



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:38 PM UTC

PDB ID : 9I9L / pdb_00009i9l
EMDB ID : EMD-52762
Title : Structure of Far-Red Photosystem I from *C. thermalis* PCC 7203
Authors : Consoli, G.; Tufail, F.; Murray, J.W.; Fantuzzi, A.; Rutherford, A.W.
Deposited on : 2025-02-06
Resolution : 1.89 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

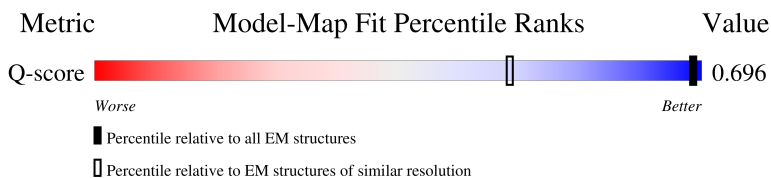
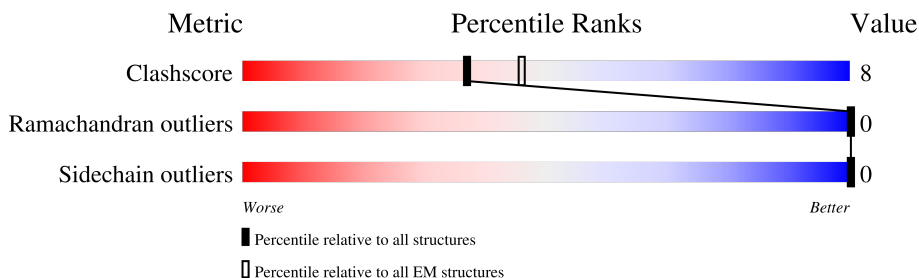
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.89 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.






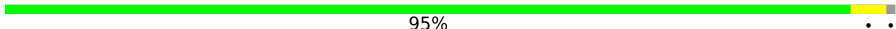





















Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1004 (1.39 - 2.38)

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

Mol	Chain	Length	Quality of chain
1	A	782	 81% 15% .
1	N	782	 84% 12% .
1	a	782	 83% 13% .
2	B	740	 86% 14%





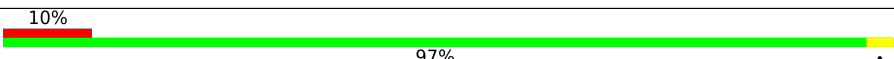
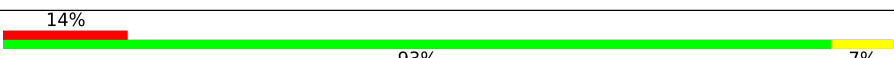
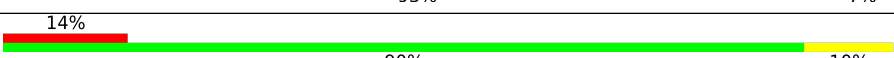
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Mol	Chain	Length	Quality of chain
2	O	740	 88% 12%
2	b	740	 89% 11%
3	C	81	 90% 9% .
3	P	81	 95% . .
3	c	81	 90% 9% .
4	D	142	 87% 11% .
4	Q	142	 84% 14% .
4	d	142	 91% 7% .
5	E	66	 89% 9% .
5	R	66	 89% 9% .
5	e	66	 92% 6% .
6	F	161	 73% 12% 15%
6	S	161	 74% 11% 15%
6	f	161	 75% 10% 15%
7	I	51	 57% 25% 18%
7	T	51	 63% 20% 18%
7	g	51	 65% 18% 18%
8	J	46	 83% 17%
8	U	46	 80% 20%
8	h	46	 85% 15%
9	K	80	 12% 84% 10% 6%
9	V	80	 11% 84% 10% 6%
9	i	80	 10% 80% 14% 6%
10	L	183	 84% 10% 6%
10	W	183	 87% 7% 6%

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Mol	Chain	Length	Quality of chain
10	j	183	
11	M	32	
11	Y	32	
11	k	32	
12	X	29	
12	Z	29	
12	l	29	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
13	CL0	N	801	X	-	-	-
13	CL0	a	801	X	-	-	-
14	F6C	A	802	X	-	-	-
14	F6C	A	824	X	-	-	-
14	F6C	A	826	X	-	-	-
14	F6C	A	856	X	-	-	-
14	F6C	B	832	X	-	-	-
14	F6C	B	839	X	-	-	-
14	F6C	L	201	X	-	-	-
14	F6C	L	204	X	-	-	-
14	F6C	N	802	X	-	-	-
14	F6C	N	824	X	-	-	-
14	F6C	N	826	X	-	-	-
14	F6C	N	856	X	-	-	-
14	F6C	O	832	X	-	-	-
14	F6C	O	839	X	-	-	-
14	F6C	W	201	X	-	-	-
14	F6C	W	204	X	-	-	-
14	F6C	a	802	X	-	-	-
14	F6C	a	824	X	-	-	-
14	F6C	a	826	X	-	-	-
14	F6C	a	855	X	-	-	-
14	F6C	b	832	X	-	-	-
14	F6C	b	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	F6C	j	201	X	-	-	-
14	F6C	j	204	X	-	-	-
15	CLA	A	803	X	-	-	-
15	CLA	A	804	X	-	-	-
15	CLA	A	805	X	-	-	-
15	CLA	A	806	X	-	-	-
15	CLA	A	807	X	-	-	-
15	CLA	A	808	X	-	-	-
15	CLA	A	809	X	-	-	-
15	CLA	A	810	X	-	-	-
15	CLA	A	811	X	-	-	-
15	CLA	A	812	X	-	-	-
15	CLA	A	813	X	-	-	-
15	CLA	A	814	X	-	-	-
15	CLA	A	815	X	-	-	-
15	CLA	A	816	X	-	-	-
15	CLA	A	817	X	-	-	-
15	CLA	A	818	X	-	-	-
15	CLA	A	819	X	-	-	-
15	CLA	A	820	X	-	-	-
15	CLA	A	821	X	-	-	-
15	CLA	A	822	X	-	-	-
15	CLA	A	823	X	-	-	-
15	CLA	A	825	X	-	-	-
15	CLA	A	827	X	-	-	-
15	CLA	A	828	X	-	-	-
15	CLA	A	829	X	-	-	-
15	CLA	A	830	X	-	-	-
15	CLA	A	831	X	-	-	-
15	CLA	A	832	X	-	-	-
15	CLA	A	833	X	-	-	-
15	CLA	A	834	X	-	-	-
15	CLA	A	835	X	-	-	-
15	CLA	A	836	X	-	-	-
15	CLA	A	837	X	-	-	-
15	CLA	A	838	X	-	-	-
15	CLA	A	839	X	-	-	-
15	CLA	A	840	X	-	-	-
15	CLA	A	841	X	-	-	-
15	CLA	A	842	X	-	-	-
15	CLA	B	801	X	-	-	-
15	CLA	B	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	803	X	-	-	-
15	CLA	B	804	X	-	-	-
15	CLA	B	805	X	-	-	-
15	CLA	B	806	X	-	-	-
15	CLA	B	807	X	-	-	-
15	CLA	B	808	X	-	-	-
15	CLA	B	809	X	-	-	-
15	CLA	B	810	X	-	-	-
15	CLA	B	811	X	-	-	-
15	CLA	B	813	X	-	-	-
15	CLA	B	814	X	-	-	-
15	CLA	B	815	X	-	-	-
15	CLA	B	816	X	-	-	-
15	CLA	B	817	X	-	-	-
15	CLA	B	818	X	-	-	-
15	CLA	B	819	X	-	-	-
15	CLA	B	820	X	-	-	-
15	CLA	B	821	X	-	-	-
15	CLA	B	822	X	-	-	-
15	CLA	B	823	X	-	-	-
15	CLA	B	824	X	-	-	-
15	CLA	B	825	X	-	-	-
15	CLA	B	826	X	-	-	-
15	CLA	B	827	X	-	-	-
15	CLA	B	828	X	-	-	-
15	CLA	B	829	X	-	-	-
15	CLA	B	830	X	-	-	-
15	CLA	B	831	X	-	-	-
15	CLA	B	833	X	-	-	-
15	CLA	B	834	X	-	-	-
15	CLA	B	835	X	-	-	-
15	CLA	B	836	X	-	-	-
15	CLA	B	837	X	-	-	-
15	CLA	B	838	X	-	-	-
15	CLA	B	840	X	-	-	-
15	CLA	F	201	X	-	-	-
15	CLA	K	102	X	-	-	-
15	CLA	K	103	X	-	-	-
15	CLA	L	202	X	-	-	-
15	CLA	L	203	X	-	-	-
15	CLA	N	803	X	-	-	-
15	CLA	N	804	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	O	807	X	-	-	-
15	CLA	O	808	X	-	-	-
15	CLA	O	809	X	-	-	-
15	CLA	O	810	X	-	-	-
15	CLA	O	811	X	-	-	-
15	CLA	O	813	X	-	-	-
15	CLA	O	814	X	-	-	-
15	CLA	O	815	X	-	-	-
15	CLA	O	816	X	-	-	-
15	CLA	O	817	X	-	-	-
15	CLA	O	818	X	-	-	-
15	CLA	O	819	X	-	-	-
15	CLA	O	820	X	-	-	-
15	CLA	O	821	X	-	-	-
15	CLA	O	822	X	-	-	-
15	CLA	O	823	X	-	-	-
15	CLA	O	824	X	-	-	-
15	CLA	O	825	X	-	-	-
15	CLA	O	826	X	-	-	-
15	CLA	O	827	X	-	-	-
15	CLA	O	828	X	-	-	-
15	CLA	O	829	X	-	-	-
15	CLA	O	830	X	-	-	-
15	CLA	O	831	X	-	-	-
15	CLA	O	833	X	-	-	-
15	CLA	O	834	X	-	-	-
15	CLA	O	835	X	-	-	-
15	CLA	O	836	X	-	-	-
15	CLA	O	837	X	-	-	-
15	CLA	O	838	X	-	-	-
15	CLA	O	840	X	-	-	-
15	CLA	S	201	X	-	-	-
15	CLA	V	102	X	-	-	-
15	CLA	V	103	X	-	-	-
15	CLA	W	202	X	-	-	-
15	CLA	W	203	X	-	-	-
15	CLA	X	102	X	-	-	-
15	CLA	Z	102	X	-	-	-
15	CLA	a	803	X	-	-	-
15	CLA	a	804	X	-	-	-
15	CLA	a	805	X	-	-	-
15	CLA	a	806	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	b	809	X	-	-	-
15	CLA	b	810	X	-	-	-
15	CLA	b	811	X	-	-	-
15	CLA	b	813	X	-	-	-
15	CLA	b	814	X	-	-	-
15	CLA	b	815	X	-	-	-
15	CLA	b	816	X	-	-	-
15	CLA	b	817	X	-	-	-
15	CLA	b	818	X	-	-	-
15	CLA	b	819	X	-	-	-
15	CLA	b	820	X	-	-	-
15	CLA	b	821	X	-	-	-
15	CLA	b	822	X	-	-	-
15	CLA	b	823	X	-	-	-
15	CLA	b	824	X	-	-	-
15	CLA	b	825	X	-	-	-
15	CLA	b	826	X	-	-	-
15	CLA	b	827	X	-	-	-
15	CLA	b	828	X	-	-	-
15	CLA	b	829	X	-	-	-
15	CLA	b	830	X	-	-	-
15	CLA	b	831	X	-	-	-
15	CLA	b	833	X	-	-	-
15	CLA	b	834	X	-	-	-
15	CLA	b	835	X	-	-	-
15	CLA	b	836	X	-	-	-
15	CLA	b	837	X	-	-	-
15	CLA	b	838	X	-	-	-
15	CLA	b	840	X	-	-	-
15	CLA	f	201	X	-	-	-
15	CLA	i	102	X	-	-	-
15	CLA	i	103	X	-	-	-
15	CLA	j	202	X	-	-	-
15	CLA	j	203	X	-	-	-
15	CLA	l	102	X	-	-	-

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 75954 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	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		
1	N	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		
1	a	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		
2	O	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		
2	b	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	368	103	118	11		
3	P	80	Total	C	N	O	S	0	0
			600	368	103	118	11		
3	c	80	Total	C	N	O	S	0	0
			600	368	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		
4	d	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	65	Total	C	N	O		0	0
			530	341	92	97			
5	R	65	Total	C	N	O		0	0
			530	341	92	97			
5	e	65	Total	C	N	O		0	0
			530	341	92	97			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		
6	S	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		
6	f	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	42	Total	C	N	O	S	0	0
			351	247	47	55	2		
7	T	42	Total	C	N	O	S	0	0
			351	247	47	55	2		
7	g	42	Total	C	N	O	S	0	0
			351	247	47	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	46	Total	C	N	O	S	0	0
			373	256	54	59	4		
8	U	46	Total	C	N	O	S	0	0
			373	256	54	59	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	46	Total	C	N	O	S	0	0
			373	256	54	59	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	75	Total	C	N	O	S	0	0
			539	356	88	94	1		
9	V	75	Total	C	N	O	S	0	0
			539	356	88	94	1		
9	i	75	Total	C	N	O	S	0	0
			539	356	88	94	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	12	MET	-	initiating methionine	UNP K9TX25
V	12	MET	-	initiating methionine	UNP K9TX25
i	12	MET	-	initiating methionine	UNP K9TX25

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		
10	W	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		
10	j	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		

- 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
			240	160	37	42	1		
11	Y	31	Total	C	N	O	S	0	0
			240	160	37	42	1		
11	k	31	Total	C	N	O	S	0	0
			240	160	37	42	1		

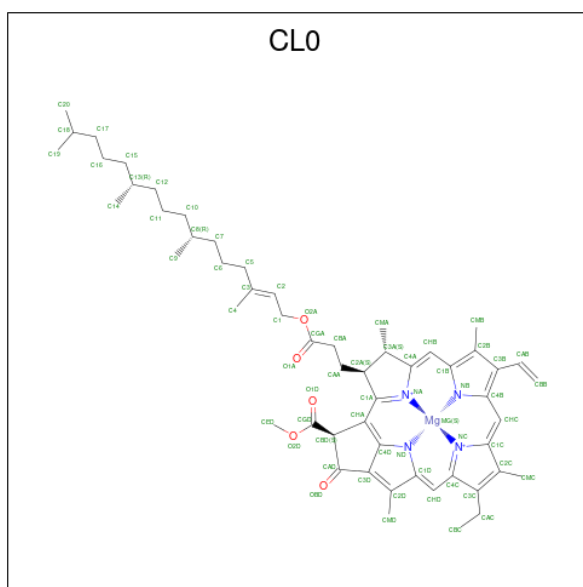
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	initiating methionine	UNP K9TSY6
Y	0	MET	-	initiating methionine	UNP K9TSY6
k	0	MET	-	initiating methionine	UNP K9TSY6

- Molecule 12 is a protein called Photosystem one Psax.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	29	Total	C	N	O	0	0
			227	157	36	34		
12	Z	29	Total	C	N	O	0	0
			227	157	36	34		
12	l	29	Total	C	N	O	0	0
			227	157	36	34		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 14 is Chlorophyll F (CCD ID: F6C) (formula: $C_{55}H_{68}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).

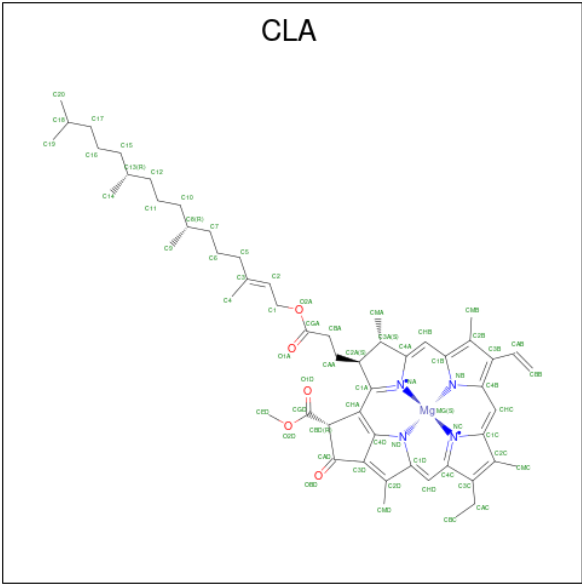


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Mol	Chain	Residues	Atoms					AltConf
14	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 62	C 52	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	N	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	N	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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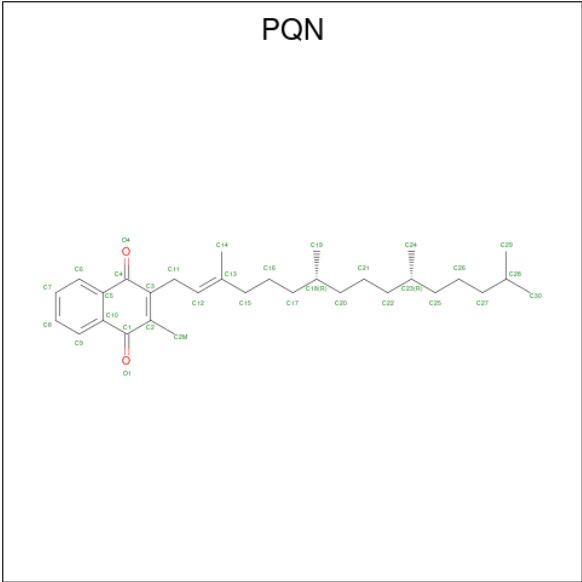
Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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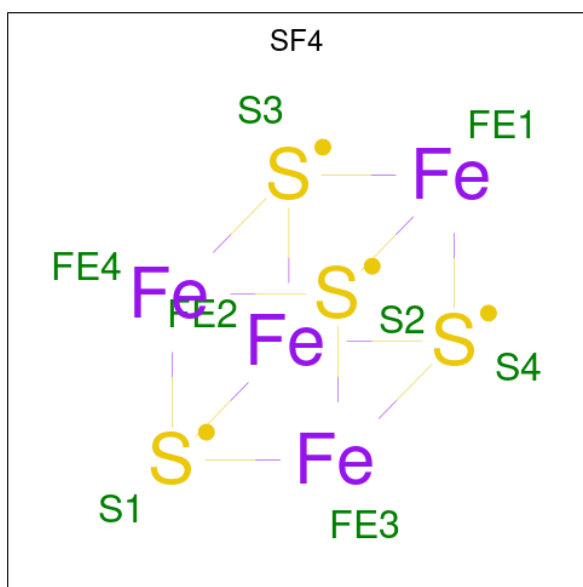
Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	i	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	i	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	j	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	l	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



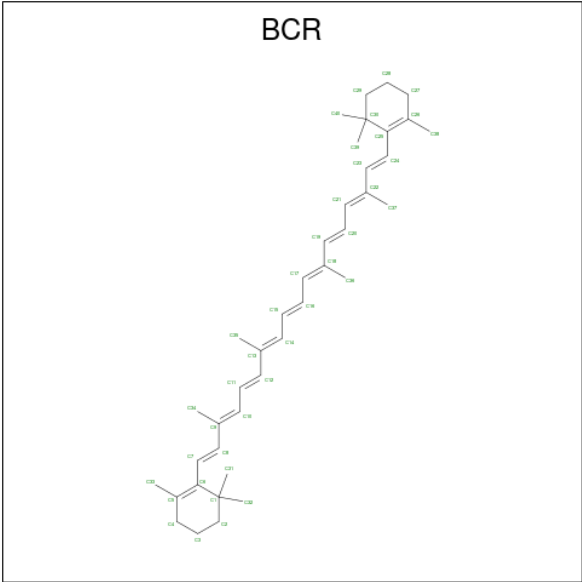
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			33	31	2	
16	B	1	Total	C	O	0
			33	31	2	
16	N	1	Total	C	O	0
			33	31	2	
16	O	1	Total	C	O	0
			33	31	2	
16	a	1	Total	C	O	0
			33	31	2	
16	b	1	Total	C	O	0
			33	31	2	

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	F	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	I	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	K	1	Total C 25 25	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	M	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0

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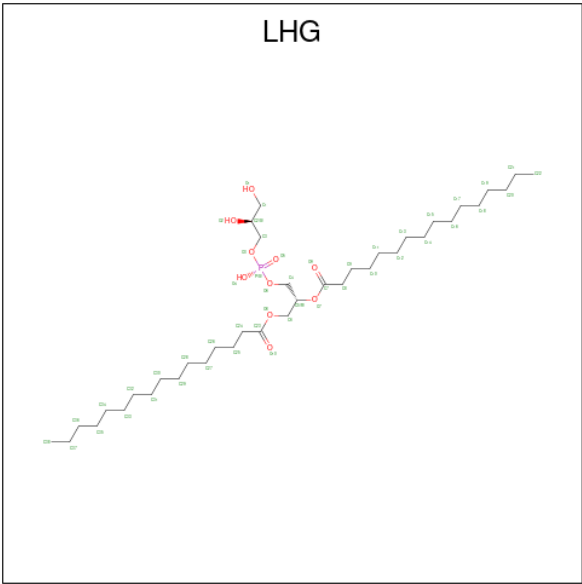
Mol	Chain	Residues	Atoms	AltConf
18	O	1	Total C 40 40	0
18	S	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 25 25	0
18	W	1	Total C 40 40	0
18	W	1	Total C 40 40	0
18	Y	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
18	b	1	Total	C	0
			40	40	
18	b	1	Total	C	0
			40	40	
18	f	1	Total	C	0
			40	40	
18	g	1	Total	C	0
			40	40	
18	g	1	Total	C	0
			40	40	
18	h	1	Total	C	0
			40	40	
18	h	1	Total	C	0
			40	40	
18	i	1	Total	C	0
			25	25	
18	j	1	Total	C	0
			40	40	
18	k	1	Total	C	0
			40	40	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



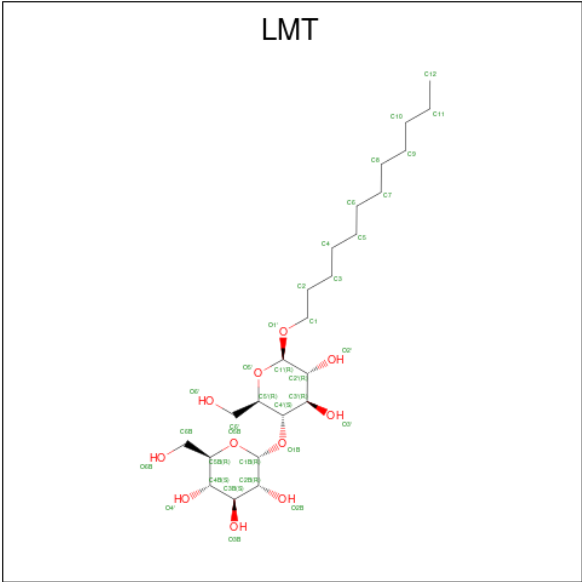
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			42	31	10	1	

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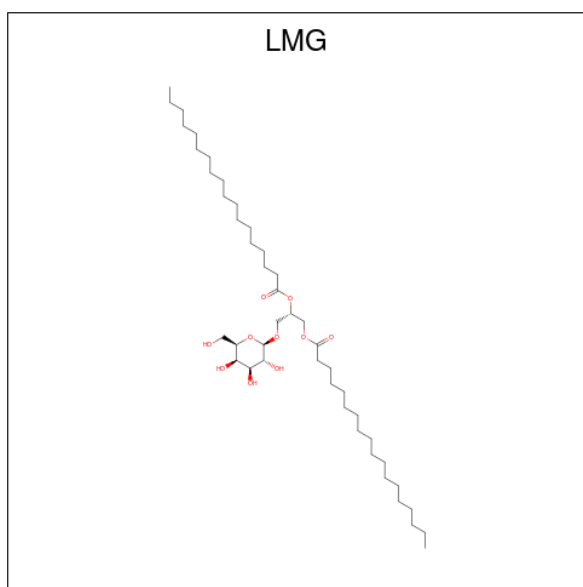
Mol	Chain	Residues	Atoms				AltConf
19	B	1	Total	C	O	P	0
			49	38	10	1	
19	F	1	Total	C	O	P	0
			49	38	10	1	
19	L	1	Total	C	O	P	0
			49	38	10	1	
19	X	1	Total	C	O	P	0
			44	33	10	1	
19	N	1	Total	C	O	P	0
			42	31	10	1	
19	N	1	Total	C	O	P	0
			49	38	10	1	
19	W	1	Total	C	O	P	0
			49	38	10	1	
19	Y	1	Total	C	O	P	0
			49	38	10	1	
19	Z	1	Total	C	O	P	0
			44	33	10	1	
19	a	1	Total	C	O	P	0
			42	31	10	1	
19	f	1	Total	C	O	P	0
			49	38	10	1	
19	j	1	Total	C	O	P	0
			49	38	10	1	
19	k	1	Total	C	O	P	0
			49	38	10	1	
19	l	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 20 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			31	20	11	
20	A	1	Total	C	O	0
			28	17	11	
20	A	1	Total	C	O	0
			35	24	11	
20	N	1	Total	C	O	0
			31	20	11	
20	N	1	Total	C	O	0
			28	17	11	
20	N	1	Total	C	O	0
			35	24	11	
20	a	1	Total	C	O	0
			31	20	11	
20	a	1	Total	C	O	0
			28	17	11	
20	a	1	Total	C	O	0
			35	24	11	

- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



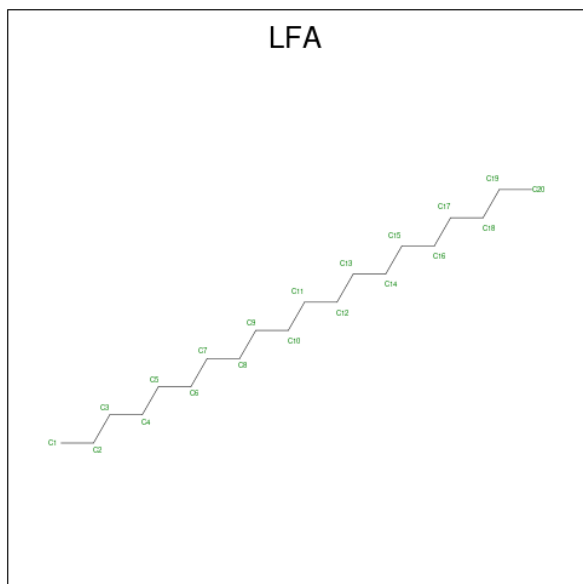
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			44	34	10	
21	B	1	Total	C	O	0
			55	45	10	
21	B	1	Total	C	O	0
			44	34	10	
21	I	1	Total	C	O	0
			37	27	10	
21	J	1	Total	C	O	0
			55	45	10	
21	L	1	Total	C	O	0
			50	40	10	
21	N	1	Total	C	O	0
			44	34	10	
21	O	1	Total	C	O	0
			55	45	10	
21	T	1	Total	C	O	0
			37	27	10	
21	U	1	Total	C	O	0
			55	45	10	
21	W	1	Total	C	O	0
			50	40	10	
21	b	1	Total	C	O	0
			55	45	10	
21	g	1	Total	C	O	0
			37	27	10	
21	h	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms			AltConf
21	j	1	Total	C	O	0
			50	40	10	

- Molecule 22 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	C	0
			16	16	
22	L	1	Total	C	0
			15	15	
22	O	1	Total	C	0
			16	16	
22	W	1	Total	C	0
			15	15	
22	b	1	Total	C	0
			16	16	
22	j	1	Total	C	0
			15	15	

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
23	L	1	Total	Ca	0
			1	1	
23	W	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
23	j	1	Total 1	Ca 1	0

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	A	50	Total 50	O 50	0
24	B	55	Total 55	O 55	0
24	C	4	Total 4	O 4	0
24	D	10	Total 10	O 10	0
24	E	2	Total 2	O 2	0
24	F	2	Total 2	O 2	0
24	I	2	Total 2	O 2	0
24	K	1	Total 1	O 1	0
24	L	9	Total 9	O 9	0
24	N	51	Total 51	O 51	0
24	O	51	Total 51	O 51	0
24	P	3	Total 3	O 3	0
24	Q	12	Total 12	O 12	0
24	R	2	Total 2	O 2	0
24	S	2	Total 2	O 2	0
24	T	2	Total 2	O 2	0
24	V	1	Total 1	O 1	0
24	W	12	Total 12	O 12	0

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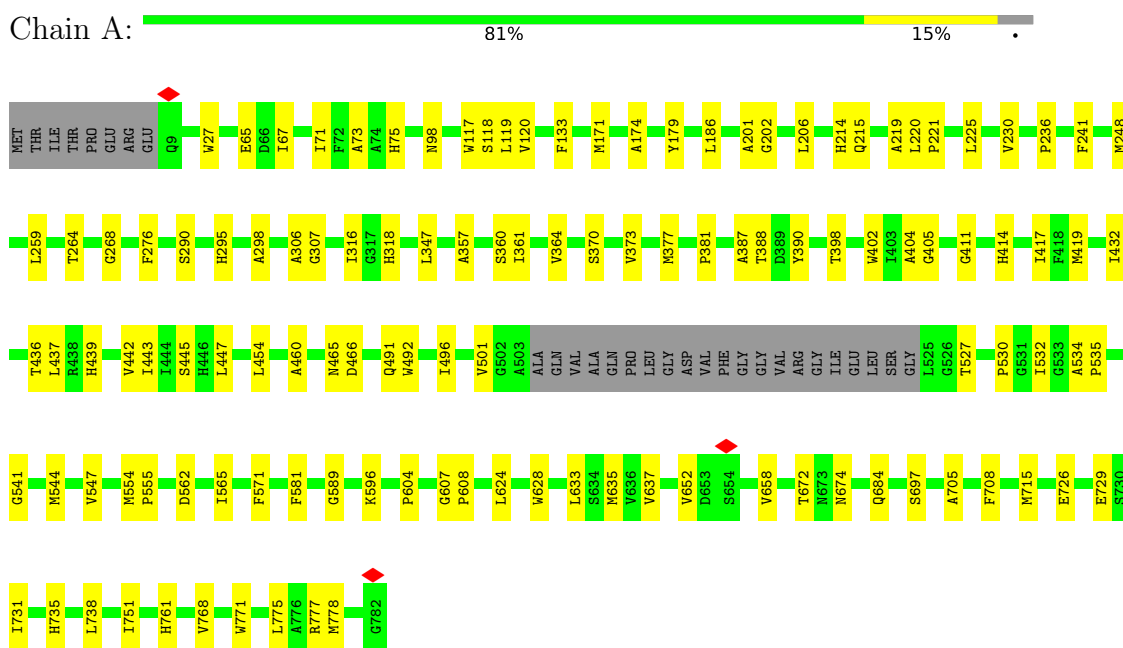
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Mol	Chain	Residues	Atoms		AltConf
24	a	51	Total 51	O 51	0
24	b	54	Total 54	O 54	0
24	c	2	Total 2	O 2	0
24	d	12	Total 12	O 12	0
24	e	2	Total 2	O 2	0
24	f	2	Total 2	O 2	0
24	g	2	Total 2	O 2	0
24	i	1	Total 1	O 1	0
24	j	8	Total 8	O 8	0

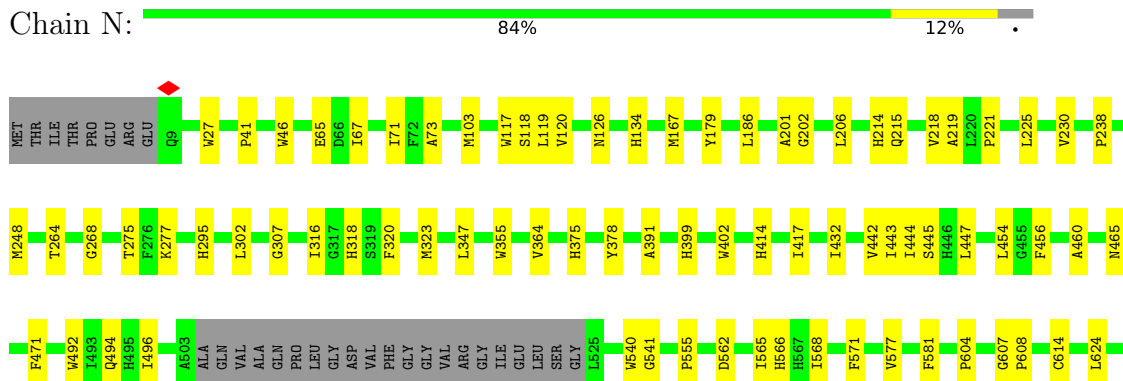
3 Residue-property plots

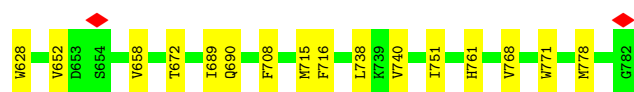
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



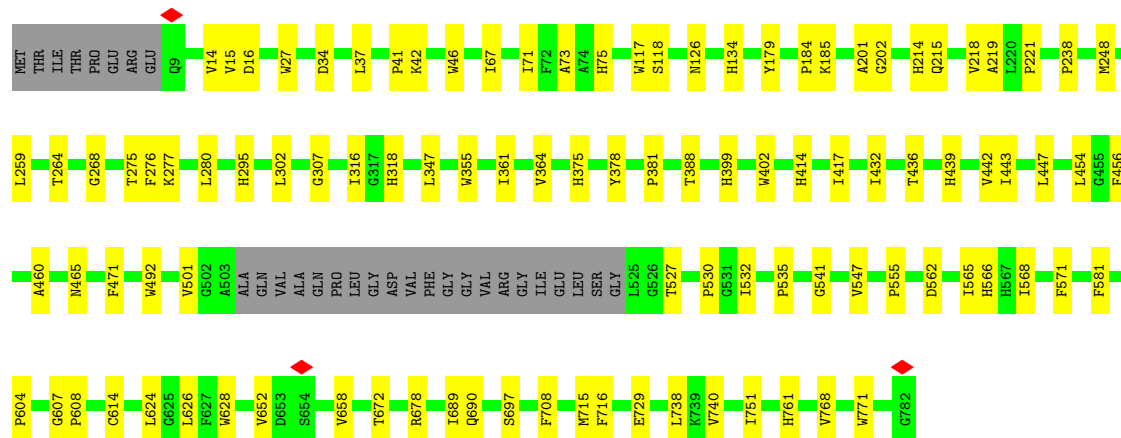
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 83% 13%



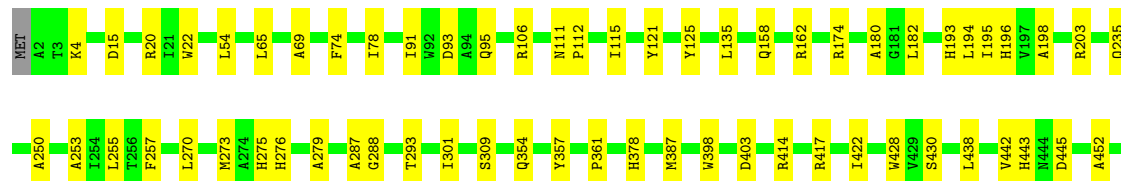
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

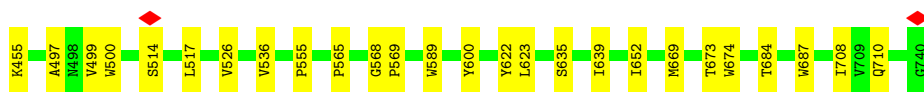
Chain B: 86% 14%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain O: 88% 12%





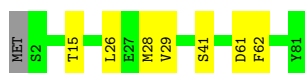
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 89% 11%



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 90% 9%



- Molecule 3: Photosystem I iron-sulfur center

Chain P: 95%



- Molecule 3: Photosystem I iron-sulfur center

Chain c: 90% 9%



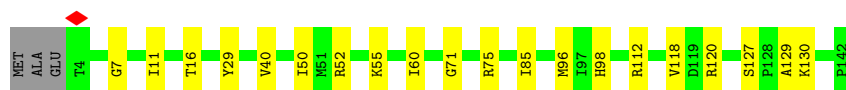
- Molecule 4: Photosystem I reaction center subunit II

Chain D: 87% 11%

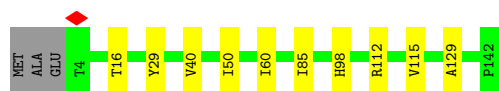
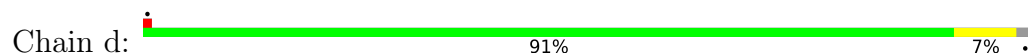


- Molecule 4: Photosystem I reaction center subunit II

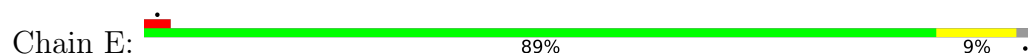
Chain Q: 84% 14%



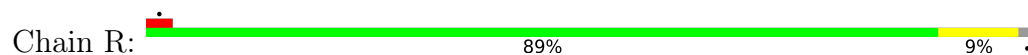
- Molecule 4: Photosystem I reaction center subunit II



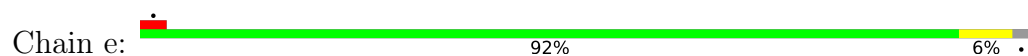
- Molecule 5: Photosystem I reaction center subunit IV



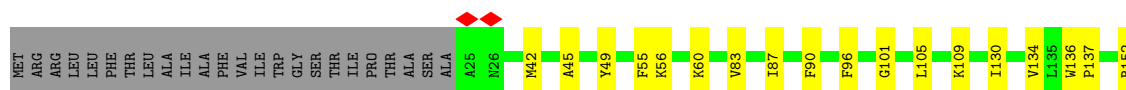
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV

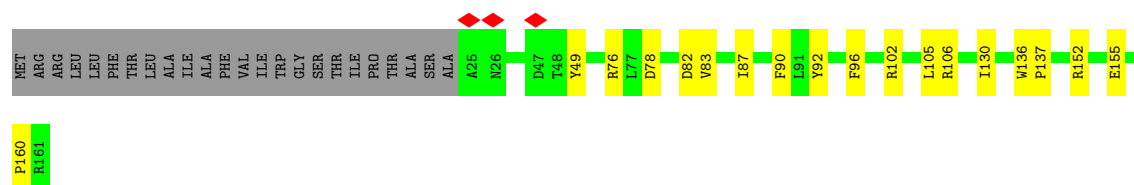


- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III

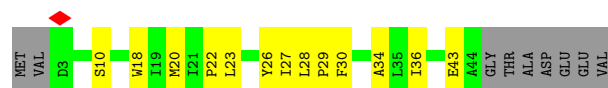




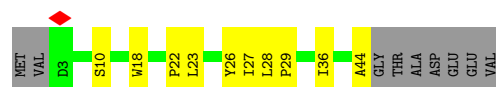
• Molecule 6: Photosystem I reaction center subunit III



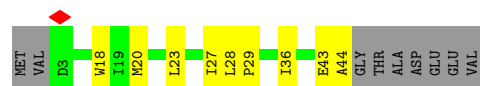
• Molecule 7: Photosystem I reaction center subunit VIII



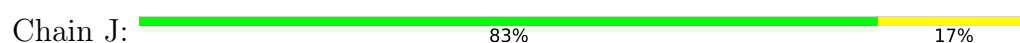
• Molecule 7: Photosystem I reaction center subunit VIII



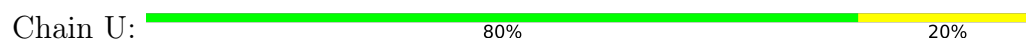
• Molecule 7: Photosystem I reaction center subunit VIII




• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 8: Photosystem I reaction center subunit IX




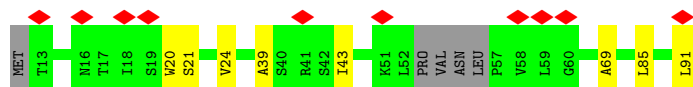
- Molecule 8: Photosystem I reaction center subunit IX

Chain h:  85% 15%




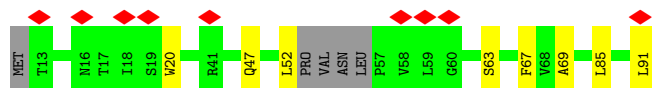
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:  12% 84% 10% 6%




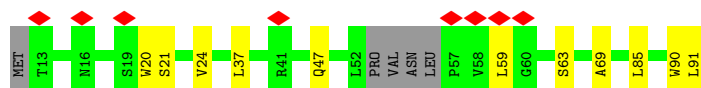
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain V:  11% 84% 10% 6%




- Molecule 9: Photosystem I reaction center subunit PsaK

Chain i:  10% 80% 14% 6%




- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  84% 10% 6%




- Molecule 10: Photosystem I reaction center subunit XI

Chain W:  87% 7% 6%




- Molecule 10: Photosystem I reaction center subunit XI

Chain j:  85% 9% 6%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  84% 12%




- Molecule 11: Photosystem I reaction center subunit XII

Chain Y:  91% 6%



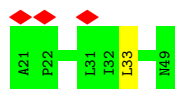
- Molecule 11: Photosystem I reaction center subunit XII

Chain k:  88% 9%



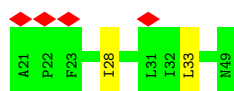
- Molecule 12: Photosystem one PsaX

Chain X:  10% 97%

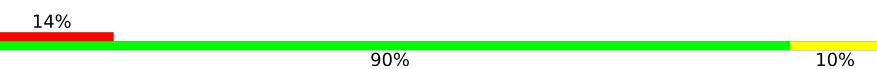


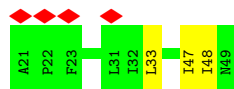
- Molecule 12: Photosystem one PsaX

Chain Z:  14% 93% 7%



- Molecule 12: Photosystem one PsaX

Chain l:  14% 90% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	300000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.172	Depositor
Minimum map value	-0.295	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	469.96, 469.96, 469.96	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.78326666, 0.78326666, 0.78326666	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, LHG, CL0, SF4, CLA, CA, BCR, LMG, F6C, LFA, 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	0.12	0/6106	0.28	0/8323
1	N	0.09	0/6106	0.24	0/8323
1	a	0.09	0/6106	0.24	0/8323
2	B	0.12	0/6139	0.29	0/8394
2	O	0.10	0/6139	0.24	0/8394
2	b	0.10	0/6139	0.25	0/8394
3	C	0.10	0/610	0.27	0/827
3	P	0.09	0/610	0.27	0/827
3	c	0.10	0/610	0.28	0/827
4	D	0.10	0/1115	0.30	0/1501
4	Q	0.09	0/1115	0.26	0/1501
4	d	0.08	0/1115	0.26	0/1501
5	E	0.08	0/540	0.23	0/728
5	R	0.08	0/540	0.23	0/728
5	e	0.08	0/540	0.26	0/728
6	F	0.13	0/1104	0.32	0/1501
6	S	0.10	0/1104	0.28	0/1501
6	f	0.10	0/1104	0.28	0/1501
7	I	0.14	0/366	0.45	0/503
7	T	0.13	0/366	0.36	0/503
7	g	0.13	0/366	0.35	0/503
8	J	0.11	0/386	0.29	0/526
8	U	0.08	0/386	0.25	0/526
8	h	0.08	0/386	0.24	0/526
9	K	0.11	0/550	0.31	0/751
9	V	0.08	0/550	0.27	0/751
9	i	0.08	0/550	0.25	0/751
10	L	0.12	0/1340	0.32	0/1821
10	W	0.09	0/1340	0.24	0/1821
10	j	0.09	0/1340	0.24	0/1821
11	M	0.10	0/243	0.20	0/329
11	Y	0.07	0/243	0.17	0/329

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	k	0.07	0/243	0.16	0/329
12	X	0.12	0/233	0.29	0/319
12	Z	0.07	0/233	0.23	0/319
12	l	0.07	0/233	0.22	0/319
All	All	0.10	0/56196	0.26	0/76569

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5900	0	5735	94	0
1	N	5900	0	5735	78	0
1	a	5900	0	5735	81	0
2	B	5913	0	5649	90	0
2	O	5913	0	5649	71	0
2	b	5913	0	5649	68	0
3	C	600	0	579	4	0
3	P	600	0	579	2	0
3	c	600	0	579	5	0
4	D	1090	0	1097	11	0
4	Q	1090	0	1097	13	0
4	d	1090	0	1097	8	0
5	E	530	0	535	3	0
5	R	530	0	535	3	0
5	e	530	0	535	2	0
6	F	1075	0	1081	18	0
6	S	1075	0	1081	15	0
6	f	1075	0	1081	13	0
7	I	351	0	354	10	0
7	T	351	0	354	8	0
7	g	351	0	354	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	373	0	390	10	0
8	U	373	0	390	8	0
8	h	373	0	390	6	0
9	K	539	0	578	6	0
9	V	539	0	578	6	0
9	i	539	0	578	7	0
10	L	1309	0	1289	14	0
10	W	1309	0	1289	12	0
10	j	1309	0	1289	14	0
11	M	240	0	261	4	0
11	Y	240	0	261	2	0
11	k	240	0	261	3	0
12	X	227	0	244	1	0
12	Z	227	0	244	2	0
12	l	227	0	244	2	0
13	A	65	0	72	3	0
13	N	65	0	72	2	0
13	a	65	0	72	2	0
14	A	250	0	0	0	0
14	B	132	0	0	1	0
14	L	132	0	0	2	0
14	N	250	0	0	0	0
14	O	132	0	0	1	0
14	W	132	0	0	1	0
14	a	250	0	0	0	0
14	b	132	0	0	1	0
14	j	132	0	0	1	0
15	A	2259	0	2271	100	0
15	B	2303	0	2383	108	0
15	F	65	0	72	0	0
15	K	95	0	72	1	0
15	L	125	0	131	3	0
15	N	2259	0	2271	94	0
15	O	2303	0	2383	98	0
15	S	65	0	72	1	0
15	V	95	0	72	1	0
15	W	125	0	131	3	0
15	X	55	0	49	1	0
15	Z	55	0	49	1	0
15	a	2259	0	2271	85	0
15	b	2303	0	2383	98	0
15	f	65	0	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	i	95	0	72	1	0
15	j	125	0	131	3	0
15	l	55	0	49	1	0
16	A	33	0	46	1	0
16	B	33	0	46	3	0
16	N	33	0	46	2	0
16	O	33	0	46	4	0
16	a	33	0	46	2	0
16	b	33	0	46	4	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
17	N	8	0	0	0	0
17	P	16	0	0	0	0
17	a	8	0	0	0	0
17	c	16	0	0	1	0
18	A	240	0	336	19	0
18	B	240	0	336	21	0
18	F	80	0	112	5	0
18	I	80	0	112	4	0
18	J	80	0	112	7	0
18	K	25	0	33	0	0
18	L	120	0	168	7	0
18	M	40	0	56	4	0
18	N	240	0	336	17	0
18	O	280	0	392	17	0
18	S	40	0	56	3	0
18	T	80	0	112	6	0
18	U	80	0	112	6	0
18	V	25	0	33	0	0
18	W	80	0	112	7	0
18	Y	40	0	56	3	0
18	a	240	0	336	16	0
18	b	280	0	392	20	0
18	f	40	0	56	4	0
18	g	80	0	112	5	0
18	h	80	0	112	7	0
18	i	25	0	33	0	0
18	j	40	0	56	1	0
18	k	40	0	56	4	0
19	A	42	0	54	0	0
19	B	49	0	74	4	0
19	F	49	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	49	0	74	6	0
19	N	91	0	128	2	0
19	W	49	0	74	8	0
19	X	44	0	61	3	0
19	Y	49	0	74	4	0
19	Z	44	0	61	1	0
19	a	42	0	54	0	0
19	f	49	0	74	2	0
19	j	49	0	74	7	0
19	k	49	0	74	5	0
19	l	44	0	61	3	0
20	A	94	0	110	5	0
20	N	94	0	110	3	0
20	a	94	0	110	3	0
21	A	44	0	61	1	0
21	B	99	0	147	4	0
21	I	37	0	44	4	0
21	J	55	0	86	0	0
21	L	50	0	70	4	0
21	N	44	0	61	0	0
21	O	55	0	86	6	0
21	T	37	0	44	2	0
21	U	55	0	86	1	0
21	W	50	0	70	4	0
21	b	55	0	86	5	0
21	g	37	0	44	3	0
21	h	55	0	86	2	0
21	j	50	0	70	3	0
22	B	16	0	28	1	0
22	L	15	0	29	2	0
22	O	16	0	28	1	0
22	W	15	0	29	1	0
22	b	16	0	28	2	0
22	j	15	0	29	1	0
23	L	1	0	0	0	0
23	W	1	0	0	0	0
23	j	1	0	0	0	0
24	A	50	0	0	0	0
24	B	55	0	0	1	0
24	C	4	0	0	0	0
24	D	10	0	0	0	0
24	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	2	0	0	0	0
24	I	2	0	0	0	0
24	K	1	0	0	0	0
24	L	9	0	0	0	0
24	N	51	0	0	0	0
24	O	51	0	0	1	0
24	P	3	0	0	0	0
24	Q	12	0	0	0	0
24	R	2	0	0	0	0
24	S	2	0	0	0	0
24	T	2	0	0	0	0
24	V	1	0	0	0	0
24	W	12	0	0	0	0
24	a	51	0	0	0	0
24	b	54	0	0	1	0
24	c	2	0	0	0	0
24	d	12	0	0	0	0
24	e	2	0	0	0	0
24	f	2	0	0	0	0
24	g	2	0	0	0	0
24	i	1	0	0	0	0
24	j	8	0	0	0	0
All	All	75954	0	74982	1150	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 8.

All (1150) 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)
8:U:37:GLN:HE21	8:U:38:TYR:H	1.13	0.91
8:J:37:GLN:HE21	8:J:38:TYR:H	1.20	0.85
8:h:37:GLN:HE21	8:h:38:TYR:H	1.27	0.83
18:N:850:BCR:H362	15:O:802:CLA:H42	1.67	0.76
18:A:850:BCR:H362	15:B:802:CLA:H42	1.67	0.75
18:a:850:BCR:H362	15:b:802:CLA:H42	1.67	0.74
15:a:804:CLA:HHC	15:a:804:CLA:HBB1	1.69	0.74
2:O:257:PHE:HE2	2:O:500:TRP:HE3	1.38	0.72
10:W:177:ARG:HH21	21:W:206:LMG:H341	1.55	0.72
10:L:177:ARG:HH21	21:L:207:LMG:H341	1.55	0.71
19:W:207:LHG:H322	15:b:804:CLA:H102	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:MET:HB3	15:A:803:CLA:C1C	2.20	0.71
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.70	0.71
15:N:806:CLA:H72	15:N:814:CLA:H2	1.73	0.71
15:B:804:CLA:H102	19:j:207:LHG:H322	1.73	0.70
1:A:347:LEU:HD11	1:A:432:ILE:HD11	1.72	0.70
19:L:208:LHG:H322	15:O:804:CLA:H102	1.73	0.70
10:j:177:ARG:HH21	21:j:206:LMG:H341	1.55	0.69
1:A:652:VAL:HG22	1:A:658:VAL:HG22	1.71	0.69
15:A:806:CLA:H72	15:A:814:CLA:H2	1.73	0.69
1:A:268:GLY:HA2	15:A:818:CLA:HAA2	1.75	0.69
2:O:257:PHE:CE2	2:O:500:TRP:HE3	2.10	0.69
1:N:347:LEU:HD11	1:N:432:ILE:HD11	1.73	0.69
15:B:809:CLA:H51	21:B:848:LMG:H273	1.75	0.69
15:N:841:CLA:H2	15:O:831:CLA:H42	1.75	0.68
10:L:71:HIS:HA	10:L:74:PHE:CE1	2.29	0.68
2:B:669:MET:HB2	15:B:803:CLA:C1C	2.24	0.68
1:a:347:LEU:HD11	1:a:432:ILE:HD11	1.75	0.67
2:b:257:PHE:CE2	2:b:500:TRP:HE3	2.13	0.67
2:B:257:PHE:HD2	2:B:499:VAL:HG23	1.60	0.67
7:T:36:ILE:HG21	18:W:205:BCR:HC8	1.77	0.67
15:a:841:CLA:H2	15:b:831:CLA:H42	1.77	0.67
5:R:7:LYS:HB3	5:R:62:GLU:HB3	1.76	0.66
15:a:806:CLA:H72	15:a:814:CLA:H2	1.77	0.66
15:A:841:CLA:H2	15:B:831:CLA:H42	1.76	0.66
2:O:669:MET:HB2	15:O:803:CLA:C1C	2.26	0.66
2:b:15:ASP:HB3	2:b:20:ARG:HB2	1.78	0.65
3:C:15:THR:HG22	3:C:28:MET:HG3	1.79	0.65
15:b:807:CLA:H43	7:g:20:MET:HE2	1.78	0.65
1:N:268:GLY:HA2	15:N:818:CLA:HAA2	1.76	0.65
4:D:85:ILE:HB	4:D:98:HIS:HB3	1.80	0.64
1:A:67:ILE:O	1:A:71:ILE:HG12	1.97	0.64
2:B:174:ARG:HB2	15:B:812:CLA:HBC2	1.79	0.64
1:a:715:MET:HB3	15:a:803:CLA:C1C	2.27	0.64
15:B:830:CLA:HBC2	15:B:838:CLA:HMC2	1.78	0.63
2:O:15:ASP:HB3	2:O:20:ARG:HB2	1.79	0.63
1:N:715:MET:HB3	15:N:803:CLA:C1C	2.28	0.63
8:h:20:VAL:HG22	18:h:102:BCR:H15C	1.81	0.63
10:W:175:ILE:HG23	14:j:201:F6C:O1A	1.97	0.63
1:a:268:GLY:HA2	15:a:818:CLA:HAA2	1.79	0.63
15:B:811:CLA:HBB2	15:B:819:CLA:H92	1.79	0.63
15:A:806:CLA:H101	15:A:814:CLA:H42	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:851:LHG:H282	19:j:207:LHG:H131	1.80	0.63
2:B:652:ILE:HD13	15:B:809:CLA:CHD	2.29	0.62
15:a:806:CLA:H101	15:a:814:CLA:H42	1.79	0.62
2:b:257:PHE:HE2	2:b:500:TRP:HE3	1.44	0.62
15:b:812:CLA:H102	15:b:817:CLA:H92	1.80	0.62
15:B:812:CLA:H102	15:B:817:CLA:H92	1.79	0.62
15:N:806:CLA:H101	15:N:814:CLA:H42	1.80	0.62
8:U:20:VAL:HG22	18:U:102:BCR:H15C	1.82	0.62
15:B:803:CLA:H143	18:B:847:BCR:H362	1.81	0.62
2:b:174:ARG:HB2	15:b:812:CLA:HBC2	1.81	0.62
15:O:803:CLA:H142	18:T:101:BCR:H271	1.81	0.61
2:B:257:PHE:HE2	2:B:500:TRP:HE3	1.47	0.61
1:A:624:LEU:HD22	2:B:673:THR:HG22	1.82	0.61
2:B:257:PHE:CE2	2:B:500:TRP:HB3	2.35	0.61
1:N:316:ILE:HD13	9:V:69:ALA:HB2	1.83	0.61
4:Q:11:ILE:HG13	4:Q:52:ARG:HE	1.66	0.61
19:W:207:LHG:H131	19:k:101:LHG:H282	1.83	0.61
1:N:318:HIS:NE2	15:N:823:CLA:ND	2.49	0.61
15:O:803:CLA:H143	18:O:848:BCR:H362	1.81	0.60
15:a:811:CLA:H11	15:a:813:CLA:H2	1.81	0.60
2:O:414:ARG:HG2	2:O:417:ARG:HH22	1.66	0.60
15:O:826:CLA:H141	18:O:848:BCR:H342	1.84	0.60
15:O:812:CLA:H102	15:O:817:CLA:H92	1.82	0.60
4:Q:71:GLY:HA2	4:Q:75:ARG:HE	1.67	0.60
1:a:316:ILE:HD13	9:i:69:ALA:HB2	1.82	0.60
6:F:42:MET:HE2	6:F:55:PHE:HB3	1.84	0.60
15:A:811:CLA:H11	15:A:813:CLA:H2	1.82	0.60
15:N:811:CLA:H11	15:N:813:CLA:H2	1.83	0.60
15:B:803:CLA:H142	18:I:101:BCR:H271	1.84	0.59
15:b:803:CLA:H142	18:g:101:BCR:H271	1.84	0.59
10:L:50:ASN:HB3	15:L:202:CLA:HAC1	1.85	0.59
2:O:652:ILE:HD13	15:O:809:CLA:CHD	2.33	0.59
8:J:20:VAL:HG22	18:J:102:BCR:H15C	1.85	0.59
15:a:816:CLA:HBB1	18:a:845:BCR:H382	1.84	0.59
18:a:850:BCR:H372	2:b:442:VAL:HG21	1.84	0.59
1:A:119:LEU:HG	1:A:120:VAL:HG13	1.85	0.59
18:N:850:BCR:H372	2:O:442:VAL:HG21	1.85	0.59
3:c:15:THR:HG22	3:c:28:MET:HG3	1.84	0.59
1:A:768:VAL:HG22	18:A:850:BCR:H323	1.85	0.59
2:O:174:ARG:HB2	15:O:812:CLA:HBC2	1.84	0.59
15:O:830:CLA:HBC2	15:O:838:CLA:HMC2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:803:CLA:H143	18:b:848:BCR:H362	1.84	0.59
7:I:36:ILE:HG21	18:L:205:BCR:HC8	1.84	0.59
10:W:50:ASN:HB3	15:W:202:CLA:HAC1	1.85	0.59
1:A:442:VAL:HG22	2:B:687:TRP:CH2	2.37	0.58
18:A:850:BCR:H372	2:B:442:VAL:HG21	1.85	0.58
2:b:180:ALA:HB2	2:b:288:GLY:HA3	1.86	0.58
15:b:820:CLA:HMD2	18:b:842:BCR:H23C	1.84	0.58
5:e:7:LYS:HB3	5:e:62:GLU:HB3	1.85	0.58
1:a:221:PRO:HD3	1:a:248:MET:HE1	1.84	0.58
15:O:811:CLA:HBB2	15:O:819:CLA:H92	1.85	0.58
6:f:82:ASP:HB3	8:h:39:GLY:HA2	1.86	0.58
15:b:834:CLA:HBB1	18:b:846:BCR:HC32	1.86	0.58
1:A:201:ALA:HB2	1:A:307:GLY:HA3	1.86	0.58
1:A:370:SER:HB3	1:A:404:ALA:HB2	1.85	0.58
9:V:91:LEU:HD21	18:b:844:BCR:H343	1.86	0.58
3:c:29:VAL:HG12	4:d:112:ARG:HB3	1.85	0.58
15:O:834:CLA:HBB1	18:O:846:BCR:HC32	1.85	0.57
15:B:824:CLA:H43	15:B:837:CLA:HBA1	1.86	0.57
2:B:74:PHE:O	2:B:78:ILE:HG12	2.03	0.57
4:D:29:TYR:HB2	4:D:60:ILE:HG13	1.87	0.57
15:O:820:CLA:HMD2	18:O:842:BCR:H23C	1.86	0.57
1:A:171:MET:HE1	15:A:814:CLA:H92	1.85	0.57
15:b:811:CLA:HBB2	15:b:819:CLA:H92	1.85	0.57
1:a:447:LEU:HD22	15:a:840:CLA:HBB1	1.86	0.57
15:a:834:CLA:H152	15:b:840:CLA:H91	1.87	0.57
1:N:447:LEU:HD22	15:N:840:CLA:HBB1	1.86	0.56
1:A:544:MET:HG3	1:A:554:MET:HB3	1.86	0.56
15:N:820:CLA:H91	15:N:830:CLA:H172	1.86	0.56
1:A:276:PHE:CE2	1:A:532:ILE:HG13	2.41	0.56
4:Q:85:ILE:HB	4:Q:98:HIS:HB3	1.87	0.56
18:W:209:BCR:H291	10:j:160:VAL:HG21	1.87	0.56
1:a:768:VAL:HG22	18:a:850:BCR:H323	1.86	0.56
15:B:804:CLA:H51	18:M:101:BCR:HC22	1.87	0.56
10:L:175:ILE:HG23	14:W:201:F6C:O1A	2.06	0.56
2:b:129:MET:HE3	2:b:135:LEU:HD23	1.85	0.56
10:j:50:ASN:HB3	15:j:202:CLA:HAC1	1.88	0.56
15:A:834:CLA:H152	15:B:840:CLA:H91	1.86	0.56
1:N:624:LEU:HD22	2:O:673:THR:HG22	1.88	0.56
15:a:803:CLA:HBA1	15:b:802:CLA:HBB2	1.88	0.56
15:B:831:CLA:HAC2	6:F:87:ILE:HG12	1.86	0.56
15:B:834:CLA:HBB1	18:B:846:BCR:HC32	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:318:HIS:HB3	1:N:323:MET:HE3	1.88	0.56
18:L:210:BCR:H291	10:W:160:VAL:HG21	1.86	0.55
15:O:809:CLA:H51	21:O:849:LMG:H273	1.88	0.55
1:a:201:ALA:HB2	1:a:307:GLY:HA3	1.88	0.55
14:L:201:F6C:O1A	10:j:175:ILE:HG23	2.07	0.55
1:N:442:VAL:HG23	4:Q:16:THR:HG21	1.88	0.55
1:a:624:LEU:HD22	2:b:673:THR:HG22	1.89	0.55
2:b:405:GLU:HA	2:b:408:LYS:HE2	1.88	0.55
1:N:201:ALA:HB2	1:N:307:GLY:HA3	1.87	0.55
1:a:492:TRP:HA	20:a:852:LMT:H6E	1.89	0.55
1:A:214:HIS:CE1	15:A:815:CLA:NA	2.74	0.55
10:W:172:LEU:HA	10:W:175:ILE:HD12	1.87	0.55
1:a:15:VAL:HG12	1:a:184:PRO:HA	1.88	0.55
1:N:768:VAL:HG22	18:N:850:BCR:H323	1.89	0.55
15:A:803:CLA:HBA1	15:B:802:CLA:HBB2	1.89	0.55
6:S:152:ARG:HB2	6:S:155:GLU:HG3	1.88	0.55
2:B:275:HIS:HB3	15:B:816:CLA:HMB2	1.87	0.55
2:B:606:LEU:HD22	2:B:738:LYS:HZ2	1.72	0.55
15:N:834:CLA:H152	15:O:840:CLA:H91	1.88	0.54
16:B:841:PQN:H302	21:B:848:LMG:H222	1.89	0.54
21:I:103:LMG:H332	18:M:101:BCR:H272	1.90	0.54
21:g:103:LMG:H332	18:k:102:BCR:H272	1.89	0.54
2:b:54:LEU:HD12	15:b:812:CLA:HED1	1.89	0.54
15:b:830:CLA:HBC2	15:b:838:CLA:HMC2	1.89	0.54
2:B:193:HIS:CE1	15:B:813:CLA:NA	2.76	0.54
15:B:829:CLA:H2	19:F:204:LHG:HC92	1.90	0.54
22:B:849:LFA:H52	6:F:83:VAL:HG22	1.90	0.54
4:Q:7:GLY:HA2	4:Q:55:LYS:HG3	1.88	0.54
2:O:74:PHE:O	2:O:78:ILE:HG12	2.08	0.54
2:b:669:MET:HB2	15:b:803:CLA:C1C	2.38	0.54
1:N:492:TRP:HA	20:N:852:LMT:H6E	1.88	0.54
15:b:838:CLA:H51	19:l:101:LHG:H372	1.90	0.54
15:N:803:CLA:HBA1	15:O:802:CLA:HBB2	1.90	0.54
15:N:813:CLA:HBC1	15:N:814:CLA:H142	1.88	0.54
15:A:807:CLA:H151	15:A:830:CLA:HBB2	1.90	0.54
15:A:833:CLA:H2	15:L:203:CLA:H43	1.90	0.54
2:B:203:ARG:HG2	2:B:250:ALA:HB1	1.91	0.54
15:a:807:CLA:H151	15:a:830:CLA:HBB2	1.89	0.54
9:K:91:LEU:HD21	18:O:844:BCR:H343	1.89	0.53
21:T:103:LMG:H332	18:Y:102:BCR:H272	1.88	0.53
2:b:526:VAL:HG21	2:b:600:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:180:ALA:HB2	2:O:288:GLY:HA3	1.91	0.53
1:a:465:ASN:HB3	1:a:672:THR:HG22	1.89	0.53
2:b:403:ASP:HB3	4:d:129:ALA:HB3	1.90	0.53
4:d:29:TYR:HB2	4:d:60:ILE:HG13	1.91	0.53
2:B:257:PHE:CD2	2:B:499:VAL:HG23	2.43	0.53
1:N:221:PRO:HD3	1:N:248:MET:HE1	1.91	0.53
15:N:833:CLA:H2	15:W:203:CLA:H43	1.89	0.53
11:k:9:PHE:HB3	18:k:102:BCR:H381	1.90	0.53
19:B:851:LHG:H111	19:j:207:LHG:H271	1.91	0.53
1:N:465:ASN:HB3	1:N:672:THR:HG22	1.91	0.53
15:N:816:CLA:HBB1	18:N:845:BCR:H382	1.90	0.53
6:S:82:ASP:HB3	8:U:39:GLY:HA2	1.90	0.53
2:b:193:HIS:CE1	15:b:813:CLA:NA	2.76	0.53
15:N:803:CLA:H122	16:N:843:PQN:H241	1.91	0.53
2:b:257:PHE:CE2	2:b:500:TRP:HB3	2.43	0.53
1:A:492:TRP:HA	20:A:852:LMT:H6E	1.90	0.53
15:A:803:CLA:CGA	15:A:803:CLA:H3A	2.38	0.53
2:B:526:VAL:HG21	2:B:600:TYR:HB2	1.90	0.53
2:O:193:HIS:CE1	15:O:813:CLA:NA	2.76	0.53
15:a:803:CLA:H122	16:a:843:PQN:H241	1.90	0.53
1:A:635:MET:HE1	13:A:801:CL0:H53	1.91	0.53
15:A:816:CLA:HBB1	18:A:845:BCR:H382	1.91	0.53
15:O:808:CLA:O1A	15:O:826:CLA:HBD	2.09	0.53
15:B:838:CLA:H51	19:X:101:LHG:H372	1.90	0.52
6:F:56:LYS:HB3	8:J:46:PRO:HG2	1.91	0.52
8:J:28:MET:HA	8:J:28:MET:HE3	1.90	0.52
2:O:422:ILE:HG23	15:O:838:CLA:HBB2	1.91	0.52
1:a:67:ILE:O	1:a:71:ILE:HG12	2.09	0.52
15:b:804:CLA:H51	18:k:102:BCR:HC22	1.92	0.52
6:F:45:ALA:HB2	6:F:55:PHE:HE2	1.75	0.52
15:a:833:CLA:H2	15:j:203:CLA:H43	1.90	0.52
15:b:810:CLA:H151	18:b:843:BCR:H10C	1.91	0.52
22:b:850:LFA:H52	6:f:83:VAL:HG22	1.90	0.52
2:B:623:LEU:HD12	15:B:802:CLA:H11	1.91	0.52
7:I:28:LEU:N	7:I:29:PRO:HD2	2.24	0.52
15:O:830:CLA:H11	18:S:202:BCR:H353	1.91	0.52
1:a:414:HIS:HA	1:a:417:ILE:HD12	1.91	0.52
1:a:442:VAL:HG23	4:d:16:THR:HG21	1.90	0.52
2:B:65:LEU:HD11	18:B:844:BCR:H281	1.90	0.52
2:B:387:MET:HE1	18:B:846:BCR:H361	1.91	0.52
15:B:808:CLA:O1A	15:B:826:CLA:HBD	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:850:LFA:H52	6:S:83:VAL:HG22	1.92	0.52
1:a:276:PHE:CE2	1:a:532:ILE:HG13	2.44	0.52
2:B:361:PRO:HG3	15:B:817:CLA:HBA1	1.90	0.52
15:O:831:CLA:HAC2	6:S:87:ILE:HG12	1.92	0.52
2:b:257:PHE:HD2	2:b:499:VAL:HG23	1.74	0.52
4:d:85:ILE:HB	4:d:98:HIS:HB3	1.90	0.52
19:L:208:LHG:H131	19:Y:101:LHG:H282	1.92	0.52
15:A:803:CLA:H122	16:A:843:PQN:H241	1.91	0.52
15:b:808:CLA:O1A	15:b:826:CLA:HBD	2.09	0.52
15:B:823:CLA:H71	15:B:825:CLA:H42	1.91	0.52
4:D:71:GLY:HA2	4:D:75:ARG:HE	1.74	0.52
1:A:402:TRP:CD1	15:A:829:CLA:HAB	2.44	0.52
15:O:803:CLA:H72	18:O:848:BCR:H363	1.92	0.52
15:B:837:CLA:H93	15:B:838:CLA:HBC1	1.92	0.52
5:E:7:LYS:HB2	5:E:62:GLU:HB3	1.92	0.52
1:N:738:LEU:HD13	18:S:202:BCR:H321	1.91	0.52
12:l:47:ILE:HG22	12:l:48:ILE:HG23	1.91	0.52
2:O:526:VAL:HG21	2:O:600:TYR:HB2	1.91	0.51
4:Q:29:TYR:HB2	4:Q:60:ILE:HG13	1.91	0.51
10:W:71:HIS:HA	10:W:74:PHE:CE2	2.45	0.51
10:j:101:ILE:HA	10:j:156:MET:HE1	1.91	0.51
1:A:295:HIS:HB2	15:A:819:CLA:C1B	2.40	0.51
11:Y:9:PHE:HB3	18:Y:102:BCR:H381	1.92	0.51
1:a:442:VAL:HG22	2:b:687:TRP:CH2	2.45	0.51
15:a:818:CLA:HBA1	15:a:818:CLA:HBD	1.92	0.51
2:B:438:LEU:O	2:B:442:VAL:HG22	2.10	0.51
1:N:67:ILE:O	1:N:71:ILE:HG12	2.09	0.51
1:N:117:TRP:CD2	15:N:810:CLA:HED3	2.46	0.51
15:b:809:CLA:H71	18:g:101:BCR:H342	1.92	0.51
1:a:402:TRP:CD1	15:a:829:CLA:HAB	2.45	0.51
15:b:824:CLA:H43	15:b:837:CLA:HBA1	1.93	0.51
10:L:160:VAL:HG21	18:L:206:BCR:H291	1.93	0.51
1:N:494:GLN:HG2	1:N:540:TRP:HD1	1.76	0.51
7:T:28:LEU:N	7:T:29:PRO:HD2	2.26	0.51
1:a:541:GLY:HA2	1:a:555:PRO:HG3	1.92	0.51
2:b:361:PRO:HG3	15:b:817:CLA:HBA1	1.91	0.51
15:A:820:CLA:O2D	15:A:820:CLA:H2A	2.10	0.51
15:B:806:CLA:H43	21:B:848:LMG:H321	1.93	0.51
6:F:152:ARG:HB2	6:F:155:GLU:OE1	2.10	0.51
15:a:820:CLA:H91	15:a:830:CLA:H172	1.93	0.51
8:h:22:LEU:HD21	21:h:103:LMG:H251	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:HD12	15:B:812:CLA:HED1	1.92	0.51
4:D:7:GLY:HA2	4:D:55:LYS:HG3	1.92	0.51
1:N:541:GLY:HA2	1:N:555:PRO:HG3	1.93	0.51
15:a:803:CLA:CGA	15:a:803:CLA:H3A	2.40	0.51
15:N:804:CLA:H61	15:N:841:CLA:H91	1.93	0.51
15:b:829:CLA:H2	19:f:203:LHG:HC92	1.93	0.51
2:B:610:GLU:HG3	2:B:738:LYS:HZ3	1.76	0.50
10:W:171:ALA:O	10:W:175:ILE:HG13	2.11	0.50
8:J:26:LEU:HD13	18:J:101:BCR:HC7	1.93	0.50
10:L:58:LEU:HD22	10:L:62:MET:HB3	1.93	0.50
1:N:214:HIS:CE1	15:N:815:CLA:NA	2.78	0.50
1:N:442:VAL:HG22	2:O:687:TRP:CH2	2.46	0.50
15:N:806:CLA:H142	18:N:847:BCR:H372	1.93	0.50
15:b:826:CLA:H141	18:b:848:BCR:H342	1.91	0.50
15:b:829:CLA:H143	19:l:101:LHG:H122	1.93	0.50
1:A:215:GLN:HA	1:A:219:ALA:HB3	1.93	0.50
1:A:697:SER:HB2	2:B:449:ALA:HB1	1.93	0.50
1:N:414:HIS:HA	1:N:417:ILE:HD12	1.92	0.50
15:O:809:CLA:H71	18:T:101:BCR:H342	1.92	0.50
10:j:71:HIS:HA	10:j:74:PHE:CE2	2.47	0.50
1:A:541:GLY:HA2	1:A:555:PRO:HG3	1.92	0.50
2:O:361:PRO:HG3	15:O:817:CLA:HBA1	1.92	0.50
15:O:838:CLA:H51	19:Z:101:LHG:H372	1.92	0.50
15:B:809:CLA:O1A	18:B:847:BCR:HC41	2.11	0.50
15:O:808:CLA:H91	15:O:809:CLA:H52	1.94	0.50
15:b:831:CLA:HAC2	6:f:87:ILE:HG12	1.92	0.50
10:L:156:MET:HG3	18:L:206:BCR:H382	1.94	0.50
15:a:806:CLA:H151	18:a:846:BCR:H323	1.94	0.50
16:b:841:PQN:H302	21:b:849:LMG:H222	1.93	0.50
3:C:29:VAL:HG12	4:D:112:ARG:HB3	1.93	0.50
1:N:402:TRP:CD1	15:N:829:CLA:HAB	2.46	0.50
1:a:14:VAL:HG13	1:a:185:LYS:HG2	1.94	0.50
1:a:214:HIS:CE1	15:a:815:CLA:NA	2.80	0.50
7:g:28:LEU:N	7:g:29:PRO:HD2	2.26	0.50
10:L:156:MET:SD	18:L:206:BCR:H24C	2.52	0.50
15:N:807:CLA:H151	15:N:830:CLA:HBB2	1.93	0.50
1:a:27:TRP:CD1	15:a:812:CLA:H2	2.47	0.50
15:b:808:CLA:H102	15:b:808:CLA:H2	1.93	0.50
1:A:447:LEU:HD22	15:A:840:CLA:HBB1	1.93	0.50
4:D:38:GLU:HA	4:D:51:MET:O	2.12	0.50
6:F:90:PHE:HB2	18:F:202:BCR:H321	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:9:PHE:HB3	18:M:101:BCR:H381	1.94	0.50
15:N:818:CLA:HBA1	15:N:818:CLA:HBD	1.94	0.50
15:a:820:CLA:O2D	15:a:820:CLA:H2A	2.11	0.50
2:B:68:VAL:HG11	2:B:124:TRP:HZ3	1.77	0.49
15:O:823:CLA:H71	15:O:825:CLA:H42	1.94	0.49
2:b:22:TRP:CG	2:b:710:GLN:HE22	2.29	0.49
15:A:818:CLA:HBA1	15:A:818:CLA:HBD	1.93	0.49
2:B:158:GLN:O	2:B:162:ARG:HG3	2.12	0.49
2:B:422:ILE:HG23	15:B:838:CLA:HBB2	1.94	0.49
2:B:454:GLU:HG3	6:F:55:PHE:HE1	1.76	0.49
1:N:445:SER:HB3	2:O:684:THR:HG22	1.93	0.49
1:N:604:PRO:HB3	1:N:751:ILE:HB	1.93	0.49
1:a:771:TRP:CG	18:a:850:BCR:HC22	2.46	0.49
15:b:809:CLA:H51	21:b:849:LMG:H273	1.93	0.49
15:A:820:CLA:H91	15:A:830:CLA:H172	1.94	0.49
2:B:718:HIS:NE2	15:B:840:CLA:NA	2.60	0.49
3:C:26:LEU:HA	3:C:41:SER:O	2.12	0.49
18:S:202:BCR:H281	15:Z:102:CLA:H11	1.93	0.49
7:g:36:ILE:HG21	18:j:205:BCR:HC8	1.94	0.49
1:A:442:VAL:HG23	4:D:16:THR:HG21	1.93	0.49
15:A:820:CLA:H201	15:A:822:CLA:H51	1.94	0.49
15:B:803:CLA:H72	18:B:847:BCR:H363	1.94	0.49
6:F:96:PHE:HZ	6:F:130:ILE:HG23	1.77	0.49
19:L:208:LHG:H271	19:Y:101:LHG:H111	1.94	0.49
3:P:29:VAL:HG12	4:Q:112:ARG:HB3	1.93	0.49
1:A:454:LEU:HB3	1:A:571:PHE:HB2	1.95	0.49
15:A:804:CLA:H61	15:A:841:CLA:H91	1.94	0.49
1:a:652:VAL:HG22	1:a:658:VAL:HG22	1.95	0.49
2:B:276:HIS:HB2	15:B:816:CLA:C1B	2.42	0.49
1:N:215:GLN:HA	1:N:219:ALA:HB3	1.95	0.49
1:a:215:GLN:HA	1:a:219:ALA:HB3	1.95	0.49
15:B:807:CLA:HMC1	15:B:807:CLA:H92	1.95	0.49
7:I:23:LEU:HA	7:I:27:ILE:HB	1.92	0.49
1:N:73:ALA:HB2	1:N:179:TYR:HB2	1.95	0.49
15:A:836:CLA:H62	15:A:836:CLA:H2	1.60	0.49
2:b:275:HIS:HB3	15:b:816:CLA:HMB2	1.94	0.49
1:A:221:PRO:HB2	1:A:241:PHE:CE1	2.48	0.49
15:B:810:CLA:H151	18:B:843:BCR:H10C	1.95	0.49
1:N:568:ILE:HD12	13:N:801:CL0:H61	1.94	0.49
1:N:771:TRP:CG	18:N:850:BCR:HC22	2.48	0.49
15:O:804:CLA:H51	18:Y:102:BCR:HC22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:816:CLA:H3A	15:b:816:CLA:HBA2	1.45	0.49
15:B:829:CLA:H42	19:F:204:LHG:H111	1.95	0.48
2:O:275:HIS:HB3	15:O:816:CLA:HMB2	1.94	0.48
6:S:96:PHE:HZ	6:S:130:ILE:HG23	1.77	0.48
15:a:818:CLA:H62	15:a:818:CLA:H41	1.53	0.48
2:b:326:LEU:O	2:b:330:ILE:HD12	2.12	0.48
15:b:823:CLA:H71	15:b:825:CLA:H42	1.95	0.48
1:A:117:TRP:CD2	15:A:810:CLA:HED3	2.48	0.48
1:A:405:GLY:HA3	1:A:633:LEU:HD21	1.95	0.48
2:B:414:ARG:HG2	2:B:417:ARG:HH22	1.78	0.48
10:L:65:LEU:O	10:L:69:MET:HG3	2.13	0.48
2:O:195:ILE:HD11	2:O:255:LEU:HD21	1.95	0.48
15:b:803:CLA:H72	18:b:848:BCR:H363	1.94	0.48
1:A:466:ASP:OD1	1:A:672:THR:HB	2.13	0.48
2:B:22:TRP:CG	2:B:710:GLN:HE22	2.31	0.48
1:N:275:THR:HG21	1:N:277:LYS:HE3	1.96	0.48
15:O:824:CLA:H43	15:O:837:CLA:HBA1	1.95	0.48
6:f:96:PHE:HZ	6:f:130:ILE:HG23	1.78	0.48
1:N:391:ALA:HA	1:N:778:MET:HB3	1.94	0.48
15:N:838:CLA:H12	15:N:839:CLA:O1A	2.14	0.48
19:N:857:LHG:HC92	15:O:829:CLA:H2	1.95	0.48
2:O:438:LEU:O	2:O:442:VAL:HG22	2.14	0.48
1:a:568:ILE:HD12	13:a:801:CL0:H61	1.95	0.48
10:j:65:LEU:O	10:j:69:MET:HG3	2.13	0.48
2:B:378:HIS:HB2	15:B:826:CLA:C1B	2.43	0.48
15:N:818:CLA:CHD	15:N:819:CLA:HBB2	2.43	0.48
2:O:403:ASP:HB3	4:Q:129:ALA:HB3	1.96	0.48
1:a:604:PRO:HB3	1:a:751:ILE:HB	1.95	0.48
10:j:86:ARG:HA	10:j:92:ALA:HB2	1.96	0.48
1:A:436:THR:HA	1:A:439:HIS:CE1	2.48	0.48
15:A:819:CLA:H93	15:A:819:CLA:H111	1.73	0.48
2:B:287:ALA:HB2	15:B:818:CLA:HBC2	1.96	0.48
2:O:257:PHE:HE2	2:O:500:TRP:CE3	2.24	0.48
1:a:628:TRP:HE1	15:b:803:CLA:C1D	2.26	0.48
2:b:257:PHE:HE2	2:b:500:TRP:CE3	2.28	0.48
2:b:422:ILE:HG23	15:b:838:CLA:HBB2	1.96	0.48
15:A:807:CLA:H42	15:A:831:CLA:H51	1.95	0.48
15:B:814:CLA:HAA2	9:i:91:LEU:HG	1.95	0.48
19:W:207:LHG:H192	19:k:101:LHG:H362	1.96	0.48
15:a:818:CLA:H111	15:a:818:CLA:H151	1.48	0.48
1:A:316:ILE:HD13	9:K:69:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TRP:HA	1:A:633:LEU:HD23	1.95	0.48
15:B:804:CLA:H43	19:j:207:LHG:H281	1.95	0.48
15:K:102:CLA:H3A	15:K:102:CLA:HBA2	1.57	0.48
19:N:857:LHG:H111	15:O:829:CLA:H42	1.96	0.48
2:O:257:PHE:CE2	2:O:500:TRP:HB3	2.48	0.48
15:a:806:CLA:H61	18:a:847:BCR:H24C	1.96	0.48
2:b:91:ILE:HB	2:b:112:PRO:HB2	1.96	0.48
15:b:831:CLA:HAB	18:b:847:BCR:H323	1.96	0.48
15:B:809:CLA:H3A	15:B:809:CLA:HBA2	1.46	0.48
15:B:816:CLA:H3A	15:B:816:CLA:HBA2	1.41	0.48
2:O:203:ARG:HG2	2:O:250:ALA:HB1	1.95	0.48
15:O:808:CLA:H2	15:O:808:CLA:H61	1.68	0.48
15:a:803:CLA:H112	18:a:850:BCR:H23C	1.95	0.48
18:f:202:BCR:H281	15:l:102:CLA:H11	1.96	0.48
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.95	0.48
15:N:804:CLA:HHC	15:N:804:CLA:HBB1	1.94	0.48
15:N:807:CLA:H62	15:N:807:CLA:H41	1.57	0.48
15:N:812:CLA:H91	15:N:812:CLA:H142	1.96	0.48
15:b:837:CLA:HMA3	15:b:838:CLA:HED2	1.95	0.48
1:A:604:PRO:HB3	1:A:751:ILE:HB	1.95	0.47
14:L:204:F6C:OMB	22:L:209:LFA:H61	2.13	0.47
15:V:102:CLA:HBA2	15:V:102:CLA:H3A	1.59	0.47
15:b:806:CLA:H43	21:b:849:LMG:H321	1.95	0.47
21:g:103:LMG:H352	18:k:102:BCR:H383	1.96	0.47
15:A:807:CLA:H193	15:A:807:CLA:H161	1.72	0.47
2:B:514:SER:HA	2:B:517:LEU:HD21	1.96	0.47
15:B:818:CLA:H162	15:B:818:CLA:H122	1.62	0.47
15:O:809:CLA:H3A	15:O:809:CLA:HBA2	1.54	0.47
16:O:841:PQN:H302	21:O:849:LMG:H222	1.95	0.47
1:a:738:LEU:HD13	18:f:202:BCR:H321	1.96	0.47
15:a:812:CLA:H61	15:a:812:CLA:H41	1.63	0.47
15:b:837:CLA:H93	15:b:838:CLA:HBC1	1.96	0.47
15:A:814:CLA:H61	15:A:814:CLA:H102	1.53	0.47
8:J:24:VAL:HG22	18:J:102:BCR:H341	1.97	0.47
18:L:210:BCR:H382	10:W:156:MET:HG3	1.96	0.47
15:N:820:CLA:H201	15:N:822:CLA:H51	1.95	0.47
2:O:445:ASP:OD1	2:O:622:TYR:HB2	2.14	0.47
19:W:207:LHG:H271	19:k:101:LHG:H111	1.96	0.47
1:a:218:VAL:HG13	1:a:238:PRO:HB3	1.96	0.47
2:b:203:ARG:HG2	2:b:250:ALA:HB1	1.96	0.47
1:A:443:ILE:HG21	1:A:581:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:SER:O	2:B:304:MET:HG3	2.13	0.47
1:N:375:HIS:HA	1:N:378:TYR:HE1	1.79	0.47
2:b:330:ILE:HG13	2:b:336:PHE:CE2	2.49	0.47
15:b:829:CLA:H42	19:f:203:LHG:H111	1.97	0.47
15:A:814:CLA:H41	15:A:814:CLA:H62	1.57	0.47
15:A:831:CLA:H101	15:A:842:CLA:HAA2	1.95	0.47
2:B:536:VAL:HG11	2:B:589:TRP:CE2	2.50	0.47
10:L:86:ARG:HA	10:L:92:ALA:HB2	1.96	0.47
15:N:803:CLA:H112	18:N:850:BCR:H23C	1.96	0.47
15:j:202:CLA:H72	19:j:207:LHG:H222	1.96	0.47
2:B:54:LEU:HD11	15:B:812:CLA:HBA2	1.96	0.47
15:B:809:CLA:H71	18:I:101:BCR:H342	1.95	0.47
15:N:820:CLA:H93	15:N:820:CLA:H62	1.75	0.47
2:b:652:ILE:HD13	15:b:809:CLA:CHD	2.45	0.47
9:i:37:LEU:HD23	9:i:59:LEU:HD23	1.96	0.47
1:A:398:THR:HG23	1:A:637:VAL:HG11	1.97	0.47
1:A:628:TRP:HE1	15:B:803:CLA:C1D	2.27	0.47
15:A:818:CLA:H62	15:A:818:CLA:H41	1.54	0.47
2:B:195:ILE:HD11	2:B:255:LEU:HD21	1.97	0.47
16:B:841:PQN:H142	18:B:847:BCR:H271	1.96	0.47
9:K:39:ALA:O	9:K:43:ILE:HG12	2.15	0.47
1:N:167:MET:HG3	18:N:846:BCR:H322	1.97	0.47
15:N:806:CLA:H151	18:N:846:BCR:H323	1.97	0.47
15:N:807:CLA:H42	15:N:831:CLA:H51	1.96	0.47
15:N:822:CLA:H93	15:N:822:CLA:H112	1.75	0.47
2:O:565:PRO:HB3	2:O:708:ILE:HB	1.97	0.47
15:O:802:CLA:HBB1	15:O:802:CLA:HMB1	1.97	0.47
15:O:829:CLA:HMA3	15:O:830:CLA:HED2	1.97	0.47
1:a:73:ALA:HB2	1:a:179:TYR:HB2	1.95	0.47
1:a:117:TRP:CD2	15:a:810:CLA:HED3	2.48	0.47
1:a:708:PHE:CG	18:a:850:BCR:H363	2.50	0.47
15:a:804:CLA:H61	15:a:841:CLA:H91	1.96	0.47
2:b:378:HIS:HB2	15:b:826:CLA:CHB	2.45	0.47
1:A:771:TRP:CG	18:A:850:BCR:HC22	2.50	0.47
15:A:838:CLA:HBA1	15:A:838:CLA:H3A	1.67	0.47
2:B:378:HIS:HB2	15:B:826:CLA:CHB	2.45	0.47
2:O:378:HIS:HB2	15:O:826:CLA:CHB	2.44	0.47
2:O:623:LEU:HD12	15:O:802:CLA:H11	1.96	0.47
15:a:820:CLA:HBC2	15:a:820:CLA:HMC1	1.96	0.47
4:d:40:VAL:HG22	4:d:50:ILE:HG12	1.96	0.47
1:A:236:PRO:HG2	1:A:241:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:PHE:CD2	18:A:850:BCR:H363	2.50	0.47
15:A:812:CLA:H41	15:A:812:CLA:H61	1.67	0.47
1:N:264:THR:HB	9:V:20:TRP:HB2	1.97	0.47
15:O:837:CLA:H142	15:O:837:CLA:H111	1.71	0.47
1:a:614:CYS:HB2	2:b:674:TRP:HB3	1.97	0.47
2:b:445:ASP:OD1	2:b:622:TYR:HB2	2.14	0.47
1:A:492:TRP:O	1:A:496:ILE:HG12	2.14	0.47
2:B:180:ALA:HB2	2:B:288:GLY:HA3	1.97	0.47
15:B:807:CLA:H43	7:I:20:MET:HE2	1.97	0.47
1:N:614:CYS:HB2	2:O:674:TRP:HB3	1.97	0.47
15:N:820:CLA:HMC1	15:N:820:CLA:HBC2	1.96	0.47
15:N:838:CLA:H41	15:N:838:CLA:H61	1.54	0.47
2:O:54:LEU:HD12	15:O:812:CLA:HED1	1.97	0.47
2:b:438:LEU:O	2:b:442:VAL:HG22	2.14	0.47
15:b:817:CLA:HBA2	15:b:817:CLA:H3A	1.39	0.47
15:b:830:CLA:H11	18:f:202:BCR:H353	1.96	0.47
1:A:562:ASP:HA	1:A:565:ILE:HG22	1.97	0.46
15:A:803:CLA:H112	18:A:850:BCR:H23C	1.97	0.46
15:A:820:CLA:HMC1	15:A:820:CLA:HBC2	1.97	0.46
15:A:825:CLA:H62	15:A:825:CLA:H41	1.59	0.46
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.97	0.46
2:B:531:ALA:HB2	15:B:837:CLA:HMA1	1.98	0.46
2:B:635:SER:O	2:B:639:ILE:HG12	2.14	0.46
1:N:708:PHE:CG	18:N:850:BCR:H363	2.50	0.46
15:N:804:CLA:H91	15:N:804:CLA:H112	1.73	0.46
15:N:814:CLA:H61	15:N:814:CLA:H102	1.55	0.46
15:N:834:CLA:H61	15:N:834:CLA:H2	1.74	0.46
15:O:818:CLA:H162	15:O:818:CLA:H122	1.61	0.46
15:b:805:CLA:H3A	15:b:805:CLA:HBA1	1.46	0.46
7:g:23:LEU:HA	7:g:27:ILE:HB	1.96	0.46
18:A:845:BCR:H24C	18:A:845:BCR:H371	1.77	0.46
15:B:829:CLA:H41	15:B:829:CLA:H62	1.63	0.46
1:N:318:HIS:CE1	15:N:823:CLA:NA	2.83	0.46
15:N:818:CLA:H151	15:N:818:CLA:H111	1.48	0.46
15:b:808:CLA:H2	15:b:808:CLA:H61	1.66	0.46
15:b:824:CLA:H41	15:b:836:CLA:H2	1.98	0.46
5:e:32:ILE:HD11	5:e:35:PRO:HA	1.97	0.46
2:B:111:ASN:HD22	7:I:10:SER:H	1.64	0.46
8:U:37:GLN:HE21	8:U:38:TYR:N	1.95	0.46
15:a:818:CLA:CHD	15:a:819:CLA:HBB2	2.46	0.46
15:a:820:CLA:H3A	15:a:820:CLA:HBA2	1.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:806:CLA:H193	15:b:806:CLA:H161	1.78	0.46
15:b:829:CLA:H41	15:b:829:CLA:H62	1.65	0.46
15:B:830:CLA:H11	18:F:203:BCR:H353	1.97	0.46
18:F:203:BCR:H281	15:X:102:CLA:H11	1.98	0.46
15:a:806:CLA:H142	18:a:847:BCR:H372	1.98	0.46
1:A:761:HIS:CE1	15:A:842:CLA:NA	2.83	0.46
15:A:807:CLA:H41	15:A:807:CLA:H62	1.56	0.46
15:O:806:CLA:H43	21:O:849:LMG:H321	1.97	0.46
8:U:26:LEU:HD13	18:U:101:BCR:HC7	1.98	0.46
15:a:807:CLA:H42	15:a:831:CLA:H51	1.97	0.46
2:B:345:LEU:HD13	15:B:806:CLA:HBB1	1.96	0.46
7:I:34:ALA:HB1	10:L:113:ILE:HG21	1.98	0.46
1:N:218:VAL:HG13	1:N:238:PRO:HB3	1.97	0.46
15:N:821:CLA:HBA2	15:N:821:CLA:H3A	1.62	0.46
16:O:841:PQN:H142	18:O:848:BCR:H271	1.98	0.46
2:b:65:LEU:HD11	18:b:844:BCR:H281	1.96	0.46
18:h:102:BCR:HC8	18:h:102:BCR:H311	1.98	0.46
2:B:377:THR:HG23	2:B:598:THR:HG21	1.98	0.46
15:B:817:CLA:H3A	15:B:817:CLA:HBA2	1.39	0.46
7:I:22:PRO:HB3	7:I:26:TYR:CZ	2.50	0.46
1:a:264:THR:HB	9:i:20:TRP:HB2	1.98	0.46
2:b:287:ALA:HB2	15:b:818:CLA:HBC2	1.97	0.46
6:f:136:TRP:CG	6:f:137:PRO:HD3	2.51	0.46
1:A:214:HIS:HB2	15:A:815:CLA:CHC	2.46	0.46
1:A:361:ILE:HD11	18:A:848:BCR:HC7	1.98	0.46
15:A:806:CLA:H151	18:A:846:BCR:H323	1.98	0.46
15:B:804:CLA:H12	15:B:804:CLA:C4D	2.46	0.46
15:B:838:CLA:H151	12:X:33:LEU:HB3	1.98	0.46
6:F:45:ALA:CB	6:F:55:PHE:HE2	2.29	0.46
1:N:562:ASP:HA	1:N:565:ILE:HG22	1.98	0.46
15:N:809:CLA:HBA2	15:N:809:CLA:H3A	1.26	0.46
15:O:804:CLA:H12	15:O:804:CLA:C4D	2.46	0.46
15:O:823:CLA:H141	15:O:823:CLA:H162	1.76	0.46
15:O:824:CLA:H41	15:O:836:CLA:H2	1.97	0.46
2:b:565:PRO:HB3	2:b:708:ILE:HB	1.96	0.46
18:b:847:BCR:H321	6:f:90:PHE:HB2	1.98	0.46
1:A:65:GLU:HB2	1:A:186:LEU:HB2	1.98	0.46
15:A:806:CLA:H2	15:A:806:CLA:H62	1.73	0.46
15:A:821:CLA:H3A	15:A:821:CLA:HBA2	1.62	0.46
15:B:804:CLA:H62	15:B:804:CLA:H41	1.55	0.46
21:I:103:LMG:H352	18:M:101:BCR:H383	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:65:GLU:HB2	1:N:186:LEU:HB2	1.97	0.46
1:N:375:HIS:HA	1:N:378:TYR:CE1	2.51	0.46
15:a:831:CLA:H111	15:a:831:CLA:H142	1.71	0.46
2:b:158:GLN:O	2:b:162:ARG:HG3	2.16	0.46
1:A:73:ALA:HB2	1:A:179:TYR:HB2	1.97	0.46
1:A:264:THR:HB	9:K:20:TRP:HB2	1.98	0.46
15:a:839:CLA:H92	20:a:853:LMT:H31	1.97	0.46
15:b:826:CLA:H143	15:b:826:CLA:H111	1.75	0.46
1:A:220:LEU:HD21	1:A:290:SER:HA	1.98	0.45
1:A:248:MET:HG3	15:A:816:CLA:HED1	1.97	0.45
15:N:806:CLA:H61	18:N:847:BCR:H24C	1.97	0.45
18:U:102:BCR:HC8	18:U:102:BCR:H311	1.98	0.45
1:a:295:HIS:HB2	15:a:819:CLA:C1B	2.46	0.45
15:a:837:CLA:H3A	15:a:837:CLA:HBA2	1.72	0.45
2:b:536:VAL:HG11	2:b:589:TRP:CE2	2.51	0.45
15:b:828:CLA:H112	15:b:828:CLA:H93	1.72	0.45
1:A:298:ALA:HA	15:A:818:CLA:HMC2	1.99	0.45
2:B:638:LEU:HD22	2:B:730:PHE:HA	1.98	0.45
15:B:822:CLA:H61	15:B:822:CLA:H2	1.60	0.45
19:L:208:LHG:H192	19:Y:101:LHG:H362	1.98	0.45
15:N:803:CLA:CGA	15:N:803:CLA:H3A	2.42	0.45
15:N:837:CLA:HBA2	15:N:837:CLA:H3A	1.67	0.45
2:O:414:ARG:HG2	2:O:417:ARG:NH2	2.30	0.45
10:W:86:ARG:HA	10:W:92:ALA:HB2	1.97	0.45
15:a:803:CLA:HBB1	15:a:803:CLA:HMB3	1.97	0.45
15:a:810:CLA:H61	18:h:102:BCR:H363	1.97	0.45
15:a:838:CLA:H3A	15:a:838:CLA:HBA1	1.70	0.45
2:b:635:SER:O	2:b:639:ILE:HG12	2.17	0.45
15:b:824:CLA:HMA1	18:b:846:BCR:H14C	1.99	0.45
1:A:225:LEU:O	1:A:230:VAL:HG12	2.16	0.45
1:A:357:ALA:HB1	18:A:848:BCR:H312	1.99	0.45
6:F:105:LEU:O	6:F:109:LYS:HG2	2.16	0.45
10:L:176:LEU:HD12	7:T:18:TRP:CZ2	2.52	0.45
15:N:833:CLA:HBB1	15:N:833:CLA:HMB3	1.98	0.45
2:O:91:ILE:HB	2:O:112:PRO:HB2	1.98	0.45
1:a:607:GLY:HA2	2:b:569:PRO:HD3	1.99	0.45
15:b:807:CLA:HMC1	15:b:807:CLA:H92	1.97	0.45
6:f:28:THR:HG23	6:f:29:LEU:HD12	1.98	0.45
1:A:465:ASN:HB3	1:A:672:THR:HG22	1.97	0.45
15:B:802:CLA:HMB1	15:B:802:CLA:HBB1	1.97	0.45
15:B:808:CLA:H91	15:B:809:CLA:H52	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ASP:HA	3:C:62:PHE:HA	1.80	0.45
2:O:22:TRP:CG	2:O:710:GLN:HE22	2.35	0.45
15:O:828:CLA:H161	15:O:828:CLA:H122	1.74	0.45
1:a:761:HIS:CE1	15:a:842:CLA:NA	2.85	0.45
15:b:828:CLA:HBB1	15:b:828:CLA:HMB1	1.98	0.45
15:B:829:CLA:H143	19:X:101:LHG:H122	1.97	0.45
15:B:831:CLA:HAB	18:F:202:BCR:H323	1.99	0.45
6:F:130:ILE:O	6:F:134:VAL:HG23	2.17	0.45
15:N:829:CLA:H41	15:N:829:CLA:H62	1.67	0.45
15:O:807:CLA:H92	15:O:807:CLA:HMC1	1.99	0.45
15:O:838:CLA:H151	12:Z:33:LEU:HB3	1.99	0.45
1:a:715:MET:HA	15:a:803:CLA:HBC2	1.97	0.45
2:b:195:ILE:HD11	2:b:255:LEU:HD21	1.98	0.45
1:A:364:VAL:HG21	18:A:849:BCR:H331	1.98	0.45
15:A:809:CLA:CHC	15:A:810:CLA:HMD2	2.47	0.45
15:B:824:CLA:H41	15:B:836:CLA:H2	1.97	0.45
15:B:826:CLA:H61	15:B:826:CLA:H41	1.77	0.45
15:N:839:CLA:H92	20:N:853:LMT:H31	1.99	0.45
15:O:829:CLA:H62	15:O:829:CLA:H41	1.64	0.45
1:a:118:SER:HB3	6:f:49:TYR:CE1	2.52	0.45
1:a:562:ASP:HA	1:a:565:ILE:HG22	1.99	0.45
1:a:608:PRO:HD3	2:b:568:GLY:HA2	1.99	0.45
15:a:806:CLA:HBA1	15:a:806:CLA:H3A	1.52	0.45
11:k:30:TYR:CG	19:k:101:LHG:HC92	2.51	0.45
15:A:803:CLA:HMB3	15:A:803:CLA:HBB1	1.98	0.45
15:A:839:CLA:H92	20:A:853:LMT:H31	1.98	0.45
2:B:655:TRP:HZ3	18:B:847:BCR:HC32	1.82	0.45
2:B:727:TYR:HB2	15:B:801:CLA:HED3	1.98	0.45
15:B:829:CLA:H3A	15:B:830:CLA:OBD	2.17	0.45
21:I:103:LMG:H362	21:I:103:LMG:H142	1.98	0.45
1:N:494:GLN:HG2	1:N:540:TRP:CD1	2.52	0.45
18:N:845:BCR:H24C	18:N:845:BCR:H371	1.77	0.45
15:O:805:CLA:H3A	15:O:805:CLA:HBA1	1.47	0.45
2:b:623:LEU:HD12	15:b:802:CLA:H11	1.97	0.45
1:A:708:PHE:CG	18:A:850:BCR:H363	2.52	0.45
13:A:801:CL0:CGD	13:A:801:CL0:H8	2.47	0.45
2:B:182:LEU:HD13	15:B:812:CLA:HBB	1.98	0.45
19:L:208:LHG:H281	15:O:804:CLA:H43	1.98	0.45
1:N:444:ILE:HB	2:O:684:THR:HG21	1.97	0.45
1:N:471:PHE:CZ	2:O:95:GLN:HG3	2.52	0.45
15:N:803:CLA:HBB1	15:N:803:CLA:HMB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:809:CLA:CHC	15:N:810:CLA:HMD2	2.47	0.45
2:O:555:PRO:HB3	6:S:160:PRO:HG3	1.99	0.45
1:a:375:HIS:HA	1:a:378:TYR:HE1	1.82	0.45
15:a:829:CLA:H62	15:a:829:CLA:H41	1.70	0.45
2:b:387:MET:HE1	18:b:846:BCR:H361	1.98	0.45
1:A:118:SER:HB3	6:F:49:TYR:CE1	2.52	0.45
15:A:820:CLA:H202	15:A:820:CLA:H161	1.79	0.45
2:O:443:HIS:CE1	14:O:832:F6C:NA	2.85	0.45
18:O:847:BCR:H321	6:S:90:PHE:HB2	1.98	0.45
1:a:355:TRP:HB3	15:a:806:CLA:HAC1	1.98	0.45
1:a:678:ARG:HG3	2:b:639:ILE:HD12	1.99	0.45
9:i:21:SER:O	9:i:24:VAL:HG22	2.17	0.45
1:A:674:ASN:HB2	2:B:658:LEU:HD11	1.99	0.45
15:A:811:CLA:H62	20:A:854:LMT:H62	1.99	0.45
15:A:827:CLA:H3A	15:A:827:CLA:HBA2	1.83	0.45
15:O:829:CLA:H3A	15:O:830:CLA:OBD	2.17	0.45
15:O:836:CLA:HBB1	15:O:836:CLA:HMB1	1.99	0.45
1:A:705:ALA:HB1	18:A:850:BCR:C15	2.47	0.44
2:B:270:LEU:HD23	2:B:273:MET:HE3	1.98	0.44
15:N:827:CLA:HBA2	15:N:827:CLA:H3A	1.82	0.44
15:O:803:CLA:CGA	15:O:803:CLA:H3A	2.47	0.44
4:Q:127:SER:HB2	4:Q:130:LYS:HZ3	1.82	0.44
6:S:102:ARG:O	6:S:106:ARG:HG3	2.18	0.44
2:b:700:ARG:HH22	7:g:43:GLU:HG2	1.81	0.44
16:b:841:PQN:H142	18:b:848:BCR:H271	1.99	0.44
2:B:369:PHE:HB3	2:B:609:TRP:CZ3	2.53	0.44
19:B:851:LHG:HC92	11:M:30:TYR:CG	2.52	0.44
18:I:101:BCR:H332	19:j:207:LHG:H382	1.99	0.44
2:O:270:LEU:HD23	2:O:273:MET:HE3	1.99	0.44
2:O:635:SER:O	2:O:639:ILE:HG12	2.17	0.44
15:O:824:CLA:HBA2	15:O:824:CLA:H3A	1.75	0.44
15:O:826:CLA:H61	15:O:826:CLA:H41	1.77	0.44
15:a:825:CLA:H41	15:a:825:CLA:H62	1.60	0.44
15:a:841:CLA:HBB2	6:f:101:GLY:HA3	1.99	0.44
15:b:823:CLA:H141	15:b:823:CLA:H162	1.77	0.44
15:A:818:CLA:CHD	15:A:819:CLA:HBB2	2.47	0.44
15:A:838:CLA:H61	15:A:838:CLA:H41	1.61	0.44
2:B:405:GLU:OE2	4:D:130:LYS:HE3	2.16	0.44
15:B:836:CLA:HBB1	15:B:836:CLA:HMB1	1.99	0.44
18:J:102:BCR:HC8	18:J:102:BCR:H311	1.99	0.44
1:N:355:TRP:HB3	15:N:806:CLA:HAC1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:78:ILE:HD12	2:O:125:TYR:CD1	2.52	0.44
15:O:803:CLA:H202	15:O:803:CLA:H162	1.80	0.44
1:a:527:THR:HG22	1:a:530:PRO:HG3	1.99	0.44
2:b:270:LEU:HD23	2:b:273:MET:HE3	1.98	0.44
15:b:802:CLA:HMB1	15:b:802:CLA:HBB1	1.99	0.44
15:b:809:CLA:H72	21:b:849:LMG:H273	1.99	0.44
1:A:738:LEU:HD13	18:F:203:BCR:H321	1.99	0.44
15:A:812:CLA:H142	15:A:812:CLA:H91	1.98	0.44
2:B:430:SER:HB3	2:B:536:VAL:HG22	1.99	0.44
16:B:841:PQN:H172	16:B:841:PQN:H211	1.81	0.44
1:N:320:PHE:CE1	15:N:822:CLA:HED2	2.53	0.44
15:N:810:CLA:H61	18:U:102:BCR:H363	1.99	0.44
9:V:47:GLN:HA	9:V:63:SER:HB3	1.98	0.44
15:a:809:CLA:CHC	15:a:810:CLA:HMD2	2.48	0.44
15:a:814:CLA:H41	15:a:814:CLA:H62	1.62	0.44
15:a:819:CLA:H3A	15:a:819:CLA:HBA2	1.55	0.44
2:b:430:SER:HB3	2:b:536:VAL:HG22	2.00	0.44
15:b:826:CLA:H61	15:b:826:CLA:H41	1.73	0.44
15:A:809:CLA:H3A	15:A:809:CLA:HBA2	1.25	0.44
2:B:398:TRP:HE1	18:B:846:BCR:H271	1.83	0.44
15:B:820:CLA:HBA2	18:B:842:BCR:H282	1.99	0.44
15:B:836:CLA:H52	15:B:836:CLA:H8	1.86	0.44
15:N:818:CLA:H161	15:N:818:CLA:H141	1.68	0.44
15:N:820:CLA:HBA2	15:N:820:CLA:H3A	1.52	0.44
2:O:536:VAL:HG11	2:O:589:TRP:CE2	2.51	0.44
11:Y:30:TYR:CG	19:Y:101:LHG:HC92	2.52	0.44
15:a:813:CLA:HBC1	15:a:814:CLA:H142	1.99	0.44
2:b:301:ILE:HG21	15:b:823:CLA:HAC1	2.00	0.44
2:B:257:PHE:CE2	2:B:500:TRP:HE3	2.30	0.44
15:B:837:CLA:H91	15:B:837:CLA:H111	1.75	0.44
6:F:96:PHE:CZ	6:F:130:ILE:HG23	2.53	0.44
1:a:259:LEU:HD11	18:a:845:BCR:H391	1.99	0.44
15:b:837:CLA:HBB1	15:b:837:CLA:HMB1	2.00	0.44
10:j:58:LEU:HD22	10:j:62:MET:HB3	2.00	0.44
1:A:259:LEU:HD11	18:A:845:BCR:H391	2.00	0.44
15:A:833:CLA:HBB1	15:A:833:CLA:HMB3	1.98	0.44
15:B:826:CLA:H141	18:B:847:BCR:H342	1.99	0.44
1:N:119:LEU:HG	1:N:120:VAL:HG13	2.00	0.44
1:N:295:HIS:HB2	15:N:819:CLA:C1B	2.48	0.44
1:N:689:ILE:HG23	1:N:690:GLN:HG3	2.00	0.44
15:O:824:CLA:H41	15:O:824:CLA:H61	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:837:CLA:H93	15:O:838:CLA:HBC1	1.98	0.44
15:W:202:CLA:H72	19:W:207:LHG:H222	1.99	0.44
15:b:806:CLA:HMD3	15:b:808:CLA:H201	1.99	0.44
1:A:202:GLY:HA3	15:A:814:CLA:HBB1	1.99	0.44
15:A:813:CLA:HBC1	15:A:814:CLA:H142	2.00	0.44
18:A:847:BCR:H20C	18:A:847:BCR:H361	1.78	0.44
2:B:414:ARG:HG2	2:B:417:ARG:NH2	2.33	0.44
15:B:803:CLA:H202	15:B:803:CLA:H162	1.81	0.44
15:B:837:CLA:H111	15:B:837:CLA:H142	1.72	0.44
2:O:158:GLN:O	2:O:162:ARG:HG3	2.18	0.44
2:O:257:PHE:HD2	2:O:499:VAL:HG23	1.82	0.44
15:O:809:CLA:H72	21:O:849:LMG:H273	2.00	0.44
15:O:831:CLA:H2	15:O:831:CLA:H62	1.79	0.44
18:W:209:BCR:H393	10:j:156:MET:HB3	2.00	0.44
2:b:398:TRP:HE1	18:b:846:BCR:H271	1.83	0.44
15:b:838:CLA:H151	12:l:33:LEU:HB3	1.99	0.44
1:A:491:GLN:HB3	20:A:852:LMT:H5B	1.99	0.44
15:A:805:CLA:HBA2	15:A:805:CLA:H3A	1.60	0.44
2:B:48:ALA:HB3	11:M:29:LEU:HD21	2.00	0.44
18:W:209:BCR:H24C	10:j:156:MET:SD	2.57	0.44
1:a:436:THR:HA	1:a:439:HIS:CE1	2.53	0.44
15:b:805:CLA:H61	15:b:805:CLA:H2	1.71	0.44
3:c:55:GLU:HG2	3:c:63:LEU:HD13	2.00	0.44
15:A:818:CLA:H111	15:A:818:CLA:H151	1.48	0.43
15:B:824:CLA:HBA2	15:B:824:CLA:H3A	1.75	0.43
1:N:214:HIS:HB2	15:N:815:CLA:CHC	2.48	0.43
1:N:456:PHE:O	1:N:460:ALA:HB3	2.18	0.43
15:N:812:CLA:H3A	15:N:812:CLA:HBA2	1.74	0.43
2:O:398:TRP:HE1	18:O:846:BCR:H271	1.83	0.43
16:O:841:PQN:H302	21:O:849:LMG:H191	2.00	0.43
7:T:23:LEU:HA	7:T:27:ILE:HB	2.00	0.43
15:b:804:CLA:H12	15:b:804:CLA:C4D	2.47	0.43
15:B:824:CLA:HMA1	18:B:846:BCR:H14C	2.00	0.43
1:N:27:TRP:CD1	15:N:812:CLA:H2	2.53	0.43
1:N:126:ASN:HB3	1:N:134:HIS:HB3	2.00	0.43
1:a:443:ILE:HG21	1:a:581:PHE:HE2	1.83	0.43
15:a:812:CLA:H91	15:a:812:CLA:H142	2.00	0.43
15:a:820:CLA:H201	15:a:822:CLA:H51	2.00	0.43
15:a:834:CLA:H61	15:a:834:CLA:H2	1.74	0.43
2:b:336:PHE:CD1	18:b:846:BCR:H391	2.53	0.43
15:b:829:CLA:H3A	15:b:830:CLA:OBD	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLY:HA2	2:B:569:PRO:HD3	2.00	0.43
15:A:810:CLA:H11	15:A:810:CLA:H52	1.79	0.43
2:B:655:TRP:CZ3	18:B:847:BCR:HC32	2.53	0.43
4:D:40:VAL:HG22	4:D:50:ILE:HG12	2.00	0.43
4:D:85:ILE:HD12	4:D:98:HIS:CD2	2.54	0.43
13:N:801:CL0:CGD	13:N:801:CL0:H8	2.48	0.43
15:N:814:CLA:H62	15:N:814:CLA:H41	1.57	0.43
15:O:806:CLA:H41	15:O:806:CLA:H61	1.49	0.43
10:W:176:LEU:HD12	7:g:18:TRP:CZ2	2.53	0.43
1:a:126:ASN:HB3	1:a:134:HIS:HB3	2.00	0.43
15:A:810:CLA:H61	18:J:102:BCR:H363	2.00	0.43
15:B:810:CLA:H122	15:B:810:CLA:H162	1.80	0.43
15:B:820:CLA:HMD1	18:B:842:BCR:H23C	1.99	0.43
9:K:21:SER:O	9:K:24:VAL:HG22	2.18	0.43
1:N:202:GLY:HA3	15:N:814:CLA:HBB1	2.01	0.43
21:W:206:LMG:H342	21:g:103:LMG:HC61	2.01	0.43
13:a:801:CL0:CGD	13:a:801:CL0:H8	2.47	0.43
1:A:318:HIS:NE2	15:A:823:CLA:ND	2.66	0.43
18:A:846:BCR:H20C	18:A:846:BCR:H361	1.80	0.43
18:J:102:BCR:H15C	18:J:102:BCR:H351	1.82	0.43
1:N:118:SER:HB3	6:S:49:TYR:CE1	2.53	0.43
15:O:817:CLA:H3A	15:O:817:CLA:HBA2	1.40	0.43
6:S:136:TRP:CG	6:S:137:PRO:HD3	2.52	0.43
8:U:24:VAL:O	8:U:28:MET:HG2	2.19	0.43
15:a:805:CLA:H3A	15:a:805:CLA:HBA2	1.58	0.43
1:A:318:HIS:CE1	15:A:823:CLA:NA	2.86	0.43
2:B:150:LEU:HD22	11:M:22:ALA:HA	2.00	0.43
15:B:824:CLA:H41	15:B:824:CLA:H61	1.67	0.43
21:L:207:LMG:H371	7:T:18:TRP:CE3	2.53	0.43
1:N:443:ILE:HG21	1:N:581:PHE:HE2	1.83	0.43
15:N:837:CLA:HED2	15:N:837:CLA:HBD	1.62	0.43
19:W:207:LHG:H312	19:k:101:LHG:H321	2.00	0.43
1:a:375:HIS:HA	1:a:378:TYR:CE1	2.54	0.43
15:b:808:CLA:C1A	15:b:808:CLA:CGA	2.97	0.43
15:b:824:CLA:H41	15:b:824:CLA:H61	1.74	0.43
15:b:837:CLA:H141	15:b:837:CLA:H161	1.73	0.43
15:A:820:CLA:HBA2	15:A:820:CLA:H3A	1.53	0.43
18:B:844:BCR:H24C	18:B:844:BCR:H371	1.86	0.43
1:N:761:HIS:CE1	15:N:842:CLA:NA	2.87	0.43
15:N:841:CLA:HBA2	2:O:428:TRP:CD1	2.54	0.43
2:O:4:LYS:HG3	7:T:44:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:806:CLA:H91	21:O:849:LMG:H421	2.00	0.43
18:U:102:BCR:H15C	18:U:102:BCR:H351	1.82	0.43
15:a:807:CLA:H193	15:a:807:CLA:H161	1.69	0.43
15:b:804:CLA:H41	15:b:804:CLA:H62	1.55	0.43
15:f:201:CLA:H141	15:f:201:CLA:H162	1.84	0.43
1:A:501:VAL:HG21	1:A:535:PRO:HA	2.01	0.43
15:A:819:CLA:H3A	15:A:819:CLA:HBA2	1.57	0.43
15:A:839:CLA:C4A	15:A:839:CLA:HBA2	2.48	0.43
2:B:454:GLU:HG3	6:F:55:PHE:CE1	2.53	0.43
15:B:804:CLA:HHC	15:B:806:CLA:OBD	2.19	0.43
15:B:805:CLA:HBA1	15:B:805:CLA:H3A	1.46	0.43
21:L:207:LMG:H191	22:L:209:LFA:H122	2.00	0.43
15:O:837:CLA:HMA3	15:O:838:CLA:HED2	1.99	0.43
19:W:207:LHG:H281	15:b:804:CLA:H43	1.99	0.43
15:a:804:CLA:H91	15:a:804:CLA:H112	1.72	0.43
15:b:803:CLA:CGA	15:b:803:CLA:H3A	2.48	0.43
15:b:806:CLA:HED3	15:b:828:CLA:H203	2.01	0.43
15:b:809:CLA:HBA1	15:b:809:CLA:H11	1.80	0.43
15:A:831:CLA:H142	15:A:831:CLA:H111	1.67	0.43
15:B:808:CLA:C1A	15:B:808:CLA:CGA	2.97	0.43
19:B:851:LHG:H362	19:j:207:LHG:H192	1.99	0.43
7:I:18:TRP:CZ2	10:j:176:LEU:HD12	2.54	0.43
15:N:836:CLA:H2	15:N:836:CLA:H62	1.63	0.43
2:O:106:ARG:NH2	2:O:115:ILE:HG12	2.34	0.43
2:O:111:ASN:HD22	7:T:10:SER:H	1.67	0.43
2:O:428:TRP:HZ3	15:O:838:CLA:HBC2	1.84	0.43
15:O:831:CLA:H151	15:O:831:CLA:H111	1.82	0.43
4:Q:40:VAL:HG22	4:Q:50:ILE:HG12	2.01	0.43
18:h:102:BCR:H341	18:h:102:BCR:H11C	1.81	0.43
1:A:527:THR:HG22	1:A:530:PRO:HG3	1.99	0.43
15:A:809:CLA:H91	15:A:809:CLA:H111	1.79	0.43
15:A:829:CLA:H62	15:A:829:CLA:H41	1.69	0.43
15:A:841:CLA:HBB2	6:F:101:GLY:HA3	2.01	0.43
15:B:828:CLA:H93	15:B:828:CLA:H112	1.76	0.43
15:B:838:CLA:H93	15:B:838:CLA:H62	1.73	0.43
15:B:840:CLA:H162	7:I:30:PHE:CZ	2.54	0.43
1:N:399:HIS:CE1	15:N:829:CLA:ND	2.86	0.43
1:N:740:VAL:HG23	6:S:102:ARG:HA	2.00	0.43
15:N:807:CLA:H193	15:N:807:CLA:H161	1.69	0.43
2:O:65:LEU:HD11	18:O:844:BCR:H281	2.00	0.43
2:O:194:LEU:HA	2:O:198:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:41:PRO:HB3	1:a:46:TRP:CE3	2.54	0.43
1:A:306:ALA:HB2	15:A:822:CLA:HBC2	1.99	0.42
1:A:731:ILE:HD13	15:A:841:CLA:HMD2	2.01	0.42
15:A:834:CLA:H61	15:A:834:CLA:H2	1.74	0.42
2:B:443:HIS:CE1	14:B:832:F6C:NA	2.87	0.42
5:E:32:ILE:HD11	5:E:35:PRO:HA	2.01	0.42
18:L:210:BCR:H393	10:W:156:MET:HB3	1.99	0.42
1:N:447:LEU:HD21	1:N:577:VAL:HG12	2.00	0.42
15:N:806:CLA:HBA1	15:N:806:CLA:H3A	1.53	0.42
2:O:279:ALA:HA	15:O:815:CLA:HMC2	2.01	0.42
1:a:697:SER:HB2	2:b:449:ALA:HB1	2.01	0.42
1:a:708:PHE:CD2	18:a:850:BCR:H363	2.54	0.42
2:b:497:ALA:HB3	15:b:834:CLA:HED1	1.99	0.42
2:b:514:SER:HA	2:b:517:LEU:HD21	1.99	0.42
2:b:555:PRO:HB3	6:f:160:PRO:HG3	2.00	0.42
15:f:201:CLA:H93	15:f:201:CLA:H62	1.82	0.42
2:B:452:ALA:HB1	2:B:455:LYS:HG3	2.01	0.42
1:N:41:PRO:HB3	1:N:46:TRP:CE3	2.54	0.42
1:N:708:PHE:CD2	18:N:850:BCR:H363	2.53	0.42
15:N:804:CLA:C1D	8:U:12:PRO:HG3	2.50	0.42
15:O:836:CLA:H52	15:O:836:CLA:H8	1.87	0.42
6:S:92:TYR:HE1	21:U:103:LMG:H452	1.84	0.42
7:T:22:PRO:HB3	7:T:26:TYR:CZ	2.54	0.42
8:U:29:LEU:HD23	8:U:29:LEU:HA	1.92	0.42
1:a:388:THR:HG21	1:a:547:VAL:HB	2.01	0.42
15:b:807:CLA:H11	15:b:807:CLA:C4D	2.49	0.42
18:f:202:BCR:H20C	18:f:202:BCR:H361	1.91	0.42
1:A:390:TYR:HB3	1:A:778:MET:HE3	2.01	0.42
1:A:726:GLU:O	1:A:729:GLU:HB2	2.20	0.42
15:A:837:CLA:HBD	15:A:837:CLA:HED2	1.74	0.42
21:I:103:LMG:HC61	21:j:206:LMG:H342	2.02	0.42
1:N:492:TRP:O	1:N:496:ILE:HG12	2.20	0.42
15:N:823:CLA:H61	15:N:823:CLA:H2	1.84	0.42
1:a:275:THR:HG21	1:a:277:LYS:HE3	2.02	0.42
1:a:295:HIS:HB2	15:a:819:CLA:CHB	2.50	0.42
1:a:361:ILE:HD11	18:a:848:BCR:HC7	2.01	0.42
2:b:443:HIS:CE1	14:b:832:F6C:NA	2.87	0.42
2:b:452:ALA:HB1	2:b:455:LYS:HG3	2.02	0.42
15:b:838:CLA:H62	15:b:838:CLA:H93	1.71	0.42
15:A:814:CLA:H143	15:A:814:CLA:H161	1.84	0.42
15:N:811:CLA:H62	20:N:854:LMT:H62	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:76:ARG:HB3	6:S:78:ASP:OD1	2.19	0.42
15:b:808:CLA:H91	15:b:809:CLA:H52	2.01	0.42
15:b:837:CLA:H161	15:b:837:CLA:H202	1.83	0.42
22:b:850:LFA:H132	22:b:850:LFA:H102	1.87	0.42
6:f:92:TYR:HE1	21:h:103:LMG:H452	1.85	0.42
1:A:202:GLY:O	1:A:206:LEU:HB2	2.20	0.42
1:A:608:PRO:HD3	2:B:568:GLY:HA2	2.00	0.42
15:A:809:CLA:O1A	15:A:829:CLA:H2	2.20	0.42
2:B:652:ILE:HD11	18:B:847:BCR:HC31	2.00	0.42
15:B:806:CLA:H193	15:B:806:CLA:H161	1.82	0.42
8:J:24:VAL:O	8:J:28:MET:HG2	2.19	0.42
1:N:628:TRP:HE1	15:O:803:CLA:C1D	2.32	0.42
1:N:715:MET:HA	15:N:803:CLA:HBC2	2.00	0.42
2:O:121:TYR:HB2	24:O:948:HOH:O	2.19	0.42
18:T:101:BCR:HC8	18:T:101:BCR:H331	2.00	0.42
18:U:102:BCR:H341	18:U:102:BCR:H11C	1.81	0.42
15:a:841:CLA:HBA2	2:b:428:TRP:CD1	2.55	0.42
18:b:848:BCR:H24C	18:b:848:BCR:H371	1.91	0.42
1:A:27:TRP:CD1	15:A:812:CLA:H2	2.55	0.42
15:A:819:CLA:HBB1	15:A:819:CLA:H92	2.02	0.42
2:B:121:TYR:HB2	24:B:953:HOH:O	2.20	0.42
1:N:607:GLY:HA2	2:O:569:PRO:HD3	2.02	0.42
15:N:810:CLA:H93	15:N:810:CLA:H112	1.72	0.42
15:N:819:CLA:H3A	15:N:819:CLA:HBA2	1.57	0.42
15:O:829:CLA:H201	18:O:845:BCR:H17C	2.01	0.42
15:O:838:CLA:H93	15:O:838:CLA:H62	1.71	0.42
4:Q:118:VAL:HG12	4:Q:120:ARG:HG2	2.02	0.42
1:a:456:PHE:O	1:a:460:ALA:HB3	2.19	0.42
1:a:501:VAL:HG21	1:a:535:PRO:HA	2.02	0.42
2:b:257:PHE:HE2	2:b:500:TRP:HB3	1.83	0.42
15:b:803:CLA:H202	15:b:803:CLA:H162	1.80	0.42
15:b:828:CLA:H161	15:b:828:CLA:H122	1.83	0.42
9:i:47:GLN:HA	9:i:63:SER:HB3	2.01	0.42
1:A:360:SER:HA	1:A:411:GLY:HA2	2.02	0.42
15:A:804:CLA:H91	15:A:804:CLA:H112	1.74	0.42
15:A:809:CLA:H62	15:A:809:CLA:H41	1.78	0.42
15:B:820:CLA:HBA1	15:B:820:CLA:H3A	1.82	0.42
15:O:808:CLA:H2	15:O:808:CLA:H102	2.01	0.42
15:O:813:CLA:H142	15:O:813:CLA:H112	1.79	0.42
6:S:96:PHE:CZ	6:S:130:ILE:HG23	2.54	0.42
21:W:206:LMG:H191	22:W:208:LFA:H122	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:471:PHE:CZ	2:b:95:GLN:HG3	2.55	0.42
15:a:815:CLA:HBA1	15:a:815:CLA:H3A	1.92	0.42
2:b:194:LEU:HA	2:b:198:ALA:HB3	2.00	0.42
1:A:295:HIS:HB2	15:A:819:CLA:CHB	2.49	0.42
2:B:222:LEU:HD23	2:B:222:LEU:HA	1.93	0.42
2:B:336:PHE:HE2	2:B:340:PHE:CZ	2.38	0.42
2:B:428:TRP:HZ3	15:B:838:CLA:HBC2	1.85	0.42
2:B:700:ARG:HH22	7:I:43:GLU:HG2	1.85	0.42
2:O:182:LEU:HD13	15:O:812:CLA:HHB	2.01	0.42
2:O:276:HIS:HB2	15:O:816:CLA:C1B	2.50	0.42
15:O:804:CLA:HHC	15:O:806:CLA:OBD	2.19	0.42
4:Q:96:MET:HE3	4:Q:96:MET:HB3	1.89	0.42
9:V:52:LEU:HD11	9:V:67:PHE:HB2	2.02	0.42
9:V:85:LEU:HD23	9:V:91:LEU:HB2	2.02	0.42
15:b:834:CLA:HBB1	15:b:834:CLA:HMB1	2.01	0.42
3:c:43:PRO:HA	4:d:115:VAL:HG11	2.02	0.42
21:j:206:LMG:H191	22:j:208:LFA:H122	2.01	0.42
1:A:75:HIS:NE2	15:A:806:CLA:ND	2.68	0.42
1:A:373:VAL:O	1:A:377:MET:HB2	2.19	0.42
15:N:831:CLA:H142	15:N:831:CLA:H111	1.68	0.42
15:O:808:CLA:CGA	15:O:808:CLA:C1A	2.97	0.42
15:O:828:CLA:H62	15:O:828:CLA:H41	1.72	0.42
18:T:101:BCR:HC7	18:T:101:BCR:H311	1.76	0.42
1:a:34:ASP:HB3	1:a:37:LEU:HB2	2.02	0.42
1:a:689:ILE:HG23	1:a:690:GLN:HG3	2.00	0.42
1:a:716:PHE:HA	16:a:843:PQN:H9	2.00	0.42
15:a:814:CLA:H102	15:a:814:CLA:H61	1.64	0.42
15:a:819:CLA:HBB1	15:a:819:CLA:H92	2.00	0.42
15:a:821:CLA:H3A	15:a:821:CLA:HBA2	1.66	0.42
15:b:804:CLA:HHC	15:b:806:CLA:OBD	2.20	0.42
16:b:841:PQN:H302	21:b:849:LMG:H191	2.02	0.42
1:A:414:HIS:HA	1:A:417:ILE:HD12	2.01	0.42
15:A:806:CLA:HBA1	15:A:806:CLA:H3A	1.54	0.42
21:A:855:LMG:H211	21:A:855:LMG:H182	1.87	0.42
2:B:276:HIS:HB2	15:B:816:CLA:CHB	2.49	0.42
15:B:813:CLA:H142	15:B:813:CLA:H112	1.76	0.42
1:N:566:HIS:CG	15:N:839:CLA:HED3	2.55	0.42
2:O:497:ALA:HB3	15:O:834:CLA:HED1	2.02	0.42
15:O:810:CLA:H151	18:O:843:BCR:H10C	2.02	0.42
4:Q:85:ILE:HD12	4:Q:98:HIS:CD2	2.55	0.42
1:a:399:HIS:CE1	15:a:829:CLA:ND	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:740:VAL:HG23	6:f:102:ARG:HA	2.01	0.42
15:a:804:CLA:C1D	8:h:12:PRO:HG3	2.50	0.42
15:a:806:CLA:H62	15:a:806:CLA:H2	1.71	0.42
2:b:4:LYS:HG3	7:g:44:ALA:HA	2.02	0.42
1:A:445:SER:HB2	2:B:688:ALA:HB2	2.02	0.41
15:A:831:CLA:H91	15:A:831:CLA:H112	1.88	0.41
15:B:807:CLA:C4D	15:B:807:CLA:H11	2.50	0.41
15:B:809:CLA:H72	21:B:848:LMG:H273	2.02	0.41
15:B:837:CLA:H141	15:B:837:CLA:H161	1.71	0.41
1:N:364:VAL:HG21	18:N:849:BCR:H331	2.01	0.41
18:N:849:BCR:H392	18:N:849:BCR:H24C	1.81	0.41
2:O:93:ASP:OD1	2:O:95:GLN:HG2	2.20	0.41
2:O:430:SER:HB3	2:O:536:VAL:HG22	2.00	0.41
1:a:364:VAL:HG21	18:a:849:BCR:H331	2.02	0.41
15:b:836:CLA:HBB1	15:b:836:CLA:HMB1	2.01	0.41
15:A:822:CLA:H93	15:A:822:CLA:H112	1.75	0.41
15:B:802:CLA:H142	15:B:802:CLA:H112	1.88	0.41
9:K:85:LEU:HD23	9:K:91:LEU:HB2	2.02	0.41
1:N:302:LEU:HG	15:N:822:CLA:HMC1	2.02	0.41
18:N:846:BCR:H20C	18:N:846:BCR:H361	1.80	0.41
2:O:301:ILE:HG21	15:O:823:CLA:HAC1	2.01	0.41
1:a:302:LEU:HG	15:a:822:CLA:HMC1	2.02	0.41
15:a:820:CLA:H93	15:a:820:CLA:H62	1.75	0.41
6:f:105:LEU:HD23	6:f:105:LEU:HA	1.93	0.41
15:A:803:CLA:O1A	2:B:431:LEU:HA	2.19	0.41
2:B:309:SER:O	15:B:821:CLA:HAA1	2.20	0.41
15:N:818:CLA:H62	15:N:818:CLA:H41	1.56	0.41
2:O:69:ALA:HB2	2:O:135:LEU:HB2	2.03	0.41
18:T:101:BCR:H382	18:T:101:BCR:H23C	2.03	0.41
18:W:209:BCR:H20C	18:W:209:BCR:H361	1.91	0.41
15:a:814:CLA:H161	15:a:814:CLA:H143	1.81	0.41
2:b:182:LEU:HD13	15:b:812:CLA:HHB	2.01	0.41
15:b:815:CLA:H92	15:b:815:CLA:H61	1.81	0.41
3:c:17:CYS:HB3	17:c:102:SF4:S4	2.61	0.41
1:A:381:PRO:HG2	1:A:387:ALA:HB2	2.03	0.41
1:A:635:MET:HE2	13:A:801:CL0:H60	2.02	0.41
2:B:78:ILE:HD12	2:B:125:TYR:CD1	2.55	0.41
2:B:484:ASN:HB3	2:B:487:SER:HB2	2.03	0.41
2:B:590:MET:HG2	15:B:824:CLA:HBC1	2.03	0.41
10:L:140:ASN:HB2	10:L:143:GLU:HG3	2.02	0.41
15:L:202:CLA:H72	19:L:208:LHG:H222	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:225:LEU:O	1:N:230:VAL:HG12	2.20	0.41
15:N:818:CLA:OBD	15:N:837:CLA:HED1	2.20	0.41
3:P:61:ASP:HA	3:P:62:PHE:HA	1.80	0.41
5:R:10:ILE:HB	5:R:17:TRP:O	2.21	0.41
6:S:105:LEU:HD23	6:S:105:LEU:HA	1.94	0.41
15:S:201:CLA:H141	15:S:201:CLA:H162	1.92	0.41
12:Z:28:ILE:HD13	12:Z:28:ILE:HA	1.92	0.41
2:b:121:TYR:HB2	24:b:952:HOH:O	2.21	0.41
15:b:803:CLA:H143	15:b:803:CLA:H111	1.93	0.41
18:g:101:BCR:H24C	18:g:101:BCR:H392	1.81	0.41
18:h:102:BCR:H15C	18:h:102:BCR:H351	1.81	0.41
18:h:102:BCR:H24C	18:h:102:BCR:H371	1.87	0.41
1:A:460:ALA:HB3	15:A:835:CLA:HAB	2.03	0.41
1:A:735:HIS:HE1	15:A:841:CLA:C4D	2.34	0.41
15:A:820:CLA:H61	15:A:820:CLA:H2	1.74	0.41
15:A:841:CLA:HBA2	2:B:428:TRP:CD1	2.55	0.41
6:F:60:LYS:HD2	8:J:46:PRO:HB3	2.03	0.41
18:J:102:BCR:H341	18:J:102:BCR:H11C	1.81	0.41
15:O:822:CLA:H2	15:O:822:CLA:H61	1.60	0.41
15:O:833:CLA:H12	15:O:833:CLA:H52	1.90	0.41
1:a:202:GLY:HA3	15:a:814:CLA:HBB1	2.02	0.41
15:a:803:CLA:O1A	2:b:431:LEU:HA	2.21	0.41
15:a:812:CLA:H92	15:a:812:CLA:H62	1.92	0.41
2:b:276:HIS:HB2	15:b:816:CLA:C1B	2.51	0.41
18:b:843:BCR:H24C	18:b:843:BCR:H371	1.91	0.41
18:g:101:BCR:HC7	18:g:101:BCR:H311	1.79	0.41
8:h:24:VAL:HG22	18:h:102:BCR:H341	2.02	0.41
1:A:98:ASN:HB3	1:A:133:PHE:CG	2.55	0.41
1:A:388:THR:HG21	1:A:547:VAL:HB	2.03	0.41
1:N:103:MET:HE3	1:N:103:MET:HB3	1.95	0.41
15:N:822:CLA:H143	15:N:822:CLA:H111	1.91	0.41
15:N:838:CLA:H3A	15:N:838:CLA:HBA1	1.74	0.41
2:O:387:MET:HE1	18:O:846:BCR:H361	2.02	0.41
15:O:805:CLA:HBD	15:O:805:CLA:H122	2.03	0.41
15:O:820:CLA:HBA2	18:O:842:BCR:H282	2.03	0.41
15:O:829:CLA:H71	15:O:829:CLA:H111	1.95	0.41
16:O:841:PQN:H211	16:O:841:PQN:H172	1.79	0.41
1:a:42:LYS:HA	1:a:42:LYS:HD2	1.88	0.41
15:a:836:CLA:H2	15:a:836:CLA:H62	1.60	0.41
18:a:846:BCR:H361	18:a:846:BCR:H20C	1.79	0.41
15:b:833:CLA:H12	15:b:833:CLA:H52	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:815:CLA:HBA1	15:A:815:CLA:H3A	1.95	0.41
15:B:812:CLA:H51	15:B:812:CLA:H11	1.85	0.41
15:B:829:CLA:H142	19:X:101:LHG:H281	2.02	0.41
6:F:136:TRP:CG	6:F:137:PRO:HD3	2.55	0.41
1:N:716:PHE:HA	16:N:843:PQN:H9	2.02	0.41
2:O:287:ALA:HB2	15:O:818:CLA:HBC2	2.01	0.41
15:O:824:CLA:HMA1	18:O:846:BCR:H14C	2.02	0.41
15:O:830:CLA:H92	15:O:830:CLA:H61	1.89	0.41
15:a:804:CLA:H12	15:a:804:CLA:H51	1.87	0.41
15:a:841:CLA:H2	15:a:841:CLA:H61	1.75	0.41
15:b:806:CLA:H61	15:b:806:CLA:H41	1.47	0.41
16:b:841:PQN:H172	16:b:841:PQN:H211	1.81	0.41
18:b:843:BCR:H20C	18:b:843:BCR:H361	1.95	0.41
15:A:806:CLA:H142	18:A:847:BCR:H372	2.02	0.41
15:B:834:CLA:HBB1	15:B:834:CLA:HMB1	2.02	0.41
1:N:402:TRP:HB3	15:N:829:CLA:HMC3	2.03	0.41
1:N:608:PRO:HD3	2:O:568:GLY:HA2	2.03	0.41
15:N:816:CLA:CBB	18:N:845:BCR:H382	2.50	0.41
15:N:825:CLA:H62	15:N:825:CLA:H41	1.61	0.41
2:O:235:GLN:O	2:O:253:ALA:HB2	2.21	0.41
2:O:293:THR:H	15:O:819:CLA:HED2	1.86	0.41
18:O:844:BCR:H24C	18:O:844:BCR:H371	1.85	0.41
18:W:209:BCR:H24C	18:W:209:BCR:H371	1.88	0.41
1:a:402:TRP:HB3	15:a:829:CLA:HMC3	2.02	0.41
15:a:810:CLA:H11	15:a:810:CLA:H52	1.78	0.41
15:b:822:CLA:H2	15:b:822:CLA:H61	1.61	0.41
1:A:419:MET:HE1	1:A:437:LEU:HD11	2.02	0.41
15:A:804:CLA:C1D	8:J:12:PRO:HG3	2.51	0.41
2:B:355:HIS:CE1	15:B:825:CLA:NB	2.89	0.41
15:B:803:CLA:CGA	15:B:803:CLA:H3A	2.50	0.41
15:B:803:CLA:HED3	18:B:847:BCR:H401	2.03	0.41
15:B:827:CLA:H3A	15:B:827:CLA:HBA2	1.70	0.41
5:E:51:ASN:HB3	5:E:53:PHE:CE2	2.56	0.41
18:I:101:BCR:H311	18:I:101:BCR:HC7	1.81	0.41
8:J:37:GLN:HE21	8:J:38:TYR:N	2.02	0.41
10:L:59:THR:O	10:L:63:ARG:HG3	2.21	0.41
15:N:813:CLA:H12	15:N:813:CLA:HBA2	1.89	0.41
2:O:196:HIS:CE1	15:O:814:CLA:NA	2.89	0.41
15:O:812:CLA:H11	15:O:812:CLA:H51	1.85	0.41
10:W:139:ARG:HA	10:W:139:ARG:HD3	1.88	0.41
18:W:209:BCR:H382	10:j:156:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:16:ASP:OD2	1:a:185:LYS:HE2	2.20	0.41
1:a:214:HIS:HB2	15:a:815:CLA:CHC	2.50	0.41
1:a:566:HIS:CG	15:a:839:CLA:HED3	2.55	0.41
15:a:811:CLA:H62	20:a:854:LMT:H62	2.03	0.41
15:b:820:CLA:HBA2	18:b:842:BCR:H282	2.02	0.41
9:i:85:LEU:HB3	9:i:90:TRP:HA	2.03	0.41
15:i:102:CLA:H3A	15:i:102:CLA:HBA2	1.58	0.41
10:j:59:THR:O	10:j:63:ARG:HG3	2.20	0.41
1:A:771:TRP:CE2	1:A:775:LEU:HD22	2.56	0.41
2:B:106:ARG:NH2	2:B:115:ILE:HG12	2.35	0.41
15:B:805:CLA:H2	15:B:805:CLA:H61	1.77	0.41
2:O:514:SER:HA	2:O:517:LEU:HD21	2.02	0.41
15:O:803:CLA:H122	18:T:101:BCR:H281	2.03	0.41
2:b:428:TRP:HZ3	15:b:838:CLA:HBC2	1.86	0.41
1:A:443:ILE:HG21	1:A:581:PHE:CE2	2.57	0.40
15:A:835:CLA:H62	15:A:835:CLA:H2	1.85	0.40
2:B:653:TRP:CZ2	2:B:732:ILE:HG21	2.56	0.40
18:B:846:BCR:H15C	18:B:846:BCR:H351	1.95	0.40
21:L:207:LMG:H342	21:T:103:LMG:HC61	2.03	0.40
1:N:454:LEU:HB3	1:N:571:PHE:HB2	2.03	0.40
15:N:808:CLA:HBB1	15:N:808:CLA:HMB1	2.02	0.40
15:N:820:CLA:H161	15:N:820:CLA:H202	1.76	0.40
15:O:801:CLA:H143	15:O:801:CLA:H111	1.91	0.40
1:a:280:LEU:HD21	1:a:381:PRO:HD2	2.03	0.40
15:a:842:CLA:H3A	15:a:842:CLA:HBA2	1.70	0.40
2:b:321:LEU:HD21	19:l:101:LHG:HC5	2.03	0.40
15:b:837:CLA:H52	15:b:837:CLA:H12	1.83	0.40
1:A:684:GLN:HB3	1:A:777:ARG:CD	2.52	0.40
2:B:50:HIS:NE2	15:B:805:CLA:NA	2.69	0.40
2:B:638:LEU:HD21	2:B:657:PHE:CD1	2.56	0.40
15:B:808:CLA:H141	15:B:808:CLA:H161	1.96	0.40
18:B:842:BCR:H20C	18:B:842:BCR:H361	1.80	0.40
1:N:652:VAL:HG22	1:N:658:VAL:HG22	2.03	0.40
15:N:809:CLA:O1A	15:N:829:CLA:H2	2.19	0.40
15:N:825:CLA:H51	15:N:825:CLA:H11	1.92	0.40
2:O:354:GLN:HA	2:O:357:TYR:HE1	1.86	0.40
21:W:206:LMG:H371	7:g:18:TRP:CE3	2.57	0.40
1:a:71:ILE:HG22	1:a:75:HIS:CE1	2.56	0.40
1:a:626:LEU:HD21	15:a:831:CLA:HBC1	2.03	0.40
18:a:845:BCR:H24C	18:a:845:BCR:H371	1.77	0.40
18:b:844:BCR:H20C	18:b:844:BCR:H361	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:23:LEU:HA	7:g:23:LEU:HD23	1.93	0.40
1:A:565:ILE:HD12	1:A:565:ILE:HA	1.95	0.40
15:A:816:CLA:CBB	18:A:845:BCR:H382	2.51	0.40
20:A:854:LMT:H101	20:A:854:LMT:H72	1.90	0.40
2:B:301:ILE:HG21	15:B:823:CLA:HAC1	2.03	0.40
1:N:202:GLY:O	1:N:206:LEU:HB2	2.22	0.40
15:N:819:CLA:H141	15:N:819:CLA:H161	1.86	0.40
15:O:827:CLA:H3A	15:O:827:CLA:HBA2	1.73	0.40
1:a:454:LEU:HB3	1:a:571:PHE:HB2	2.03	0.40
2:b:309:SER:O	15:b:821:CLA:HAA1	2.21	0.40
15:b:807:CLA:HBC2	11:k:12:LEU:HD23	2.02	0.40
4:d:85:ILE:HD12	4:d:98:HIS:CD2	2.57	0.40
1:A:532:ILE:HG22	1:A:534:ALA:O	2.21	0.40
1:A:589:GLY:HA2	1:A:596:LYS:HD3	2.04	0.40
1:N:295:HIS:HB2	15:N:819:CLA:CHB	2.51	0.40
15:N:820:CLA:O2D	15:N:820:CLA:H2A	2.21	0.40
2:O:452:ALA:HB1	2:O:455:LYS:HG3	2.03	0.40
18:O:842:BCR:H20C	18:O:842:BCR:H361	1.78	0.40
5:R:32:ILE:HD11	5:R:35:PRO:HA	2.03	0.40
1:a:295:HIS:CE1	15:a:819:CLA:ND	2.89	0.40
1:a:318:HIS:NE2	15:a:823:CLA:ND	2.69	0.40
1:a:729:GLU:CD	2:b:552:LYS:HB2	2.47	0.40
1:A:174:ALA:HB2	15:A:811:CLA:HBC2	2.03	0.40
15:A:813:CLA:H12	15:A:813:CLA:HBA2	1.92	0.40
15:A:830:CLA:HMB3	15:A:830:CLA:HBB1	2.03	0.40
15:A:837:CLA:HBA2	15:A:837:CLA:H3A	1.72	0.40
2:B:403:ASP:HB3	4:D:129:ALA:HB3	2.03	0.40
15:B:806:CLA:H61	15:B:806:CLA:H41	1.48	0.40
18:B:847:BCR:H371	18:B:847:BCR:H24C	1.88	0.40
15:N:809:CLA:H91	15:N:809:CLA:H111	1.81	0.40
2:O:309:SER:O	15:O:821:CLA:HAA1	2.22	0.40
19:W:207:LHG:H382	18:g:101:BCR:H332	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	749/782 (96%)	732 (98%)	17 (2%)	0	100	100
1	N	749/782 (96%)	736 (98%)	13 (2%)	0	100	100
1	a	749/782 (96%)	736 (98%)	13 (2%)	0	100	100
2	B	737/740 (100%)	722 (98%)	15 (2%)	0	100	100
2	O	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
2	b	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
3	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	P	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	D	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
4	Q	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
4	d	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
5	E	63/66 (96%)	63 (100%)	0	0	100	100
5	R	63/66 (96%)	63 (100%)	0	0	100	100
5	e	63/66 (96%)	63 (100%)	0	0	100	100
6	F	135/161 (84%)	132 (98%)	3 (2%)	0	100	100
6	S	135/161 (84%)	132 (98%)	3 (2%)	0	100	100
6	f	135/161 (84%)	132 (98%)	3 (2%)	0	100	100
7	I	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
7	T	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
7	g	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
8	J	44/46 (96%)	44 (100%)	0	0	100	100
8	U	44/46 (96%)	44 (100%)	0	0	100	100
8	h	44/46 (96%)	44 (100%)	0	0	100	100
9	K	71/80 (89%)	68 (96%)	3 (4%)	0	100	100
9	V	71/80 (89%)	69 (97%)	2 (3%)	0	100	100
9	i	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
10	L	170/183 (93%)	169 (99%)	1 (1%)	0	100	100
10	W	170/183 (93%)	170 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	j	170/183 (93%)	170 (100%)	0	0	100	100
11	M	29/32 (91%)	29 (100%)	0	0	100	100
11	Y	29/32 (91%)	29 (100%)	0	0	100	100
11	k	29/32 (91%)	29 (100%)	0	0	100	100
12	X	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
12	Z	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
12	l	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	6840/7179 (95%)	6716 (98%)	124 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/623 (96%)	600 (100%)	0	100	100
1	N	600/623 (96%)	600 (100%)	0	100	100
1	a	600/623 (96%)	600 (100%)	0	100	100
2	B	594/595 (100%)	594 (100%)	0	100	100
2	O	594/595 (100%)	594 (100%)	0	100	100
2	b	594/595 (100%)	594 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
3	P	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	114/116 (98%)	114 (100%)	0	100	100
4	Q	114/116 (98%)	114 (100%)	0	100	100
4	d	114/116 (98%)	114 (100%)	0	100	100
5	E	57/58 (98%)	57 (100%)	0	100	100
5	R	57/58 (98%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	57/58 (98%)	57 (100%)	0	100	100
6	F	116/135 (86%)	116 (100%)	0	100	100
6	S	116/135 (86%)	116 (100%)	0	100	100
6	f	116/135 (86%)	116 (100%)	0	100	100
7	I	37/44 (84%)	37 (100%)	0	100	100
7	T	37/44 (84%)	37 (100%)	0	100	100
7	g	37/44 (84%)	37 (100%)	0	100	100
8	J	41/41 (100%)	41 (100%)	0	100	100
8	U	41/41 (100%)	41 (100%)	0	100	100
8	h	41/41 (100%)	41 (100%)	0	100	100
9	K	60/65 (92%)	60 (100%)	0	100	100
9	V	60/65 (92%)	60 (100%)	0	100	100
9	i	60/65 (92%)	60 (100%)	0	100	100
10	L	135/146 (92%)	135 (100%)	0	100	100
10	W	135/146 (92%)	135 (100%)	0	100	100
10	j	135/146 (92%)	135 (100%)	0	100	100
11	M	26/27 (96%)	26 (100%)	0	100	100
11	Y	26/27 (96%)	26 (100%)	0	100	100
11	k	26/27 (96%)	26 (100%)	0	100	100
12	X	24/24 (100%)	24 (100%)	0	100	100
12	Z	24/24 (100%)	24 (100%)	0	100	100
12	l	24/24 (100%)	24 (100%)	0	100	100
All	All	5616/5829 (96%)	5616 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	180	HIS
1	A	223	ASN
2	B	76	GLN
2	B	111	ASN

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Mol	Chain	Res	Type
2	B	196	HIS
2	B	235	GLN
2	B	236	ASN
2	B	248	GLN
2	B	266	GLN
2	B	443	HIS
2	B	496	HIS
2	B	637	GLN
4	D	110	GLN
4	D	137	GLN
5	E	19	GLN
6	F	52	ASN
6	F	142	GLN
8	J	37	GLN
10	L	90	HIS
10	L	140	ASN
10	L	181	ASN
12	X	37	ASN
1	N	114	GLN
1	N	215	GLN
1	N	266	GLN
1	N	269	GLN
1	N	294	HIS
2	O	111	ASN
2	O	132	ASN
2	O	156	HIS
2	O	196	HIS
2	O	235	GLN
2	O	406	GLN
2	O	443	HIS
2	O	634	HIS
4	Q	110	GLN
4	Q	137	GLN
5	R	19	GLN
8	U	3	HIS
8	U	37	GLN
10	W	50	ASN
10	W	148	ASN
12	Z	37	ASN
1	a	114	GLN
1	a	153	ASN
1	a	178	HIS

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Mol	Chain	Res	Type
1	a	215	GLN
1	a	239	HIS
1	a	690	GLN
2	b	111	ASN
2	b	156	HIS
2	b	193	HIS
2	b	196	HIS
2	b	235	GLN
2	b	248	GLN
2	b	443	HIS
2	b	496	HIS
2	b	634	HIS
2	b	637	GLN
4	d	110	GLN
8	h	37	GLN
10	j	148	ASN
12	l	37	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 402 ligands modelled in this entry, 3 are monoatomic - leaving 399 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	810	2	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
14	F6C	L	204	24	72,74,74	1.59	8 (11%)	83,114,114	2.02	15 (18%)
15	CLA	O	833	2	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
15	CLA	b	822	2	59,63,73	1.30	9 (15%)	70,101,113	1.21	5 (7%)
19	LHG	Y	101	-	48,48,48	0.50	0	51,54,54	0.48	0
15	CLA	b	810	2	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	B	835	24	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
15	CLA	A	806	1	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
15	CLA	A	825	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	O	814	2	49,53,73	1.37	6 (12%)	58,89,113	1.46	6 (10%)
15	CLA	B	806	2	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
15	CLA	b	828	2	69,73,73	1.17	8 (11%)	82,113,113	1.30	8 (9%)
15	CLA	A	809	1	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
15	CLA	a	821	1	64,68,73	1.22	8 (12%)	76,107,113	1.29	6 (7%)
15	CLA	B	809	2	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
14	F6C	b	839	24	72,74,74	1.58	8 (11%)	83,114,114	2.07	15 (18%)
15	CLA	B	816	2	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
18	BCR	O	848	-	41,41,41	0.29	0	56,56,56	0.62	0
15	CLA	b	820	2	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
15	CLA	V	103	24	54,58,73	1.33	8 (14%)	64,95,113	1.40	6 (9%)
21	LMG	T	103	-	37,37,55	0.56	0	45,45,63	0.65	0
18	BCR	B	846	-	41,41,41	0.31	0	56,56,56	0.87	1 (1%)
15	CLA	B	831	2	69,73,73	1.16	7 (10%)	82,113,113	1.25	8 (9%)
15	CLA	O	801	2	69,73,73	1.17	8 (11%)	82,113,113	1.21	6 (7%)
15	CLA	N	808	1	49,53,73	1.38	7 (14%)	58,89,113	1.45	6 (10%)
18	BCR	S	202	-	41,41,41	0.30	0	56,56,56	0.51	0
20	LMT	A	852	-	32,32,36	0.56	0	43,43,47	0.69	0
15	CLA	N	842	1	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
15	CLA	O	835	24	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
18	BCR	N	846	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
15	CLA	b	809	2	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
19	LHG	N	851	-	41,41,48	0.54	0	44,47,54	0.49	0
15	CLA	A	837	1	55,59,73	1.31	7 (12%)	64,96,113	1.37	8 (12%)
20	LMT	N	853	-	29,29,36	0.56	0	40,40,47	1.42	4 (10%)
15	CLA	N	804	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	4 (4%)
15	CLA	A	804	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	LHG	F	204	-	48,48,48	0.50	0	51,54,54	0.46	0
15	CLA	O	820	2	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
15	CLA	N	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	4 (4%)
15	CLA	B	826	2	66,70,73	1.19	7 (10%)	78,109,113	1.25	5 (6%)
18	BCR	B	842	-	41,41,41	0.31	0	56,56,56	0.56	0
13	CL0	N	801	1	58,73,73	2.24	9 (15%)	60,113,113	1.63	13 (21%)
15	CLA	a	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	4 (4%)
18	BCR	A	847	-	41,41,41	0.31	0	56,56,56	0.60	0
15	CLA	O	807	2	69,73,73	1.16	7 (10%)	82,113,113	1.25	7 (8%)
15	CLA	A	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.33	5 (6%)
15	CLA	A	830	1	69,73,73	1.17	7 (10%)	82,113,113	1.24	7 (8%)
13	CL0	a	801	1	58,73,73	2.24	9 (15%)	60,113,113	1.63	13 (21%)
21	LMG	j	206	-	50,50,55	0.50	0	58,58,63	0.61	0
15	CLA	a	819	1	69,73,73	1.18	9 (13%)	82,113,113	1.25	6 (7%)
18	BCR	N	845	-	41,41,41	0.35	0	56,56,56	0.93	2 (3%)
19	LHG	j	207	-	48,48,48	0.50	0	51,54,54	0.46	0
15	CLA	A	839	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
15	CLA	a	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	7 (8%)
18	BCR	a	845	-	41,41,41	0.35	0	56,56,56	0.93	2 (3%)
15	CLA	A	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	4 (4%)
14	F6C	j	201	2	72,74,74	1.61	8 (11%)	83,114,114	1.97	14 (16%)
15	CLA	N	805	1,15	64,68,73	1.22	7 (10%)	76,107,113	1.29	4 (5%)
20	LMT	a	854	-	36,36,36	0.54	0	47,47,47	0.64	0
18	BCR	A	848	-	41,41,41	0.31	0	56,56,56	0.54	0
14	F6C	A	802	24	72,74,74	1.59	10 (13%)	83,114,114	2.01	14 (16%)
14	F6C	a	802	24	72,74,74	1.59	10 (13%)	83,114,114	1.99	13 (15%)
15	CLA	a	806	1	69,73,73	1.16	6 (8%)	82,113,113	1.24	5 (6%)
15	CLA	O	830	2	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
15	CLA	a	804	1	69,73,73	1.19	8 (11%)	82,113,113	1.26	4 (4%)
15	CLA	A	822	24	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	N	833	1	59,63,73	1.26	8 (13%)	70,101,113	1.34	6 (8%)
15	CLA	a	809	1	64,68,73	1.20	7 (10%)	76,107,113	1.29	6 (7%)
15	CLA	a	816	1	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
18	BCR	B	843	-	41,41,41	0.31	0	56,56,56	0.61	0
18	BCR	b	848	-	41,41,41	0.29	0	56,56,56	0.63	0
14	F6C	a	855	24	72,74,74	1.57	8 (11%)	83,114,114	2.08	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	F6C	a	826	24	72,74,74	1.61	8 (11%)	83,114,114	2.08	19 (22%)
18	BCR	U	102	-	41,41,41	0.37	0	56,56,56	1.30	8 (14%)
18	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.44	0
22	LFA	b	850	-	15,15,19	0.23	0	14,14,18	0.19	0
15	CLA	a	842	1	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	a	823	1	60,64,73	1.25	7 (11%)	71,102,113	1.35	6 (8%)
15	CLA	N	832	1	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
16	PQN	b	841	-	34,34,34	0.35	0	43,45,45	0.61	1 (2%)
15	CLA	B	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
15	CLA	j	202	10	69,73,73	1.16	8 (11%)	82,113,113	1.27	7 (8%)
18	BCR	F	202	-	41,41,41	0.32	0	56,56,56	0.94	2 (3%)
15	CLA	b	807	2	69,73,73	1.16	8 (11%)	82,113,113	1.25	7 (8%)
15	CLA	N	822	24	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	B	824	24	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
15	CLA	N	838	1	59,63,73	1.26	7 (11%)	70,101,113	1.32	5 (7%)
15	CLA	W	202	10	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
15	CLA	O	829	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
15	CLA	B	815	2	61,65,73	1.24	7 (11%)	72,103,113	1.34	8 (11%)
14	F6C	L	201	2	72,74,74	1.62	8 (11%)	83,114,114	1.94	13 (15%)
18	BCR	a	846	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
18	BCR	b	842	-	41,41,41	0.31	0	56,56,56	0.55	0
15	CLA	a	831	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
15	CLA	b	835	24	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
18	BCR	N	848	-	41,41,41	0.31	0	56,56,56	0.50	0
15	CLA	O	818	24	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
21	LMG	O	849	-	55,55,55	0.49	0	63,63,63	0.58	0
22	LFA	B	849	-	15,15,19	0.23	0	14,14,18	0.20	0
19	LHG	B	851	-	48,48,48	0.50	0	51,54,54	0.48	0
15	CLA	O	821	24	57,61,73	1.28	6 (10%)	67,98,113	1.39	8 (11%)
15	CLA	i	103	24	54,58,73	1.33	7 (12%)	64,95,113	1.38	6 (9%)
14	F6C	j	204	24	72,74,74	1.59	8 (11%)	83,114,114	2.04	16 (19%)
15	CLA	A	819	1	69,73,73	1.18	9 (13%)	82,113,113	1.25	6 (7%)
18	BCR	a	848	-	41,41,41	0.31	0	56,56,56	0.50	0
15	CLA	b	838	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
17	SF4	C	102	3	0,12,12	-	-	-	-	-
14	F6C	N	802	24	72,74,74	1.59	10 (13%)	83,114,114	1.98	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	F6C	W	204	24	72,74,74	1.59	8 (11%)	83,114,114	2.04	16 (19%)
21	LMG	L	207	-	50,50,55	0.50	0	58,58,63	0.61	0
14	F6C	B	839	24	72,74,74	1.58	8 (11%)	83,114,114	2.07	15 (18%)
15	CLA	A	838	1	59,63,73	1.26	7 (11%)	70,101,113	1.32	5 (7%)
15	CLA	B	819	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
14	F6C	b	832	2	72,74,74	1.60	9 (12%)	83,114,114	2.02	17 (20%)
15	CLA	N	814	1	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
19	LHG	f	203	-	48,48,48	0.50	0	51,54,54	0.46	0
18	BCR	J	102	-	41,41,41	0.38	0	56,56,56	1.28	9 (16%)
15	CLA	A	829	1	64,68,73	1.20	7 (10%)	76,107,113	1.25	5 (6%)
15	CLA	O	828	2	69,73,73	1.17	8 (11%)	82,113,113	1.30	8 (9%)
15	CLA	b	812	2	60,64,73	1.26	7 (11%)	71,102,113	1.37	6 (8%)
15	CLA	N	823	1	60,64,73	1.25	7 (11%)	71,102,113	1.34	5 (7%)
15	CLA	b	819	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
19	LHG	k	101	-	48,48,48	0.50	0	51,54,54	0.48	0
15	CLA	A	810	1	61,65,73	1.24	7 (11%)	72,103,113	1.36	7 (9%)
14	F6C	W	201	2	72,74,74	1.62	8 (11%)	83,114,114	1.94	13 (15%)
18	BCR	B	845	-	41,41,41	0.31	0	56,56,56	0.55	0
18	BCR	N	849	-	41,41,41	0.31	0	56,56,56	0.58	0
19	LHG	A	851	-	41,41,48	0.54	0	44,47,54	0.49	0
15	CLA	O	802	24	69,73,73	1.17	7 (10%)	82,113,113	1.21	6 (7%)
18	BCR	g	102	-	41,41,41	0.29	0	56,56,56	0.45	0
15	CLA	O	817	2	64,68,73	1.21	8 (12%)	76,107,113	1.24	4 (5%)
15	CLA	O	809	2	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	a	837	1	55,59,73	1.31	7 (12%)	64,96,113	1.37	8 (12%)
15	CLA	O	816	2	69,73,73	1.19	8 (11%)	82,113,113	1.25	6 (7%)
15	CLA	A	816	1	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
15	CLA	N	835	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
15	CLA	a	840	1	54,58,73	1.31	7 (12%)	64,95,113	1.40	6 (9%)
15	CLA	b	827	2	69,73,73	1.16	7 (10%)	82,113,113	1.23	8 (9%)
15	CLA	N	829	1	64,68,73	1.20	7 (10%)	76,107,113	1.25	5 (6%)
15	CLA	A	805	1,15	64,68,73	1.22	7 (10%)	76,107,113	1.29	5 (6%)
15	CLA	N	821	1	64,68,73	1.22	8 (12%)	76,107,113	1.29	6 (7%)
15	CLA	A	841	1	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
15	CLA	b	804	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	b	826	2	66,70,73	1.19	8 (12%)	78,109,113	1.25	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	SF4	C	101	3	0,12,12	-	-	-		
15	CLA	O	826	2	66,70,73	1.19	8 (12%)	78,109,113	1.25	5 (6%)
15	CLA	O	810	2	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
14	F6C	O	832	2	72,74,74	1.60	9 (12%)	83,114,114	2.02	17 (20%)
18	BCR	B	847	-	41,41,41	0.32	0	56,56,56	0.77	1 (1%)
15	CLA	B	837	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
21	LMG	I	103	-	37,37,55	0.56	0	45,45,63	0.65	0
15	CLA	A	823	1	60,64,73	1.25	7 (11%)	71,102,113	1.34	6 (8%)
15	CLA	B	840	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
18	BCR	g	101	-	41,41,41	0.33	0	56,56,56	0.71	0
18	BCR	L	205	-	41,41,41	0.32	0	56,56,56	0.63	0
15	CLA	N	841	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
15	CLA	N	836	1	58,62,73	1.27	8 (13%)	68,99,113	1.35	6 (8%)
15	CLA	N	818	1	69,73,73	1.16	9 (13%)	82,113,113	1.31	5 (6%)
15	CLA	N	831	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	7 (8%)
22	LFA	W	208	-	14,14,19	0.23	0	13,13,18	0.24	0
15	CLA	A	813	1	58,62,73	1.28	7 (12%)	68,99,113	1.36	7 (10%)
15	CLA	A	812	1,15	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
18	BCR	b	847	-	41,41,41	0.32	0	56,56,56	0.93	1 (1%)
15	CLA	B	812	2	60,64,73	1.26	8 (13%)	71,102,113	1.37	6 (8%)
15	CLA	X	102	12	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
21	LMG	N	855	-	44,44,55	0.53	0	52,52,63	0.63	0
19	LHG	W	207	-	48,48,48	0.50	0	51,54,54	0.46	0
20	LMT	N	852	-	32,32,36	0.56	0	43,43,47	0.68	0
15	CLA	b	833	2	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
15	CLA	O	825	2	69,73,73	1.17	9 (13%)	82,113,113	1.27	6 (7%)
18	BCR	W	209	-	41,41,41	0.29	0	56,56,56	0.64	0
15	CLA	A	831	1	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
15	CLA	l	102	12	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
21	LMG	B	850	-	44,44,55	0.53	0	52,52,63	0.64	0
15	CLA	b	815	2	61,65,73	1.24	7 (11%)	72,103,113	1.34	8 (11%)
15	CLA	a	838	1	59,63,73	1.26	7 (11%)	70,101,113	1.32	5 (7%)
15	CLA	O	823	24	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
15	CLA	A	815	1	59,63,73	1.27	7 (11%)	70,101,113	1.34	6 (8%)
15	CLA	B	818	24	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
17	SF4	N	844	2,1	0,12,12	-	-	-		
15	CLA	B	834	24	49,53,73	1.39	8 (16%)	58,89,113	1.42	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	M	101	-	41,41,41	0.31	0	56,56,56	0.65	1 (1%)
15	CLA	b	808	2	69,73,73	1.15	8 (11%)	82,113,113	1.29	8 (9%)
15	CLA	N	810	1	61,65,73	1.24	7 (11%)	72,103,113	1.36	7 (9%)
15	CLA	b	837	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
18	BCR	A	850	-	41,41,41	0.31	0	56,56,56	0.83	0
18	BCR	b	845	-	41,41,41	0.31	0	56,56,56	0.55	0
21	LMG	b	849	-	55,55,55	0.49	0	63,63,63	0.58	0
15	CLA	b	831	2	69,73,73	1.17	7 (10%)	82,113,113	1.26	8 (9%)
15	CLA	A	808	1	49,53,73	1.38	7 (14%)	58,89,113	1.44	6 (10%)
18	BCR	O	844	-	41,41,41	0.30	0	56,56,56	0.49	0
15	CLA	F	201	24	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
19	LHG	a	851	-	41,41,48	0.54	0	44,47,54	0.49	0
15	CLA	A	811	1	61,65,73	1.24	6 (9%)	72,103,113	1.31	5 (6%)
15	CLA	O	819	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
18	BCR	O	843	-	41,41,41	0.31	0	56,56,56	0.61	0
15	CLA	b	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	7 (8%)
22	LFA	L	209	-	14,14,19	0.23	0	13,13,18	0.22	0
16	PQN	B	841	-	34,34,34	0.35	0	43,45,45	0.62	1 (2%)
15	CLA	N	816	1	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
13	CL0	A	801	1	58,73,73	2.25	9 (15%)	60,113,113	1.62	13 (21%)
15	CLA	O	831	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
14	F6C	A	856	24	72,74,74	1.57	8 (11%)	83,114,114	2.08	15 (18%)
15	CLA	Z	102	12	59,63,73	1.27	7 (11%)	70,101,113	1.32	6 (8%)
15	CLA	a	805	1,15	64,68,73	1.22	7 (10%)	76,107,113	1.29	4 (5%)
16	PQN	a	843	-	34,34,34	0.35	0	43,45,45	0.61	1 (2%)
15	CLA	b	806	2	69,73,73	1.17	7 (10%)	82,113,113	1.27	4 (4%)
15	CLA	O	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	7 (8%)
15	CLA	N	820	1	69,73,73	1.17	8 (11%)	82,113,113	1.32	7 (8%)
15	CLA	B	836	2	69,73,73	1.17	7 (10%)	82,113,113	1.27	8 (9%)
15	CLA	a	812	1,15	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	O	805	2	69,73,73	1.16	7 (10%)	82,113,113	1.28	8 (9%)
15	CLA	N	807	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
15	CLA	a	813	1	58,62,73	1.28	7 (12%)	68,99,113	1.36	7 (10%)
20	LMT	A	854	-	36,36,36	0.54	0	47,47,47	0.64	0
18	BCR	a	850	-	41,41,41	0.31	0	56,56,56	0.84	0
15	CLA	O	806	2	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
18	BCR	T	102	-	41,41,41	0.29	0	56,56,56	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	L	203	10	64,68,73	1.21	8 (12%)	76,107,113	1.30	7 (9%)
18	BCR	L	210	-	41,41,41	0.29	0	56,56,56	0.66	0
15	CLA	A	835	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	O	813	2	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
15	CLA	B	813	2	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
15	CLA	a	822	24	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	a	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.33	6 (7%)
18	BCR	a	847	-	41,41,41	0.31	0	56,56,56	0.63	1 (1%)
15	CLA	N	815	1	59,63,73	1.27	7 (11%)	70,101,113	1.34	5 (7%)
15	CLA	A	820	1	69,73,73	1.16	8 (11%)	82,113,113	1.34	8 (9%)
17	SF4	P	101	3	0,12,12	-	-	-	-	-
14	F6C	a	824	24	58,60,74	1.79	7 (12%)	65,97,114	2.22	14 (21%)
15	CLA	A	827	24	59,63,73	1.25	7 (11%)	70,101,113	1.38	8 (11%)
18	BCR	O	846	-	41,41,41	0.32	0	56,56,56	0.80	2 (3%)
15	CLA	a	827	24	59,63,73	1.25	7 (11%)	70,101,113	1.37	7 (10%)
15	CLA	b	824	24	69,73,73	1.17	7 (10%)	82,113,113	1.28	7 (8%)
18	BCR	O	845	-	41,41,41	0.31	0	56,56,56	0.55	0
15	CLA	A	807	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
15	CLA	N	830	1	69,73,73	1.17	7 (10%)	82,113,113	1.24	6 (7%)
18	BCR	N	850	-	41,41,41	0.31	0	56,56,56	0.83	0
15	CLA	A	832	1	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
15	CLA	W	203	10	64,68,73	1.21	8 (12%)	76,107,113	1.31	7 (9%)
15	CLA	B	838	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
19	LHG	L	208	-	48,48,48	0.50	0	51,54,54	0.46	0
15	CLA	O	815	2	61,65,73	1.24	7 (11%)	72,103,113	1.33	7 (9%)
15	CLA	b	818	24	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	N	811	1	61,65,73	1.24	8 (13%)	72,103,113	1.31	5 (6%)
15	CLA	B	827	2	69,73,73	1.16	7 (10%)	82,113,113	1.22	7 (8%)
15	CLA	N	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	7 (8%)
18	BCR	Y	102	-	41,41,41	0.31	0	56,56,56	0.65	1 (1%)
15	CLA	B	808	2	69,73,73	1.15	7 (10%)	82,113,113	1.27	8 (9%)
15	CLA	O	824	24	69,73,73	1.16	7 (10%)	82,113,113	1.29	7 (8%)
15	CLA	a	811	1	61,65,73	1.24	6 (9%)	72,103,113	1.31	5 (6%)
15	CLA	b	829	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
20	LMT	A	853	-	29,29,36	0.56	0	40,40,47	1.41	4 (10%)
15	CLA	a	832	1	54,58,73	1.31	8 (14%)	64,95,113	1.39	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	L	202	10	69,73,73	1.16	8 (11%)	82,113,113	1.27	7 (8%)
21	LMG	B	848	-	55,55,55	0.49	0	63,63,63	0.59	0
17	SF4	c	101	3	0,12,12	-	-	-	-	-
15	CLA	N	819	1	69,73,73	1.18	9 (13%)	82,113,113	1.25	6 (7%)
14	F6C	N	856	24	72,74,74	1.57	8 (11%)	83,114,114	2.08	15 (18%)
15	CLA	N	825	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
18	BCR	F	203	-	41,41,41	0.30	0	56,56,56	0.52	0
15	CLA	a	814	1	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
15	CLA	a	833	1	59,63,73	1.26	8 (13%)	70,101,113	1.35	6 (8%)
18	BCR	V	101	-	25,25,41	0.52	1 (4%)	33,33,56	0.50	0
15	CLA	O	834	24	49,53,73	1.38	8 (16%)	58,89,113	1.43	7 (12%)
14	F6C	N	826	24	72,74,74	1.61	8 (11%)	83,114,114	2.03	15 (18%)
15	CLA	b	816	2	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
14	F6C	O	839	24	72,74,74	1.58	8 (11%)	83,114,114	2.07	15 (18%)
15	CLA	O	804	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
18	BCR	a	849	-	41,41,41	0.31	0	56,56,56	0.57	0
19	LHG	X	101	-	43,43,48	0.52	0	46,49,54	0.48	0
15	CLA	B	814	2	49,53,73	1.38	6 (12%)	58,89,113	1.45	6 (10%)
18	BCR	f	202	-	41,41,41	0.30	0	56,56,56	0.51	0
21	LMG	g	103	-	37,37,55	0.56	0	45,45,63	0.64	0
18	BCR	K	101	-	25,25,41	0.52	1 (4%)	33,33,56	0.51	0
15	CLA	a	835	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
18	BCR	N	847	-	41,41,41	0.30	0	56,56,56	0.60	1 (1%)
15	CLA	B	801	2	69,73,73	1.17	8 (11%)	82,113,113	1.21	6 (7%)
15	CLA	B	805	2	69,73,73	1.16	7 (10%)	82,113,113	1.28	7 (8%)
18	BCR	j	205	-	41,41,41	0.32	0	56,56,56	0.62	0
14	F6C	N	824	24	58,60,74	1.79	8 (13%)	65,97,114	2.22	14 (21%)
18	BCR	b	846	-	41,41,41	0.31	0	56,56,56	0.86	2 (3%)
15	CLA	b	840	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	a	836	1	58,62,73	1.27	8 (13%)	68,99,113	1.35	7 (10%)
15	CLA	b	805	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	7 (8%)
21	LMG	h	103	-	55,55,55	0.49	0	63,63,63	0.59	0
18	BCR	A	846	-	41,41,41	0.32	0	56,56,56	0.65	1 (1%)
15	CLA	B	820	2	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
15	CLA	V	102	9	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
18	BCR	h	102	-	41,41,41	0.38	0	56,56,56	1.31	8 (14%)
18	BCR	I	101	-	41,41,41	0.33	0	56,56,56	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	b	825	2	69,73,73	1.17	9 (13%)	82,113,113	1.27	6 (7%)
15	CLA	K	103	24	54,58,73	1.33	8 (14%)	64,95,113	1.40	6 (9%)
18	BCR	A	845	-	41,41,41	0.35	0	56,56,56	0.93	2 (3%)
15	CLA	a	808	1	49,53,73	1.38	7 (14%)	58,89,113	1.44	6 (10%)
15	CLA	O	840	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	B	807	2	69,73,73	1.16	8 (11%)	82,113,113	1.25	7 (8%)
14	F6C	A	824	24	58,60,74	1.79	8 (13%)	65,97,114	2.22	14 (21%)
15	CLA	N	813	1	58,62,73	1.28	7 (12%)	68,99,113	1.36	7 (10%)
15	CLA	O	822	2	59,63,73	1.27	8 (13%)	70,101,113	1.34	6 (8%)
15	CLA	b	801	2	69,73,73	1.17	7 (10%)	82,113,113	1.21	6 (7%)
15	CLA	f	201	24	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
20	LMT	a	853	-	29,29,36	0.56	0	40,40,47	1.41	4 (10%)
15	CLA	b	821	24	57,61,73	1.28	6 (10%)	67,98,113	1.38	8 (11%)
15	CLA	b	814	2	49,53,73	1.37	6 (12%)	58,89,113	1.45	5 (8%)
22	LFA	j	208	-	14,14,19	0.23	0	13,13,18	0.23	0
15	CLA	b	817	2	64,68,73	1.21	8 (12%)	76,107,113	1.25	4 (5%)
18	BCR	O	847	-	41,41,41	0.31	0	56,56,56	0.93	1 (1%)
20	LMT	a	852	-	32,32,36	0.56	0	43,43,47	0.69	0
15	CLA	A	840	1	54,58,73	1.32	7 (12%)	64,95,113	1.39	6 (9%)
15	CLA	i	102	9	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
18	BCR	U	101	-	41,41,41	0.31	0	56,56,56	0.48	0
15	CLA	b	823	24	69,73,73	1.17	8 (11%)	82,113,113	1.30	5 (6%)
15	CLA	A	821	1	64,68,73	1.22	8 (12%)	76,107,113	1.29	6 (7%)
15	CLA	B	802	24	69,73,73	1.17	6 (8%)	82,113,113	1.22	6 (7%)
15	CLA	a	830	1	69,73,73	1.17	7 (10%)	82,113,113	1.23	7 (8%)
15	CLA	b	834	24	49,53,73	1.39	8 (16%)	58,89,113	1.41	7 (12%)
18	BCR	T	101	-	41,41,41	0.33	0	56,56,56	0.71	0
22	LFA	O	850	-	15,15,19	0.23	0	14,14,18	0.19	0
18	BCR	L	206	-	41,41,41	0.30	0	56,56,56	0.67	0
15	CLA	N	817	24	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
21	LMG	J	103	-	55,55,55	0.49	0	63,63,63	0.59	0
15	CLA	B	830	2	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
16	PQN	O	841	-	34,34,34	0.35	0	43,45,45	0.61	1 (2%)
15	CLA	N	828	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
17	SF4	a	844	2,1	0,12,12	-	-	-	-	-
15	CLA	A	828	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	O	837	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	8 (9%)
15	CLA	O	838	2	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
21	LMG	A	855	-	44,44,55	0.53	0	52,52,63	0.63	0
20	LMT	N	854	-	36,36,36	0.54	0	47,47,47	0.64	0
18	BCR	h	101	-	41,41,41	0.31	0	56,56,56	0.48	0
15	CLA	N	840	1	54,58,73	1.31	7 (12%)	64,95,113	1.39	6 (9%)
15	CLA	N	809	1	64,68,73	1.21	8 (12%)	76,107,113	1.28	6 (7%)
15	CLA	A	817	24	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
15	CLA	B	833	2	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
15	CLA	B	825	2	69,73,73	1.17	9 (13%)	82,113,113	1.28	7 (8%)
15	CLA	K	102	9	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
18	BCR	B	844	-	41,41,41	0.30	0	56,56,56	0.47	0
15	CLA	a	820	1	69,73,73	1.17	8 (11%)	82,113,113	1.36	8 (9%)
19	LHG	l	101	-	43,43,48	0.52	0	46,49,54	0.48	0
17	SF4	A	844	2,1	0,12,12	-	-	-	-	-
15	CLA	B	822	2	59,63,73	1.31	9 (15%)	70,101,113	1.21	5 (7%)
18	BCR	b	843	-	41,41,41	0.30	0	56,56,56	0.61	0
15	CLA	b	811	2	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
17	SF4	P	102	3	0,12,12	-	-	-	-	-
18	BCR	W	205	-	41,41,41	0.32	0	56,56,56	0.58	0
19	LHG	N	857	-	48,48,48	0.50	0	51,54,54	0.46	0
15	CLA	a	807	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
15	CLA	a	841	1	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
15	CLA	N	837	1	55,59,73	1.31	7 (12%)	64,96,113	1.37	7 (10%)
15	CLA	a	810	1	61,65,73	1.24	7 (11%)	72,103,113	1.36	7 (9%)
18	BCR	i	101	-	25,25,41	0.52	1 (4%)	33,33,56	0.51	0
15	CLA	b	830	2	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
18	BCR	J	101	-	41,41,41	0.31	0	56,56,56	0.49	0
15	CLA	A	836	1	58,62,73	1.27	8 (13%)	68,99,113	1.35	6 (8%)
15	CLA	b	813	2	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
16	PQN	A	843	-	34,34,34	0.35	0	43,45,45	0.60	1 (2%)
15	CLA	a	829	1	64,68,73	1.21	7 (10%)	76,107,113	1.25	5 (6%)
15	CLA	O	812	2	60,64,73	1.26	8 (13%)	71,102,113	1.37	6 (8%)
15	CLA	B	821	24	57,61,73	1.28	6 (10%)	67,98,113	1.38	8 (11%)
18	BCR	k	102	-	41,41,41	0.31	0	56,56,56	0.65	1 (1%)
15	CLA	b	836	2	69,73,73	1.17	8 (11%)	82,113,113	1.27	8 (9%)
18	BCR	O	842	-	41,41,41	0.31	0	56,56,56	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	b	844	-	41,41,41	0.30	0	56,56,56	0.48	0
19	LHG	Z	101	-	43,43,48	0.52	0	46,49,54	0.48	0
14	F6C	A	826	24	72,74,74	1.61	8 (11%)	83,114,114	2.03	16 (19%)
15	CLA	N	827	24	59,63,73	1.26	7 (11%)	70,101,113	1.38	8 (11%)
15	CLA	A	842	1	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
15	CLA	B	829	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
15	CLA	B	828	2	69,73,73	1.16	8 (11%)	82,113,113	1.30	8 (9%)
14	F6C	B	832	2	72,74,74	1.60	9 (12%)	83,114,114	2.02	17 (20%)
15	CLA	N	839	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
15	CLA	O	836	2	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
18	BCR	A	849	-	41,41,41	0.31	0	56,56,56	0.57	0
15	CLA	A	833	1	59,63,73	1.26	8 (13%)	70,101,113	1.34	6 (8%)
15	CLA	a	839	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	j	203	10	64,68,73	1.21	8 (12%)	76,107,113	1.31	7 (9%)
15	CLA	a	825	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	a	817	24	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
15	CLA	B	811	2	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
15	CLA	B	804	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	O	827	2	69,73,73	1.16	8 (11%)	82,113,113	1.22	7 (8%)
15	CLA	a	815	1	59,63,73	1.27	8 (13%)	70,101,113	1.33	6 (8%)
15	CLA	N	806	1	69,73,73	1.16	6 (8%)	82,113,113	1.25	5 (6%)
15	CLA	O	808	2	69,73,73	1.15	7 (10%)	82,113,113	1.30	8 (9%)
15	CLA	A	814	1	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
17	SF4	c	102	3	0,12,12	-	-	-	-	-
16	PQN	N	843	-	34,34,34	0.34	0	43,45,45	0.60	1 (2%)
15	CLA	O	811	2	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
15	CLA	a	828	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
15	CLA	B	817	2	64,68,73	1.21	8 (12%)	76,107,113	1.25	4 (5%)
21	LMG	W	206	-	50,50,55	0.50	0	58,58,63	0.60	0
15	CLA	B	823	24	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
15	CLA	S	201	24	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	b	802	24	69,73,73	1.17	6 (8%)	82,113,113	1.22	6 (7%)
15	CLA	N	812	1,15	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	A	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	8 (9%)
21	LMG	U	103	-	55,55,55	0.49	0	63,63,63	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	810	2	1/1/15/20	11/39/115/115	-
14	F6C	L	204	24	1/1/10/16	11/41/97/97	-
15	CLA	O	833	2	1/1/13/20	8/27/103/115	-
15	CLA	b	822	2	1/1/13/20	8/27/103/115	-
19	LHG	Y	101	-	-	17/53/53/53	-
15	CLA	b	810	2	1/1/15/20	12/39/115/115	-
15	CLA	B	835	24	1/1/11/20	10/15/91/115	-
15	CLA	A	806	1	1/1/15/20	15/39/115/115	-
15	CLA	A	825	1	1/1/15/20	10/39/115/115	-
15	CLA	O	814	2	1/1/11/20	5/15/91/115	-
15	CLA	B	806	2	1/1/15/20	20/39/115/115	-
15	CLA	b	828	2	1/1/15/20	15/39/115/115	-
15	CLA	A	809	1	1/1/14/20	16/33/109/115	-
15	CLA	a	821	1	1/1/14/20	4/33/109/115	-
15	CLA	B	809	2	1/1/15/20	13/39/115/115	-
14	F6C	b	839	24	1/1/10/16	13/41/97/97	-
15	CLA	B	816	2	1/1/15/20	11/39/115/115	-
18	BCR	O	848	-	-	3/29/63/63	0/2/2/2
15	CLA	b	820	2	1/1/11/20	2/15/91/115	-
15	CLA	V	103	24	1/1/12/20	4/21/97/115	-
21	LMG	T	103	-	-	15/32/52/70	0/1/1/1
18	BCR	B	846	-	-	0/29/63/63	0/2/2/2
15	CLA	B	831	2	1/1/15/20	10/39/115/115	-
15	CLA	O	801	2	1/1/15/20	10/39/115/115	-
15	CLA	N	808	1	1/1/11/20	0/15/91/115	-
18	BCR	S	202	-	-	2/29/63/63	0/2/2/2
20	LMT	A	852	-	-	0/17/57/61	0/2/2/2
15	CLA	N	842	1	1/1/15/20	15/39/115/115	-
15	CLA	O	835	24	1/1/11/20	10/15/91/115	-
18	BCR	N	846	-	-	7/29/63/63	0/2/2/2
15	CLA	b	809	2	1/1/15/20	16/39/115/115	-
19	LHG	N	851	-	-	12/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	837	1	1/1/12/20	8/23/99/115	-
20	LMT	N	853	-	-	8/14/54/61	0/2/2/2
15	CLA	N	804	1	1/1/15/20	5/39/115/115	-
15	CLA	A	804	1	1/1/15/20	5/39/115/115	-
19	LHG	F	204	-	-	24/53/53/53	-
15	CLA	O	820	2	1/1/11/20	2/15/91/115	-
15	CLA	N	834	1	1/1/15/20	7/39/115/115	-
15	CLA	B	826	2	1/1/14/20	13/36/112/115	-
18	BCR	B	842	-	-	3/29/63/63	0/2/2/2
13	CL0	N	801	1	3/3/20/25	9/37/135/135	-
15	CLA	a	834	1	1/1/15/20	6/39/115/115	-
18	BCR	A	847	-	-	4/29/63/63	0/2/2/2
15	CLA	O	807	2	1/1/15/20	4/39/115/115	-
15	CLA	A	818	1	1/1/15/20	21/39/115/115	-
15	CLA	A	830	1	1/1/15/20	7/39/115/115	-
13	CL0	a	801	1	3/3/20/25	9/37/135/135	-
21	LMG	j	206	-	-	10/45/65/70	0/1/1/1
15	CLA	a	819	1	1/1/15/20	11/39/115/115	-
18	BCR	N	845	-	-	3/29/63/63	0/2/2/2
19	LHG	j	207	-	-	12/53/53/53	-
15	CLA	A	839	1	1/1/15/20	18/39/115/115	-
15	CLA	a	803	-	1/1/15/20	9/39/115/115	-
18	BCR	a	845	-	-	3/29/63/63	0/2/2/2
15	CLA	A	834	1	1/1/15/20	6/39/115/115	-
14	F6C	j	201	2	1/1/10/16	8/41/97/97	-
15	CLA	N	805	1,15	1/1/14/20	9/33/109/115	-
20	LMT	a	854	-	-	4/21/61/61	0/2/2/2
18	BCR	A	848	-	-	6/29/63/63	0/2/2/2
14	F6C	A	802	24	1/1/10/16	7/41/97/97	-
14	F6C	a	802	24	1/1/10/16	7/41/97/97	-
15	CLA	a	806	1	1/1/15/20	16/39/115/115	-
15	CLA	O	830	2	1/1/15/20	11/39/115/115	-
15	CLA	a	804	1	1/1/15/20	5/39/115/115	-
15	CLA	A	822	24	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	833	1	1/1/13/20	3/27/103/115	-
15	CLA	a	809	1	1/1/14/20	12/33/109/115	-
15	CLA	a	816	1	1/1/11/20	6/15/91/115	-
18	BCR	B	843	-	-	3/29/63/63	0/2/2/2
18	BCR	b	848	-	-	3/29/63/63	0/2/2/2
14	F6C	a	855	24	1/1/10/16	14/41/97/97	-
14	F6C	a	826	24	1/1/10/16	17/41/97/97	-
18	BCR	U	102	-	-	8/29/63/63	0/2/2/2
18	BCR	I	102	-	-	4/29/63/63	0/2/2/2
22	LFA	b	850	-	-	5/13/13/17	-
15	CLA	a	842	1	1/1/15/20	15/39/115/115	-
15	CLA	a	823	1	1/1/13/20	6/29/105/115	-
15	CLA	N	832	1	1/1/12/20	2/21/97/115	-
16	PQN	b	841	-	-	0/23/43/43	0/2/2/2
15	CLA	B	803	-	1/1/15/20	5/39/115/115	-
15	CLA	j	202	10	1/1/15/20	4/39/115/115	-
18	BCR	F	202	-	-	6/29/63/63	0/2/2/2
15	CLA	b	807	2	1/1/15/20	4/39/115/115	-
15	CLA	N	822	24	1/1/15/20	14/39/115/115	-
15	CLA	B	824	24	1/1/15/20	14/39/115/115	-
15	CLA	N	838	1	1/1/13/20	11/27/103/115	-
15	CLA	W	202	10	1/1/15/20	5/39/115/115	-
15	CLA	O	829	2	1/1/15/20	15/39/115/115	-
15	CLA	B	815	2	1/1/13/20	6/30/106/115	-
14	F6C	L	201	2	1/1/10/16	8/41/97/97	-
18	BCR	a	846	-	-	8/29/63/63	0/2/2/2
18	BCR	b	842	-	-	3/29/63/63	0/2/2/2
15	CLA	a	831	1	1/1/15/20	12/39/115/115	-
15	CLA	b	835	24	1/1/11/20	10/15/91/115	-
18	BCR	N	848	-	-	5/29/63/63	0/2/2/2
15	CLA	O	818	24	1/1/15/20	8/39/115/115	-
21	LMG	O	849	-	-	5/50/70/70	0/1/1/1
22	LFA	B	849	-	-	5/13/13/17	-
19	LHG	B	851	-	-	17/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	O	821	24	1/1/12/20	9/25/101/115	-
15	CLA	i	103	24	1/1/12/20	2/21/97/115	-
14	F6C	j	204	24	1/1/10/16	9/41/97/97	-
15	CLA	A	819	1	1/1/15/20	13/39/115/115	-
18	BCR	a	848	-	-	6/29/63/63	0/2/2/2
15	CLA	b	838	2	1/1/15/20	8/39/115/115	-
17	SF4	C	102	3	-	-	0/6/5/5
14	F6C	N	802	24	1/1/10/16	9/41/97/97	-
14	F6C	W	204	24	1/1/10/16	10/41/97/97	-
21	LMG	L	207	-	-	10/45/65/70	0/1/1/1
14	F6C	B	839	24	1/1/10/16	13/41/97/97	-
15	CLA	A	838	1	1/1/13/20	10/27/103/115	-
15	CLA	B	819	2	1/1/13/20	12/27/103/115	-
14	F6C	b	832	2	1/1/10/16	5/41/97/97	-
15	CLA	N	814	1	1/1/15/20	8/39/115/115	-
19	LHG	f	203	-	-	26/53/53/53	-
18	BCR	J	102	-	-	8/29/63/63	0/2/2/2
15	CLA	A	829	1	1/1/14/20	17/33/109/115	-
15	CLA	O	828	2	1/1/15/20	13/39/115/115	-
15	CLA	b	812	2	-	11/29/105/115	-
15	CLA	N	823	1	1/1/13/20	6/29/105/115	-
15	CLA	b	819	2	1/1/13/20	12/27/103/115	-
19	LHG	k	101	-	-	15/53/53/53	-
15	CLA	A	810	1	1/1/13/20	7/30/106/115	-
14	F6C	W	201	2	1/1/10/16	8/41/97/97	-
18	BCR	B	845	-	-	8/29/63/63	0/2/2/2
18	BCR	N	849	-	-	3/29/63/63	0/2/2/2
19	LHG	A	851	-	-	12/46/46/53	-
15	CLA	O	802	24	1/1/15/20	12/39/115/115	-
18	BCR	g	102	-	-	4/29/63/63	0/2/2/2
15	CLA	O	817	2	1/1/14/20	13/33/109/115	-
15	CLA	O	809	2	1/1/15/20	15/39/115/115	-
15	CLA	a	837	1	1/1/12/20	8/23/99/115	-
15	CLA	O	816	2	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	816	1	1/1/11/20	6/15/91/115	-
15	CLA	N	835	1	1/1/15/20	9/39/115/115	-
15	CLA	a	840	1	1/1/12/20	0/21/97/115	-
15	CLA	b	827	2	1/1/15/20	6/39/115/115	-
15	CLA	N	829	1	1/1/14/20	15/33/109/115	-
15	CLA	A	805	1,15	1/1/14/20	9/33/109/115	-
15	CLA	N	821	1	1/1/14/20	6/33/109/115	-
15	CLA	A	841	1	1/1/15/20	14/39/115/115	-
15	CLA	b	804	2	1/1/15/20	9/39/115/115	-
15	CLA	b	826	2	1/1/14/20	11/36/112/115	-
17	SF4	C	101	3	-	-	0/6/5/5
15	CLA	O	826	2	1/1/14/20	11/36/112/115	-
15	CLA	O	810	2	1/1/15/20	10/39/115/115	-
14	F6C	O	832	2	1/1/10/16	7/41/97/97	-
18	BCR	B	847	-	-	3/29/63/63	0/2/2/2
15	CLA	B	837	2	1/1/15/20	11/39/115/115	-
21	LMG	I	103	-	-	14/32/52/70	0/1/1/1
15	CLA	A	823	1	1/1/13/20	6/29/105/115	-
15	CLA	B	840	2	1/1/15/20	12/39/115/115	-
18	BCR	g	101	-	-	8/29/63/63	0/2/2/2
18	BCR	L	205	-	-	4/29/63/63	0/2/2/2
15	CLA	N	841	1	1/1/15/20	13/39/115/115	-
15	CLA	N	836	1	1/1/12/20	7/26/102/115	-
15	CLA	N	818	1	1/1/15/20	20/39/115/115	-
15	CLA	N	831	1	1/1/15/20	12/39/115/115	-
22	LFA	W	208	-	-	0/12/12/17	-
15	CLA	A	813	1	1/1/12/20	7/26/102/115	-
15	CLA	A	812	1,15	1/1/15/20	20/39/115/115	-
18	BCR	b	847	-	-	6/29/63/63	0/2/2/2
15	CLA	B	812	2	-	11/29/105/115	-
15	CLA	X	102	12	1/1/13/20	2/27/103/115	-
21	LMG	N	855	-	-	10/39/59/70	0/1/1/1
19	LHG	W	207	-	-	14/53/53/53	-
20	LMT	N	852	-	-	0/17/57/61	0/2/2/2
15	CLA	b	833	2	1/1/13/20	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	O	825	2	1/1/15/20	3/39/115/115	-
18	BCR	W	209	-	-	1/29/63/63	0/2/2/2
15	CLA	A	831	1	1/1/15/20	12/39/115/115	-
15	CLA	l	102	12	1/1/13/20	2/27/103/115	-
21	LMG	B	850	-	-	10/39/59/70	0/1/1/1
15	CLA	b	815	2	1/1/13/20	4/30/106/115	-
15	CLA	a	838	1	1/1/13/20	11/27/103/115	-
15	CLA	O	823	24	1/1/15/20	9/39/115/115	-
15	CLA	A	815	1	1/1/13/20	2/27/103/115	-
15	CLA	B	818	24	1/1/15/20	7/39/115/115	-
17	SF4	N	844	2,1	-	-	0/6/5/5
15	CLA	B	834	24	1/1/11/20	6/15/91/115	-
18	BCR	M	101	-	-	6/29/63/63	0/2/2/2
15	CLA	b	808	2	1/1/15/20	7/39/115/115	-
15	CLA	N	810	1	1/1/13/20	8/30/106/115	-
15	CLA	b	837	2	1/1/15/20	11/39/115/115	-
18	BCR	A	850	-	-	13/29/63/63	0/2/2/2
18	BCR	b	845	-	-	8/29/63/63	0/2/2/2
21	LMG	b	849	-	-	6/50/70/70	0/1/1/1
15	CLA	b	831	2	1/1/15/20	10/39/115/115	-
15	CLA	A	808	1	1/1/11/20	2/15/91/115	-
18	BCR	O	844	-	-	4/29/63/63	0/2/2/2
15	CLA	F	201	24	1/1/15/20	10/39/115/115	-
19	LHG	a	851	-	-	12/46/46/53	-
15	CLA	A	811	1	1/1/13/20	11/30/106/115	-
15	CLA	O	819	2	1/1/13/20	12/27/103/115	-
18	BCR	O	843	-	-	3/29/63/63	0/2/2/2
15	CLA	b	803	-	1/1/15/20	3/39/115/115	-
22	LFA	L	209	-	-	0/12/12/17	-
16	PQN	B	841	-	-	0/23/43/43	0/2/2/2
15	CLA	N	816	1	1/1/11/20	6/15/91/115	-
13	CL0	A	801	1	3/3/20/25	5/37/135/135	-
15	CLA	O	831	2	1/1/15/20	10/39/115/115	-
14	F6C	A	856	24	1/1/10/16	15/41/97/97	-
15	CLA	Z	102	12	1/1/13/20	2/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a	805	1,15	1/1/14/20	9/33/109/115	-
16	PQN	a	843	-	-	0/23/43/43	0/2/2/2
15	CLA	b	806	2	1/1/15/20	19/39/115/115	-
15	CLA	O	803	-	1/1/15/20	3/39/115/115	-
15	CLA	N	820	1	1/1/15/20	22/39/115/115	-
15	CLA	B	836	2	1/1/15/20	7/39/115/115	-
15	CLA	a	812	1,15	1/1/15/20	17/39/115/115	-
15	CLA	O	805	2	1/1/15/20	10/39/115/115	-
15	CLA	N	807	1	1/1/15/20	18/39/115/115	-
15	CLA	a	813	1	1/1/12/20	6/26/102/115	-
20	LMT	A	854	-	-	4/21/61/61	0/2/2/2
18	BCR	a	850	-	-	13/29/63/63	0/2/2/2
15	CLA	O	806	2	1/1/15/20	19/39/115/115	-
18	BCR	T	102	-	-	4/29/63/63	0/2/2/2
15	CLA	L	203	10	1/1/14/20	11/33/109/115	-
18	BCR	L	210	-	-	1/29/63/63	0/2/2/2
15	CLA	A	835	1	1/1/15/20	9/39/115/115	-
15	CLA	O	813	2	1/1/15/20	13/39/115/115	-
15	CLA	B	813	2	1/1/15/20	13/39/115/115	-
15	CLA	a	822	24	1/1/15/20	13/39/115/115	-
15	CLA	a	818	1	1/1/15/20	19/39/115/115	-
18	BCR	a	847	-	-	4/29/63/63	0/2/2/2
15	CLA	N	815	1	1/1/13/20	2/27/103/115	-
15	CLA	A	820	1	1/1/15/20	19/39/115/115	-
17	SF4	P	101	3	-	-	0/6/5/5
14	F6C	a	824	24	1/1/7/16	7/25/81/97	-
15	CLA	A	827	24	1/1/13/20	1/27/103/115	-
18	BCR	O	846	-	-	1/29/63/63	0/2/2/2
15	CLA	a	827	24	1/1/13/20	1/27/103/115	-
15	CLA	b	824	24	1/1/15/20	14/39/115/115	-
18	BCR	O	845	-	-	8/29/63/63	0/2/2/2
15	CLA	A	807	1	1/1/15/20	17/39/115/115	-
15	CLA	N	830	1	1/1/15/20	6/39/115/115	-
18	BCR	N	850	-	-	13/29/63/63	0/2/2/2
15	CLA	A	832	1	1/1/12/20	2/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	W	203	10	1/1/14/20	9/33/109/115	-
15	CLA	B	838	2	1/1/15/20	9/39/115/115	-
19	LHG	L	208	-	-	13/53/53/53	-
15	CLA	O	815	2	1/1/13/20	8/30/106/115	-
15	CLA	b	818	24	1/1/15/20	8/39/115/115	-
15	CLA	N	811	1	1/1/13/20	12/30/106/115	-
15	CLA	B	827	2	1/1/15/20	6/39/115/115	-
15	CLA	N	803	-	1/1/15/20	9/39/115/115	-
18	BCR	Y	102	-	-	6/29/63/63	0/2/2/2
15	CLA	B	808	2	1/1/15/20	8/39/115/115	-
15	CLA	O	824	24	1/1/15/20	14/39/115/115	-
15	CLA	a	811	1	1/1/13/20	11/30/106/115	-
15	CLA	b	829	2	1/1/15/20	16/39/115/115	-
20	LMT	A	853	-	-	8/14/54/61	0/2/2/2
15	CLA	a	832	1	1/1/12/20	2/21/97/115	-
15	CLA	L	202	10	1/1/15/20	5/39/115/115	-
21	LMG	B	848	-	-	4/50/70/70	0/1/1/1
17	SF4	c	101	3	-	-	0/6/5/5
15	CLA	N	819	1	1/1/15/20	13/39/115/115	-
14	F6C	N	856	24	1/1/10/16	15/41/97/97	-
15	CLA	N	825	1	1/1/15/20	11/39/115/115	-
18	BCR	F	203	-	-	2/29/63/63	0/2/2/2
15	CLA	a	814	1	1/1/15/20	7/39/115/115	-
15	CLA	a	833	1	1/1/13/20	4/27/103/115	-
18	BCR	V	101	-	-	0/18/35/63	0/1/1/2
15	CLA	O	834	24	1/1/11/20	6/15/91/115	-
14	F6C	N	826	24	1/1/10/16	13/41/97/97	-
15	CLA	b	816	2	1/1/15/20	11/39/115/115	-
14	F6C	O	839	24	1/1/10/16	13/41/97/97	-
15	CLA	O	804	2	1/1/15/20	8/39/115/115	-
18	BCR	a	849	-	-	3/29/63/63	0/2/2/2
19	LHG	X	101	-	-	21/48/48/53	-
15	CLA	B	814	2	1/1/11/20	4/15/91/115	-
18	BCR	f	202	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMG	g	103	-	-	16/32/52/70	0/1/1/1
18	BCR	K	101	-	-	0/18/35/63	0/1/1/2
15	CLA	a	835	1	1/1/15/20	8/39/115/115	-
18	BCR	N	847	-	-	5/29/63/63	0/2/2/2
15	CLA	B	801	2	1/1/15/20	10/39/115/115	-
15	CLA	B	805	2	1/1/15/20	11/39/115/115	-
18	BCR	j	205	-	-	2/29/63/63	0/2/2/2
14	F6C	N	824	24	1/1/7/16	7/25/81/97	-
18	BCR	b	846	-	-	0/29/63/63	0/2/2/2
15	CLA	b	840	2	1/1/15/20	13/39/115/115	-
15	CLA	a	836	1	1/1/12/20	7/26/102/115	-
15	CLA	b	805	2	1/1/15/20	8/39/115/115	-
21	LMG	h	103	-	-	15/50/70/70	0/1/1/1
18	BCR	A	846	-	-	8/29/63/63	0/2/2/2
15	CLA	B	820	2	1/1/11/20	4/15/91/115	-
15	CLA	V	102	9	1/1/11/20	9/15/91/115	-
18	BCR	h	102	-	-	8/29/63/63	0/2/2/2
18	BCR	I	101	-	-	8/29/63/63	0/2/2/2
15	CLA	b	825	2	1/1/15/20	3/39/115/115	-
15	CLA	K	103	24	1/1/12/20	2/21/97/115	-
18	BCR	A	845	-	-	3/29/63/63	0/2/2/2
15	CLA	a	808	1	1/1/11/20	2/15/91/115	-
15	CLA	O	840	2	1/1/15/20	13/39/115/115	-
15	CLA	B	807	2	1/1/15/20	4/39/115/115	-
14	F6C	A	824	24	1/1/7/16	8/25/81/97	-
15	CLA	N	813	1	1/1/12/20	6/26/102/115	-
15	CLA	O	822	2	1/1/13/20	10/27/103/115	-
15	CLA	b	801	2	1/1/15/20	9/39/115/115	-
15	CLA	f	201	24	1/1/15/20	9/39/115/115	-
20	LMT	a	853	-	-	8/14/54/61	0/2/2/2
15	CLA	b	821	24	1/1/12/20	9/25/101/115	-
15	CLA	b	814	2	1/1/11/20	6/15/91/115	-
22	LFA	j	208	-	-	0/12/12/17	-
15	CLA	b	817	2	1/1/14/20	13/33/109/115	-
18	BCR	O	847	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMT	a	852	-	-	0/17/57/61	0/2/2/2
15	CLA	A	840	1	1/1/12/20	2/21/97/115	-
15	CLA	i	102	9	1/1/11/20	9/15/91/115	-
18	BCR	U	101	-	-	7/29/63/63	0/2/2/2
15	CLA	b	823	24	1/1/15/20	9/39/115/115	-
15	CLA	A	821	1	1/1/14/20	6/33/109/115	-
15	CLA	B	802	24	1/1/15/20	12/39/115/115	-
15	CLA	a	830	1	1/1/15/20	5/39/115/115	-
15	CLA	b	834	24	1/1/11/20	4/15/91/115	-
18	BCR	T	101	-	-	8/29/63/63	0/2/2/2
22	LFA	O	850	-	-	7/13/13/17	-
18	BCR	L	206	-	-	2/29/63/63	0/2/2/2
15	CLA	N	817	24	1/1/11/20	6/15/91/115	-
21	LMG	J	103	-	-	16/50/70/70	0/1/1/1
15	CLA	B	830	2	1/1/15/20	11/39/115/115	-
16	PQN	O	841	-	-	0/23/43/43	0/2/2/2
15	CLA	N	828	1	1/1/15/20	8/39/115/115	-
17	SF4	a	844	2,1	-	-	0/6/5/5
15	CLA	A	828	1	1/1/15/20	8/39/115/115	-
15	CLA	O	837	2	1/1/15/20	10/39/115/115	-
15	CLA	O	838	2	1/1/15/20	6/39/115/115	-
21	LMG	A	855	-	-	11/39/59/70	0/1/1/1
20	LMT	N	854	-	-	4/21/61/61	0/2/2/2
18	BCR	h	101	-	-	7/29/63/63	0/2/2/2
15	CLA	N	840	1	1/1/12/20	2/21/97/115	-
15	CLA	N	809	1	1/1/14/20	14/33/109/115	-
15	CLA	A	817	24	1/1/11/20	6/15/91/115	-
15	CLA	B	833	2	1/1/13/20	6/27/103/115	-
15	CLA	B	825	2	1/1/15/20	3/39/115/115	-
15	CLA	K	102	9	1/1/11/20	8/15/91/115	-
18	BCR	B	844	-	-	4/29/63/63	0/2/2/2
15	CLA	a	820	1	1/1/15/20	19/39/115/115	-
19	LHG	l	101	-	-	23/48/48/53	-
17	SF4	A	844	2,1	-	-	0/6/5/5
15	CLA	B	822	2	1/1/13/20	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	b	843	-	-	3/29/63/63	0/2/2/2
15	CLA	b	811	2	1/1/11/20	3/15/91/115	-
19	LHG	N	857	-	-	24/53/53/53	-
18	BCR	W	205	-	-	4/29/63/63	0/2/2/2
17	SF4	P	102	3	-	-	0/6/5/5
15	CLA	a	807	1	1/1/15/20	18/39/115/115	-
15	CLA	a	841	1	1/1/15/20	13/39/115/115	-
15	CLA	N	837	1	1/1/12/20	7/23/99/115	-
15	CLA	a	810	1	1/1/13/20	8/30/106/115	-
18	BCR	i	101	-	-	0/18/35/63	0/1/1/2
15	CLA	b	830	2	1/1/15/20	11/39/115/115	-
18	BCR	J	101	-	-	7/29/63/63	0/2/2/2
15	CLA	A	836	1	1/1/12/20	7/26/102/115	-
15	CLA	b	813	2	1/1/15/20	11/39/115/115	-
16	PQN	A	843	-	-	0/23/43/43	0/2/2/2
15	CLA	a	829	1	1/1/14/20	14/33/109/115	-
15	CLA	O	812	2	-	10/29/105/115	-
15	CLA	B	821	24	1/1/12/20	10/25/101/115	-
18	BCR	k	102	-	-	6/29/63/63	0/2/2/2
15	CLA	b	836	2	1/1/15/20	8/39/115/115	-
18	BCR	O	842	-	-	3/29/63/63	0/2/2/2
18	BCR	b	844	-	-	4/29/63/63	0/2/2/2
19	LHG	Z	101	-	-	23/48/48/53	-
14	F6C	A	826	24	1/1/10/16	12/41/97/97	-
15	CLA	N	827	24	1/1/13/20	1/27/103/115	-
15	CLA	A	842	1	1/1/15/20	15/39/115/115	-
15	CLA	B	829	2	1/1/15/20	18/39/115/115	-
15	CLA	B	828	2	1/1/15/20	12/39/115/115	-
14	F6C	B	832	2	1/1/10/16	5/41/97/97	-
15	CLA	N	839	1	1/1/15/20	17/39/115/115	-
15	CLA	O	836	2	1/1/15/20	8/39/115/115	-
18	BCR	A	849	-	-	3/29/63/63	0/2/2/2
15	CLA	A	833	1	1/1/13/20	3/27/103/115	-
15	CLA	a	839	1	1/1/15/20	15/39/115/115	-
15	CLA	j	203	10	1/1/14/20	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a	825	1	1/1/15/20	11/39/115/115	-
15	CLA	a	817	24	1/1/11/20	6/15/91/115	-
15	CLA	B	811	2	1/1/11/20	3/15/91/115	-
15	CLA	B	804	2	1/1/15/20	9/39/115/115	-
15	CLA	O	827	2	1/1/15/20	6/39/115/115	-
15	CLA	a	815	1	1/1/13/20	2/27/103/115	-
15	CLA	N	806	1	1/1/15/20	16/39/115/115	-
15	CLA	O	808	2	1/1/15/20	8/39/115/115	-
15	CLA	A	814	1	1/1/15/20	8/39/115/115	-
17	SF4	c	102	3	-	-	0/6/5/5
16	PQN	N	843	-	-	0/23/43/43	0/2/2/2
15	CLA	O	811	2	1/1/11/20	3/15/91/115	-
15	CLA	a	828	1	1/1/15/20	7/39/115/115	-
15	CLA	B	817	2	1/1/14/20	13/33/109/115	-
21	LMG	W	206	-	-	10/45/65/70	0/1/1/1
15	CLA	B	823	24	1/1/15/20	9/39/115/115	-
15	CLA	S	201	24	1/1/15/20	10/39/115/115	-
15	CLA	b	802	24	1/1/15/20	12/39/115/115	-
15	CLA	N	812	1,15	1/1/15/20	19/39/115/115	-
15	CLA	A	803	-	1/1/15/20	11/39/115/115	-
21	LMG	U	103	-	-	14/50/70/70	0/1/1/1

All (2099) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	801	CL0	C1B-C2B	9.06	1.49	1.39
13	N	801	CL0	C1B-C2B	9.06	1.49	1.39
13	A	801	CL0	C1B-C2B	9.04	1.49	1.39
14	j	201	F6C	C2A-C3A	8.65	1.55	1.36
14	W	201	F6C	C2A-C3A	8.61	1.55	1.36
14	L	201	F6C	C2A-C3A	8.61	1.55	1.36
14	A	826	F6C	C2A-C3A	8.61	1.55	1.36
14	N	826	F6C	C2A-C3A	8.60	1.55	1.36
14	a	826	F6C	C2A-C3A	8.60	1.55	1.36
14	N	802	F6C	C2A-C3A	8.58	1.55	1.36
14	A	824	F6C	C2A-C3A	8.55	1.55	1.36
14	a	824	F6C	C2A-C3A	8.55	1.55	1.36
14	N	824	F6C	C2A-C3A	8.55	1.55	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	802	F6C	C2A-C3A	8.53	1.55	1.36
14	A	802	F6C	C2A-C3A	8.53	1.55	1.36
14	O	832	F6C	C2A-C3A	8.51	1.55	1.36
14	b	832	F6C	C2A-C3A	8.51	1.55	1.36
14	B	832	F6C	C2A-C3A	8.51	1.55	1.36
14	j	204	F6C	C2A-C3A	8.45	1.55	1.36
14	b	839	F6C	C2A-C3A	8.45	1.55	1.36
14	B	839	F6C	C2A-C3A	8.44	1.55	1.36
14	O	839	F6C	C2A-C3A	8.44	1.55	1.36
14	L	204	F6C	C2A-C3A	8.44	1.55	1.36
14	W	204	F6C	C2A-C3A	8.43	1.54	1.36
14	N	856	F6C	C2A-C3A	8.29	1.54	1.36
14	a	855	F6C	C2A-C3A	8.28	1.54	1.36
14	A	856	F6C	C2A-C3A	8.28	1.54	1.36
13	A	801	CL0	C3B-C4B	8.04	1.49	1.41
13	N	801	CL0	C3B-C4B	8.00	1.49	1.41
13	a	801	CL0	C3B-C4B	8.00	1.49	1.41
13	A	801	CL0	C1D-C2D	7.78	1.48	1.39
13	N	801	CL0	C1D-C2D	7.73	1.48	1.39
13	a	801	CL0	C1D-C2D	7.73	1.48	1.39
13	A	801	CL0	C3D-C4D	4.26	1.48	1.41
13	a	801	CL0	C3D-C4D	4.24	1.48	1.41
13	N	801	CL0	C3D-C4D	4.23	1.48	1.41
14	L	204	F6C	C4A-C3A	4.21	1.53	1.45
14	L	201	F6C	C1A-C2A	4.21	1.54	1.45
14	W	201	F6C	C1A-C2A	4.21	1.54	1.45
14	b	839	F6C	C4A-C3A	4.11	1.53	1.45
14	B	839	F6C	C4A-C3A	4.10	1.53	1.45
14	W	204	F6C	C4A-C3A	4.10	1.53	1.45
14	j	201	F6C	C1A-C2A	4.10	1.54	1.45
14	j	204	F6C	C4A-C3A	4.09	1.53	1.45
14	O	839	F6C	C4A-C3A	4.09	1.53	1.45
14	N	824	F6C	C4A-C3A	4.08	1.53	1.45
14	N	802	F6C	C4A-C3A	4.08	1.53	1.45
14	A	824	F6C	C4A-C3A	4.08	1.53	1.45
14	a	802	F6C	C4A-C3A	4.07	1.53	1.45
14	a	824	F6C	C4A-C3A	4.07	1.53	1.45
14	A	802	F6C	C4A-C3A	4.05	1.53	1.45
14	B	832	F6C	C4A-C3A	4.05	1.53	1.45
14	O	832	F6C	C4A-C3A	4.04	1.53	1.45
14	b	832	F6C	C4A-C3A	4.04	1.53	1.45
14	a	826	F6C	C4A-C3A	4.04	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	826	F6C	C4A-C3A	4.01	1.53	1.45
14	N	826	F6C	C4A-C3A	4.01	1.53	1.45
14	N	826	F6C	C1A-C2A	4.00	1.53	1.45
14	A	826	F6C	C1A-C2A	3.98	1.53	1.45
14	a	826	F6C	C1A-C2A	3.96	1.53	1.45
14	a	855	F6C	C4A-C3A	3.95	1.53	1.45
14	N	856	F6C	C4A-C3A	3.95	1.53	1.45
14	A	856	F6C	C4A-C3A	3.92	1.53	1.45
14	W	201	F6C	C4A-C3A	3.88	1.53	1.45
14	L	201	F6C	C4A-C3A	3.88	1.53	1.45
14	j	201	F6C	C4A-C3A	3.81	1.52	1.45
14	a	824	F6C	C1A-C2A	3.79	1.53	1.45
14	A	824	F6C	C1A-C2A	3.78	1.53	1.45
14	N	824	F6C	C1A-C2A	3.74	1.53	1.45
14	b	832	F6C	C1A-C2A	3.73	1.53	1.45
14	O	832	F6C	C1A-C2A	3.73	1.53	1.45
14	B	832	F6C	C1A-C2A	3.70	1.53	1.45
14	j	204	F6C	C1A-C2A	3.67	1.53	1.45
14	L	204	F6C	C1A-C2A	3.67	1.53	1.45
15	B	812	CLA	C1D-ND	3.67	1.42	1.37
14	a	802	F6C	C1A-C2A	3.66	1.53	1.45
14	W	204	F6C	C1A-C2A	3.65	1.53	1.45
14	A	802	F6C	C1A-C2A	3.65	1.53	1.45
15	O	812	CLA	C1D-ND	3.65	1.42	1.37
15	b	812	CLA	C1D-ND	3.64	1.42	1.37
15	a	828	CLA	C1D-ND	3.63	1.42	1.37
14	N	802	F6C	C1A-C2A	3.60	1.53	1.45
15	K	102	CLA	C1D-ND	3.59	1.42	1.37
15	A	840	CLA	C1D-ND	3.58	1.42	1.37
15	A	828	CLA	C1D-ND	3.58	1.42	1.37
15	B	835	CLA	C1D-ND	3.58	1.42	1.37
15	V	102	CLA	C1D-ND	3.58	1.42	1.37
15	N	840	CLA	C1D-ND	3.58	1.42	1.37
15	i	102	CLA	C1D-ND	3.57	1.42	1.37
15	N	815	CLA	C1D-ND	3.57	1.42	1.37
15	a	804	CLA	C1D-ND	3.57	1.42	1.37
15	B	825	CLA	C1D-ND	3.57	1.42	1.37
15	a	815	CLA	C1D-ND	3.57	1.42	1.37
15	a	817	CLA	C1D-ND	3.57	1.42	1.37
15	A	815	CLA	C1D-ND	3.57	1.42	1.37
15	A	817	CLA	C1D-ND	3.57	1.42	1.37
15	N	804	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	835	CLA	C1D-ND	3.57	1.42	1.37
15	B	833	CLA	C1D-ND	3.57	1.42	1.37
15	N	828	CLA	C1D-ND	3.56	1.42	1.37
15	b	835	CLA	C1D-ND	3.56	1.42	1.37
15	A	822	CLA	C1D-ND	3.55	1.42	1.37
15	N	817	CLA	C1D-ND	3.55	1.42	1.37
15	O	801	CLA	C1D-ND	3.55	1.42	1.37
15	N	822	CLA	C1D-ND	3.55	1.42	1.37
15	a	822	CLA	C1D-ND	3.55	1.42	1.37
15	A	811	CLA	C1D-ND	3.55	1.42	1.37
15	B	814	CLA	C1D-ND	3.55	1.42	1.37
15	O	825	CLA	C1D-ND	3.55	1.42	1.37
15	N	825	CLA	C1D-ND	3.54	1.42	1.37
15	N	811	CLA	C1D-ND	3.54	1.42	1.37
15	A	837	CLA	C1D-ND	3.54	1.42	1.37
15	A	804	CLA	C1D-ND	3.54	1.42	1.37
15	b	825	CLA	C1D-ND	3.54	1.42	1.37
14	A	856	F6C	C1A-C2A	3.54	1.52	1.45
15	a	814	CLA	C1D-ND	3.54	1.42	1.37
15	O	816	CLA	C1D-ND	3.54	1.42	1.37
14	a	855	F6C	C1A-C2A	3.54	1.52	1.45
15	A	807	CLA	C1D-ND	3.54	1.42	1.37
15	N	816	CLA	C1D-ND	3.54	1.42	1.37
15	a	820	CLA	C1D-ND	3.54	1.42	1.37
15	b	801	CLA	C1D-ND	3.54	1.42	1.37
15	b	806	CLA	C1D-ND	3.54	1.42	1.37
14	O	839	F6C	C1A-C2A	3.54	1.52	1.45
15	B	820	CLA	C1D-ND	3.54	1.42	1.37
15	B	823	CLA	C1D-ND	3.54	1.42	1.37
15	a	837	CLA	C1D-ND	3.53	1.42	1.37
15	N	808	CLA	C1D-ND	3.53	1.42	1.37
15	N	814	CLA	C1D-ND	3.53	1.42	1.37
15	N	837	CLA	C1D-ND	3.53	1.42	1.37
15	a	840	CLA	C1D-ND	3.53	1.42	1.37
15	a	816	CLA	C1D-ND	3.53	1.42	1.37
15	A	814	CLA	C1D-ND	3.53	1.42	1.37
15	b	820	CLA	C1D-ND	3.53	1.42	1.37
15	b	823	CLA	C1D-ND	3.53	1.42	1.37
14	b	839	F6C	C1A-C2A	3.53	1.52	1.45
15	O	811	CLA	C1D-ND	3.53	1.42	1.37
15	b	816	CLA	C1D-ND	3.53	1.42	1.37
15	O	820	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	819	CLA	C1D-ND	3.53	1.42	1.37
14	N	856	F6C	C1A-C2A	3.53	1.52	1.45
15	B	806	CLA	C1D-ND	3.53	1.42	1.37
15	O	813	CLA	C1D-ND	3.53	1.42	1.37
15	a	807	CLA	C1D-ND	3.52	1.42	1.37
15	b	811	CLA	C1D-ND	3.52	1.42	1.37
15	N	835	CLA	C1D-ND	3.52	1.42	1.37
15	a	811	CLA	C1D-ND	3.52	1.42	1.37
15	b	813	CLA	C1D-ND	3.52	1.42	1.37
15	O	834	CLA	C1D-ND	3.52	1.42	1.37
15	b	831	CLA	C1D-ND	3.52	1.42	1.37
15	b	838	CLA	C1D-ND	3.52	1.42	1.37
15	A	819	CLA	C1D-ND	3.52	1.42	1.37
15	B	811	CLA	C1D-ND	3.52	1.42	1.37
15	O	823	CLA	C1D-ND	3.52	1.42	1.37
15	B	815	CLA	C1D-ND	3.52	1.42	1.37
15	A	816	CLA	C1D-ND	3.52	1.42	1.37
15	b	834	CLA	C1D-ND	3.52	1.42	1.37
15	a	808	CLA	C1D-ND	3.52	1.42	1.37
15	l	102	CLA	C1D-ND	3.52	1.42	1.37
15	B	801	CLA	C1D-ND	3.52	1.42	1.37
15	B	819	CLA	C1D-ND	3.52	1.42	1.37
15	A	813	CLA	C1D-ND	3.52	1.42	1.37
15	B	813	CLA	C1D-ND	3.52	1.42	1.37
15	V	103	CLA	C1D-ND	3.52	1.42	1.37
15	A	820	CLA	C1D-ND	3.52	1.42	1.37
15	B	807	CLA	C1D-ND	3.52	1.42	1.37
15	Z	102	CLA	C1D-ND	3.52	1.42	1.37
15	B	826	CLA	C1D-ND	3.51	1.42	1.37
15	K	103	CLA	C1D-ND	3.51	1.42	1.37
14	B	839	F6C	C1A-C2A	3.51	1.52	1.45
15	O	806	CLA	C1D-ND	3.51	1.42	1.37
15	A	812	CLA	C1D-ND	3.51	1.42	1.37
15	B	829	CLA	C1D-ND	3.51	1.42	1.37
15	X	102	CLA	C1D-ND	3.51	1.42	1.37
15	N	813	CLA	C1D-ND	3.51	1.42	1.37
15	O	819	CLA	C1D-ND	3.51	1.42	1.37
15	O	840	CLA	C1D-ND	3.51	1.42	1.37
15	A	808	CLA	C1D-ND	3.51	1.42	1.37
15	O	815	CLA	C1D-ND	3.51	1.42	1.37
15	A	825	CLA	C1D-ND	3.51	1.42	1.37
15	B	840	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	838	CLA	C1D-ND	3.51	1.42	1.37
15	b	814	CLA	C1D-ND	3.51	1.42	1.37
15	A	809	CLA	C1D-ND	3.51	1.42	1.37
15	N	823	CLA	C1D-ND	3.51	1.42	1.37
15	b	826	CLA	C1D-ND	3.51	1.42	1.37
15	b	829	CLA	C1D-ND	3.51	1.42	1.37
15	N	807	CLA	C1D-ND	3.51	1.42	1.37
15	a	825	CLA	C1D-ND	3.51	1.42	1.37
15	a	842	CLA	C1D-ND	3.51	1.42	1.37
15	i	103	CLA	C1D-ND	3.51	1.42	1.37
15	N	820	CLA	C1D-ND	3.51	1.42	1.37
15	O	831	CLA	C1D-ND	3.51	1.42	1.37
15	b	815	CLA	C1D-ND	3.51	1.42	1.37
15	B	831	CLA	C1D-ND	3.51	1.42	1.37
15	N	809	CLA	C1D-ND	3.51	1.42	1.37
15	N	832	CLA	C1D-ND	3.51	1.42	1.37
15	a	831	CLA	C1D-ND	3.51	1.42	1.37
15	a	835	CLA	C1D-ND	3.51	1.42	1.37
15	B	821	CLA	C1D-ND	3.50	1.42	1.37
15	A	835	CLA	C1D-ND	3.50	1.42	1.37
15	N	819	CLA	C1D-ND	3.50	1.42	1.37
15	N	831	CLA	C1D-ND	3.50	1.42	1.37
15	O	807	CLA	C1D-ND	3.50	1.42	1.37
15	a	813	CLA	C1D-ND	3.50	1.42	1.37
15	f	201	CLA	C1D-ND	3.50	1.42	1.37
15	O	826	CLA	C1D-ND	3.50	1.42	1.37
15	a	805	CLA	C1D-ND	3.50	1.42	1.37
15	B	816	CLA	C1D-ND	3.50	1.42	1.37
15	A	842	CLA	C1D-ND	3.50	1.42	1.37
15	N	812	CLA	C1D-ND	3.50	1.42	1.37
15	N	842	CLA	C1D-ND	3.50	1.42	1.37
15	a	806	CLA	C1D-ND	3.50	1.42	1.37
15	b	817	CLA	C1D-ND	3.50	1.42	1.37
15	A	832	CLA	C1D-ND	3.50	1.42	1.37
15	b	824	CLA	C1D-ND	3.50	1.42	1.37
15	A	823	CLA	C1D-ND	3.50	1.42	1.37
15	B	838	CLA	C1D-ND	3.50	1.42	1.37
15	a	809	CLA	C1D-ND	3.50	1.42	1.37
15	a	839	CLA	C1D-ND	3.50	1.42	1.37
15	O	818	CLA	C1D-ND	3.50	1.42	1.37
15	a	841	CLA	C1D-ND	3.50	1.42	1.37
15	B	836	CLA	C1D-ND	3.50	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	824	CLA	C1D-ND	3.49	1.42	1.37
15	O	833	CLA	C1D-ND	3.49	1.42	1.37
15	a	832	CLA	C1D-ND	3.49	1.42	1.37
15	A	839	CLA	C1D-ND	3.49	1.42	1.37
15	b	807	CLA	C1D-ND	3.49	1.42	1.37
15	b	840	CLA	C1D-ND	3.49	1.42	1.37
15	N	839	CLA	C1D-ND	3.49	1.42	1.37
15	O	836	CLA	C1D-ND	3.49	1.42	1.37
15	b	818	CLA	C1D-ND	3.49	1.42	1.37
15	b	830	CLA	C1D-ND	3.49	1.42	1.37
15	b	821	CLA	C1D-ND	3.49	1.42	1.37
15	F	201	CLA	C1D-ND	3.49	1.42	1.37
15	a	819	CLA	C1D-ND	3.49	1.42	1.37
15	a	823	CLA	C1D-ND	3.49	1.42	1.37
15	a	827	CLA	C1D-ND	3.49	1.42	1.37
15	N	841	CLA	C1D-ND	3.49	1.42	1.37
15	B	818	CLA	C1D-ND	3.49	1.42	1.37
15	a	812	CLA	C1D-ND	3.49	1.42	1.37
15	A	805	CLA	C1D-ND	3.49	1.42	1.37
15	A	806	CLA	C1D-ND	3.49	1.42	1.37
15	O	821	CLA	C1D-ND	3.49	1.42	1.37
15	O	817	CLA	C1D-ND	3.49	1.42	1.37
15	a	821	CLA	C1D-ND	3.49	1.42	1.37
15	N	805	CLA	C1D-ND	3.48	1.42	1.37
15	O	814	CLA	C1D-ND	3.48	1.42	1.37
15	a	834	CLA	C1D-ND	3.48	1.42	1.37
15	N	821	CLA	C1D-ND	3.48	1.42	1.37
15	N	838	CLA	C1D-ND	3.48	1.42	1.37
15	b	833	CLA	C1D-ND	3.48	1.42	1.37
15	A	821	CLA	C1D-ND	3.48	1.42	1.37
15	O	830	CLA	C1D-ND	3.48	1.42	1.37
15	a	833	CLA	C1D-ND	3.48	1.42	1.37
15	b	810	CLA	C1D-ND	3.48	1.42	1.37
15	O	804	CLA	C1D-ND	3.48	1.42	1.37
15	S	201	CLA	C1D-ND	3.48	1.42	1.37
15	O	824	CLA	C1D-ND	3.48	1.42	1.37
15	O	822	CLA	C1D-ND	3.48	1.42	1.37
15	W	203	CLA	C1D-ND	3.47	1.42	1.37
15	b	804	CLA	C1D-ND	3.47	1.42	1.37
15	A	831	CLA	C1D-ND	3.47	1.42	1.37
15	B	837	CLA	C1D-ND	3.47	1.42	1.37
15	O	810	CLA	C1D-ND	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	828	CLA	C1D-ND	3.47	1.42	1.37
15	A	841	CLA	C1D-ND	3.47	1.42	1.37
15	O	837	CLA	C1D-ND	3.47	1.42	1.37
15	A	834	CLA	C1D-ND	3.47	1.42	1.37
15	B	804	CLA	C1D-ND	3.47	1.42	1.37
15	b	828	CLA	C1D-ND	3.47	1.42	1.37
15	B	817	CLA	C1D-ND	3.47	1.42	1.37
15	O	829	CLA	C1D-ND	3.47	1.42	1.37
15	N	806	CLA	C1D-ND	3.47	1.42	1.37
15	A	827	CLA	C1D-ND	3.47	1.42	1.37
15	B	805	CLA	C1D-ND	3.47	1.42	1.37
15	N	827	CLA	C1D-ND	3.46	1.42	1.37
15	A	838	CLA	C1D-ND	3.46	1.42	1.37
15	b	837	CLA	C1D-ND	3.46	1.42	1.37
15	B	810	CLA	C1D-ND	3.46	1.42	1.37
15	j	203	CLA	C1D-ND	3.46	1.42	1.37
15	A	830	CLA	C1D-ND	3.46	1.42	1.37
15	b	805	CLA	C1D-ND	3.46	1.42	1.37
15	N	833	CLA	C1D-ND	3.46	1.42	1.37
15	N	834	CLA	C1D-ND	3.46	1.42	1.37
15	b	836	CLA	C1D-ND	3.46	1.42	1.37
15	A	833	CLA	C1D-ND	3.46	1.42	1.37
15	A	829	CLA	C1D-ND	3.46	1.42	1.37
15	N	830	CLA	C1D-ND	3.46	1.42	1.37
15	B	834	CLA	C1D-ND	3.45	1.42	1.37
15	L	203	CLA	C1D-ND	3.45	1.42	1.37
15	O	805	CLA	C1D-ND	3.45	1.42	1.37
15	B	830	CLA	C1D-ND	3.45	1.42	1.37
15	a	830	CLA	C1D-ND	3.45	1.42	1.37
15	B	802	CLA	C1D-ND	3.45	1.42	1.37
15	a	829	CLA	C1D-ND	3.45	1.42	1.37
15	a	838	CLA	C1D-ND	3.45	1.42	1.37
15	B	828	CLA	C1D-ND	3.45	1.42	1.37
15	N	829	CLA	C1D-ND	3.44	1.42	1.37
15	O	802	CLA	C1D-ND	3.44	1.42	1.37
15	A	836	CLA	C1D-ND	3.43	1.42	1.37
15	b	802	CLA	C1D-ND	3.43	1.42	1.37
15	a	836	CLA	C1D-ND	3.43	1.42	1.37
15	b	808	CLA	C1D-ND	3.42	1.42	1.37
15	O	808	CLA	C1D-ND	3.42	1.42	1.37
15	A	810	CLA	C1D-ND	3.41	1.42	1.37
15	B	822	CLA	C1D-ND	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	836	CLA	C1D-ND	3.41	1.42	1.37
15	a	810	CLA	C1D-ND	3.41	1.42	1.37
15	N	810	CLA	C1D-ND	3.41	1.42	1.37
15	B	827	CLA	C1D-ND	3.40	1.42	1.37
15	b	822	CLA	C1D-ND	3.40	1.42	1.37
15	B	808	CLA	C1D-ND	3.40	1.42	1.37
15	A	803	CLA	C1D-ND	3.40	1.42	1.37
15	B	809	CLA	C1D-ND	3.39	1.42	1.37
15	b	827	CLA	C1D-ND	3.39	1.42	1.37
15	O	827	CLA	C1D-ND	3.38	1.42	1.37
15	j	202	CLA	C1D-ND	3.38	1.42	1.37
15	B	803	CLA	C1D-ND	3.38	1.42	1.37
15	W	202	CLA	C1D-ND	3.38	1.42	1.37
15	N	803	CLA	C1D-ND	3.38	1.42	1.37
15	b	809	CLA	C1D-ND	3.38	1.42	1.37
15	a	803	CLA	C1D-ND	3.37	1.42	1.37
15	b	803	CLA	C1D-ND	3.36	1.42	1.37
15	O	803	CLA	C1D-ND	3.34	1.42	1.37
15	L	202	CLA	C1D-ND	3.31	1.42	1.37
15	O	809	CLA	C1D-ND	3.30	1.42	1.37
15	N	818	CLA	C1D-ND	3.27	1.42	1.37
15	a	804	CLA	C4B-NB	3.27	1.42	1.37
15	N	804	CLA	C4B-NB	3.21	1.42	1.37
15	a	842	CLA	C4B-NB	3.20	1.42	1.37
15	A	842	CLA	C4B-NB	3.18	1.42	1.37
15	N	816	CLA	C4B-NB	3.17	1.42	1.37
15	N	842	CLA	C4B-NB	3.17	1.42	1.37
15	A	816	CLA	C4B-NB	3.17	1.42	1.37
15	a	818	CLA	C1D-ND	3.16	1.42	1.37
15	a	816	CLA	C4B-NB	3.16	1.42	1.37
15	K	103	CLA	C4B-NB	3.16	1.42	1.37
15	i	103	CLA	C4B-NB	3.16	1.42	1.37
15	b	835	CLA	C4B-NB	3.15	1.42	1.37
15	V	103	CLA	C4B-NB	3.15	1.42	1.37
15	O	835	CLA	C4B-NB	3.14	1.42	1.37
15	A	818	CLA	C1D-ND	3.14	1.42	1.37
15	O	816	CLA	C4B-NB	3.14	1.42	1.37
15	B	835	CLA	C4B-NB	3.14	1.42	1.37
15	S	201	CLA	C4B-NB	3.13	1.42	1.37
15	N	817	CLA	C4B-NB	3.13	1.42	1.37
15	a	817	CLA	C4B-NB	3.13	1.42	1.37
15	A	817	CLA	C4B-NB	3.12	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	201	CLA	C4B-NB	3.12	1.42	1.37
15	A	804	CLA	C4B-NB	3.12	1.42	1.37
15	b	816	CLA	C4B-NB	3.10	1.41	1.37
15	f	201	CLA	C4B-NB	3.10	1.41	1.37
15	a	812	CLA	C4B-NB	3.10	1.41	1.37
15	O	819	CLA	C4B-NB	3.10	1.41	1.37
15	b	819	CLA	C4B-NB	3.09	1.41	1.37
15	B	819	CLA	C4B-NB	3.09	1.41	1.37
15	A	819	CLA	C4B-NB	3.09	1.41	1.37
15	N	812	CLA	C4B-NB	3.08	1.41	1.37
15	a	819	CLA	C4B-NB	3.08	1.41	1.37
15	A	812	CLA	C4B-NB	3.08	1.41	1.37
15	A	834	CLA	C4B-NB	3.08	1.41	1.37
15	O	818	CLA	C4B-NB	3.08	1.41	1.37
15	O	811	CLA	C4B-NB	3.08	1.41	1.37
15	b	818	CLA	C4B-NB	3.08	1.41	1.37
15	N	834	CLA	C4B-NB	3.07	1.41	1.37
15	B	811	CLA	C4B-NB	3.07	1.41	1.37
15	B	818	CLA	C4B-NB	3.07	1.41	1.37
15	N	819	CLA	C4B-NB	3.07	1.41	1.37
15	b	811	CLA	C4B-NB	3.06	1.41	1.37
15	a	834	CLA	C4B-NB	3.06	1.41	1.37
15	N	805	CLA	C4B-NB	3.06	1.41	1.37
15	A	805	CLA	C4B-NB	3.05	1.41	1.37
15	b	817	CLA	C4B-NB	3.05	1.41	1.37
15	B	817	CLA	C4B-NB	3.05	1.41	1.37
15	a	805	CLA	C4B-NB	3.05	1.41	1.37
15	O	817	CLA	C4B-NB	3.05	1.41	1.37
15	a	835	CLA	C4B-NB	3.05	1.41	1.37
15	A	839	CLA	C4B-NB	3.04	1.41	1.37
15	B	804	CLA	C4B-NB	3.04	1.41	1.37
15	O	804	CLA	C4B-NB	3.04	1.41	1.37
15	A	831	CLA	C4B-NB	3.04	1.41	1.37
15	K	102	CLA	C4B-NB	3.04	1.41	1.37
15	X	102	CLA	C4B-NB	3.04	1.41	1.37
15	Z	102	CLA	C4B-NB	3.03	1.41	1.37
15	a	839	CLA	C4B-NB	3.03	1.41	1.37
15	V	102	CLA	C4B-NB	3.03	1.41	1.37
15	b	804	CLA	C4B-NB	3.03	1.41	1.37
15	A	825	CLA	C4B-NB	3.03	1.41	1.37
15	b	840	CLA	C4B-NB	3.03	1.41	1.37
15	O	826	CLA	C4B-NB	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	839	CLA	C4B-NB	3.03	1.41	1.37
15	B	840	CLA	C4B-NB	3.03	1.41	1.37
15	b	807	CLA	C4B-NB	3.03	1.41	1.37
15	l	102	CLA	C4B-NB	3.03	1.41	1.37
15	N	818	CLA	C4B-NB	3.03	1.41	1.37
15	b	826	CLA	C4B-NB	3.03	1.41	1.37
15	B	822	CLA	C4B-NB	3.02	1.41	1.37
15	a	825	CLA	C4B-NB	3.02	1.41	1.37
15	i	102	CLA	C4B-NB	3.02	1.41	1.37
15	N	815	CLA	C4B-NB	3.02	1.41	1.37
15	L	203	CLA	C4B-NB	3.02	1.41	1.37
15	B	816	CLA	C4B-NB	3.02	1.41	1.37
15	N	831	CLA	C4B-NB	3.02	1.41	1.37
15	A	822	CLA	C4B-NB	3.02	1.41	1.37
15	b	802	CLA	C4B-NB	3.02	1.41	1.37
15	O	840	CLA	C4B-NB	3.02	1.41	1.37
15	B	802	CLA	C4B-NB	3.01	1.41	1.37
15	B	813	CLA	C4B-NB	3.01	1.41	1.37
15	a	829	CLA	C4B-NB	3.01	1.41	1.37
15	O	802	CLA	C4B-NB	3.01	1.41	1.37
15	a	831	CLA	C4B-NB	3.01	1.41	1.37
15	B	831	CLA	C4B-NB	3.01	1.41	1.37
15	O	820	CLA	C4B-NB	3.01	1.41	1.37
15	N	825	CLA	C4B-NB	3.00	1.41	1.37
15	j	203	CLA	C4B-NB	3.00	1.41	1.37
15	N	821	CLA	C4B-NB	3.00	1.41	1.37
15	N	822	CLA	C4B-NB	3.00	1.41	1.37
15	a	822	CLA	C4B-NB	3.00	1.41	1.37
15	b	820	CLA	C4B-NB	3.00	1.41	1.37
15	A	815	CLA	C4B-NB	3.00	1.41	1.37
15	A	835	CLA	C4B-NB	3.00	1.41	1.37
15	B	810	CLA	C4B-NB	3.00	1.41	1.37
15	N	807	CLA	C4B-NB	3.00	1.41	1.37
15	A	818	CLA	C4B-NB	3.00	1.41	1.37
15	N	835	CLA	C4B-NB	3.00	1.41	1.37
15	a	818	CLA	C4B-NB	3.00	1.41	1.37
15	A	821	CLA	C4B-NB	3.00	1.41	1.37
15	O	807	CLA	C4B-NB	3.00	1.41	1.37
15	a	821	CLA	C4B-NB	3.00	1.41	1.37
15	a	837	CLA	C4B-NB	3.00	1.41	1.37
15	b	831	CLA	C4B-NB	3.00	1.41	1.37
15	N	841	CLA	C4B-NB	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	838	CLA	C4B-NB	2.99	1.41	1.37
15	A	837	CLA	C4B-NB	2.99	1.41	1.37
15	B	830	CLA	C4B-NB	2.99	1.41	1.37
15	O	810	CLA	C4B-NB	2.99	1.41	1.37
15	O	813	CLA	C4B-NB	2.99	1.41	1.37
15	b	823	CLA	C4B-NB	2.99	1.41	1.37
15	a	815	CLA	C4B-NB	2.99	1.41	1.37
15	A	840	CLA	C4B-NB	2.99	1.41	1.37
15	B	820	CLA	C4B-NB	2.99	1.41	1.37
15	O	831	CLA	C4B-NB	2.99	1.41	1.37
15	b	813	CLA	C4B-NB	2.99	1.41	1.37
15	B	826	CLA	C4B-NB	2.99	1.41	1.37
15	O	822	CLA	C4B-NB	2.99	1.41	1.37
15	L	202	CLA	C4B-NB	2.99	1.41	1.37
15	a	832	CLA	C4B-NB	2.98	1.41	1.37
15	b	821	CLA	C4B-NB	2.98	1.41	1.37
15	O	815	CLA	C4B-NB	2.98	1.41	1.37
15	O	828	CLA	C4B-NB	2.98	1.41	1.37
15	b	833	CLA	C4B-NB	2.98	1.41	1.37
15	O	833	CLA	C4B-NB	2.98	1.41	1.37
15	a	811	CLA	C4B-NB	2.98	1.41	1.37
15	b	810	CLA	C4B-NB	2.98	1.41	1.37
15	a	840	CLA	C4B-NB	2.98	1.41	1.37
15	B	823	CLA	C4B-NB	2.98	1.41	1.37
15	b	830	CLA	C4B-NB	2.98	1.41	1.37
15	B	833	CLA	C4B-NB	2.98	1.41	1.37
15	B	834	CLA	C4B-NB	2.98	1.41	1.37
15	N	829	CLA	C4B-NB	2.98	1.41	1.37
15	b	812	CLA	C4B-NB	2.98	1.41	1.37
15	O	823	CLA	C4B-NB	2.97	1.41	1.37
15	B	812	CLA	C4B-NB	2.97	1.41	1.37
15	N	811	CLA	C4B-NB	2.97	1.41	1.37
15	N	840	CLA	C4B-NB	2.97	1.41	1.37
15	a	807	CLA	C4B-NB	2.97	1.41	1.37
15	b	824	CLA	C4B-NB	2.97	1.41	1.37
15	B	824	CLA	C4B-NB	2.97	1.41	1.37
15	O	830	CLA	C4B-NB	2.97	1.41	1.37
15	b	828	CLA	C4B-NB	2.97	1.41	1.37
15	B	838	CLA	C4B-NB	2.97	1.41	1.37
15	A	829	CLA	C4B-NB	2.97	1.41	1.37
15	B	821	CLA	C4B-NB	2.97	1.41	1.37
15	N	832	CLA	C4B-NB	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	829	CLA	C4B-NB	2.97	1.41	1.37
15	O	809	CLA	C4B-NB	2.97	1.41	1.37
15	B	815	CLA	C4B-NB	2.97	1.41	1.37
15	A	813	CLA	C4B-NB	2.97	1.41	1.37
15	W	203	CLA	C4B-NB	2.97	1.41	1.37
15	b	838	CLA	C4B-NB	2.96	1.41	1.37
15	B	807	CLA	C4B-NB	2.96	1.41	1.37
15	N	823	CLA	C4B-NB	2.96	1.41	1.37
15	A	811	CLA	C4B-NB	2.96	1.41	1.37
15	B	829	CLA	C4B-NB	2.96	1.41	1.37
15	O	821	CLA	C4B-NB	2.96	1.41	1.37
15	A	836	CLA	C4B-NB	2.96	1.41	1.37
15	a	823	CLA	C4B-NB	2.96	1.41	1.37
15	N	813	CLA	C4B-NB	2.96	1.41	1.37
15	A	823	CLA	C4B-NB	2.96	1.41	1.37
15	B	828	CLA	C4B-NB	2.96	1.41	1.37
15	O	824	CLA	C4B-NB	2.96	1.41	1.37
15	a	813	CLA	C4B-NB	2.96	1.41	1.37
15	O	814	CLA	C4B-NB	2.96	1.41	1.37
15	B	827	CLA	C4B-NB	2.95	1.41	1.37
15	b	822	CLA	C4B-NB	2.95	1.41	1.37
15	N	837	CLA	C4B-NB	2.95	1.41	1.37
15	b	806	CLA	C4B-NB	2.95	1.41	1.37
15	A	832	CLA	C4B-NB	2.95	1.41	1.37
15	b	815	CLA	C4B-NB	2.95	1.41	1.37
15	O	827	CLA	C4B-NB	2.95	1.41	1.37
15	O	829	CLA	C4B-NB	2.95	1.41	1.37
15	b	814	CLA	C4B-NB	2.95	1.41	1.37
15	A	807	CLA	C4B-NB	2.95	1.41	1.37
15	N	809	CLA	C4B-NB	2.95	1.41	1.37
15	b	837	CLA	C4B-NB	2.95	1.41	1.37
15	O	812	CLA	C4B-NB	2.95	1.41	1.37
15	B	814	CLA	C4B-NB	2.95	1.41	1.37
15	B	837	CLA	C4B-NB	2.94	1.41	1.37
15	A	809	CLA	C4B-NB	2.94	1.41	1.37
15	B	801	CLA	C4B-NB	2.94	1.41	1.37
15	O	837	CLA	C4B-NB	2.94	1.41	1.37
15	O	806	CLA	C4B-NB	2.94	1.41	1.37
15	B	801	CLA	C1B-C2B	2.94	1.50	1.43
15	O	801	CLA	C4B-NB	2.94	1.41	1.37
15	a	820	CLA	C4B-NB	2.94	1.41	1.37
15	a	808	CLA	C4B-NB	2.94	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	805	CLA	C4B-NB	2.94	1.41	1.37
15	N	808	CLA	C4B-NB	2.94	1.41	1.37
15	N	827	CLA	C4B-NB	2.93	1.41	1.37
15	a	830	CLA	C4B-NB	2.93	1.41	1.37
15	a	809	CLA	C4B-NB	2.93	1.41	1.37
15	N	836	CLA	C4B-NB	2.93	1.41	1.37
15	B	808	CLA	C4B-NB	2.93	1.41	1.37
15	W	202	CLA	C4B-NB	2.93	1.41	1.37
15	b	834	CLA	C4B-NB	2.93	1.41	1.37
15	b	827	CLA	C4B-NB	2.93	1.41	1.37
15	b	801	CLA	C4B-NB	2.92	1.41	1.37
15	A	810	CLA	C4B-NB	2.92	1.41	1.37
15	A	830	CLA	C4B-NB	2.92	1.41	1.37
15	b	805	CLA	C4B-NB	2.92	1.41	1.37
15	A	808	CLA	C4B-NB	2.92	1.41	1.37
15	O	834	CLA	C4B-NB	2.92	1.41	1.37
15	b	808	CLA	C4B-NB	2.92	1.41	1.37
15	O	801	CLA	C1B-C2B	2.92	1.50	1.43
15	j	202	CLA	C4B-NB	2.92	1.41	1.37
15	a	838	CLA	C4B-NB	2.92	1.41	1.37
15	a	810	CLA	C4B-NB	2.92	1.41	1.37
15	N	810	CLA	C4B-NB	2.92	1.41	1.37
15	B	825	CLA	C4B-NB	2.92	1.41	1.37
15	N	833	CLA	C4B-NB	2.92	1.41	1.37
15	b	801	CLA	C1B-C2B	2.92	1.50	1.43
15	N	820	CLA	C4B-NB	2.92	1.41	1.37
15	O	808	CLA	C4B-NB	2.91	1.41	1.37
15	A	827	CLA	C4B-NB	2.91	1.41	1.37
15	N	806	CLA	C4B-NB	2.91	1.41	1.37
15	b	809	CLA	C4B-NB	2.91	1.41	1.37
15	A	820	CLA	C4B-NB	2.91	1.41	1.37
15	a	836	CLA	C4B-NB	2.91	1.41	1.37
15	B	809	CLA	C4B-NB	2.91	1.41	1.37
15	a	841	CLA	C4B-NB	2.91	1.41	1.37
15	A	841	CLA	C4B-NB	2.91	1.41	1.37
15	a	833	CLA	C4B-NB	2.91	1.41	1.37
15	O	805	CLA	C4B-NB	2.91	1.41	1.37
15	A	833	CLA	C4B-NB	2.91	1.41	1.37
15	N	803	CLA	C4B-NB	2.90	1.41	1.37
15	N	830	CLA	C4B-NB	2.90	1.41	1.37
15	a	806	CLA	C4B-NB	2.90	1.41	1.37
15	a	803	CLA	C4B-NB	2.90	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	838	CLA	C4B-NB	2.90	1.41	1.37
15	a	814	CLA	C4B-NB	2.90	1.41	1.37
15	a	827	CLA	C4B-NB	2.89	1.41	1.37
15	A	828	CLA	C4B-NB	2.89	1.41	1.37
15	B	806	CLA	C4B-NB	2.89	1.41	1.37
15	A	803	CLA	C4B-NB	2.89	1.41	1.37
15	O	836	CLA	C4B-NB	2.89	1.41	1.37
15	b	836	CLA	C4B-NB	2.88	1.41	1.37
15	A	806	CLA	C4B-NB	2.88	1.41	1.37
15	O	825	CLA	C4B-NB	2.88	1.41	1.37
15	B	836	CLA	C4B-NB	2.88	1.41	1.37
15	a	828	CLA	C4B-NB	2.87	1.41	1.37
15	A	838	CLA	C4B-NB	2.87	1.41	1.37
15	N	828	CLA	C4B-NB	2.87	1.41	1.37
15	N	814	CLA	C4B-NB	2.86	1.41	1.37
15	B	803	CLA	C4B-NB	2.86	1.41	1.37
14	A	856	F6C	C3B-C4B	2.86	1.50	1.44
15	b	822	CLA	C1B-C2B	2.86	1.49	1.43
14	A	824	F6C	C1D-ND	2.86	1.42	1.37
15	A	814	CLA	C4B-NB	2.86	1.41	1.37
14	N	824	F6C	C1D-ND	2.86	1.42	1.37
14	N	826	F6C	C1D-ND	2.86	1.42	1.37
14	W	201	F6C	C1D-ND	2.86	1.42	1.37
14	b	832	F6C	C1D-ND	2.86	1.42	1.37
15	b	825	CLA	C4B-NB	2.85	1.41	1.37
14	a	826	F6C	C1D-ND	2.85	1.42	1.37
14	B	832	F6C	C1D-ND	2.85	1.42	1.37
15	B	822	CLA	C1B-C2B	2.85	1.49	1.43
15	b	803	CLA	C4B-NB	2.85	1.41	1.37
14	O	832	F6C	C1D-ND	2.84	1.42	1.37
14	A	826	F6C	C1D-ND	2.84	1.42	1.37
14	N	856	F6C	C3B-C4B	2.84	1.50	1.44
14	a	824	F6C	C1D-ND	2.84	1.42	1.37
14	a	855	F6C	C3B-C4B	2.84	1.50	1.44
14	L	201	F6C	C1D-ND	2.84	1.42	1.37
15	O	803	CLA	C4B-NB	2.83	1.41	1.37
14	j	204	F6C	C1D-ND	2.83	1.42	1.37
14	A	802	F6C	C1D-ND	2.83	1.42	1.37
14	a	802	F6C	C1D-ND	2.83	1.42	1.37
14	W	204	F6C	C1D-ND	2.83	1.42	1.37
14	L	204	F6C	C1D-ND	2.81	1.42	1.37
14	j	201	F6C	C1D-ND	2.80	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	802	F6C	C1D-ND	2.80	1.42	1.37
15	N	838	CLA	C1B-C2B	2.80	1.49	1.43
15	O	822	CLA	C1B-C2B	2.79	1.49	1.43
15	b	814	CLA	C1B-C2B	2.79	1.49	1.43
15	A	838	CLA	C1B-C2B	2.78	1.49	1.43
14	a	855	F6C	C1D-ND	2.78	1.42	1.37
15	a	814	CLA	C1B-C2B	2.78	1.49	1.43
15	a	838	CLA	C1B-C2B	2.78	1.49	1.43
15	N	814	CLA	C1B-C2B	2.78	1.49	1.43
15	A	814	CLA	C1B-C2B	2.78	1.49	1.43
15	V	102	CLA	C1B-C2B	2.77	1.49	1.43
15	K	102	CLA	C1B-C2B	2.77	1.49	1.43
15	i	102	CLA	C1B-C2B	2.77	1.49	1.43
15	N	815	CLA	C1B-C2B	2.77	1.49	1.43
15	O	833	CLA	C1B-C2B	2.77	1.49	1.43
15	A	807	CLA	C1B-C2B	2.77	1.49	1.43
15	A	828	CLA	C1B-C2B	2.77	1.49	1.43
15	a	815	CLA	C1B-C2B	2.77	1.49	1.43
15	A	815	CLA	C1B-C2B	2.77	1.49	1.43
15	B	814	CLA	C1B-C2B	2.76	1.49	1.43
15	O	814	CLA	C1B-C2B	2.76	1.49	1.43
15	b	833	CLA	C1B-C2B	2.76	1.49	1.43
14	N	856	F6C	C1D-ND	2.76	1.42	1.37
14	A	856	F6C	C1D-ND	2.76	1.42	1.37
15	a	807	CLA	C1B-C2B	2.76	1.49	1.43
15	N	828	CLA	C1B-C2B	2.76	1.49	1.43
15	b	810	CLA	C1B-C2B	2.76	1.49	1.43
15	a	828	CLA	C1B-C2B	2.75	1.49	1.43
15	O	810	CLA	C1B-C2B	2.75	1.49	1.43
15	B	826	CLA	C1B-C2B	2.75	1.49	1.43
15	A	818	CLA	C1B-C2B	2.75	1.49	1.43
15	a	818	CLA	C1B-C2B	2.75	1.49	1.43
15	b	820	CLA	C1B-C2B	2.75	1.49	1.43
15	N	818	CLA	C1B-C2B	2.74	1.49	1.43
15	B	805	CLA	C1B-C2B	2.74	1.49	1.43
15	b	812	CLA	C1B-C2B	2.74	1.49	1.43
15	B	812	CLA	C1B-C2B	2.74	1.49	1.43
15	O	820	CLA	C1B-C2B	2.74	1.49	1.43
15	A	830	CLA	C1B-C2B	2.74	1.49	1.43
15	B	837	CLA	C1B-C2B	2.74	1.49	1.43
15	a	840	CLA	C1B-C2B	2.74	1.49	1.43
15	Z	102	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	l	102	CLA	C1B-C2B	2.74	1.49	1.43
15	A	823	CLA	C1B-C2B	2.74	1.49	1.43
15	B	820	CLA	C1B-C2B	2.74	1.49	1.43
15	X	102	CLA	C1B-C2B	2.74	1.49	1.43
15	O	829	CLA	C1B-C2B	2.74	1.49	1.43
15	B	810	CLA	C1B-C2B	2.74	1.49	1.43
15	b	829	CLA	C1B-C2B	2.74	1.49	1.43
15	A	811	CLA	C1B-C2B	2.74	1.49	1.43
15	b	815	CLA	C1B-C2B	2.74	1.49	1.43
15	B	815	CLA	C1B-C2B	2.74	1.49	1.43
15	N	807	CLA	C1B-C2B	2.74	1.49	1.43
15	O	815	CLA	C1B-C2B	2.74	1.49	1.43
15	O	807	CLA	C1B-C2B	2.74	1.49	1.43
15	a	834	CLA	C1B-C2B	2.74	1.49	1.43
15	a	823	CLA	C1B-C2B	2.74	1.49	1.43
15	A	822	CLA	C1B-C2B	2.73	1.49	1.43
15	a	811	CLA	C1B-C2B	2.73	1.49	1.43
15	b	805	CLA	C1B-C2B	2.73	1.49	1.43
15	N	830	CLA	C1B-C2B	2.73	1.49	1.43
15	a	830	CLA	C1B-C2B	2.73	1.49	1.43
15	N	808	CLA	C1B-C2B	2.73	1.49	1.43
15	b	837	CLA	C1B-C2B	2.73	1.49	1.43
15	N	809	CLA	C1B-C2B	2.73	1.49	1.43
15	N	834	CLA	C1B-C2B	2.73	1.49	1.43
15	N	823	CLA	C1B-C2B	2.73	1.49	1.43
15	N	831	CLA	C1B-C2B	2.73	1.49	1.43
15	O	837	CLA	C1B-C2B	2.73	1.49	1.43
15	N	821	CLA	C1B-C2B	2.73	1.49	1.43
15	b	807	CLA	C1B-C2B	2.73	1.49	1.43
15	A	821	CLA	C1B-C2B	2.73	1.49	1.43
15	a	821	CLA	C1B-C2B	2.73	1.49	1.43
15	a	822	CLA	C1B-C2B	2.73	1.49	1.43
15	B	807	CLA	C1B-C2B	2.73	1.49	1.43
15	N	813	CLA	C1B-C2B	2.73	1.49	1.43
15	B	806	CLA	C1B-C2B	2.73	1.49	1.43
15	N	811	CLA	C1B-C2B	2.73	1.49	1.43
15	A	841	CLA	C1B-C2B	2.73	1.49	1.43
15	b	827	CLA	C1B-C2B	2.73	1.49	1.43
15	A	813	CLA	C1B-C2B	2.73	1.49	1.43
15	O	812	CLA	C1B-C2B	2.73	1.49	1.43
15	j	202	CLA	C1B-C2B	2.73	1.49	1.43
15	a	806	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	829	CLA	C1B-C2B	2.72	1.49	1.43
15	a	832	CLA	C1B-C2B	2.72	1.49	1.43
15	B	833	CLA	C1B-C2B	2.72	1.49	1.43
15	N	806	CLA	C1B-C2B	2.72	1.49	1.43
15	O	805	CLA	C1B-C2B	2.72	1.49	1.43
15	O	806	CLA	C1B-C2B	2.72	1.49	1.43
15	A	808	CLA	C1B-C2B	2.72	1.49	1.43
15	A	809	CLA	C1B-C2B	2.72	1.49	1.43
15	B	809	CLA	C1B-C2B	2.72	1.49	1.43
15	A	840	CLA	C1B-C2B	2.72	1.49	1.43
15	O	827	CLA	C1B-C2B	2.72	1.49	1.43
15	b	825	CLA	C1B-C2B	2.72	1.49	1.43
15	B	829	CLA	C1B-C2B	2.72	1.49	1.43
15	a	813	CLA	C1B-C2B	2.72	1.49	1.43
15	B	813	CLA	C1B-C2B	2.72	1.49	1.43
15	O	838	CLA	C1B-C2B	2.72	1.49	1.43
15	a	808	CLA	C1B-C2B	2.72	1.49	1.43
15	b	838	CLA	C1B-C2B	2.72	1.49	1.43
15	B	819	CLA	C1B-C2B	2.72	1.49	1.43
15	A	806	CLA	C1B-C2B	2.72	1.49	1.43
15	O	819	CLA	C1B-C2B	2.72	1.49	1.43
15	b	806	CLA	C1B-C2B	2.72	1.49	1.43
15	O	825	CLA	C1B-C2B	2.72	1.49	1.43
15	a	809	CLA	C1B-C2B	2.72	1.49	1.43
15	B	827	CLA	C1B-C2B	2.71	1.49	1.43
15	W	202	CLA	C1B-C2B	2.71	1.49	1.43
15	B	821	CLA	C1B-C2B	2.71	1.49	1.43
15	A	834	CLA	C1B-C2B	2.71	1.49	1.43
15	b	826	CLA	C1B-C2B	2.71	1.49	1.43
15	b	819	CLA	C1B-C2B	2.71	1.49	1.43
15	B	838	CLA	C1B-C2B	2.71	1.49	1.43
15	O	840	CLA	C1B-C2B	2.71	1.49	1.43
15	N	822	CLA	C1B-C2B	2.71	1.49	1.43
15	b	830	CLA	C1B-C2B	2.71	1.49	1.43
15	N	840	CLA	C1B-C2B	2.71	1.49	1.43
15	a	836	CLA	C1B-C2B	2.71	1.49	1.43
15	A	831	CLA	C1B-C2B	2.71	1.49	1.43
15	N	837	CLA	C1B-C2B	2.71	1.49	1.43
15	b	813	CLA	C1B-C2B	2.70	1.49	1.43
14	B	839	F6C	C1D-ND	2.70	1.42	1.37
15	A	825	CLA	C1B-C2B	2.70	1.49	1.43
15	a	831	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	826	CLA	C1B-C2B	2.70	1.49	1.43
15	N	832	CLA	C1B-C2B	2.70	1.49	1.43
15	F	201	CLA	C1B-C2B	2.70	1.49	1.43
15	A	810	CLA	C1B-C2B	2.70	1.49	1.43
15	a	825	CLA	C1B-C2B	2.70	1.49	1.43
15	B	831	CLA	C1B-C2B	2.70	1.49	1.43
15	a	837	CLA	C1B-C2B	2.70	1.49	1.43
15	b	803	CLA	C1B-C2B	2.70	1.49	1.43
15	a	841	CLA	C1B-C2B	2.70	1.49	1.43
15	a	842	CLA	C1B-C2B	2.70	1.49	1.43
15	b	821	CLA	C1B-C2B	2.70	1.49	1.43
15	B	825	CLA	C1B-C2B	2.70	1.49	1.43
14	O	839	F6C	C1D-ND	2.70	1.42	1.37
15	O	813	CLA	C1B-C2B	2.70	1.49	1.43
15	O	821	CLA	C1B-C2B	2.70	1.49	1.43
15	S	201	CLA	C1B-C2B	2.70	1.49	1.43
15	b	840	CLA	C1B-C2B	2.70	1.49	1.43
15	f	201	CLA	C1B-C2B	2.70	1.49	1.43
15	A	832	CLA	C1B-C2B	2.70	1.49	1.43
15	A	837	CLA	C1B-C2B	2.70	1.49	1.43
15	O	830	CLA	C1B-C2B	2.70	1.49	1.43
15	b	831	CLA	C1B-C2B	2.70	1.49	1.43
15	A	836	CLA	C1B-C2B	2.69	1.49	1.43
15	N	842	CLA	C1B-C2B	2.69	1.49	1.43
15	N	810	CLA	C1B-C2B	2.69	1.49	1.43
15	a	829	CLA	C1B-C2B	2.69	1.49	1.43
15	a	812	CLA	C1B-C2B	2.69	1.49	1.43
15	L	202	CLA	C1B-C2B	2.69	1.49	1.43
15	N	829	CLA	C1B-C2B	2.69	1.49	1.43
15	b	811	CLA	C1B-C2B	2.69	1.49	1.43
15	a	810	CLA	C1B-C2B	2.69	1.49	1.43
15	b	835	CLA	C1B-C2B	2.69	1.49	1.43
15	B	840	CLA	C1B-C2B	2.69	1.49	1.43
15	O	831	CLA	C1B-C2B	2.69	1.49	1.43
15	B	811	CLA	C1B-C2B	2.69	1.49	1.43
15	A	812	CLA	C1B-C2B	2.69	1.49	1.43
15	N	812	CLA	C1B-C2B	2.69	1.49	1.43
14	b	839	F6C	C1D-ND	2.69	1.42	1.37
15	O	836	CLA	C1B-C2B	2.69	1.49	1.43
15	O	803	CLA	C1B-C2B	2.69	1.49	1.43
15	B	830	CLA	C1B-C2B	2.69	1.49	1.43
15	O	811	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	835	CLA	C1B-C2B	2.68	1.49	1.43
15	B	835	CLA	C1B-C2B	2.68	1.49	1.43
15	W	203	CLA	C1B-C2B	2.68	1.49	1.43
15	O	823	CLA	C1B-C2B	2.68	1.49	1.43
15	A	835	CLA	C1B-C2B	2.68	1.49	1.43
15	a	819	CLA	C1B-C2B	2.68	1.49	1.43
15	A	842	CLA	C1B-C2B	2.68	1.49	1.43
15	N	825	CLA	C1B-C2B	2.68	1.49	1.43
15	j	203	CLA	C1B-C2B	2.67	1.49	1.43
15	B	802	CLA	C1B-C2B	2.67	1.49	1.43
15	A	805	CLA	C1B-C2B	2.67	1.49	1.43
15	B	836	CLA	C1B-C2B	2.67	1.49	1.43
15	B	823	CLA	C1B-C2B	2.67	1.49	1.43
15	O	824	CLA	C1B-C2B	2.67	1.49	1.43
15	b	823	CLA	C1B-C2B	2.67	1.49	1.43
15	a	805	CLA	C1B-C2B	2.67	1.49	1.43
15	O	808	CLA	C1B-C2B	2.67	1.49	1.43
15	N	836	CLA	C1B-C2B	2.67	1.49	1.43
15	N	805	CLA	C1B-C2B	2.67	1.49	1.43
15	N	841	CLA	C1B-C2B	2.67	1.49	1.43
15	b	802	CLA	C1B-C2B	2.67	1.49	1.43
15	b	808	CLA	C1B-C2B	2.67	1.49	1.43
15	A	819	CLA	C1B-C2B	2.67	1.49	1.43
15	a	804	CLA	C3B-C4B	2.66	1.50	1.42
15	b	836	CLA	C1B-C2B	2.66	1.49	1.43
15	N	803	CLA	C1B-C2B	2.66	1.49	1.43
15	O	802	CLA	C1B-C2B	2.66	1.49	1.43
15	A	804	CLA	C1B-C2B	2.66	1.49	1.43
15	a	803	CLA	C1B-C2B	2.66	1.49	1.43
15	L	203	CLA	C1B-C2B	2.66	1.49	1.43
15	O	804	CLA	C1B-C2B	2.66	1.49	1.43
15	B	803	CLA	C1B-C2B	2.66	1.49	1.43
15	b	824	CLA	C1B-C2B	2.66	1.49	1.43
15	N	819	CLA	C1B-C2B	2.65	1.49	1.43
15	B	804	CLA	C1B-C2B	2.65	1.49	1.43
15	B	824	CLA	C1B-C2B	2.65	1.49	1.43
15	B	834	CLA	C1B-C2B	2.65	1.49	1.43
15	A	803	CLA	C1B-C2B	2.64	1.49	1.43
15	B	817	CLA	C1B-C2B	2.64	1.49	1.43
15	i	103	CLA	C1B-C2B	2.64	1.49	1.43
15	b	804	CLA	C1B-C2B	2.64	1.49	1.43
15	N	835	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	827	CLA	C1B-C2B	2.64	1.49	1.43
15	N	804	CLA	C1B-C2B	2.63	1.49	1.43
15	b	817	CLA	C1B-C2B	2.63	1.49	1.43
14	N	856	F6C	C4B-NB	2.63	1.42	1.37
15	a	839	CLA	C1B-C2B	2.63	1.49	1.43
15	A	839	CLA	C1B-C2B	2.63	1.49	1.43
15	O	834	CLA	C1B-C2B	2.63	1.49	1.43
15	b	834	CLA	C1B-C2B	2.63	1.49	1.43
15	a	835	CLA	C1B-C2B	2.63	1.49	1.43
15	N	839	CLA	C1B-C2B	2.63	1.49	1.43
15	N	827	CLA	C1B-C2B	2.63	1.49	1.43
15	a	827	CLA	C1B-C2B	2.63	1.49	1.43
15	O	817	CLA	C1B-C2B	2.63	1.49	1.43
15	K	103	CLA	C1B-C2B	2.62	1.49	1.43
14	a	855	F6C	C4B-NB	2.62	1.42	1.37
15	N	820	CLA	C1B-C2B	2.62	1.49	1.43
15	O	809	CLA	C1B-C2B	2.62	1.49	1.43
13	a	801	CL0	CMD-C2D	-2.61	1.46	1.51
13	N	801	CL0	CMD-C2D	-2.61	1.46	1.51
15	b	828	CLA	C1B-C2B	2.61	1.49	1.43
15	O	828	CLA	C1B-C2B	2.61	1.49	1.43
15	A	817	CLA	C1B-C2B	2.61	1.49	1.43
15	b	809	CLA	C1B-C2B	2.61	1.49	1.43
14	A	856	F6C	C4B-NB	2.61	1.42	1.37
15	A	820	CLA	C1B-C2B	2.61	1.49	1.43
15	B	808	CLA	C1B-C2B	2.60	1.49	1.43
15	a	817	CLA	C1B-C2B	2.60	1.49	1.43
15	a	816	CLA	C1B-C2B	2.60	1.49	1.43
15	N	817	CLA	C1B-C2B	2.60	1.49	1.43
15	b	818	CLA	C1B-C2B	2.60	1.49	1.43
15	a	820	CLA	C1B-C2B	2.59	1.49	1.43
15	B	828	CLA	C1B-C2B	2.59	1.49	1.43
15	N	816	CLA	C1B-C2B	2.59	1.49	1.43
15	B	818	CLA	C1B-C2B	2.59	1.49	1.43
15	a	804	CLA	C1B-C2B	2.58	1.49	1.43
15	N	804	CLA	C3B-C4B	2.58	1.50	1.42
15	O	818	CLA	C1B-C2B	2.58	1.49	1.43
15	A	816	CLA	C1B-C2B	2.58	1.49	1.43
15	V	103	CLA	C1B-C2B	2.57	1.49	1.43
15	A	833	CLA	C1B-C2B	2.57	1.49	1.43
15	N	833	CLA	C1B-C2B	2.56	1.49	1.43
13	A	801	CL0	CMD-C2D	-2.56	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	833	CLA	C1B-C2B	2.54	1.49	1.43
15	A	816	CLA	C3B-C4B	2.54	1.50	1.42
15	B	816	CLA	C1B-C2B	2.53	1.49	1.43
15	N	816	CLA	C3B-C4B	2.53	1.50	1.42
14	a	802	F6C	C4B-NB	2.52	1.42	1.37
14	A	802	F6C	C4B-NB	2.52	1.42	1.37
15	a	816	CLA	C3B-C4B	2.51	1.50	1.42
14	N	802	F6C	C4B-NB	2.50	1.41	1.37
14	W	201	F6C	C3B-C4B	2.49	1.49	1.44
14	A	824	F6C	C4B-NB	2.49	1.41	1.37
14	N	824	F6C	C4B-NB	2.48	1.41	1.37
15	A	804	CLA	C3B-C4B	2.48	1.49	1.42
15	b	816	CLA	C1B-C2B	2.47	1.48	1.43
14	b	832	F6C	C2B-C1B	2.47	1.49	1.44
14	a	824	F6C	C4B-NB	2.47	1.41	1.37
13	a	801	CL0	CMB-C2B	-2.47	1.46	1.51
14	j	201	F6C	C3B-C4B	2.47	1.49	1.44
13	a	801	CL0	CMC-C2C	-2.47	1.46	1.50
14	B	832	F6C	C2B-C1B	2.47	1.49	1.44
14	L	204	F6C	C4B-NB	2.46	1.41	1.37
13	N	801	CL0	CMB-C2B	-2.46	1.46	1.51
13	A	801	CL0	CMC-C2C	-2.45	1.46	1.50
15	B	822	CLA	CHC-C1C	2.45	1.43	1.38
13	A	801	CL0	CMB-C2B	-2.45	1.46	1.51
13	N	801	CL0	CMC-C2C	-2.45	1.46	1.50
14	O	832	F6C	C2B-C1B	2.45	1.49	1.44
13	N	801	CL0	CAC-C3C	-2.45	1.47	1.51
15	i	103	CLA	C3B-C4B	2.44	1.49	1.42
14	a	826	F6C	C2B-C1B	2.44	1.49	1.44
14	j	201	F6C	C4B-NB	2.44	1.41	1.37
13	a	801	CL0	CAC-C3C	-2.44	1.47	1.51
15	b	835	CLA	C3B-C4B	2.43	1.49	1.42
14	W	201	F6C	C4B-NB	2.43	1.41	1.37
15	b	822	CLA	CHC-C1C	2.43	1.43	1.38
15	O	835	CLA	C3B-C4B	2.43	1.49	1.42
15	B	835	CLA	C3B-C4B	2.43	1.49	1.42
13	A	801	CL0	CAC-C3C	-2.43	1.47	1.51
15	N	819	CLA	C3B-C4B	2.42	1.49	1.42
15	A	819	CLA	C3B-C4B	2.42	1.49	1.42
13	N	801	CL0	C1A-CHA	-2.42	1.37	1.40
14	j	204	F6C	C4B-NB	2.42	1.41	1.37
14	A	826	F6C	C2B-C1B	2.42	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	S	201	CLA	C3B-C4B	2.42	1.49	1.42
15	F	201	CLA	C3B-C4B	2.42	1.49	1.42
15	a	839	CLA	C3B-C4B	2.42	1.49	1.42
14	O	832	F6C	C4B-NB	2.42	1.41	1.37
15	O	816	CLA	C3B-C4B	2.42	1.49	1.42
15	a	819	CLA	C3B-C4B	2.41	1.49	1.42
14	W	204	F6C	C4B-NB	2.41	1.41	1.37
15	A	839	CLA	C3B-C4B	2.41	1.49	1.42
14	B	832	F6C	C4B-NB	2.41	1.41	1.37
14	b	832	F6C	C4B-NB	2.41	1.41	1.37
15	f	201	CLA	C3B-C4B	2.41	1.49	1.42
15	B	804	CLA	C3B-C4B	2.41	1.49	1.42
14	L	201	F6C	C3B-C4B	2.41	1.49	1.44
15	N	839	CLA	C3B-C4B	2.41	1.49	1.42
13	a	801	CL0	C1A-CHA	-2.41	1.37	1.40
14	N	826	F6C	C4B-NB	2.41	1.41	1.37
14	N	824	F6C	C2B-C1B	2.40	1.49	1.44
14	L	201	F6C	C4B-NB	2.40	1.41	1.37
15	B	811	CLA	C3B-C4B	2.40	1.49	1.42
15	N	842	CLA	C3B-C4B	2.40	1.49	1.42
15	A	842	CLA	C3B-C4B	2.40	1.49	1.42
15	B	804	CLA	CHC-C1C	2.40	1.43	1.38
15	b	804	CLA	C3B-C4B	2.40	1.49	1.42
15	O	811	CLA	C3B-C4B	2.40	1.49	1.42
15	a	842	CLA	C3B-C4B	2.40	1.49	1.42
14	N	826	F6C	C2B-C1B	2.40	1.49	1.44
15	N	805	CLA	C3B-C4B	2.40	1.49	1.42
15	A	819	CLA	CHC-C1C	2.40	1.43	1.38
15	a	817	CLA	C3B-C4B	2.39	1.49	1.42
14	B	839	F6C	C4B-NB	2.39	1.41	1.37
15	B	822	CLA	C3B-C4B	2.39	1.49	1.42
15	b	811	CLA	C3B-C4B	2.39	1.49	1.42
14	a	826	F6C	C4B-NB	2.39	1.41	1.37
15	b	804	CLA	CHC-C1C	2.39	1.43	1.38
15	A	805	CLA	C3B-C4B	2.39	1.49	1.42
15	O	804	CLA	C3B-C4B	2.39	1.49	1.42
15	A	817	CLA	C3B-C4B	2.39	1.49	1.42
14	A	824	F6C	C2B-C1B	2.39	1.49	1.44
15	B	814	CLA	C3B-C4B	2.39	1.49	1.42
15	O	816	CLA	C1B-C2B	2.39	1.48	1.43
15	V	103	CLA	C3B-C4B	2.39	1.49	1.42
15	N	812	CLA	C3B-C4B	2.39	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	812	CLA	C3B-C4B	2.38	1.49	1.42
15	N	817	CLA	C3B-C4B	2.38	1.49	1.42
15	N	819	CLA	CHC-C1C	2.38	1.43	1.38
14	a	824	F6C	C2B-C1B	2.38	1.49	1.44
15	A	812	CLA	C3B-C4B	2.38	1.49	1.42
15	O	814	CLA	C3B-C4B	2.38	1.49	1.42
15	a	805	CLA	C3B-C4B	2.38	1.49	1.42
15	O	804	CLA	CHC-C1C	2.38	1.43	1.38
15	A	803	CLA	C3B-C4B	2.38	1.49	1.42
15	K	103	CLA	C3B-C4B	2.38	1.49	1.42
15	b	814	CLA	C3B-C4B	2.38	1.49	1.42
15	b	819	CLA	C3B-C4B	2.38	1.49	1.42
15	N	827	CLA	C3B-C4B	2.38	1.49	1.42
15	O	819	CLA	C3B-C4B	2.38	1.49	1.42
15	a	803	CLA	C3B-C4B	2.38	1.49	1.42
14	O	839	F6C	C4B-NB	2.38	1.41	1.37
14	A	824	F6C	C3B-C4B	2.37	1.49	1.44
15	a	819	CLA	CHC-C1C	2.37	1.43	1.38
15	B	824	CLA	C3B-C4B	2.37	1.49	1.42
15	B	819	CLA	C3B-C4B	2.37	1.49	1.42
14	A	826	F6C	C4B-NB	2.37	1.41	1.37
14	b	839	F6C	C4B-NB	2.37	1.41	1.37
15	N	825	CLA	C3B-C4B	2.37	1.49	1.42
15	N	803	CLA	C3B-C4B	2.37	1.49	1.42
14	N	824	F6C	C3B-C4B	2.36	1.49	1.44
14	a	824	F6C	C3B-C4B	2.36	1.49	1.44
15	O	816	CLA	CHC-C1C	2.36	1.43	1.38
13	A	801	CL0	C1A-CHA	-2.36	1.37	1.40
15	O	824	CLA	C3B-C4B	2.36	1.49	1.42
15	a	827	CLA	C3B-C4B	2.36	1.49	1.42
15	B	809	CLA	CMB-C2B	-2.36	1.45	1.50
15	A	825	CLA	C3B-C4B	2.36	1.49	1.42
15	a	825	CLA	C3B-C4B	2.36	1.49	1.42
15	N	805	CLA	CHC-C1C	2.36	1.43	1.38
15	A	827	CLA	C3B-C4B	2.36	1.49	1.42
14	L	201	F6C	C2B-C1B	2.36	1.49	1.44
15	A	834	CLA	C3B-C4B	2.36	1.49	1.42
15	N	841	CLA	C3B-C4B	2.36	1.49	1.42
15	i	103	CLA	CHC-C1C	2.36	1.43	1.38
15	B	808	CLA	C3B-C4B	2.35	1.49	1.42
15	b	824	CLA	C3B-C4B	2.35	1.49	1.42
15	B	831	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	809	CLA	CMB-C2B	-2.35	1.46	1.50
15	b	809	CLA	CMB-C2B	-2.35	1.46	1.50
15	B	818	CLA	C3B-C4B	2.35	1.49	1.42
15	b	818	CLA	C3B-C4B	2.35	1.49	1.42
15	A	805	CLA	CHC-C1C	2.35	1.43	1.38
15	b	816	CLA	CMB-C2B	-2.35	1.46	1.50
15	O	818	CLA	C3B-C4B	2.35	1.49	1.42
15	b	822	CLA	C3B-C4B	2.35	1.49	1.42
15	N	833	CLA	C3B-C4B	2.35	1.49	1.42
15	O	816	CLA	CMB-C2B	-2.35	1.46	1.50
15	b	828	CLA	C3B-C4B	2.35	1.49	1.42
15	a	833	CLA	C3B-C4B	2.35	1.49	1.42
15	b	831	CLA	C3B-C4B	2.34	1.49	1.42
15	N	811	CLA	C3B-C4B	2.34	1.49	1.42
15	b	821	CLA	C3B-C4B	2.34	1.49	1.42
15	O	831	CLA	C3B-C4B	2.34	1.49	1.42
15	A	833	CLA	C3B-C4B	2.34	1.49	1.42
15	A	803	CLA	CHC-C1C	2.34	1.43	1.38
15	O	828	CLA	C3B-C4B	2.34	1.49	1.42
15	b	805	CLA	C3B-C4B	2.34	1.49	1.42
15	b	825	CLA	C3B-C4B	2.34	1.49	1.42
15	a	805	CLA	CHC-C1C	2.34	1.43	1.38
15	a	811	CLA	C3B-C4B	2.34	1.49	1.42
15	B	805	CLA	C3B-C4B	2.34	1.49	1.42
14	b	839	F6C	C2B-C1B	2.34	1.49	1.44
15	B	830	CLA	C3B-C4B	2.34	1.49	1.42
15	O	821	CLA	C3B-C4B	2.34	1.49	1.42
15	O	825	CLA	C3B-C4B	2.34	1.49	1.42
15	A	837	CLA	C3B-C4B	2.34	1.49	1.42
15	a	829	CLA	C3B-C4B	2.34	1.49	1.42
14	j	204	F6C	C2B-C1B	2.34	1.49	1.44
15	A	811	CLA	C3B-C4B	2.33	1.49	1.42
15	L	202	CLA	C3B-C4B	2.33	1.49	1.42
15	b	840	CLA	C3B-C4B	2.33	1.49	1.42
15	A	808	CLA	C3B-C4B	2.33	1.49	1.42
15	X	102	CLA	C3B-C4B	2.33	1.49	1.42
15	a	837	CLA	C3B-C4B	2.33	1.49	1.42
15	B	825	CLA	C3B-C4B	2.33	1.49	1.42
15	O	805	CLA	C3B-C4B	2.33	1.49	1.42
15	B	818	CLA	CHC-C1C	2.33	1.43	1.38
15	A	813	CLA	C3B-C4B	2.33	1.49	1.42
15	O	830	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	816	CLA	CHC-C1C	2.33	1.43	1.38
15	N	829	CLA	C3B-C4B	2.33	1.49	1.42
14	B	839	F6C	C2B-C1B	2.33	1.49	1.44
15	a	803	CLA	CHC-C1C	2.33	1.43	1.38
15	B	828	CLA	C3B-C4B	2.33	1.49	1.42
15	N	837	CLA	C3B-C4B	2.33	1.49	1.42
15	a	813	CLA	C3B-C4B	2.33	1.49	1.42
14	N	826	F6C	C3B-C4B	2.33	1.49	1.44
15	O	813	CLA	C3B-C4B	2.33	1.49	1.42
15	l	102	CLA	C3B-C4B	2.33	1.49	1.42
15	B	813	CLA	C3B-C4B	2.33	1.49	1.42
15	B	836	CLA	C3B-C4B	2.33	1.49	1.42
15	O	802	CLA	C3B-C4B	2.33	1.49	1.42
15	Z	102	CLA	C3B-C4B	2.33	1.49	1.42
15	B	802	CLA	C3B-C4B	2.33	1.49	1.42
15	B	821	CLA	C3B-C4B	2.33	1.49	1.42
15	O	820	CLA	C3B-C4B	2.33	1.49	1.42
15	N	834	CLA	C3B-C4B	2.33	1.49	1.42
15	b	834	CLA	C3B-C4B	2.33	1.49	1.42
14	W	204	F6C	C3B-C4B	2.33	1.49	1.44
15	O	822	CLA	C3B-C4B	2.32	1.49	1.42
15	B	827	CLA	C3B-C4B	2.32	1.49	1.42
15	O	840	CLA	C3B-C4B	2.32	1.49	1.42
15	b	815	CLA	C3B-C4B	2.32	1.49	1.42
14	L	204	F6C	C2B-C1B	2.32	1.49	1.44
15	A	829	CLA	C3B-C4B	2.32	1.49	1.42
15	O	815	CLA	C3B-C4B	2.32	1.49	1.42
15	b	813	CLA	C3B-C4B	2.32	1.49	1.42
15	A	816	CLA	CHC-C1C	2.32	1.43	1.38
15	O	818	CLA	CHC-C1C	2.32	1.43	1.38
15	a	810	CLA	C3B-C4B	2.32	1.49	1.42
15	B	840	CLA	C3B-C4B	2.32	1.49	1.42
15	b	802	CLA	C3B-C4B	2.32	1.49	1.42
15	O	834	CLA	C3B-C4B	2.32	1.49	1.42
15	N	810	CLA	C3B-C4B	2.32	1.49	1.42
15	a	839	CLA	CHC-C1C	2.32	1.43	1.38
14	W	204	F6C	C2B-C1B	2.32	1.49	1.44
15	b	818	CLA	CHC-C1C	2.32	1.43	1.38
15	B	815	CLA	C3B-C4B	2.32	1.49	1.42
15	L	203	CLA	C3B-C4B	2.32	1.49	1.42
14	W	201	F6C	C2B-C1B	2.32	1.49	1.44
15	A	810	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	j	203	CLA	C3B-C4B	2.32	1.49	1.42
15	b	812	CLA	C3B-C4B	2.32	1.49	1.42
15	N	813	CLA	C3B-C4B	2.32	1.49	1.42
15	b	830	CLA	C3B-C4B	2.32	1.49	1.42
14	j	204	F6C	C3B-C4B	2.32	1.49	1.44
15	b	816	CLA	C3B-C4B	2.32	1.49	1.42
15	O	836	CLA	C3B-C4B	2.32	1.49	1.42
15	a	828	CLA	C3B-C4B	2.32	1.49	1.42
15	B	824	CLA	CHC-C1C	2.32	1.43	1.38
15	A	806	CLA	C3B-C4B	2.32	1.49	1.42
15	a	806	CLA	C3B-C4B	2.32	1.49	1.42
15	b	820	CLA	C3B-C4B	2.32	1.49	1.42
15	b	837	CLA	C3B-C4B	2.32	1.49	1.42
15	N	836	CLA	C3B-C4B	2.32	1.49	1.42
15	O	837	CLA	C3B-C4B	2.32	1.49	1.42
15	B	820	CLA	C3B-C4B	2.31	1.49	1.42
15	O	812	CLA	C3B-C4B	2.31	1.49	1.42
15	B	834	CLA	C3B-C4B	2.31	1.49	1.42
15	B	833	CLA	C3B-C4B	2.31	1.49	1.42
15	B	812	CLA	C3B-C4B	2.31	1.49	1.42
15	a	808	CLA	C3B-C4B	2.31	1.49	1.42
15	A	828	CLA	C3B-C4B	2.31	1.49	1.42
15	N	816	CLA	CHC-C1C	2.31	1.43	1.38
15	A	823	CLA	C3B-C4B	2.31	1.49	1.42
15	B	803	CLA	C3B-C4B	2.31	1.49	1.42
15	N	803	CLA	CHC-C1C	2.31	1.43	1.38
15	N	808	CLA	C3B-C4B	2.31	1.49	1.42
15	N	823	CLA	C3B-C4B	2.31	1.49	1.42
15	a	823	CLA	C3B-C4B	2.31	1.49	1.42
15	b	833	CLA	C3B-C4B	2.31	1.49	1.42
15	b	824	CLA	CHC-C1C	2.31	1.43	1.38
15	N	821	CLA	C3B-C4B	2.31	1.49	1.42
15	B	816	CLA	C3B-C4B	2.31	1.49	1.42
15	a	834	CLA	C3B-C4B	2.31	1.49	1.42
15	N	830	CLA	C3B-C4B	2.31	1.49	1.42
15	O	813	CLA	CHC-C1C	2.31	1.43	1.38
15	b	808	CLA	C3B-C4B	2.31	1.49	1.42
15	b	836	CLA	C3B-C4B	2.31	1.49	1.42
15	A	808	CLA	CHC-C1C	2.31	1.43	1.38
15	B	813	CLA	CHC-C1C	2.31	1.43	1.38
15	O	806	CLA	C3B-C4B	2.31	1.49	1.42
15	a	830	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	826	F6C	C3B-C4B	2.31	1.49	1.44
15	a	832	CLA	C3B-C4B	2.31	1.49	1.42
15	N	806	CLA	C3B-C4B	2.31	1.49	1.42
15	B	837	CLA	C3B-C4B	2.31	1.49	1.42
15	N	828	CLA	C3B-C4B	2.31	1.49	1.42
15	B	808	CLA	CHC-C1C	2.31	1.43	1.38
15	A	830	CLA	C3B-C4B	2.30	1.49	1.42
15	O	824	CLA	CHC-C1C	2.30	1.43	1.38
15	A	836	CLA	C3B-C4B	2.30	1.49	1.42
15	a	821	CLA	C3B-C4B	2.30	1.49	1.42
15	b	806	CLA	C3B-C4B	2.30	1.49	1.42
14	a	826	F6C	C3B-C4B	2.30	1.49	1.44
15	A	839	CLA	CHC-C1C	2.30	1.43	1.38
15	a	815	CLA	C3B-C4B	2.30	1.49	1.42
15	N	839	CLA	CHC-C1C	2.30	1.43	1.38
15	b	833	CLA	CHC-C1C	2.30	1.43	1.38
15	A	821	CLA	C3B-C4B	2.30	1.49	1.42
15	O	833	CLA	C3B-C4B	2.30	1.49	1.42
15	b	827	CLA	C3B-C4B	2.30	1.49	1.42
15	B	830	CLA	CHC-C1C	2.30	1.43	1.38
15	O	808	CLA	C3B-C4B	2.30	1.49	1.42
14	N	802	F6C	C3B-C4B	2.30	1.49	1.44
15	B	806	CLA	C3B-C4B	2.30	1.49	1.42
14	A	802	F6C	C3B-C4B	2.30	1.49	1.44
15	a	809	CLA	C3B-C4B	2.30	1.49	1.42
15	K	102	CLA	C3B-C4B	2.30	1.49	1.42
15	a	835	CLA	C3B-C4B	2.30	1.49	1.42
15	B	833	CLA	CHC-C1C	2.30	1.43	1.38
15	N	835	CLA	C3B-C4B	2.30	1.49	1.42
15	A	815	CLA	C3B-C4B	2.30	1.49	1.42
15	N	822	CLA	C3B-C4B	2.30	1.49	1.42
15	i	102	CLA	C3B-C4B	2.30	1.49	1.42
15	A	809	CLA	C3B-C4B	2.30	1.49	1.42
15	N	815	CLA	C3B-C4B	2.30	1.49	1.42
14	O	839	F6C	C3B-C4B	2.30	1.49	1.44
15	B	827	CLA	CHC-C1C	2.29	1.43	1.38
15	B	805	CLA	CHC-C1C	2.29	1.43	1.38
14	O	832	F6C	C3B-C4B	2.29	1.49	1.44
15	j	202	CLA	C3B-C4B	2.29	1.49	1.42
15	V	102	CLA	C3B-C4B	2.29	1.49	1.42
15	B	810	CLA	C3B-C4B	2.29	1.49	1.42
15	O	827	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	831	CLA	CHC-C1C	2.29	1.43	1.38
15	B	822	CLA	CMD-C2D	-2.29	1.46	1.50
15	a	836	CLA	C3B-C4B	2.29	1.49	1.42
15	A	837	CLA	CHC-C1C	2.29	1.43	1.38
15	N	825	CLA	CHC-C1C	2.29	1.43	1.38
15	O	826	CLA	C3B-C4B	2.29	1.49	1.42
15	b	805	CLA	CHC-C1C	2.29	1.43	1.38
15	b	813	CLA	CHC-C1C	2.29	1.43	1.38
15	b	814	CLA	CHC-C1C	2.29	1.43	1.38
15	L	203	CLA	CHC-C1C	2.29	1.43	1.38
15	N	827	CLA	CHC-C1C	2.29	1.43	1.38
15	a	829	CLA	CHC-C1C	2.29	1.43	1.38
15	N	820	CLA	C3B-C4B	2.29	1.49	1.42
15	B	834	CLA	CHC-C1C	2.29	1.43	1.38
15	B	836	CLA	CHC-C1C	2.29	1.43	1.38
15	N	833	CLA	CHC-C1C	2.29	1.43	1.38
15	N	837	CLA	CHC-C1C	2.29	1.43	1.38
15	A	835	CLA	C3B-C4B	2.29	1.49	1.42
15	N	809	CLA	C3B-C4B	2.29	1.49	1.42
15	b	831	CLA	CHC-C1C	2.29	1.43	1.38
15	N	832	CLA	C3B-C4B	2.29	1.49	1.42
15	W	203	CLA	C3B-C4B	2.29	1.49	1.42
15	b	835	CLA	CHC-C1C	2.29	1.43	1.38
15	W	202	CLA	C3B-C4B	2.29	1.49	1.42
15	F	201	CLA	CHC-C1C	2.29	1.43	1.38
15	O	835	CLA	CHC-C1C	2.29	1.43	1.38
15	A	833	CLA	CHC-C1C	2.29	1.43	1.38
15	a	811	CLA	CHC-C1C	2.29	1.43	1.38
15	a	833	CLA	CHC-C1C	2.29	1.43	1.38
14	a	802	F6C	C3B-C4B	2.29	1.49	1.44
15	O	810	CLA	C3B-C4B	2.29	1.49	1.42
15	b	821	CLA	CHC-C1C	2.29	1.43	1.38
15	A	820	CLA	C3B-C4B	2.29	1.49	1.42
15	B	831	CLA	CHC-C1C	2.29	1.43	1.38
15	B	817	CLA	C3B-C4B	2.29	1.49	1.42
15	a	820	CLA	C3B-C4B	2.29	1.49	1.42
15	A	834	CLA	CHC-C1C	2.29	1.43	1.38
15	A	832	CLA	C3B-C4B	2.28	1.49	1.42
15	V	103	CLA	CHC-C1C	2.28	1.43	1.38
15	a	825	CLA	CHC-C1C	2.28	1.43	1.38
15	a	814	CLA	C3B-C4B	2.28	1.49	1.42
15	O	817	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	X	102	CLA	CHC-C1C	2.28	1.43	1.38
15	O	836	CLA	CHC-C1C	2.28	1.43	1.38
14	O	839	F6C	C2B-C1B	2.28	1.49	1.44
15	B	829	CLA	C3B-C4B	2.28	1.49	1.42
15	N	818	CLA	C3B-C4B	2.28	1.49	1.42
15	a	827	CLA	CHC-C1C	2.28	1.43	1.38
15	b	834	CLA	CHC-C1C	2.28	1.43	1.38
15	a	837	CLA	CHC-C1C	2.28	1.43	1.38
15	A	829	CLA	CHC-C1C	2.28	1.43	1.38
15	b	829	CLA	C3B-C4B	2.28	1.49	1.42
15	B	807	CLA	C3B-C4B	2.28	1.49	1.42
15	Z	102	CLA	CHC-C1C	2.28	1.43	1.38
15	b	817	CLA	C3B-C4B	2.28	1.49	1.42
15	B	819	CLA	CHC-C1C	2.28	1.43	1.38
15	B	835	CLA	CHC-C1C	2.28	1.43	1.38
15	N	811	CLA	CHC-C1C	2.28	1.43	1.38
15	l	102	CLA	CHC-C1C	2.28	1.43	1.38
14	O	839	F6C	CMD-C2D	-2.28	1.46	1.50
15	L	202	CLA	CHC-C1C	2.28	1.43	1.38
15	O	814	CLA	CHC-C1C	2.28	1.43	1.38
15	O	827	CLA	CHC-C1C	2.28	1.43	1.38
15	N	814	CLA	C3B-C4B	2.28	1.49	1.42
15	b	807	CLA	C3B-C4B	2.28	1.49	1.42
15	b	826	CLA	C3B-C4B	2.28	1.49	1.42
14	B	839	F6C	CMD-C2D	-2.28	1.46	1.50
15	B	823	CLA	C3B-C4B	2.28	1.49	1.42
15	O	829	CLA	C3B-C4B	2.28	1.49	1.42
15	N	812	CLA	CHC-C1C	2.28	1.43	1.38
15	a	812	CLA	CHC-C1C	2.28	1.43	1.38
15	b	819	CLA	CHC-C1C	2.28	1.43	1.38
15	b	822	CLA	CMD-C2D	-2.28	1.46	1.50
15	b	823	CLA	C3B-C4B	2.28	1.49	1.42
15	b	803	CLA	CMC-C2C	-2.28	1.46	1.50
15	B	814	CLA	CHC-C1C	2.28	1.43	1.38
14	B	839	F6C	C3B-C4B	2.28	1.49	1.44
15	O	833	CLA	CHC-C1C	2.28	1.43	1.38
15	a	841	CLA	C3B-C4B	2.27	1.49	1.42
15	A	842	CLA	CHC-C1C	2.27	1.43	1.38
15	b	816	CLA	CHC-C1C	2.27	1.43	1.38
15	O	821	CLA	CHC-C1C	2.27	1.43	1.38
15	O	823	CLA	C3B-C4B	2.27	1.49	1.42
15	b	810	CLA	C3B-C4B	2.27	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	832	F6C	C3B-C4B	2.27	1.49	1.44
14	b	839	F6C	C3B-C4B	2.27	1.49	1.44
15	A	822	CLA	C3B-C4B	2.27	1.49	1.42
15	A	827	CLA	CHC-C1C	2.27	1.43	1.38
15	O	837	CLA	CHC-C1C	2.27	1.43	1.38
15	a	809	CLA	CHC-C1C	2.27	1.43	1.38
15	O	807	CLA	C3B-C4B	2.27	1.49	1.42
15	N	808	CLA	CHC-C1C	2.27	1.43	1.38
15	b	830	CLA	CHC-C1C	2.27	1.43	1.38
15	N	810	CLA	CHC-C1C	2.27	1.43	1.38
15	O	805	CLA	CHC-C1C	2.27	1.43	1.38
14	b	839	F6C	CMD-C2D	-2.27	1.46	1.50
15	A	825	CLA	CHC-C1C	2.27	1.43	1.38
15	O	803	CLA	C3B-C4B	2.27	1.49	1.42
15	O	830	CLA	CHC-C1C	2.27	1.43	1.38
15	a	808	CLA	CHC-C1C	2.27	1.43	1.38
14	B	832	F6C	C3B-C4B	2.27	1.49	1.44
15	A	821	CLA	CHC-C1C	2.27	1.43	1.38
15	N	842	CLA	CHC-C1C	2.27	1.43	1.38
15	a	835	CLA	CHC-C1C	2.27	1.43	1.38
15	A	812	CLA	CHC-C1C	2.27	1.43	1.38
15	A	813	CLA	CHC-C1C	2.27	1.43	1.38
15	B	810	CLA	CHC-C1C	2.27	1.43	1.38
15	N	829	CLA	CHC-C1C	2.27	1.43	1.38
15	b	838	CLA	C3B-C4B	2.27	1.49	1.42
15	S	201	CLA	CHC-C1C	2.27	1.43	1.38
15	a	810	CLA	CHC-C1C	2.27	1.43	1.38
15	b	837	CLA	CHC-C1C	2.27	1.43	1.38
15	j	203	CLA	CHC-C1C	2.27	1.43	1.38
15	O	819	CLA	CHC-C1C	2.27	1.43	1.38
15	N	835	CLA	CHC-C1C	2.27	1.43	1.38
15	B	803	CLA	CHC-C1C	2.27	1.43	1.38
15	B	838	CLA	C3B-C4B	2.27	1.49	1.42
15	A	811	CLA	CHC-C1C	2.27	1.43	1.38
15	N	821	CLA	CHC-C1C	2.27	1.43	1.38
15	O	802	CLA	CHC-C1C	2.27	1.43	1.38
15	a	813	CLA	CHC-C1C	2.27	1.43	1.38
15	N	807	CLA	C3B-C4B	2.27	1.49	1.42
15	a	821	CLA	CHC-C1C	2.27	1.43	1.38
15	a	822	CLA	C3B-C4B	2.27	1.49	1.42
15	A	806	CLA	CHC-C1C	2.27	1.43	1.38
15	N	830	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	804	CLA	CHC-C1C	2.27	1.43	1.38
15	b	836	CLA	CHC-C1C	2.27	1.43	1.38
15	A	841	CLA	C3B-C4B	2.27	1.49	1.42
15	A	814	CLA	C3B-C4B	2.26	1.49	1.42
14	j	201	F6C	C2B-C1B	2.26	1.49	1.44
15	A	810	CLA	CHC-C1C	2.26	1.43	1.38
15	N	813	CLA	CHC-C1C	2.26	1.43	1.38
15	a	830	CLA	CHC-C1C	2.26	1.43	1.38
15	B	837	CLA	CHC-C1C	2.26	1.43	1.38
15	b	806	CLA	CHC-C1C	2.26	1.43	1.38
15	a	818	CLA	C3B-C4B	2.26	1.49	1.42
15	O	811	CLA	CHC-C1C	2.26	1.43	1.38
15	B	826	CLA	C3B-C4B	2.26	1.49	1.42
15	A	815	CLA	CHC-C1C	2.26	1.43	1.38
15	O	810	CLA	CHC-C1C	2.26	1.43	1.38
15	b	827	CLA	CHC-C1C	2.26	1.43	1.38
15	A	809	CLA	CHC-C1C	2.26	1.43	1.38
15	O	815	CLA	CHC-C1C	2.26	1.43	1.38
15	A	818	CLA	C3B-C4B	2.26	1.49	1.42
15	b	803	CLA	C3B-C4B	2.26	1.49	1.42
15	K	103	CLA	CHC-C1C	2.26	1.43	1.38
15	N	809	CLA	CHC-C1C	2.26	1.43	1.38
15	f	201	CLA	CHC-C1C	2.26	1.43	1.38
15	A	831	CLA	C3B-C4B	2.26	1.49	1.42
15	a	806	CLA	CHC-C1C	2.26	1.43	1.38
15	a	842	CLA	CHC-C1C	2.26	1.43	1.38
15	b	815	CLA	CHC-C1C	2.26	1.43	1.38
15	B	815	CLA	CHC-C1C	2.26	1.43	1.38
15	N	834	CLA	CHC-C1C	2.26	1.43	1.38
15	B	811	CLA	CHC-C1C	2.26	1.43	1.38
15	N	815	CLA	CHC-C1C	2.26	1.43	1.38
15	N	822	CLA	CHC-C1C	2.26	1.43	1.38
15	O	803	CLA	CMC-C2C	-2.25	1.46	1.50
15	N	841	CLA	CHC-C1C	2.25	1.43	1.38
15	O	806	CLA	CHC-C1C	2.25	1.43	1.38
15	O	834	CLA	CHC-C1C	2.25	1.43	1.38
15	b	811	CLA	CHC-C1C	2.25	1.43	1.38
15	a	834	CLA	CHC-C1C	2.25	1.43	1.38
15	O	820	CLA	CHC-C1C	2.25	1.43	1.38
15	B	820	CLA	CHC-C1C	2.25	1.43	1.38
15	B	821	CLA	CHC-C1C	2.25	1.43	1.38
15	O	822	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	802	CLA	CHC-C1C	2.25	1.43	1.38
15	B	825	CLA	CHC-C1C	2.25	1.43	1.38
15	a	815	CLA	CHC-C1C	2.25	1.43	1.38
15	A	830	CLA	CHC-C1C	2.25	1.43	1.38
15	a	832	CLA	CHC-C1C	2.25	1.43	1.38
15	B	816	CLA	CHC-C1C	2.25	1.43	1.38
15	N	838	CLA	C3B-C4B	2.25	1.49	1.42
15	b	820	CLA	CHC-C1C	2.25	1.43	1.38
15	O	838	CLA	C3B-C4B	2.25	1.49	1.42
15	N	831	CLA	C3B-C4B	2.25	1.49	1.42
15	b	802	CLA	CHC-C1C	2.25	1.43	1.38
15	a	831	CLA	C3B-C4B	2.25	1.49	1.42
15	A	836	CLA	CHC-C1C	2.25	1.43	1.38
15	N	836	CLA	CHC-C1C	2.25	1.43	1.38
15	A	832	CLA	CHC-C1C	2.25	1.43	1.38
15	N	807	CLA	CHC-C1C	2.25	1.43	1.38
15	K	102	CLA	CHC-C1C	2.24	1.43	1.38
15	W	203	CLA	CHC-C1C	2.24	1.43	1.38
15	A	823	CLA	CHC-C1C	2.24	1.43	1.38
15	a	838	CLA	C3B-C4B	2.24	1.49	1.42
15	O	828	CLA	CHC-C1C	2.24	1.43	1.38
15	A	835	CLA	CHC-C1C	2.24	1.43	1.38
15	a	804	CLA	CHC-C1C	2.24	1.43	1.38
15	B	829	CLA	CHC-C1C	2.24	1.43	1.38
15	A	838	CLA	C3B-C4B	2.24	1.49	1.42
15	N	823	CLA	CHC-C1C	2.24	1.43	1.38
15	b	808	CLA	CHC-C1C	2.24	1.43	1.38
15	b	828	CLA	CHC-C1C	2.24	1.43	1.38
15	i	102	CLA	CHC-C1C	2.24	1.43	1.38
15	N	804	CLA	CHC-C1C	2.24	1.43	1.38
15	N	832	CLA	CHC-C1C	2.24	1.43	1.38
15	O	826	CLA	CHC-C1C	2.24	1.43	1.38
15	a	823	CLA	CHC-C1C	2.24	1.43	1.38
15	a	807	CLA	C3B-C4B	2.24	1.49	1.42
15	b	810	CLA	CHC-C1C	2.24	1.43	1.38
15	B	806	CLA	CHC-C1C	2.24	1.43	1.38
15	V	102	CLA	CHC-C1C	2.23	1.43	1.38
15	b	801	CLA	C3B-C4B	2.23	1.49	1.42
15	A	831	CLA	CMB-C2B	-2.23	1.46	1.50
15	N	840	CLA	C3B-C4B	2.23	1.49	1.42
15	B	828	CLA	CHC-C1C	2.23	1.43	1.38
15	O	829	CLA	CHC-C1C	2.23	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	j	202	CLA	CHC-C1C	2.23	1.43	1.38
15	N	806	CLA	CHC-C1C	2.23	1.43	1.38
15	b	826	CLA	CHC-C1C	2.23	1.42	1.38
15	B	817	CLA	CHC-C1C	2.23	1.42	1.38
15	b	812	CLA	CHC-C1C	2.23	1.42	1.38
15	O	801	CLA	C3B-C4B	2.23	1.49	1.42
14	L	204	F6C	C3B-C4B	2.23	1.49	1.44
15	W	202	CLA	CHC-C1C	2.23	1.42	1.38
15	N	828	CLA	CMC-C2C	-2.22	1.46	1.50
15	O	812	CLA	CHC-C1C	2.22	1.42	1.38
15	A	807	CLA	C3B-C4B	2.22	1.49	1.42
15	a	836	CLA	CHC-C1C	2.22	1.42	1.38
15	b	829	CLA	CHC-C1C	2.22	1.42	1.38
15	B	812	CLA	CHC-C1C	2.22	1.42	1.38
15	a	817	CLA	CHC-C1C	2.22	1.42	1.38
15	N	831	CLA	CMB-C2B	-2.22	1.46	1.50
15	B	801	CLA	C3B-C4B	2.22	1.49	1.42
15	b	803	CLA	CHC-C1C	2.22	1.42	1.38
15	N	818	CLA	CHC-C1C	2.22	1.42	1.38
15	N	828	CLA	CHC-C1C	2.22	1.42	1.38
15	O	817	CLA	CHC-C1C	2.22	1.42	1.38
15	a	831	CLA	CMB-C2B	-2.22	1.46	1.50
15	A	828	CLA	CHC-C1C	2.22	1.42	1.38
15	A	822	CLA	CHC-C1C	2.22	1.42	1.38
15	O	825	CLA	CHC-C1C	2.22	1.42	1.38
15	b	809	CLA	MG-NB	-2.22	2.01	2.05
15	B	803	CLA	CMC-C2C	-2.22	1.46	1.50
15	O	803	CLA	CHC-C1C	2.22	1.42	1.38
15	A	828	CLA	CMC-C2C	-2.21	1.46	1.50
15	O	808	CLA	CHC-C1C	2.21	1.42	1.38
15	O	823	CLA	CHC-C1C	2.21	1.42	1.38
15	B	826	CLA	CHC-C1C	2.21	1.42	1.38
15	a	814	CLA	CHC-C1C	2.21	1.42	1.38
15	B	823	CLA	CHC-C1C	2.21	1.42	1.38
15	a	840	CLA	C3B-C4B	2.21	1.49	1.42
15	B	801	CLA	CHC-C1C	2.21	1.42	1.38
15	a	822	CLA	CHC-C1C	2.21	1.42	1.38
15	b	801	CLA	CHC-C1C	2.21	1.42	1.38
15	b	817	CLA	CHC-C1C	2.21	1.42	1.38
15	b	823	CLA	CHC-C1C	2.21	1.42	1.38
15	A	840	CLA	C3B-C4B	2.21	1.49	1.42
15	A	817	CLA	CHC-C1C	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	817	CLA	CHC-C1C	2.21	1.42	1.38
15	a	828	CLA	CHC-C1C	2.21	1.42	1.38
15	B	816	CLA	CMB-C2B	-2.21	1.46	1.50
15	O	801	CLA	CHC-C1C	2.21	1.42	1.38
15	A	818	CLA	CHC-C1C	2.21	1.42	1.38
15	O	809	CLA	MG-NB	-2.20	2.01	2.05
15	a	818	CLA	CHC-C1C	2.20	1.42	1.38
15	b	825	CLA	CHC-C1C	2.20	1.42	1.38
15	a	828	CLA	CMC-C2C	-2.20	1.46	1.50
15	N	814	CLA	CHC-C1C	2.20	1.42	1.38
15	A	814	CLA	CHC-C1C	2.20	1.42	1.38
15	b	838	CLA	CHC-C1C	2.20	1.42	1.38
15	N	840	CLA	CHC-C1C	2.20	1.42	1.38
15	a	807	CLA	CHC-C1C	2.20	1.42	1.38
15	A	807	CLA	CHC-C1C	2.20	1.42	1.38
15	B	838	CLA	CHC-C1C	2.20	1.42	1.38
15	O	809	CLA	CHC-C1C	2.20	1.42	1.38
15	b	818	CLA	CMB-C2B	-2.20	1.46	1.50
15	O	809	CLA	C3B-C4B	2.19	1.49	1.42
15	a	838	CLA	CHC-C1C	2.19	1.42	1.38
15	b	840	CLA	CHC-C1C	2.19	1.42	1.38
15	b	822	CLA	MG-NB	-2.19	2.01	2.05
15	N	817	CLA	CMB-C2B	-2.19	1.46	1.50
15	B	840	CLA	CHC-C1C	2.18	1.42	1.38
15	O	838	CLA	CHC-C1C	2.18	1.42	1.38
15	O	840	CLA	CHC-C1C	2.18	1.42	1.38
15	a	841	CLA	CHC-C1C	2.18	1.42	1.38
15	N	838	CLA	CHC-C1C	2.18	1.42	1.38
15	O	818	CLA	CMB-C2B	-2.18	1.46	1.50
15	O	822	CLA	CMC-C2C	-2.18	1.46	1.50
15	b	809	CLA	C3B-C4B	2.18	1.49	1.42
15	B	818	CLA	CMB-C2B	-2.18	1.46	1.50
15	a	817	CLA	CMB-C2B	-2.18	1.46	1.50
15	N	810	CLA	CMD-C2D	-2.18	1.46	1.50
15	A	817	CLA	CMB-C2B	-2.18	1.46	1.50
15	a	810	CLA	CMD-C2D	-2.17	1.46	1.50
15	A	818	CLA	CMD-C2D	-2.17	1.46	1.50
15	V	103	CLA	CMB-C2B	-2.17	1.46	1.50
15	A	810	CLA	CMD-C2D	-2.17	1.46	1.50
15	a	840	CLA	CHC-C1C	2.17	1.42	1.38
15	A	841	CLA	CHC-C1C	2.17	1.42	1.38
15	N	820	CLA	CHC-C1C	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	816	CLA	MG-NB	-2.17	2.01	2.05
15	B	808	CLA	CMD-C2D	-2.17	1.46	1.50
15	A	820	CLA	CHC-C1C	2.16	1.42	1.38
15	A	840	CLA	CHC-C1C	2.16	1.42	1.38
15	A	838	CLA	CHC-C1C	2.16	1.42	1.38
15	a	820	CLA	CMB-C2B	-2.16	1.46	1.50
15	a	818	CLA	CMD-C2D	-2.16	1.46	1.50
15	B	822	CLA	MG-NB	-2.16	2.01	2.05
15	b	809	CLA	CHC-C1C	2.15	1.42	1.38
15	b	808	CLA	CMD-C2D	-2.15	1.46	1.50
15	a	820	CLA	CHC-C1C	2.15	1.42	1.38
15	O	808	CLA	CMD-C2D	-2.15	1.46	1.50
15	O	807	CLA	CHC-C1C	2.15	1.42	1.38
15	b	807	CLA	CHC-C1C	2.15	1.42	1.38
15	A	831	CLA	CHC-C1C	2.14	1.42	1.38
15	b	816	CLA	MG-NB	-2.14	2.01	2.05
15	a	833	CLA	MG-NB	-2.14	2.01	2.05
15	K	103	CLA	CMB-C2B	-2.14	1.46	1.50
15	O	829	CLA	CMD-C2D	-2.14	1.46	1.50
15	A	818	CLA	MG-NB	-2.14	2.01	2.05
15	b	836	CLA	MG-NB	-2.14	2.01	2.05
15	S	201	CLA	CMD-C2D	-2.14	1.46	1.50
14	A	856	F6C	C2B-C1B	2.14	1.49	1.44
15	B	809	CLA	C3B-C4B	2.13	1.49	1.42
15	F	201	CLA	CMD-C2D	-2.13	1.46	1.50
15	a	830	CLA	CMD-C2D	-2.13	1.46	1.50
14	a	802	F6C	C2B-C1B	2.13	1.49	1.44
15	B	827	CLA	CMD-C2D	-2.13	1.46	1.50
14	N	802	F6C	C2B-C1B	2.13	1.49	1.44
15	A	833	CLA	MG-NB	-2.13	2.01	2.05
15	f	201	CLA	CMD-C2D	-2.13	1.46	1.50
15	N	820	CLA	CMB-C2B	-2.13	1.46	1.50
15	b	827	CLA	CMD-C2D	-2.13	1.46	1.50
15	b	801	CLA	CMD-C2D	-2.13	1.46	1.50
15	O	822	CLA	CMD-C2D	-2.13	1.46	1.50
15	A	830	CLA	CMD-C2D	-2.13	1.46	1.50
15	a	831	CLA	CHC-C1C	2.13	1.42	1.38
15	B	801	CLA	CMD-C2D	-2.13	1.46	1.50
15	B	807	CLA	CHC-C1C	2.13	1.42	1.38
15	A	820	CLA	CMB-C2B	-2.13	1.46	1.50
15	O	827	CLA	CMD-C2D	-2.12	1.46	1.50
15	B	836	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	818	CLA	MG-NB	-2.12	2.01	2.05
15	a	803	CLA	CMC-C2C	-2.12	1.46	1.50
15	b	822	CLA	CMC-C2C	-2.12	1.46	1.50
14	A	802	F6C	C2B-C1B	2.12	1.49	1.44
15	A	838	CLA	MG-NB	-2.12	2.01	2.05
15	N	833	CLA	MG-NB	-2.12	2.01	2.05
15	B	809	CLA	CHC-C1C	2.12	1.42	1.38
15	N	803	CLA	CMC-C2C	-2.12	1.46	1.50
15	V	102	CLA	CMD-C2D	-2.12	1.46	1.50
15	A	822	CLA	CMB-C2B	-2.12	1.46	1.50
15	N	830	CLA	CMD-C2D	-2.12	1.46	1.50
15	O	836	CLA	MG-NB	-2.12	2.01	2.05
15	O	834	CLA	MG-NB	-2.12	2.01	2.05
14	N	856	F6C	C2B-C1B	2.12	1.49	1.44
15	B	825	CLA	MG-NB	-2.12	2.01	2.05
15	O	825	CLA	MG-NB	-2.12	2.01	2.05
14	a	855	F6C	C2B-C1B	2.11	1.49	1.44
15	a	822	CLA	CMB-C2B	-2.11	1.46	1.50
15	a	835	CLA	MG-NB	-2.11	2.01	2.05
15	b	834	CLA	MG-NB	-2.11	2.01	2.05
15	a	838	CLA	MG-NB	-2.11	2.01	2.05
15	B	823	CLA	CMD-C2D	-2.11	1.46	1.50
15	N	831	CLA	CHC-C1C	2.11	1.42	1.38
15	O	801	CLA	CMD-C2D	-2.11	1.46	1.50
14	B	832	F6C	CMC-C2C	-2.11	1.46	1.50
15	N	818	CLA	CMD-C2D	-2.11	1.46	1.50
15	a	827	CLA	MG-NB	-2.11	2.01	2.05
15	B	809	CLA	MG-NB	-2.11	2.01	2.05
15	a	810	CLA	MG-NB	-2.11	2.01	2.05
15	B	834	CLA	MG-NB	-2.11	2.01	2.05
15	W	202	CLA	MG-NB	-2.11	2.01	2.05
15	b	825	CLA	MG-NB	-2.11	2.01	2.05
15	N	829	CLA	CMD-C2D	-2.11	1.46	1.50
15	O	816	CLA	MG-NB	-2.11	2.01	2.05
15	N	838	CLA	MG-NB	-2.10	2.01	2.05
15	B	825	CLA	CMC-C2C	-2.10	1.46	1.50
15	A	810	CLA	MG-NB	-2.10	2.01	2.05
15	N	810	CLA	MG-NB	-2.10	2.01	2.05
15	a	819	CLA	CMC-C2C	-2.10	1.46	1.50
15	B	806	CLA	MG-NB	-2.10	2.01	2.05
15	a	829	CLA	CMD-C2D	-2.10	1.46	1.50
15	N	840	CLA	MG-NB	-2.10	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	j	202	CLA	MG-NB	-2.10	2.01	2.05
15	A	814	CLA	MG-NB	-2.10	2.01	2.05
15	a	822	CLA	MG-NB	-2.10	2.01	2.05
15	N	834	CLA	CMD-C2D	-2.10	1.46	1.50
15	L	202	CLA	CMD-C2D	-2.10	1.46	1.50
15	A	822	CLA	MG-NB	-2.10	2.01	2.05
15	N	819	CLA	CMC-C2C	-2.10	1.46	1.50
15	N	821	CLA	MG-NB	-2.10	2.01	2.05
15	A	821	CLA	MG-NB	-2.10	2.01	2.05
15	N	835	CLA	MG-NB	-2.10	2.01	2.05
15	O	809	CLA	CMD-C2D	-2.10	1.46	1.50
15	W	202	CLA	CMD-C2D	-2.10	1.46	1.50
15	A	840	CLA	MG-NB	-2.10	2.01	2.05
15	O	817	CLA	MG-NB	-2.10	2.01	2.05
15	b	823	CLA	CMD-C2D	-2.10	1.46	1.50
15	L	202	CLA	MG-NB	-2.10	2.01	2.05
15	N	822	CLA	MG-NB	-2.10	2.01	2.05
15	O	818	CLA	MG-NB	-2.10	2.01	2.05
15	B	818	CLA	MG-NB	-2.10	2.01	2.05
15	a	834	CLA	CMD-C2D	-2.09	1.46	1.50
15	B	822	CLA	CMC-C2C	-2.09	1.46	1.50
15	O	825	CLA	CMC-C2C	-2.09	1.46	1.50
15	j	202	CLA	CMD-C2D	-2.09	1.46	1.50
18	V	101	BCR	C19-C18	-2.09	1.44	1.50
15	b	823	CLA	MG-NB	-2.09	2.01	2.05
18	i	101	BCR	C19-C18	-2.09	1.44	1.50
15	B	840	CLA	CMB-C2B	-2.09	1.46	1.50
18	K	101	BCR	C19-C18	-2.09	1.44	1.50
15	A	834	CLA	CMD-C2D	-2.09	1.46	1.50
15	a	821	CLA	MG-NB	-2.09	2.01	2.05
15	A	819	CLA	CMC-C2C	-2.09	1.46	1.50
15	a	838	CLA	CMD-C2D	-2.09	1.46	1.50
15	b	809	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	826	F6C	CMD-C2D	-2.09	1.46	1.50
15	O	834	CLA	CMD-C2D	-2.09	1.46	1.50
15	A	835	CLA	MG-NB	-2.09	2.01	2.05
15	i	103	CLA	CMD-C2D	-2.09	1.46	1.50
15	A	829	CLA	CMD-C2D	-2.09	1.46	1.50
15	O	828	CLA	CMB-C2B	-2.09	1.46	1.50
15	A	832	CLA	MG-NB	-2.09	2.01	2.05
15	N	827	CLA	MG-NB	-2.09	2.01	2.05
15	a	830	CLA	MG-NB	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	826	F6C	CMD-C2D	-2.09	1.46	1.50
15	O	813	CLA	CMD-C2D	-2.09	1.46	1.50
15	O	817	CLA	CMB-C2B	-2.09	1.46	1.50
15	b	818	CLA	MG-NB	-2.09	2.01	2.05
15	a	833	CLA	CMB-C2B	-2.09	1.46	1.50
15	b	840	CLA	CMB-C2B	-2.09	1.46	1.50
15	V	103	CLA	MG-NB	-2.08	2.01	2.05
14	b	832	F6C	CMC-C2C	-2.08	1.46	1.50
15	A	838	CLA	CMD-C2D	-2.08	1.46	1.50
15	O	806	CLA	MG-NB	-2.08	2.01	2.05
15	O	823	CLA	CMD-C2D	-2.08	1.46	1.50
14	O	832	F6C	CMC-C2C	-2.08	1.46	1.50
15	A	833	CLA	CMB-C2B	-2.08	1.46	1.50
15	B	828	CLA	MG-NB	-2.08	2.01	2.05
14	a	826	F6C	CMD-C2D	-2.08	1.46	1.50
15	B	828	CLA	CMB-C2B	-2.08	1.46	1.50
15	b	817	CLA	MG-NB	-2.08	2.01	2.05
15	B	813	CLA	CMD-C2D	-2.08	1.46	1.50
15	b	813	CLA	CMD-C2D	-2.08	1.46	1.50
15	N	814	CLA	MG-NB	-2.08	2.01	2.05
15	N	837	CLA	MG-NB	-2.08	2.01	2.05
15	A	803	CLA	CMC-C2C	-2.08	1.46	1.50
15	N	822	CLA	CMB-C2B	-2.08	1.46	1.50
15	b	807	CLA	CMD-C2D	-2.08	1.46	1.50
15	N	832	CLA	MG-NB	-2.08	2.01	2.05
15	i	102	CLA	CMD-C2D	-2.08	1.46	1.50
15	A	807	CLA	MG-NB	-2.08	2.01	2.05
15	b	806	CLA	MG-NB	-2.08	2.01	2.05
15	N	830	CLA	MG-NB	-2.08	2.01	2.05
15	a	840	CLA	MG-NB	-2.08	2.01	2.05
15	a	834	CLA	CMB-C2B	-2.08	1.46	1.50
15	b	828	CLA	CMB-C2B	-2.08	1.46	1.50
15	B	823	CLA	MG-NB	-2.08	2.01	2.05
15	a	831	CLA	MG-NB	-2.08	2.01	2.05
15	B	809	CLA	CMD-C2D	-2.08	1.46	1.50
15	K	102	CLA	CMD-C2D	-2.08	1.46	1.50
15	B	806	CLA	CMD-C2D	-2.08	1.46	1.50
15	a	821	CLA	CMD-C2D	-2.08	1.46	1.50
15	O	837	CLA	MG-NB	-2.08	2.01	2.05
15	A	821	CLA	CMD-C2D	-2.08	1.46	1.50
15	b	806	CLA	CMD-C2D	-2.08	1.46	1.50
15	A	830	CLA	MG-NB	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	817	CLA	MG-NB	-2.08	2.01	2.05
15	X	102	CLA	CMD-C2D	-2.08	1.46	1.50
15	O	806	CLA	CMD-C2D	-2.08	1.46	1.50
15	O	840	CLA	CMB-C2B	-2.08	1.46	1.50
15	N	836	CLA	MG-NB	-2.08	2.01	2.05
15	B	834	CLA	CMD-C2D	-2.08	1.46	1.50
15	a	833	CLA	CMD-C2D	-2.08	1.46	1.50
15	B	837	CLA	MG-NB	-2.08	2.01	2.05
15	O	807	CLA	CMD-C2D	-2.08	1.46	1.50
15	l	102	CLA	CMD-C2D	-2.08	1.46	1.50
15	A	837	CLA	MG-NB	-2.08	2.01	2.05
15	b	813	CLA	MG-NB	-2.08	2.01	2.05
15	b	837	CLA	MG-NB	-2.08	2.01	2.05
15	W	203	CLA	MG-NB	-2.07	2.01	2.05
15	B	838	CLA	MG-NB	-2.07	2.01	2.05
15	b	810	CLA	MG-NB	-2.07	2.01	2.05
15	b	825	CLA	CMC-C2C	-2.07	1.46	1.50
15	N	818	CLA	MG-NB	-2.07	2.01	2.05
15	a	836	CLA	MG-NB	-2.07	2.01	2.05
15	Z	102	CLA	CMD-C2D	-2.07	1.46	1.50
15	O	828	CLA	MG-NB	-2.07	2.01	2.05
15	N	833	CLA	CMB-C2B	-2.07	1.46	1.50
15	N	834	CLA	CMB-C2B	-2.07	1.46	1.50
15	a	835	CLA	CMD-C2D	-2.07	1.46	1.50
15	B	807	CLA	MG-NB	-2.07	2.01	2.05
15	N	807	CLA	MG-NB	-2.07	2.01	2.05
15	b	838	CLA	MG-NB	-2.07	2.01	2.05
15	N	806	CLA	CMD-C2D	-2.07	1.46	1.50
15	N	821	CLA	CMD-C2D	-2.07	1.46	1.50
15	A	827	CLA	MG-NB	-2.07	2.01	2.05
15	a	837	CLA	MG-NB	-2.07	2.01	2.05
15	a	807	CLA	MG-NB	-2.07	2.01	2.05
15	N	825	CLA	MG-NB	-2.07	2.01	2.05
15	O	823	CLA	MG-NB	-2.07	2.01	2.05
15	A	812	CLA	CMD-C2D	-2.07	1.46	1.50
15	O	819	CLA	MG-NB	-2.07	2.01	2.05
15	A	833	CLA	CMD-C2D	-2.07	1.46	1.50
15	O	803	CLA	CMD-C2D	-2.07	1.46	1.50
15	K	103	CLA	MG-NB	-2.07	2.01	2.05
15	A	818	CLA	CMC-C2C	-2.07	1.46	1.50
15	B	829	CLA	MG-NB	-2.07	2.01	2.05
15	K	102	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	814	CLA	MG-NB	-2.07	2.01	2.05
15	O	838	CLA	CMD-C2D	-2.07	1.46	1.50
15	B	815	CLA	MG-NB	-2.07	2.01	2.05
15	N	838	CLA	CMD-C2D	-2.07	1.46	1.50
15	a	803	CLA	CMD-C2D	-2.07	1.46	1.50
15	b	840	CLA	CMD-C2D	-2.07	1.46	1.50
15	B	819	CLA	MG-NB	-2.07	2.01	2.05
15	b	815	CLA	MG-NB	-2.07	2.01	2.05
15	N	833	CLA	CMD-C2D	-2.07	1.46	1.50
14	O	832	F6C	CMD-C2D	-2.07	1.46	1.50
15	A	834	CLA	CMB-C2B	-2.07	1.46	1.50
15	L	203	CLA	MG-NB	-2.07	2.01	2.05
15	Z	102	CLA	MG-NB	-2.07	2.01	2.05
15	O	810	CLA	MG-NB	-2.07	2.01	2.05
15	O	829	CLA	MG-NB	-2.07	2.01	2.05
15	b	819	CLA	MG-NB	-2.07	2.01	2.05
15	b	803	CLA	CMD-C2D	-2.06	1.46	1.50
15	O	807	CLA	MG-NB	-2.06	2.01	2.05
15	O	815	CLA	MG-NB	-2.06	2.01	2.05
15	l	102	CLA	MG-NB	-2.06	2.01	2.05
14	A	856	F6C	CMD-C2D	-2.06	1.46	1.50
15	A	832	CLA	CMD-C2D	-2.06	1.46	1.50
15	V	102	CLA	MG-NB	-2.06	2.01	2.05
15	A	842	CLA	CMB-C2B	-2.06	1.46	1.50
15	A	836	CLA	MG-NB	-2.06	2.01	2.05
15	O	834	CLA	CMB-C2B	-2.06	1.46	1.50
15	A	831	CLA	MG-NB	-2.06	2.01	2.05
15	N	817	CLA	MG-NB	-2.06	2.01	2.05
15	N	828	CLA	MG-NB	-2.06	2.01	2.05
15	O	813	CLA	MG-NB	-2.06	2.01	2.05
15	B	807	CLA	CMD-C2D	-2.06	1.46	1.50
15	X	102	CLA	MG-NB	-2.06	2.01	2.05
15	N	813	CLA	MG-NB	-2.06	2.01	2.05
15	i	102	CLA	MG-NB	-2.06	2.01	2.05
15	N	803	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	820	CLA	MG-NB	-2.06	2.01	2.05
15	a	823	CLA	MG-NB	-2.06	2.01	2.05
14	a	855	F6C	CMD-C2D	-2.06	1.46	1.50
15	O	827	CLA	MG-NB	-2.06	2.01	2.05
15	N	807	CLA	CMD-C2D	-2.06	1.46	1.50
15	O	824	CLA	CMD-C2D	-2.06	1.46	1.50
15	B	805	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	837	CLA	CMD-C2D	-2.06	1.46	1.50
15	O	803	CLA	MG-NB	-2.06	2.01	2.05
14	j	201	F6C	CMD-C2D	-2.06	1.46	1.50
15	A	806	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	836	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	804	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	832	CLA	CMD-C2D	-2.06	1.46	1.50
15	b	837	CLA	CMD-C2D	-2.06	1.46	1.50
15	b	838	CLA	CMD-C2D	-2.06	1.46	1.50
15	B	810	CLA	MG-NB	-2.06	2.01	2.05
15	O	814	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	804	CLA	CMB-C2B	-2.06	1.46	1.50
15	a	842	CLA	CMD-C2D	-2.06	1.46	1.50
15	B	840	CLA	MG-NB	-2.06	2.01	2.05
15	A	803	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	819	CLA	CMD-C2D	-2.06	1.46	1.50
15	b	817	CLA	CMB-C2B	-2.06	1.46	1.50
15	b	827	CLA	MG-NB	-2.06	2.01	2.05
15	O	805	CLA	CMD-C2D	-2.06	1.46	1.50
15	O	837	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	820	CLA	MG-NB	-2.06	2.01	2.05
15	a	813	CLA	MG-NB	-2.06	2.01	2.05
14	b	832	F6C	CMD-C2D	-2.06	1.46	1.50
15	O	831	CLA	MG-NB	-2.06	2.01	2.05
15	L	203	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	822	CLA	CMD-C2D	-2.06	1.46	1.50
15	W	203	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	832	CLA	CMD-C2D	-2.06	1.46	1.50
15	O	838	CLA	MG-NB	-2.06	2.01	2.05
15	A	839	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	841	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	842	CLA	CMB-C2B	-2.06	1.46	1.50
15	A	819	CLA	MG-NB	-2.06	2.01	2.05
15	b	807	CLA	MG-NB	-2.06	2.01	2.05
15	A	804	CLA	CMB-C2B	-2.06	1.46	1.50
15	A	807	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	825	CLA	CMD-C2D	-2.06	1.46	1.50
15	N	842	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	825	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	841	CLA	CMD-C2D	-2.06	1.46	1.50
15	b	814	CLA	CMD-C2D	-2.06	1.46	1.50
15	B	838	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	833	CLA	CMD-C2D	-2.06	1.46	1.50
15	N	820	CLA	MG-NB	-2.06	2.01	2.05
15	b	828	CLA	MG-NB	-2.06	2.01	2.05
15	B	817	CLA	CMB-C2B	-2.05	1.46	1.50
15	B	813	CLA	MG-NB	-2.05	2.01	2.05
15	O	820	CLA	MG-NB	-2.05	2.01	2.05
15	N	836	CLA	CMB-C2B	-2.05	1.46	1.50
15	a	819	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	819	CLA	CMD-C2D	-2.05	1.46	1.50
14	N	856	F6C	CMD-C2D	-2.05	1.46	1.50
15	L	203	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	812	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	805	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	831	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	841	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	841	CLA	CMB-C2B	-2.05	1.46	1.50
15	B	820	CLA	MG-NB	-2.05	2.01	2.05
15	N	831	CLA	MG-NB	-2.05	2.01	2.05
15	a	808	CLA	MG-NB	-2.05	2.01	2.05
14	N	802	F6C	CMD-C2D	-2.05	1.46	1.50
15	N	820	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	831	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	842	CLA	CMB-C2B	-2.05	1.46	1.50
15	j	203	CLA	CMB-C2B	-2.05	1.46	1.50
15	B	819	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	827	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	828	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	823	CLA	CMB-C2B	-2.05	1.46	1.50
15	f	201	CLA	CMB-C2B	-2.05	1.46	1.50
15	a	817	CLA	MG-NB	-2.05	2.01	2.05
15	b	840	CLA	MG-NB	-2.05	2.01	2.05
15	j	203	CLA	MG-NB	-2.05	2.01	2.05
14	A	802	F6C	CMD-C2D	-2.05	1.46	1.50
15	A	842	CLA	CMD-C2D	-2.05	1.46	1.50
15	F	201	CLA	CMB-C2B	-2.05	1.46	1.50
15	O	840	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	820	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	811	CLA	CMB-C2B	-2.05	1.46	1.50
15	O	817	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	834	CLA	CMB-C2B	-2.05	1.46	1.50
15	A	817	CLA	MG-NB	-2.05	2.01	2.05
14	L	201	F6C	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	840	CLA	CMD-C2D	-2.05	1.46	1.50
15	j	203	CLA	CMD-C2D	-2.05	1.46	1.50
15	B	828	CLA	CMD-C2D	-2.05	1.46	1.50
15	B	810	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	810	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	819	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	828	CLA	MG-NB	-2.05	2.01	2.05
15	N	819	CLA	MG-NB	-2.05	2.01	2.05
15	b	820	CLA	MG-NB	-2.05	2.01	2.05
15	A	820	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	841	CLA	CMC-C2C	-2.05	1.46	1.50
15	B	823	CLA	CMB-C2B	-2.05	1.46	1.50
15	N	836	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	815	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	813	CLA	MG-NB	-2.05	2.01	2.05
15	A	823	CLA	MG-NB	-2.05	2.01	2.05
14	B	832	F6C	CMD-C2D	-2.05	1.46	1.50
15	B	824	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	809	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	839	CLA	CMB-C2B	-2.05	1.46	1.50
15	B	821	CLA	CMD-C2D	-2.05	1.46	1.50
15	W	203	CLA	CMB-C2B	-2.05	1.46	1.50
15	a	806	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	807	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	829	CLA	MG-NB	-2.05	2.01	2.05
15	B	812	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	833	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	812	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	808	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	841	CLA	CMB-C2B	-2.05	1.46	1.50
15	W	202	CLA	CMB-C2B	-2.05	1.46	1.50
15	a	841	CLA	CMC-C2C	-2.05	1.46	1.50
15	b	817	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	808	CLA	MG-NB	-2.05	2.01	2.05
15	N	823	CLA	MG-NB	-2.05	2.01	2.05
15	A	809	CLA	CMD-C2D	-2.05	1.46	1.50
15	S	201	CLA	CMB-C2B	-2.05	1.46	1.50
15	a	836	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	836	CLA	CMD-C2D	-2.05	1.46	1.50
15	i	103	CLA	CMB-C2B	-2.05	1.46	1.50
15	L	202	CLA	CMB-C2B	-2.05	1.46	1.50
15	b	830	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	808	CLA	MG-NB	-2.05	2.01	2.05
15	a	819	CLA	MG-NB	-2.05	2.01	2.05
14	L	204	F6C	CMD-C2D	-2.05	1.46	1.50
15	N	819	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	839	CLA	CMB-C2B	-2.05	1.46	1.50
15	j	202	CLA	CMB-C2B	-2.05	1.46	1.50
15	a	832	CLA	MG-NB	-2.05	2.01	2.05
15	b	831	CLA	MG-NB	-2.05	2.01	2.05
15	N	841	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	812	CLA	CMB-C2B	-2.04	1.46	1.50
15	B	802	CLA	CMD-C2D	-2.04	1.46	1.50
15	B	811	CLA	CMB-C2B	-2.04	1.46	1.50
15	N	825	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	808	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	811	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	836	CLA	CMB-C2B	-2.04	1.46	1.50
15	N	811	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	812	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	840	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	812	CLA	MG-NB	-2.04	2.01	2.05
14	a	802	F6C	CMD-C2D	-2.04	1.46	1.50
15	A	815	CLA	CMD-C2D	-2.04	1.46	1.50
15	A	832	CLA	CMB-C2B	-2.04	1.46	1.50
15	a	841	CLA	MG-NB	-2.04	2.01	2.05
15	B	831	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	831	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	839	CLA	MG-NB	-2.04	2.01	2.05
15	b	811	CLA	CMB-C2B	-2.04	1.46	1.50
15	B	808	CLA	MG-NB	-2.04	2.01	2.05
15	b	803	CLA	MG-NB	-2.04	2.01	2.05
15	B	803	CLA	CMD-C2D	-2.04	1.46	1.50
15	B	826	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	810	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	828	CLA	MG-NB	-2.04	2.01	2.05
15	b	808	CLA	MG-NB	-2.04	2.01	2.05
14	W	204	F6C	CMD-C2D	-2.04	1.46	1.50
15	A	811	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	812	CLA	CMB-C2B	-2.04	1.46	1.50
15	a	803	CLA	MG-NB	-2.04	2.01	2.05
14	N	824	F6C	CMD-C2D	-2.04	1.46	1.50
15	B	835	CLA	CMB-C2B	-2.04	1.46	1.50
15	a	812	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	822	CLA	CMD-C2D	-2.04	1.46	1.50
15	B	827	CLA	MG-NB	-2.04	2.01	2.05
15	O	830	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	802	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	834	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	824	CLA	MG-NB	-2.04	2.01	2.05
15	A	804	CLA	CMD-C2D	-2.04	1.46	1.50
15	B	830	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	808	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	812	CLA	CMB-C2B	-2.04	1.46	1.50
15	N	816	CLA	CMB-C2B	-2.04	1.46	1.50
15	O	826	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	809	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	804	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	830	CLA	MG-NB	-2.04	2.01	2.05
15	N	839	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	807	CLA	CMB-C2B	-2.04	1.46	1.50
14	N	802	F6C	C4D-ND	-2.04	1.33	1.37
14	j	204	F6C	CMD-C2D	-2.04	1.46	1.50
15	B	817	CLA	CMD-C2D	-2.04	1.46	1.50
15	B	818	CLA	CMD-C2D	-2.04	1.46	1.50
15	A	836	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	826	CLA	MG-NB	-2.04	2.01	2.05
15	b	829	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	825	CLA	MG-NB	-2.04	2.01	2.05
15	b	812	CLA	MG-NB	-2.04	2.01	2.05
15	B	814	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	813	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	831	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	815	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	828	CLA	CMD-C2D	-2.04	1.46	1.50
15	A	813	CLA	CMD-C2D	-2.04	1.46	1.50
15	A	817	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	831	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	821	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	804	CLA	CMD-C2D	-2.04	1.46	1.50
15	B	836	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	807	CLA	CMB-C2B	-2.04	1.46	1.50
15	N	832	CLA	CMB-C2B	-2.04	1.46	1.50
15	N	841	CLA	CMC-C2C	-2.04	1.46	1.50
15	O	828	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	836	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	835	CLA	CMB-C2B	-2.04	1.46	1.50
15	O	818	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	823	CLA	CMB-C2B	-2.04	1.46	1.50
15	a	813	CLA	CMD-C2D	-2.04	1.46	1.50
15	A	825	CLA	MG-NB	-2.04	2.01	2.05
15	b	811	CLA	MG-NB	-2.04	2.01	2.05
15	A	835	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	816	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	814	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	803	CLA	MG-NB	-2.04	2.01	2.05
15	A	807	CLA	CMB-C2B	-2.03	1.46	1.50
15	A	835	CLA	CMB-C2B	-2.03	1.46	1.50
15	B	815	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	815	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	835	CLA	CMB-C2B	-2.03	1.46	1.50
15	b	804	CLA	CMC-C2C	-2.03	1.46	1.50
15	b	818	CLA	CMD-C2D	-2.03	1.46	1.50
15	A	815	CLA	MG-NB	-2.03	2.01	2.05
15	B	811	CLA	MG-NB	-2.03	2.01	2.05
15	a	815	CLA	MG-NB	-2.03	2.01	2.05
15	A	816	CLA	CMB-C2B	-2.03	1.46	1.50
15	A	827	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	804	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	804	CLA	CMD-C2D	-2.03	1.46	1.50
15	a	817	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	826	CLA	CMD-C2D	-2.03	1.46	1.50
14	W	201	F6C	CMD-C2D	-2.03	1.46	1.50
15	A	839	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	804	CLA	CMC-C2C	-2.03	1.46	1.50
15	B	822	CLA	CMB-C2B	-2.03	1.46	1.50
15	N	804	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	840	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	802	CLA	CMD-C2D	-2.03	1.46	1.50
15	a	818	CLA	CMC-C2C	-2.03	1.46	1.50
15	A	822	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	820	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	821	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	833	CLA	MG-NB	-2.03	2.01	2.05
15	N	817	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	823	CLA	CMD-C2D	-2.03	1.46	1.50
15	a	816	CLA	CMB-C2B	-2.03	1.46	1.50
15	B	820	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	103	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	825	CLA	CMB-C2B	-2.03	1.46	1.50
15	A	816	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	829	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	804	CLA	CMC-C2C	-2.03	1.46	1.50
15	b	835	CLA	CMB-C2B	-2.03	1.46	1.50
15	N	815	CLA	MG-NB	-2.03	2.01	2.05
15	O	822	CLA	MG-NB	-2.03	2.01	2.05
15	O	840	CLA	MG-NB	-2.03	2.01	2.05
15	a	839	CLA	MG-NB	-2.03	2.01	2.05
15	A	840	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	828	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	835	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	830	CLA	MG-NB	-2.03	2.01	2.05
15	B	825	CLA	CMB-C2B	-2.03	1.46	1.50
15	N	814	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	824	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	830	CLA	MG-NB	-2.03	2.01	2.05
15	N	815	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	829	CLA	MG-NB	-2.03	2.01	2.05
15	A	814	CLA	CMD-C2D	-2.03	1.46	1.50
15	A	819	CLA	CMB-C2B	-2.03	1.46	1.50
15	A	823	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	833	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	835	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	816	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	812	CLA	MG-NB	-2.03	2.01	2.05
15	O	819	CLA	CMB-C2B	-2.03	1.46	1.50
15	O	825	CLA	CMD-C2D	-2.03	1.46	1.50
15	a	823	CLA	CMD-C2D	-2.03	1.46	1.50
15	a	825	CLA	CMB-C2B	-2.03	1.46	1.50
15	b	835	CLA	CMD-C2D	-2.03	1.46	1.50
15	A	803	CLA	MG-NB	-2.03	2.01	2.05
15	a	829	CLA	MG-NB	-2.03	2.01	2.05
15	N	827	CLA	CMD-C2D	-2.03	1.46	1.50
15	a	819	CLA	CMB-C2B	-2.03	1.46	1.50
15	a	837	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	820	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	825	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	834	CLA	MG-NB	-2.03	2.01	2.05
15	a	816	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	811	CLA	MG-NB	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	828	CLA	CMD-C2D	-2.03	1.46	1.50
15	A	837	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	816	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	819	CLA	CMB-C2B	-2.03	1.46	1.50
15	B	831	CLA	MG-NB	-2.03	2.01	2.05
15	B	834	CLA	CMB-C2B	-2.03	1.46	1.50
15	O	825	CLA	CMB-C2B	-2.03	1.46	1.50
15	B	826	CLA	MG-NB	-2.03	2.01	2.05
15	O	824	CLA	MG-NB	-2.03	2.01	2.05
15	a	805	CLA	MG-NB	-2.03	2.01	2.05
15	a	834	CLA	MG-NB	-2.03	2.01	2.05
15	a	839	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	819	CLA	CMB-C2B	-2.03	1.46	1.50
15	b	803	CLA	CMB-C2B	-2.03	1.46	1.50
15	A	841	CLA	MG-NB	-2.03	2.01	2.05
15	A	825	CLA	CMB-C2B	-2.03	1.46	1.50
15	B	825	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	837	CLA	CMD-C2D	-2.03	1.46	1.50
15	V	103	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	825	CLA	CMB-C2B	-2.03	1.46	1.50
15	O	805	CLA	MG-NB	-2.03	2.01	2.05
15	B	829	CLA	CMB-C2B	-2.03	1.46	1.50
15	b	811	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	808	CLA	MG-NB	-2.02	2.01	2.05
15	B	819	CLA	CMB-C2B	-2.02	1.46	1.50
15	O	826	CLA	MG-NB	-2.02	2.01	2.05
15	N	835	CLA	CMB-C2B	-2.02	1.46	1.50
15	b	801	CLA	CMB-C2B	-2.02	1.46	1.50
15	A	805	CLA	MG-NB	-2.02	2.01	2.05
15	A	809	CLA	MG-NB	-2.02	2.01	2.05
15	b	822	CLA	CMB-C2B	-2.02	1.46	1.50
15	N	809	CLA	MG-NB	-2.02	2.01	2.05
15	O	803	CLA	CMB-C2B	-2.02	1.46	1.50
15	O	811	CLA	CMD-C2D	-2.02	1.46	1.50
15	B	803	CLA	MG-NB	-2.02	2.01	2.05
15	B	811	CLA	CMD-C2D	-2.02	1.46	1.50
15	A	839	CLA	MG-NB	-2.02	2.01	2.05
15	O	833	CLA	MG-NB	-2.02	2.01	2.05
15	a	832	CLA	CMB-C2B	-2.02	1.46	1.50
15	A	834	CLA	MG-NB	-2.02	2.01	2.05
15	b	816	CLA	CMD-C2D	-2.02	1.46	1.50
15	A	842	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	805	CLA	MG-NB	-2.02	2.01	2.05
15	A	812	CLA	MG-NB	-2.02	2.01	2.05
15	B	824	CLA	MG-NB	-2.02	2.01	2.05
15	b	805	CLA	MG-NB	-2.02	2.01	2.05
15	O	801	CLA	CMB-C2B	-2.02	1.46	1.50
15	f	201	CLA	MG-NB	-2.02	2.01	2.05
15	N	805	CLA	CMD-C2D	-2.02	1.46	1.50
15	b	833	CLA	MG-NB	-2.02	2.01	2.05
15	a	805	CLA	CMD-C2D	-2.02	1.46	1.50
15	N	804	CLA	CMC-C2C	-2.02	1.46	1.50
15	S	201	CLA	MG-NB	-2.02	2.01	2.05
15	A	805	CLA	CMD-C2D	-2.01	1.46	1.50
15	A	821	CLA	CMB-C2B	-2.01	1.46	1.50
15	A	829	CLA	MG-NB	-2.01	2.01	2.05
15	F	201	CLA	MG-NB	-2.01	2.01	2.05
15	N	811	CLA	CMC-C2C	-2.01	1.46	1.50
15	O	835	CLA	MG-NB	-2.01	2.01	2.05
15	A	804	CLA	CMC-C2C	-2.01	1.46	1.50
15	B	801	CLA	CMC-C2C	-2.01	1.46	1.50
15	a	804	CLA	CMC-C2C	-2.01	1.46	1.50
15	A	809	CLA	CMB-C2B	-2.01	1.46	1.50
14	a	802	F6C	C4D-ND	-2.01	1.33	1.37
15	B	835	CLA	MG-NB	-2.01	2.01	2.05
15	N	842	CLA	MG-NB	-2.01	2.01	2.05
15	a	809	CLA	MG-NB	-2.01	2.01	2.05
15	b	835	CLA	MG-NB	-2.01	2.01	2.05
15	a	818	CLA	CMB-C2B	-2.01	1.46	1.50
15	B	801	CLA	CMB-C2B	-2.01	1.46	1.50
15	B	810	CLA	CMB-C2B	-2.01	1.46	1.50
15	N	841	CLA	MG-NB	-2.01	2.01	2.05
15	N	812	CLA	MG-NB	-2.01	2.01	2.05
15	b	804	CLA	MG-NB	-2.01	2.01	2.05
15	b	810	CLA	CMB-C2B	-2.01	1.46	1.50
15	N	835	CLA	CMD-C2D	-2.01	1.46	1.50
15	b	808	CLA	CMC-C2C	-2.01	1.46	1.50
15	O	804	CLA	MG-NB	-2.01	2.01	2.05
15	b	829	CLA	CMB-C2B	-2.01	1.46	1.50
15	B	805	CLA	MG-NB	-2.01	2.01	2.05
15	O	829	CLA	CMB-C2B	-2.01	1.46	1.50
14	A	802	F6C	C4D-ND	-2.01	1.33	1.37
15	N	809	CLA	CMB-C2B	-2.01	1.46	1.50
15	a	821	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	836	CLA	CMB-C2B	-2.01	1.46	1.50
15	N	831	CLA	CMC-C2C	-2.01	1.46	1.50
15	B	803	CLA	CMB-C2B	-2.01	1.46	1.50
15	B	804	CLA	MG-NB	-2.01	2.01	2.05
14	a	802	F6C	C1D-C2D	2.01	1.48	1.44
15	N	811	CLA	MG-NB	-2.01	2.01	2.05
15	O	801	CLA	CMC-C2C	-2.01	1.46	1.50
15	a	842	CLA	MG-NB	-2.01	2.01	2.05
15	N	821	CLA	CMB-C2B	-2.00	1.46	1.50
15	O	826	CLA	CMB-C2B	-2.00	1.46	1.50
15	N	818	CLA	CMB-C2B	-2.00	1.46	1.50
15	O	810	CLA	CMB-C2B	-2.00	1.46	1.50
15	O	827	CLA	CMB-C2B	-2.00	1.46	1.50
15	O	802	CLA	MG-NB	-2.00	2.01	2.05
14	A	802	F6C	C1D-C2D	2.00	1.48	1.44
15	N	818	CLA	CMC-C2C	-2.00	1.46	1.50
15	O	838	CLA	CMC-C2C	-2.00	1.46	1.50
15	O	812	CLA	CMC-C2C	-2.00	1.46	1.50
15	a	815	CLA	CMC-C2C	-2.00	1.46	1.50
15	b	807	CLA	CMB-C2B	-2.00	1.46	1.50
15	b	826	CLA	CMB-C2B	-2.00	1.46	1.50
15	A	806	CLA	MG-NB	-2.00	2.01	2.05
15	a	812	CLA	MG-NB	-2.00	2.01	2.05
15	A	818	CLA	CMB-C2B	-2.00	1.46	1.50
15	B	807	CLA	CMB-C2B	-2.00	1.46	1.50
15	B	812	CLA	CMB-C2B	-2.00	1.46	1.50
14	N	802	F6C	C1D-C2D	2.00	1.48	1.44
14	A	824	F6C	CMD-C2D	-2.00	1.46	1.50

All (1915) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	839	F6C	CAA-C2A-C3A	-9.85	109.43	127.87
14	O	839	F6C	CAA-C2A-C3A	-9.83	109.46	127.87
14	B	839	F6C	CAA-C2A-C3A	-9.83	109.46	127.87
14	a	826	F6C	CAA-C2A-C3A	-9.77	109.56	127.87
14	W	204	F6C	CAA-C2A-C3A	-9.64	109.81	127.87
14	L	204	F6C	CAA-C2A-C3A	-9.58	109.92	127.87
14	A	826	F6C	CAA-C2A-C3A	-9.56	109.96	127.87
14	N	826	F6C	CAA-C2A-C3A	-9.55	109.99	127.87
14	j	204	F6C	CAA-C2A-C3A	-9.53	110.01	127.87
14	N	856	F6C	CAA-C2A-C3A	-9.30	110.45	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	855	F6C	CAA-C2A-C3A	-9.29	110.46	127.87
14	A	856	F6C	CAA-C2A-C3A	-9.27	110.50	127.87
14	a	824	F6C	CAA-C2A-C3A	-9.16	110.70	127.87
14	A	824	F6C	CAA-C2A-C3A	-9.16	110.71	127.87
14	N	824	F6C	CAA-C2A-C3A	-9.10	110.82	127.87
14	a	802	F6C	CAA-C2A-C3A	-8.76	111.46	127.87
14	A	802	F6C	CAA-C2A-C3A	-8.68	111.61	127.87
14	B	832	F6C	CAA-C2A-C3A	-8.62	111.72	127.87
14	O	832	F6C	CAA-C2A-C3A	-8.56	111.83	127.87
14	L	201	F6C	CAA-C2A-C3A	-8.54	111.87	127.87
14	b	832	F6C	CAA-C2A-C3A	-8.49	111.97	127.87
14	N	802	F6C	CAA-C2A-C3A	-8.49	111.97	127.87
14	W	201	F6C	CAA-C2A-C3A	-8.48	111.99	127.87
14	j	201	F6C	CAA-C2A-C3A	-8.40	112.13	127.87
14	A	856	F6C	CMA-C3A-C4A	-8.09	110.49	124.73
14	j	201	F6C	CMA-C3A-C4A	-7.91	110.80	124.73
14	a	855	F6C	CMA-C3A-C4A	-7.90	110.82	124.73
14	N	856	F6C	CMA-C3A-C4A	-7.89	110.83	124.73
14	b	832	F6C	CMA-C3A-C4A	-7.66	111.24	124.73
14	O	832	F6C	CMA-C3A-C4A	-7.61	111.33	124.73
14	B	832	F6C	CMA-C3A-C4A	-7.55	111.43	124.73
14	L	201	F6C	CMA-C3A-C4A	-7.50	111.52	124.73
14	W	201	F6C	CMA-C3A-C4A	-7.48	111.55	124.73
14	N	824	F6C	CMA-C3A-C4A	-7.21	112.04	124.73
14	N	802	F6C	CMA-C3A-C4A	-7.20	112.04	124.73
14	a	824	F6C	CMA-C3A-C4A	-7.20	112.05	124.73
14	O	839	F6C	CMA-C3A-C4A	-7.18	112.08	124.73
14	A	802	F6C	CMA-C3A-C4A	-7.18	112.08	124.73
14	A	824	F6C	CMA-C3A-C4A	-7.18	112.09	124.73
14	a	802	F6C	CMA-C3A-C4A	-7.16	112.12	124.73
14	B	839	F6C	CMA-C3A-C4A	-7.13	112.16	124.73
14	b	839	F6C	CMA-C3A-C4A	-7.07	112.28	124.73
15	A	818	CLA	C4A-NA-C1A	6.94	109.84	106.68
15	A	828	CLA	C4A-NA-C1A	6.93	109.84	106.68
14	B	839	F6C	CAA-C2A-C1A	-6.92	108.67	128.01
14	b	839	F6C	CAA-C2A-C1A	-6.91	108.70	128.01
14	O	839	F6C	CAA-C2A-C1A	-6.89	108.76	128.01
15	O	814	CLA	C4A-NA-C1A	6.89	109.82	106.68
15	b	814	CLA	C4A-NA-C1A	6.88	109.82	106.68
14	N	826	F6C	CMA-C3A-C4A	-6.87	112.62	124.73
15	a	818	CLA	C4A-NA-C1A	6.87	109.81	106.68
14	j	204	F6C	CMA-C3A-C4A	-6.87	112.64	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	841	CLA	C4A-NA-C1A	6.85	109.80	106.68
15	N	828	CLA	C4A-NA-C1A	6.84	109.80	106.68
14	A	826	F6C	CMA-C3A-C4A	-6.83	112.70	124.73
15	O	803	CLA	C4A-NA-C1A	6.83	109.79	106.68
14	a	826	F6C	CMA-C3A-C4A	-6.81	112.74	124.73
14	W	204	F6C	CMA-C3A-C4A	-6.80	112.75	124.73
15	B	814	CLA	C4A-NA-C1A	6.80	109.78	106.68
15	a	828	CLA	C4A-NA-C1A	6.80	109.78	106.68
15	a	841	CLA	C4A-NA-C1A	6.78	109.77	106.68
15	N	818	CLA	C4A-NA-C1A	6.76	109.76	106.68
15	b	803	CLA	C4A-NA-C1A	6.76	109.76	106.68
15	N	831	CLA	C4A-NA-C1A	6.71	109.74	106.68
15	B	826	CLA	C4A-NA-C1A	6.70	109.74	106.68
15	B	809	CLA	C4A-NA-C1A	6.67	109.72	106.68
15	a	840	CLA	C4A-NA-C1A	6.67	109.72	106.68
15	B	801	CLA	C4A-NA-C1A	6.67	109.72	106.68
15	O	823	CLA	C4A-NA-C1A	6.65	109.71	106.68
15	W	202	CLA	C4A-NA-C1A	6.65	109.71	106.68
15	a	831	CLA	C4A-NA-C1A	6.65	109.71	106.68
15	b	823	CLA	C4A-NA-C1A	6.64	109.71	106.68
15	j	202	CLA	C4A-NA-C1A	6.63	109.71	106.68
15	A	807	CLA	C4A-NA-C1A	6.63	109.70	106.68
15	N	841	CLA	C4A-NA-C1A	6.63	109.70	106.68
15	O	801	CLA	C4A-NA-C1A	6.63	109.70	106.68
15	O	815	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	A	815	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	A	820	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	a	823	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	O	840	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	b	815	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	O	820	CLA	C4A-NA-C1A	6.61	109.70	106.68
15	b	820	CLA	C4A-NA-C1A	6.61	109.70	106.68
15	L	202	CLA	C4A-NA-C1A	6.61	109.69	106.68
15	O	826	CLA	C4A-NA-C1A	6.61	109.69	106.68
15	j	203	CLA	C4A-NA-C1A	6.61	109.69	106.68
15	A	823	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	a	820	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	A	829	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	A	831	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	N	815	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	O	805	CLA	C4A-NA-C1A	6.59	109.69	106.68
15	b	805	CLA	C4A-NA-C1A	6.59	109.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	803	CLA	C4A-NA-C1A	6.59	109.68	106.68
15	b	840	CLA	C4A-NA-C1A	6.59	109.68	106.68
15	B	820	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	B	823	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	a	815	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	N	829	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	B	815	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	B	840	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	N	823	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	a	829	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	b	801	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	b	826	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	B	805	CLA	C4A-NA-C1A	6.57	109.68	106.68
15	N	820	CLA	C4A-NA-C1A	6.57	109.68	106.68
15	a	822	CLA	C4A-NA-C1A	6.57	109.67	106.68
15	a	809	CLA	C4A-NA-C1A	6.56	109.67	106.68
15	A	839	CLA	C4A-NA-C1A	6.56	109.67	106.68
15	a	832	CLA	C4A-NA-C1A	6.55	109.67	106.68
15	O	829	CLA	C4A-NA-C1A	6.55	109.67	106.68
15	a	807	CLA	C4A-NA-C1A	6.55	109.67	106.68
15	O	838	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	b	829	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	W	203	CLA	C4A-NA-C1A	6.53	109.66	106.68
15	A	822	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	B	838	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	O	822	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	B	807	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	B	825	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	N	808	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	A	838	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	b	807	CLA	C4A-NA-C1A	6.50	109.65	106.68
15	A	809	CLA	C4A-NA-C1A	6.50	109.64	106.68
15	K	102	CLA	C4A-NA-C1A	6.50	109.64	106.68
15	O	807	CLA	C4A-NA-C1A	6.50	109.64	106.68
15	B	837	CLA	C4A-NA-C1A	6.50	109.64	106.68
15	O	808	CLA	C4A-NA-C1A	6.50	109.64	106.68
15	b	825	CLA	C4A-NA-C1A	6.50	109.64	106.68
15	N	839	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	N	802	F6C	CAA-C2A-C1A	-6.49	109.88	128.01
15	O	825	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	N	809	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	B	828	CLA	C4A-NA-C1A	6.49	109.64	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	813	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	O	828	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	A	808	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	b	837	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	V	102	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	b	838	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	b	812	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	N	838	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	O	834	CLA	C4A-NA-C1A	6.46	109.63	106.68
15	A	813	CLA	C4A-NA-C1A	6.46	109.63	106.68
15	S	201	CLA	C4A-NA-C1A	6.46	109.63	106.68
15	B	812	CLA	C4A-NA-C1A	6.46	109.62	106.68
15	a	808	CLA	C4A-NA-C1A	6.46	109.62	106.68
15	N	803	CLA	C4A-NA-C1A	6.46	109.62	106.68
15	O	812	CLA	C4A-NA-C1A	6.46	109.62	106.68
15	i	102	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	N	807	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	O	819	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	O	833	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	O	837	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	a	811	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	L	203	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	N	822	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	B	804	CLA	C4A-NA-C1A	6.44	109.62	106.68
15	B	819	CLA	C4A-NA-C1A	6.44	109.62	106.68
15	a	838	CLA	C4A-NA-C1A	6.44	109.62	106.68
15	O	811	CLA	C4A-NA-C1A	6.44	109.61	106.68
15	a	813	CLA	C4A-NA-C1A	6.44	109.61	106.68
15	a	834	CLA	C4A-NA-C1A	6.44	109.61	106.68
15	N	840	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	b	808	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	b	828	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	a	805	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	X	102	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	a	839	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	b	819	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	a	812	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	B	811	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	l	102	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	A	805	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	b	811	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	B	829	CLA	C4A-NA-C1A	6.42	109.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	102	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	f	201	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	A	811	CLA	C4A-NA-C1A	6.41	109.61	106.68
15	A	840	CLA	C4A-NA-C1A	6.41	109.60	106.68
15	O	804	CLA	C4A-NA-C1A	6.41	109.60	106.68
15	F	201	CLA	C4A-NA-C1A	6.41	109.60	106.68
15	b	833	CLA	C4A-NA-C1A	6.41	109.60	106.68
15	N	814	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	N	834	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	a	803	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	B	832	F6C	CAA-C2A-C1A	-6.40	110.12	128.01
15	N	812	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	N	832	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	b	806	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	a	814	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	A	832	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	N	811	CLA	C4A-NA-C1A	6.39	109.60	106.68
15	a	821	CLA	C4A-NA-C1A	6.39	109.60	106.68
15	a	825	CLA	C4A-NA-C1A	6.39	109.60	106.68
15	A	821	CLA	C4A-NA-C1A	6.39	109.59	106.68
15	N	817	CLA	C4A-NA-C1A	6.39	109.59	106.68
15	A	817	CLA	C4A-NA-C1A	6.39	109.59	106.68
15	B	806	CLA	C4A-NA-C1A	6.39	109.59	106.68
15	N	805	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	L	204	F6C	CMA-C3A-C4A	-6.39	113.48	124.73
15	N	821	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	a	836	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	b	810	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	A	812	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	A	836	CLA	C4A-NA-C1A	6.37	109.59	106.68
15	a	817	CLA	C4A-NA-C1A	6.37	109.59	106.68
15	O	806	CLA	C4A-NA-C1A	6.37	109.58	106.68
15	A	804	CLA	C4A-NA-C1A	6.36	109.58	106.68
15	A	825	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	a	802	F6C	CAA-C2A-C1A	-6.35	110.28	128.01
15	B	824	CLA	C4A-NA-C1A	6.35	109.57	106.68
15	a	842	CLA	C4A-NA-C1A	6.35	109.57	106.68
15	A	814	CLA	C4A-NA-C1A	6.34	109.57	106.68
15	A	803	CLA	C4A-NA-C1A	6.34	109.57	106.68
15	b	813	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	b	804	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	O	810	CLA	C4A-NA-C1A	6.33	109.57	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	816	CLA	C4A-NA-C1A	6.33	109.56	106.68
15	B	817	CLA	C4A-NA-C1A	6.32	109.56	106.68
15	B	813	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	O	832	F6C	CAA-C2A-C1A	-6.31	110.37	128.01
15	N	804	CLA	C4A-NA-C1A	6.31	109.56	106.68
15	a	806	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	b	832	F6C	CAA-C2A-C1A	-6.31	110.38	128.01
14	N	856	F6C	CAA-C2A-C1A	-6.31	110.38	128.01
15	b	831	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	A	802	F6C	CAA-C2A-C1A	-6.31	110.39	128.01
15	B	833	CLA	C4A-NA-C1A	6.30	109.56	106.68
15	O	824	CLA	C4A-NA-C1A	6.30	109.56	106.68
15	N	816	CLA	C4A-NA-C1A	6.30	109.55	106.68
15	A	834	CLA	C4A-NA-C1A	6.30	109.55	106.68
15	O	809	CLA	C4A-NA-C1A	6.30	109.55	106.68
15	b	834	CLA	C4A-NA-C1A	6.30	109.55	106.68
15	O	813	CLA	C4A-NA-C1A	6.29	109.55	106.68
15	A	816	CLA	C4A-NA-C1A	6.29	109.55	106.68
15	N	806	CLA	C4A-NA-C1A	6.28	109.55	106.68
15	A	827	CLA	C4A-NA-C1A	6.28	109.54	106.68
14	a	855	F6C	CAA-C2A-C1A	-6.28	110.47	128.01
15	K	103	CLA	C4A-NA-C1A	6.27	109.54	106.68
15	N	827	CLA	C4A-NA-C1A	6.27	109.54	106.68
15	b	817	CLA	C4A-NA-C1A	6.27	109.54	106.68
15	O	817	CLA	C4A-NA-C1A	6.27	109.54	106.68
15	N	836	CLA	C4A-NA-C1A	6.26	109.54	106.68
15	N	837	CLA	C4A-NA-C1A	6.25	109.53	106.68
15	N	842	CLA	C4A-NA-C1A	6.25	109.53	106.68
15	B	810	CLA	C4A-NA-C1A	6.25	109.53	106.68
15	b	830	CLA	C4A-NA-C1A	6.25	109.53	106.68
14	A	856	F6C	CAA-C2A-C1A	-6.25	110.55	128.01
15	O	831	CLA	C4A-NA-C1A	6.25	109.53	106.68
15	B	830	CLA	C4A-NA-C1A	6.24	109.53	106.68
15	O	835	CLA	C4A-NA-C1A	6.24	109.53	106.68
15	A	806	CLA	C4A-NA-C1A	6.24	109.53	106.68
15	B	831	CLA	C4A-NA-C1A	6.23	109.52	106.68
15	B	835	CLA	C4A-NA-C1A	6.23	109.52	106.68
15	B	834	CLA	C4A-NA-C1A	6.23	109.52	106.68
15	O	830	CLA	C4A-NA-C1A	6.23	109.52	106.68
15	a	819	CLA	C4A-NA-C1A	6.23	109.52	106.68
15	b	827	CLA	C4A-NA-C1A	6.23	109.52	106.68
15	b	824	CLA	C4A-NA-C1A	6.22	109.52	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	842	CLA	C4A-NA-C1A	6.22	109.52	106.68
15	b	835	CLA	C4A-NA-C1A	6.21	109.51	106.68
15	A	810	CLA	C4A-NA-C1A	6.21	109.51	106.68
15	a	833	CLA	C4A-NA-C1A	6.21	109.51	106.68
15	N	825	CLA	C4A-NA-C1A	6.21	109.51	106.68
15	a	804	CLA	C4A-NA-C1A	6.20	109.51	106.68
15	N	810	CLA	C4A-NA-C1A	6.19	109.50	106.68
15	A	819	CLA	C4A-NA-C1A	6.19	109.50	106.68
15	a	810	CLA	C4A-NA-C1A	6.18	109.50	106.68
15	i	103	CLA	C4A-NA-C1A	6.18	109.50	106.68
15	A	830	CLA	C4A-NA-C1A	6.18	109.50	106.68
15	B	821	CLA	C4A-NA-C1A	6.18	109.50	106.68
15	b	818	CLA	C4A-NA-C1A	6.18	109.50	106.68
15	N	819	CLA	C4A-NA-C1A	6.18	109.50	106.68
13	a	801	CL0	C1B-CHB-C4A	6.17	125.30	121.32
15	b	809	CLA	C4A-NA-C1A	6.17	109.50	106.68
15	A	833	CLA	C4A-NA-C1A	6.16	109.49	106.68
15	N	830	CLA	C4A-NA-C1A	6.16	109.49	106.68
15	V	103	CLA	C4A-NA-C1A	6.15	109.49	106.68
15	N	833	CLA	C4A-NA-C1A	6.15	109.48	106.68
15	O	836	CLA	C4A-NA-C1A	6.14	109.48	106.68
14	W	204	F6C	CAA-C2A-C1A	-6.14	110.86	128.01
15	a	830	CLA	C4A-NA-C1A	6.14	109.48	106.68
15	B	827	CLA	C4A-NA-C1A	6.13	109.48	106.68
15	O	827	CLA	C4A-NA-C1A	6.13	109.48	106.68
15	a	827	CLA	C4A-NA-C1A	6.12	109.47	106.68
15	a	837	CLA	C4A-NA-C1A	6.12	109.47	106.68
15	B	818	CLA	C4A-NA-C1A	6.12	109.47	106.68
15	O	821	CLA	C4A-NA-C1A	6.12	109.47	106.68
13	N	801	CL0	C1B-CHB-C4A	6.11	125.25	121.32
15	A	837	CLA	C4A-NA-C1A	6.11	109.47	106.68
15	B	836	CLA	C4A-NA-C1A	6.08	109.45	106.68
15	O	818	CLA	C4A-NA-C1A	6.07	109.45	106.68
14	j	204	F6C	CAA-C2A-C1A	-6.07	111.06	128.01
15	B	802	CLA	C4A-NA-C1A	6.06	109.45	106.68
13	A	801	CL0	C1B-CHB-C4A	6.06	125.22	121.32
15	B	816	CLA	C4A-NA-C1A	6.06	109.44	106.68
15	B	808	CLA	C4A-NA-C1A	6.05	109.44	106.68
15	b	821	CLA	C4A-NA-C1A	6.03	109.43	106.68
15	b	802	CLA	C4A-NA-C1A	6.03	109.43	106.68
15	b	836	CLA	C4A-NA-C1A	6.02	109.43	106.68
14	L	204	F6C	CAA-C2A-C1A	-6.01	111.22	128.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	835	CLA	C4A-NA-C1A	5.99	109.41	106.68
15	O	802	CLA	C4A-NA-C1A	5.96	109.40	106.68
15	N	835	CLA	C4A-NA-C1A	5.95	109.39	106.68
15	b	816	CLA	C4A-NA-C1A	5.92	109.38	106.68
14	A	856	F6C	CMA-C3A-C2A	-5.91	110.16	126.15
14	N	824	F6C	CAA-C2A-C1A	-5.91	111.50	128.01
14	a	855	F6C	CMA-C3A-C2A	-5.88	110.25	126.15
14	N	856	F6C	CMA-C3A-C2A	-5.85	110.32	126.15
15	a	835	CLA	C4A-NA-C1A	5.85	109.35	106.68
14	a	826	F6C	CAA-C2A-C1A	-5.83	111.72	128.01
14	A	824	F6C	CAA-C2A-C1A	-5.83	111.73	128.01
14	a	824	F6C	CAA-C2A-C1A	-5.81	111.78	128.01
15	O	816	CLA	C4A-NA-C1A	5.68	109.27	106.68
14	A	826	F6C	CAA-C2A-C1A	-5.54	112.53	128.01
14	j	201	F6C	C4A-NA-C1A	5.52	110.18	106.31
14	L	204	F6C	CMA-C3A-C2A	-5.49	111.29	126.15
14	N	826	F6C	CAA-C2A-C1A	-5.46	112.74	128.01
14	W	201	F6C	C4A-NA-C1A	5.43	110.12	106.31
14	b	832	F6C	CMA-C3A-C2A	-5.43	111.47	126.15
14	O	832	F6C	CMA-C3A-C2A	-5.42	111.48	126.15
14	L	201	F6C	C4A-NA-C1A	5.42	110.12	106.31
14	B	832	F6C	CMA-C3A-C2A	-5.40	111.54	126.15
14	W	204	F6C	CMA-C3A-C2A	-5.36	111.66	126.15
14	j	204	F6C	CMA-C3A-C2A	-5.34	111.72	126.15
14	b	839	F6C	CMA-C3A-C2A	-5.27	111.90	126.15
14	B	839	F6C	CMA-C3A-C2A	-5.25	111.94	126.15
14	O	839	F6C	CMA-C3A-C2A	-5.22	112.03	126.15
14	N	824	F6C	CMA-C3A-C2A	-5.21	112.06	126.15
14	A	802	F6C	CMA-C3A-C2A	-5.18	112.14	126.15
14	A	824	F6C	CMA-C3A-C2A	-5.16	112.19	126.15
14	a	824	F6C	CMA-C3A-C2A	-5.15	112.21	126.15
14	a	802	F6C	CMA-C3A-C2A	-5.10	112.35	126.15
14	N	802	F6C	CMA-C3A-C2A	-5.08	112.41	126.15
14	W	201	F6C	CMA-C3A-C2A	-5.04	112.51	126.15
14	L	201	F6C	CMA-C3A-C2A	-5.02	112.57	126.15
14	A	826	F6C	C4A-NA-C1A	4.99	109.81	106.31
14	a	826	F6C	C4A-NA-C1A	4.98	109.81	106.31
14	N	826	F6C	C4A-NA-C1A	4.95	109.78	106.31
14	j	201	F6C	CMA-C3A-C2A	-4.92	112.83	126.15
14	B	832	F6C	C4A-NA-C1A	4.91	109.76	106.31
14	O	832	F6C	C4A-NA-C1A	4.88	109.73	106.31
14	b	832	F6C	C4A-NA-C1A	4.87	109.73	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	824	F6C	C4A-NA-C1A	4.85	109.71	106.31
14	N	824	F6C	C4A-NA-C1A	4.84	109.71	106.31
14	a	824	F6C	C4A-NA-C1A	4.84	109.71	106.31
14	j	201	F6C	CAA-C2A-C1A	-4.82	114.55	128.01
14	L	204	F6C	C4A-NA-C1A	4.77	109.66	106.31
14	b	839	F6C	C4A-NA-C1A	4.76	109.65	106.31
14	j	204	F6C	C4A-NA-C1A	4.75	109.64	106.31
14	a	826	F6C	CMA-C3A-C2A	-4.71	113.42	126.15
14	O	839	F6C	C4A-NA-C1A	4.70	109.61	106.31
14	W	204	F6C	C4A-NA-C1A	4.70	109.61	106.31
14	N	826	F6C	CMA-C3A-C2A	-4.69	113.46	126.15
14	B	839	F6C	C4A-NA-C1A	4.68	109.60	106.31
14	A	826	F6C	CMA-C3A-C2A	-4.65	113.58	126.15
14	A	856	F6C	C4A-NA-C1A	4.54	109.50	106.31
14	a	855	F6C	C4A-NA-C1A	4.48	109.45	106.31
14	N	856	F6C	C4A-NA-C1A	4.47	109.45	106.31
14	W	201	F6C	CAA-C2A-C1A	-4.45	115.57	128.01
14	L	201	F6C	CAA-C2A-C1A	-4.44	115.62	128.01
14	A	802	F6C	C4A-NA-C1A	4.20	109.26	106.31
14	N	802	F6C	C4A-NA-C1A	4.19	109.25	106.31
14	a	802	F6C	C4A-NA-C1A	4.17	109.24	106.31
15	b	822	CLA	C4A-NA-C1A	4.16	108.58	106.68
15	B	822	CLA	C4A-NA-C1A	4.12	108.56	106.68
20	N	853	LMT	C1B-O5B-C5B	4.12	121.76	113.72
20	A	853	LMT	C1B-O5B-C5B	4.09	121.71	113.72
20	a	853	LMT	C1B-O5B-C5B	4.09	121.70	113.72
14	a	802	F6C	C1A-C2A-C3A	-3.74	103.03	106.97
14	N	802	F6C	C1A-C2A-C3A	-3.73	103.04	106.97
14	A	802	F6C	C1A-C2A-C3A	-3.68	103.09	106.97
18	h	102	BCR	C15-C14-C13	-3.59	122.24	127.28
20	A	853	LMT	C1B-O1B-C4'	3.56	126.43	117.98
20	N	853	LMT	C1B-O1B-C4'	3.56	126.41	117.98
18	U	102	BCR	C15-C14-C13	-3.54	122.31	127.28
14	A	856	F6C	C1A-C2A-C3A	-3.53	103.25	106.97
20	a	853	LMT	C1B-O1B-C4'	3.53	126.35	117.98
14	a	855	F6C	C1A-C2A-C3A	-3.51	103.27	106.97
14	N	856	F6C	C1A-C2A-C3A	-3.50	103.28	106.97
15	a	820	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
18	h	102	BCR	C11-C10-C9	-3.50	122.37	127.28
15	B	812	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
18	U	102	BCR	C11-C10-C9	-3.48	122.39	127.28
15	O	812	CLA	O2D-CGD-O1D	-3.47	117.10	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	812	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
18	J	102	BCR	C15-C14-C13	-3.46	122.43	127.28
18	J	102	BCR	C11-C10-C9	-3.43	122.46	127.28
14	a	826	F6C	C1A-C2A-C3A	-3.35	103.44	106.97
15	a	835	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
15	A	819	CLA	C3B-C4B-NB	-3.27	107.61	110.53
14	A	826	F6C	C1A-C2A-C3A	-3.27	103.53	106.97
15	A	811	CLA	O2D-CGD-O1D	-3.26	117.49	123.85
15	N	819	CLA	C3B-C4B-NB	-3.26	107.62	110.53
15	a	811	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
15	a	827	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
15	A	820	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
14	N	826	F6C	C1A-C2A-C3A	-3.23	103.56	106.97
15	N	811	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
15	a	819	CLA	C3B-C4B-NB	-3.23	107.64	110.53
15	b	813	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
13	N	801	CL0	O2D-CGD-CBD	3.19	114.45	110.95
15	L	203	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
15	A	835	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
14	N	824	F6C	C1A-C2A-C3A	-3.16	103.64	106.97
14	b	832	F6C	C1A-C2A-C3A	-3.16	103.64	106.97
15	W	203	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
14	a	824	F6C	C1A-C2A-C3A	-3.15	103.65	106.97
14	O	832	F6C	C1A-C2A-C3A	-3.15	103.66	106.97
14	a	826	F6C	O2D-CGD-O1D	-3.15	117.72	123.85
15	B	816	CLA	C3B-C4B-NB	-3.14	107.72	110.53
15	j	203	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
15	N	827	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
15	N	835	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
15	O	821	CLA	CAA-C2A-C3A	-3.13	104.53	113.00
15	A	827	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
14	B	839	F6C	C1A-C2A-C3A	-3.13	103.67	106.97
15	B	835	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	A	824	F6C	C1A-C2A-C3A	-3.12	103.68	106.97
15	a	831	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
15	A	831	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
15	O	808	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
15	A	816	CLA	C3B-C4B-NB	-3.11	107.75	110.53
14	B	832	F6C	C1A-C2A-C3A	-3.11	103.69	106.97
15	A	818	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
15	O	824	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
15	O	801	CLA	O2D-CGD-O1D	-3.11	117.80	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	813	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
15	b	808	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
15	O	816	CLA	C3B-C4B-NB	-3.10	107.76	110.53
15	N	831	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
15	N	818	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
15	b	824	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
15	O	828	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
15	b	835	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
15	a	837	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
15	B	801	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
15	B	821	CLA	CAA-C2A-C3A	-3.10	104.64	113.00
15	a	818	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
15	O	813	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	A	802	F6C	C1-C2-C3	-3.09	121.13	126.20
15	b	821	CLA	CAA-C2A-C3A	-3.09	104.64	113.00
15	b	801	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	b	839	F6C	C1A-C2A-C3A	-3.09	103.72	106.97
15	O	835	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
15	N	816	CLA	C3B-C4B-NB	-3.09	107.78	110.53
15	N	825	CLA	C3B-C4B-NB	-3.09	107.78	110.53
15	a	816	CLA	C3B-C4B-NB	-3.09	107.78	110.53
15	L	203	CLA	C3B-C4B-NB	-3.08	107.78	110.53
14	j	201	F6C	CBD-CHA-C4D	-3.08	105.07	108.54
14	O	839	F6C	C1A-C2A-C3A	-3.08	103.72	106.97
15	B	815	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
15	b	807	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
15	B	824	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
13	A	801	CL0	O2D-CGD-CBD	3.08	114.33	110.95
15	b	816	CLA	C3B-C4B-NB	-3.07	107.79	110.53
15	B	819	CLA	C3B-C4B-NB	-3.07	107.79	110.53
15	O	819	CLA	C3B-C4B-NB	-3.07	107.79	110.53
15	B	807	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
15	A	837	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
15	b	802	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
15	b	819	CLA	C3B-C4B-NB	-3.06	107.80	110.53
15	B	816	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
15	B	828	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
15	b	815	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
18	h	102	BCR	C7-C8-C9	-3.05	121.72	126.23
14	N	826	F6C	O2D-CGD-O1D	-3.05	117.91	123.85
15	b	823	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	a	801	CL0	O2D-CGD-CBD	3.05	114.30	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	828	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
14	B	839	F6C	O2D-CGD-O1D	-3.05	117.91	123.85
15	O	802	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
14	j	204	F6C	O2D-CGD-O1D	-3.05	117.92	123.85
15	B	823	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
15	O	807	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
15	B	804	CLA	C3B-C4B-NB	-3.04	107.81	110.53
14	A	826	F6C	O2D-CGD-O1D	-3.04	117.93	123.85
15	O	816	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	W	201	F6C	CBD-CHA-C4D	-3.04	105.12	108.54
15	N	839	CLA	C3B-C4B-NB	-3.04	107.82	110.53
15	O	814	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
15	V	103	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
15	i	103	CLA	C3B-C4B-NB	-3.04	107.82	110.53
15	B	814	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
14	W	204	F6C	O2D-CGD-O1D	-3.03	117.94	123.85
15	b	816	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
18	J	102	BCR	C7-C8-C9	-3.03	121.75	126.23
14	L	204	F6C	O2D-CGD-O1D	-3.03	117.95	123.85
15	S	201	CLA	C3B-C4B-NB	-3.03	107.83	110.53
15	N	820	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
15	F	201	CLA	C3B-C4B-NB	-3.03	107.83	110.53
15	B	802	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
15	O	823	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
15	a	839	CLA	C3B-C4B-NB	-3.02	107.83	110.53
15	O	815	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	L	204	F6C	C1A-C2A-C3A	-3.02	103.79	106.97
14	L	201	F6C	CBD-CHA-C4D	-3.01	105.14	108.54
15	B	811	CLA	C3B-C4B-NB	-3.01	107.84	110.53
15	b	814	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
18	U	102	BCR	C7-C8-C9	-3.01	121.78	126.23
13	N	801	CL0	O2D-CGD-O1D	-3.01	117.99	123.85
15	a	817	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
15	b	804	CLA	C3B-C4B-NB	-3.01	107.84	110.53
15	b	838	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
15	f	201	CLA	C3B-C4B-NB	-3.01	107.85	110.53
14	a	802	F6C	C4A-C3A-C2A	-3.01	102.51	106.97
15	A	812	CLA	C3B-C4B-NB	-3.01	107.85	110.53
15	N	812	CLA	C3B-C4B-NB	-3.01	107.85	110.53
15	B	818	CLA	C3B-C4B-NB	-3.00	107.85	110.53
14	j	204	F6C	C1A-C2A-C3A	-3.00	103.81	106.97
15	a	804	CLA	C3B-C4B-NB	-3.00	107.85	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	840	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
15	a	804	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
15	a	825	CLA	C3B-C4B-NB	-3.00	107.85	110.53
15	j	203	CLA	C3B-C4B-NB	-3.00	107.86	110.53
15	O	804	CLA	C3B-C4B-NB	-3.00	107.86	110.53
15	b	811	CLA	C3B-C4B-NB	-3.00	107.86	110.53
15	O	811	CLA	C3B-C4B-NB	-2.99	107.86	110.53
15	a	812	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	b	832	F6C	O2D-CGD-O1D	-2.99	118.03	123.85
15	A	809	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
15	A	825	CLA	C3B-C4B-NB	-2.99	107.86	110.53
15	B	838	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	W	204	F6C	C1A-C2A-C3A	-2.99	103.83	106.97
15	N	804	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
15	A	817	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
15	A	810	CLA	CAA-C2A-C3A	-2.98	104.94	113.00
15	N	817	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
15	A	839	CLA	C3B-C4B-NB	-2.98	107.87	110.53
15	B	808	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	O	832	F6C	O2D-CGD-O1D	-2.98	118.05	123.85
15	B	822	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
15	b	817	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
15	N	840	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
15	K	103	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
15	A	804	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
15	A	840	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
15	b	818	CLA	C3B-C4B-NB	-2.97	107.88	110.53
14	B	832	F6C	O2D-CGD-O1D	-2.97	118.06	123.85
15	N	809	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
15	A	838	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
15	W	203	CLA	C3B-C4B-NB	-2.97	107.88	110.53
15	N	825	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
15	a	808	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
15	a	833	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
15	O	838	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
15	b	822	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
15	a	838	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
15	O	818	CLA	C3B-C4B-NB	-2.97	107.88	110.53
15	B	817	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
15	a	809	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
15	N	805	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
15	B	805	CLA	O2D-CGD-O1D	-2.96	118.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	818	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
15	N	808	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
15	B	837	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
15	N	833	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	a	801	CL0	O2D-CGD-O1D	-2.96	118.09	123.85
14	N	802	F6C	C4A-C3A-C2A	-2.96	102.59	106.97
15	O	806	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
15	a	805	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
13	N	801	CL0	CHA-C1A-C2A	-2.95	126.37	133.31
15	A	808	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
14	W	201	F6C	C4A-C3A-C2A	-2.95	102.59	106.97
15	N	842	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	b	837	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	b	839	F6C	O2D-CGD-O1D	-2.95	118.11	123.85
15	b	818	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	A	823	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	A	833	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	A	805	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	O	837	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	B	806	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	a	810	CLA	CAA-C2A-C3A	-2.94	105.06	113.00
15	O	822	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
15	b	806	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
15	b	822	CLA	C3B-C4B-NB	-2.94	107.91	110.53
13	A	801	CL0	O2D-CGD-O1D	-2.94	118.13	123.85
14	a	824	F6C	O2D-CGD-O1D	-2.94	118.13	123.85
15	a	823	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
15	a	839	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
15	N	838	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
15	A	842	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
15	a	807	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
15	A	822	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
14	j	201	F6C	C4A-C3A-C2A	-2.93	102.62	106.97
15	B	803	CLA	C3B-C4B-NB	-2.93	107.91	110.53
15	V	103	CLA	C3B-C4B-NB	-2.93	107.91	110.53
15	N	823	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
15	i	103	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
15	B	822	CLA	C3B-C4B-NB	-2.93	107.92	110.53
15	N	804	CLA	C3B-C4B-NB	-2.93	107.92	110.53
14	A	802	F6C	C4A-C3A-C2A	-2.93	102.63	106.97
15	N	807	CLA	C3B-C4B-NB	-2.93	107.92	110.53
14	L	201	F6C	C4A-C3A-C2A	-2.93	102.63	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	801	CL0	CHA-C1A-C2A	-2.93	126.44	133.31
15	O	818	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
15	a	842	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	A	824	F6C	O2D-CGD-O1D	-2.92	118.16	123.85
15	B	836	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
15	A	804	CLA	C3B-C4B-NB	-2.92	107.92	110.53
15	N	821	CLA	C3B-C4B-NB	-2.92	107.92	110.53
14	O	839	F6C	O2D-CGD-O1D	-2.92	118.16	123.85
15	A	839	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
15	N	839	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	N	810	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
15	O	817	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	K	103	CLA	C3B-C4B-NB	-2.92	107.93	110.53
15	O	805	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
15	A	821	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
15	A	821	CLA	C3B-C4B-NB	-2.91	107.93	110.53
14	a	855	F6C	O2D-CGD-O1D	-2.91	118.18	123.85
15	N	837	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
15	B	827	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
13	A	801	CL0	CHA-C1A-C2A	-2.91	126.47	133.31
15	B	809	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	b	805	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	b	836	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	N	807	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	b	820	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	a	821	CLA	C3B-C4B-NB	-2.91	107.94	110.53
15	N	806	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	N	828	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
15	O	825	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
15	B	810	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
15	A	819	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
15	N	805	CLA	C3B-C4B-NB	-2.90	107.94	110.53
15	O	835	CLA	C3B-C4B-NB	-2.90	107.94	110.53
15	B	811	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	A	802	F6C	O2D-CGD-O1D	-2.90	118.20	123.85
15	b	811	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
15	a	821	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
15	b	810	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
15	b	835	CLA	C3B-C4B-NB	-2.90	107.94	110.53
15	A	807	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
15	b	819	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
15	N	821	CLA	O2D-CGD-O1D	-2.90	118.21	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	830	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
14	a	802	F6C	O2D-CGD-O1D	-2.90	118.21	123.85
18	h	102	BCR	C16-C15-C14	2.89	129.44	123.52
15	O	810	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	N	841	CLA	C3B-C4B-NB	-2.89	107.95	110.53
15	a	813	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	O	836	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	a	819	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	O	819	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	O	831	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	B	820	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	O	820	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	B	840	CLA	C3B-C4B-NB	-2.89	107.95	110.53
15	O	803	CLA	C3B-C4B-NB	-2.89	107.95	110.53
15	A	813	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	A	814	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	B	829	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	B	830	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	O	811	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
15	B	831	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
14	W	201	F6C	O2D-CGD-O1D	-2.89	118.23	123.85
15	B	835	CLA	C3B-C4B-NB	-2.88	107.95	110.53
15	O	829	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	b	830	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	B	825	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	a	812	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	A	828	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	a	806	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	B	819	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	a	814	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	b	804	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	b	825	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	a	817	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	N	814	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	N	836	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	O	827	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	b	829	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	A	806	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	A	805	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	A	812	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	a	825	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	b	840	CLA	O2D-CGD-O1D	-2.88	118.25	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	822	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	B	804	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	N	813	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	N	817	CLA	C3B-C4B-NB	-2.87	107.96	110.53
15	b	833	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	N	824	F6C	O2D-CGD-O1D	-2.87	118.26	123.85
15	N	812	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
15	a	827	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	B	812	CLA	O2D-CGD-CBD	2.87	116.25	111.23
15	B	840	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
15	N	819	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
15	O	840	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
15	a	822	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
15	O	833	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
14	N	826	F6C	CHA-C4D-ND	2.87	135.79	133.05
14	a	826	F6C	CHA-C4D-ND	2.87	135.79	133.05
15	a	807	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	A	856	F6C	O2D-CGD-O1D	-2.86	118.27	123.85
15	A	829	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
15	N	834	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
14	A	826	F6C	CHA-C4D-ND	2.86	135.79	133.05
15	j	202	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	A	803	CLA	C3B-C4B-NB	-2.86	107.97	110.53
15	W	202	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	A	825	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	A	832	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	a	818	CLA	C3B-C4B-NB	-2.86	107.98	110.53
15	b	803	CLA	C3B-C4B-NB	-2.86	107.98	110.53
15	Z	102	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
14	j	201	F6C	O2D-CGD-O1D	-2.86	118.29	123.85
14	N	802	F6C	O2D-CGD-O1D	-2.86	118.29	123.85
15	a	829	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
15	a	836	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
15	X	102	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
15	O	804	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
15	A	834	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
15	A	818	CLA	C3B-C4B-NB	-2.85	107.98	110.53
15	A	817	CLA	C3B-C4B-NB	-2.85	107.98	110.53
15	A	836	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
15	l	102	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
15	a	820	CLA	O2D-CGD-CBD	2.85	116.21	111.23
14	L	201	F6C	O2D-CGD-O1D	-2.85	118.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	856	F6C	O2D-CGD-O1D	-2.85	118.31	123.85
15	a	805	CLA	C3B-C4B-NB	-2.85	107.99	110.53
15	b	840	CLA	C3B-C4B-NB	-2.85	107.99	110.53
15	A	816	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
15	N	832	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
15	b	831	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
15	Z	102	CLA	C3B-C4B-NB	-2.84	107.99	110.53
15	a	816	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
15	O	812	CLA	O2D-CGD-CBD	2.84	116.20	111.23
15	b	826	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
15	O	826	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
15	N	829	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
15	B	829	CLA	C3B-C4B-NB	-2.84	107.99	110.53
14	L	201	F6C	C1A-C2A-C3A	-2.84	103.98	106.97
14	B	839	F6C	CHA-C4D-ND	2.84	135.76	133.05
15	N	816	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
15	A	834	CLA	C3B-C4B-NB	-2.83	108.00	110.53
15	a	832	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
15	A	807	CLA	C3B-C4B-NB	-2.83	108.00	110.53
15	O	813	CLA	C3B-C4B-NB	-2.83	108.00	110.53
15	a	803	CLA	C3B-C4B-NB	-2.83	108.00	110.53
15	L	202	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
15	b	827	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
15	K	102	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	a	801	CL0	C1C-CHC-C4B	2.83	126.19	116.07
15	B	833	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
15	i	102	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
15	a	834	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
15	V	102	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
18	U	102	BCR	C16-C15-C14	2.82	129.30	123.52
13	A	801	CL0	C1C-CHC-C4B	2.82	126.17	116.07
15	B	825	CLA	C3B-C4B-NB	-2.82	108.01	110.53
15	a	841	CLA	C3B-C4B-NB	-2.82	108.01	110.53
15	l	102	CLA	C3B-C4B-NB	-2.82	108.01	110.53
13	N	801	CL0	C1C-CHC-C4B	2.82	126.15	116.07
14	A	802	F6C	CHA-C4D-ND	2.81	135.74	133.05
15	L	202	CLA	C3B-C4B-NB	-2.81	108.02	110.53
15	N	803	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
15	B	813	CLA	C3B-C4B-NB	-2.81	108.02	110.53
15	X	102	CLA	C3B-C4B-NB	-2.81	108.02	110.53
15	b	812	CLA	O2D-CGD-CBD	2.81	116.14	111.23
15	a	803	CLA	O2D-CGD-O1D	-2.81	118.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	818	CLA	C3B-C4B-NB	-2.80	108.03	110.53
15	b	813	CLA	C3B-C4B-NB	-2.80	108.03	110.53
13	A	801	CL0	C4D-CHA-CBD	-2.80	106.14	108.97
15	N	815	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
15	a	835	CLA	C3B-C4B-NB	-2.80	108.03	110.53
15	O	821	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
15	N	803	CLA	C3B-C4B-NB	-2.80	108.03	110.53
15	O	840	CLA	C3B-C4B-NB	-2.80	108.03	110.53
15	N	827	CLA	C3B-C4B-NB	-2.80	108.03	110.53
15	A	830	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
18	J	102	BCR	C16-C15-C14	2.80	129.24	123.52
15	N	835	CLA	C3B-C4B-NB	-2.79	108.03	110.53
15	B	826	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
15	O	825	CLA	C3B-C4B-NB	-2.79	108.04	110.53
14	b	839	F6C	CHA-C4D-ND	2.79	135.72	133.05
15	A	822	CLA	C3B-C4B-NB	-2.79	108.04	110.53
15	N	830	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
14	O	839	F6C	CHA-C4D-ND	2.78	135.71	133.05
15	O	809	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
15	A	841	CLA	C3B-C4B-NB	-2.78	108.05	110.53
15	O	829	CLA	C3B-C4B-NB	-2.78	108.05	110.53
15	B	821	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
15	a	810	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
15	A	810	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
15	A	803	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
15	O	809	CLA	C3B-C4B-NB	-2.78	108.05	110.53
14	a	802	F6C	CHA-C4D-ND	2.78	135.71	133.05
15	a	828	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
15	b	821	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
15	A	841	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
15	b	809	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
15	a	823	CLA	C3B-C4B-NB	-2.77	108.06	110.53
14	W	201	F6C	C1A-C2A-C3A	-2.76	104.06	106.97
15	N	810	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
15	b	829	CLA	C3B-C4B-NB	-2.76	108.06	110.53
15	B	833	CLA	C3B-C4B-NB	-2.76	108.06	110.53
15	N	834	CLA	C3B-C4B-NB	-2.76	108.06	110.53
15	N	809	CLA	C3B-C4B-NB	-2.76	108.07	110.53
15	N	842	CLA	C3B-C4B-NB	-2.76	108.07	110.53
15	N	823	CLA	C3B-C4B-NB	-2.76	108.07	110.53
15	A	827	CLA	C3B-C4B-NB	-2.76	108.07	110.53
15	b	809	CLA	C3B-C4B-NB	-2.76	108.07	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	808	CLA	O2A-CGA-O1A	-2.76	116.73	123.63
15	a	830	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
15	b	806	CLA	C3B-C4B-NB	-2.75	108.07	110.53
15	b	825	CLA	C3B-C4B-NB	-2.75	108.07	110.53
15	b	808	CLA	O2A-CGA-O1A	-2.75	116.74	123.63
14	j	201	F6C	C1A-C2A-C3A	-2.75	104.07	106.97
15	A	842	CLA	C3B-C4B-NB	-2.75	108.07	110.53
20	N	853	LMT	O5B-C1B-C2B	2.75	116.02	110.37
15	A	809	CLA	C3B-C4B-NB	-2.75	108.08	110.53
15	a	841	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
15	a	809	CLA	C3B-C4B-NB	-2.74	108.08	110.53
15	a	833	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
15	A	823	CLA	C3B-C4B-NB	-2.74	108.08	110.53
15	O	806	CLA	C3B-C4B-NB	-2.74	108.08	110.53
15	a	842	CLA	C3B-C4B-NB	-2.74	108.08	110.53
15	A	815	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
15	N	841	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
15	a	815	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
15	B	810	CLA	C3B-C4B-NB	-2.74	108.09	110.53
13	a	801	CL0	C4D-CHA-CBD	-2.74	106.21	108.97
15	b	833	CLA	C3B-C4B-NB	-2.73	108.09	110.53
15	B	808	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
15	A	835	CLA	C3B-C4B-NB	-2.73	108.09	110.53
15	O	833	CLA	C3B-C4B-NB	-2.73	108.09	110.53
15	a	822	CLA	C3B-C4B-NB	-2.73	108.09	110.53
15	A	814	CLA	C3B-C4B-NB	-2.72	108.10	110.53
15	N	833	CLA	CMB-C2B-C1B	-2.72	121.27	125.42
15	a	834	CLA	C3B-C4B-NB	-2.72	108.10	110.53
14	j	201	F6C	CHB-C4A-C3A	-2.72	119.83	125.49
14	j	201	F6C	OMB-CMB-C2B	-2.72	119.49	125.62
15	O	810	CLA	C3B-C4B-NB	-2.72	108.11	110.53
15	A	833	CLA	CMB-C2B-C1B	-2.71	121.28	125.42
15	a	813	CLA	C3B-C4B-NB	-2.71	108.11	110.53
20	a	853	LMT	O5B-C1B-C2B	2.71	115.94	110.37
14	N	802	F6C	CHA-C4D-ND	2.71	135.64	133.05
15	A	813	CLA	C3B-C4B-NB	-2.71	108.11	110.53
15	N	822	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
15	O	820	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	a	814	CLA	C3B-C4B-NB	-2.70	108.12	110.53
13	N	801	CL0	C4D-CHA-CBD	-2.70	106.24	108.97
15	N	811	CLA	C3B-C4B-NB	-2.70	108.12	110.53
20	A	853	LMT	O5B-C1B-C2B	2.70	115.92	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	824	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	N	814	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	N	813	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	b	810	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	W	201	F6C	CHB-C4A-C3A	-2.70	119.88	125.49
14	O	832	F6C	CHA-C4D-ND	2.70	135.63	133.05
15	B	820	CLA	C3B-C4B-NB	-2.69	108.12	110.53
15	i	102	CLA	C3B-C4B-NB	-2.69	108.12	110.53
15	b	820	CLA	C3B-C4B-NB	-2.69	108.13	110.53
14	L	201	F6C	CHB-C4A-C3A	-2.69	119.89	125.49
15	A	832	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	a	833	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	j	202	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	b	823	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	a	832	CLA	C3B-C4B-NB	-2.69	108.13	110.53
14	b	832	F6C	CHA-C4D-ND	2.68	135.62	133.05
14	N	824	F6C	CHA-C4D-ND	2.68	135.62	133.05
15	a	811	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	V	102	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	W	202	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	A	811	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	b	805	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	O	834	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
14	W	204	F6C	CHA-C4D-ND	2.67	135.60	133.05
15	a	810	CLA	C3B-C4B-NB	-2.67	108.15	110.53
15	A	808	CLA	C3B-C4B-NB	-2.66	108.15	110.53
15	N	832	CLA	C3B-C4B-NB	-2.66	108.15	110.53
15	N	810	CLA	C3B-C4B-NB	-2.66	108.15	110.53
15	K	102	CLA	C3B-C4B-NB	-2.66	108.15	110.53
14	A	824	F6C	CHA-C4D-ND	2.66	135.59	133.05
18	O	847	BCR	C20-C21-C22	-2.66	123.55	127.28
15	O	812	CLA	C3B-C4B-NB	-2.66	108.16	110.53
14	B	832	F6C	CHA-C4D-ND	2.66	135.59	133.05
15	B	805	CLA	C3B-C4B-NB	-2.66	108.16	110.53
15	O	801	CLA	C3B-C4B-NB	-2.65	108.16	110.53
15	A	810	CLA	C3B-C4B-NB	-2.65	108.16	110.53
15	A	833	CLA	C3B-C4B-NB	-2.65	108.16	110.53
15	B	803	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	N	826	F6C	CHB-C4A-C3A	-2.65	119.97	125.49
15	B	812	CLA	C3B-C4B-NB	-2.65	108.16	110.53
15	O	824	CLA	C3B-C4B-NB	-2.65	108.17	110.53
14	j	204	F6C	CHA-C4D-ND	2.65	135.58	133.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	837	CLA	C3B-C4B-NB	-2.65	108.17	110.53
15	O	808	CLA	C1-C2-C3	-2.64	121.86	126.20
15	B	806	CLA	C3B-C4B-NB	-2.64	108.17	110.53
15	N	833	CLA	C3B-C4B-NB	-2.64	108.17	110.53
13	A	801	CL0	C3D-C4D-CHA	2.64	112.56	108.54
15	b	834	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
14	a	855	F6C	CHA-C4D-ND	2.64	135.58	133.05
14	a	824	F6C	CHA-C4D-ND	2.64	135.57	133.05
14	B	839	F6C	OMB-CMB-C2B	-2.64	119.67	125.62
15	A	841	CLA	CHB-C4A-NA	2.64	128.21	124.40
15	a	808	CLA	C3B-C4B-NB	-2.64	108.18	110.53
14	L	201	F6C	CHA-C4D-ND	2.64	135.57	133.05
15	A	836	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	b	824	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	O	815	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	N	836	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	b	801	CLA	C3B-C4B-NB	-2.63	108.18	110.53
14	A	824	F6C	CHB-C4A-C3A	-2.63	120.02	125.49
14	a	824	F6C	CHB-C4A-C3A	-2.63	120.02	125.49
15	a	841	CLA	CHB-C4A-NA	2.63	128.19	124.40
15	b	812	CLA	C3B-C4B-NB	-2.63	108.19	110.53
14	L	204	F6C	OMB-CMB-C2B	-2.63	119.69	125.62
15	B	834	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
15	B	836	CLA	C3B-C4B-NB	-2.62	108.19	110.53
15	a	820	CLA	CHB-C4A-NA	2.62	128.19	124.40
14	W	201	F6C	CHA-C4D-ND	2.62	135.56	133.05
15	B	809	CLA	C3B-C4B-NB	-2.62	108.19	110.53
15	B	823	CLA	C3B-C4B-NB	-2.62	108.19	110.53
15	a	806	CLA	C3B-C4B-NB	-2.62	108.19	110.53
14	W	201	F6C	OMB-CMB-C2B	-2.61	119.72	125.62
14	A	826	F6C	CHB-C4A-C3A	-2.61	120.05	125.49
14	N	802	F6C	OMB-CMB-C2B	-2.61	119.72	125.62
13	a	801	CL0	C3D-C4D-CHA	2.61	112.51	108.54
15	A	815	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	O	839	F6C	OMB-CMB-C2B	-2.61	119.73	125.62
15	B	830	CLA	C3B-C4B-NB	-2.61	108.20	110.53
15	A	820	CLA	CHB-C4A-NA	2.61	128.16	124.40
15	N	806	CLA	C3B-C4B-NB	-2.61	108.20	110.53
18	M	101	BCR	C7-C8-C9	-2.61	122.38	126.23
15	B	828	CLA	C3B-C4B-NB	-2.60	108.21	110.53
13	N	801	CL0	C3D-C4D-CHA	2.60	112.49	108.54
14	N	824	F6C	CHB-C4A-C3A	-2.60	120.08	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	808	CLA	C1-C2-C3	-2.60	121.94	126.20
15	A	837	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	O	823	CLA	C3B-C4B-NB	-2.60	108.21	110.53
14	L	204	F6C	CHA-C4D-ND	2.60	135.54	133.05
14	j	201	F6C	CHA-C4D-ND	2.60	135.54	133.05
13	N	801	CL0	CMB-C2B-C3B	2.60	129.88	124.68
15	b	830	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	O	837	CLA	C1-C2-C3	-2.60	121.94	126.20
13	a	801	CL0	CMB-C2B-C3B	2.60	129.87	124.68
15	B	815	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	O	805	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	b	836	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	B	834	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
14	A	856	F6C	CHA-C4D-ND	2.59	135.53	133.05
15	a	837	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	O	830	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	B	808	CLA	C1-C2-C3	-2.59	121.95	126.20
14	W	204	F6C	OMB-CMB-C2B	-2.59	119.78	125.62
14	N	856	F6C	CHA-C4D-ND	2.59	135.52	133.05
13	A	801	CL0	CMB-C2B-C3B	2.59	129.85	124.68
14	O	832	F6C	CHB-C4A-C3A	-2.59	120.11	125.49
13	N	801	CL0	C4C-CHD-C1D	2.59	125.32	116.07
15	N	841	CLA	CHB-C4A-NA	2.58	128.13	124.40
15	A	806	CLA	C3B-C4B-NB	-2.58	108.22	110.53
14	L	201	F6C	OMB-CMB-C2B	-2.58	119.80	125.62
14	b	832	F6C	CHB-C4A-C3A	-2.58	120.12	125.49
14	j	204	F6C	CHB-C4A-C3A	-2.58	120.12	125.49
14	a	826	F6C	C1-C2-C3	-2.58	121.97	126.20
14	W	204	F6C	CHB-C4A-C3A	-2.58	120.12	125.49
14	b	839	F6C	OMB-CMB-C2B	-2.58	119.80	125.62
15	B	801	CLA	C3B-C4B-NB	-2.58	108.23	110.53
13	A	801	CL0	C4C-CHD-C1D	2.58	125.29	116.07
15	B	828	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
15	B	808	CLA	C3B-C4B-NB	-2.58	108.23	110.53
15	O	821	CLA	CHB-C4A-NA	2.57	128.12	124.40
13	a	801	CL0	C4C-CHD-C1D	2.57	125.28	116.07
14	A	802	F6C	CMB-C2B-C1B	-2.57	121.82	128.37
14	a	826	F6C	CBD-CHA-C4D	-2.57	105.64	108.54
15	A	832	CLA	C1-C2-C3	-2.57	122.60	126.76
14	j	204	F6C	OMB-CMB-C2B	-2.57	119.82	125.62
14	O	839	F6C	CHB-C4A-C3A	-2.57	120.14	125.49
15	N	808	CLA	C3B-C4B-NB	-2.57	108.24	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	815	CLA	C3B-C4B-NB	-2.57	108.24	110.53
14	A	826	F6C	CBD-CHA-C4D	-2.57	105.65	108.54
14	B	832	F6C	CHB-C4A-C3A	-2.57	120.15	125.49
15	b	808	CLA	C3B-C4B-NB	-2.57	108.24	110.53
15	O	828	CLA	C3B-C4B-NB	-2.56	108.24	110.53
18	k	102	BCR	C7-C8-C9	-2.56	122.45	126.23
15	b	828	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
15	O	836	CLA	C3B-C4B-NB	-2.56	108.25	110.53
15	a	838	CLA	C3B-C4B-NB	-2.55	108.25	110.53
15	b	823	CLA	C1-C2-C3	-2.55	122.01	126.20
14	a	826	F6C	CHB-C4A-C3A	-2.55	120.18	125.49
15	N	820	CLA	CHB-C4A-NA	2.55	128.09	124.40
15	F	201	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
18	b	847	BCR	C20-C21-C22	-2.55	123.70	127.28
14	N	826	F6C	CBD-CHA-C4D	-2.55	105.66	108.54
15	S	201	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
15	A	838	CLA	C3B-C4B-NB	-2.55	108.26	110.53
15	b	831	CLA	C3B-C4B-NB	-2.55	108.26	110.53
13	N	801	CL0	CMA-C3A-C4A	-2.55	109.13	114.61
14	N	802	F6C	CMB-C2B-C1B	-2.55	121.89	128.37
15	a	832	CLA	C1-C2-C3	-2.54	122.64	126.76
14	N	826	F6C	C4A-C3A-C2A	-2.54	103.20	106.97
15	B	821	CLA	CHB-C4A-NA	2.54	128.07	124.40
14	A	826	F6C	C4A-C3A-C2A	-2.54	103.20	106.97
14	B	839	F6C	CHB-C4A-C3A	-2.54	120.20	125.49
15	O	831	CLA	C3B-C4B-NB	-2.54	108.26	110.53
15	f	201	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
18	Y	102	BCR	C7-C8-C9	-2.54	122.48	126.23
15	O	814	CLA	C3B-C4B-NB	-2.54	108.26	110.53
15	b	814	CLA	CHB-C4A-NA	2.54	128.06	124.40
15	N	815	CLA	C3B-C4B-NB	-2.54	108.27	110.53
15	a	818	CLA	CHB-C4A-NA	2.53	128.06	124.40
15	b	814	CLA	C3B-C4B-NB	-2.53	108.27	110.53
15	O	834	CLA	C3B-C4B-NB	-2.53	108.27	110.53
15	i	103	CLA	C1-C2-C3	-2.53	122.67	126.76
14	a	802	F6C	OMB-CMB-C2B	-2.53	119.91	125.62
15	A	818	CLA	CHB-C4A-NA	2.53	128.05	124.40
15	O	828	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
14	b	839	F6C	CHB-C4A-C3A	-2.53	120.23	125.49
15	B	831	CLA	C3B-C4B-NB	-2.52	108.28	110.53
15	N	838	CLA	C3B-C4B-NB	-2.52	108.28	110.53
15	b	834	CLA	C3B-C4B-NB	-2.52	108.28	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	103	CLA	C1-C2-C3	-2.52	122.68	126.76
15	V	103	CLA	C1-C2-C3	-2.52	122.68	126.76
15	O	823	CLA	CHB-C4A-NA	2.52	128.04	124.40
15	N	832	CLA	C1-C2-C3	-2.52	122.69	126.76
14	a	802	F6C	CMB-C2B-C1B	-2.52	121.96	128.37
15	b	815	CLA	C3B-C4B-NB	-2.52	108.28	110.53
14	O	832	F6C	OMB-CMB-C2B	-2.52	119.94	125.62
18	a	846	BCR	C11-C10-C9	-2.52	123.75	127.28
15	A	807	CLA	CHB-C4A-NA	2.52	128.03	124.40
15	a	809	CLA	CHB-C4A-NA	2.51	128.03	124.40
15	N	818	CLA	CHB-C4A-NA	2.51	128.03	124.40
14	A	802	F6C	OMB-CMB-C2B	-2.51	119.95	125.62
15	b	833	CLA	CHB-C4A-NA	2.51	128.03	124.40
15	a	836	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	O	833	CLA	CHB-C4A-NA	2.51	128.03	124.40
15	b	828	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	a	830	CLA	C3B-C4B-NB	-2.51	108.29	110.53
14	a	826	F6C	CMC-C2C-C3C	2.51	130.94	125.62
15	A	831	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	O	808	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	B	837	CLA	C1-C2-C3	-2.51	122.09	126.20
15	O	827	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	O	837	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	A	805	CLA	CHB-C4A-NA	2.51	128.02	124.40
15	B	814	CLA	CHB-C4A-NA	2.50	128.01	124.40
15	a	816	CLA	CHB-C4A-NA	2.50	128.01	124.40
18	F	202	BCR	C20-C21-C22	-2.50	123.77	127.28
15	B	814	CLA	C3B-C4B-NB	-2.50	108.30	110.53
18	N	846	BCR	C11-C10-C9	-2.50	123.77	127.28
15	a	807	CLA	CHB-C4A-NA	2.50	128.01	124.40
15	B	833	CLA	CHB-C4A-NA	2.50	128.00	124.40
15	b	821	CLA	CHB-C4A-NA	2.50	128.00	124.40
15	b	837	CLA	C1-C2-C3	-2.50	122.11	126.20
15	O	822	CLA	C3B-C4B-NB	-2.50	108.30	110.53
15	A	816	CLA	CHB-C4A-NA	2.50	128.00	124.40
15	B	820	CLA	CHB-C4A-NA	2.50	128.00	124.40
15	b	827	CLA	C3B-C4B-NB	-2.49	108.30	110.53
15	A	809	CLA	CHB-C4A-NA	2.49	128.00	124.40
15	B	840	CLA	CHB-C4A-NA	2.49	128.00	124.40
15	N	807	CLA	CHB-C4A-NA	2.49	127.99	124.40
15	b	823	CLA	CHB-C4A-NA	2.49	127.99	124.40
18	A	846	BCR	C11-C10-C9	-2.49	123.79	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	823	CLA	CHB-C4A-NA	2.49	127.99	124.40
15	O	820	CLA	CHB-C4A-NA	2.49	127.99	124.40
15	a	828	CLA	CHB-C4A-NA	2.49	127.99	124.40
15	S	201	CLA	C1-C2-C3	-2.49	122.12	126.20
15	b	805	CLA	CHB-C4A-NA	2.49	127.99	124.40
14	A	856	F6C	CHB-C4A-C3A	-2.49	120.31	125.49
15	b	815	CLA	CHB-C4A-NA	2.49	127.99	124.40
15	N	828	CLA	C3B-C4B-NB	-2.49	108.31	110.53
15	a	831	CLA	C3B-C4B-NB	-2.49	108.31	110.53
15	N	828	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	O	814	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	j	203	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	N	856	F6C	OMB-CMB-C2B	-2.48	120.02	125.62
15	B	823	CLA	C1-C2-C3	-2.48	122.13	126.20
15	N	830	CLA	C3B-C4B-NB	-2.48	108.31	110.53
15	N	823	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	O	815	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	N	809	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	b	820	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	a	828	CLA	C3B-C4B-NB	-2.48	108.32	110.53
15	V	102	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	O	840	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	B	827	CLA	C3B-C4B-NB	-2.48	108.32	110.53
15	K	102	CLA	CHB-C4A-NA	2.48	127.97	124.40
15	N	816	CLA	CHB-C4A-NA	2.48	127.97	124.40
14	j	201	F6C	CHB-C4A-NA	2.47	128.29	124.80
15	a	805	CLA	CHB-C4A-NA	2.47	127.97	124.40
15	A	830	CLA	C3B-C4B-NB	-2.47	108.32	110.53
15	O	823	CLA	C1-C2-C3	-2.47	122.15	126.20
15	a	806	CLA	CHB-C4A-NA	2.47	127.97	124.40
16	B	841	PQN	C11-C3-C4	-2.47	115.98	118.58
15	N	814	CLA	CHB-C4A-NA	2.47	127.96	124.40
15	b	829	CLA	CHB-C4A-NA	2.47	127.96	124.40
15	N	840	CLA	C3B-C4B-NB	-2.47	108.33	110.53
15	i	102	CLA	CHB-C4A-NA	2.47	127.96	124.40
15	B	815	CLA	CHB-C4A-NA	2.47	127.96	124.40
15	N	805	CLA	CHB-C4A-NA	2.47	127.96	124.40
18	h	102	BCR	C8-C7-C6	2.47	133.59	127.00
15	O	805	CLA	CHB-C4A-NA	2.47	127.96	124.40
15	B	805	CLA	CHB-C4A-NA	2.46	127.96	124.40
15	O	812	CLA	CHB-C4A-NA	2.46	127.96	124.40
15	a	814	CLA	CHB-C4A-NA	2.46	127.96	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	837	CLA	C3B-C4B-NB	-2.46	108.33	110.53
14	W	204	F6C	C4A-C3A-C2A	-2.46	103.32	106.97
14	A	826	F6C	CMC-C2C-C3C	2.46	130.85	125.62
15	O	829	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	A	828	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	A	806	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	a	824	F6C	OMB-CMB-C2B	-2.46	120.06	125.62
15	b	811	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	A	828	CLA	C3B-C4B-NB	-2.46	108.33	110.53
15	B	829	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	W	203	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	a	823	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	A	808	CLA	CHB-C4A-NA	2.46	127.94	124.40
15	O	811	CLA	CHB-C4A-NA	2.46	127.94	124.40
15	a	808	CLA	CHB-C4A-NA	2.46	127.94	124.40
18	J	102	BCR	C8-C7-C6	2.46	133.56	127.00
18	B	847	BCR	C11-C10-C9	-2.46	123.83	127.28
14	N	856	F6C	CHB-C4A-C3A	-2.45	120.38	125.49
15	N	808	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	N	821	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	b	806	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	a	813	CLA	C1-C2-C3	-2.45	122.18	126.20
14	j	204	F6C	C4A-C3A-C2A	-2.45	103.33	106.97
15	F	201	CLA	C1-C2-C3	-2.45	122.18	126.20
15	A	823	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	B	811	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	a	821	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	i	103	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	j	202	CLA	CHB-C4A-NA	2.45	127.94	124.40
14	A	824	F6C	OMB-CMB-C2B	-2.45	120.09	125.62
14	N	826	F6C	OMB-CMB-C2B	-2.45	120.09	125.62
14	A	826	F6C	OMB-CMB-C2B	-2.45	120.09	125.62
15	b	812	CLA	CHB-C4A-NA	2.45	127.93	124.40
14	B	832	F6C	OMB-CMB-C2B	-2.45	120.09	125.62
15	B	806	CLA	CHB-C4A-NA	2.45	127.93	124.40
15	X	102	CLA	CHB-C4A-NA	2.45	127.93	124.40
13	a	801	CL0	CMA-C3A-C4A	-2.45	109.34	114.61
14	a	855	F6C	CHB-C4A-C3A	-2.45	120.40	125.49
15	A	817	CLA	CHB-C4A-NA	2.45	127.93	124.40
14	b	832	F6C	OMB-CMB-C2B	-2.45	120.10	125.62
15	B	837	CLA	C3B-C4B-NB	-2.45	108.35	110.53
15	A	814	CLA	CHB-C4A-NA	2.45	127.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	817	CLA	CHB-C4A-NA	2.44	127.93	124.40
15	N	817	CLA	CHB-C4A-NA	2.44	127.93	124.40
15	b	825	CLA	CHB-C4A-NA	2.44	127.93	124.40
15	A	815	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	N	806	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	O	806	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	b	840	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	A	804	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	B	812	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	N	813	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	A	813	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	B	824	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	L	203	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	b	819	CLA	CHB-C4A-NA	2.44	127.92	124.40
18	U	102	BCR	C8-C7-C6	2.44	133.51	127.00
15	a	825	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	A	811	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	B	804	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	A	839	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	O	819	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	a	812	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	N	824	F6C	OMB-CMB-C2B	-2.44	120.12	125.62
15	B	819	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	a	813	CLA	CHB-C4A-NA	2.44	127.91	124.40
15	A	836	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	B	816	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	O	825	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	B	813	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	A	840	CLA	C1-C2-C3	-2.43	122.83	126.76
15	N	840	CLA	C1-C2-C3	-2.43	122.83	126.76
15	O	804	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	O	824	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	a	811	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	a	815	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	A	821	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	l	102	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	f	201	CLA	C1-C2-C3	-2.43	122.22	126.20
15	N	839	CLA	CHB-C4A-NA	2.43	127.90	124.40
15	a	832	CLA	CHB-C4A-NA	2.43	127.90	124.40
14	L	201	F6C	CHB-C4A-NA	2.43	128.22	124.80
15	K	103	CLA	CHB-C4A-NA	2.43	127.90	124.40
14	a	855	F6C	OMB-CMB-C2B	-2.43	120.14	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	855	F6C	C4A-C3A-C2A	-2.43	103.37	106.97
15	Z	102	CLA	CHB-C4A-NA	2.43	127.90	124.40
15	N	832	CLA	CHB-C4A-NA	2.42	127.90	124.40
15	N	836	CLA	CHB-C4A-NA	2.42	127.90	124.40
15	O	813	CLA	CHB-C4A-NA	2.42	127.90	124.40
15	a	836	CLA	CHB-C4A-NA	2.42	127.90	124.40
15	b	813	CLA	CHB-C4A-NA	2.42	127.89	124.40
15	a	839	CLA	CHB-C4A-NA	2.42	127.89	124.40
15	b	804	CLA	CHB-C4A-NA	2.42	127.89	124.40
15	a	840	CLA	C1-C2-C3	-2.42	122.85	126.76
15	N	812	CLA	CHB-C4A-NA	2.42	127.89	124.40
14	N	826	F6C	CMC-C2C-C3C	2.42	130.75	125.62
14	L	204	F6C	C4A-C3A-C2A	-2.42	103.39	106.97
15	B	825	CLA	CHB-C4A-NA	2.42	127.89	124.40
14	a	826	F6C	OMB-CMB-C2B	-2.42	120.17	125.62
15	N	815	CLA	CHB-C4A-NA	2.41	127.89	124.40
15	A	812	CLA	CHB-C4A-NA	2.41	127.88	124.40
15	B	834	CLA	C3B-C4B-NB	-2.41	108.38	110.53
15	A	825	CLA	CHB-C4A-NA	2.41	127.88	124.40
14	a	826	F6C	C4A-C3A-C2A	-2.41	103.39	106.97
14	N	856	F6C	C4A-C3A-C2A	-2.41	103.40	106.97
14	N	856	F6C	C1-C2-C3	-2.41	122.25	126.20
15	N	804	CLA	CHB-C4A-NA	2.41	127.88	124.40
15	N	833	CLA	CHB-C4A-NA	2.41	127.88	124.40
15	a	833	CLA	CHB-C4A-NA	2.41	127.88	124.40
15	a	820	CLA	C1-C2-C3	-2.41	122.25	126.20
14	L	204	F6C	CHB-C4A-C3A	-2.41	120.48	125.49
15	A	810	CLA	CHB-C4A-NA	2.41	127.87	124.40
14	W	201	F6C	CHB-C4A-NA	2.41	128.19	124.80
15	A	832	CLA	CHB-C4A-NA	2.41	127.87	124.40
15	V	103	CLA	CHB-C4A-NA	2.41	127.87	124.40
15	B	828	CLA	CHB-C4A-NA	2.40	127.87	124.40
15	a	810	CLA	CHB-C4A-NA	2.40	127.87	124.40
15	W	202	CLA	CHB-C4A-NA	2.40	127.87	124.40
15	N	810	CLA	CHB-C4A-NA	2.40	127.86	124.40
15	O	830	CLA	CHB-C4A-NA	2.40	127.86	124.40
15	N	813	CLA	C1-C2-C3	-2.40	122.27	126.20
15	N	811	CLA	CHB-C4A-NA	2.40	127.86	124.40
15	b	830	CLA	CHB-C4A-NA	2.40	127.86	124.40
15	O	835	CLA	CHB-C4A-NA	2.40	127.86	124.40
15	B	830	CLA	CHB-C4A-NA	2.40	127.86	124.40
15	B	835	CLA	CHB-C4A-NA	2.40	127.86	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	819	CLA	CHB-C4A-NA	2.40	127.86	124.40
15	O	828	CLA	CHB-C4A-NA	2.40	127.86	124.40
15	O	803	CLA	CHB-C4A-NA	2.39	127.86	124.40
15	b	818	CLA	CHB-C4A-NA	2.39	127.86	124.40
15	O	834	CLA	O2D-CGD-CBD	2.39	115.42	111.23
15	a	819	CLA	CHB-C4A-NA	2.39	127.85	124.40
14	A	856	F6C	OMB-CMB-C2B	-2.39	120.22	125.62
15	B	818	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	A	833	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	B	808	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	L	202	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	N	819	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	B	836	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
15	A	813	CLA	C1-C2-C3	-2.39	122.29	126.20
15	A	840	CLA	C3B-C4B-NB	-2.39	108.40	110.53
15	b	828	CLA	CHB-C4A-NA	2.39	127.84	124.40
15	a	804	CLA	CHB-C4A-NA	2.38	127.84	124.40
15	b	835	CLA	CHB-C4A-NA	2.38	127.84	124.40
15	A	803	CLA	CHB-C4A-NA	2.38	127.84	124.40
15	b	836	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
14	a	855	F6C	C1-C2-C3	-2.38	122.30	126.20
15	b	810	CLA	CHB-C4A-NA	2.38	127.84	124.40
16	O	841	PQN	C11-C3-C4	-2.38	116.07	118.58
15	O	808	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	O	839	F6C	C4A-C3A-C2A	-2.38	103.44	106.97
15	b	816	CLA	CHB-C4A-NA	2.38	127.83	124.40
15	N	831	CLA	CHB-C4A-NA	2.38	127.83	124.40
15	a	831	CLA	CHB-C4A-NA	2.38	127.83	124.40
15	N	810	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
15	a	840	CLA	C3B-C4B-NB	-2.37	108.41	110.53
15	b	831	CLA	CHB-C4A-NA	2.37	127.83	124.40
15	B	826	CLA	C3B-C4B-NB	-2.37	108.41	110.53
15	A	829	CLA	C3B-C4B-NB	-2.37	108.41	110.53
14	A	826	F6C	CHB-C4A-NA	2.37	128.14	124.80
15	b	803	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	O	834	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
15	N	825	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	N	822	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	N	834	CLA	CHB-C4A-NA	2.37	127.82	124.40
13	a	801	CL0	CMD-C2D-C3D	2.37	129.41	124.68
15	O	803	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
15	A	831	CLA	CHB-C4A-NA	2.37	127.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	831	CLA	CHB-C4A-NA	2.37	127.81	124.40
15	N	803	CLA	CHB-C4A-NA	2.37	127.81	124.40
15	O	818	CLA	CHB-C4A-NA	2.36	127.81	124.40
14	B	832	F6C	CBD-CHA-C4D	-2.36	105.88	108.54
18	a	847	BCR	C20-C21-C22	-2.36	123.96	127.28
15	a	840	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	O	826	CLA	C3B-C4B-NB	-2.36	108.42	110.53
15	b	826	CLA	C3B-C4B-NB	-2.36	108.42	110.53
14	A	856	F6C	C4A-C3A-C2A	-2.36	103.47	106.97
13	A	801	CL0	CMD-C2D-C3D	2.36	129.40	124.68
15	O	827	CLA	C1-C2-C3	-2.36	122.33	126.20
15	F	201	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	O	831	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	O	836	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	a	803	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
15	O	810	CLA	CHB-C4A-NA	2.36	127.80	124.40
15	B	803	CLA	CHB-C4A-NA	2.36	127.80	124.40
15	A	810	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
15	A	820	CLA	O2D-CGD-CBD	2.36	115.35	111.23
15	b	808	CLA	CHB-C4A-NA	2.36	127.80	124.40
15	B	810	CLA	CHB-C4A-NA	2.36	127.80	124.40
15	B	817	CLA	C3B-C4B-NB	-2.36	108.43	110.53
15	a	810	CLA	CMB-C2B-C1B	-2.35	121.83	125.42
15	O	816	CLA	CHB-C4A-NA	2.35	127.80	124.40
14	N	826	F6C	CHB-C4A-NA	2.35	128.12	124.80
15	N	803	CLA	CMB-C2B-C1B	-2.35	121.83	125.42
15	N	820	CLA	C1-C2-C3	-2.35	122.34	126.20
15	a	803	CLA	CHB-C4A-NA	2.35	127.80	124.40
13	N	801	CL0	CMD-C2D-C3D	2.35	129.38	124.68
15	N	831	CLA	C3B-C4B-NB	-2.35	108.43	110.53
15	N	819	CLA	C1-C2-C3	-2.35	122.34	126.20
15	O	837	CLA	CHB-C4A-NA	2.35	127.79	124.40
14	b	832	F6C	CBD-CHA-C4D	-2.35	105.89	108.54
14	A	824	F6C	C4A-C3A-C2A	-2.35	103.48	106.97
15	B	837	CLA	CHB-C4A-NA	2.35	127.79	124.40
15	f	201	CLA	CHB-C4A-NA	2.35	127.79	124.40
13	A	801	CL0	C3C-C4C-NC	-2.35	108.91	114.65
14	N	824	F6C	C4A-C3A-C2A	-2.35	103.49	106.97
14	O	832	F6C	CBD-CHA-C4D	-2.35	105.89	108.54
15	A	803	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
14	B	839	F6C	C4A-C3A-C2A	-2.35	103.49	106.97
15	b	837	CLA	CHB-C4A-NA	2.35	127.79	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	839	F6C	C4A-C3A-C2A	-2.35	103.49	106.97
15	a	822	CLA	CHB-C4A-NA	2.35	127.78	124.40
15	O	822	CLA	CHB-C4A-NA	2.34	127.78	124.40
15	A	827	CLA	CHB-C4A-NA	2.34	127.78	124.40
16	b	841	PQN	C11-C3-C4	-2.34	116.11	118.58
15	b	836	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	a	824	F6C	C4A-C3A-C2A	-2.34	103.50	106.97
15	b	824	CLA	CHB-C4A-NA	2.34	127.78	124.40
15	S	201	CLA	CHB-C4A-NA	2.34	127.78	124.40
15	b	827	CLA	C1-C2-C3	-2.34	122.36	126.20
15	B	807	CLA	C3B-C4B-NB	-2.34	108.44	110.53
13	N	801	CL0	C3C-C4C-NC	-2.34	108.94	114.65
15	O	817	CLA	C3B-C4B-NB	-2.34	108.44	110.53
15	b	807	CLA	C3B-C4B-NB	-2.34	108.44	110.53
18	N	845	BCR	C33-C5-C6	2.33	127.03	124.48
14	A	856	F6C	C1-C2-C3	-2.33	122.37	126.20
15	A	834	CLA	CHB-C4A-NA	2.33	127.77	124.40
14	B	832	F6C	C4A-C3A-C2A	-2.33	103.51	106.97
15	a	834	CLA	CHB-C4A-NA	2.33	127.77	124.40
15	a	836	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
13	a	801	CL0	C3C-C4C-NC	-2.33	108.95	114.65
15	a	827	CLA	CHB-C4A-NA	2.33	127.76	124.40
15	B	807	CLA	CHB-C4A-NA	2.33	127.76	124.40
15	b	803	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
15	a	819	CLA	C1-C2-C3	-2.33	122.38	126.20
15	N	835	CLA	CHB-C4A-NA	2.33	127.76	124.40
15	B	836	CLA	CHB-C4A-NA	2.33	127.76	124.40
14	a	802	F6C	C1-C2-C3	-2.32	122.39	126.20
15	N	840	CLA	CHB-C4A-NA	2.32	127.75	124.40
15	L	203	CLA	O2D-CGD-CBD	2.32	115.29	111.23
15	A	838	CLA	CHB-C4A-NA	2.32	127.75	124.40
15	O	838	CLA	CHB-C4A-NA	2.32	127.75	124.40
15	b	834	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
15	N	829	CLA	C3B-C4B-NB	-2.32	108.46	110.53
15	b	817	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	W	204	F6C	C1-C2-C3	-2.32	122.40	126.20
15	a	829	CLA	C3B-C4B-NB	-2.32	108.46	110.53
15	N	827	CLA	CHB-C4A-NA	2.32	127.74	124.40
15	A	822	CLA	CHB-C4A-NA	2.32	127.74	124.40
15	B	817	CLA	CHB-C4A-NA	2.32	127.74	124.40
15	A	820	CLA	C3B-C4B-NB	-2.31	108.46	110.53
15	A	835	CLA	CHB-C4A-NA	2.31	127.74	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	838	CLA	CHB-C4A-NA	2.31	127.73	124.40
15	O	836	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
14	a	826	F6C	CHB-C4A-NA	2.31	128.05	124.80
14	j	204	F6C	C1-C2-C3	-2.31	122.42	126.20
15	a	838	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	O	832	F6C	C4A-C3A-C2A	-2.31	103.55	106.97
14	O	839	F6C	CMB-C2B-C1B	-2.31	122.50	128.37
15	B	834	CLA	CHB-C4A-NA	2.31	127.73	124.40
15	B	826	CLA	CHB-C4A-NA	2.30	127.73	124.40
15	N	830	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
15	O	817	CLA	CHB-C4A-NA	2.30	127.72	124.40
14	b	832	F6C	C4A-C3A-C2A	-2.30	103.56	106.97
15	A	820	CLA	C1-C2-C3	-2.30	122.43	126.20
15	b	838	CLA	CHB-C4A-NA	2.30	127.71	124.40
15	B	827	CLA	C1-C2-C3	-2.29	122.44	126.20
15	N	837	CLA	CHB-C4A-NA	2.29	127.71	124.40
15	b	817	CLA	C3B-C4B-NB	-2.29	108.48	110.53
15	A	840	CLA	CHB-C4A-NA	2.29	127.71	124.40
15	B	838	CLA	CHB-C4A-NA	2.29	127.70	124.40
15	O	807	CLA	CHB-C4A-NA	2.29	127.70	124.40
15	A	819	CLA	C1-C2-C3	-2.29	122.45	126.20
15	N	839	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
15	B	806	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
15	a	833	CLA	CMB-C2B-C3B	2.28	131.92	126.55
15	O	807	CLA	C3B-C4B-NB	-2.28	108.49	110.53
15	b	815	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
15	b	807	CLA	CHB-C4A-NA	2.28	127.69	124.40
15	O	837	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
15	a	835	CLA	O2D-CGD-CBD	2.28	115.21	111.23
18	a	845	BCR	C33-C5-C6	2.28	126.97	124.48
15	A	809	CLA	C1-C2-C3	-2.27	122.47	126.20
14	B	839	F6C	CMB-C2B-C1B	-2.27	122.58	128.37
15	a	835	CLA	CHB-C4A-NA	2.27	127.68	124.40
20	N	853	LMT	O1B-C1B-O5B	2.27	116.68	110.69
15	A	830	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
15	A	829	CLA	CHB-C4A-NA	2.27	127.68	124.40
15	b	826	CLA	CHB-C4A-NA	2.27	127.68	124.40
15	j	203	CLA	O2D-CGD-CBD	2.27	115.20	111.23
15	N	833	CLA	CMB-C2B-C3B	2.27	131.89	126.55
15	N	820	CLA	C3B-C4B-NB	-2.27	108.50	110.53
15	O	821	CLA	C3B-C4B-NB	-2.27	108.50	110.53
15	O	826	CLA	CHB-C4A-NA	2.27	127.68	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	820	CLA	C3B-C4B-NB	-2.27	108.50	110.53
20	a	853	LMT	O1B-C1B-O5B	2.27	116.66	110.69
14	L	204	F6C	C1-C2-C3	-2.27	122.48	126.20
18	b	846	BCR	C15-C16-C17	-2.27	118.88	123.52
15	O	834	CLA	CHB-C4A-NA	2.27	127.67	124.40
15	N	836	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
14	W	204	F6C	CMB-C2B-C1B	-2.27	122.60	128.37
15	A	833	CLA	CMB-C2B-C3B	2.26	131.88	126.55
20	A	853	LMT	O1B-C1B-O5B	2.26	116.65	110.69
16	a	843	PQN	C11-C3-C4	-2.26	116.19	118.58
15	W	203	CLA	O2D-CGD-CBD	2.26	115.19	111.23
15	a	829	CLA	CHB-C4A-NA	2.26	127.67	124.40
14	b	839	F6C	CMB-C2B-C1B	-2.26	122.61	128.37
15	B	808	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
14	L	204	F6C	O2A-CGA-O1A	-2.26	117.98	123.63
15	N	829	CLA	CHB-C4A-NA	2.26	127.66	124.40
15	a	842	CLA	CHB-C4A-NA	2.26	127.66	124.40
15	b	834	CLA	O2D-CGD-CBD	2.26	115.18	111.23
18	N	847	BCR	C20-C21-C22	-2.26	124.11	127.28
15	S	201	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
15	B	837	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
15	O	814	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
15	b	827	CLA	CHB-C4A-NA	2.25	127.65	124.40
15	b	827	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
15	B	829	CLA	C1-C2-C3	-2.25	122.52	126.20
15	O	831	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
15	N	842	CLA	CHB-C4A-NA	2.25	127.64	124.40
15	B	821	CLA	C3B-C4B-NB	-2.24	108.53	110.53
15	b	837	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
15	A	839	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
18	b	846	BCR	C19-C18-C17	-2.24	115.48	119.01
15	A	837	CLA	CHB-C4A-NA	2.24	127.63	124.40
15	a	837	CLA	CHB-C4A-NA	2.24	127.63	124.40
15	a	820	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
14	a	826	F6C	O2A-CGA-O1A	-2.24	118.03	123.63
15	b	818	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
15	N	820	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
18	A	845	BCR	C33-C5-C6	2.24	126.92	124.48
15	A	820	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
15	A	835	CLA	O2D-CGD-CBD	2.23	115.14	111.23
15	B	827	CLA	CHB-C4A-NA	2.23	127.62	124.40
15	B	818	CLA	O2A-CGA-O1A	-2.23	118.04	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	831	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
15	b	831	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
15	N	830	CLA	CHB-C4A-NA	2.23	127.62	124.40
15	b	834	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	A	856	F6C	CHB-C4A-NA	2.23	127.94	124.80
15	A	835	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
15	F	201	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
15	A	830	CLA	CHB-C4A-NA	2.23	127.62	124.40
15	N	820	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
15	O	827	CLA	CHB-C4A-NA	2.23	127.61	124.40
15	O	805	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
15	b	834	CLA	CMB-C2B-C3B	2.23	131.79	126.55
14	j	204	F6C	O2A-CGA-O1A	-2.23	118.06	123.63
15	O	834	CLA	CMB-C2B-C3B	2.22	131.78	126.55
15	j	203	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
15	A	806	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
15	a	827	CLA	O2D-CGD-CBD	2.22	115.11	111.23
15	L	203	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
15	A	842	CLA	CHB-C4A-NA	2.22	127.60	124.40
15	B	814	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
15	a	820	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
15	O	822	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
15	B	809	CLA	CHB-C4A-NA	2.22	127.60	124.40
15	W	203	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
14	j	204	F6C	CMB-C2B-C1B	-2.22	122.72	128.37
15	b	807	CLA	O2D-CGD-CBD	2.22	115.11	111.23
15	b	838	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
14	W	204	F6C	O2A-CGA-O1A	-2.22	118.08	123.63
16	A	843	PQN	C11-C3-C4	-2.22	116.25	118.58
15	O	808	CLA	O2D-CGD-CBD	2.21	115.10	111.23
15	b	808	CLA	O2D-CGD-CBD	2.21	115.10	111.23
15	b	821	CLA	C3B-C4B-NB	-2.21	108.56	110.53
15	a	827	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
15	a	830	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
14	A	824	F6C	CHB-C4A-NA	2.21	127.92	124.80
15	A	822	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
14	N	824	F6C	CHB-C4A-NA	2.21	127.91	124.80
15	B	834	CLA	CMB-C2B-C3B	2.21	131.75	126.55
15	B	838	CLA	C3B-C4B-NB	-2.21	108.56	110.53
14	a	824	F6C	CHB-C4A-NA	2.21	127.91	124.80
13	N	801	CL0	O2A-CGA-O1A	-2.21	118.11	123.63
15	f	201	CLA	O2A-CGA-O1A	-2.21	118.11	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	807	CLA	C1-C2-C3	-2.21	122.58	126.20
15	N	818	CLA	O2D-CGD-CBD	2.21	115.09	111.23
18	O	846	BCR	C15-C16-C17	-2.20	119.01	123.52
13	A	801	CL0	O2A-CGA-O1A	-2.20	118.12	123.63
15	B	805	CLA	C1-C2-C3	-2.20	122.59	126.20
15	a	835	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
15	A	827	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
14	N	856	F6C	O2A-CGA-O1A	-2.20	118.12	123.63
15	N	822	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
15	B	827	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
15	N	835	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
15	a	830	CLA	CHB-C4A-NA	2.20	127.57	124.40
15	b	804	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
15	A	820	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
15	A	838	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
15	B	804	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
18	U	102	BCR	C11-C12-C13	-2.19	120.36	126.36
15	a	823	CLA	C1-C2-C3	-2.19	122.61	126.20
15	O	801	CLA	CHB-C4A-NA	2.19	127.56	124.40
15	B	807	CLA	C1-C2-C3	-2.19	122.61	126.20
15	B	802	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
14	A	856	F6C	O2A-CGA-O1A	-2.19	118.16	123.63
13	a	801	CL0	O2A-CGA-O1A	-2.19	118.16	123.63
15	O	802	CLA	CMB-C2B-C1B	-2.18	122.09	125.42
15	A	839	CLA	C1-C2-C3	-2.18	122.62	126.20
15	O	804	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
15	A	821	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
15	b	802	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
15	a	822	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
15	B	807	CLA	O2D-CGD-CBD	2.18	115.04	111.23
15	N	835	CLA	O2D-CGD-CBD	2.18	115.04	111.23
14	A	826	F6C	CMB-C2B-C1B	-2.18	122.82	128.37
15	N	827	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
14	a	826	F6C	CAC-C3C-C2C	2.18	130.34	126.89
15	B	828	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
15	N	838	CLA	CMB-C2B-C1B	-2.18	122.11	125.42
13	A	801	CL0	CMA-C3A-C4A	-2.18	109.92	114.61
15	b	801	CLA	CHB-C4A-NA	2.18	127.54	124.40
15	B	802	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
14	a	855	F6C	CHB-C4A-NA	2.17	127.86	124.80
14	a	855	F6C	O2A-CGA-O1A	-2.17	118.19	123.63
18	h	102	BCR	C11-C12-C13	-2.17	120.41	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	806	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
14	A	824	F6C	CBD-CHA-C4D	-2.17	106.09	108.54
15	O	805	CLA	C1-C2-C3	-2.17	122.64	126.20
18	U	102	BCR	C12-C13-C14	2.17	122.42	119.01
15	B	828	CLA	CMB-C2B-C3B	2.17	131.65	126.55
15	A	818	CLA	O2D-CGD-CBD	2.17	115.02	111.23
15	B	831	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
15	N	813	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
15	A	813	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
15	a	829	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
14	a	824	F6C	CBD-CHA-C4D	-2.16	106.10	108.54
15	b	838	CLA	C3B-C4B-NB	-2.16	108.60	110.53
15	B	801	CLA	CHB-C4A-NA	2.16	127.52	124.40
14	O	832	F6C	CHB-C4A-NA	2.16	127.85	124.80
18	N	845	BCR	C7-C6-C5	2.16	126.54	121.56
15	a	818	CLA	O2D-CGD-CBD	2.16	115.01	111.23
15	O	818	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
15	O	825	CLA	C1-C2-C3	-2.16	122.65	126.20
15	B	827	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
15	a	813	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
15	A	836	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
15	W	202	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
15	A	829	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
14	L	204	F6C	CMB-C2B-C1B	-2.16	122.87	128.37
15	O	802	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	b	840	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	N	856	F6C	CHB-C4A-NA	2.16	127.84	124.80
15	a	821	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	O	838	CLA	C3B-C4B-NB	-2.16	108.60	110.53
15	B	838	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	b	832	F6C	CHB-C4A-NA	2.16	127.84	124.80
15	N	829	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	O	830	CLA	C1-C2-C3	-2.16	122.66	126.20
15	b	802	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
14	a	855	F6C	CMB-C2B-C1B	-2.16	122.89	128.37
14	b	832	F6C	O2A-CGA-O1A	-2.15	118.24	123.63
14	A	856	F6C	CMB-C2B-C1B	-2.15	122.89	128.37
15	L	202	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
15	O	803	CLA	O1D-CGD-CBD	2.15	128.76	124.52
15	B	825	CLA	C1-C2-C3	-2.15	122.67	126.20
15	a	809	CLA	C1-C2-C3	-2.15	122.67	126.20
14	O	839	F6C	CHB-C4A-NA	2.15	127.83	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	826	F6C	CMB-C2B-C1B	-2.15	122.89	128.37
15	O	827	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
15	b	827	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
15	b	824	CLA	O2D-CGD-CBD	2.15	114.99	111.23
18	h	102	BCR	C12-C13-C14	2.15	122.39	119.01
15	b	822	CLA	C1-C2-C3	-2.15	122.67	126.20
15	b	831	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
14	N	826	F6C	CMB-C2B-C1B	-2.15	122.90	128.37
15	b	821	CLA	C1-C2-C3	-2.15	122.68	126.20
14	B	839	F6C	CHB-C4A-NA	2.15	127.83	124.80
15	N	821	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
15	b	813	CLA	O2D-CGD-CBD	2.15	114.98	111.23
15	N	809	CLA	C1-C2-C3	-2.15	122.68	126.20
15	b	825	CLA	C1-C2-C3	-2.15	122.68	126.20
15	O	838	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
15	B	821	CLA	C1-C2-C3	-2.15	122.68	126.20
15	O	831	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
14	b	839	F6C	CHB-C4A-NA	2.14	127.82	124.80
15	b	838	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
15	W	203	CLA	C1-C2-C3	-2.14	122.68	126.20
15	j	203	CLA	C1-C2-C3	-2.14	122.68	126.20
15	B	824	CLA	O2D-CGD-CBD	2.14	114.98	111.23
18	J	102	BCR	C12-C13-C14	2.14	122.38	119.01
18	a	845	BCR	C7-C6-C5	2.14	126.49	121.56
15	B	838	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
15	B	809	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
15	A	831	CLA	O2D-CGD-CBD	2.14	114.98	111.23
16	N	843	PQN	C11-C3-C4	-2.14	116.32	118.58
15	O	826	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
15	b	828	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
15	N	842	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
15	B	824	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	B	832	F6C	CHB-C4A-NA	2.14	127.82	124.80
15	b	828	CLA	CMB-C2B-C3B	2.14	131.59	126.55
18	A	845	BCR	C7-C6-C5	2.14	126.48	121.56
14	N	856	F6C	CMB-C2B-C1B	-2.14	122.92	128.37
15	O	821	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
15	a	836	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
15	O	809	CLA	CHB-C4A-NA	2.14	127.48	124.40
15	B	815	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
14	N	824	F6C	CBD-CHA-C4D	-2.13	106.13	108.54
15	a	838	CLA	CMB-C2B-C1B	-2.13	122.17	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	824	CLA	O2D-CGD-CBD	2.13	114.96	111.23
15	a	842	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
15	B	801	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
14	O	832	F6C	O2A-CGA-O1A	-2.13	118.29	123.63
15	B	815	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
15	A	836	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
15	O	807	CLA	O2D-CGD-CBD	2.13	114.96	111.23
15	a	812	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
15	A	842	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
15	b	815	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
15	O	840	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
15	O	801	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
18	J	102	BCR	C11-C12-C13	-2.13	120.53	126.36
14	B	832	F6C	O2A-CGA-O1A	-2.13	118.30	123.63
15	a	819	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
15	O	831	CLA	C1-C2-C3	-2.13	122.71	126.20
15	B	826	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
15	B	840	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
15	N	836	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
15	B	810	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
15	N	831	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
15	b	801	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
15	N	815	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
15	a	815	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
15	O	824	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
15	b	824	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
14	L	204	F6C	CBD-CHA-C4D	-2.12	106.15	108.54
15	O	825	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
15	a	827	CLA	C1-C2-C3	-2.12	122.72	126.20
15	b	831	CLA	C1-C2-C3	-2.12	122.72	126.20
15	B	822	CLA	C1-C2-C3	-2.12	122.72	126.20
15	b	826	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
15	i	103	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
15	N	808	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
15	N	827	CLA	C1-C2-C3	-2.12	122.72	126.20
15	A	803	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	b	825	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	a	831	CLA	O2D-CGD-CBD	2.12	114.93	111.23
15	N	825	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	O	810	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	O	828	CLA	CMB-C2B-C3B	2.12	131.53	126.55
15	Z	102	CLA	O2A-CGA-O1A	-2.12	118.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	j	204	F6C	CHB-C4A-NA	2.12	127.78	124.80
15	L	203	CLA	C1-C2-C3	-2.12	122.73	126.20
15	A	815	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	O	815	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	O	830	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	b	810	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	a	825	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
15	B	825	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
15	N	831	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
15	A	825	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
15	a	831	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
15	a	803	CLA	CMB-C2B-C3B	2.11	131.52	126.55
15	V	103	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
15	A	827	CLA	C1-C2-C3	-2.11	122.74	126.20
15	O	828	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
15	b	836	CLA	CMB-C2B-C3B	2.11	131.51	126.55
15	A	831	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
15	O	827	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
15	O	829	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
15	O	829	CLA	C1-C2-C3	-2.11	122.74	126.20
18	B	846	BCR	C15-C16-C17	-2.11	119.21	123.52
15	A	837	CLA	O2D-CGD-CBD	2.11	114.91	111.23
14	W	204	F6C	CHB-C4A-NA	2.11	127.77	124.80
15	B	833	CLA	C1-C2-C3	-2.11	122.75	126.20
15	A	803	CLA	C1-C2-C3	-2.11	122.75	126.20
14	b	832	F6C	C1-C2-C3	-2.11	122.75	126.20
15	X	102	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
15	b	809	CLA	CHB-C4A-NA	2.10	127.44	124.40
15	A	803	CLA	CMB-C2B-C3B	2.10	131.50	126.55
15	B	836	CLA	CMB-C2B-C3B	2.10	131.50	126.55
15	N	819	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
15	N	807	CLA	C1-C2-C3	-2.10	122.75	126.20
15	B	837	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
15	l	102	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
15	A	814	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
15	b	829	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
15	A	819	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
15	N	827	CLA	O2D-CGD-CBD	2.10	114.90	111.23
15	A	840	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
15	B	830	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
15	a	839	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
15	B	833	CLA	O2A-CGA-O1A	-2.10	118.38	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	803	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
15	B	821	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
15	b	803	CLA	O1D-CGD-CBD	2.10	128.66	124.52
15	b	836	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
15	N	810	CLA	CMB-C2B-C3B	2.10	131.48	126.55
15	N	812	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
15	N	803	CLA	CMB-C2B-C3B	2.09	131.48	126.55
15	b	830	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
15	b	828	CLA	C1-C2-C3	-2.09	122.77	126.20
15	a	807	CLA	C1-C2-C3	-2.09	122.77	126.20
15	A	812	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
15	A	807	CLA	C1-C2-C3	-2.09	122.77	126.20
15	B	829	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
15	a	840	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
15	O	809	CLA	C1-C2-C3	-2.09	122.77	126.20
14	O	839	F6C	O2A-CGA-O1A	-2.09	118.40	123.63
15	N	814	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
14	A	802	F6C	CHB-C4A-C3A	-2.09	121.14	125.49
15	B	815	CLA	C1-C2-C3	-2.09	122.77	126.20
15	N	837	CLA	C1-C2-C3	-2.09	122.77	126.20
15	b	807	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
15	A	808	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
15	b	833	CLA	C1-C2-C3	-2.09	122.78	126.20
14	b	839	F6C	CBD-CHA-C4D	-2.09	106.19	108.54
14	j	204	F6C	CBD-CHA-C4D	-2.09	106.19	108.54
15	b	821	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
15	j	202	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
15	a	810	CLA	CMB-C2B-C3B	2.08	131.45	126.55
15	B	807	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
15	b	837	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
15	O	822	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
15	a	814	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
14	b	839	F6C	O2A-CGA-O1A	-2.08	118.42	123.63
15	B	836	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
15	B	828	CLA	C1-C2-C3	-2.08	122.79	126.20
15	N	840	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
15	O	837	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
15	B	831	CLA	C1-C2-C3	-2.08	122.79	126.20
15	K	103	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
14	O	832	F6C	CMB-C2B-C1B	-2.08	123.08	128.37
15	O	819	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
15	A	810	CLA	CMB-C2B-C3B	2.08	131.44	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	837	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
15	B	808	CLA	CMB-C2B-C3B	2.08	131.44	126.55
15	O	813	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
15	a	806	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
15	b	807	CLA	C1-C2-C3	-2.08	122.79	126.20
15	a	832	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
15	b	809	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
18	F	202	BCR	C24-C23-C22	-2.08	123.16	126.23
14	B	839	F6C	O2A-CGA-O1A	-2.08	118.44	123.63
15	N	803	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
15	b	814	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
15	A	837	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	b	819	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	N	807	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	N	837	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	b	836	CLA	C1-C2-C3	-2.07	122.80	126.20
15	B	819	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	O	836	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
15	B	803	CLA	O1D-CGD-CBD	2.07	128.60	124.52
15	O	833	CLA	C1-C2-C3	-2.07	122.80	126.20
15	A	832	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
15	O	816	CLA	CHB-C1B-NB	2.07	127.15	124.05
15	O	807	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
15	N	830	CLA	CMB-C2B-C3B	2.07	131.42	126.55
15	A	830	CLA	CMB-C2B-C3B	2.07	131.42	126.55
15	B	830	CLA	C1-C2-C3	-2.07	122.81	126.20
15	O	815	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
15	a	813	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
14	O	839	F6C	CBD-CHA-C4D	-2.07	106.21	108.54
15	O	802	CLA	CMB-C2B-C3B	2.07	131.41	126.55
15	a	837	CLA	C1-C2-C3	-2.07	122.81	126.20
14	W	204	F6C	CBD-CHA-C4D	-2.07	106.21	108.54
15	B	813	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
15	O	838	CLA	C1-C2-C3	-2.07	122.81	126.20
15	b	819	CLA	C1-C2-C3	-2.07	122.81	126.20
15	O	837	CLA	CMB-C2B-C3B	2.07	131.41	126.55
15	N	832	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
15	b	833	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
15	b	830	CLA	C1-C2-C3	-2.07	122.81	126.20
15	B	809	CLA	CAA-CBA-CGA	-2.07	107.34	113.21
15	b	815	CLA	C1-C2-C3	-2.07	122.81	126.20
15	B	802	CLA	CMB-C2B-C3B	2.07	131.41	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	838	CLA	CMB-C2B-C3B	2.06	131.41	126.55
15	O	815	CLA	C1-C2-C3	-2.06	122.81	126.20
15	O	836	CLA	CMB-C2B-C3B	2.06	131.41	126.55
15	b	838	CLA	C1-C2-C3	-2.06	122.82	126.20
15	b	802	CLA	CMB-C2B-C3B	2.06	131.40	126.55
15	N	842	CLA	C1-C2-C3	-2.06	122.82	126.20
15	b	821	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
15	b	813	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
15	B	819	CLA	C1-C2-C3	-2.06	122.82	126.20
15	j	202	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
15	b	808	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
15	a	842	CLA	C1-C2-C3	-2.06	122.82	126.20
15	L	202	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
15	a	837	CLA	O2D-CGD-CBD	2.06	114.83	111.23
15	b	829	CLA	C1-C2-C3	-2.06	122.83	126.20
15	B	812	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
15	B	816	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
15	b	822	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
15	A	837	CLA	C1-C2-C3	-2.06	122.83	126.20
15	N	827	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
15	b	805	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
15	a	830	CLA	C1-C2-C3	-2.05	122.83	126.20
15	b	803	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
15	b	805	CLA	C1-C2-C3	-2.05	122.83	126.20
15	l	102	CLA	C1-C2-C3	-2.05	122.83	126.20
15	B	822	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
15	N	813	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
15	W	202	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
15	B	821	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
15	a	807	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
15	a	811	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
15	b	815	CLA	CMB-C2B-C3B	2.05	131.37	126.55
15	A	830	CLA	C1-C2-C3	-2.05	122.84	126.20
15	b	801	CLA	C1-C2-C3	-2.05	122.84	126.20
14	A	826	F6C	CAC-C3C-C2C	2.05	130.13	126.89
15	O	809	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
15	j	202	CLA	C1-C2-C3	-2.05	122.84	126.20
15	O	812	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
14	a	826	F6C	O2D-CGD-CBD	2.05	114.81	111.23
15	O	833	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
15	A	808	CLA	O2A-CGA-O1A	-2.05	118.06	123.33
15	O	821	CLA	O2A-CGA-O1A	-2.05	118.51	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	837	CLA	CMB-C2B-C3B	2.05	131.37	126.55
14	O	832	F6C	O2D-CGD-CBD	2.05	114.81	111.23
15	N	831	CLA	O2D-CGD-CBD	2.05	114.81	111.23
15	A	842	CLA	C1-C2-C3	-2.05	122.85	126.20
15	B	806	CLA	CMB-C2B-C3B	2.04	131.36	126.55
15	B	837	CLA	CMB-C2B-C3B	2.04	131.36	126.55
15	B	805	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
15	B	824	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
15	b	824	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
14	B	832	F6C	C1-C2-C3	-2.04	122.85	126.20
15	N	811	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
15	b	812	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
15	O	802	CLA	C3B-C4B-NB	-2.04	108.71	110.53
14	b	832	F6C	O2D-CGD-CBD	2.04	114.80	111.23
15	A	815	CLA	C1-C2-C3	-2.04	122.85	126.20
15	A	827	CLA	O2D-CGD-CBD	2.04	114.80	111.23
15	A	823	CLA	C1-C2-C3	-2.04	122.86	126.20
15	a	823	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
15	A	811	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
15	O	803	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	O	832	F6C	C1-C2-C3	-2.04	122.86	126.20
15	O	806	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
14	b	832	F6C	CMB-C2B-C1B	-2.04	123.19	128.37
15	a	815	CLA	C1-C2-C3	-2.04	122.86	126.20
18	U	102	BCR	C10-C11-C12	2.04	129.10	123.20
14	a	802	F6C	CHB-C4A-C3A	-2.04	121.25	125.49
15	N	809	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
15	X	102	CLA	C1-C2-C3	-2.04	122.86	126.20
15	B	838	CLA	C1-C2-C3	-2.03	122.86	126.20
15	a	836	CLA	CMB-C2B-C3B	2.03	131.34	126.55
14	N	802	F6C	CHB-C4A-C3A	-2.03	121.26	125.49
18	O	846	BCR	C15-C14-C13	-2.03	124.43	127.28
15	A	823	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
15	a	809	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
15	N	808	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
15	A	807	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
15	a	808	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
15	N	828	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
15	O	819	CLA	C1-C2-C3	-2.03	122.87	126.20
15	a	830	CLA	CMB-C2B-C3B	2.03	131.33	126.55
15	b	816	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
15	A	813	CLA	CMB-C2B-C1B	-2.03	122.33	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	827	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
15	N	821	CLA	C1-C2-C3	-2.03	122.87	126.20
15	O	801	CLA	C1-C2-C3	-2.03	122.87	126.20
14	j	201	F6C	CMB-C2B-C1B	-2.03	123.21	128.37
15	O	816	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
14	N	824	F6C	O2A-CGA-O1A	-2.03	118.56	123.63
15	O	821	CLA	CMB-C2B-C3B	2.03	131.32	126.55
15	A	821	CLA	C1-C2-C3	-2.03	122.88	126.20
15	O	828	CLA	C1-C2-C3	-2.03	122.88	126.20
15	O	831	CLA	CMB-C2B-C3B	2.03	131.32	126.55
18	J	102	BCR	C10-C11-C12	2.03	129.07	123.20
15	O	814	CLA	CMB-C2B-C3B	2.03	131.31	126.55
15	a	828	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
14	a	824	F6C	O2A-CGA-O1A	-2.02	118.57	123.63
14	A	824	F6C	O2A-CGA-O1A	-2.02	118.57	123.63
15	N	823	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
15	Z	102	CLA	C1-C2-C3	-2.02	122.89	126.20
15	a	808	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
15	B	803	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
15	a	837	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
15	B	802	CLA	C3B-C4B-NB	-2.02	108.73	110.53
15	b	809	CLA	C1-C2-C3	-2.02	122.89	126.20
14	B	832	F6C	CMB-C2B-C1B	-2.02	123.23	128.37
15	a	841	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
15	A	809	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
15	A	837	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
15	O	808	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
15	A	806	CLA	CMB-C2B-C3B	2.02	131.29	126.55
18	J	102	BCR	C8-C9-C10	2.02	122.18	119.01
15	A	841	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
15	b	827	CLA	CMB-C2B-C3B	2.02	131.29	126.55
15	b	831	CLA	CMB-C2B-C3B	2.02	131.29	126.55
18	h	102	BCR	C10-C11-C12	2.02	129.04	123.20
15	O	805	CLA	CMB-C2B-C3B	2.01	131.29	126.55
15	B	805	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
14	A	802	F6C	O2A-CGA-O1A	-2.01	118.59	123.63
15	B	831	CLA	CMB-C2B-C3B	2.01	131.29	126.55
15	B	825	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
15	B	836	CLA	C1-C2-C3	-2.01	122.90	126.20
15	B	838	CLA	CMB-C2B-C3B	2.01	131.28	126.55
15	N	841	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
15	O	803	CLA	C1-C2-C3	-2.01	122.91	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	801	CLA	O1D-CGD-CBD	2.01	128.48	124.52
15	B	815	CLA	O2D-CGD-CBD	2.01	114.74	111.23
15	O	824	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
15	b	802	CLA	C3B-C4B-NB	-2.01	108.74	110.53
15	a	818	CLA	CBA-CAA-C2A	2.01	119.77	113.79
14	B	832	F6C	O2D-CGD-CBD	2.01	114.74	111.23
15	N	837	CLA	CMB-C2B-C1B	-2.01	122.37	125.42
15	a	821	CLA	C1-C2-C3	-2.00	122.91	126.20
14	B	839	F6C	CBD-CHA-C4D	-2.00	106.28	108.54
15	L	202	CLA	C1-C2-C3	-2.00	122.92	126.20
15	A	805	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	O	805	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	b	803	CLA	C1-C2-C3	-2.00	122.92	126.20
15	b	805	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	B	814	CLA	CMB-C2B-C3B	2.00	131.25	126.55

All (276) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NC
13	A	801	CL0	NA
13	A	801	CL0	ND
13	N	801	CL0	NC
13	N	801	CL0	NA
13	N	801	CL0	ND
13	a	801	CL0	NC
13	a	801	CL0	NA
13	a	801	CL0	ND
14	A	802	F6C	NA
14	A	824	F6C	NA
14	A	826	F6C	NA
14	A	856	F6C	NA
14	B	832	F6C	NA
14	B	839	F6C	NA
14	L	201	F6C	NA
14	L	204	F6C	NA
14	N	802	F6C	NA
14	N	824	F6C	NA
14	N	826	F6C	NA
14	N	856	F6C	NA
14	O	832	F6C	NA
14	O	839	F6C	NA

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Mol	Chain	Res	Type	Atom
14	W	201	F6C	NA
14	W	204	F6C	NA
14	a	802	F6C	NA
14	a	824	F6C	NA
14	a	826	F6C	NA
14	a	855	F6C	NA
14	b	832	F6C	NA
14	b	839	F6C	NA
14	j	201	F6C	NA
14	j	204	F6C	NA
15	A	803	CLA	ND
15	A	804	CLA	ND
15	A	805	CLA	ND
15	A	806	CLA	ND
15	A	807	CLA	ND
15	A	808	CLA	ND
15	A	809	CLA	ND
15	A	810	CLA	ND
15	A	811	CLA	ND
15	A	812	CLA	ND
15	A	813	CLA	ND
15	A	814	CLA	ND
15	A	815	CLA	ND
15	A	816	CLA	ND
15	A	817	CLA	ND
15	A	818	CLA	ND
15	A	819	CLA	ND
15	A	820	CLA	ND
15	A	821	CLA	ND
15	A	822	CLA	ND
15	A	823	CLA	ND
15	A	825	CLA	ND
15	A	827	CLA	ND
15	A	828	CLA	ND
15	A	829	CLA	ND
15	A	830	CLA	ND
15	A	831	CLA	ND
15	A	832	CLA	ND
15	A	833	CLA	ND
15	A	834	CLA	ND
15	A	835	CLA	ND
15	A	836	CLA	ND

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Mol	Chain	Res	Type	Atom
15	A	837	CLA	ND
15	A	838	CLA	ND
15	A	839	CLA	ND
15	A	840	CLA	ND
15	A	841	CLA	ND
15	A	842	CLA	ND
15	B	801	CLA	ND
15	B	802	CLA	ND
15	B	803	CLA	ND
15	B	804	CLA	ND
15	B	805	CLA	ND
15	B	806	CLA	ND
15	B	807	CLA	ND
15	B	808	CLA	ND
15	B	809	CLA	ND
15	B	810	CLA	ND
15	B	811	CLA	ND
15	B	813	CLA	ND
15	B	814	CLA	ND
15	B	815	CLA	ND
15	B	816	CLA	ND
15	B	817	CLA	ND
15	B	818	CLA	ND
15	B	819	CLA	ND
15	B	820	CLA	ND
15	B	821	CLA	ND
15	B	822	CLA	ND
15	B	823	CLA	ND
15	B	824	CLA	ND
15	B	825	CLA	ND
15	B	826	CLA	ND
15	B	827	CLA	ND
15	B	828	CLA	ND
15	B	829	CLA	ND
15	B	830	CLA	ND
15	B	831	CLA	ND
15	B	833	CLA	ND
15	B	834	CLA	ND
15	B	835	CLA	ND
15	B	836	CLA	ND
15	B	837	CLA	ND
15	B	838	CLA	ND

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Mol	Chain	Res	Type	Atom
15	B	840	CLA	ND
15	F	201	CLA	ND
15	K	102	CLA	ND
15	K	103	CLA	ND
15	L	202	CLA	ND
15	L	203	CLA	ND
15	X	102	CLA	ND
15	N	803	CLA	ND
15	N	804	CLA	ND
15	N	805	CLA	ND
15	N	806	CLA	ND
15	N	807	CLA	ND
15	N	808	CLA	ND
15	N	809	CLA	ND
15	N	810	CLA	ND
15	N	811	CLA	ND
15	N	812	CLA	ND
15	N	813	CLA	ND
15	N	814	CLA	ND
15	N	815	CLA	ND
15	N	816	CLA	ND
15	N	817	CLA	ND
15	N	818	CLA	ND
15	N	819	CLA	ND
15	N	820	CLA	ND
15	N	821	CLA	ND
15	N	822	CLA	ND
15	N	823	CLA	ND
15	N	825	CLA	ND
15	N	827	CLA	ND
15	N	828	CLA	ND
15	N	829	CLA	ND
15	N	830	CLA	ND
15	N	831	CLA	ND
15	N	832	CLA	ND
15	N	833	CLA	ND
15	N	834	CLA	ND
15	N	835	CLA	ND
15	N	836	CLA	ND
15	N	837	CLA	ND
15	N	838	CLA	ND
15	N	839	CLA	ND

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Mol	Chain	Res	Type	Atom
15	N	840	CLA	ND
15	N	841	CLA	ND
15	N	842	CLA	ND
15	O	801	CLA	ND
15	O	802	CLA	ND
15	O	803	CLA	ND
15	O	804	CLA	ND
15	O	805	CLA	ND
15	O	806	CLA	ND
15	O	807	CLA	ND
15	O	808	CLA	ND
15	O	809	CLA	ND
15	O	810	CLA	ND
15	O	811	CLA	ND
15	O	813	CLA	ND
15	O	814	CLA	ND
15	O	815	CLA	ND
15	O	816	CLA	ND
15	O	817	CLA	ND
15	O	818	CLA	ND
15	O	819	CLA	ND
15	O	820	CLA	ND
15	O	821	CLA	ND
15	O	822	CLA	ND
15	O	823	CLA	ND
15	O	824	CLA	ND
15	O	825	CLA	ND
15	O	826	CLA	ND
15	O	827	CLA	ND
15	O	828	CLA	ND
15	O	829	CLA	ND
15	O	830	CLA	ND
15	O	831	CLA	ND
15	O	833	CLA	ND
15	O	834	CLA	ND
15	O	835	CLA	ND
15	O	836	CLA	ND
15	O	837	CLA	ND
15	O	838	CLA	ND
15	O	840	CLA	ND
15	S	201	CLA	ND
15	V	102	CLA	ND

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Mol	Chain	Res	Type	Atom
15	V	103	CLA	ND
15	W	202	CLA	ND
15	W	203	CLA	ND
15	Z	102	CLA	ND
15	a	803	CLA	ND
15	a	804	CLA	ND
15	a	805	CLA	ND
15	a	806	CLA	ND
15	a	807	CLA	ND
15	a	808	CLA	ND
15	a	809	CLA	ND
15	a	810	CLA	ND
15	a	811	CLA	ND
15	a	812	CLA	ND
15	a	813	CLA	ND
15	a	814	CLA	ND
15	a	815	CLA	ND
15	a	816	CLA	ND
15	a	817	CLA	ND
15	a	818	CLA	ND
15	a	819	CLA	ND
15	a	820	CLA	ND
15	a	821	CLA	ND
15	a	822	CLA	ND
15	a	823	CLA	ND
15	a	825	CLA	ND
15	a	827	CLA	ND
15	a	828	CLA	ND
15	a	829	CLA	ND
15	a	830	CLA	ND
15	a	831	CLA	ND
15	a	832	CLA	ND
15	a	833	CLA	ND
15	a	834	CLA	ND
15	a	835	CLA	ND
15	a	836	CLA	ND
15	a	837	CLA	ND
15	a	838	CLA	ND
15	a	839	CLA	ND
15	a	840	CLA	ND
15	a	841	CLA	ND
15	a	842	CLA	ND

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Mol	Chain	Res	Type	Atom
15	b	801	CLA	ND
15	b	802	CLA	ND
15	b	803	CLA	ND
15	b	804	CLA	ND
15	b	805	CLA	ND
15	b	806	CLA	ND
15	b	807	CLA	ND
15	b	808	CLA	ND
15	b	809	CLA	ND
15	b	810	CLA	ND
15	b	811	CLA	ND
15	b	813	CLA	ND
15	b	814	CLA	ND
15	b	815	CLA	ND
15	b	816	CLA	ND
15	b	817	CLA	ND
15	b	818	CLA	ND
15	b	819	CLA	ND
15	b	820	CLA	ND
15	b	821	CLA	ND
15	b	822	CLA	ND
15	b	823	CLA	ND
15	b	824	CLA	ND
15	b	825	CLA	ND
15	b	826	CLA	ND
15	b	827	CLA	ND
15	b	828	CLA	ND
15	b	829	CLA	ND
15	b	830	CLA	ND
15	b	831	CLA	ND
15	b	833	CLA	ND
15	b	834	CLA	ND
15	b	835	CLA	ND
15	b	836	CLA	ND
15	b	837	CLA	ND
15	b	838	CLA	ND
15	b	840	CLA	ND
15	f	201	CLA	ND
15	i	102	CLA	ND
15	i	103	CLA	ND
15	j	202	CLA	ND
15	j	203	CLA	ND

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Mol	Chain	Res	Type	Atom
15	1	102	CLA	ND

All (3325) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	F6C	C1B-C2B-CMB-OMB
14	A	802	F6C	C3B-C2B-CMB-OMB
14	A	824	F6C	C1B-C2B-CMB-OMB
14	A	824	F6C	C3B-C2B-CMB-OMB
14	A	826	F6C	CHA-CBD-CGD-O2D
14	A	826	F6C	C3B-C2B-CMB-OMB
14	A	856	F6C	C1B-C2B-CMB-OMB
14	A	856	F6C	C3B-C2B-CMB-OMB
14	B	832	F6C	CHA-CBD-CGD-O1D
14	B	832	F6C	CHA-CBD-CGD-O2D
14	B	839	F6C	C1B-C2B-CMB-OMB
14	B	839	F6C	C3B-C2B-CMB-OMB
14	L	201	F6C	C1B-C2B-CMB-OMB
14	L	201	F6C	C3B-C2B-CMB-OMB
14	L	204	F6C	CBA-CGA-O2A-C1
14	L	204	F6C	O1A-CGA-O2A-C1
14	L	204	F6C	C1B-C2B-CMB-OMB
14	L	204	F6C	C3B-C2B-CMB-OMB
14	N	802	F6C	C1B-C2B-CMB-OMB
14	N	802	F6C	C3B-C2B-CMB-OMB
14	N	824	F6C	C1B-C2B-CMB-OMB
14	N	824	F6C	C3B-C2B-CMB-OMB
14	N	826	F6C	CHA-CBD-CGD-O2D
14	N	826	F6C	C3B-C2B-CMB-OMB
14	N	856	F6C	C1B-C2B-CMB-OMB
14	O	832	F6C	CHA-CBD-CGD-O1D
14	O	832	F6C	CHA-CBD-CGD-O2D
14	O	832	F6C	C3B-C2B-CMB-OMB
14	O	839	F6C	C1B-C2B-CMB-OMB
14	O	839	F6C	C3B-C2B-CMB-OMB
14	W	201	F6C	C1B-C2B-CMB-OMB
14	W	201	F6C	C3B-C2B-CMB-OMB
14	W	204	F6C	C1A-C2A-CAA-CBA
14	W	204	F6C	CBA-CGA-O2A-C1
14	W	204	F6C	O1A-CGA-O2A-C1
14	W	204	F6C	C1B-C2B-CMB-OMB
14	W	204	F6C	C3B-C2B-CMB-OMB

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Mol	Chain	Res	Type	Atoms
14	W	204	F6C	C2-C3-C5-C6
14	W	204	F6C	C4-C3-C5-C6
14	a	802	F6C	C1B-C2B-CMB-OMB
14	a	802	F6C	C3B-C2B-CMB-OMB
14	a	824	F6C	C1B-C2B-CMB-OMB
14	a	824	F6C	C3B-C2B-CMB-OMB
14	a	826	F6C	CHA-CBD-CGD-O1D
14	a	826	F6C	CHA-CBD-CGD-O2D
14	a	826	F6C	C3B-C2B-CMB-OMB
14	a	855	F6C	C2A-CAA-CBA-CGA
14	a	855	F6C	C1B-C2B-CMB-OMB
14	b	832	F6C	CHA-CBD-CGD-O1D
14	b	832	F6C	CHA-CBD-CGD-O2D
14	b	839	F6C	C1B-C2B-CMB-OMB
14	b	839	F6C	C3B-C2B-CMB-OMB
14	j	201	F6C	C1B-C2B-CMB-OMB
14	j	201	F6C	C3B-C2B-CMB-OMB
14	j	204	F6C	CBA-CGA-O2A-C1
14	j	204	F6C	O1A-CGA-O2A-C1
14	j	204	F6C	C1B-C2B-CMB-OMB
14	j	204	F6C	C3B-C2B-CMB-OMB
14	j	204	F6C	C2-C3-C5-C6
14	j	204	F6C	C4-C3-C5-C6
15	A	803	CLA	C3A-C2A-CAA-CBA
15	A	805	CLA	C3A-C2A-CAA-CBA
15	A	806	CLA	C1A-C2A-CAA-CBA
15	A	806	CLA	C3A-C2A-CAA-CBA
15	A	806	CLA	CAD-CBD-CGD-O1D
15	A	806	CLA	CAD-CBD-CGD-O2D
15	A	809	CLA	C3A-C2A-CAA-CBA
15	A	809	CLA	CHA-CBD-CGD-O1D
15	A	809	CLA	CHA-CBD-CGD-O2D
15	A	810	CLA	C1A-C2A-CAA-CBA
15	A	811	CLA	CAD-CBD-CGD-O1D
15	A	811	CLA	CAD-CBD-CGD-O2D
15	A	811	CLA	CBD-CGD-O2D-CED
15	A	811	CLA	C6-C7-C8-C9
15	A	812	CLA	C1A-C2A-CAA-CBA
15	A	815	CLA	C1A-C2A-CAA-CBA
15	A	818	CLA	C1A-C2A-CAA-CBA
15	A	818	CLA	C3A-C2A-CAA-CBA
15	A	818	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	A	818	CLA	CHA-CBD-CGD-O2D
15	A	819	CLA	C3A-C2A-CAA-CBA
15	A	820	CLA	C1A-C2A-CAA-CBA
15	A	820	CLA	C3A-C2A-CAA-CBA
15	A	825	CLA	C4-C3-C5-C6
15	A	831	CLA	CHA-CBD-CGD-O1D
15	A	831	CLA	CHA-CBD-CGD-O2D
15	A	837	CLA	CBD-CGD-O2D-CED
15	A	841	CLA	C1A-C2A-CAA-CBA
15	A	841	CLA	C4B-C3B-CAB-CBB
15	A	842	CLA	C1A-C2A-CAA-CBA
15	B	802	CLA	CAD-CBD-CGD-O1D
15	B	802	CLA	CAD-CBD-CGD-O2D
15	B	805	CLA	C3A-C2A-CAA-CBA
15	B	806	CLA	CHA-CBD-CGD-O1D
15	B	806	CLA	CHA-CBD-CGD-O2D
15	B	806	CLA	CBD-CGD-O2D-CED
15	B	808	CLA	CHA-CBD-CGD-O1D
15	B	808	CLA	CHA-CBD-CGD-O2D
15	B	809	CLA	C1A-C2A-CAA-CBA
15	B	809	CLA	C3A-C2A-CAA-CBA
15	B	810	CLA	C12-C13-C15-C16
15	B	814	CLA	CHA-CBD-CGD-O1D
15	B	814	CLA	CHA-CBD-CGD-O2D
15	B	815	CLA	CHA-CBD-CGD-O1D
15	B	815	CLA	CHA-CBD-CGD-O2D
15	B	816	CLA	C3A-C2A-CAA-CBA
15	B	817	CLA	C1A-C2A-CAA-CBA
15	B	817	CLA	C3A-C2A-CAA-CBA
15	B	818	CLA	C2B-C3B-CAB-CBB
15	B	818	CLA	C4B-C3B-CAB-CBB
15	B	819	CLA	C1A-C2A-CAA-CBA
15	B	819	CLA	C3A-C2A-CAA-CBA
15	B	823	CLA	CHA-CBD-CGD-O1D
15	B	823	CLA	CHA-CBD-CGD-O2D
15	B	824	CLA	CHA-CBD-CGD-O1D
15	B	824	CLA	CHA-CBD-CGD-O2D
15	B	826	CLA	CBD-CGD-O2D-CED
15	B	827	CLA	C1A-C2A-CAA-CBA
15	B	827	CLA	C3A-C2A-CAA-CBA
15	B	828	CLA	C4-C3-C5-C6
15	B	829	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	B	834	CLA	C1A-C2A-CAA-CBA
15	B	835	CLA	CAD-CBD-CGD-O1D
15	B	835	CLA	CAD-CBD-CGD-O2D
15	K	102	CLA	C1A-C2A-CAA-CBA
15	K	102	CLA	C3A-C2A-CAA-CBA
15	L	203	CLA	C2B-C3B-CAB-CBB
15	L	203	CLA	C4B-C3B-CAB-CBB
15	N	803	CLA	C3A-C2A-CAA-CBA
15	N	805	CLA	C3A-C2A-CAA-CBA
15	N	806	CLA	C1A-C2A-CAA-CBA
15	N	806	CLA	C3A-C2A-CAA-CBA
15	N	806	CLA	CAD-CBD-CGD-O1D
15	N	806	CLA	CAD-CBD-CGD-O2D
15	N	806	CLA	CBD-CGD-O2D-CED
15	N	809	CLA	C3A-C2A-CAA-CBA
15	N	809	CLA	CHA-CBD-CGD-O1D
15	N	809	CLA	CHA-CBD-CGD-O2D
15	N	810	CLA	C1A-C2A-CAA-CBA
15	N	811	CLA	CAD-CBD-CGD-O1D
15	N	811	CLA	CAD-CBD-CGD-O2D
15	N	811	CLA	CBD-CGD-O2D-CED
15	N	812	CLA	C1A-C2A-CAA-CBA
15	N	818	CLA	C1A-C2A-CAA-CBA
15	N	818	CLA	C3A-C2A-CAA-CBA
15	N	818	CLA	CHA-CBD-CGD-O1D
15	N	818	CLA	CHA-CBD-CGD-O2D
15	N	819	CLA	C3A-C2A-CAA-CBA
15	N	820	CLA	C1A-C2A-CAA-CBA
15	N	820	CLA	C3A-C2A-CAA-CBA
15	N	822	CLA	C2-C3-C5-C6
15	N	822	CLA	C4-C3-C5-C6
15	N	825	CLA	C2-C3-C5-C6
15	N	825	CLA	C4-C3-C5-C6
15	N	831	CLA	CHA-CBD-CGD-O1D
15	N	831	CLA	CHA-CBD-CGD-O2D
15	N	837	CLA	CBD-CGD-O2D-CED
15	N	841	CLA	C1A-C2A-CAA-CBA
15	N	841	CLA	C4B-C3B-CAB-CBB
15	N	842	CLA	C1A-C2A-CAA-CBA
15	O	802	CLA	CAD-CBD-CGD-O2D
15	O	805	CLA	C3A-C2A-CAA-CBA
15	O	806	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	O	806	CLA	CHA-CBD-CGD-O2D
15	O	806	CLA	CBD-CGD-O2D-CED
15	O	808	CLA	CHA-CBD-CGD-O1D
15	O	808	CLA	CHA-CBD-CGD-O2D
15	O	809	CLA	C1A-C2A-CAA-CBA
15	O	809	CLA	C3A-C2A-CAA-CBA
15	O	810	CLA	C12-C13-C15-C16
15	O	814	CLA	CHA-CBD-CGD-O1D
15	O	814	CLA	CHA-CBD-CGD-O2D
15	O	815	CLA	CHA-CBD-CGD-O1D
15	O	815	CLA	CHA-CBD-CGD-O2D
15	O	816	CLA	C3A-C2A-CAA-CBA
15	O	817	CLA	C1A-C2A-CAA-CBA
15	O	817	CLA	C3A-C2A-CAA-CBA
15	O	818	CLA	C2B-C3B-CAB-CBB
15	O	818	CLA	C4B-C3B-CAB-CBB
15	O	819	CLA	C1A-C2A-CAA-CBA
15	O	819	CLA	C3A-C2A-CAA-CBA
15	O	823	CLA	CHA-CBD-CGD-O1D
15	O	823	CLA	CHA-CBD-CGD-O2D
15	O	824	CLA	CHA-CBD-CGD-O1D
15	O	824	CLA	CHA-CBD-CGD-O2D
15	O	824	CLA	C4-C3-C5-C6
15	O	826	CLA	CBD-CGD-O2D-CED
15	O	827	CLA	C1A-C2A-CAA-CBA
15	O	827	CLA	C3A-C2A-CAA-CBA
15	O	829	CLA	CBD-CGD-O2D-CED
15	O	834	CLA	C1A-C2A-CAA-CBA
15	O	834	CLA	CBD-CGD-O2D-CED
15	O	835	CLA	CAD-CBD-CGD-O1D
15	O	835	CLA	CAD-CBD-CGD-O2D
15	V	102	CLA	C1A-C2A-CAA-CBA
15	V	102	CLA	C3A-C2A-CAA-CBA
15	W	203	CLA	C2B-C3B-CAB-CBB
15	W	203	CLA	C4B-C3B-CAB-CBB
15	a	803	CLA	C3A-C2A-CAA-CBA
15	a	805	CLA	C3A-C2A-CAA-CBA
15	a	806	CLA	C1A-C2A-CAA-CBA
15	a	806	CLA	C3A-C2A-CAA-CBA
15	a	806	CLA	CAD-CBD-CGD-O1D
15	a	806	CLA	CAD-CBD-CGD-O2D
15	a	809	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	a	809	CLA	CHA-CBD-CGD-O1D
15	a	809	CLA	CHA-CBD-CGD-O2D
15	a	809	CLA	C6-C7-C8-C9
15	a	810	CLA	C1A-C2A-CAA-CBA
15	a	811	CLA	CAD-CBD-CGD-O1D
15	a	811	CLA	CAD-CBD-CGD-O2D
15	a	811	CLA	CBD-CGD-O2D-CED
15	a	811	CLA	C6-C7-C8-C9
15	a	812	CLA	C1A-C2A-CAA-CBA
15	a	814	CLA	C4-C3-C5-C6
15	a	815	CLA	C1A-C2A-CAA-CBA
15	a	818	CLA	C1A-C2A-CAA-CBA
15	a	818	CLA	C3A-C2A-CAA-CBA
15	a	818	CLA	CHA-CBD-CGD-O1D
15	a	818	CLA	CHA-CBD-CGD-O2D
15	a	819	CLA	C3A-C2A-CAA-CBA
15	a	820	CLA	C1A-C2A-CAA-CBA
15	a	820	CLA	C3A-C2A-CAA-CBA
15	a	822	CLA	C2-C3-C5-C6
15	a	822	CLA	C4-C3-C5-C6
15	a	825	CLA	C4-C3-C5-C6
15	a	831	CLA	CHA-CBD-CGD-O1D
15	a	831	CLA	CHA-CBD-CGD-O2D
15	a	834	CLA	C4B-C3B-CAB-CBB
15	a	837	CLA	CBD-CGD-O2D-CED
15	a	841	CLA	C1A-C2A-CAA-CBA
15	a	841	CLA	C2B-C3B-CAB-CBB
15	a	841	CLA	C4B-C3B-CAB-CBB
15	a	842	CLA	C1A-C2A-CAA-CBA
15	b	802	CLA	CAD-CBD-CGD-O2D
15	b	805	CLA	C3A-C2A-CAA-CBA
15	b	806	CLA	CHA-CBD-CGD-O1D
15	b	806	CLA	CHA-CBD-CGD-O2D
15	b	806	CLA	CBD-CGD-O2D-CED
15	b	808	CLA	CHA-CBD-CGD-O1D
15	b	808	CLA	CHA-CBD-CGD-O2D
15	b	809	CLA	C1A-C2A-CAA-CBA
15	b	809	CLA	C3A-C2A-CAA-CBA
15	b	814	CLA	CHA-CBD-CGD-O1D
15	b	814	CLA	CHA-CBD-CGD-O2D
15	b	815	CLA	CHA-CBD-CGD-O1D
15	b	815	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	b	816	CLA	C3A-C2A-CAA-CBA
15	b	817	CLA	C1A-C2A-CAA-CBA
15	b	817	CLA	C3A-C2A-CAA-CBA
15	b	818	CLA	C2B-C3B-CAB-CBB
15	b	818	CLA	C4B-C3B-CAB-CBB
15	b	819	CLA	C1A-C2A-CAA-CBA
15	b	819	CLA	C3A-C2A-CAA-CBA
15	b	823	CLA	CHA-CBD-CGD-O1D
15	b	823	CLA	CHA-CBD-CGD-O2D
15	b	824	CLA	CHA-CBD-CGD-O1D
15	b	824	CLA	CHA-CBD-CGD-O2D
15	b	826	CLA	CBD-CGD-O2D-CED
15	b	827	CLA	C1A-C2A-CAA-CBA
15	b	827	CLA	C3A-C2A-CAA-CBA
15	b	828	CLA	C4-C3-C5-C6
15	b	829	CLA	C1A-C2A-CAA-CBA
15	b	834	CLA	C1A-C2A-CAA-CBA
15	b	835	CLA	CAD-CBD-CGD-O1D
15	b	835	CLA	CAD-CBD-CGD-O2D
15	i	102	CLA	C1A-C2A-CAA-CBA
15	i	102	CLA	C3A-C2A-CAA-CBA
15	j	203	CLA	C2B-C3B-CAB-CBB
15	j	203	CLA	C4B-C3B-CAB-CBB
18	A	845	BCR	C17-C18-C19-C20
18	A	846	BCR	C5-C6-C7-C8
18	A	846	BCR	C21-C22-C23-C24
18	A	847	BCR	C21-C22-C23-C24
18	A	847	BCR	C37-C22-C23-C24
18	A	848	BCR	C23-C24-C25-C26
18	A	849	BCR	C21-C22-C23-C24
18	A	849	BCR	C37-C22-C23-C24
18	A	850	BCR	C7-C8-C9-C10
18	A	850	BCR	C7-C8-C9-C34
18	A	850	BCR	C21-C22-C23-C24
18	A	850	BCR	C37-C22-C23-C24
18	A	850	BCR	C23-C24-C25-C26
18	A	850	BCR	C23-C24-C25-C30
18	B	842	BCR	C21-C22-C23-C24
18	B	842	BCR	C37-C22-C23-C24
18	B	845	BCR	C5-C6-C7-C8
18	F	202	BCR	C17-C18-C19-C20
18	F	202	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
18	F	202	BCR	C21-C22-C23-C24
18	F	202	BCR	C37-C22-C23-C24
18	I	101	BCR	C11-C12-C13-C14
18	I	101	BCR	C21-C22-C23-C24
18	I	101	BCR	C23-C24-C25-C26
18	J	101	BCR	C11-C12-C13-C14
18	J	101	BCR	C11-C12-C13-C35
18	J	101	BCR	C23-C24-C25-C26
18	J	101	BCR	C23-C24-C25-C30
18	M	101	BCR	C1-C6-C7-C8
18	M	101	BCR	C5-C6-C7-C8
18	M	101	BCR	C7-C8-C9-C10
18	M	101	BCR	C7-C8-C9-C34
18	N	845	BCR	C17-C18-C19-C20
18	N	846	BCR	C5-C6-C7-C8
18	N	846	BCR	C21-C22-C23-C24
18	N	847	BCR	C21-C22-C23-C24
18	N	847	BCR	C37-C22-C23-C24
18	N	848	BCR	C23-C24-C25-C26
18	N	849	BCR	C21-C22-C23-C24
18	N	849	BCR	C37-C22-C23-C24
18	N	850	BCR	C7-C8-C9-C10
18	N	850	BCR	C7-C8-C9-C34
18	N	850	BCR	C21-C22-C23-C24
18	N	850	BCR	C37-C22-C23-C24
18	N	850	BCR	C23-C24-C25-C26
18	N	850	BCR	C23-C24-C25-C30
18	O	842	BCR	C21-C22-C23-C24
18	O	845	BCR	C5-C6-C7-C8
18	O	847	BCR	C17-C18-C19-C20
18	O	847	BCR	C36-C18-C19-C20
18	O	847	BCR	C21-C22-C23-C24
18	O	847	BCR	C37-C22-C23-C24
18	T	101	BCR	C21-C22-C23-C24
18	T	101	BCR	C37-C22-C23-C24
18	T	101	BCR	C23-C24-C25-C30
18	U	101	BCR	C11-C12-C13-C14
18	U	101	BCR	C11-C12-C13-C35
18	U	101	BCR	C23-C24-C25-C26
18	U	101	BCR	C23-C24-C25-C30
18	W	205	BCR	C7-C8-C9-C10
18	Y	102	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	Y	102	BCR	C5-C6-C7-C8
18	Y	102	BCR	C7-C8-C9-C10
18	Y	102	BCR	C7-C8-C9-C34
18	a	845	BCR	C17-C18-C19-C20
18	a	846	BCR	C5-C6-C7-C8
18	a	846	BCR	C21-C22-C23-C24
18	a	847	BCR	C37-C22-C23-C24
18	a	848	BCR	C23-C24-C25-C26
18	a	849	BCR	C21-C22-C23-C24
18	a	849	BCR	C37-C22-C23-C24
18	a	850	BCR	C7-C8-C9-C10
18	a	850	BCR	C21-C22-C23-C24
18	a	850	BCR	C37-C22-C23-C24
18	a	850	BCR	C23-C24-C25-C26
18	a	850	BCR	C23-C24-C25-C30
18	b	842	BCR	C21-C22-C23-C24
18	b	842	BCR	C37-C22-C23-C24
18	b	845	BCR	C5-C6-C7-C8
18	b	847	BCR	C17-C18-C19-C20
18	b	847	BCR	C36-C18-C19-C20
18	b	847	BCR	C21-C22-C23-C24
18	g	101	BCR	C21-C22-C23-C24
18	g	101	BCR	C37-C22-C23-C24
18	g	101	BCR	C23-C24-C25-C30
18	h	101	BCR	C11-C12-C13-C14
18	h	101	BCR	C11-C12-C13-C35
18	h	101	BCR	C23-C24-C25-C26
18	h	101	BCR	C23-C24-C25-C30
18	j	205	BCR	C21-C22-C23-C24
18	k	102	BCR	C1-C6-C7-C8
18	k	102	BCR	C5-C6-C7-C8
18	k	102	BCR	C7-C8-C9-C10
18	k	102	BCR	C7-C8-C9-C34
18	k	102	BCR	C17-C18-C19-C20
19	B	851	LHG	O9-C7-O7-C5
19	F	204	LHG	C3-O3-P-O5
19	F	204	LHG	C3-O3-P-O6
19	L	208	LHG	C4-O6-P-O3
19	L	208	LHG	C4-O6-P-O5
19	X	101	LHG	C3-O3-P-O5
19	X	101	LHG	C3-O3-P-O6
19	X	101	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
19	X	101	LHG	C4-O6-P-O5
19	X	101	LHG	O7-C5-C6-O8
19	N	857	LHG	C3-O3-P-O5
19	N	857	LHG	C3-O3-P-O6
19	W	207	LHG	C4-O6-P-O3
19	W	207	LHG	C4-O6-P-O5
19	Y	101	LHG	O9-C7-O7-C5
19	Z	101	LHG	C3-O3-P-O5
19	Z	101	LHG	C3-O3-P-O6
19	Z	101	LHG	C4-O6-P-O3
19	Z	101	LHG	C4-O6-P-O5
19	Z	101	LHG	O7-C5-C6-O8
19	f	203	LHG	C3-O3-P-O5
19	f	203	LHG	C3-O3-P-O6
19	j	207	LHG	C4-O6-P-O3
19	j	207	LHG	C4-O6-P-O5
19	k	101	LHG	O9-C7-O7-C5
19	l	101	LHG	C3-O3-P-O5
19	l	101	LHG	C3-O3-P-O6
19	l	101	LHG	C4-O6-P-O3
19	l	101	LHG	C4-O6-P-O5
19	l	101	LHG	O7-C5-C6-O8
21	A	855	LMG	O9-C10-O7-C8
21	B	850	LMG	O9-C10-O7-C8
21	I	103	LMG	C11-C10-O7-C8
21	J	103	LMG	C2-C1-O1-C7
21	J	103	LMG	O6-C1-O1-C7
21	N	855	LMG	O9-C10-O7-C8
21	N	855	LMG	C11-C10-O7-C8
21	T	103	LMG	C11-C10-O7-C8
21	U	103	LMG	O6-C1-O1-C7
21	g	103	LMG	C11-C10-O7-C8
21	h	103	LMG	C2-C1-O1-C7
21	h	103	LMG	O6-C1-O1-C7
15	A	812	CLA	O1D-CGD-O2D-CED
15	A	837	CLA	O1D-CGD-O2D-CED
15	a	812	CLA	O1D-CGD-O2D-CED
15	a	837	CLA	O1D-CGD-O2D-CED
15	A	807	CLA	CBD-CGD-O2D-CED
15	A	812	CLA	CBD-CGD-O2D-CED
15	A	816	CLA	CBD-CGD-O2D-CED
15	B	801	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	804	CLA	CBD-CGD-O2D-CED
15	B	813	CLA	CBD-CGD-O2D-CED
15	B	829	CLA	CBD-CGD-O2D-CED
15	X	102	CLA	CBD-CGD-O2D-CED
15	N	807	CLA	CBD-CGD-O2D-CED
15	N	812	CLA	CBD-CGD-O2D-CED
15	N	822	CLA	CBD-CGD-O2D-CED
15	N	828	CLA	CBD-CGD-O2D-CED
15	O	801	CLA	CBD-CGD-O2D-CED
15	O	804	CLA	CBD-CGD-O2D-CED
15	O	813	CLA	CBD-CGD-O2D-CED
15	O	819	CLA	CBD-CGD-O2D-CED
15	V	102	CLA	CBD-CGD-O2D-CED
15	Z	102	CLA	CBD-CGD-O2D-CED
15	a	807	CLA	CBD-CGD-O2D-CED
15	a	812	CLA	CBD-CGD-O2D-CED
15	a	816	CLA	CBD-CGD-O2D-CED
15	a	820	CLA	CBD-CGD-O2D-CED
15	b	801	CLA	CBD-CGD-O2D-CED
15	b	804	CLA	CBD-CGD-O2D-CED
15	b	819	CLA	CBD-CGD-O2D-CED
15	b	820	CLA	CBD-CGD-O2D-CED
15	b	834	CLA	CBD-CGD-O2D-CED
15	i	102	CLA	CBD-CGD-O2D-CED
15	l	102	CLA	CBD-CGD-O2D-CED
14	A	856	F6C	O1A-CGA-O2A-C1
14	N	856	F6C	O1A-CGA-O2A-C1
14	a	855	F6C	O1A-CGA-O2A-C1
15	A	813	CLA	O1A-CGA-O2A-C1
15	N	813	CLA	O1A-CGA-O2A-C1
15	N	822	CLA	O1A-CGA-O2A-C1
15	O	809	CLA	O1A-CGA-O2A-C1
15	a	813	CLA	O1A-CGA-O2A-C1
15	b	809	CLA	O1A-CGA-O2A-C1
15	A	807	CLA	O1D-CGD-O2D-CED
15	B	801	CLA	O1D-CGD-O2D-CED
15	N	807	CLA	O1D-CGD-O2D-CED
15	N	822	CLA	O1D-CGD-O2D-CED
15	N	837	CLA	O1D-CGD-O2D-CED
15	O	801	CLA	O1D-CGD-O2D-CED
15	a	807	CLA	O1D-CGD-O2D-CED
14	A	856	F6C	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	N	856	F6C	CBA-CGA-O2A-C1
14	a	855	F6C	CBA-CGA-O2A-C1
15	A	813	CLA	CBA-CGA-O2A-C1
15	N	813	CLA	CBA-CGA-O2A-C1
15	O	809	CLA	CBA-CGA-O2A-C1
15	a	813	CLA	CBA-CGA-O2A-C1
15	b	809	CLA	CBA-CGA-O2A-C1
15	K	102	CLA	CBD-CGD-O2D-CED
15	N	816	CLA	CBD-CGD-O2D-CED
14	a	826	F6C	O1A-CGA-O2A-C1
15	A	820	CLA	O1A-CGA-O2A-C1
15	A	822	CLA	O1A-CGA-O2A-C1
15	B	809	CLA	O1A-CGA-O2A-C1
15	B	818	CLA	O1A-CGA-O2A-C1
15	B	826	CLA	O1A-CGA-O2A-C1
15	B	828	CLA	O1A-CGA-O2A-C1
15	B	830	CLA	O1A-CGA-O2A-C1
15	N	820	CLA	O1A-CGA-O2A-C1
15	N	842	CLA	O1A-CGA-O2A-C1
15	O	818	CLA	O1A-CGA-O2A-C1
15	O	826	CLA	O1A-CGA-O2A-C1
15	O	828	CLA	O1A-CGA-O2A-C1
15	O	830	CLA	O1A-CGA-O2A-C1
15	a	822	CLA	O1A-CGA-O2A-C1
15	a	842	CLA	O1A-CGA-O2A-C1
15	b	818	CLA	O1A-CGA-O2A-C1
15	b	826	CLA	O1A-CGA-O2A-C1
15	b	828	CLA	O1A-CGA-O2A-C1
15	b	830	CLA	O1A-CGA-O2A-C1
19	F	204	LHG	O10-C23-O8-C6
19	L	208	LHG	O10-C23-O8-C6
19	N	857	LHG	O10-C23-O8-C6
19	W	207	LHG	O10-C23-O8-C6
19	f	203	LHG	O10-C23-O8-C6
19	j	207	LHG	O10-C23-O8-C6
21	I	103	LMG	O10-C28-O8-C9
21	T	103	LMG	O10-C28-O8-C9
21	g	103	LMG	O10-C28-O8-C9
15	N	806	CLA	O1D-CGD-O2D-CED
15	N	812	CLA	O1D-CGD-O2D-CED
15	b	801	CLA	O1D-CGD-O2D-CED
15	b	806	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	806	CLA	O1D-CGD-O2D-CED
15	O	806	CLA	O1D-CGD-O2D-CED
15	a	811	CLA	O1D-CGD-O2D-CED
20	A	853	LMT	O5B-C1B-O1B-C4'
20	N	853	LMT	O5B-C1B-O1B-C4'
20	a	853	LMT	O5B-C1B-O1B-C4'
15	A	842	CLA	O1A-CGA-O2A-C1
15	a	820	CLA	O1A-CGA-O2A-C1
21	I	103	LMG	O9-C10-O7-C8
21	T	103	LMG	O9-C10-O7-C8
21	g	103	LMG	O9-C10-O7-C8
14	a	826	F6C	C3-C5-C6-C7
15	A	804	CLA	C3-C5-C6-C7
15	A	831	CLA	C3-C5-C6-C7
15	A	839	CLA	C3-C5-C6-C7
15	B	804	CLA	C3-C5-C6-C7
15	B	819	CLA	C3-C5-C6-C7
15	B	822	CLA	C3-C5-C6-C7
15	B	824	CLA	C3-C5-C6-C7
15	B	828	CLA	C3-C5-C6-C7
15	N	804	CLA	C3-C5-C6-C7
15	N	831	CLA	C3-C5-C6-C7
15	O	804	CLA	C3-C5-C6-C7
15	O	819	CLA	C3-C5-C6-C7
15	O	822	CLA	C3-C5-C6-C7
15	O	824	CLA	C3-C5-C6-C7
15	O	828	CLA	C3-C5-C6-C7
15	a	804	CLA	C3-C5-C6-C7
15	a	831	CLA	C3-C5-C6-C7
15	b	804	CLA	C3-C5-C6-C7
15	b	819	CLA	C3-C5-C6-C7
15	b	822	CLA	C3-C5-C6-C7
15	b	824	CLA	C3-C5-C6-C7
15	b	828	CLA	C3-C5-C6-C7
14	a	826	F6C	C2C-C3C-CAC-CBC
15	A	811	CLA	O1D-CGD-O2D-CED
14	a	826	F6C	CBA-CGA-O2A-C1
15	A	822	CLA	CBA-CGA-O2A-C1
15	B	809	CLA	CBA-CGA-O2A-C1
15	B	819	CLA	CBA-CGA-O2A-C1
15	B	826	CLA	CBA-CGA-O2A-C1
15	B	833	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	N	822	CLA	CBA-CGA-O2A-C1
15	O	819	CLA	CBA-CGA-O2A-C1
15	O	826	CLA	CBA-CGA-O2A-C1
15	O	830	CLA	CBA-CGA-O2A-C1
15	b	817	CLA	CBA-CGA-O2A-C1
15	b	819	CLA	CBA-CGA-O2A-C1
15	b	826	CLA	CBA-CGA-O2A-C1
15	b	830	CLA	CBA-CGA-O2A-C1
15	b	833	CLA	CBA-CGA-O2A-C1
21	I	103	LMG	C29-C28-O8-C9
21	T	103	LMG	C29-C28-O8-C9
21	g	103	LMG	C29-C28-O8-C9
15	A	818	CLA	CBD-CGD-O2D-CED
15	A	820	CLA	CBD-CGD-O2D-CED
15	A	828	CLA	CBD-CGD-O2D-CED
15	A	829	CLA	CBD-CGD-O2D-CED
15	B	819	CLA	CBD-CGD-O2D-CED
15	B	834	CLA	CBD-CGD-O2D-CED
15	N	823	CLA	CBD-CGD-O2D-CED
15	N	829	CLA	CBD-CGD-O2D-CED
15	O	820	CLA	CBD-CGD-O2D-CED
15	a	818	CLA	CBD-CGD-O2D-CED
15	b	829	CLA	CBD-CGD-O2D-CED
19	B	851	LHG	C8-C7-O7-C5
19	Y	101	LHG	C8-C7-O7-C5
19	k	101	LHG	C8-C7-O7-C5
21	A	855	LMG	C11-C10-O7-C8
21	B	850	LMG	C11-C10-O7-C8
15	B	826	CLA	O1D-CGD-O2D-CED
15	N	811	CLA	O1D-CGD-O2D-CED
15	O	834	CLA	O1D-CGD-O2D-CED
15	V	102	CLA	O1D-CGD-O2D-CED
15	b	826	CLA	O1D-CGD-O2D-CED
14	A	826	F6C	C2C-C3C-CAC-CBC
15	O	826	CLA	O1D-CGD-O2D-CED
15	O	829	CLA	O1D-CGD-O2D-CED
14	A	856	F6C	C4-C3-C5-C6
14	B	839	F6C	C4-C3-C5-C6
14	L	204	F6C	C4-C3-C5-C6
14	O	839	F6C	C4-C3-C5-C6
14	b	839	F6C	C4-C3-C5-C6
15	A	807	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	A	814	CLA	C4-C3-C5-C6
15	A	822	CLA	C4-C3-C5-C6
15	A	838	CLA	C4-C3-C5-C6
15	B	804	CLA	C4-C3-C5-C6
15	B	824	CLA	C4-C3-C5-C6
15	B	829	CLA	C4-C3-C5-C6
15	N	807	CLA	C4-C3-C5-C6
15	N	814	CLA	C4-C3-C5-C6
15	N	838	CLA	C4-C3-C5-C6
15	O	804	CLA	C4-C3-C5-C6
15	O	806	CLA	C4-C3-C5-C6
15	O	828	CLA	C4-C3-C5-C6
15	O	829	CLA	C4-C3-C5-C6
15	a	807	CLA	C4-C3-C5-C6
15	a	812	CLA	C4-C3-C5-C6
15	a	838	CLA	C4-C3-C5-C6
15	b	804	CLA	C4-C3-C5-C6
15	b	806	CLA	C4-C3-C5-C6
15	b	824	CLA	C4-C3-C5-C6
15	b	829	CLA	C4-C3-C5-C6
14	B	839	F6C	C2-C3-C5-C6
15	A	807	CLA	C2-C3-C5-C6
15	A	814	CLA	C2-C3-C5-C6
15	A	822	CLA	C2-C3-C5-C6
15	A	825	CLA	C2-C3-C5-C6
15	A	838	CLA	C2-C3-C5-C6
15	B	828	CLA	C2-C3-C5-C6
15	B	829	CLA	C2-C3-C5-C6
15	N	807	CLA	C2-C3-C5-C6
15	N	814	CLA	C2-C3-C5-C6
15	N	838	CLA	C2-C3-C5-C6
15	O	824	CLA	C2-C3-C5-C6
15	O	828	CLA	C2-C3-C5-C6
15	O	829	CLA	C2-C3-C5-C6
15	a	807	CLA	C2-C3-C5-C6
15	a	814	CLA	C2-C3-C5-C6
15	a	825	CLA	C2-C3-C5-C6
15	a	838	CLA	C2-C3-C5-C6
15	b	828	CLA	C2-C3-C5-C6
14	N	826	F6C	C2C-C3C-CAC-CBC
15	A	823	CLA	CBD-CGD-O2D-CED
15	B	804	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	O	804	CLA	O1D-CGD-O2D-CED
15	b	804	CLA	O1D-CGD-O2D-CED
14	B	832	F6C	C3A-C2A-CAA-CBA
14	b	832	F6C	C3A-C2A-CAA-CBA
15	N	830	CLA	C2A-CAA-CBA-CGA
15	a	830	CLA	C2A-CAA-CBA-CGA
14	a	826	F6C	C4C-C3C-CAC-CBC
15	A	836	CLA	C3-C5-C6-C7
15	A	841	CLA	C3-C5-C6-C7
15	N	836	CLA	C3-C5-C6-C7
15	N	841	CLA	C3-C5-C6-C7
15	a	836	CLA	C3-C5-C6-C7
15	a	841	CLA	C3-C5-C6-C7
15	A	820	CLA	CBA-CGA-O2A-C1
15	A	842	CLA	CBA-CGA-O2A-C1
15	B	806	CLA	CBA-CGA-O2A-C1
15	B	817	CLA	CBA-CGA-O2A-C1
15	B	818	CLA	CBA-CGA-O2A-C1
15	B	828	CLA	CBA-CGA-O2A-C1
15	B	830	CLA	CBA-CGA-O2A-C1
15	N	820	CLA	CBA-CGA-O2A-C1
15	N	841	CLA	CBA-CGA-O2A-C1
15	N	842	CLA	CBA-CGA-O2A-C1
15	O	806	CLA	CBA-CGA-O2A-C1
15	O	817	CLA	CBA-CGA-O2A-C1
15	O	818	CLA	CBA-CGA-O2A-C1
15	O	824	CLA	CBA-CGA-O2A-C1
15	O	828	CLA	CBA-CGA-O2A-C1
15	O	833	CLA	CBA-CGA-O2A-C1
15	a	820	CLA	CBA-CGA-O2A-C1
15	a	822	CLA	CBA-CGA-O2A-C1
15	a	841	CLA	CBA-CGA-O2A-C1
15	a	842	CLA	CBA-CGA-O2A-C1
15	b	806	CLA	CBA-CGA-O2A-C1
15	b	818	CLA	CBA-CGA-O2A-C1
15	b	824	CLA	CBA-CGA-O2A-C1
15	b	828	CLA	CBA-CGA-O2A-C1
19	F	204	LHG	C24-C23-O8-C6
19	L	208	LHG	C24-C23-O8-C6
19	N	857	LHG	C24-C23-O8-C6
19	W	207	LHG	C24-C23-O8-C6
19	f	203	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
19	j	207	LHG	C24-C23-O8-C6
15	A	837	CLA	O1A-CGA-O2A-C1
15	A	841	CLA	O1A-CGA-O2A-C1
15	B	806	CLA	O1A-CGA-O2A-C1
15	B	819	CLA	O1A-CGA-O2A-C1
15	B	824	CLA	O1A-CGA-O2A-C1
15	B	833	CLA	O1A-CGA-O2A-C1
15	N	837	CLA	O1A-CGA-O2A-C1
15	N	841	CLA	O1A-CGA-O2A-C1
15	O	806	CLA	O1A-CGA-O2A-C1
15	O	819	CLA	O1A-CGA-O2A-C1
15	O	824	CLA	O1A-CGA-O2A-C1
15	a	837	CLA	O1A-CGA-O2A-C1
15	a	841	CLA	O1A-CGA-O2A-C1
15	b	806	CLA	O1A-CGA-O2A-C1
15	b	819	CLA	O1A-CGA-O2A-C1
15	b	824	CLA	O1A-CGA-O2A-C1
14	A	802	F6C	C1A-C2A-CAA-CBA
14	A	826	F6C	C1A-C2A-CAA-CBA
14	A	856	F6C	C1A-C2A-CAA-CBA
14	L	204	F6C	C1A-C2A-CAA-CBA
14	N	802	F6C	C1A-C2A-CAA-CBA
14	N	826	F6C	C1A-C2A-CAA-CBA
14	N	856	F6C	C1A-C2A-CAA-CBA
14	a	802	F6C	C1A-C2A-CAA-CBA
14	a	826	F6C	C1A-C2A-CAA-CBA
14	a	855	F6C	C1A-C2A-CAA-CBA
14	j	204	F6C	C1A-C2A-CAA-CBA
15	X	102	CLA	O1D-CGD-O2D-CED
14	A	826	F6C	C4C-C3C-CAC-CBC
15	a	820	CLA	C2C-C3C-CAC-CBC
15	O	819	CLA	O1D-CGD-O2D-CED
15	b	819	CLA	O1D-CGD-O2D-CED
14	L	201	F6C	C3-C5-C6-C7
15	A	813	CLA	C3-C5-C6-C7
15	B	802	CLA	C3-C5-C6-C7
15	N	813	CLA	C3-C5-C6-C7
15	N	839	CLA	C3-C5-C6-C7
15	O	802	CLA	C3-C5-C6-C7
15	a	813	CLA	C3-C5-C6-C7
15	b	802	CLA	C3-C5-C6-C7
15	A	836	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	B	803	CLA	CBD-CGD-O2D-CED
15	a	823	CLA	CBD-CGD-O2D-CED
15	b	828	CLA	CBD-CGD-O2D-CED
15	N	828	CLA	O1D-CGD-O2D-CED
15	Z	102	CLA	O1D-CGD-O2D-CED
15	i	102	CLA	O1D-CGD-O2D-CED
15	A	837	CLA	CBA-CGA-O2A-C1
15	B	824	CLA	CBA-CGA-O2A-C1
15	N	837	CLA	CBA-CGA-O2A-C1
15	a	837	CLA	CBA-CGA-O2A-C1
15	B	817	CLA	O1A-CGA-O2A-C1
15	O	817	CLA	O1A-CGA-O2A-C1
15	b	817	CLA	O1A-CGA-O2A-C1
15	b	833	CLA	O1A-CGA-O2A-C1
15	b	834	CLA	O1D-CGD-O2D-CED
15	l	102	CLA	O1D-CGD-O2D-CED
15	B	816	CLA	CBD-CGD-O2D-CED
15	N	836	CLA	CBD-CGD-O2D-CED
15	O	840	CLA	CBD-CGD-O2D-CED
15	a	836	CLA	CBD-CGD-O2D-CED
15	A	820	CLA	C2C-C3C-CAC-CBC
15	N	820	CLA	C2C-C3C-CAC-CBC
15	A	816	CLA	O1D-CGD-O2D-CED
15	B	813	CLA	O1D-CGD-O2D-CED
15	O	813	CLA	O1D-CGD-O2D-CED
15	a	816	CLA	O1D-CGD-O2D-CED
15	b	820	CLA	O1D-CGD-O2D-CED
14	W	201	F6C	C3-C5-C6-C7
15	O	830	CLA	C3-C5-C6-C7
15	S	201	CLA	C3-C5-C6-C7
15	a	822	CLA	C3-C5-C6-C7
15	A	806	CLA	CBD-CGD-O2D-CED
15	B	828	CLA	CBD-CGD-O2D-CED
15	B	829	CLA	O1D-CGD-O2D-CED
15	A	841	CLA	CBA-CGA-O2A-C1
15	A	818	CLA	C4-C3-C5-C6
15	N	818	CLA	C4-C3-C5-C6
15	a	818	CLA	C4-C3-C5-C6
14	A	856	F6C	C2-C3-C5-C6
14	O	839	F6C	C2-C3-C5-C6
15	A	818	CLA	C2-C3-C5-C6
15	B	804	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	N	818	CLA	C2-C3-C5-C6
15	a	818	CLA	C2-C3-C5-C6
15	b	804	CLA	C2-C3-C5-C6
15	b	829	CLA	C2-C3-C5-C6
14	N	826	F6C	C4C-C3C-CAC-CBC
15	B	835	CLA	CBD-CGD-O2D-CED
15	B	840	CLA	CBD-CGD-O2D-CED
15	V	103	CLA	CBD-CGD-O2D-CED
15	a	829	CLA	CBD-CGD-O2D-CED
15	b	835	CLA	CBD-CGD-O2D-CED
15	a	820	CLA	O1D-CGD-O2D-CED
14	O	832	F6C	C3A-C2A-CAA-CBA
14	A	856	F6C	C2A-CAA-CBA-CGA
14	B	839	F6C	C2A-CAA-CBA-CGA
14	N	856	F6C	C2A-CAA-CBA-CGA
14	O	839	F6C	C2A-CAA-CBA-CGA
14	b	839	F6C	C2A-CAA-CBA-CGA
15	A	830	CLA	C2A-CAA-CBA-CGA
15	O	833	CLA	O1A-CGA-O2A-C1
15	N	816	CLA	O1D-CGD-O2D-CED
15	A	823	CLA	CBA-CGA-O2A-C1
15	B	804	CLA	CBA-CGA-O2A-C1
15	B	805	CLA	CBA-CGA-O2A-C1
15	B	840	CLA	CBA-CGA-O2A-C1
15	O	804	CLA	CBA-CGA-O2A-C1
15	O	813	CLA	CBA-CGA-O2A-C1
15	a	811	CLA	CBA-CGA-O2A-C1
15	a	823	CLA	CBA-CGA-O2A-C1
15	b	804	CLA	CBA-CGA-O2A-C1
14	a	802	F6C	CBD-CGD-O2D-CED
15	A	838	CLA	CBD-CGD-O2D-CED
15	N	818	CLA	CBD-CGD-O2D-CED
15	O	828	CLA	CBD-CGD-O2D-CED
15	a	806	CLA	CBD-CGD-O2D-CED
15	a	838	CLA	CBD-CGD-O2D-CED
15	b	840	CLA	CBD-CGD-O2D-CED
15	b	804	CLA	O1A-CGA-O2A-C1
15	K	102	CLA	O1D-CGD-O2D-CED
15	B	820	CLA	CBD-CGD-O2D-CED
15	N	838	CLA	CBD-CGD-O2D-CED
15	O	835	CLA	CBD-CGD-O2D-CED
15	b	816	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	b	838	CLA	CBD-CGD-O2D-CED
15	a	820	CLA	C4C-C3C-CAC-CBC
14	j	201	F6C	C3-C5-C6-C7
15	B	804	CLA	O1A-CGA-O2A-C1
15	B	840	CLA	O1A-CGA-O2A-C1
15	O	804	CLA	O1A-CGA-O2A-C1
15	a	804	CLA	O1A-CGA-O2A-C1
15	A	804	CLA	CBA-CGA-O2A-C1
15	A	811	CLA	CBA-CGA-O2A-C1
15	A	821	CLA	CBA-CGA-O2A-C1
15	A	831	CLA	CBA-CGA-O2A-C1
15	A	838	CLA	CBA-CGA-O2A-C1
15	B	810	CLA	CBA-CGA-O2A-C1
15	B	813	CLA	CBA-CGA-O2A-C1
15	N	804	CLA	CBA-CGA-O2A-C1
15	N	811	CLA	CBA-CGA-O2A-C1
15	N	821	CLA	CBA-CGA-O2A-C1
15	N	823	CLA	CBA-CGA-O2A-C1
15	N	831	CLA	CBA-CGA-O2A-C1
15	N	838	CLA	CBA-CGA-O2A-C1
15	O	810	CLA	CBA-CGA-O2A-C1
15	O	829	CLA	CBA-CGA-O2A-C1
15	O	840	CLA	CBA-CGA-O2A-C1
15	a	804	CLA	CBA-CGA-O2A-C1
15	a	831	CLA	CBA-CGA-O2A-C1
15	a	838	CLA	CBA-CGA-O2A-C1
15	b	810	CLA	CBA-CGA-O2A-C1
15	b	840	CLA	CBA-CGA-O2A-C1
15	O	816	CLA	CBD-CGD-O2D-CED
15	A	804	CLA	O1A-CGA-O2A-C1
15	N	804	CLA	O1A-CGA-O2A-C1
14	N	856	F6C	C4-C3-C5-C6
14	a	855	F6C	C4-C3-C5-C6
15	B	806	CLA	C4-C3-C5-C6
14	L	204	F6C	C2-C3-C5-C6
14	N	856	F6C	C2-C3-C5-C6
14	a	855	F6C	C2-C3-C5-C6
14	b	839	F6C	C2-C3-C5-C6
15	B	806	CLA	C2-C3-C5-C6
15	B	824	CLA	C2-C3-C5-C6
15	O	804	CLA	C2-C3-C5-C6
15	O	806	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	a	812	CLA	C2-C3-C5-C6
15	b	806	CLA	C2-C3-C5-C6
15	b	824	CLA	C2-C3-C5-C6
14	N	826	F6C	C3-C5-C6-C7
15	A	822	CLA	C3-C5-C6-C7
15	F	201	CLA	C3-C5-C6-C7
15	N	822	CLA	C3-C5-C6-C7
15	a	810	CLA	C3-C5-C6-C7
15	b	808	CLA	C3-C5-C6-C7
14	A	802	F6C	CBD-CGD-O2D-CED
15	b	823	CLA	CBD-CGD-O2D-CED
14	A	856	F6C	C11-C10-C8-C9
14	N	856	F6C	C6-C7-C8-C9
14	N	856	F6C	C11-C10-C8-C9
14	a	855	F6C	C6-C7-C8-C9
14	a	855	F6C	C11-C10-C8-C9
15	A	809	CLA	C6-C7-C8-C9
15	A	829	CLA	C6-C7-C8-C9
15	B	806	CLA	C11-C10-C8-C9
15	B	813	CLA	C11-C12-C13-C14
15	B	829	CLA	C11-C12-C13-C14
15	B	840	CLA	C11-C12-C13-C14
15	F	201	CLA	C6-C7-C8-C9
15	L	203	CLA	C11-C10-C8-C9
15	N	809	CLA	C6-C7-C8-C9
15	N	811	CLA	C6-C7-C8-C9
15	N	829	CLA	C6-C7-C8-C9
15	O	806	CLA	C11-C10-C8-C9
15	O	813	CLA	C11-C12-C13-C14
15	O	829	CLA	C11-C12-C13-C14
15	O	837	CLA	C14-C13-C15-C16
15	S	201	CLA	C6-C7-C8-C9
15	W	203	CLA	C11-C10-C8-C9
15	a	810	CLA	C11-C10-C8-C9
15	a	829	CLA	C6-C7-C8-C9
15	b	806	CLA	C11-C10-C8-C9
15	b	813	CLA	C11-C12-C13-C14
15	b	829	CLA	C11-C12-C13-C14
15	b	837	CLA	C14-C13-C15-C16
15	j	203	CLA	C11-C10-C8-C9
15	B	834	CLA	O1D-CGD-O2D-CED
21	U	103	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
15	A	831	CLA	O1A-CGA-O2A-C1
15	B	810	CLA	O1A-CGA-O2A-C1
15	O	840	CLA	O1A-CGA-O2A-C1
15	b	810	CLA	O1A-CGA-O2A-C1
15	A	820	CLA	O1D-CGD-O2D-CED
15	b	829	CLA	O1D-CGD-O2D-CED
18	A	845	BCR	C36-C18-C19-C20
18	A	846	BCR	C37-C22-C23-C24
18	B	845	BCR	C7-C8-C9-C34
18	I	101	BCR	C7-C8-C9-C34
18	I	101	BCR	C11-C12-C13-C35
18	I	101	BCR	C37-C22-C23-C24
18	J	101	BCR	C37-C22-C23-C24
18	L	205	BCR	C37-C22-C23-C24
18	M	101	BCR	C36-C18-C19-C20
18	N	845	BCR	C36-C18-C19-C20
18	N	846	BCR	C37-C22-C23-C24
18	N	850	BCR	C36-C18-C19-C20
18	O	842	BCR	C37-C22-C23-C24
18	O	845	BCR	C7-C8-C9-C34
18	T	101	BCR	C11-C12-C13-C35
18	U	101	BCR	C37-C22-C23-C24
18	W	205	BCR	C7-C8-C9-C34
18	W	205	BCR	C37-C22-C23-C24
18	Y	102	BCR	C36-C18-C19-C20
18	a	845	BCR	C36-C18-C19-C20
18	a	846	BCR	C37-C22-C23-C24
18	a	850	BCR	C7-C8-C9-C34
18	a	850	BCR	C36-C18-C19-C20
18	b	845	BCR	C7-C8-C9-C34
18	b	847	BCR	C37-C22-C23-C24
18	g	101	BCR	C11-C12-C13-C35
18	h	101	BCR	C37-C22-C23-C24
18	j	205	BCR	C37-C22-C23-C24
18	k	102	BCR	C36-C18-C19-C20
18	B	845	BCR	C7-C8-C9-C10
18	I	101	BCR	C7-C8-C9-C10
18	O	845	BCR	C7-C8-C9-C10
18	W	205	BCR	C21-C22-C23-C24
18	b	845	BCR	C7-C8-C9-C10
18	g	101	BCR	C7-C8-C9-C10
15	N	831	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	O	810	CLA	O1A-CGA-O2A-C1
15	a	831	CLA	O1A-CGA-O2A-C1
15	b	840	CLA	O1A-CGA-O2A-C1
15	B	829	CLA	C5-C6-C7-C8
15	O	805	CLA	CBA-CGA-O2A-C1
15	a	821	CLA	CBA-CGA-O2A-C1
15	b	805	CLA	CBA-CGA-O2A-C1
15	b	813	CLA	CBA-CGA-O2A-C1
15	A	820	CLA	C5-C6-C7-C8
15	a	820	CLA	C5-C6-C7-C8
15	b	840	CLA	C15-C16-C17-C18
15	B	828	CLA	C2-C1-O2A-CGA
15	O	828	CLA	C2-C1-O2A-CGA
15	b	828	CLA	C2-C1-O2A-CGA
15	A	828	CLA	O1D-CGD-O2D-CED
15	A	829	CLA	O1D-CGD-O2D-CED
15	O	820	CLA	O1D-CGD-O2D-CED
15	j	202	CLA	CBD-CGD-O2D-CED
15	A	820	CLA	C4C-C3C-CAC-CBC
14	N	802	F6C	C15-C16-C17-C18
15	N	811	CLA	C5-C6-C7-C8
15	N	831	CLA	C10-C11-C12-C13
15	O	829	CLA	C5-C6-C7-C8
15	N	818	CLA	C3-C5-C6-C7
15	B	819	CLA	O1D-CGD-O2D-CED
14	a	802	F6C	C15-C16-C17-C18
15	B	814	CLA	CBD-CGD-O2D-CED
15	a	814	CLA	CBD-CGD-O2D-CED
15	N	820	CLA	C4C-C3C-CAC-CBC
15	B	829	CLA	C11-C10-C8-C7
15	O	829	CLA	C11-C10-C8-C7
15	b	829	CLA	C11-C10-C8-C7
15	O	827	CLA	CBA-CGA-O2A-C1
15	b	827	CLA	CBA-CGA-O2A-C1
15	N	812	CLA	C4-C3-C5-C6
19	l	101	LHG	C23-C24-C25-C26
21	I	103	LMG	C28-C29-C30-C31
14	N	856	F6C	C3-C5-C6-C7
14	a	855	F6C	C3-C5-C6-C7
15	N	820	CLA	C3-C5-C6-C7
15	O	817	CLA	C3-C5-C6-C7
14	L	204	F6C	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	N	819	CLA	C15-C16-C17-C18
15	O	817	CLA	C10-C11-C12-C13
15	a	830	CLA	C8-C10-C11-C12
15	b	829	CLA	C5-C6-C7-C8
15	b	831	CLA	C10-C11-C12-C13
19	A	851	LHG	C23-C24-C25-C26
19	N	857	LHG	C7-C8-C9-C10
19	Z	101	LHG	C23-C24-C25-C26
21	T	103	LMG	C28-C29-C30-C31
21	g	103	LMG	C28-C29-C30-C31
15	A	838	CLA	O1A-CGA-O2A-C1
15	B	805	CLA	O1A-CGA-O2A-C1
15	B	813	CLA	O1A-CGA-O2A-C1
15	N	811	CLA	O1A-CGA-O2A-C1
15	N	821	CLA	O1A-CGA-O2A-C1
15	b	814	CLA	CBD-CGD-O2D-CED
15	b	833	CLA	CBD-CGD-O2D-CED
14	A	802	F6C	C15-C16-C17-C18
15	A	803	CLA	C13-C15-C16-C17
15	A	811	CLA	C5-C6-C7-C8
15	B	810	CLA	C5-C6-C7-C8
15	B	812	CLA	C5-C6-C7-C8
15	B	813	CLA	C10-C11-C12-C13
15	B	817	CLA	C10-C11-C12-C13
15	B	822	CLA	C5-C6-C7-C8
15	N	819	CLA	C10-C11-C12-C13
15	N	830	CLA	C8-C10-C11-C12
15	O	813	CLA	C5-C6-C7-C8
15	O	813	CLA	C10-C11-C12-C13
15	b	813	CLA	C5-C6-C7-C8
15	A	809	CLA	C2A-CAA-CBA-CGA
15	B	829	CLA	C2A-CAA-CBA-CGA
15	N	809	CLA	C2A-CAA-CBA-CGA
15	O	829	CLA	C2A-CAA-CBA-CGA
15	a	809	CLA	C2A-CAA-CBA-CGA
15	b	829	CLA	C2A-CAA-CBA-CGA
15	A	818	CLA	O1D-CGD-O2D-CED
15	A	812	CLA	C5-C6-C7-C8
15	A	829	CLA	C8-C10-C11-C12
15	B	828	CLA	C8-C10-C11-C12
15	B	838	CLA	C5-C6-C7-C8
15	N	812	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	N	818	CLA	C8-C10-C11-C12
15	O	812	CLA	C5-C6-C7-C8
15	O	828	CLA	C10-C11-C12-C13
15	a	809	CLA	C5-C6-C7-C8
15	a	811	CLA	C5-C6-C7-C8
15	a	818	CLA	C8-C10-C11-C12
15	b	813	CLA	C10-C11-C12-C13
15	b	822	CLA	C5-C6-C7-C8
19	F	204	LHG	C7-C8-C9-C10
19	f	203	LHG	C7-C8-C9-C10
15	N	823	CLA	O1A-CGA-O2A-C1
15	N	838	CLA	O1A-CGA-O2A-C1
15	O	829	CLA	O1A-CGA-O2A-C1
14	b	839	F6C	C3-C5-C6-C7
15	A	806	CLA	C3-C5-C6-C7
15	B	817	CLA	C3-C5-C6-C7
15	N	806	CLA	C3-C5-C6-C7
15	a	806	CLA	C3-C5-C6-C7
15	b	817	CLA	C3-C5-C6-C7
15	f	201	CLA	C3-C5-C6-C7
15	O	833	CLA	CBD-CGD-O2D-CED
21	g	103	LMG	O6-C1-O1-C7
15	a	818	CLA	O1D-CGD-O2D-CED
14	a	826	F6C	C5-C6-C7-C8
15	A	812	CLA	C10-C11-C12-C13
15	A	819	CLA	C15-C16-C17-C18
15	A	822	CLA	C5-C6-C7-C8
15	A	831	CLA	C10-C11-C12-C13
15	B	813	CLA	C5-C6-C7-C8
15	B	831	CLA	C10-C11-C12-C13
15	N	803	CLA	C13-C15-C16-C17
15	N	812	CLA	C10-C11-C12-C13
15	N	820	CLA	C5-C6-C7-C8
15	N	829	CLA	C8-C10-C11-C12
15	O	806	CLA	C10-C11-C12-C13
15	O	810	CLA	C5-C6-C7-C8
15	O	822	CLA	C5-C6-C7-C8
15	O	831	CLA	C10-C11-C12-C13
15	O	838	CLA	C5-C6-C7-C8
15	a	812	CLA	C10-C11-C12-C13
15	a	819	CLA	C15-C16-C17-C18
15	a	829	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	a	831	CLA	C10-C11-C12-C13
15	b	810	CLA	C5-C6-C7-C8
15	b	812	CLA	C5-C6-C7-C8
15	b	828	CLA	C10-C11-C12-C13
21	h	103	LMG	C19-C20-C21-C22
15	O	802	CLA	CBD-CGD-O2D-CED
15	O	823	CLA	CBD-CGD-O2D-CED
15	A	811	CLA	O1A-CGA-O2A-C1
15	A	823	CLA	O1A-CGA-O2A-C1
15	a	811	CLA	O1A-CGA-O2A-C1
15	a	823	CLA	O1A-CGA-O2A-C1
15	a	838	CLA	O1A-CGA-O2A-C1
15	N	810	CLA	C8-C10-C11-C12
19	F	204	LHG	C23-C24-C25-C26
19	X	101	LHG	C23-C24-C25-C26
14	j	204	F6C	C8-C10-C11-C12
15	a	803	CLA	C13-C15-C16-C17
15	b	828	CLA	O1D-CGD-O2D-CED
15	A	823	CLA	O1D-CGD-O2D-CED
15	N	823	CLA	O1D-CGD-O2D-CED
15	N	829	CLA	O1D-CGD-O2D-CED
14	A	856	F6C	C10-C11-C12-C13
15	A	830	CLA	C8-C10-C11-C12
15	B	837	CLA	C8-C10-C11-C12
15	N	819	CLA	C8-C10-C11-C12
15	O	840	CLA	C15-C16-C17-C18
15	b	837	CLA	C8-C10-C11-C12
15	A	835	CLA	CBD-CGD-O2D-CED
15	B	823	CLA	CBD-CGD-O2D-CED
15	A	812	CLA	C4-C3-C5-C6
15	A	821	CLA	O1A-CGA-O2A-C1
15	O	805	CLA	O1A-CGA-O2A-C1
15	O	813	CLA	O1A-CGA-O2A-C1
15	a	821	CLA	O1A-CGA-O2A-C1
15	A	836	CLA	O1D-CGD-O2D-CED
15	a	823	CLA	O1D-CGD-O2D-CED
14	W	204	F6C	C8-C10-C11-C12
14	a	855	F6C	C10-C11-C12-C13
15	A	819	CLA	C8-C10-C11-C12
15	A	819	CLA	C10-C11-C12-C13
15	A	841	CLA	C5-C6-C7-C8
15	B	828	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	N	822	CLA	C5-C6-C7-C8
15	a	812	CLA	C5-C6-C7-C8
15	a	812	CLA	C15-C16-C17-C18
15	a	819	CLA	C8-C10-C11-C12
15	a	819	CLA	C10-C11-C12-C13
15	a	822	CLA	C5-C6-C7-C8
15	a	839	CLA	C13-C15-C16-C17
15	a	841	CLA	C5-C6-C7-C8
15	b	838	CLA	C5-C6-C7-C8
15	A	833	CLA	CBA-CGA-O2A-C1
15	B	827	CLA	CBA-CGA-O2A-C1
15	N	833	CLA	CBA-CGA-O2A-C1
15	b	829	CLA	CBA-CGA-O2A-C1
15	N	825	CLA	CBD-CGD-O2D-CED
15	O	814	CLA	CBD-CGD-O2D-CED
15	b	802	CLA	CBD-CGD-O2D-CED
15	b	805	CLA	O1A-CGA-O2A-C1
15	b	813	CLA	O1A-CGA-O2A-C1
15	B	803	CLA	O1D-CGD-O2D-CED
19	f	203	LHG	C23-C24-C25-C26
15	b	808	CLA	C10-C11-C12-C13
14	O	839	F6C	C3-C5-C6-C7
15	B	830	CLA	C3-C5-C6-C7
15	A	810	CLA	C8-C10-C11-C12
14	A	826	F6C	C10-C11-C12-C13
14	N	826	F6C	C10-C11-C12-C13
15	A	806	CLA	C8-C10-C11-C12
15	A	822	CLA	C8-C10-C11-C12
15	N	822	CLA	C8-C10-C11-C12
15	A	812	CLA	C2A-CAA-CBA-CGA
15	A	839	CLA	C2A-CAA-CBA-CGA
15	B	827	CLA	C2A-CAA-CBA-CGA
15	N	812	CLA	C2A-CAA-CBA-CGA
15	O	827	CLA	C2A-CAA-CBA-CGA
15	a	812	CLA	C2A-CAA-CBA-CGA
15	b	827	CLA	C2A-CAA-CBA-CGA
15	A	829	CLA	CBA-CGA-O2A-C1
15	B	829	CLA	CBA-CGA-O2A-C1
15	N	829	CLA	CBA-CGA-O2A-C1
15	a	829	CLA	CBA-CGA-O2A-C1
15	N	812	CLA	C15-C16-C17-C18
15	N	831	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	O	828	CLA	C8-C10-C11-C12
15	b	817	CLA	C10-C11-C12-C13
15	A	817	CLA	CBD-CGD-O2D-CED
15	L	202	CLA	CBD-CGD-O2D-CED
14	a	826	F6C	C10-C11-C12-C13
15	A	818	CLA	C8-C10-C11-C12
15	A	831	CLA	C5-C6-C7-C8
15	B	806	CLA	C10-C11-C12-C13
15	N	806	CLA	C8-C10-C11-C12
15	N	809	CLA	C5-C6-C7-C8
15	O	824	CLA	C13-C15-C16-C17
15	a	831	CLA	C5-C6-C7-C8
15	b	828	CLA	C8-C10-C11-C12
15	A	809	CLA	C5-C6-C7-C8
15	A	812	CLA	C15-C16-C17-C18
15	B	808	CLA	C10-C11-C12-C13
15	B	824	CLA	C13-C15-C16-C17
15	N	841	CLA	C5-C6-C7-C8
15	O	837	CLA	C8-C10-C11-C12
15	b	806	CLA	C10-C11-C12-C13
15	b	806	CLA	C15-C16-C17-C18
15	B	816	CLA	O1D-CGD-O2D-CED
15	B	837	CLA	CBA-CGA-O2A-C1
15	b	837	CLA	CBA-CGA-O2A-C1
15	a	810	CLA	C8-C10-C11-C12
15	N	829	CLA	C4-C3-C5-C6
20	N	854	LMT	C3-C4-C5-C6
15	N	820	CLA	C10-C11-C12-C13
15	O	808	CLA	C10-C11-C12-C13
15	a	806	CLA	C8-C10-C11-C12
15	a	822	CLA	C8-C10-C11-C12
15	b	824	CLA	C13-C15-C16-C17
14	A	826	F6C	C3-C5-C6-C7
14	A	856	F6C	C3-C5-C6-C7
15	N	810	CLA	C3-C5-C6-C7
15	O	808	CLA	C3-C5-C6-C7
15	f	201	CLA	C6-C7-C8-C9
20	A	854	LMT	C3-C4-C5-C6
20	a	854	LMT	C3-C4-C5-C6
21	J	103	LMG	C19-C20-C21-C22
15	O	840	CLA	O1D-CGD-O2D-CED
15	a	836	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	I	103	LMG	C2-C1-O1-C7
21	T	103	LMG	C2-C1-O1-C7
21	g	103	LMG	C2-C1-O1-C7
14	O	832	F6C	C15-C16-C17-C18
15	B	828	CLA	O1D-CGD-O2D-CED
15	N	836	CLA	O1D-CGD-O2D-CED
15	N	840	CLA	CBD-CGD-O2D-CED
15	a	829	CLA	C11-C12-C13-C14
15	b	817	CLA	C11-C12-C13-C15
15	A	820	CLA	C10-C11-C12-C13
15	A	806	CLA	O1D-CGD-O2D-CED
15	B	824	CLA	C5-C6-C7-C8
15	O	806	CLA	C15-C16-C17-C18
15	b	802	CLA	C15-C16-C17-C18
18	A	846	BCR	C7-C8-C9-C34
18	A	850	BCR	C36-C18-C19-C20
18	J	102	BCR	C7-C8-C9-C34
18	N	846	BCR	C7-C8-C9-C34
18	O	847	BCR	C11-C12-C13-C35
18	T	101	BCR	C7-C8-C9-C34
18	U	102	BCR	C7-C8-C9-C34
18	a	846	BCR	C7-C8-C9-C34
18	g	101	BCR	C7-C8-C9-C34
18	A	846	BCR	C7-C8-C9-C10
18	J	101	BCR	C21-C22-C23-C24
18	M	101	BCR	C17-C18-C19-C20
18	N	846	BCR	C7-C8-C9-C10
18	T	101	BCR	C7-C8-C9-C10
18	T	101	BCR	C11-C12-C13-C14
18	Y	102	BCR	C17-C18-C19-C20
18	a	846	BCR	C7-C8-C9-C10
18	a	847	BCR	C21-C22-C23-C24
18	g	101	BCR	C11-C12-C13-C14
18	h	101	BCR	C21-C22-C23-C24
15	N	829	CLA	O1A-CGA-O2A-C1
15	N	833	CLA	O1A-CGA-O2A-C1
15	O	827	CLA	O1A-CGA-O2A-C1
15	a	829	CLA	O1A-CGA-O2A-C1
15	b	827	CLA	O1A-CGA-O2A-C1
15	b	829	CLA	O1A-CGA-O2A-C1
20	A	854	LMT	C7-C8-C9-C10
15	A	813	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	B	830	CLA	C2A-CAA-CBA-CGA
15	N	813	CLA	C2A-CAA-CBA-CGA
15	a	813	CLA	C2A-CAA-CBA-CGA
15	a	831	CLA	C2A-CAA-CBA-CGA
19	a	851	LHG	C23-C24-C25-C26
15	b	835	CLA	O1D-CGD-O2D-CED
15	A	803	CLA	C16-C17-C18-C20
15	A	829	CLA	C11-C12-C13-C14
15	B	802	CLA	C16-C17-C18-C19
15	N	803	CLA	C16-C17-C18-C20
15	N	829	CLA	C11-C12-C13-C14
15	O	802	CLA	C16-C17-C18-C19
15	a	803	CLA	C16-C17-C18-C20
15	b	802	CLA	C16-C17-C18-C19
15	A	829	CLA	O1A-CGA-O2A-C1
15	B	827	CLA	O1A-CGA-O2A-C1
14	B	839	F6C	C3-C5-C6-C7
15	A	818	CLA	C3-C5-C6-C7
15	A	820	CLA	C3-C5-C6-C7
15	B	808	CLA	C3-C5-C6-C7
15	a	818	CLA	C3-C5-C6-C7
15	b	806	CLA	C3-C5-C6-C7
15	b	830	CLA	C3-C5-C6-C7
15	A	810	CLA	C5-C6-C7-C8
15	j	202	CLA	C13-C15-C16-C17
20	N	854	LMT	C7-C8-C9-C10
21	I	103	LMG	O6-C1-O1-C7
21	T	103	LMG	O6-C1-O1-C7
15	a	820	CLA	C10-C11-C12-C13
15	V	103	CLA	O1D-CGD-O2D-CED
15	B	835	CLA	O1D-CGD-O2D-CED
15	O	837	CLA	CBA-CGA-O2A-C1
15	a	809	CLA	CBA-CGA-O2A-C1
15	a	833	CLA	CBA-CGA-O2A-C1
15	f	201	CLA	CBA-CGA-O2A-C1
21	U	103	LMG	C19-C20-C21-C22
19	N	857	LHG	C23-C24-C25-C26
15	B	806	CLA	C3-C5-C6-C7
14	a	826	F6C	C2-C1-O2A-CGA
15	A	803	CLA	C16-C17-C18-C19
15	A	829	CLA	C11-C12-C13-C15
15	B	817	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
15	a	803	CLA	C16-C17-C18-C19
15	a	829	CLA	C11-C12-C13-C15
15	B	829	CLA	O1A-CGA-O2A-C1
15	O	803	CLA	C13-C15-C16-C17
19	Z	101	LHG	C25-C26-C27-C28
21	B	850	LMG	C13-C14-C15-C16
21	J	103	LMG	C39-C40-C41-C42
15	A	842	CLA	CBD-CGD-O2D-CED
20	a	854	LMT	C7-C8-C9-C10
21	U	103	LMG	C39-C40-C41-C42
21	b	849	LMG	C22-C23-C24-C25
15	B	840	CLA	O1D-CGD-O2D-CED
15	a	829	CLA	O1D-CGD-O2D-CED
21	W	206	LMG	O6-C5-C6-O5
15	N	839	CLA	C13-C15-C16-C17
15	b	824	CLA	C5-C6-C7-C8
21	B	850	LMG	C20-C21-C22-C23
21	N	855	LMG	C20-C21-C22-C23
22	b	850	LFA	C11-C12-C13-C14
15	A	833	CLA	O1A-CGA-O2A-C1
15	N	818	CLA	O1D-CGD-O2D-CED
19	W	207	LHG	C29-C30-C31-C32
20	A	853	LMT	C2-C1-O1'-C1'
20	N	853	LMT	C2-C1-O1'-C1'
20	a	853	LMT	C2-C1-O1'-C1'
20	a	854	LMT	C2-C1-O1'-C1'
22	O	850	LFA	C11-C12-C13-C14
14	a	802	F6C	O1D-CGD-O2D-CED
15	O	829	CLA	C8-C10-C11-C12
15	B	816	CLA	C4B-C3B-CAB-CBB
15	N	807	CLA	C4B-C3B-CAB-CBB
15	N	834	CLA	C4B-C3B-CAB-CBB
15	O	816	CLA	C4B-C3B-CAB-CBB
15	a	807	CLA	C4B-C3B-CAB-CBB
15	a	825	CLA	C4B-C3B-CAB-CBB
15	b	816	CLA	C4B-C3B-CAB-CBB
13	N	801	CL0	C16-C17-C18-C20
13	a	801	CL0	C16-C17-C18-C19
13	a	801	CL0	C16-C17-C18-C20
15	B	802	CLA	C16-C17-C18-C20
15	N	803	CLA	C16-C17-C18-C19
15	N	829	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
15	O	802	CLA	C16-C17-C18-C20
15	b	802	CLA	C16-C17-C18-C20
15	a	806	CLA	O1D-CGD-O2D-CED
21	h	103	LMG	C39-C40-C41-C42
15	B	806	CLA	C15-C16-C17-C18
15	O	830	CLA	C8-C10-C11-C12
15	b	803	CLA	C13-C15-C16-C17
19	f	203	LHG	C8-C7-O7-C5
19	l	101	LHG	C25-C26-C27-C28
15	A	807	CLA	C12-C13-C15-C16
15	A	818	CLA	C11-C12-C13-C15
15	B	802	CLA	C6-C7-C8-C10
15	N	818	CLA	C11-C12-C13-C15
15	O	802	CLA	C6-C7-C8-C10
15	a	818	CLA	C11-C12-C13-C15
15	b	802	CLA	C6-C7-C8-C10
15	b	810	CLA	C12-C13-C15-C16
19	k	101	LHG	C23-C24-C25-C26
15	F	201	CLA	CBA-CGA-O2A-C1
14	N	856	F6C	C10-C11-C12-C13
15	B	809	CLA	C5-C6-C7-C8
19	j	207	LHG	C13-C14-C15-C16
15	O	806	CLA	C3-C5-C6-C7
15	a	820	CLA	C3-C5-C6-C7
15	A	812	CLA	C3A-C2A-CAA-CBA
15	A	841	CLA	C3A-C2A-CAA-CBA
15	B	806	CLA	C3A-C2A-CAA-CBA
15	B	823	CLA	C3A-C2A-CAA-CBA
15	B	835	CLA	C3A-C2A-CAA-CBA
15	N	812	CLA	C3A-C2A-CAA-CBA
15	N	841	CLA	C3A-C2A-CAA-CBA
15	O	806	CLA	C3A-C2A-CAA-CBA
15	O	823	CLA	C3A-C2A-CAA-CBA
15	O	835	CLA	C3A-C2A-CAA-CBA
15	a	812	CLA	C3A-C2A-CAA-CBA
15	a	841	CLA	C3A-C2A-CAA-CBA
15	b	806	CLA	C3A-C2A-CAA-CBA
15	b	823	CLA	C3A-C2A-CAA-CBA
15	b	835	CLA	C3A-C2A-CAA-CBA
21	B	848	LMG	C22-C23-C24-C25
21	O	849	LMG	C22-C23-C24-C25
15	A	840	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	L	208	LHG	C29-C30-C31-C32
15	A	839	CLA	C13-C15-C16-C17
15	B	802	CLA	C15-C16-C17-C18
15	N	810	CLA	C5-C6-C7-C8
15	N	818	CLA	C10-C11-C12-C13
15	a	818	CLA	C10-C11-C12-C13
15	O	828	CLA	O1D-CGD-O2D-CED
19	N	851	LHG	C23-C24-C25-C26
13	N	801	CL0	C16-C17-C18-C19
15	O	817	CLA	C11-C12-C13-C15
15	B	837	CLA	O1A-CGA-O2A-C1
15	b	837	CLA	O1A-CGA-O2A-C1
19	F	204	LHG	C13-C14-C15-C16
19	l	101	LHG	C30-C31-C32-C33
21	O	849	LMG	C40-C41-C42-C43
15	N	817	CLA	CBD-CGD-O2D-CED
21	N	855	LMG	C21-C22-C23-C24
15	a	838	CLA	O1D-CGD-O2D-CED
15	b	840	CLA	O1D-CGD-O2D-CED
15	N	809	CLA	CBA-CGA-O2A-C1
15	S	201	CLA	CBA-CGA-O2A-C1
19	B	851	LHG	C12-C13-C14-C15
19	j	207	LHG	C29-C30-C31-C32
21	A	855	LMG	C21-C22-C23-C24
19	Y	101	LHG	C23-C24-C25-C26
21	L	207	LMG	C28-C29-C30-C31
15	B	816	CLA	C13-C15-C16-C17
19	N	857	LHG	C13-C14-C15-C16
22	B	849	LFA	C11-C12-C13-C14
15	O	837	CLA	O1A-CGA-O2A-C1
21	B	848	LMG	C40-C41-C42-C43
21	A	855	LMG	C20-C21-C22-C23
15	B	817	CLA	C11-C12-C13-C14
19	B	851	LHG	C23-C24-C25-C26
21	W	206	LMG	C28-C29-C30-C31
21	j	206	LMG	C28-C29-C30-C31
15	A	841	CLA	C2B-C3B-CAB-CBB
15	B	816	CLA	C2B-C3B-CAB-CBB
15	N	825	CLA	C2B-C3B-CAB-CBB
15	N	834	CLA	C2B-C3B-CAB-CBB
15	N	841	CLA	C2B-C3B-CAB-CBB
15	O	816	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	a	825	CLA	C2B-C3B-CAB-CBB
15	a	834	CLA	C2B-C3B-CAB-CBB
15	b	816	CLA	C2B-C3B-CAB-CBB
18	A	846	BCR	C1-C6-C7-C8
18	A	848	BCR	C23-C24-C25-C30
18	B	845	BCR	C1-C6-C7-C8
18	I	101	BCR	C23-C24-C25-C30
18	J	102	BCR	C23-C24-C25-C26
18	J	102	BCR	C23-C24-C25-C30
18	N	846	BCR	C1-C6-C7-C8
18	N	848	BCR	C23-C24-C25-C30
18	O	845	BCR	C1-C6-C7-C8
18	T	101	BCR	C23-C24-C25-C26
18	U	102	BCR	C23-C24-C25-C26
18	a	846	BCR	C1-C6-C7-C8
18	a	848	BCR	C23-C24-C25-C30
18	b	845	BCR	C1-C6-C7-C8
18	g	101	BCR	C23-C24-C25-C26
18	h	102	BCR	C23-C24-C25-C26
18	h	102	BCR	C23-C24-C25-C30
19	Y	101	LHG	C12-C13-C14-C15
21	L	207	LMG	C19-C20-C21-C22
21	b	849	LMG	C40-C41-C42-C43
15	B	802	CLA	CBD-CGD-O2D-CED
15	W	202	CLA	CBD-CGD-O2D-CED
14	B	832	F6C	C15-C16-C17-C18
15	O	809	CLA	C3-C5-C6-C7
19	L	208	LHG	C15-C16-C17-C18
19	N	851	LHG	C25-C26-C27-C28
21	W	206	LMG	C19-C20-C21-C22
15	N	831	CLA	C2A-CAA-CBA-CGA
15	O	821	CLA	C2A-CAA-CBA-CGA
15	O	824	CLA	C5-C6-C7-C8
15	a	809	CLA	O1A-CGA-O2A-C1
15	a	833	CLA	O1A-CGA-O2A-C1
15	f	201	CLA	O1A-CGA-O2A-C1
15	N	842	CLA	CBD-CGD-O2D-CED
19	f	203	LHG	O9-C7-O7-C5
15	O	812	CLA	C11-C10-C8-C7
15	b	812	CLA	C11-C10-C8-C7
15	A	829	CLA	C4-C3-C5-C6
15	A	812	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	N	812	CLA	C2-C3-C5-C6
15	N	829	CLA	C2-C3-C5-C6
15	A	838	CLA	O1D-CGD-O2D-CED
15	A	814	CLA	CBA-CGA-O2A-C1
15	A	818	CLA	CBA-CGA-O2A-C1
15	N	814	CLA	CBA-CGA-O2A-C1
15	N	832	CLA	CBA-CGA-O2A-C1
15	B	837	CLA	C14-C13-C15-C16
15	N	810	CLA	C11-C10-C8-C9
19	W	207	LHG	C13-C14-C15-C16
21	B	850	LMG	C21-C22-C23-C24
20	A	853	LMT	O5'-C1'-O1'-C1
15	a	810	CLA	C5-C6-C7-C8
15	F	201	CLA	O1A-CGA-O2A-C1
15	O	835	CLA	O1D-CGD-O2D-CED
19	k	101	LHG	C12-C13-C14-C15
21	j	206	LMG	C19-C20-C21-C22
21	g	103	LMG	C11-C12-C13-C14
15	A	810	CLA	C3-C5-C6-C7
15	a	814	CLA	CBA-CGA-O2A-C1
15	b	817	CLA	C11-C12-C13-C14
19	A	851	LHG	C8-C7-O7-C5
19	F	204	LHG	C8-C7-O7-C5
19	L	208	LHG	C8-C7-O7-C5
19	N	851	LHG	C8-C7-O7-C5
19	N	857	LHG	C8-C7-O7-C5
19	W	207	LHG	C8-C7-O7-C5
19	j	207	LHG	C8-C7-O7-C5
15	B	840	CLA	C15-C16-C17-C18
15	O	833	CLA	C5-C6-C7-C8
15	O	837	CLA	C15-C16-C17-C18
15	b	810	CLA	C13-C15-C16-C17
15	b	830	CLA	C8-C10-C11-C12
19	F	204	LHG	O9-C7-O7-C5
19	N	857	LHG	O9-C7-O7-C5
14	a	826	F6C	C8-C10-C11-C12
15	A	806	CLA	C5-C6-C7-C8
15	B	803	CLA	C15-C16-C17-C18
18	h	102	BCR	C7-C8-C9-C34
15	B	809	CLA	C3-C5-C6-C7
15	b	809	CLA	C3-C5-C6-C7
18	O	847	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	A	831	CLA	C2A-CAA-CBA-CGA
15	b	830	CLA	C2A-CAA-CBA-CGA
15	O	817	CLA	C11-C12-C13-C14
15	b	826	CLA	C4-C3-C5-C6
14	A	824	F6C	C2B-C3B-CAB-CBB
14	N	824	F6C	C2B-C3B-CAB-CBB
14	a	824	F6C	C2B-C3B-CAB-CBB
20	A	853	LMT	C2B-C1B-O1B-C4'
15	L	202	CLA	C13-C15-C16-C17
15	O	816	CLA	C13-C15-C16-C17
15	b	837	CLA	C15-C16-C17-C18
15	S	201	CLA	O1A-CGA-O2A-C1
15	B	833	CLA	C5-C6-C7-C8
15	N	806	CLA	C5-C6-C7-C8
15	N	828	CLA	C5-C6-C7-C8
15	N	839	CLA	C8-C10-C11-C12
15	W	202	CLA	C13-C15-C16-C17
15	a	806	CLA	C5-C6-C7-C8
15	B	820	CLA	O1D-CGD-O2D-CED
21	W	206	LMG	C29-C30-C31-C32
14	b	832	F6C	C15-C16-C17-C18
15	A	818	CLA	C10-C11-C12-C13
15	N	809	CLA	O1A-CGA-O2A-C1
19	Z	101	LHG	C31-C32-C33-C34
15	B	830	CLA	C8-C10-C11-C12
15	N	807	CLA	C15-C16-C17-C18
15	b	803	CLA	C15-C16-C17-C18
19	a	851	LHG	C25-C26-C27-C28
19	f	203	LHG	C24-C25-C26-C27
21	B	850	LMG	O6-C5-C6-O5
15	A	825	CLA	C3-C5-C6-C7
15	a	825	CLA	C3-C5-C6-C7
19	N	851	LHG	O7-C5-C6-O8
19	Z	101	LHG	C30-C31-C32-C33
19	f	203	LHG	C13-C14-C15-C16
15	b	838	CLA	O1D-CGD-O2D-CED
15	O	816	CLA	CBA-CGA-O2A-C1
15	b	816	CLA	CBA-CGA-O2A-C1
15	N	830	CLA	C5-C6-C7-C8
21	J	103	LMG	O6-C5-C6-O5
21	j	206	LMG	O6-C5-C6-O5
19	N	857	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
19	l	101	LHG	C31-C32-C33-C34
15	b	816	CLA	O1D-CGD-O2D-CED
14	j	201	F6C	C3A-C2A-CAA-CBA
21	h	103	LMG	C13-C14-C15-C16
14	B	832	F6C	C1A-C2A-CAA-CBA
15	A	822	CLA	C2A-CAA-CBA-CGA
15	B	802	CLA	C2A-CAA-CBA-CGA
15	B	821	CLA	C2A-CAA-CBA-CGA
15	N	822	CLA	C2A-CAA-CBA-CGA
15	N	839	CLA	C2A-CAA-CBA-CGA
15	O	802	CLA	C2A-CAA-CBA-CGA
15	a	804	CLA	C2A-CAA-CBA-CGA
15	a	822	CLA	C2A-CAA-CBA-CGA
15	b	802	CLA	C2A-CAA-CBA-CGA
15	b	821	CLA	C2A-CAA-CBA-CGA
15	N	819	CLA	CBD-CGD-O2D-CED
15	a	842	CLA	CBD-CGD-O2D-CED
15	N	838	CLA	O1D-CGD-O2D-CED
15	O	816	CLA	O1D-CGD-O2D-CED
15	A	814	CLA	O1A-CGA-O2A-C1
15	A	803	CLA	C1A-C2A-CAA-CBA
15	A	805	CLA	C1A-C2A-CAA-CBA
15	A	809	CLA	C1A-C2A-CAA-CBA
15	A	819	CLA	C1A-C2A-CAA-CBA
15	B	805	CLA	C1A-C2A-CAA-CBA
15	B	806	CLA	C1A-C2A-CAA-CBA
15	B	811	CLA	C1A-C2A-CAA-CBA
15	B	816	CLA	C1A-C2A-CAA-CBA
15	B	823	CLA	C1A-C2A-CAA-CBA
15	B	830	CLA	C1A-C2A-CAA-CBA
15	B	835	CLA	C1A-C2A-CAA-CBA
15	N	803	CLA	C1A-C2A-CAA-CBA
15	N	805	CLA	C1A-C2A-CAA-CBA
15	N	809	CLA	C1A-C2A-CAA-CBA
15	N	815	CLA	C1A-C2A-CAA-CBA
15	N	819	CLA	C1A-C2A-CAA-CBA
15	N	837	CLA	C1A-C2A-CAA-CBA
15	O	805	CLA	C1A-C2A-CAA-CBA
15	O	806	CLA	C1A-C2A-CAA-CBA
15	O	811	CLA	C1A-C2A-CAA-CBA
15	O	816	CLA	C1A-C2A-CAA-CBA
15	O	823	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	O	829	CLA	C1A-C2A-CAA-CBA
15	O	830	CLA	C1A-C2A-CAA-CBA
15	O	835	CLA	C1A-C2A-CAA-CBA
15	a	803	CLA	C1A-C2A-CAA-CBA
15	a	805	CLA	C1A-C2A-CAA-CBA
15	a	809	CLA	C1A-C2A-CAA-CBA
15	a	819	CLA	C1A-C2A-CAA-CBA
15	b	805	CLA	C1A-C2A-CAA-CBA
15	b	806	CLA	C1A-C2A-CAA-CBA
15	b	811	CLA	C1A-C2A-CAA-CBA
15	b	816	CLA	C1A-C2A-CAA-CBA
15	b	823	CLA	C1A-C2A-CAA-CBA
15	b	830	CLA	C1A-C2A-CAA-CBA
15	b	835	CLA	C1A-C2A-CAA-CBA
15	O	802	CLA	C15-C16-C17-C18
15	a	807	CLA	C15-C16-C17-C18
20	N	853	LMT	O5'-C1'-O1'-C1
15	N	814	CLA	O1A-CGA-O2A-C1
15	B	813	CLA	C8-C10-C11-C12
19	W	207	LHG	O9-C7-O7-C5
15	N	836	CLA	C5-C6-C7-C8
19	F	204	LHG	C24-C25-C26-C27
21	T	103	LMG	C30-C31-C32-C33
15	a	839	CLA	C3-C5-C6-C7
14	B	839	F6C	C11-C10-C8-C7
14	O	839	F6C	C11-C10-C8-C7
15	A	839	CLA	C6-C7-C8-C10
15	A	839	CLA	C11-C12-C13-C15
15	A	839	CLA	C12-C13-C15-C16
15	A	841	CLA	C6-C7-C8-C10
15	A	842	CLA	C11-C10-C8-C7
15	B	806	CLA	C11-C10-C8-C7
15	B	809	CLA	C12-C13-C15-C16
15	B	823	CLA	C11-C12-C13-C15
15	B	826	CLA	C12-C13-C15-C16
15	B	829	CLA	C11-C12-C13-C15
15	B	830	CLA	C11-C12-C13-C15
15	B	836	CLA	C12-C13-C15-C16
15	B	840	CLA	C12-C13-C15-C16
15	N	807	CLA	C12-C13-C15-C16
15	N	811	CLA	C6-C7-C8-C10
15	N	839	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	N	841	CLA	C6-C7-C8-C10
15	N	842	CLA	C11-C10-C8-C7
15	O	809	CLA	C12-C13-C15-C16
15	O	810	CLA	C6-C7-C8-C10
15	O	823	CLA	C11-C12-C13-C15
15	O	826	CLA	C12-C13-C15-C16
15	O	831	CLA	C6-C7-C8-C10
15	O	840	CLA	C12-C13-C15-C16
15	a	807	CLA	C12-C13-C15-C16
15	a	811	CLA	C6-C7-C8-C10
15	a	820	CLA	C12-C13-C15-C16
15	a	831	CLA	C6-C7-C8-C10
15	a	839	CLA	C6-C7-C8-C10
15	a	839	CLA	C11-C10-C8-C7
15	a	839	CLA	C12-C13-C15-C16
15	a	841	CLA	C6-C7-C8-C10
15	a	842	CLA	C11-C10-C8-C7
15	b	806	CLA	C11-C10-C8-C7
15	b	809	CLA	C12-C13-C15-C16
15	b	823	CLA	C11-C12-C13-C15
15	b	826	CLA	C12-C13-C15-C16
15	b	830	CLA	C11-C12-C13-C15
15	b	831	CLA	C6-C7-C8-C10
15	b	836	CLA	C12-C13-C15-C16
15	a	842	CLA	C16-C17-C18-C20
15	A	818	CLA	O1A-CGA-O2A-C1
15	N	832	CLA	O1A-CGA-O2A-C1
21	j	206	LMG	C29-C30-C31-C32
15	B	822	CLA	CBD-CGD-O2D-CED
14	A	826	F6C	C8-C10-C11-C12
20	a	853	LMT	C2B-C1B-O1B-C4'
15	N	841	CLA	C2-C3-C5-C6
15	O	817	CLA	C2-C3-C5-C6
15	b	817	CLA	C2-C3-C5-C6
19	j	207	LHG	C17-C18-C19-C20
14	N	826	F6C	C8-C10-C11-C12
15	A	842	CLA	C13-C15-C16-C17
15	B	837	CLA	C5-C6-C7-C8
15	O	813	CLA	C8-C10-C11-C12
14	A	802	F6C	O1D-CGD-O2D-CED
15	A	804	CLA	C2A-CAA-CBA-CGA
15	B	809	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	N	804	CLA	C2A-CAA-CBA-CGA
14	L	201	F6C	C11-C12-C13-C14
14	b	839	F6C	C11-C10-C8-C9
15	A	812	CLA	C11-C12-C13-C14
15	A	831	CLA	C6-C7-C8-C9
15	A	839	CLA	C6-C7-C8-C9
15	A	839	CLA	C11-C10-C8-C9
15	A	839	CLA	C11-C12-C13-C14
15	A	839	CLA	C14-C13-C15-C16
15	B	830	CLA	C11-C12-C13-C14
15	B	836	CLA	C14-C13-C15-C16
15	N	805	CLA	C11-C10-C8-C9
15	N	812	CLA	C11-C12-C13-C14
15	N	818	CLA	C14-C13-C15-C16
15	N	831	CLA	C6-C7-C8-C9
15	O	840	CLA	C14-C13-C15-C16
15	a	812	CLA	C11-C12-C13-C14
15	a	820	CLA	C14-C13-C15-C16
15	a	831	CLA	C6-C7-C8-C9
15	a	839	CLA	C6-C7-C8-C9
15	a	839	CLA	C11-C10-C8-C9
15	a	839	CLA	C11-C12-C13-C14
15	a	839	CLA	C14-C13-C15-C16
15	b	801	CLA	C11-C10-C8-C9
15	b	818	CLA	C11-C10-C8-C9
15	b	824	CLA	C11-C12-C13-C14
15	b	830	CLA	C11-C12-C13-C14
15	b	836	CLA	C14-C13-C15-C16
21	N	855	LMG	C29-C30-C31-C32
15	A	809	CLA	CBA-CGA-O2A-C1
15	B	812	CLA	CBA-CGA-O2A-C1
15	N	836	CLA	CBA-CGA-O2A-C1
15	O	812	CLA	CBA-CGA-O2A-C1
15	O	836	CLA	CBA-CGA-O2A-C1
15	a	818	CLA	CBA-CGA-O2A-C1
15	b	812	CLA	CBA-CGA-O2A-C1
15	b	836	CLA	CBA-CGA-O2A-C1
21	L	207	LMG	C29-C30-C31-C32
21	j	206	LMG	C33-C34-C35-C36
14	O	832	F6C	C1A-C2A-CAA-CBA
14	b	832	F6C	C1A-C2A-CAA-CBA
14	b	839	F6C	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	L	208	LHG	C13-C14-C15-C16
19	L	208	LHG	O9-C7-O7-C5
19	j	207	LHG	O9-C7-O7-C5
19	A	851	LHG	C4-C5-C6-O8
19	X	101	LHG	C4-C5-C6-O8
19	N	851	LHG	C4-C5-C6-O8
19	Z	101	LHG	C4-C5-C6-O8
19	l	101	LHG	C4-C5-C6-O8
20	N	853	LMT	C2B-C1B-O1B-C4'
15	j	202	CLA	O1D-CGD-O2D-CED
21	A	855	LMG	O6-C5-C6-O5
19	Z	101	LHG	C24-C25-C26-C27
15	A	839	CLA	C8-C10-C11-C12
15	B	803	CLA	C13-C15-C16-C17
15	B	810	CLA	C13-C15-C16-C17
19	N	851	LHG	C27-C28-C29-C30
15	b	823	CLA	O1D-CGD-O2D-CED
20	A	853	LMT	O5B-C5B-C6B-O6B
20	N	853	LMT	O5B-C5B-C6B-O6B
20	a	853	LMT	O5B-C5B-C6B-O6B
21	L	207	LMG	O6-C5-C6-O5
21	U	103	LMG	O6-C5-C6-O5
21	h	103	LMG	O6-C5-C6-O5
15	N	842	CLA	C16-C17-C18-C20
15	b	840	CLA	C16-C17-C18-C19
15	B	814	CLA	O1D-CGD-O2D-CED
15	a	842	CLA	C13-C15-C16-C17
15	b	833	CLA	C5-C6-C7-C8
21	J	103	LMG	C13-C14-C15-C16
15	a	814	CLA	O1A-CGA-O2A-C1
15	N	841	CLA	C4-C3-C5-C6
15	O	817	CLA	C4-C3-C5-C6
15	a	829	CLA	C4-C3-C5-C6
15	A	841	CLA	C2-C3-C5-C6
15	a	841	CLA	C2-C3-C5-C6
18	B	847	BCR	C7-C8-C9-C34
18	F	202	BCR	C11-C12-C13-C35
18	b	848	BCR	C7-C8-C9-C34
15	b	822	CLA	C6-C7-C8-C9
21	g	103	LMG	O6-C5-C6-O5
18	U	101	BCR	C21-C22-C23-C24
18	a	850	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
15	O	816	CLA	O1A-CGA-O2A-C1
15	b	816	CLA	O1A-CGA-O2A-C1
15	O	809	CLA	C5-C6-C7-C8
15	S	201	CLA	C5-C6-C7-C8
15	b	813	CLA	C8-C10-C11-C12
15	N	825	CLA	C3-C5-C6-C7
21	I	103	LMG	O6-C5-C6-O5
21	N	855	LMG	O6-C5-C6-O5
21	T	103	LMG	O6-C5-C6-O5
15	A	805	CLA	CBA-CGA-O2A-C1
15	B	816	CLA	CBA-CGA-O2A-C1
15	A	841	CLA	C15-C16-C17-C18
15	a	830	CLA	C5-C6-C7-C8
15	a	839	CLA	C8-C10-C11-C12
15	a	814	CLA	O1D-CGD-O2D-CED
14	N	856	F6C	C3B-C2B-CMB-OMB
14	a	855	F6C	C3B-C2B-CMB-OMB
15	a	842	CLA	C16-C17-C18-C19
14	B	839	F6C	C1A-C2A-CAA-CBA
19	Y	101	LHG	C25-C26-C27-C28
21	U	103	LMG	C12-C13-C14-C15
19	N	851	LHG	O9-C7-O7-C5
15	A	836	CLA	CBA-CGA-O2A-C1
15	N	818	CLA	CBA-CGA-O2A-C1
15	a	805	CLA	CBA-CGA-O2A-C1
19	X	101	LHG	C24-C23-O8-C6
19	N	851	LHG	C24-C23-O8-C6
19	X	101	LHG	C24-C25-C26-C27
19	W	207	LHG	C15-C16-C17-C18
19	k	101	LHG	C11-C12-C13-C14
15	A	841	CLA	C4-C3-C5-C6
15	a	841	CLA	C4-C3-C5-C6
21	I	103	LMG	C30-C31-C32-C33
19	X	101	LHG	C25-C26-C27-C28
21	L	207	LMG	C30-C31-C32-C33
21	j	206	LMG	C30-C31-C32-C33
15	N	825	CLA	CBA-CGA-O2A-C1
15	a	825	CLA	CBA-CGA-O2A-C1
14	A	824	F6C	C3A-C2A-CAA-CBA
14	L	201	F6C	C3A-C2A-CAA-CBA
14	N	824	F6C	C3A-C2A-CAA-CBA
14	W	201	F6C	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	W	207	LHG	C14-C15-C16-C17
19	j	207	LHG	C14-C15-C16-C17
15	O	833	CLA	O1D-CGD-O2D-CED
15	b	833	CLA	O1D-CGD-O2D-CED
15	A	821	CLA	CAA-CBA-CGA-O2A
15	a	819	CLA	C2A-CAA-CBA-CGA
15	j	203	CLA	C2A-CAA-CBA-CGA
15	O	838	CLA	C3-C5-C6-C7
19	a	851	LHG	C27-C28-C29-C30
15	b	814	CLA	O1D-CGD-O2D-CED
21	g	103	LMG	C12-C13-C14-C15
15	N	842	CLA	C16-C17-C18-C19
15	B	812	CLA	O1A-CGA-O2A-C1
15	O	812	CLA	O1A-CGA-O2A-C1
15	a	818	CLA	O1A-CGA-O2A-C1
21	j	206	LMG	C10-C11-C12-C13
15	A	832	CLA	CBA-CGA-O2A-C1
15	B	838	CLA	CBA-CGA-O2A-C1
15	N	805	CLA	CBA-CGA-O2A-C1
15	N	806	CLA	CBA-CGA-O2A-C1
15	a	836	CLA	CBA-CGA-O2A-C1
19	l	101	LHG	C24-C23-O8-C6
19	B	851	LHG	C25-C26-C27-C28
15	B	812	CLA	CBD-CGD-O2D-CED
15	N	820	CLA	CBD-CGD-O2D-CED
15	N	834	CLA	CBD-CGD-O2D-CED
15	O	822	CLA	CBD-CGD-O2D-CED
19	k	101	LHG	C25-C26-C27-C28
19	l	101	LHG	C24-C25-C26-C27
21	B	850	LMG	C29-C30-C31-C32
21	T	103	LMG	C32-C33-C34-C35
15	B	838	CLA	C3-C5-C6-C7
15	A	835	CLA	O1D-CGD-O2D-CED
15	N	812	CLA	C8-C10-C11-C12
15	f	201	CLA	C5-C6-C7-C8
15	b	840	CLA	C16-C17-C18-C20
15	b	817	CLA	C4-C3-C5-C6
15	b	831	CLA	C2-C3-C5-C6
21	L	207	LMG	C34-C35-C36-C37
15	A	825	CLA	CBA-CGA-O2A-C1
15	B	836	CLA	CBA-CGA-O2A-C1
15	A	836	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	B	851	LHG	C11-C12-C13-C14
19	F	204	LHG	C28-C29-C30-C31
14	O	839	F6C	C1A-C2A-CAA-CBA
19	A	851	LHG	O9-C7-O7-C5
20	A	854	LMT	C2-C1-O1'-C1'
20	N	854	LMT	C2-C1-O1'-C1'
14	A	856	F6C	C6-C7-C8-C9
14	B	839	F6C	C11-C10-C8-C9
14	O	839	F6C	C11-C10-C8-C9
15	A	805	CLA	C11-C10-C8-C9
15	A	807	CLA	C14-C13-C15-C16
15	A	810	CLA	C11-C10-C8-C9
15	A	818	CLA	C14-C13-C15-C16
15	A	828	CLA	C6-C7-C8-C9
15	A	831	CLA	C11-C12-C13-C14
15	A	841	CLA	C6-C7-C8-C9
15	B	801	CLA	C11-C10-C8-C9
15	B	809	CLA	C14-C13-C15-C16
15	B	823	CLA	C11-C12-C13-C14
15	B	826	CLA	C14-C13-C15-C16
15	B	840	CLA	C14-C13-C15-C16
15	N	807	CLA	C14-C13-C15-C16
15	N	839	CLA	C6-C7-C8-C9
15	N	839	CLA	C11-C12-C13-C14
15	N	839	CLA	C14-C13-C15-C16
15	N	841	CLA	C6-C7-C8-C9
15	N	842	CLA	C11-C10-C8-C9
15	O	801	CLA	C11-C10-C8-C9
15	O	809	CLA	C14-C13-C15-C16
15	O	818	CLA	C11-C10-C8-C9
15	O	823	CLA	C11-C12-C13-C14
15	O	826	CLA	C14-C13-C15-C16
15	O	836	CLA	C14-C13-C15-C16
15	O	840	CLA	C11-C12-C13-C14
15	a	805	CLA	C11-C10-C8-C9
15	a	807	CLA	C14-C13-C15-C16
15	a	818	CLA	C14-C13-C15-C16
15	a	830	CLA	C14-C13-C15-C16
15	a	841	CLA	C6-C7-C8-C9
15	b	809	CLA	C14-C13-C15-C16
15	b	823	CLA	C11-C12-C13-C14
15	b	826	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	b	840	CLA	C11-C12-C13-C14
15	B	837	CLA	C15-C16-C17-C18
15	N	818	CLA	C13-C15-C16-C17
15	N	842	CLA	C13-C15-C16-C17
15	a	841	CLA	C15-C16-C17-C18
19	X	101	LHG	C2-C3-O3-P
19	Z	101	LHG	C2-C3-O3-P
19	l	101	LHG	C2-C3-O3-P
15	A	807	CLA	C4B-C3B-CAB-CBB
15	A	825	CLA	C4B-C3B-CAB-CBB
15	A	834	CLA	C4B-C3B-CAB-CBB
15	B	819	CLA	C4B-C3B-CAB-CBB
15	N	825	CLA	C4B-C3B-CAB-CBB
15	O	801	CLA	C4B-C3B-CAB-CBB
15	O	819	CLA	C4B-C3B-CAB-CBB
15	b	801	CLA	C4B-C3B-CAB-CBB
15	i	103	CLA	C4B-C3B-CAB-CBB
19	f	203	LHG	C31-C32-C33-C34
15	O	802	CLA	O1D-CGD-O2D-CED
15	O	823	CLA	O1D-CGD-O2D-CED
15	N	821	CLA	CAA-CBA-CGA-O2A
21	W	206	LMG	C33-C34-C35-C36
14	a	824	F6C	C3A-C2A-CAA-CBA
15	A	828	CLA	C5-C6-C7-C8
15	F	201	CLA	C5-C6-C7-C8
15	b	809	CLA	C5-C6-C7-C8
14	L	201	F6C	C16-C17-C18-C20
15	A	835	CLA	C2A-CAA-CBA-CGA
15	N	819	CLA	C2A-CAA-CBA-CGA
15	A	818	CLA	C13-C15-C16-C17
15	b	837	CLA	C13-C15-C16-C17
15	A	819	CLA	CBD-CGD-O2D-CED
19	W	207	LHG	C17-C18-C19-C20
21	J	103	LMG	C12-C13-C14-C15
21	U	103	LMG	C13-C14-C15-C16
22	B	849	LFA	C13-C14-C15-C16
15	O	814	CLA	O1D-CGD-O2D-CED
14	L	201	F6C	C11-C12-C13-C15
14	O	839	F6C	C11-C12-C13-C15
14	b	839	F6C	C11-C10-C8-C7
14	b	839	F6C	C11-C12-C13-C15
15	A	805	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	A	805	CLA	C11-C10-C8-C7
15	A	811	CLA	C6-C7-C8-C10
15	A	812	CLA	C11-C12-C13-C15
15	A	828	CLA	C6-C7-C8-C10
15	A	830	CLA	C12-C13-C15-C16
15	A	831	CLA	C6-C7-C8-C10
15	A	839	CLA	C11-C10-C8-C7
15	B	801	CLA	C11-C10-C8-C7
15	B	807	CLA	C12-C13-C15-C16
15	B	813	CLA	C11-C12-C13-C15
15	B	824	CLA	C11-C12-C13-C15
15	N	805	CLA	C6-C7-C8-C10
15	N	805	CLA	C11-C10-C8-C7
15	N	812	CLA	C11-C12-C13-C15
15	N	830	CLA	C12-C13-C15-C16
15	N	831	CLA	C6-C7-C8-C10
15	N	839	CLA	C6-C7-C8-C10
15	N	839	CLA	C11-C12-C13-C15
15	O	801	CLA	C11-C10-C8-C7
15	O	806	CLA	C6-C7-C8-C10
15	O	806	CLA	C12-C13-C15-C16
15	O	807	CLA	C12-C13-C15-C16
15	O	812	CLA	C6-C7-C8-C10
15	O	818	CLA	C11-C10-C8-C7
15	O	824	CLA	C11-C12-C13-C15
15	O	836	CLA	C12-C13-C15-C16
15	a	805	CLA	C11-C10-C8-C7
15	a	809	CLA	C6-C7-C8-C10
15	a	812	CLA	C11-C12-C13-C15
15	a	830	CLA	C12-C13-C15-C16
15	a	839	CLA	C11-C12-C13-C15
15	b	801	CLA	C11-C10-C8-C7
15	b	806	CLA	C6-C7-C8-C10
15	b	807	CLA	C12-C13-C15-C16
15	b	812	CLA	C6-C7-C8-C10
15	b	818	CLA	C11-C10-C8-C7
15	b	824	CLA	C11-C12-C13-C15
15	b	829	CLA	C11-C12-C13-C15
15	A	812	CLA	C8-C10-C11-C12
15	N	820	CLA	C15-C16-C17-C18
15	B	823	CLA	O1D-CGD-O2D-CED
21	W	206	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
15	A	815	CLA	C3A-C2A-CAA-CBA
15	A	838	CLA	C3A-C2A-CAA-CBA
15	A	842	CLA	C3A-C2A-CAA-CBA
15	B	829	CLA	C3A-C2A-CAA-CBA
15	B	834	CLA	C3A-C2A-CAA-CBA
15	L	203	CLA	C3A-C2A-CAA-CBA
15	N	837	CLA	C3A-C2A-CAA-CBA
15	N	842	CLA	C3A-C2A-CAA-CBA
15	O	829	CLA	C3A-C2A-CAA-CBA
15	O	834	CLA	C3A-C2A-CAA-CBA
15	W	203	CLA	C3A-C2A-CAA-CBA
15	a	815	CLA	C3A-C2A-CAA-CBA
15	a	838	CLA	C3A-C2A-CAA-CBA
15	a	842	CLA	C3A-C2A-CAA-CBA
15	b	829	CLA	C3A-C2A-CAA-CBA
15	b	834	CLA	C3A-C2A-CAA-CBA
15	j	203	CLA	C3A-C2A-CAA-CBA
15	B	801	CLA	C13-C15-C16-C17
15	a	821	CLA	CAA-CBA-CGA-O2A
15	A	829	CLA	C2-C3-C5-C6
15	B	817	CLA	C2-C3-C5-C6
15	B	831	CLA	C2-C3-C5-C6
15	L	202	CLA	O1D-CGD-O2D-CED
20	a	853	LMT	O5'-C1'-O1'-C1
15	A	809	CLA	O1A-CGA-O2A-C1
15	N	836	CLA	O1A-CGA-O2A-C1
15	O	836	CLA	O1A-CGA-O2A-C1
15	b	812	CLA	O1A-CGA-O2A-C1
15	b	836	CLA	O1A-CGA-O2A-C1
15	a	812	CLA	C8-C10-C11-C12
15	O	838	CLA	CBA-CGA-O2A-C1
15	a	806	CLA	CBA-CGA-O2A-C1
15	O	833	CLA	C3-C5-C6-C7
15	a	807	CLA	C3-C5-C6-C7
14	b	839	F6C	C5-C6-C7-C8
18	b	847	BCR	C11-C12-C13-C35
15	A	805	CLA	O1A-CGA-O2A-C1
15	a	805	CLA	O1A-CGA-O2A-C1
15	A	817	CLA	O1D-CGD-O2D-CED
15	O	837	CLA	C10-C11-C12-C13
18	L	205	BCR	C21-C22-C23-C24
21	I	103	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
15	N	835	CLA	C2A-CAA-CBA-CGA
15	O	830	CLA	C2A-CAA-CBA-CGA
15	a	835	CLA	C2A-CAA-CBA-CGA
15	b	819	CLA	C2A-CAA-CBA-CGA
15	N	825	CLA	O1D-CGD-O2D-CED
19	A	851	LHG	C25-C26-C27-C28
15	N	838	CLA	C3-C5-C6-C7
15	b	838	CLA	C3-C5-C6-C7
15	b	822	CLA	C6-C7-C8-C10
19	f	203	LHG	C12-C13-C14-C15
15	B	816	CLA	O1A-CGA-O2A-C1
21	g	103	LMG	C29-C30-C31-C32
15	O	803	CLA	C15-C16-C17-C18
15	O	837	CLA	C13-C15-C16-C17
19	Y	101	LHG	C11-C12-C13-C14
21	g	103	LMG	C32-C33-C34-C35
15	B	817	CLA	C4-C3-C5-C6
15	B	831	CLA	C4-C3-C5-C6
15	b	831	CLA	C4-C3-C5-C6
19	X	101	LHG	C26-C27-C28-C29
15	N	840	CLA	O1D-CGD-O2D-CED
15	b	802	CLA	O1D-CGD-O2D-CED
15	A	842	CLA	C16-C17-C18-C20
15	A	825	CLA	C2B-C3B-CAB-CBB
15	A	834	CLA	C2B-C3B-CAB-CBB
15	B	819	CLA	C2B-C3B-CAB-CBB
15	i	103	CLA	C2B-C3B-CAB-CBB
18	B	843	BCR	C23-C24-C25-C26
18	I	102	BCR	C23-C24-C25-C30
18	U	102	BCR	C23-C24-C25-C30
21	T	103	LMG	C29-C30-C31-C32
15	B	821	CLA	CAA-CBA-CGA-O2A
15	B	837	CLA	C13-C15-C16-C17
15	A	807	CLA	C3-C5-C6-C7
21	W	206	LMG	C10-C11-C12-C13
15	N	841	CLA	C15-C16-C17-C18
15	b	816	CLA	C13-C15-C16-C17
15	b	829	CLA	C8-C10-C11-C12
14	O	839	F6C	C3A-C2A-CAA-CBA
14	N	802	F6C	C2A-CAA-CBA-CGA
13	A	801	CL0	CAA-CBA-CGA-O2A
15	b	821	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	B	819	CLA	C2A-CAA-CBA-CGA
15	W	203	CLA	C2A-CAA-CBA-CGA
19	A	851	LHG	O7-C5-C6-O8
19	N	857	LHG	O7-C5-C6-O8
19	f	203	LHG	O7-C5-C6-O8
21	J	103	LMG	O7-C8-C9-O8
21	U	103	LMG	O7-C8-C9-O8
15	B	812	CLA	C11-C10-C8-C7
15	N	818	CLA	O1A-CGA-O2A-C1
14	a	826	F6C	C4-C3-C5-C6
15	A	823	CLA	C4-C3-C5-C6
15	N	823	CLA	C4-C3-C5-C6
15	N	834	CLA	C4-C3-C5-C6
15	A	840	CLA	O1D-CGD-O2D-CED
14	a	826	F6C	C2-C3-C5-C6
14	W	201	F6C	C16-C17-C18-C20
15	a	806	CLA	C16-C17-C18-C20
19	f	203	LHG	C28-C29-C30-C31
15	A	842	CLA	O1D-CGD-O2D-CED
19	Z	101	LHG	C24-C23-O8-C6
15	b	833	CLA	C3-C5-C6-C7
15	B	807	CLA	C14-C13-C15-C16
15	B	810	CLA	C14-C13-C15-C16
15	B	818	CLA	C11-C10-C8-C9
15	B	824	CLA	C11-C12-C13-C14
15	N	828	CLA	C6-C7-C8-C9
15	N	830	CLA	C14-C13-C15-C16
15	O	807	CLA	C14-C13-C15-C16
15	O	810	CLA	C6-C7-C8-C9
15	O	810	CLA	C14-C13-C15-C16
15	O	824	CLA	C11-C12-C13-C14
15	O	830	CLA	C11-C12-C13-C14
15	a	828	CLA	C6-C7-C8-C9
15	a	842	CLA	C11-C10-C8-C9
15	b	807	CLA	C14-C13-C15-C16
19	X	101	LHG	C12-C13-C14-C15
21	h	103	LMG	C12-C13-C14-C15
15	a	836	CLA	C5-C6-C7-C8
21	h	103	LMG	C28-C29-C30-C31
19	X	101	LHG	O10-C23-O8-C6
21	j	206	LMG	C34-C35-C36-C37
20	N	854	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	O	822	CLA	C6-C7-C8-C10
15	N	817	CLA	O1D-CGD-O2D-CED
15	W	202	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	C3-C5-C6-C7
13	N	801	CL0	C3-C5-C6-C7
19	Z	101	LHG	C12-C13-C14-C15
14	B	839	F6C	C3A-C2A-CAA-CBA
20	a	854	LMT	C9-C10-C11-C12
15	L	203	CLA	C2A-CAA-CBA-CGA
15	N	807	CLA	C3-C5-C6-C7
15	b	805	CLA	C3-C5-C6-C7
15	N	835	CLA	C4-C3-C5-C6
19	N	857	LHG	C28-C29-C30-C31
15	O	821	CLA	CAA-CBA-CGA-O2A
15	N	823	CLA	C2-C3-C5-C6
15	A	842	CLA	C16-C17-C18-C19
15	b	812	CLA	CBD-CGD-O2D-CED
19	a	851	LHG	C8-C7-O7-C5
15	a	818	CLA	C13-C15-C16-C17
15	b	837	CLA	C10-C11-C12-C13
21	W	206	LMG	C34-C35-C36-C37
21	g	103	LMG	C30-C31-C32-C33
15	N	825	CLA	O1A-CGA-O2A-C1
15	a	825	CLA	O1A-CGA-O2A-C1
13	a	801	CL0	C3-C5-C6-C7
15	B	833	CLA	C3-C5-C6-C7
15	N	819	CLA	C3-C5-C6-C7
15	A	806	CLA	CBA-CGA-O2A-C1
15	b	838	CLA	CBA-CGA-O2A-C1
15	A	807	CLA	C15-C16-C17-C18
19	Y	101	LHG	C28-C29-C30-C31
15	B	822	CLA	C6-C7-C8-C10
19	F	204	LHG	C31-C32-C33-C34
15	B	808	CLA	C13-C15-C16-C17
15	B	837	CLA	C10-C11-C12-C13
15	a	828	CLA	C5-C6-C7-C8
18	A	848	BCR	C36-C18-C19-C20
18	O	848	BCR	C7-C8-C9-C34
18	a	848	BCR	C36-C18-C19-C20
19	l	101	LHG	C12-C13-C14-C15
14	B	839	F6C	C11-C12-C13-C15
15	A	809	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	A	812	CLA	C11-C10-C8-C7
15	B	812	CLA	C6-C7-C8-C10
15	B	818	CLA	C11-C10-C8-C7
15	N	809	CLA	C6-C7-C8-C10
15	N	812	CLA	C11-C10-C8-C7
15	N	828	CLA	C6-C7-C8-C10
15	O	806	CLA	C11-C10-C8-C7
15	O	813	CLA	C11-C12-C13-C15
15	O	830	CLA	C11-C12-C13-C15
15	a	805	CLA	C6-C7-C8-C10
15	a	812	CLA	C11-C10-C8-C7
15	a	828	CLA	C6-C7-C8-C10
15	b	809	CLA	C6-C7-C8-C10
15	b	824	CLA	C12-C13-C15-C16
21	L	207	LMG	C10-C11-C12-C13
21	J	103	LMG	C18-C19-C20-C21
21	U	103	LMG	C18-C19-C20-C21
19	B	851	LHG	C13-C14-C15-C16
19	k	101	LHG	C11-C10-C9-C8
15	O	836	CLA	C13-C15-C16-C17
18	A	850	BCR	C17-C18-C19-C20
18	B	847	BCR	C7-C8-C9-C10
18	F	202	BCR	C11-C12-C13-C14
18	J	102	BCR	C7-C8-C9-C10
18	N	850	BCR	C17-C18-C19-C20
18	O	848	BCR	C7-C8-C9-C10
18	U	102	BCR	C7-C8-C9-C10
18	b	848	BCR	C7-C8-C9-C10
14	A	802	F6C	C2A-CAA-CBA-CGA
14	A	824	F6C	C2A-CAA-CBA-CGA
14	a	802	F6C	C2A-CAA-CBA-CGA
14	a	824	F6C	C2A-CAA-CBA-CGA
15	A	825	CLA	O1A-CGA-O2A-C1
15	A	832	CLA	O1A-CGA-O2A-C1
15	A	836	CLA	O1A-CGA-O2A-C1
15	B	836	CLA	O1A-CGA-O2A-C1
15	A	819	CLA	C2A-CAA-CBA-CGA
15	O	828	CLA	C2A-CAA-CBA-CGA
19	L	208	LHG	C14-C15-C16-C17
15	B	812	CLA	C11-C10-C8-C9
15	O	812	CLA	C11-C10-C8-C9
15	b	812	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	A	806	CLA	C16-C17-C18-C20
15	O	822	CLA	C6-C7-C8-C9
21	I	103	LMG	C29-C30-C31-C32
13	N	801	CL0	CAA-CBA-CGA-O2A
15	B	838	CLA	O1A-CGA-O2A-C1
15	N	806	CLA	O1A-CGA-O2A-C1
15	O	838	CLA	O1A-CGA-O2A-C1
19	N	851	LHG	O10-C23-O8-C6
15	A	823	CLA	C2-C3-C5-C6
15	N	834	CLA	C2-C3-C5-C6
21	L	207	LMG	C33-C34-C35-C36
15	B	802	CLA	O1D-CGD-O2D-CED
15	N	835	CLA	CBD-CGD-O2D-CED
15	N	842	CLA	O1D-CGD-O2D-CED
15	N	805	CLA	O1A-CGA-O2A-C1
18	A	846	BCR	C9-C10-C11-C12
18	a	846	BCR	C9-C10-C11-C12
15	A	803	CLA	CBD-CGD-O2D-CED
22	b	850	LFA	C7-C8-C9-C10
21	A	855	LMG	C13-C14-C15-C16
22	b	850	LFA	C13-C14-C15-C16
20	A	854	LMT	C9-C10-C11-C12
15	a	806	CLA	O1A-CGA-O2A-C1
15	a	836	CLA	O1A-CGA-O2A-C1
19	l	101	LHG	O10-C23-O8-C6
15	O	837	CLA	C5-C6-C7-C8
19	a	851	LHG	C4-C5-C6-O8
21	J	103	LMG	C7-C8-C9-O8
14	L	201	F6C	C16-C17-C18-C19
15	B	812	CLA	C3-C5-C6-C7
15	B	805	CLA	C4-C3-C5-C6
15	O	831	CLA	C4-C3-C5-C6
15	a	835	CLA	C4-C3-C5-C6
15	B	828	CLA	C2A-CAA-CBA-CGA
15	O	819	CLA	C2A-CAA-CBA-CGA
15	b	828	CLA	C2A-CAA-CBA-CGA
15	N	835	CLA	C2-C3-C5-C6
15	b	826	CLA	C2-C3-C5-C6
21	U	103	LMG	C28-C29-C30-C31
15	A	820	CLA	C15-C16-C17-C18
19	F	204	LHG	O7-C5-C6-O8
19	a	851	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
21	h	103	LMG	O7-C8-C9-O8
15	N	820	CLA	C6-C7-C8-C9
15	N	831	CLA	C11-C12-C13-C14
15	b	809	CLA	C6-C7-C8-C9
15	a	806	CLA	C16-C17-C18-C19
15	b	833	CLA	C6-C7-C8-C10
15	A	839	CLA	CBA-CGA-O2A-C1
19	Z	101	LHG	O10-C23-O8-C6
13	a	801	CL0	C10-C11-C12-C13
14	W	201	F6C	C16-C17-C18-C19
15	O	808	CLA	C13-C15-C16-C17
15	B	826	CLA	C4-C3-C5-C6
15	O	830	CLA	C4-C3-C5-C6
14	N	824	F6C	C2A-CAA-CBA-CGA
15	O	812	CLA	C3-C5-C6-C7
15	N	819	CLA	O1D-CGD-O2D-CED
15	j	203	CLA	C10-C11-C12-C13
15	B	804	CLA	C2A-CAA-CBA-CGA
15	O	804	CLA	C2A-CAA-CBA-CGA
15	b	804	CLA	C2A-CAA-CBA-CGA
14	j	201	F6C	C16-C17-C18-C19
15	A	806	CLA	C16-C17-C18-C19
15	B	833	CLA	C6-C7-C8-C10
15	A	806	CLA	O1A-CGA-O2A-C1
15	b	838	CLA	O1A-CGA-O2A-C1
15	N	814	CLA	C5-C6-C7-C8
15	a	842	CLA	O1D-CGD-O2D-CED
19	N	857	LHG	C31-C32-C33-C34
19	B	851	LHG	C28-C29-C30-C31
15	b	812	CLA	C3-C5-C6-C7
15	O	810	CLA	C13-C15-C16-C17
21	N	855	LMG	C12-C13-C14-C15
15	A	812	CLA	C4B-C3B-CAB-CBB
15	A	817	CLA	C4B-C3B-CAB-CBB
15	A	819	CLA	C4B-C3B-CAB-CBB
15	A	839	CLA	C4B-C3B-CAB-CBB
15	A	842	CLA	C4B-C3B-CAB-CBB
15	B	811	CLA	C4B-C3B-CAB-CBB
15	B	831	CLA	C1A-C2A-CAA-CBA
15	B	835	CLA	C4B-C3B-CAB-CBB
15	B	840	CLA	C4B-C3B-CAB-CBB
15	F	201	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	K	103	CLA	C4B-C3B-CAB-CBB
15	N	812	CLA	C4B-C3B-CAB-CBB
15	N	817	CLA	C4B-C3B-CAB-CBB
15	N	819	CLA	C4B-C3B-CAB-CBB
15	N	839	CLA	C4B-C3B-CAB-CBB
15	N	842	CLA	C4B-C3B-CAB-CBB
15	O	811	CLA	C4B-C3B-CAB-CBB
15	O	835	CLA	C4B-C3B-CAB-CBB
15	O	840	CLA	C4B-C3B-CAB-CBB
15	V	103	CLA	C4B-C3B-CAB-CBB
15	a	812	CLA	C4B-C3B-CAB-CBB
15	a	817	CLA	C4B-C3B-CAB-CBB
15	a	819	CLA	C4B-C3B-CAB-CBB
15	a	839	CLA	C4B-C3B-CAB-CBB
15	a	842	CLA	C4B-C3B-CAB-CBB
15	b	811	CLA	C4B-C3B-CAB-CBB
15	b	819	CLA	C4B-C3B-CAB-CBB
15	b	825	CLA	C1A-C2A-CAA-CBA
15	b	835	CLA	C4B-C3B-CAB-CBB
15	b	840	CLA	C4B-C3B-CAB-CBB
15	f	201	CLA	C4B-C3B-CAB-CBB
15	O	821	CLA	CBA-CGA-O2A-C1
14	b	839	F6C	C3A-C2A-CAA-CBA
18	b	847	BCR	C11-C12-C13-C14
18	h	102	BCR	C7-C8-C9-C10
14	j	201	F6C	C16-C17-C18-C20
15	B	822	CLA	C6-C7-C8-C9
15	O	809	CLA	C2A-CAA-CBA-CGA
15	b	809	CLA	C2A-CAA-CBA-CGA
21	N	855	LMG	C13-C14-C15-C16
19	Y	101	LHG	C26-C27-C28-C29
22	O	850	LFA	C7-C8-C9-C10
15	a	838	CLA	C3-C5-C6-C7
15	B	806	CLA	C6-C7-C8-C10
15	B	806	CLA	C12-C13-C15-C16
15	B	808	CLA	C11-C12-C13-C15
15	B	813	CLA	C11-C10-C8-C7
15	B	824	CLA	C12-C13-C15-C16
15	N	820	CLA	C11-C12-C13-C15
15	O	813	CLA	C11-C10-C8-C7
15	O	817	CLA	C6-C7-C8-C10
15	a	829	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
15	b	806	CLA	C12-C13-C15-C16
15	b	813	CLA	C11-C10-C8-C7
15	b	813	CLA	C11-C12-C13-C15
19	Y	101	LHG	C30-C31-C32-C33
15	A	831	CLA	C16-C17-C18-C20
15	N	806	CLA	C16-C17-C18-C19
15	a	831	CLA	C16-C17-C18-C20
15	O	831	CLA	CAA-CBA-CGA-O2A
19	l	101	LHG	C9-C10-C11-C12
15	A	814	CLA	C5-C6-C7-C8
15	b	826	CLA	C10-C11-C12-C13
15	A	810	CLA	C3A-C2A-CAA-CBA
15	N	810	CLA	C3A-C2A-CAA-CBA
15	N	815	CLA	C3A-C2A-CAA-CBA
15	a	810	CLA	C3A-C2A-CAA-CBA
15	b	814	CLA	C3A-C2A-CAA-CBA
15	N	831	CLA	C16-C17-C18-C20
21	A	855	LMG	C12-C13-C14-C15
19	k	101	LHG	C13-C14-C15-C16
19	a	851	LHG	O9-C7-O7-C5
15	O	822	CLA	O1D-CGD-O2D-CED
15	A	842	CLA	C2A-CAA-CBA-CGA
15	N	842	CLA	C2A-CAA-CBA-CGA
14	O	839	F6C	C11-C12-C13-C14
15	A	812	CLA	C11-C10-C8-C9
15	A	842	CLA	C11-C10-C8-C9
15	B	812	CLA	C6-C7-C8-C9
15	B	829	CLA	C11-C10-C8-C9
15	N	805	CLA	C6-C7-C8-C9
15	N	812	CLA	C11-C10-C8-C9
15	O	812	CLA	C6-C7-C8-C9
15	O	829	CLA	C11-C10-C8-C9
15	O	831	CLA	C6-C7-C8-C9
15	a	805	CLA	C6-C7-C8-C9
15	a	812	CLA	C11-C10-C8-C9
15	b	829	CLA	C14-C13-C15-C16
15	b	831	CLA	C6-C7-C8-C9
15	O	801	CLA	C13-C15-C16-C17
18	h	102	BCR	C15-C16-C17-C18
15	b	833	CLA	C6-C7-C8-C9
15	A	830	CLA	C5-C6-C7-C8
15	a	835	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	A	826	F6C	C1B-C2B-CMB-OMB
14	N	826	F6C	C1B-C2B-CMB-OMB
14	O	832	F6C	C1B-C2B-CMB-OMB
14	a	826	F6C	C1B-C2B-CMB-OMB
15	b	808	CLA	C13-C15-C16-C17
19	A	851	LHG	C27-C28-C29-C30
15	N	835	CLA	C5-C6-C7-C8
15	O	805	CLA	C15-C16-C17-C18
15	a	803	CLA	C8-C10-C11-C12
15	b	801	CLA	C13-C15-C16-C17
21	h	103	LMG	C18-C19-C20-C21
21	U	103	LMG	C7-C8-C9-O8
21	h	103	LMG	C7-C8-C9-O8
15	B	815	CLA	C5-C6-C7-C8
15	b	805	CLA	C15-C16-C17-C18
19	k	101	LHG	C30-C31-C32-C33
15	A	816	CLA	CAD-CBD-CGD-O2D
15	B	822	CLA	CAD-CBD-CGD-O2D
15	N	816	CLA	CAD-CBD-CGD-O2D
15	O	822	CLA	CAD-CBD-CGD-O2D
15	a	816	CLA	CAD-CBD-CGD-O2D
15	b	822	CLA	CAD-CBD-CGD-O2D
15	N	834	CLA	O1D-CGD-O2D-CED
19	a	851	LHG	C11-C12-C13-C14
15	N	807	CLA	O1A-CGA-O2A-C1
15	a	807	CLA	O1A-CGA-O2A-C1
15	A	807	CLA	CBA-CGA-O2A-C1
15	N	807	CLA	CBA-CGA-O2A-C1
15	a	807	CLA	CBA-CGA-O2A-C1
15	O	831	CLA	C8-C10-C11-C12
15	O	833	CLA	C6-C7-C8-C10
15	a	842	CLA	C2A-CAA-CBA-CGA
15	B	838	CLA	C10-C11-C12-C13
15	A	807	CLA	O1A-CGA-O2A-C1
15	O	821	CLA	O1A-CGA-O2A-C1
15	A	819	CLA	O1D-CGD-O2D-CED
19	F	204	LHG	C12-C13-C14-C15
19	Y	101	LHG	C11-C10-C9-C8
19	B	851	LHG	C11-C10-C9-C8
14	A	826	F6C	CHA-CBD-CGD-O1D
14	N	826	F6C	CHA-CBD-CGD-O1D
15	A	807	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
15	A	807	CLA	CHA-CBD-CGD-O2D
15	A	816	CLA	CAD-CBD-CGD-O1D
15	A	817	CLA	CHA-CBD-CGD-O1D
15	A	817	CLA	CHA-CBD-CGD-O2D
15	A	825	CLA	CHA-CBD-CGD-O2D
15	B	820	CLA	CAD-CBD-CGD-O1D
15	B	822	CLA	CAD-CBD-CGD-O1D
15	N	807	CLA	CHA-CBD-CGD-O1D
15	N	807	CLA	CHA-CBD-CGD-O2D
15	N	816	CLA	CAD-CBD-CGD-O1D
15	N	817	CLA	CHA-CBD-CGD-O1D
15	N	817	CLA	CHA-CBD-CGD-O2D
15	O	802	CLA	CAD-CBD-CGD-O1D
15	O	822	CLA	CAD-CBD-CGD-O1D
15	V	102	CLA	CHA-CBD-CGD-O1D
15	V	102	CLA	CHA-CBD-CGD-O2D
15	a	807	CLA	CHA-CBD-CGD-O1D
15	a	807	CLA	CHA-CBD-CGD-O2D
15	a	816	CLA	CAD-CBD-CGD-O1D
15	a	817	CLA	CHA-CBD-CGD-O1D
15	a	817	CLA	CHA-CBD-CGD-O2D
15	a	825	CLA	CHA-CBD-CGD-O1D
15	a	825	CLA	CHA-CBD-CGD-O2D
15	b	802	CLA	CAD-CBD-CGD-O1D
15	b	822	CLA	CAD-CBD-CGD-O1D
15	b	828	CLA	CHA-CBD-CGD-O1D
15	i	102	CLA	CHA-CBD-CGD-O1D
15	i	102	CLA	CHA-CBD-CGD-O2D
18	J	102	BCR	C15-C16-C17-C18
18	N	846	BCR	C9-C10-C11-C12
18	U	102	BCR	C15-C16-C17-C18
19	A	851	LHG	C3-O3-P-O5
19	X	101	LHG	C3-O3-P-O4
19	X	101	LHG	C4-O6-P-O4
19	W	207	LHG	C3-O3-P-O6
19	Z	101	LHG	C3-O3-P-O4
19	Z	101	LHG	C4-O6-P-O4
19	l	101	LHG	C3-O3-P-O4
19	l	101	LHG	C4-O6-P-O4
19	X	101	LHG	C31-C32-C33-C34
21	A	855	LMG	C29-C30-C31-C32
22	O	850	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	A	834	CLA	C4-C3-C5-C6
15	L	203	CLA	C4-C3-C5-C6
15	O	826	CLA	C4-C3-C5-C6
15	A	812	CLA	C2B-C3B-CAB-CBB
15	A	819	CLA	C2B-C3B-CAB-CBB
15	A	839	CLA	C2B-C3B-CAB-CBB
15	B	840	CLA	C2B-C3B-CAB-CBB
15	K	103	CLA	C2B-C3B-CAB-CBB
15	N	807	CLA	C2B-C3B-CAB-CBB
15	N	812	CLA	C2B-C3B-CAB-CBB
15	N	819	CLA	C2B-C3B-CAB-CBB
15	N	839	CLA	C2B-C3B-CAB-CBB
15	O	819	CLA	C2B-C3B-CAB-CBB
15	O	840	CLA	C2B-C3B-CAB-CBB
15	S	201	CLA	C2B-C3B-CAB-CBB
15	V	103	CLA	C2B-C3B-CAB-CBB
15	a	807	CLA	C2B-C3B-CAB-CBB
15	a	812	CLA	C2B-C3B-CAB-CBB
15	a	819	CLA	C2B-C3B-CAB-CBB
15	a	839	CLA	C2B-C3B-CAB-CBB
15	b	819	CLA	C2B-C3B-CAB-CBB
15	b	840	CLA	C2B-C3B-CAB-CBB
15	B	805	CLA	C2-C3-C5-C6
15	O	830	CLA	C2-C3-C5-C6
15	O	831	CLA	C2-C3-C5-C6
15	a	829	CLA	C2-C3-C5-C6
15	a	835	CLA	C2-C3-C5-C6
15	N	820	CLA	O1D-CGD-O2D-CED
19	X	101	LHG	C5-C4-O6-P
19	B	851	LHG	C30-C31-C32-C33
15	N	803	CLA	C8-C10-C11-C12
22	B	849	LFA	C10-C11-C12-C13
15	B	833	CLA	C6-C7-C8-C9
15	N	806	CLA	C16-C17-C18-C20
15	A	839	CLA	O1A-CGA-O2A-C1
15	B	822	CLA	O1D-CGD-O2D-CED
15	A	836	CLA	C6-C7-C8-C9
14	O	839	F6C	C5-C6-C7-C8
15	a	820	CLA	C15-C16-C17-C18
15	b	831	CLA	CAA-CBA-CGA-O2A
15	L	203	CLA	C10-C11-C12-C13
15	b	815	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	b	837	CLA	C5-C6-C7-C8
15	a	839	CLA	C16-C17-C18-C20
15	O	815	CLA	C5-C6-C7-C8
19	N	857	LHG	C12-C13-C14-C15
14	B	839	F6C	C11-C12-C13-C14
14	b	839	F6C	C11-C12-C13-C14
15	A	805	CLA	C6-C7-C8-C9
15	A	819	CLA	C11-C10-C8-C9
15	A	820	CLA	C14-C13-C15-C16
15	A	830	CLA	C14-C13-C15-C16
15	B	810	CLA	C6-C7-C8-C9
15	B	817	CLA	C6-C7-C8-C9
15	L	202	CLA	C11-C10-C8-C9
15	O	806	CLA	C14-C13-C15-C16
15	O	817	CLA	C6-C7-C8-C9
15	a	819	CLA	C11-C10-C8-C9
15	a	831	CLA	C11-C12-C13-C14
15	b	806	CLA	C6-C7-C8-C9
15	b	812	CLA	C6-C7-C8-C9
15	b	817	CLA	C6-C7-C8-C9
15	b	829	CLA	C11-C10-C8-C9
15	N	813	CLA	C6-C7-C8-C9
15	A	820	CLA	C12-C13-C15-C16
15	B	810	CLA	C6-C7-C8-C10
15	B	817	CLA	C6-C7-C8-C10
15	B	831	CLA	C6-C7-C8-C10
15	N	829	CLA	C11-C10-C8-C7
15	O	809	CLA	C6-C7-C8-C10
15	O	824	CLA	C12-C13-C15-C16
15	b	817	CLA	C6-C7-C8-C10
15	A	839	CLA	C16-C17-C18-C20
15	N	839	CLA	C16-C17-C18-C20
19	Y	101	LHG	C13-C14-C15-C16
22	O	850	LFA	C13-C14-C15-C16
20	A	853	LMT	C2'-C1'-O1'-C1
20	N	853	LMT	C2'-C1'-O1'-C1
20	a	853	LMT	C2'-C1'-O1'-C1
15	A	809	CLA	CBD-CGD-O2D-CED
15	A	829	CLA	C10-C11-C12-C13
15	a	834	CLA	C4-C3-C5-C6
15	j	203	CLA	C4-C3-C5-C6
19	l	101	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
21	J	103	LMG	C28-C29-C30-C31
19	L	208	LHG	C17-C18-C19-C20
19	L	208	LHG	C33-C34-C35-C36
19	Z	101	LHG	C5-C4-O6-P
15	B	831	CLA	CAA-CBA-CGA-O2A
15	N	812	CLA	C16-C17-C18-C19
15	O	833	CLA	C6-C7-C8-C9
19	Z	101	LHG	C11-C10-C9-C8
15	O	805	CLA	C3-C5-C6-C7
15	a	829	CLA	C10-C11-C12-C13
15	W	203	CLA	C4-C3-C5-C6
13	a	801	CL0	CAA-CBA-CGA-O2A
22	B	849	LFA	C7-C8-C9-C10
15	N	835	CLA	O1D-CGD-O2D-CED
15	N	829	CLA	C10-C11-C12-C13
19	j	207	LHG	C15-C16-C17-C18
18	B	845	BCR	C36-C18-C19-C20
15	B	837	CLA	C16-C17-C18-C20
21	W	206	LMG	C29-C28-O8-C9
15	O	824	CLA	C10-C11-C12-C13
21	A	855	LMG	C8-C7-O1-C1
21	N	855	LMG	C8-C7-O1-C1
15	A	814	CLA	C2A-CAA-CBA-CGA
15	A	837	CLA	C2A-CAA-CBA-CGA
15	N	814	CLA	C2A-CAA-CBA-CGA
15	a	837	CLA	C2A-CAA-CBA-CGA
15	b	807	CLA	C2A-CAA-CBA-CGA
15	A	803	CLA	O1D-CGD-O2D-CED
15	B	812	CLA	O1D-CGD-O2D-CED
15	N	822	CLA	C16-C17-C18-C20
15	L	203	CLA	C2-C3-C5-C6
19	k	101	LHG	C28-C29-C30-C31
15	B	831	CLA	C8-C10-C11-C12
15	B	806	CLA	C6-C7-C8-C9
15	B	806	CLA	C14-C13-C15-C16
15	B	813	CLA	C11-C10-C8-C9
15	B	813	CLA	C14-C13-C15-C16
15	B	831	CLA	C6-C7-C8-C9
15	O	806	CLA	C6-C7-C8-C9
15	O	809	CLA	C6-C7-C8-C9
15	O	813	CLA	C11-C10-C8-C9
15	b	806	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	b	810	CLA	C6-C7-C8-C9
15	b	813	CLA	C11-C10-C8-C9
15	O	826	CLA	C10-C11-C12-C13
15	A	813	CLA	C6-C7-C8-C9
15	B	801	CLA	C4B-C3B-CAB-CBB
15	S	201	CLA	C4B-C3B-CAB-CBB
15	a	822	CLA	CBD-CGD-O2D-CED
15	A	822	CLA	C16-C17-C18-C20
15	O	837	CLA	C16-C17-C18-C20
15	b	837	CLA	C16-C17-C18-C20
15	B	821	CLA	CBA-CGA-O2A-C1
15	N	803	CLA	CBA-CGA-O2A-C1
15	b	821	CLA	CBA-CGA-O2A-C1
21	L	207	LMG	C29-C28-O8-C9
15	B	824	CLA	C10-C11-C12-C13
15	B	829	CLA	C8-C10-C11-C12
15	O	823	CLA	C8-C10-C11-C12
15	B	830	CLA	C4-C3-C5-C6
19	B	851	LHG	C26-C27-C28-C29
19	A	851	LHG	C11-C12-C13-C14
21	W	206	LMG	O10-C28-O8-C9
18	A	845	BCR	C15-C16-C17-C18
14	A	824	F6C	C4B-C3B-CAB-CBB
14	N	824	F6C	C4B-C3B-CAB-CBB
14	a	824	F6C	C4B-C3B-CAB-CBB
22	b	850	LFA	C6-C7-C8-C9
19	N	857	LHG	C34-C35-C36-C37
15	B	809	CLA	C6-C7-C8-C10
15	B	813	CLA	C12-C13-C15-C16
15	N	839	CLA	C11-C10-C8-C7
15	B	826	CLA	C10-C11-C12-C13
15	b	812	CLA	O1D-CGD-O2D-CED
15	W	203	CLA	C10-C11-C12-C13
15	a	803	CLA	CBA-CGA-O2A-C1
19	a	851	LHG	C24-C23-O8-C6
15	N	812	CLA	C16-C17-C18-C20
15	A	821	CLA	CAA-CBA-CGA-O1A
15	N	807	CLA	C5-C6-C7-C8
21	L	207	LMG	O10-C28-O8-C9
15	A	809	CLA	O1D-CGD-O2D-CED
15	A	809	CLA	C4-C3-C5-C6
15	A	821	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	837	CLA	C3A-C2A-CAA-CBA
15	N	838	CLA	C3A-C2A-CAA-CBA
15	O	814	CLA	C3A-C2A-CAA-CBA
15	a	837	CLA	C3A-C2A-CAA-CBA
15	b	825	CLA	C3A-C2A-CAA-CBA
13	N	801	CL0	C13-C15-C16-C17
19	B	851	LHG	C10-C11-C12-C13
15	j	203	CLA	C2-C3-C5-C6
19	Y	101	LHG	C33-C34-C35-C36
22	b	850	LFA	C10-C11-C12-C13
18	A	848	BCR	C16-C17-C18-C36
18	A	850	BCR	C11-C10-C9-C34
18	A	850	BCR	C16-C17-C18-C36
18	B	843	BCR	C11-C10-C9-C34
18	B	844	BCR	C11-C10-C9-C34
18	B	844	BCR	C20-C21-C22-C37
18	F	203	BCR	C35-C13-C14-C15
18	I	102	BCR	C20-C21-C22-C37
18	J	102	BCR	C16-C17-C18-C36
18	N	848	BCR	C16-C17-C18-C36
18	N	850	BCR	C11-C10-C9-C34
18	N	850	BCR	C16-C17-C18-C36
18	O	843	BCR	C11-C10-C9-C34
18	O	844	BCR	C11-C10-C9-C34
18	O	844	BCR	C20-C21-C22-C37
18	S	202	BCR	C35-C13-C14-C15
18	T	102	BCR	C20-C21-C22-C37
18	U	102	BCR	C16-C17-C18-C36
18	a	848	BCR	C16-C17-C18-C36
18	a	850	BCR	C11-C10-C9-C34
18	a	850	BCR	C16-C17-C18-C36
18	b	843	BCR	C11-C10-C9-C34
18	b	844	BCR	C11-C10-C9-C34
18	b	844	BCR	C20-C21-C22-C37
18	f	202	BCR	C35-C13-C14-C15
18	g	102	BCR	C20-C21-C22-C37
18	h	102	BCR	C16-C17-C18-C36
15	A	835	CLA	C5-C6-C7-C8
15	O	808	CLA	C8-C10-C11-C12
15	B	821	CLA	O1A-CGA-O2A-C1
15	O	840	CLA	C13-C15-C16-C17
15	b	824	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	b	840	CLA	C13-C15-C16-C17
18	N	848	BCR	C36-C18-C19-C20
18	O	845	BCR	C36-C18-C19-C20
19	l	101	LHG	C5-C4-O6-P
15	a	811	CLA	C4-C3-C5-C6
15	b	830	CLA	C4-C3-C5-C6
15	A	842	CLA	C15-C16-C17-C18
15	B	823	CLA	C8-C10-C11-C12
15	B	807	CLA	C2A-CAA-CBA-CGA
15	O	826	CLA	C2A-CAA-CBA-CGA
15	O	809	CLA	C10-C11-C12-C13
19	N	857	LHG	C17-C18-C19-C20
19	k	101	LHG	C26-C27-C28-C29
15	A	804	CLA	C14-C13-C15-C16
15	A	820	CLA	C6-C7-C8-C9
15	B	809	CLA	C6-C7-C8-C9
15	B	815	CLA	C6-C7-C8-C9
15	B	837	CLA	C11-C10-C8-C9
15	B	838	CLA	C6-C7-C8-C9
15	N	804	CLA	C14-C13-C15-C16
15	N	820	CLA	C14-C13-C15-C16
15	N	839	CLA	C11-C10-C8-C9
15	O	813	CLA	C14-C13-C15-C16
15	O	831	CLA	C11-C10-C8-C9
15	O	838	CLA	C6-C7-C8-C9
15	W	202	CLA	C11-C10-C8-C9
15	a	820	CLA	C6-C7-C8-C9
15	b	813	CLA	C14-C13-C15-C16
15	b	828	CLA	C11-C10-C8-C9
15	b	838	CLA	C6-C7-C8-C9
21	U	103	LMG	C17-C18-C19-C20
19	Y	101	LHG	O1-C1-C2-C3
15	a	822	CLA	O1D-CGD-O2D-CED
15	F	201	CLA	C16-C17-C18-C20
15	B	805	CLA	C15-C16-C17-C18
15	B	836	CLA	C13-C15-C16-C17
15	N	828	CLA	C13-C15-C16-C17
20	N	853	LMT	C5'-C4'-O1B-C1B
15	O	812	CLA	CBD-CGD-O2D-CED
15	b	808	CLA	C5-C6-C7-C8
18	O	846	BCR	C15-C16-C17-C18
19	f	203	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
15	O	805	CLA	C4-C3-C5-C6
15	O	840	CLA	C4-C3-C5-C6
15	B	815	CLA	CBA-CGA-O2A-C1
22	B	849	LFA	C6-C7-C8-C9
15	a	817	CLA	CBD-CGD-O2D-CED
15	N	819	CLA	CAA-CBA-CGA-O2A
15	W	203	CLA	C2-C3-C5-C6
15	b	830	CLA	C2-C3-C5-C6
19	Y	101	LHG	O1-C1-C2-O2
15	b	821	CLA	O1A-CGA-O2A-C1
15	B	835	CLA	CAA-CBA-CGA-O2A
15	b	835	CLA	CAA-CBA-CGA-O1A
15	B	803	CLA	C2A-CAA-CBA-CGA
15	B	826	CLA	C2A-CAA-CBA-CGA
15	N	837	CLA	C2A-CAA-CBA-CGA
15	O	807	CLA	C2A-CAA-CBA-CGA
15	a	814	CLA	C2A-CAA-CBA-CGA
15	b	826	CLA	C2A-CAA-CBA-CGA
15	A	837	CLA	C1A-C2A-CAA-CBA
15	A	838	CLA	C1A-C2A-CAA-CBA
15	B	810	CLA	C1A-C2A-CAA-CBA
15	B	825	CLA	C1A-C2A-CAA-CBA
15	O	821	CLA	C1A-C2A-CAA-CBA
15	O	825	CLA	C1A-C2A-CAA-CBA
15	W	203	CLA	C1A-C2A-CAA-CBA
15	a	837	CLA	C1A-C2A-CAA-CBA
15	a	838	CLA	C1A-C2A-CAA-CBA
15	b	821	CLA	C1A-C2A-CAA-CBA
15	b	831	CLA	C1A-C2A-CAA-CBA
15	j	203	CLA	C1A-C2A-CAA-CBA
18	A	848	BCR	C16-C17-C18-C19
18	A	850	BCR	C11-C10-C9-C8
18	A	850	BCR	C16-C17-C18-C19
18	B	843	BCR	C11-C10-C9-C8
18	B	844	BCR	C11-C10-C9-C8
18	B	844	BCR	C20-C21-C22-C23
18	F	203	BCR	C12-C13-C14-C15
18	I	102	BCR	C20-C21-C22-C23
18	J	102	BCR	C16-C17-C18-C19
18	N	848	BCR	C16-C17-C18-C19
18	N	850	BCR	C11-C10-C9-C8
18	N	850	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	O	843	BCR	C11-C10-C9-C8
18	O	844	BCR	C11-C10-C9-C8
18	O	844	BCR	C20-C21-C22-C23
18	S	202	BCR	C12-C13-C14-C15
18	T	102	BCR	C20-C21-C22-C23
18	U	102	BCR	C16-C17-C18-C19
18	a	848	BCR	C16-C17-C18-C19
18	a	850	BCR	C11-C10-C9-C8
18	a	850	BCR	C16-C17-C18-C19
18	b	843	BCR	C11-C10-C9-C8
18	b	844	BCR	C11-C10-C9-C8
18	b	844	BCR	C20-C21-C22-C23
18	f	202	BCR	C12-C13-C14-C15
18	g	102	BCR	C20-C21-C22-C23
18	h	102	BCR	C16-C17-C18-C19
19	k	101	LHG	C33-C34-C35-C36
19	j	207	LHG	C33-C34-C35-C36
15	N	821	CLA	CAA-CBA-CGA-O1A
15	A	807	CLA	C2B-C3B-CAB-CBB
15	A	817	CLA	C2B-C3B-CAB-CBB
15	A	842	CLA	C2B-C3B-CAB-CBB
15	B	801	CLA	C2B-C3B-CAB-CBB
15	B	811	CLA	C2B-C3B-CAB-CBB
15	B	835	CLA	C2B-C3B-CAB-CBB
15	F	201	CLA	C2B-C3B-CAB-CBB
15	N	817	CLA	C2B-C3B-CAB-CBB
15	N	842	CLA	C2B-C3B-CAB-CBB
15	O	811	CLA	C2B-C3B-CAB-CBB
15	O	835	CLA	C2B-C3B-CAB-CBB
15	a	817	CLA	C2B-C3B-CAB-CBB
15	a	842	CLA	C2B-C3B-CAB-CBB
15	b	811	CLA	C2B-C3B-CAB-CBB
15	b	835	CLA	C2B-C3B-CAB-CBB
15	f	201	CLA	C2B-C3B-CAB-CBB
18	A	847	BCR	C1-C6-C7-C8
18	A	847	BCR	C5-C6-C7-C8
18	A	849	BCR	C1-C6-C7-C8
18	A	850	BCR	C5-C6-C7-C8
18	B	842	BCR	C23-C24-C25-C26
18	B	845	BCR	C23-C24-C25-C26
18	B	845	BCR	C23-C24-C25-C30
18	B	847	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	I	102	BCR	C23-C24-C25-C26
18	J	102	BCR	C1-C6-C7-C8
18	L	206	BCR	C5-C6-C7-C8
18	L	210	BCR	C5-C6-C7-C8
18	N	847	BCR	C1-C6-C7-C8
18	N	847	BCR	C5-C6-C7-C8
18	N	847	BCR	C23-C24-C25-C26
18	N	849	BCR	C1-C6-C7-C8
18	N	850	BCR	C5-C6-C7-C8
18	O	845	BCR	C23-C24-C25-C26
18	O	845	BCR	C23-C24-C25-C30
18	O	848	BCR	C5-C6-C7-C8
18	T	102	BCR	C23-C24-C25-C26
18	T	102	BCR	C23-C24-C25-C30
18	U	102	BCR	C1-C6-C7-C8
18	W	209	BCR	C5-C6-C7-C8
18	a	847	BCR	C5-C6-C7-C8
18	a	847	BCR	C23-C24-C25-C26
18	a	849	BCR	C1-C6-C7-C8
18	a	850	BCR	C5-C6-C7-C8
18	b	842	BCR	C23-C24-C25-C26
18	b	843	BCR	C23-C24-C25-C26
18	b	845	BCR	C23-C24-C25-C26
18	b	845	BCR	C23-C24-C25-C30
18	b	848	BCR	C5-C6-C7-C8
18	g	102	BCR	C23-C24-C25-C26
18	g	102	BCR	C23-C24-C25-C30
18	h	102	BCR	C1-C6-C7-C8
15	b	831	CLA	C8-C10-C11-C12
21	T	103	LMG	C33-C34-C35-C36
15	A	814	CLA	C3-C5-C6-C7
15	B	835	CLA	CAA-CBA-CGA-O1A
15	b	835	CLA	CAA-CBA-CGA-O2A
15	b	821	CLA	C4-C3-C5-C6
19	f	203	LHG	C32-C33-C34-C35
14	N	856	F6C	C11-C10-C8-C7
15	A	818	CLA	C11-C10-C8-C7
15	A	829	CLA	C11-C10-C8-C7
15	B	826	CLA	C6-C7-C8-C10
15	N	820	CLA	C11-C10-C8-C7
15	N	825	CLA	C11-C10-C8-C7
15	O	829	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
15	a	810	CLA	C11-C10-C8-C7
15	a	820	CLA	C11-C12-C13-C15
15	a	825	CLA	C11-C10-C8-C7
15	b	810	CLA	C6-C7-C8-C10
15	A	820	CLA	C16-C17-C18-C20
15	N	822	CLA	C16-C17-C18-C19
15	f	201	CLA	C16-C17-C18-C20
20	A	853	LMT	C5'-C4'-O1B-C1B
15	A	838	CLA	C2A-CAA-CBA-CGA
15	O	803	CLA	C2A-CAA-CBA-CGA
15	b	803	CLA	C2A-CAA-CBA-CGA
19	l	101	LHG	C33-C34-C35-C36
19	f	203	LHG	C15-C16-C17-C18
15	b	836	CLA	C13-C15-C16-C17
15	A	819	CLA	C3-C5-C6-C7
15	O	835	CLA	CAA-CBA-CGA-O2A
19	W	207	LHG	C33-C34-C35-C36
15	a	813	CLA	C6-C7-C8-C9
18	L	205	BCR	C7-C8-C9-C34
19	B	851	LHG	C29-C30-C31-C32
15	a	823	CLA	C4-C3-C5-C6
15	A	834	CLA	C2-C3-C5-C6
15	B	830	CLA	C2-C3-C5-C6
15	a	834	CLA	C2-C3-C5-C6
15	N	818	CLA	C5-C6-C7-C8
15	O	801	CLA	C8-C10-C11-C12
15	A	812	CLA	C16-C17-C18-C19
15	a	803	CLA	C15-C16-C17-C18
15	b	823	CLA	C8-C10-C11-C12
15	a	817	CLA	O1D-CGD-O2D-CED
15	N	814	CLA	C3-C5-C6-C7
20	a	853	LMT	C5'-C4'-O1B-C1B
15	A	829	CLA	C2A-CAA-CBA-CGA
14	W	201	F6C	C11-C12-C13-C14
15	B	831	CLA	C11-C10-C8-C9
15	b	818	CLA	C11-C12-C13-C14
19	k	101	LHG	C31-C32-C33-C34
19	f	203	LHG	C11-C10-C9-C8
21	b	849	LMG	C31-C32-C33-C34
14	A	826	F6C	O1A-CGA-O2A-C1
15	A	803	CLA	C15-C16-C17-C18
19	B	851	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
15	O	835	CLA	CAA-CBA-CGA-O1A
15	b	821	CLA	C5-C6-C7-C8
15	N	803	CLA	O1A-CGA-O2A-C1
15	S	201	CLA	C15-C16-C17-C18
15	A	819	CLA	CAA-CBA-CGA-O2A
15	B	826	CLA	C2-C3-C5-C6
14	L	204	F6C	C10-C11-C12-C13
15	N	842	CLA	C15-C16-C17-C18
15	A	822	CLA	C16-C17-C18-C19
19	N	851	LHG	C11-C12-C13-C14
15	A	816	CLA	CAA-CBA-CGA-O2A
15	B	840	CLA	C13-C15-C16-C17
15	B	815	CLA	O1A-CGA-O2A-C1
19	a	851	LHG	O10-C23-O8-C6
19	X	101	LHG	C28-C29-C30-C31
19	f	203	LHG	C17-C18-C19-C20
15	N	836	CLA	C6-C7-C8-C9
15	O	815	CLA	O1D-CGD-O2D-CED
15	a	816	CLA	CAA-CBA-CGA-O2A
15	a	803	CLA	O1A-CGA-O2A-C1
15	N	829	CLA	C2A-CAA-CBA-CGA
15	a	829	CLA	C2A-CAA-CBA-CGA
15	b	805	CLA	C2A-CAA-CBA-CGA
15	B	801	CLA	CAA-CBA-CGA-O2A
15	a	822	CLA	C13-C15-C16-C17
19	B	851	LHG	O1-C1-C2-O2
19	F	204	LHG	O1-C1-C2-O2
19	N	857	LHG	O1-C1-C2-O2
19	f	203	LHG	O1-C1-C2-O2
19	k	101	LHG	O1-C1-C2-O2
21	A	855	LMG	C15-C16-C17-C18
15	N	811	CLA	C4-C3-C5-C6
15	N	813	CLA	C4-C3-C5-C6
18	a	845	BCR	C15-C16-C17-C18
15	N	806	CLA	C10-C11-C12-C13
15	B	809	CLA	C4B-C3B-CAB-CBB
15	K	102	CLA	C4B-C3B-CAB-CBB
15	N	835	CLA	C4B-C3B-CAB-CBB
15	O	809	CLA	C4B-C3B-CAB-CBB
15	V	102	CLA	C4B-C3B-CAB-CBB
15	b	809	CLA	C4B-C3B-CAB-CBB
21	j	206	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
15	a	821	CLA	CAA-CBA-CGA-O1A
15	B	805	CLA	C3-C5-C6-C7
15	a	819	CLA	CAA-CBA-CGA-O2A
15	O	821	CLA	C5-C6-C7-C8
15	B	838	CLA	C16-C17-C18-C20
15	N	807	CLA	C16-C17-C18-C19
15	a	822	CLA	C16-C17-C18-C20
13	A	801	CL0	CHA-CBD-CGD-O1D
13	A	801	CL0	CHA-CBD-CGD-O2D
13	N	801	CL0	CHA-CBD-CGD-O1D
13	N	801	CL0	CHA-CBD-CGD-O2D
13	a	801	CL0	CHA-CBD-CGD-O1D
13	a	801	CL0	CHA-CBD-CGD-O2D
13	a	801	CL0	C15-C16-C17-C18
15	O	801	CLA	CAA-CBA-CGA-O2A
22	O	850	LFA	C5-C6-C7-C8
21	j	206	LMG	C29-C28-O8-C9
15	N	816	CLA	CAA-CBA-CGA-O2A
15	i	102	CLA	CAA-CBA-CGA-O2A
21	J	103	LMG	C15-C16-C17-C18
15	N	818	CLA	C16-C17-C18-C20
15	N	820	CLA	C4-C3-C5-C6
15	a	842	CLA	C15-C16-C17-C18
15	B	821	CLA	CAA-CBA-CGA-O1A
15	O	826	CLA	C2-C3-C5-C6
15	A	803	CLA	C8-C10-C11-C12
15	A	818	CLA	C5-C6-C7-C8
15	B	830	CLA	C5-C6-C7-C8
15	A	825	CLA	C11-C10-C8-C7
15	O	813	CLA	C12-C13-C15-C16
15	b	813	CLA	C12-C13-C15-C16
19	N	857	LHG	C25-C26-C27-C28
19	F	204	LHG	C17-C18-C19-C20
22	O	850	LFA	C10-C11-C12-C13
18	N	845	BCR	C15-C16-C17-C18
15	a	832	CLA	O1A-CGA-O2A-C1
21	J	103	LMG	C17-C18-C19-C20
15	B	821	CLA	C5-C6-C7-C8
19	N	857	LHG	C30-C31-C32-C33
15	K	102	CLA	CAA-CBA-CGA-O2A
15	A	818	CLA	C11-C12-C13-C14
15	A	822	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	B	802	CLA	C6-C7-C8-C9
15	L	203	CLA	C6-C7-C8-C9
15	O	818	CLA	C11-C12-C13-C14
15	b	802	CLA	C6-C7-C8-C9
15	b	804	CLA	C6-C7-C8-C9
15	b	831	CLA	C11-C10-C8-C9
15	b	840	CLA	C14-C13-C15-C16
19	Y	101	LHG	C10-C11-C12-C13
21	B	850	LMG	C8-C7-O1-C1
19	Y	101	LHG	C29-C30-C31-C32
15	V	102	CLA	CAA-CBA-CGA-O2A
15	a	838	CLA	C2A-CAA-CBA-CGA
15	N	827	CLA	C2-C1-O2A-CGA
15	a	827	CLA	C2-C1-O2A-CGA
14	N	824	F6C	C1A-C2A-CAA-CBA
14	a	824	F6C	C1A-C2A-CAA-CBA
15	F	201	CLA	C16-C17-C18-C19
15	a	807	CLA	C16-C17-C18-C19
15	a	834	CLA	C16-C17-C18-C20
15	b	808	CLA	C8-C10-C11-C12
14	A	826	F6C	CBA-CGA-O2A-C1
21	J	103	LMG	O9-C10-O7-C8
15	B	825	CLA	C3A-C2A-CAA-CBA
15	N	821	CLA	C3A-C2A-CAA-CBA
15	O	825	CLA	C3A-C2A-CAA-CBA
13	A	801	CL0	CAA-CBA-CGA-O1A
15	b	801	CLA	CAA-CBA-CGA-O2A
15	a	811	CLA	C2-C3-C5-C6
15	a	819	CLA	C3-C5-C6-C7
19	X	101	LHG	C33-C34-C35-C36
15	N	803	CLA	C15-C16-C17-C18
15	b	821	CLA	CAA-CBA-CGA-O1A
15	A	834	CLA	C16-C17-C18-C20
15	a	818	CLA	C16-C17-C18-C20
15	a	820	CLA	C16-C17-C18-C20
15	A	803	CLA	CBA-CGA-O2A-C1
15	a	832	CLA	CBA-CGA-O2A-C1
19	A	851	LHG	C24-C23-O8-C6
15	A	816	CLA	CAA-CBA-CGA-O1A
15	a	816	CLA	CAA-CBA-CGA-O1A
15	a	813	CLA	C4-C3-C5-C6
15	K	102	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	N	816	CLA	CAA-CBA-CGA-O1A
15	O	805	CLA	C2-C3-C5-C6
15	a	823	CLA	C2-C3-C5-C6
15	a	806	CLA	C10-C11-C12-C13
14	A	824	F6C	C1A-C2A-CAA-CBA
15	N	833	CLA	C6-C7-C8-C10
15	V	102	CLA	CAA-CBA-CGA-O1A
19	A	851	LHG	O10-C23-O8-C6
13	a	801	CL0	C13-C15-C16-C17
15	b	830	CLA	C5-C6-C7-C8
14	A	856	F6C	C4B-C3B-CAB-CBB
19	N	857	LHG	C11-C10-C9-C8
19	F	204	LHG	C32-C33-C34-C35
19	Z	101	LHG	C28-C29-C30-C31
15	N	820	CLA	C2-C3-C5-C6
15	N	834	CLA	C16-C17-C18-C20
19	F	204	LHG	C30-C31-C32-C33
15	O	830	CLA	C10-C11-C12-C13
15	A	808	CLA	CBD-CGD-O2D-CED
19	L	208	LHG	C9-C10-C11-C12
21	U	103	LMG	C15-C16-C17-C18
15	O	819	CLA	CAA-CBA-CGA-O2A
21	T	103	LMG	O7-C10-C11-C12
15	O	815	CLA	CBD-CGD-O2D-CED
14	a	826	F6C	C6-C7-C8-C9
15	B	804	CLA	C6-C7-C8-C9
15	B	808	CLA	C11-C12-C13-C14
15	N	806	CLA	C6-C7-C8-C9
15	N	818	CLA	C11-C12-C13-C14
15	N	819	CLA	C11-C10-C8-C9
15	O	802	CLA	C6-C7-C8-C9
15	a	818	CLA	C11-C12-C13-C14
15	a	829	CLA	C11-C10-C8-C9
15	b	810	CLA	C14-C13-C15-C16
15	j	203	CLA	C6-C7-C8-C9
15	A	812	CLA	C16-C17-C18-C20
15	B	810	CLA	C16-C17-C18-C20
15	f	201	CLA	C16-C17-C18-C19
15	B	819	CLA	CAA-CBA-CGA-O2A
15	O	816	CLA	CAA-CBA-CGA-O2A
15	b	816	CLA	CAA-CBA-CGA-O2A
19	f	203	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
21	g	103	LMG	O7-C10-C11-C12
15	a	836	CLA	C6-C7-C8-C9
18	B	845	BCR	C17-C18-C19-C20
15	B	808	CLA	C8-C10-C11-C12
15	b	825	CLA	C8-C10-C11-C12
15	A	811	CLA	C4-C3-C5-C6
15	B	816	CLA	CAA-CBA-CGA-O2A
21	B	848	LMG	O7-C10-C11-C12
15	N	811	CLA	C2-C3-C5-C6
15	B	805	CLA	C2A-CAA-CBA-CGA
14	N	856	F6C	C6-C7-C8-C10
14	W	201	F6C	C11-C12-C13-C15
14	a	855	F6C	C6-C7-C8-C10
15	A	814	CLA	C6-C7-C8-C10
15	A	822	CLA	C12-C13-C15-C16
15	A	829	CLA	C6-C7-C8-C10
15	B	831	CLA	C11-C10-C8-C7
15	F	201	CLA	C6-C7-C8-C10
15	N	820	CLA	C12-C13-C15-C16
15	O	831	CLA	C11-C10-C8-C7
15	S	201	CLA	C6-C7-C8-C10
15	b	818	CLA	C11-C12-C13-C15
15	b	831	CLA	C11-C10-C8-C7
15	b	836	CLA	C6-C7-C8-C10
15	b	840	CLA	C12-C13-C15-C16
15	b	809	CLA	C10-C11-C12-C13
15	A	803	CLA	O1A-CGA-O2A-C1
15	O	821	CLA	CAA-CBA-CGA-O1A
20	N	853	LMT	C3'-C4'-O1B-C1B
15	B	834	CLA	CAA-CBA-CGA-O2A
15	A	830	CLA	C2B-C3B-CAB-CBB
15	B	829	CLA	C2B-C3B-CAB-CBB
15	K	102	CLA	C2B-C3B-CAB-CBB
15	N	830	CLA	C2B-C3B-CAB-CBB
15	O	801	CLA	C2B-C3B-CAB-CBB
15	O	809	CLA	C2B-C3B-CAB-CBB
15	b	801	CLA	C2B-C3B-CAB-CBB
15	b	809	CLA	C2B-C3B-CAB-CBB
15	b	836	CLA	C2B-C3B-CAB-CBB
18	A	846	BCR	C23-C24-C25-C26
18	J	101	BCR	C5-C6-C7-C8
18	L	206	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	O	842	BCR	C23-C24-C25-C26
18	O	843	BCR	C23-C24-C25-C26
18	U	101	BCR	C5-C6-C7-C8
18	a	846	BCR	C23-C24-C25-C26
18	h	101	BCR	C5-C6-C7-C8
15	N	839	CLA	CAA-CBA-CGA-O2A
19	F	204	LHG	O8-C23-C24-C25
21	I	103	LMG	O7-C10-C11-C12
21	I	103	LMG	C33-C34-C35-C36
15	A	827	CLA	C2-C1-O2A-CGA
15	B	838	CLA	C2-C1-O2A-CGA
15	O	802	CLA	C2-C1-O2A-CGA
15	N	828	CLA	C16-C17-C18-C19
15	a	828	CLA	C16-C17-C18-C19
15	i	102	CLA	CAA-CBA-CGA-O1A
15	O	825	CLA	C8-C10-C11-C12
19	a	851	LHG	C29-C30-C31-C32
15	O	822	CLA	CAA-CBA-CGA-O2A
15	b	819	CLA	CAA-CBA-CGA-O2A
19	N	857	LHG	O8-C23-C24-C25
15	a	808	CLA	CBD-CGD-O2D-CED
15	a	822	CLA	C16-C17-C18-C19
15	a	833	CLA	C3-C5-C6-C7
21	N	855	LMG	C15-C16-C17-C18
15	A	811	CLA	C2-C3-C5-C6
15	O	805	CLA	C2A-CAA-CBA-CGA
21	J	103	LMG	C11-C10-O7-C8
20	A	853	LMT	C3'-C4'-O1B-C1B
15	A	838	CLA	C3-C5-C6-C7
21	J	103	LMG	C38-C39-C40-C41
15	b	822	CLA	CAA-CBA-CGA-O2A
22	O	850	LFA	C15-C16-C17-C18
15	O	801	CLA	C16-C17-C18-C20
19	f	203	LHG	C25-C26-C27-C28
15	a	818	CLA	C5-C6-C7-C8
15	A	830	CLA	C4-C3-C5-C6
15	O	821	CLA	C4-C3-C5-C6
21	h	103	LMG	C15-C16-C17-C18
15	A	806	CLA	C10-C11-C12-C13
15	A	835	CLA	C2-C3-C5-C6
15	a	808	CLA	O1D-CGD-O2D-CED
15	O	834	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	A	828	CLA	C13-C15-C16-C17
19	X	101	LHG	C30-C31-C32-C33
21	O	849	LMG	C13-C14-C15-C16
15	B	806	CLA	C8-C10-C11-C12
19	Z	101	LHG	C9-C10-C11-C12
20	a	853	LMT	C3'-C4'-O1B-C1B
15	A	809	CLA	C11-C10-C8-C9
15	A	818	CLA	C11-C10-C8-C9
15	A	829	CLA	C11-C10-C8-C9
15	B	824	CLA	C14-C13-C15-C16
15	B	829	CLA	C14-C13-C15-C16
15	N	820	CLA	C11-C12-C13-C14
15	O	809	CLA	C11-C12-C13-C14
15	O	815	CLA	C6-C7-C8-C9
15	O	828	CLA	C11-C10-C8-C9
15	a	820	CLA	C11-C12-C13-C14
15	b	809	CLA	C11-C12-C13-C14
15	b	815	CLA	C6-C7-C8-C9
15	b	824	CLA	C14-C13-C15-C16
18	b	845	BCR	C36-C18-C19-C20
15	A	807	CLA	CAA-CBA-CGA-O2A
15	a	807	CLA	CAA-CBA-CGA-O2A
21	O	849	LMG	O7-C10-C11-C12
21	B	850	LMG	C18-C19-C20-C21
15	B	825	CLA	C8-C10-C11-C12
15	A	821	CLA	C1A-C2A-CAA-CBA
15	B	812	CLA	C1A-C2A-CAA-CBA
15	B	821	CLA	C1A-C2A-CAA-CBA
15	B	829	CLA	C4B-C3B-CAB-CBB
15	B	836	CLA	C1A-C2A-CAA-CBA
15	L	203	CLA	C1A-C2A-CAA-CBA
15	N	811	CLA	C1A-C2A-CAA-CBA
15	N	821	CLA	C1A-C2A-CAA-CBA
15	N	838	CLA	C1A-C2A-CAA-CBA
15	O	810	CLA	C1A-C2A-CAA-CBA
15	O	831	CLA	C1A-C2A-CAA-CBA
15	O	836	CLA	C1A-C2A-CAA-CBA
15	a	828	CLA	C1A-C2A-CAA-CBA
15	a	835	CLA	C4B-C3B-CAB-CBB
15	b	810	CLA	C1A-C2A-CAA-CBA
15	b	812	CLA	C1A-C2A-CAA-CBA
15	b	814	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	b	836	CLA	C1A-C2A-CAA-CBA
15	i	102	CLA	C4B-C3B-CAB-CBB
15	O	812	CLA	O1D-CGD-O2D-CED
21	A	855	LMG	C18-C19-C20-C21
15	B	821	CLA	C4-C3-C5-C6
15	B	840	CLA	C4-C3-C5-C6
15	N	809	CLA	C4-C3-C5-C6
15	b	801	CLA	C8-C10-C11-C12
15	N	807	CLA	CAA-CBA-CGA-O2A
19	W	207	LHG	C9-C10-C11-C12
15	A	809	CLA	C2-C3-C5-C6
18	A	848	BCR	C17-C18-C19-C20
18	L	205	BCR	C7-C8-C9-C10
18	O	845	BCR	C17-C18-C19-C20
18	a	848	BCR	C17-C18-C19-C20
18	b	845	BCR	C17-C18-C19-C20
15	A	818	CLA	C16-C17-C18-C20
15	N	820	CLA	C16-C17-C18-C20
13	N	801	CL0	CAA-CBA-CGA-O1A
21	U	103	LMG	C38-C39-C40-C41
15	B	817	CLA	C2A-CAA-CBA-CGA
15	N	809	CLA	O1D-CGD-O2D-CED
14	B	839	F6C	C5-C6-C7-C8
15	A	808	CLA	O1D-CGD-O2D-CED
15	B	801	CLA	C16-C17-C18-C20
15	B	807	CLA	C16-C17-C18-C20
15	B	838	CLA	C16-C17-C18-C19
15	N	814	CLA	C16-C17-C18-C19
15	a	806	CLA	CAA-CBA-CGA-O2A
19	l	101	LHG	O7-C7-C8-C9
14	A	824	F6C	C2-C3-C5-C6
15	A	809	CLA	C8-C10-C11-C12
15	B	801	CLA	C8-C10-C11-C12
15	A	813	CLA	C4-C3-C5-C6
15	A	835	CLA	C4-C3-C5-C6
14	j	201	F6C	C2-C1-O2A-CGA
15	A	820	CLA	C2-C1-O2A-CGA
15	A	828	CLA	C2-C1-O2A-CGA
15	A	829	CLA	C2-C1-O2A-CGA
15	A	835	CLA	C2-C1-O2A-CGA
15	A	837	CLA	C2-C1-O2A-CGA
15	A	839	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	B	802	CLA	C2-C1-O2A-CGA
15	N	828	CLA	C2-C1-O2A-CGA
15	N	835	CLA	C2-C1-O2A-CGA
15	a	820	CLA	C2-C1-O2A-CGA
15	a	828	CLA	C2-C1-O2A-CGA
15	a	835	CLA	C2-C1-O2A-CGA
15	a	837	CLA	C2-C1-O2A-CGA
14	A	856	F6C	C11-C10-C8-C7
14	L	204	F6C	C11-C10-C8-C7
14	L	204	F6C	C12-C13-C15-C16
14	N	802	F6C	C11-C10-C8-C7
14	W	204	F6C	C11-C10-C8-C7
14	j	204	F6C	C11-C10-C8-C7
15	A	820	CLA	C11-C12-C13-C15
15	A	835	CLA	C12-C13-C15-C16
15	B	805	CLA	C12-C13-C15-C16
15	B	836	CLA	C6-C7-C8-C10
15	N	818	CLA	C11-C10-C8-C7
15	O	808	CLA	C11-C12-C13-C15
15	O	818	CLA	C11-C12-C13-C15
15	O	836	CLA	C6-C7-C8-C10
15	a	835	CLA	C12-C13-C15-C16
15	b	828	CLA	C11-C12-C13-C15
15	A	833	CLA	C6-C7-C8-C10
15	N	835	CLA	C16-C17-C18-C20
15	O	807	CLA	C16-C17-C18-C20
15	a	835	CLA	C16-C17-C18-C20
15	b	810	CLA	C16-C17-C18-C20
15	B	822	CLA	CAA-CBA-CGA-O2A
19	N	851	LHG	O8-C23-C24-C25
19	Z	101	LHG	O7-C7-C8-C9
21	b	849	LMG	O7-C10-C11-C12
15	A	822	CLA	C13-C15-C16-C17
15	a	807	CLA	C5-C6-C7-C8
15	a	809	CLA	O1D-CGD-O2D-CED
15	b	817	CLA	C2A-CAA-CBA-CGA
15	b	838	CLA	C10-C11-C12-C13
15	A	828	CLA	C16-C17-C18-C19
15	O	810	CLA	C16-C17-C18-C20
15	a	833	CLA	C6-C7-C8-C10
15	b	807	CLA	C16-C17-C18-C20
15	A	841	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	N	822	CLA	C13-C15-C16-C17
15	b	819	CLA	CAA-CBA-CGA-O1A
15	a	828	CLA	C13-C15-C16-C17
15	b	802	CLA	C13-C15-C16-C17
15	B	821	CLA	C3A-C2A-CAA-CBA
15	O	836	CLA	C3A-C2A-CAA-CBA
15	B	819	CLA	CAA-CBA-CGA-O1A
14	N	826	F6C	O1A-CGA-O2A-C1
15	B	810	CLA	C10-C11-C12-C13
15	O	840	CLA	C2-C3-C5-C6
15	b	821	CLA	C2-C3-C5-C6
15	B	834	CLA	CAA-CBA-CGA-O1A
21	h	103	LMG	C38-C39-C40-C41
21	g	103	LMG	O9-C10-C11-C12
15	O	815	CLA	CBA-CGA-O2A-C1
15	a	804	CLA	C8-C10-C11-C12
21	b	849	LMG	C13-C14-C15-C16
15	O	815	CLA	O1A-CGA-O2A-C1
19	N	851	LHG	C29-C30-C31-C32
15	N	838	CLA	C2A-CAA-CBA-CGA
15	O	817	CLA	C2A-CAA-CBA-CGA
14	W	204	F6C	C11-C10-C8-C9
15	A	825	CLA	C11-C10-C8-C9
15	B	809	CLA	C11-C12-C13-C14
15	B	818	CLA	C11-C12-C13-C14
15	N	820	CLA	C11-C10-C8-C9
15	N	822	CLA	C14-C13-C15-C16
15	N	829	CLA	C11-C10-C8-C9
15	O	824	CLA	C14-C13-C15-C16
15	a	806	CLA	C6-C7-C8-C9
15	b	828	CLA	C11-C12-C13-C14
15	O	837	CLA	CAA-CBA-CGA-O2A
15	N	807	CLA	CAA-CBA-CGA-O1A
19	F	204	LHG	C25-C26-C27-C28
15	O	834	CLA	CAA-CBA-CGA-O1A
15	A	807	CLA	C5-C6-C7-C8
14	N	826	F6C	C4-C3-C5-C6
19	F	204	LHG	O10-C23-C24-C25
14	N	802	F6C	O1D-CGD-O2D-CED
15	A	829	CLA	CAA-CBA-CGA-O2A
15	N	805	CLA	CAA-CBA-CGA-O2A
14	N	826	F6C	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	h	103	LMG	C17-C18-C19-C20
19	f	203	LHG	O10-C23-C24-C25
19	l	101	LHG	O9-C7-C8-C9
15	B	805	CLA	CAA-CBA-CGA-O2A
15	b	810	CLA	C10-C11-C12-C13
15	N	839	CLA	CAA-CBA-CGA-O1A
15	O	816	CLA	CAA-CBA-CGA-O1A
15	O	822	CLA	CAA-CBA-CGA-O1A
19	N	857	LHG	O10-C23-C24-C25
21	I	103	LMG	O9-C10-C11-C12
21	T	103	LMG	O9-C10-C11-C12
15	O	819	CLA	CAA-CBA-CGA-O1A
15	b	816	CLA	CAA-CBA-CGA-O1A
21	b	849	LMG	O9-C10-C11-C12
19	A	851	LHG	O8-C23-C24-C25
21	T	103	LMG	O8-C28-C29-C30
15	W	202	CLA	C2A-CAA-CBA-CGA
15	a	839	CLA	C2A-CAA-CBA-CGA
15	j	202	CLA	C2A-CAA-CBA-CGA
19	F	204	LHG	C15-C16-C17-C18
15	S	201	CLA	C16-C17-C18-C20
14	N	802	F6C	CBD-CGD-O2D-CED
15	N	809	CLA	CBD-CGD-O2D-CED
19	F	204	LHG	C4-C5-C6-O8
19	N	857	LHG	C4-C5-C6-O8
19	f	203	LHG	C4-C5-C6-O8
15	B	816	CLA	CAA-CBA-CGA-O1A
21	B	848	LMG	O9-C10-C11-C12
21	O	849	LMG	O9-C10-C11-C12
15	O	808	CLA	C5-C6-C7-C8
19	F	204	LHG	C2-C3-O3-P
19	N	857	LHG	C2-C3-O3-P
19	f	203	LHG	C2-C3-O3-P
15	A	806	CLA	CAA-CBA-CGA-O2A
15	N	806	CLA	CAA-CBA-CGA-O2A
15	O	805	CLA	CAA-CBA-CGA-O2A
15	b	837	CLA	CAA-CBA-CGA-O2A
21	B	850	LMG	C12-C13-C14-C15
15	B	822	CLA	CAA-CBA-CGA-O1A
15	b	822	CLA	CAA-CBA-CGA-O1A
19	Z	101	LHG	O9-C7-C8-C9
15	A	820	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	B	820	CLA	CAD-CBD-CGD-O2D
15	B	821	CLA	CAD-CBD-CGD-O2D
15	N	810	CLA	CAD-CBD-CGD-O2D
15	O	821	CLA	CAD-CBD-CGD-O2D
15	a	834	CLA	CAD-CBD-CGD-O2D
15	N	809	CLA	C8-C10-C11-C12
14	a	855	F6C	CAA-CBA-CGA-O2A
15	b	805	CLA	CAA-CBA-CGA-O2A
15	b	827	CLA	CAA-CBA-CGA-O2A
19	f	203	LHG	C34-C35-C36-C37
15	A	812	CLA	C3-C5-C6-C7
15	b	810	CLA	C3-C5-C6-C7
15	A	807	CLA	CAA-CBA-CGA-O1A
15	a	807	CLA	CAA-CBA-CGA-O1A
14	j	201	F6C	C2A-CAA-CBA-CGA
15	N	829	CLA	C2-C1-O2A-CGA
14	A	856	F6C	CAA-CBA-CGA-O2A
15	N	810	CLA	CAA-CBA-CGA-O2A
15	a	805	CLA	CAA-CBA-CGA-O2A
19	a	851	LHG	O8-C23-C24-C25
15	A	835	CLA	C16-C17-C18-C20
15	L	202	CLA	C2A-CAA-CBA-CGA
14	N	802	F6C	C13-C15-C16-C17
15	O	826	CLA	C6-C7-C8-C10
15	A	805	CLA	CAA-CBA-CGA-O2A
15	B	826	CLA	CAA-CBA-CGA-O2A
15	B	827	CLA	CAA-CBA-CGA-O2A
15	B	837	CLA	CAA-CBA-CGA-O2A
15	N	825	CLA	CAA-CBA-CGA-O2A
15	O	827	CLA	CAA-CBA-CGA-O2A
15	b	826	CLA	CAA-CBA-CGA-O2A
19	k	101	LHG	O7-C7-C8-C9
21	h	103	LMG	O8-C28-C29-C30
15	O	838	CLA	C10-C11-C12-C13
15	b	809	CLA	C8-C10-C11-C12
15	A	834	CLA	CBD-CGD-O2D-CED
15	B	826	CLA	CAA-CBA-CGA-O1A
15	b	837	CLA	CAA-CBA-CGA-O1A
15	a	809	CLA	CBD-CGD-O2D-CED
14	N	856	F6C	CAA-CBA-CGA-O2A
15	A	810	CLA	CAA-CBA-CGA-O2A
15	A	813	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	B	828	CLA	CAA-CBA-CGA-O2A
15	N	838	CLA	CAA-CBA-CGA-O2A
15	O	828	CLA	CAA-CBA-CGA-O2A
15	a	810	CLA	CAA-CBA-CGA-O2A
15	a	825	CLA	CAA-CBA-CGA-O2A
15	a	838	CLA	CAA-CBA-CGA-O2A
19	B	851	LHG	O7-C7-C8-C9
19	Y	101	LHG	O7-C7-C8-C9
21	g	103	LMG	O8-C28-C29-C30
13	N	801	CL0	C10-C11-C12-C13
15	L	203	CLA	C5-C6-C7-C8
19	B	851	LHG	C27-C28-C29-C30

There are no ring outliers.

331 monomers are involved in 769 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	810	CLA	2	0
14	L	204	F6C	1	0
15	O	833	CLA	1	0
15	b	822	CLA	1	0
19	Y	101	LHG	4	0
15	b	810	CLA	1	0
15	A	806	CLA	7	0
15	A	825	CLA	1	0
15	O	814	CLA	1	0
15	B	806	CLA	5	0
15	b	828	CLA	4	0
15	A	809	CLA	5	0
15	a	821	CLA	1	0
15	B	809	CLA	7	0
15	B	816	CLA	4	0
18	O	848	BCR	4	0
15	b	820	CLA	2	0
21	T	103	LMG	2	0
18	B	846	BCR	5	0
15	B	831	CLA	3	0
15	O	801	CLA	1	0
15	N	808	CLA	1	0
18	S	202	BCR	3	0
20	A	852	LMT	2	0
15	N	842	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	846	BCR	3	0
15	b	809	CLA	6	0
15	A	837	CLA	2	0
20	N	853	LMT	1	0
15	N	804	CLA	4	0
15	A	804	CLA	3	0
19	F	204	LHG	2	0
15	O	820	CLA	2	0
15	N	834	CLA	2	0
15	B	826	CLA	5	0
18	B	842	BCR	3	0
13	N	801	CL0	2	0
15	a	834	CLA	2	0
18	A	847	BCR	2	0
15	O	807	CLA	1	0
15	A	818	CLA	6	0
15	A	830	CLA	3	0
13	a	801	CL0	2	0
21	j	206	LMG	3	0
15	a	819	CLA	6	0
18	N	845	BCR	3	0
19	j	207	LHG	7	0
15	A	839	CLA	2	0
15	a	803	CLA	8	0
18	a	845	BCR	3	0
15	A	834	CLA	2	0
14	j	201	F6C	1	0
20	a	854	LMT	1	0
18	A	848	BCR	2	0
15	a	806	CLA	8	0
15	O	830	CLA	5	0
15	a	804	CLA	5	0
15	A	822	CLA	3	0
15	N	833	CLA	2	0
15	a	809	CLA	1	0
15	a	816	CLA	1	0
18	B	843	BCR	1	0
18	b	848	BCR	5	0
18	U	102	BCR	5	0
22	b	850	LFA	2	0
15	a	842	CLA	2	0
15	a	823	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	841	PQN	4	0
15	B	803	CLA	8	0
15	j	202	CLA	2	0
18	F	202	BCR	2	0
15	b	807	CLA	4	0
15	N	822	CLA	5	0
15	B	824	CLA	6	0
15	N	838	CLA	3	0
15	W	202	CLA	2	0
15	O	829	CLA	7	0
14	L	201	F6C	1	0
18	a	846	BCR	2	0
18	b	842	BCR	2	0
15	a	831	CLA	3	0
15	O	818	CLA	2	0
21	O	849	LMG	6	0
22	B	849	LFA	1	0
19	B	851	LHG	4	0
15	O	821	CLA	1	0
15	A	819	CLA	6	0
18	a	848	BCR	1	0
15	b	838	CLA	8	0
21	L	207	LMG	4	0
15	A	838	CLA	2	0
15	B	819	CLA	1	0
14	b	832	F6C	1	0
15	N	814	CLA	6	0
19	f	203	LHG	2	0
18	J	102	BCR	6	0
15	A	829	CLA	3	0
15	O	828	CLA	2	0
15	b	812	CLA	4	0
15	N	823	CLA	3	0
15	b	819	CLA	1	0
19	k	101	LHG	5	0
15	A	810	CLA	4	0
14	W	201	F6C	1	0
18	N	849	BCR	2	0
15	O	802	CLA	4	0
15	O	817	CLA	3	0
15	O	809	CLA	6	0
15	a	837	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	816	CLA	2	0
15	A	816	CLA	3	0
15	a	840	CLA	1	0
15	N	829	CLA	5	0
15	A	805	CLA	1	0
15	N	821	CLA	1	0
15	A	841	CLA	6	0
15	b	804	CLA	6	0
15	b	826	CLA	5	0
15	O	826	CLA	4	0
15	O	810	CLA	1	0
14	O	832	F6C	1	0
18	B	847	BCR	10	0
15	B	837	CLA	6	0
21	I	103	LMG	4	0
15	A	823	CLA	2	0
15	B	840	CLA	3	0
18	g	101	BCR	5	0
18	L	205	BCR	1	0
15	N	841	CLA	3	0
15	N	836	CLA	1	0
15	N	818	CLA	7	0
15	N	831	CLA	2	0
22	W	208	LFA	1	0
15	A	813	CLA	3	0
15	A	812	CLA	3	0
18	b	847	BCR	2	0
15	B	812	CLA	6	0
15	X	102	CLA	1	0
19	W	207	LHG	8	0
20	N	852	LMT	1	0
15	b	833	CLA	1	0
15	O	825	CLA	1	0
18	W	209	BCR	6	0
15	A	831	CLA	4	0
15	l	102	CLA	1	0
15	b	815	CLA	1	0
15	a	838	CLA	1	0
15	O	823	CLA	3	0
15	A	815	CLA	3	0
15	B	818	CLA	2	0
15	B	834	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	M	101	BCR	4	0
15	b	808	CLA	6	0
15	N	810	CLA	4	0
15	b	837	CLA	7	0
18	A	850	BCR	8	0
21	b	849	LMG	5	0
15	b	831	CLA	3	0
18	O	844	BCR	3	0
15	A	811	CLA	3	0
15	O	819	CLA	2	0
18	O	843	BCR	1	0
15	b	803	CLA	8	0
22	L	209	LFA	2	0
16	B	841	PQN	3	0
15	N	816	CLA	2	0
13	A	801	CL0	3	0
15	O	831	CLA	4	0
15	Z	102	CLA	1	0
15	a	805	CLA	1	0
16	a	843	PQN	2	0
15	b	806	CLA	6	0
15	O	803	CLA	8	0
15	N	820	CLA	7	0
15	B	836	CLA	3	0
15	a	812	CLA	4	0
15	O	805	CLA	2	0
15	N	807	CLA	4	0
15	a	813	CLA	2	0
20	A	854	LMT	2	0
18	a	850	BCR	7	0
15	O	806	CLA	4	0
15	L	203	CLA	1	0
18	L	210	BCR	3	0
15	A	835	CLA	2	0
15	O	813	CLA	2	0
15	B	813	CLA	2	0
15	a	822	CLA	2	0
15	a	818	CLA	5	0
18	a	847	BCR	2	0
15	N	815	CLA	2	0
15	A	820	CLA	7	0
15	A	827	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	O	846	BCR	4	0
15	b	824	CLA	4	0
18	O	845	BCR	1	0
15	A	807	CLA	4	0
15	N	830	CLA	2	0
18	N	850	BCR	7	0
15	W	203	CLA	1	0
15	B	838	CLA	7	0
19	L	208	LHG	6	0
15	O	815	CLA	1	0
15	b	818	CLA	1	0
15	N	811	CLA	2	0
15	B	827	CLA	1	0
15	N	803	CLA	7	0
18	Y	102	BCR	3	0
15	B	808	CLA	4	0
15	O	824	CLA	5	0
15	a	811	CLA	2	0
15	b	829	CLA	5	0
20	A	853	LMT	1	0
15	L	202	CLA	2	0
21	B	848	LMG	4	0
15	N	819	CLA	5	0
15	N	825	CLA	2	0
18	F	203	BCR	3	0
15	a	814	CLA	7	0
15	a	833	CLA	1	0
15	O	834	CLA	2	0
15	b	816	CLA	3	0
15	O	804	CLA	5	0
18	a	849	BCR	1	0
19	X	101	LHG	3	0
15	B	814	CLA	1	0
18	f	202	BCR	4	0
21	g	103	LMG	3	0
18	N	847	BCR	2	0
15	B	801	CLA	1	0
15	B	805	CLA	3	0
18	j	205	BCR	1	0
18	b	846	BCR	5	0
15	b	840	CLA	1	0
15	a	836	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b	805	CLA	2	0
21	h	103	LMG	2	0
18	A	846	BCR	2	0
15	B	820	CLA	3	0
15	V	102	CLA	1	0
18	h	102	BCR	7	0
18	I	101	BCR	4	0
15	b	825	CLA	1	0
18	A	845	BCR	4	0
15	O	840	CLA	1	0
15	B	807	CLA	3	0
15	N	813	CLA	3	0
15	O	822	CLA	1	0
15	f	201	CLA	2	0
20	a	853	LMT	1	0
15	b	821	CLA	1	0
22	j	208	LFA	1	0
15	b	817	CLA	3	0
18	O	847	BCR	1	0
20	a	852	LMT	1	0
15	A	840	CLA	1	0
15	i	102	CLA	1	0
18	U	101	BCR	1	0
15	b	823	CLA	3	0
15	A	821	CLA	1	0
15	B	802	CLA	5	0
15	a	830	CLA	2	0
15	b	834	CLA	3	0
18	T	101	BCR	6	0
22	O	850	LFA	1	0
18	L	206	BCR	3	0
15	B	830	CLA	3	0
16	O	841	PQN	4	0
15	O	837	CLA	4	0
15	O	838	CLA	8	0
21	A	855	LMG	1	0
20	N	854	LMT	1	0
15	N	840	CLA	1	0
15	N	809	CLA	4	0
15	B	825	CLA	2	0
15	K	102	CLA	1	0
18	B	844	BCR	2	0

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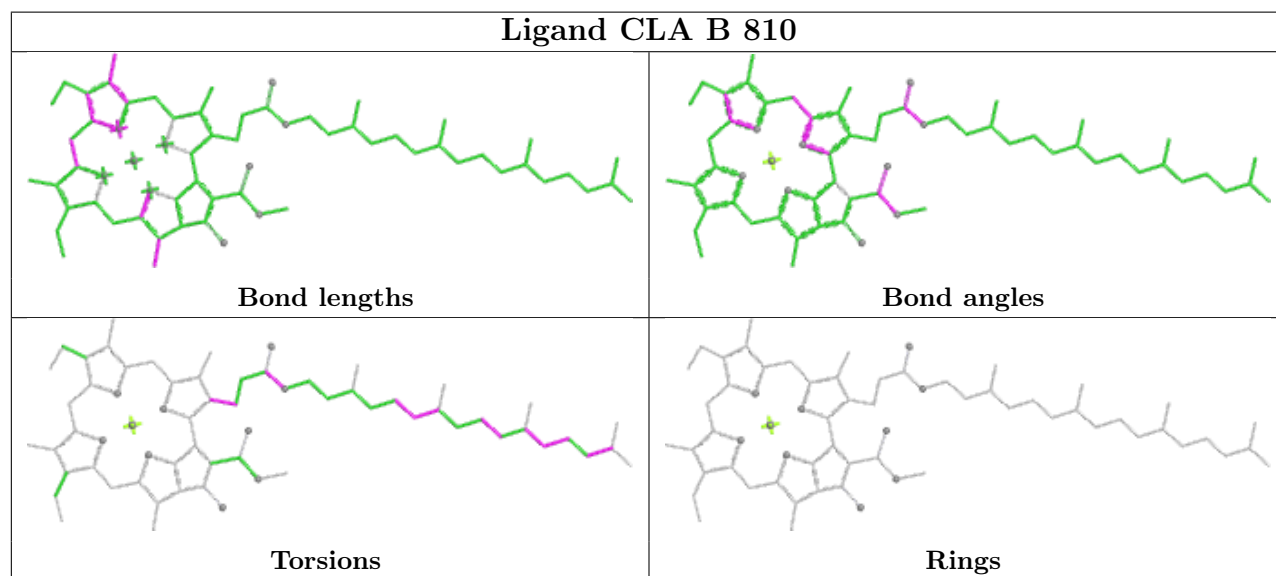
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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19	l	101	LHG	3	0
15	B	822	CLA	1	0
18	b	843	BCR	3	0
15	b	811	CLA	1	0
18	W	205	BCR	1	0
19	N	857	LHG	2	0
15	a	807	CLA	3	0
15	a	841	CLA	5	0
15	N	837	CLA	3	0
15	a	810	CLA	4	0
15	b	830	CLA	3	0
18	J	101	BCR	1	0
15	A	836	CLA	1	0
15	b	813	CLA	1	0
16	A	843	PQN	1	0
15	a	829	CLA	4	0
15	O	812	CLA	5	0
15	B	821	CLA	1	0
18	k	102	BCR	4	0
15	b	836	CLA	2	0
18	O	842	BCR	3	0
18	b	844	BCR	3	0
19	Z	101	LHG	1	0
15	N	827	CLA	1	0
15	A	842	CLA	2	0
15	B	829	CLA	6	0
15	B	828	CLA	1	0
14	B	832	F6C	1	0
15	N	839	CLA	3	0
15	O	836	CLA	3	0
18	A	849	BCR	1	0
15	A	833	CLA	2	0
15	a	839	CLA	2	0
15	j	203	CLA	1	0
15	a	825	CLA	1	0
15	B	811	CLA	1	0
15	B	804	CLA	6	0
15	O	827	CLA	1	0
15	a	815	CLA	3	0
15	N	806	CLA	7	0
15	O	808	CLA	5	0

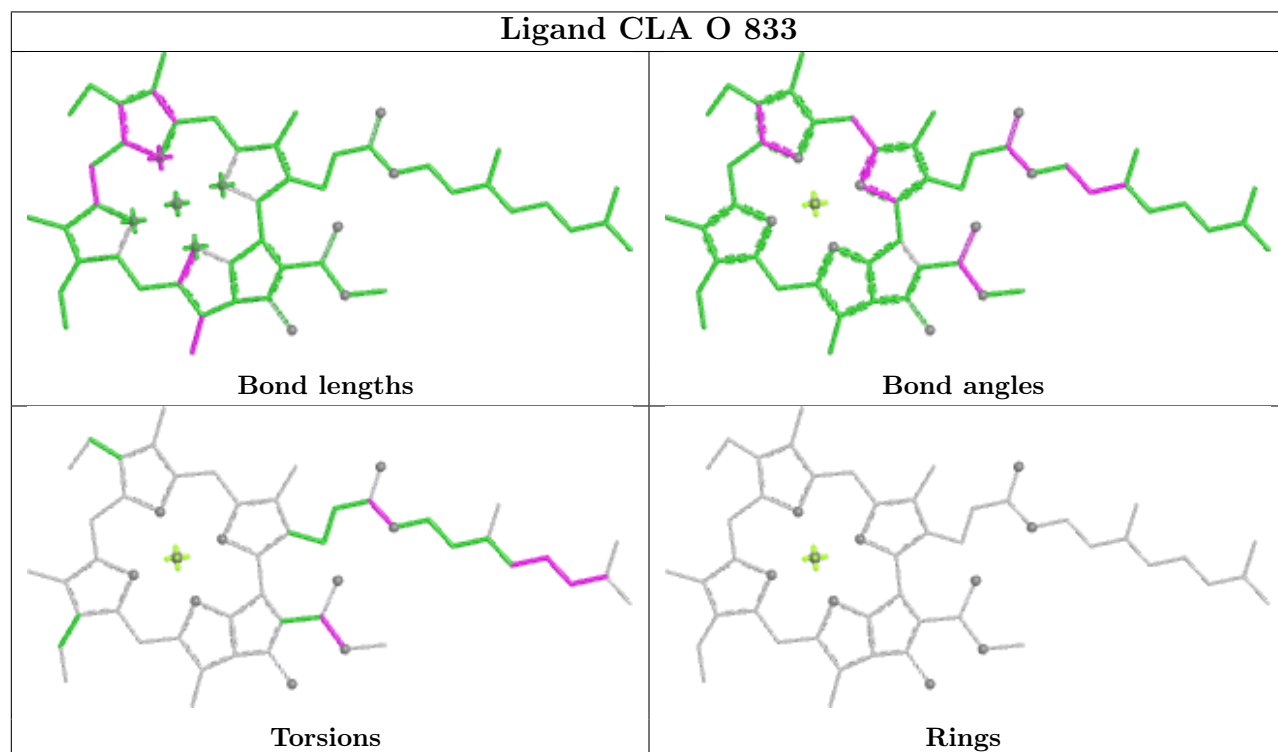
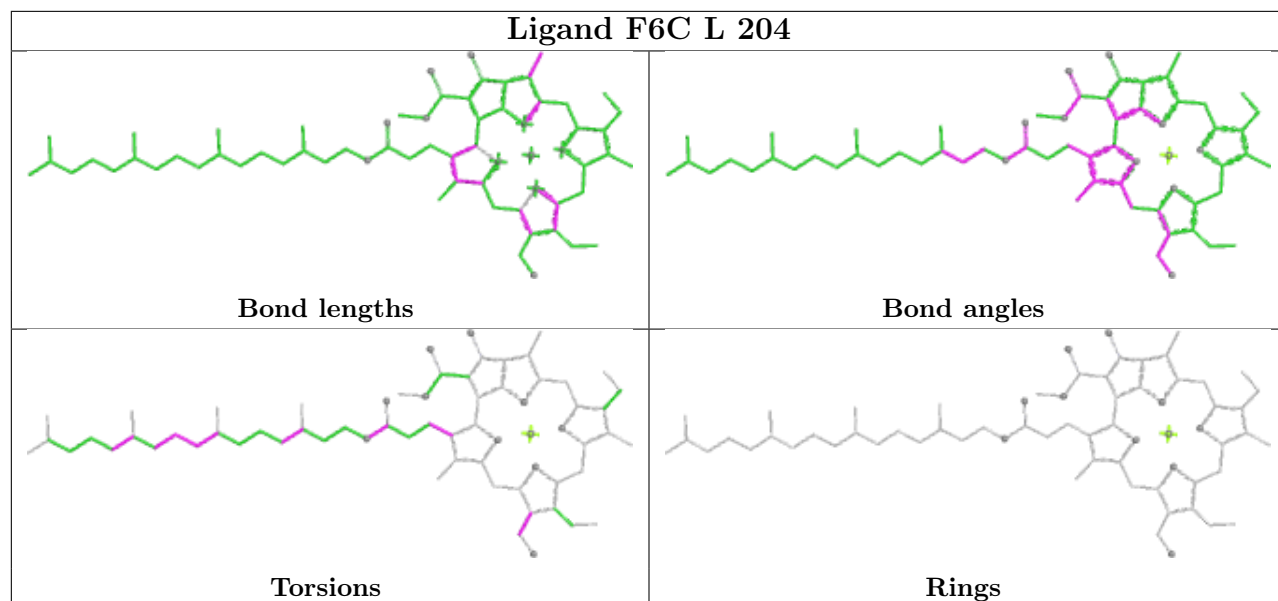
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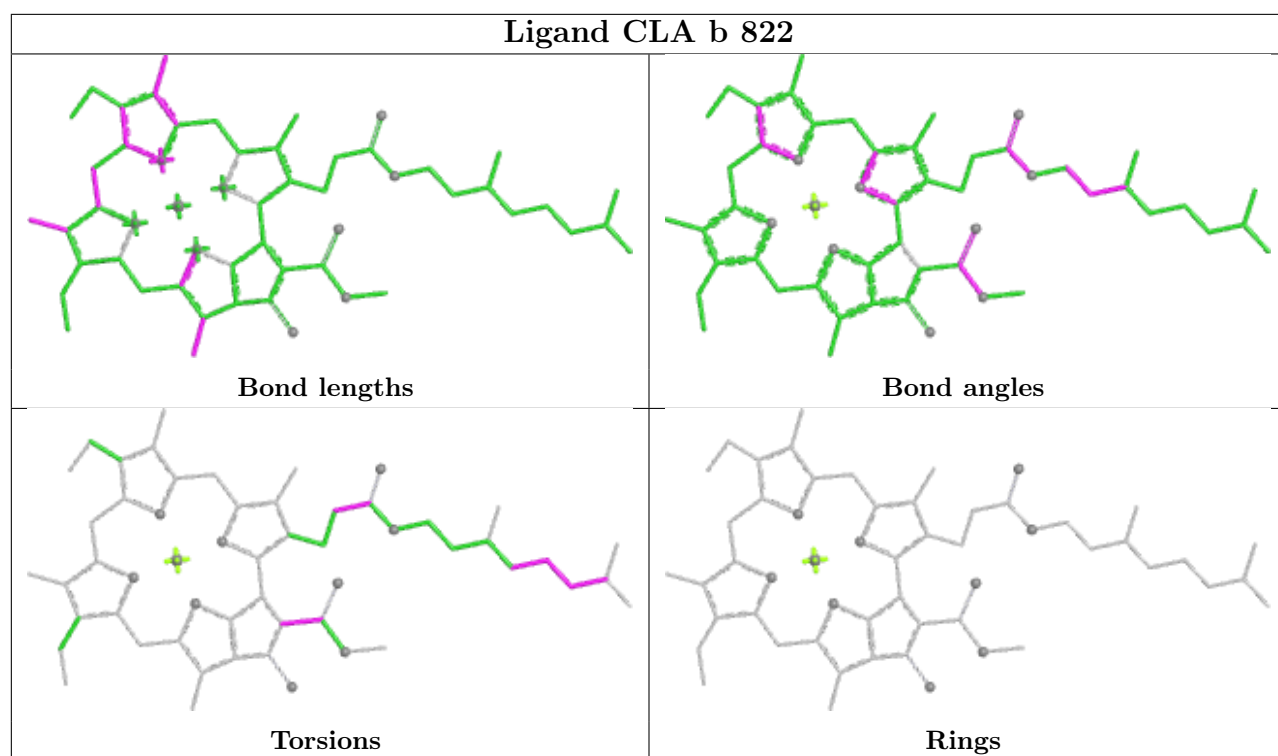
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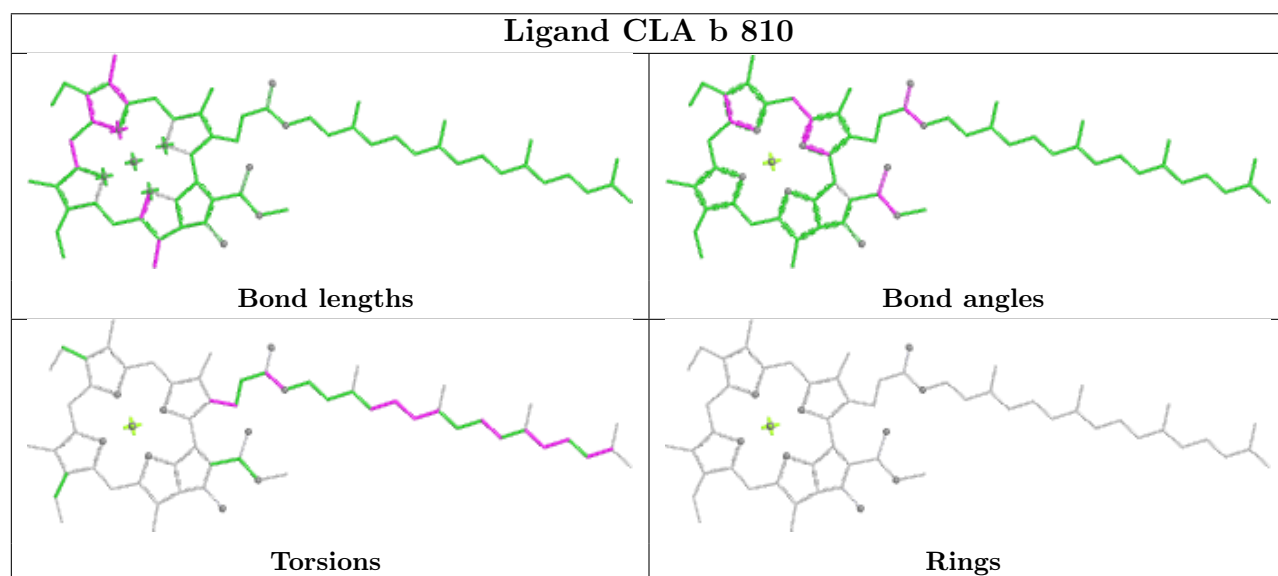
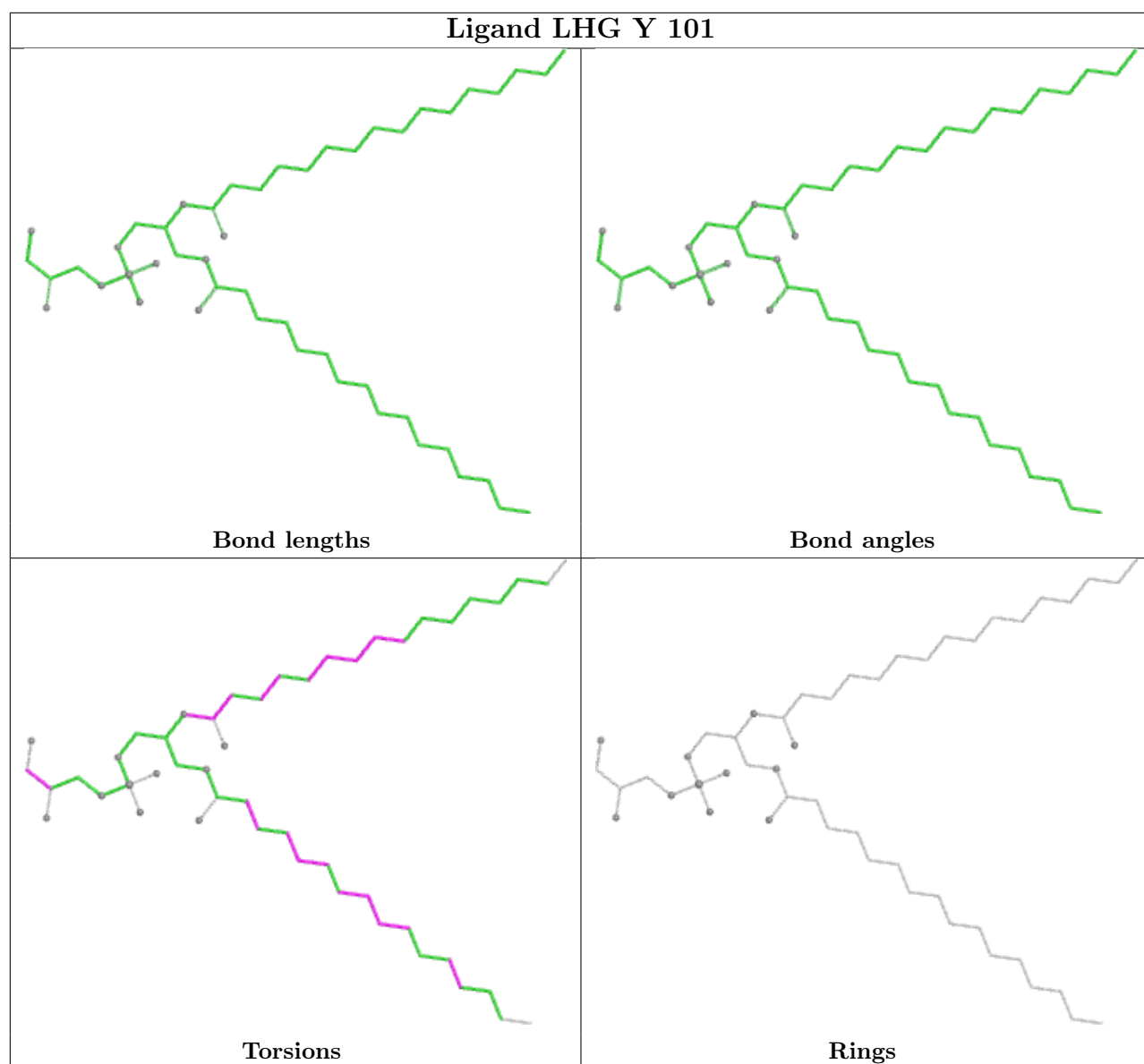
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	814	CLA	8	0
17	c	102	SF4	1	0
16	N	843	PQN	2	0
15	O	811	CLA	1	0
15	B	817	CLA	3	0
21	W	206	LMG	4	0
15	B	823	CLA	2	0
15	S	201	CLA	1	0
15	b	802	CLA	4	0
15	N	812	CLA	3	0
15	A	803	CLA	7	0
21	U	103	LMG	1	0

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.

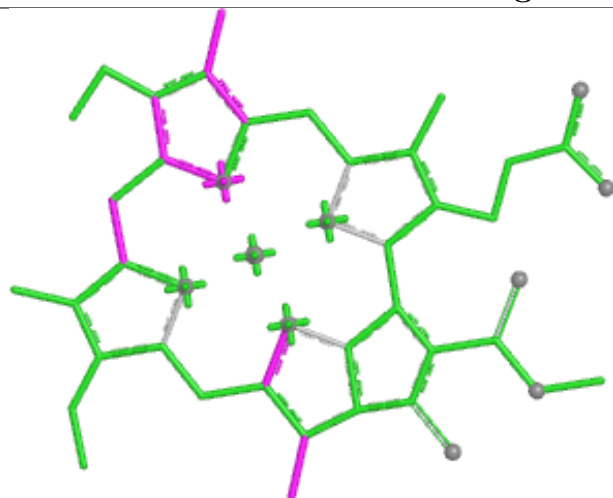




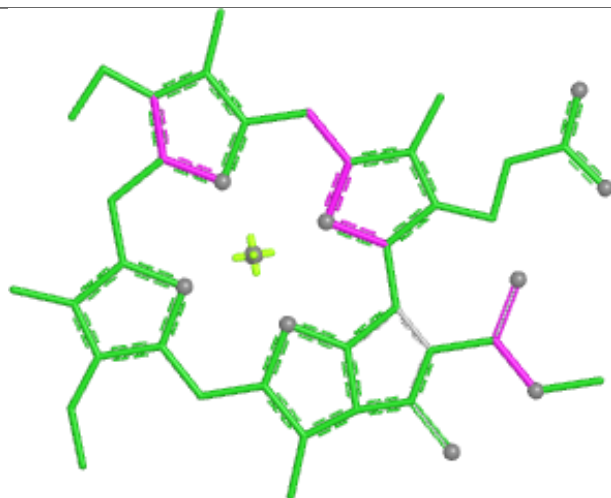




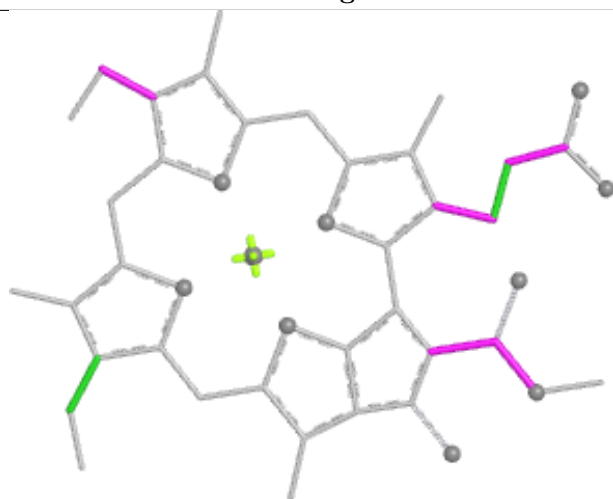
Ligand CLA B 835



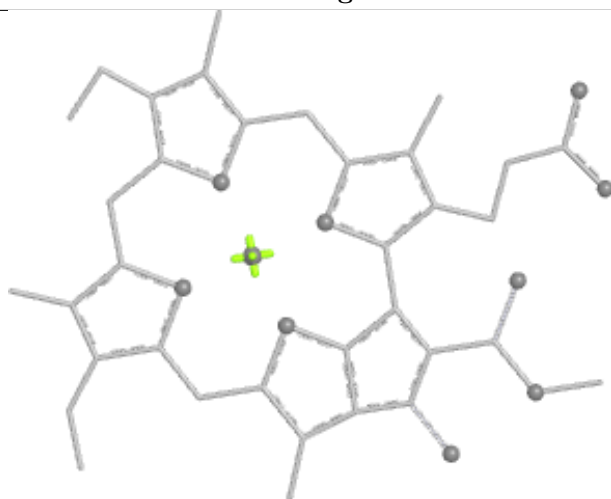
Bond lengths



Bond angles

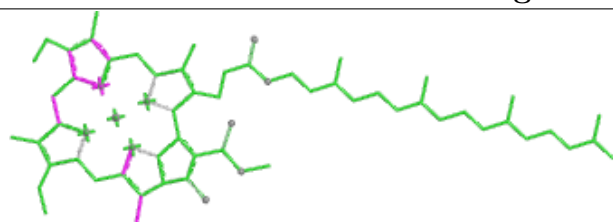


Torsions

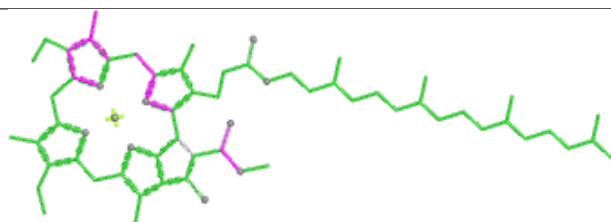


Rings

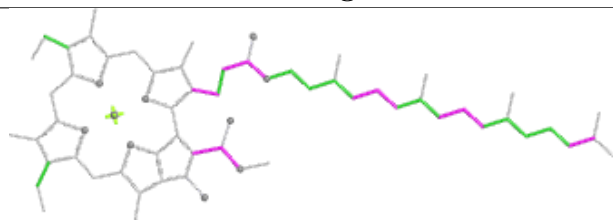
Ligand CLA A 806



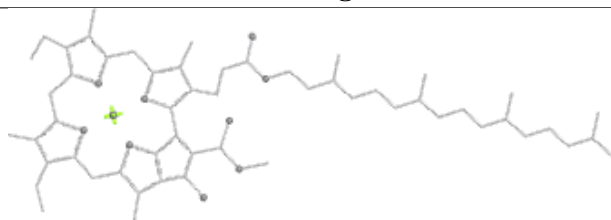
Bond lengths



Bond angles

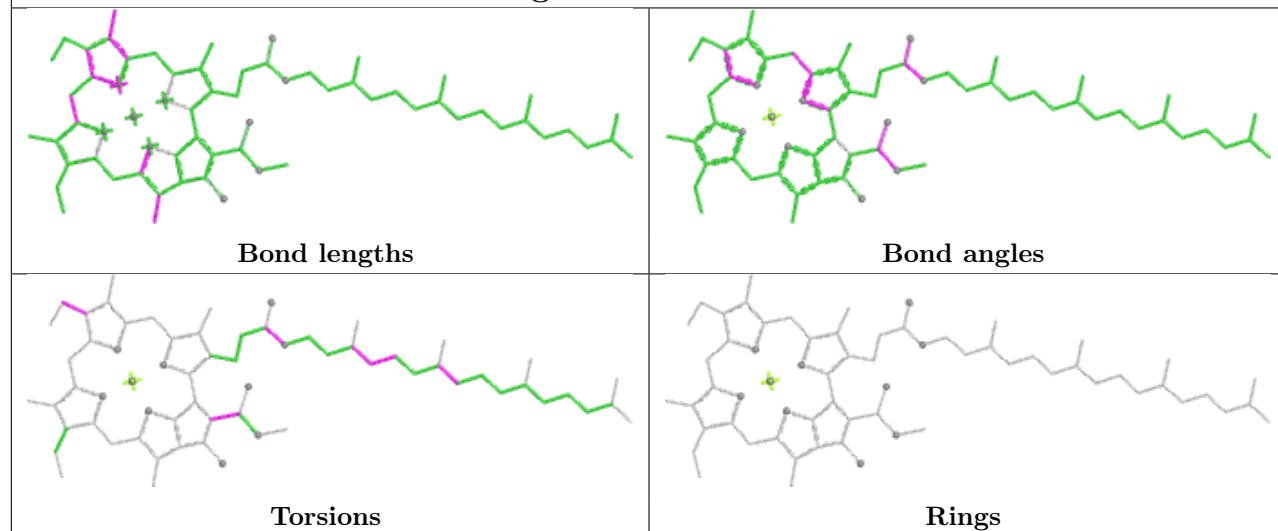


Torsions

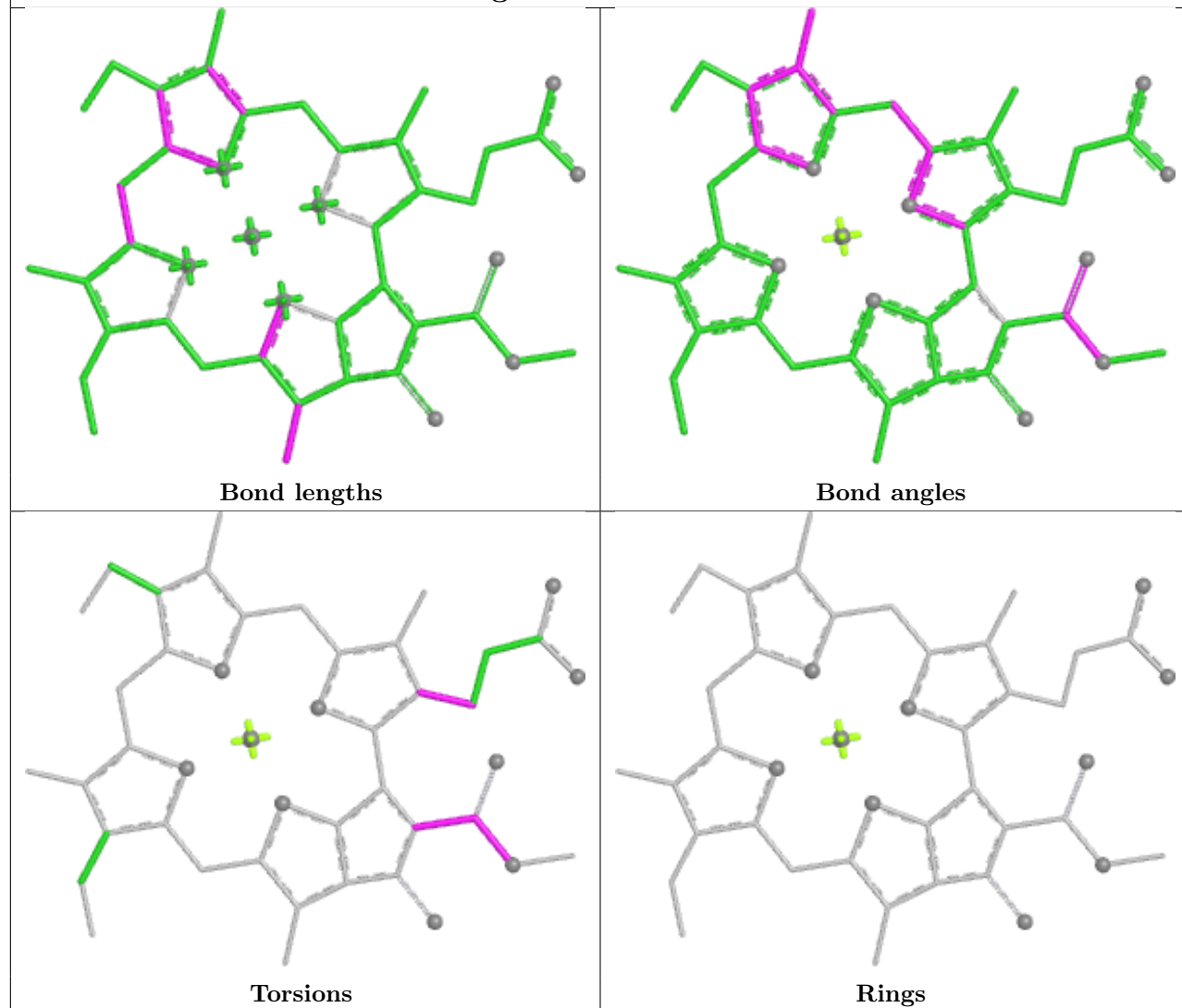


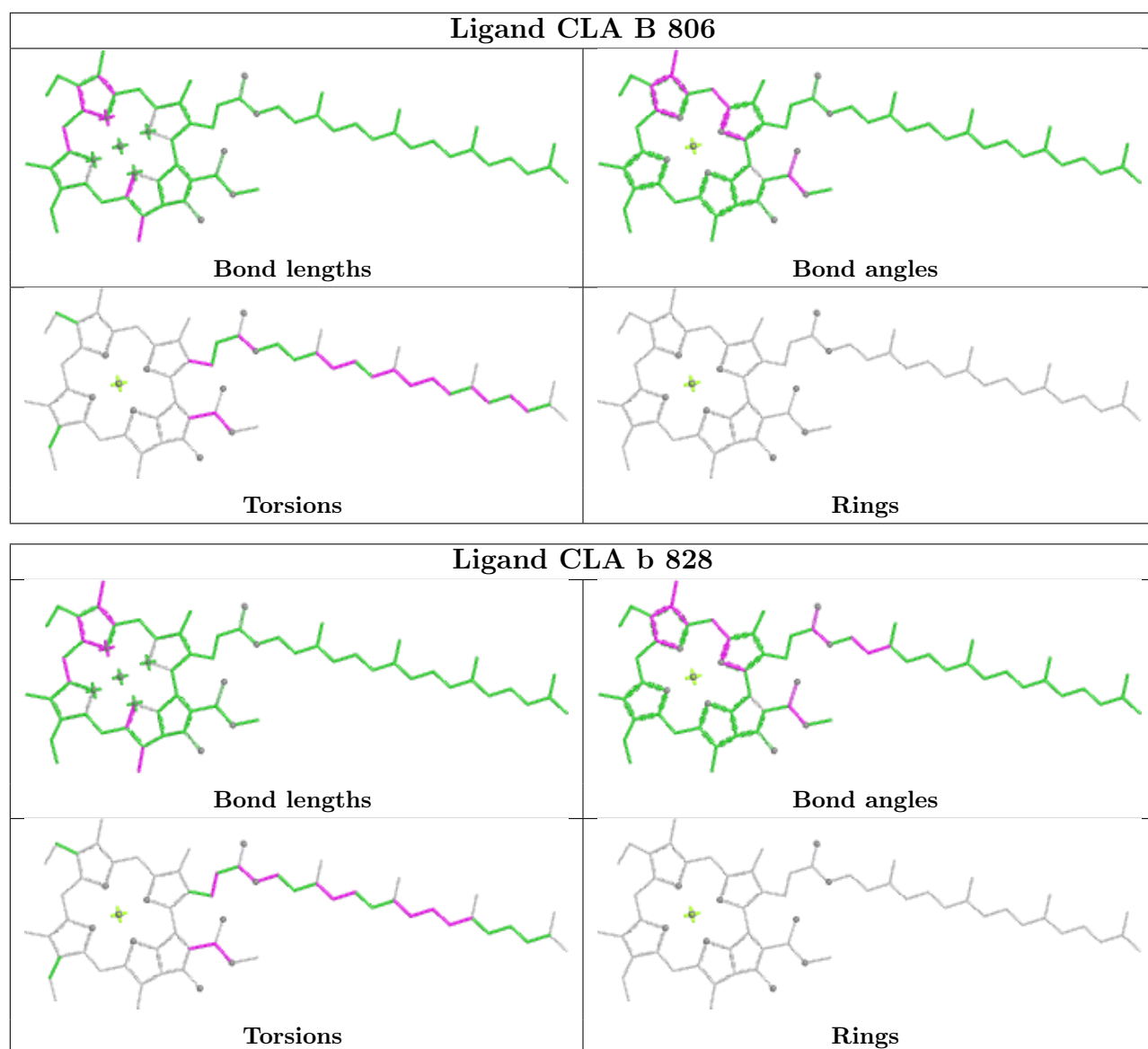
Rings

Ligand CLA A 825

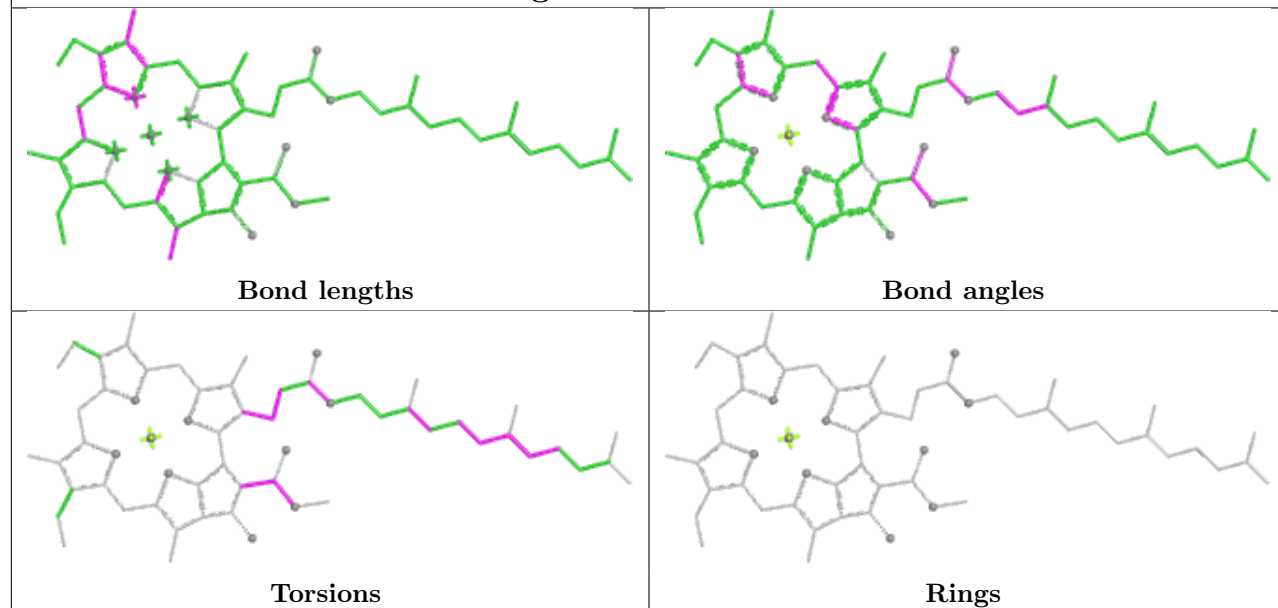


Ligand CLA O 814

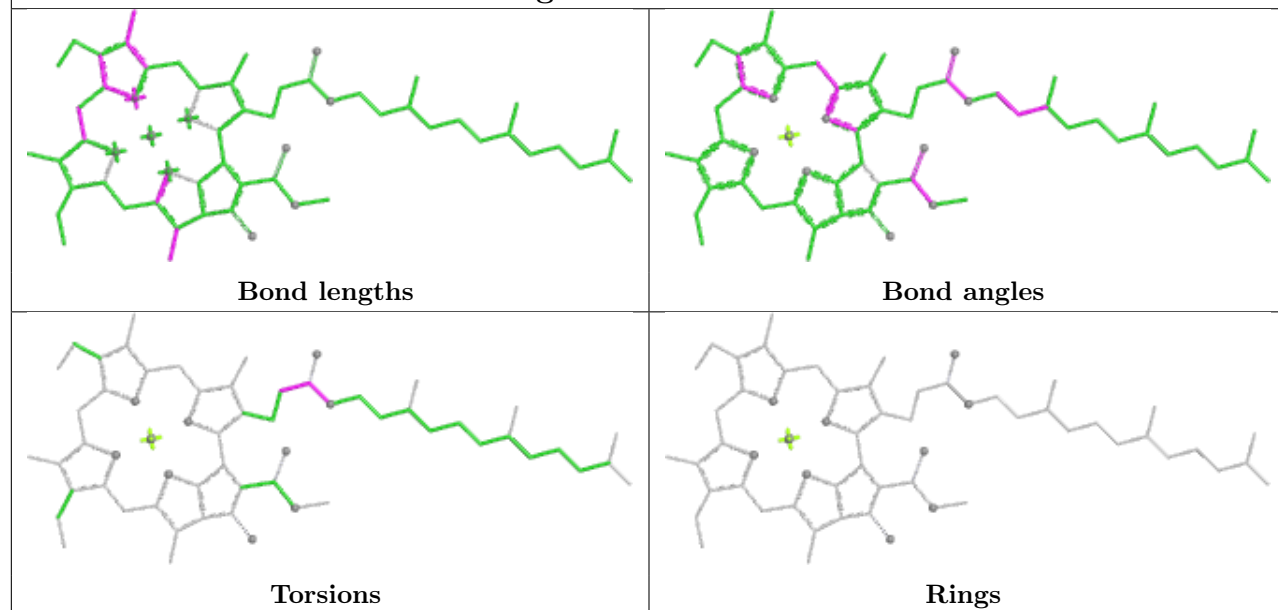


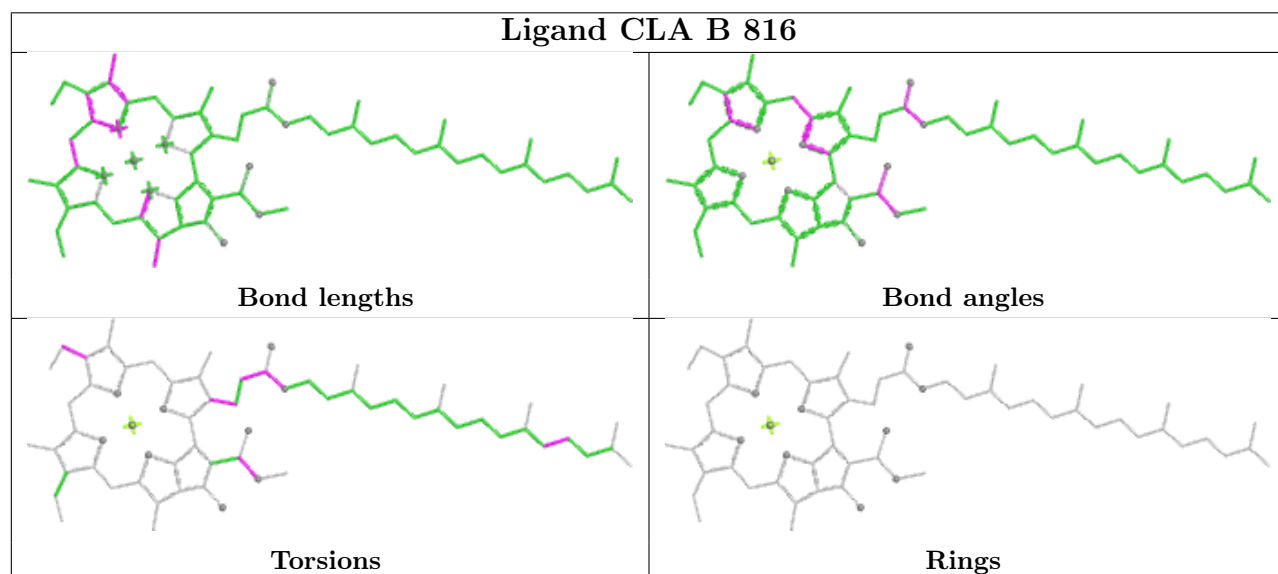
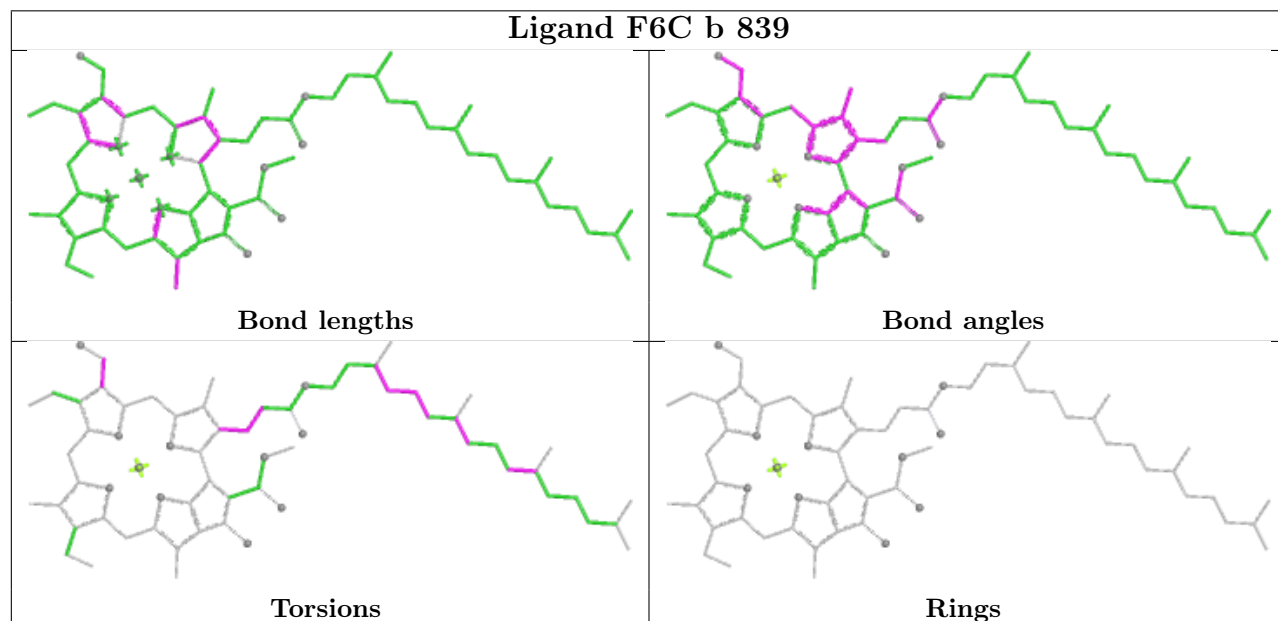
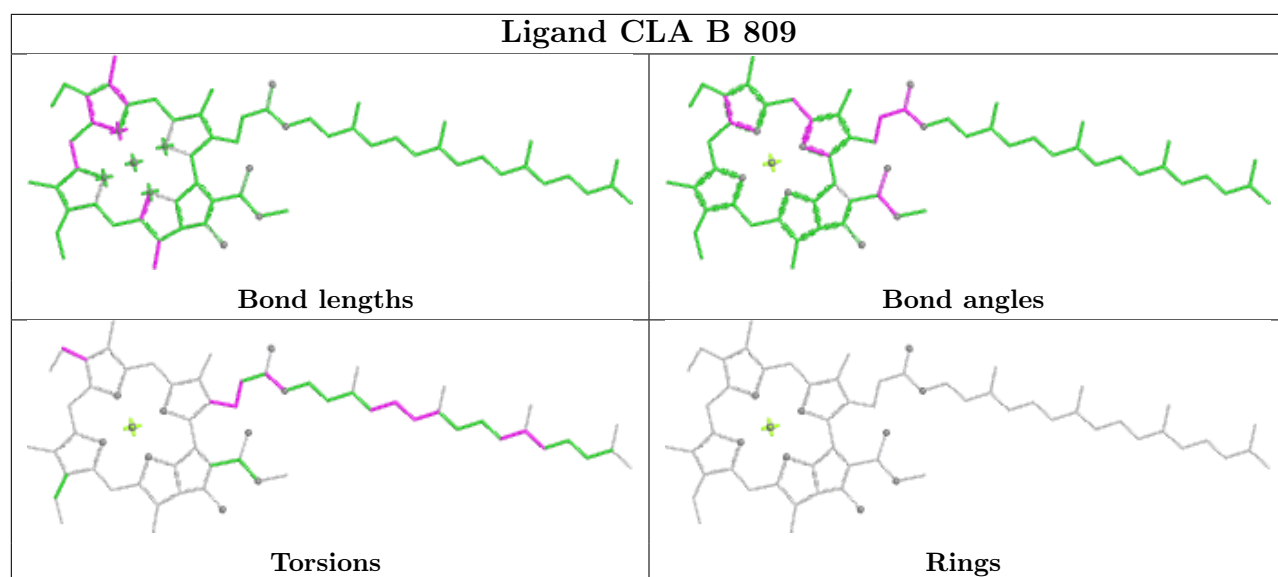


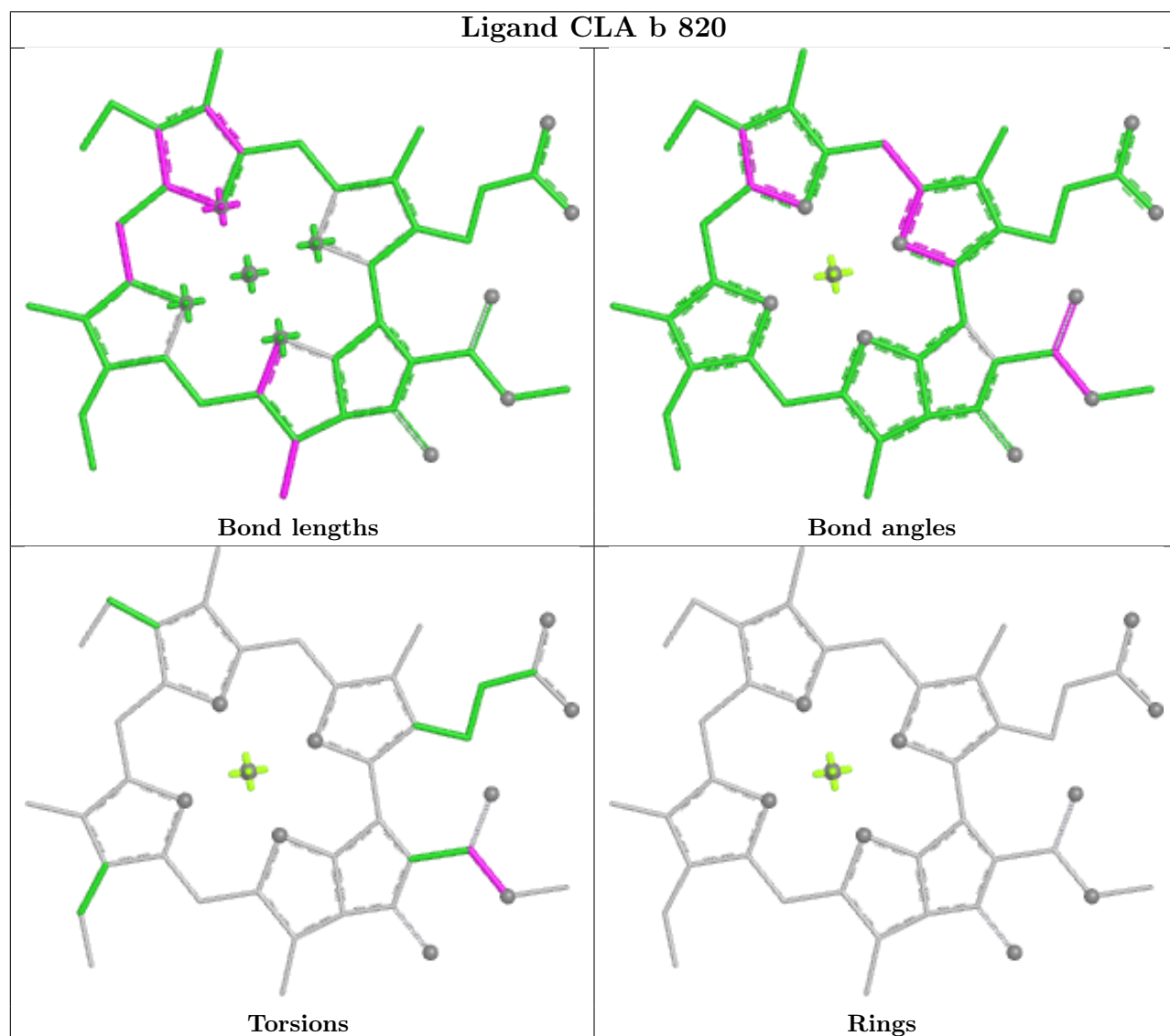
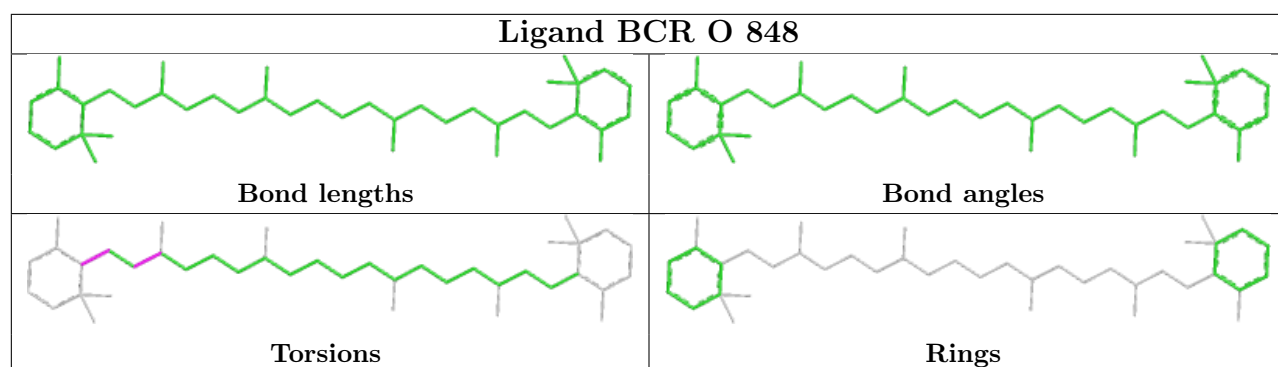
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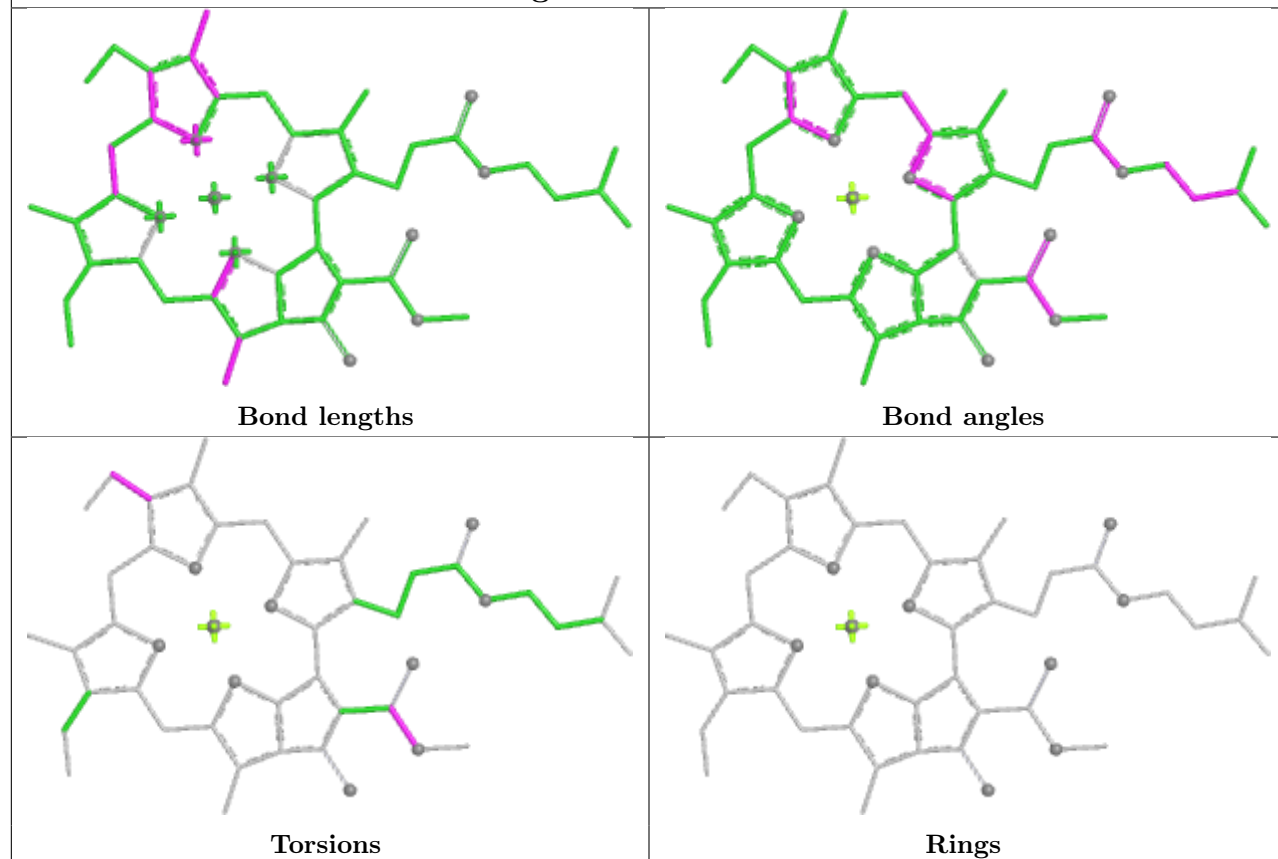
Ligand CLA a 821



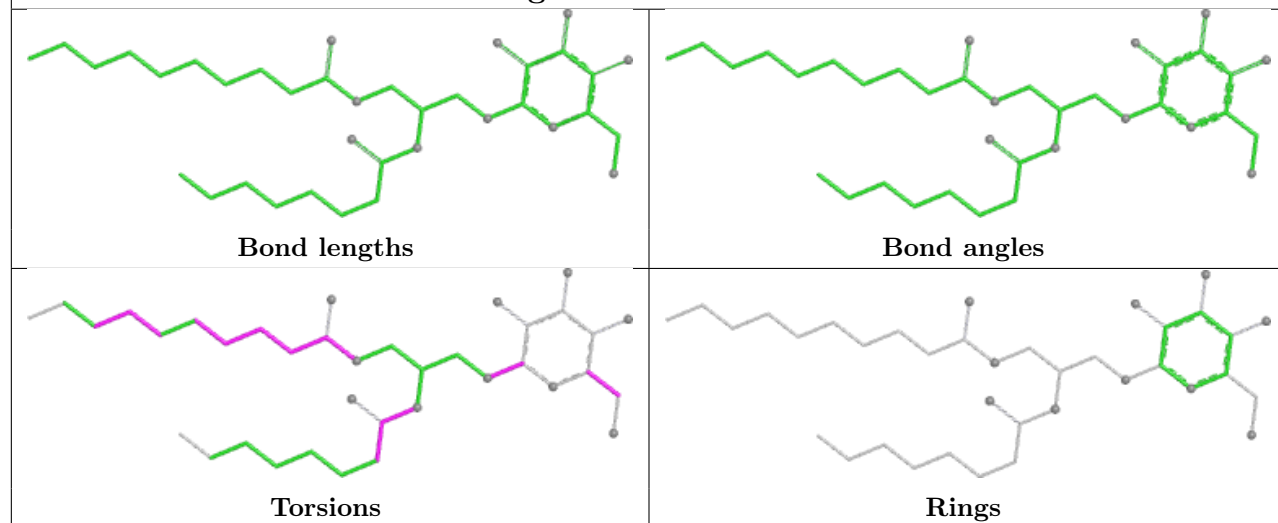


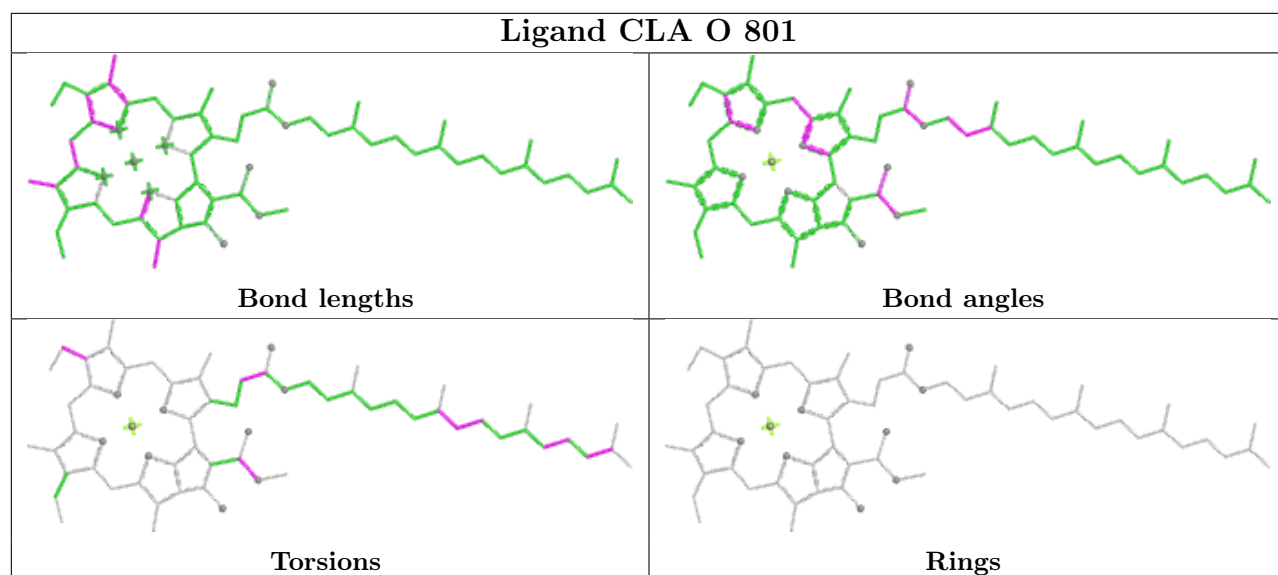
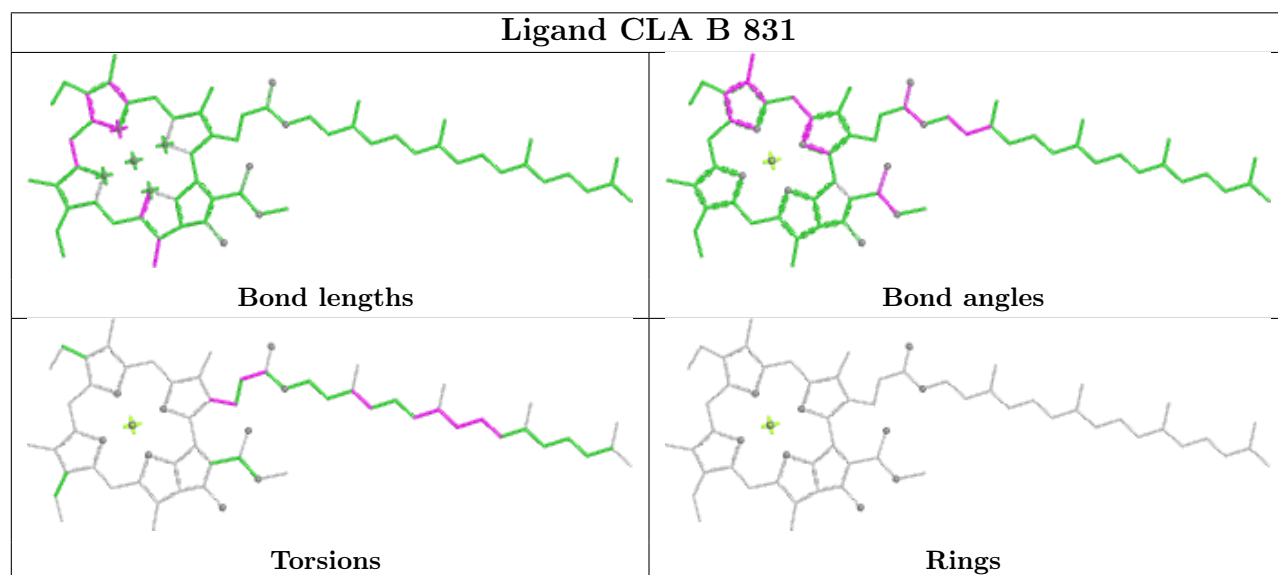
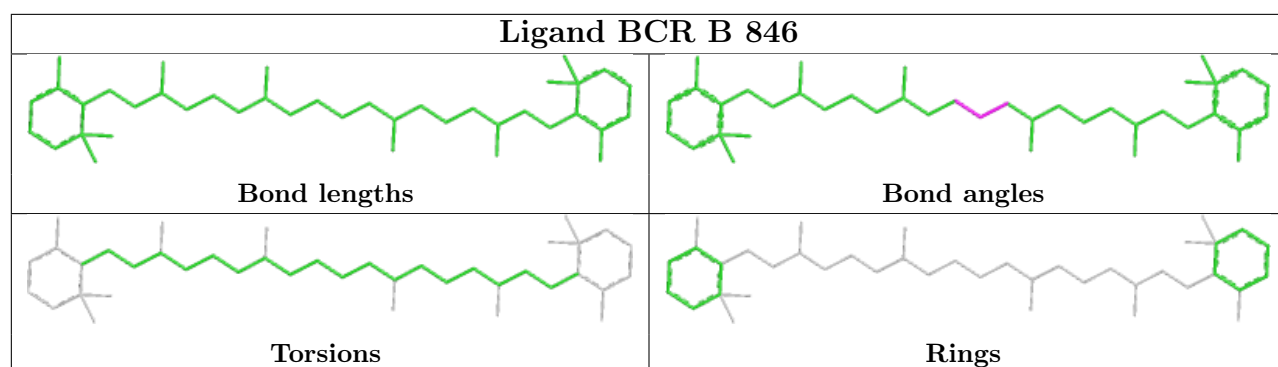


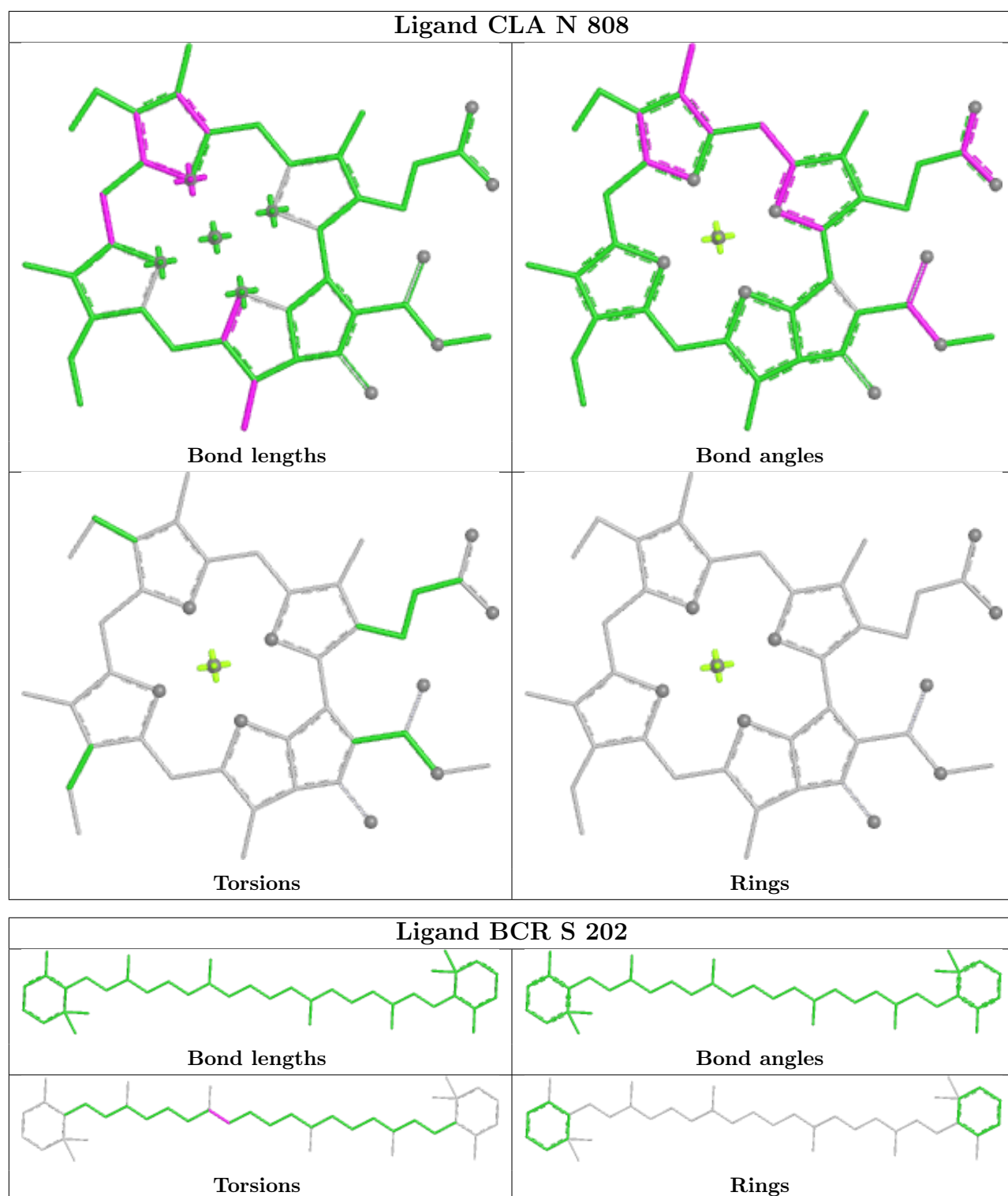
Ligand CLA V 103



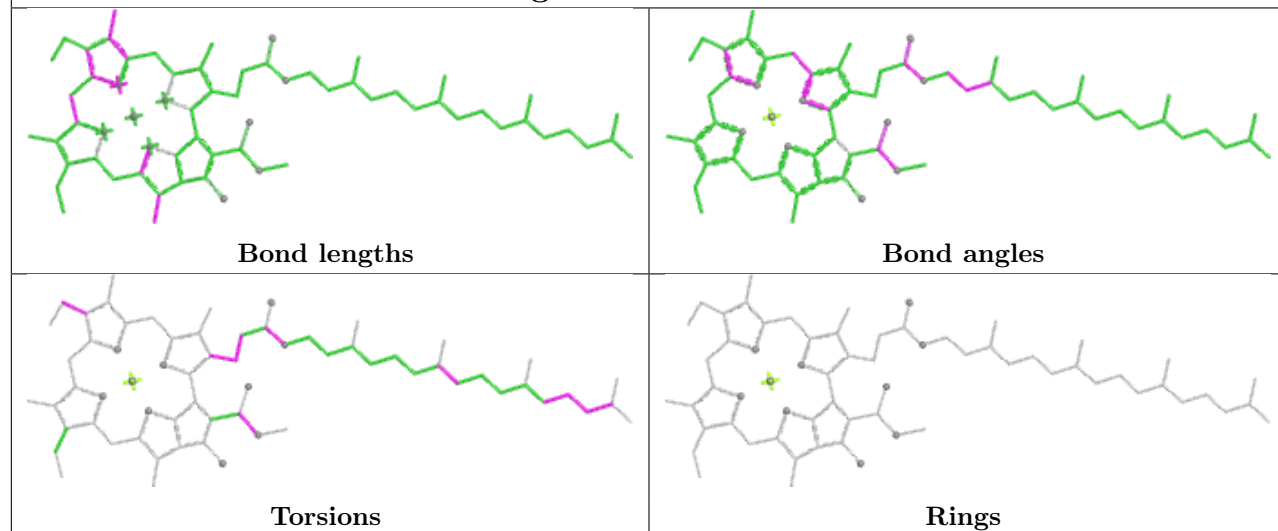
Ligand LMG T 103



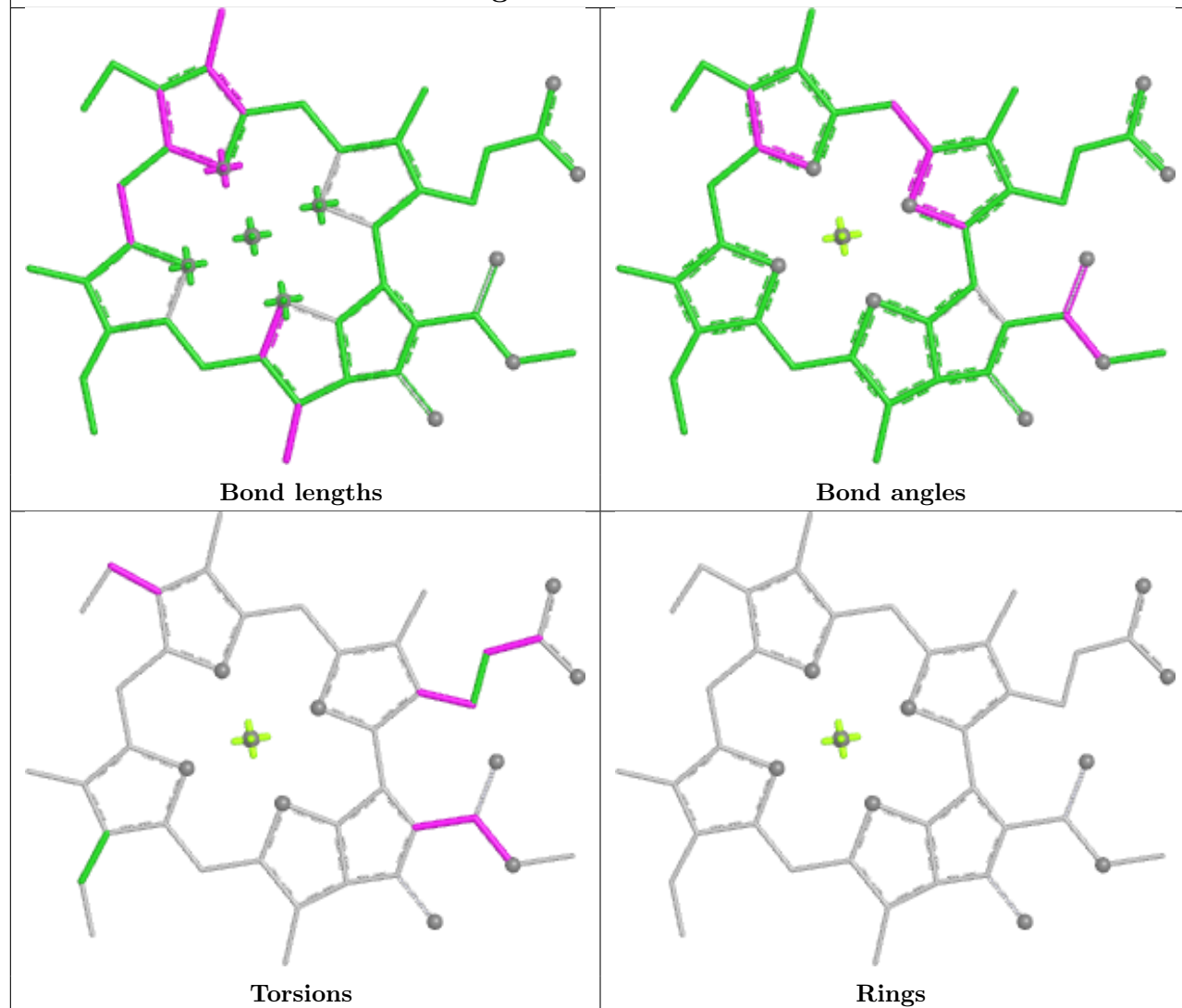


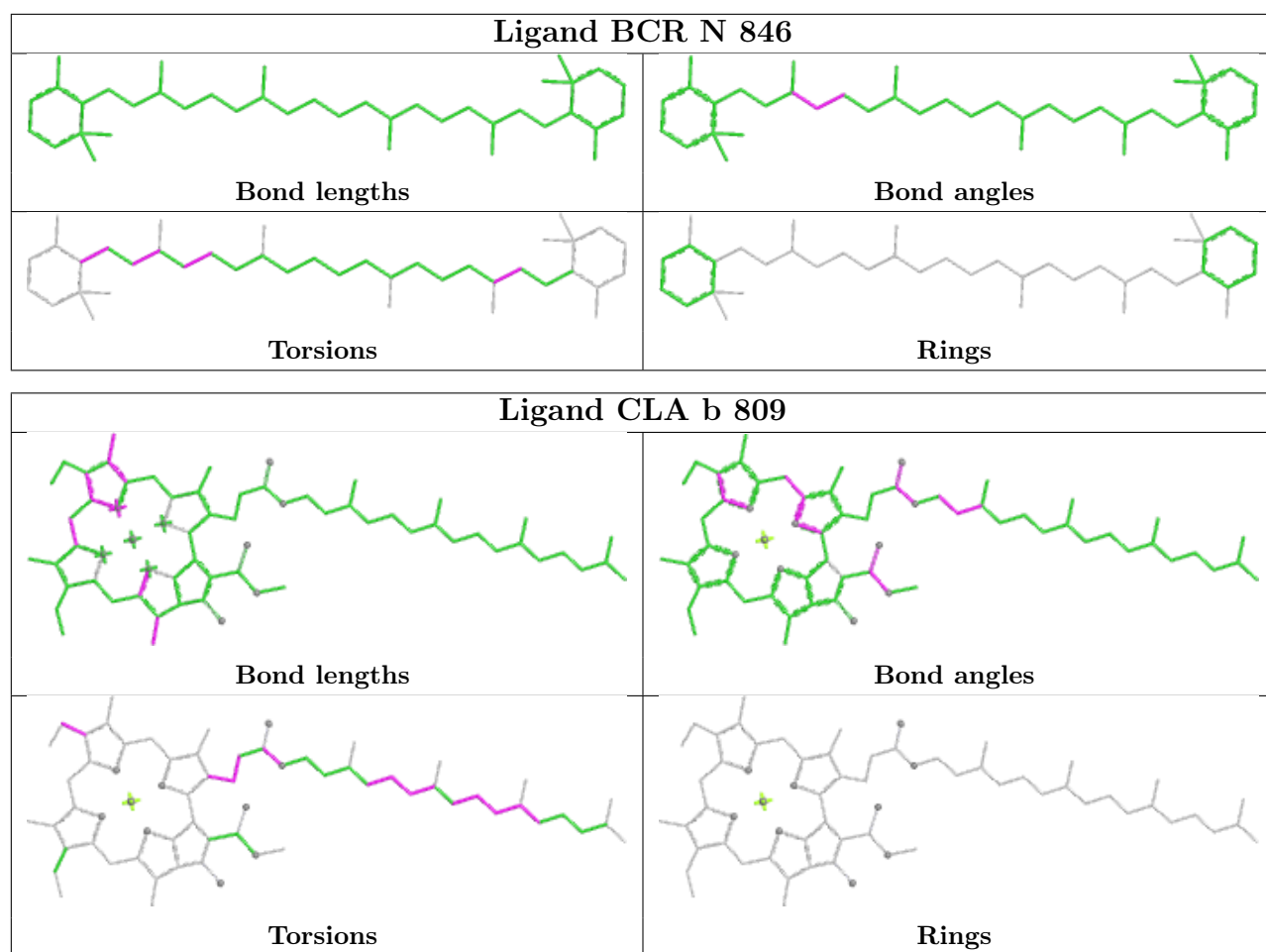


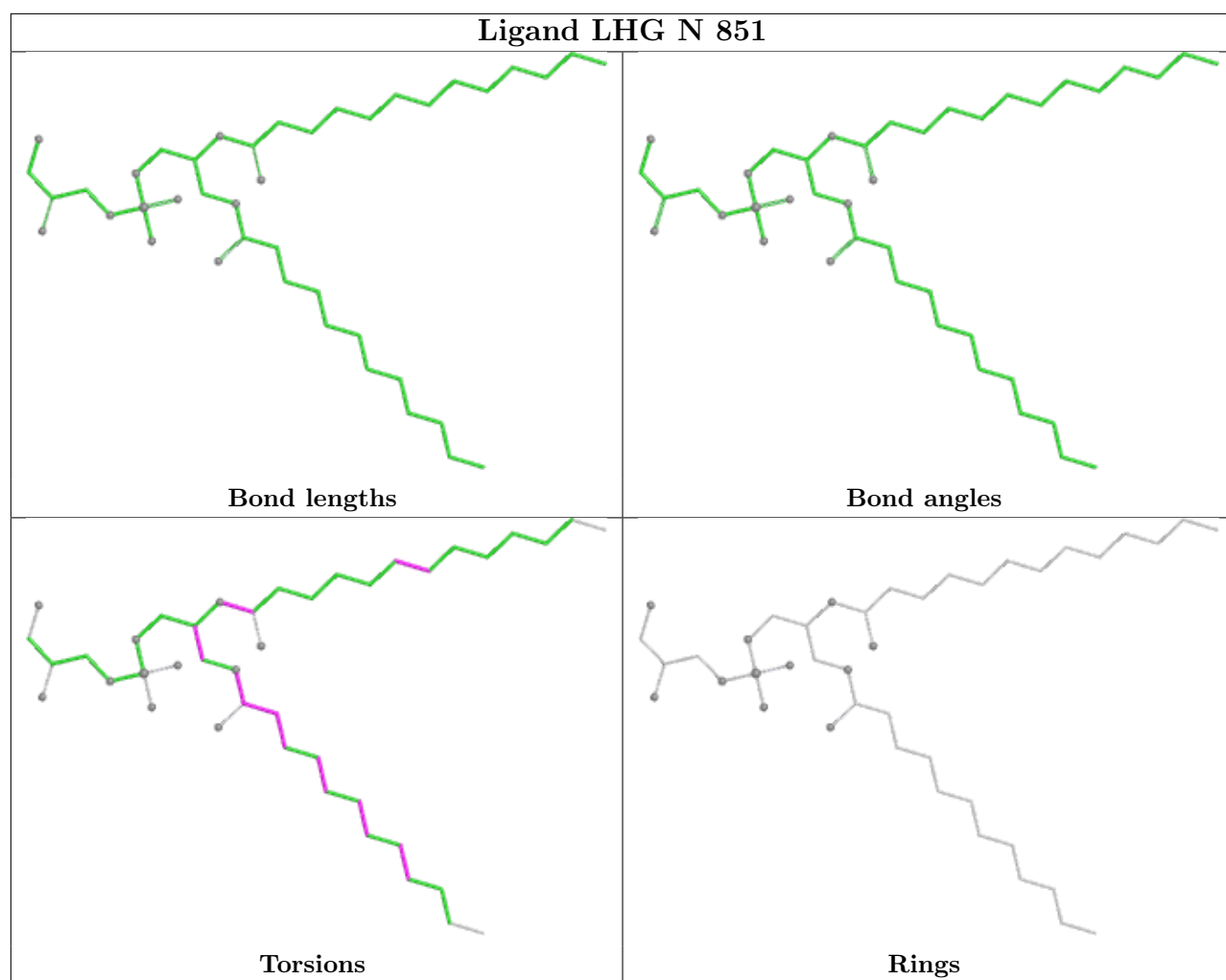
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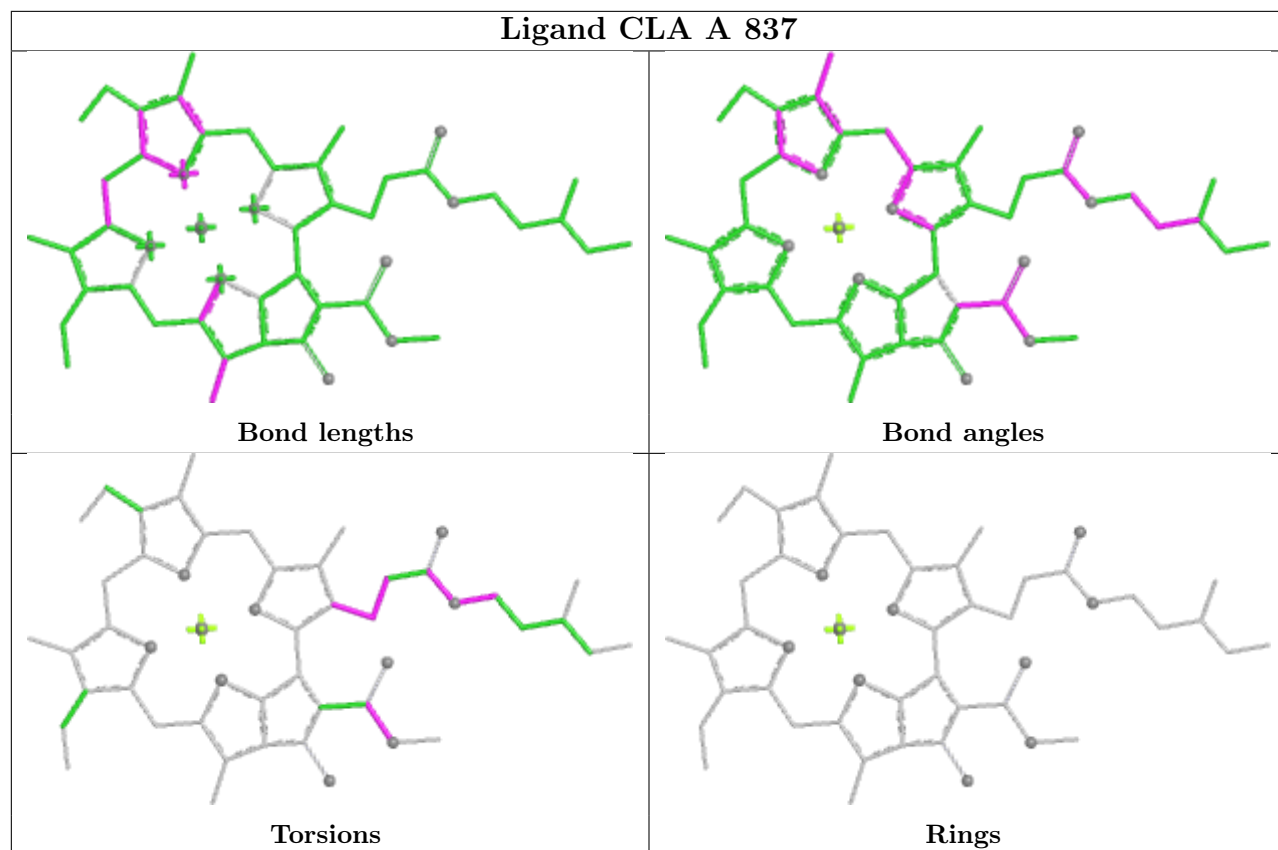
Ligand CLA O 835



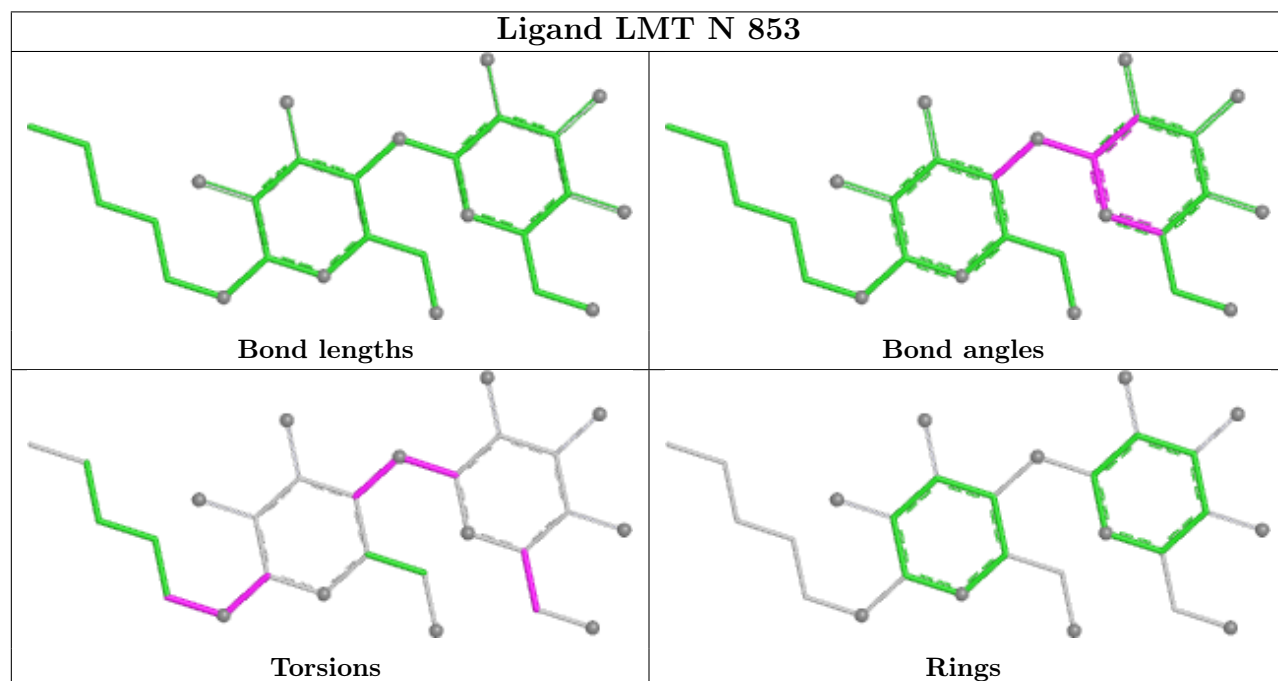


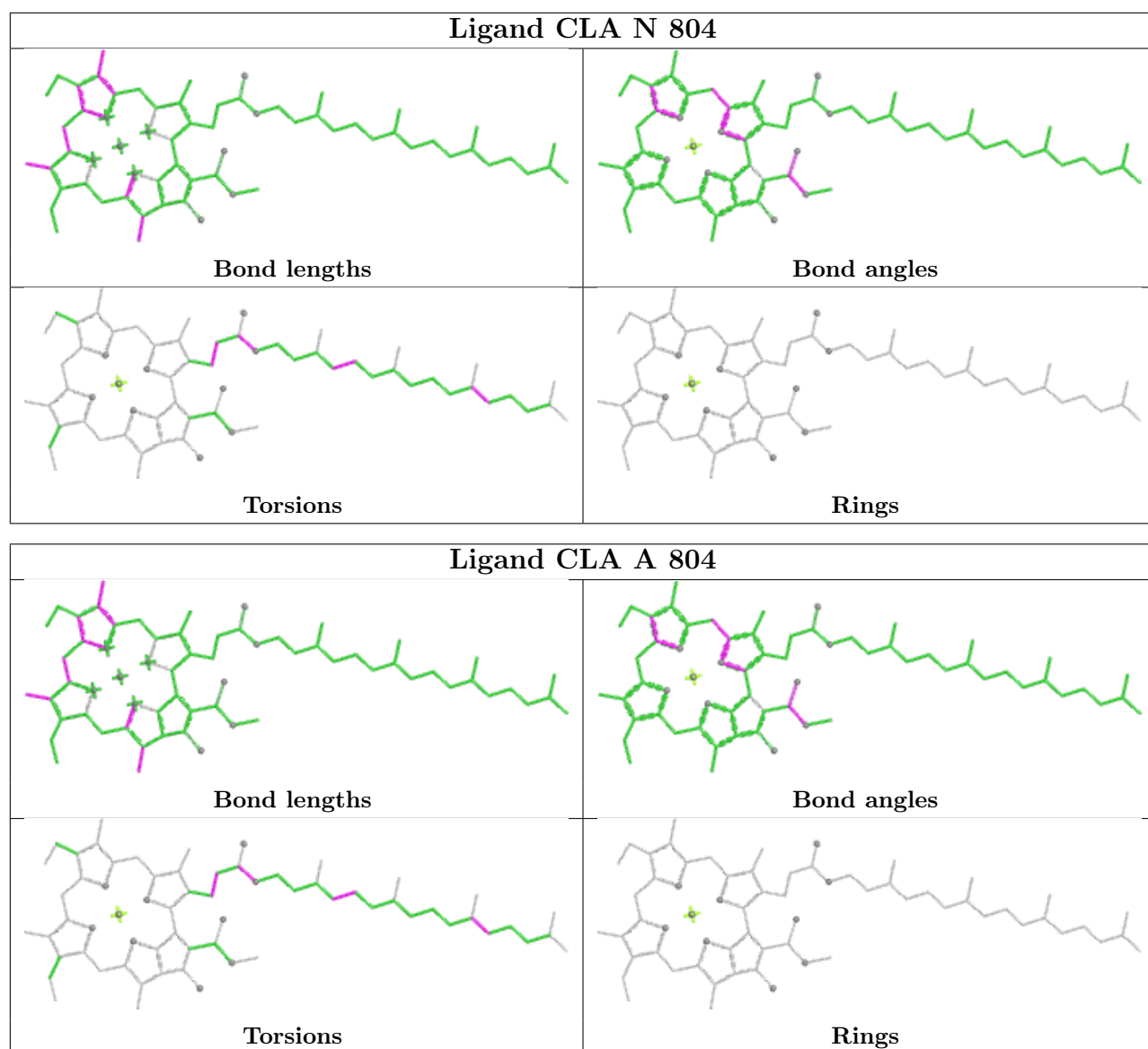


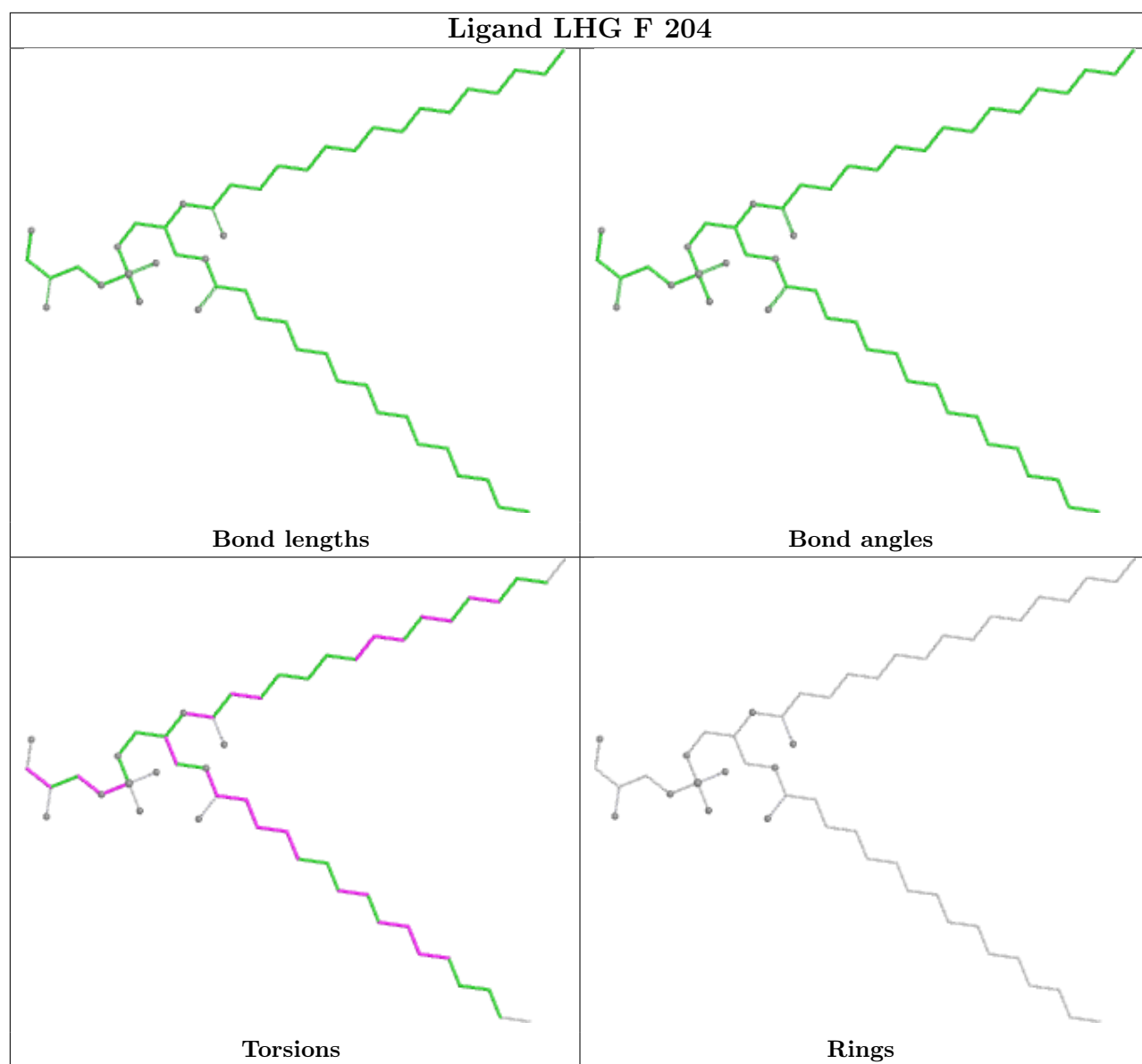
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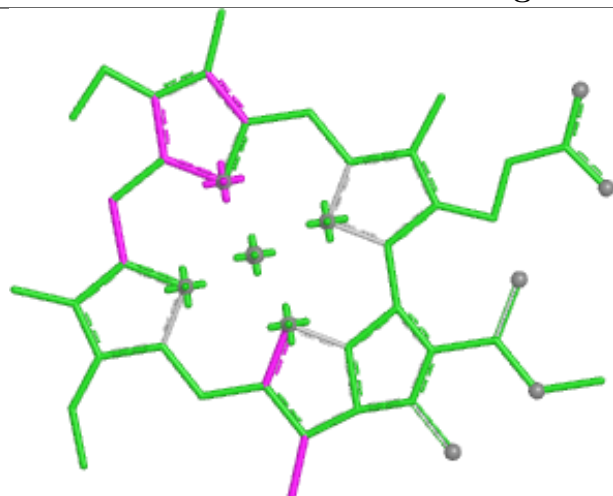
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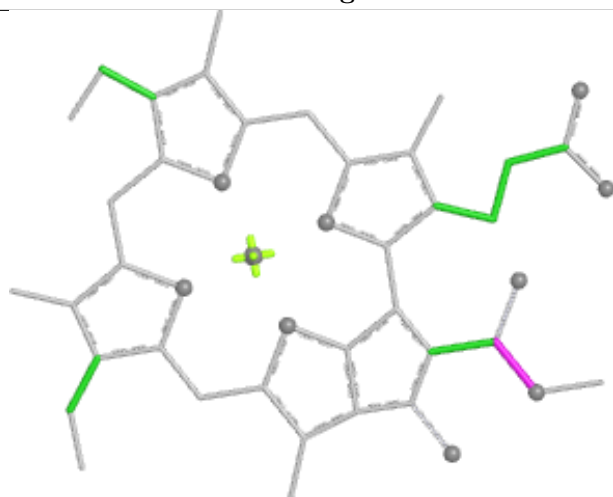
Ligand CLA O 820



Bond lengths



Bond angles

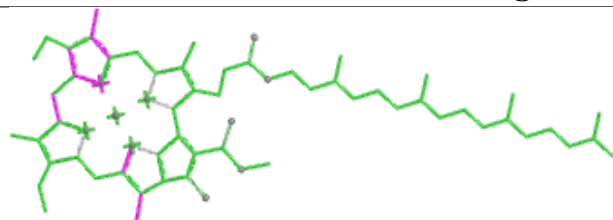


Torsions

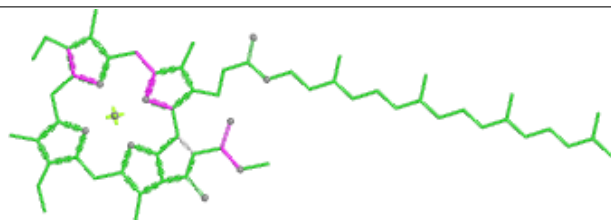


Rings

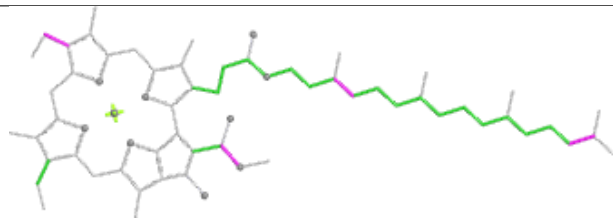
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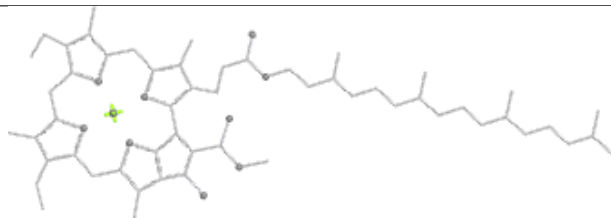
Bond lengths



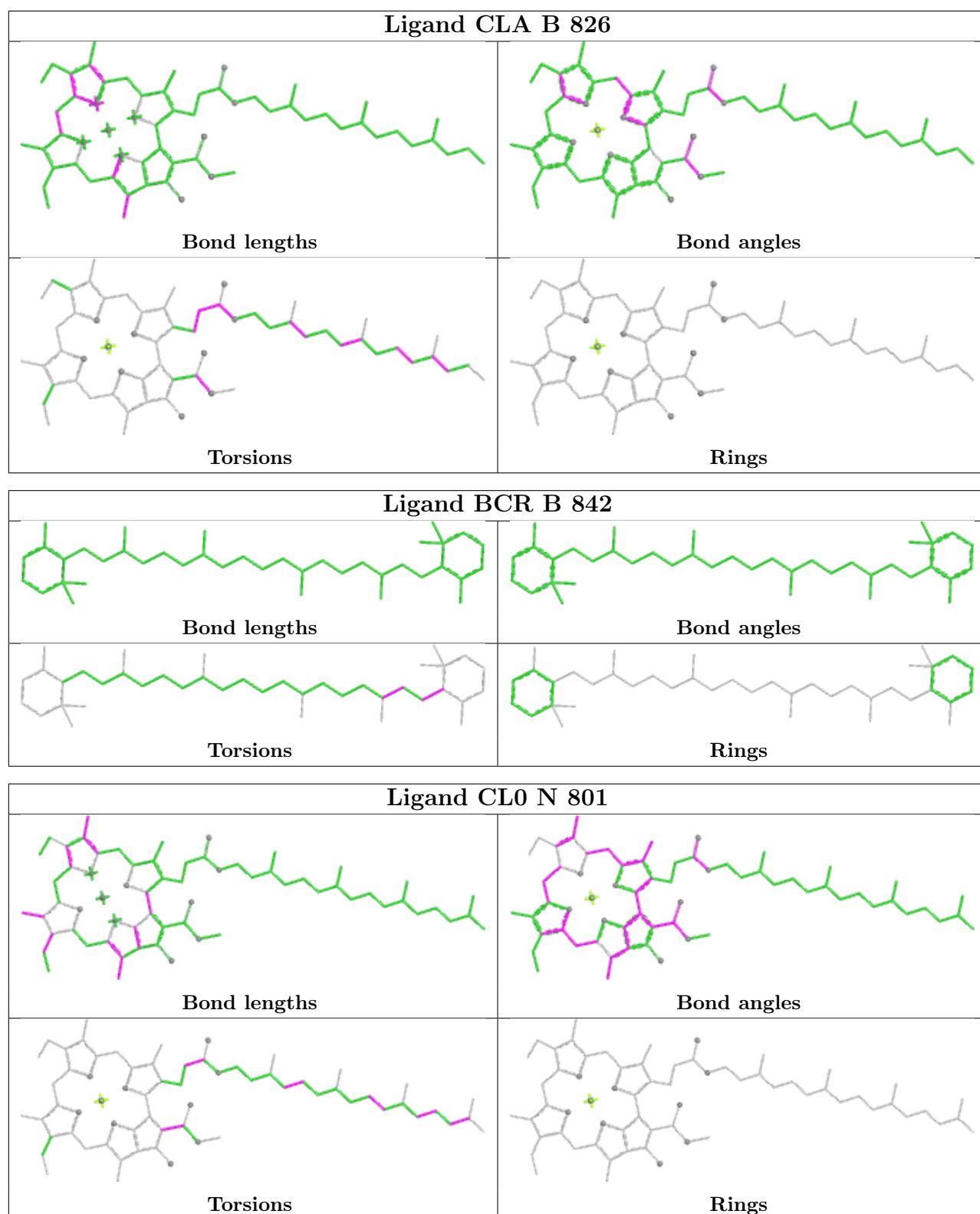
Bond angles



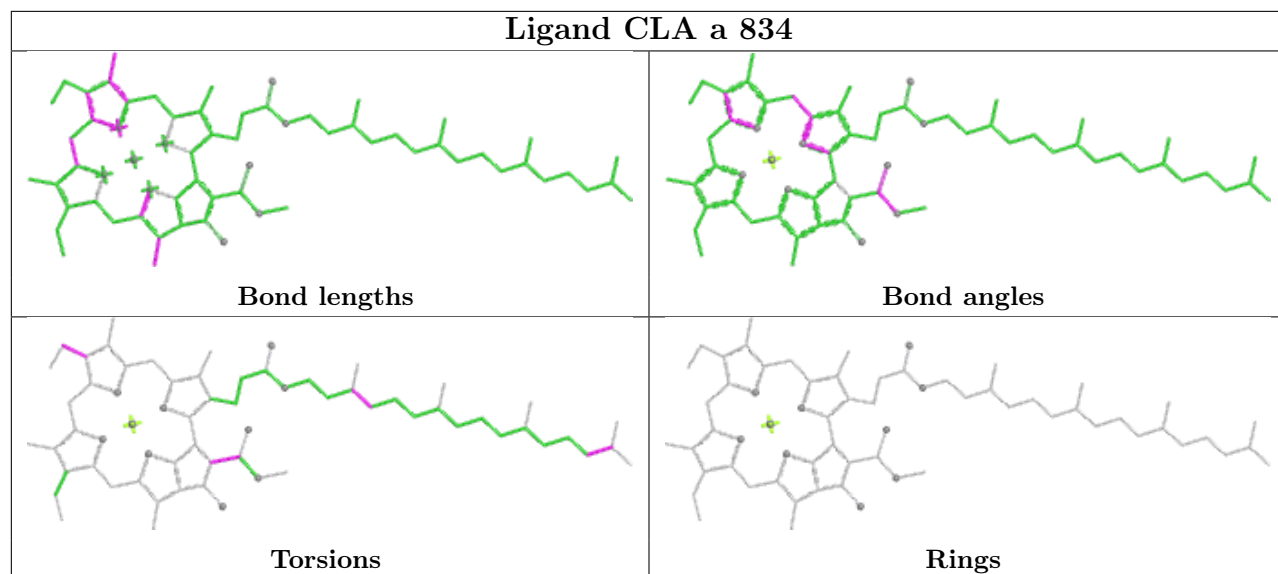
Torsions



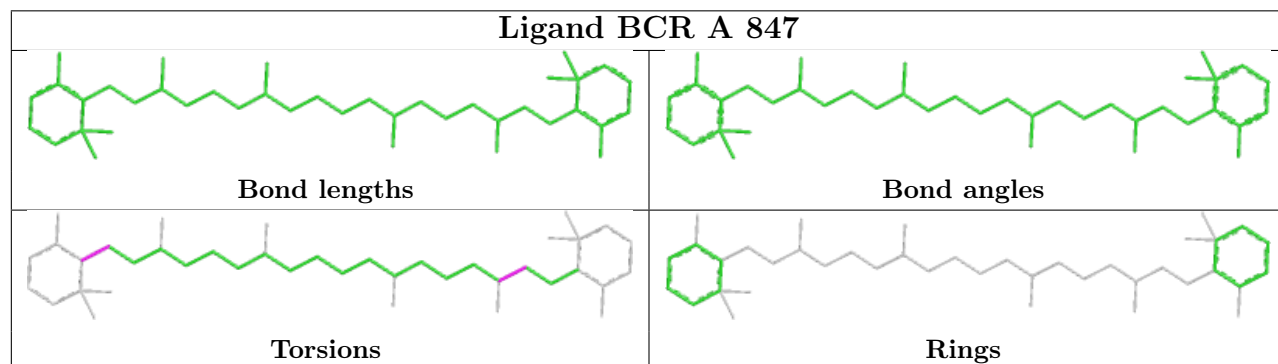
Rings



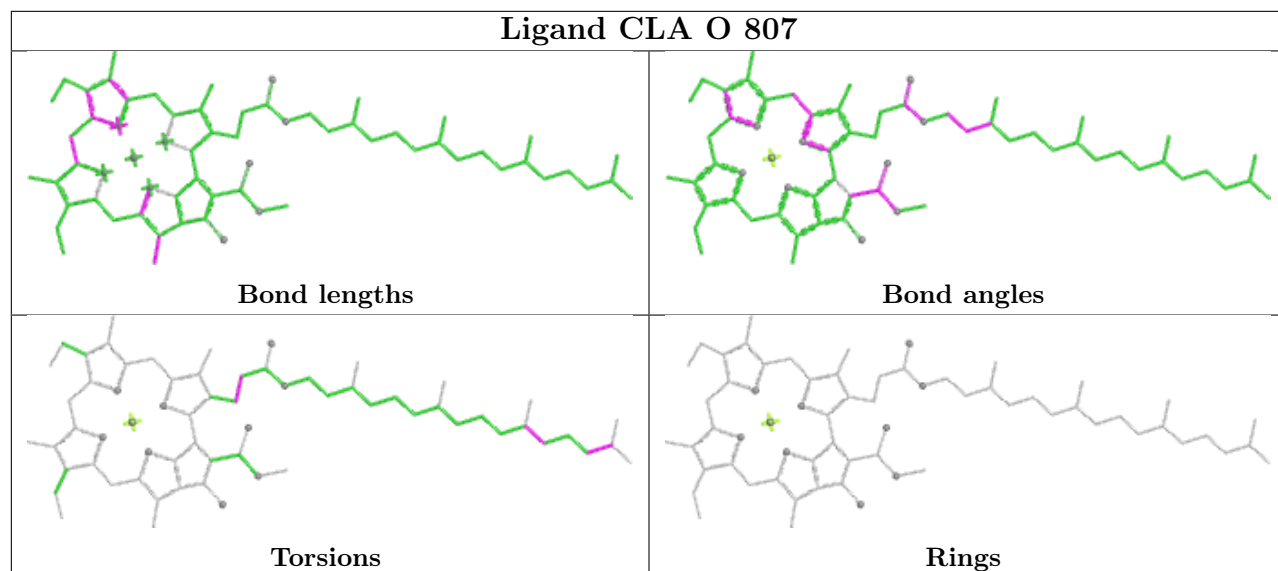
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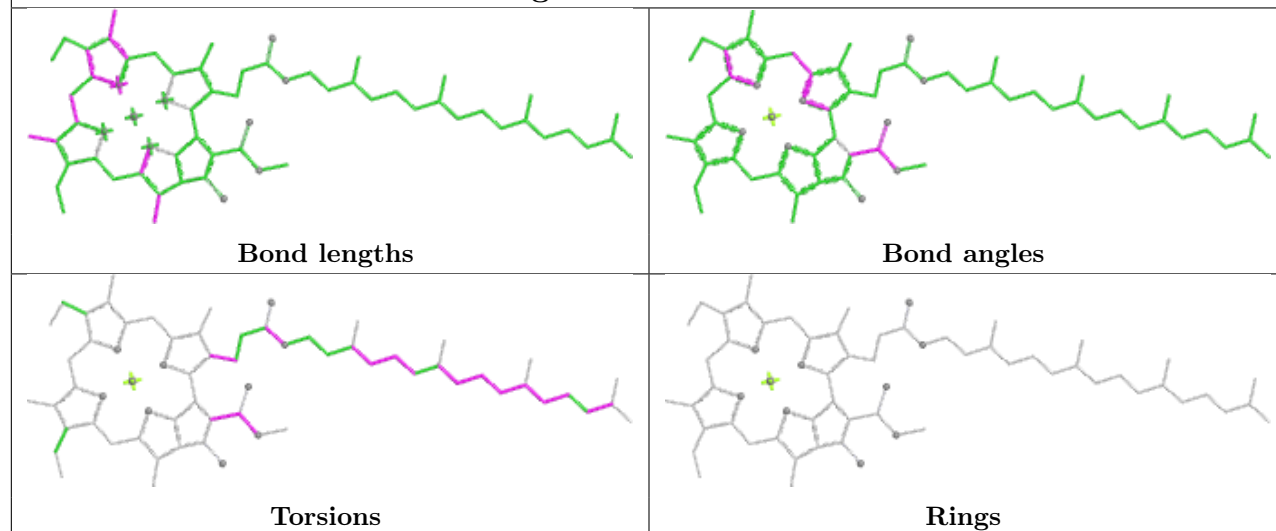
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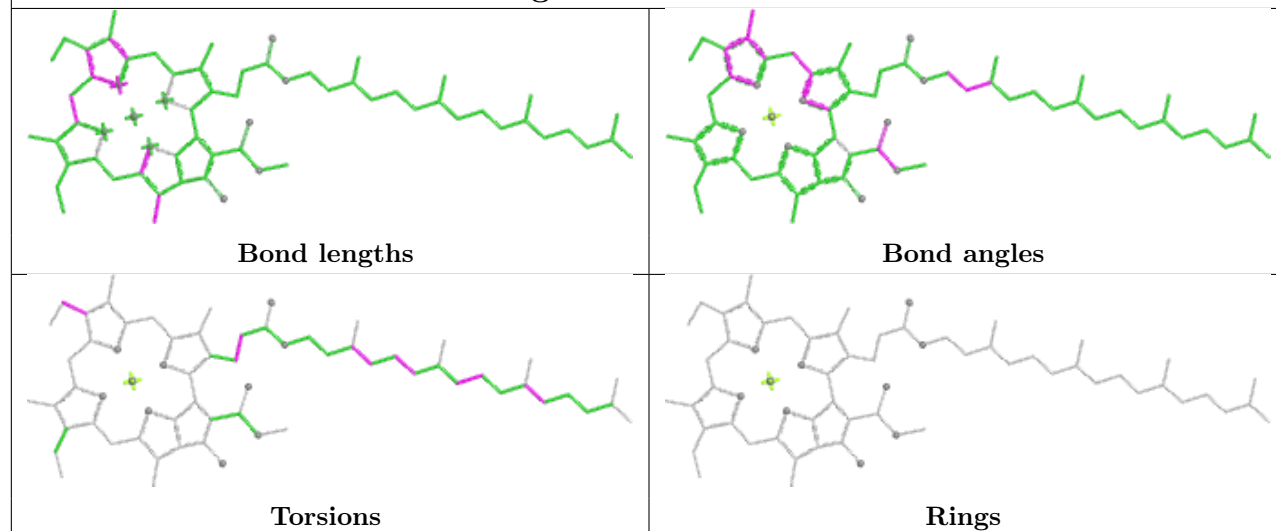
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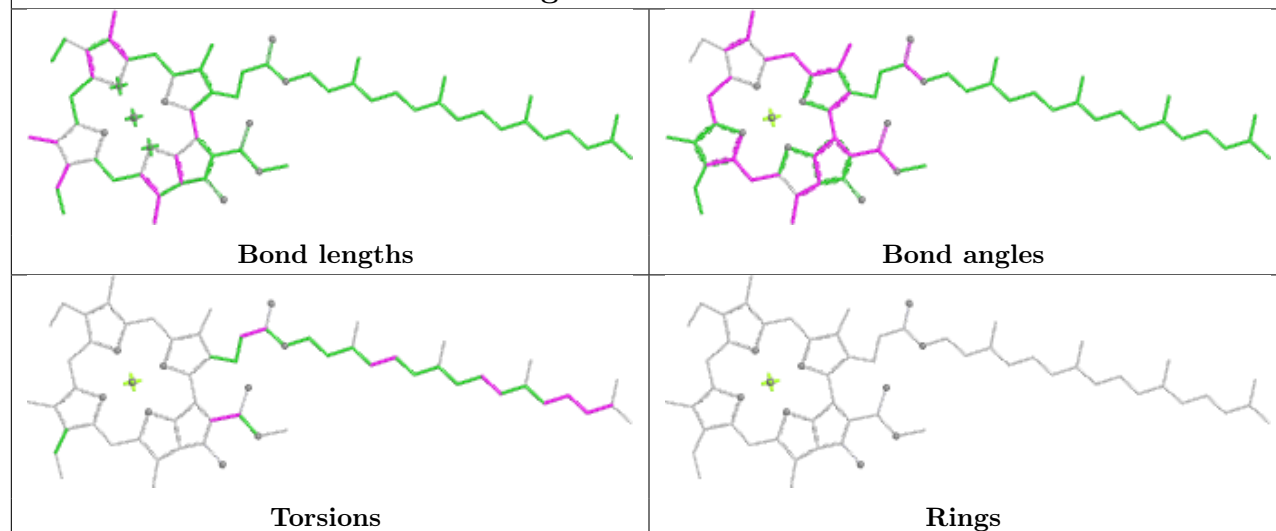
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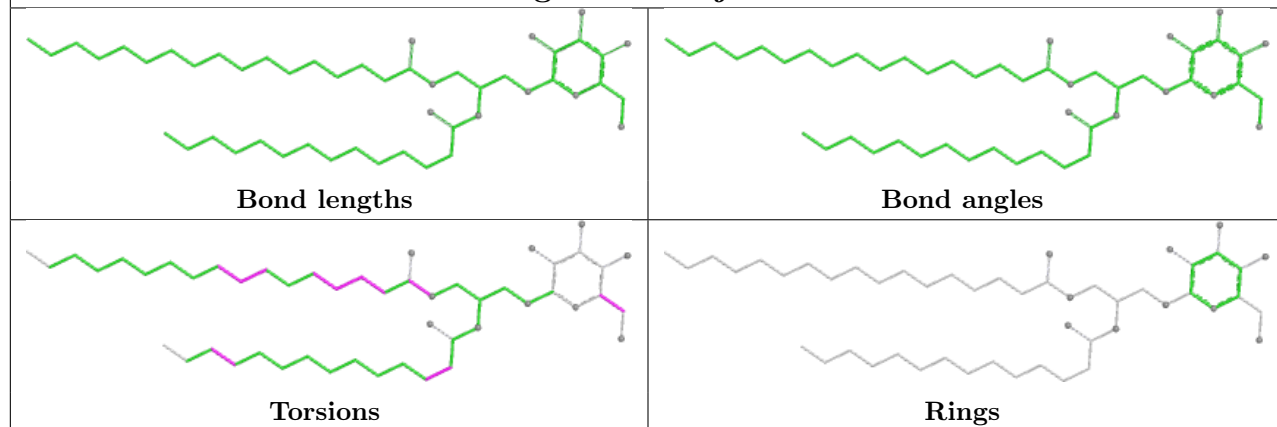
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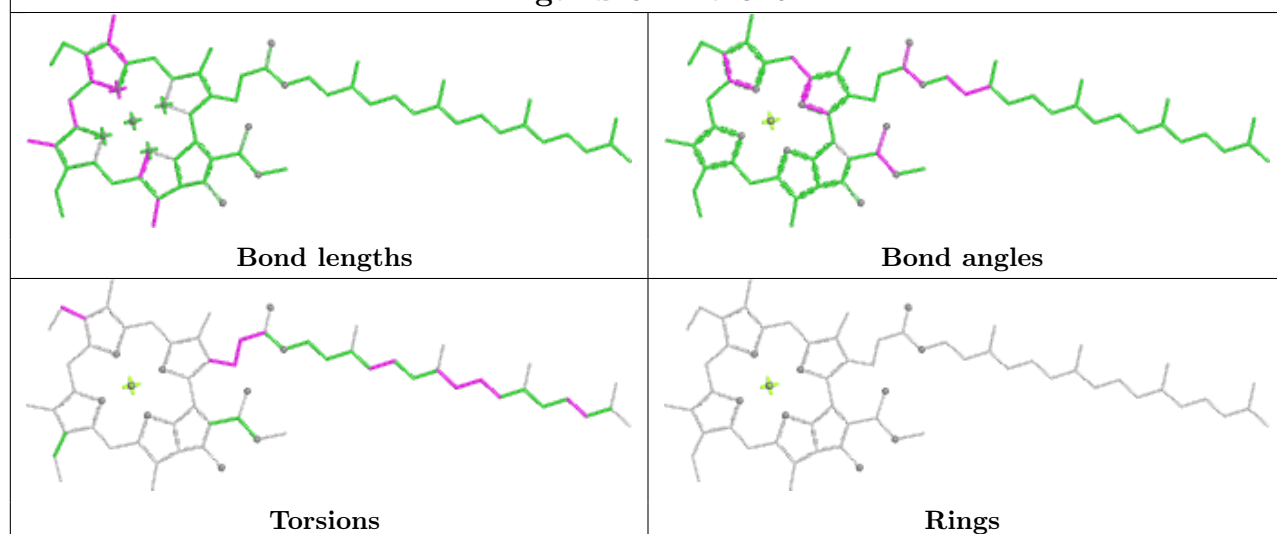
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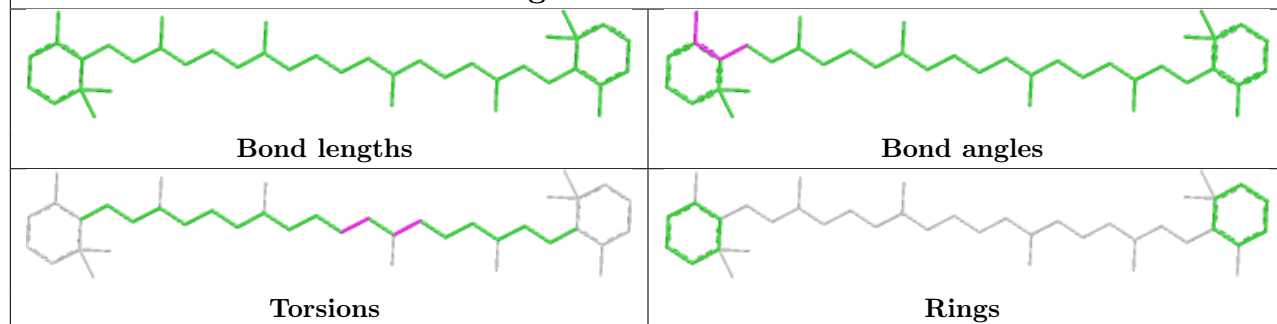
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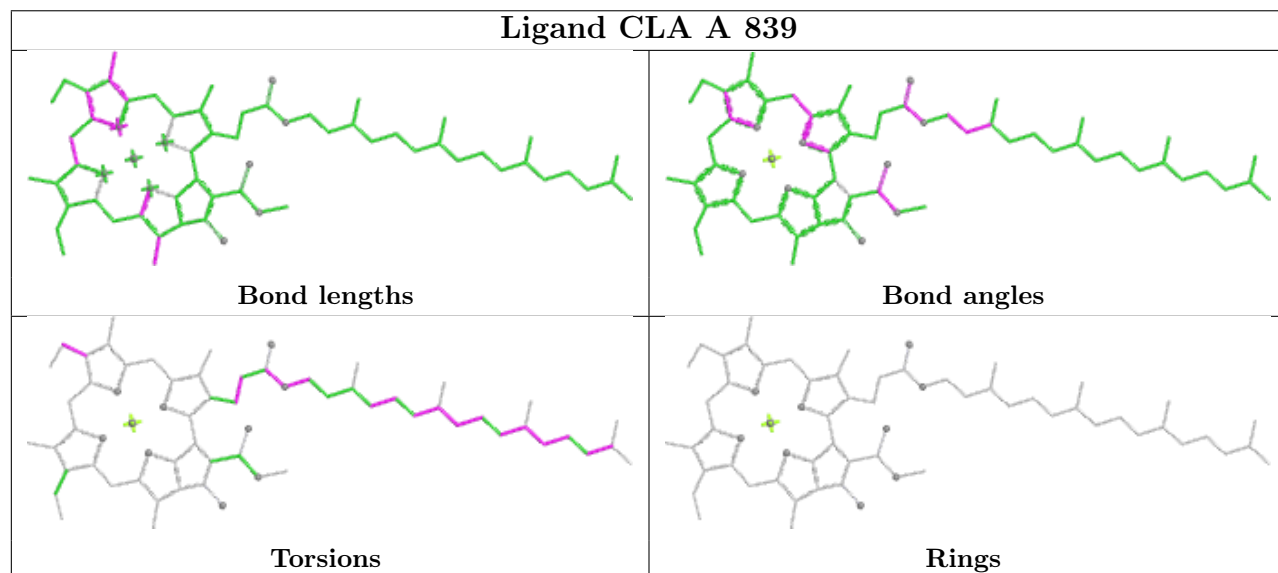
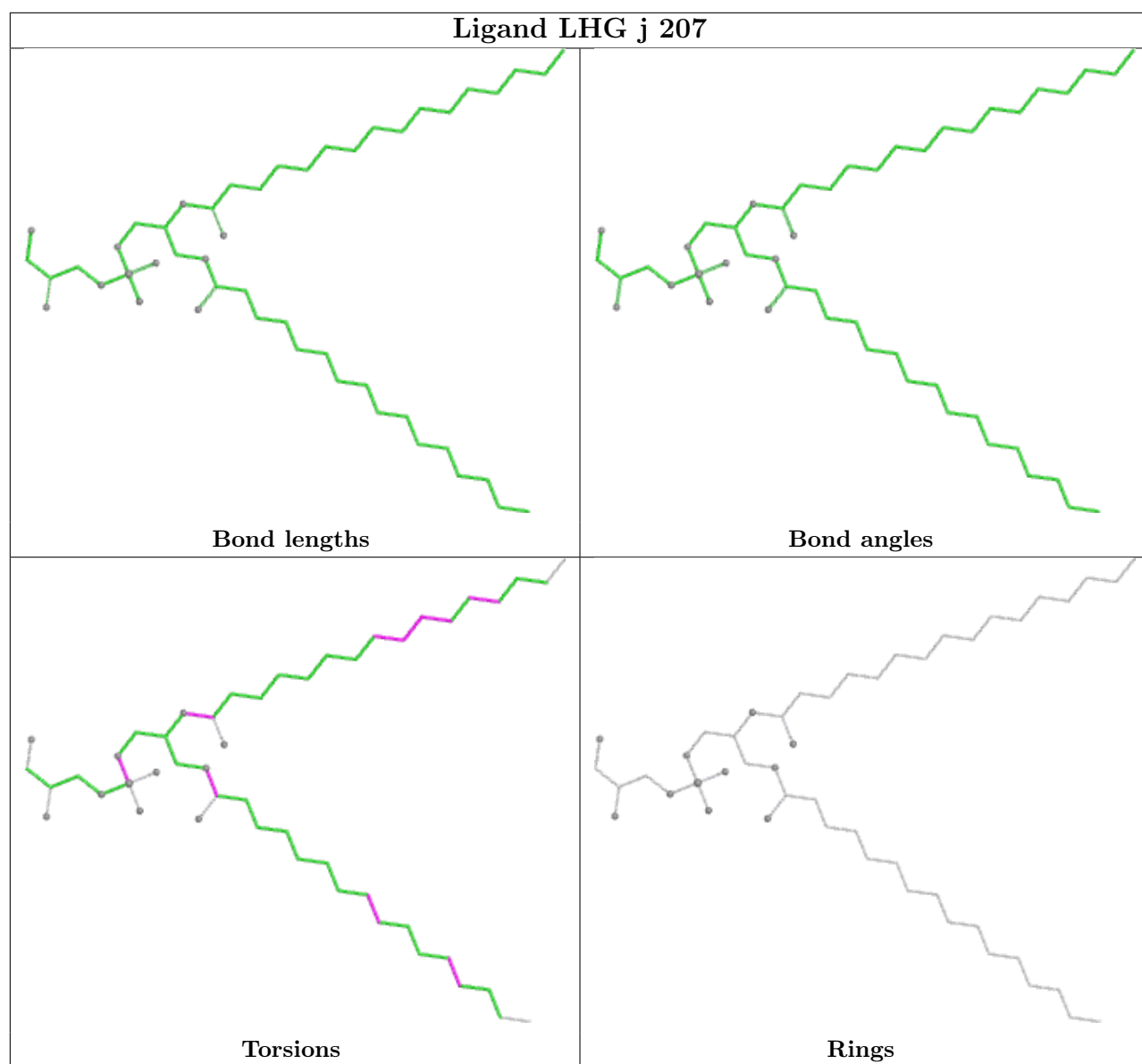


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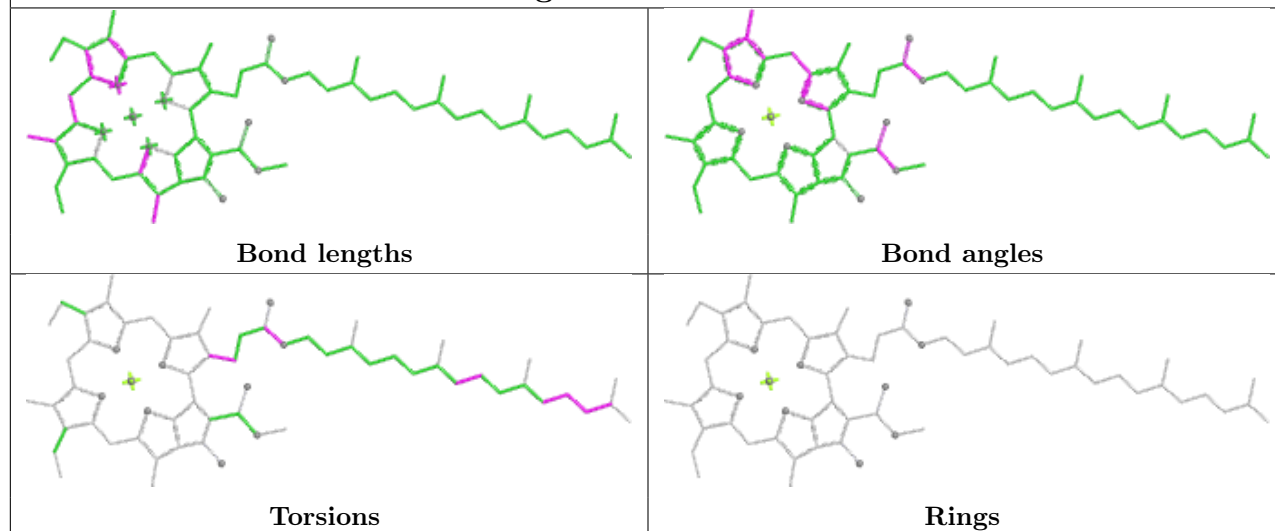


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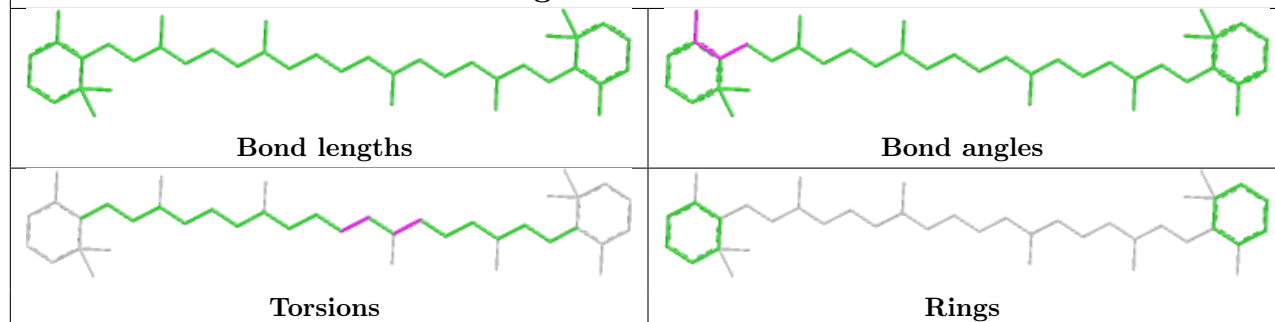




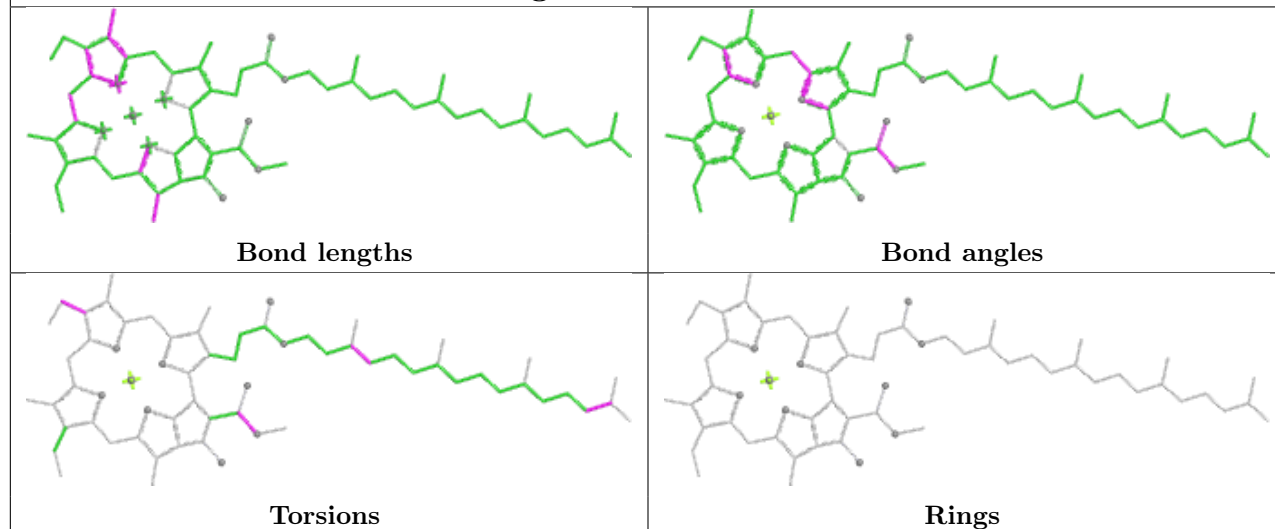
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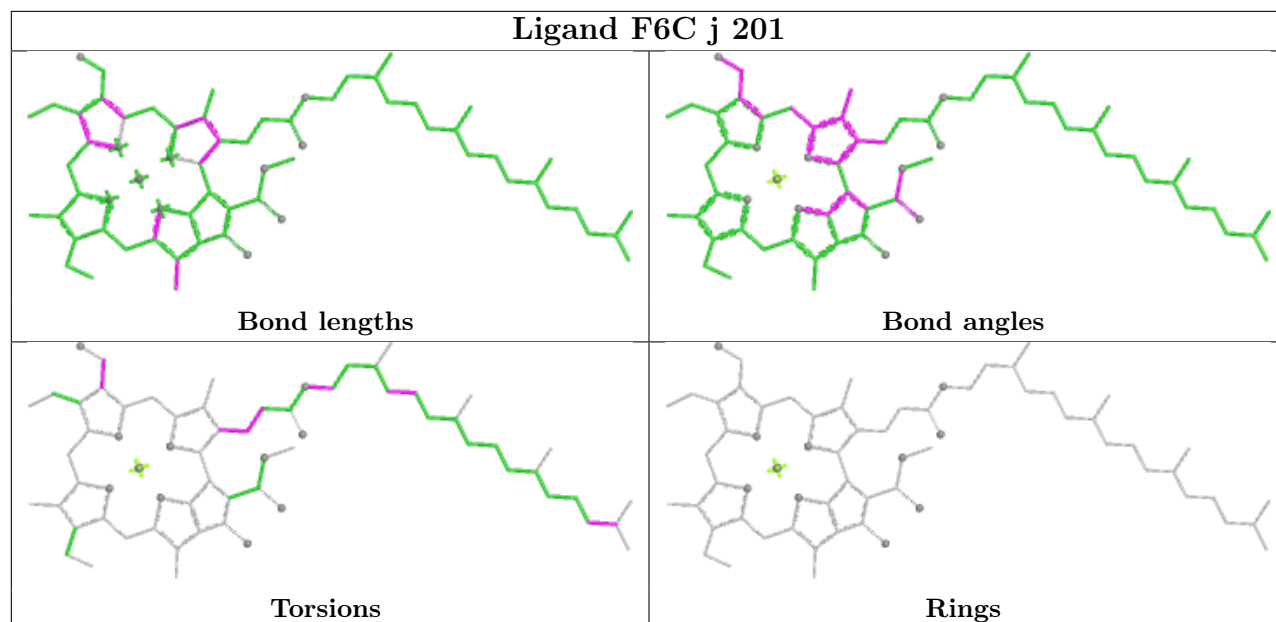
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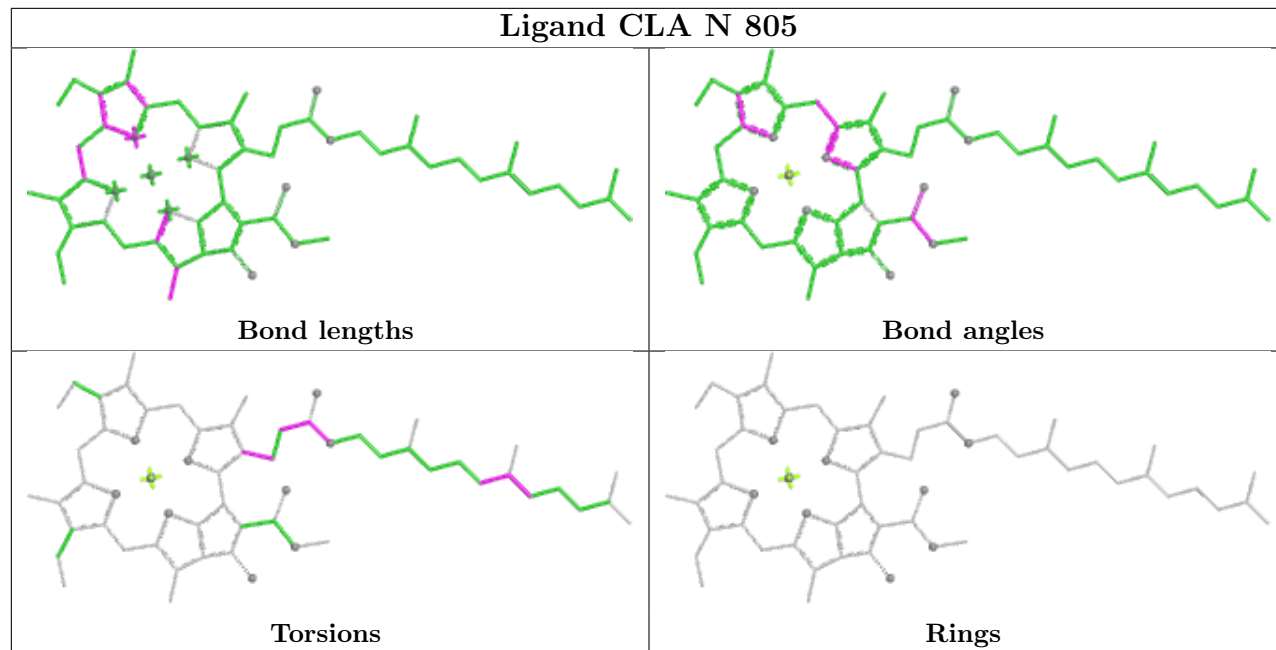
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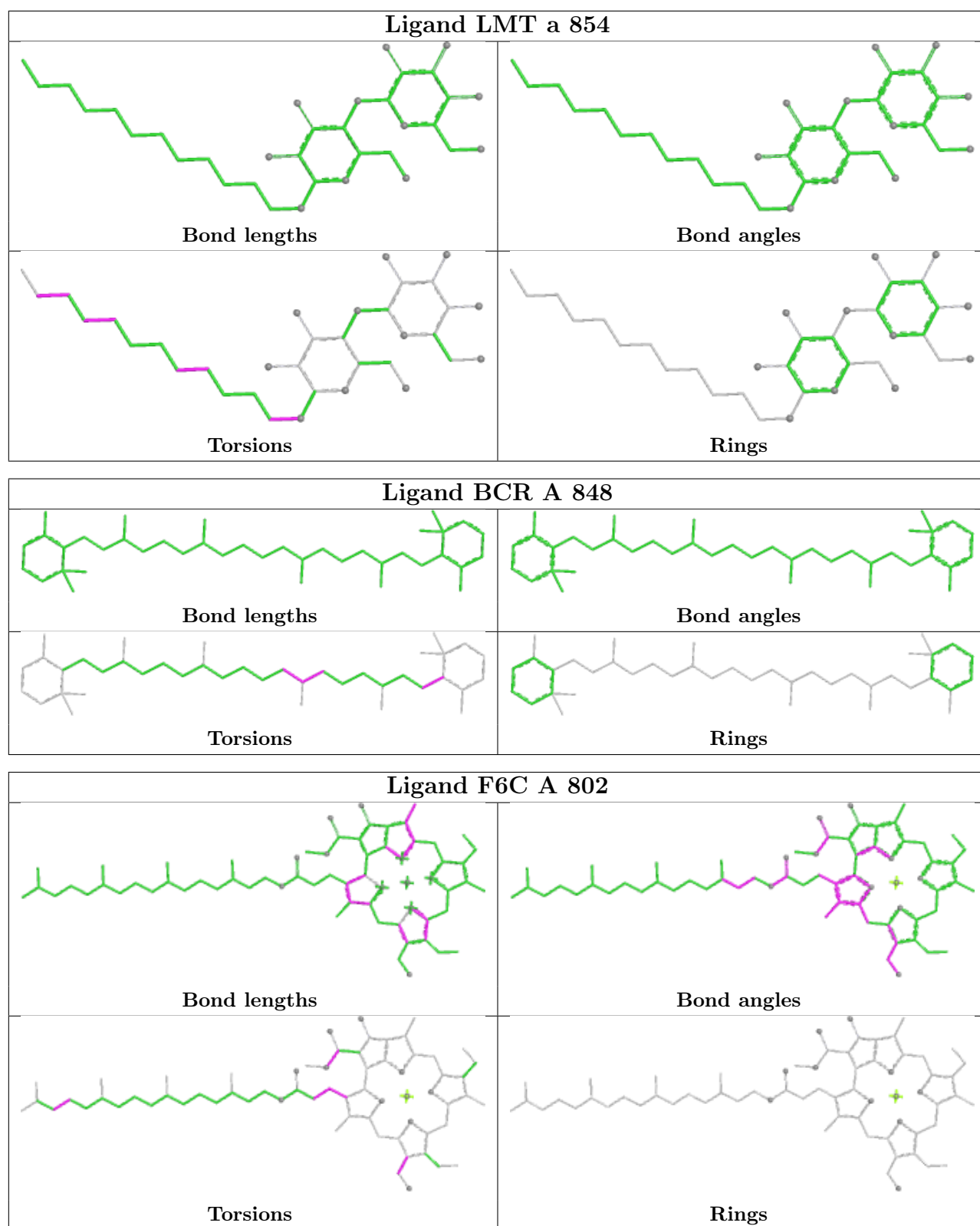


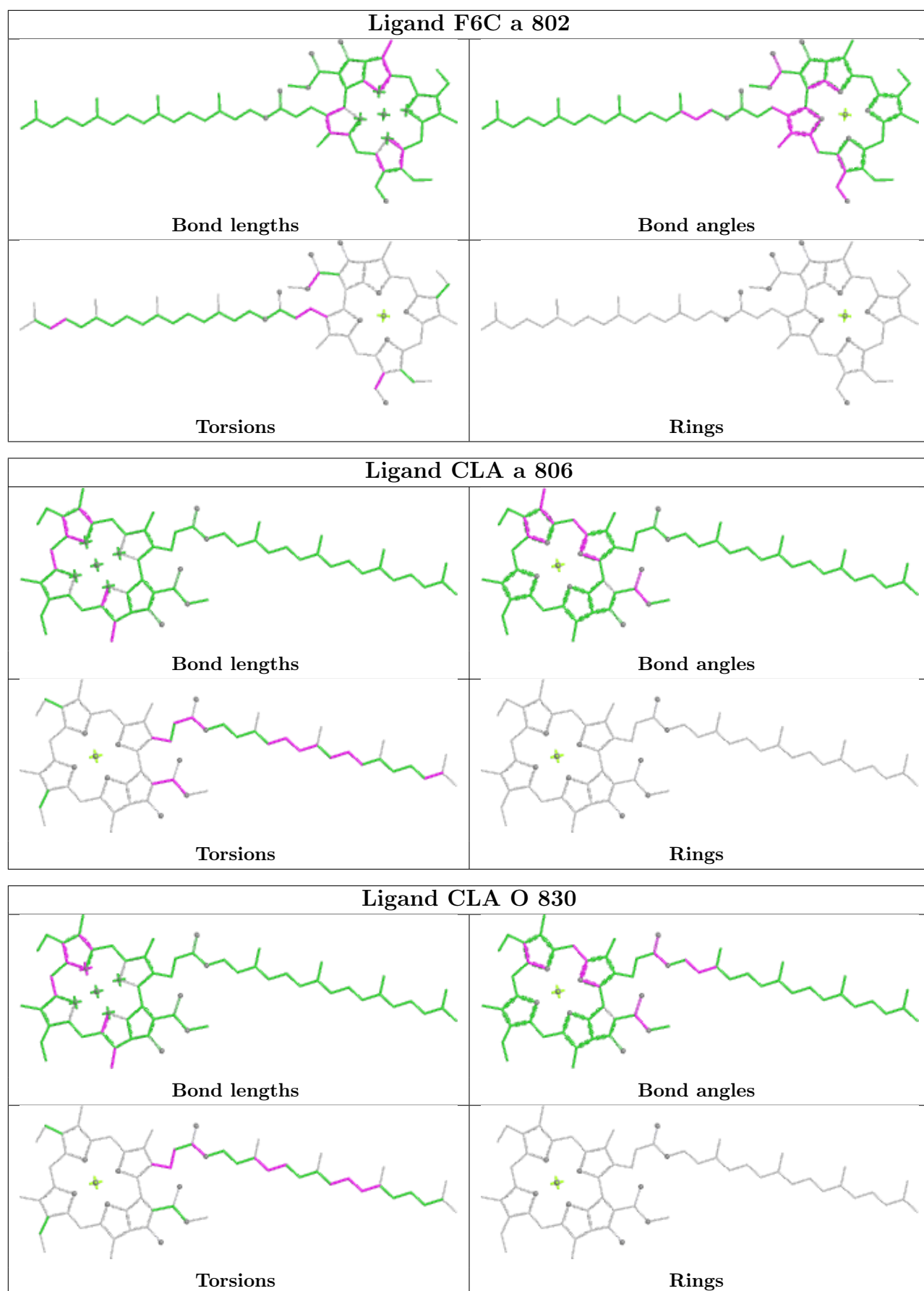
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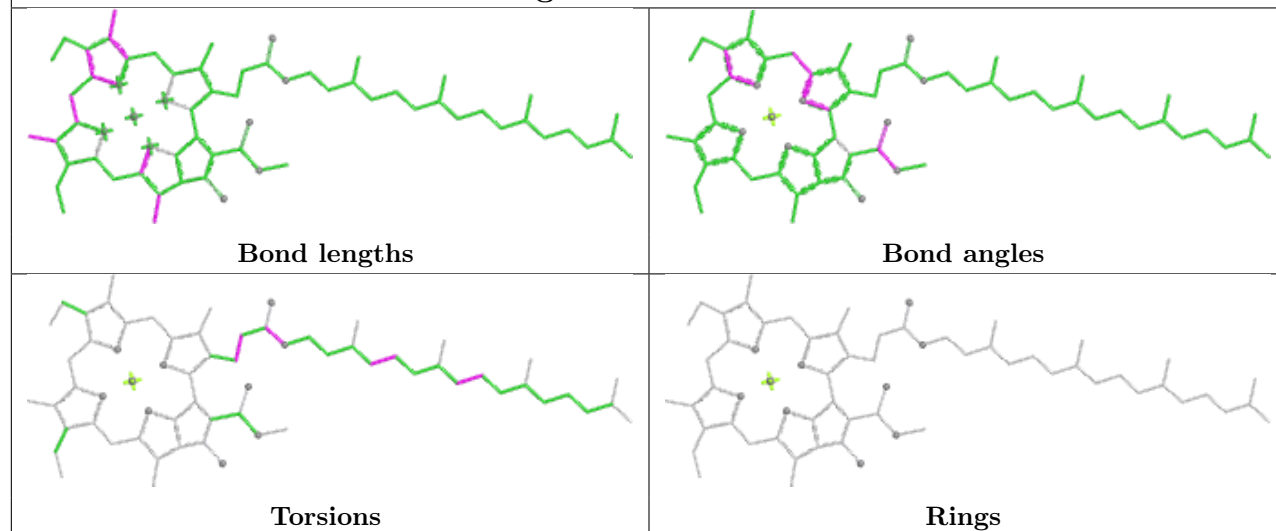
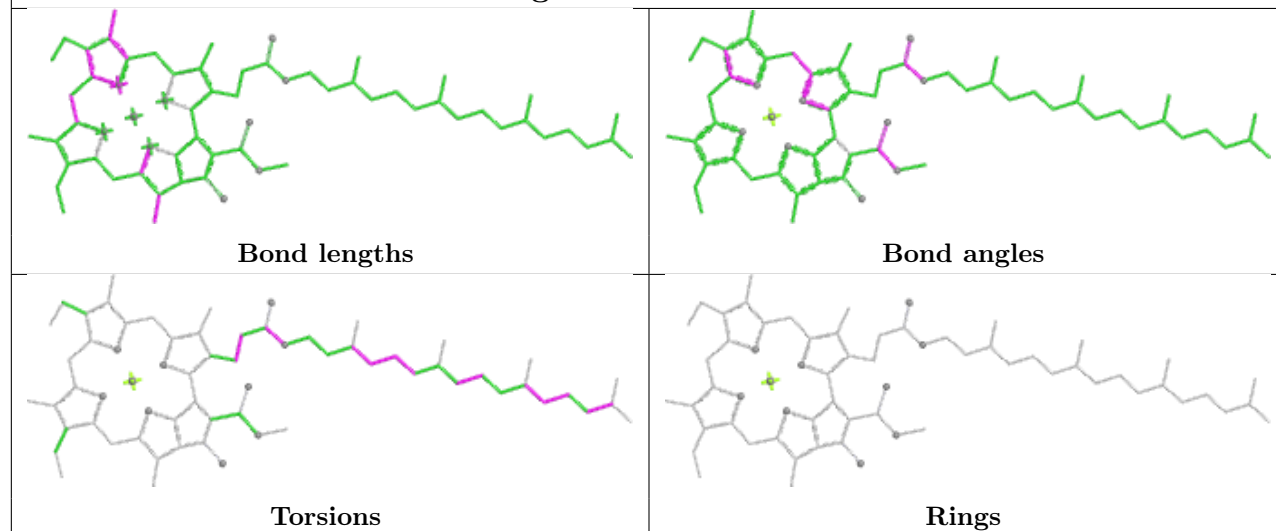


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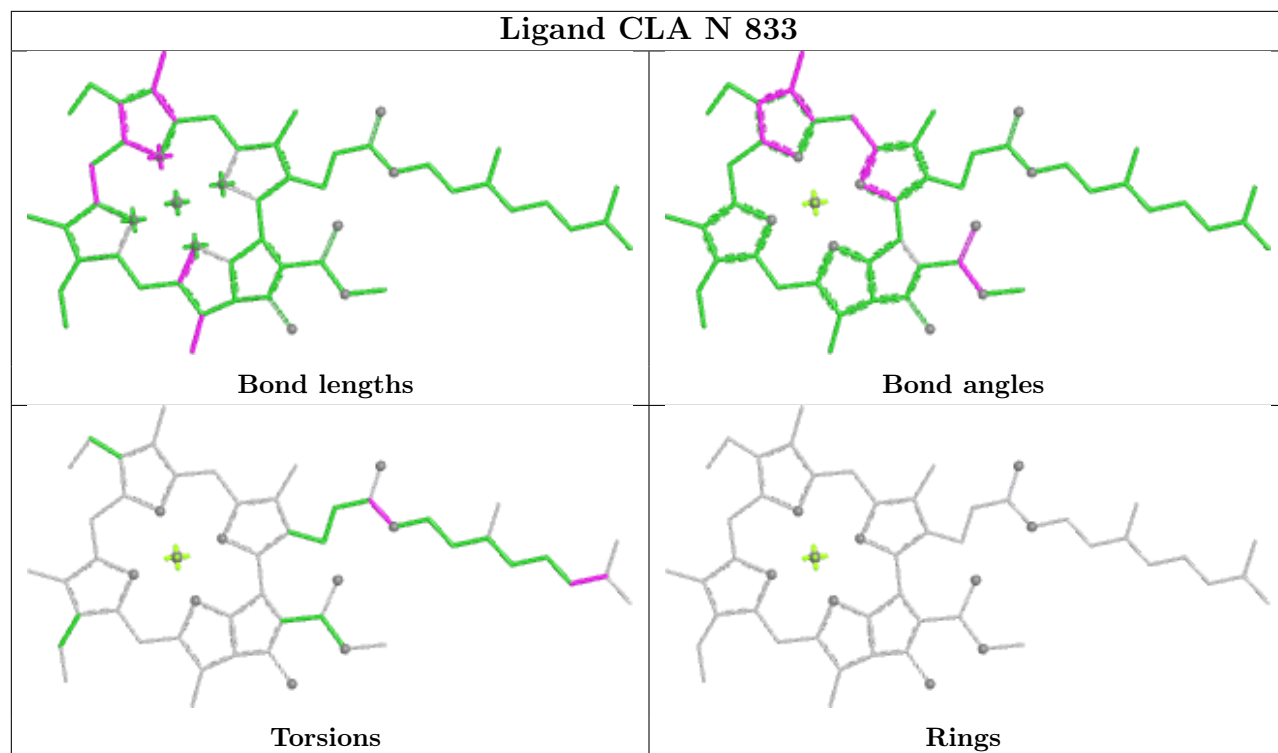




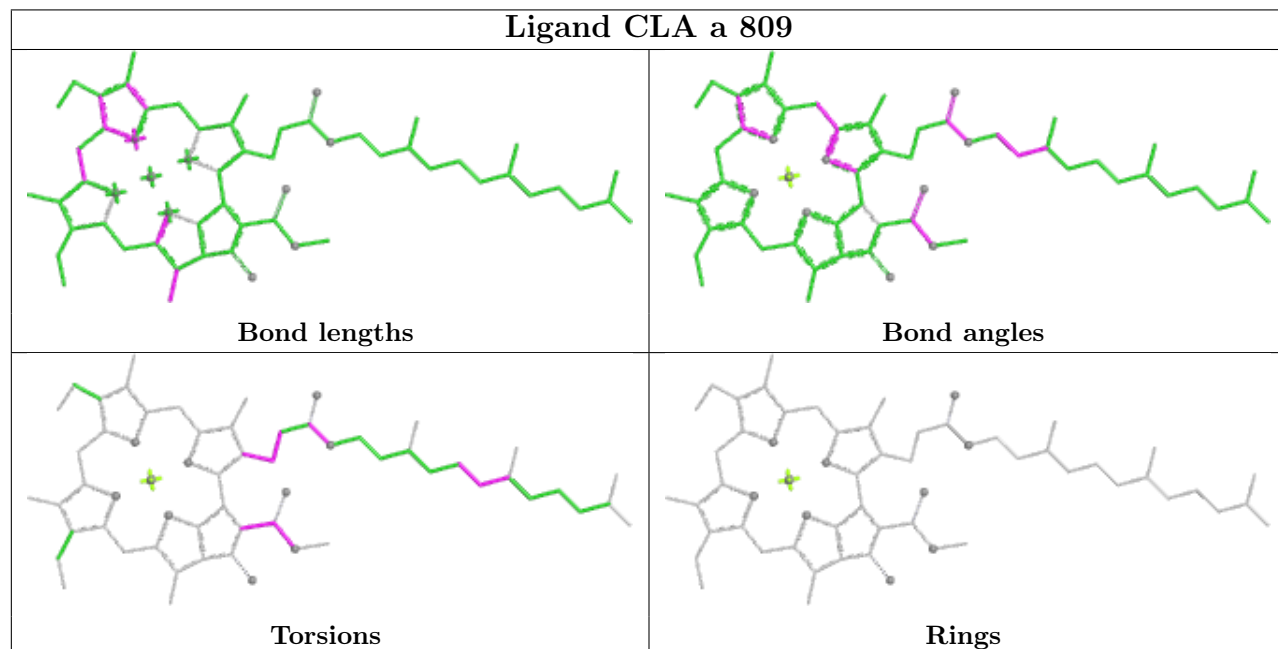


Ligand CLA a 804**Ligand CLA A 822**

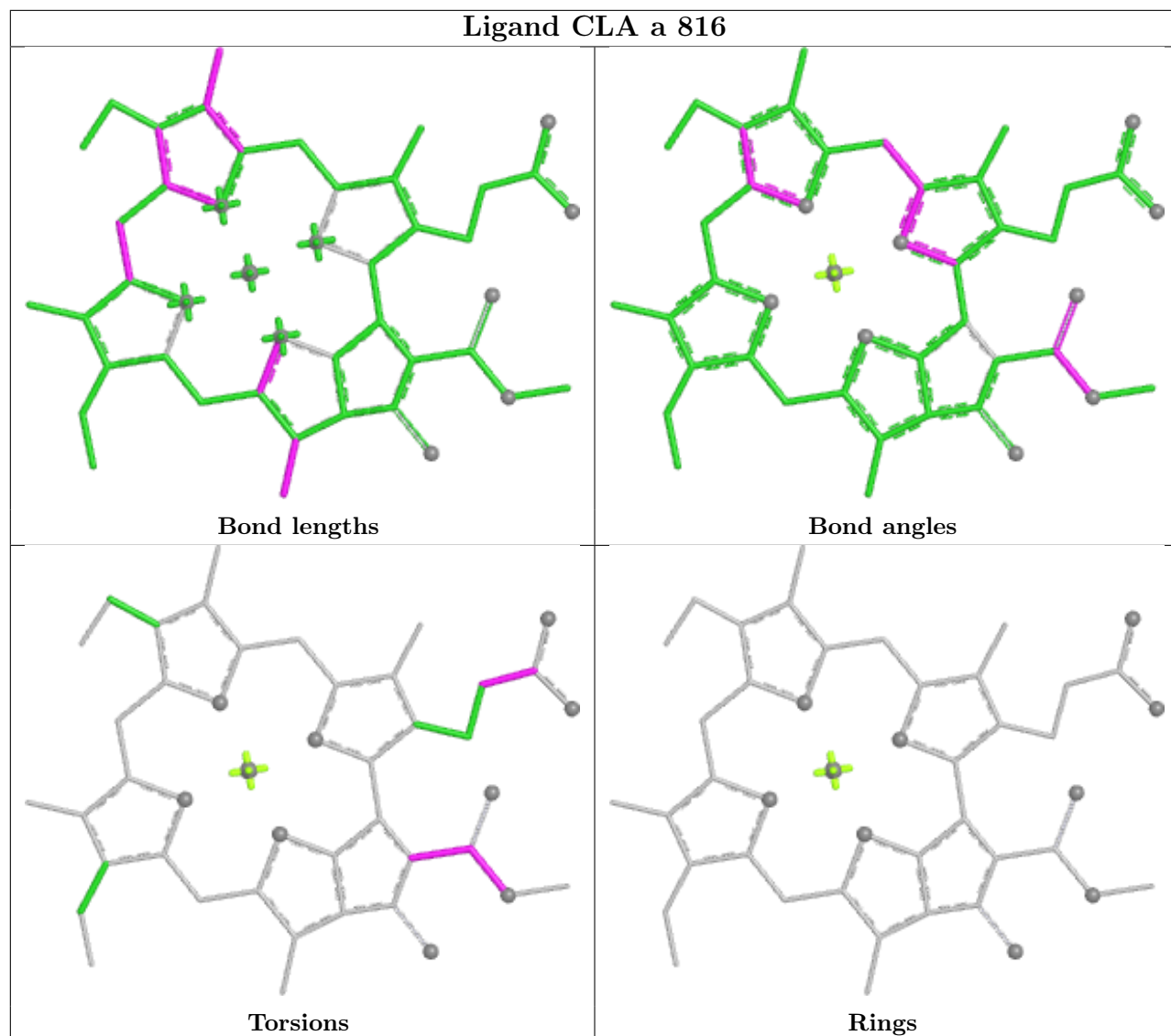
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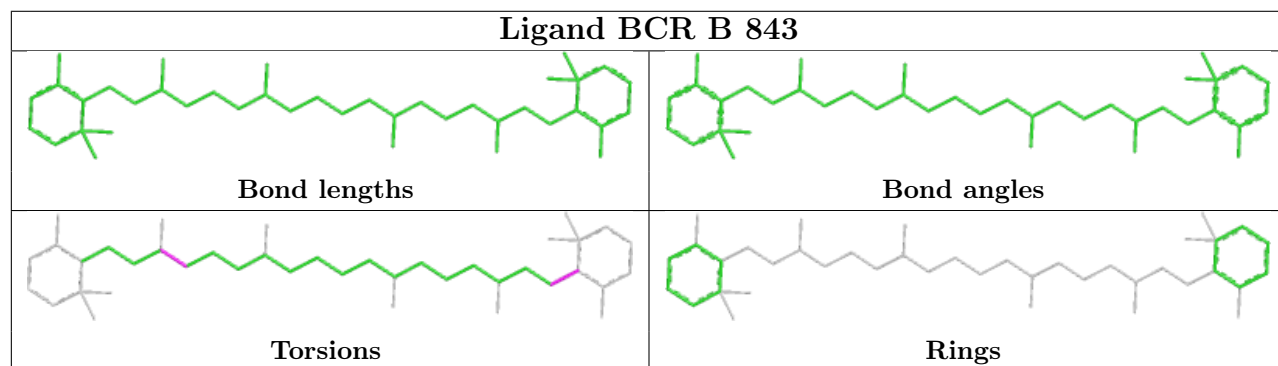
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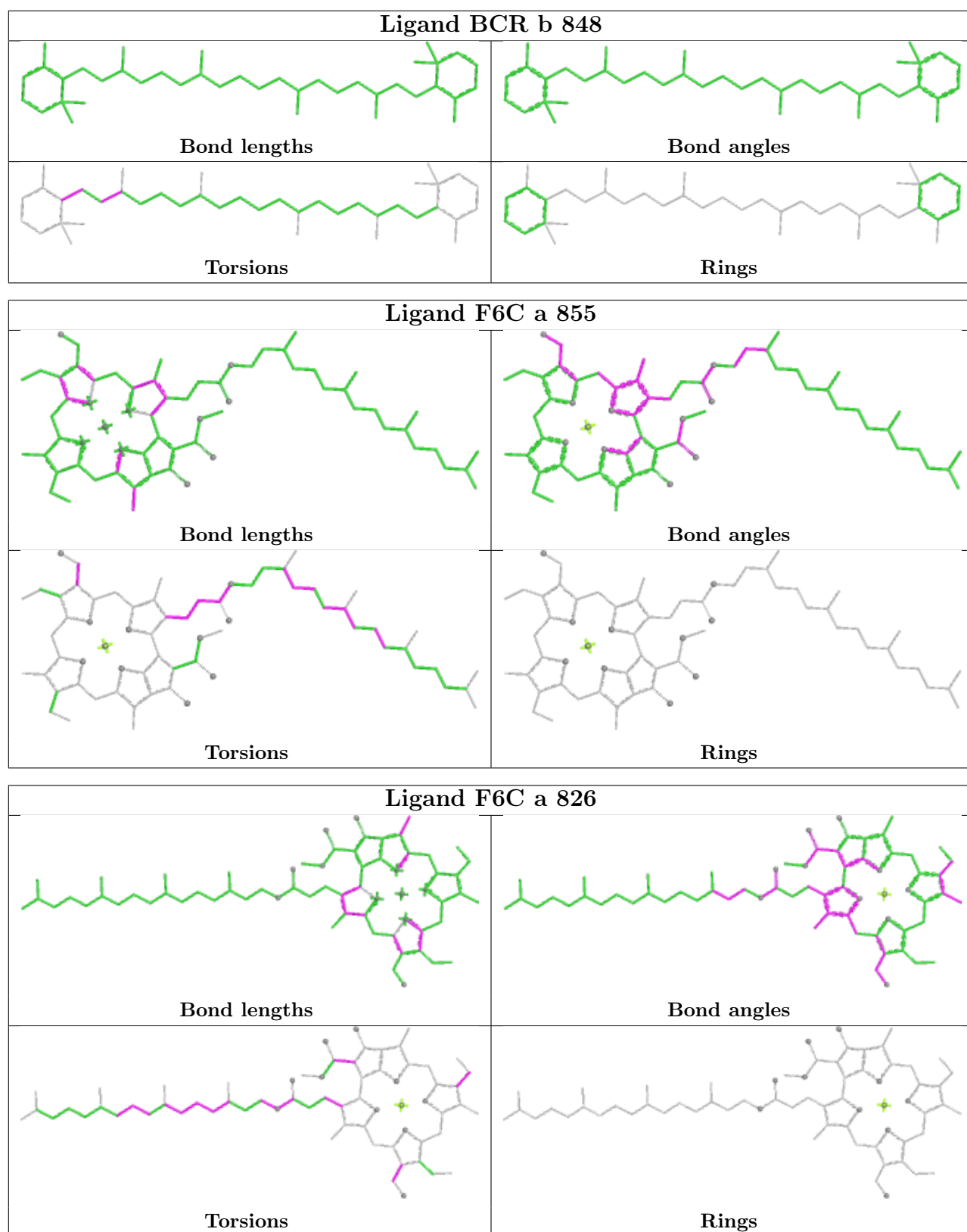


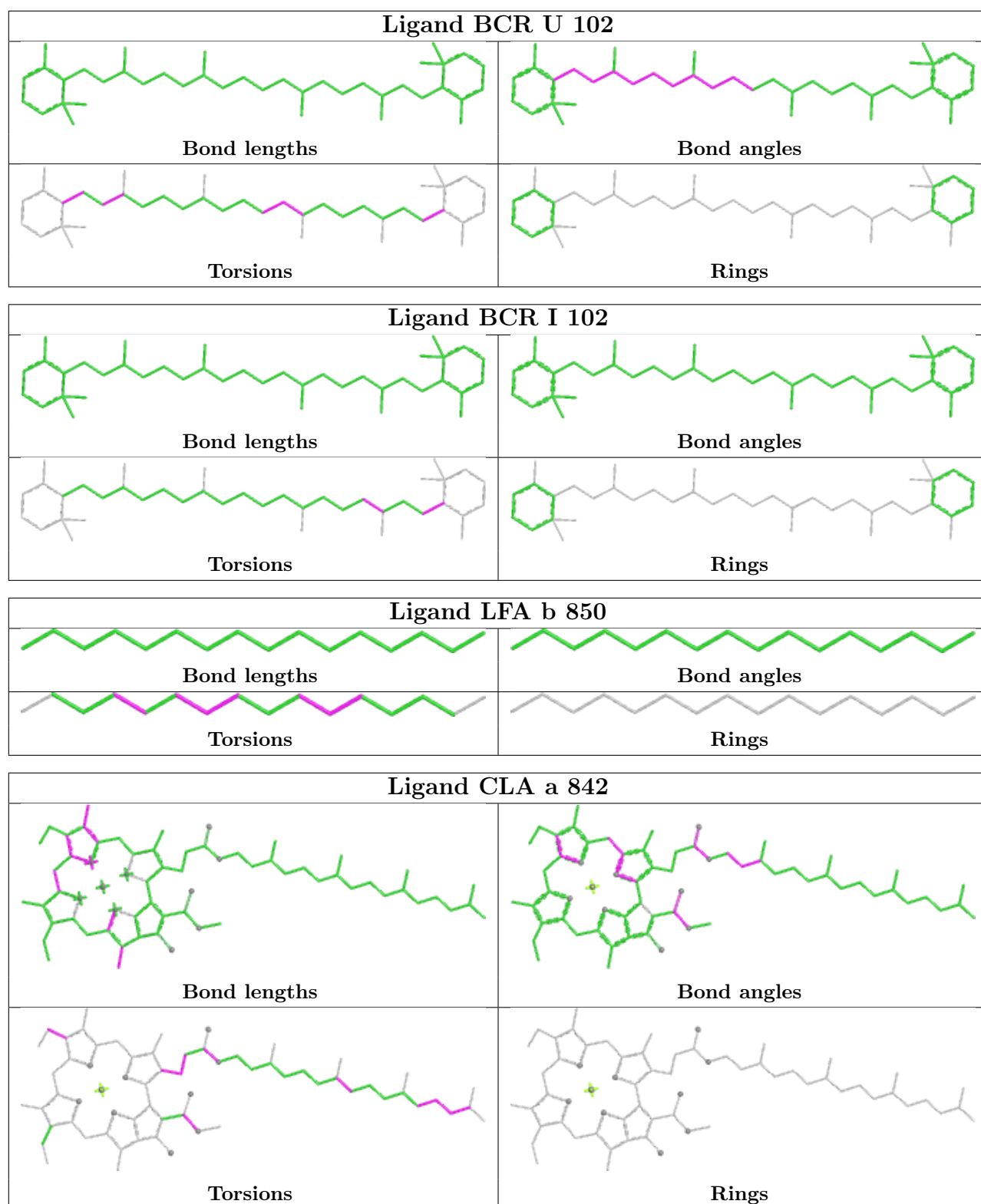
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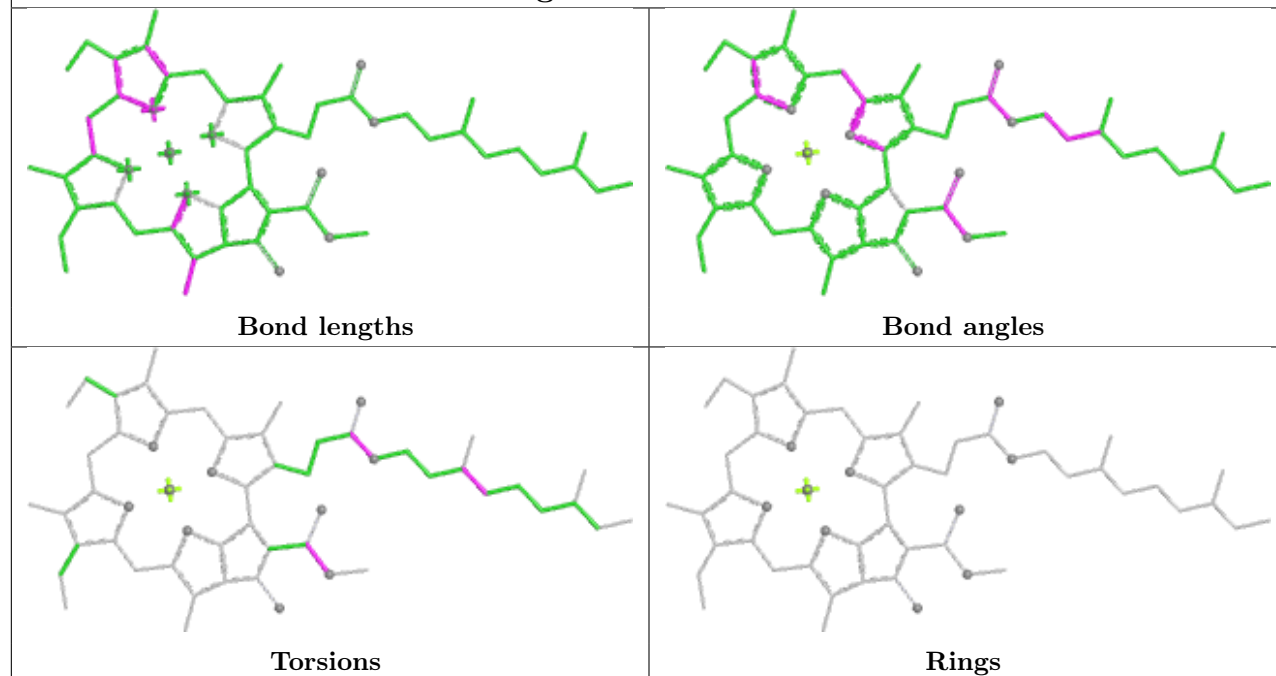
Ligand BCR B 843



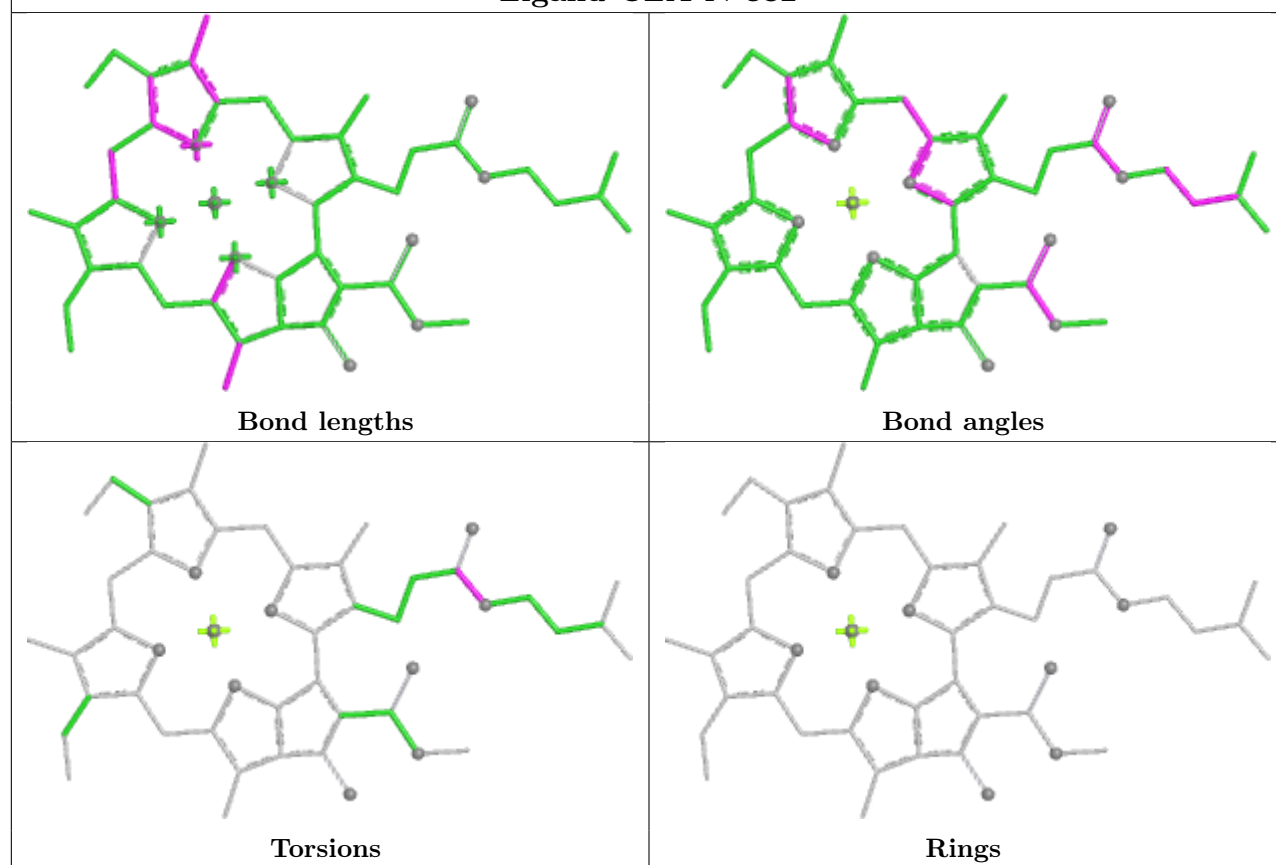


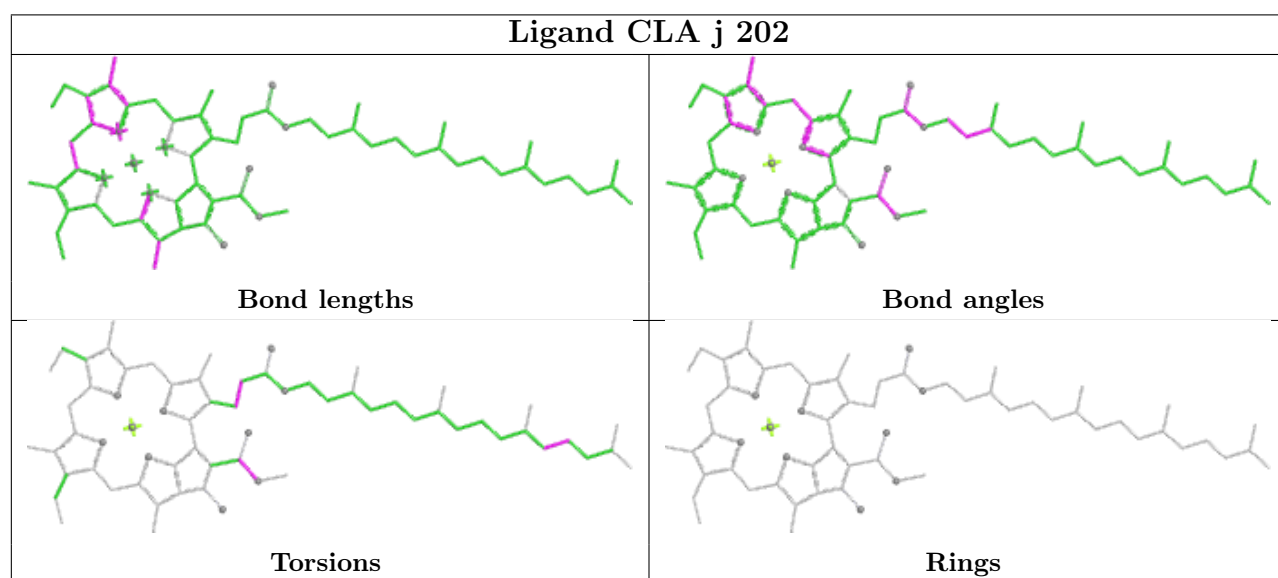
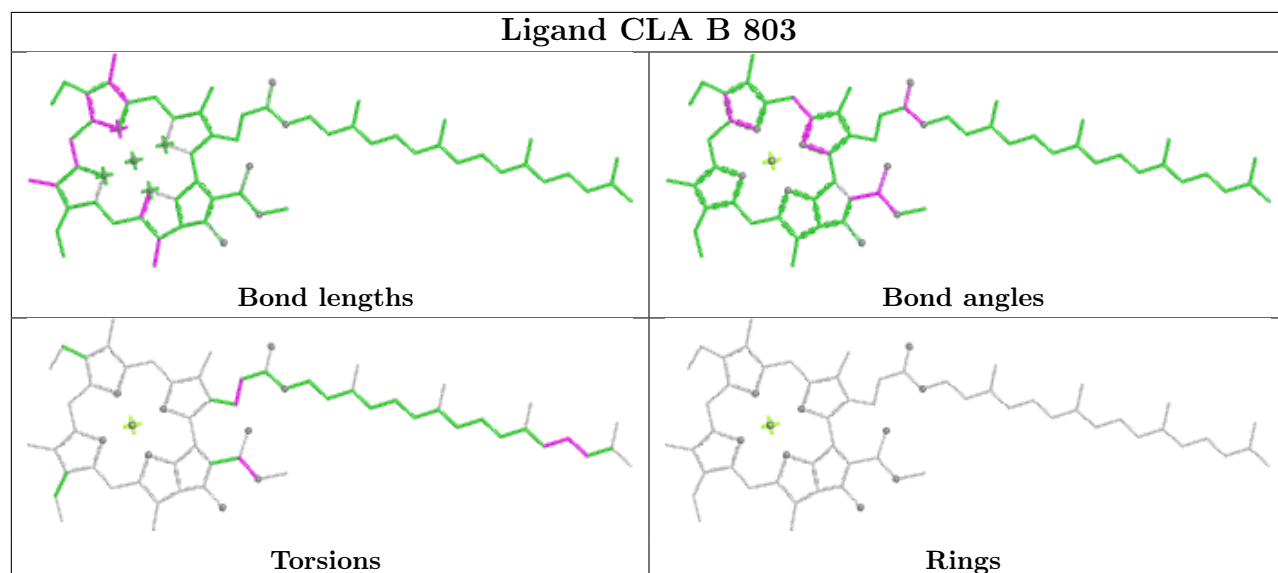
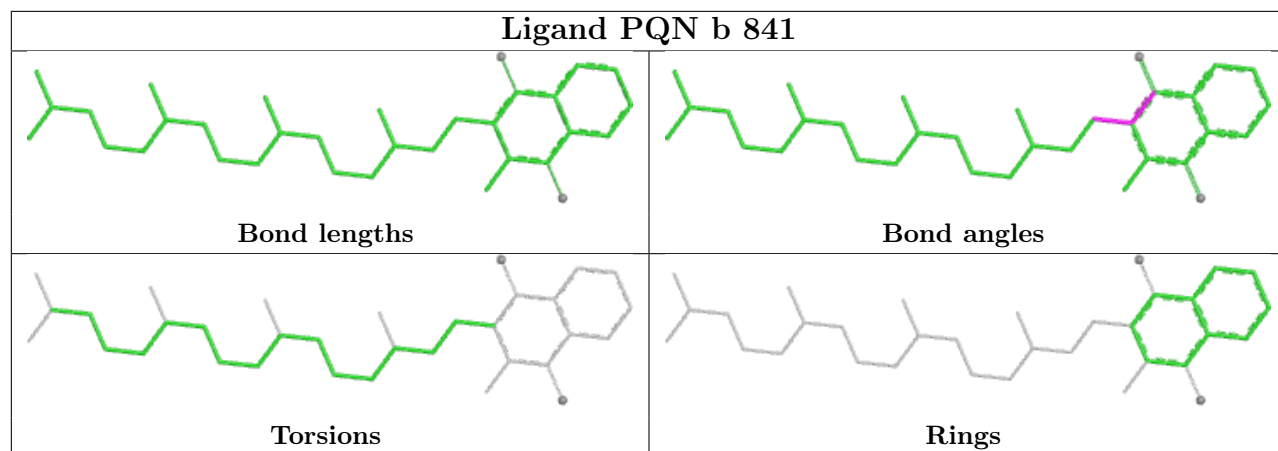


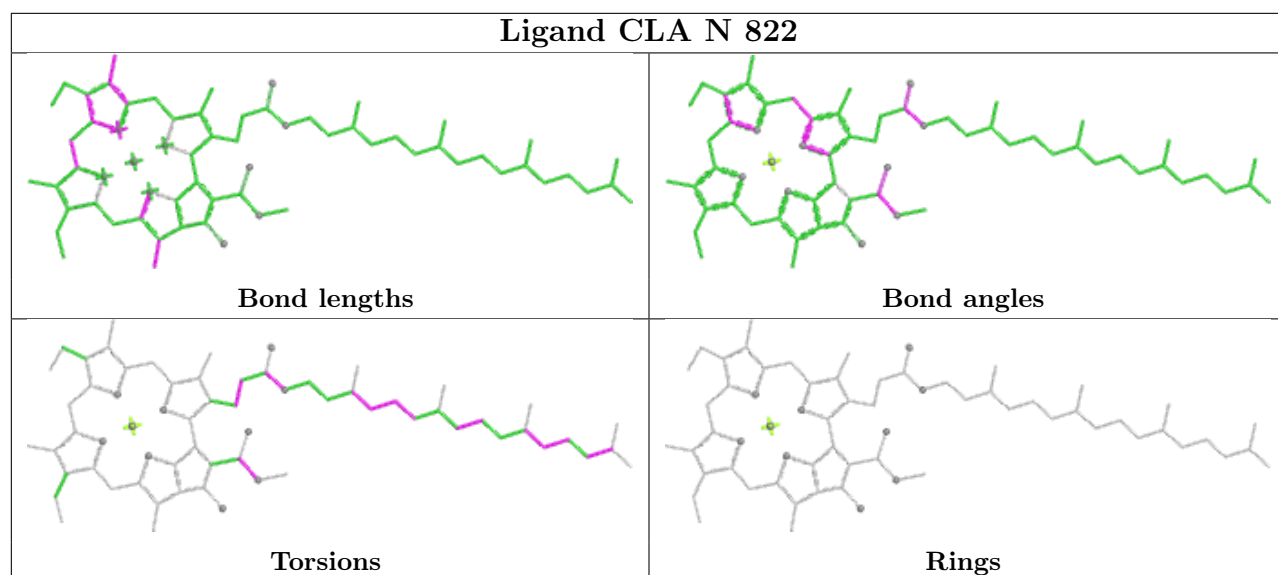
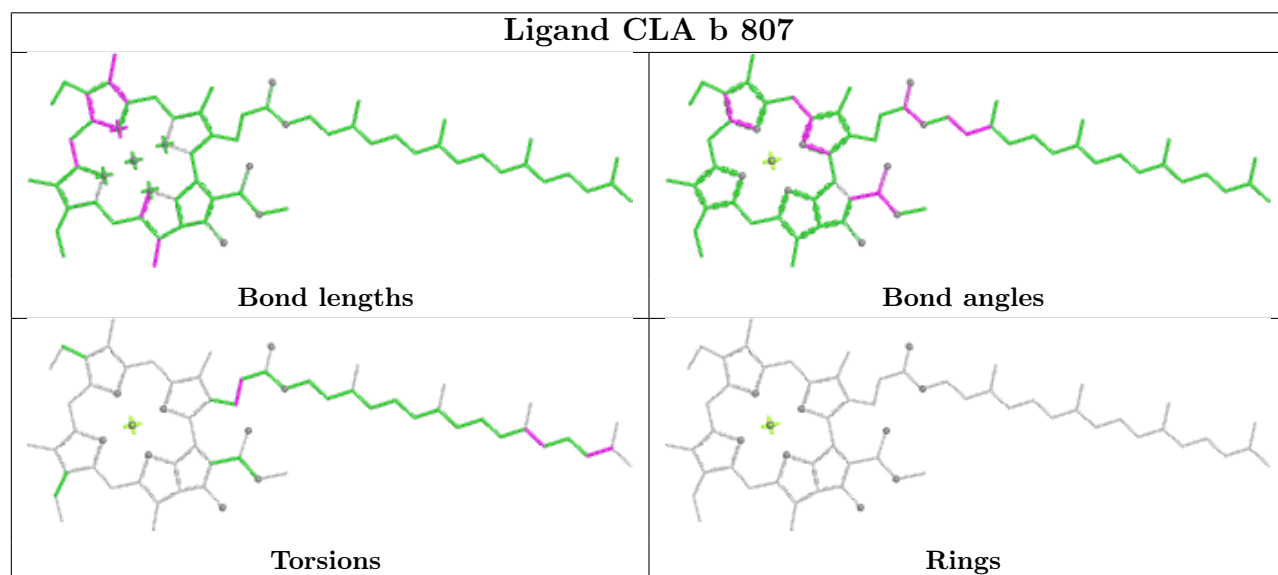
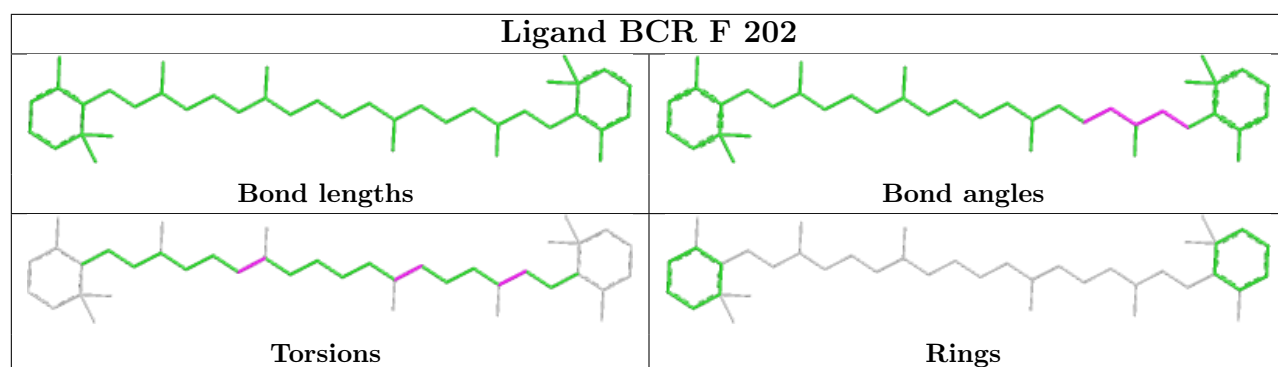
Ligand CLA a 823

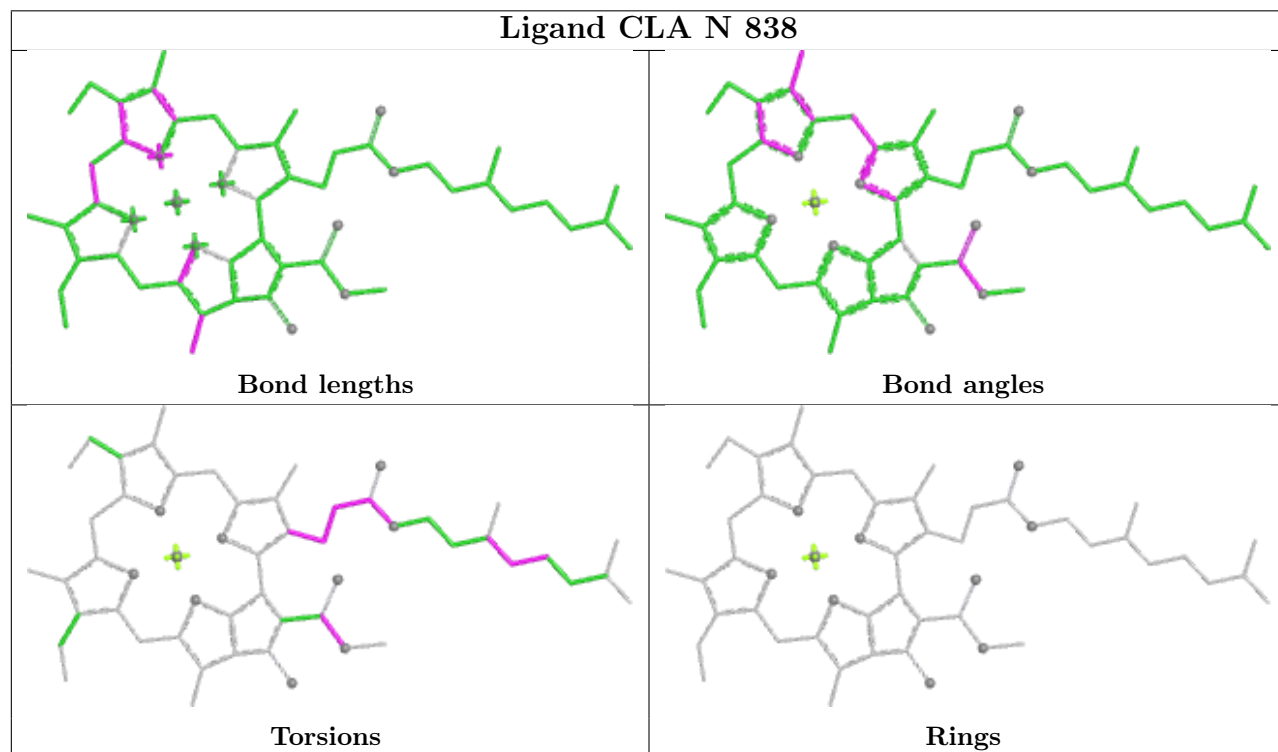
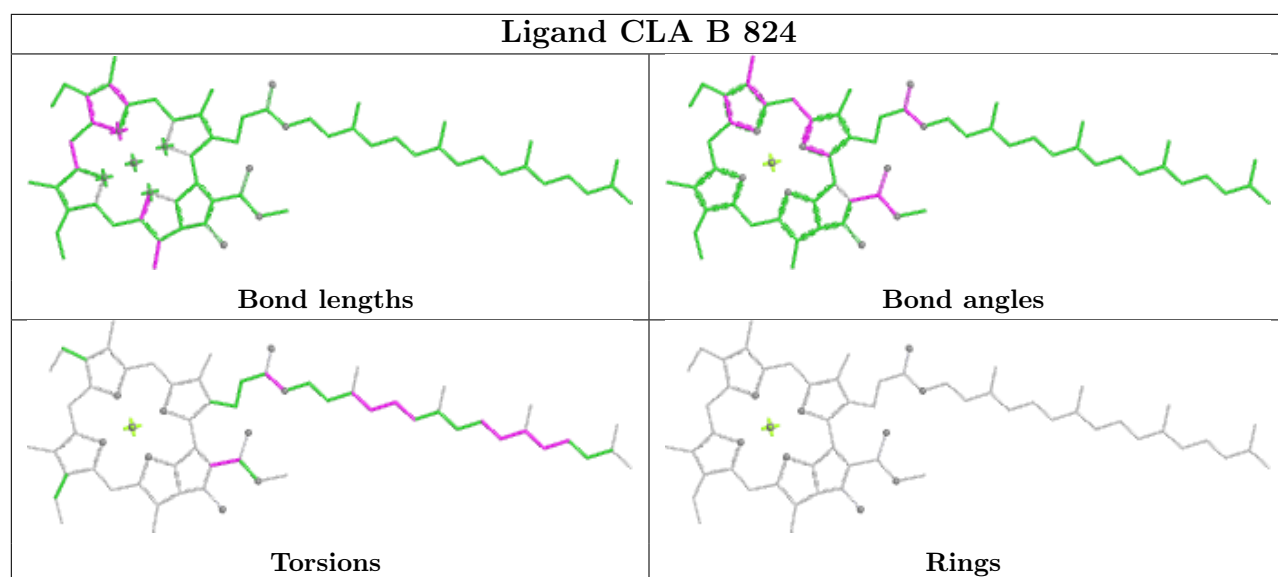


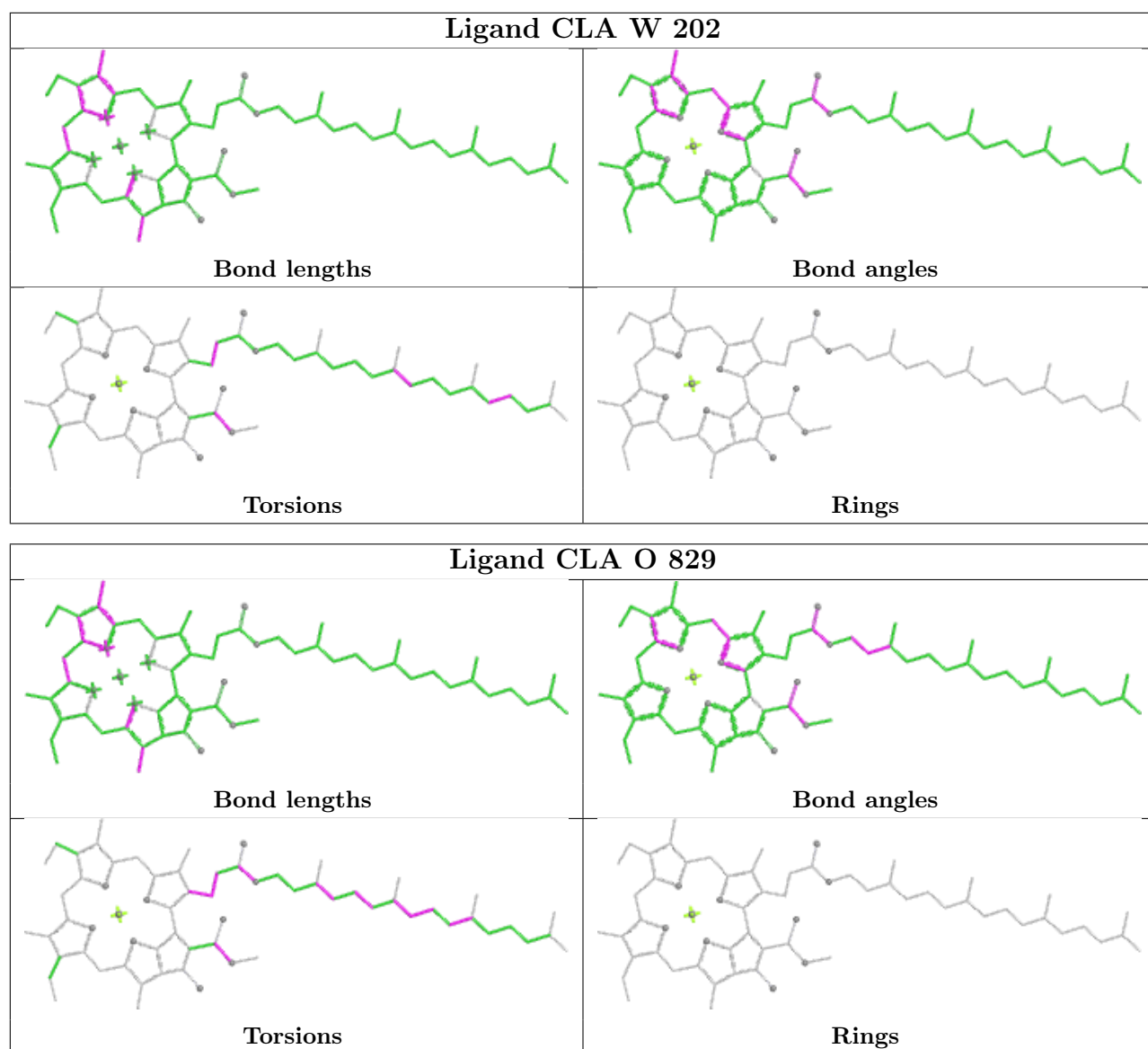
Ligand CLA N 832

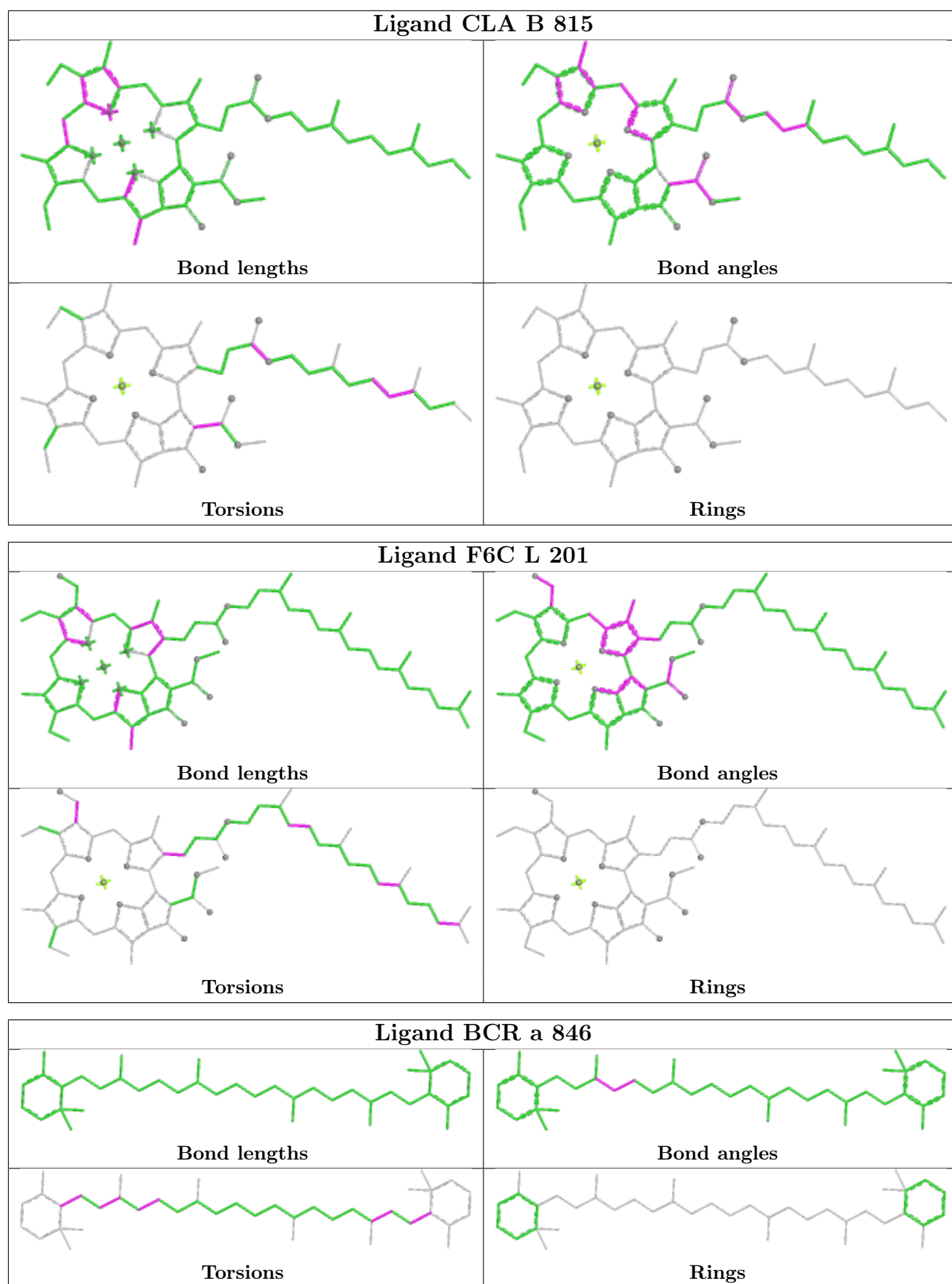


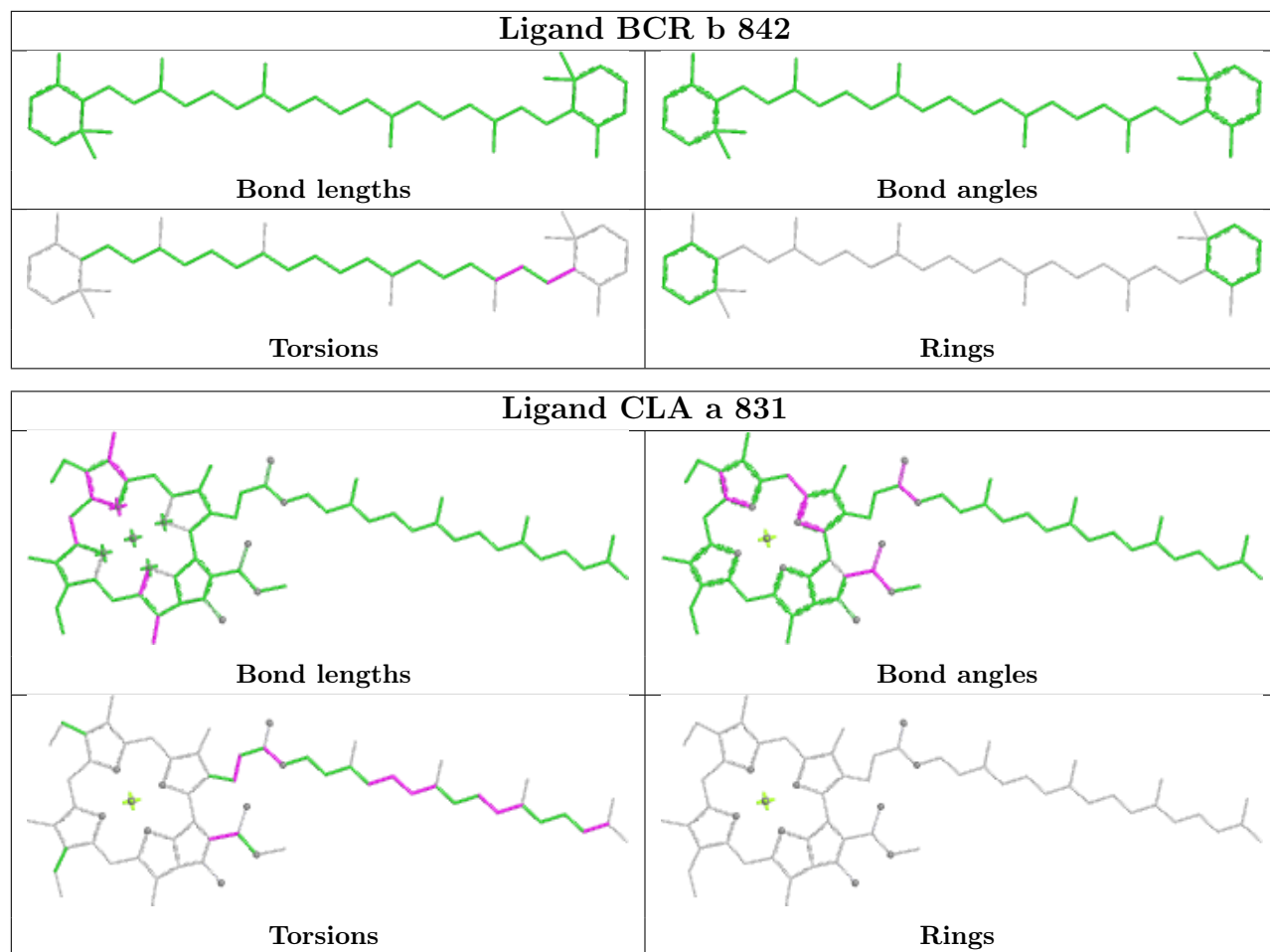




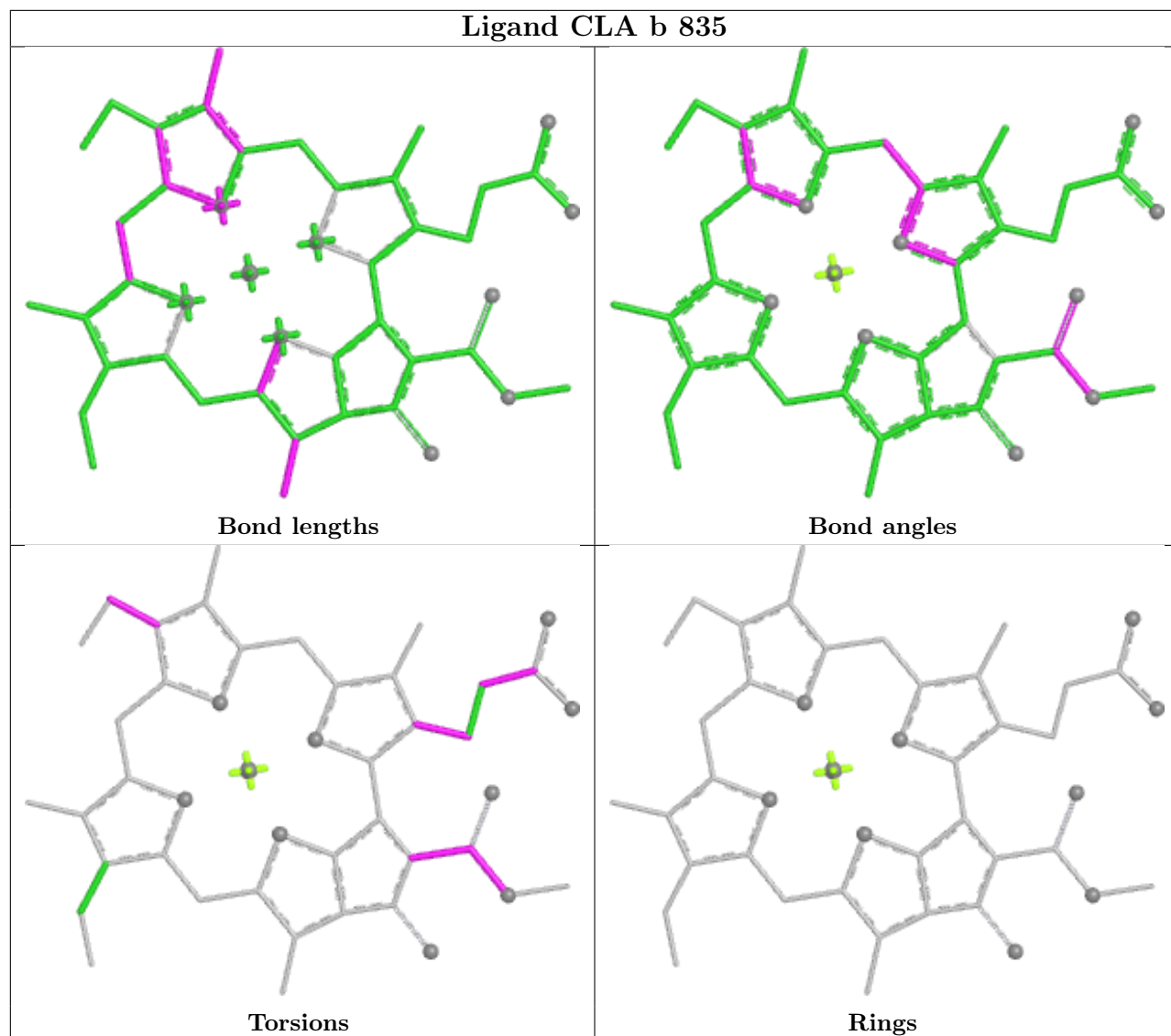




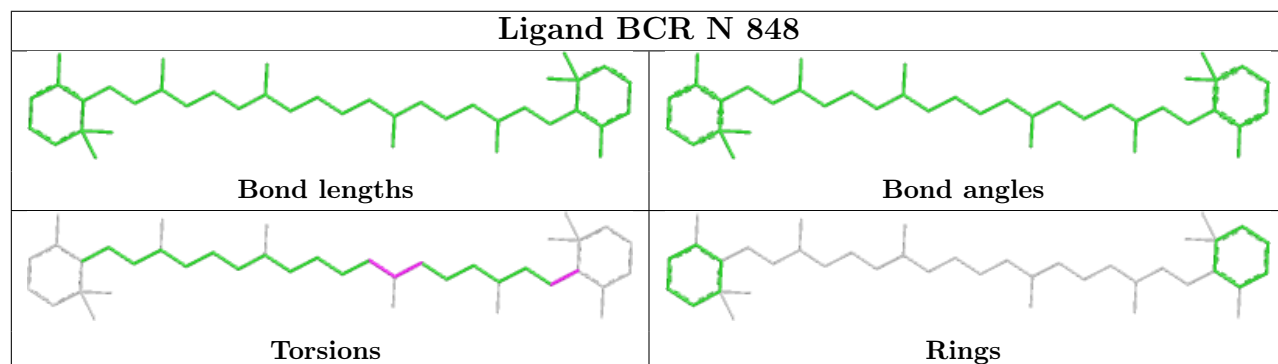


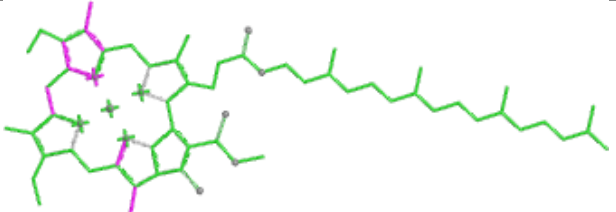
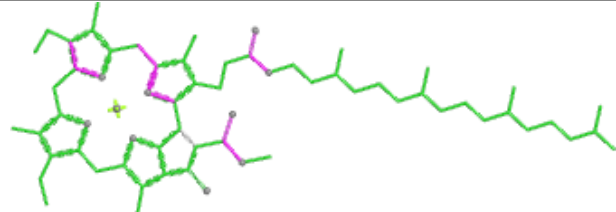
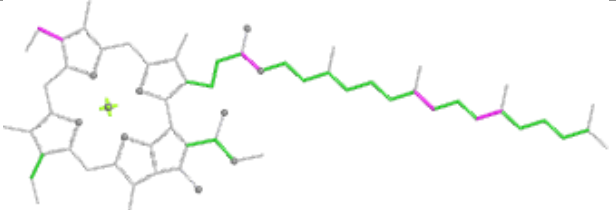
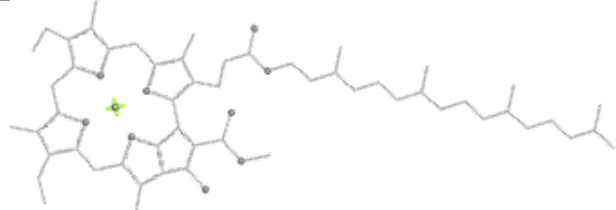


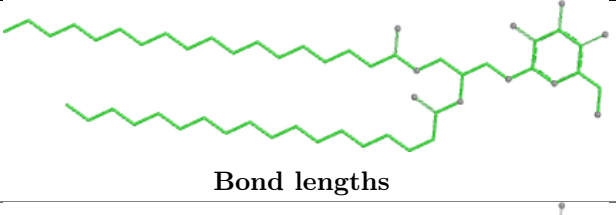
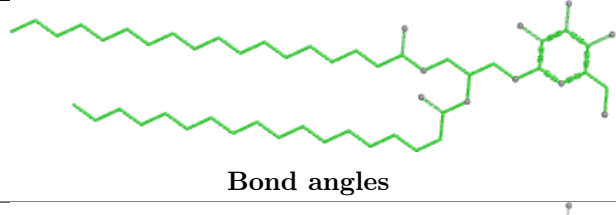
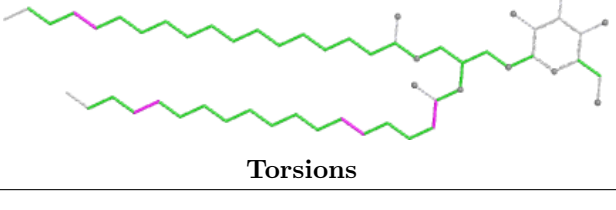
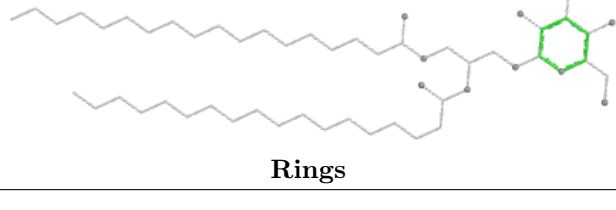
Ligand CLA b 835

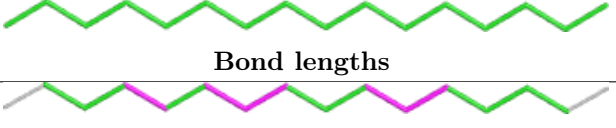





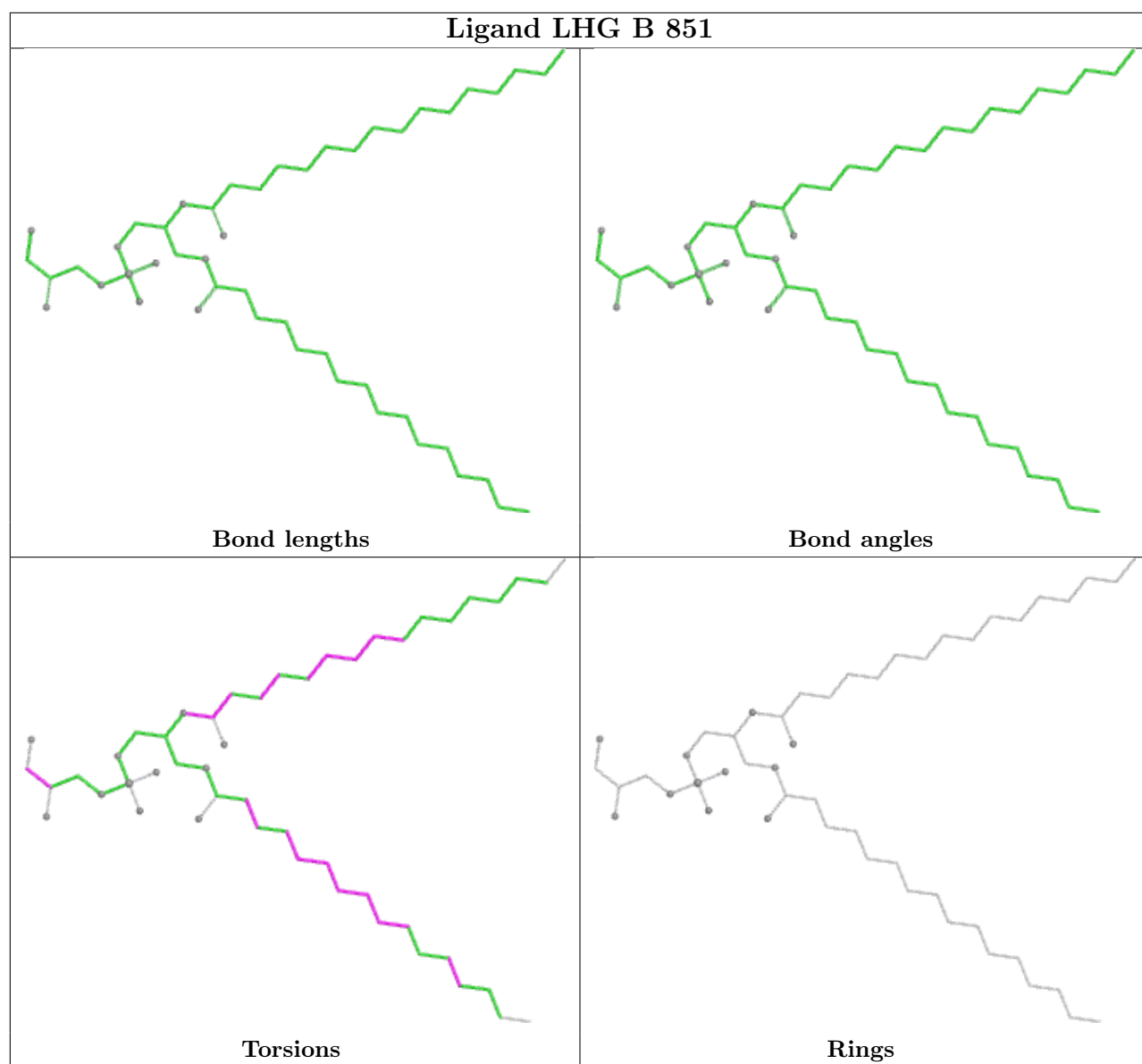
Ligand BCR N 848



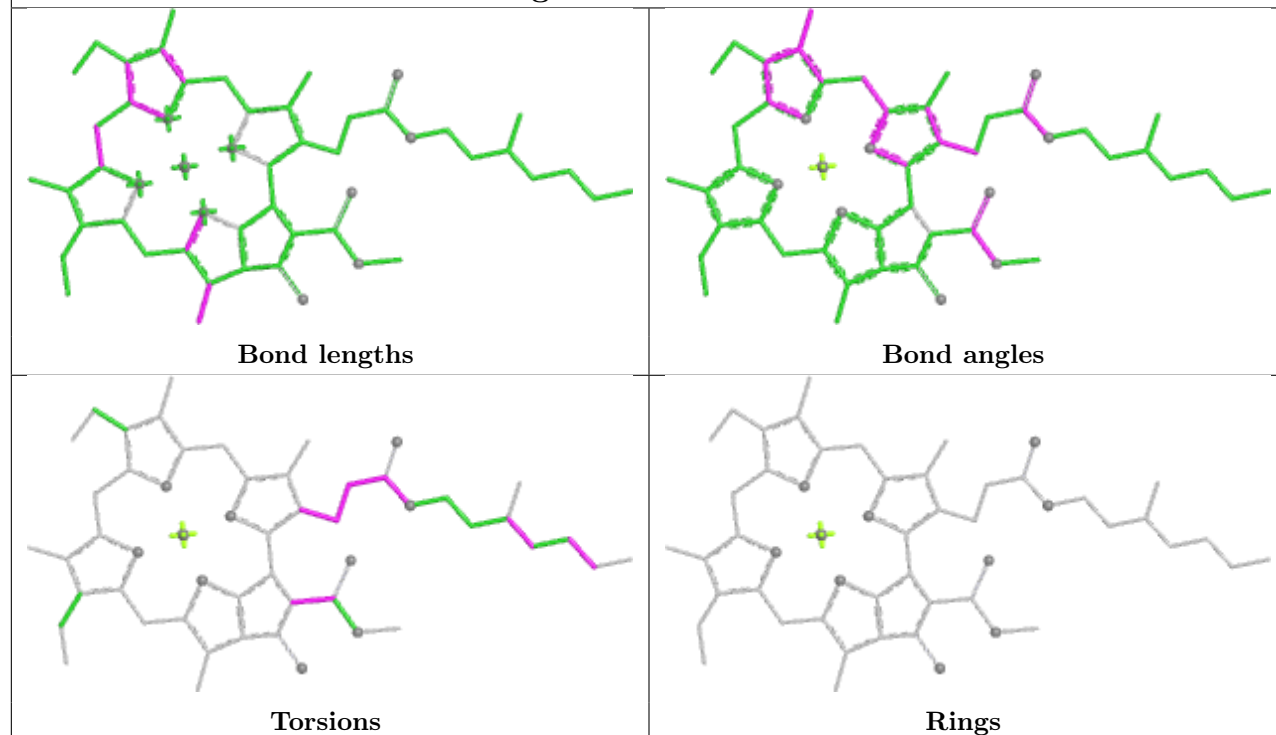
Ligand CLA O 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG O 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

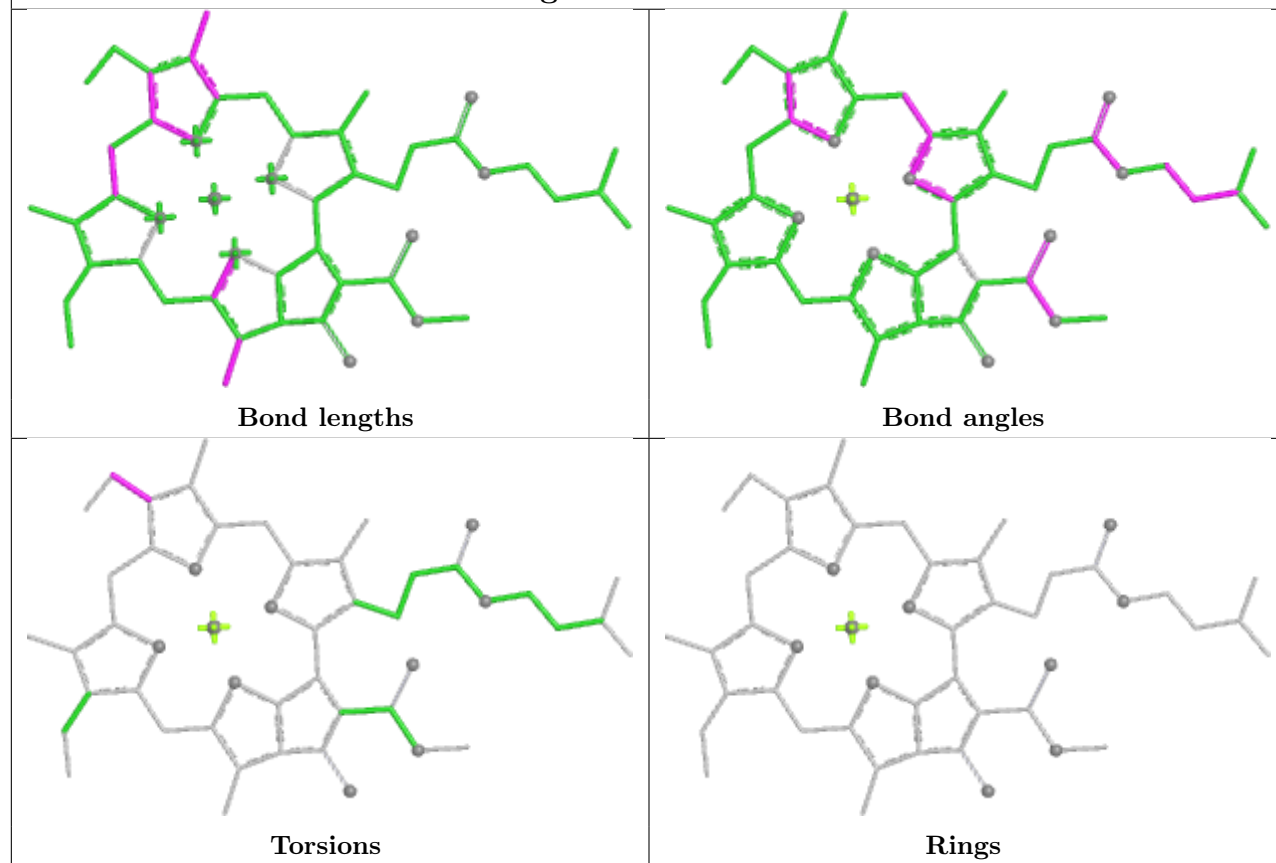
Ligand LFA B 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

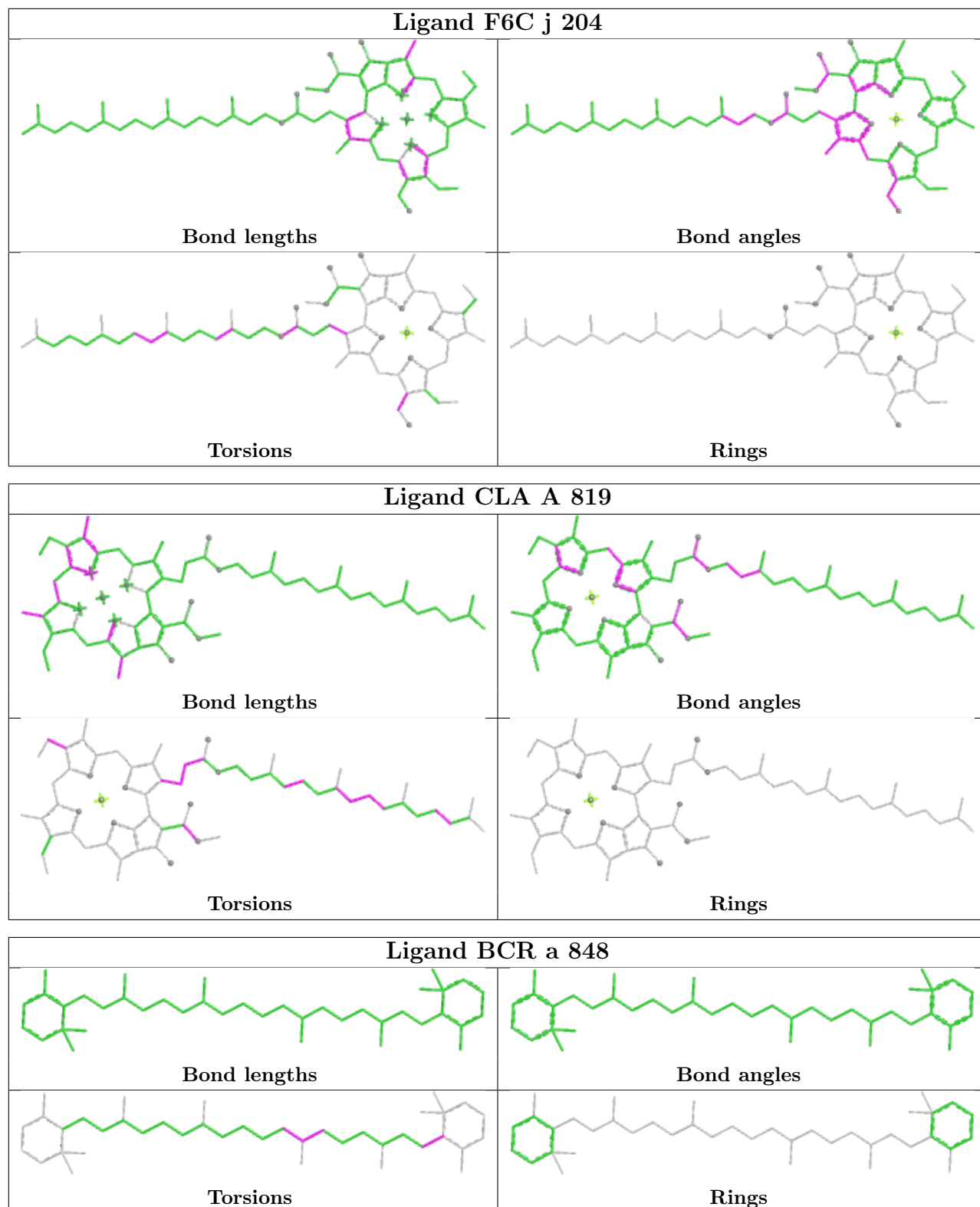


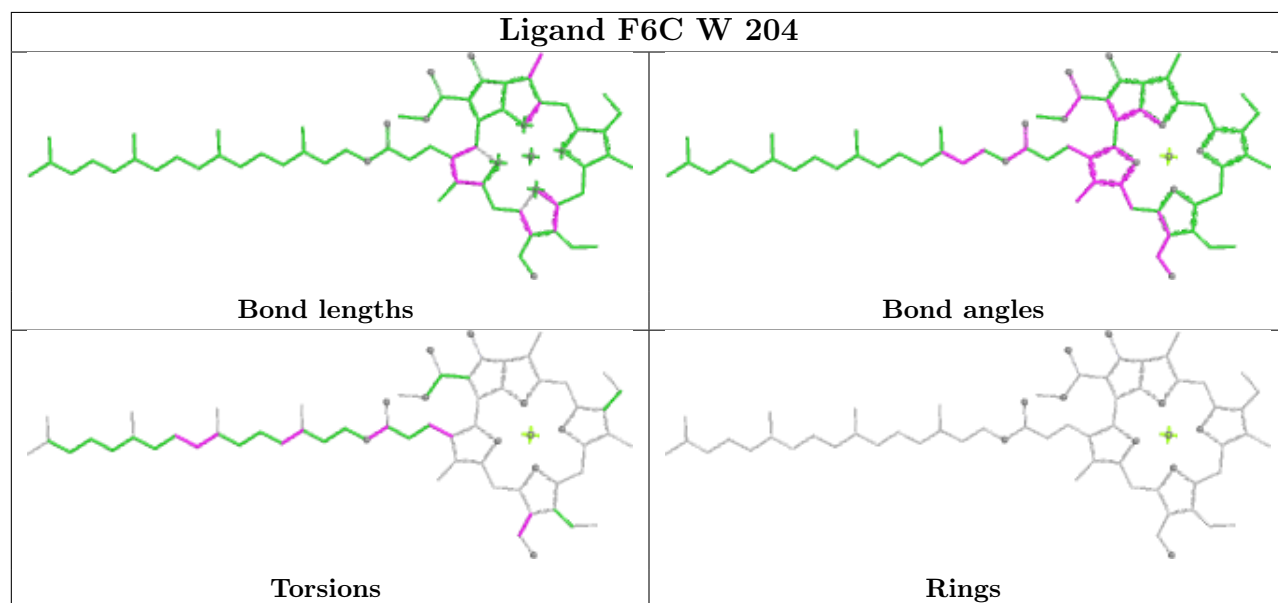
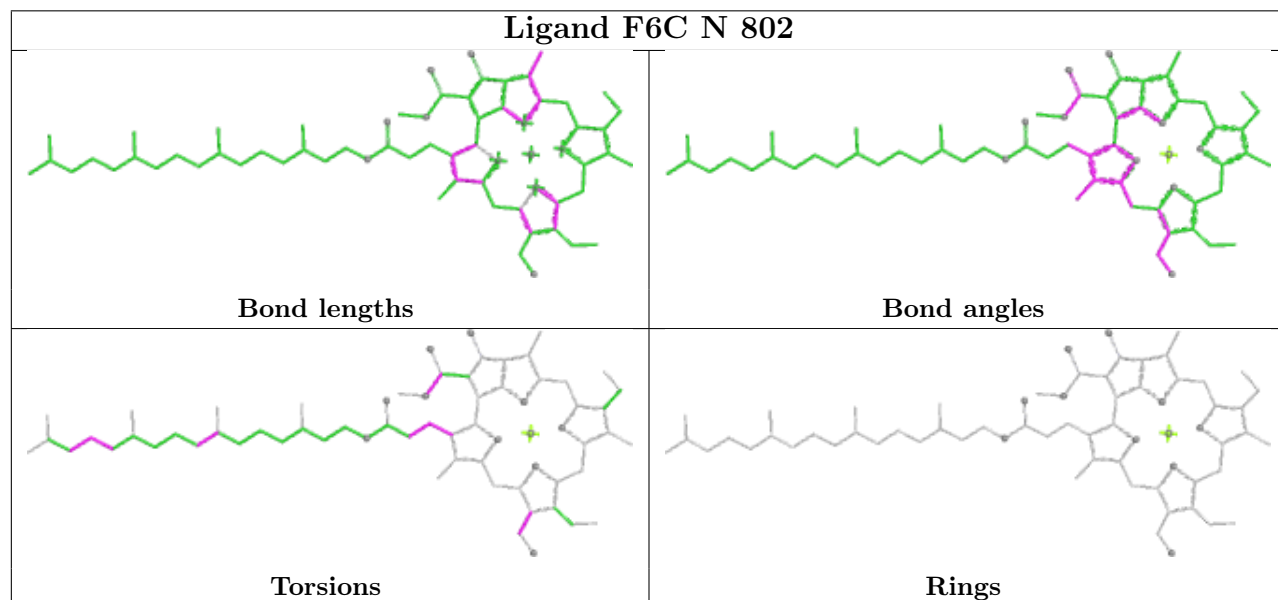
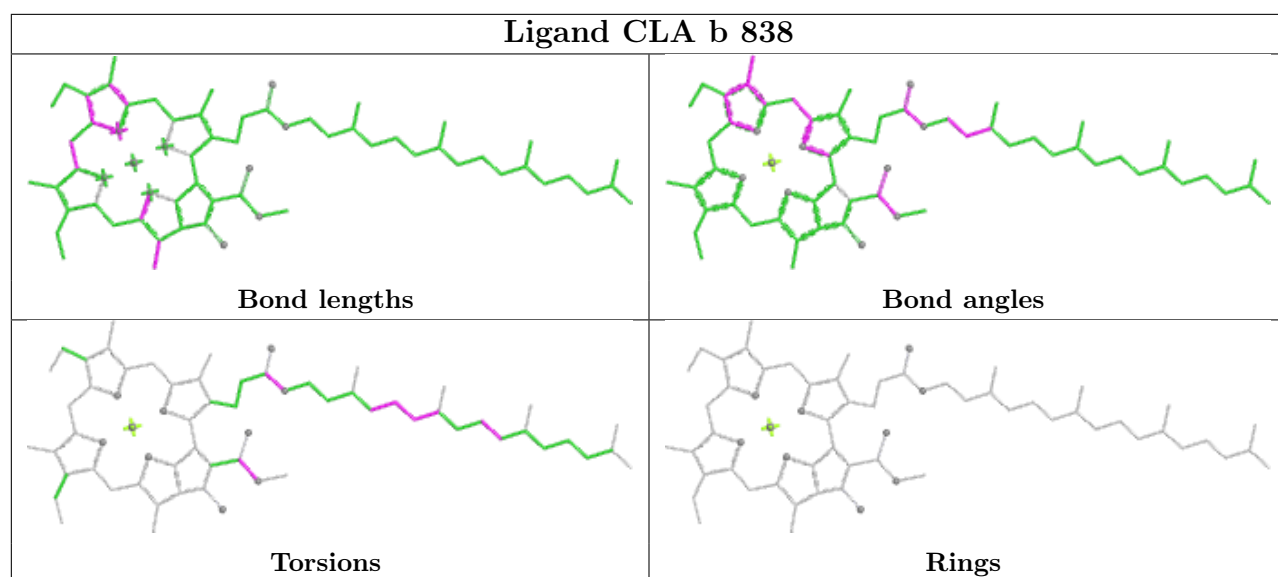
Ligand CLA O 821

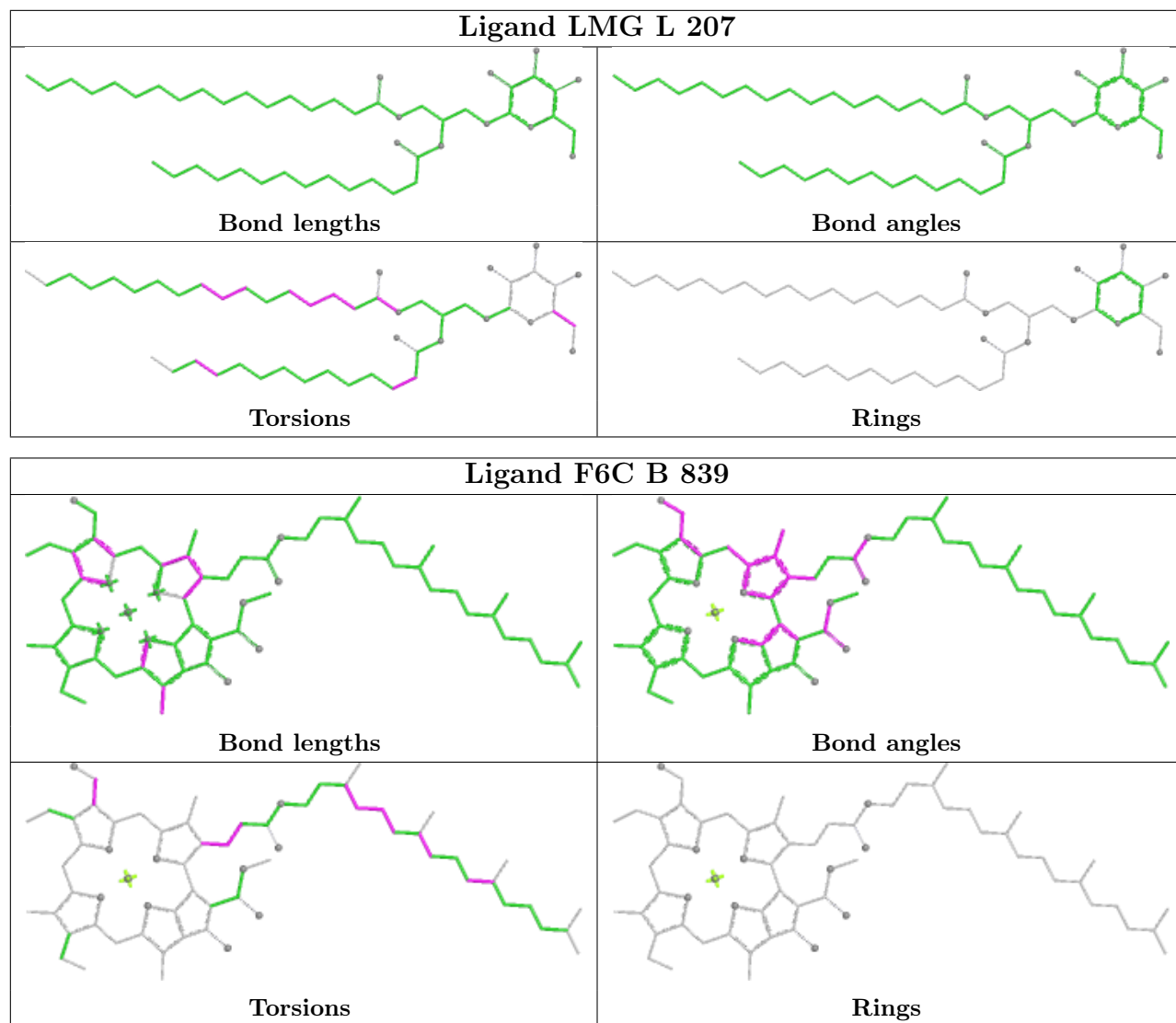


Ligand CLA i 103

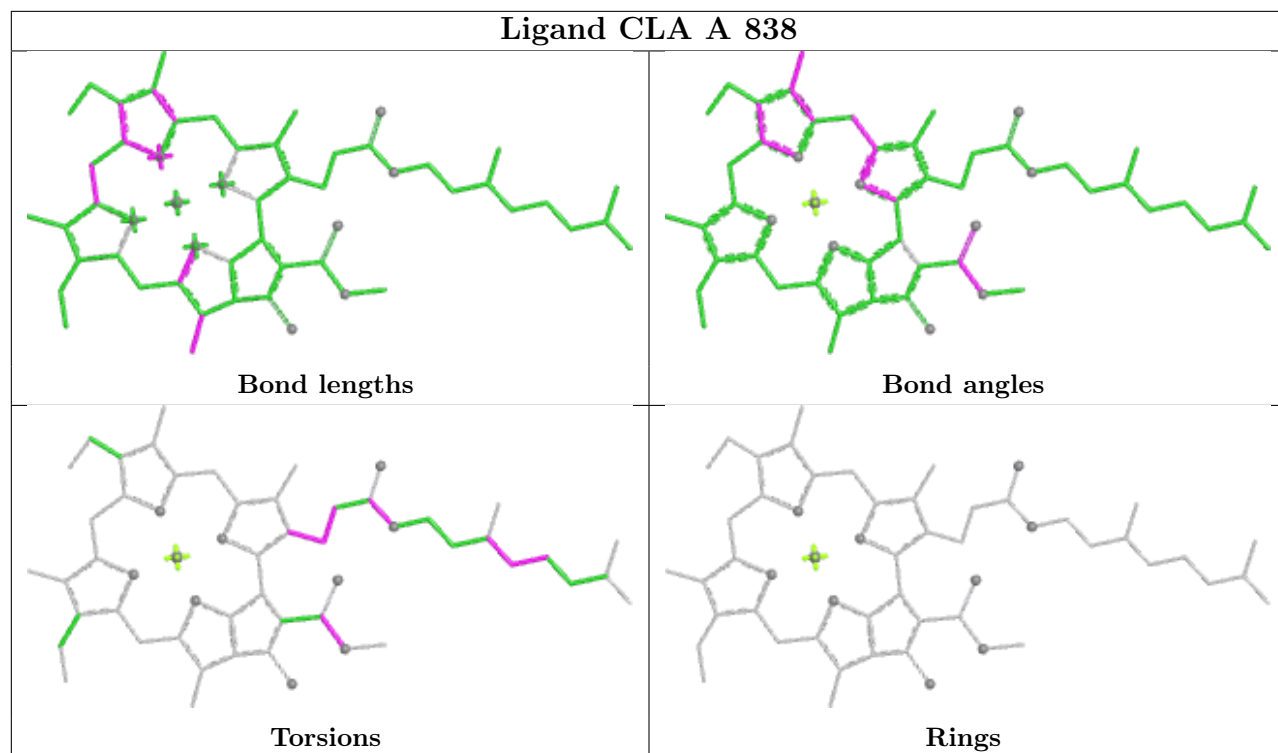




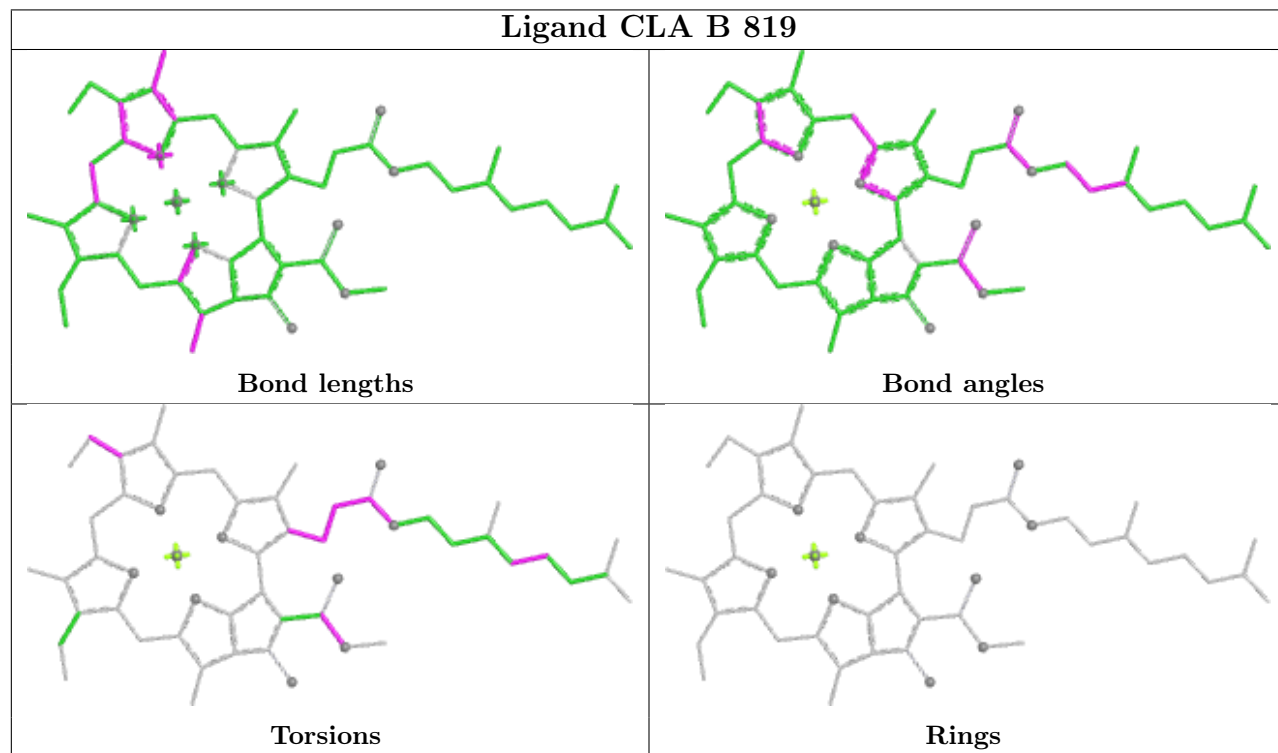


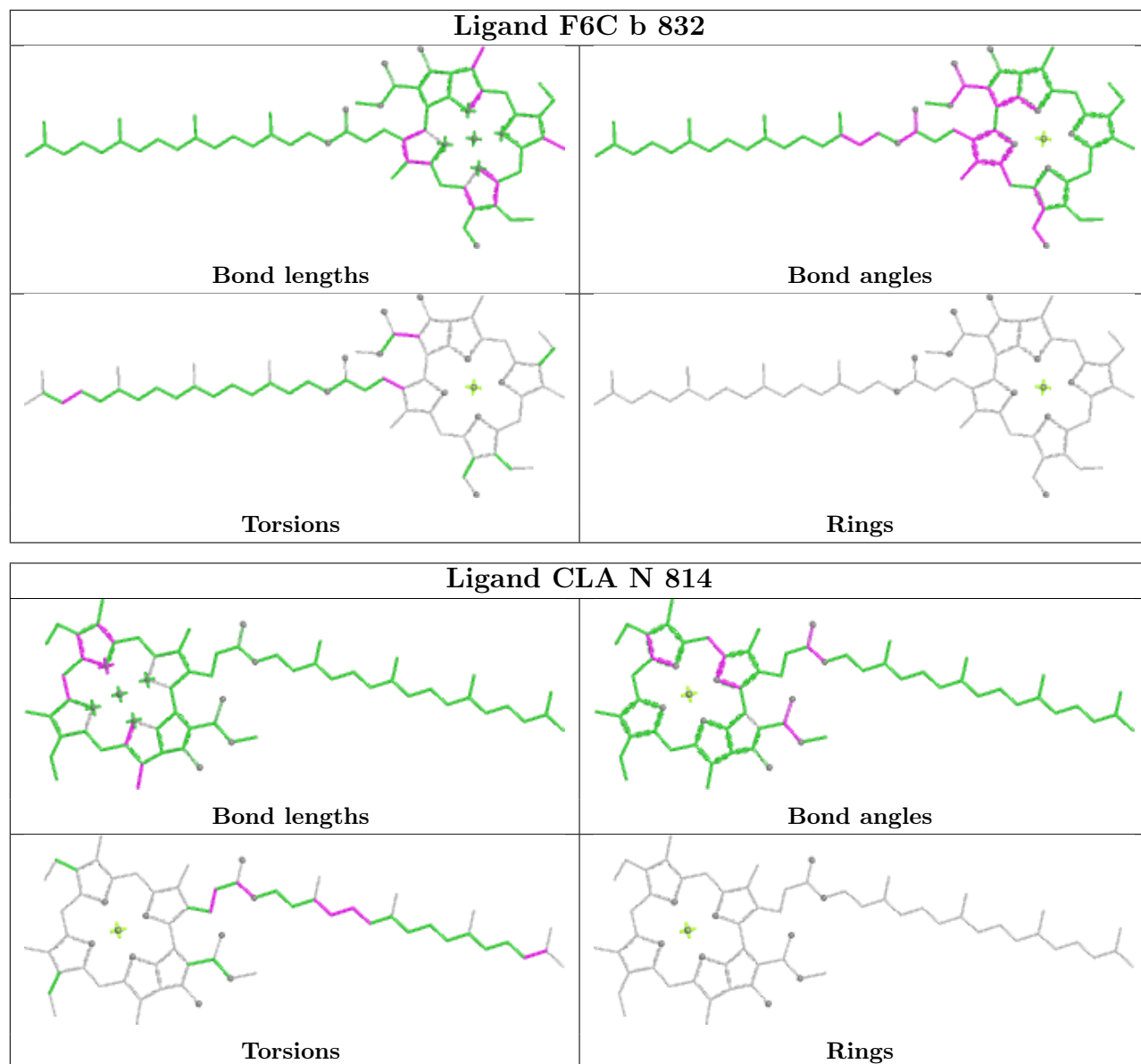


Ligand CLA A 838

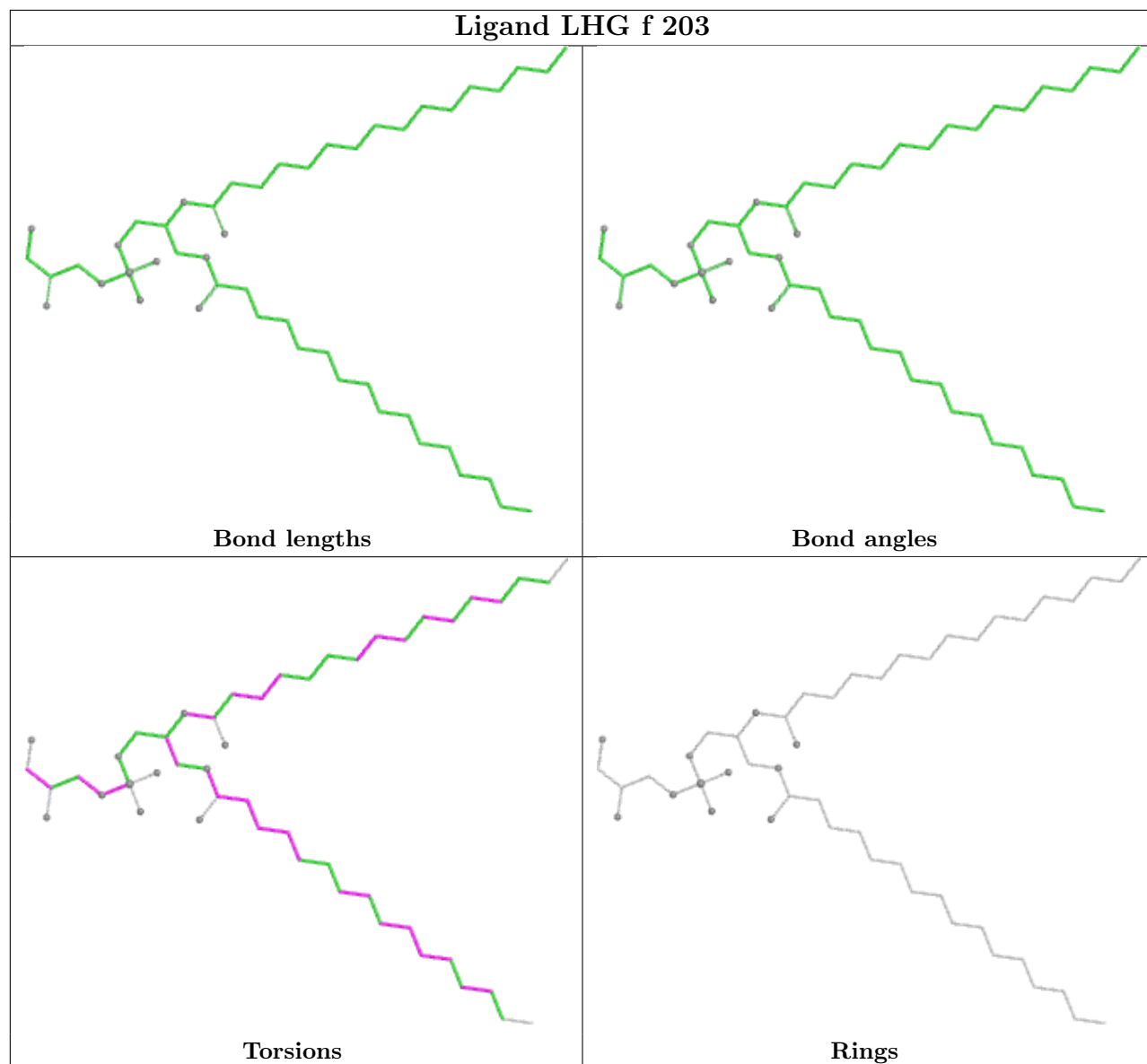


Ligand CLA B 819

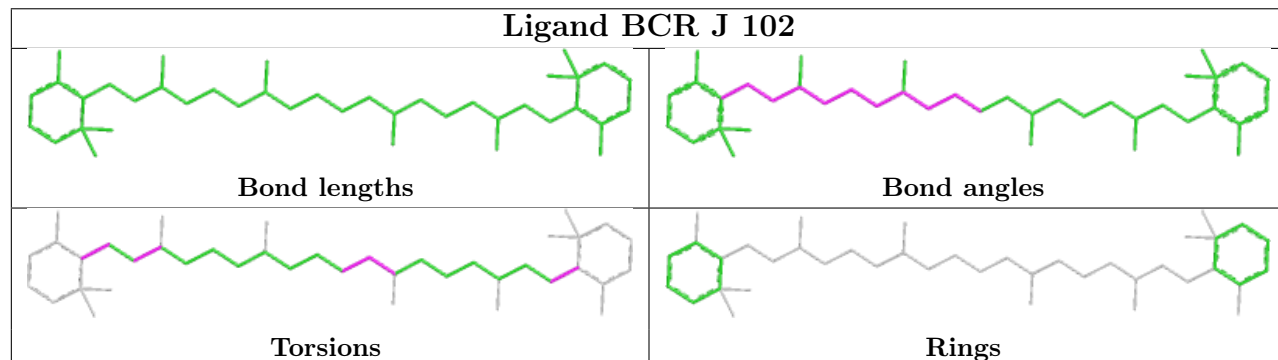


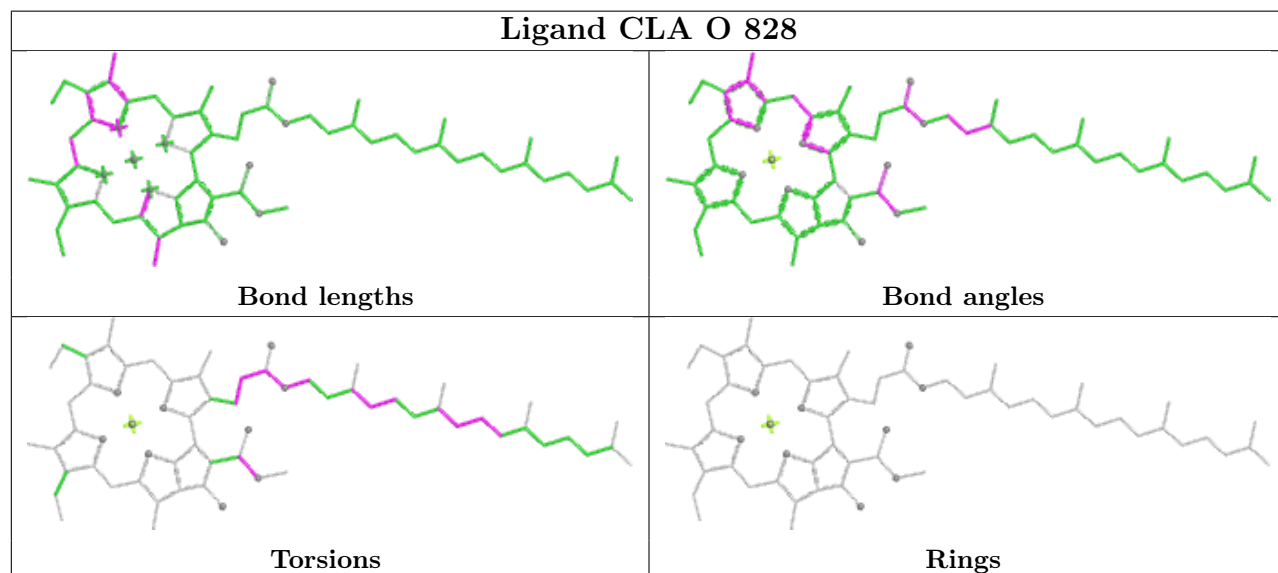
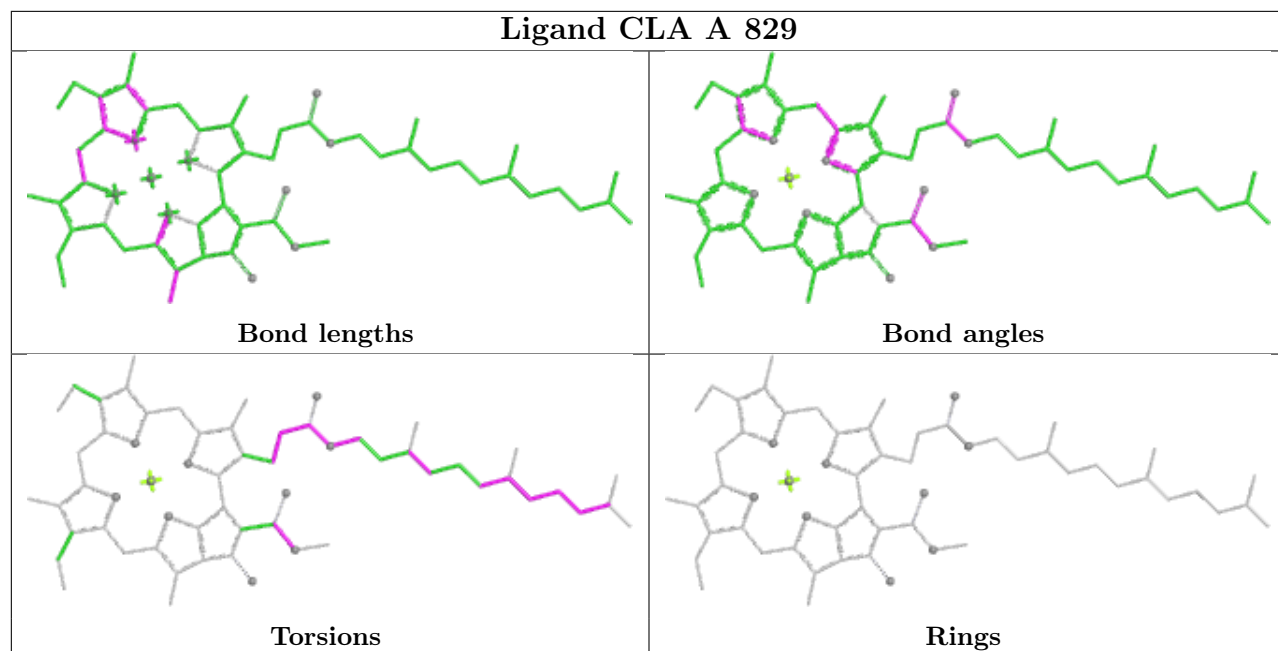


Ligand LHG f 203

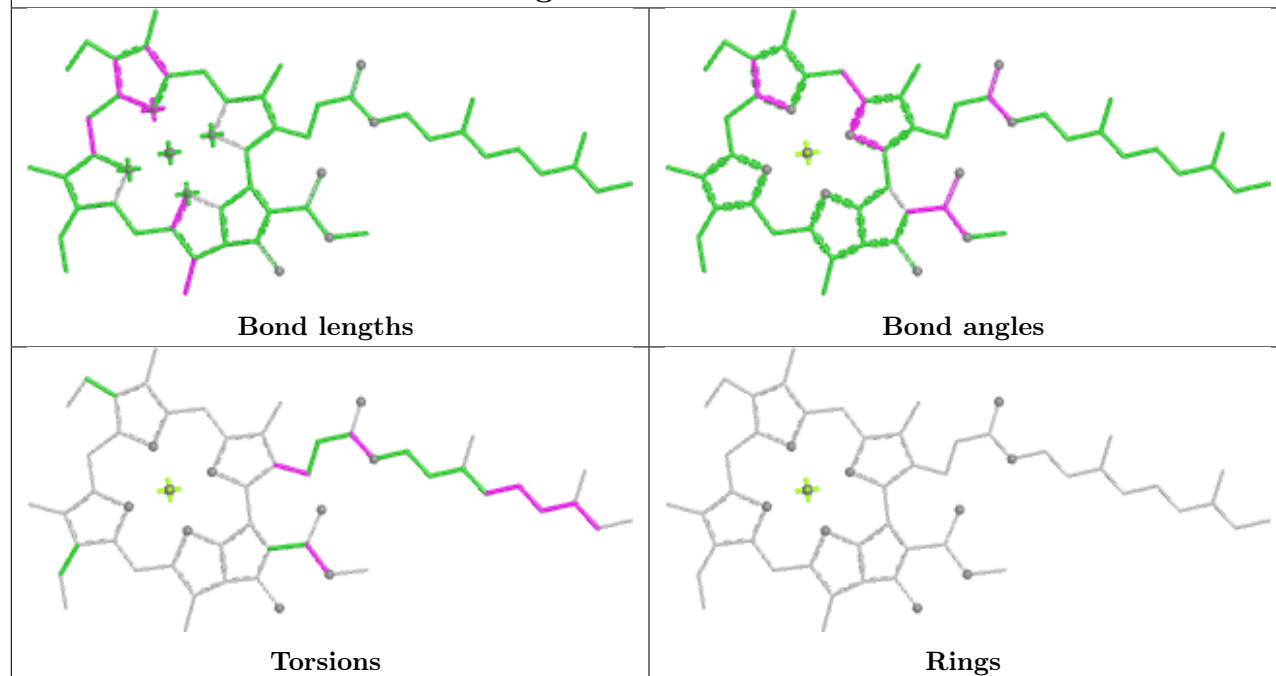


Ligand BCR J 102

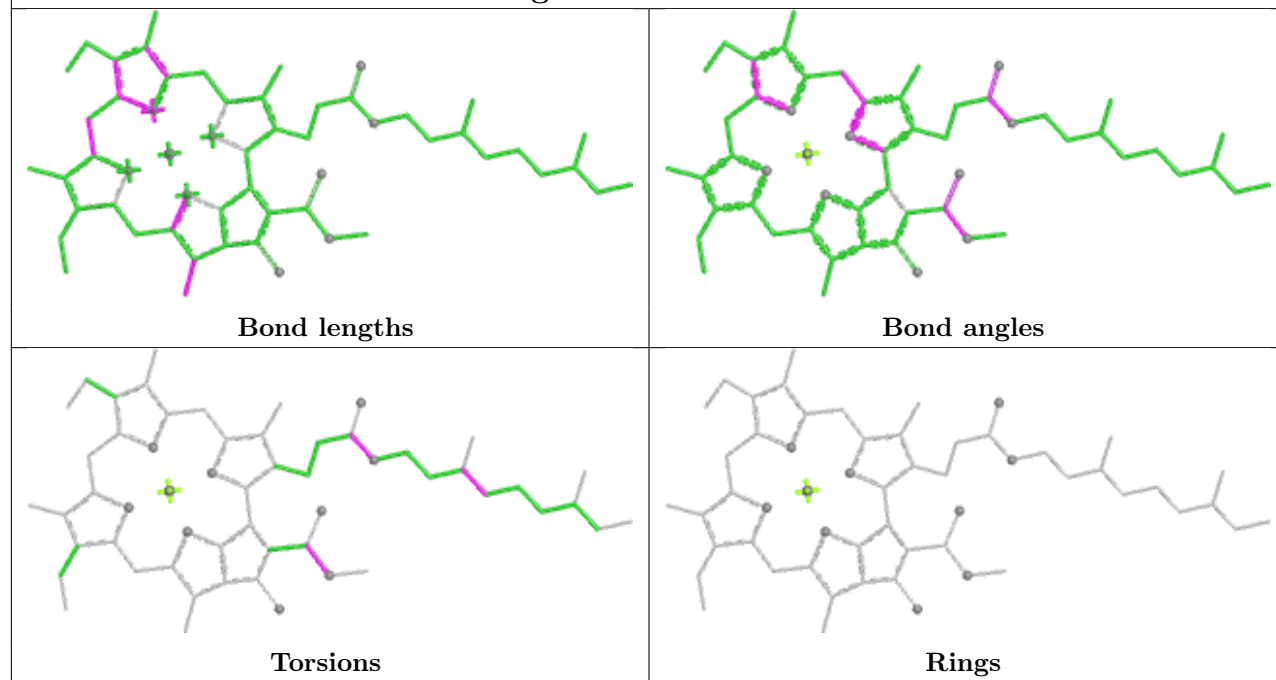


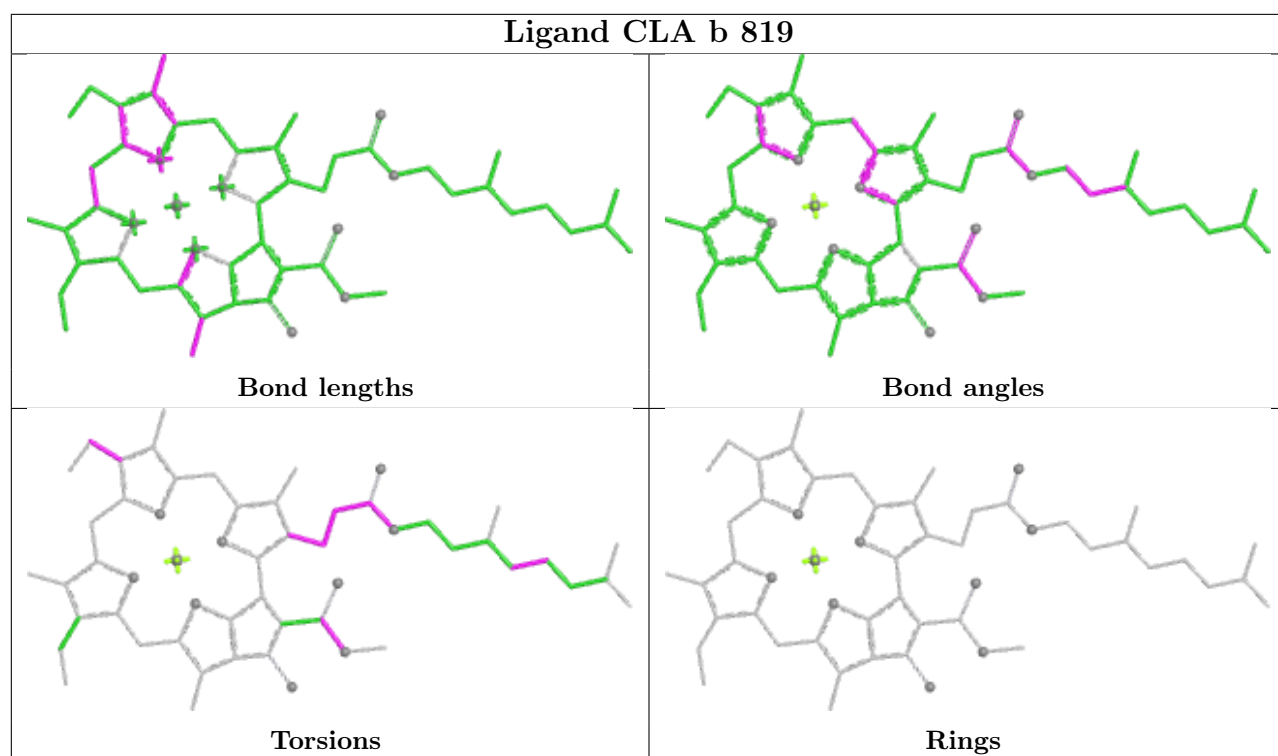


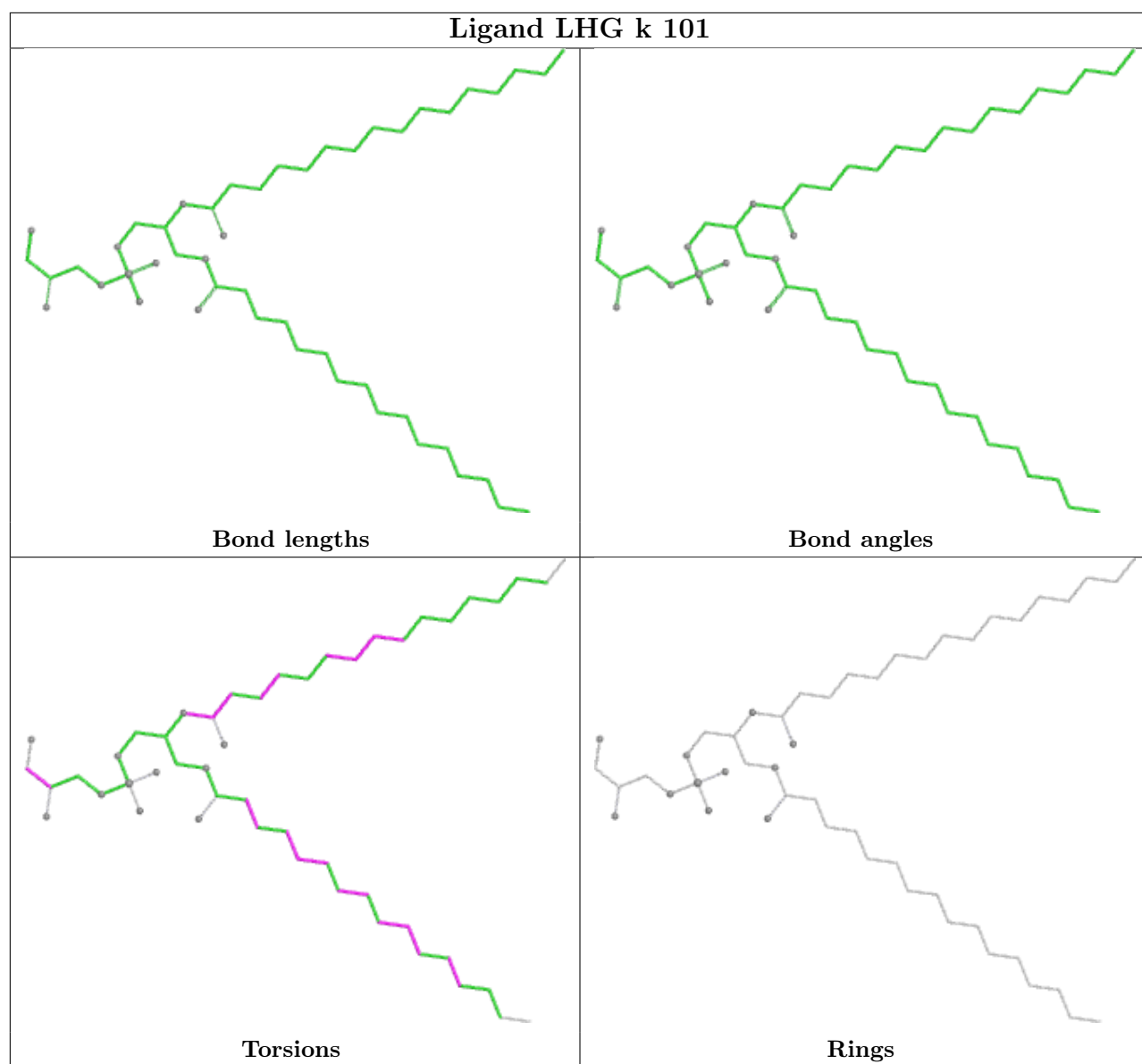
Ligand CLA b 812

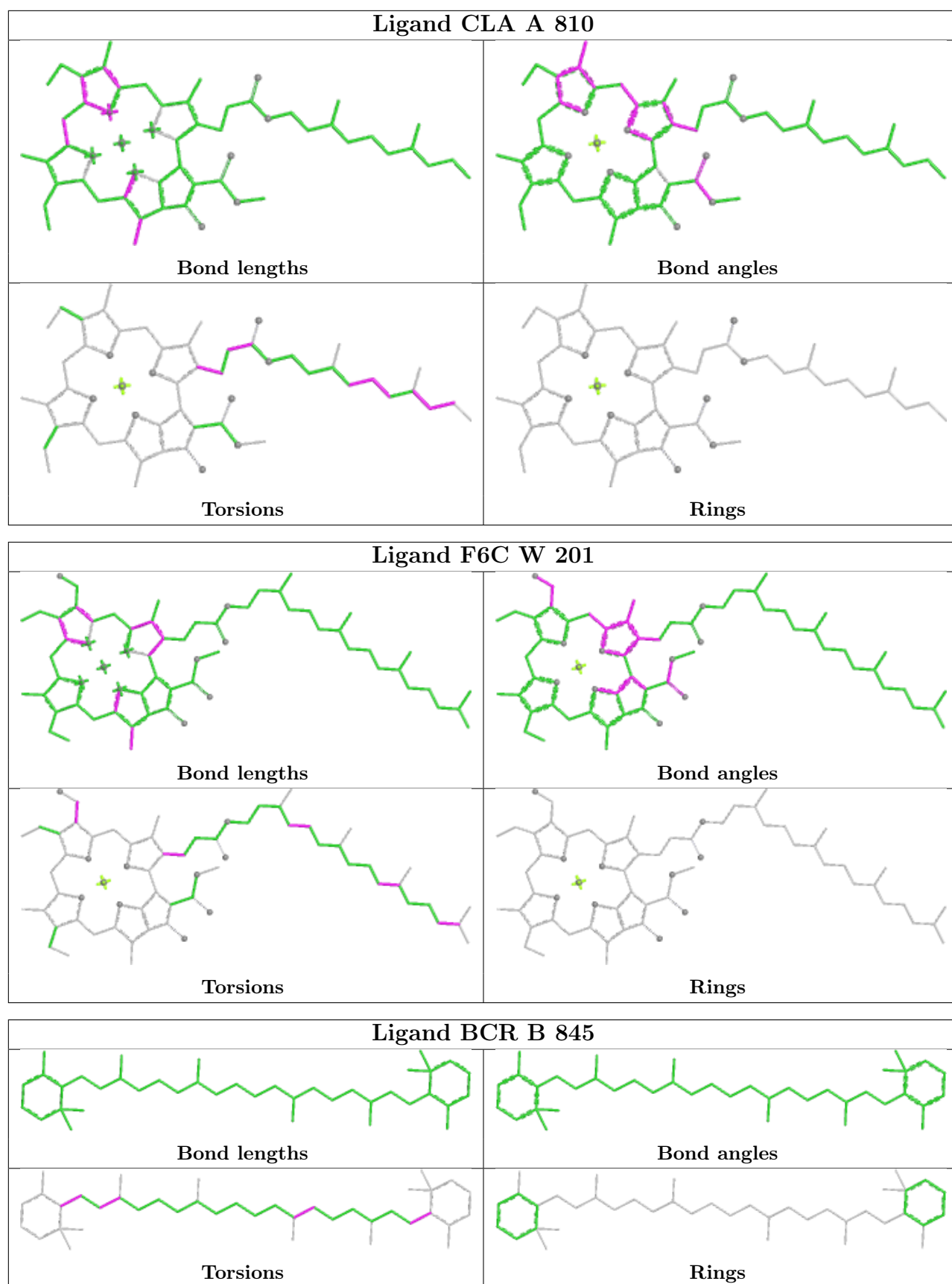


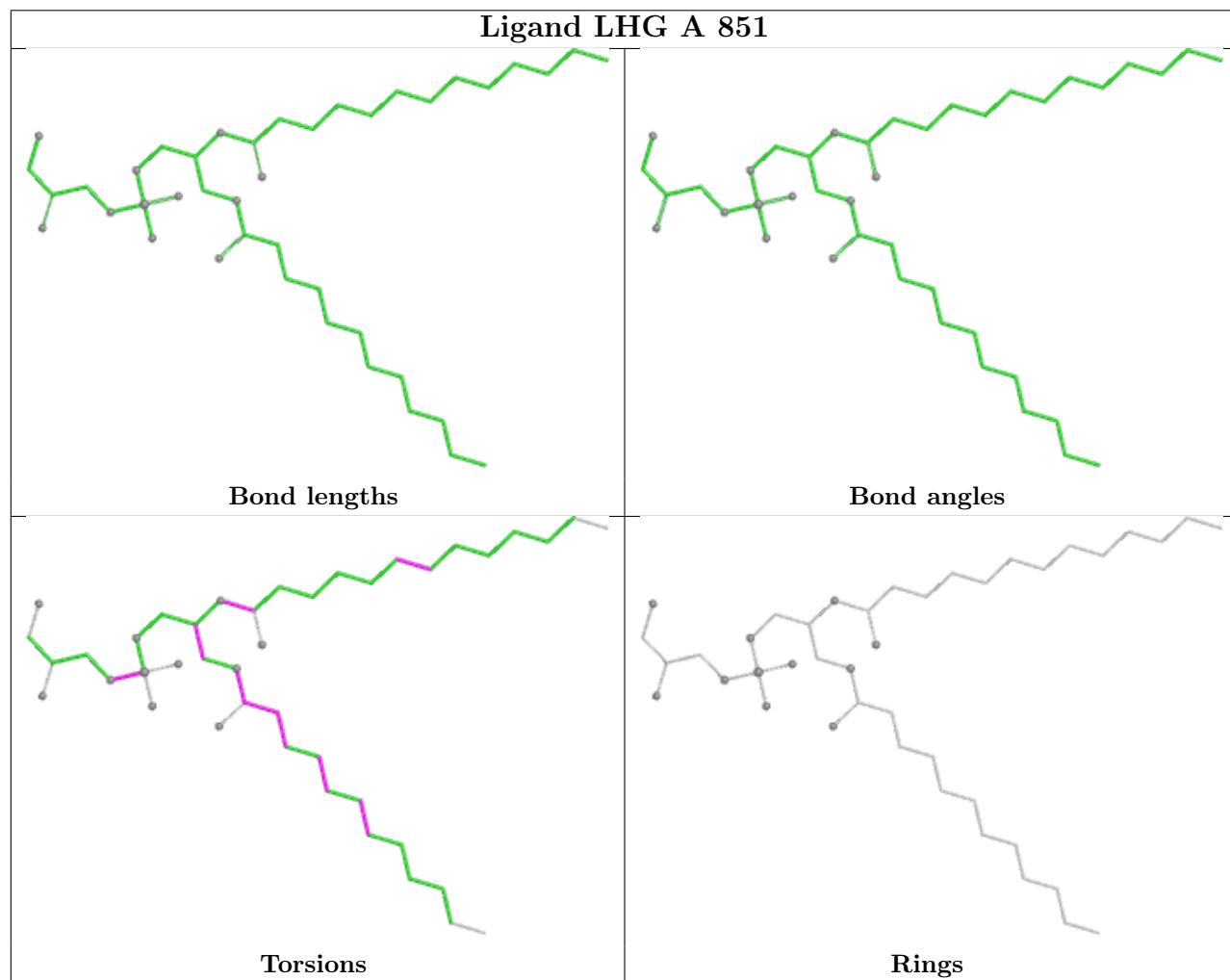
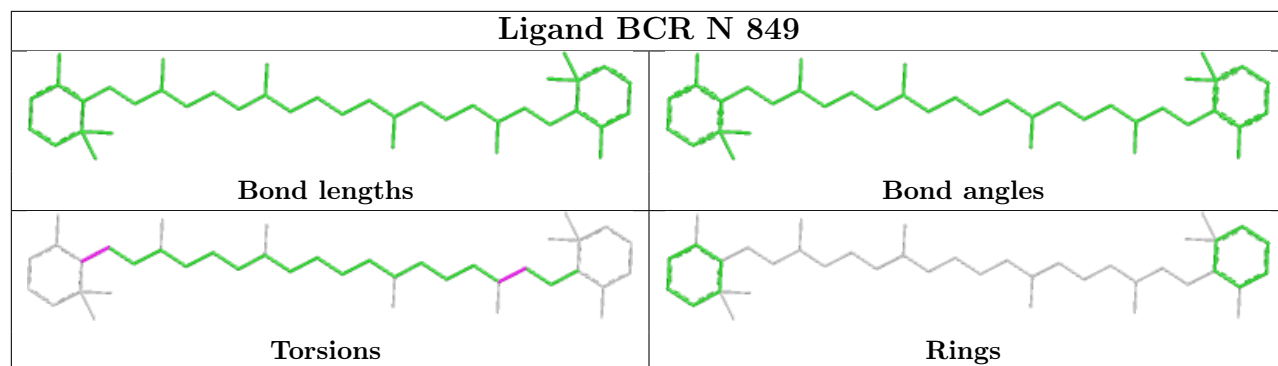
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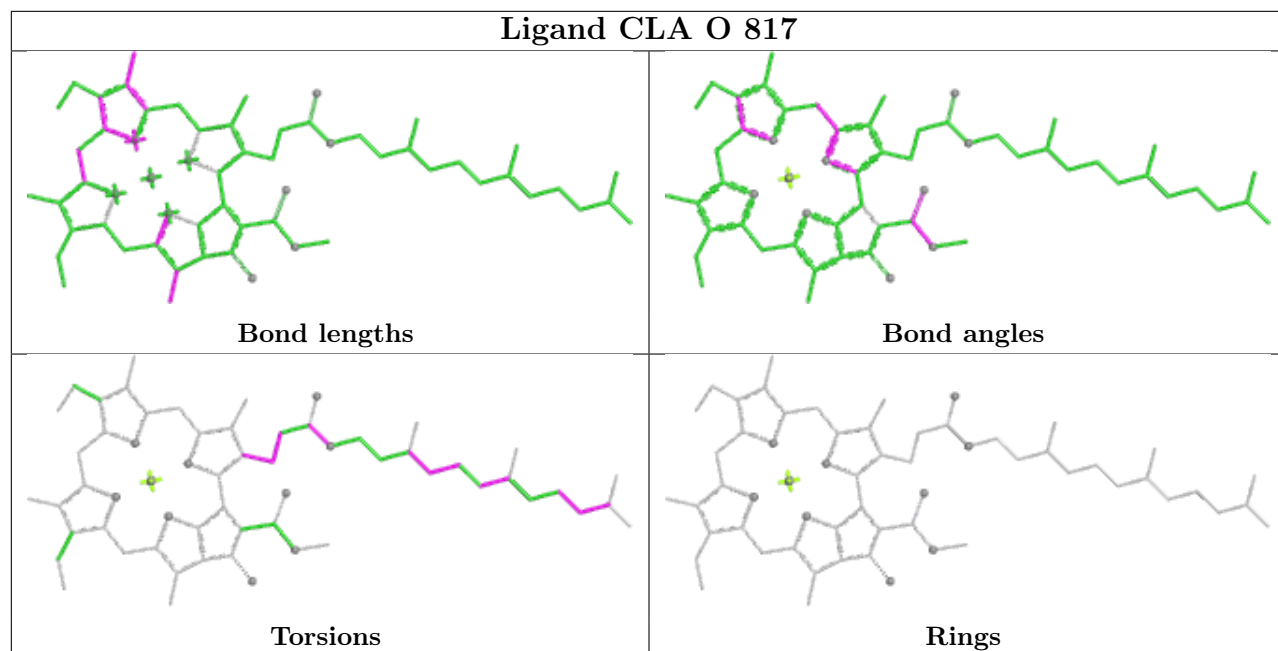
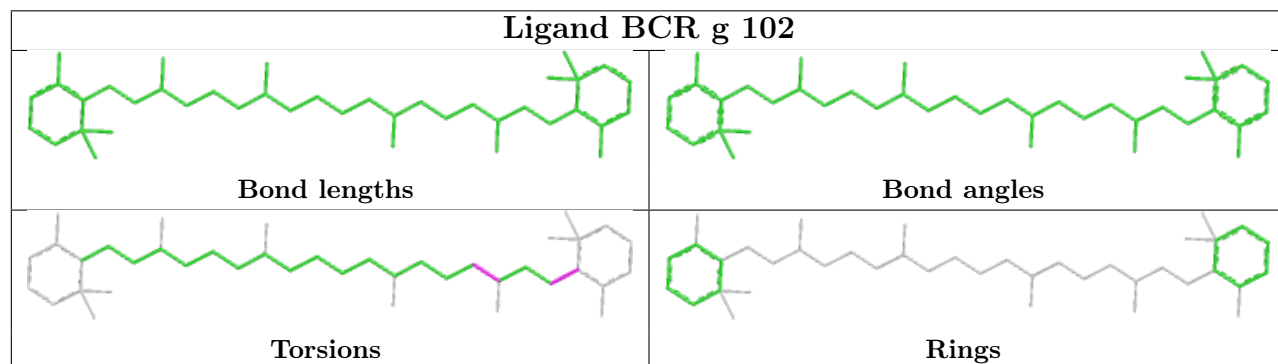
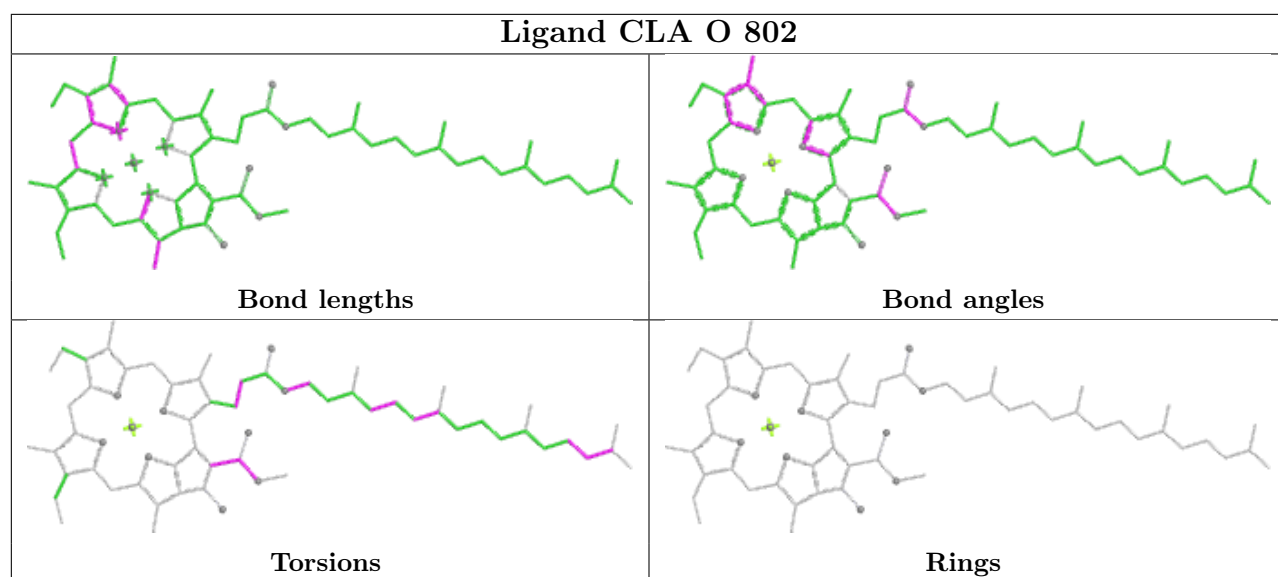




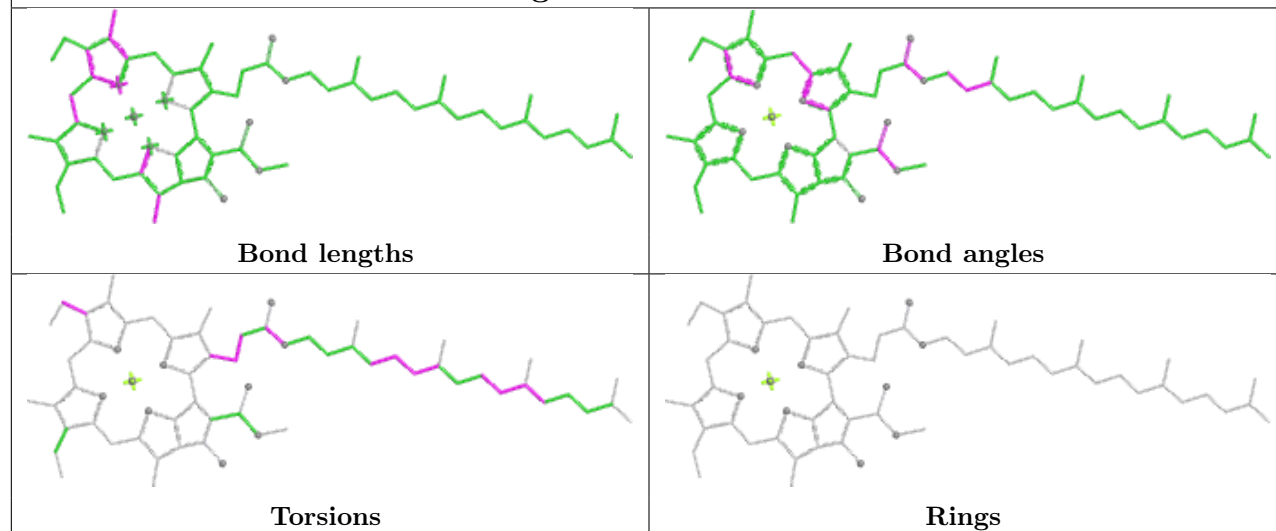




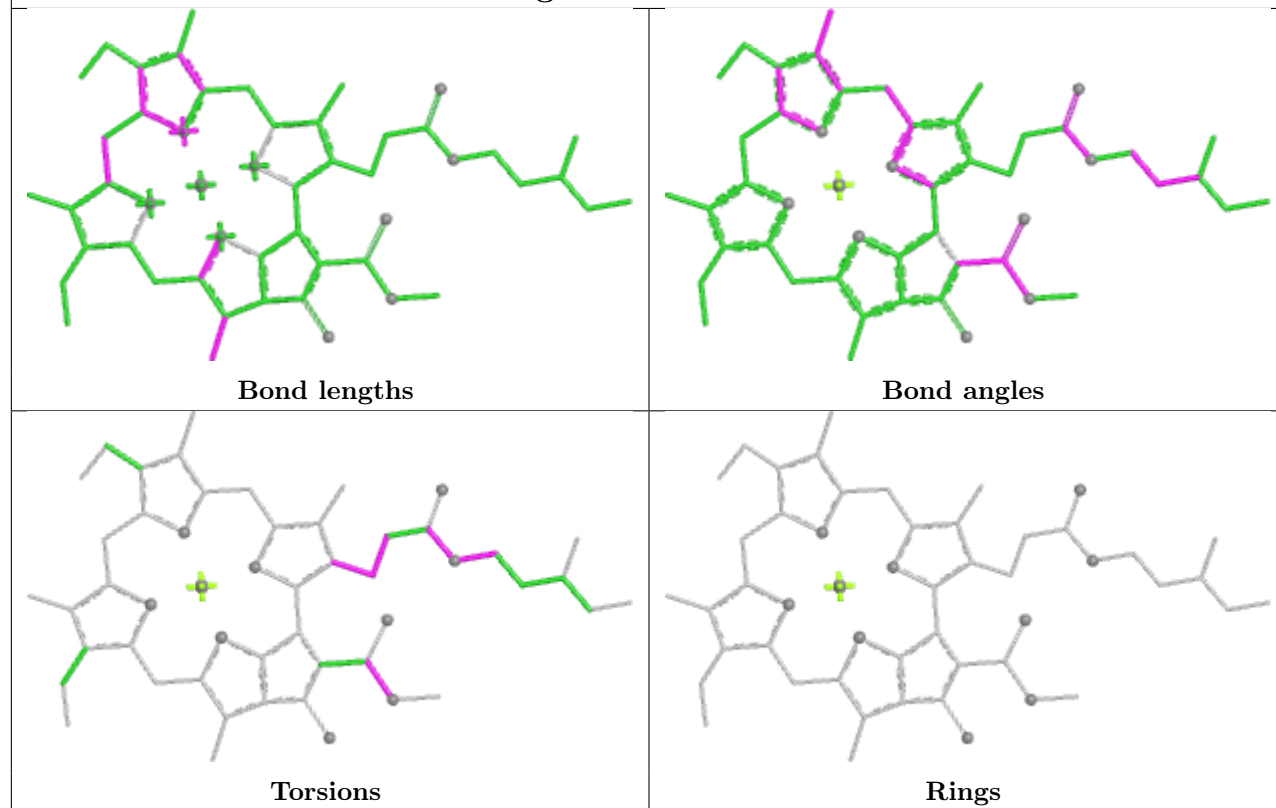




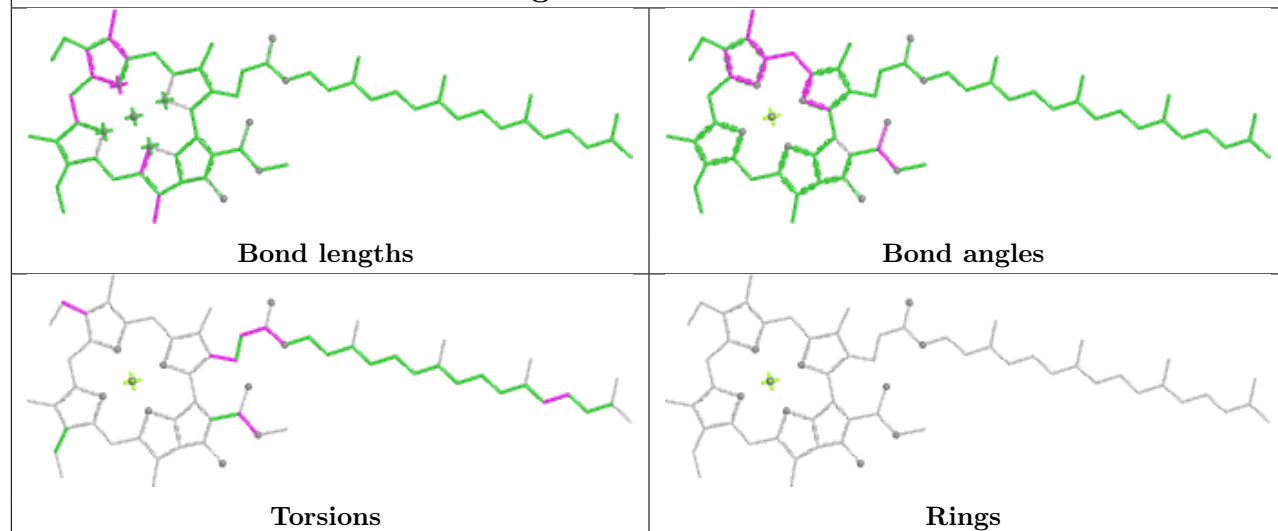
Ligand CLA O 809



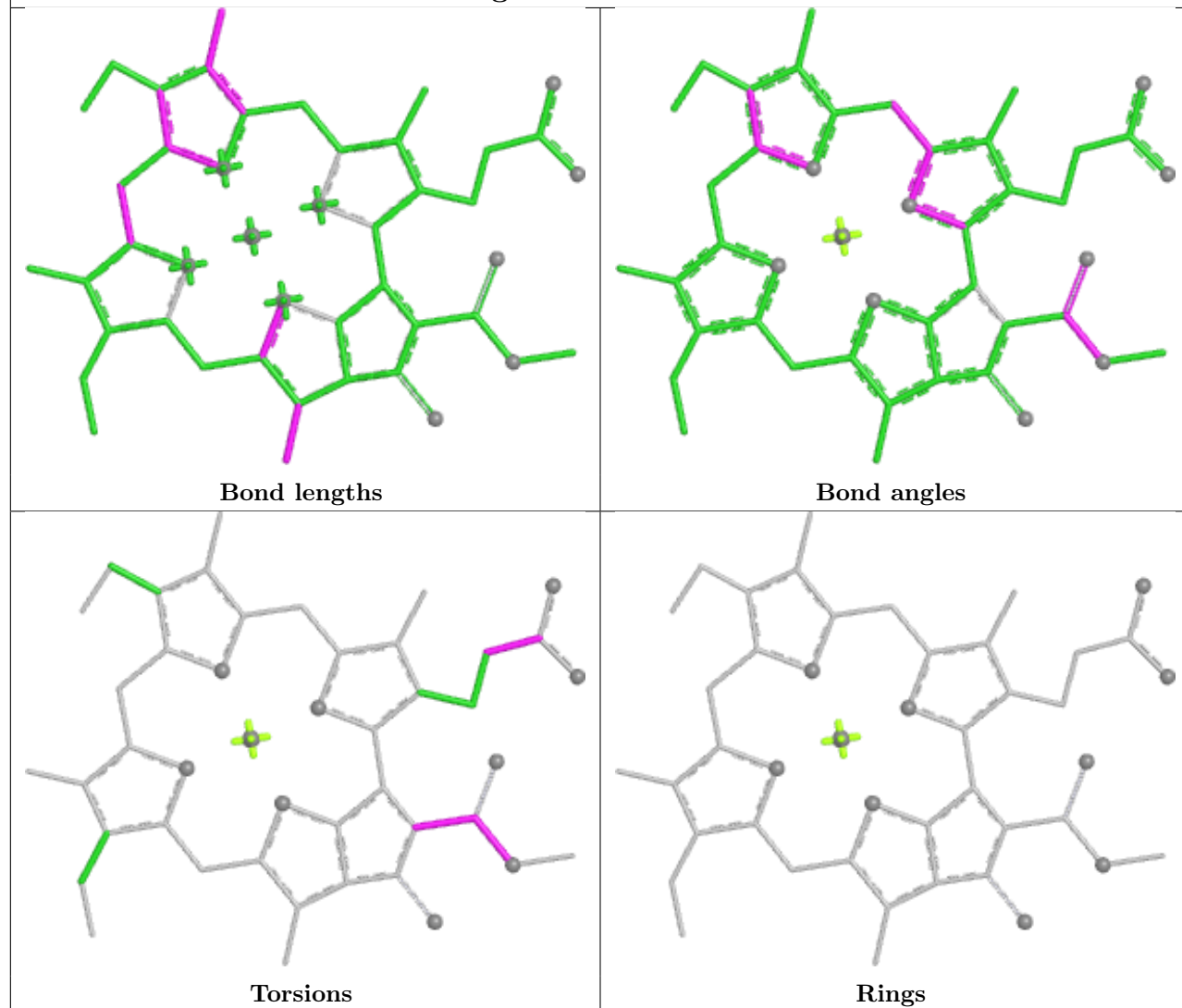
Ligand CLA a 837



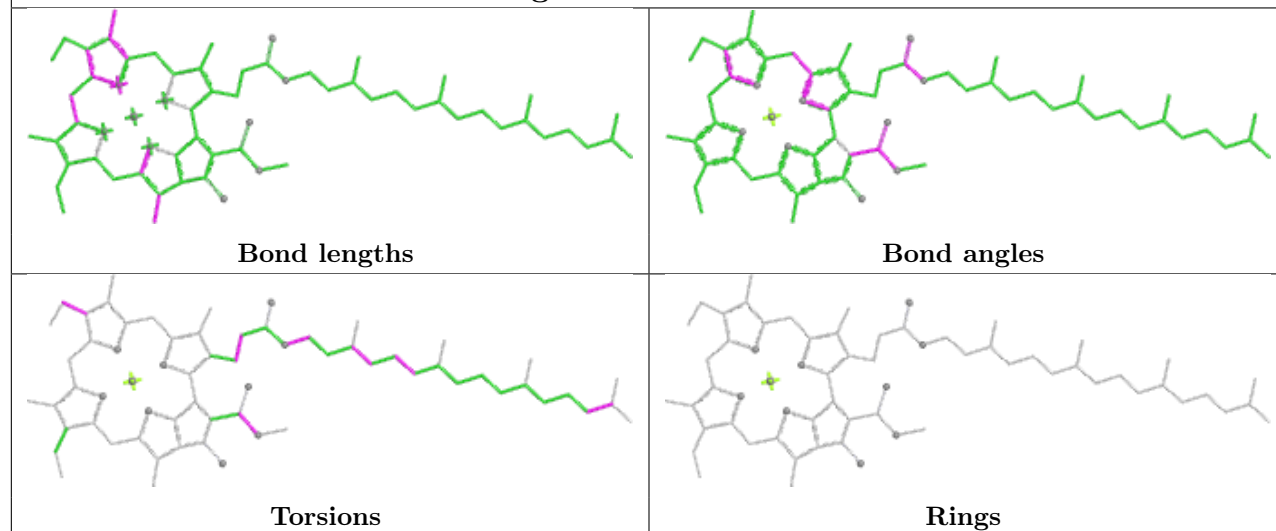
Ligand CLA O 816



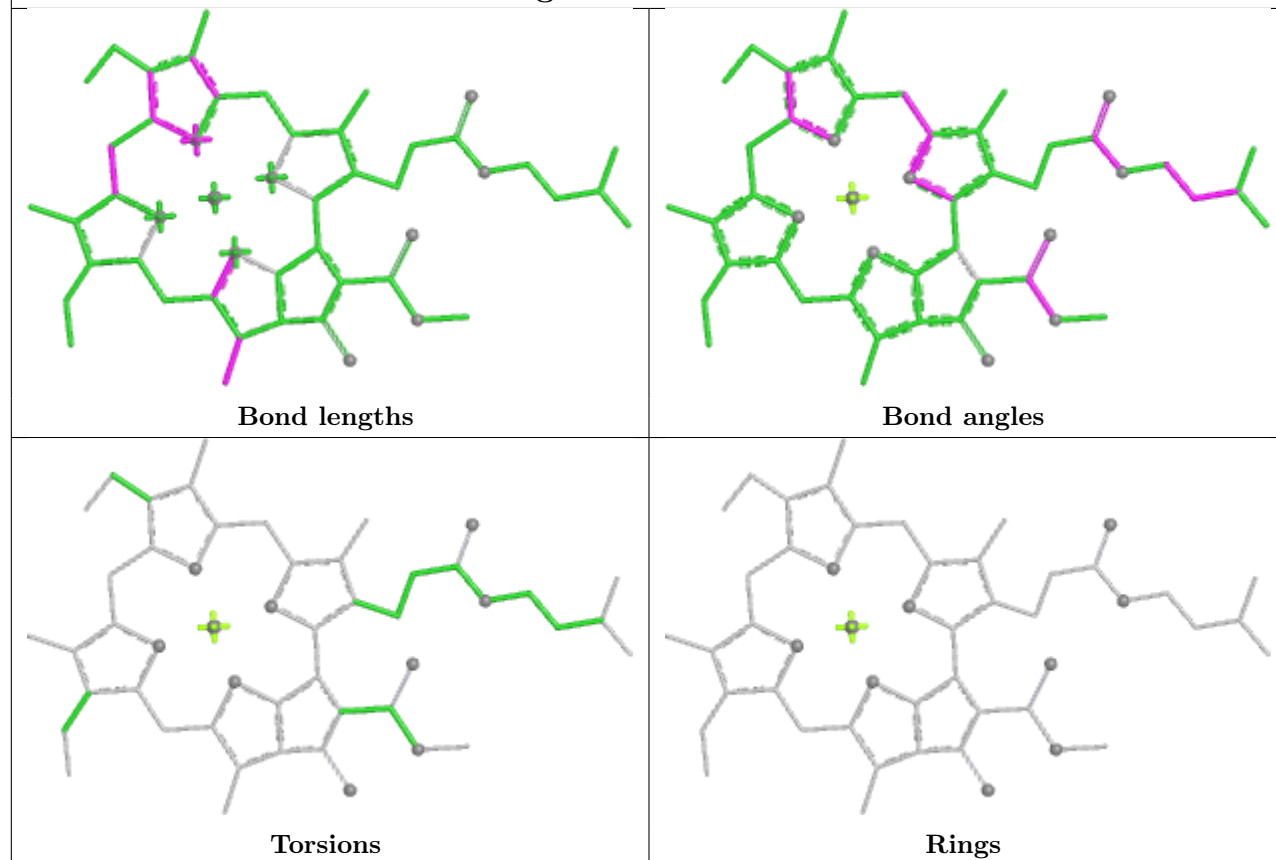
Ligand CLA A 816



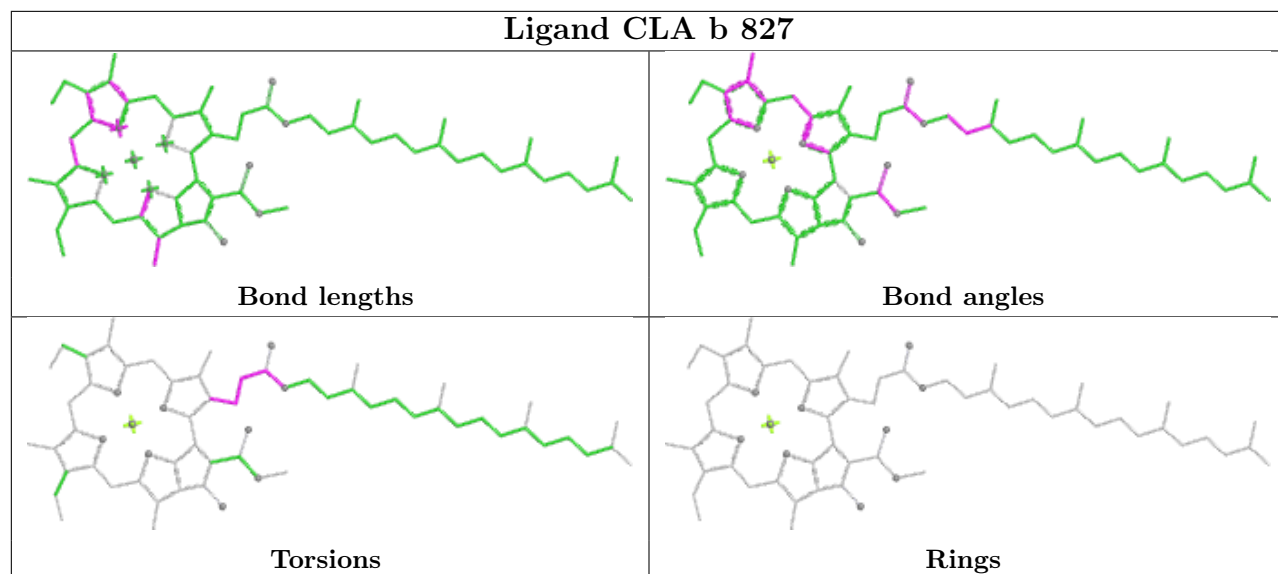
Ligand CLA N 835



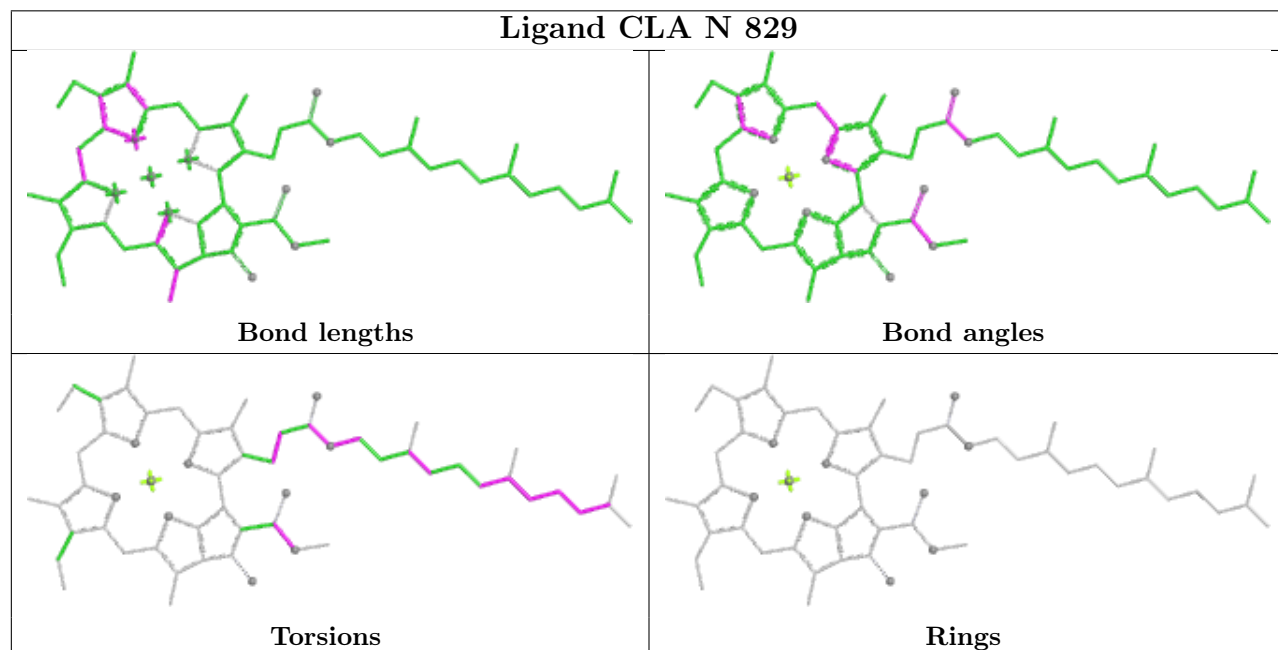
Ligand CLA a 840



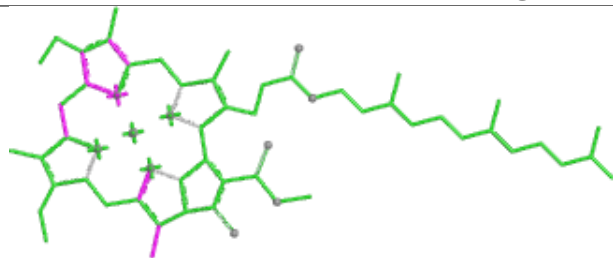
Ligand CLA b 827



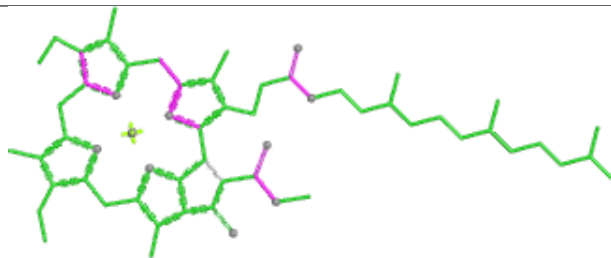
Ligand CLA N 829



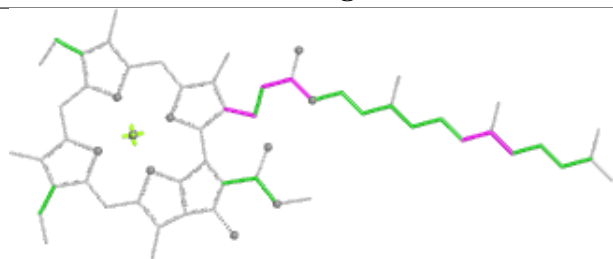
Ligand CLA A 805



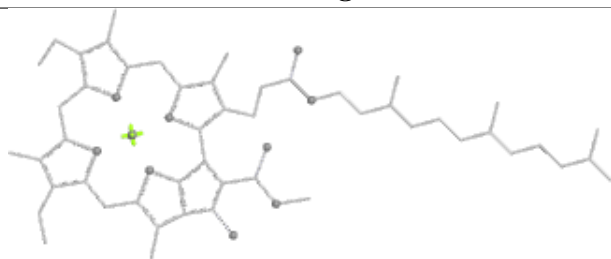
Bond lengths



Bond angles

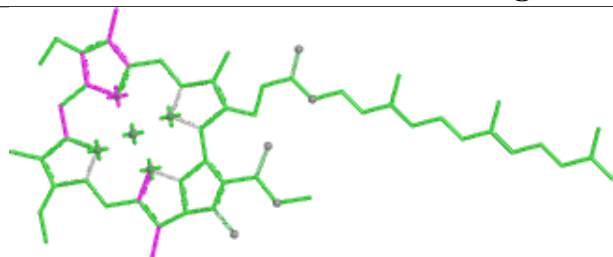


Torsions

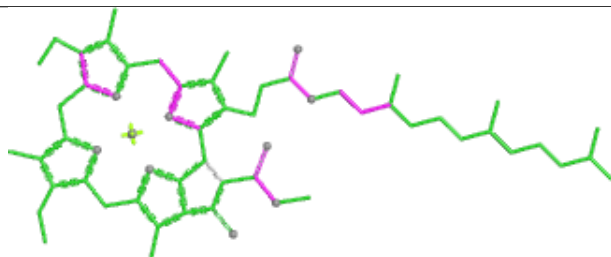


Rings

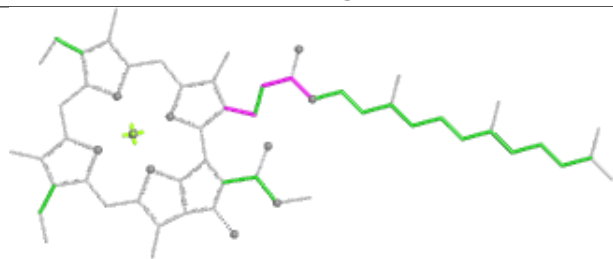
Ligand CLA N 821



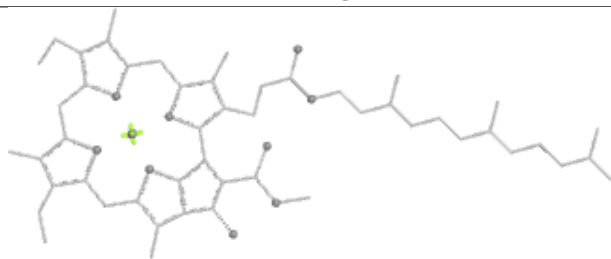
Bond lengths



Bond angles

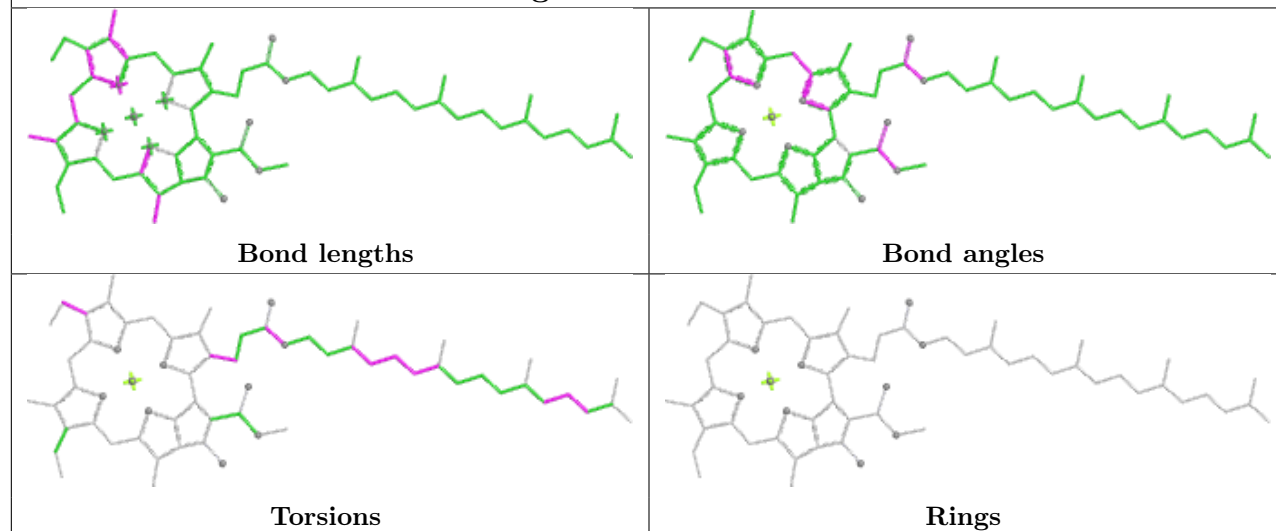


Torsions

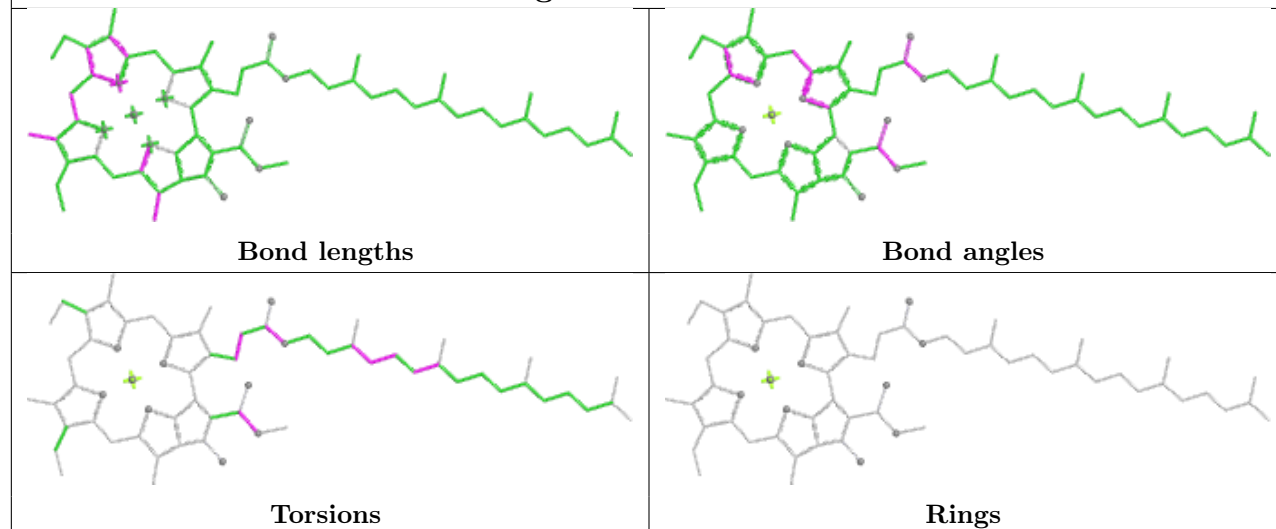


Rings

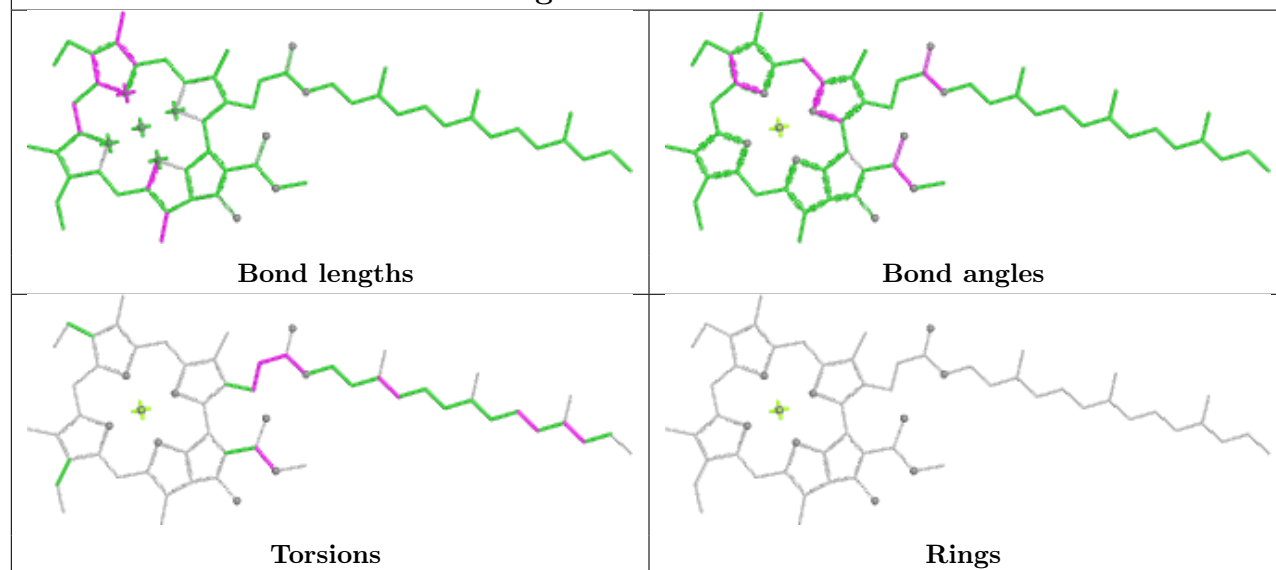
Ligand CLA A 841



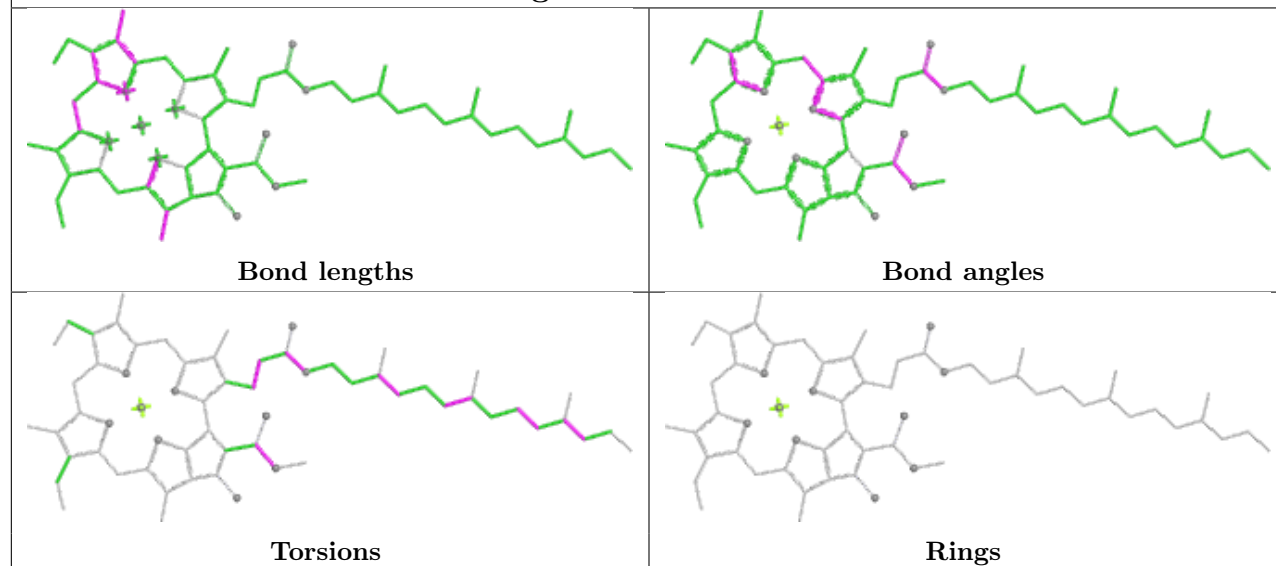
Ligand CLA b 804



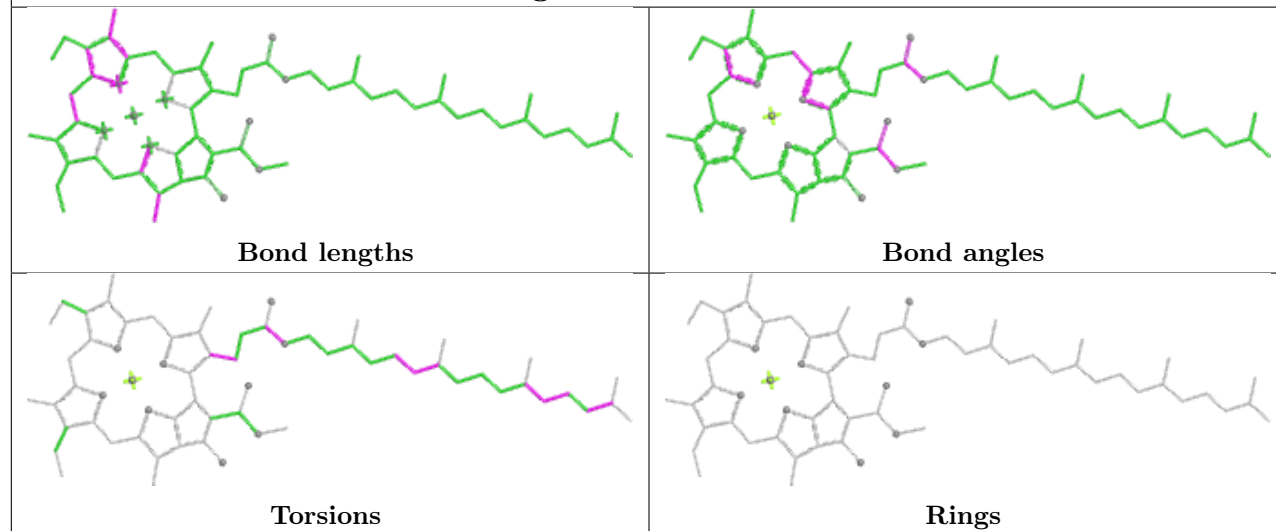
Ligand CLA b 826

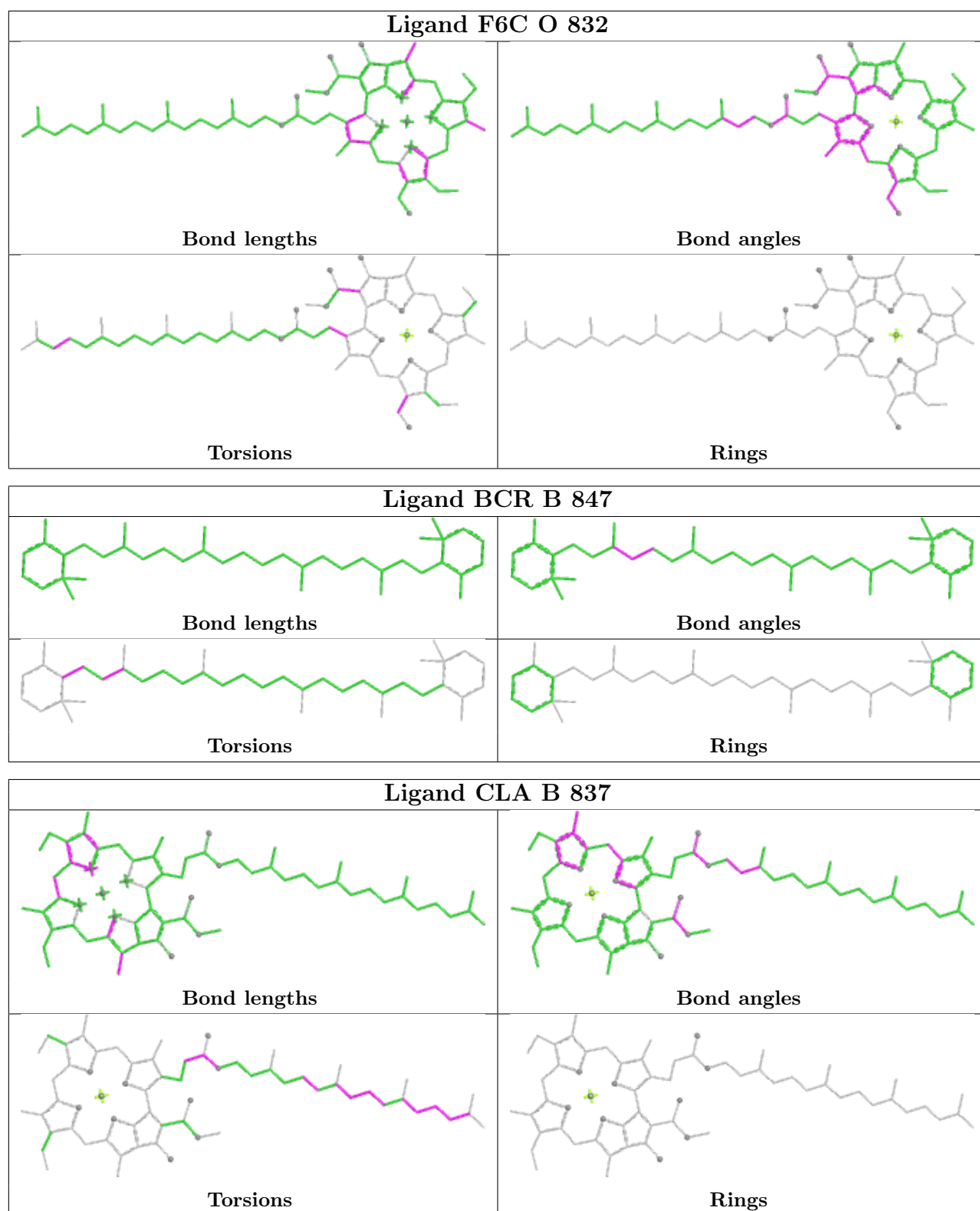


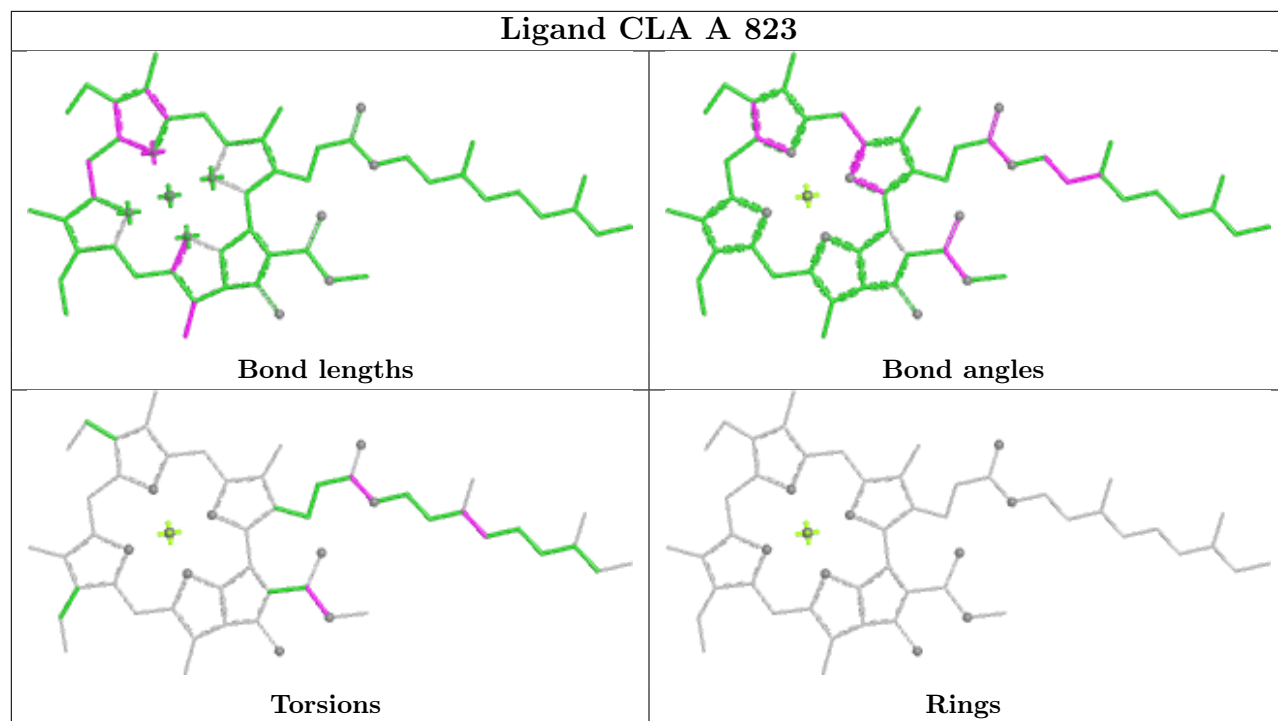
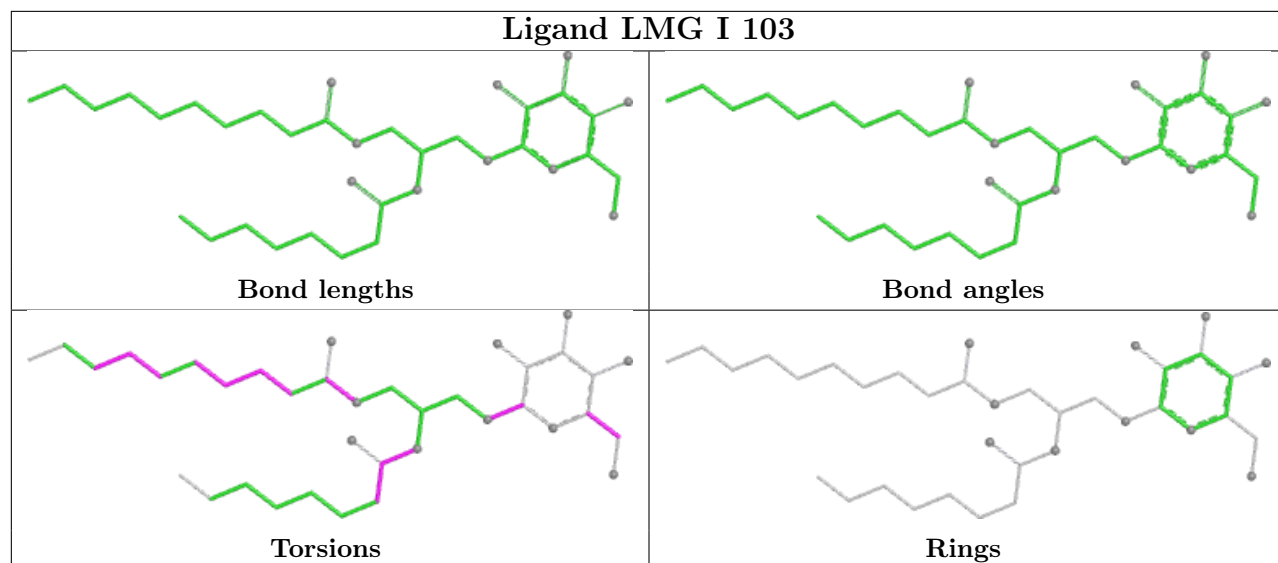
Ligand CLA O 826

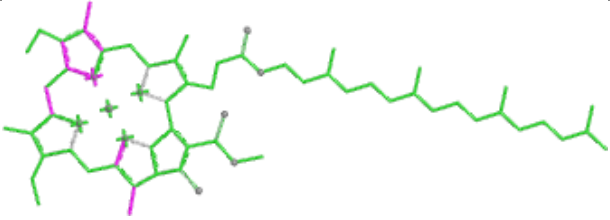
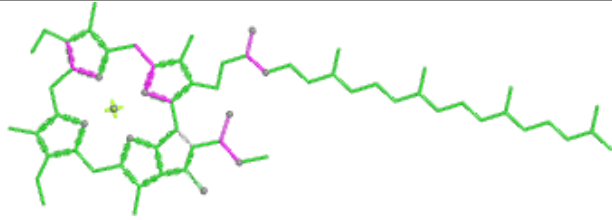
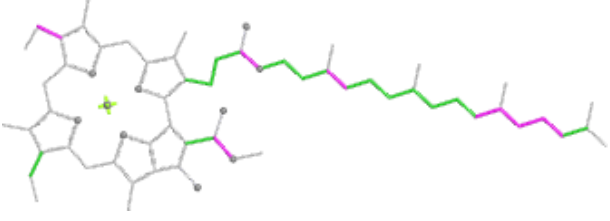
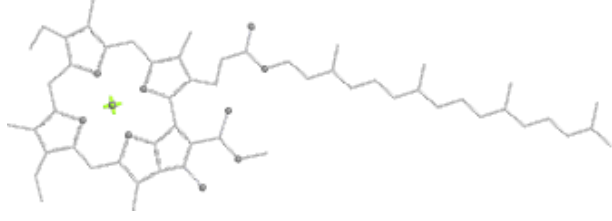
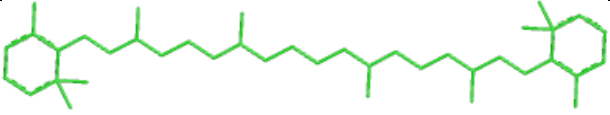
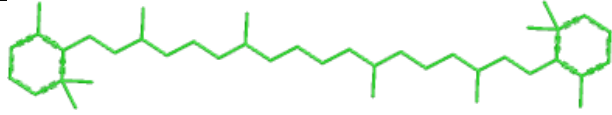
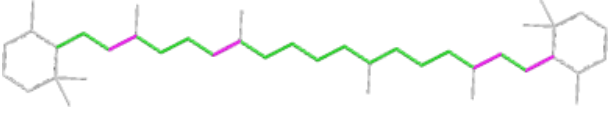
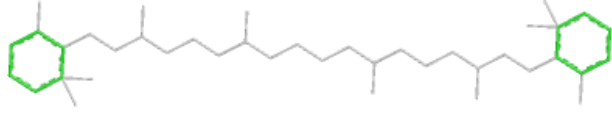
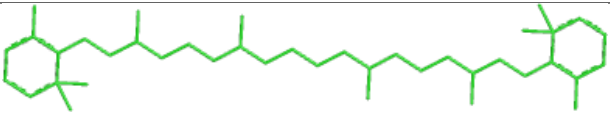
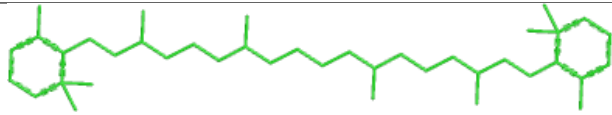
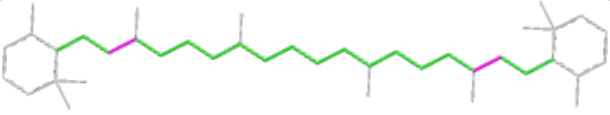
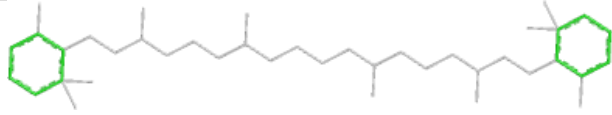


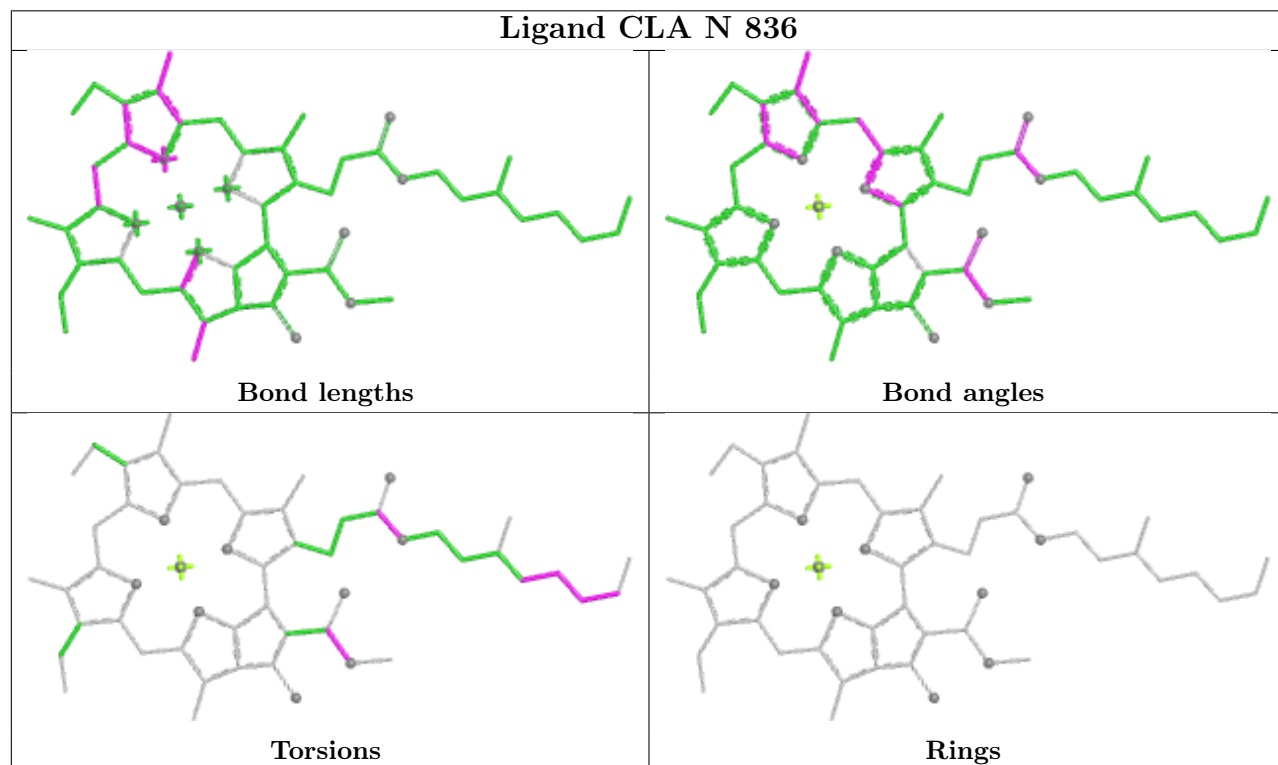
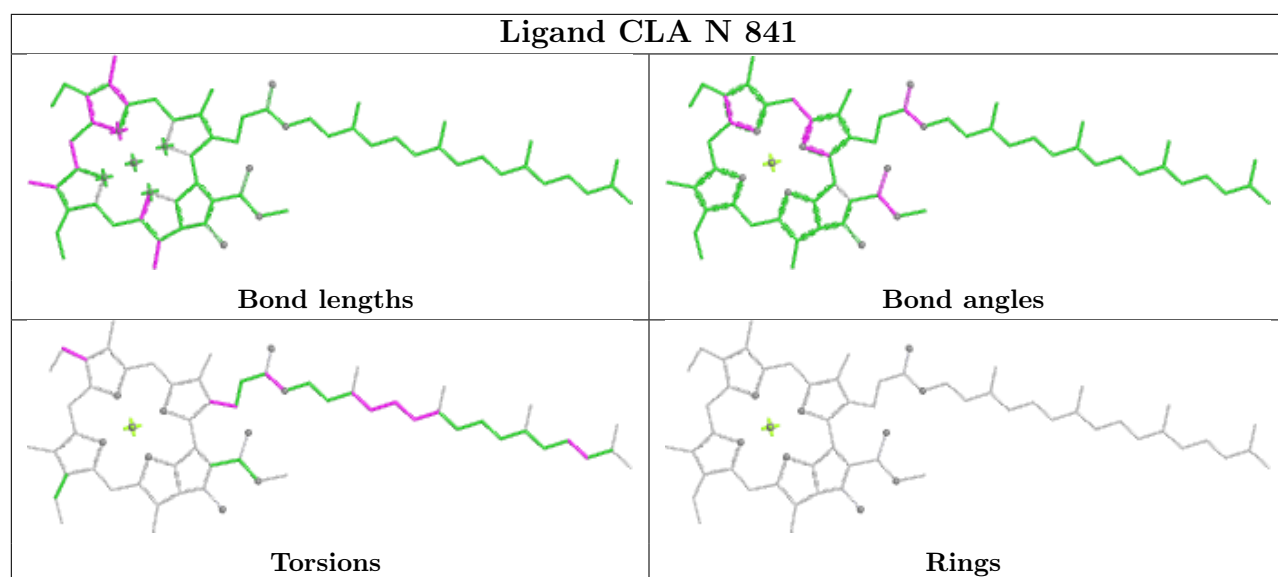
Ligand CLA O 810

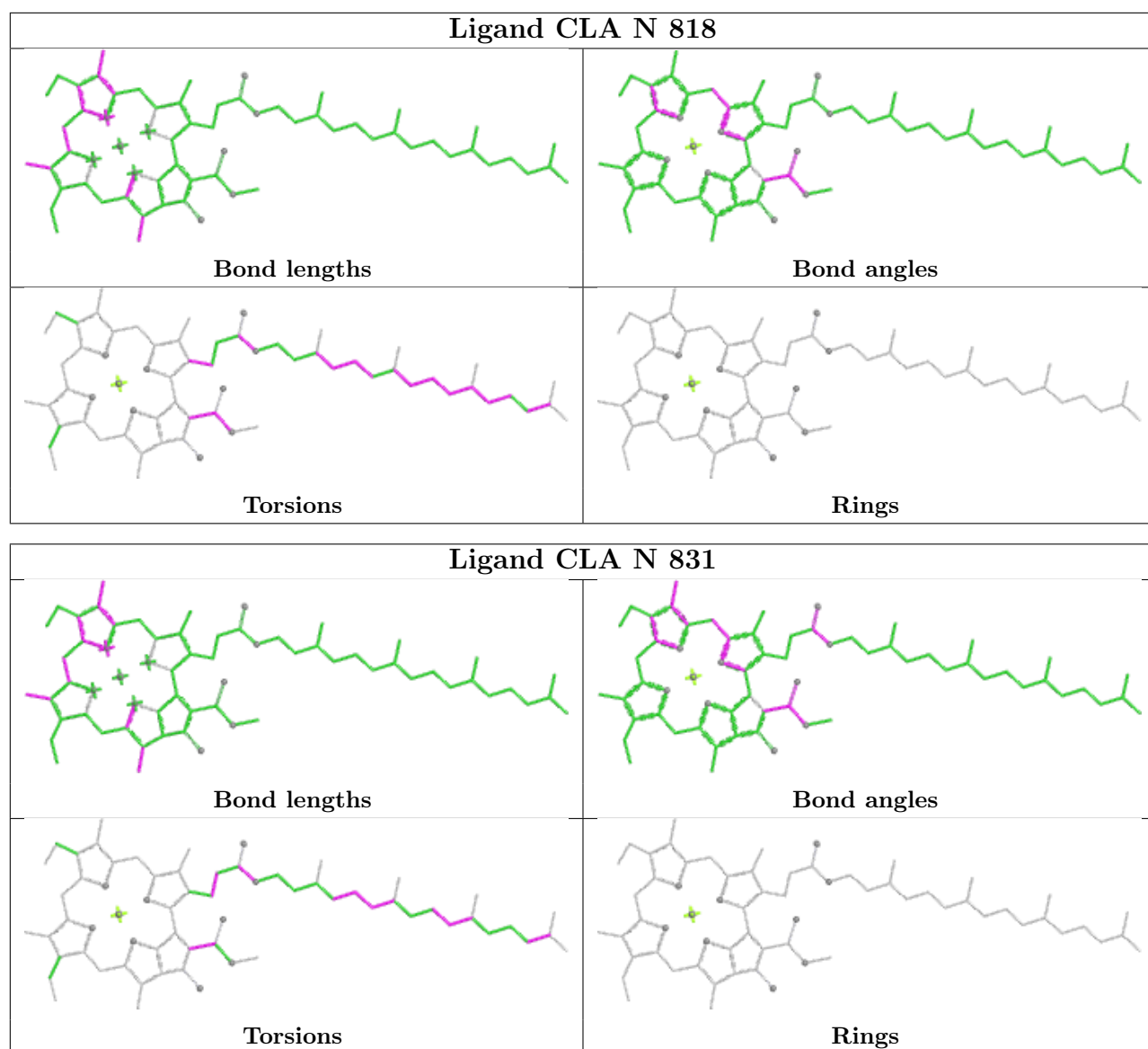


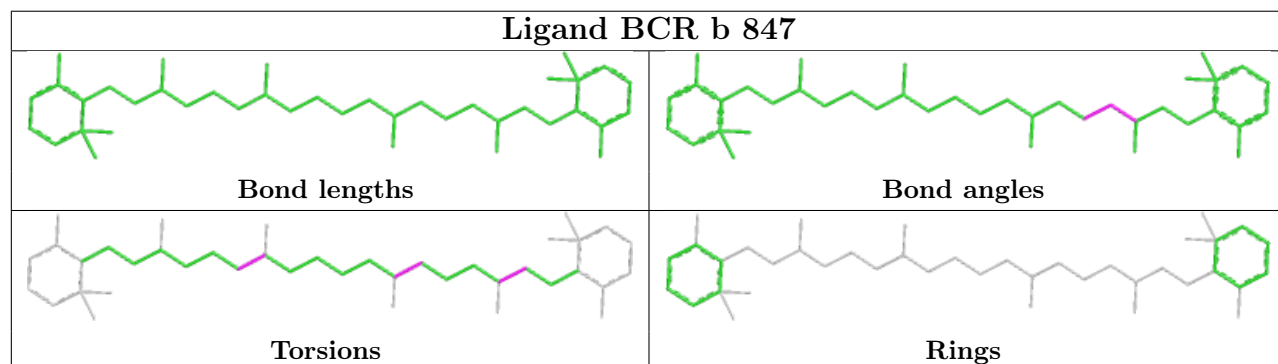
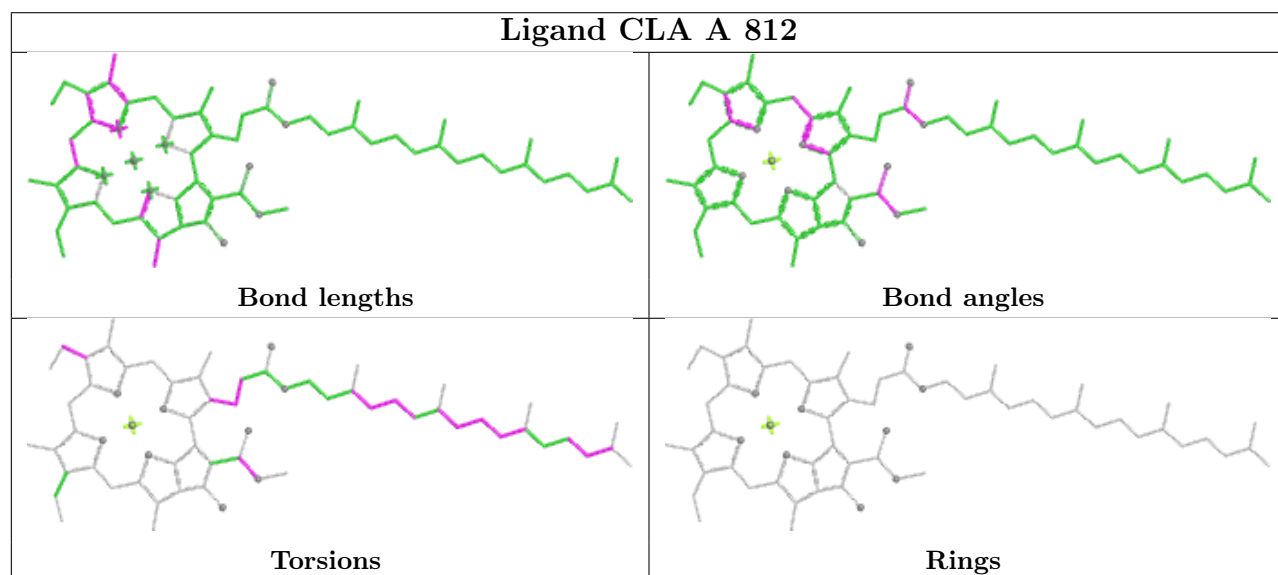
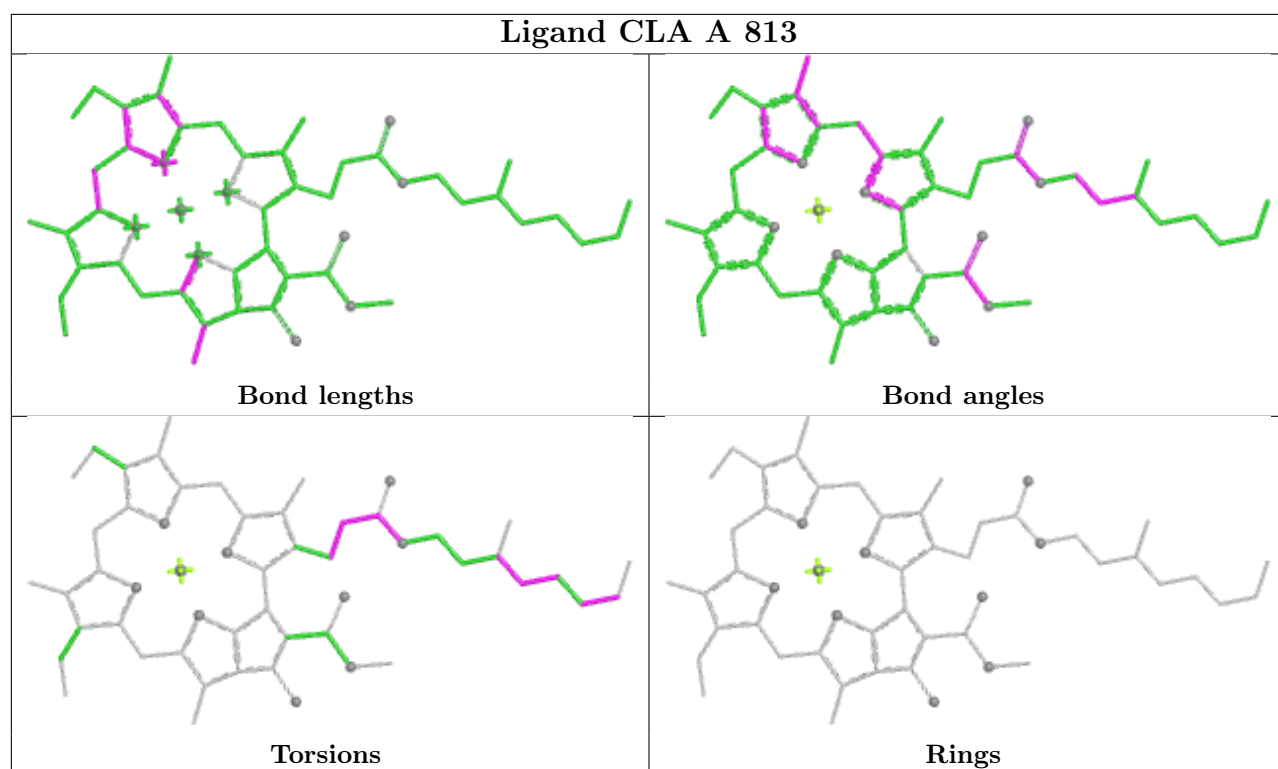




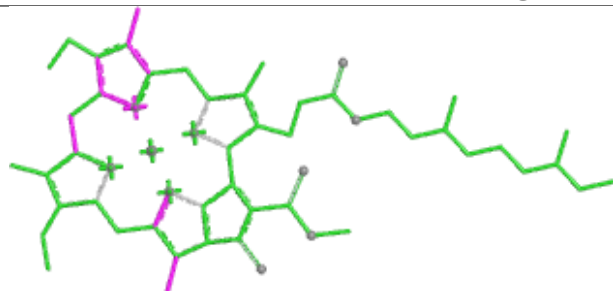
Ligand CLA B 840	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR g 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR L 205	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



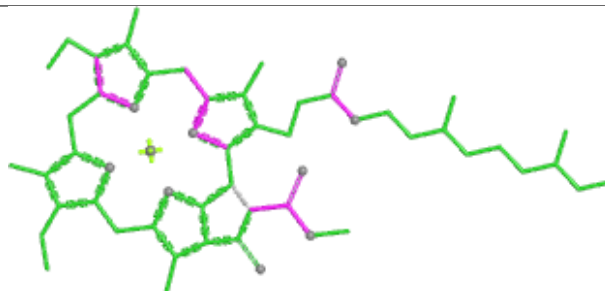




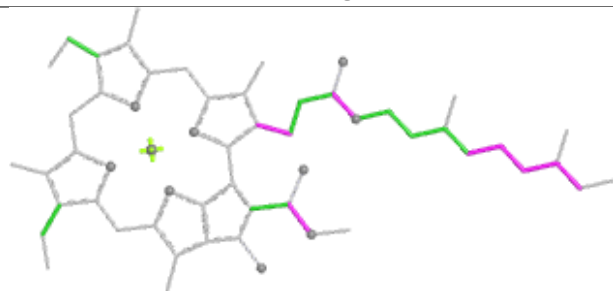
Ligand CLA B 812



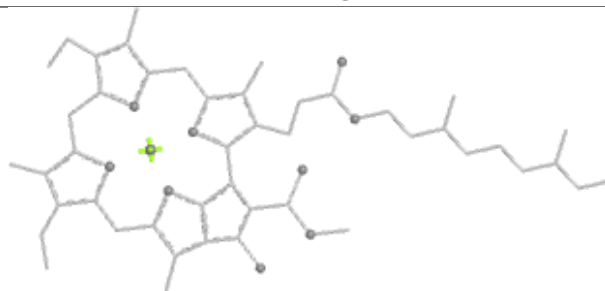
Bond lengths



Bond angles

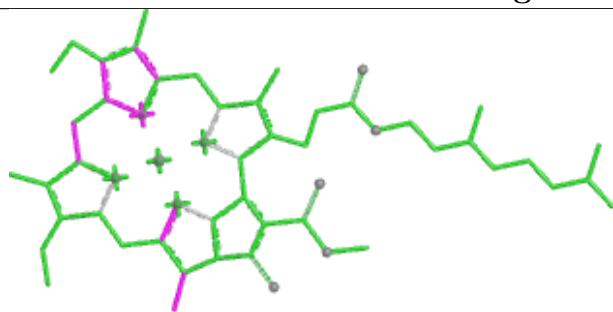


Torsions

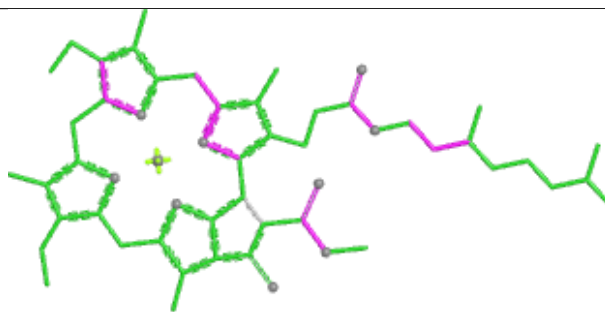


Rings

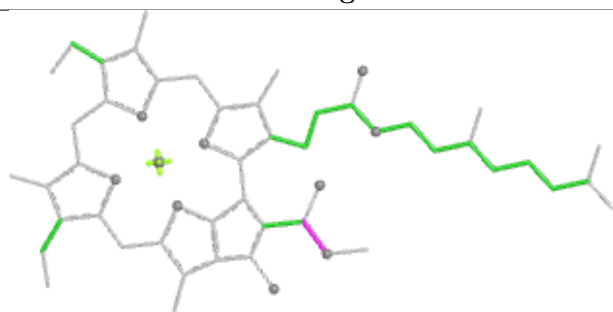
Ligand CLA X 102



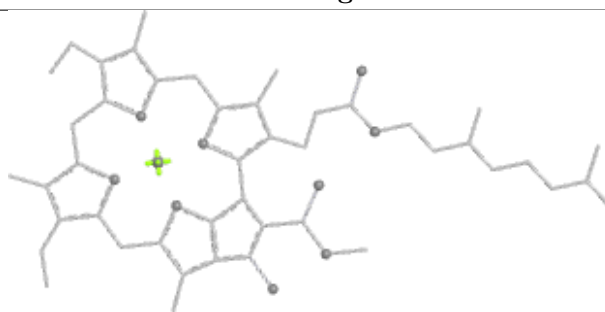
Bond lengths



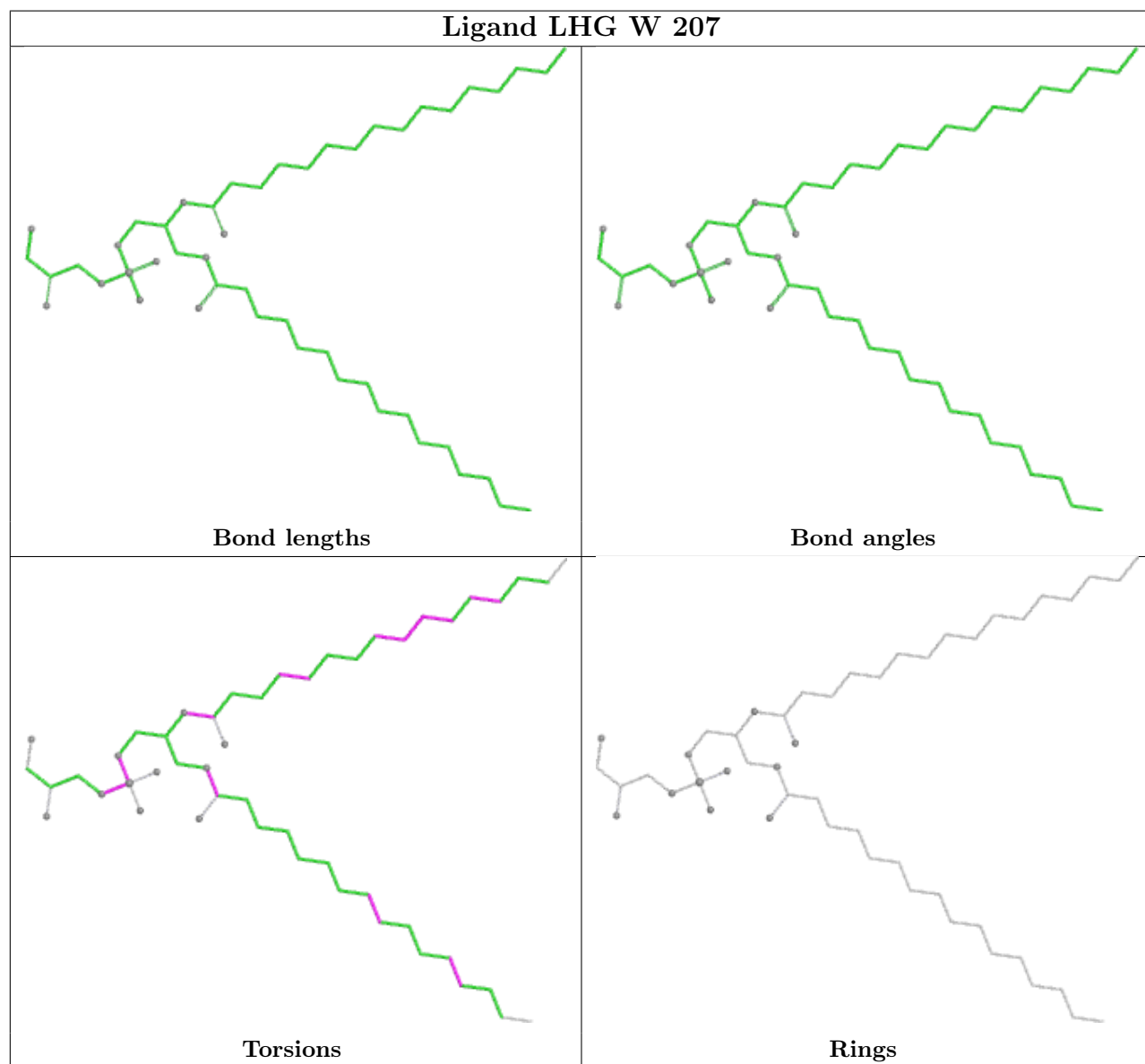
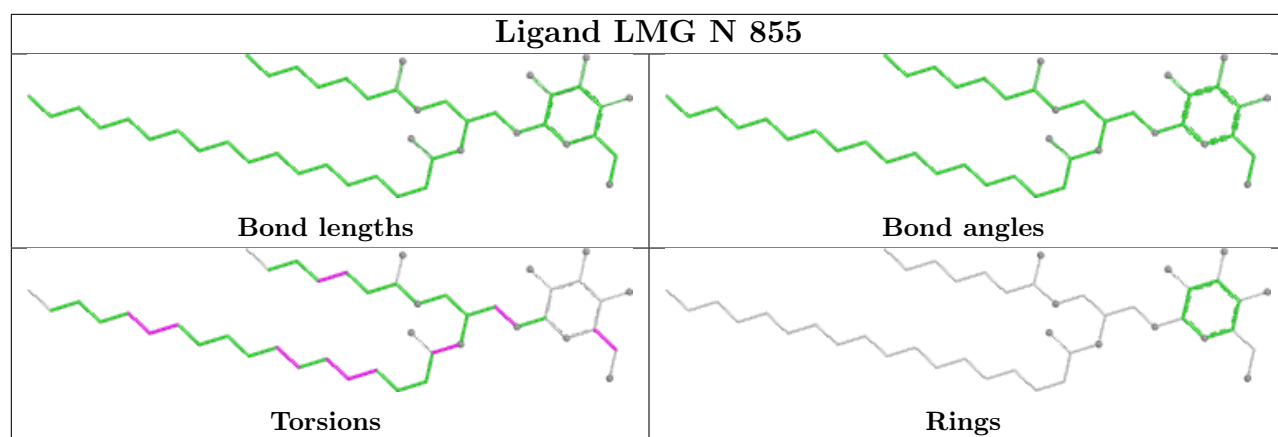
Bond angles



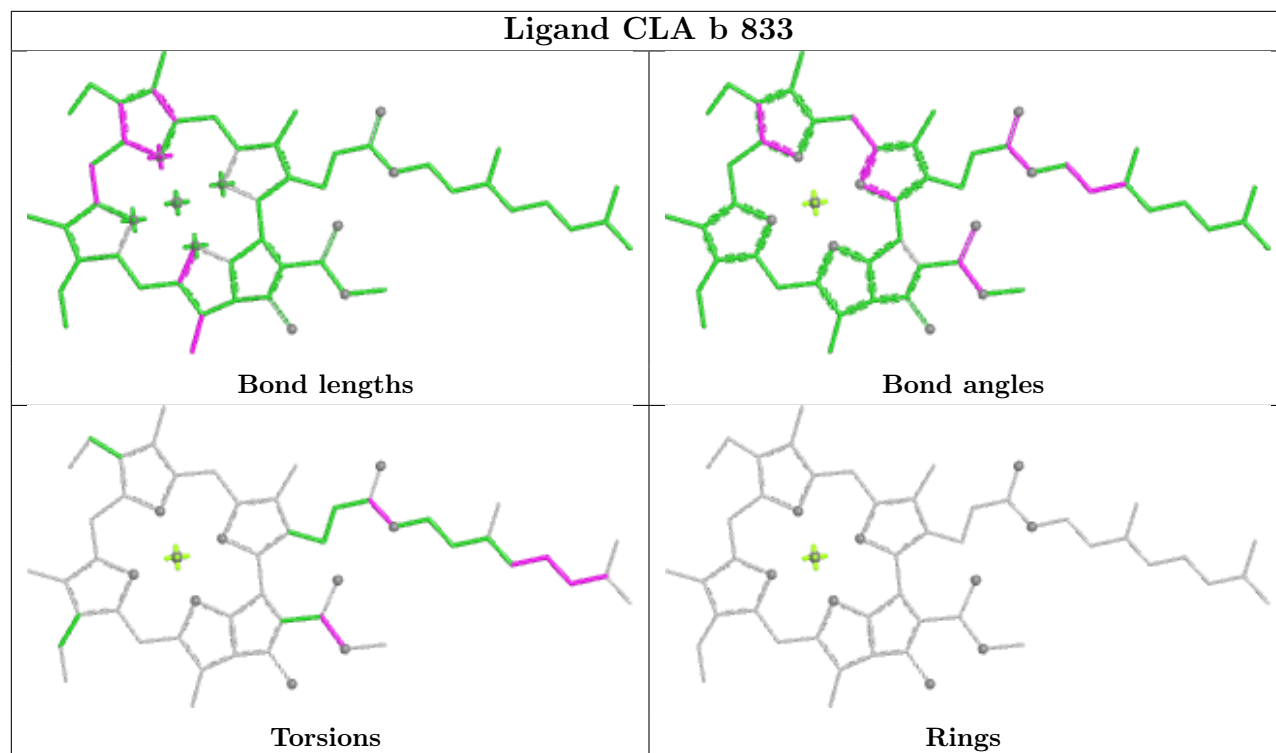
Torsions



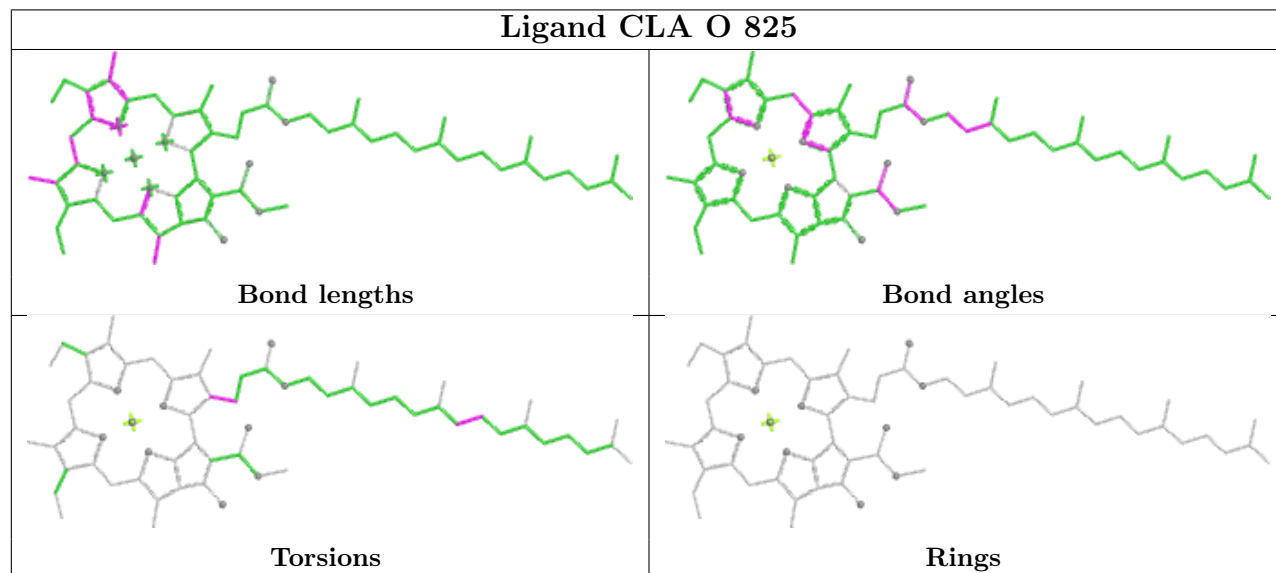
Rings



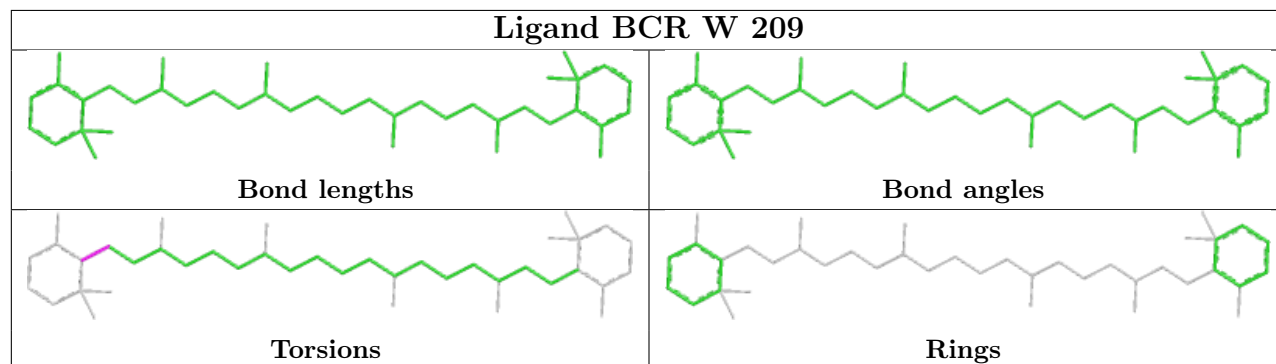
Ligand CLA b 833



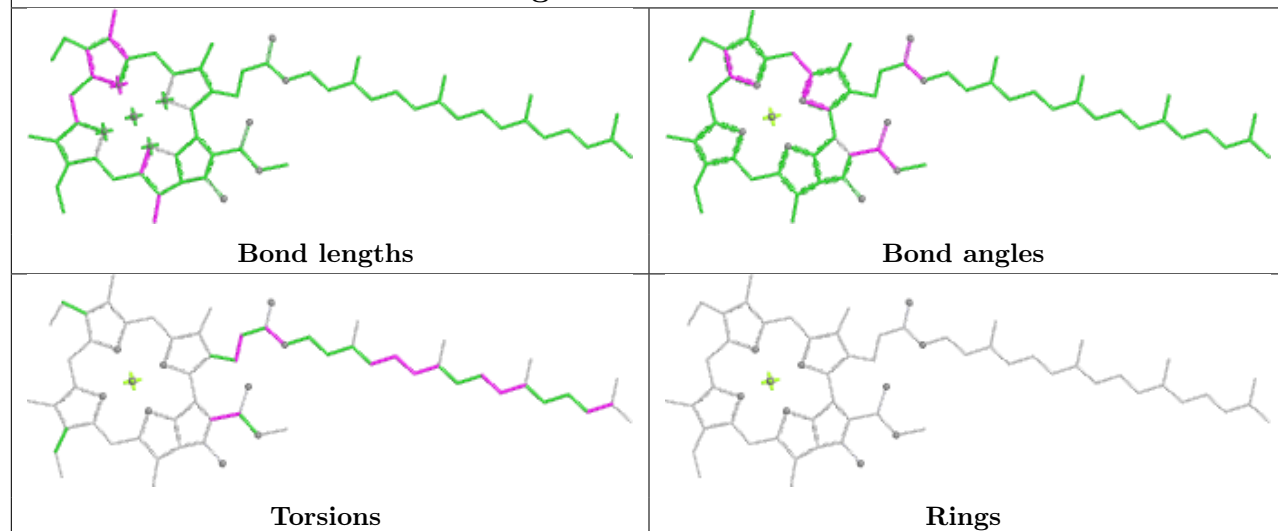
Ligand CLA O 825



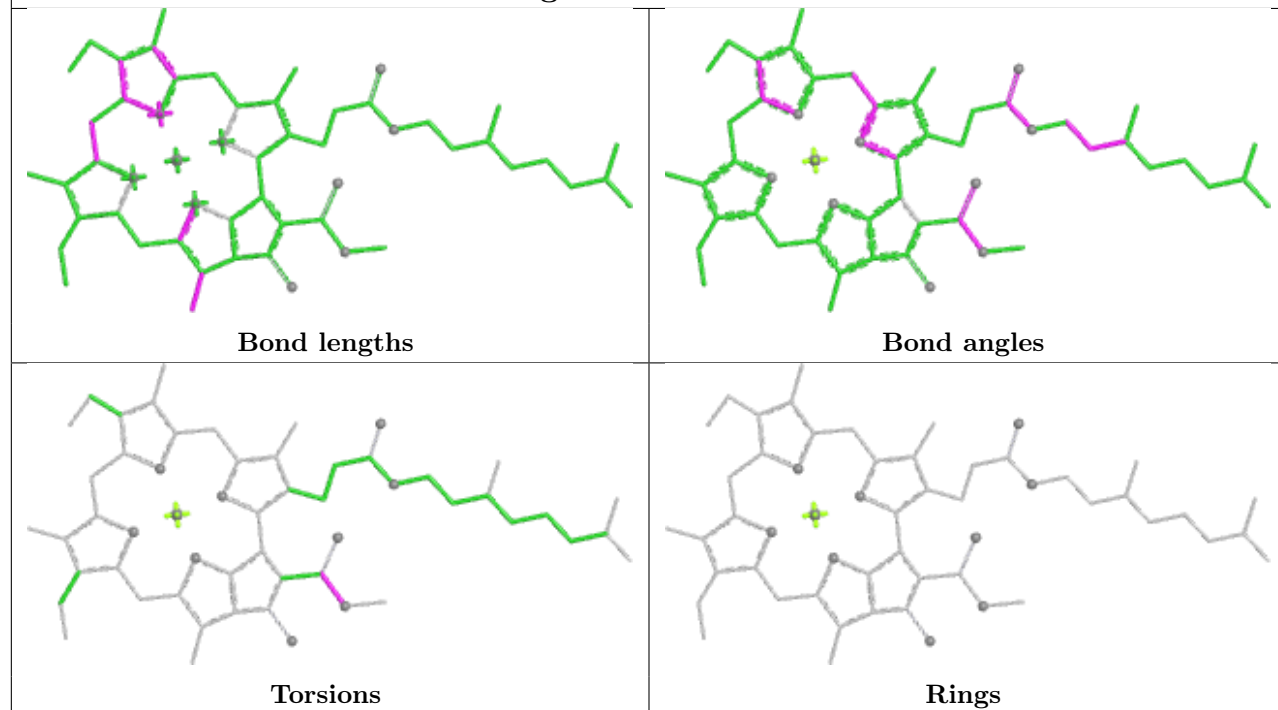
Ligand BCR W 209



Ligand CLA A 831



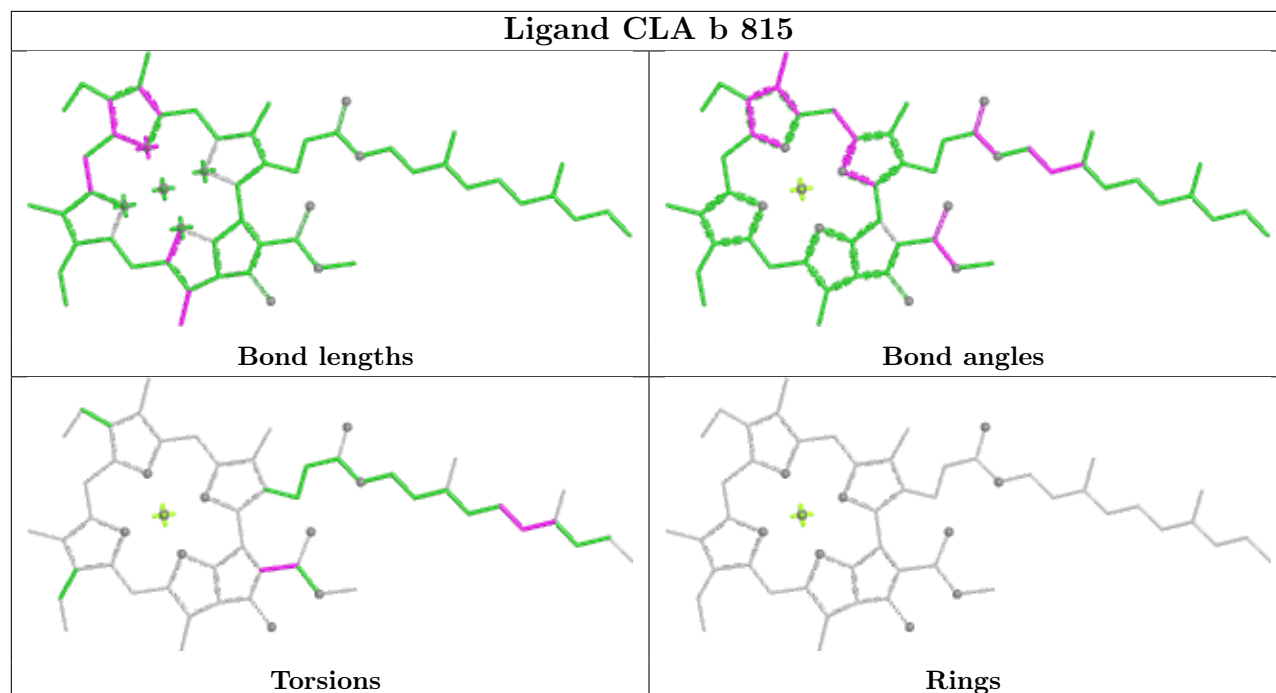
Ligand CLA I 102



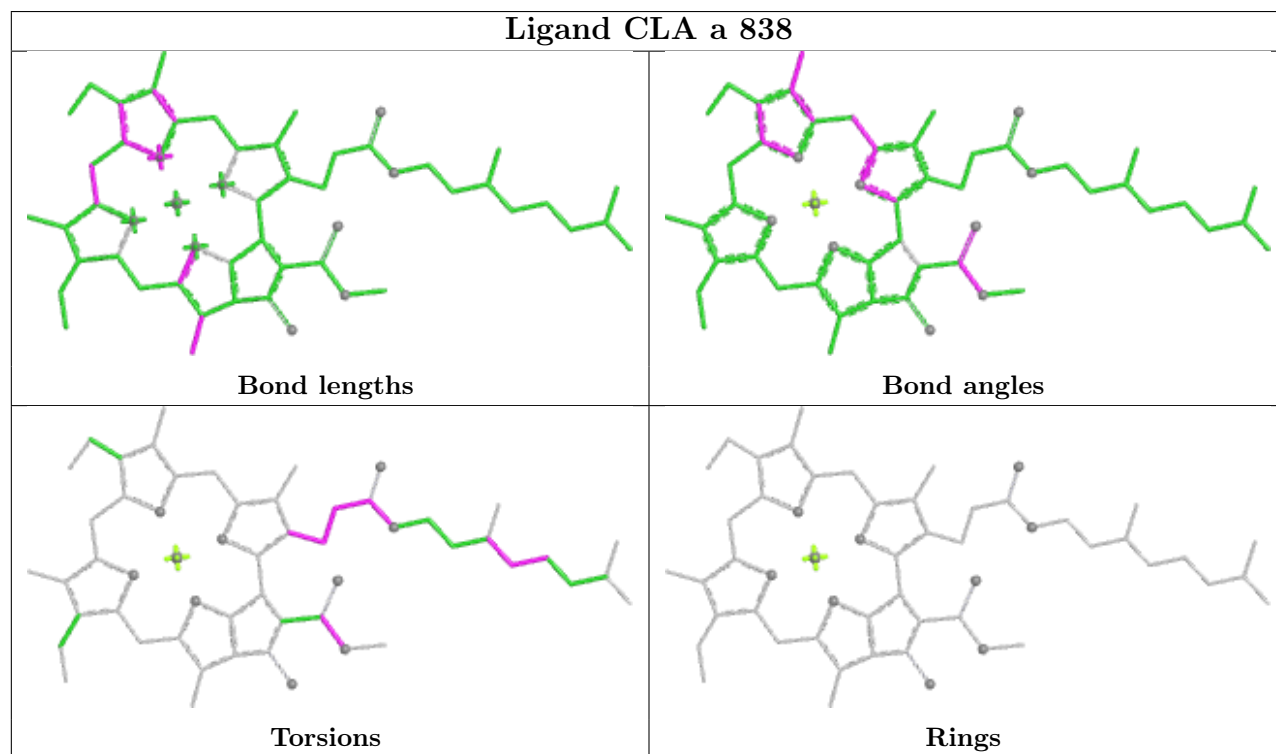
Ligand LMG B 850



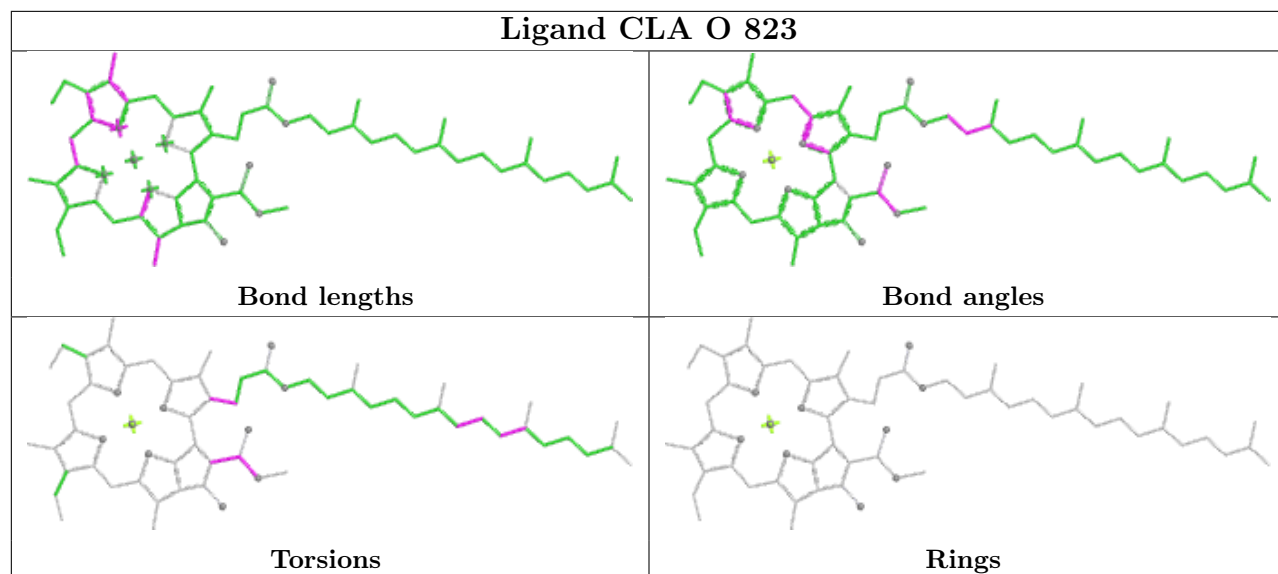
Ligand CLA b 815



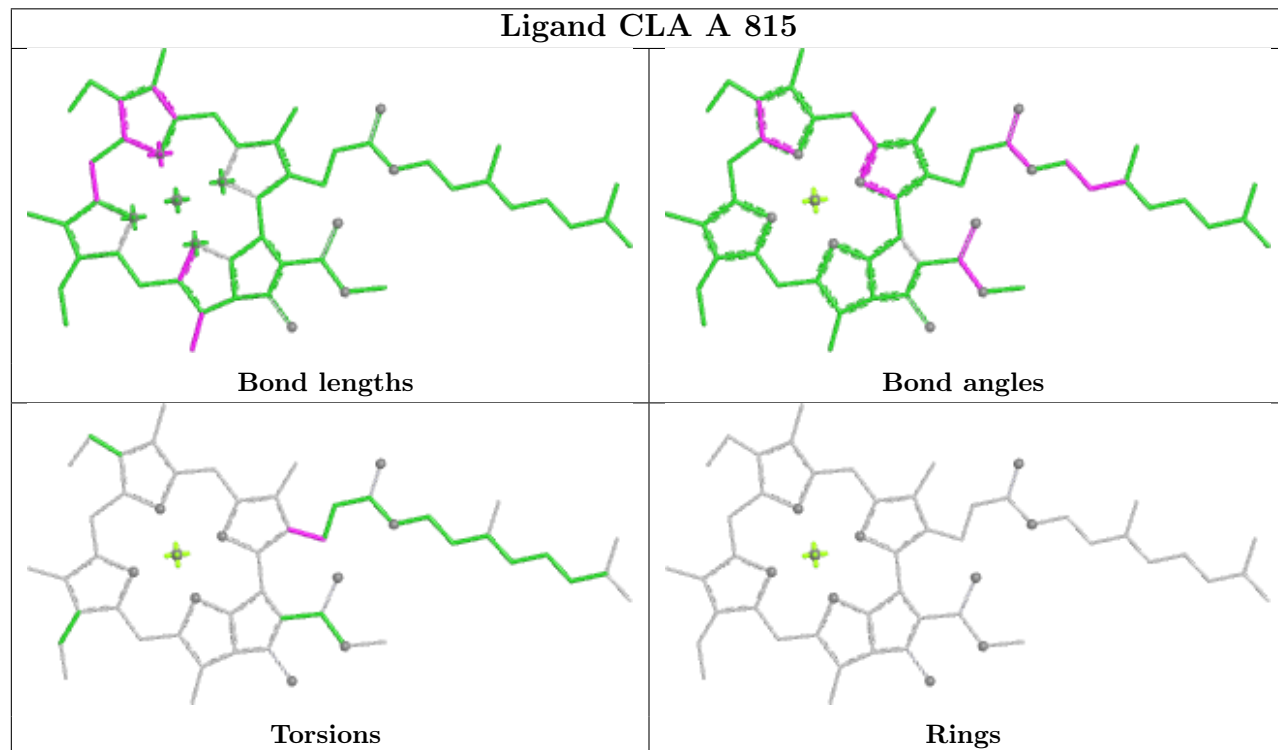
Ligand CLA a 838



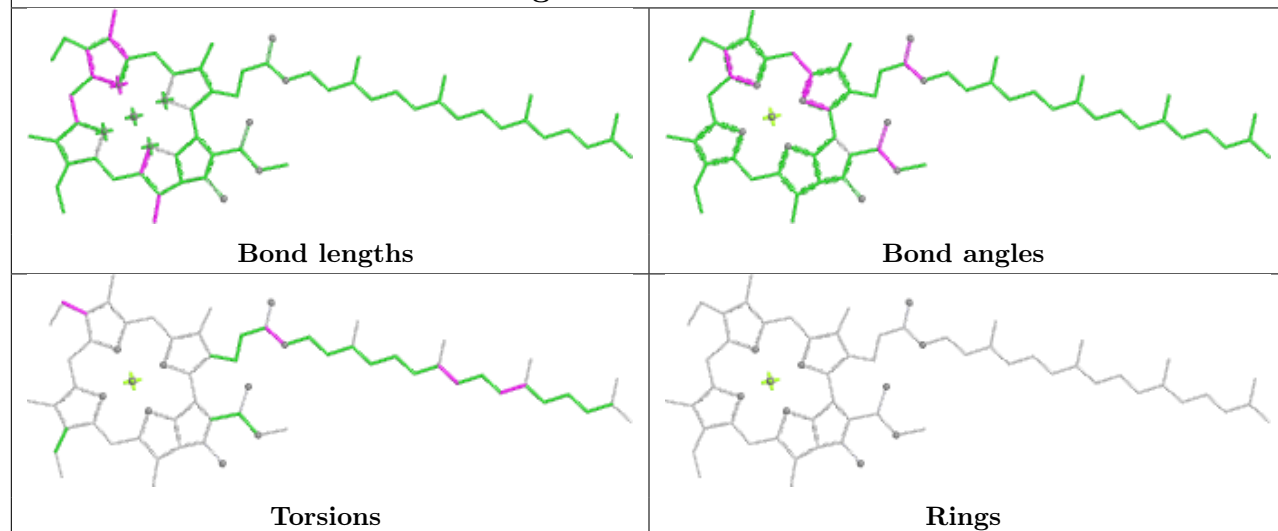
Ligand CLA O 823



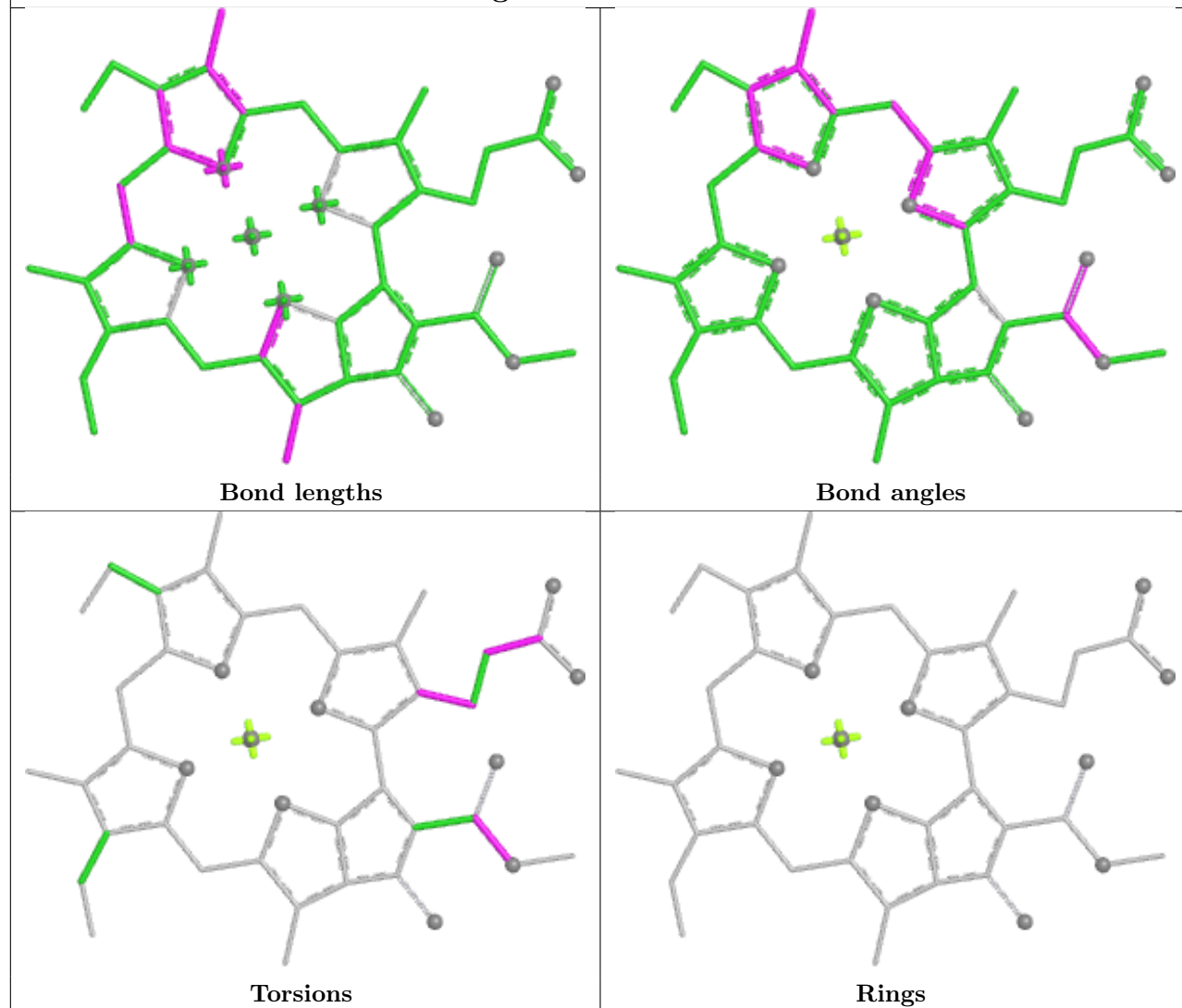
Ligand CLA A 815

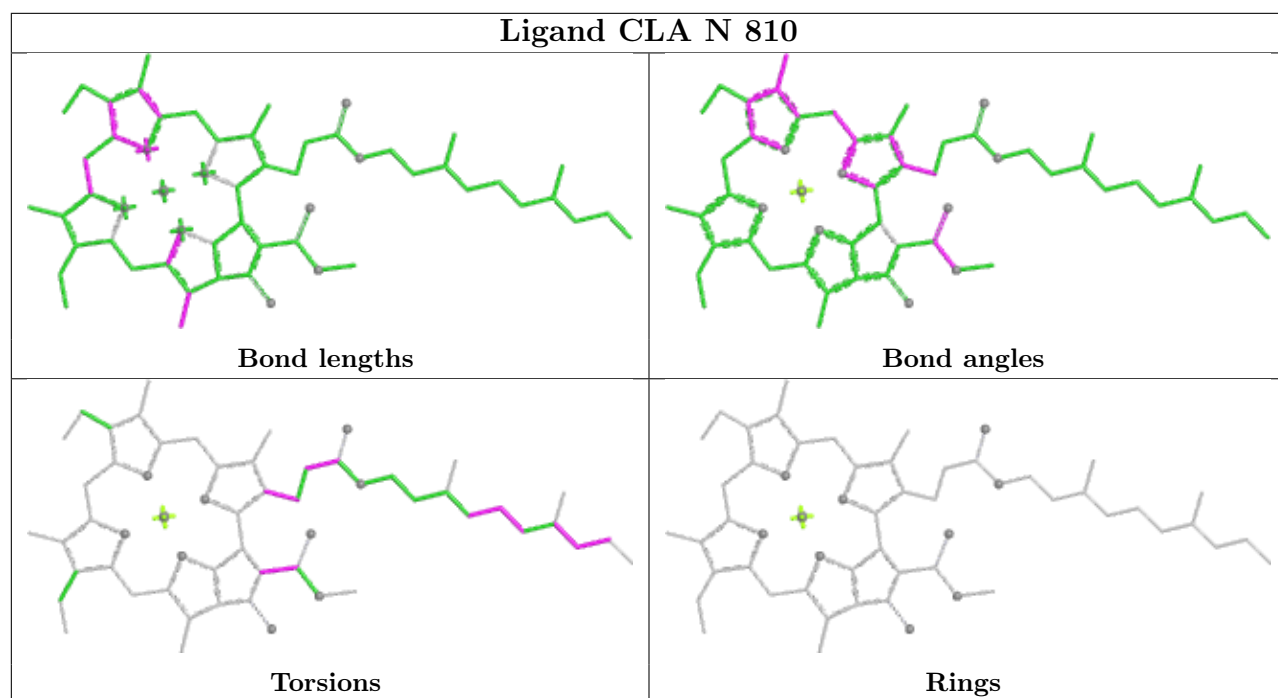
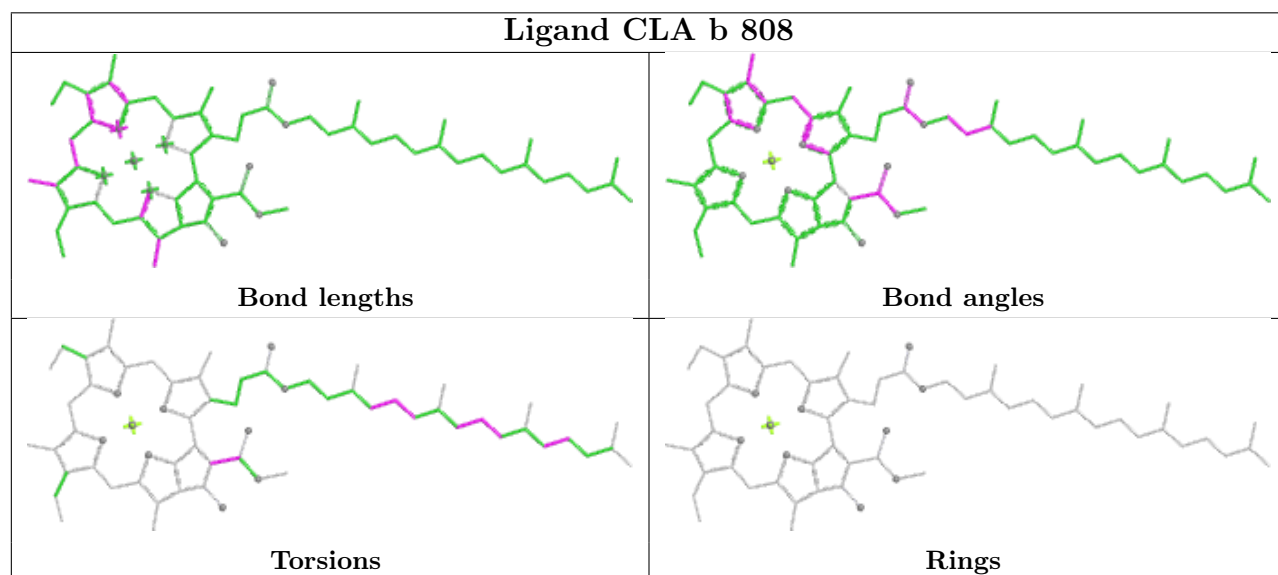
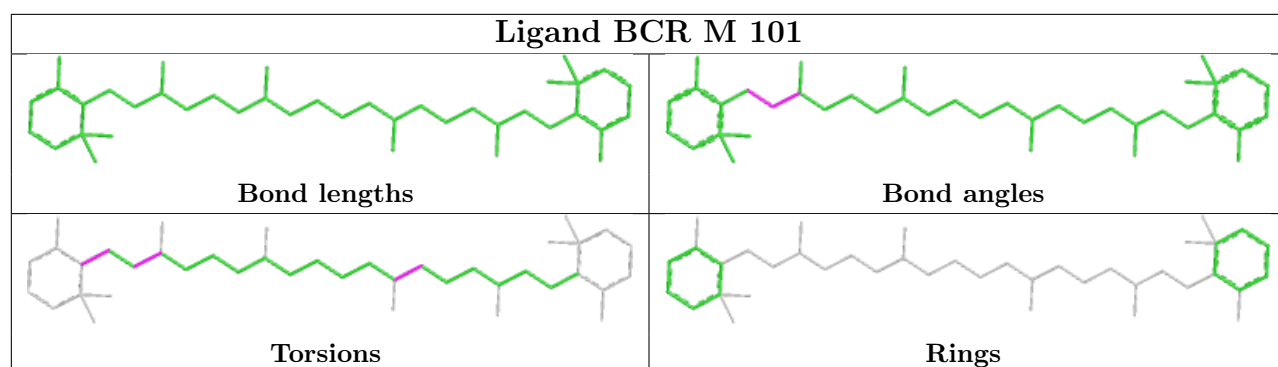


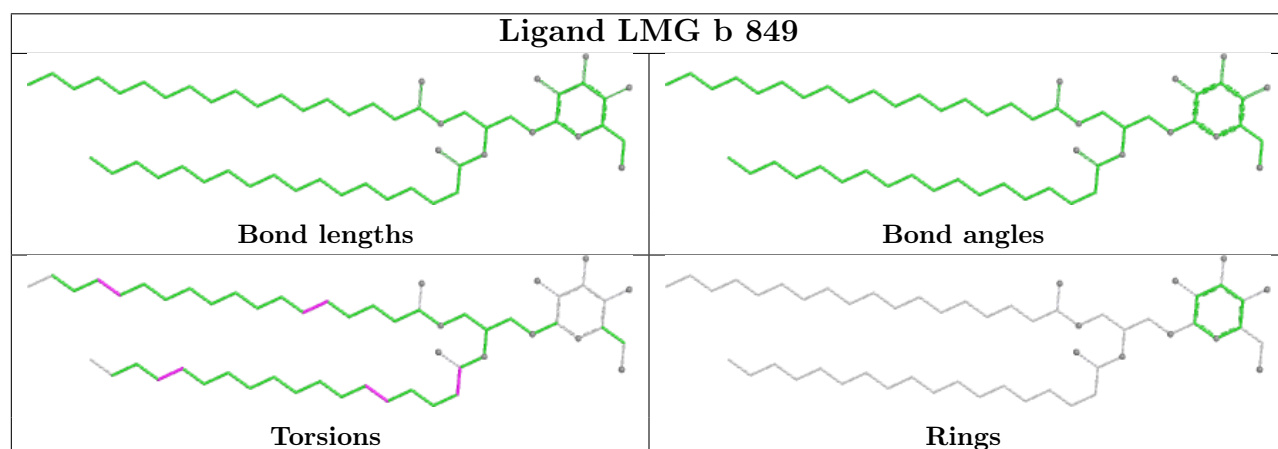
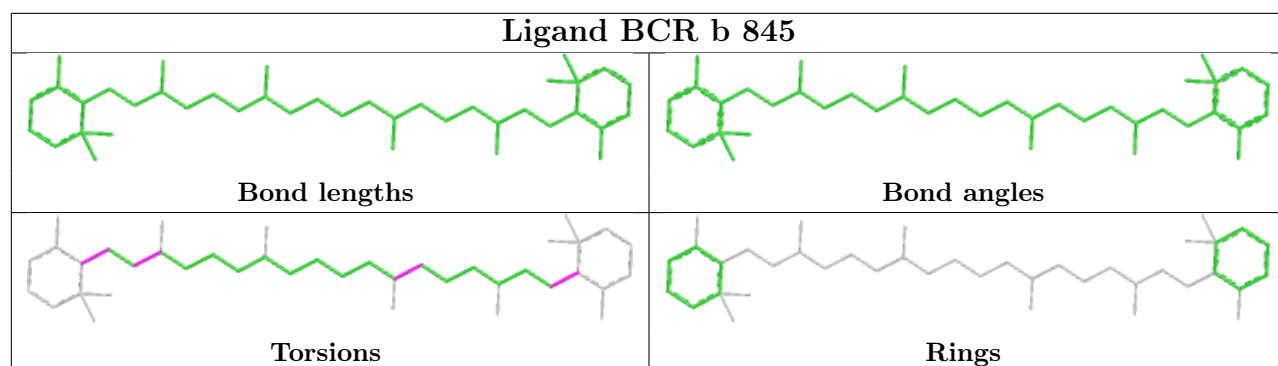
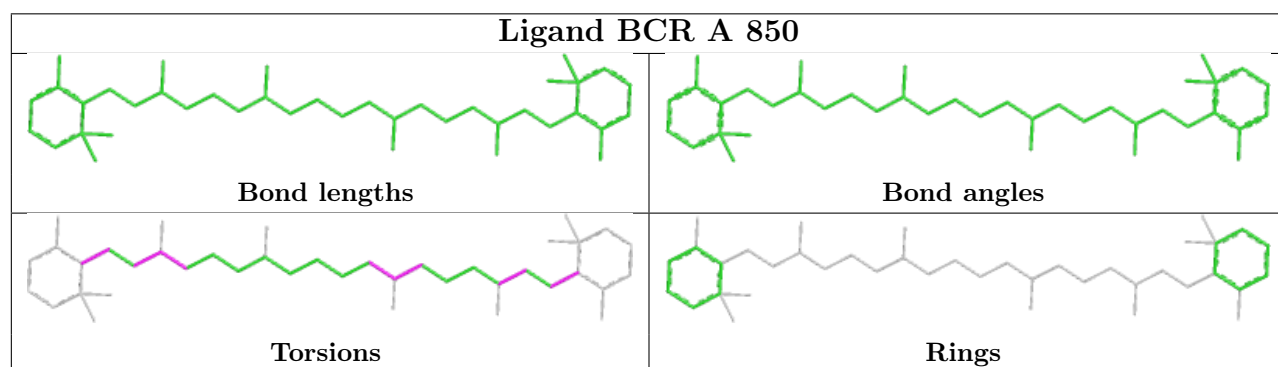
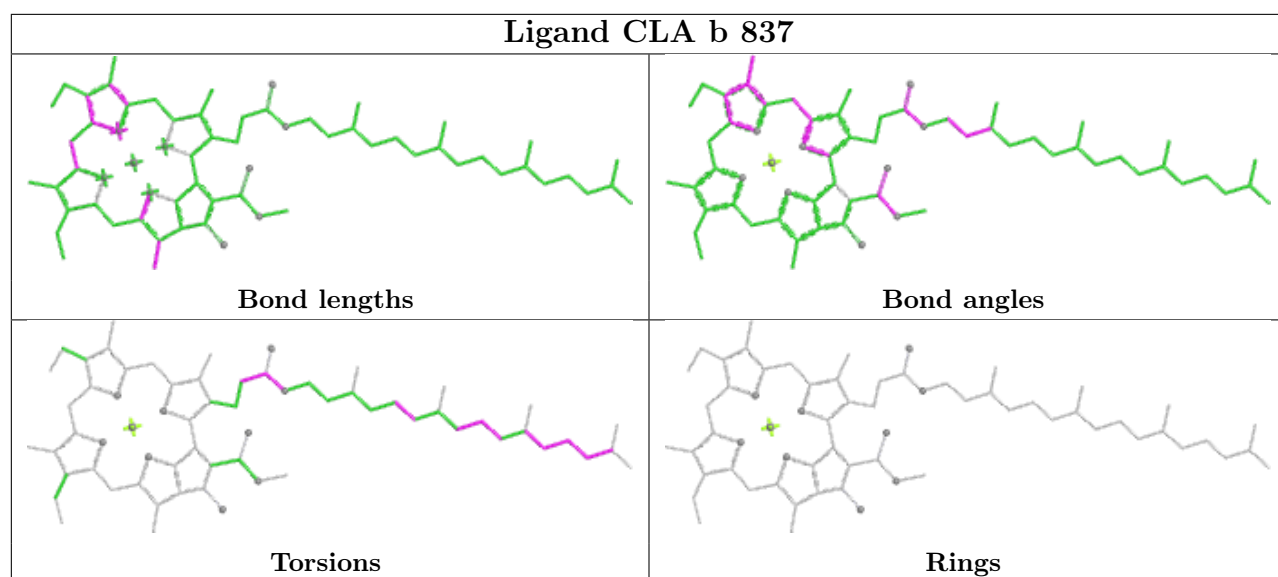
Ligand CLA B 818



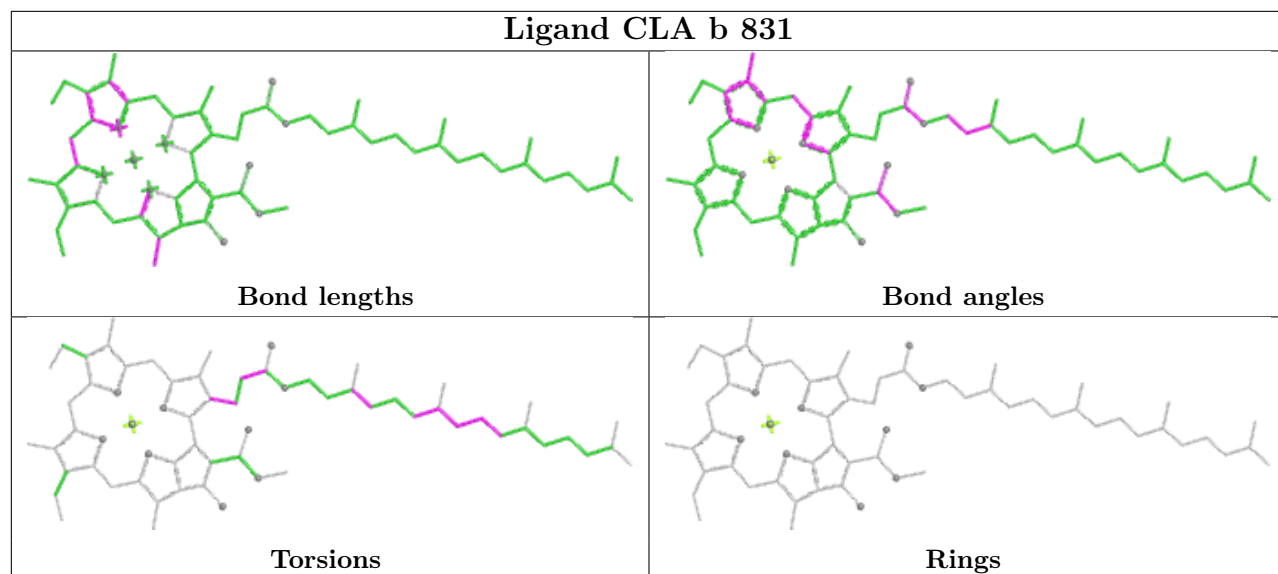
Ligand CLA B 834



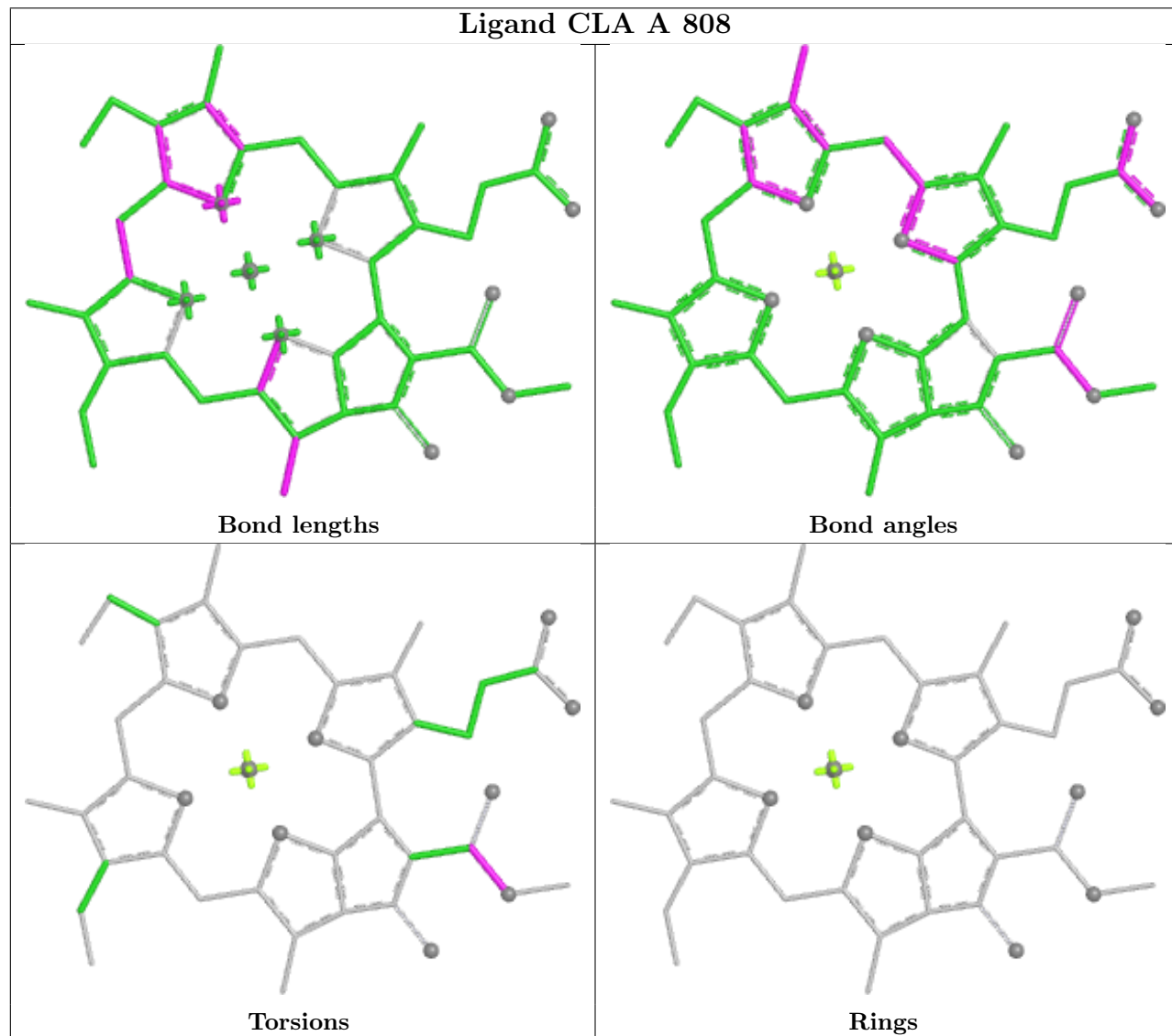


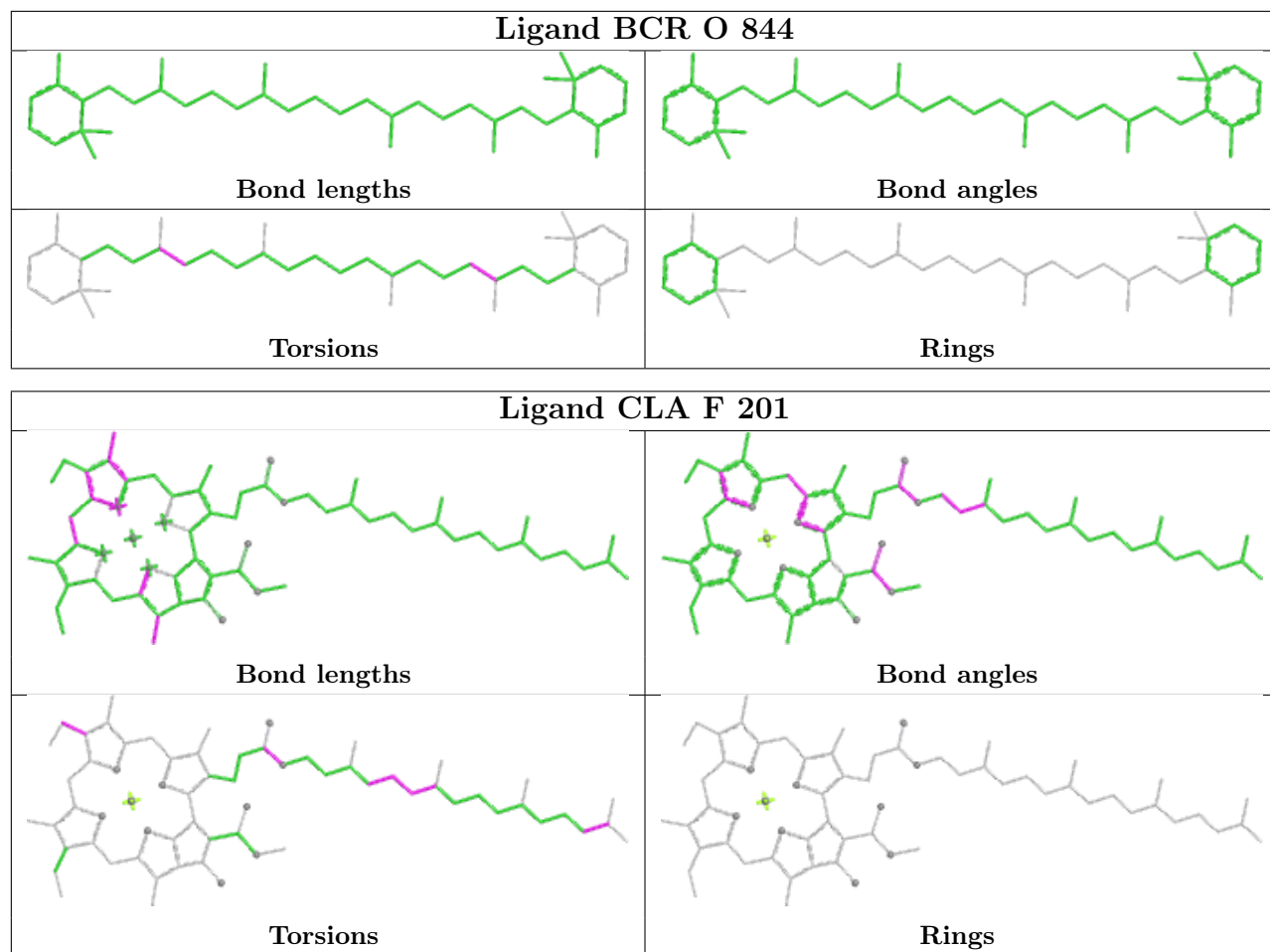


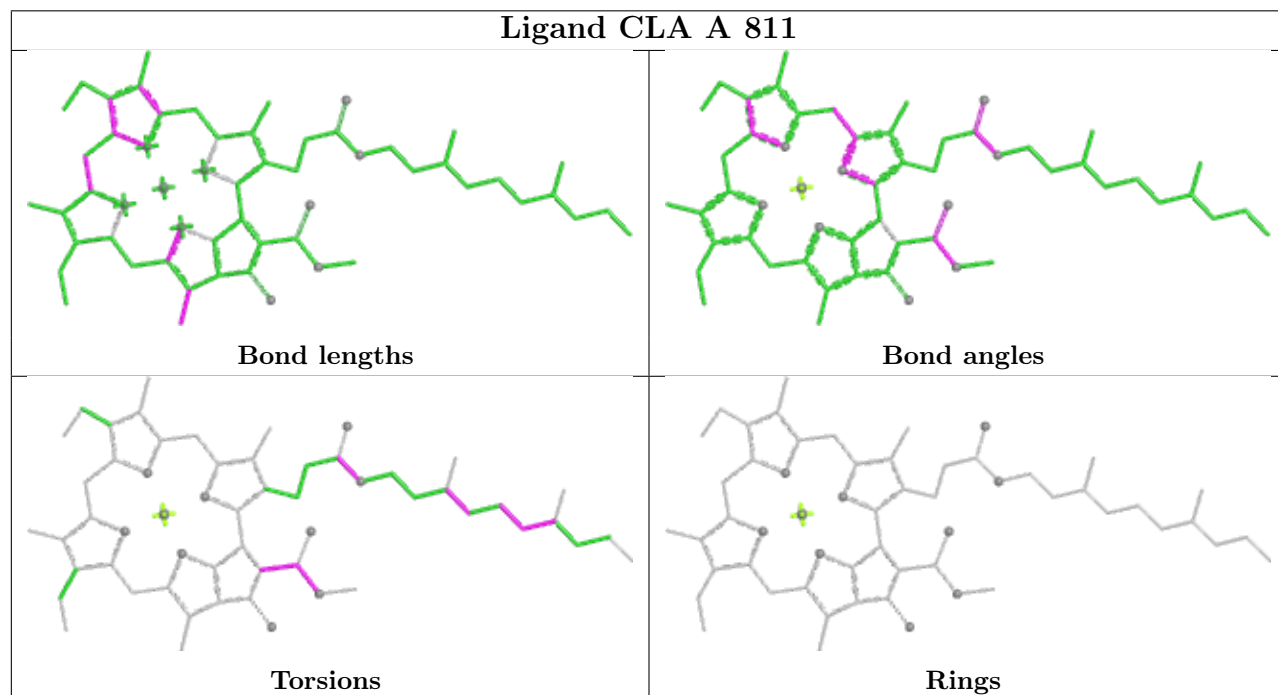
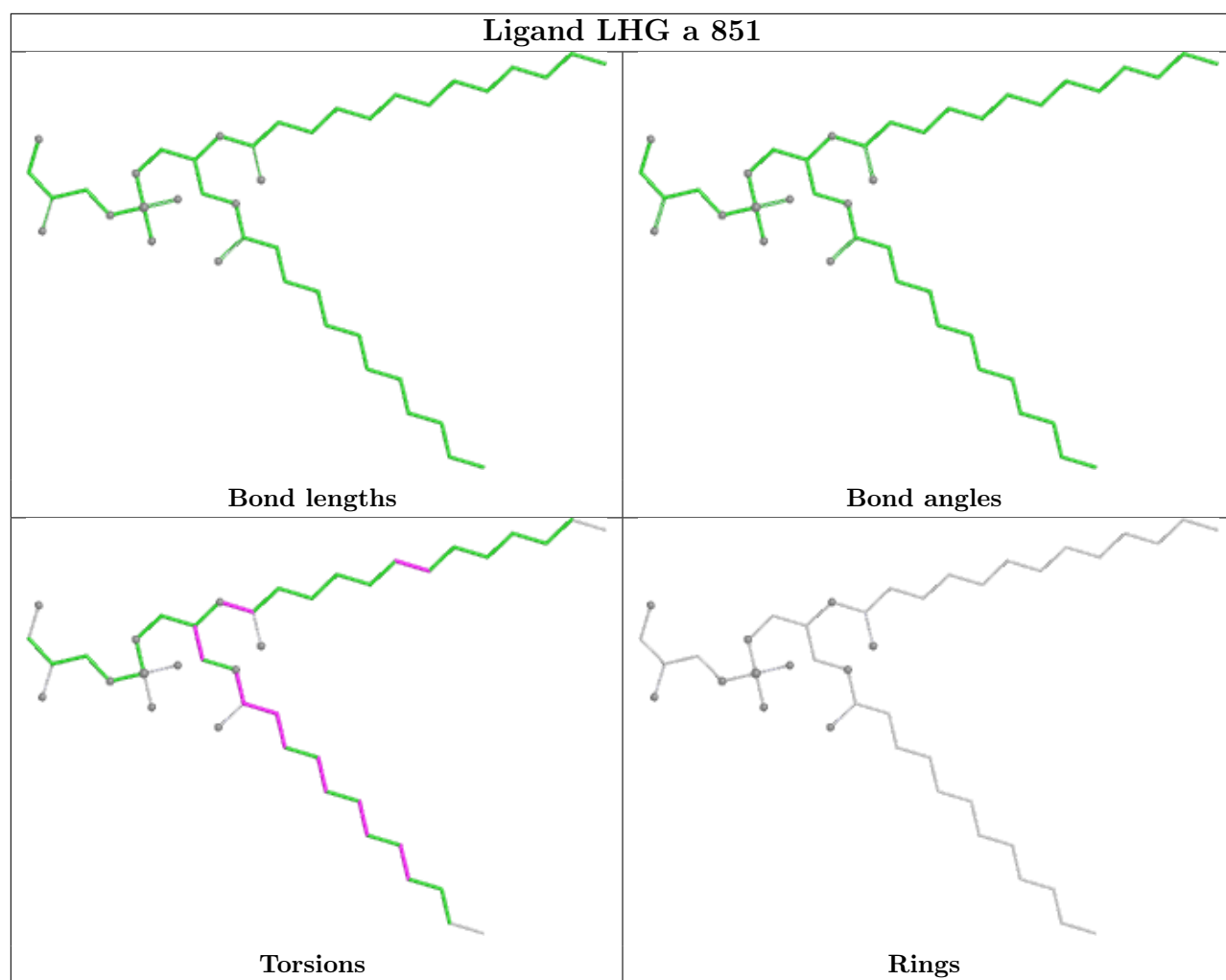
Ligand CLA b 831

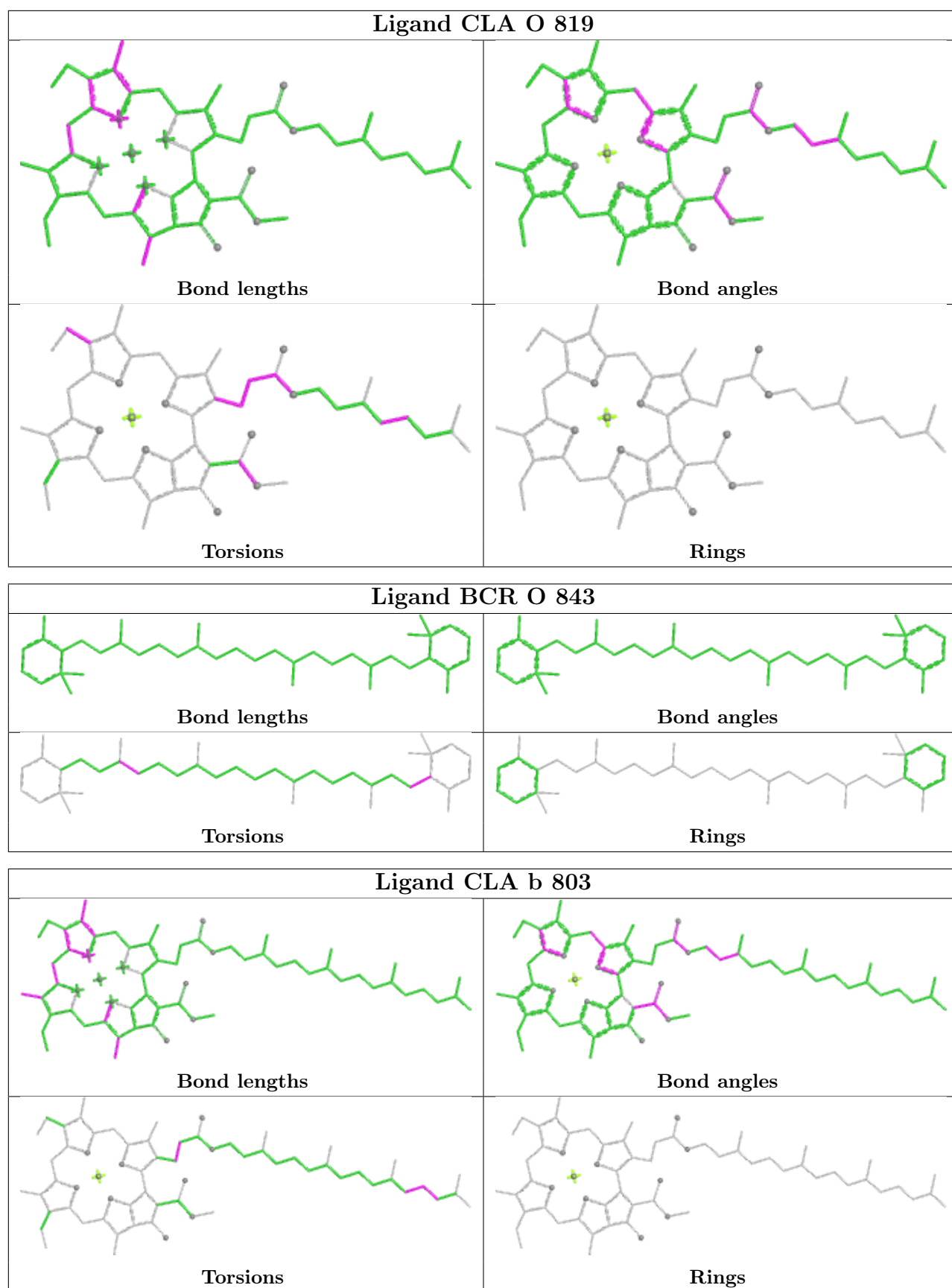


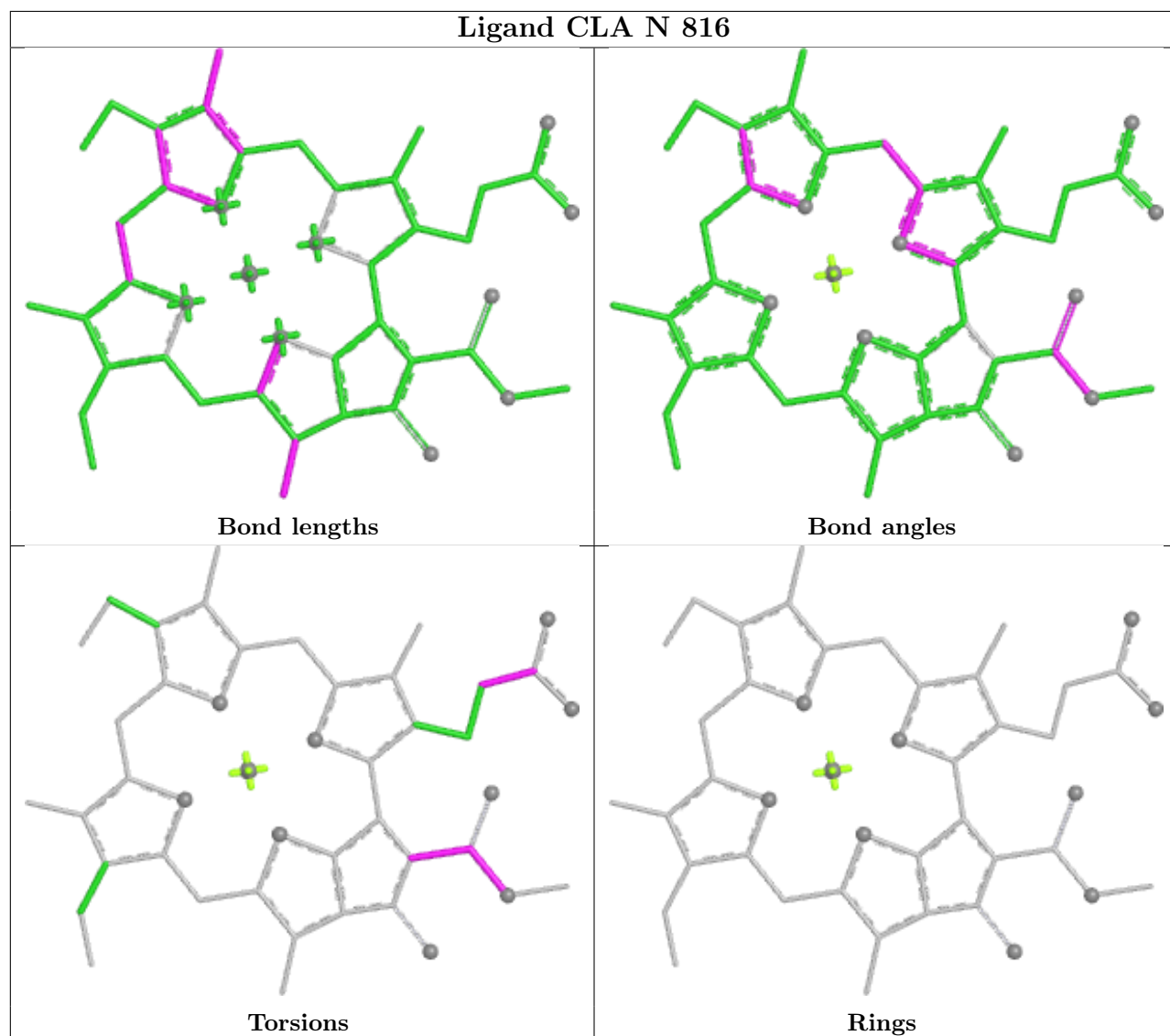
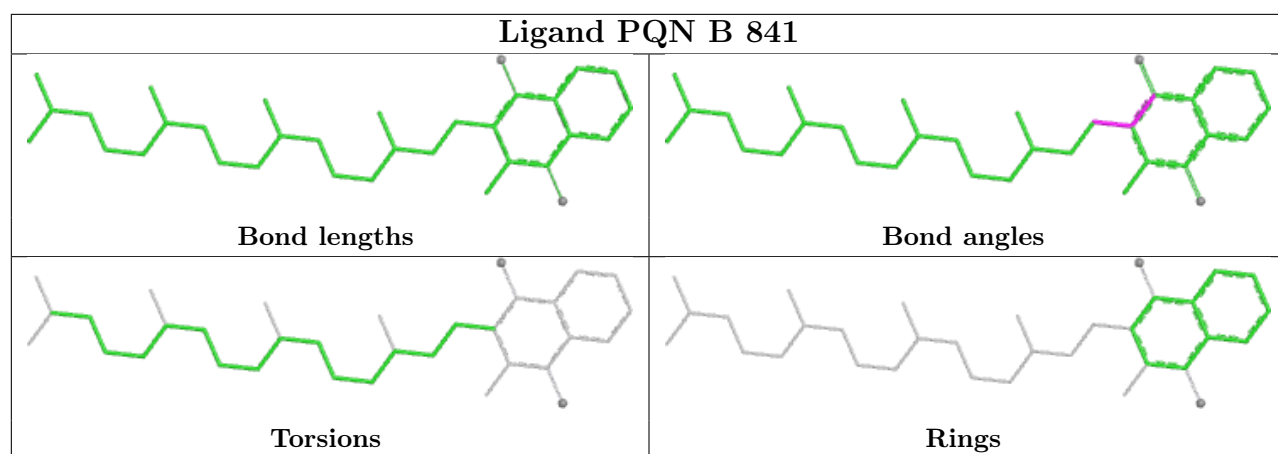
Ligand CLA A 808



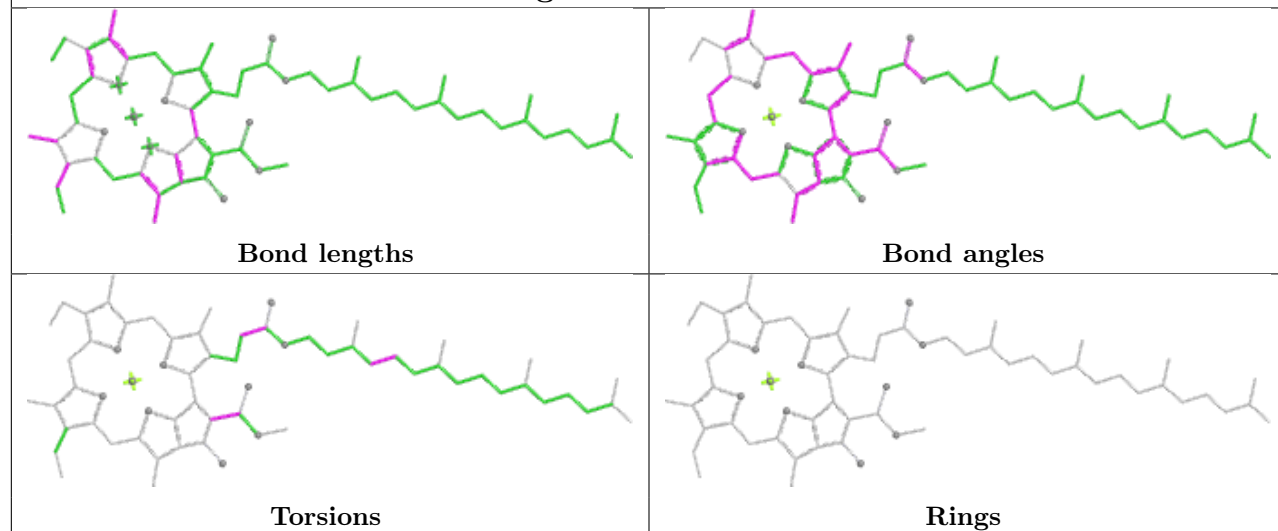




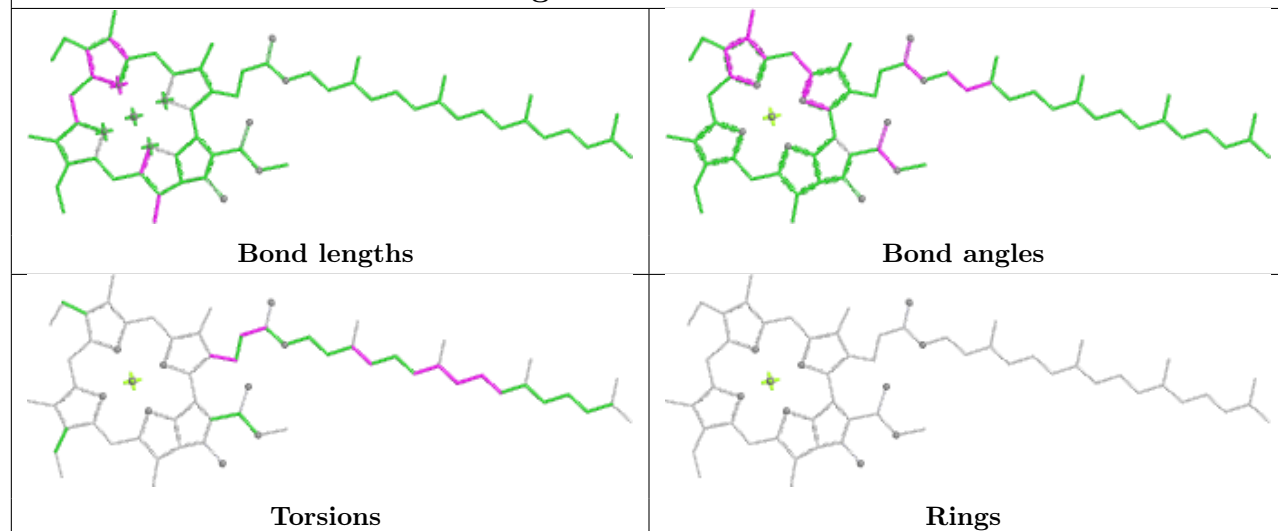




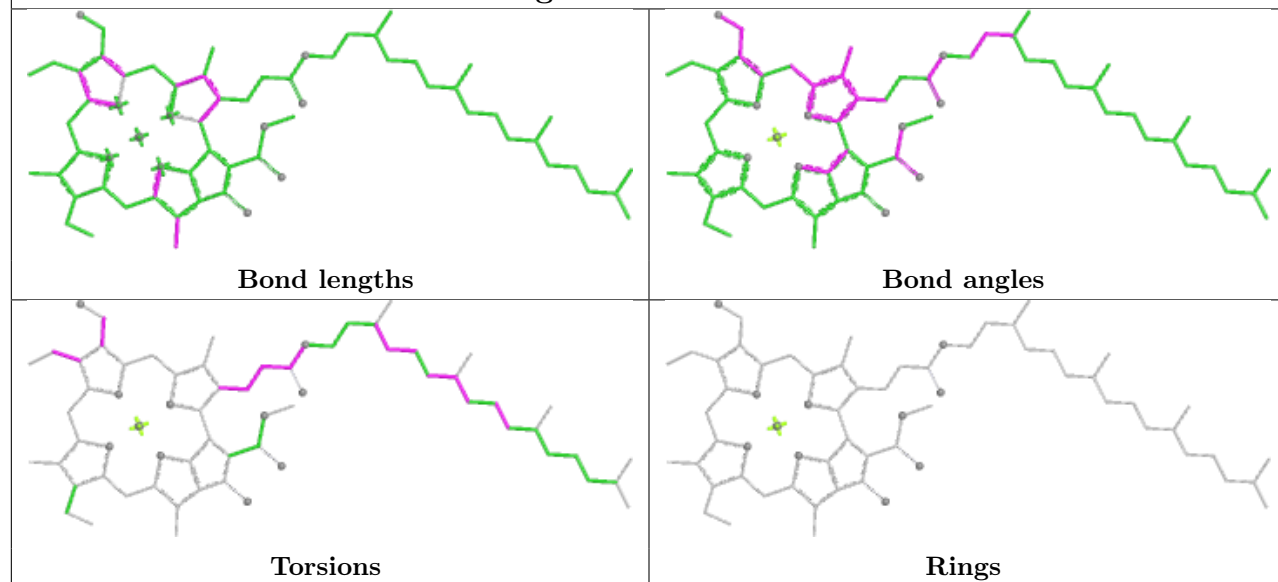
Ligand CL0 A 801



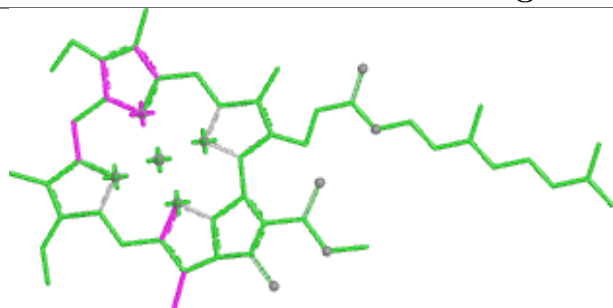
Ligand CLA O 831



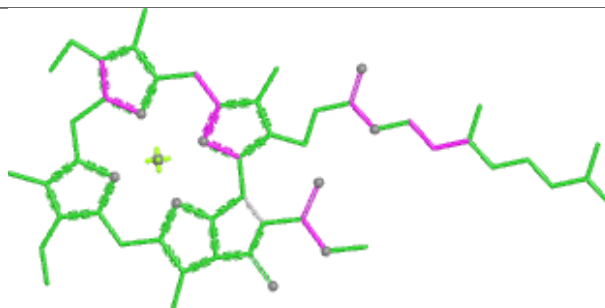
Ligand F6C A 856



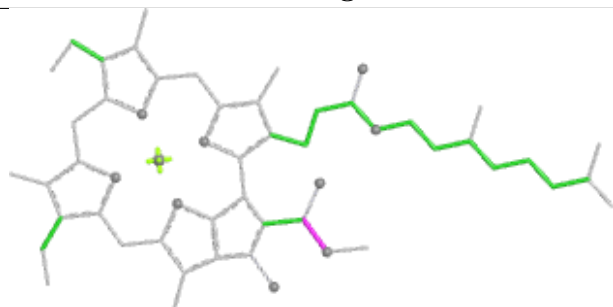
Ligand CLA Z 102



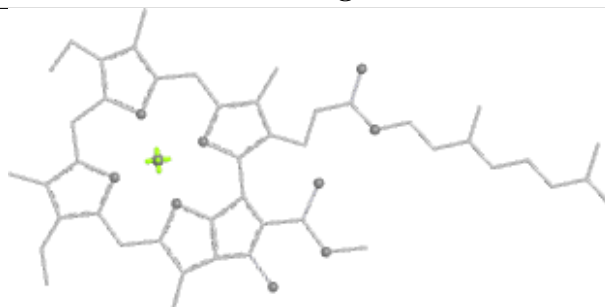
Bond lengths



Bond angles

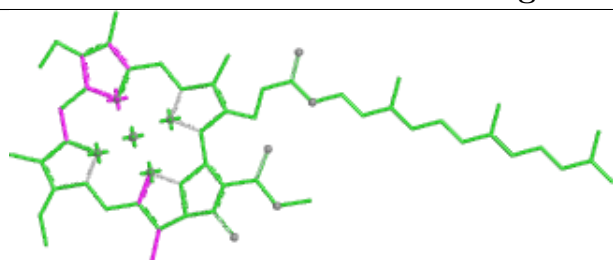


Torsions

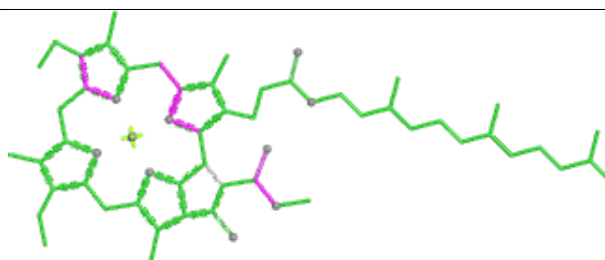


Rings

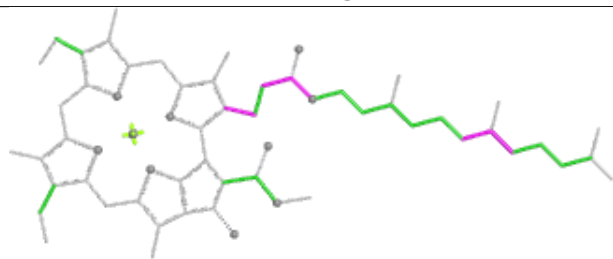
Ligand CLA a 805



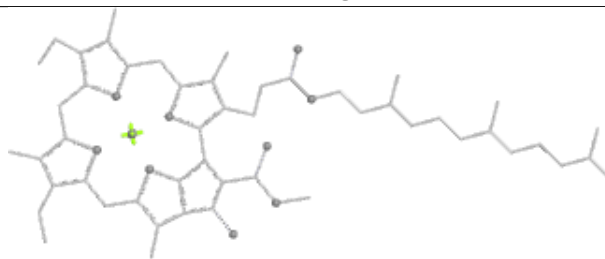
Bond lengths



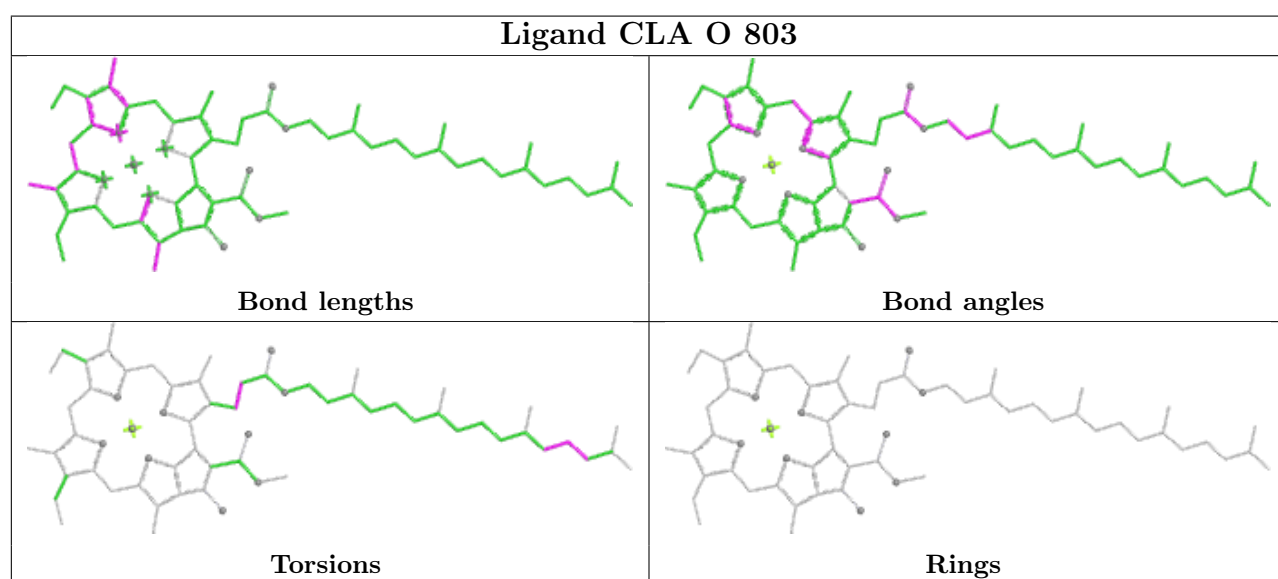
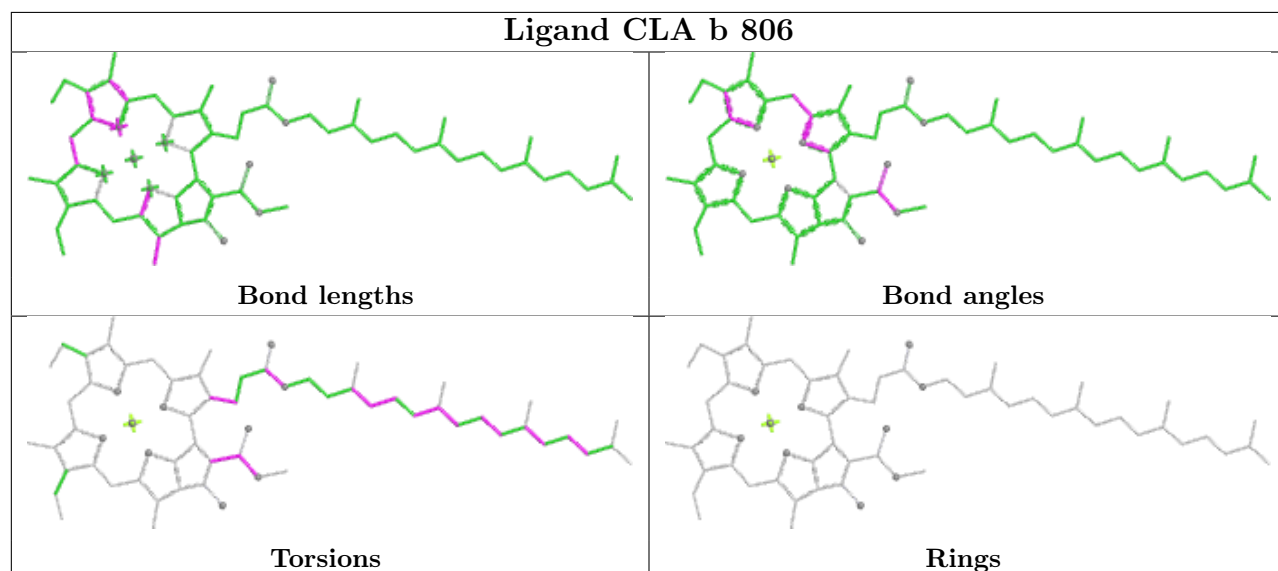
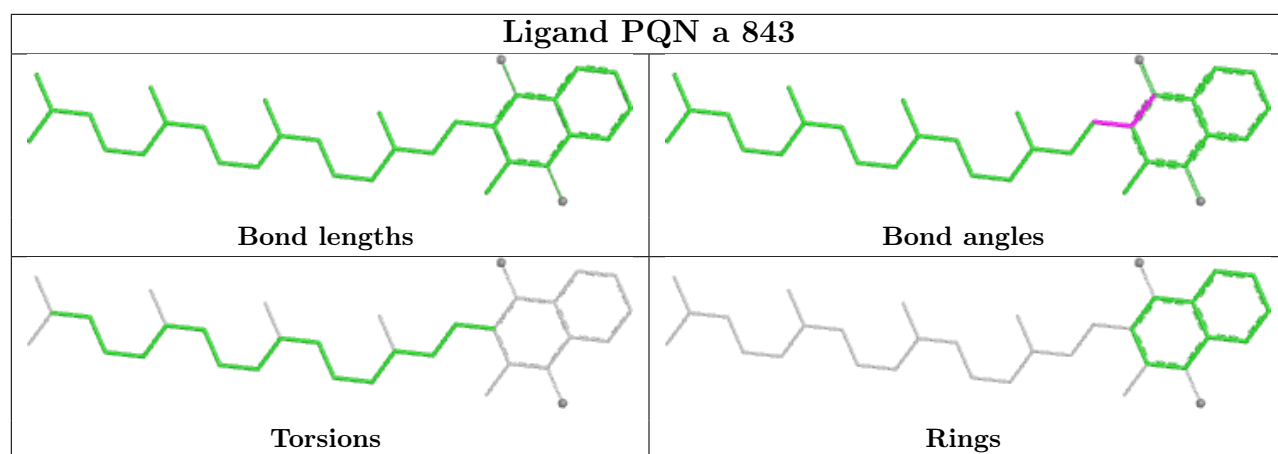
Bond angles

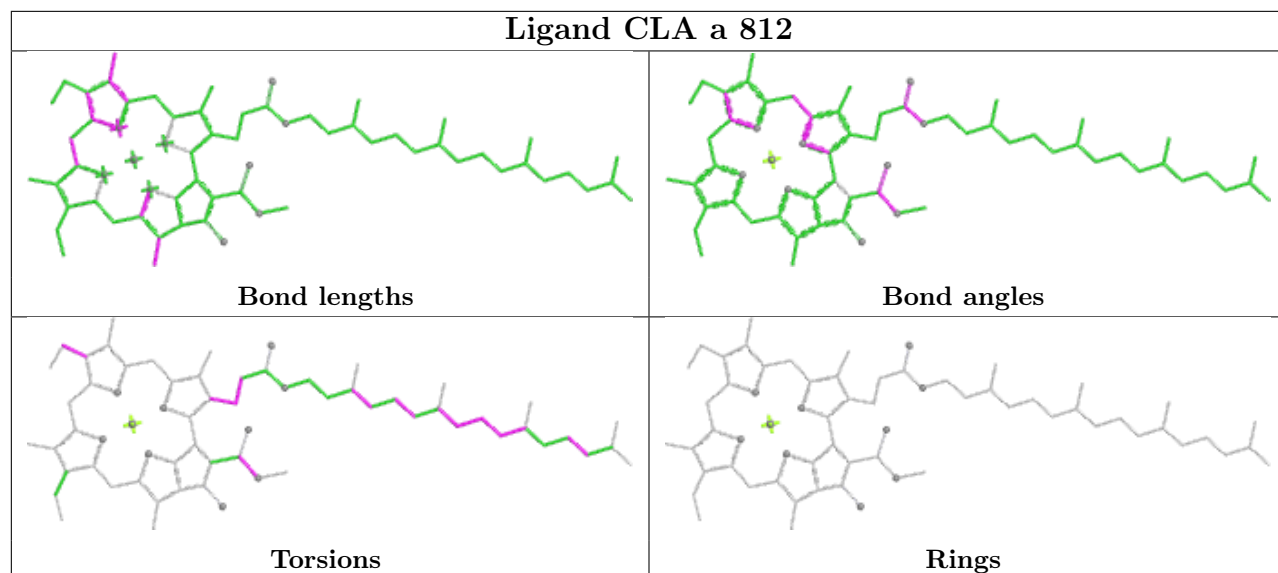
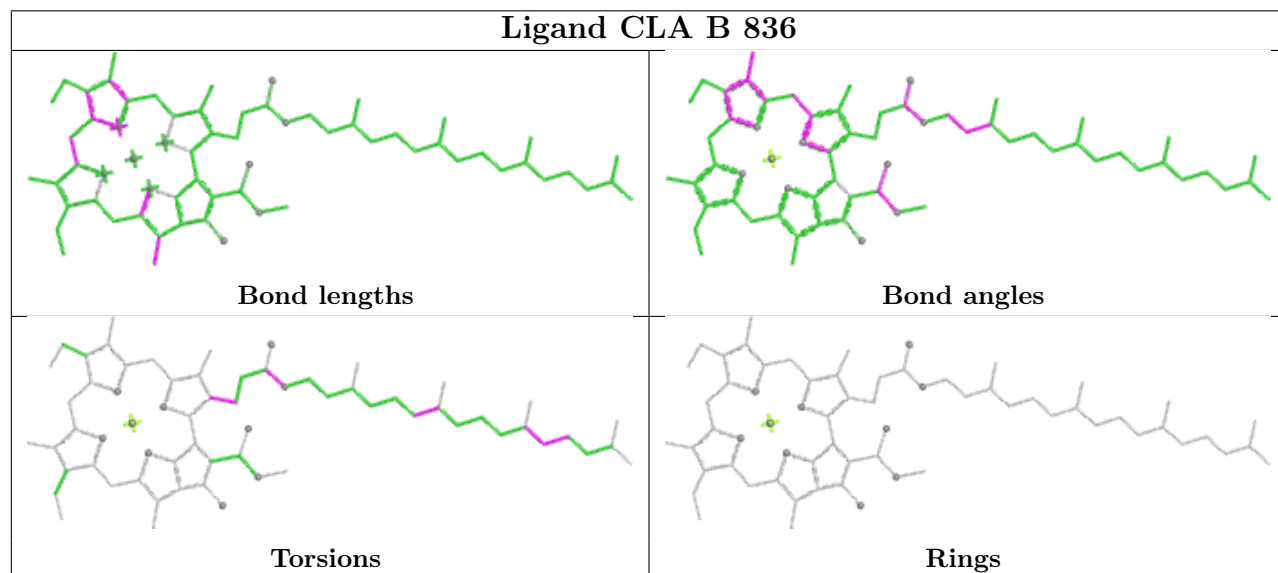
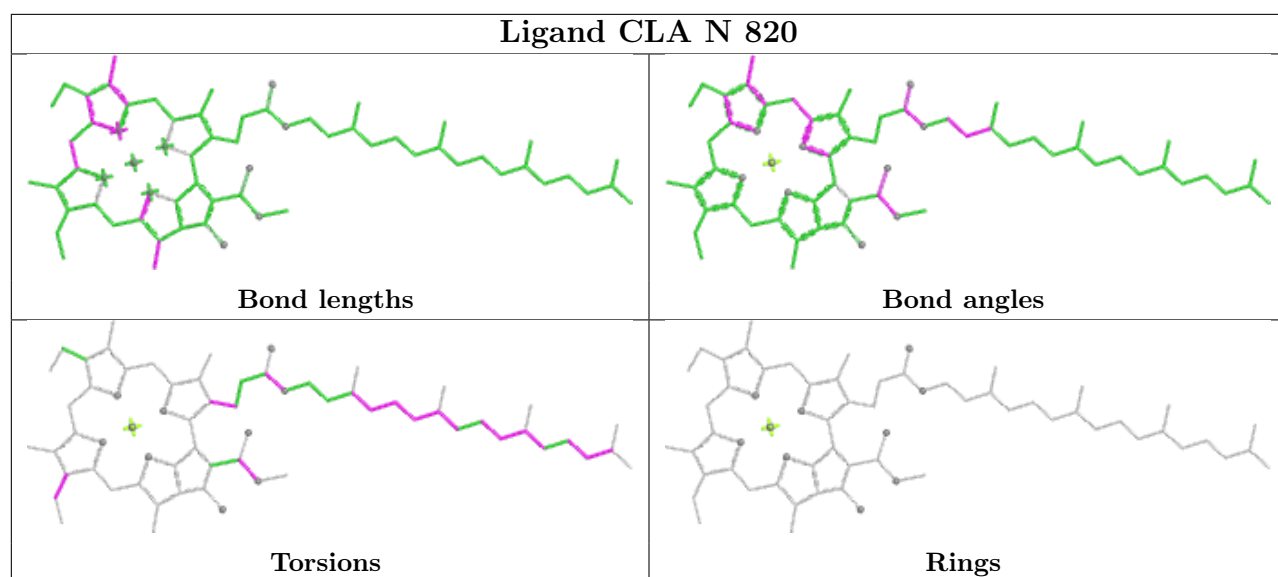


Torsions

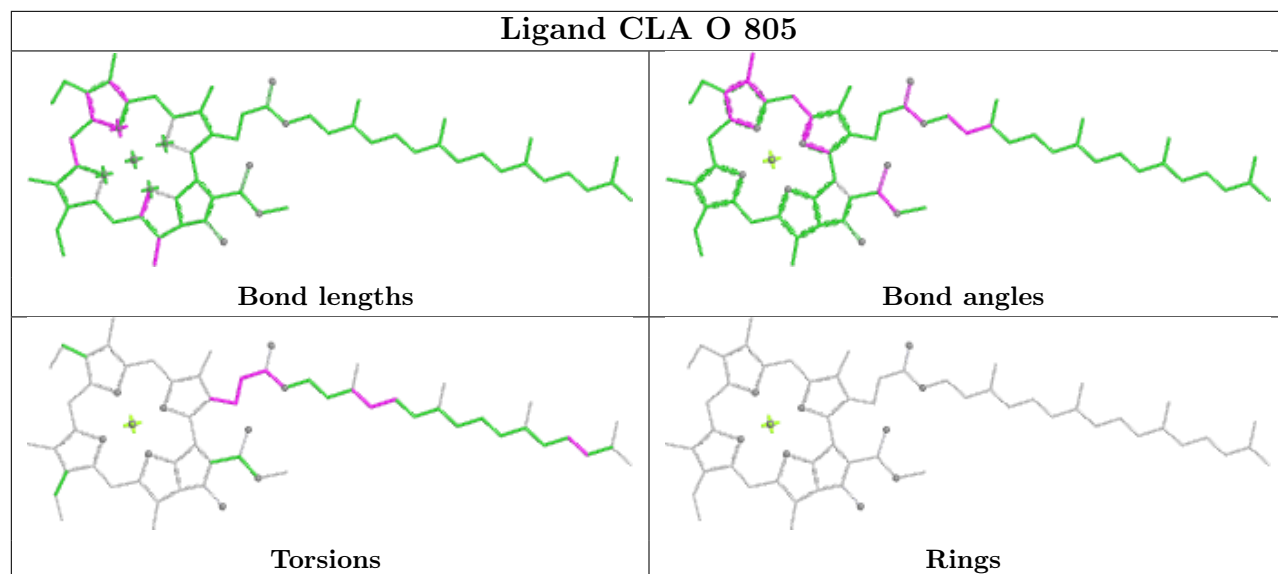


Rings

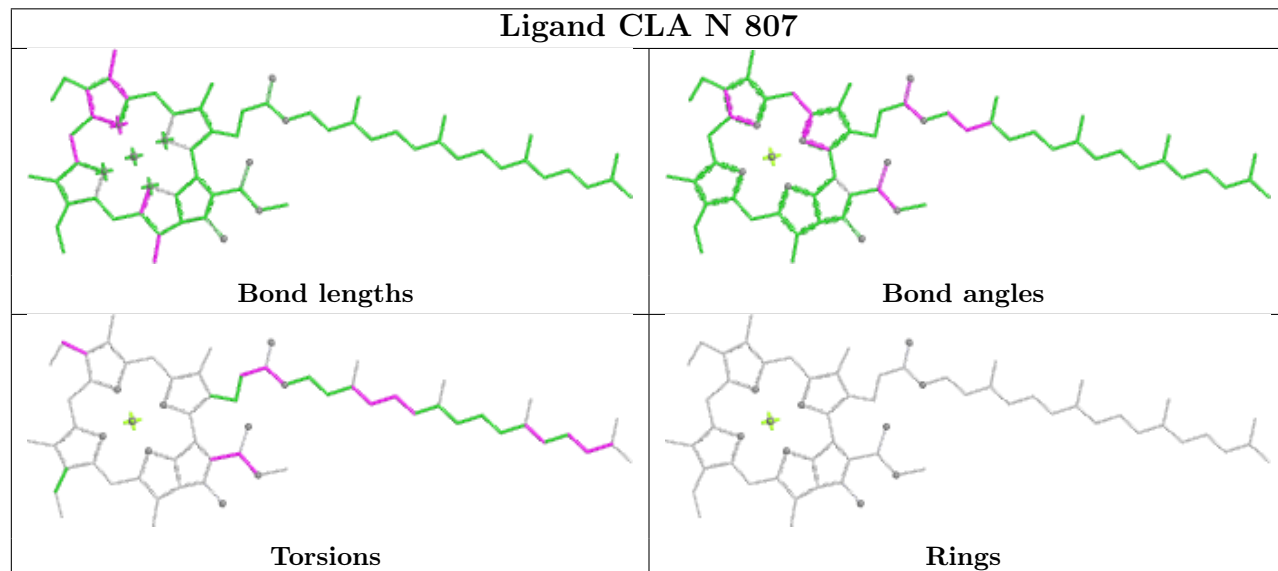




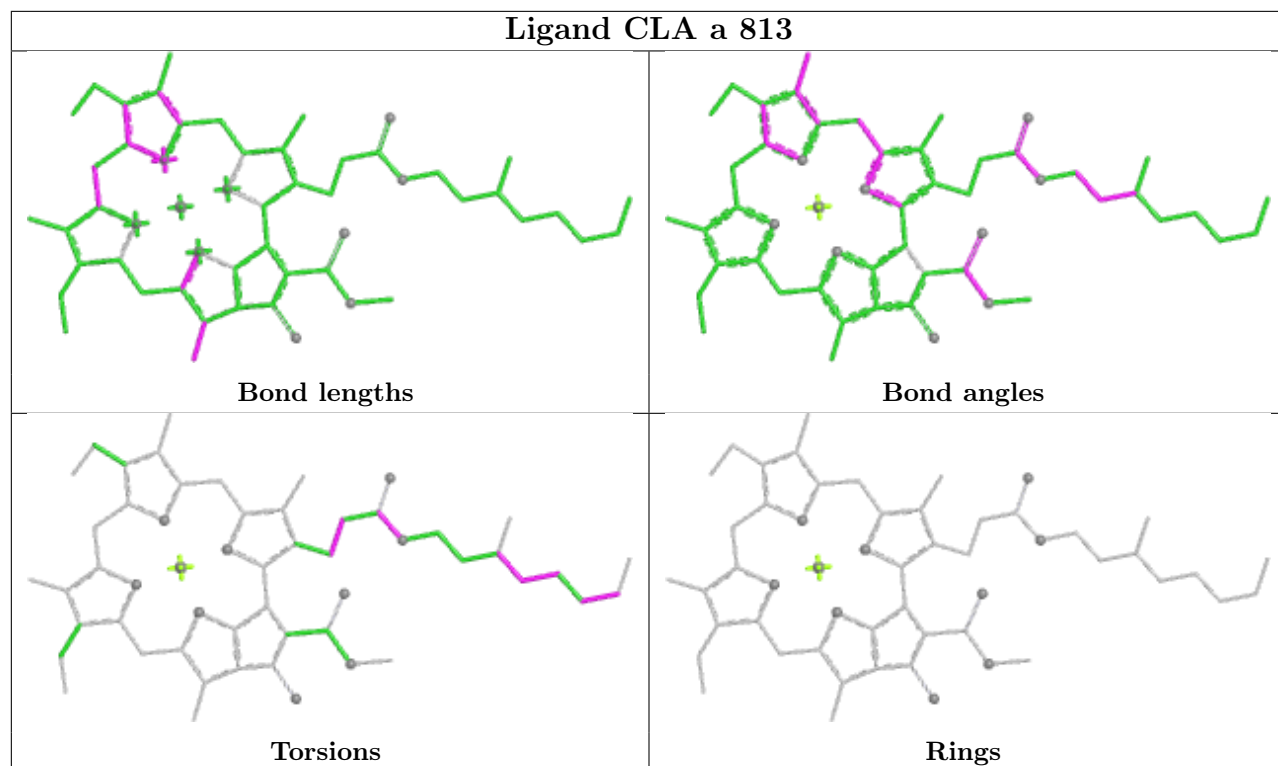
Ligand CLA O 805



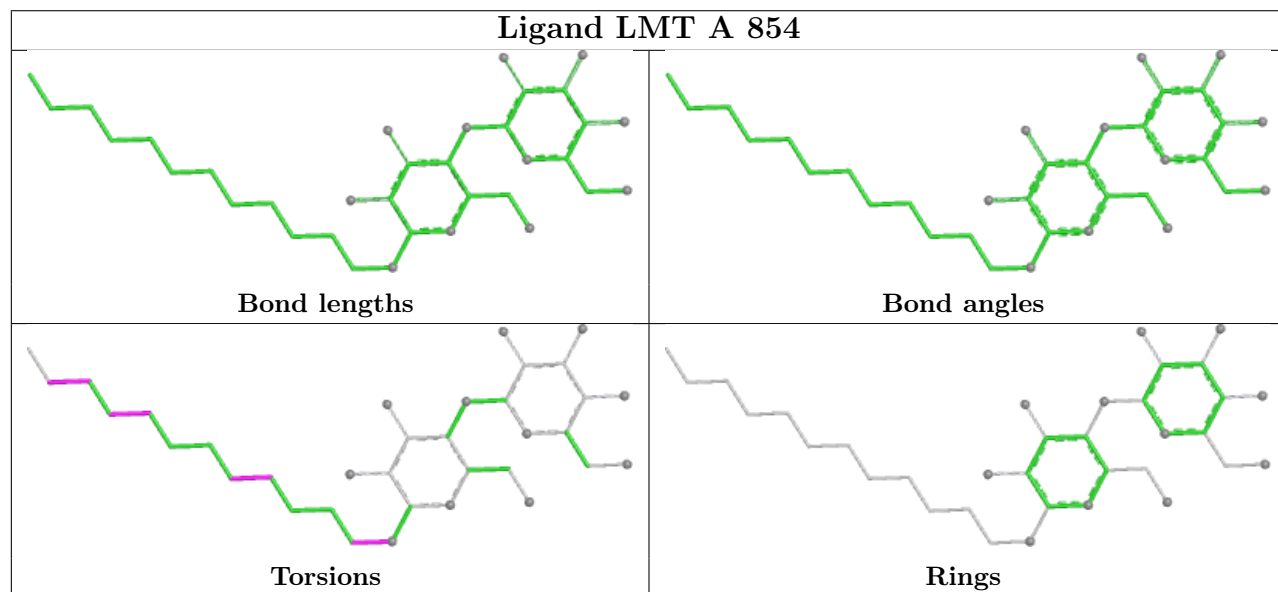
Ligand CLA N 807



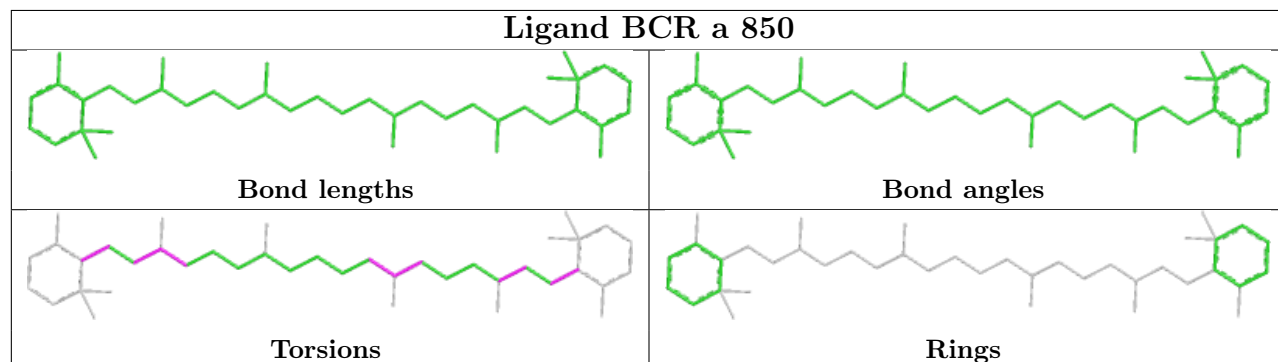
Ligand CLA a 813

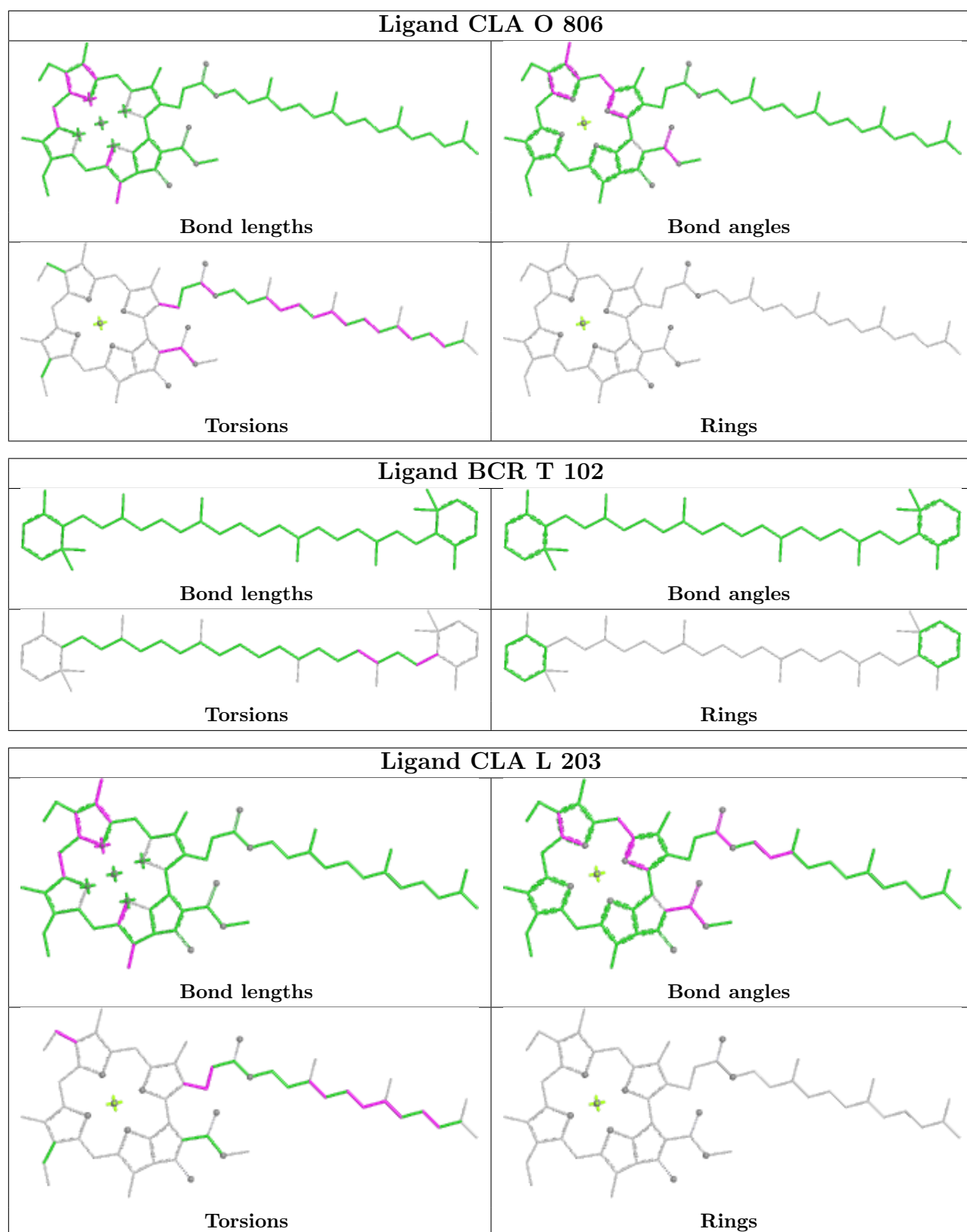


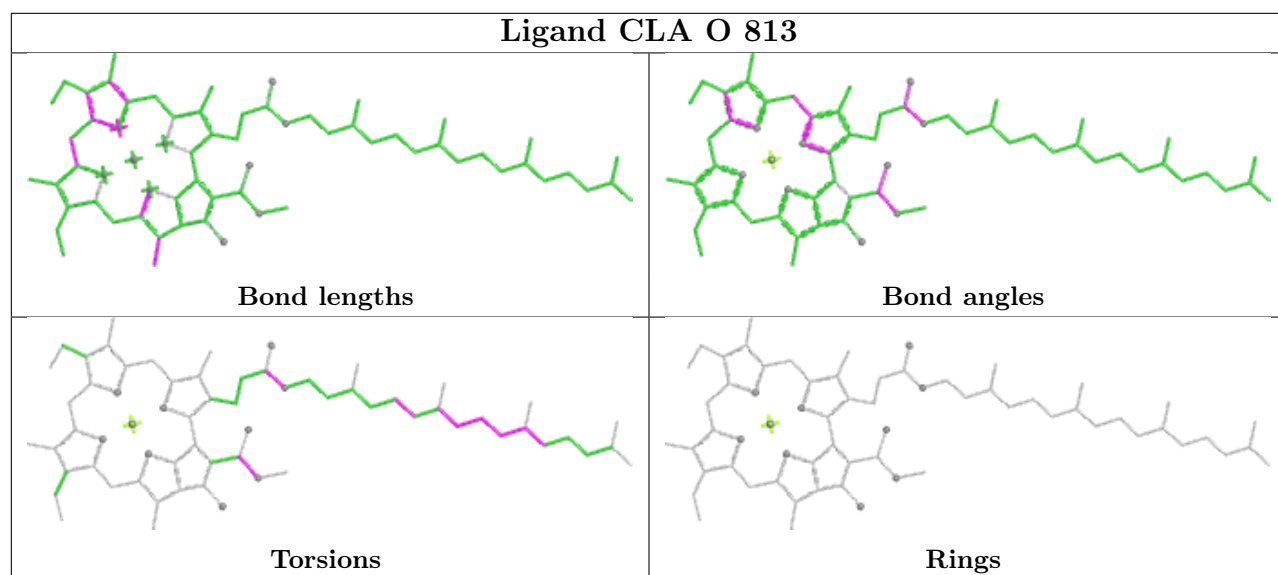
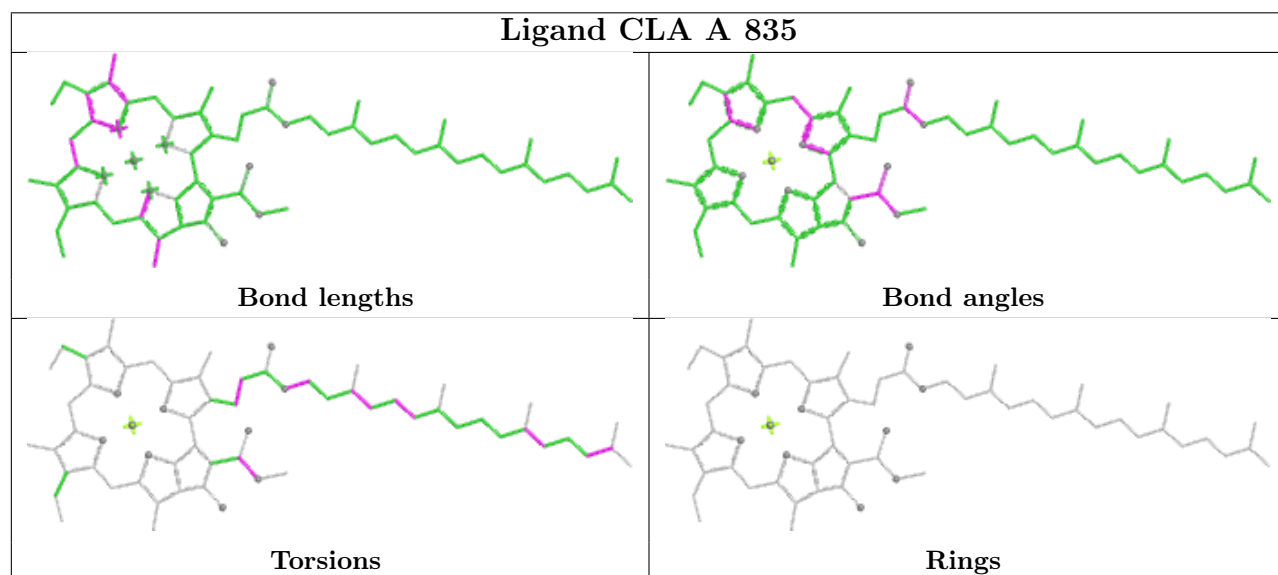
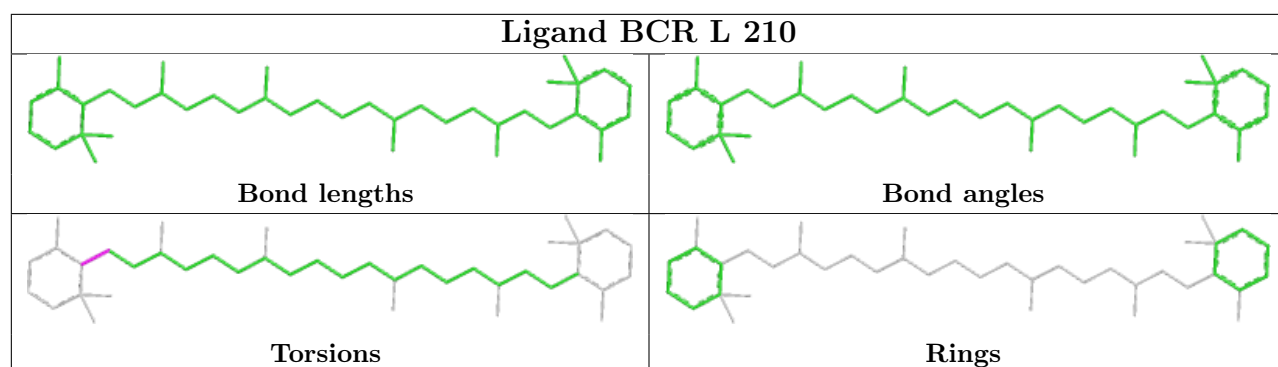
Ligand LMT A 854

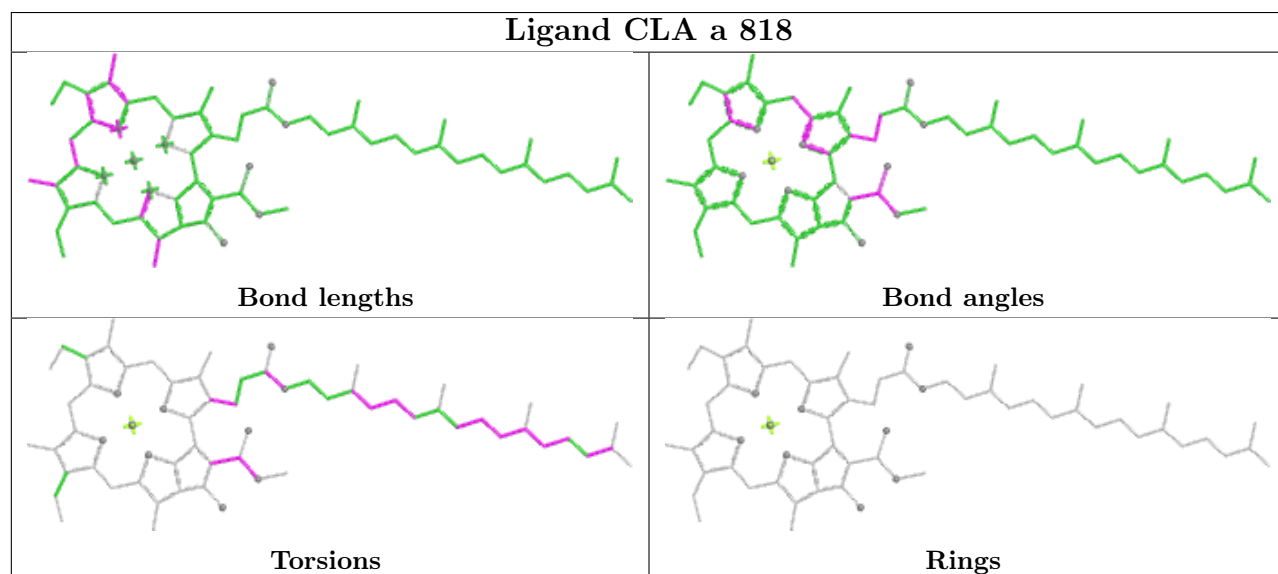
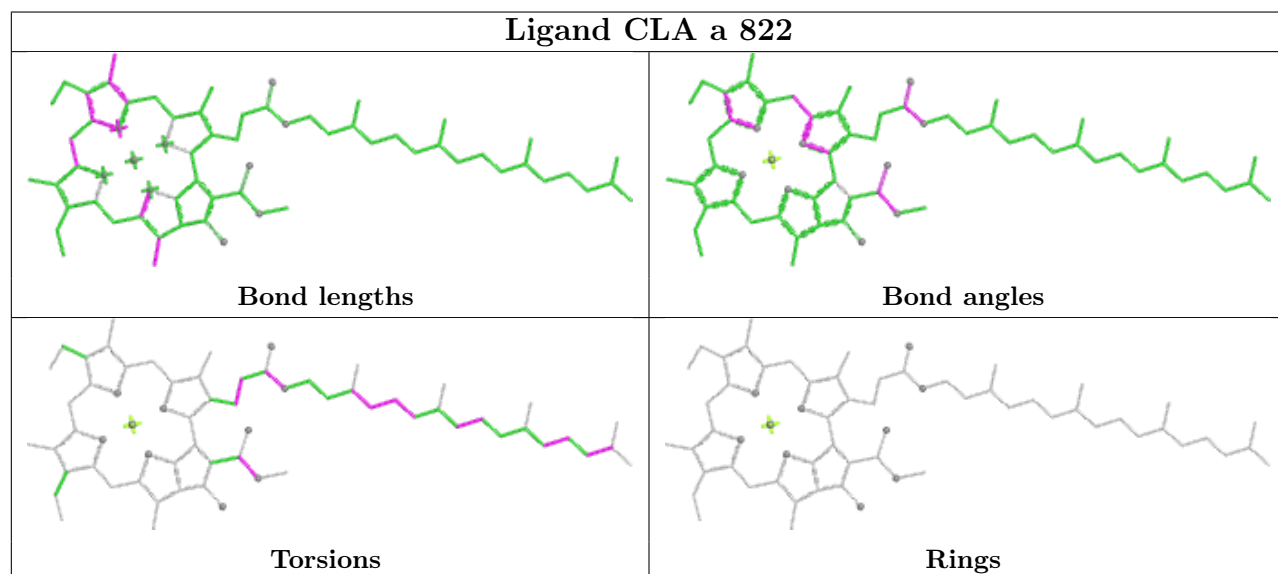
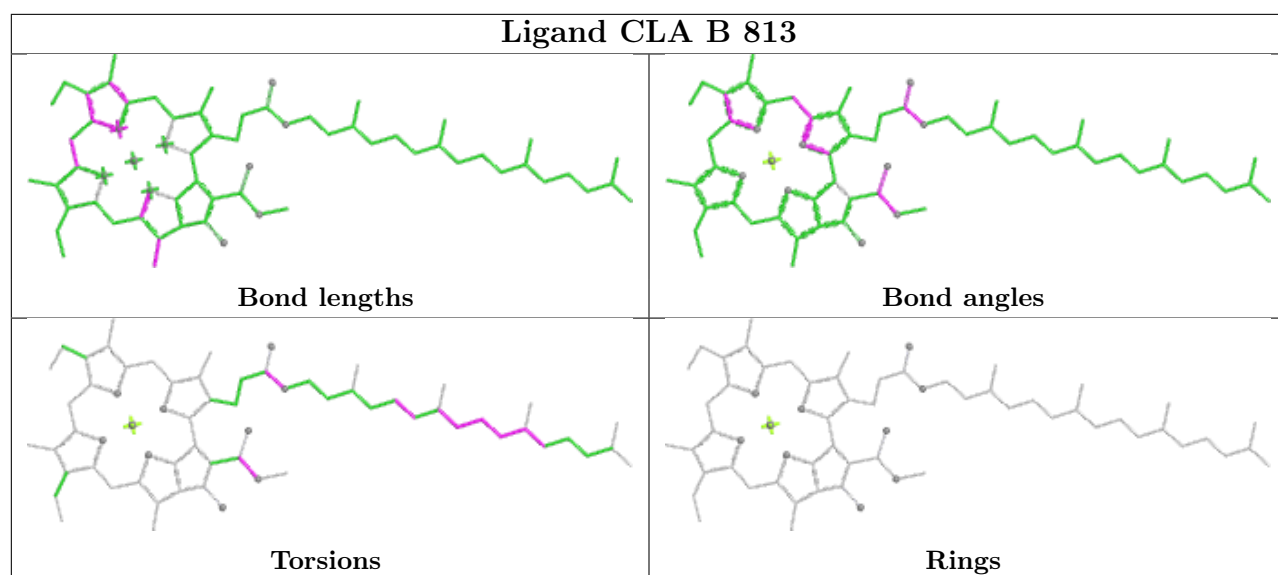


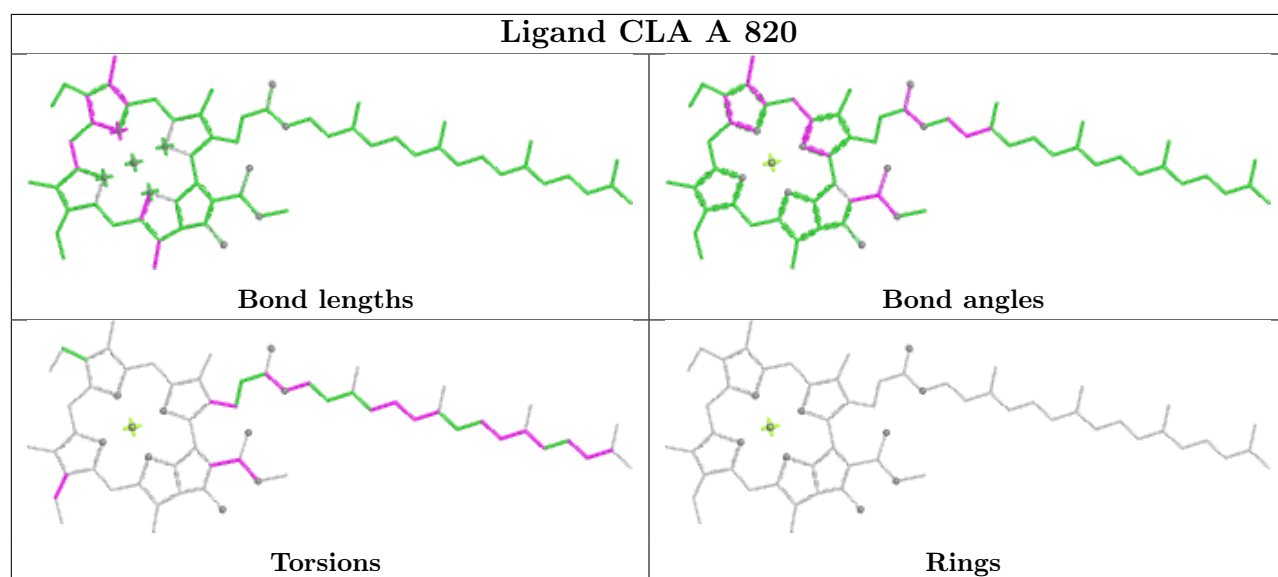
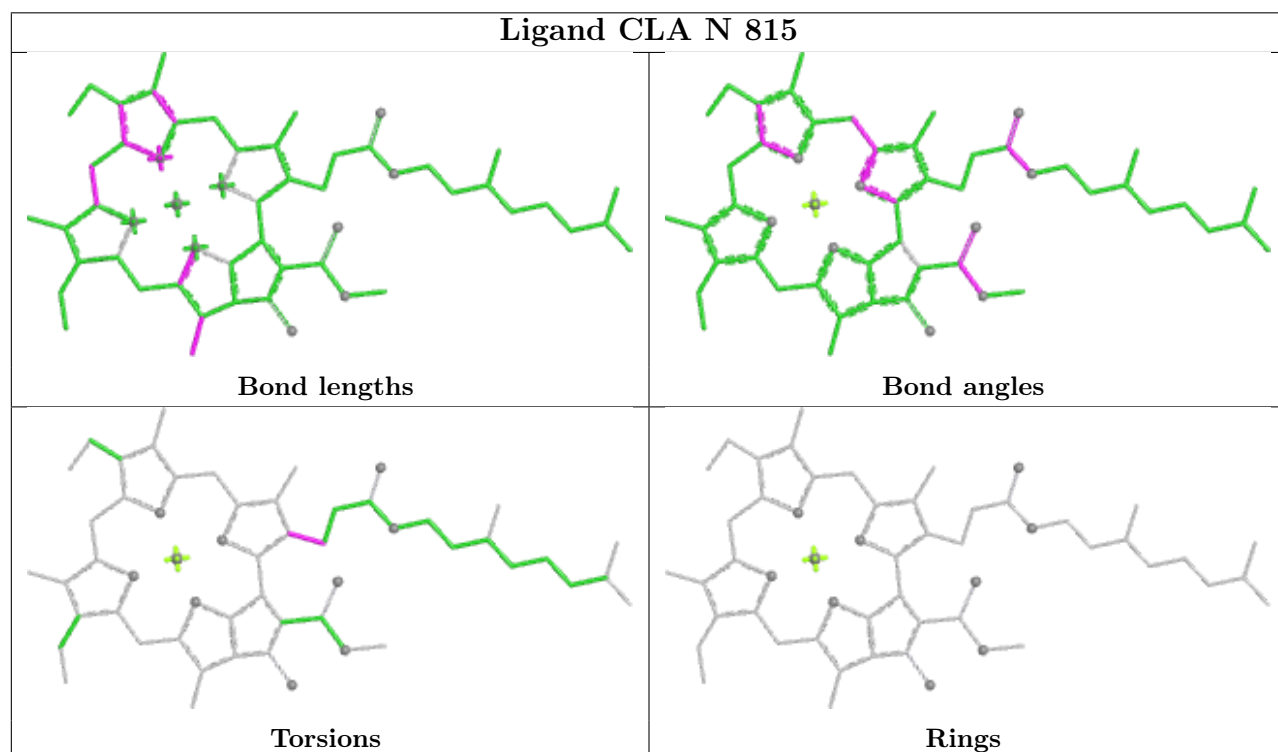
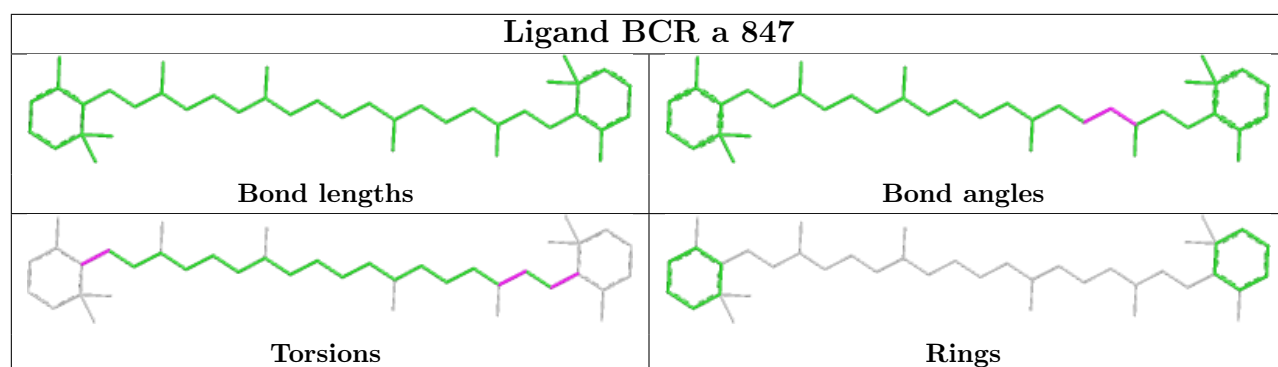
Ligand BCR a 850



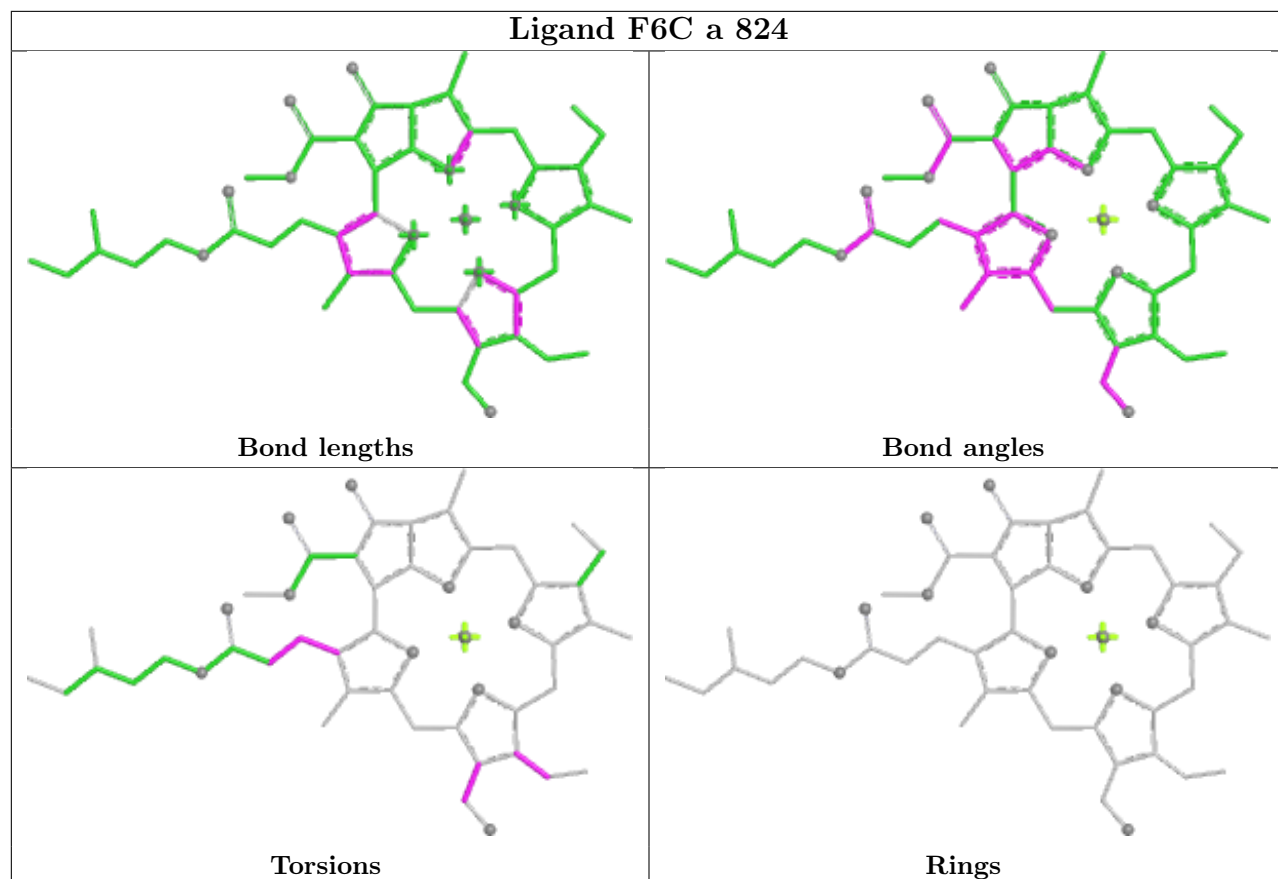




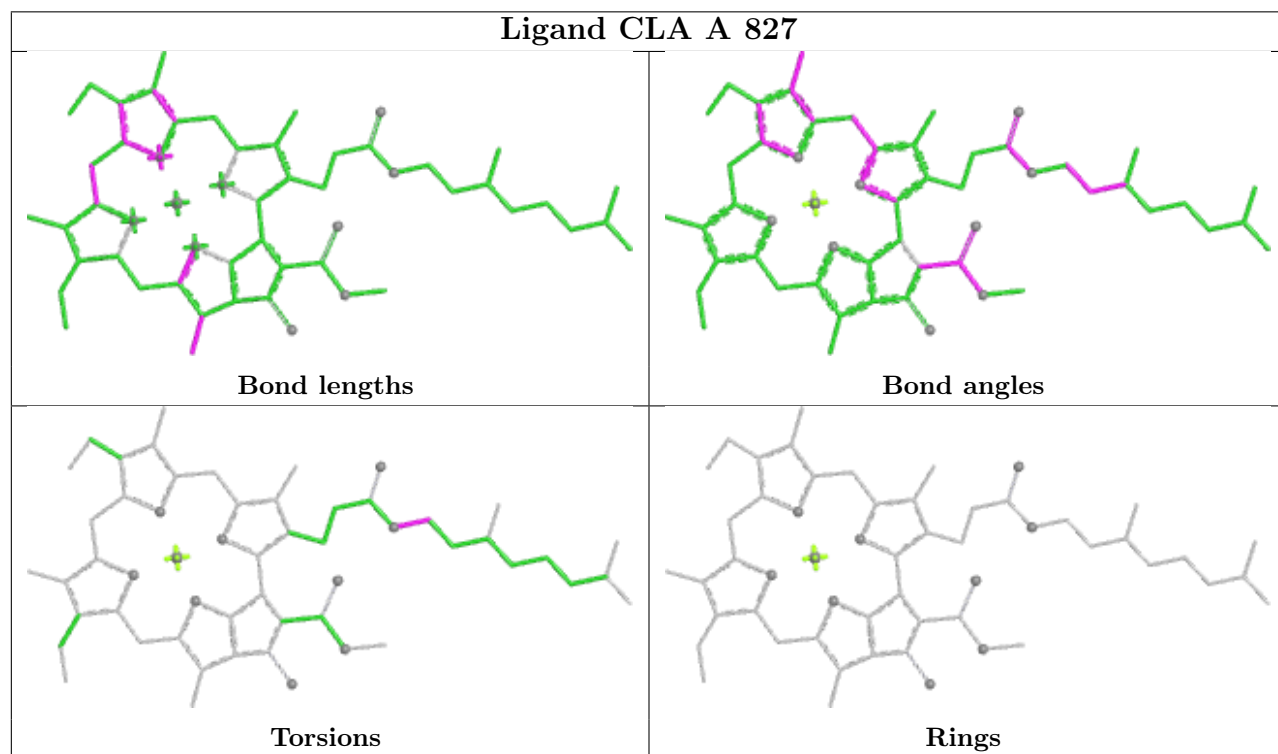


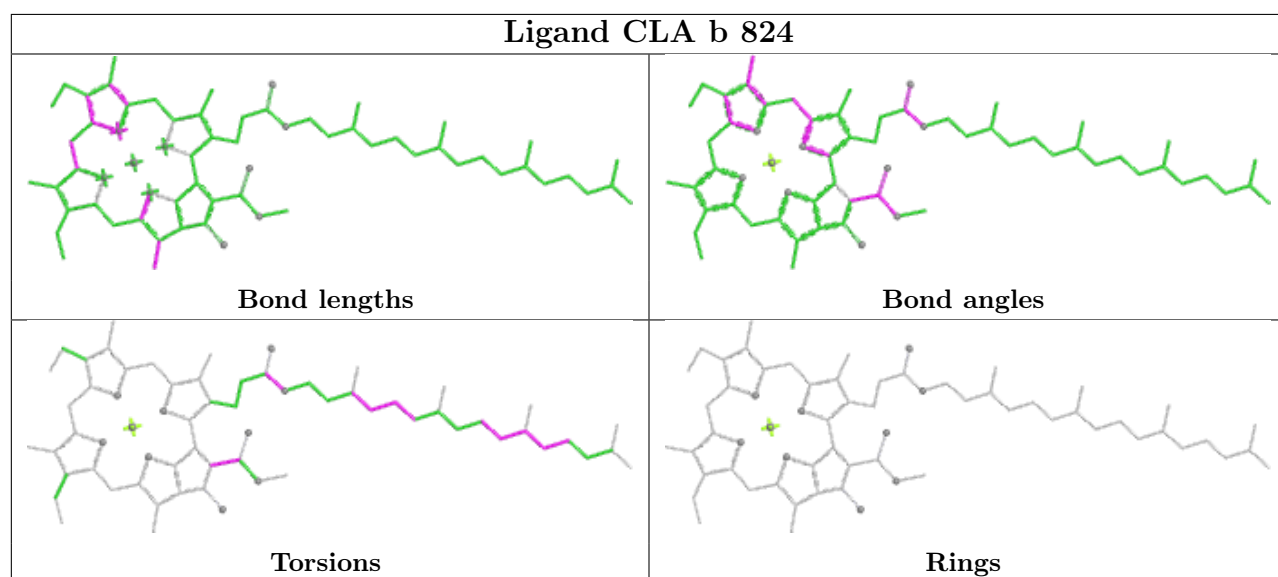
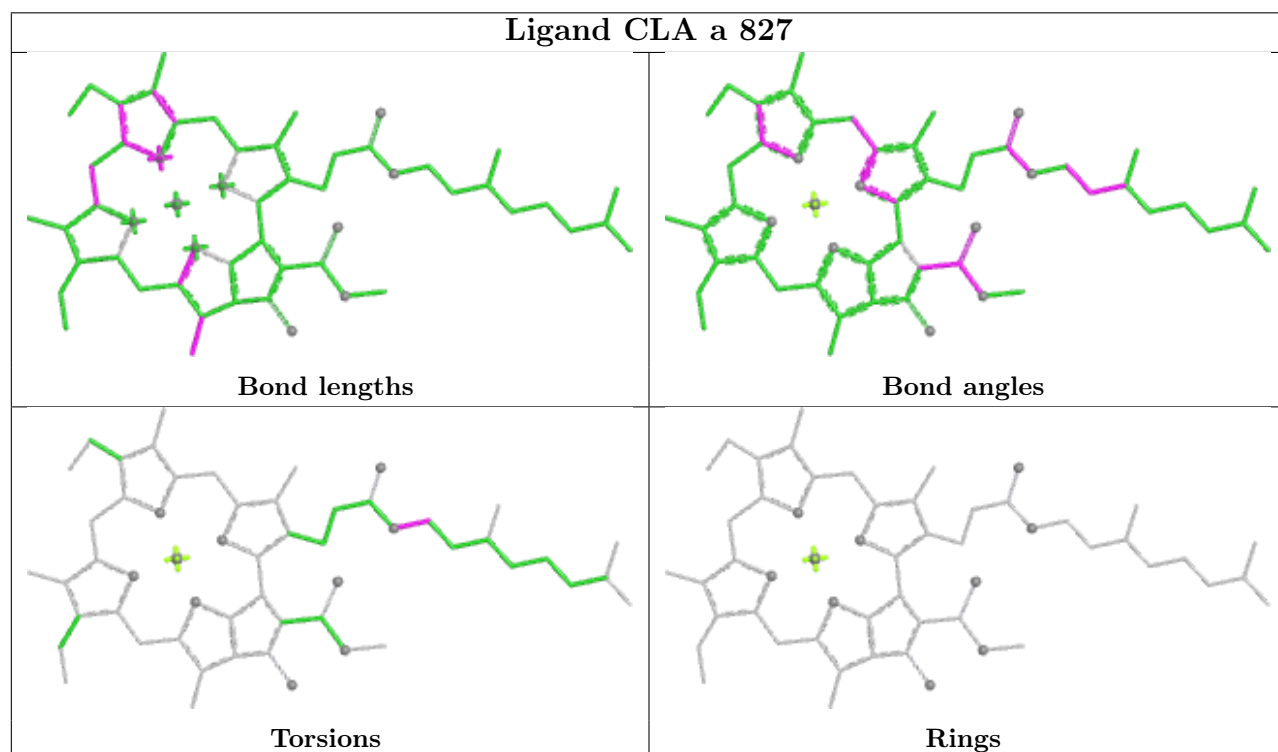
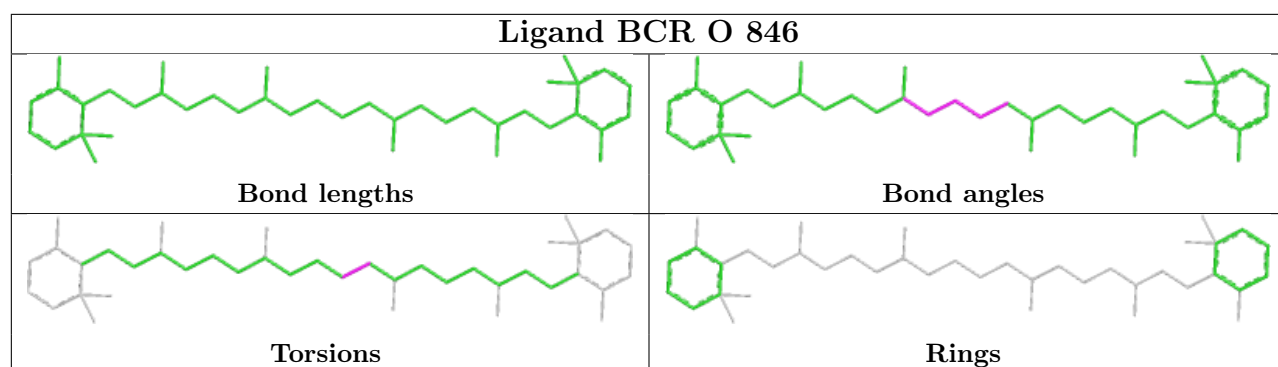


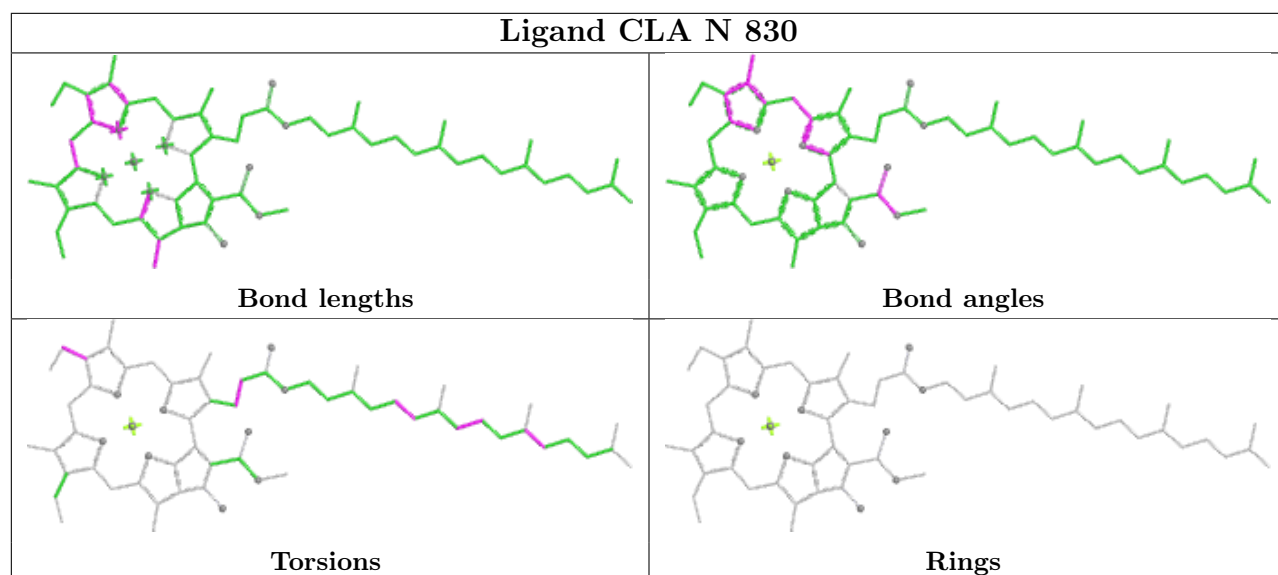
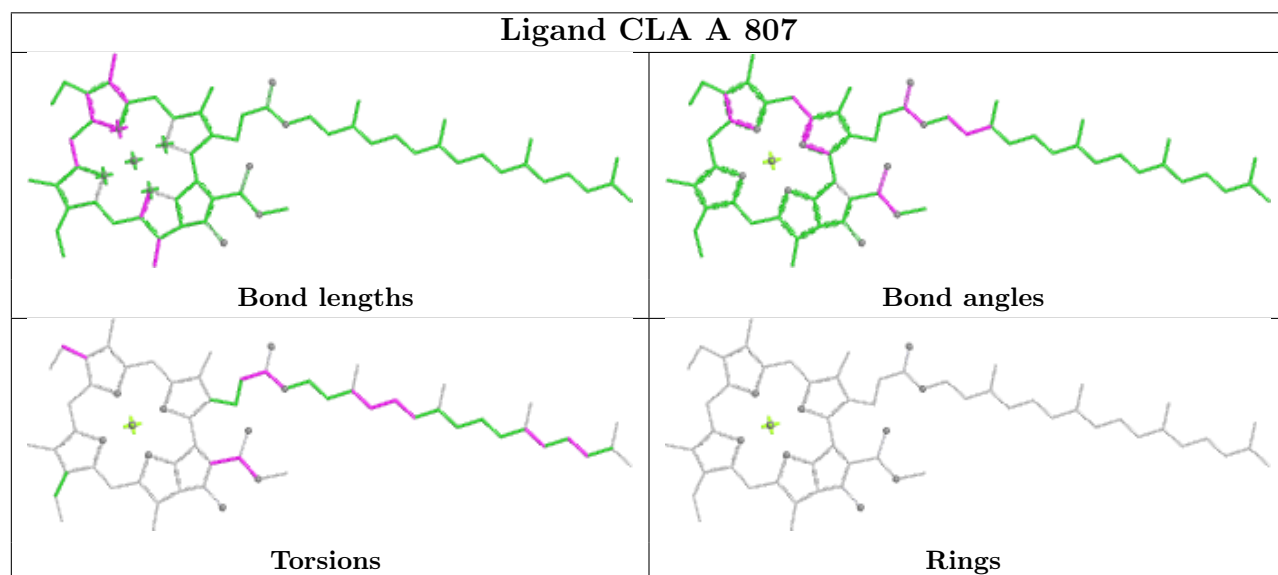
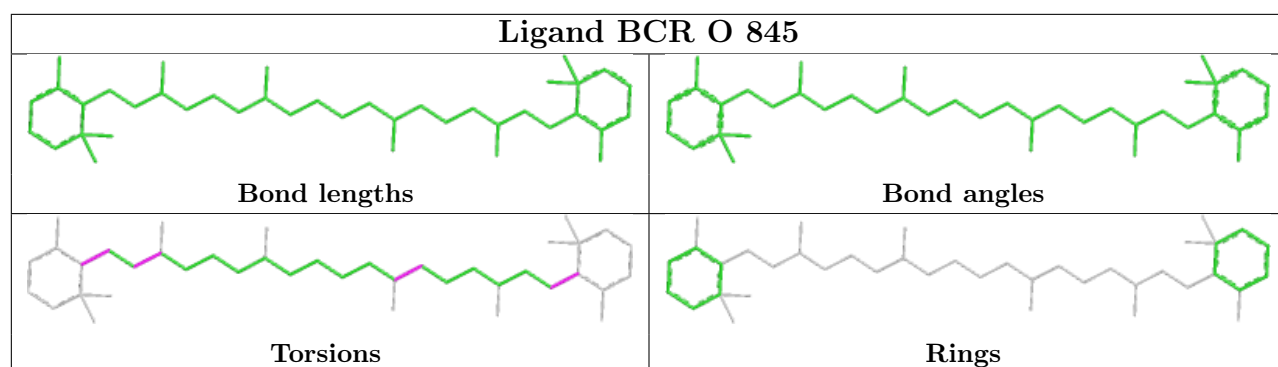
Ligand F6C a 824

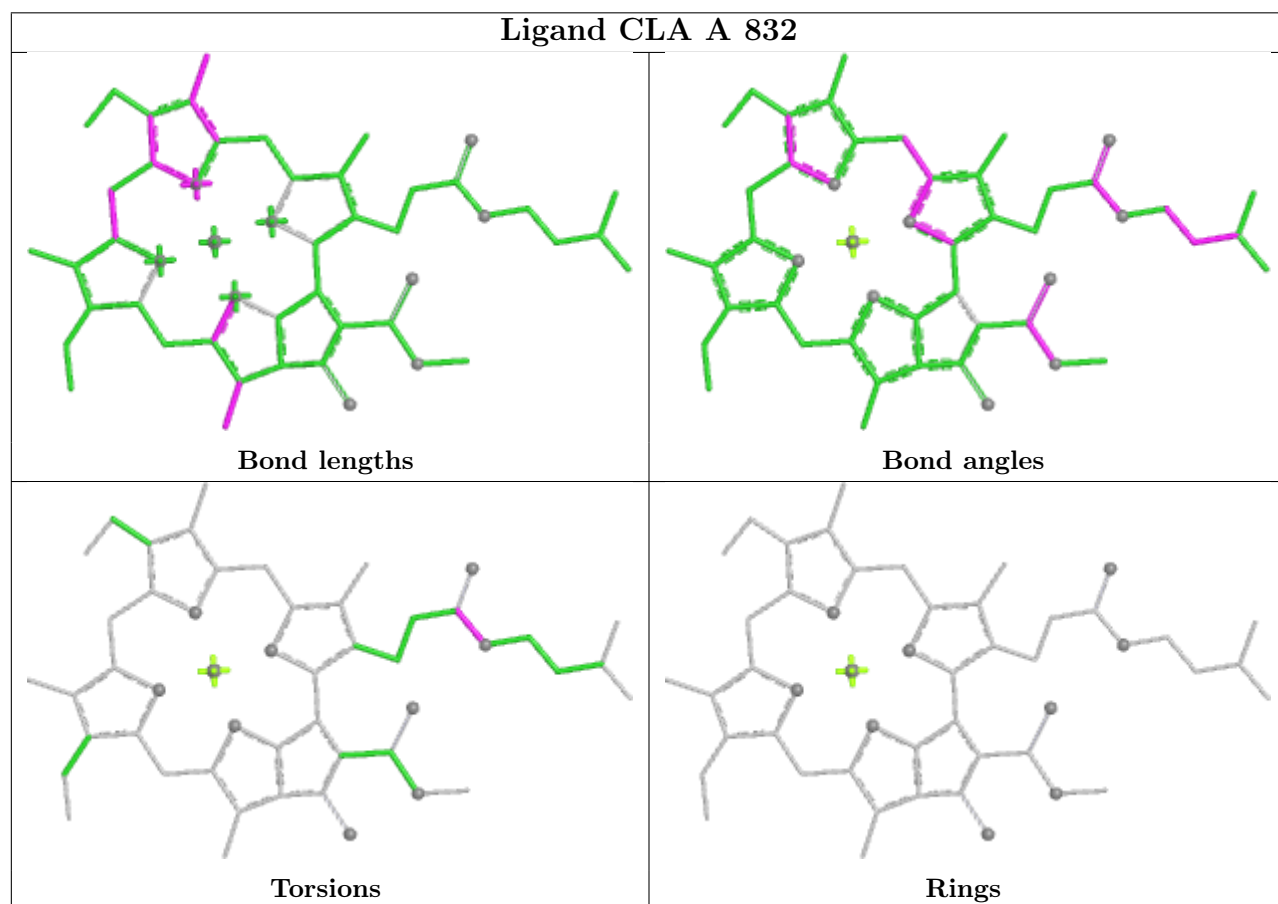
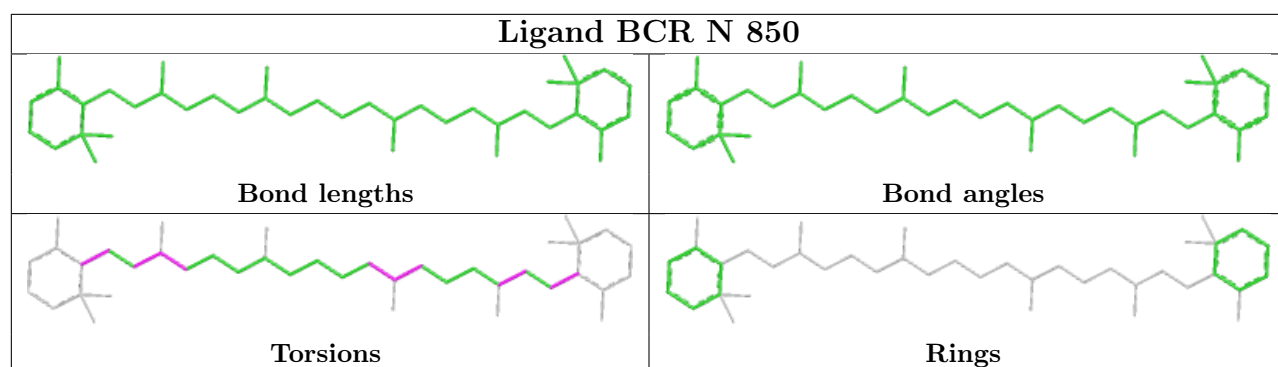


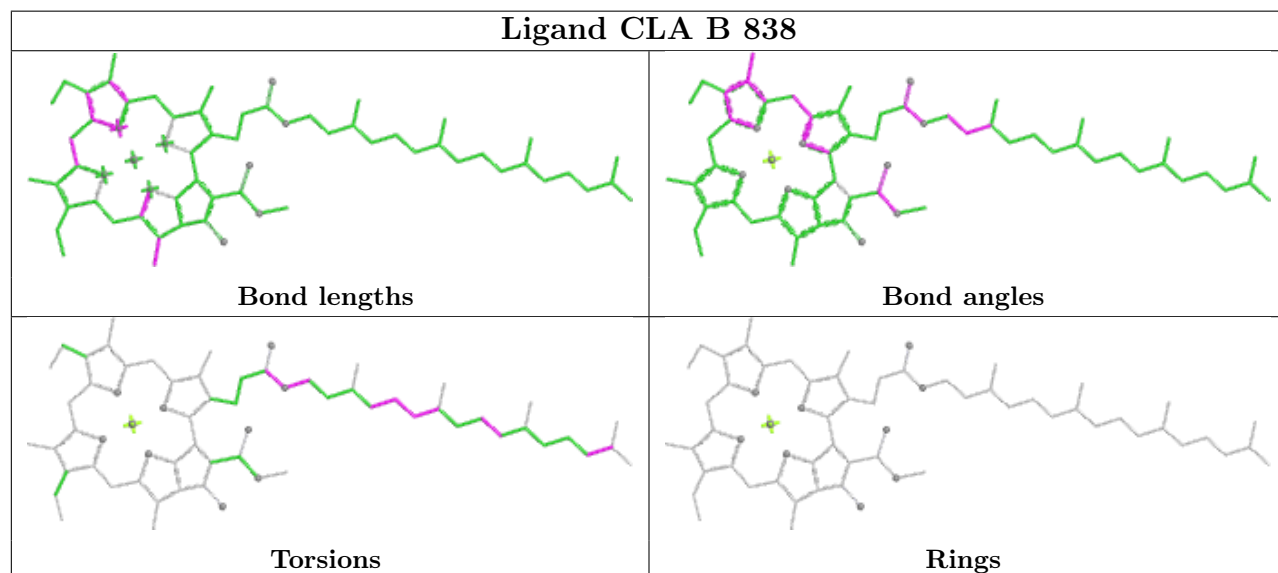
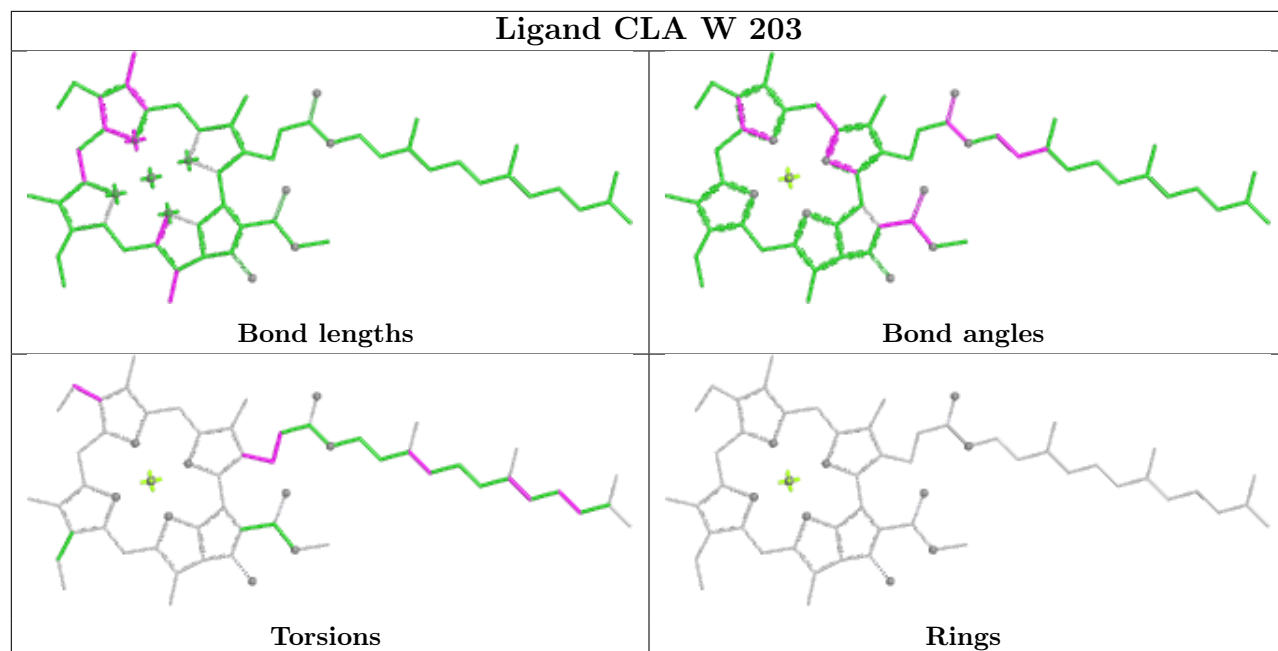
Ligand CLA A 827

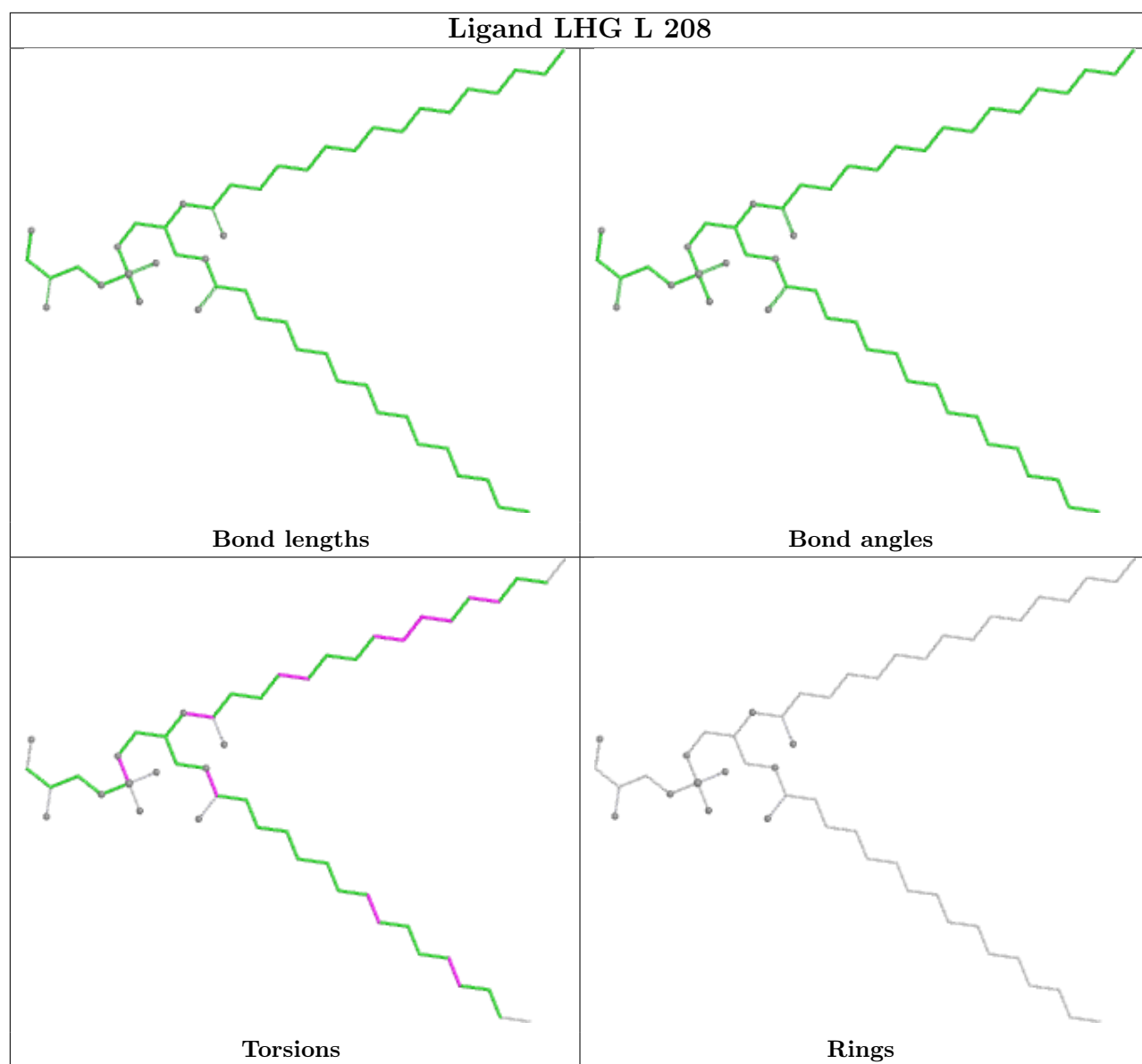




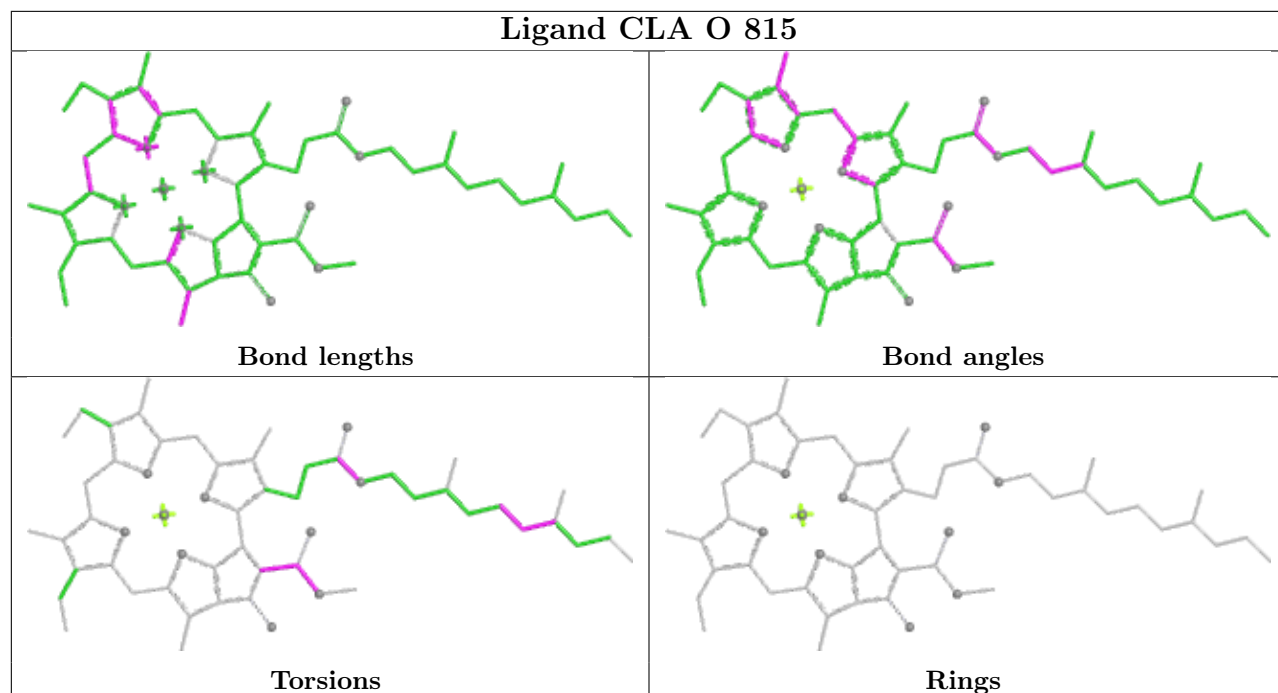




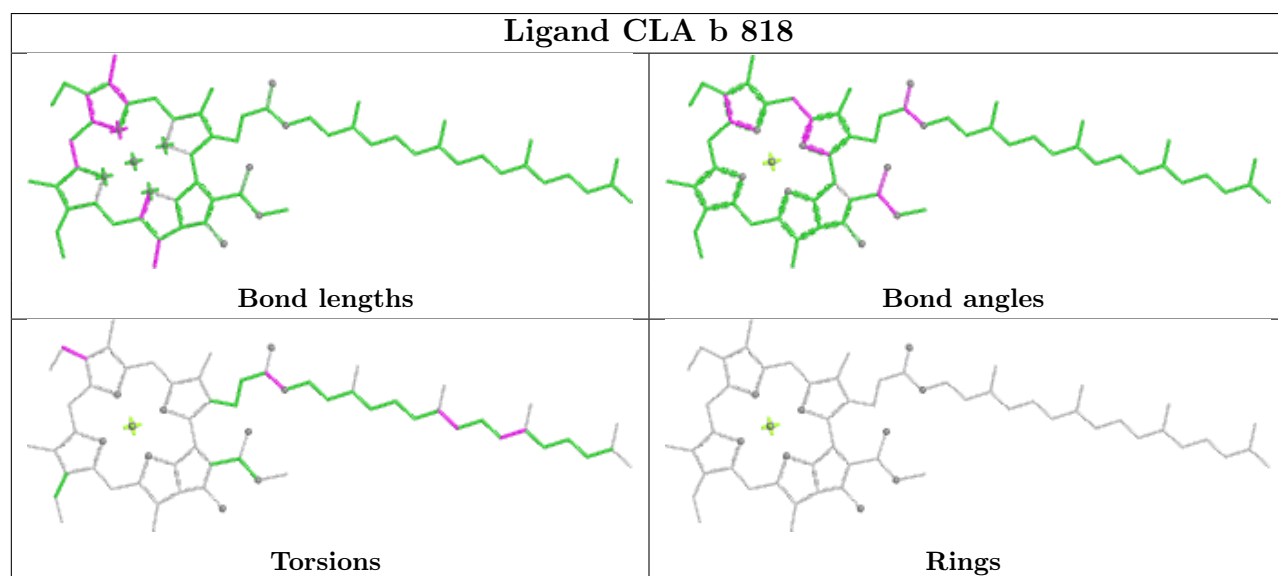




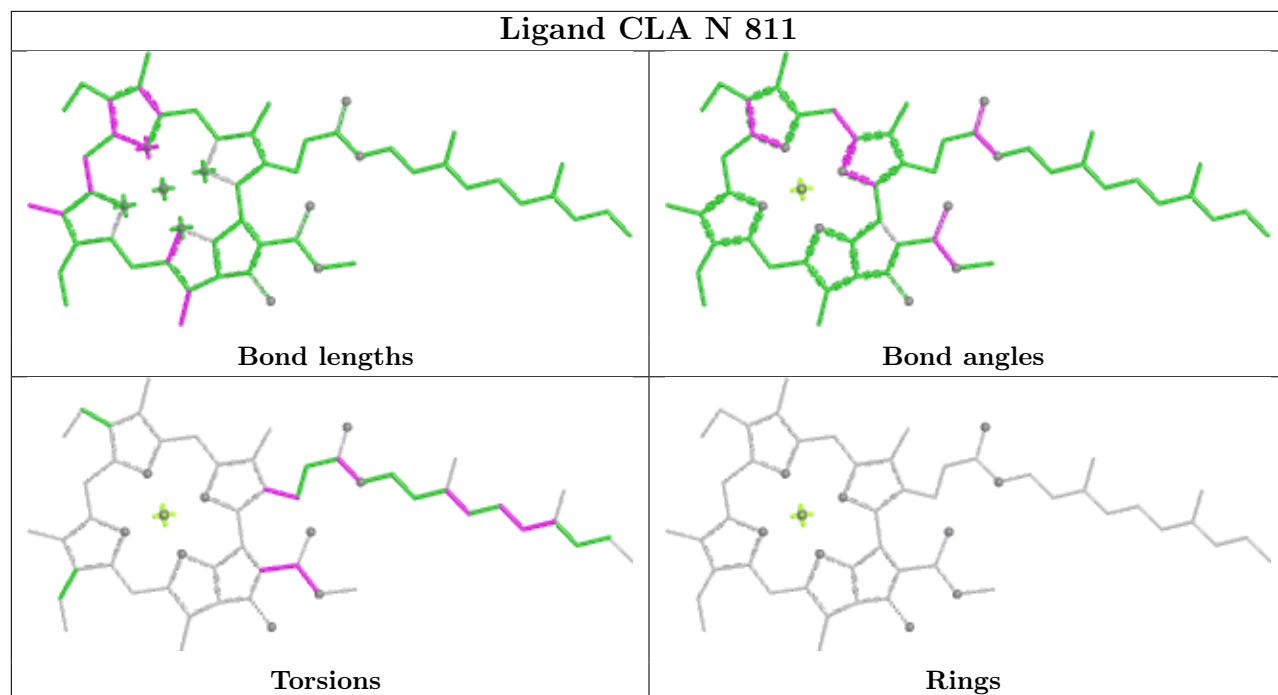
Ligand CLA O 815



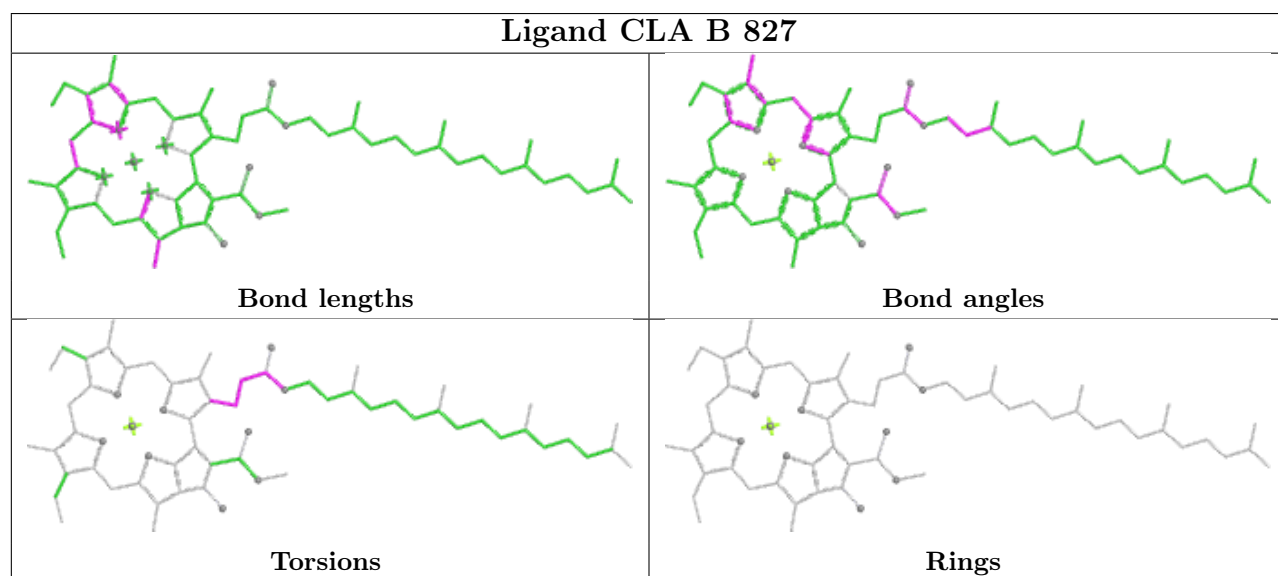
Ligand CLA b 818

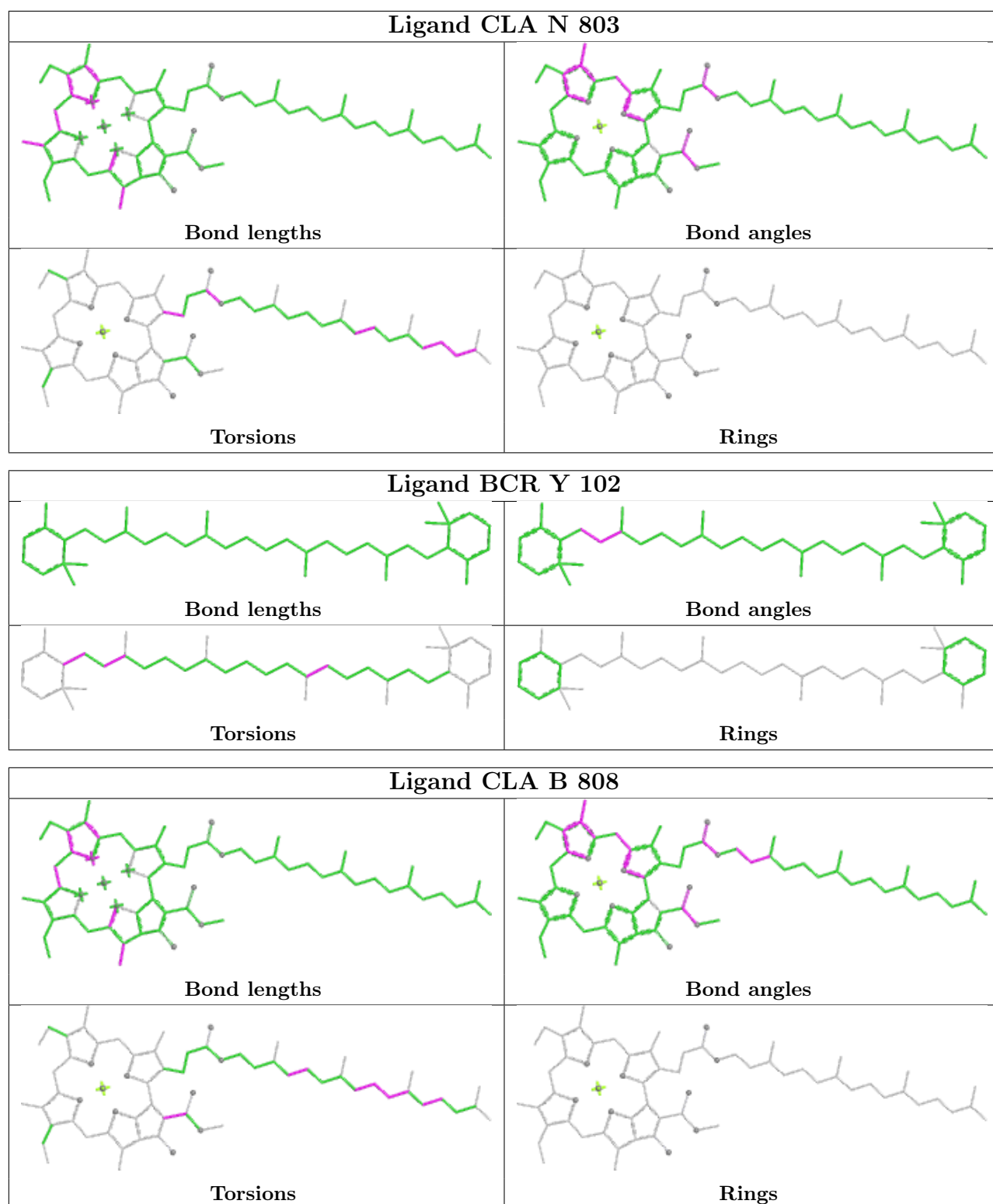


Ligand CLA N 811

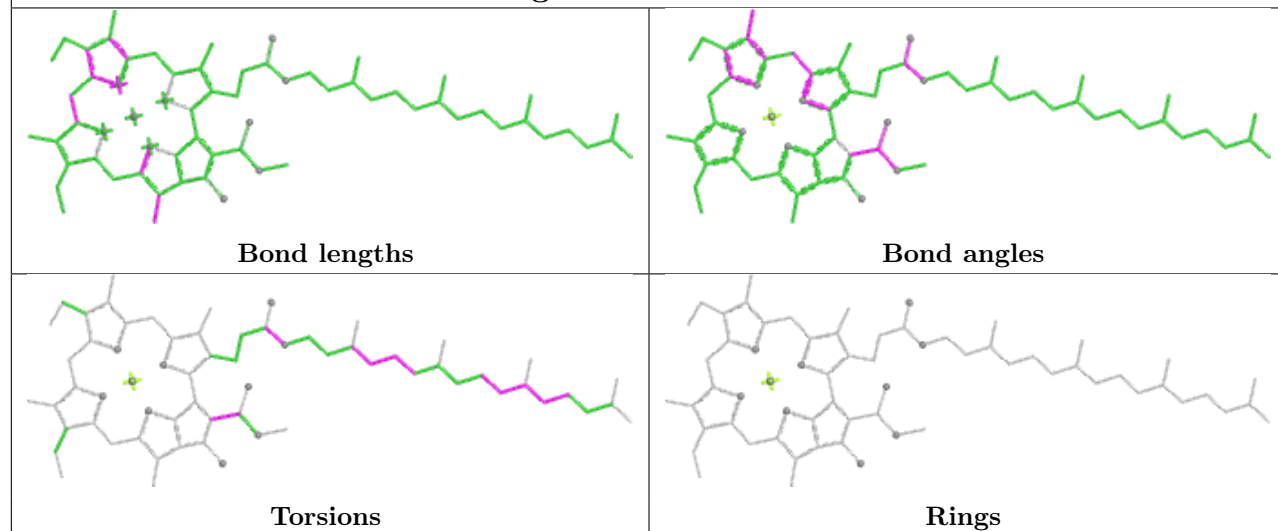


Ligand CLA B 827

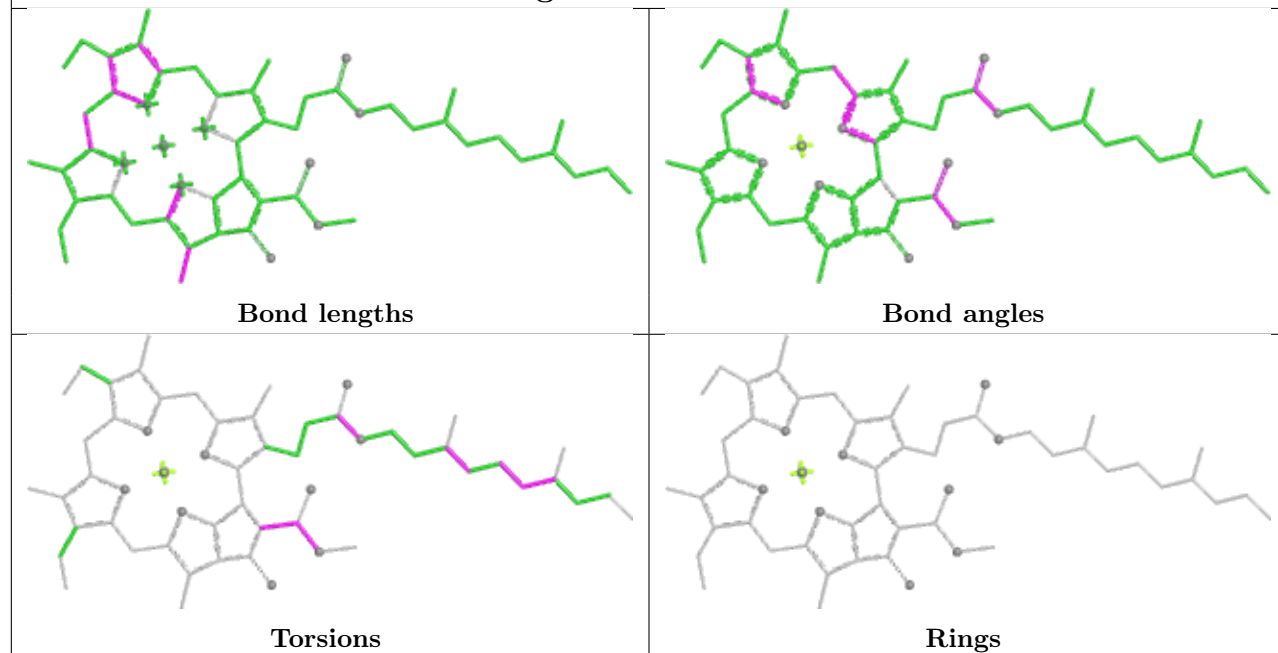


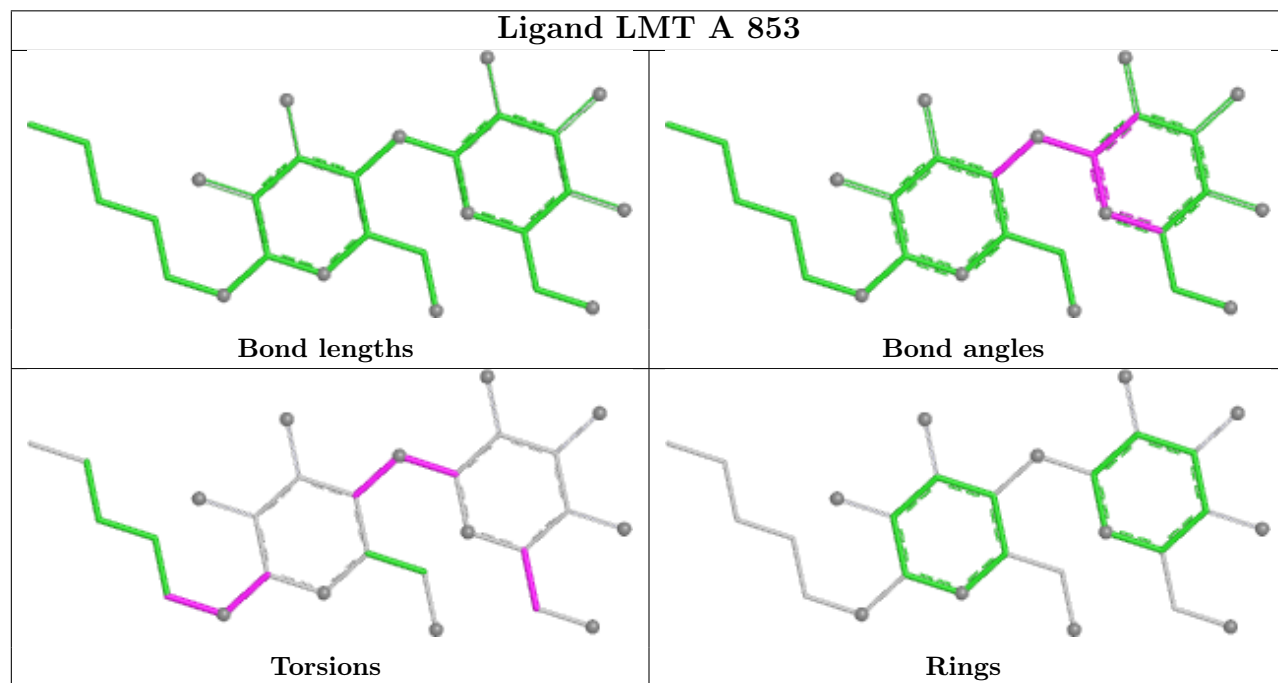
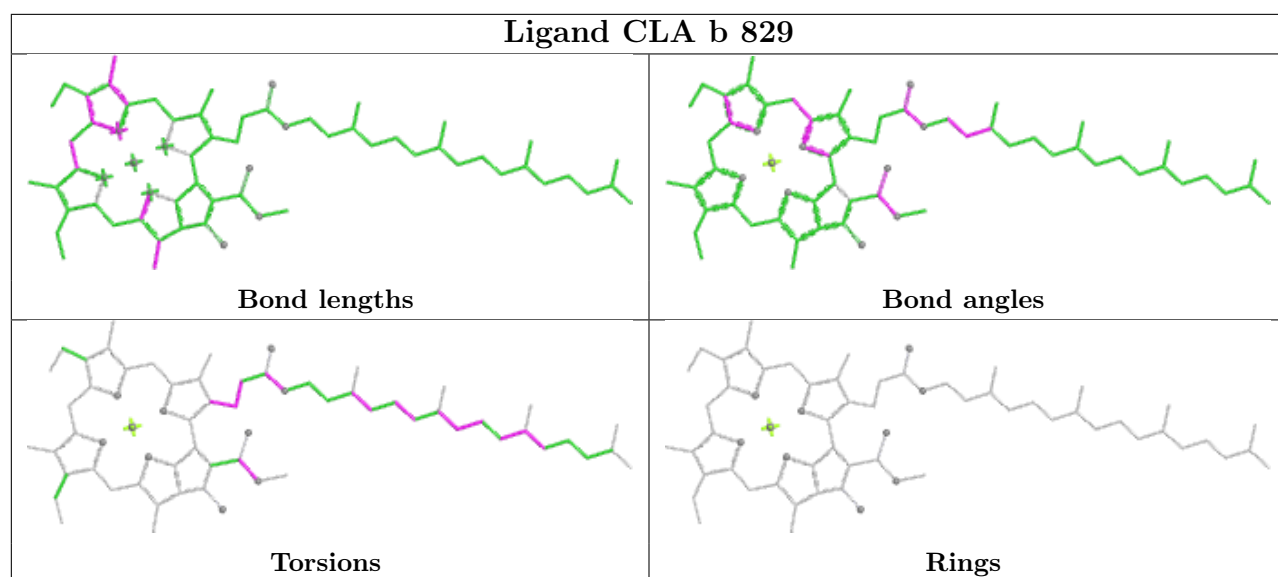


Ligand CLA O 824

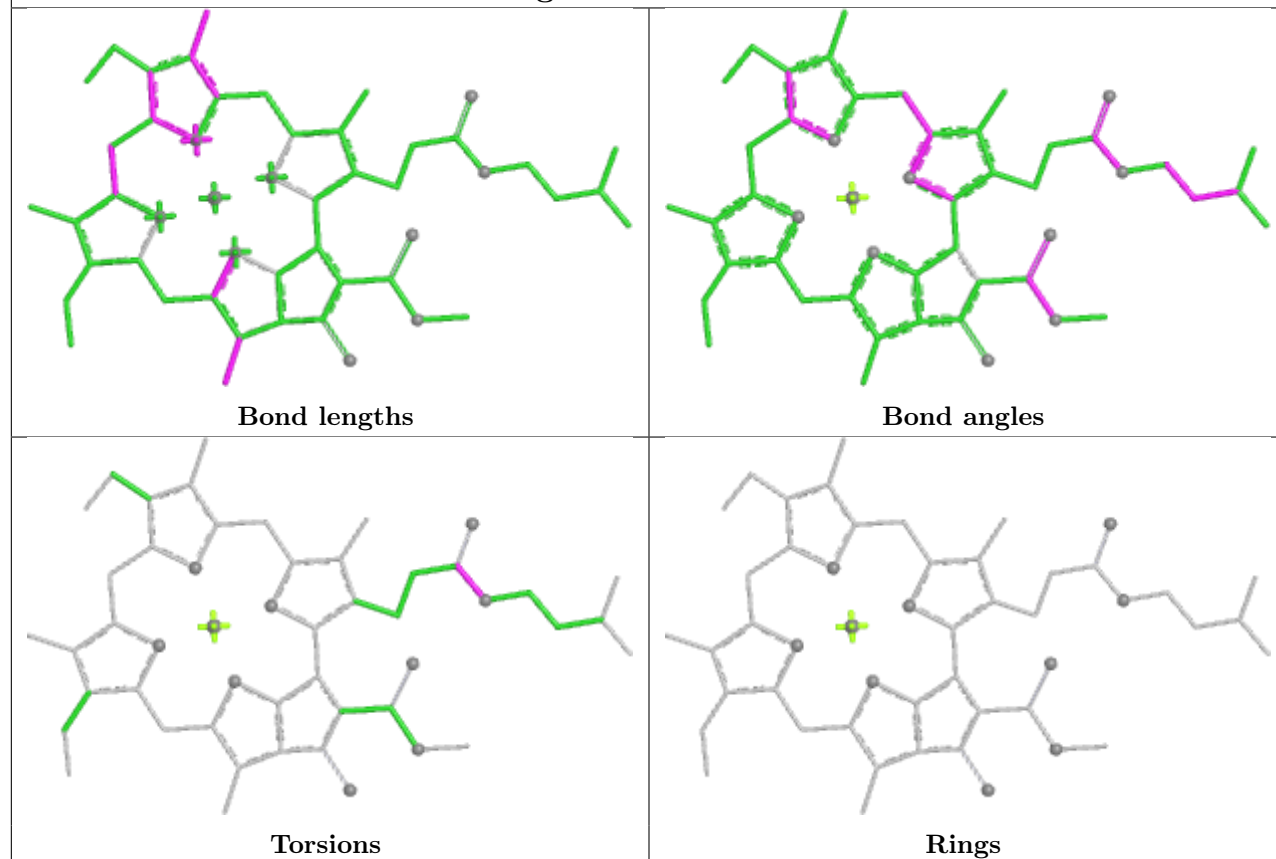


Ligand CLA a 811

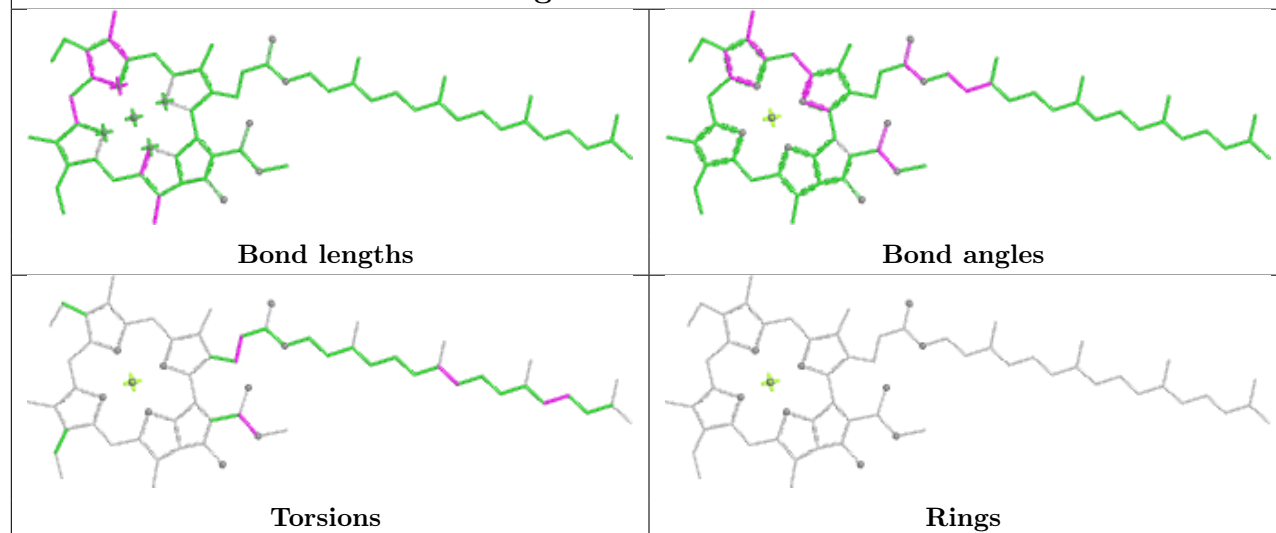


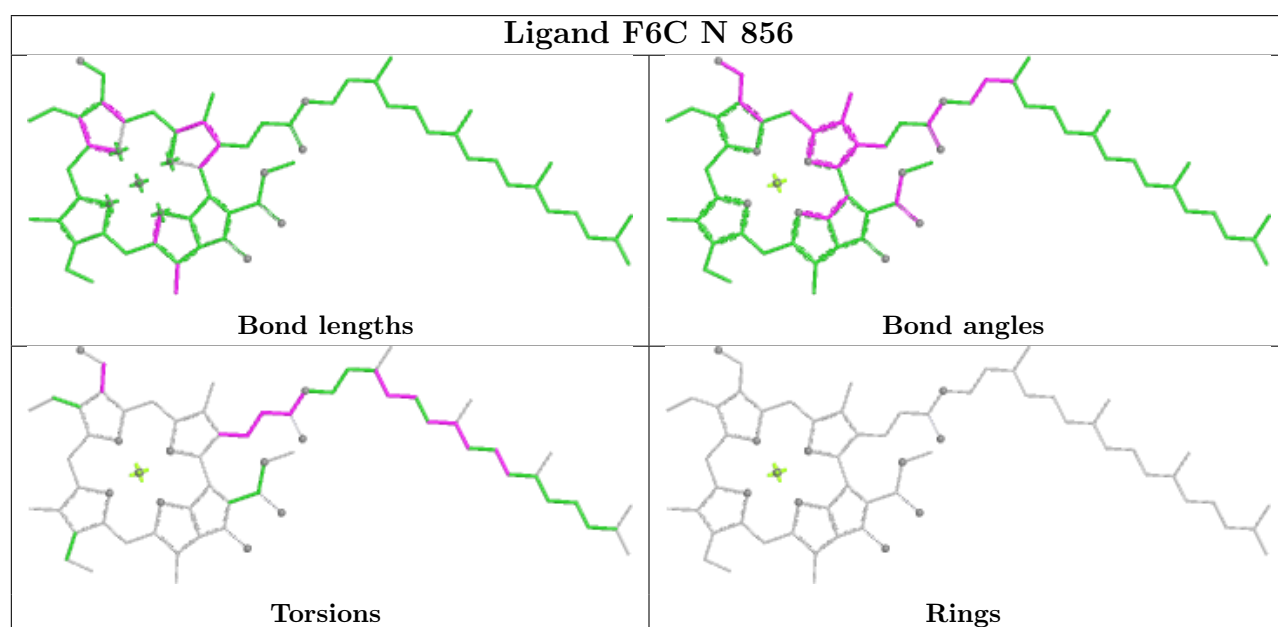
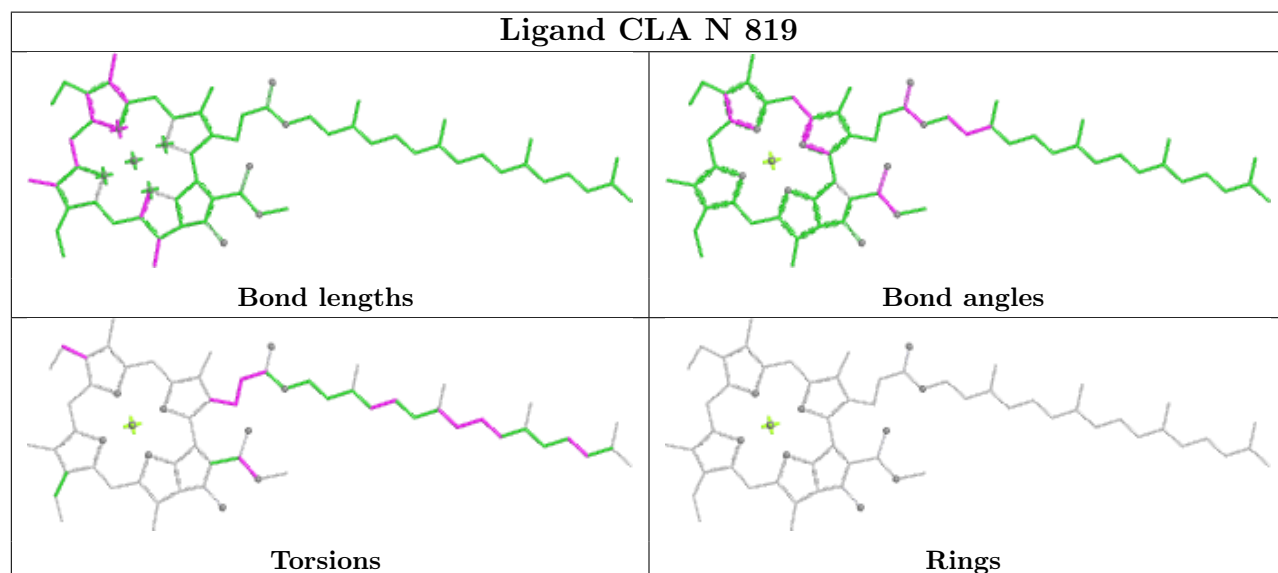
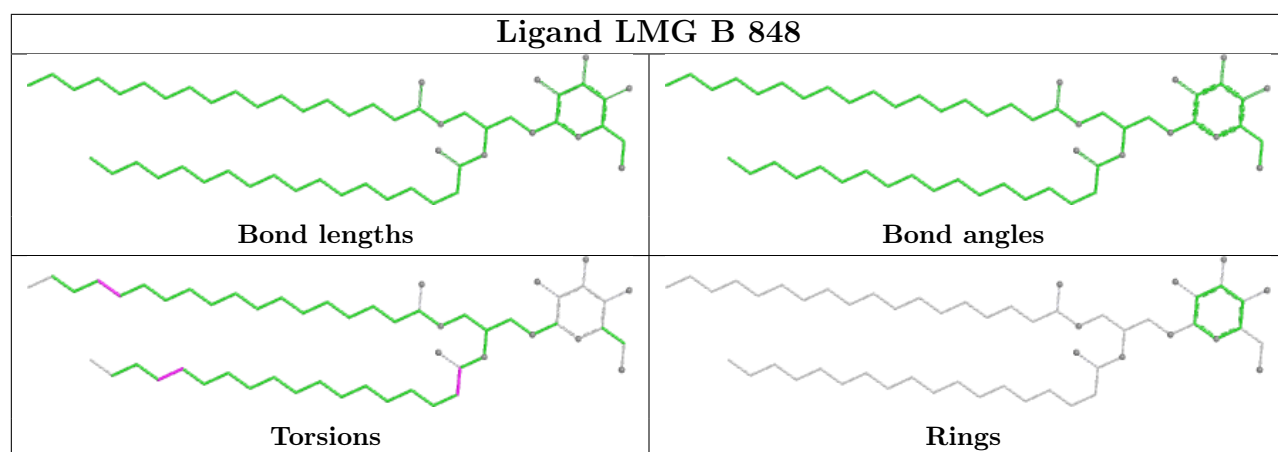


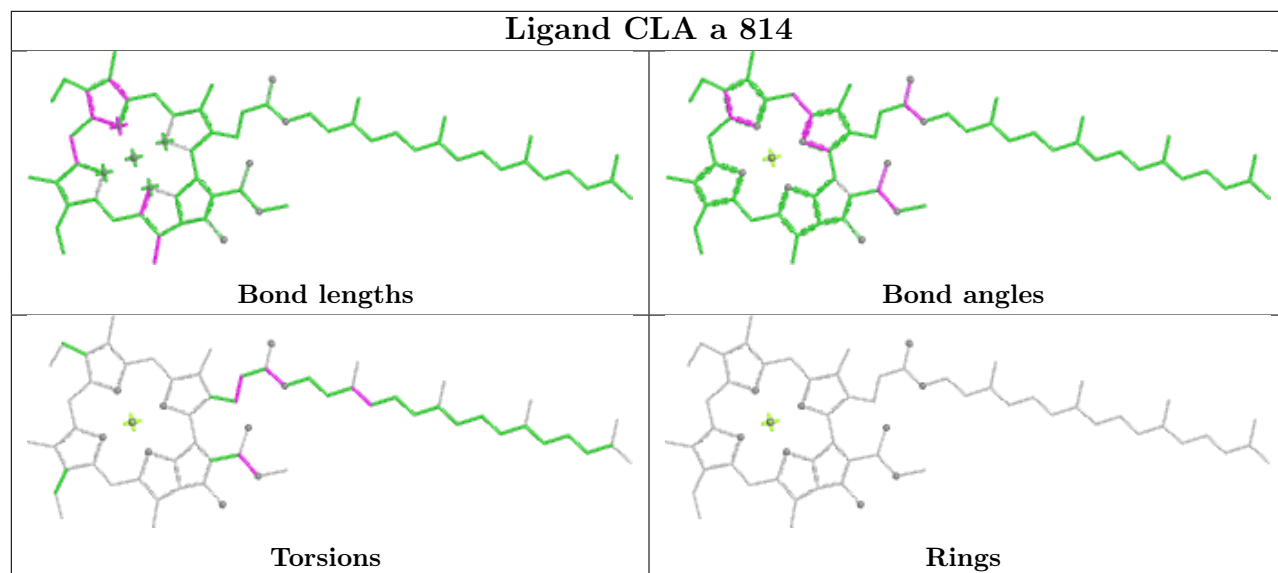
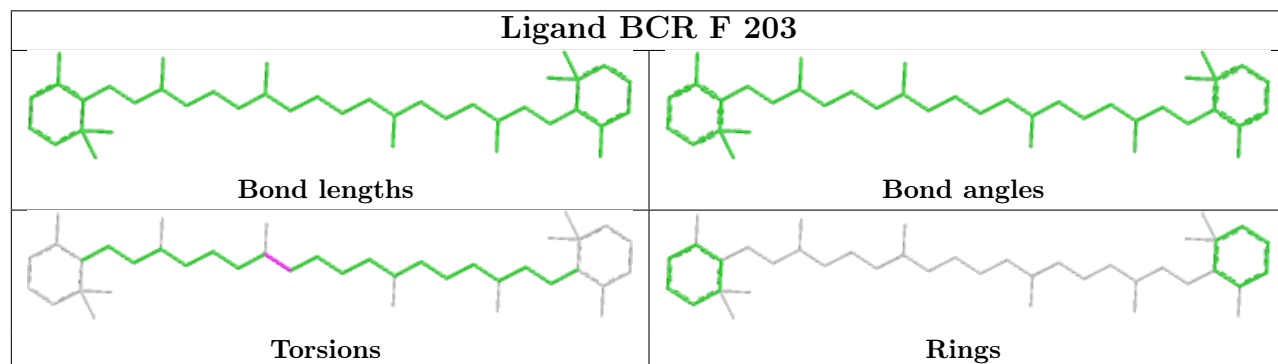
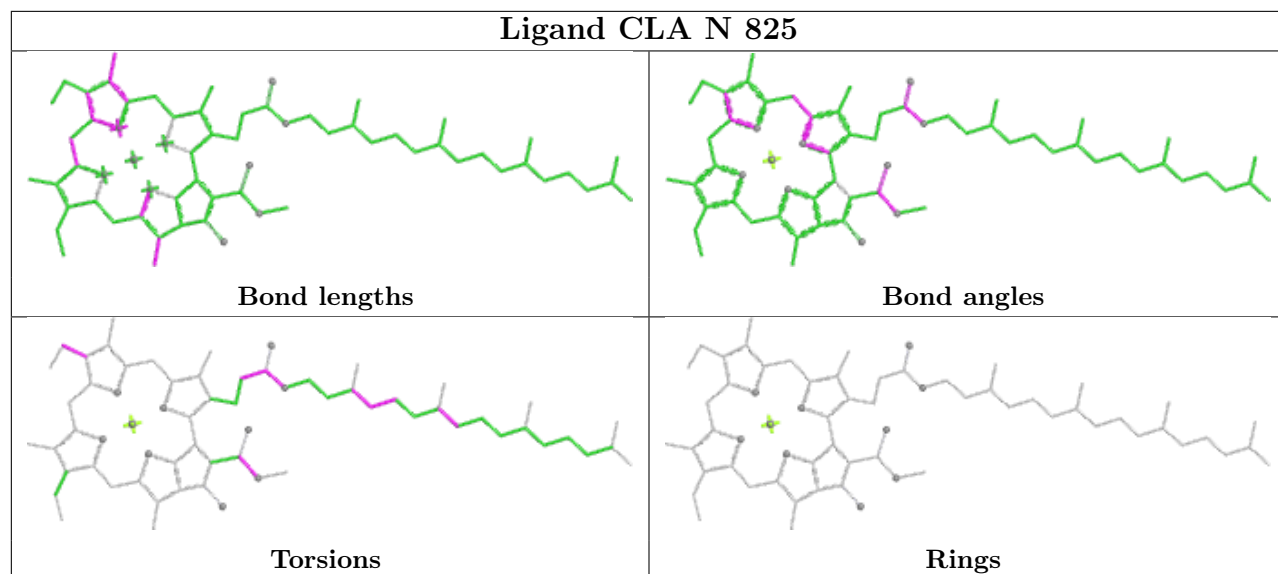
Ligand CLA a 832



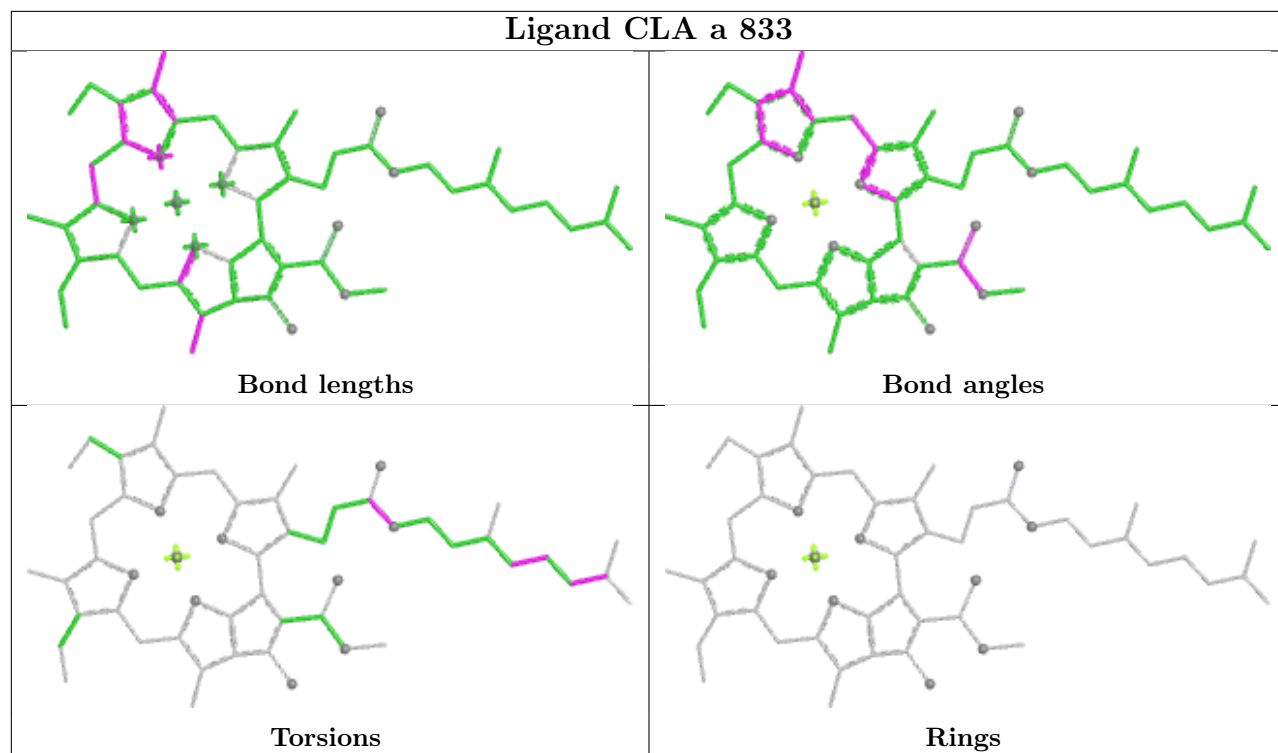
Ligand CLA L 202



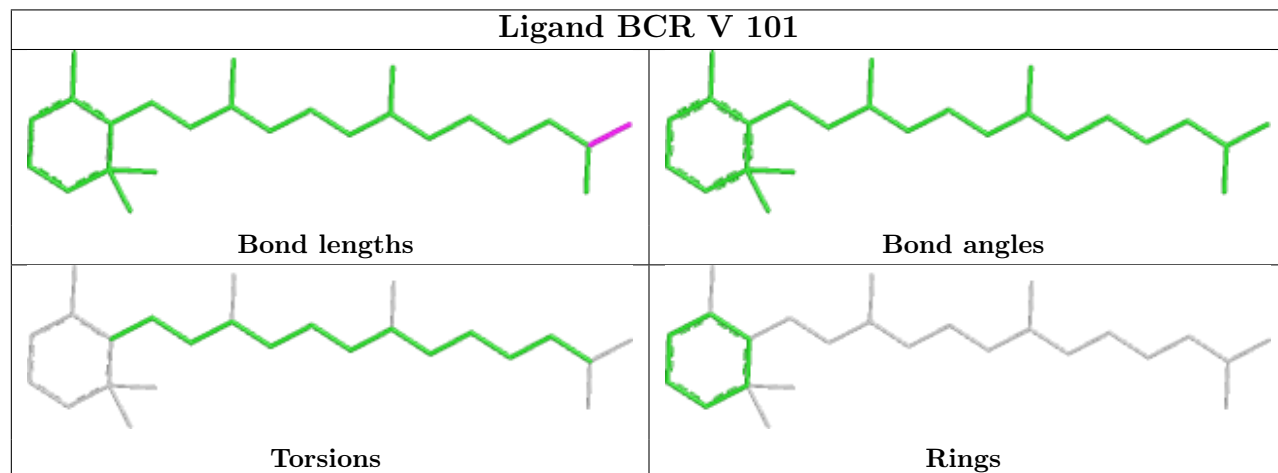




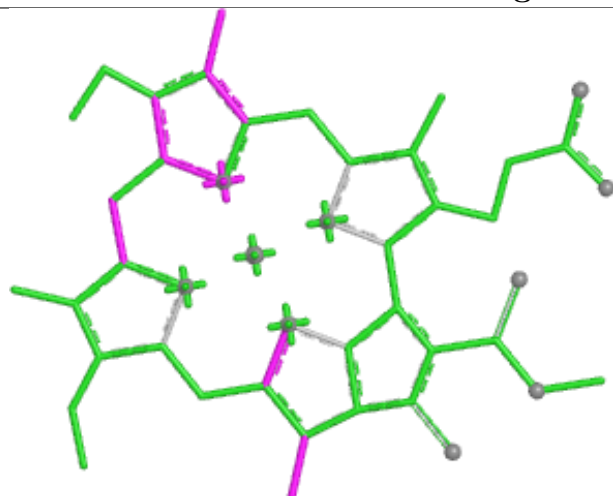
Ligand CLA a 833



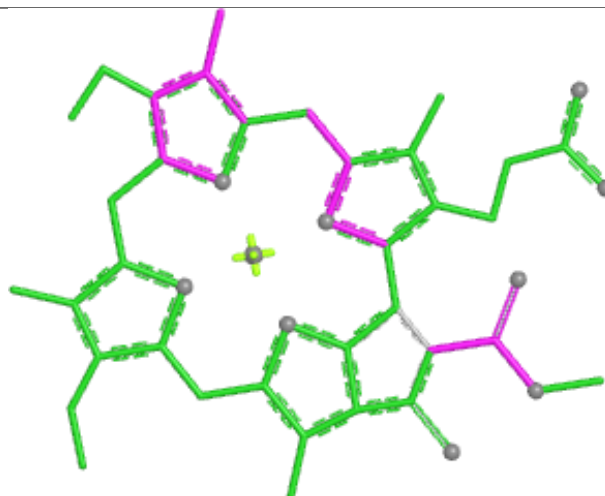
Ligand BCR V 101



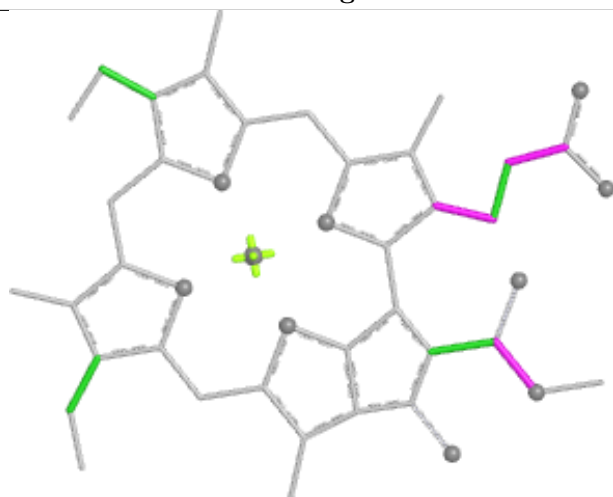
Ligand CLA O 834



Bond lengths



Bond angles

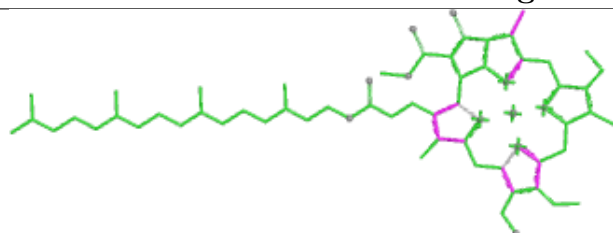


Torsions

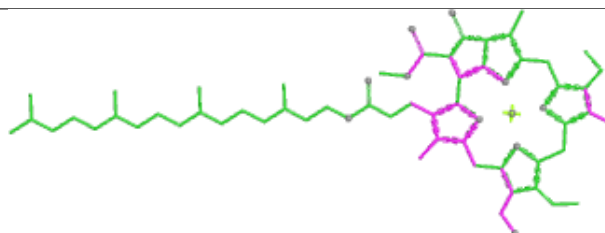


Rings

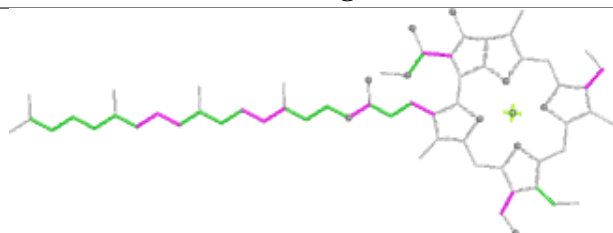
Ligand F6C N 826



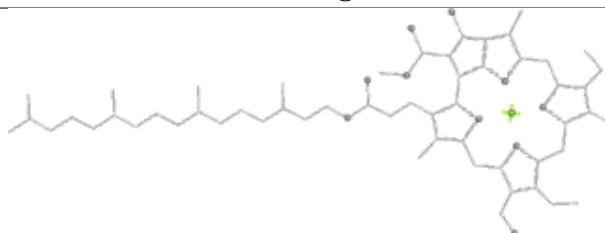
Bond lengths



Bond angles

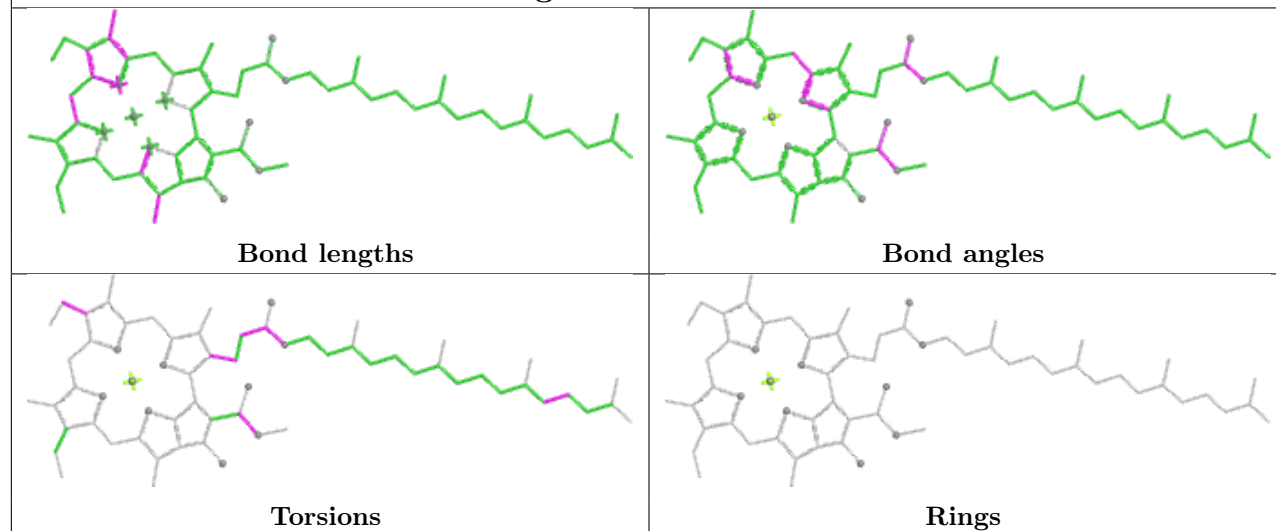


Torsions

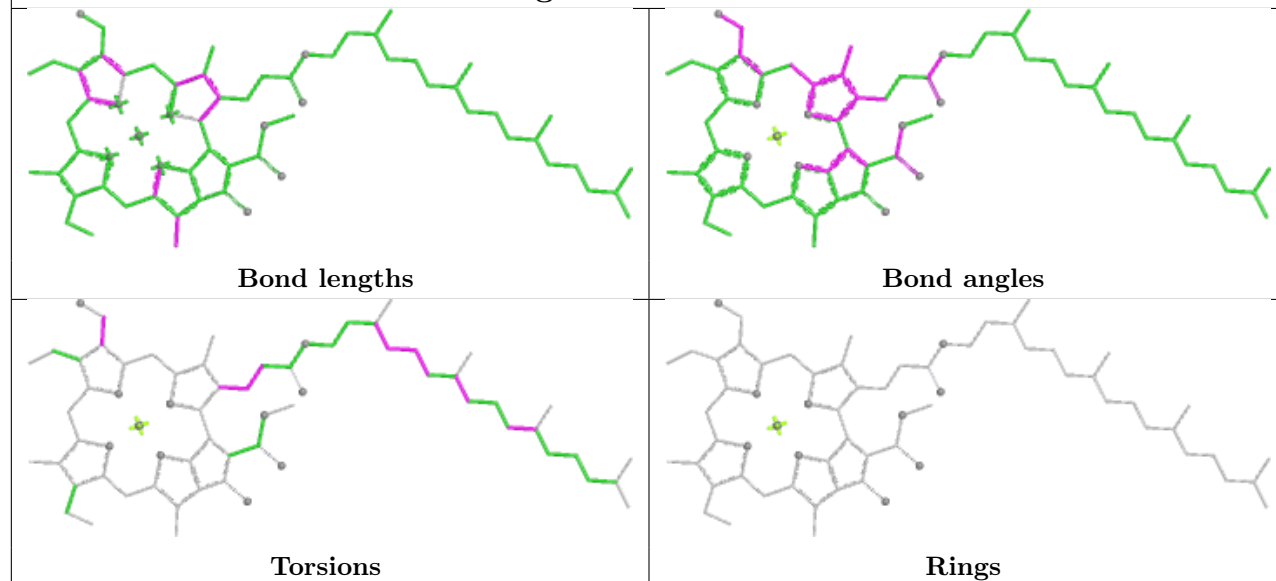


Rings

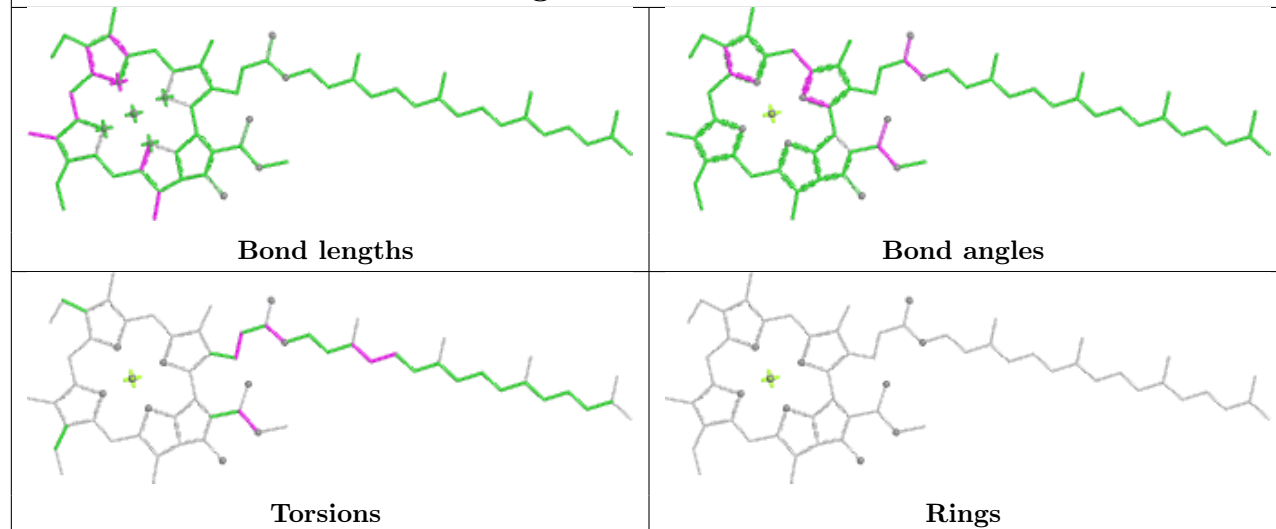
Ligand CLA b 816

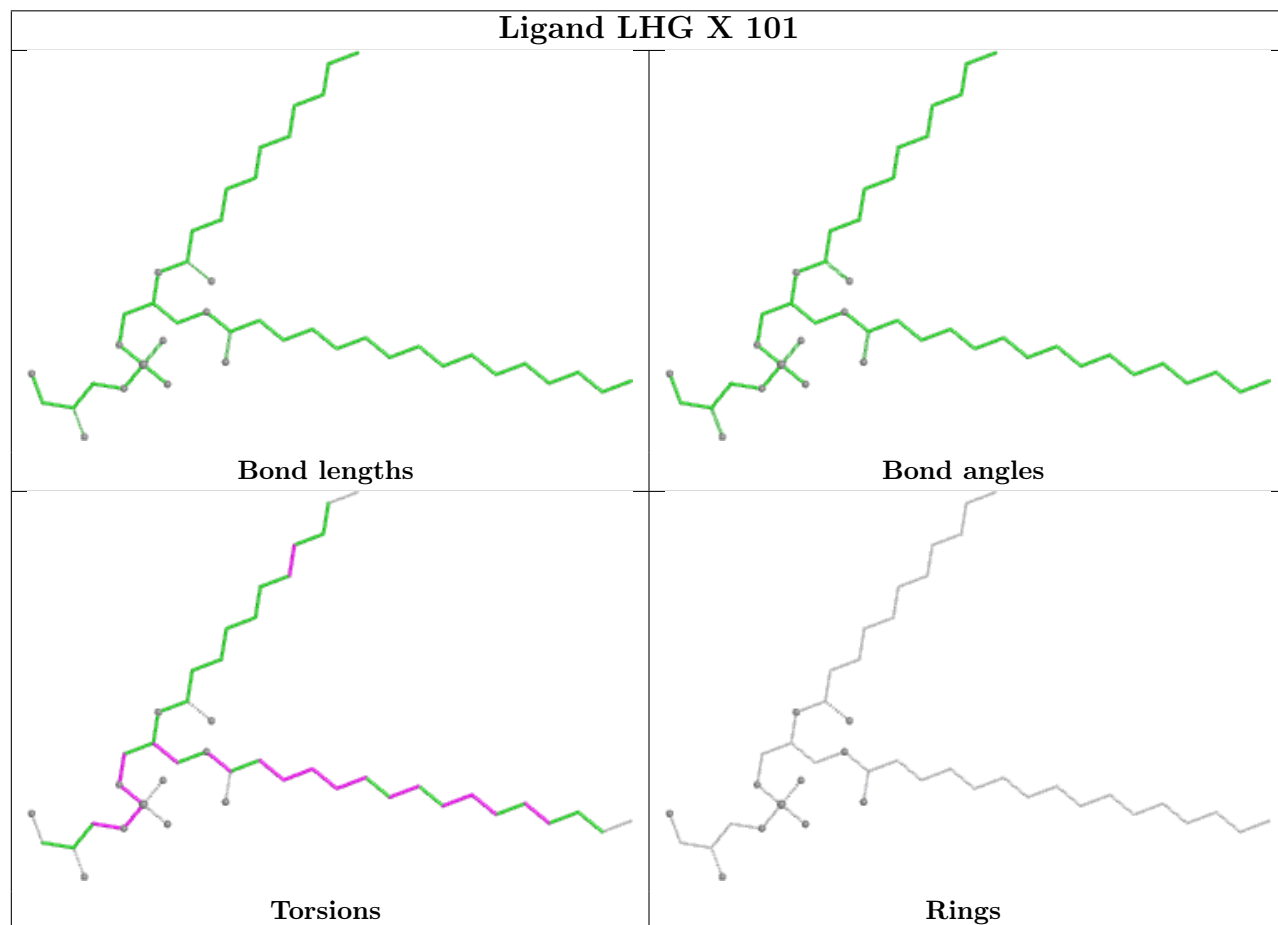
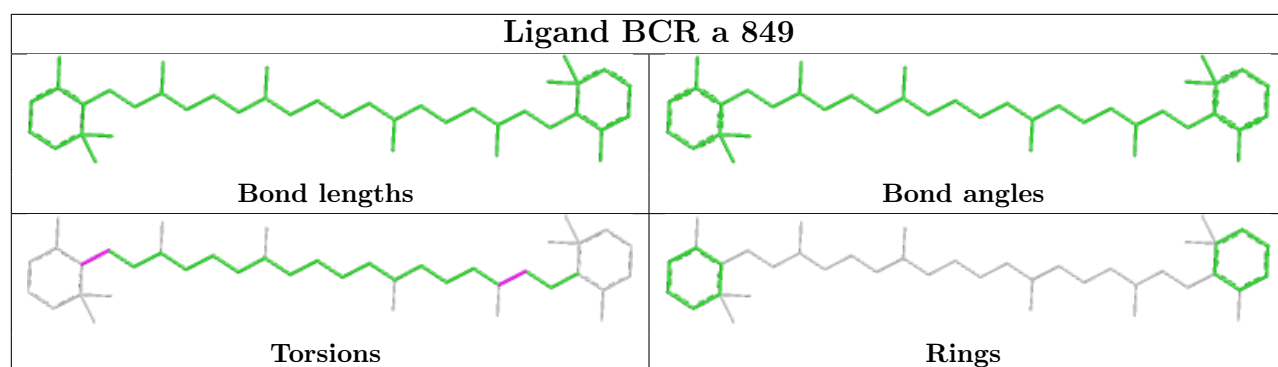


Ligand F6C O 839

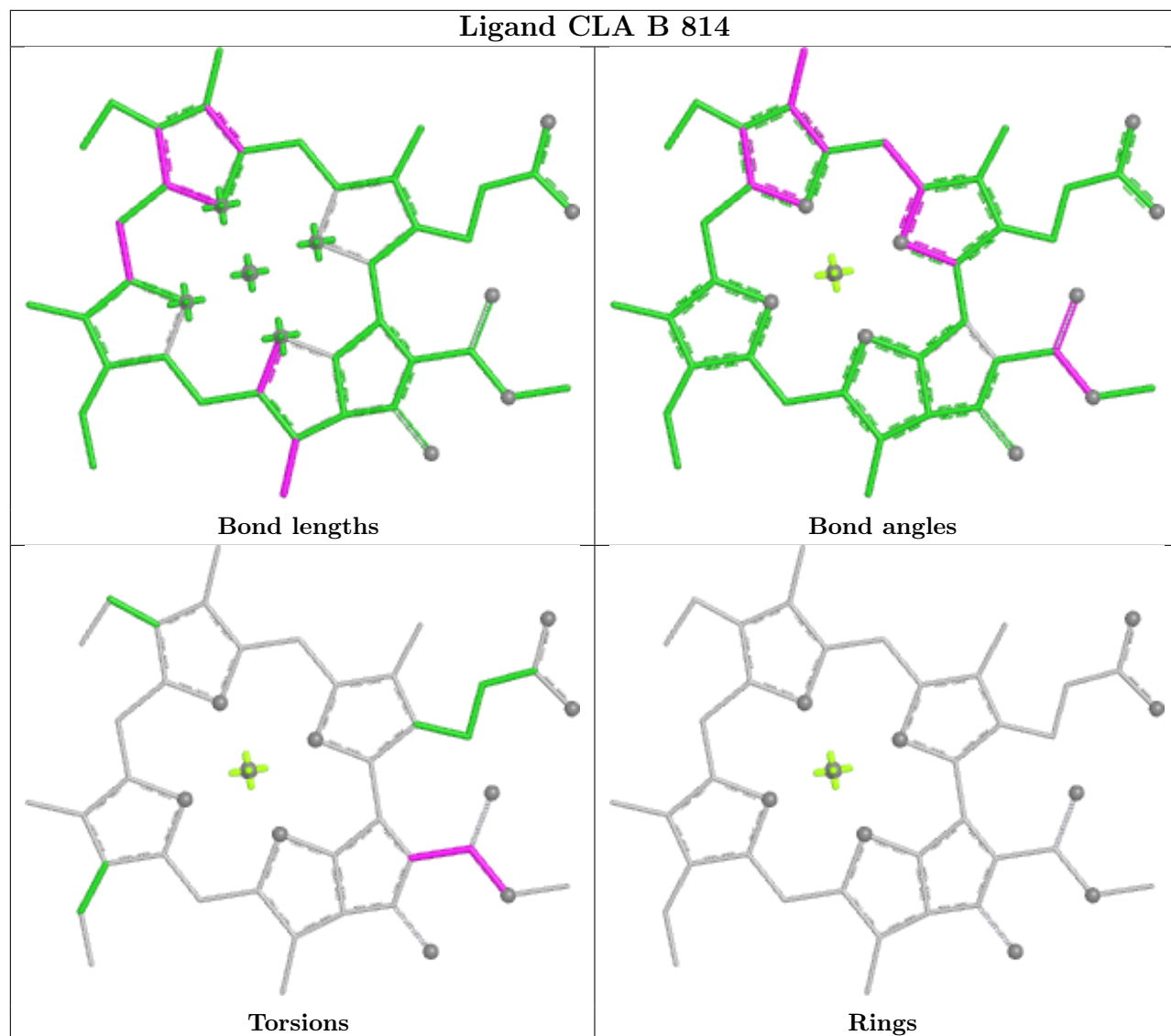


Ligand CLA O 804

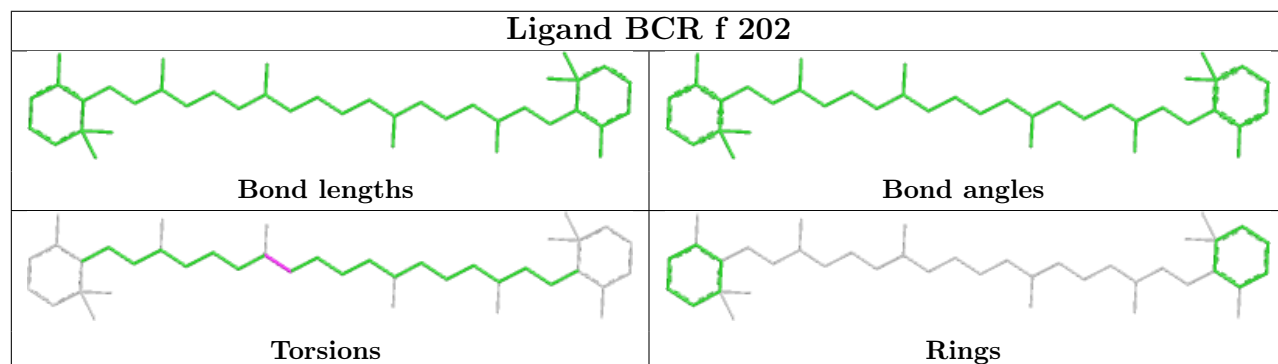


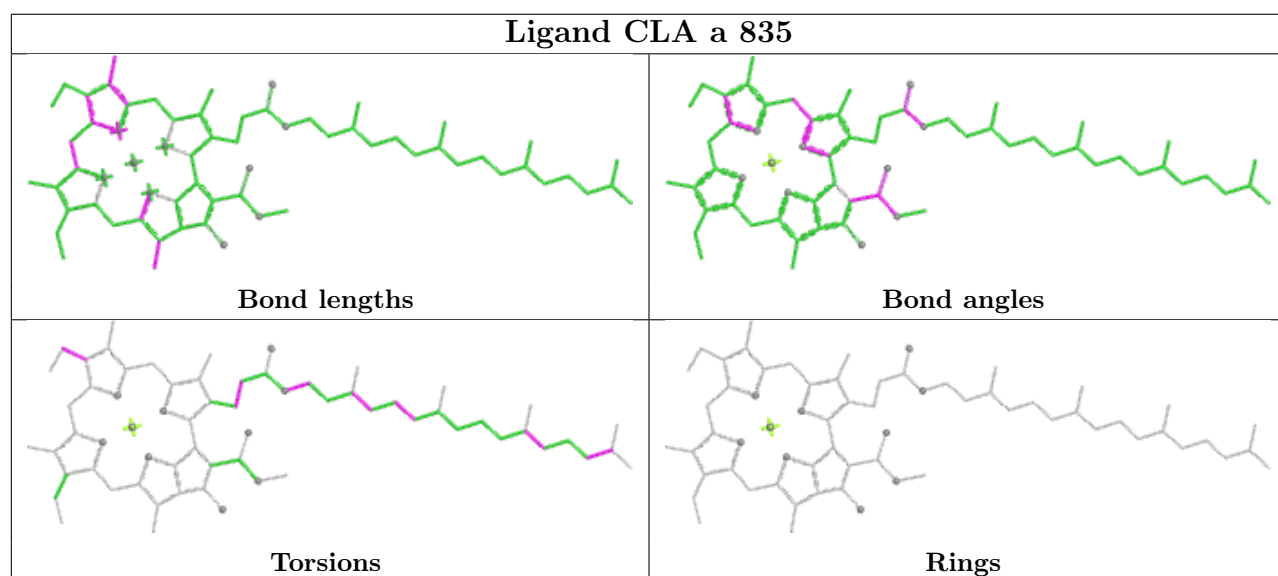
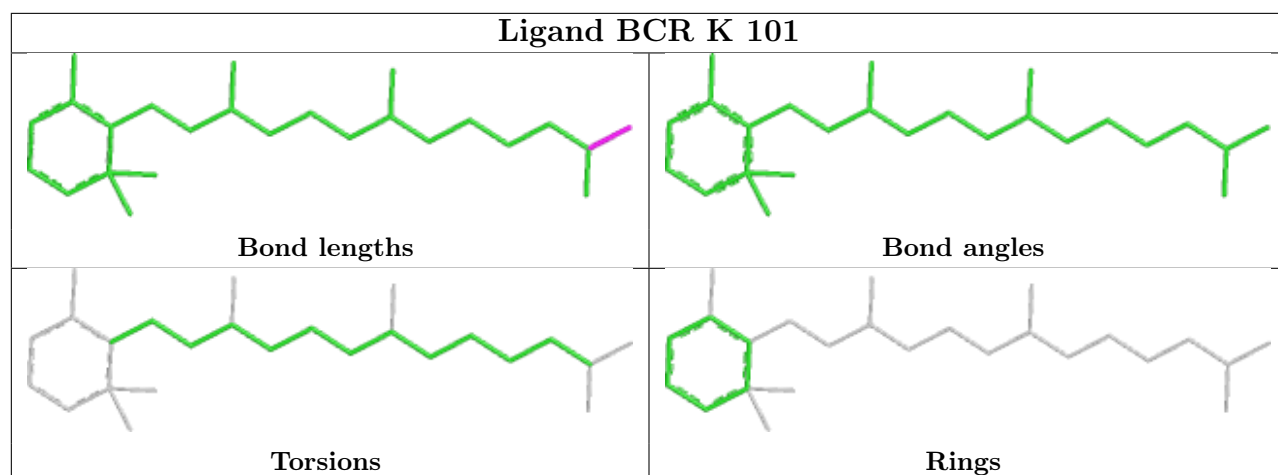
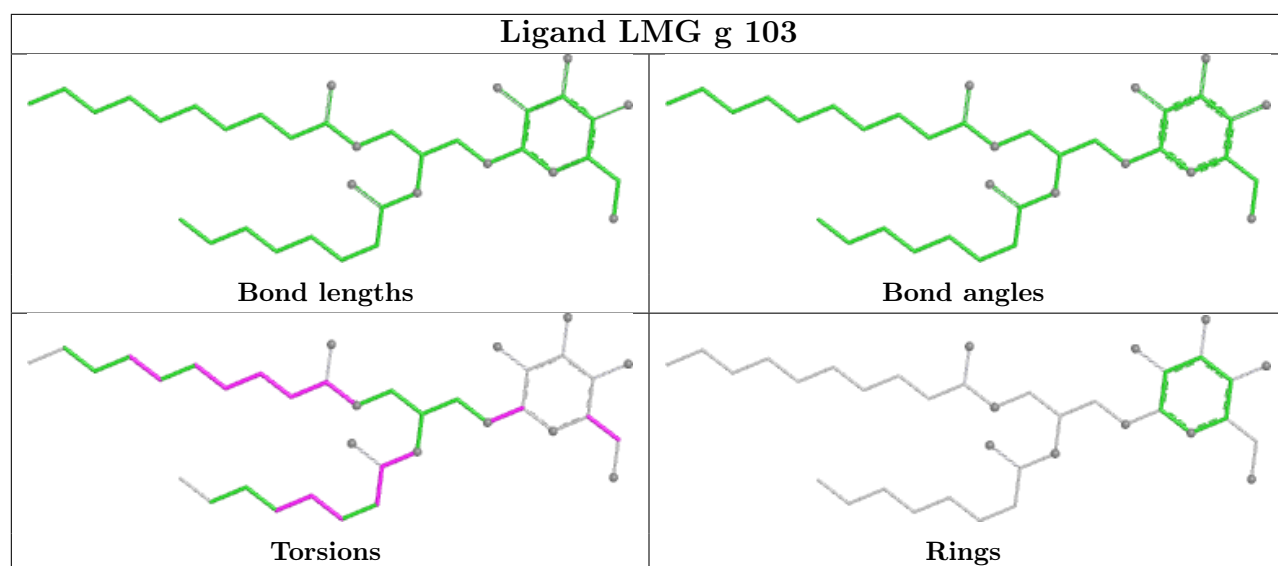


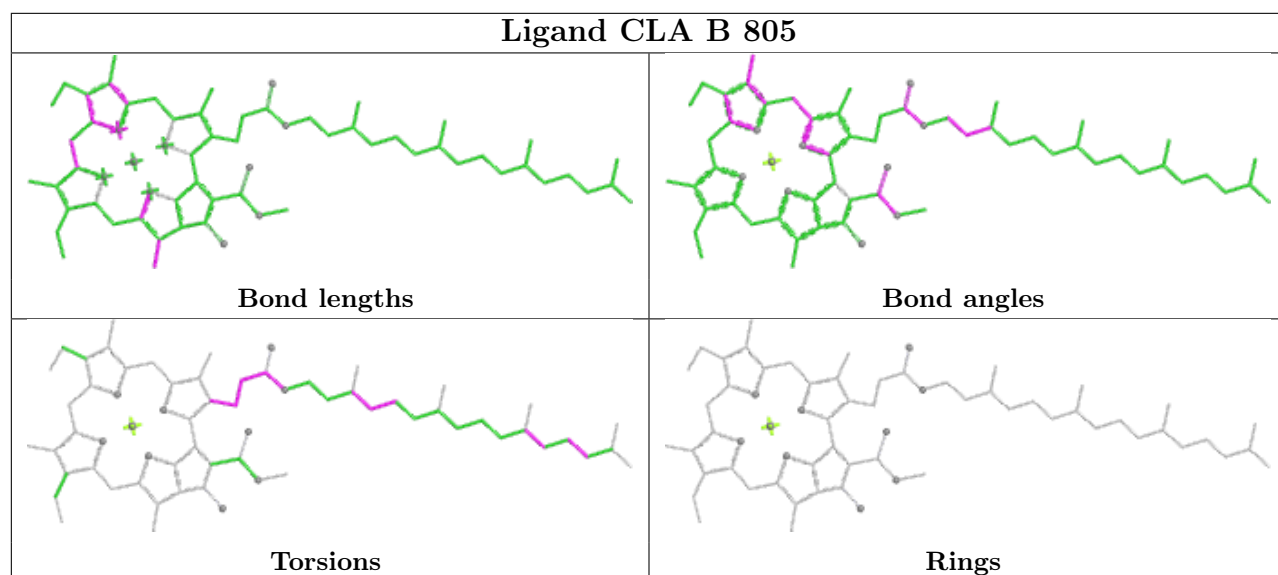
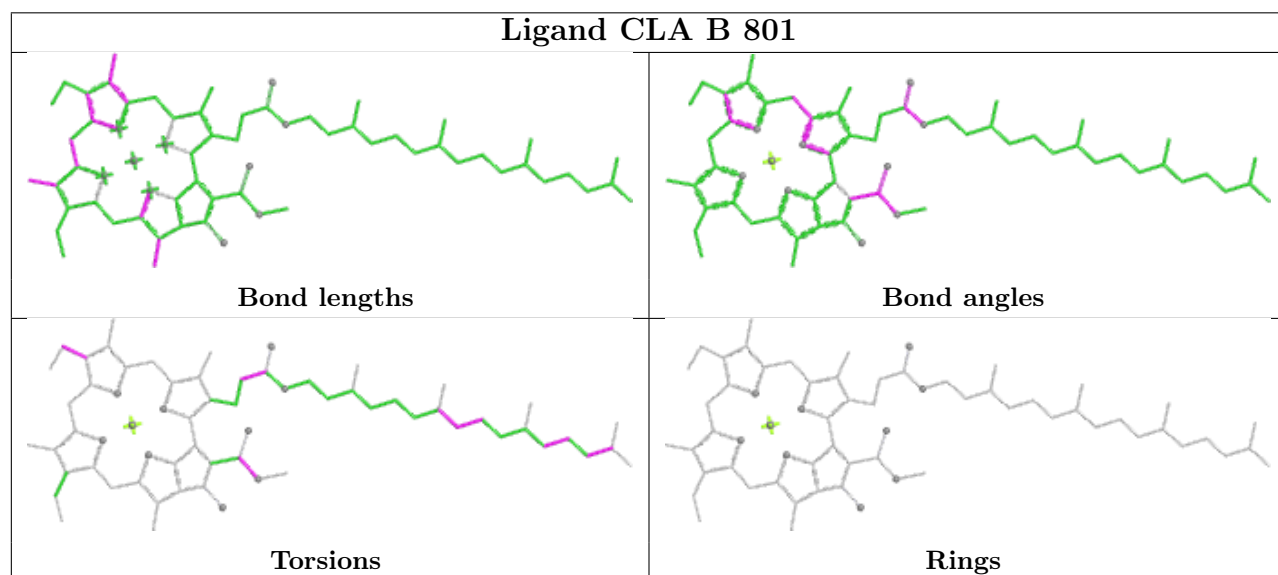
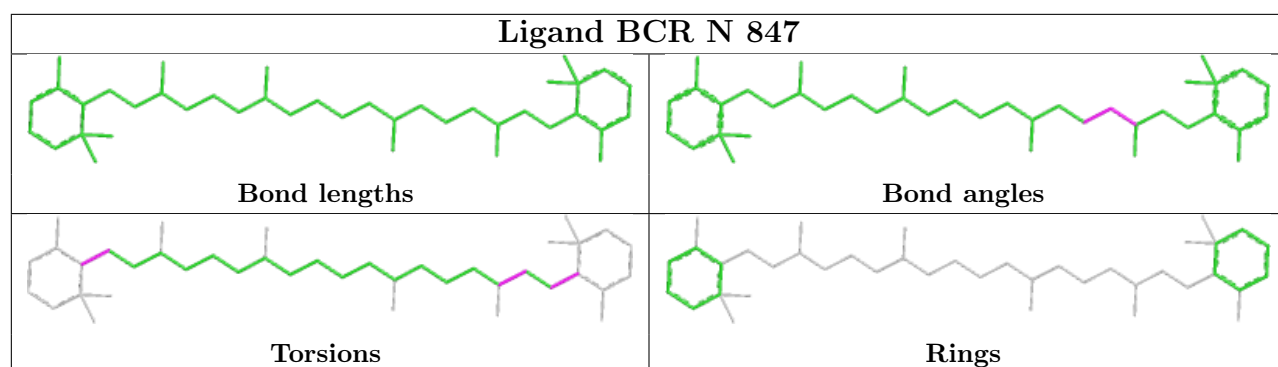
Ligand CLA B 814

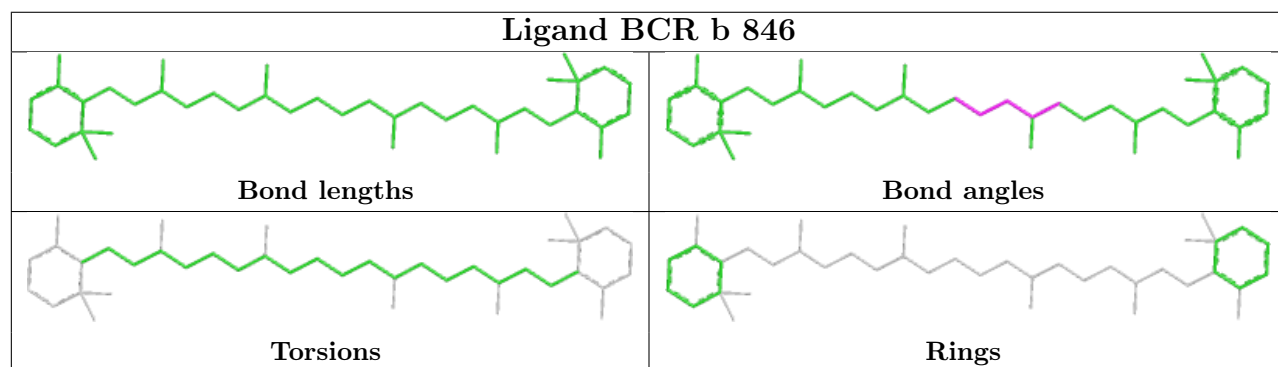
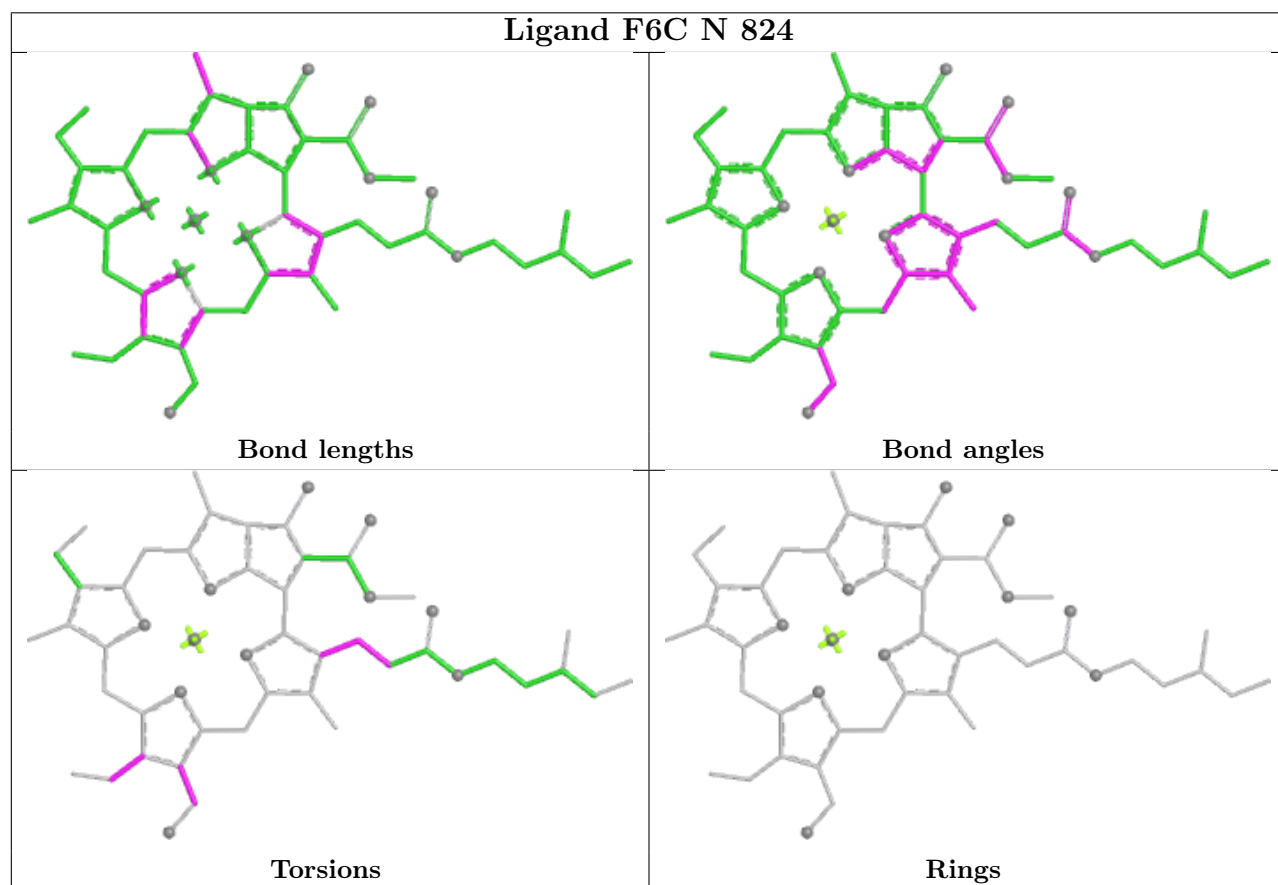
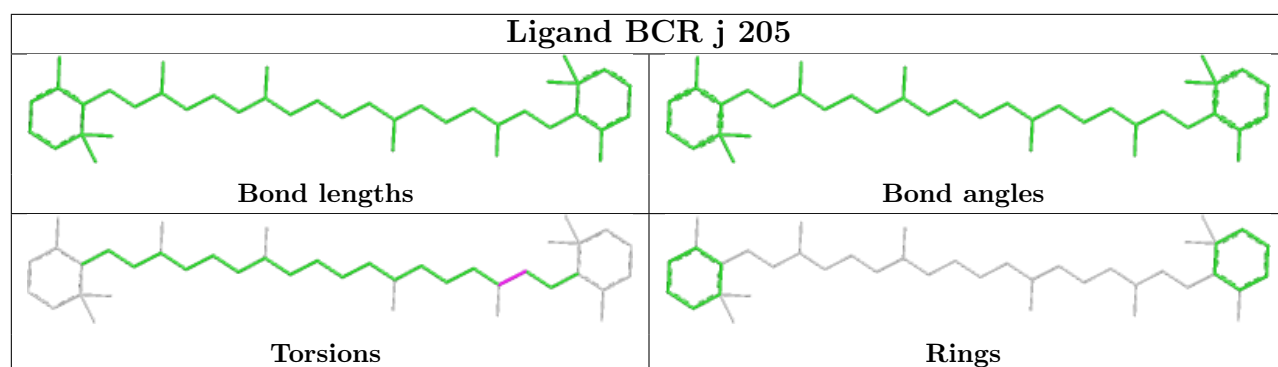


Ligand BCR f 202

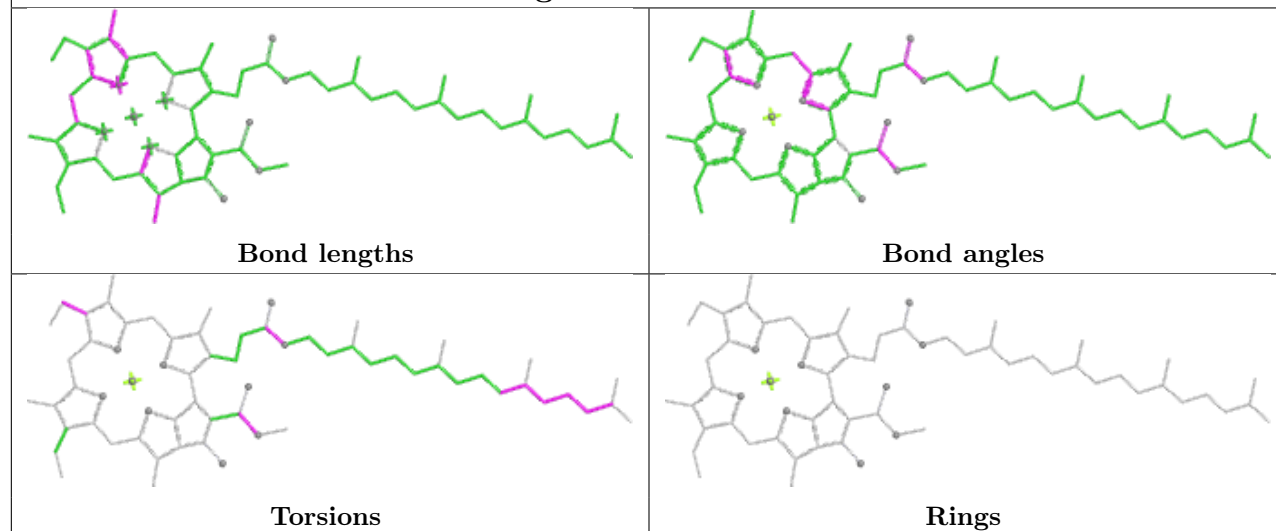




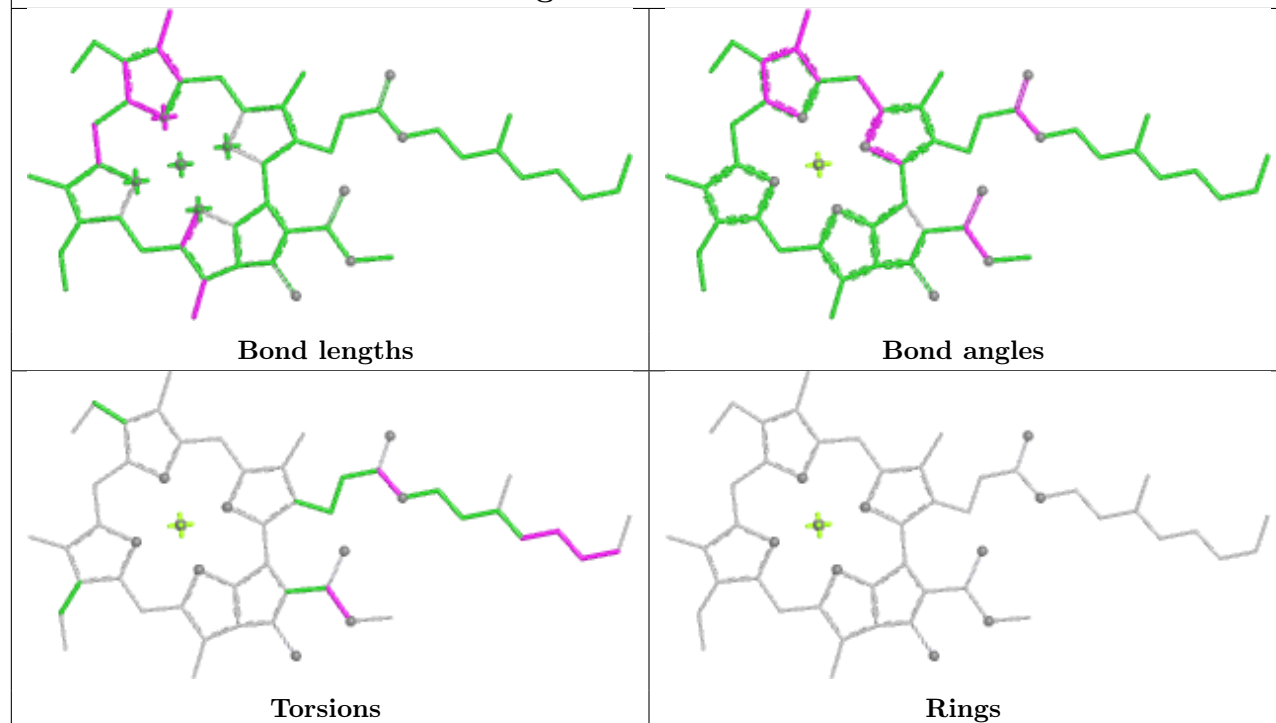


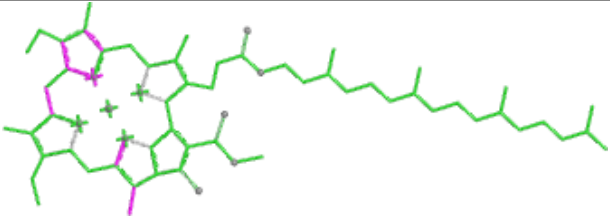
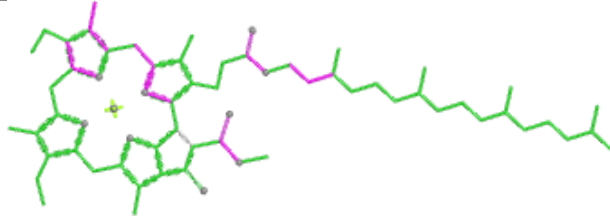
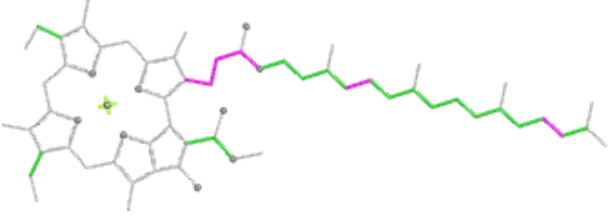
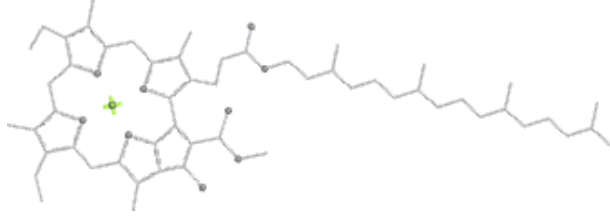
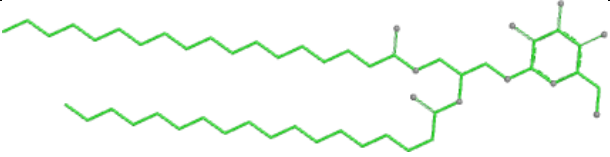
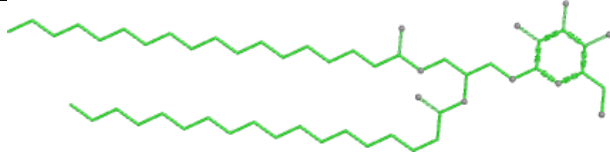

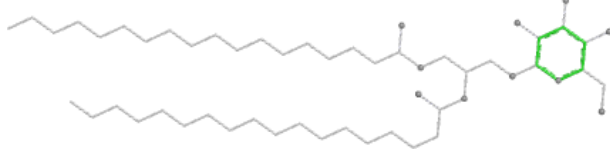

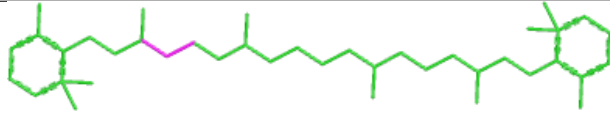
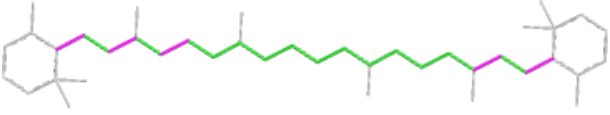
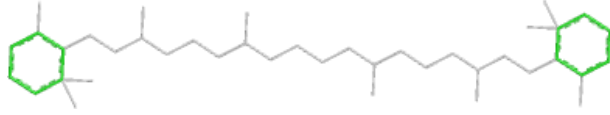


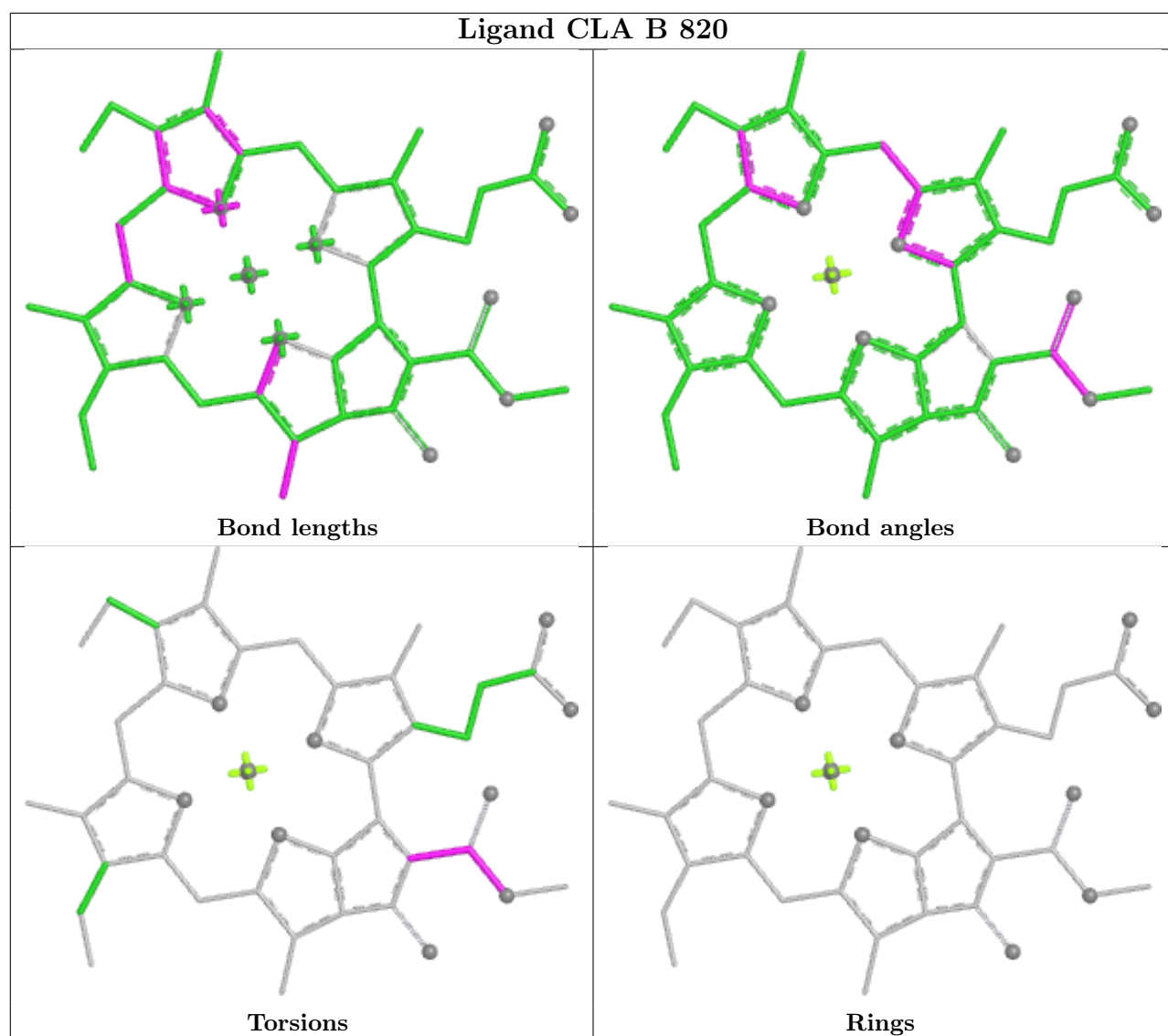
Ligand CLA b 840

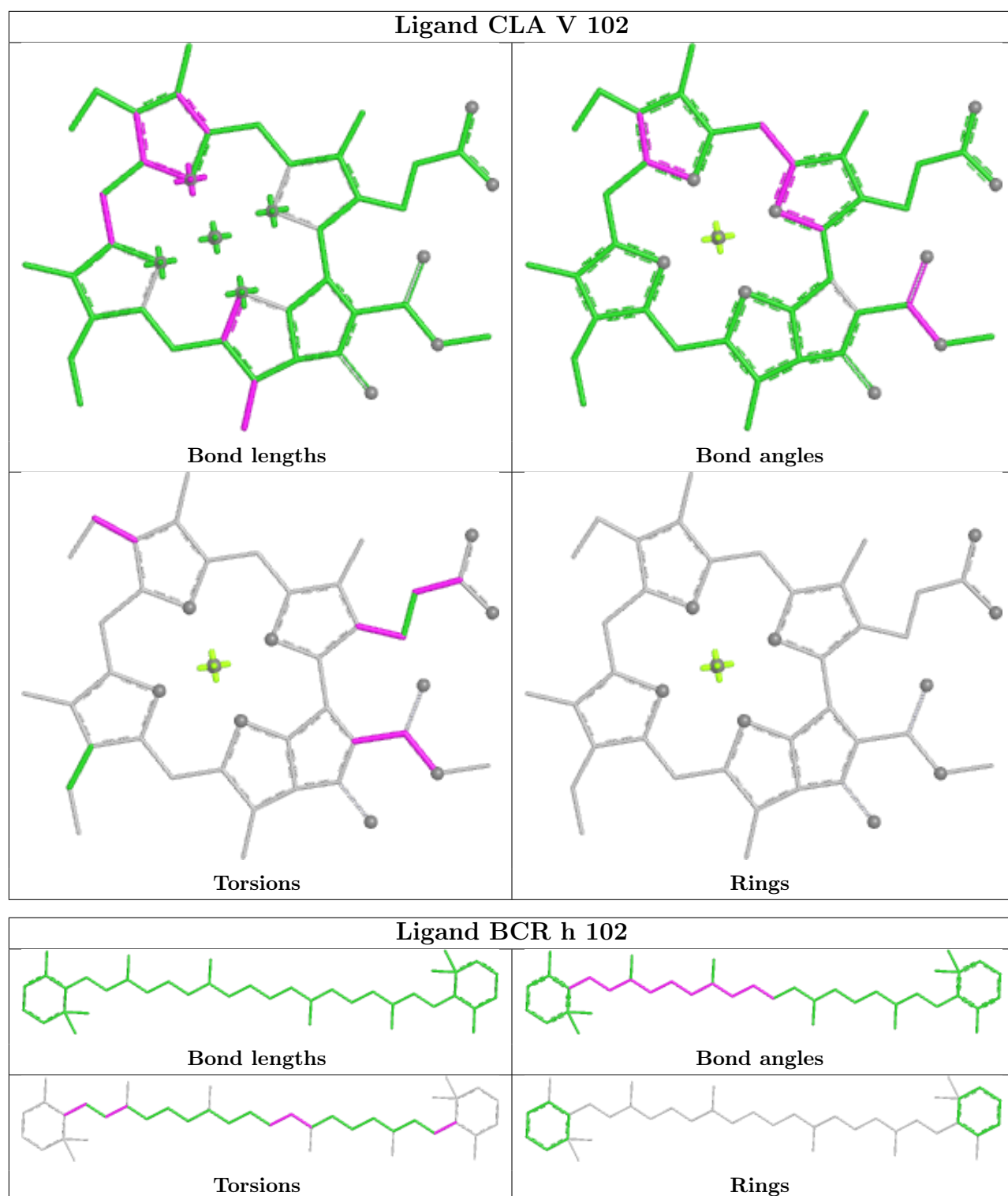


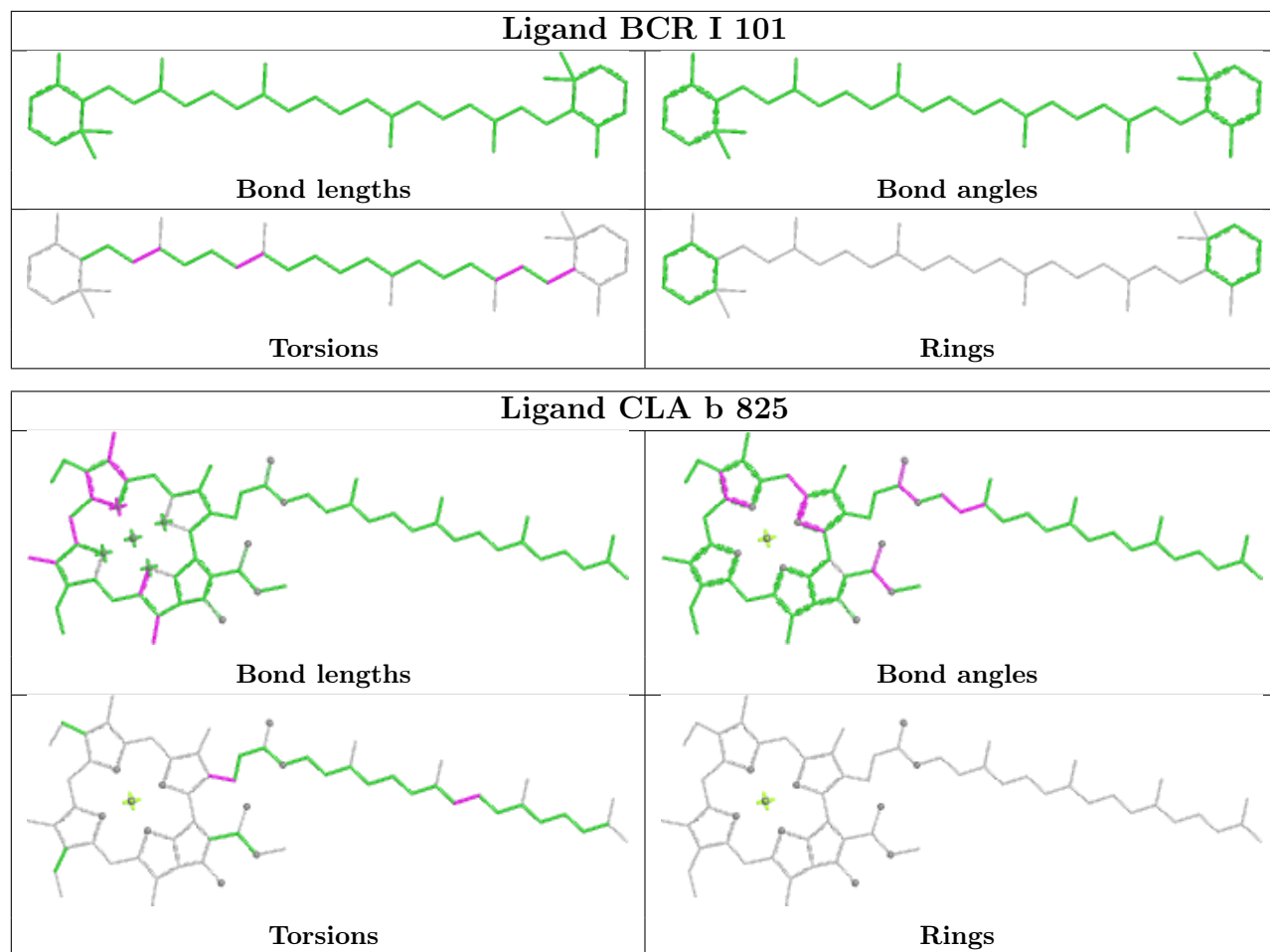
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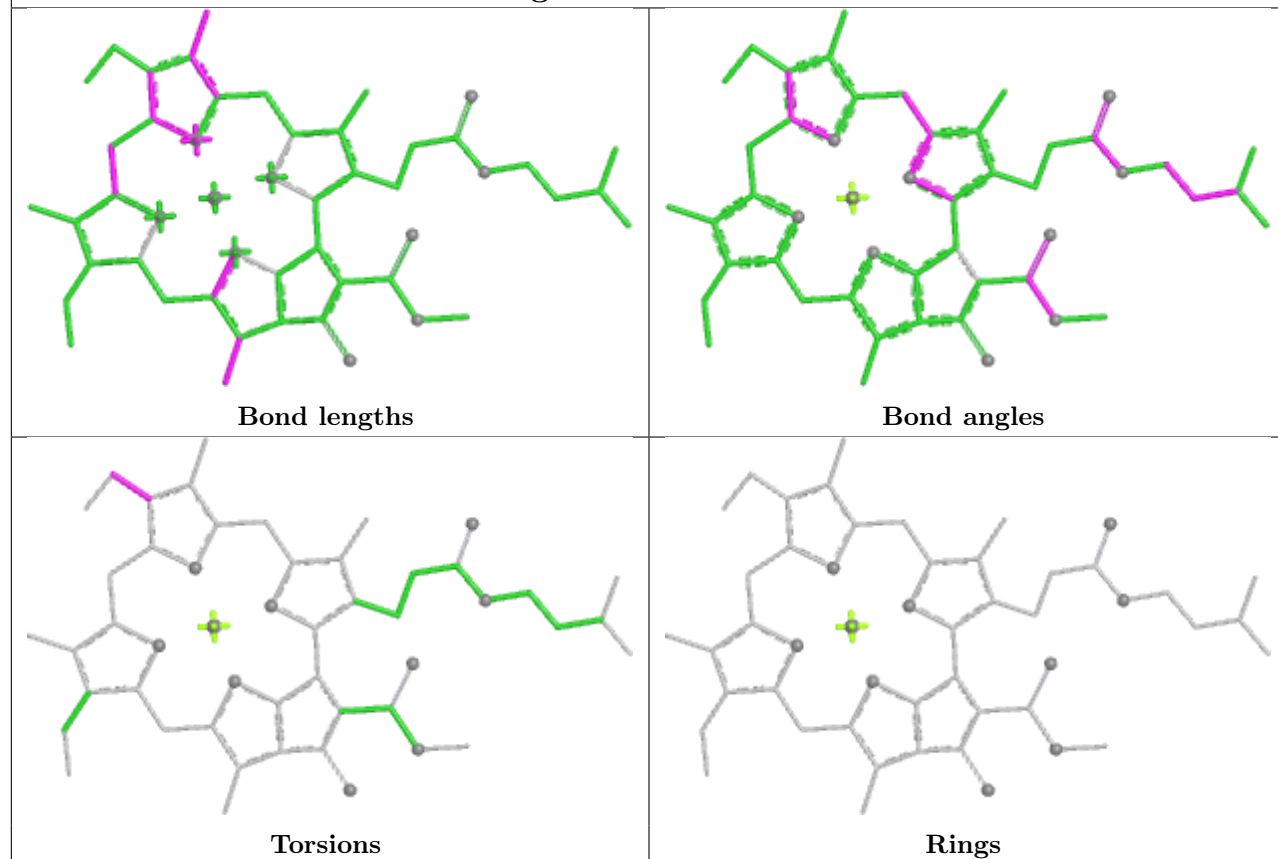
Ligand CLA b 805	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG h 103	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 846	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



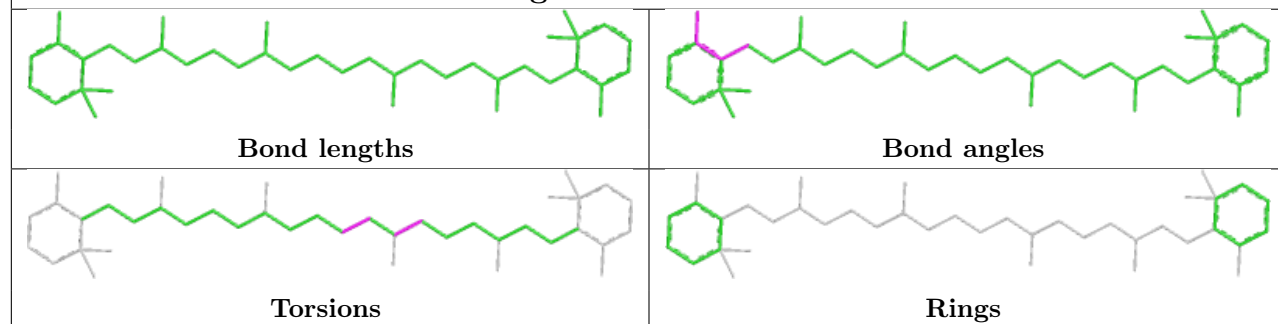




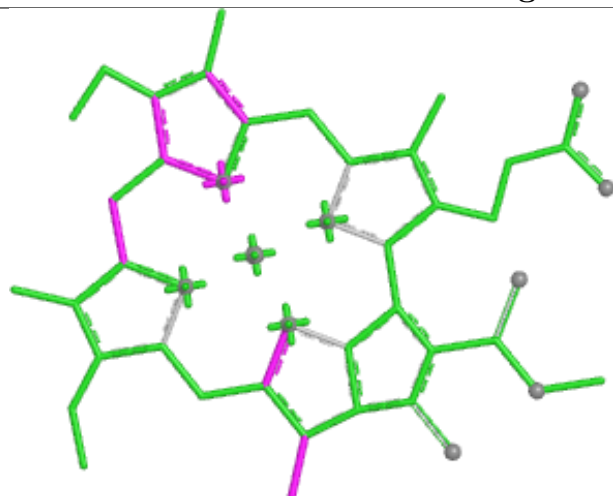
Ligand CLA K 103



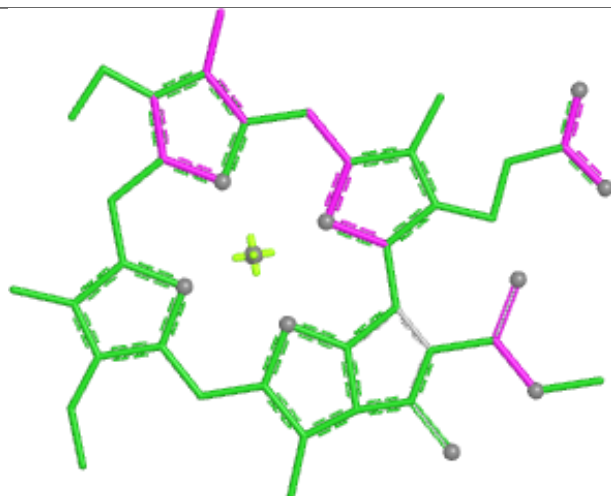
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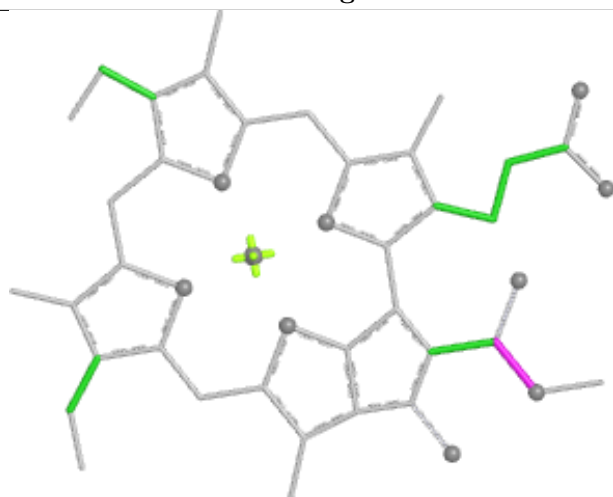
Ligand CLA a 808



Bond lengths



Bond angles

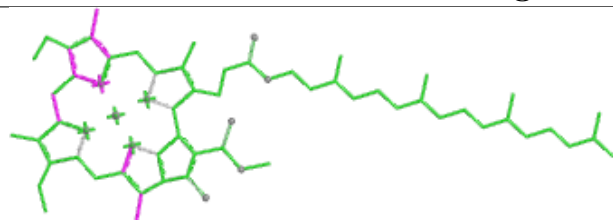


Torsions

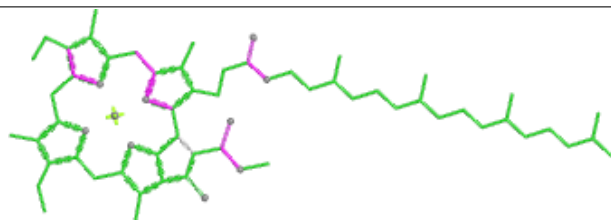


Rings

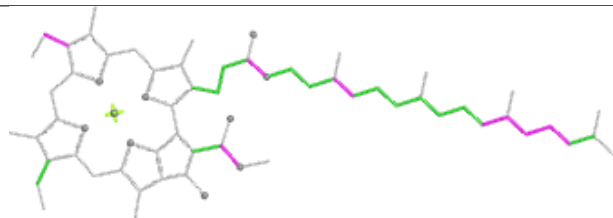
Ligand CLA O 840



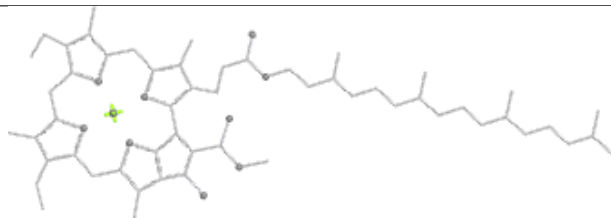
Bond lengths



Bond angles

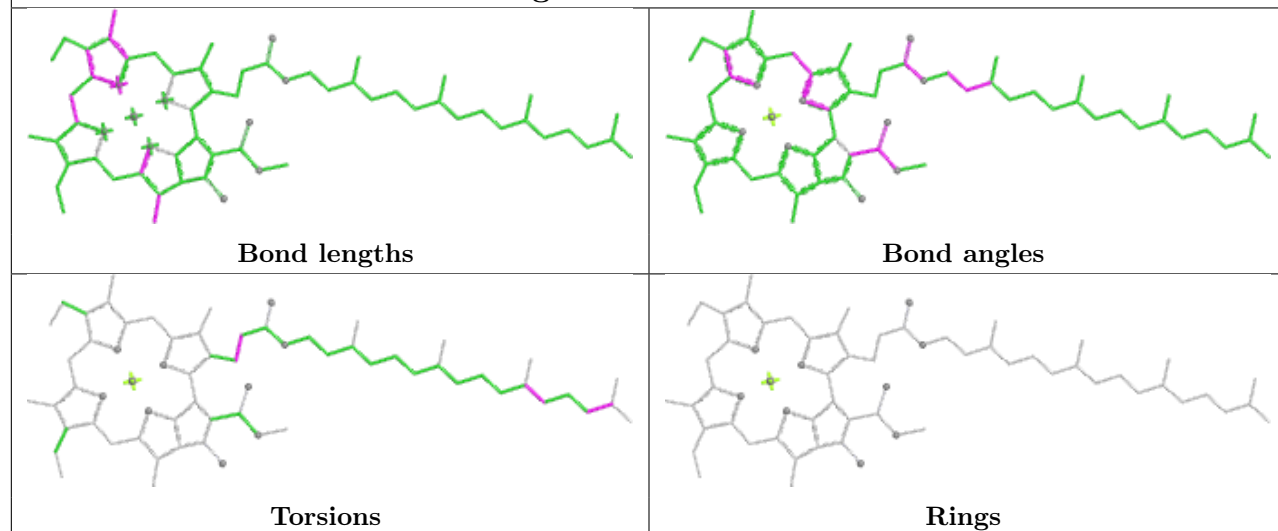


Torsions

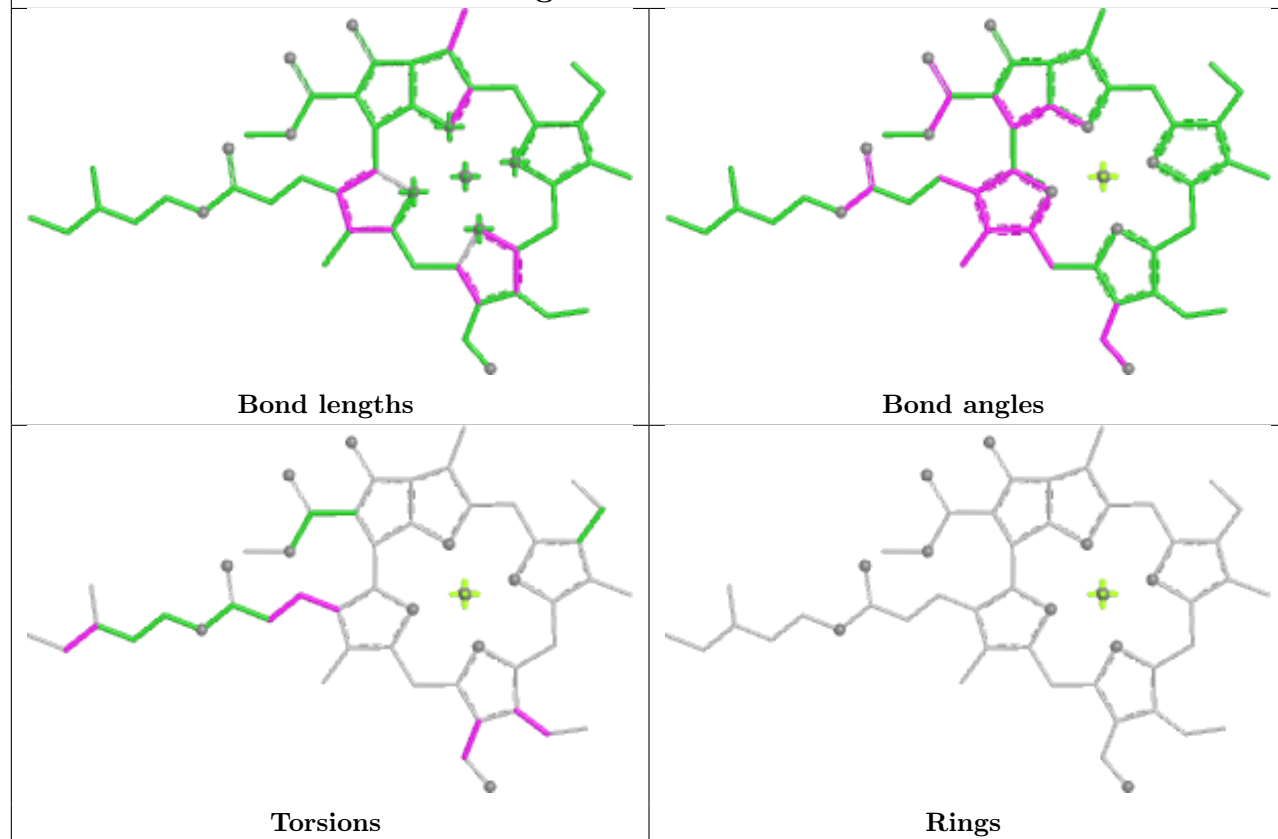


Rings

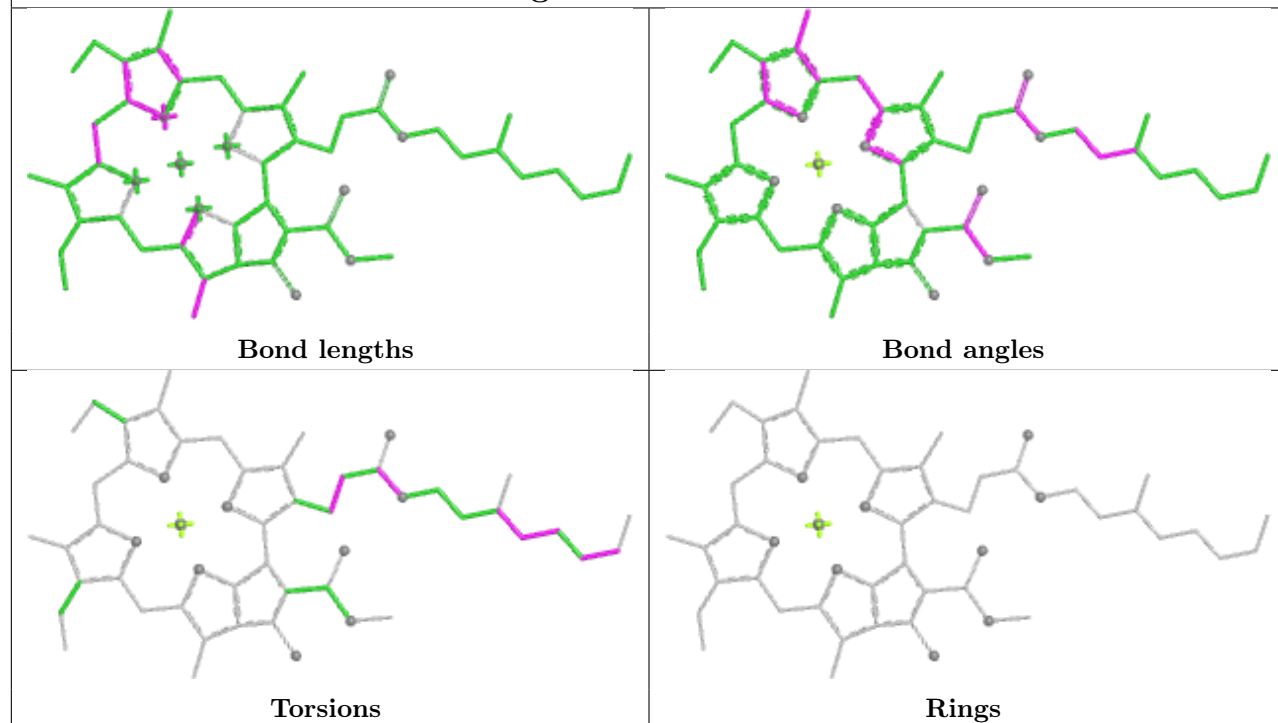
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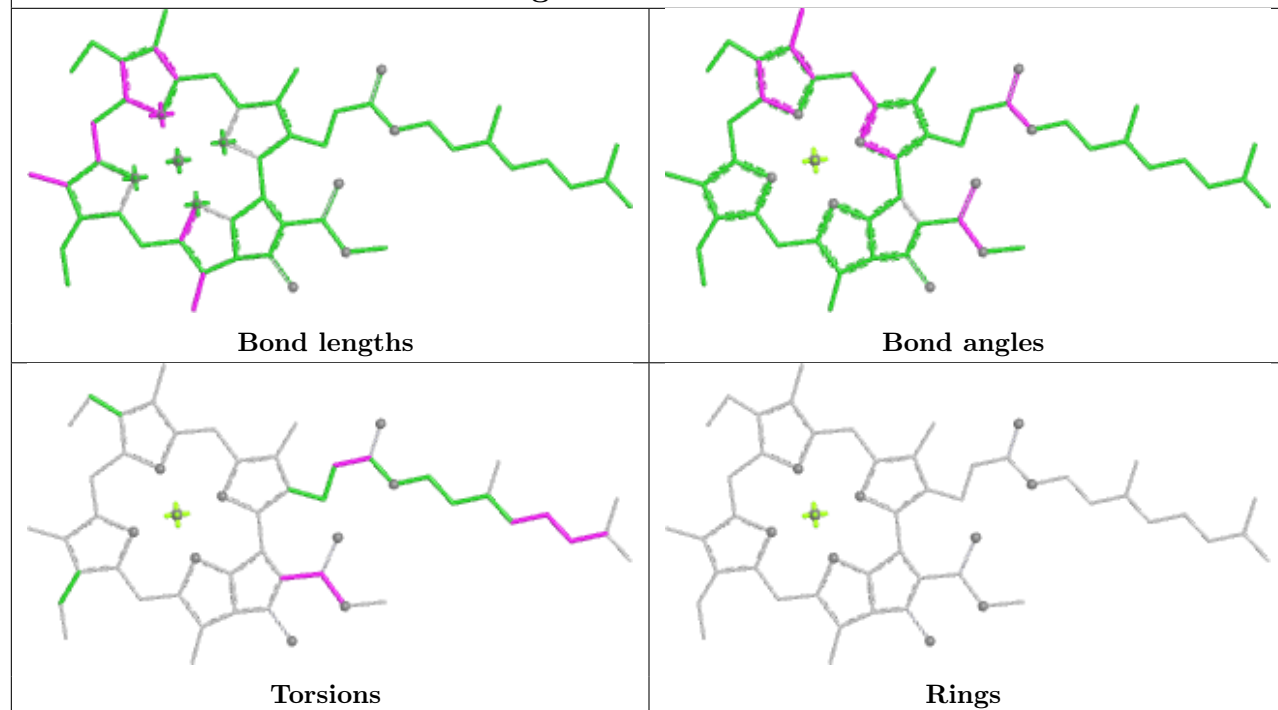
Ligand F6C A 824



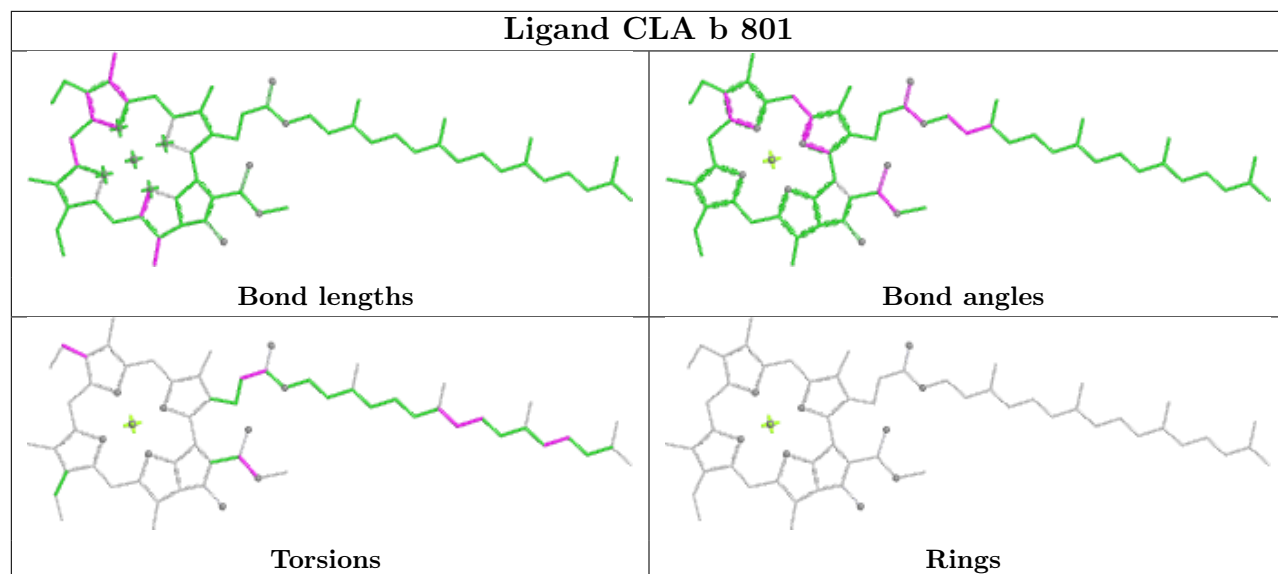
Ligand CLA N 813



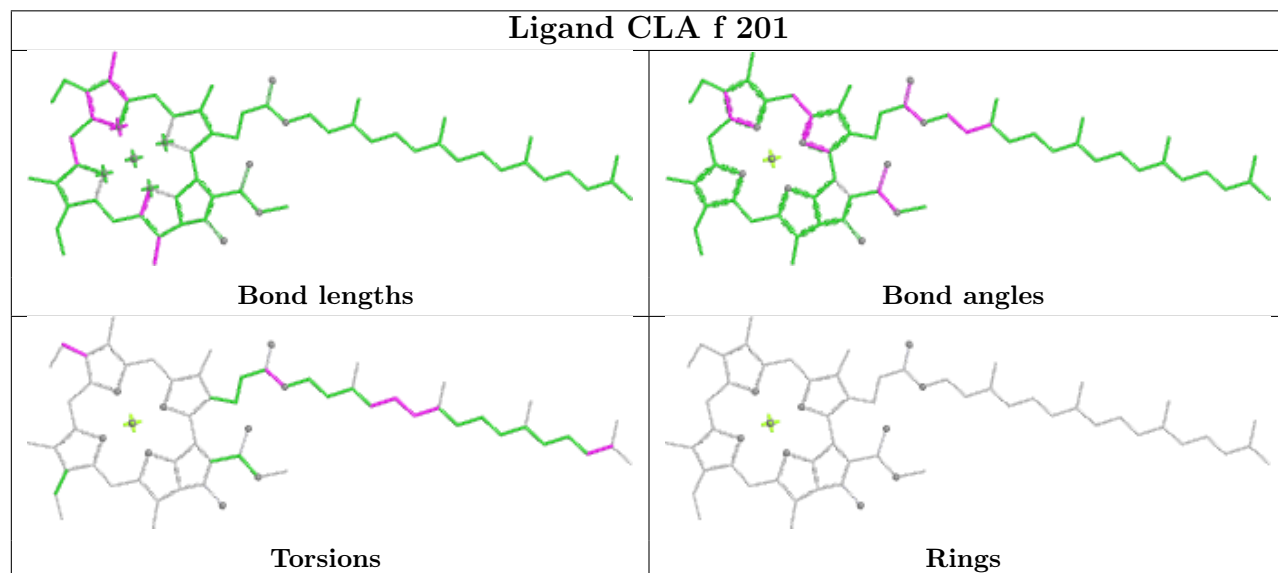
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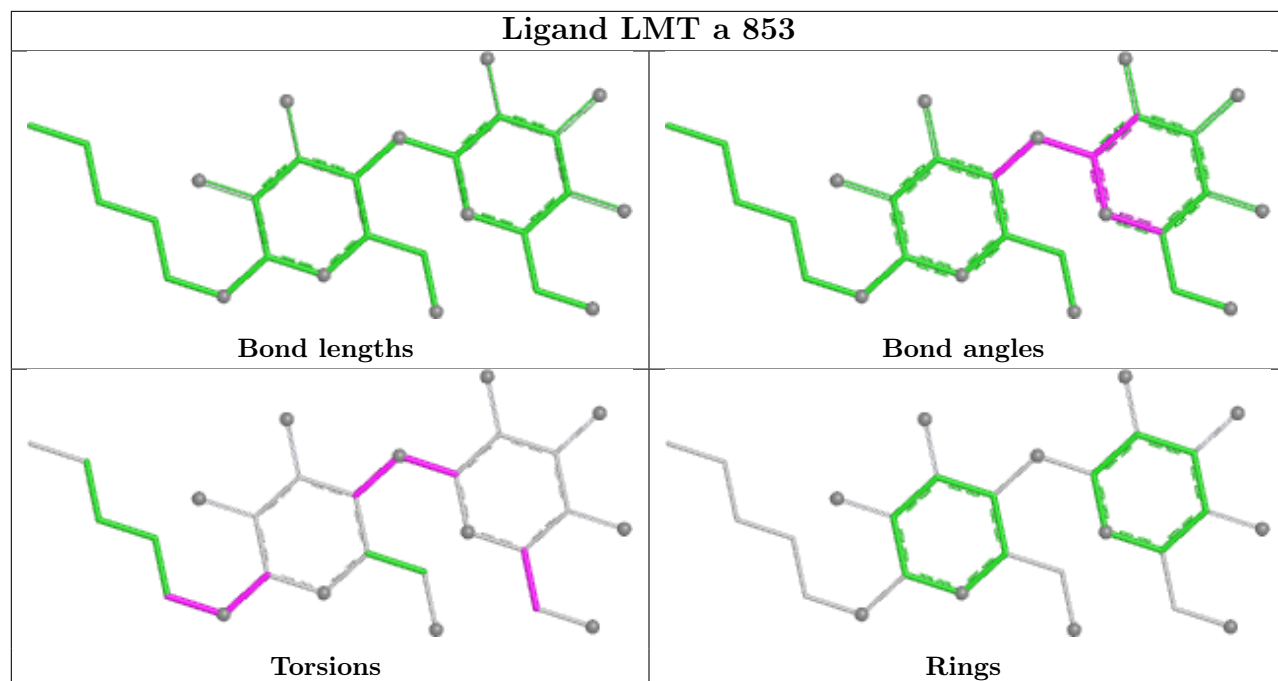
Ligand CLA b 801



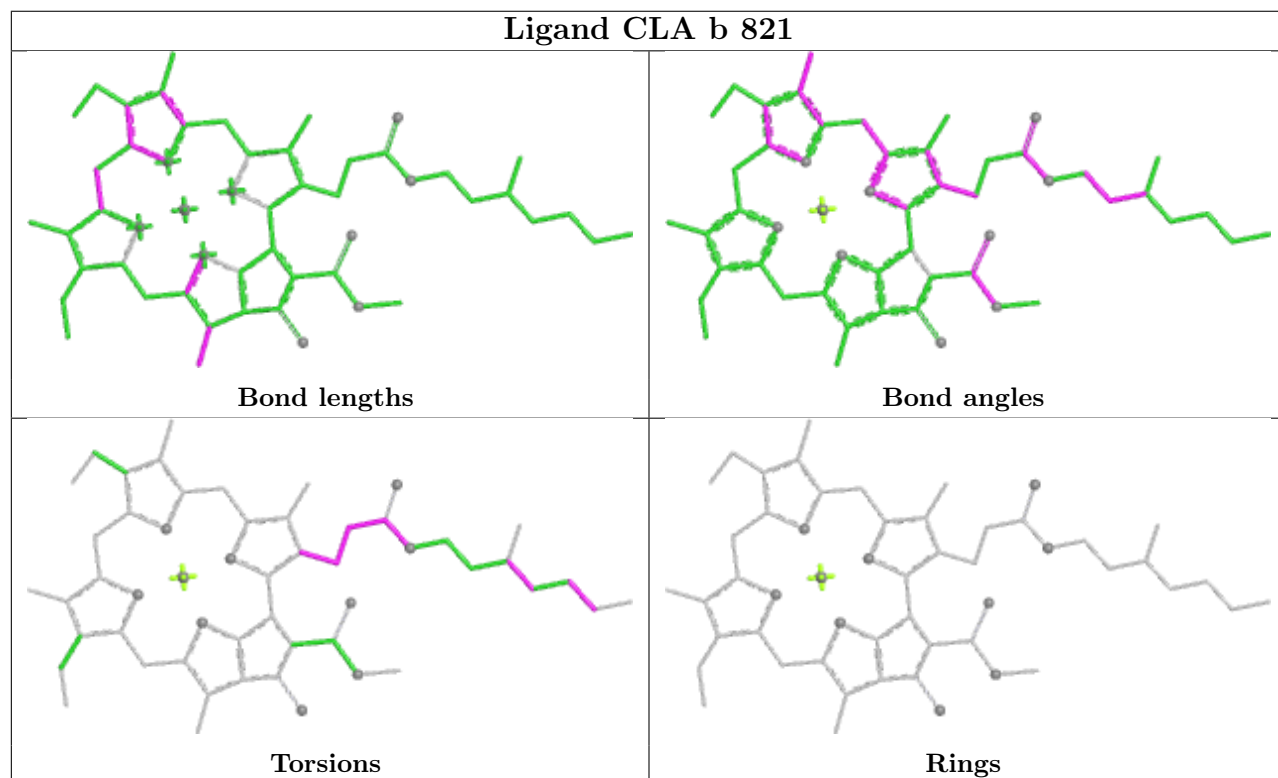
Ligand CLA f 201



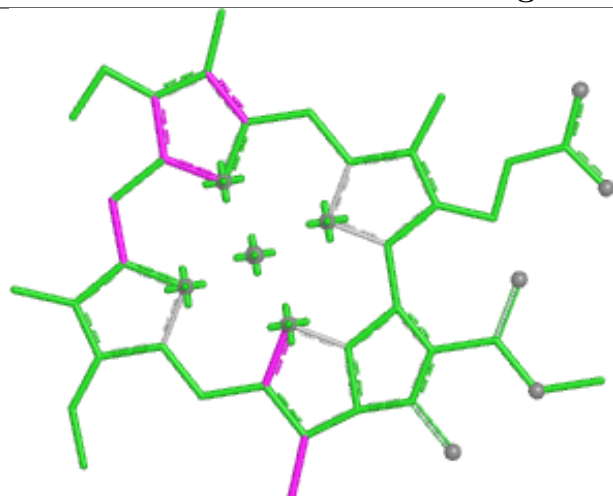
Ligand LMT a 853



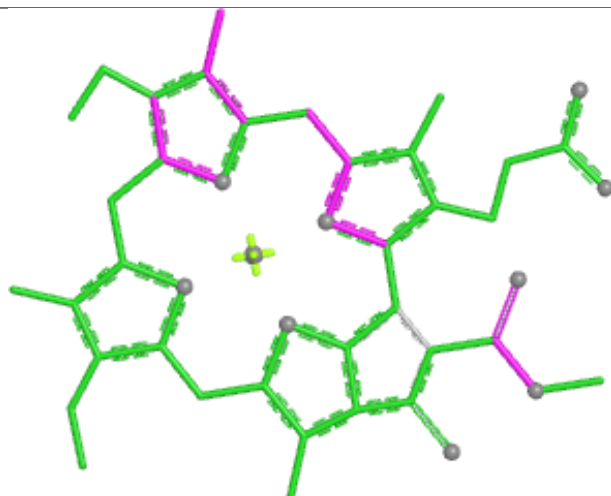
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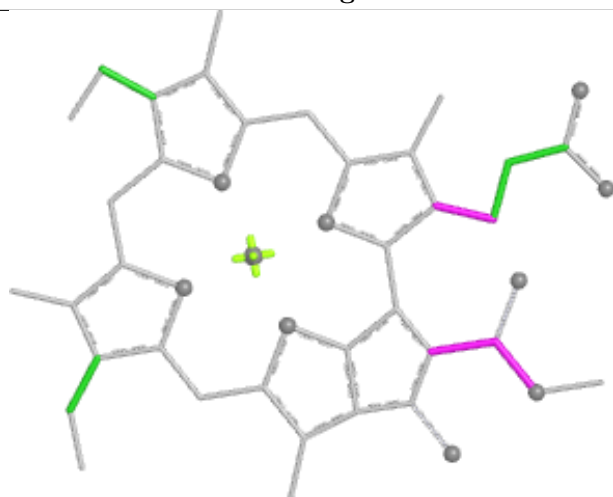
Ligand CLA b 814



Bond lengths



Bond angles

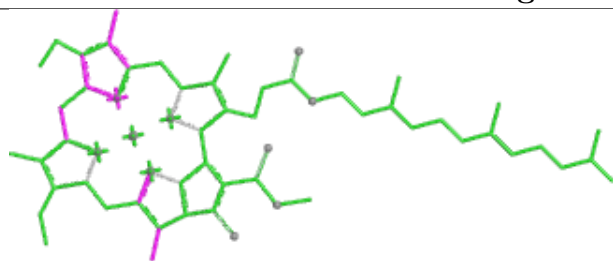


Torsions

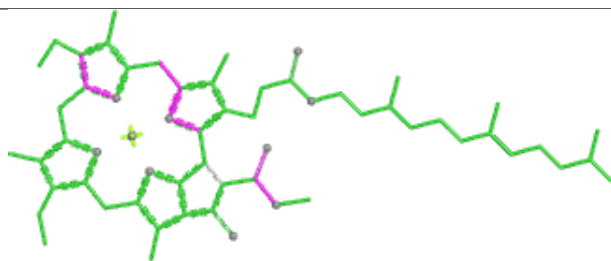


Rings

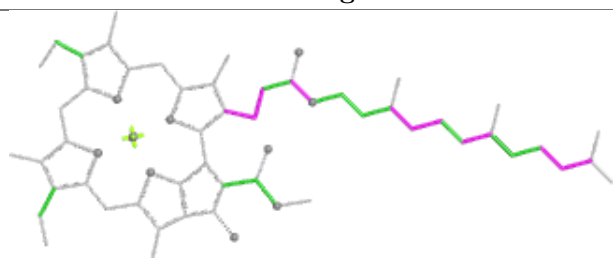
Ligand CLA b 817



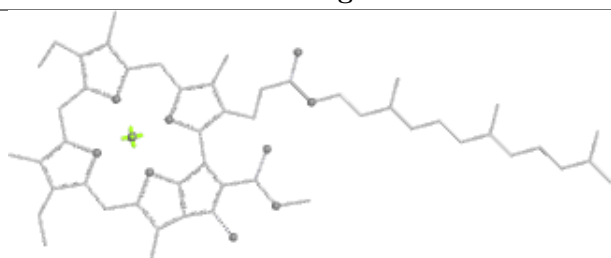
Bond lengths



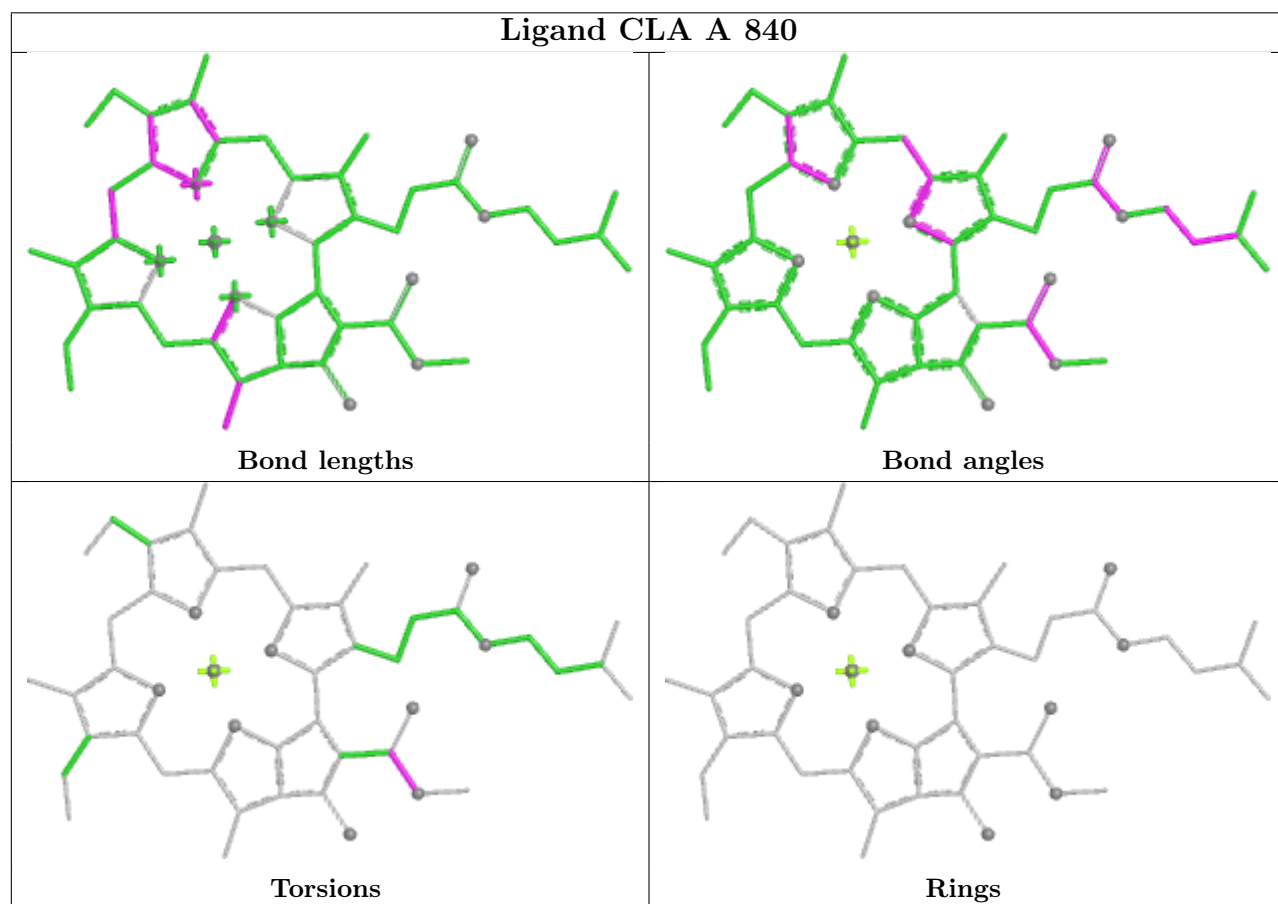
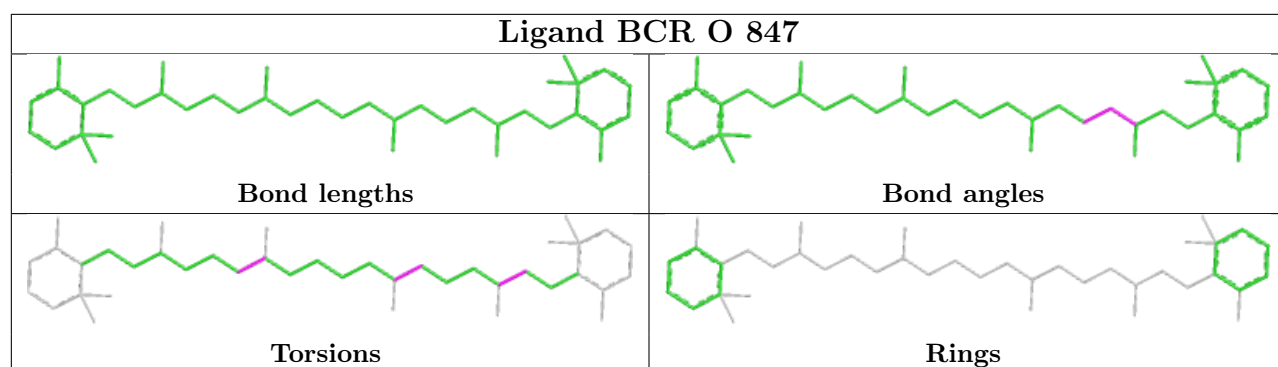
Bond angles



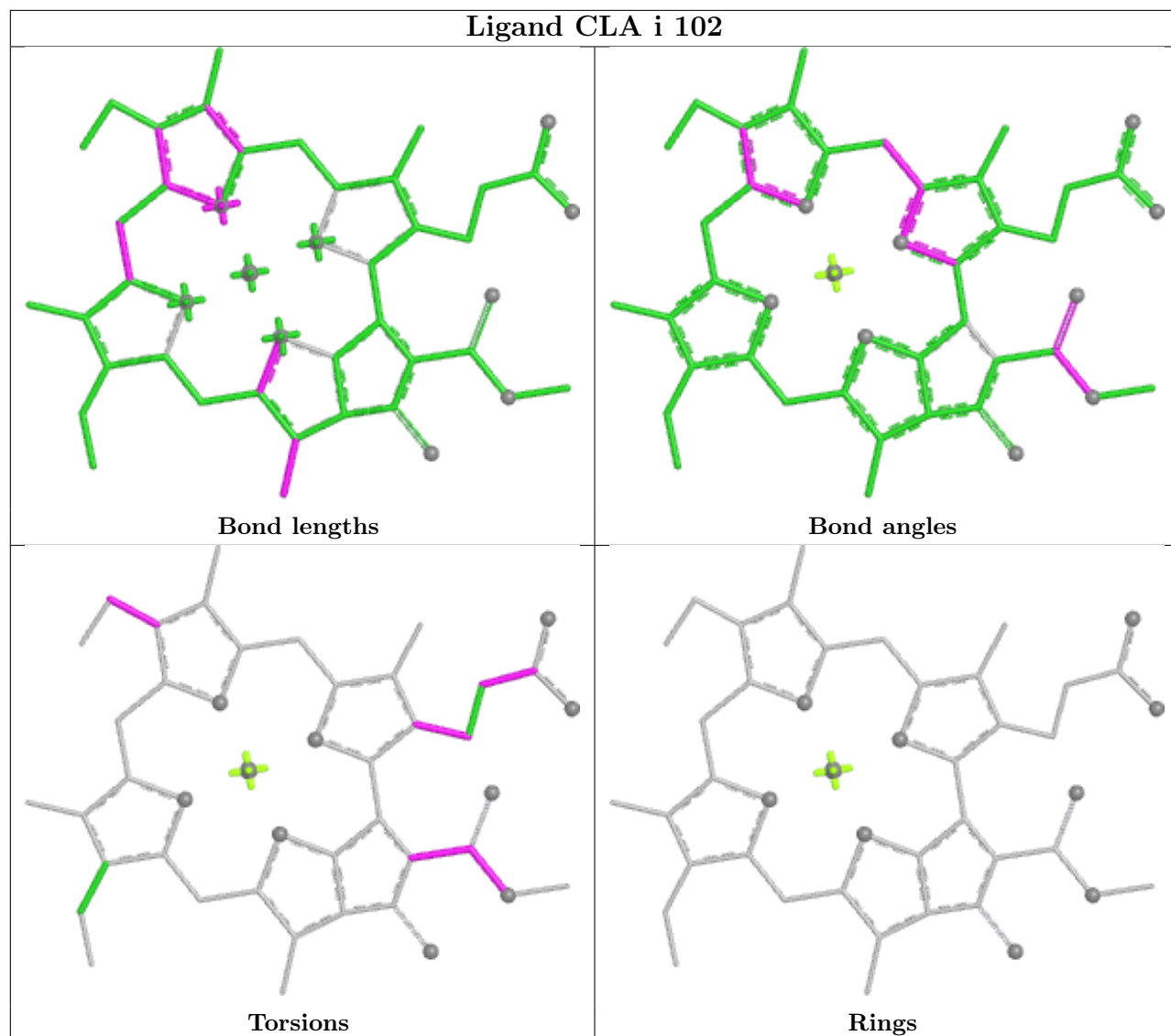
Torsions



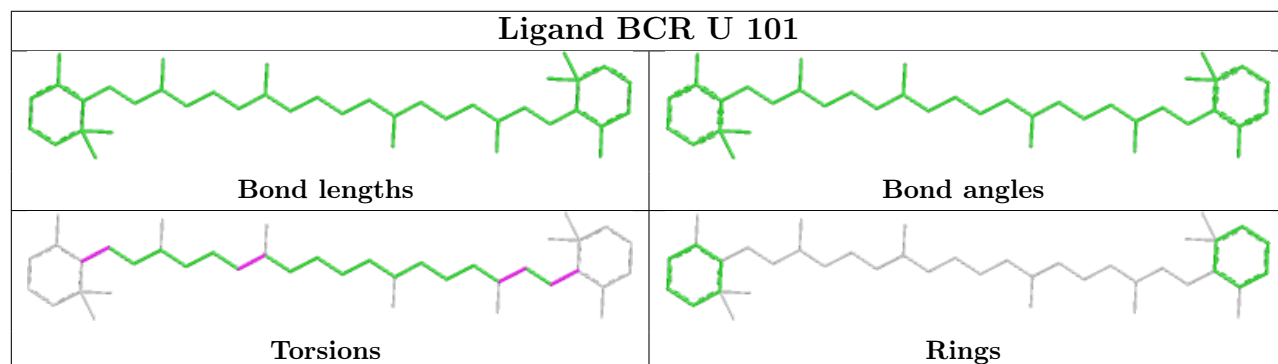
Rings

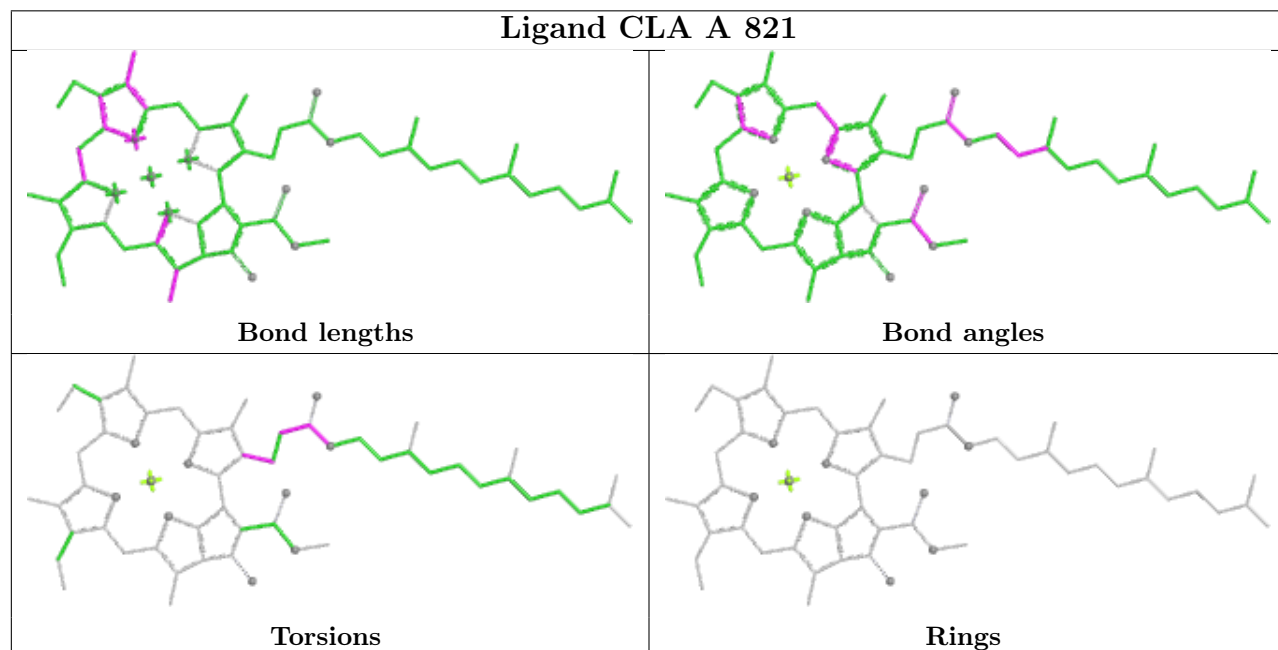
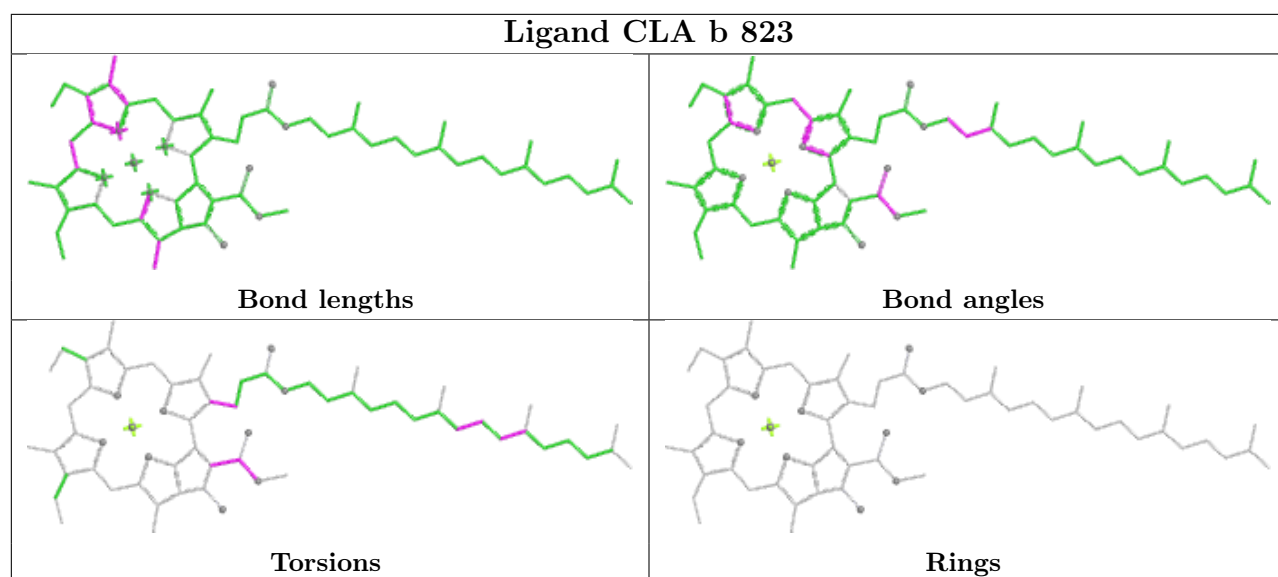


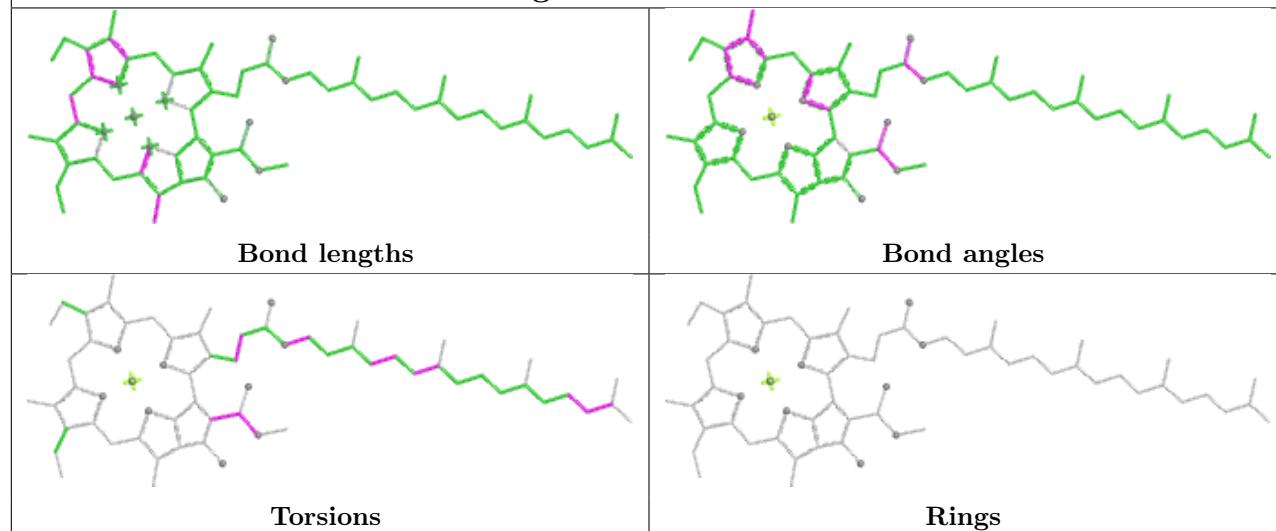
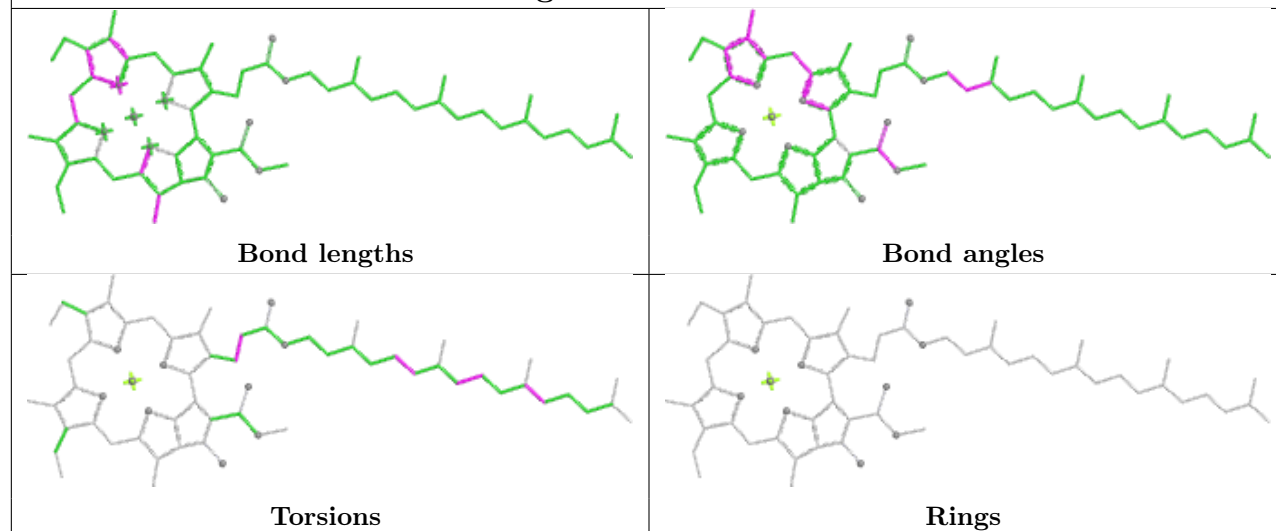
Ligand CLA i 102



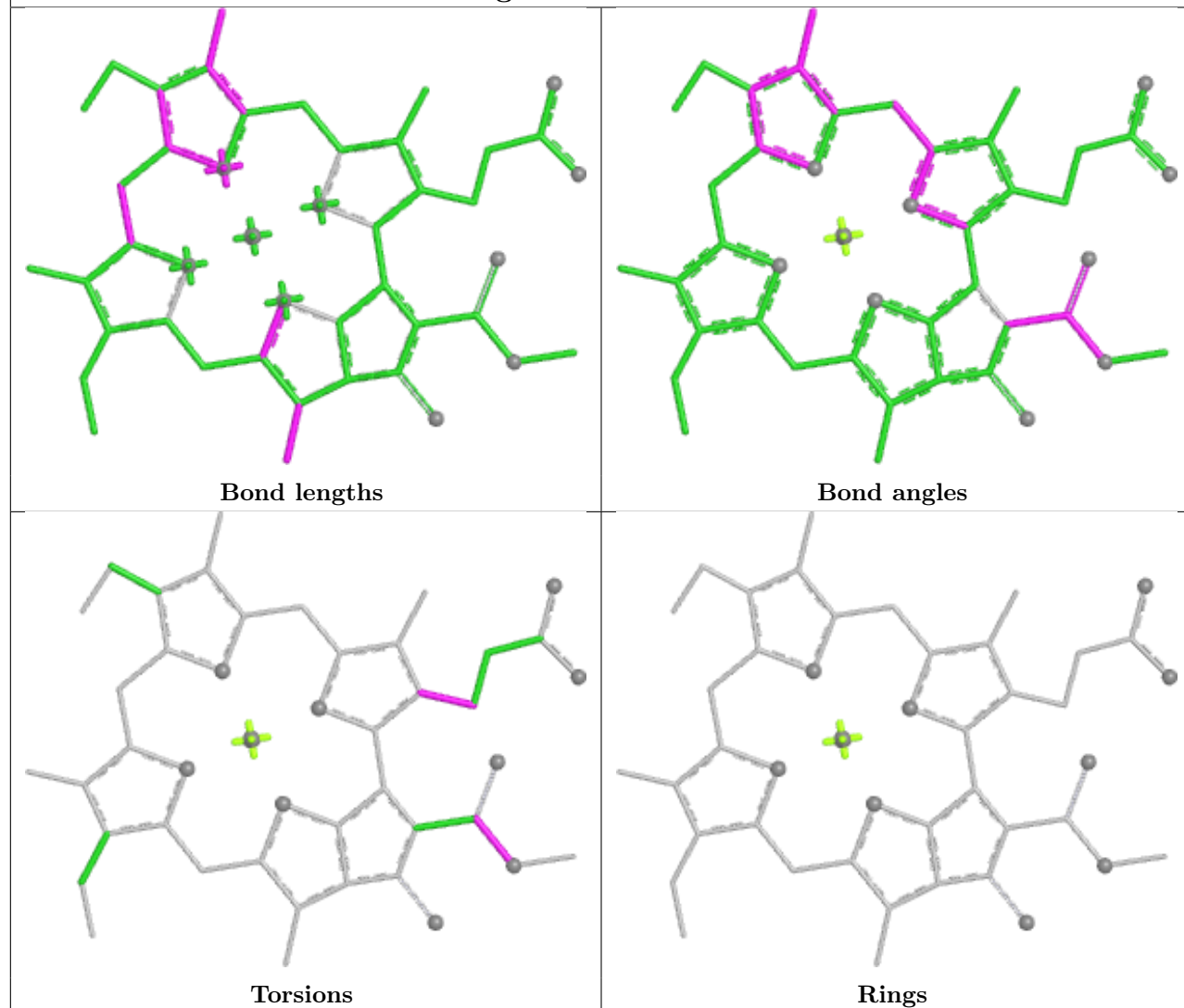
Ligand BCR U 101



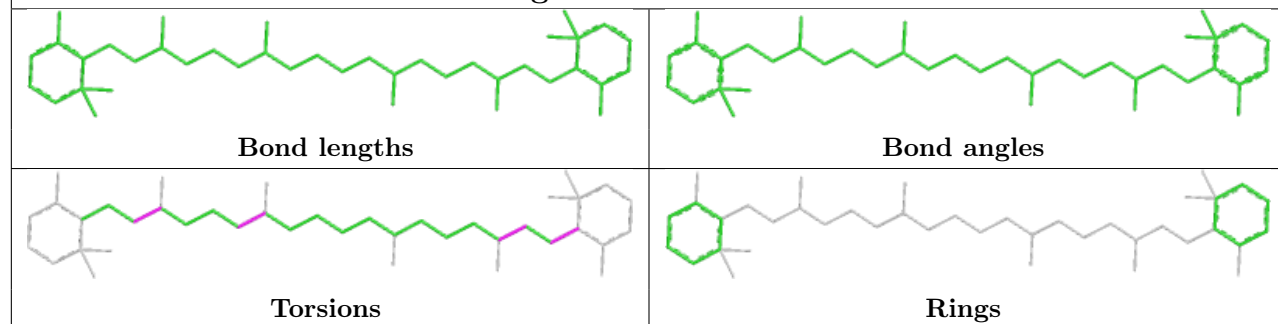


Ligand CLA B 802**Ligand CLA a 830**

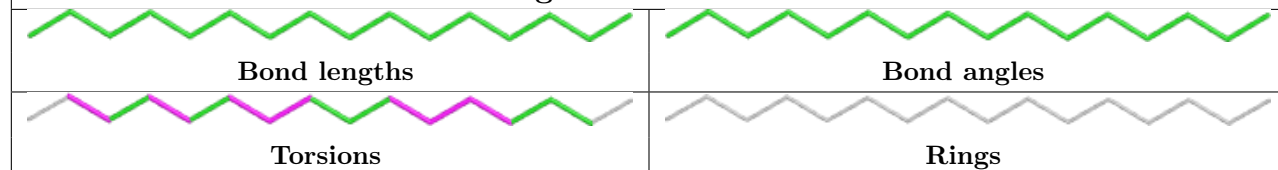
Ligand CLA b 834

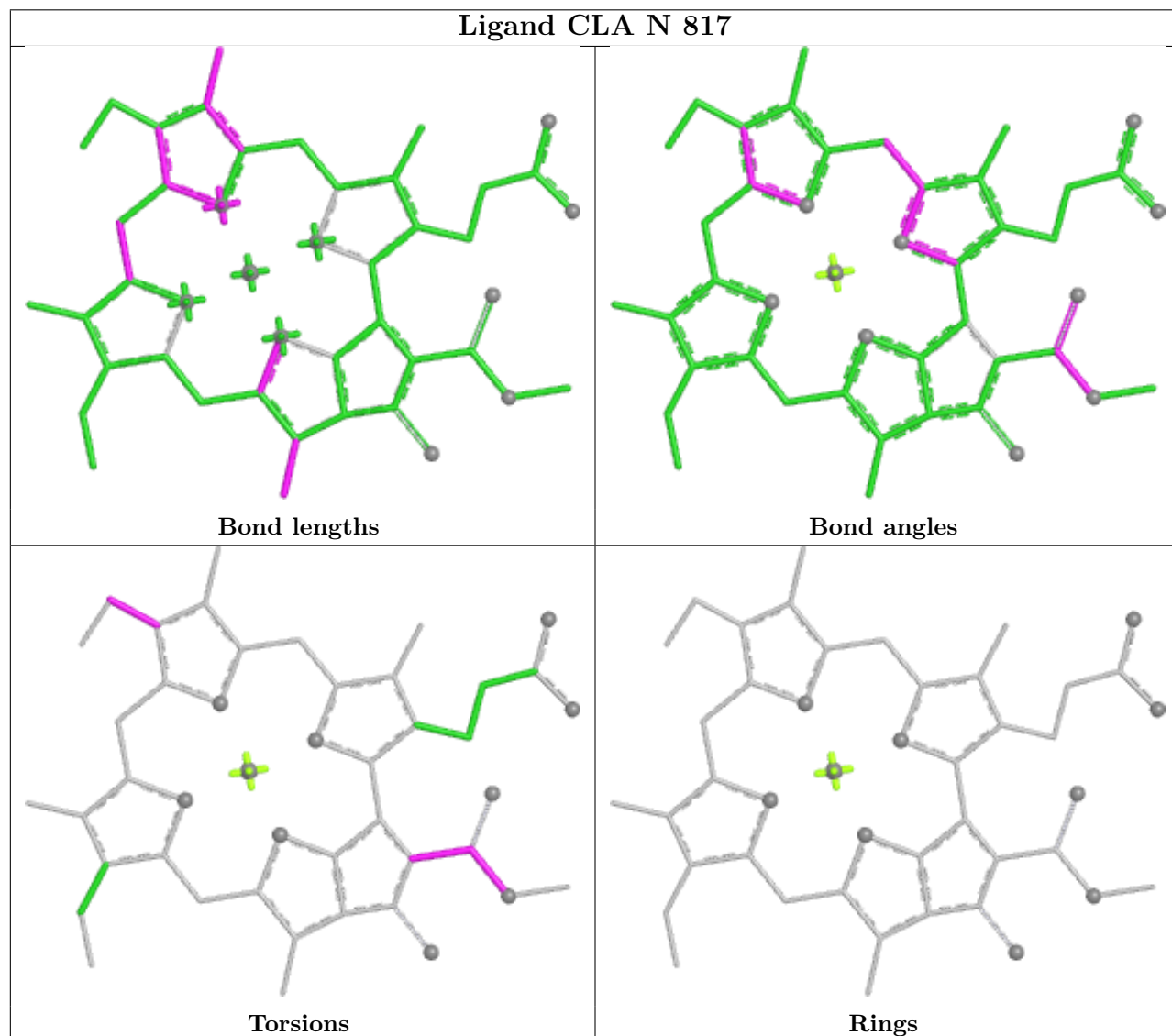
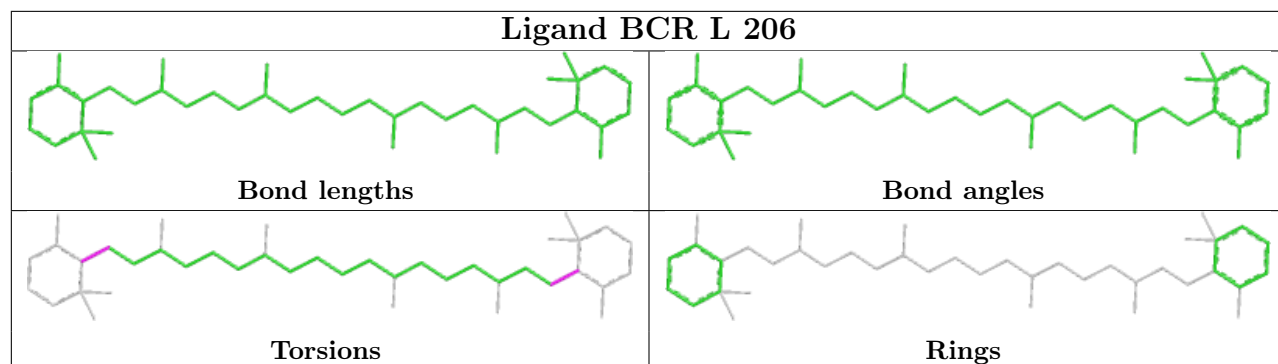


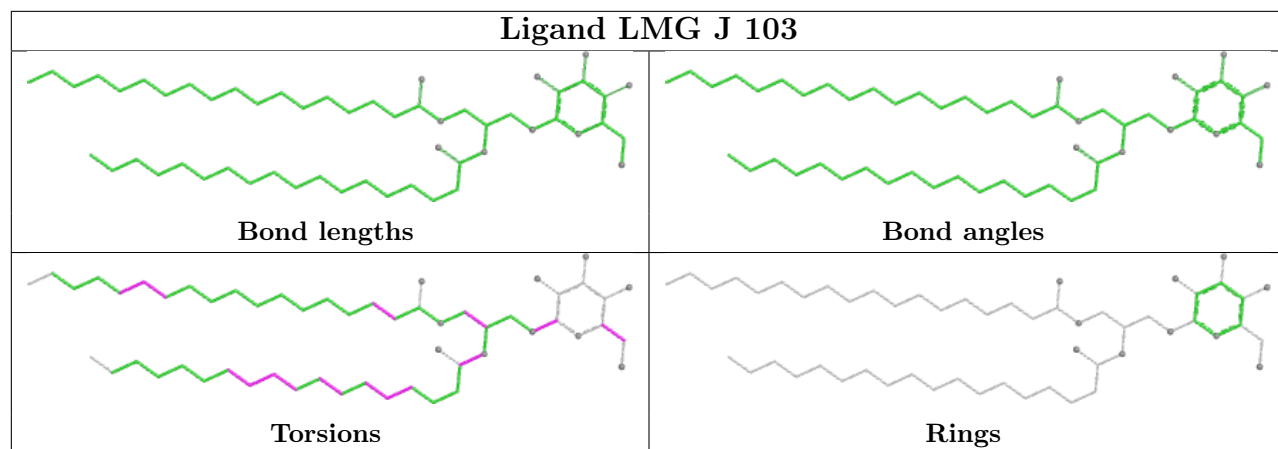
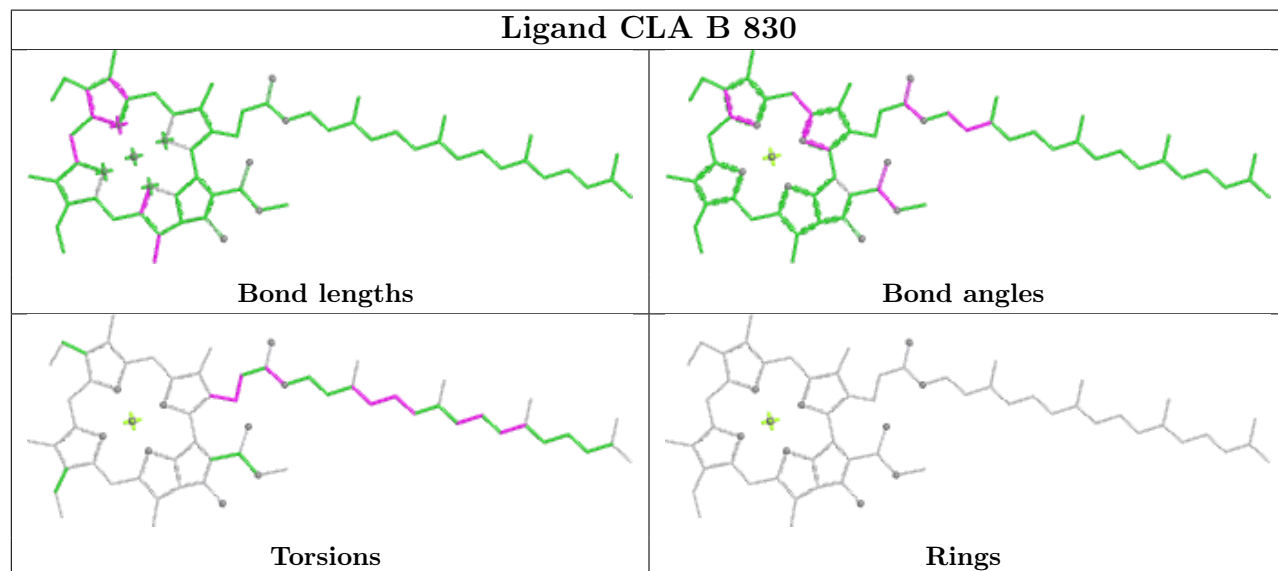
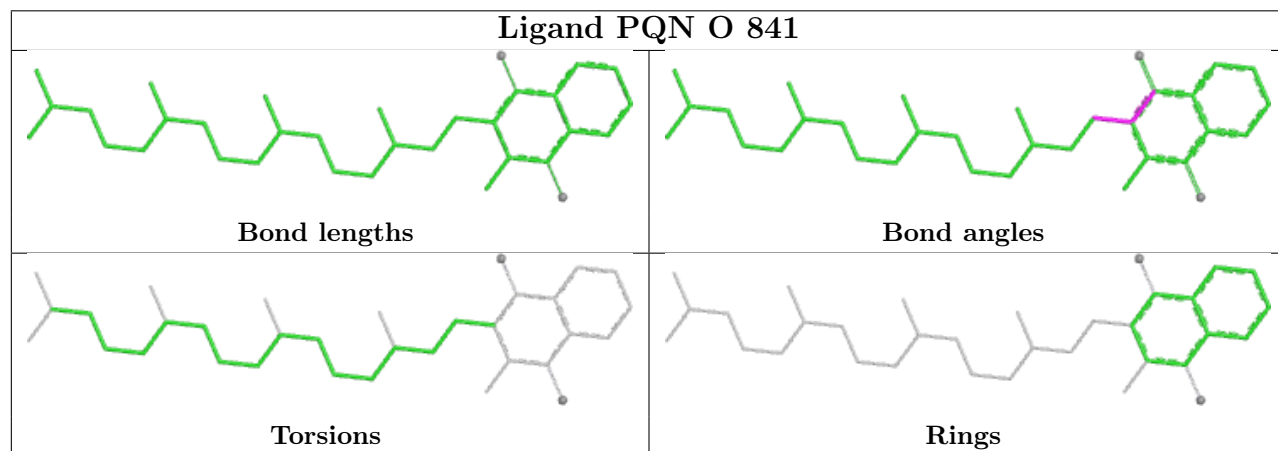
Ligand BCR T 101

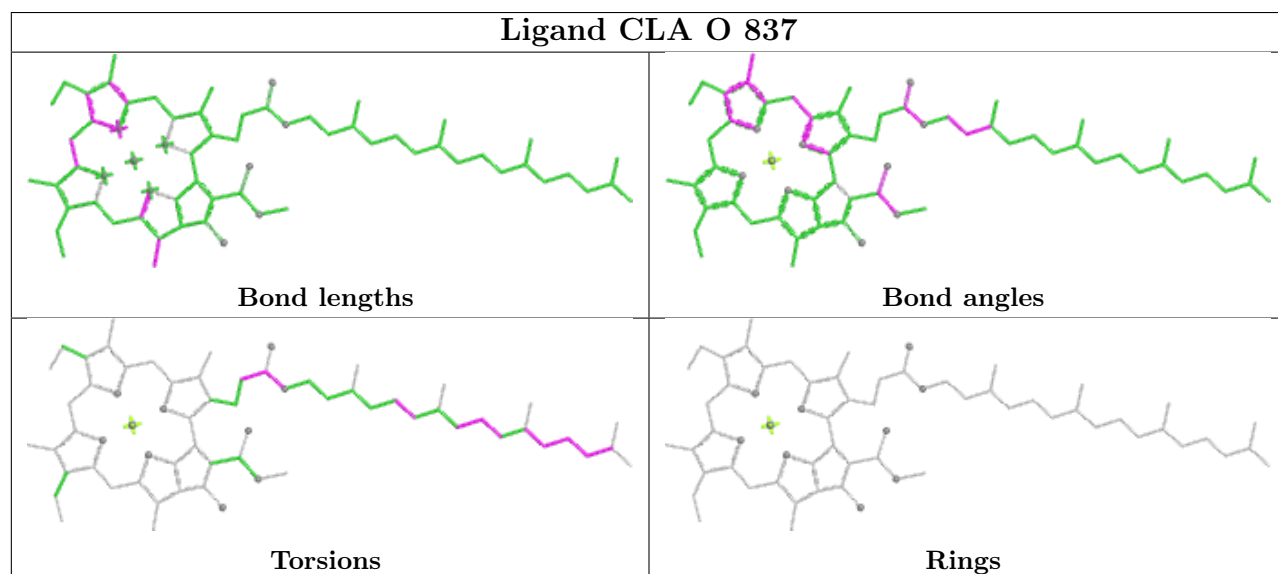
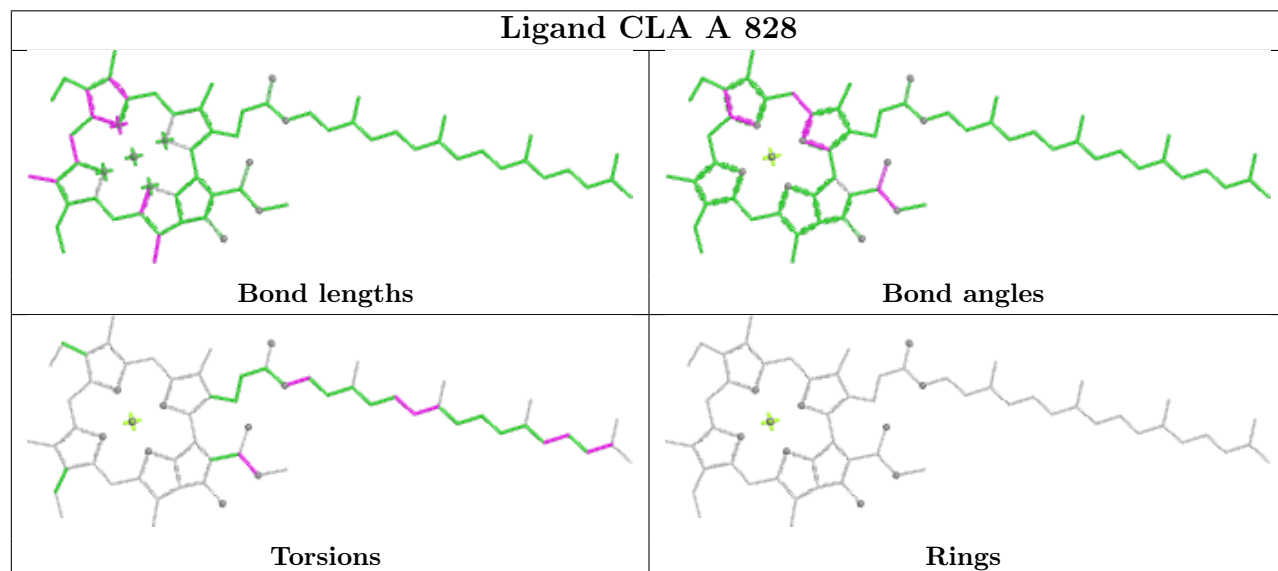
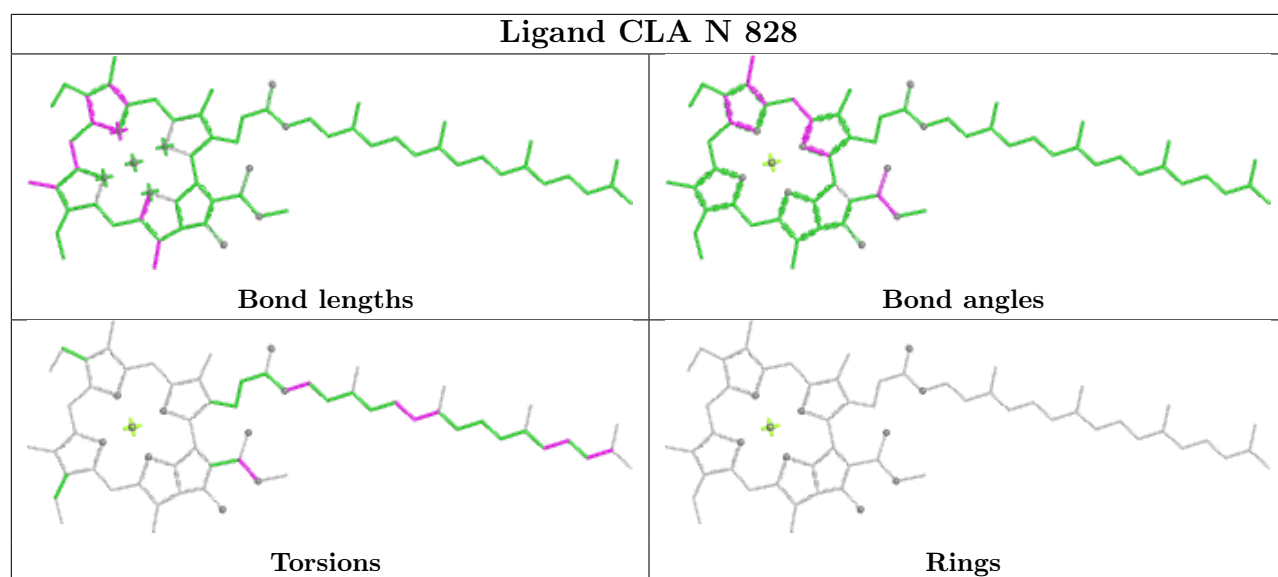


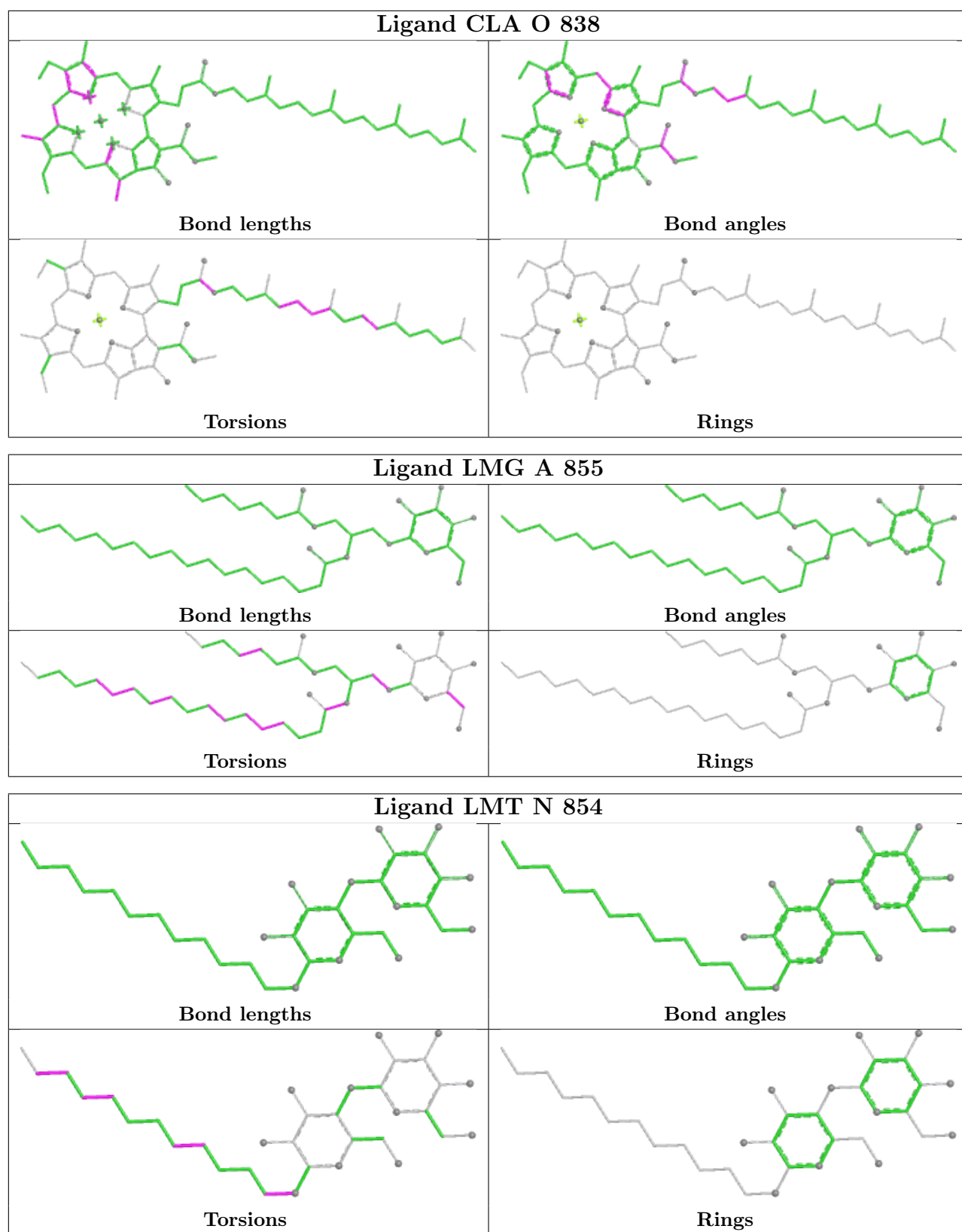
Ligand LFA O 850

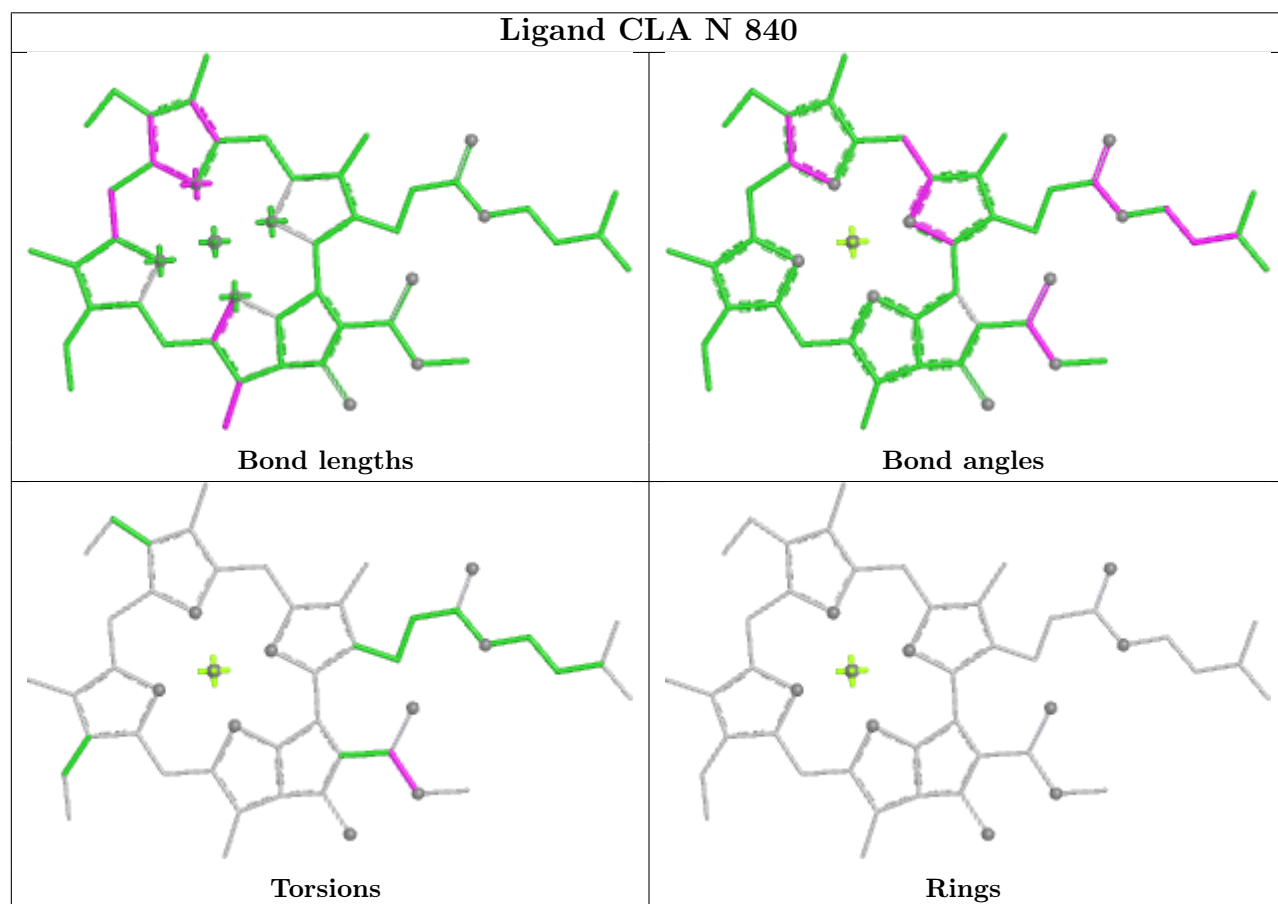
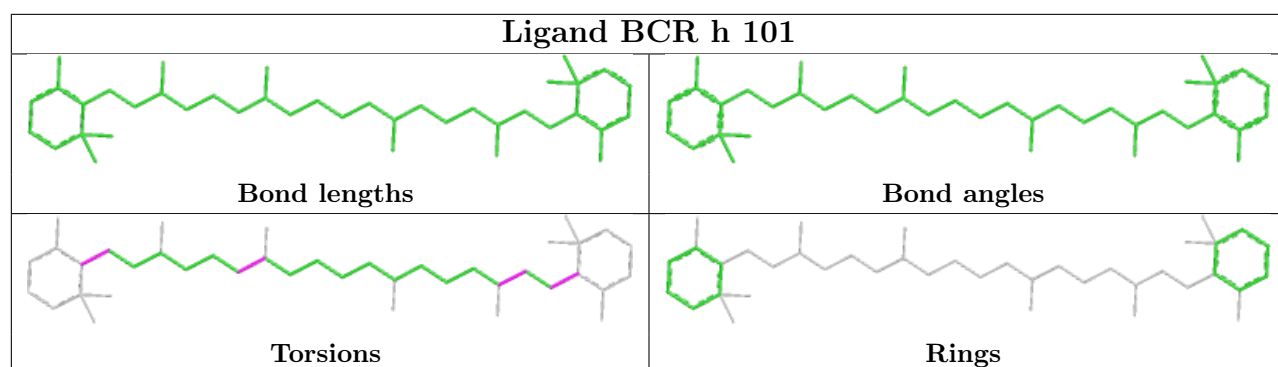




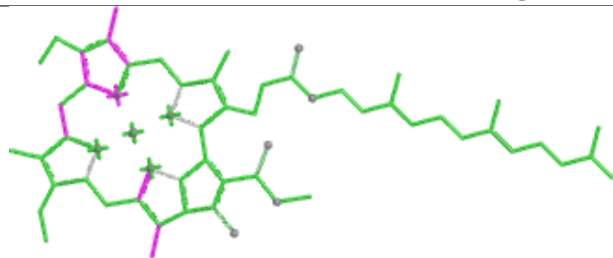
Ligand LMG J 103**Ligand CLA B 830****Ligand PQN O 841**



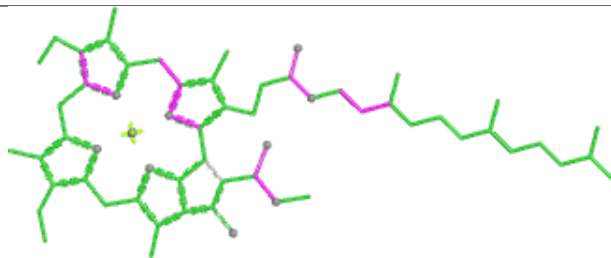




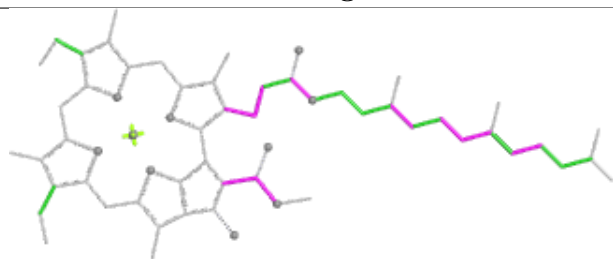
Ligand CLA N 809



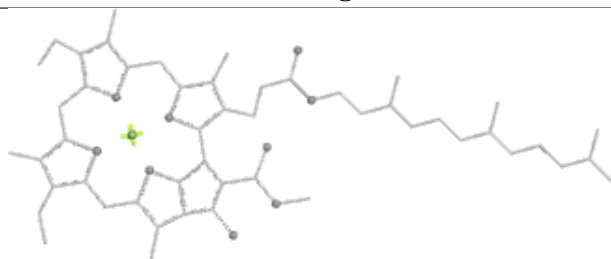
Bond lengths



Bond angles

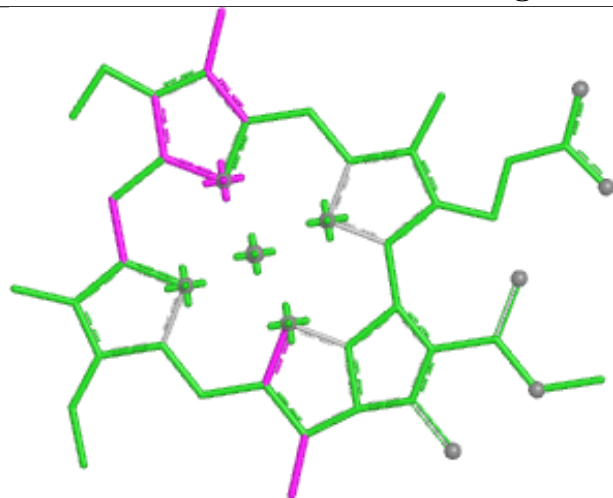


Torsions

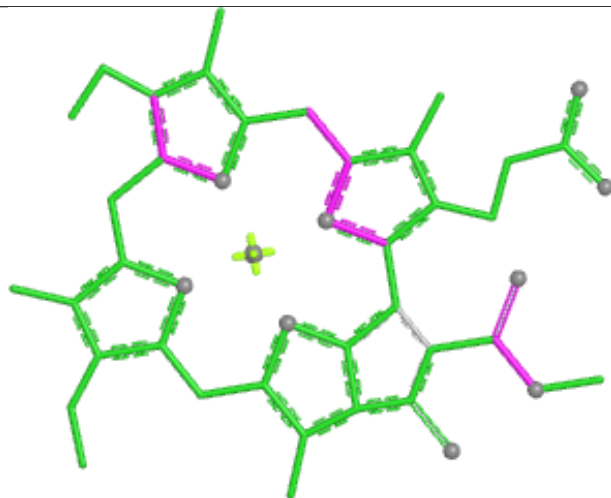


Rings

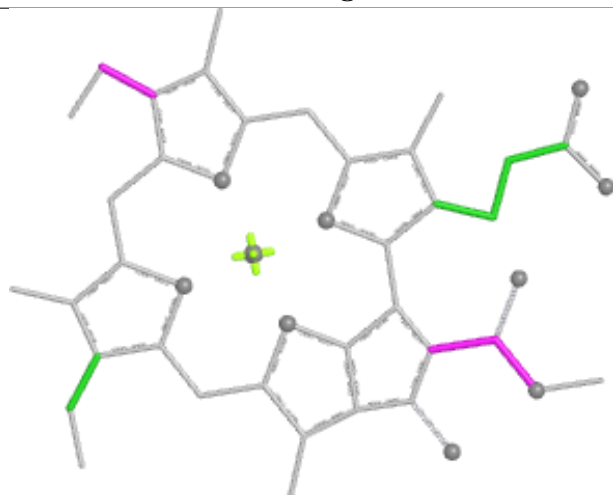
Ligand CLA A 817



Bond lengths



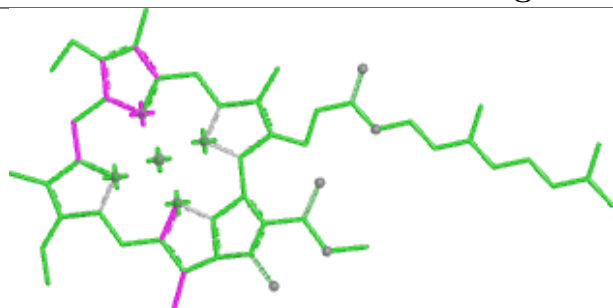
Bond angles



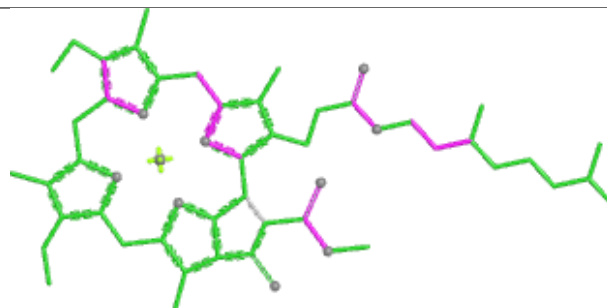
Torsions



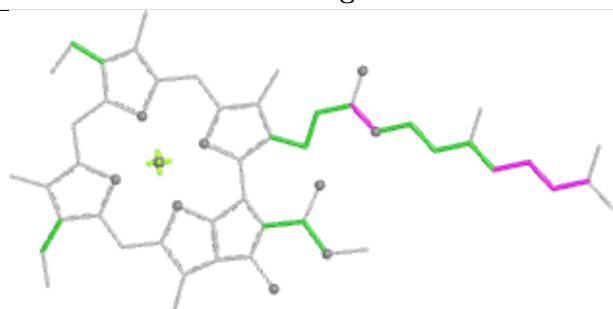
Rings

Ligand CLA B 833

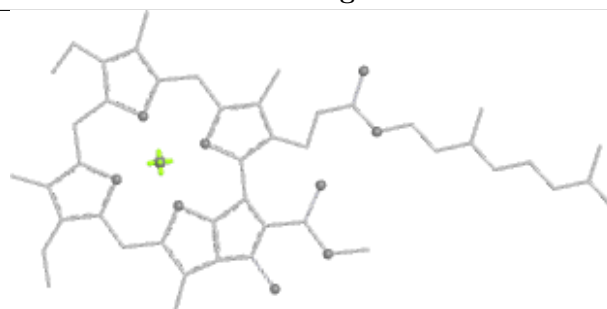
Bond lengths



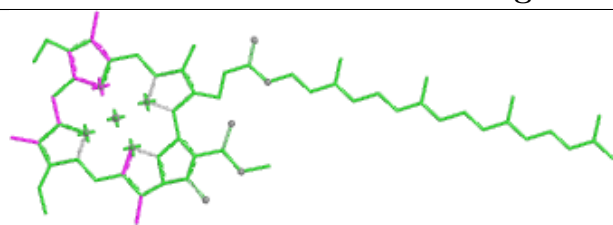
Bond angles



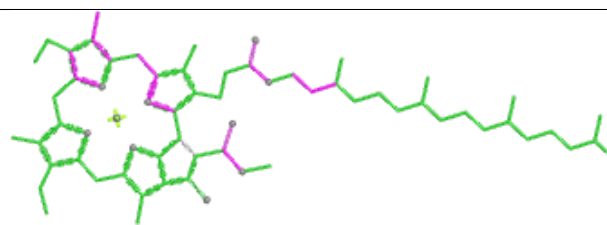
Torsions



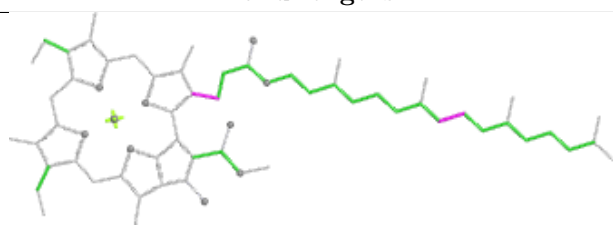
Rings

Ligand CLA B 825

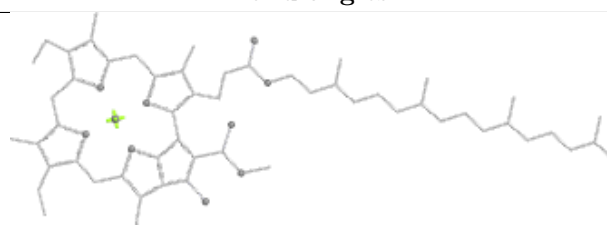
Bond lengths



Bond angles

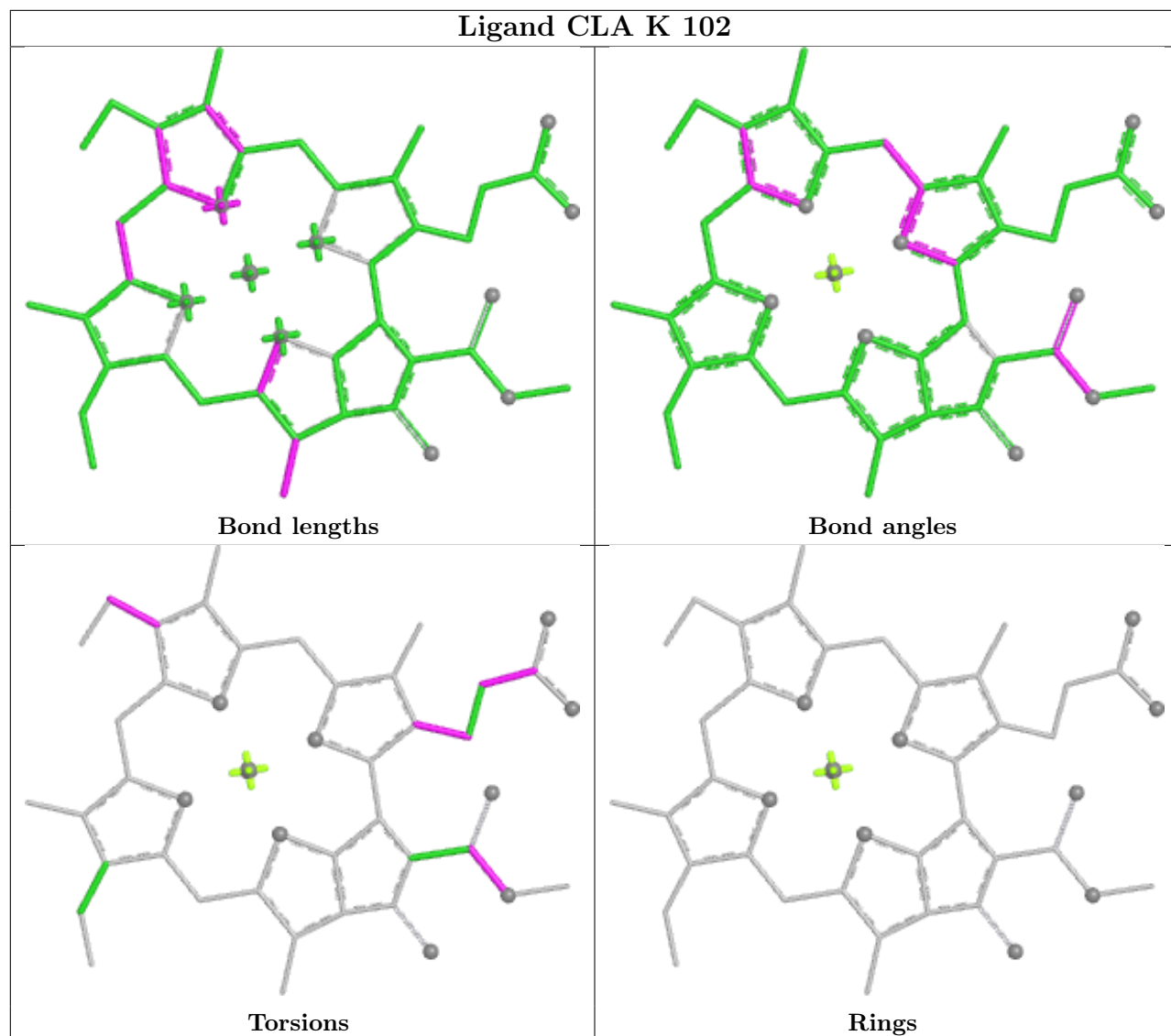


Torsions

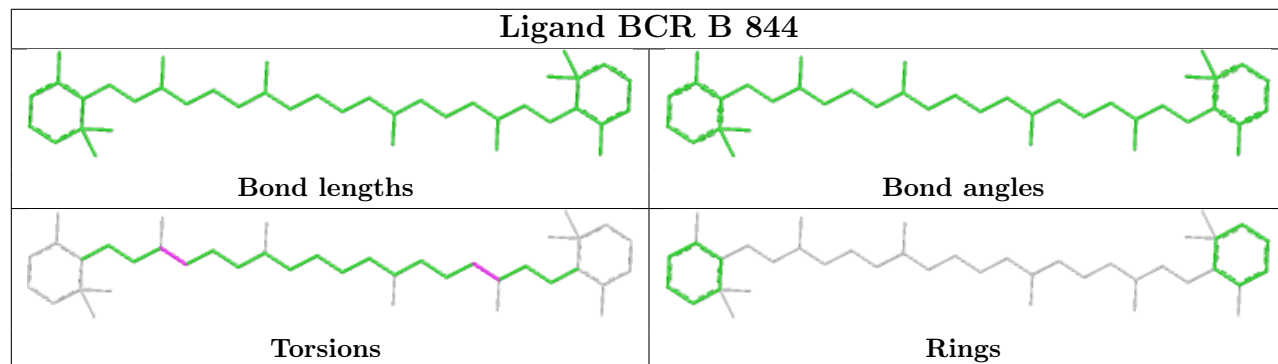


Rings

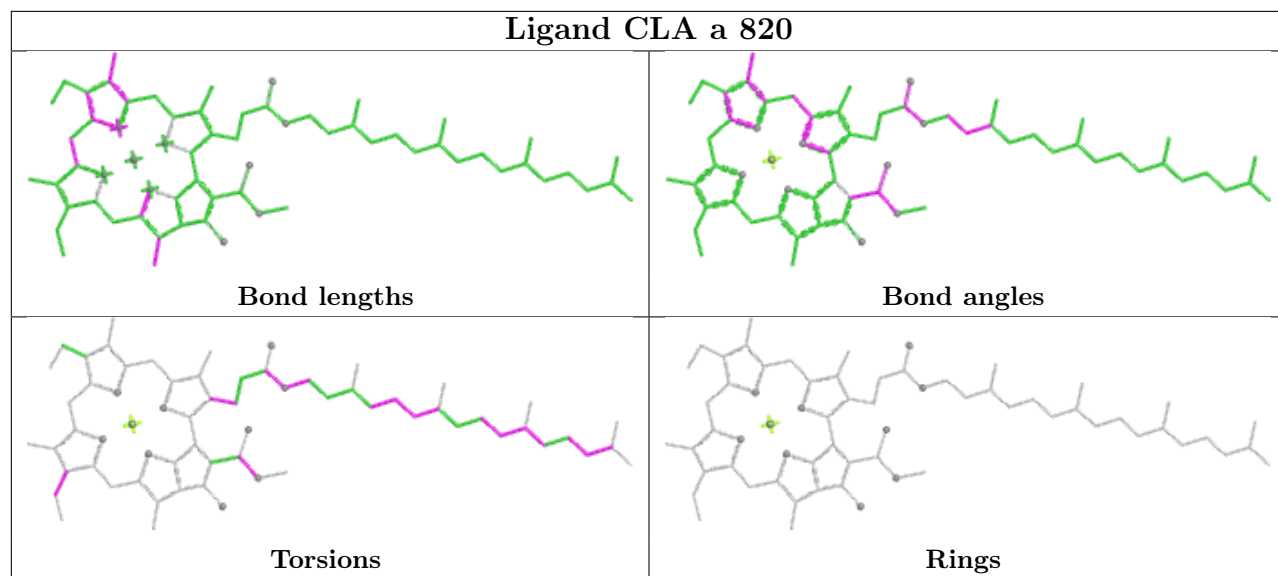
Ligand CLA K 102



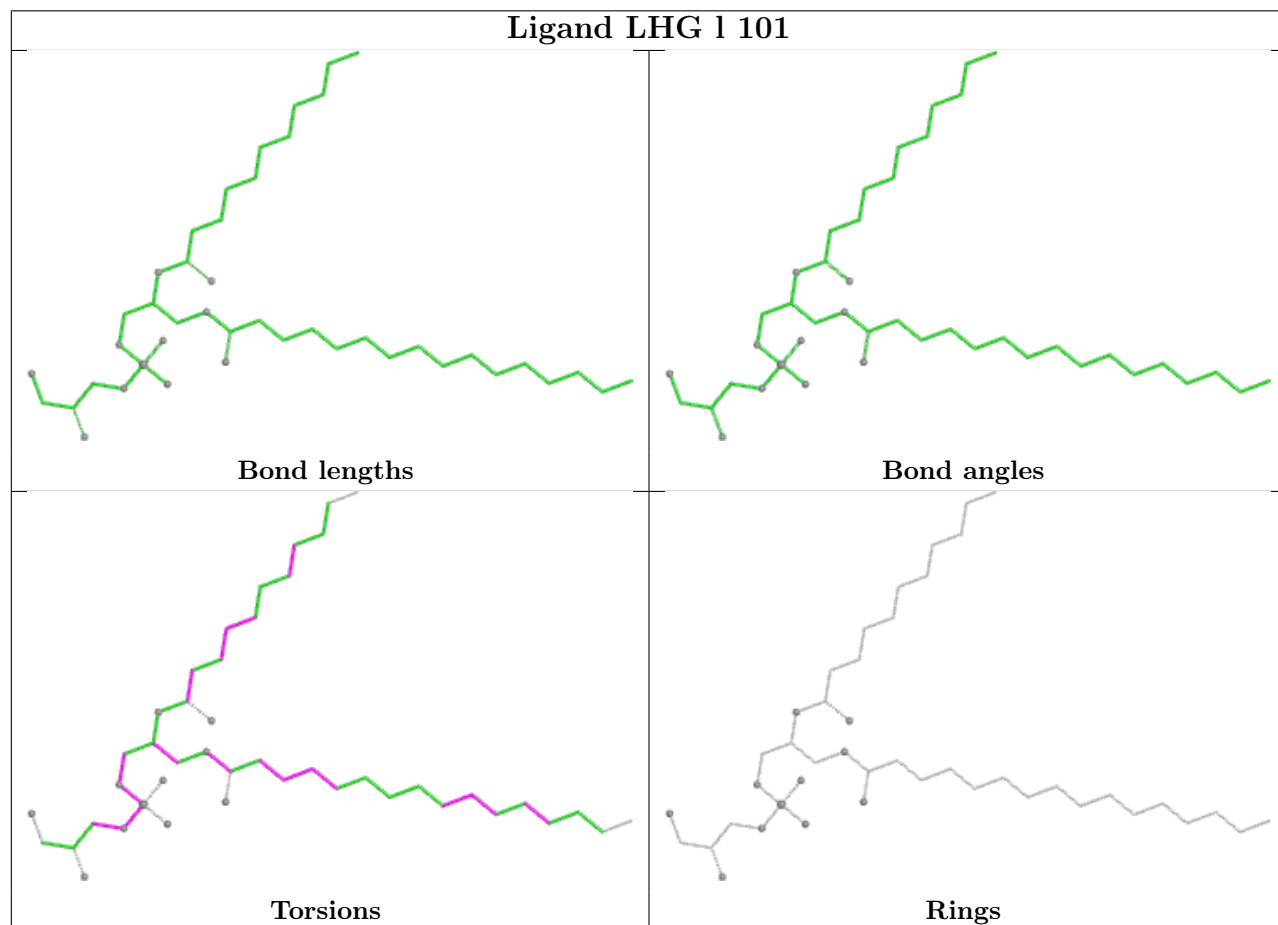
Ligand BCR B 844

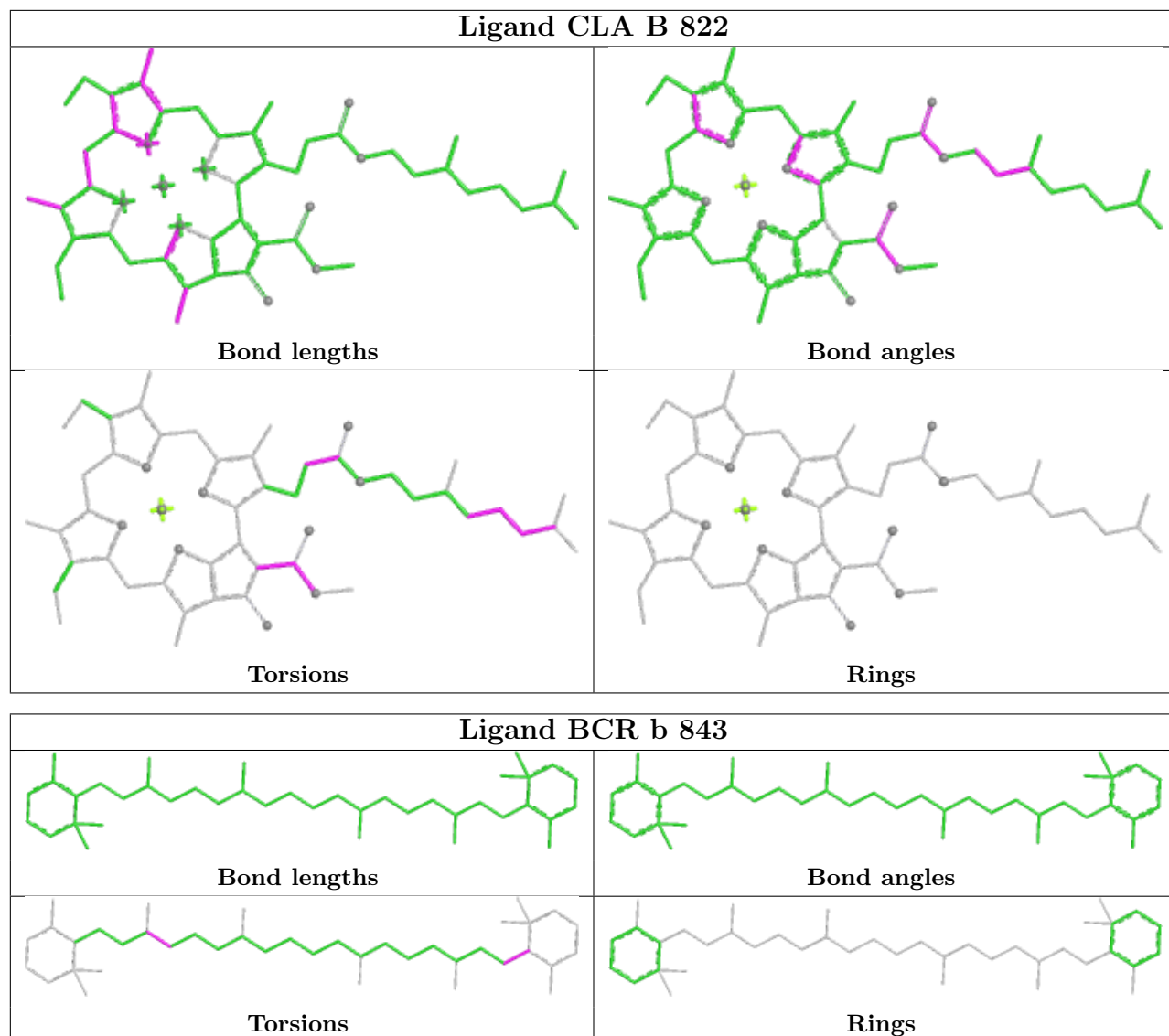


Ligand CLA a 820

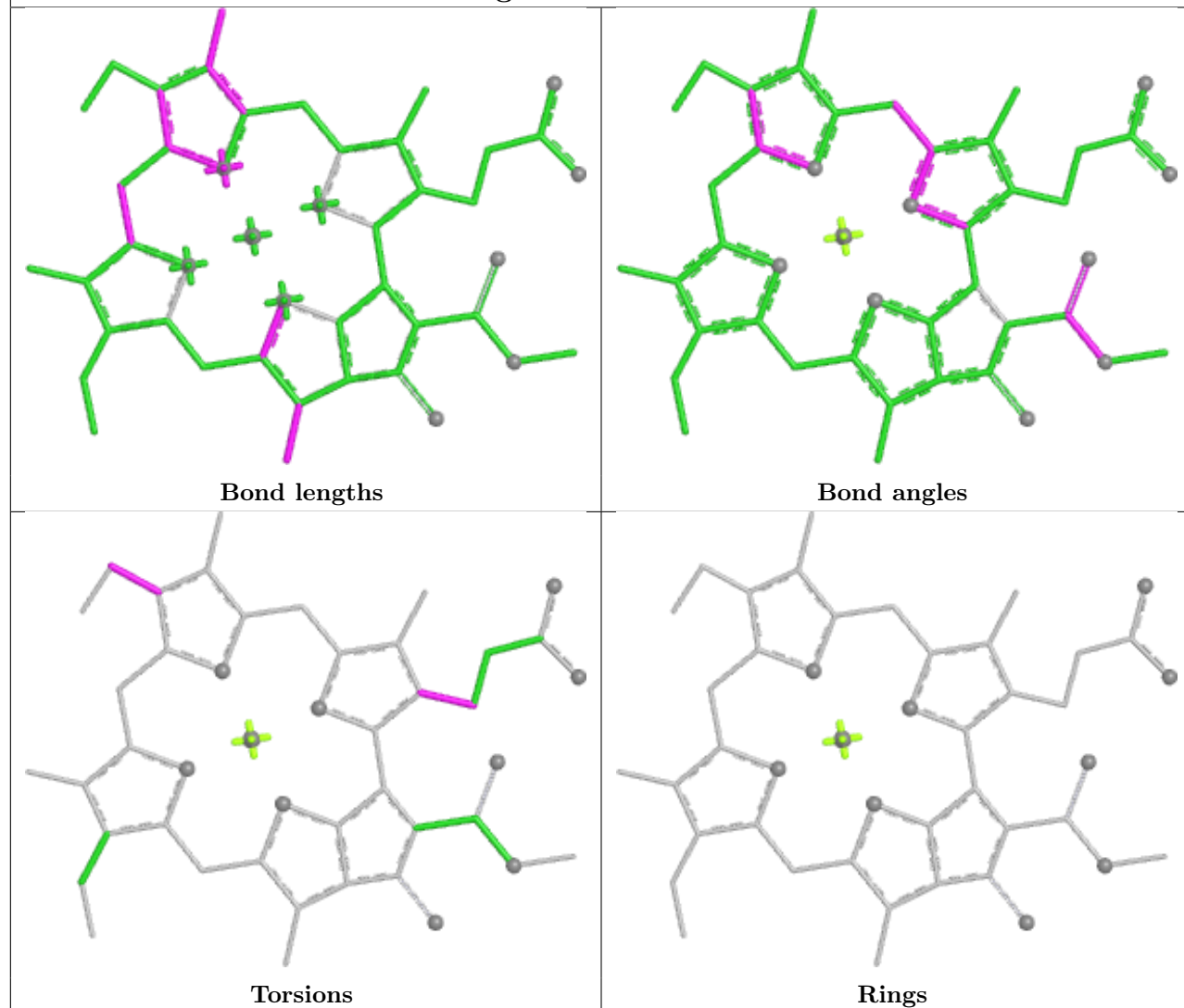


Ligand LHG 1 101

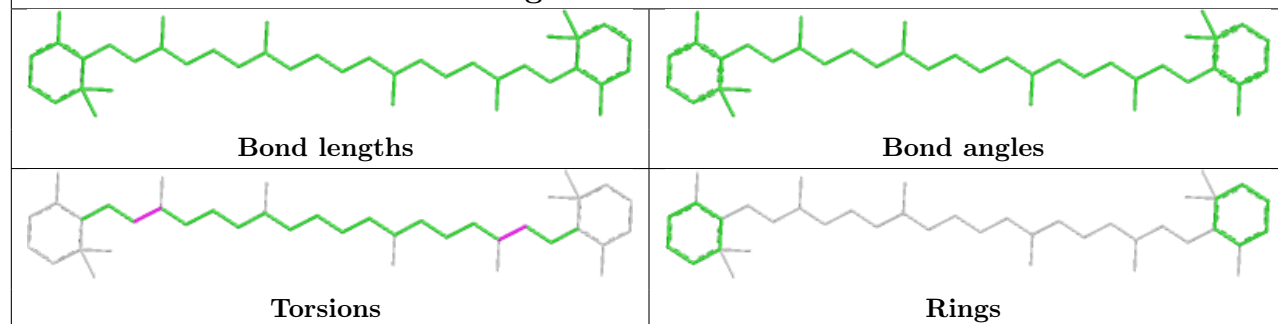


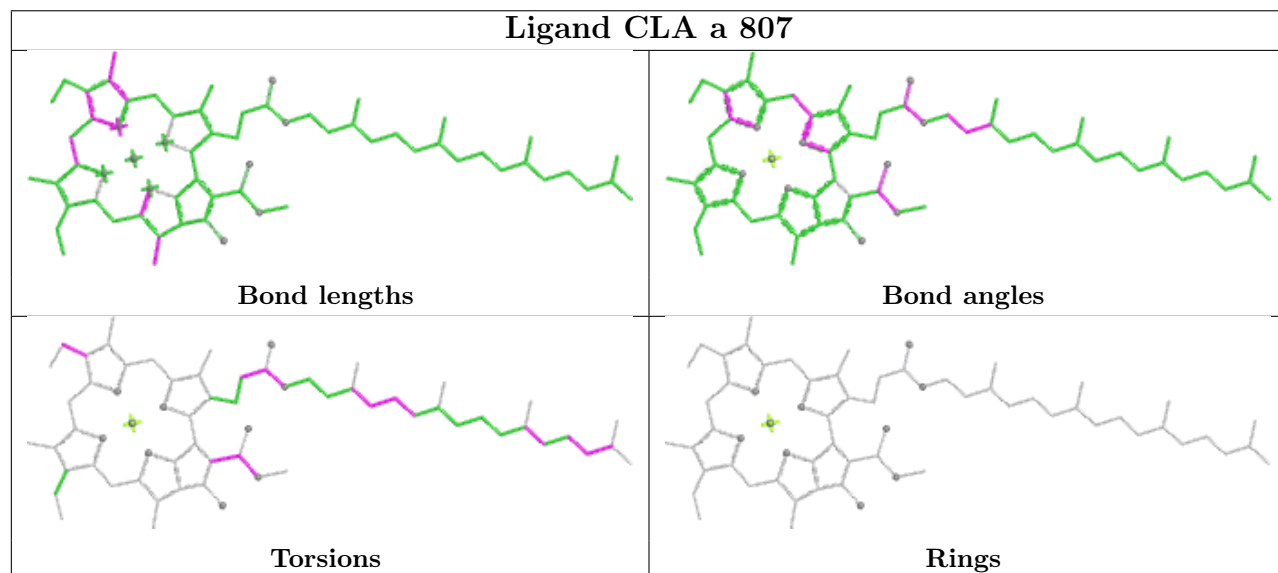
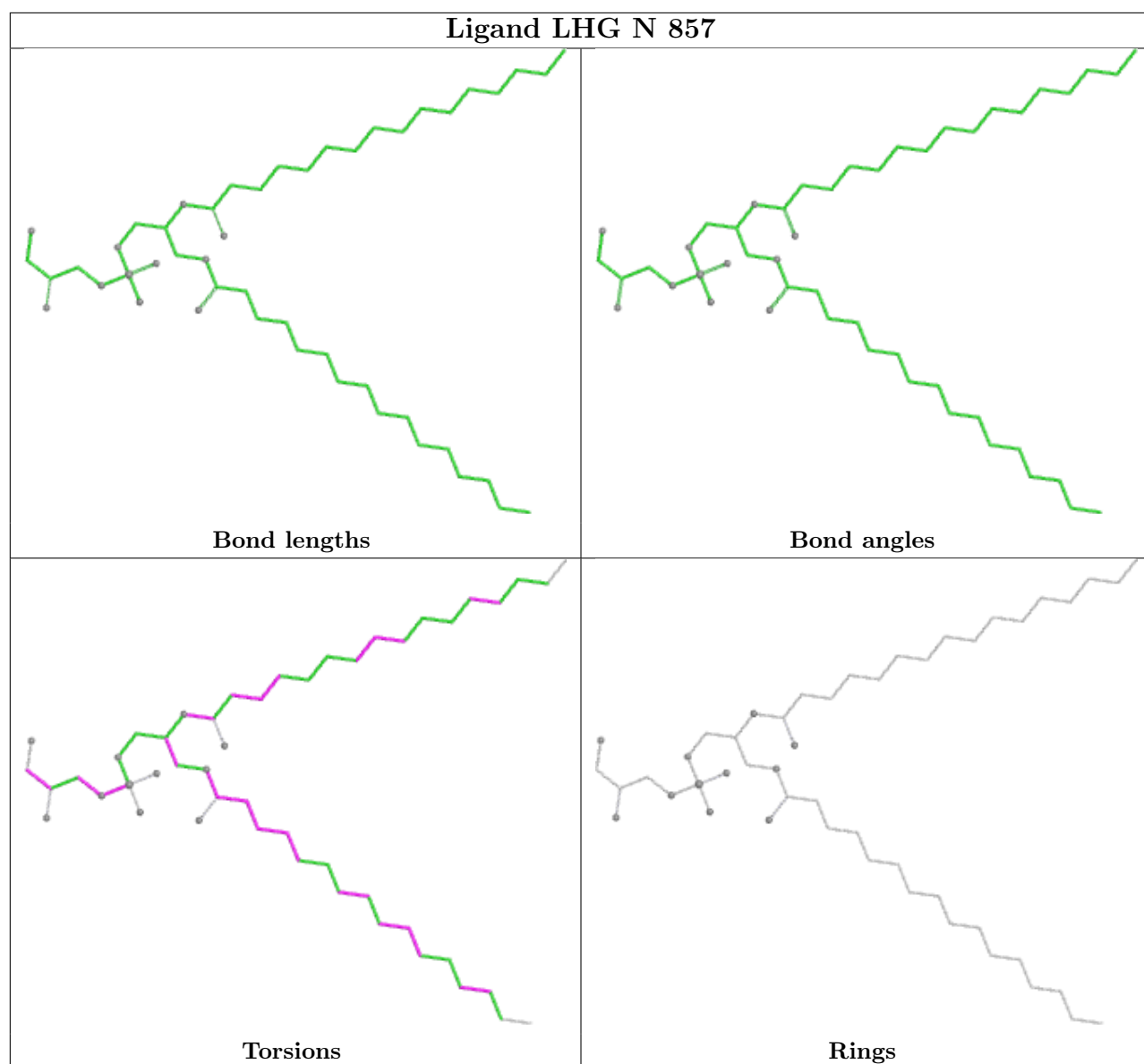


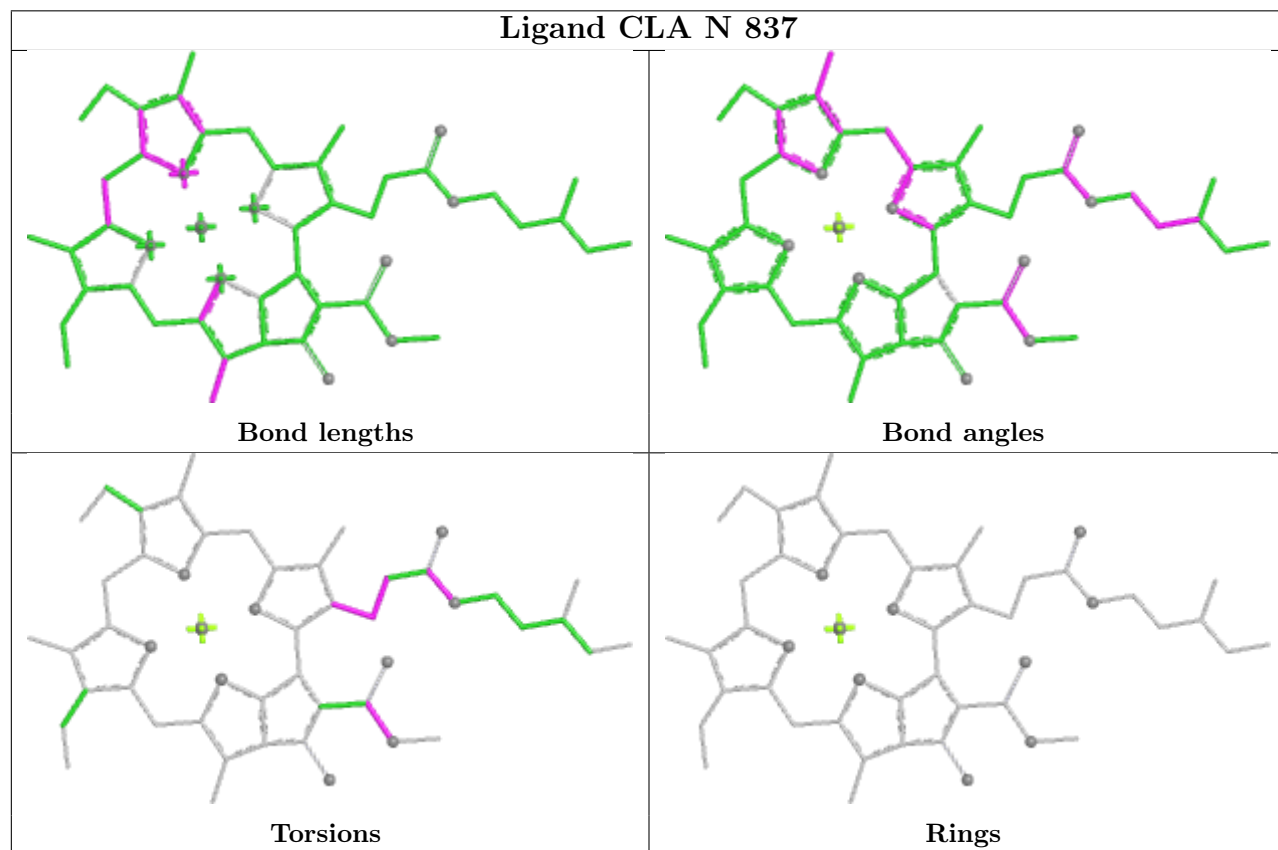
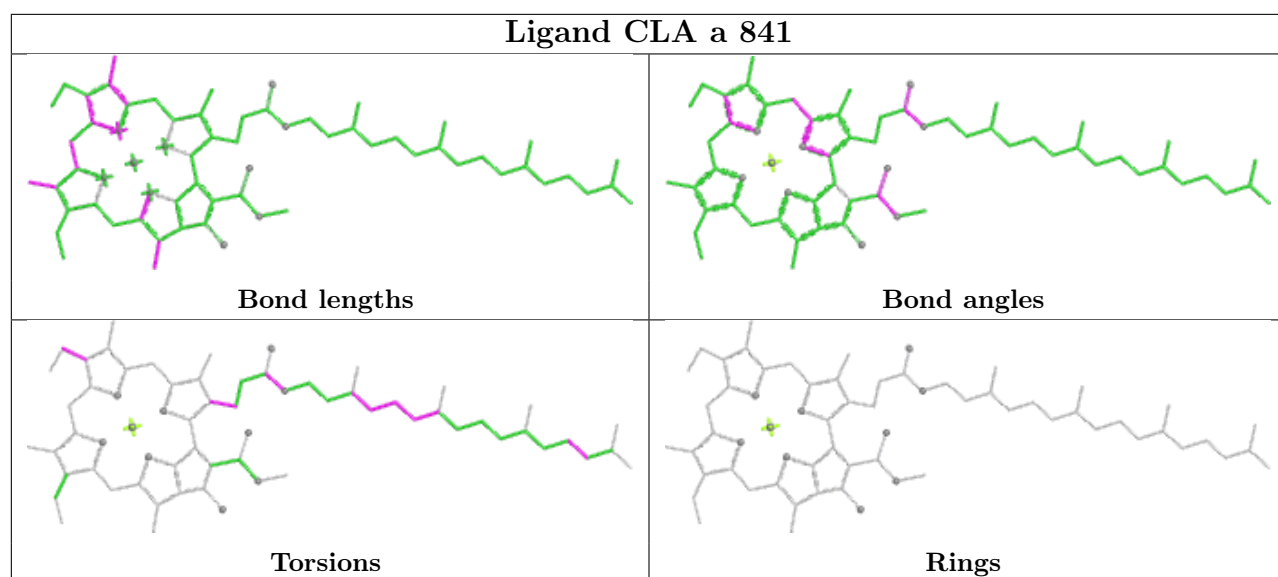
Ligand CLA b 811



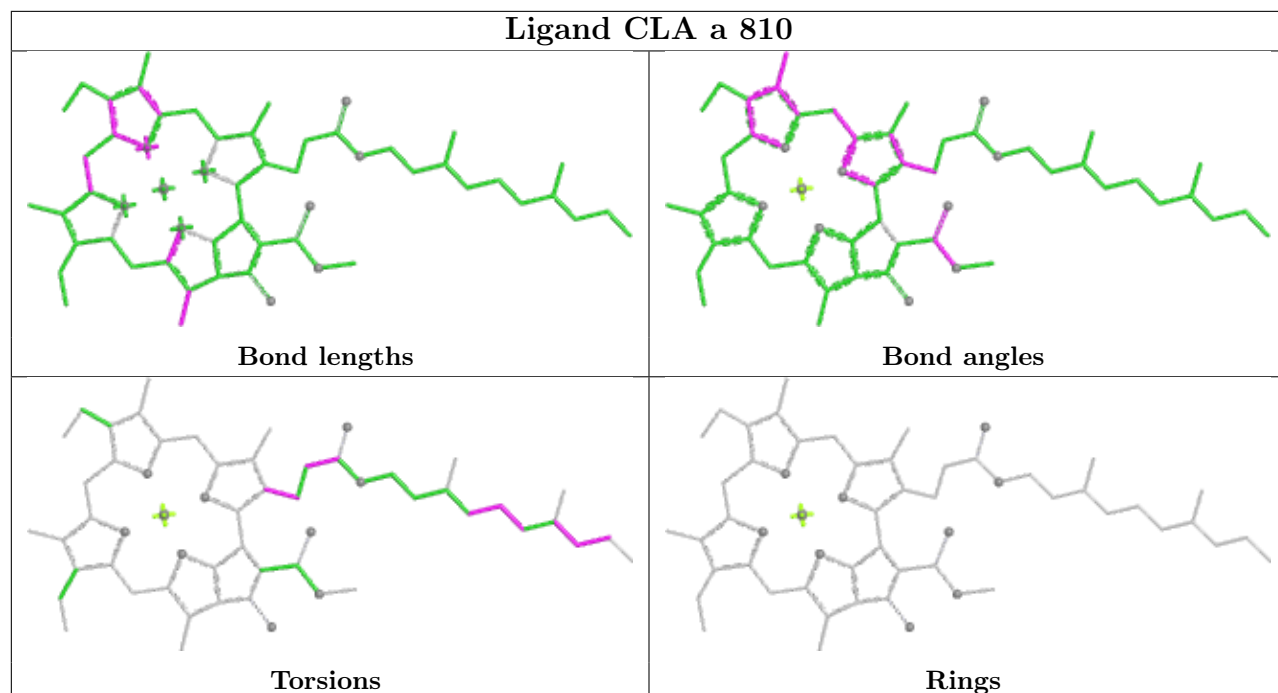
Ligand BCR W 205



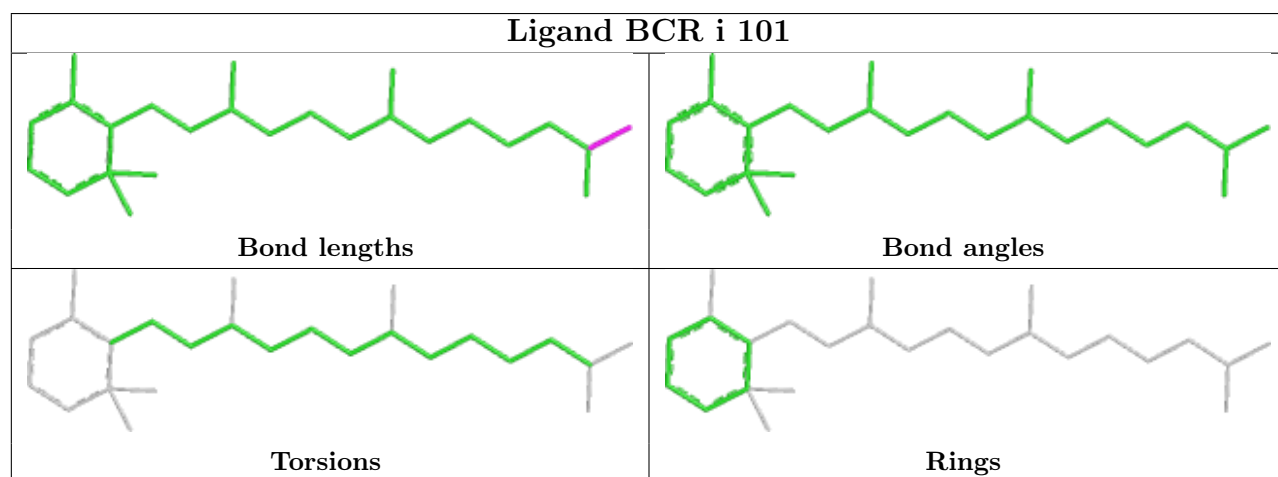




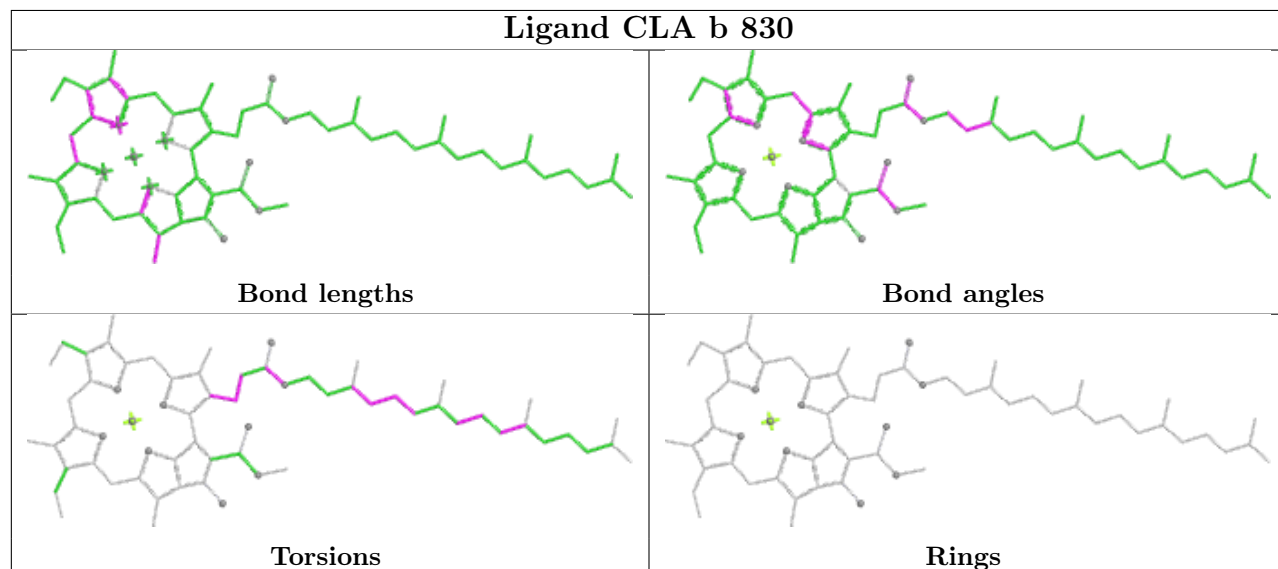
Ligand CLA a 810



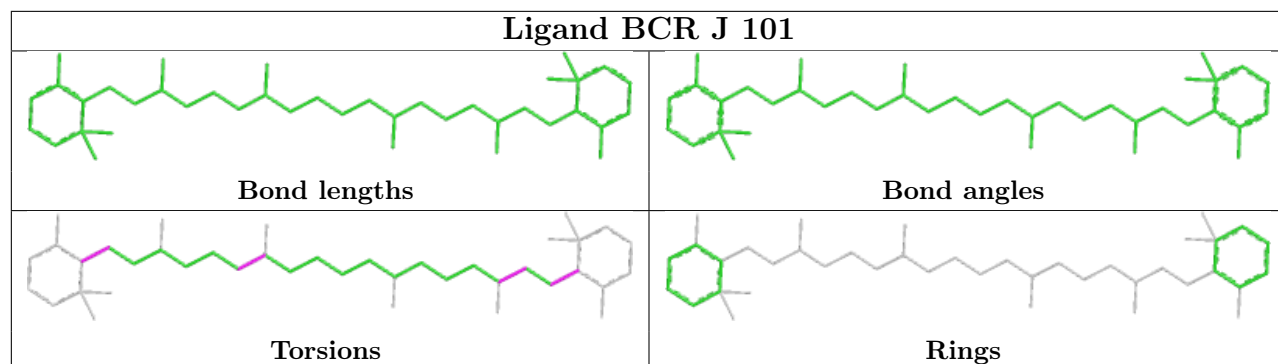
Ligand BCR i 101



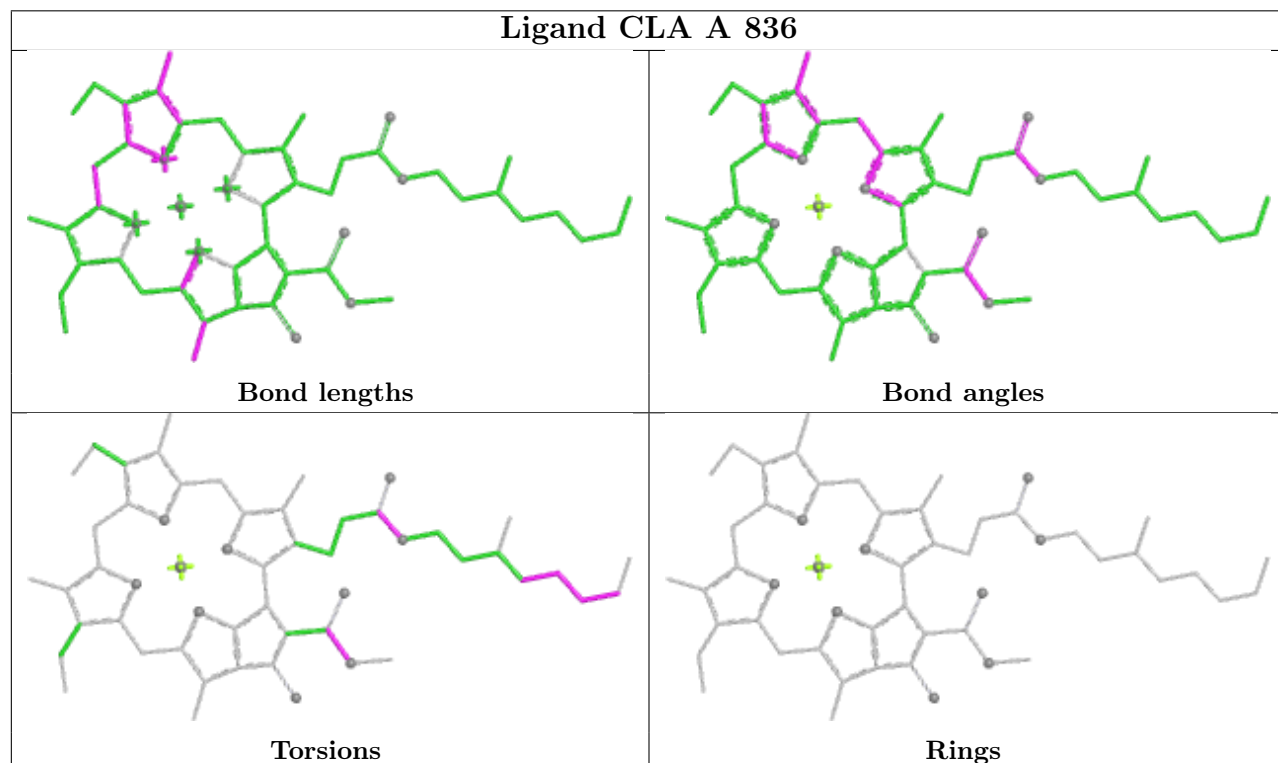
Ligand CLA b 830



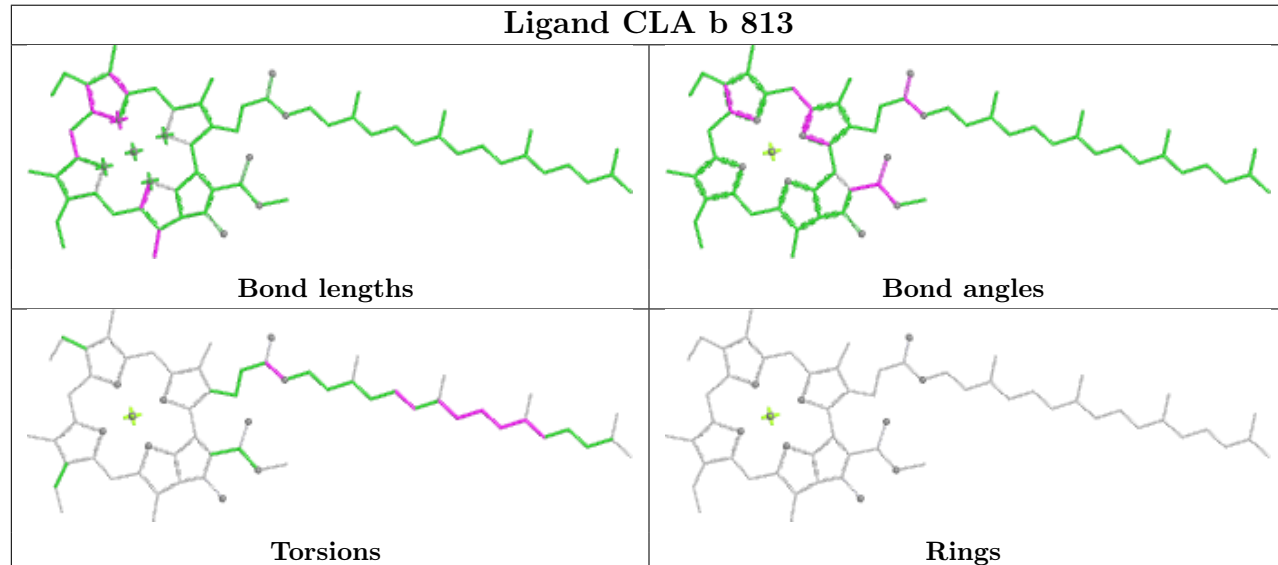
Ligand BCR J 101

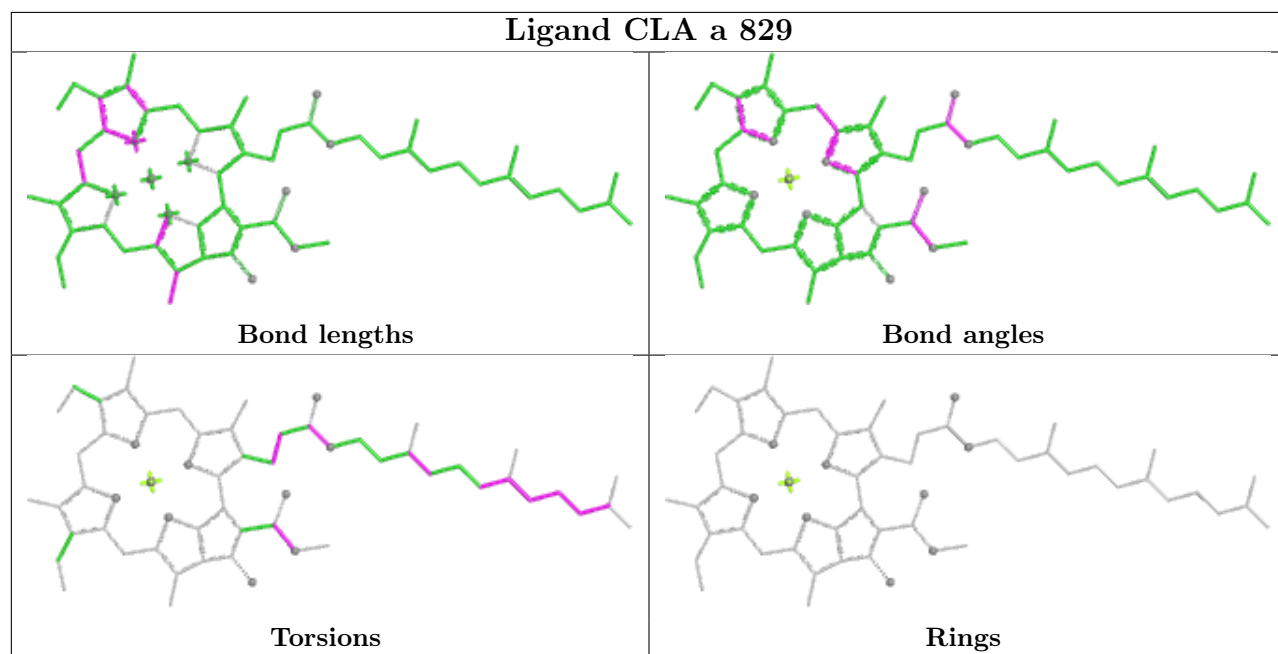
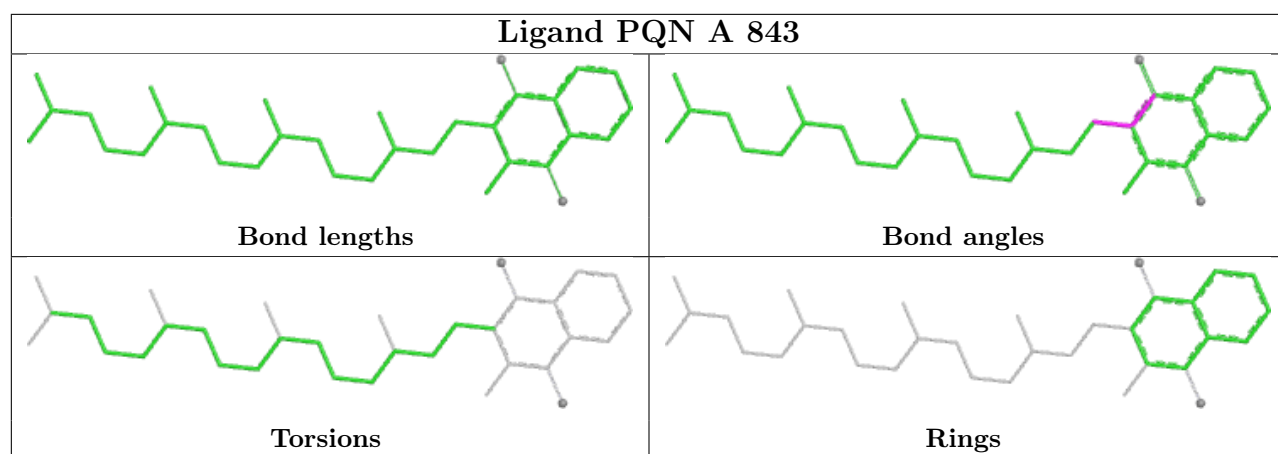


Ligand CLA A 836

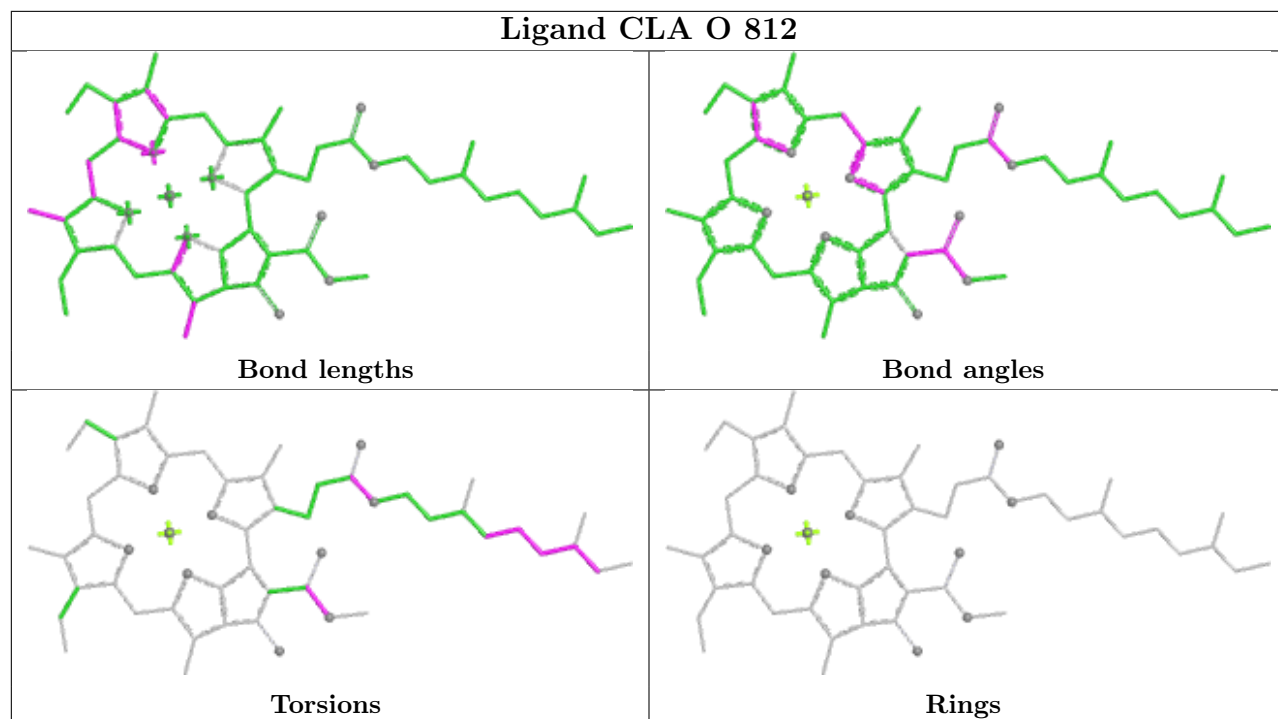


Ligand CLA b 813

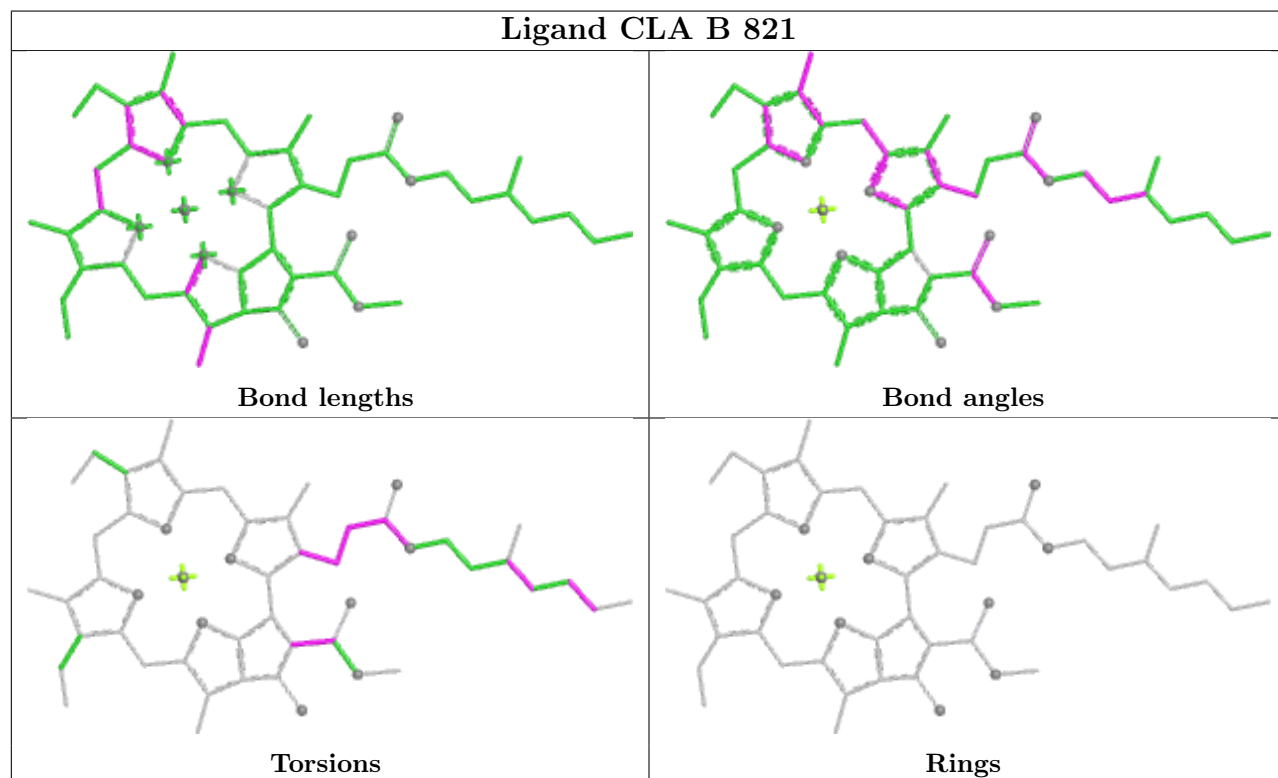


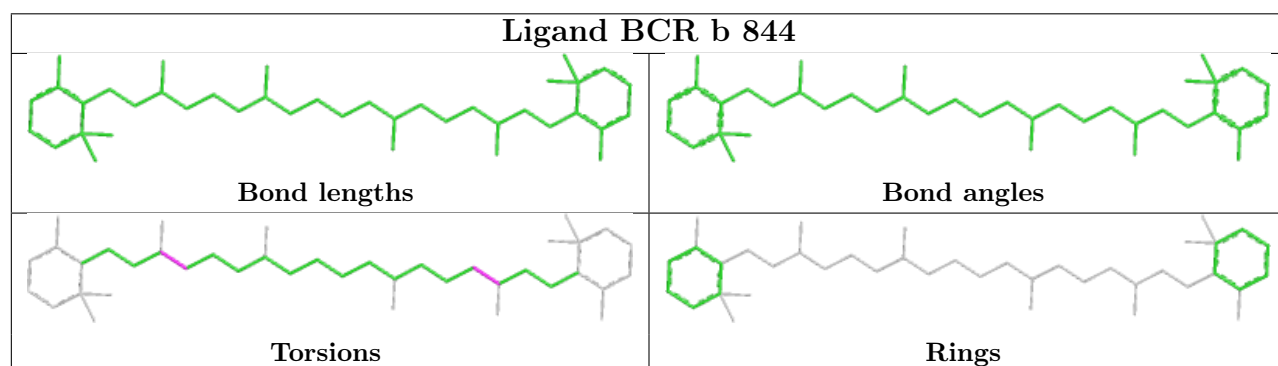
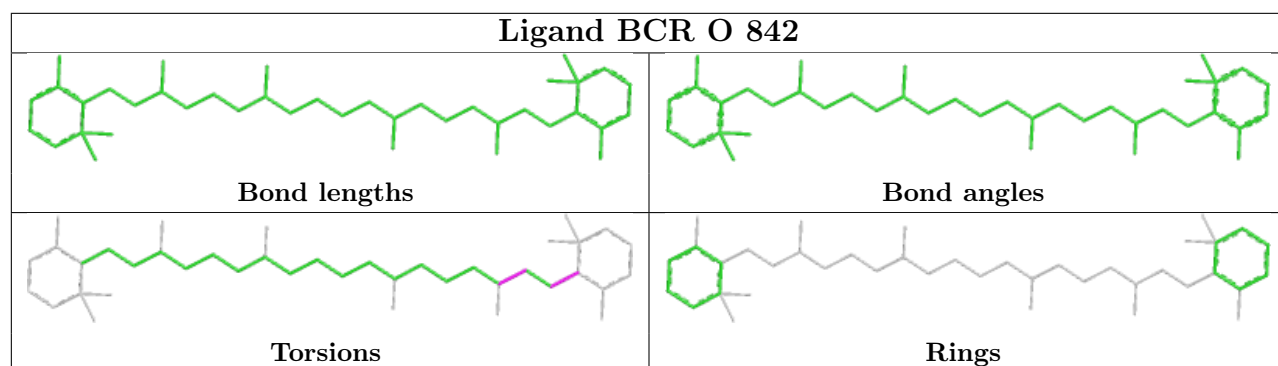
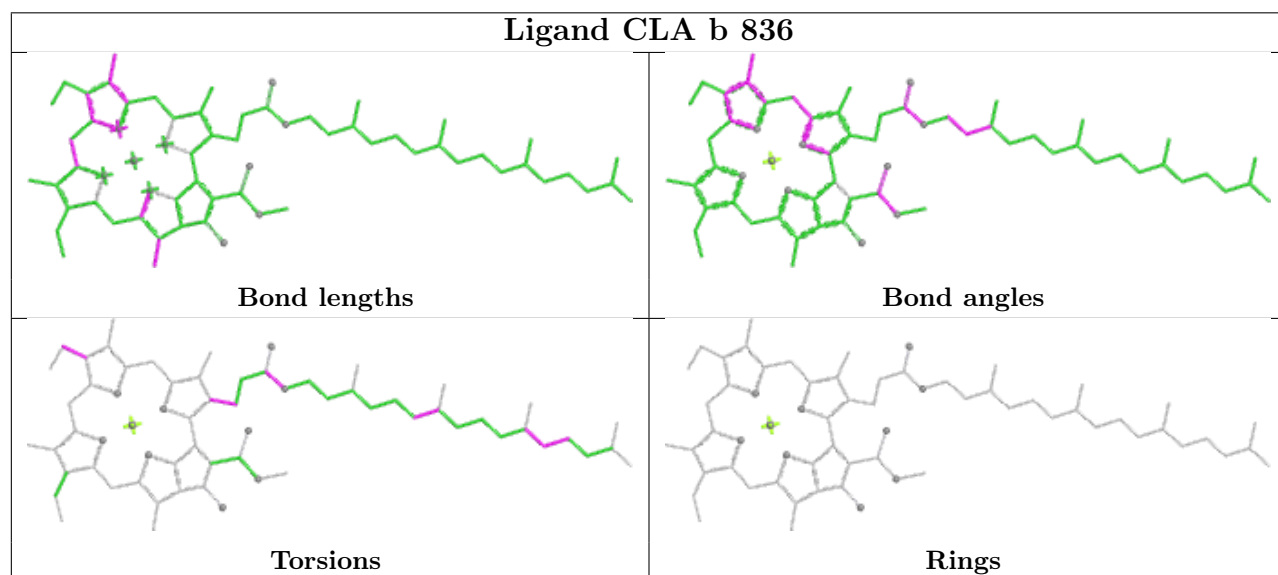
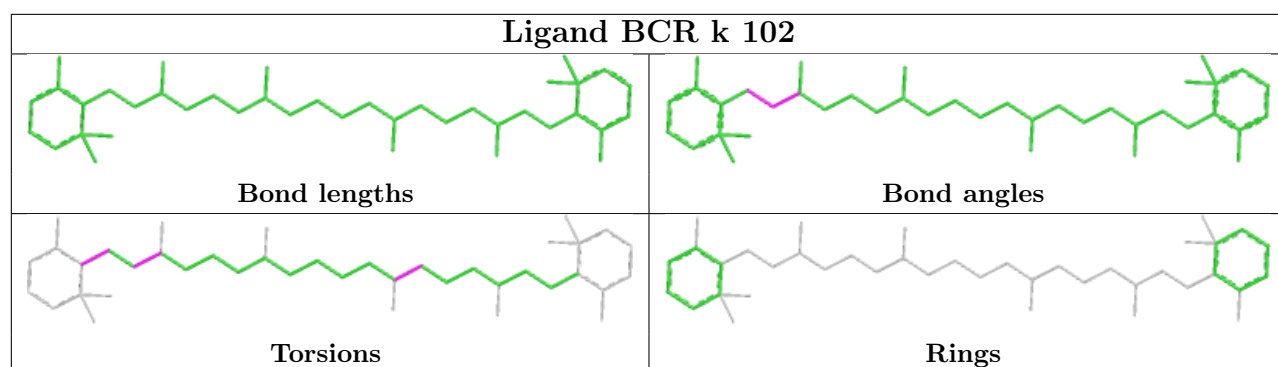


Ligand CLA O 812

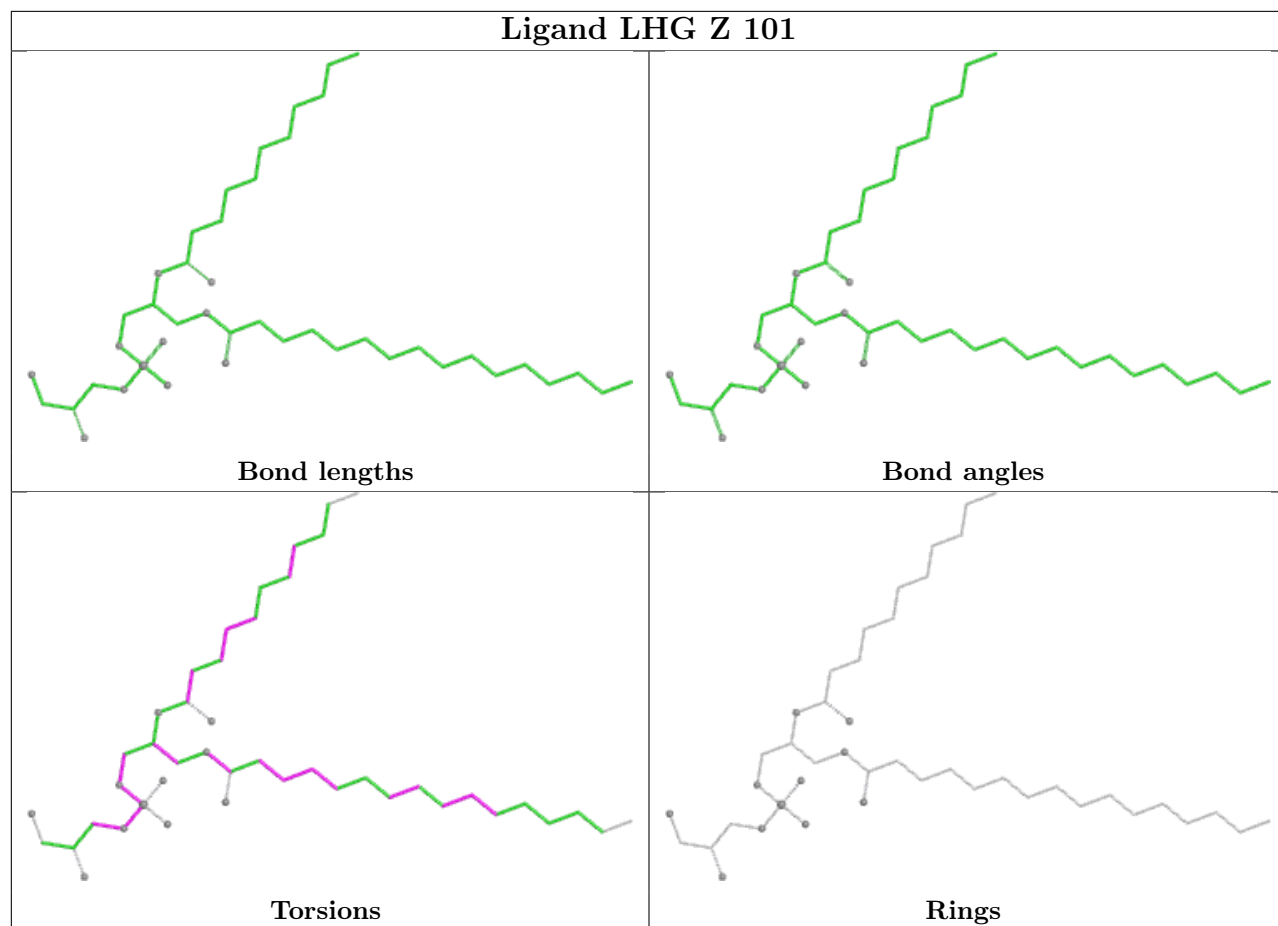


Ligand CLA B 821

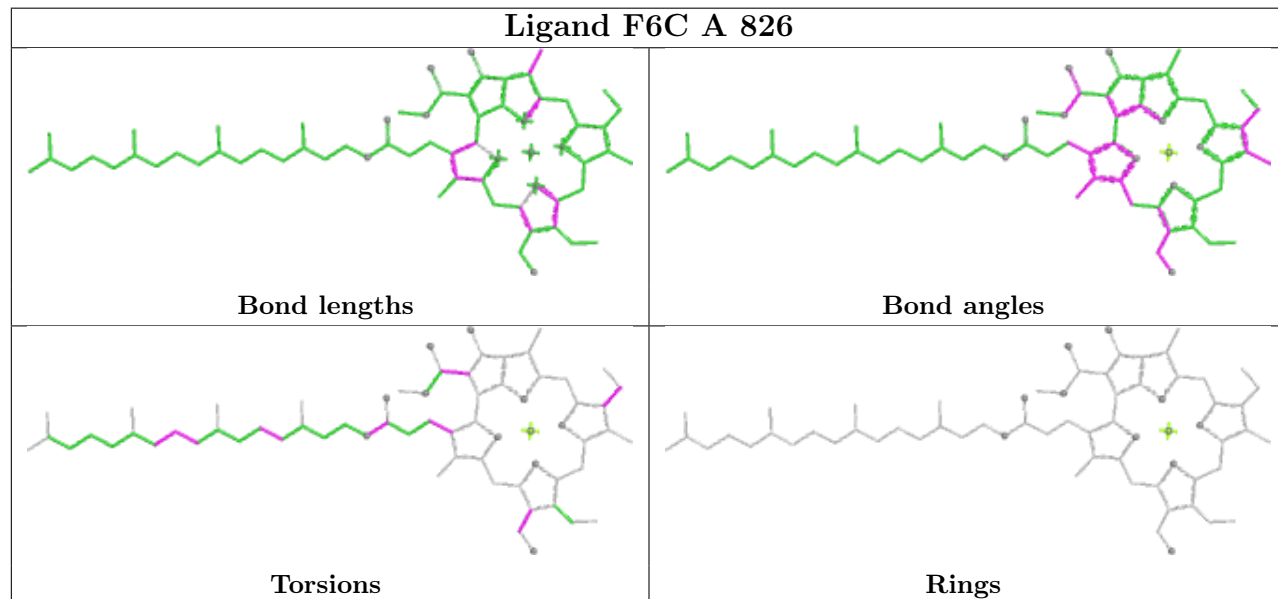




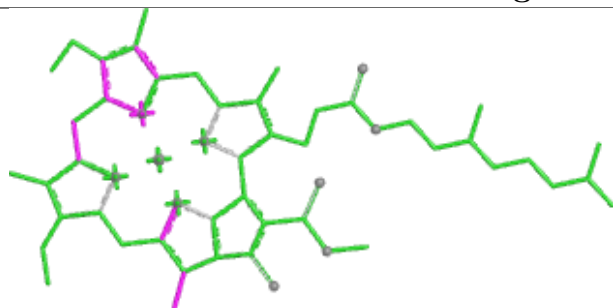
Ligand LHG Z 101



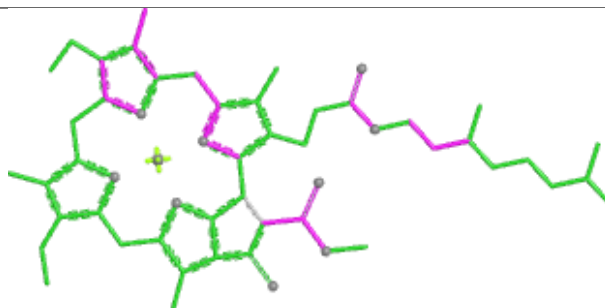
Ligand F6C A 826



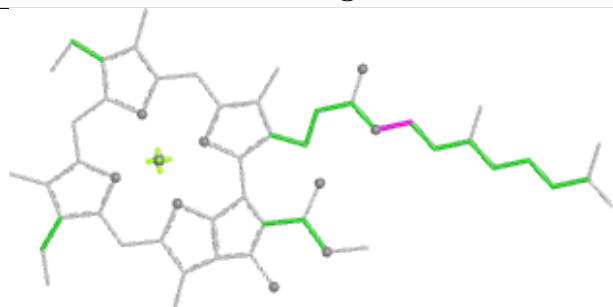
Ligand CLA N 827



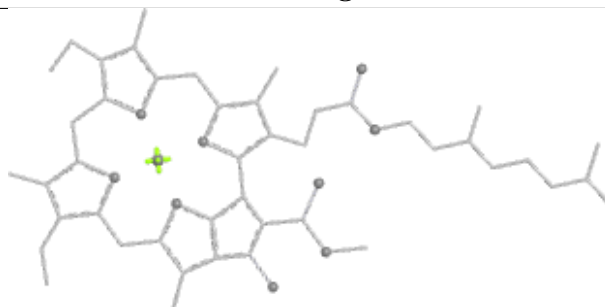
Bond lengths



Bond angles

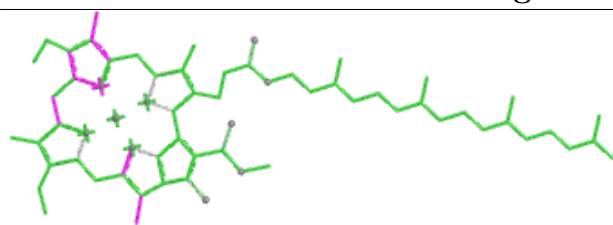


Torsions

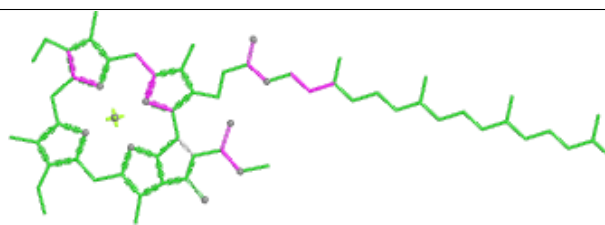


Rings

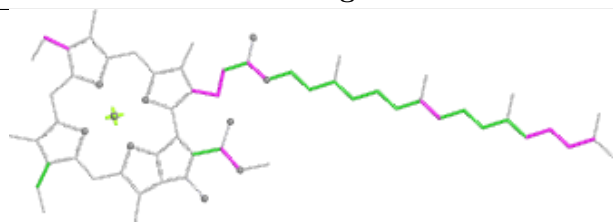
Ligand CLA A 842



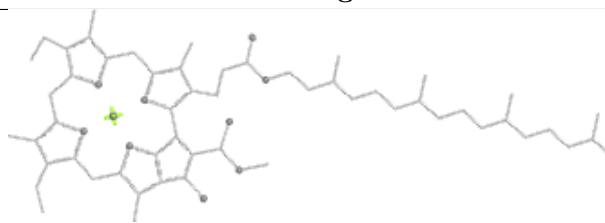
Bond lengths



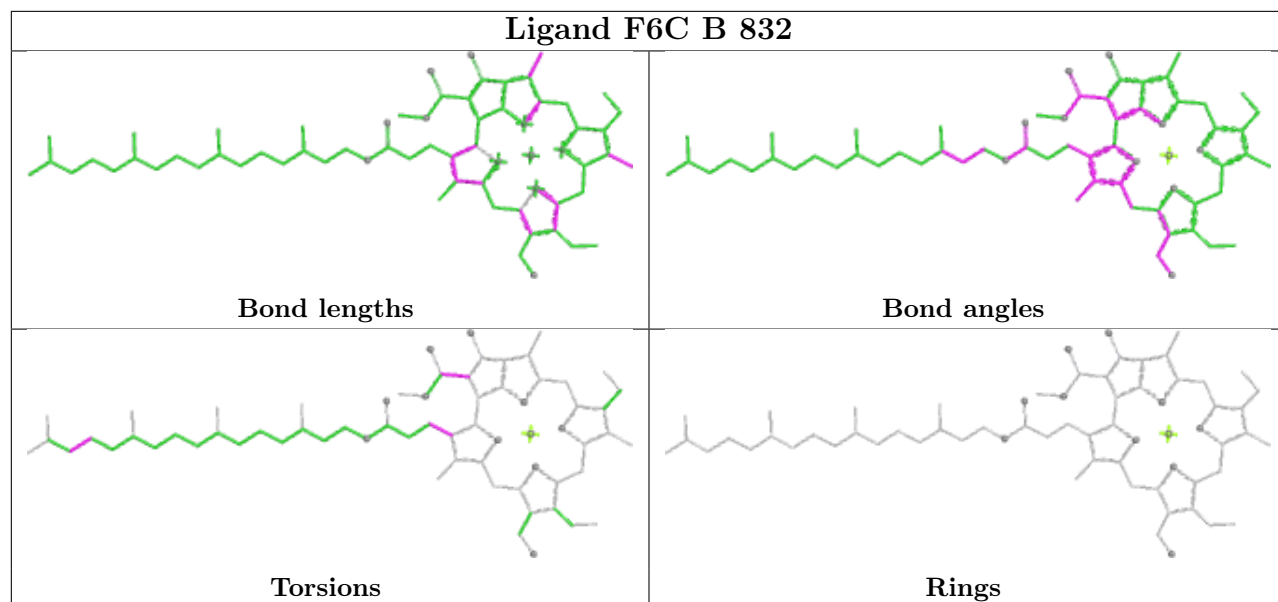
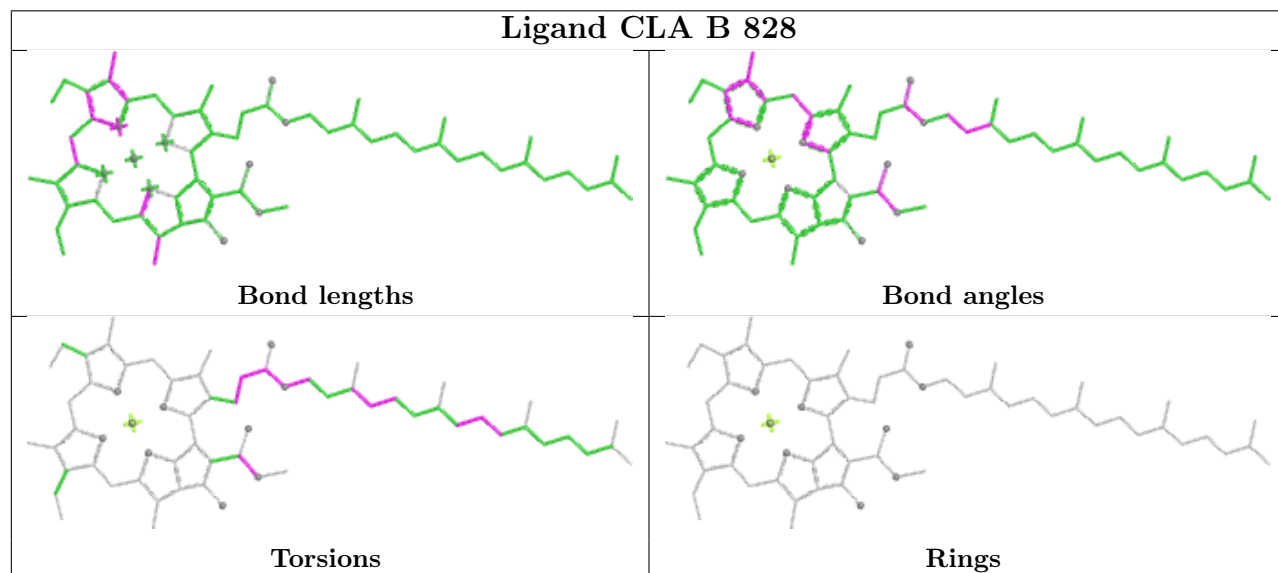
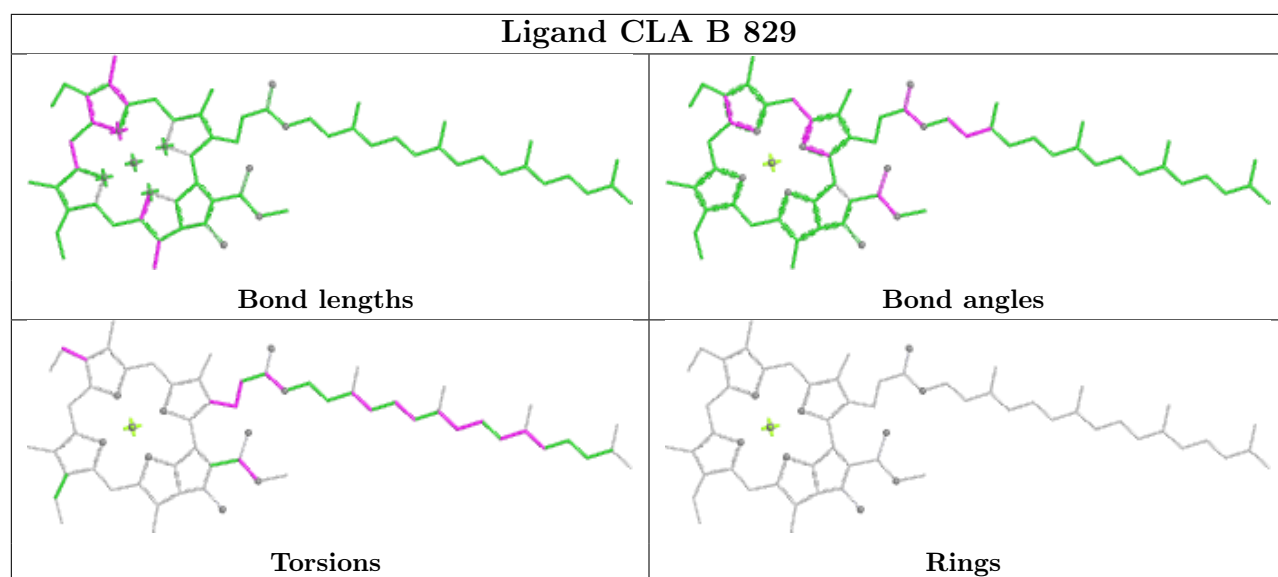
Bond angles

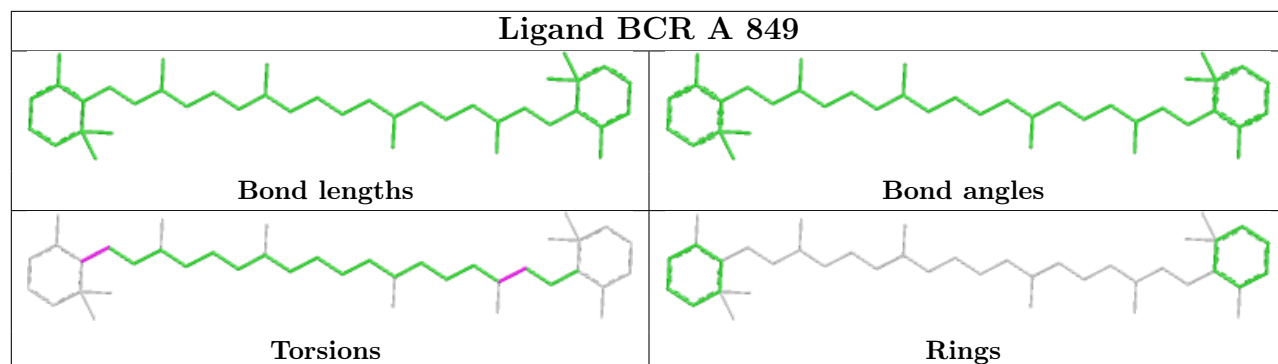
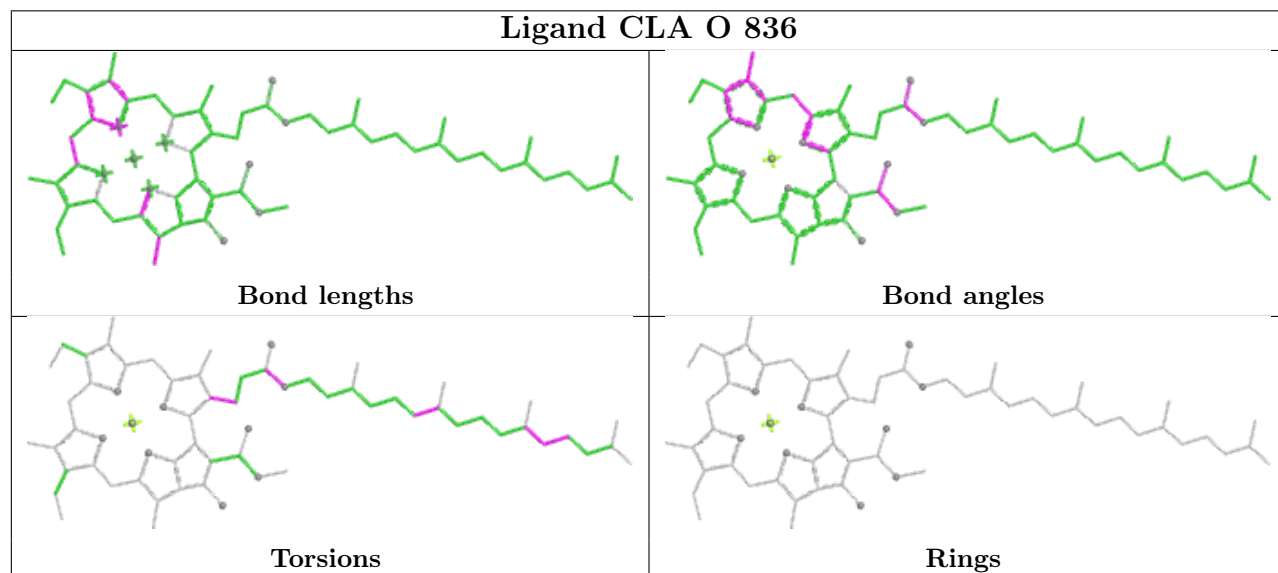
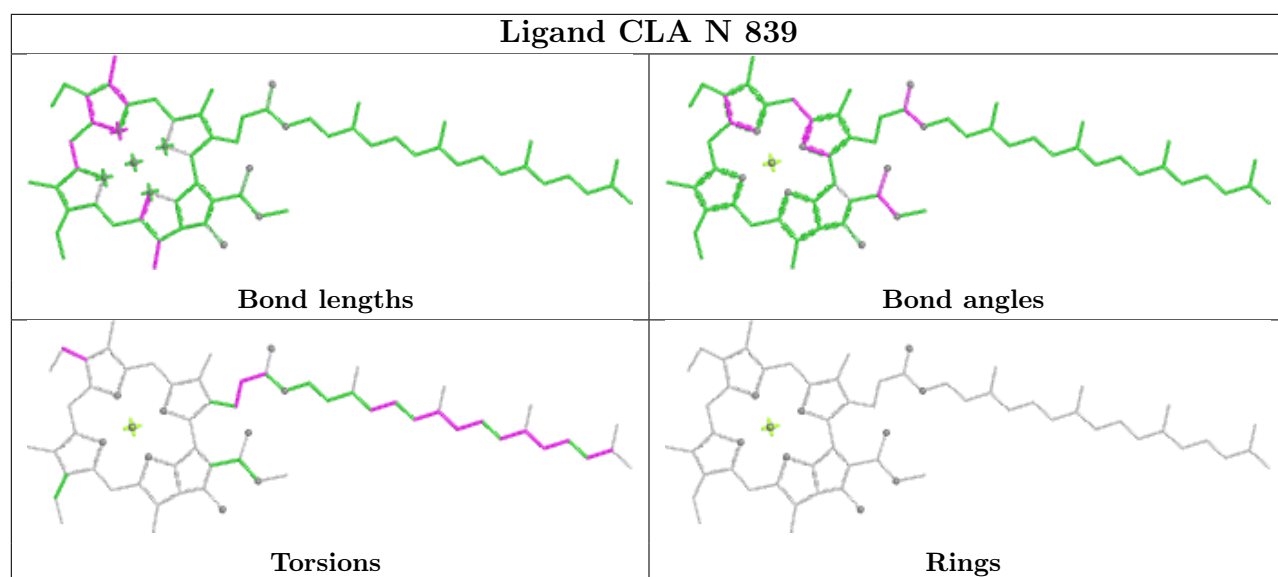


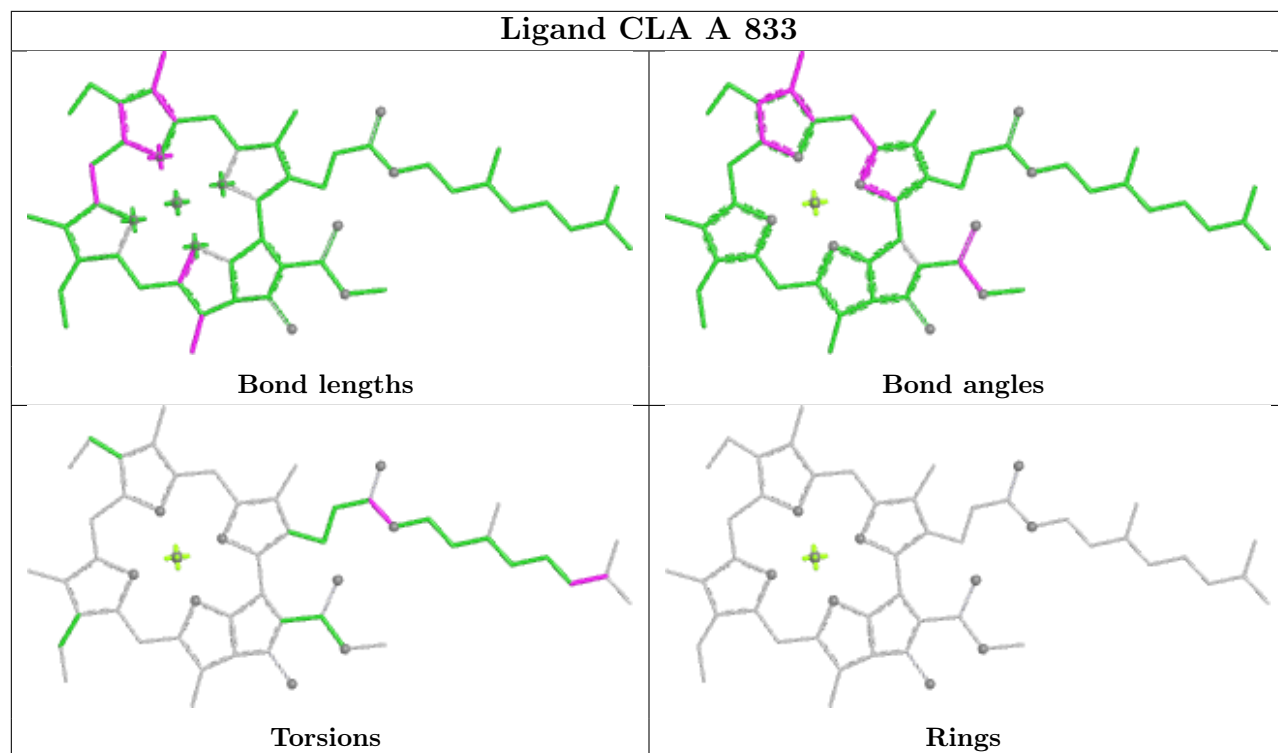
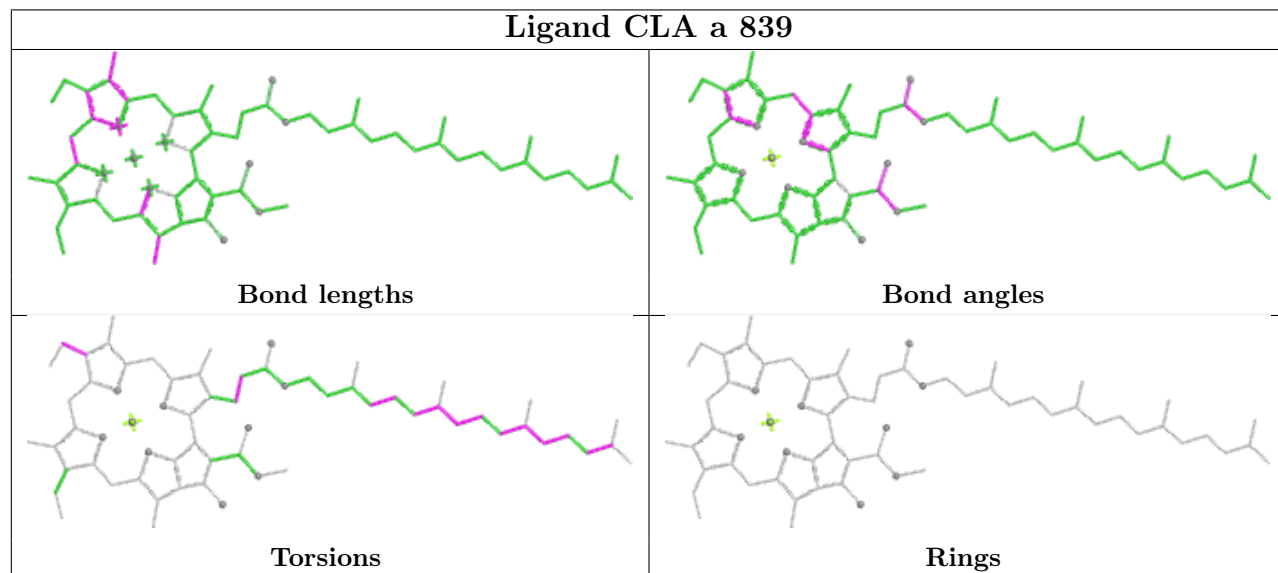
Torsions



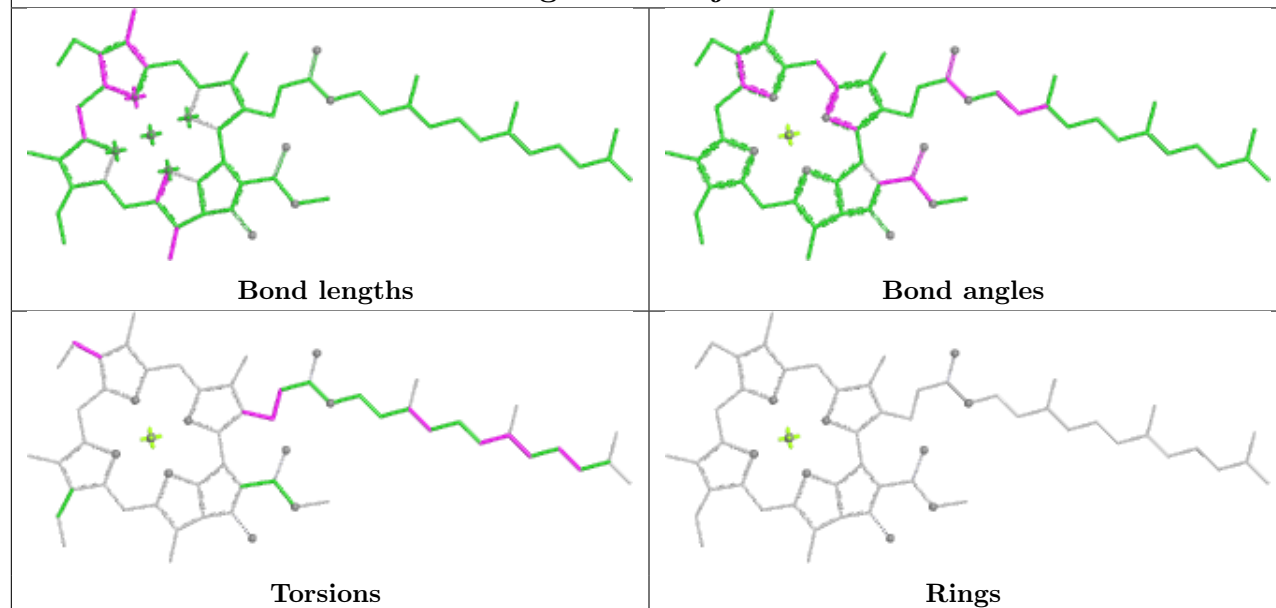
Rings



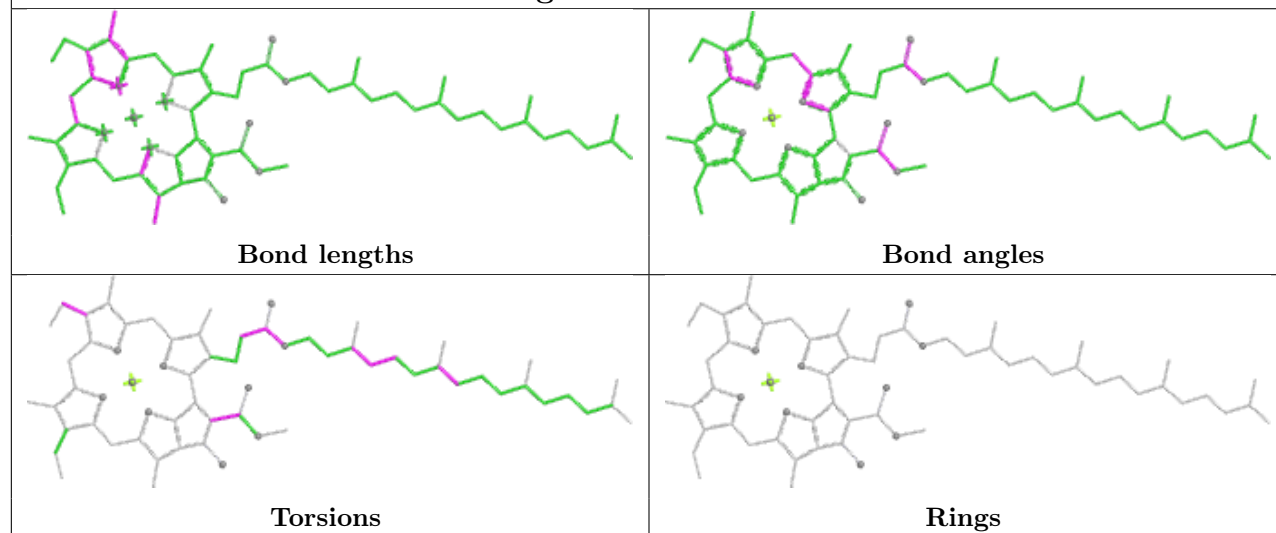


Ligand CLA A 833**Ligand CLA a 839**

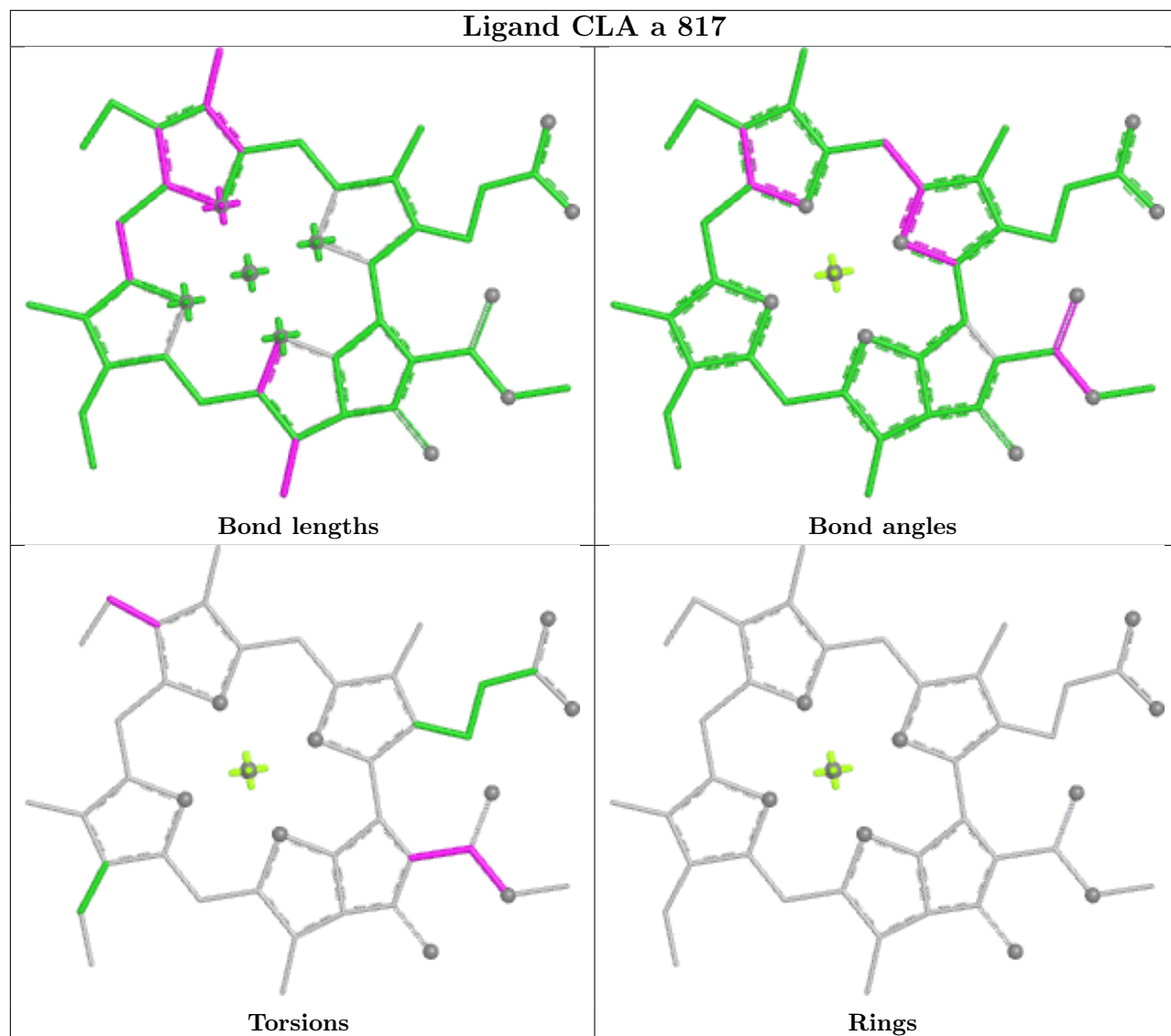
Ligand CLA j 203



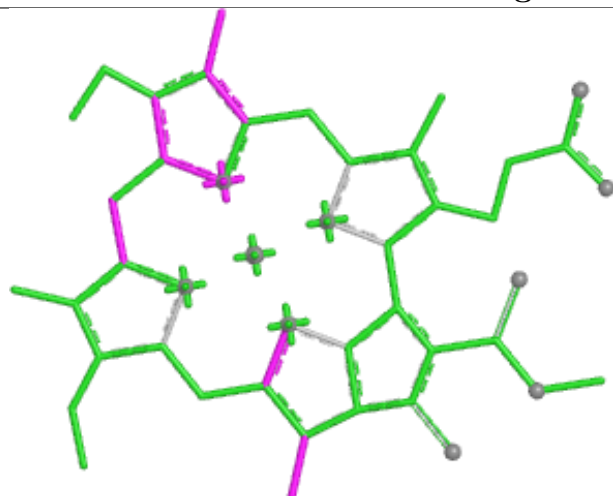
Ligand CLA a 825



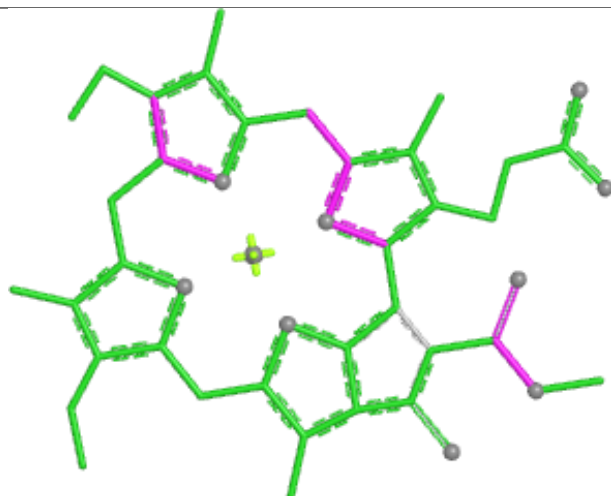
Ligand CLA a 817



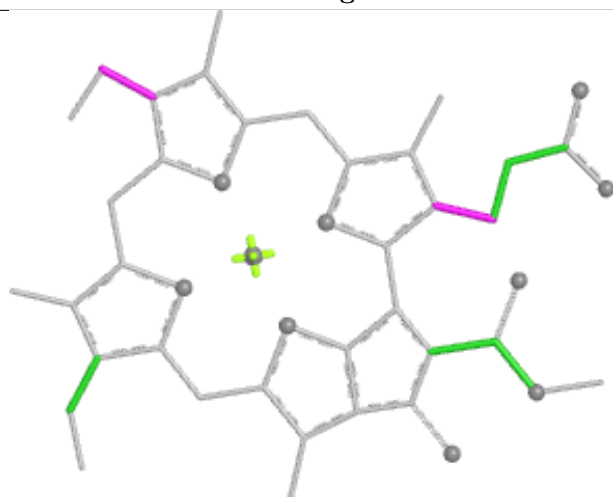
Ligand CLA B 811



Bond lengths



Bond angles

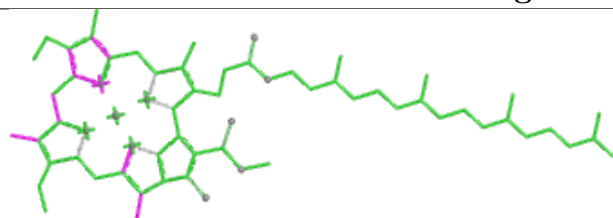


Torsions

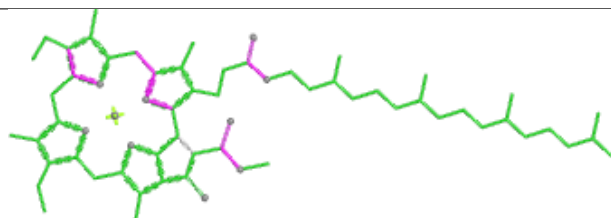


Rings

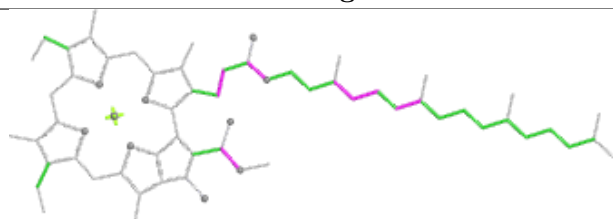
Ligand CLA B 804



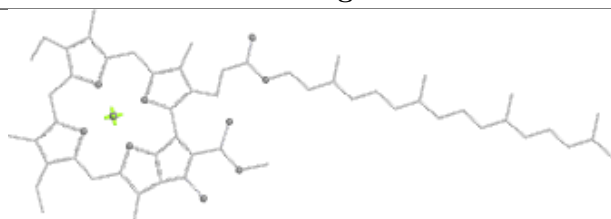
Bond lengths



Bond angles

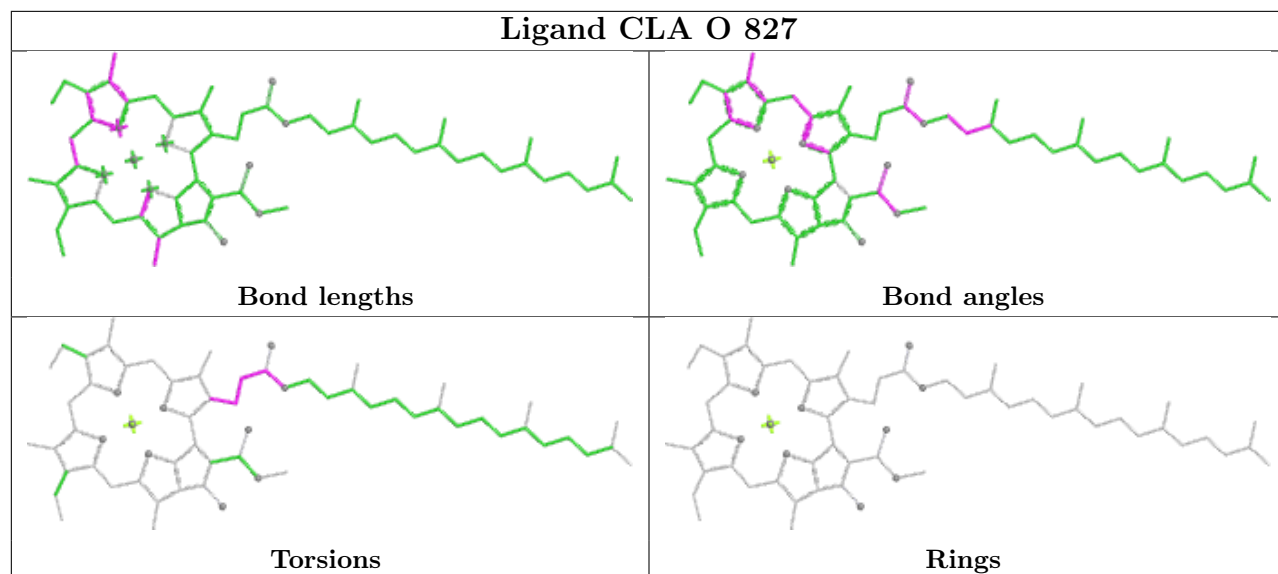


Torsions

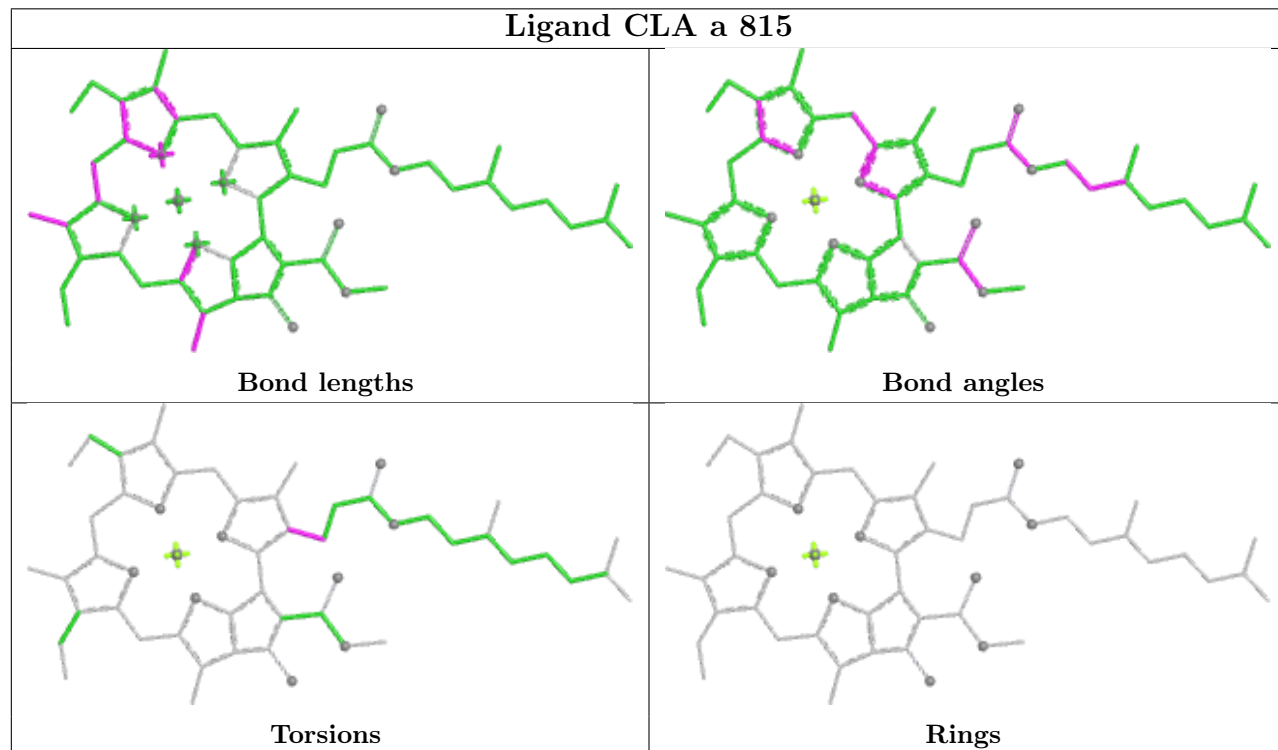


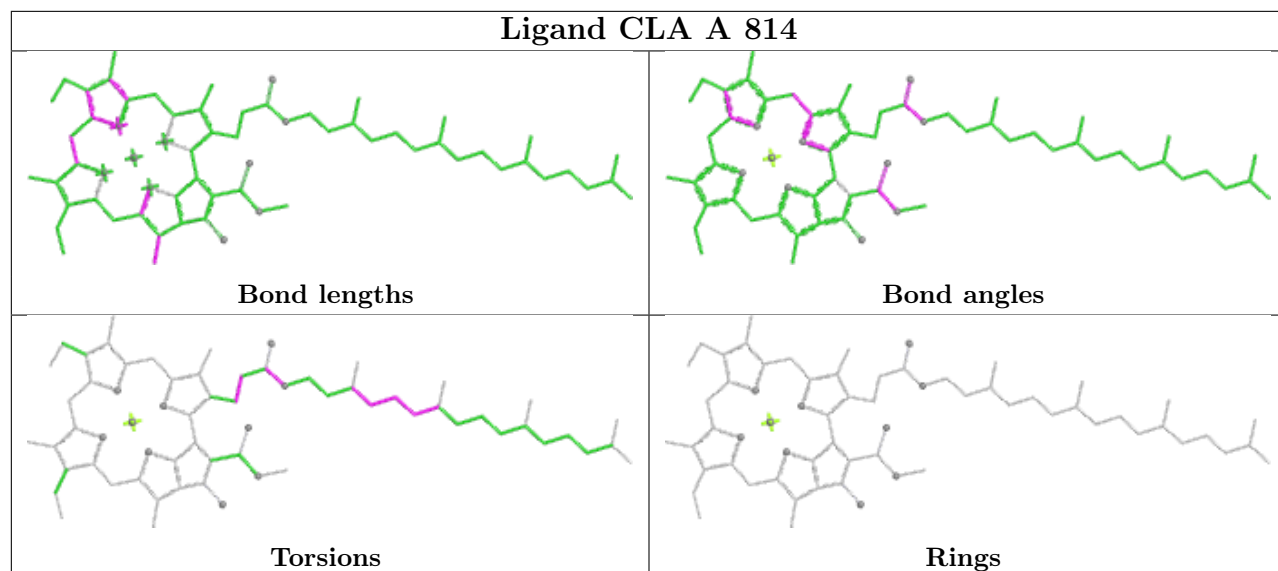
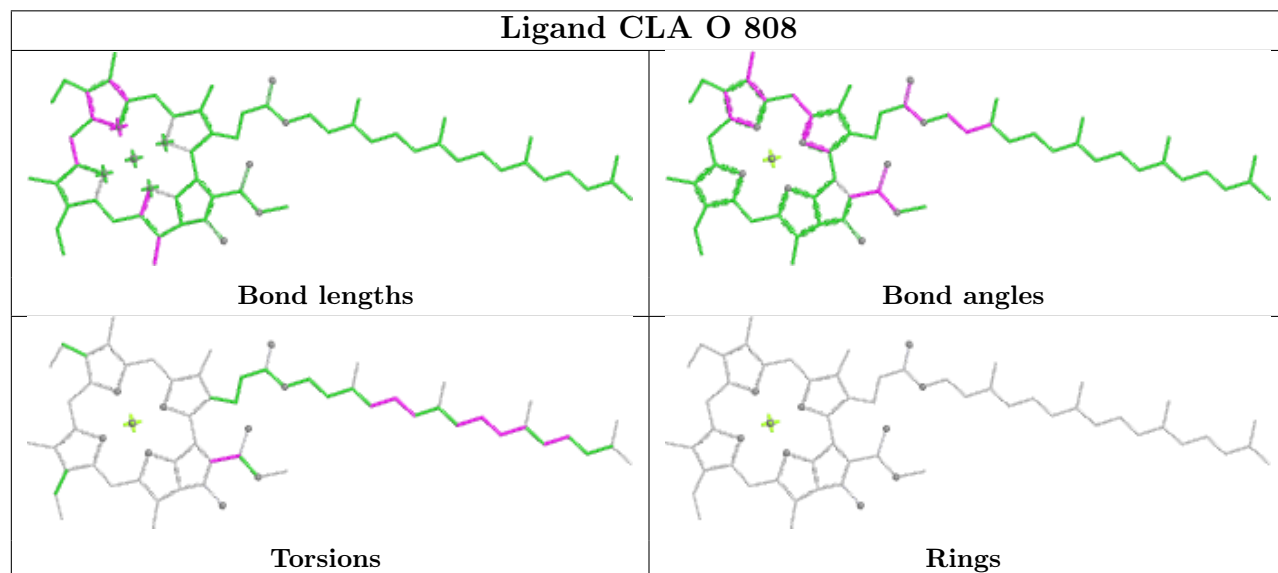
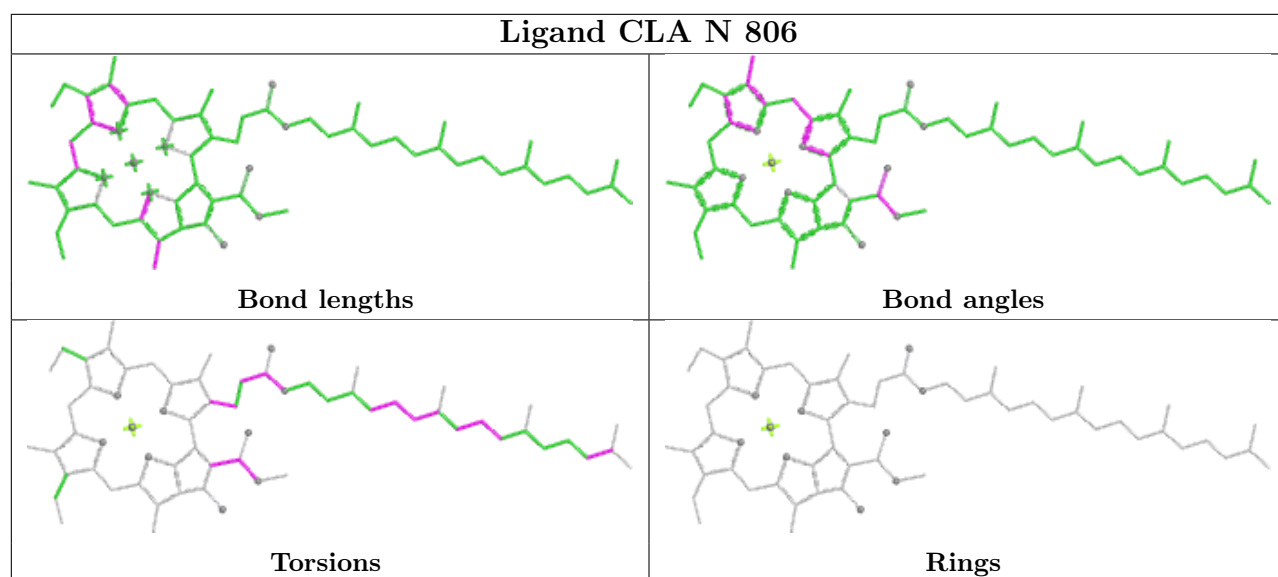
Rings

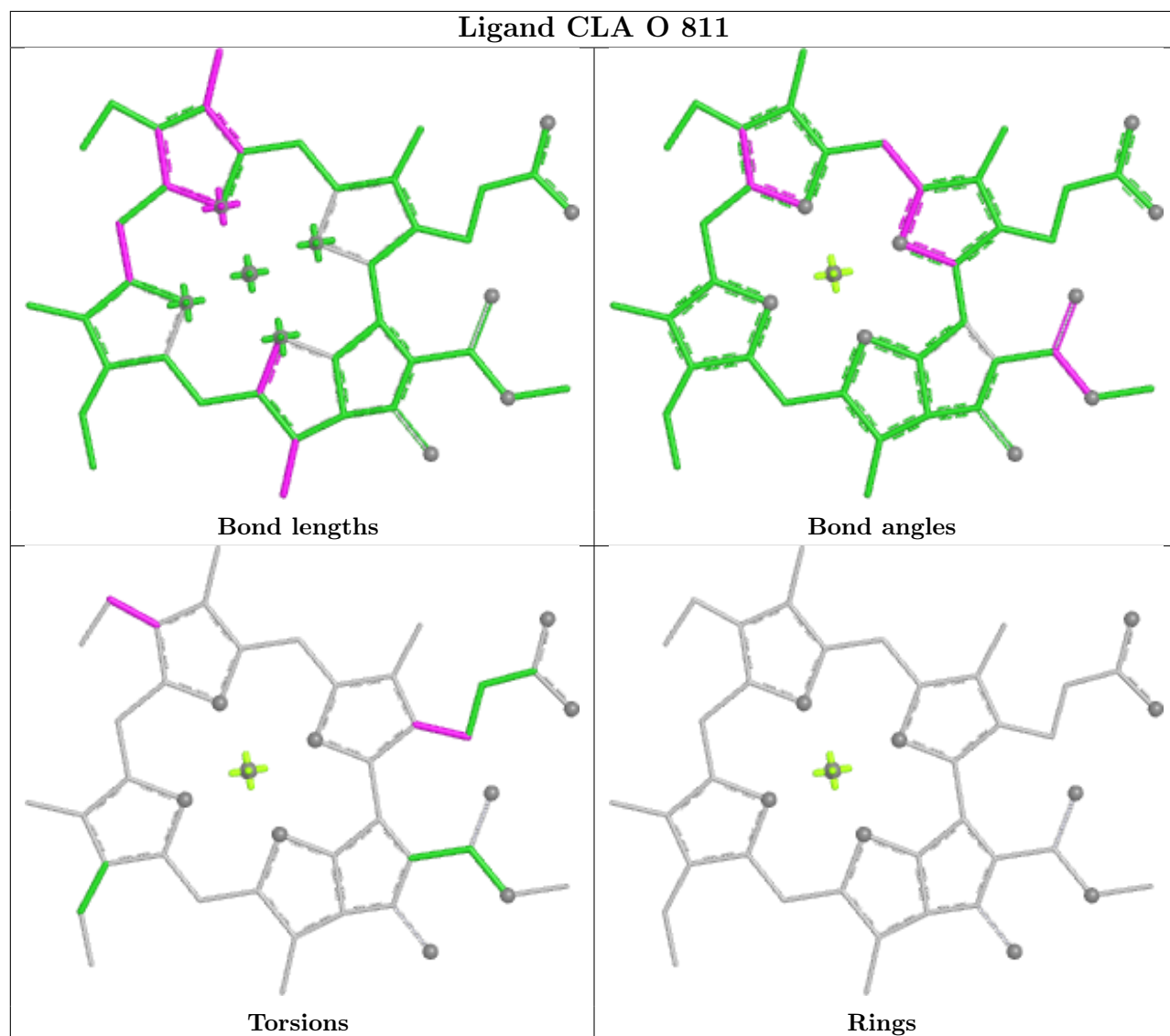
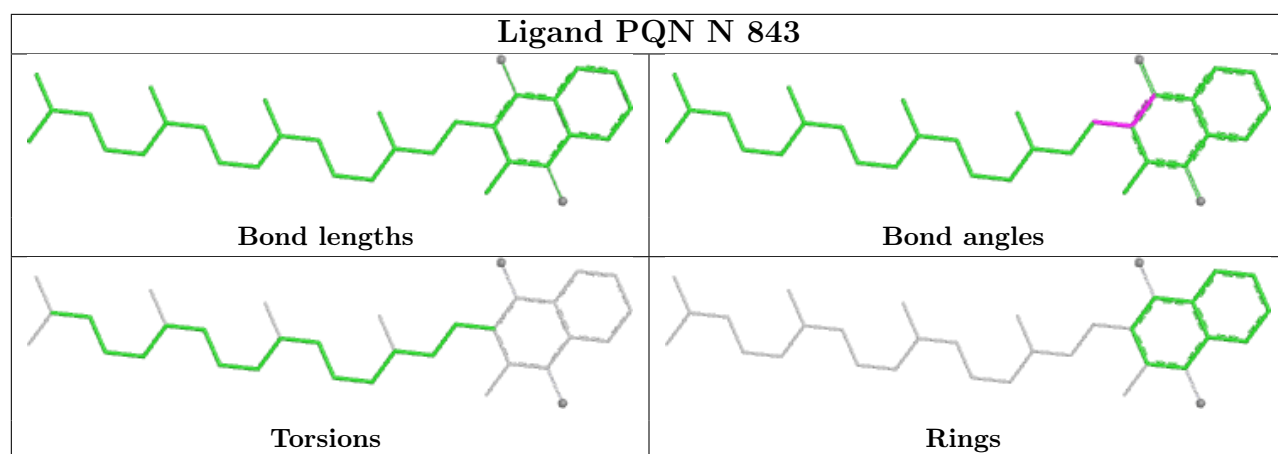
Ligand CLA O 827

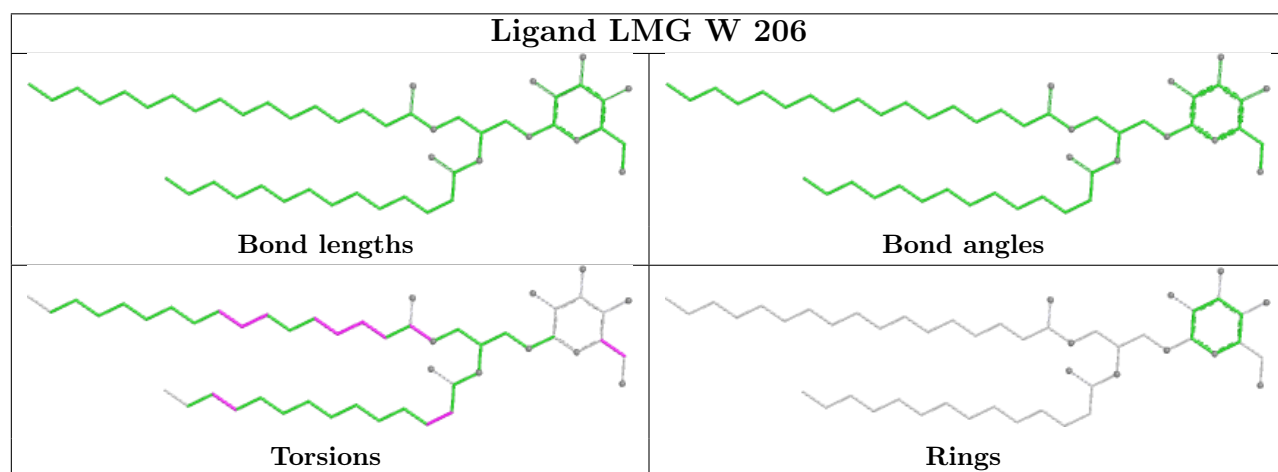
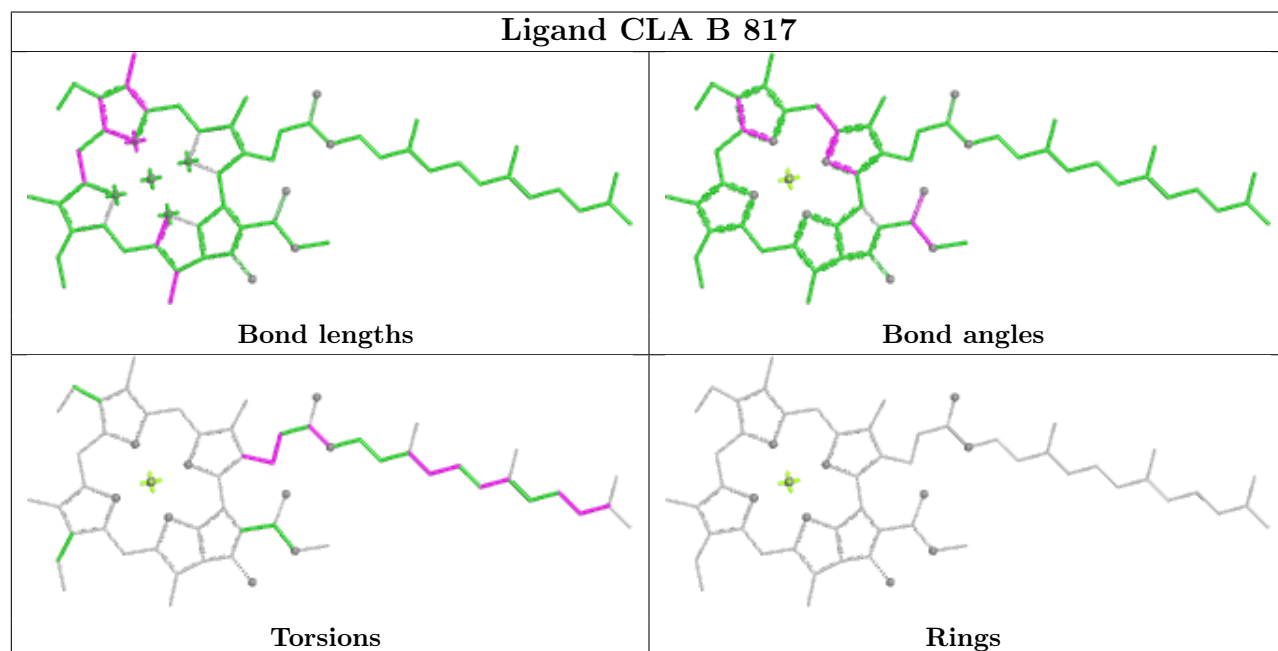
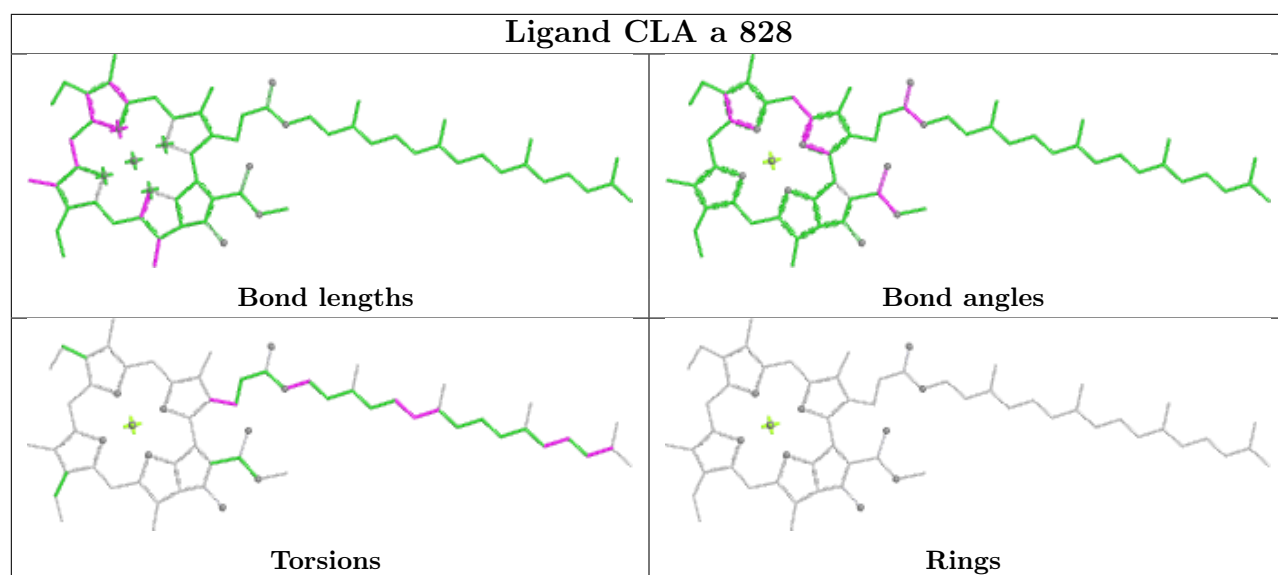


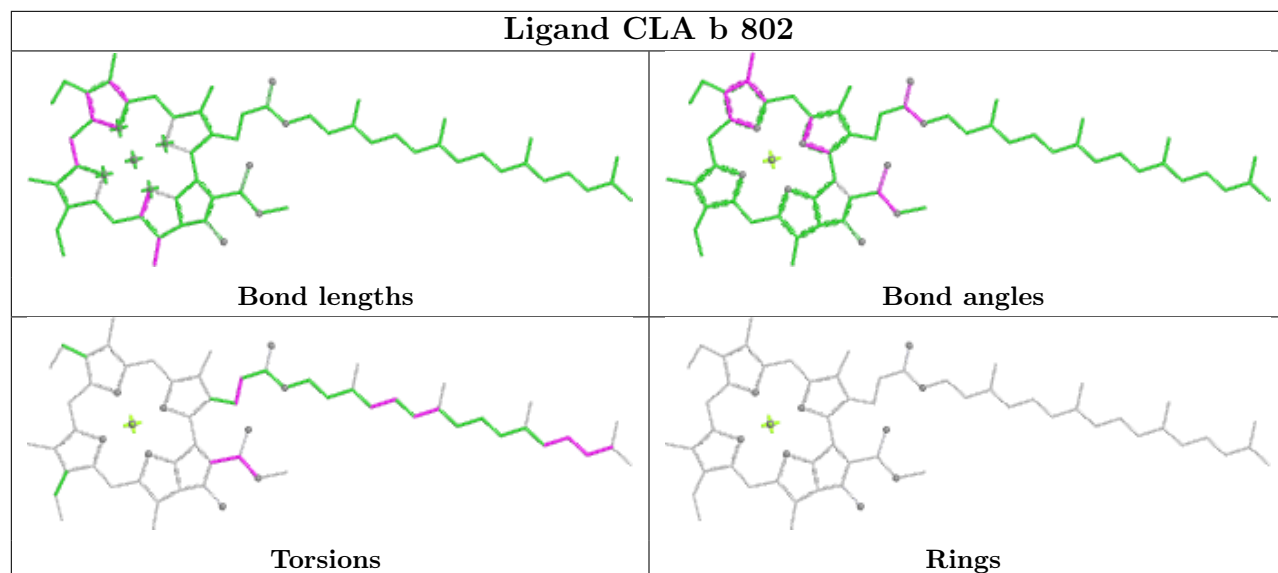
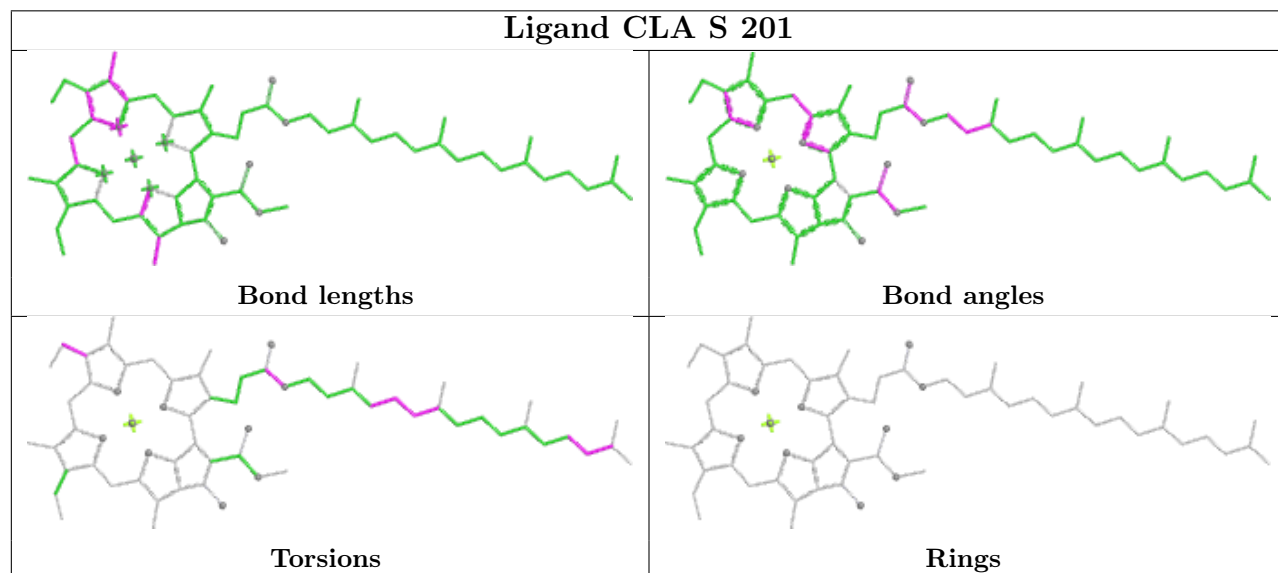
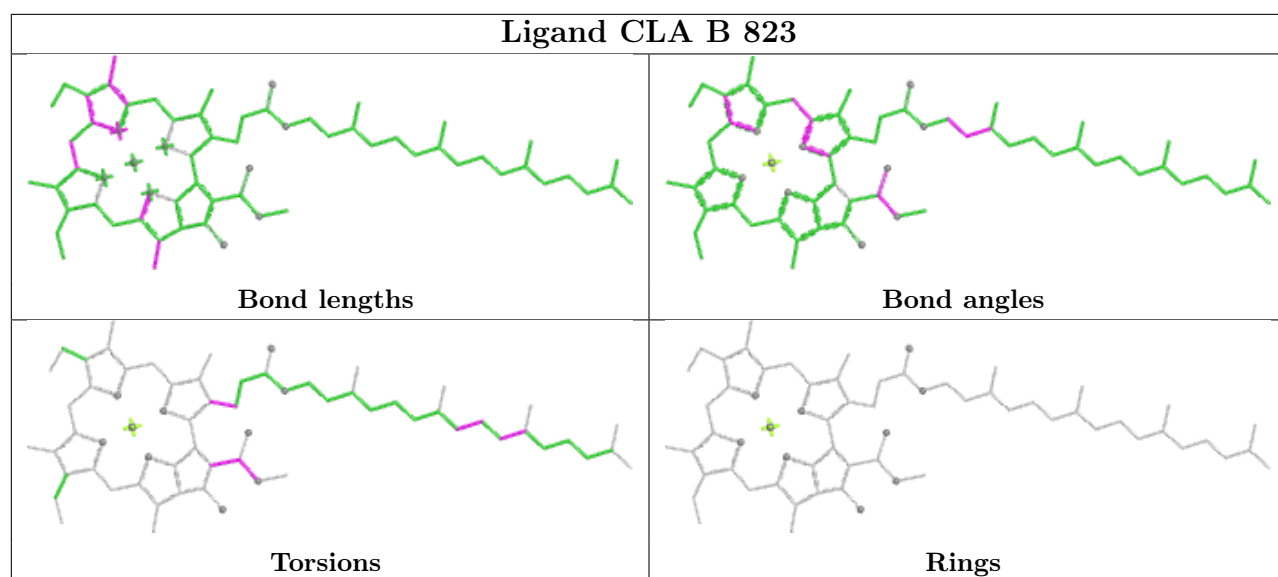
Ligand CLA a 815

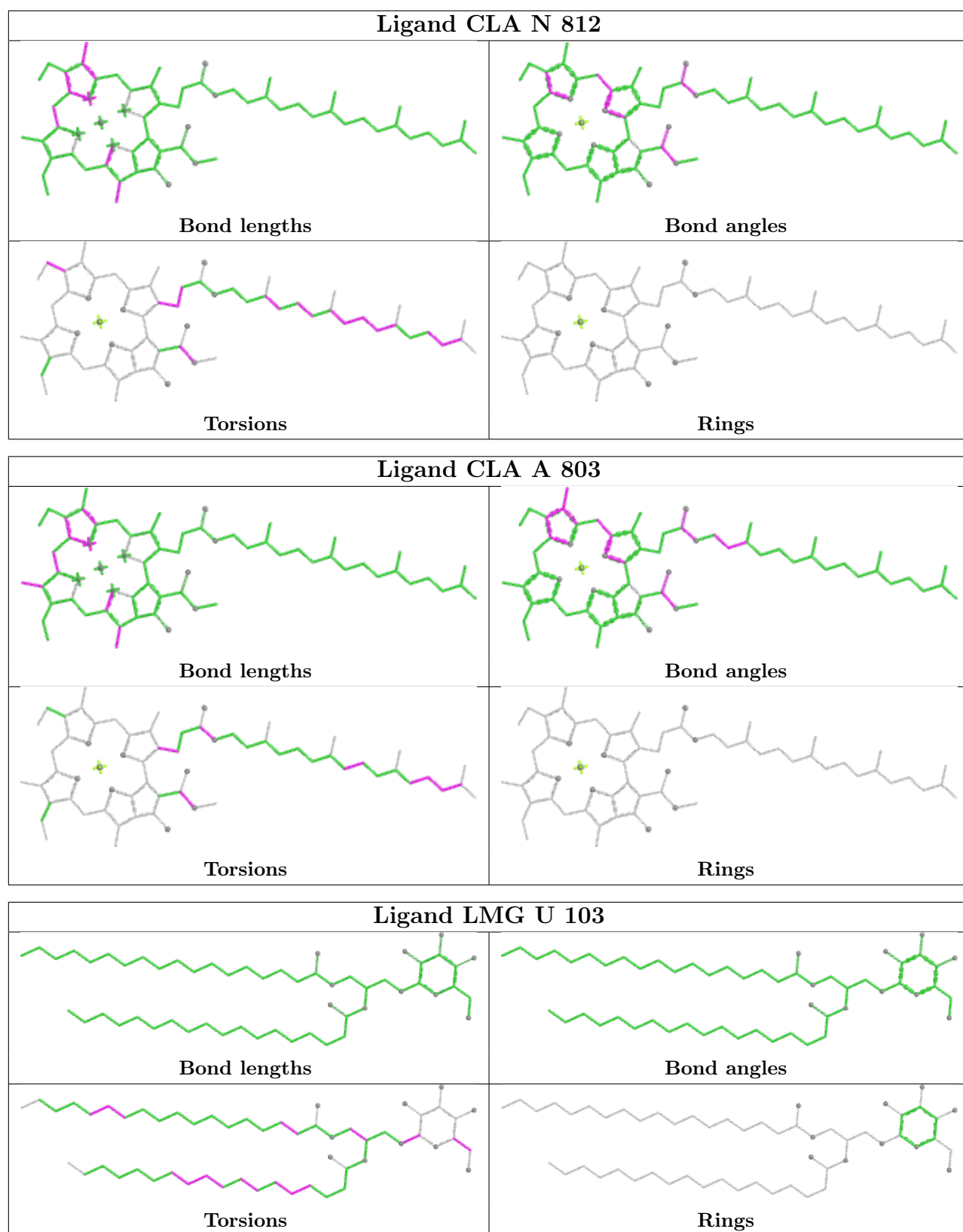












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

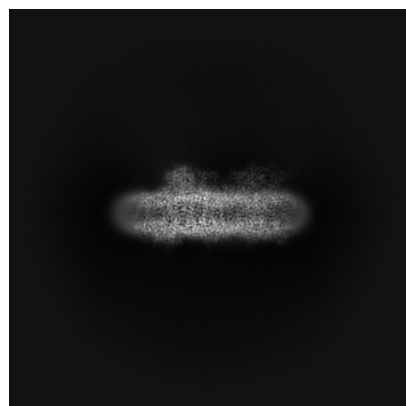
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52762. These allow visual inspection of the internal detail of the map and identification of artifacts.

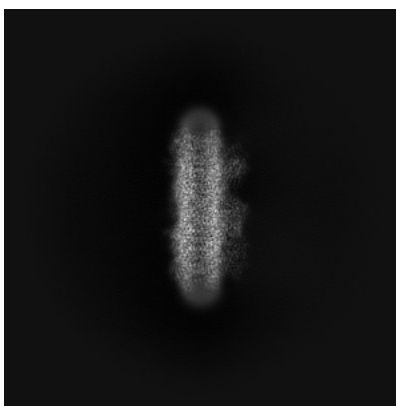
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

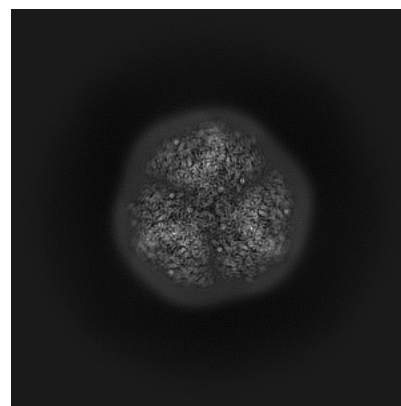
6.1.1 Primary map



X

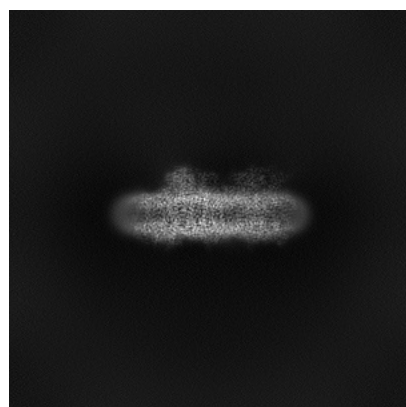


Y

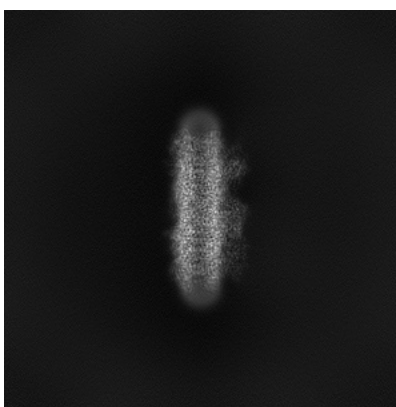


Z

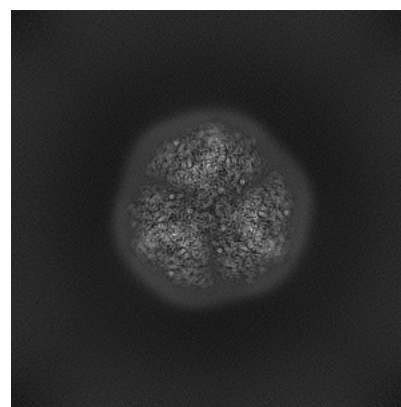
6.1.2 Raw map



X



Y

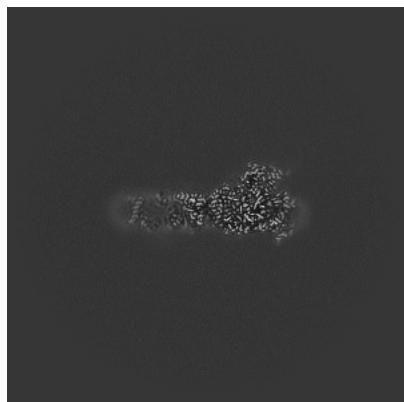


Z

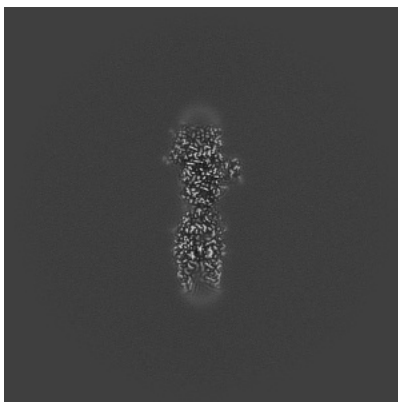
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

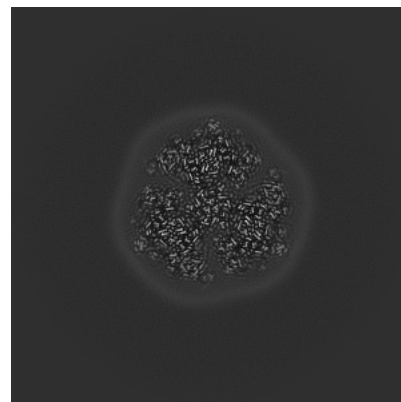
6.2.1 Primary map



X Index: 300

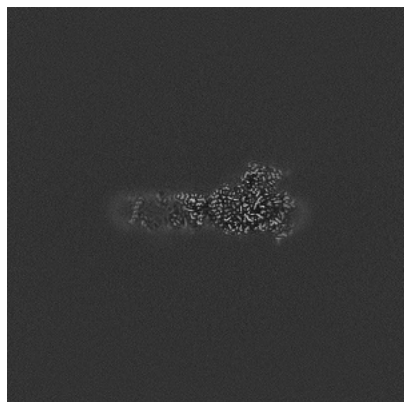


Y Index: 300

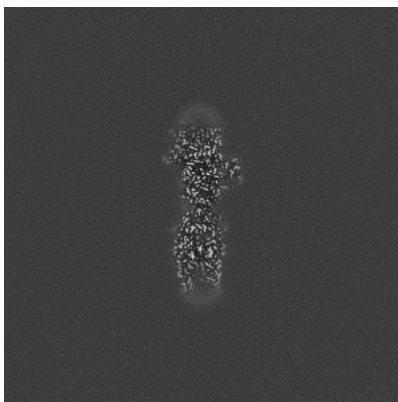


Z Index: 300

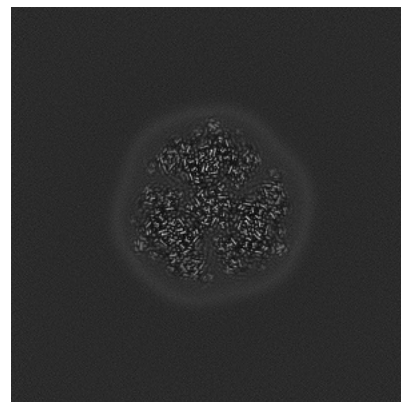
6.2.2 Raw map



X Index: 300



Y Index: 300

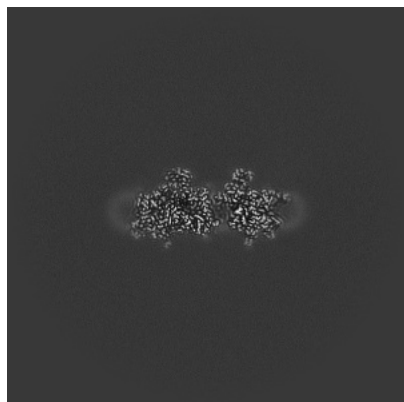


Z Index: 300

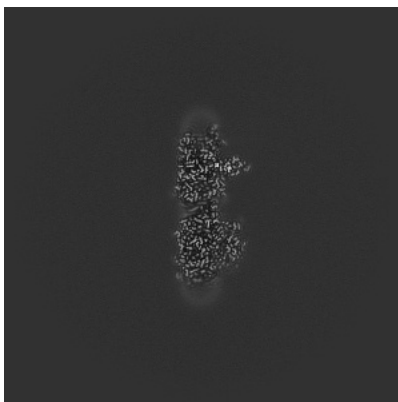
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

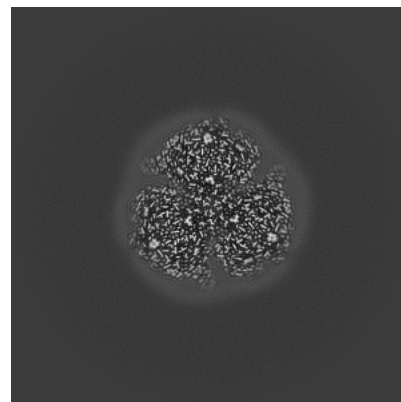
6.3.1 Primary map



X Index: 267

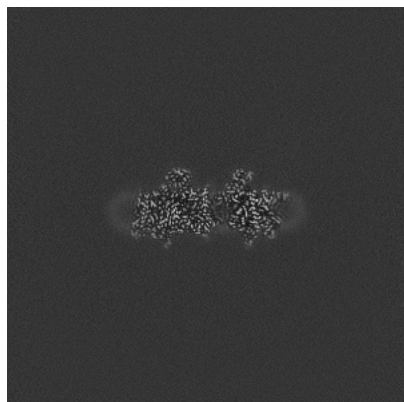


Y Index: 270

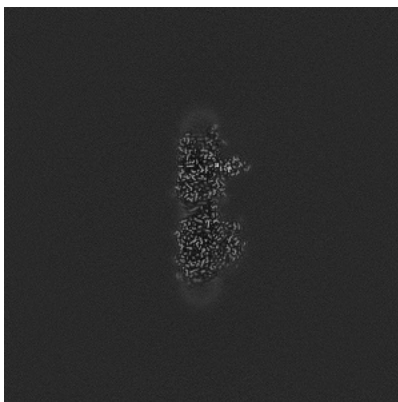


Z Index: 311

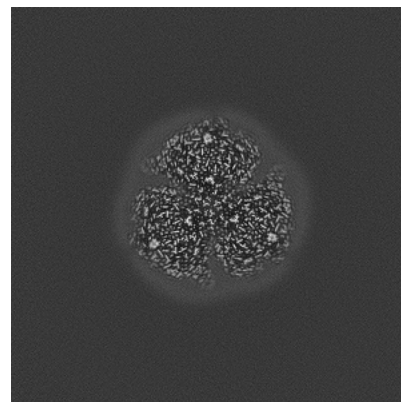
6.3.2 Raw map



X Index: 266



Y Index: 270

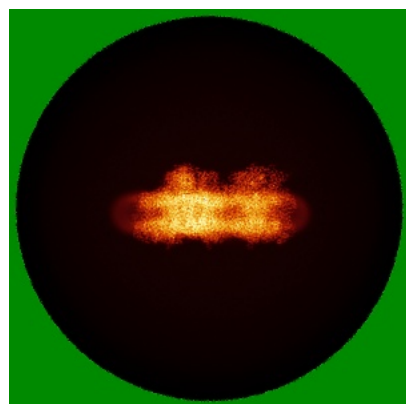


Z Index: 311

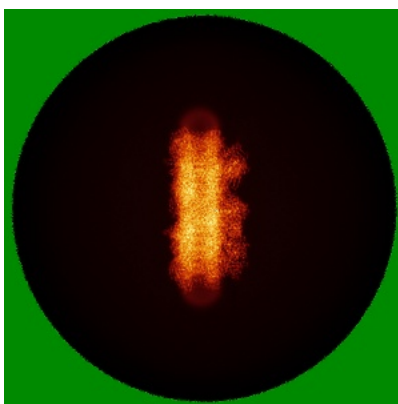
The images above show the largest variance slices of the map in three orthogonal directions.

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

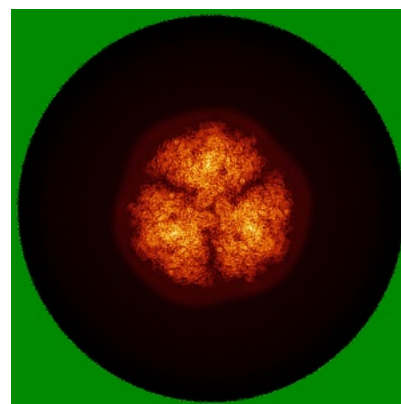
6.4.1 Primary map



X

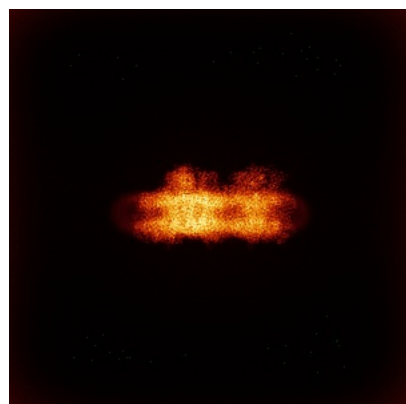


Y

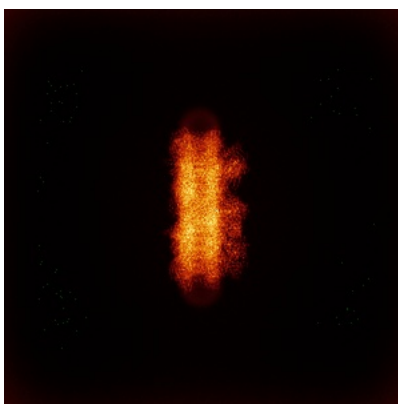


Z

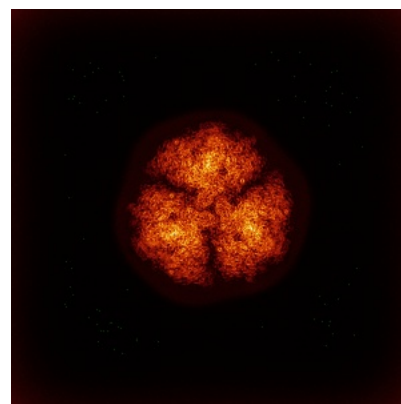
6.4.2 Raw map



X



Y

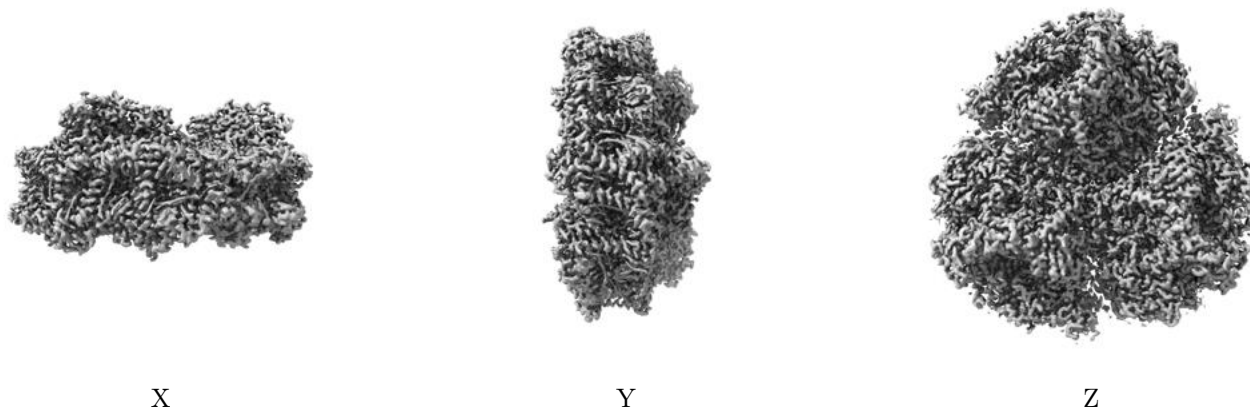


Z

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

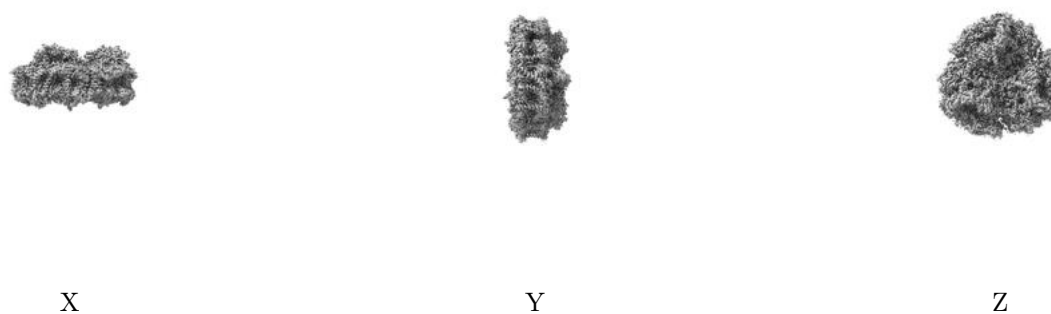
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

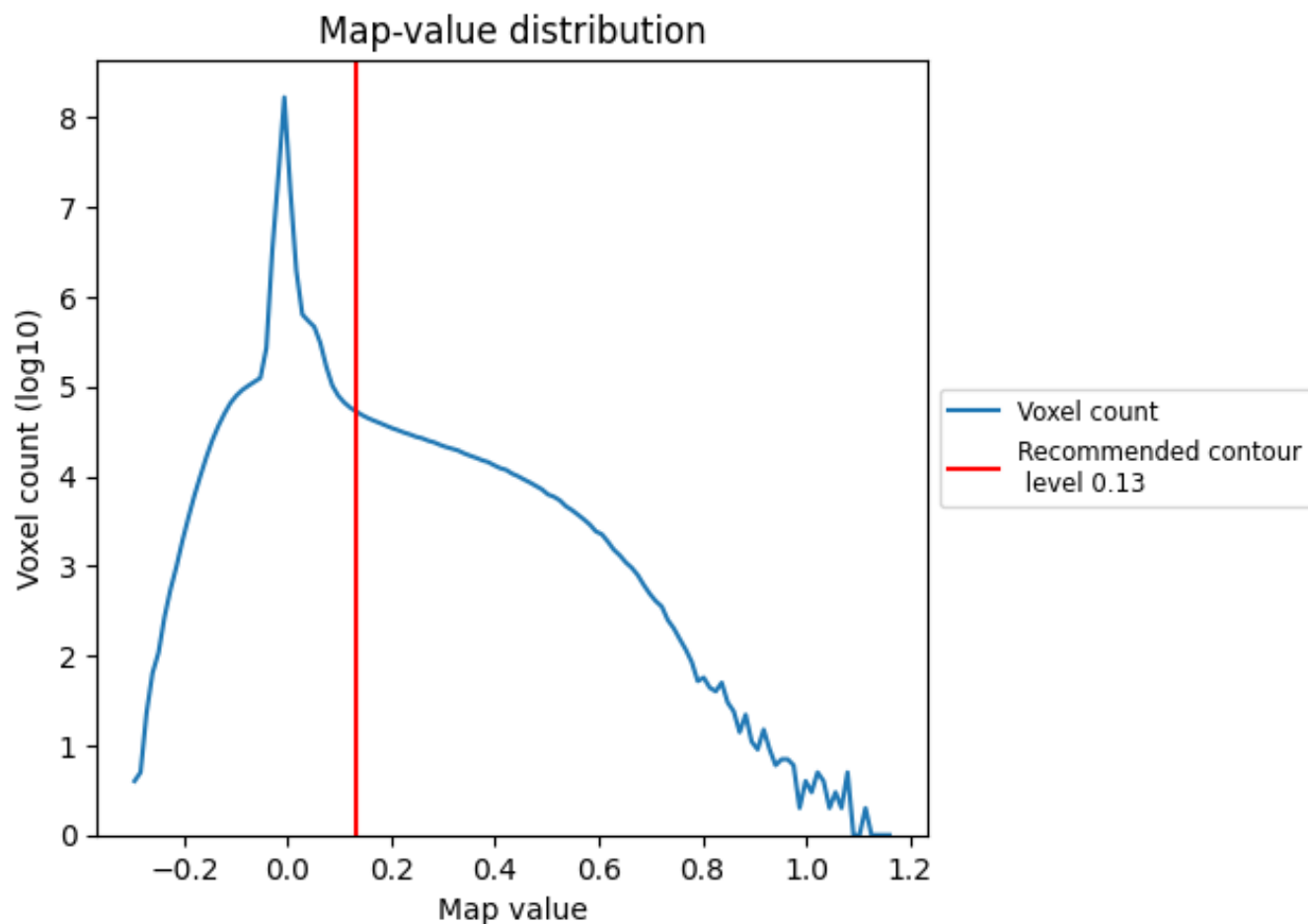
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

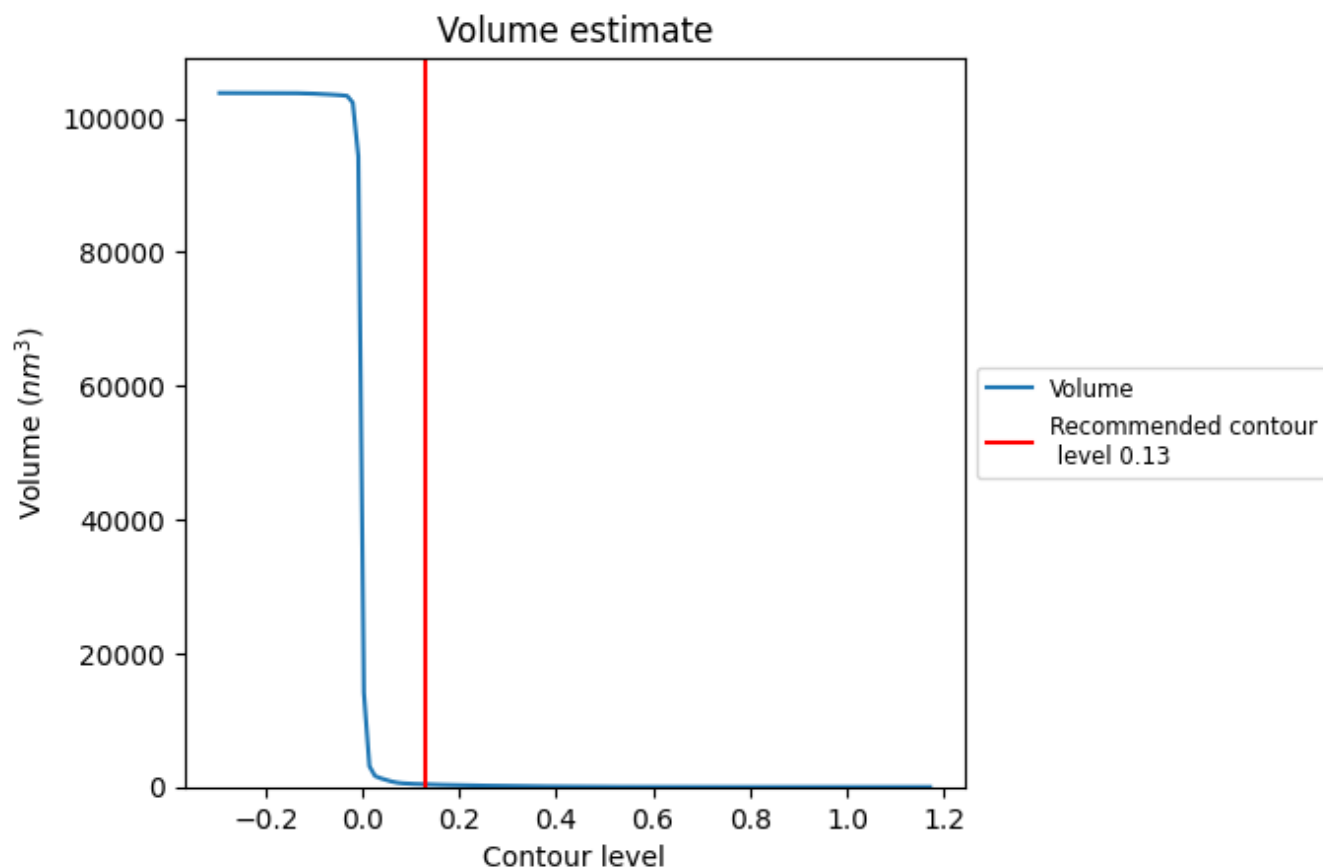
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

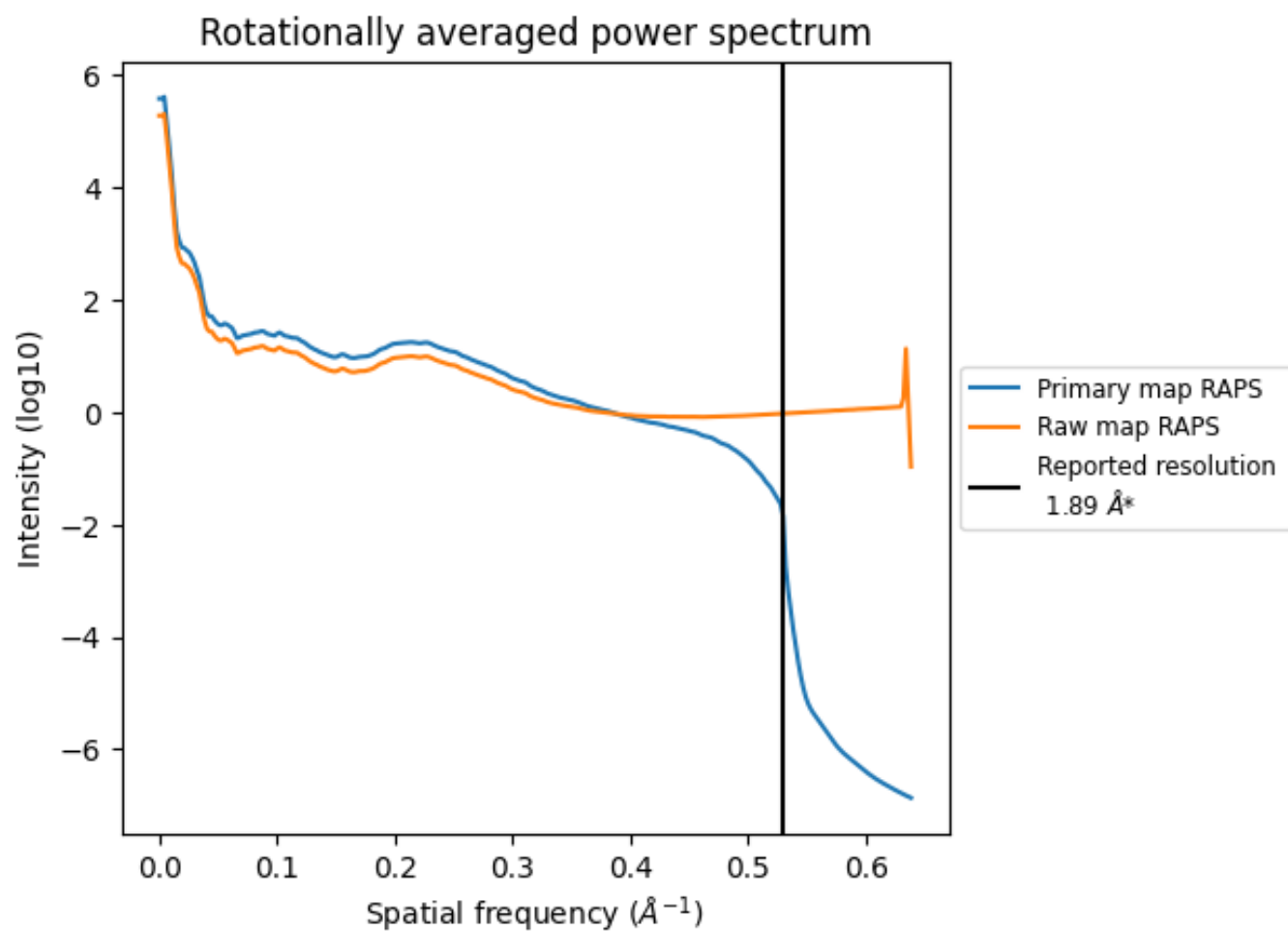
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 389 nm^3 ; this corresponds to an approximate mass of 352 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

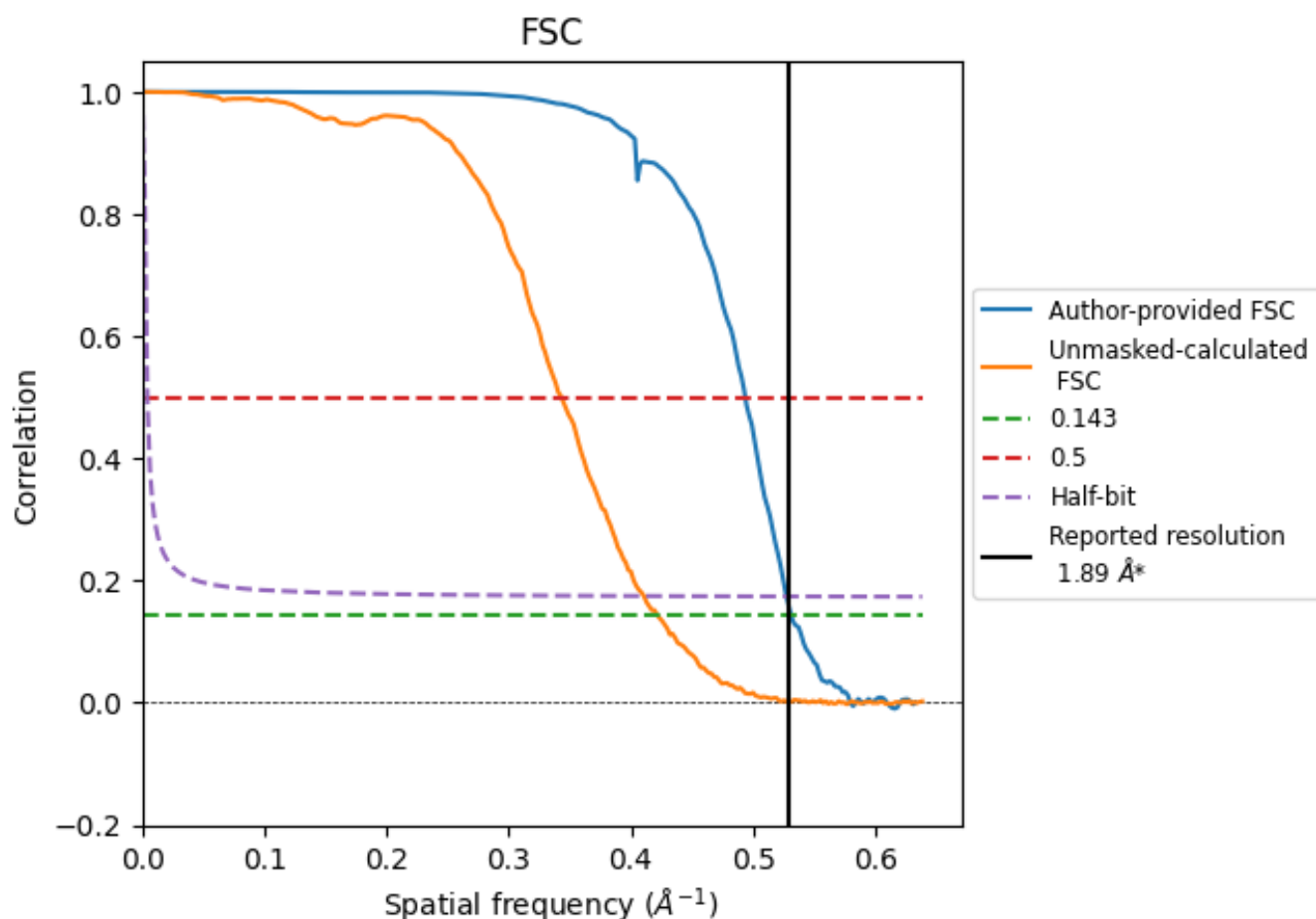


*Reported resolution corresponds to spatial frequency of 0.529 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.529 Å⁻¹

8.2 Resolution estimates [i](#)

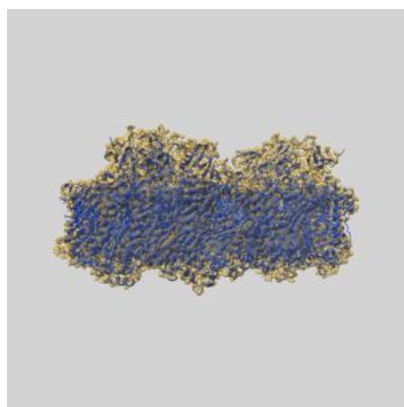
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.89	-	-
Author-provided FSC curve	1.88	2.03	1.90
Unmasked-calculated*	2.37	2.91	2.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.37 differs from the reported value 1.89 by more than 10 %

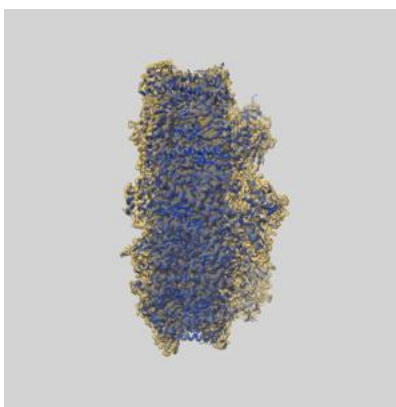
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52762 and PDB model 9I9L. Per-residue inclusion information can be found in section [3](#) on page [41](#).

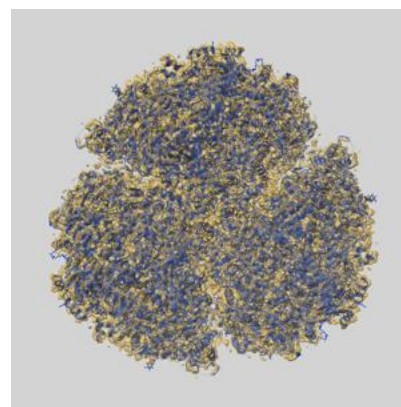
9.1 Map-model overlay [i](#)



X



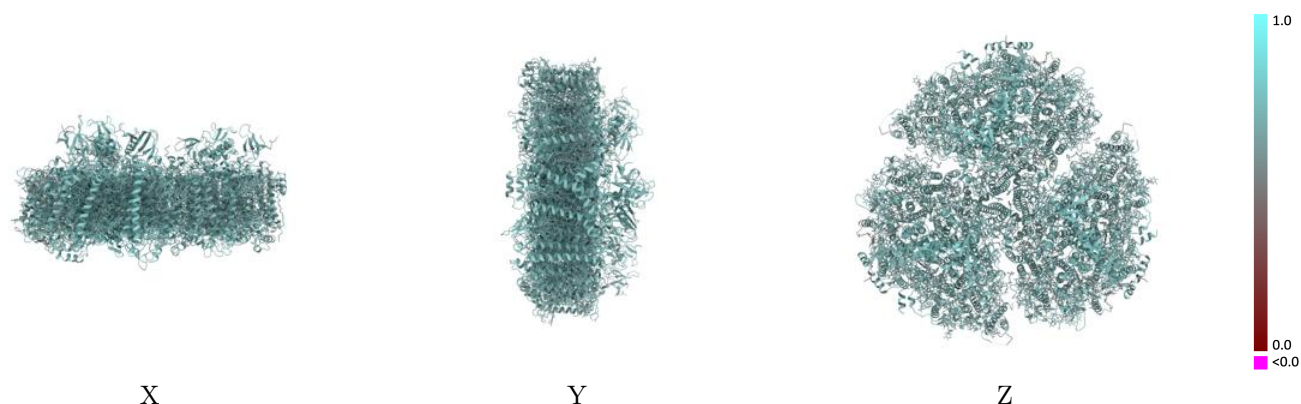
Y



Z

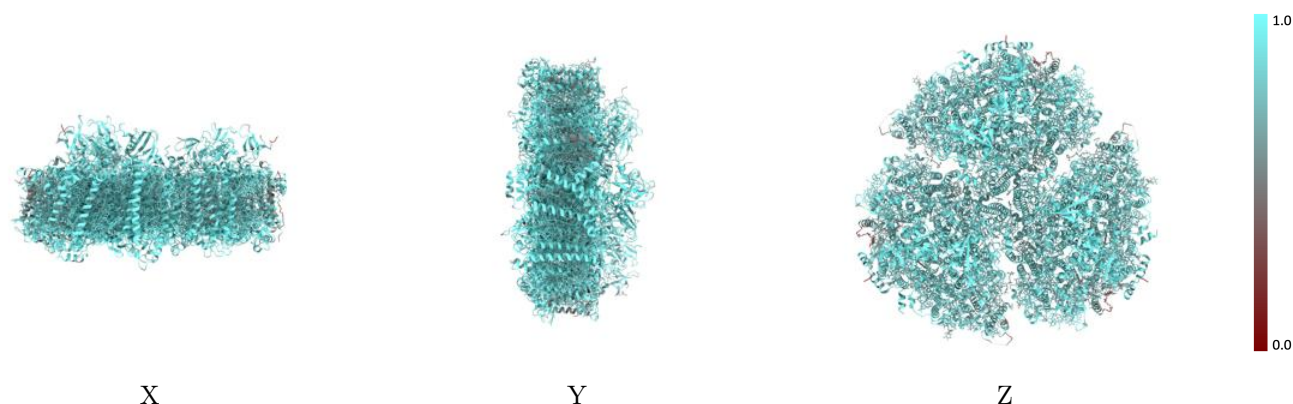
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



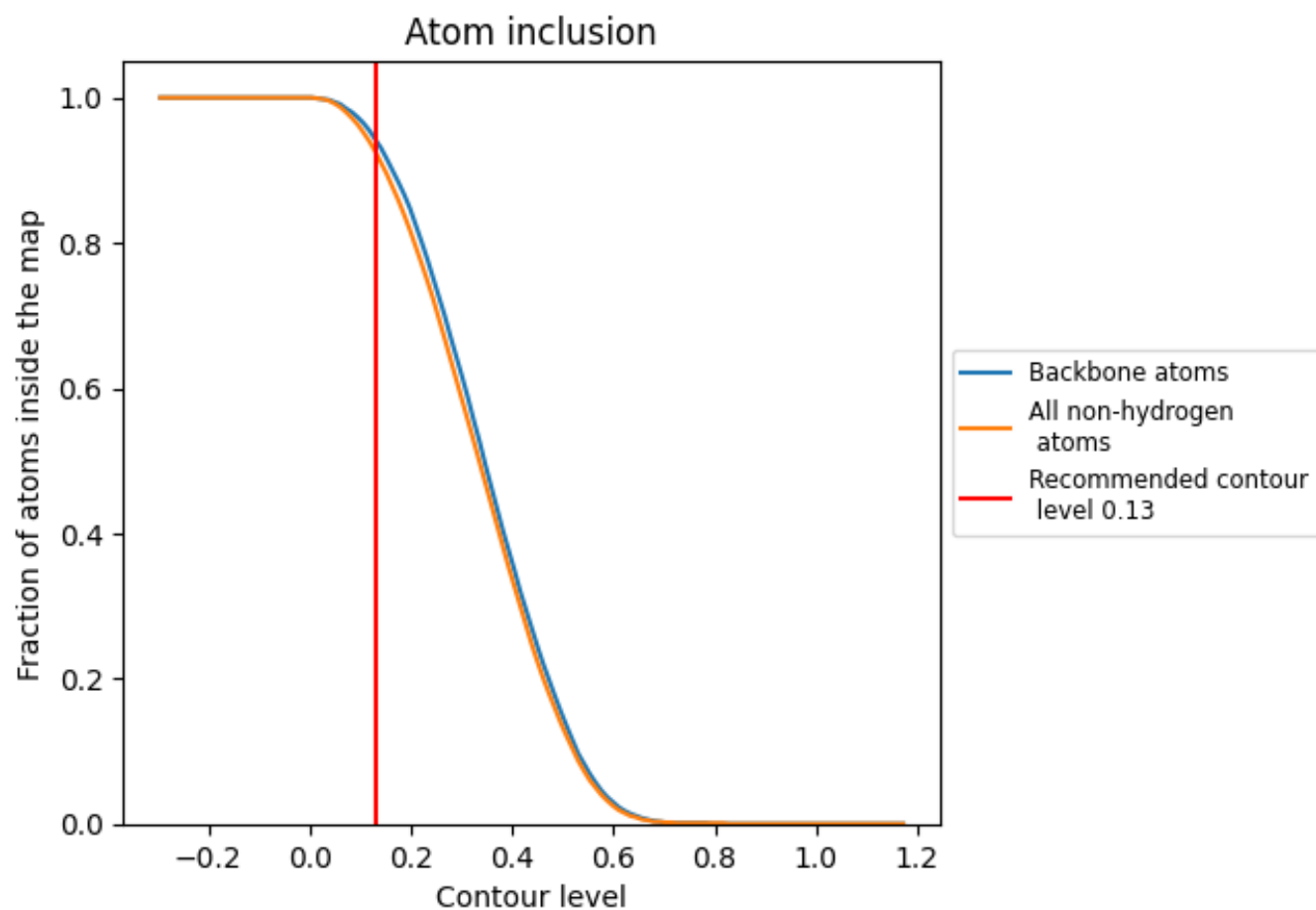
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ




The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.6960
A	 0.9400	 0.6990
B	 0.9400	 0.7000
C	 0.9880	 0.7270
D	 0.9310	 0.6920
E	 0.8470	 0.6580
F	 0.8290	 0.6420
I	 0.9550	 0.7160
J	 0.8330	 0.6500
K	 0.7150	 0.6260
L	 0.9560	 0.7200
M	 0.9390	 0.7080
N	 0.9360	 0.7010
O	 0.9440	 0.7040
P	 0.9920	 0.7290
Q	 0.9340	 0.6980
R	 0.8470	 0.6600
S	 0.8560	 0.6530
T	 0.9500	 0.7190
U	 0.8450	 0.6540
V	 0.7140	 0.6210
W	 0.9550	 0.7210
X	 0.6580	 0.6300
Y	 0.8930	 0.6890
Z	 0.6580	 0.6320
a	 0.9420	 0.7030
b	 0.9440	 0.7030
c	 0.9870	 0.7260
d	 0.9260	 0.6960
e	 0.8520	 0.6570
f	 0.8360	 0.6460
g	 0.9500	 0.7210
h	 0.8430	 0.6530
i	 0.7180	 0.6270
j	 0.9580	 0.7220



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Chain	Atom inclusion	Q-score
k	 0.8930	 0.6890
l	 0.6580	 0.6270