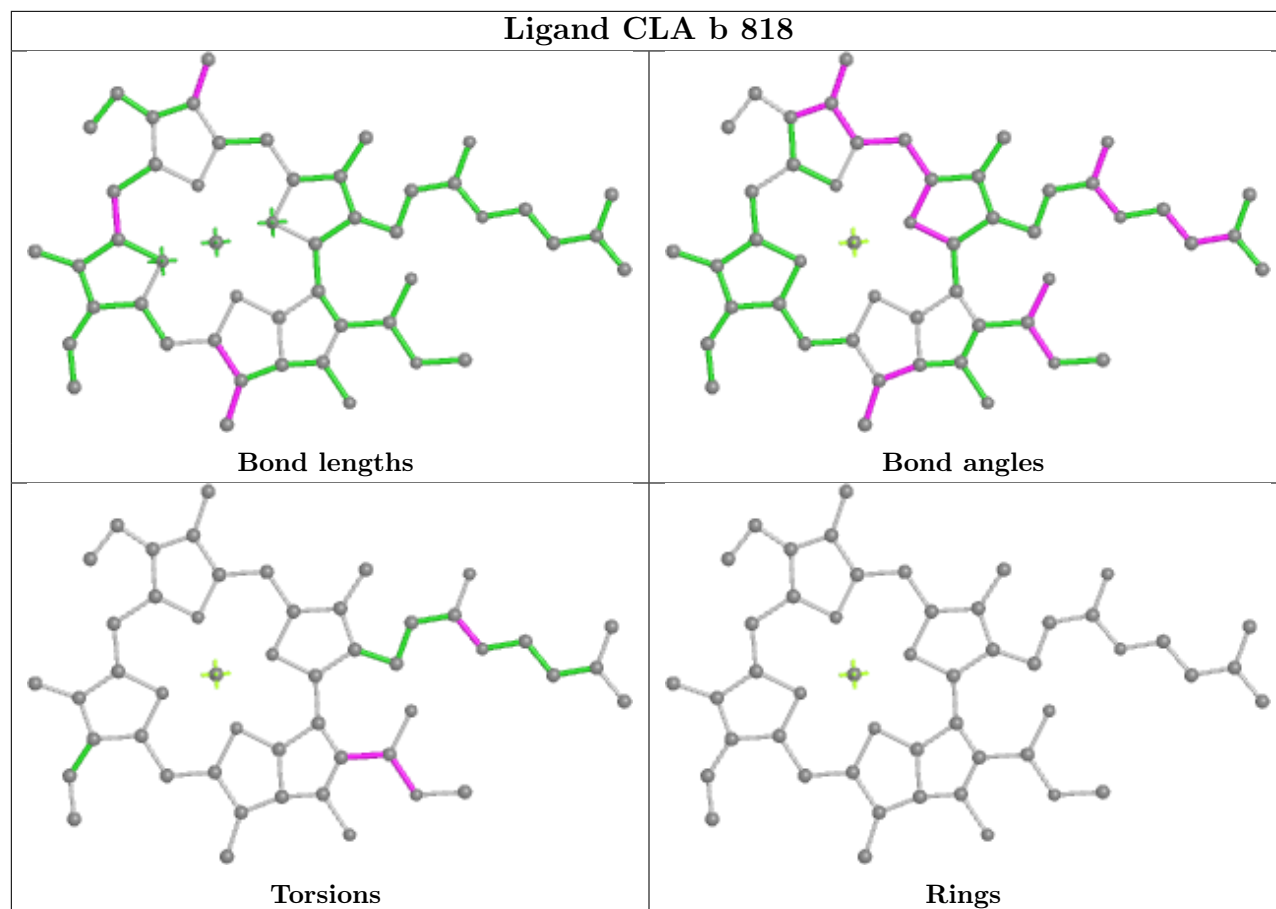
Ligand CLA b 816



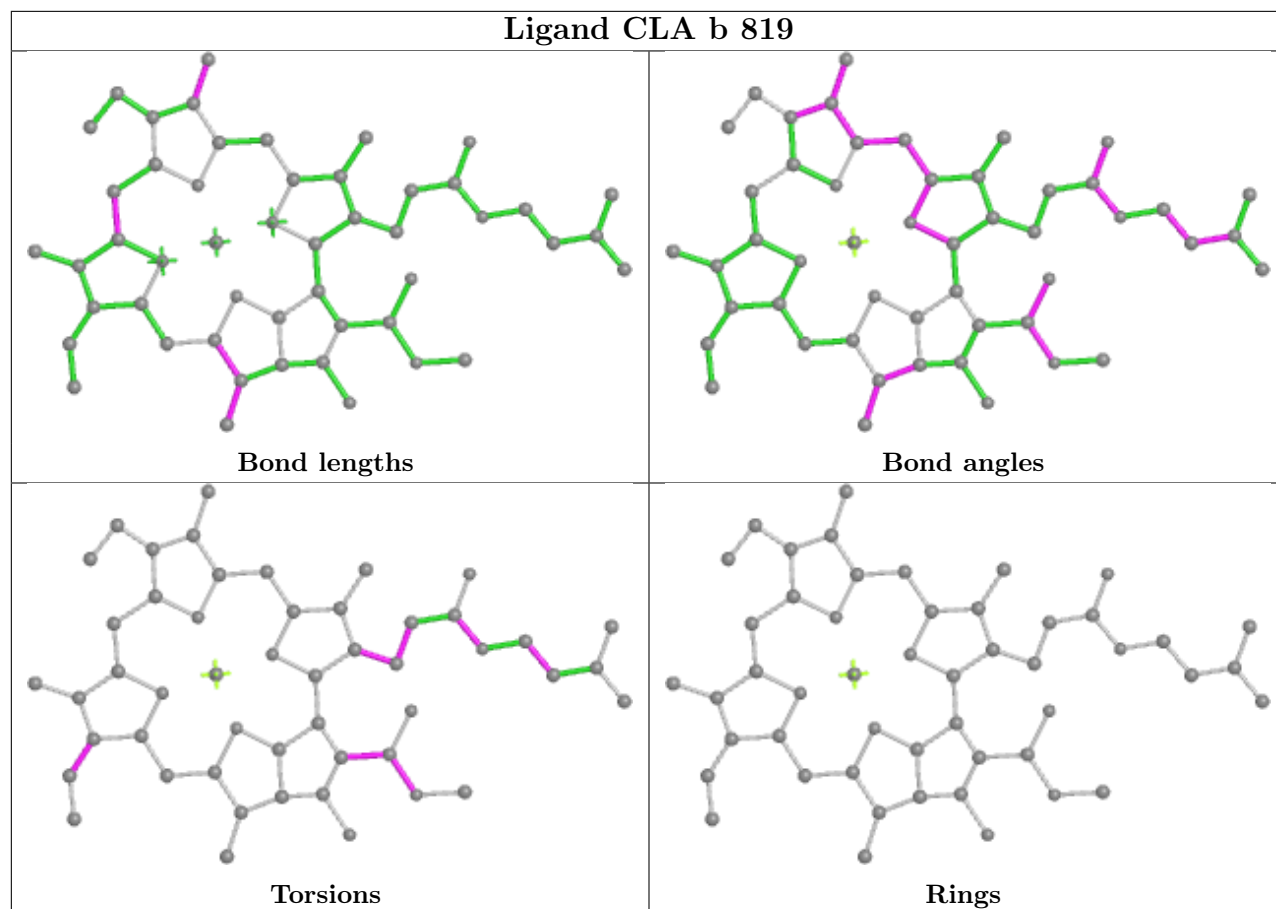
Ligand CLA b 817



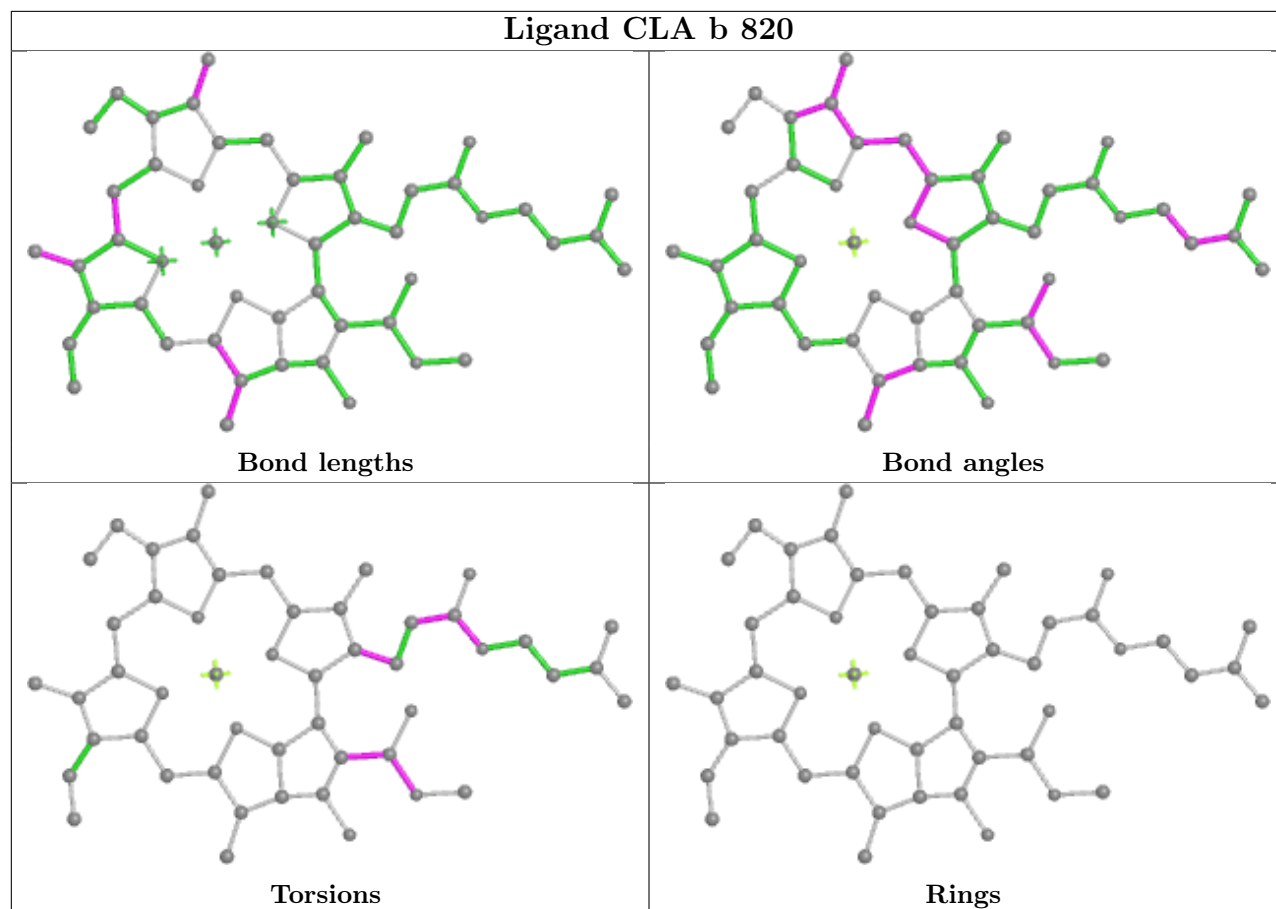
Ligand CLA b 818



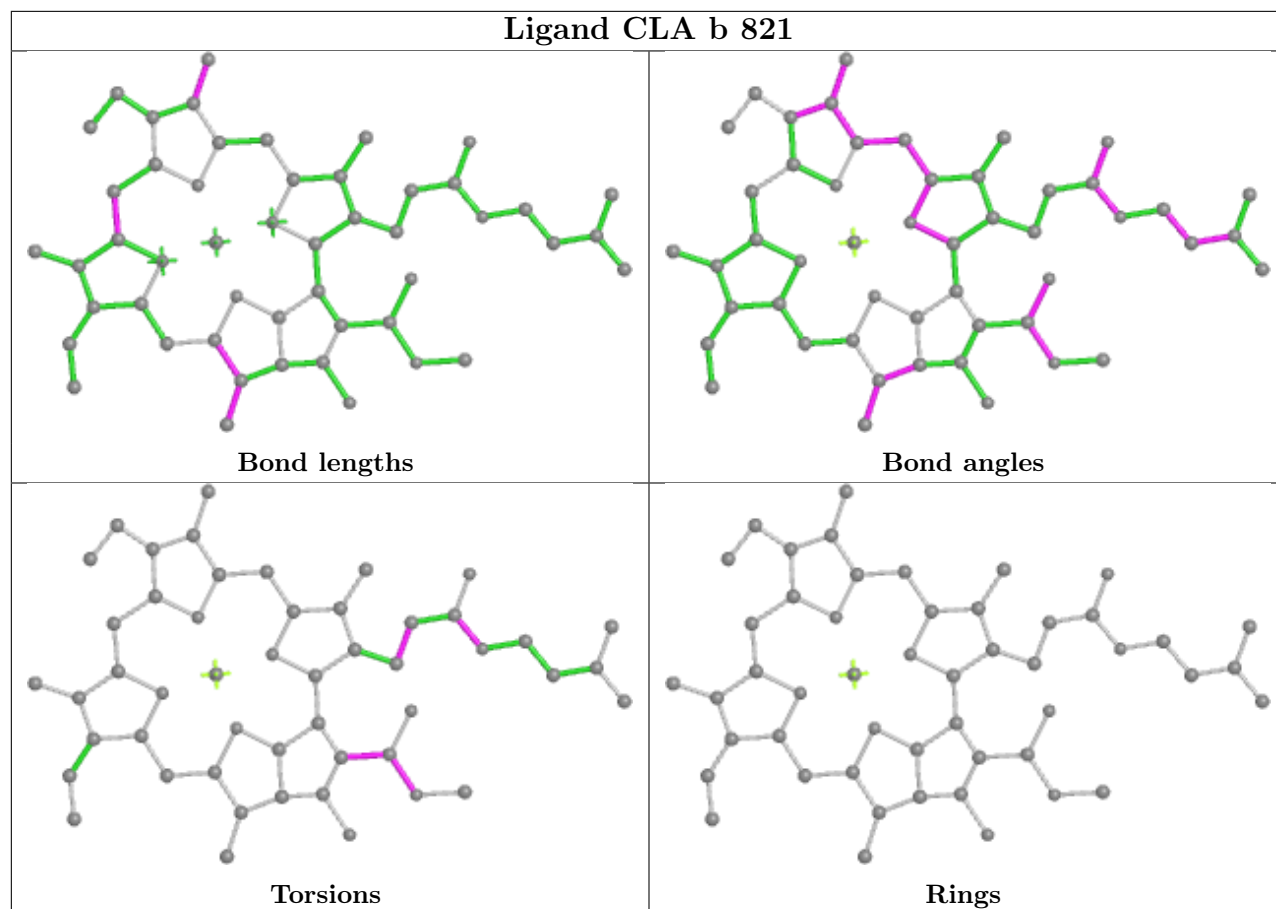
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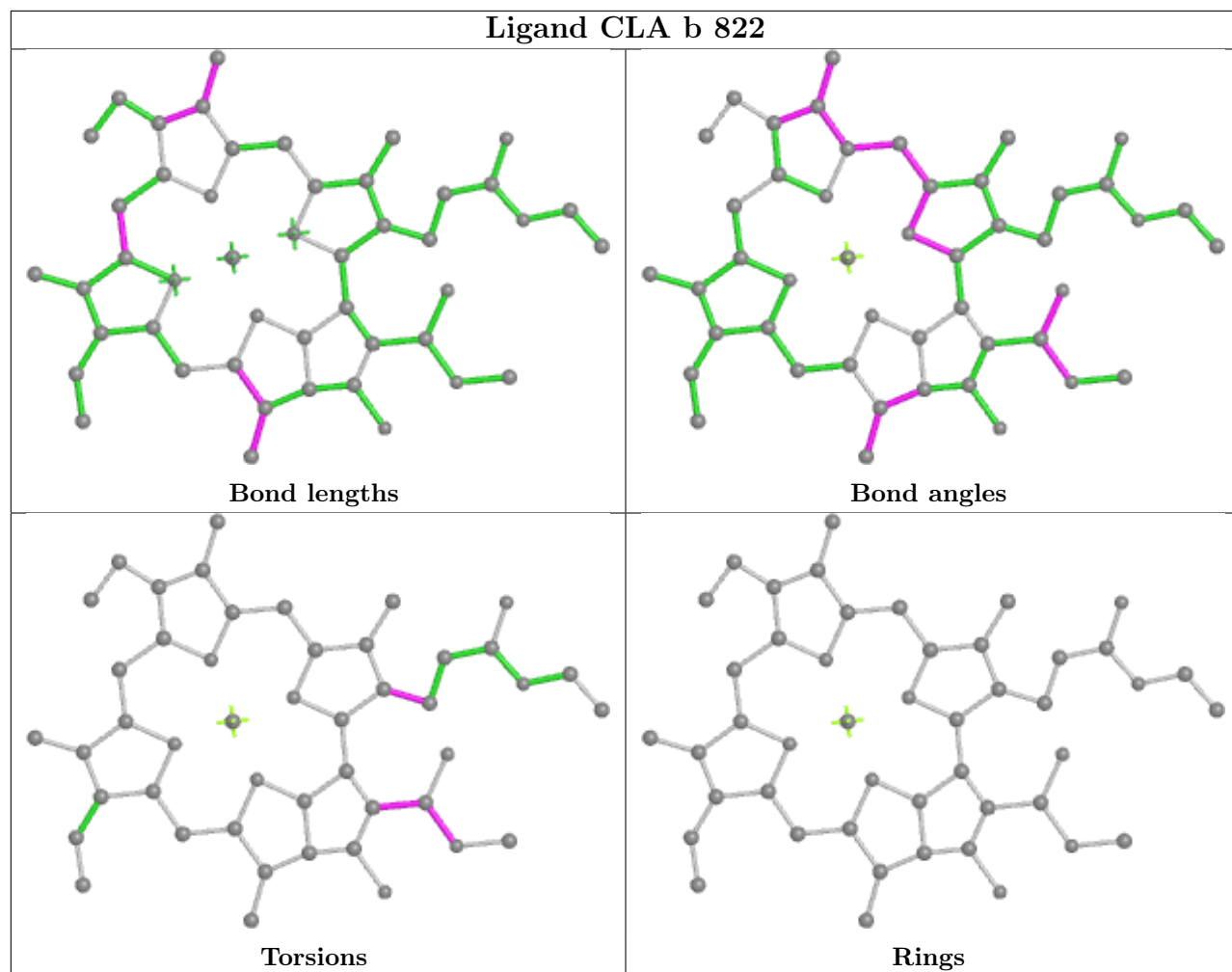
Ligand CLA b 820



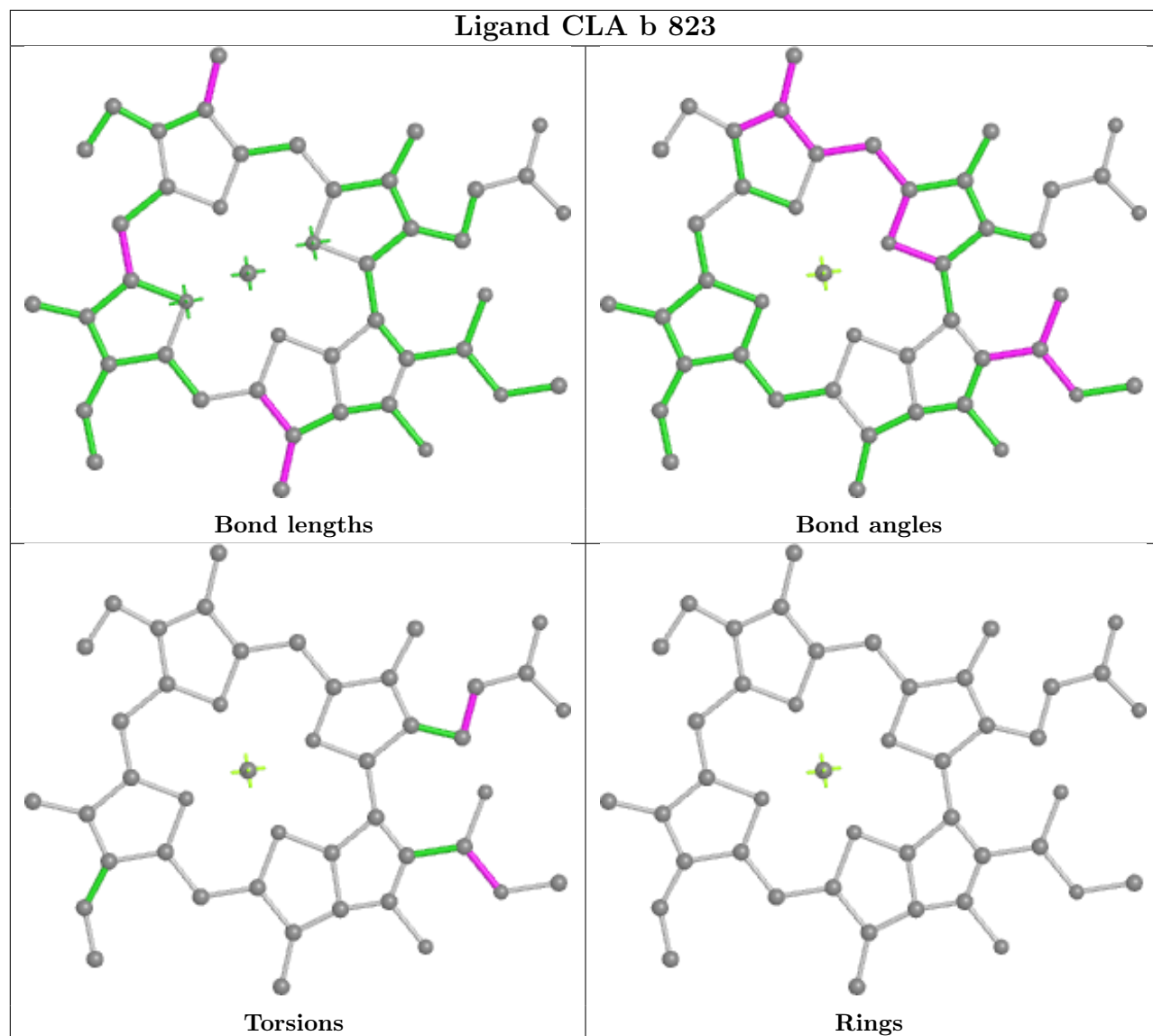
Ligand CLA b 821

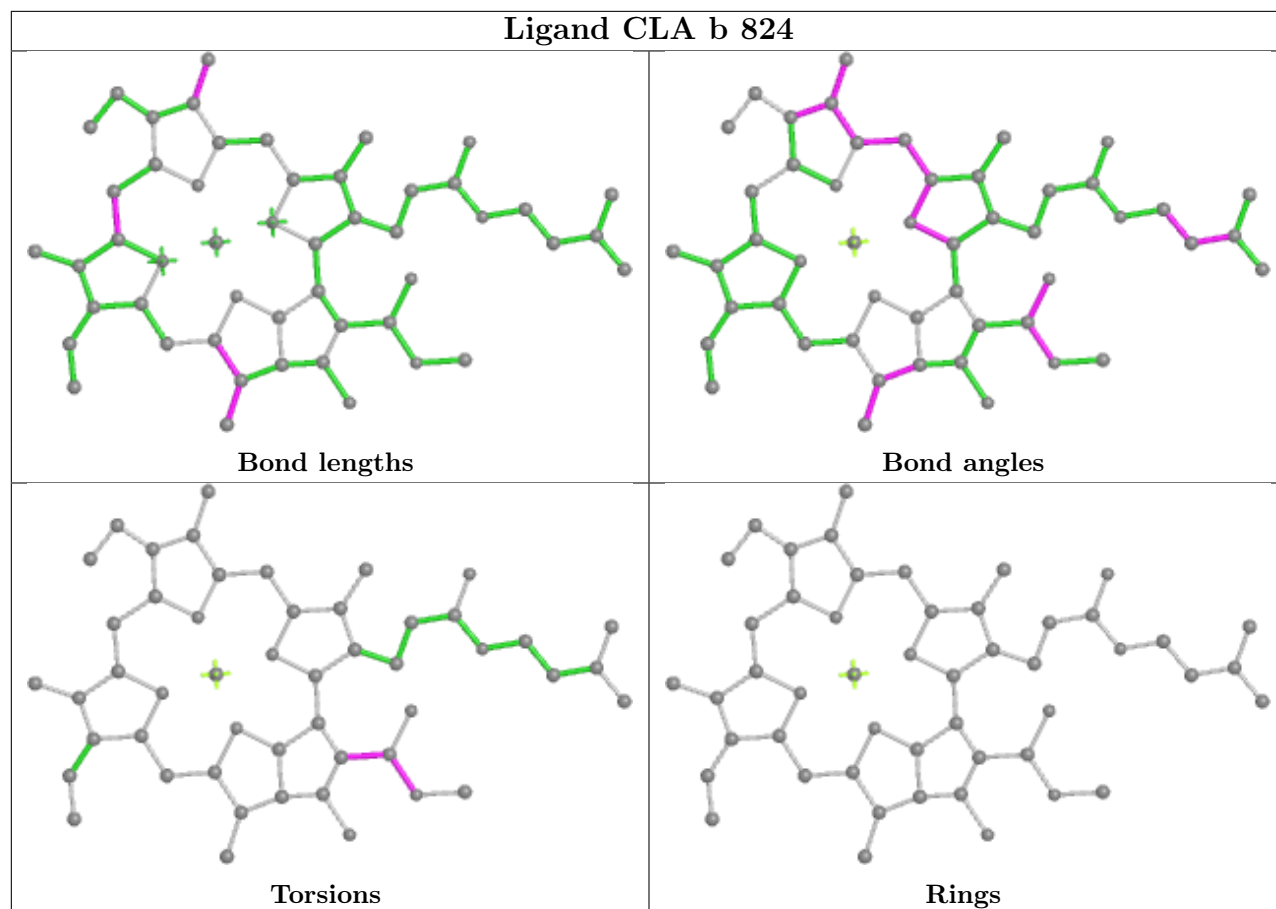


Ligand CLA b 822

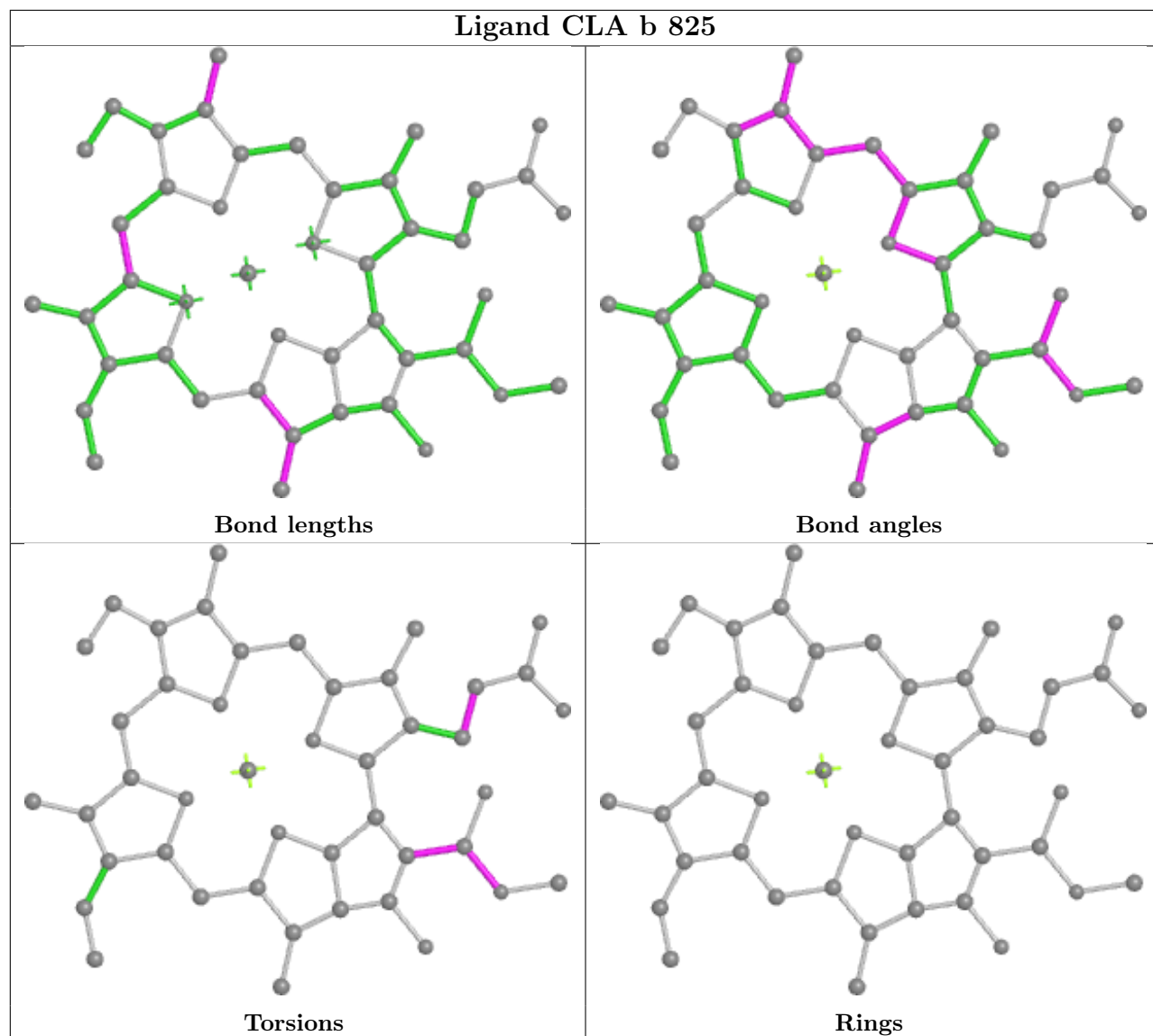


Ligand CLA b 823

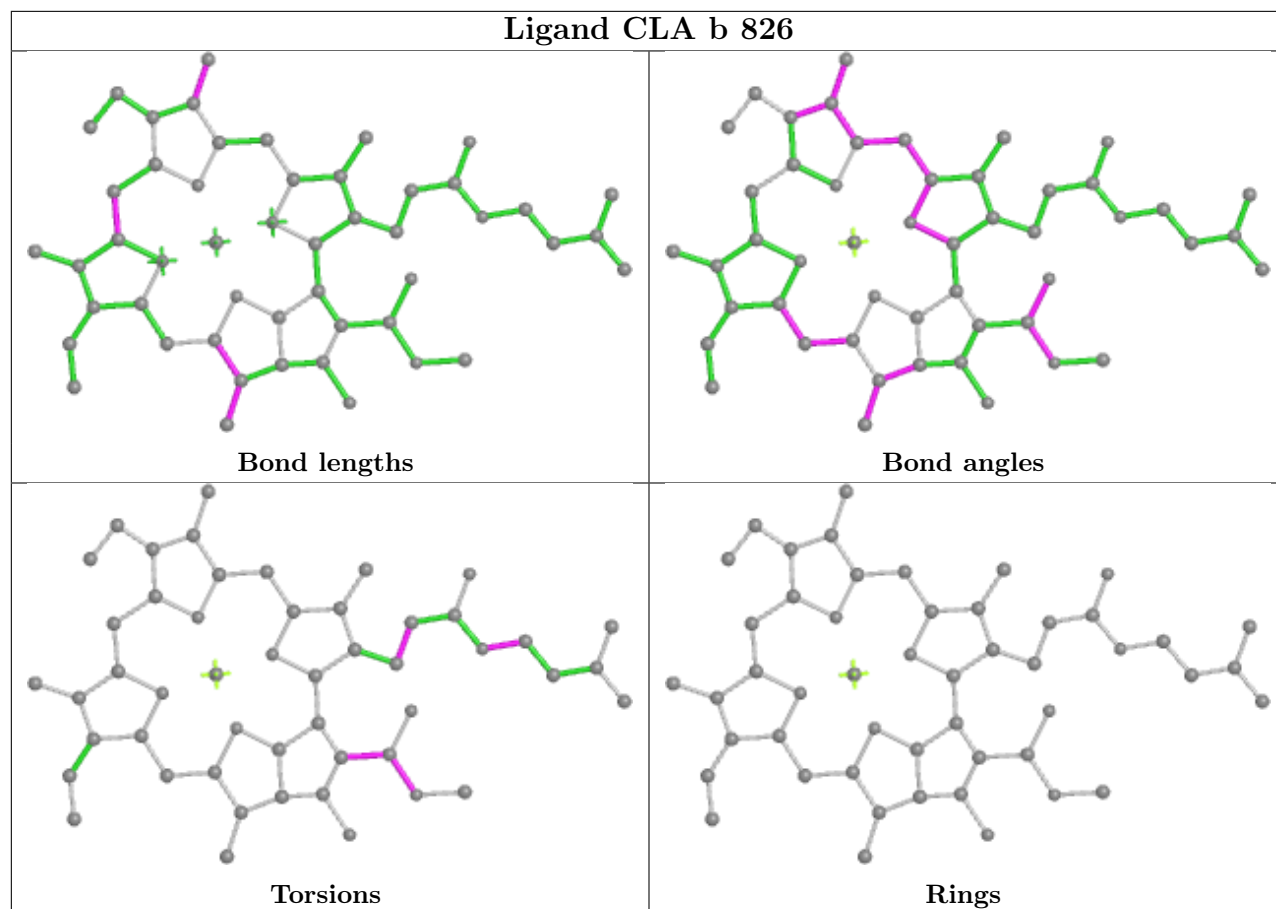




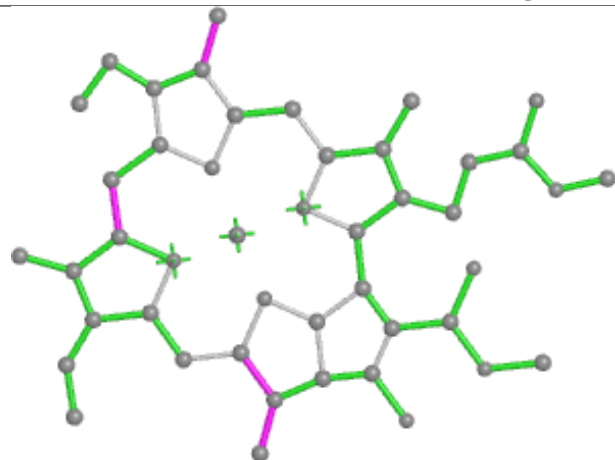
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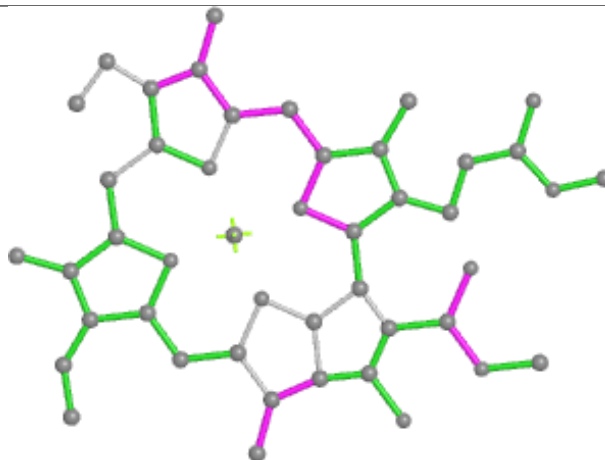
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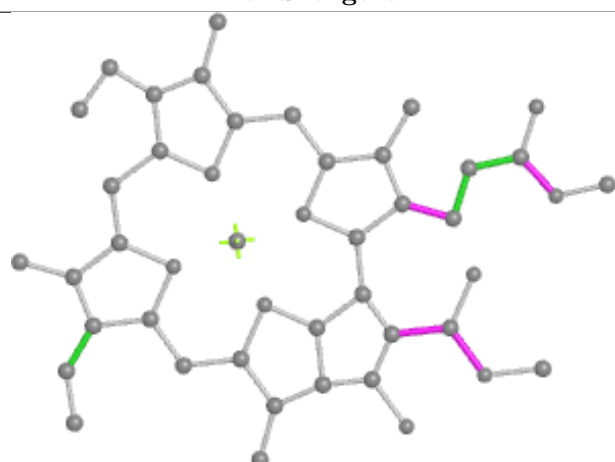
Ligand CLA b 827



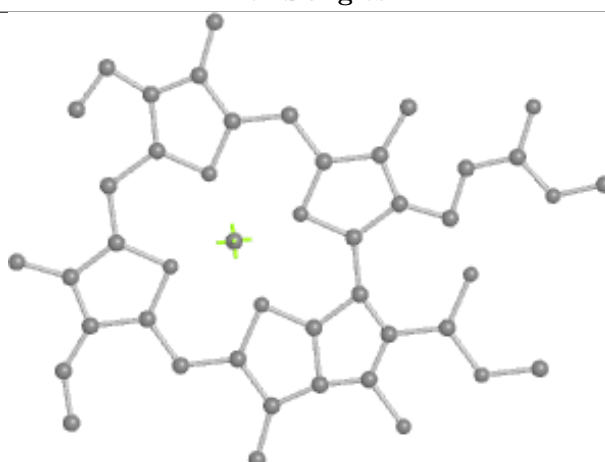
Bond lengths



Bond angles

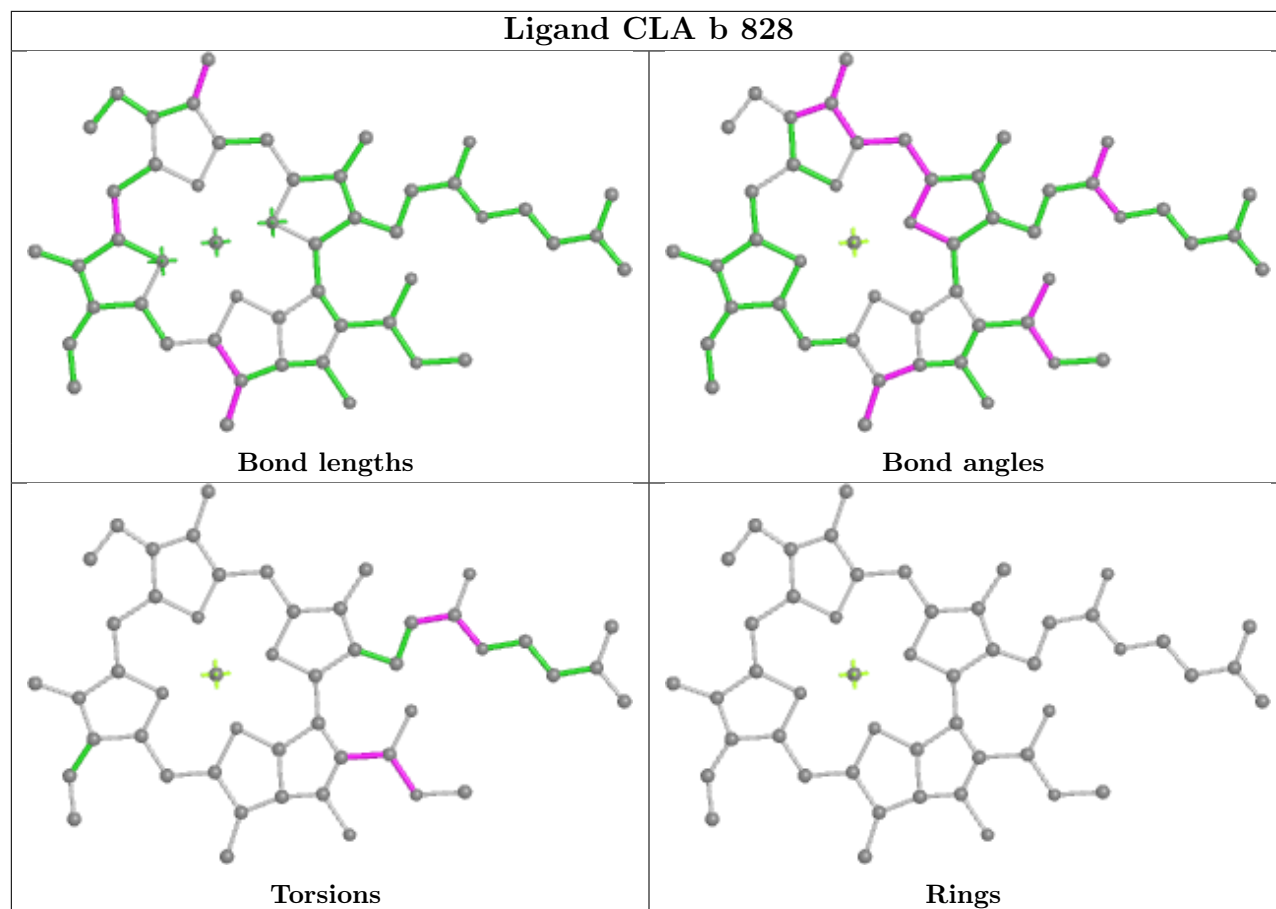


Torsions

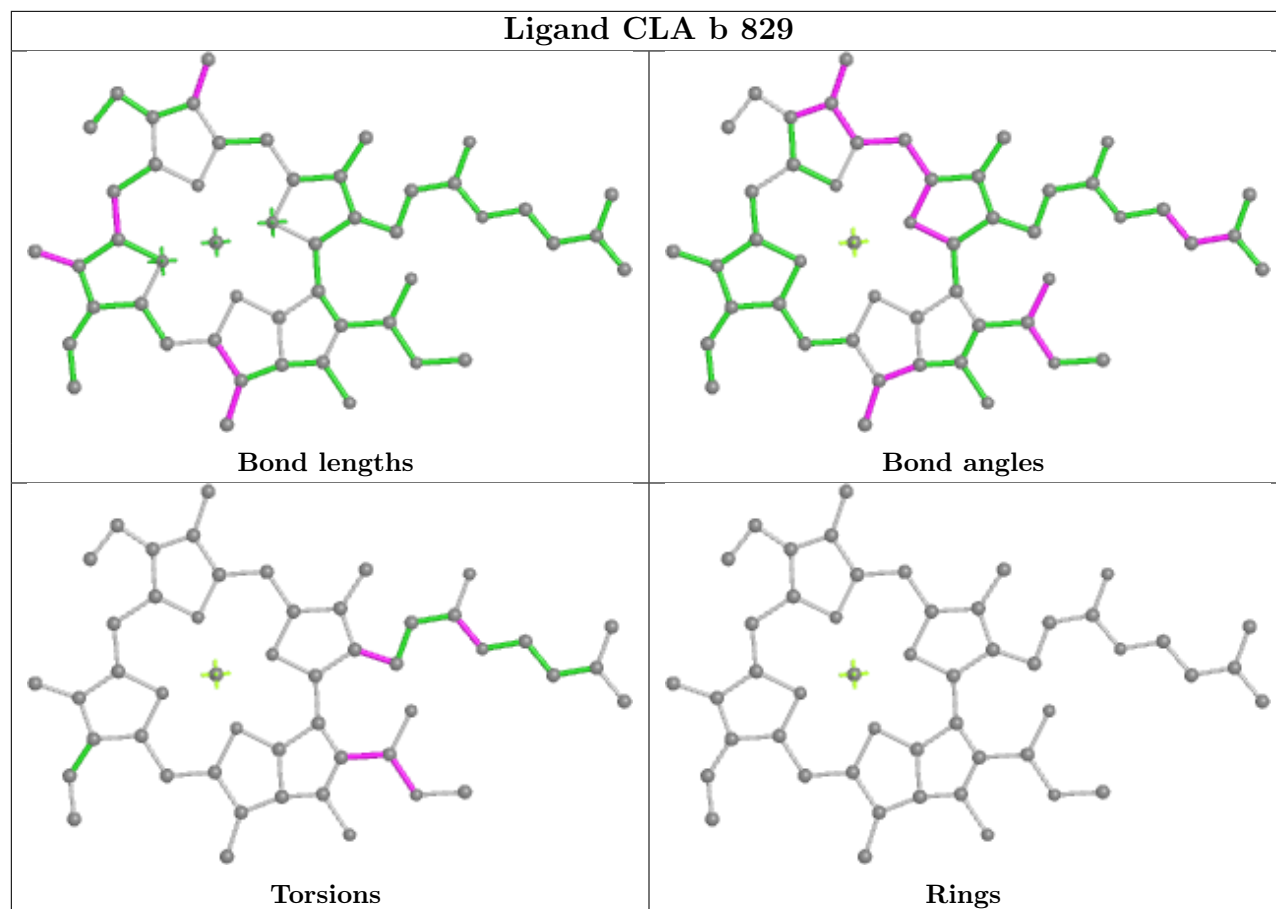


Rings

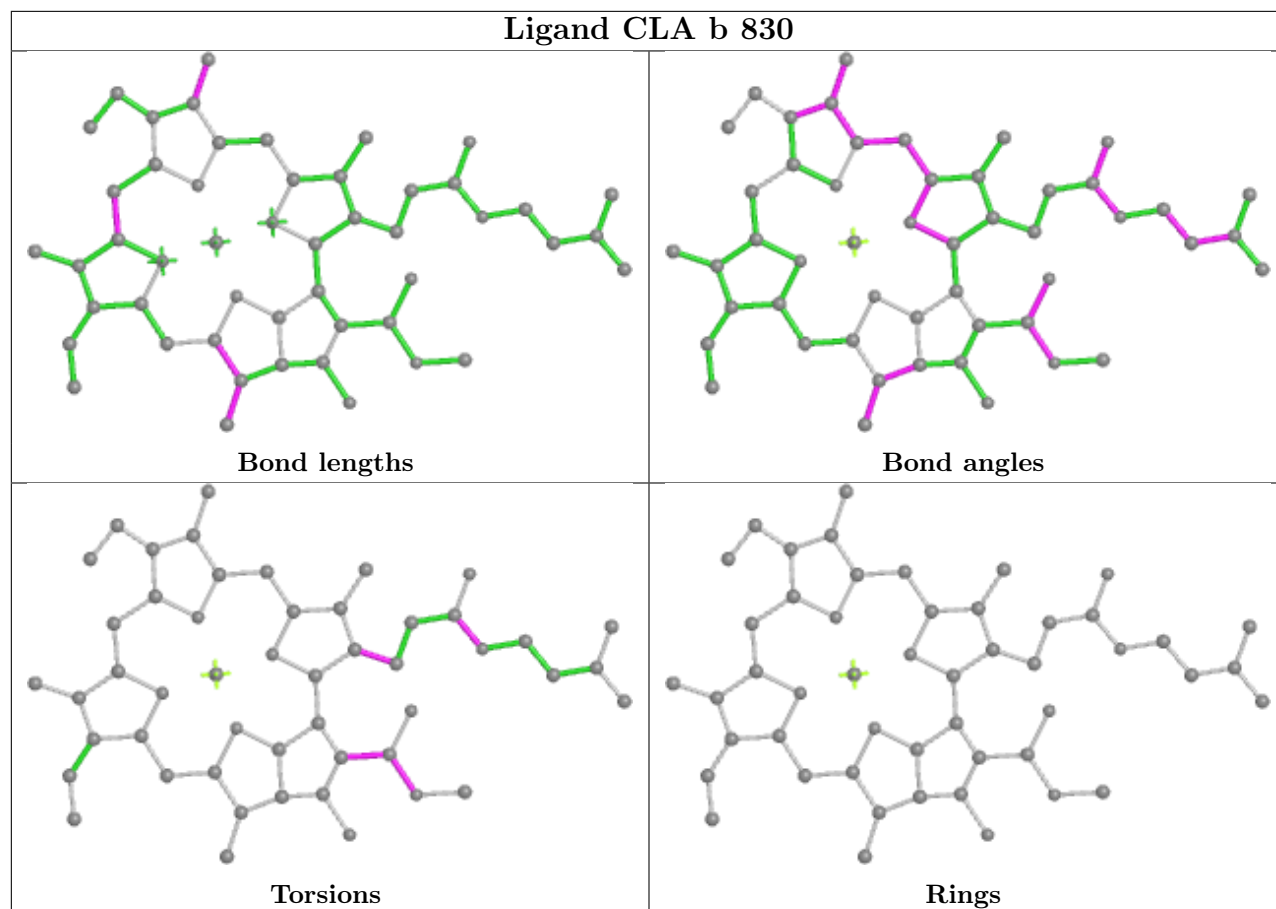
Ligand CLA b 828



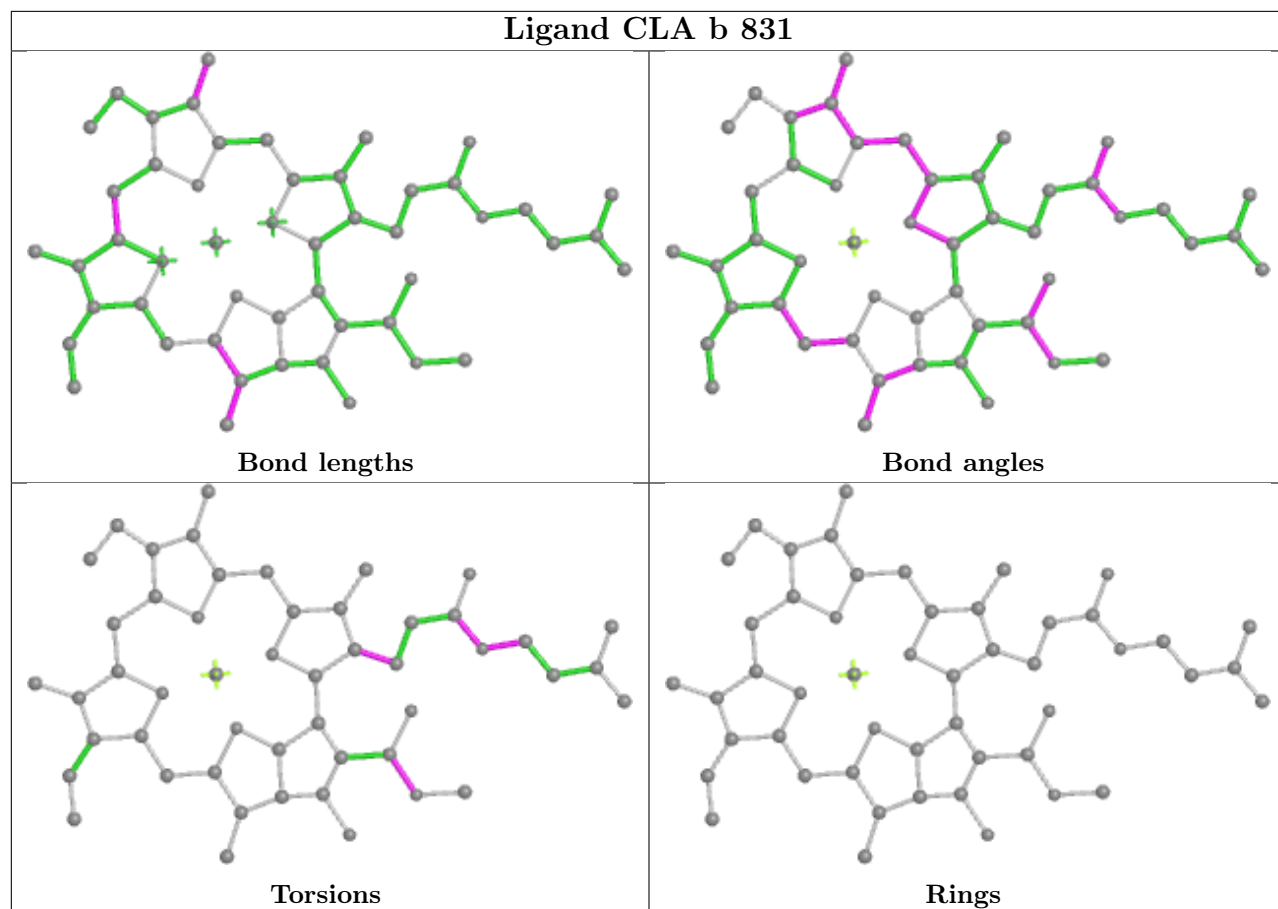
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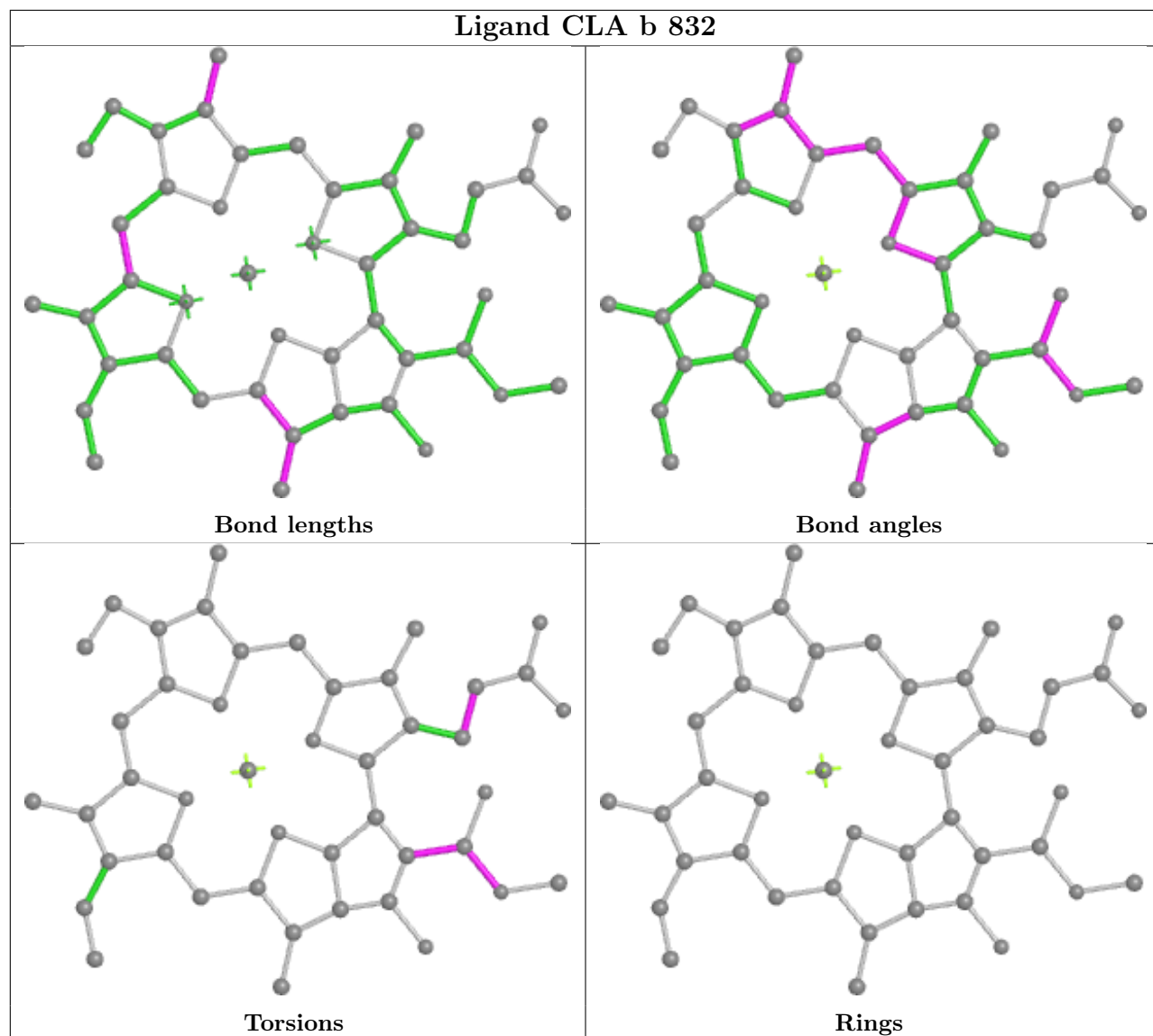
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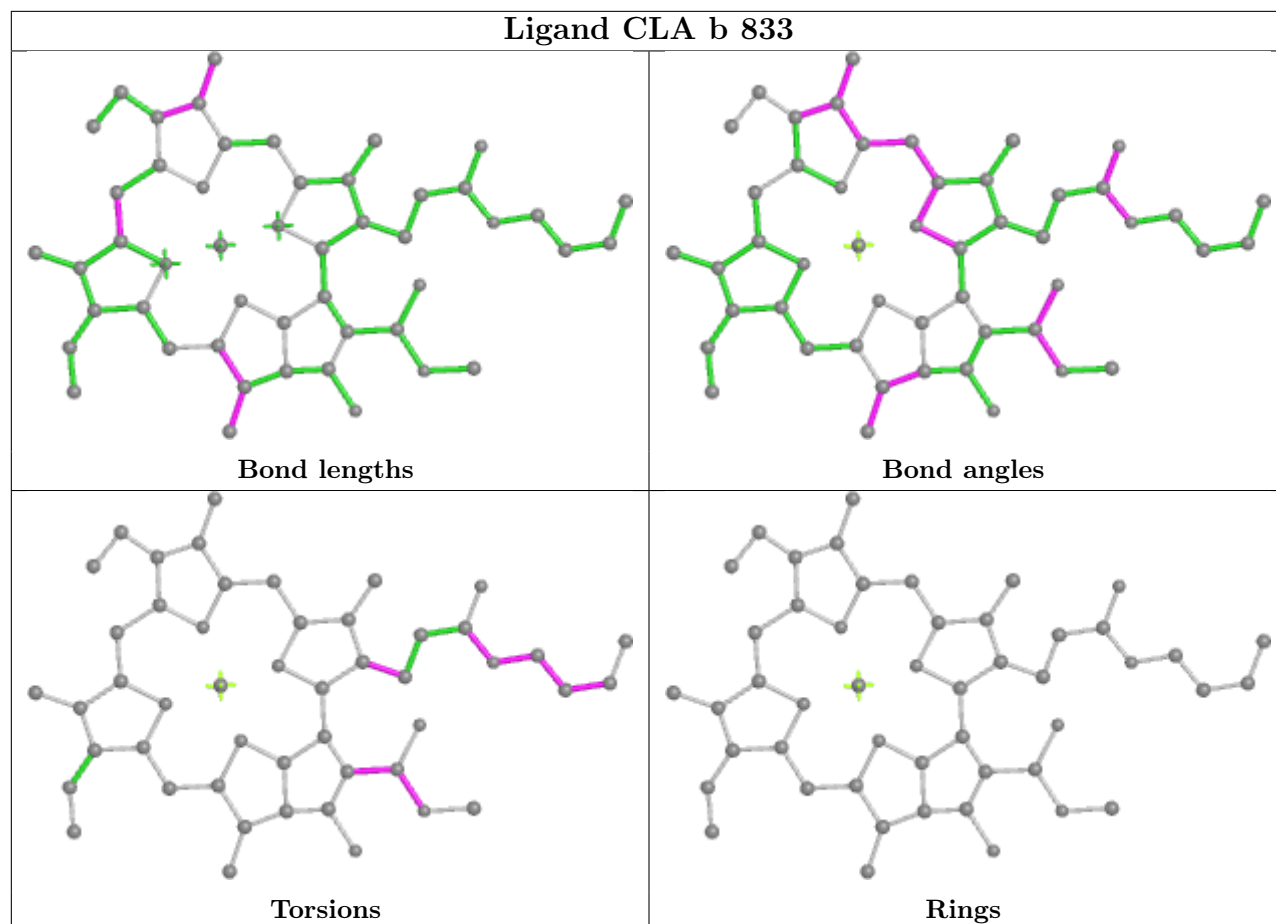
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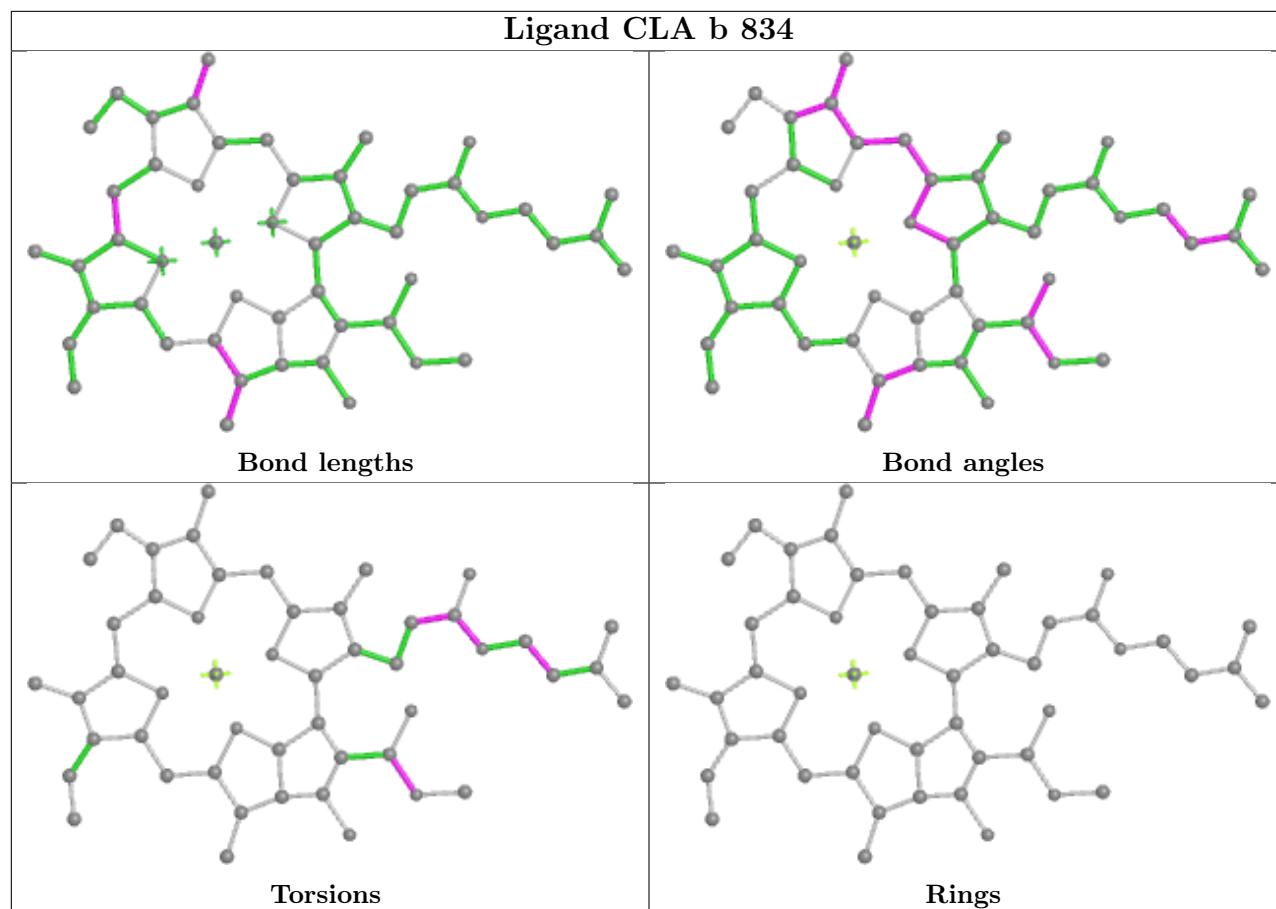
Ligand CLA b 832



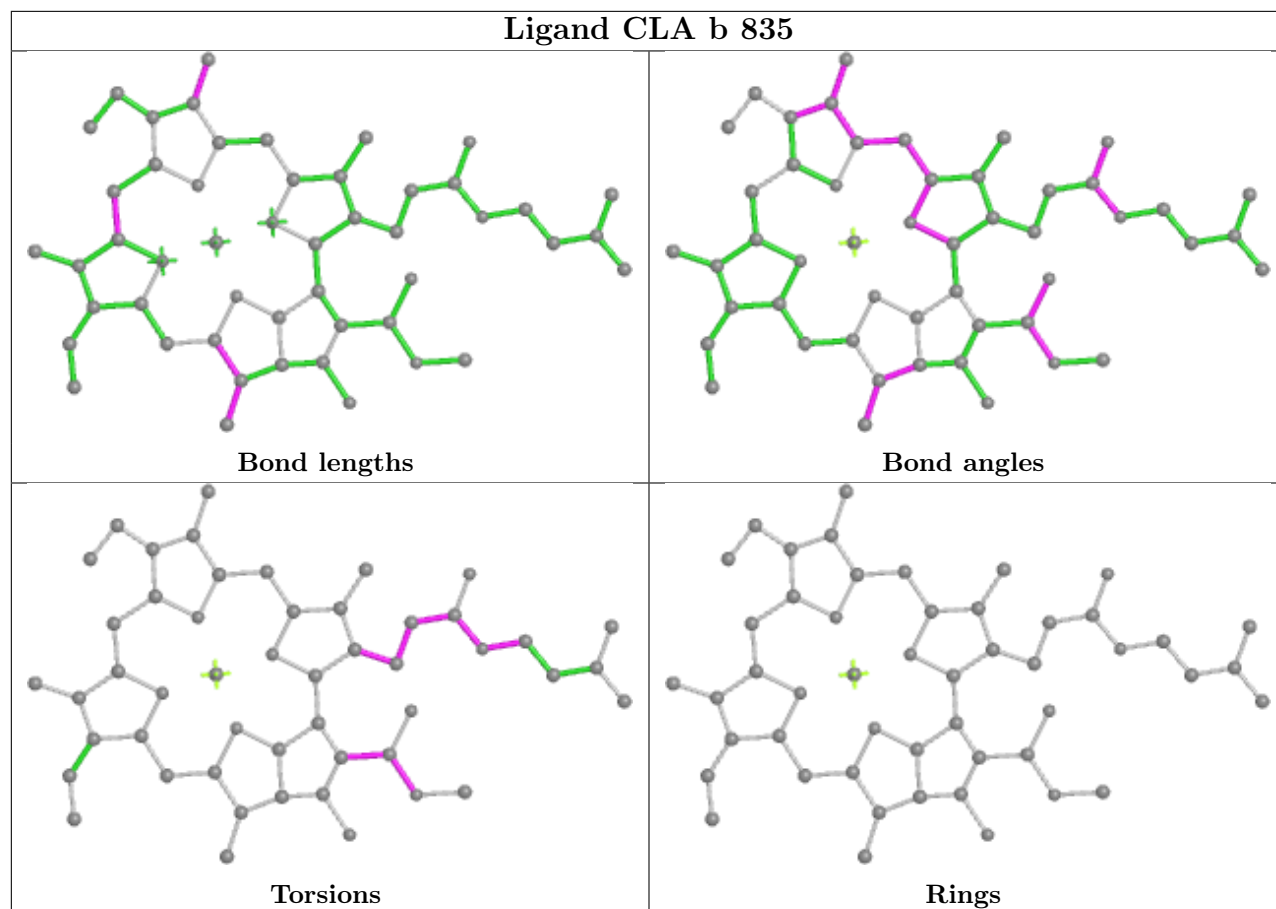
Ligand CLA b 833



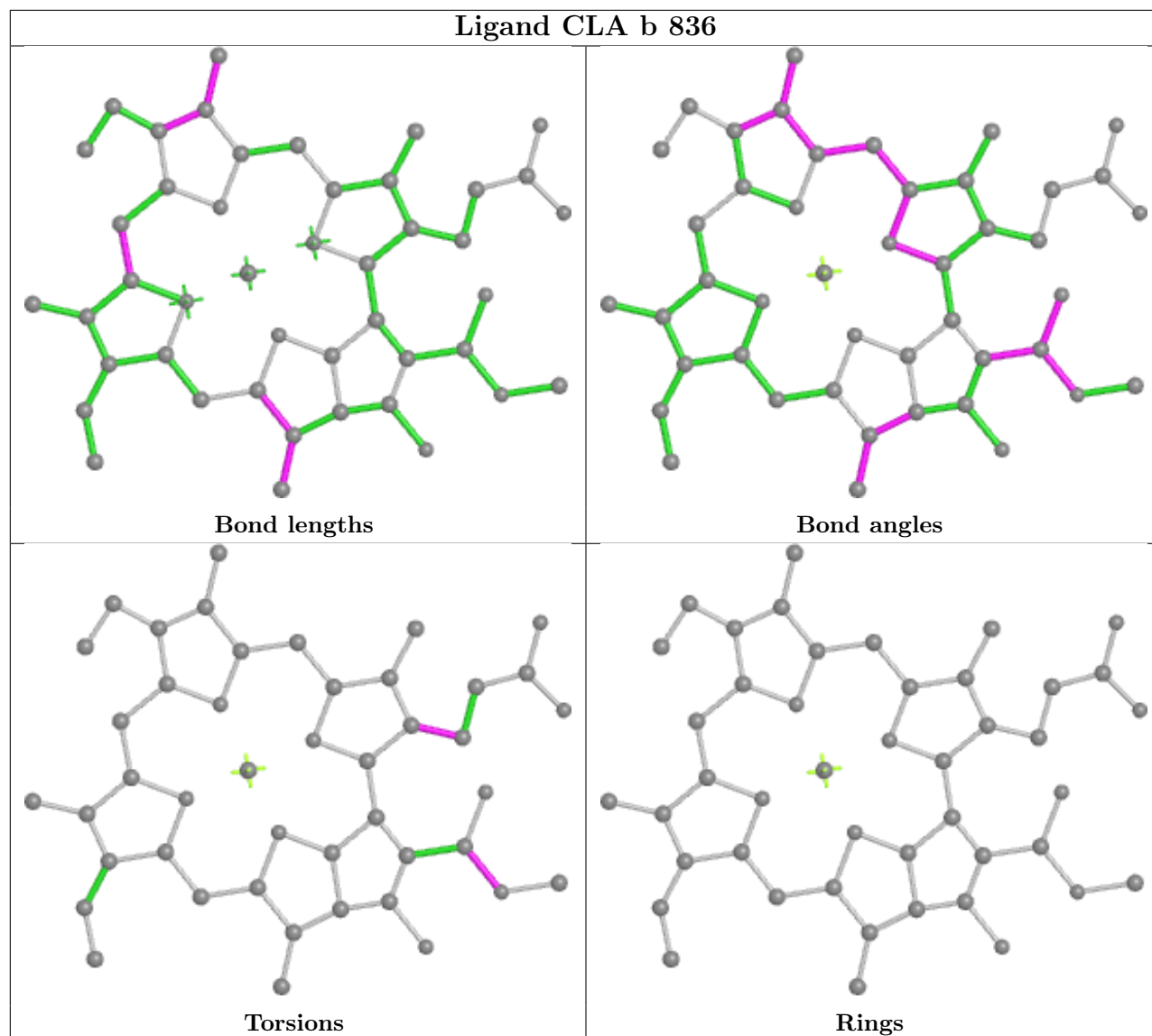
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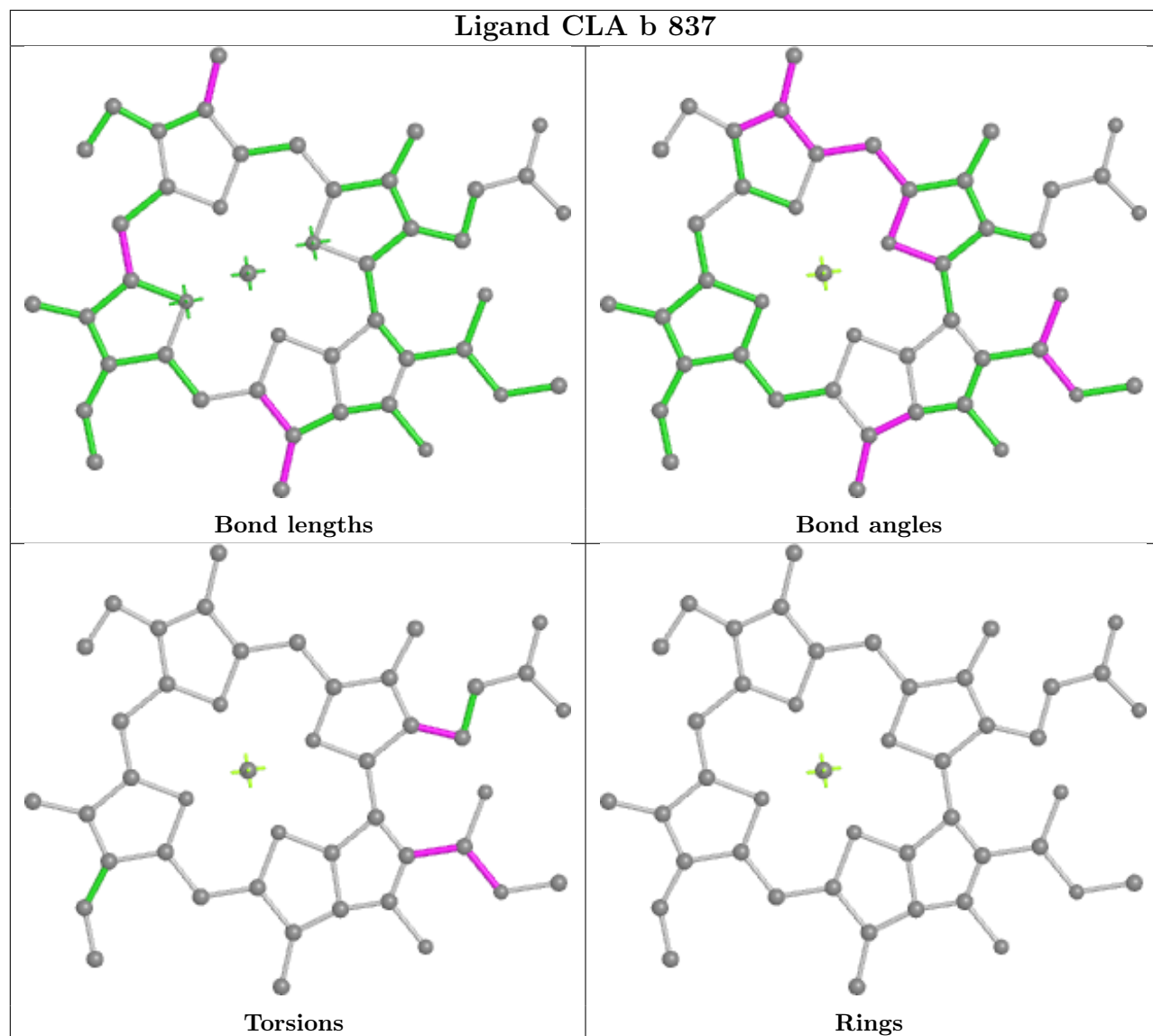
Ligand CLA b 835



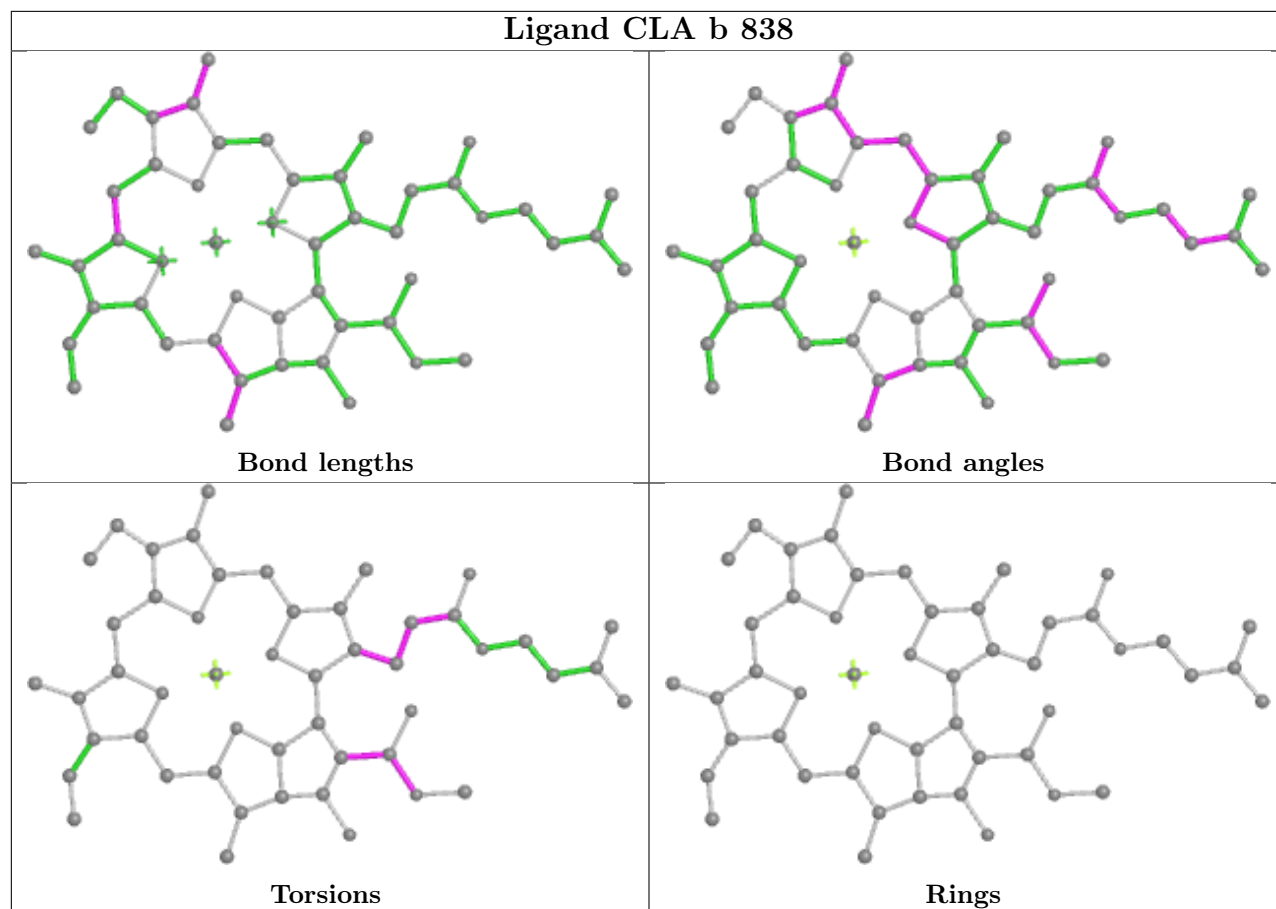
Ligand CLA b 836



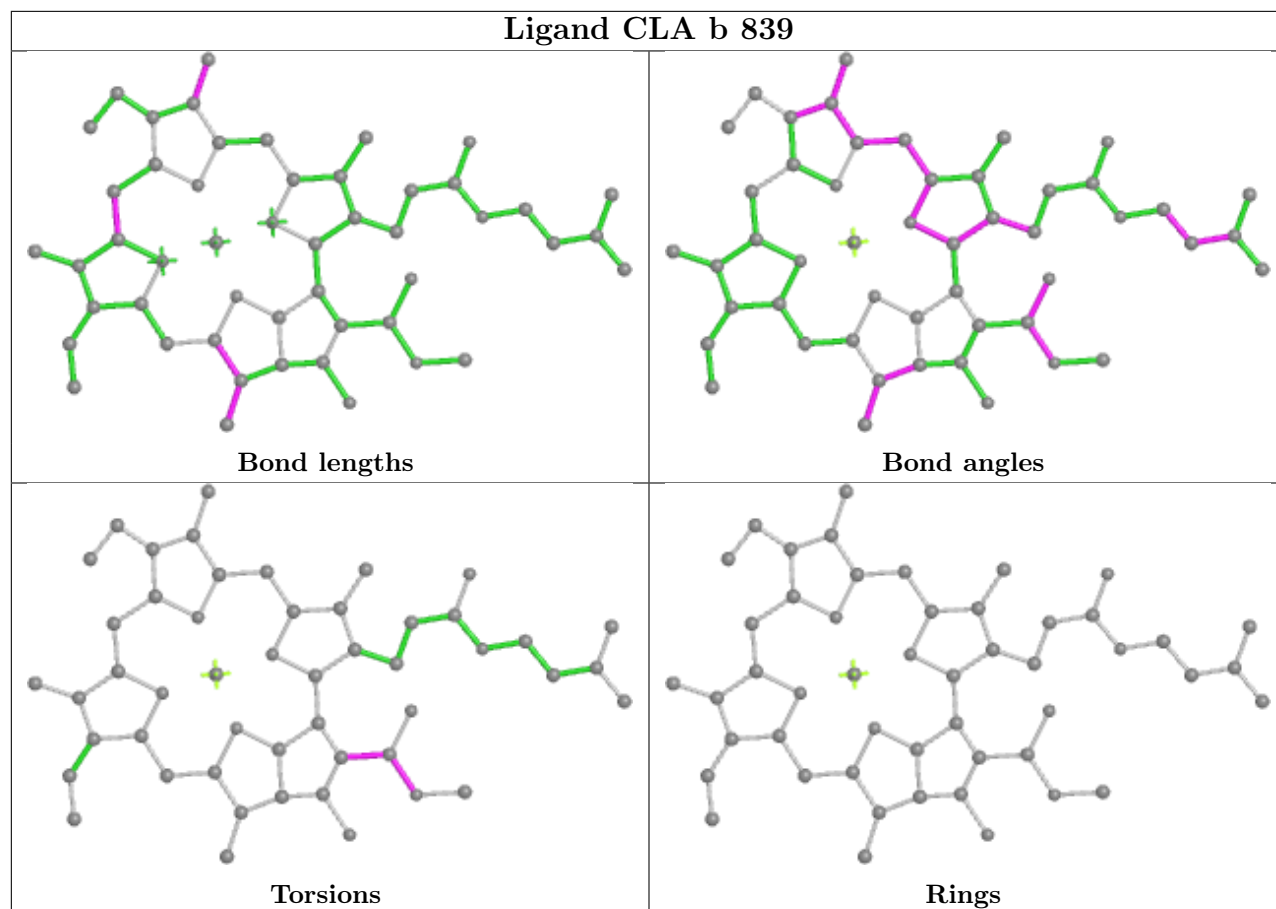
Ligand CLA b 837



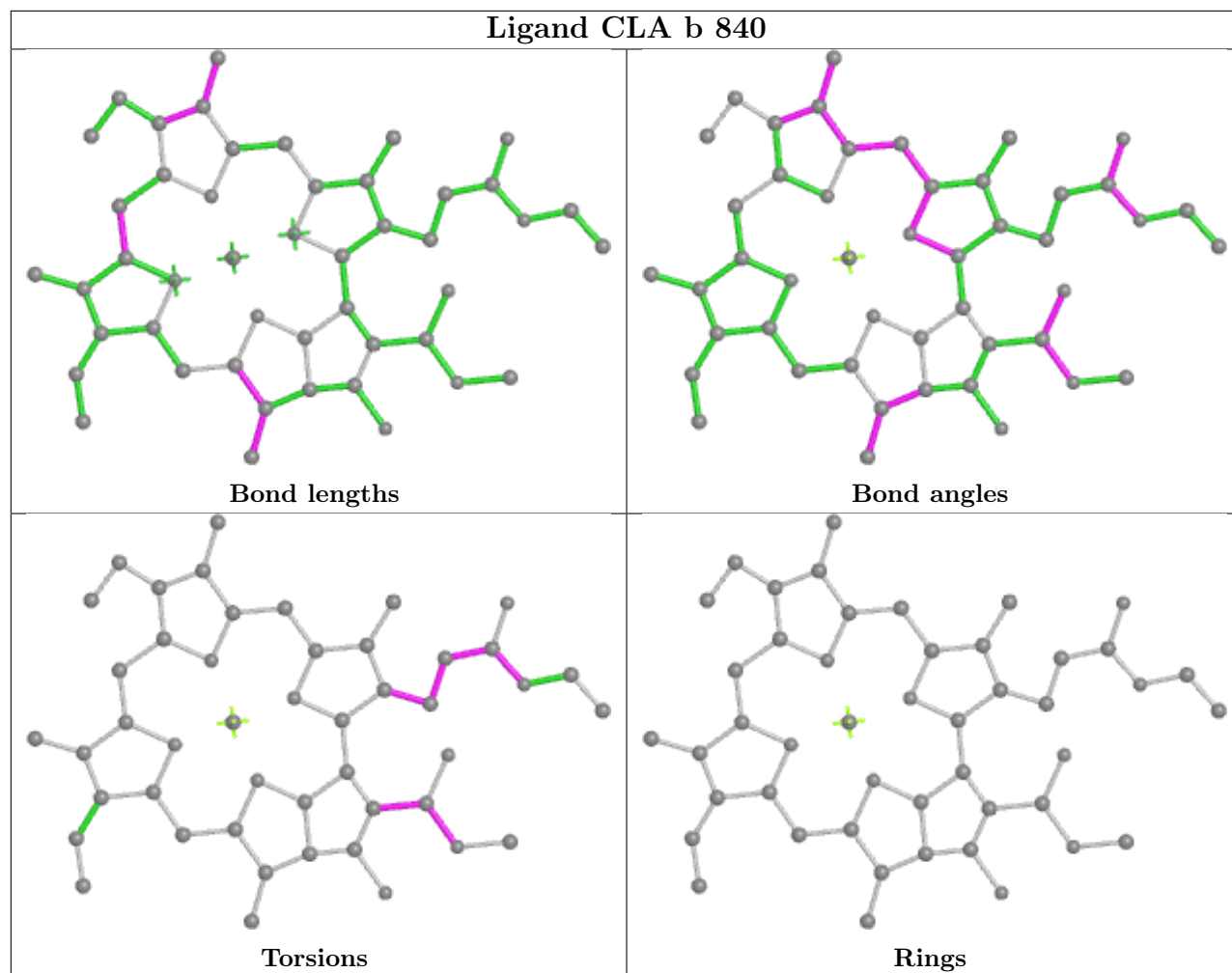
Ligand CLA b 838



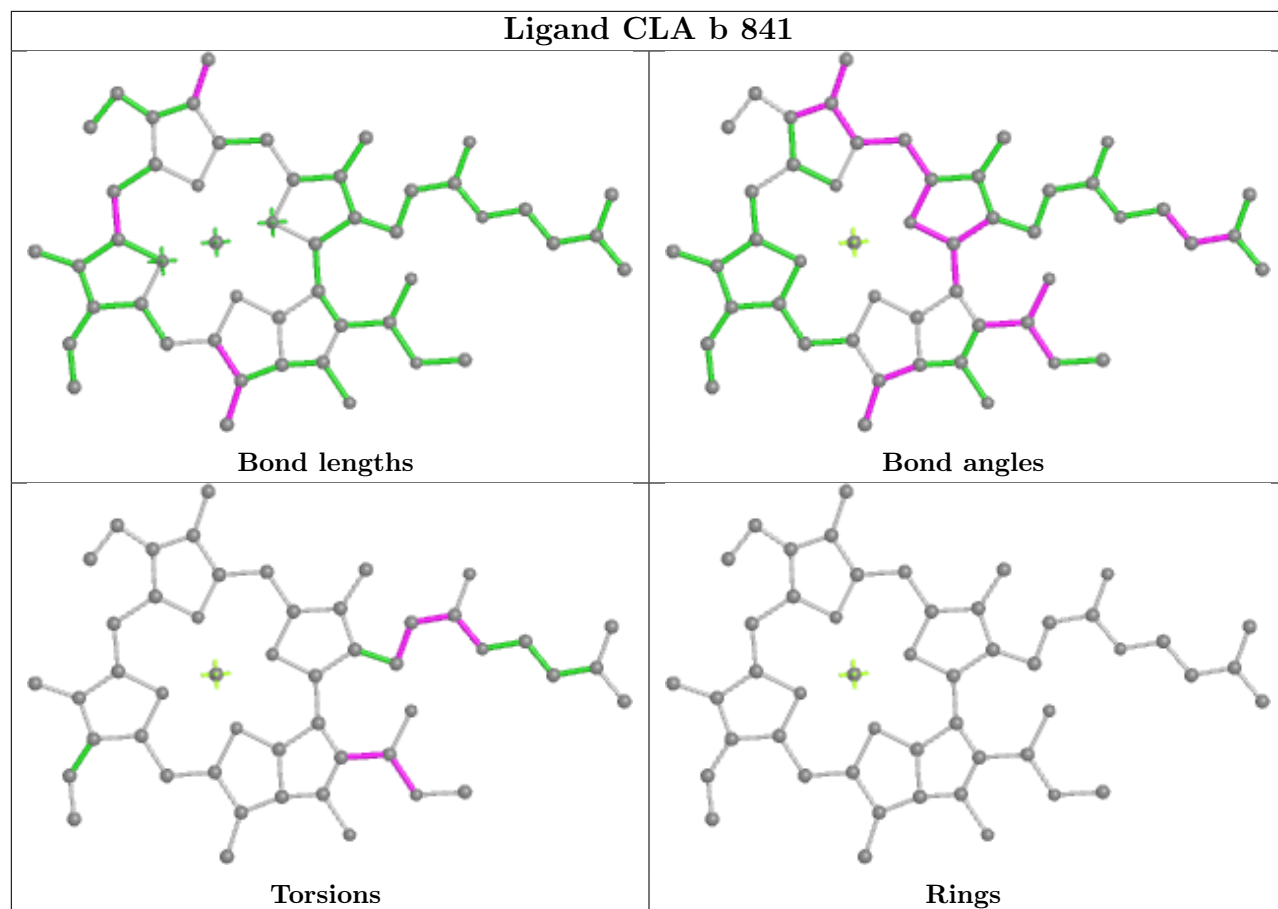
Ligand CLA b 839

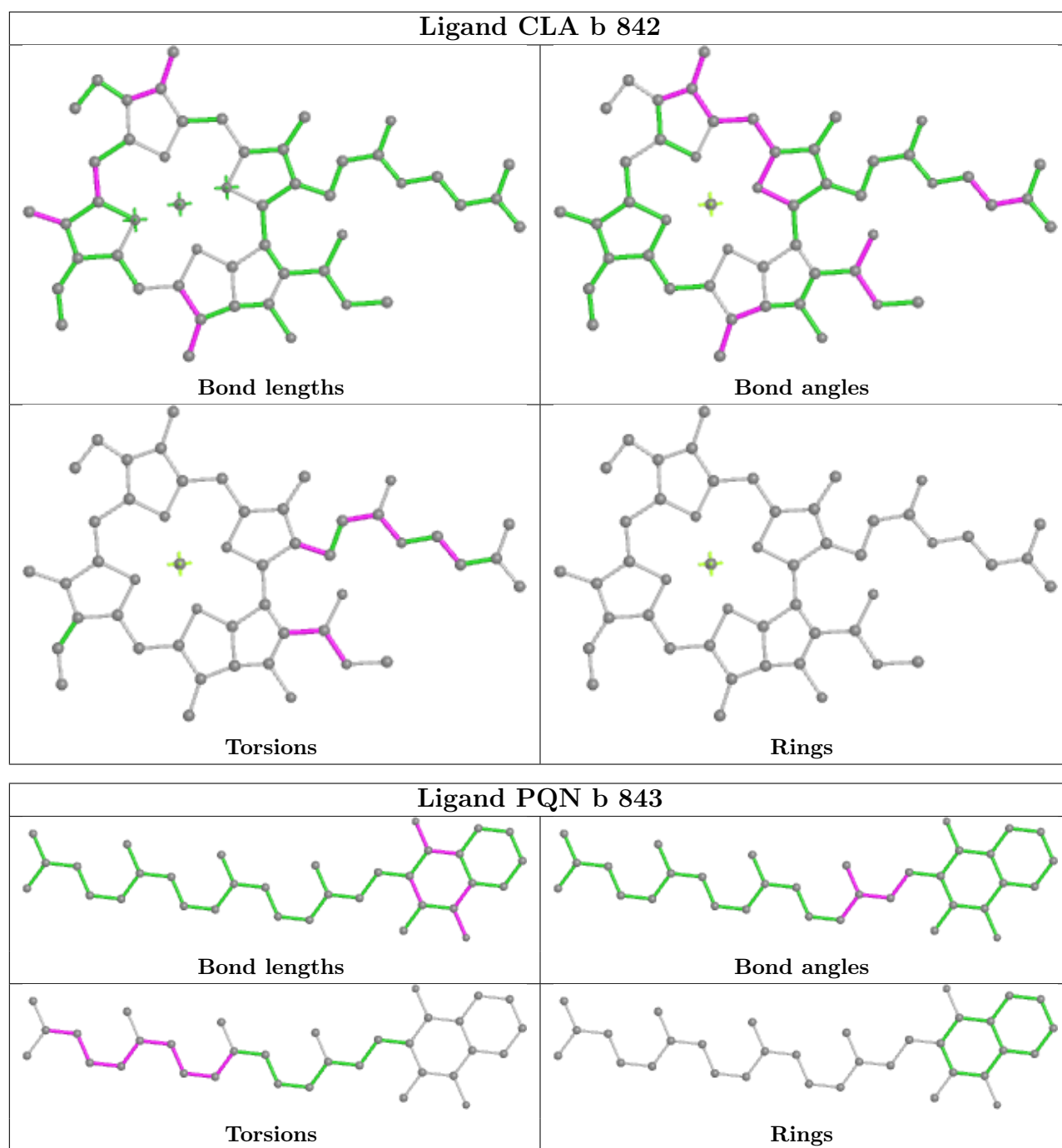


Ligand CLA b 840

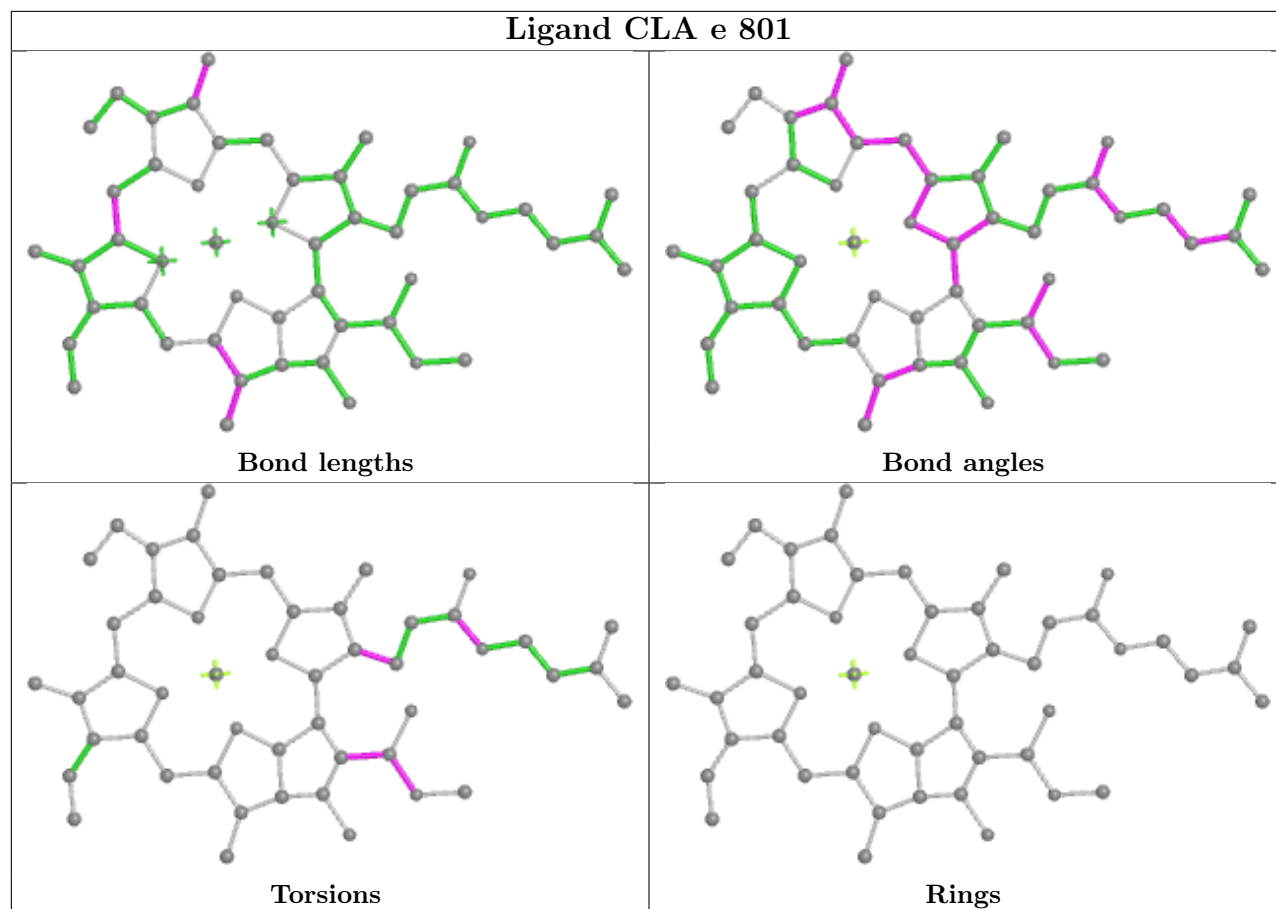


Ligand CLA b 841

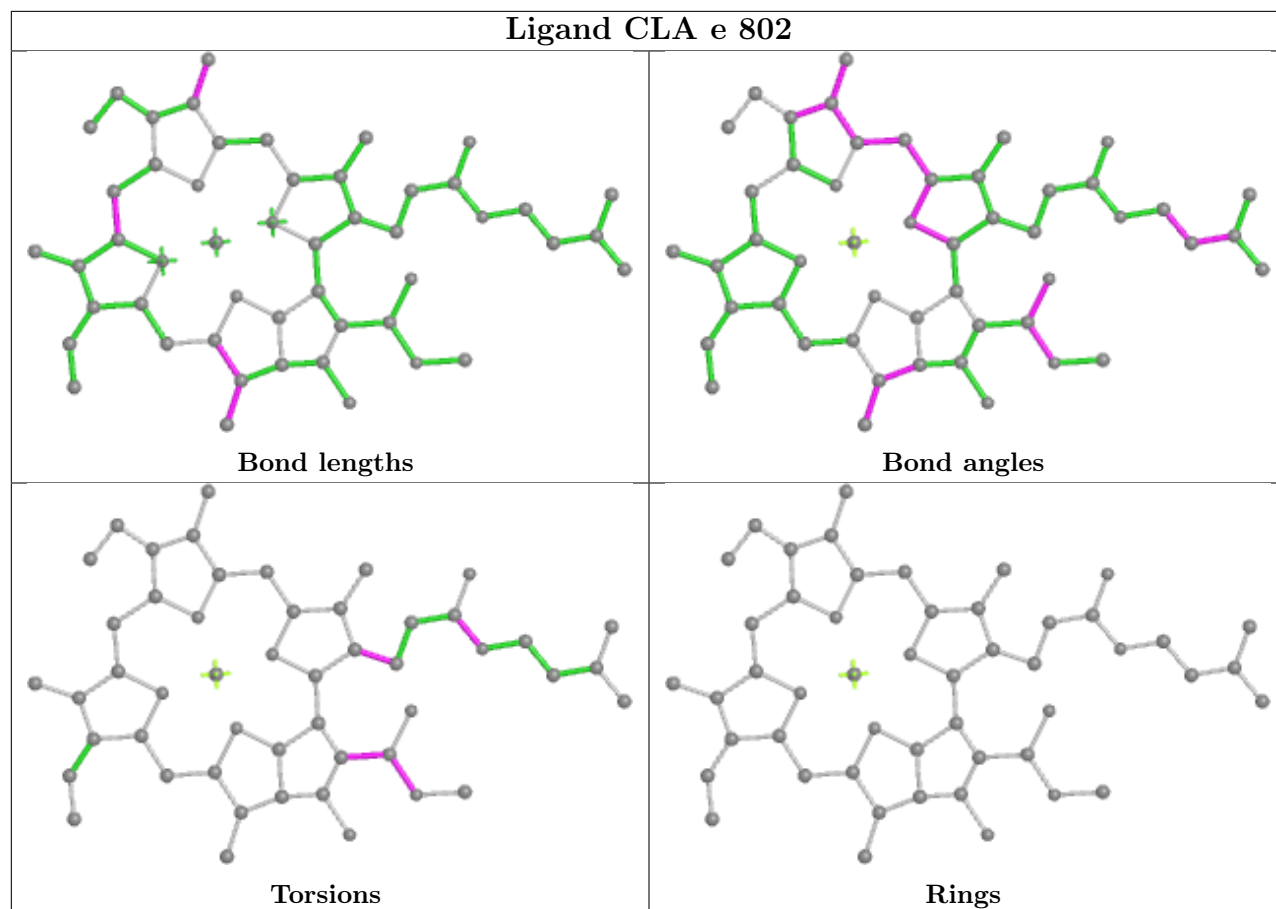




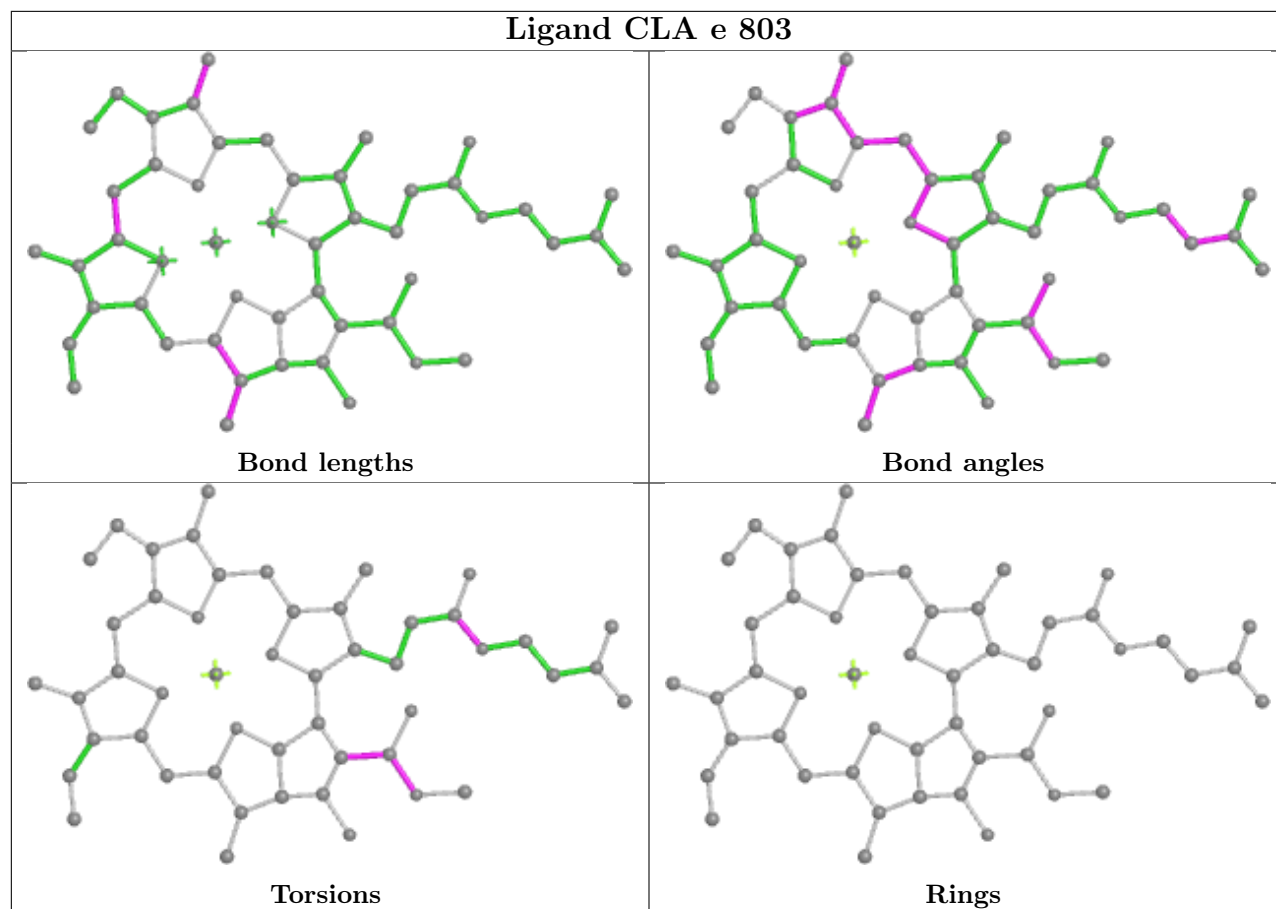
Ligand CLA e 801



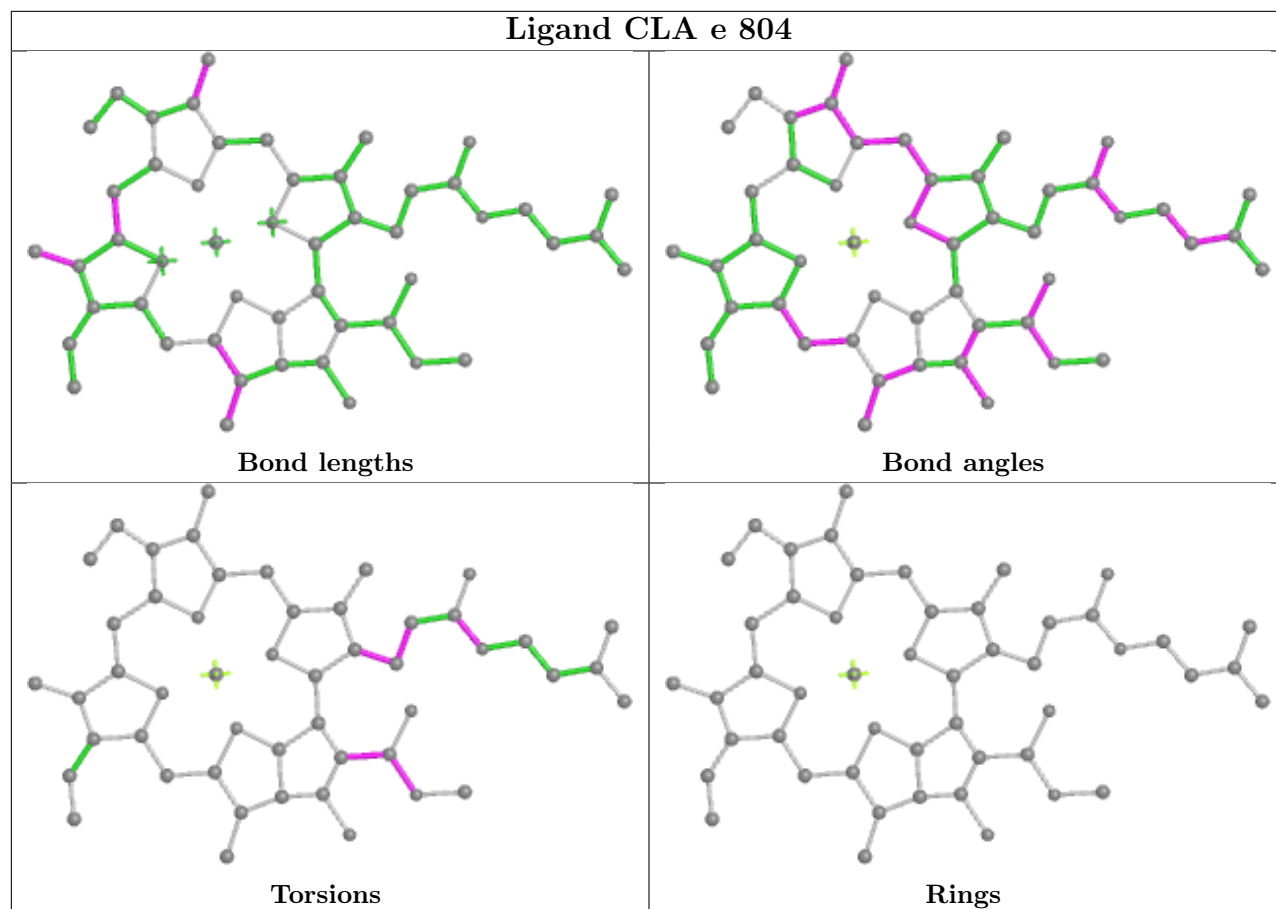
Ligand CLA e 802



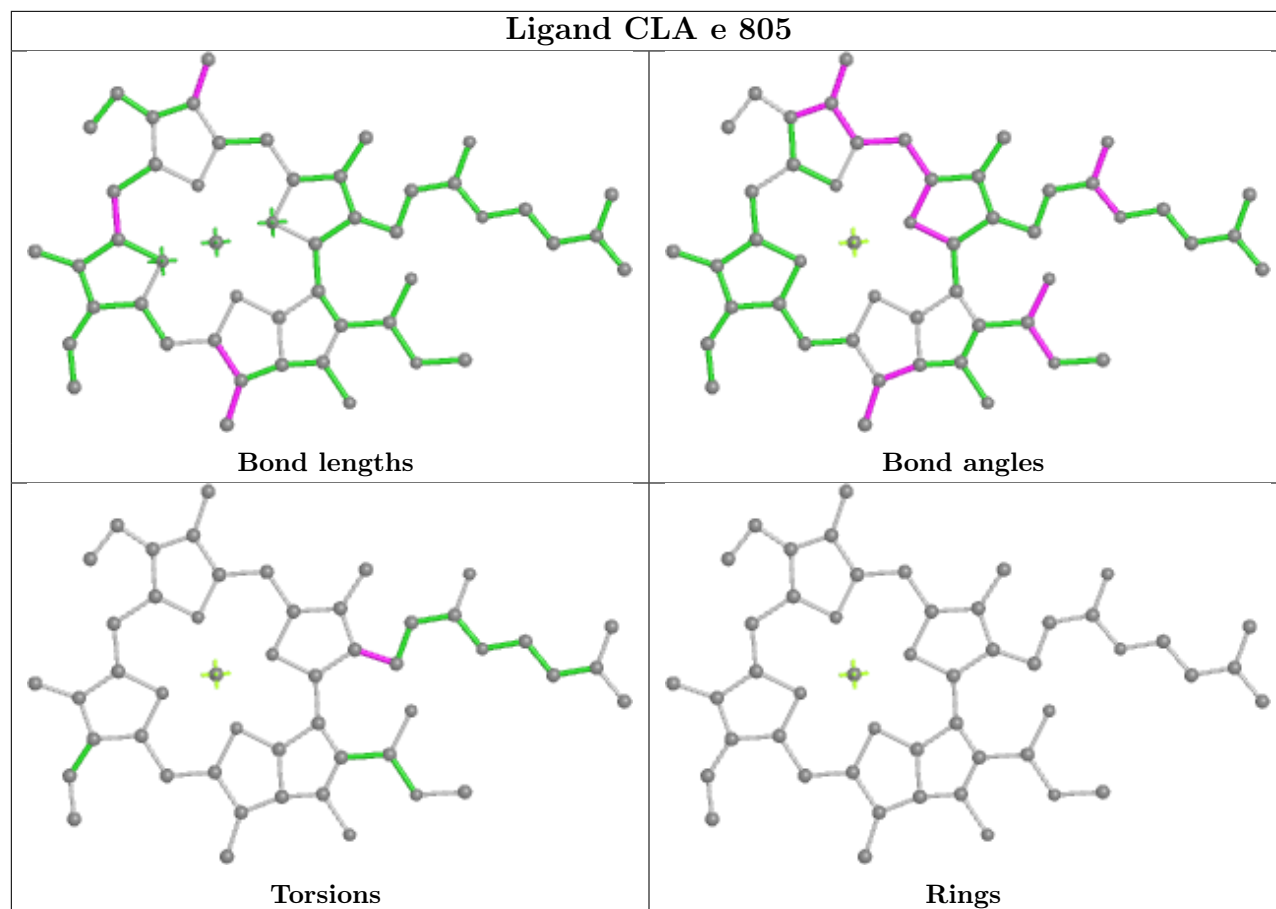
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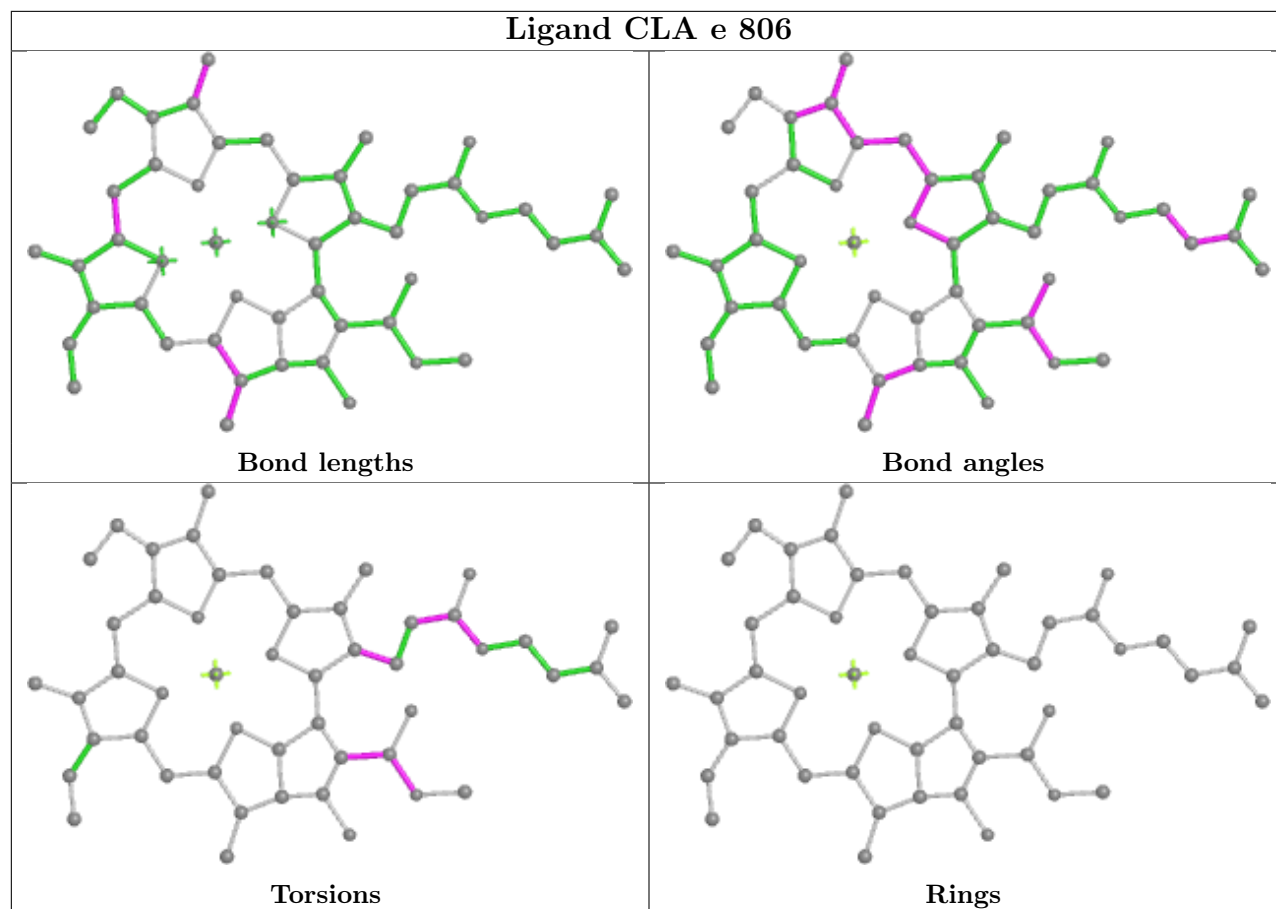
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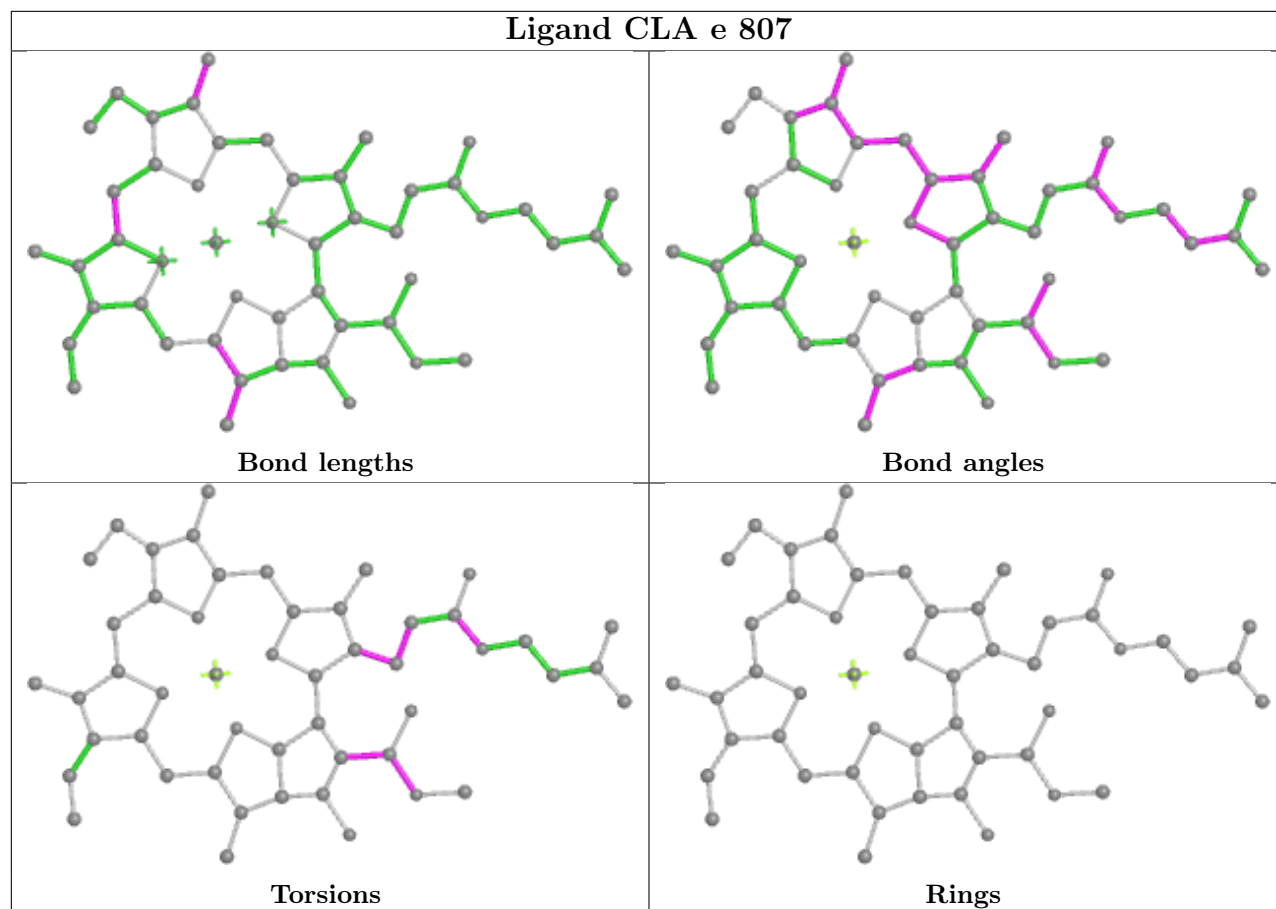
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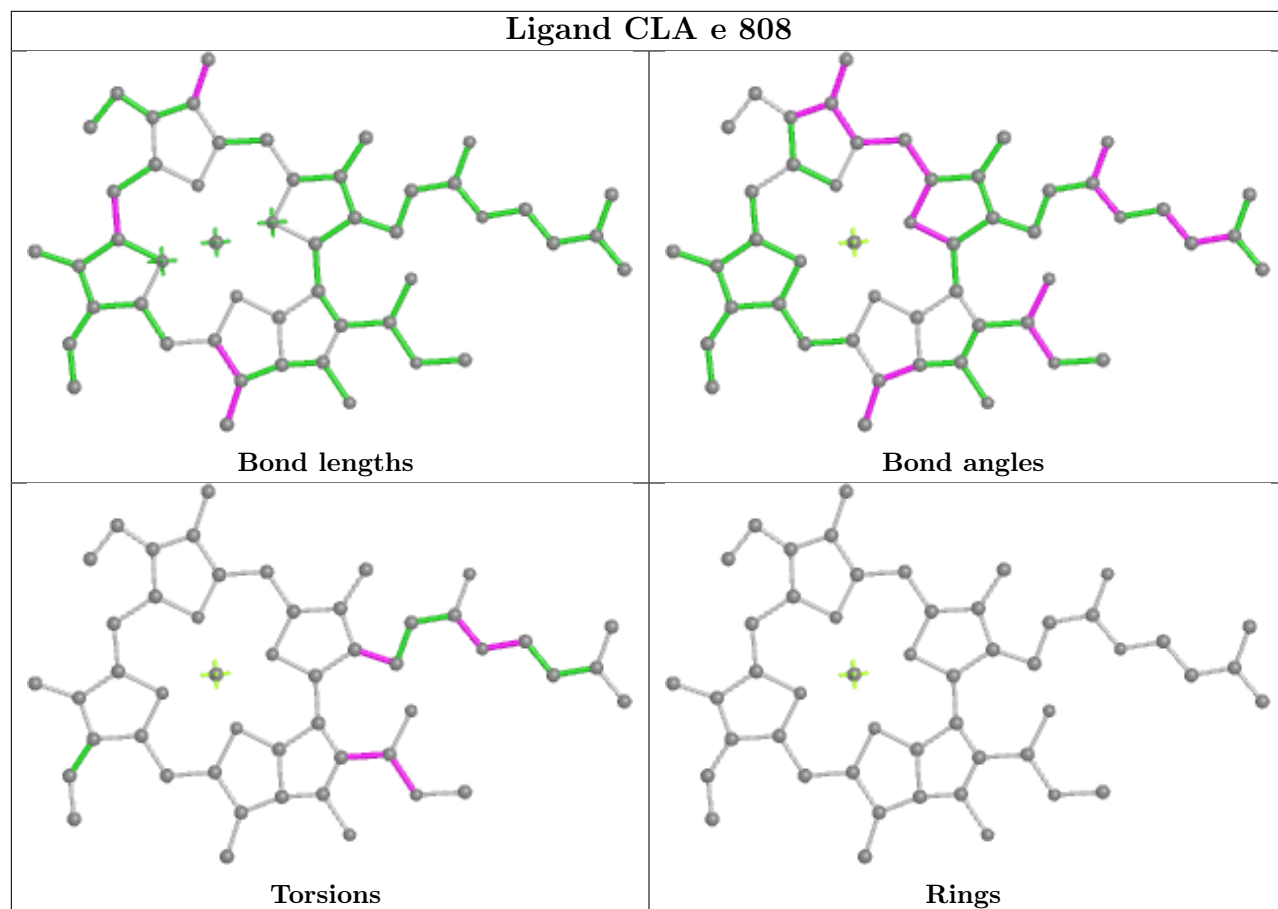
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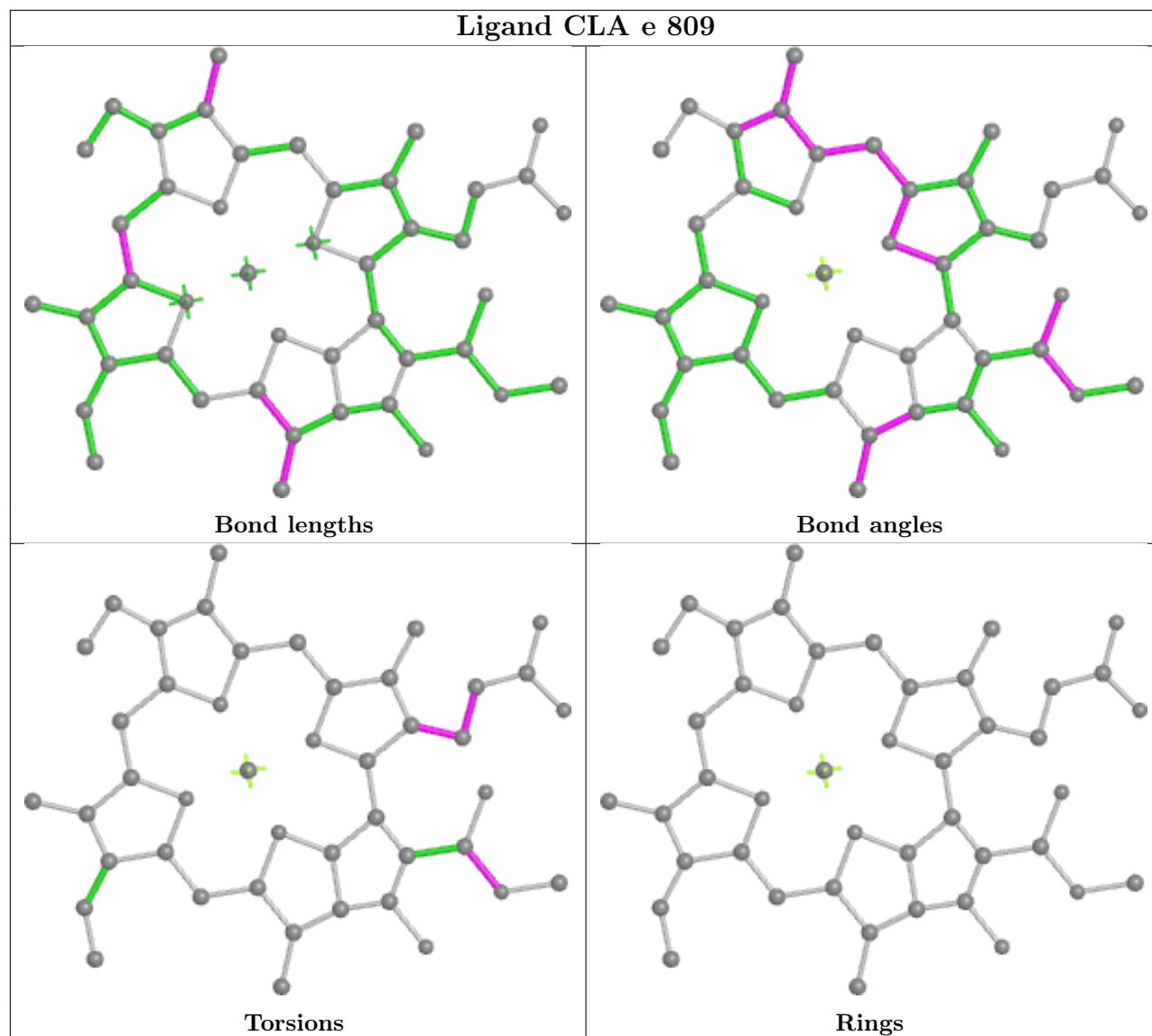
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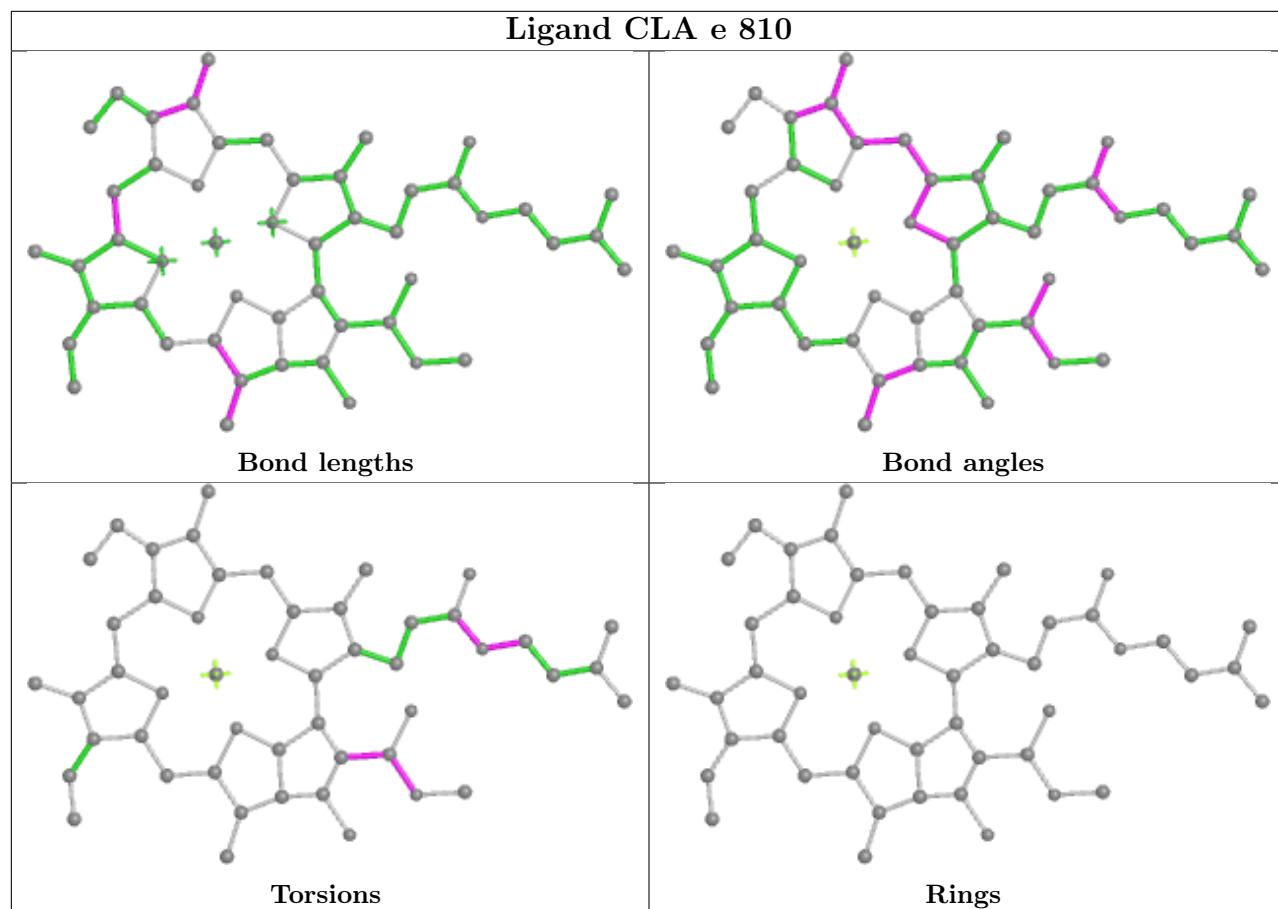
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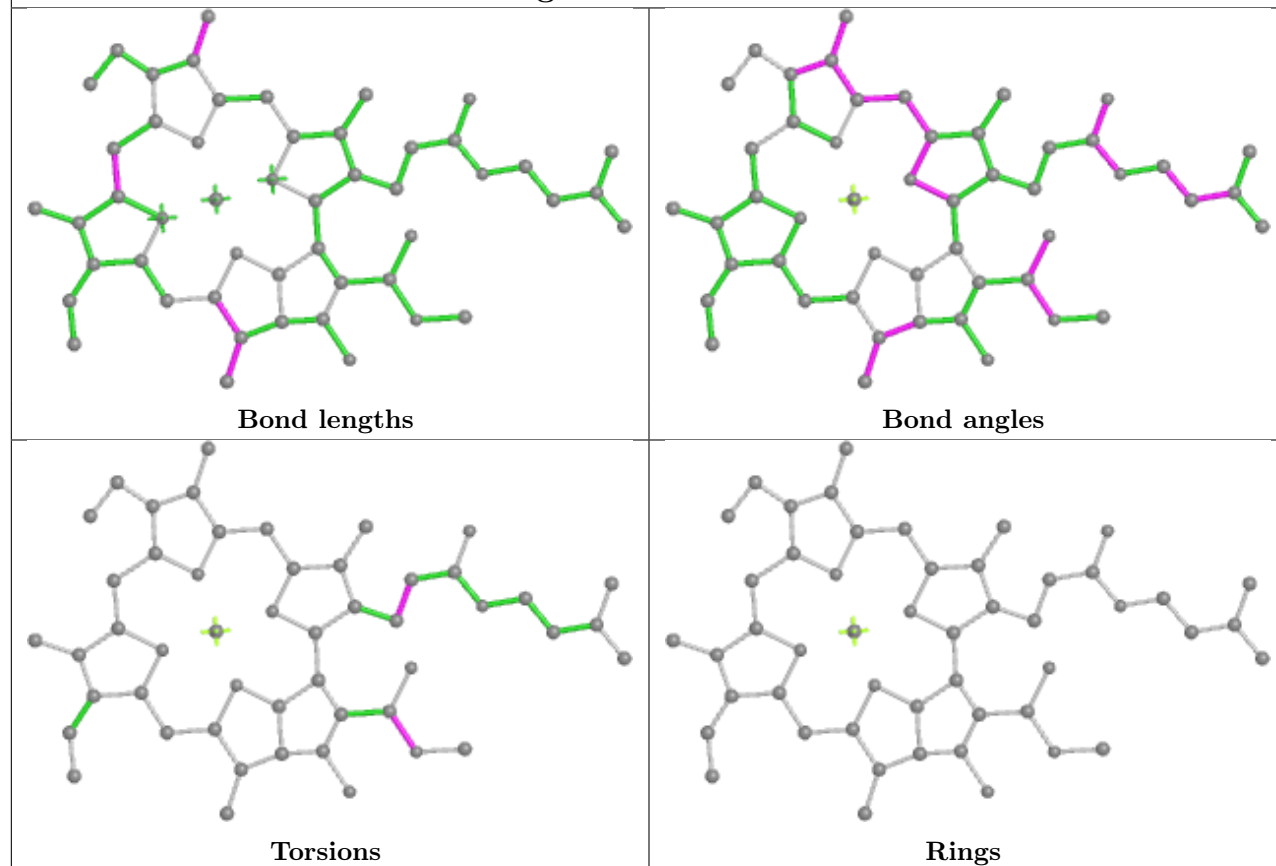
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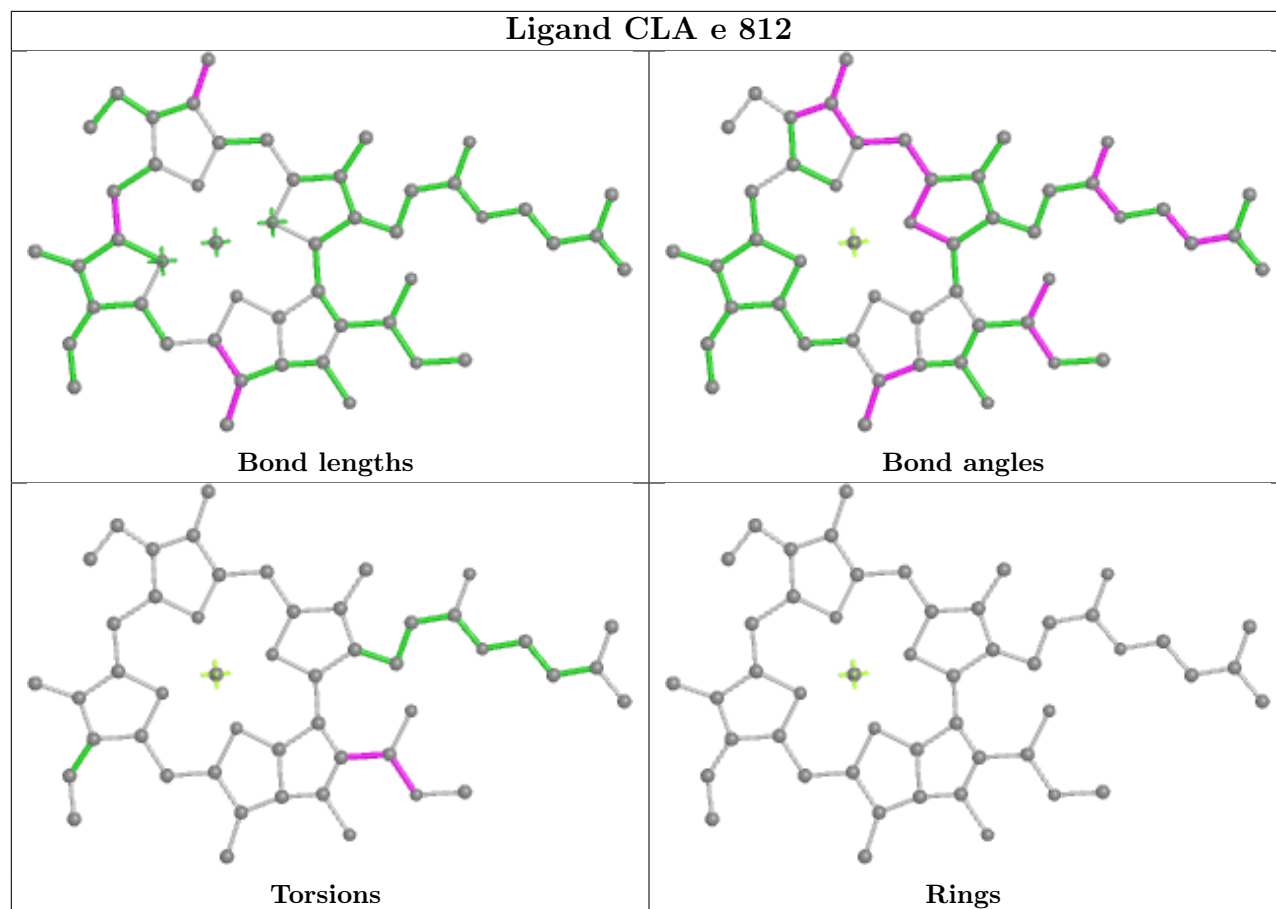
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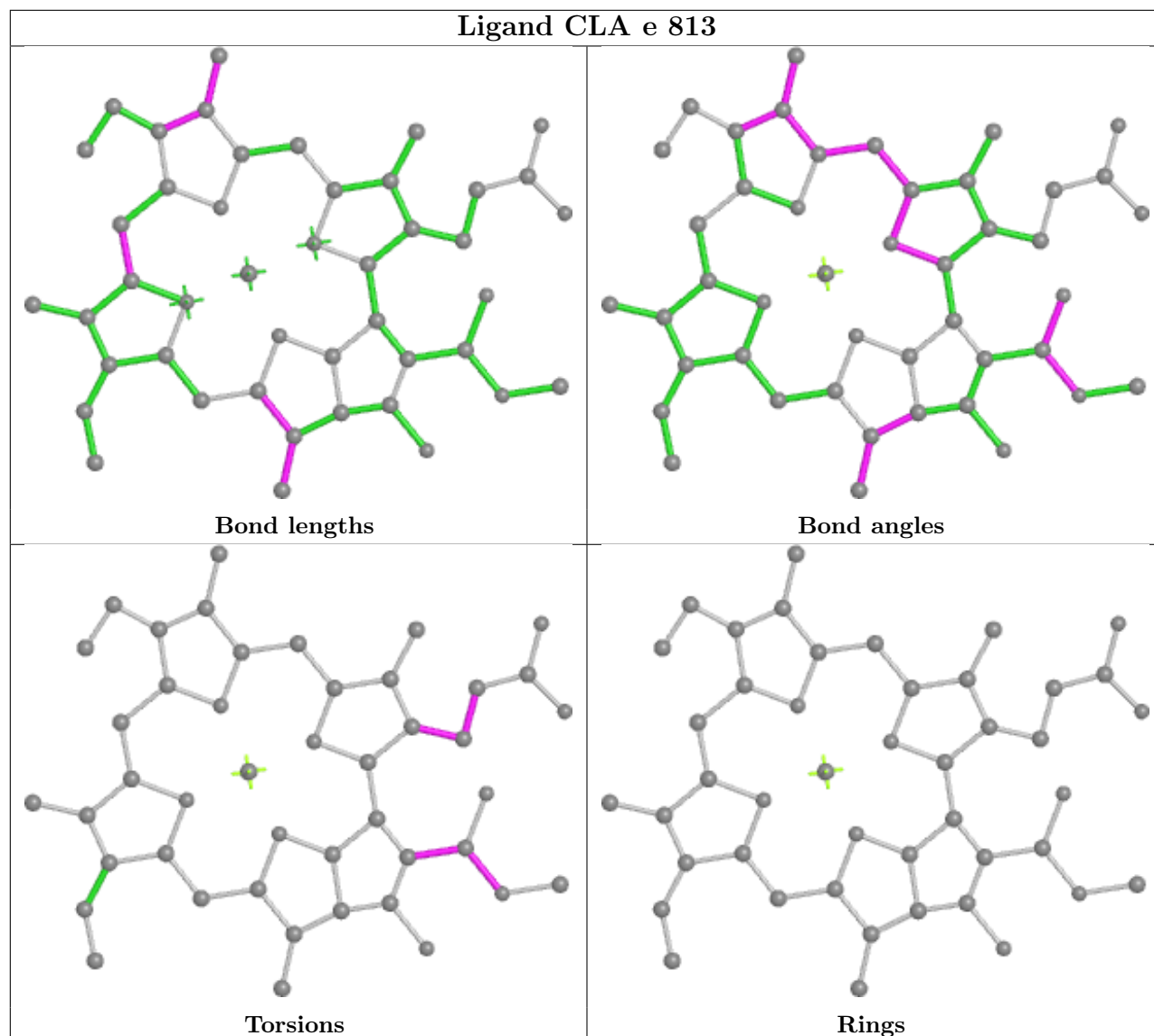
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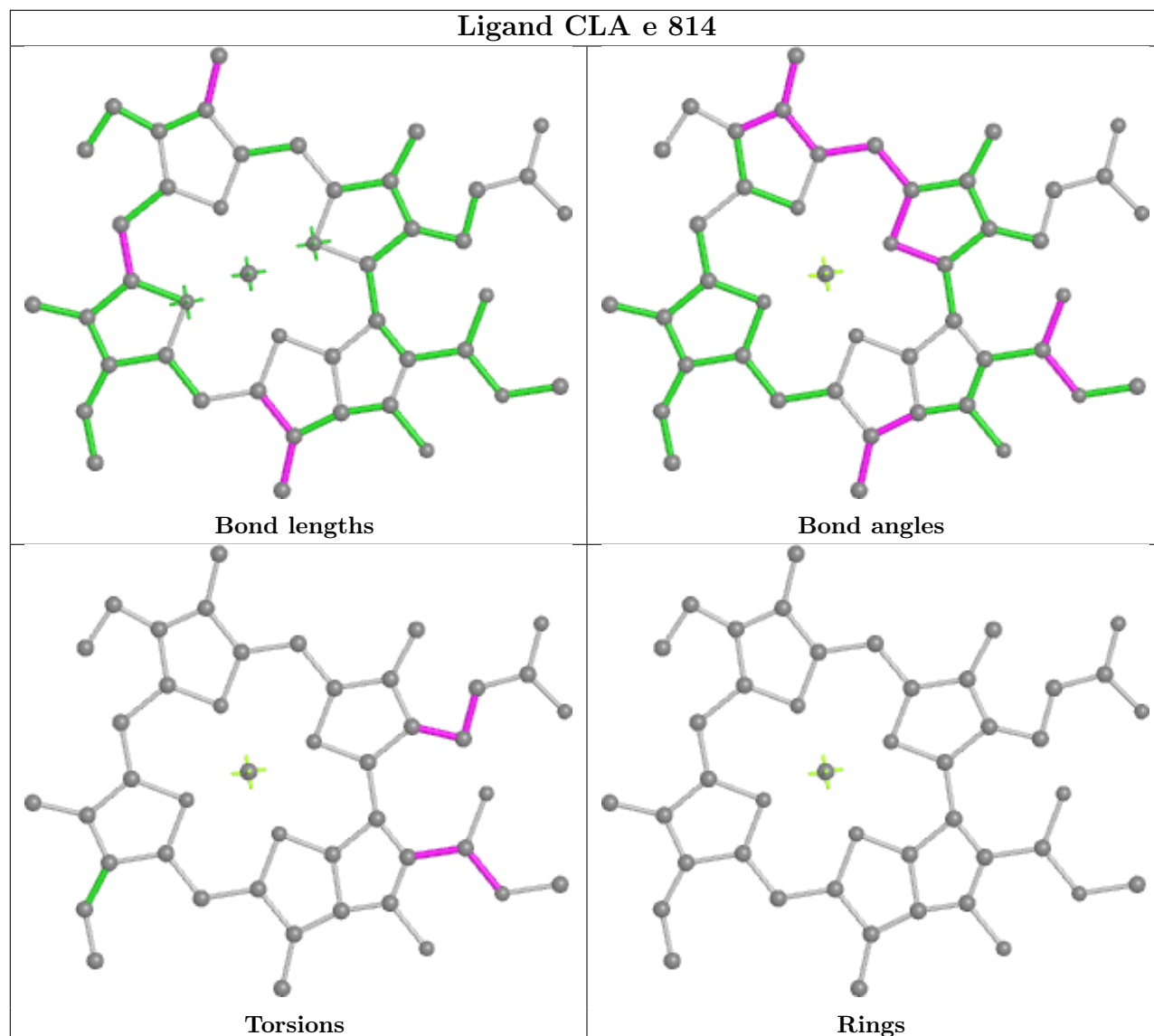
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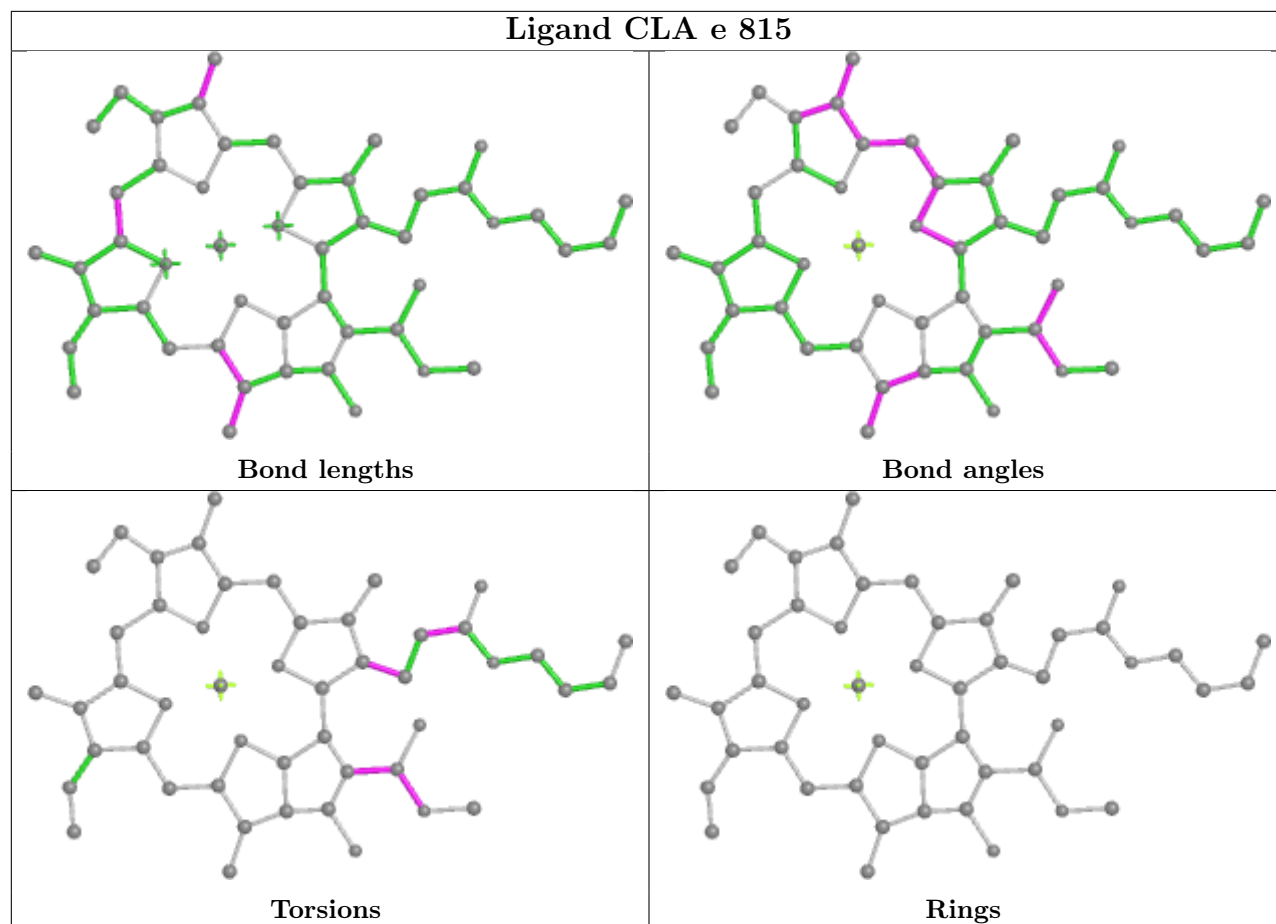
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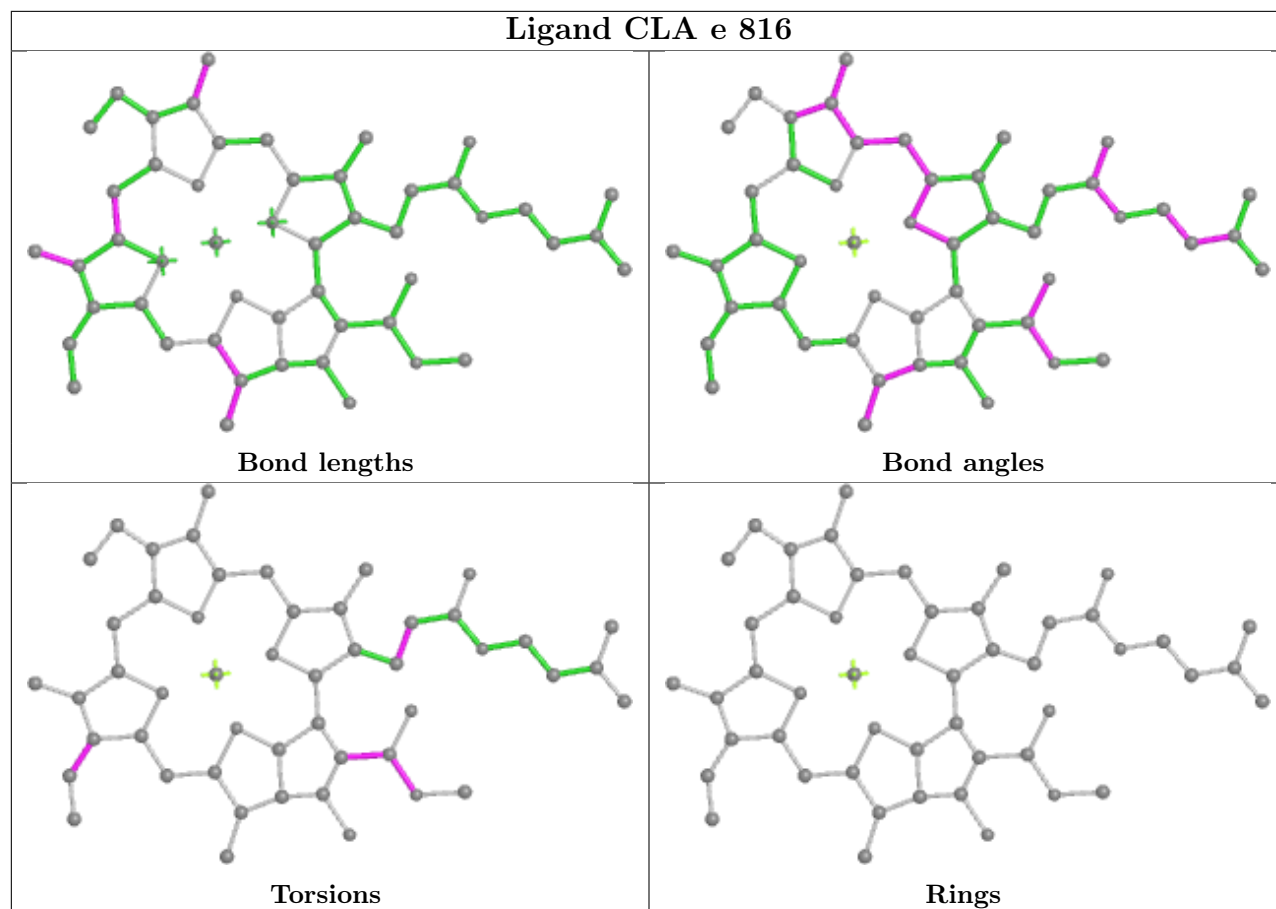
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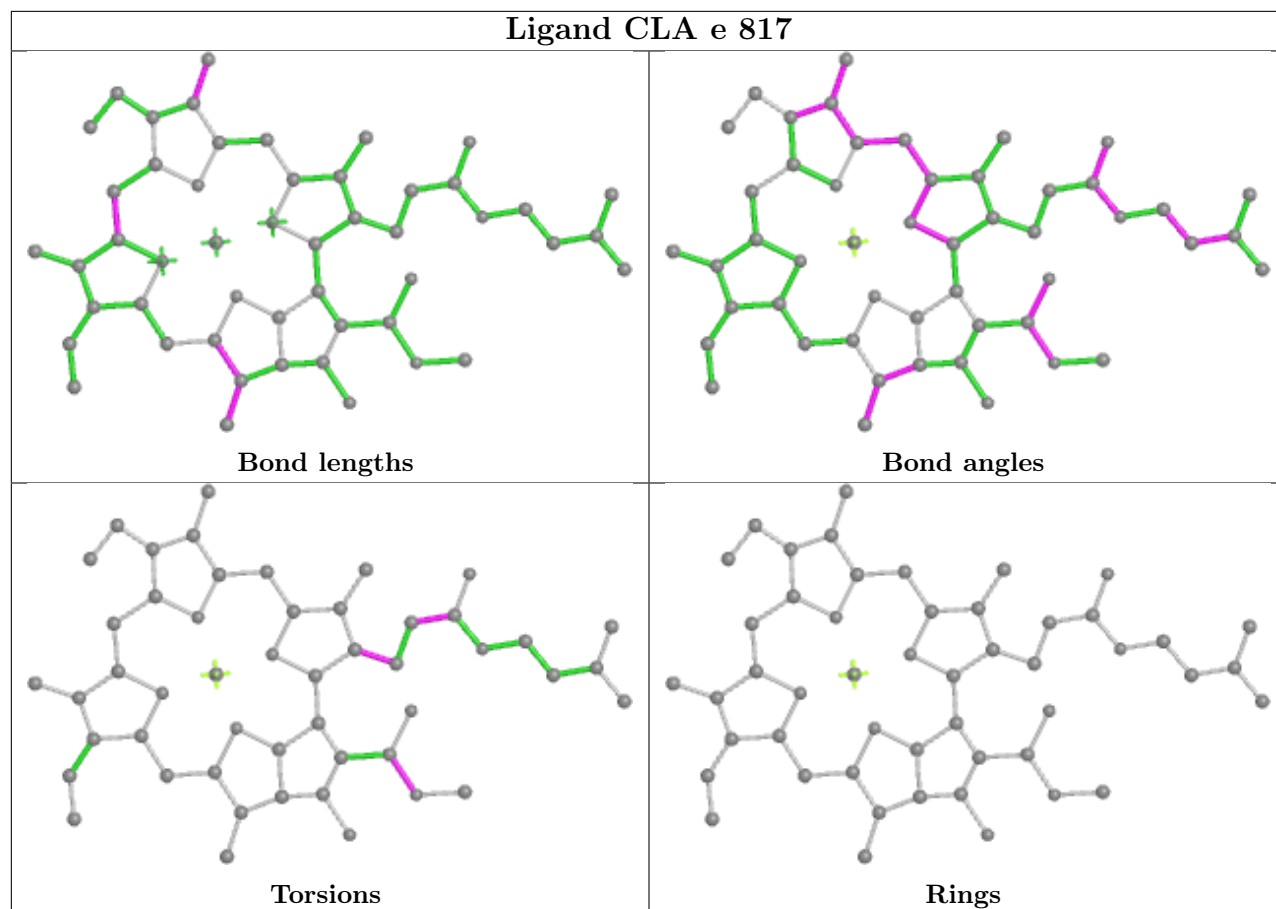
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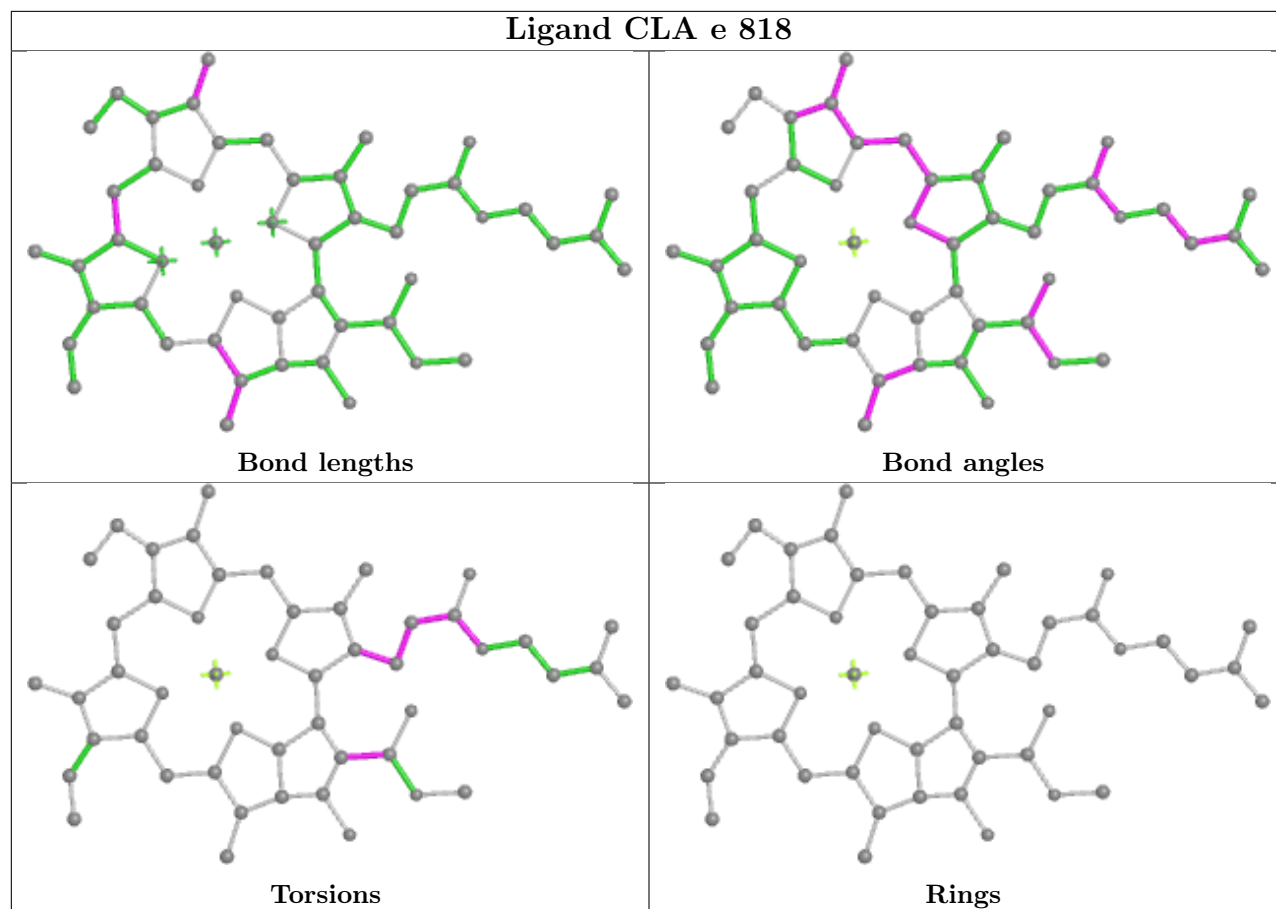
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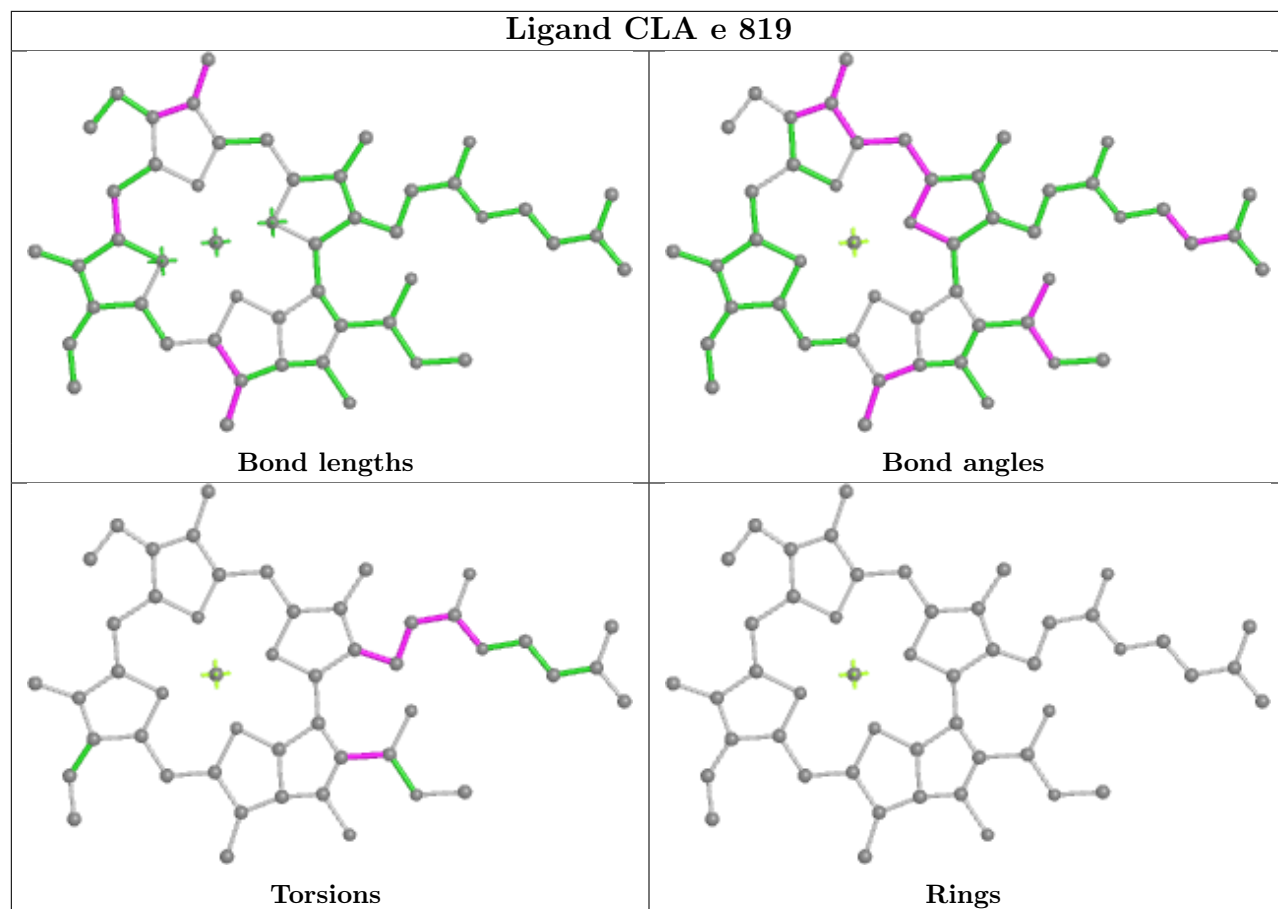
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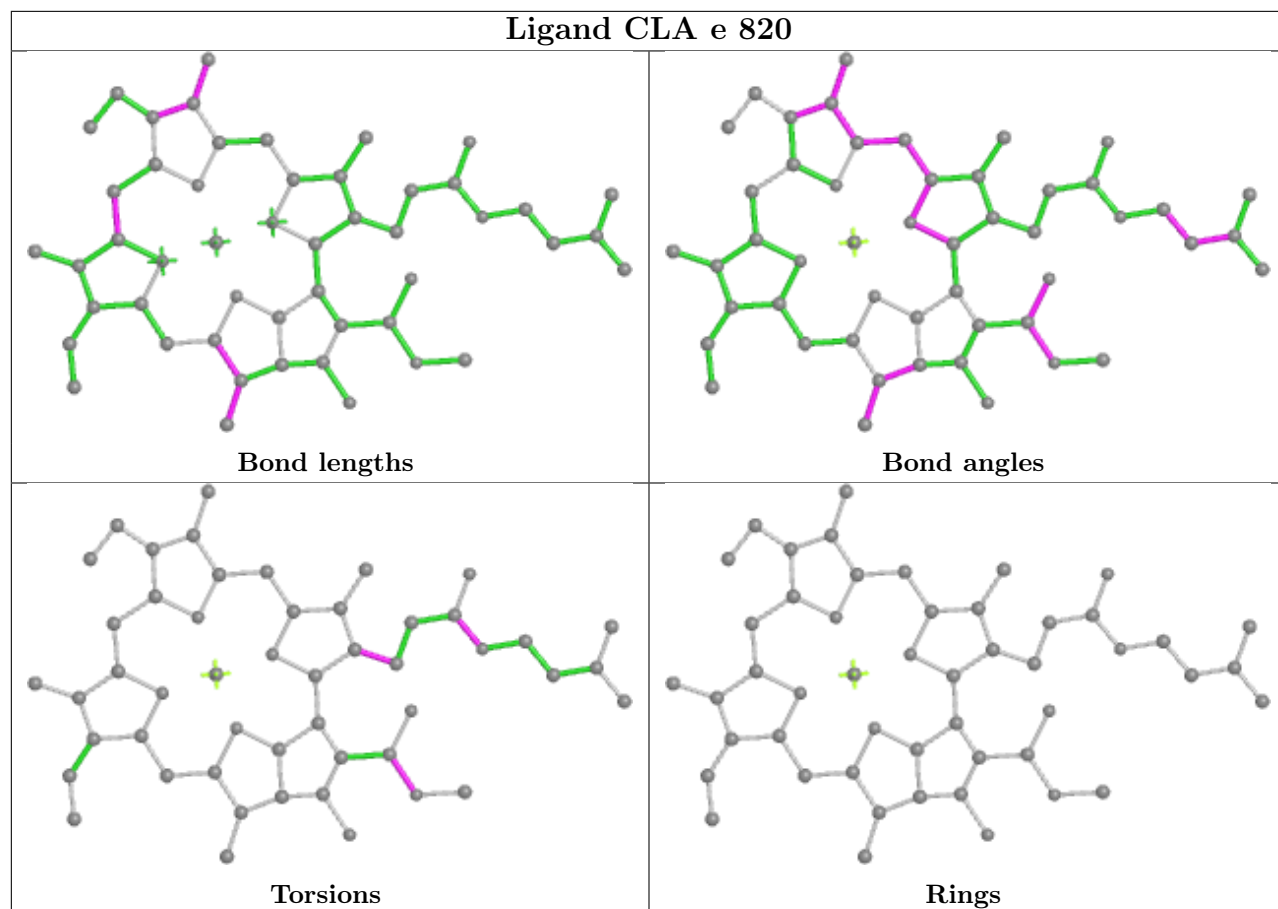
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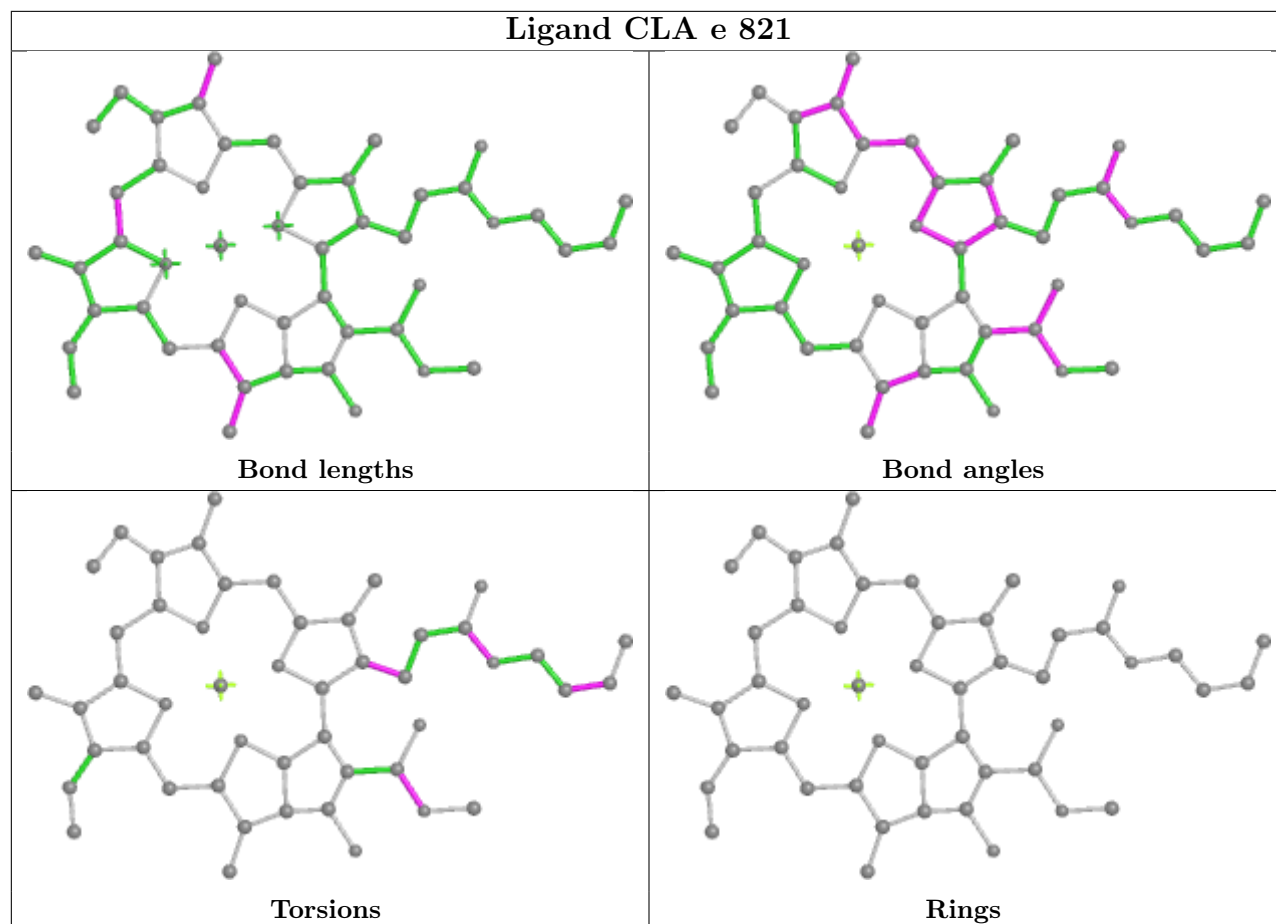
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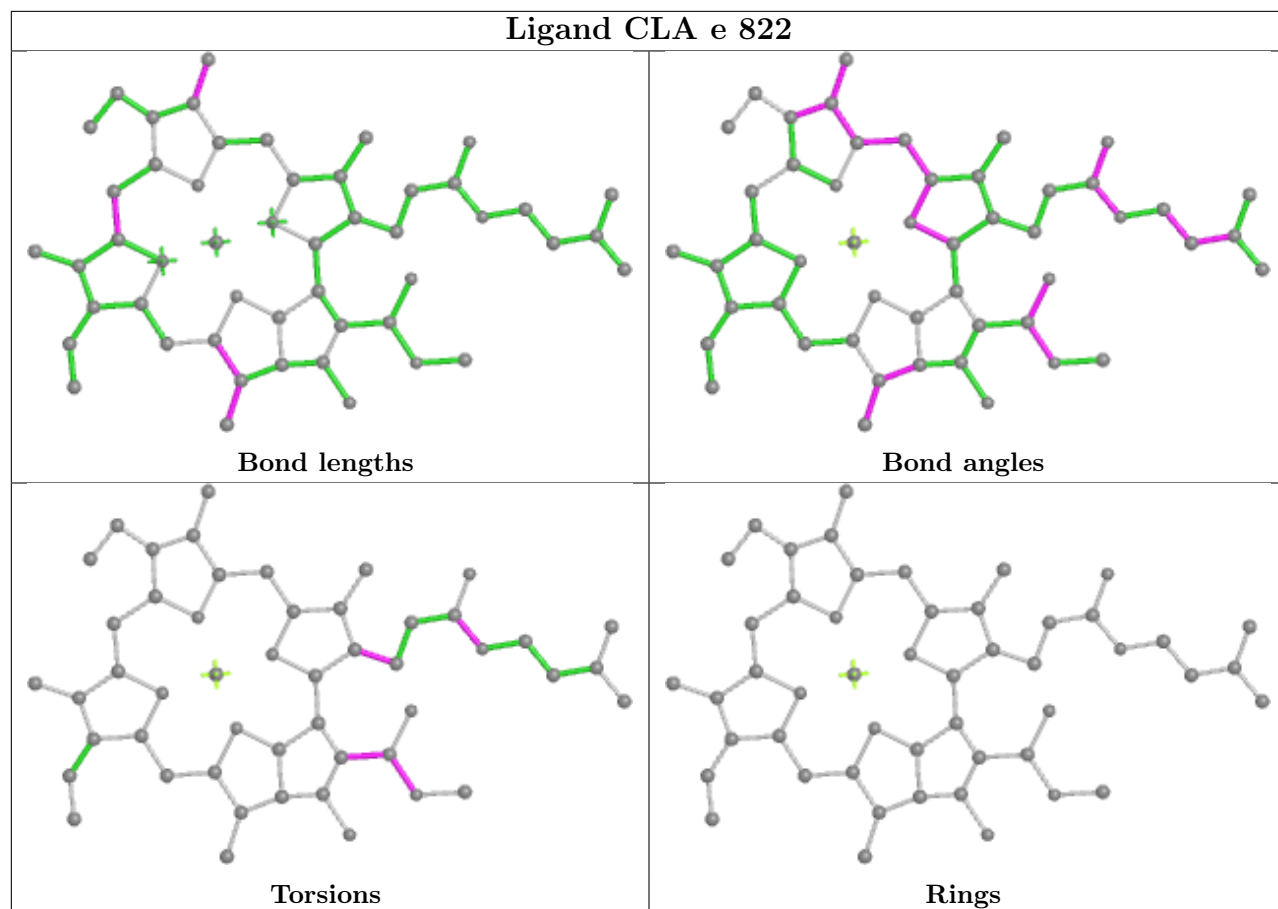
Ligand CLA e 820



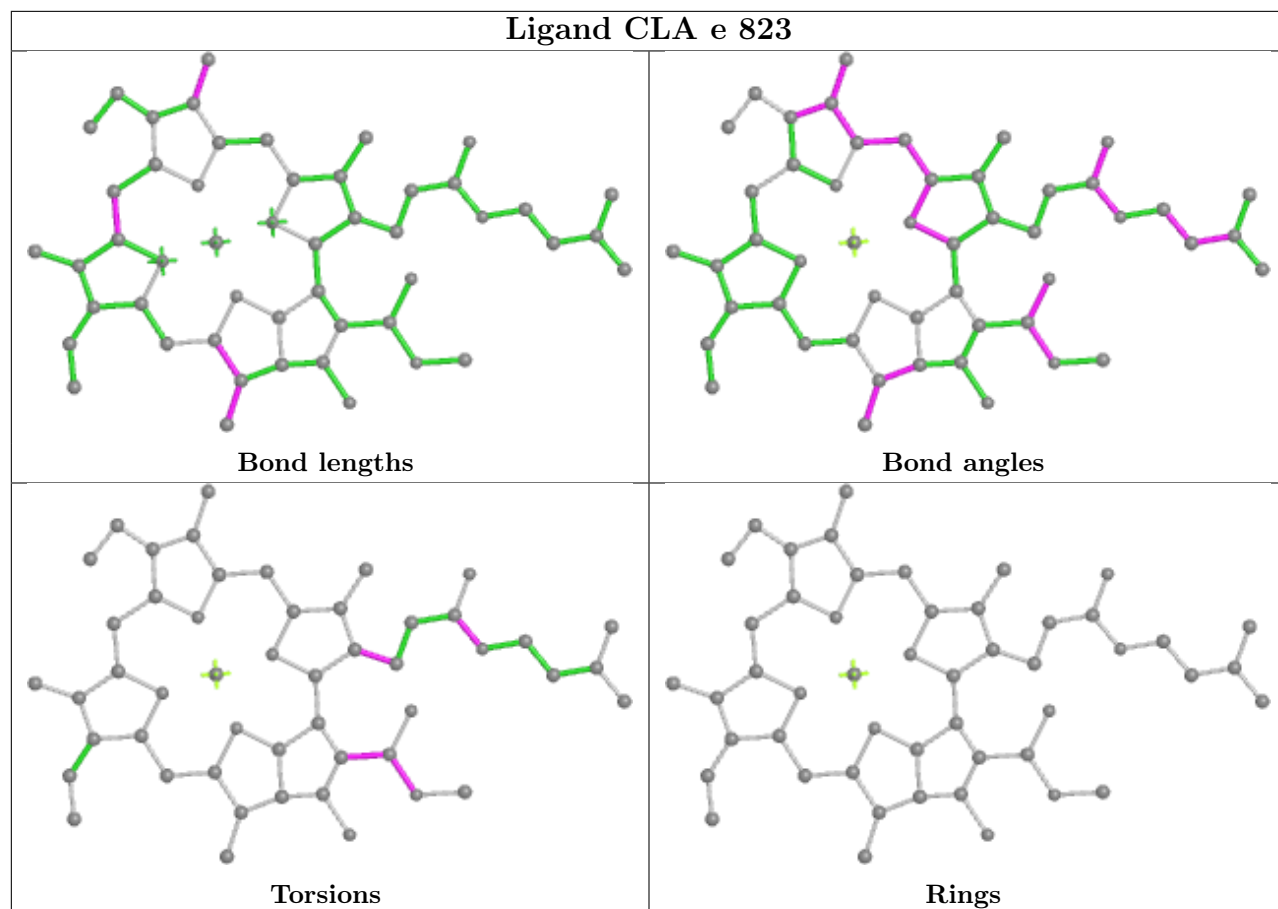
Ligand CLA e 821



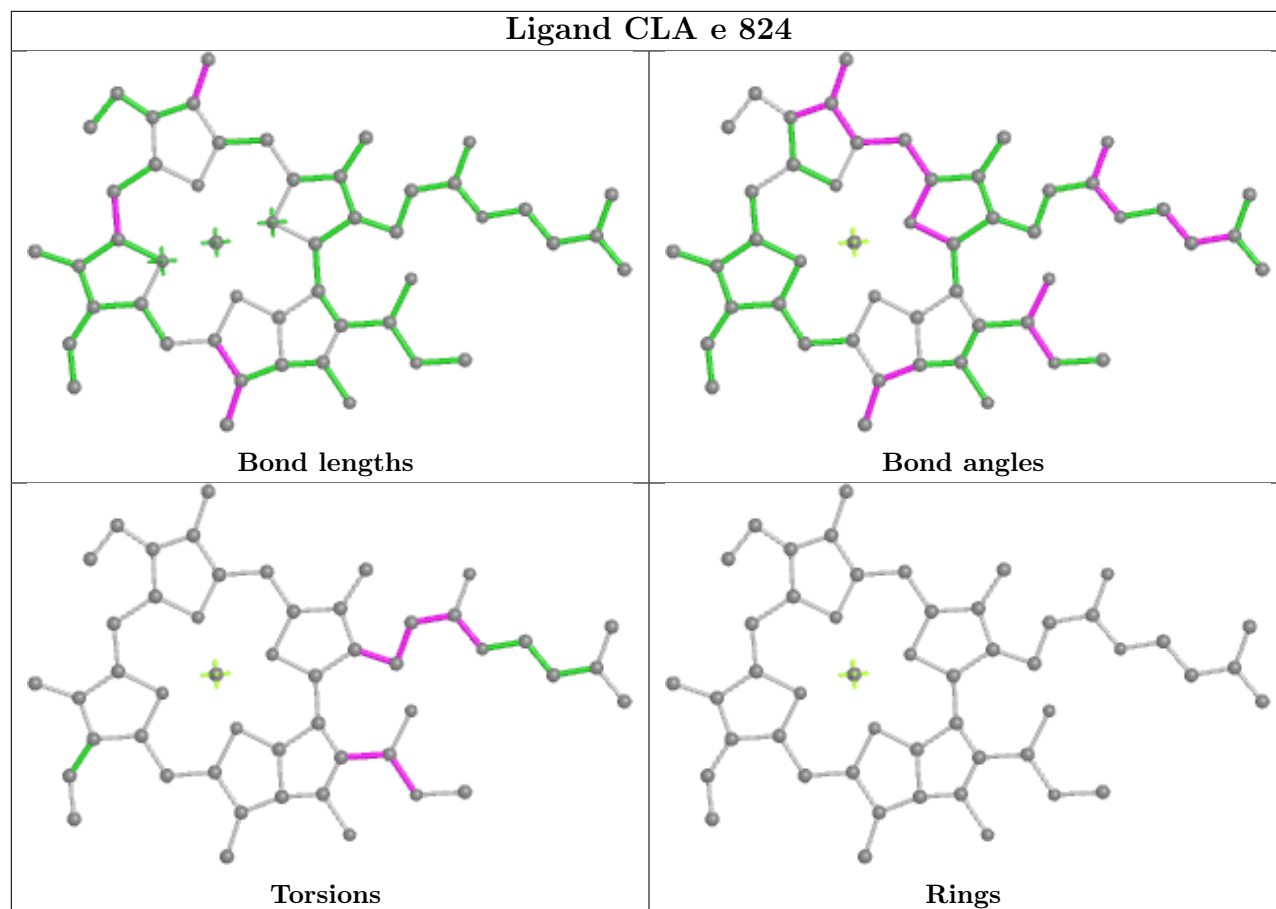
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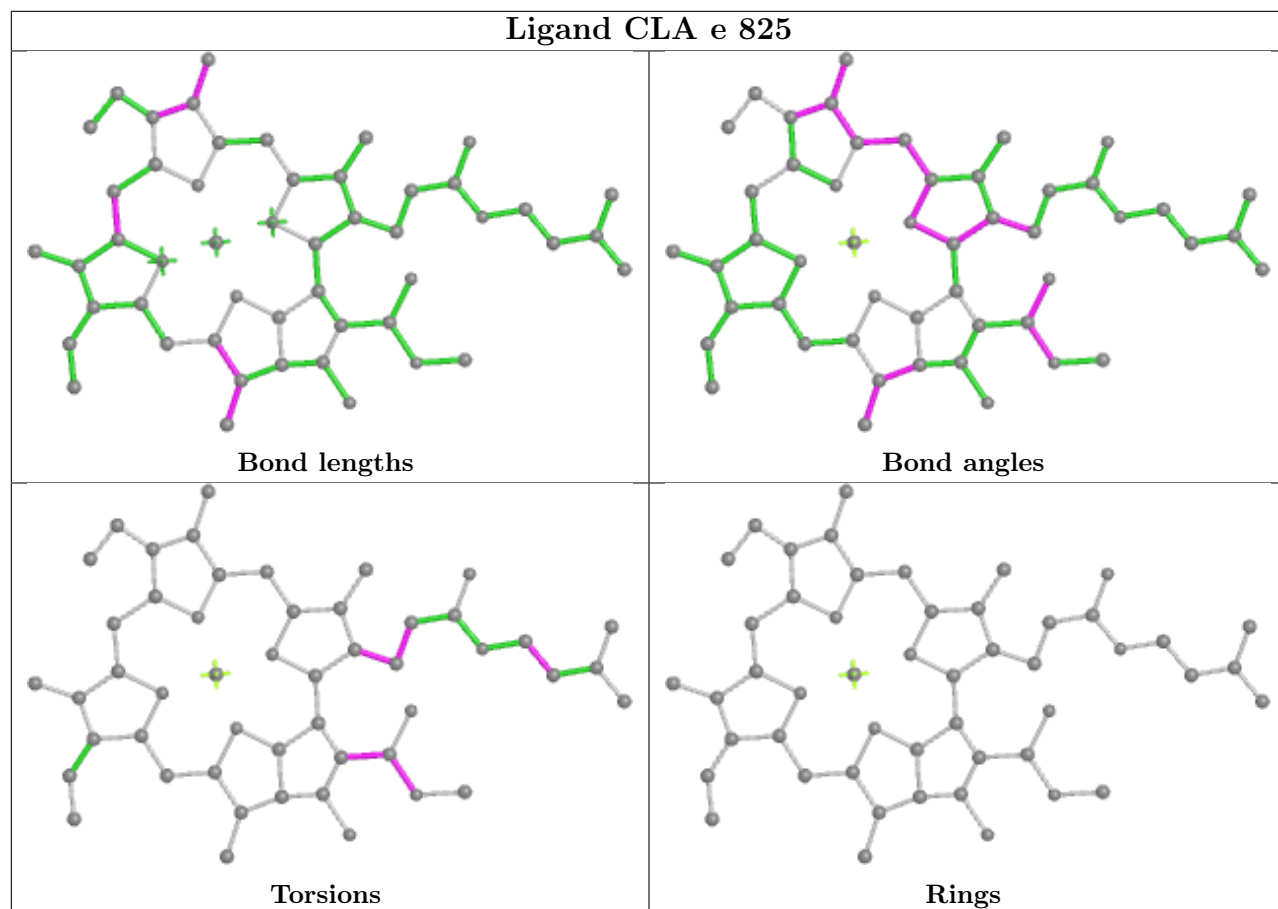
Ligand CLA e 823



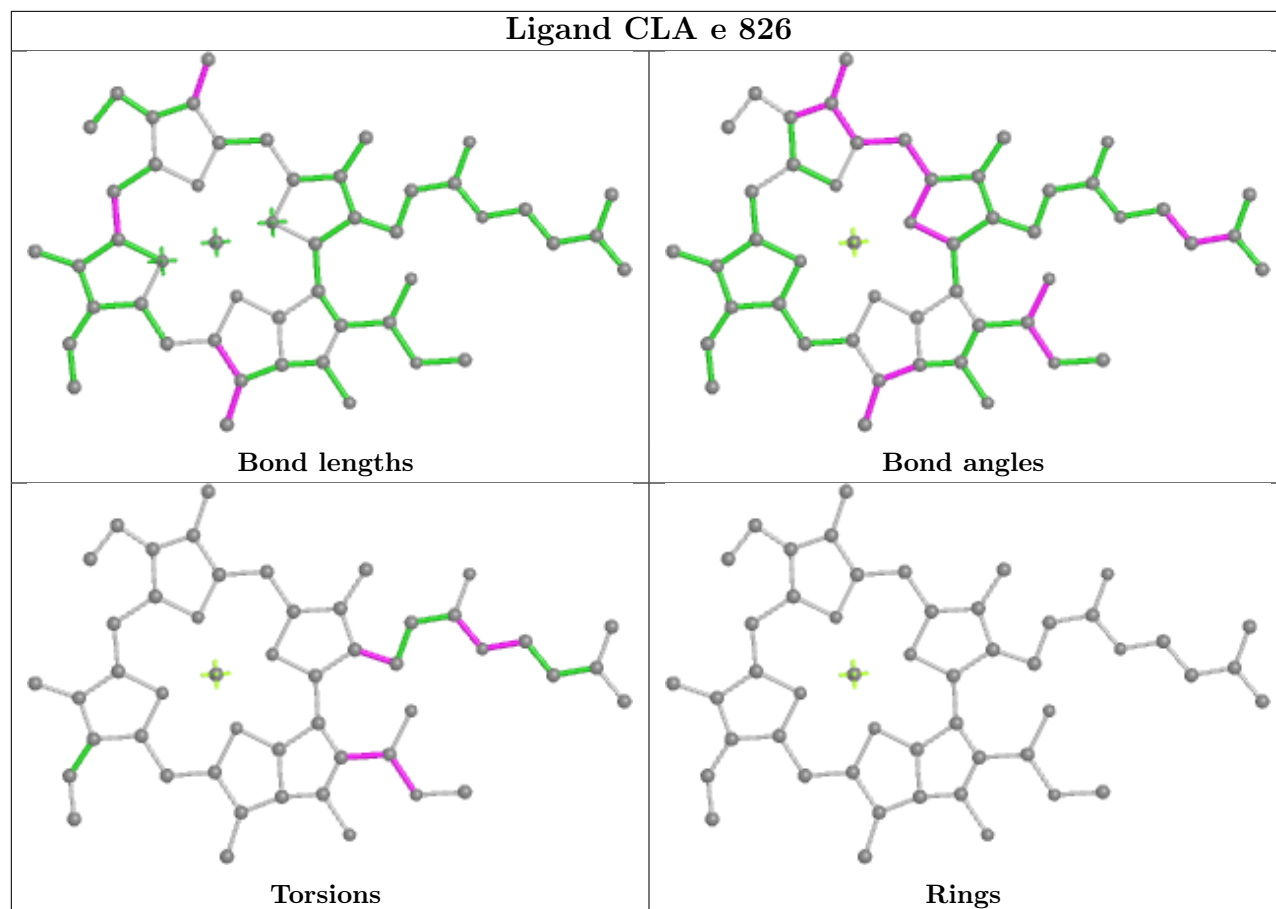
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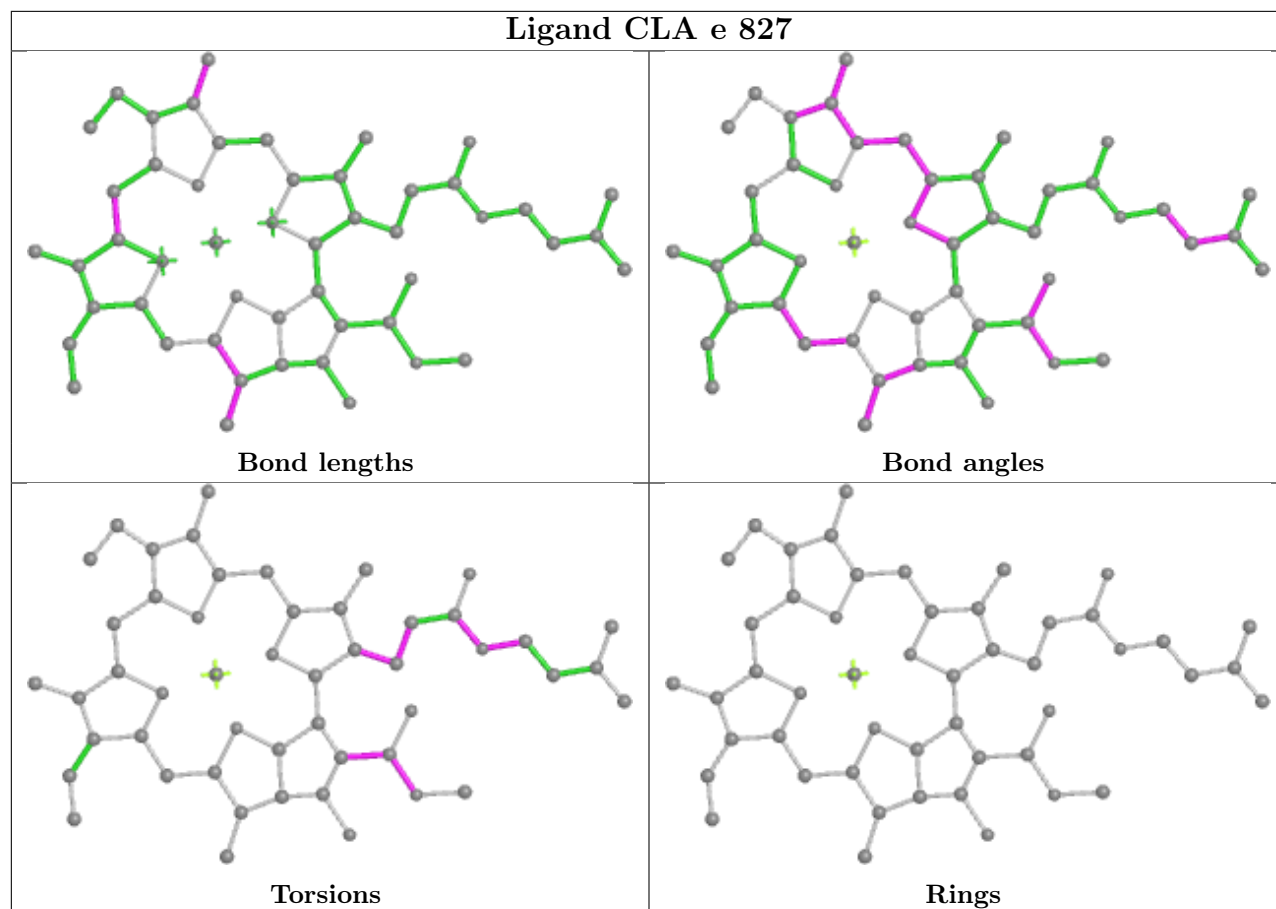
Ligand CLA e 825



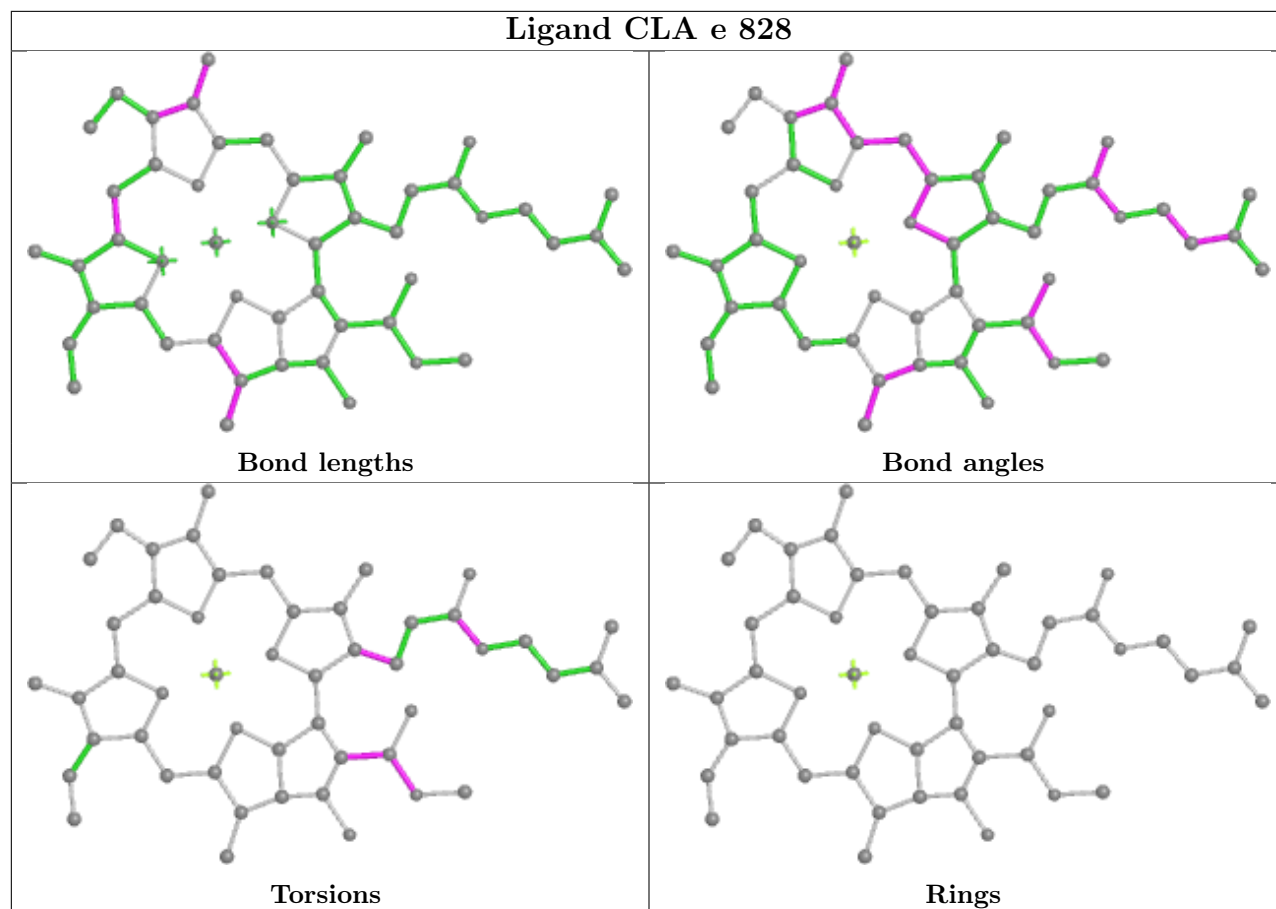
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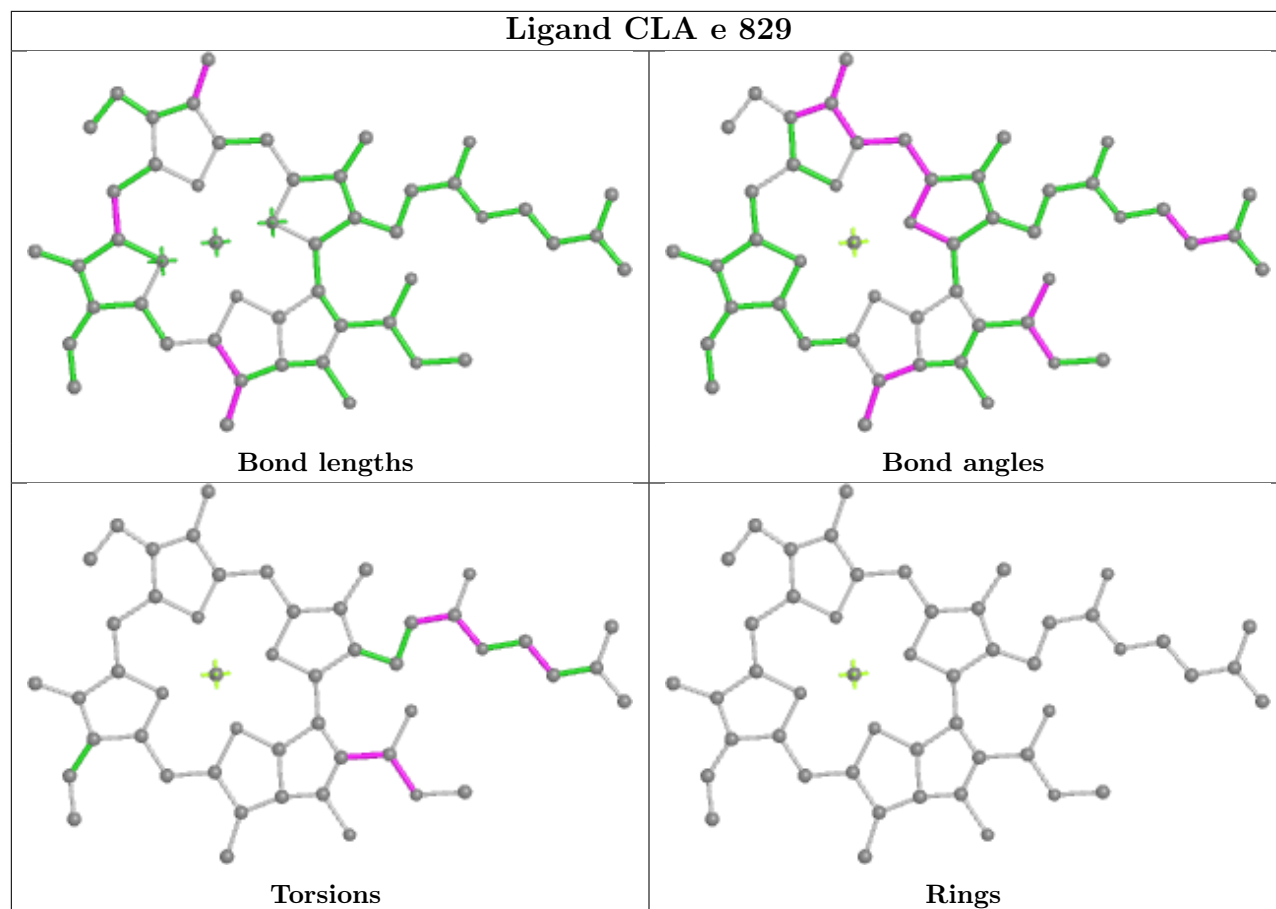
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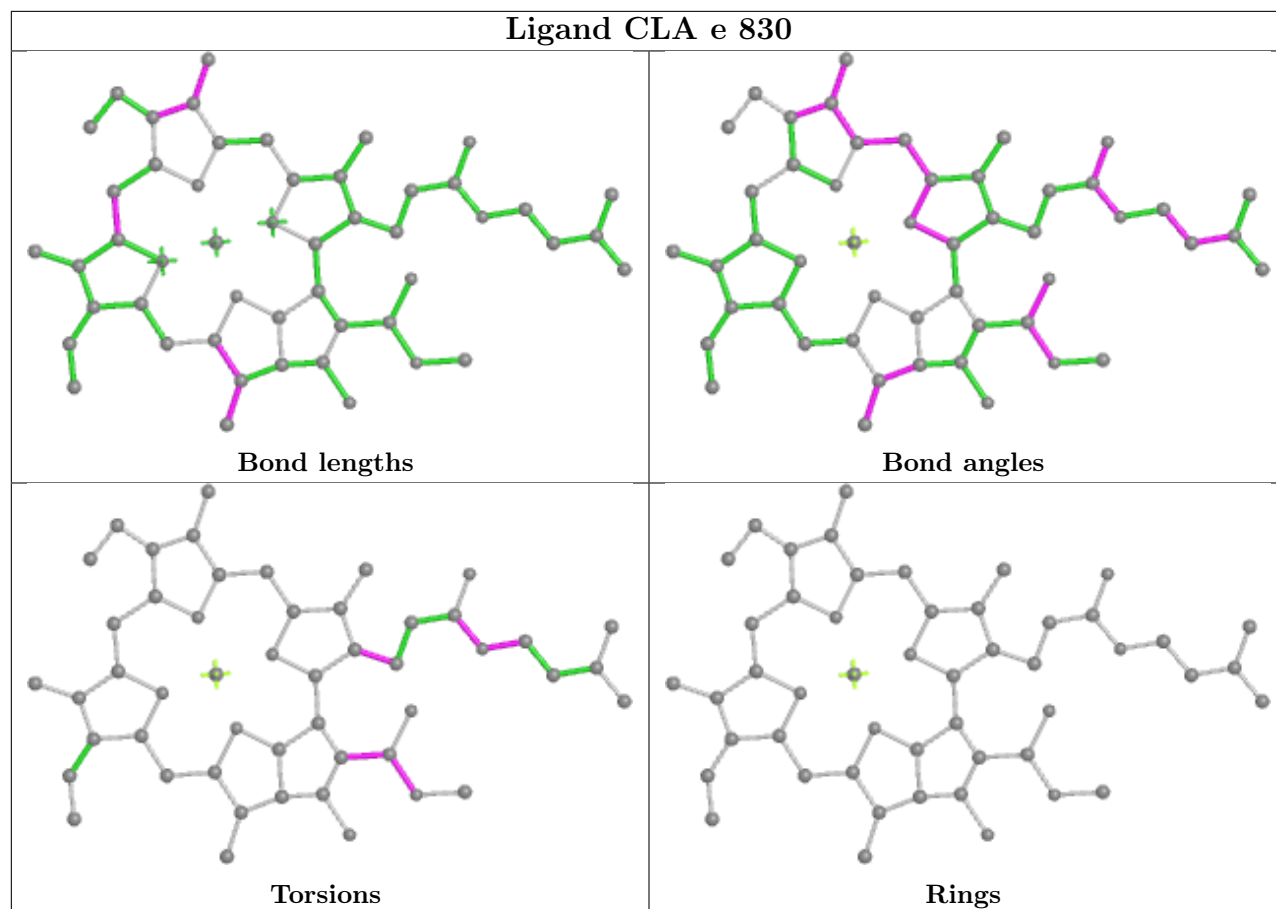
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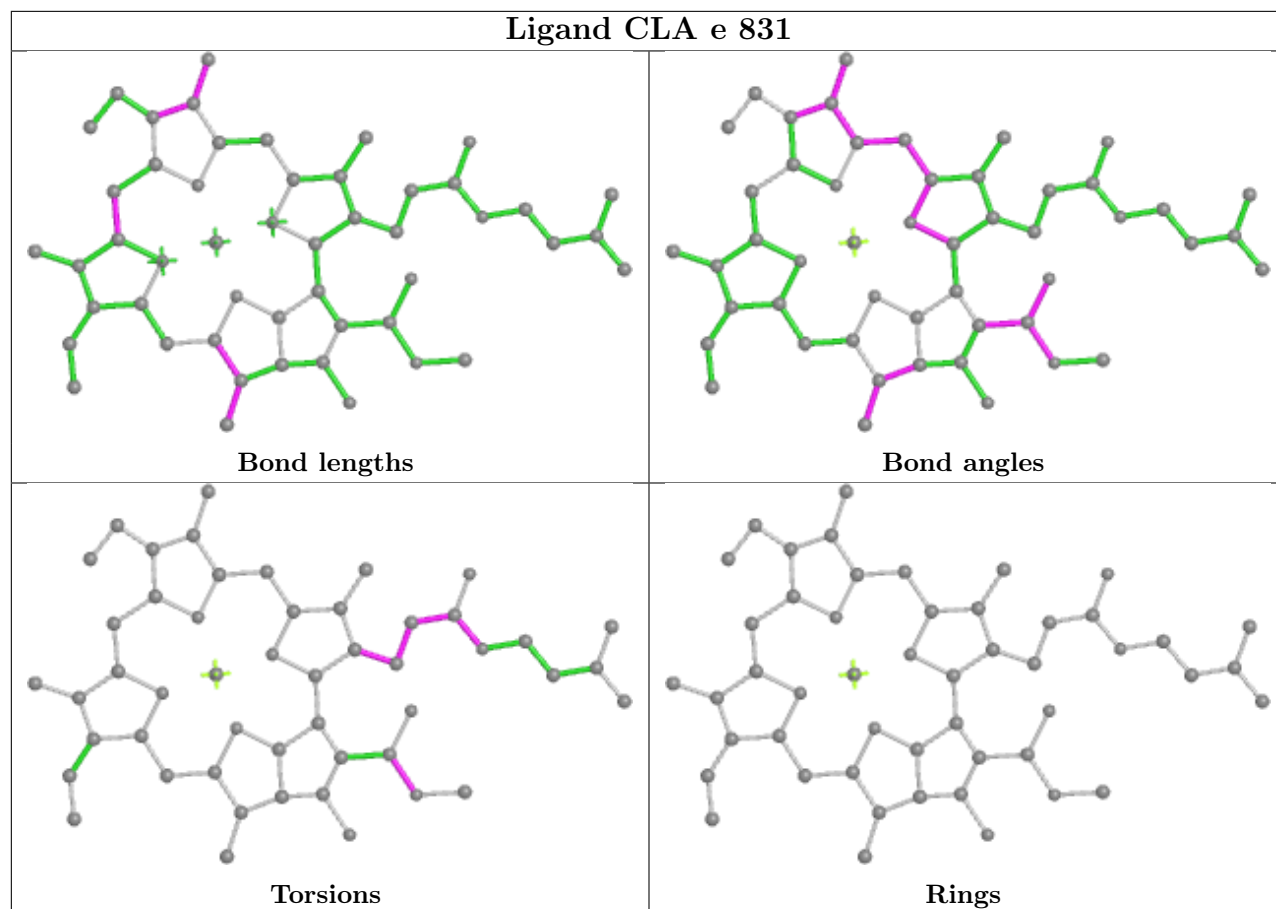
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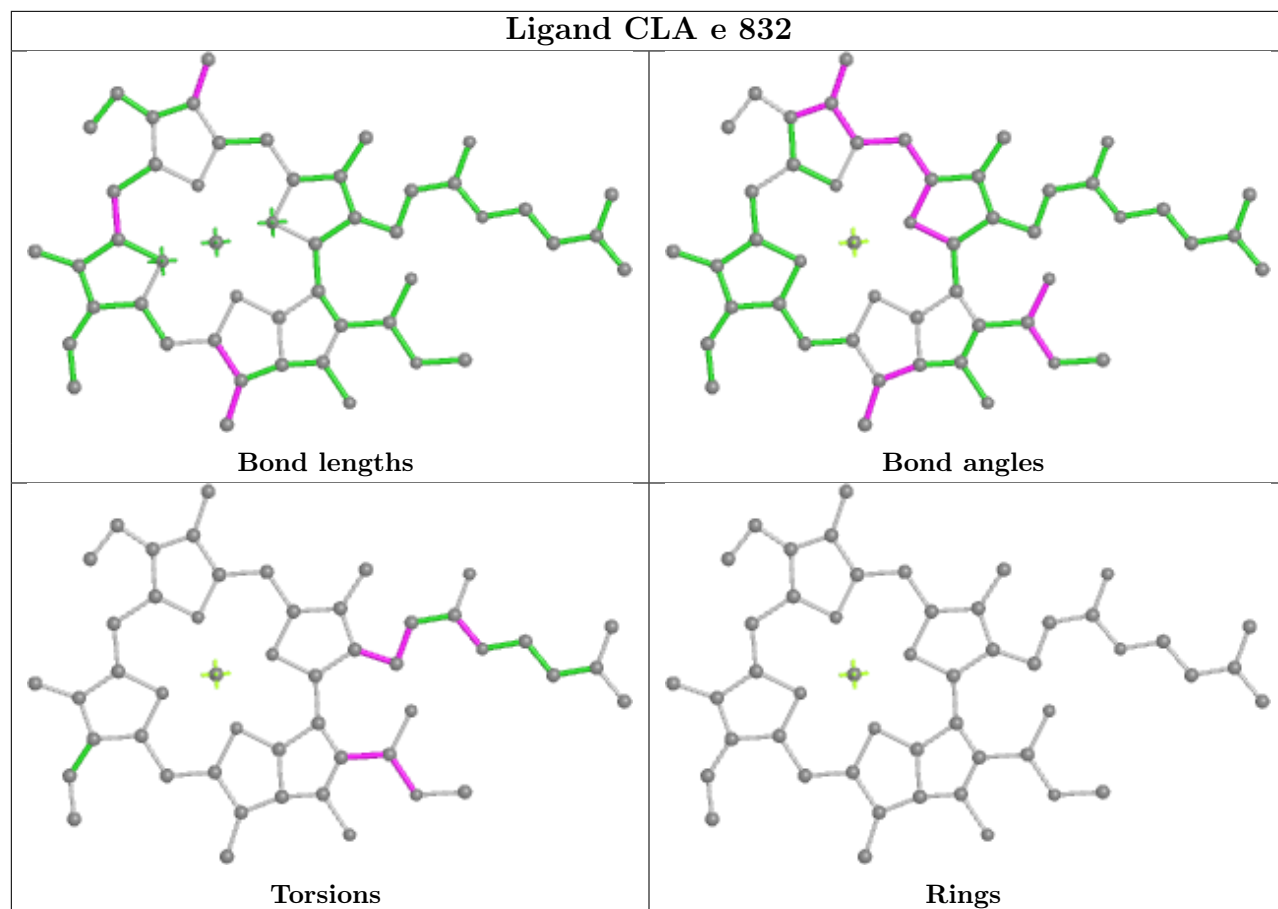
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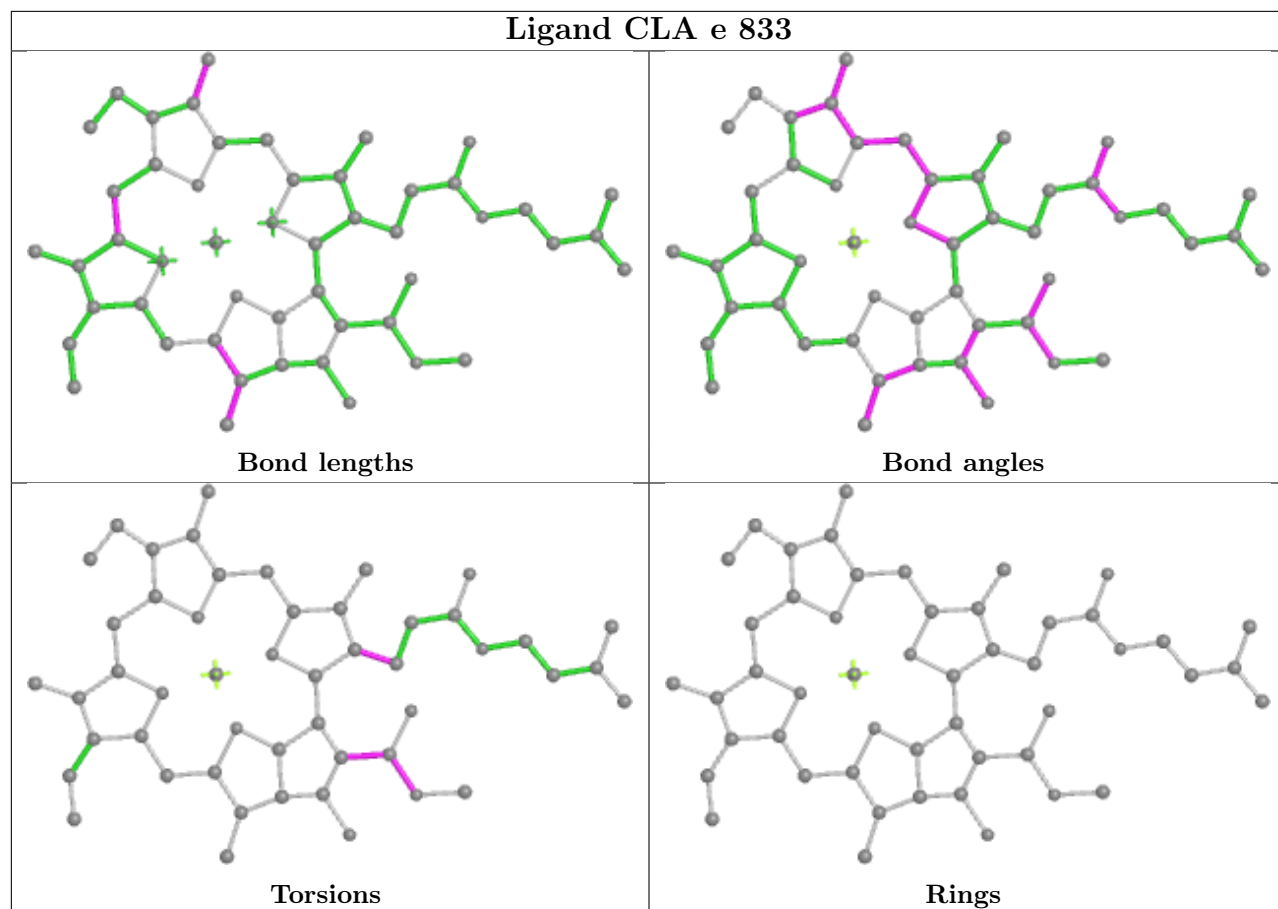
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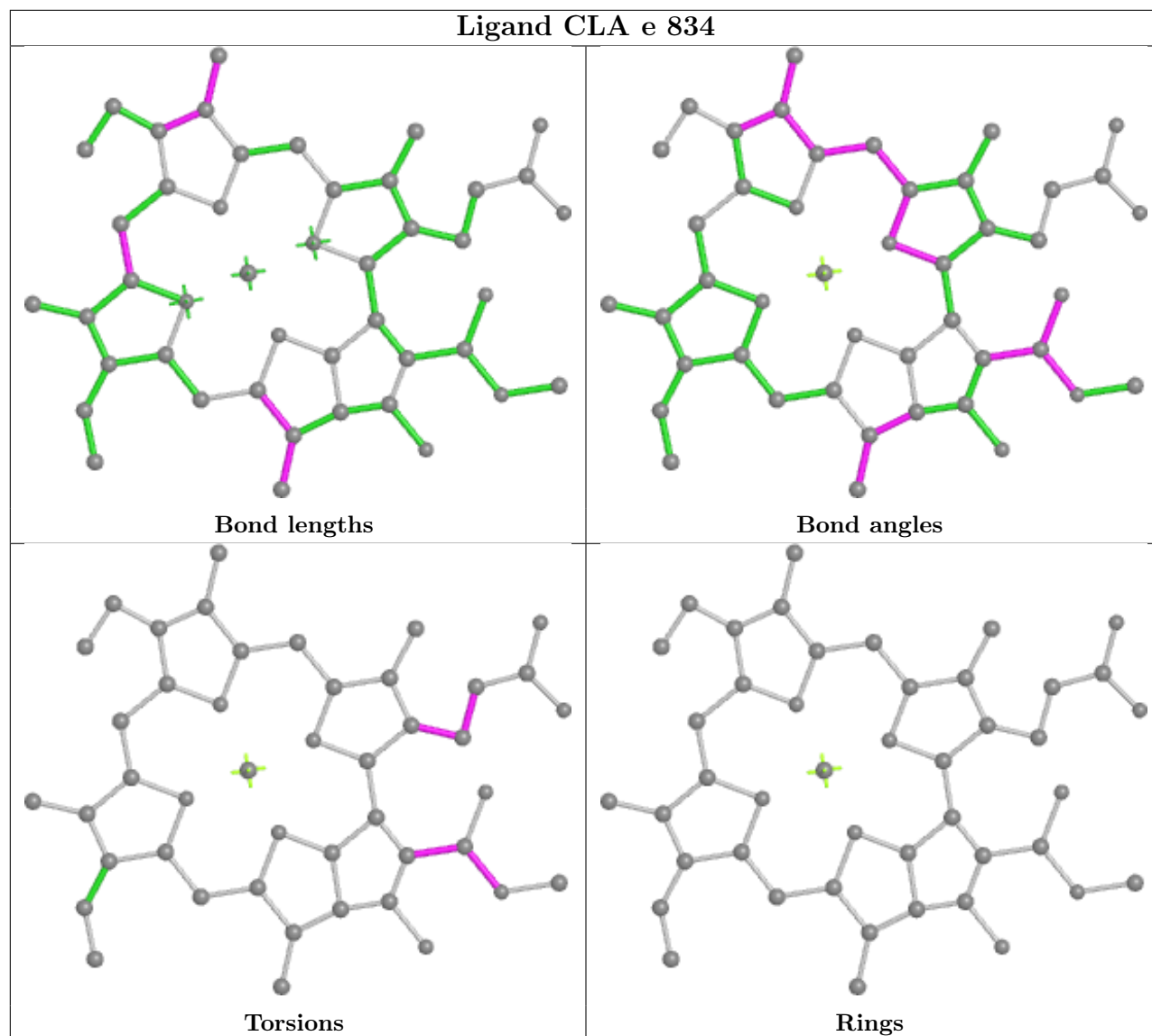
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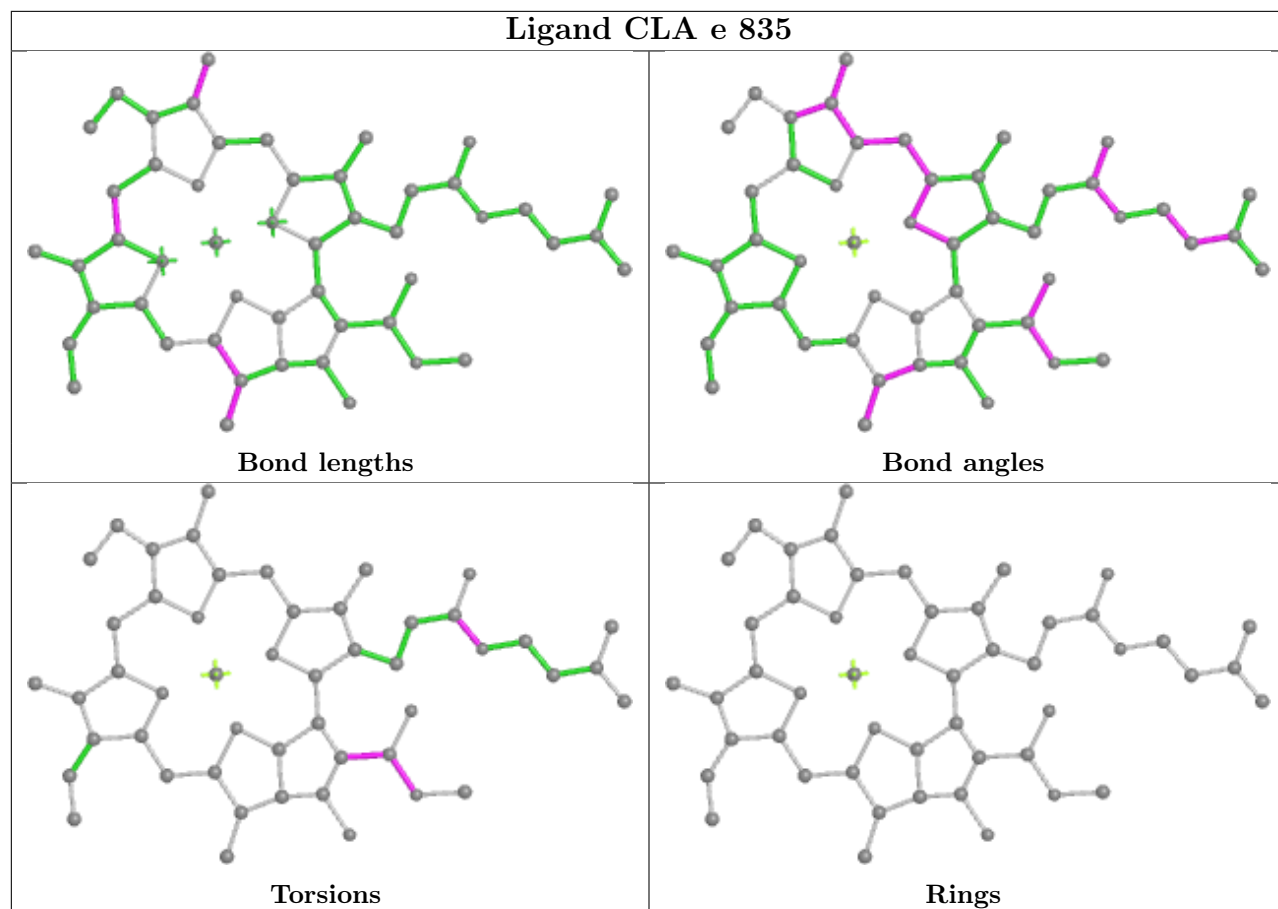
Ligand CLA e 833



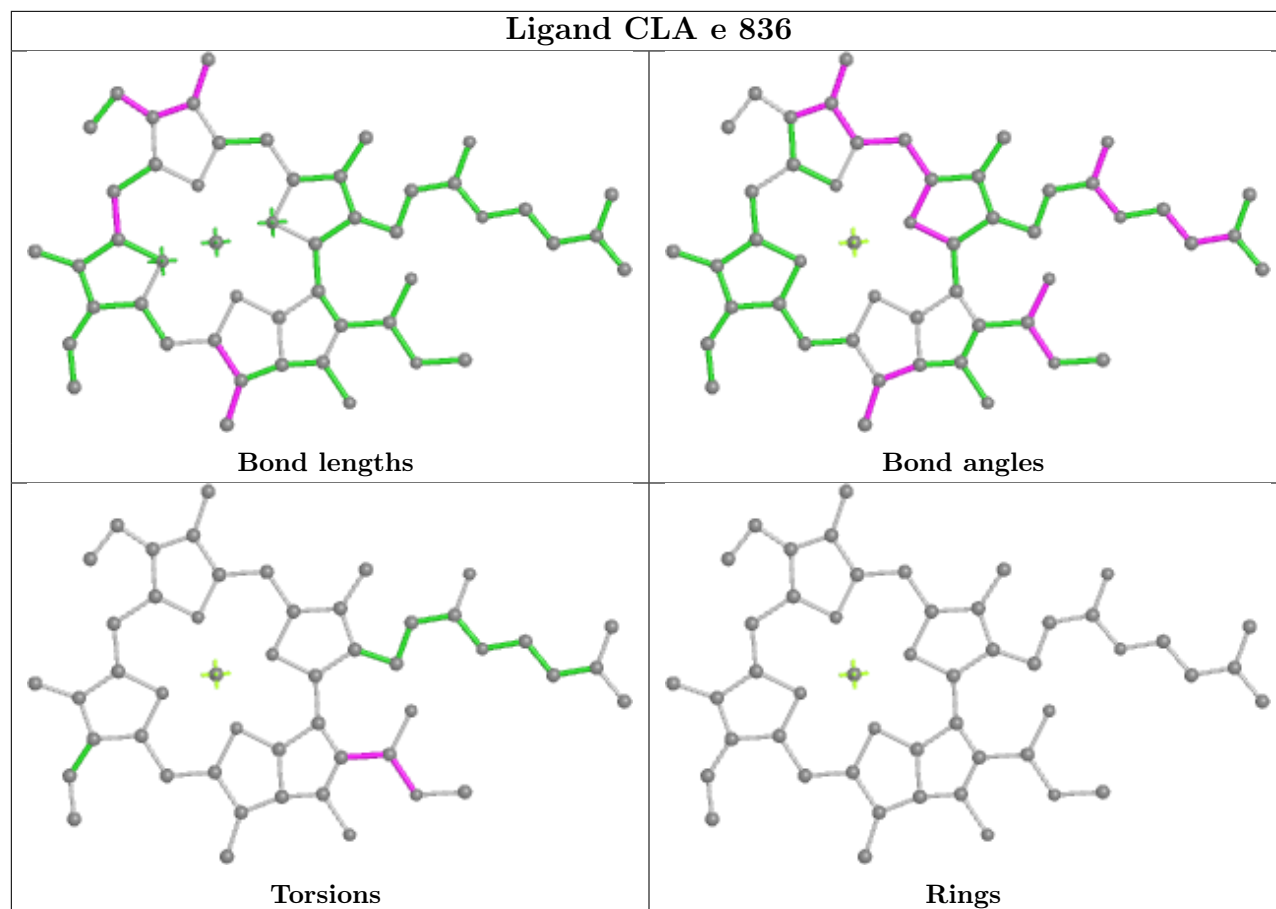
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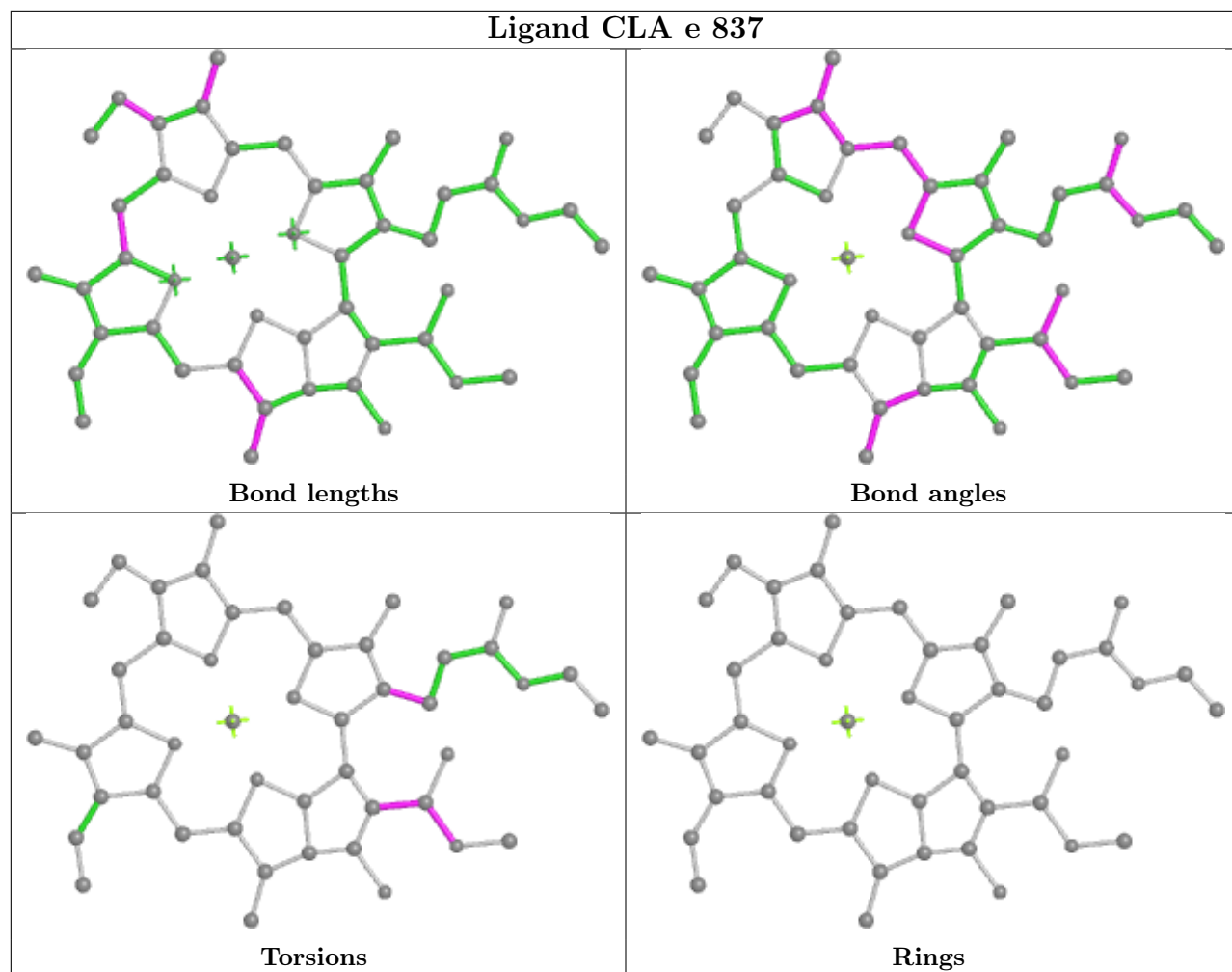
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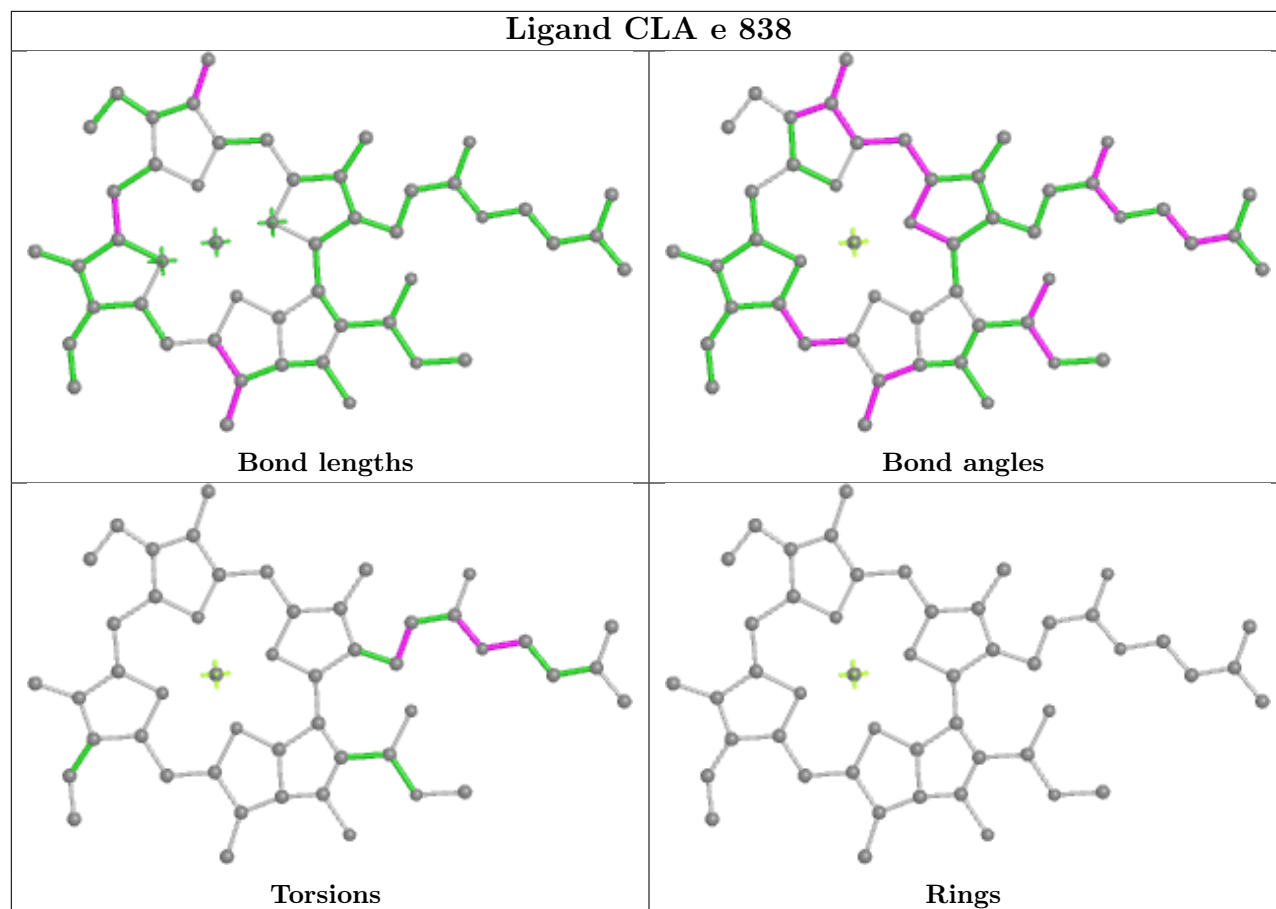
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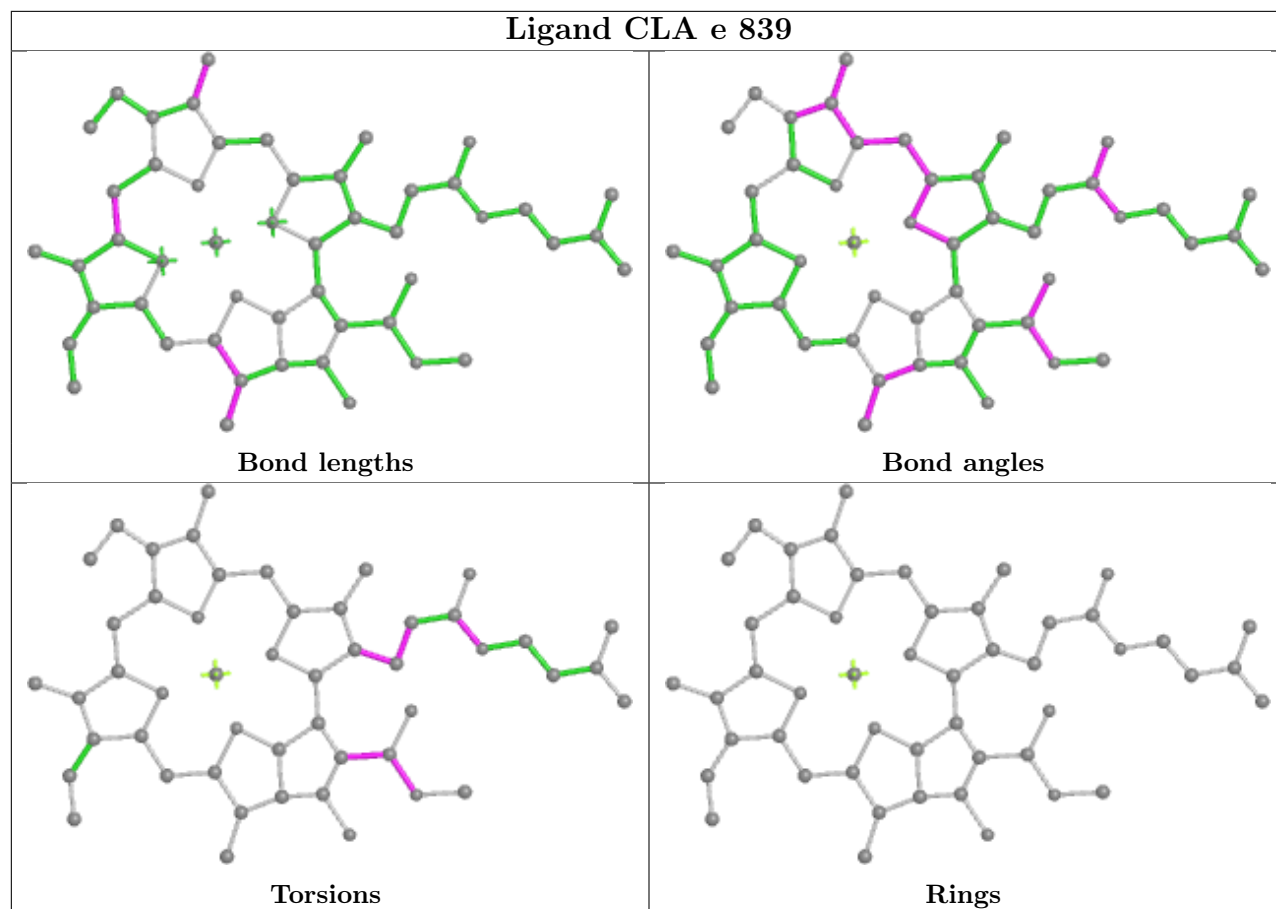
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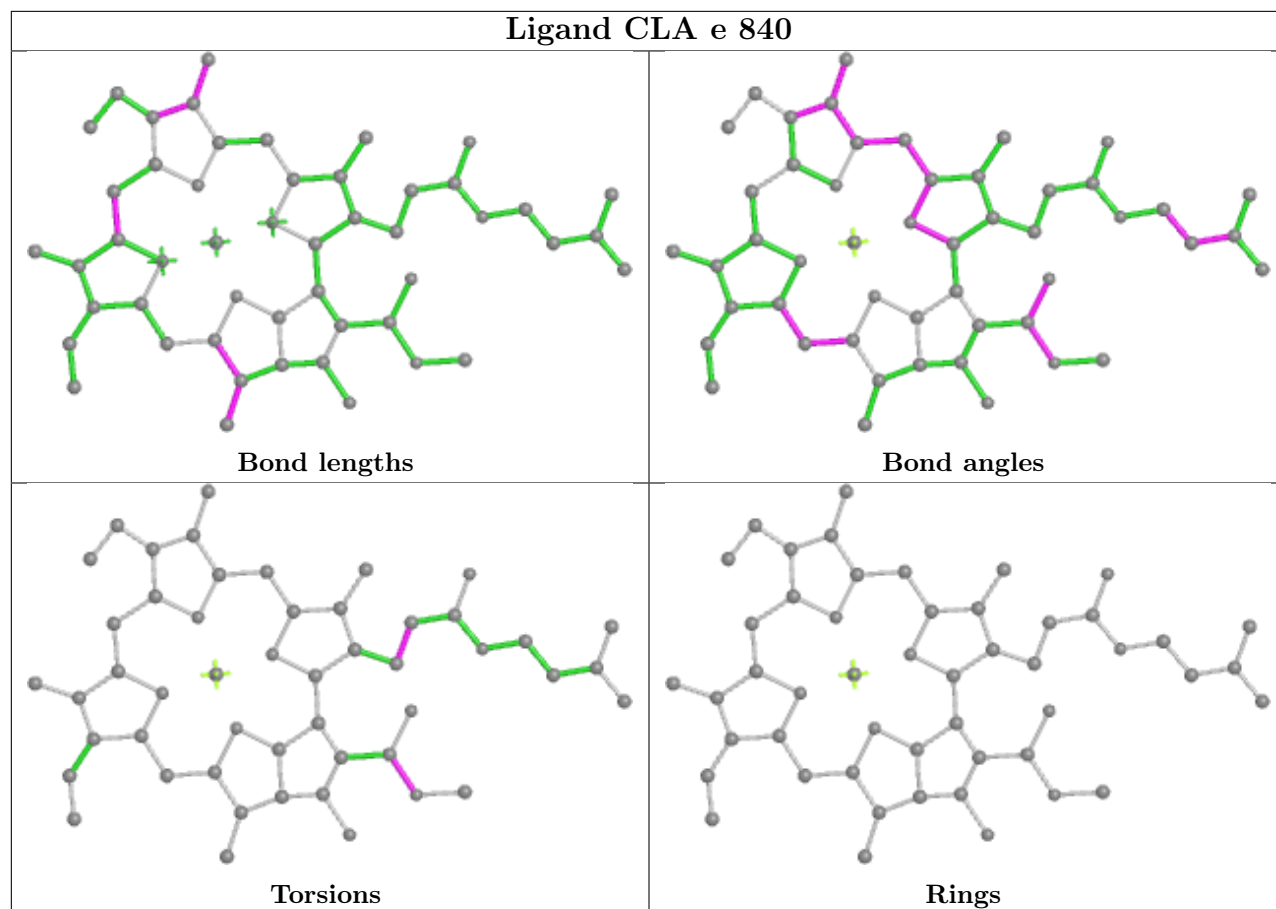
Ligand CLA e 838

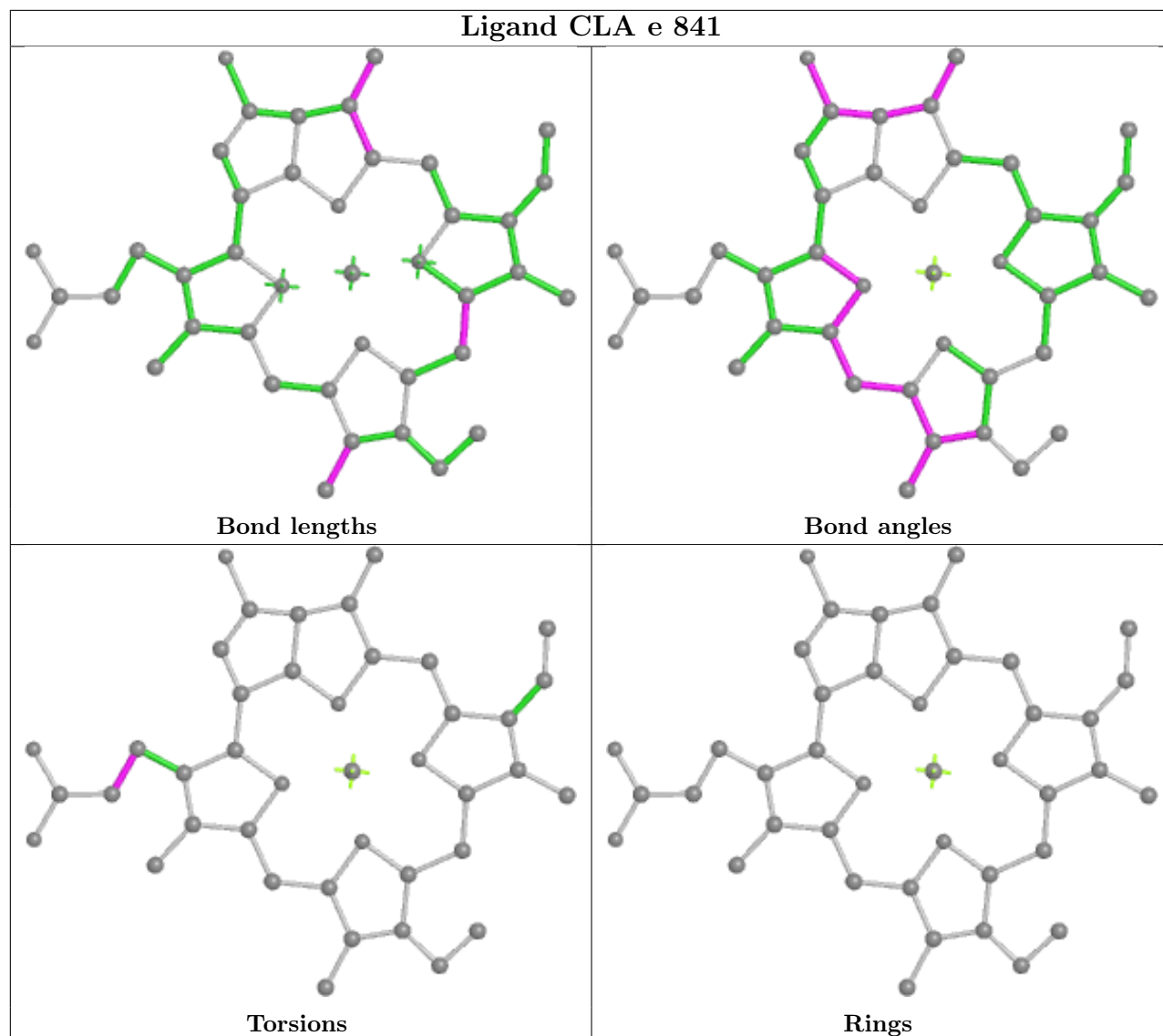


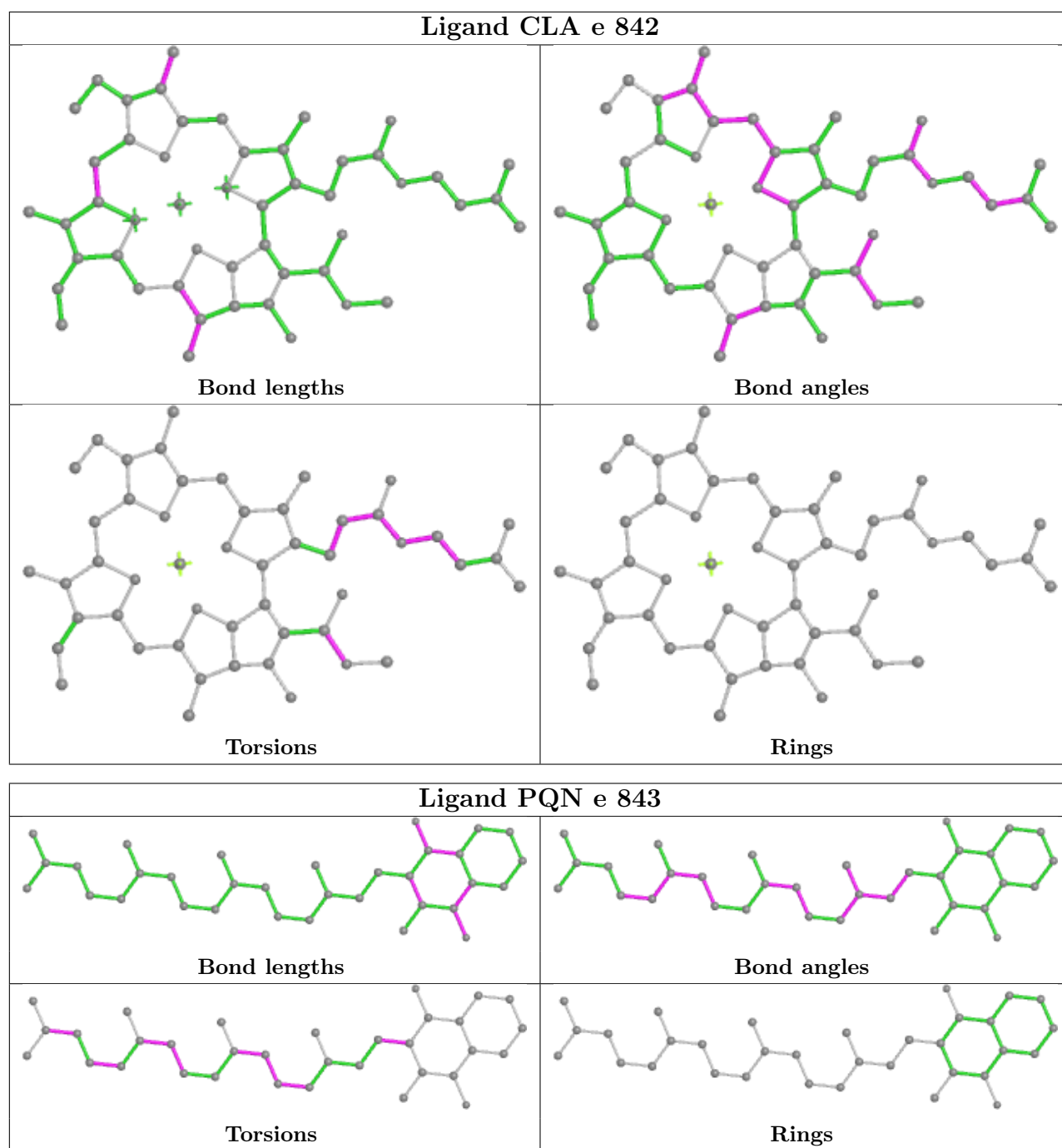
Ligand CLA e 839

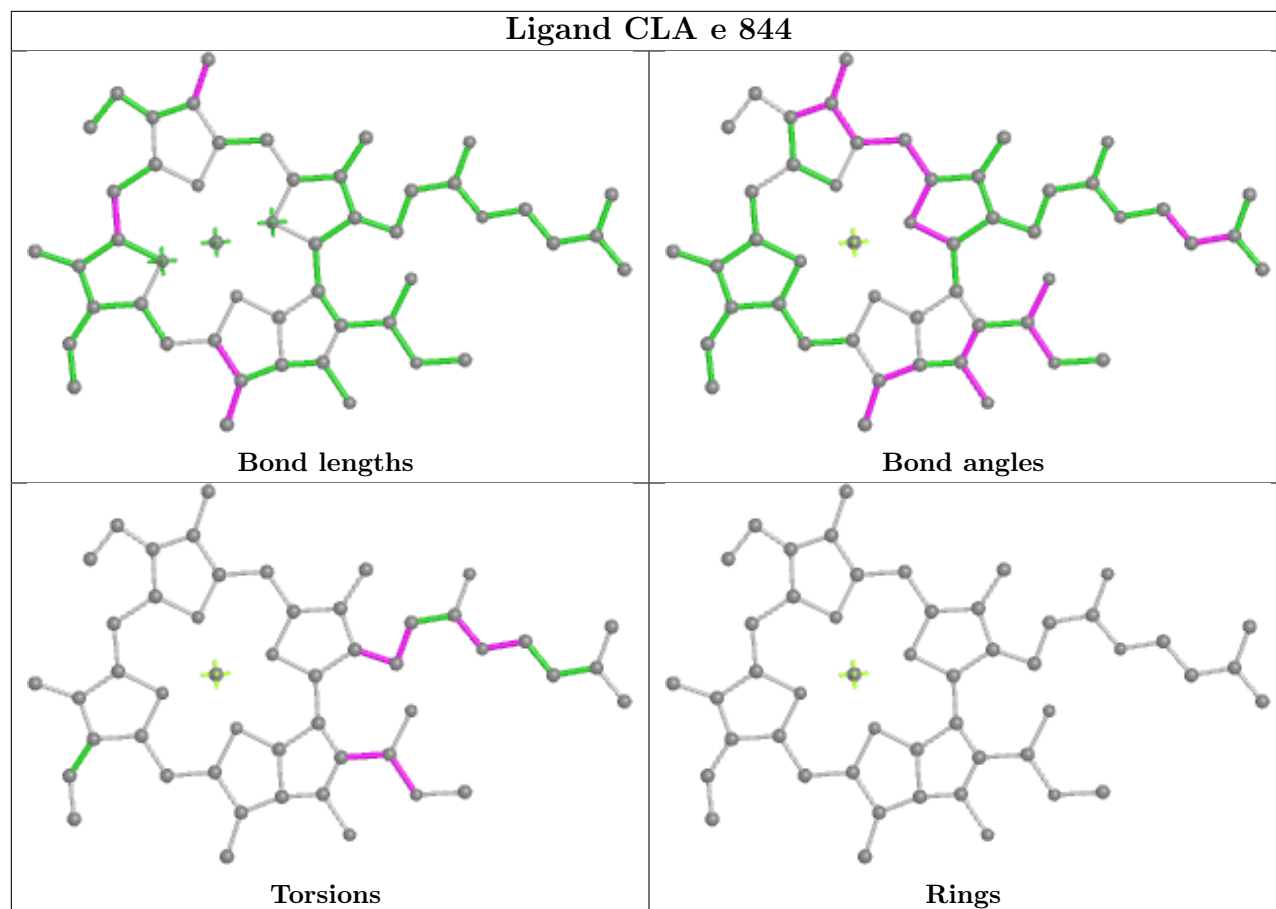


Ligand CLA e 840

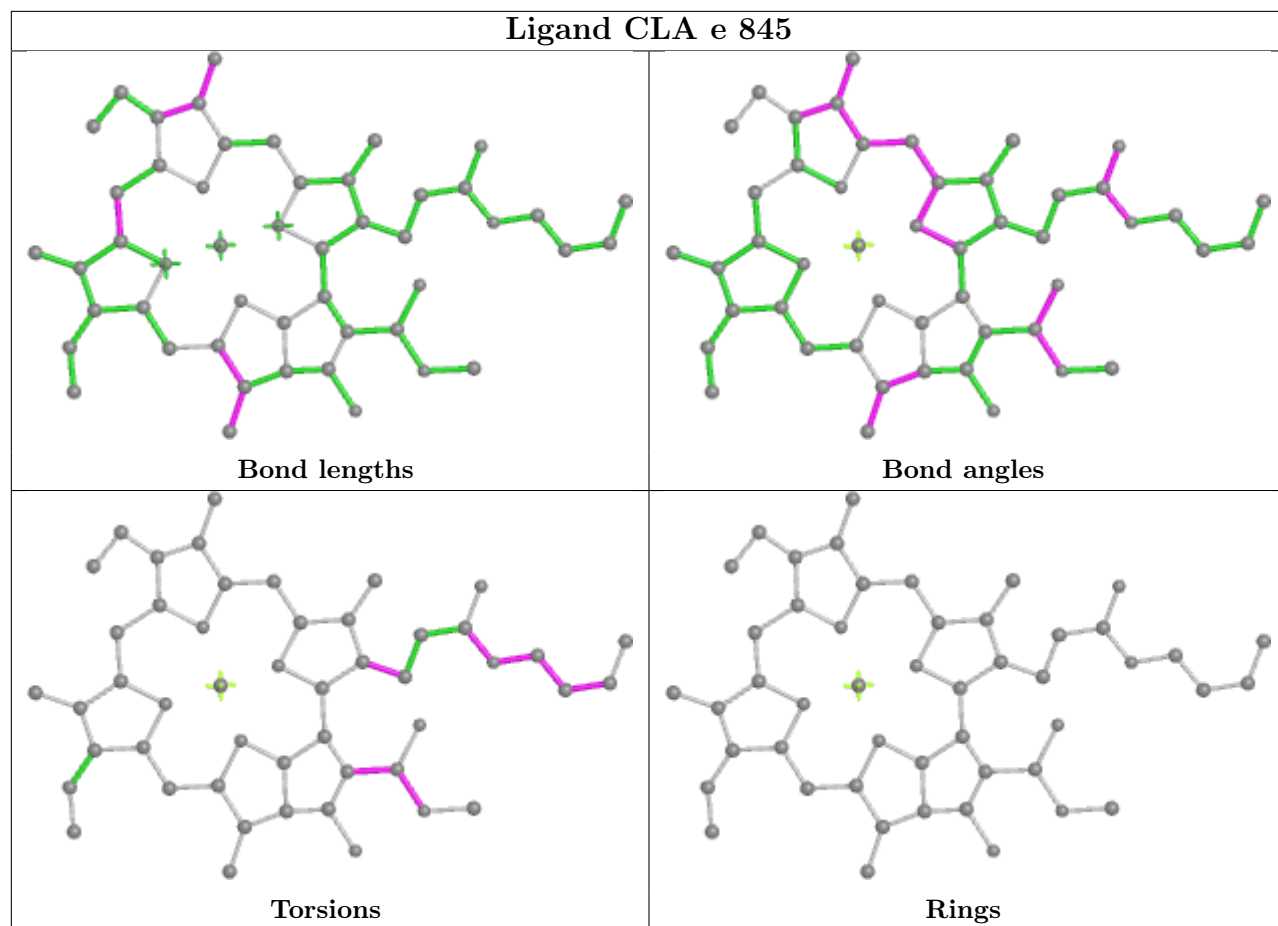




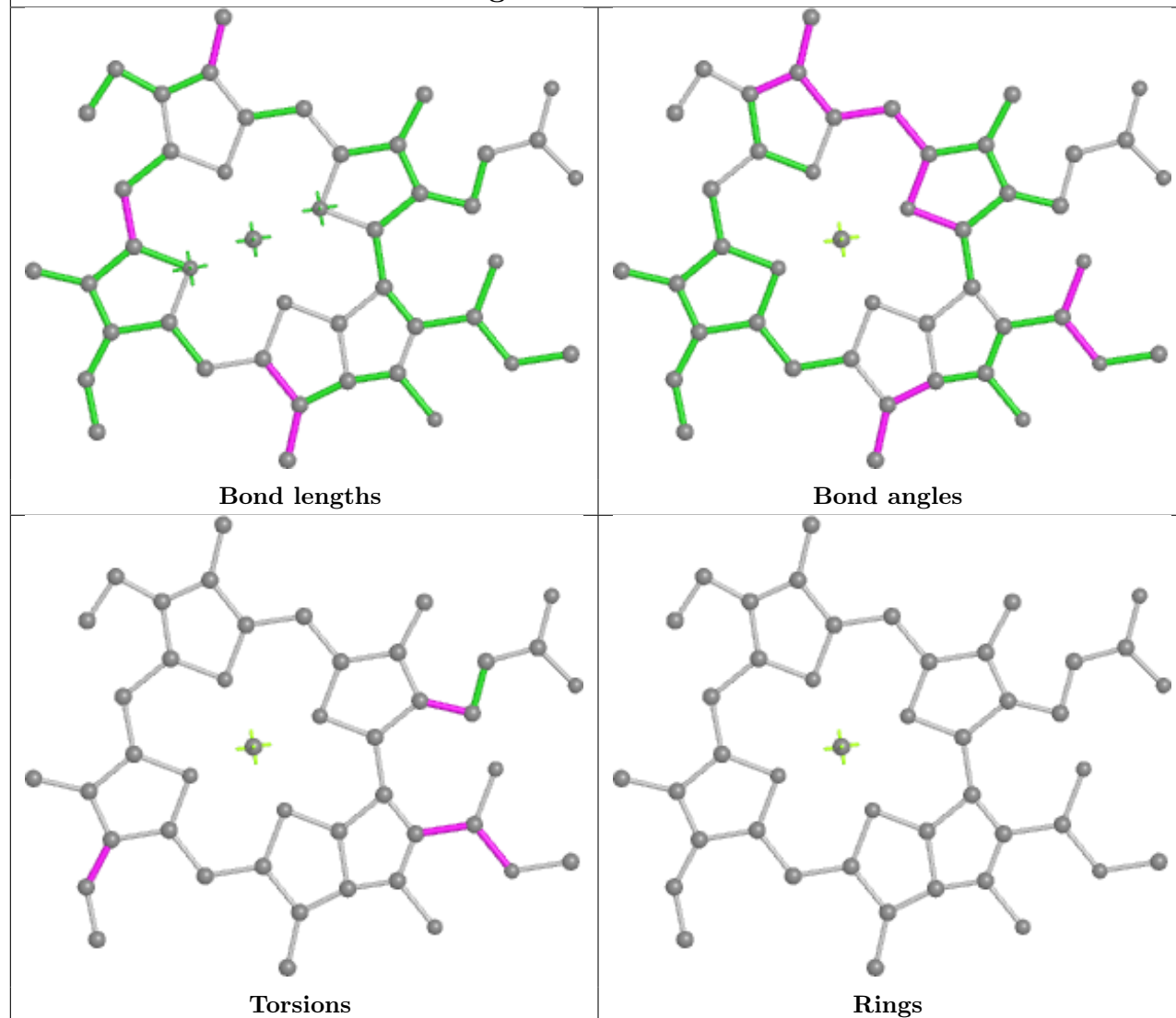


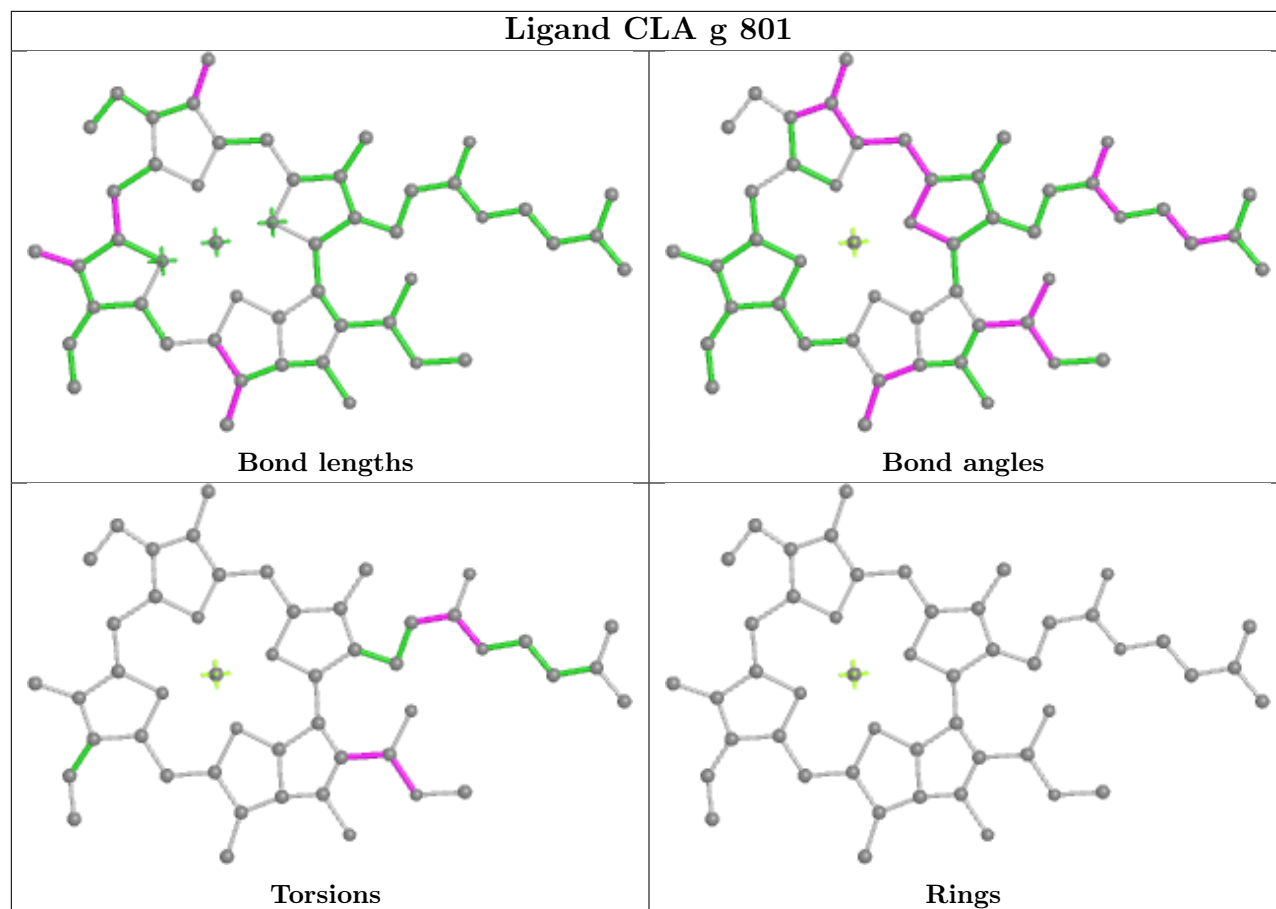


Ligand CLA e 845

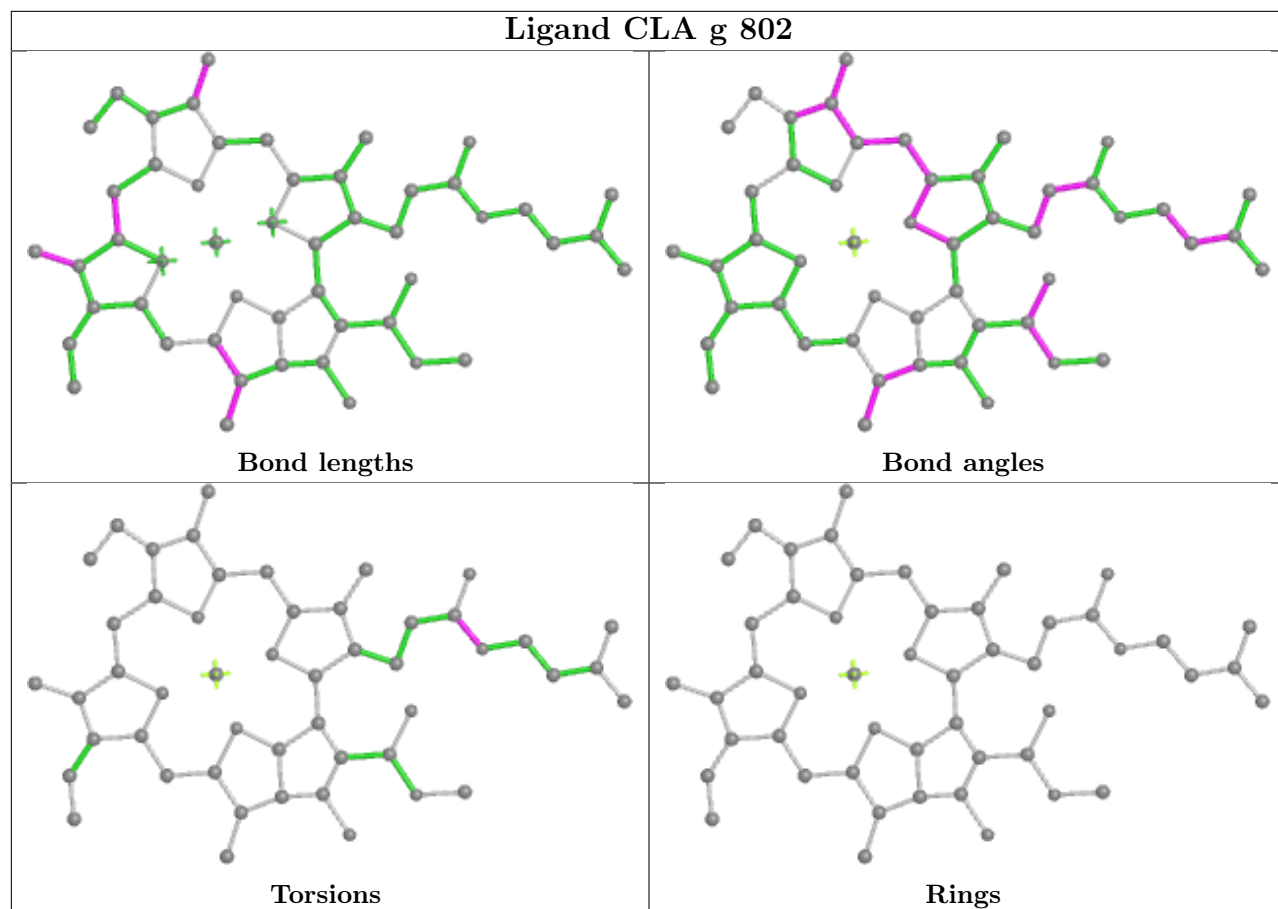


Ligand CLA f 1301

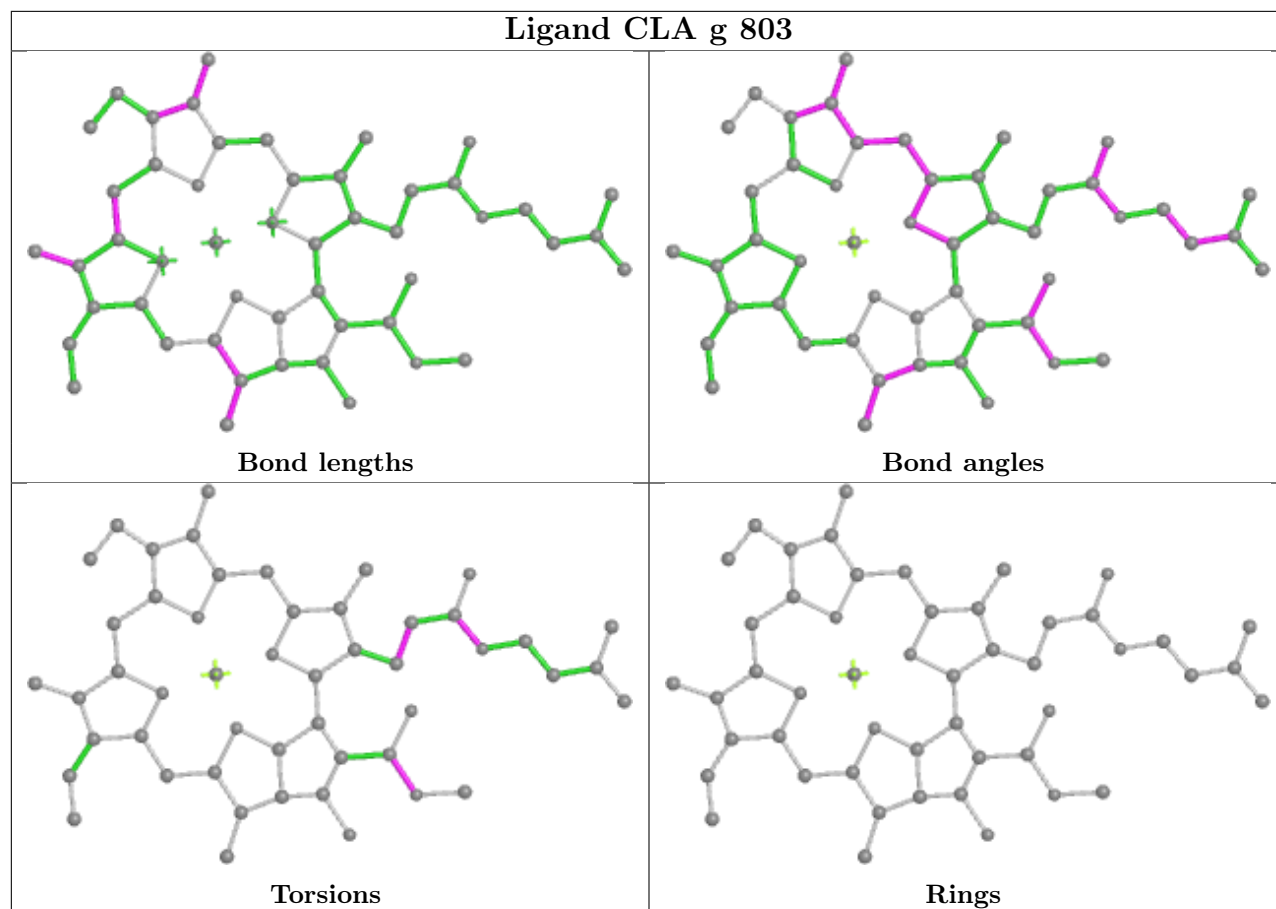




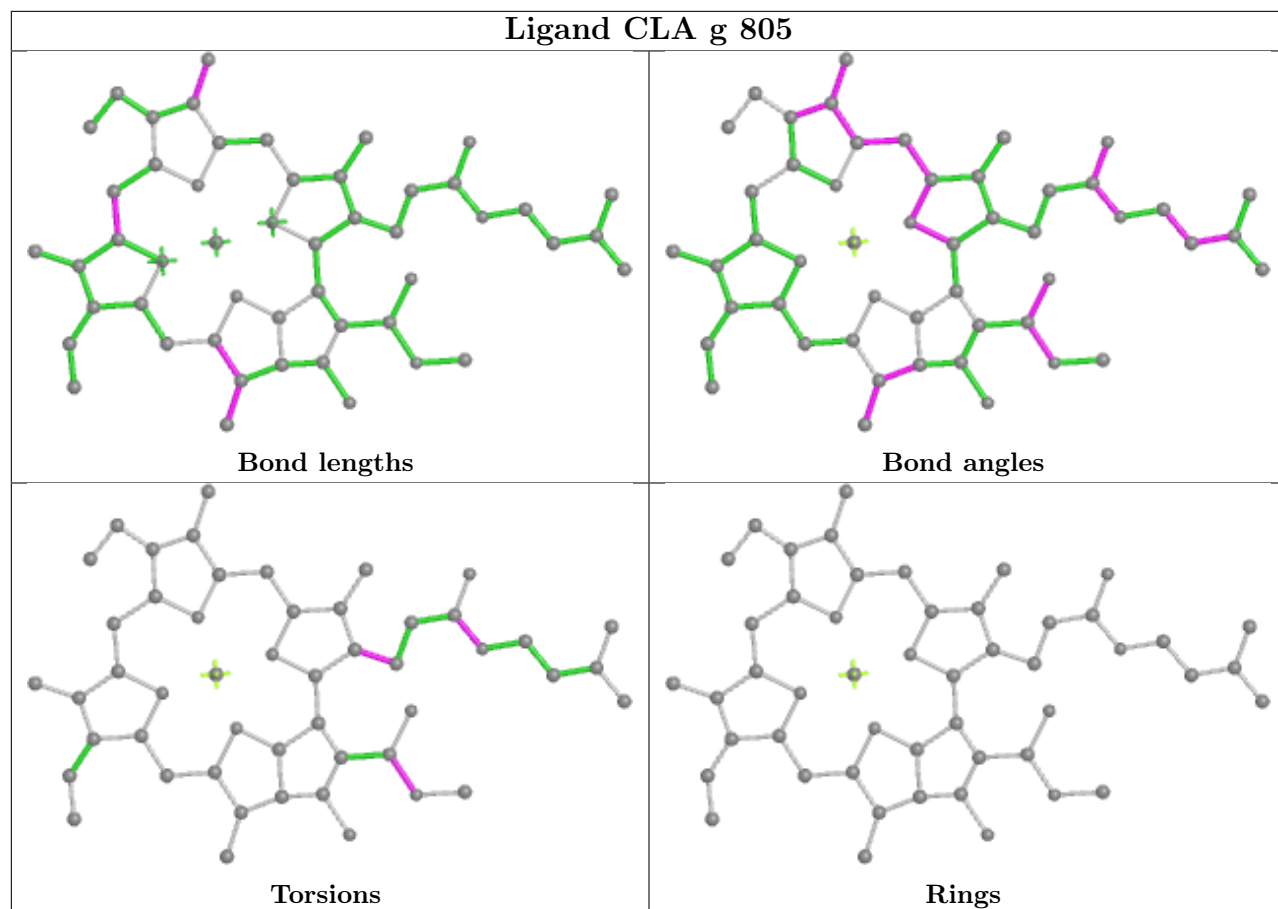
Ligand CLA g 802



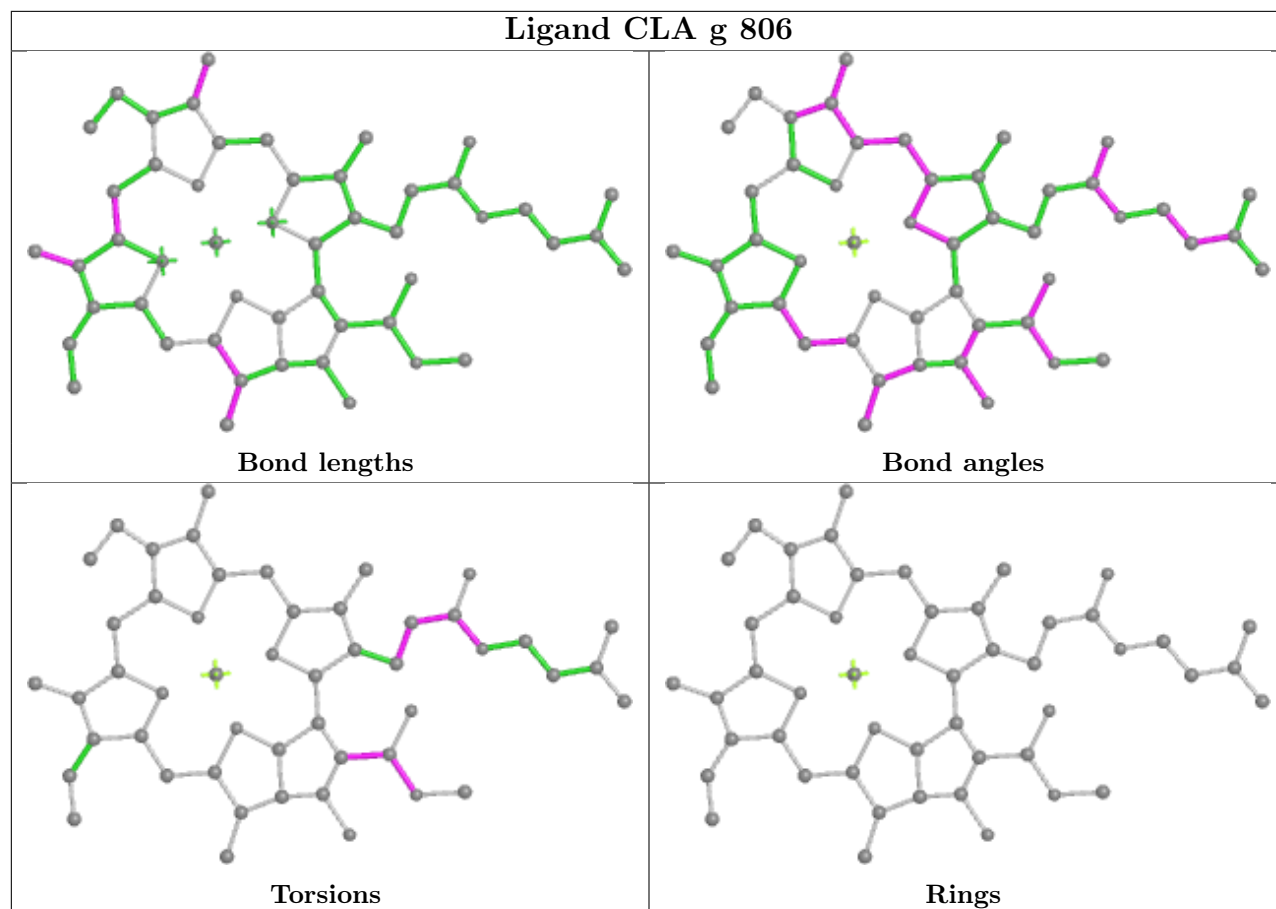
Ligand CLA g 803



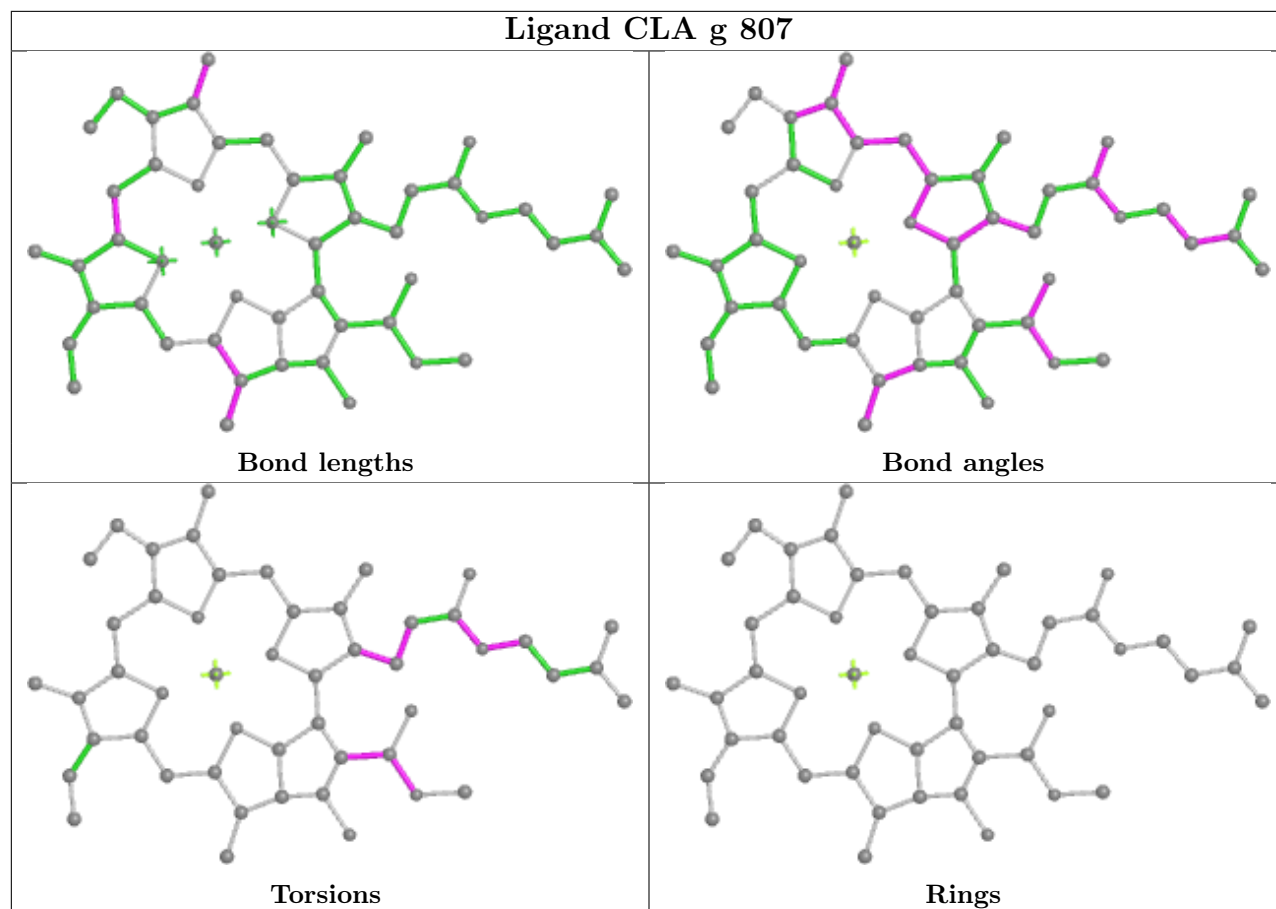
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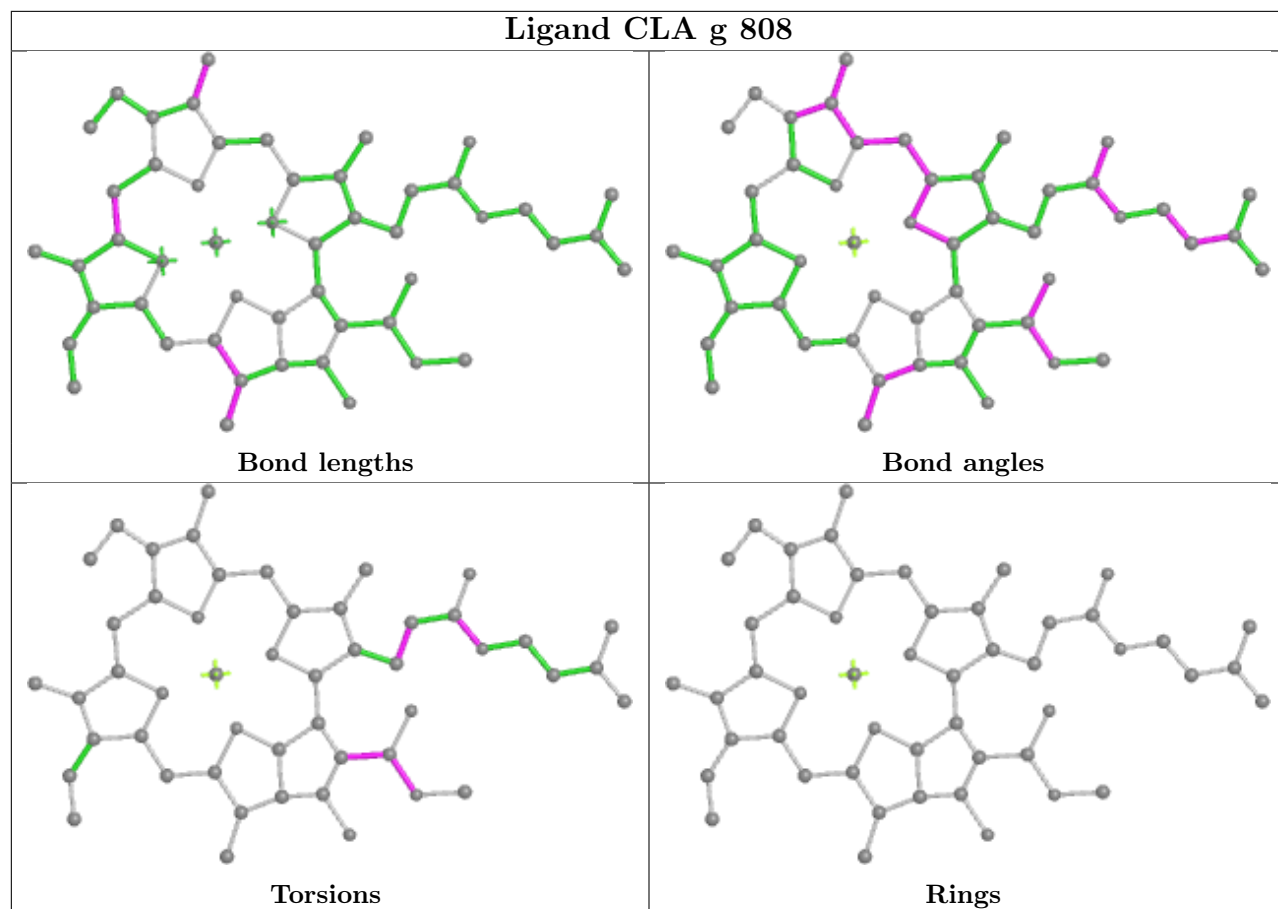
Ligand CLA g 806



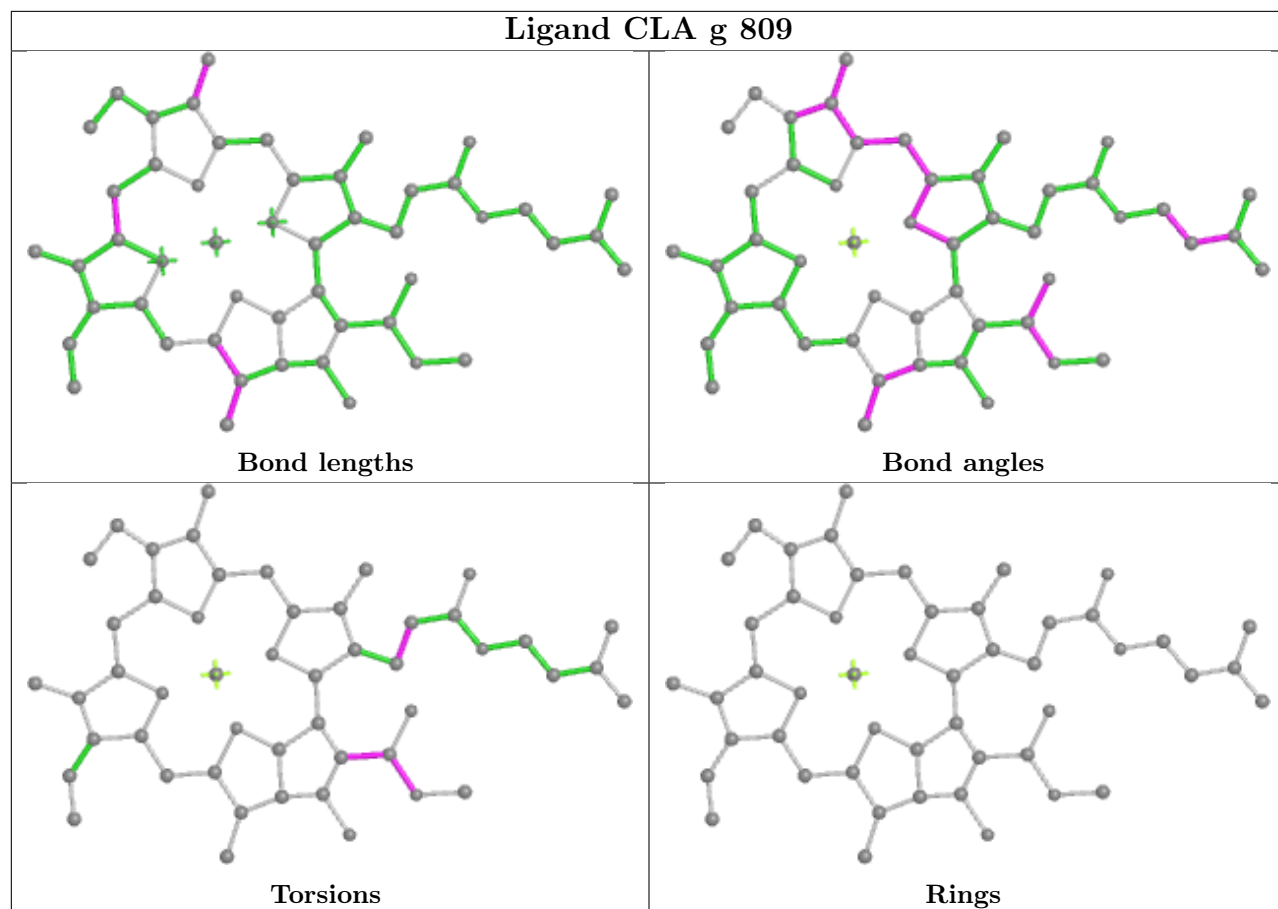
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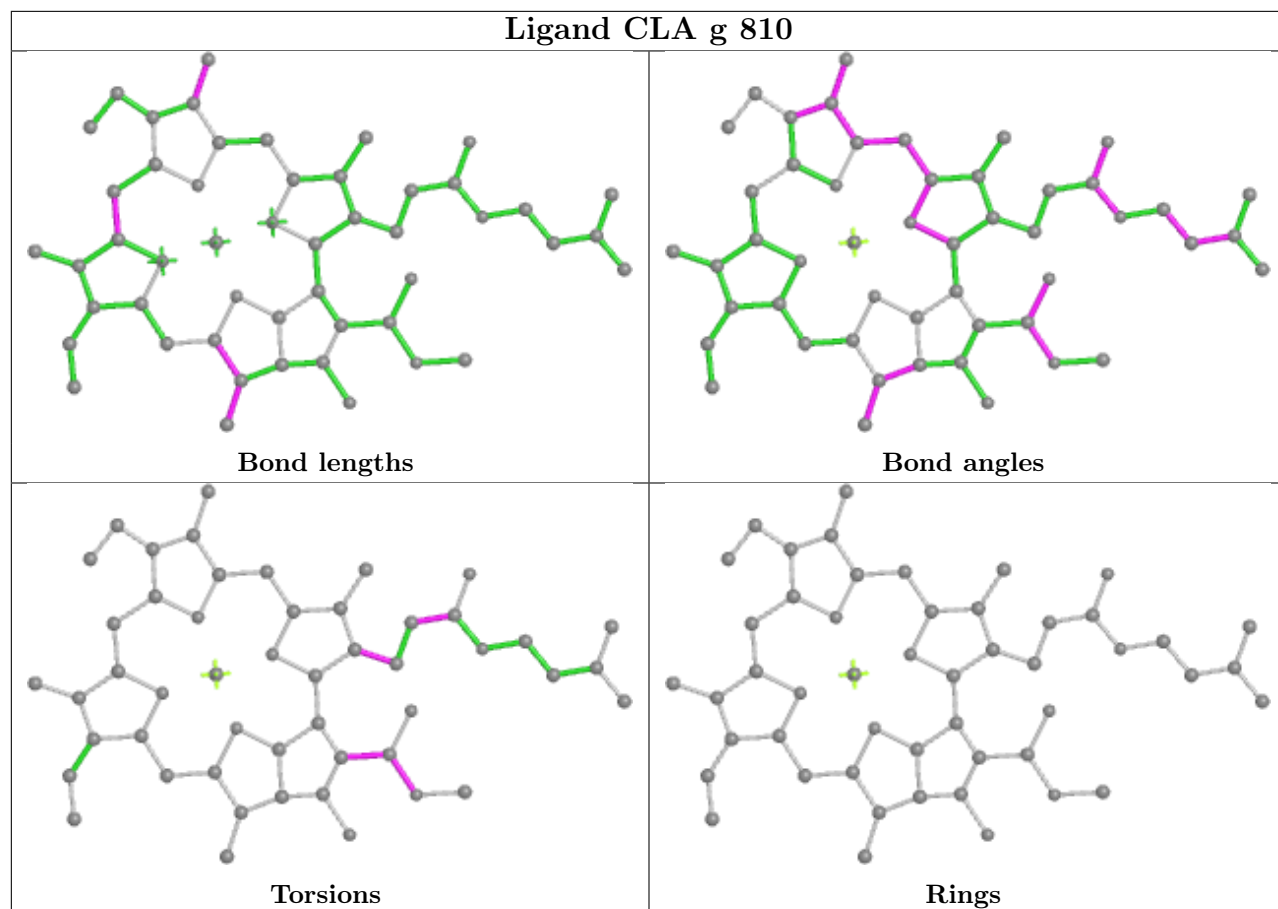
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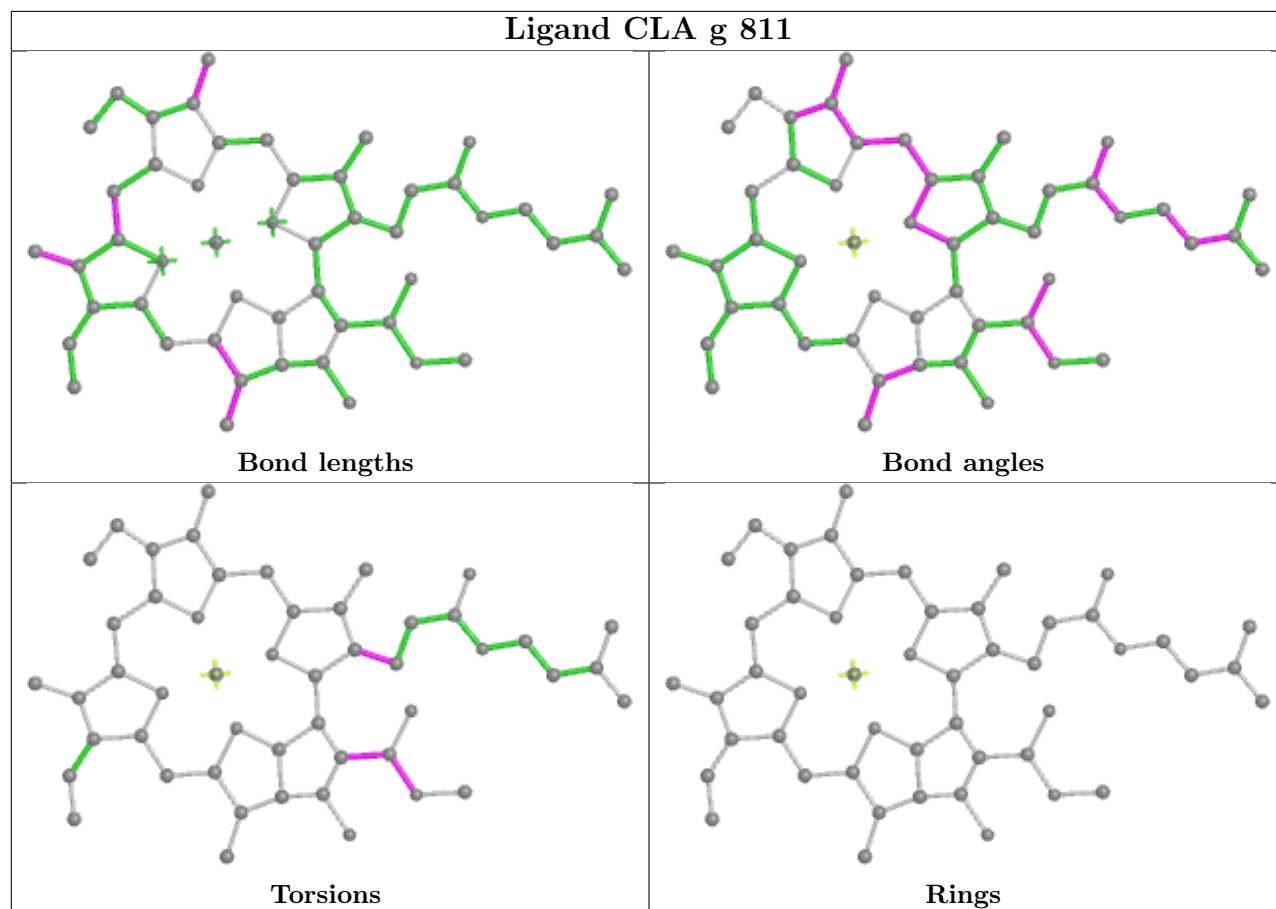
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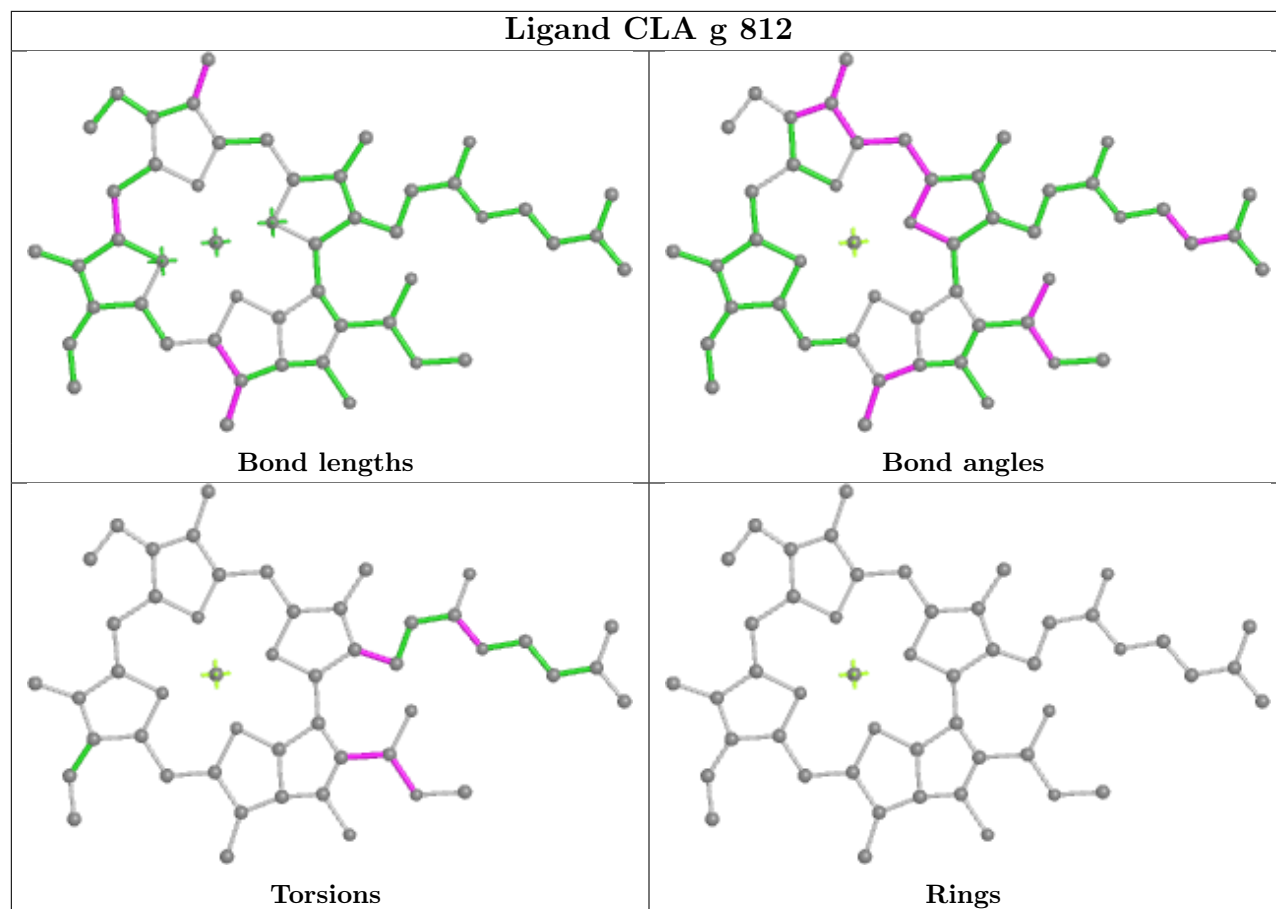
Ligand CLA g 810



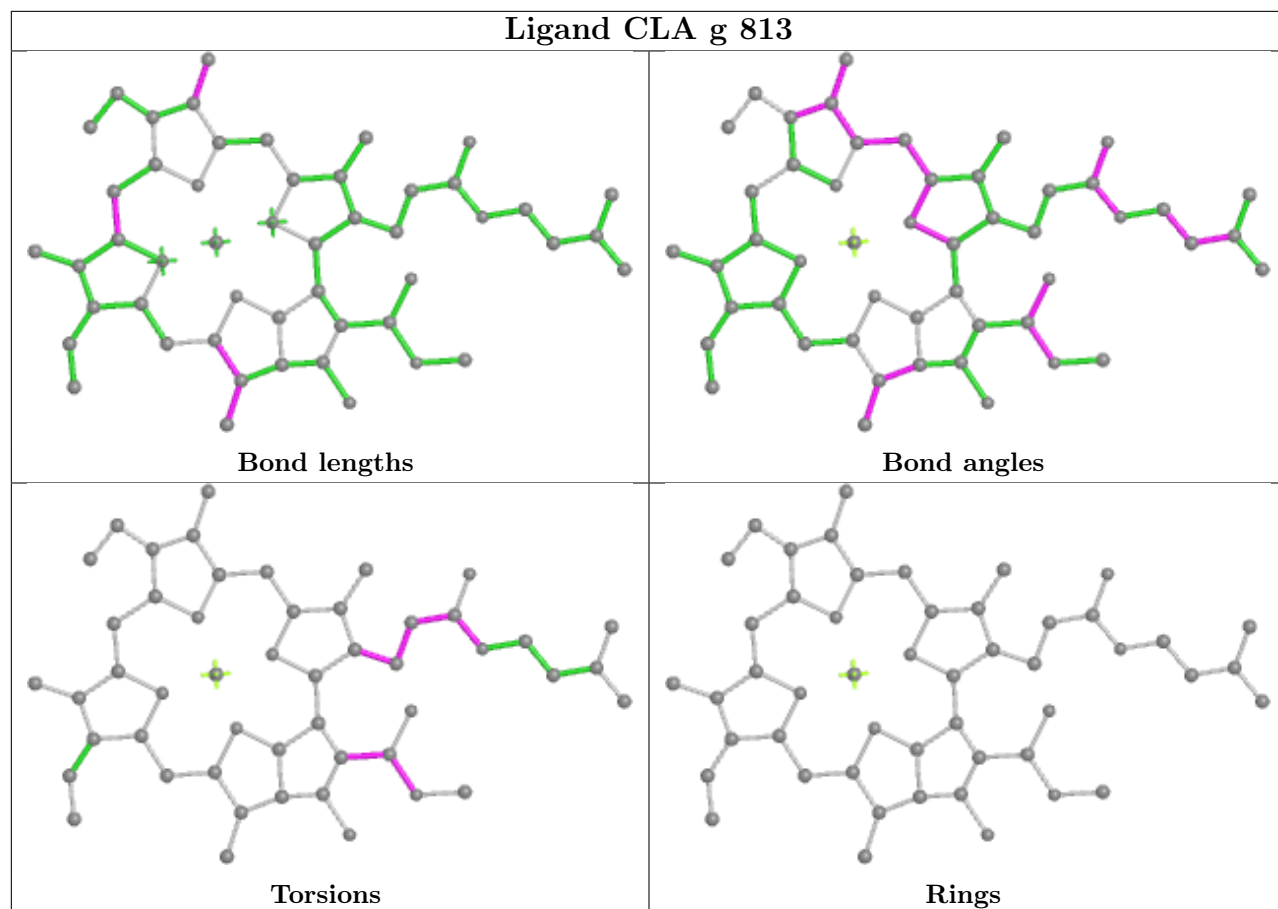
Ligand CLA g 811



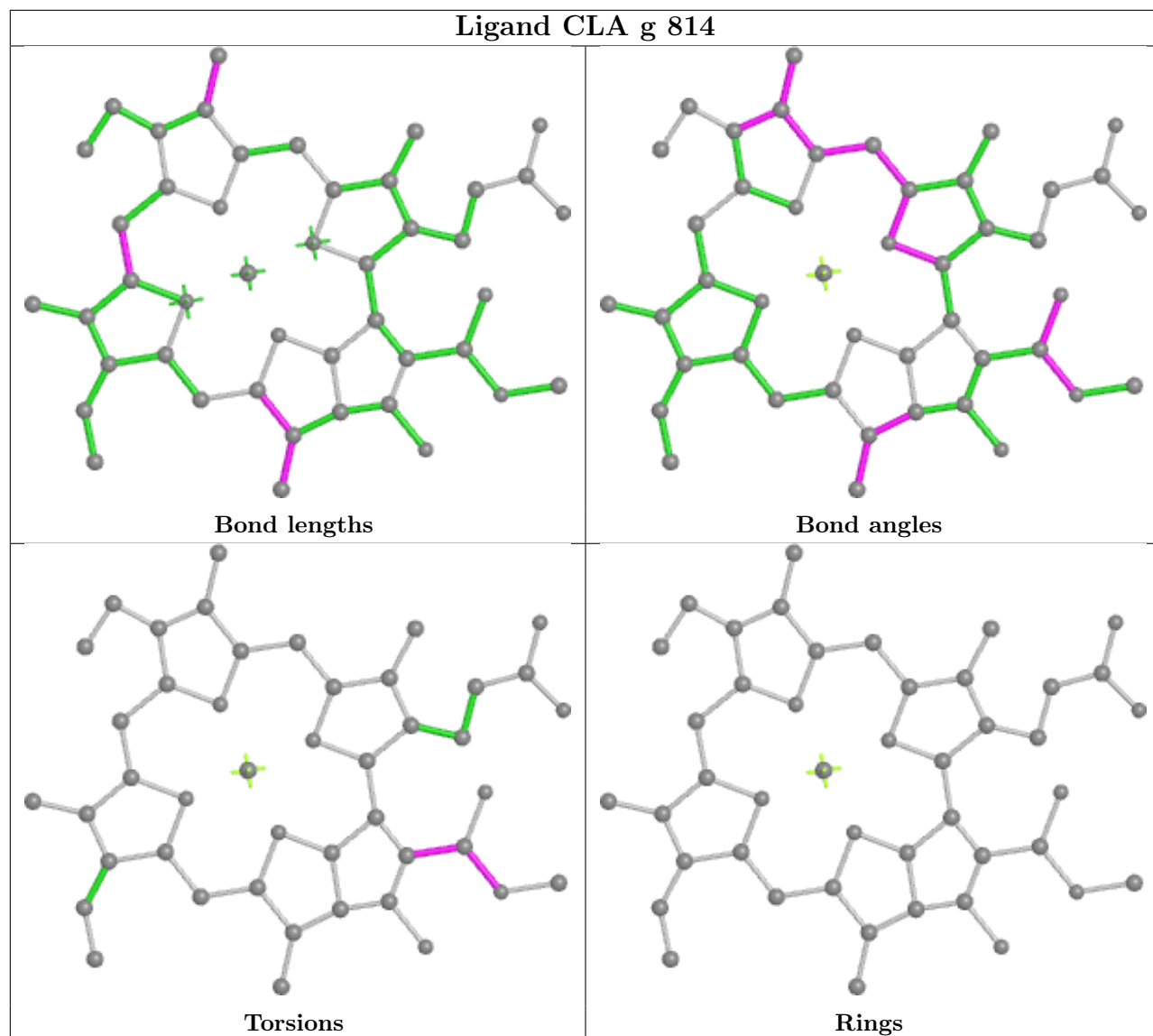
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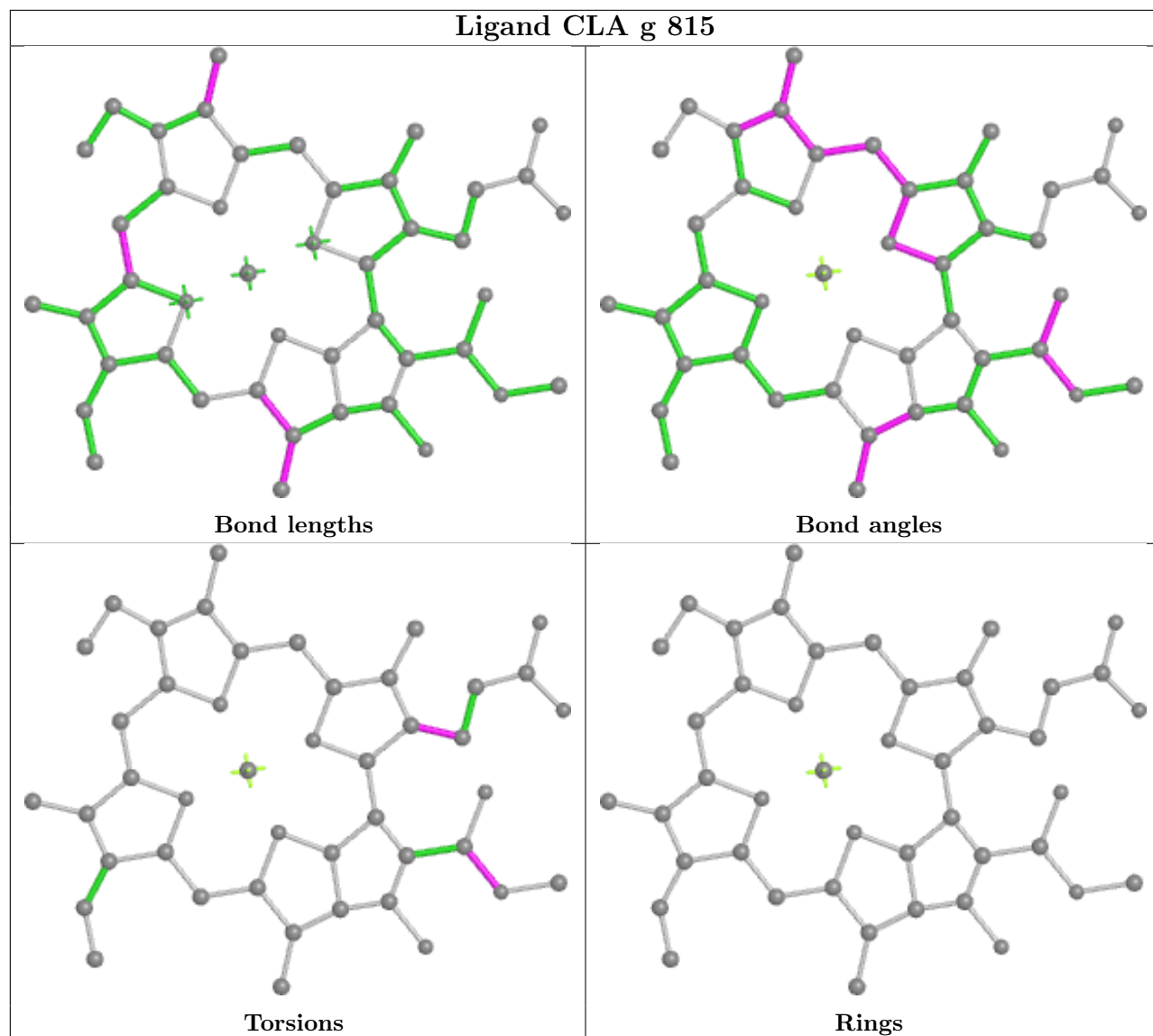
Ligand CLA g 813



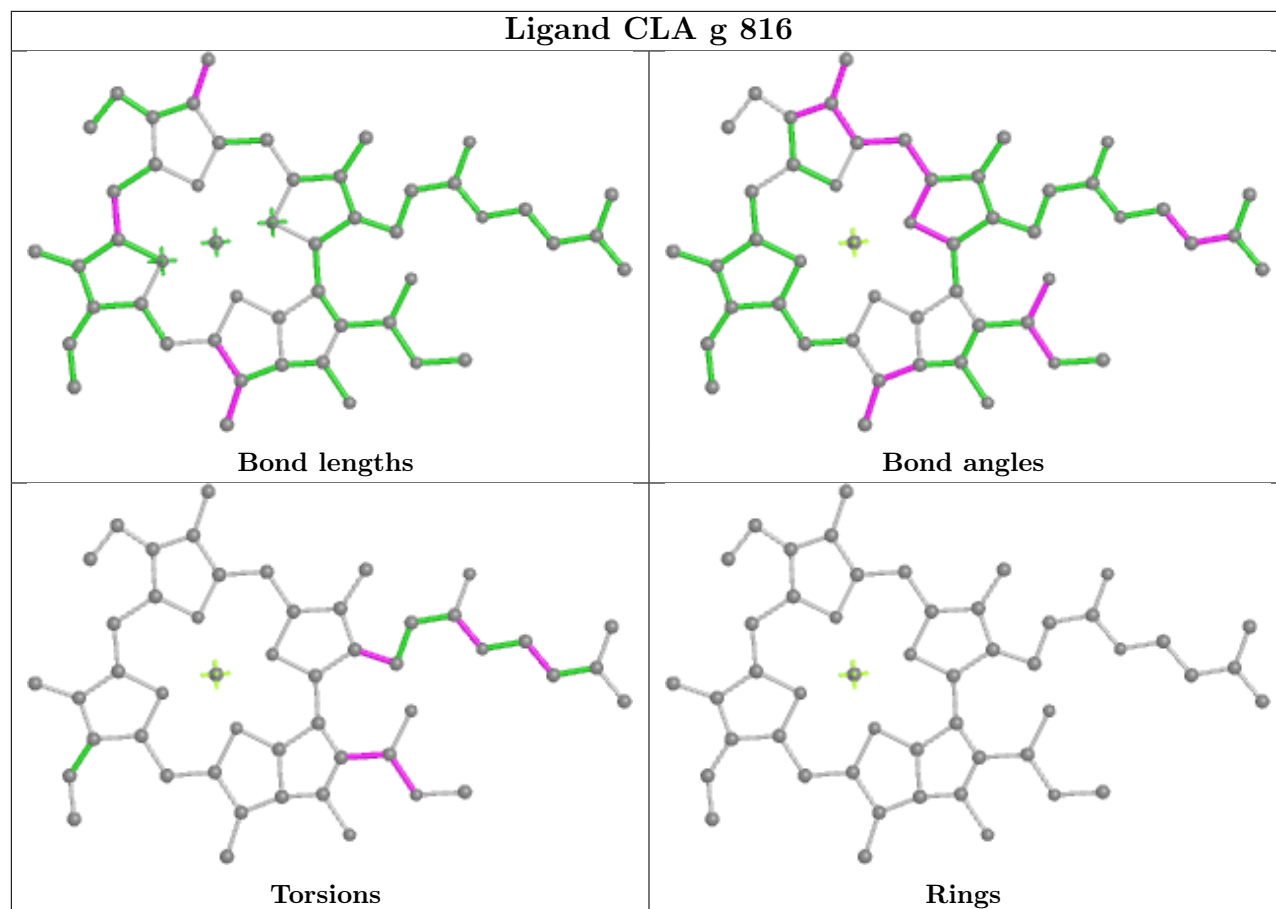
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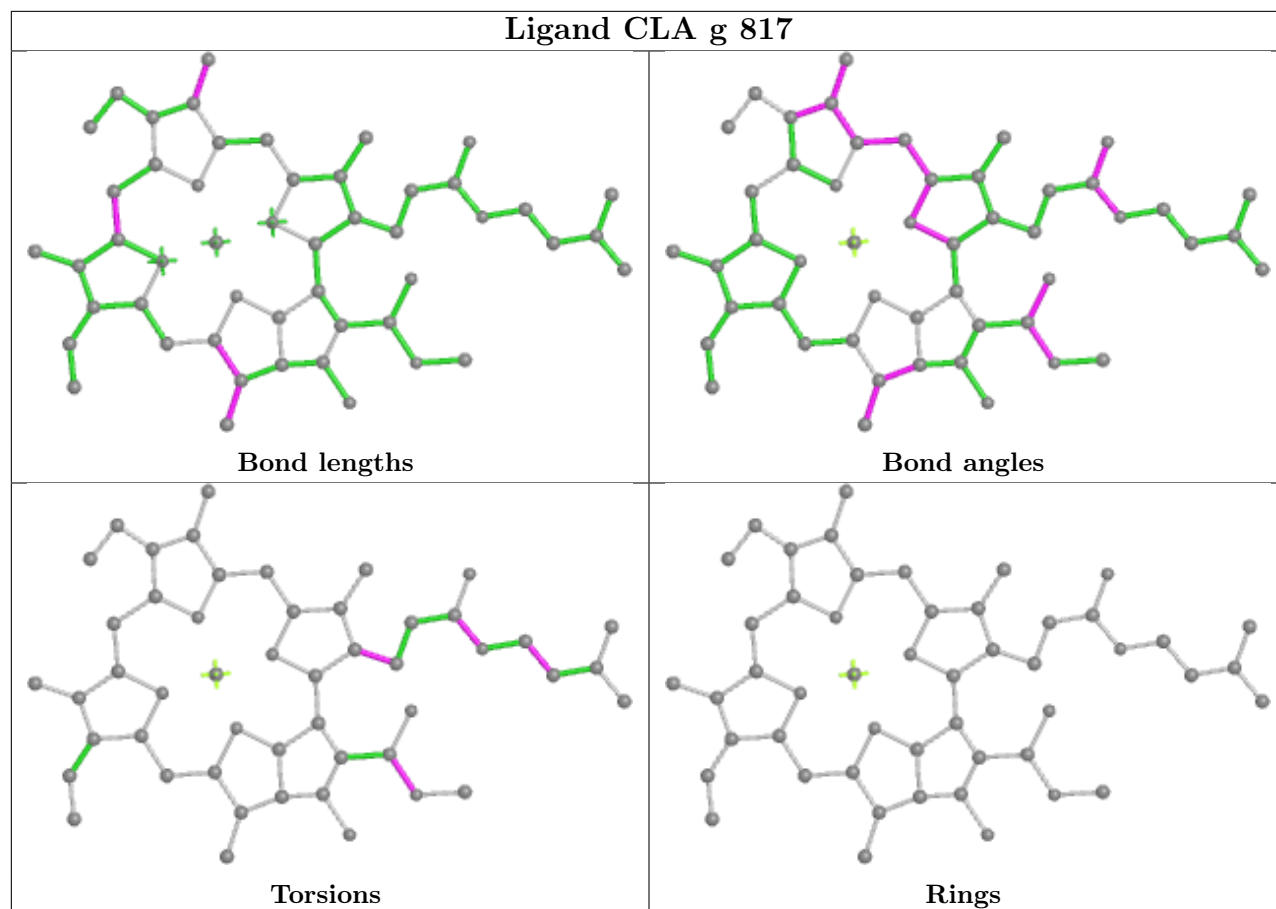
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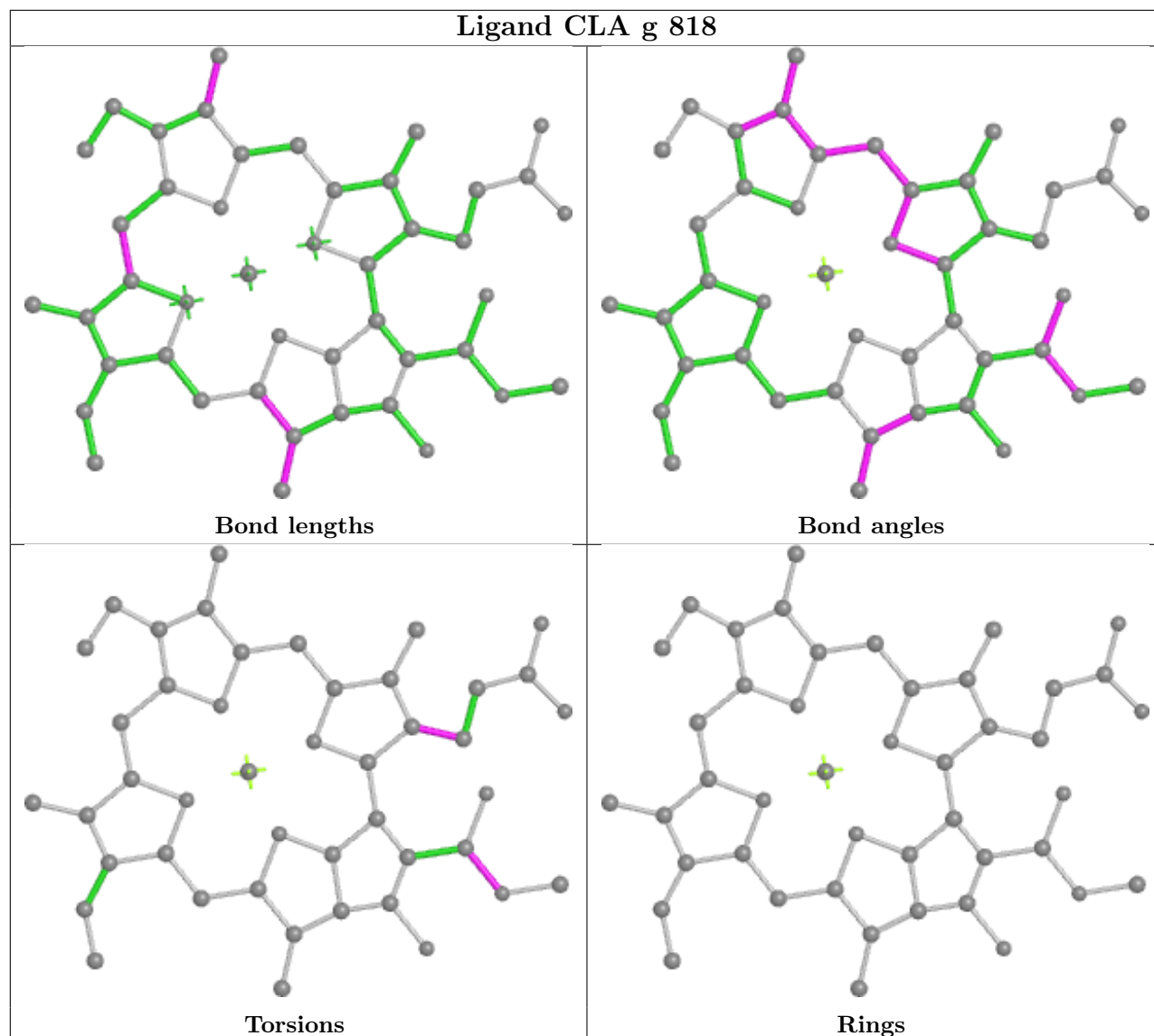
Ligand CLA g 816



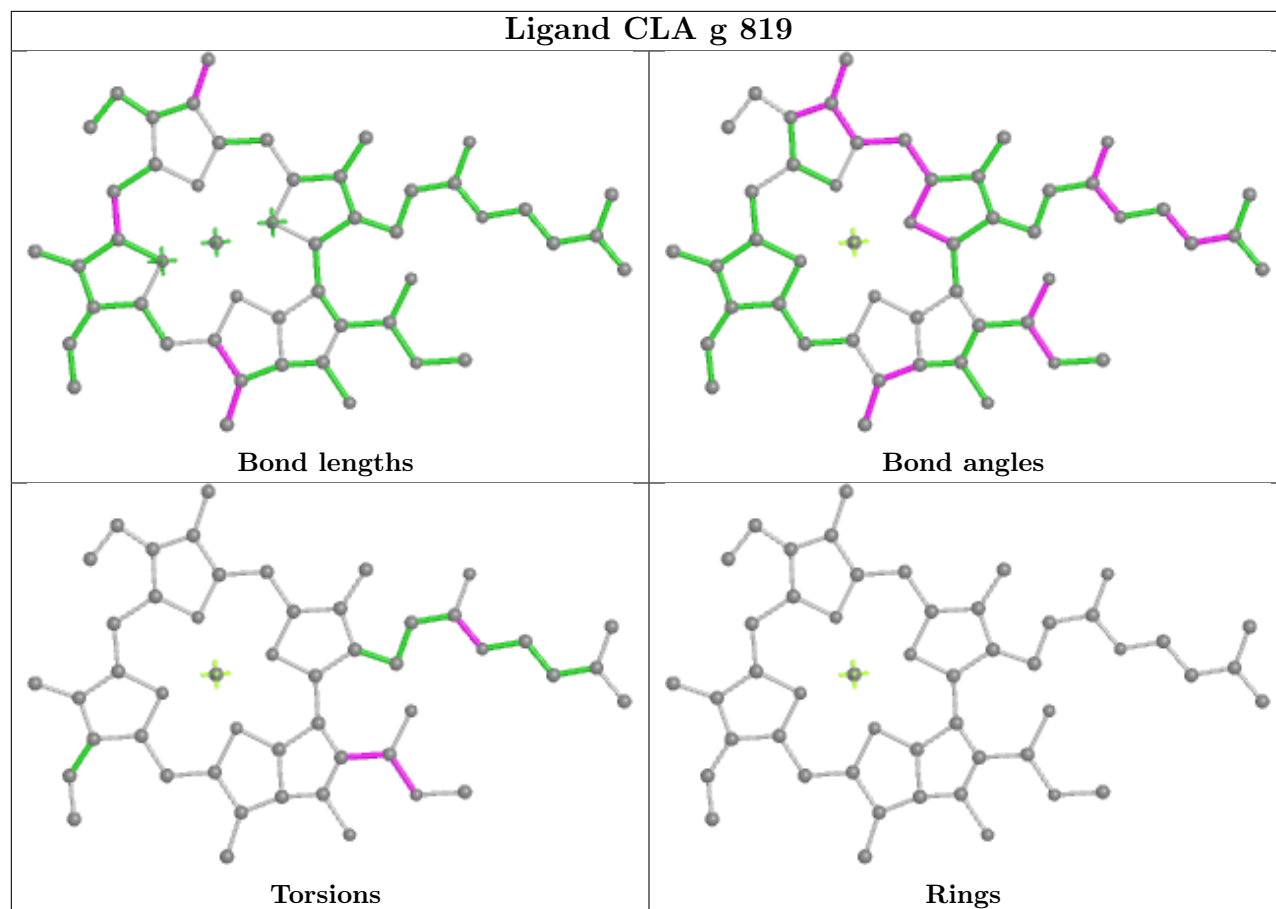
Ligand CLA g 817

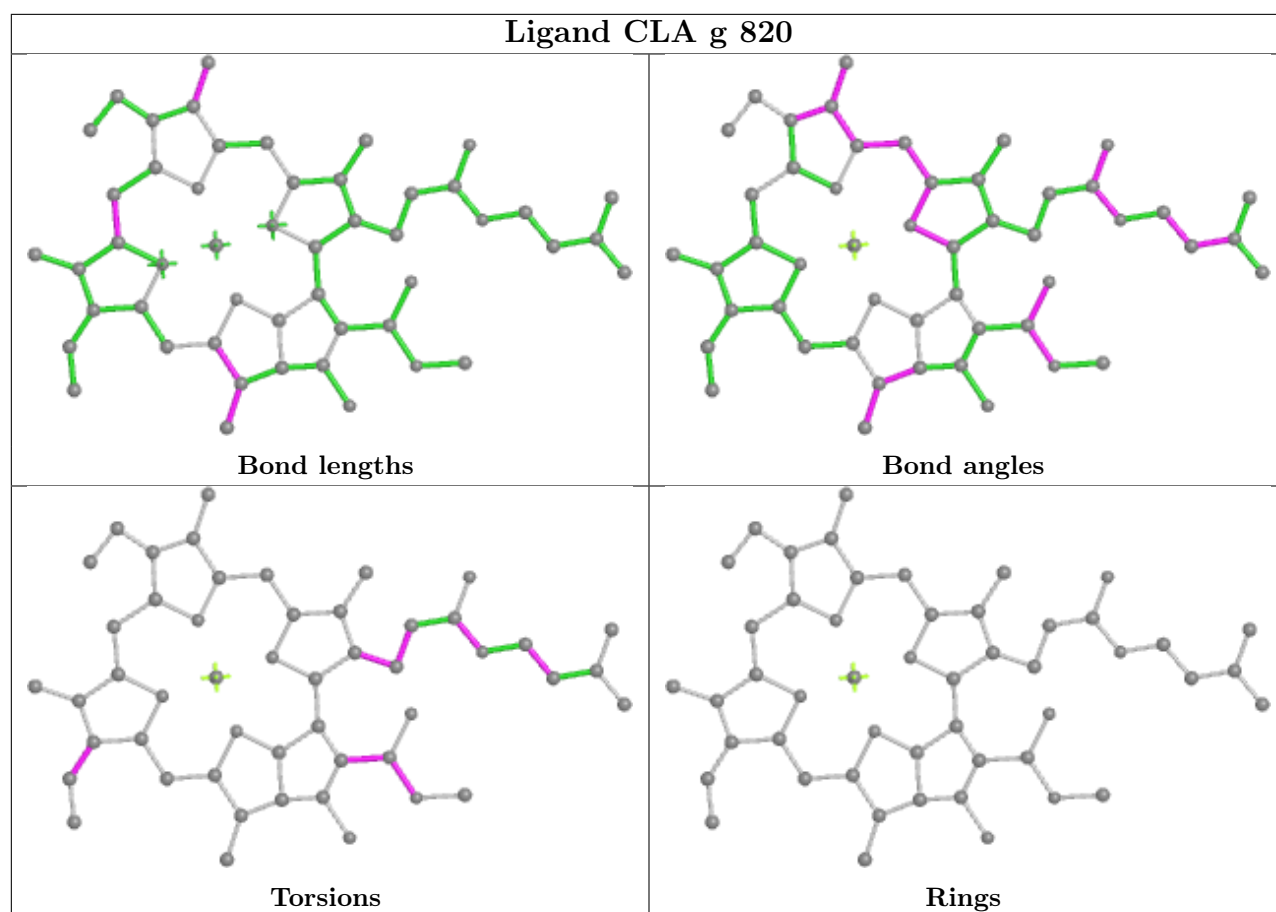


Ligand CLA g 818

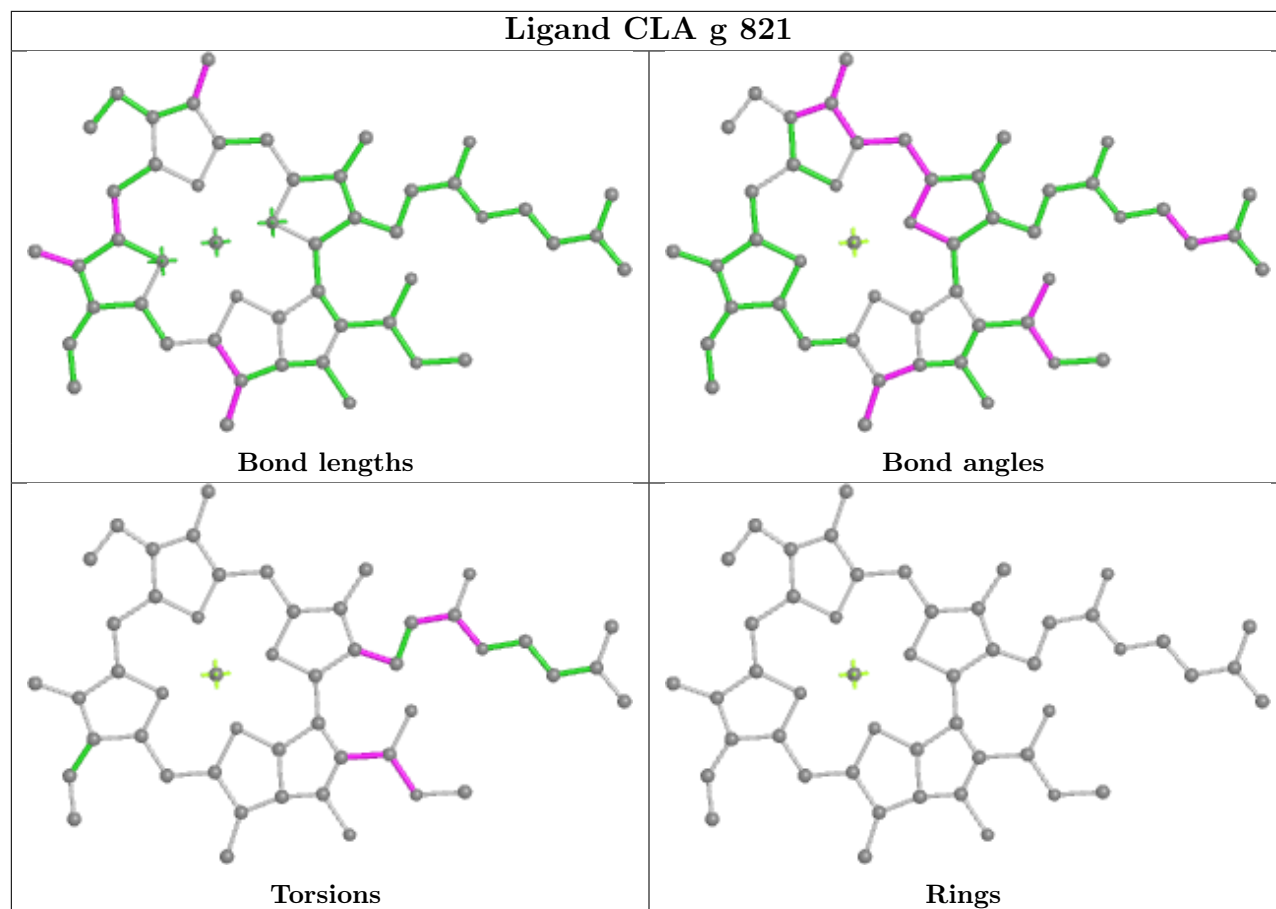


Ligand CLA g 819

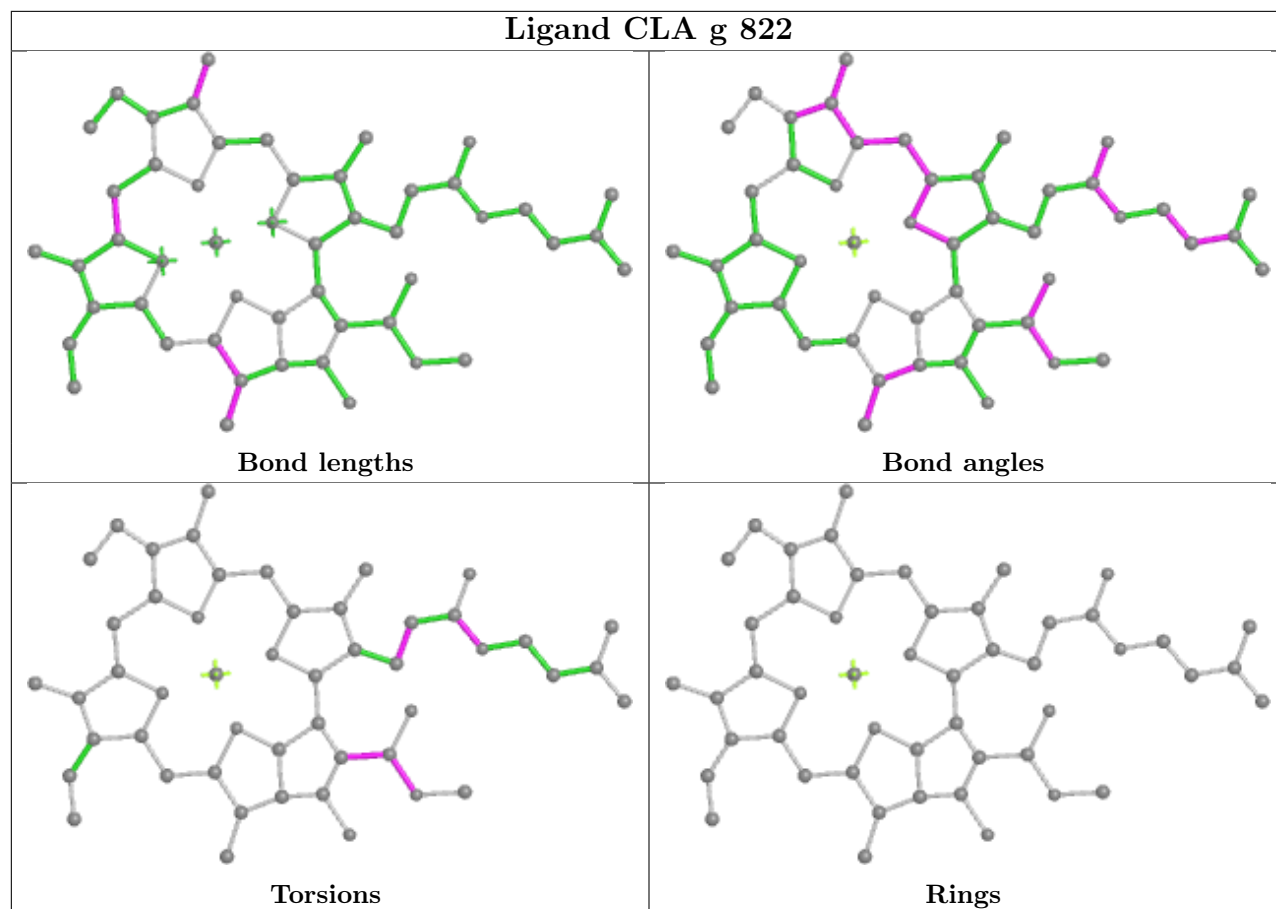




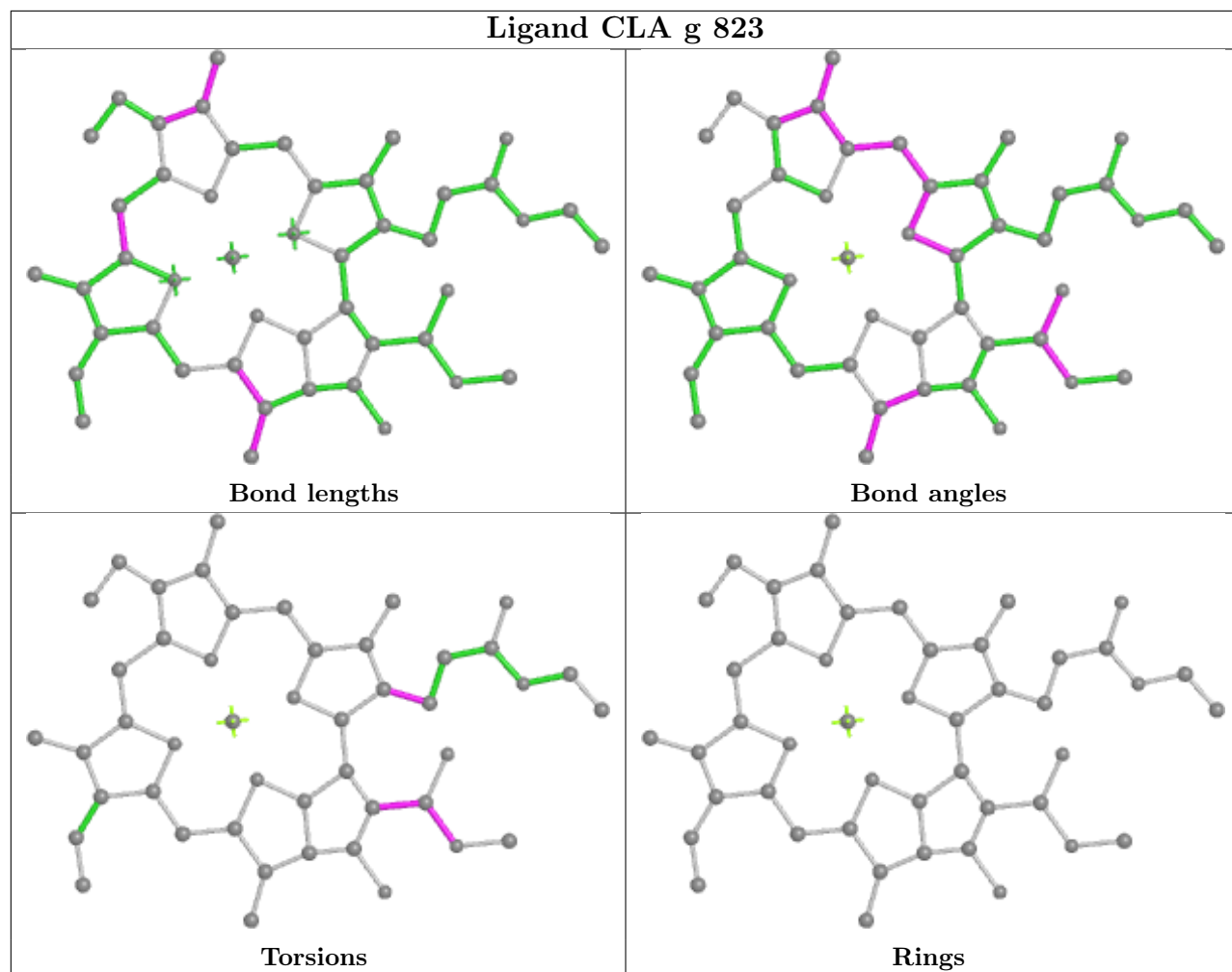
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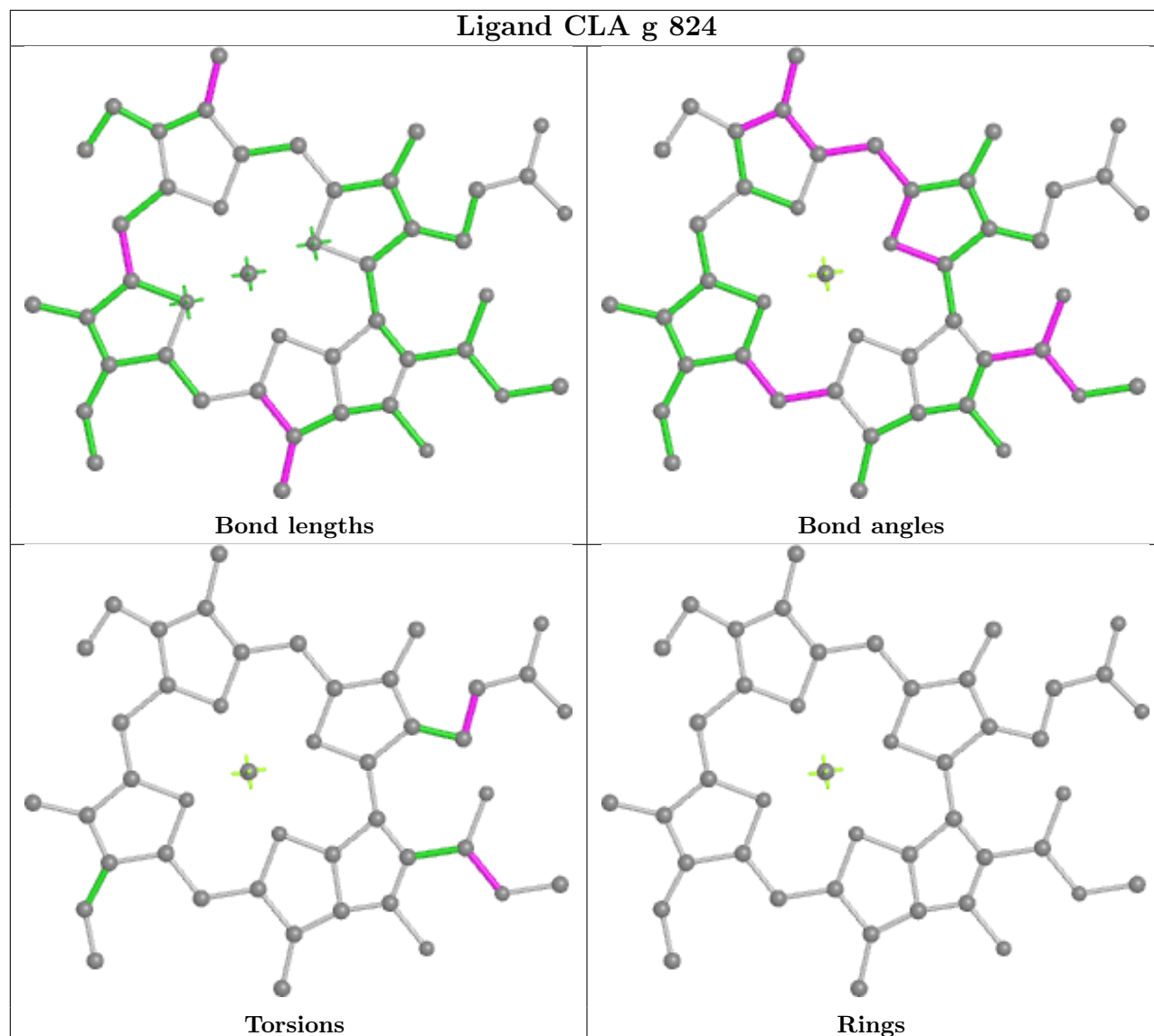
Ligand CLA g 822



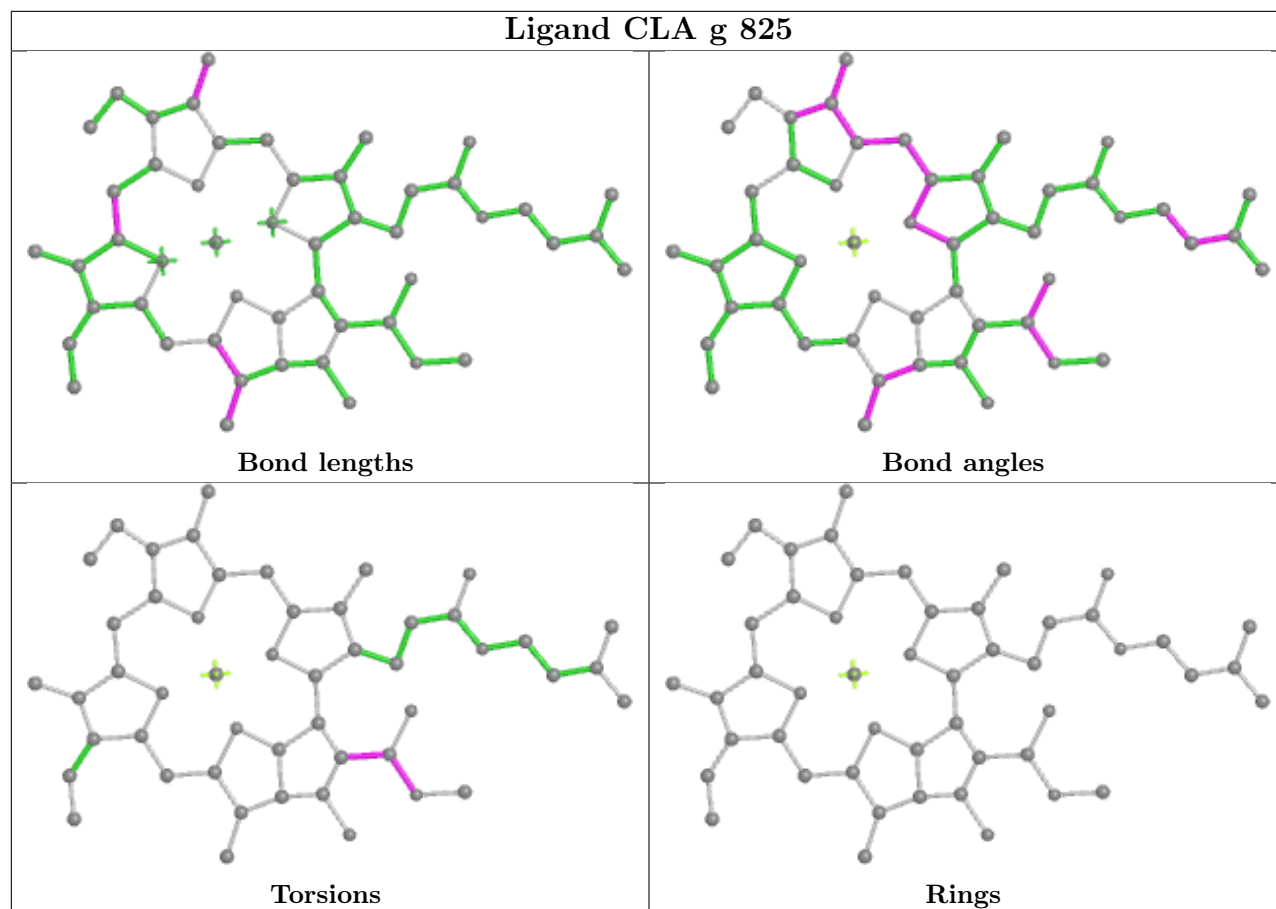
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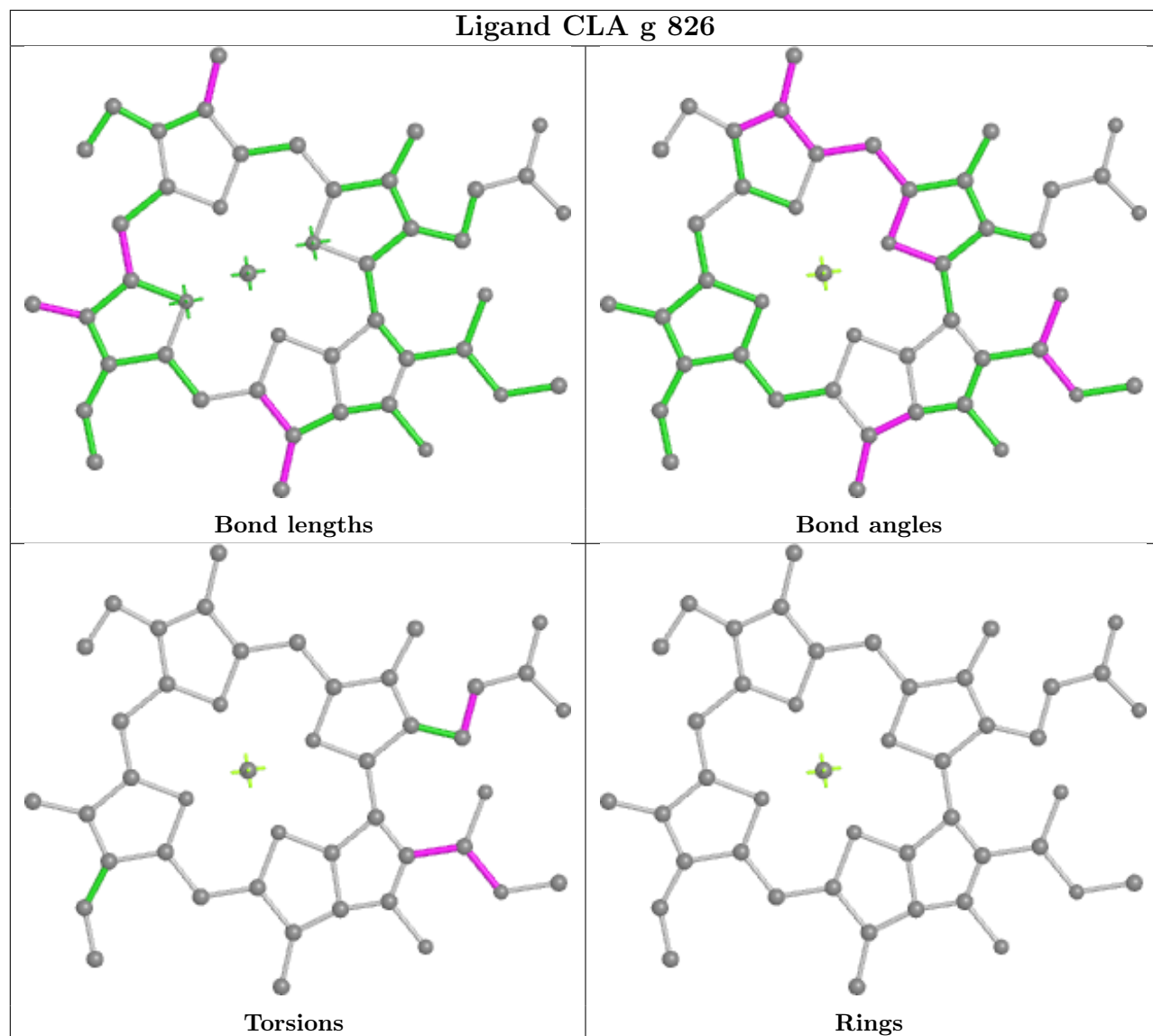
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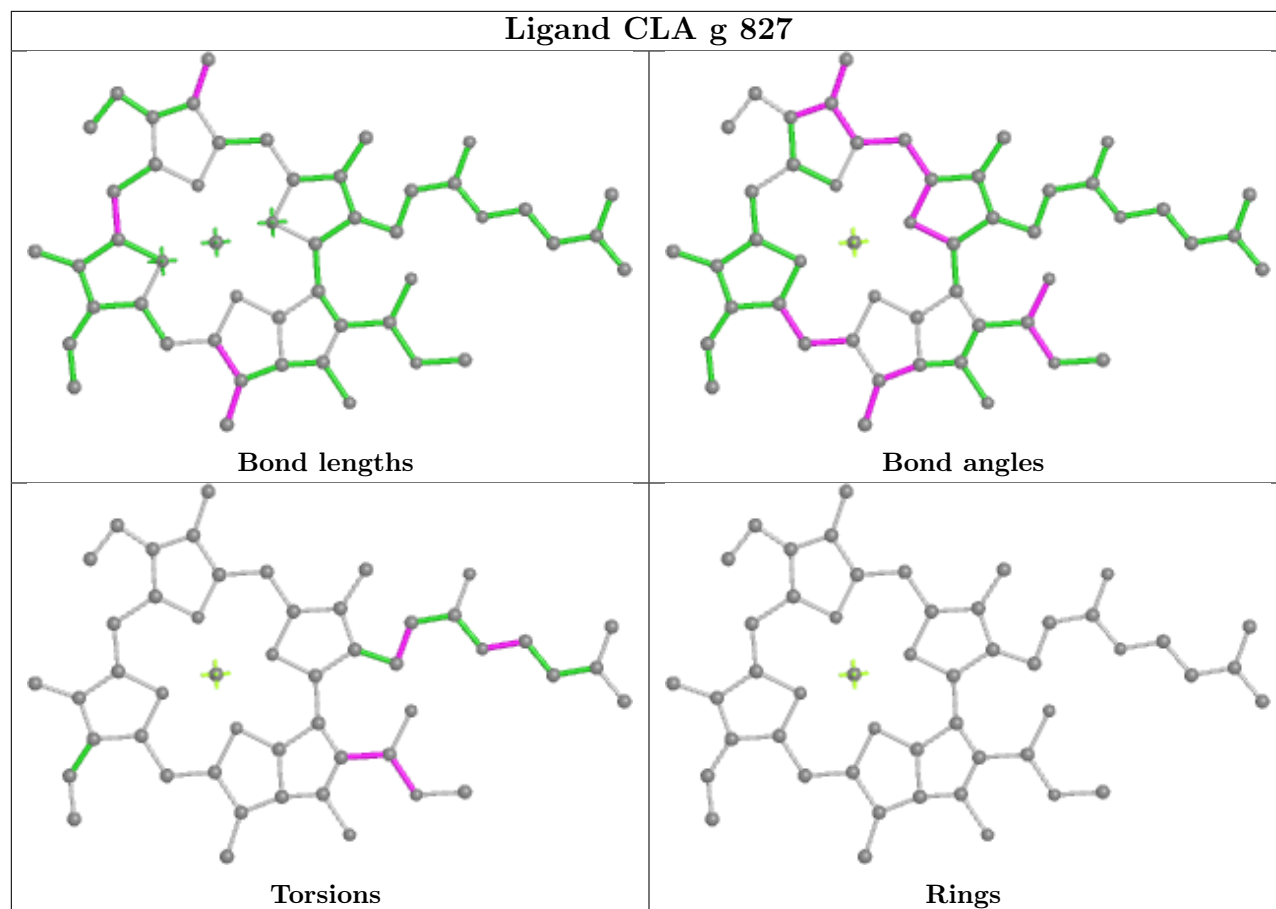
Ligand CLA g 825



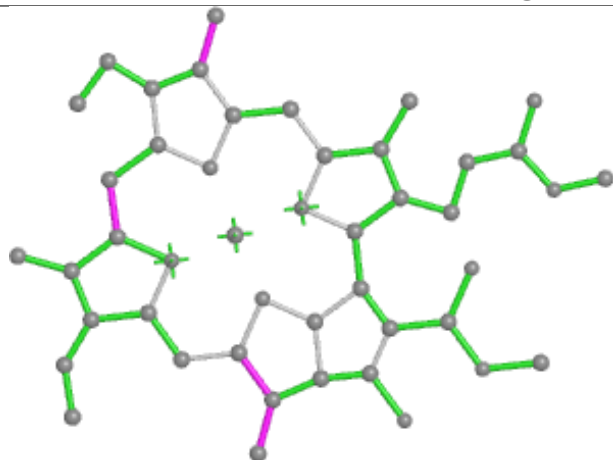
Ligand CLA g 826



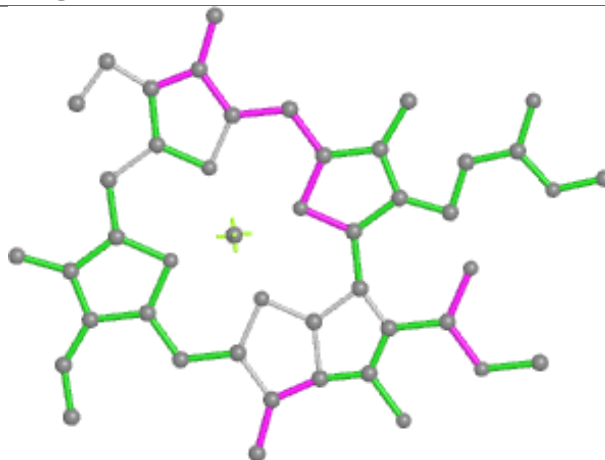
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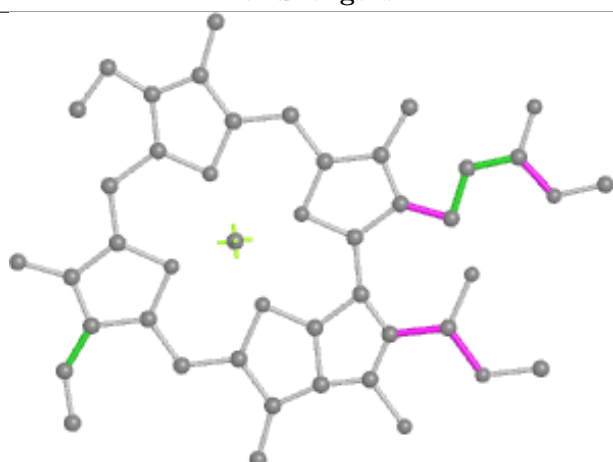
Ligand CLA g 828



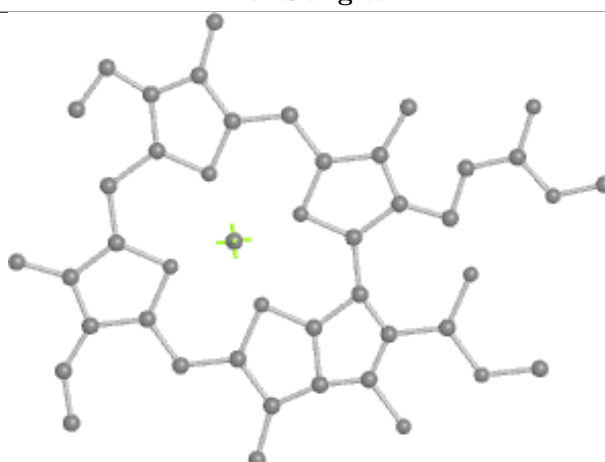
Bond lengths



Bond angles

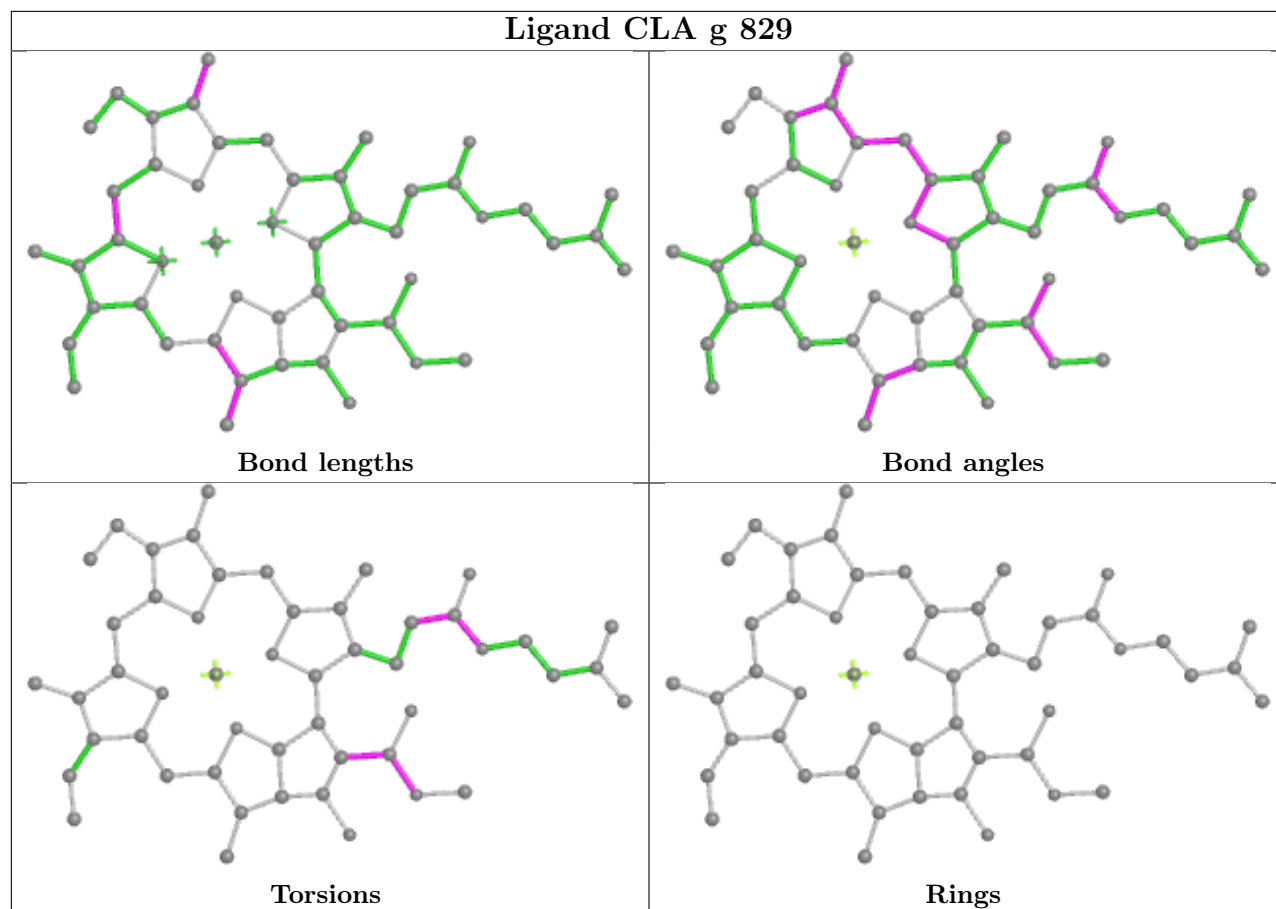


Torsions

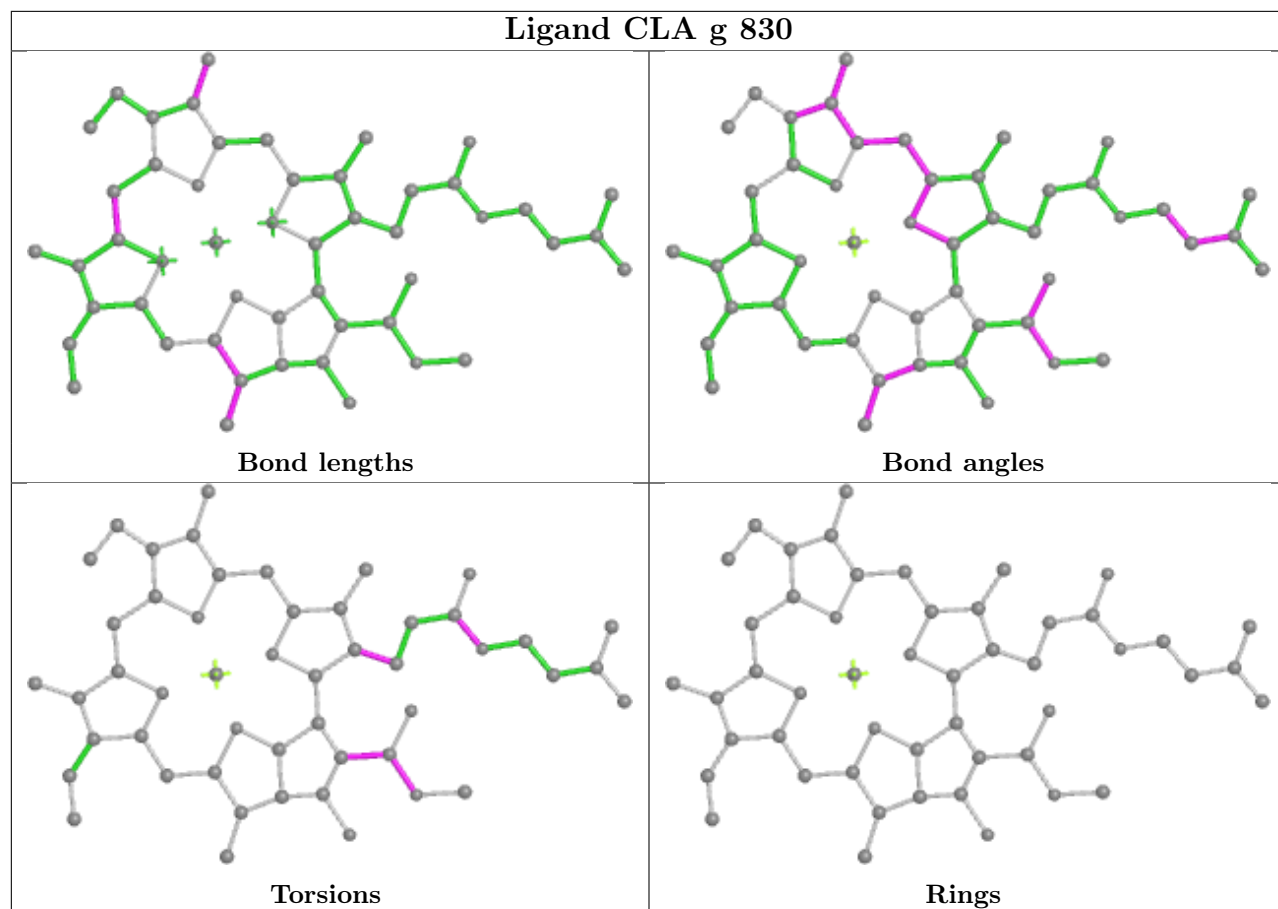


Rings

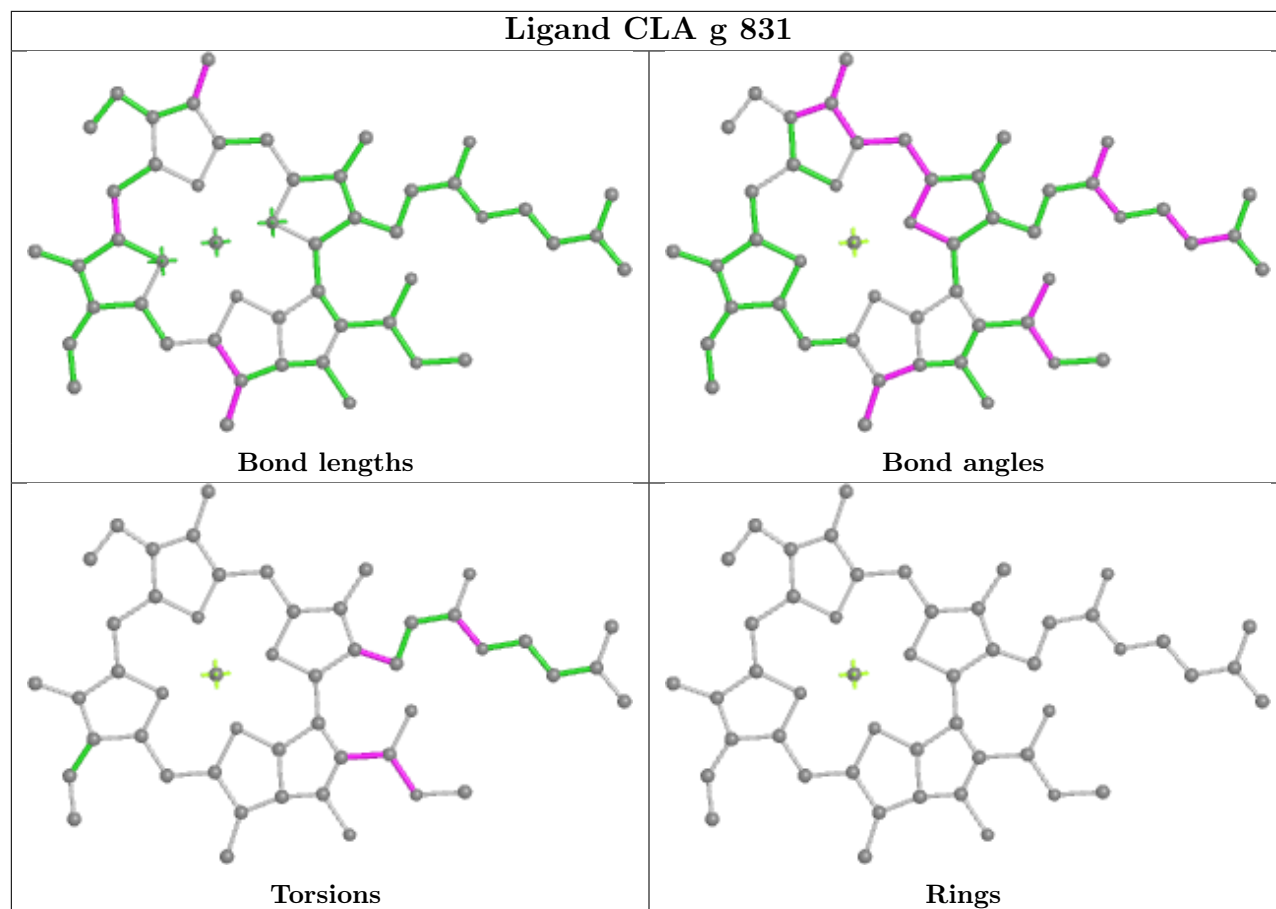
Ligand CLA g 829



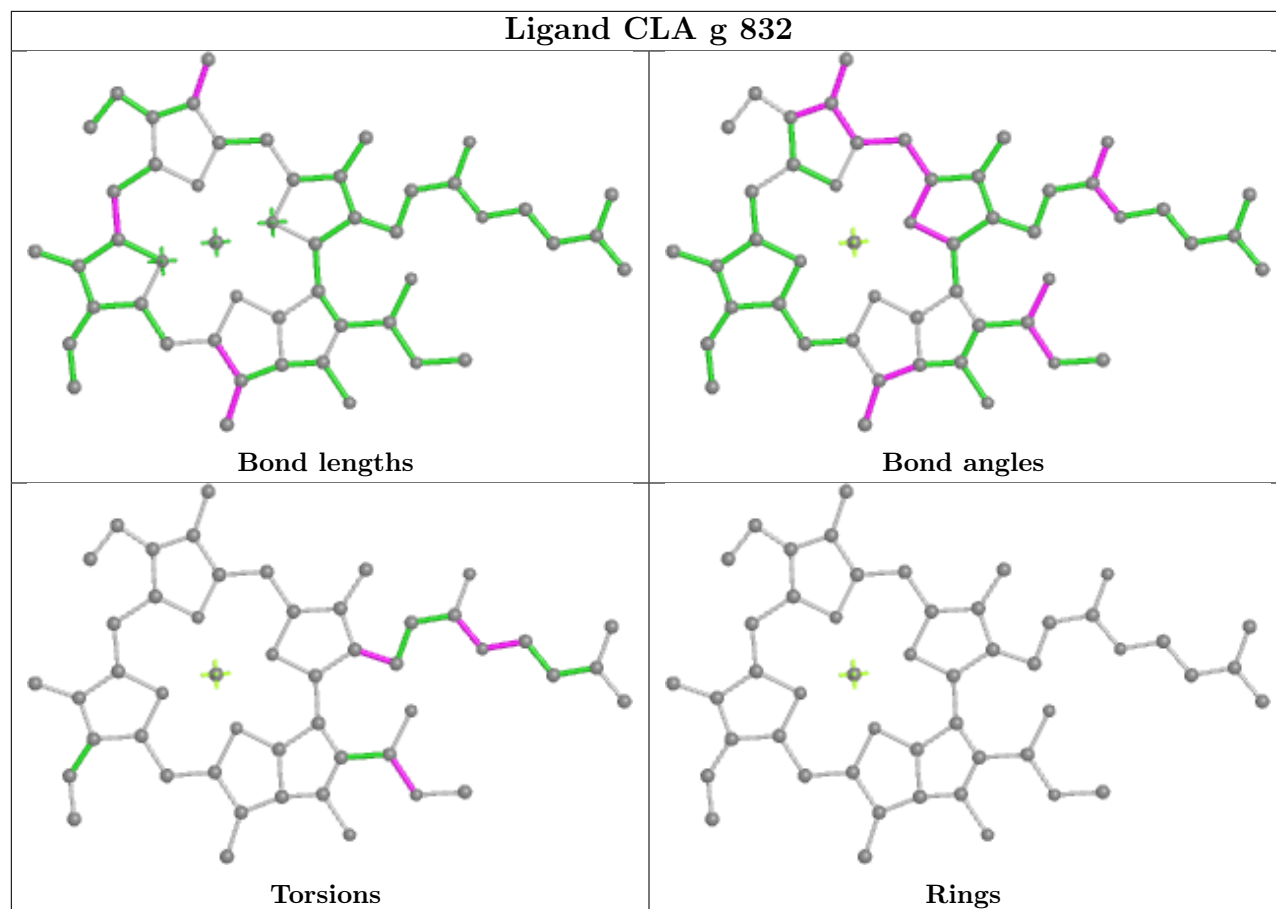
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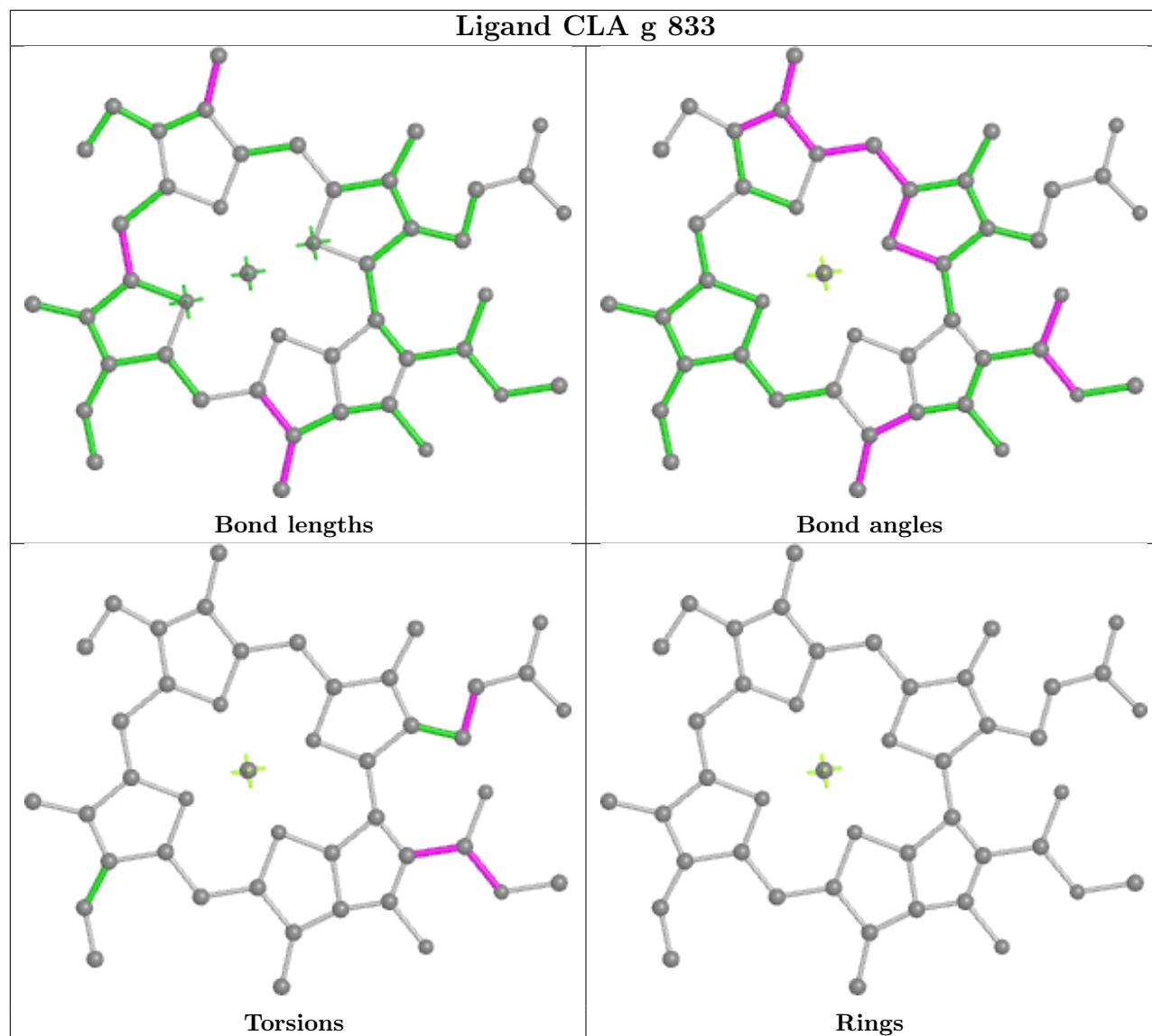
Ligand CLA g 831

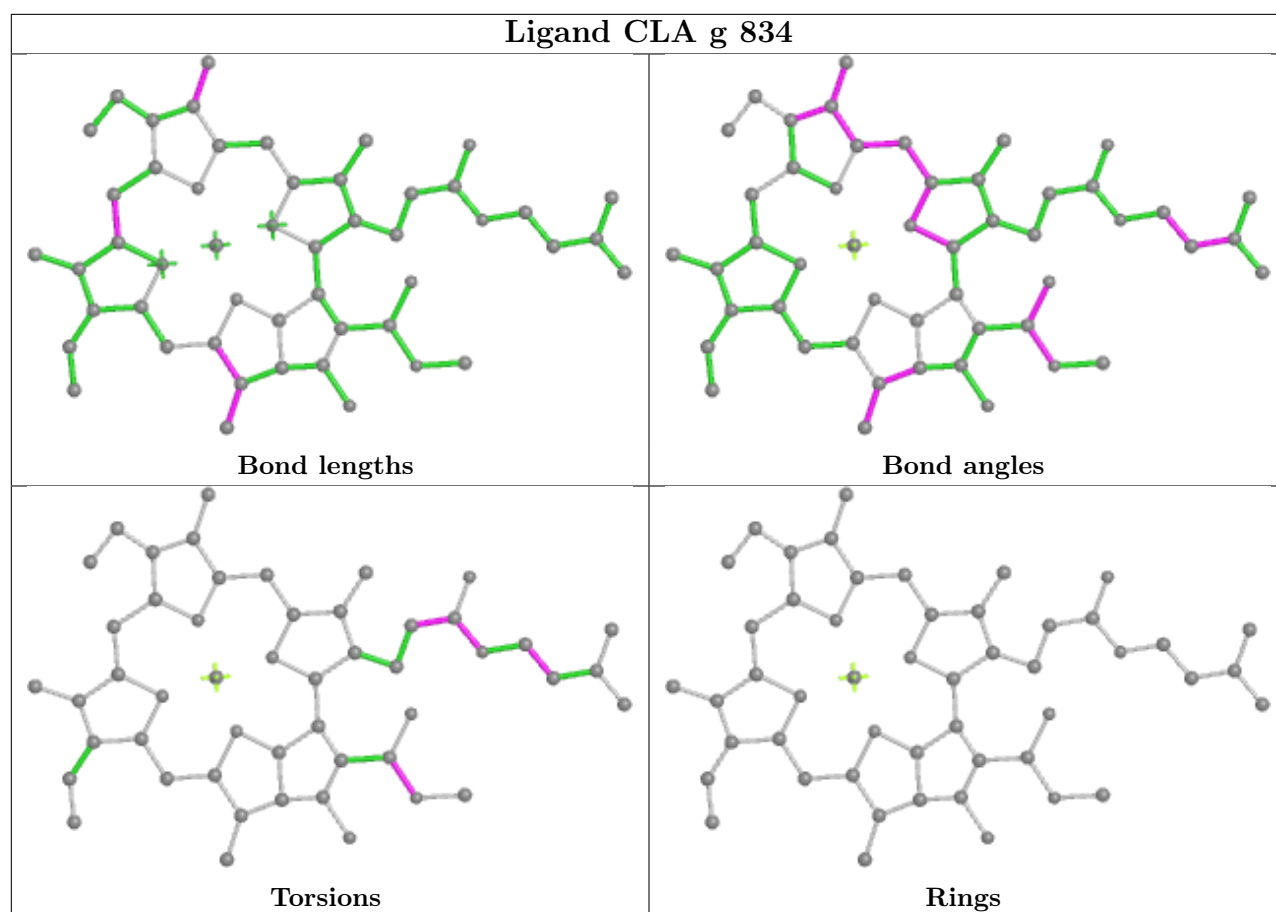


Ligand CLA g 832

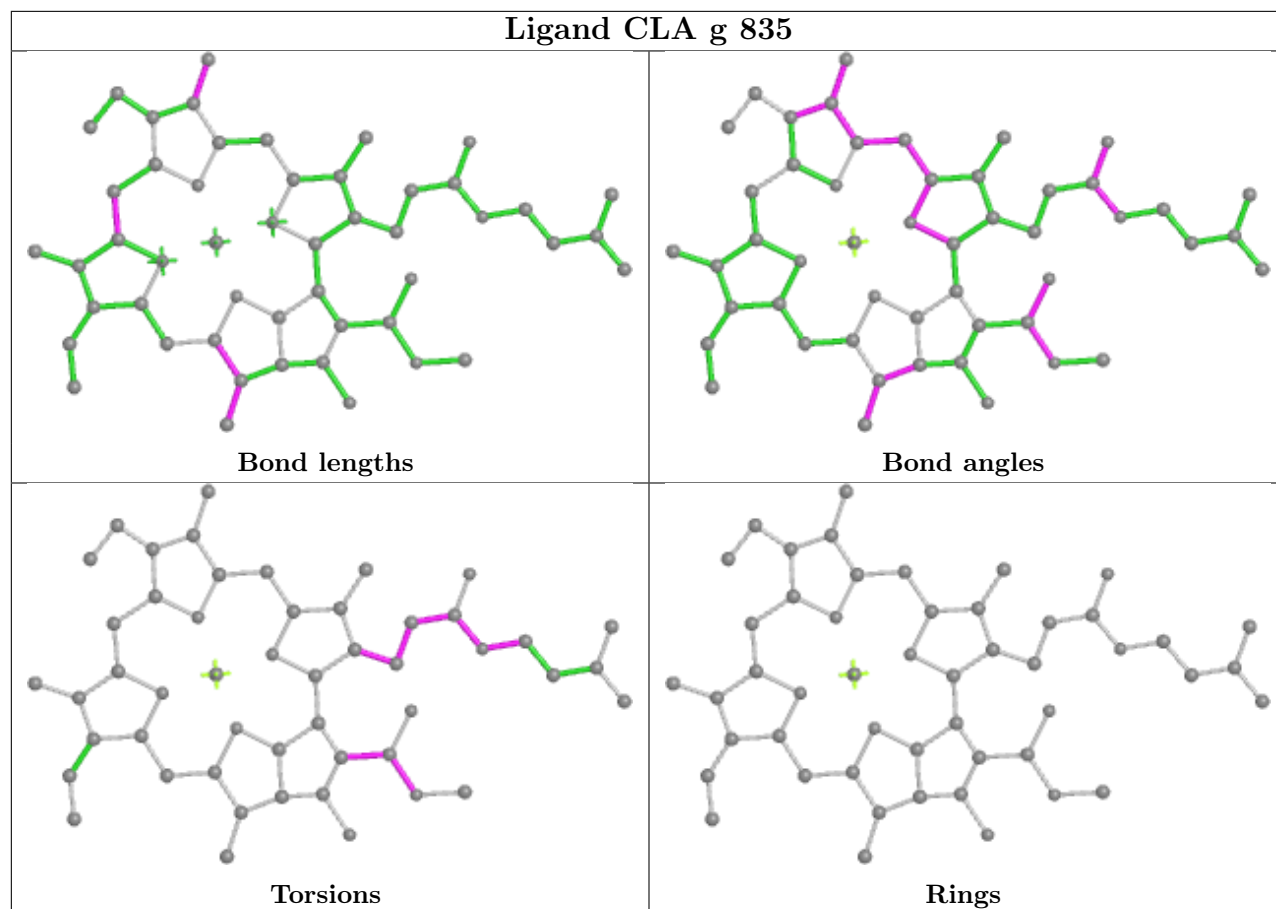


Ligand CLA g 833

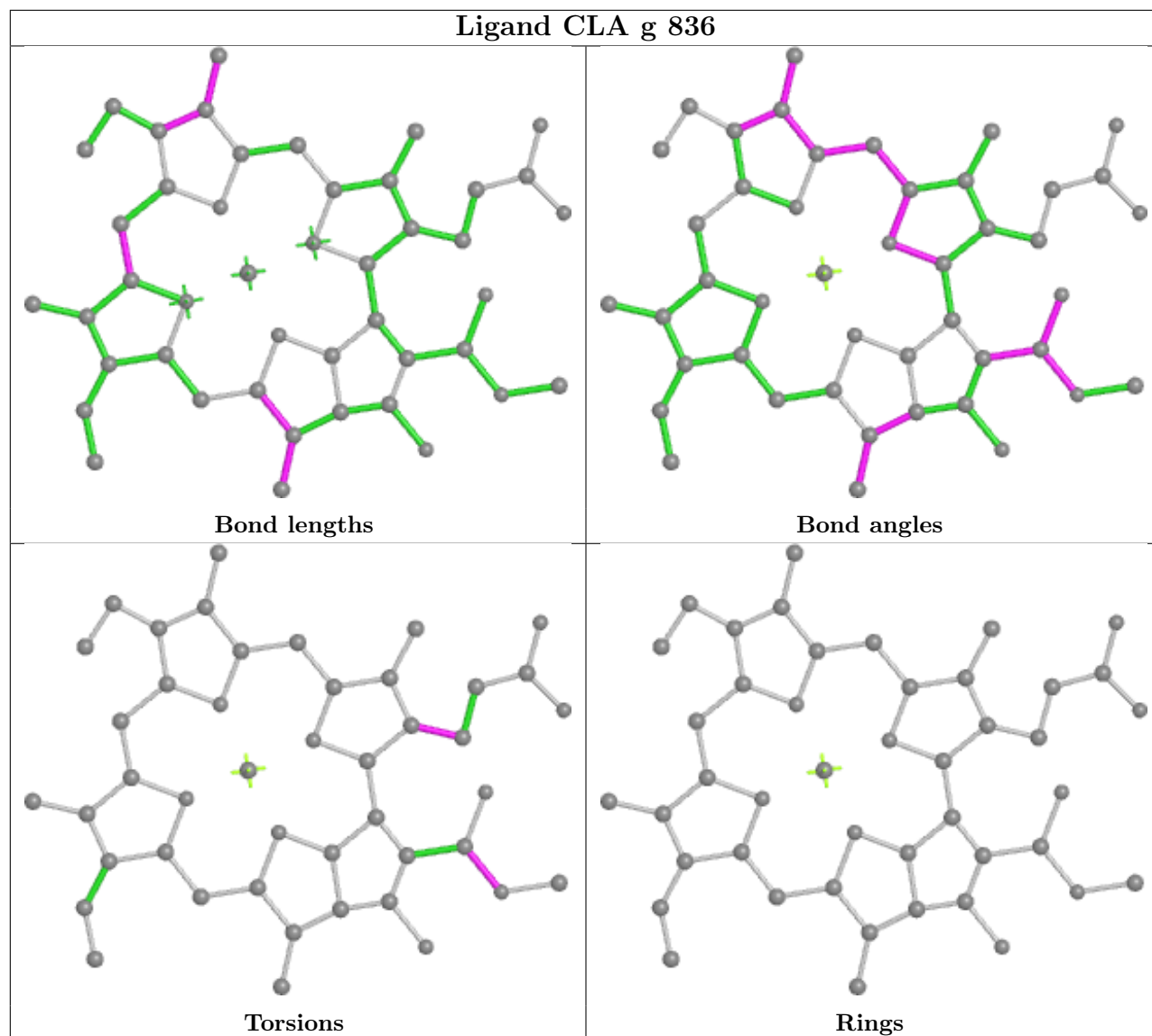




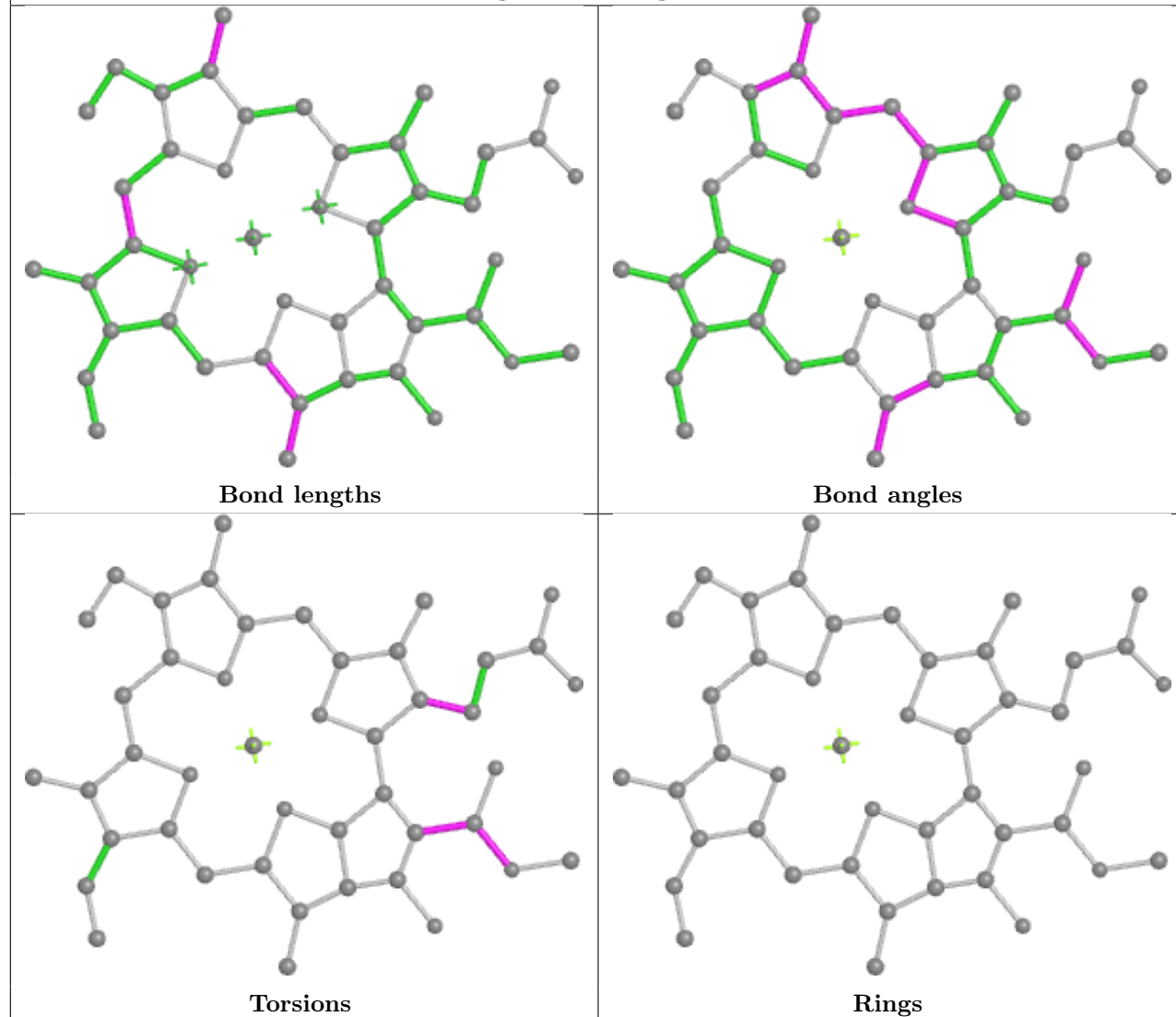
Ligand CLA g 835



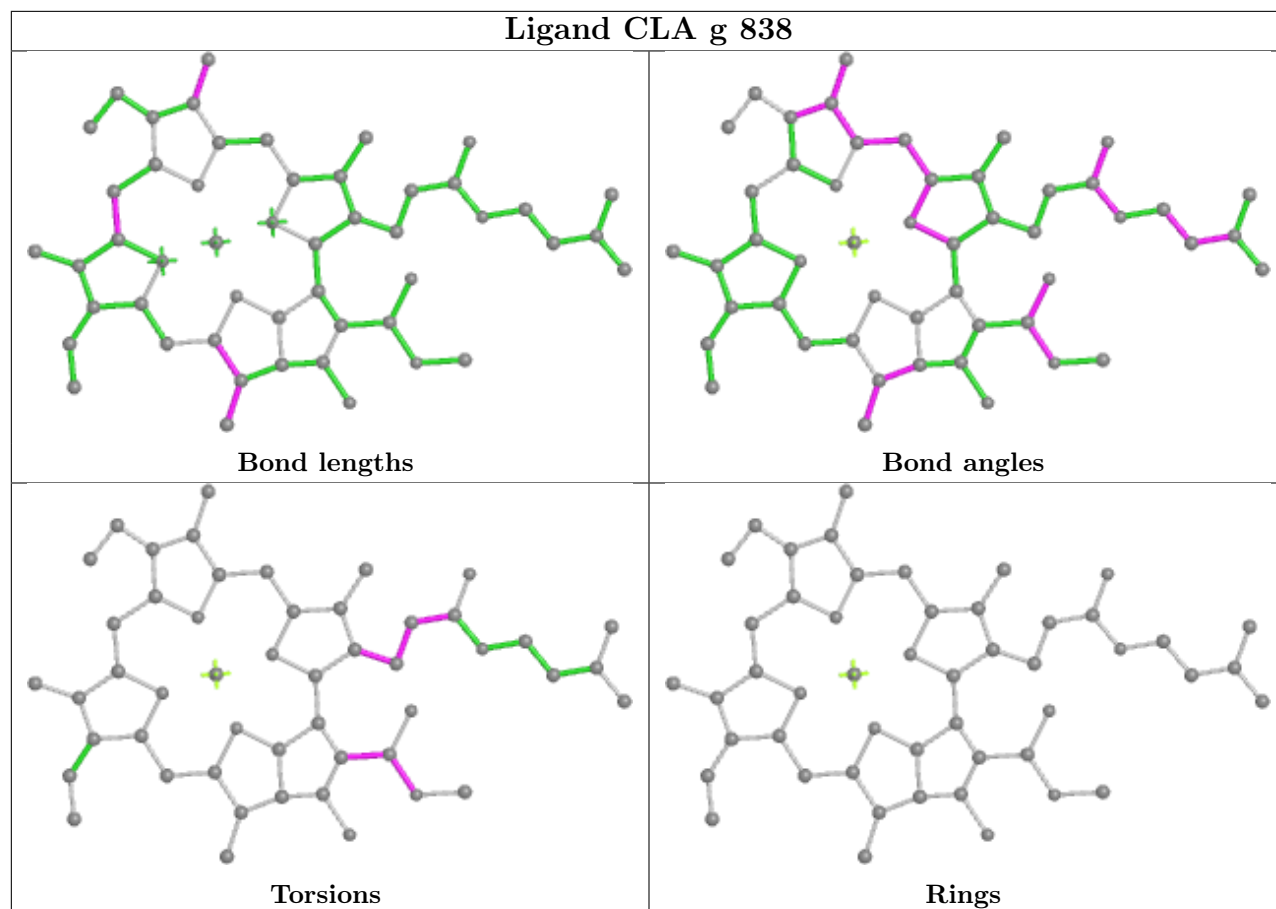
Ligand CLA g 836



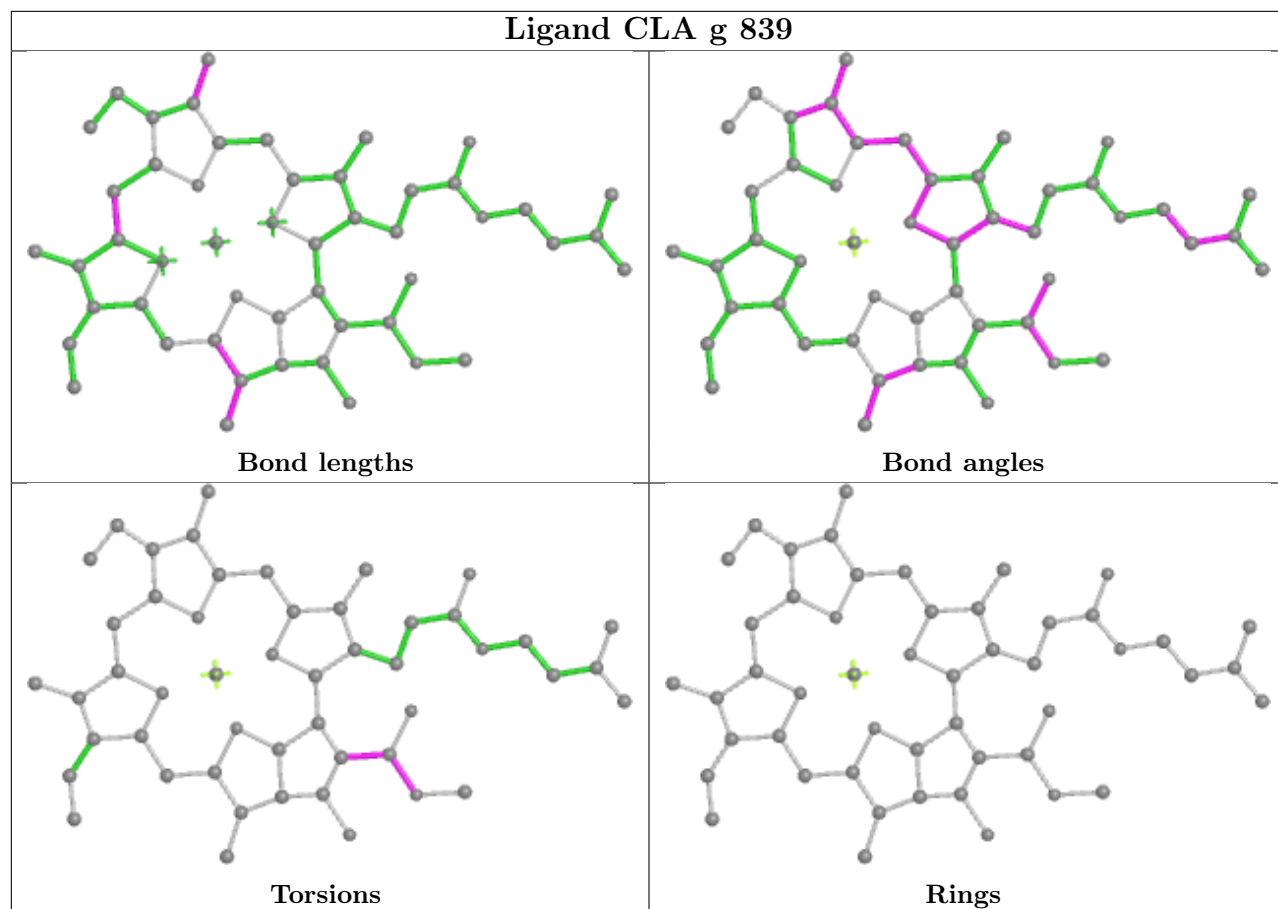
Ligand CLA g 837



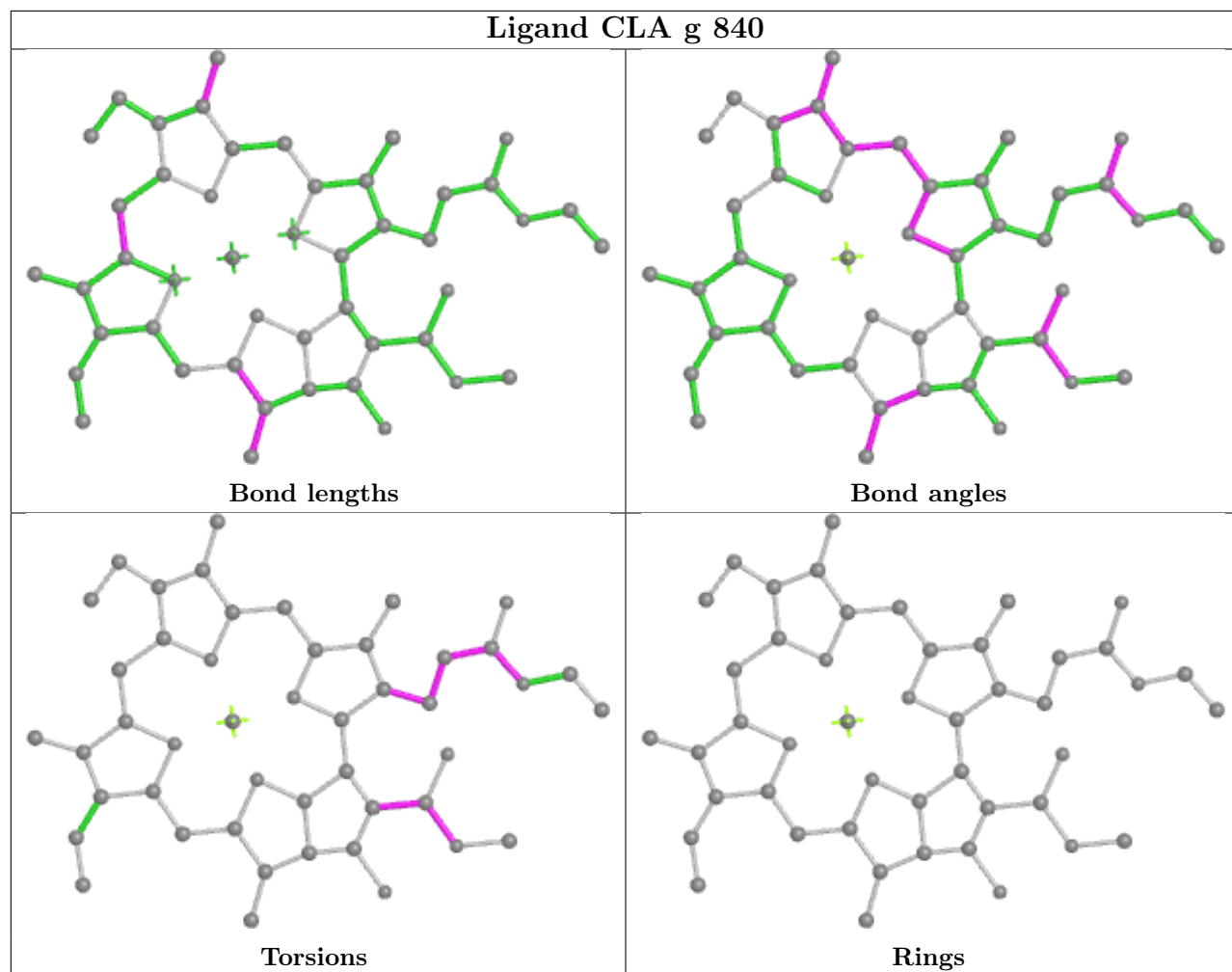
Ligand CLA g 838



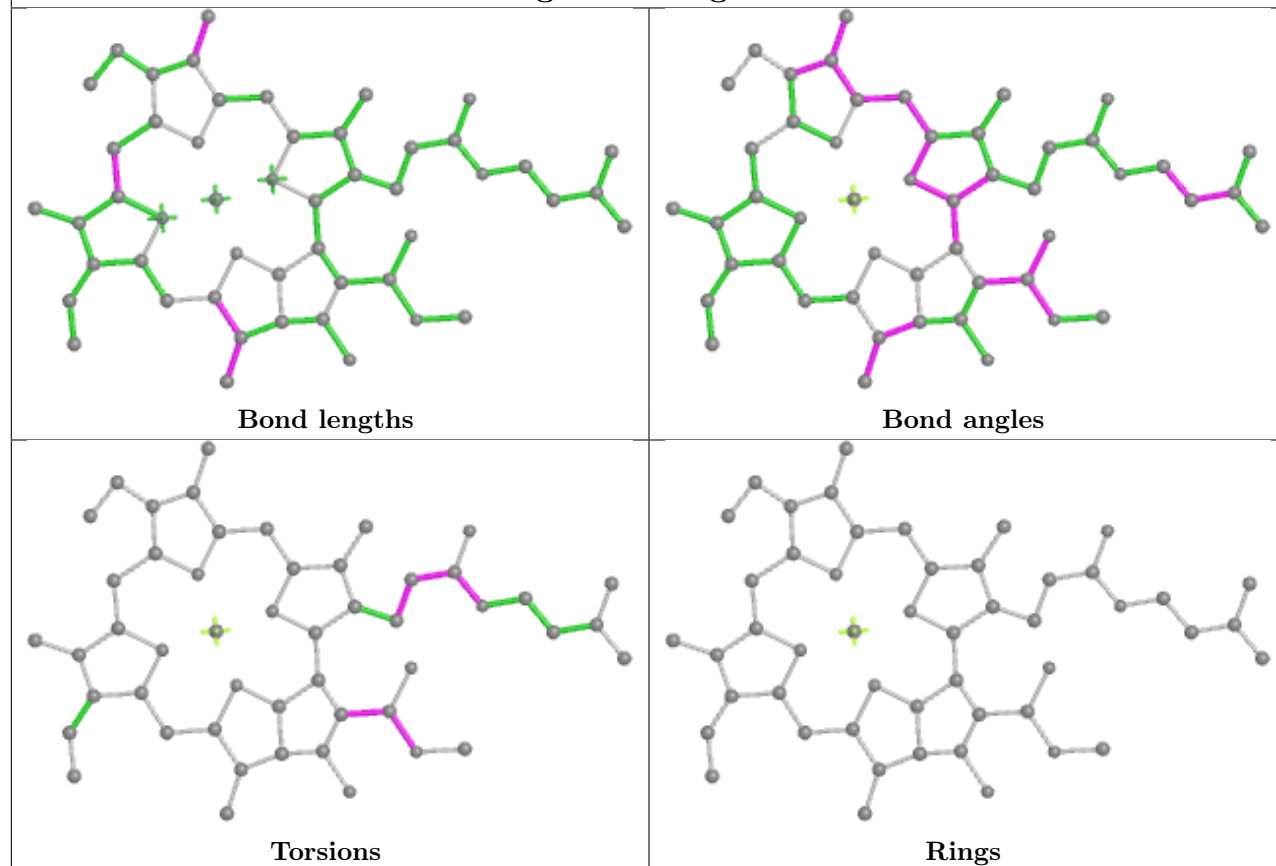
Ligand CLA g 839



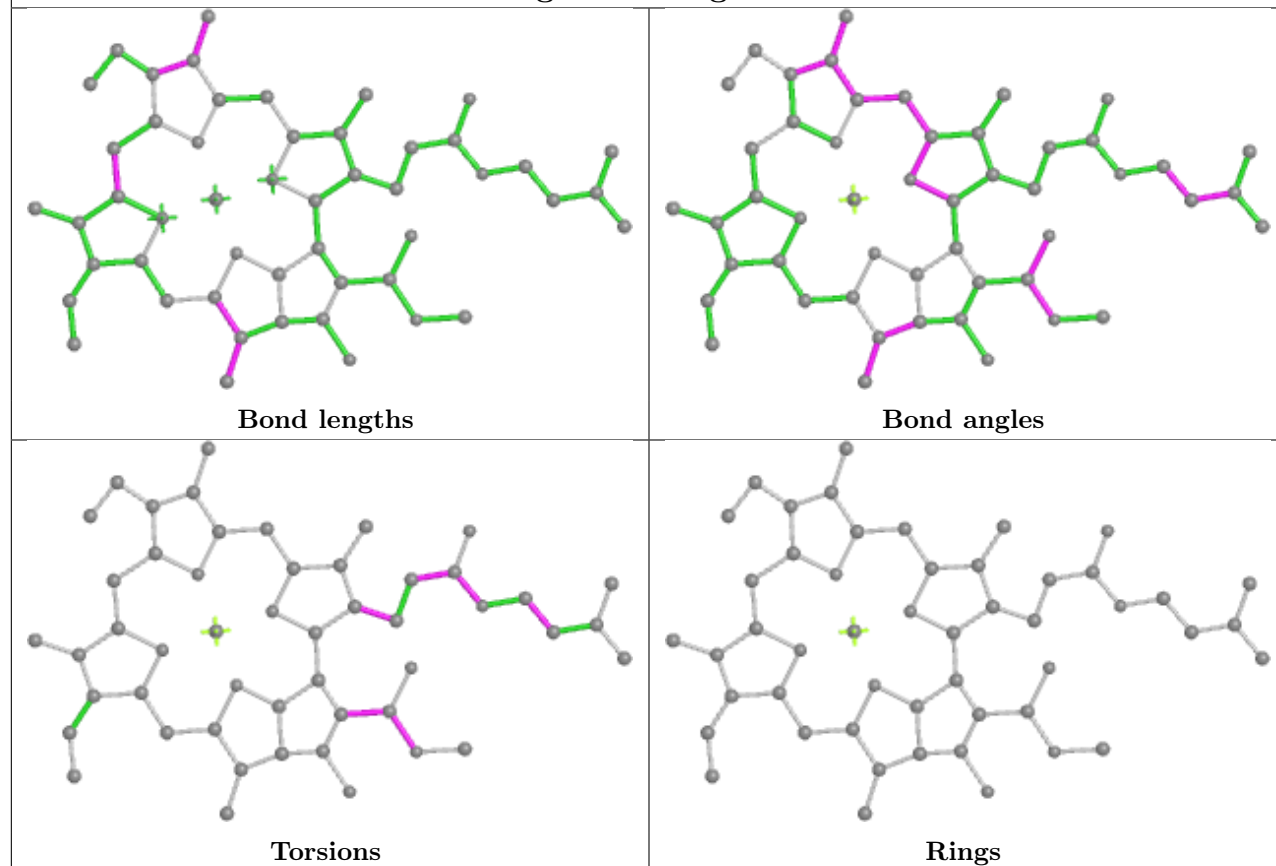
Ligand CLA g 840



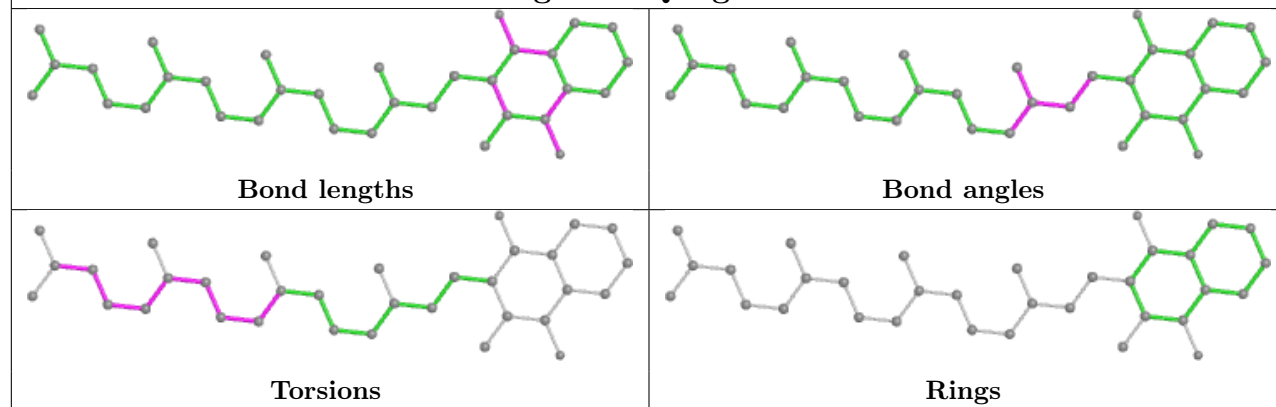
Ligand CLA g 841

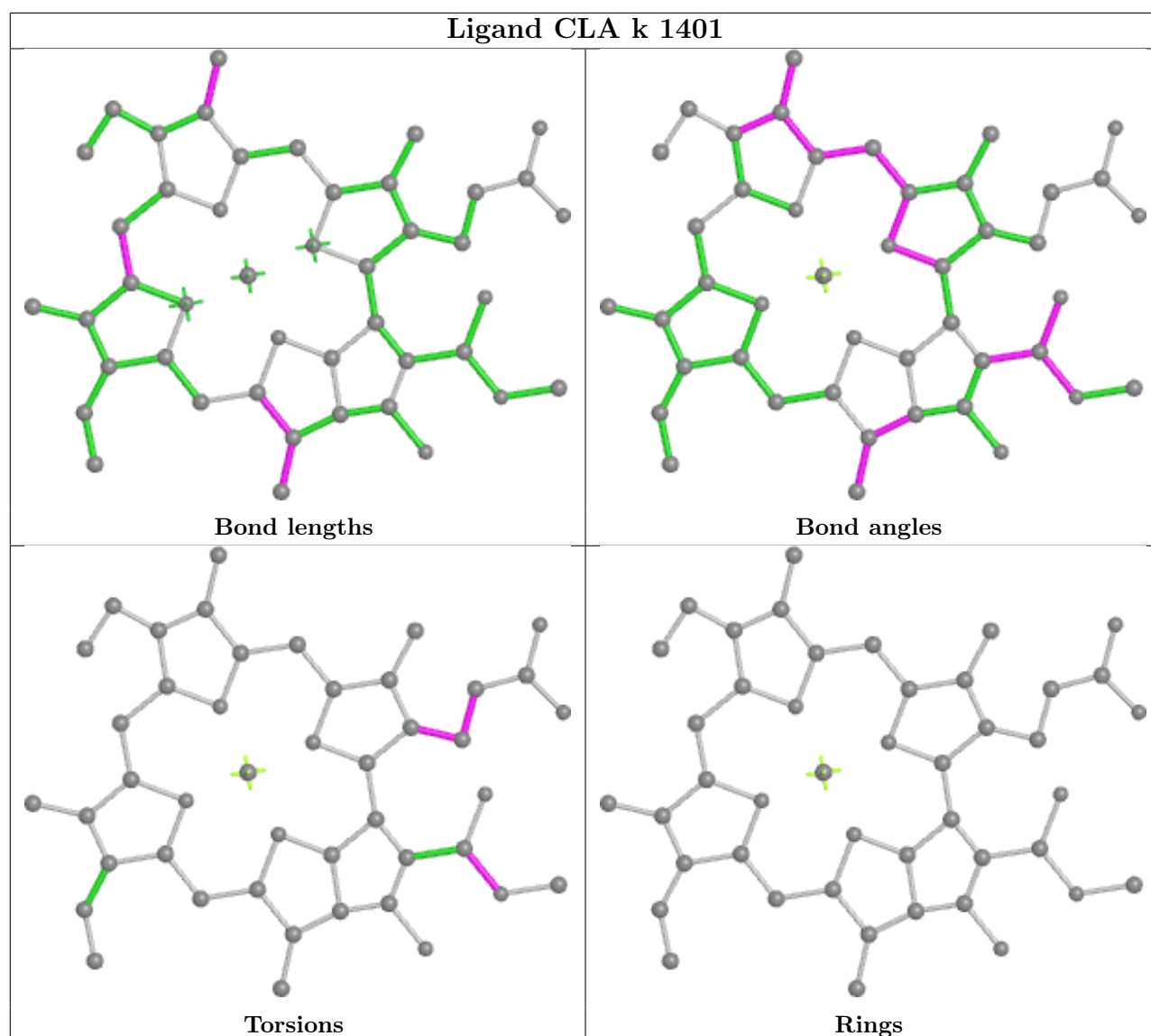


Ligand CLA g 842

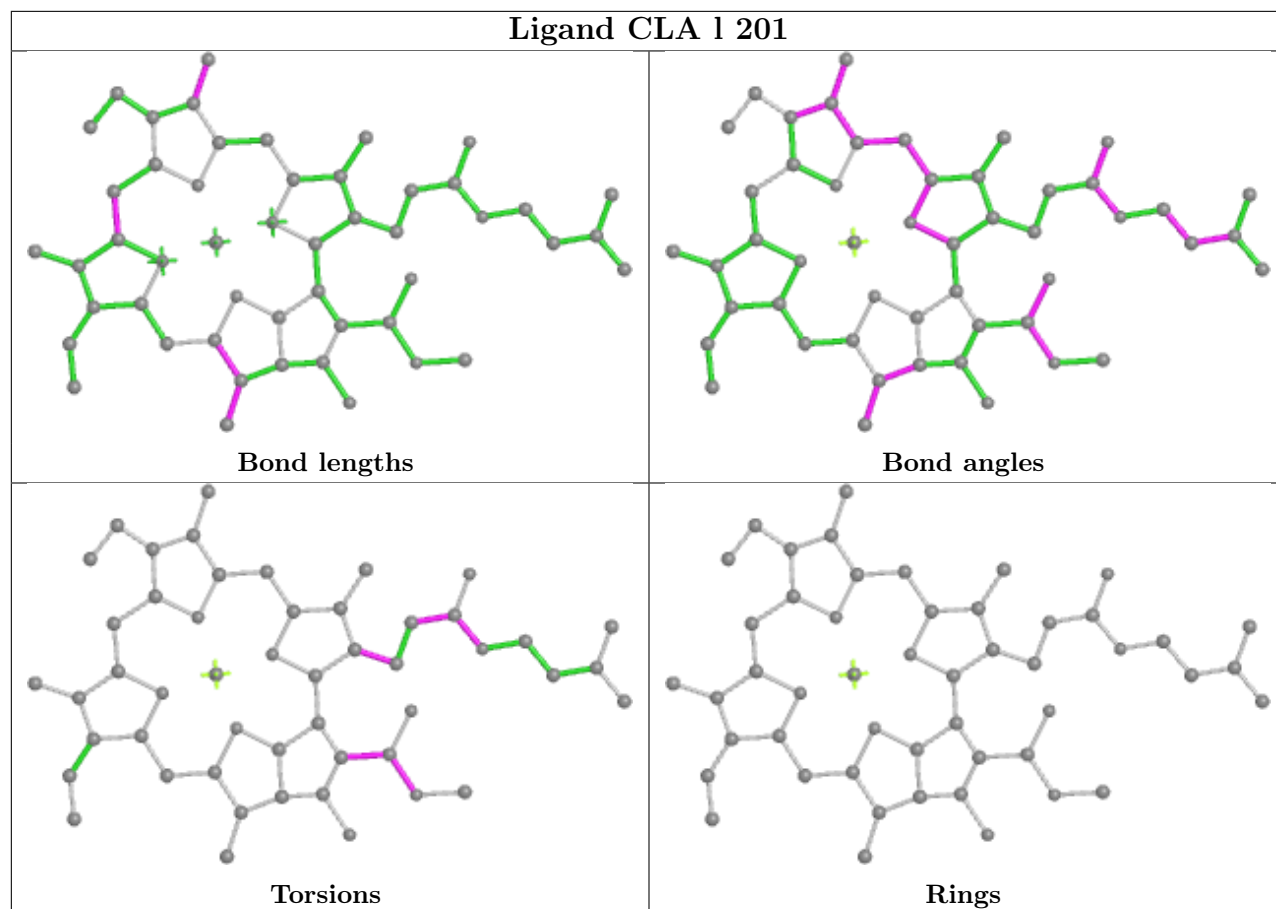


Ligand PQN g 843

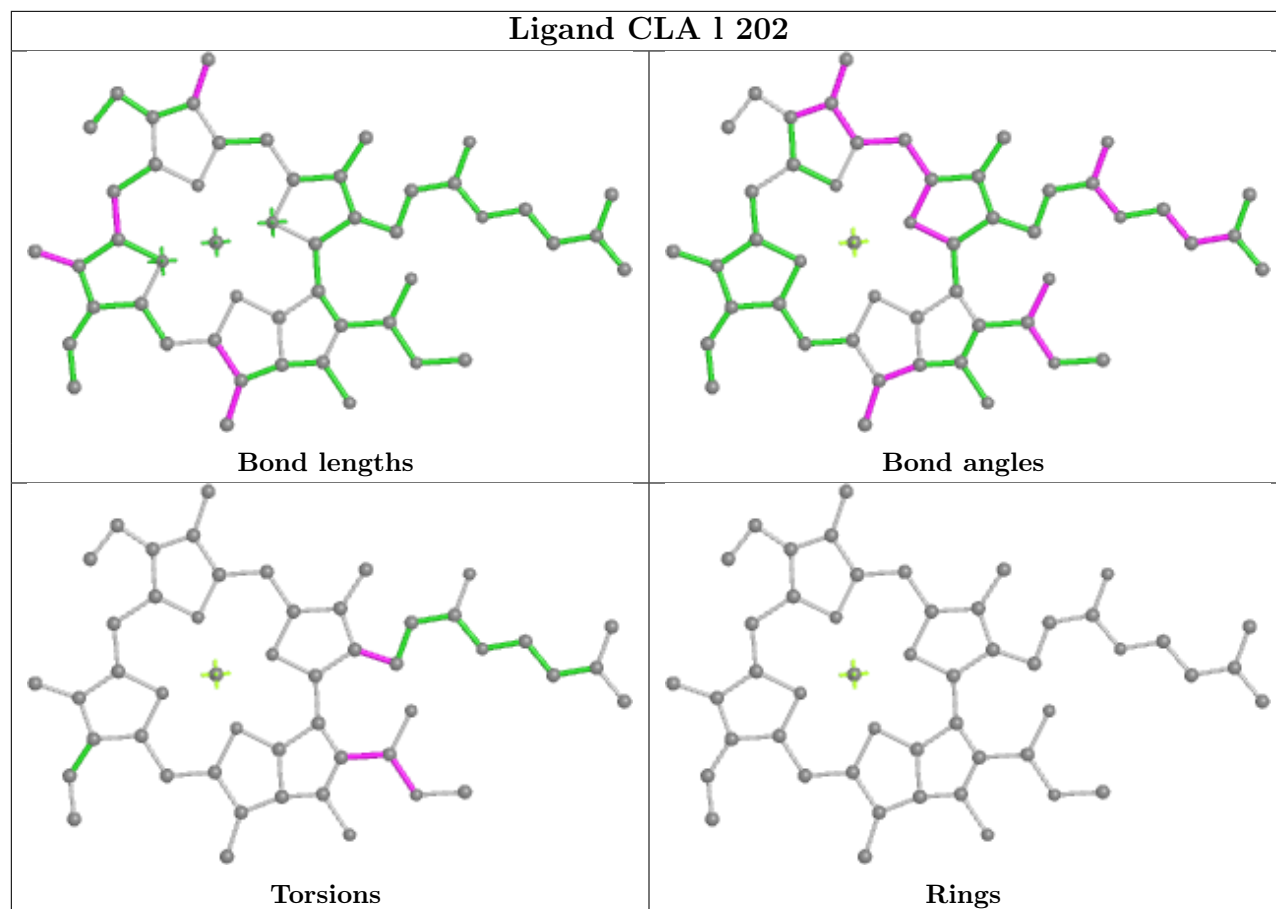




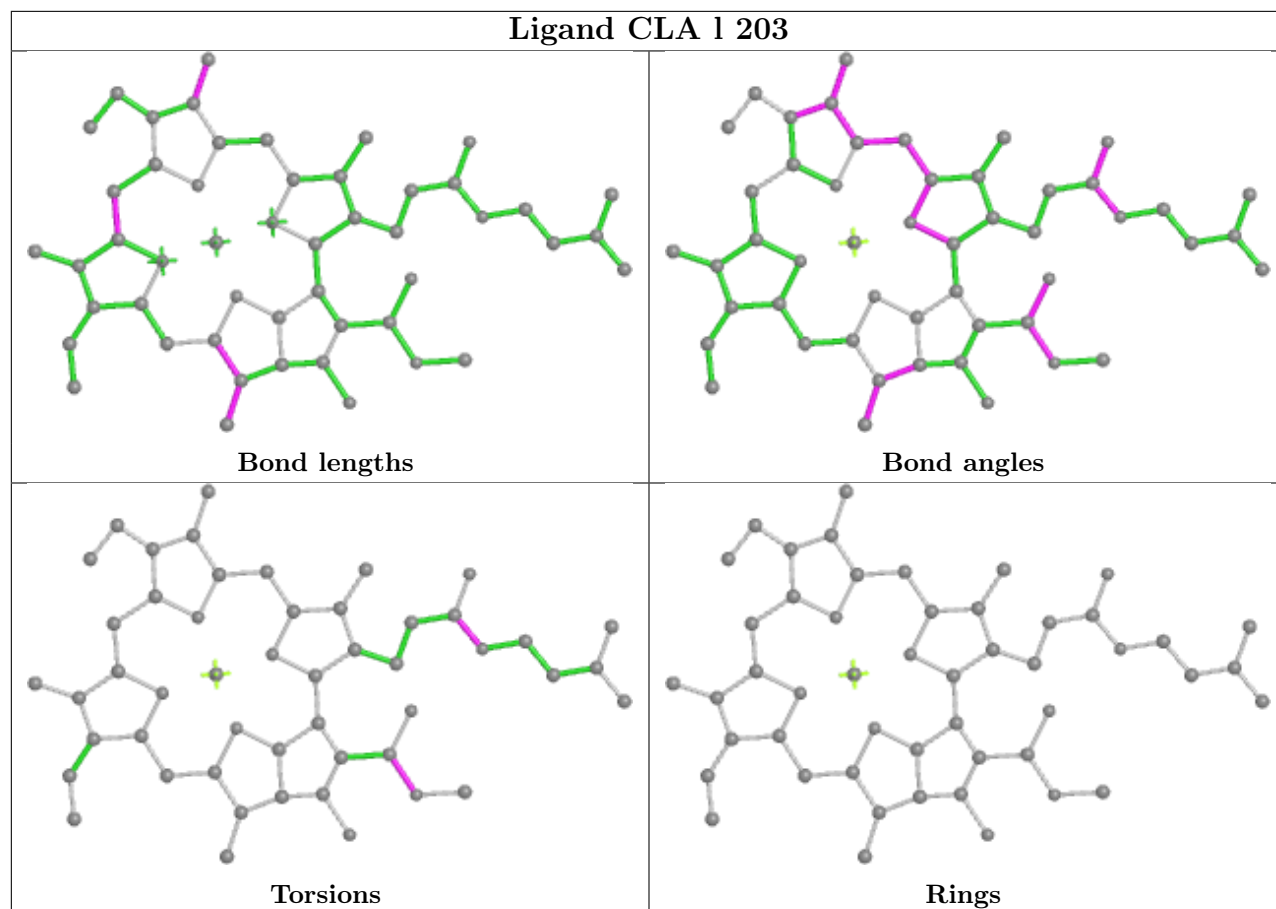
Ligand CLA 1 201



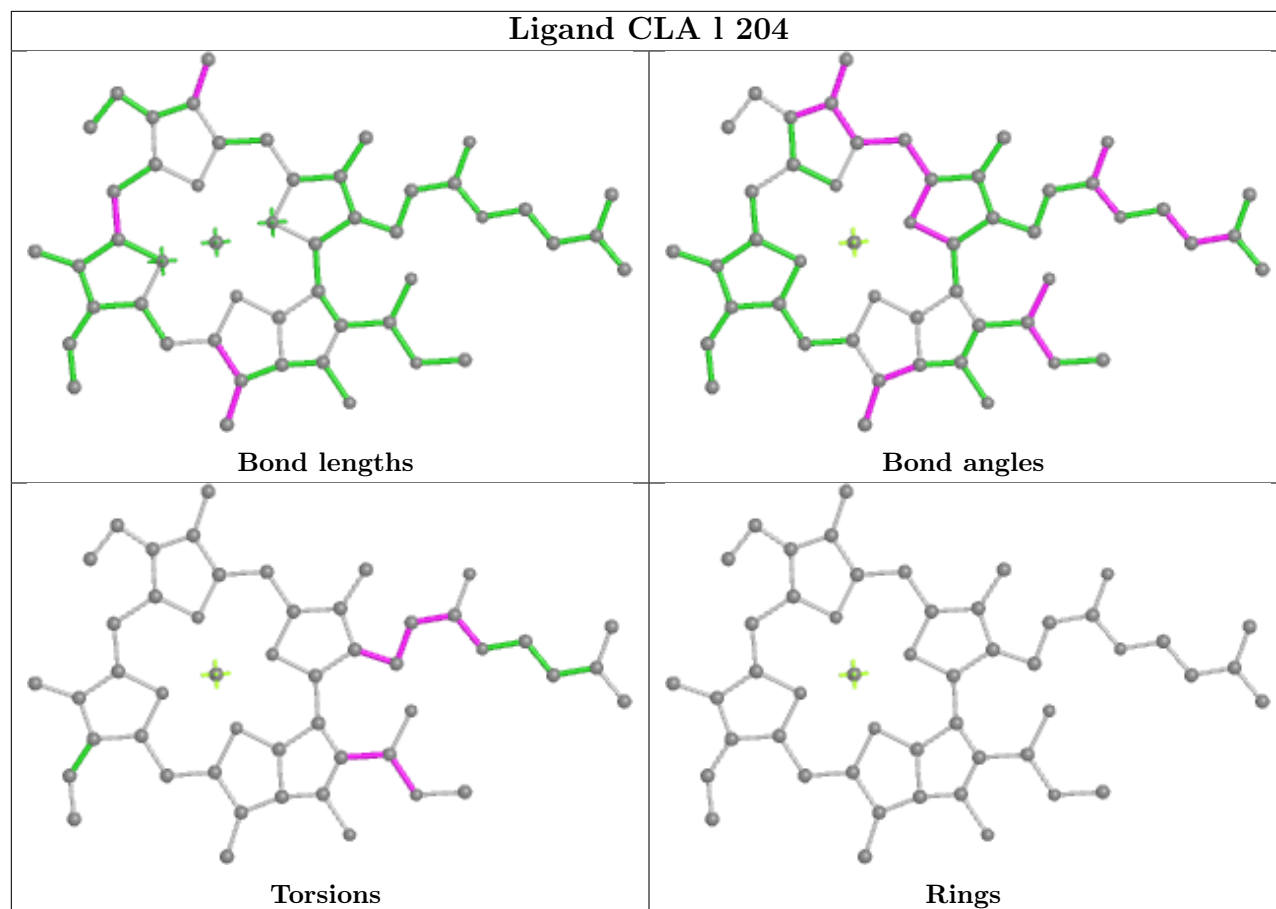
Ligand CLA 1 202

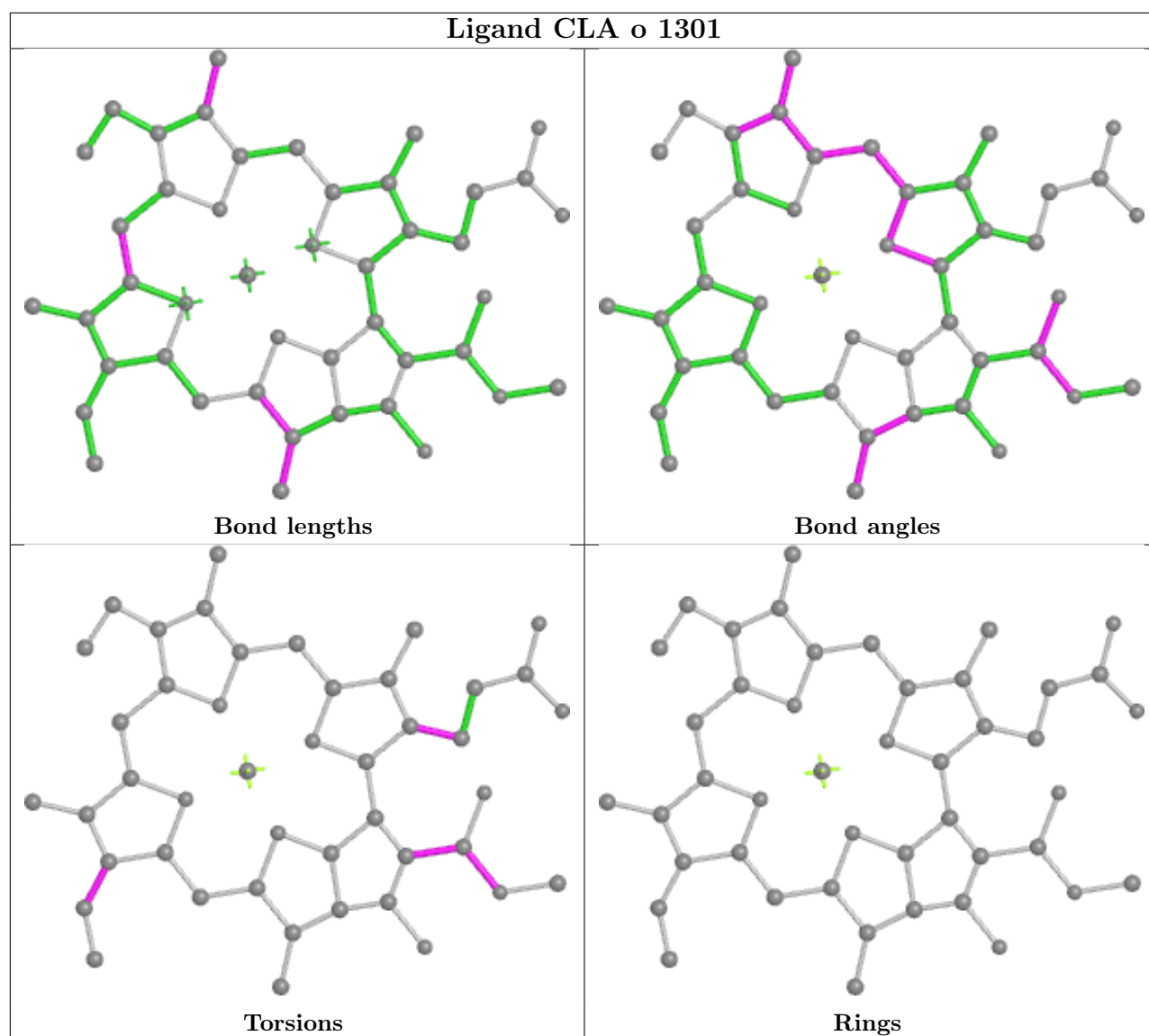


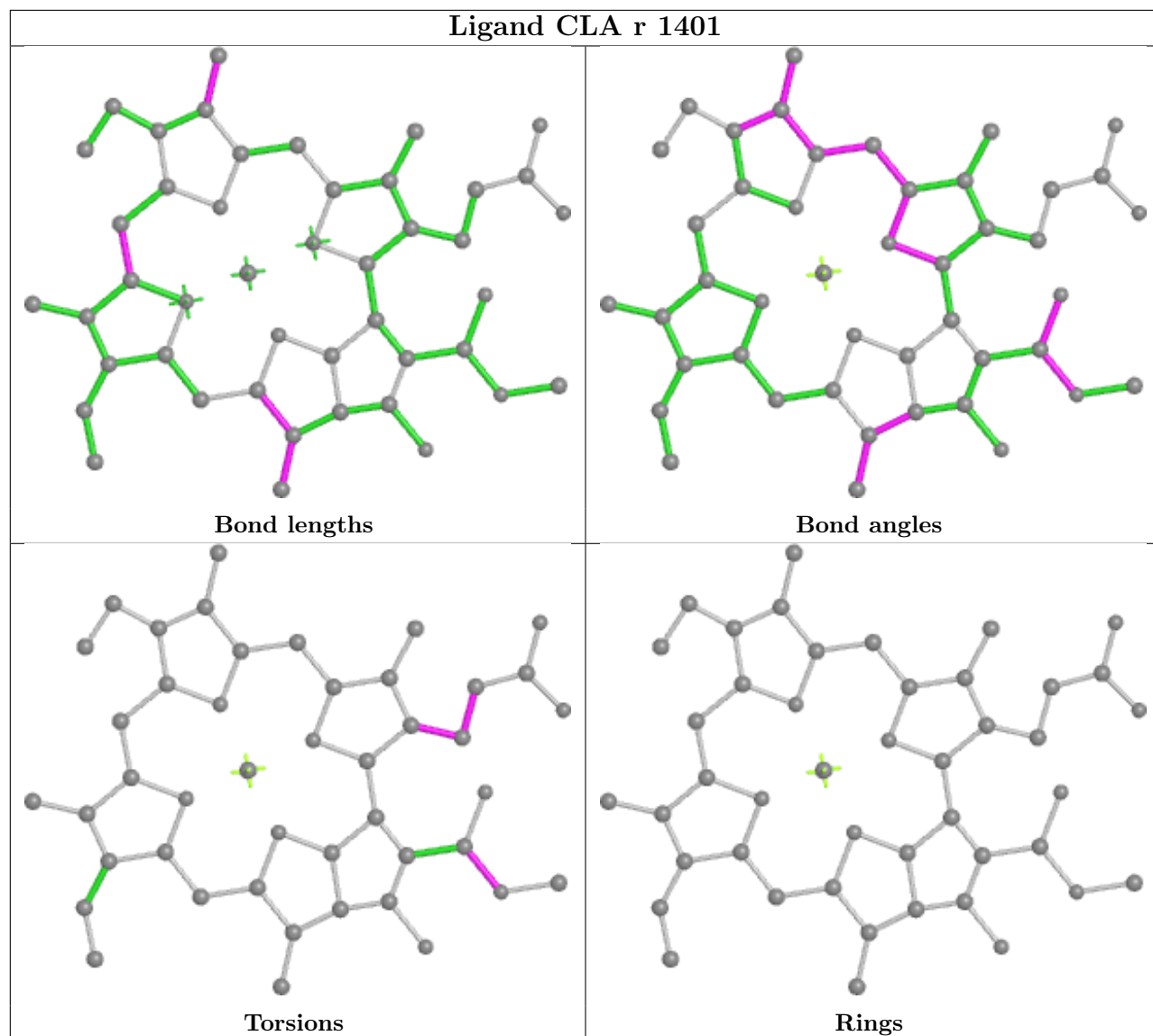
Ligand CLA 1 203



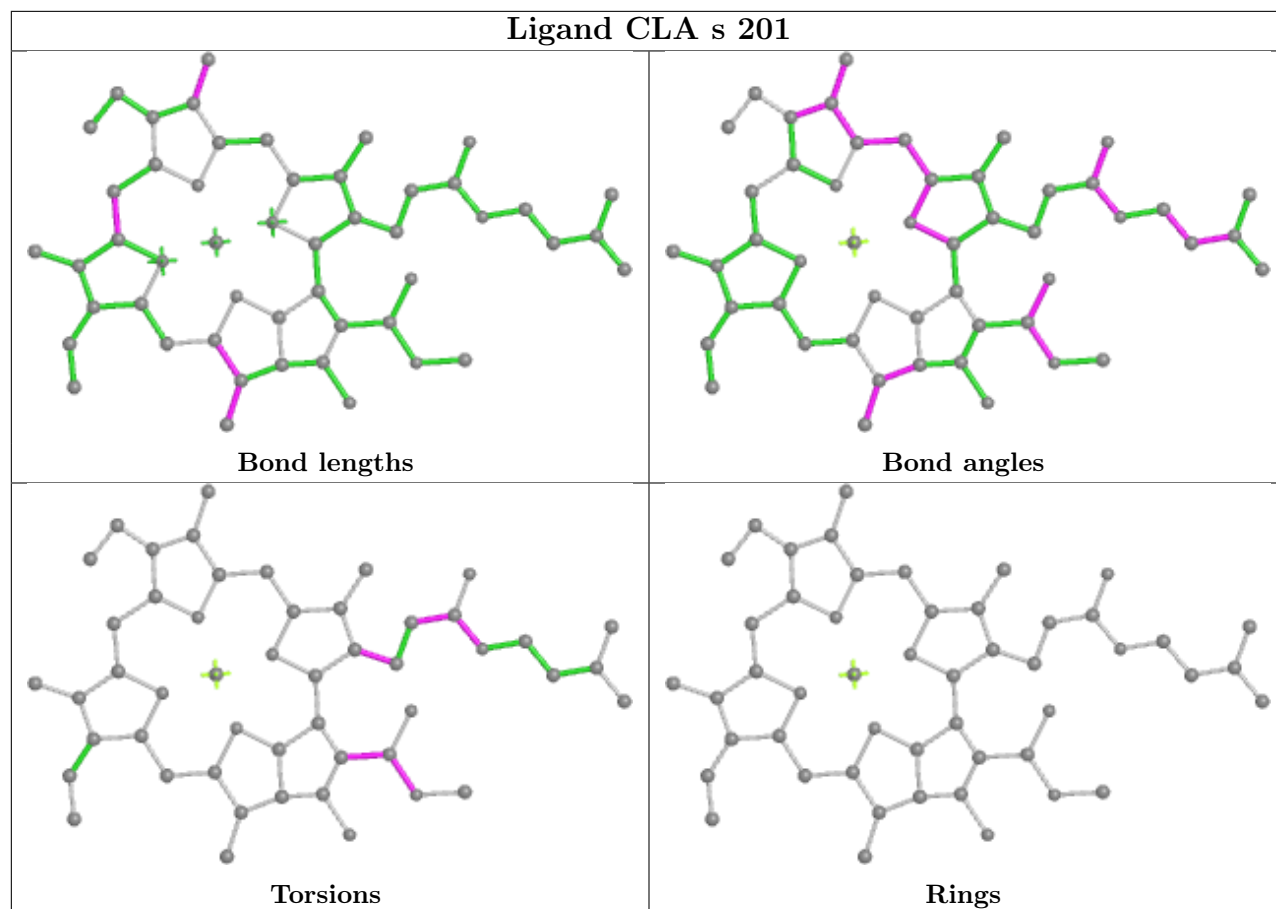
Ligand CLA 1 204



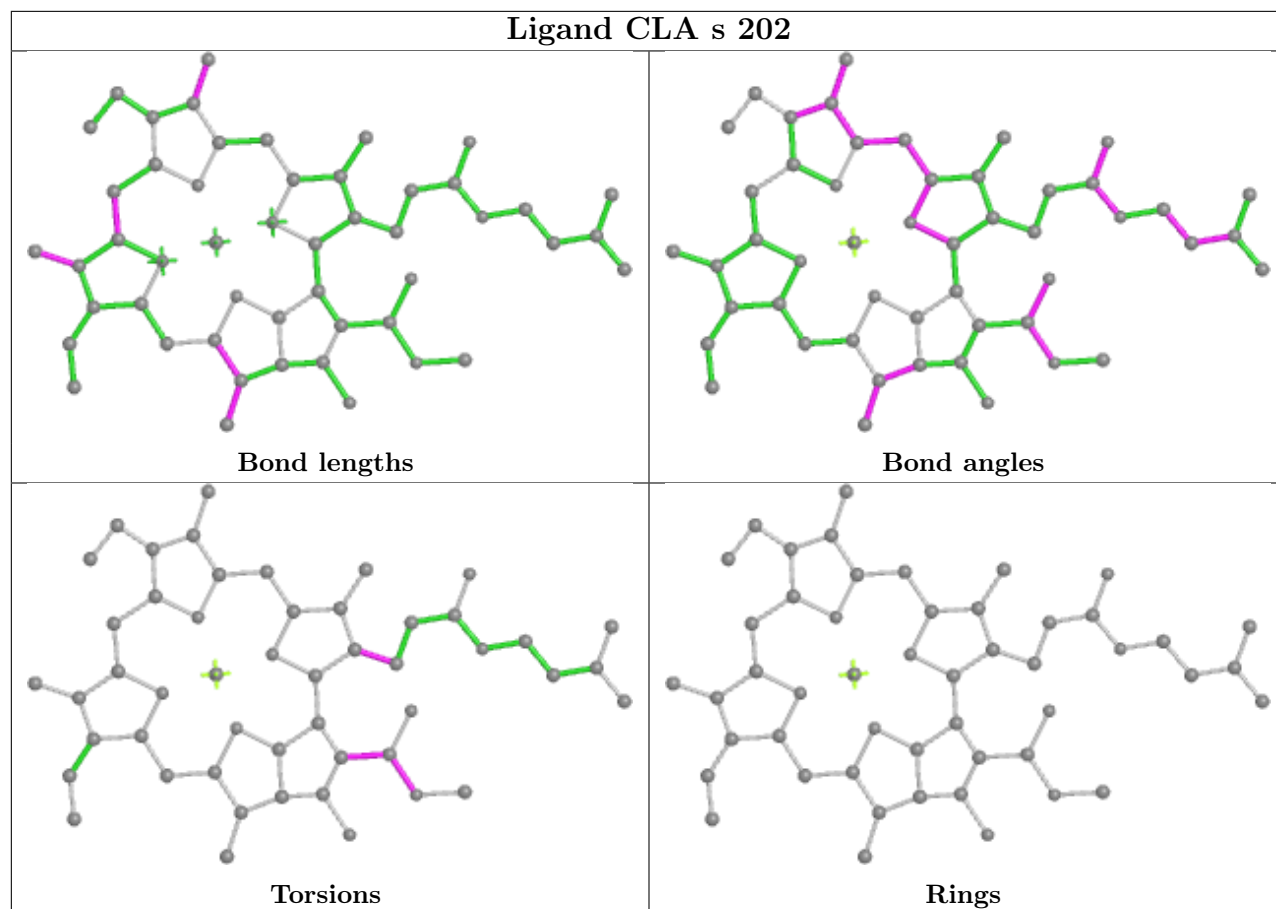




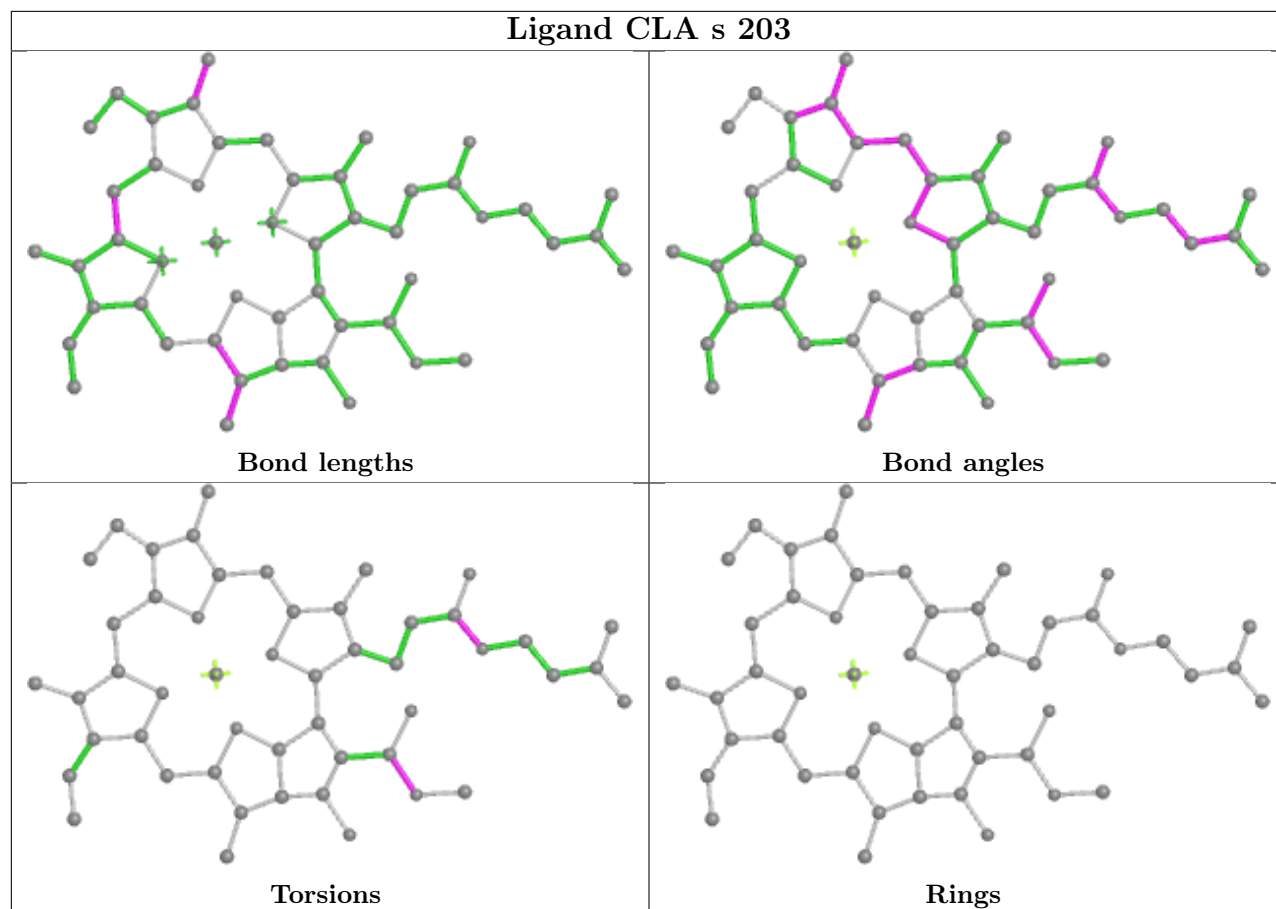
Ligand CLA s 201

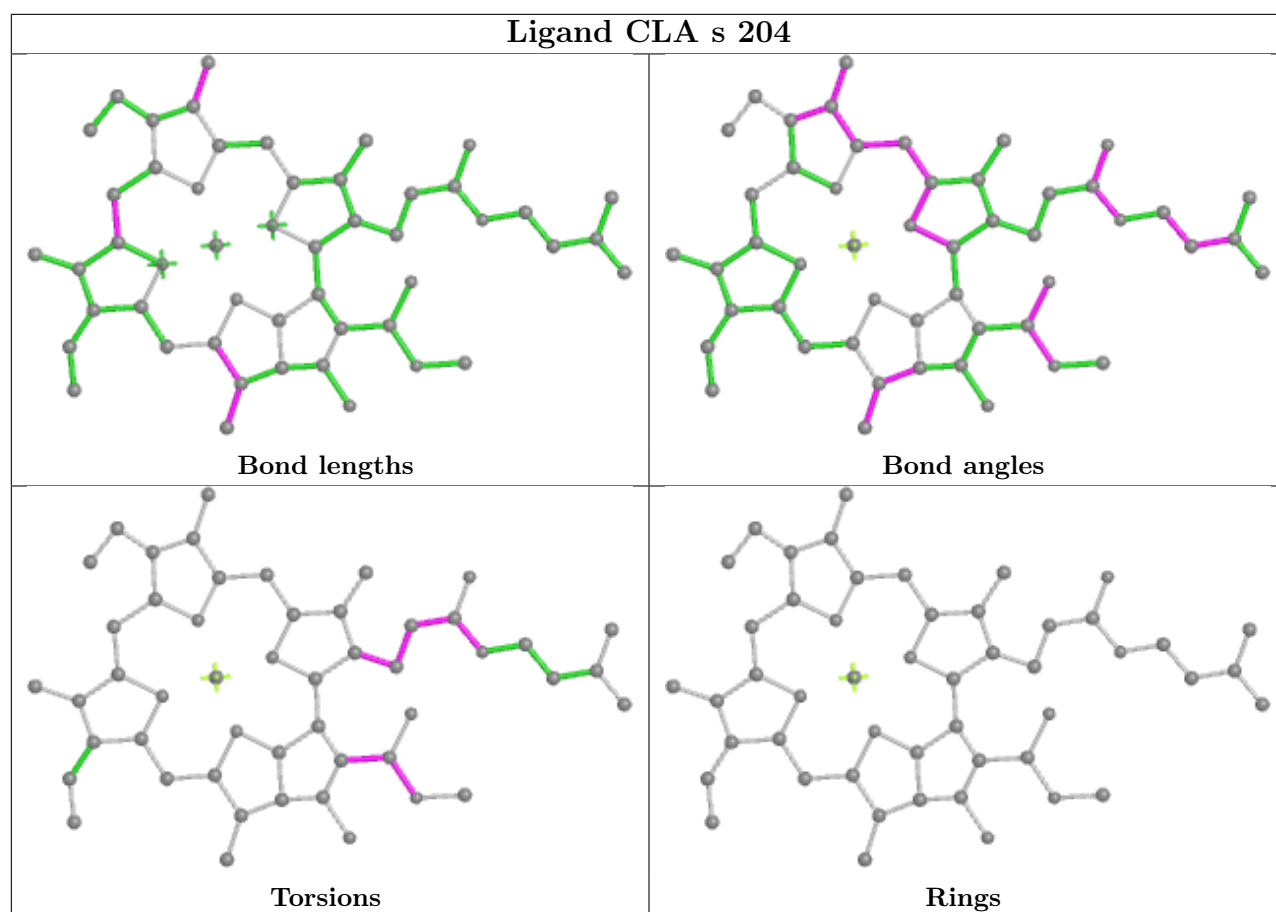


Ligand CLA s 202



Ligand CLA s 203





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.