



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 12:32 PM UTC

PDB ID : 9EYS / pdb_00009eys
EMDB ID : EMD-50063
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 : 2024-04-09
Resolution : 2.01 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:

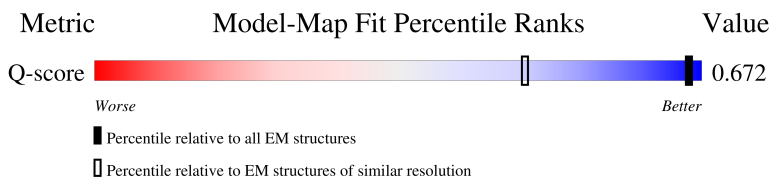
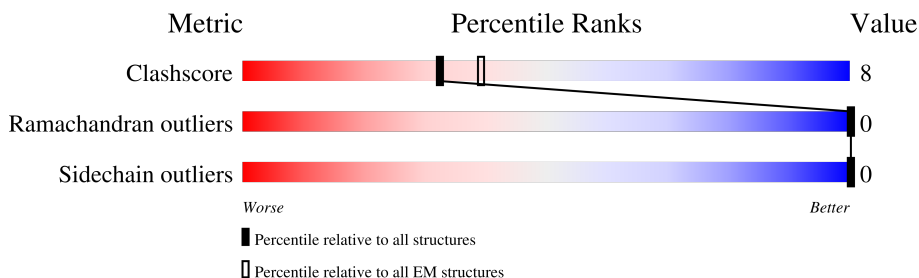
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.01 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	1691 (1.52 - 2.51)

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	 79% 17% .
1	N	782	 81% 15% .
1	a	782	 82% 15% .
2	B	740	 84% 16%

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Mol	Chain	Length	Quality of chain
2	O	740	
2	b	740	
3	C	81	
3	P	81	
3	c	81	
4	D	142	
4	Q	142	
4	d	142	
5	E	66	
5	R	66	
5	e	66	
6	F	161	
6	S	161	
6	f	161	
7	I	51	
7	T	51	
7	g	51	
8	J	46	
8	U	46	
8	h	46	
9	K	80	
9	V	80	
9	i	80	
10	L	183	
10	W	183	

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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	857	X	-	-	-
14	F6C	B	831	X	-	-	-
14	F6C	B	838	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	810	X	-	-	-
14	F6C	O	833	X	-	-	-
14	F6C	O	840	X	-	-	-
14	F6C	W	1503	X	-	-	-
14	F6C	a	802	X	-	-	-
14	F6C	a	824	X	-	-	-
14	F6C	a	826	X	-	-	-
14	F6C	a	856	X	-	-	-
14	F6C	b	810	X	-	-	-
14	F6C	b	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	F6C	b	840	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	A	856	X	-	-	-
15	CLA	B	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
15	CLA	B	809	X	-	-	-
15	CLA	B	810	X	-	-	-
15	CLA	B	812	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	832	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	839	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	811	X	-	-	-
15	CLA	O	812	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	832	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	839	X	-	-	-
15	CLA	O	841	X	-	-	-
15	CLA	S	201	X	-	-	-
15	CLA	V	102	X	-	-	-
15	CLA	V	103	X	-	-	-
15	CLA	W	1501	X	-	-	-
15	CLA	W	1502	X	-	-	-
15	CLA	X	103	X	-	-	-
15	CLA	Z	103	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	811	X	-	-	-
15	CLA	b	812	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	832	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	839	X	-	-	-
15	CLA	b	841	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	103	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		

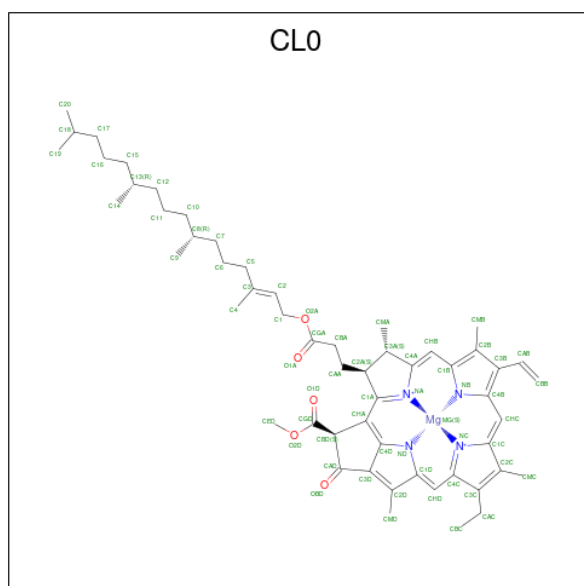
There are 3 discrepancies between the modelled and reference sequences:

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.

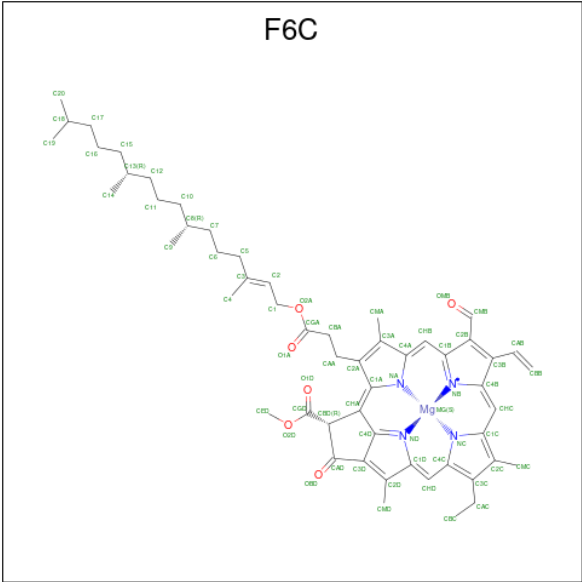
Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	29	Total	C	N	O	0	0
			227	157	36	34		
12	Z	29	Total	C	N	O	0	0
			227	157	36	34		
12	l	29	Total	C	N	O	0	0
			227	157	36	34		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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).



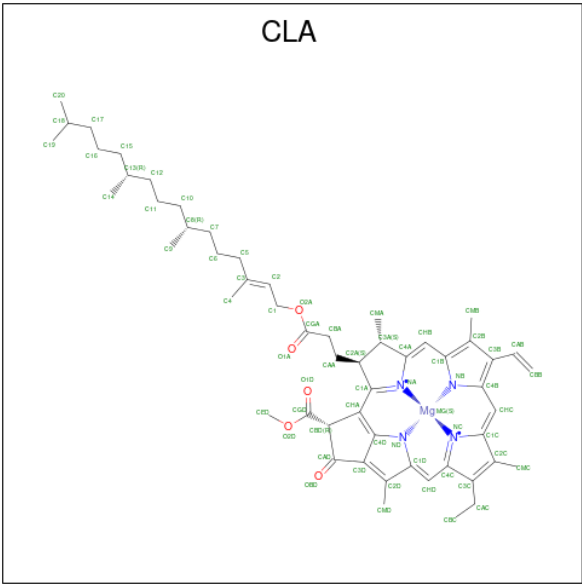
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	A	1	Total 52	C 41	Mg 1	N 4	O 6	0
14	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	N	1	Total 52	C 41	Mg 1	N 4	O 6	0
14	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
14	O	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
14	O	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	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	

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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	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

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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
			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	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			56	46	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
			45	35	1	4	5	
15	B	1	Total	C	Mg	N	O	0
			57	47	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
			60	50	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
			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
			53	43	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
			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
			62	52	1	4	5	

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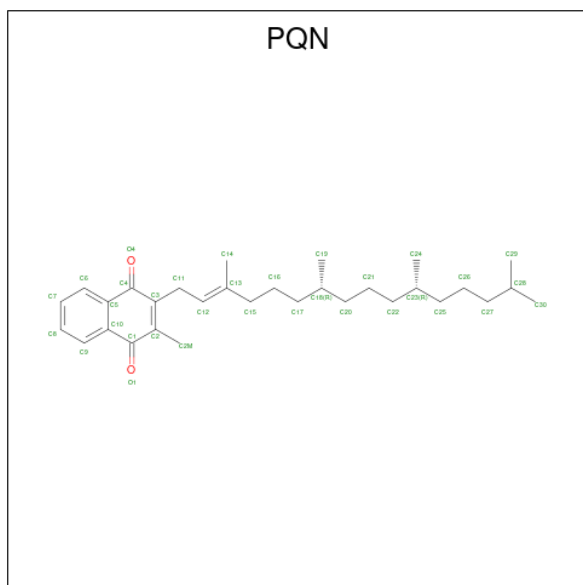
Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
15	b	1	Total	C	Mg	N	O	0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

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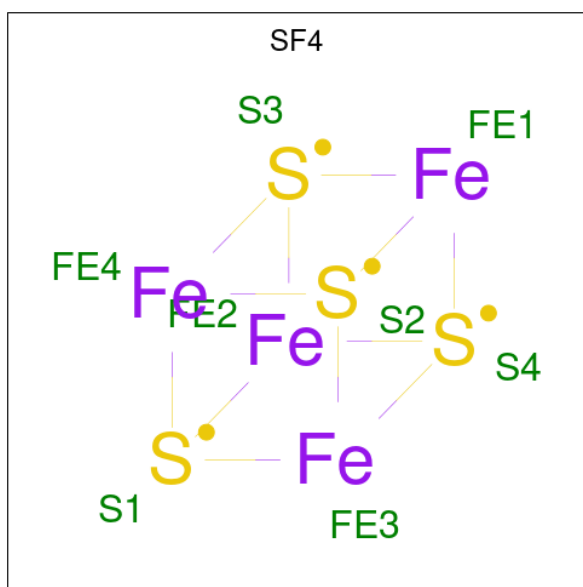
Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b	1	Total	C	Mg	N	O	0
			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: C₃₁H₄₆O₂).



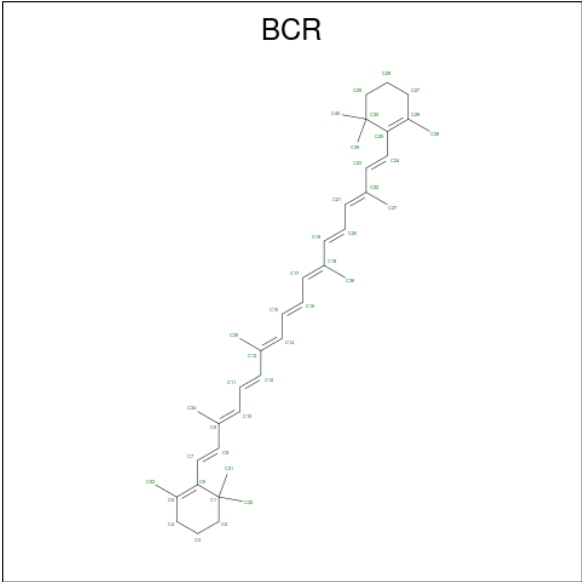
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			33	31	2	
16	B	1	Total	C	O	0
			33	31	2	
16	N	1	Total	C	O	0
			33	31	2	
16	O	1	Total	C	O	0
			33	31	2	
16	a	1	Total	C	O	0
			33	31	2	
16	b	1	Total	C	O	0
			33	31	2	

- 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	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	F	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
18	F	1	Total C 40 40	0
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	K	1	Total C 25 25	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	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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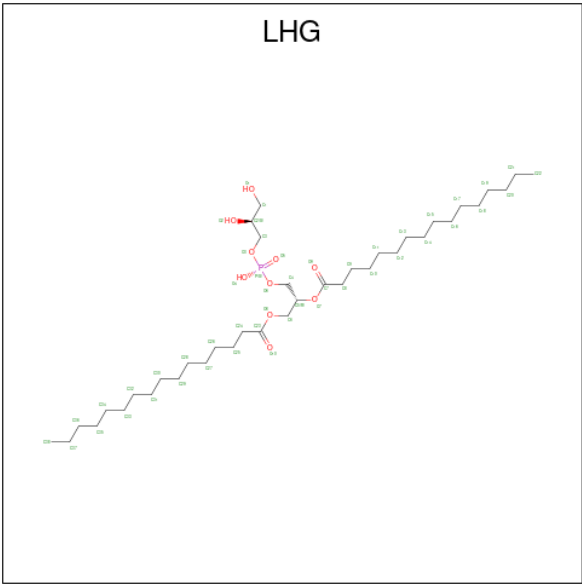
Mol	Chain	Residues	Atoms	AltConf
18	O	1	Total C 40 40	0
18	S	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 25 25	0
18	W	1	Total C 40 40	0
18	W	1	Total C 40 40	0
18	Y	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 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	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	f	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	i	1	Total	C	0
			25	25	
18	j	1	Total	C	0
			40	40	
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).



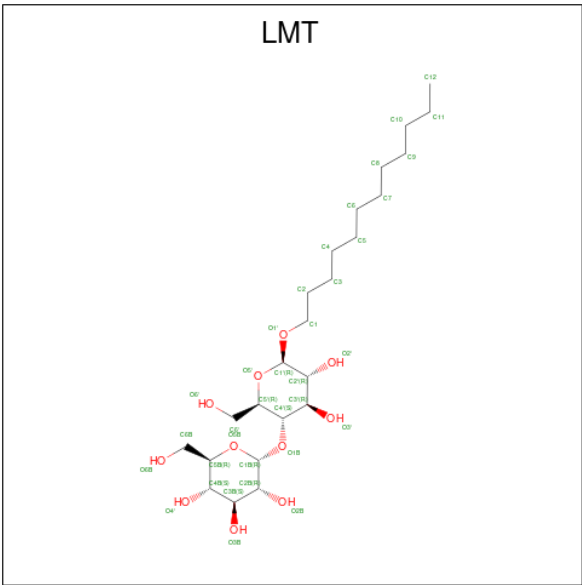
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			42	31	10	1	

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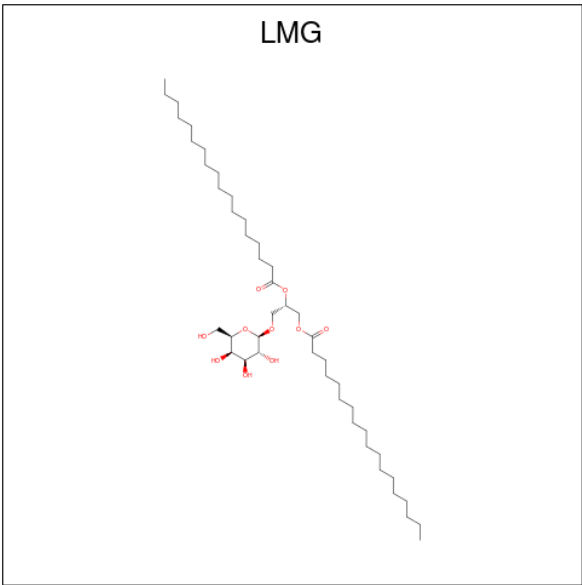
Mol	Chain	Residues	Atoms				AltConf
19	L	1	Total	C	O	P	0
			49	38	10	1	
19	M	1	Total	C	O	P	0
			49	38	10	1	
19	X	1	Total	C	O	P	0
			44	33	10	1	
19	X	1	Total	C	O	P	0
			49	38	10	1	
19	N	1	Total	C	O	P	0
			42	31	10	1	
19	W	1	Total	C	O	P	0
			49	38	10	1	
19	Y	1	Total	C	O	P	0
			49	38	10	1	
19	Z	1	Total	C	O	P	0
			44	33	10	1	
19	Z	1	Total	C	O	P	0
			49	38	10	1	
19	a	1	Total	C	O	P	0
			42	31	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	
19	l	1	Total	C	O	P	0
			49	38	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).



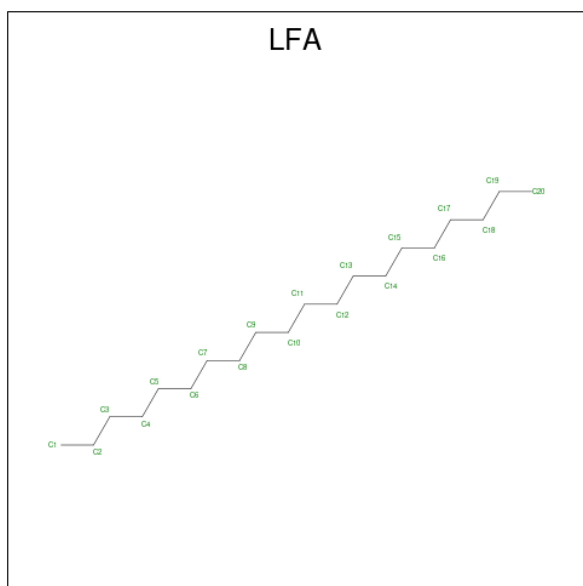
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			44	34	10	
21	B	1	Total	C	O	0
			55	45	10	
21	I	1	Total	C	O	0
			37	27	10	
21	J	1	Total	C	O	0
			55	45	10	
21	L	1	Total	C	O	0
			50	40	10	
21	N	1	Total	C	O	0
			44	34	10	
21	O	1	Total	C	O	0
			55	45	10	
21	T	1	Total	C	O	0
			37	27	10	
21	U	1	Total	C	O	0
			55	45	10	
21	W	1	Total	C	O	0
			50	40	10	
21	a	1	Total	C	O	0
			44	34	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	f	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	3	Total 3	O 3	0
24	D	11	Total 11	O 11	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	8	Total 8	O 8	0
24	N	51	Total 51	O 51	0
24	O	55	Total 55	O 55	0
24	P	2	Total 2	O 2	0
24	Q	11	Total 11	O 11	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	9	Total 9	O 9	0

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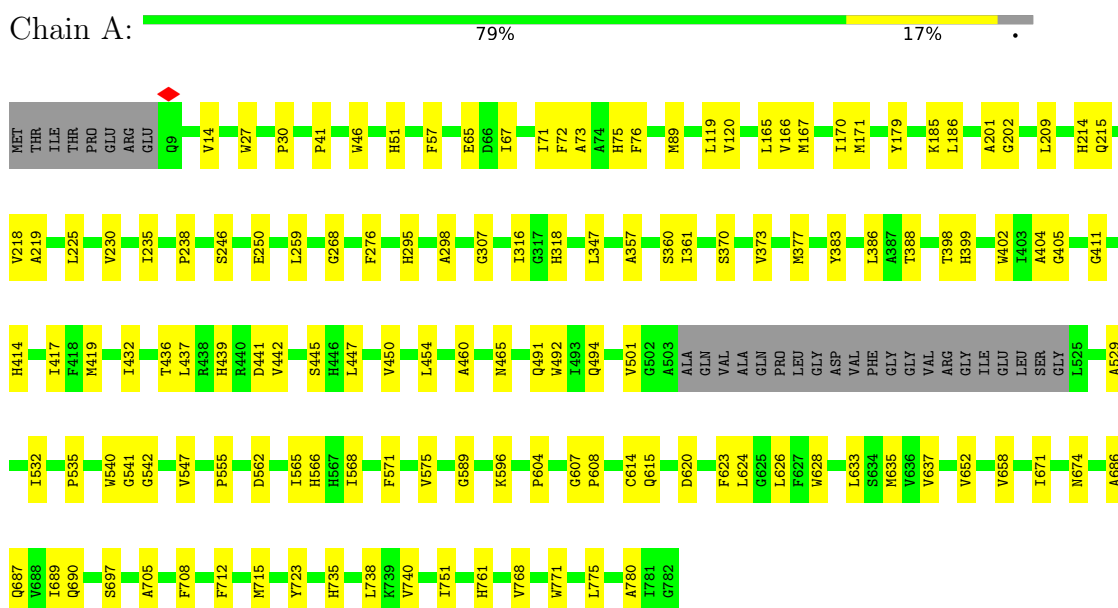
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Mol	Chain	Residues	Atoms		AltConf
24	a	52	Total 52	O 52	0
24	b	55	Total 55	O 55	0
24	c	3	Total 3	O 3	0
24	d	10	Total 10	O 10	0
24	e	2	Total 2	O 2	0
24	f	2	Total 2	O 2	0
24	g	3	Total 3	O 3	0
24	i	1	Total 1	O 1	0
24	j	8	Total 8	O 8	0

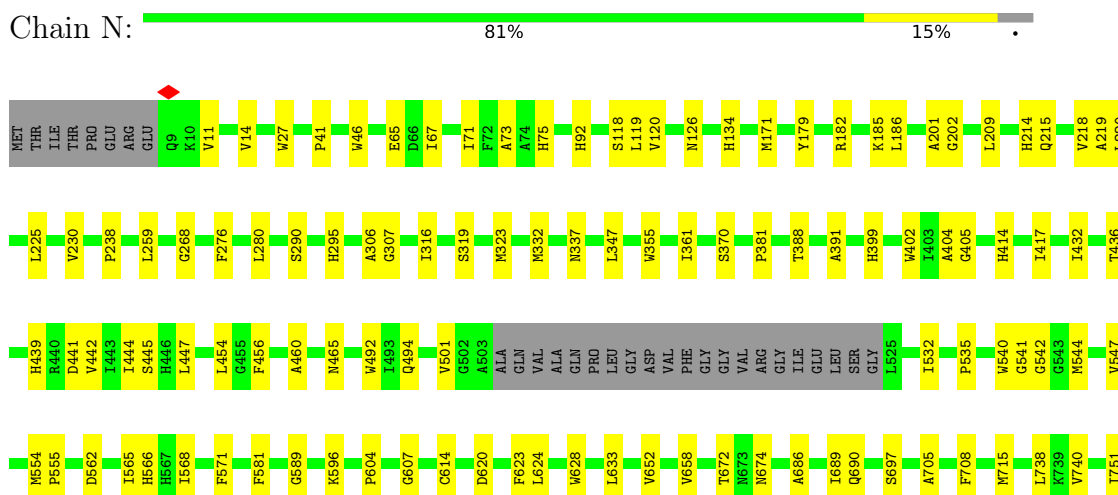
3 Residue-property plots [i](#)

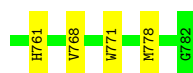
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



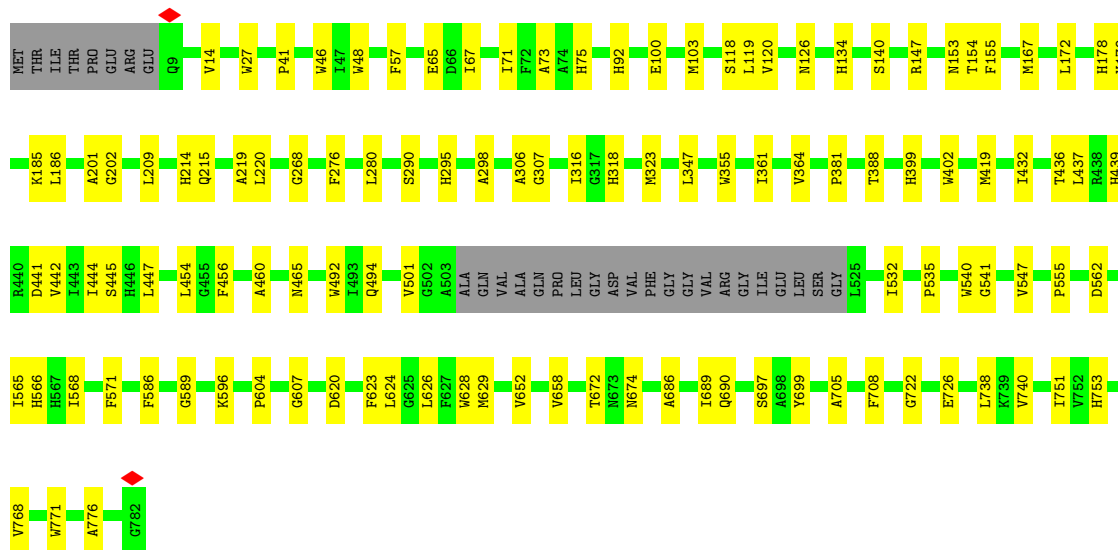
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





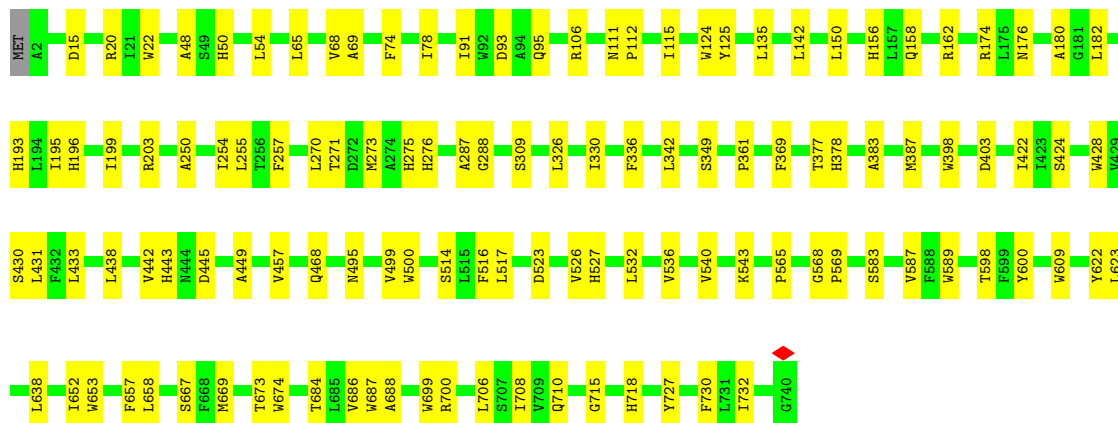
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 82% 15%



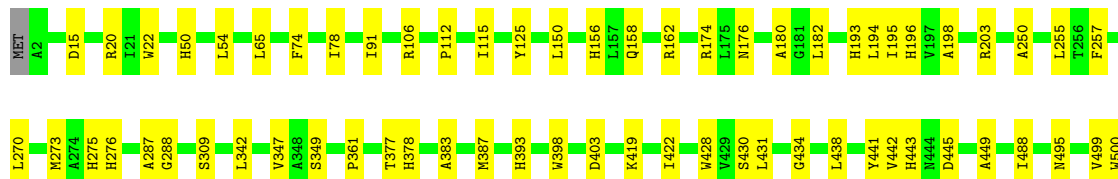
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

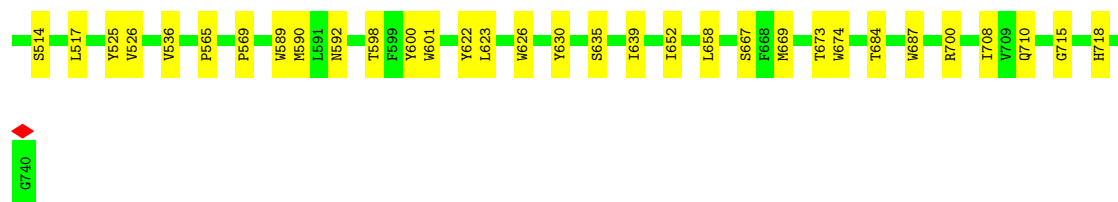
Chain B: 84% 16%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

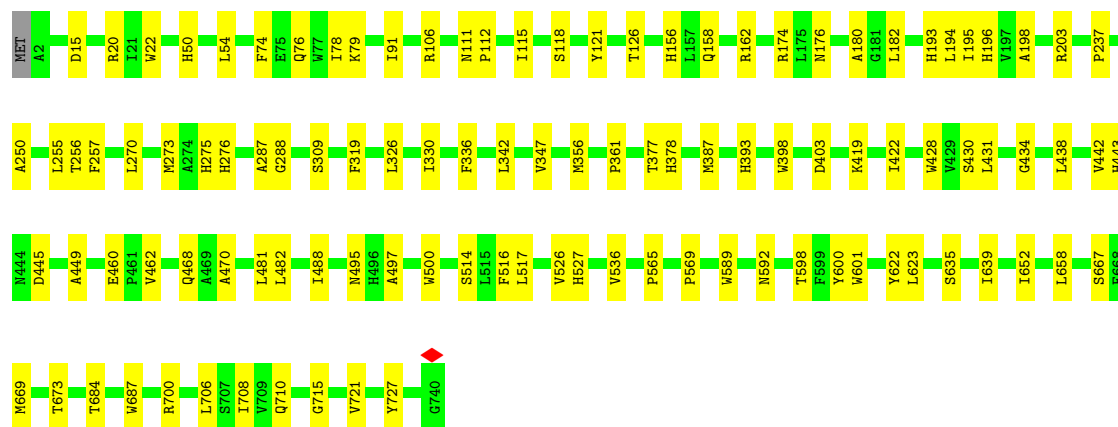
Chain O: 87% 13%





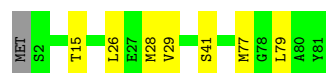
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 85% 15%



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 90% 9%



- Molecule 3: Photosystem I iron-sulfur center

Chain P: 89% 10%



- Molecule 3: Photosystem I iron-sulfur center

Chain c: 94% 5%



- Molecule 4: Photosystem I reaction center subunit II

Chain D: 84% 14%



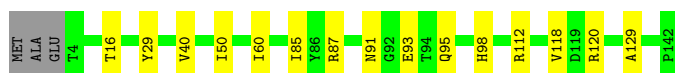
- Molecule 4: Photosystem I reaction center subunit II

Chain Q: 87% 11% .



- Molecule 4: Photosystem I reaction center subunit II

Chain d: 87% 11% .



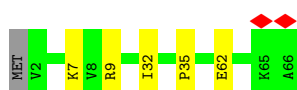
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 92% 6% .



- Molecule 5: Photosystem I reaction center subunit IV

Chain R: 91% 8% .



- Molecule 5: Photosystem I reaction center subunit IV

Chain e: 91% 8% .



- Molecule 6: Photosystem I reaction center subunit III

Chain F: 71% 14% 15%



- Molecule 6: Photosystem I reaction center subunit III

Chain S:  73% 12% 15%



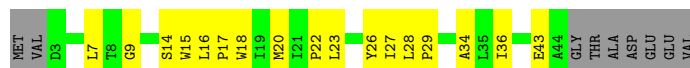
- Molecule 6: Photosystem I reaction center subunit III

Chain f:  75% 11% 15%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  49% 33% 18%



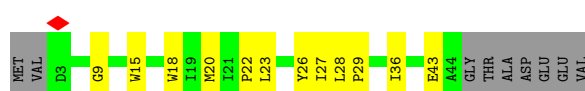
- Molecule 7: Photosystem I reaction center subunit VIII

Chain T:  57% 25% 18%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain g:  59% 24% 18%



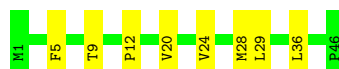
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  80% 20%



- Molecule 8: Photosystem I reaction center subunit IX

Chain U:  83% 17%



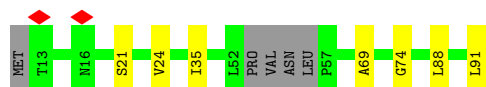
- Molecule 8: Photosystem I reaction center subunit IX

Chain h:  87% 13%



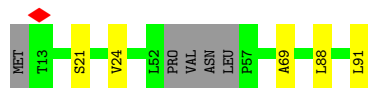
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:  85% 9% 6%



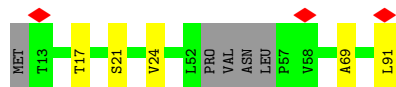
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain V:  88% 6% 6%



- Molecule 9: Photosystem I reaction center subunit PsaK

Chain i:  88% 6% 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:  75% 22% .



- Molecule 11: Photosystem I reaction center subunit XII

Chain Y:  88% 9% .



- Molecule 11: Photosystem I reaction center subunit XII

Chain k:  91% 6% .



- Molecule 12: Photosystem one PsaX

Chain X:  93% 7%



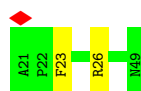
- Molecule 12: Photosystem one PsaX

Chain Z:  86% 14%



- Molecule 12: Photosystem one PsaX

Chain l:  93% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	83138	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)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.504	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.054	Depositor
Map size (Å)	552.6, 552.6, 552.6	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92099994, 0.92099994, 0.92099994	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, BCR, SF4, CL0, LMT, CA, PQN, LMG, LFA, CLA, F6C

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	0.13	0/6106	0.29	0/8323
1	N	0.11	0/6106	0.25	0/8323
1	a	0.11	0/6106	0.25	0/8323
2	B	0.13	0/6139	0.29	0/8394
2	O	0.11	0/6139	0.25	0/8394
2	b	0.11	0/6139	0.26	0/8394
3	C	0.12	0/610	0.29	0/827
3	P	0.11	0/610	0.28	0/827
3	c	0.13	0/610	0.29	0/827
4	D	0.11	0/1115	0.31	0/1501
4	Q	0.10	0/1115	0.26	0/1501
4	d	0.10	0/1115	0.26	0/1501
5	E	0.10	0/540	0.26	0/728
5	R	0.09	0/540	0.22	0/728
5	e	0.09	0/540	0.23	0/728
6	F	0.12	0/1104	0.30	0/1501
6	S	0.11	0/1104	0.28	0/1501
6	f	0.10	0/1104	0.27	0/1501
7	I	0.16	0/366	0.43	0/503
7	T	0.15	0/366	0.37	0/503
7	g	0.15	0/366	0.38	0/503
8	J	0.10	0/386	0.25	0/526
8	U	0.09	0/386	0.24	0/526
8	h	0.08	0/386	0.23	0/526
9	K	0.12	0/550	0.32	0/751
9	V	0.10	0/550	0.31	0/751
9	i	0.10	0/550	0.29	0/751
10	L	0.13	0/1340	0.30	0/1821
10	W	0.10	0/1340	0.26	0/1821
10	j	0.10	0/1340	0.26	0/1821
11	M	0.11	0/243	0.21	0/329
11	Y	0.09	0/243	0.18	0/329

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	k	0.08	0/243	0.17	0/329
12	X	0.11	0/233	0.28	0/319
12	Z	0.07	0/233	0.24	0/319
12	l	0.07	0/233	0.23	0/319
All	All	0.11	0/56196	0.27	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5900	0	5735	113	0
1	N	5900	0	5735	89	0
1	a	5900	0	5735	93	0
2	B	5913	0	5649	102	0
2	O	5913	0	5649	85	0
2	b	5913	0	5649	93	0
3	C	600	0	579	4	0
3	P	600	0	579	7	0
3	c	600	0	579	3	0
4	D	1090	0	1097	13	0
4	Q	1090	0	1097	11	0
4	d	1090	0	1097	9	0
5	E	530	0	535	2	0
5	R	530	0	535	3	0
5	e	530	0	535	3	0
6	F	1075	0	1081	17	0
6	S	1075	0	1081	15	0
6	f	1075	0	1081	15	0
7	I	351	0	354	15	0
7	T	351	0	354	11	0
7	g	351	0	354	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	373	0	390	9	0
8	U	373	0	390	7	0
8	h	373	0	390	6	0
9	K	539	0	578	7	0
9	V	539	0	578	5	0
9	i	539	0	578	4	0
10	L	1309	0	1289	15	0
10	W	1309	0	1289	11	0
10	j	1309	0	1289	12	0
11	M	240	0	261	6	0
11	Y	240	0	261	3	0
11	k	240	0	261	2	0
12	X	227	0	244	2	0
12	Z	227	0	244	5	0
12	l	227	0	244	3	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	198	0	0	3	0
14	W	66	0	0	0	0
14	a	250	0	0	0	0
14	b	198	0	0	3	0
14	j	66	0	0	1	0
15	A	2324	0	2343	115	0
15	B	2238	0	2311	112	0
15	F	65	0	72	1	0
15	K	95	0	72	1	0
15	L	125	0	131	4	0
15	N	2259	0	2271	98	0
15	O	2303	0	2383	124	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	3	0
15	Z	55	0	49	2	0
15	a	2259	0	2271	98	0
15	b	2303	0	2383	127	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	4	0
15	l	55	0	49	2	0
16	A	33	0	46	1	0
16	B	33	0	46	1	0
16	N	33	0	46	1	0
16	O	33	0	46	1	0
16	a	33	0	46	1	0
16	b	33	0	46	3	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	1	0
17	a	8	0	0	0	0
17	c	16	0	0	1	0
18	A	280	0	392	29	0
18	B	240	0	336	16	0
18	F	80	0	112	9	0
18	I	80	0	112	5	0
18	J	40	0	56	1	0
18	K	25	0	33	0	0
18	L	80	0	112	5	0
18	M	40	0	56	4	0
18	N	280	0	392	23	0
18	O	280	0	392	18	0
18	S	40	0	56	5	0
18	T	80	0	112	3	0
18	U	40	0	56	0	0
18	V	25	0	33	0	0
18	W	80	0	112	3	0
18	Y	40	0	56	4	0
18	a	280	0	392	20	0
18	b	240	0	336	15	0
18	f	80	0	112	6	0
18	g	80	0	112	4	0
18	h	40	0	56	1	0
18	i	25	0	33	1	0
18	j	80	0	112	6	0
18	k	40	0	56	3	0
19	A	42	0	54	0	0
19	L	49	0	74	5	0
19	M	49	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	42	0	54	0	0
19	W	49	0	74	5	0
19	X	93	0	135	3	0
19	Y	49	0	74	5	0
19	Z	93	0	135	4	0
19	a	42	0	54	0	0
19	j	49	0	74	5	0
19	k	49	0	74	5	0
19	l	93	0	135	4	0
20	A	94	0	110	3	0
20	N	94	0	110	2	0
20	a	94	0	110	2	0
21	A	44	0	61	1	0
21	B	55	0	86	4	0
21	I	37	0	44	3	0
21	J	55	0	86	1	0
21	L	50	0	70	4	0
21	N	44	0	61	0	0
21	O	55	0	86	5	0
21	T	37	0	44	5	0
21	U	55	0	86	3	0
21	W	50	0	70	4	0
21	a	44	0	61	1	0
21	b	55	0	86	5	0
21	g	37	0	44	3	0
21	h	55	0	86	3	0
21	j	50	0	70	2	0
22	B	16	0	31	1	0
22	L	15	0	29	1	0
22	O	16	0	31	1	0
22	W	15	0	29	1	0
22	f	16	0	31	1	0
22	j	15	0	29	2	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	0	0
24	C	3	0	0	0	0
24	D	11	0	0	0	0
24	E	2	0	0	0	0
24	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	I	2	0	0	0	0
24	K	1	0	0	0	0
24	L	8	0	0	0	0
24	N	51	0	0	0	0
24	O	55	0	0	0	0
24	P	2	0	0	0	0
24	Q	11	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	9	0	0	0	0
24	a	52	0	0	0	0
24	b	55	0	0	1	0
24	c	3	0	0	0	0
24	d	10	0	0	0	0
24	e	2	0	0	0	0
24	f	2	0	0	0	0
24	g	3	0	0	0	0
24	i	1	0	0	0	0
24	j	8	0	0	0	0
All	All	75954	0	74991	1279	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 (1279) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:PHE:HE2	2:B:500:TRP:HE3	1.32	0.78
18:A:850:BCR:H362	15:A:856:CLA:H42	1.67	0.76
18:a:850:BCR:H362	15:b:802:CLA:H42	1.66	0.76
18:N:850:BCR:H362	15:O:802:CLA:H42	1.69	0.75
2:O:257:PHE:HE2	2:O:500:TRP:HE3	1.34	0.75
15:N:804:CLA:HHC	15:N:804:CLA:HBB1	1.68	0.75
15:O:812:CLA:HBB2	15:O:820:CLA:H92	1.68	0.74
15:B:810:CLA:HBB2	15:B:818:CLA:H92	1.70	0.73
15:b:812:CLA:HBB2	15:b:820:CLA:H92	1.70	0.73
15:a:804:CLA:HHC	15:a:804:CLA:HBB1	1.68	0.73
1:A:652:VAL:HG22	1:A:658:VAL:HG22	1.71	0.71
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:806:CLA:H72	15:N:814:CLA:H2	1.73	0.71
15:A:806:CLA:H72	15:A:814:CLA:H2	1.72	0.71
15:B:808:CLA:H51	21:B:847:LMG:H273	1.73	0.70
15:A:804:CLA:HHC	15:A:804:CLA:HBB1	1.74	0.69
19:M:102:LHG:H362	19:j:207:LHG:H192	1.74	0.69
1:N:347:LEU:HD11	1:N:432:ILE:HD11	1.73	0.69
2:B:111:ASN:HD22	7:I:9:GLY:HA2	1.57	0.69
1:A:347:LEU:HD11	1:A:432:ILE:HD11	1.74	0.69
2:O:441:TYR:HE1	2:O:525:TYR:HB3	1.56	0.69
1:A:316:ILE:HD13	9:K:69:ALA:HB2	1.75	0.68
15:O:831:CLA:HBC2	15:O:839:CLA:HMC2	1.75	0.68
1:a:347:LEU:HD11	1:a:432:ILE:HD11	1.74	0.68
15:a:841:CLA:H2	15:b:832:CLA:H42	1.75	0.67
15:N:806:CLA:H101	15:N:814:CLA:H42	1.76	0.67
15:N:841:CLA:H2	15:O:832:CLA:H42	1.75	0.66
2:b:111:ASN:HD22	7:g:9:GLY:HA2	1.59	0.66
15:A:841:CLA:H2	15:B:830:CLA:H42	1.76	0.66
1:N:119:LEU:HG	1:N:120:VAL:HG13	1.78	0.66
2:b:257:PHE:CE2	2:b:500:TRP:HB3	2.30	0.66
1:N:316:ILE:HD13	9:V:69:ALA:HB2	1.78	0.66
15:B:829:CLA:HBC2	15:B:837:CLA:HMC2	1.77	0.66
15:a:806:CLA:H72	15:a:814:CLA:H2	1.76	0.66
2:b:257:PHE:HE2	2:b:500:TRP:HB3	1.61	0.66
19:W:1506:LHG:H192	19:k:101:LHG:H362	1.76	0.66
15:A:806:CLA:H101	15:A:814:CLA:H42	1.76	0.66
5:e:7:LYS:HB3	5:e:62:GLU:HB3	1.78	0.66
1:N:652:VAL:HG22	1:N:658:VAL:HG22	1.75	0.65
15:O:831:CLA:H11	18:S:202:BCR:H353	1.78	0.65
15:a:806:CLA:H101	15:a:814:CLA:H42	1.77	0.65
19:L:207:LHG:H192	19:Y:101:LHG:H362	1.79	0.65
15:b:816:CLA:H92	15:b:816:CLA:H41	1.78	0.65
15:b:808:CLA:H91	15:b:809:CLA:H52	1.76	0.65
10:W:177:ARG:HH21	21:W:1505:LMG:H341	1.62	0.65
1:A:119:LEU:HG	1:A:120:VAL:HG13	1.78	0.65
15:B:829:CLA:H11	18:F:203:BCR:H353	1.78	0.64
10:L:177:ARG:HH21	21:L:206:LMG:H341	1.60	0.64
2:O:15:ASP:HB3	2:O:20:ARG:HB2	1.78	0.64
15:O:807:CLA:H43	7:T:20:MET:HE2	1.78	0.64
2:O:669:MET:HB2	15:O:803:CLA:C1C	2.27	0.64
15:b:831:CLA:HBC2	15:b:839:CLA:HMC2	1.78	0.64
2:b:15:ASP:HB3	2:b:20:ARG:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:825:CLA:H141	18:B:846:BCR:H342	1.79	0.64
2:O:54:LEU:HD12	15:O:813:CLA:HED1	1.80	0.64
15:O:827:CLA:H141	18:O:849:BCR:H342	1.80	0.63
1:a:14:VAL:HG12	1:a:185:LYS:HG3	1.80	0.63
6:F:60:LYS:HD2	8:J:46:PRO:HB3	1.80	0.63
2:b:257:PHE:CE2	2:b:500:TRP:HE3	2.16	0.63
10:L:160:VAL:HG21	18:j:201:BCR:H291	1.81	0.63
15:O:809:CLA:H51	21:O:850:LMG:H273	1.80	0.63
15:O:816:CLA:H41	15:O:816:CLA:H92	1.78	0.63
10:L:175:ILE:HG23	14:O:810:F6C:O1A	1.99	0.63
5:R:7:LYS:HB3	5:R:62:GLU:HB3	1.81	0.63
10:j:140:ASN:HB2	10:j:143:GLU:HG3	1.81	0.63
15:B:828:CLA:H101	15:B:837:CLA:H152	1.80	0.62
7:I:36:ILE:HG21	18:L:205:BCR:HC8	1.81	0.62
1:a:318:HIS:HB3	1:a:323:MET:HE2	1.81	0.62
2:B:174:ARG:HB2	15:B:811:CLA:HBC2	1.81	0.62
14:L:201:F6C:O1A	10:j:175:ILE:HG23	1.99	0.62
2:b:174:ARG:HB2	15:b:813:CLA:HBC2	1.82	0.62
15:O:803:CLA:H143	18:O:849:BCR:H362	1.81	0.62
15:B:814:CLA:H92	15:B:814:CLA:H41	1.82	0.62
15:N:803:CLA:HBA1	15:O:802:CLA:HBB2	1.82	0.62
6:f:28:THR:HG23	6:f:29:LEU:HD12	1.82	0.62
15:O:803:CLA:H142	18:T:101:BCR:H271	1.82	0.62
15:b:830:CLA:H101	15:b:839:CLA:H152	1.82	0.62
1:a:316:ILE:HD13	9:i:69:ALA:HB2	1.81	0.61
2:b:237:PRO:HB3	2:b:256:THR:HG21	1.81	0.61
18:L:209:BCR:H291	10:W:160:VAL:HG21	1.82	0.61
15:a:816:CLA:HBB1	18:a:845:BCR:H382	1.81	0.61
1:A:14:VAL:HG12	1:A:185:LYS:HG3	1.82	0.61
10:W:175:ILE:HG23	14:b:810:F6C:O1A	2.00	0.61
15:b:809:CLA:H51	21:b:849:LMG:H273	1.83	0.61
1:A:624:LEU:HD22	2:B:673:THR:HG22	1.83	0.61
2:B:669:MET:HB2	15:B:802:CLA:C1C	2.31	0.60
1:A:370:SER:HB3	1:A:404:ALA:HB2	1.83	0.60
15:B:807:CLA:H91	15:B:808:CLA:H52	1.83	0.60
6:F:28:THR:HG23	6:F:29:LEU:HD12	1.82	0.60
18:N:850:BCR:H372	2:O:442:VAL:HG21	1.83	0.60
15:a:803:CLA:HBA1	15:b:802:CLA:HBB2	1.83	0.60
1:A:67:ILE:O	1:A:71:ILE:HG12	2.01	0.60
2:B:257:PHE:HE2	2:B:500:TRP:CE3	2.17	0.60
15:A:811:CLA:H62	20:A:854:LMT:H62	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:VAL:HG21	2:B:600:TYR:HB2	1.82	0.60
15:B:806:CLA:H43	7:I:20:MET:HE2	1.84	0.60
10:L:50:ASN:HB3	15:L:202:CLA:HAC1	1.84	0.60
2:O:342:LEU:HD21	15:O:829:CLA:HAB	1.84	0.60
15:O:806:CLA:H91	21:O:850:LMG:H421	1.84	0.60
7:g:36:ILE:HG21	18:j:205:BCR:HC8	1.83	0.60
2:O:180:ALA:HB2	2:O:288:GLY:HA3	1.84	0.60
2:O:441:TYR:CE1	2:O:525:TYR:HB3	2.36	0.60
1:N:768:VAL:HG22	18:N:850:BCR:H323	1.84	0.60
1:a:624:LEU:HD22	2:b:673:THR:HG22	1.84	0.60
1:a:768:VAL:HG22	18:a:850:BCR:H323	1.84	0.60
18:W:1508:BCR:H291	10:j:160:VAL:HG21	1.84	0.59
2:B:54:LEU:HD12	15:B:811:CLA:HED1	1.85	0.59
15:N:816:CLA:HBB1	18:N:845:BCR:H382	1.84	0.59
1:N:182:ARG:HD2	15:N:811:CLA:HED1	1.83	0.59
4:Q:40:VAL:HG22	4:Q:50:ILE:HG12	1.85	0.59
8:h:29:LEU:HD21	21:h:102:LMG:H161	1.84	0.59
2:O:652:ILE:HD13	15:O:809:CLA:CHD	2.33	0.59
1:a:652:VAL:HG22	1:a:658:VAL:HG22	1.84	0.59
18:a:857:BCR:H15C	8:h:20:VAL:HG22	1.85	0.59
16:B:840:PQN:H302	21:B:847:LMG:H222	1.85	0.59
15:B:805:CLA:H91	21:B:847:LMG:H421	1.83	0.58
4:D:40:VAL:HG22	4:D:50:ILE:HG12	1.85	0.58
15:b:803:CLA:H143	18:b:848:BCR:H362	1.83	0.58
18:N:857:BCR:H15C	8:U:20:VAL:HG22	1.85	0.58
15:b:806:CLA:H43	21:b:849:LMG:H321	1.86	0.58
15:O:830:CLA:H101	15:O:839:CLA:H152	1.85	0.58
15:b:835:CLA:HBB1	18:b:847:BCR:HC32	1.86	0.58
15:B:830:CLA:HAC2	6:F:87:ILE:HG12	1.85	0.58
15:N:803:CLA:H112	18:N:850:BCR:H23C	1.84	0.58
10:j:101:ILE:HA	10:j:156:MET:HE1	1.86	0.58
1:A:442:VAL:HG22	2:B:687:TRP:CH2	2.39	0.58
15:B:805:CLA:H43	21:B:847:LMG:H321	1.86	0.58
4:D:29:TYR:HB2	4:D:60:ILE:HG13	1.86	0.57
3:c:15:THR:HG22	3:c:28:MET:HG3	1.86	0.57
3:C:15:THR:HG22	3:C:28:MET:HG3	1.85	0.57
10:L:101:ILE:HA	10:L:156:MET:HE1	1.86	0.57
2:b:180:ALA:HB2	2:b:288:GLY:HA3	1.85	0.57
15:B:802:CLA:H142	18:I:101:BCR:H271	1.86	0.57
1:N:214:HIS:CE1	15:N:815:CLA:NA	2.72	0.57
2:O:174:ARG:HB2	15:O:813:CLA:HBC2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:842:PQN:H302	21:O:850:LMG:H222	1.86	0.57
2:B:193:HIS:CE1	15:B:812:CLA:NA	2.73	0.57
15:B:803:CLA:H102	19:j:207:LHG:H322	1.87	0.57
6:S:28:THR:HG23	6:S:29:LEU:HD12	1.85	0.57
21:g:103:LMG:H332	18:k:102:BCR:H272	1.85	0.57
1:A:768:VAL:HG22	18:A:850:BCR:H323	1.87	0.57
10:W:101:ILE:HA	10:W:156:MET:HE1	1.86	0.57
15:b:803:CLA:H142	18:g:101:BCR:H271	1.86	0.57
15:a:803:CLA:H112	18:a:850:BCR:H23C	1.86	0.57
15:b:831:CLA:H11	18:f:203:BCR:H353	1.85	0.57
19:L:207:LHG:H322	15:O:804:CLA:H102	1.87	0.57
1:N:201:ALA:HB2	1:N:307:GLY:HA3	1.87	0.57
16:b:842:PQN:H302	21:b:849:LMG:H222	1.86	0.57
18:A:850:BCR:H372	2:B:442:VAL:HG21	1.87	0.56
2:B:652:ILE:HD13	15:B:808:CLA:CHD	2.35	0.56
15:B:802:CLA:H143	18:B:846:BCR:H362	1.87	0.56
2:O:193:HIS:CE1	15:O:814:CLA:NA	2.74	0.56
4:D:11:ILE:HG13	4:D:52:ARG:HE	1.70	0.56
15:a:811:CLA:H11	15:a:813:CLA:H2	1.87	0.56
15:A:803:CLA:HBA1	15:A:856:CLA:HBB2	1.87	0.56
2:B:203:ARG:HG2	2:B:250:ALA:HB1	1.86	0.56
9:K:35:ILE:HD12	9:K:74:GLY:HA2	1.86	0.56
1:N:715:MET:HB2	15:N:803:CLA:C1C	2.35	0.56
15:a:834:CLA:H152	15:b:841:CLA:H91	1.86	0.56
6:f:83:VAL:HG22	22:f:204:LFA:H32	1.87	0.56
2:O:257:PHE:CE2	2:O:500:TRP:HB3	2.41	0.56
1:N:589:GLY:HA2	1:N:596:LYS:HD3	1.87	0.56
1:a:201:ALA:HB2	1:a:307:GLY:HA3	1.87	0.56
2:O:276:HIS:HE1	15:O:817:CLA:ND	2.02	0.56
1:A:201:ALA:HB2	1:A:307:GLY:HA3	1.88	0.56
2:B:257:PHE:CE2	2:B:500:TRP:HB3	2.40	0.56
2:B:275:HIS:HB3	15:B:815:CLA:HMB2	1.87	0.56
3:P:13:GLY:HA2	3:P:28:MET:HE1	1.87	0.56
21:T:103:LMG:H332	18:Y:102:BCR:H272	1.87	0.56
18:a:850:BCR:H372	2:b:442:VAL:HG21	1.87	0.56
2:O:441:TYR:CD2	15:O:801:CLA:H203	2.41	0.56
15:A:816:CLA:HBB1	18:A:845:BCR:H382	1.88	0.55
7:T:36:ILE:HG21	18:W:1504:BCR:HC8	1.88	0.55
1:a:388:THR:HG21	1:a:547:VAL:HB	1.89	0.55
1:a:568:ILE:HD12	13:a:801:CL0:H61	1.87	0.55
22:B:848:LFA:H32	6:F:83:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:270:LEU:HD23	2:O:273:MET:HE3	1.88	0.55
1:a:492:TRP:HA	20:a:852:LMT:H6E	1.88	0.55
2:b:342:LEU:HD21	15:b:829:CLA:HAB	1.88	0.55
21:j:206:LMG:H191	22:j:208:LFA:H122	1.87	0.55
1:N:541:GLY:HA2	1:N:555:PRO:HG3	1.87	0.55
1:a:268:GLY:HA2	15:a:818:CLA:HAA2	1.88	0.55
2:b:526:VAL:HG21	2:b:600:TYR:HB2	1.86	0.55
10:j:50:ASN:HB3	15:j:202:CLA:HAC1	1.88	0.55
1:a:67:ILE:O	1:a:71:ILE:HG12	2.06	0.55
1:a:445:SER:HB3	2:b:684:THR:HG22	1.88	0.55
2:b:193:HIS:CE1	15:b:814:CLA:NA	2.74	0.55
15:b:825:CLA:H43	15:b:838:CLA:HBA1	1.89	0.55
2:B:74:PHE:O	2:B:78:ILE:HG12	2.06	0.55
15:O:830:CLA:H142	19:Z:101:LHG:H282	1.88	0.55
1:A:697:SER:HB2	2:B:449:ALA:HB1	1.89	0.55
1:a:214:HIS:CE1	15:a:815:CLA:NA	2.73	0.55
2:B:65:LEU:HD11	18:B:843:BCR:H281	1.89	0.55
15:N:811:CLA:H62	20:N:854:LMT:H62	1.89	0.55
10:L:71:HIS:HA	10:L:74:PHE:CE1	2.42	0.55
22:O:851:LFA:H32	6:S:83:VAL:HG22	1.88	0.55
1:a:722:GLY:O	1:a:726:GLU:HG3	2.07	0.55
1:A:615:GLN:HA	1:A:620:ASP:OD2	2.07	0.54
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.89	0.54
18:F:203:BCR:H281	15:X:103:CLA:H11	1.89	0.54
1:N:494:GLN:HG2	1:N:540:TRP:HD1	1.72	0.54
3:P:15:THR:HG22	3:P:28:MET:HE2	1.88	0.54
1:a:465:ASN:HB3	1:a:672:THR:HG22	1.89	0.54
6:f:92:TYR:HE2	21:h:102:LMG:H452	1.72	0.54
1:A:454:LEU:HB3	1:A:571:PHE:HB2	1.88	0.54
15:A:833:CLA:H2	15:L:203:CLA:H43	1.87	0.54
2:B:468:GLN:HG2	2:B:516:PHE:HB3	1.90	0.54
10:L:58:LEU:HD22	10:L:62:MET:HB3	1.88	0.54
6:S:92:TYR:HE2	21:U:102:LMG:H452	1.72	0.54
1:A:529:ALA:HB1	1:A:532:ILE:HD13	1.89	0.54
15:N:807:CLA:H42	15:N:831:CLA:H51	1.89	0.54
2:b:257:PHE:HE2	2:b:500:TRP:HE3	1.56	0.54
15:A:807:CLA:H151	15:A:830:CLA:HBB2	1.90	0.54
2:O:275:HIS:HB3	15:O:817:CLA:HMB2	1.88	0.54
15:O:804:CLA:H51	18:Y:102:BCR:HC22	1.88	0.54
15:A:811:CLA:H11	15:A:813:CLA:H2	1.90	0.54
2:b:74:PHE:O	2:b:78:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ALA:HB2	2:B:288:GLY:HA3	1.89	0.54
1:N:388:THR:HG21	1:N:547:VAL:HB	1.90	0.54
2:b:270:LEU:HD23	2:b:273:MET:HE3	1.90	0.54
15:b:827:CLA:H141	18:b:848:BCR:H342	1.90	0.54
15:A:834:CLA:H152	15:B:839:CLA:H91	1.88	0.54
2:O:526:VAL:HG21	2:O:600:TYR:HB2	1.89	0.54
1:N:771:TRP:CG	18:N:850:BCR:HC22	2.43	0.54
1:a:276:PHE:CE2	1:a:532:ILE:HG13	2.43	0.54
2:b:319:PHE:CD2	15:b:823:CLA:HMA1	2.43	0.54
2:b:468:GLN:HG2	2:b:516:PHE:HB3	1.90	0.54
1:A:214:HIS:CE1	15:A:815:CLA:NA	2.75	0.54
21:I:103:LMG:H362	21:I:103:LMG:H142	1.89	0.54
1:N:442:VAL:HG22	2:O:687:TRP:CH2	2.42	0.54
2:b:54:LEU:HD12	15:b:813:CLA:HED1	1.90	0.54
15:A:803:CLA:H112	18:A:850:BCR:H23C	1.90	0.53
2:B:342:LEU:HD21	15:B:827:CLA:HAB	1.90	0.53
2:O:91:ILE:HB	2:O:112:PRO:HB2	1.91	0.53
1:a:442:VAL:HG22	2:b:687:TRP:CH2	2.43	0.53
1:A:628:TRP:HE1	15:B:802:CLA:C1D	2.20	0.53
15:B:833:CLA:HBB1	18:B:845:BCR:HC32	1.90	0.53
19:M:102:LHG:H321	19:j:207:LHG:H312	1.90	0.53
11:Y:9:PHE:HB3	18:Y:102:BCR:H381	1.91	0.53
1:A:268:GLY:HA2	15:A:818:CLA:HAA2	1.90	0.53
2:O:422:ILE:HG23	15:O:839:CLA:HBB2	1.91	0.53
15:O:806:CLA:H43	21:O:850:LMG:H321	1.91	0.53
15:b:806:CLA:H91	21:b:849:LMG:H421	1.89	0.53
15:O:825:CLA:H122	15:O:835:CLA:HBB2	1.89	0.53
1:A:492:TRP:HA	20:A:852:LMT:H6E	1.90	0.53
15:A:803:CLA:H122	16:A:843:PQN:H241	1.90	0.53
21:I:103:LMG:H332	18:M:101:BCR:H272	1.90	0.53
1:N:620:ASP:HA	1:N:623:PHE:HB3	1.90	0.53
3:P:29:VAL:HG12	4:Q:112:ARG:HB3	1.90	0.53
15:a:811:CLA:H62	20:a:854:LMT:H62	1.91	0.53
2:b:700:ARG:HH22	7:g:43:GLU:HG2	1.74	0.53
4:d:40:VAL:HG22	4:d:50:ILE:HG12	1.91	0.53
2:B:445:ASP:OD1	2:B:622:TYR:HB2	2.09	0.53
1:N:215:GLN:HA	1:N:219:ALA:HB3	1.91	0.53
8:U:29:LEU:HD21	21:U:102:LMG:H161	1.89	0.53
15:a:833:CLA:H2	15:j:203:CLA:H43	1.91	0.53
2:b:422:ILE:HG23	15:b:839:CLA:HBB2	1.91	0.53
18:f:203:BCR:H281	15:l:103:CLA:H11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:71:HIS:HA	10:j:74:PHE:CE2	2.44	0.53
1:N:494:GLN:HG2	1:N:540:TRP:CD1	2.45	0.52
15:A:818:CLA:CHD	15:A:819:CLA:HBB2	2.40	0.52
15:B:822:CLA:H71	15:B:824:CLA:H42	1.91	0.52
2:O:257:PHE:CE2	2:O:500:TRP:HE3	2.21	0.52
15:a:803:CLA:H122	16:a:843:PQN:H241	1.90	0.52
15:b:808:CLA:O1A	15:b:827:CLA:HBD	2.08	0.52
15:B:807:CLA:O1A	15:B:825:CLA:HBD	2.09	0.52
4:D:85:ILE:HB	4:D:98:HIS:HB3	1.91	0.52
15:N:834:CLA:H152	15:O:841:CLA:H91	1.92	0.52
19:L:207:LHG:H271	19:Y:101:LHG:H111	1.90	0.52
15:a:823:CLA:H42	18:a:845:BCR:HC21	1.91	0.52
2:b:76:GLN:HA	2:b:79:LYS:HE3	1.91	0.52
2:b:276:HIS:HE1	15:b:817:CLA:ND	2.07	0.52
14:j:204:F6C:OMB	22:j:208:LFA:H61	2.10	0.52
1:A:589:GLY:HA2	1:A:596:LYS:HD3	1.92	0.52
15:N:818:CLA:HBA1	15:N:818:CLA:HBD	1.92	0.52
1:A:73:ALA:HB2	1:A:179:TYR:HB2	1.92	0.52
15:B:819:CLA:HMD2	18:B:841:BCR:H23C	1.91	0.52
11:M:9:PHE:HB3	18:M:101:BCR:H381	1.92	0.52
1:N:624:LEU:HD22	2:O:673:THR:HG22	1.92	0.52
19:W:1506:LHG:H312	19:k:101:LHG:H321	1.91	0.52
1:a:103:MET:HE1	1:a:147:ARG:HG3	1.91	0.52
15:b:821:CLA:HMD2	18:b:843:BCR:H23C	1.92	0.52
15:b:824:CLA:H71	15:b:826:CLA:H42	1.92	0.52
1:N:492:TRP:HA	20:N:852:LMT:H6E	1.91	0.52
15:a:818:CLA:HBA1	15:a:818:CLA:HBD	1.91	0.52
15:b:804:CLA:H51	18:k:102:BCR:HC22	1.92	0.52
8:J:26:LEU:HD13	18:J:101:BCR:HC7	1.92	0.52
1:N:67:ILE:O	1:N:71:ILE:HG12	2.09	0.52
15:O:809:CLA:H71	18:T:101:BCR:H342	1.92	0.52
15:O:838:CLA:HMA3	15:O:839:CLA:HED2	1.92	0.52
7:I:23:LEU:HA	7:I:27:ILE:HB	1.92	0.52
7:I:28:LEU:N	7:I:29:PRO:HD2	2.24	0.52
10:W:71:HIS:HA	10:W:74:PHE:CE2	2.45	0.52
15:A:818:CLA:HBA1	15:A:818:CLA:HBD	1.92	0.51
15:N:813:CLA:HBC1	15:N:814:CLA:H142	1.92	0.51
2:O:445:ASP:OD1	2:O:622:TYR:HB2	2.10	0.51
1:a:402:TRP:CD1	15:a:829:CLA:HAB	2.45	0.51
1:a:494:GLN:HG2	1:a:540:TRP:HD1	1.75	0.51
15:b:825:CLA:H122	15:b:835:CLA:HBB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:58:LEU:HD22	10:j:62:MET:HB3	1.92	0.51
9:K:91:LEU:HD21	18:O:845:BCR:H343	1.93	0.51
21:L:206:LMG:H191	22:L:208:LFA:H122	1.91	0.51
2:O:441:TYR:HD2	15:O:801:CLA:H203	1.75	0.51
15:O:832:CLA:HAC2	6:S:87:ILE:HG12	1.93	0.51
10:W:50:ASN:HB3	15:W:1501:CLA:HAC1	1.91	0.51
2:b:91:ILE:HB	2:b:112:PRO:HB2	1.93	0.51
15:b:825:CLA:H41	15:b:837:CLA:H2	1.92	0.51
3:c:29:VAL:HG12	4:d:112:ARG:HB3	1.93	0.51
2:B:718:HIS:NE2	15:B:839:CLA:NA	2.59	0.51
7:g:28:LEU:N	7:g:29:PRO:HD2	2.25	0.51
1:A:388:THR:HG21	1:A:547:VAL:HB	1.92	0.51
15:A:806:CLA:H61	18:A:847:BCR:H24C	1.92	0.51
15:A:823:CLA:H42	18:A:845:BCR:HC21	1.92	0.51
1:N:628:TRP:HE1	15:O:803:CLA:C1D	2.23	0.51
1:a:771:TRP:CG	18:a:850:BCR:HC22	2.46	0.51
5:R:32:ILE:HD11	5:R:35:PRO:HA	1.93	0.51
15:a:807:CLA:H42	15:a:831:CLA:H51	1.91	0.51
2:b:669:MET:HB2	15:b:803:CLA:C1C	2.40	0.51
1:A:361:ILE:HD11	18:A:848:BCR:HC7	1.92	0.51
11:k:9:PHE:HB3	18:k:102:BCR:H381	1.92	0.51
1:A:535:PRO:HG2	1:A:542:GLY:HA3	1.91	0.51
1:N:73:ALA:HB2	1:N:179:TYR:HB2	1.92	0.51
1:a:604:PRO:HB3	1:a:751:ILE:HB	1.93	0.51
15:B:823:CLA:H122	15:B:833:CLA:HBB2	1.91	0.51
1:N:738:LEU:HD13	18:S:202:BCR:H321	1.93	0.51
1:A:604:PRO:HB3	1:A:751:ILE:HB	1.93	0.51
18:A:858:BCR:H15C	8:J:20:VAL:HG22	1.92	0.51
2:B:403:ASP:HB3	4:D:129:ALA:HB3	1.93	0.51
1:N:465:ASN:HB3	1:N:672:THR:HG22	1.93	0.51
15:N:818:CLA:CHD	15:N:819:CLA:HBB2	2.41	0.51
15:A:807:CLA:H42	15:A:831:CLA:H51	1.93	0.51
19:L:207:LHG:H282	7:T:36:ILE:HG12	1.93	0.51
2:B:430:SER:HB3	2:B:536:VAL:HG22	1.93	0.50
10:L:156:MET:SD	18:j:201:BCR:H24C	2.51	0.50
15:N:833:CLA:H2	15:W:1502:CLA:H43	1.92	0.50
7:T:23:LEU:HA	7:T:27:ILE:HB	1.92	0.50
5:e:32:ILE:HD11	5:e:35:PRO:HA	1.94	0.50
1:A:167:MET:HG3	18:A:846:BCR:H322	1.94	0.50
1:A:295:HIS:HB2	15:A:819:CLA:C1B	2.41	0.50
6:F:93:VAL:O	6:F:97:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:28:LEU:N	7:T:29:PRO:HD2	2.26	0.50
1:a:215:GLN:HA	1:a:219:ALA:HB3	1.92	0.50
1:a:501:VAL:HG21	1:a:535:PRO:HA	1.94	0.50
15:a:823:CLA:H11	18:a:845:BCR:HC31	1.92	0.50
15:A:803:CLA:CGA	15:A:803:CLA:H3A	2.41	0.50
3:C:29:VAL:HG12	4:D:112:ARG:HB3	1.94	0.50
15:O:808:CLA:O1A	15:O:827:CLA:HBD	2.11	0.50
2:b:445:ASP:OD1	2:b:622:TYR:HB2	2.12	0.50
12:l:26:ARG:HG3	19:l:101:LHG:HC42	1.93	0.50
1:A:405:GLY:HA3	1:A:633:LEU:HD21	1.92	0.50
2:O:718:HIS:NE2	15:O:841:CLA:NA	2.60	0.50
15:B:823:CLA:H43	15:B:836:CLA:HBA1	1.94	0.50
15:B:837:CLA:H203	12:X:30:SER:HB3	1.94	0.50
5:E:7:LYS:HB2	5:E:62:GLU:HB3	1.93	0.50
1:N:708:PHE:CG	18:N:850:BCR:H363	2.47	0.50
18:S:202:BCR:H281	15:Z:103:CLA:H11	1.93	0.50
1:a:441:ASP:H	4:d:16:THR:HG21	1.76	0.50
2:b:203:ARG:HG2	2:b:250:ALA:HB1	1.93	0.50
2:b:495:ASN:HB3	15:b:836:CLA:HED2	1.94	0.50
2:B:257:PHE:HD2	2:B:499:VAL:HG23	1.76	0.50
1:a:589:GLY:HA2	1:a:596:LYS:HD3	1.92	0.50
2:b:182:LEU:HD13	15:b:813:CLA:HHB	1.94	0.50
1:A:738:LEU:HD13	18:F:203:BCR:H321	1.93	0.50
15:B:805:CLA:HMD3	15:B:807:CLA:H201	1.92	0.50
2:O:565:PRO:HB3	2:O:708:ILE:HB	1.93	0.50
5:E:32:ILE:HD11	5:E:35:PRO:HA	1.94	0.50
1:a:494:GLN:HG2	1:a:540:TRP:CD1	2.46	0.50
2:b:403:ASP:HB3	4:d:129:ALA:HB3	1.93	0.50
15:b:807:CLA:H43	7:g:20:MET:HE2	1.94	0.50
15:N:823:CLA:H42	18:N:845:BCR:HC21	1.94	0.49
1:a:73:ALA:HB2	1:a:179:TYR:HB2	1.94	0.49
15:B:836:CLA:H93	15:B:837:CLA:HBC1	1.94	0.49
1:A:27:TRP:CD1	15:A:812:CLA:H2	2.47	0.49
1:A:614:CYS:HB2	2:B:674:TRP:HB3	1.93	0.49
15:B:830:CLA:HAB	18:F:202:BCR:H323	1.94	0.49
1:N:268:GLY:HA2	15:N:818:CLA:HAA2	1.95	0.49
15:O:825:CLA:H41	15:O:837:CLA:H2	1.94	0.49
4:Q:29:TYR:HB2	4:Q:60:ILE:HG13	1.94	0.49
1:a:697:SER:HB2	2:b:449:ALA:HB1	1.95	0.49
15:N:803:CLA:H122	16:N:843:PQN:H241	1.93	0.49
1:A:541:GLY:HA2	1:A:555:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ALA:HB3	11:M:29:LEU:HD21	1.94	0.49
2:B:150:LEU:HD22	11:M:22:ALA:HA	1.93	0.49
15:N:841:CLA:H172	6:S:101:GLY:HA2	1.94	0.49
15:b:830:CLA:H2	19:l:102:LHG:HC92	1.95	0.49
1:A:215:GLN:HA	1:A:219:ALA:HB3	1.95	0.49
15:A:823:CLA:H11	18:A:845:BCR:HC31	1.95	0.49
2:B:387:MET:HE1	18:B:845:BCR:H361	1.93	0.49
15:B:836:CLA:HMA3	15:B:837:CLA:HED2	1.95	0.49
19:M:102:LHG:HC62	19:M:102:LHG:HC12	1.93	0.49
2:O:22:TRP:CG	2:O:710:GLN:HE22	2.30	0.49
15:b:838:CLA:H93	15:b:839:CLA:HBC1	1.93	0.49
1:A:419:MET:HE1	1:A:437:LEU:HD11	1.95	0.49
2:B:349:SER:HB3	2:B:383:ALA:HB2	1.95	0.49
2:O:257:PHE:HD2	2:O:499:VAL:HG23	1.77	0.49
2:O:361:PRO:HG3	15:O:818:CLA:HBA1	1.93	0.49
1:a:628:TRP:HE1	15:b:803:CLA:C1D	2.26	0.49
15:a:820:CLA:HBC2	15:a:820:CLA:HMC1	1.95	0.49
2:B:361:PRO:HG3	15:B:816:CLA:HBA1	1.93	0.49
2:B:378:HIS:HB2	15:B:825:CLA:CHB	2.43	0.49
15:O:825:CLA:H43	15:O:838:CLA:HBA1	1.95	0.49
1:A:771:TRP:CG	18:A:850:BCR:HC22	2.48	0.49
2:B:422:ILE:HG23	15:B:837:CLA:HBB2	1.95	0.49
4:D:11:ILE:HB	4:D:50:ILE:HB	1.94	0.49
1:N:391:ALA:HA	1:N:778:MET:HB3	1.95	0.49
4:Q:75:ARG:HG3	4:Q:83:TYR:HE1	1.77	0.49
2:b:378:HIS:HB2	15:b:827:CLA:CHB	2.42	0.49
15:A:820:CLA:HBA2	15:A:820:CLA:H3A	1.54	0.49
7:I:22:PRO:HB3	7:I:26:TYR:CZ	2.48	0.49
15:N:820:CLA:H91	15:N:830:CLA:H172	1.94	0.49
15:O:808:CLA:H91	15:O:809:CLA:H52	1.95	0.49
2:b:257:PHE:HE2	2:b:500:TRP:CE3	2.31	0.49
1:A:402:TRP:CD1	15:A:829:CLA:HAB	2.48	0.48
15:A:825:CLA:H62	18:A:848:BCR:H352	1.95	0.48
2:B:158:GLN:O	2:B:162:ARG:HG3	2.13	0.48
15:B:811:CLA:H91	15:B:822:CLA:H43	1.95	0.48
15:B:828:CLA:H143	19:X:101:LHG:H122	1.95	0.48
1:N:276:PHE:CE2	1:N:532:ILE:HG13	2.48	0.48
1:N:319:SER:O	1:N:323:MET:HG3	2.12	0.48
1:N:604:PRO:HB3	1:N:751:ILE:HB	1.94	0.48
21:T:103:LMG:H142	21:T:103:LMG:H362	1.95	0.48
21:W:1505:LMG:H191	22:W:1507:LFA:H122	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:818:CLA:CHD	15:a:819:CLA:HBB2	2.43	0.48
2:b:158:GLN:O	2:b:162:ARG:HG3	2.12	0.48
2:b:565:PRO:HB3	2:b:708:ILE:HB	1.94	0.48
10:L:140:ASN:HB2	10:L:143:GLU:HG3	1.95	0.48
19:L:207:LHG:H312	19:Y:101:LHG:H321	1.94	0.48
1:N:280:LEU:HD21	1:N:381:PRO:HD2	1.94	0.48
1:N:697:SER:HB2	2:O:449:ALA:HB1	1.95	0.48
2:O:378:HIS:HB2	15:O:827:CLA:CHB	2.43	0.48
1:a:620:ASP:HA	1:a:623:PHE:HB3	1.93	0.48
1:a:708:PHE:CG	18:a:850:BCR:H363	2.48	0.48
15:a:841:CLA:HBA2	2:b:428:TRP:CD1	2.48	0.48
15:b:802:CLA:HMB1	15:b:802:CLA:HBB1	1.95	0.48
15:b:806:CLA:H151	15:b:828:CLA:HBB2	1.95	0.48
15:A:841:CLA:HBA2	2:B:428:TRP:CD1	2.48	0.48
15:N:803:CLA:CGA	15:N:803:CLA:H3A	2.41	0.48
1:a:419:MET:HE1	1:a:437:LEU:HD11	1.94	0.48
4:D:32:THR:O	4:D:83:TYR:HA	2.13	0.48
19:M:102:LHG:H111	19:j:207:LHG:H271	1.96	0.48
2:O:158:GLN:O	2:O:162:ARG:HG3	2.13	0.48
15:b:809:CLA:H71	18:g:101:BCR:H342	1.96	0.48
1:A:715:MET:HB2	15:A:803:CLA:C1C	2.44	0.48
18:B:843:BCR:H343	9:i:91:LEU:HD21	1.95	0.48
1:N:126:ASN:HB3	1:N:134:HIS:HB3	1.96	0.48
2:O:403:ASP:HB3	4:Q:129:ALA:HB3	1.96	0.48
1:A:562:ASP:HA	1:A:565:ILE:HG22	1.96	0.48
8:J:37:GLN:HE21	8:J:38:TYR:H	1.61	0.48
1:N:535:PRO:HG2	1:N:542:GLY:HA3	1.95	0.48
15:O:832:CLA:HAB	18:O:848:BCR:H323	1.95	0.48
15:b:830:CLA:HMA3	15:b:831:CLA:HED2	1.95	0.48
2:O:441:TYR:HB3	2:O:623:LEU:HG	1.96	0.48
15:O:805:CLA:HBD	15:O:805:CLA:H122	1.96	0.48
15:O:835:CLA:HBB1	18:O:847:BCR:HC32	1.94	0.48
1:a:202:GLY:HA3	15:a:814:CLA:HBB1	1.96	0.48
19:k:101:LHG:HC62	19:k:101:LHG:HC12	1.95	0.48
15:A:835:CLA:O2D	15:A:835:CLA:H2A	2.14	0.48
15:B:828:CLA:H3A	15:B:829:CLA:OBD	2.13	0.48
15:N:806:CLA:H61	18:N:847:BCR:H24C	1.95	0.48
15:N:823:CLA:HBA1	15:N:823:CLA:H3A	1.72	0.48
1:a:541:GLY:HA2	1:a:555:PRO:HG3	1.95	0.48
15:b:832:CLA:HAC2	6:f:87:ILE:HG12	1.96	0.48
6:F:90:PHE:HB2	18:F:202:BCR:H321	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:818:CLA:H62	15:N:818:CLA:H41	1.52	0.48
15:a:841:CLA:H172	6:f:101:GLY:HA2	1.95	0.48
15:b:838:CLA:HMA3	15:b:839:CLA:HED2	1.95	0.48
15:A:814:CLA:H62	15:A:814:CLA:H41	1.60	0.48
2:B:377:THR:HG23	2:B:598:THR:HG21	1.95	0.48
18:B:842:BCR:H392	18:B:842:BCR:H24C	1.70	0.48
6:F:96:PHE:HZ	6:F:130:ILE:HG23	1.79	0.48
2:O:65:LEU:HD11	18:O:845:BCR:H281	1.95	0.48
2:O:430:SER:HB3	2:O:536:VAL:HG22	1.96	0.48
9:V:91:LEU:HD22	15:b:815:CLA:HAA2	1.96	0.48
1:A:491:GLN:HB3	20:A:852:LMT:H5B	1.94	0.47
1:N:214:HIS:HB2	15:N:815:CLA:CHC	2.44	0.47
15:N:811:CLA:H11	15:N:813:CLA:H2	1.96	0.47
1:a:318:HIS:NE2	15:a:823:CLA:ND	2.61	0.47
1:A:568:ILE:HD12	13:A:801:CL0:H61	1.96	0.47
1:A:705:ALA:HB2	15:A:856:CLA:H71	1.96	0.47
1:A:708:PHE:CD2	18:A:850:BCR:H363	2.49	0.47
2:B:495:ASN:HB3	15:B:834:CLA:HED2	1.96	0.47
15:B:808:CLA:H71	18:I:101:BCR:H342	1.95	0.47
21:W:1505:LMG:H342	21:g:103:LMG:HC61	1.96	0.47
1:A:218:VAL:HG13	1:A:238:PRO:HB3	1.96	0.47
15:A:820:CLA:HMC1	15:A:820:CLA:HBC2	1.96	0.47
2:B:727:TYR:HB2	15:B:801:CLA:HED3	1.95	0.47
1:N:740:VAL:HG23	6:S:102:ARG:HA	1.96	0.47
15:O:830:CLA:H3A	15:O:831:CLA:OBD	2.14	0.47
15:B:816:CLA:H3A	15:B:816:CLA:HBA2	1.43	0.47
15:B:817:CLA:H162	15:B:817:CLA:H122	1.48	0.47
7:I:18:TRP:CZ2	10:j:176:LEU:HD12	2.50	0.47
1:N:445:SER:HB3	2:O:684:THR:HG22	1.96	0.47
15:N:807:CLA:H151	15:N:830:CLA:HBB2	1.95	0.47
15:N:820:CLA:HMC1	15:N:820:CLA:HBC2	1.95	0.47
1:a:214:HIS:HB2	15:a:815:CLA:CHC	2.44	0.47
15:a:820:CLA:H91	15:a:830:CLA:H172	1.97	0.47
2:b:361:PRO:HG3	15:b:818:CLA:HBA1	1.95	0.47
1:N:441:ASP:H	4:Q:16:THR:HG21	1.80	0.47
2:O:176:ASN:HB3	15:O:820:CLA:HMD1	1.97	0.47
4:Q:30:VAL:HG22	4:Q:59:GLU:HG2	1.96	0.47
15:a:803:CLA:CGA	15:a:803:CLA:H3A	2.42	0.47
15:a:838:CLA:H61	15:a:838:CLA:H41	1.60	0.47
2:b:430:SER:HB3	2:b:536:VAL:HG22	1.96	0.47
2:B:195:ILE:HD11	2:B:255:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:LEU:O	2:B:442:VAL:HG22	2.14	0.47
15:B:818:CLA:H8	15:B:818:CLA:HBB1	1.96	0.47
1:N:402:TRP:CD1	15:N:829:CLA:HAB	2.49	0.47
15:O:821:CLA:HMD1	18:O:843:BCR:H23C	1.96	0.47
1:a:167:MET:HG3	18:a:846:BCR:H322	1.95	0.47
15:b:805:CLA:H3A	15:b:805:CLA:HBA1	1.49	0.47
15:b:830:CLA:H3A	15:b:831:CLA:OBD	2.15	0.47
15:A:804:CLA:H91	15:A:804:CLA:H112	1.70	0.47
15:A:807:CLA:H41	15:A:807:CLA:H62	1.53	0.47
2:B:378:HIS:HB2	15:B:825:CLA:C1B	2.44	0.47
15:B:828:CLA:HMA2	15:B:829:CLA:HED2	1.97	0.47
6:F:130:ILE:O	6:F:134:VAL:HG23	2.14	0.47
1:N:259:LEU:HD11	18:N:845:BCR:H291	1.96	0.47
1:N:568:ILE:HD12	13:N:801:CL0:H61	1.97	0.47
15:N:823:CLA:H11	18:N:845:BCR:HC31	1.96	0.47
2:O:182:LEU:HD13	15:O:813:CLA:HHB	1.96	0.47
15:O:803:CLA:H72	18:O:849:BCR:H363	1.96	0.47
15:O:809:CLA:H3A	15:O:809:CLA:HBA2	1.56	0.47
1:a:65:GLU:HB3	1:a:186:LEU:HB2	1.97	0.47
18:a:845:BCR:H24C	18:a:845:BCR:H371	1.76	0.47
2:b:275:HIS:HB3	15:b:817:CLA:HMB2	1.96	0.47
2:b:398:TRP:HE1	18:b:847:BCR:H271	1.80	0.47
15:b:819:CLA:O1A	15:b:823:CLA:HAA2	2.15	0.47
12:l:23:PHE:HB3	12:l:26:ARG:HB2	1.97	0.47
1:A:708:PHE:CG	18:A:850:BCR:H363	2.50	0.47
15:A:856:CLA:H11	2:B:623:LEU:HD12	1.97	0.47
2:B:270:LEU:HD23	2:B:273:MET:HE3	1.96	0.47
15:B:821:CLA:H52	15:B:822:CLA:H172	1.96	0.47
15:N:812:CLA:H61	15:N:812:CLA:H41	1.62	0.47
15:O:832:CLA:H201	15:O:838:CLA:H143	1.97	0.47
2:O:495:ASN:HB3	15:O:836:CLA:HED2	1.96	0.47
15:O:830:CLA:H2	19:Z:102:LHG:HC92	1.97	0.47
4:Q:43:MET:HE1	4:Q:58:LEU:HD11	1.95	0.47
1:a:454:LEU:HB3	1:a:571:PHE:HB2	1.97	0.47
4:d:87:ARG:HD2	4:d:95:GLN:HE21	1.80	0.47
15:A:856:CLA:HBB1	15:A:856:CLA:HMB1	1.96	0.47
15:B:836:CLA:H142	15:B:836:CLA:H111	1.74	0.47
15:K:102:CLA:H3A	15:K:102:CLA:HBA2	1.67	0.47
21:L:206:LMG:H371	7:T:18:TRP:CE3	2.50	0.47
15:N:809:CLA:CHC	15:N:810:CLA:HMD2	2.45	0.47
15:O:832:CLA:H142	6:S:136:TRP:HH2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:26:ARG:HG3	19:Z:101:LHG:HC42	1.97	0.47
2:b:126:THR:HG22	2:b:270:LEU:HD21	1.96	0.47
15:b:838:CLA:H91	15:b:838:CLA:H111	1.73	0.47
15:b:838:CLA:H111	15:b:838:CLA:H142	1.73	0.47
2:B:106:ARG:NH2	2:B:115:ILE:HG12	2.30	0.46
2:B:514:SER:HA	2:B:517:LEU:HD21	1.96	0.46
15:N:820:CLA:H93	15:N:820:CLA:H62	1.76	0.46
1:A:318:HIS:NE2	15:A:823:CLA:ND	2.64	0.46
15:A:839:CLA:C4A	15:A:839:CLA:HBA2	2.45	0.46
2:B:276:HIS:HE1	15:B:815:CLA:ND	2.11	0.46
10:L:71:HIS:HA	10:L:74:PHE:CD1	2.50	0.46
1:N:454:LEU:HB3	1:N:571:PHE:HB2	1.97	0.46
15:N:803:CLA:HBB1	15:N:803:CLA:HMB3	1.98	0.46
15:N:805:CLA:H3A	15:N:805:CLA:HBA2	1.62	0.46
15:O:804:CLA:H12	15:O:804:CLA:C4D	2.45	0.46
15:O:819:CLA:H122	15:O:819:CLA:H162	1.50	0.46
15:a:819:CLA:HBB1	15:a:819:CLA:H92	1.96	0.46
15:b:830:CLA:H142	19:l:101:LHG:H281	1.97	0.46
15:b:832:CLA:HAB	18:f:202:BCR:H323	1.97	0.46
1:A:723:TYR:HA	2:B:543:LYS:HZ1	1.80	0.46
15:A:842:CLA:H3A	15:A:842:CLA:HBA2	1.74	0.46
15:B:823:CLA:H41	15:B:835:CLA:H2	1.96	0.46
18:I:102:BCR:H402	15:L:203:CLA:H51	1.97	0.46
1:N:705:ALA:HB2	15:O:802:CLA:H71	1.97	0.46
2:O:635:SER:O	2:O:639:ILE:HG12	2.15	0.46
3:P:15:THR:HG22	3:P:28:MET:HG3	1.97	0.46
19:W:1506:LHG:H271	19:k:101:LHG:H111	1.97	0.46
15:a:807:CLA:H151	15:a:830:CLA:HBB2	1.97	0.46
15:a:812:CLA:H61	15:a:812:CLA:H41	1.60	0.46
2:B:565:PRO:HB3	2:B:708:ILE:HB	1.97	0.46
15:O:806:CLA:H41	15:O:806:CLA:H61	1.47	0.46
10:W:58:LEU:HD22	10:W:62:MET:HB3	1.98	0.46
19:W:1506:LHG:H282	7:g:36:ILE:HG12	1.98	0.46
15:a:803:CLA:HBB1	15:a:803:CLA:HMB3	1.97	0.46
15:a:809:CLA:CHC	15:a:810:CLA:HMD2	2.45	0.46
15:b:838:CLA:H141	15:b:838:CLA:H161	1.74	0.46
15:i:102:CLA:H3A	15:i:102:CLA:HBA2	1.67	0.46
1:A:436:THR:HA	1:A:439:HIS:CE1	2.50	0.46
15:B:804:CLA:H122	15:B:804:CLA:HBD	1.97	0.46
15:B:808:CLA:H3A	15:B:808:CLA:HBA2	1.53	0.46
15:B:835:CLA:HMB1	15:B:835:CLA:HBB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:176:LEU:HD12	7:T:18:TRP:CZ2	2.51	0.46
15:N:818:CLA:H111	15:N:818:CLA:H151	1.59	0.46
15:O:829:CLA:H122	15:O:829:CLA:H161	1.70	0.46
15:O:837:CLA:HMB1	15:O:837:CLA:HBB1	1.97	0.46
15:O:839:CLA:H203	12:Z:30:SER:HB3	1.97	0.46
1:a:355:TRP:HB3	15:a:806:CLA:HAC1	1.98	0.46
1:a:562:ASP:HA	1:a:565:ILE:HG22	1.98	0.46
1:a:740:VAL:HG23	6:f:102:ARG:HA	1.97	0.46
2:b:536:VAL:HG11	2:b:589:TRP:CE2	2.50	0.46
15:b:811:CLA:H122	15:b:811:CLA:H162	1.75	0.46
1:A:398:THR:HG23	1:A:637:VAL:HG11	1.98	0.46
1:A:402:TRP:HA	1:A:633:LEU:HD23	1.96	0.46
15:B:808:CLA:HBA1	15:B:808:CLA:H11	1.67	0.46
15:N:806:CLA:HBA1	15:N:806:CLA:H3A	1.52	0.46
2:O:195:ILE:HD11	2:O:255:LEU:HD21	1.97	0.46
1:a:402:TRP:HB3	15:a:829:CLA:HMC3	1.98	0.46
1:a:436:THR:HA	1:a:439:HIS:CE1	2.50	0.46
2:b:419:LYS:HE2	6:f:161:ARG:HH11	1.80	0.46
15:b:807:CLA:HMC1	15:b:807:CLA:H92	1.97	0.46
7:g:22:PRO:HB3	7:g:26:TYR:CZ	2.50	0.46
2:B:700:ARG:HH22	7:I:43:GLU:HG2	1.81	0.46
15:B:803:CLA:H62	15:B:803:CLA:H41	1.53	0.46
15:B:830:CLA:H201	15:B:836:CLA:H143	1.96	0.46
1:N:456:PHE:O	1:N:460:ALA:HB3	2.16	0.46
2:O:194:LEU:HA	2:O:198:ALA:HB3	1.98	0.46
15:O:805:CLA:H61	15:O:805:CLA:H2	1.71	0.46
15:b:804:CLA:H12	15:b:804:CLA:C4D	2.45	0.46
15:b:828:CLA:H3A	15:b:828:CLA:HBA2	1.70	0.46
1:A:689:ILE:HG23	1:A:690:GLN:HG3	1.98	0.46
15:B:836:CLA:H111	15:B:836:CLA:H91	1.72	0.46
15:a:829:CLA:H62	15:a:829:CLA:H41	1.67	0.46
18:a:857:BCR:H11C	18:a:857:BCR:H341	1.80	0.46
15:b:809:CLA:H3A	15:b:809:CLA:HBA2	1.52	0.46
15:b:837:CLA:HBB1	15:b:837:CLA:HMB1	1.97	0.46
15:A:809:CLA:CHC	15:A:810:CLA:HMD2	2.46	0.46
15:A:810:CLA:H112	15:A:810:CLA:H93	1.70	0.46
15:A:820:CLA:H91	15:A:830:CLA:H172	1.98	0.46
2:O:150:LEU:HD22	11:Y:22:ALA:HA	1.98	0.46
3:P:18:VAL:HG21	3:P:28:MET:HG2	1.97	0.46
9:V:88:LEU:HB2	9:V:91:LEU:HA	1.97	0.46
19:Y:101:LHG:HC12	19:Y:101:LHG:HC62	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:818:CLA:H141	15:a:818:CLA:H161	1.71	0.46
15:b:823:CLA:H52	15:b:824:CLA:H172	1.98	0.46
15:b:830:CLA:H62	15:b:830:CLA:H41	1.55	0.46
2:B:182:LEU:HD11	15:B:811:CLA:H2	1.97	0.46
15:B:828:CLA:H142	19:X:101:LHG:H281	1.98	0.46
1:N:171:MET:HE1	15:N:814:CLA:H92	1.97	0.46
15:a:822:CLA:H93	15:a:822:CLA:H112	1.74	0.46
2:b:22:TRP:CG	2:b:710:GLN:HE22	2.34	0.46
15:b:804:CLA:H41	15:b:804:CLA:H62	1.51	0.46
1:A:635:MET:HE2	13:A:801:CL0:H58	1.97	0.45
15:B:804:CLA:HBA1	15:B:804:CLA:H3A	1.47	0.45
10:L:156:MET:HG3	18:j:201:BCR:H382	1.99	0.45
1:N:355:TRP:HB3	15:N:806:CLA:HAC1	1.98	0.45
1:a:118:SER:HB3	6:f:49:TYR:CE1	2.50	0.45
1:a:220:LEU:HD21	1:a:290:SER:HA	1.98	0.45
2:b:635:SER:O	2:b:639:ILE:HG12	2.17	0.45
15:b:823:CLA:H61	15:b:823:CLA:H2	1.62	0.45
9:i:21:SER:O	9:i:24:VAL:HG22	2.16	0.45
1:A:166:VAL:O	1:A:170:ILE:HG12	2.16	0.45
15:B:827:CLA:H93	15:B:827:CLA:H112	1.77	0.45
2:b:194:LEU:HA	2:b:198:ALA:HB3	1.98	0.45
15:b:825:CLA:HBA2	15:b:825:CLA:H3A	1.74	0.45
1:A:65:GLU:HB2	1:A:186:LEU:HB2	1.97	0.45
2:B:398:TRP:HE1	18:B:845:BCR:H271	1.81	0.45
15:B:803:CLA:H51	18:M:101:BCR:HC22	1.97	0.45
1:N:414:HIS:HA	1:N:417:ILE:HD12	1.98	0.45
15:O:804:CLA:H62	15:O:804:CLA:H41	1.53	0.45
18:O:844:BCR:H24C	18:O:844:BCR:H392	1.71	0.45
15:a:810:CLA:H112	15:a:810:CLA:H93	1.71	0.45
1:A:501:VAL:HG21	1:A:535:PRO:HA	1.98	0.45
15:B:815:CLA:HBA2	15:B:815:CLA:H3A	1.37	0.45
6:F:96:PHE:CZ	6:F:130:ILE:HG23	2.52	0.45
7:I:36:ILE:HG12	19:j:207:LHG:H282	1.98	0.45
1:N:65:GLU:HB2	1:N:186:LEU:HB2	1.98	0.45
15:N:825:CLA:H41	15:N:825:CLA:H62	1.61	0.45
2:O:257:PHE:HE2	2:O:500:TRP:CE3	2.24	0.45
2:O:700:ARG:HH22	7:T:43:GLU:HG2	1.80	0.45
6:f:90:PHE:HB2	18:f:202:BCR:H321	1.98	0.45
6:f:96:PHE:HZ	6:f:130:ILE:HG23	1.81	0.45
7:g:23:LEU:HA	7:g:27:ILE:HB	1.97	0.45
18:L:209:BCR:H24C	10:W:156:MET:SD	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:14:VAL:HG12	1:N:185:LYS:HG3	1.97	0.45
2:O:78:ILE:HD12	2:O:125:TYR:CD1	2.51	0.45
15:O:809:CLA:HBA1	15:O:809:CLA:H11	1.71	0.45
8:U:36:LEU:HD21	21:U:102:LMG:HC71	1.98	0.45
1:a:126:ASN:HB3	1:a:134:HIS:HB3	1.97	0.45
2:b:195:ILE:HD11	2:b:255:LEU:HD21	1.98	0.45
2:b:443:HIS:CE1	14:b:833:F6C:NA	2.85	0.45
6:f:136:TRP:CG	6:f:137:PRO:HD3	2.52	0.45
1:A:30:PRO:HB2	1:A:46:TRP:HH2	1.80	0.45
2:O:438:LEU:O	2:O:442:VAL:HG22	2.17	0.45
15:O:826:CLA:H72	15:O:826:CLA:H112	1.64	0.45
21:W:1505:LMG:H371	7:g:18:TRP:CE3	2.52	0.45
1:a:626:LEU:HD21	15:a:831:CLA:HBC1	1.98	0.45
15:a:839:CLA:C4A	15:a:839:CLA:HBA2	2.47	0.45
15:b:832:CLA:H201	15:b:838:CLA:H143	1.98	0.45
2:B:287:ALA:HB2	15:B:817:CLA:HBC2	1.99	0.45
1:N:761:HIS:CE1	15:N:842:CLA:NA	2.85	0.45
18:O:848:BCR:H321	6:S:90:PHE:HB2	1.99	0.45
21:T:103:LMG:H352	18:Y:102:BCR:H383	1.98	0.45
9:V:91:LEU:HD21	18:b:845:BCR:H343	1.98	0.45
1:a:444:ILE:HB	2:b:684:THR:HG21	1.98	0.45
15:a:806:CLA:H3A	15:a:806:CLA:HBA1	1.47	0.45
2:b:182:LEU:HD11	15:b:813:CLA:H2	1.99	0.45
15:A:818:CLA:H193	15:A:822:CLA:HBC1	1.98	0.45
15:A:819:CLA:H3A	15:A:819:CLA:HBA2	1.50	0.45
2:B:50:HIS:NE2	15:B:804:CLA:NA	2.65	0.45
2:B:433:LEU:HB3	2:B:532:LEU:HB2	1.98	0.45
1:N:501:VAL:HG21	1:N:535:PRO:HA	1.98	0.45
15:O:830:CLA:H162	15:O:830:CLA:H141	1.77	0.45
15:a:806:CLA:H62	15:a:806:CLA:H2	1.71	0.45
15:b:806:CLA:H41	15:b:806:CLA:H61	1.46	0.45
6:f:82:ASP:HB3	8:h:39:GLY:HA2	1.98	0.45
1:A:214:HIS:HB2	15:A:815:CLA:CHC	2.46	0.45
15:A:820:CLA:H93	15:A:820:CLA:H62	1.76	0.45
2:B:182:LEU:HD13	15:B:811:CLA:HHB	1.98	0.45
15:B:806:CLA:H92	15:B:806:CLA:HMC1	1.99	0.45
15:B:808:CLA:HHB	14:L:201:F6C:CBB	2.47	0.45
1:N:276:PHE:HD1	15:N:819:CLA:HMB2	1.82	0.45
15:N:804:CLA:H91	15:N:804:CLA:H112	1.68	0.45
15:O:838:CLA:H93	15:O:839:CLA:HBC1	1.98	0.45
9:V:21:SER:O	9:V:24:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:838:CLA:H3A	15:a:838:CLA:HBA1	1.63	0.45
2:b:721:VAL:HG13	15:b:827:CLA:H112	1.99	0.45
15:b:811:CLA:H18	15:b:814:CLA:H122	1.97	0.45
1:A:494:GLN:HG2	1:A:540:TRP:HD1	1.81	0.45
15:A:837:CLA:HED2	15:A:837:CLA:HBD	1.70	0.45
15:B:817:CLA:O1A	15:B:821:CLA:HAA2	2.17	0.45
1:N:447:LEU:HD22	15:N:840:CLA:HBB1	1.99	0.45
15:O:824:CLA:H71	15:O:826:CLA:H42	1.99	0.45
11:Y:30:TYR:CG	19:Y:101:LHG:HC92	2.52	0.45
15:a:813:CLA:HBC1	15:a:814:CLA:H142	1.99	0.45
15:a:814:CLA:H62	15:a:814:CLA:H41	1.64	0.45
15:a:818:CLA:H41	15:a:818:CLA:H62	1.52	0.45
2:b:106:ARG:NH2	2:b:115:ILE:HG12	2.32	0.45
15:b:829:CLA:H122	15:b:829:CLA:H161	1.67	0.45
1:A:202:GLY:HA3	15:A:814:CLA:HBB1	1.99	0.44
1:A:276:PHE:HD1	15:A:819:CLA:HMB2	1.82	0.44
2:B:257:PHE:CE2	2:B:500:TRP:HE3	2.23	0.44
1:N:689:ILE:HG23	1:N:690:GLN:HG3	1.99	0.44
15:N:837:CLA:HED2	15:N:837:CLA:HBD	1.69	0.44
18:N:857:BCR:HC8	18:N:857:BCR:H311	1.99	0.44
2:O:203:ARG:HG2	2:O:250:ALA:HB1	1.99	0.44
15:O:803:CLA:CGA	15:O:803:CLA:H3A	2.47	0.44
15:O:823:CLA:H2	15:O:823:CLA:H61	1.59	0.44
1:a:456:PHE:O	1:a:460:ALA:HB3	2.16	0.44
15:b:832:CLA:H142	6:f:136:TRP:HH2	1.82	0.44
16:b:842:PQN:H172	16:b:842:PQN:H211	1.76	0.44
1:A:246:SER:O	1:A:250:GLU:HG3	2.18	0.44
1:A:419:MET:HE2	1:A:437:LEU:HD21	2.00	0.44
15:A:803:CLA:HMB3	15:A:803:CLA:HBB1	1.97	0.44
15:A:819:CLA:H93	15:A:819:CLA:H111	1.78	0.44
15:B:821:CLA:H61	15:B:821:CLA:H2	1.63	0.44
18:B:841:BCR:H20C	18:B:841:BCR:H361	1.80	0.44
2:O:514:SER:HA	2:O:517:LEU:HD21	1.98	0.44
1:a:399:HIS:CE1	15:a:829:CLA:ND	2.85	0.44
1:A:295:HIS:HB2	15:A:819:CLA:CHB	2.47	0.44
15:A:820:CLA:H202	15:A:820:CLA:H161	1.82	0.44
2:B:638:LEU:HD22	2:B:730:PHE:HA	1.98	0.44
15:B:804:CLA:H61	15:B:804:CLA:H2	1.70	0.44
6:F:82:ASP:HB3	8:J:39:GLY:HA2	2.00	0.44
6:F:92:TYR:HE2	21:J:102:LMG:H452	1.82	0.44
1:N:41:PRO:HB3	1:N:46:TRP:CE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:306:ALA:HB2	15:N:822:CLA:HBC2	2.00	0.44
15:N:820:CLA:O2D	15:N:820:CLA:H2A	2.17	0.44
15:O:827:CLA:H61	15:O:827:CLA:H41	1.68	0.44
1:a:119:LEU:HG	1:a:120:VAL:HG13	2.00	0.44
2:b:470:ALA:HB1	2:b:481:LEU:HD12	2.00	0.44
1:A:41:PRO:HG3	6:F:119:ILE:HG21	1.99	0.44
15:B:803:CLA:HHC	15:B:805:CLA:OBD	2.16	0.44
7:I:15:TRP:CD1	21:I:103:LMG:HC1	2.53	0.44
1:N:295:HIS:HB2	15:N:819:CLA:CHB	2.48	0.44
15:O:802:CLA:HBB1	15:O:802:CLA:HMB3	2.00	0.44
15:O:832:CLA:H62	15:O:832:CLA:H2	1.76	0.44
6:S:96:PHE:HZ	6:S:130:ILE:HG23	1.82	0.44
1:a:306:ALA:HB2	15:a:822:CLA:HBC2	1.99	0.44
15:a:809:CLA:HBA2	15:a:809:CLA:H3A	1.27	0.44
15:a:841:CLA:H2	15:a:841:CLA:H61	1.71	0.44
1:A:607:GLY:HA2	2:B:569:PRO:HD3	1.99	0.44
15:A:806:CLA:HBA1	15:A:806:CLA:H3A	1.51	0.44
15:A:810:CLA:H61	15:A:810:CLA:H92	1.83	0.44
15:A:841:CLA:H71	18:F:202:BCR:H17C	2.00	0.44
18:A:858:BCR:HC8	18:A:858:BCR:H311	1.99	0.44
15:O:838:CLA:H52	15:O:838:CLA:H12	1.82	0.44
18:W:1508:BCR:H24C	10:j:156:MET:SD	2.57	0.44
1:a:41:PRO:HB3	1:a:46:TRP:CE3	2.52	0.44
15:a:804:CLA:H12	15:a:804:CLA:H51	1.86	0.44
18:a:857:BCR:HC8	18:a:857:BCR:H311	2.00	0.44
1:A:738:LEU:HD11	18:F:203:BCR:H342	1.98	0.44
2:B:309:SER:O	15:B:820:CLA:HAA1	2.18	0.44
1:N:295:HIS:HB2	15:N:819:CLA:C1B	2.48	0.44
1:N:544:MET:HG3	1:N:554:MET:HB3	2.00	0.44
1:N:562:ASP:HA	1:N:565:ILE:HG22	1.99	0.44
2:O:349:SER:HB3	2:O:383:ALA:HB2	1.98	0.44
10:W:176:LEU:HD12	7:g:18:TRP:CZ2	2.52	0.44
12:Z:23:PHE:HB3	12:Z:26:ARG:HB2	1.99	0.44
2:b:387:MET:HE1	18:b:847:BCR:H361	1.99	0.44
18:b:846:BCR:H24C	18:b:846:BCR:H371	1.85	0.44
7:g:15:TRP:CD1	21:g:103:LMG:HC1	2.53	0.44
18:g:102:BCR:H402	15:j:203:CLA:H51	2.00	0.44
15:A:833:CLA:HBB1	15:A:833:CLA:HMB3	2.00	0.44
2:B:22:TRP:CG	2:B:710:GLN:HE22	2.36	0.44
2:B:176:ASN:HB3	15:B:818:CLA:HMD2	2.00	0.44
2:B:653:TRP:CZ2	2:B:732:ILE:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:MET:HB2	3:C:79:LEU:HG	1.99	0.44
1:N:220:LEU:HD21	1:N:290:SER:HA	1.98	0.44
7:T:22:PRO:HB3	7:T:26:TYR:CZ	2.53	0.44
15:b:827:CLA:H41	15:b:827:CLA:H61	1.69	0.44
1:A:357:ALA:HB1	18:A:848:BCR:H312	2.00	0.44
1:A:674:ASN:HB2	2:B:658:LEU:HD11	1.99	0.44
1:A:705:ALA:HB1	18:A:850:BCR:C15	2.48	0.44
13:A:801:CL0:CGD	13:A:801:CL0:H8	2.48	0.44
15:A:812:CLA:H41	15:A:812:CLA:H61	1.56	0.44
15:b:808:CLA:H2	15:b:808:CLA:H61	1.73	0.44
15:A:809:CLA:H3A	15:A:809:CLA:HBA2	1.28	0.44
18:A:858:BCR:H341	8:J:24:VAL:HG22	1.99	0.44
18:L:209:BCR:H24C	18:L:209:BCR:H371	1.87	0.44
15:O:804:CLA:HHC	15:O:806:CLA:OBD	2.17	0.44
15:O:827:CLA:H111	15:O:827:CLA:H143	1.74	0.44
6:S:122:ASP:OD1	6:S:124:PRO:HD2	2.18	0.44
1:a:57:PHE:HD2	1:a:71:ILE:HD13	1.82	0.44
2:b:347:VAL:HG13	15:b:825:CLA:HED1	1.99	0.44
10:j:86:ARG:HA	10:j:92:ALA:HB2	2.00	0.44
1:A:298:ALA:HA	15:A:818:CLA:HMC2	2.00	0.43
1:A:360:SER:HA	1:A:411:GLY:HA2	1.99	0.43
1:A:445:SER:HB2	2:B:688:ALA:HB2	2.00	0.43
15:A:806:CLA:H8	18:A:847:BCR:H402	2.00	0.43
15:A:818:CLA:H141	15:A:818:CLA:H161	1.72	0.43
15:A:820:CLA:O2D	15:A:820:CLA:H2A	2.18	0.43
2:B:276:HIS:HB2	15:B:815:CLA:C1B	2.48	0.43
2:B:369:PHE:HB3	2:B:609:TRP:CZ3	2.53	0.43
15:N:833:CLA:HBB1	15:N:833:CLA:HMB3	2.00	0.43
2:O:536:VAL:HG11	2:O:589:TRP:CE2	2.53	0.43
6:S:136:TRP:CG	6:S:137:PRO:HD3	2.53	0.43
2:b:497:ALA:HB3	15:b:835:CLA:HED1	2.00	0.43
2:b:601:TRP:CD1	15:b:837:CLA:HBC2	2.53	0.43
1:A:72:PHE:CE2	1:A:76:PHE:HE2	2.36	0.43
15:A:838:CLA:H3A	15:A:838:CLA:HBA1	1.61	0.43
18:A:858:BCR:H341	18:A:858:BCR:H11C	1.80	0.43
2:B:457:VAL:HG22	8:J:37:GLN:HE22	1.84	0.43
15:B:802:CLA:H143	15:B:802:CLA:H111	1.81	0.43
15:B:803:CLA:H12	15:B:803:CLA:C4D	2.47	0.43
10:L:86:ARG:HA	10:L:92:ALA:HB2	2.00	0.43
1:N:402:TRP:HB3	15:N:829:CLA:HMC3	1.99	0.43
15:N:838:CLA:HBA1	15:N:838:CLA:H3A	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:857:BCR:H11C	18:N:857:BCR:H341	1.80	0.43
2:O:393:HIS:CE1	15:O:829:CLA:NA	2.86	0.43
19:W:1506:LHG:H322	15:b:804:CLA:H102	1.99	0.43
1:a:92:HIS:CE1	15:a:808:CLA:NA	2.87	0.43
1:a:172:LEU:HD12	1:a:172:LEU:HA	1.88	0.43
1:a:699:TYR:HB3	1:a:776:ALA:HB2	2.00	0.43
1:A:494:GLN:HG2	1:A:540:TRP:CD1	2.54	0.43
15:A:823:CLA:H61	15:A:823:CLA:H2	1.77	0.43
15:B:807:CLA:C1A	15:B:807:CLA:CGA	2.96	0.43
18:L:209:BCR:H382	10:W:156:MET:HG3	1.99	0.43
1:N:11:VAL:HG13	15:N:813:CLA:HED3	2.00	0.43
18:O:849:BCR:H24C	18:O:849:BCR:H371	1.90	0.43
4:Q:118:VAL:HG12	4:Q:120:ARG:HG2	2.00	0.43
2:b:356:MET:HE2	2:b:356:MET:HB3	1.83	0.43
15:b:808:CLA:C1A	15:b:808:CLA:CGA	2.96	0.43
15:b:809:CLA:H72	21:b:849:LMG:H273	1.99	0.43
15:b:825:CLA:H142	15:b:837:CLA:H101	2.00	0.43
15:b:829:CLA:H112	15:b:829:CLA:H93	1.75	0.43
1:A:447:LEU:HA	1:A:450:VAL:HG12	1.99	0.43
2:B:336:PHE:CE1	18:B:845:BCR:H291	2.54	0.43
11:M:30:TYR:CG	19:M:102:LHG:HC92	2.53	0.43
15:N:804:CLA:C1D	8:U:12:PRO:HG3	2.48	0.43
2:O:74:PHE:O	2:O:78:ILE:HG12	2.18	0.43
2:O:156:HIS:CE1	15:O:811:CLA:NA	2.87	0.43
18:S:202:BCR:H20C	18:S:202:BCR:H361	1.89	0.43
1:a:153:ASN:ND2	1:a:155:PHE:HB3	2.32	0.43
15:a:809:CLA:H93	15:a:809:CLA:H61	1.84	0.43
15:a:833:CLA:HBB1	15:a:833:CLA:HMB3	1.99	0.43
1:A:399:HIS:CE1	15:A:829:CLA:ND	2.86	0.43
15:A:821:CLA:H3A	15:A:821:CLA:HBA2	1.63	0.43
9:K:21:SER:O	9:K:24:VAL:HG22	2.18	0.43
11:M:14:VAL:O	11:M:18:PRO:HD2	2.18	0.43
15:N:810:CLA:HBD	15:N:810:CLA:HBA1	2.01	0.43
15:N:839:CLA:C4A	15:N:839:CLA:HBA2	2.47	0.43
15:O:816:CLA:H92	15:O:816:CLA:H61	1.79	0.43
15:O:838:CLA:H161	15:O:838:CLA:H141	1.75	0.43
1:a:280:LEU:HD21	1:a:381:PRO:HD2	2.01	0.43
2:b:287:ALA:HB2	15:b:819:CLA:HBC2	2.00	0.43
2:b:438:LEU:O	2:b:442:VAL:HG22	2.19	0.43
15:b:830:CLA:H42	19:l:102:LHG:H111	2.00	0.43
4:d:118:VAL:HG12	4:d:120:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:LEU:HD21	15:A:831:CLA:HBC1	2.00	0.43
15:A:809:CLA:H93	15:A:809:CLA:H61	1.81	0.43
1:N:674:ASN:HB2	2:O:658:LEU:HD11	2.01	0.43
15:N:841:CLA:HBA2	2:O:428:TRP:CD1	2.52	0.43
18:N:847:BCR:H361	18:N:847:BCR:H20C	1.79	0.43
2:O:443:HIS:CE1	14:O:833:F6C:NA	2.86	0.43
15:O:803:CLA:H202	15:O:803:CLA:H162	1.83	0.43
15:O:808:CLA:H2	15:O:808:CLA:H102	2.00	0.43
5:R:9:ARG:NH2	6:S:155:GLU:HG2	2.33	0.43
15:b:819:CLA:H162	15:b:819:CLA:H122	1.50	0.43
15:b:832:CLA:H62	15:b:832:CLA:H2	1.80	0.43
1:A:414:HIS:HA	1:A:417:ILE:HD12	1.99	0.43
2:B:69:ALA:HB2	2:B:135:LEU:HB2	2.01	0.43
2:B:93:ASP:OD1	2:B:95:GLN:HG2	2.18	0.43
15:N:811:CLA:H93	15:N:811:CLA:H61	1.85	0.43
15:O:830:CLA:H41	15:O:830:CLA:H62	1.55	0.43
15:O:835:CLA:HBA1	15:O:835:CLA:H3A	1.78	0.43
1:a:27:TRP:HA	15:a:812:CLA:H2	1.99	0.43
1:a:295:HIS:HB2	15:a:819:CLA:C1B	2.48	0.43
13:a:801:CL0:CGD	13:a:801:CL0:H8	2.49	0.43
15:b:803:CLA:CGA	15:b:803:CLA:H3A	2.49	0.43
15:b:803:CLA:H72	18:b:848:BCR:H363	2.00	0.43
18:b:843:BCR:H361	18:b:843:BCR:H20C	1.79	0.43
15:A:816:CLA:CBB	18:A:845:BCR:H382	2.49	0.43
2:B:78:ILE:HD12	2:B:125:TYR:CD1	2.53	0.43
15:B:801:CLA:H62	15:B:801:CLA:H102	1.81	0.43
15:B:804:CLA:HMB1	15:B:804:CLA:HBB1	2.01	0.43
3:C:26:LEU:HA	3:C:41:SER:O	2.17	0.43
15:O:809:CLA:HHB	14:O:810:F6C:CBB	2.49	0.43
1:a:738:LEU:HD11	18:f:203:BCR:H342	2.01	0.43
15:a:818:CLA:H193	15:a:822:CLA:HBC1	2.01	0.43
4:d:29:TYR:HB2	4:d:60:ILE:HG13	2.01	0.43
15:A:825:CLA:H51	15:A:825:CLA:H11	1.80	0.43
15:B:811:CLA:H11	15:B:811:CLA:H51	1.87	0.43
21:L:206:LMG:H342	21:T:103:LMG:HC61	2.01	0.43
1:N:436:THR:HA	1:N:439:HIS:CE1	2.54	0.43
2:O:347:VAL:HG13	15:O:825:CLA:HED1	2.01	0.43
2:O:398:TRP:HE1	18:O:847:BCR:H271	1.83	0.43
15:O:808:CLA:CGA	15:O:808:CLA:C1A	2.97	0.43
15:O:828:CLA:H3A	15:O:828:CLA:HBA2	1.65	0.43
1:a:364:VAL:HG21	18:a:849:BCR:H331	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:514:SER:HA	2:b:517:LEU:HD21	2.00	0.43
15:b:805:CLA:H61	15:b:805:CLA:H2	1.70	0.43
15:b:809:CLA:H11	15:b:809:CLA:HBA1	1.74	0.43
1:A:209:LEU:HG	15:A:816:CLA:CBB	2.49	0.43
15:A:831:CLA:H111	15:A:831:CLA:H142	1.68	0.43
2:B:532:LEU:O	2:B:536:VAL:HG23	2.19	0.43
15:N:807:CLA:H62	15:N:807:CLA:H41	1.52	0.43
18:N:857:BCR:H341	8:U:24:VAL:HG22	2.00	0.43
15:O:814:CLA:H142	15:O:814:CLA:H112	1.83	0.43
1:a:48:TRP:CD2	1:a:753:HIS:HE1	2.37	0.43
1:a:447:LEU:HB2	15:a:840:CLA:CBB	2.49	0.43
1:a:689:ILE:HG23	1:a:690:GLN:HG3	2.01	0.43
15:a:837:CLA:HBA2	15:a:837:CLA:H3A	1.66	0.43
15:b:804:CLA:HHC	15:b:806:CLA:OBD	2.19	0.43
15:f:201:CLA:H121	15:f:201:CLA:H8	1.88	0.43
1:A:75:HIS:NE2	15:A:806:CLA:ND	2.66	0.42
15:A:821:CLA:H62	15:A:821:CLA:H2	1.75	0.42
15:B:823:CLA:H3A	15:B:823:CLA:HBA2	1.71	0.42
15:B:828:CLA:H141	15:B:828:CLA:H162	1.75	0.42
15:N:804:CLA:H12	15:N:804:CLA:H51	1.87	0.42
15:N:820:CLA:H2	15:N:820:CLA:H61	1.76	0.42
2:O:669:MET:HB2	15:O:803:CLA:NC	2.34	0.42
15:O:830:CLA:H42	19:Z:102:LHG:H111	2.01	0.42
8:U:5:PHE:O	8:U:9:THR:HG23	2.19	0.42
2:b:667:SER:HB2	2:b:715:GLY:O	2.19	0.42
8:h:36:LEU:HD21	21:h:102:LMG:HC71	1.99	0.42
1:A:259:LEU:HD11	18:A:845:BCR:H291	1.99	0.42
1:A:608:PRO:HD3	2:B:568:GLY:HA2	2.00	0.42
2:B:536:VAL:O	2:B:540:VAL:HG23	2.19	0.42
18:B:843:BCR:H20C	18:B:843:BCR:H361	1.89	0.42
2:O:667:SER:HB2	2:O:715:GLY:O	2.19	0.42
1:a:178:HIS:CE1	15:a:811:CLA:NA	2.87	0.42
2:b:428:TRP:HZ3	15:b:839:CLA:HBC2	1.84	0.42
18:b:847:BCR:H24C	18:b:847:BCR:H371	1.88	0.42
3:c:58:CYS:HA	17:c:102:SF4:S4	2.59	0.42
8:h:26:LEU:HD13	18:h:101:BCR:HC7	2.01	0.42
15:j:202:CLA:H193	15:j:202:CLA:H162	1.79	0.42
1:A:171:MET:HE1	15:A:814:CLA:H92	2.01	0.42
15:A:830:CLA:H143	15:A:830:CLA:H111	1.86	0.42
6:F:122:ASP:OD1	6:F:124:PRO:HD2	2.20	0.42
2:O:488:ILE:HG12	15:O:835:CLA:HMD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:816:CLA:CBB	18:a:845:BCR:H382	2.49	0.42
15:a:821:CLA:H3A	15:a:821:CLA:HBA2	1.62	0.42
21:a:855:LMG:H182	21:a:855:LMG:H211	1.92	0.42
1:A:460:ALA:HB3	15:A:835:CLA:HAB	2.02	0.42
1:A:686:ALA:HA	1:A:689:ILE:HG22	2.02	0.42
15:A:813:CLA:HBC1	15:A:814:CLA:H142	2.01	0.42
2:B:523:ASP:HA	2:B:526:VAL:HG12	2.01	0.42
15:O:825:CLA:HBA2	15:O:825:CLA:H3A	1.72	0.42
15:O:839:CLA:H93	15:O:839:CLA:H62	1.71	0.42
2:b:319:PHE:HD2	15:b:823:CLA:HMA1	1.84	0.42
2:b:652:ILE:HD13	15:b:809:CLA:CHD	2.48	0.42
1:A:687:GLN:HG2	1:A:780:ALA:HB3	2.01	0.42
7:I:34:ALA:HB1	10:L:113:ILE:HG21	2.01	0.42
9:K:88:LEU:HB2	9:K:91:LEU:HA	2.02	0.42
2:O:623:LEU:HD12	15:O:802:CLA:H11	2.01	0.42
15:O:807:CLA:H92	15:O:807:CLA:HMC1	2.00	0.42
15:O:816:CLA:HMB3	15:O:816:CLA:HBB1	2.02	0.42
15:O:839:CLA:H161	15:Z:103:CLA:HMC2	2.01	0.42
1:a:708:PHE:CD2	18:a:850:BCR:H363	2.54	0.42
15:a:814:CLA:H102	15:a:814:CLA:H61	1.60	0.42
15:b:805:CLA:HMB1	15:b:805:CLA:HBB1	2.00	0.42
15:b:806:CLA:HMD3	15:b:808:CLA:H201	2.00	0.42
15:b:839:CLA:H161	15:l:103:CLA:HMC2	2.01	0.42
4:d:91:ASN:OD1	4:d:93:GLU:HG2	2.19	0.42
5:e:13:ARG:NH2	6:f:161:ARG:H	2.18	0.42
1:A:75:HIS:CD2	15:A:806:CLA:NA	2.88	0.42
1:A:89:MET:SD	15:A:809:CLA:HAA2	2.59	0.42
1:A:441:ASP:H	4:D:16:THR:HG21	1.85	0.42
15:A:818:CLA:H151	15:A:818:CLA:H111	1.55	0.42
15:B:823:CLA:H142	15:B:835:CLA:H101	2.01	0.42
15:B:837:CLA:H151	12:X:33:LEU:HB3	2.02	0.42
1:N:75:HIS:NE2	15:N:806:CLA:NA	2.68	0.42
1:N:370:SER:HB3	1:N:404:ALA:HB2	2.02	0.42
13:N:801:CL0:CGD	13:N:801:CL0:H8	2.49	0.42
15:N:807:CLA:H193	15:N:807:CLA:H161	1.86	0.42
15:N:810:CLA:H61	18:N:857:BCR:H363	2.01	0.42
15:N:835:CLA:H92	15:N:835:CLA:H61	1.87	0.42
2:O:106:ARG:NH2	2:O:115:ILE:HG12	2.34	0.42
15:O:806:CLA:HMD3	15:O:808:CLA:H201	2.01	0.42
15:O:825:CLA:H142	15:O:837:CLA:H101	2.01	0.42
1:a:607:GLY:HA2	2:b:569:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:674:ASN:HB2	2:b:658:LEU:HD11	2.01	0.42
2:b:118:SER:HA	15:b:827:CLA:HMA2	2.00	0.42
2:b:309:SER:O	15:b:822:CLA:HAA1	2.19	0.42
1:A:51:HIS:CE1	15:A:804:CLA:ND	2.87	0.42
1:A:373:VAL:O	1:A:377:MET:HB2	2.19	0.42
15:A:804:CLA:C1D	8:J:12:PRO:HG3	2.50	0.42
2:B:199:ILE:HD13	2:B:271:THR:HG22	2.01	0.42
15:B:805:CLA:H61	15:B:805:CLA:H41	1.46	0.42
18:F:203:BCR:H20C	18:F:203:BCR:H361	1.88	0.42
1:N:361:ILE:HD11	18:N:848:BCR:HC7	2.01	0.42
15:N:822:CLA:NC	15:N:822:CLA:H52	2.35	0.42
2:O:287:ALA:HB2	15:O:819:CLA:HBC2	2.01	0.42
15:O:821:CLA:HBA1	15:O:821:CLA:H3A	1.84	0.42
15:a:810:CLA:H61	15:a:810:CLA:H92	1.83	0.42
11:k:30:TYR:CG	19:k:101:LHG:HC92	2.54	0.42
1:A:383:TYR:HD2	1:A:386:LEU:HD22	1.85	0.42
21:A:855:LMG:H182	21:A:855:LMG:H211	1.87	0.42
2:B:536:VAL:HG11	2:B:589:TRP:CE2	2.55	0.42
15:B:808:CLA:H18	15:B:825:CLA:H71	2.02	0.42
15:B:832:CLA:H52	15:B:832:CLA:H12	1.82	0.42
18:F:203:BCR:H382	15:X:103:CLA:HBA2	2.02	0.42
1:N:581:PHE:HA	18:N:849:BCR:HC22	2.02	0.42
15:N:814:CLA:H102	15:N:814:CLA:H61	1.58	0.42
15:N:820:CLA:HBA2	15:N:820:CLA:H3A	1.53	0.42
2:O:193:HIS:HE1	15:O:814:CLA:C1A	2.32	0.42
15:O:829:CLA:H93	15:O:829:CLA:H112	1.75	0.42
15:a:807:CLA:H62	15:a:807:CLA:H41	1.53	0.42
1:A:71:ILE:HD12	15:A:806:CLA:C2C	2.50	0.42
1:A:445:SER:HB3	2:B:684:THR:HG22	2.00	0.42
15:A:820:CLA:H2	15:A:820:CLA:H61	1.77	0.42
18:A:846:BCR:H20C	18:A:846:BCR:H361	1.80	0.42
2:B:254:ILE:HG13	2:B:255:LEU:HG	2.01	0.42
9:K:91:LEU:HD22	15:O:815:CLA:HAA2	2.00	0.42
1:N:405:GLY:HA3	1:N:633:LEU:HD21	2.01	0.42
1:N:738:LEU:HD11	18:S:202:BCR:H342	2.02	0.42
15:N:810:CLA:H11	15:N:810:CLA:H52	1.77	0.42
15:N:818:CLA:H141	15:N:818:CLA:H161	1.73	0.42
2:O:590:MET:HG2	15:O:825:CLA:HBC1	2.02	0.42
15:O:809:CLA:H72	21:O:850:LMG:H273	2.01	0.42
15:a:820:CLA:H3A	15:a:820:CLA:HBA2	1.51	0.42
15:a:842:CLA:H3A	15:a:842:CLA:HBA2	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:121:TYR:HB2	24:b:952:HOH:O	2.19	0.42
2:b:176:ASN:HB3	15:b:820:CLA:HMD2	2.01	0.42
6:F:51:PHE:O	6:F:55:PHE:HB2	2.20	0.42
1:N:27:TRP:CD1	15:N:812:CLA:H2	2.55	0.42
1:N:202:GLY:HA3	15:N:814:CLA:HBB1	2.01	0.42
15:N:819:CLA:H3A	15:N:819:CLA:HBA2	1.54	0.42
2:O:309:SER:O	15:O:822:CLA:HAA1	2.20	0.42
15:O:817:CLA:HBA2	15:O:817:CLA:H3A	1.51	0.42
1:a:71:ILE:HG22	1:a:75:HIS:CE1	2.55	0.42
1:a:444:ILE:HG13	1:a:586:PHE:HE2	1.85	0.42
15:a:805:CLA:HBA2	15:a:805:CLA:H3A	1.62	0.42
2:b:193:HIS:HE1	15:b:814:CLA:C1A	2.32	0.42
2:b:527:HIS:CG	15:b:838:CLA:HED3	2.55	0.42
1:A:225:LEU:O	1:A:230:VAL:HG22	2.19	0.41
15:A:841:CLA:HED2	2:B:424:SER:HB2	2.01	0.41
2:B:196:HIS:CE1	15:B:813:CLA:NA	2.88	0.41
2:B:443:HIS:CE1	14:B:831:F6C:NA	2.88	0.41
11:M:23:PHE:CE2	10:j:43:LEU:HD22	2.55	0.41
1:N:225:LEU:O	1:N:230:VAL:HG22	2.20	0.41
1:N:708:PHE:CD2	18:N:850:BCR:H363	2.54	0.41
15:N:818:CLA:H193	15:N:822:CLA:HBC1	2.01	0.41
15:N:837:CLA:H3A	15:N:837:CLA:HBA2	1.59	0.41
15:N:838:CLA:H61	15:N:838:CLA:H41	1.60	0.41
18:N:857:BCR:H15C	18:N:857:BCR:H351	1.80	0.41
2:O:377:THR:HG23	2:O:598:THR:HG21	2.02	0.41
15:O:813:CLA:H51	15:O:813:CLA:H11	1.85	0.41
15:O:837:CLA:H52	15:O:837:CLA:H8	1.91	0.41
18:O:845:BCR:H24C	18:O:845:BCR:H371	1.89	0.41
3:P:61:ASP:HA	3:P:62:PHE:HA	1.82	0.41
10:W:172:LEU:HD22	10:j:94:LEU:HD21	2.02	0.41
1:a:209:LEU:HG	15:a:816:CLA:CBB	2.50	0.41
15:a:804:CLA:C1D	8:h:12:PRO:HG3	2.49	0.41
15:a:822:CLA:NC	15:a:822:CLA:H52	2.35	0.41
15:b:809:CLA:HHB	14:b:810:F6C:CBB	2.50	0.41
1:A:57:PHE:HD2	1:A:71:ILE:HD13	1.85	0.41
1:A:402:TRP:HB3	15:A:829:CLA:HMC3	2.02	0.41
1:A:735:HIS:HE1	15:A:841:CLA:C4D	2.34	0.41
15:A:807:CLA:H193	15:A:807:CLA:H161	1.83	0.41
2:B:142:LEU:HG	18:B:843:BCR:H382	2.02	0.41
2:B:667:SER:HB2	2:B:715:GLY:O	2.20	0.41
4:D:38:GLU:HA	4:D:51:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:15:TRP:HB2	21:j:206:LMG:H372	2.01	0.41
15:L:203:CLA:H91	15:L:203:CLA:H111	1.77	0.41
1:N:399:HIS:CE1	15:N:829:CLA:ND	2.89	0.41
1:N:566:HIS:CG	15:N:839:CLA:HED3	2.55	0.41
15:N:828:CLA:H13	18:N:848:BCR:H362	2.01	0.41
15:N:834:CLA:H2	15:N:834:CLA:H61	1.76	0.41
15:O:808:CLA:H2	15:O:808:CLA:H61	1.67	0.41
7:T:14:SER:O	7:T:17:PRO:HD2	2.21	0.41
1:a:75:HIS:NE2	15:a:806:CLA:NA	2.68	0.41
15:a:806:CLA:H61	18:a:847:BCR:H24C	2.02	0.41
15:a:828:CLA:H141	15:a:828:CLA:H161	1.88	0.41
15:a:841:CLA:H18	15:f:201:CLA:H61	2.01	0.41
2:b:393:HIS:CE1	15:b:829:CLA:NA	2.88	0.41
6:f:122:ASP:OD1	6:f:124:PRO:HD2	2.20	0.41
18:j:201:BCR:H24C	18:j:201:BCR:H371	1.87	0.41
15:A:819:CLA:H162	15:A:819:CLA:H203	1.84	0.41
15:A:820:CLA:CAD	15:A:830:CLA:H41	2.51	0.41
15:A:841:CLA:H2	15:A:841:CLA:H61	1.69	0.41
15:B:817:CLA:H61	15:B:821:CLA:H43	2.02	0.41
15:B:836:CLA:H3A	15:B:836:CLA:HBA2	1.91	0.41
15:N:803:CLA:O1A	2:O:431:LEU:HA	2.21	0.41
15:N:803:CLA:O2A	2:O:434:GLY:HA3	2.20	0.41
2:O:50:HIS:NE2	15:O:805:CLA:NA	2.68	0.41
2:O:196:HIS:CE1	15:O:815:CLA:NA	2.88	0.41
2:O:387:MET:HE1	18:O:847:BCR:H361	2.03	0.41
15:a:820:CLA:CAD	15:a:830:CLA:H41	2.50	0.41
2:b:460:GLU:HB3	2:b:462:VAL:HG13	2.02	0.41
18:A:845:BCR:H343	9:K:69:ALA:HB1	2.02	0.41
15:B:837:CLA:HBB1	15:B:837:CLA:HMB3	2.03	0.41
18:B:845:BCR:H24C	18:B:845:BCR:H371	1.90	0.41
1:N:332:MET:HB2	1:N:337:ASN:OD1	2.21	0.41
15:N:827:CLA:H3A	15:N:827:CLA:HBA2	1.82	0.41
15:O:803:CLA:H143	15:O:803:CLA:H111	1.94	0.41
1:a:318:HIS:CE1	15:a:823:CLA:NA	2.88	0.41
1:a:566:HIS:CG	15:a:839:CLA:HED3	2.55	0.41
15:a:827:CLA:HBA2	15:a:827:CLA:H3A	1.81	0.41
15:a:834:CLA:HMA1	18:g:101:BCR:H292	2.03	0.41
15:b:822:CLA:H62	15:b:822:CLA:H41	1.94	0.41
16:b:842:PQN:H142	18:b:848:BCR:H271	2.03	0.41
1:A:89:MET:N	1:A:89:MET:HE2	2.35	0.41
15:A:841:CLA:HBA2	2:B:428:TRP:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:847:BCR:H361	18:A:847:BCR:H20C	1.80	0.41
2:B:156:HIS:CE1	15:B:809:CLA:NA	2.88	0.41
15:B:809:CLA:H162	15:B:809:CLA:H122	1.74	0.41
15:B:827:CLA:H62	15:B:827:CLA:H41	1.76	0.41
15:N:810:CLA:H61	15:N:810:CLA:H92	1.86	0.41
15:N:821:CLA:H3A	15:N:821:CLA:HBA2	1.61	0.41
4:Q:120:ARG:HD2	4:Q:124:SER:HB2	2.03	0.41
1:a:705:ALA:HB2	15:b:802:CLA:H71	2.01	0.41
18:a:857:BCR:H15C	18:a:857:BCR:H351	1.82	0.41
2:b:156:HIS:CE1	15:b:811:CLA:NA	2.89	0.41
2:b:257:PHE:HD1	15:b:817:CLA:CMB	2.34	0.41
2:b:336:PHE:CE1	18:b:847:BCR:H291	2.55	0.41
15:b:821:CLA:H3A	15:b:821:CLA:HBA1	1.79	0.41
15:b:827:CLA:H143	15:b:827:CLA:H111	1.72	0.41
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.93	0.41
15:A:805:CLA:HBA2	15:A:805:CLA:H3A	1.59	0.41
2:B:527:HIS:CG	15:B:836:CLA:HED3	2.56	0.41
6:F:58:TYR:O	6:F:62:GLU:HB2	2.20	0.41
18:M:101:BCR:H24C	18:M:101:BCR:H371	1.92	0.41
1:N:92:HIS:CE1	15:N:808:CLA:NA	2.88	0.41
2:O:419:LYS:HE2	6:S:161:ARG:HH11	1.85	0.41
2:O:652:ILE:HG12	15:O:808:CLA:HAC1	2.02	0.41
15:O:834:CLA:H12	15:O:834:CLA:H52	1.80	0.41
6:S:93:VAL:O	6:S:97:ILE:HG13	2.21	0.41
15:a:822:CLA:H92	15:a:822:CLA:H61	1.80	0.41
15:b:826:CLA:H112	15:b:826:CLA:H72	1.62	0.41
1:A:447:LEU:HB2	15:A:840:CLA:CBB	2.51	0.41
1:A:712:PHE:HZ	15:A:842:CLA:HBC2	1.86	0.41
15:A:837:CLA:H3A	15:A:837:CLA:HBA2	1.60	0.41
2:B:68:VAL:HG11	2:B:124:TRP:HZ3	1.85	0.41
2:B:93:ASP:C	7:I:7:LEU:HD11	2.46	0.41
7:I:16:LEU:HD23	7:I:16:LEU:HA	1.96	0.41
15:N:821:CLA:H2	15:N:821:CLA:H62	1.76	0.41
3:P:58:CYS:HA	17:P:102:SF4:S4	2.60	0.41
1:a:140:SER:HA	15:a:829:CLA:HMA2	2.03	0.41
1:a:298:ALA:HA	15:a:818:CLA:HMC2	2.01	0.41
2:b:50:HIS:NE2	15:b:805:CLA:NA	2.68	0.41
2:b:488:ILE:HG12	15:b:835:CLA:HMD3	2.02	0.41
2:b:592:ASN:HB2	15:b:802:CLA:HBC2	2.02	0.41
15:b:807:CLA:HHB	15:b:808:CLA:HHB	2.02	0.41
15:b:813:CLA:H91	15:b:824:CLA:H43	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:818:CLA:HBA2	15:b:818:CLA:H3A	1.43	0.41
15:A:821:CLA:H92	15:A:821:CLA:H61	1.92	0.41
2:B:686:VAL:HG13	2:B:699:TRP:CH2	2.56	0.41
18:B:846:BCR:H20C	18:B:846:BCR:H361	1.87	0.41
1:N:686:ALA:HA	1:N:689:ILE:HG22	2.02	0.41
1:a:295:HIS:CE1	15:a:819:CLA:ND	2.89	0.41
15:a:803:CLA:O1A	2:b:431:LEU:HA	2.21	0.41
15:a:819:CLA:H152	15:a:819:CLA:H112	1.73	0.41
2:b:623:LEU:HD12	15:b:802:CLA:H11	2.01	0.41
15:b:817:CLA:HBA2	15:b:817:CLA:H3A	1.36	0.41
15:b:830:CLA:O1A	12:l:26:ARG:HD3	2.20	0.41
1:A:51:HIS:HE1	15:A:804:CLA:C4D	2.34	0.41
1:A:259:LEU:HD11	18:A:845:BCR:H391	2.03	0.41
1:A:614:CYS:HB3	2:B:674:TRP:HE3	1.86	0.41
1:A:740:VAL:HG23	6:F:102:ARG:HA	2.02	0.41
15:A:806:CLA:H2	15:A:806:CLA:H62	1.71	0.41
15:A:810:CLA:HBA1	15:A:810:CLA:HBD	2.02	0.41
15:A:827:CLA:CHB	15:A:840:CLA:HAA2	2.51	0.41
15:A:842:CLA:H192	18:A:850:BCR:H401	2.02	0.41
2:B:276:HIS:HB2	15:B:815:CLA:CHB	2.50	0.41
15:B:821:CLA:HMB1	15:B:821:CLA:HBB1	2.02	0.41
4:D:43:MET:HE1	4:D:58:LEU:HD11	2.02	0.41
18:I:102:BCR:H24C	18:I:102:BCR:H371	1.94	0.41
15:N:808:CLA:HBB1	15:N:808:CLA:HMB1	2.02	0.41
15:N:819:CLA:HBB1	15:N:819:CLA:H92	2.03	0.41
15:N:820:CLA:CHB	15:N:820:CLA:H12	2.51	0.41
18:T:102:BCR:H402	15:W:1502:CLA:H51	2.03	0.41
15:V:102:CLA:HBA2	15:V:102:CLA:H3A	1.64	0.41
1:a:100:GLU:HG3	1:a:154:THR:HG23	2.03	0.41
1:a:276:PHE:HD1	15:a:819:CLA:HMB2	1.84	0.41
1:a:629:MET:HE3	1:a:629:MET:HB3	2.01	0.41
1:a:738:LEU:HD13	18:f:203:BCR:H321	2.01	0.41
15:a:803:CLA:O2A	2:b:434:GLY:HA3	2.21	0.41
15:a:822:CLA:H112	15:a:822:CLA:H152	1.94	0.41
15:A:803:CLA:O1A	2:B:431:LEU:HA	2.21	0.41
2:B:326:LEU:O	2:B:330:ILE:HD12	2.21	0.41
2:B:583:SER:O	2:B:587:VAL:HG23	2.21	0.41
4:D:28:LYS:HB3	4:D:28:LYS:HE2	1.82	0.41
15:N:827:CLA:CHB	15:N:840:CLA:HAA2	2.51	0.41
18:O:843:BCR:H361	18:O:843:BCR:H20C	1.77	0.41
15:S:201:CLA:H141	15:S:201:CLA:H162	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ASN:HD22	1:A:671:ILE:HB	1.86	0.40
18:A:850:BCR:H20C	18:A:850:BCR:H361	1.92	0.40
2:B:257:PHE:HD1	15:B:815:CLA:CMB	2.34	0.40
15:B:802:CLA:H3A	15:B:802:CLA:CGA	2.51	0.40
19:X:101:LHG:H361	19:X:101:LHG:H332	1.89	0.40
1:N:209:LEU:HG	15:N:816:CLA:CBB	2.51	0.40
1:N:444:ILE:HB	2:O:684:THR:HG21	2.03	0.40
2:O:257:PHE:HD1	15:O:817:CLA:HMB3	1.87	0.40
2:O:592:ASN:HB2	15:O:802:CLA:HBC2	2.03	0.40
15:O:830:CLA:H72	15:O:830:CLA:H111	1.75	0.40
15:O:830:CLA:O1A	12:Z:26:ARG:HD3	2.22	0.40
1:a:686:ALA:HA	1:a:689:ILE:HG22	2.02	0.40
2:b:378:HIS:HB2	15:b:827:CLA:C1B	2.51	0.40
1:A:75:HIS:NE2	15:A:806:CLA:NA	2.69	0.40
1:A:225:LEU:HD12	1:A:235:ILE:HG23	2.03	0.40
1:A:566:HIS:CG	15:A:839:CLA:HED3	2.56	0.40
15:A:812:CLA:H42	8:J:7:TYR:CE2	2.56	0.40
2:B:638:LEU:HD21	2:B:657:PHE:CD1	2.55	0.40
2:B:706:LEU:HD22	2:B:710:GLN:NE2	2.36	0.40
15:B:819:CLA:H3A	15:B:819:CLA:HBA1	1.81	0.40
15:B:828:CLA:H41	15:B:828:CLA:H62	1.49	0.40
15:B:833:CLA:HBA1	15:B:833:CLA:H3A	1.85	0.40
10:L:65:LEU:O	10:L:69:MET:HG3	2.21	0.40
1:N:118:SER:HB3	6:S:49:TYR:CE1	2.57	0.40
1:N:607:GLY:HA2	2:O:569:PRO:HD3	2.03	0.40
1:N:614:CYS:HB2	2:O:674:TRP:HB3	2.03	0.40
15:N:803:CLA:HBA1	15:N:803:CLA:H3A	1.79	0.40
15:N:806:CLA:H8	18:N:847:BCR:H402	2.04	0.40
18:O:845:BCR:H20C	18:O:845:BCR:H361	1.89	0.40
2:b:326:LEU:O	2:b:330:ILE:HD12	2.21	0.40
2:b:377:THR:HG23	2:b:598:THR:HG21	2.03	0.40
2:b:727:TYR:HB2	15:b:801:CLA:HED3	2.02	0.40
18:b:845:BCR:H20C	18:b:845:BCR:H361	1.89	0.40
4:d:85:ILE:HB	4:d:98:HIS:HB3	2.02	0.40
1:A:575:VAL:HG11	1:A:628:TRP:CZ2	2.56	0.40
1:A:620:ASP:HA	1:A:623:PHE:HB3	2.03	0.40
1:A:761:HIS:CE1	15:A:842:CLA:NA	2.89	0.40
15:A:828:CLA:H141	15:A:828:CLA:H161	1.88	0.40
15:B:811:CLA:H102	15:B:816:CLA:H92	2.03	0.40
4:D:118:VAL:HG12	4:D:120:ARG:HG2	2.03	0.40
15:F:201:CLA:H162	15:F:201:CLA:H141	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:14:SER:O	7:I:17:PRO:HD2	2.22	0.40
15:X:103:CLA:H62	15:X:103:CLA:H41	1.91	0.40
1:N:441:ASP:HB2	4:Q:16:THR:OG1	2.21	0.40
15:N:823:CLA:H61	15:N:823:CLA:H2	1.80	0.40
2:O:601:TRP:CD1	15:O:837:CLA:HBC2	2.56	0.40
7:T:15:TRP:CD1	21:T:103:LMG:HC1	2.56	0.40
8:U:24:VAL:O	8:U:28:MET:HG2	2.22	0.40
1:a:268:GLY:H	9:i:17:THR:HG21	1.86	0.40
1:a:295:HIS:HB2	15:a:819:CLA:CHB	2.51	0.40
1:a:361:ILE:HD11	18:a:848:BCR:HC7	2.04	0.40
1:a:460:ALA:HB1	15:a:835:CLA:HMC1	2.03	0.40
15:a:834:CLA:H61	15:a:834:CLA:H2	1.78	0.40
2:b:196:HIS:CE1	15:b:815:CLA:NA	2.90	0.40
2:b:706:LEU:HD22	2:b:710:GLN:NE2	2.36	0.40
15:b:821:CLA:C3D	18:b:843:BCR:H393	2.52	0.40
15:A:810:CLA:H52	15:A:810:CLA:H11	1.79	0.40
15:A:828:CLA:H41	15:A:828:CLA:H62	1.87	0.40
2:B:193:HIS:HE1	15:B:812:CLA:C1A	2.33	0.40
6:F:42:MET:HG3	6:F:55:PHE:HB3	2.03	0.40
1:N:218:VAL:HG13	1:N:238:PRO:HB3	2.04	0.40
1:N:447:LEU:HB2	15:N:840:CLA:CBB	2.51	0.40
2:O:626:TRP:O	2:O:630:TYR:HB3	2.22	0.40
15:O:821:CLA:HBA2	18:O:843:BCR:H282	2.02	0.40
15:a:820:CLA:H2	15:a:820:CLA:H61	1.73	0.40
15:b:830:CLA:H162	15:b:830:CLA:H141	1.76	0.40
1:A:771:TRP:CE2	1:A:775:LEU:HD22	2.57	0.40
15:A:809:CLA:O1A	15:A:829:CLA:H2	2.21	0.40
15:B:812:CLA:HMA2	18:B:843:BCR:H292	2.03	0.40
15:B:830:CLA:H62	15:B:830:CLA:H2	1.79	0.40
18:I:101:BCR:H382	18:I:101:BCR:H23C	2.04	0.40
18:O:844:BCR:H23C	18:O:844:BCR:H382	2.03	0.40
12:Z:28:ILE:HD13	12:Z:28:ILE:HA	1.90	0.40
15:a:810:CLA:HBA1	15:a:810:CLA:HBD	2.02	0.40
15:a:821:CLA:HBB1	18:i:101:BCR:H342	2.02	0.40
15:a:823:CLA:H3A	15:a:823:CLA:HBA1	1.76	0.40
2:b:470:ALA:O	2:b:482:LEU:HB2	2.22	0.40
18:j:201:BCR:H20C	18:j:201:BCR:H361	1.91	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%)	730 (98%)	19 (2%)	0	100	100
1	N	749/782 (96%)	736 (98%)	13 (2%)	0	100	100
1	a	749/782 (96%)	735 (98%)	14 (2%)	0	100	100
2	B	737/740 (100%)	723 (98%)	14 (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%)	76 (97%)	2 (3%)	0	100	100
3	P	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
4	Q	137/142 (96%)	134 (98%)	3 (2%)	0	100	100
4	d	137/142 (96%)	136 (99%)	1 (1%)	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%)	131 (97%)	4 (3%)	0	100	100
6	f	135/161 (84%)	131 (97%)	4 (3%)	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%)	70 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	V	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
9	i	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
10	L	170/183 (93%)	170 (100%)	0	0	100	100
10	W	170/183 (93%)	170 (100%)	0	0	100	100
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%)	25 (93%)	2 (7%)	0	100	100
12	Z	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
12	l	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
All	All	6840/7179 (95%)	6715 (98%)	125 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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 (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	665	ASN
2	B	76	GLN
2	B	111	ASN
2	B	156	HIS
2	B	196	HIS
2	B	248	GLN
2	B	443	HIS
2	B	605	HIS
8	J	37	GLN
10	L	148	ASN
10	L	181	ASN
12	X	37	ASN
1	N	134	HIS
1	N	178	HIS
1	N	269	GLN
2	O	76	GLN
2	O	95	GLN
2	O	156	HIS
2	O	196	HIS
2	O	235	GLN
2	O	443	HIS
4	Q	95	GLN
4	Q	137	GLN
6	S	52	ASN
6	S	142	GLN
10	W	50	ASN
10	W	140	ASN
10	W	146	GLN
10	W	148	ASN
10	W	181	ASN
12	Z	37	ASN
1	a	153	ASN
1	a	239	HIS
1	a	269	GLN
1	a	294	HIS
1	a	665	ASN
2	b	76	GLN
2	b	95	GLN
2	b	111	ASN
2	b	193	HIS
2	b	196	HIS
2	b	235	GLN
2	b	443	HIS

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Mol	Chain	Res	Type
2	b	615	GLN
4	d	53	GLN
4	d	81	ASN
4	d	95	GLN
5	e	19	GLN
6	f	39	GLN
6	f	44	ASN
6	f	52	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	821	2	59,63,73	1.30	8 (13%)	70,101,113	1.23	6 (8%)
18	BCR	g	101	-	41,41,41	0.32	0	56,56,56	0.70	0
22	LFA	L	208	-	14,14,19	0.23	0	13,13,18	0.23	0
15	CLA	N	816	1	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	N	827	24	59,63,73	1.25	8 (13%)	70,101,113	1.37	8 (11%)
15	CLA	a	807	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
15	CLA	N	829	1	64,68,73	1.20	7 (10%)	76,107,113	1.26	7 (9%)
15	CLA	b	837	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
15	CLA	F	201	24	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	B	816	2	64,68,73	1.20	8 (12%)	76,107,113	1.23	4 (5%)
15	CLA	a	823	1	60,64,73	1.25	8 (13%)	71,102,113	1.35	5 (7%)
15	CLA	j	202	10	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
15	CLA	B	829	2	69,73,73	1.16	7 (10%)	82,113,113	1.25	6 (7%)
18	BCR	N	848	-	41,41,41	0.31	0	56,56,56	0.54	0
15	CLA	A	808	1	49,53,73	1.38	8 (16%)	58,89,113	1.45	6 (10%)
15	CLA	b	802	24	69,73,73	1.16	7 (10%)	82,113,113	1.21	6 (7%)
17	SF4	C	101	3	0,12,12	-	-	-	-	-
22	LFA	f	204	-	15,15,19	0.23	0	14,14,18	0.19	0
15	CLA	A	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	7 (8%)
15	CLA	N	836	1	58,62,73	1.27	8 (13%)	68,99,113	1.35	6 (8%)
15	CLA	a	806	1	69,73,73	1.16	7 (10%)	82,113,113	1.26	6 (7%)
15	CLA	N	815	1	59,63,73	1.27	8 (13%)	70,101,113	1.34	5 (7%)
15	CLA	A	813	1	58,62,73	1.27	7 (12%)	68,99,113	1.37	7 (10%)
18	BCR	O	849	-	41,41,41	0.29	0	56,56,56	0.60	0
18	BCR	a	857	-	41,41,41	0.38	0	56,56,56	1.29	8 (14%)
18	BCR	O	844	-	41,41,41	0.31	0	56,56,56	0.68	0
20	LMT	A	854	-	36,36,36	0.55	0	47,47,47	0.63	0
14	F6C	O	810	2	72,74,74	1.60	8 (11%)	83,114,114	1.97	13 (15%)
22	LFA	j	208	-	14,14,19	0.23	0	13,13,18	0.23	0
15	CLA	A	856	24	69,73,73	1.16	8 (11%)	82,113,113	1.22	6 (7%)
15	CLA	N	822	24	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
22	LFA	W	1507	-	14,14,19	0.23	0	13,13,18	0.23	0
15	CLA	N	838	1	59,63,73	1.25	8 (13%)	70,101,113	1.32	5 (7%)
15	CLA	O	820	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
15	CLA	a	808	1	49,53,73	1.38	8 (16%)	58,89,113	1.45	6 (10%)
15	CLA	N	805	15,1	64,68,73	1.21	7 (10%)	76,107,113	1.29	5 (6%)
21	LMG	O	850	-	55,55,55	0.50	0	63,63,63	0.59	0
15	CLA	a	829	1	64,68,73	1.20	7 (10%)	76,107,113	1.26	7 (9%)
21	LMG	a	855	-	44,44,55	0.53	0	52,52,63	0.61	0
15	CLA	N	817	24	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
15	CLA	a	832	1	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	a	831	1	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
15	CLA	a	811	1	61,65,73	1.23	6 (9%)	72,103,113	1.31	6 (8%)
15	CLA	B	804	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	6 (7%)
15	CLA	N	812	15,1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	A	816	1	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
20	LMT	N	854	-	36,36,36	0.55	0	47,47,47	0.63	0
15	CLA	A	806	1	69,73,73	1.16	7 (10%)	82,113,113	1.26	7 (8%)
18	BCR	F	203	-	41,41,41	0.30	0	56,56,56	0.50	0
15	CLA	b	827	2	66,70,73	1.18	9 (13%)	78,109,113	1.26	5 (6%)
15	CLA	O	817	2	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
19	LHG	l	101	-	43,43,48	0.54	0	46,49,54	0.51	0
18	BCR	N	845	-	41,41,41	0.35	0	56,56,56	0.93	0
15	CLA	A	833	1	59,63,73	1.25	8 (13%)	70,101,113	1.34	6 (8%)
18	BCR	T	101	-	41,41,41	0.32	0	56,56,56	0.72	0
18	BCR	N	849	-	41,41,41	0.32	0	56,56,56	0.58	0
15	CLA	O	830	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
18	BCR	a	849	-	41,41,41	0.31	0	56,56,56	0.58	0
21	LMG	W	1505	-	50,50,55	0.50	0	58,58,63	0.59	0
20	LMT	a	852	-	32,32,36	0.57	0	43,43,47	0.69	0
15	CLA	A	840	1	54,58,73	1.30	8 (14%)	64,95,113	1.40	6 (9%)
18	BCR	g	102	-	41,41,41	0.29	0	56,56,56	0.49	0
18	BCR	O	845	-	41,41,41	0.30	0	56,56,56	0.47	0
15	CLA	N	823	1	60,64,73	1.25	8 (13%)	71,102,113	1.34	5 (7%)
15	CLA	N	842	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
15	CLA	O	828	2	69,73,73	1.15	8 (11%)	82,113,113	1.24	8 (9%)
15	CLA	B	813	2	49,53,73	1.37	6 (12%)	58,89,113	1.45	6 (10%)
17	SF4	N	844	2,1	0,12,12	-	-	-	-	-
15	CLA	N	809	1	64,68,73	1.20	8 (12%)	76,107,113	1.28	6 (7%)
22	LFA	O	851	-	15,15,19	0.23	0	14,14,18	0.19	0
14	F6C	b	833	2	72,74,74	1.59	9 (12%)	83,114,114	2.03	16 (19%)
15	CLA	a	813	1	58,62,73	1.27	7 (12%)	68,99,113	1.37	7 (10%)
19	LHG	L	207	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	A	841	1	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
16	PQN	O	842	-	34,34,34	0.36	0	43,45,45	0.63	1 (2%)
15	CLA	N	833	1	59,63,73	1.26	8 (13%)	70,101,113	1.35	6 (8%)
18	BCR	a	845	-	41,41,41	0.35	0	56,56,56	0.95	1 (1%)
15	CLA	N	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	Y	102	-	41,41,41	0.31	0	56,56,56	0.65	1 (1%)
18	BCR	I	101	-	41,41,41	0.33	0	56,56,56	0.73	0
15	CLA	a	822	24	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
21	LMG	I	103	-	37,37,55	0.56	0	45,45,63	0.66	0
15	CLA	V	103	24	54,58,73	1.33	8 (14%)	64,95,113	1.40	7 (10%)
21	LMG	N	855	-	44,44,55	0.54	0	52,52,63	0.64	0
15	CLA	A	837	1	55,59,73	1.31	8 (14%)	64,96,113	1.37	8 (12%)
16	PQN	a	843	-	34,34,34	0.35	0	43,45,45	0.61	1 (2%)
15	CLA	a	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
15	CLA	b	807	2	69,73,73	1.16	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	B	815	2	69,73,73	1.18	8 (11%)	82,113,113	1.27	7 (8%)
15	CLA	a	838	1	59,63,73	1.25	8 (13%)	70,101,113	1.32	5 (7%)
15	CLA	b	812	2	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
18	BCR	N	850	-	41,41,41	0.31	0	56,56,56	0.87	0
14	F6C	a	802	24	72,74,74	1.59	9 (12%)	83,114,114	1.99	13 (15%)
18	BCR	b	847	-	41,41,41	0.32	0	56,56,56	0.87	2 (3%)
15	CLA	a	830	1	69,73,73	1.16	8 (11%)	82,113,113	1.25	7 (8%)
15	CLA	O	824	24	69,73,73	1.17	8 (11%)	82,113,113	1.30	7 (8%)
18	BCR	B	842	-	41,41,41	0.31	0	56,56,56	0.65	0
18	BCR	W	1508	-	41,41,41	0.30	0	56,56,56	0.65	0
17	SF4	a	844	2,1	0,12,12	-	-	-	-	-
18	BCR	B	845	-	41,41,41	0.32	0	56,56,56	0.87	2 (3%)
15	CLA	A	814	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	O	816	2	61,65,73	1.23	7 (11%)	72,103,113	1.34	8 (11%)
20	LMT	N	852	-	32,32,36	0.56	0	43,43,47	0.68	0
17	SF4	c	102	3	0,12,12	-	-	-	-	-
15	CLA	B	835	2	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
15	CLA	a	819	1	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
15	CLA	K	103	24	54,58,73	1.33	8 (14%)	64,95,113	1.40	7 (10%)
15	CLA	W	1502	10	64,68,73	1.20	8 (12%)	76,107,113	1.31	7 (9%)
15	CLA	N	841	1	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
15	CLA	S	201	24	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	N	837	1	55,59,73	1.30	8 (14%)	64,96,113	1.37	8 (12%)
15	CLA	N	808	1	49,53,73	1.38	8 (16%)	58,89,113	1.46	6 (10%)
18	BCR	A	849	-	41,41,41	0.32	0	56,56,56	0.60	0
18	BCR	j	201	-	41,41,41	0.30	0	56,56,56	0.67	0
18	BCR	O	843	-	41,41,41	0.30	0	56,56,56	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	a	825	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
18	BCR	A	845	-	41,41,41	0.35	0	56,56,56	0.97	2 (3%)
15	CLA	N	806	1	69,73,73	1.16	6 (8%)	82,113,113	1.27	7 (8%)
15	CLA	a	805	15,1	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
17	SF4	c	101	3	0,12,12	-	-	-	-	-
15	CLA	B	806	2	69,73,73	1.15	8 (11%)	82,113,113	1.25	6 (7%)
15	CLA	O	819	24	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
14	F6C	a	824	24	58,60,74	1.78	8 (13%)	65,97,114	2.22	14 (21%)
18	BCR	L	205	-	41,41,41	0.33	0	56,56,56	0.66	0
21	LMG	h	102	-	55,55,55	0.49	0	63,63,63	0.61	0
14	F6C	A	824	24	58,60,74	1.78	8 (13%)	65,97,114	2.23	14 (21%)
15	CLA	A	825	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	a	835	1	69,73,73	1.16	8 (11%)	82,113,113	1.24	6 (7%)
18	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.48	0
15	CLA	A	839	1	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
15	CLA	O	827	2	66,70,73	1.18	9 (13%)	78,109,113	1.25	5 (6%)
14	F6C	A	826	24	72,74,74	1.60	8 (11%)	83,114,114	2.06	19 (22%)
18	BCR	a	846	-	41,41,41	0.31	0	56,56,56	0.67	1 (1%)
15	CLA	O	836	24	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
15	CLA	b	822	24	57,61,73	1.28	6 (10%)	67,98,113	1.37	7 (10%)
15	CLA	A	812	15,1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	a	816	1	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
19	LHG	Z	101	-	43,43,48	0.54	0	46,49,54	0.51	0
15	CLA	A	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
15	CLA	B	833	24	49,53,73	1.39	8 (16%)	58,89,113	1.42	6 (10%)
18	BCR	A	850	-	41,41,41	0.31	0	56,56,56	0.88	1 (1%)
15	CLA	O	815	2	49,53,73	1.38	6 (12%)	58,89,113	1.45	5 (8%)
15	CLA	N	830	1	69,73,73	1.16	7 (10%)	82,113,113	1.24	5 (6%)
18	BCR	S	202	-	41,41,41	0.30	0	56,56,56	0.51	0
15	CLA	A	804	1	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
15	CLA	b	835	24	49,53,73	1.39	8 (16%)	58,89,113	1.41	6 (10%)
15	CLA	A	830	1	69,73,73	1.16	7 (10%)	82,113,113	1.24	7 (8%)
18	BCR	O	846	-	41,41,41	0.30	0	56,56,56	0.60	0
15	CLA	B	837	2	69,73,73	1.15	8 (11%)	82,113,113	1.28	9 (10%)
21	LMG	b	849	-	55,55,55	0.49	0	63,63,63	0.59	0
18	BCR	f	203	-	41,41,41	0.30	0	56,56,56	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	a	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.33	7 (8%)
15	CLA	N	835	1	69,73,73	1.16	9 (13%)	82,113,113	1.24	6 (7%)
15	CLA	B	808	2	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
18	BCR	i	101	-	25,25,41	0.52	1 (4%)	33,33,56	0.50	0
15	CLA	O	832	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	8 (9%)
21	LMG	j	206	-	50,50,55	0.50	0	58,58,63	0.59	0
20	LMT	a	853	-	29,29,36	0.57	0	40,40,47	1.45	4 (10%)
15	CLA	N	825	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	a	815	1	59,63,73	1.27	8 (13%)	70,101,113	1.34	6 (8%)
15	CLA	W	1501	10	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
14	F6C	N	802	24	72,74,74	1.58	9 (12%)	83,114,114	1.99	13 (15%)
15	CLA	a	809	1	64,68,73	1.20	8 (12%)	76,107,113	1.28	7 (9%)
18	BCR	W	1504	-	41,41,41	0.32	0	56,56,56	0.57	0
21	LMG	B	847	-	55,55,55	0.50	0	63,63,63	0.59	0
15	CLA	l	103	12	59,63,73	1.27	7 (11%)	70,101,113	1.33	5 (7%)
19	LHG	W	1506	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	b	823	2	59,63,73	1.30	8 (13%)	70,101,113	1.24	6 (8%)
15	CLA	b	813	2	60,64,73	1.26	9 (15%)	71,102,113	1.36	6 (8%)
15	CLA	B	812	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	A	827	24	59,63,73	1.25	7 (11%)	70,101,113	1.38	8 (11%)
15	CLA	O	839	2	69,73,73	1.15	8 (11%)	82,113,113	1.27	8 (9%)
14	F6C	N	826	24	72,74,74	1.62	8 (11%)	83,114,114	2.02	17 (20%)
15	CLA	O	802	24	69,73,73	1.16	7 (10%)	82,113,113	1.21	6 (7%)
15	CLA	b	832	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
15	CLA	a	833	1	59,63,73	1.26	8 (13%)	70,101,113	1.34	6 (8%)
15	CLA	a	810	1	61,65,73	1.24	8 (13%)	72,103,113	1.37	8 (11%)
15	CLA	b	831	2	69,73,73	1.16	7 (10%)	82,113,113	1.25	6 (7%)
15	CLA	a	812	15,1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	b	806	2	69,73,73	1.16	7 (10%)	82,113,113	1.30	6 (7%)
15	CLA	A	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
15	CLA	A	836	1	58,62,73	1.27	8 (13%)	68,99,113	1.35	6 (8%)
14	F6C	a	826	24	72,74,74	1.60	8 (11%)	83,114,114	2.02	16 (19%)
19	LHG	j	207	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	b	801	2	69,73,73	1.16	8 (11%)	82,113,113	1.22	6 (7%)
15	CLA	b	834	2	59,63,73	1.26	7 (11%)	70,101,113	1.33	6 (8%)
18	BCR	V	101	-	25,25,41	0.52	1 (4%)	33,33,56	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	PQN	N	843	-	34,34,34	0.35	0	43,45,45	0.58	1 (2%)
19	LHG	Z	102	-	48,48,48	0.51	0	51,54,54	0.48	0
18	BCR	N	847	-	41,41,41	0.29	0	56,56,56	0.60	1 (1%)
15	CLA	O	835	24	49,53,73	1.39	8 (16%)	58,89,113	1.42	6 (10%)
15	CLA	B	832	2	59,63,73	1.26	7 (11%)	70,101,113	1.33	5 (7%)
18	BCR	O	847	-	41,41,41	0.32	0	56,56,56	0.84	3 (5%)
14	F6C	b	840	24	72,74,74	1.57	9 (12%)	83,114,114	2.08	15 (18%)
15	CLA	b	829	2	69,73,73	1.16	8 (11%)	82,113,113	1.30	7 (8%)
14	F6C	W	1503	24	72,74,74	1.58	8 (11%)	83,114,114	2.06	17 (20%)
15	CLA	N	819	1	69,73,73	1.18	9 (13%)	82,113,113	1.25	6 (7%)
15	CLA	A	815	1	59,63,73	1.27	8 (13%)	70,101,113	1.34	6 (8%)
15	CLA	A	820	1	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
18	BCR	b	848	-	41,41,41	0.29	0	56,56,56	0.63	0
15	CLA	b	811	2	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
18	BCR	M	101	-	41,41,41	0.31	0	56,56,56	0.68	1 (1%)
15	CLA	B	834	24	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
15	CLA	O	821	2	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
15	CLA	N	814	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
20	LMT	a	854	-	36,36,36	0.55	0	47,47,47	0.63	0
15	CLA	N	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
14	F6C	A	802	24	72,74,74	1.59	10 (13%)	83,114,114	1.99	14 (16%)
15	CLA	b	808	2	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
15	CLA	A	819	1	69,73,73	1.18	9 (13%)	82,113,113	1.25	6 (7%)
15	CLA	A	809	1	64,68,73	1.20	8 (12%)	76,107,113	1.29	7 (9%)
15	CLA	O	818	2	64,68,73	1.20	8 (12%)	76,107,113	1.23	4 (5%)
15	CLA	B	817	24	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	a	840	1	54,58,73	1.30	8 (14%)	64,95,113	1.40	6 (9%)
15	CLA	A	807	1	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
15	CLA	N	820	1	69,73,73	1.16	8 (11%)	82,113,113	1.37	9 (10%)
16	PQN	B	840	-	34,34,34	0.37	0	43,45,45	0.63	1 (2%)
15	CLA	N	828	1	69,73,73	1.17	9 (13%)	82,113,113	1.26	4 (4%)
16	PQN	A	843	-	34,34,34	0.36	0	43,45,45	0.61	1 (2%)
15	CLA	B	830	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
18	BCR	A	847	-	41,41,41	0.29	0	56,56,56	0.61	1 (1%)
15	CLA	B	828	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMT	A	853	-	29,29,36	0.57	0	40,40,47	1.45	4 (10%)
14	F6C	b	810	2	72,74,74	1.60	8 (11%)	83,114,114	1.96	14 (16%)
15	CLA	O	801	2	69,73,73	1.16	8 (11%)	82,113,113	1.21	7 (8%)
22	LFA	B	848	-	15,15,19	0.23	0	14,14,18	0.19	0
18	BCR	A	858	-	41,41,41	0.38	0	56,56,56	1.31	9 (16%)
15	CLA	b	841	2	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	a	814	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
15	CLA	B	819	2	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
19	LHG	Y	101	-	48,48,48	0.51	0	51,54,54	0.50	0
15	CLA	O	823	2	59,63,73	1.26	9 (15%)	70,101,113	1.37	6 (8%)
15	CLA	B	803	2	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
14	F6C	j	204	24	72,74,74	1.58	8 (11%)	83,114,114	2.07	17 (20%)
17	SF4	A	844	2,1	0,12,12	-	-	-	-	-
15	CLA	A	810	1	61,65,73	1.24	7 (11%)	72,103,113	1.37	8 (11%)
15	CLA	B	805	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
15	CLA	O	829	2	69,73,73	1.17	8 (11%)	82,113,113	1.29	8 (9%)
15	CLA	B	822	24	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
20	LMT	N	853	-	29,29,36	0.57	0	40,40,47	1.43	4 (10%)
18	BCR	A	846	-	41,41,41	0.31	0	56,56,56	0.65	1 (1%)
15	CLA	O	809	2	69,73,73	1.17	9 (13%)	82,113,113	1.26	5 (6%)
15	CLA	a	841	1	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
15	CLA	O	831	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	7 (8%)
15	CLA	A	838	1	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
15	CLA	A	823	1	60,64,73	1.25	8 (13%)	71,102,113	1.34	6 (8%)
15	CLA	a	839	1	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
18	BCR	U	101	-	41,41,41	0.31	0	56,56,56	0.54	0
15	CLA	b	819	24	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
14	F6C	O	833	2	72,74,74	1.59	9 (12%)	83,114,114	2.03	15 (18%)
15	CLA	j	203	10	64,68,73	1.20	8 (12%)	76,107,113	1.32	7 (9%)
19	LHG	A	851	-	41,41,48	0.56	0	44,47,54	0.51	0
18	BCR	b	844	-	41,41,41	0.31	0	56,56,56	0.63	0
15	CLA	N	832	1	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
15	CLA	a	817	24	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
15	CLA	A	832	1	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
14	F6C	A	857	24	72,74,74	1.56	8 (11%)	83,114,114	2.10	15 (18%)
14	F6C	a	856	24	72,74,74	1.56	8 (11%)	83,114,114	2.09	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	O	838	2	69,73,73	1.16	7 (10%)	82,113,113	1.28	8 (9%)
15	CLA	b	814	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
18	BCR	j	205	-	41,41,41	0.33	0	56,56,56	0.67	0
15	CLA	b	817	2	69,73,73	1.18	8 (11%)	82,113,113	1.26	7 (8%)
15	CLA	a	828	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
18	BCR	N	846	-	41,41,41	0.31	0	56,56,56	0.67	1 (1%)
21	LMG	g	103	-	37,37,55	0.56	0	45,45,63	0.66	0
18	BCR	b	843	-	41,41,41	0.30	0	56,56,56	0.61	0
15	CLA	O	834	2	59,63,73	1.26	8 (13%)	70,101,113	1.33	6 (8%)
13	CL0	N	801	1	58,73,73	2.23	10 (17%)	60,113,113	1.63	14 (23%)
15	CLA	b	828	2	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
15	CLA	B	809	2	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	a	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
13	CL0	A	801	1	58,73,73	2.23	9 (15%)	60,113,113	1.62	13 (21%)
15	CLA	a	827	24	59,63,73	1.25	8 (13%)	70,101,113	1.38	7 (10%)
18	BCR	b	845	-	41,41,41	0.29	0	56,56,56	0.47	0
15	CLA	B	818	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	5 (7%)
15	CLA	b	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	7 (8%)
15	CLA	b	825	24	69,73,73	1.16	6 (8%)	82,113,113	1.31	7 (8%)
15	CLA	N	831	1	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
15	CLA	a	836	1	58,62,73	1.27	8 (13%)	68,99,113	1.35	6 (8%)
17	SF4	P	101	3	0,12,12	-	-	-	-	-
15	CLA	b	805	2	69,73,73	1.15	6 (8%)	82,113,113	1.28	6 (7%)
14	F6C	B	831	2	72,74,74	1.58	9 (12%)	83,114,114	2.05	16 (19%)
15	CLA	b	830	2	69,73,73	1.16	8 (11%)	82,113,113	1.25	6 (7%)
15	CLA	b	826	2	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
15	CLA	B	801	2	69,73,73	1.16	8 (11%)	82,113,113	1.22	6 (7%)
15	CLA	O	813	2	60,64,73	1.26	9 (15%)	71,102,113	1.36	6 (8%)
21	LMG	U	102	-	55,55,55	0.49	0	63,63,63	0.60	0
15	CLA	B	825	2	66,70,73	1.19	9 (13%)	78,109,113	1.25	5 (6%)
15	CLA	N	840	1	54,58,73	1.30	8 (14%)	64,95,113	1.40	6 (9%)
19	LHG	M	102	-	48,48,48	0.51	0	51,54,54	0.50	0
15	CLA	O	814	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
17	SF4	C	102	3	0,12,12	-	-	-	-	-
14	F6C	L	204	24	72,74,74	1.58	8 (11%)	83,114,114	2.05	16 (19%)
18	BCR	a	848	-	41,41,41	0.31	0	56,56,56	0.50	0
21	LMG	A	855	-	44,44,55	0.53	0	52,52,63	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	b	846	-	41,41,41	0.31	0	56,56,56	0.57	0
18	BCR	B	841	-	41,41,41	0.30	0	56,56,56	0.60	0
15	CLA	b	821	2	49,53,73	1.38	7 (14%)	58,89,113	1.44	4 (6%)
19	LHG	a	851	-	41,41,48	0.55	0	44,47,54	0.52	0
15	CLA	N	811	1	61,65,73	1.23	7 (11%)	72,103,113	1.33	6 (8%)
15	CLA	b	816	2	61,65,73	1.24	7 (11%)	72,103,113	1.32	7 (9%)
18	BCR	a	850	-	41,41,41	0.31	0	56,56,56	0.88	1 (1%)
14	F6C	O	840	24	72,74,74	1.57	8 (11%)	83,114,114	2.07	15 (18%)
14	F6C	B	838	24	72,74,74	1.57	8 (11%)	83,114,114	2.08	15 (18%)
15	CLA	A	805	15,1	64,68,73	1.21	7 (10%)	76,107,113	1.29	5 (6%)
15	CLA	B	836	2	69,73,73	1.16	7 (10%)	82,113,113	1.28	8 (9%)
15	CLA	N	839	1	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
18	BCR	k	102	-	41,41,41	0.31	0	56,56,56	0.69	1 (1%)
15	CLA	a	804	1	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
15	CLA	O	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
18	BCR	B	843	-	41,41,41	0.30	0	56,56,56	0.48	0
18	BCR	h	101	-	41,41,41	0.31	0	56,56,56	0.54	0
15	CLA	N	810	1	61,65,73	1.24	8 (13%)	72,103,113	1.37	8 (11%)
15	CLA	O	841	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	a	842	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
15	CLA	B	810	2	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
15	CLA	a	820	1	69,73,73	1.16	8 (11%)	82,113,113	1.36	9 (10%)
14	F6C	N	856	24	72,74,74	1.56	9 (12%)	83,114,114	2.09	15 (18%)
19	LHG	X	102	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	A	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)
15	CLA	X	103	12	59,63,73	1.27	7 (11%)	70,101,113	1.33	5 (7%)
15	CLA	f	201	24	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	b	818	2	64,68,73	1.20	8 (12%)	76,107,113	1.24	4 (5%)
15	CLA	b	836	24	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
19	LHG	N	851	-	41,41,48	0.55	0	44,47,54	0.50	0
15	CLA	N	813	1	58,62,73	1.27	8 (13%)	68,99,113	1.36	7 (10%)
15	CLA	B	827	2	69,73,73	1.16	8 (11%)	82,113,113	1.29	8 (9%)
15	CLA	O	805	2	69,73,73	1.15	7 (10%)	82,113,113	1.28	7 (8%)
15	CLA	O	822	24	57,61,73	1.28	7 (12%)	67,98,113	1.39	8 (11%)
18	BCR	L	209	-	41,41,41	0.30	0	56,56,56	0.65	0
15	CLA	B	826	2	69,73,73	1.15	7 (10%)	82,113,113	1.22	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	829	1	64,68,73	1.20	7 (10%)	76,107,113	1.26	6 (7%)
15	CLA	B	814	2	61,65,73	1.23	7 (11%)	72,103,113	1.34	8 (11%)
17	SF4	P	102	3	0,12,12	-	-	-		
14	F6C	N	824	24	58,60,74	1.78	7 (12%)	65,97,114	2.20	14 (21%)
15	CLA	A	811	1	61,65,73	1.23	6 (9%)	72,103,113	1.31	6 (8%)
18	BCR	T	102	-	41,41,41	0.29	0	56,56,56	0.48	0
15	CLA	b	809	2	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
19	LHG	l	102	-	48,48,48	0.52	0	51,54,54	0.48	0
15	CLA	b	815	2	49,53,73	1.38	6 (12%)	58,89,113	1.45	7 (12%)
15	CLA	A	831	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	7 (8%)
15	CLA	B	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
13	CL0	a	801	1	58,73,73	2.23	9 (15%)	60,113,113	1.64	14 (23%)
18	BCR	A	848	-	41,41,41	0.31	0	56,56,56	0.52	0
15	CLA	i	103	24	54,58,73	1.33	8 (14%)	64,95,113	1.39	6 (9%)
19	LHG	X	101	-	43,43,48	0.54	0	46,49,54	0.52	0
15	CLA	b	820	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
18	BCR	a	847	-	41,41,41	0.30	0	56,56,56	0.61	1 (1%)
15	CLA	A	828	1	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
15	CLA	A	835	1	69,73,73	1.16	8 (11%)	82,113,113	1.27	7 (8%)
18	BCR	B	846	-	41,41,41	0.29	0	56,56,56	0.61	0
15	CLA	V	102	9	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
15	CLA	O	806	2	69,73,73	1.16	7 (10%)	82,113,113	1.30	6 (7%)
15	CLA	b	804	2	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	i	102	9	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
15	CLA	K	102	9	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
15	CLA	B	811	2	60,64,73	1.26	9 (15%)	71,102,113	1.36	6 (8%)
18	BCR	B	844	-	41,41,41	0.31	0	56,56,56	0.60	0
20	LMT	A	852	-	32,32,36	0.57	0	43,43,47	0.68	0
15	CLA	L	202	10	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
15	CLA	B	820	24	57,61,73	1.27	7 (12%)	67,98,113	1.38	7 (10%)
18	BCR	F	202	-	41,41,41	0.31	0	56,56,56	1.02	4 (7%)
15	CLA	L	203	10	64,68,73	1.20	9 (14%)	76,107,113	1.33	7 (9%)
21	LMG	L	206	-	50,50,55	0.50	0	58,58,63	0.59	0
16	PQN	b	842	-	34,34,34	0.36	0	43,45,45	0.62	1 (2%)
15	CLA	N	807	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
15	CLA	B	807	2	69,73,73	1.14	9 (13%)	82,113,113	1.30	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	O	811	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	A	842	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
18	BCR	N	857	-	41,41,41	0.38	0	56,56,56	1.32	8 (14%)
15	CLA	Z	103	12	59,63,73	1.27	7 (11%)	70,101,113	1.33	5 (7%)
21	LMG	T	103	-	37,37,55	0.56	0	45,45,63	0.65	0
15	CLA	O	804	2	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	N	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
18	BCR	O	848	-	41,41,41	0.31	0	56,56,56	1.00	4 (7%)
15	CLA	B	839	2	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
18	BCR	J	101	-	41,41,41	0.31	0	56,56,56	0.54	0
19	LHG	k	101	-	48,48,48	0.51	0	51,54,54	0.50	0
15	CLA	O	812	2	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
18	BCR	K	101	-	25,25,41	0.52	1 (4%)	33,33,56	0.51	0
21	LMG	J	102	-	55,55,55	0.49	0	63,63,63	0.60	0
15	CLA	O	807	2	69,73,73	1.16	8 (11%)	82,113,113	1.25	7 (8%)
15	CLA	O	825	24	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
15	CLA	O	837	2	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
15	CLA	b	824	24	69,73,73	1.17	8 (11%)	82,113,113	1.30	7 (8%)
15	CLA	N	804	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	b	838	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	8 (9%)
14	F6C	L	201	2	72,74,74	1.60	8 (11%)	83,114,114	1.97	14 (16%)
15	CLA	a	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
15	CLA	O	826	2	69,73,73	1.17	9 (13%)	82,113,113	1.30	7 (8%)
15	CLA	b	839	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	9 (10%)
15	CLA	O	808	2	69,73,73	1.14	9 (13%)	82,113,113	1.31	9 (10%)
18	BCR	f	202	-	41,41,41	0.31	0	56,56,56	1.00	4 (7%)
15	CLA	A	817	24	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
15	CLA	A	822	24	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	a	837	1	55,59,73	1.30	7 (12%)	64,96,113	1.37	7 (10%)
15	CLA	N	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	7 (8%)
15	CLA	B	824	2	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
15	CLA	B	823	24	69,73,73	1.16	6 (8%)	82,113,113	1.31	6 (7%)

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	821	2	1/1/13/20	11/27/103/115	-
18	BCR	g	101	-	-	7/29/63/63	0/2/2/2
22	LFA	L	208	-	-	0/12/12/17	-
15	CLA	N	816	1	1/1/11/20	8/15/91/115	-
15	CLA	N	827	24	1/1/13/20	0/27/103/115	-
15	CLA	a	807	1	1/1/15/20	18/39/115/115	-
15	CLA	N	829	1	1/1/14/20	16/33/109/115	-
15	CLA	b	837	2	1/1/15/20	9/39/115/115	-
15	CLA	F	201	24	1/1/15/20	10/39/115/115	-
15	CLA	B	816	2	1/1/14/20	13/33/109/115	-
15	CLA	a	823	1	1/1/13/20	5/29/105/115	-
15	CLA	j	202	10	1/1/15/20	6/39/115/115	-
15	CLA	B	829	2	1/1/15/20	14/39/115/115	-
18	BCR	N	848	-	-	8/29/63/63	0/2/2/2
15	CLA	A	808	1	1/1/11/20	0/15/91/115	-
15	CLA	b	802	24	1/1/15/20	12/39/115/115	-
17	SF4	C	101	3	-	-	0/6/5/5
22	LFA	f	204	-	-	6/13/13/17	-
15	CLA	A	803	-	1/1/15/20	11/39/115/115	-
15	CLA	N	836	1	1/1/12/20	7/26/102/115	-
15	CLA	a	806	1	1/1/15/20	17/39/115/115	-
15	CLA	N	815	1	1/1/13/20	2/27/103/115	-
15	CLA	A	813	1	1/1/12/20	7/26/102/115	-
18	BCR	O	849	-	-	4/29/63/63	0/2/2/2
18	BCR	a	857	-	-	10/29/63/63	0/2/2/2
18	BCR	O	844	-	-	5/29/63/63	0/2/2/2
20	LMT	A	854	-	-	5/21/61/61	0/2/2/2
14	F6C	O	810	2	1/1/10/16	8/41/97/97	-
22	LFA	j	208	-	-	0/12/12/17	-
15	CLA	A	856	24	1/1/15/20	12/39/115/115	-
15	CLA	N	822	24	1/1/15/20	18/39/115/115	-
22	LFA	W	1507	-	-	0/12/12/17	-
15	CLA	N	838	1	1/1/13/20	10/27/103/115	-
15	CLA	O	820	2	1/1/13/20	13/27/103/115	-
15	CLA	a	808	1	1/1/11/20	0/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	805	15,1	1/1/14/20	8/33/109/115	-
21	LMG	O	850	-	-	7/50/70/70	0/1/1/1
15	CLA	a	829	1	1/1/14/20	17/33/109/115	-
21	LMG	a	855	-	-	8/39/59/70	0/1/1/1
15	CLA	N	817	24	1/1/11/20	5/15/91/115	-
15	CLA	a	832	1	1/1/12/20	3/21/97/115	-
15	CLA	a	831	1	1/1/15/20	14/39/115/115	-
15	CLA	a	811	1	1/1/13/20	11/30/106/115	-
15	CLA	B	804	2	1/1/15/20	14/39/115/115	-
15	CLA	N	812	15,1	1/1/15/20	19/39/115/115	-
15	CLA	A	816	1	1/1/11/20	7/15/91/115	-
20	LMT	N	854	-	-	5/21/61/61	0/2/2/2
15	CLA	A	806	1	1/1/15/20	17/39/115/115	-
18	BCR	F	203	-	-	2/29/63/63	0/2/2/2
15	CLA	b	827	2	1/1/14/20	12/36/112/115	-
15	CLA	O	817	2	1/1/15/20	11/39/115/115	-
19	LHG	l	101	-	-	22/48/48/53	-
18	BCR	N	845	-	-	3/29/63/63	0/2/2/2
15	CLA	A	833	1	1/1/13/20	4/27/103/115	-
18	BCR	T	101	-	-	9/29/63/63	0/2/2/2
18	BCR	N	849	-	-	3/29/63/63	0/2/2/2
15	CLA	O	830	2	1/1/15/20	17/39/115/115	-
18	BCR	a	849	-	-	3/29/63/63	0/2/2/2
21	LMG	W	1505	-	-	11/45/65/70	0/1/1/1
20	LMT	a	852	-	-	0/17/57/61	0/2/2/2
15	CLA	A	840	1	1/1/12/20	0/21/97/115	-
18	BCR	g	102	-	-	4/29/63/63	0/2/2/2
18	BCR	O	845	-	-	4/29/63/63	0/2/2/2
15	CLA	N	823	1	1/1/13/20	6/29/105/115	-
15	CLA	N	842	1	1/1/15/20	12/39/115/115	-
15	CLA	O	828	2	1/1/15/20	6/39/115/115	-
15	CLA	B	813	2	1/1/11/20	7/15/91/115	-
17	SF4	N	844	2,1	-	-	0/6/5/5
15	CLA	N	809	1	1/1/14/20	14/33/109/115	-
22	LFA	O	851	-	-	6/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	F6C	b	833	2	1/1/10/16	5/41/97/97	-
15	CLA	a	813	1	1/1/12/20	4/26/102/115	-
19	LHG	L	207	-	-	16/53/53/53	-
15	CLA	A	841	1	1/1/15/20	14/39/115/115	-
16	PQN	O	842	-	-	0/23/43/43	0/2/2/2
15	CLA	N	833	1	1/1/13/20	3/27/103/115	-
18	BCR	a	845	-	-	3/29/63/63	0/2/2/2
15	CLA	N	834	1	1/1/15/20	8/39/115/115	-
18	BCR	Y	102	-	-	6/29/63/63	0/2/2/2
18	BCR	I	101	-	-	9/29/63/63	0/2/2/2
15	CLA	a	822	24	1/1/15/20	17/39/115/115	-
21	LMG	I	103	-	-	11/32/52/70	0/1/1/1
15	CLA	V	103	24	1/1/12/20	2/21/97/115	-
21	LMG	N	855	-	-	6/39/59/70	0/1/1/1
15	CLA	A	837	1	1/1/12/20	8/23/99/115	-
16	PQN	a	843	-	-	0/23/43/43	0/2/2/2
15	CLA	a	803	-	1/1/15/20	11/39/115/115	-
15	CLA	b	807	2	1/1/15/20	3/39/115/115	-
15	CLA	B	815	2	1/1/15/20	12/39/115/115	-
15	CLA	a	838	1	1/1/13/20	10/27/103/115	-
15	CLA	b	812	2	1/1/11/20	5/15/91/115	-
18	BCR	N	850	-	-	13/29/63/63	0/2/2/2
14	F6C	a	802	24	1/1/10/16	7/41/97/97	-
18	BCR	b	847	-	-	1/29/63/63	0/2/2/2
15	CLA	a	830	1	1/1/15/20	6/39/115/115	-
15	CLA	O	824	24	1/1/15/20	9/39/115/115	-
18	BCR	B	842	-	-	5/29/63/63	0/2/2/2
18	BCR	W	1508	-	-	2/29/63/63	0/2/2/2
17	SF4	a	844	2,1	-	-	0/6/5/5
18	BCR	B	845	-	-	2/29/63/63	0/2/2/2
15	CLA	A	814	1	1/1/15/20	11/39/115/115	-
15	CLA	O	816	2	1/1/13/20	6/30/106/115	-
20	LMT	N	852	-	-	2/17/57/61	0/2/2/2
17	SF4	c	102	3	-	-	0/6/5/5
15	CLA	B	835	2	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a	819	1	1/1/15/20	14/39/115/115	-
15	CLA	K	103	24	1/1/12/20	2/21/97/115	-
15	CLA	W	1502	10	1/1/14/20	12/33/109/115	-
15	CLA	N	841	1	1/1/15/20	15/39/115/115	-
15	CLA	S	201	24	1/1/15/20	10/39/115/115	-
15	CLA	N	837	1	1/1/12/20	8/23/99/115	-
15	CLA	N	808	1	1/1/11/20	2/15/91/115	-
18	BCR	A	849	-	-	3/29/63/63	0/2/2/2
18	BCR	j	201	-	-	4/29/63/63	0/2/2/2
18	BCR	O	843	-	-	3/29/63/63	0/2/2/2
15	CLA	a	825	1	1/1/15/20	10/39/115/115	-
18	BCR	A	845	-	-	3/29/63/63	0/2/2/2
15	CLA	N	806	1	1/1/15/20	17/39/115/115	-
15	CLA	a	805	15,1	1/1/14/20	9/33/109/115	-
17	SF4	c	101	3	-	-	0/6/5/5
15	CLA	B	806	2	1/1/15/20	5/39/115/115	-
15	CLA	O	819	24	1/1/15/20	9/39/115/115	-
14	F6C	a	824	24	1/1/7/16	9/25/81/97	-
18	BCR	L	205	-	-	4/29/63/63	0/2/2/2
21	LMG	h	102	-	-	16/50/70/70	0/1/1/1
14	F6C	A	824	24	1/1/7/16	9/25/81/97	-
15	CLA	A	825	1	1/1/15/20	6/39/115/115	-
15	CLA	a	835	1	1/1/15/20	7/39/115/115	-
18	BCR	I	102	-	-	4/29/63/63	0/2/2/2
15	CLA	A	839	1	1/1/15/20	17/39/115/115	-
15	CLA	O	827	2	1/1/14/20	12/36/112/115	-
14	F6C	A	826	24	1/1/10/16	14/41/97/97	-
18	BCR	a	846	-	-	8/29/63/63	0/2/2/2
15	CLA	O	836	24	1/1/11/20	8/15/91/115	-
15	CLA	b	822	24	1/1/12/20	9/25/101/115	-
15	CLA	A	812	15,1	1/1/15/20	19/39/115/115	-
15	CLA	a	816	1	1/1/11/20	7/15/91/115	-
19	LHG	Z	101	-	-	22/48/48/53	-
15	CLA	A	821	1	1/1/14/20	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	833	24	1/1/11/20	2/15/91/115	-
18	BCR	A	850	-	-	13/29/63/63	0/2/2/2
15	CLA	O	815	2	1/1/11/20	6/15/91/115	-
15	CLA	N	830	1	1/1/15/20	6/39/115/115	-
18	BCR	S	202	-	-	2/29/63/63	0/2/2/2
15	CLA	A	804	1	1/1/15/20	6/39/115/115	-
15	CLA	b	835	24	1/1/11/20	4/15/91/115	-
15	CLA	A	830	1	1/1/15/20	7/39/115/115	-
18	BCR	O	846	-	-	8/29/63/63	0/2/2/2
15	CLA	B	837	2	1/1/15/20	10/39/115/115	-
21	LMG	b	849	-	-	7/50/70/70	0/1/1/1
18	BCR	f	203	-	-	2/29/63/63	0/2/2/2
15	CLA	a	818	1	1/1/15/20	22/39/115/115	-
15	CLA	N	835	1	1/1/15/20	10/39/115/115	-
15	CLA	B	808	2	1/1/15/20	13/39/115/115	-
18	BCR	i	101	-	-	0/18/35/63	0/1/1/2
15	CLA	O	832	2	1/1/15/20	9/39/115/115	-
21	LMG	j	206	-	-	10/45/65/70	0/1/1/1
20	LMT	a	853	-	-	10/14/54/61	0/2/2/2
15	CLA	N	825	1	1/1/15/20	9/39/115/115	-
15	CLA	a	815	1	1/1/13/20	4/27/103/115	-
15	CLA	W	1501	10	1/1/15/20	7/39/115/115	-
14	F6C	N	802	24	1/1/10/16	7/41/97/97	-
15	CLA	a	809	1	1/1/14/20	10/33/109/115	-
18	BCR	W	1504	-	-	4/29/63/63	0/2/2/2
21	LMG	B	847	-	-	7/50/70/70	0/1/1/1
15	CLA	l	103	12	1/1/13/20	2/27/103/115	-
19	LHG	W	1506	-	-	16/53/53/53	-
15	CLA	b	823	2	1/1/13/20	6/27/103/115	-
15	CLA	b	813	2	-	10/29/105/115	-
15	CLA	B	812	2	1/1/15/20	14/39/115/115	-
15	CLA	A	827	24	1/1/13/20	0/27/103/115	-
15	CLA	O	839	2	1/1/15/20	12/39/115/115	-
14	F6C	N	826	24	1/1/10/16	15/41/97/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	O	802	24	1/1/15/20	12/39/115/115	-
15	CLA	b	832	2	1/1/15/20	10/39/115/115	-
15	CLA	a	833	1	1/1/13/20	3/27/103/115	-
15	CLA	a	810	1	1/1/13/20	7/30/106/115	-
15	CLA	b	831	2	1/1/15/20	11/39/115/115	-
15	CLA	a	812	15,1	1/1/15/20	18/39/115/115	-
15	CLA	b	806	2	1/1/15/20	18/39/115/115	-
15	CLA	A	818	1	1/1/15/20	19/39/115/115	-
15	CLA	A	836	1	1/1/12/20	6/26/102/115	-
14	F6C	a	826	24	1/1/10/16	12/41/97/97	-
19	LHG	j	207	-	-	17/53/53/53	-
15	CLA	b	801	2	1/1/15/20	10/39/115/115	-
15	CLA	b	834	2	1/1/13/20	8/27/103/115	-
18	BCR	V	101	-	-	0/18/35/63	0/1/1/2
16	PQN	N	843	-	-	1/23/43/43	0/2/2/2
19	LHG	Z	102	-	-	23/53/53/53	-
18	BCR	N	847	-	-	6/29/63/63	0/2/2/2
15	CLA	O	835	24	1/1/11/20	2/15/91/115	-
15	CLA	B	832	2	1/1/13/20	8/27/103/115	-
18	BCR	O	847	-	-	1/29/63/63	0/2/2/2
14	F6C	b	840	24	1/1/10/16	13/41/97/97	-
15	CLA	b	829	2	1/1/15/20	11/39/115/115	-
14	F6C	W	1503	24	1/1/10/16	14/41/97/97	-
15	CLA	N	819	1	1/1/15/20	12/39/115/115	-
15	CLA	A	815	1	1/1/13/20	4/27/103/115	-
15	CLA	A	820	1	1/1/15/20	19/39/115/115	-
18	BCR	b	848	-	-	3/29/63/63	0/2/2/2
15	CLA	b	811	2	1/1/15/20	10/39/115/115	-
18	BCR	M	101	-	-	6/29/63/63	0/2/2/2
15	CLA	B	834	24	1/1/11/20	9/15/91/115	-
15	CLA	O	821	2	1/1/11/20	4/15/91/115	-
15	CLA	N	814	1	1/1/15/20	9/39/115/115	-
20	LMT	a	854	-	-	4/21/61/61	0/2/2/2
15	CLA	N	818	1	1/1/15/20	19/39/115/115	-
14	F6C	A	802	24	1/1/10/16	9/41/97/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b	808	2	1/1/15/20	12/39/115/115	-
15	CLA	A	819	1	1/1/15/20	11/39/115/115	-
15	CLA	A	809	1	1/1/14/20	10/33/109/115	-
15	CLA	O	818	2	1/1/14/20	13/33/109/115	-
15	CLA	B	817	24	1/1/15/20	10/39/115/115	-
15	CLA	a	840	1	1/1/12/20	0/21/97/115	-
15	CLA	A	807	1	1/1/15/20	18/39/115/115	-
15	CLA	N	820	1	1/1/15/20	19/39/115/115	-
16	PQN	B	840	-	-	0/23/43/43	0/2/2/2
15	CLA	N	828	1	1/1/15/20	5/39/115/115	-
16	PQN	A	843	-	-	0/23/43/43	0/2/2/2
15	CLA	B	830	2	1/1/15/20	12/39/115/115	-
18	BCR	A	847	-	-	6/29/63/63	0/2/2/2
15	CLA	B	828	2	1/1/15/20	19/39/115/115	-
20	LMT	A	853	-	-	10/14/54/61	0/2/2/2
14	F6C	b	810	2	1/1/10/16	8/41/97/97	-
15	CLA	O	801	2	1/1/15/20	11/39/115/115	-
22	LFA	B	848	-	-	6/13/13/17	-
18	BCR	A	858	-	-	9/29/63/63	0/2/2/2
15	CLA	b	841	2	1/1/15/20	14/39/115/115	-
15	CLA	a	814	1	1/1/15/20	8/39/115/115	-
15	CLA	B	819	2	1/1/11/20	4/15/91/115	-
19	LHG	Y	101	-	-	17/53/53/53	-
15	CLA	O	823	2	1/1/13/20	10/27/103/115	-
15	CLA	B	803	2	1/1/15/20	8/39/115/115	-
14	F6C	j	204	24	1/1/10/16	13/41/97/97	-
17	SF4	A	844	2,1	-	-	0/6/5/5
15	CLA	A	810	1	1/1/13/20	7/30/106/115	-
15	CLA	B	805	2	1/1/15/20	17/39/115/115	-
15	CLA	O	829	2	1/1/15/20	11/39/115/115	-
15	CLA	B	822	24	1/1/15/20	9/39/115/115	-
20	LMT	N	853	-	-	10/14/54/61	0/2/2/2
18	BCR	A	846	-	-	8/29/63/63	0/2/2/2
15	CLA	O	809	2	1/1/15/20	15/39/115/115	-
15	CLA	a	841	1	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	O	831	2	1/1/15/20	15/39/115/115	-
15	CLA	A	838	1	1/1/13/20	9/27/103/115	-
15	CLA	A	823	1	1/1/13/20	5/29/105/115	-
15	CLA	a	839	1	1/1/15/20	16/39/115/115	-
18	BCR	U	101	-	-	7/29/63/63	0/2/2/2
15	CLA	b	819	24	1/1/15/20	9/39/115/115	-
14	F6C	O	833	2	1/1/10/16	5/41/97/97	-
15	CLA	j	203	10	1/1/14/20	13/33/109/115	-
19	LHG	A	851	-	-	11/46/46/53	-
18	BCR	b	844	-	-	5/29/63/63	0/2/2/2
15	CLA	N	832	1	1/1/12/20	3/21/97/115	-
15	CLA	a	817	24	1/1/11/20	5/15/91/115	-
15	CLA	A	832	1	1/1/12/20	3/21/97/115	-
14	F6C	A	857	24	1/1/10/16	18/41/97/97	-
14	F6C	a	856	24	1/1/10/16	18/41/97/97	-
15	CLA	O	838	2	1/1/15/20	10/39/115/115	-
15	CLA	b	814	2	1/1/15/20	14/39/115/115	-
18	BCR	j	205	-	-	4/29/63/63	0/2/2/2
15	CLA	b	817	2	1/1/15/20	11/39/115/115	-
15	CLA	a	828	1	1/1/15/20	7/39/115/115	-
18	BCR	N	846	-	-	8/29/63/63	0/2/2/2
21	LMG	g	103	-	-	14/32/52/70	0/1/1/1
18	BCR	b	843	-	-	3/29/63/63	0/2/2/2
15	CLA	O	834	2	1/1/13/20	8/27/103/115	-
13	CL0	N	801	1	3/3/20/25	11/37/135/135	-
15	CLA	b	828	2	1/1/15/20	10/39/115/115	-
15	CLA	B	809	2	1/1/15/20	10/39/115/115	-
15	CLA	a	821	1	1/1/14/20	7/33/109/115	-
13	CL0	A	801	1	3/3/20/25	9/37/135/135	-
15	CLA	a	827	24	1/1/13/20	1/27/103/115	-
18	BCR	b	845	-	-	4/29/63/63	0/2/2/2
15	CLA	B	818	2	1/1/13/20	11/27/103/115	-
15	CLA	b	803	-	1/1/15/20	7/39/115/115	-
15	CLA	b	825	24	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	831	1	1/1/15/20	13/39/115/115	-
15	CLA	a	836	1	1/1/12/20	6/26/102/115	-
17	SF4	P	101	3	-	-	0/6/5/5
15	CLA	b	805	2	1/1/15/20	11/39/115/115	-
14	F6C	B	831	2	1/1/10/16	7/41/97/97	-
15	CLA	b	830	2	1/1/15/20	17/39/115/115	-
15	CLA	b	826	2	1/1/15/20	5/39/115/115	-
15	CLA	B	801	2	1/1/15/20	10/39/115/115	-
15	CLA	O	813	2	-	9/29/105/115	-
21	LMG	U	102	-	-	19/50/70/70	0/1/1/1
15	CLA	B	825	2	1/1/14/20	13/36/112/115	-
15	CLA	N	840	1	1/1/12/20	0/21/97/115	-
19	LHG	M	102	-	-	17/53/53/53	-
15	CLA	O	814	2	1/1/15/20	14/39/115/115	-
17	SF4	C	102	3	-	-	0/6/5/5
14	F6C	L	204	24	1/1/10/16	11/41/97/97	-
18	BCR	a	848	-	-	6/29/63/63	0/2/2/2
21	LMG	A	855	-	-	10/39/59/70	0/1/1/1
18	BCR	b	846	-	-	5/29/63/63	0/2/2/2
18	BCR	B	841	-	-	3/29/63/63	0/2/2/2
15	CLA	b	821	2	1/1/11/20	5/15/91/115	-
19	LHG	a	851	-	-	12/46/46/53	-
15	CLA	N	811	1	1/1/13/20	11/30/106/115	-
15	CLA	b	816	2	1/1/13/20	7/30/106/115	-
18	BCR	a	850	-	-	13/29/63/63	0/2/2/2
14	F6C	O	840	24	1/1/10/16	13/41/97/97	-
14	F6C	B	838	24	1/1/10/16	13/41/97/97	-
15	CLA	A	805	15,1	1/1/14/20	9/33/109/115	-
15	CLA	B	836	2	1/1/15/20	12/39/115/115	-
15	CLA	N	839	1	1/1/15/20	19/39/115/115	-
18	BCR	k	102	-	-	7/29/63/63	0/2/2/2
15	CLA	a	804	1	1/1/15/20	6/39/115/115	-
15	CLA	O	803	-	1/1/15/20	6/39/115/115	-
18	BCR	B	843	-	-	4/29/63/63	0/2/2/2
18	BCR	h	101	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	810	1	1/1/13/20	6/30/106/115	-
15	CLA	O	841	2	1/1/15/20	15/39/115/115	-
15	CLA	a	842	1	1/1/15/20	12/39/115/115	-
15	CLA	B	810	2	1/1/11/20	5/15/91/115	-
15	CLA	a	820	1	1/1/15/20	20/39/115/115	-
14	F6C	N	856	24	1/1/10/16	17/41/97/97	-
19	LHG	X	102	-	-	22/53/53/53	-
15	CLA	A	834	1	1/1/15/20	6/39/115/115	-
15	CLA	X	103	12	1/1/13/20	2/27/103/115	-
15	CLA	f	201	24	1/1/15/20	10/39/115/115	-
15	CLA	b	818	2	1/1/14/20	12/33/109/115	-
15	CLA	b	836	24	1/1/11/20	8/15/91/115	-
19	LHG	N	851	-	-	12/46/46/53	-
15	CLA	N	813	1	1/1/12/20	8/26/102/115	-
15	CLA	B	827	2	1/1/15/20	11/39/115/115	-
15	CLA	O	805	2	1/1/15/20	10/39/115/115	-
15	CLA	O	822	24	1/1/12/20	8/25/101/115	-
18	BCR	L	209	-	-	2/29/63/63	0/2/2/2
15	CLA	B	826	2	1/1/15/20	7/39/115/115	-
15	CLA	A	829	1	1/1/14/20	15/33/109/115	-
15	CLA	B	814	2	1/1/13/20	5/30/106/115	-
17	SF4	P	102	3	-	-	0/6/5/5
14	F6C	N	824	24	1/1/7/16	11/25/81/97	-
15	CLA	A	811	1	1/1/13/20	10/30/106/115	-
18	BCR	T	102	-	-	4/29/63/63	0/2/2/2
15	CLA	b	809	2	1/1/15/20	15/39/115/115	-
19	LHG	l	102	-	-	23/53/53/53	-
15	CLA	b	815	2	1/1/11/20	6/15/91/115	-
15	CLA	A	831	1	1/1/15/20	12/39/115/115	-
15	CLA	B	802	-	1/1/15/20	7/39/115/115	-
13	CL0	a	801	1	3/3/20/25	10/37/135/135	-
18	BCR	A	848	-	-	6/29/63/63	0/2/2/2
15	CLA	i	103	24	1/1/12/20	2/21/97/115	-
19	LHG	X	101	-	-	21/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b	820	2	1/1/13/20	13/27/103/115	-
18	BCR	a	847	-	-	6/29/63/63	0/2/2/2
15	CLA	A	828	1	1/1/15/20	5/39/115/115	-
15	CLA	A	835	1	1/1/15/20	6/39/115/115	-
18	BCR	B	846	-	-	4/29/63/63	0/2/2/2
15	CLA	V	102	9	1/1/11/20	8/15/91/115	-
15	CLA	O	806	2	1/1/15/20	16/39/115/115	-
15	CLA	b	804	2	1/1/15/20	8/39/115/115	-
15	CLA	i	102	9	1/1/11/20	6/15/91/115	-
15	CLA	K	102	9	1/1/11/20	6/15/91/115	-
15	CLA	B	811	2	-	9/29/105/115	-
18	BCR	B	844	-	-	8/29/63/63	0/2/2/2
20	LMT	A	852	-	-	1/17/57/61	0/2/2/2
15	CLA	L	202	10	1/1/15/20	7/39/115/115	-
15	CLA	B	820	24	1/1/12/20	10/25/101/115	-
18	BCR	F	202	-	-	6/29/63/63	0/2/2/2
15	CLA	L	203	10	1/1/14/20	12/33/109/115	-
21	LMG	L	206	-	-	12/45/65/70	0/1/1/1
16	PQN	b	842	-	-	0/23/43/43	0/2/2/2
15	CLA	N	807	1	1/1/15/20	19/39/115/115	-
15	CLA	B	807	2	1/1/15/20	10/39/115/115	-
15	CLA	O	811	2	1/1/15/20	9/39/115/115	-
15	CLA	A	842	1	1/1/15/20	11/39/115/115	-
18	BCR	N	857	-	-	9/29/63/63	0/2/2/2
15	CLA	Z	103	12	1/1/13/20	4/27/103/115	-
21	LMG	T	103	-	-	12/32/52/70	0/1/1/1
15	CLA	O	804	2	1/1/15/20	8/39/115/115	-
15	CLA	N	821	1	1/1/14/20	8/33/109/115	-
18	BCR	O	848	-	-	6/29/63/63	0/2/2/2
15	CLA	B	839	2	1/1/15/20	15/39/115/115	-
18	BCR	J	101	-	-	6/29/63/63	0/2/2/2
19	LHG	k	101	-	-	18/53/53/53	-
15	CLA	O	812	2	1/1/11/20	5/15/91/115	-
18	BCR	K	101	-	-	0/18/35/63	0/1/1/2
21	LMG	J	102	-	-	19/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	O	807	2	1/1/15/20	6/39/115/115	-
15	CLA	O	825	24	1/1/15/20	14/39/115/115	-
15	CLA	O	837	2	1/1/15/20	9/39/115/115	-
15	CLA	b	824	24	1/1/15/20	9/39/115/115	-
15	CLA	N	804	1	1/1/15/20	6/39/115/115	-
15	CLA	b	838	2	1/1/15/20	13/39/115/115	-
14	F6C	L	201	2	1/1/10/16	9/41/97/97	-
15	CLA	a	834	1	1/1/15/20	8/39/115/115	-
15	CLA	O	826	2	1/1/15/20	4/39/115/115	-
15	CLA	b	839	2	1/1/15/20	9/39/115/115	-
15	CLA	O	808	2	1/1/15/20	8/39/115/115	-
18	BCR	f	202	-	-	6/29/63/63	0/2/2/2
15	CLA	A	817	24	1/1/11/20	6/15/91/115	-
15	CLA	A	822	24	1/1/15/20	17/39/115/115	-
15	CLA	a	837	1	1/1/12/20	7/23/99/115	-
15	CLA	N	803	-	1/1/15/20	11/39/115/115	-
15	CLA	B	824	2	1/1/15/20	4/39/115/115	-
15	CLA	B	823	24	1/1/15/20	15/39/115/115	-

All (2175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	C1B-C2B	9.00	1.49	1.39
13	N	801	CL0	C1B-C2B	8.99	1.49	1.39
13	a	801	CL0	C1B-C2B	8.99	1.49	1.39
14	N	826	F6C	C2A-C3A	8.63	1.55	1.36
14	L	201	F6C	C2A-C3A	8.59	1.55	1.36
14	A	826	F6C	C2A-C3A	8.58	1.55	1.36
14	O	810	F6C	C2A-C3A	8.57	1.55	1.36
14	a	826	F6C	C2A-C3A	8.57	1.55	1.36
14	b	810	F6C	C2A-C3A	8.56	1.55	1.36
14	A	802	F6C	C2A-C3A	8.55	1.55	1.36
14	N	824	F6C	C2A-C3A	8.55	1.55	1.36
14	A	824	F6C	C2A-C3A	8.54	1.55	1.36
14	a	824	F6C	C2A-C3A	8.53	1.55	1.36
14	a	802	F6C	C2A-C3A	8.53	1.55	1.36
14	N	802	F6C	C2A-C3A	8.52	1.55	1.36
14	O	833	F6C	C2A-C3A	8.47	1.55	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	833	F6C	C2A-C3A	8.47	1.55	1.36
14	B	831	F6C	C2A-C3A	8.43	1.55	1.36
14	B	838	F6C	C2A-C3A	8.40	1.54	1.36
14	W	1503	F6C	C2A-C3A	8.40	1.54	1.36
14	b	840	F6C	C2A-C3A	8.39	1.54	1.36
14	O	840	F6C	C2A-C3A	8.39	1.54	1.36
14	j	204	F6C	C2A-C3A	8.36	1.54	1.36
14	L	204	F6C	C2A-C3A	8.34	1.54	1.36
14	a	856	F6C	C2A-C3A	8.23	1.54	1.36
14	N	856	F6C	C2A-C3A	8.22	1.54	1.36
14	A	857	F6C	C2A-C3A	8.20	1.54	1.36
13	a	801	CL0	C3B-C4B	7.88	1.49	1.41
13	A	801	CL0	C3B-C4B	7.85	1.49	1.41
13	N	801	CL0	C3B-C4B	7.84	1.49	1.41
13	A	801	CL0	C1D-C2D	7.77	1.48	1.39
13	N	801	CL0	C1D-C2D	7.73	1.48	1.39
13	a	801	CL0	C1D-C2D	7.64	1.48	1.39
14	L	204	F6C	C4A-C3A	4.17	1.53	1.45
13	A	801	CL0	C3D-C4D	4.17	1.47	1.41
13	a	801	CL0	C3D-C4D	4.14	1.47	1.41
14	N	826	F6C	C4A-C3A	4.14	1.53	1.45
14	L	201	F6C	C1A-C2A	4.13	1.54	1.45
13	N	801	CL0	C3D-C4D	4.12	1.47	1.41
14	b	810	F6C	C1A-C2A	4.11	1.54	1.45
14	O	840	F6C	C4A-C3A	4.09	1.53	1.45
14	j	204	F6C	C4A-C3A	4.09	1.53	1.45
14	A	824	F6C	C4A-C3A	4.09	1.53	1.45
14	B	838	F6C	C4A-C3A	4.08	1.53	1.45
14	N	824	F6C	C4A-C3A	4.07	1.53	1.45
14	b	840	F6C	C4A-C3A	4.07	1.53	1.45
14	O	810	F6C	C1A-C2A	4.07	1.54	1.45
14	W	1503	F6C	C4A-C3A	4.06	1.53	1.45
14	a	824	F6C	C4A-C3A	4.05	1.53	1.45
14	A	802	F6C	C4A-C3A	4.04	1.53	1.45
14	N	826	F6C	C1A-C2A	4.03	1.53	1.45
14	N	802	F6C	C4A-C3A	4.03	1.53	1.45
14	a	826	F6C	C1A-C2A	4.03	1.53	1.45
14	a	802	F6C	C4A-C3A	4.02	1.53	1.45
14	A	826	F6C	C1A-C2A	4.01	1.53	1.45
14	a	826	F6C	C4A-C3A	4.01	1.53	1.45
14	O	833	F6C	C4A-C3A	4.00	1.53	1.45
14	b	833	F6C	C4A-C3A	3.99	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	826	F6C	C4A-C3A	3.98	1.53	1.45
14	B	831	F6C	C4A-C3A	3.98	1.53	1.45
14	N	856	F6C	C4A-C3A	3.94	1.53	1.45
14	a	856	F6C	C4A-C3A	3.93	1.53	1.45
14	A	857	F6C	C4A-C3A	3.91	1.53	1.45
14	O	810	F6C	C4A-C3A	3.83	1.52	1.45
14	b	810	F6C	C4A-C3A	3.82	1.52	1.45
14	L	201	F6C	C4A-C3A	3.78	1.52	1.45
14	N	824	F6C	C1A-C2A	3.72	1.53	1.45
14	A	824	F6C	C1A-C2A	3.72	1.53	1.45
14	a	824	F6C	C1A-C2A	3.71	1.53	1.45
15	O	815	CLA	C1D-ND	3.67	1.42	1.37
15	b	815	CLA	C1D-ND	3.67	1.42	1.37
14	a	802	F6C	C1A-C2A	3.66	1.53	1.45
14	b	833	F6C	C1A-C2A	3.66	1.53	1.45
14	O	833	F6C	C1A-C2A	3.66	1.53	1.45
14	A	802	F6C	C1A-C2A	3.64	1.53	1.45
15	b	813	CLA	C1D-ND	3.64	1.42	1.37
15	O	813	CLA	C1D-ND	3.63	1.42	1.37
14	B	831	F6C	C1A-C2A	3.63	1.53	1.45
14	N	802	F6C	C1A-C2A	3.62	1.53	1.45
15	B	811	CLA	C1D-ND	3.62	1.42	1.37
15	N	806	CLA	C1D-ND	3.61	1.42	1.37
14	W	1503	F6C	C1A-C2A	3.61	1.53	1.45
14	L	204	F6C	C1A-C2A	3.58	1.53	1.45
15	N	815	CLA	C1D-ND	3.57	1.42	1.37
14	j	204	F6C	C1A-C2A	3.57	1.53	1.45
15	A	828	CLA	C1D-ND	3.57	1.42	1.37
15	A	817	CLA	C1D-ND	3.57	1.42	1.37
15	a	811	CLA	C1D-ND	3.56	1.42	1.37
15	A	815	CLA	C1D-ND	3.55	1.42	1.37
15	a	815	CLA	C1D-ND	3.55	1.42	1.37
15	N	811	CLA	C1D-ND	3.55	1.42	1.37
15	a	817	CLA	C1D-ND	3.55	1.42	1.37
15	A	811	CLA	C1D-ND	3.55	1.42	1.37
15	N	817	CLA	C1D-ND	3.55	1.42	1.37
15	N	804	CLA	C1D-ND	3.55	1.42	1.37
15	a	814	CLA	C1D-ND	3.55	1.42	1.37
15	A	804	CLA	C1D-ND	3.55	1.42	1.37
15	O	826	CLA	C1D-ND	3.55	1.42	1.37
15	A	814	CLA	C1D-ND	3.54	1.42	1.37
15	N	814	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	824	CLA	C1D-ND	3.54	1.42	1.37
15	V	102	CLA	C1D-ND	3.54	1.42	1.37
15	B	834	CLA	C1D-ND	3.53	1.42	1.37
15	O	832	CLA	C1D-ND	3.53	1.42	1.37
15	A	832	CLA	C1D-ND	3.53	1.42	1.37
15	N	822	CLA	C1D-ND	3.53	1.42	1.37
15	b	824	CLA	C1D-ND	3.53	1.42	1.37
15	N	832	CLA	C1D-ND	3.53	1.42	1.37
15	a	820	CLA	C1D-ND	3.53	1.42	1.37
15	N	820	CLA	C1D-ND	3.53	1.42	1.37
15	a	837	CLA	C1D-ND	3.53	1.42	1.37
15	A	822	CLA	C1D-ND	3.53	1.42	1.37
15	N	837	CLA	C1D-ND	3.53	1.42	1.37
15	b	839	CLA	C1D-ND	3.53	1.42	1.37
15	N	840	CLA	C1D-ND	3.52	1.42	1.37
15	a	840	CLA	C1D-ND	3.52	1.42	1.37
15	i	102	CLA	C1D-ND	3.52	1.42	1.37
15	K	102	CLA	C1D-ND	3.52	1.42	1.37
15	a	822	CLA	C1D-ND	3.52	1.42	1.37
15	b	836	CLA	C1D-ND	3.52	1.42	1.37
15	b	832	CLA	C1D-ND	3.52	1.42	1.37
15	a	804	CLA	C1D-ND	3.52	1.42	1.37
15	A	808	CLA	C1D-ND	3.52	1.42	1.37
15	O	812	CLA	C1D-ND	3.52	1.42	1.37
15	a	828	CLA	C1D-ND	3.52	1.42	1.37
15	A	819	CLA	C1D-ND	3.52	1.42	1.37
15	A	837	CLA	C1D-ND	3.52	1.42	1.37
15	N	823	CLA	C1D-ND	3.51	1.42	1.37
15	A	840	CLA	C1D-ND	3.51	1.42	1.37
15	B	810	CLA	C1D-ND	3.51	1.42	1.37
15	b	817	CLA	C1D-ND	3.51	1.42	1.37
15	b	822	CLA	C1D-ND	3.51	1.42	1.37
15	B	814	CLA	C1D-ND	3.51	1.42	1.37
15	N	808	CLA	C1D-ND	3.51	1.42	1.37
15	O	836	CLA	C1D-ND	3.51	1.42	1.37
15	b	812	CLA	C1D-ND	3.51	1.42	1.37
15	b	814	CLA	C1D-ND	3.51	1.42	1.37
15	B	815	CLA	C1D-ND	3.51	1.42	1.37
15	N	828	CLA	C1D-ND	3.51	1.42	1.37
15	N	807	CLA	C1D-ND	3.51	1.42	1.37
15	O	825	CLA	C1D-ND	3.51	1.42	1.37
15	a	831	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	820	CLA	C1D-ND	3.51	1.42	1.37
15	B	837	CLA	C1D-ND	3.51	1.42	1.37
15	A	809	CLA	C1D-ND	3.51	1.42	1.37
15	b	826	CLA	C1D-ND	3.51	1.42	1.37
15	B	822	CLA	C1D-ND	3.51	1.42	1.37
15	i	103	CLA	C1D-ND	3.51	1.42	1.37
15	O	806	CLA	C1D-ND	3.50	1.42	1.37
15	a	816	CLA	C1D-ND	3.50	1.42	1.37
15	B	817	CLA	C1D-ND	3.50	1.42	1.37
15	B	824	CLA	C1D-ND	3.50	1.42	1.37
15	B	830	CLA	C1D-ND	3.50	1.42	1.37
15	b	834	CLA	C1D-ND	3.50	1.42	1.37
15	O	816	CLA	C1D-ND	3.50	1.42	1.37
15	N	816	CLA	C1D-ND	3.50	1.42	1.37
15	O	814	CLA	C1D-ND	3.50	1.42	1.37
15	O	839	CLA	C1D-ND	3.50	1.42	1.37
15	a	808	CLA	C1D-ND	3.50	1.42	1.37
15	X	103	CLA	C1D-ND	3.50	1.42	1.37
15	N	842	CLA	C1D-ND	3.50	1.42	1.37
15	b	819	CLA	C1D-ND	3.50	1.42	1.37
15	A	816	CLA	C1D-ND	3.50	1.42	1.37
15	B	813	CLA	C1D-ND	3.50	1.42	1.37
15	B	819	CLA	C1D-ND	3.50	1.42	1.37
15	O	817	CLA	C1D-ND	3.50	1.42	1.37
15	Z	103	CLA	C1D-ND	3.50	1.42	1.37
15	a	809	CLA	C1D-ND	3.50	1.42	1.37
15	b	816	CLA	C1D-ND	3.50	1.42	1.37
15	O	819	CLA	C1D-ND	3.50	1.42	1.37
15	N	809	CLA	C1D-ND	3.50	1.42	1.37
15	a	807	CLA	C1D-ND	3.49	1.42	1.37
15	K	103	CLA	C1D-ND	3.49	1.42	1.37
15	b	829	CLA	C1D-ND	3.49	1.42	1.37
15	O	822	CLA	C1D-ND	3.49	1.42	1.37
15	a	832	CLA	C1D-ND	3.49	1.42	1.37
15	B	823	CLA	C1D-ND	3.49	1.42	1.37
15	O	821	CLA	C1D-ND	3.49	1.42	1.37
15	V	103	CLA	C1D-ND	3.49	1.42	1.37
15	b	804	CLA	C1D-ND	3.49	1.42	1.37
14	B	838	F6C	C1A-C2A	3.49	1.52	1.45
15	b	820	CLA	C1D-ND	3.49	1.42	1.37
15	N	825	CLA	C1D-ND	3.49	1.42	1.37
15	b	821	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	807	CLA	C1D-ND	3.49	1.42	1.37
14	O	840	F6C	C1A-C2A	3.49	1.52	1.45
15	A	823	CLA	C1D-ND	3.49	1.42	1.37
15	B	818	CLA	C1D-ND	3.49	1.42	1.37
15	b	835	CLA	C1D-ND	3.49	1.42	1.37
15	b	825	CLA	C1D-ND	3.48	1.42	1.37
15	l	103	CLA	C1D-ND	3.48	1.42	1.37
15	B	825	CLA	C1D-ND	3.48	1.42	1.37
15	B	806	CLA	C1D-ND	3.48	1.42	1.37
15	B	820	CLA	C1D-ND	3.48	1.42	1.37
15	B	832	CLA	C1D-ND	3.48	1.42	1.37
15	a	821	CLA	C1D-ND	3.48	1.42	1.37
15	A	806	CLA	C1D-ND	3.48	1.42	1.37
15	O	841	CLA	C1D-ND	3.48	1.42	1.37
14	N	856	F6C	C1A-C2A	3.48	1.52	1.45
15	N	819	CLA	C1D-ND	3.48	1.42	1.37
15	a	823	CLA	C1D-ND	3.48	1.42	1.37
15	a	806	CLA	C1D-ND	3.48	1.42	1.37
15	A	813	CLA	C1D-ND	3.48	1.42	1.37
15	O	834	CLA	C1D-ND	3.48	1.42	1.37
14	b	840	F6C	C1A-C2A	3.48	1.52	1.45
14	a	856	F6C	C1A-C2A	3.48	1.52	1.45
15	a	819	CLA	C1D-ND	3.47	1.42	1.37
15	N	833	CLA	C1D-ND	3.47	1.42	1.37
15	a	835	CLA	C1D-ND	3.47	1.42	1.37
15	O	820	CLA	C1D-ND	3.47	1.42	1.37
15	O	831	CLA	C1D-ND	3.47	1.42	1.37
15	a	813	CLA	C1D-ND	3.47	1.42	1.37
15	A	842	CLA	C1D-ND	3.47	1.42	1.37
15	N	821	CLA	C1D-ND	3.47	1.42	1.37
15	b	806	CLA	C1D-ND	3.47	1.42	1.37
15	j	203	CLA	C1D-ND	3.47	1.42	1.37
15	B	805	CLA	C1D-ND	3.47	1.42	1.37
15	O	804	CLA	C1D-ND	3.47	1.42	1.37
15	N	813	CLA	C1D-ND	3.46	1.42	1.37
15	O	829	CLA	C1D-ND	3.46	1.42	1.37
15	b	811	CLA	C1D-ND	3.46	1.42	1.37
15	O	807	CLA	C1D-ND	3.46	1.42	1.37
15	b	827	CLA	C1D-ND	3.46	1.42	1.37
15	N	812	CLA	C1D-ND	3.46	1.42	1.37
15	b	818	CLA	C1D-ND	3.46	1.42	1.37
15	b	801	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	801	CLA	C1D-ND	3.46	1.42	1.37
15	A	812	CLA	C1D-ND	3.46	1.42	1.37
15	A	825	CLA	C1D-ND	3.46	1.42	1.37
15	B	812	CLA	C1D-ND	3.46	1.42	1.37
15	B	827	CLA	C1D-ND	3.46	1.42	1.37
15	N	835	CLA	C1D-ND	3.46	1.42	1.37
15	a	838	CLA	C1D-ND	3.46	1.42	1.37
15	A	838	CLA	C1D-ND	3.46	1.42	1.37
15	O	818	CLA	C1D-ND	3.46	1.42	1.37
15	N	838	CLA	C1D-ND	3.46	1.42	1.37
15	O	811	CLA	C1D-ND	3.46	1.42	1.37
15	b	831	CLA	C1D-ND	3.46	1.42	1.37
15	B	829	CLA	C1D-ND	3.45	1.42	1.37
15	A	821	CLA	C1D-ND	3.45	1.42	1.37
15	O	827	CLA	C1D-ND	3.45	1.42	1.37
15	a	839	CLA	C1D-ND	3.45	1.42	1.37
15	B	839	CLA	C1D-ND	3.45	1.42	1.37
15	B	804	CLA	C1D-ND	3.45	1.42	1.37
15	B	816	CLA	C1D-ND	3.45	1.42	1.37
15	a	842	CLA	C1D-ND	3.45	1.42	1.37
15	O	830	CLA	C1D-ND	3.45	1.42	1.37
15	O	837	CLA	C1D-ND	3.45	1.42	1.37
14	A	857	F6C	C1A-C2A	3.44	1.52	1.45
15	O	823	CLA	C1D-ND	3.44	1.42	1.37
15	a	825	CLA	C1D-ND	3.44	1.42	1.37
15	A	831	CLA	C1D-ND	3.44	1.42	1.37
15	B	833	CLA	C1D-ND	3.44	1.42	1.37
15	O	805	CLA	C1D-ND	3.44	1.42	1.37
15	b	805	CLA	C1D-ND	3.44	1.42	1.37
15	A	827	CLA	C1D-ND	3.44	1.42	1.37
15	B	801	CLA	C1D-ND	3.44	1.42	1.37
15	a	805	CLA	C1D-ND	3.44	1.42	1.37
15	b	841	CLA	C1D-ND	3.44	1.42	1.37
15	B	803	CLA	C1D-ND	3.44	1.42	1.37
15	N	839	CLA	C1D-ND	3.44	1.42	1.37
15	a	812	CLA	C1D-ND	3.44	1.42	1.37
15	b	807	CLA	C1D-ND	3.44	1.42	1.37
15	N	805	CLA	C1D-ND	3.43	1.42	1.37
15	A	829	CLA	C1D-ND	3.43	1.42	1.37
15	a	829	CLA	C1D-ND	3.43	1.42	1.37
15	A	805	CLA	C1D-ND	3.43	1.42	1.37
15	S	201	CLA	C1D-ND	3.43	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	809	CLA	C1D-ND	3.43	1.42	1.37
15	O	835	CLA	C1D-ND	3.43	1.42	1.37
15	N	834	CLA	C1D-ND	3.43	1.42	1.37
15	a	830	CLA	C1D-ND	3.43	1.42	1.37
15	a	841	CLA	C1D-ND	3.43	1.42	1.37
15	b	838	CLA	C1D-ND	3.43	1.42	1.37
15	A	835	CLA	C1D-ND	3.42	1.42	1.37
15	A	836	CLA	C1D-ND	3.42	1.42	1.37
15	b	830	CLA	C1D-ND	3.42	1.42	1.37
15	a	834	CLA	C1D-ND	3.42	1.42	1.37
15	B	835	CLA	C1D-ND	3.42	1.42	1.37
15	N	829	CLA	C1D-ND	3.42	1.42	1.37
15	A	834	CLA	C1D-ND	3.42	1.42	1.37
15	N	830	CLA	C1D-ND	3.42	1.42	1.37
15	O	838	CLA	C1D-ND	3.42	1.42	1.37
15	N	831	CLA	C1D-ND	3.42	1.42	1.37
15	W	1502	CLA	C1D-ND	3.42	1.42	1.37
15	a	836	CLA	C1D-ND	3.42	1.42	1.37
15	A	841	CLA	C1D-ND	3.42	1.42	1.37
15	F	201	CLA	C1D-ND	3.42	1.42	1.37
15	N	841	CLA	C1D-ND	3.41	1.42	1.37
15	A	830	CLA	C1D-ND	3.41	1.42	1.37
15	A	839	CLA	C1D-ND	3.41	1.42	1.37
15	a	833	CLA	C1D-ND	3.41	1.42	1.37
15	b	802	CLA	C1D-ND	3.41	1.42	1.37
15	f	201	CLA	C1D-ND	3.41	1.42	1.37
15	N	827	CLA	C1D-ND	3.41	1.42	1.37
15	b	837	CLA	C1D-ND	3.40	1.42	1.37
15	N	810	CLA	C1D-ND	3.40	1.42	1.37
15	a	827	CLA	C1D-ND	3.40	1.42	1.37
15	b	809	CLA	C1D-ND	3.40	1.42	1.37
15	B	807	CLA	C1D-ND	3.40	1.42	1.37
15	A	833	CLA	C1D-ND	3.40	1.42	1.37
15	L	203	CLA	C1D-ND	3.40	1.42	1.37
15	B	828	CLA	C1D-ND	3.40	1.42	1.37
15	O	802	CLA	C1D-ND	3.40	1.42	1.37
15	A	810	CLA	C1D-ND	3.39	1.42	1.37
15	B	836	CLA	C1D-ND	3.39	1.42	1.37
15	N	836	CLA	C1D-ND	3.39	1.42	1.37
15	a	810	CLA	C1D-ND	3.39	1.42	1.37
15	b	808	CLA	C1D-ND	3.38	1.42	1.37
15	O	808	CLA	C1D-ND	3.37	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	828	CLA	C1D-ND	3.36	1.42	1.37
15	B	826	CLA	C1D-ND	3.36	1.42	1.37
15	O	828	CLA	C1D-ND	3.36	1.42	1.37
15	A	856	CLA	C1D-ND	3.35	1.42	1.37
15	b	823	CLA	C1D-ND	3.34	1.42	1.37
15	a	803	CLA	C1D-ND	3.34	1.42	1.37
15	A	803	CLA	C1D-ND	3.34	1.42	1.37
15	b	803	CLA	C1D-ND	3.33	1.42	1.37
15	B	821	CLA	C1D-ND	3.33	1.42	1.37
15	N	803	CLA	C1D-ND	3.33	1.42	1.37
15	O	803	CLA	C1D-ND	3.31	1.42	1.37
15	B	802	CLA	C1D-ND	3.31	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	B	808	CLA	C1D-ND	3.29	1.42	1.37
15	W	1501	CLA	C1D-ND	3.26	1.42	1.37
15	j	202	CLA	C1D-ND	3.24	1.42	1.37
15	a	804	CLA	C4B-NB	3.22	1.42	1.37
15	A	804	CLA	C4B-NB	3.19	1.42	1.37
15	N	804	CLA	C4B-NB	3.18	1.42	1.37
15	O	836	CLA	C4B-NB	3.17	1.42	1.37
15	a	842	CLA	C4B-NB	3.17	1.42	1.37
15	A	816	CLA	C4B-NB	3.16	1.42	1.37
15	A	817	CLA	C4B-NB	3.16	1.42	1.37
15	b	836	CLA	C4B-NB	3.16	1.42	1.37
15	a	817	CLA	C4B-NB	3.15	1.42	1.37
15	N	816	CLA	C4B-NB	3.15	1.42	1.37
15	B	834	CLA	C4B-NB	3.15	1.42	1.37
15	N	842	CLA	C4B-NB	3.15	1.42	1.37
15	A	842	CLA	C4B-NB	3.15	1.42	1.37
15	a	816	CLA	C4B-NB	3.14	1.42	1.37
15	N	817	CLA	C4B-NB	3.14	1.42	1.37
15	N	818	CLA	C1D-ND	3.14	1.42	1.37
15	a	818	CLA	C1D-ND	3.13	1.42	1.37
15	K	103	CLA	C4B-NB	3.12	1.42	1.37
15	V	103	CLA	C4B-NB	3.12	1.42	1.37
15	A	818	CLA	C1D-ND	3.10	1.41	1.37
15	O	820	CLA	C4B-NB	3.10	1.41	1.37
15	i	103	CLA	C4B-NB	3.10	1.41	1.37
15	B	818	CLA	C4B-NB	3.09	1.41	1.37
15	F	201	CLA	C4B-NB	3.09	1.41	1.37
15	b	820	CLA	C4B-NB	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	S	201	CLA	C4B-NB	3.09	1.41	1.37
15	f	201	CLA	C4B-NB	3.08	1.41	1.37
15	N	822	CLA	C4B-NB	3.07	1.41	1.37
15	b	819	CLA	C4B-NB	3.07	1.41	1.37
15	O	819	CLA	C4B-NB	3.06	1.41	1.37
15	b	817	CLA	C4B-NB	3.06	1.41	1.37
15	a	819	CLA	C4B-NB	3.05	1.41	1.37
15	B	817	CLA	C4B-NB	3.05	1.41	1.37
15	A	812	CLA	C4B-NB	3.04	1.41	1.37
15	N	812	CLA	C4B-NB	3.03	1.41	1.37
15	B	810	CLA	C4B-NB	3.03	1.41	1.37
15	a	812	CLA	C4B-NB	3.03	1.41	1.37
15	N	819	CLA	C4B-NB	3.03	1.41	1.37
15	B	812	CLA	C4B-NB	3.02	1.41	1.37
15	b	812	CLA	C4B-NB	3.02	1.41	1.37
15	N	834	CLA	C4B-NB	3.02	1.41	1.37
15	a	805	CLA	C4B-NB	3.02	1.41	1.37
15	B	803	CLA	C4B-NB	3.01	1.41	1.37
15	a	822	CLA	C4B-NB	3.01	1.41	1.37
15	B	815	CLA	C4B-NB	3.01	1.41	1.37
15	A	805	CLA	C4B-NB	3.00	1.41	1.37
15	b	815	CLA	C4B-NB	3.00	1.41	1.37
15	B	830	CLA	C4B-NB	3.00	1.41	1.37
15	O	814	CLA	C4B-NB	3.00	1.41	1.37
15	b	818	CLA	C4B-NB	3.00	1.41	1.37
15	A	834	CLA	C4B-NB	3.00	1.41	1.37
15	A	819	CLA	C4B-NB	2.99	1.41	1.37
15	A	822	CLA	C4B-NB	2.99	1.41	1.37
15	A	841	CLA	C4B-NB	2.99	1.41	1.37
15	O	841	CLA	C4B-NB	2.99	1.41	1.37
15	O	812	CLA	C4B-NB	2.99	1.41	1.37
15	O	804	CLA	C4B-NB	2.99	1.41	1.37
15	N	825	CLA	C4B-NB	2.99	1.41	1.37
15	A	856	CLA	C4B-NB	2.99	1.41	1.37
15	a	818	CLA	C4B-NB	2.99	1.41	1.37
15	b	802	CLA	C4B-NB	2.99	1.41	1.37
15	N	823	CLA	C4B-NB	2.99	1.41	1.37
15	N	815	CLA	C4B-NB	2.98	1.41	1.37
15	K	102	CLA	C4B-NB	2.98	1.41	1.37
15	O	815	CLA	C4B-NB	2.98	1.41	1.37
15	i	102	CLA	C4B-NB	2.98	1.41	1.37
15	X	103	CLA	C4B-NB	2.98	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	805	CLA	C4B-NB	2.98	1.41	1.37
15	b	804	CLA	C4B-NB	2.98	1.41	1.37
15	Z	103	CLA	C4B-NB	2.98	1.41	1.37
15	a	815	CLA	C4B-NB	2.98	1.41	1.37
15	O	817	CLA	C4B-NB	2.98	1.41	1.37
15	A	815	CLA	C4B-NB	2.98	1.41	1.37
15	N	818	CLA	C4B-NB	2.98	1.41	1.37
15	O	832	CLA	C4B-NB	2.98	1.41	1.37
15	a	834	CLA	C4B-NB	2.97	1.41	1.37
15	l	103	CLA	C4B-NB	2.97	1.41	1.37
15	B	816	CLA	C4B-NB	2.97	1.41	1.37
15	b	814	CLA	C4B-NB	2.97	1.41	1.37
15	b	841	CLA	C4B-NB	2.97	1.41	1.37
15	O	818	CLA	C4B-NB	2.97	1.41	1.37
15	N	829	CLA	C4B-NB	2.97	1.41	1.37
15	N	835	CLA	C4B-NB	2.97	1.41	1.37
15	V	102	CLA	C4B-NB	2.97	1.41	1.37
15	a	825	CLA	C4B-NB	2.97	1.41	1.37
15	A	825	CLA	C4B-NB	2.97	1.41	1.37
15	A	835	CLA	C4B-NB	2.97	1.41	1.37
15	B	819	CLA	C4B-NB	2.97	1.41	1.37
15	A	821	CLA	C4B-NB	2.97	1.41	1.37
15	A	839	CLA	C4B-NB	2.97	1.41	1.37
15	N	821	CLA	C4B-NB	2.96	1.41	1.37
15	O	827	CLA	C4B-NB	2.96	1.41	1.37
15	a	841	CLA	C4B-NB	2.96	1.41	1.37
15	N	807	CLA	C4B-NB	2.96	1.41	1.37
15	a	821	CLA	C4B-NB	2.96	1.41	1.37
15	b	807	CLA	C4B-NB	2.96	1.41	1.37
15	A	823	CLA	C4B-NB	2.96	1.41	1.37
15	a	831	CLA	C4B-NB	2.96	1.41	1.37
15	b	827	CLA	C4B-NB	2.96	1.41	1.37
15	N	839	CLA	C4B-NB	2.95	1.41	1.37
15	a	835	CLA	C4B-NB	2.95	1.41	1.37
15	a	837	CLA	C4B-NB	2.95	1.41	1.37
15	a	839	CLA	C4B-NB	2.95	1.41	1.37
15	A	837	CLA	C4B-NB	2.95	1.41	1.37
15	O	829	CLA	C4B-NB	2.95	1.41	1.37
15	A	818	CLA	C4B-NB	2.95	1.41	1.37
15	N	841	CLA	C4B-NB	2.95	1.41	1.37
15	O	811	CLA	C4B-NB	2.95	1.41	1.37
15	B	827	CLA	C4B-NB	2.95	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	832	CLA	C4B-NB	2.95	1.41	1.37
15	b	821	CLA	C4B-NB	2.95	1.41	1.37
15	a	823	CLA	C4B-NB	2.95	1.41	1.37
15	A	831	CLA	C4B-NB	2.95	1.41	1.37
15	O	821	CLA	C4B-NB	2.95	1.41	1.37
15	N	811	CLA	C4B-NB	2.95	1.41	1.37
15	B	839	CLA	C4B-NB	2.94	1.41	1.37
15	O	835	CLA	C4B-NB	2.94	1.41	1.37
15	B	809	CLA	C4B-NB	2.94	1.41	1.37
15	B	825	CLA	C4B-NB	2.94	1.41	1.37
15	N	837	CLA	C4B-NB	2.94	1.41	1.37
15	O	807	CLA	C4B-NB	2.94	1.41	1.37
15	b	823	CLA	C4B-NB	2.94	1.41	1.37
15	a	829	CLA	C4B-NB	2.94	1.41	1.37
15	B	821	CLA	C4B-NB	2.94	1.41	1.37
15	O	831	CLA	C4B-NB	2.94	1.41	1.37
15	b	831	CLA	C4B-NB	2.93	1.41	1.37
15	b	829	CLA	C4B-NB	2.93	1.41	1.37
15	O	813	CLA	C4B-NB	2.93	1.41	1.37
15	N	831	CLA	C4B-NB	2.93	1.41	1.37
15	L	203	CLA	C4B-NB	2.93	1.41	1.37
15	W	1501	CLA	C4B-NB	2.93	1.41	1.37
15	W	1502	CLA	C4B-NB	2.93	1.41	1.37
15	b	811	CLA	C4B-NB	2.93	1.41	1.37
15	A	813	CLA	C4B-NB	2.93	1.41	1.37
15	B	811	CLA	C4B-NB	2.93	1.41	1.37
15	B	832	CLA	C4B-NB	2.93	1.41	1.37
15	a	813	CLA	C4B-NB	2.93	1.41	1.37
15	b	839	CLA	C4B-NB	2.93	1.41	1.37
15	j	203	CLA	C4B-NB	2.93	1.41	1.37
15	A	829	CLA	C4B-NB	2.93	1.41	1.37
15	a	808	CLA	C4B-NB	2.93	1.41	1.37
15	O	825	CLA	C4B-NB	2.93	1.41	1.37
15	B	829	CLA	C4B-NB	2.92	1.41	1.37
15	B	833	CLA	C4B-NB	2.92	1.41	1.37
15	b	834	CLA	C4B-NB	2.92	1.41	1.37
15	N	827	CLA	C4B-NB	2.92	1.41	1.37
15	a	827	CLA	C4B-NB	2.92	1.41	1.37
15	A	836	CLA	C4B-NB	2.92	1.41	1.37
15	N	813	CLA	C4B-NB	2.92	1.41	1.37
15	O	823	CLA	C4B-NB	2.92	1.41	1.37
15	O	830	CLA	C4B-NB	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	832	CLA	C4B-NB	2.92	1.41	1.37
15	b	835	CLA	C4B-NB	2.92	1.41	1.37
15	N	840	CLA	C4B-NB	2.92	1.41	1.37
15	a	807	CLA	C4B-NB	2.92	1.41	1.37
15	a	832	CLA	C4B-NB	2.92	1.41	1.37
15	A	811	CLA	C4B-NB	2.92	1.41	1.37
15	a	809	CLA	C4B-NB	2.92	1.41	1.37
15	B	823	CLA	C4B-NB	2.91	1.41	1.37
15	O	834	CLA	C4B-NB	2.91	1.41	1.37
15	a	836	CLA	C4B-NB	2.91	1.41	1.37
15	b	822	CLA	C4B-NB	2.91	1.41	1.37
15	B	837	CLA	C4B-NB	2.91	1.41	1.37
15	b	801	CLA	C1B-C2B	2.91	1.50	1.43
15	A	832	CLA	C4B-NB	2.91	1.41	1.37
15	a	840	CLA	C4B-NB	2.91	1.41	1.37
15	b	813	CLA	C4B-NB	2.91	1.41	1.37
15	b	825	CLA	C4B-NB	2.91	1.41	1.37
15	b	824	CLA	C4B-NB	2.91	1.41	1.37
15	A	807	CLA	C4B-NB	2.91	1.41	1.37
15	N	836	CLA	C4B-NB	2.91	1.41	1.37
15	O	824	CLA	C4B-NB	2.91	1.41	1.37
15	A	820	CLA	C4B-NB	2.91	1.41	1.37
15	a	811	CLA	C4B-NB	2.91	1.41	1.37
15	b	830	CLA	C4B-NB	2.91	1.41	1.37
15	b	805	CLA	C4B-NB	2.90	1.41	1.37
15	N	809	CLA	C4B-NB	2.90	1.41	1.37
15	B	828	CLA	C4B-NB	2.90	1.41	1.37
15	b	816	CLA	C4B-NB	2.90	1.41	1.37
14	N	856	F6C	C3B-C4B	2.90	1.50	1.44
14	A	857	F6C	C3B-C4B	2.90	1.50	1.44
15	B	801	CLA	C1B-C2B	2.90	1.49	1.43
15	N	808	CLA	C4B-NB	2.90	1.41	1.37
15	A	840	CLA	C4B-NB	2.90	1.41	1.37
15	O	822	CLA	C4B-NB	2.90	1.41	1.37
15	O	839	CLA	C4B-NB	2.90	1.41	1.37
15	B	814	CLA	C4B-NB	2.90	1.41	1.37
15	B	822	CLA	C4B-NB	2.89	1.41	1.37
15	A	809	CLA	C4B-NB	2.89	1.41	1.37
15	O	816	CLA	C4B-NB	2.89	1.41	1.37
15	B	836	CLA	C4B-NB	2.89	1.41	1.37
15	O	801	CLA	C1B-C2B	2.89	1.49	1.43
15	O	802	CLA	C4B-NB	2.89	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	804	CLA	C4B-NB	2.89	1.41	1.37
15	B	806	CLA	C4B-NB	2.88	1.41	1.37
15	O	808	CLA	C4B-NB	2.88	1.41	1.37
15	b	801	CLA	C4B-NB	2.88	1.41	1.37
15	b	828	CLA	C4B-NB	2.88	1.41	1.37
15	B	801	CLA	C4B-NB	2.88	1.41	1.37
15	B	826	CLA	C4B-NB	2.88	1.41	1.37
15	O	805	CLA	C4B-NB	2.88	1.41	1.37
15	O	809	CLA	C4B-NB	2.88	1.41	1.37
15	O	801	CLA	C4B-NB	2.88	1.41	1.37
15	a	810	CLA	C4B-NB	2.88	1.41	1.37
15	B	813	CLA	C4B-NB	2.88	1.41	1.37
15	L	202	CLA	C4B-NB	2.88	1.41	1.37
14	a	856	F6C	C3B-C4B	2.88	1.50	1.44
15	N	828	CLA	C4B-NB	2.88	1.41	1.37
15	B	824	CLA	C4B-NB	2.88	1.41	1.37
15	A	810	CLA	C4B-NB	2.87	1.41	1.37
15	a	828	CLA	C4B-NB	2.87	1.41	1.37
15	N	830	CLA	C4B-NB	2.87	1.41	1.37
15	b	838	CLA	C4B-NB	2.87	1.41	1.37
15	B	821	CLA	C1B-C2B	2.87	1.49	1.43
15	O	838	CLA	C4B-NB	2.87	1.41	1.37
15	A	830	CLA	C4B-NB	2.87	1.41	1.37
15	N	820	CLA	C4B-NB	2.87	1.41	1.37
15	B	820	CLA	C4B-NB	2.87	1.41	1.37
15	N	810	CLA	C4B-NB	2.87	1.41	1.37
14	N	824	F6C	C1D-ND	2.87	1.42	1.37
15	A	808	CLA	C4B-NB	2.86	1.41	1.37
15	N	833	CLA	C4B-NB	2.86	1.41	1.37
15	a	806	CLA	C4B-NB	2.86	1.41	1.37
15	B	835	CLA	C4B-NB	2.86	1.41	1.37
15	O	826	CLA	C4B-NB	2.86	1.41	1.37
15	b	823	CLA	C1B-C2B	2.86	1.49	1.43
15	O	828	CLA	C4B-NB	2.86	1.41	1.37
15	b	808	CLA	C4B-NB	2.86	1.41	1.37
15	A	827	CLA	C4B-NB	2.86	1.41	1.37
15	a	830	CLA	C4B-NB	2.86	1.41	1.37
15	A	833	CLA	C4B-NB	2.86	1.41	1.37
14	a	824	F6C	C1D-ND	2.86	1.42	1.37
15	b	826	CLA	C4B-NB	2.85	1.41	1.37
14	b	833	F6C	C1D-ND	2.85	1.42	1.37
15	A	803	CLA	C4B-NB	2.85	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	833	CLA	C4B-NB	2.85	1.41	1.37
15	b	809	CLA	C4B-NB	2.85	1.41	1.37
15	j	202	CLA	C4B-NB	2.85	1.41	1.37
15	a	803	CLA	C4B-NB	2.84	1.41	1.37
15	A	828	CLA	C4B-NB	2.84	1.41	1.37
14	O	833	F6C	C1D-ND	2.84	1.42	1.37
15	O	806	CLA	C4B-NB	2.84	1.41	1.37
15	b	815	CLA	C1B-C2B	2.84	1.49	1.43
14	b	810	F6C	C1D-ND	2.83	1.42	1.37
14	A	826	F6C	C1D-ND	2.83	1.42	1.37
14	B	831	F6C	C1D-ND	2.83	1.42	1.37
15	O	815	CLA	C1B-C2B	2.83	1.49	1.43
15	N	803	CLA	C4B-NB	2.83	1.41	1.37
15	B	807	CLA	C4B-NB	2.83	1.41	1.37
15	b	806	CLA	C4B-NB	2.83	1.41	1.37
14	N	826	F6C	C1D-ND	2.83	1.42	1.37
15	a	820	CLA	C4B-NB	2.82	1.41	1.37
14	L	204	F6C	C1D-ND	2.82	1.42	1.37
14	j	204	F6C	C1D-ND	2.82	1.42	1.37
15	B	808	CLA	C4B-NB	2.82	1.41	1.37
15	O	837	CLA	C4B-NB	2.82	1.41	1.37
15	b	837	CLA	C4B-NB	2.82	1.41	1.37
14	a	826	F6C	C1D-ND	2.82	1.42	1.37
15	A	838	CLA	C1B-C2B	2.82	1.49	1.43
15	a	838	CLA	C4B-NB	2.82	1.41	1.37
14	A	824	F6C	C1D-ND	2.81	1.42	1.37
15	A	806	CLA	C4B-NB	2.81	1.41	1.37
15	B	805	CLA	C4B-NB	2.81	1.41	1.37
14	O	810	F6C	C1D-ND	2.81	1.42	1.37
15	B	802	CLA	C4B-NB	2.81	1.41	1.37
15	A	838	CLA	C4B-NB	2.80	1.41	1.37
14	L	201	F6C	C1D-ND	2.80	1.42	1.37
14	N	802	F6C	C1D-ND	2.80	1.42	1.37
15	a	814	CLA	C4B-NB	2.80	1.41	1.37
15	N	814	CLA	C4B-NB	2.80	1.41	1.37
14	a	802	F6C	C1D-ND	2.80	1.42	1.37
15	b	803	CLA	C4B-NB	2.80	1.41	1.37
14	W	1503	F6C	C1D-ND	2.79	1.42	1.37
15	N	838	CLA	C4B-NB	2.79	1.41	1.37
15	a	838	CLA	C1B-C2B	2.79	1.49	1.43
15	A	814	CLA	C4B-NB	2.79	1.41	1.37
15	N	838	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	802	F6C	C1D-ND	2.78	1.42	1.37
15	i	102	CLA	C1B-C2B	2.77	1.49	1.43
15	N	806	CLA	C4B-NB	2.77	1.41	1.37
15	a	814	CLA	C1B-C2B	2.77	1.49	1.43
15	O	803	CLA	C4B-NB	2.77	1.41	1.37
15	N	815	CLA	C1B-C2B	2.76	1.49	1.43
15	V	102	CLA	C1B-C2B	2.76	1.49	1.43
15	N	814	CLA	C1B-C2B	2.76	1.49	1.43
15	K	102	CLA	C1B-C2B	2.76	1.49	1.43
15	A	815	CLA	C1B-C2B	2.76	1.49	1.43
15	O	811	CLA	C1B-C2B	2.75	1.49	1.43
15	N	823	CLA	C1B-C2B	2.75	1.49	1.43
15	A	807	CLA	C1B-C2B	2.75	1.49	1.43
15	a	815	CLA	C1B-C2B	2.74	1.49	1.43
15	N	821	CLA	C1B-C2B	2.74	1.49	1.43
15	a	828	CLA	C1B-C2B	2.74	1.49	1.43
15	B	809	CLA	C1B-C2B	2.74	1.49	1.43
15	A	814	CLA	C1B-C2B	2.74	1.49	1.43
15	a	818	CLA	C1B-C2B	2.74	1.49	1.43
15	a	807	CLA	C1B-C2B	2.74	1.49	1.43
14	N	856	F6C	C1D-ND	2.74	1.42	1.37
15	b	811	CLA	C1B-C2B	2.74	1.49	1.43
15	a	821	CLA	C1B-C2B	2.74	1.49	1.43
15	a	834	CLA	C1B-C2B	2.74	1.49	1.43
15	O	834	CLA	C1B-C2B	2.74	1.49	1.43
15	A	818	CLA	C1B-C2B	2.73	1.49	1.43
15	B	813	CLA	C1B-C2B	2.73	1.49	1.43
15	N	818	CLA	C1B-C2B	2.73	1.49	1.43
15	N	822	CLA	C1B-C2B	2.73	1.49	1.43
15	O	813	CLA	C1B-C2B	2.73	1.49	1.43
15	b	838	CLA	C1B-C2B	2.73	1.49	1.43
15	A	821	CLA	C1B-C2B	2.73	1.49	1.43
15	B	819	CLA	C1B-C2B	2.73	1.49	1.43
15	N	807	CLA	C1B-C2B	2.73	1.49	1.43
15	B	811	CLA	C1B-C2B	2.73	1.49	1.43
15	A	834	CLA	C1B-C2B	2.73	1.49	1.43
15	B	806	CLA	C1B-C2B	2.73	1.49	1.43
15	B	832	CLA	C1B-C2B	2.73	1.49	1.43
15	O	821	CLA	C1B-C2B	2.73	1.49	1.43
15	l	103	CLA	C1B-C2B	2.73	1.49	1.43
15	a	823	CLA	C1B-C2B	2.73	1.49	1.43
15	b	821	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	836	CLA	C1B-C2B	2.73	1.49	1.43
14	A	857	F6C	C1D-ND	2.73	1.42	1.37
15	O	807	CLA	C1B-C2B	2.73	1.49	1.43
15	b	834	CLA	C1B-C2B	2.72	1.49	1.43
15	b	827	CLA	C1B-C2B	2.72	1.49	1.43
15	O	838	CLA	C1B-C2B	2.72	1.49	1.43
15	X	103	CLA	C1B-C2B	2.72	1.49	1.43
15	Z	103	CLA	C1B-C2B	2.72	1.49	1.43
14	a	856	F6C	C1D-ND	2.72	1.42	1.37
15	A	823	CLA	C1B-C2B	2.72	1.49	1.43
15	b	807	CLA	C1B-C2B	2.72	1.49	1.43
15	N	828	CLA	C1B-C2B	2.72	1.49	1.43
15	a	822	CLA	C1B-C2B	2.72	1.49	1.43
15	B	818	CLA	C1B-C2B	2.71	1.49	1.43
15	O	823	CLA	C1B-C2B	2.71	1.49	1.43
15	O	816	CLA	C1B-C2B	2.71	1.49	1.43
15	O	806	CLA	C1B-C2B	2.71	1.49	1.43
15	A	809	CLA	C1B-C2B	2.71	1.49	1.43
15	b	806	CLA	C1B-C2B	2.71	1.49	1.43
15	A	806	CLA	C1B-C2B	2.71	1.49	1.43
15	b	814	CLA	C1B-C2B	2.71	1.49	1.43
15	O	830	CLA	C1B-C2B	2.71	1.49	1.43
15	B	814	CLA	C1B-C2B	2.71	1.49	1.43
15	A	811	CLA	C1B-C2B	2.70	1.49	1.43
15	b	816	CLA	C1B-C2B	2.70	1.49	1.43
15	b	830	CLA	C1B-C2B	2.70	1.49	1.43
15	N	813	CLA	C1B-C2B	2.70	1.49	1.43
15	N	834	CLA	C1B-C2B	2.70	1.49	1.43
15	b	820	CLA	C1B-C2B	2.70	1.49	1.43
15	N	842	CLA	C1B-C2B	2.70	1.49	1.43
15	A	808	CLA	C1B-C2B	2.70	1.49	1.43
15	N	809	CLA	C1B-C2B	2.70	1.49	1.43
15	O	820	CLA	C1B-C2B	2.70	1.49	1.43
13	a	801	CL0	CMD-C2D	-2.70	1.46	1.51
15	B	820	CLA	C1B-C2B	2.70	1.49	1.43
15	A	813	CLA	C1B-C2B	2.70	1.49	1.43
15	O	827	CLA	C1B-C2B	2.70	1.49	1.43
15	b	822	CLA	C1B-C2B	2.70	1.49	1.43
15	A	822	CLA	C1B-C2B	2.70	1.49	1.43
15	a	809	CLA	C1B-C2B	2.70	1.49	1.43
15	N	808	CLA	C1B-C2B	2.70	1.49	1.43
15	a	813	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	828	CLA	C1B-C2B	2.70	1.49	1.43
15	b	813	CLA	C1B-C2B	2.70	1.49	1.43
15	B	825	CLA	C1B-C2B	2.69	1.49	1.43
15	O	826	CLA	C1B-C2B	2.69	1.49	1.43
15	a	808	CLA	C1B-C2B	2.69	1.49	1.43
15	N	832	CLA	C1B-C2B	2.69	1.49	1.43
15	B	826	CLA	C1B-C2B	2.69	1.49	1.43
15	N	830	CLA	C1B-C2B	2.69	1.49	1.43
15	a	811	CLA	C1B-C2B	2.69	1.49	1.43
15	a	806	CLA	C1B-C2B	2.69	1.49	1.43
15	A	836	CLA	C1B-C2B	2.69	1.49	1.43
15	N	836	CLA	C1B-C2B	2.69	1.49	1.43
15	B	812	CLA	C1B-C2B	2.69	1.49	1.43
15	A	829	CLA	C1B-C2B	2.69	1.49	1.43
15	a	842	CLA	C1B-C2B	2.69	1.49	1.43
13	N	801	CL0	CMD-C2D	-2.69	1.46	1.51
15	N	840	CLA	C1B-C2B	2.69	1.49	1.43
15	O	814	CLA	C1B-C2B	2.69	1.49	1.43
15	N	811	CLA	C1B-C2B	2.69	1.49	1.43
15	b	826	CLA	C1B-C2B	2.69	1.49	1.43
15	a	830	CLA	C1B-C2B	2.68	1.49	1.43
15	O	841	CLA	C1B-C2B	2.68	1.49	1.43
15	b	841	CLA	C1B-C2B	2.68	1.49	1.43
15	B	805	CLA	C1B-C2B	2.68	1.49	1.43
15	O	828	CLA	C1B-C2B	2.68	1.49	1.43
15	O	839	CLA	C1B-C2B	2.68	1.49	1.43
15	B	824	CLA	C1B-C2B	2.68	1.49	1.43
15	a	836	CLA	C1B-C2B	2.68	1.49	1.43
15	a	837	CLA	C1B-C2B	2.68	1.49	1.43
15	B	804	CLA	C1B-C2B	2.68	1.49	1.43
15	B	839	CLA	C1B-C2B	2.68	1.49	1.43
15	b	832	CLA	C1B-C2B	2.68	1.49	1.43
15	B	837	CLA	C1B-C2B	2.68	1.49	1.43
15	N	810	CLA	C1B-C2B	2.68	1.49	1.43
15	a	832	CLA	C1B-C2B	2.68	1.49	1.43
15	N	806	CLA	C1B-C2B	2.67	1.49	1.43
15	B	830	CLA	C1B-C2B	2.67	1.49	1.43
15	O	824	CLA	C1B-C2B	2.67	1.49	1.43
15	O	832	CLA	C1B-C2B	2.67	1.49	1.43
15	b	839	CLA	C1B-C2B	2.67	1.49	1.43
15	A	830	CLA	C1B-C2B	2.67	1.49	1.43
15	A	842	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	837	CLA	C1B-C2B	2.67	1.49	1.43
15	b	828	CLA	C1B-C2B	2.67	1.49	1.43
15	A	810	CLA	C1B-C2B	2.67	1.49	1.43
15	O	805	CLA	C1B-C2B	2.67	1.49	1.43
15	A	812	CLA	C1B-C2B	2.67	1.49	1.43
15	O	803	CLA	C1B-C2B	2.67	1.49	1.43
15	b	805	CLA	C1B-C2B	2.67	1.49	1.43
15	N	837	CLA	C1B-C2B	2.66	1.49	1.43
15	a	810	CLA	C1B-C2B	2.66	1.49	1.43
15	a	840	CLA	C1B-C2B	2.66	1.49	1.43
15	A	840	CLA	C1B-C2B	2.66	1.49	1.43
15	A	832	CLA	C1B-C2B	2.66	1.49	1.43
15	O	822	CLA	C1B-C2B	2.66	1.49	1.43
15	N	829	CLA	C1B-C2B	2.66	1.49	1.43
15	i	103	CLA	C1B-C2B	2.66	1.49	1.43
15	B	835	CLA	C1B-C2B	2.66	1.49	1.43
15	b	836	CLA	C1B-C2B	2.66	1.49	1.43
15	B	822	CLA	C1B-C2B	2.66	1.49	1.43
15	O	836	CLA	C1B-C2B	2.66	1.49	1.43
15	f	201	CLA	C1B-C2B	2.66	1.49	1.43
15	A	831	CLA	C1B-C2B	2.66	1.49	1.43
15	B	828	CLA	C1B-C2B	2.66	1.49	1.43
15	O	809	CLA	C1B-C2B	2.66	1.49	1.43
15	a	804	CLA	C3B-C4B	2.66	1.50	1.42
15	B	834	CLA	C1B-C2B	2.65	1.49	1.43
15	N	804	CLA	C3B-C4B	2.65	1.50	1.42
15	L	202	CLA	C1B-C2B	2.65	1.49	1.43
15	N	812	CLA	C1B-C2B	2.65	1.49	1.43
15	j	203	CLA	C1B-C2B	2.65	1.49	1.43
15	b	824	CLA	C1B-C2B	2.65	1.49	1.43
15	W	1501	CLA	C1B-C2B	2.65	1.49	1.43
15	N	805	CLA	C1B-C2B	2.65	1.49	1.43
15	b	831	CLA	C1B-C2B	2.65	1.49	1.43
15	a	819	CLA	C1B-C2B	2.65	1.49	1.43
15	a	829	CLA	C1B-C2B	2.65	1.49	1.43
15	a	812	CLA	C1B-C2B	2.65	1.49	1.43
15	F	201	CLA	C1B-C2B	2.65	1.49	1.43
14	O	840	F6C	C1D-ND	2.65	1.42	1.37
15	a	805	CLA	C1B-C2B	2.65	1.49	1.43
15	b	812	CLA	C1B-C2B	2.65	1.49	1.43
15	a	825	CLA	C1B-C2B	2.65	1.49	1.43
15	B	829	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	841	CLA	C1B-C2B	2.64	1.49	1.43
15	A	805	CLA	C1B-C2B	2.64	1.49	1.43
15	O	837	CLA	C1B-C2B	2.64	1.49	1.43
15	N	825	CLA	C1B-C2B	2.64	1.49	1.43
15	j	202	CLA	C1B-C2B	2.64	1.49	1.43
15	N	831	CLA	C1B-C2B	2.64	1.49	1.43
15	O	831	CLA	C1B-C2B	2.64	1.49	1.43
15	b	804	CLA	C1B-C2B	2.64	1.49	1.43
15	A	804	CLA	C3B-C4B	2.64	1.50	1.42
15	A	825	CLA	C1B-C2B	2.64	1.49	1.43
15	O	812	CLA	C1B-C2B	2.64	1.49	1.43
15	N	819	CLA	C1B-C2B	2.64	1.49	1.43
15	a	831	CLA	C1B-C2B	2.64	1.49	1.43
15	A	841	CLA	C1B-C2B	2.63	1.49	1.43
15	B	810	CLA	C1B-C2B	2.63	1.49	1.43
15	O	802	CLA	C1B-C2B	2.63	1.49	1.43
15	N	841	CLA	C1B-C2B	2.63	1.49	1.43
15	B	802	CLA	C1B-C2B	2.63	1.49	1.43
15	S	201	CLA	C1B-C2B	2.63	1.49	1.43
15	L	203	CLA	C1B-C2B	2.63	1.49	1.43
15	b	803	CLA	C1B-C2B	2.63	1.49	1.43
15	b	837	CLA	C1B-C2B	2.63	1.49	1.43
15	b	809	CLA	C1B-C2B	2.63	1.49	1.43
14	B	838	F6C	C1D-ND	2.62	1.42	1.37
15	b	808	CLA	C1B-C2B	2.62	1.49	1.43
15	a	820	CLA	C1B-C2B	2.62	1.49	1.43
14	b	840	F6C	C1D-ND	2.62	1.42	1.37
15	N	803	CLA	C1B-C2B	2.62	1.49	1.43
15	O	825	CLA	C1B-C2B	2.62	1.49	1.43
15	b	825	CLA	C1B-C2B	2.62	1.49	1.43
15	N	820	CLA	C1B-C2B	2.62	1.49	1.43
15	B	808	CLA	C1B-C2B	2.62	1.49	1.43
15	a	835	CLA	C1B-C2B	2.62	1.49	1.43
15	A	835	CLA	C1B-C2B	2.61	1.49	1.43
15	N	839	CLA	C1B-C2B	2.61	1.49	1.43
15	A	827	CLA	C1B-C2B	2.61	1.49	1.43
15	A	820	CLA	C1B-C2B	2.61	1.49	1.43
15	O	818	CLA	C1B-C2B	2.61	1.49	1.43
15	B	823	CLA	C1B-C2B	2.61	1.49	1.43
13	A	801	CL0	CMD-C2D	-2.60	1.46	1.51
15	A	819	CLA	C1B-C2B	2.60	1.49	1.43
15	a	839	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	803	CLA	C1B-C2B	2.60	1.49	1.43
15	a	827	CLA	C1B-C2B	2.60	1.49	1.43
15	N	817	CLA	C1B-C2B	2.60	1.49	1.43
15	W	1502	CLA	C1B-C2B	2.60	1.49	1.43
15	B	807	CLA	C1B-C2B	2.60	1.49	1.43
15	O	804	CLA	C1B-C2B	2.60	1.49	1.43
15	a	817	CLA	C1B-C2B	2.60	1.49	1.43
15	a	803	CLA	C1B-C2B	2.59	1.49	1.43
15	N	835	CLA	C1B-C2B	2.59	1.49	1.43
15	A	804	CLA	C1B-C2B	2.59	1.49	1.43
15	A	839	CLA	C1B-C2B	2.59	1.49	1.43
15	A	817	CLA	C1B-C2B	2.59	1.49	1.43
15	N	827	CLA	C1B-C2B	2.59	1.49	1.43
14	A	857	F6C	C4B-NB	2.59	1.42	1.37
15	B	817	CLA	C1B-C2B	2.58	1.49	1.43
15	b	818	CLA	C1B-C2B	2.58	1.49	1.43
14	N	856	F6C	C4B-NB	2.57	1.42	1.37
14	a	856	F6C	C4B-NB	2.57	1.42	1.37
15	B	816	CLA	C1B-C2B	2.57	1.49	1.43
15	O	808	CLA	C1B-C2B	2.57	1.49	1.43
15	A	856	CLA	C1B-C2B	2.57	1.49	1.43
15	O	819	CLA	C1B-C2B	2.56	1.49	1.43
15	A	803	CLA	C1B-C2B	2.56	1.49	1.43
15	b	835	CLA	C1B-C2B	2.56	1.49	1.43
15	N	804	CLA	C1B-C2B	2.56	1.49	1.43
15	b	802	CLA	C1B-C2B	2.56	1.49	1.43
15	N	833	CLA	C1B-C2B	2.56	1.49	1.43
15	a	804	CLA	C1B-C2B	2.56	1.49	1.43
15	a	833	CLA	C1B-C2B	2.56	1.49	1.43
15	A	816	CLA	C3B-C4B	2.55	1.50	1.42
15	a	816	CLA	C1B-C2B	2.55	1.49	1.43
15	N	816	CLA	C1B-C2B	2.54	1.49	1.43
15	b	819	CLA	C1B-C2B	2.54	1.49	1.43
15	b	829	CLA	C1B-C2B	2.54	1.49	1.43
15	B	827	CLA	C1B-C2B	2.54	1.49	1.43
15	N	816	CLA	C3B-C4B	2.53	1.50	1.42
15	A	816	CLA	C1B-C2B	2.53	1.49	1.43
15	O	829	CLA	C1B-C2B	2.52	1.49	1.43
15	B	833	CLA	C1B-C2B	2.52	1.49	1.43
15	A	833	CLA	C1B-C2B	2.52	1.49	1.43
13	N	801	CL0	CMC-C2C	-2.52	1.46	1.50
15	O	835	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	816	CLA	C3B-C4B	2.52	1.50	1.42
14	N	826	F6C	C2B-C1B	2.51	1.49	1.44
13	N	801	CL0	C1A-CHA	-2.51	1.37	1.40
13	A	801	CL0	CAC-C3C	-2.50	1.47	1.51
15	B	821	CLA	CHC-C1C	2.50	1.43	1.38
13	A	801	CL0	CMC-C2C	-2.50	1.46	1.50
15	V	103	CLA	C1B-C2B	2.50	1.49	1.43
14	O	833	F6C	C2B-C1B	2.49	1.49	1.44
13	N	801	CL0	CAC-C3C	-2.49	1.47	1.51
13	a	801	CL0	C1A-CHA	-2.49	1.37	1.40
13	N	801	CL0	CMB-C2B	-2.49	1.46	1.51
15	b	823	CLA	CHC-C1C	2.49	1.43	1.38
13	a	801	CL0	CMB-C2B	-2.48	1.46	1.51
14	b	833	F6C	C2B-C1B	2.48	1.49	1.44
15	O	836	CLA	C3B-C4B	2.48	1.50	1.42
13	a	801	CL0	CMC-C2C	-2.48	1.46	1.50
13	A	801	CL0	CMB-C2B	-2.48	1.46	1.51
14	N	826	F6C	C4B-NB	2.47	1.41	1.37
14	N	824	F6C	C4B-NB	2.47	1.41	1.37
13	a	801	CL0	CAC-C3C	-2.47	1.47	1.51
14	N	802	F6C	C4B-NB	2.46	1.41	1.37
15	b	836	CLA	C3B-C4B	2.46	1.49	1.42
15	K	103	CLA	C1B-C2B	2.46	1.48	1.43
15	B	834	CLA	C3B-C4B	2.45	1.49	1.42
14	a	824	F6C	C4B-NB	2.45	1.41	1.37
14	B	831	F6C	C2B-C1B	2.44	1.49	1.44
14	A	824	F6C	C4B-NB	2.44	1.41	1.37
14	a	802	F6C	C4B-NB	2.43	1.41	1.37
13	A	801	CL0	C1A-CHA	-2.43	1.37	1.40
14	A	802	F6C	C4B-NB	2.43	1.41	1.37
15	b	815	CLA	C3B-C4B	2.43	1.49	1.42
15	b	817	CLA	CMB-C2B	-2.42	1.45	1.50
15	A	817	CLA	C3B-C4B	2.42	1.49	1.42
15	A	819	CLA	C3B-C4B	2.42	1.49	1.42
14	O	810	F6C	C3B-C4B	2.42	1.49	1.44
15	B	821	CLA	C3B-C4B	2.42	1.49	1.42
15	a	819	CLA	C3B-C4B	2.42	1.49	1.42
15	N	819	CLA	C3B-C4B	2.42	1.49	1.42
14	b	810	F6C	C3B-C4B	2.41	1.49	1.44
15	B	803	CLA	CHC-C1C	2.41	1.43	1.38
15	O	815	CLA	C3B-C4B	2.41	1.49	1.42
15	O	820	CLA	C3B-C4B	2.41	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	823	CLA	C3B-C4B	2.41	1.49	1.42
15	B	803	CLA	C3B-C4B	2.41	1.49	1.42
14	L	204	F6C	C4B-NB	2.41	1.41	1.37
15	b	820	CLA	C3B-C4B	2.41	1.49	1.42
15	B	808	CLA	CMB-C2B	-2.40	1.45	1.50
15	B	815	CLA	C1B-C2B	2.40	1.48	1.43
15	S	201	CLA	C3B-C4B	2.40	1.49	1.42
15	N	825	CLA	C3B-C4B	2.40	1.49	1.42
15	b	817	CLA	C1B-C2B	2.40	1.48	1.43
15	a	805	CLA	C3B-C4B	2.40	1.49	1.42
14	j	204	F6C	C4B-NB	2.40	1.41	1.37
15	A	819	CLA	CHC-C1C	2.40	1.43	1.38
15	N	817	CLA	C3B-C4B	2.40	1.49	1.42
15	O	804	CLA	C3B-C4B	2.40	1.49	1.42
15	O	817	CLA	C3B-C4B	2.40	1.49	1.42
15	a	817	CLA	C3B-C4B	2.40	1.49	1.42
15	a	805	CLA	CHC-C1C	2.39	1.43	1.38
15	F	201	CLA	C3B-C4B	2.39	1.49	1.42
15	B	818	CLA	C3B-C4B	2.39	1.49	1.42
15	N	805	CLA	C3B-C4B	2.39	1.49	1.42
15	A	803	CLA	CHC-C1C	2.39	1.43	1.38
15	A	805	CLA	C3B-C4B	2.39	1.49	1.42
14	A	824	F6C	C2B-C1B	2.39	1.49	1.44
15	f	201	CLA	C3B-C4B	2.39	1.49	1.42
15	O	804	CLA	CHC-C1C	2.39	1.43	1.38
15	A	803	CLA	C3B-C4B	2.39	1.49	1.42
15	N	819	CLA	CHC-C1C	2.39	1.43	1.38
14	a	826	F6C	C2B-C1B	2.38	1.49	1.44
15	a	841	CLA	C3B-C4B	2.38	1.49	1.42
15	O	809	CLA	CMB-C2B	-2.38	1.45	1.50
15	a	825	CLA	C3B-C4B	2.38	1.49	1.42
15	O	817	CLA	C1B-C2B	2.38	1.48	1.43
15	a	839	CLA	C3B-C4B	2.38	1.49	1.42
15	A	805	CLA	CHC-C1C	2.38	1.43	1.38
14	B	838	F6C	CMD-C2D	-2.38	1.45	1.50
15	b	815	CLA	CHC-C1C	2.38	1.43	1.38
15	A	828	CLA	C3B-C4B	2.38	1.49	1.42
14	W	1503	F6C	C4B-NB	2.38	1.41	1.37
15	a	842	CLA	C3B-C4B	2.38	1.49	1.42
14	a	824	F6C	C2B-C1B	2.38	1.49	1.44
15	A	825	CLA	C3B-C4B	2.38	1.49	1.42
15	A	841	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	839	CLA	C3B-C4B	2.38	1.49	1.42
15	N	827	CLA	C3B-C4B	2.38	1.49	1.42
15	A	842	CLA	C3B-C4B	2.38	1.49	1.42
14	L	201	F6C	C3B-C4B	2.38	1.49	1.44
15	A	812	CLA	C3B-C4B	2.37	1.49	1.42
15	A	827	CLA	C3B-C4B	2.37	1.49	1.42
15	a	819	CLA	CHC-C1C	2.37	1.43	1.38
15	b	804	CLA	C3B-C4B	2.37	1.49	1.42
15	N	841	CLA	C3B-C4B	2.37	1.49	1.42
15	a	803	CLA	C3B-C4B	2.37	1.49	1.42
15	B	802	CLA	CMC-C2C	-2.37	1.45	1.50
15	N	805	CLA	CHC-C1C	2.37	1.43	1.38
15	B	810	CLA	C3B-C4B	2.37	1.49	1.42
15	b	812	CLA	C3B-C4B	2.37	1.49	1.42
14	A	826	F6C	C2B-C1B	2.37	1.49	1.44
15	a	827	CLA	C3B-C4B	2.37	1.49	1.42
15	b	804	CLA	CHC-C1C	2.37	1.43	1.38
15	N	839	CLA	C3B-C4B	2.37	1.49	1.42
14	O	810	F6C	C4B-NB	2.37	1.41	1.37
15	i	103	CLA	C3B-C4B	2.37	1.49	1.42
15	B	815	CLA	C3B-C4B	2.36	1.49	1.42
14	O	833	F6C	C4B-NB	2.36	1.41	1.37
15	a	812	CLA	C3B-C4B	2.36	1.49	1.42
15	O	803	CLA	CMC-C2C	-2.36	1.45	1.50
14	a	824	F6C	C3B-C4B	2.36	1.49	1.44
15	N	812	CLA	C3B-C4B	2.36	1.49	1.42
15	K	103	CLA	C3B-C4B	2.36	1.49	1.42
15	O	812	CLA	C3B-C4B	2.36	1.49	1.42
15	a	803	CLA	CHC-C1C	2.36	1.43	1.38
14	L	201	F6C	C4B-NB	2.36	1.41	1.37
14	O	840	F6C	C4B-NB	2.36	1.41	1.37
15	N	842	CLA	C3B-C4B	2.35	1.49	1.42
14	N	824	F6C	C3B-C4B	2.35	1.49	1.44
15	B	813	CLA	C3B-C4B	2.35	1.49	1.42
15	V	103	CLA	C3B-C4B	2.35	1.49	1.42
14	a	826	F6C	C4B-NB	2.35	1.41	1.37
14	B	831	F6C	C4B-NB	2.35	1.41	1.37
15	b	825	CLA	C3B-C4B	2.35	1.49	1.42
15	O	835	CLA	C3B-C4B	2.35	1.49	1.42
15	B	823	CLA	C3B-C4B	2.35	1.49	1.42
15	A	856	CLA	C3B-C4B	2.35	1.49	1.42
15	O	829	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	810	F6C	C4B-NB	2.35	1.41	1.37
15	A	816	CLA	CHC-C1C	2.35	1.43	1.38
15	O	815	CLA	CHC-C1C	2.35	1.43	1.38
15	b	803	CLA	CMC-C2C	-2.35	1.46	1.50
15	b	835	CLA	C3B-C4B	2.35	1.49	1.42
14	N	824	F6C	C2B-C1B	2.35	1.49	1.44
14	b	833	F6C	C4B-NB	2.35	1.41	1.37
15	N	803	CLA	C3B-C4B	2.34	1.49	1.42
15	a	816	CLA	CHC-C1C	2.34	1.43	1.38
15	b	802	CLA	C3B-C4B	2.34	1.49	1.42
15	N	811	CLA	C3B-C4B	2.34	1.49	1.42
14	W	1503	F6C	C3B-C4B	2.34	1.49	1.44
14	A	826	F6C	C4B-NB	2.34	1.41	1.37
15	B	833	CLA	C3B-C4B	2.34	1.49	1.42
15	b	819	CLA	C3B-C4B	2.34	1.49	1.42
14	b	840	F6C	C4B-NB	2.34	1.41	1.37
15	a	829	CLA	C3B-C4B	2.34	1.49	1.42
15	B	830	CLA	C3B-C4B	2.34	1.49	1.42
15	N	816	CLA	CHC-C1C	2.34	1.43	1.38
15	O	831	CLA	C3B-C4B	2.34	1.49	1.42
15	b	809	CLA	CMB-C2B	-2.34	1.46	1.50
15	O	817	CLA	CHC-C1C	2.34	1.43	1.38
15	a	811	CLA	C3B-C4B	2.33	1.49	1.42
15	Z	103	CLA	C3B-C4B	2.33	1.49	1.42
15	B	827	CLA	C3B-C4B	2.33	1.49	1.42
15	O	819	CLA	C3B-C4B	2.33	1.49	1.42
15	A	831	CLA	CMB-C2B	-2.33	1.46	1.50
15	N	829	CLA	C3B-C4B	2.33	1.49	1.42
15	N	827	CLA	CHC-C1C	2.33	1.43	1.38
15	O	822	CLA	C3B-C4B	2.33	1.49	1.42
15	O	825	CLA	C3B-C4B	2.33	1.49	1.42
15	X	103	CLA	C3B-C4B	2.33	1.49	1.42
15	A	811	CLA	C3B-C4B	2.33	1.49	1.42
15	O	805	CLA	C3B-C4B	2.33	1.49	1.42
15	N	803	CLA	CHC-C1C	2.33	1.43	1.38
15	b	819	CLA	CHC-C1C	2.33	1.43	1.38
14	j	204	F6C	C3B-C4B	2.33	1.49	1.44
15	l	103	CLA	C3B-C4B	2.33	1.49	1.42
15	O	832	CLA	C3B-C4B	2.33	1.49	1.42
15	a	813	CLA	C3B-C4B	2.33	1.49	1.42
15	b	832	CLA	C3B-C4B	2.33	1.49	1.42
15	B	815	CLA	CMB-C2B	-2.32	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	813	CLA	C3B-C4B	2.32	1.49	1.42
15	N	828	CLA	C3B-C4B	2.32	1.49	1.42
15	O	819	CLA	CHC-C1C	2.32	1.43	1.38
15	b	829	CLA	C3B-C4B	2.32	1.49	1.42
15	B	812	CLA	C3B-C4B	2.32	1.49	1.42
15	O	841	CLA	C3B-C4B	2.32	1.49	1.42
15	b	841	CLA	C3B-C4B	2.32	1.49	1.42
15	O	808	CLA	C3B-C4B	2.32	1.49	1.42
15	a	828	CLA	CMC-C2C	-2.32	1.46	1.50
15	b	805	CLA	C3B-C4B	2.32	1.49	1.42
14	A	824	F6C	C3B-C4B	2.32	1.49	1.44
15	A	813	CLA	C3B-C4B	2.32	1.49	1.42
15	B	804	CLA	C3B-C4B	2.32	1.49	1.42
15	O	814	CLA	C3B-C4B	2.32	1.49	1.42
15	b	817	CLA	C3B-C4B	2.32	1.49	1.42
15	O	823	CLA	C3B-C4B	2.32	1.49	1.42
15	A	829	CLA	C3B-C4B	2.32	1.49	1.42
15	B	817	CLA	C3B-C4B	2.32	1.49	1.42
15	O	835	CLA	CHC-C1C	2.32	1.43	1.38
15	b	835	CLA	CHC-C1C	2.32	1.43	1.38
15	a	831	CLA	CMB-C2B	-2.31	1.46	1.50
15	b	825	CLA	CHC-C1C	2.31	1.43	1.38
14	b	840	F6C	CMD-C2D	-2.31	1.46	1.50
15	b	816	CLA	C3B-C4B	2.31	1.49	1.42
15	B	815	CLA	CHC-C1C	2.31	1.43	1.38
15	B	814	CLA	C3B-C4B	2.31	1.49	1.42
14	B	838	F6C	C4B-NB	2.31	1.41	1.37
14	O	840	F6C	CMD-C2D	-2.31	1.46	1.50
15	B	812	CLA	CHC-C1C	2.31	1.43	1.38
15	b	831	CLA	C3B-C4B	2.31	1.49	1.42
15	b	813	CLA	C3B-C4B	2.31	1.49	1.42
15	B	824	CLA	C3B-C4B	2.31	1.49	1.42
15	A	837	CLA	C3B-C4B	2.31	1.49	1.42
15	O	816	CLA	C3B-C4B	2.31	1.49	1.42
15	B	835	CLA	C3B-C4B	2.31	1.49	1.42
15	a	833	CLA	C3B-C4B	2.31	1.49	1.42
15	b	834	CLA	C3B-C4B	2.31	1.49	1.42
15	A	808	CLA	C3B-C4B	2.31	1.49	1.42
15	B	819	CLA	C3B-C4B	2.31	1.49	1.42
15	B	807	CLA	C3B-C4B	2.30	1.49	1.42
15	a	837	CLA	C3B-C4B	2.30	1.49	1.42
15	A	823	CLA	C3B-C4B	2.30	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	827	CLA	CHC-C1C	2.30	1.43	1.38
15	W	1502	CLA	C3B-C4B	2.30	1.49	1.42
14	L	204	F6C	C3B-C4B	2.30	1.49	1.44
15	B	833	CLA	CHC-C1C	2.30	1.43	1.38
15	N	823	CLA	C3B-C4B	2.30	1.49	1.42
15	N	837	CLA	C3B-C4B	2.30	1.49	1.42
14	L	204	F6C	C2B-C1B	2.30	1.49	1.44
15	b	834	CLA	CHC-C1C	2.30	1.43	1.38
15	a	829	CLA	CHC-C1C	2.30	1.43	1.38
15	b	803	CLA	C3B-C4B	2.30	1.49	1.42
15	B	823	CLA	CHC-C1C	2.30	1.43	1.38
15	B	832	CLA	C3B-C4B	2.30	1.49	1.42
15	A	835	CLA	C3B-C4B	2.30	1.49	1.42
15	L	203	CLA	C3B-C4B	2.30	1.49	1.42
15	B	839	CLA	C3B-C4B	2.30	1.49	1.42
15	a	823	CLA	C3B-C4B	2.30	1.49	1.42
15	N	828	CLA	CMC-C2C	-2.30	1.46	1.50
15	O	802	CLA	C3B-C4B	2.30	1.49	1.42
15	O	821	CLA	C3B-C4B	2.30	1.49	1.42
15	a	828	CLA	C3B-C4B	2.30	1.49	1.42
15	b	837	CLA	C3B-C4B	2.30	1.49	1.42
15	N	835	CLA	CHC-C1C	2.30	1.43	1.38
15	O	814	CLA	CHC-C1C	2.30	1.43	1.38
15	B	829	CLA	C3B-C4B	2.30	1.49	1.42
15	A	828	CLA	CMC-C2C	-2.30	1.46	1.50
15	N	831	CLA	CMB-C2B	-2.30	1.46	1.50
15	N	808	CLA	C3B-C4B	2.30	1.49	1.42
15	B	832	CLA	CHC-C1C	2.30	1.43	1.38
15	a	815	CLA	C3B-C4B	2.30	1.49	1.42
15	N	806	CLA	C3B-C4B	2.30	1.49	1.42
15	N	834	CLA	C3B-C4B	2.30	1.49	1.42
15	A	827	CLA	CHC-C1C	2.30	1.43	1.38
15	a	808	CLA	C3B-C4B	2.30	1.49	1.42
15	O	825	CLA	CHC-C1C	2.30	1.43	1.38
15	O	831	CLA	CHC-C1C	2.30	1.43	1.38
15	O	813	CLA	C3B-C4B	2.30	1.49	1.42
15	N	829	CLA	CHC-C1C	2.30	1.43	1.38
15	A	820	CLA	C3B-C4B	2.30	1.49	1.42
15	B	811	CLA	C3B-C4B	2.30	1.49	1.42
15	a	810	CLA	C3B-C4B	2.30	1.49	1.42
15	b	826	CLA	C3B-C4B	2.30	1.49	1.42
15	a	830	CLA	CHC-C1C	2.29	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	821	CLA	C3B-C4B	2.29	1.49	1.42
15	V	102	CLA	C3B-C4B	2.29	1.49	1.42
15	O	834	CLA	C3B-C4B	2.29	1.49	1.42
15	A	832	CLA	C3B-C4B	2.29	1.49	1.42
15	N	835	CLA	C3B-C4B	2.29	1.49	1.42
15	b	814	CLA	C3B-C4B	2.29	1.49	1.42
15	K	102	CLA	C3B-C4B	2.29	1.49	1.42
15	A	834	CLA	C3B-C4B	2.29	1.49	1.42
15	b	822	CLA	C3B-C4B	2.29	1.49	1.42
15	A	815	CLA	C3B-C4B	2.29	1.49	1.42
15	W	1502	CLA	CHC-C1C	2.29	1.43	1.38
15	N	809	CLA	C3B-C4B	2.29	1.49	1.42
15	a	832	CLA	C3B-C4B	2.29	1.49	1.42
15	B	805	CLA	C3B-C4B	2.29	1.49	1.42
15	N	810	CLA	C3B-C4B	2.29	1.49	1.42
15	A	810	CLA	C3B-C4B	2.29	1.49	1.42
15	B	836	CLA	C3B-C4B	2.29	1.49	1.42
15	A	856	CLA	CHC-C1C	2.29	1.43	1.38
15	N	809	CLA	CHC-C1C	2.29	1.43	1.38
15	B	802	CLA	C3B-C4B	2.29	1.49	1.42
15	a	820	CLA	C3B-C4B	2.29	1.49	1.42
15	B	804	CLA	CHC-C1C	2.29	1.43	1.38
15	N	820	CLA	C3B-C4B	2.29	1.49	1.42
15	a	806	CLA	C3B-C4B	2.29	1.49	1.42
15	B	817	CLA	CHC-C1C	2.29	1.43	1.38
15	b	802	CLA	CHC-C1C	2.29	1.43	1.38
15	i	102	CLA	C3B-C4B	2.29	1.49	1.42
15	A	825	CLA	CHC-C1C	2.29	1.43	1.38
15	N	811	CLA	CHC-C1C	2.29	1.43	1.38
15	K	103	CLA	CMB-C2B	-2.29	1.46	1.50
15	A	830	CLA	C3B-C4B	2.28	1.49	1.42
15	b	831	CLA	CHC-C1C	2.28	1.43	1.38
15	B	826	CLA	C3B-C4B	2.28	1.49	1.42
15	b	808	CLA	C3B-C4B	2.28	1.49	1.42
15	O	838	CLA	C3B-C4B	2.28	1.49	1.42
15	a	830	CLA	C3B-C4B	2.28	1.49	1.42
15	N	815	CLA	C3B-C4B	2.28	1.49	1.42
15	a	835	CLA	C3B-C4B	2.28	1.49	1.42
15	A	809	CLA	C3B-C4B	2.28	1.49	1.42
15	A	837	CLA	CHC-C1C	2.28	1.43	1.38
15	b	838	CLA	C3B-C4B	2.28	1.49	1.42
15	O	823	CLA	CHC-C1C	2.28	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	836	CLA	CHC-C1C	2.28	1.43	1.38
15	A	833	CLA	C3B-C4B	2.28	1.49	1.42
15	Z	103	CLA	CHC-C1C	2.28	1.43	1.38
15	N	833	CLA	C3B-C4B	2.28	1.49	1.42
15	a	809	CLA	C3B-C4B	2.28	1.49	1.42
14	a	826	F6C	C3B-C4B	2.28	1.49	1.44
15	A	829	CLA	CHC-C1C	2.28	1.43	1.38
15	b	814	CLA	CHC-C1C	2.28	1.43	1.38
15	N	830	CLA	C3B-C4B	2.28	1.49	1.42
15	X	103	CLA	CHC-C1C	2.28	1.43	1.38
15	O	837	CLA	C3B-C4B	2.28	1.49	1.42
15	A	821	CLA	C3B-C4B	2.28	1.49	1.42
15	W	1501	CLA	C3B-C4B	2.28	1.49	1.42
15	O	820	CLA	CHC-C1C	2.28	1.43	1.38
15	b	836	CLA	CHC-C1C	2.28	1.43	1.38
15	b	828	CLA	C3B-C4B	2.28	1.49	1.42
15	A	830	CLA	CHC-C1C	2.28	1.43	1.38
15	O	834	CLA	CHC-C1C	2.28	1.43	1.38
15	b	817	CLA	CHC-C1C	2.28	1.43	1.38
15	l	103	CLA	CHC-C1C	2.28	1.43	1.38
15	O	826	CLA	C3B-C4B	2.28	1.49	1.42
15	B	829	CLA	CHC-C1C	2.27	1.43	1.38
15	B	830	CLA	CHC-C1C	2.27	1.43	1.38
15	O	805	CLA	CHC-C1C	2.27	1.43	1.38
15	N	832	CLA	C3B-C4B	2.27	1.49	1.42
15	j	202	CLA	C3B-C4B	2.27	1.49	1.42
15	b	837	CLA	CHC-C1C	2.27	1.43	1.38
15	B	820	CLA	C3B-C4B	2.27	1.49	1.42
15	b	807	CLA	C3B-C4B	2.27	1.49	1.42
15	B	810	CLA	CHC-C1C	2.27	1.43	1.38
15	b	806	CLA	C3B-C4B	2.27	1.49	1.42
15	B	834	CLA	CHC-C1C	2.27	1.43	1.38
15	B	835	CLA	CHC-C1C	2.27	1.43	1.38
15	a	809	CLA	CHC-C1C	2.27	1.43	1.38
15	b	823	CLA	CMD-C2D	-2.27	1.46	1.50
15	A	836	CLA	C3B-C4B	2.27	1.49	1.42
15	O	828	CLA	C3B-C4B	2.27	1.49	1.42
15	O	818	CLA	C3B-C4B	2.27	1.49	1.42
15	a	836	CLA	C3B-C4B	2.27	1.49	1.42
15	L	203	CLA	CHC-C1C	2.27	1.43	1.38
15	a	808	CLA	CHC-C1C	2.27	1.43	1.38
15	a	837	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	803	CLA	CHC-C1C	2.27	1.43	1.38
15	N	837	CLA	CHC-C1C	2.27	1.43	1.38
15	A	806	CLA	C3B-C4B	2.27	1.49	1.42
15	N	825	CLA	CHC-C1C	2.27	1.43	1.38
15	a	835	CLA	CHC-C1C	2.27	1.43	1.38
15	N	830	CLA	CHC-C1C	2.27	1.43	1.38
15	a	815	CLA	CHC-C1C	2.27	1.43	1.38
15	L	202	CLA	C3B-C4B	2.27	1.49	1.42
15	O	806	CLA	C3B-C4B	2.27	1.49	1.42
15	a	821	CLA	C3B-C4B	2.27	1.49	1.42
15	a	825	CLA	CHC-C1C	2.27	1.43	1.38
15	b	811	CLA	C3B-C4B	2.27	1.49	1.42
15	N	821	CLA	C3B-C4B	2.27	1.49	1.42
15	A	833	CLA	CHC-C1C	2.27	1.43	1.38
15	b	805	CLA	CHC-C1C	2.27	1.43	1.38
14	O	810	F6C	C2B-C1B	2.26	1.49	1.44
15	A	812	CLA	CHC-C1C	2.26	1.43	1.38
15	B	802	CLA	CHC-C1C	2.26	1.43	1.38
15	O	817	CLA	CMB-C2B	-2.26	1.46	1.50
15	N	836	CLA	C3B-C4B	2.26	1.49	1.42
15	A	811	CLA	CHC-C1C	2.26	1.43	1.38
15	N	839	CLA	CHC-C1C	2.26	1.43	1.38
15	b	818	CLA	C3B-C4B	2.26	1.49	1.42
15	A	808	CLA	CHC-C1C	2.26	1.43	1.38
15	B	826	CLA	CHC-C1C	2.26	1.43	1.38
15	A	814	CLA	C3B-C4B	2.26	1.49	1.42
15	A	809	CLA	CHC-C1C	2.26	1.43	1.38
15	i	103	CLA	CHC-C1C	2.26	1.43	1.38
15	B	821	CLA	CMD-C2D	-2.26	1.46	1.50
15	B	806	CLA	C3B-C4B	2.26	1.49	1.42
15	j	203	CLA	C3B-C4B	2.26	1.49	1.42
15	N	812	CLA	CHC-C1C	2.26	1.43	1.38
15	A	813	CLA	CHC-C1C	2.26	1.43	1.38
15	a	839	CLA	CHC-C1C	2.26	1.43	1.38
14	j	204	F6C	C2B-C1B	2.26	1.49	1.44
15	B	816	CLA	C3B-C4B	2.26	1.49	1.42
15	O	830	CLA	C3B-C4B	2.26	1.49	1.42
15	a	813	CLA	CHC-C1C	2.26	1.43	1.38
15	a	811	CLA	CHC-C1C	2.26	1.43	1.38
14	A	826	F6C	C3B-C4B	2.26	1.49	1.44
14	W	1503	F6C	C2B-C1B	2.26	1.49	1.44
15	A	835	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	811	CLA	C3B-C4B	2.26	1.49	1.42
15	B	809	CLA	C3B-C4B	2.26	1.49	1.42
15	V	103	CLA	CMB-C2B	-2.26	1.46	1.50
15	a	812	CLA	CHC-C1C	2.26	1.43	1.38
15	A	818	CLA	C3B-C4B	2.26	1.49	1.42
15	B	818	CLA	CHC-C1C	2.26	1.43	1.38
15	a	810	CLA	CHC-C1C	2.26	1.43	1.38
15	b	812	CLA	CHC-C1C	2.26	1.43	1.38
15	B	836	CLA	CHC-C1C	2.26	1.43	1.38
15	N	815	CLA	CHC-C1C	2.26	1.43	1.38
15	b	820	CLA	CHC-C1C	2.26	1.43	1.38
15	b	830	CLA	C3B-C4B	2.26	1.49	1.42
15	O	829	CLA	CHC-C1C	2.26	1.43	1.38
15	O	832	CLA	CHC-C1C	2.26	1.43	1.38
15	A	815	CLA	CHC-C1C	2.26	1.43	1.38
15	K	103	CLA	CHC-C1C	2.26	1.43	1.38
15	N	806	CLA	CHC-C1C	2.25	1.43	1.38
15	N	818	CLA	C3B-C4B	2.25	1.49	1.42
15	B	828	CLA	C3B-C4B	2.25	1.49	1.42
15	O	803	CLA	C3B-C4B	2.25	1.49	1.42
15	O	837	CLA	CHC-C1C	2.25	1.43	1.38
15	S	201	CLA	CHC-C1C	2.25	1.43	1.38
15	B	825	CLA	C3B-C4B	2.25	1.49	1.42
15	B	837	CLA	C3B-C4B	2.25	1.49	1.42
15	O	816	CLA	CHC-C1C	2.25	1.43	1.38
15	N	808	CLA	CHC-C1C	2.25	1.43	1.38
15	V	103	CLA	CHC-C1C	2.25	1.43	1.38
15	a	804	CLA	CHC-C1C	2.25	1.43	1.38
15	N	814	CLA	C3B-C4B	2.25	1.49	1.42
15	A	834	CLA	CHC-C1C	2.25	1.43	1.38
15	B	827	CLA	CHC-C1C	2.25	1.43	1.38
15	N	833	CLA	CHC-C1C	2.25	1.43	1.38
15	b	828	CLA	CHC-C1C	2.25	1.43	1.38
15	O	807	CLA	C3B-C4B	2.25	1.49	1.42
15	A	804	CLA	CHC-C1C	2.25	1.43	1.38
15	N	810	CLA	CHC-C1C	2.25	1.43	1.38
15	F	201	CLA	CHC-C1C	2.25	1.43	1.38
15	a	834	CLA	C3B-C4B	2.25	1.49	1.42
15	N	813	CLA	CHC-C1C	2.25	1.43	1.38
15	O	822	CLA	CHC-C1C	2.25	1.43	1.38
15	f	201	CLA	CHC-C1C	2.25	1.43	1.38
15	a	814	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	810	CLA	CHC-C1C	2.24	1.43	1.38
15	O	838	CLA	CHC-C1C	2.24	1.43	1.38
14	b	840	F6C	C2B-C1B	2.24	1.49	1.44
15	A	822	CLA	C3B-C4B	2.24	1.49	1.42
15	a	818	CLA	C3B-C4B	2.24	1.49	1.42
15	O	812	CLA	CHC-C1C	2.24	1.43	1.38
15	O	827	CLA	C3B-C4B	2.24	1.49	1.42
15	O	802	CLA	CHC-C1C	2.24	1.43	1.38
15	N	834	CLA	CHC-C1C	2.24	1.43	1.38
15	b	816	CLA	CHC-C1C	2.24	1.43	1.38
15	B	814	CLA	CHC-C1C	2.24	1.43	1.38
15	a	817	CLA	CMB-C2B	-2.24	1.46	1.50
14	N	826	F6C	C3B-C4B	2.24	1.49	1.44
14	b	810	F6C	C2B-C1B	2.24	1.49	1.44
15	O	821	CLA	CHC-C1C	2.24	1.43	1.38
15	b	839	CLA	C3B-C4B	2.24	1.49	1.42
15	N	807	CLA	C3B-C4B	2.24	1.49	1.42
15	N	804	CLA	CHC-C1C	2.24	1.43	1.38
14	N	802	F6C	C3B-C4B	2.24	1.49	1.44
15	A	832	CLA	CHC-C1C	2.24	1.43	1.38
15	A	821	CLA	CHC-C1C	2.24	1.43	1.38
15	B	819	CLA	CHC-C1C	2.24	1.43	1.38
15	b	832	CLA	CHC-C1C	2.24	1.43	1.38
15	b	838	CLA	CHC-C1C	2.24	1.43	1.38
14	O	833	F6C	C3B-C4B	2.24	1.49	1.44
15	B	805	CLA	CHC-C1C	2.24	1.43	1.38
15	N	807	CLA	CHC-C1C	2.23	1.43	1.38
15	b	823	CLA	CMC-C2C	-2.23	1.46	1.50
15	B	809	CLA	CHC-C1C	2.23	1.43	1.38
15	B	822	CLA	C3B-C4B	2.23	1.49	1.42
15	b	827	CLA	C3B-C4B	2.23	1.49	1.42
15	A	839	CLA	CHC-C1C	2.23	1.43	1.38
15	b	824	CLA	C3B-C4B	2.23	1.49	1.42
15	a	833	CLA	CHC-C1C	2.23	1.43	1.38
15	A	842	CLA	CHC-C1C	2.23	1.43	1.38
15	B	813	CLA	CHC-C1C	2.23	1.43	1.38
14	B	831	F6C	C3B-C4B	2.23	1.49	1.44
15	B	807	CLA	CHC-C1C	2.23	1.43	1.38
14	A	802	F6C	C3B-C4B	2.23	1.49	1.44
15	N	828	CLA	CHC-C1C	2.23	1.43	1.38
15	O	830	CLA	CHC-C1C	2.23	1.42	1.38
15	a	834	CLA	CHC-C1C	2.23	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	808	CLA	CHC-C1C	2.23	1.42	1.38
15	O	811	CLA	CHC-C1C	2.22	1.42	1.38
15	W	1501	CLA	CHC-C1C	2.22	1.42	1.38
15	B	828	CLA	CMD-C2D	-2.22	1.46	1.50
15	N	822	CLA	CMB-C2B	-2.22	1.46	1.50
15	O	824	CLA	C3B-C4B	2.22	1.49	1.42
15	A	828	CLA	CHC-C1C	2.22	1.42	1.38
15	a	842	CLA	CHC-C1C	2.22	1.42	1.38
15	a	810	CLA	CMD-C2D	-2.22	1.46	1.50
15	B	824	CLA	CHC-C1C	2.22	1.42	1.38
15	O	806	CLA	CHC-C1C	2.22	1.42	1.38
15	a	828	CLA	CHC-C1C	2.22	1.42	1.38
15	b	821	CLA	CHC-C1C	2.22	1.42	1.38
15	N	821	CLA	CHC-C1C	2.22	1.42	1.38
15	A	810	CLA	CMD-C2D	-2.22	1.46	1.50
15	O	828	CLA	CHC-C1C	2.22	1.42	1.38
15	a	821	CLA	CHC-C1C	2.22	1.42	1.38
15	A	823	CLA	CHC-C1C	2.22	1.42	1.38
15	j	203	CLA	CHC-C1C	2.22	1.42	1.38
15	N	810	CLA	CMD-C2D	-2.22	1.46	1.50
15	a	831	CLA	C3B-C4B	2.22	1.49	1.42
15	a	822	CLA	C3B-C4B	2.22	1.49	1.42
15	A	806	CLA	CHC-C1C	2.22	1.42	1.38
15	B	811	CLA	CHC-C1C	2.22	1.42	1.38
15	b	830	CLA	CHC-C1C	2.22	1.42	1.38
15	B	828	CLA	CHC-C1C	2.22	1.42	1.38
15	b	822	CLA	CHC-C1C	2.22	1.42	1.38
14	O	840	F6C	C3B-C4B	2.22	1.49	1.44
15	A	836	CLA	CHC-C1C	2.22	1.42	1.38
15	b	819	CLA	CMB-C2B	-2.22	1.46	1.50
15	K	102	CLA	CHC-C1C	2.22	1.42	1.38
15	O	801	CLA	CHC-C1C	2.22	1.42	1.38
15	b	829	CLA	CHC-C1C	2.22	1.42	1.38
15	O	818	CLA	CHC-C1C	2.22	1.42	1.38
15	O	839	CLA	C3B-C4B	2.22	1.49	1.42
15	a	836	CLA	CHC-C1C	2.21	1.42	1.38
14	L	201	F6C	C2B-C1B	2.21	1.49	1.44
15	B	816	CLA	CHC-C1C	2.21	1.42	1.38
15	V	102	CLA	CHC-C1C	2.21	1.42	1.38
15	b	806	CLA	CHC-C1C	2.21	1.42	1.38
15	N	823	CLA	CHC-C1C	2.21	1.42	1.38
15	b	811	CLA	CHC-C1C	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	806	CLA	CHC-C1C	2.21	1.42	1.38
15	O	801	CLA	C3B-C4B	2.21	1.49	1.42
15	N	842	CLA	CHC-C1C	2.21	1.42	1.38
15	N	817	CLA	CMB-C2B	-2.21	1.46	1.50
15	N	822	CLA	C3B-C4B	2.21	1.49	1.42
15	b	801	CLA	C3B-C4B	2.21	1.49	1.42
15	A	841	CLA	CHC-C1C	2.21	1.42	1.38
15	a	832	CLA	CHC-C1C	2.21	1.42	1.38
14	B	838	F6C	C2B-C1B	2.21	1.49	1.44
15	N	832	CLA	CHC-C1C	2.21	1.42	1.38
15	a	838	CLA	C3B-C4B	2.21	1.49	1.42
15	b	813	CLA	CHC-C1C	2.21	1.42	1.38
15	i	102	CLA	CHC-C1C	2.21	1.42	1.38
15	L	202	CLA	CHC-C1C	2.21	1.42	1.38
15	N	831	CLA	C3B-C4B	2.21	1.49	1.42
14	b	833	F6C	C3B-C4B	2.20	1.49	1.44
15	B	820	CLA	CHC-C1C	2.20	1.42	1.38
15	A	831	CLA	C3B-C4B	2.20	1.49	1.42
14	O	840	F6C	C2B-C1B	2.20	1.49	1.44
15	O	813	CLA	CHC-C1C	2.20	1.42	1.38
15	a	807	CLA	C3B-C4B	2.20	1.49	1.42
15	B	825	CLA	CHC-C1C	2.20	1.42	1.38
15	a	823	CLA	CHC-C1C	2.20	1.42	1.38
15	O	827	CLA	CHC-C1C	2.20	1.42	1.38
15	O	819	CLA	CMB-C2B	-2.20	1.46	1.50
15	f	201	CLA	CMD-C2D	-2.20	1.46	1.50
15	A	817	CLA	CMB-C2B	-2.20	1.46	1.50
15	N	838	CLA	C3B-C4B	2.20	1.49	1.42
15	N	841	CLA	CHC-C1C	2.20	1.42	1.38
15	b	818	CLA	CHC-C1C	2.20	1.42	1.38
14	B	838	F6C	C3B-C4B	2.20	1.49	1.44
15	A	818	CLA	CHC-C1C	2.20	1.42	1.38
15	B	808	CLA	MG-NB	-2.20	2.01	2.05
15	B	807	CLA	CMD-C2D	-2.20	1.46	1.50
15	B	817	CLA	CMB-C2B	-2.20	1.46	1.50
15	a	818	CLA	CHC-C1C	2.20	1.42	1.38
15	b	828	CLA	CMD-C2D	-2.19	1.46	1.50
15	O	803	CLA	CHC-C1C	2.19	1.42	1.38
15	A	822	CLA	CHC-C1C	2.19	1.42	1.38
15	a	807	CLA	CHC-C1C	2.19	1.42	1.38
15	A	817	CLA	CHC-C1C	2.19	1.42	1.38
14	b	840	F6C	C3B-C4B	2.19	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	801	CLA	CHC-C1C	2.19	1.42	1.38
15	j	202	CLA	CHC-C1C	2.19	1.42	1.38
15	a	803	CLA	CMC-C2C	-2.19	1.46	1.50
15	b	808	CLA	CMD-C2D	-2.19	1.46	1.50
15	b	809	CLA	C3B-C4B	2.19	1.49	1.42
15	b	808	CLA	CHC-C1C	2.19	1.42	1.38
15	a	818	CLA	CMD-C2D	-2.19	1.46	1.50
15	A	818	CLA	CMD-C2D	-2.19	1.46	1.50
15	a	822	CLA	CMB-C2B	-2.19	1.46	1.50
14	a	802	F6C	C3B-C4B	2.19	1.49	1.44
15	A	814	CLA	CHC-C1C	2.19	1.42	1.38
15	O	809	CLA	MG-NB	-2.19	2.01	2.05
15	O	826	CLA	CHC-C1C	2.19	1.42	1.38
15	b	826	CLA	CHC-C1C	2.19	1.42	1.38
15	B	821	CLA	CMC-C2C	-2.19	1.46	1.50
15	B	801	CLA	C3B-C4B	2.19	1.49	1.42
15	a	841	CLA	CHC-C1C	2.19	1.42	1.38
15	N	836	CLA	CHC-C1C	2.18	1.42	1.38
15	A	820	CLA	CHC-C1C	2.18	1.42	1.38
15	B	837	CLA	CHC-C1C	2.18	1.42	1.38
15	N	817	CLA	CHC-C1C	2.18	1.42	1.38
15	A	830	CLA	CMD-C2D	-2.18	1.46	1.50
15	a	822	CLA	CHC-C1C	2.18	1.42	1.38
15	N	818	CLA	CHC-C1C	2.18	1.42	1.38
15	O	808	CLA	CMD-C2D	-2.18	1.46	1.50
15	O	823	CLA	CMC-C2C	-2.18	1.46	1.50
15	A	807	CLA	C3B-C4B	2.18	1.49	1.42
15	a	817	CLA	CHC-C1C	2.18	1.42	1.38
15	K	103	CLA	MG-NB	-2.18	2.01	2.05
15	b	841	CLA	CHC-C1C	2.18	1.42	1.38
15	B	801	CLA	CMD-C2D	-2.18	1.46	1.50
15	N	830	CLA	CMD-C2D	-2.18	1.46	1.50
15	N	818	CLA	CMD-C2D	-2.18	1.46	1.50
15	A	822	CLA	CMB-C2B	-2.18	1.46	1.50
15	O	828	CLA	CMD-C2D	-2.17	1.46	1.50
15	S	201	CLA	CMD-C2D	-2.17	1.46	1.50
15	B	801	CLA	CHC-C1C	2.17	1.42	1.38
15	O	841	CLA	CHC-C1C	2.17	1.42	1.38
15	b	839	CLA	CHC-C1C	2.17	1.42	1.38
15	b	827	CLA	CHC-C1C	2.17	1.42	1.38
15	N	819	CLA	CMC-C2C	-2.17	1.46	1.50
15	b	817	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	838	CLA	C3B-C4B	2.17	1.49	1.42
15	O	817	CLA	MG-NB	-2.17	2.01	2.05
15	j	202	CLA	MG-NB	-2.17	2.01	2.05
15	a	830	CLA	CMD-C2D	-2.17	1.46	1.50
15	b	826	CLA	CMC-C2C	-2.17	1.46	1.50
15	i	102	CLA	CMD-C2D	-2.17	1.46	1.50
15	A	833	CLA	MG-NB	-2.17	2.01	2.05
15	O	839	CLA	CHC-C1C	2.16	1.42	1.38
15	B	826	CLA	CMD-C2D	-2.16	1.46	1.50
15	N	814	CLA	CHC-C1C	2.16	1.42	1.38
15	B	828	CLA	MG-NB	-2.16	2.01	2.05
15	K	102	CLA	CMD-C2D	-2.16	1.46	1.50
15	O	830	CLA	CMD-C2D	-2.16	1.46	1.50
15	b	807	CLA	CHC-C1C	2.16	1.42	1.38
15	B	824	CLA	CMC-C2C	-2.16	1.46	1.50
15	a	838	CLA	CHC-C1C	2.16	1.42	1.38
15	A	819	CLA	CMC-C2C	-2.16	1.46	1.50
15	O	801	CLA	CMD-C2D	-2.16	1.46	1.50
15	O	809	CLA	C3B-C4B	2.16	1.49	1.42
15	b	829	CLA	CMB-C2B	-2.16	1.46	1.50
15	a	840	CLA	C3B-C4B	2.16	1.49	1.42
15	N	822	CLA	CHC-C1C	2.16	1.42	1.38
15	V	103	CLA	MG-NB	-2.16	2.01	2.05
15	b	824	CLA	CHC-C1C	2.15	1.42	1.38
15	a	833	CLA	MG-NB	-2.15	2.01	2.05
15	A	840	CLA	MG-NB	-2.15	2.01	2.05
15	O	826	CLA	CMC-C2C	-2.15	1.46	1.50
15	a	819	CLA	CMC-C2C	-2.15	1.46	1.50
15	A	840	CLA	C3B-C4B	2.15	1.49	1.42
15	B	839	CLA	CHC-C1C	2.15	1.42	1.38
15	F	201	CLA	CMD-C2D	-2.15	1.46	1.50
15	b	830	CLA	CMD-C2D	-2.15	1.46	1.50
15	a	814	CLA	CHC-C1C	2.15	1.42	1.38
15	A	807	CLA	CHC-C1C	2.15	1.42	1.38
15	B	815	CLA	MG-NB	-2.15	2.01	2.05
14	O	833	F6C	CMC-C2C	-2.15	1.46	1.50
15	b	809	CLA	MG-NB	-2.14	2.01	2.05
15	N	820	CLA	CHC-C1C	2.14	1.42	1.38
15	N	840	CLA	MG-NB	-2.14	2.01	2.05
15	B	822	CLA	CMD-C2D	-2.14	1.46	1.50
15	A	829	CLA	CMD-C2D	-2.14	1.46	1.50
14	B	831	F6C	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	833	CLA	CMB-C2B	-2.14	1.46	1.50
15	a	840	CLA	MG-NB	-2.14	2.01	2.05
15	O	824	CLA	CHC-C1C	2.14	1.42	1.38
15	b	801	CLA	CMD-C2D	-2.14	1.46	1.50
15	a	818	CLA	MG-NB	-2.14	2.01	2.05
15	b	809	CLA	CHC-C1C	2.14	1.42	1.38
15	O	809	CLA	CHC-C1C	2.14	1.42	1.38
15	b	818	CLA	MG-NB	-2.14	2.01	2.05
15	N	803	CLA	CMC-C2C	-2.14	1.46	1.50
15	a	829	CLA	CMD-C2D	-2.14	1.46	1.50
15	B	822	CLA	CHC-C1C	2.14	1.42	1.38
15	N	822	CLA	MG-NB	-2.14	2.01	2.05
15	N	840	CLA	C3B-C4B	2.14	1.49	1.42
15	N	829	CLA	CMD-C2D	-2.13	1.46	1.50
15	V	102	CLA	CMD-C2D	-2.13	1.46	1.50
15	B	833	CLA	MG-NB	-2.13	2.01	2.05
15	N	838	CLA	CHC-C1C	2.13	1.42	1.38
15	A	818	CLA	MG-NB	-2.13	2.01	2.05
14	N	826	F6C	CMD-C2D	-2.13	1.46	1.50
15	O	807	CLA	CHC-C1C	2.13	1.42	1.38
15	O	824	CLA	CMD-C2D	-2.13	1.46	1.50
15	a	820	CLA	CHC-C1C	2.13	1.42	1.38
15	b	826	CLA	MG-NB	-2.13	2.01	2.05
15	N	820	CLA	CMB-C2B	-2.13	1.46	1.50
15	O	835	CLA	CMD-C2D	-2.13	1.46	1.50
15	N	818	CLA	MG-NB	-2.13	2.01	2.05
15	B	808	CLA	C3B-C4B	2.13	1.48	1.42
15	B	812	CLA	CMD-C2D	-2.13	1.46	1.50
15	B	808	CLA	CMD-C2D	-2.13	1.46	1.50
15	O	835	CLA	CMB-C2B	-2.13	1.46	1.50
14	b	833	F6C	CMC-C2C	-2.13	1.46	1.50
15	L	202	CLA	CMB-C2B	-2.13	1.46	1.50
15	O	829	CLA	CMB-C2B	-2.13	1.46	1.50
15	B	824	CLA	MG-NB	-2.13	2.01	2.05
15	N	834	CLA	CMB-C2B	-2.13	1.46	1.50
15	A	834	CLA	CMD-C2D	-2.13	1.46	1.50
15	b	814	CLA	CMD-C2D	-2.13	1.46	1.50
15	A	818	CLA	CMC-C2C	-2.13	1.46	1.50
15	O	809	CLA	CMD-C2D	-2.13	1.46	1.50
15	W	1501	CLA	MG-NB	-2.13	2.01	2.05
15	a	834	CLA	CMB-C2B	-2.12	1.46	1.50
15	N	836	CLA	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	820	CLA	CMB-C2B	-2.12	1.46	1.50
15	B	816	CLA	CMB-C2B	-2.12	1.46	1.50
15	O	835	CLA	MG-NB	-2.12	2.01	2.05
15	W	1501	CLA	CMB-C2B	-2.12	1.46	1.50
15	B	833	CLA	CMD-C2D	-2.12	1.46	1.50
15	b	809	CLA	CMD-C2D	-2.12	1.46	1.50
15	L	202	CLA	MG-NB	-2.12	2.01	2.05
15	O	814	CLA	CMD-C2D	-2.12	1.46	1.50
15	O	837	CLA	MG-NB	-2.12	2.01	2.05
15	L	202	CLA	CMD-C2D	-2.12	1.46	1.50
15	B	827	CLA	CMB-C2B	-2.12	1.46	1.50
15	b	835	CLA	CMD-C2D	-2.12	1.46	1.50
15	b	830	CLA	MG-NB	-2.12	2.01	2.05
14	N	856	F6C	C2B-C1B	2.12	1.49	1.44
15	N	814	CLA	MG-NB	-2.12	2.01	2.05
15	b	837	CLA	MG-NB	-2.12	2.01	2.05
15	B	805	CLA	CMD-C2D	-2.12	1.46	1.50
15	W	1502	CLA	MG-NB	-2.12	2.01	2.05
15	B	833	CLA	CMB-C2B	-2.12	1.46	1.50
15	A	840	CLA	CHC-C1C	2.12	1.42	1.38
15	B	816	CLA	MG-NB	-2.12	2.01	2.05
15	O	823	CLA	CMD-C2D	-2.11	1.46	1.50
15	N	834	CLA	CMD-C2D	-2.11	1.46	1.50
14	a	802	F6C	C2B-C1B	2.11	1.49	1.44
15	N	833	CLA	MG-NB	-2.11	2.01	2.05
15	N	828	CLA	MG-NB	-2.11	2.01	2.05
15	l	103	CLA	CMD-C2D	-2.11	1.46	1.50
15	B	806	CLA	CHC-C1C	2.11	1.42	1.38
15	b	818	CLA	CMB-C2B	-2.11	1.46	1.50
15	a	840	CLA	CHC-C1C	2.11	1.42	1.38
14	A	857	F6C	C2B-C1B	2.11	1.49	1.44
15	a	818	CLA	CMC-C2C	-2.11	1.46	1.50
15	j	202	CLA	CMB-C2B	-2.11	1.46	1.50
15	W	1501	CLA	CMD-C2D	-2.11	1.46	1.50
15	b	824	CLA	CMD-C2D	-2.11	1.46	1.50
15	a	833	CLA	CMB-C2B	-2.11	1.46	1.50
15	a	838	CLA	CMD-C2D	-2.11	1.46	1.50
15	A	807	CLA	MG-NB	-2.11	2.01	2.05
15	b	834	CLA	CMD-C2D	-2.11	1.46	1.50
15	b	841	CLA	CMB-C2B	-2.11	1.46	1.50
15	A	838	CLA	CHC-C1C	2.11	1.42	1.38
15	A	835	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	830	CLA	MG-NB	-2.11	2.01	2.05
15	B	836	CLA	CMD-C2D	-2.11	1.46	1.50
15	b	801	CLA	CMC-C2C	-2.11	1.46	1.50
15	b	835	CLA	MG-NB	-2.11	2.01	2.05
15	B	839	CLA	CMB-C2B	-2.11	1.46	1.50
15	A	814	CLA	MG-NB	-2.11	2.01	2.05
15	a	807	CLA	MG-NB	-2.11	2.01	2.05
15	N	833	CLA	CMB-C2B	-2.11	1.46	1.50
15	O	818	CLA	MG-NB	-2.11	2.01	2.05
15	b	806	CLA	CMD-C2D	-2.11	1.46	1.50
15	N	835	CLA	MG-NB	-2.11	2.01	2.05
15	b	819	CLA	MG-NB	-2.11	2.01	2.05
15	j	202	CLA	CMD-C2D	-2.11	1.46	1.50
15	O	826	CLA	MG-NB	-2.11	2.01	2.05
15	a	834	CLA	CMD-C2D	-2.11	1.46	1.50
15	a	822	CLA	MG-NB	-2.11	2.01	2.05
15	A	833	CLA	CMD-C2D	-2.10	1.46	1.50
15	b	838	CLA	CMD-C2D	-2.10	1.46	1.50
15	B	817	CLA	MG-NB	-2.10	2.01	2.05
15	A	836	CLA	CMB-C2B	-2.10	1.46	1.50
14	a	856	F6C	C2B-C1B	2.10	1.49	1.44
15	N	838	CLA	CMD-C2D	-2.10	1.46	1.50
15	O	806	CLA	CMD-C2D	-2.10	1.46	1.50
15	A	837	CLA	MG-NB	-2.10	2.01	2.05
15	b	835	CLA	CMB-C2B	-2.10	1.46	1.50
15	b	807	CLA	CMD-C2D	-2.10	1.46	1.50
15	N	831	CLA	MG-NB	-2.10	2.01	2.05
15	O	838	CLA	MG-NB	-2.10	2.01	2.05
15	A	821	CLA	CMD-C2D	-2.10	1.46	1.50
15	O	841	CLA	CMB-C2B	-2.10	1.46	1.50
14	O	833	F6C	CMD-C2D	-2.10	1.46	1.50
15	B	805	CLA	MG-NB	-2.10	2.01	2.05
15	A	838	CLA	CMD-C2D	-2.10	1.46	1.50
15	O	838	CLA	CMD-C2D	-2.10	1.46	1.50
14	N	856	F6C	CMD-C2D	-2.10	1.46	1.50
15	A	825	CLA	CMD-C2D	-2.10	1.46	1.50
15	a	821	CLA	CMD-C2D	-2.10	1.46	1.50
15	B	828	CLA	CMB-C2B	-2.10	1.46	1.50
15	N	837	CLA	MG-NB	-2.10	2.01	2.05
18	V	101	BCR	C19-C18	-2.10	1.44	1.50
18	K	101	BCR	C19-C18	-2.10	1.44	1.50
15	A	834	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	803	CLA	CMD-C2D	-2.10	1.46	1.50
15	a	833	CLA	CMD-C2D	-2.10	1.46	1.50
15	A	842	CLA	CMB-C2B	-2.10	1.46	1.50
15	N	833	CLA	CMD-C2D	-2.10	1.46	1.50
15	N	821	CLA	CMD-C2D	-2.09	1.46	1.50
15	A	831	CLA	MG-NB	-2.09	2.01	2.05
15	L	203	CLA	MG-NB	-2.09	2.01	2.05
14	b	833	F6C	CMD-C2D	-2.09	1.46	1.50
15	A	810	CLA	MG-NB	-2.09	2.01	2.05
15	B	835	CLA	MG-NB	-2.09	2.01	2.05
15	O	819	CLA	MG-NB	-2.09	2.01	2.05
15	b	827	CLA	CMD-C2D	-2.09	1.46	1.50
15	N	840	CLA	CHC-C1C	2.09	1.42	1.38
15	A	835	CLA	MG-NB	-2.09	2.01	2.05
18	i	101	BCR	C19-C18	-2.09	1.44	1.50
15	O	807	CLA	CMD-C2D	-2.09	1.46	1.50
15	a	836	CLA	CMB-C2B	-2.09	1.46	1.50
15	a	825	CLA	CMD-C2D	-2.09	1.46	1.50
15	N	836	CLA	MG-NB	-2.09	2.01	2.05
15	a	810	CLA	MG-NB	-2.09	2.01	2.05
15	a	831	CLA	MG-NB	-2.09	2.01	2.05
15	b	806	CLA	MG-NB	-2.09	2.01	2.05
15	i	103	CLA	CMB-C2B	-2.09	1.46	1.50
15	A	821	CLA	MG-NB	-2.09	2.01	2.05
15	O	801	CLA	CMC-C2C	-2.09	1.46	1.50
15	A	822	CLA	MG-NB	-2.09	2.01	2.05
15	B	809	CLA	MG-NB	-2.09	2.01	2.05
15	a	814	CLA	MG-NB	-2.09	2.01	2.05
15	j	203	CLA	CMB-C2B	-2.09	1.46	1.50
15	b	838	CLA	MG-NB	-2.09	2.01	2.05
15	Z	103	CLA	CMD-C2D	-2.09	1.46	1.50
15	a	820	CLA	CMB-C2B	-2.09	1.46	1.50
15	A	832	CLA	MG-NB	-2.09	2.01	2.05
15	N	818	CLA	CMC-C2C	-2.09	1.46	1.50
15	a	835	CLA	MG-NB	-2.09	2.01	2.05
15	B	836	CLA	MG-NB	-2.09	2.01	2.05
14	a	856	F6C	CMD-C2D	-2.09	1.46	1.50
15	B	804	CLA	CMD-C2D	-2.09	1.46	1.50
15	A	819	CLA	MG-NB	-2.09	2.01	2.05
15	A	838	CLA	MG-NB	-2.09	2.01	2.05
15	B	822	CLA	MG-NB	-2.09	2.01	2.05
15	K	102	CLA	MG-NB	-2.09	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	816	CLA	MG-NB	-2.09	2.01	2.05
15	O	827	CLA	CMD-C2D	-2.09	1.46	1.50
15	N	813	CLA	MG-NB	-2.09	2.01	2.05
15	a	821	CLA	MG-NB	-2.09	2.01	2.05
15	a	832	CLA	MG-NB	-2.09	2.01	2.05
15	N	825	CLA	CMD-C2D	-2.09	1.46	1.50
15	b	837	CLA	CMD-C2D	-2.09	1.46	1.50
15	j	203	CLA	MG-NB	-2.09	2.01	2.05
15	A	812	CLA	CMD-C2D	-2.09	1.46	1.50
15	N	810	CLA	MG-NB	-2.09	2.01	2.05
15	N	838	CLA	MG-NB	-2.09	2.01	2.05
15	N	831	CLA	CMD-C2D	-2.09	1.46	1.50
15	B	808	CLA	CHC-C1C	2.08	1.42	1.38
15	O	806	CLA	MG-NB	-2.08	2.01	2.05
15	A	841	CLA	CMB-C2B	-2.08	1.46	1.50
15	X	103	CLA	CMD-C2D	-2.08	1.46	1.50
15	a	804	CLA	CMC-C2C	-2.08	1.46	1.50
15	a	837	CLA	MG-NB	-2.08	2.01	2.05
15	B	813	CLA	CMD-C2D	-2.08	1.46	1.50
15	a	803	CLA	CMD-C2D	-2.08	1.46	1.50
15	N	821	CLA	MG-NB	-2.08	2.01	2.05
14	A	826	F6C	CMD-C2D	-2.08	1.46	1.50
14	B	831	F6C	CMD-C2D	-2.08	1.46	1.50
15	A	828	CLA	CMB-C2B	-2.08	1.46	1.50
15	N	807	CLA	CMD-C2D	-2.08	1.46	1.50
15	O	837	CLA	CMD-C2D	-2.08	1.46	1.50
15	a	841	CLA	CMB-C2B	-2.08	1.46	1.50
15	b	823	CLA	MG-NB	-2.08	2.01	2.05
15	A	803	CLA	CMC-C2C	-2.08	1.46	1.50
15	A	803	CLA	CMD-C2D	-2.08	1.46	1.50
15	b	824	CLA	MG-NB	-2.08	2.01	2.05
15	i	102	CLA	MG-NB	-2.08	2.01	2.05
15	N	832	CLA	CMD-C2D	-2.08	1.46	1.50
15	N	841	CLA	CMB-C2B	-2.08	1.46	1.50
14	N	802	F6C	CMD-C2D	-2.08	1.46	1.50
14	a	826	F6C	CMD-C2D	-2.08	1.46	1.50
15	N	836	CLA	CMD-C2D	-2.08	1.46	1.50
15	a	815	CLA	CMD-C2D	-2.08	1.46	1.50
15	b	804	CLA	CMC-C2C	-2.08	1.46	1.50
15	A	806	CLA	CMD-C2D	-2.08	1.46	1.50
15	W	1502	CLA	CMB-C2B	-2.08	1.46	1.50
15	b	803	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	821	CLA	MG-NB	-2.08	2.01	2.05
15	N	832	CLA	MG-NB	-2.08	2.01	2.05
15	O	816	CLA	MG-NB	-2.08	2.01	2.05
15	a	832	CLA	CMD-C2D	-2.08	1.46	1.50
15	V	102	CLA	MG-NB	-2.08	2.01	2.05
14	A	802	F6C	C2B-C1B	2.08	1.49	1.44
14	A	802	F6C	CMD-C2D	-2.08	1.46	1.50
15	N	839	CLA	CMB-C2B	-2.08	1.46	1.50
15	N	841	CLA	CMC-C2C	-2.08	1.46	1.50
15	O	808	CLA	CMB-C2B	-2.08	1.46	1.50
15	B	825	CLA	CMD-C2D	-2.08	1.46	1.50
15	F	201	CLA	CMB-C2B	-2.08	1.46	1.50
15	a	839	CLA	CMB-C2B	-2.08	1.46	1.50
15	A	804	CLA	CMC-C2C	-2.08	1.46	1.50
15	A	832	CLA	CMD-C2D	-2.08	1.46	1.50
15	b	839	CLA	CMD-C2D	-2.08	1.46	1.50
15	O	813	CLA	CMC-C2C	-2.08	1.46	1.50
15	b	820	CLA	CMD-C2D	-2.08	1.46	1.50
15	b	811	CLA	MG-NB	-2.08	2.01	2.05
15	L	203	CLA	CMB-C2B	-2.08	1.46	1.50
15	a	806	CLA	CMD-C2D	-2.07	1.46	1.50
15	N	819	CLA	MG-NB	-2.07	2.01	2.05
15	A	836	CLA	CMD-C2D	-2.07	1.46	1.50
15	O	818	CLA	CMB-C2B	-2.07	1.46	1.50
15	a	841	CLA	CMC-C2C	-2.07	1.46	1.50
15	B	806	CLA	CMD-C2D	-2.07	1.46	1.50
15	A	825	CLA	MG-NB	-2.07	2.01	2.05
14	A	857	F6C	CMD-C2D	-2.07	1.46	1.50
15	b	831	CLA	CMD-C2D	-2.07	1.46	1.50
15	O	824	CLA	MG-NB	-2.07	2.01	2.05
15	A	839	CLA	CMB-C2B	-2.07	1.46	1.50
15	a	836	CLA	MG-NB	-2.07	2.01	2.05
15	B	835	CLA	CMD-C2D	-2.07	1.46	1.50
15	O	834	CLA	CMD-C2D	-2.07	1.46	1.50
15	a	842	CLA	CMB-C2B	-2.07	1.46	1.50
15	a	827	CLA	MG-NB	-2.07	2.01	2.05
15	O	824	CLA	CMB-C2B	-2.07	1.46	1.50
15	O	829	CLA	MG-NB	-2.07	2.01	2.05
15	N	812	CLA	CMB-C2B	-2.07	1.46	1.50
15	A	836	CLA	MG-NB	-2.07	2.01	2.05
15	B	829	CLA	MG-NB	-2.07	2.01	2.05
15	A	819	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	818	CLA	CMD-C2D	-2.07	1.46	1.50
15	B	829	CLA	CMD-C2D	-2.07	1.46	1.50
15	N	815	CLA	CMD-C2D	-2.07	1.46	1.50
15	O	831	CLA	CMD-C2D	-2.07	1.46	1.50
15	a	811	CLA	CMD-C2D	-2.07	1.46	1.50
14	a	802	F6C	CMD-C2D	-2.07	1.46	1.50
15	N	842	CLA	CMB-C2B	-2.07	1.46	1.50
15	b	808	CLA	CMB-C2B	-2.07	1.46	1.50
15	A	831	CLA	CMD-C2D	-2.07	1.46	1.50
15	a	807	CLA	CMD-C2D	-2.07	1.46	1.50
15	b	824	CLA	CMB-C2B	-2.07	1.46	1.50
15	B	814	CLA	MG-NB	-2.07	2.01	2.05
15	a	828	CLA	MG-NB	-2.07	2.01	2.05
15	b	821	CLA	MG-NB	-2.07	2.01	2.05
15	a	836	CLA	CMD-C2D	-2.07	1.46	1.50
15	O	811	CLA	MG-NB	-2.07	2.01	2.05
15	B	803	CLA	CMC-C2C	-2.07	1.46	1.50
15	A	807	CLA	CMD-C2D	-2.07	1.46	1.50
15	A	822	CLA	CMD-C2D	-2.07	1.46	1.50
15	N	832	CLA	CMB-C2B	-2.07	1.46	1.50
15	A	813	CLA	MG-NB	-2.07	2.01	2.05
15	B	810	CLA	CMB-C2B	-2.07	1.46	1.50
15	B	820	CLA	CMD-C2D	-2.07	1.46	1.50
15	b	827	CLA	CMC-C2C	-2.07	1.46	1.50
15	X	103	CLA	MG-NB	-2.07	2.01	2.05
15	O	812	CLA	MG-NB	-2.07	2.01	2.05
15	O	805	CLA	CMD-C2D	-2.06	1.46	1.50
15	O	839	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	830	CLA	MG-NB	-2.06	2.01	2.05
15	N	827	CLA	MG-NB	-2.06	2.01	2.05
15	N	839	CLA	MG-NB	-2.06	2.01	2.05
15	a	838	CLA	MG-NB	-2.06	2.01	2.05
15	A	804	CLA	CMB-C2B	-2.06	1.46	1.50
14	L	201	F6C	CMD-C2D	-2.06	1.46	1.50
15	i	103	CLA	MG-NB	-2.06	2.01	2.05
14	A	824	F6C	CMD-C2D	-2.06	1.46	1.50
15	B	811	CLA	CMD-C2D	-2.06	1.46	1.50
15	B	822	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	819	CLA	CMD-C2D	-2.06	1.46	1.50
15	f	201	CLA	CMB-C2B	-2.06	1.46	1.50
15	B	806	CLA	MG-NB	-2.06	2.01	2.05
15	B	819	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	807	CLA	MG-NB	-2.06	2.01	2.05
15	A	841	CLA	CMC-C2C	-2.06	1.46	1.50
15	N	804	CLA	CMC-C2C	-2.06	1.46	1.50
15	a	804	CLA	CMB-C2B	-2.06	1.46	1.50
15	A	815	CLA	CMD-C2D	-2.06	1.46	1.50
15	N	804	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	842	CLA	CMD-C2D	-2.06	1.46	1.50
15	N	803	CLA	MG-NB	-2.06	2.01	2.05
15	A	831	CLA	CHC-C1C	2.06	1.42	1.38
15	O	820	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	812	CLA	CMB-C2B	-2.06	1.46	1.50
15	B	837	CLA	MG-NB	-2.06	2.01	2.05
15	b	803	CLA	MG-NB	-2.06	2.01	2.05
15	A	819	CLA	CMB-C2B	-2.06	1.46	1.50
15	B	824	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	816	CLA	CMB-C2B	-2.06	1.46	1.50
15	O	804	CLA	CMC-C2C	-2.06	1.46	1.50
15	A	827	CLA	MG-NB	-2.06	2.01	2.05
15	O	831	CLA	MG-NB	-2.06	2.01	2.05
15	A	811	CLA	CMD-C2D	-2.06	1.46	1.50
15	N	807	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	828	CLA	CMD-C2D	-2.06	1.46	1.50
15	Z	103	CLA	MG-NB	-2.06	2.01	2.05
15	b	814	CLA	MG-NB	-2.06	2.01	2.05
15	b	839	CLA	MG-NB	-2.06	2.01	2.05
15	N	814	CLA	CMD-C2D	-2.06	1.46	1.50
15	N	822	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	822	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	841	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	819	CLA	MG-NB	-2.06	2.01	2.05
15	b	831	CLA	MG-NB	-2.06	2.01	2.05
15	B	832	CLA	CMD-C2D	-2.06	1.46	1.50
15	B	839	CLA	CMD-C2D	-2.06	1.46	1.50
15	N	811	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	814	CLA	CMD-C2D	-2.06	1.46	1.50
15	B	802	CLA	CMD-C2D	-2.06	1.46	1.50
15	N	808	CLA	CMD-C2D	-2.06	1.46	1.50
15	b	805	CLA	CMD-C2D	-2.06	1.46	1.50
15	b	819	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	816	CLA	CMB-C2B	-2.06	1.46	1.50
15	O	812	CLA	CMB-C2B	-2.06	1.46	1.50
15	a	816	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	830	CLA	MG-NB	-2.06	2.01	2.05
14	L	204	F6C	CMD-C2D	-2.06	1.46	1.50
15	A	808	CLA	CMD-C2D	-2.06	1.46	1.50
15	A	835	CLA	CMB-C2B	-2.06	1.46	1.50
15	B	837	CLA	CMD-C2D	-2.06	1.46	1.50
15	N	819	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	835	CLA	CMB-C2B	-2.06	1.46	1.50
15	O	803	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	819	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	828	CLA	CMD-C2D	-2.06	1.46	1.50
15	b	822	CLA	CMD-C2D	-2.06	1.46	1.50
15	l	103	CLA	MG-NB	-2.06	2.01	2.05
15	B	807	CLA	CMB-C2B	-2.06	1.46	1.50
15	S	201	CLA	CMB-C2B	-2.06	1.46	1.50
15	B	807	CLA	CMC-C2C	-2.06	1.46	1.50
15	B	834	CLA	CMB-C2B	-2.06	1.46	1.50
15	a	807	CLA	CMB-C2B	-2.06	1.46	1.50
15	A	842	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	814	CLA	CMD-C2D	-2.06	1.46	1.50
15	O	828	CLA	MG-NB	-2.06	2.01	2.05
15	A	839	CLA	CMD-C2D	-2.06	1.46	1.50
15	B	801	CLA	CMC-C2C	-2.06	1.46	1.50
15	b	813	CLA	CMD-C2D	-2.06	1.46	1.50
15	a	812	CLA	MG-NB	-2.06	2.01	2.05
15	b	829	CLA	MG-NB	-2.06	2.01	2.05
15	O	836	CLA	CMB-C2B	-2.06	1.46	1.50
15	b	813	CLA	MG-NB	-2.06	2.01	2.05
15	A	832	CLA	CMB-C2B	-2.06	1.46	1.50
15	N	811	CLA	CMC-C2C	-2.06	1.46	1.50
15	b	826	CLA	CMB-C2B	-2.06	1.46	1.50
15	B	811	CLA	MG-NB	-2.06	2.01	2.05
15	O	839	CLA	MG-NB	-2.06	2.01	2.05
15	B	811	CLA	CMC-C2C	-2.05	1.46	1.50
15	B	814	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	836	CLA	CMB-C2B	-2.05	1.46	1.50
15	B	810	CLA	MG-NB	-2.05	2.01	2.05
15	B	818	CLA	MG-NB	-2.05	2.01	2.05
15	A	841	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	812	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	819	CLA	CMB-C2B	-2.05	1.46	1.50
15	A	828	CLA	MG-NB	-2.05	2.01	2.05
15	O	821	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	W	1503	F6C	CMD-C2D	-2.05	1.46	1.50
15	B	825	CLA	CMC-C2C	-2.05	1.46	1.50
15	O	803	CLA	MG-NB	-2.05	2.01	2.05
15	b	820	CLA	MG-NB	-2.05	2.01	2.05
15	A	812	CLA	CMB-C2B	-2.05	1.46	1.50
15	a	808	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	820	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	839	CLA	MG-NB	-2.05	2.01	2.05
15	O	807	CLA	MG-NB	-2.05	2.01	2.05
15	A	837	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	841	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	831	CLA	CHC-C1C	2.05	1.42	1.38
15	O	803	CLA	CMB-C2B	-2.05	1.46	1.50
15	W	1502	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	812	CLA	CMB-C2B	-2.05	1.46	1.50
15	a	823	CLA	MG-NB	-2.05	2.01	2.05
15	a	825	CLA	MG-NB	-2.05	2.01	2.05
15	A	828	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	809	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	816	CLA	CMD-C2D	-2.05	1.46	1.50
15	B	812	CLA	MG-NB	-2.05	2.01	2.05
14	j	204	F6C	CMD-C2D	-2.05	1.46	1.50
15	N	812	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	813	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	816	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	808	CLA	MG-NB	-2.05	2.01	2.05
15	a	808	CLA	MG-NB	-2.05	2.01	2.05
15	O	819	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	827	CLA	CMB-C2B	-2.05	1.46	1.50
15	b	821	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	820	CLA	MG-NB	-2.05	2.01	2.05
15	N	806	CLA	CMB-C2B	-2.05	1.46	1.50
15	a	827	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	839	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	813	CLA	CMC-C2C	-2.05	1.46	1.50
15	A	803	CLA	MG-NB	-2.05	2.01	2.05
15	O	813	CLA	MG-NB	-2.05	2.01	2.05
15	a	803	CLA	MG-NB	-2.05	2.01	2.05
15	a	813	CLA	MG-NB	-2.05	2.01	2.05
15	N	827	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	822	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	826	CLA	CMB-C2B	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	840	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	856	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	811	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	818	CLA	CMB-C2B	-2.05	1.46	1.50
15	O	832	CLA	MG-NB	-2.05	2.01	2.05
15	B	827	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	837	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	821	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	816	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	811	CLA	CMD-C2D	-2.05	1.46	1.50
14	N	802	F6C	C2B-C1B	2.05	1.48	1.44
15	A	804	CLA	CMD-C2D	-2.05	1.46	1.50
15	B	819	CLA	CMD-C2D	-2.05	1.46	1.50
15	O	827	CLA	CMC-C2C	-2.05	1.46	1.50
15	a	817	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	842	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	841	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	827	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	820	CLA	CMD-C2D	-2.05	1.46	1.50
15	A	823	CLA	MG-NB	-2.05	2.01	2.05
15	B	809	CLA	CMB-C2B	-2.05	1.46	1.50
15	B	817	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	821	CLA	CMB-C2B	-2.05	1.46	1.50
15	N	830	CLA	MG-NB	-2.05	2.01	2.05
15	A	820	CLA	CMD-C2D	-2.05	1.46	1.50
15	B	803	CLA	CMD-C2D	-2.05	1.46	1.50
15	L	203	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	817	CLA	CMD-C2D	-2.05	1.46	1.50
15	a	831	CLA	CMD-C2D	-2.05	1.46	1.50
15	b	812	CLA	MG-NB	-2.05	2.01	2.05
15	A	817	CLA	CMD-C2D	-2.05	1.46	1.50
15	B	809	CLA	CMD-C2D	-2.05	1.46	1.50
15	N	839	CLA	CMD-C2D	-2.05	1.46	1.50
15	B	825	CLA	MG-NB	-2.04	2.01	2.05
14	a	824	F6C	CMD-C2D	-2.04	1.46	1.50
15	A	809	CLA	CMD-C2D	-2.04	1.46	1.50
15	B	825	CLA	CMB-C2B	-2.04	1.46	1.50
15	a	837	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	827	CLA	CMB-C2B	-2.04	1.46	1.50
15	b	832	CLA	MG-NB	-2.04	2.01	2.05
15	B	816	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	802	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	802	CLA	MG-NB	-2.04	2.01	2.05
15	A	816	CLA	CMD-C2D	-2.04	1.46	1.50
15	B	802	CLA	CMB-C2B	-2.04	1.46	1.50
15	O	809	CLA	CMC-C2C	-2.04	1.46	1.50
15	a	804	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	809	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	816	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	825	CLA	CMB-C2B	-2.04	1.46	1.50
15	O	804	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	830	CLA	CMB-C2B	-2.04	1.46	1.50
15	O	814	CLA	MG-NB	-2.04	2.01	2.05
15	O	818	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	841	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	832	CLA	CMB-C2B	-2.04	1.46	1.50
14	a	802	F6C	C4D-ND	-2.04	1.33	1.37
15	A	808	CLA	MG-NB	-2.04	2.01	2.05
14	b	810	F6C	CMD-C2D	-2.04	1.46	1.50
15	N	805	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	829	CLA	CMD-C2D	-2.04	1.46	1.50
15	O	830	CLA	CMB-C2B	-2.04	1.46	1.50
15	a	835	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	840	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	817	CLA	MG-NB	-2.04	2.01	2.05
15	b	802	CLA	CMD-C2D	-2.04	1.46	1.50
15	A	809	CLA	MG-NB	-2.04	2.01	2.05
15	N	834	CLA	MG-NB	-2.04	2.01	2.05
15	a	834	CLA	MG-NB	-2.04	2.01	2.05
15	A	807	CLA	CMB-C2B	-2.04	1.46	1.50
15	a	831	CLA	CMC-C2C	-2.04	1.46	1.50
15	B	827	CLA	MG-NB	-2.04	2.01	2.05
15	B	823	CLA	CMD-C2D	-2.04	1.46	1.50
15	j	203	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	809	CLA	MG-NB	-2.04	2.01	2.05
15	O	827	CLA	MG-NB	-2.04	2.01	2.05
15	a	839	CLA	MG-NB	-2.04	2.01	2.05
15	A	805	CLA	MG-NB	-2.04	2.01	2.05
15	B	832	CLA	MG-NB	-2.04	2.01	2.05
15	A	825	CLA	CMB-C2B	-2.04	1.46	1.50
15	B	830	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	817	CLA	MG-NB	-2.04	2.01	2.05
15	a	820	CLA	MG-NB	-2.04	2.01	2.05
15	b	827	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	804	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	813	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	823	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	835	CLA	CMB-C2B	-2.04	1.46	1.50
15	b	808	CLA	CMC-C2C	-2.04	1.46	1.50
15	O	836	CLA	CMD-C2D	-2.04	1.46	1.50
15	i	103	CLA	CMD-C2D	-2.04	1.46	1.50
15	a	825	CLA	CMB-C2B	-2.04	1.46	1.50
15	b	832	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	820	CLA	MG-NB	-2.04	2.01	2.05
15	A	805	CLA	CMD-C2D	-2.04	1.46	1.50
15	A	820	CLA	MG-NB	-2.04	2.01	2.05
15	a	828	CLA	CMB-C2B	-2.04	1.46	1.50
15	b	825	CLA	CMD-C2D	-2.04	1.46	1.50
15	A	812	CLA	MG-NB	-2.04	2.01	2.05
15	b	807	CLA	MG-NB	-2.04	2.01	2.05
15	B	834	CLA	CMD-C2D	-2.04	1.46	1.50
15	b	836	CLA	CMD-C2D	-2.04	1.46	1.50
15	N	812	CLA	MG-NB	-2.04	2.01	2.05
15	b	804	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	839	CLA	MG-NB	-2.03	2.01	2.05
15	a	809	CLA	MG-NB	-2.03	2.01	2.05
14	O	810	F6C	CMD-C2D	-2.03	1.46	1.50
15	a	805	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	840	CLA	CMD-C2D	-2.03	1.46	1.50
15	a	813	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	812	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	805	CLA	MG-NB	-2.03	2.01	2.05
15	O	834	CLA	MG-NB	-2.03	2.01	2.05
15	A	821	CLA	CMB-C2B	-2.03	1.46	1.50
15	b	829	CLA	CMD-C2D	-2.03	1.46	1.50
15	B	802	CLA	MG-NB	-2.03	2.01	2.05
15	N	825	CLA	MG-NB	-2.03	2.01	2.05
15	b	808	CLA	MG-NB	-2.03	2.01	2.05
15	B	815	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	826	CLA	CMD-C2D	-2.03	1.46	1.50
14	A	802	F6C	C4D-ND	-2.03	1.33	1.37
15	B	808	CLA	CMC-C2C	-2.03	1.46	1.50
15	B	824	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	840	CLA	CMB-C2B	-2.03	1.46	1.50
15	V	103	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	817	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	815	CLA	CMC-C2C	-2.03	1.46	1.50
15	a	809	CLA	CMB-C2B	-2.03	1.46	1.50
15	b	801	CLA	CMB-C2B	-2.03	1.46	1.50
15	b	818	CLA	CMD-C2D	-2.03	1.46	1.50
15	A	842	CLA	MG-NB	-2.03	2.01	2.05
15	O	832	CLA	CMD-C2D	-2.03	1.46	1.50
15	A	856	CLA	MG-NB	-2.03	2.01	2.05
15	N	828	CLA	CMB-C2B	-2.03	1.46	1.50
15	O	808	CLA	CMC-C2C	-2.03	1.46	1.50
15	a	842	CLA	MG-NB	-2.03	2.01	2.05
15	N	810	CLA	CMC-C2C	-2.03	1.46	1.50
15	A	817	CLA	MG-NB	-2.03	2.01	2.05
15	N	823	CLA	MG-NB	-2.03	2.01	2.05
15	O	812	CLA	CMD-C2D	-2.03	1.46	1.50
15	A	834	CLA	MG-NB	-2.03	2.01	2.05
15	b	802	CLA	MG-NB	-2.03	2.01	2.05
15	b	834	CLA	MG-NB	-2.03	2.01	2.05
15	B	818	CLA	CMB-C2B	-2.03	1.46	1.50
15	O	813	CLA	CMB-C2B	-2.03	1.46	1.50
15	O	837	CLA	CMB-C2B	-2.03	1.46	1.50
15	b	826	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	839	CLA	CMC-C2C	-2.03	1.46	1.50
15	A	813	CLA	CMD-C2D	-2.03	1.46	1.50
15	N	818	CLA	CMB-C2B	-2.03	1.46	1.50
15	N	805	CLA	MG-NB	-2.03	2.01	2.05
15	N	842	CLA	MG-NB	-2.03	2.01	2.05
15	K	103	CLA	CMD-C2D	-2.03	1.46	1.50
15	O	820	CLA	CMB-C2B	-2.03	1.46	1.50
15	B	835	CLA	CMB-C2B	-2.03	1.46	1.50
15	N	809	CLA	CMB-C2B	-2.03	1.46	1.50
15	N	838	CLA	CMB-C2B	-2.03	1.46	1.50
15	a	805	CLA	MG-NB	-2.03	2.01	2.05
15	O	825	CLA	CMD-C2D	-2.03	1.46	1.50
15	b	820	CLA	CMB-C2B	-2.03	1.46	1.50
15	N	823	CLA	CMD-C2D	-2.03	1.46	1.50
15	a	821	CLA	CMB-C2B	-2.03	1.46	1.50
15	b	813	CLA	CMB-C2B	-2.03	1.46	1.50
15	B	826	CLA	MG-NB	-2.02	2.01	2.05
15	B	830	CLA	MG-NB	-2.02	2.01	2.05
15	B	810	CLA	CMD-C2D	-2.02	1.46	1.50
15	a	829	CLA	MG-NB	-2.02	2.01	2.05
15	b	828	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	809	CLA	CMB-C2B	-2.02	1.46	1.50
15	A	823	CLA	CMD-C2D	-2.02	1.46	1.50
15	O	823	CLA	MG-NB	-2.02	2.01	2.05
15	O	815	CLA	CMC-C2C	-2.02	1.46	1.50
15	O	801	CLA	CMB-C2B	-2.02	1.46	1.50
15	a	840	CLA	CMB-C2B	-2.02	1.46	1.50
15	b	828	CLA	CMB-C2B	-2.02	1.46	1.50
15	N	831	CLA	CHC-C1C	2.02	1.42	1.38
15	B	801	CLA	CMB-C2B	-2.02	1.46	1.50
15	O	811	CLA	CMB-C2B	-2.02	1.46	1.50
15	B	837	CLA	CMC-C2C	-2.02	1.46	1.50
15	L	203	CLA	CMC-C2C	-2.02	1.46	1.50
15	O	808	CLA	MG-NB	-2.02	2.01	2.05
15	N	835	CLA	CMD-C2D	-2.02	1.46	1.50
15	O	817	CLA	CMD-C2D	-2.02	1.46	1.50
14	N	802	F6C	C4D-ND	-2.02	1.33	1.37
15	A	815	CLA	MG-NB	-2.02	2.01	2.05
15	b	836	CLA	MG-NB	-2.02	2.01	2.05
15	b	809	CLA	CMC-C2C	-2.02	1.46	1.50
15	B	834	CLA	MG-NB	-2.02	2.01	2.05
15	a	815	CLA	MG-NB	-2.02	2.01	2.05
15	A	840	CLA	CMB-C2B	-2.02	1.46	1.50
15	b	841	CLA	MG-NB	-2.02	2.01	2.05
15	A	838	CLA	CMB-C2B	-2.02	1.46	1.50
15	b	807	CLA	CMB-C2B	-2.02	1.46	1.50
15	B	804	CLA	MG-NB	-2.02	2.01	2.05
15	S	201	CLA	MG-NB	-2.02	2.01	2.05
15	B	811	CLA	CMB-C2B	-2.02	1.46	1.50
15	O	807	CLA	CMB-C2B	-2.02	1.46	1.50
15	B	807	CLA	MG-NB	-2.02	2.01	2.05
15	A	815	CLA	CMC-C2C	-2.02	1.46	1.50
15	b	803	CLA	CMB-C2B	-2.02	1.46	1.50
15	N	815	CLA	MG-NB	-2.02	2.01	2.05
15	a	815	CLA	CMC-C2C	-2.02	1.46	1.50
15	A	823	CLA	CMB-C2B	-2.01	1.46	1.50
15	a	806	CLA	CMB-C2B	-2.01	1.46	1.50
15	a	838	CLA	CMB-C2B	-2.01	1.46	1.50
15	O	841	CLA	MG-NB	-2.01	2.01	2.05
15	N	814	CLA	CMB-C2B	-2.01	1.46	1.50
15	N	814	CLA	CMC-C2C	-2.01	1.46	1.50
15	a	827	CLA	CMB-C2B	-2.01	1.46	1.50
14	b	840	F6C	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	806	CLA	CMB-C2B	-2.01	1.46	1.50
15	a	808	CLA	CMB-C2B	-2.01	1.46	1.50
15	O	804	CLA	MG-NB	-2.01	2.01	2.05
15	O	828	CLA	CMB-C2B	-2.01	1.46	1.50
15	a	814	CLA	CMB-C2B	-2.01	1.46	1.50
15	N	827	CLA	CMB-C2B	-2.01	1.46	1.50
15	O	825	CLA	CMB-C2B	-2.01	1.46	1.50
15	B	820	CLA	MG-NB	-2.01	2.01	2.05
15	F	201	CLA	MG-NB	-2.01	2.01	2.05
15	a	810	CLA	CMC-C2C	-2.01	1.46	1.50
15	b	837	CLA	CMB-C2B	-2.01	1.46	1.50
15	N	841	CLA	MG-NB	-2.01	2.01	2.05
15	N	837	CLA	CMB-C2B	-2.01	1.46	1.50
15	b	814	CLA	CMB-C2B	-2.01	1.46	1.50
15	f	201	CLA	MG-NB	-2.01	2.01	2.05
15	N	829	CLA	CMC-C2C	-2.01	1.46	1.50
15	b	811	CLA	CMB-C2B	-2.01	1.46	1.50
15	A	806	CLA	CMB-C2B	-2.01	1.46	1.50
15	N	831	CLA	CMC-C2C	-2.01	1.46	1.50
15	A	814	CLA	CMB-C2B	-2.01	1.46	1.50
15	N	823	CLA	CMB-C2B	-2.01	1.46	1.50
15	O	814	CLA	CMB-C2B	-2.01	1.46	1.50
15	b	839	CLA	CMC-C2C	-2.01	1.46	1.50
15	a	841	CLA	MG-NB	-2.01	2.01	2.05
15	a	814	CLA	CMC-C2C	-2.01	1.46	1.50
15	A	837	CLA	CMB-C2B	-2.01	1.46	1.50
15	O	837	CLA	CMC-C2C	-2.01	1.46	1.50
15	B	803	CLA	MG-NB	-2.01	2.01	2.05
14	N	856	F6C	CMC-C2C	-2.00	1.46	1.50
15	A	829	CLA	CMC-C2C	-2.00	1.46	1.50
15	B	835	CLA	CMC-C2C	-2.00	1.46	1.50
15	K	102	CLA	CMB-C2B	-2.00	1.46	1.50
15	N	803	CLA	CMB-C2B	-2.00	1.46	1.50
15	i	102	CLA	CMB-C2B	-2.00	1.46	1.50
15	A	808	CLA	CMB-C2B	-2.00	1.46	1.50
15	B	812	CLA	CMB-C2B	-2.00	1.46	1.50
15	N	813	CLA	CMB-C2B	-2.00	1.46	1.50
15	O	821	CLA	CMB-C2B	-2.00	1.46	1.50
15	O	823	CLA	CMB-C2B	-2.00	1.46	1.50
15	V	102	CLA	CMB-C2B	-2.00	1.46	1.50
15	a	803	CLA	CMB-C2B	-2.00	1.46	1.50
15	a	823	CLA	CMB-C2B	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	836	CLA	MG-NB	-2.00	2.01	2.05
15	b	804	CLA	MG-NB	-2.00	2.01	2.05
15	A	818	CLA	CMB-C2B	-2.00	1.46	1.50
15	A	856	CLA	CMB-C2B	-2.00	1.46	1.50
15	N	835	CLA	CMC-C2C	-2.00	1.46	1.50
15	a	805	CLA	CMC-C2C	-2.00	1.46	1.50
15	b	815	CLA	CMC-C2C	-2.00	1.46	1.50
14	A	802	F6C	C1D-C2D	2.00	1.48	1.44
15	B	805	CLA	CMC-C2C	-2.00	1.46	1.50
15	a	830	CLA	CMC-C2C	-2.00	1.46	1.50
15	O	825	CLA	CMC-C2C	-2.00	1.46	1.50
15	O	822	CLA	MG-NB	-2.00	2.01	2.05
15	A	838	CLA	CMC-C2C	-2.00	1.46	1.50
15	N	808	CLA	CMB-C2B	-2.00	1.46	1.50
15	O	834	CLA	CMC-C2C	-2.00	1.46	1.50
13	N	801	CL0	MG-NB	-2.00	2.01	2.05
15	A	841	CLA	MG-NB	-2.00	2.01	2.05

All (1961) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	840	F6C	CAA-C2A-C3A	-10.01	109.11	127.87
14	B	838	F6C	CAA-C2A-C3A	-10.00	109.14	127.87
14	b	840	F6C	CAA-C2A-C3A	-9.96	109.21	127.87
14	L	204	F6C	CAA-C2A-C3A	-9.94	109.25	127.87
14	j	204	F6C	CAA-C2A-C3A	-9.90	109.33	127.87
14	W	1503	F6C	CAA-C2A-C3A	-9.81	109.49	127.87
14	A	826	F6C	CAA-C2A-C3A	-9.68	109.73	127.87
14	a	826	F6C	CAA-C2A-C3A	-9.55	109.98	127.87
14	N	826	F6C	CAA-C2A-C3A	-9.53	110.02	127.87
14	N	856	F6C	CAA-C2A-C3A	-9.38	110.30	127.87
14	A	857	F6C	CAA-C2A-C3A	-9.35	110.35	127.87
14	a	856	F6C	CAA-C2A-C3A	-9.31	110.43	127.87
14	A	824	F6C	CAA-C2A-C3A	-9.18	110.67	127.87
14	a	824	F6C	CAA-C2A-C3A	-9.13	110.77	127.87
14	N	824	F6C	CAA-C2A-C3A	-8.92	111.17	127.87
14	O	810	F6C	CAA-C2A-C3A	-8.82	111.35	127.87
14	a	802	F6C	CAA-C2A-C3A	-8.77	111.45	127.87
14	N	802	F6C	CAA-C2A-C3A	-8.71	111.55	127.87
14	b	810	F6C	CAA-C2A-C3A	-8.69	111.59	127.87
14	L	201	F6C	CAA-C2A-C3A	-8.69	111.59	127.87
14	B	831	F6C	CAA-C2A-C3A	-8.59	111.78	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	802	F6C	CAA-C2A-C3A	-8.58	111.80	127.87
14	b	833	F6C	CAA-C2A-C3A	-8.40	112.13	127.87
14	O	833	F6C	CAA-C2A-C3A	-8.34	112.25	127.87
14	A	857	F6C	CMA-C3A-C4A	-8.15	110.38	124.73
14	a	856	F6C	CMA-C3A-C4A	-7.99	110.66	124.73
14	N	856	F6C	CMA-C3A-C4A	-7.90	110.81	124.73
14	b	833	F6C	CMA-C3A-C4A	-7.76	111.05	124.73
14	B	831	F6C	CMA-C3A-C4A	-7.75	111.08	124.73
14	O	833	F6C	CMA-C3A-C4A	-7.74	111.10	124.73
14	L	201	F6C	CMA-C3A-C4A	-7.70	111.17	124.73
14	b	810	F6C	CMA-C3A-C4A	-7.54	111.44	124.73
14	O	810	F6C	CMA-C3A-C4A	-7.49	111.54	124.73
14	a	824	F6C	CMA-C3A-C4A	-7.22	112.02	124.73
14	N	824	F6C	CMA-C3A-C4A	-7.17	112.09	124.73
14	A	802	F6C	CMA-C3A-C4A	-7.17	112.10	124.73
14	b	840	F6C	CMA-C3A-C4A	-7.14	112.15	124.73
14	a	802	F6C	CMA-C3A-C4A	-7.13	112.17	124.73
14	A	824	F6C	CMA-C3A-C4A	-7.13	112.18	124.73
14	B	838	F6C	CMA-C3A-C4A	-7.08	112.26	124.73
14	N	802	F6C	CMA-C3A-C4A	-7.04	112.33	124.73
14	O	840	F6C	CMA-C3A-C4A	-7.00	112.40	124.73
14	b	840	F6C	CAA-C2A-C1A	-6.96	108.56	128.01
14	O	840	F6C	CAA-C2A-C1A	-6.95	108.61	128.01
14	B	838	F6C	CAA-C2A-C1A	-6.94	108.61	128.01
15	a	828	CLA	C4A-NA-C1A	6.92	109.83	106.68
15	A	818	CLA	C4A-NA-C1A	6.90	109.83	106.68
15	b	803	CLA	C4A-NA-C1A	6.89	109.82	106.68
15	a	818	CLA	C4A-NA-C1A	6.86	109.81	106.68
15	N	818	CLA	C4A-NA-C1A	6.85	109.81	106.68
15	B	802	CLA	C4A-NA-C1A	6.82	109.79	106.68
15	N	831	CLA	C4A-NA-C1A	6.82	109.79	106.68
15	O	803	CLA	C4A-NA-C1A	6.81	109.78	106.68
15	A	828	CLA	C4A-NA-C1A	6.81	109.78	106.68
14	W	1503	F6C	CMA-C3A-C4A	-6.80	112.75	124.73
14	A	826	F6C	CMA-C3A-C4A	-6.77	112.80	124.73
14	a	826	F6C	CMA-C3A-C4A	-6.76	112.82	124.73
15	O	826	CLA	C4A-NA-C1A	6.76	109.76	106.68
15	a	823	CLA	C4A-NA-C1A	6.75	109.76	106.68
15	B	813	CLA	C4A-NA-C1A	6.73	109.75	106.68
14	j	204	F6C	CMA-C3A-C4A	-6.71	112.92	124.73
15	N	841	CLA	C4A-NA-C1A	6.70	109.74	106.68
15	b	826	CLA	C4A-NA-C1A	6.70	109.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	820	CLA	C4A-NA-C1A	6.70	109.73	106.68
15	b	801	CLA	C4A-NA-C1A	6.70	109.73	106.68
15	N	828	CLA	C4A-NA-C1A	6.69	109.73	106.68
15	A	807	CLA	C4A-NA-C1A	6.68	109.73	106.68
15	N	823	CLA	C4A-NA-C1A	6.68	109.73	106.68
15	b	805	CLA	C4A-NA-C1A	6.68	109.73	106.68
15	b	824	CLA	C4A-NA-C1A	6.68	109.72	106.68
15	N	838	CLA	C4A-NA-C1A	6.67	109.72	106.68
15	A	823	CLA	C4A-NA-C1A	6.67	109.72	106.68
15	A	838	CLA	C4A-NA-C1A	6.67	109.72	106.68
15	O	805	CLA	C4A-NA-C1A	6.67	109.72	106.68
15	B	801	CLA	C4A-NA-C1A	6.66	109.72	106.68
15	b	827	CLA	C4A-NA-C1A	6.65	109.72	106.68
15	B	822	CLA	C4A-NA-C1A	6.64	109.71	106.68
15	A	839	CLA	C4A-NA-C1A	6.64	109.71	106.68
15	b	806	CLA	C4A-NA-C1A	6.63	109.71	106.68
15	N	839	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	O	827	CLA	C4A-NA-C1A	6.62	109.70	106.68
15	N	815	CLA	C4A-NA-C1A	6.61	109.69	106.68
15	O	809	CLA	C4A-NA-C1A	6.61	109.69	106.68
15	a	839	CLA	C4A-NA-C1A	6.61	109.69	106.68
15	O	821	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	a	820	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	O	841	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	B	824	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	b	821	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	A	841	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	B	839	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	L	202	CLA	C4A-NA-C1A	6.59	109.69	106.68
15	O	824	CLA	C4A-NA-C1A	6.59	109.69	106.68
15	X	103	CLA	C4A-NA-C1A	6.59	109.69	106.68
15	B	804	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	O	815	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	B	819	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	a	807	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	b	839	CLA	C4A-NA-C1A	6.58	109.68	106.68
14	N	826	F6C	CMA-C3A-C4A	-6.57	113.15	124.73
15	A	831	CLA	C4A-NA-C1A	6.57	109.68	106.68
15	N	807	CLA	C4A-NA-C1A	6.57	109.68	106.68
15	A	815	CLA	C4A-NA-C1A	6.57	109.68	106.68
15	a	815	CLA	C4A-NA-C1A	6.57	109.68	106.68
15	B	837	CLA	C4A-NA-C1A	6.56	109.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	801	CLA	C4A-NA-C1A	6.56	109.67	106.68
15	O	816	CLA	C4A-NA-C1A	6.56	109.67	106.68
15	O	839	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	B	831	F6C	CAA-C2A-C1A	-6.56	109.69	128.01
15	a	838	CLA	C4A-NA-C1A	6.56	109.67	106.68
15	O	838	CLA	C4A-NA-C1A	6.56	109.67	106.68
15	b	841	CLA	C4A-NA-C1A	6.56	109.67	106.68
15	B	836	CLA	C4A-NA-C1A	6.55	109.67	106.68
15	Z	103	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	a	841	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	L	203	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	O	806	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	A	820	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	j	203	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	b	816	CLA	C4A-NA-C1A	6.53	109.66	106.68
15	A	809	CLA	C4A-NA-C1A	6.53	109.66	106.68
15	l	103	CLA	C4A-NA-C1A	6.52	109.66	106.68
15	b	815	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	B	814	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	a	809	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	N	809	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	N	840	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	a	831	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	j	202	CLA	C4A-NA-C1A	6.52	109.65	106.68
15	A	840	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	B	825	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	a	803	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	N	808	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	O	830	CLA	C4A-NA-C1A	6.51	109.65	106.68
15	A	829	CLA	C4A-NA-C1A	6.50	109.65	106.68
15	b	838	CLA	C4A-NA-C1A	6.50	109.64	106.68
14	b	833	F6C	CAA-C2A-C1A	-6.50	109.86	128.01
15	W	1501	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	N	811	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	b	830	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	a	814	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	N	829	CLA	C4A-NA-C1A	6.49	109.64	106.68
15	A	813	CLA	C4A-NA-C1A	6.48	109.64	106.68
15	b	820	CLA	C4A-NA-C1A	6.48	109.64	106.68
15	N	803	CLA	C4A-NA-C1A	6.48	109.63	106.68
15	N	817	CLA	C4A-NA-C1A	6.48	109.63	106.68
15	N	821	CLA	C4A-NA-C1A	6.48	109.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	808	CLA	C4A-NA-C1A	6.48	109.63	106.68
14	O	833	F6C	CAA-C2A-C1A	-6.47	109.92	128.01
15	O	820	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	A	822	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	A	808	CLA	C4A-NA-C1A	6.47	109.63	106.68
15	a	813	CLA	C4A-NA-C1A	6.46	109.63	106.68
15	a	822	CLA	C4A-NA-C1A	6.46	109.63	106.68
15	f	201	CLA	C4A-NA-C1A	6.46	109.63	106.68
15	B	818	CLA	C4A-NA-C1A	6.46	109.63	106.68
15	B	808	CLA	C4A-NA-C1A	6.46	109.62	106.68
15	F	201	CLA	C4A-NA-C1A	6.46	109.62	106.68
15	a	811	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	a	817	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	b	808	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	A	821	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	a	821	CLA	C4A-NA-C1A	6.45	109.62	106.68
14	j	204	F6C	CAA-C2A-C1A	-6.44	110.02	128.01
15	B	823	CLA	C4A-NA-C1A	6.44	109.62	106.68
15	b	807	CLA	C4A-NA-C1A	6.44	109.62	106.68
15	b	829	CLA	C4A-NA-C1A	6.44	109.62	106.68
15	V	102	CLA	C4A-NA-C1A	6.44	109.61	106.68
15	N	813	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	O	811	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	O	807	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	N	842	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	a	840	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	a	808	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	i	102	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	O	813	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	K	102	CLA	C4A-NA-C1A	6.42	109.61	106.68
15	N	814	CLA	C4A-NA-C1A	6.41	109.61	106.68
14	A	857	F6C	CAA-C2A-C1A	-6.41	110.10	128.01
15	A	814	CLA	C4A-NA-C1A	6.41	109.60	106.68
15	O	825	CLA	C4A-NA-C1A	6.41	109.60	106.68
15	B	811	CLA	C4A-NA-C1A	6.41	109.60	106.68
14	a	856	F6C	CAA-C2A-C1A	-6.41	110.12	128.01
15	N	805	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	N	802	F6C	CAA-C2A-C1A	-6.40	110.12	128.01
15	a	806	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	B	806	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	O	834	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	a	829	CLA	C4A-NA-C1A	6.40	109.60	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	817	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	a	842	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	B	803	CLA	C4A-NA-C1A	6.39	109.59	106.68
15	B	807	CLA	C4A-NA-C1A	6.39	109.59	106.68
15	A	811	CLA	C4A-NA-C1A	6.39	109.59	106.68
15	a	805	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	A	832	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	b	811	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	B	832	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	N	836	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	A	806	CLA	C4A-NA-C1A	6.37	109.59	106.68
15	b	812	CLA	C4A-NA-C1A	6.37	109.59	106.68
15	B	805	CLA	C4A-NA-C1A	6.37	109.58	106.68
14	N	856	F6C	CAA-C2A-C1A	-6.37	110.22	128.01
15	O	814	CLA	C4A-NA-C1A	6.37	109.58	106.68
15	b	835	CLA	C4A-NA-C1A	6.37	109.58	106.68
15	N	832	CLA	C4A-NA-C1A	6.36	109.58	106.68
15	b	804	CLA	C4A-NA-C1A	6.36	109.58	106.68
15	b	809	CLA	C4A-NA-C1A	6.36	109.58	106.68
15	A	804	CLA	C4A-NA-C1A	6.35	109.58	106.68
15	O	812	CLA	C4A-NA-C1A	6.35	109.58	106.68
15	B	810	CLA	C4A-NA-C1A	6.35	109.58	106.68
15	B	812	CLA	C4A-NA-C1A	6.35	109.58	106.68
15	N	806	CLA	C4A-NA-C1A	6.35	109.58	106.68
15	b	813	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	A	802	F6C	CAA-C2A-C1A	-6.35	110.28	128.01
15	O	804	CLA	C4A-NA-C1A	6.34	109.57	106.68
15	A	842	CLA	C4A-NA-C1A	6.34	109.57	106.68
15	B	833	CLA	C4A-NA-C1A	6.34	109.57	106.68
15	B	809	CLA	C4A-NA-C1A	6.34	109.57	106.68
15	W	1502	CLA	C4A-NA-C1A	6.34	109.57	106.68
15	b	814	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	O	835	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	b	825	CLA	C4A-NA-C1A	6.33	109.57	106.68
14	W	1503	F6C	CAA-C2A-C1A	-6.33	110.32	128.01
15	O	823	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	a	836	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	A	805	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	i	103	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	A	803	CLA	C4A-NA-C1A	6.33	109.56	106.68
15	B	827	CLA	C4A-NA-C1A	6.33	109.56	106.68
15	a	827	CLA	C4A-NA-C1A	6.33	109.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	812	CLA	C4A-NA-C1A	6.32	109.56	106.68
15	a	819	CLA	C4A-NA-C1A	6.32	109.56	106.68
15	S	201	CLA	C4A-NA-C1A	6.31	109.56	106.68
15	O	832	CLA	C4A-NA-C1A	6.31	109.56	106.68
15	N	810	CLA	C4A-NA-C1A	6.31	109.56	106.68
15	a	810	CLA	C4A-NA-C1A	6.31	109.56	106.68
15	N	812	CLA	C4A-NA-C1A	6.31	109.56	106.68
15	b	834	CLA	C4A-NA-C1A	6.31	109.56	106.68
15	A	836	CLA	C4A-NA-C1A	6.30	109.55	106.68
15	A	827	CLA	C4A-NA-C1A	6.29	109.55	106.68
15	a	812	CLA	C4A-NA-C1A	6.29	109.55	106.68
15	a	834	CLA	C4A-NA-C1A	6.29	109.55	106.68
15	A	810	CLA	C4A-NA-C1A	6.29	109.55	106.68
15	a	832	CLA	C4A-NA-C1A	6.28	109.55	106.68
15	A	834	CLA	C4A-NA-C1A	6.28	109.54	106.68
15	O	829	CLA	C4A-NA-C1A	6.28	109.54	106.68
15	B	828	CLA	C4A-NA-C1A	6.28	109.54	106.68
14	L	204	F6C	CMA-C3A-C4A	-6.27	113.69	124.73
15	N	804	CLA	C4A-NA-C1A	6.27	109.54	106.68
14	a	802	F6C	CAA-C2A-C1A	-6.26	110.51	128.01
15	N	822	CLA	C4A-NA-C1A	6.26	109.53	106.68
15	N	816	CLA	C4A-NA-C1A	6.26	109.53	106.68
15	A	816	CLA	C4A-NA-C1A	6.25	109.53	106.68
15	a	816	CLA	C4A-NA-C1A	6.25	109.53	106.68
15	b	832	CLA	C4A-NA-C1A	6.25	109.53	106.68
15	a	804	CLA	C4A-NA-C1A	6.24	109.53	106.68
15	N	833	CLA	C4A-NA-C1A	6.24	109.53	106.68
15	a	825	CLA	C4A-NA-C1A	6.22	109.52	106.68
15	O	836	CLA	C4A-NA-C1A	6.21	109.51	106.68
15	b	836	CLA	C4A-NA-C1A	6.21	109.51	106.68
15	N	834	CLA	C4A-NA-C1A	6.21	109.51	106.68
15	N	830	CLA	C4A-NA-C1A	6.20	109.51	106.68
15	b	822	CLA	C4A-NA-C1A	6.20	109.51	106.68
14	L	204	F6C	CAA-C2A-C1A	-6.19	110.70	128.01
15	B	834	CLA	C4A-NA-C1A	6.19	109.50	106.68
15	a	830	CLA	C4A-NA-C1A	6.19	109.50	106.68
15	A	825	CLA	C4A-NA-C1A	6.18	109.50	106.68
15	O	822	CLA	C4A-NA-C1A	6.18	109.50	106.68
15	B	830	CLA	C4A-NA-C1A	6.17	109.49	106.68
15	N	825	CLA	C4A-NA-C1A	6.16	109.49	106.68
15	N	827	CLA	C4A-NA-C1A	6.16	109.49	106.68
15	b	831	CLA	C4A-NA-C1A	6.16	109.49	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	820	CLA	C4A-NA-C1A	6.15	109.49	106.68
15	N	819	CLA	C4A-NA-C1A	6.15	109.48	106.68
15	A	835	CLA	C4A-NA-C1A	6.15	109.48	106.68
15	B	817	CLA	C4A-NA-C1A	6.15	109.48	106.68
15	A	833	CLA	C4A-NA-C1A	6.15	109.48	106.68
15	a	837	CLA	C4A-NA-C1A	6.15	109.48	106.68
15	A	837	CLA	C4A-NA-C1A	6.14	109.48	106.68
15	B	829	CLA	C4A-NA-C1A	6.13	109.47	106.68
15	O	828	CLA	C4A-NA-C1A	6.13	109.47	106.68
15	O	831	CLA	C4A-NA-C1A	6.13	109.47	106.68
15	B	835	CLA	C4A-NA-C1A	6.13	109.47	106.68
15	A	830	CLA	C4A-NA-C1A	6.12	109.47	106.68
15	b	818	CLA	C4A-NA-C1A	6.12	109.47	106.68
15	N	837	CLA	C4A-NA-C1A	6.12	109.47	106.68
15	b	837	CLA	C4A-NA-C1A	6.10	109.46	106.68
15	O	818	CLA	C4A-NA-C1A	6.09	109.46	106.68
15	A	819	CLA	C4A-NA-C1A	6.08	109.45	106.68
15	a	833	CLA	C4A-NA-C1A	6.08	109.45	106.68
15	b	819	CLA	C4A-NA-C1A	6.08	109.45	106.68
13	A	801	CL0	C1B-CHB-C4A	6.08	125.23	121.32
14	A	857	F6C	CMA-C3A-C2A	-6.08	109.70	126.15
15	O	837	CLA	C4A-NA-C1A	6.07	109.45	106.68
15	b	828	CLA	C4A-NA-C1A	6.07	109.45	106.68
15	O	819	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	N	856	F6C	CMA-C3A-C2A	-6.05	109.80	126.15
15	V	103	CLA	C4A-NA-C1A	6.03	109.43	106.68
13	N	801	CL0	C1B-CHB-C4A	6.01	125.19	121.32
15	B	816	CLA	C4A-NA-C1A	6.01	109.42	106.68
14	a	856	F6C	CMA-C3A-C2A	-6.00	109.91	126.15
15	N	835	CLA	C4A-NA-C1A	6.00	109.42	106.68
15	a	835	CLA	C4A-NA-C1A	6.00	109.42	106.68
15	B	826	CLA	C4A-NA-C1A	5.99	109.41	106.68
13	a	801	CL0	C1B-CHB-C4A	5.96	125.15	121.32
15	A	856	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	A	824	F6C	CAA-C2A-C1A	-5.95	111.38	128.01
15	K	103	CLA	C4A-NA-C1A	5.94	109.39	106.68
14	a	824	F6C	CAA-C2A-C1A	-5.94	111.42	128.01
15	O	802	CLA	C4A-NA-C1A	5.89	109.36	106.68
14	N	824	F6C	CAA-C2A-C1A	-5.88	111.58	128.01
15	B	815	CLA	C4A-NA-C1A	5.79	109.32	106.68
15	b	802	CLA	C4A-NA-C1A	5.79	109.32	106.68
15	b	817	CLA	C4A-NA-C1A	5.71	109.28	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	817	CLA	C4A-NA-C1A	5.69	109.28	106.68
14	B	831	F6C	CMA-C3A-C2A	-5.65	110.87	126.15
14	L	204	F6C	CMA-C3A-C2A	-5.60	111.01	126.15
14	O	833	F6C	CMA-C3A-C2A	-5.58	111.05	126.15
14	N	826	F6C	CAA-C2A-C1A	-5.57	112.46	128.01
14	b	833	F6C	CMA-C3A-C2A	-5.55	111.13	126.15
14	L	201	F6C	C4A-NA-C1A	5.52	110.18	106.31
14	A	826	F6C	CAA-C2A-C1A	-5.44	112.82	128.01
14	O	810	F6C	C4A-NA-C1A	5.43	110.12	106.31
14	j	204	F6C	CMA-C3A-C2A	-5.41	111.53	126.15
14	b	840	F6C	CMA-C3A-C2A	-5.38	111.59	126.15
14	O	840	F6C	CMA-C3A-C2A	-5.37	111.62	126.15
14	W	1503	F6C	CMA-C3A-C2A	-5.34	111.70	126.15
14	B	838	F6C	CMA-C3A-C2A	-5.34	111.71	126.15
14	a	826	F6C	CAA-C2A-C1A	-5.27	113.29	128.01
14	N	824	F6C	CMA-C3A-C2A	-5.25	111.95	126.15
14	b	810	F6C	C4A-NA-C1A	5.24	109.99	106.31
14	A	824	F6C	CMA-C3A-C2A	-5.21	112.05	126.15
14	a	824	F6C	CMA-C3A-C2A	-5.18	112.15	126.15
14	A	826	F6C	C4A-NA-C1A	5.11	109.90	106.31
14	N	802	F6C	CMA-C3A-C2A	-5.05	112.50	126.15
14	A	802	F6C	CMA-C3A-C2A	-5.04	112.51	126.15
14	a	802	F6C	CMA-C3A-C2A	-5.02	112.56	126.15
14	L	201	F6C	CMA-C3A-C2A	-5.02	112.58	126.15
14	b	810	F6C	CMA-C3A-C2A	-5.00	112.62	126.15
14	b	833	F6C	C4A-NA-C1A	4.99	109.82	106.31
14	a	826	F6C	C4A-NA-C1A	4.98	109.81	106.31
14	O	833	F6C	C4A-NA-C1A	4.97	109.80	106.31
14	B	831	F6C	C4A-NA-C1A	4.96	109.79	106.31
14	O	810	F6C	CMA-C3A-C2A	-4.96	112.74	126.15
14	A	824	F6C	C4A-NA-C1A	4.94	109.78	106.31
14	a	824	F6C	C4A-NA-C1A	4.92	109.77	106.31
14	N	826	F6C	C4A-NA-C1A	4.87	109.73	106.31
14	O	810	F6C	CAA-C2A-C1A	-4.86	114.43	128.01
14	b	840	F6C	C4A-NA-C1A	4.84	109.71	106.31
14	N	824	F6C	C4A-NA-C1A	4.83	109.70	106.31
14	B	838	F6C	C4A-NA-C1A	4.71	109.62	106.31
14	N	826	F6C	CMA-C3A-C2A	-4.69	113.46	126.15
14	b	810	F6C	CAA-C2A-C1A	-4.68	114.93	128.01
14	W	1503	F6C	C4A-NA-C1A	4.68	109.60	106.31
14	L	204	F6C	C4A-NA-C1A	4.68	109.60	106.31
14	a	826	F6C	CMA-C3A-C2A	-4.68	113.49	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	840	F6C	C4A-NA-C1A	4.65	109.58	106.31
14	L	201	F6C	CAA-C2A-C1A	-4.64	115.06	128.01
14	j	204	F6C	C4A-NA-C1A	4.61	109.55	106.31
14	A	826	F6C	CMA-C3A-C2A	-4.58	113.75	126.15
14	N	856	F6C	C4A-NA-C1A	4.54	109.50	106.31
14	A	857	F6C	C4A-NA-C1A	4.49	109.46	106.31
14	a	856	F6C	C4A-NA-C1A	4.47	109.45	106.31
20	a	853	LMT	C1B-O5B-C5B	4.36	122.24	113.72
20	N	853	LMT	C1B-O5B-C5B	4.32	122.15	113.72
20	A	853	LMT	C1B-O5B-C5B	4.32	122.15	113.72
14	a	802	F6C	C4A-NA-C1A	4.24	109.29	106.31
14	A	802	F6C	C4A-NA-C1A	4.16	109.23	106.31
14	N	802	F6C	C4A-NA-C1A	4.13	109.21	106.31
15	B	821	CLA	C4A-NA-C1A	4.05	108.53	106.68
15	b	823	CLA	C4A-NA-C1A	3.89	108.45	106.68
14	A	802	F6C	C1A-C2A-C3A	-3.72	103.06	106.97
20	a	853	LMT	C1B-O1B-C4'	3.67	126.69	117.98
14	N	802	F6C	C1A-C2A-C3A	-3.67	103.11	106.97
18	N	857	BCR	C15-C14-C13	-3.67	122.14	127.28
20	A	853	LMT	C1B-O1B-C4'	3.65	126.64	117.98
14	A	857	F6C	C1A-C2A-C3A	-3.65	103.13	106.97
18	A	858	BCR	C15-C14-C13	-3.64	122.17	127.28
20	N	853	LMT	C1B-O1B-C4'	3.59	126.48	117.98
14	a	802	F6C	C1A-C2A-C3A	-3.58	103.20	106.97
15	A	835	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
15	N	811	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
18	a	857	BCR	C15-C14-C13	-3.56	122.29	127.28
14	a	856	F6C	C1A-C2A-C3A	-3.54	103.24	106.97
18	a	857	BCR	C11-C10-C9	-3.52	122.34	127.28
18	N	857	BCR	C11-C10-C9	-3.52	122.35	127.28
15	B	811	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
14	N	856	F6C	C1A-C2A-C3A	-3.51	103.27	106.97
15	O	813	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
15	b	813	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
18	A	858	BCR	C11-C10-C9	-3.48	122.40	127.28
15	N	820	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
15	A	820	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
14	N	826	F6C	C1A-C2A-C3A	-3.45	103.34	106.97
15	N	806	CLA	O2D-CGD-O1D	-3.44	117.14	123.85
15	a	820	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
15	A	819	CLA	C3B-C4B-NB	-3.40	107.49	110.53
14	N	826	F6C	O2D-CGD-O1D	-3.36	117.31	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	801	CL0	O2D-CGD-CBD	3.35	114.63	110.95
15	L	203	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
15	A	811	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
15	a	819	CLA	C3B-C4B-NB	-3.32	107.57	110.53
15	O	817	CLA	C3B-C4B-NB	-3.32	107.57	110.53
15	N	819	CLA	C3B-C4B-NB	-3.31	107.58	110.53
14	a	826	F6C	C1A-C2A-C3A	-3.29	103.50	106.97
15	a	811	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
15	a	835	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
13	N	801	CL0	O2D-CGD-CBD	3.23	114.50	110.95
15	W	1502	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
13	A	801	CL0	O2D-CGD-CBD	3.22	114.49	110.95
15	j	203	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
15	b	808	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	A	826	F6C	C1A-C2A-C3A	-3.21	103.59	106.97
14	N	824	F6C	C1A-C2A-C3A	-3.20	103.60	106.97
15	A	816	CLA	C3B-C4B-NB	-3.20	107.67	110.53
14	j	204	F6C	O2D-CGD-O1D	-3.20	117.63	123.85
15	B	806	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
15	N	835	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
15	b	817	CLA	C3B-C4B-NB	-3.19	107.68	110.53
15	W	1502	CLA	C3B-C4B-NB	-3.19	107.69	110.53
14	L	204	F6C	O2D-CGD-O1D	-3.18	117.66	123.85
15	B	803	CLA	C3B-C4B-NB	-3.18	107.69	110.53
15	B	815	CLA	C3B-C4B-NB	-3.17	107.70	110.53
15	N	810	CLA	CAA-C2A-C3A	-3.17	104.43	113.00
15	b	807	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
14	A	826	F6C	O2D-CGD-O1D	-3.17	117.69	123.85
15	N	816	CLA	C3B-C4B-NB	-3.16	107.71	110.53
15	b	825	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
15	O	808	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
15	O	807	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
15	b	815	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
15	B	801	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
15	A	818	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
15	A	825	CLA	C3B-C4B-NB	-3.14	107.73	110.53
15	a	816	CLA	C3B-C4B-NB	-3.14	107.73	110.53
15	B	807	CLA	O2D-CGD-O1D	-3.14	117.75	123.85
14	a	824	F6C	C1A-C2A-C3A	-3.13	103.67	106.97
15	a	818	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
15	O	836	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
15	b	801	CLA	O2D-CGD-O1D	-3.13	117.76	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	804	CLA	C3B-C4B-NB	-3.12	107.74	110.53
15	L	203	CLA	C3B-C4B-NB	-3.12	107.75	110.53
14	A	824	F6C	C1A-C2A-C3A	-3.12	103.69	106.97
14	a	826	F6C	O2D-CGD-O1D	-3.12	117.78	123.85
15	N	818	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
15	O	815	CLA	O2D-CGD-O1D	-3.11	117.78	123.85
15	b	824	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
15	a	810	CLA	CAA-C2A-C3A	-3.11	104.58	113.00
15	a	831	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
15	O	820	CLA	C3B-C4B-NB	-3.11	107.75	110.53
15	B	834	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
14	W	1503	F6C	O2D-CGD-O1D	-3.11	117.80	123.85
15	A	827	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
15	O	824	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
14	O	840	F6C	C1A-C2A-C3A	-3.11	103.70	106.97
14	b	833	F6C	O2D-CGD-O1D	-3.10	117.81	123.85
15	B	822	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
15	N	831	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
15	b	836	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
14	B	838	F6C	C1A-C2A-C3A	-3.10	103.70	106.97
15	A	831	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
15	O	822	CLA	CAA-C2A-C3A	-3.10	104.63	113.00
15	B	812	CLA	O2D-CGD-O1D	-3.09	117.82	123.85
14	O	833	F6C	C1A-C2A-C3A	-3.09	103.71	106.97
14	B	831	F6C	O2D-CGD-O1D	-3.09	117.83	123.85
15	O	814	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
15	B	823	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	L	201	F6C	CBD-CHA-C4D	-3.09	105.06	108.54
15	B	818	CLA	C3B-C4B-NB	-3.09	107.77	110.53
15	b	820	CLA	C3B-C4B-NB	-3.09	107.78	110.53
14	b	833	F6C	C1A-C2A-C3A	-3.08	103.72	106.97
15	a	812	CLA	C3B-C4B-NB	-3.08	107.78	110.53
15	A	810	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
14	O	833	F6C	O2D-CGD-O1D	-3.08	117.85	123.85
15	N	822	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
15	A	803	CLA	C3B-C4B-NB	-3.08	107.78	110.53
15	A	812	CLA	C3B-C4B-NB	-3.08	107.78	110.53
15	b	817	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
15	a	809	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
15	B	837	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
15	O	801	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
15	B	810	CLA	C3B-C4B-NB	-3.07	107.79	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	812	CLA	C3B-C4B-NB	-3.07	107.79	110.53
15	a	840	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
15	O	825	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
15	N	809	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
15	N	825	CLA	C3B-C4B-NB	-3.06	107.80	110.53
14	B	831	F6C	C1A-C2A-C3A	-3.06	103.75	106.97
15	b	823	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
15	B	813	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
14	N	802	F6C	C4A-C3A-C2A	-3.05	102.44	106.97
15	A	809	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
15	b	814	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
15	O	812	CLA	C3B-C4B-NB	-3.05	107.81	110.53
15	S	201	CLA	C3B-C4B-NB	-3.05	107.81	110.53
15	a	837	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
15	b	839	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
15	a	825	CLA	C3B-C4B-NB	-3.05	107.81	110.53
15	b	829	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
15	A	837	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
15	O	829	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
15	A	833	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
15	a	827	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
15	N	827	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
15	a	822	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
15	b	804	CLA	C3B-C4B-NB	-3.04	107.82	110.53
13	a	801	CL0	O2D-CGD-O1D	-3.04	117.93	123.85
15	O	816	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
15	A	817	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
15	B	816	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
15	N	808	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
13	A	801	CL0	O2D-CGD-O1D	-3.03	117.94	123.85
15	A	805	CLA	C3B-C4B-NB	-3.03	107.82	110.53
14	b	840	F6C	C1A-C2A-C3A	-3.03	103.78	106.97
15	a	817	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
15	B	836	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
15	O	802	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
15	N	817	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
15	b	812	CLA	C3B-C4B-NB	-3.03	107.83	110.53
15	a	839	CLA	C3B-C4B-NB	-3.03	107.83	110.53
15	N	837	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
15	b	822	CLA	CAA-C2A-C3A	-3.02	104.83	113.00
15	B	815	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
15	A	840	CLA	O2D-CGD-O1D	-3.02	117.97	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	808	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
15	V	103	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
15	A	839	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
15	a	804	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
15	A	856	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
15	a	804	CLA	C3B-C4B-NB	-3.01	107.84	110.53
15	B	821	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
15	K	103	CLA	C3B-C4B-NB	-3.01	107.84	110.53
14	B	838	F6C	O2D-CGD-O1D	-3.01	117.98	123.85
15	O	838	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
13	N	801	CL0	O2D-CGD-O1D	-3.01	117.99	123.85
15	a	805	CLA	C3B-C4B-NB	-3.01	107.84	110.53
15	N	840	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
15	N	835	CLA	C3B-C4B-NB	-3.01	107.85	110.53
15	i	103	CLA	C3B-C4B-NB	-3.01	107.85	110.53
15	b	838	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
15	N	804	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
15	A	808	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
15	B	814	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
15	A	839	CLA	C3B-C4B-NB	-3.00	107.85	110.53
15	A	804	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
15	B	827	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
14	a	802	F6C	C4A-C3A-C2A	-3.00	102.52	106.97
15	B	830	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
15	V	103	CLA	C3B-C4B-NB	-3.00	107.85	110.53
15	i	103	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
15	b	802	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
15	K	103	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
15	O	839	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
15	B	820	CLA	CAA-C2A-C3A	-2.99	104.91	113.00
15	N	839	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
15	a	818	CLA	C3B-C4B-NB	-2.99	107.86	110.53
15	N	839	CLA	C3B-C4B-NB	-2.99	107.86	110.53
15	b	826	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
15	B	828	CLA	C3B-C4B-NB	-2.98	107.87	110.53
18	k	102	BCR	C7-C8-C9	-2.98	121.83	126.23
15	b	819	CLA	C3B-C4B-NB	-2.98	107.87	110.53
15	O	817	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	L	204	F6C	C1A-C2A-C3A	-2.98	103.84	106.97
15	b	837	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
14	j	204	F6C	C1A-C2A-C3A	-2.97	103.84	106.97
15	O	823	CLA	O2D-CGD-O1D	-2.97	118.06	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	831	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
15	a	805	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
15	F	201	CLA	C3B-C4B-NB	-2.97	107.88	110.53
15	N	804	CLA	C3B-C4B-NB	-2.97	107.88	110.53
15	a	803	CLA	C3B-C4B-NB	-2.97	107.88	110.53
14	A	802	F6C	C4A-C3A-C2A	-2.97	102.56	106.97
15	N	833	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
15	A	804	CLA	C3B-C4B-NB	-2.97	107.88	110.53
15	O	826	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
15	b	819	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
15	f	201	CLA	C3B-C4B-NB	-2.97	107.88	110.53
15	B	802	CLA	C3B-C4B-NB	-2.97	107.88	110.53
15	O	819	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
15	B	835	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
15	N	805	CLA	C3B-C4B-NB	-2.97	107.88	110.53
15	b	803	CLA	C3B-C4B-NB	-2.97	107.88	110.53
14	N	826	F6C	CHA-C4D-ND	2.96	135.88	133.05
15	N	805	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
14	W	1503	F6C	C1A-C2A-C3A	-2.96	103.85	106.97
15	b	811	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
15	b	836	CLA	C3B-C4B-NB	-2.96	107.89	110.53
14	L	201	F6C	C4A-C3A-C2A	-2.96	102.58	106.97
15	O	837	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
15	A	805	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
15	B	809	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
15	O	803	CLA	C3B-C4B-NB	-2.96	107.89	110.53
13	a	801	CL0	CHA-C1A-C2A	-2.95	126.37	133.31
15	A	806	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
15	A	823	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
15	b	818	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
15	O	836	CLA	C3B-C4B-NB	-2.95	107.90	110.53
15	O	806	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	O	818	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	A	832	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	B	817	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	a	833	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	O	830	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	b	810	F6C	O2D-CGD-O1D	-2.95	118.11	123.85
15	b	806	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	N	823	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	O	819	CLA	C3B-C4B-NB	-2.95	107.90	110.53
15	a	807	CLA	C3B-C4B-NB	-2.95	107.90	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	826	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	O	810	F6C	CBD-CHA-C4D	-2.94	105.22	108.54
15	b	841	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	A	813	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	b	830	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	B	839	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
15	N	807	CLA	C3B-C4B-NB	-2.94	107.91	110.53
15	B	828	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
15	A	814	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
15	N	803	CLA	C3B-C4B-NB	-2.94	107.91	110.53
15	N	813	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
14	O	810	F6C	O2D-CGD-O1D	-2.93	118.14	123.85
14	b	840	F6C	O2D-CGD-O1D	-2.93	118.14	123.85
14	O	840	F6C	O2D-CGD-O1D	-2.93	118.14	123.85
15	b	805	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
15	j	203	CLA	C3B-C4B-NB	-2.93	107.91	110.53
15	a	842	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
15	N	838	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	a	806	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	a	823	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	a	838	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	A	812	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	B	805	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	O	811	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	W	1501	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	B	817	CLA	C3B-C4B-NB	-2.93	107.92	110.53
15	a	839	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	A	842	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	b	812	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
15	O	841	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
15	b	816	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	N	801	CL0	CHA-C1A-C2A	-2.92	126.44	133.31
15	a	807	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
15	a	814	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	A	824	F6C	O2D-CGD-O1D	-2.92	118.16	123.85
14	a	824	F6C	O2D-CGD-O1D	-2.92	118.16	123.85
15	a	825	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
15	N	814	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	A	822	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	B	819	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	O	809	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	a	813	CLA	O2D-CGD-O1D	-2.92	118.17	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	834	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	B	824	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	B	829	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	a	821	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	O	828	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	B	804	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
15	O	821	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
15	b	831	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
15	N	842	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
14	N	824	F6C	O2D-CGD-O1D	-2.91	118.19	123.85
15	O	804	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	a	812	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	A	801	CL0	CHA-C1A-C2A	-2.91	126.48	133.31
15	N	821	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
15	O	834	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	a	856	F6C	O2D-CGD-O1D	-2.90	118.20	123.85
15	b	828	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	b	810	F6C	C4A-C3A-C2A	-2.90	102.67	106.97
15	b	820	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
15	A	820	CLA	O2D-CGD-CBD	2.90	116.30	111.23
15	O	830	CLA	C3B-C4B-NB	-2.90	107.94	110.53
15	O	805	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
15	N	807	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
15	b	804	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
15	O	820	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
15	O	827	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
15	b	821	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
15	a	832	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	A	807	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	B	825	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	N	812	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	B	821	CLA	C3B-C4B-NB	-2.89	107.95	110.53
15	B	834	CLA	C3B-C4B-NB	-2.89	107.95	110.53
15	B	818	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	L	202	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	O	812	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	A	825	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	A	821	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
15	A	838	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
15	b	823	CLA	C3B-C4B-NB	-2.88	107.96	110.53
14	N	802	F6C	O2D-CGD-O1D	-2.88	118.24	123.85
15	N	832	CLA	O2D-CGD-O1D	-2.88	118.24	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	841	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	A	834	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	a	834	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	b	832	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
15	A	836	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	N	822	CLA	C3B-C4B-NB	-2.88	107.96	110.53
14	A	802	F6C	O2D-CGD-O1D	-2.88	118.25	123.85
15	a	822	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	B	810	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	B	803	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
15	b	841	CLA	C3B-C4B-NB	-2.88	107.96	110.53
15	a	819	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
18	A	858	BCR	C16-C15-C14	2.88	129.40	123.52
15	b	827	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
15	N	818	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	N	841	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	B	832	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
15	O	841	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	W	1501	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	b	830	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	N	827	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	a	841	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	A	819	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
15	B	824	CLA	C3B-C4B-NB	-2.87	107.97	110.53
15	O	832	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
14	L	201	F6C	O2D-CGD-O1D	-2.86	118.27	123.85
15	X	103	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
14	b	810	F6C	CBD-CHA-C4D	-2.86	105.31	108.54
15	A	828	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	a	827	CLA	C3B-C4B-NB	-2.86	107.97	110.53
15	N	828	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	A	830	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	l	103	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	N	825	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
14	A	857	F6C	O2D-CGD-O1D	-2.86	118.29	123.85
15	N	819	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
15	N	820	CLA	O2D-CGD-CBD	2.86	116.22	111.23
15	N	829	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
15	a	835	CLA	C3B-C4B-NB	-2.86	107.98	110.53
15	a	821	CLA	C3B-C4B-NB	-2.85	107.98	110.53
15	Z	103	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
15	a	816	CLA	O2D-CGD-O1D	-2.85	118.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	817	CLA	C3B-C4B-NB	-2.85	107.98	110.53
15	N	830	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
15	B	839	CLA	C3B-C4B-NB	-2.85	107.99	110.53
15	B	807	CLA	O2A-CGA-O1A	-2.85	116.50	123.63
14	B	838	F6C	CHA-C4D-ND	2.85	135.78	133.05
13	N	801	CL0	C1C-CHC-C4B	2.85	126.26	116.07
15	A	821	CLA	C3B-C4B-NB	-2.85	107.99	110.53
15	B	811	CLA	O2D-CGD-CBD	2.85	116.21	111.23
18	N	857	BCR	C16-C15-C14	2.85	129.34	123.52
15	a	836	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
15	X	103	CLA	C3B-C4B-NB	-2.84	107.99	110.53
15	N	836	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
15	A	803	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
15	N	834	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
15	A	822	CLA	C3B-C4B-NB	-2.84	107.99	110.53
14	a	802	F6C	O2D-CGD-O1D	-2.84	118.32	123.85
13	a	801	CL0	C1C-CHC-C4B	2.84	126.23	116.07
15	N	821	CLA	C3B-C4B-NB	-2.84	108.00	110.53
15	b	813	CLA	O2D-CGD-CBD	2.84	116.19	111.23
15	A	816	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
15	a	830	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
13	A	801	CL0	C1C-CHC-C4B	2.84	126.23	116.07
14	a	802	F6C	CHA-C4D-ND	2.84	135.76	133.05
15	V	102	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
15	b	809	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
18	A	858	BCR	C7-C8-C9	-2.84	122.04	126.23
15	a	809	CLA	C3B-C4B-NB	-2.84	108.00	110.53
15	K	102	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
15	N	834	CLA	C3B-C4B-NB	-2.83	108.00	110.53
15	N	816	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
15	i	102	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
15	O	813	CLA	O2D-CGD-CBD	2.83	116.18	111.23
20	A	853	LMT	O5B-C1B-C2B	2.83	116.19	110.37
15	A	818	CLA	C3B-C4B-NB	-2.83	108.00	110.53
15	N	817	CLA	C3B-C4B-NB	-2.83	108.00	110.53
15	a	829	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
15	A	835	CLA	C3B-C4B-NB	-2.83	108.01	110.53
14	A	826	F6C	CHA-C4D-ND	2.83	135.75	133.05
15	a	817	CLA	C3B-C4B-NB	-2.83	108.01	110.53
15	a	828	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
15	A	807	CLA	C3B-C4B-NB	-2.82	108.01	110.53
15	B	812	CLA	C3B-C4B-NB	-2.82	108.01	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	826	CLA	C3B-C4B-NB	-2.82	108.01	110.53
15	l	103	CLA	C3B-C4B-NB	-2.82	108.01	110.53
15	A	829	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	N	809	CLA	C3B-C4B-NB	-2.82	108.01	110.53
15	B	823	CLA	C3B-C4B-NB	-2.82	108.01	110.53
14	N	856	F6C	O2D-CGD-O1D	-2.82	118.36	123.85
15	A	834	CLA	C3B-C4B-NB	-2.82	108.02	110.53
15	B	808	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
15	a	820	CLA	O2D-CGD-CBD	2.81	116.15	111.23
15	A	809	CLA	C3B-C4B-NB	-2.81	108.02	110.53
15	N	841	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
15	Z	103	CLA	C3B-C4B-NB	-2.81	108.02	110.53
14	O	810	F6C	C4A-C3A-C2A	-2.81	102.80	106.97
18	a	857	BCR	C7-C8-C9	-2.81	122.08	126.23
18	N	857	BCR	C7-C8-C9	-2.80	122.09	126.23
15	O	814	CLA	C3B-C4B-NB	-2.80	108.03	110.53
15	A	827	CLA	C3B-C4B-NB	-2.80	108.03	110.53
15	A	833	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
15	j	202	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	O	840	F6C	CHA-C4D-ND	2.80	135.73	133.05
15	b	808	CLA	O2A-CGA-O1A	-2.80	116.64	123.63
14	N	802	F6C	CHA-C4D-ND	2.79	135.72	133.05
15	b	834	CLA	C3B-C4B-NB	-2.79	108.04	110.53
15	j	202	CLA	C3B-C4B-NB	-2.79	108.04	110.53
15	O	808	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
15	A	810	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
15	N	832	CLA	C3B-C4B-NB	-2.79	108.04	110.53
14	A	802	F6C	CHA-C4D-ND	2.79	135.72	133.05
15	N	803	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
18	M	101	BCR	C7-C8-C9	-2.78	122.12	126.23
15	a	810	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
15	b	814	CLA	C3B-C4B-NB	-2.78	108.05	110.53
15	L	202	CLA	C3B-C4B-NB	-2.78	108.05	110.53
15	O	811	CLA	C3B-C4B-NB	-2.78	108.05	110.53
14	a	826	F6C	CHA-C4D-ND	2.78	135.71	133.05
15	a	841	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
15	b	809	CLA	C3B-C4B-NB	-2.77	108.05	110.53
14	b	810	F6C	CHB-C4A-C3A	-2.77	119.72	125.49
18	a	857	BCR	C16-C15-C14	2.77	129.19	123.52
15	N	810	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
15	A	832	CLA	C3B-C4B-NB	-2.77	108.06	110.53
14	b	810	F6C	C1A-C2A-C3A	-2.77	104.06	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	822	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
14	O	833	F6C	CHA-C4D-ND	2.77	135.69	133.05
15	O	826	CLA	C3B-C4B-NB	-2.76	108.06	110.53
15	O	835	CLA	C3B-C4B-NB	-2.76	108.06	110.53
14	N	824	F6C	CHA-C4D-ND	2.76	135.69	133.05
15	a	834	CLA	C3B-C4B-NB	-2.76	108.06	110.53
15	B	832	CLA	C3B-C4B-NB	-2.76	108.07	110.53
15	A	815	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	O	810	F6C	C1A-C2A-C3A	-2.76	104.06	106.97
15	O	823	CLA	C3B-C4B-NB	-2.76	108.07	110.53
14	b	833	F6C	CHA-C4D-ND	2.75	135.69	133.05
15	N	811	CLA	C3B-C4B-NB	-2.75	108.07	110.53
15	N	813	CLA	C3B-C4B-NB	-2.75	108.07	110.53
15	B	833	CLA	C3B-C4B-NB	-2.75	108.07	110.53
20	a	853	LMT	O5B-C1B-C2B	2.75	116.03	110.37
15	a	803	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
15	B	829	CLA	C3B-C4B-NB	-2.75	108.07	110.53
15	A	813	CLA	C3B-C4B-NB	-2.75	108.08	110.53
14	L	204	F6C	C1-C2-C3	-2.75	121.70	126.20
15	a	811	CLA	C3B-C4B-NB	-2.75	108.08	110.53
14	b	840	F6C	CHA-C4D-ND	2.75	135.68	133.05
15	b	822	CLA	O2D-CGD-O1D	-2.74	118.50	123.85
15	B	809	CLA	C3B-C4B-NB	-2.74	108.08	110.53
15	B	807	CLA	C1-C2-C3	-2.74	121.70	126.20
15	N	833	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
13	a	801	CL0	CMA-C3A-C4A	-2.74	108.71	114.61
14	O	810	F6C	CHB-C4A-C3A	-2.74	119.79	125.49
20	N	853	LMT	O5B-C1B-C2B	2.74	115.99	110.37
15	A	811	CLA	C3B-C4B-NB	-2.74	108.09	110.53
15	O	834	CLA	C3B-C4B-NB	-2.73	108.09	110.53
15	A	841	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
15	B	820	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
15	N	815	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
15	a	813	CLA	C3B-C4B-NB	-2.72	108.10	110.53
14	b	840	F6C	OMB-CMB-C2B	-2.72	119.49	125.62
15	B	819	CLA	C3B-C4B-NB	-2.72	108.10	110.53
14	L	201	F6C	CHB-C4A-C3A	-2.72	119.84	125.49
15	A	823	CLA	C3B-C4B-NB	-2.71	108.11	110.53
15	b	806	CLA	C3B-C4B-NB	-2.71	108.11	110.53
15	b	813	CLA	C3B-C4B-NB	-2.71	108.11	110.53
14	B	831	F6C	CHA-C4D-ND	2.71	135.64	133.05
15	B	805	CLA	C3B-C4B-NB	-2.71	108.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	813	CLA	C3B-C4B-NB	-2.71	108.11	110.53
15	A	814	CLA	C3B-C4B-NB	-2.71	108.11	110.53
15	a	823	CLA	C3B-C4B-NB	-2.71	108.11	110.53
15	b	825	CLA	C3B-C4B-NB	-2.71	108.11	110.53
15	O	805	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	O	825	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	L	201	F6C	C1A-C2A-C3A	-2.70	104.12	106.97
15	A	842	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	b	831	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	b	810	F6C	CHA-C4D-ND	2.70	135.63	133.05
14	B	838	F6C	OMB-CMB-C2B	-2.70	119.52	125.62
15	O	808	CLA	C1-C2-C3	-2.70	121.77	126.20
15	a	815	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
15	B	808	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	N	814	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	a	814	CLA	C3B-C4B-NB	-2.70	108.12	110.53
18	O	848	BCR	C20-C21-C22	-2.70	123.50	127.28
15	O	831	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	V	102	CLA	C3B-C4B-NB	-2.69	108.12	110.53
15	a	832	CLA	C3B-C4B-NB	-2.69	108.12	110.53
15	O	821	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	A	801	CL0	C4D-CHA-CBD	-2.69	106.26	108.97
15	O	809	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	b	837	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	A	833	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	b	821	CLA	C3B-C4B-NB	-2.68	108.13	110.53
15	B	811	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	b	835	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
15	a	833	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	O	801	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	O	829	CLA	C3B-C4B-NB	-2.68	108.14	110.53
15	a	810	CLA	C3B-C4B-NB	-2.67	108.14	110.53
15	b	801	CLA	C3B-C4B-NB	-2.67	108.14	110.53
15	b	835	CLA	C3B-C4B-NB	-2.67	108.14	110.53
15	a	833	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
15	K	102	CLA	C3B-C4B-NB	-2.67	108.14	110.53
15	b	816	CLA	C3B-C4B-NB	-2.67	108.14	110.53
14	j	204	F6C	C1-C2-C3	-2.67	121.82	126.20
15	b	808	CLA	C1-C2-C3	-2.67	121.82	126.20
15	a	808	CLA	C3B-C4B-NB	-2.67	108.15	110.53
15	B	833	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
14	A	826	F6C	CMC-C2C-C3C	2.67	131.28	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	815	CLA	CHB-C4A-NA	2.67	128.25	124.40
15	N	823	CLA	C3B-C4B-NB	-2.67	108.15	110.53
15	b	811	CLA	C3B-C4B-NB	-2.67	108.15	110.53
14	A	826	F6C	CBD-CHA-C4D	-2.67	105.54	108.54
14	O	840	F6C	OMB-CMB-C2B	-2.66	119.62	125.62
14	a	824	F6C	CHA-C4D-ND	2.66	135.59	133.05
15	A	828	CLA	C3B-C4B-NB	-2.66	108.16	110.53
15	a	828	CLA	C3B-C4B-NB	-2.65	108.16	110.53
15	O	829	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
14	L	201	F6C	OMB-CMB-C2B	-2.65	119.63	125.62
15	N	828	CLA	C3B-C4B-NB	-2.65	108.16	110.53
15	i	102	CLA	C3B-C4B-NB	-2.65	108.16	110.53
15	O	837	CLA	C3B-C4B-NB	-2.65	108.17	110.53
15	O	831	CLA	C1-C2-C3	-2.65	121.86	126.20
15	A	837	CLA	C3B-C4B-NB	-2.64	108.17	110.53
15	N	810	CLA	C3B-C4B-NB	-2.64	108.17	110.53
14	b	810	F6C	OMB-CMB-C2B	-2.64	119.66	125.62
14	L	201	F6C	CHA-C4D-ND	2.64	135.58	133.05
15	O	808	CLA	C3B-C4B-NB	-2.64	108.17	110.53
15	A	810	CLA	C3B-C4B-NB	-2.64	108.17	110.53
15	O	835	CLA	CMB-C2B-C1B	-2.64	121.41	125.42
15	N	820	CLA	CHB-C4A-NA	2.64	128.20	124.40
15	b	815	CLA	CHB-C4A-NA	2.63	128.20	124.40
13	a	801	CL0	C4D-CHA-CBD	-2.63	106.31	108.97
14	A	826	F6C	CHB-C4A-C3A	-2.63	120.01	125.49
15	B	835	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	A	820	CLA	CHB-C4A-NA	2.63	128.20	124.40
15	A	835	CLA	O2D-CGD-CBD	2.63	115.83	111.23
14	a	824	F6C	CHB-C4A-C3A	-2.63	120.02	125.49
15	b	828	CLA	C3B-C4B-NB	-2.63	108.19	110.53
14	N	802	F6C	OMB-CMB-C2B	-2.62	119.70	125.62
15	B	801	CLA	C3B-C4B-NB	-2.62	108.19	110.53
18	Y	102	BCR	C7-C8-C9	-2.62	122.35	126.23
18	f	202	BCR	C20-C21-C22	-2.62	123.60	127.28
15	F	201	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
15	b	805	CLA	C3B-C4B-NB	-2.62	108.19	110.53
15	a	820	CLA	CHB-C4A-NA	2.62	128.18	124.40
15	B	804	CLA	C3B-C4B-NB	-2.62	108.19	110.53
14	W	1503	F6C	OMB-CMB-C2B	-2.62	119.71	125.62
15	O	803	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
13	N	801	CL0	CMB-C2B-C3B	2.62	129.92	124.68
15	a	806	CLA	C3B-C4B-NB	-2.62	108.19	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	824	F6C	CHA-C4D-ND	2.62	135.55	133.05
15	N	830	CLA	C3B-C4B-NB	-2.62	108.19	110.53
15	O	806	CLA	C3B-C4B-NB	-2.61	108.20	110.53
13	a	801	CL0	CMB-C2B-C3B	2.61	129.91	124.68
15	a	836	CLA	C3B-C4B-NB	-2.61	108.20	110.53
18	F	202	BCR	C20-C21-C22	-2.61	123.61	127.28
13	a	801	CL0	C3D-C4D-CHA	2.61	112.50	108.54
15	B	827	CLA	C3B-C4B-NB	-2.61	108.20	110.53
15	N	837	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	j	204	F6C	CHA-C4D-ND	2.61	135.54	133.05
15	B	829	CLA	C1-C2-C3	-2.61	121.93	126.20
14	j	204	F6C	OMB-CMB-C2B	-2.61	119.74	125.62
15	K	103	CLA	C1-C2-C3	-2.60	122.55	126.76
14	W	1503	F6C	CHA-C4D-ND	2.60	135.54	133.05
14	a	856	F6C	CHA-C4D-ND	2.60	135.54	133.05
15	A	808	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	A	815	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	A	836	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	N	808	CLA	C3B-C4B-NB	-2.60	108.21	110.53
15	A	832	CLA	C1-C2-C3	-2.60	122.56	126.76
14	L	204	F6C	OMB-CMB-C2B	-2.60	119.75	125.62
14	a	826	F6C	CHB-C4A-C3A	-2.60	120.08	125.49
15	B	814	CLA	C3B-C4B-NB	-2.60	108.21	110.53
14	a	826	F6C	CBD-CHA-C4D	-2.60	105.61	108.54
15	B	827	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
14	A	826	F6C	OMB-CMB-C2B	-2.60	119.76	125.62
15	i	103	CLA	C1-C2-C3	-2.60	122.56	126.76
14	L	204	F6C	CHA-C4D-ND	2.60	135.53	133.05
14	A	824	F6C	CHB-C4A-C3A	-2.60	120.09	125.49
15	O	824	CLA	C1-C2-C3	-2.60	121.94	126.20
15	N	815	CLA	C3B-C4B-NB	-2.59	108.21	110.53
15	a	815	CLA	C3B-C4B-NB	-2.59	108.21	110.53
15	A	806	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	b	829	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
15	O	816	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	b	829	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	S	201	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
15	N	841	CLA	CHB-C4A-NA	2.59	128.14	124.40
13	N	801	CL0	C4D-CHA-CBD	-2.59	106.36	108.97
14	a	826	F6C	C4A-C3A-C2A	-2.59	103.13	106.97
15	N	842	CLA	C3B-C4B-NB	-2.59	108.22	110.53
15	a	837	CLA	C3B-C4B-NB	-2.59	108.22	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	831	F6C	CHB-C4A-C3A	-2.59	120.11	125.49
14	B	838	F6C	CMB-C2B-C1B	-2.59	121.79	128.37
15	V	103	CLA	C1-C2-C3	-2.58	122.58	126.76
15	N	836	CLA	C3B-C4B-NB	-2.58	108.22	110.53
15	B	813	CLA	C3B-C4B-NB	-2.58	108.23	110.53
15	O	822	CLA	CHB-C4A-NA	2.58	128.12	124.40
14	W	1503	F6C	CHB-C4A-C3A	-2.58	120.12	125.49
15	N	833	CLA	C3B-C4B-NB	-2.58	108.23	110.53
14	A	826	F6C	C4A-C3A-C2A	-2.58	103.14	106.97
13	A	801	CL0	C4C-CHD-C1D	2.58	125.29	116.07
15	B	836	CLA	C1-C2-C3	-2.58	121.97	126.20
14	b	833	F6C	CHB-C4A-C3A	-2.58	120.13	125.49
15	a	842	CLA	C3B-C4B-NB	-2.58	108.23	110.53
13	N	801	CL0	C4C-CHD-C1D	2.57	125.28	116.07
13	a	801	CL0	C4C-CHD-C1D	2.57	125.28	116.07
15	b	808	CLA	C3B-C4B-NB	-2.57	108.23	110.53
14	A	857	F6C	CHA-C4D-ND	2.57	135.51	133.05
14	A	802	F6C	OMB-CMB-C2B	-2.57	119.81	125.62
13	N	801	CL0	CMA-C3A-C4A	-2.57	109.07	114.61
13	A	801	CL0	C3D-C4D-CHA	2.57	112.45	108.54
14	N	824	F6C	CHB-C4A-C3A	-2.57	120.14	125.49
14	O	833	F6C	CHB-C4A-C3A	-2.57	120.14	125.49
15	B	802	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
15	B	807	CLA	C3B-C4B-NB	-2.57	108.24	110.53
15	O	838	CLA	C3B-C4B-NB	-2.57	108.24	110.53
16	b	842	PQN	C11-C3-C4	-2.56	115.88	118.58
15	f	201	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
15	N	818	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	A	801	CL0	CMB-C2B-C3B	2.56	129.79	124.68
14	a	802	F6C	OMB-CMB-C2B	-2.56	119.85	125.62
14	N	856	F6C	CHA-C4D-ND	2.56	135.50	133.05
15	b	834	CLA	CHB-C4A-NA	2.55	128.08	124.40
15	a	818	CLA	CHB-C4A-NA	2.55	128.08	124.40
15	O	838	CLA	C1-C2-C3	-2.55	122.02	126.20
18	N	857	BCR	C8-C7-C6	2.54	133.79	127.00
15	a	832	CLA	C1-C2-C3	-2.54	122.65	126.76
15	A	818	CLA	CHB-C4A-NA	2.54	128.07	124.40
15	O	832	CLA	C3B-C4B-NB	-2.54	108.26	110.53
14	O	810	F6C	CHA-C4D-ND	2.54	135.48	133.05
15	B	826	CLA	C3B-C4B-NB	-2.54	108.26	110.53
13	N	801	CL0	C3D-C4D-CHA	2.54	112.40	108.54
15	a	814	CLA	CHB-C4A-NA	2.54	128.06	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	810	F6C	OMB-CMB-C2B	-2.54	119.90	125.62
15	b	806	CLA	CHB-C4A-NA	2.54	128.06	124.40
14	j	204	F6C	CHB-C4A-C3A	-2.53	120.22	125.49
15	O	834	CLA	CHB-C4A-NA	2.53	128.06	124.40
15	O	828	CLA	C3B-C4B-NB	-2.53	108.27	110.53
15	b	815	CLA	C3B-C4B-NB	-2.53	108.27	110.53
15	b	832	CLA	C3B-C4B-NB	-2.53	108.27	110.53
15	b	824	CLA	CHB-C4A-NA	2.53	128.05	124.40
15	O	824	CLA	CHB-C4A-NA	2.53	128.05	124.40
14	N	826	F6C	CMC-C2C-C3C	2.53	130.98	125.62
15	a	807	CLA	CHB-C4A-NA	2.52	128.04	124.40
15	b	805	CLA	CHB-C4A-NA	2.52	128.04	124.40
15	A	841	CLA	CHB-C4A-NA	2.52	128.04	124.40
14	N	826	F6C	CBD-CHA-C4D	-2.52	105.70	108.54
15	A	807	CLA	CHB-C4A-NA	2.52	128.04	124.40
15	X	103	CLA	CHB-C4A-NA	2.52	128.04	124.40
15	b	838	CLA	C3B-C4B-NB	-2.52	108.28	110.53
15	N	805	CLA	CHB-C4A-NA	2.52	128.03	124.40
15	a	816	CLA	CHB-C4A-NA	2.52	128.03	124.40
15	A	830	CLA	C3B-C4B-NB	-2.51	108.28	110.53
18	a	857	BCR	C8-C7-C6	2.51	133.72	127.00
15	A	813	CLA	C1-C2-C3	-2.51	122.08	126.20
15	Z	103	CLA	CHB-C4A-NA	2.51	128.03	124.40
15	O	805	CLA	CHB-C4A-NA	2.51	128.03	124.40
15	O	815	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	A	816	CLA	CHB-C4A-NA	2.51	128.02	124.40
15	N	807	CLA	CHB-C4A-NA	2.51	128.02	124.40
15	b	822	CLA	CHB-C4A-NA	2.51	128.02	124.40
15	B	836	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	N	832	CLA	C1-C2-C3	-2.51	122.70	126.76
15	a	830	CLA	C3B-C4B-NB	-2.51	108.29	110.53
15	B	832	CLA	CHB-C4A-NA	2.51	128.02	124.40
15	B	822	CLA	CHB-C4A-NA	2.51	128.02	124.40
15	a	841	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	B	838	F6C	CHB-C4A-C3A	-2.51	120.28	125.49
15	A	806	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	O	840	F6C	CHB-C4A-C3A	-2.51	120.28	125.49
15	A	814	CLA	CHB-C4A-NA	2.50	128.01	124.40
15	B	823	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	A	802	F6C	CMB-C2B-C1B	-2.50	122.00	128.37
15	A	828	CLA	CHB-C4A-NA	2.50	128.01	124.40
15	B	813	CLA	CHB-C4A-NA	2.50	128.01	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	839	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	N	802	F6C	CMB-C2B-C1B	-2.50	122.01	128.37
15	O	806	CLA	CHB-C4A-NA	2.50	128.01	124.40
15	O	826	CLA	CHB-C4A-NA	2.50	128.01	124.40
15	B	822	CLA	C1-C2-C3	-2.50	122.10	126.20
15	B	839	CLA	CHB-C4A-NA	2.50	128.00	124.40
15	b	816	CLA	CHB-C4A-NA	2.50	128.00	124.40
15	B	814	CLA	CHB-C4A-NA	2.50	128.00	124.40
14	j	204	F6C	C4A-C3A-C2A	-2.50	103.27	106.97
15	B	820	CLA	CHB-C4A-NA	2.50	128.00	124.40
15	N	814	CLA	CHB-C4A-NA	2.50	128.00	124.40
14	B	831	F6C	OMB-CMB-C2B	-2.50	119.99	125.62
15	l	103	CLA	CHB-C4A-NA	2.49	128.00	124.40
15	O	825	CLA	CHB-C4A-NA	2.49	128.00	124.40
15	L	202	CLA	CHB-C4A-NA	2.49	128.00	124.40
15	b	812	CLA	CHB-C4A-NA	2.49	127.99	124.40
15	B	830	CLA	C3B-C4B-NB	-2.49	108.31	110.53
14	W	1503	F6C	C4A-C3A-C2A	-2.49	103.28	106.97
15	a	806	CLA	CHB-C4A-NA	2.49	127.99	124.40
15	A	820	CLA	C1-C2-C3	-2.49	122.12	126.20
14	b	840	F6C	CHB-C4A-C3A	-2.49	120.31	125.49
15	A	805	CLA	CHB-C4A-NA	2.49	127.99	124.40
15	O	821	CLA	CHB-C4A-NA	2.49	127.99	124.40
14	N	856	F6C	OMB-CMB-C2B	-2.49	120.01	125.62
15	L	203	CLA	O2D-CGD-CBD	2.49	115.58	111.23
15	b	821	CLA	CHB-C4A-NA	2.49	127.99	124.40
14	a	802	F6C	CMB-C2B-C1B	-2.48	122.05	128.37
15	A	821	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	N	809	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	j	203	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	B	804	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	A	808	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	a	805	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	B	805	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	N	808	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	b	824	CLA	C1-C2-C3	-2.48	122.13	126.20
15	N	816	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	b	841	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	A	809	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	O	812	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	b	826	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	N	820	CLA	C1-C2-C3	-2.48	122.14	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	819	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	O	841	CLA	CHB-C4A-NA	2.48	127.98	124.40
15	L	203	CLA	CHB-C4A-NA	2.48	127.97	124.40
15	V	102	CLA	CHB-C4A-NA	2.48	127.97	124.40
14	a	856	F6C	OMB-CMB-C2B	-2.48	120.03	125.62
15	a	809	CLA	CHB-C4A-NA	2.48	127.97	124.40
15	O	816	CLA	CHB-C4A-NA	2.47	127.97	124.40
15	B	825	CLA	C3B-C4B-NB	-2.47	108.32	110.53
15	W	1502	CLA	CHB-C4A-NA	2.47	127.97	124.40
15	B	810	CLA	CHB-C4A-NA	2.47	127.97	124.40
15	A	836	CLA	CHB-C4A-NA	2.47	127.97	124.40
15	N	815	CLA	CHB-C4A-NA	2.47	127.97	124.40
15	N	839	CLA	CHB-C4A-NA	2.47	127.96	124.40
15	b	828	CLA	C1-C2-C3	-2.47	122.15	126.20
15	a	828	CLA	CHB-C4A-NA	2.47	127.96	124.40
14	A	824	F6C	OMB-CMB-C2B	-2.47	120.06	125.62
18	N	846	BCR	C11-C10-C9	-2.47	123.82	127.28
15	B	822	CLA	C3B-C4B-NB	-2.47	108.33	110.53
15	b	838	CLA	C1-C2-C3	-2.47	122.16	126.20
15	a	821	CLA	CHB-C4A-NA	2.46	127.96	124.40
15	a	815	CLA	CHB-C4A-NA	2.46	127.96	124.40
15	a	813	CLA	C1-C2-C3	-2.46	122.16	126.20
15	N	821	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	i	102	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	K	102	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	811	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	B	826	CLA	C1-C2-C3	-2.46	122.17	126.20
14	N	826	F6C	C4A-C3A-C2A	-2.46	103.32	106.97
15	a	808	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	O	830	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	N	838	CLA	C3B-C4B-NB	-2.46	108.34	110.53
15	b	804	CLA	CHB-C4A-NA	2.46	127.94	124.40
15	a	838	CLA	C3B-C4B-NB	-2.45	108.34	110.53
15	B	824	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	b	825	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	O	817	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	a	813	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	b	820	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	A	815	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	O	820	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	a	823	CLA	CHB-C4A-NA	2.45	127.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	813	CLA	C1-C2-C3	-2.45	122.18	126.20
15	N	817	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	O	814	CLA	CHB-C4A-NA	2.45	127.94	124.40
15	b	803	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
15	N	806	CLA	C3B-C4B-NB	-2.45	108.34	110.53
15	O	828	CLA	C1-C2-C3	-2.45	122.19	126.20
15	A	810	CLA	CHB-C4A-NA	2.45	127.93	124.40
15	b	830	CLA	CHB-C4A-NA	2.45	127.93	124.40
15	A	813	CLA	CHB-C4A-NA	2.45	127.93	124.40
14	N	826	F6C	O2D-CGD-CBD	2.45	115.50	111.23
14	W	1503	F6C	C1-C2-C3	-2.45	122.19	126.20
15	B	815	CLA	CHB-C4A-NA	2.44	127.93	124.40
15	a	810	CLA	CHB-C4A-NA	2.44	127.93	124.40
15	N	810	CLA	CHB-C4A-NA	2.44	127.93	124.40
14	L	204	F6C	C4A-C3A-C2A	-2.44	103.35	106.97
15	A	811	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	A	817	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	a	856	F6C	CHB-C4A-C3A	-2.44	120.41	125.49
14	N	856	F6C	CHB-C4A-C3A	-2.44	120.41	125.49
15	B	818	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	b	814	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	N	836	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	N	823	CLA	CHB-C4A-NA	2.44	127.92	124.40
15	B	812	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	A	857	F6C	CHB-C4A-C3A	-2.44	120.42	125.49
15	A	804	CLA	CHB-C4A-NA	2.43	127.91	124.40
15	N	811	CLA	CHB-C4A-NA	2.43	127.91	124.40
14	N	856	F6C	C1-C2-C3	-2.43	122.21	126.20
15	A	839	CLA	CHB-C4A-NA	2.43	127.91	124.40
18	A	858	BCR	C8-C7-C6	2.43	133.50	127.00
14	L	201	F6C	CHB-C4A-NA	2.43	128.23	124.80
15	A	838	CLA	C3B-C4B-NB	-2.43	108.36	110.53
15	O	831	CLA	CHB-C4A-NA	2.43	127.91	124.40
18	a	846	BCR	C11-C10-C9	-2.43	123.87	127.28
15	b	824	CLA	C3B-C4B-NB	-2.43	108.36	110.53
15	a	836	CLA	CHB-C4A-NA	2.43	127.91	124.40
14	A	857	F6C	C1-C2-C3	-2.43	122.22	126.20
15	a	830	CLA	C1-C2-C3	-2.43	122.22	126.20
15	a	831	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	O	810	F6C	CHB-C4A-NA	2.43	128.22	124.80
15	N	804	CLA	CHB-C4A-NA	2.43	127.90	124.40
15	N	825	CLA	CHB-C4A-NA	2.43	127.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	826	F6C	CMC-C2C-C3C	2.43	130.77	125.62
15	N	828	CLA	CHB-C4A-NA	2.43	127.90	124.40
15	N	831	CLA	CHB-C4A-NA	2.43	127.90	124.40
15	B	829	CLA	CHB-C4A-NA	2.43	127.90	124.40
16	O	842	PQN	C11-C3-C4	-2.42	116.03	118.58
15	j	202	CLA	CHB-C4A-NA	2.42	127.90	124.40
14	L	204	F6C	CHB-C4A-C3A	-2.42	120.45	125.49
15	a	817	CLA	CHB-C4A-NA	2.42	127.89	124.40
14	b	833	F6C	OMB-CMB-C2B	-2.42	120.16	125.62
15	b	818	CLA	C3B-C4B-NB	-2.42	108.37	110.53
15	B	803	CLA	CHB-C4A-NA	2.42	127.89	124.40
15	N	838	CLA	CHB-C4A-NA	2.42	127.89	124.40
15	L	203	CLA	C1-C2-C3	-2.42	122.23	126.20
15	A	820	CLA	C3B-C4B-NB	-2.42	108.37	110.53
15	b	831	CLA	CHB-C4A-NA	2.42	127.89	124.40
14	N	826	F6C	CHB-C4A-C3A	-2.42	120.46	125.49
14	a	826	F6C	OMB-CMB-C2B	-2.42	120.17	125.62
15	N	806	CLA	CHB-C4A-NA	2.42	127.89	124.40
15	a	829	CLA	C3B-C4B-NB	-2.42	108.37	110.53
15	N	832	CLA	CHB-C4A-NA	2.42	127.89	124.40
15	N	813	CLA	CHB-C4A-NA	2.41	127.89	124.40
15	O	836	CLA	CHB-C4A-NA	2.41	127.89	124.40
15	A	803	CLA	CMB-C2B-C1B	-2.41	121.74	125.42
15	A	832	CLA	CHB-C4A-NA	2.41	127.88	124.40
15	B	828	CLA	CHB-C4A-NA	2.41	127.88	124.40
15	b	829	CLA	CHB-C4A-NA	2.41	127.88	124.40
15	N	840	CLA	C3B-C4B-NB	-2.41	108.38	110.53
15	a	820	CLA	C1-C2-C3	-2.41	122.25	126.20
16	B	840	PQN	C11-C3-C4	-2.41	116.04	118.58
15	O	824	CLA	C3B-C4B-NB	-2.41	108.38	110.53
13	a	801	CL0	CMD-C2D-C3D	2.41	129.49	124.68
15	B	811	CLA	CHB-C4A-NA	2.40	127.87	124.40
15	A	831	CLA	C3B-C4B-NB	-2.40	108.39	110.53
14	O	840	F6C	CMB-C2B-C1B	-2.40	122.25	128.37
15	B	802	CLA	CHB-C4A-NA	2.40	127.87	124.40
15	i	103	CLA	CHB-C4A-NA	2.40	127.87	124.40
15	A	819	CLA	CHB-C4A-NA	2.40	127.87	124.40
14	N	826	F6C	OMB-CMB-C2B	-2.40	120.20	125.62
15	a	803	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
15	b	813	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	W	1503	F6C	CMB-C2B-C1B	-2.40	122.26	128.37
15	N	812	CLA	CHB-C4A-NA	2.40	127.86	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	804	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	b	840	F6C	CMB-C2B-C1B	-2.40	122.26	128.37
14	b	810	F6C	CHB-C4A-NA	2.40	128.18	124.80
15	O	838	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	A	826	F6C	CHB-C4A-NA	2.40	128.18	124.80
15	O	823	CLA	CHB-C4A-NA	2.40	127.86	124.40
15	b	838	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	b	833	F6C	CBD-CHA-C4D	-2.40	105.84	108.54
15	O	813	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	N	803	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
15	A	812	CLA	CHB-C4A-NA	2.39	127.85	124.40
14	j	204	F6C	CMB-C2B-C1B	-2.39	122.28	128.37
15	a	832	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	A	803	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	A	829	CLA	C3B-C4B-NB	-2.39	108.40	110.53
15	b	815	CLA	O2D-CGD-CBD	2.39	115.41	111.23
15	a	812	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	b	807	CLA	C3B-C4B-NB	-2.39	108.40	110.53
15	a	819	CLA	CHB-C4A-NA	2.39	127.85	124.40
15	b	836	CLA	CHB-C4A-NA	2.39	127.85	124.40
13	A	801	CL0	C3C-C4C-NC	-2.39	108.81	114.65
15	N	831	CLA	C3B-C4B-NB	-2.39	108.40	110.53
15	a	825	CLA	CHB-C4A-NA	2.39	127.84	124.40
15	b	819	CLA	CHB-C4A-NA	2.39	127.84	124.40
15	W	1502	CLA	C1-C2-C3	-2.39	122.29	126.20
15	A	825	CLA	CHB-C4A-NA	2.39	127.84	124.40
15	O	837	CLA	CHB-C4A-NA	2.39	127.84	124.40
15	a	840	CLA	C1-C2-C3	-2.39	122.90	126.76
15	B	834	CLA	CHB-C4A-NA	2.38	127.84	124.40
15	b	803	CLA	CHB-C4A-NA	2.38	127.84	124.40
18	A	847	BCR	C20-C21-C22	-2.38	123.94	127.28
14	B	831	F6C	CBD-CHA-C4D	-2.38	105.86	108.54
15	a	804	CLA	CHB-C4A-NA	2.38	127.84	124.40
13	N	801	CL0	C3C-C4C-NC	-2.38	108.83	114.65
15	W	1501	CLA	CHB-C4A-NA	2.38	127.84	124.40
15	B	836	CLA	CHB-C4A-NA	2.38	127.83	124.40
15	O	811	CLA	CHB-C4A-NA	2.38	127.83	124.40
15	a	835	CLA	CHB-C4A-NA	2.38	127.83	124.40
15	O	818	CLA	C3B-C4B-NB	-2.38	108.41	110.53
13	A	801	CL0	CMA-C3A-C4A	-2.38	109.49	114.61
15	b	808	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	N	824	F6C	C4A-C3A-C2A	-2.38	103.45	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	840	CLA	C1-C2-C3	-2.38	122.92	126.76
14	O	833	F6C	CBD-CHA-C4D	-2.37	105.86	108.54
15	A	833	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	B	817	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	N	803	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	a	838	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	b	837	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	a	840	CLA	C3B-C4B-NB	-2.37	108.41	110.53
15	N	833	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	O	835	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	B	809	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	b	832	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	j	203	CLA	O2D-CGD-CBD	2.37	115.37	111.23
15	a	810	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
15	N	819	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	O	832	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	b	811	CLA	CHB-C4A-NA	2.37	127.81	124.40
15	a	819	CLA	C1-C2-C3	-2.37	122.32	126.20
15	b	817	CLA	CHB-C4A-NA	2.37	127.81	124.40
15	b	839	CLA	CHB-C4A-NA	2.37	127.81	124.40
15	b	837	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
15	a	820	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
15	N	835	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	O	839	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	O	808	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	a	833	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	S	201	CLA	C1-C2-C3	-2.36	122.33	126.20
15	B	827	CLA	CHB-C4A-NA	2.36	127.81	124.40
15	B	830	CLA	CHB-C4A-NA	2.36	127.81	124.40
14	A	802	F6C	C1-C2-C3	-2.36	122.33	126.20
15	A	838	CLA	CHB-C4A-NA	2.36	127.80	124.40
15	B	835	CLA	CHB-C4A-NA	2.36	127.80	124.40
15	W	1502	CLA	O2D-CGD-CBD	2.36	115.35	111.23
15	O	807	CLA	C3B-C4B-NB	-2.36	108.43	110.53
15	B	816	CLA	C3B-C4B-NB	-2.36	108.43	110.53
15	A	840	CLA	C1-C2-C3	-2.35	122.95	126.76
14	a	824	F6C	C4A-C3A-C2A	-2.35	103.48	106.97
15	f	201	CLA	C1-C2-C3	-2.35	122.34	126.20
15	A	827	CLA	CHB-C4A-NA	2.35	127.80	124.40
15	j	203	CLA	C1-C2-C3	-2.35	122.34	126.20
15	B	807	CLA	CHB-C4A-NA	2.35	127.79	124.40
15	B	833	CLA	CHB-C4A-NA	2.35	127.79	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	837	CLA	CHB-C4A-NA	2.35	127.79	124.40
13	a	801	CL0	C3C-C4C-NC	-2.35	108.91	114.65
15	O	829	CLA	CHB-C4A-NA	2.35	127.79	124.40
15	b	835	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
15	a	803	CLA	CHB-C4A-NA	2.35	127.79	124.40
15	N	829	CLA	C3B-C4B-NB	-2.35	108.43	110.53
15	A	835	CLA	CHB-C4A-NA	2.35	127.79	124.40
15	F	201	CLA	CHB-C4A-NA	2.35	127.79	124.40
14	A	857	F6C	OMB-CMB-C2B	-2.35	120.32	125.62
15	A	810	CLA	CMB-C2B-C1B	-2.35	121.85	125.42
14	O	840	F6C	C4A-C3A-C2A	-2.35	103.49	106.97
15	A	840	CLA	C3B-C4B-NB	-2.35	108.44	110.53
15	O	827	CLA	C3B-C4B-NB	-2.35	108.44	110.53
15	b	823	CLA	C1-C2-C3	-2.35	122.35	126.20
15	B	835	CLA	CMB-C2B-C1B	-2.35	121.85	125.42
15	O	803	CLA	CHB-C4A-NA	2.34	127.78	124.40
15	O	819	CLA	CHB-C4A-NA	2.34	127.78	124.40
15	a	827	CLA	CHB-C4A-NA	2.34	127.78	124.40
15	O	806	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
15	N	810	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
14	b	840	F6C	C4A-C3A-C2A	-2.34	103.50	106.97
14	N	824	F6C	OMB-CMB-C2B	-2.34	120.34	125.62
14	L	204	F6C	CMB-C2B-C1B	-2.34	122.42	128.37
14	A	824	F6C	C4A-C3A-C2A	-2.34	103.50	106.97
14	a	826	F6C	CHB-C4A-NA	2.34	128.09	124.80
15	A	831	CLA	CHB-C4A-NA	2.34	127.77	124.40
15	F	201	CLA	C1-C2-C3	-2.34	122.37	126.20
14	A	826	F6C	CMB-C2B-C1B	-2.34	122.43	128.37
14	O	833	F6C	OMB-CMB-C2B	-2.33	120.35	125.62
14	a	824	F6C	OMB-CMB-C2B	-2.33	120.36	125.62
15	K	103	CLA	CHB-C4A-NA	2.33	127.76	124.40
15	V	103	CLA	CHB-C4A-NA	2.33	127.76	124.40
14	N	856	F6C	C4A-C3A-C2A	-2.33	103.51	106.97
15	O	835	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
15	f	201	CLA	CHB-C4A-NA	2.33	127.76	124.40
15	b	827	CLA	C3B-C4B-NB	-2.32	108.46	110.53
15	a	831	CLA	CHB-C4A-NA	2.32	127.75	124.40
18	a	847	BCR	C20-C21-C22	-2.32	124.02	127.28
15	S	201	CLA	CHB-C4A-NA	2.32	127.75	124.40
15	N	820	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
15	b	827	CLA	CHB-C4A-NA	2.32	127.75	124.40
15	B	806	CLA	O2D-CGD-CBD	2.32	115.28	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	838	F6C	C4A-C3A-C2A	-2.32	103.54	106.97
14	B	831	F6C	O2D-CGD-CBD	2.32	115.28	111.23
15	A	840	CLA	CHB-C4A-NA	2.31	127.74	124.40
15	N	840	CLA	CHB-C4A-NA	2.31	127.74	124.40
15	A	834	CLA	CHB-C4A-NA	2.31	127.73	124.40
15	O	815	CLA	O2D-CGD-CBD	2.31	115.27	111.23
15	A	822	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	B	831	F6C	C4A-C3A-C2A	-2.31	103.55	106.97
18	F	202	BCR	C2-C1-C6	2.31	113.79	110.44
15	a	820	CLA	C3B-C4B-NB	-2.31	108.47	110.53
15	B	825	CLA	CHB-C4A-NA	2.31	127.73	124.40
15	N	834	CLA	CHB-C4A-NA	2.31	127.73	124.40
15	b	807	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	a	856	F6C	C4A-C3A-C2A	-2.31	103.55	106.97
15	b	808	CLA	O2D-CGD-CBD	2.30	115.26	111.23
15	a	840	CLA	CHB-C4A-NA	2.30	127.72	124.40
15	O	807	CLA	CHB-C4A-NA	2.30	127.72	124.40
15	B	804	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
15	N	819	CLA	C1-C2-C3	-2.30	122.43	126.20
15	a	822	CLA	CHB-C4A-NA	2.30	127.72	124.40
15	b	805	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
15	A	833	CLA	CMB-C2B-C3B	2.30	131.95	126.55
15	a	835	CLA	O2D-CGD-CBD	2.29	115.24	111.23
18	A	846	BCR	C11-C10-C9	-2.29	124.06	127.28
15	B	826	CLA	CHB-C4A-NA	2.29	127.71	124.40
18	b	847	BCR	C15-C16-C17	-2.29	118.83	123.52
15	b	818	CLA	CHB-C4A-NA	2.29	127.71	124.40
14	b	833	F6C	C4A-C3A-C2A	-2.29	103.57	106.97
15	N	827	CLA	CHB-C4A-NA	2.29	127.71	124.40
14	O	833	F6C	C4A-C3A-C2A	-2.29	103.57	106.97
15	S	201	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
15	a	834	CLA	CHB-C4A-NA	2.29	127.70	124.40
15	A	839	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
14	b	833	F6C	O2D-CGD-CBD	2.29	115.23	111.23
14	O	833	F6C	O2D-CGD-CBD	2.29	115.23	111.23
15	O	837	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
15	B	833	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
15	b	835	CLA	CHB-C4A-NA	2.29	127.70	124.40
15	b	822	CLA	C3B-C4B-NB	-2.29	108.49	110.53
15	F	201	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
15	O	816	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
15	B	806	CLA	C3B-C4B-NB	-2.28	108.49	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	857	F6C	C4A-C3A-C2A	-2.28	103.59	106.97
15	b	828	CLA	CHB-C4A-NA	2.28	127.69	124.40
15	a	818	CLA	O2D-CGD-CBD	2.28	115.21	111.23
14	N	802	F6C	C1-C2-C3	-2.28	122.47	126.20
15	b	831	CLA	C1-C2-C3	-2.28	122.47	126.20
15	A	818	CLA	O2D-CGD-CBD	2.28	115.21	111.23
14	a	824	F6C	CHB-C4A-NA	2.27	128.00	124.80
15	N	833	CLA	CMB-C2B-C3B	2.27	131.90	126.55
20	a	853	LMT	O1B-C1B-O5B	2.27	116.67	110.69
15	a	830	CLA	CHB-C4A-NA	2.27	127.68	124.40
20	A	853	LMT	O1B-C1B-O5B	2.27	116.67	110.69
13	A	801	CL0	CMD-C2D-C3D	2.27	129.22	124.68
15	O	818	CLA	CHB-C4A-NA	2.27	127.68	124.40
15	B	816	CLA	CHB-C4A-NA	2.27	127.67	124.40
15	N	820	CLA	C3B-C4B-NB	-2.27	108.50	110.53
15	B	837	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
15	O	828	CLA	CHB-C4A-NA	2.27	127.67	124.40
15	A	820	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
15	O	822	CLA	C3B-C4B-NB	-2.27	108.51	110.53
15	a	829	CLA	CHB-C4A-NA	2.26	127.67	124.40
13	N	801	CL0	CMD-C2D-C3D	2.26	129.21	124.68
18	N	847	BCR	C20-C21-C22	-2.26	124.10	127.28
14	N	826	F6C	CMB-C2B-C1B	-2.26	122.61	128.37
15	a	839	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
15	K	103	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
15	b	802	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
15	B	837	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
15	b	801	CLA	CHB-C4A-NA	2.26	127.66	124.40
15	f	201	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
18	A	858	BCR	C12-C13-C14	2.26	122.56	119.01
15	A	837	CLA	CHB-C4A-NA	2.26	127.66	124.40
14	a	826	F6C	CMB-C2B-C1B	-2.26	122.62	128.37
15	b	802	CLA	C3B-C4B-NB	-2.26	108.52	110.53
14	a	856	F6C	C1-C2-C3	-2.26	122.50	126.20
15	B	805	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
15	A	829	CLA	CHB-C4A-NA	2.26	127.66	124.40
15	a	837	CLA	CHB-C4A-NA	2.26	127.66	124.40
15	B	806	CLA	CHB-C4A-NA	2.25	127.65	124.40
15	B	836	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
15	A	830	CLA	CHB-C4A-NA	2.25	127.65	124.40
15	N	830	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	A	826	F6C	CAC-C3C-C2C	2.25	130.45	126.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	856	CLA	C3B-C4B-NB	-2.25	108.53	110.53
15	A	856	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
15	N	829	CLA	CHB-C4A-NA	2.25	127.64	124.40
15	N	837	CLA	CHB-C4A-NA	2.25	127.64	124.40
15	a	829	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
15	a	830	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
15	a	833	CLA	CMB-C2B-C3B	2.24	131.83	126.55
15	b	839	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
15	b	807	CLA	O2D-CGD-CBD	2.24	115.15	111.23
15	A	830	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
15	B	801	CLA	CHB-C4A-NA	2.24	127.63	124.40
15	O	801	CLA	CHB-C4A-NA	2.24	127.63	124.40
15	O	822	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
18	B	845	BCR	C15-C16-C17	-2.24	118.94	123.52
15	B	820	CLA	C3B-C4B-NB	-2.24	108.53	110.53
18	f	202	BCR	C24-C23-C22	-2.24	122.92	126.23
18	b	847	BCR	C19-C18-C17	-2.24	115.49	119.01
15	N	829	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
15	B	830	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
15	O	827	CLA	CHB-C4A-NA	2.24	127.63	124.40
18	O	847	BCR	C15-C16-C17	-2.24	118.94	123.52
15	b	838	CLA	CMB-C2B-C1B	-2.24	122.02	125.42
15	O	805	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
15	A	829	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
15	N	839	CLA	C1-C2-C3	-2.23	122.54	126.20
18	F	202	BCR	C24-C23-C22	-2.23	122.93	126.23
15	O	807	CLA	O2D-CGD-CBD	2.23	115.13	111.23
15	A	839	CLA	C1-C2-C3	-2.23	122.54	126.20
15	b	819	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
15	N	831	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
15	O	828	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
18	N	857	BCR	C12-C13-C14	2.23	122.52	119.01
15	a	820	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
15	b	804	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
15	O	808	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
15	B	808	CLA	CHB-C4A-NA	2.23	127.62	124.40
15	b	839	CLA	C3B-C4B-NB	-2.23	108.54	110.53
15	N	835	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
15	O	838	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
15	A	821	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
15	O	808	CLA	O2D-CGD-CBD	2.23	115.12	111.23
15	b	832	CLA	CMB-C2B-C1B	-2.23	122.03	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	824	F6C	CHB-C4A-NA	2.22	127.93	124.80
15	a	835	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
15	O	839	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
20	N	853	LMT	O1B-C1B-O5B	2.22	116.54	110.69
15	O	832	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
15	b	806	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
15	B	817	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
15	b	835	CLA	CMB-C2B-C3B	2.22	131.77	126.55
15	O	804	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
15	b	809	CLA	CHB-C4A-NA	2.22	127.60	124.40
13	A	801	CL0	O2A-CGA-O1A	-2.22	118.08	123.63
15	N	839	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
15	B	833	CLA	CMB-C2B-C3B	2.21	131.76	126.55
15	N	842	CLA	CHB-C4A-NA	2.21	127.59	124.40
15	a	804	CLA	C1-C2-C3	-2.21	122.57	126.20
14	L	204	F6C	O2D-CGD-CBD	2.21	115.09	111.23
15	N	820	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
15	O	832	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
15	A	856	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
15	b	802	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
15	O	829	CLA	CMB-C2B-C3B	2.21	131.75	126.55
15	B	803	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
15	A	819	CLA	C1-C2-C3	-2.21	122.58	126.20
15	B	829	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
15	O	811	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
16	a	843	PQN	C11-C3-C4	-2.20	116.26	118.58
14	A	857	F6C	CHB-C4A-NA	2.20	127.91	124.80
14	A	826	F6C	O2D-CGD-CBD	2.20	115.08	111.23
15	a	821	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
14	B	831	F6C	CHB-C4A-NA	2.20	127.90	124.80
15	B	814	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
18	O	848	BCR	C24-C23-C22	-2.20	122.98	126.23
15	b	839	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
15	O	831	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
15	O	802	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
15	B	827	CLA	CMB-C2B-C3B	2.20	131.72	126.55
15	a	837	CLA	O2D-CGD-CBD	2.20	115.07	111.23
15	a	815	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
15	B	809	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
15	B	830	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
15	N	818	CLA	O2D-CGD-CBD	2.20	115.07	111.23
14	b	833	F6C	CHB-C4A-NA	2.20	127.90	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	808	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
15	A	835	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
15	a	842	CLA	CHB-C4A-NA	2.19	127.56	124.40
15	N	821	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
15	O	819	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
15	B	837	CLA	C3B-C4B-NB	-2.19	108.57	110.53
14	A	857	F6C	CMB-C2B-C1B	-2.19	122.79	128.37
15	j	203	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
15	A	812	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
15	A	815	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
15	N	815	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
15	A	813	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
15	A	842	CLA	CHB-C4A-NA	2.19	127.56	124.40
15	a	813	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
15	b	828	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
15	O	835	CLA	CMB-C2B-C3B	2.19	131.70	126.55
15	N	811	CLA	O2D-CGD-CBD	2.19	115.06	111.23
14	O	833	F6C	CHB-C4A-NA	2.19	127.88	124.80
15	O	832	CLA	C1-C2-C3	-2.19	122.61	126.20
15	L	203	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
14	b	840	F6C	CBD-CHA-C4D	-2.19	106.08	108.54
15	B	825	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
14	A	824	F6C	CBD-CHA-C4D	-2.18	106.08	108.54
13	N	801	CL0	O2A-CGA-O1A	-2.18	118.17	123.63
15	B	813	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
14	N	856	F6C	CMB-C2B-C1B	-2.18	122.82	128.37
15	b	801	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
14	N	856	F6C	CHB-C4A-NA	2.18	127.87	124.80
15	O	809	CLA	CHB-C4A-NA	2.18	127.55	124.40
15	N	812	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
15	B	821	CLA	C1-C2-C3	-2.18	122.63	126.20
15	a	812	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
15	b	811	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
15	a	839	CLA	C1-C2-C3	-2.18	122.63	126.20
15	A	841	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
15	N	813	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
15	a	807	CLA	C1-C2-C3	-2.17	122.64	126.20
15	b	824	CLA	O2D-CGD-CBD	2.17	115.03	111.23
15	a	827	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
15	N	823	CLA	C1-C2-C3	-2.17	122.64	126.20
15	W	1502	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
15	B	822	CLA	O2D-CGD-CBD	2.17	115.02	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	803	CLA	O1D-CGD-CBD	2.17	128.79	124.52
15	O	828	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
15	N	827	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
13	a	801	CL0	O2A-CGA-O1A	-2.17	118.21	123.63
15	B	826	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
15	N	840	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
15	A	803	CLA	CMB-C2B-C3B	2.16	131.64	126.55
14	a	856	F6C	CMB-C2B-C1B	-2.16	122.86	128.37
15	a	825	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
15	O	802	CLA	C3B-C4B-NB	-2.16	108.60	110.53
14	W	1503	F6C	O2A-CGA-O1A	-2.16	118.22	123.63
15	O	824	CLA	O2D-CGD-CBD	2.16	115.01	111.23
15	A	842	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	B	814	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	a	841	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	j	204	F6C	O2D-CGD-CBD	2.16	115.00	111.23
15	A	827	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	b	829	CLA	CMB-C2B-C3B	2.16	131.62	126.55
15	B	824	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	O	816	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
15	b	830	CLA	C1-C2-C3	-2.16	122.67	126.20
18	O	848	BCR	C2-C1-C6	2.15	113.57	110.44
15	b	802	CLA	CMB-C2B-C3B	2.15	131.61	126.55
14	a	856	F6C	CHB-C4A-NA	2.15	127.83	124.80
15	j	202	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
15	O	825	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
15	b	816	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
14	N	824	F6C	CHB-C4A-NA	2.15	127.83	124.80
15	b	832	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
15	B	807	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
14	A	857	F6C	O2A-CGA-O1A	-2.15	118.25	123.63
15	O	826	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	836	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
18	a	857	BCR	C12-C13-C14	2.15	122.38	119.01
15	N	842	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
15	b	829	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
18	f	202	BCR	C20-C19-C18	-2.15	120.48	126.36
15	N	803	CLA	CMB-C2B-C3B	2.14	131.59	126.55
15	N	822	CLA	CHB-C4A-NA	2.14	127.50	124.40
15	A	804	CLA	C1-C2-C3	-2.14	122.68	126.20
15	N	825	CLA	O2A-CGA-O1A	-2.14	118.27	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	f	202	BCR	C2-C1-C6	2.14	113.55	110.44
15	b	826	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
15	A	829	CLA	C1-C2-C3	-2.14	122.69	126.20
14	N	856	F6C	O2A-CGA-O1A	-2.14	118.27	123.63
15	a	842	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
18	A	858	BCR	C11-C12-C13	-2.14	120.49	126.36
15	A	809	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
15	B	808	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
15	N	835	CLA	O2D-CGD-CBD	2.14	114.97	111.23
14	a	824	F6C	CBD-CHA-C4D	-2.14	106.13	108.54
15	B	823	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	N	826	F6C	CHB-C4A-NA	2.14	127.81	124.80
15	a	818	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
15	A	856	CLA	CMB-C2B-C3B	2.14	131.57	126.55
15	O	827	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
15	V	103	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
15	b	841	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
15	A	806	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
15	B	828	CLA	C1-C2-C3	-2.13	122.70	126.20
15	A	822	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
15	b	838	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
15	B	824	CLA	C1-C2-C3	-2.13	122.70	126.20
15	a	840	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
14	j	204	F6C	O2A-CGA-O1A	-2.13	118.30	123.63
15	B	839	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
15	O	839	CLA	C3B-C4B-NB	-2.13	108.63	110.53
15	A	808	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
15	b	827	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
15	a	803	CLA	CMB-C2B-C3B	2.13	131.56	126.55
15	O	841	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
15	A	840	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
14	B	831	F6C	O2A-CGA-O1A	-2.13	118.31	123.63
15	O	801	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
15	b	825	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
15	N	830	CLA	C1-C2-C3	-2.12	122.72	126.20
18	N	857	BCR	C11-C12-C13	-2.12	120.54	126.36
18	a	857	BCR	C11-C12-C13	-2.12	120.54	126.36
15	O	809	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
14	a	802	F6C	CHB-C4A-C3A	-2.12	121.07	125.49
15	a	836	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
15	A	830	CLA	C1-C2-C3	-2.12	122.72	126.20
14	b	840	F6C	CHB-C4A-NA	2.12	127.79	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	806	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
15	N	808	CLA	O2A-CGA-O1A	-2.12	117.88	123.33
15	O	803	CLA	O1D-CGD-CBD	2.12	128.70	124.52
15	N	836	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
15	a	814	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	N	804	CLA	C1-C2-C3	-2.12	122.73	126.20
15	O	839	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
15	a	838	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
14	B	838	F6C	CBD-CHA-C4D	-2.12	106.15	108.54
15	a	818	CLA	CBA-CAA-C2A	2.12	120.09	113.79
15	O	838	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	a	809	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	B	820	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
15	A	809	CLA	C1-C2-C3	-2.11	122.73	126.20
15	A	827	CLA	C1-C2-C3	-2.11	122.73	126.20
15	N	827	CLA	C1-C2-C3	-2.11	122.73	126.20
15	Z	103	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
15	b	825	CLA	O2D-CGD-CBD	2.11	114.93	111.23
15	B	801	CLA	O1D-CGD-CBD	2.11	128.69	124.52
15	B	807	CLA	O2D-CGD-CBD	2.11	114.93	111.23
15	l	103	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
14	L	204	F6C	O2A-CGA-O1A	-2.11	118.34	123.63
14	b	833	F6C	O2A-CGA-O1A	-2.11	118.34	123.63
15	A	808	CLA	O2A-CGA-O1A	-2.11	117.90	123.33
15	K	103	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
15	O	814	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
15	i	103	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
14	B	838	F6C	CHB-C4A-NA	2.11	127.77	124.80
15	b	809	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
15	b	837	CLA	CMB-C2B-C3B	2.11	131.51	126.55
15	N	837	CLA	O2D-CGD-CBD	2.11	114.92	111.23
15	b	831	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
15	O	826	CLA	C1-C2-C3	-2.11	122.74	126.20
14	a	802	F6C	C1-C2-C3	-2.11	122.74	126.20
15	B	808	CLA	C1-C2-C3	-2.11	122.74	126.20
15	A	820	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
15	A	836	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
14	a	856	F6C	O2A-CGA-O1A	-2.11	118.36	123.63
15	V	103	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
14	a	826	F6C	O2D-CGD-CBD	2.11	114.91	111.23
15	B	802	CLA	O1D-CGD-CBD	2.11	128.67	124.52
15	B	837	CLA	CMB-C2B-C3B	2.10	131.50	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	822	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
15	O	839	CLA	C1-C2-C3	-2.10	122.75	126.20
15	a	810	CLA	CMB-C2B-C3B	2.10	131.50	126.55
15	a	813	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
14	L	201	F6C	CMB-C2B-C1B	-2.10	123.02	128.37
15	A	813	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
15	a	819	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
15	B	812	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
15	O	822	CLA	CMB-C2B-C3B	2.10	131.49	126.55
15	N	807	CLA	C1-C2-C3	-2.10	122.76	126.20
14	A	802	F6C	CHB-C4A-C3A	-2.10	121.12	125.49
14	N	824	F6C	CBD-CHA-C4D	-2.10	106.18	108.54
15	a	808	CLA	O2A-CGA-O1A	-2.10	117.94	123.33
14	O	833	F6C	O2A-CGA-O1A	-2.10	118.38	123.63
15	A	836	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
15	O	802	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
15	A	825	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
15	a	836	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
16	A	843	PQN	C11-C3-C4	-2.10	116.37	118.58
15	b	822	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
14	O	840	F6C	CHB-C4A-NA	2.09	127.75	124.80
15	b	826	CLA	C1-C2-C3	-2.09	122.77	126.20
15	N	836	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
15	b	814	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
18	O	848	BCR	C20-C19-C18	-2.09	120.63	126.36
15	N	809	CLA	C1-C2-C3	-2.09	122.77	126.20
15	A	814	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
15	N	809	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
15	b	805	CLA	CMB-C2B-C3B	2.09	131.47	126.55
15	A	818	CLA	CBA-CAA-C2A	2.09	120.01	113.79
15	N	814	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
15	A	810	CLA	CMB-C2B-C3B	2.09	131.46	126.55
15	L	202	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
15	N	819	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
15	A	811	CLA	O2D-CGD-CBD	2.09	114.88	111.23
15	a	822	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
15	N	810	CLA	CMB-C2B-C3B	2.09	131.46	126.55
15	O	829	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
15	O	830	CLA	C1-C2-C3	-2.09	122.78	126.20
14	b	840	F6C	O2A-CGA-O1A	-2.09	118.41	123.63
15	a	831	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
18	A	845	BCR	C7-C6-C5	2.08	126.36	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	W	1503	F6C	CBD-CHA-C4D	-2.08	106.19	108.54
18	B	845	BCR	C19-C18-C17	-2.08	115.73	119.01
15	N	813	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
15	O	806	CLA	CMB-C2B-C3B	2.08	131.45	126.55
15	N	818	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
15	O	817	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
15	b	834	CLA	C1-C2-C3	-2.08	122.78	126.20
14	W	1503	F6C	CHB-C4A-NA	2.08	127.73	124.80
14	A	802	F6C	O2A-CGA-O1A	-2.08	118.42	123.63
15	A	818	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
15	b	839	CLA	C1-C2-C3	-2.08	122.79	126.20
15	O	820	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
18	O	847	BCR	C19-C18-C17	-2.08	115.74	119.01
14	O	840	F6C	CBD-CHA-C4D	-2.08	106.19	108.54
15	b	808	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
14	O	840	F6C	O2A-CGA-O1A	-2.08	118.42	123.63
15	N	827	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
15	B	821	CLA	CHB-C4A-NA	2.08	127.40	124.40
15	B	835	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
15	a	830	CLA	CMB-C2B-C3B	2.08	131.44	126.55
15	a	809	CLA	C1-C2-C3	-2.08	122.79	126.20
15	O	837	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
15	b	839	CLA	CMB-C2B-C3B	2.08	131.43	126.55
15	A	837	CLA	C1-C2-C3	-2.08	122.80	126.20
18	A	850	BCR	C27-C26-C25	-2.08	119.90	122.70
15	b	809	CLA	C1-C2-C3	-2.08	122.80	126.20
15	O	823	CLA	CAA-CBA-CGA	-2.07	107.32	113.21
15	b	825	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
15	N	806	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	a	837	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	A	830	CLA	CMB-C2B-C3B	2.07	131.43	126.55
14	N	826	F6C	O2A-CGA-O1A	-2.07	118.44	123.63
15	N	837	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	a	827	CLA	C1-C2-C3	-2.07	122.80	126.20
15	N	831	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	b	820	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
15	a	821	CLA	C1-C2-C3	-2.07	122.80	126.20
15	B	818	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
15	a	842	CLA	C1-C2-C3	-2.07	122.80	126.20
15	O	802	CLA	CMB-C2B-C3B	2.07	131.42	126.55
15	A	837	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
15	O	817	CLA	O2A-CGA-O1A	-2.07	118.45	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	804	CLA	CMB-C2B-C3B	2.07	131.42	126.55
15	B	837	CLA	C1-C2-C3	-2.07	122.81	126.20
15	A	838	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
15	b	817	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
15	B	835	CLA	CMB-C2B-C3B	2.07	131.41	126.55
15	A	827	CLA	O2D-CGD-CBD	2.07	114.84	111.23
14	A	824	F6C	O2A-CGA-O1A	-2.07	118.46	123.63
15	a	831	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
15	b	837	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
15	B	822	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
15	A	819	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
15	L	202	CLA	C1-C2-C3	-2.06	122.81	126.20
15	N	837	CLA	C1-C2-C3	-2.06	122.81	126.20
15	a	820	CLA	CMB-C2B-C3B	2.06	131.41	126.55
16	N	843	PQN	C11-C3-C4	-2.06	116.41	118.58
15	B	802	CLA	C1-C2-C3	-2.06	122.82	126.20
15	A	831	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
18	F	202	BCR	C20-C19-C18	-2.06	120.71	126.36
15	O	816	CLA	CMB-C2B-C3B	2.06	131.40	126.55
15	b	801	CLA	O1D-CGD-CBD	2.06	128.59	124.52
15	B	836	CLA	CMB-C2B-C3B	2.06	131.40	126.55
15	A	823	CLA	C1-C2-C3	-2.06	122.82	126.20
15	N	842	CLA	C1-C2-C3	-2.06	122.82	126.20
15	b	817	CLA	O2D-CGD-CBD	2.06	114.83	111.23
15	A	803	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
15	a	829	CLA	C1-C2-C3	-2.06	122.82	126.20
15	B	801	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
15	O	807	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
18	A	858	BCR	C10-C11-C12	2.06	129.17	123.20
14	A	826	F6C	CBC-CAC-C3C	2.06	118.00	112.42
15	O	801	CLA	O1D-CGD-CBD	2.06	128.58	124.52
15	A	807	CLA	C1-C2-C3	-2.06	122.82	126.20
14	B	831	F6C	CMB-C2B-C1B	-2.06	123.13	128.37
15	a	808	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
15	a	806	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
15	B	815	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
15	b	807	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
15	a	837	CLA	C1-C2-C3	-2.06	122.83	126.20
15	b	820	CLA	C1-C2-C3	-2.05	122.83	126.20
14	B	838	F6C	O2A-CGA-O1A	-2.05	118.49	123.63
15	b	817	CLA	CHB-C1B-NB	2.05	127.13	124.05
15	O	837	CLA	CMB-C2B-C3B	2.05	131.38	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	805	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
14	N	802	F6C	CHB-C4A-C3A	-2.05	121.22	125.49
15	O	830	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
15	a	811	CLA	O2D-CGD-CBD	2.05	114.81	111.23
15	O	831	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
15	O	823	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
13	N	801	CL0	C4D-ND-C1D	2.05	106.77	105.22
15	N	829	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
15	B	820	CLA	CMB-C2B-C3B	2.05	131.37	126.55
15	N	829	CLA	C1-C2-C3	-2.05	122.84	126.20
15	b	819	CLA	C1-C2-C3	-2.05	122.84	126.20
15	A	809	CLA	O2D-CGD-CBD	2.05	114.81	111.23
15	b	813	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
15	b	838	CLA	CMB-C2B-C3B	2.04	131.36	126.55
15	B	805	CLA	CMB-C2B-C3B	2.04	131.36	126.55
18	N	857	BCR	C10-C11-C12	2.04	129.12	123.20
15	N	821	CLA	C1-C2-C3	-2.04	122.85	126.20
15	A	810	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
15	A	828	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	a	824	F6C	O2A-CGA-O1A	-2.04	118.52	123.63
18	A	845	BCR	C24-C25-C26	2.04	126.26	121.56
15	b	824	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
15	X	103	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
15	N	834	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	N	824	F6C	O2A-CGA-O1A	-2.04	118.52	123.63
18	a	850	BCR	C27-C26-C25	-2.04	119.95	122.70
15	O	805	CLA	CMB-C2B-C3B	2.04	131.35	126.55
14	A	826	F6C	CMC-C2C-C1C	-2.04	122.31	125.42
15	B	821	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
15	B	817	CLA	C1-C2-C3	-2.04	122.86	126.20
15	N	818	CLA	CBA-CAA-C2A	2.04	119.86	113.79
15	A	837	CLA	O2D-CGD-CBD	2.04	114.79	111.23
15	B	806	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
15	O	824	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
15	a	806	CLA	C1-C2-C3	-2.04	122.86	126.20
15	O	838	CLA	CMB-C2B-C3B	2.04	131.34	126.55
15	N	803	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
15	N	811	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
15	b	823	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
15	B	826	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
15	a	815	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
14	j	204	F6C	CHB-C4A-NA	2.03	127.66	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	807	CLA	C1-C2-C3	-2.03	122.87	126.20
15	A	831	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
14	j	204	F6C	CBD-CHA-C4D	-2.03	106.25	108.54
15	a	809	CLA	O2D-CGD-CBD	2.03	114.78	111.23
15	b	823	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
15	b	816	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
15	b	834	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
15	B	832	CLA	C1-C2-C3	-2.03	122.87	126.20
15	a	823	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
18	A	858	BCR	C8-C9-C10	2.03	122.20	119.01
15	a	834	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
15	b	815	CLA	CHD-C1D-ND	-2.03	121.95	124.80
15	B	814	CLA	C1-C2-C3	-2.03	122.87	126.20
15	b	815	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
18	a	845	BCR	C7-C6-C5	2.03	126.22	121.56
15	O	834	CLA	C1-C2-C3	-2.03	122.88	126.20
15	N	832	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
13	a	801	CL0	C4D-ND-C1D	2.03	106.76	105.22
15	b	830	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
15	B	811	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
15	W	1501	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
15	B	822	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
15	O	820	CLA	C1-C2-C3	-2.03	122.88	126.20
14	L	204	F6C	CBD-CHA-C4D	-2.03	106.26	108.54
15	N	810	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
15	O	828	CLA	CMB-C2B-C3B	2.03	131.31	126.55
15	O	839	CLA	CMB-C2B-C3B	2.02	131.31	126.55
14	W	1503	F6C	C3A-C4A-NA	2.02	112.13	110.13
15	N	838	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
15	N	806	CLA	C1-C2-C3	-2.02	122.88	126.20
15	b	803	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
15	B	827	CLA	C1-C2-C3	-2.02	122.88	126.20
15	b	806	CLA	CMB-C2B-C3B	2.02	131.31	126.55
15	N	827	CLA	CAA-C2A-C1A	-2.02	105.35	111.97
15	j	202	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
15	O	816	CLA	C1-C2-C3	-2.02	122.89	126.20
15	b	816	CLA	C1-C2-C3	-2.02	122.89	126.20
15	b	822	CLA	CMB-C2B-C3B	2.02	131.30	126.55
15	B	813	CLA	O2D-CGD-CBD	2.02	114.76	111.23
15	B	823	CLA	O2D-CGD-CBD	2.02	114.76	111.23
15	a	810	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
15	b	839	CLA	O2D-CGD-CBD	2.02	114.76	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	810	F6C	CMB-C2B-C1B	-2.02	123.23	128.37
15	A	827	CLA	CAA-C2A-C1A	-2.02	105.36	111.97
15	a	829	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
15	A	811	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
15	O	808	CLA	CMB-C2B-C3B	2.02	131.29	126.55
15	B	837	CLA	O2D-CGD-CBD	2.02	114.75	111.23
15	O	826	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
18	O	847	BCR	C15-C14-C13	-2.02	124.45	127.28
15	O	829	CLA	C1-C2-C3	-2.01	122.90	126.20
15	a	811	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
15	O	801	CLA	C1-C2-C3	-2.01	122.90	126.20
15	A	834	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
15	B	830	CLA	CMB-C2B-C3B	2.01	131.29	126.55
15	N	805	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
15	a	803	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
15	B	814	CLA	CMB-C2B-C3B	2.01	131.28	126.55
15	A	823	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
15	N	807	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
15	a	807	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
15	A	805	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
15	A	835	CLA	C1-C2-C3	-2.01	122.90	126.20
15	O	825	CLA	O2D-CGD-CBD	2.01	114.75	111.23
18	a	857	BCR	C10-C11-C12	2.01	129.02	123.20
15	a	832	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
15	A	831	CLA	O2D-CGD-CBD	2.01	114.74	111.23
15	A	806	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
15	b	832	CLA	CMB-C2B-C3B	2.01	131.27	126.55
15	B	815	CLA	CHB-C1B-NB	2.01	127.06	124.05
15	A	815	CLA	C1-C2-C3	-2.01	122.91	126.20
15	O	832	CLA	CMB-C2B-C3B	2.01	131.27	126.55
15	L	202	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
15	O	803	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
15	A	832	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
15	O	805	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
15	b	803	CLA	C1-C2-C3	-2.00	122.91	126.20
15	b	832	CLA	C1-C2-C3	-2.00	122.91	126.20
15	B	815	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
15	O	813	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	a	827	CLA	CAA-C2A-C1A	-2.00	105.41	111.97
14	b	833	F6C	CMB-C2B-C1B	-2.00	123.27	128.37
15	N	820	CLA	CMB-C2B-C3B	2.00	131.26	126.55
15	N	837	CLA	CMB-C2B-C1B	-2.00	122.37	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	828	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	A	837	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
15	B	824	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
15	O	822	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	O	834	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	A	806	CLA	C1-C2-C3	-2.00	122.92	126.20
15	a	828	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	B	830	CLA	C1-C2-C3	-2.00	122.92	126.20

All (276) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	ND
13	A	801	CL0	NC
13	A	801	CL0	NA
13	N	801	CL0	ND
13	N	801	CL0	NC
13	N	801	CL0	NA
13	a	801	CL0	ND
13	a	801	CL0	NC
13	a	801	CL0	NA
14	A	802	F6C	NA
14	A	824	F6C	NA
14	A	826	F6C	NA
14	A	857	F6C	NA
14	B	831	F6C	NA
14	B	838	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	810	F6C	NA
14	O	833	F6C	NA
14	O	840	F6C	NA
14	W	1503	F6C	NA
14	a	802	F6C	NA
14	a	824	F6C	NA
14	a	826	F6C	NA
14	a	856	F6C	NA
14	b	810	F6C	NA

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Mol	Chain	Res	Type	Atom
14	b	833	F6C	NA
14	b	840	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
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	A	856	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	812	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	832	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	839	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	103	CLA	ND

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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	811	CLA	ND
15	O	812	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	832	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	839	CLA	ND
15	O	841	CLA	ND
15	S	201	CLA	ND
15	V	102	CLA	ND
15	V	103	CLA	ND
15	W	1501	CLA	ND
15	W	1502	CLA	ND
15	Z	103	CLA	ND
15	a	803	CLA	ND
15	a	804	CLA	ND
15	a	805	CLA	ND

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
15	b	808	CLA	ND
15	b	809	CLA	ND
15	b	811	CLA	ND
15	b	812	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	832	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	839	CLA	ND
15	b	841	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
15	l	103	CLA	ND

All (3474) 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

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Mol	Chain	Res	Type	Atoms
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	857	F6C	C3B-C2B-CMB-OMB
14	B	831	F6C	CHA-CBD-CGD-O1D
14	B	831	F6C	CHA-CBD-CGD-O2D
14	B	831	F6C	C3B-C2B-CMB-OMB
14	B	838	F6C	C1B-C2B-CMB-OMB
14	B	838	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	C1A-C2A-CAA-CBA
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	C2B-C3B-CAB-CBB
14	N	824	F6C	C3B-C2B-CMB-OMB
14	N	826	F6C	CHA-CBD-CGD-O1D
14	N	826	F6C	CHA-CBD-CGD-O2D
14	N	856	F6C	C2A-CAA-CBA-CGA
14	O	810	F6C	C1B-C2B-CMB-OMB
14	O	810	F6C	C3B-C2B-CMB-OMB
14	O	833	F6C	CHA-CBD-CGD-O1D
14	O	833	F6C	CHA-CBD-CGD-O2D
14	O	840	F6C	C1B-C2B-CMB-OMB
14	O	840	F6C	C3B-C2B-CMB-OMB
14	W	1503	F6C	C1A-C2A-CAA-CBA
14	W	1503	F6C	CBA-CGA-O2A-C1
14	W	1503	F6C	C1B-C2B-CMB-OMB
14	W	1503	F6C	C3B-C2B-CMB-OMB
14	W	1503	F6C	C2-C3-C5-C6
14	W	1503	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	C2B-C3B-CAB-CBB
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

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Mol	Chain	Res	Type	Atoms
14	a	856	F6C	C2A-CAA-CBA-CGA
14	a	856	F6C	C3B-C2B-CMB-OMB
14	b	810	F6C	C1B-C2B-CMB-OMB
14	b	810	F6C	C3B-C2B-CMB-OMB
14	b	833	F6C	CHA-CBD-CGD-O1D
14	b	833	F6C	CHA-CBD-CGD-O2D
14	b	840	F6C	C1B-C2B-CMB-OMB
14	b	840	F6C	C3B-C2B-CMB-OMB
14	j	204	F6C	C1A-C2A-CAA-CBA
14	j	204	F6C	C1B-C2B-CMB-OMB
14	j	204	F6C	C3B-C2B-CMB-OMB
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	807	CLA	CBD-CGD-O2D-CED
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	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	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	820	CLA	CHA-CBD-CGD-O1D
15	A	820	CLA	CHA-CBD-CGD-O2D
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	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	A	837	CLA	CBD-CGD-O2D-CED
15	A	838	CLA	C1A-C2A-CAA-CBA
15	A	838	CLA	C3A-C2A-CAA-CBA
15	A	838	CLA	C4-C3-C5-C6
15	A	841	CLA	C1A-C2A-CAA-CBA
15	A	841	CLA	CBA-CGA-O2A-C1
15	A	841	CLA	O1A-CGA-O2A-C1
15	A	842	CLA	C1A-C2A-CAA-CBA
15	B	803	CLA	CBD-CGD-O2D-CED
15	B	804	CLA	C3A-C2A-CAA-CBA
15	B	805	CLA	CHA-CBD-CGD-O1D
15	B	805	CLA	CHA-CBD-CGD-O2D
15	B	805	CLA	CBD-CGD-O2D-CED
15	B	808	CLA	C1A-C2A-CAA-CBA
15	B	808	CLA	C3A-C2A-CAA-CBA
15	B	812	CLA	CBD-CGD-O2D-CED
15	B	813	CLA	C1A-C2A-CAA-CBA
15	B	813	CLA	C3A-C2A-CAA-CBA
15	B	813	CLA	CHA-CBD-CGD-O1D
15	B	813	CLA	CHA-CBD-CGD-O2D
15	B	814	CLA	CHA-CBD-CGD-O1D
15	B	814	CLA	CHA-CBD-CGD-O2D
15	B	815	CLA	C3A-C2A-CAA-CBA
15	B	816	CLA	C1A-C2A-CAA-CBA
15	B	816	CLA	C3A-C2A-CAA-CBA
15	B	817	CLA	C2B-C3B-CAB-CBB
15	B	817	CLA	C4B-C3B-CAB-CBB
15	B	818	CLA	C1A-C2A-CAA-CBA
15	B	818	CLA	C3A-C2A-CAA-CBA
15	B	818	CLA	CBD-CGD-O2D-CED
15	B	820	CLA	C1A-C2A-CAA-CBA
15	B	822	CLA	CHA-CBD-CGD-O1D
15	B	822	CLA	CHA-CBD-CGD-O2D
15	B	823	CLA	CHA-CBD-CGD-O1D
15	B	823	CLA	CHA-CBD-CGD-O2D
15	B	823	CLA	C2-C3-C5-C6
15	B	823	CLA	C4-C3-C5-C6
15	B	826	CLA	C1A-C2A-CAA-CBA
15	B	826	CLA	C3A-C2A-CAA-CBA
15	B	834	CLA	CAD-CBD-CGD-O1D
15	B	834	CLA	CAD-CBD-CGD-O2D
15	B	835	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	K	102	CLA	CBD-CGD-O2D-CED
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	807	CLA	C2B-C3B-CAB-CBB
15	N	807	CLA	C4B-C3B-CAB-CBB
15	N	807	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	809	CLA	C6-C7-C8-C9
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	C6-C7-C8-C9
15	N	812	CLA	C1A-C2A-CAA-CBA
15	N	812	CLA	CBD-CGD-O2D-CED
15	N	812	CLA	C4-C3-C5-C6
15	N	814	CLA	C4-C3-C5-C6
15	N	815	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	820	CLA	CHA-CBD-CGD-O1D
15	N	820	CLA	CHA-CBD-CGD-O2D
15	N	823	CLA	C1A-C2A-CAA-CBA
15	N	823	CLA	C3A-C2A-CAA-CBA
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	C1A-C2A-CAA-CBA
15	N	837	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	N	841	CLA	C1A-C2A-CAA-CBA
15	N	842	CLA	C1A-C2A-CAA-CBA
15	O	801	CLA	CBD-CGD-O2D-CED
15	O	804	CLA	CBD-CGD-O2D-CED
15	O	805	CLA	C3A-C2A-CAA-CBA
15	O	806	CLA	CHA-CBD-CGD-O1D
15	O	806	CLA	CHA-CBD-CGD-O2D
15	O	806	CLA	CBD-CGD-O2D-CED
15	O	809	CLA	C1A-C2A-CAA-CBA
15	O	809	CLA	C3A-C2A-CAA-CBA
15	O	814	CLA	C11-C12-C13-C14
15	O	815	CLA	C1A-C2A-CAA-CBA
15	O	815	CLA	CHA-CBD-CGD-O1D
15	O	815	CLA	CHA-CBD-CGD-O2D
15	O	816	CLA	CHA-CBD-CGD-O1D
15	O	816	CLA	CHA-CBD-CGD-O2D
15	O	817	CLA	C3A-C2A-CAA-CBA
15	O	818	CLA	C1A-C2A-CAA-CBA
15	O	818	CLA	C3A-C2A-CAA-CBA
15	O	819	CLA	C2B-C3B-CAB-CBB
15	O	819	CLA	C4B-C3B-CAB-CBB
15	O	820	CLA	C1A-C2A-CAA-CBA
15	O	820	CLA	C3A-C2A-CAA-CBA
15	O	820	CLA	CBD-CGD-O2D-CED
15	O	822	CLA	C1A-C2A-CAA-CBA
15	O	824	CLA	CHA-CBD-CGD-O1D
15	O	824	CLA	CHA-CBD-CGD-O2D
15	O	825	CLA	CHA-CBD-CGD-O1D
15	O	825	CLA	CHA-CBD-CGD-O2D
15	O	825	CLA	C4-C3-C5-C6
15	O	827	CLA	CBD-CGD-O2D-CED
15	O	828	CLA	C1A-C2A-CAA-CBA
15	O	828	CLA	C3A-C2A-CAA-CBA
15	O	830	CLA	C11-C10-C8-C7
15	O	835	CLA	C1A-C2A-CAA-CBA
15	O	836	CLA	CAD-CBD-CGD-O1D
15	O	836	CLA	CAD-CBD-CGD-O2D
15	O	837	CLA	C1A-C2A-CAA-CBA
15	O	841	CLA	C1A-C2A-CAA-CBA
15	V	102	CLA	CBD-CGD-O2D-CED
15	W	1502	CLA	C2B-C3B-CAB-CBB
15	W	1502	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
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	807	CLA	CBD-CGD-O2D-CED
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	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	C6-C7-C8-C9
15	a	812	CLA	C1A-C2A-CAA-CBA
15	a	812	CLA	C3A-C2A-CAA-CBA
15	a	812	CLA	CBD-CGD-O2D-CED
15	a	814	CLA	C2-C3-C5-C6
15	a	814	CLA	C4-C3-C5-C6
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	820	CLA	CHA-CBD-CGD-O1D
15	a	820	CLA	CHA-CBD-CGD-O2D
15	a	825	CLA	C2-C3-C5-C6
15	a	825	CLA	C4-C3-C5-C6
15	a	831	CLA	CHA-CBD-CGD-O2D
15	a	834	CLA	C2B-C3B-CAB-CBB
15	a	834	CLA	C4B-C3B-CAB-CBB
15	a	837	CLA	C1A-C2A-CAA-CBA
15	a	837	CLA	CBD-CGD-O2D-CED
15	a	841	CLA	C1A-C2A-CAA-CBA
15	a	841	CLA	CBA-CGA-O2A-C1
15	a	841	CLA	O1A-CGA-O2A-C1
15	a	842	CLA	C1A-C2A-CAA-CBA
15	b	804	CLA	CBD-CGD-O2D-CED
15	b	805	CLA	C3A-C2A-CAA-CBA
15	b	806	CLA	CHA-CBD-CGD-O2D
15	b	806	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	b	809	CLA	C1A-C2A-CAA-CBA
15	b	809	CLA	C3A-C2A-CAA-CBA
15	b	811	CLA	C12-C13-C15-C16
15	b	814	CLA	CBD-CGD-O2D-CED
15	b	815	CLA	C1A-C2A-CAA-CBA
15	b	815	CLA	C3A-C2A-CAA-CBA
15	b	815	CLA	CHA-CBD-CGD-O1D
15	b	815	CLA	CHA-CBD-CGD-O2D
15	b	816	CLA	CHA-CBD-CGD-O1D
15	b	816	CLA	CHA-CBD-CGD-O2D
15	b	817	CLA	C3A-C2A-CAA-CBA
15	b	818	CLA	C1A-C2A-CAA-CBA
15	b	818	CLA	C3A-C2A-CAA-CBA
15	b	819	CLA	C2B-C3B-CAB-CBB
15	b	819	CLA	C4B-C3B-CAB-CBB
15	b	820	CLA	C1A-C2A-CAA-CBA
15	b	820	CLA	C3A-C2A-CAA-CBA
15	b	820	CLA	CBD-CGD-O2D-CED
15	b	822	CLA	C1A-C2A-CAA-CBA
15	b	823	CLA	C1A-C2A-CAA-CBA
15	b	823	CLA	C3A-C2A-CAA-CBA
15	b	824	CLA	CHA-CBD-CGD-O1D
15	b	824	CLA	CHA-CBD-CGD-O2D
15	b	825	CLA	CHA-CBD-CGD-O1D
15	b	825	CLA	CHA-CBD-CGD-O2D
15	b	828	CLA	C1A-C2A-CAA-CBA
15	b	828	CLA	C3A-C2A-CAA-CBA
15	b	829	CLA	C4-C3-C5-C6
15	b	835	CLA	C1A-C2A-CAA-CBA
15	b	836	CLA	CAD-CBD-CGD-O1D
15	b	836	CLA	CAD-CBD-CGD-O2D
15	b	837	CLA	C1A-C2A-CAA-CBA
15	b	841	CLA	C1A-C2A-CAA-CBA
15	i	102	CLA	CBD-CGD-O2D-CED
15	j	203	CLA	C2B-C3B-CAB-CBB
15	j	203	CLA	C4B-C3B-CAB-CBB
15	j	203	CLA	C11-C10-C8-C9
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	846	BCR	C37-C22-C23-C24
18	A	848	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
18	A	848	BCR	C23-C24-C25-C26
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	858	BCR	C23-C24-C25-C26
18	B	842	BCR	C21-C22-C23-C24
18	B	844	BCR	C5-C6-C7-C8
18	F	202	BCR	C17-C18-C19-C20
18	F	202	BCR	C21-C22-C23-C24
18	F	202	BCR	C37-C22-C23-C24
18	I	101	BCR	C7-C8-C9-C10
18	I	101	BCR	C11-C12-C13-C14
18	I	101	BCR	C21-C22-C23-C24
18	I	101	BCR	C37-C22-C23-C24
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	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	846	BCR	C37-C22-C23-C24
18	N	848	BCR	C17-C18-C19-C20
18	N	848	BCR	C23-C24-C25-C26
18	N	850	BCR	C7-C8-C9-C10
18	N	850	BCR	C17-C18-C19-C20
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	N	857	BCR	C23-C24-C25-C26
18	O	844	BCR	C21-C22-C23-C24
18	O	848	BCR	C11-C12-C13-C14
18	O	848	BCR	C17-C18-C19-C20
18	O	848	BCR	C36-C18-C19-C20
18	O	848	BCR	C21-C22-C23-C24
18	T	101	BCR	C7-C8-C9-C10
18	T	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
18	T	101	BCR	C11-C12-C13-C14
18	T	101	BCR	C11-C12-C13-C35
18	T	101	BCR	C21-C22-C23-C24
18	T	101	BCR	C23-C24-C25-C26
18	U	101	BCR	C11-C12-C13-C14
18	U	101	BCR	C11-C12-C13-C35
18	U	101	BCR	C21-C22-C23-C24
18	U	101	BCR	C23-C24-C25-C26
18	W	1504	BCR	C7-C8-C9-C10
18	W	1504	BCR	C7-C8-C9-C34
18	W	1504	BCR	C37-C22-C23-C24
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	846	BCR	C37-C22-C23-C24
18	a	848	BCR	C17-C18-C19-C20
18	a	848	BCR	C23-C24-C25-C26
18	a	848	BCR	C23-C24-C25-C30
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	857	BCR	C23-C24-C25-C26
18	b	844	BCR	C21-C22-C23-C24
18	b	846	BCR	C5-C6-C7-C8
18	f	202	BCR	C11-C12-C13-C14
18	f	202	BCR	C17-C18-C19-C20
18	f	202	BCR	C21-C22-C23-C24
18	f	202	BCR	C37-C22-C23-C24
18	g	101	BCR	C7-C8-C9-C10
18	g	101	BCR	C7-C8-C9-C34
18	g	101	BCR	C11-C12-C13-C14
18	g	101	BCR	C11-C12-C13-C35
18	g	101	BCR	C23-C24-C25-C26
18	h	101	BCR	C11-C12-C13-C14
18	h	101	BCR	C11-C12-C13-C35
18	h	101	BCR	C21-C22-C23-C24
18	h	101	BCR	C23-C24-C25-C26
18	j	205	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
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
19	A	851	LHG	C3-O3-P-O5
19	L	207	LHG	C3-O3-P-O5
19	L	207	LHG	C3-O3-P-O6
19	L	207	LHG	C4-O6-P-O3
19	L	207	LHG	C4-O6-P-O4
19	M	102	LHG	O9-C7-O7-C5
19	X	101	LHG	C4-O6-P-O3
19	X	101	LHG	C4-O6-P-O4
19	X	102	LHG	C3-O3-P-O4
19	X	102	LHG	C3-O3-P-O6
19	N	851	LHG	C3-O3-P-O5
19	W	1506	LHG	C3-O3-P-O5
19	W	1506	LHG	C4-O6-P-O3
19	W	1506	LHG	C4-O6-P-O4
19	Y	101	LHG	O9-C7-O7-C5
19	Z	101	LHG	C3-O3-P-O4
19	Z	101	LHG	C3-O3-P-O6
19	Z	101	LHG	C4-O6-P-O3
19	Z	101	LHG	C4-O6-P-O4
19	Z	102	LHG	C3-O3-P-O4
19	Z	102	LHG	C3-O3-P-O6
19	j	207	LHG	C3-O3-P-O5
19	j	207	LHG	C3-O3-P-O6
19	j	207	LHG	C4-O6-P-O3
19	j	207	LHG	C4-O6-P-O4
19	k	101	LHG	O9-C7-O7-C5
19	l	101	LHG	C3-O3-P-O6
19	l	101	LHG	C4-O6-P-O3
19	l	101	LHG	C4-O6-P-O4
19	l	102	LHG	C3-O3-P-O4
19	l	102	LHG	C3-O3-P-O6
20	A	853	LMT	C2-C1-O1'-C1'
20	N	853	LMT	C2-C1-O1'-C1'
20	a	853	LMT	C2-C1-O1'-C1'
21	A	855	LMG	O9-C10-O7-C8
21	A	855	LMG	C11-C10-O7-C8
21	I	103	LMG	C11-C10-O7-C8
21	J	102	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
21	J	102	LMG	O6-C1-O1-C7
21	N	855	LMG	O9-C10-O7-C8
21	T	103	LMG	C11-C10-O7-C8
21	U	102	LMG	C2-C1-O1-C7
21	U	102	LMG	O6-C1-O1-C7
21	a	855	LMG	O9-C10-O7-C8
21	a	855	LMG	C11-C10-O7-C8
21	g	103	LMG	C11-C10-O7-C8
21	h	102	LMG	C2-C1-O1-C7
21	h	102	LMG	O6-C1-O1-C7
15	N	837	CLA	O1D-CGD-O2D-CED
14	A	826	F6C	C2C-C3C-CAC-CBC
15	A	812	CLA	O1D-CGD-O2D-CED
15	A	837	CLA	O1D-CGD-O2D-CED
15	N	806	CLA	O1D-CGD-O2D-CED
15	A	811	CLA	CBD-CGD-O2D-CED
15	A	812	CLA	CBD-CGD-O2D-CED
15	A	820	CLA	CBD-CGD-O2D-CED
15	B	801	CLA	CBD-CGD-O2D-CED
15	B	825	CLA	CBD-CGD-O2D-CED
15	B	828	CLA	CBD-CGD-O2D-CED
15	N	806	CLA	CBD-CGD-O2D-CED
15	N	811	CLA	CBD-CGD-O2D-CED
15	N	820	CLA	CBD-CGD-O2D-CED
15	O	814	CLA	CBD-CGD-O2D-CED
15	a	811	CLA	CBD-CGD-O2D-CED
15	b	801	CLA	CBD-CGD-O2D-CED
15	b	827	CLA	CBD-CGD-O2D-CED
14	A	857	F6C	O1A-CGA-O2A-C1
14	L	204	F6C	O1A-CGA-O2A-C1
14	N	856	F6C	O1A-CGA-O2A-C1
14	W	1503	F6C	O1A-CGA-O2A-C1
14	a	856	F6C	O1A-CGA-O2A-C1
14	j	204	F6C	O1A-CGA-O2A-C1
15	A	813	CLA	O1A-CGA-O2A-C1
15	B	808	CLA	O1A-CGA-O2A-C1
15	N	813	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	B	801	CLA	O1D-CGD-O2D-CED
15	a	837	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	b	801	CLA	O1D-CGD-O2D-CED
14	A	857	F6C	CBA-CGA-O2A-C1
14	L	204	F6C	CBA-CGA-O2A-C1
14	N	856	F6C	CBA-CGA-O2A-C1
14	j	204	F6C	CBA-CGA-O2A-C1
15	A	813	CLA	CBA-CGA-O2A-C1
15	B	808	CLA	CBA-CGA-O2A-C1
15	B	829	CLA	CBA-CGA-O2A-C1
15	N	813	CLA	CBA-CGA-O2A-C1
15	O	809	CLA	CBA-CGA-O2A-C1
15	O	831	CLA	CBA-CGA-O2A-C1
15	a	813	CLA	CBA-CGA-O2A-C1
15	b	809	CLA	CBA-CGA-O2A-C1
15	A	816	CLA	CBD-CGD-O2D-CED
15	A	820	CLA	O1A-CGA-O2A-C1
15	A	822	CLA	O1A-CGA-O2A-C1
15	A	842	CLA	O1A-CGA-O2A-C1
15	B	817	CLA	O1A-CGA-O2A-C1
15	B	825	CLA	O1A-CGA-O2A-C1
15	B	827	CLA	O1A-CGA-O2A-C1
15	B	829	CLA	O1A-CGA-O2A-C1
15	N	820	CLA	O1A-CGA-O2A-C1
15	N	822	CLA	O1A-CGA-O2A-C1
15	N	842	CLA	O1A-CGA-O2A-C1
15	O	819	CLA	O1A-CGA-O2A-C1
15	O	827	CLA	O1A-CGA-O2A-C1
15	O	829	CLA	O1A-CGA-O2A-C1
15	O	831	CLA	O1A-CGA-O2A-C1
15	a	842	CLA	O1A-CGA-O2A-C1
15	b	819	CLA	O1A-CGA-O2A-C1
15	b	827	CLA	O1A-CGA-O2A-C1
15	b	829	CLA	O1A-CGA-O2A-C1
15	b	831	CLA	O1A-CGA-O2A-C1
19	W	1506	LHG	O10-C23-O8-C6
19	j	207	LHG	O10-C23-O8-C6
19	l	102	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
14	A	826	F6C	C4C-C3C-CAC-CBC
15	A	807	CLA	O1D-CGD-O2D-CED
15	B	803	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	N	807	CLA	O1D-CGD-O2D-CED
15	N	812	CLA	O1D-CGD-O2D-CED
15	O	801	CLA	O1D-CGD-O2D-CED
15	O	820	CLA	O1D-CGD-O2D-CED
15	a	807	CLA	O1D-CGD-O2D-CED
15	a	812	CLA	O1D-CGD-O2D-CED
15	b	820	CLA	O1D-CGD-O2D-CED
15	B	805	CLA	O1D-CGD-O2D-CED
15	B	818	CLA	O1D-CGD-O2D-CED
15	K	102	CLA	O1D-CGD-O2D-CED
15	O	804	CLA	O1D-CGD-O2D-CED
15	O	806	CLA	O1D-CGD-O2D-CED
15	V	102	CLA	O1D-CGD-O2D-CED
15	b	804	CLA	O1D-CGD-O2D-CED
15	b	806	CLA	O1D-CGD-O2D-CED
15	b	814	CLA	O1D-CGD-O2D-CED
15	i	102	CLA	O1D-CGD-O2D-CED
15	O	830	CLA	CBD-CGD-O2D-CED
15	a	820	CLA	O1A-CGA-O2A-C1
19	L	207	LHG	O10-C23-O8-C6
21	I	103	LMG	O9-C10-O7-C8
21	g	103	LMG	O9-C10-O7-C8
14	A	826	F6C	C3-C5-C6-C7
14	a	826	F6C	C3-C5-C6-C7
15	A	813	CLA	C3-C5-C6-C7
15	A	829	CLA	C3-C5-C6-C7
15	A	831	CLA	C3-C5-C6-C7
15	A	836	CLA	C3-C5-C6-C7
15	A	856	CLA	C3-C5-C6-C7
15	B	818	CLA	C3-C5-C6-C7
15	B	821	CLA	C3-C5-C6-C7
15	B	823	CLA	C3-C5-C6-C7
15	B	827	CLA	C3-C5-C6-C7
15	B	828	CLA	C3-C5-C6-C7
15	N	804	CLA	C3-C5-C6-C7
15	N	813	CLA	C3-C5-C6-C7
15	N	829	CLA	C3-C5-C6-C7
15	N	831	CLA	C3-C5-C6-C7
15	N	836	CLA	C3-C5-C6-C7
15	N	839	CLA	C3-C5-C6-C7
15	N	841	CLA	C3-C5-C6-C7
15	O	802	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	O	804	CLA	C3-C5-C6-C7
15	O	820	CLA	C3-C5-C6-C7
15	O	823	CLA	C3-C5-C6-C7
15	O	829	CLA	C3-C5-C6-C7
15	O	830	CLA	C3-C5-C6-C7
15	a	813	CLA	C3-C5-C6-C7
15	a	829	CLA	C3-C5-C6-C7
15	a	831	CLA	C3-C5-C6-C7
15	a	836	CLA	C3-C5-C6-C7
15	b	802	CLA	C3-C5-C6-C7
15	b	820	CLA	C3-C5-C6-C7
15	b	825	CLA	C3-C5-C6-C7
15	b	829	CLA	C3-C5-C6-C7
15	b	830	CLA	C3-C5-C6-C7
15	b	831	CLA	C3-C5-C6-C7
14	N	826	F6C	C2C-C3C-CAC-CBC
15	B	812	CLA	O1D-CGD-O2D-CED
14	a	856	F6C	CBA-CGA-O2A-C1
15	B	805	CLA	CBA-CGA-O2A-C1
15	B	818	CLA	CBA-CGA-O2A-C1
15	B	825	CLA	CBA-CGA-O2A-C1
15	N	841	CLA	CBA-CGA-O2A-C1
15	O	806	CLA	CBA-CGA-O2A-C1
15	O	820	CLA	CBA-CGA-O2A-C1
15	O	825	CLA	CBA-CGA-O2A-C1
15	O	827	CLA	CBA-CGA-O2A-C1
15	b	806	CLA	CBA-CGA-O2A-C1
15	b	827	CLA	CBA-CGA-O2A-C1
15	b	831	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	806	CLA	CBD-CGD-O2D-CED
15	A	818	CLA	CBD-CGD-O2D-CED
15	A	822	CLA	CBD-CGD-O2D-CED
15	B	827	CLA	CBD-CGD-O2D-CED
15	X	103	CLA	CBD-CGD-O2D-CED
15	N	816	CLA	CBD-CGD-O2D-CED
15	N	818	CLA	CBD-CGD-O2D-CED
15	O	831	CLA	CBD-CGD-O2D-CED
15	W	1501	CLA	CBD-CGD-O2D-CED
15	a	816	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	a	820	CLA	CBD-CGD-O2D-CED
15	a	822	CLA	CBD-CGD-O2D-CED
15	b	830	CLA	CBD-CGD-O2D-CED
19	M	102	LHG	C8-C7-O7-C5
19	Y	101	LHG	C8-C7-O7-C5
19	k	101	LHG	C8-C7-O7-C5
21	N	855	LMG	C11-C10-O7-C8
15	O	827	CLA	O1D-CGD-O2D-CED
14	N	826	F6C	C4C-C3C-CAC-CBC
15	a	820	CLA	C2C-C3C-CAC-CBC
20	a	853	LMT	O5B-C1B-O1B-C4'
14	A	857	F6C	C4-C3-C5-C6
14	B	838	F6C	C4-C3-C5-C6
14	L	204	F6C	C4-C3-C5-C6
14	O	840	F6C	C4-C3-C5-C6
14	a	856	F6C	C4-C3-C5-C6
14	b	840	F6C	C4-C3-C5-C6
15	A	807	CLA	C4-C3-C5-C6
15	A	812	CLA	C4-C3-C5-C6
15	B	827	CLA	C4-C3-C5-C6
15	B	828	CLA	C4-C3-C5-C6
15	N	807	CLA	C4-C3-C5-C6
15	N	829	CLA	C4-C3-C5-C6
15	N	838	CLA	C4-C3-C5-C6
15	O	804	CLA	C4-C3-C5-C6
15	O	829	CLA	C4-C3-C5-C6
15	O	830	CLA	C4-C3-C5-C6
15	a	807	CLA	C4-C3-C5-C6
15	a	812	CLA	C4-C3-C5-C6
15	a	829	CLA	C4-C3-C5-C6
15	a	838	CLA	C4-C3-C5-C6
15	b	830	CLA	C4-C3-C5-C6
14	B	838	F6C	C2-C3-C5-C6
14	O	840	F6C	C2-C3-C5-C6
14	b	840	F6C	C2-C3-C5-C6
15	A	807	CLA	C2-C3-C5-C6
15	A	812	CLA	C2-C3-C5-C6
15	A	814	CLA	C2-C3-C5-C6
15	A	838	CLA	C2-C3-C5-C6
15	B	827	CLA	C2-C3-C5-C6
15	N	807	CLA	C2-C3-C5-C6
15	N	812	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	N	814	CLA	C2-C3-C5-C6
15	N	829	CLA	C2-C3-C5-C6
15	N	838	CLA	C2-C3-C5-C6
15	O	825	CLA	C2-C3-C5-C6
15	O	829	CLA	C2-C3-C5-C6
15	O	830	CLA	C2-C3-C5-C6
15	a	807	CLA	C2-C3-C5-C6
15	a	812	CLA	C2-C3-C5-C6
15	a	838	CLA	C2-C3-C5-C6
15	b	829	CLA	C2-C3-C5-C6
15	b	830	CLA	C2-C3-C5-C6
14	a	826	F6C	C2C-C3C-CAC-CBC
15	a	820	CLA	C4C-C3C-CAC-CBC
15	O	841	CLA	CBD-CGD-O2D-CED
15	b	827	CLA	O1D-CGD-O2D-CED
14	B	831	F6C	C3A-C2A-CAA-CBA
15	B	803	CLA	C3-C5-C6-C7
15	O	825	CLA	C3-C5-C6-C7
15	a	825	CLA	C3-C5-C6-C7
15	a	841	CLA	C3-C5-C6-C7
15	b	823	CLA	C3-C5-C6-C7
15	A	820	CLA	CBA-CGA-O2A-C1
15	A	822	CLA	CBA-CGA-O2A-C1
15	A	837	CLA	CBA-CGA-O2A-C1
15	A	842	CLA	CBA-CGA-O2A-C1
15	B	816	CLA	CBA-CGA-O2A-C1
15	B	817	CLA	CBA-CGA-O2A-C1
15	B	823	CLA	CBA-CGA-O2A-C1
15	B	827	CLA	CBA-CGA-O2A-C1
15	N	820	CLA	CBA-CGA-O2A-C1
15	N	822	CLA	CBA-CGA-O2A-C1
15	N	837	CLA	CBA-CGA-O2A-C1
15	N	842	CLA	CBA-CGA-O2A-C1
15	O	818	CLA	CBA-CGA-O2A-C1
15	O	819	CLA	CBA-CGA-O2A-C1
15	O	829	CLA	CBA-CGA-O2A-C1
15	a	820	CLA	CBA-CGA-O2A-C1
15	a	837	CLA	CBA-CGA-O2A-C1
15	a	842	CLA	CBA-CGA-O2A-C1
15	b	818	CLA	CBA-CGA-O2A-C1
15	b	819	CLA	CBA-CGA-O2A-C1
15	b	820	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	b	825	CLA	CBA-CGA-O2A-C1
15	b	829	CLA	CBA-CGA-O2A-C1
19	L	207	LHG	C24-C23-O8-C6
19	W	1506	LHG	C24-C23-O8-C6
19	j	207	LHG	C24-C23-O8-C6
19	l	102	LHG	C24-C23-O8-C6
20	A	853	LMT	O5B-C1B-O1B-C4'
15	A	837	CLA	O1A-CGA-O2A-C1
15	B	805	CLA	O1A-CGA-O2A-C1
15	B	823	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	820	CLA	O1A-CGA-O2A-C1
15	O	825	CLA	O1A-CGA-O2A-C1
15	a	837	CLA	O1A-CGA-O2A-C1
15	b	806	CLA	O1A-CGA-O2A-C1
15	b	825	CLA	O1A-CGA-O2A-C1
19	X	102	LHG	O10-C23-O8-C6
15	N	820	CLA	C2C-C3C-CAC-CBC
14	A	802	F6C	C1A-C2A-CAA-CBA
14	A	826	F6C	C1A-C2A-CAA-CBA
14	A	857	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
21	T	103	LMG	O9-C10-O7-C8
15	N	811	CLA	O1D-CGD-O2D-CED
14	N	826	F6C	C3-C5-C6-C7
14	b	810	F6C	C3-C5-C6-C7
15	A	804	CLA	C3-C5-C6-C7
15	A	841	CLA	C3-C5-C6-C7
15	B	808	CLA	C3-C5-C6-C7
15	B	829	CLA	C3-C5-C6-C7
15	F	201	CLA	C3-C5-C6-C7
15	S	201	CLA	C3-C5-C6-C7
15	a	804	CLA	C3-C5-C6-C7
15	b	804	CLA	C3-C5-C6-C7
15	f	201	CLA	C3-C5-C6-C7
15	B	802	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	O	829	CLA	CBD-CGD-O2D-CED
15	a	803	CLA	CBD-CGD-O2D-CED
15	a	818	CLA	CBD-CGD-O2D-CED
15	b	829	CLA	CBD-CGD-O2D-CED
15	A	820	CLA	C2C-C3C-CAC-CBC
15	B	825	CLA	O1D-CGD-O2D-CED
15	O	814	CLA	O1D-CGD-O2D-CED
15	a	811	CLA	O1D-CGD-O2D-CED
15	B	809	CLA	CBA-CGA-O2A-C1
15	O	811	CLA	CBA-CGA-O2A-C1
15	O	841	CLA	CBA-CGA-O2A-C1
15	a	804	CLA	CBA-CGA-O2A-C1
15	a	822	CLA	CBA-CGA-O2A-C1
15	b	811	CLA	CBA-CGA-O2A-C1
15	b	834	CLA	CBA-CGA-O2A-C1
15	b	841	CLA	CBA-CGA-O2A-C1
19	X	102	LHG	C24-C23-O8-C6
19	Z	102	LHG	C24-C23-O8-C6
14	a	826	F6C	C4C-C3C-CAC-CBC
15	B	816	CLA	O1A-CGA-O2A-C1
15	B	818	CLA	O1A-CGA-O2A-C1
15	O	818	CLA	O1A-CGA-O2A-C1
15	a	822	CLA	O1A-CGA-O2A-C1
15	b	820	CLA	O1A-CGA-O2A-C1
19	Z	102	LHG	O10-C23-O8-C6
15	A	819	CLA	CBD-CGD-O2D-CED
15	N	819	CLA	CBD-CGD-O2D-CED
15	N	836	CLA	CBD-CGD-O2D-CED
15	O	803	CLA	CBD-CGD-O2D-CED
15	Z	103	CLA	CBD-CGD-O2D-CED
15	b	841	CLA	CBD-CGD-O2D-CED
15	N	820	CLA	C4C-C3C-CAC-CBC
15	A	811	CLA	O1D-CGD-O2D-CED
14	L	201	F6C	C3-C5-C6-C7
14	O	810	F6C	C3-C5-C6-C7
15	N	825	CLA	C3-C5-C6-C7
15	A	836	CLA	CBD-CGD-O2D-CED
15	B	839	CLA	CBD-CGD-O2D-CED
15	N	803	CLA	CBD-CGD-O2D-CED
15	a	819	CLA	CBD-CGD-O2D-CED
15	A	820	CLA	O1D-CGD-O2D-CED
15	B	828	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	N	820	CLA	O1D-CGD-O2D-CED
14	j	204	F6C	C4-C3-C5-C6
15	A	829	CLA	C4-C3-C5-C6
15	B	805	CLA	C4-C3-C5-C6
15	N	818	CLA	C4-C3-C5-C6
15	O	806	CLA	C4-C3-C5-C6
15	b	804	CLA	C4-C3-C5-C6
15	b	806	CLA	C4-C3-C5-C6
14	A	857	F6C	C2-C3-C5-C6
14	L	204	F6C	C2-C3-C5-C6
14	N	856	F6C	C2-C3-C5-C6
15	B	805	CLA	C2-C3-C5-C6
15	B	828	CLA	C2-C3-C5-C6
15	N	818	CLA	C2-C3-C5-C6
15	O	806	CLA	C2-C3-C5-C6
15	a	829	CLA	C2-C3-C5-C6
15	b	804	CLA	C2-C3-C5-C6
15	b	806	CLA	C2-C3-C5-C6
15	b	818	CLA	O1A-CGA-O2A-C1
15	A	803	CLA	CBD-CGD-O2D-CED
15	A	838	CLA	CBD-CGD-O2D-CED
15	N	825	CLA	CBD-CGD-O2D-CED
15	a	829	CLA	CBD-CGD-O2D-CED
15	b	834	CLA	CBD-CGD-O2D-CED
14	O	833	F6C	C3A-C2A-CAA-CBA
14	b	833	F6C	C3A-C2A-CAA-CBA
14	A	857	F6C	C2A-CAA-CBA-CGA
14	B	838	F6C	C2A-CAA-CBA-CGA
14	O	840	F6C	C2A-CAA-CBA-CGA
14	b	840	F6C	C2A-CAA-CBA-CGA
15	B	809	CLA	O1A-CGA-O2A-C1
15	O	811	CLA	O1A-CGA-O2A-C1
15	a	804	CLA	O1A-CGA-O2A-C1
15	b	811	CLA	O1A-CGA-O2A-C1
15	b	834	CLA	O1A-CGA-O2A-C1
15	b	841	CLA	O1A-CGA-O2A-C1
15	B	832	CLA	CBA-CGA-O2A-C1
15	B	839	CLA	CBA-CGA-O2A-C1
15	O	804	CLA	CBA-CGA-O2A-C1
15	O	834	CLA	CBA-CGA-O2A-C1
15	a	811	CLA	CBA-CGA-O2A-C1
15	a	829	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	b	804	CLA	CBA-CGA-O2A-C1
14	a	802	F6C	CBD-CGD-O2D-CED
15	A	829	CLA	CBD-CGD-O2D-CED
15	A	835	CLA	CBD-CGD-O2D-CED
15	B	815	CLA	CBD-CGD-O2D-CED
15	N	822	CLA	CBD-CGD-O2D-CED
15	O	834	CLA	CBD-CGD-O2D-CED
15	a	823	CLA	CBD-CGD-O2D-CED
15	a	825	CLA	CBD-CGD-O2D-CED
15	a	834	CLA	CBD-CGD-O2D-CED
15	a	836	CLA	CBD-CGD-O2D-CED
20	N	853	LMT	O5B-C1B-O1B-C4'
15	O	841	CLA	O1A-CGA-O2A-C1
15	A	816	CLA	O1D-CGD-O2D-CED
15	B	832	CLA	CBD-CGD-O2D-CED
15	N	829	CLA	CBD-CGD-O2D-CED
15	a	835	CLA	CBD-CGD-O2D-CED
15	b	802	CLA	CBD-CGD-O2D-CED
15	b	821	CLA	CBD-CGD-O2D-CED
15	b	835	CLA	CBD-CGD-O2D-CED
15	A	820	CLA	C4C-C3C-CAC-CBC
15	b	806	CLA	C3-C5-C6-C7
15	B	803	CLA	O1A-CGA-O2A-C1
15	B	832	CLA	O1A-CGA-O2A-C1
15	B	839	CLA	O1A-CGA-O2A-C1
15	O	804	CLA	O1A-CGA-O2A-C1
15	O	834	CLA	O1A-CGA-O2A-C1
15	b	804	CLA	O1A-CGA-O2A-C1
15	A	804	CLA	CBA-CGA-O2A-C1
15	A	809	CLA	CBA-CGA-O2A-C1
15	A	811	CLA	CBA-CGA-O2A-C1
15	A	823	CLA	CBA-CGA-O2A-C1
15	A	829	CLA	CBA-CGA-O2A-C1
15	A	831	CLA	CBA-CGA-O2A-C1
15	B	803	CLA	CBA-CGA-O2A-C1
15	N	804	CLA	CBA-CGA-O2A-C1
15	N	811	CLA	CBA-CGA-O2A-C1
15	N	829	CLA	CBA-CGA-O2A-C1
15	N	831	CLA	CBA-CGA-O2A-C1
15	a	823	CLA	CBA-CGA-O2A-C1
15	a	831	CLA	CBA-CGA-O2A-C1
21	U	102	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
15	O	839	CLA	CBD-CGD-O2D-CED
15	a	838	CLA	CBD-CGD-O2D-CED
15	B	827	CLA	O1D-CGD-O2D-CED
15	N	816	CLA	O1D-CGD-O2D-CED
15	O	830	CLA	O1D-CGD-O2D-CED
15	b	830	CLA	O1D-CGD-O2D-CED
14	N	856	F6C	C4-C3-C5-C6
15	A	818	CLA	C4-C3-C5-C6
15	B	803	CLA	C4-C3-C5-C6
15	a	818	CLA	C4-C3-C5-C6
14	a	856	F6C	C2-C3-C5-C6
14	j	204	F6C	C2-C3-C5-C6
15	A	818	CLA	C2-C3-C5-C6
15	B	803	CLA	C2-C3-C5-C6
15	O	804	CLA	C2-C3-C5-C6
15	a	818	CLA	C2-C3-C5-C6
15	O	831	CLA	C3-C5-C6-C7
15	a	810	CLA	C3-C5-C6-C7
15	B	822	CLA	CBD-CGD-O2D-CED
15	N	834	CLA	CBD-CGD-O2D-CED
15	N	838	CLA	CBD-CGD-O2D-CED
15	b	824	CLA	CBD-CGD-O2D-CED
14	A	857	F6C	C6-C7-C8-C9
14	A	857	F6C	C11-C10-C8-C9
14	N	856	F6C	C6-C7-C8-C9
14	N	856	F6C	C11-C10-C8-C9
14	a	856	F6C	C6-C7-C8-C9
14	a	856	F6C	C11-C10-C8-C9
15	B	812	CLA	C11-C12-C13-C14
15	B	828	CLA	C11-C12-C13-C14
15	B	839	CLA	C11-C12-C13-C14
15	F	201	CLA	C6-C7-C8-C9
15	L	203	CLA	C11-C10-C8-C9
15	S	201	CLA	C6-C7-C8-C9
15	W	1502	CLA	C11-C10-C8-C9
15	b	814	CLA	C11-C12-C13-C14
15	b	830	CLA	C11-C12-C13-C14
15	f	201	CLA	C6-C7-C8-C9
15	A	806	CLA	O1D-CGD-O2D-CED
15	A	822	CLA	O1D-CGD-O2D-CED
15	a	820	CLA	O1D-CGD-O2D-CED
15	b	805	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	A	804	CLA	O1A-CGA-O2A-C1
15	A	831	CLA	O1A-CGA-O2A-C1
15	N	804	CLA	O1A-CGA-O2A-C1
15	N	831	CLA	O1A-CGA-O2A-C1
15	a	831	CLA	O1A-CGA-O2A-C1
14	a	824	F6C	CBD-CGD-O2D-CED
15	B	834	CLA	CBD-CGD-O2D-CED
15	l	103	CLA	CBD-CGD-O2D-CED
18	A	845	BCR	C36-C18-C19-C20
18	A	846	BCR	C7-C8-C9-C34
18	A	848	BCR	C36-C18-C19-C20
18	A	849	BCR	C37-C22-C23-C24
18	A	850	BCR	C36-C18-C19-C20
18	A	858	BCR	C7-C8-C9-C34
18	B	841	BCR	C37-C22-C23-C24
18	B	842	BCR	C37-C22-C23-C24
18	F	202	BCR	C36-C18-C19-C20
18	I	101	BCR	C7-C8-C9-C34
18	I	101	BCR	C11-C12-C13-C35
18	J	101	BCR	C37-C22-C23-C24
18	L	205	BCR	C7-C8-C9-C34
18	N	845	BCR	C36-C18-C19-C20
18	N	846	BCR	C7-C8-C9-C34
18	N	848	BCR	C36-C18-C19-C20
18	N	850	BCR	C7-C8-C9-C34
18	N	850	BCR	C36-C18-C19-C20
18	O	843	BCR	C37-C22-C23-C24
18	O	844	BCR	C37-C22-C23-C24
18	O	846	BCR	C7-C8-C9-C34
18	O	848	BCR	C11-C12-C13-C35
18	O	848	BCR	C37-C22-C23-C24
18	T	101	BCR	C37-C22-C23-C24
18	U	101	BCR	C37-C22-C23-C24
18	a	845	BCR	C36-C18-C19-C20
18	a	846	BCR	C7-C8-C9-C34
18	a	848	BCR	C36-C18-C19-C20
18	a	850	BCR	C7-C8-C9-C34
18	a	850	BCR	C36-C18-C19-C20
18	b	843	BCR	C37-C22-C23-C24
18	b	844	BCR	C37-C22-C23-C24
18	b	846	BCR	C7-C8-C9-C34
18	f	202	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
18	f	202	BCR	C36-C18-C19-C20
18	h	101	BCR	C37-C22-C23-C24
18	j	205	BCR	C7-C8-C9-C34
18	A	846	BCR	C7-C8-C9-C10
18	A	849	BCR	C21-C22-C23-C24
18	B	841	BCR	C21-C22-C23-C24
18	N	846	BCR	C7-C8-C9-C10
18	O	843	BCR	C21-C22-C23-C24
18	O	846	BCR	C7-C8-C9-C10
18	W	1504	BCR	C21-C22-C23-C24
18	a	846	BCR	C7-C8-C9-C10
18	b	843	BCR	C21-C22-C23-C24
18	b	846	BCR	C7-C8-C9-C10
15	A	830	CLA	C2A-CAA-CBA-CGA
15	N	809	CLA	C2A-CAA-CBA-CGA
15	N	830	CLA	C2A-CAA-CBA-CGA
15	N	839	CLA	C2A-CAA-CBA-CGA
15	O	828	CLA	C2A-CAA-CBA-CGA
15	O	830	CLA	C2A-CAA-CBA-CGA
15	a	830	CLA	C2A-CAA-CBA-CGA
15	a	823	CLA	O1A-CGA-O2A-C1
15	A	806	CLA	C3-C5-C6-C7
15	B	805	CLA	C3-C5-C6-C7
15	a	806	CLA	C3-C5-C6-C7
19	X	101	LHG	O7-C5-C6-O8
19	l	101	LHG	O7-C5-C6-O8
15	N	833	CLA	CBA-CGA-O2A-C1
15	N	838	CLA	CBA-CGA-O2A-C1
19	Z	101	LHG	C23-C24-C25-C26
19	Z	102	LHG	C7-C8-C9-C10
15	b	829	CLA	C2-C1-O2A-CGA
15	O	829	CLA	C10-C11-C12-C13
15	O	841	CLA	C15-C16-C17-C18
15	b	829	CLA	C10-C11-C12-C13
15	N	830	CLA	C8-C10-C11-C12
15	A	818	CLA	C11-C12-C13-C15
15	A	856	CLA	C6-C7-C8-C10
15	B	809	CLA	C12-C13-C15-C16
15	B	828	CLA	C11-C10-C8-C7
15	N	818	CLA	C11-C12-C13-C15
15	O	802	CLA	C6-C7-C8-C10
15	O	811	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	a	818	CLA	C11-C12-C13-C15
15	b	802	CLA	C6-C7-C8-C10
15	b	830	CLA	C11-C10-C8-C7
15	A	821	CLA	CBA-CGA-O2A-C1
15	B	804	CLA	CBA-CGA-O2A-C1
15	N	821	CLA	CBA-CGA-O2A-C1
15	O	805	CLA	CBA-CGA-O2A-C1
15	a	821	CLA	CBA-CGA-O2A-C1
15	A	822	CLA	C4-C3-C5-C6
15	O	827	CLA	C4-C3-C5-C6
15	b	827	CLA	C4-C3-C5-C6
15	B	827	CLA	C10-C11-C12-C13
15	a	819	CLA	C15-C16-C17-C18
15	b	830	CLA	C5-C6-C7-C8
15	X	103	CLA	O1D-CGD-O2D-CED
19	X	102	LHG	C7-C8-C9-C10
14	a	856	F6C	C1A-C2A-CAA-CBA
15	A	810	CLA	C3-C5-C6-C7
15	O	806	CLA	C3-C5-C6-C7
15	O	808	CLA	C3-C5-C6-C7
15	A	819	CLA	C15-C16-C17-C18
15	B	828	CLA	C5-C6-C7-C8
15	O	814	CLA	C10-C11-C12-C13
15	O	830	CLA	C8-C10-C11-C12
19	A	851	LHG	C23-C24-C25-C26
19	X	101	LHG	C23-C24-C25-C26
19	X	102	LHG	C23-C24-C25-C26
19	a	851	LHG	C23-C24-C25-C26
15	A	809	CLA	O1A-CGA-O2A-C1
15	N	811	CLA	O1A-CGA-O2A-C1
15	b	805	CLA	O1A-CGA-O2A-C1
15	A	825	CLA	CBD-CGD-O2D-CED
15	B	830	CLA	CBD-CGD-O2D-CED
15	O	817	CLA	CBD-CGD-O2D-CED
15	O	831	CLA	O1D-CGD-O2D-CED
15	W	1501	CLA	O1D-CGD-O2D-CED
15	a	822	CLA	O1D-CGD-O2D-CED
14	L	204	F6C	C8-C10-C11-C12
14	a	802	F6C	C15-C16-C17-C18
14	b	833	F6C	C15-C16-C17-C18
14	j	204	F6C	C8-C10-C11-C12
15	A	812	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	A	812	CLA	C15-C16-C17-C18
15	A	819	CLA	C10-C11-C12-C13
15	A	820	CLA	C5-C6-C7-C8
15	A	830	CLA	C8-C10-C11-C12
15	N	812	CLA	C15-C16-C17-C18
15	O	838	CLA	C8-C10-C11-C12
15	W	1501	CLA	C13-C15-C16-C17
15	a	812	CLA	C5-C6-C7-C8
15	b	811	CLA	C5-C6-C7-C8
15	b	814	CLA	C10-C11-C12-C13
15	b	838	CLA	C8-C10-C11-C12
15	b	841	CLA	C15-C16-C17-C18
15	j	202	CLA	C13-C15-C16-C17
15	A	809	CLA	C2A-CAA-CBA-CGA
15	A	812	CLA	C2A-CAA-CBA-CGA
15	A	839	CLA	C2A-CAA-CBA-CGA
15	B	828	CLA	C2A-CAA-CBA-CGA
15	N	812	CLA	C2A-CAA-CBA-CGA
15	a	809	CLA	C2A-CAA-CBA-CGA
15	a	812	CLA	C2A-CAA-CBA-CGA
15	a	839	CLA	C2A-CAA-CBA-CGA
15	b	828	CLA	C2A-CAA-CBA-CGA
15	b	830	CLA	C2A-CAA-CBA-CGA
14	A	802	F6C	C15-C16-C17-C18
15	A	803	CLA	C13-C15-C16-C17
15	A	809	CLA	C5-C6-C7-C8
15	A	810	CLA	C5-C6-C7-C8
15	B	809	CLA	C5-C6-C7-C8
15	B	836	CLA	C8-C10-C11-C12
15	N	803	CLA	C13-C15-C16-C17
15	N	812	CLA	C5-C6-C7-C8
15	N	812	CLA	C10-C11-C12-C13
15	N	820	CLA	C5-C6-C7-C8
15	O	830	CLA	C5-C6-C7-C8
15	O	832	CLA	C10-C11-C12-C13
15	a	812	CLA	C15-C16-C17-C18
15	b	803	CLA	C15-C16-C17-C18
15	b	811	CLA	C13-C15-C16-C17
15	b	817	CLA	C13-C15-C16-C17
19	Z	102	LHG	C23-C24-C25-C26
19	l	102	LHG	C23-C24-C25-C26
21	T	103	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
21	g	103	LMG	C28-C29-C30-C31
15	a	816	CLA	O1D-CGD-O2D-CED
15	A	823	CLA	O1A-CGA-O2A-C1
15	A	829	CLA	O1A-CGA-O2A-C1
14	N	856	F6C	C3-C5-C6-C7
15	N	806	CLA	C3-C5-C6-C7
15	N	820	CLA	C3-C5-C6-C7
15	a	820	CLA	C3-C5-C6-C7
21	J	102	LMG	C19-C20-C21-C22
15	A	818	CLA	O1D-CGD-O2D-CED
14	B	831	F6C	C15-C16-C17-C18
14	O	833	F6C	C15-C16-C17-C18
15	A	811	CLA	C5-C6-C7-C8
15	B	812	CLA	C5-C6-C7-C8
15	B	812	CLA	C10-C11-C12-C13
15	B	830	CLA	C10-C11-C12-C13
15	N	811	CLA	C5-C6-C7-C8
15	N	819	CLA	C10-C11-C12-C13
15	N	819	CLA	C15-C16-C17-C18
15	O	811	CLA	C5-C6-C7-C8
15	O	814	CLA	C5-C6-C7-C8
15	O	817	CLA	C13-C15-C16-C17
15	a	803	CLA	C13-C15-C16-C17
15	a	820	CLA	C5-C6-C7-C8
15	a	830	CLA	C8-C10-C11-C12
15	b	814	CLA	C5-C6-C7-C8
15	b	832	CLA	C10-C11-C12-C13
20	A	853	LMT	O1'-C1-C2-C3
15	N	818	CLA	O1D-CGD-O2D-CED
15	A	811	CLA	O1A-CGA-O2A-C1
15	N	829	CLA	O1A-CGA-O2A-C1
15	a	811	CLA	O1A-CGA-O2A-C1
15	a	829	CLA	O1A-CGA-O2A-C1
15	A	810	CLA	C8-C10-C11-C12
15	a	810	CLA	C8-C10-C11-C12
19	l	101	LHG	C23-C24-C25-C26
19	l	102	LHG	C7-C8-C9-C10
15	A	812	CLA	C10-C11-C12-C13
15	A	819	CLA	C8-C10-C11-C12
15	a	810	CLA	C5-C6-C7-C8
15	a	812	CLA	C10-C11-C12-C13
15	O	841	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	N	854	LMT	C7-C8-C9-C10
15	B	802	CLA	O1D-CGD-O2D-CED
15	O	829	CLA	O1D-CGD-O2D-CED
14	N	802	F6C	C15-C16-C17-C18
14	W	1503	F6C	C8-C10-C11-C12
15	B	828	CLA	C8-C10-C11-C12
15	N	819	CLA	C8-C10-C11-C12
15	N	839	CLA	C13-C15-C16-C17
15	a	819	CLA	C8-C10-C11-C12
15	N	833	CLA	O1A-CGA-O2A-C1
15	a	818	CLA	O1D-CGD-O2D-CED
15	b	829	CLA	O1D-CGD-O2D-CED
14	A	857	F6C	C10-C11-C12-C13
14	a	856	F6C	C10-C11-C12-C13
15	A	839	CLA	C13-C15-C16-C17
15	B	802	CLA	C15-C16-C17-C18
15	a	839	CLA	C13-C15-C16-C17
15	A	838	CLA	CBA-CGA-O2A-C1
15	B	812	CLA	CBA-CGA-O2A-C1
15	B	826	CLA	CBA-CGA-O2A-C1
15	N	809	CLA	CBA-CGA-O2A-C1
15	N	823	CLA	CBA-CGA-O2A-C1
15	O	814	CLA	CBA-CGA-O2A-C1
15	a	809	CLA	CBA-CGA-O2A-C1
15	b	814	CLA	CBA-CGA-O2A-C1
15	b	828	CLA	CBA-CGA-O2A-C1
15	b	838	CLA	CBA-CGA-O2A-C1
15	O	824	CLA	CBD-CGD-O2D-CED
15	O	836	CLA	CBD-CGD-O2D-CED
15	b	803	CLA	CBD-CGD-O2D-CED
15	B	804	CLA	O1A-CGA-O2A-C1
14	a	856	F6C	C3-C5-C6-C7
15	B	816	CLA	C3-C5-C6-C7
15	O	834	CLA	C3-C5-C6-C7
15	a	822	CLA	C3-C5-C6-C7
15	b	818	CLA	C3-C5-C6-C7
15	B	819	CLA	CBD-CGD-O2D-CED
20	A	854	LMT	C7-C8-C9-C10
15	O	839	CLA	C5-C6-C7-C8
15	N	821	CLA	O1A-CGA-O2A-C1
15	N	838	CLA	O1A-CGA-O2A-C1
15	O	805	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	N	853	LMT	C2B-C1B-O1B-C4'
15	B	826	CLA	C2A-CAA-CBA-CGA
15	A	833	CLA	CBA-CGA-O2A-C1
15	O	828	CLA	CBA-CGA-O2A-C1
15	O	838	CLA	CBA-CGA-O2A-C1
15	a	833	CLA	CBA-CGA-O2A-C1
15	a	838	CLA	CBA-CGA-O2A-C1
20	a	854	LMT	C3-C4-C5-C6
20	a	854	LMT	C7-C8-C9-C10
14	N	826	F6C	C10-C11-C12-C13
15	A	831	CLA	C10-C11-C12-C13
15	B	821	CLA	C5-C6-C7-C8
15	B	823	CLA	C13-C15-C16-C17
15	N	818	CLA	C8-C10-C11-C12
15	N	822	CLA	C5-C6-C7-C8
15	O	825	CLA	C13-C15-C16-C17
15	a	811	CLA	C5-C6-C7-C8
15	a	819	CLA	C10-C11-C12-C13
15	a	822	CLA	C8-C10-C11-C12
15	b	825	CLA	C13-C15-C16-C17
15	N	823	CLA	CBD-CGD-O2D-CED
15	O	823	CLA	CBD-CGD-O2D-CED
15	b	816	CLA	CBD-CGD-O2D-CED
15	O	803	CLA	O1D-CGD-O2D-CED
15	Z	103	CLA	O1D-CGD-O2D-CED
15	a	803	CLA	O1D-CGD-O2D-CED
14	A	826	F6C	C10-C11-C12-C13
14	a	826	F6C	C10-C11-C12-C13
15	A	818	CLA	C8-C10-C11-C12
15	B	808	CLA	C5-C6-C7-C8
15	B	827	CLA	C8-C10-C11-C12
15	B	837	CLA	C5-C6-C7-C8
15	O	808	CLA	C10-C11-C12-C13
15	O	823	CLA	C5-C6-C7-C8
15	a	809	CLA	C5-C6-C7-C8
15	b	829	CLA	C8-C10-C11-C12
15	b	839	CLA	C5-C6-C7-C8
15	A	822	CLA	C8-C10-C11-C12
15	L	202	CLA	C13-C15-C16-C17
15	N	829	CLA	C8-C10-C11-C12
15	a	806	CLA	C8-C10-C11-C12
15	a	818	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
15	b	830	CLA	C8-C10-C11-C12
15	j	202	CLA	C10-C11-C12-C13
15	B	836	CLA	CBA-CGA-O2A-C1
15	N	810	CLA	C8-C10-C11-C12
21	I	103	LMG	C28-C29-C30-C31
15	b	825	CLA	C4-C3-C5-C6
15	N	836	CLA	O1D-CGD-O2D-CED
15	b	841	CLA	O1D-CGD-O2D-CED
15	A	806	CLA	C8-C10-C11-C12
15	A	822	CLA	C5-C6-C7-C8
15	B	839	CLA	C15-C16-C17-C18
15	N	806	CLA	C8-C10-C11-C12
15	N	809	CLA	C5-C6-C7-C8
15	O	829	CLA	C8-C10-C11-C12
15	b	823	CLA	C5-C6-C7-C8
15	N	822	CLA	C3-C5-C6-C7
15	O	818	CLA	C3-C5-C6-C7
15	N	841	CLA	CBD-CGD-O2D-CED
15	N	819	CLA	O1D-CGD-O2D-CED
15	a	821	CLA	O1A-CGA-O2A-C1
15	N	803	CLA	O1D-CGD-O2D-CED
20	A	854	LMT	C3-C4-C5-C6
15	A	819	CLA	O1D-CGD-O2D-CED
15	N	810	CLA	C5-C6-C7-C8
15	A	821	CLA	O1A-CGA-O2A-C1
15	N	835	CLA	CBD-CGD-O2D-CED
15	O	821	CLA	CBD-CGD-O2D-CED
15	a	829	CLA	C8-C10-C11-C12
18	B	844	BCR	C7-C8-C9-C34
18	F	202	BCR	C11-C12-C13-C35
18	L	205	BCR	C37-C22-C23-C24
18	M	101	BCR	C36-C18-C19-C20
18	N	849	BCR	C37-C22-C23-C24
18	Y	102	BCR	C36-C18-C19-C20
18	a	849	BCR	C37-C22-C23-C24
18	a	857	BCR	C7-C8-C9-C34
18	k	102	BCR	C36-C18-C19-C20
14	A	824	F6C	C3A-C2A-CAA-CBA
18	B	844	BCR	C7-C8-C9-C10
18	N	849	BCR	C21-C22-C23-C24
18	a	849	BCR	C21-C22-C23-C24
18	a	850	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
15	B	812	CLA	O1A-CGA-O2A-C1
15	B	826	CLA	O1A-CGA-O2A-C1
15	O	814	CLA	O1A-CGA-O2A-C1
20	N	854	LMT	C3-C4-C5-C6
15	A	813	CLA	C2A-CAA-CBA-CGA
15	A	831	CLA	C2A-CAA-CBA-CGA
15	B	820	CLA	C2A-CAA-CBA-CGA
15	N	813	CLA	C2A-CAA-CBA-CGA
15	N	831	CLA	C2A-CAA-CBA-CGA
15	a	813	CLA	C2A-CAA-CBA-CGA
15	a	831	CLA	C2A-CAA-CBA-CGA
15	b	822	CLA	C2A-CAA-CBA-CGA
15	N	831	CLA	C10-C11-C12-C13
13	N	801	CL0	C16-C17-C18-C19
13	N	801	CL0	C16-C17-C18-C20
13	a	801	CL0	C16-C17-C18-C19
15	A	803	CLA	C16-C17-C18-C20
15	B	816	CLA	C11-C12-C13-C15
15	N	803	CLA	C16-C17-C18-C20
15	b	802	CLA	C16-C17-C18-C20
15	b	818	CLA	C11-C12-C13-C15
15	A	836	CLA	O1D-CGD-O2D-CED
15	B	839	CLA	O1D-CGD-O2D-CED
15	a	809	CLA	O1A-CGA-O2A-C1
15	b	814	CLA	O1A-CGA-O2A-C1
14	A	857	F6C	C3-C5-C6-C7
15	N	810	CLA	C3-C5-C6-C7
15	N	818	CLA	C3-C5-C6-C7
15	b	834	CLA	C3-C5-C6-C7
20	N	853	LMT	O5'-C1'-O1'-C1
19	N	851	LHG	C23-C24-C25-C26
15	A	829	CLA	C2-C3-C5-C6
15	b	834	CLA	O1D-CGD-O2D-CED
15	A	803	CLA	O1D-CGD-O2D-CED
15	a	819	CLA	O1D-CGD-O2D-CED
15	S	201	CLA	CBA-CGA-O2A-C1
15	b	818	CLA	C10-C11-C12-C13
15	O	802	CLA	CBD-CGD-O2D-CED
15	B	827	CLA	C2-C1-O2A-CGA
15	O	829	CLA	C2-C1-O2A-CGA
13	a	801	CL0	C16-C17-C18-C20
14	b	810	F6C	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	A	803	CLA	C16-C17-C18-C19
15	A	829	CLA	C11-C12-C13-C14
15	A	842	CLA	C16-C17-C18-C19
15	A	856	CLA	C16-C17-C18-C20
15	N	829	CLA	C11-C12-C13-C14
15	O	818	CLA	C11-C12-C13-C15
15	a	803	CLA	C16-C17-C18-C20
15	a	829	CLA	C11-C12-C13-C14
15	a	842	CLA	C16-C17-C18-C19
15	b	802	CLA	C16-C17-C18-C19
15	A	833	CLA	O1A-CGA-O2A-C1
15	a	833	CLA	O1A-CGA-O2A-C1
15	a	838	CLA	O1A-CGA-O2A-C1
15	b	838	CLA	O1A-CGA-O2A-C1
15	A	838	CLA	O1D-CGD-O2D-CED
21	J	102	LMG	O6-C5-C6-O5
19	k	101	LHG	C12-C13-C14-C15
21	T	103	LMG	C11-C12-C13-C14
15	A	817	CLA	CBD-CGD-O2D-CED
21	B	847	LMG	C22-C23-C24-C25
21	I	103	LMG	C11-C12-C13-C14
21	O	850	LMG	C22-C23-C24-C25
15	N	825	CLA	O1D-CGD-O2D-CED
15	a	829	CLA	O1D-CGD-O2D-CED
15	A	839	CLA	C8-C10-C11-C12
21	U	102	LMG	C39-C40-C41-C42
15	N	809	CLA	O1A-CGA-O2A-C1
15	A	818	CLA	CBA-CGA-O2A-C1
21	b	849	LMG	C22-C23-C24-C25
21	h	102	LMG	C39-C40-C41-C42
20	A	854	LMT	C2-C1-O1'-C1'
20	N	854	LMT	C2-C1-O1'-C1'
20	a	854	LMT	C2-C1-O1'-C1'
15	A	820	CLA	C3-C5-C6-C7
21	J	102	LMG	C39-C40-C41-C42
21	b	849	LMG	C40-C41-C42-C43
15	A	835	CLA	O1D-CGD-O2D-CED
15	a	834	CLA	O1D-CGD-O2D-CED
15	B	815	CLA	C4B-C3B-CAB-CBB
15	N	834	CLA	C4B-C3B-CAB-CBB
15	a	807	CLA	C4B-C3B-CAB-CBB
15	b	817	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	A	801	CL0	C16-C17-C18-C19
14	L	201	F6C	C16-C17-C18-C20
15	A	856	CLA	C16-C17-C18-C19
15	B	816	CLA	C11-C12-C13-C14
15	N	803	CLA	C16-C17-C18-C19
15	N	829	CLA	C11-C12-C13-C15
15	N	842	CLA	C16-C17-C18-C20
15	O	802	CLA	C16-C17-C18-C19
15	O	802	CLA	C16-C17-C18-C20
15	a	803	CLA	C16-C17-C18-C19
15	a	829	CLA	C11-C12-C13-C15
15	b	818	CLA	C11-C12-C13-C14
14	a	802	F6C	O1D-CGD-O2D-CED
15	N	822	CLA	O1D-CGD-O2D-CED
15	N	823	CLA	O1A-CGA-O2A-C1
15	b	828	CLA	O1A-CGA-O2A-C1
15	A	856	CLA	C2A-CAA-CBA-CGA
15	N	822	CLA	C8-C10-C11-C12
15	b	806	CLA	C15-C16-C17-C18
19	l	102	LHG	C8-C7-O7-C5
19	Y	101	LHG	C12-C13-C14-C15
21	O	850	LMG	C40-C41-C42-C43
14	B	838	F6C	C11-C10-C8-C7
15	A	820	CLA	C12-C13-C15-C16
15	B	816	CLA	C6-C7-C8-C10
15	B	817	CLA	C12-C13-C15-C16
15	B	825	CLA	C12-C13-C15-C16
15	O	811	CLA	C6-C7-C8-C10
15	a	819	CLA	C11-C12-C13-C15
15	f	201	CLA	CBA-CGA-O2A-C1
15	N	831	CLA	C5-C6-C7-C8
15	a	822	CLA	C5-C6-C7-C8
21	g	103	LMG	C11-C12-C13-C14
15	B	836	CLA	O1A-CGA-O2A-C1
15	O	828	CLA	O1A-CGA-O2A-C1
14	B	838	F6C	C3-C5-C6-C7
14	O	840	F6C	C3-C5-C6-C7
14	b	840	F6C	C3-C5-C6-C7
15	A	807	CLA	C3-C5-C6-C7
15	A	812	CLA	C3A-C2A-CAA-CBA
15	B	805	CLA	C3A-C2A-CAA-CBA
15	B	821	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	B	822	CLA	C3A-C2A-CAA-CBA
15	B	834	CLA	C3A-C2A-CAA-CBA
15	B	835	CLA	C3A-C2A-CAA-CBA
15	N	837	CLA	C3A-C2A-CAA-CBA
15	N	841	CLA	C3A-C2A-CAA-CBA
15	O	806	CLA	C3A-C2A-CAA-CBA
15	O	815	CLA	C3A-C2A-CAA-CBA
15	O	823	CLA	C3A-C2A-CAA-CBA
15	O	824	CLA	C3A-C2A-CAA-CBA
15	O	826	CLA	C3A-C2A-CAA-CBA
15	O	835	CLA	C3A-C2A-CAA-CBA
15	O	836	CLA	C3A-C2A-CAA-CBA
15	O	837	CLA	C3A-C2A-CAA-CBA
15	a	838	CLA	C3A-C2A-CAA-CBA
15	b	806	CLA	C3A-C2A-CAA-CBA
15	b	824	CLA	C3A-C2A-CAA-CBA
15	b	836	CLA	C3A-C2A-CAA-CBA
15	b	837	CLA	C3A-C2A-CAA-CBA
15	O	834	CLA	O1D-CGD-O2D-CED
22	B	848	LFA	C9-C10-C11-C12
15	O	827	CLA	C2-C3-C5-C6
20	A	853	LMT	C2B-C1B-O1B-C4'
19	M	102	LHG	C12-C13-C14-C15
15	O	837	CLA	C13-C15-C16-C17
15	a	806	CLA	C5-C6-C7-C8
15	B	815	CLA	O1D-CGD-O2D-CED
15	a	825	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	C16-C17-C18-C20
15	A	829	CLA	C11-C12-C13-C15
15	B	832	CLA	C6-C7-C8-C10
15	N	842	CLA	C16-C17-C18-C19
15	O	823	CLA	C6-C7-C8-C9
20	a	853	LMT	C2B-C1B-O1B-C4'
15	A	838	CLA	O1A-CGA-O2A-C1
15	O	838	CLA	O1A-CGA-O2A-C1
15	a	817	CLA	CBD-CGD-O2D-CED
15	b	836	CLA	CBD-CGD-O2D-CED
19	W	1506	LHG	C9-C10-C11-C12
15	a	818	CLA	CBA-CGA-O2A-C1
21	B	847	LMG	C40-C41-C42-C43
15	A	818	CLA	C3-C5-C6-C7
15	A	822	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	B	807	CLA	C3-C5-C6-C7
15	B	832	CLA	C3-C5-C6-C7
15	a	818	CLA	C3-C5-C6-C7
19	Y	101	LHG	C23-C24-C25-C26
15	A	829	CLA	C8-C10-C11-C12
19	X	102	LHG	C28-C29-C30-C31
15	A	829	CLA	O1D-CGD-O2D-CED
19	j	207	LHG	C29-C30-C31-C32
19	N	851	LHG	C25-C26-C27-C28
15	O	818	CLA	C11-C12-C13-C14
15	A	834	CLA	C2B-C3B-CAB-CBB
15	B	815	CLA	C2B-C3B-CAB-CBB
15	N	834	CLA	C2B-C3B-CAB-CBB
15	O	817	CLA	C2B-C3B-CAB-CBB
15	a	812	CLA	C2B-C3B-CAB-CBB
15	b	817	CLA	C2B-C3B-CAB-CBB
18	A	846	BCR	C1-C6-C7-C8
18	A	847	BCR	C5-C6-C7-C8
18	A	847	BCR	C23-C24-C25-C26
18	A	848	BCR	C23-C24-C25-C30
18	A	850	BCR	C23-C24-C25-C26
18	A	850	BCR	C23-C24-C25-C30
18	A	858	BCR	C23-C24-C25-C30
18	B	842	BCR	C23-C24-C25-C30
18	B	844	BCR	C1-C6-C7-C8
18	B	846	BCR	C5-C6-C7-C8
18	I	101	BCR	C23-C24-C25-C26
18	I	101	BCR	C23-C24-C25-C30
18	J	101	BCR	C23-C24-C25-C30
18	N	846	BCR	C1-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	848	BCR	C23-C24-C25-C30
18	N	857	BCR	C23-C24-C25-C30
18	O	844	BCR	C23-C24-C25-C30
18	O	846	BCR	C1-C6-C7-C8
18	O	846	BCR	C5-C6-C7-C8
18	O	849	BCR	C5-C6-C7-C8
18	T	101	BCR	C23-C24-C25-C30
18	U	101	BCR	C23-C24-C25-C30
18	Y	102	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	a	846	BCR	C1-C6-C7-C8
18	a	847	BCR	C1-C6-C7-C8
18	a	847	BCR	C5-C6-C7-C8
18	a	847	BCR	C23-C24-C25-C26
18	a	850	BCR	C23-C24-C25-C30
18	a	857	BCR	C23-C24-C25-C30
18	b	844	BCR	C23-C24-C25-C30
18	b	846	BCR	C1-C6-C7-C8
18	h	101	BCR	C23-C24-C25-C30
19	l	101	LHG	C24-C25-C26-C27
19	l	102	LHG	C28-C29-C30-C31
15	B	813	CLA	CBD-CGD-O2D-CED
15	B	837	CLA	CBD-CGD-O2D-CED
15	F	201	CLA	CBA-CGA-O2A-C1
15	b	830	CLA	CBA-CGA-O2A-C1
15	B	807	CLA	C10-C11-C12-C13
15	B	804	CLA	C3-C5-C6-C7
15	a	807	CLA	C3-C5-C6-C7
15	b	805	CLA	C3-C5-C6-C7
19	Z	102	LHG	C12-C13-C14-C15
14	a	824	F6C	C3A-C2A-CAA-CBA
15	a	836	CLA	O1D-CGD-O2D-CED
15	O	822	CLA	C2A-CAA-CBA-CGA
19	k	101	LHG	C23-C24-C25-C26
21	U	102	LMG	C10-C11-C12-C13
21	J	102	LMG	C17-C18-C19-C20
15	S	201	CLA	O1A-CGA-O2A-C1
15	f	201	CLA	O1A-CGA-O2A-C1
19	X	102	LHG	C12-C13-C14-C15
21	U	102	LMG	C17-C18-C19-C20
19	l	102	LHG	O9-C7-O7-C5
15	b	818	CLA	C4-C3-C5-C6
19	l	102	LHG	C12-C13-C14-C15
22	f	204	LFA	C9-C10-C11-C12
15	A	856	CLA	C13-C15-C16-C17
15	A	822	CLA	C2-C3-C5-C6
15	b	825	CLA	C2-C3-C5-C6
15	b	827	CLA	C2-C3-C5-C6
19	X	101	LHG	C24-C25-C26-C27
21	j	206	LMG	C29-C30-C31-C32
15	A	814	CLA	CBA-CGA-O2A-C1
15	B	828	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	N	818	CLA	CBA-CGA-O2A-C1
15	O	830	CLA	CBA-CGA-O2A-C1
15	N	810	CLA	C11-C10-C8-C9
15	O	839	CLA	C6-C7-C8-C9
19	Z	101	LHG	C25-C26-C27-C28
14	N	856	F6C	C10-C11-C12-C13
15	O	806	CLA	C15-C16-C17-C18
19	L	207	LHG	C17-C18-C19-C20
21	a	855	LMG	C21-C22-C23-C24
20	a	853	LMT	O5'-C1'-O1'-C1
21	A	855	LMG	C21-C22-C23-C24
21	j	206	LMG	C19-C20-C21-C22
15	a	823	CLA	O1D-CGD-O2D-CED
14	N	826	F6C	C8-C10-C11-C12
15	A	831	CLA	C5-C6-C7-C8
15	A	818	CLA	O1A-CGA-O2A-C1
21	N	855	LMG	C21-C22-C23-C24
15	O	809	CLA	C3-C5-C6-C7
15	b	823	CLA	C6-C7-C8-C9
15	b	841	CLA	C16-C17-C18-C19
19	X	102	LHG	C8-C7-O7-C5
19	Z	102	LHG	C8-C7-O7-C5
19	a	851	LHG	C8-C7-O7-C5
19	j	207	LHG	C8-C7-O7-C5
21	J	102	LMG	C11-C10-O7-C8
15	O	801	CLA	C13-C15-C16-C17
15	b	802	CLA	C13-C15-C16-C17
19	Z	102	LHG	O9-C7-O7-C5
19	Z	101	LHG	C24-C25-C26-C27
18	N	857	BCR	C7-C8-C9-C34
19	M	102	LHG	C23-C24-C25-C26
19	l	101	LHG	C25-C26-C27-C28
15	N	807	CLA	C3-C5-C6-C7
14	L	201	F6C	C3A-C2A-CAA-CBA
18	A	858	BCR	C7-C8-C9-C10
18	J	101	BCR	C21-C22-C23-C24
18	L	205	BCR	C7-C8-C9-C10
21	L	206	LMG	C19-C20-C21-C22
15	A	835	CLA	C2A-CAA-CBA-CGA
15	N	835	CLA	C2A-CAA-CBA-CGA
15	O	831	CLA	C2A-CAA-CBA-CGA
15	A	842	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	B	821	CLA	C6-C7-C8-C9
15	O	834	CLA	C6-C7-C8-C9
15	O	834	CLA	C6-C7-C8-C10
15	a	842	CLA	C16-C17-C18-C20
15	b	834	CLA	C6-C7-C8-C10
15	b	841	CLA	C16-C17-C18-C20
15	L	202	CLA	CBD-CGD-O2D-CED
19	A	851	LHG	C27-C28-C29-C30
21	W	1505	LMG	C19-C20-C21-C22
22	O	851	LFA	C9-C10-C11-C12
15	B	816	CLA	C4-C3-C5-C6
14	A	824	F6C	C2B-C3B-CAB-CBB
15	b	818	CLA	C2-C3-C5-C6
15	a	831	CLA	C5-C6-C7-C8
21	W	1505	LMG	C29-C30-C31-C32
15	A	804	CLA	C8-C10-C11-C12
15	N	804	CLA	C8-C10-C11-C12
15	N	806	CLA	C5-C6-C7-C8
15	a	828	CLA	C5-C6-C7-C8
15	a	839	CLA	C8-C10-C11-C12
15	b	801	CLA	C13-C15-C16-C17
15	N	805	CLA	CBA-CGA-O2A-C1
21	J	102	LMG	C10-C11-C12-C13
21	N	855	LMG	O6-C5-C6-O5
15	b	821	CLA	O1D-CGD-O2D-CED
19	W	1506	LHG	C8-C7-O7-C5
21	U	102	LMG	C11-C10-O7-C8
14	N	826	F6C	C15-C16-C17-C18
15	A	841	CLA	C5-C6-C7-C8
15	a	831	CLA	C10-C11-C12-C13
15	j	203	CLA	C10-C11-C12-C13
15	b	834	CLA	C6-C7-C8-C9
15	a	818	CLA	O1A-CGA-O2A-C1
15	A	806	CLA	C5-C6-C7-C8
15	N	841	CLA	C5-C6-C7-C8
15	O	811	CLA	C13-C15-C16-C17
15	O	838	CLA	C15-C16-C17-C18
15	a	804	CLA	C8-C10-C11-C12
15	B	832	CLA	O1D-CGD-O2D-CED
15	N	829	CLA	O1D-CGD-O2D-CED
15	b	835	CLA	O1D-CGD-O2D-CED
15	O	805	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	Z	101	LHG	O7-C5-C6-O8
19	a	851	LHG	O7-C5-C6-O8
15	F	201	CLA	O1A-CGA-O2A-C1
19	a	851	LHG	C25-C26-C27-C28
21	L	206	LMG	C34-C35-C36-C37
15	B	809	CLA	C13-C15-C16-C17
15	a	841	CLA	C5-C6-C7-C8
19	A	851	LHG	C25-C26-C27-C28
19	X	101	LHG	C25-C26-C27-C28
21	a	855	LMG	O6-C5-C6-O5
15	B	832	CLA	C6-C7-C8-C9
14	O	810	F6C	C3A-C2A-CAA-CBA
21	U	102	LMG	C21-C22-C23-C24
14	B	831	F6C	C1A-C2A-CAA-CBA
15	N	828	CLA	C5-C6-C7-C8
19	L	207	LHG	C29-C30-C31-C32
15	B	808	CLA	C2A-CAA-CBA-CGA
15	B	829	CLA	C2A-CAA-CBA-CGA
15	O	802	CLA	C2A-CAA-CBA-CGA
15	b	802	CLA	C2A-CAA-CBA-CGA
15	a	835	CLA	O1D-CGD-O2D-CED
15	b	802	CLA	O1D-CGD-O2D-CED
15	O	817	CLA	CBA-CGA-O2A-C1
15	a	806	CLA	CBA-CGA-O2A-C1
19	j	207	LHG	C14-C15-C16-C17
15	a	838	CLA	O1D-CGD-O2D-CED
15	B	835	CLA	C13-C15-C16-C17
20	a	853	LMT	O5B-C5B-C6B-O6B
21	U	102	LMG	C13-C14-C15-C16
22	f	204	LFA	C4-C5-C6-C7
15	b	830	CLA	O1A-CGA-O2A-C1
13	A	801	CL0	C3-C5-C6-C7
19	l	102	LHG	C24-C25-C26-C27
22	B	848	LFA	C4-C5-C6-C7
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	804	CLA	C1A-C2A-CAA-CBA
15	B	805	CLA	C1A-C2A-CAA-CBA
15	B	810	CLA	C1A-C2A-CAA-CBA
15	B	815	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	B	821	CLA	C1A-C2A-CAA-CBA
15	B	822	CLA	C1A-C2A-CAA-CBA
15	B	828	CLA	C1A-C2A-CAA-CBA
15	B	829	CLA	C1A-C2A-CAA-CBA
15	B	830	CLA	C1A-C2A-CAA-CBA
15	B	833	CLA	C1A-C2A-CAA-CBA
15	B	834	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	811	CLA	C1A-C2A-CAA-CBA
15	N	819	CLA	C1A-C2A-CAA-CBA
15	O	805	CLA	C1A-C2A-CAA-CBA
15	O	806	CLA	C1A-C2A-CAA-CBA
15	O	812	CLA	C1A-C2A-CAA-CBA
15	O	817	CLA	C1A-C2A-CAA-CBA
15	O	823	CLA	C1A-C2A-CAA-CBA
15	O	824	CLA	C1A-C2A-CAA-CBA
15	O	826	CLA	C1A-C2A-CAA-CBA
15	O	830	CLA	C1A-C2A-CAA-CBA
15	O	831	CLA	C1A-C2A-CAA-CBA
15	O	832	CLA	C1A-C2A-CAA-CBA
15	O	836	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	815	CLA	C1A-C2A-CAA-CBA
15	a	819	CLA	C1A-C2A-CAA-CBA
15	a	838	CLA	C1A-C2A-CAA-CBA
15	b	805	CLA	C1A-C2A-CAA-CBA
15	b	806	CLA	C1A-C2A-CAA-CBA
15	b	812	CLA	C1A-C2A-CAA-CBA
15	b	817	CLA	C1A-C2A-CAA-CBA
15	b	824	CLA	C1A-C2A-CAA-CBA
15	b	831	CLA	C1A-C2A-CAA-CBA
15	b	832	CLA	C1A-C2A-CAA-CBA
15	b	836	CLA	C1A-C2A-CAA-CBA
15	B	829	CLA	CBD-CGD-O2D-CED
14	A	826	F6C	C8-C10-C11-C12
14	a	826	F6C	C8-C10-C11-C12
21	L	206	LMG	C30-C31-C32-C33
21	j	206	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
15	B	823	CLA	C5-C6-C7-C8
15	O	814	CLA	C8-C10-C11-C12
20	A	853	LMT	O5B-C5B-C6B-O6B
21	T	103	LMG	O6-C5-C6-O5
21	W	1505	LMG	O6-C5-C6-O5
19	X	102	LHG	O9-C7-O7-C5
21	L	206	LMG	C29-C30-C31-C32
21	h	102	LMG	C10-C11-C12-C13
15	b	839	CLA	C3-C5-C6-C7
15	O	839	CLA	O1D-CGD-O2D-CED
14	L	201	F6C	C11-C12-C13-C15
14	O	810	F6C	C11-C12-C13-C15
14	b	840	F6C	C11-C10-C8-C7
15	A	812	CLA	C11-C12-C13-C15
15	A	822	CLA	C12-C13-C15-C16
15	A	839	CLA	C12-C13-C15-C16
15	B	808	CLA	C12-C13-C15-C16
15	B	811	CLA	C6-C7-C8-C10
15	B	812	CLA	C12-C13-C15-C16
15	B	817	CLA	C11-C10-C8-C7
15	B	817	CLA	C11-C12-C13-C15
15	B	822	CLA	C11-C12-C13-C15
15	B	829	CLA	C11-C12-C13-C15
15	B	839	CLA	C12-C13-C15-C16
15	N	805	CLA	C11-C10-C8-C7
15	N	812	CLA	C11-C12-C13-C15
15	N	820	CLA	C12-C13-C15-C16
15	N	839	CLA	C11-C12-C13-C15
15	O	809	CLA	C12-C13-C15-C16
15	O	814	CLA	C12-C13-C15-C16
15	O	818	CLA	C6-C7-C8-C10
15	O	819	CLA	C11-C10-C8-C7
15	O	819	CLA	C11-C12-C13-C15
15	O	819	CLA	C12-C13-C15-C16
15	O	824	CLA	C11-C12-C13-C15
15	O	827	CLA	C12-C13-C15-C16
15	O	831	CLA	C11-C12-C13-C15
15	a	804	CLA	C6-C7-C8-C10
15	a	809	CLA	C6-C7-C8-C10
15	a	812	CLA	C11-C12-C13-C15
15	a	820	CLA	C12-C13-C15-C16
15	a	822	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	a	839	CLA	C12-C13-C15-C16
15	b	809	CLA	C6-C7-C8-C10
15	b	809	CLA	C12-C13-C15-C16
15	b	813	CLA	C6-C7-C8-C10
15	b	814	CLA	C12-C13-C15-C16
15	b	818	CLA	C6-C7-C8-C10
15	b	819	CLA	C11-C12-C13-C15
15	b	819	CLA	C12-C13-C15-C16
15	b	824	CLA	C11-C12-C13-C15
15	b	827	CLA	C12-C13-C15-C16
15	b	831	CLA	C11-C12-C13-C15
19	Z	102	LHG	C28-C29-C30-C31
13	A	801	CL0	C10-C11-C12-C13
15	B	801	CLA	C13-C15-C16-C17
15	A	814	CLA	O1A-CGA-O2A-C1
15	N	805	CLA	O1A-CGA-O2A-C1
15	N	818	CLA	O1A-CGA-O2A-C1
15	O	830	CLA	O1A-CGA-O2A-C1
15	l	103	CLA	O1D-CGD-O2D-CED
15	N	820	CLA	C10-C11-C12-C13
15	O	813	CLA	C5-C6-C7-C8
21	j	206	LMG	C28-C29-C30-C31
15	B	816	CLA	C2-C3-C5-C6
15	B	828	CLA	O1A-CGA-O2A-C1
14	a	824	F6C	O1D-CGD-O2D-CED
19	L	207	LHG	C8-C7-O7-C5
19	N	851	LHG	C8-C7-O7-C5
21	h	102	LMG	C11-C10-O7-C8
15	B	834	CLA	O1D-CGD-O2D-CED
15	A	819	CLA	C2A-CAA-CBA-CGA
15	A	822	CLA	C2A-CAA-CBA-CGA
15	A	842	CLA	C2A-CAA-CBA-CGA
15	N	822	CLA	C2A-CAA-CBA-CGA
15	a	804	CLA	C2A-CAA-CBA-CGA
14	b	810	F6C	C11-C12-C13-C14
14	b	840	F6C	C11-C10-C8-C9
15	A	812	CLA	C11-C12-C13-C14
15	A	822	CLA	C14-C13-C15-C16
15	A	829	CLA	C11-C10-C8-C9
15	A	830	CLA	C14-C13-C15-C16
15	A	839	CLA	C14-C13-C15-C16
15	A	856	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	B	805	CLA	C14-C13-C15-C16
15	B	811	CLA	C6-C7-C8-C9
15	B	817	CLA	C11-C10-C8-C9
15	N	839	CLA	C11-C12-C13-C14
15	N	841	CLA	C11-C12-C13-C14
15	O	819	CLA	C11-C10-C8-C9
15	a	822	CLA	C14-C13-C15-C16
15	b	802	CLA	C6-C7-C8-C9
15	b	813	CLA	C6-C7-C8-C9
15	b	814	CLA	C14-C13-C15-C16
15	b	818	CLA	C6-C7-C8-C9
15	b	819	CLA	C11-C10-C8-C9
15	b	819	CLA	C11-C12-C13-C14
15	b	830	CLA	C11-C10-C8-C9
21	W	1505	LMG	C34-C35-C36-C37
21	b	849	LMG	C31-C32-C33-C34
22	O	851	LFA	C4-C5-C6-C7
15	A	839	CLA	CBA-CGA-O2A-C1
15	N	814	CLA	CBA-CGA-O2A-C1
15	a	805	CLA	CBA-CGA-O2A-C1
19	l	101	LHG	C24-C23-O8-C6
20	N	853	LMT	O5B-C5B-C6B-O6B
15	N	834	CLA	O1D-CGD-O2D-CED
15	N	838	CLA	O1D-CGD-O2D-CED
14	O	840	F6C	C1A-C2A-CAA-CBA
21	L	206	LMG	C33-C34-C35-C36
19	Z	102	LHG	C24-C25-C26-C27
21	g	103	LMG	O6-C5-C6-O5
15	B	811	CLA	C11-C10-C8-C9
15	O	813	CLA	C11-C10-C8-C9
19	A	851	LHG	C4-C5-C6-O8
19	N	851	LHG	C4-C5-C6-O8
19	a	851	LHG	C4-C5-C6-O8
19	j	207	LHG	C17-C18-C19-C20
15	b	824	CLA	O1D-CGD-O2D-CED
19	W	1506	LHG	C17-C18-C19-C20
15	A	841	CLA	C15-C16-C17-C18
19	W	1506	LHG	C14-C15-C16-C17
15	B	822	CLA	O1D-CGD-O2D-CED
15	B	815	CLA	CBA-CGA-O2A-C1
15	N	806	CLA	CBA-CGA-O2A-C1
15	a	814	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	W	1505	LMG	C28-C29-C30-C31
21	A	855	LMG	O6-C5-C6-O5
21	I	103	LMG	O6-C5-C6-O5
15	B	816	CLA	C10-C11-C12-C13
15	O	809	CLA	C5-C6-C7-C8
15	B	808	CLA	C10-C11-C12-C13
15	b	838	CLA	C15-C16-C17-C18
19	N	851	LHG	C27-C28-C29-C30
15	a	806	CLA	O1A-CGA-O2A-C1
19	a	851	LHG	C27-C28-C29-C30
15	A	836	CLA	C4-C3-C5-C6
15	A	836	CLA	C2-C3-C5-C6
15	O	818	CLA	C2-C3-C5-C6
15	A	820	CLA	C10-C11-C12-C13
15	O	834	CLA	C5-C6-C7-C8
15	b	834	CLA	C5-C6-C7-C8
18	A	847	BCR	C37-C22-C23-C24
18	N	847	BCR	C37-C22-C23-C24
18	a	847	BCR	C37-C22-C23-C24
18	b	848	BCR	C7-C8-C9-C34
14	O	810	F6C	C16-C17-C18-C20
19	X	102	LHG	C34-C35-C36-C37
21	h	102	LMG	O6-C5-C6-O5
21	j	206	LMG	O6-C5-C6-O5
14	B	838	F6C	C3A-C2A-CAA-CBA
18	A	847	BCR	C21-C22-C23-C24
18	N	847	BCR	C21-C22-C23-C24
18	O	849	BCR	C7-C8-C9-C10
15	a	805	CLA	O1A-CGA-O2A-C1
15	O	839	CLA	C3-C5-C6-C7
21	L	206	LMG	O6-C5-C6-O5
21	U	102	LMG	O6-C5-C6-O5
15	b	825	CLA	C5-C6-C7-C8
19	L	207	LHG	C14-C15-C16-C17
15	A	805	CLA	CBA-CGA-O2A-C1
15	A	806	CLA	CBA-CGA-O2A-C1
15	B	835	CLA	CBA-CGA-O2A-C1
21	I	103	LMG	C29-C30-C31-C32
15	O	808	CLA	C13-C15-C16-C17
15	O	818	CLA	C10-C11-C12-C13
14	N	826	F6C	C3B-C2B-CMB-OMB
15	B	812	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	O	833	F6C	C1A-C2A-CAA-CBA
14	b	833	F6C	C1A-C2A-CAA-CBA
14	b	840	F6C	C1A-C2A-CAA-CBA
19	Z	101	LHG	C30-C31-C32-C33
15	O	837	CLA	CBA-CGA-O2A-C1
15	b	822	CLA	CBA-CGA-O2A-C1
19	Z	101	LHG	C24-C23-O8-C6
19	A	851	LHG	C8-C7-O7-C5
21	j	206	LMG	C35-C36-C37-C38
15	B	830	CLA	O1D-CGD-O2D-CED
20	N	853	LMT	C2-C3-C4-C5
15	B	829	CLA	C2-C3-C5-C6
19	k	101	LHG	C33-C34-C35-C36
21	W	1505	LMG	C33-C34-C35-C36
19	Z	102	LHG	C11-C10-C9-C8
19	l	102	LHG	C15-C16-C17-C18
21	A	855	LMG	C13-C14-C15-C16
14	b	810	F6C	C3A-C2A-CAA-CBA
15	O	817	CLA	O1A-CGA-O2A-C1
15	O	817	CLA	O1D-CGD-O2D-CED
13	a	801	CL0	CAA-CBA-CGA-O2A
15	N	821	CLA	CAA-CBA-CGA-O2A
15	a	821	CLA	CAA-CBA-CGA-O2A
21	T	103	LMG	C29-C30-C31-C32
15	a	819	CLA	C2A-CAA-CBA-CGA
15	a	835	CLA	C2A-CAA-CBA-CGA
15	b	808	CLA	C3-C5-C6-C7
15	A	828	CLA	C5-C6-C7-C8
15	b	814	CLA	C8-C10-C11-C12
15	b	831	CLA	C10-C11-C12-C13
19	W	1506	LHG	O9-C7-O7-C5
19	a	851	LHG	O9-C7-O7-C5
15	N	814	CLA	O1A-CGA-O2A-C1
19	l	101	LHG	O10-C23-O8-C6
20	a	853	LMT	C2-C3-C4-C5
19	L	207	LHG	C13-C14-C15-C16
15	A	832	CLA	CBA-CGA-O2A-C1
15	N	825	CLA	CBA-CGA-O2A-C1
15	a	839	CLA	CBA-CGA-O2A-C1
15	O	822	CLA	CAA-CBA-CGA-O2A
14	A	824	F6C	CBD-CGD-O2D-CED
19	Z	102	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	A	818	CLA	C10-C11-C12-C13
15	b	808	CLA	C13-C15-C16-C17
15	B	837	CLA	C3-C5-C6-C7
15	A	825	CLA	O1D-CGD-O2D-CED
13	N	801	CL0	C10-C11-C12-C13
15	B	805	CLA	C15-C16-C17-C18
15	N	839	CLA	C8-C10-C11-C12
15	b	808	CLA	C10-C11-C12-C13
15	b	803	CLA	O1D-CGD-O2D-CED
15	b	813	CLA	C11-C10-C8-C9
15	A	815	CLA	C6-C7-C8-C9
14	N	802	F6C	CBD-CGD-O2D-CED
15	O	818	CLA	C4-C3-C5-C6
13	A	801	CL0	CAA-CBA-CGA-O2A
15	N	841	CLA	C2-C3-C5-C6
19	X	101	LHG	C31-C32-C33-C34
15	b	837	CLA	CBA-CGA-O2A-C1
19	X	101	LHG	C24-C23-O8-C6
15	O	825	CLA	C5-C6-C7-C8
15	O	838	CLA	C10-C11-C12-C13
15	a	818	CLA	C10-C11-C12-C13
15	b	837	CLA	C13-C15-C16-C17
21	J	102	LMG	O9-C10-O7-C8
20	N	852	LMT	C2-C1-O1'-C1'
14	B	838	F6C	C11-C10-C8-C9
14	L	201	F6C	C11-C12-C13-C14
14	O	810	F6C	C11-C12-C13-C14
14	O	840	F6C	C11-C10-C8-C9
15	A	805	CLA	C11-C10-C8-C9
15	A	820	CLA	C14-C13-C15-C16
15	A	831	CLA	C6-C7-C8-C9
15	A	839	CLA	C11-C12-C13-C14
15	B	806	CLA	C14-C13-C15-C16
15	B	808	CLA	C14-C13-C15-C16
15	B	812	CLA	C14-C13-C15-C16
15	B	816	CLA	C6-C7-C8-C9
15	B	817	CLA	C11-C12-C13-C14
15	B	822	CLA	C11-C12-C13-C14
15	B	823	CLA	C11-C12-C13-C14
15	B	825	CLA	C14-C13-C15-C16
15	B	829	CLA	C11-C12-C13-C14
15	B	837	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	B	839	CLA	C14-C13-C15-C16
15	N	805	CLA	C11-C10-C8-C9
15	N	812	CLA	C11-C12-C13-C14
15	N	820	CLA	C14-C13-C15-C16
15	N	839	CLA	C6-C7-C8-C9
15	N	839	CLA	C11-C10-C8-C9
15	O	806	CLA	C14-C13-C15-C16
15	O	809	CLA	C14-C13-C15-C16
15	O	811	CLA	C6-C7-C8-C9
15	O	814	CLA	C14-C13-C15-C16
15	O	818	CLA	C6-C7-C8-C9
15	O	819	CLA	C11-C12-C13-C14
15	O	824	CLA	C11-C12-C13-C14
15	O	827	CLA	C14-C13-C15-C16
15	O	830	CLA	C11-C12-C13-C14
15	O	831	CLA	C11-C12-C13-C14
15	a	805	CLA	C11-C10-C8-C9
15	a	812	CLA	C11-C12-C13-C14
15	a	819	CLA	C11-C10-C8-C9
15	a	820	CLA	C14-C13-C15-C16
15	a	828	CLA	C6-C7-C8-C9
15	a	830	CLA	C14-C13-C15-C16
15	a	839	CLA	C11-C12-C13-C14
15	a	839	CLA	C14-C13-C15-C16
15	b	809	CLA	C14-C13-C15-C16
15	b	824	CLA	C11-C12-C13-C14
15	b	825	CLA	C11-C12-C13-C14
15	b	827	CLA	C14-C13-C15-C16
15	b	831	CLA	C11-C12-C13-C14
15	b	839	CLA	C6-C7-C8-C9
15	O	802	CLA	C13-C15-C16-C17
15	O	803	CLA	C13-C15-C16-C17
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	812	CLA	C4B-C3B-CAB-CBB
15	B	808	CLA	C4B-C3B-CAB-CBB
15	B	828	CLA	C4B-C3B-CAB-CBB
15	N	812	CLA	C4B-C3B-CAB-CBB
15	N	822	CLA	C4B-C3B-CAB-CBB
15	N	839	CLA	C4B-C3B-CAB-CBB
15	O	801	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	O	817	CLA	C4B-C3B-CAB-CBB
15	a	812	CLA	C4B-C3B-CAB-CBB
15	a	818	CLA	C4B-C3B-CAB-CBB
15	a	822	CLA	C4B-C3B-CAB-CBB
19	a	851	LHG	O8-C23-C24-C25
14	a	826	F6C	C5-C6-C7-C8
15	O	832	CLA	C8-C10-C11-C12
15	a	803	CLA	C8-C10-C11-C12
15	b	827	CLA	C10-C11-C12-C13
15	N	807	CLA	CBA-CGA-O2A-C1
15	b	839	CLA	CBA-CGA-O2A-C1
15	B	803	CLA	C2A-CAA-CBA-CGA
15	N	804	CLA	C2A-CAA-CBA-CGA
15	N	819	CLA	C2A-CAA-CBA-CGA
15	O	804	CLA	C2A-CAA-CBA-CGA
15	b	804	CLA	C2A-CAA-CBA-CGA
20	N	853	LMT	C2'-C1'-O1'-C1
20	a	853	LMT	C2'-C1'-O1'-C1
19	X	101	LHG	C11-C10-C9-C8
19	k	101	LHG	C25-C26-C27-C28
19	Z	102	LHG	C34-C35-C36-C37
14	O	840	F6C	C11-C10-C8-C7
14	O	840	F6C	C11-C12-C13-C15
14	b	810	F6C	C11-C12-C13-C15
15	A	805	CLA	C11-C10-C8-C7
15	A	809	CLA	C6-C7-C8-C10
15	A	811	CLA	C6-C7-C8-C10
15	A	812	CLA	C11-C10-C8-C7
15	A	828	CLA	C6-C7-C8-C10
15	A	829	CLA	C11-C10-C8-C7
15	A	830	CLA	C12-C13-C15-C16
15	A	831	CLA	C6-C7-C8-C10
15	A	839	CLA	C11-C12-C13-C15
15	B	805	CLA	C12-C13-C15-C16
15	B	806	CLA	C12-C13-C15-C16
15	B	809	CLA	C6-C7-C8-C10
15	B	812	CLA	C11-C10-C8-C7
15	B	823	CLA	C11-C12-C13-C15
15	N	805	CLA	C6-C7-C8-C10
15	N	809	CLA	C6-C7-C8-C10
15	N	811	CLA	C6-C7-C8-C10
15	N	822	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	N	830	CLA	C12-C13-C15-C16
15	N	839	CLA	C6-C7-C8-C10
15	N	839	CLA	C11-C10-C8-C7
15	O	806	CLA	C12-C13-C15-C16
15	O	814	CLA	C11-C12-C13-C15
15	O	825	CLA	C11-C12-C13-C15
15	O	837	CLA	C12-C13-C15-C16
15	a	805	CLA	C6-C7-C8-C10
15	a	805	CLA	C11-C10-C8-C7
15	a	811	CLA	C6-C7-C8-C10
15	a	828	CLA	C6-C7-C8-C10
15	a	830	CLA	C12-C13-C15-C16
15	a	839	CLA	C11-C12-C13-C15
15	b	806	CLA	C12-C13-C15-C16
15	b	807	CLA	C12-C13-C15-C16
15	b	808	CLA	C11-C10-C8-C7
15	b	819	CLA	C11-C10-C8-C7
15	b	825	CLA	C11-C12-C13-C15
15	b	802	CLA	C15-C16-C17-C18
15	b	808	CLA	C8-C10-C11-C12
15	a	814	CLA	O1A-CGA-O2A-C1
15	B	819	CLA	O1D-CGD-O2D-CED
15	O	836	CLA	O1D-CGD-O2D-CED
15	b	816	CLA	O1D-CGD-O2D-CED
15	N	818	CLA	C10-C11-C12-C13
15	A	815	CLA	C3A-C2A-CAA-CBA
15	A	837	CLA	C3A-C2A-CAA-CBA
15	A	842	CLA	C3A-C2A-CAA-CBA
15	B	824	CLA	C3A-C2A-CAA-CBA
15	B	825	CLA	C4-C3-C5-C6
15	B	828	CLA	C3A-C2A-CAA-CBA
15	B	839	CLA	C3A-C2A-CAA-CBA
15	K	102	CLA	C3A-C2A-CAA-CBA
15	N	812	CLA	C3A-C2A-CAA-CBA
15	N	815	CLA	C3A-C2A-CAA-CBA
15	N	822	CLA	C4-C3-C5-C6
15	N	838	CLA	C3A-C2A-CAA-CBA
15	N	842	CLA	C3A-C2A-CAA-CBA
15	O	830	CLA	C3A-C2A-CAA-CBA
15	O	841	CLA	C3A-C2A-CAA-CBA
15	V	102	CLA	C3A-C2A-CAA-CBA
15	W	1502	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	a	815	CLA	C3A-C2A-CAA-CBA
15	a	837	CLA	C3A-C2A-CAA-CBA
15	a	842	CLA	C3A-C2A-CAA-CBA
15	b	830	CLA	C3A-C2A-CAA-CBA
15	b	835	CLA	C3A-C2A-CAA-CBA
15	b	841	CLA	C3A-C2A-CAA-CBA
15	i	102	CLA	C3A-C2A-CAA-CBA
15	j	203	CLA	C3A-C2A-CAA-CBA
15	a	836	CLA	C2-C3-C5-C6
15	a	841	CLA	C2-C3-C5-C6
15	O	823	CLA	O1D-CGD-O2D-CED
15	O	824	CLA	O1D-CGD-O2D-CED
15	A	839	CLA	O1A-CGA-O2A-C1
15	N	806	CLA	O1A-CGA-O2A-C1
15	B	825	CLA	C10-C11-C12-C13
15	N	828	CLA	C13-C15-C16-C17
13	N	801	CL0	CBA-CGA-O2A-C1
15	O	839	CLA	CBA-CGA-O2A-C1
15	a	825	CLA	CBA-CGA-O2A-C1
19	l	102	LHG	C31-C32-C33-C34
18	A	846	BCR	C9-C10-C11-C12
18	N	845	BCR	C15-C16-C17-C18
18	N	846	BCR	C9-C10-C11-C12
18	T	101	BCR	C9-C10-C11-C12
18	a	846	BCR	C9-C10-C11-C12
18	g	101	BCR	C9-C10-C11-C12
15	N	841	CLA	O1D-CGD-O2D-CED
15	A	815	CLA	C6-C7-C8-C10
18	N	848	BCR	C37-C22-C23-C24
18	O	849	BCR	C7-C8-C9-C34
19	X	101	LHG	C12-C13-C14-C15
15	A	805	CLA	O1A-CGA-O2A-C1
15	B	815	CLA	O1A-CGA-O2A-C1
14	N	824	F6C	C3A-C2A-CAA-CBA
18	A	850	BCR	C17-C18-C19-C20
18	Y	102	BCR	C17-C18-C19-C20
18	a	847	BCR	C21-C22-C23-C24
19	X	102	LHG	C11-C10-C9-C8
21	b	849	LMG	C13-C14-C15-C16
15	j	203	CLA	C2A-CAA-CBA-CGA
19	X	101	LHG	C4-C5-C6-O8
19	Z	101	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
19	l	101	LHG	C4-C5-C6-O8
21	J	102	LMG	C7-C8-C9-O8
21	h	102	LMG	C7-C8-C9-O8
19	l	101	LHG	C12-C13-C14-C15
15	N	817	CLA	CBD-CGD-O2D-CED
21	J	102	LMG	C13-C14-C15-C16
21	O	850	LMG	C41-C42-C43-C44
15	B	807	CLA	C13-C15-C16-C17
19	W	1506	LHG	C31-C32-C33-C34
21	W	1505	LMG	C30-C31-C32-C33
15	B	806	CLA	C4-C3-C5-C6
15	B	829	CLA	C4-C3-C5-C6
15	N	841	CLA	C4-C3-C5-C6
15	a	841	CLA	C4-C3-C5-C6
21	j	206	LMG	C10-C11-C12-C13
15	B	820	CLA	CAA-CBA-CGA-O2A
15	A	806	CLA	O1A-CGA-O2A-C1
15	b	809	CLA	C3-C5-C6-C7
19	X	102	LHG	C24-C25-C26-C27
15	N	823	CLA	O1D-CGD-O2D-CED
15	O	821	CLA	O1D-CGD-O2D-CED
19	Z	101	LHG	C28-C29-C30-C31
19	j	207	LHG	O9-C7-O7-C5
21	U	102	LMG	O9-C10-O7-C8
15	f	201	CLA	C5-C6-C7-C8
15	A	812	CLA	C2B-C3B-CAB-CBB
15	N	812	CLA	C2B-C3B-CAB-CBB
15	N	839	CLA	C2B-C3B-CAB-CBB
15	a	807	CLA	C2B-C3B-CAB-CBB
18	A	847	BCR	C1-C6-C7-C8
15	b	822	CLA	CAA-CBA-CGA-O2A
15	B	836	CLA	C15-C16-C17-C18
15	O	805	CLA	C15-C16-C17-C18
15	A	812	CLA	C8-C10-C11-C12
15	B	830	CLA	C8-C10-C11-C12
14	b	840	F6C	C3A-C2A-CAA-CBA
19	M	102	LHG	C11-C10-C9-C8
19	M	102	LHG	C25-C26-C27-C28
19	Y	101	LHG	C10-C11-C12-C13
19	j	207	LHG	C13-C14-C15-C16
15	F	201	CLA	C16-C17-C18-C20
15	O	841	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	A	821	CLA	CAA-CBA-CGA-O2A
15	O	809	CLA	C2A-CAA-CBA-CGA
15	a	822	CLA	C2A-CAA-CBA-CGA
15	A	817	CLA	O1D-CGD-O2D-CED
15	N	835	CLA	O1D-CGD-O2D-CED
15	a	812	CLA	C8-C10-C11-C12
19	A	851	LHG	O7-C5-C6-O8
19	X	102	LHG	O7-C5-C6-O8
19	N	851	LHG	O7-C5-C6-O8
19	Z	102	LHG	O7-C5-C6-O8
19	l	102	LHG	O7-C5-C6-O8
21	J	102	LMG	O7-C8-C9-O8
21	h	102	LMG	O7-C8-C9-O8
15	a	820	CLA	C10-C11-C12-C13
15	B	835	CLA	O1A-CGA-O2A-C1
15	A	834	CLA	C4-C3-C5-C6
15	A	841	CLA	C4-C3-C5-C6
15	O	807	CLA	C4-C3-C5-C6
15	a	836	CLA	C4-C3-C5-C6
15	b	832	CLA	C4-C3-C5-C6
21	h	102	LMG	C13-C14-C15-C16
15	B	832	CLA	C5-C6-C7-C8
15	S	201	CLA	C5-C6-C7-C8
15	b	809	CLA	C5-C6-C7-C8
15	b	816	CLA	C5-C6-C7-C8
15	O	807	CLA	C2-C3-C5-C6
15	b	832	CLA	C2-C3-C5-C6
14	L	201	F6C	C16-C17-C18-C19
15	B	821	CLA	C6-C7-C8-C10
19	l	102	LHG	C11-C10-C9-C8
21	h	102	LMG	C30-C31-C32-C33
14	O	840	F6C	C5-C6-C7-C8
15	B	815	CLA	C13-C15-C16-C17
15	F	201	CLA	C5-C6-C7-C8
21	L	206	LMG	C10-C11-C12-C13
15	A	807	CLA	CBA-CGA-O2A-C1
15	B	837	CLA	CBA-CGA-O2A-C1
19	X	102	LHG	C15-C16-C17-C18
15	A	810	CLA	C11-C10-C8-C9
15	A	831	CLA	C11-C12-C13-C14
15	B	828	CLA	C11-C10-C8-C9
15	B	829	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	N	822	CLA	C14-C13-C15-C16
15	N	830	CLA	C14-C13-C15-C16
15	N	831	CLA	C6-C7-C8-C9
15	O	801	CLA	C11-C10-C8-C9
15	O	802	CLA	C6-C7-C8-C9
15	O	813	CLA	C6-C7-C8-C9
15	O	825	CLA	C11-C12-C13-C14
15	O	831	CLA	C11-C10-C8-C9
15	a	829	CLA	C11-C10-C8-C9
15	a	831	CLA	C6-C7-C8-C9
15	b	806	CLA	C14-C13-C15-C16
15	b	807	CLA	C14-C13-C15-C16
15	b	808	CLA	C11-C10-C8-C9
15	b	809	CLA	C6-C7-C8-C9
21	h	102	LMG	C15-C16-C17-C18
19	Y	101	LHG	C30-C31-C32-C33
14	a	826	F6C	C15-C16-C17-C18
21	j	206	LMG	C34-C35-C36-C37
20	A	853	LMT	O5'-C1'-O1'-C1
15	O	802	CLA	O1D-CGD-O2D-CED
19	a	851	LHG	C29-C30-C31-C32
14	b	810	F6C	C16-C17-C18-C19
15	b	823	CLA	C6-C7-C8-C10
15	B	813	CLA	O1D-CGD-O2D-CED
15	a	817	CLA	O1D-CGD-O2D-CED
15	b	836	CLA	O1D-CGD-O2D-CED
15	B	814	CLA	C3-C5-C6-C7
21	J	102	LMG	C12-C13-C14-C15
19	Z	101	LHG	O10-C23-O8-C6
19	k	101	LHG	C11-C10-C9-C8
21	L	206	LMG	C28-C29-C30-C31
15	N	813	CLA	C6-C7-C8-C9
19	W	1506	LHG	C33-C34-C35-C36
21	g	103	LMG	C29-C30-C31-C32
19	M	102	LHG	C33-C34-C35-C36
21	W	1505	LMG	C10-C11-C12-C13
15	B	802	CLA	C13-C15-C16-C17
15	N	839	CLA	CBA-CGA-O2A-C1
15	N	836	CLA	C4-C3-C5-C6
19	L	207	LHG	C33-C34-C35-C36
19	Y	101	LHG	C29-C30-C31-C32
18	a	857	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	B	806	CLA	C2-C3-C5-C6
15	N	806	CLA	C16-C17-C18-C20
15	O	823	CLA	C6-C7-C8-C10
15	b	815	CLA	CBD-CGD-O2D-CED
15	N	812	CLA	C8-C10-C11-C12
15	O	802	CLA	C15-C16-C17-C18
15	N	841	CLA	C15-C16-C17-C18
15	a	818	CLA	C5-C6-C7-C8
15	b	813	CLA	C5-C6-C7-C8
15	b	838	CLA	C10-C11-C12-C13
19	N	851	LHG	O9-C7-O7-C5
21	h	102	LMG	O9-C10-O7-C8
19	l	101	LHG	C11-C10-C9-C8
15	O	837	CLA	O1A-CGA-O2A-C1
15	A	825	CLA	CBA-CGA-O2A-C1
15	a	807	CLA	CBA-CGA-O2A-C1
15	b	813	CLA	CBA-CGA-O2A-C1
15	b	817	CLA	CBA-CGA-O2A-C1
15	N	830	CLA	C5-C6-C7-C8
15	B	837	CLA	O1D-CGD-O2D-CED
14	O	810	F6C	C16-C17-C18-C19
15	B	836	CLA	C10-C11-C12-C13
15	N	818	CLA	C5-C6-C7-C8
18	B	846	BCR	C7-C8-C9-C34
18	a	857	BCR	C36-C18-C19-C20
18	j	205	BCR	C37-C22-C23-C24
14	B	838	F6C	C11-C12-C13-C15
15	B	801	CLA	C11-C10-C8-C7
15	B	812	CLA	C11-C12-C13-C15
15	B	835	CLA	C12-C13-C15-C16
15	N	807	CLA	C11-C10-C8-C7
15	N	812	CLA	C11-C10-C8-C7
15	N	828	CLA	C6-C7-C8-C10
15	N	829	CLA	C11-C10-C8-C7
15	N	831	CLA	C6-C7-C8-C10
15	O	801	CLA	C11-C10-C8-C7
15	O	807	CLA	C12-C13-C15-C16
15	O	813	CLA	C6-C7-C8-C10
15	a	812	CLA	C11-C10-C8-C7
15	a	829	CLA	C11-C10-C8-C7
15	a	831	CLA	C6-C7-C8-C10
15	b	801	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
15	b	808	CLA	C11-C12-C13-C15
15	b	814	CLA	C11-C12-C13-C15
15	b	837	CLA	C12-C13-C15-C16
22	f	204	LFA	C5-C6-C7-C8
15	A	856	CLA	C15-C16-C17-C18
18	B	846	BCR	C7-C8-C9-C10
18	F	202	BCR	C11-C12-C13-C14
18	M	101	BCR	C17-C18-C19-C20
18	a	857	BCR	C7-C8-C9-C10
18	b	848	BCR	C7-C8-C9-C10
18	k	102	BCR	C17-C18-C19-C20
15	O	813	CLA	CBA-CGA-O2A-C1
19	l	101	LHG	C31-C32-C33-C34
14	A	802	F6C	C2A-CAA-CBA-CGA
14	A	824	F6C	C2A-CAA-CBA-CGA
14	N	802	F6C	C2A-CAA-CBA-CGA
14	N	824	F6C	C2A-CAA-CBA-CGA
14	a	802	F6C	C2A-CAA-CBA-CGA
14	a	824	F6C	C2A-CAA-CBA-CGA
15	A	807	CLA	O1A-CGA-O2A-C1
15	O	839	CLA	O1A-CGA-O2A-C1
15	a	825	CLA	O1A-CGA-O2A-C1
15	b	805	CLA	C15-C16-C17-C18
15	A	804	CLA	C2A-CAA-CBA-CGA
15	A	838	CLA	C2A-CAA-CBA-CGA
15	N	816	CLA	C2A-CAA-CBA-CGA
15	a	842	CLA	C2A-CAA-CBA-CGA
15	b	809	CLA	C2A-CAA-CBA-CGA
15	b	831	CLA	C2A-CAA-CBA-CGA
15	L	202	CLA	O1D-CGD-O2D-CED
19	L	207	LHG	O9-C7-O7-C5
21	h	102	LMG	C19-C20-C21-C22
15	B	830	CLA	C4-C3-C5-C6
15	a	834	CLA	C4-C3-C5-C6
15	A	832	CLA	O1A-CGA-O2A-C1
15	a	839	CLA	O1A-CGA-O2A-C1
15	b	822	CLA	O1A-CGA-O2A-C1
15	b	837	CLA	O1A-CGA-O2A-C1
15	b	839	CLA	O1A-CGA-O2A-C1
19	X	101	LHG	O10-C23-O8-C6
15	A	834	CLA	C2-C3-C5-C6
15	A	841	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	B	830	CLA	C2-C3-C5-C6
15	N	836	CLA	C2-C3-C5-C6
15	N	835	CLA	C5-C6-C7-C8
15	O	815	CLA	CBD-CGD-O2D-CED
13	N	801	CL0	O1A-CGA-O2A-C1
15	N	825	CLA	O1A-CGA-O2A-C1
15	A	814	CLA	CBD-CGD-O2D-CED
19	Y	101	LHG	C11-C12-C13-C14
19	Z	101	LHG	C14-C15-C16-C17
15	N	807	CLA	O1A-CGA-O2A-C1
15	a	811	CLA	C3-C5-C6-C7
15	B	804	CLA	C15-C16-C17-C18
15	O	827	CLA	C10-C11-C12-C13
15	b	839	CLA	C10-C11-C12-C13
21	A	855	LMG	C29-C30-C31-C32
20	A	853	LMT	C2-C3-C4-C5
20	N	853	LMT	O1'-C1-C2-C3
15	N	836	CLA	C5-C6-C7-C8
19	Z	101	LHG	C12-C13-C14-C15
19	k	101	LHG	C30-C31-C32-C33
15	A	828	CLA	C13-C15-C16-C17
19	A	851	LHG	O9-C7-O7-C5
19	X	102	LHG	O6-C4-C5-O7
21	U	102	LMG	C7-C8-C9-O8
14	A	824	F6C	C4B-C3B-CAB-CBB
14	A	857	F6C	C4B-C3B-CAB-CBB
14	N	824	F6C	C4B-C3B-CAB-CBB
14	N	856	F6C	C4B-C3B-CAB-CBB
14	a	824	F6C	C4B-C3B-CAB-CBB
14	a	856	F6C	C4B-C3B-CAB-CBB
15	A	833	CLA	C6-C7-C8-C10
15	O	801	CLA	C16-C17-C18-C20
15	f	201	CLA	C16-C17-C18-C20
22	B	848	LFA	C5-C6-C7-C8
15	L	203	CLA	C2A-CAA-CBA-CGA
15	N	842	CLA	C2A-CAA-CBA-CGA
15	W	1502	CLA	C2A-CAA-CBA-CGA
15	O	816	CLA	C5-C6-C7-C8
15	b	832	CLA	C8-C10-C11-C12
15	b	816	CLA	C3-C5-C6-C7
21	U	102	LMG	O7-C8-C9-O8
14	b	840	F6C	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	A	818	CLA	C14-C13-C15-C16
15	B	801	CLA	C11-C10-C8-C9
15	B	836	CLA	C14-C13-C15-C16
15	N	828	CLA	C6-C7-C8-C9
15	N	829	CLA	C11-C10-C8-C9
15	O	807	CLA	C14-C13-C15-C16
15	O	830	CLA	C11-C10-C8-C9
15	O	838	CLA	C14-C13-C15-C16
15	b	801	CLA	C11-C10-C8-C9
15	b	816	CLA	C6-C7-C8-C9
15	b	837	CLA	C14-C13-C15-C16
15	b	805	CLA	C16-C17-C18-C20
21	J	102	LMG	C30-C31-C32-C33
15	A	825	CLA	O1A-CGA-O2A-C1
15	B	837	CLA	O1A-CGA-O2A-C1
15	a	807	CLA	O1A-CGA-O2A-C1
15	b	813	CLA	O1A-CGA-O2A-C1
15	A	818	CLA	C5-C6-C7-C8
15	B	802	CLA	C10-C11-C12-C13
15	O	839	CLA	C10-C11-C12-C13
20	N	854	LMT	C9-C10-C11-C12
15	b	831	CLA	C8-C10-C11-C12
19	Z	101	LHG	C11-C10-C9-C8
19	Z	101	LHG	C31-C32-C33-C34
15	N	832	CLA	CBA-CGA-O2A-C1
15	N	806	CLA	C16-C17-C18-C19
15	a	806	CLA	C16-C17-C18-C20
19	Y	101	LHG	C33-C34-C35-C36
14	O	840	F6C	C3A-C2A-CAA-CBA
14	A	826	F6C	C15-C16-C17-C18
15	B	836	CLA	C5-C6-C7-C8
15	L	203	CLA	C10-C11-C12-C13
21	T	103	LMG	C32-C33-C34-C35
15	F	201	CLA	C16-C17-C18-C19
15	N	822	CLA	C16-C17-C18-C20
15	S	201	CLA	C16-C17-C18-C20
15	a	806	CLA	C16-C17-C18-C19
15	b	841	CLA	C13-C15-C16-C17
15	O	813	CLA	O1A-CGA-O2A-C1
15	b	817	CLA	O1A-CGA-O2A-C1
13	N	801	CL0	C3-C5-C6-C7
15	O	816	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	B	811	CLA	CBA-CGA-O2A-C1
19	M	102	LHG	C10-C11-C12-C13
21	U	102	LMG	C30-C31-C32-C33
19	Z	102	LHG	C31-C32-C33-C34
22	B	848	LFA	C13-C14-C15-C16
15	O	841	CLA	C16-C17-C18-C20
20	A	854	LMT	C9-C10-C11-C12
15	b	813	CLA	CBD-CGD-O2D-CED
21	J	102	LMG	C21-C22-C23-C24
15	B	801	CLA	C8-C10-C11-C12
21	B	847	LMG	C35-C36-C37-C38
15	A	811	CLA	C1A-C2A-CAA-CBA
15	A	819	CLA	C4B-C3B-CAB-CBB
15	A	825	CLA	C4B-C3B-CAB-CBB
15	A	839	CLA	C4B-C3B-CAB-CBB
15	A	841	CLA	C4B-C3B-CAB-CBB
15	A	842	CLA	C4B-C3B-CAB-CBB
15	B	810	CLA	C4B-C3B-CAB-CBB
15	B	818	CLA	C4B-C3B-CAB-CBB
15	B	824	CLA	C1A-C2A-CAA-CBA
15	B	839	CLA	C1A-C2A-CAA-CBA
15	B	839	CLA	C4B-C3B-CAB-CBB
15	F	201	CLA	C4B-C3B-CAB-CBB
15	K	103	CLA	C4B-C3B-CAB-CBB
15	N	819	CLA	C4B-C3B-CAB-CBB
15	N	825	CLA	C4B-C3B-CAB-CBB
15	N	838	CLA	C1A-C2A-CAA-CBA
15	N	841	CLA	C4B-C3B-CAB-CBB
15	N	842	CLA	C4B-C3B-CAB-CBB
15	O	812	CLA	C4B-C3B-CAB-CBB
15	O	820	CLA	C4B-C3B-CAB-CBB
15	O	841	CLA	C4B-C3B-CAB-CBB
15	V	102	CLA	C1A-C2A-CAA-CBA
15	V	103	CLA	C4B-C3B-CAB-CBB
15	a	819	CLA	C4B-C3B-CAB-CBB
15	a	825	CLA	C4B-C3B-CAB-CBB
15	a	839	CLA	C4B-C3B-CAB-CBB
15	a	841	CLA	C4B-C3B-CAB-CBB
15	a	842	CLA	C4B-C3B-CAB-CBB
15	b	812	CLA	C4B-C3B-CAB-CBB
15	b	820	CLA	C4B-C3B-CAB-CBB
15	b	826	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	b	830	CLA	C1A-C2A-CAA-CBA
15	b	841	CLA	C4B-C3B-CAB-CBB
15	i	103	CLA	C4B-C3B-CAB-CBB
15	B	829	CLA	O1D-CGD-O2D-CED
15	O	822	CLA	CBA-CGA-O2A-C1
15	O	831	CLA	C4-C3-C5-C6
18	L	205	BCR	C21-C22-C23-C24
18	N	857	BCR	C7-C8-C9-C10
18	A	858	BCR	C15-C16-C17-C18
15	O	805	CLA	C16-C17-C18-C20
15	a	839	CLA	C3-C5-C6-C7
15	B	837	CLA	C10-C11-C12-C13
19	M	102	LHG	C26-C27-C28-C29
19	Y	101	LHG	C25-C26-C27-C28
15	B	802	CLA	C2A-CAA-CBA-CGA
14	B	838	F6C	C1A-C2A-CAA-CBA
19	X	102	LHG	O6-C4-C5-C6
15	A	823	CLA	CBD-CGD-O2D-CED
15	B	811	CLA	CBD-CGD-O2D-CED
19	k	101	LHG	C28-C29-C30-C31
14	N	824	F6C	C2-C3-C5-C6
15	N	820	CLA	C15-C16-C17-C18
14	N	856	F6C	C11-C10-C8-C7
14	W	1503	F6C	C11-C10-C8-C7
14	W	1503	F6C	C11-C12-C13-C15
14	b	840	F6C	C11-C12-C13-C15
14	j	204	F6C	C11-C10-C8-C7
15	A	805	CLA	C6-C7-C8-C10
15	A	820	CLA	C11-C12-C13-C15
15	B	805	CLA	C6-C7-C8-C10
15	B	807	CLA	C11-C10-C8-C7
15	B	807	CLA	C11-C12-C13-C15
15	B	815	CLA	C11-C12-C13-C15
15	N	820	CLA	C11-C12-C13-C15
15	O	808	CLA	C11-C12-C13-C15
15	O	814	CLA	C11-C10-C8-C7
15	a	814	CLA	C11-C10-C8-C7
15	a	820	CLA	C11-C12-C13-C15
15	b	814	CLA	C11-C10-C8-C7
15	A	806	CLA	C16-C17-C18-C19
15	O	811	CLA	C16-C17-C18-C20
14	N	824	F6C	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	N	801	CL0	CAA-CBA-CGA-O2A
15	B	820	CLA	CBA-CGA-O2A-C1
21	L	206	LMG	C36-C37-C38-C39
22	B	848	LFA	C3-C4-C5-C6
15	N	811	CLA	C3-C5-C6-C7
19	Z	101	LHG	C5-C4-O6-P
15	N	821	CLA	C3A-C2A-CAA-CBA
20	a	854	LMT	C9-C10-C11-C12
15	B	811	CLA	C5-C6-C7-C8
19	Z	102	LHG	O6-C4-C5-O7
14	B	838	F6C	C11-C12-C13-C14
14	j	204	F6C	C11-C10-C8-C9
15	A	818	CLA	C11-C12-C13-C14
15	A	828	CLA	C6-C7-C8-C9
15	B	809	CLA	C6-C7-C8-C9
15	B	812	CLA	C11-C10-C8-C9
15	B	835	CLA	C14-C13-C15-C16
15	N	812	CLA	C11-C10-C8-C9
15	N	818	CLA	C11-C12-C13-C14
15	O	837	CLA	C14-C13-C15-C16
15	a	805	CLA	C6-C7-C8-C9
15	a	812	CLA	C11-C10-C8-C9
15	b	808	CLA	C11-C12-C13-C14
15	B	811	CLA	O1A-CGA-O2A-C1
15	N	839	CLA	O1A-CGA-O2A-C1
13	a	801	CL0	C10-C11-C12-C13
15	O	803	CLA	C15-C16-C17-C18
15	W	1502	CLA	C8-C10-C11-C12
15	b	828	CLA	C15-C16-C17-C18
21	U	102	LMG	C12-C13-C14-C15
18	N	857	BCR	C15-C16-C17-C18
18	a	845	BCR	C15-C16-C17-C18
14	A	824	F6C	O1D-CGD-O2D-CED
15	A	818	CLA	C13-C15-C16-C17
15	O	831	CLA	C8-C10-C11-C12
15	b	801	CLA	C8-C10-C11-C12
21	h	102	LMG	C12-C13-C14-C15
14	A	826	F6C	C1B-C2B-CMB-OMB
14	B	831	F6C	C1B-C2B-CMB-OMB
14	N	824	F6C	C1B-C2B-CMB-OMB
14	N	826	F6C	C1B-C2B-CMB-OMB
14	a	856	F6C	C1B-C2B-CMB-OMB

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Mol	Chain	Res	Type	Atoms
15	N	832	CLA	O1A-CGA-O2A-C1
15	N	817	CLA	O1D-CGD-O2D-CED
19	l	102	LHG	C34-C35-C36-C37
15	N	803	CLA	C8-C10-C11-C12
15	b	805	CLA	C16-C17-C18-C19
14	N	802	F6C	O1D-CGD-O2D-CED
15	A	816	CLA	CAD-CBD-CGD-O2D
15	A	856	CLA	CAD-CBD-CGD-O2D
15	B	804	CLA	CAD-CBD-CGD-O2D
15	B	819	CLA	CAD-CBD-CGD-O2D
15	B	821	CLA	CAD-CBD-CGD-O2D
15	N	816	CLA	CAD-CBD-CGD-O2D
15	O	802	CLA	CAD-CBD-CGD-O2D
15	O	821	CLA	CAD-CBD-CGD-O2D
15	O	823	CLA	CAD-CBD-CGD-O2D
15	a	816	CLA	CAD-CBD-CGD-O2D
15	b	802	CLA	CAD-CBD-CGD-O2D
15	b	821	CLA	CAD-CBD-CGD-O2D
15	O	822	CLA	O1A-CGA-O2A-C1
15	A	803	CLA	CBA-CGA-O2A-C1
15	a	803	CLA	CBA-CGA-O2A-C1
15	A	835	CLA	C5-C6-C7-C8
15	a	818	CLA	C13-C15-C16-C17
15	A	822	CLA	C16-C17-C18-C20
15	B	809	CLA	C16-C17-C18-C20
15	N	822	CLA	C16-C17-C18-C19
15	N	831	CLA	C16-C17-C18-C20
15	a	831	CLA	C16-C17-C18-C20
15	a	833	CLA	C6-C7-C8-C10
15	b	811	CLA	C16-C17-C18-C20
15	f	201	CLA	C16-C17-C18-C19
19	Z	101	LHG	C33-C34-C35-C36
15	A	816	CLA	C2A-CAA-CBA-CGA
15	O	829	CLA	C2A-CAA-CBA-CGA
15	a	816	CLA	C2A-CAA-CBA-CGA
15	a	838	CLA	C2A-CAA-CBA-CGA
15	a	828	CLA	C13-C15-C16-C17
15	B	820	CLA	O1A-CGA-O2A-C1
19	j	207	LHG	C33-C34-C35-C36
13	N	801	CL0	CHA-CBD-CGD-O2D
13	a	801	CL0	CHA-CBD-CGD-O1D
13	a	801	CL0	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
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	856	CLA	CAD-CBD-CGD-O1D
15	B	804	CLA	CAD-CBD-CGD-O1D
15	B	807	CLA	CHA-CBD-CGD-O1D
15	B	807	CLA	CHA-CBD-CGD-O2D
15	B	819	CLA	CAD-CBD-CGD-O1D
15	B	821	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	O	802	CLA	CAD-CBD-CGD-O1D
15	O	808	CLA	CHA-CBD-CGD-O1D
15	O	808	CLA	CHA-CBD-CGD-O2D
15	O	821	CLA	CAD-CBD-CGD-O1D
15	O	823	CLA	CAD-CBD-CGD-O1D
15	V	102	CLA	CHA-CBD-CGD-O1D
15	V	102	CLA	CHA-CBD-CGD-O2D
15	a	806	CLA	CAD-CBD-CGD-O1D
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	831	CLA	CHA-CBD-CGD-O1D
15	b	802	CLA	CAD-CBD-CGD-O1D
15	b	806	CLA	CHA-CBD-CGD-O1D
15	b	808	CLA	CHA-CBD-CGD-O1D
15	b	808	CLA	CHA-CBD-CGD-O2D
15	b	821	CLA	CAD-CBD-CGD-O1D
18	B	845	BCR	C19-C20-C21-C22
18	O	847	BCR	C19-C20-C21-C22
19	L	207	LHG	C3-O3-P-O4
19	X	101	LHG	C3-O3-P-O5
19	X	101	LHG	C3-O3-P-O6
19	X	101	LHG	C4-O6-P-O5
19	W	1506	LHG	C3-O3-P-O4
19	W	1506	LHG	C3-O3-P-O6
19	Z	101	LHG	C3-O3-P-O5
19	Z	101	LHG	C4-O6-P-O5
19	a	851	LHG	C3-O3-P-O5
19	j	207	LHG	C3-O3-P-O4
19	l	101	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
19	l	101	LHG	C4-O6-P-O5
15	B	814	CLA	C5-C6-C7-C8
21	h	102	LMG	C29-C30-C31-C32
15	A	819	CLA	C2B-C3B-CAB-CBB
15	A	825	CLA	C2B-C3B-CAB-CBB
15	A	839	CLA	C2B-C3B-CAB-CBB
15	B	810	CLA	C2B-C3B-CAB-CBB
15	B	839	CLA	C2B-C3B-CAB-CBB
15	K	103	CLA	C2B-C3B-CAB-CBB
15	N	819	CLA	C2B-C3B-CAB-CBB
15	N	825	CLA	C2B-C3B-CAB-CBB
15	O	812	CLA	C2B-C3B-CAB-CBB
15	O	841	CLA	C2B-C3B-CAB-CBB
15	S	201	CLA	C2B-C3B-CAB-CBB
15	V	103	CLA	C2B-C3B-CAB-CBB
15	a	819	CLA	C2B-C3B-CAB-CBB
15	a	839	CLA	C2B-C3B-CAB-CBB
15	b	841	CLA	C2B-C3B-CAB-CBB
15	i	103	CLA	C2B-C3B-CAB-CBB
18	a	847	BCR	C23-C24-C25-C30
18	b	848	BCR	C5-C6-C7-C8
19	M	102	LHG	C28-C29-C30-C31
15	a	834	CLA	C2-C3-C5-C6
15	B	836	CLA	C13-C15-C16-C17
18	A	858	BCR	C36-C18-C19-C20
15	A	803	CLA	C8-C10-C11-C12
15	B	807	CLA	C8-C10-C11-C12
15	A	806	CLA	C16-C17-C18-C20
15	A	836	CLA	C5-C6-C7-C8
15	N	809	CLA	CBD-CGD-O2D-CED
15	N	812	CLA	CBA-CGA-O2A-C1
20	a	853	LMT	O1'-C1-C2-C3
19	Z	102	LHG	C35-C36-C37-C38
19	X	101	LHG	C33-C34-C35-C36
15	N	818	CLA	C13-C15-C16-C17
15	a	834	CLA	C16-C17-C18-C20
15	A	841	CLA	C13-C15-C16-C17
19	X	102	LHG	C14-C15-C16-C17
15	N	834	CLA	C4-C3-C5-C6
15	A	814	CLA	C5-C6-C7-C8
15	A	830	CLA	C5-C6-C7-C8
15	O	831	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	j	206	LMG	C30-C31-C32-C33
22	O	851	LFA	C5-C6-C7-C8
15	b	815	CLA	O1D-CGD-O2D-CED
15	S	201	CLA	C16-C17-C18-C19
15	a	822	CLA	C16-C17-C18-C20
19	Y	101	LHG	C26-C27-C28-C29
19	l	101	LHG	C14-C15-C16-C17
19	Z	102	LHG	O6-C4-C5-C6
15	O	832	CLA	CAA-CBA-CGA-O2A
14	B	838	F6C	C6-C7-C8-C9
14	O	840	F6C	C11-C12-C13-C14
15	A	812	CLA	C11-C10-C8-C9
15	A	839	CLA	C11-C10-C8-C9
15	N	805	CLA	C6-C7-C8-C9
15	N	818	CLA	C14-C13-C15-C16
15	N	822	CLA	C11-C10-C8-C9
15	O	816	CLA	C6-C7-C8-C9
15	O	841	CLA	C11-C12-C13-C14
15	a	810	CLA	C11-C10-C8-C9
15	a	818	CLA	C11-C12-C13-C14
15	a	818	CLA	C14-C13-C15-C16
15	b	814	CLA	C11-C10-C8-C9
15	b	838	CLA	C14-C13-C15-C16
15	A	804	CLA	C6-C7-C8-C10
15	A	807	CLA	C11-C10-C8-C7
15	A	839	CLA	C11-C10-C8-C7
15	O	806	CLA	C6-C7-C8-C10
15	O	827	CLA	C6-C7-C8-C10
15	W	1502	CLA	C11-C10-C8-C7
15	a	807	CLA	C11-C10-C8-C7
15	b	806	CLA	C6-C7-C8-C10
15	b	830	CLA	C11-C12-C13-C15
15	B	804	CLA	CBD-CGD-O2D-CED
15	N	820	CLA	C16-C17-C18-C20
15	L	202	CLA	C15-C16-C17-C18
15	b	832	CLA	CAA-CBA-CGA-O2A
19	j	207	LHG	C9-C10-C11-C12
15	N	812	CLA	O1A-CGA-O2A-C1
15	a	803	CLA	O1A-CGA-O2A-C1
15	N	803	CLA	CBA-CGA-O2A-C1
15	A	822	CLA	C16-C17-C18-C19
15	B	804	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	N	834	CLA	C16-C17-C18-C20
15	O	805	CLA	C16-C17-C18-C19
21	O	850	LMG	C31-C32-C33-C34
19	X	101	LHG	C5-C4-O6-P
19	l	101	LHG	C5-C4-O6-P
15	a	832	CLA	CBA-CGA-O2A-C1
18	A	845	BCR	C15-C16-C17-C18
18	I	101	BCR	C9-C10-C11-C12
19	W	1506	LHG	C29-C30-C31-C32
15	B	837	CLA	C16-C17-C18-C20
15	N	833	CLA	C6-C7-C8-C10
15	O	815	CLA	O1D-CGD-O2D-CED
15	O	825	CLA	C10-C11-C12-C13
14	L	201	F6C	C2-C1-O2A-CGA
15	L	203	CLA	C4-C3-C5-C6
15	W	1502	CLA	C4-C3-C5-C6
21	A	855	LMG	C20-C21-C22-C23
15	B	830	CLA	CAA-CBA-CGA-O2A
15	j	203	CLA	C8-C10-C11-C12
18	j	201	BCR	C7-C8-C9-C34
15	A	834	CLA	C16-C17-C18-C20
15	B	829	CLA	C10-C11-C12-C13
13	a	801	CL0	C3-C5-C6-C7
15	A	803	CLA	O1A-CGA-O2A-C1
15	N	806	CLA	C10-C11-C12-C13
15	A	814	CLA	C2A-CAA-CBA-CGA
15	N	838	CLA	C2A-CAA-CBA-CGA
15	a	837	CLA	C2A-CAA-CBA-CGA
15	b	803	CLA	C2A-CAA-CBA-CGA
19	l	101	LHG	C28-C29-C30-C31
15	B	820	CLA	C4-C3-C5-C6
15	a	830	CLA	C4-C3-C5-C6
15	b	831	CLA	C4-C3-C5-C6
15	j	203	CLA	C4-C3-C5-C6
14	N	856	F6C	C5-C6-C7-C8
15	a	832	CLA	O1A-CGA-O2A-C1
15	B	825	CLA	C2-C3-C5-C6
22	O	851	LFA	C3-C4-C5-C6
15	O	803	CLA	C2C-C3C-CAC-CBC
15	A	814	CLA	O1D-CGD-O2D-CED
13	a	801	CL0	CAA-CBA-CGA-O1A
15	N	821	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	a	821	CLA	CAA-CBA-CGA-O1A
15	A	805	CLA	C6-C7-C8-C9
15	B	807	CLA	C11-C10-C8-C9
15	B	807	CLA	C11-C12-C13-C14
15	N	807	CLA	C11-C12-C13-C14
15	N	839	CLA	C14-C13-C15-C16
15	O	841	CLA	C14-C13-C15-C16
15	a	814	CLA	C11-C10-C8-C9
15	b	811	CLA	C6-C7-C8-C9
14	N	824	F6C	O1D-CGD-O2D-CED
15	B	801	CLA	C4B-C3B-CAB-CBB
15	O	830	CLA	C4B-C3B-CAB-CBB
15	S	201	CLA	C4B-C3B-CAB-CBB
15	b	801	CLA	C4B-C3B-CAB-CBB
15	f	201	CLA	C4B-C3B-CAB-CBB
15	O	820	CLA	C6-C7-C8-C10
15	a	815	CLA	C6-C7-C8-C9
15	a	820	CLA	C15-C16-C17-C18
15	j	202	CLA	C15-C16-C17-C18
15	N	803	CLA	O1A-CGA-O2A-C1
15	b	829	CLA	C2A-CAA-CBA-CGA
19	Y	101	LHG	C11-C10-C9-C8
14	a	826	F6C	CBD-CGD-O2D-CED
19	Z	102	LHG	C14-C15-C16-C17
15	a	822	CLA	C16-C17-C18-C19
20	A	853	LMT	C5'-C4'-O1B-C1B
20	a	853	LMT	C5'-C4'-O1B-C1B
19	X	101	LHG	C9-C10-C11-C12
15	B	804	CLA	O1D-CGD-O2D-CED
14	L	204	F6C	C11-C10-C8-C7
14	N	856	F6C	C6-C7-C8-C10
15	A	807	CLA	C11-C12-C13-C15
15	B	828	CLA	C11-C12-C13-C15
15	B	830	CLA	C11-C10-C8-C7
15	a	806	CLA	C6-C7-C8-C10
15	a	839	CLA	C11-C10-C8-C7
15	a	841	CLA	C6-C7-C8-C10
15	b	827	CLA	C6-C7-C8-C10
15	b	832	CLA	C11-C10-C8-C7
15	L	203	CLA	C8-C10-C11-C12
15	A	856	CLA	CBD-CGD-O2D-CED
15	a	838	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	b	838	CLA	C13-C15-C16-C17
15	A	833	CLA	C6-C7-C8-C9
15	B	804	CLA	C16-C17-C18-C19
15	N	809	CLA	O1D-CGD-O2D-CED
15	O	831	CLA	C10-C11-C12-C13
15	b	825	CLA	C10-C11-C12-C13
15	B	802	CLA	C2C-C3C-CAC-CBC
15	A	810	CLA	C3A-C2A-CAA-CBA
15	A	821	CLA	C3A-C2A-CAA-CBA
15	B	833	CLA	C3A-C2A-CAA-CBA
15	L	203	CLA	C3A-C2A-CAA-CBA
15	N	810	CLA	C3A-C2A-CAA-CBA
15	a	810	CLA	C3A-C2A-CAA-CBA
15	a	821	CLA	C3A-C2A-CAA-CBA
15	W	1502	CLA	C2-C3-C5-C6
15	O	838	CLA	C13-C15-C16-C17
15	B	837	CLA	C16-C17-C18-C19
21	a	855	LMG	C18-C19-C20-C21
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	A	858	BCR	C16-C17-C18-C36
18	B	842	BCR	C11-C10-C9-C34
18	B	843	BCR	C11-C10-C9-C34
18	B	843	BCR	C20-C21-C22-C37
18	F	203	BCR	C35-C13-C14-C15
18	I	102	BCR	C20-C21-C22-C37
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	N	857	BCR	C16-C17-C18-C36
18	O	844	BCR	C11-C10-C9-C34
18	O	845	BCR	C11-C10-C9-C34
18	O	845	BCR	C20-C21-C22-C37
18	S	202	BCR	C35-C13-C14-C15
18	T	102	BCR	C20-C21-C22-C37
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	a	857	BCR	C16-C17-C18-C36
18	b	844	BCR	C11-C10-C9-C34
18	b	845	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
18	b	845	BCR	C20-C21-C22-C37
18	f	203	BCR	C35-C13-C14-C15
18	g	102	BCR	C20-C21-C22-C37
15	a	812	CLA	C3-C5-C6-C7
15	N	821	CLA	C5-C6-C7-C8
19	k	101	LHG	C29-C30-C31-C32
15	A	820	CLA	C15-C16-C17-C18
22	O	851	LFA	C10-C11-C12-C13
22	f	204	LFA	C3-C4-C5-C6
15	a	832	CLA	C2-C1-O2A-CGA
18	B	845	BCR	C15-C16-C17-C18
18	b	847	BCR	C19-C20-C21-C22
15	L	202	CLA	C16-C17-C18-C19
15	O	801	CLA	C8-C10-C11-C12
15	W	1501	CLA	C15-C16-C17-C18
15	a	806	CLA	C10-C11-C12-C13
14	N	824	F6C	C4-C3-C5-C6
19	Y	101	LHG	C27-C28-C29-C30
13	a	801	CL0	C13-C15-C16-C17
14	A	857	F6C	C5-C6-C7-C8
15	b	803	CLA	C10-C11-C12-C13
15	N	813	CLA	C4-C3-C5-C6
21	B	847	LMG	C41-C42-C43-C44
15	O	822	CLA	CAA-CBA-CGA-O1A
15	A	823	CLA	O1D-CGD-O2D-CED
19	M	102	LHG	C27-C28-C29-C30
19	k	101	LHG	C26-C27-C28-C29
15	B	806	CLA	C2A-CAA-CBA-CGA
15	B	827	CLA	C2A-CAA-CBA-CGA
15	B	823	CLA	C10-C11-C12-C13
15	N	842	CLA	C13-C15-C16-C17
15	a	821	CLA	C5-C6-C7-C8
14	N	826	F6C	O1A-CGA-O2A-C1
14	W	1503	F6C	C11-C10-C8-C9
14	b	840	F6C	C11-C12-C13-C14
15	A	806	CLA	C6-C7-C8-C9
15	A	807	CLA	C11-C12-C13-C14
15	A	820	CLA	C11-C12-C13-C14
15	A	842	CLA	C11-C10-C8-C9
15	B	808	CLA	C11-C12-C13-C14
15	B	814	CLA	C6-C7-C8-C9
15	B	830	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
15	B	836	CLA	C11-C12-C13-C14
15	L	202	CLA	C11-C10-C8-C9
15	N	806	CLA	C6-C7-C8-C9
15	N	819	CLA	C11-C10-C8-C9
15	O	809	CLA	C6-C7-C8-C9
15	O	814	CLA	C11-C10-C8-C9
15	O	831	CLA	C14-C13-C15-C16
15	O	832	CLA	C6-C7-C8-C9
15	O	838	CLA	C11-C12-C13-C14
15	a	806	CLA	C6-C7-C8-C9
15	a	807	CLA	C11-C12-C13-C14
15	a	820	CLA	C6-C7-C8-C9
15	a	839	CLA	C11-C10-C8-C9
15	a	841	CLA	C6-C7-C8-C9
15	a	841	CLA	C11-C12-C13-C14
15	a	842	CLA	C11-C10-C8-C9
15	b	808	CLA	C6-C7-C8-C9
15	b	811	CLA	C14-C13-C15-C16
15	b	832	CLA	C11-C10-C8-C9
15	b	838	CLA	C11-C12-C13-C14
19	L	207	LHG	C31-C32-C33-C34
21	J	102	LMG	C29-C30-C31-C32
15	O	801	CLA	C16-C17-C18-C19
21	J	102	LMG	C18-C19-C20-C21
21	g	103	LMG	C30-C31-C32-C33
14	N	826	F6C	C5-C6-C7-C8
15	N	838	CLA	C3-C5-C6-C7
15	A	839	CLA	C4-C3-C5-C6
15	A	831	CLA	C16-C17-C18-C20
15	L	203	CLA	C2-C3-C5-C6
15	a	830	CLA	C2-C3-C5-C6
15	b	831	CLA	C2-C3-C5-C6
15	A	837	CLA	C2A-CAA-CBA-CGA
15	N	814	CLA	C2A-CAA-CBA-CGA
15	O	803	CLA	C2A-CAA-CBA-CGA
15	O	807	CLA	C2A-CAA-CBA-CGA
13	A	801	CL0	CAA-CBA-CGA-O1A
15	A	829	CLA	C10-C11-C12-C13
15	B	809	CLA	C1A-C2A-CAA-CBA
15	K	102	CLA	C1A-C2A-CAA-CBA
15	N	821	CLA	C1A-C2A-CAA-CBA
15	O	811	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
15	a	811	CLA	C1A-C2A-CAA-CBA
15	i	102	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	A	858	BCR	C16-C17-C18-C19
18	B	842	BCR	C11-C10-C9-C8
18	B	843	BCR	C11-C10-C9-C8
18	B	843	BCR	C20-C21-C22-C23
18	F	203	BCR	C12-C13-C14-C15
18	I	102	BCR	C20-C21-C22-C23
18	N	848	BCR	C16-C17-C18-C19
18	N	850	BCR	C11-C10-C9-C8
18	N	850	BCR	C16-C17-C18-C19
18	N	857	BCR	C16-C17-C18-C19
18	O	844	BCR	C11-C10-C9-C8
18	O	845	BCR	C11-C10-C9-C8
18	O	845	BCR	C20-C21-C22-C23
18	S	202	BCR	C12-C13-C14-C15
18	T	102	BCR	C20-C21-C22-C23
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	a	857	BCR	C16-C17-C18-C19
18	b	844	BCR	C11-C10-C9-C8
18	b	845	BCR	C11-C10-C9-C8
18	b	845	BCR	C20-C21-C22-C23
18	f	203	BCR	C12-C13-C14-C15
18	g	102	BCR	C20-C21-C22-C23
15	b	803	CLA	C13-C15-C16-C17
15	O	841	CLA	C13-C15-C16-C17
15	A	807	CLA	C2B-C3B-CAB-CBB
15	A	822	CLA	C2B-C3B-CAB-CBB
15	A	841	CLA	C2B-C3B-CAB-CBB
15	A	842	CLA	C2B-C3B-CAB-CBB
15	B	808	CLA	C2B-C3B-CAB-CBB
15	B	818	CLA	C2B-C3B-CAB-CBB
15	F	201	CLA	C2B-C3B-CAB-CBB
15	N	822	CLA	C2B-C3B-CAB-CBB
15	N	841	CLA	C2B-C3B-CAB-CBB
15	N	842	CLA	C2B-C3B-CAB-CBB
15	O	820	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	O	830	CLA	C2B-C3B-CAB-CBB
15	a	822	CLA	C2B-C3B-CAB-CBB
15	a	825	CLA	C2B-C3B-CAB-CBB
15	a	841	CLA	C2B-C3B-CAB-CBB
15	a	842	CLA	C2B-C3B-CAB-CBB
15	b	812	CLA	C2B-C3B-CAB-CBB
15	b	820	CLA	C2B-C3B-CAB-CBB
15	f	201	CLA	C2B-C3B-CAB-CBB
18	A	846	BCR	C23-C24-C25-C26
18	A	847	BCR	C23-C24-C25-C30
18	A	849	BCR	C1-C6-C7-C8
18	A	850	BCR	C5-C6-C7-C8
18	A	858	BCR	C1-C6-C7-C8
18	B	844	BCR	C23-C24-C25-C26
18	B	844	BCR	C23-C24-C25-C30
18	I	102	BCR	C23-C24-C25-C26
18	I	102	BCR	C23-C24-C25-C30
18	L	209	BCR	C5-C6-C7-C8
18	N	847	BCR	C23-C24-C25-C30
18	N	849	BCR	C1-C6-C7-C8
18	N	850	BCR	C5-C6-C7-C8
18	O	843	BCR	C23-C24-C25-C26
18	O	846	BCR	C23-C24-C25-C30
18	T	102	BCR	C23-C24-C25-C26
18	T	102	BCR	C23-C24-C25-C30
18	W	1508	BCR	C5-C6-C7-C8
18	a	849	BCR	C1-C6-C7-C8
18	a	850	BCR	C5-C6-C7-C8
18	b	846	BCR	C23-C24-C25-C30
18	j	201	BCR	C5-C6-C7-C8
18	j	201	BCR	C23-C24-C25-C26
14	A	802	F6C	CBD-CGD-O2D-CED
19	Y	101	LHG	C28-C29-C30-C31
21	W	1505	LMG	C35-C36-C37-C38
15	B	801	CLA	C16-C17-C18-C20
15	A	813	CLA	C4-C3-C5-C6
15	N	830	CLA	C4-C3-C5-C6
15	j	203	CLA	C2-C3-C5-C6
15	O	826	CLA	C15-C16-C17-C18
14	A	857	F6C	C11-C10-C8-C7
14	L	204	F6C	C12-C13-C15-C16
14	a	856	F6C	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
15	A	814	CLA	C6-C7-C8-C10
15	A	814	CLA	C11-C10-C8-C7
15	B	823	CLA	C12-C13-C15-C16
15	B	835	CLA	C6-C7-C8-C10
15	L	203	CLA	C11-C10-C8-C7
15	N	804	CLA	C6-C7-C8-C10
15	N	807	CLA	C11-C12-C13-C15
15	N	814	CLA	C11-C10-C8-C7
15	N	821	CLA	C11-C10-C8-C7
15	N	839	CLA	C12-C13-C15-C16
15	O	809	CLA	C6-C7-C8-C10
15	O	825	CLA	C12-C13-C15-C16
15	O	832	CLA	C6-C7-C8-C10
15	O	837	CLA	C6-C7-C8-C10
15	O	841	CLA	C12-C13-C15-C16
15	a	807	CLA	C11-C12-C13-C15
15	a	818	CLA	C11-C10-C8-C7
15	a	819	CLA	C6-C7-C8-C10
15	b	811	CLA	C6-C7-C8-C10
15	b	825	CLA	C12-C13-C15-C16
15	b	837	CLA	C6-C7-C8-C10
19	a	851	LHG	O10-C23-C24-C25
15	a	835	CLA	C16-C17-C18-C20
15	N	837	CLA	C2A-CAA-CBA-CGA
15	a	814	CLA	C2A-CAA-CBA-CGA
15	b	807	CLA	C2A-CAA-CBA-CGA
15	b	827	CLA	C2A-CAA-CBA-CGA
15	N	808	CLA	CBD-CGD-O2D-CED
20	N	853	LMT	C5'-C4'-O1B-C1B
15	a	822	CLA	C15-C16-C17-C18
21	I	103	LMG	C32-C33-C34-C35
21	L	206	LMG	C18-C19-C20-C21
14	N	824	F6C	C1A-C2A-CAA-CBA
15	B	811	CLA	C11-C10-C8-C7
15	O	813	CLA	C11-C10-C8-C7
15	b	813	CLA	C11-C10-C8-C7
15	W	1502	CLA	C10-C11-C12-C13
15	a	814	CLA	C10-C11-C12-C13
18	O	846	BCR	C36-C18-C19-C20
15	b	822	CLA	C4-C3-C5-C6
15	b	801	CLA	CAA-CBA-CGA-O2A
15	N	822	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	N	834	CLA	C2-C3-C5-C6
19	k	101	LHG	C10-C11-C12-C13
15	B	811	CLA	O1D-CGD-O2D-CED
19	l	101	LHG	C33-C34-C35-C36
15	O	839	CLA	C16-C17-C18-C20
14	a	826	F6C	O1D-CGD-O2D-CED
15	a	829	CLA	C10-C11-C12-C13
15	a	835	CLA	C5-C6-C7-C8
15	b	813	CLA	O1D-CGD-O2D-CED
15	b	817	CLA	CBD-CGD-O2D-CED
19	X	102	LHG	C13-C14-C15-C16
15	B	804	CLA	C2A-CAA-CBA-CGA
15	b	805	CLA	C2A-CAA-CBA-CGA
15	N	809	CLA	C11-C10-C8-C9
15	O	809	CLA	C11-C12-C13-C14
15	b	832	CLA	C6-C7-C8-C9
15	j	203	CLA	C6-C7-C8-C9
15	a	841	CLA	C15-C16-C17-C18
21	h	102	LMG	C38-C39-C40-C41
21	g	103	LMG	C12-C13-C14-C15
14	a	856	F6C	C5-C6-C7-C8
13	A	801	CL0	C15-C16-C17-C18
15	O	820	CLA	C6-C7-C8-C9
15	b	820	CLA	C6-C7-C8-C10
19	l	102	LHG	C13-C14-C15-C16
20	A	853	LMT	C2'-C1'-O1'-C1
13	N	801	CL0	C15-C16-C17-C18
15	A	806	CLA	C10-C11-C12-C13
15	B	839	CLA	C13-C15-C16-C17
15	O	808	CLA	C5-C6-C7-C8
19	A	851	LHG	C12-C13-C14-C15
19	M	102	LHG	C30-C31-C32-C33
19	X	102	LHG	C35-C36-C37-C38
14	A	802	F6C	O1D-CGD-O2D-CED
15	B	825	CLA	C2A-CAA-CBA-CGA
15	N	829	CLA	C2A-CAA-CBA-CGA
15	O	805	CLA	C2A-CAA-CBA-CGA
15	a	829	CLA	C2A-CAA-CBA-CGA
15	N	803	CLA	C15-C16-C17-C18
19	Y	101	LHG	O1-C1-C2-O2
19	k	101	LHG	O1-C1-C2-O2
19	l	102	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	l	102	LHG	O6-C4-C5-O7
15	A	830	CLA	C4-C3-C5-C6
15	N	839	CLA	C4-C3-C5-C6
15	O	822	CLA	C4-C3-C5-C6
15	a	822	CLA	C4-C3-C5-C6
15	i	102	CLA	CAA-CBA-CGA-O2A
19	M	102	LHG	C11-C12-C13-C14
15	A	822	CLA	C4B-C3B-CAB-CBB
15	N	835	CLA	C4B-C3B-CAB-CBB
15	O	809	CLA	C4B-C3B-CAB-CBB
15	b	809	CLA	C4B-C3B-CAB-CBB
19	M	102	LHG	C29-C30-C31-C32
22	B	848	LFA	C10-C11-C12-C13
15	A	819	CLA	CAA-CBA-CGA-O2A
15	N	819	CLA	CAA-CBA-CGA-O2A
14	j	204	F6C	C16-C17-C18-C19
15	A	820	CLA	C16-C17-C18-C20
15	A	839	CLA	C16-C17-C18-C20
15	a	815	CLA	C6-C7-C8-C10
15	B	820	CLA	CAA-CBA-CGA-O1A
15	A	822	CLA	C15-C16-C17-C18
13	A	801	CL0	CHA-CBD-CGD-O1D
13	A	801	CL0	CHA-CBD-CGD-O2D
13	N	801	CL0	CHA-CBD-CGD-O1D
15	b	838	CLA	C5-C6-C7-C8
15	b	803	CLA	C2C-C3C-CAC-CBC
22	f	204	LFA	C10-C11-C12-C13
15	A	856	CLA	O1D-CGD-O2D-CED
15	a	820	CLA	C16-C17-C18-C20
15	N	835	CLA	C4-C3-C5-C6
15	b	822	CLA	CAA-CBA-CGA-O1A
21	a	855	LMG	C29-C30-C31-C32
20	N	852	LMT	O5'-C1'-O1'-C1
15	A	839	CLA	C15-C16-C17-C18
15	O	838	CLA	C5-C6-C7-C8
15	A	818	CLA	C11-C10-C8-C7
15	B	828	CLA	C6-C7-C8-C10
15	B	830	CLA	C6-C7-C8-C10
15	O	832	CLA	C11-C10-C8-C7
15	a	831	CLA	C11-C10-C8-C7
15	N	829	CLA	C10-C11-C12-C13
15	O	801	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	A	851	LHG	C26-C27-C28-C29
15	N	808	CLA	O1D-CGD-O2D-CED
15	O	813	CLA	C3-C5-C6-C7
15	A	807	CLA	C14-C13-C15-C16
15	A	841	CLA	C6-C7-C8-C9
15	B	830	CLA	C6-C7-C8-C9
15	L	203	CLA	C6-C7-C8-C9
15	N	807	CLA	C14-C13-C15-C16
15	N	842	CLA	C11-C10-C8-C9
15	O	808	CLA	C11-C12-C13-C14
15	O	832	CLA	C11-C10-C8-C9
15	O	839	CLA	C11-C12-C13-C14
15	a	807	CLA	C14-C13-C15-C16
15	a	820	CLA	C11-C12-C13-C14
15	a	822	CLA	C11-C10-C8-C9
15	b	824	CLA	C8-C10-C11-C12
19	W	1506	LHG	C13-C14-C15-C16
21	W	1505	LMG	C11-C12-C13-C14
15	B	810	CLA	CAA-CBA-CGA-O2A
15	i	102	CLA	CAA-CBA-CGA-O1A
15	O	827	CLA	C2A-CAA-CBA-CGA
14	N	826	F6C	C2-C1-O2A-CGA
15	A	829	CLA	C2-C1-O2A-CGA
15	A	832	CLA	C2-C1-O2A-CGA
21	a	855	LMG	C19-C20-C21-C22
15	a	806	CLA	O1D-CGD-O2D-CED
14	N	826	F6C	CBA-CGA-O2A-C1
21	O	850	LMG	C13-C14-C15-C16
15	A	823	CLA	C3A-C2A-CAA-CBA
15	a	823	CLA	C3A-C2A-CAA-CBA
15	a	841	CLA	C3A-C2A-CAA-CBA
15	b	821	CLA	C3A-C2A-CAA-CBA
15	b	826	CLA	C3A-C2A-CAA-CBA
15	B	834	CLA	CAA-CBA-CGA-O2A
15	V	102	CLA	CAA-CBA-CGA-O2A
19	l	101	LHG	C9-C10-C11-C12
15	B	834	CLA	CAA-CBA-CGA-O1A
15	K	102	CLA	CAA-CBA-CGA-O2A
15	b	836	CLA	CAA-CBA-CGA-O2A
15	B	801	CLA	CAA-CBA-CGA-O2A
19	X	101	LHG	C14-C15-C16-C17
21	A	855	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
19	X	102	LHG	C33-C34-C35-C36
21	U	102	LMG	C29-C30-C31-C32
15	b	817	CLA	O1D-CGD-O2D-CED
15	A	816	CLA	CAA-CBA-CGA-O2A
15	N	816	CLA	CAA-CBA-CGA-O2A
15	a	816	CLA	CAA-CBA-CGA-O2A
15	b	836	CLA	CAA-CBA-CGA-O1A
20	a	853	LMT	C3'-C4'-O1B-C1B
15	a	819	CLA	CAA-CBA-CGA-O2A
15	A	830	CLA	C13-C15-C16-C17
14	N	856	F6C	C3B-C2B-CMB-OMB
19	Y	101	LHG	C13-C14-C15-C16
15	A	821	CLA	CAA-CBA-CGA-O1A
15	b	839	CLA	C16-C17-C18-C20
15	O	812	CLA	CAA-CBA-CGA-O2A
15	b	812	CLA	CAA-CBA-CGA-O2A
15	b	827	CLA	C3-C5-C6-C7
15	b	828	CLA	C4-C3-C5-C6
20	A	853	LMT	C3'-C4'-O1B-C1B
15	b	806	CLA	C8-C10-C11-C12
15	K	102	CLA	CAA-CBA-CGA-O1A
15	B	829	CLA	C8-C10-C11-C12
15	O	824	CLA	C8-C10-C11-C12
20	A	852	LMT	C5-C6-C7-C8
19	a	851	LHG	C12-C13-C14-C15
21	U	102	LMG	C18-C19-C20-C21
15	b	822	CLA	C5-C6-C7-C8
15	N	817	CLA	CAA-CBA-CGA-O2A
15	V	102	CLA	CAA-CBA-CGA-O1A
21	J	102	LMG	C38-C39-C40-C41
15	A	813	CLA	C6-C7-C8-C9
15	b	814	CLA	C2A-CAA-CBA-CGA
21	B	847	LMG	C33-C34-C35-C36
15	B	818	CLA	CAA-CBA-CGA-O2A
15	O	812	CLA	CAA-CBA-CGA-O1A
15	b	812	CLA	CAA-CBA-CGA-O1A
18	O	849	BCR	C19-C20-C21-C22
22	O	851	LFA	C11-C10-C9-C8
15	O	836	CLA	CAA-CBA-CGA-O2A
21	b	849	LMG	O7-C10-C11-C12
13	N	801	CL0	C13-C15-C16-C17
15	O	832	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	O	836	CLA	CAA-CBA-CGA-O1A
15	a	816	CLA	CAA-CBA-CGA-O1A
15	O	826	CLA	C8-C10-C11-C12
15	b	826	CLA	C8-C10-C11-C12
14	W	1503	F6C	C11-C12-C13-C14
15	B	805	CLA	C6-C7-C8-C9
15	B	815	CLA	C11-C12-C13-C14
15	B	817	CLA	C14-C13-C15-C16
15	N	820	CLA	C11-C12-C13-C14
15	N	831	CLA	C11-C12-C13-C14
15	O	806	CLA	C6-C7-C8-C9
15	W	1502	CLA	C6-C7-C8-C9
15	b	809	CLA	C11-C12-C13-C14
15	b	841	CLA	C11-C12-C13-C14
15	b	841	CLA	C14-C13-C15-C16
15	b	820	CLA	C6-C7-C8-C9
15	B	820	CLA	C5-C6-C7-C8
19	l	102	LHG	O6-C4-C5-C6
18	j	205	BCR	C21-C22-C23-C24
15	a	828	CLA	C3-C5-C6-C7
15	O	809	CLA	C10-C11-C12-C13
21	g	103	LMG	C31-C32-C33-C34
15	A	835	CLA	C16-C17-C18-C20
15	a	839	CLA	C16-C17-C18-C20
21	T	103	LMG	C31-C32-C33-C34
15	B	812	CLA	C2A-CAA-CBA-CGA
15	O	814	CLA	C2A-CAA-CBA-CGA
14	A	857	F6C	C6-C7-C8-C10
15	A	806	CLA	C6-C7-C8-C10
15	A	807	CLA	C12-C13-C15-C16
15	A	835	CLA	C12-C13-C15-C16
15	A	841	CLA	C6-C7-C8-C10
15	A	842	CLA	C11-C10-C8-C7
15	B	824	CLA	C11-C10-C8-C7
15	B	825	CLA	C6-C7-C8-C10
15	F	201	CLA	C6-C7-C8-C10
15	L	203	CLA	C6-C7-C8-C10
15	N	806	CLA	C6-C7-C8-C10
15	N	807	CLA	C12-C13-C15-C16
15	O	839	CLA	C11-C12-C13-C15
15	S	201	CLA	C6-C7-C8-C10
15	a	807	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	a	842	CLA	C11-C10-C8-C7
15	b	806	CLA	C11-C12-C13-C15
15	b	808	CLA	C6-C7-C8-C10
15	b	826	CLA	C11-C10-C8-C7
15	b	832	CLA	C6-C7-C8-C10
15	b	838	CLA	C6-C7-C8-C10
15	f	201	CLA	C6-C7-C8-C10
15	j	203	CLA	C6-C7-C8-C10
15	j	203	CLA	C11-C10-C8-C7
19	j	207	LHG	C18-C19-C20-C21
19	k	101	LHG	C13-C14-C15-C16
15	A	816	CLA	CAA-CBA-CGA-O1A
15	B	810	CLA	CAA-CBA-CGA-O1A
15	a	817	CLA	CAA-CBA-CGA-O2A
15	B	801	CLA	C2B-C3B-CAB-CBB
15	B	821	CLA	C2B-C3B-CAB-CBB
15	B	828	CLA	C2B-C3B-CAB-CBB
15	B	836	CLA	C2B-C3B-CAB-CBB
15	N	835	CLA	C2B-C3B-CAB-CBB
15	O	801	CLA	C2B-C3B-CAB-CBB
15	O	809	CLA	C2B-C3B-CAB-CBB
15	O	816	CLA	C2B-C3B-CAB-CBB
15	a	818	CLA	C2B-C3B-CAB-CBB
15	b	801	CLA	C2B-C3B-CAB-CBB
15	b	809	CLA	C2B-C3B-CAB-CBB
18	B	841	BCR	C23-C24-C25-C26
18	B	846	BCR	C1-C6-C7-C8
18	L	209	BCR	C23-C24-C25-C26
18	N	846	BCR	C23-C24-C25-C26
18	N	857	BCR	C1-C6-C7-C8
18	O	846	BCR	C23-C24-C25-C26
18	U	101	BCR	C5-C6-C7-C8
18	W	1508	BCR	C23-C24-C25-C26
18	a	846	BCR	C23-C24-C25-C26
18	a	857	BCR	C1-C6-C7-C8
18	b	843	BCR	C23-C24-C25-C26
18	g	102	BCR	C23-C24-C25-C26
18	g	102	BCR	C23-C24-C25-C30
18	h	101	BCR	C5-C6-C7-C8
18	k	102	BCR	C23-C24-C25-C26
19	Y	101	LHG	C34-C35-C36-C37
15	N	841	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	A	812	CLA	CBA-CGA-O2A-C1
15	O	839	CLA	C16-C17-C18-C19
15	b	801	CLA	C16-C17-C18-C20
15	a	806	CLA	CBD-CGD-O2D-CED
15	A	807	CLA	CAA-CBA-CGA-O2A
15	B	821	CLA	C2-C3-C5-C6
15	N	835	CLA	C2-C3-C5-C6
15	b	828	CLA	C2-C3-C5-C6
15	B	825	CLA	C8-C10-C11-C12
15	A	812	CLA	O1A-CGA-O2A-C1
15	j	202	CLA	O1D-CGD-O2D-CED
21	a	855	LMG	C20-C21-C22-C23
15	B	836	CLA	C16-C17-C18-C20
15	a	835	CLA	C15-C16-C17-C18
15	O	820	CLA	CAA-CBA-CGA-O2A
15	a	807	CLA	CAA-CBA-CGA-O2A
15	b	809	CLA	C8-C10-C11-C12
16	N	843	PQN	C20-C21-C22-C23
15	a	836	CLA	C5-C6-C7-C8
20	A	854	LMT	C5-C6-C7-C8
15	N	807	CLA	CAA-CBA-CGA-O2A
21	I	103	LMG	O7-C10-C11-C12
21	g	103	LMG	O7-C10-C11-C12
15	B	824	CLA	C8-C10-C11-C12
15	N	831	CLA	C13-C15-C16-C17
15	B	820	CLA	C2-C3-C5-C6
15	N	816	CLA	CAA-CBA-CGA-O1A
15	N	817	CLA	CAA-CBA-CGA-O1A
21	j	206	LMG	C18-C19-C20-C21
15	b	826	CLA	C15-C16-C17-C18
21	L	206	LMG	C37-C38-C39-C40
15	B	822	CLA	C8-C10-C11-C12
21	B	847	LMG	O7-C10-C11-C12
19	L	207	LHG	C26-C27-C28-C29
15	O	822	CLA	C5-C6-C7-C8
14	L	204	F6C	C11-C10-C8-C9
15	B	823	CLA	C14-C13-C15-C16
15	O	825	CLA	C14-C13-C15-C16
15	a	818	CLA	C11-C10-C8-C9
15	a	829	CLA	C6-C7-C8-C9
15	b	806	CLA	C6-C7-C8-C9
15	b	825	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	b	838	CLA	C11-C10-C8-C9
15	b	839	CLA	C11-C12-C13-C14
19	N	851	LHG	O8-C23-C24-C25
21	J	102	LMG	C23-C24-C25-C26
19	Z	102	LHG	C4-C5-C6-O8
15	A	807	CLA	C4B-C3B-CAB-CBB
15	A	817	CLA	C4B-C3B-CAB-CBB
15	A	821	CLA	C1A-C2A-CAA-CBA
15	B	834	CLA	C4B-C3B-CAB-CBB
15	N	816	CLA	C1A-C2A-CAA-CBA
15	O	813	CLA	C1A-C2A-CAA-CBA
15	W	1502	CLA	C1A-C2A-CAA-CBA
15	a	817	CLA	C4B-C3B-CAB-CBB
15	a	821	CLA	C1A-C2A-CAA-CBA
15	b	813	CLA	C1A-C2A-CAA-CBA
15	b	830	CLA	C4B-C3B-CAB-CBB
15	j	203	CLA	C1A-C2A-CAA-CBA
15	O	827	CLA	C3-C5-C6-C7
15	B	821	CLA	C4-C3-C5-C6
15	B	839	CLA	C4-C3-C5-C6
14	N	856	F6C	CAA-CBA-CGA-O2A
15	B	826	CLA	CAA-CBA-CGA-O2A
19	k	101	LHG	O7-C7-C8-C9
21	T	103	LMG	O7-C10-C11-C12
15	N	813	CLA	C2-C3-C5-C6
18	B	844	BCR	C17-C18-C19-C20
18	N	848	BCR	C21-C22-C23-C24
18	O	846	BCR	C17-C18-C19-C20
18	a	857	BCR	C17-C18-C19-C20
15	b	828	CLA	C5-C6-C7-C8
15	j	202	CLA	CBD-CGD-O2D-CED
19	k	101	LHG	C32-C33-C34-C35
14	A	857	F6C	CAA-CBA-CGA-O2A
14	a	856	F6C	CAA-CBA-CGA-O2A
19	M	102	LHG	C13-C14-C15-C16
15	N	814	CLA	C16-C17-C18-C19
15	N	839	CLA	C16-C17-C18-C20
21	O	850	LMG	O7-C10-C11-C12
14	A	824	F6C	C2-C3-C5-C6
14	a	824	F6C	C2-C3-C5-C6
15	A	837	CLA	C2-C3-C5-C6
15	N	837	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	826	F6C	C4-C3-C5-C6
15	B	823	CLA	C2-C1-O2A-CGA
15	N	832	CLA	C2-C1-O2A-CGA
15	a	827	CLA	C2-C1-O2A-CGA
15	b	820	CLA	CAA-CBA-CGA-O2A
21	b	849	LMG	C23-C24-C25-C26
14	A	802	F6C	C11-C10-C8-C7
14	W	1503	F6C	C12-C13-C15-C16
14	a	856	F6C	C6-C7-C8-C10
14	j	204	F6C	C11-C12-C13-C15
15	A	821	CLA	C11-C10-C8-C7
15	A	834	CLA	C12-C13-C15-C16
15	B	839	CLA	C11-C12-C13-C15
15	N	818	CLA	C11-C10-C8-C7
15	N	834	CLA	C12-C13-C15-C16
15	N	835	CLA	C12-C13-C15-C16
15	N	842	CLA	C11-C10-C8-C7
15	a	834	CLA	C12-C13-C15-C16
15	a	835	CLA	C12-C13-C15-C16
15	b	805	CLA	C11-C12-C13-C15
15	N	839	CLA	C15-C16-C17-C18
15	W	1501	CLA	C10-C11-C12-C13
15	b	838	CLA	C16-C17-C18-C20
21	U	102	LMG	C11-C12-C13-C14
15	A	821	CLA	C5-C6-C7-C8
20	N	853	LMT	C3'-C4'-O1B-C1B
15	a	817	CLA	CAA-CBA-CGA-O1A
15	a	803	CLA	C15-C16-C17-C18
21	g	103	LMG	C32-C33-C34-C35
15	A	829	CLA	C2A-CAA-CBA-CGA
15	B	816	CLA	C2A-CAA-CBA-CGA
15	N	835	CLA	C16-C17-C18-C20
15	W	1501	CLA	C16-C17-C18-C19
19	M	102	LHG	C34-C35-C36-C37
15	N	806	CLA	CAA-CBA-CGA-O2A
21	U	102	LMG	C38-C39-C40-C41
15	A	841	CLA	C3A-C2A-CAA-CBA
15	N	828	CLA	C4-C3-C5-C6
21	I	103	LMG	O9-C10-C11-C12
15	N	809	CLA	C8-C10-C11-C12
14	A	826	F6C	C2-C3-C5-C6
15	A	813	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	A	839	CLA	C2-C3-C5-C6
21	W	1505	LMG	C20-C21-C22-C23
15	A	817	CLA	CAA-CBA-CGA-O2A
15	b	817	CLA	CAA-CBA-CGA-O2A
22	f	204	LFA	C11-C10-C9-C8
15	A	807	CLA	CAA-CBA-CGA-O1A
21	O	850	LMG	O9-C10-C11-C12
21	T	103	LMG	O9-C10-C11-C12
15	N	807	CLA	C13-C15-C16-C17
15	O	818	CLA	C2A-CAA-CBA-CGA
15	W	1501	CLA	C2A-CAA-CBA-CGA
15	j	202	CLA	C2A-CAA-CBA-CGA
15	A	814	CLA	C11-C10-C8-C9
15	B	809	CLA	C14-C13-C15-C16
15	B	825	CLA	C11-C12-C13-C14
15	B	835	CLA	C6-C7-C8-C9
15	N	814	CLA	C11-C10-C8-C9
15	O	837	CLA	C6-C7-C8-C9
15	a	831	CLA	C11-C10-C8-C9
15	b	837	CLA	C6-C7-C8-C9
19	M	102	LHG	O7-C7-C8-C9
18	B	844	BCR	C36-C18-C19-C20
18	N	857	BCR	C36-C18-C19-C20
19	N	851	LHG	C29-C30-C31-C32
15	O	817	CLA	CAA-CBA-CGA-O2A
19	A	851	LHG	O8-C23-C24-C25
15	b	811	CLA	C10-C11-C12-C13
14	A	857	F6C	C1B-C2B-CMB-OMB
19	Z	102	LHG	O1-C1-C2-O2
19	l	102	LHG	O1-C1-C2-O2
21	A	855	LMG	C18-C19-C20-C21
15	A	828	CLA	O1A-CGA-O2A-C1
19	l	102	LHG	O8-C23-C24-C25
15	b	839	CLA	C16-C17-C18-C19
13	a	801	CL0	C15-C16-C17-C18
18	g	101	BCR	C21-C22-C23-C24
18	j	201	BCR	C7-C8-C9-C10
14	j	204	F6C	C5-C6-C7-C8
21	A	855	LMG	C8-C7-O1-C1
21	N	855	LMG	C8-C7-O1-C1
21	L	206	LMG	C11-C12-C13-C14
14	N	856	F6C	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	B	818	CLA	CAA-CBA-CGA-O1A
21	b	849	LMG	O9-C10-C11-C12
15	B	815	CLA	CAA-CBA-CGA-O2A
15	a	805	CLA	CAA-CBA-CGA-O2A
15	a	829	CLA	CAA-CBA-CGA-O2A
15	N	822	CLA	C15-C16-C17-C18
15	L	202	CLA	C2A-CAA-CBA-CGA
19	X	102	LHG	C4-C5-C6-O8
19	l	102	LHG	C4-C5-C6-O8
14	a	856	F6C	CAA-CBA-CGA-O1A
15	N	807	CLA	CAA-CBA-CGA-O1A
15	O	820	CLA	CAA-CBA-CGA-O1A
21	B	847	LMG	O9-C10-C11-C12
21	g	103	LMG	O9-C10-C11-C12
19	N	851	LHG	C12-C13-C14-C15
15	A	803	CLA	C15-C16-C17-C18
15	a	839	CLA	C15-C16-C17-C18
19	Z	102	LHG	C2-C3-O3-P
15	A	806	CLA	CAA-CBA-CGA-O2A
15	a	806	CLA	CAA-CBA-CGA-O2A
15	b	805	CLA	CAA-CBA-CGA-O2A
15	b	822	CLA	C2-C3-C5-C6
15	B	826	CLA	CAA-CBA-CGA-O1A
15	a	807	CLA	CAA-CBA-CGA-O1A
14	W	1503	F6C	C16-C17-C18-C19
15	A	817	CLA	CAD-CBD-CGD-O2D
15	B	820	CLA	CAD-CBD-CGD-O2D
15	N	817	CLA	CAD-CBD-CGD-O2D
15	a	806	CLA	CAD-CBD-CGD-O2D
15	a	842	CLA	CAD-CBD-CGD-O2D
14	A	826	F6C	C5-C6-C7-C8
19	k	101	LHG	C11-C12-C13-C14
15	A	805	CLA	CAA-CBA-CGA-O2A
15	B	804	CLA	CAA-CBA-CGA-O2A
15	O	828	CLA	CAA-CBA-CGA-O2A
15	O	838	CLA	CAA-CBA-CGA-O2A
15	a	810	CLA	CAA-CBA-CGA-O2A
15	b	828	CLA	CAA-CBA-CGA-O2A
15	b	838	CLA	CAA-CBA-CGA-O2A
19	l	101	LHG	O7-C7-C8-C9
15	b	820	CLA	CAA-CBA-CGA-O1A
15	N	814	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	N	836	CLA	O1A-CGA-O2A-C1
21	N	855	LMG	C19-C20-C21-C22
15	a	831	CLA	C13-C15-C16-C17
15	N	829	CLA	C2-C1-O2A-CGA
15	Z	103	CLA	C2-C1-O2A-CGA
15	a	829	CLA	C2-C1-O2A-CGA
15	B	813	CLA	CAA-CBA-CGA-O2A
14	A	857	F6C	CAA-CBA-CGA-O1A
19	k	101	LHG	O9-C7-C8-C9
15	N	829	CLA	CAA-CBA-CGA-O2A
15	A	817	CLA	CAA-CBA-CGA-O1A
19	j	207	LHG	C26-C27-C28-C29
15	O	817	CLA	CAA-CBA-CGA-O1A
15	b	817	CLA	CAA-CBA-CGA-O1A
15	Z	103	CLA	O1A-CGA-O2A-C1
15	A	810	CLA	CAA-CBA-CGA-O2A
15	O	805	CLA	CAA-CBA-CGA-O2A
15	a	825	CLA	CAA-CBA-CGA-O2A
20	N	854	LMT	C5-C6-C7-C8
15	O	807	CLA	C16-C17-C18-C20
15	a	828	CLA	C16-C17-C18-C19
14	A	802	F6C	C3-C5-C6-C7
15	B	836	CLA	CAA-CBA-CGA-O2A
15	N	813	CLA	CAA-CBA-CGA-O2A
19	X	101	LHG	O7-C7-C8-C9
19	N	851	LHG	C24-C23-O8-C6
15	a	828	CLA	O1A-CGA-O2A-C1
15	B	805	CLA	C8-C10-C11-C12

There are no ring outliers.

343 monomers are involved in 870 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	821	CLA	5	0
18	g	101	BCR	3	0
22	L	208	LFA	1	0
15	N	816	CLA	2	0
15	N	827	CLA	2	0
15	a	807	CLA	3	0
15	N	829	CLA	3	0
15	b	837	CLA	4	0
15	F	201	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	816	CLA	3	0
15	a	823	CLA	5	0
15	j	202	CLA	2	0
15	B	829	CLA	4	0
18	N	848	BCR	2	0
15	b	802	CLA	6	0
22	f	204	LFA	1	0
15	A	803	CLA	7	0
15	a	806	CLA	7	0
15	N	815	CLA	2	0
15	A	813	CLA	2	0
18	O	849	BCR	4	0
18	a	857	BCR	4	0
18	O	844	BCR	2	0
20	A	854	LMT	1	0
14	O	810	F6C	2	0
22	j	208	LFA	2	0
15	A	856	CLA	5	0
15	N	822	CLA	3	0
22	W	1507	LFA	1	0
15	N	838	CLA	2	0
15	O	820	CLA	2	0
15	a	808	CLA	1	0
15	N	805	CLA	1	0
21	O	850	LMG	5	0
15	a	829	CLA	5	0
21	a	855	LMG	1	0
15	a	831	CLA	2	0
15	a	811	CLA	3	0
15	B	804	CLA	5	0
15	N	812	CLA	2	0
15	A	816	CLA	3	0
20	N	854	LMT	1	0
15	A	806	CLA	10	0
18	F	203	BCR	6	0
15	b	827	CLA	8	0
15	O	817	CLA	4	0
19	l	101	LHG	2	0
18	N	845	BCR	4	0
15	A	833	CLA	2	0
18	T	101	BCR	2	0
18	N	849	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	830	CLA	9	0
18	a	849	BCR	1	0
21	W	1505	LMG	4	0
20	a	852	LMT	1	0
15	A	840	CLA	2	0
18	g	102	BCR	1	0
18	O	845	BCR	4	0
15	N	823	CLA	4	0
15	N	842	CLA	1	0
15	O	828	CLA	1	0
15	B	813	CLA	1	0
15	N	809	CLA	1	0
22	O	851	LFA	1	0
14	b	833	F6C	1	0
15	a	813	CLA	2	0
19	L	207	LHG	5	0
15	A	841	CLA	7	0
16	O	842	PQN	1	0
15	N	833	CLA	2	0
18	a	845	BCR	5	0
15	N	834	CLA	2	0
18	Y	102	BCR	4	0
18	I	101	BCR	3	0
15	a	822	CLA	6	0
21	I	103	LMG	3	0
15	A	837	CLA	2	0
16	a	843	PQN	1	0
15	a	803	CLA	7	0
15	b	807	CLA	3	0
15	B	815	CLA	6	0
15	a	838	CLA	2	0
15	b	812	CLA	1	0
18	N	850	BCR	7	0
18	b	847	BCR	5	0
15	a	830	CLA	3	0
15	O	824	CLA	1	0
18	B	842	BCR	1	0
18	W	1508	BCR	2	0
18	B	845	BCR	5	0
15	A	814	CLA	6	0
15	O	816	CLA	3	0
20	N	852	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	c	102	SF4	1	0
15	B	835	CLA	3	0
15	a	819	CLA	7	0
15	W	1502	CLA	2	0
15	N	841	CLA	3	0
15	S	201	CLA	1	0
15	N	837	CLA	2	0
15	N	808	CLA	2	0
18	j	201	BCR	5	0
18	O	843	BCR	3	0
18	A	845	BCR	7	0
15	N	806	CLA	7	0
15	a	805	CLA	1	0
15	B	806	CLA	2	0
15	O	819	CLA	2	0
18	L	205	BCR	1	0
21	h	102	LMG	3	0
15	A	825	CLA	2	0
15	a	835	CLA	1	0
18	I	102	BCR	2	0
15	A	839	CLA	2	0
15	O	827	CLA	5	0
18	a	846	BCR	1	0
15	O	836	CLA	1	0
15	b	822	CLA	2	0
15	A	812	CLA	3	0
15	a	816	CLA	3	0
19	Z	101	LHG	2	0
15	A	821	CLA	3	0
15	B	833	CLA	3	0
18	A	850	BCR	10	0
15	O	815	CLA	2	0
15	N	830	CLA	2	0
18	S	202	BCR	5	0
15	A	804	CLA	5	0
15	b	835	CLA	4	0
15	A	830	CLA	4	0
15	B	837	CLA	8	0
21	b	849	LMG	5	0
18	f	203	BCR	4	0
15	a	818	CLA	7	0
15	N	835	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	808	CLA	8	0
18	i	101	BCR	1	0
15	O	832	CLA	6	0
21	j	206	LMG	2	0
15	N	825	CLA	1	0
15	a	815	CLA	2	0
15	W	1501	CLA	1	0
15	a	809	CLA	3	0
18	W	1504	BCR	1	0
21	B	847	LMG	4	0
15	l	103	CLA	2	0
19	W	1506	LHG	5	0
15	b	823	CLA	5	0
15	b	813	CLA	5	0
15	B	812	CLA	3	0
15	A	827	CLA	1	0
15	O	839	CLA	8	0
15	O	802	CLA	6	0
15	b	832	CLA	6	0
15	a	833	CLA	2	0
15	a	810	CLA	4	0
15	b	831	CLA	4	0
15	a	812	CLA	2	0
15	b	806	CLA	6	0
15	A	818	CLA	7	0
19	j	207	LHG	5	0
15	b	801	CLA	1	0
16	N	843	PQN	1	0
19	Z	102	LHG	2	0
18	N	847	BCR	3	0
15	O	835	CLA	4	0
15	B	832	CLA	1	0
18	O	847	BCR	3	0
15	b	829	CLA	4	0
15	N	819	CLA	6	0
15	A	815	CLA	2	0
15	A	820	CLA	8	0
18	b	848	BCR	4	0
15	b	811	CLA	3	0
18	M	101	BCR	4	0
15	B	834	CLA	1	0
15	O	821	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	814	CLA	6	0
20	a	854	LMT	1	0
15	N	818	CLA	7	0
15	b	808	CLA	6	0
15	A	819	CLA	7	0
15	A	809	CLA	5	0
15	O	818	CLA	1	0
15	B	817	CLA	4	0
15	a	840	CLA	1	0
15	A	807	CLA	4	0
15	N	820	CLA	7	0
16	B	840	PQN	1	0
15	N	828	CLA	1	0
16	A	843	PQN	1	0
15	B	830	CLA	5	0
18	A	847	BCR	3	0
15	B	828	CLA	7	0
14	b	810	F6C	2	0
15	O	801	CLA	2	0
22	B	848	LFA	1	0
18	A	858	BCR	4	0
15	b	841	CLA	1	0
15	a	814	CLA	6	0
15	B	819	CLA	2	0
19	Y	101	LHG	5	0
15	O	823	CLA	1	0
15	B	803	CLA	5	0
14	j	204	F6C	1	0
15	A	810	CLA	5	0
15	B	805	CLA	5	0
15	O	829	CLA	4	0
15	B	822	CLA	3	0
18	A	846	BCR	2	0
15	O	809	CLA	8	0
15	a	841	CLA	5	0
15	O	831	CLA	3	0
15	A	838	CLA	1	0
15	A	823	CLA	4	0
15	a	839	CLA	2	0
15	b	819	CLA	3	0
14	O	833	F6C	1	0
15	j	203	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	838	CLA	6	0
15	b	814	CLA	3	0
18	j	205	BCR	1	0
15	b	817	CLA	4	0
15	a	828	CLA	1	0
21	g	103	LMG	3	0
18	b	843	BCR	3	0
15	O	834	CLA	1	0
13	N	801	CL0	2	0
15	b	828	CLA	2	0
15	B	809	CLA	2	0
15	a	821	CLA	2	0
13	A	801	CL0	3	0
15	a	827	CLA	1	0
18	b	845	BCR	2	0
15	B	818	CLA	3	0
15	b	803	CLA	6	0
15	b	825	CLA	6	0
15	N	831	CLA	1	0
15	b	805	CLA	4	0
14	B	831	F6C	1	0
15	b	830	CLA	9	0
15	b	826	CLA	2	0
15	B	801	CLA	2	0
15	O	813	CLA	4	0
21	U	102	LMG	3	0
15	B	825	CLA	5	0
15	N	840	CLA	3	0
19	M	102	LHG	5	0
15	O	814	CLA	3	0
18	a	848	BCR	1	0
21	A	855	LMG	1	0
18	b	846	BCR	1	0
18	B	841	BCR	2	0
15	b	821	CLA	3	0
15	N	811	CLA	4	0
15	b	816	CLA	1	0
18	a	850	BCR	7	0
15	A	805	CLA	1	0
15	B	836	CLA	8	0
15	N	839	CLA	2	0
18	k	102	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a	804	CLA	3	0
15	O	803	CLA	9	0
18	B	843	BCR	5	0
18	h	101	BCR	1	0
15	N	810	CLA	5	0
15	O	841	CLA	2	0
15	a	842	CLA	1	0
15	B	810	CLA	1	0
15	a	820	CLA	5	0
15	A	834	CLA	1	0
15	X	103	CLA	3	0
15	f	201	CLA	2	0
15	b	818	CLA	2	0
15	b	836	CLA	1	0
15	N	813	CLA	3	0
15	B	827	CLA	3	0
15	O	805	CLA	3	0
15	O	822	CLA	1	0
18	L	209	BCR	4	0
15	A	829	CLA	4	0
15	B	814	CLA	1	0
17	P	102	SF4	1	0
15	A	811	CLA	2	0
18	T	102	BCR	1	0
15	b	809	CLA	8	0
19	l	102	LHG	2	0
15	b	815	CLA	2	0
15	A	831	CLA	3	0
15	B	802	CLA	6	0
13	a	801	CL0	2	0
18	A	848	BCR	3	0
19	X	101	LHG	3	0
15	b	820	CLA	2	0
18	a	847	BCR	1	0
15	A	828	CLA	2	0
15	A	835	CLA	2	0
18	B	846	BCR	3	0
15	V	102	CLA	1	0
15	O	806	CLA	5	0
15	b	804	CLA	5	0
15	i	102	CLA	1	0
15	K	102	CLA	1	0

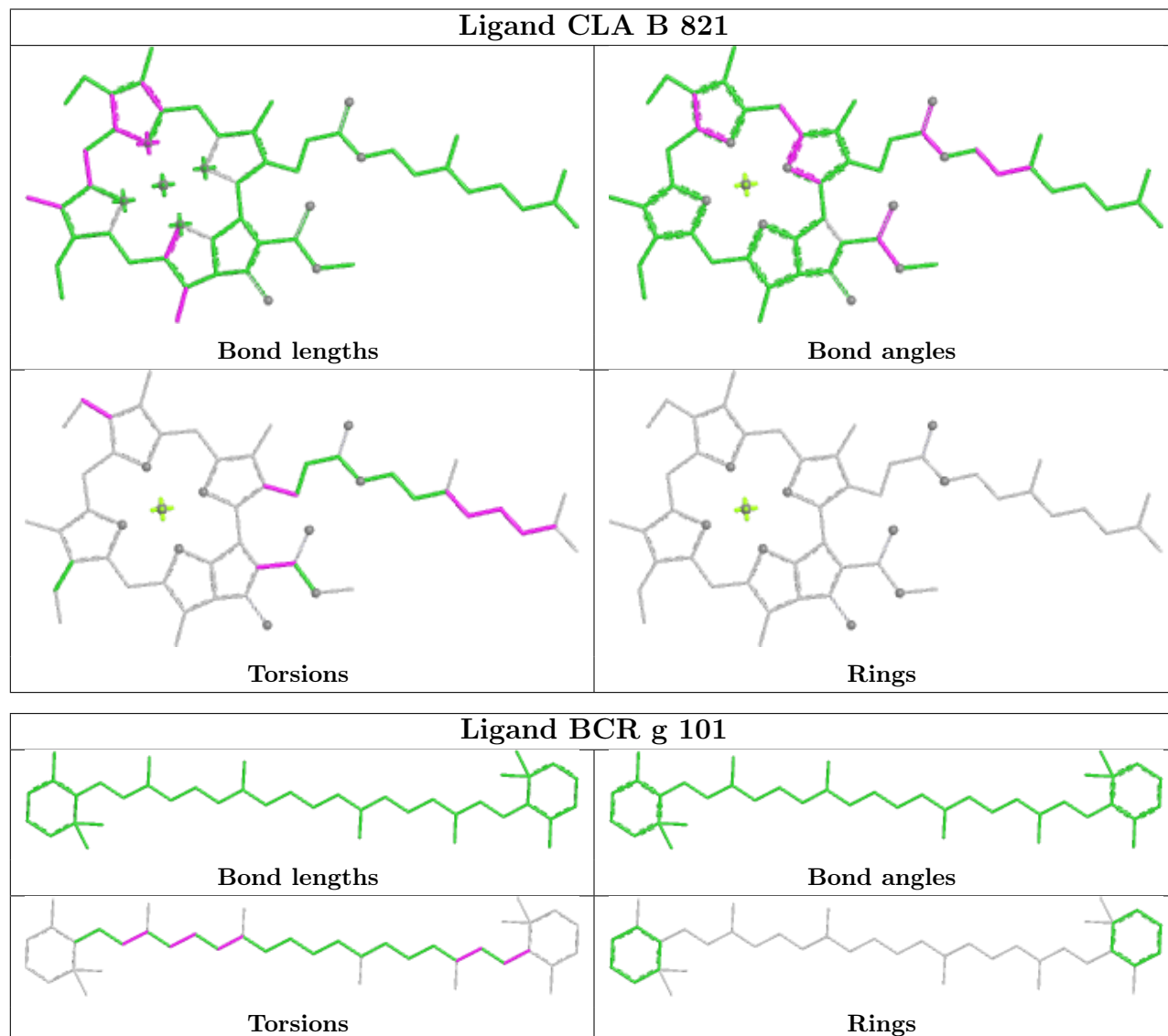
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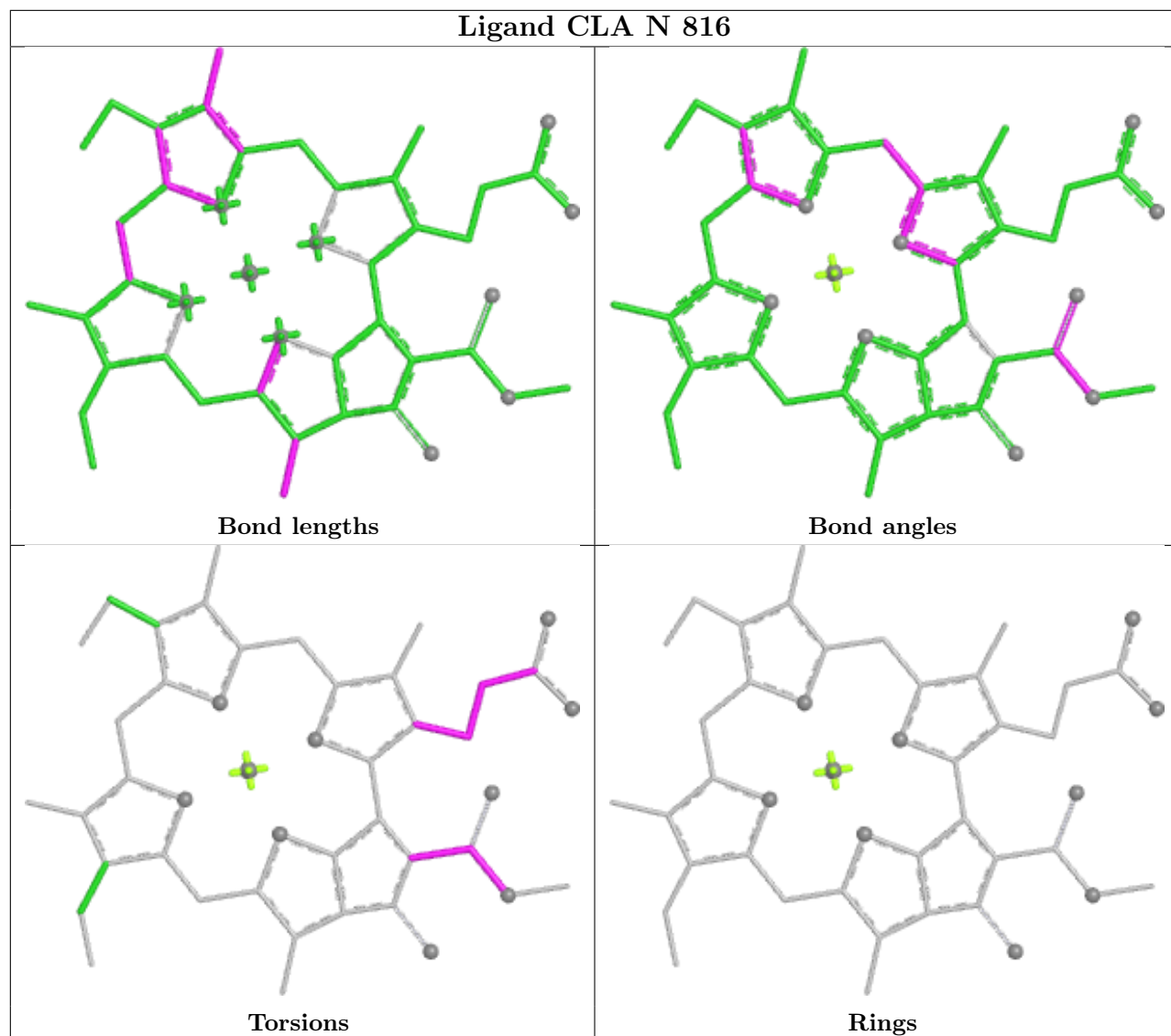
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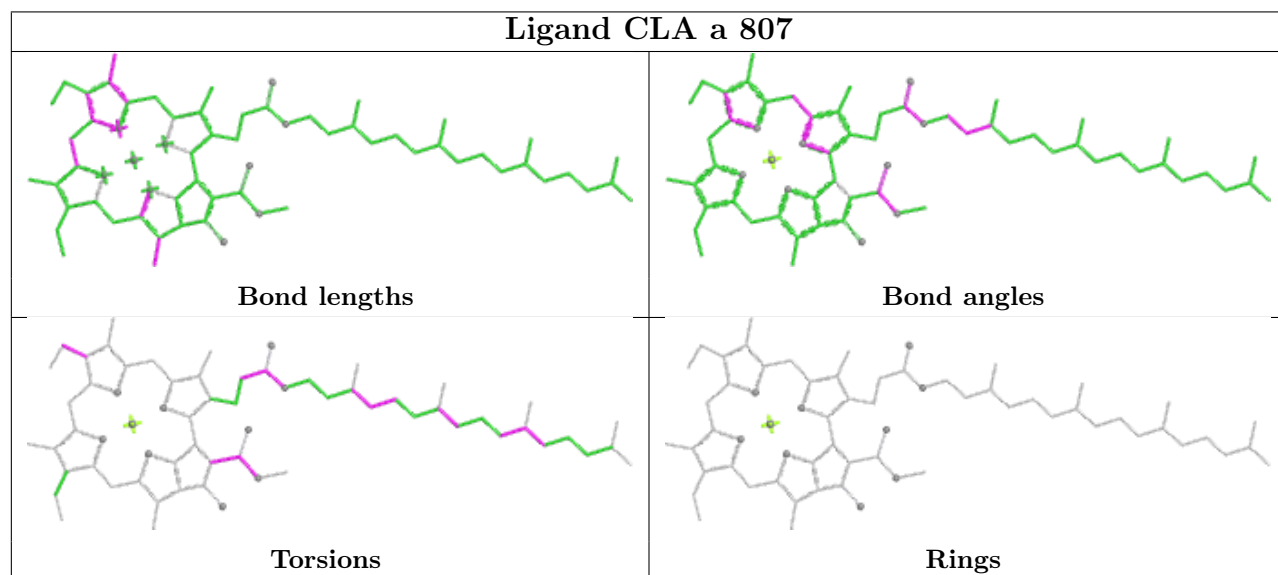
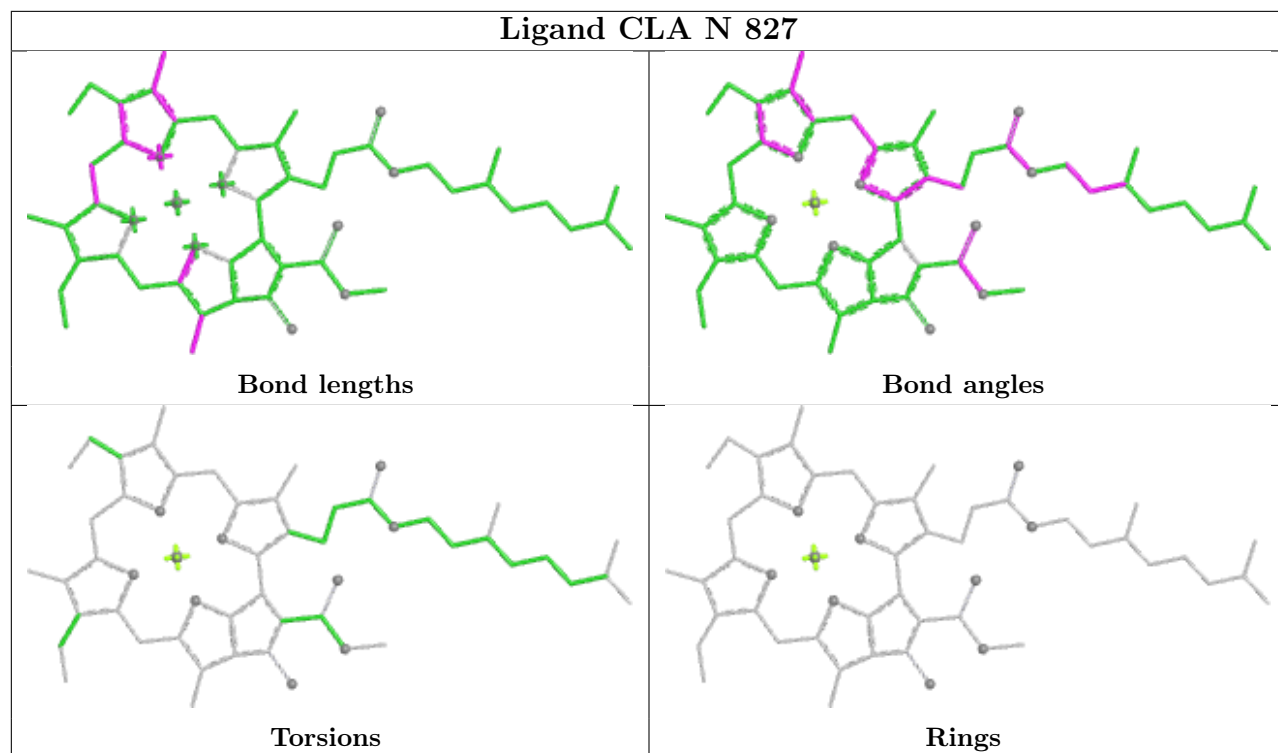
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	811	CLA	7	0
20	A	852	LMT	2	0
15	L	202	CLA	1	0
15	B	820	CLA	1	0
18	F	202	BCR	3	0
15	L	203	CLA	3	0
21	L	206	LMG	4	0
16	b	842	PQN	3	0
15	N	807	CLA	4	0
15	B	807	CLA	4	0
15	O	811	CLA	1	0
15	A	842	CLA	4	0
18	N	857	BCR	6	0
15	Z	103	CLA	2	0
21	T	103	LMG	5	0
15	O	804	CLA	5	0
15	N	821	CLA	2	0
18	O	848	BCR	2	0
15	B	839	CLA	2	0
18	J	101	BCR	1	0
19	k	101	LHG	5	0
15	O	812	CLA	1	0
21	J	102	LMG	1	0
15	O	807	CLA	2	0
15	O	825	CLA	7	0
15	O	837	CLA	5	0
15	b	824	CLA	3	0
15	N	804	CLA	4	0
15	b	838	CLA	8	0
14	L	201	F6C	2	0
15	a	834	CLA	3	0
15	O	826	CLA	2	0
15	b	839	CLA	7	0
15	O	808	CLA	7	0
18	f	202	BCR	2	0
15	A	822	CLA	1	0
15	a	837	CLA	1	0
15	N	803	CLA	9	0
15	B	824	CLA	1	0
15	B	823	CLA	5	0

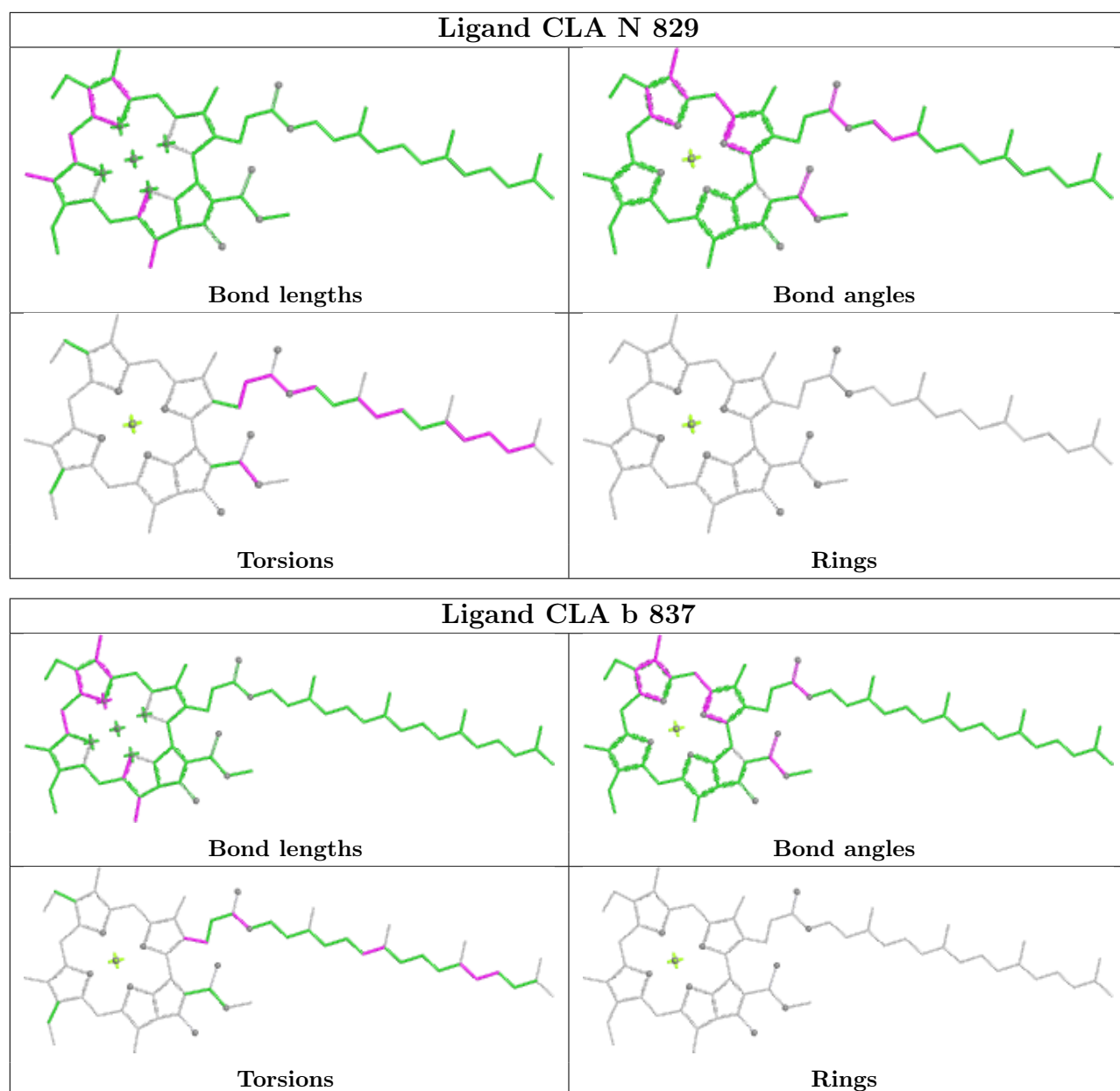
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

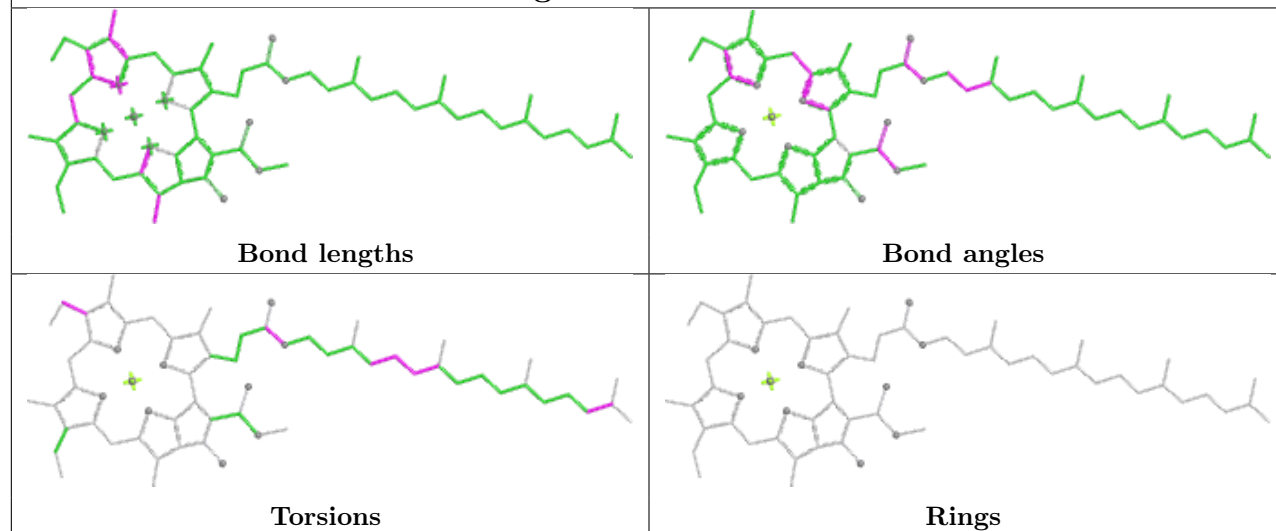




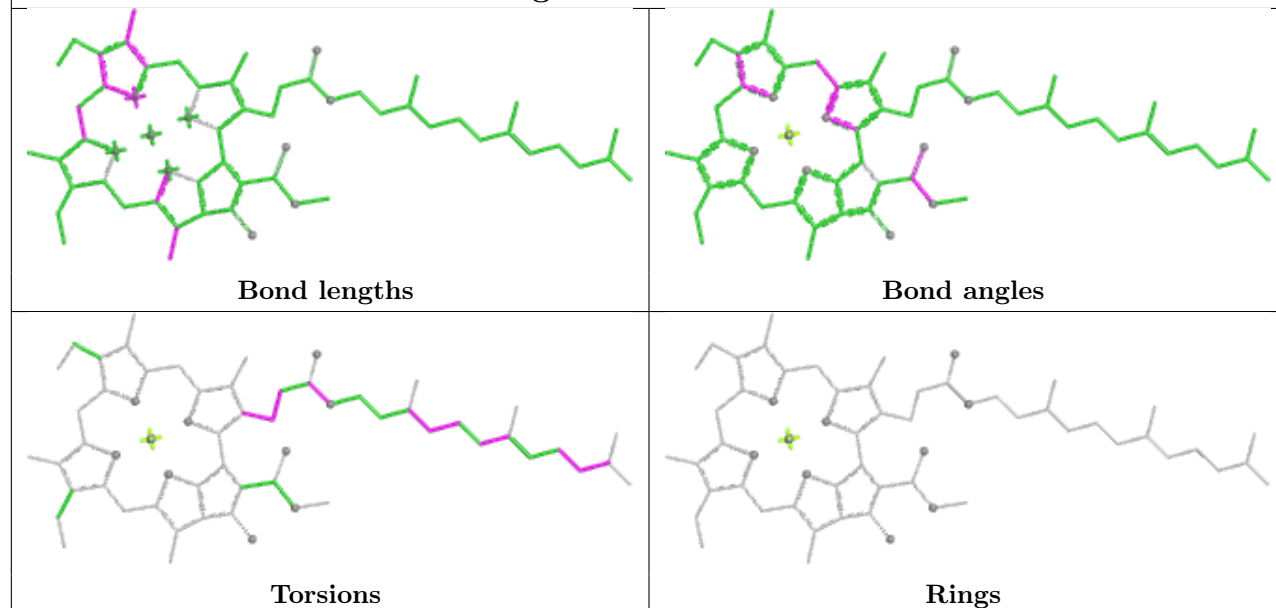




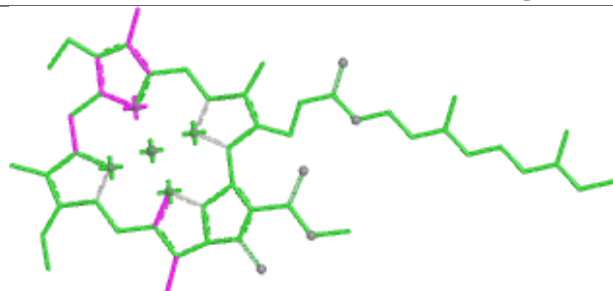
Ligand CLA F 201



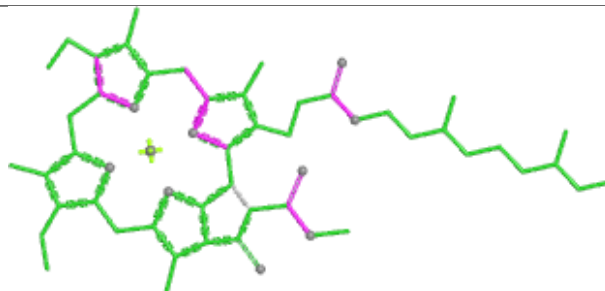
Ligand CLA B 816



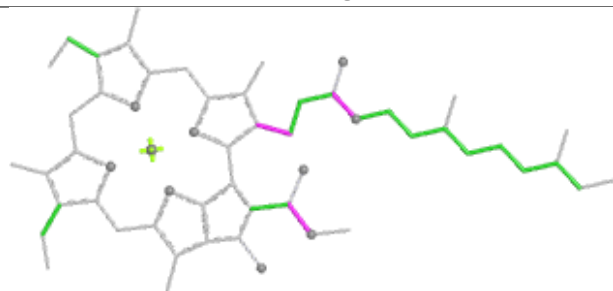
Ligand CLA a 823



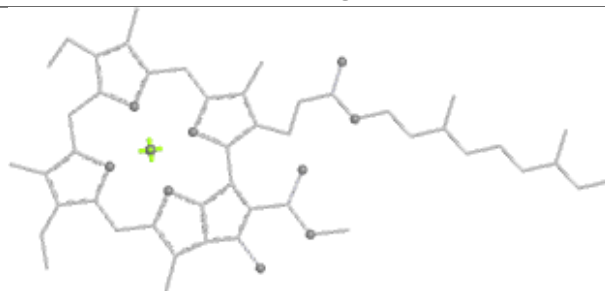
Bond lengths



Bond angles

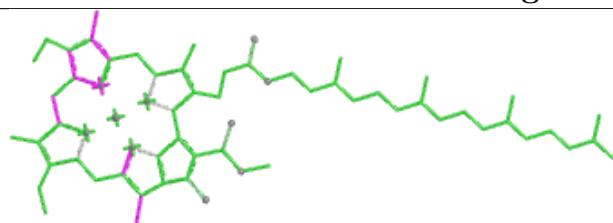


Torsions

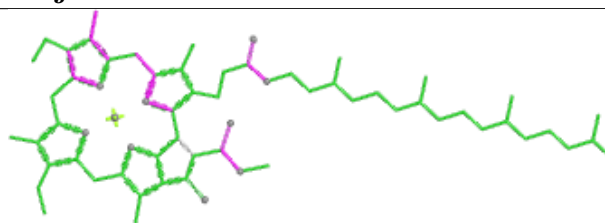


Rings

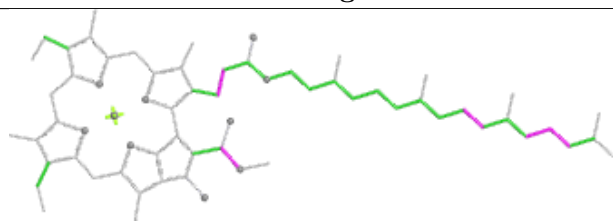
Ligand CLA j 202



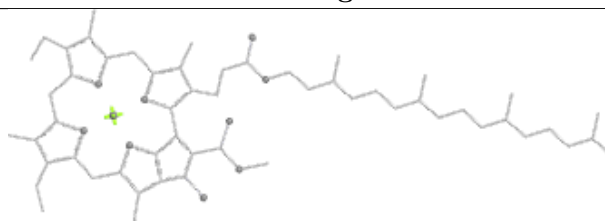
Bond lengths



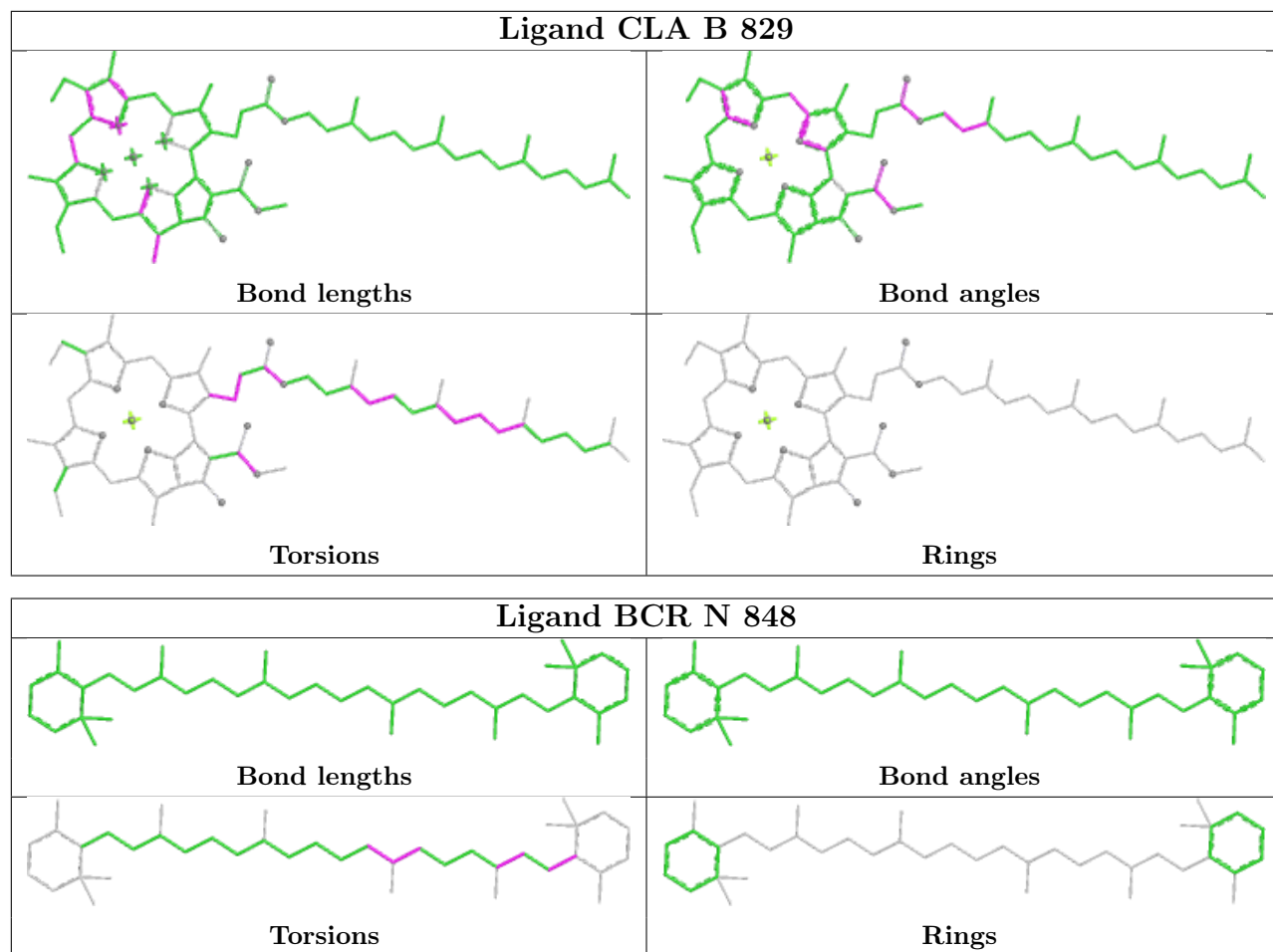
Bond angles



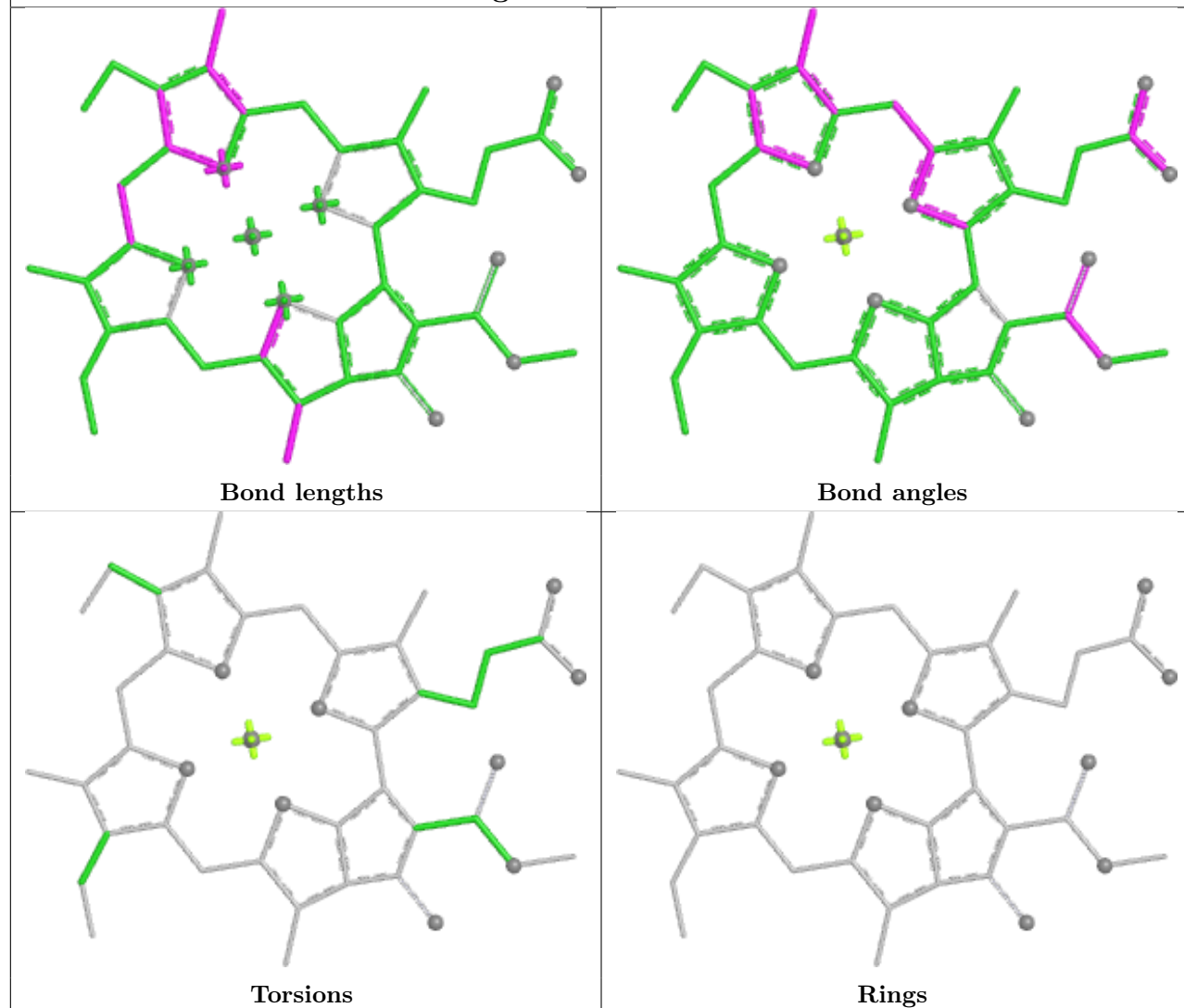
Torsions



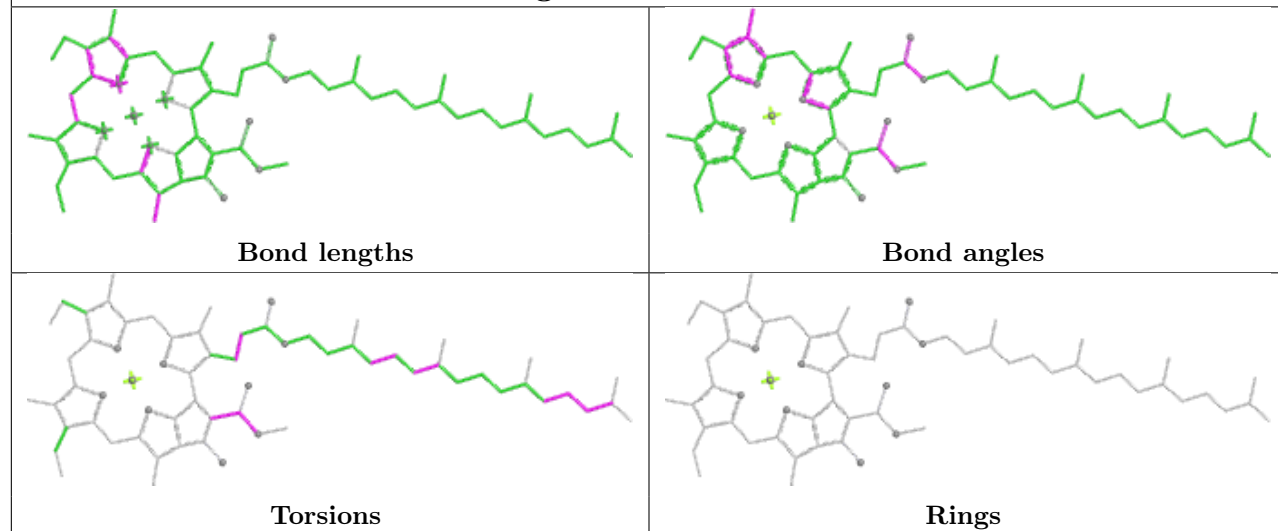
Rings

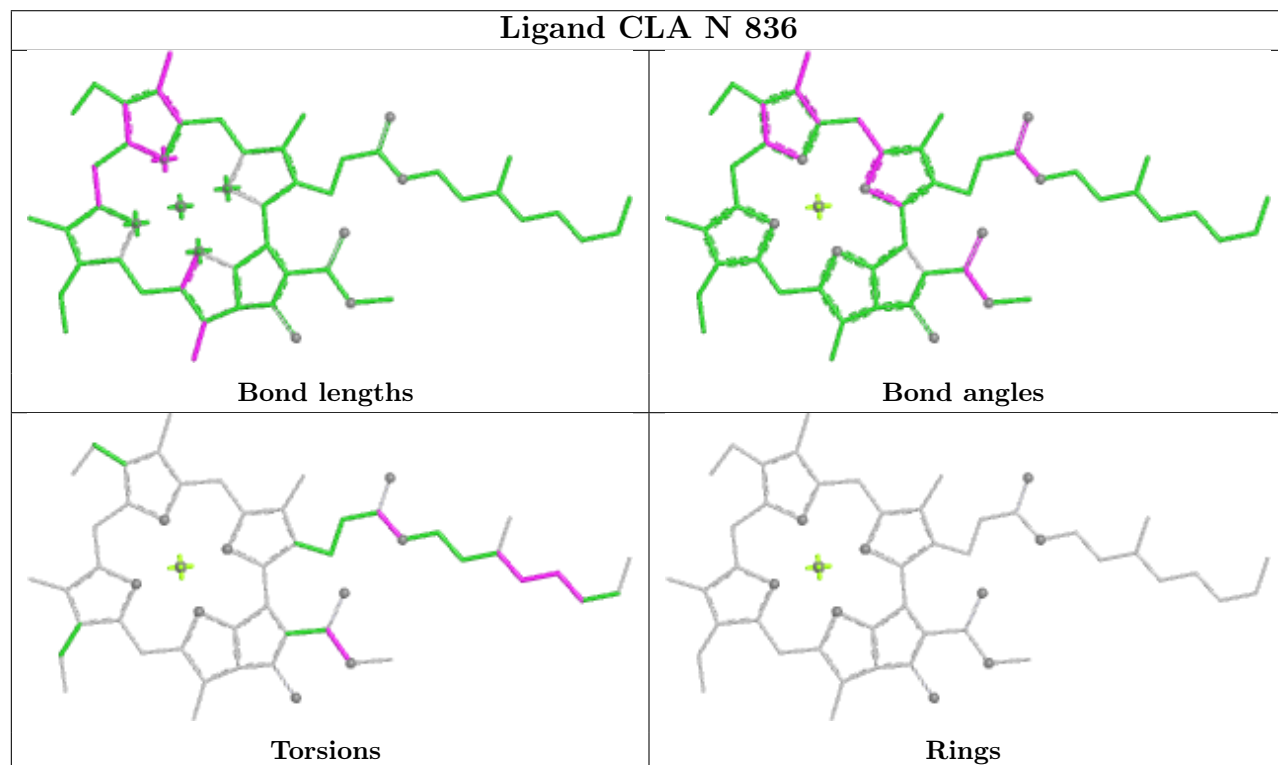
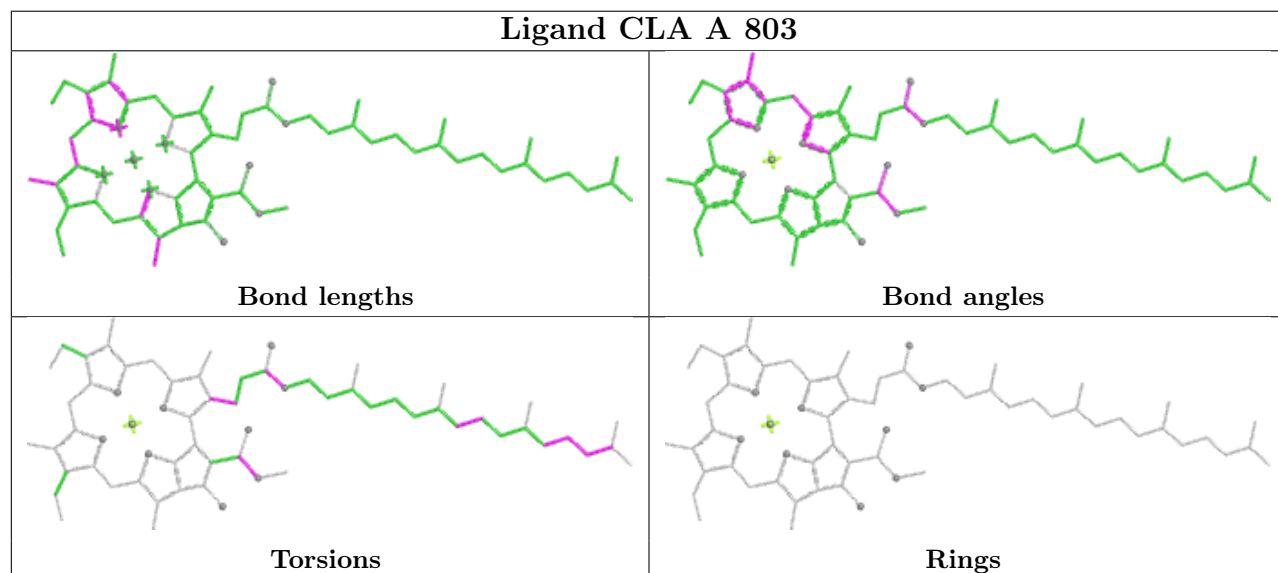
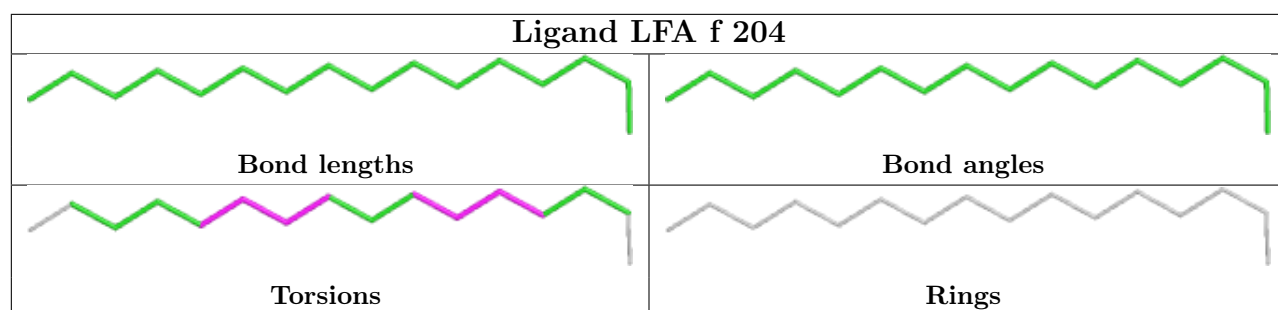


Ligand CLA A 808

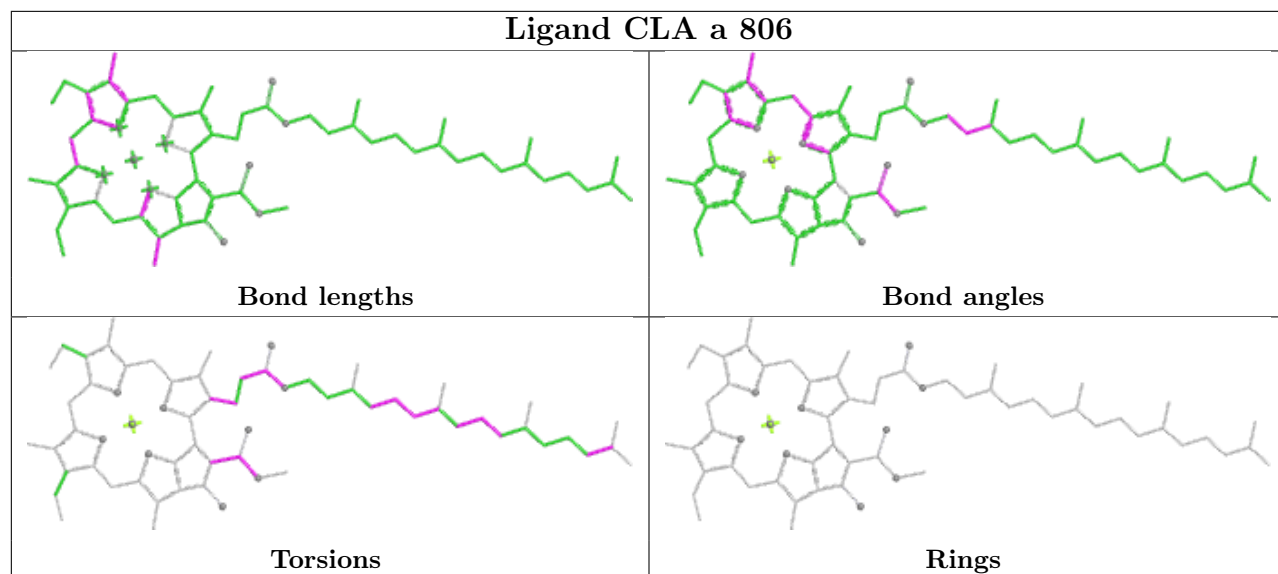


Ligand CLA b 802

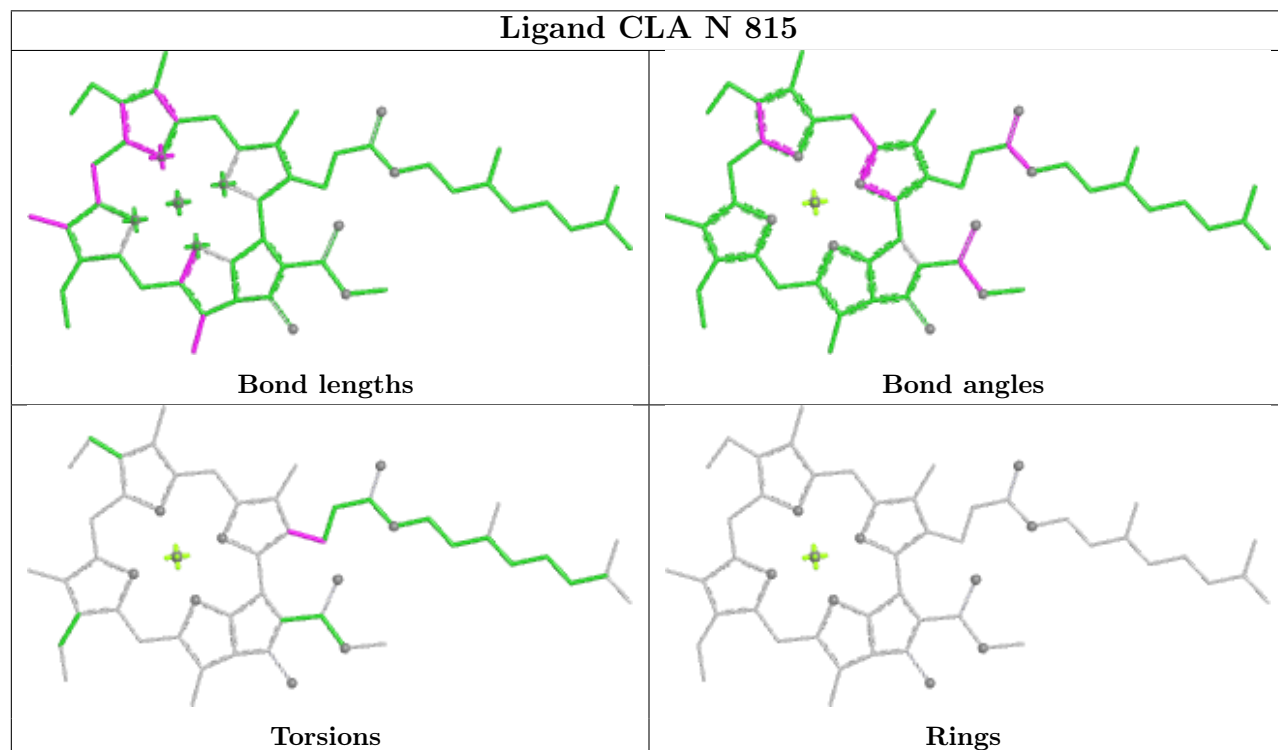


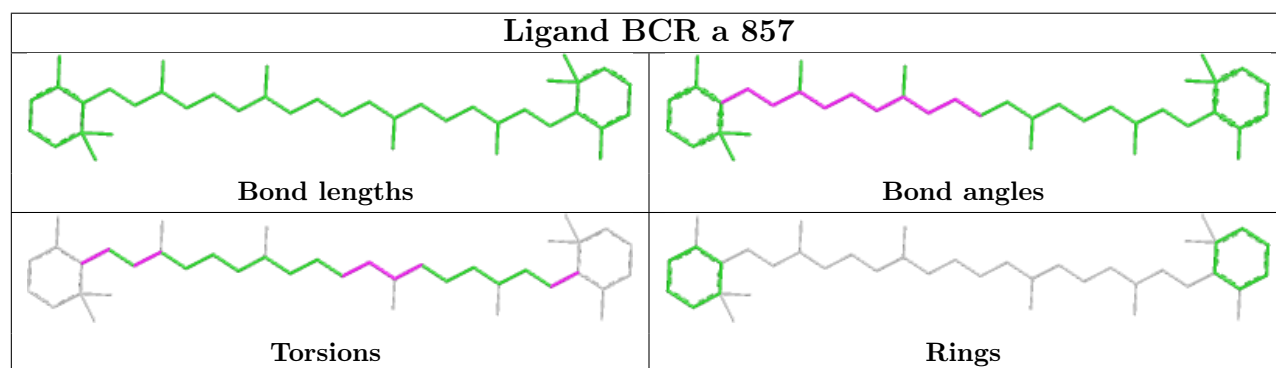
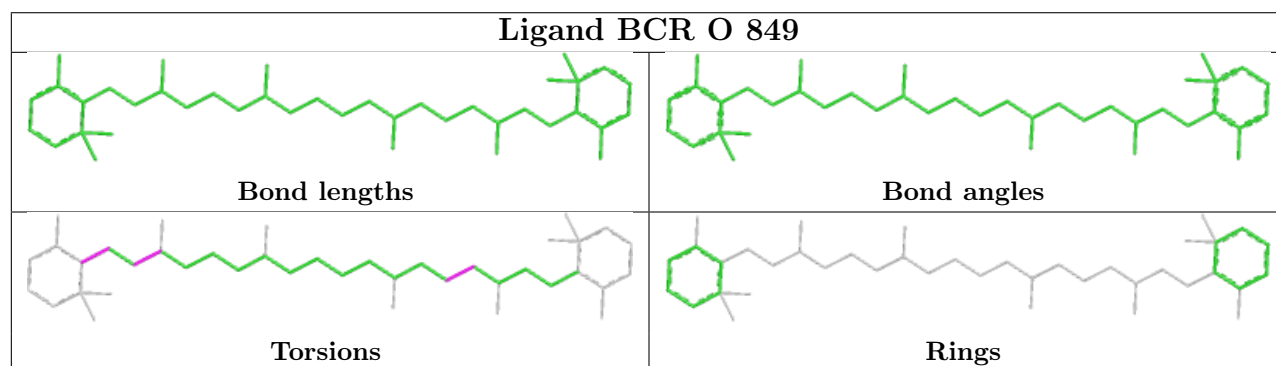
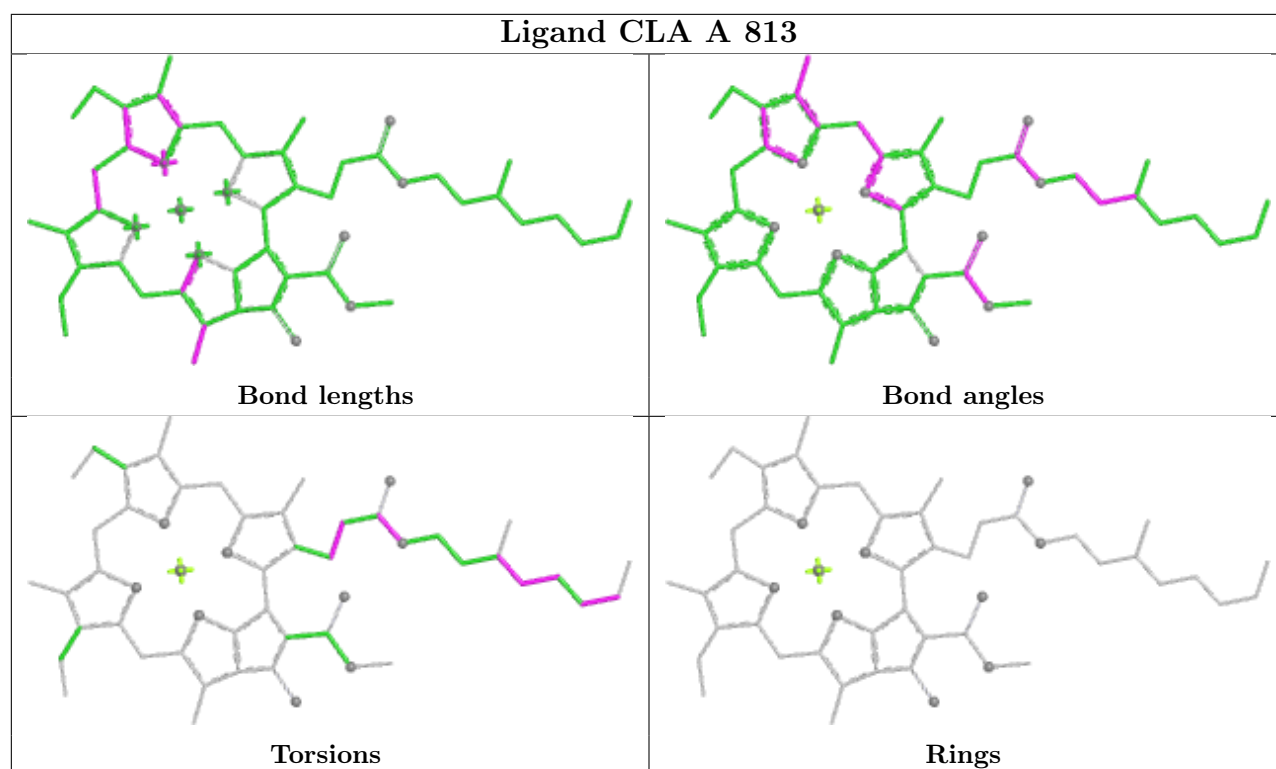


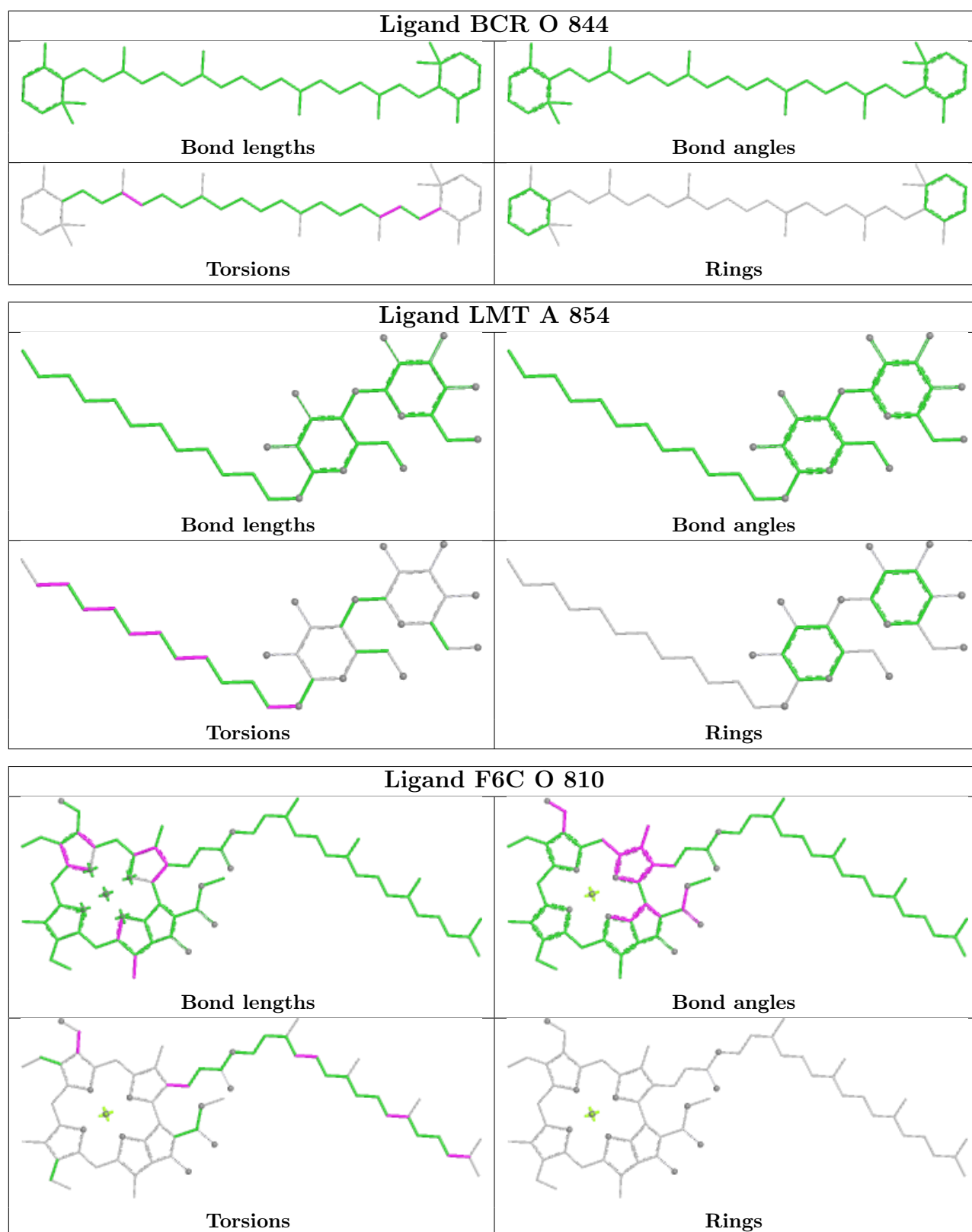
Ligand CLA a 806

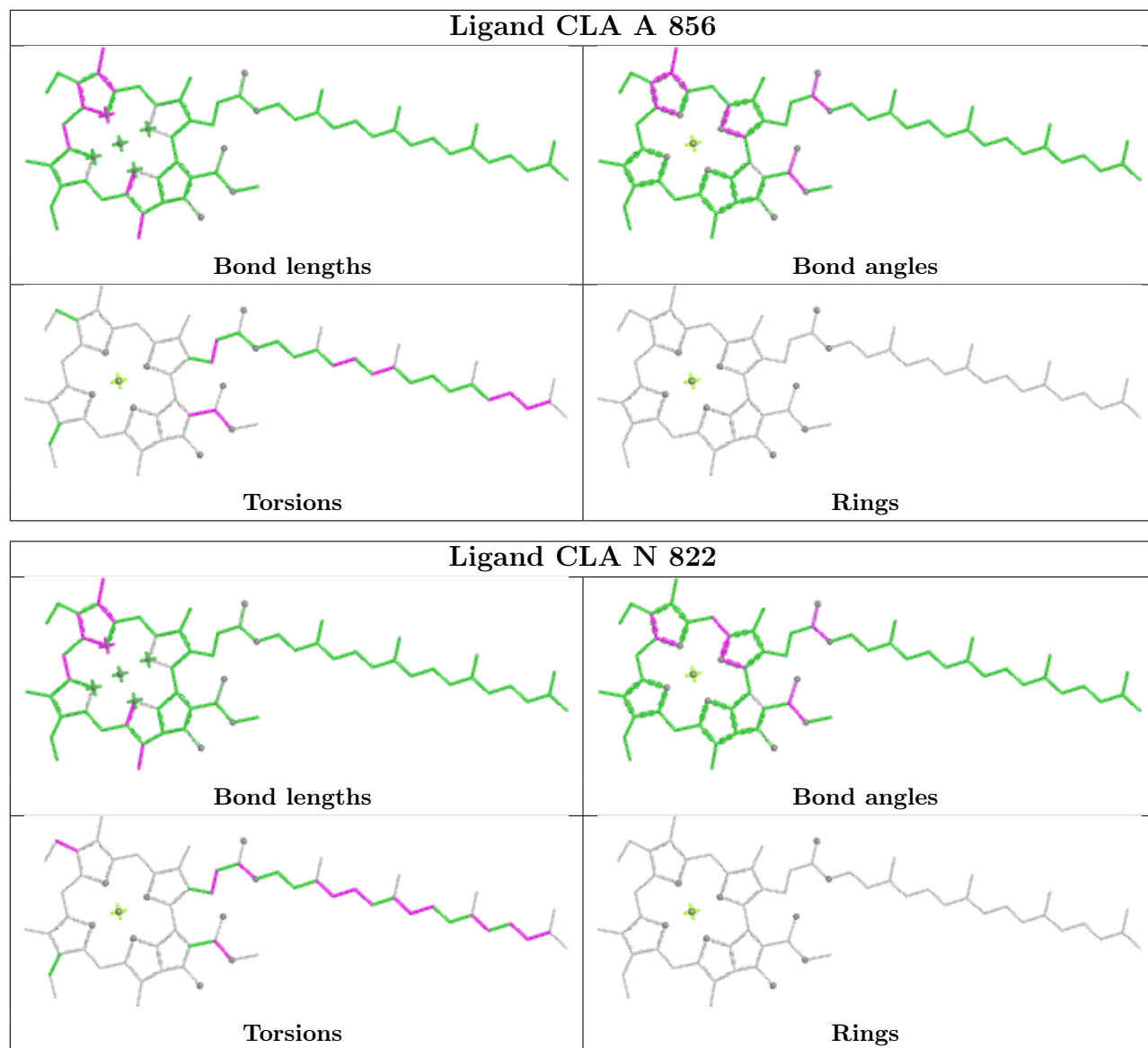


Ligand CLA N 815

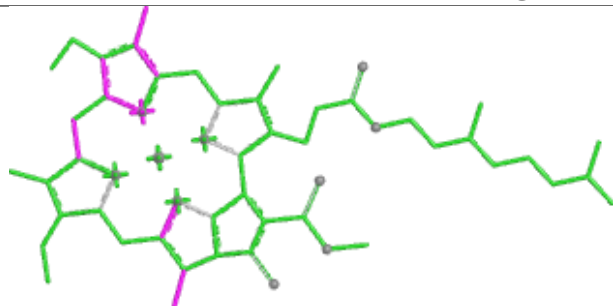




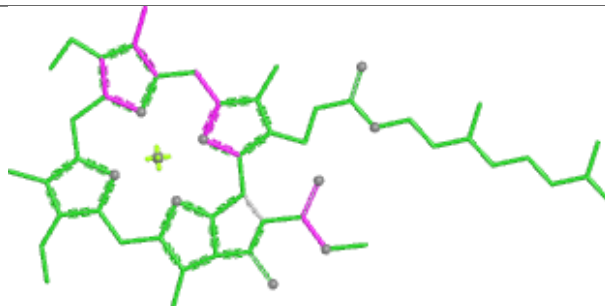




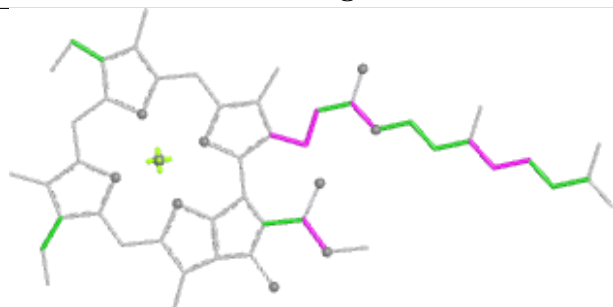
Ligand CLA N 838



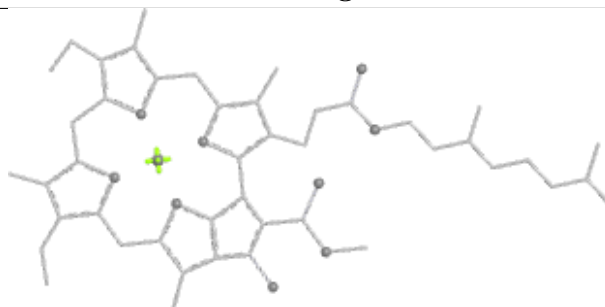
Bond lengths



Bond angles

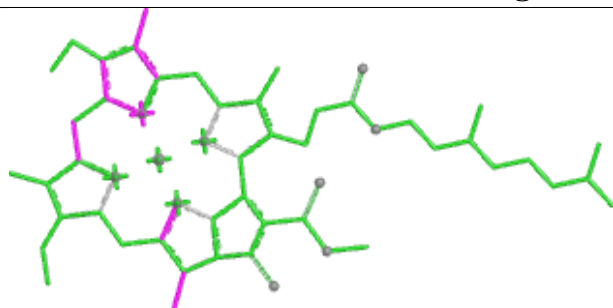


Torsions

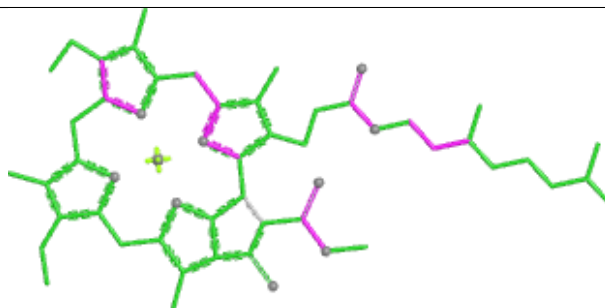


Rings

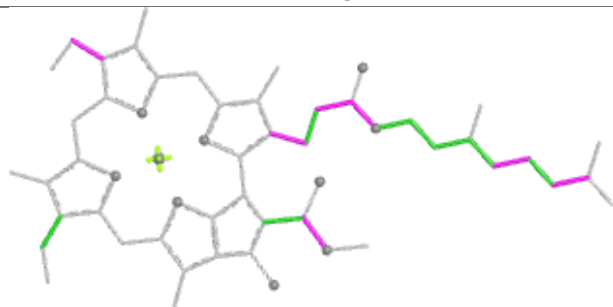
Ligand CLA O 820



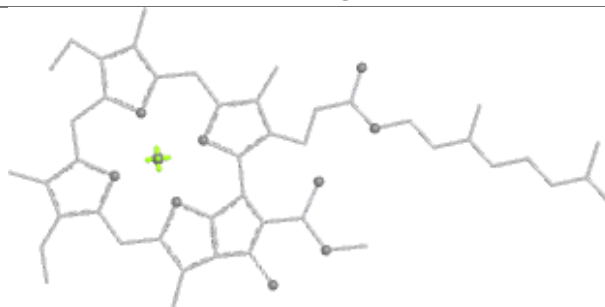
Bond lengths



Bond angles

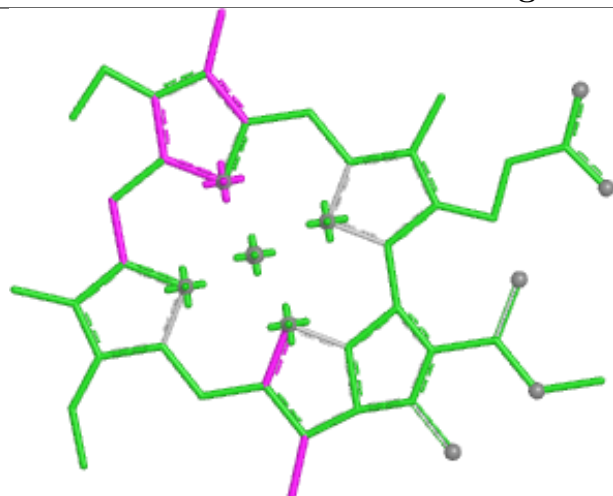


Torsions

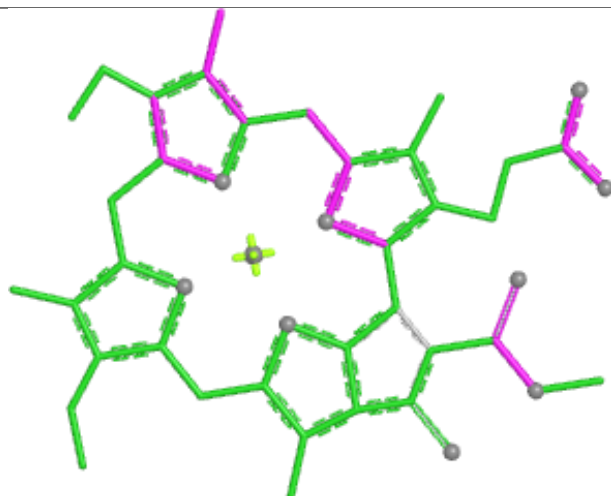


Rings

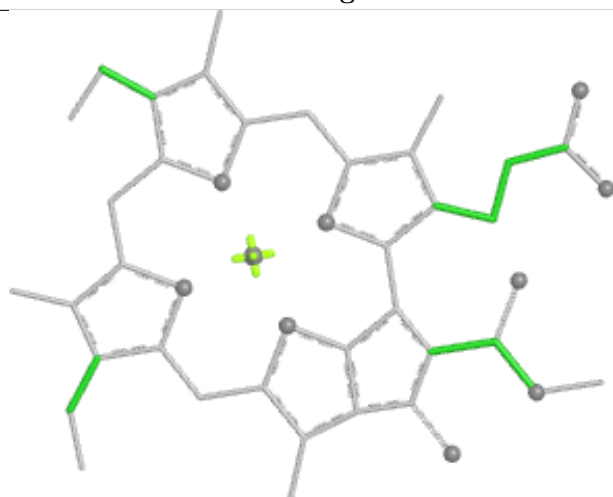
Ligand CLA a 808



Bond lengths



Bond angles

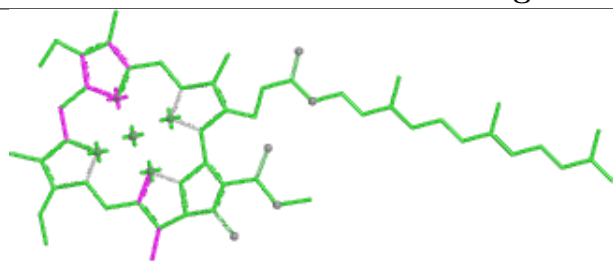


Torsions

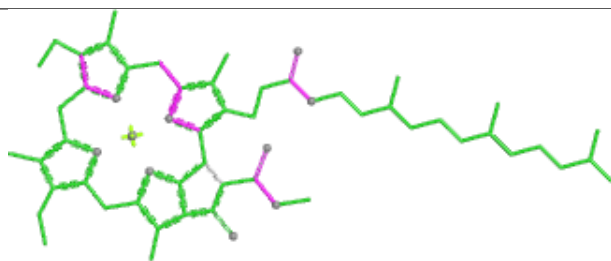


Rings

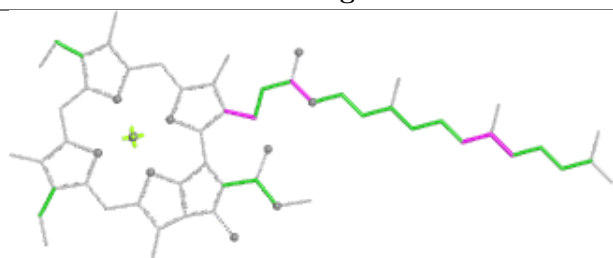
Ligand CLA N 805



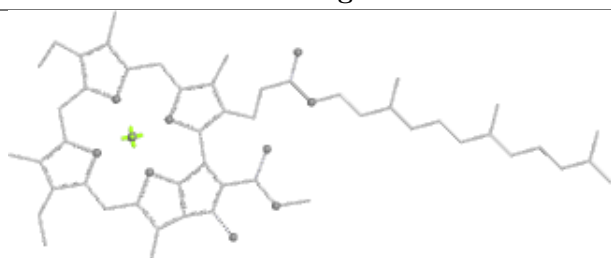
Bond lengths



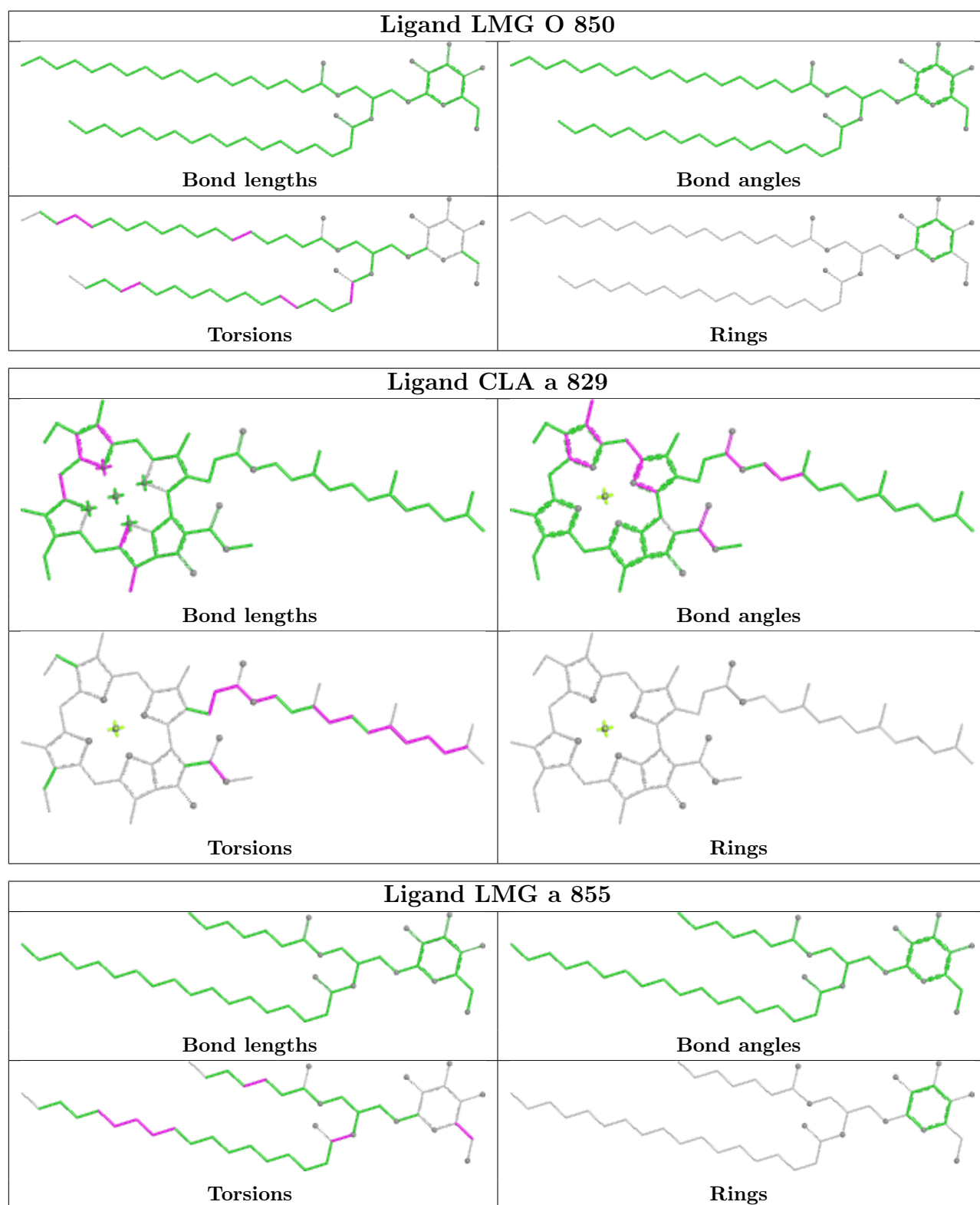
Bond angles

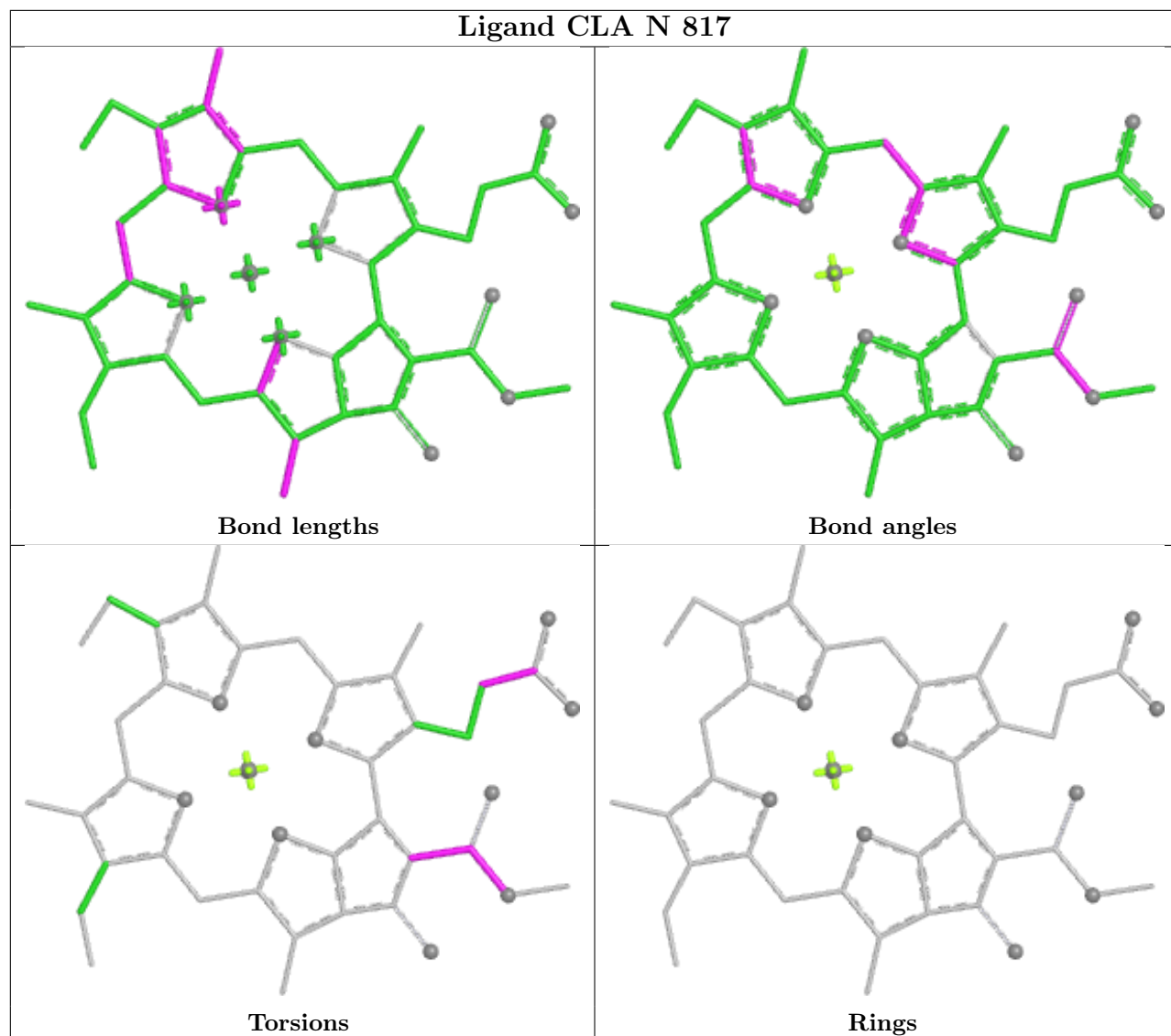


Torsions

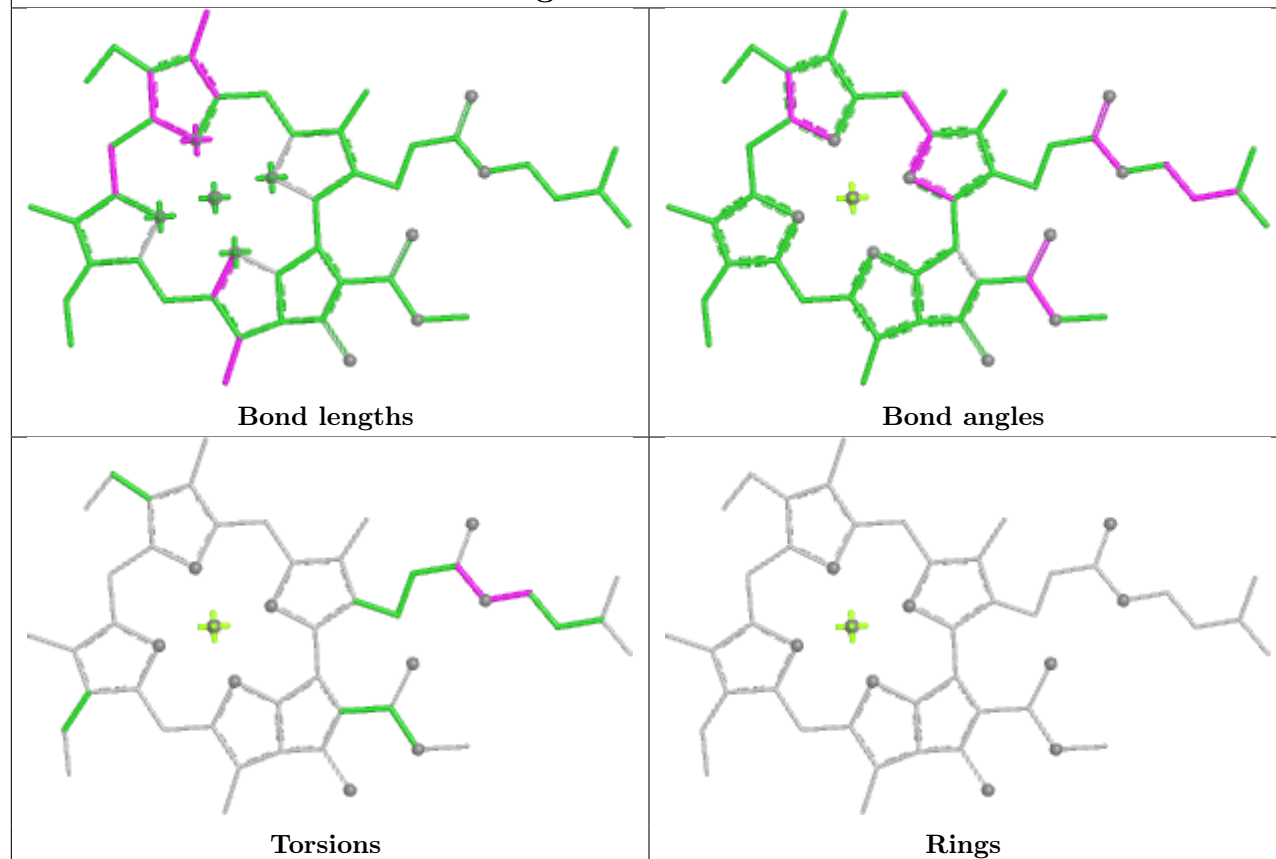


Rings

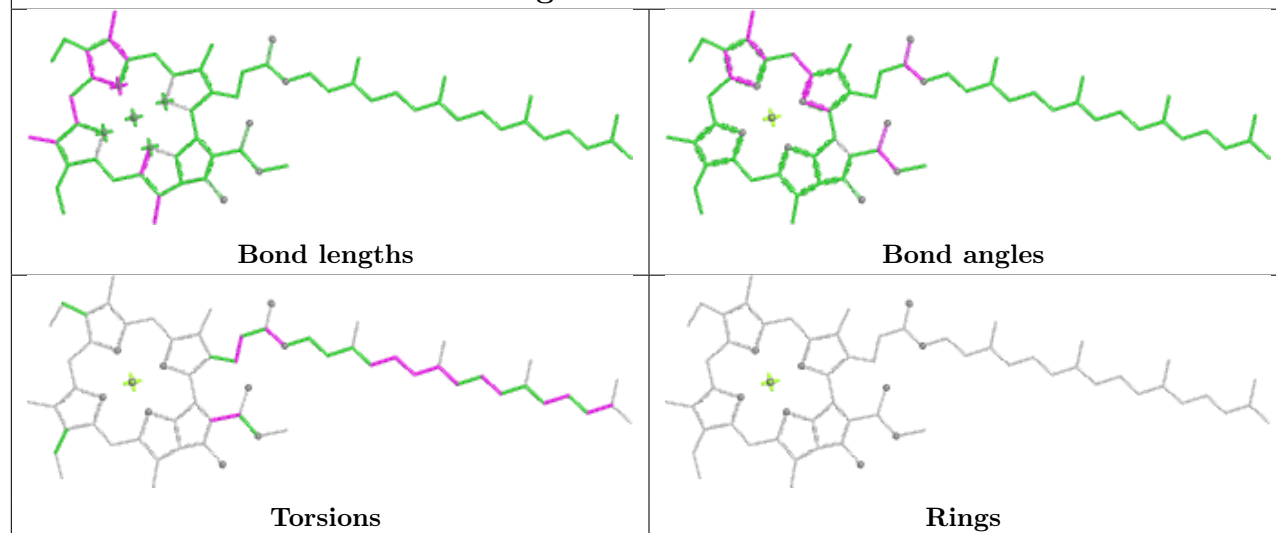




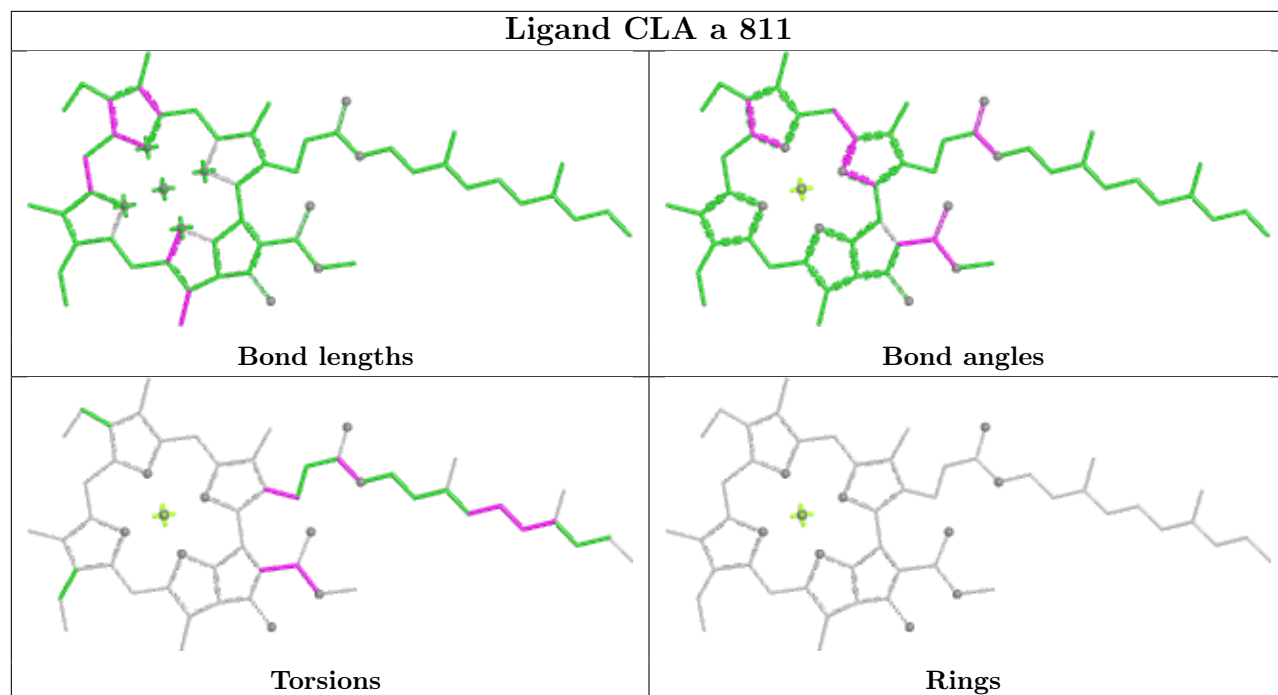
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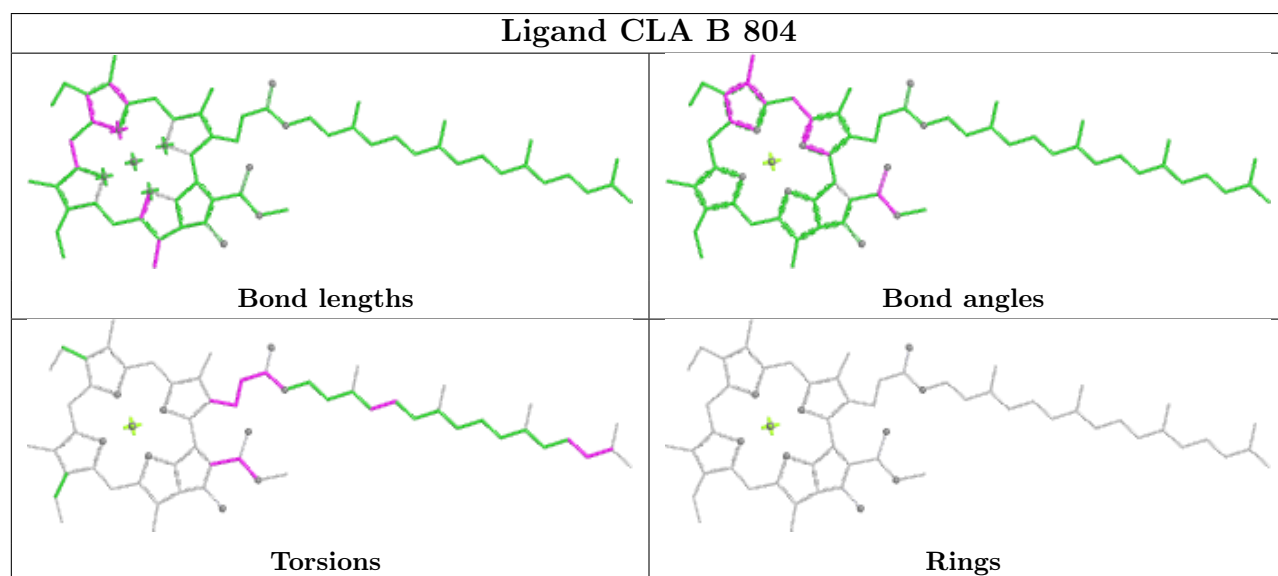
Ligand CLA a 831

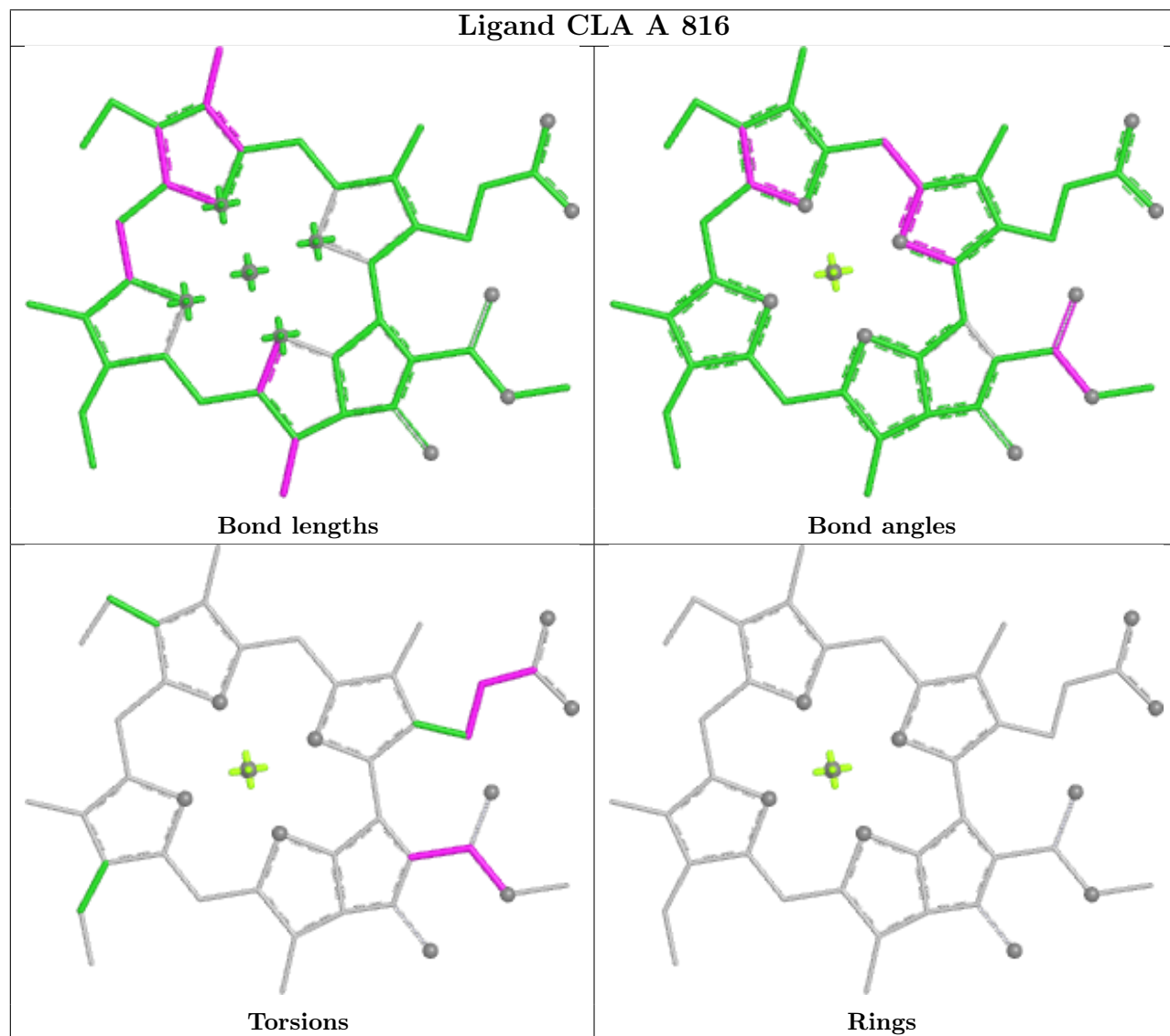
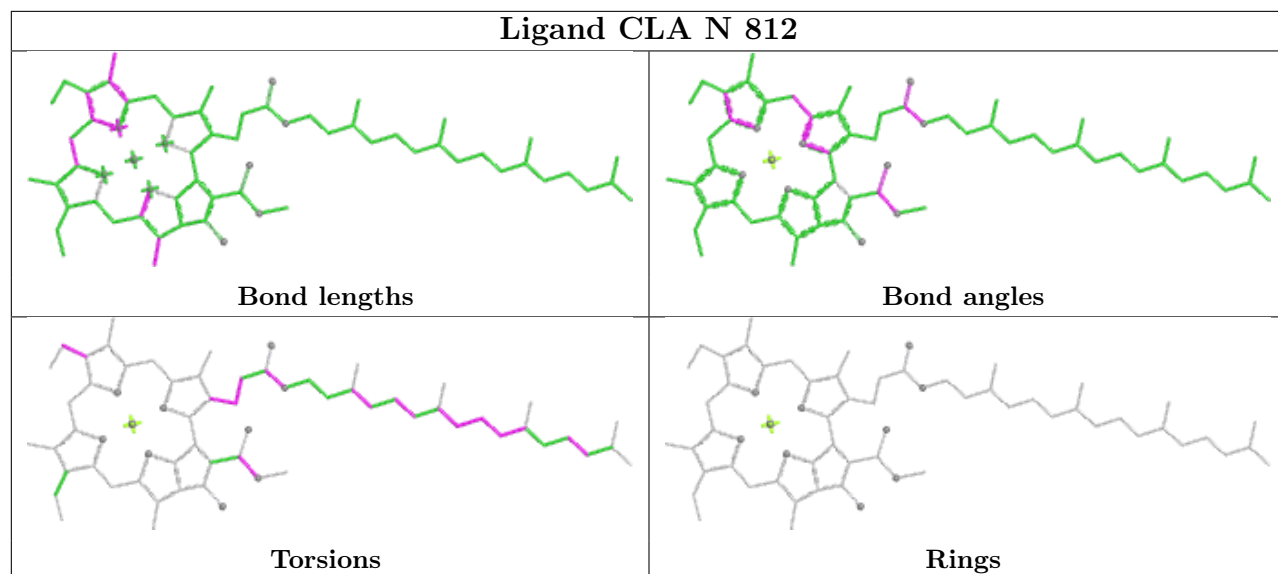


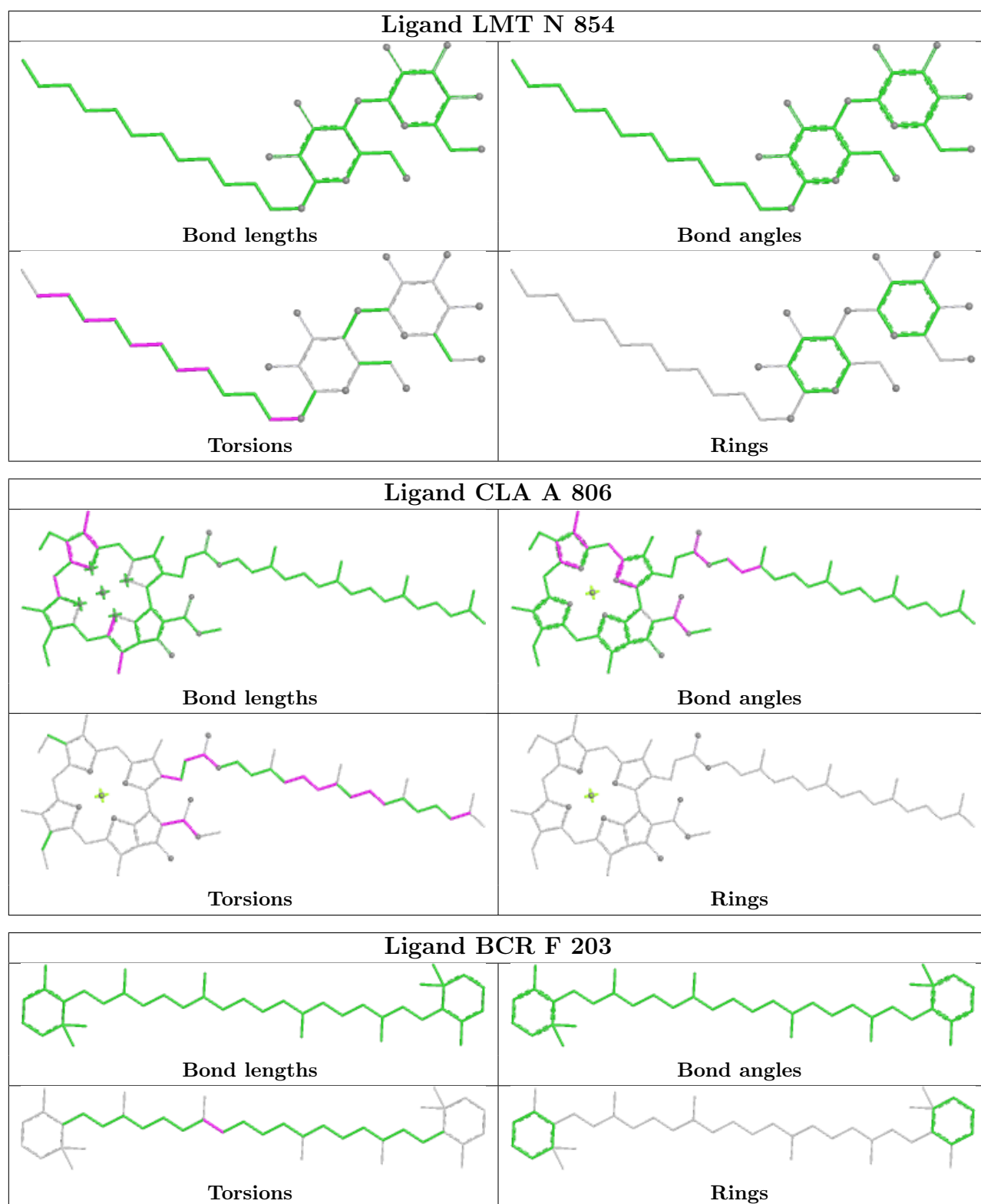
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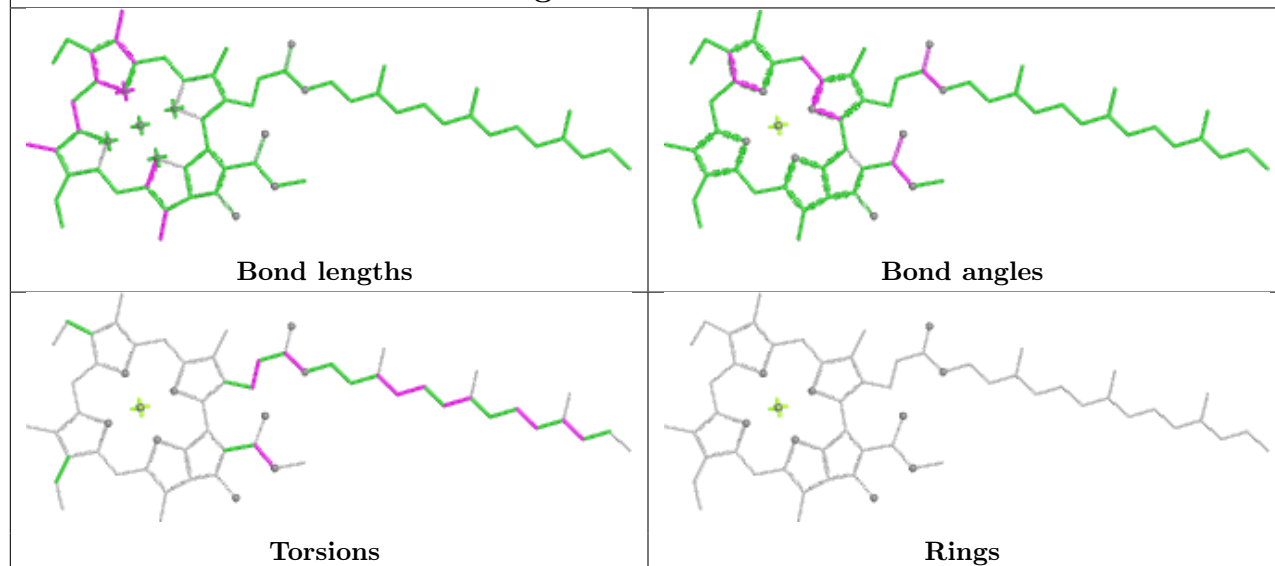
Ligand CLA B 804



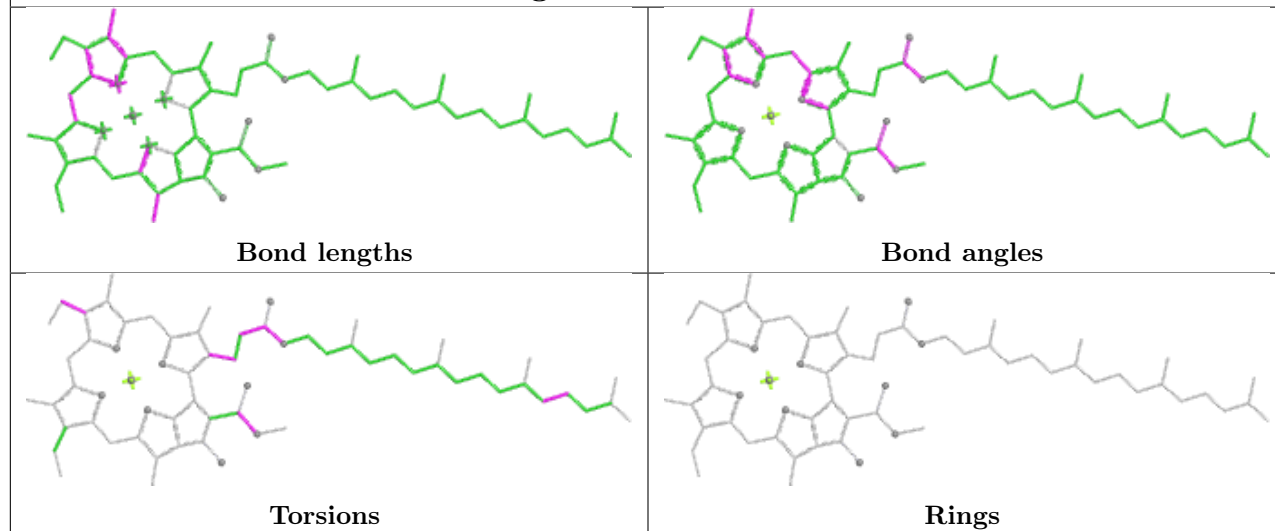


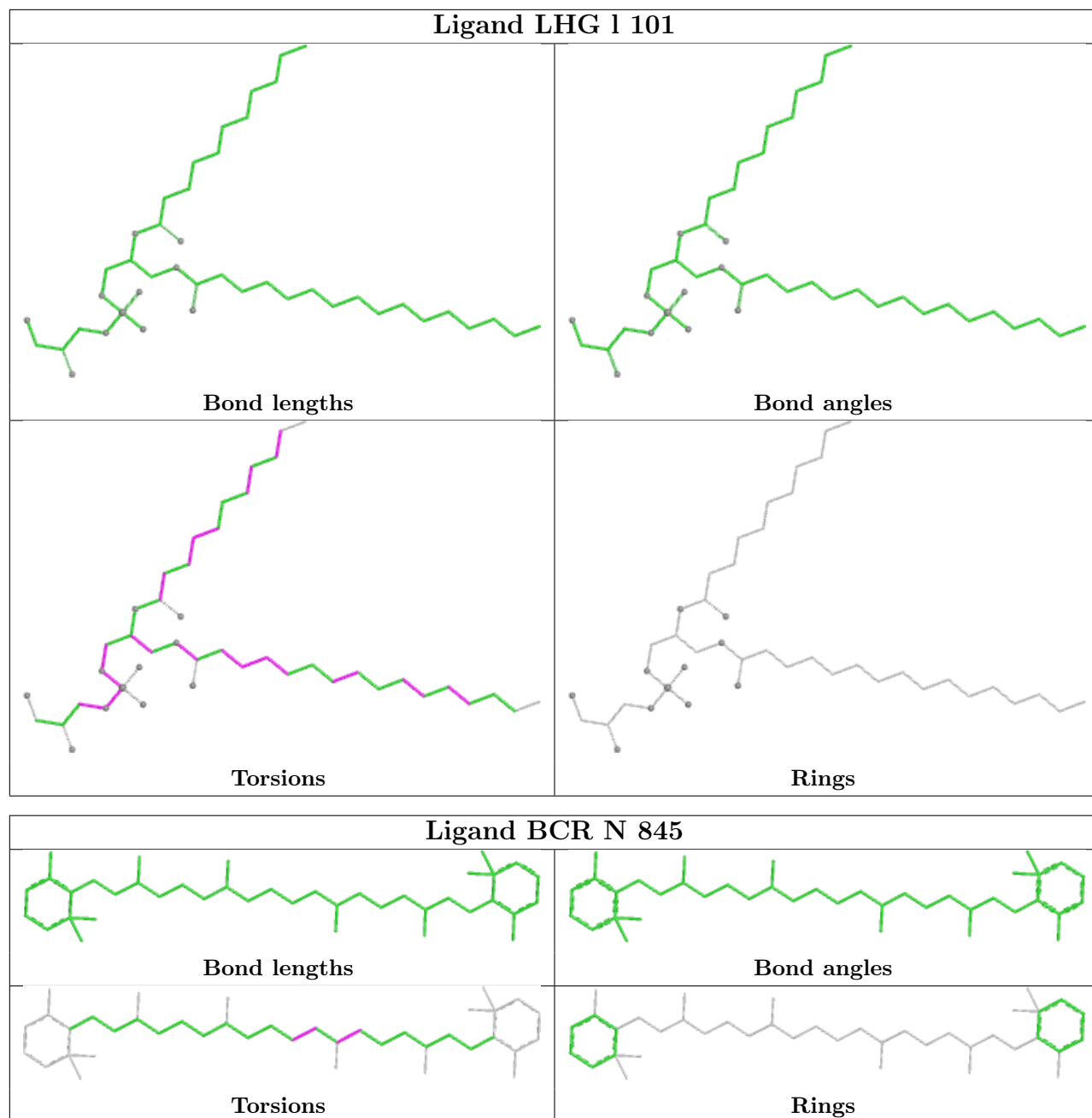


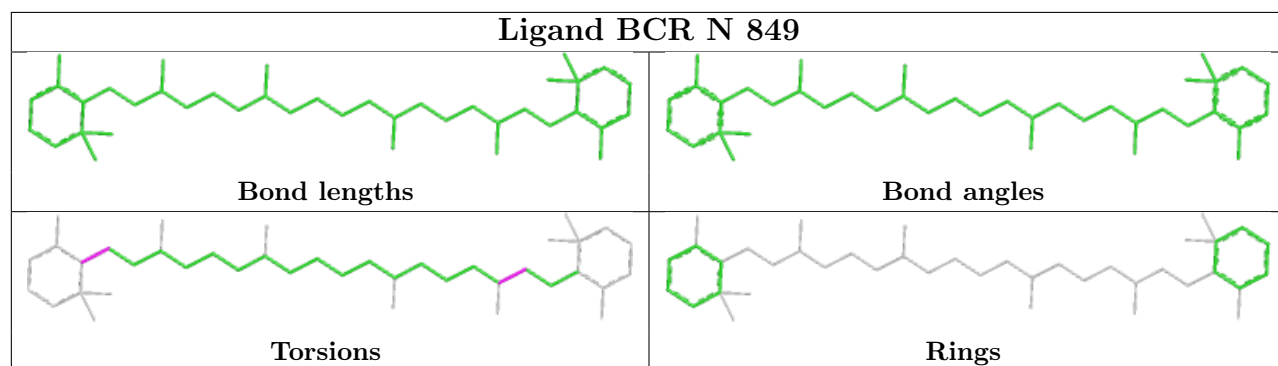
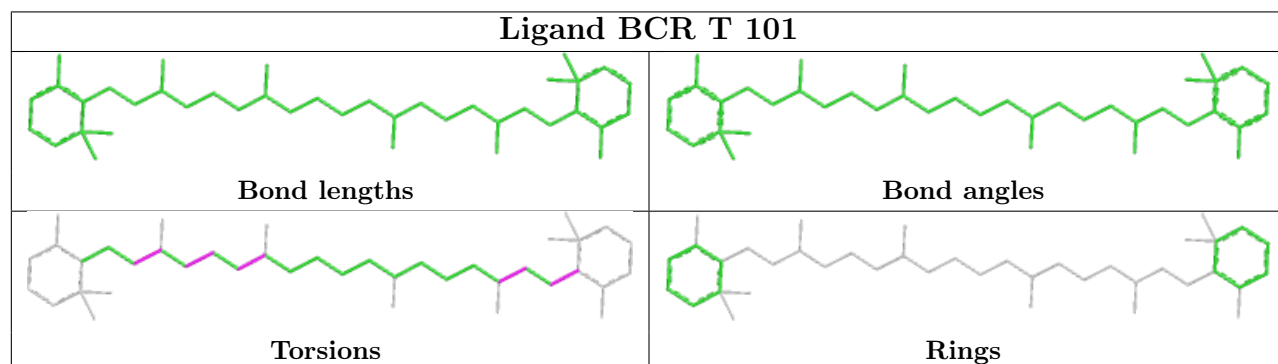
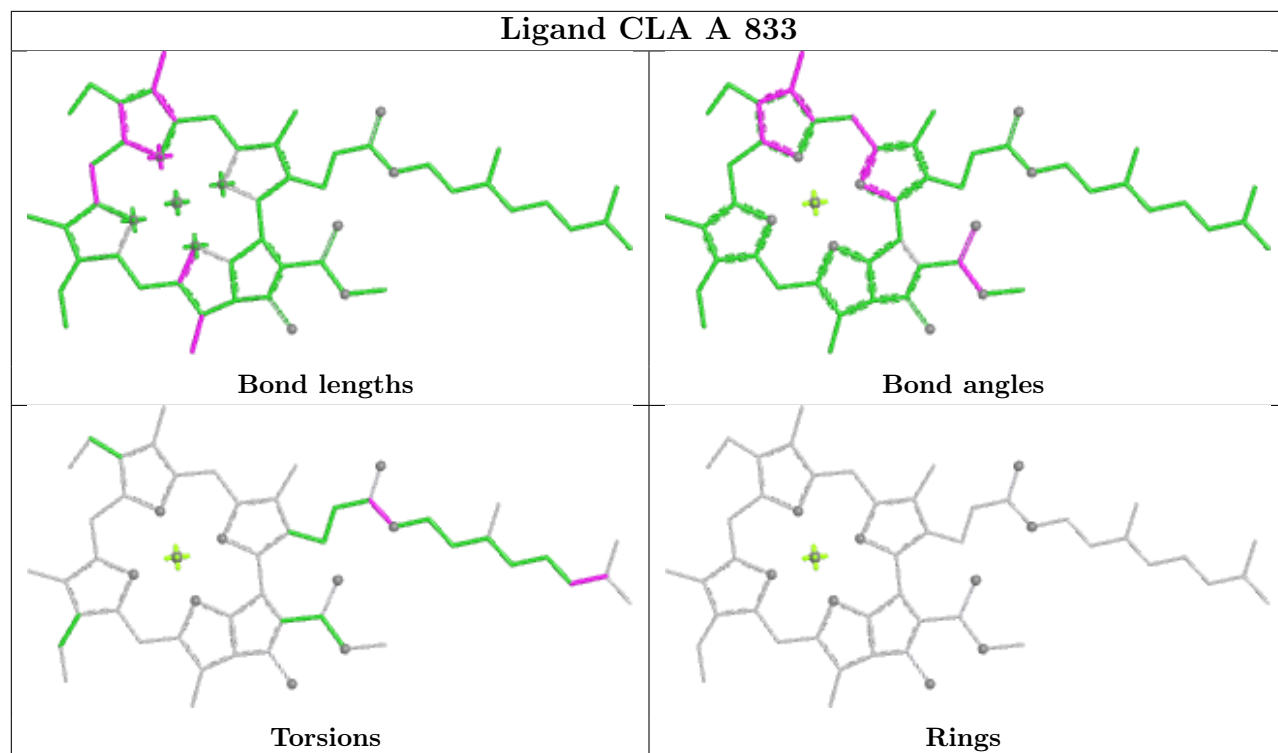
Ligand CLA b 827

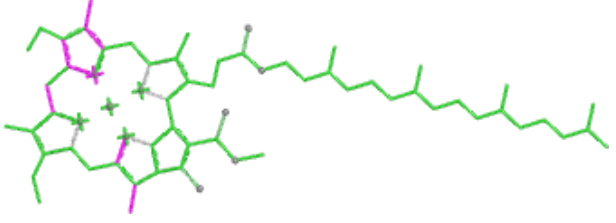
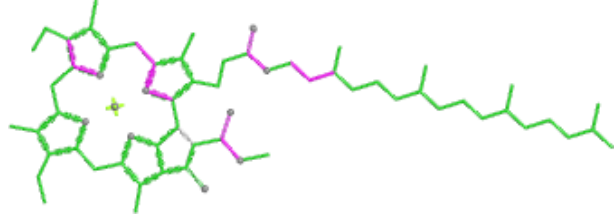
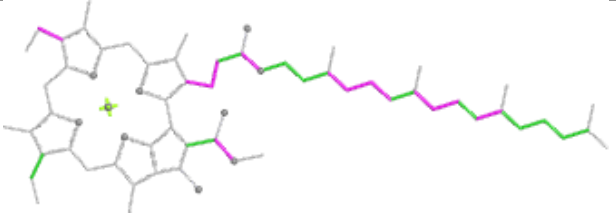
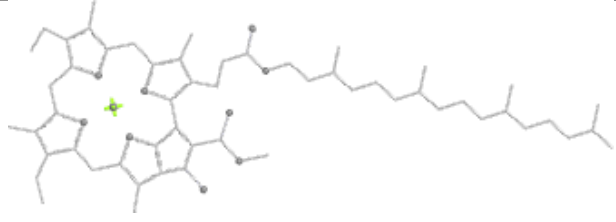
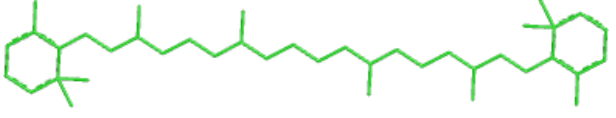
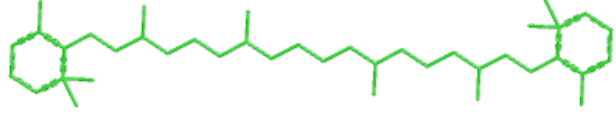
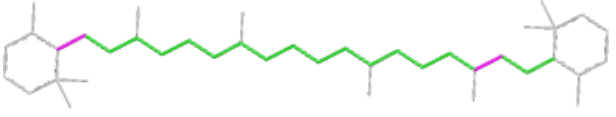
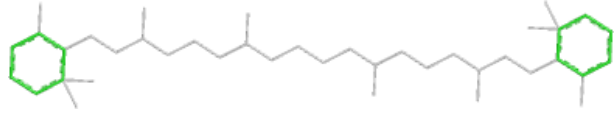
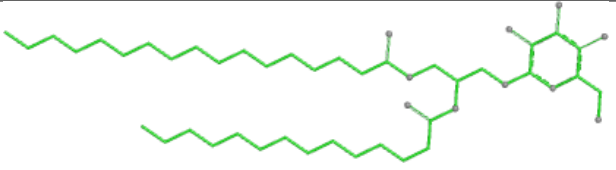
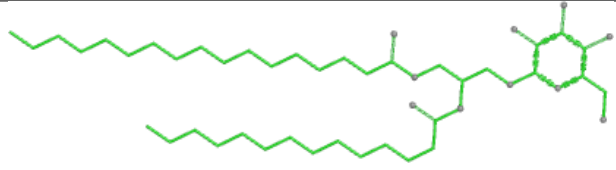
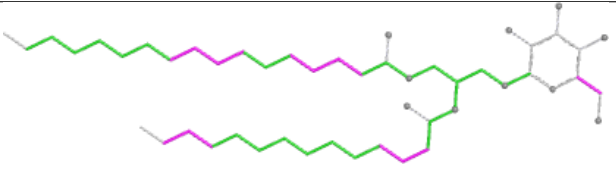
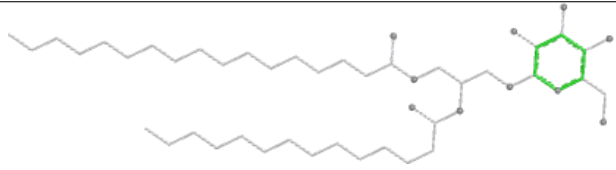


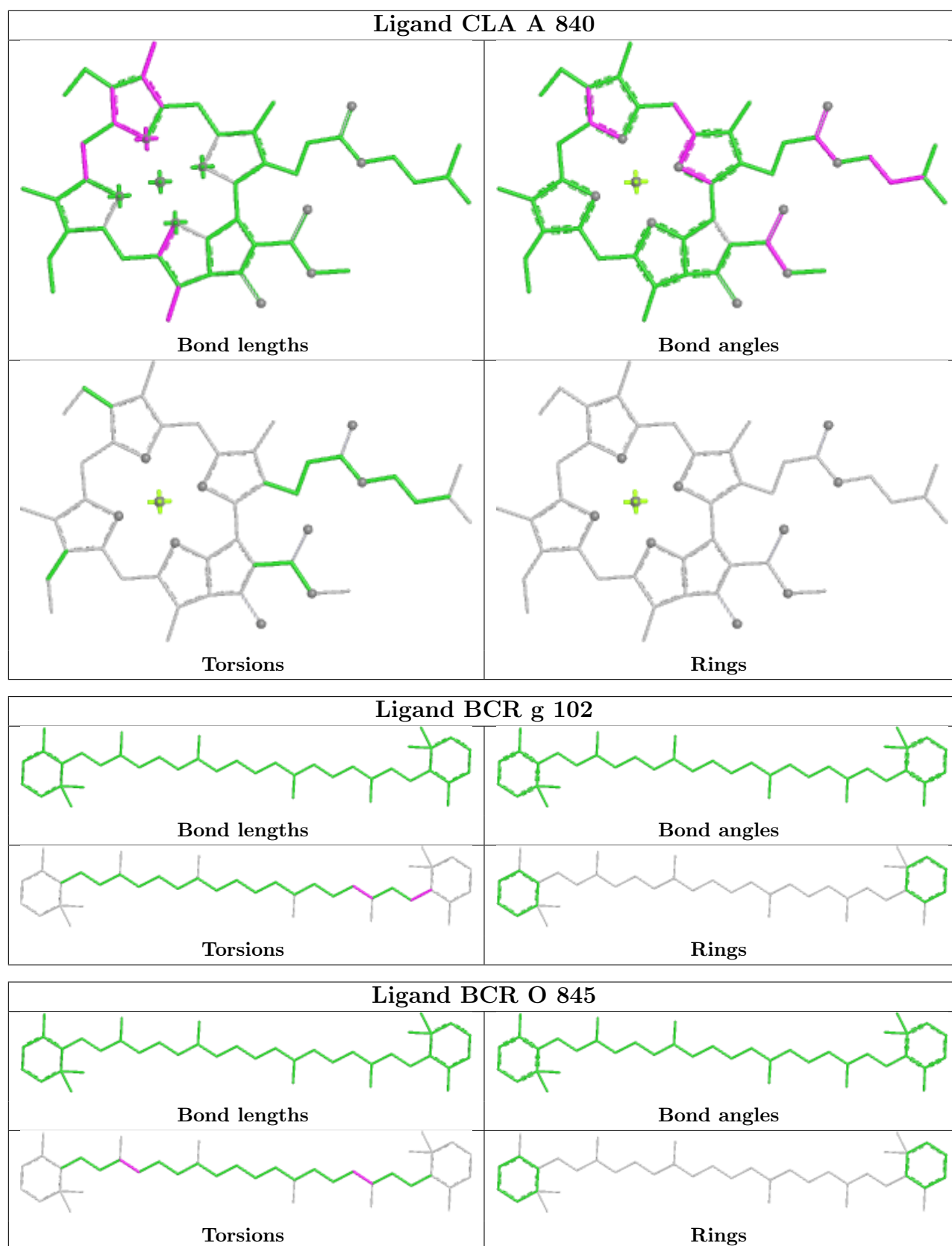
Ligand CLA O 817

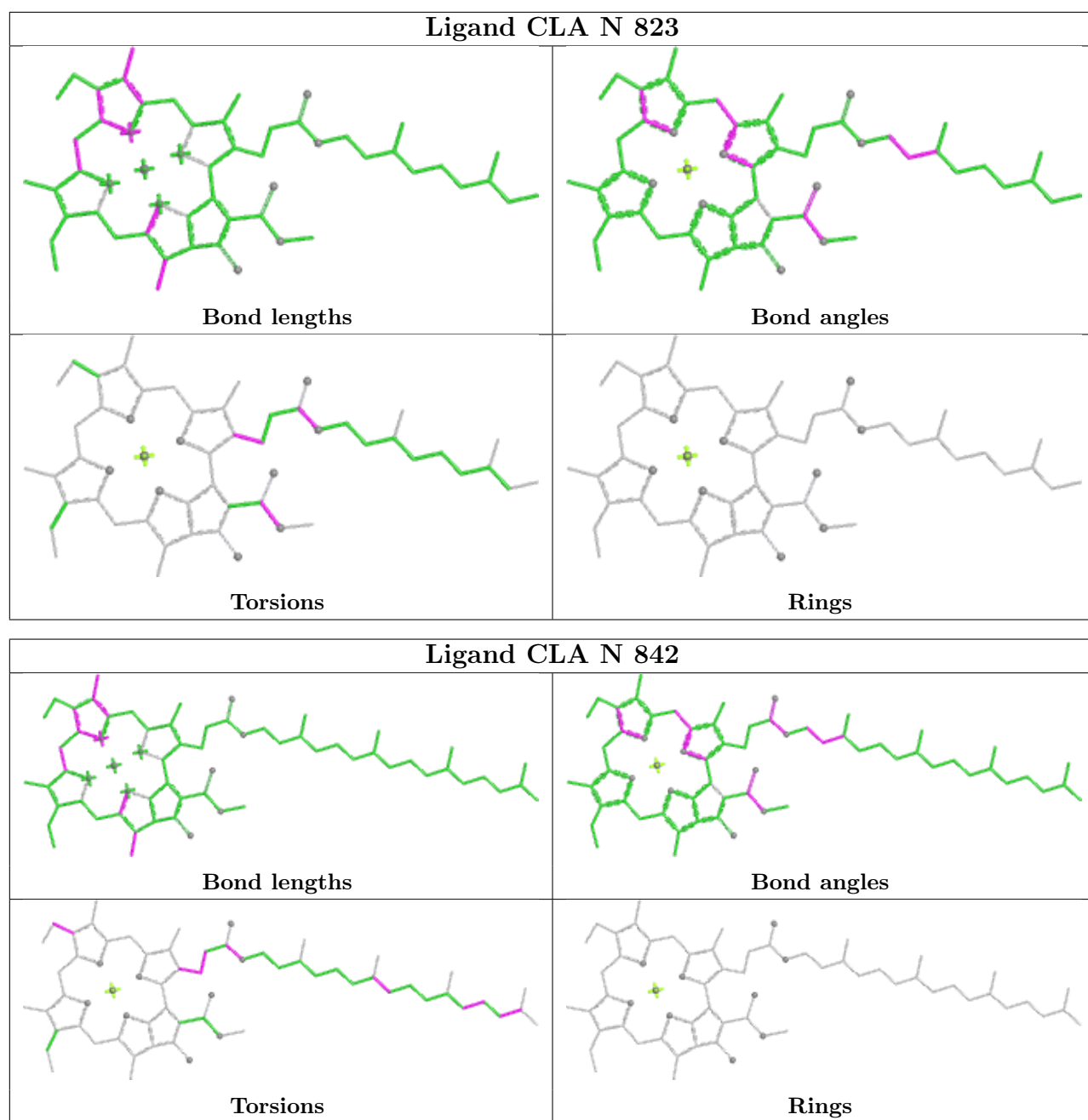




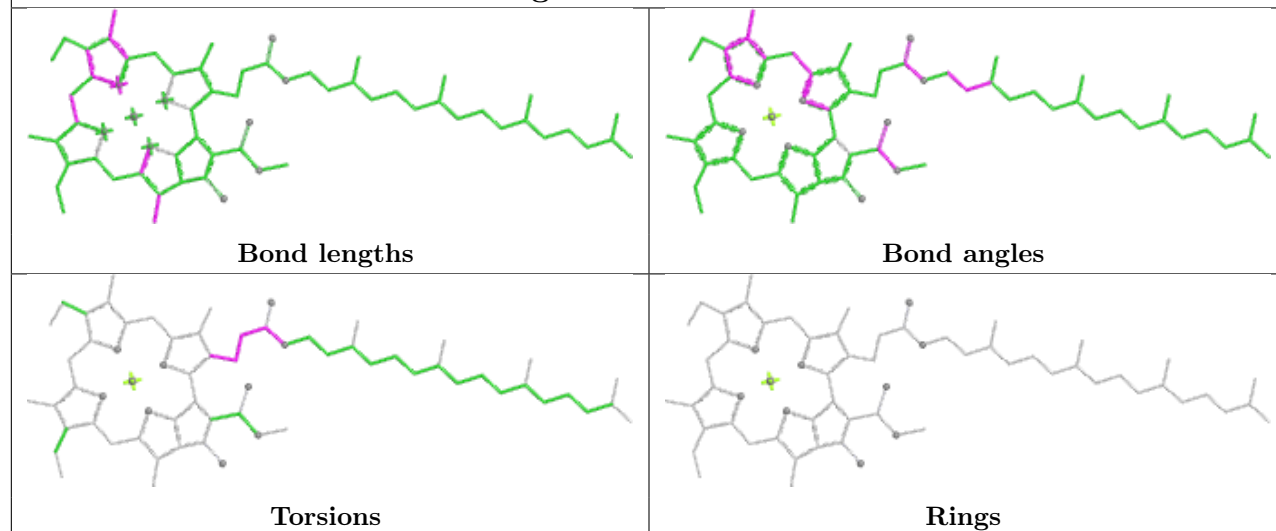


Ligand CLA O 830	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 849	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG W 1505	
 Bond lengths	 Bond angles
 Torsions	 Rings

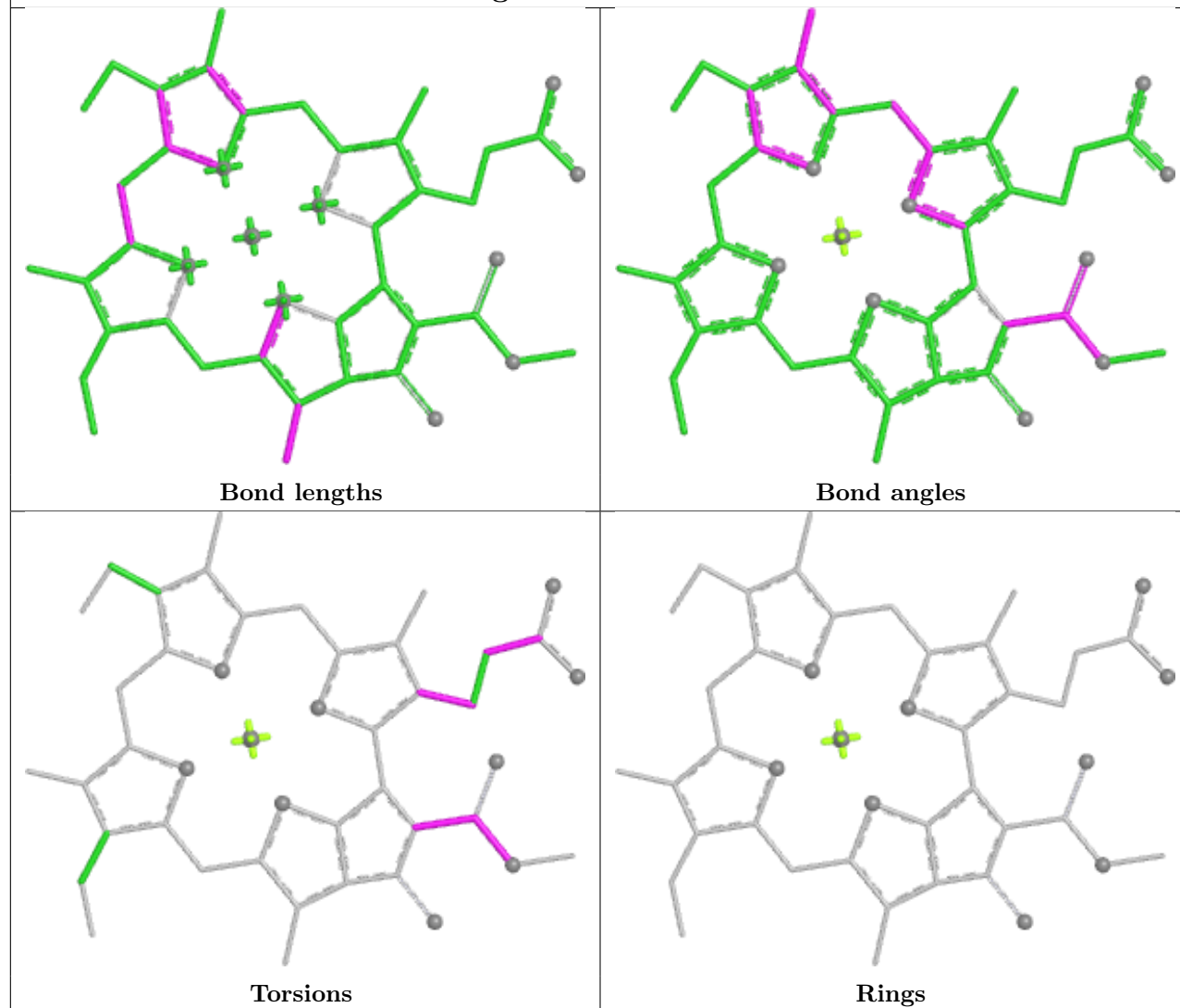


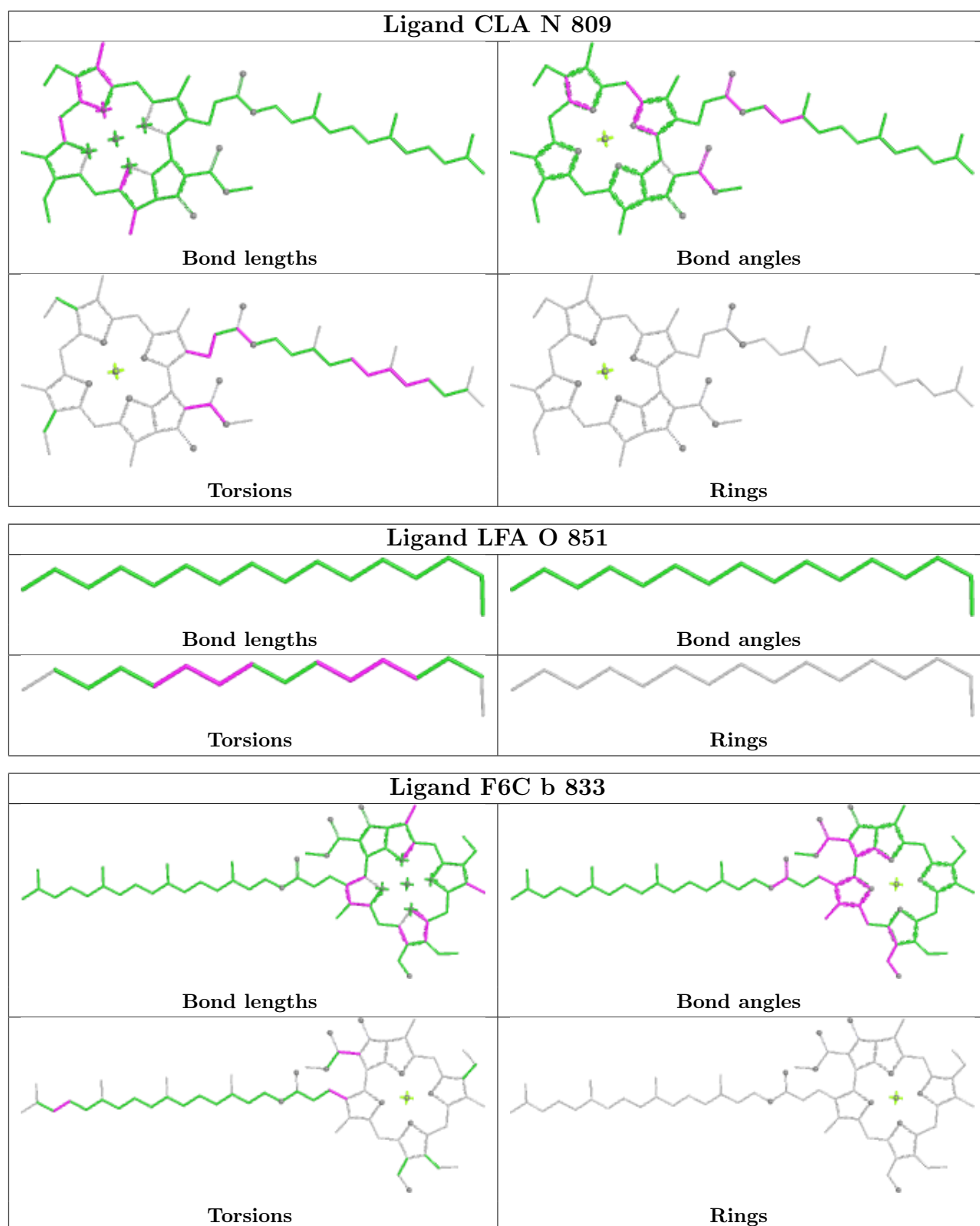


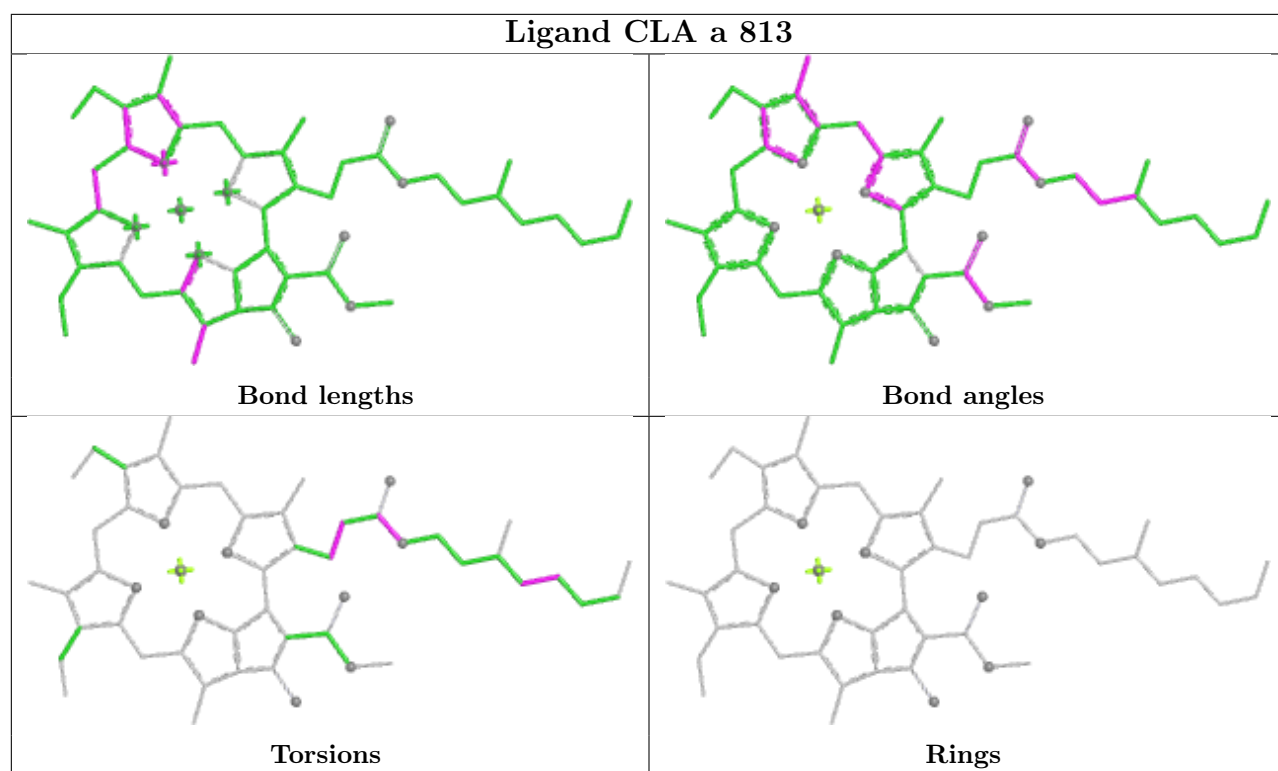
Ligand CLA O 828

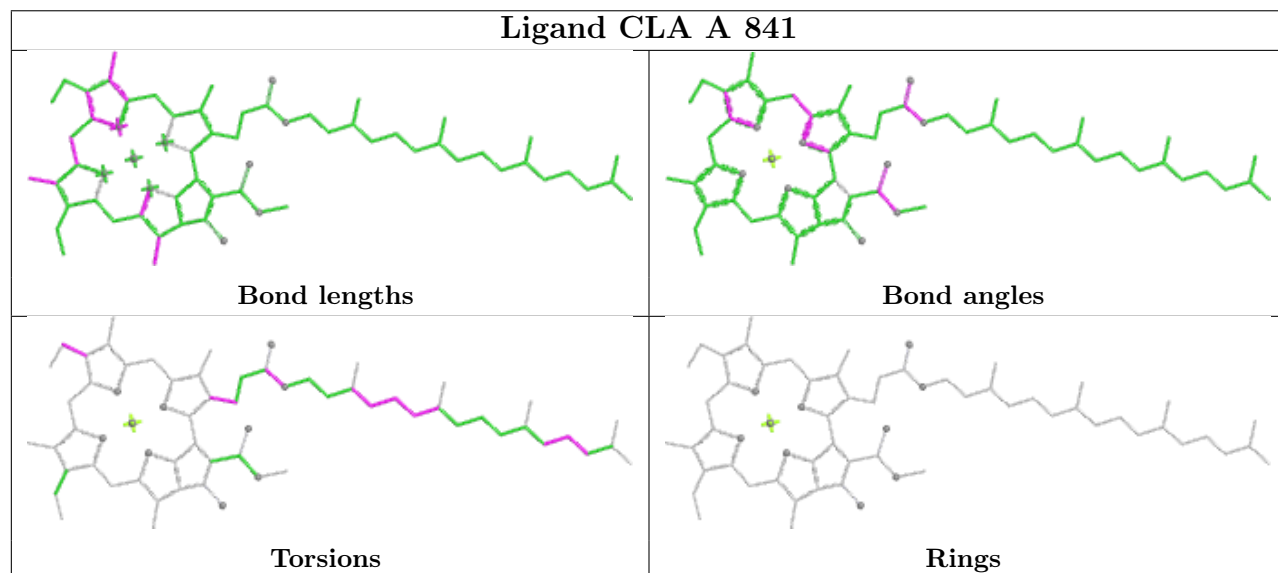
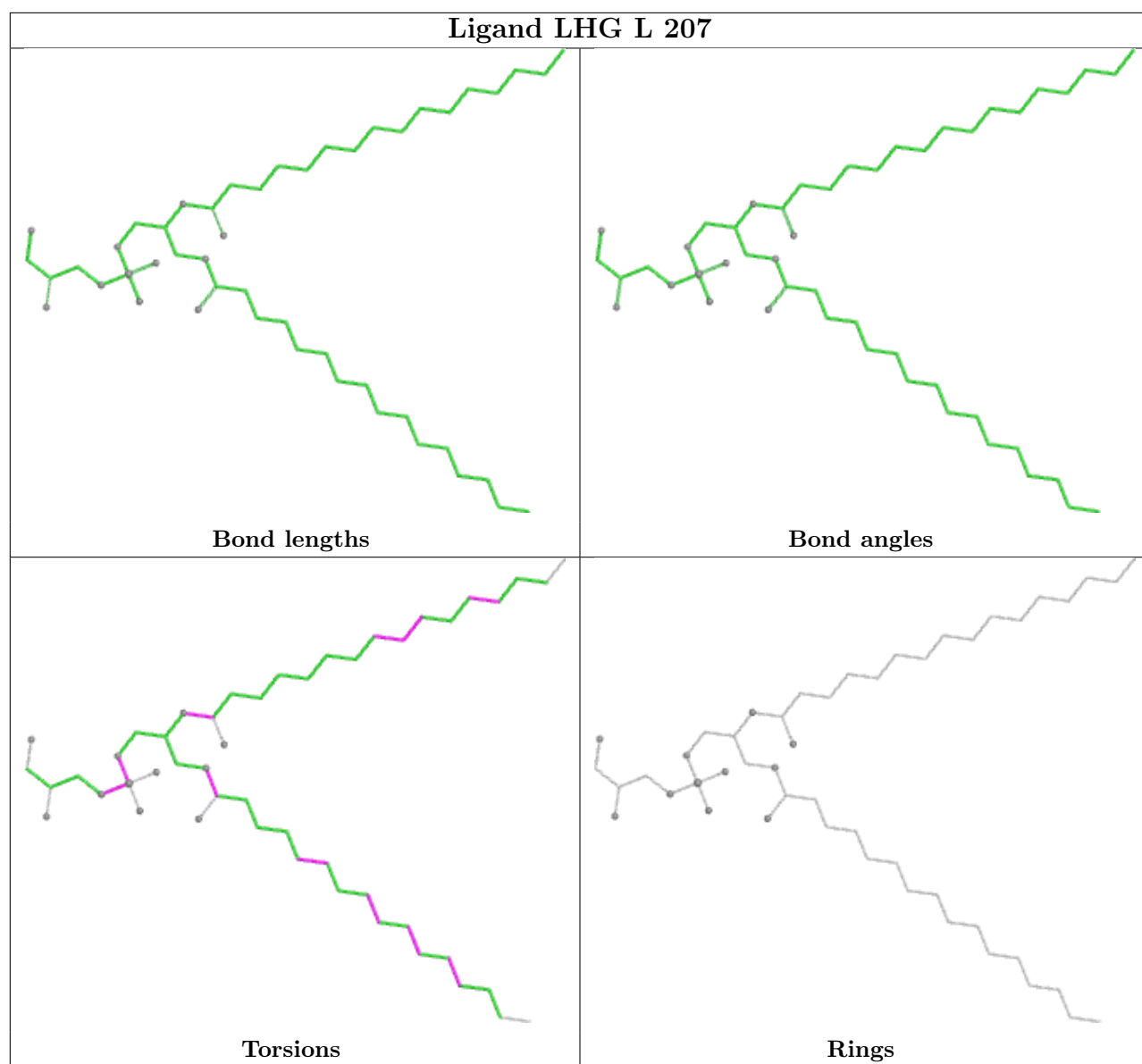


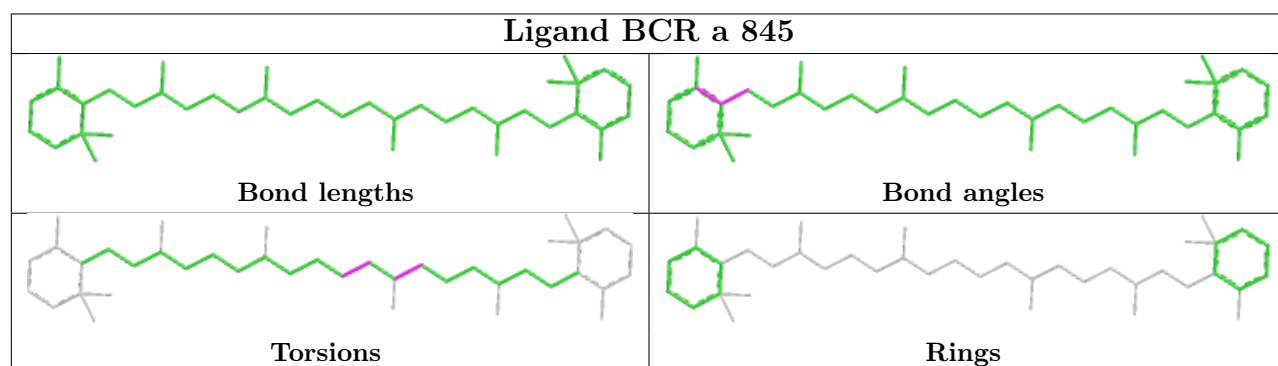
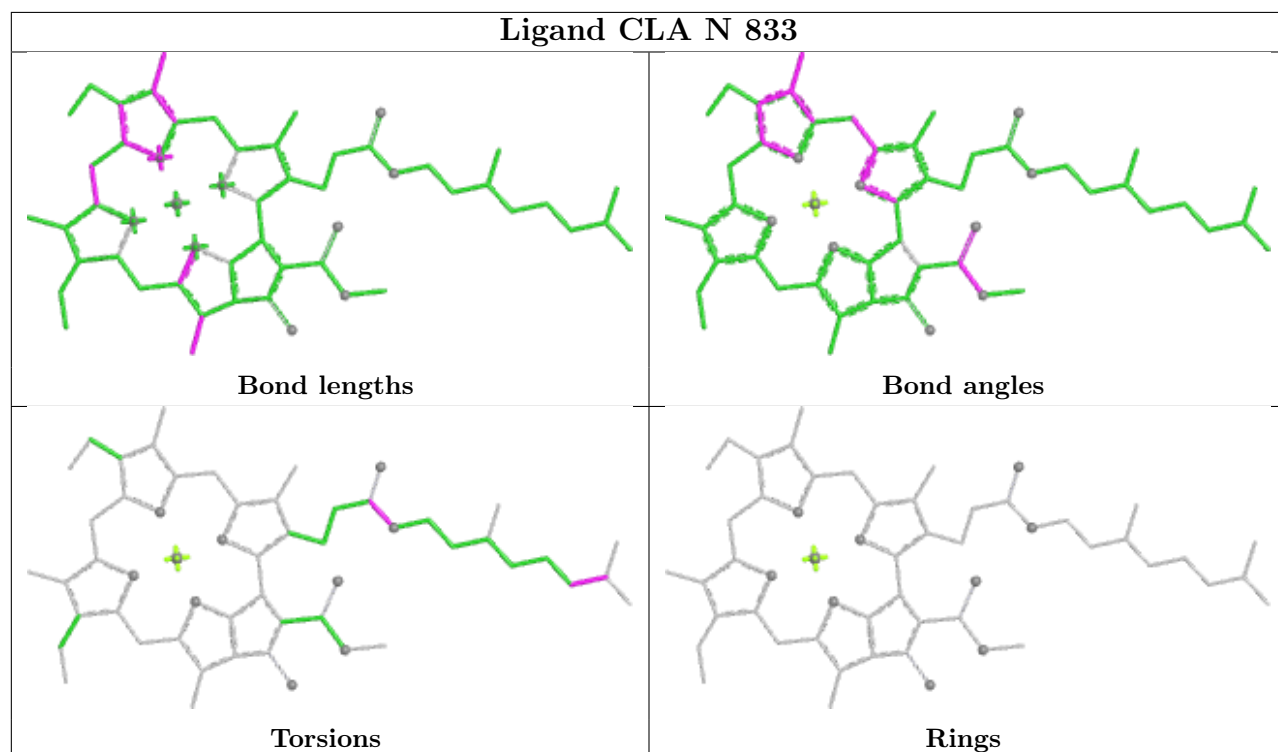
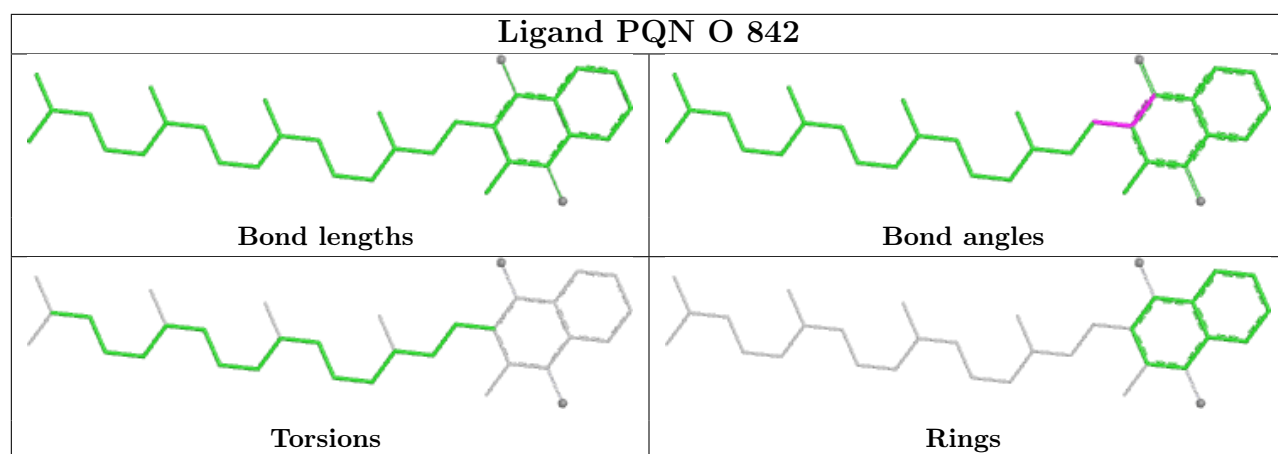
Ligand CLA B 813

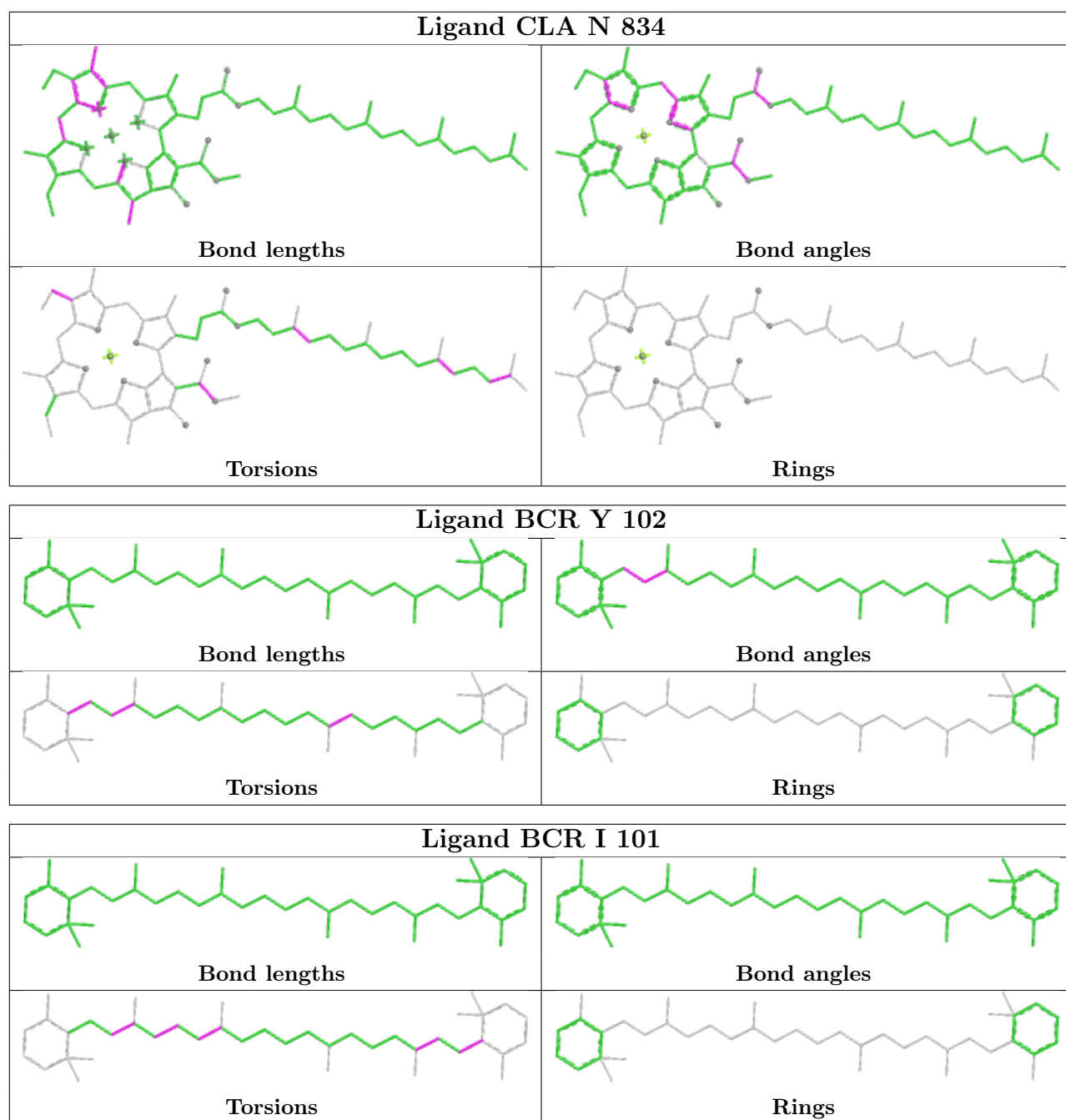


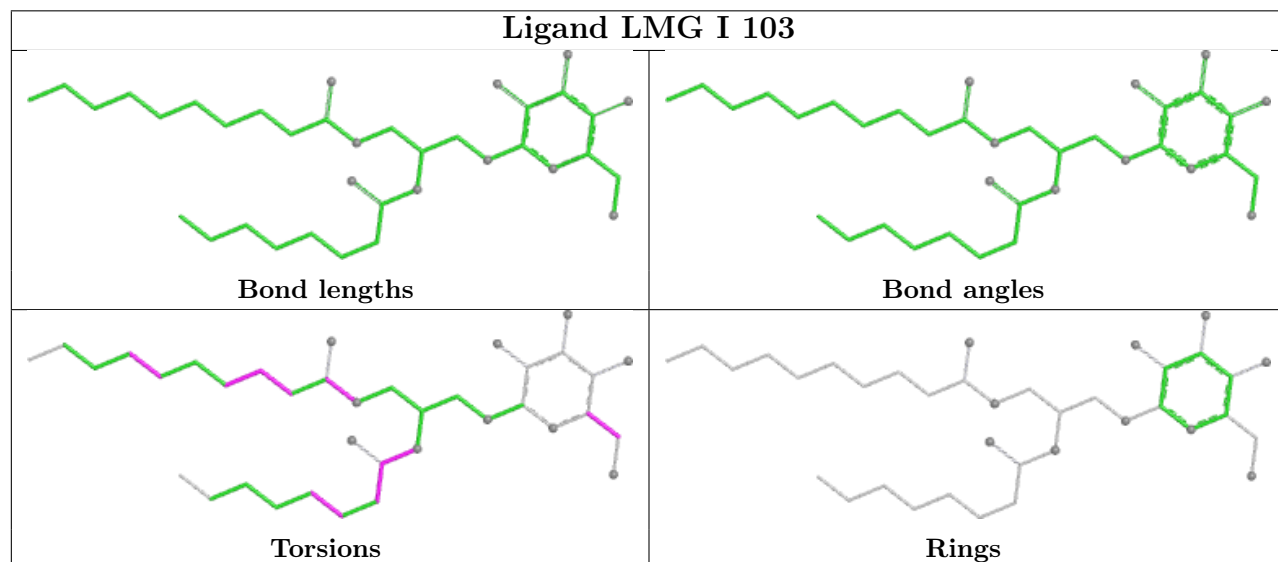
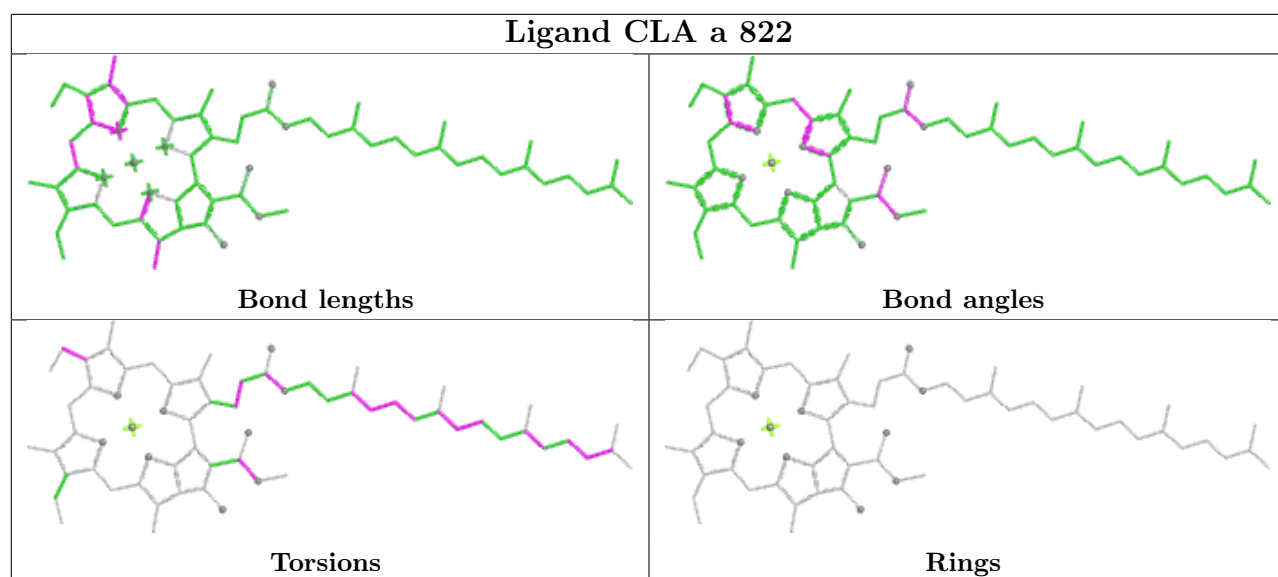




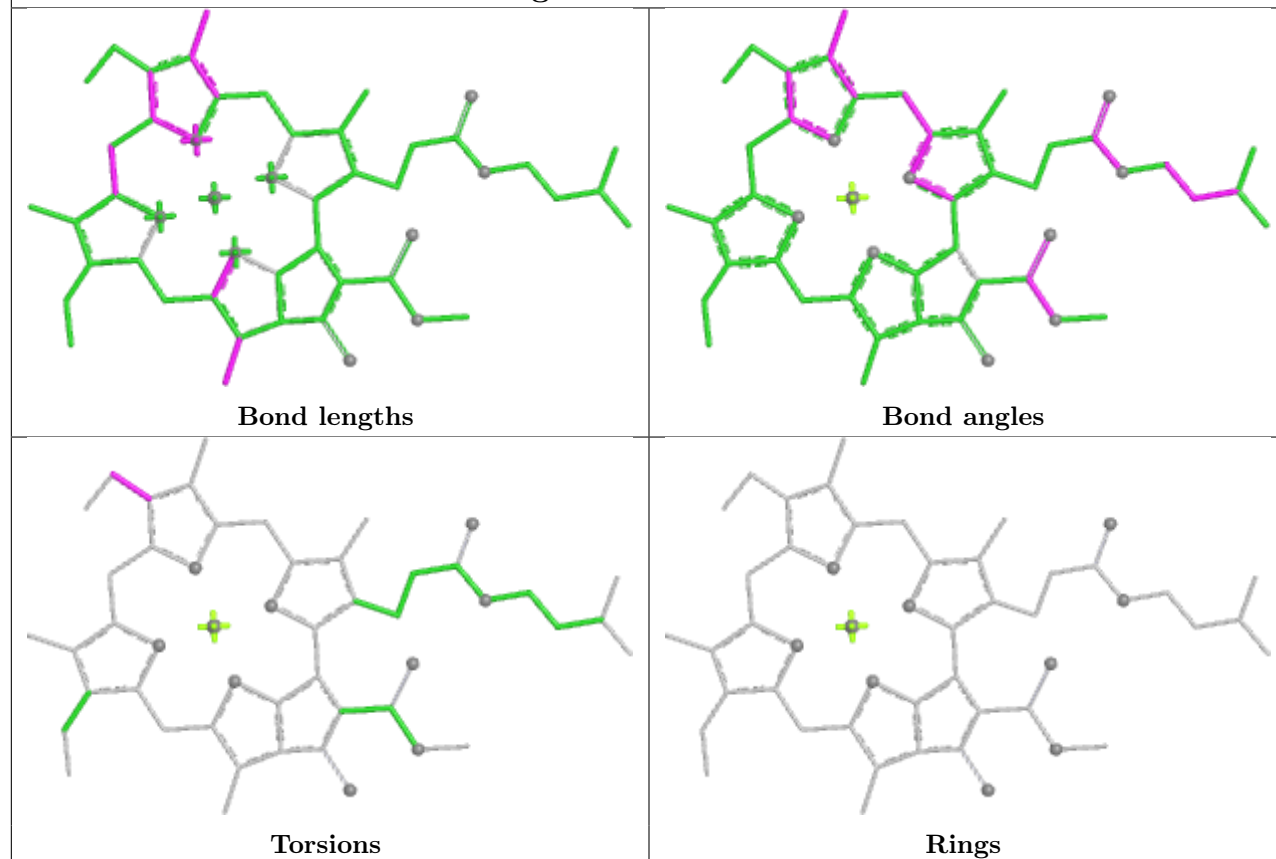




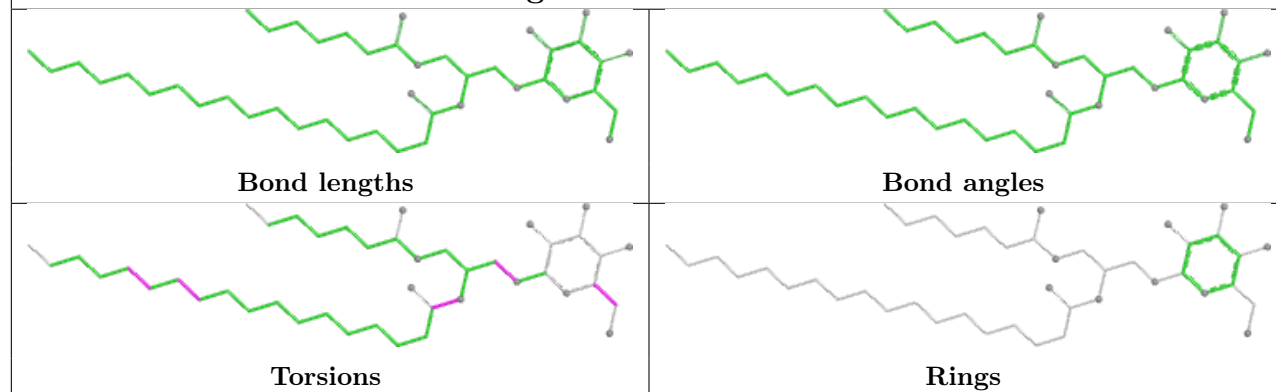




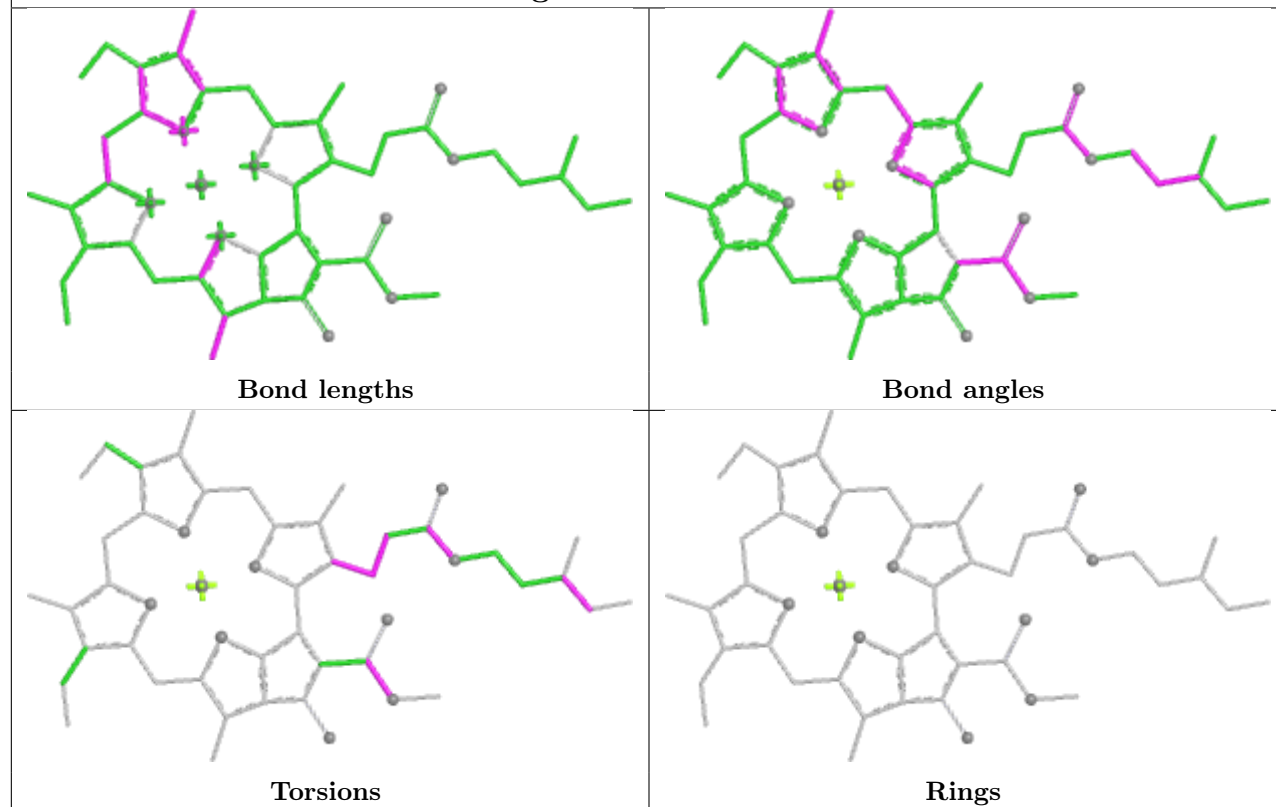
Ligand CLA V 103



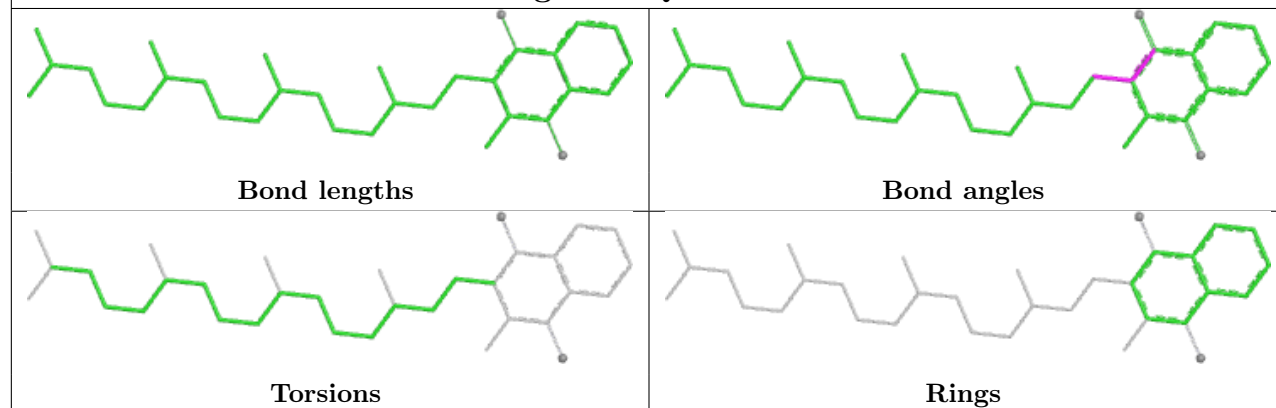
Ligand LMG N 855

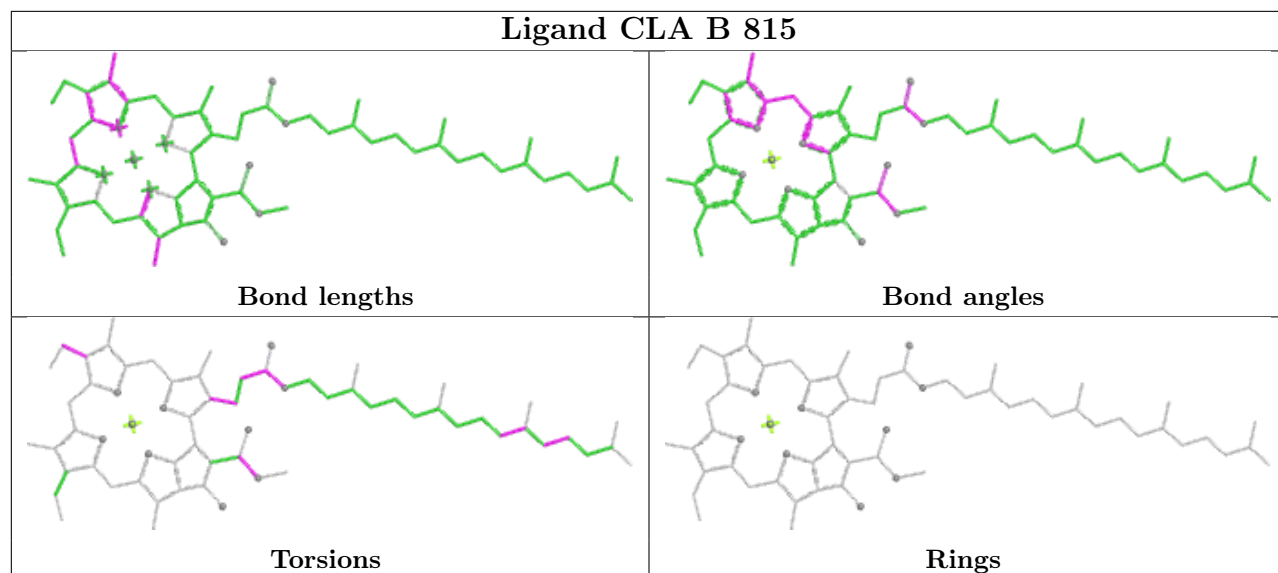
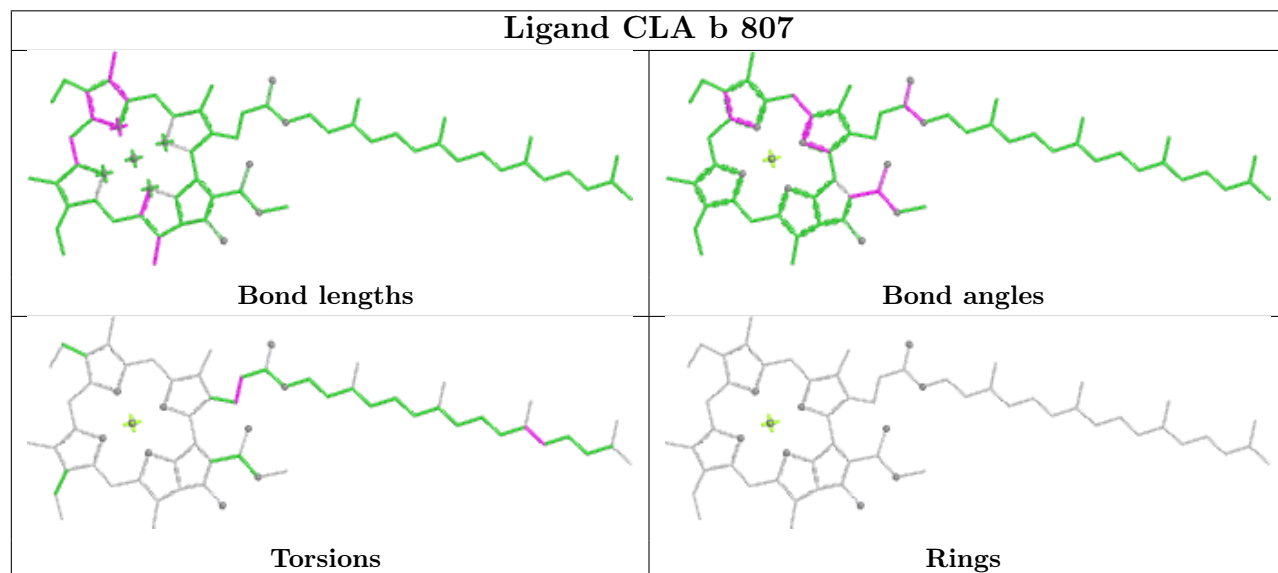
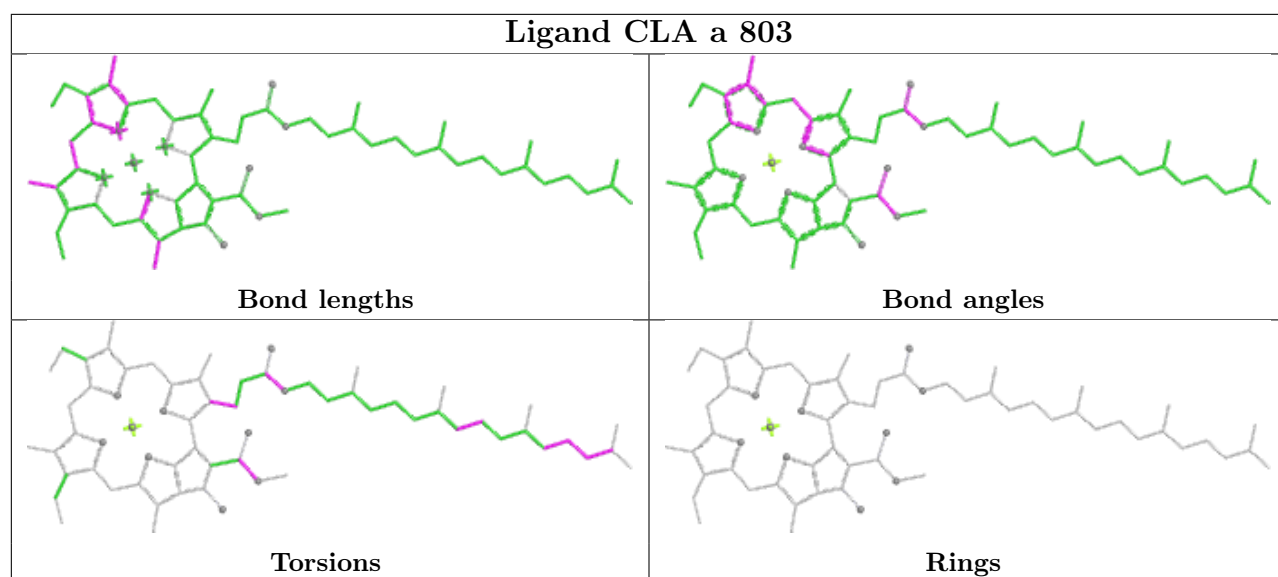


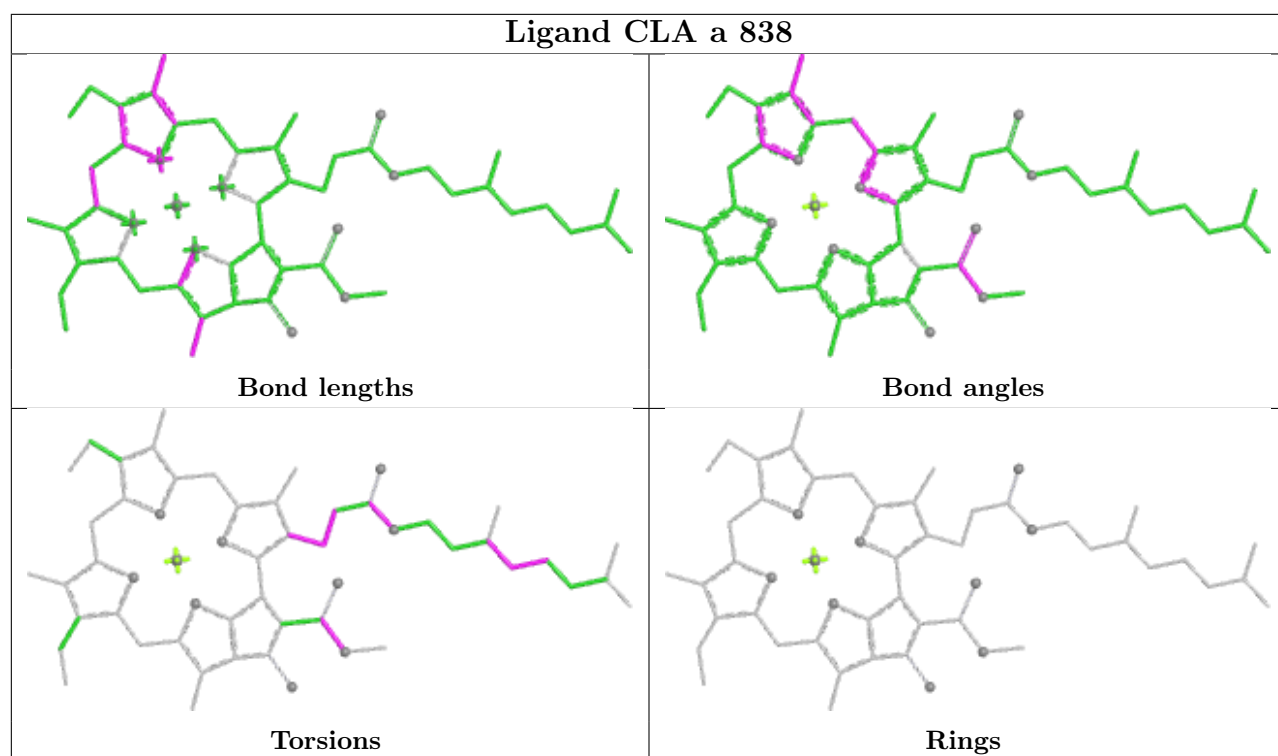
Ligand CLA A 837



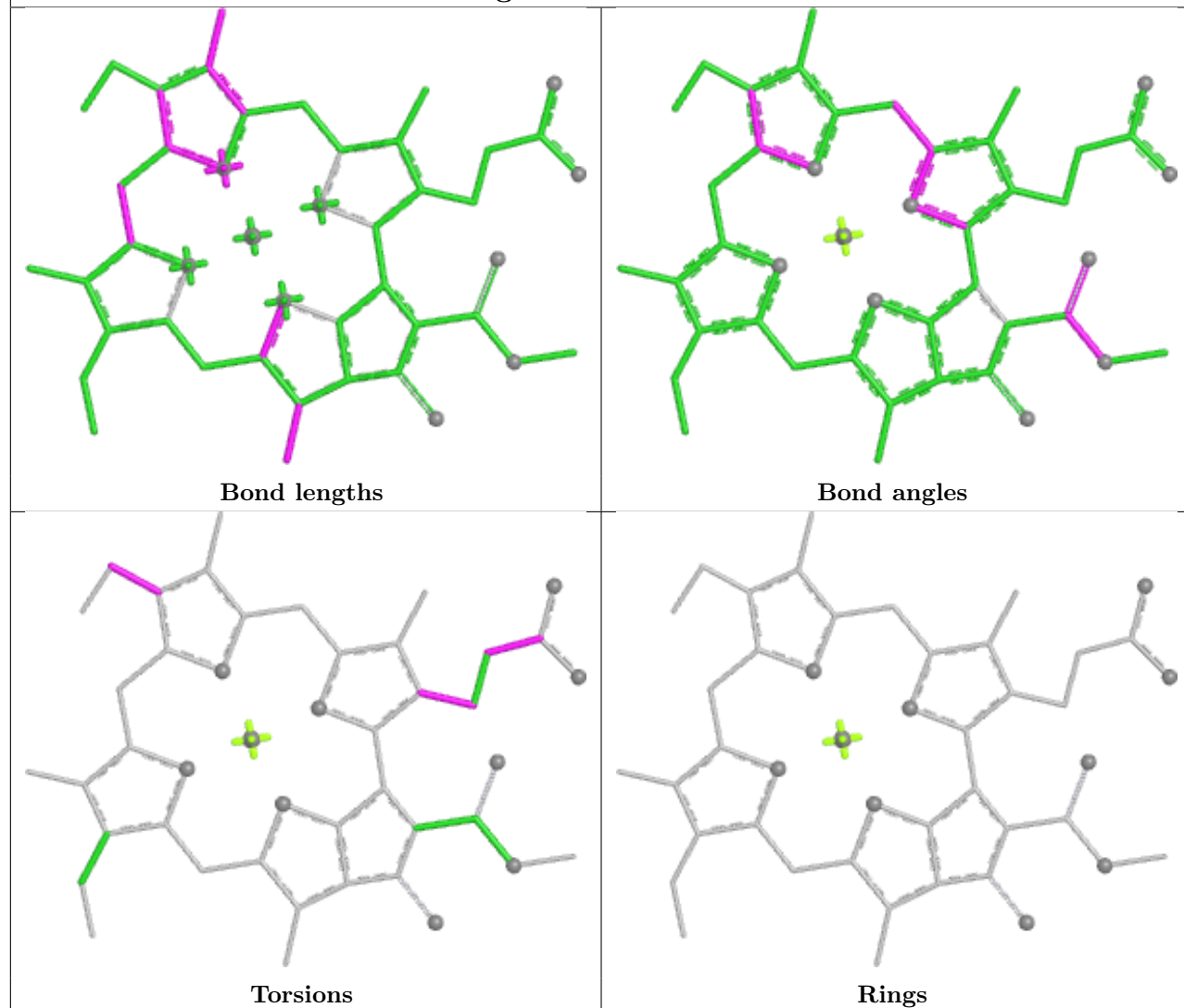
Ligand PQN a 843



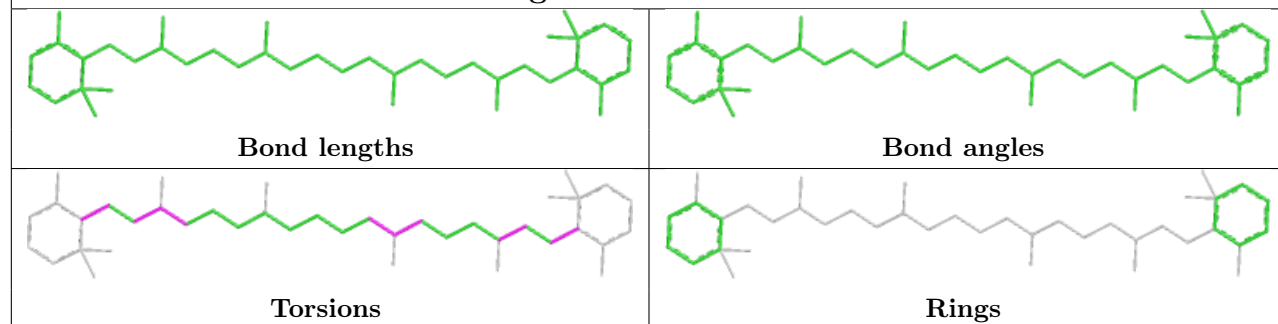


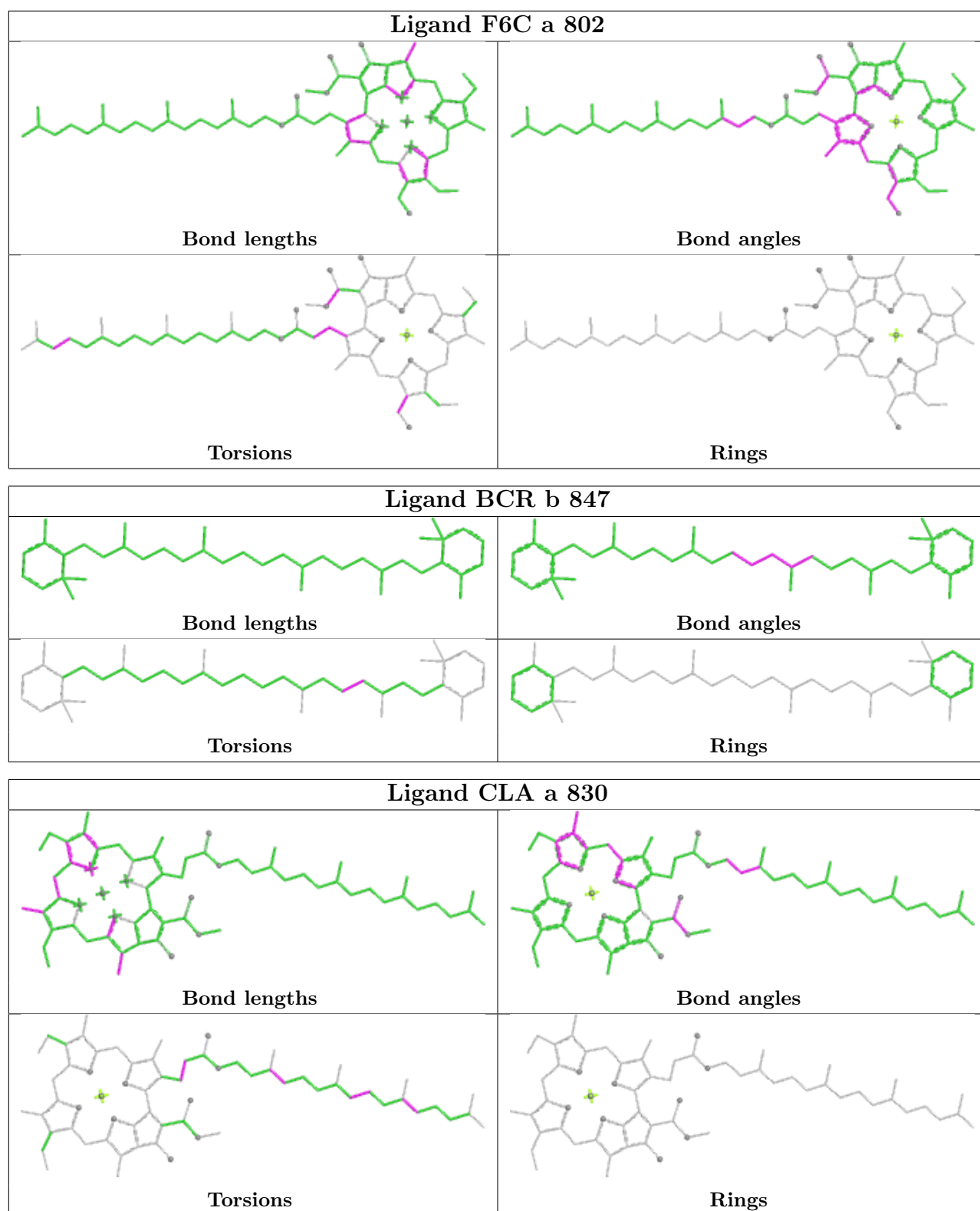


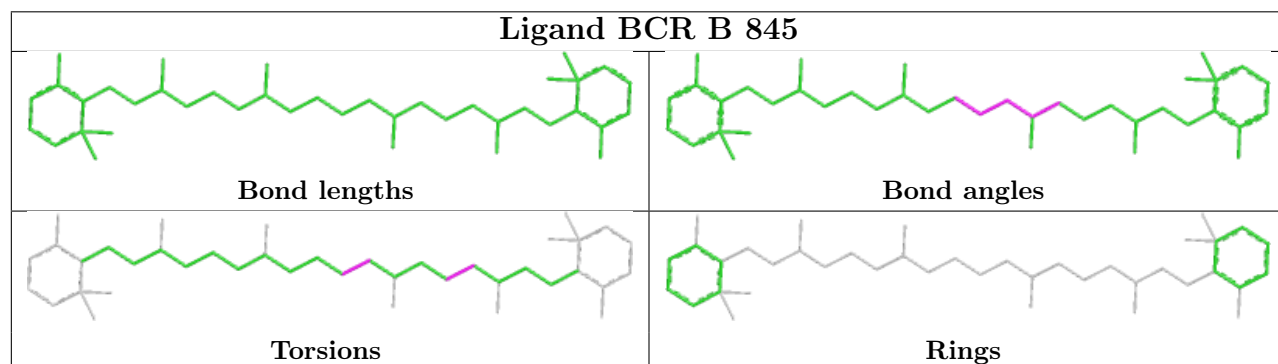
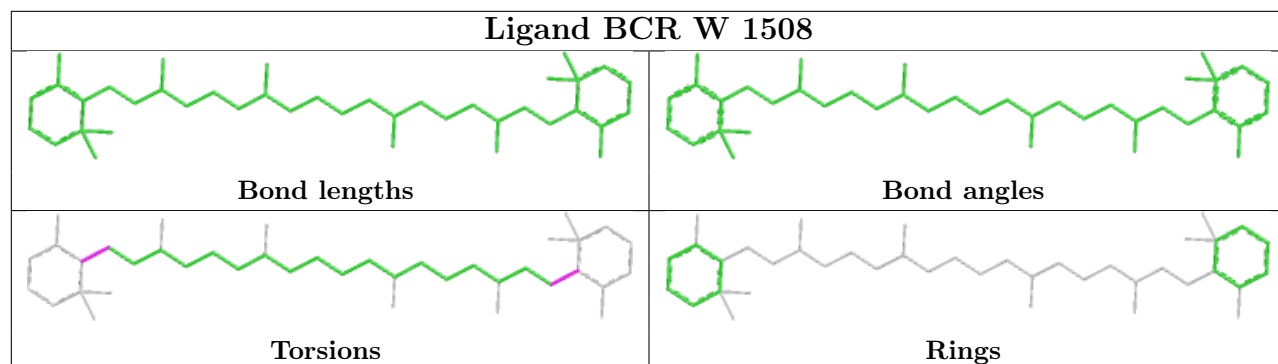
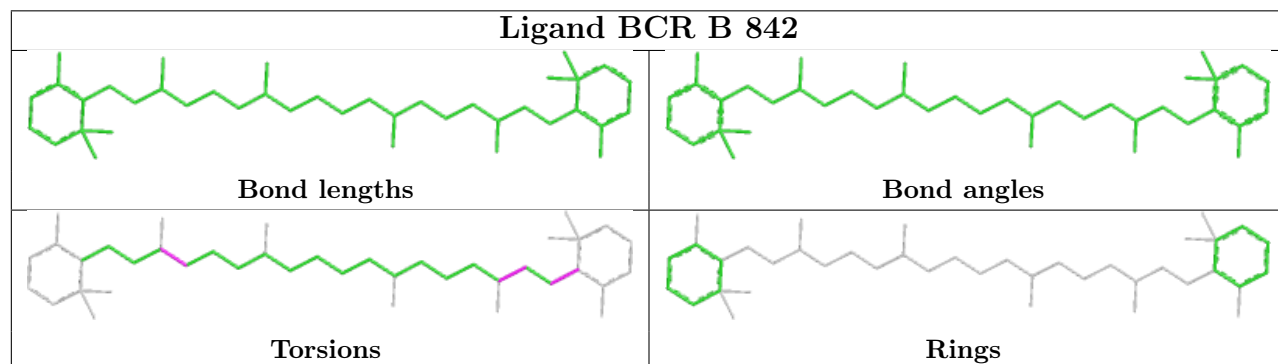
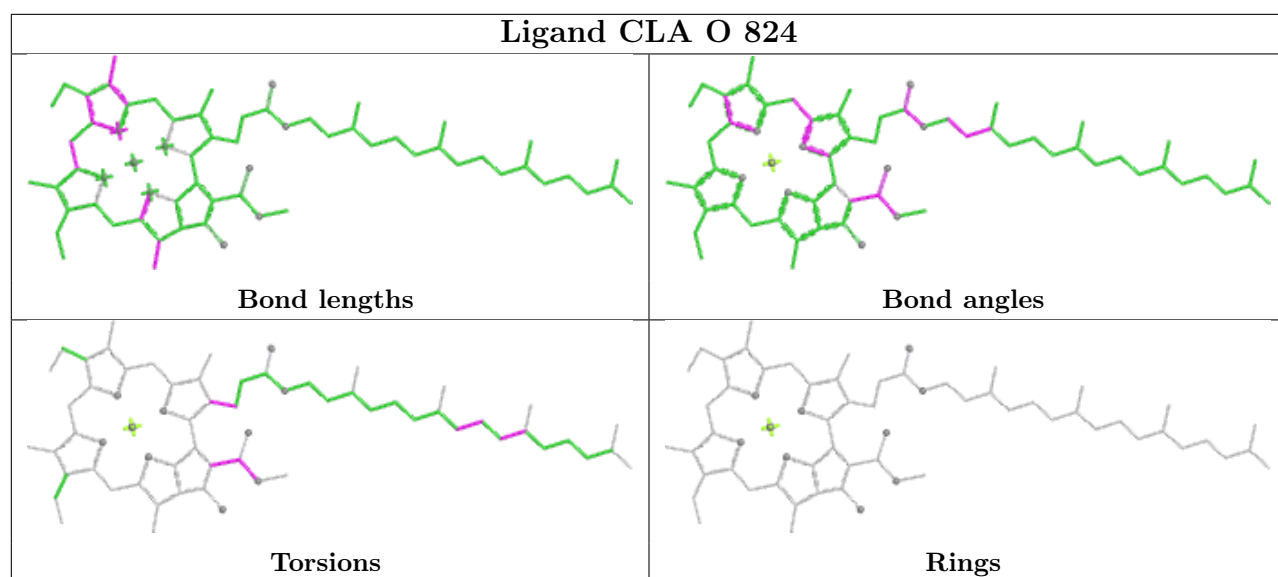
Ligand CLA b 812

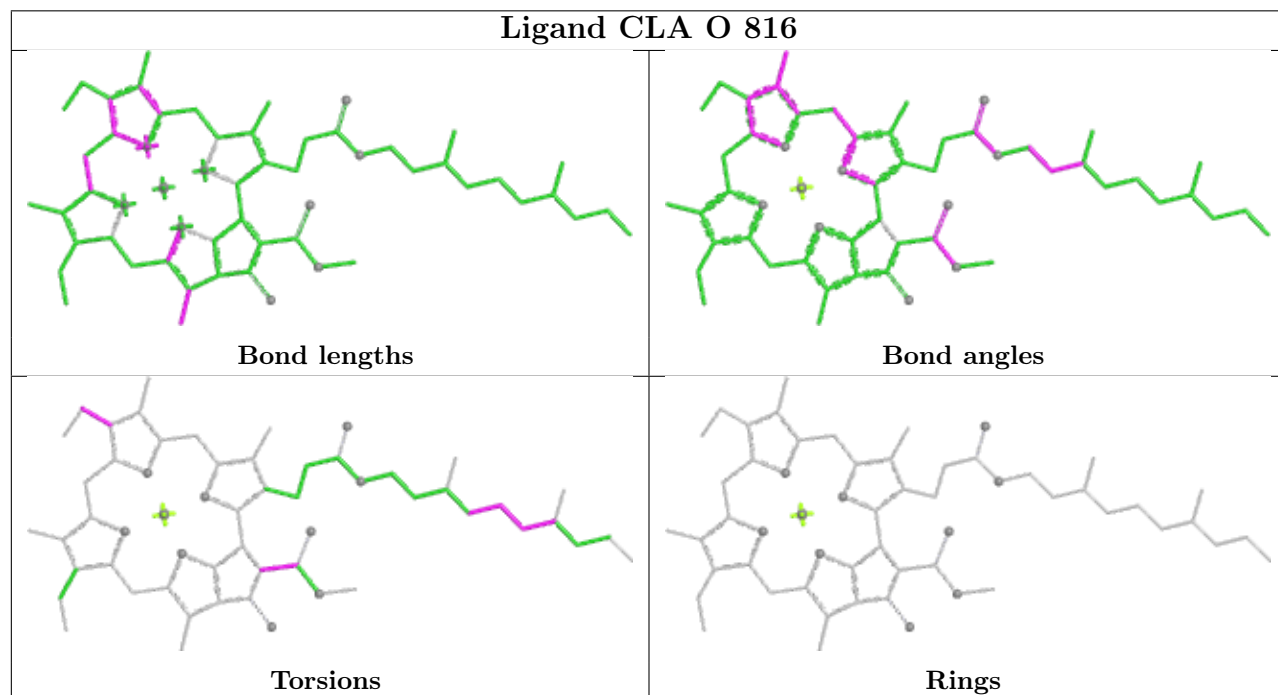
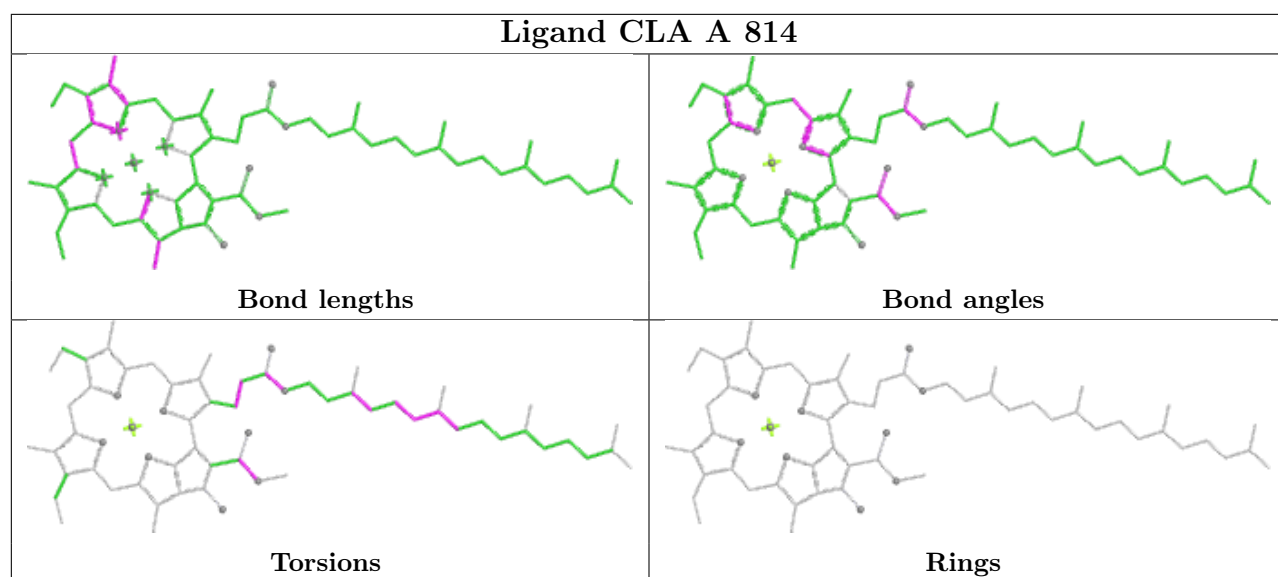


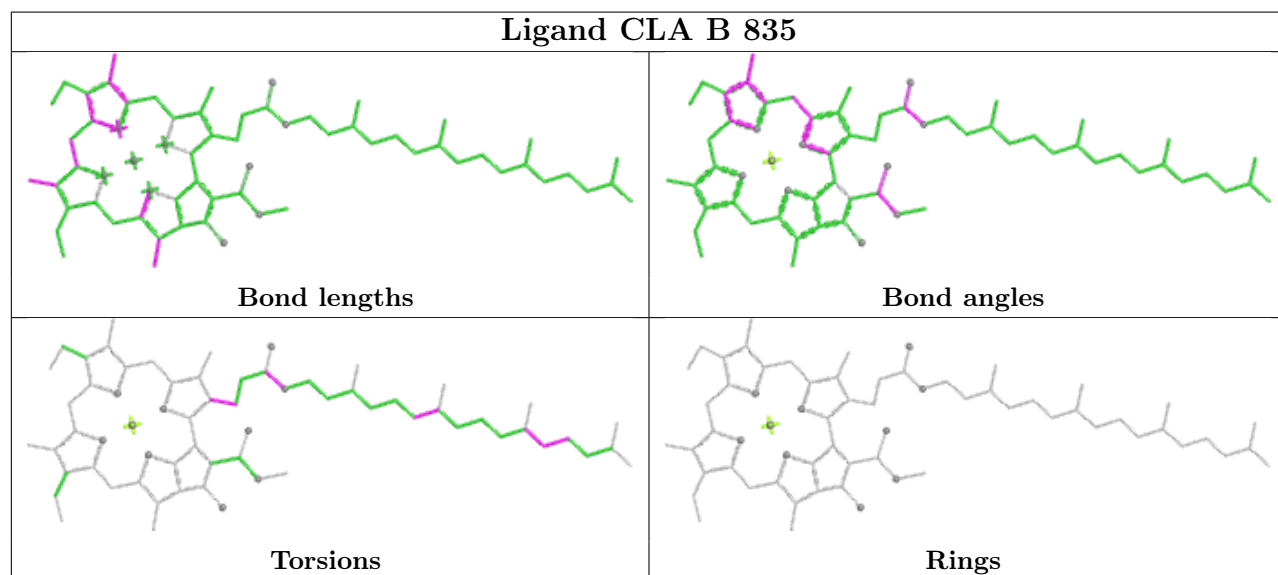
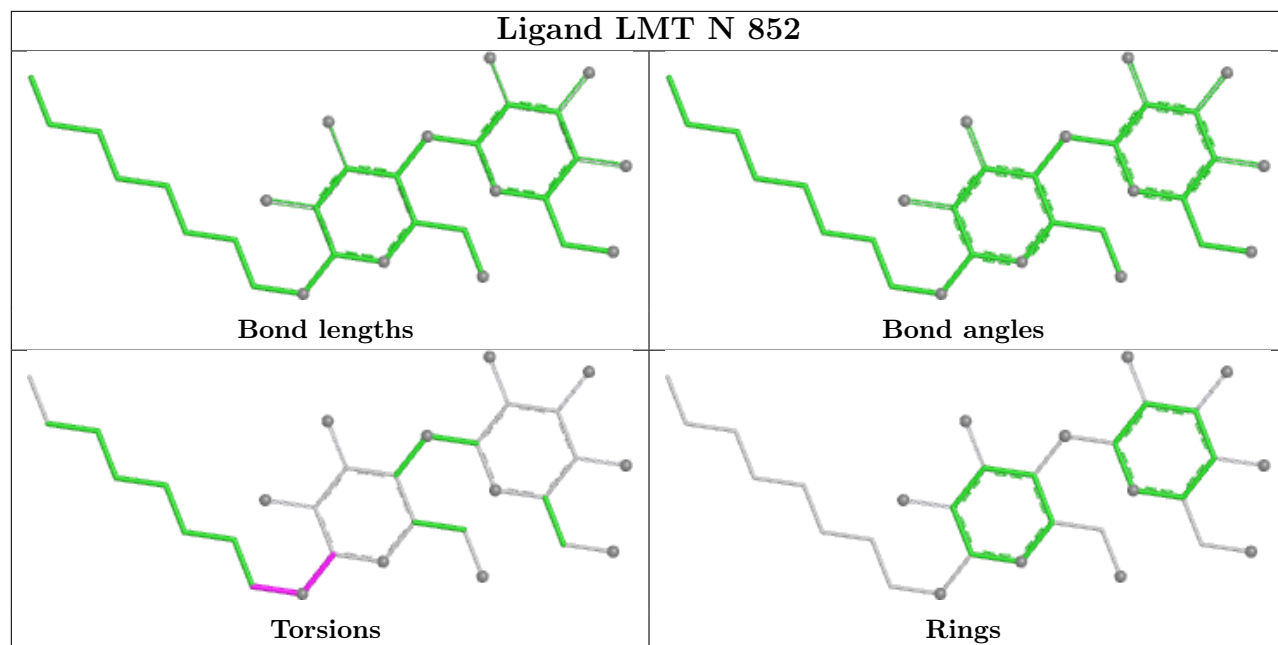
Ligand BCR N 850



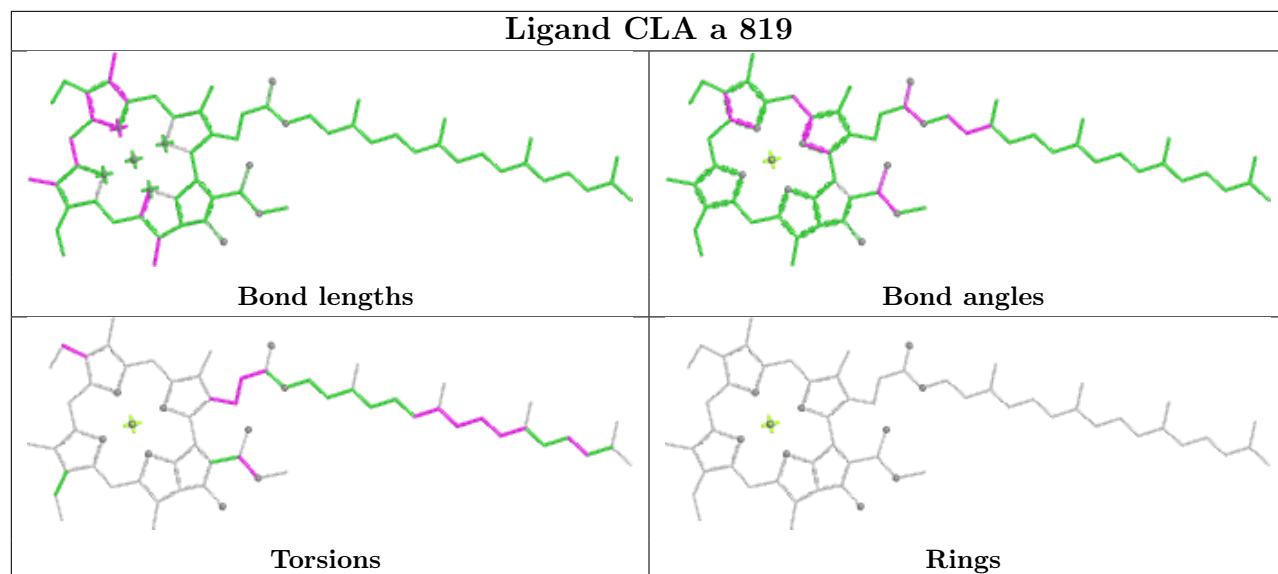




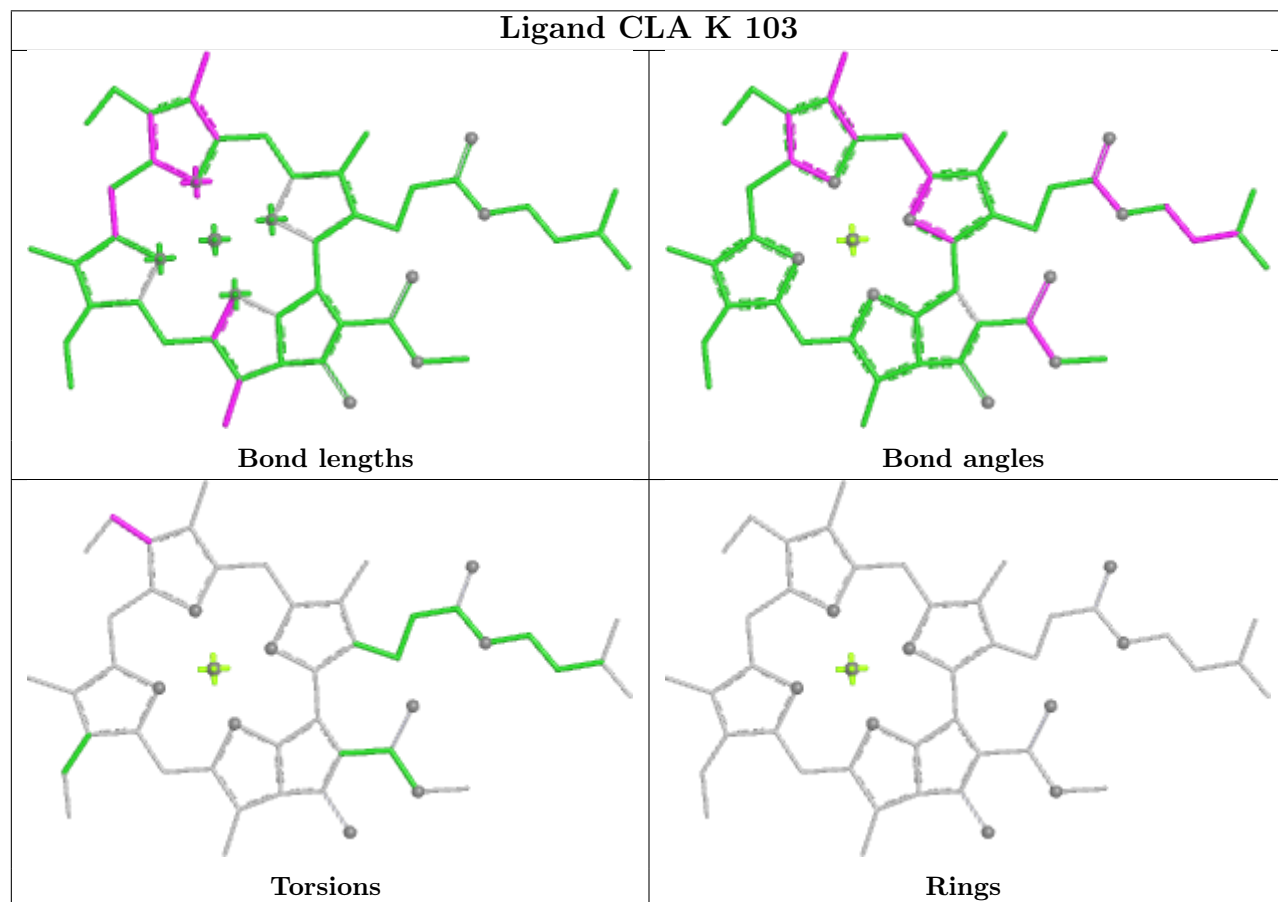


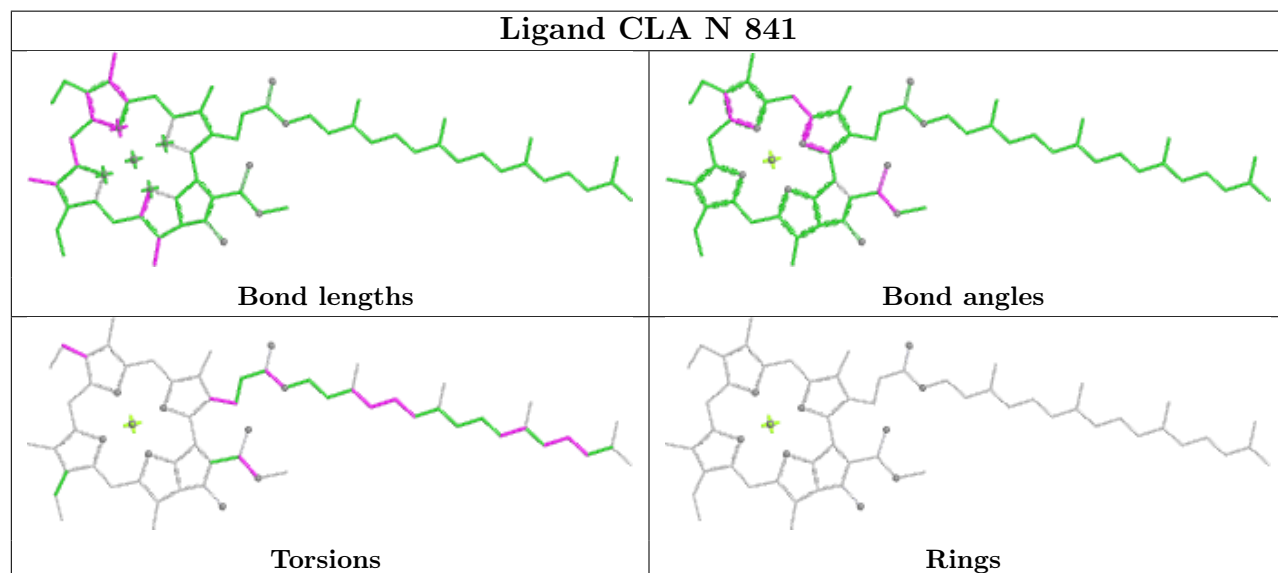
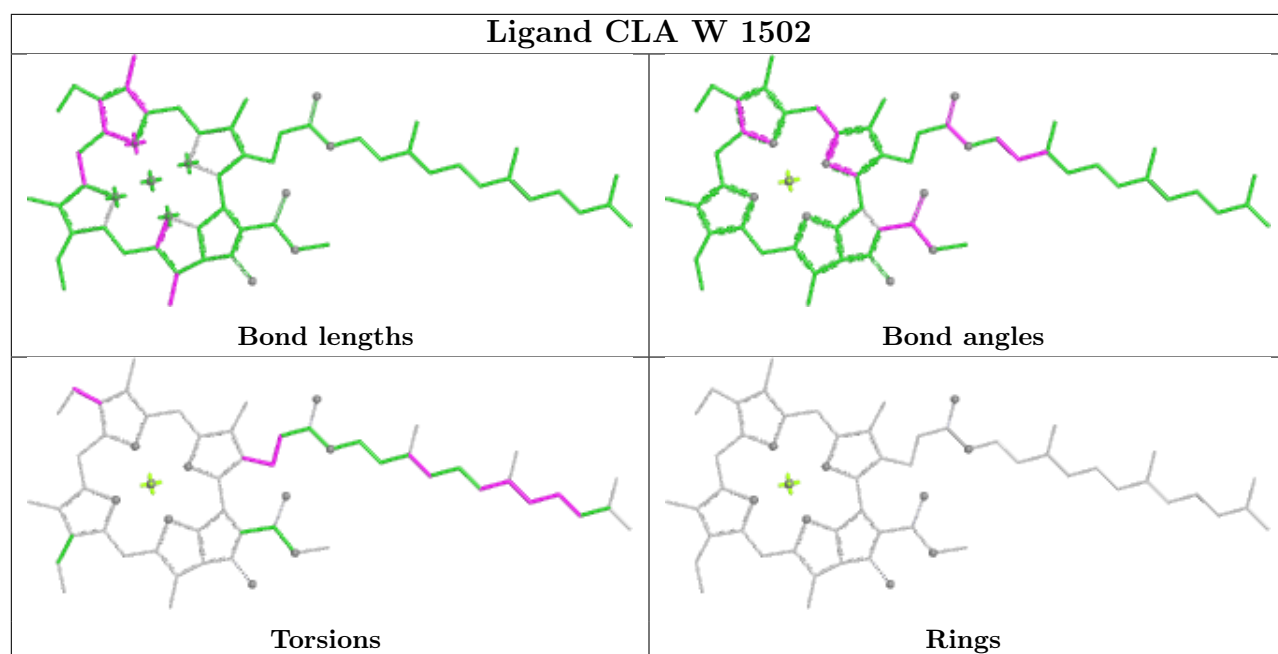


Ligand CLA a 819

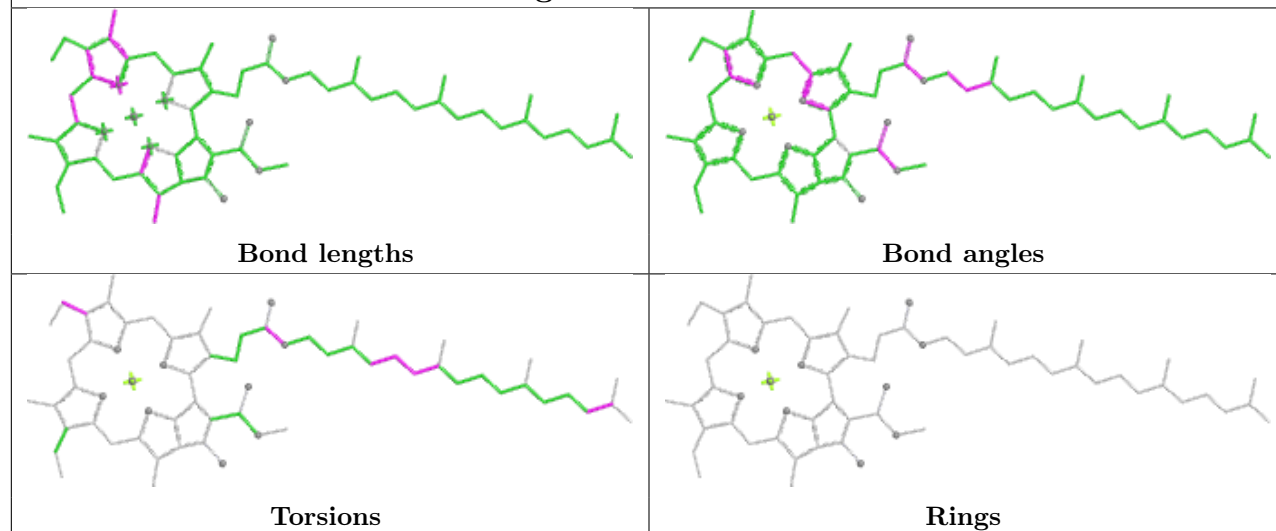


Ligand CLA K 103

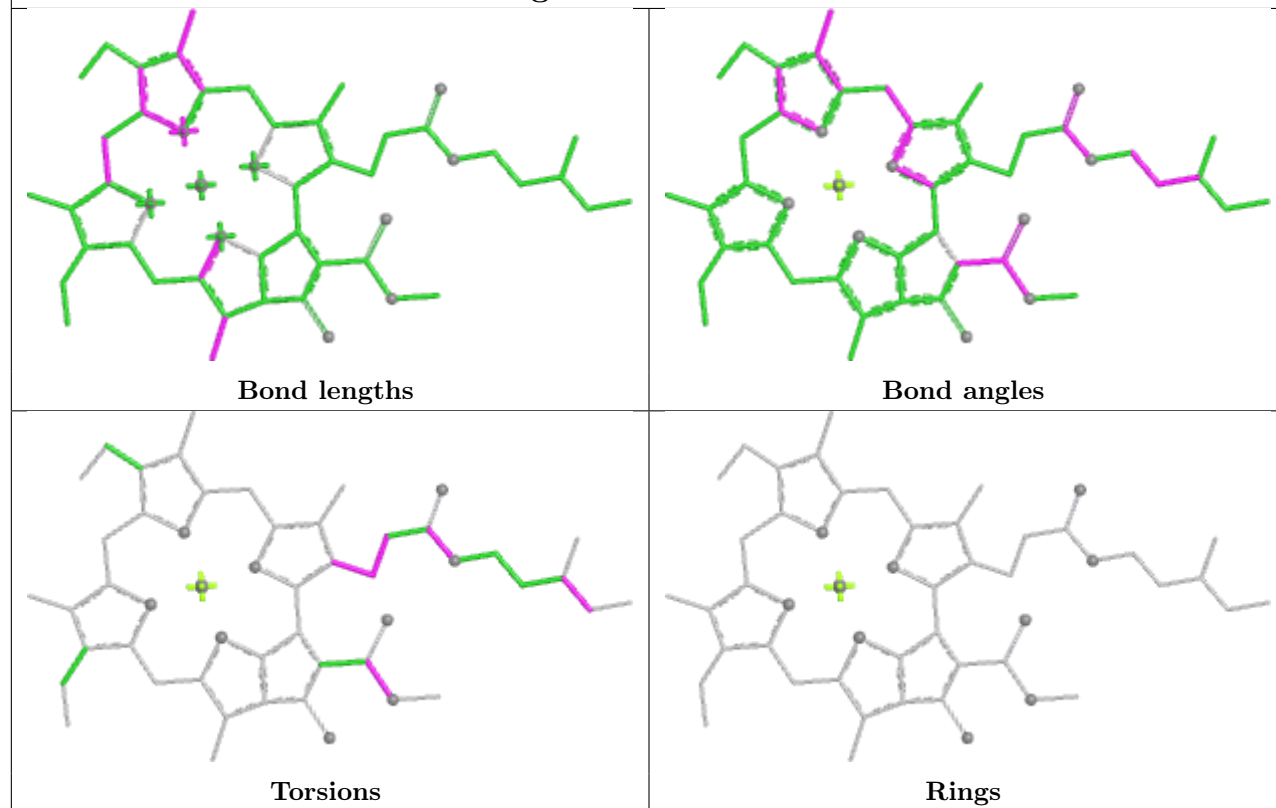


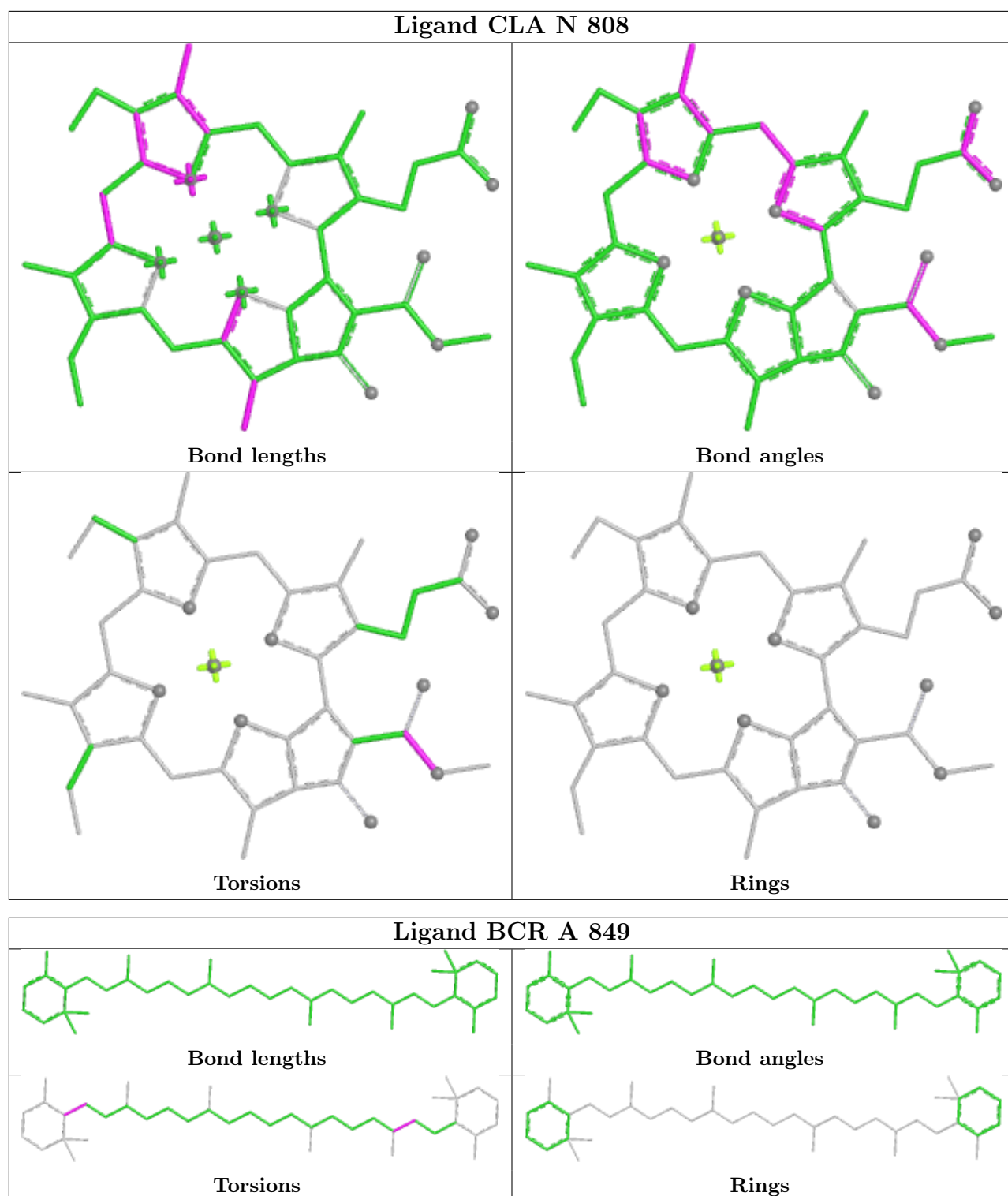


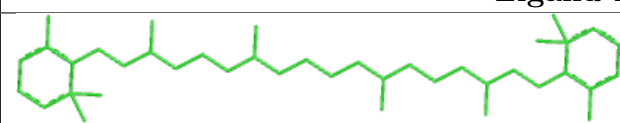
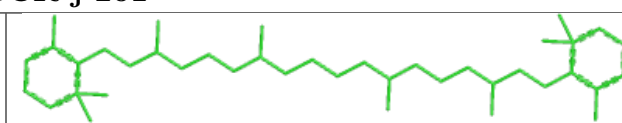
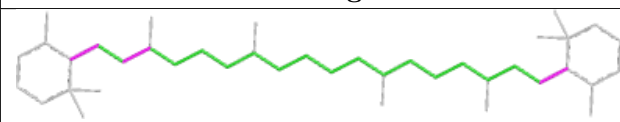
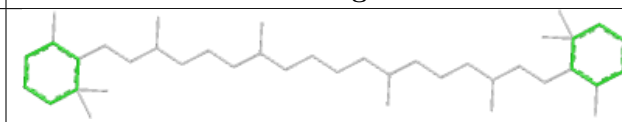
Ligand CLA S 201

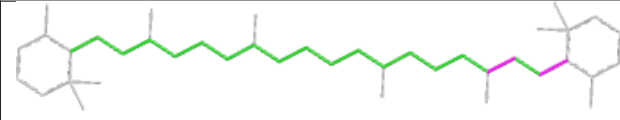
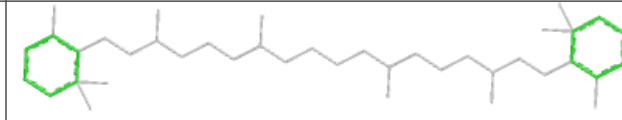


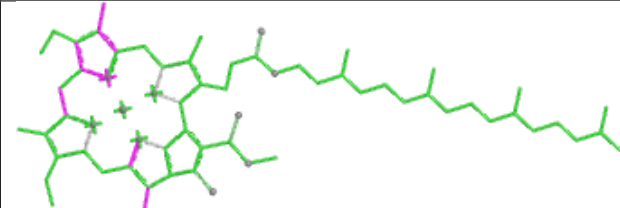
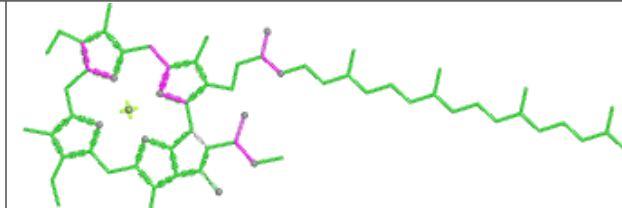
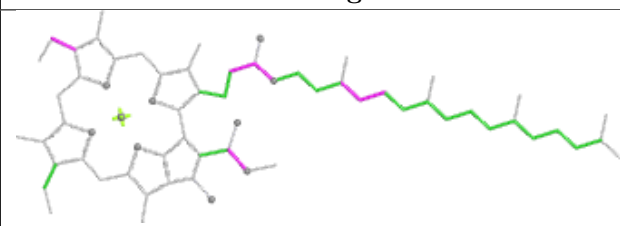
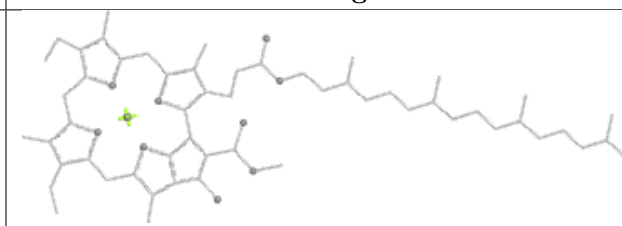
Ligand CLA N 837

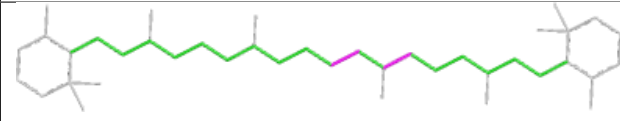
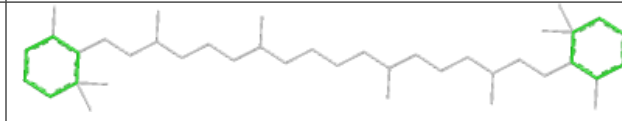


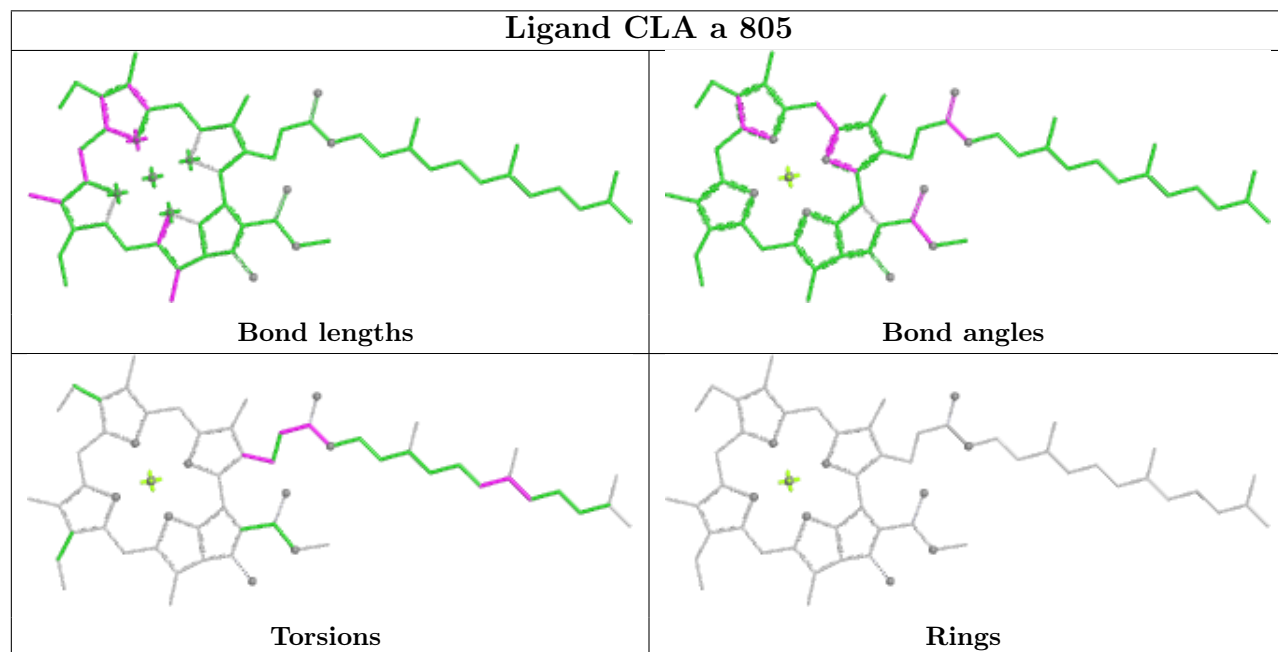
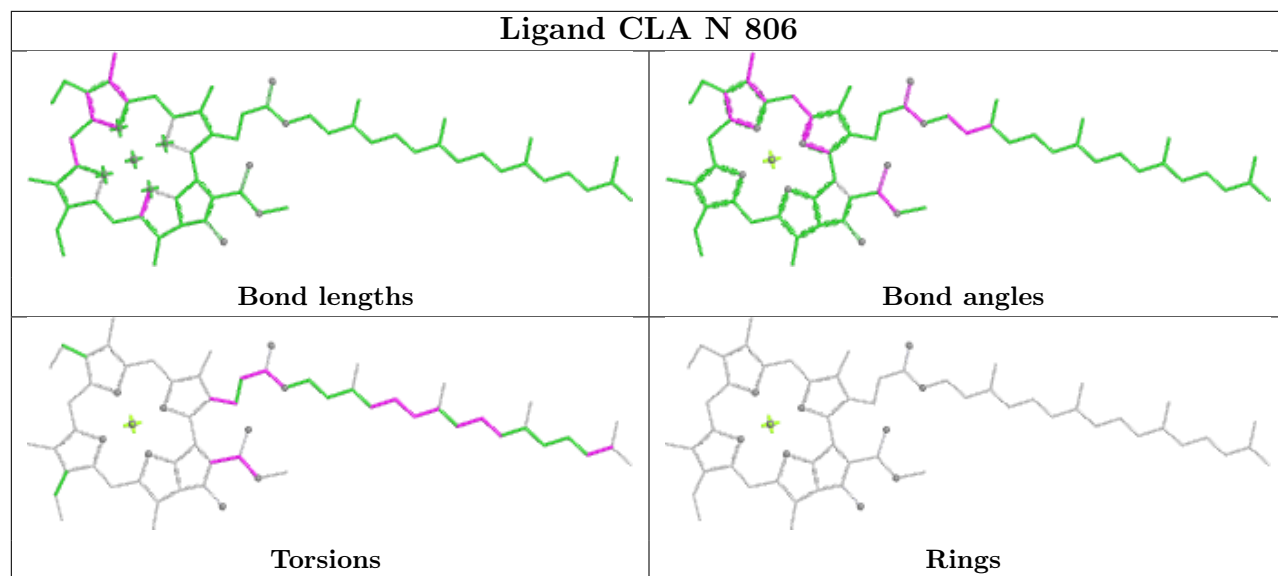


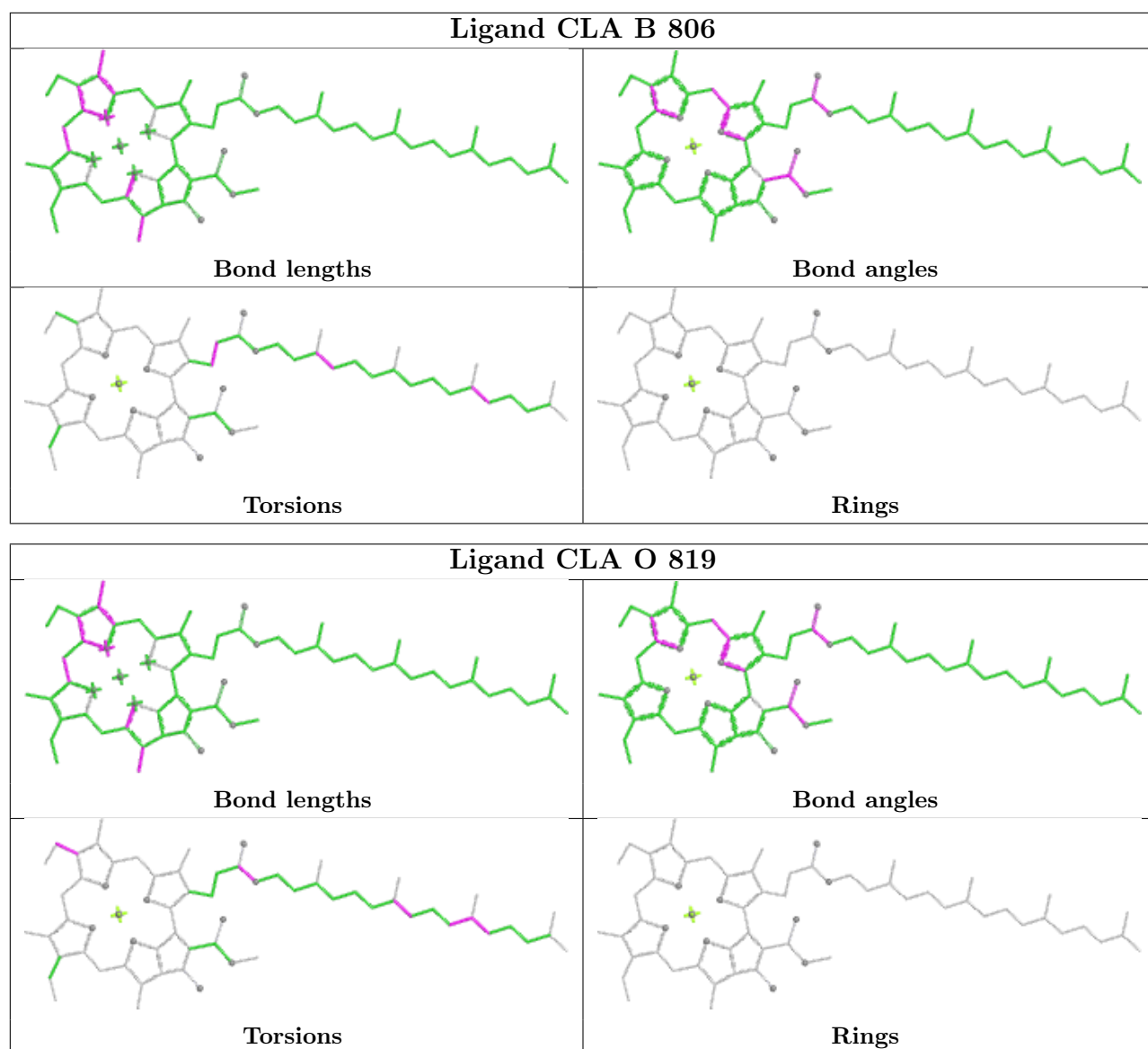
Ligand BCR j 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

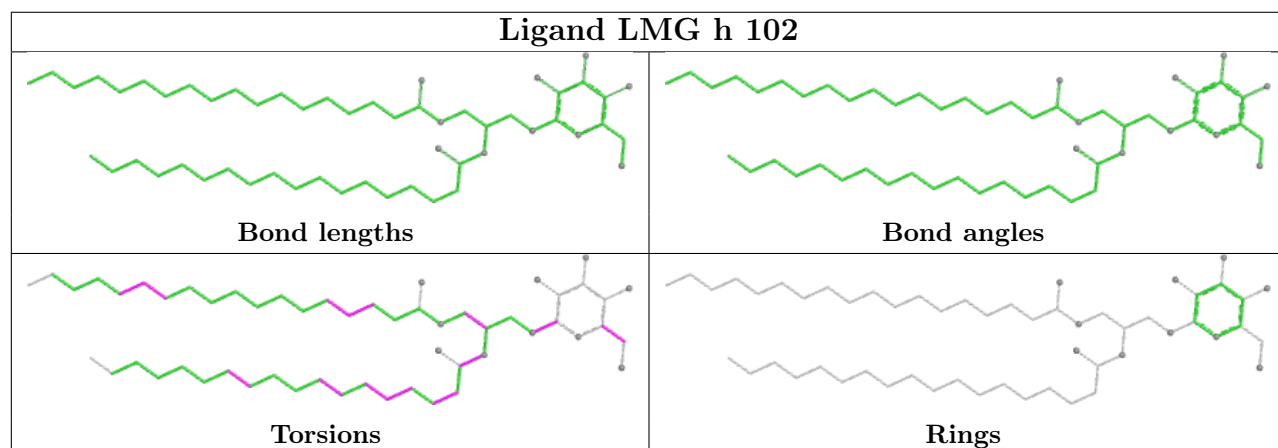
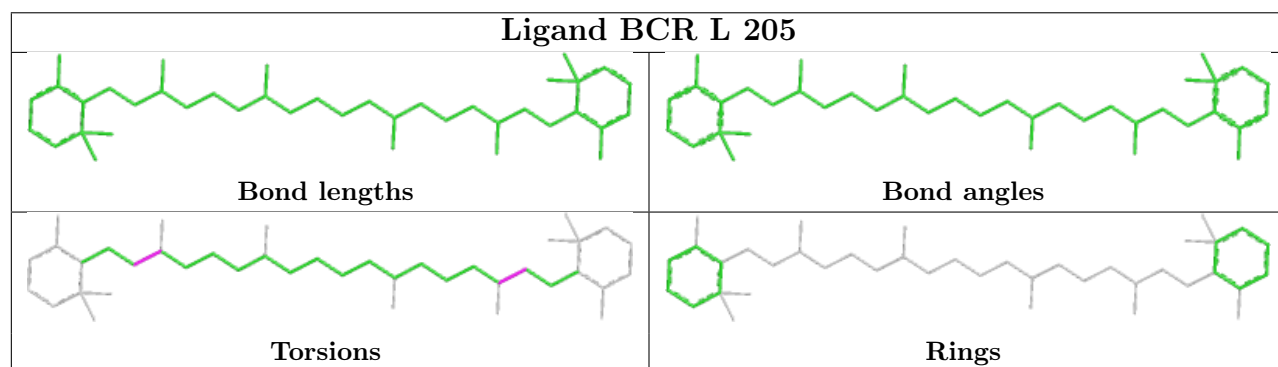
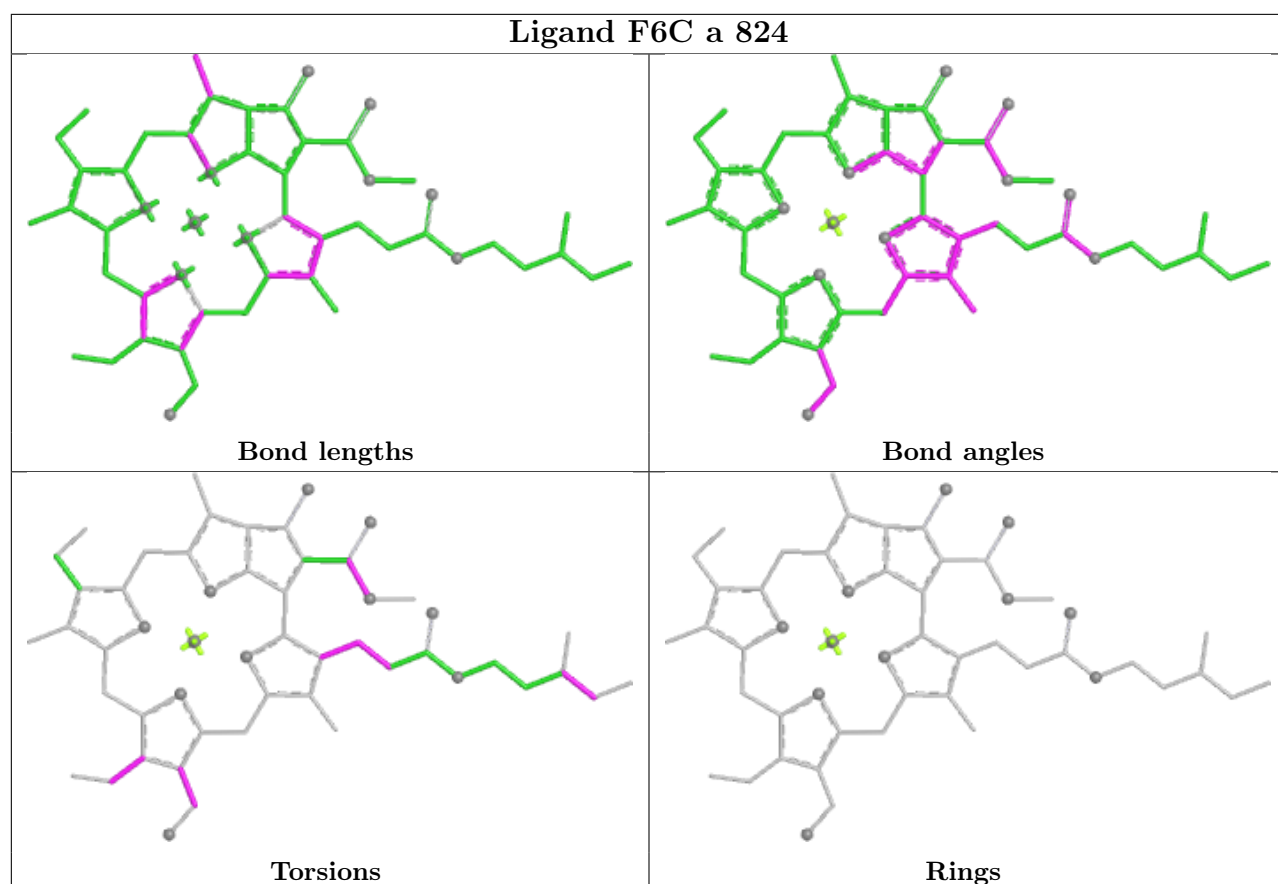
Ligand BCR O 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

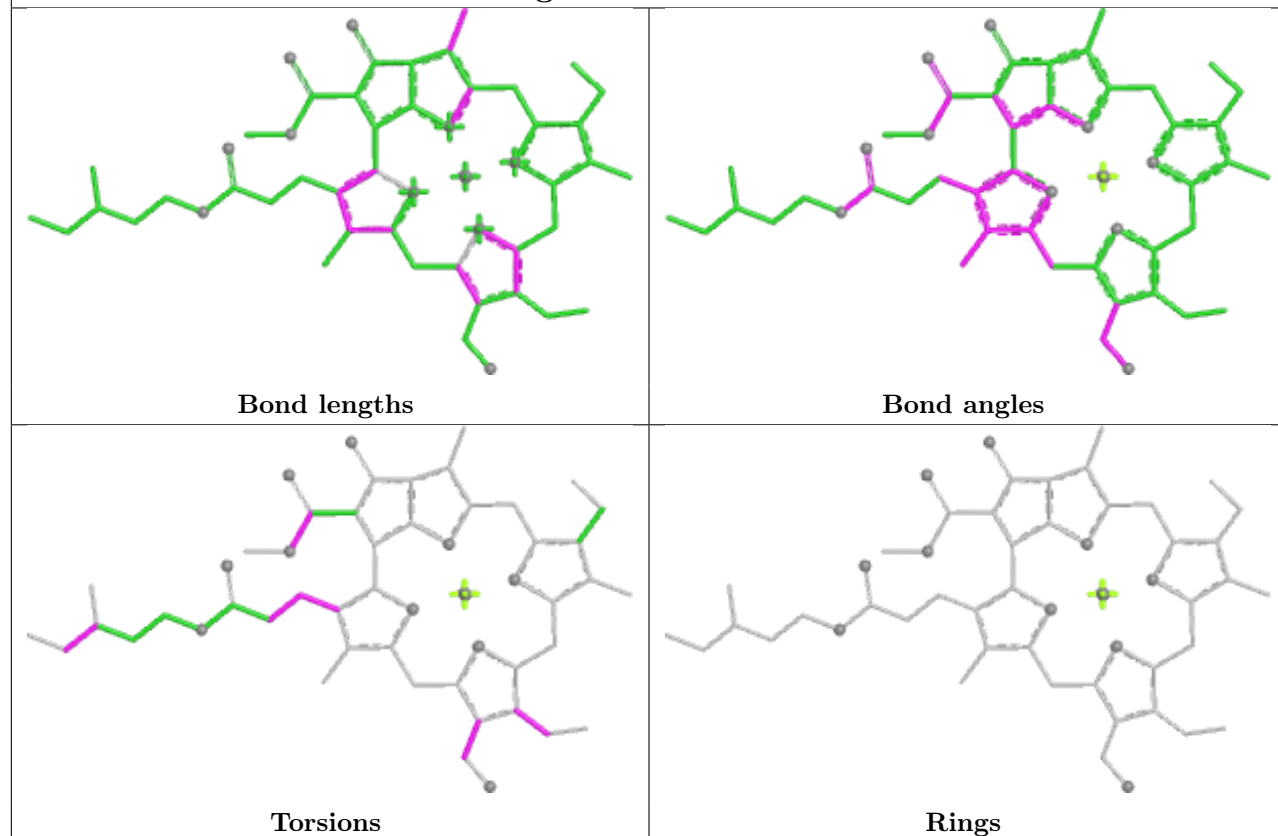
Ligand BCR A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings



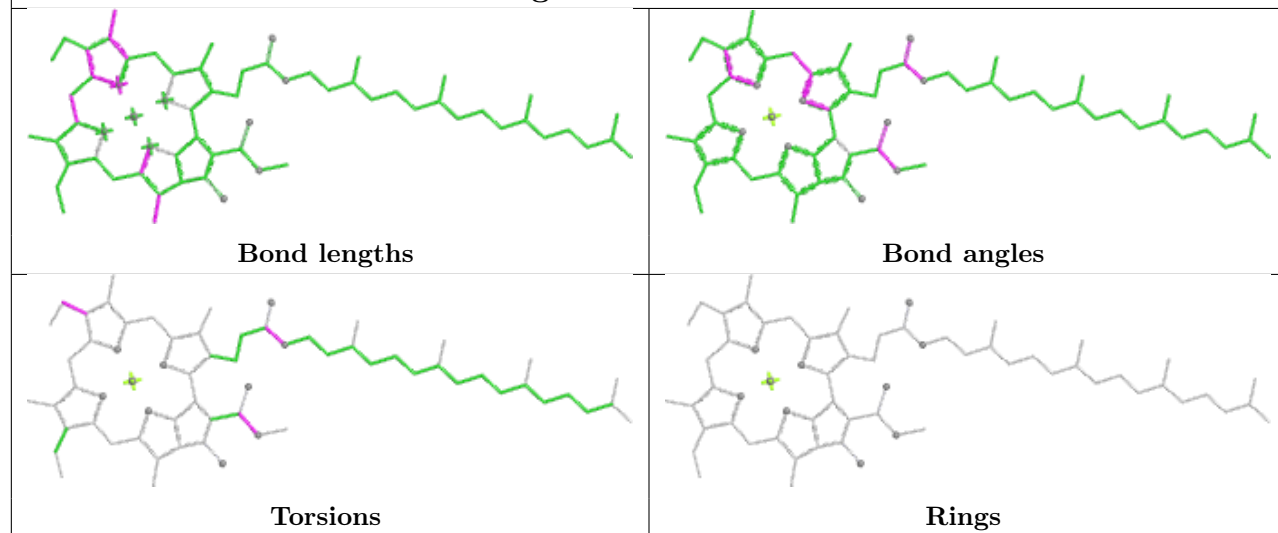


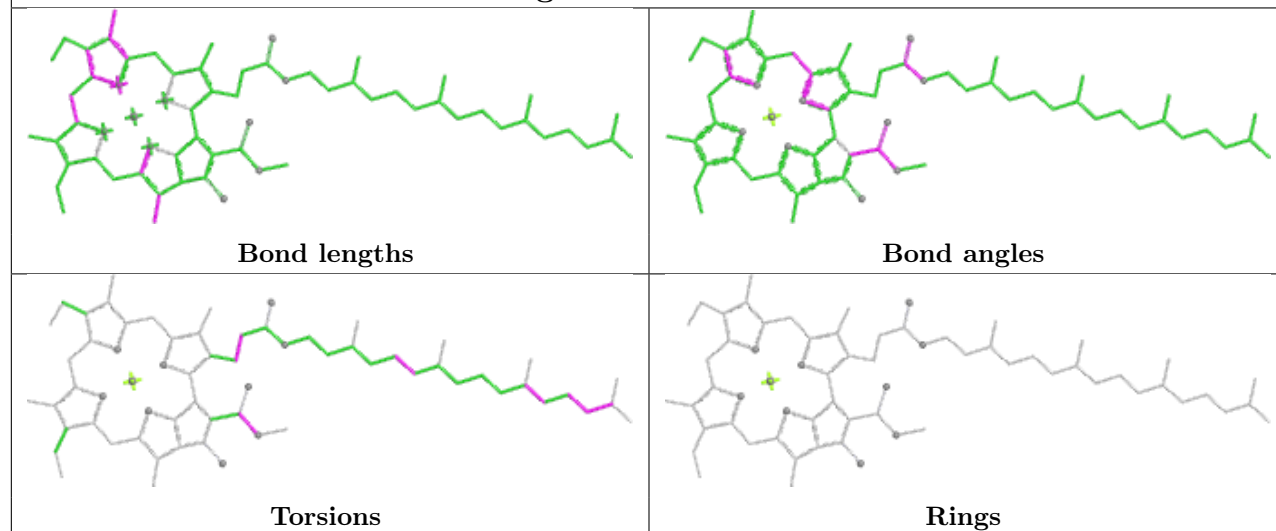
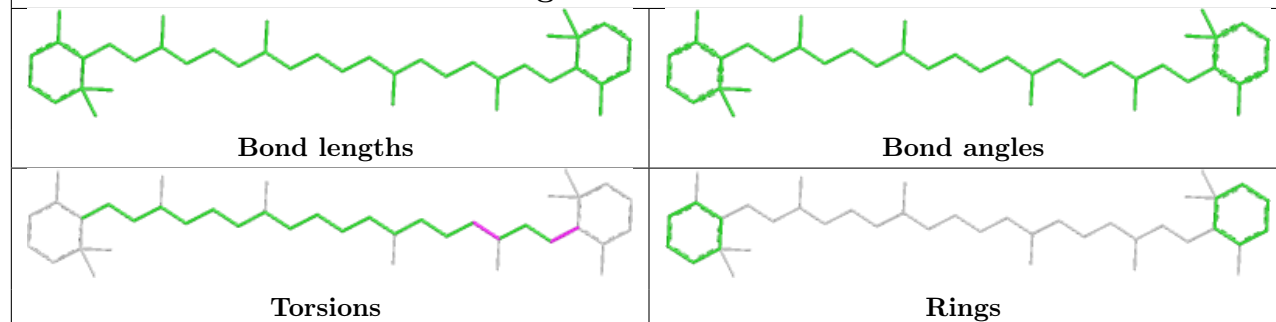
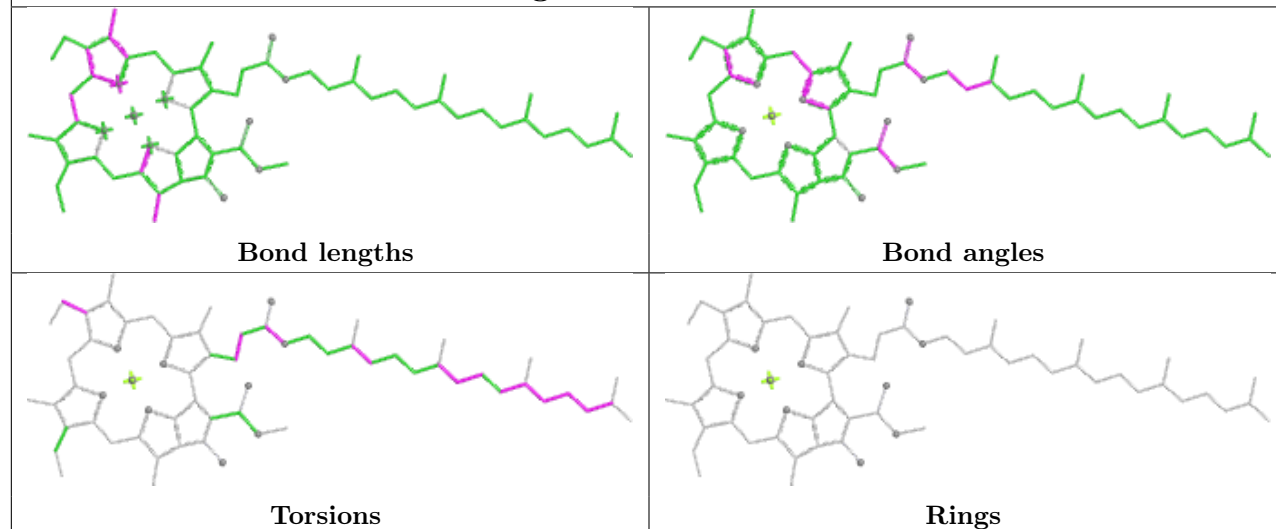


Ligand F6C A 824

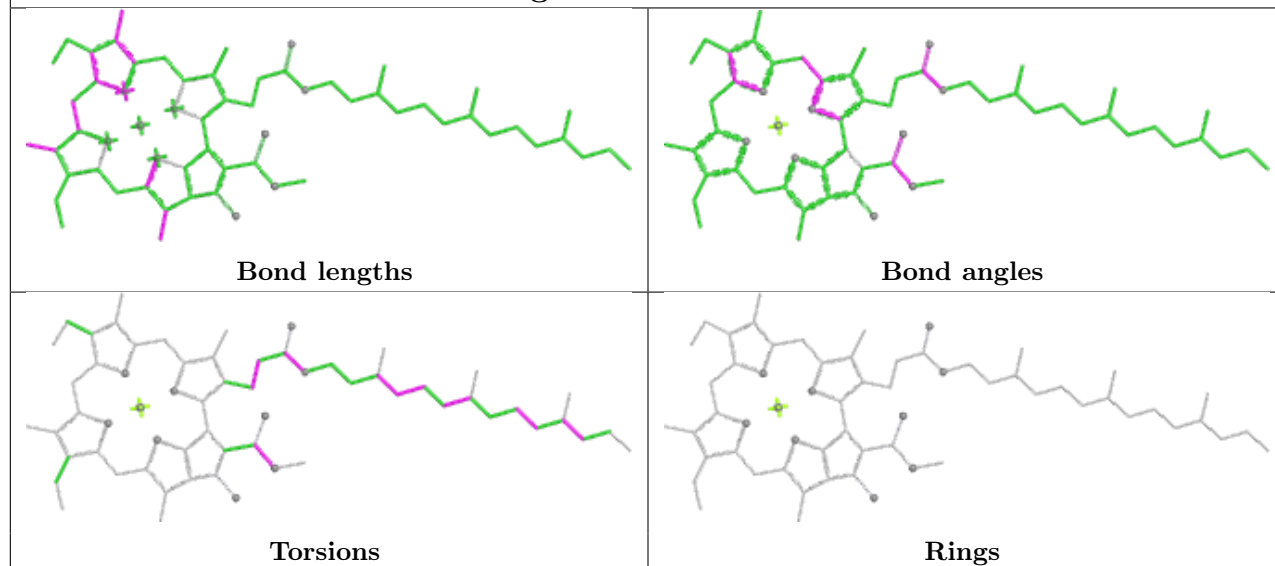


Ligand CLA A 825

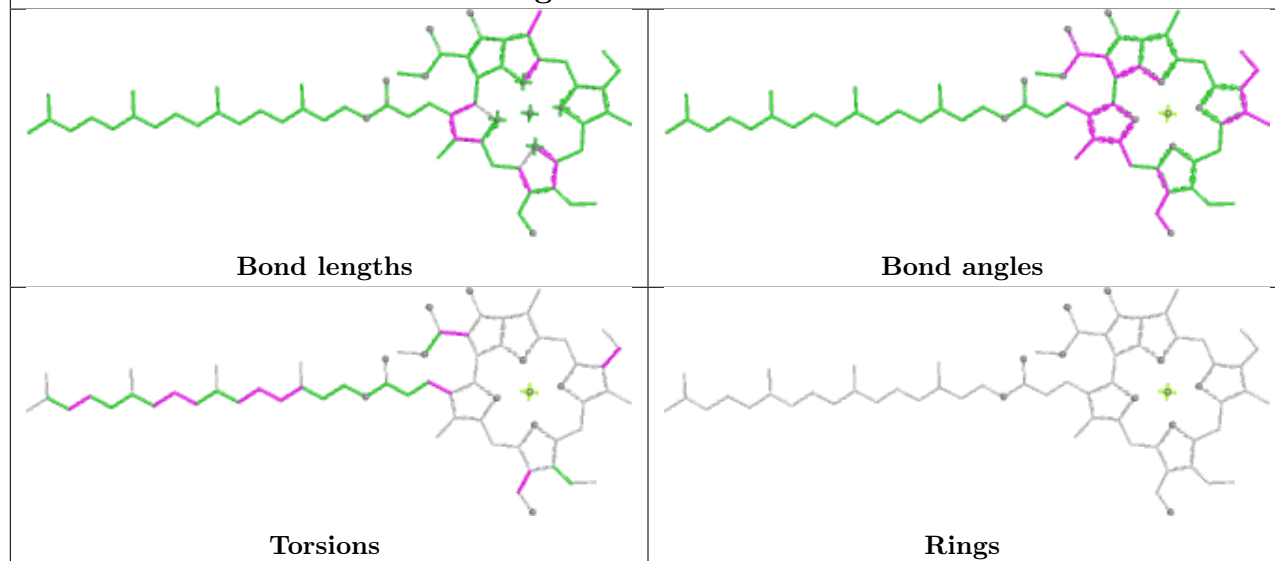


Ligand CLA a 835**Ligand BCR I 102****Ligand CLA A 839**

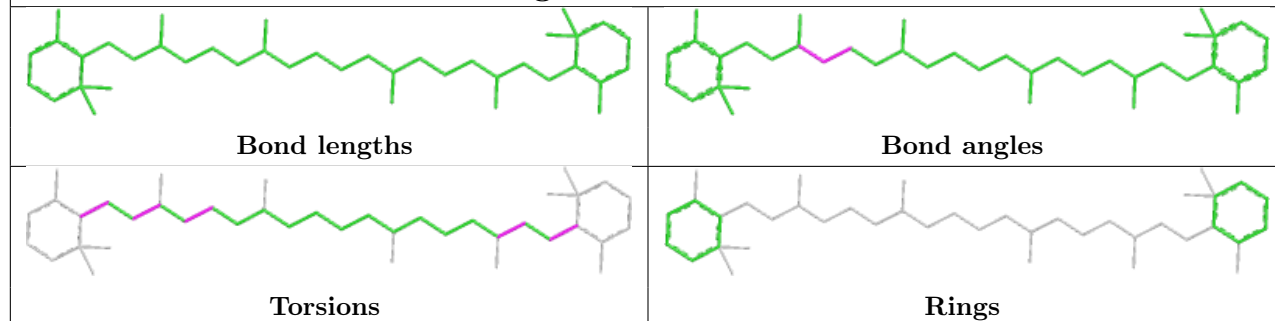
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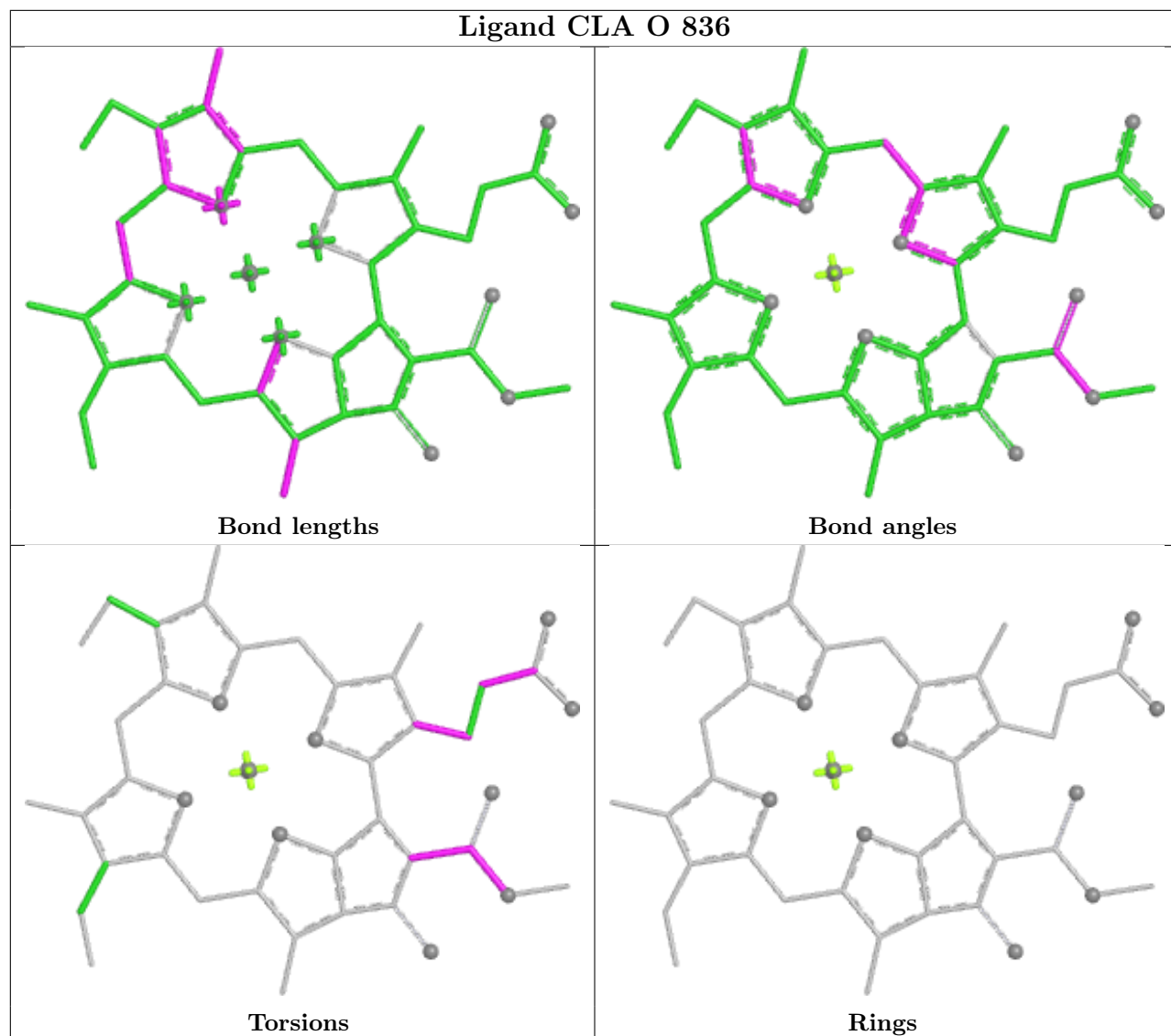


Ligand F6C A 826

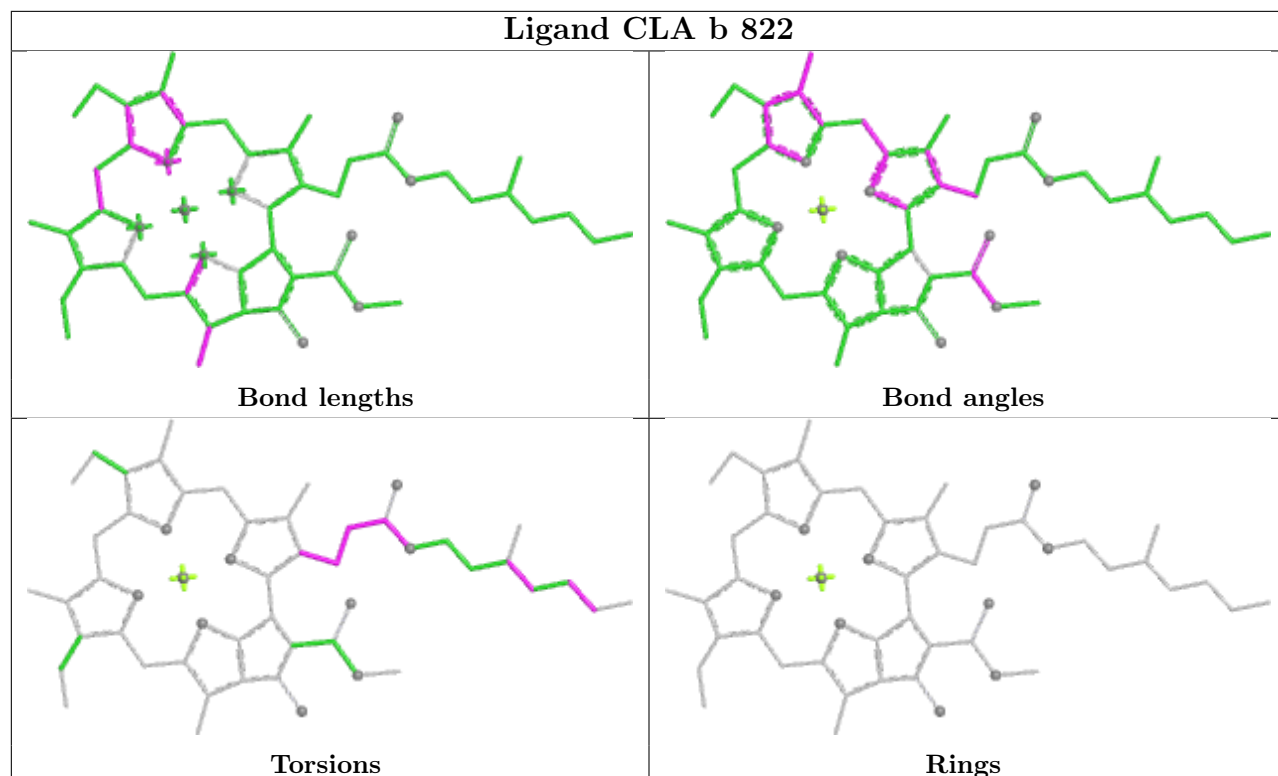


Ligand BCR a 846

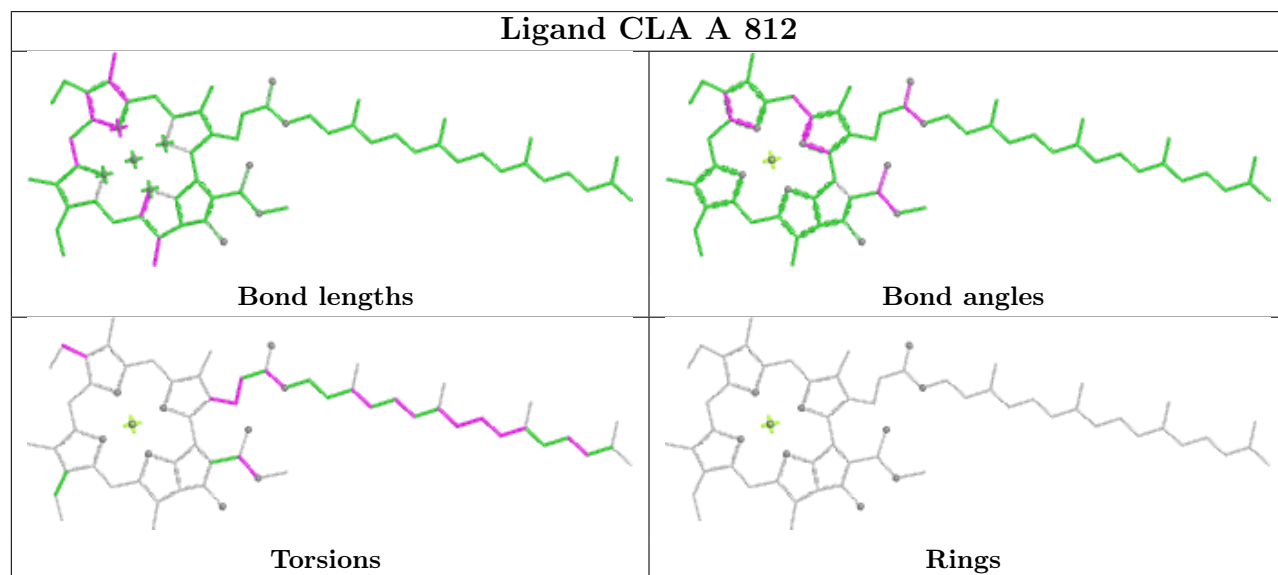




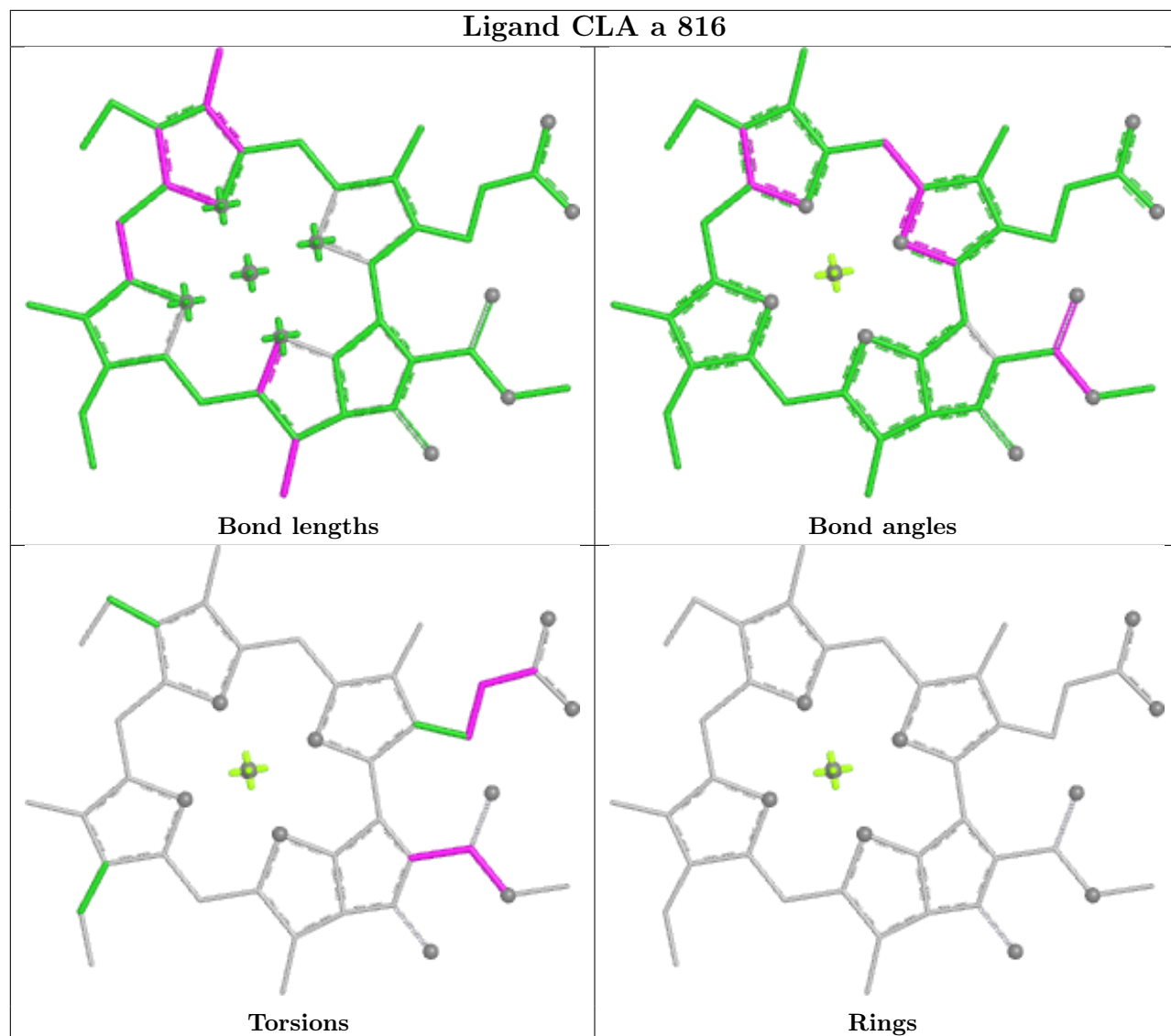
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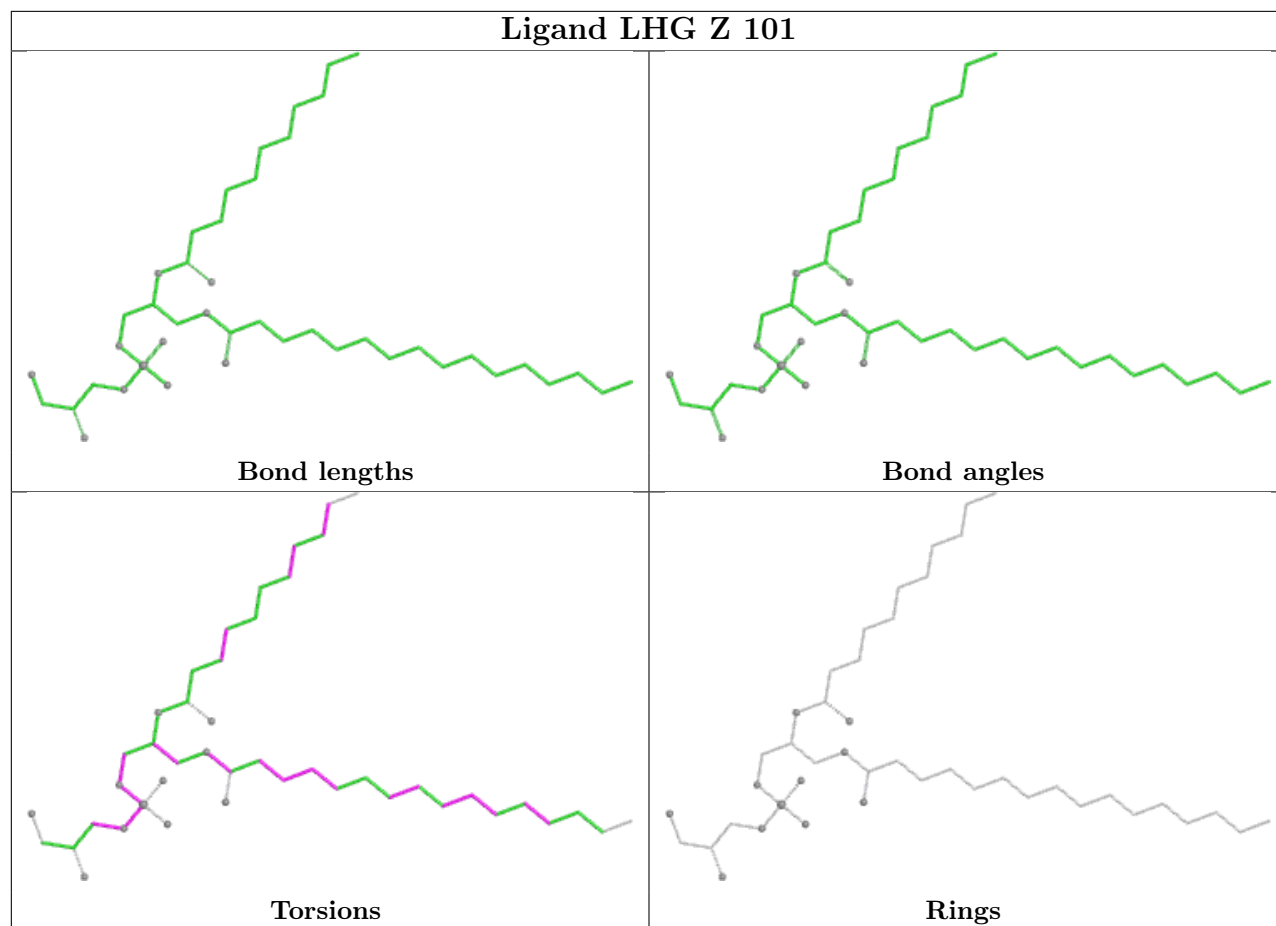
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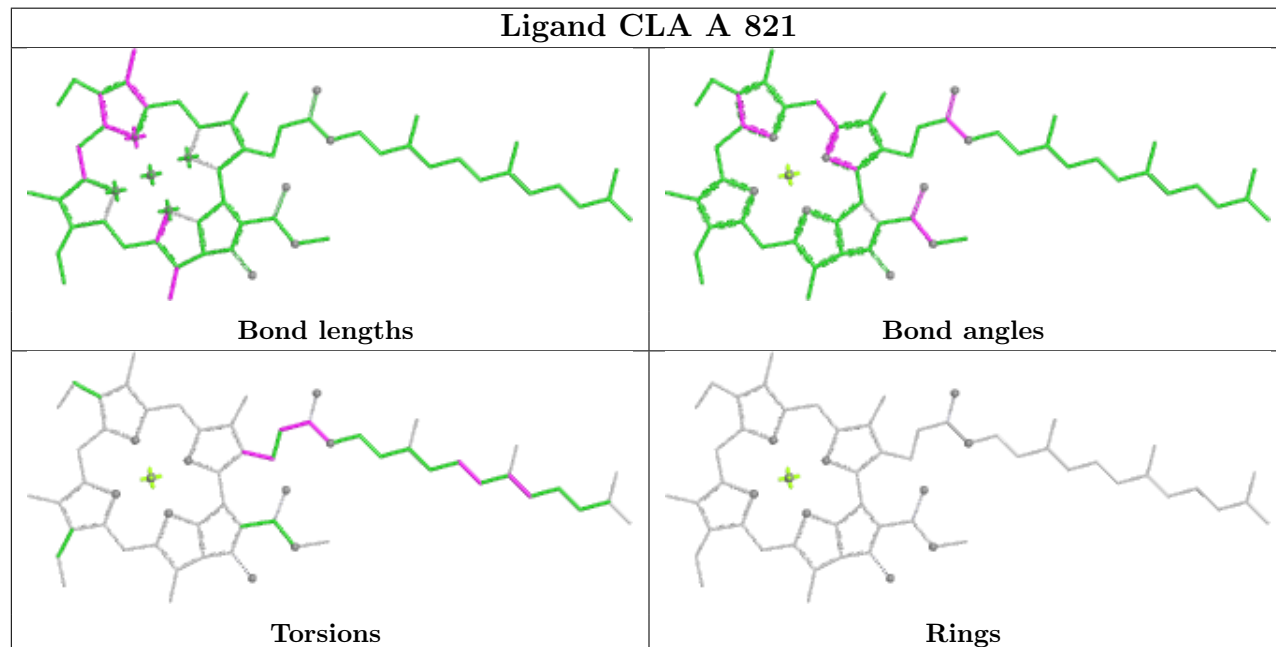
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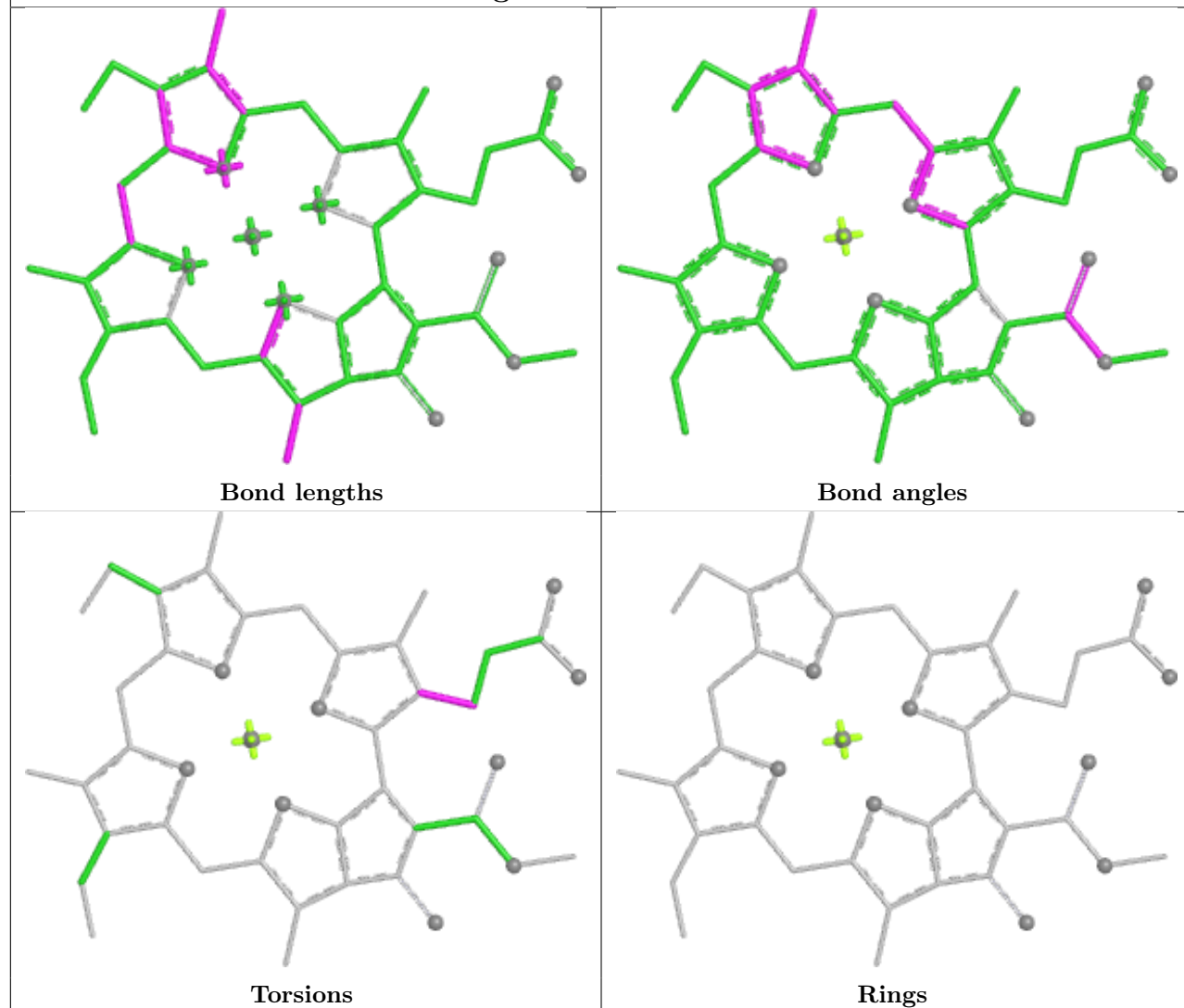
Ligand LHG Z 101



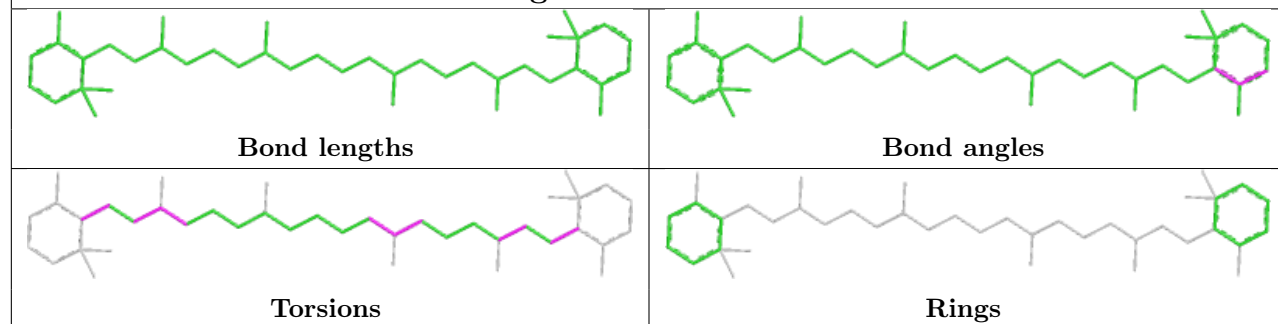
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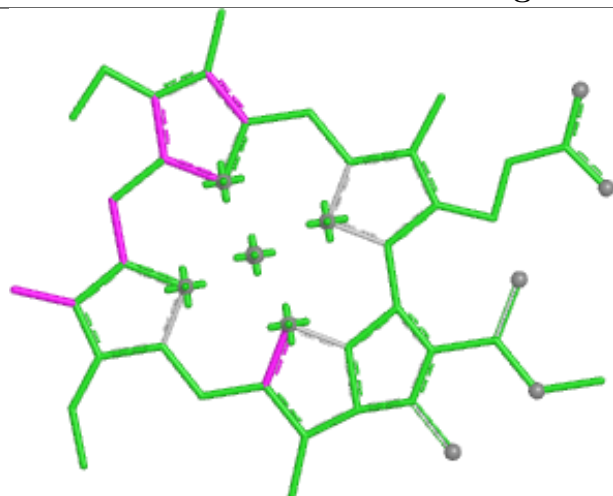
Ligand CLA B 833



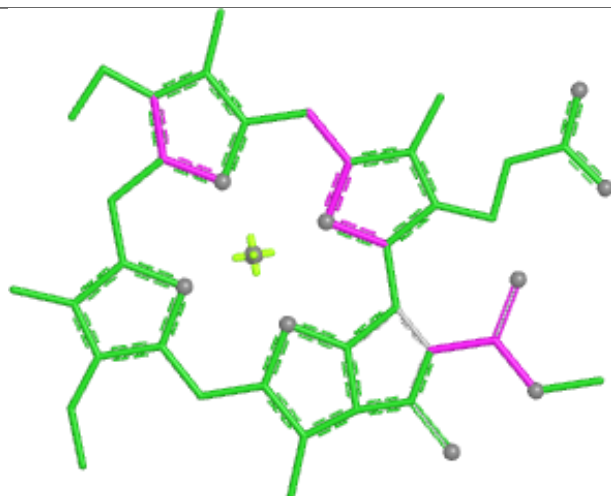
Ligand BCR A 850



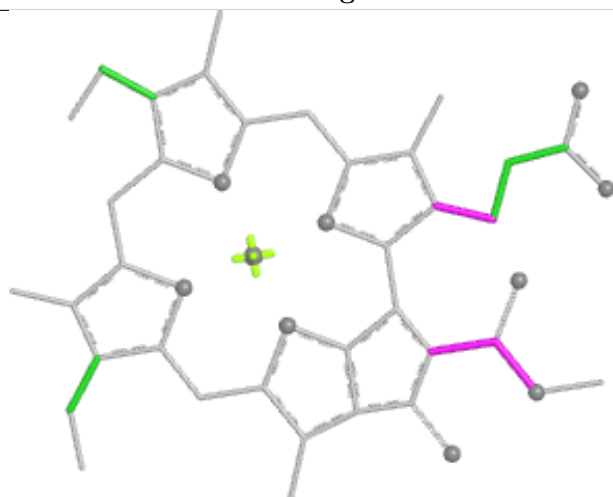
Ligand CLA O 815



Bond lengths



Bond angles

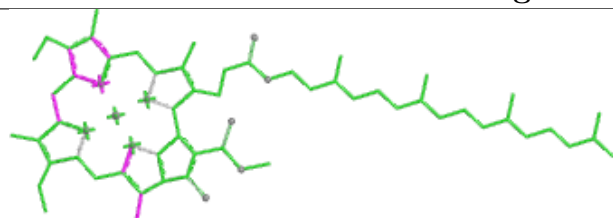


Torsions

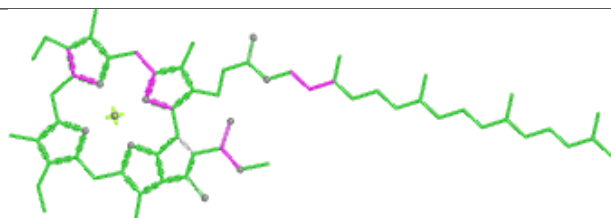


Rings

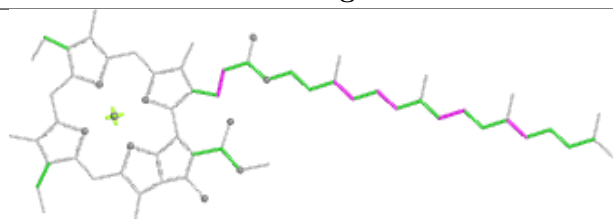
Ligand CLA N 830



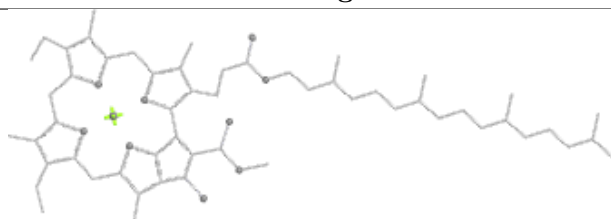
Bond lengths



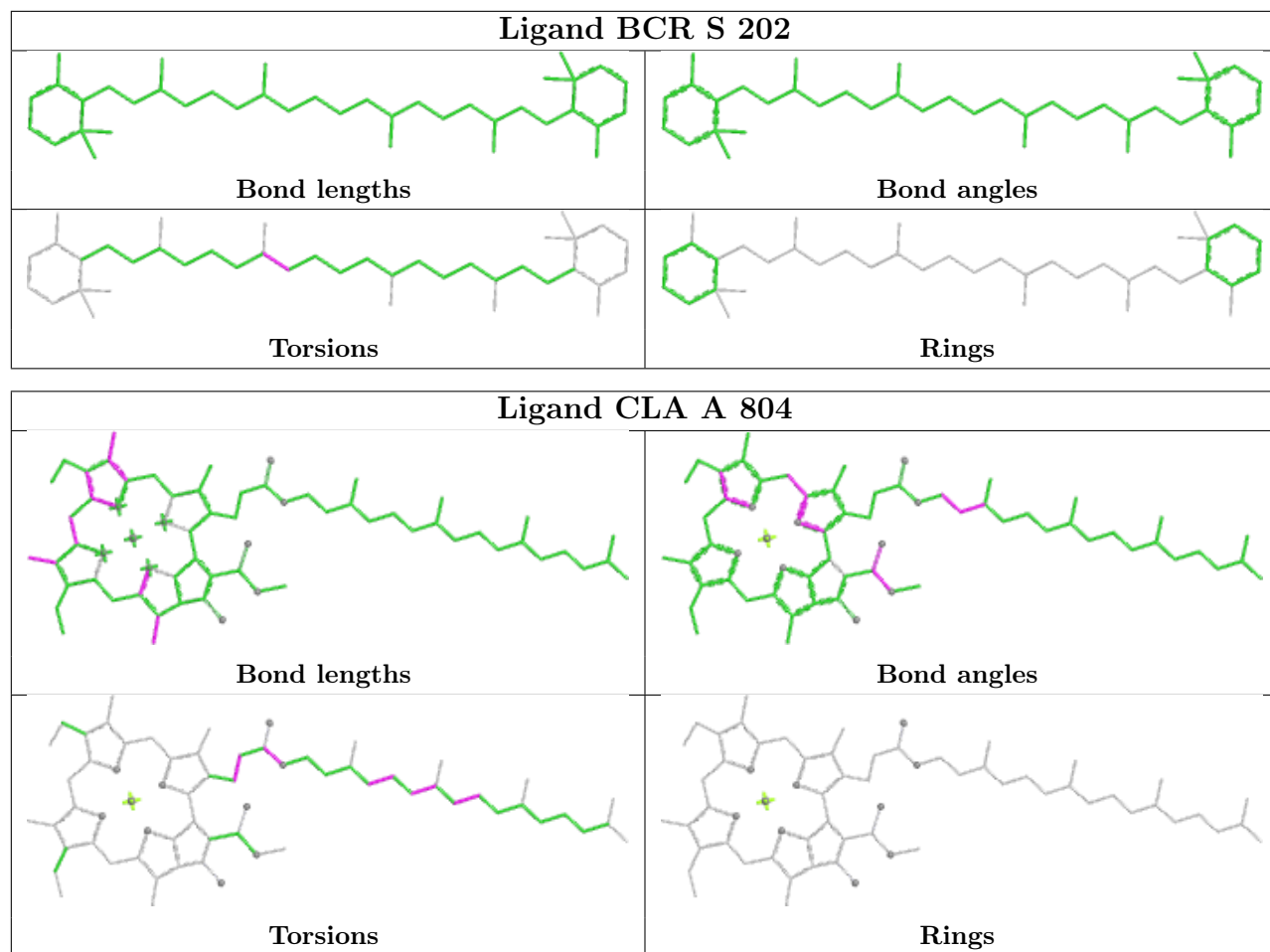
Bond angles



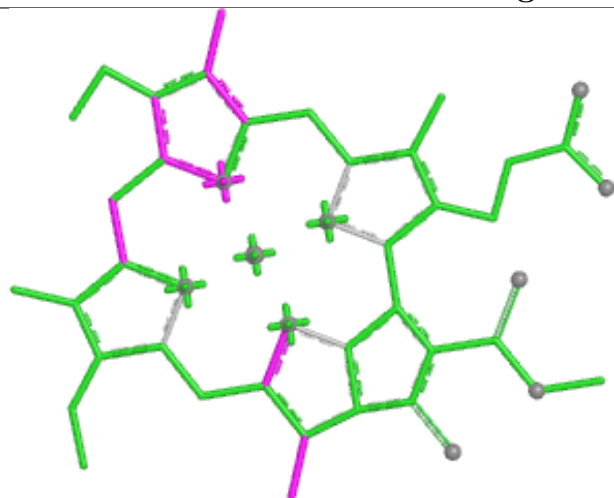
Torsions



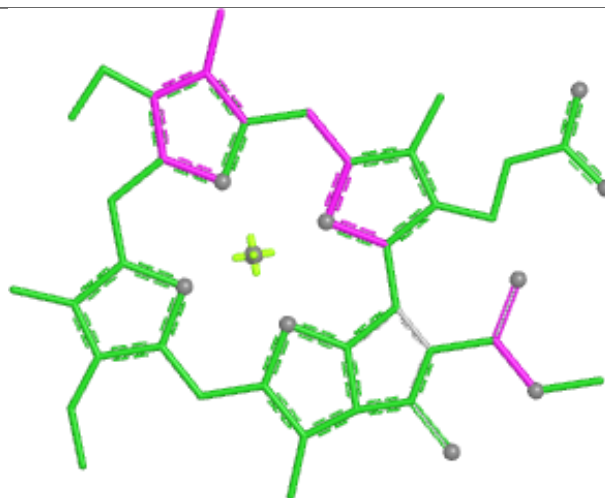
Rings



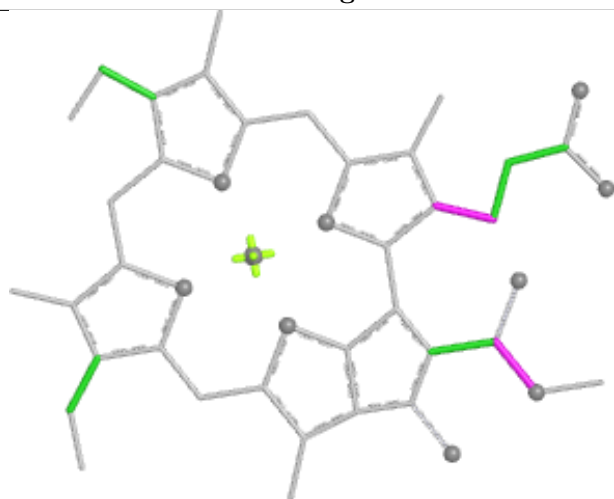
Ligand CLA b 835



Bond lengths



Bond angles

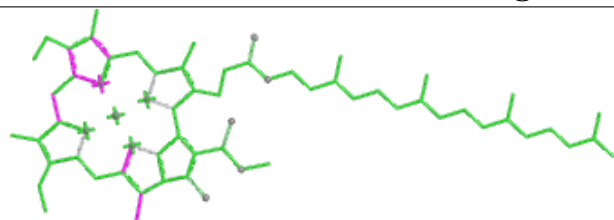


Torsions

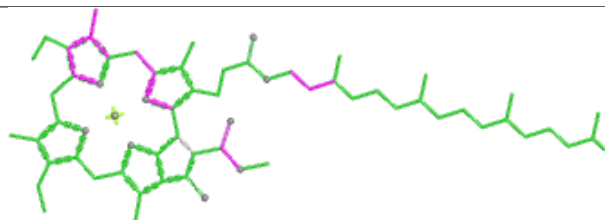


Rings

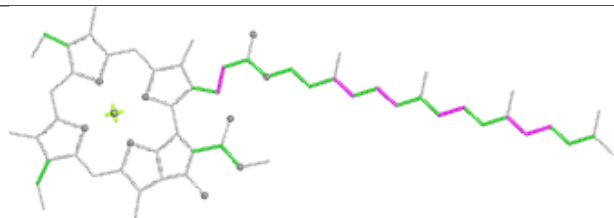
Ligand CLA A 830



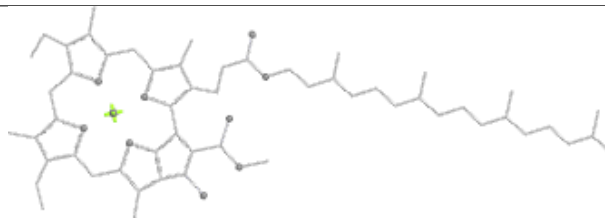
Bond lengths



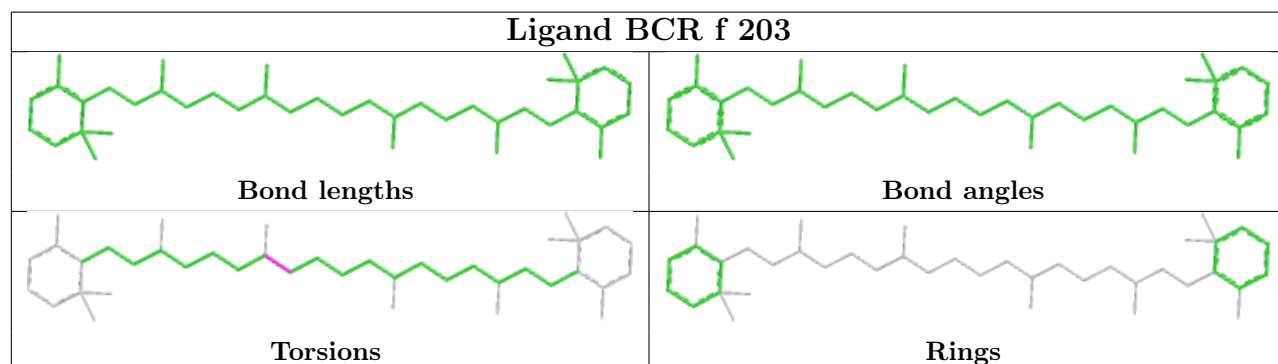
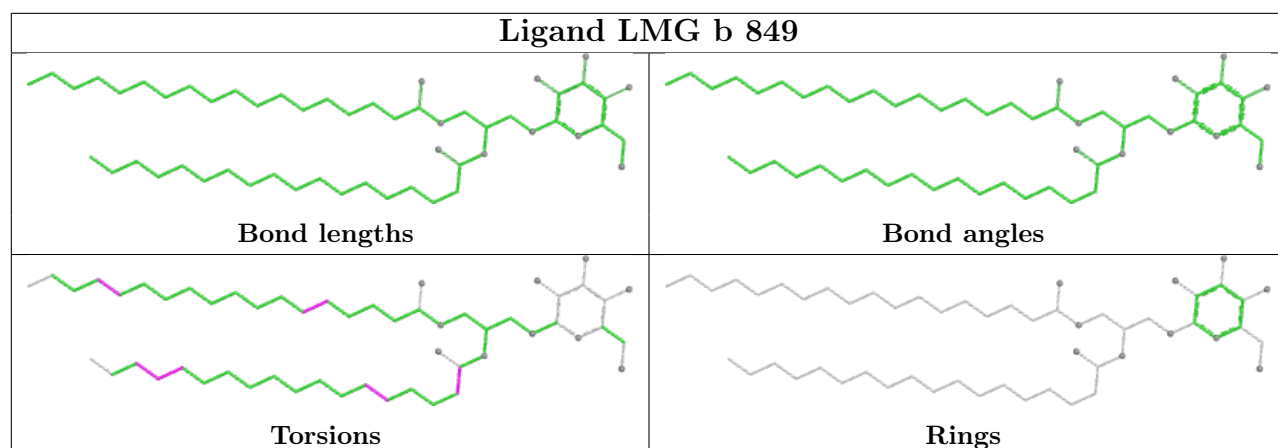
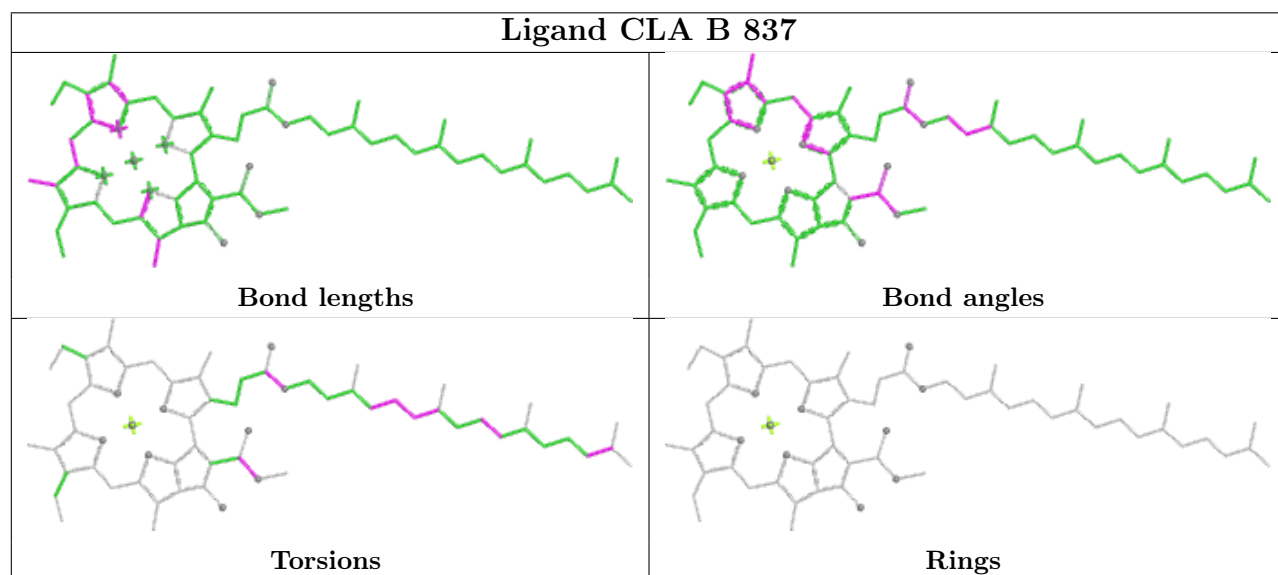
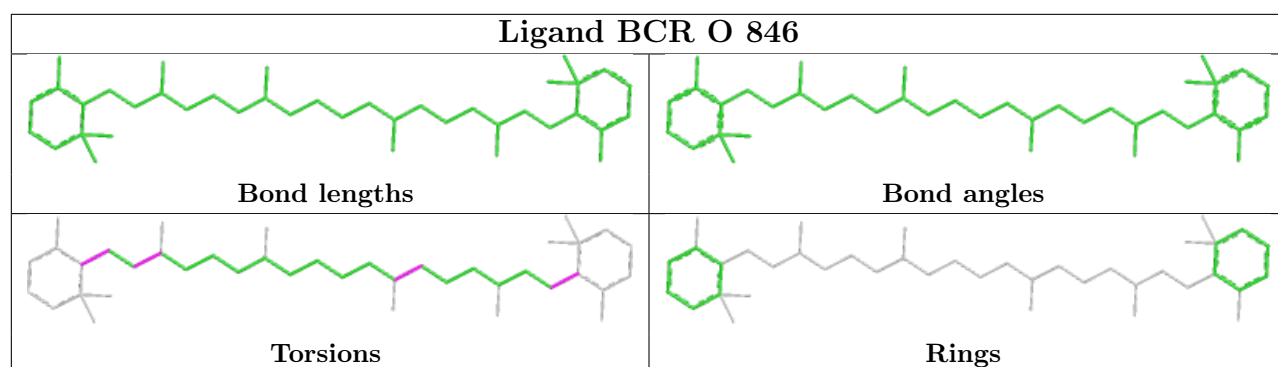
Bond angles

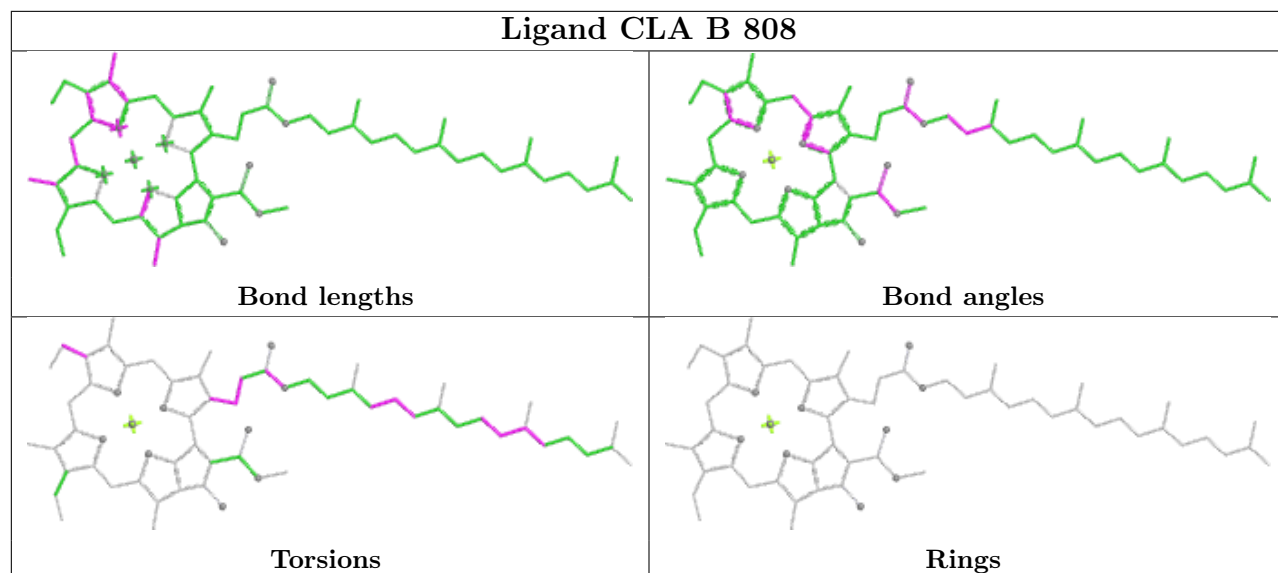
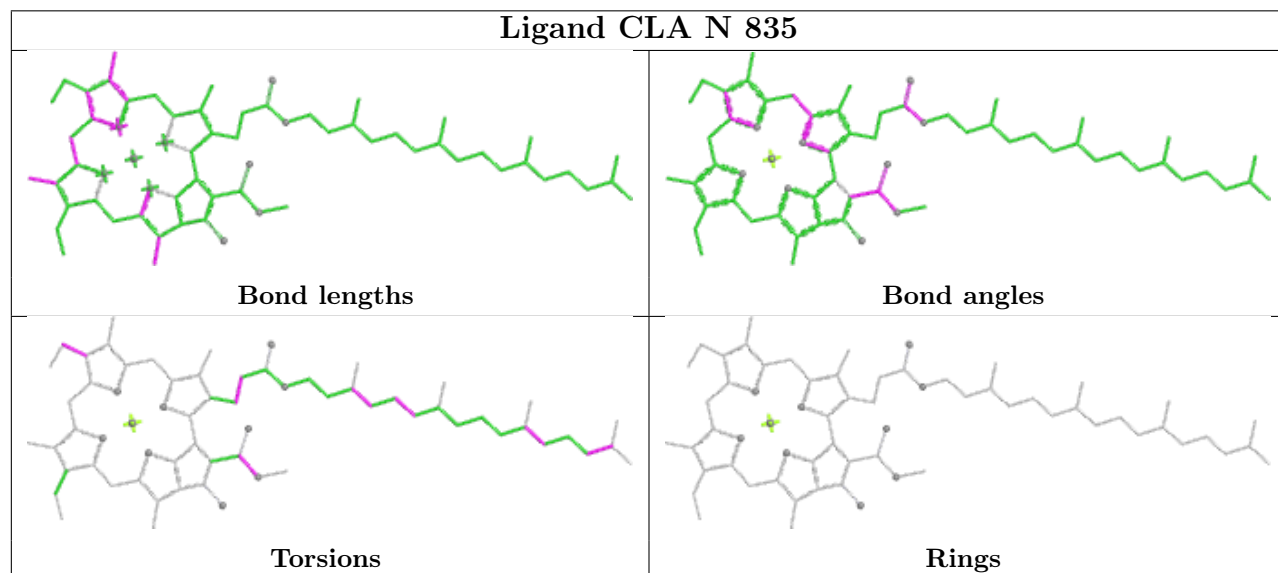
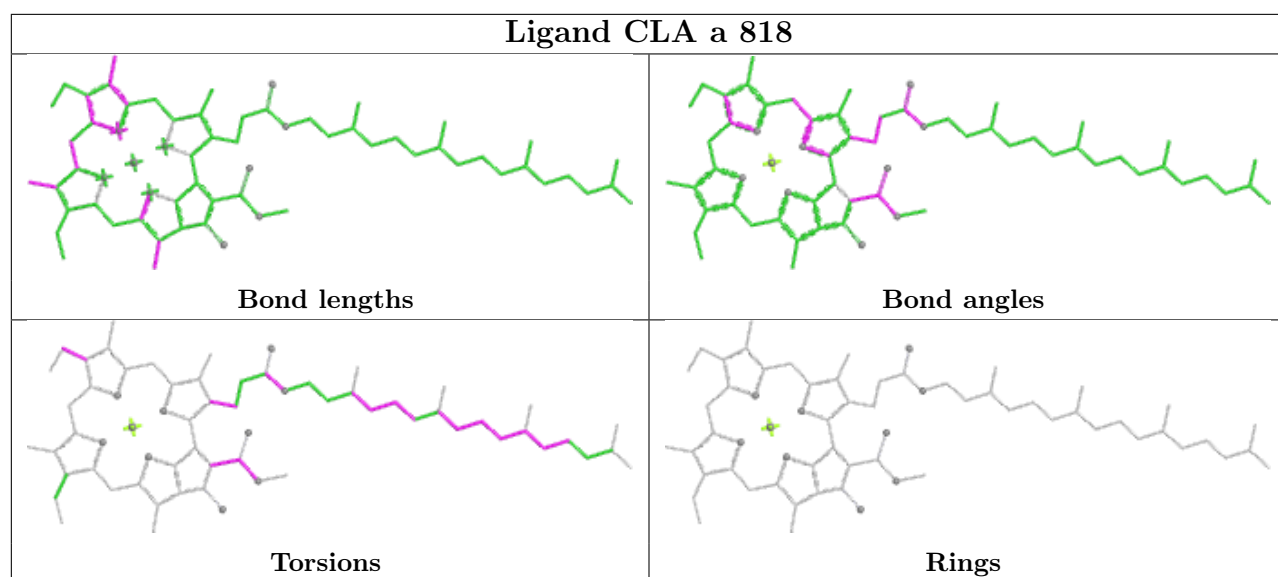


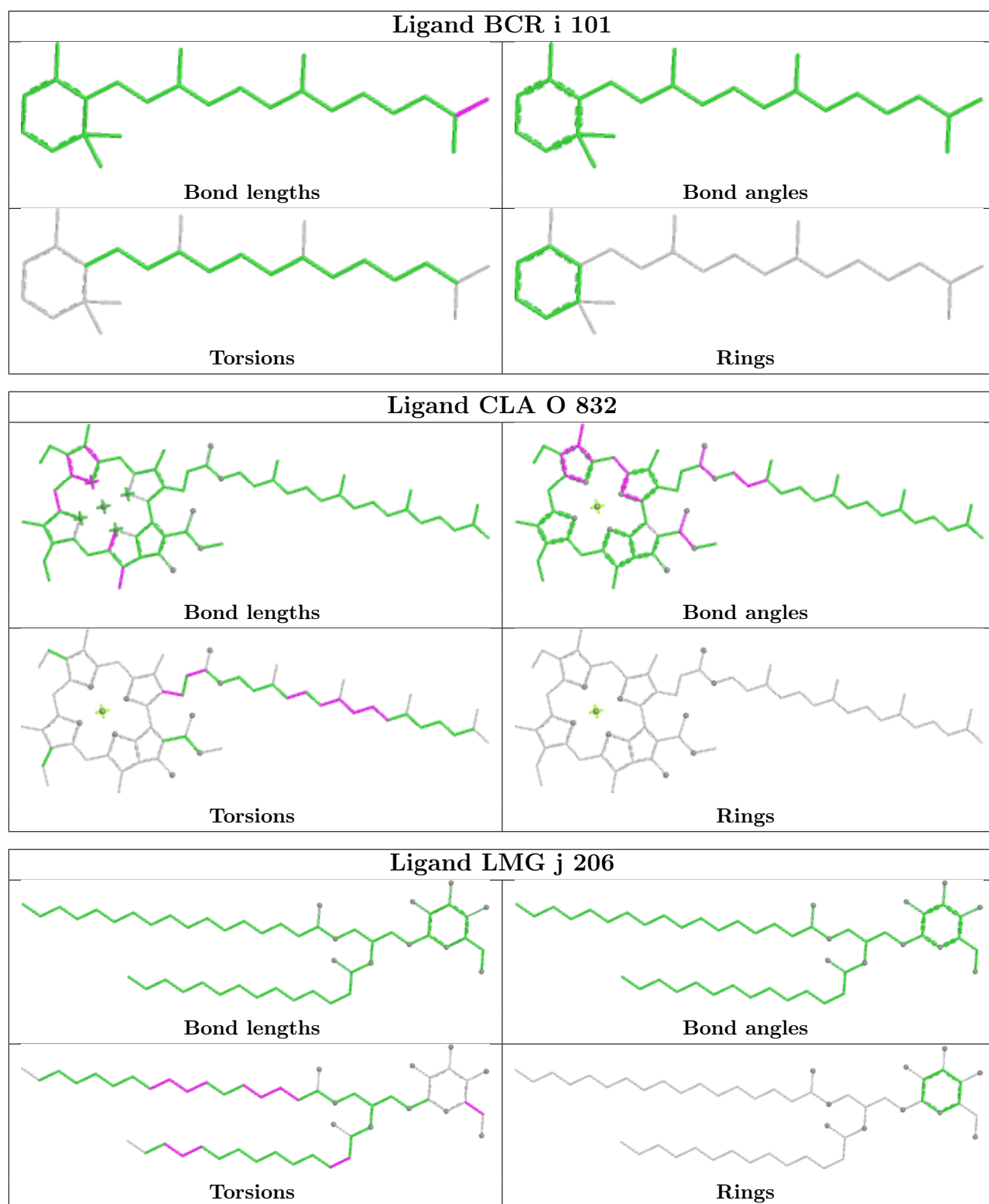
Torsions

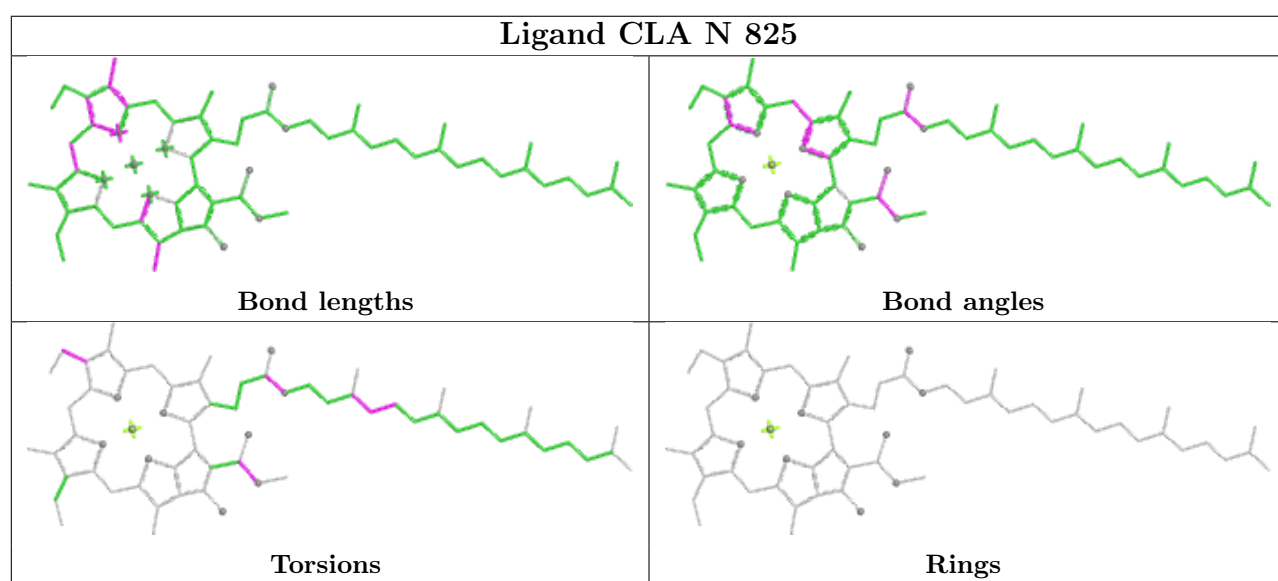
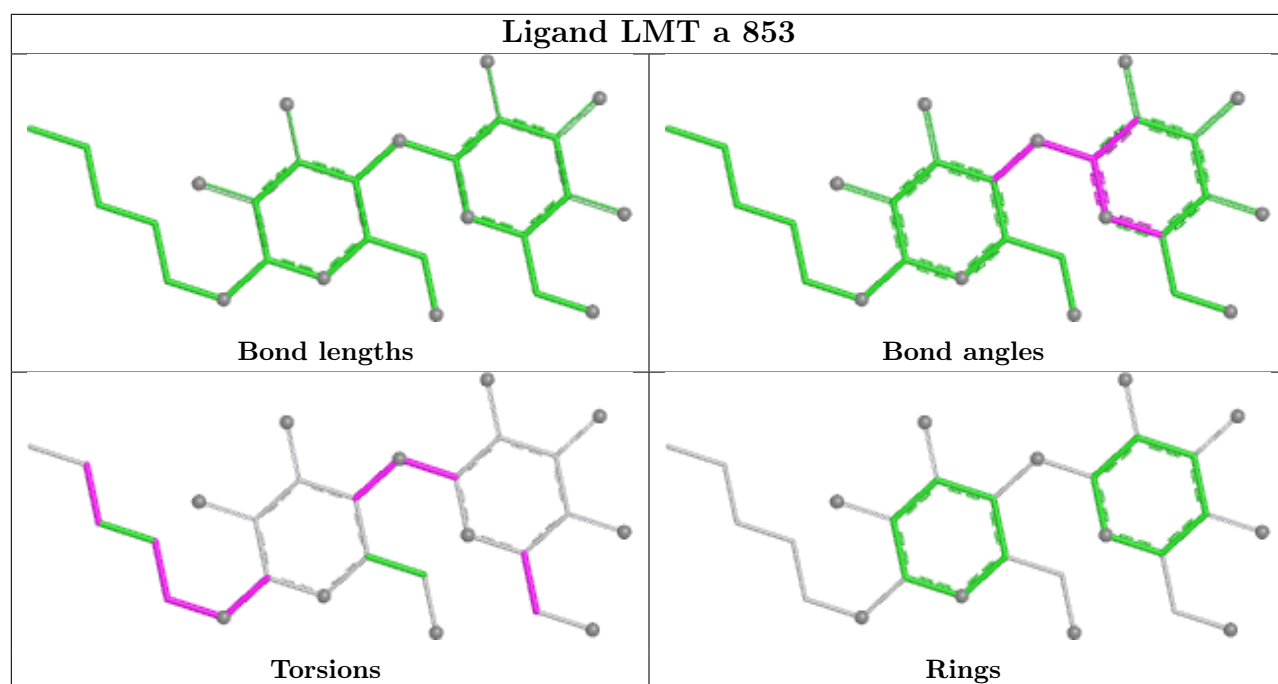


Rings

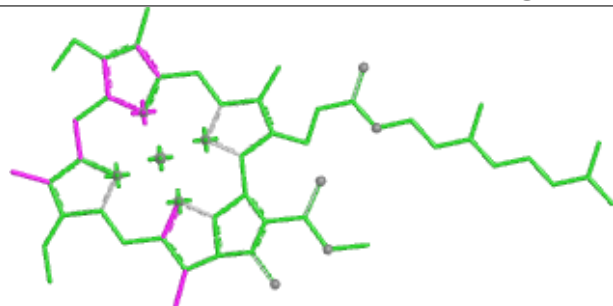




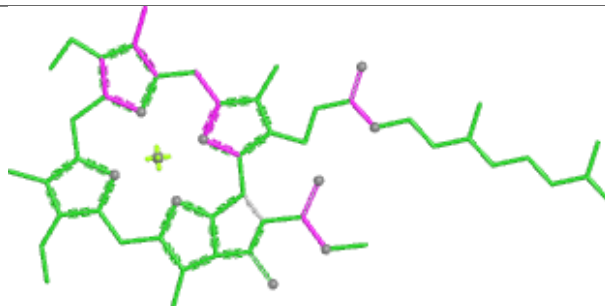




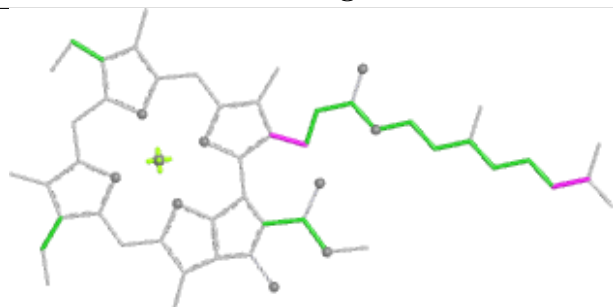
Ligand CLA a 815



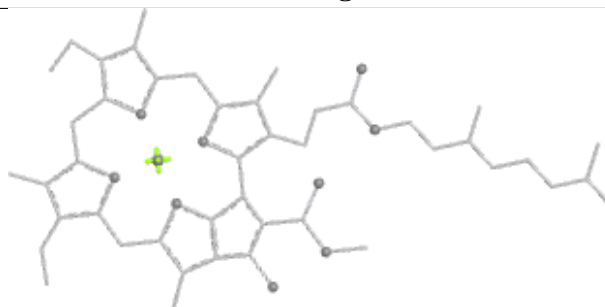
Bond lengths



Bond angles

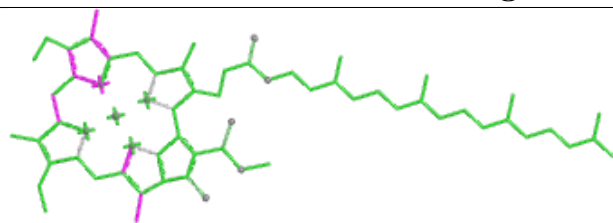


Torsions

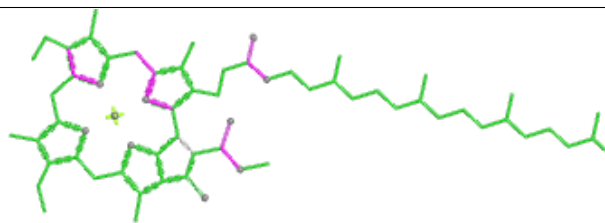


Rings

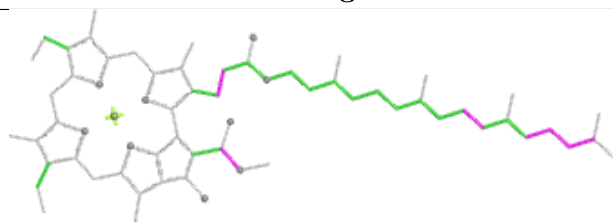
Ligand CLA W 1501



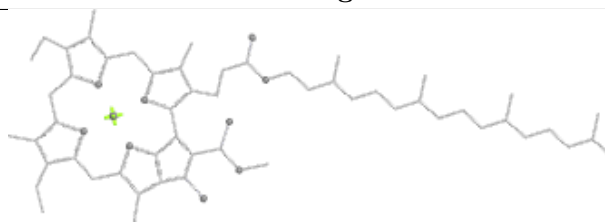
Bond lengths



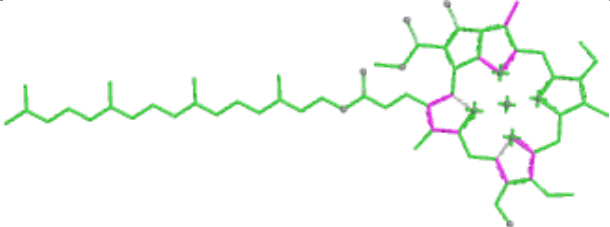
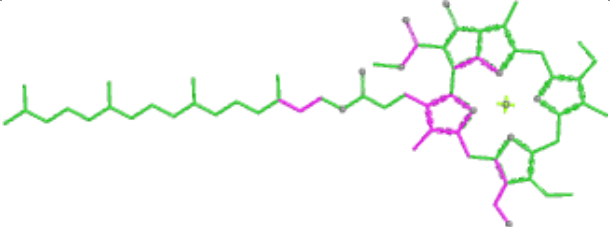
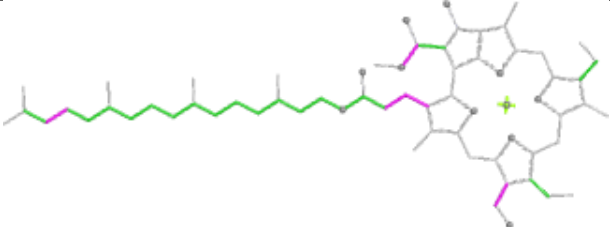
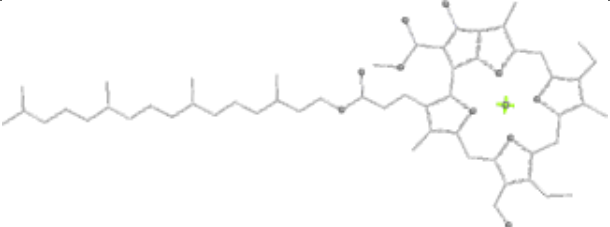
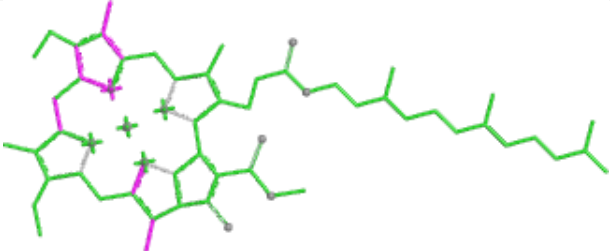
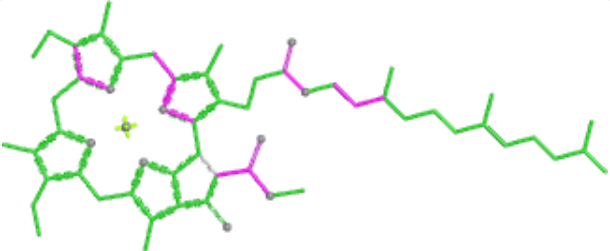
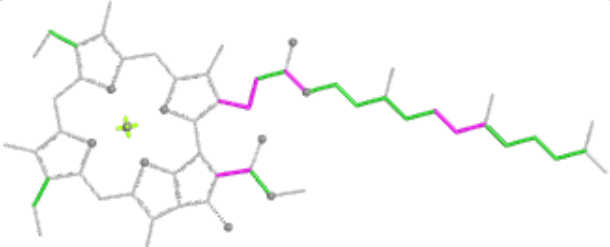
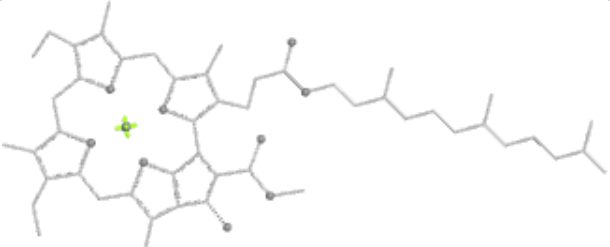
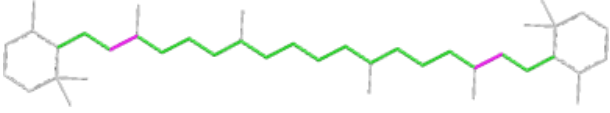
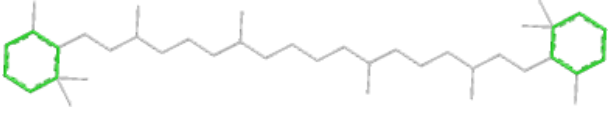
Bond angles

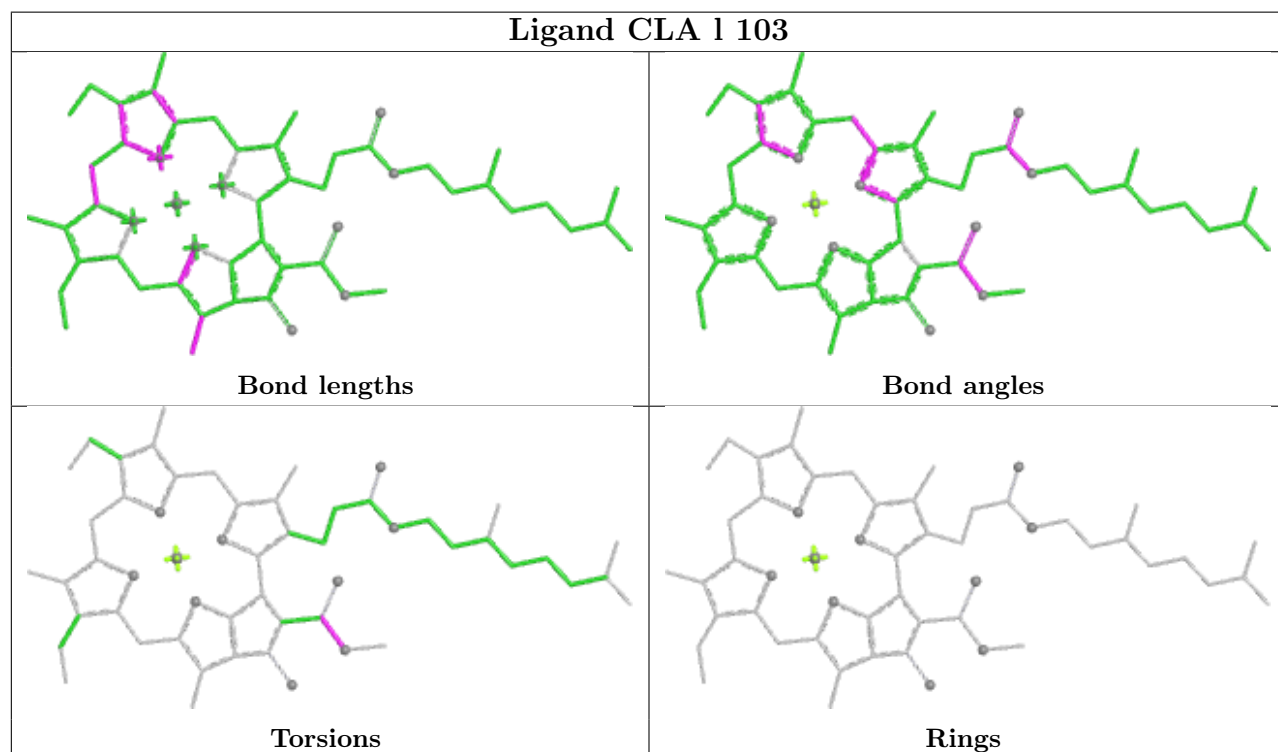
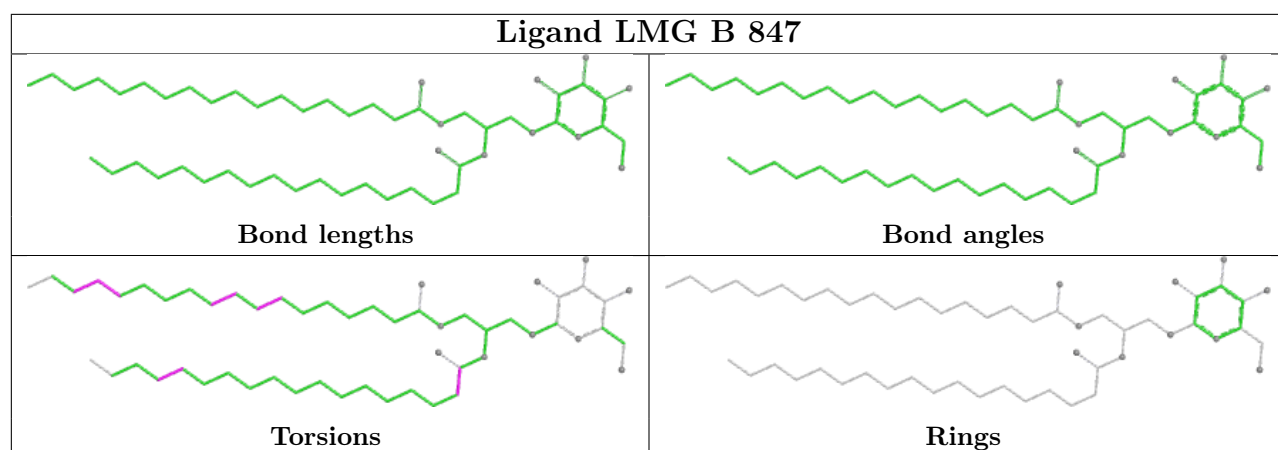


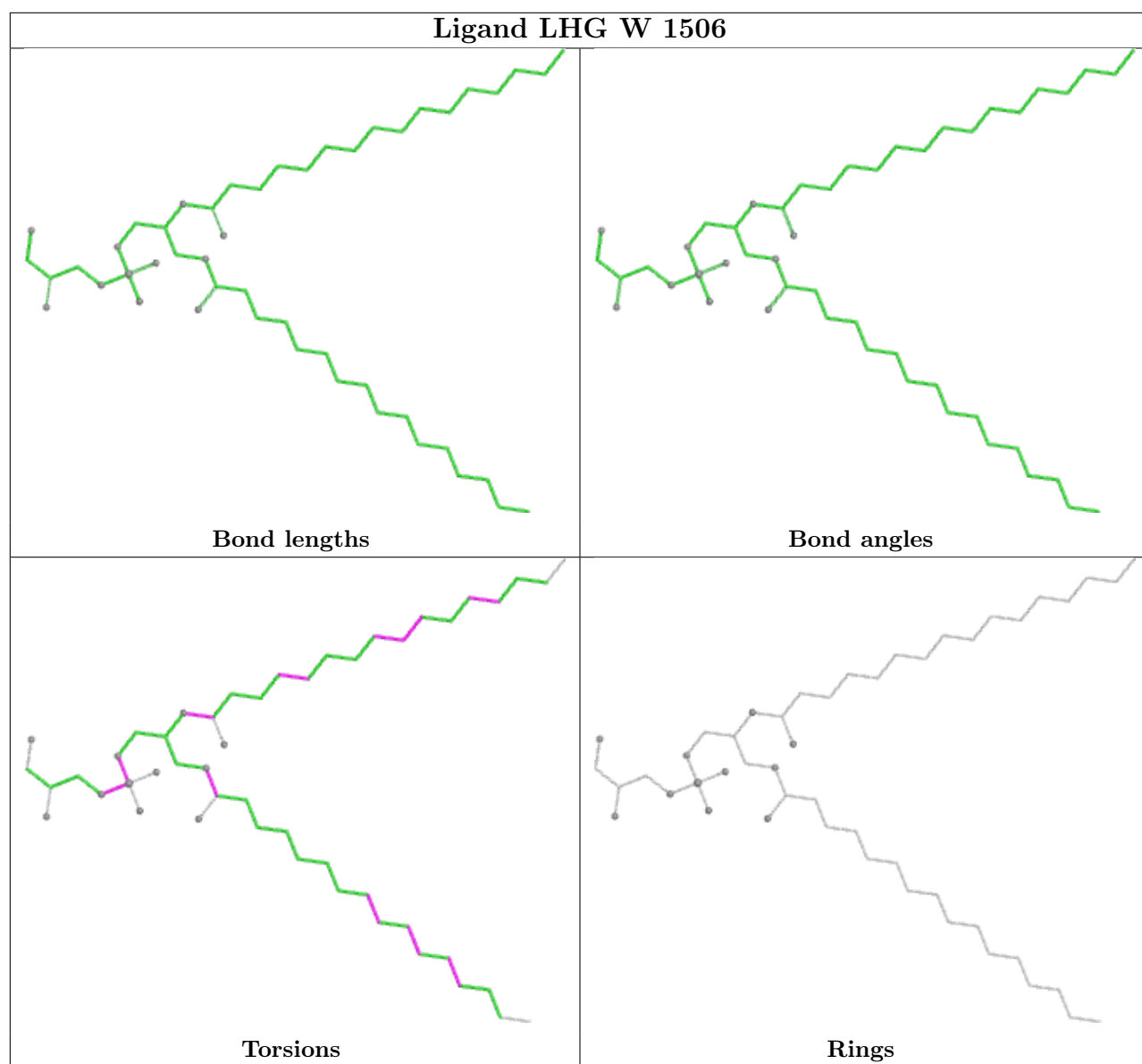
Torsions



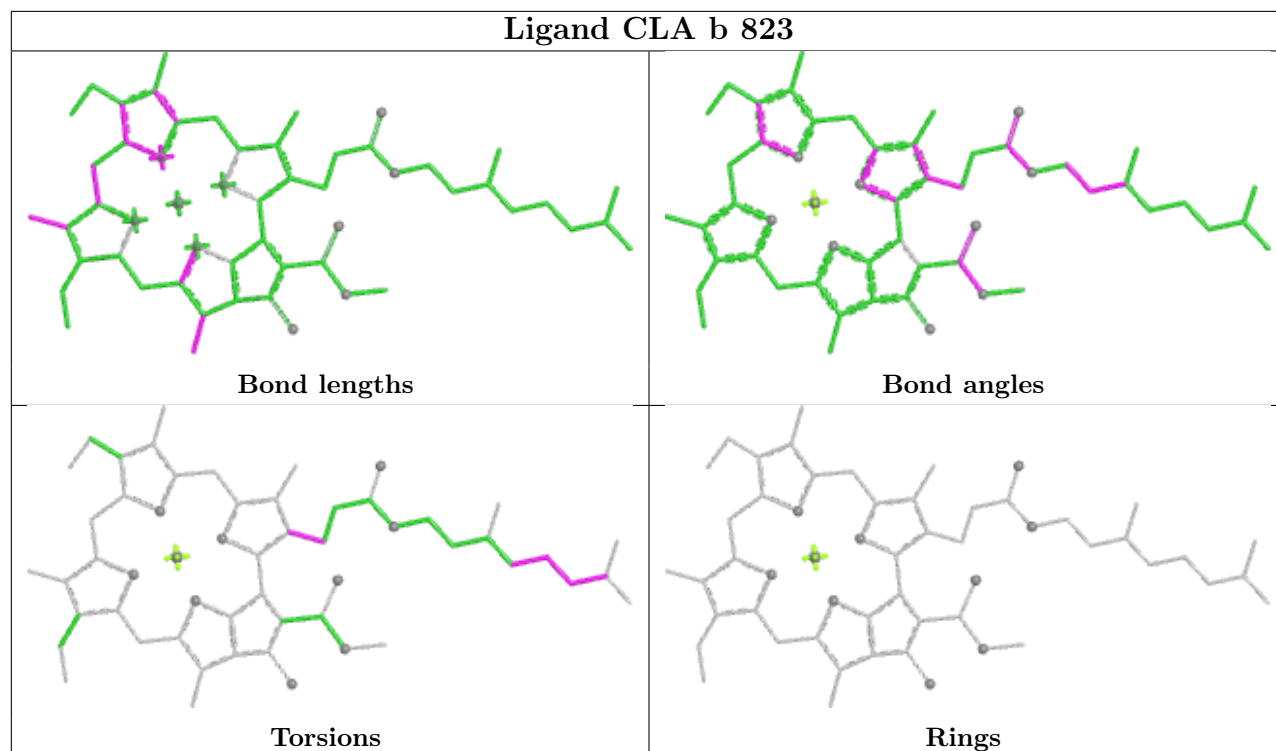
Rings

Ligand F6C N 802	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 809	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR W 1504	
 Bond lengths	 Bond angles
 Torsions	 Rings

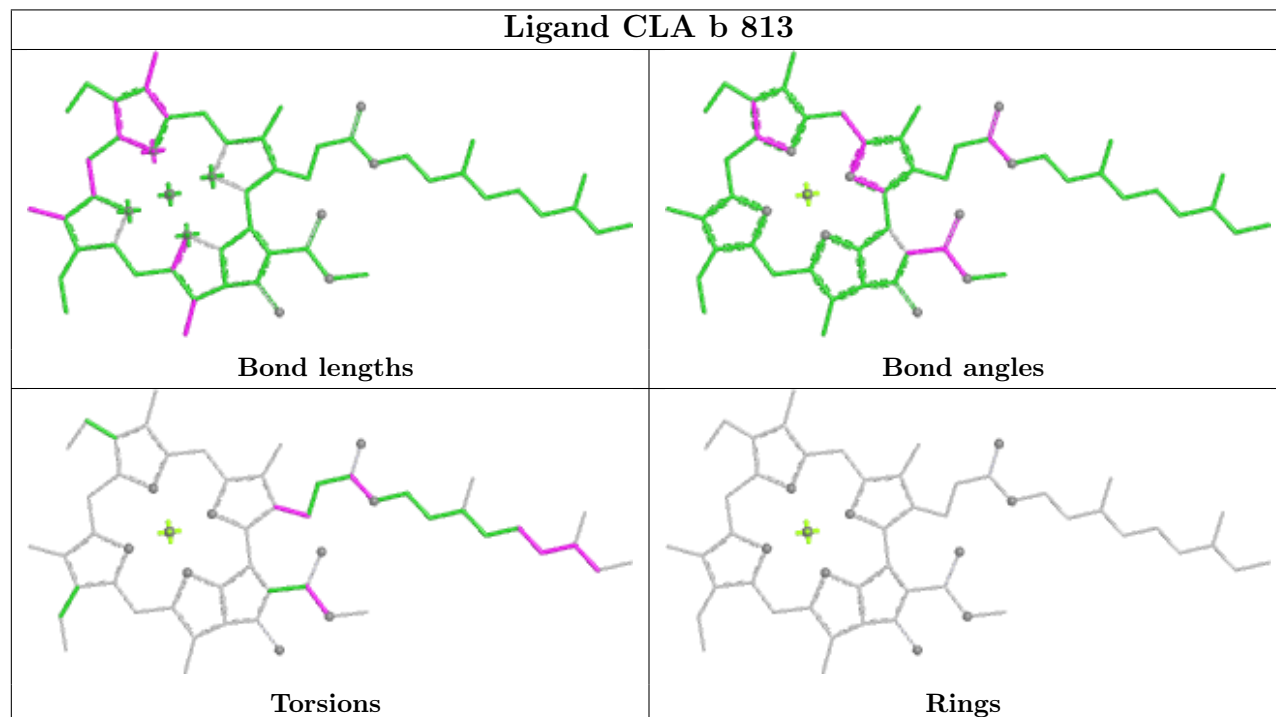


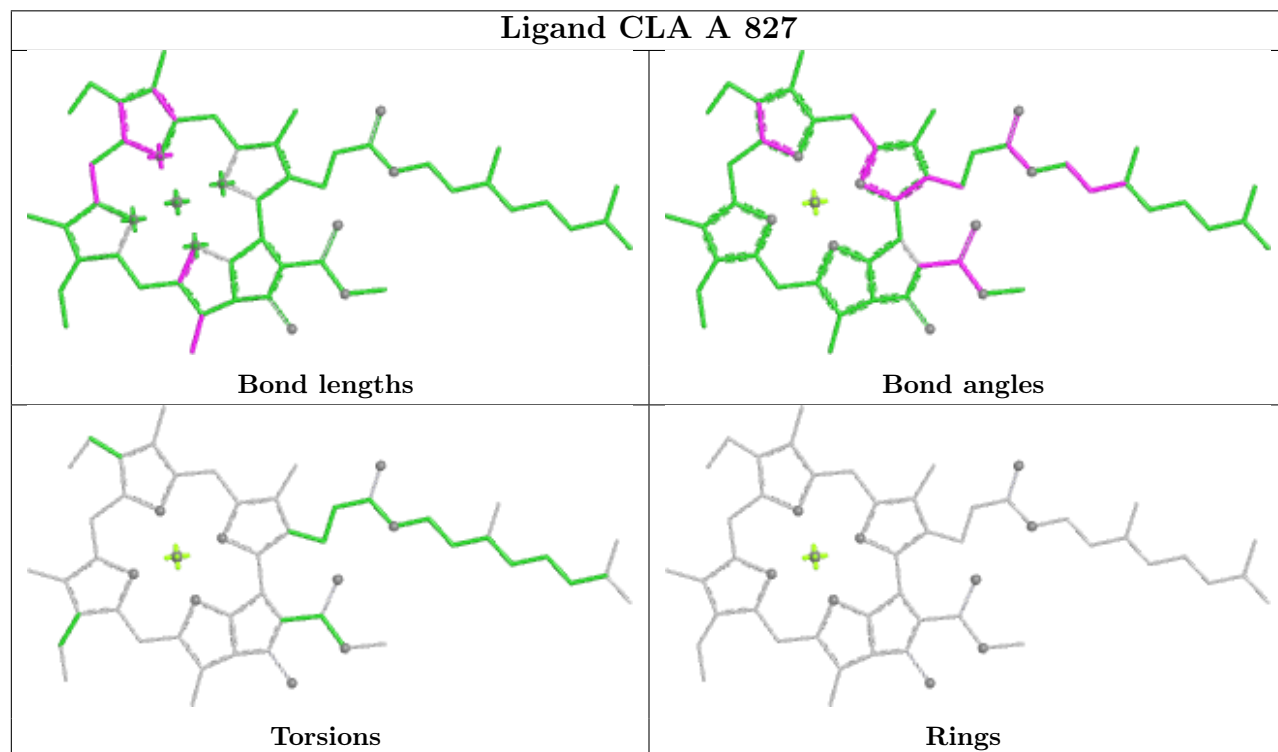
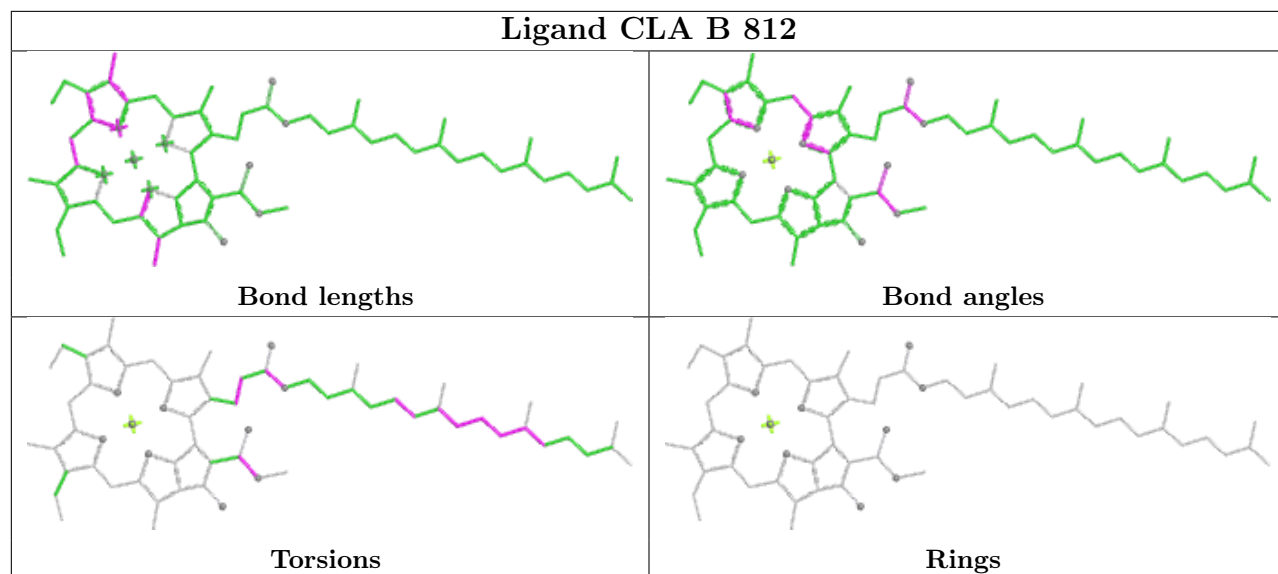


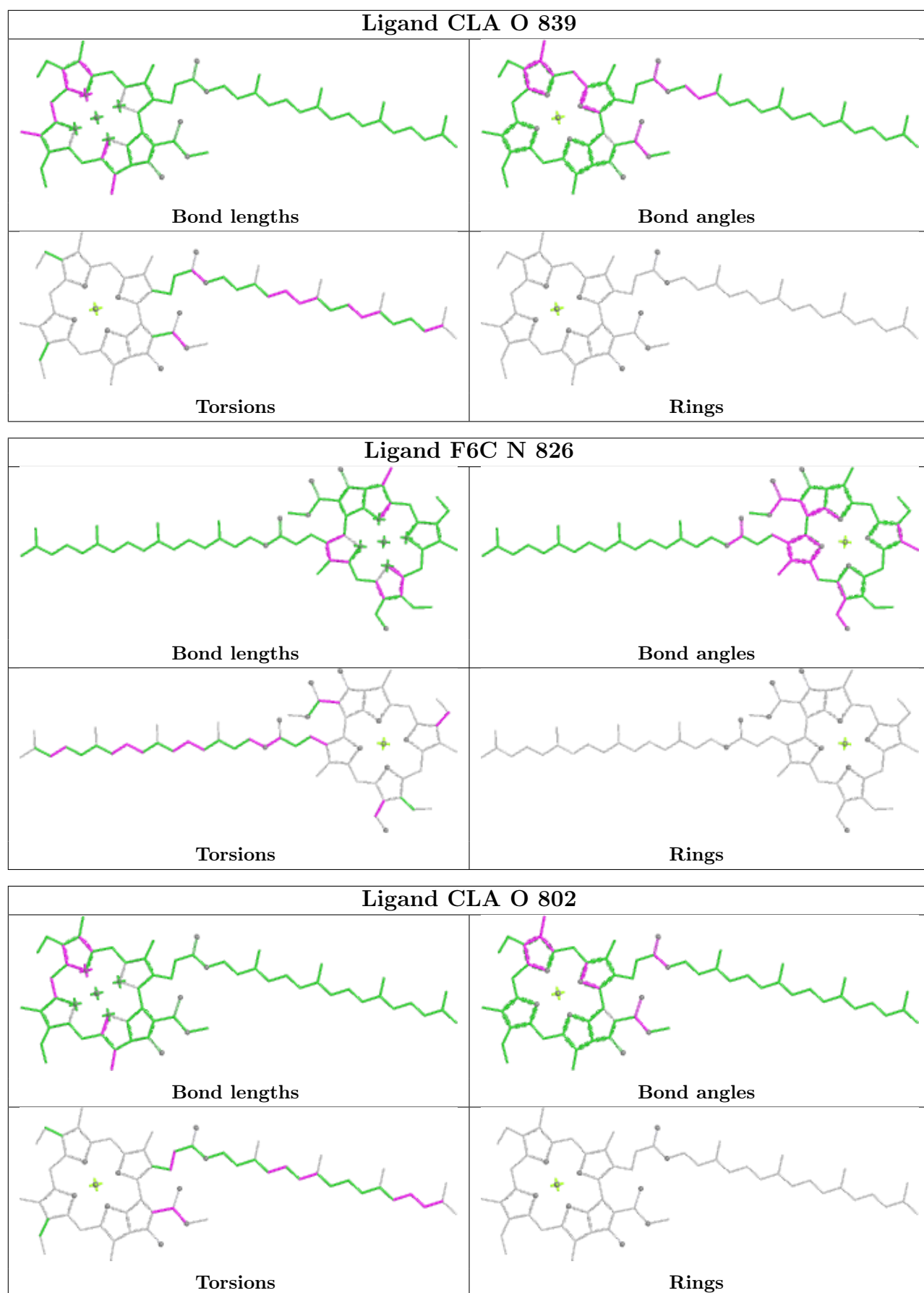
Ligand CLA b 823



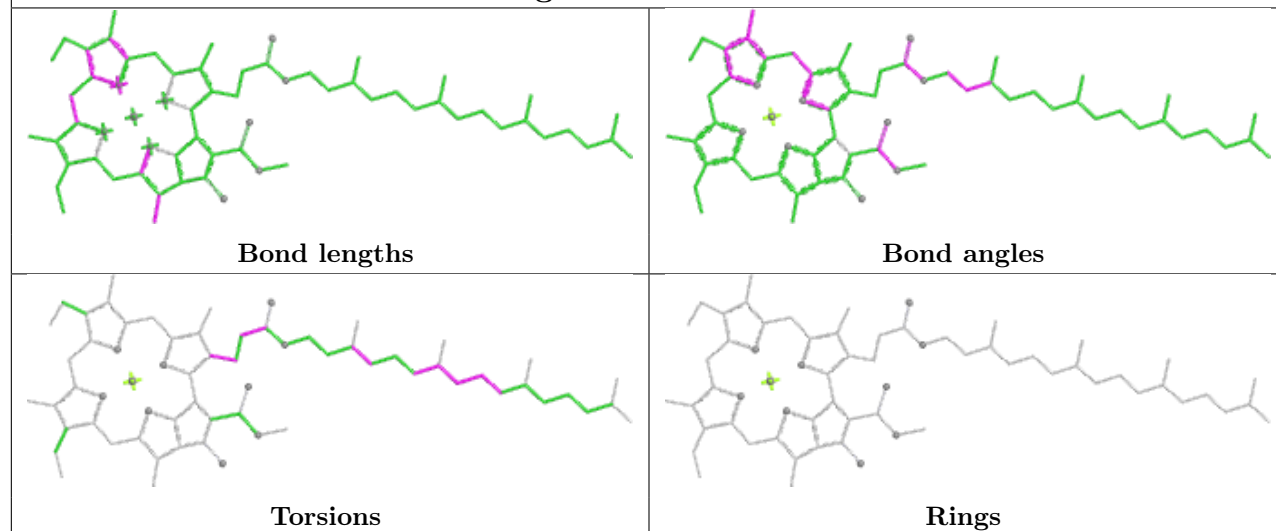
Ligand CLA b 813



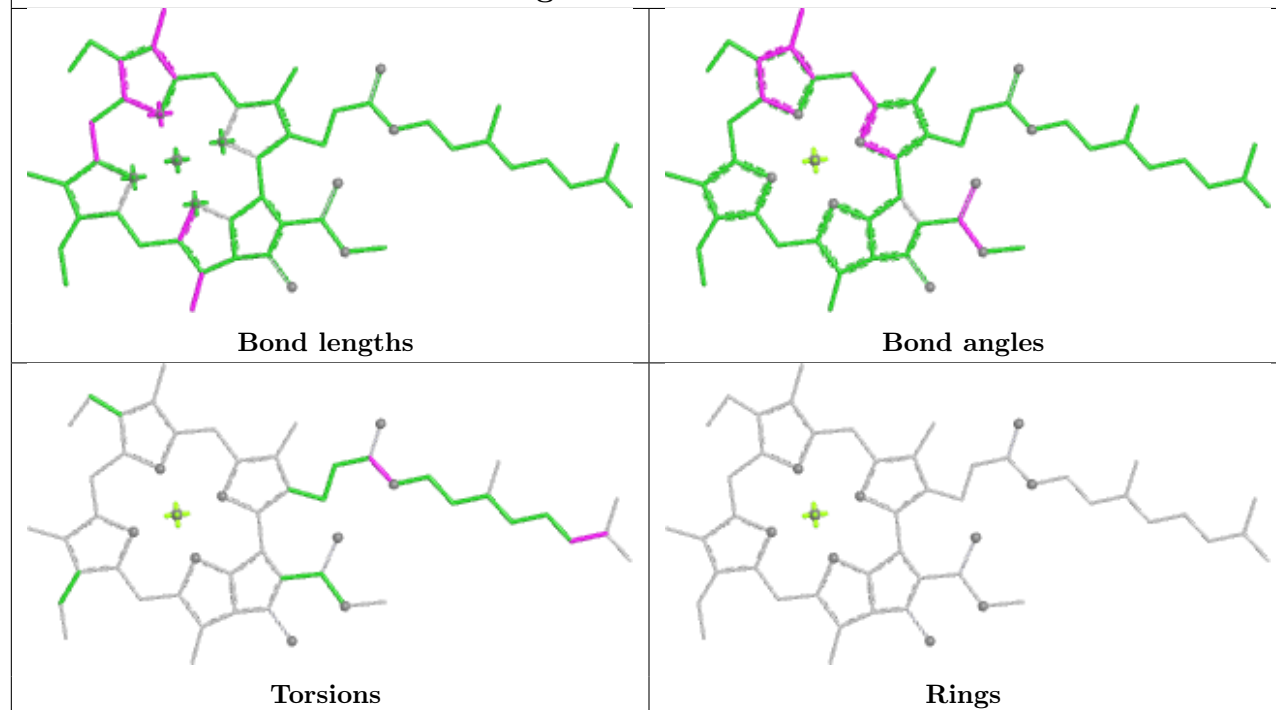




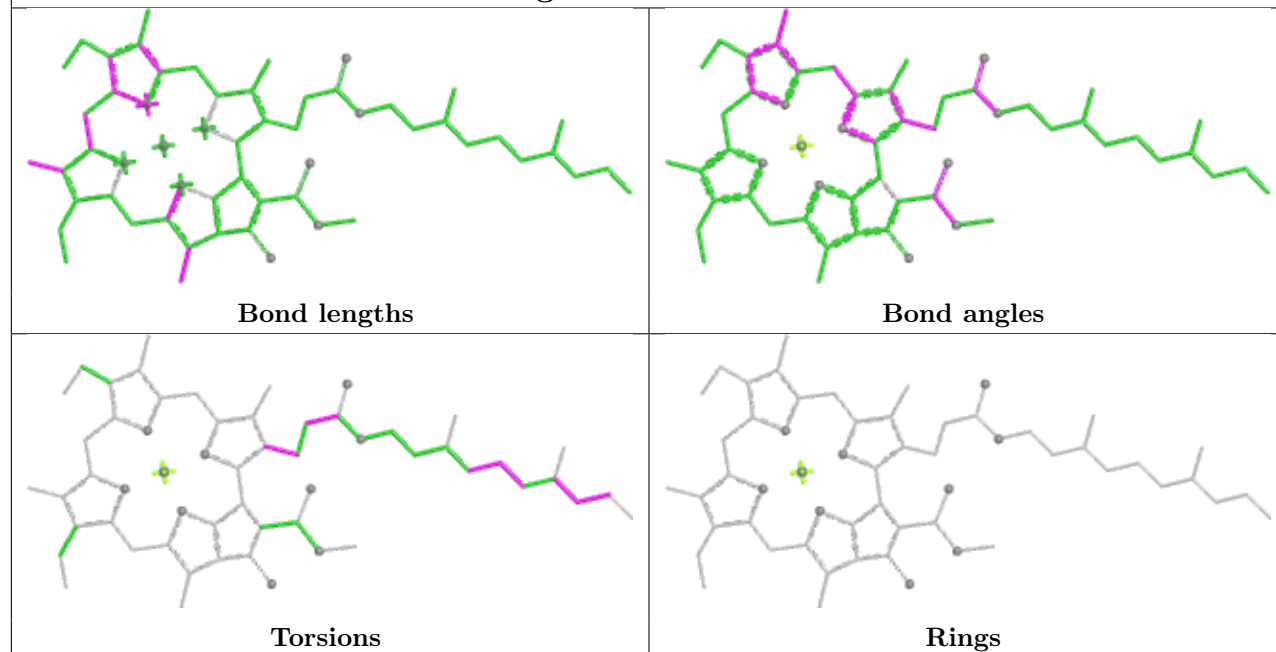
Ligand CLA b 832



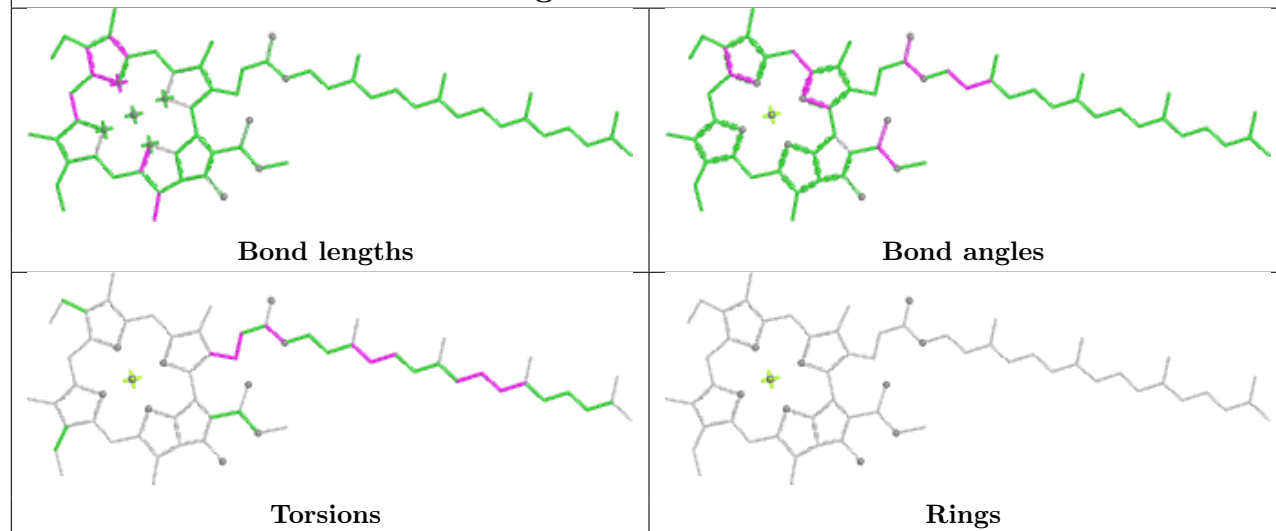
Ligand CLA a 833



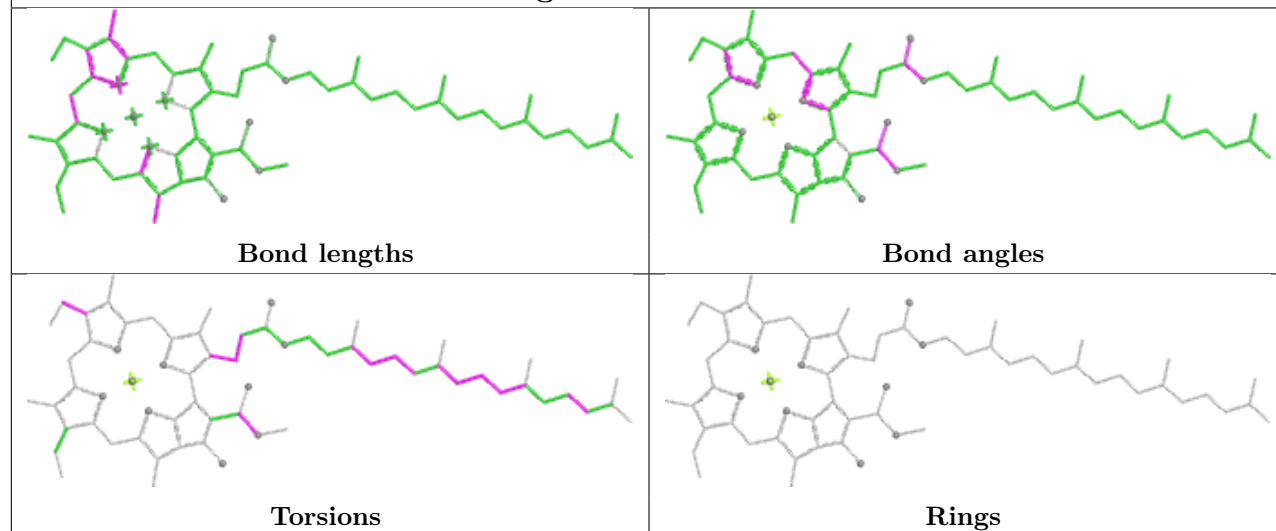
Ligand CLA a 810



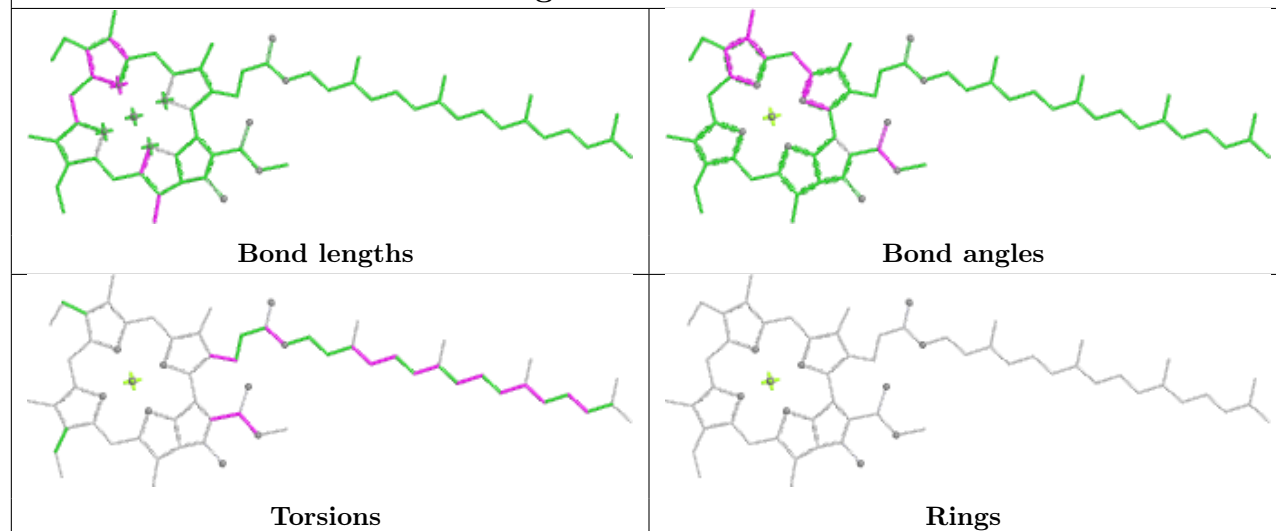
Ligand CLA b 831



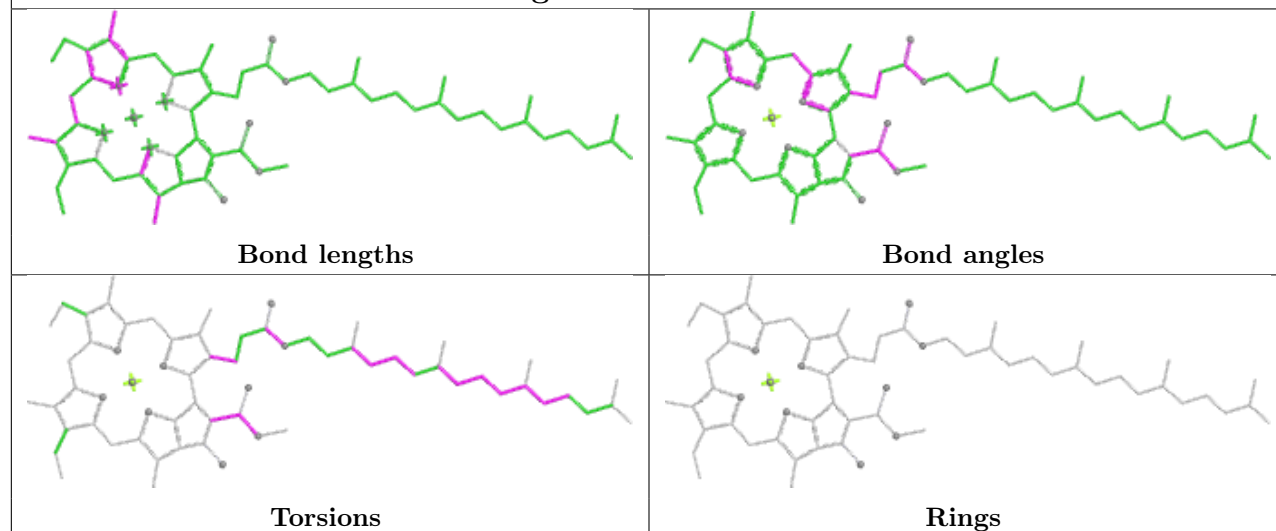
Ligand CLA a 812



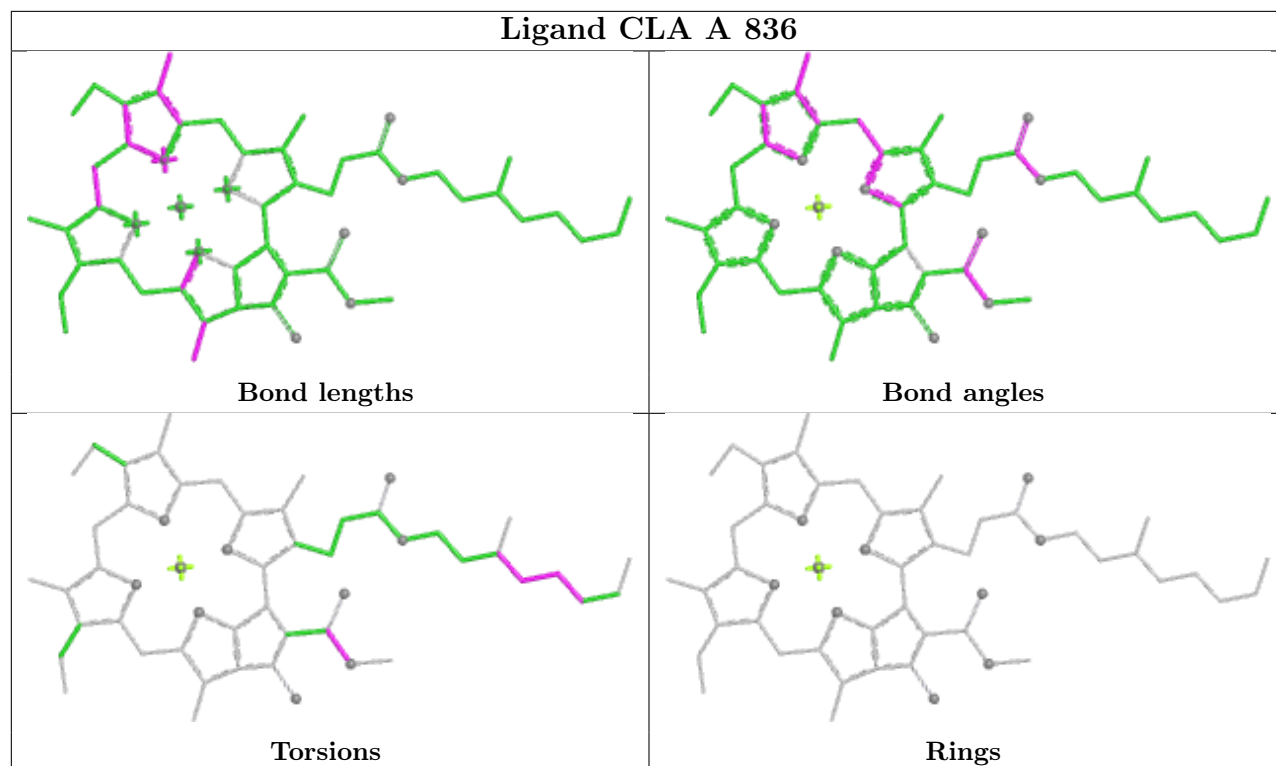
Ligand CLA b 806



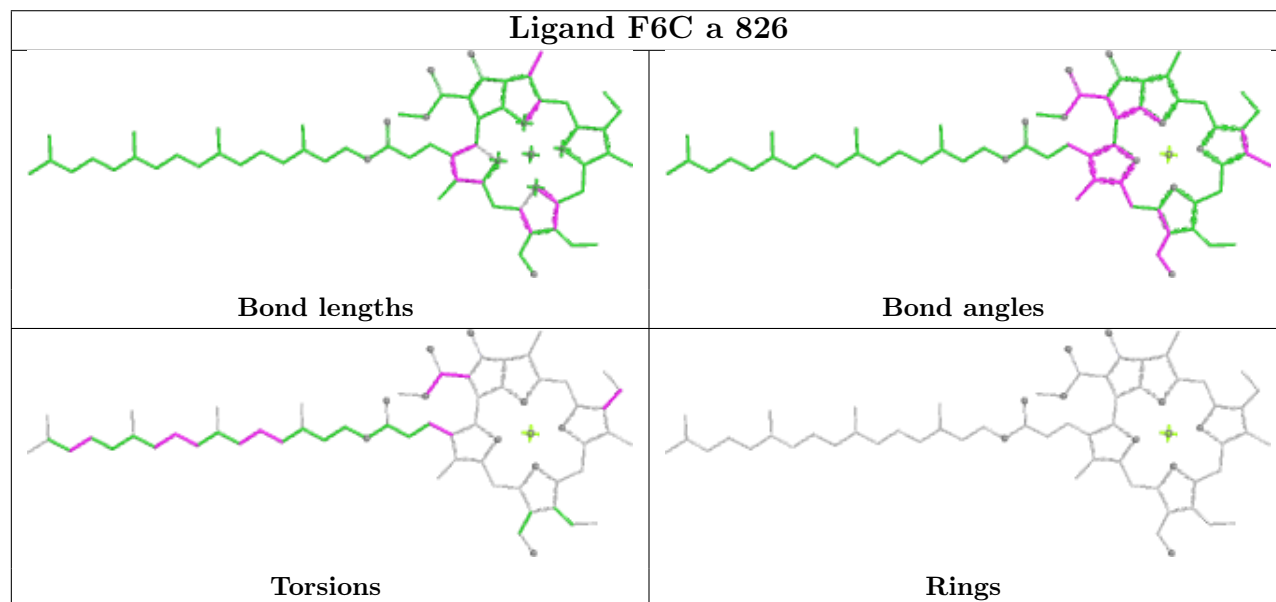
Ligand CLA A 818

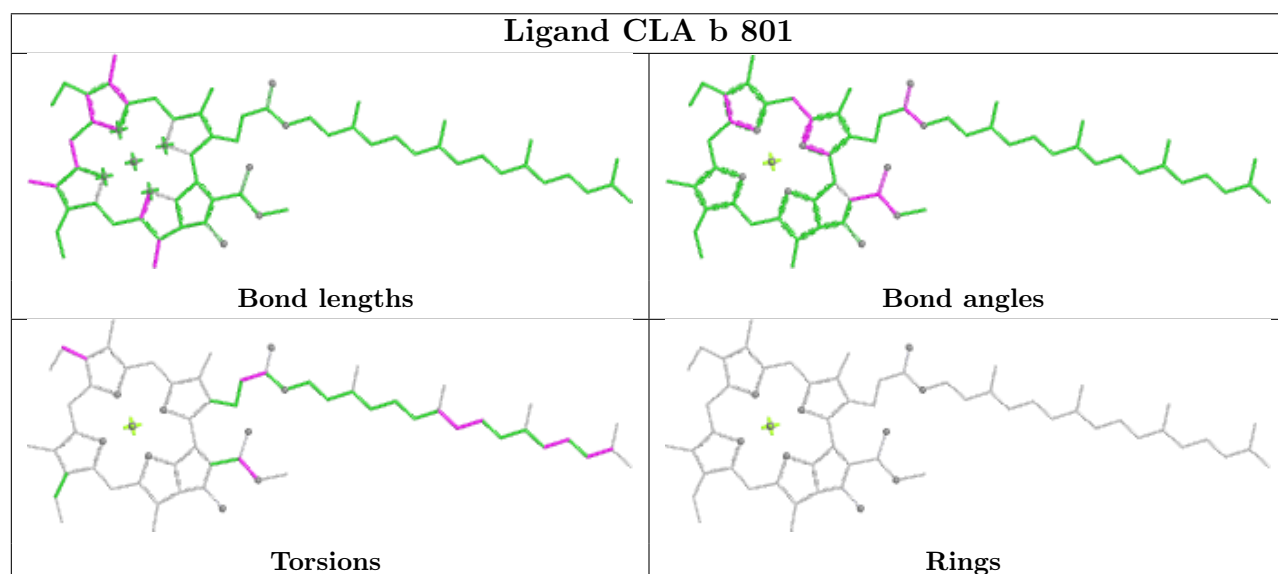
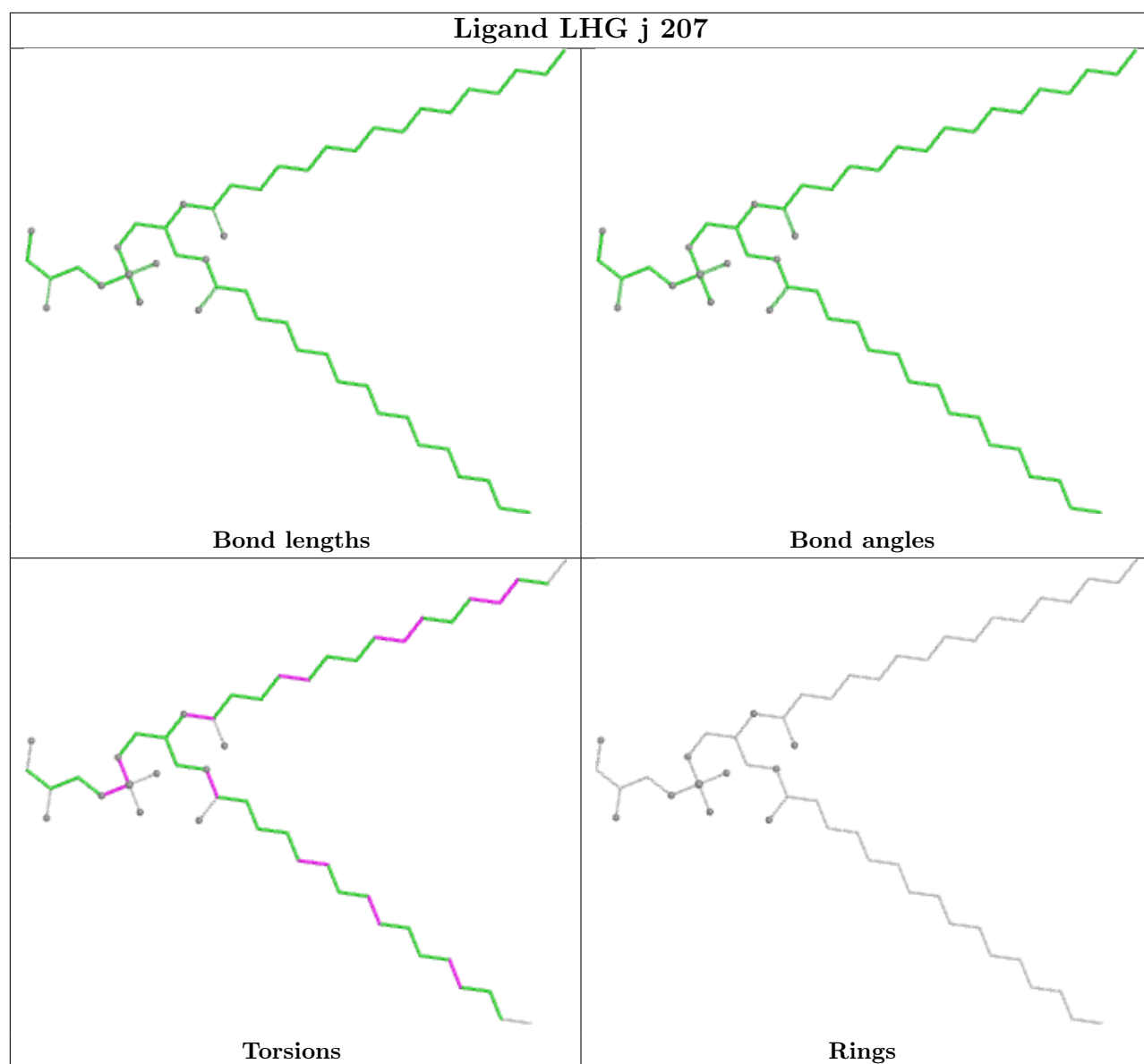


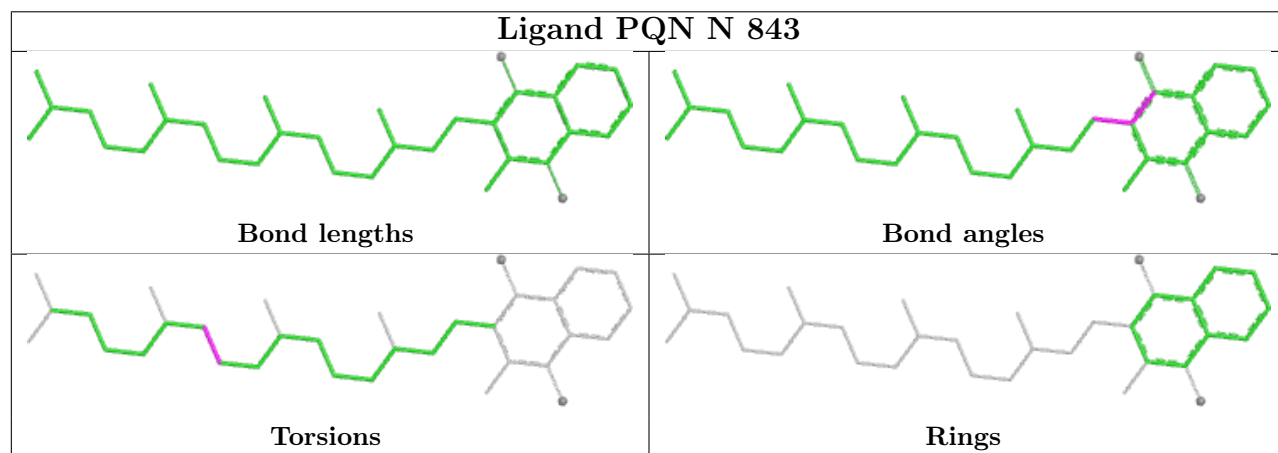
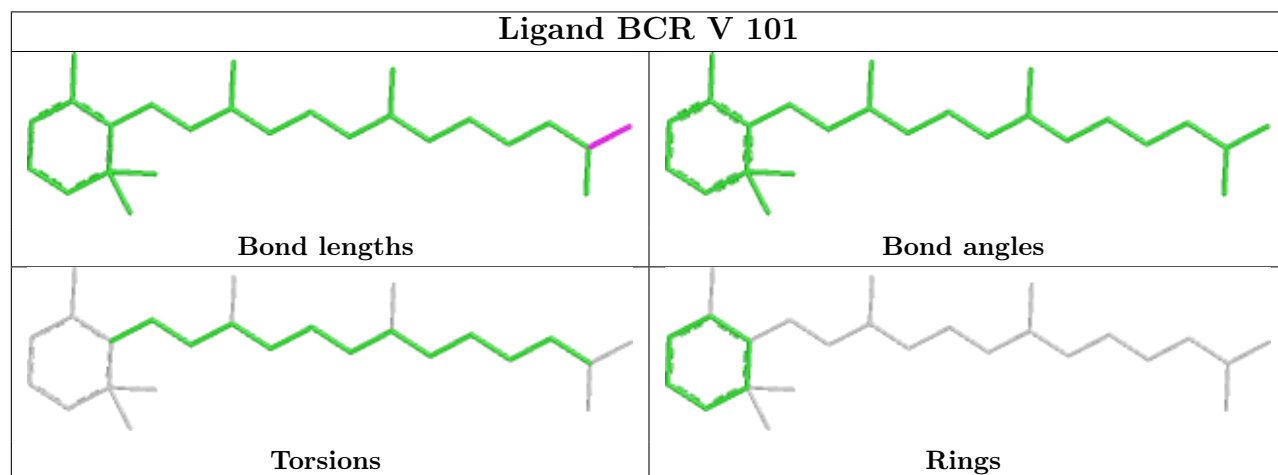
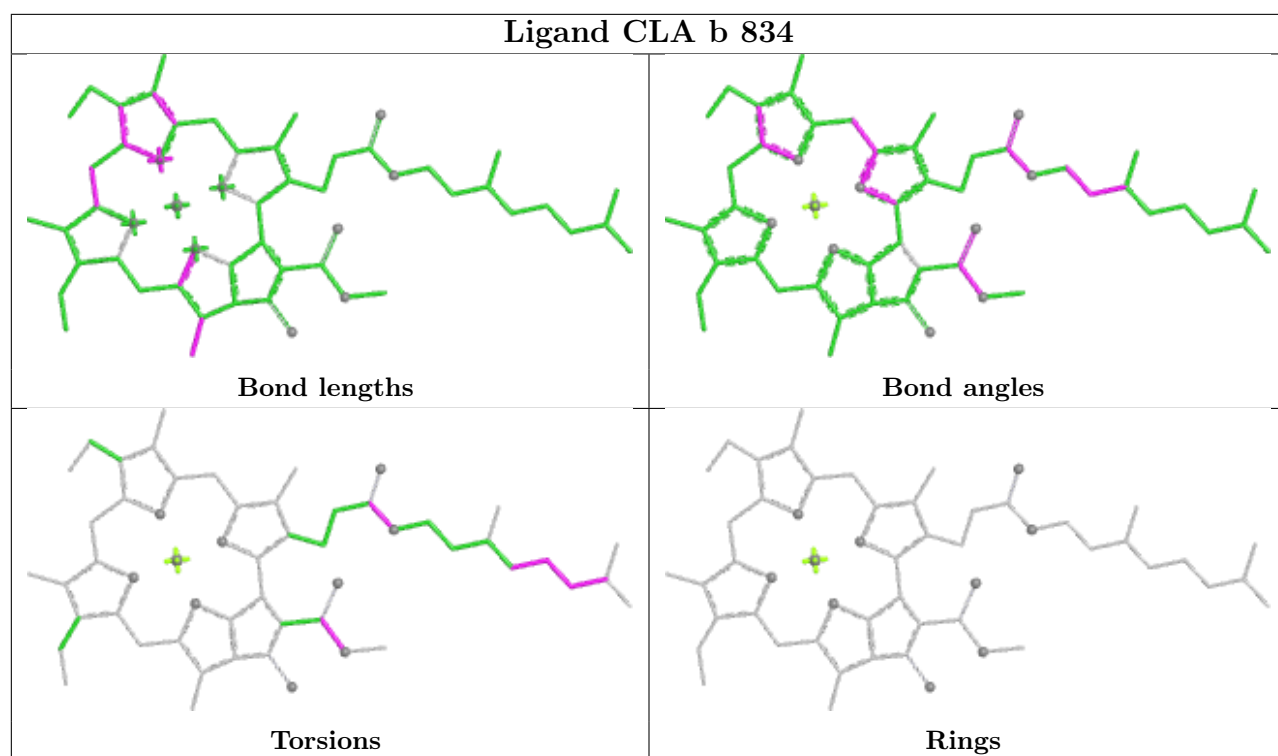
Ligand CLA A 836

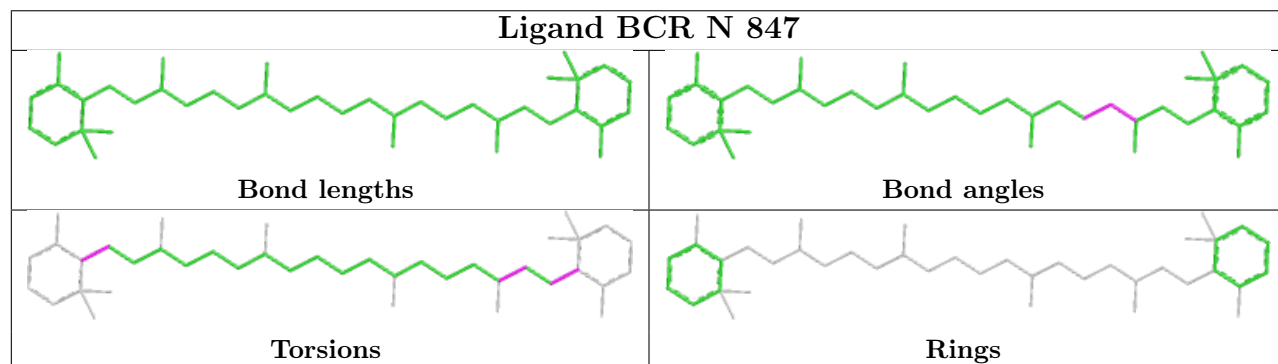
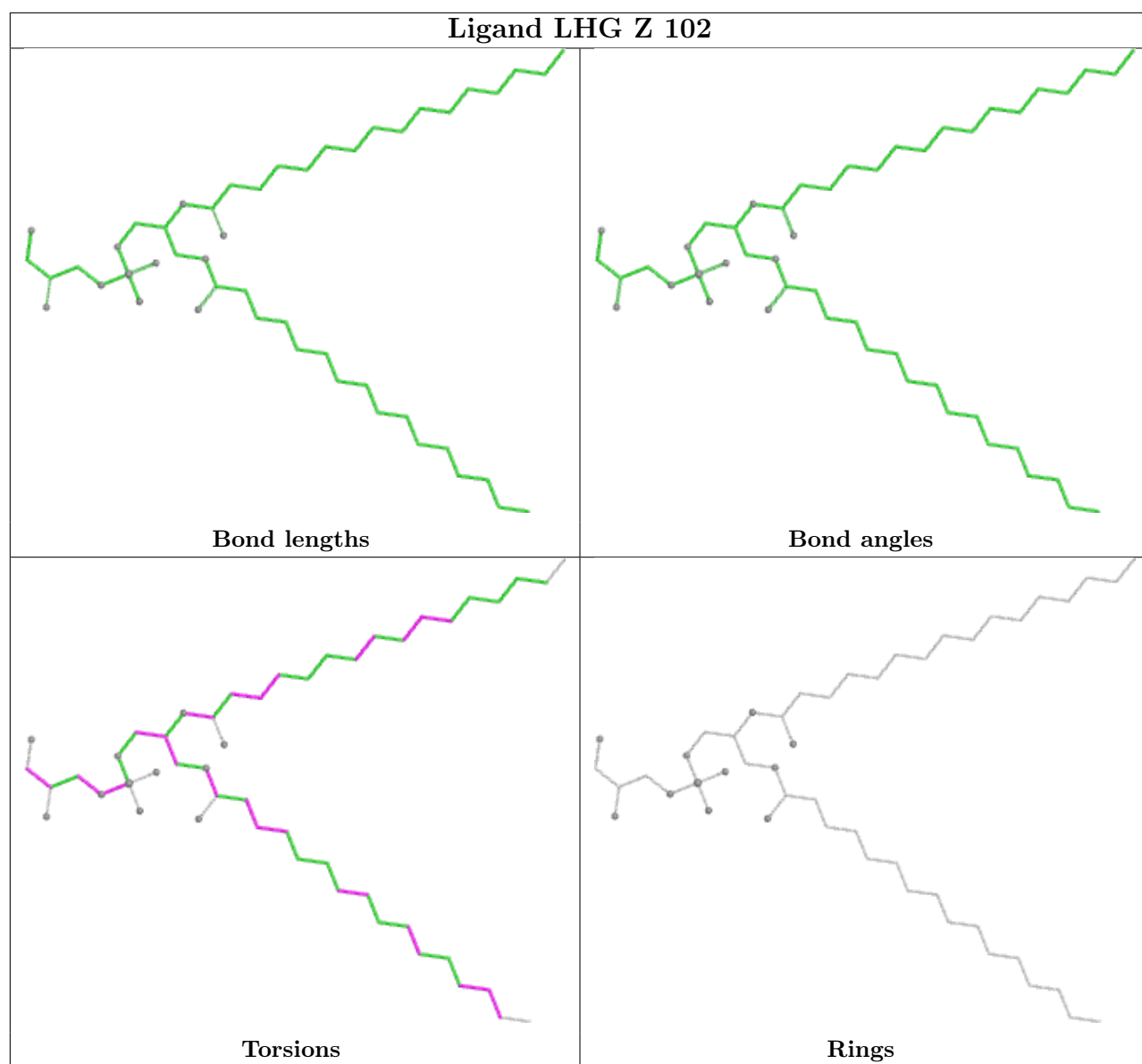


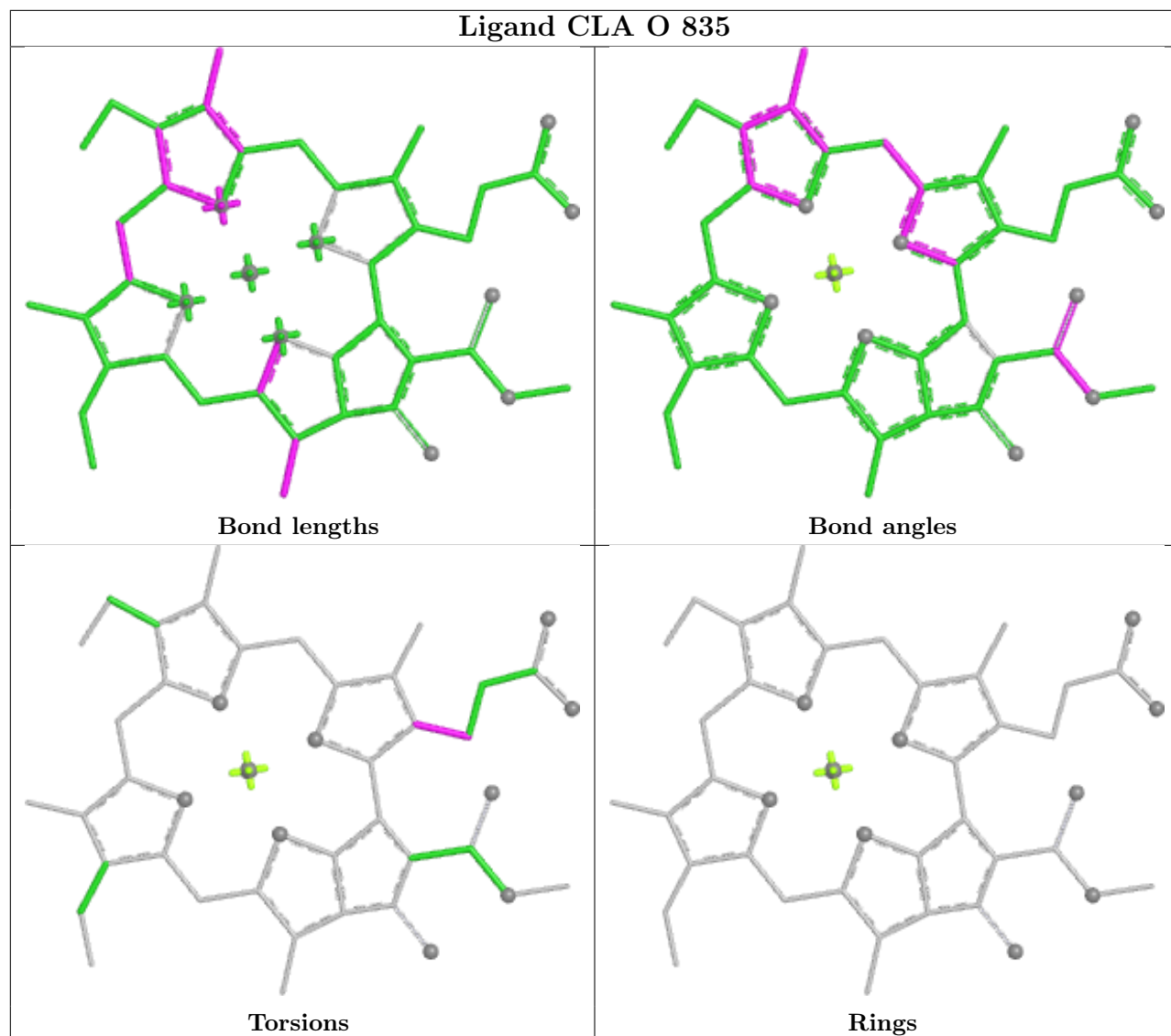
Ligand F6C a 826

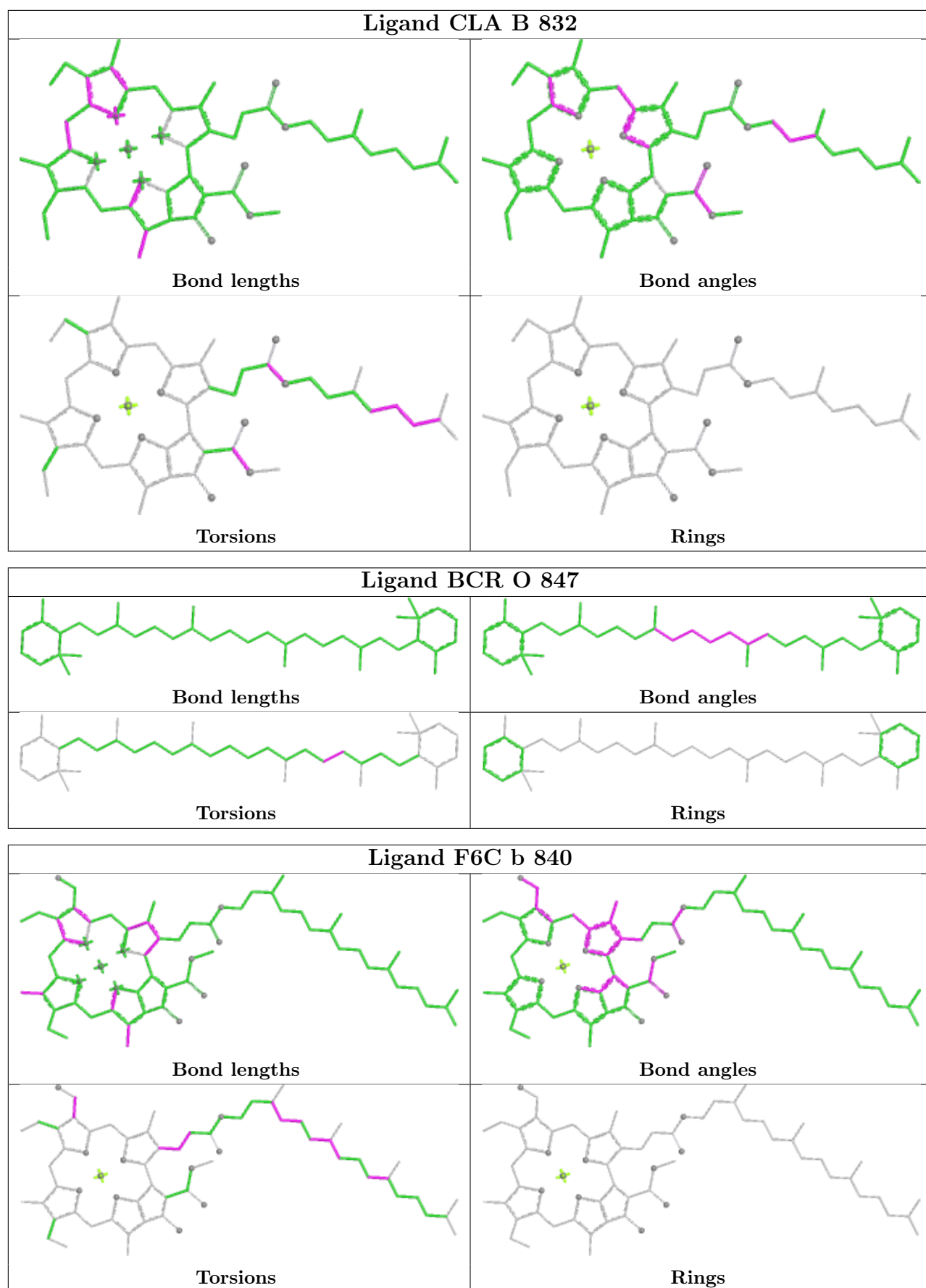


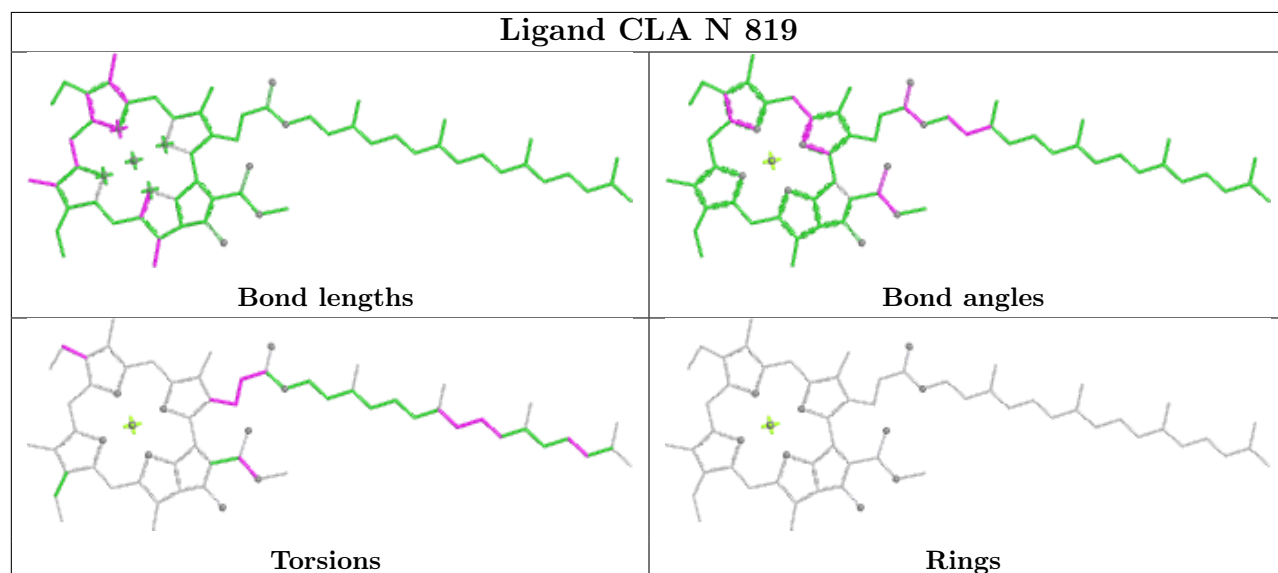
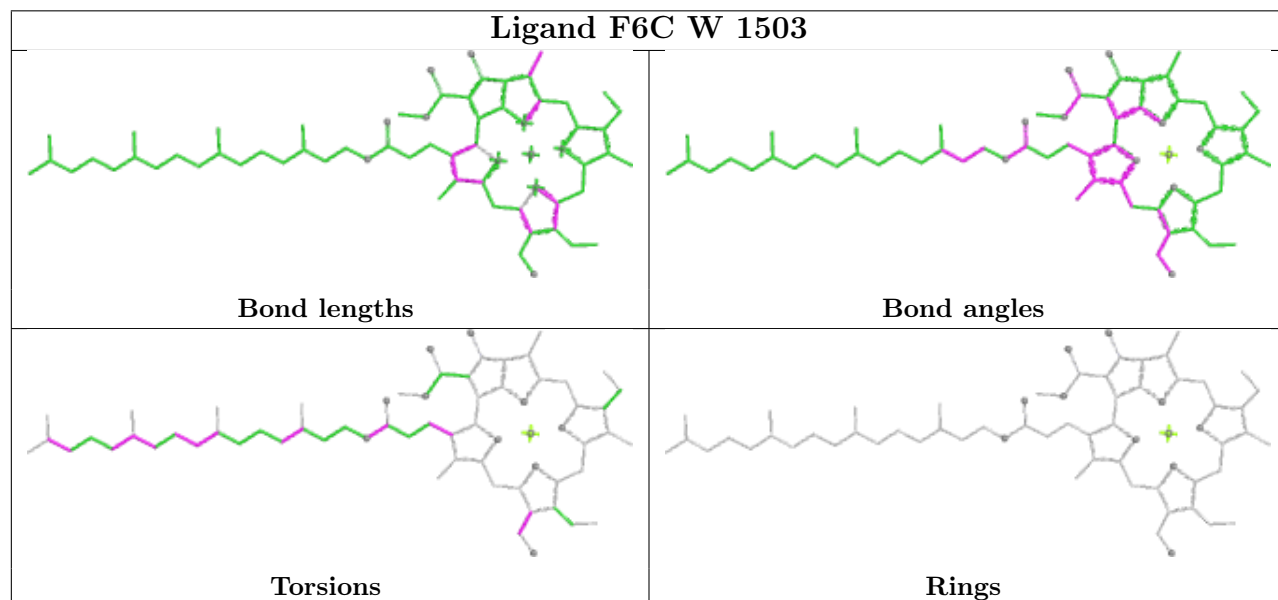
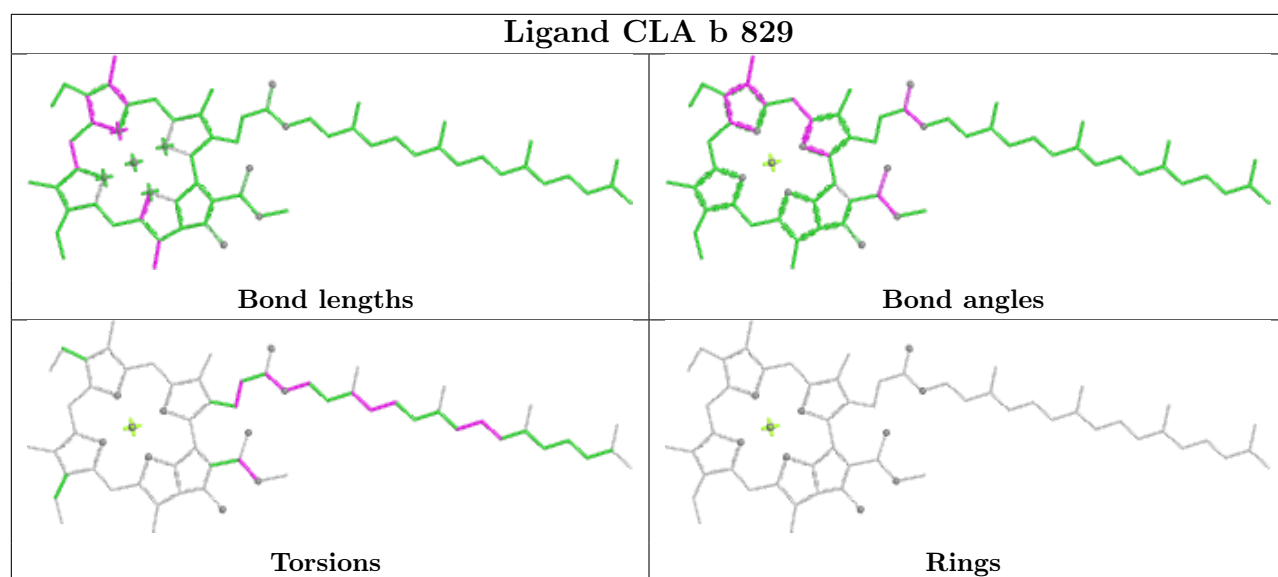




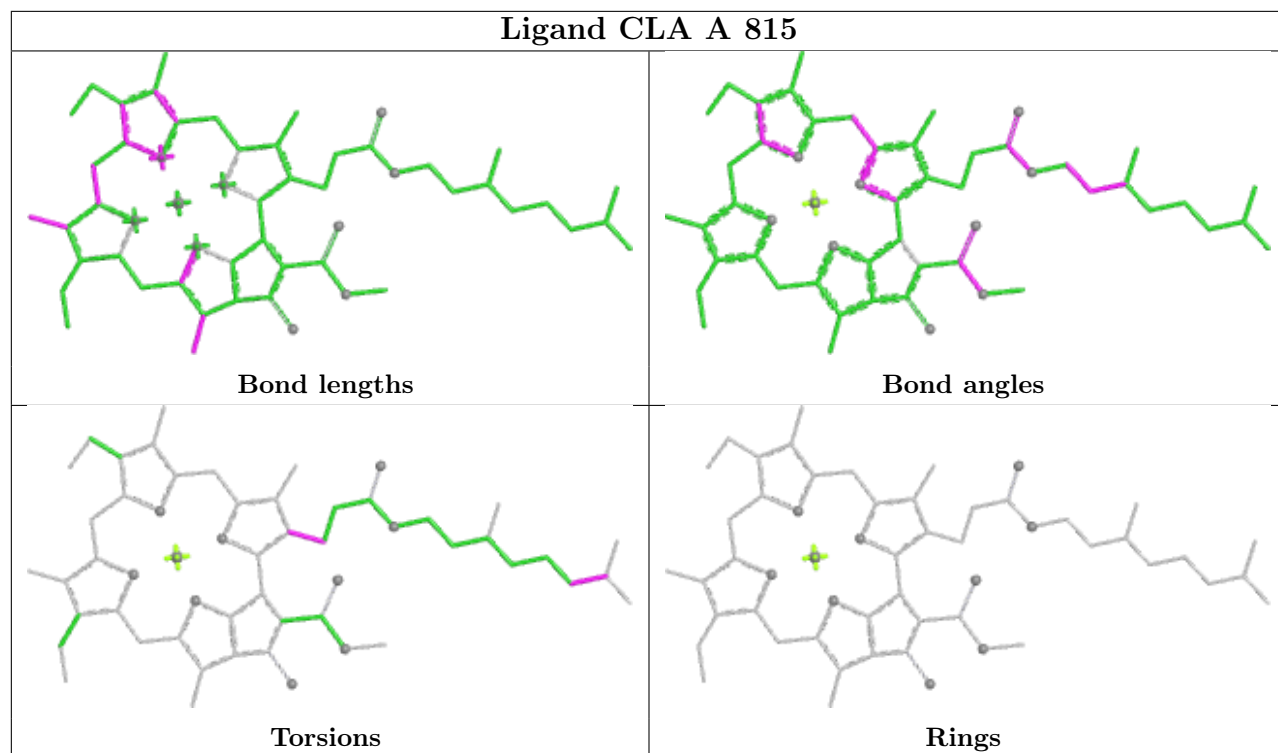




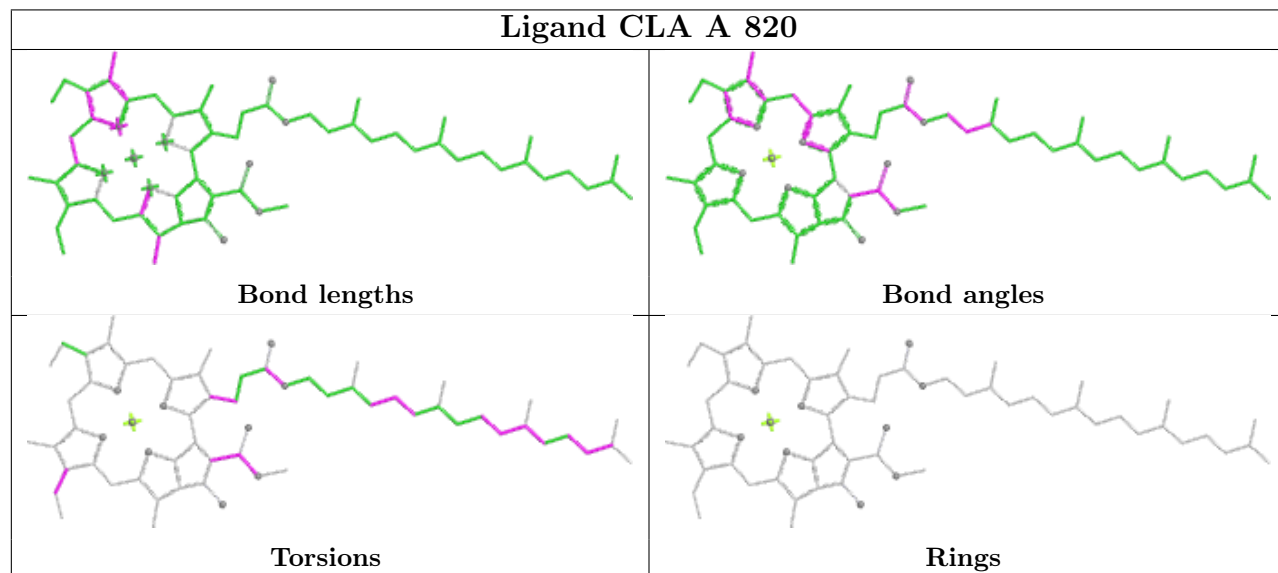




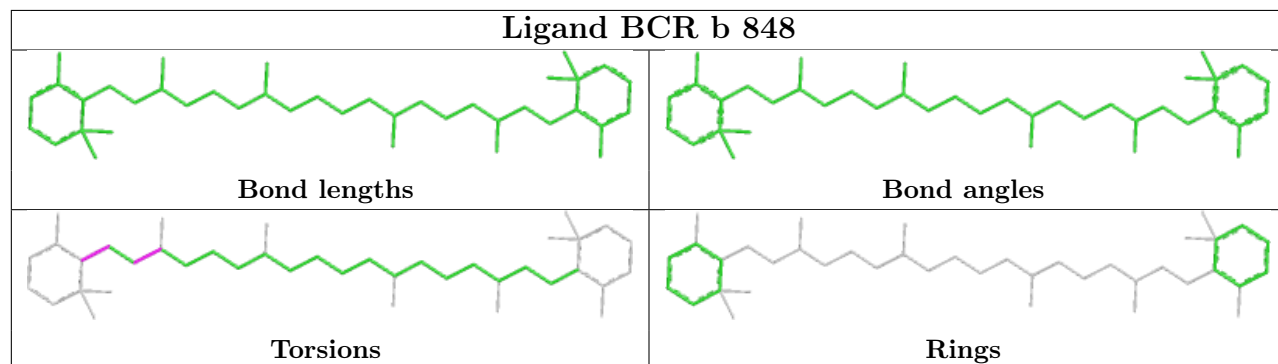
Ligand CLA A 815

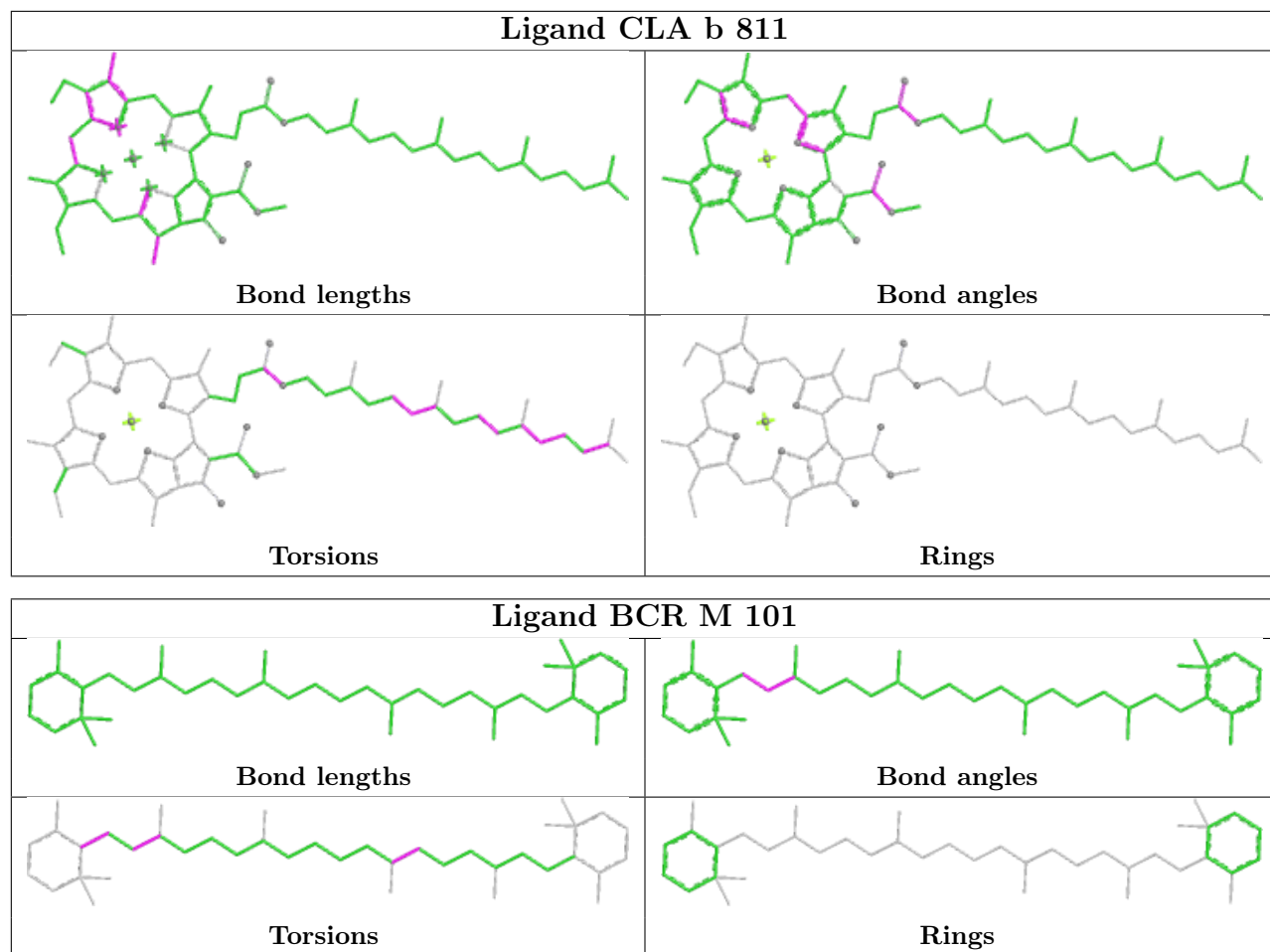


Ligand CLA A 820

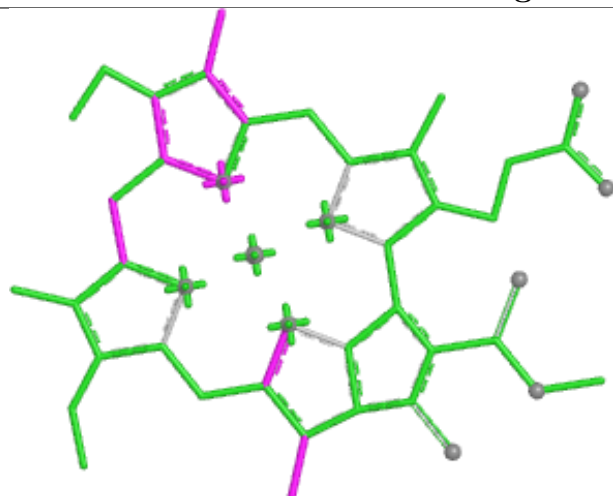


Ligand BCR b 848

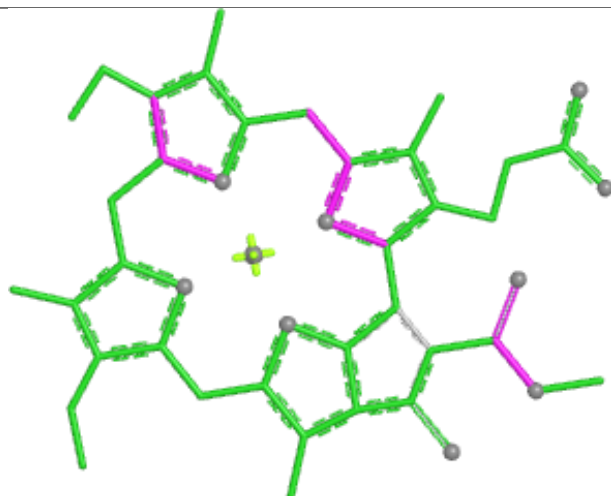




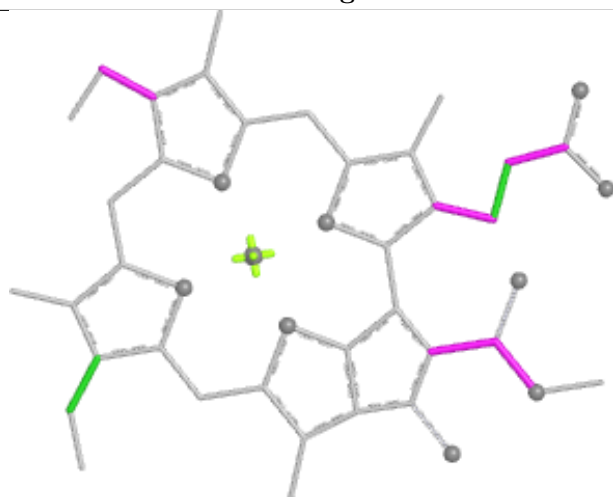
Ligand CLA B 834



Bond lengths



Bond angles

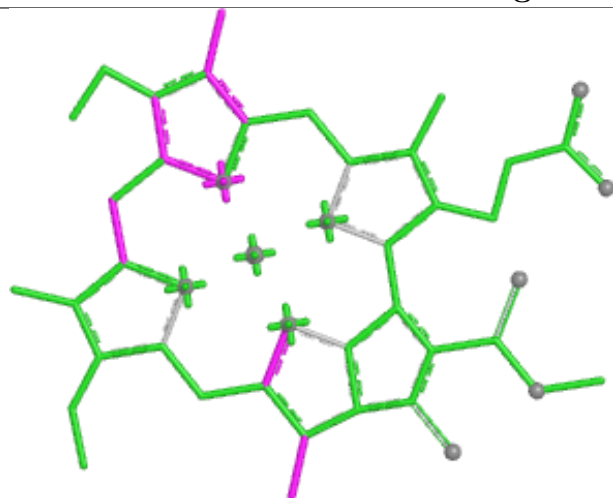


Torsions

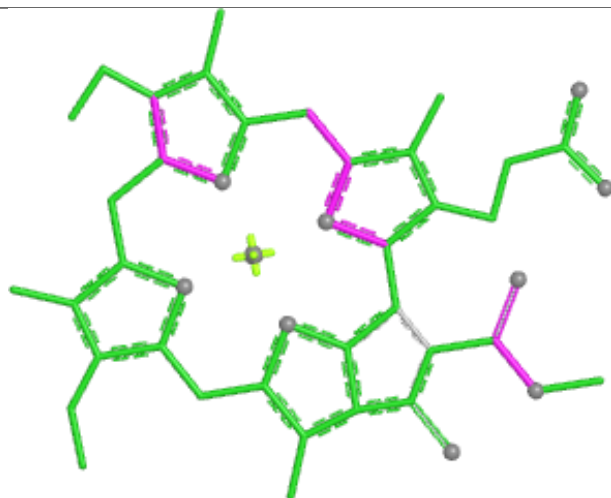


Rings

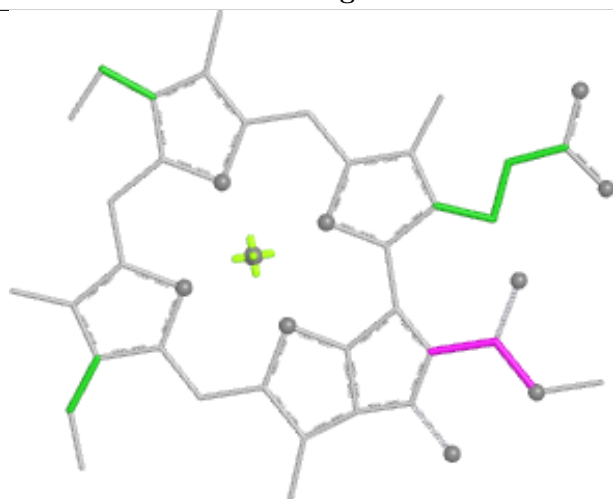
Ligand CLA O 821



Bond lengths



Bond angles

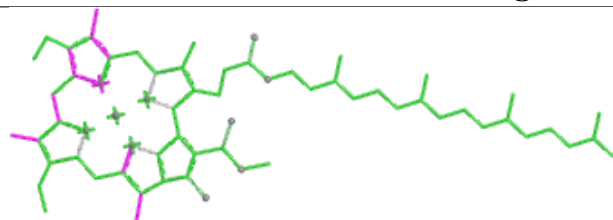


Torsions

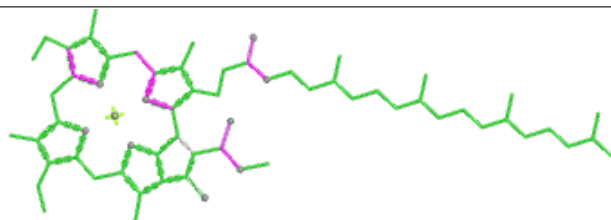


Rings

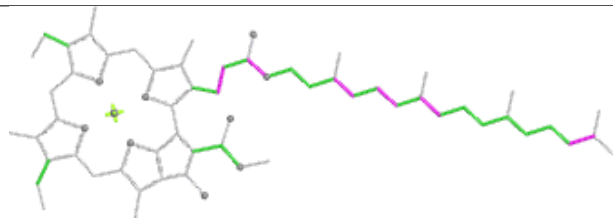
Ligand CLA N 814



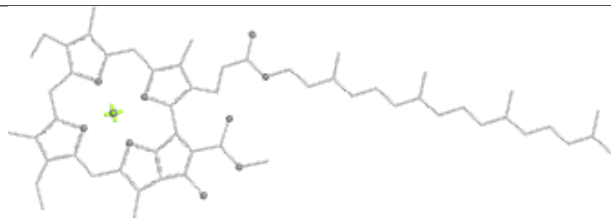
Bond lengths



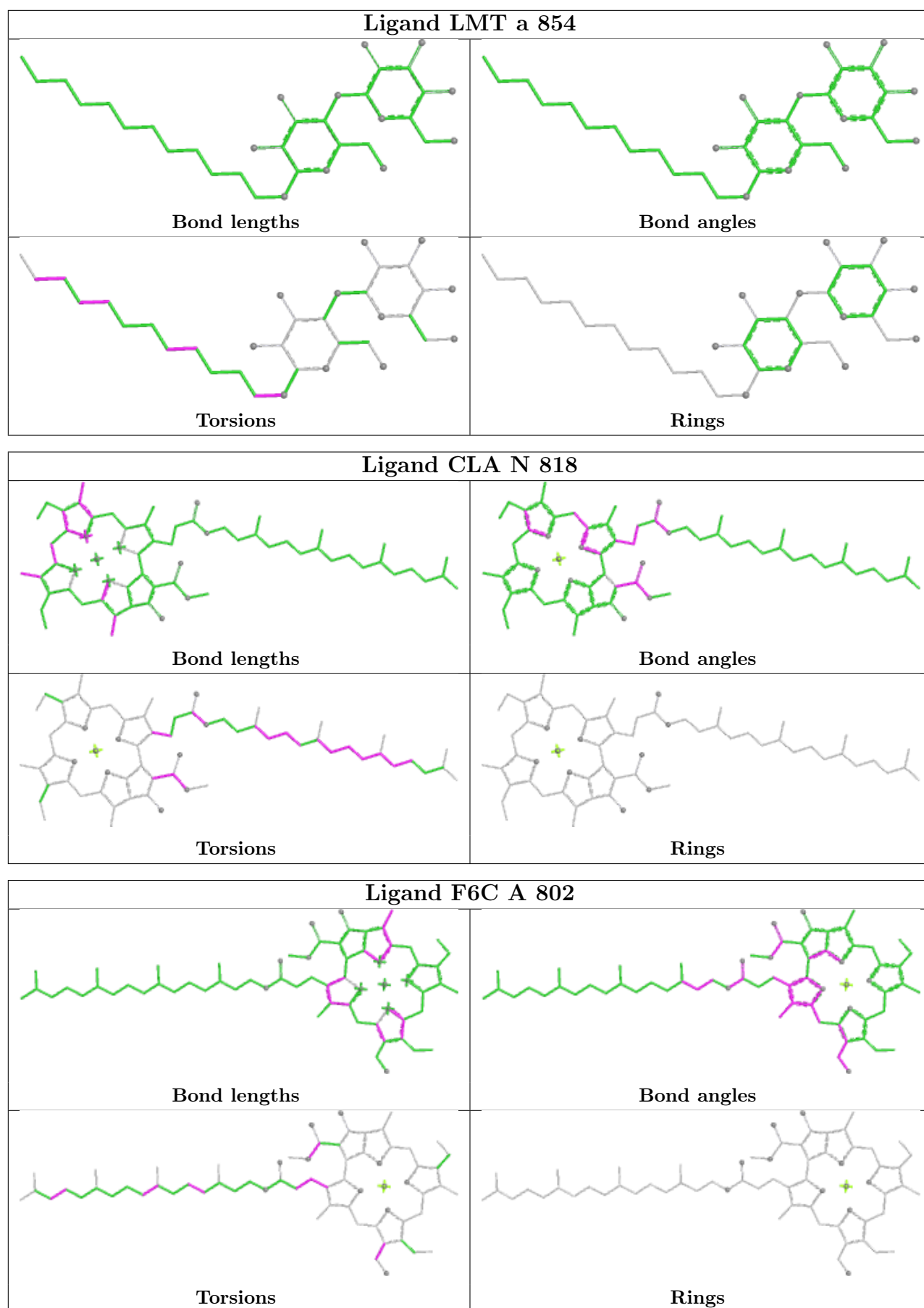
Bond angles

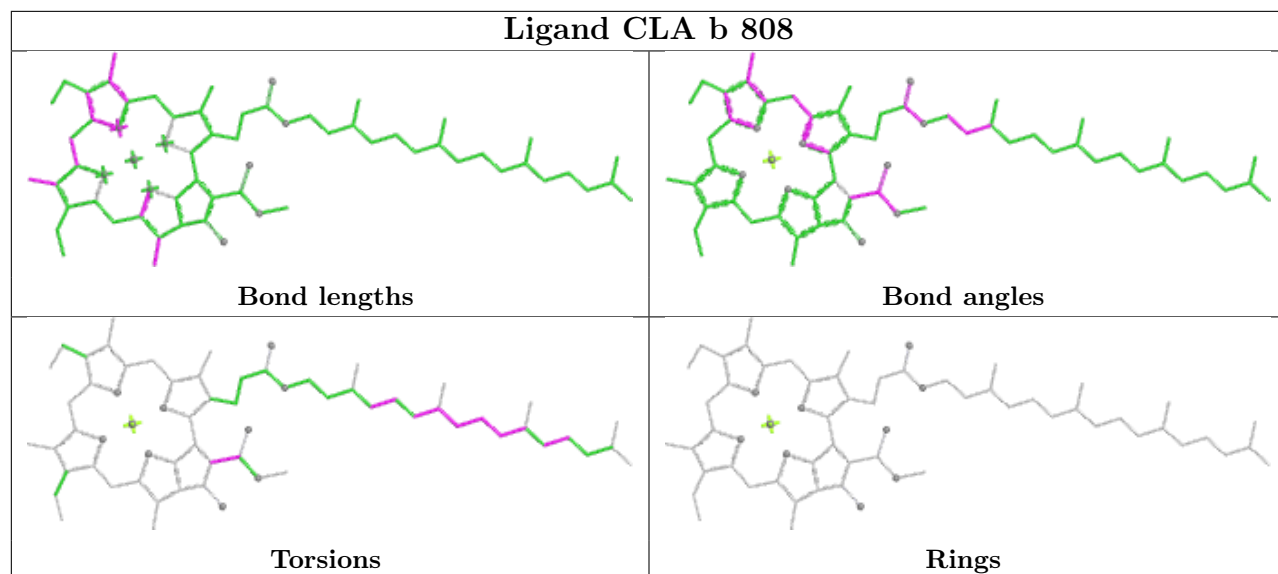
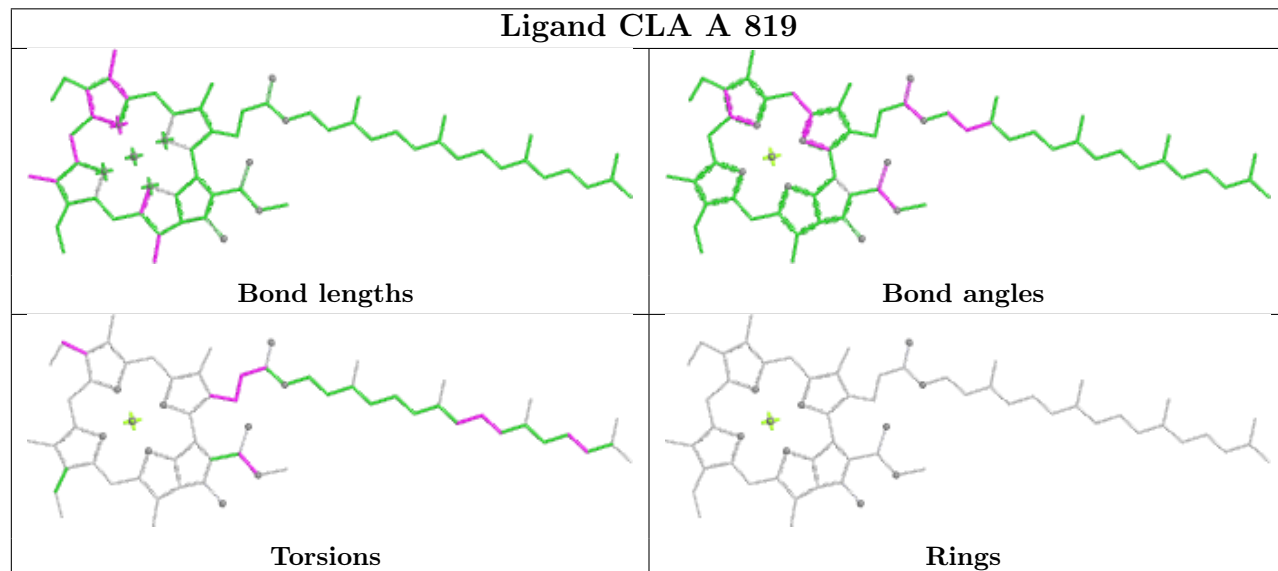


Torsions

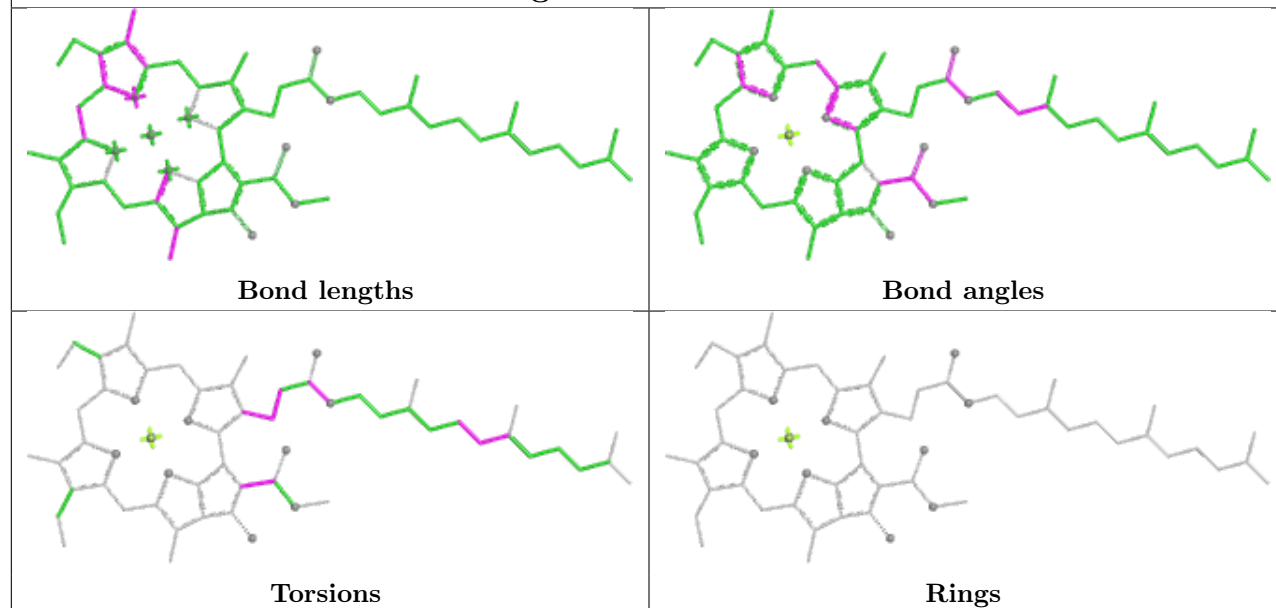


Rings

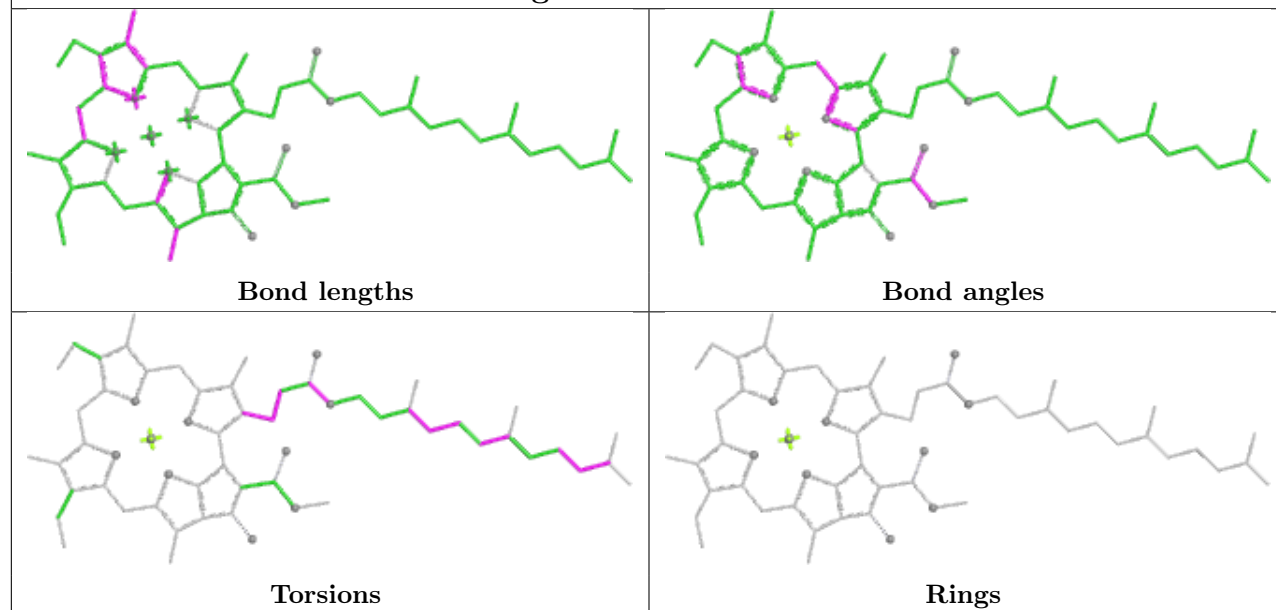


Ligand CLA b 808**Ligand CLA A 819**

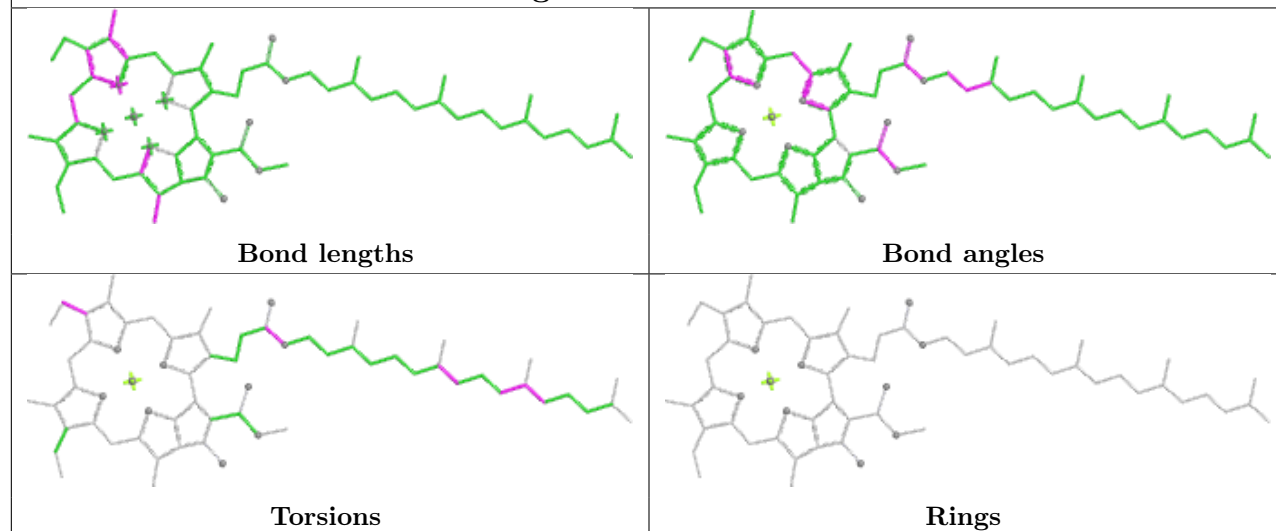
Ligand CLA A 809



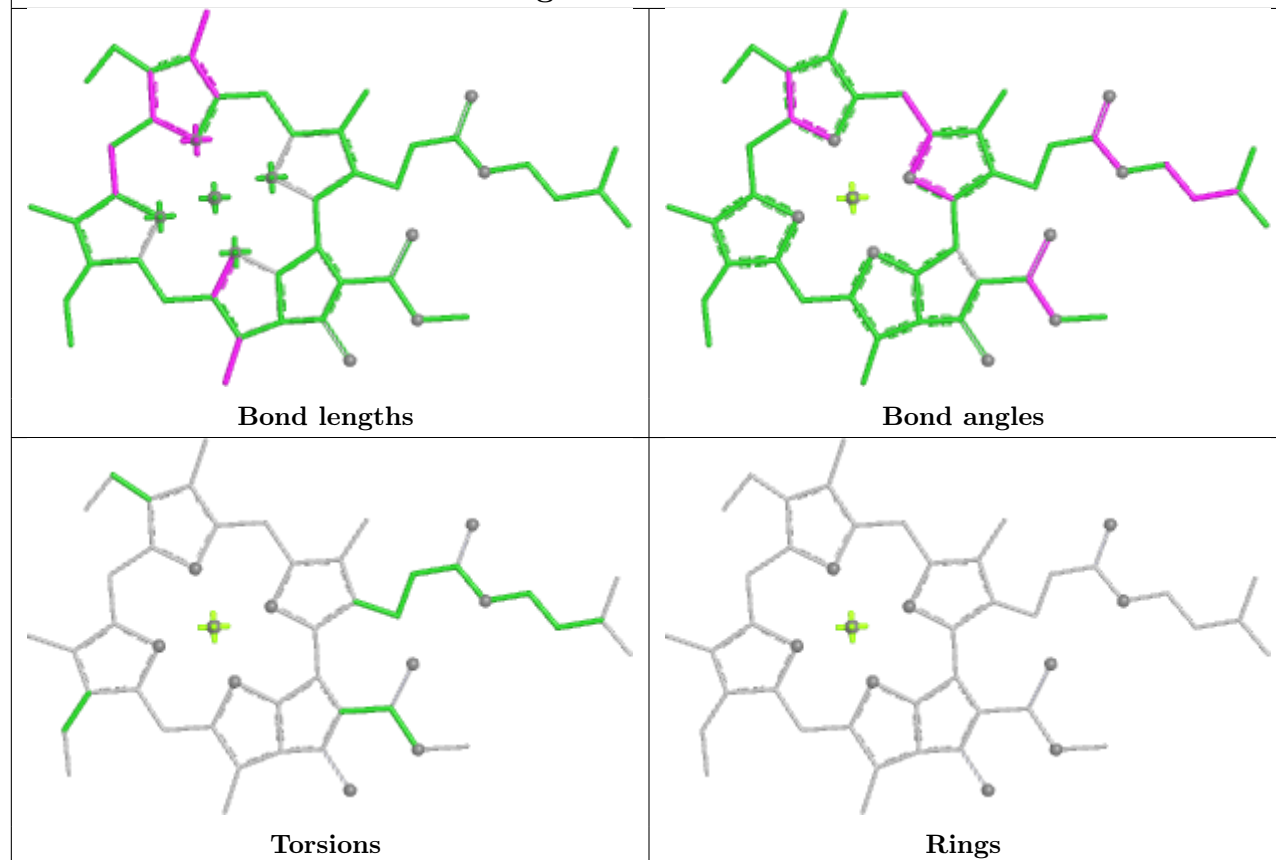
Ligand CLA O 818

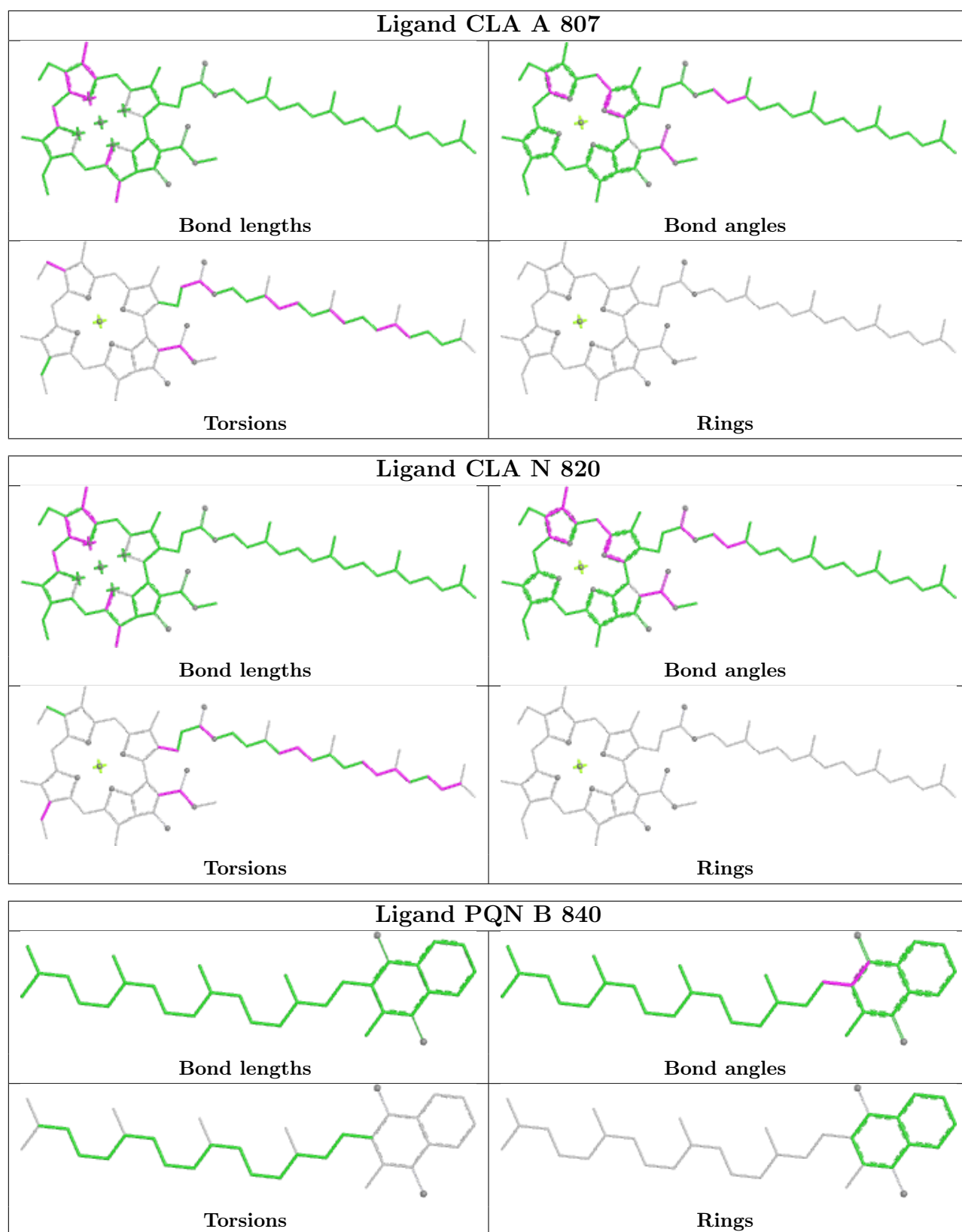


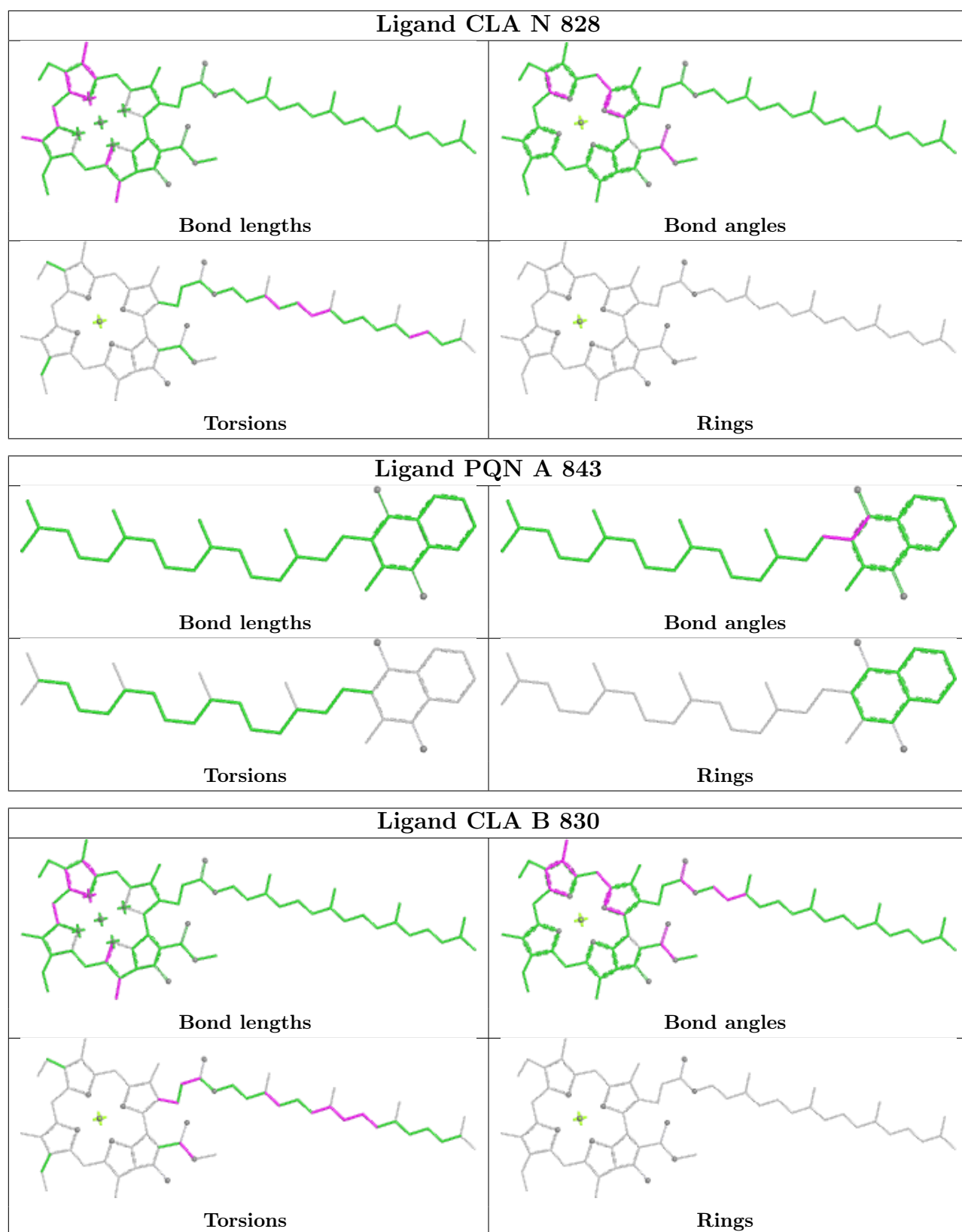
Ligand CLA B 817

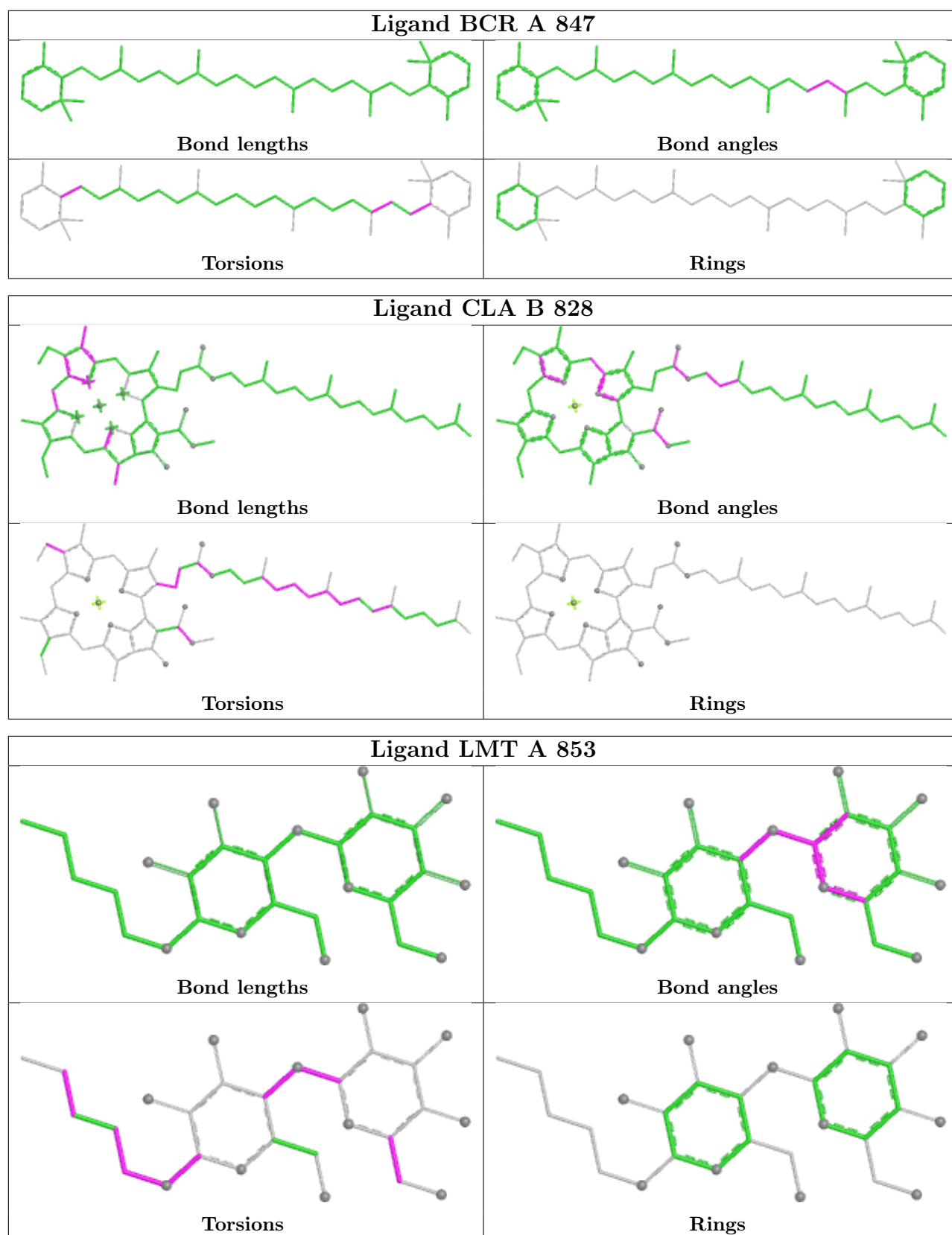


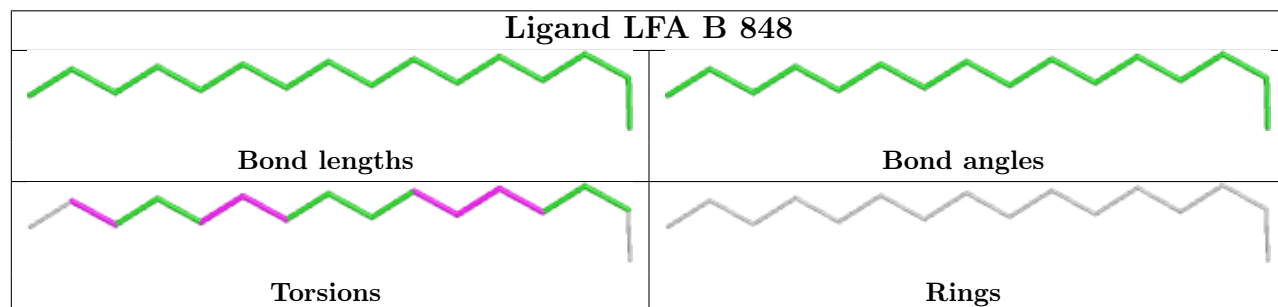
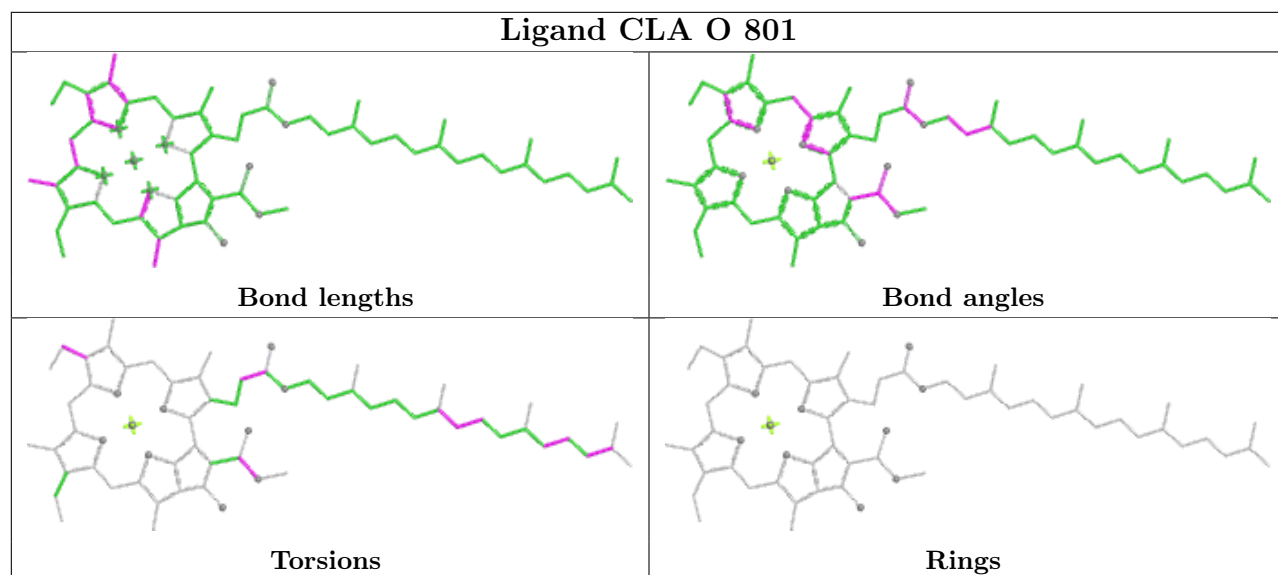
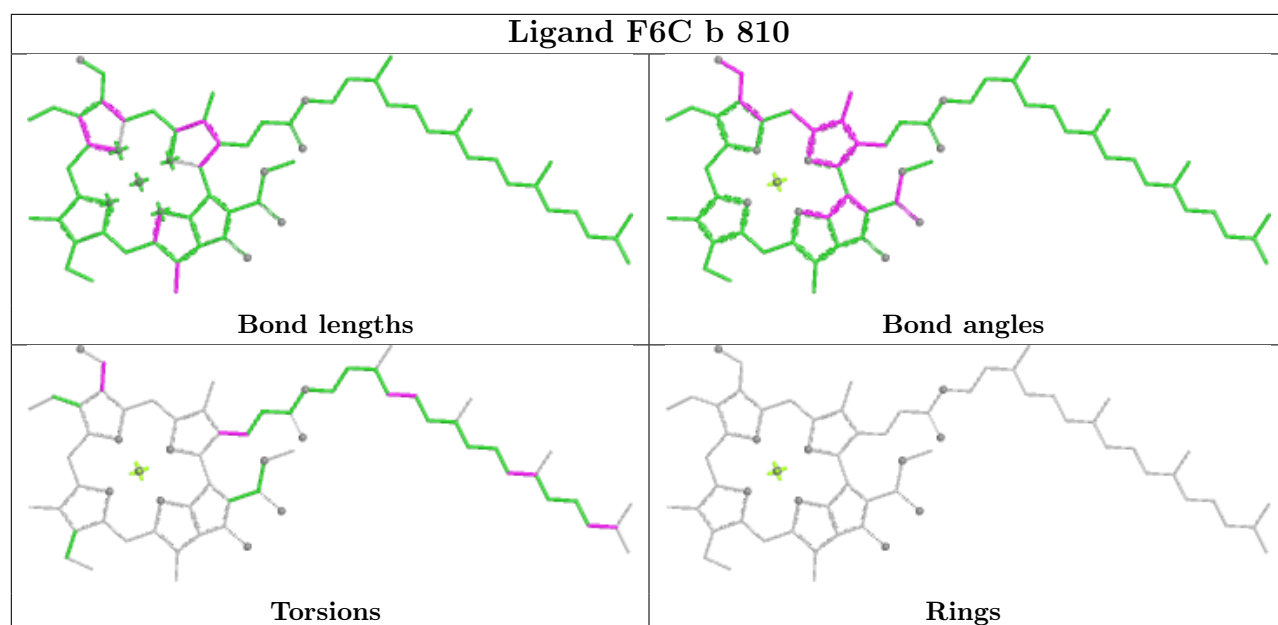
Ligand CLA a 840

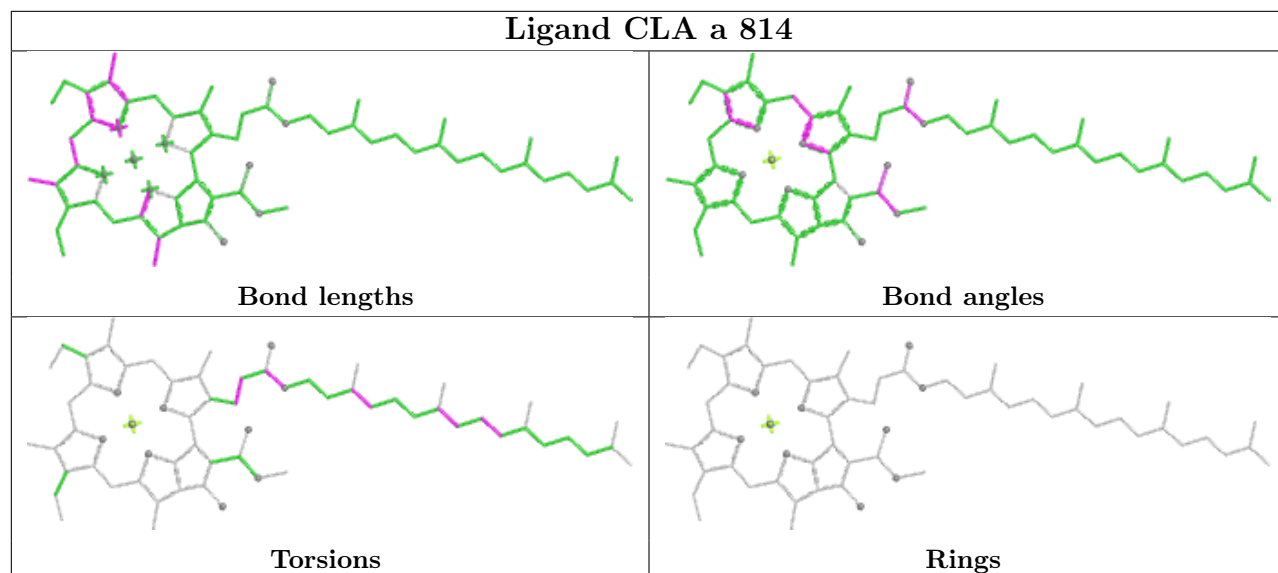
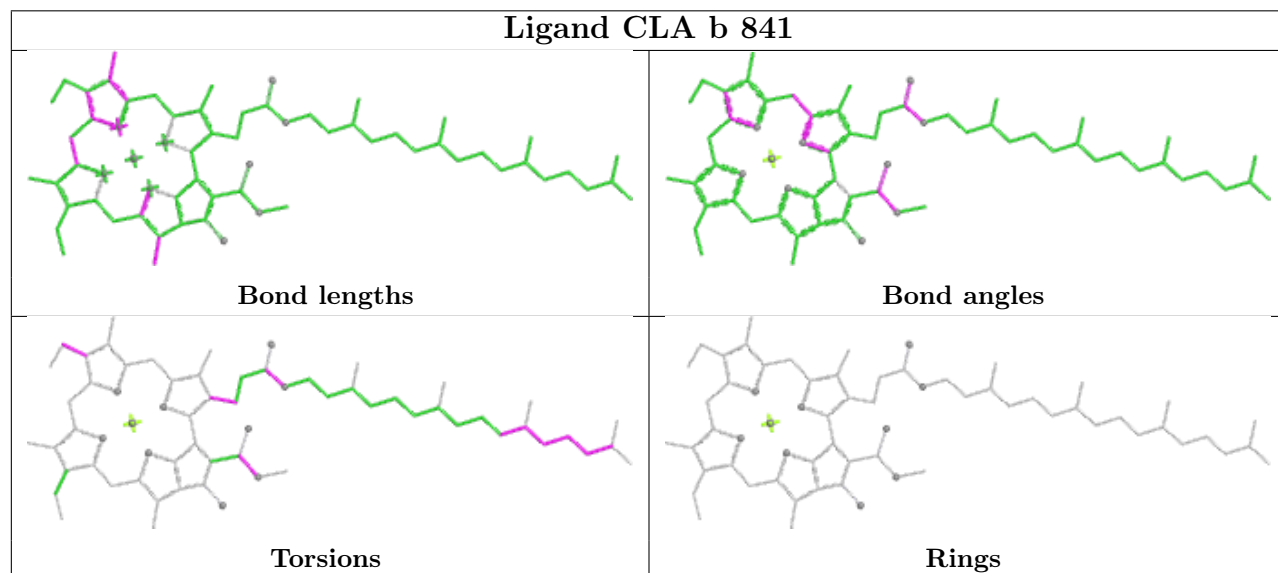
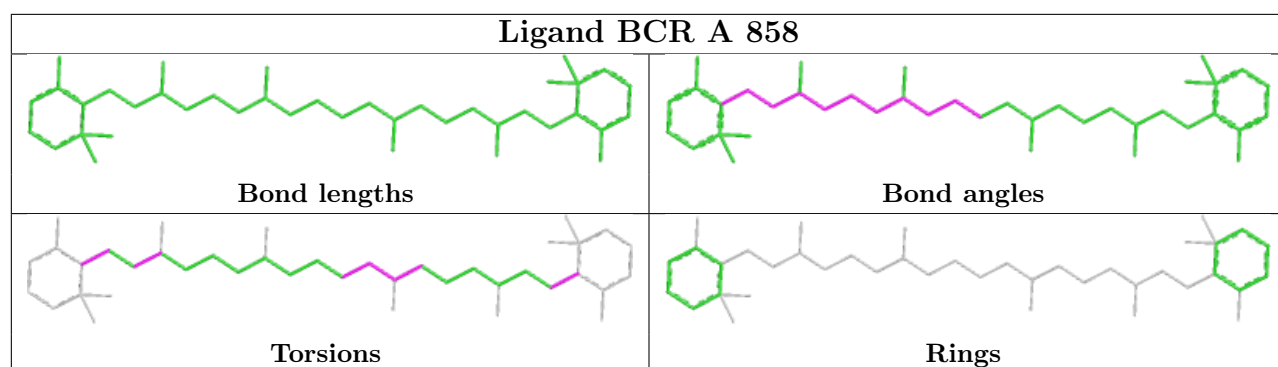


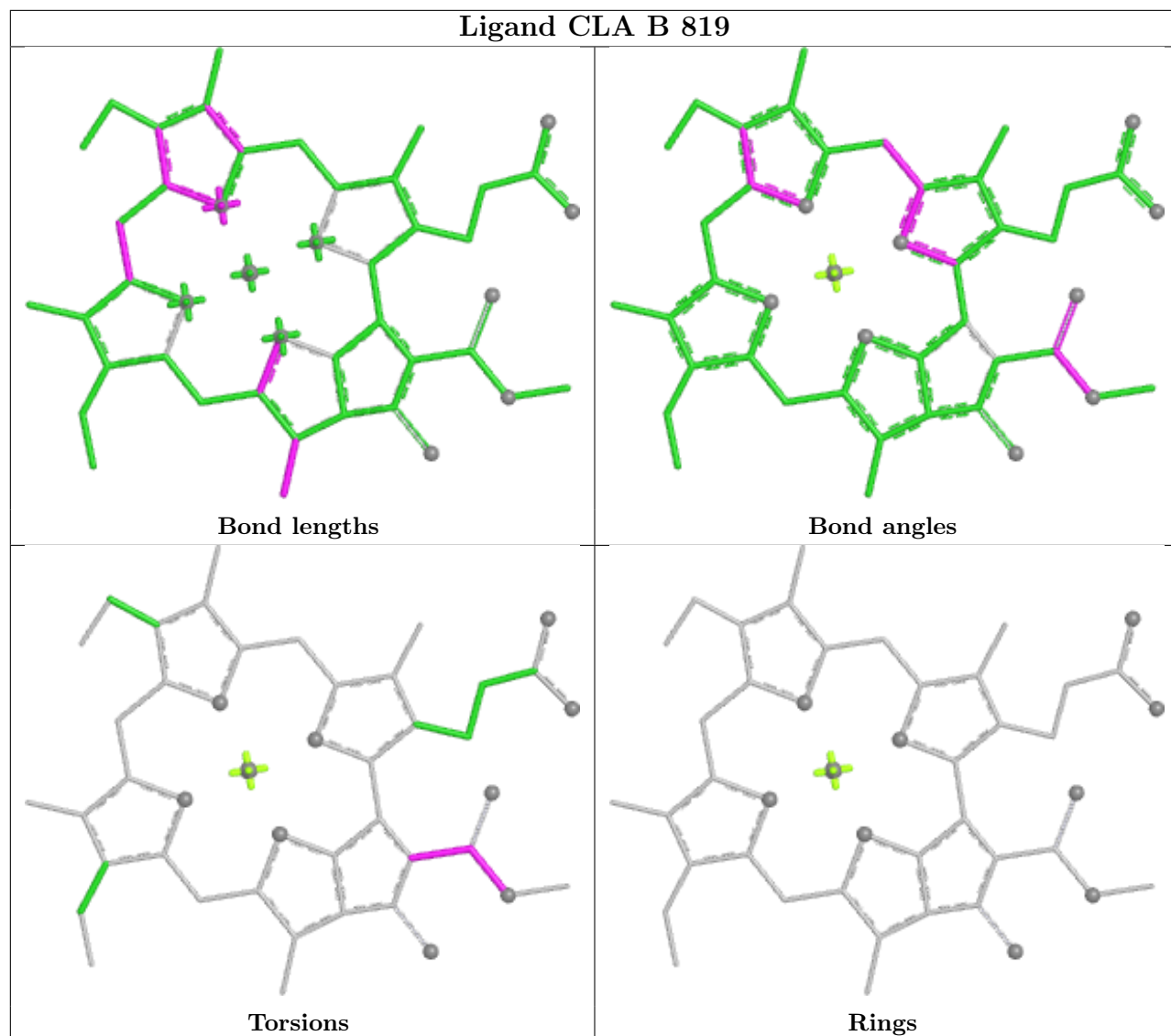


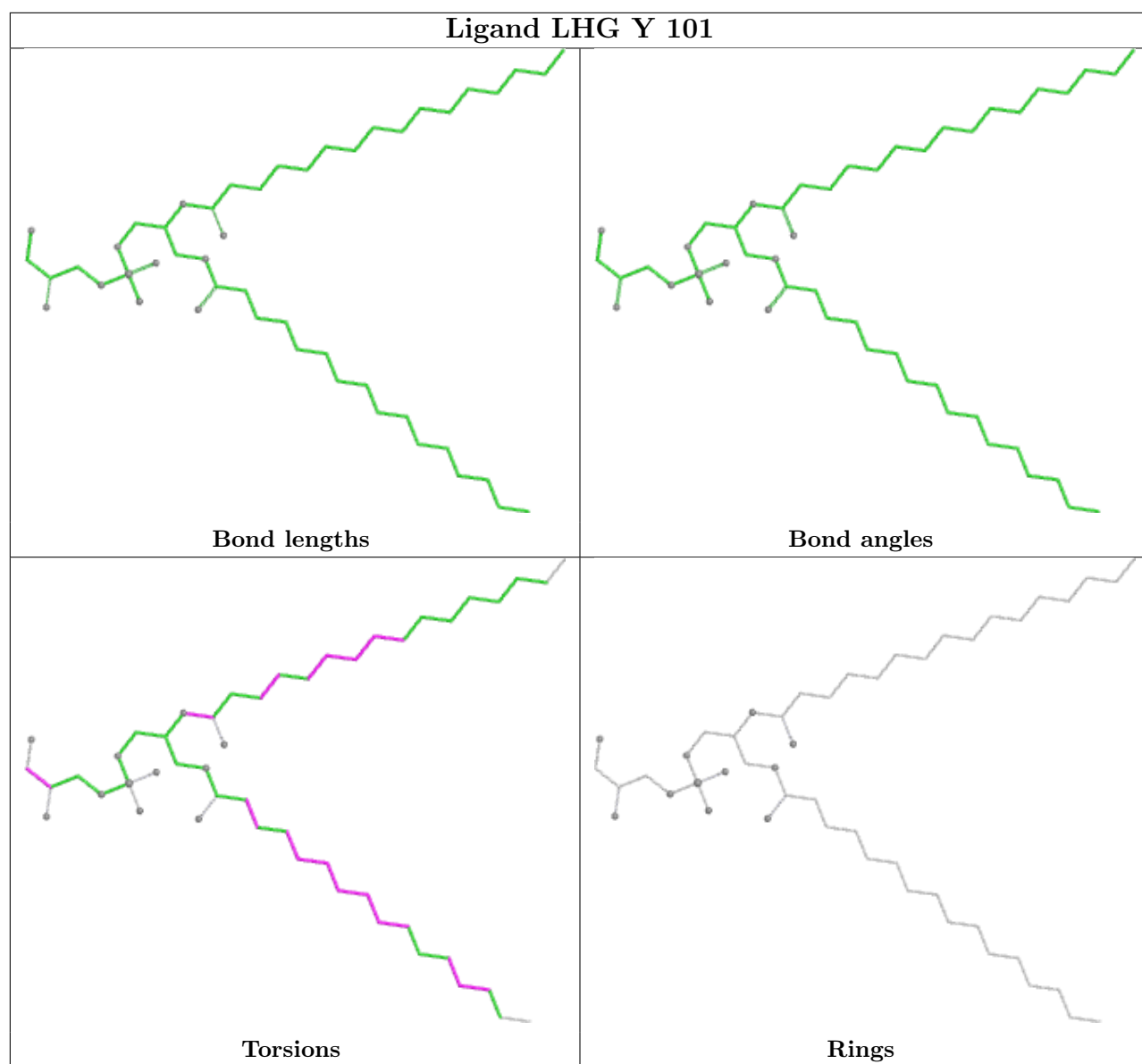




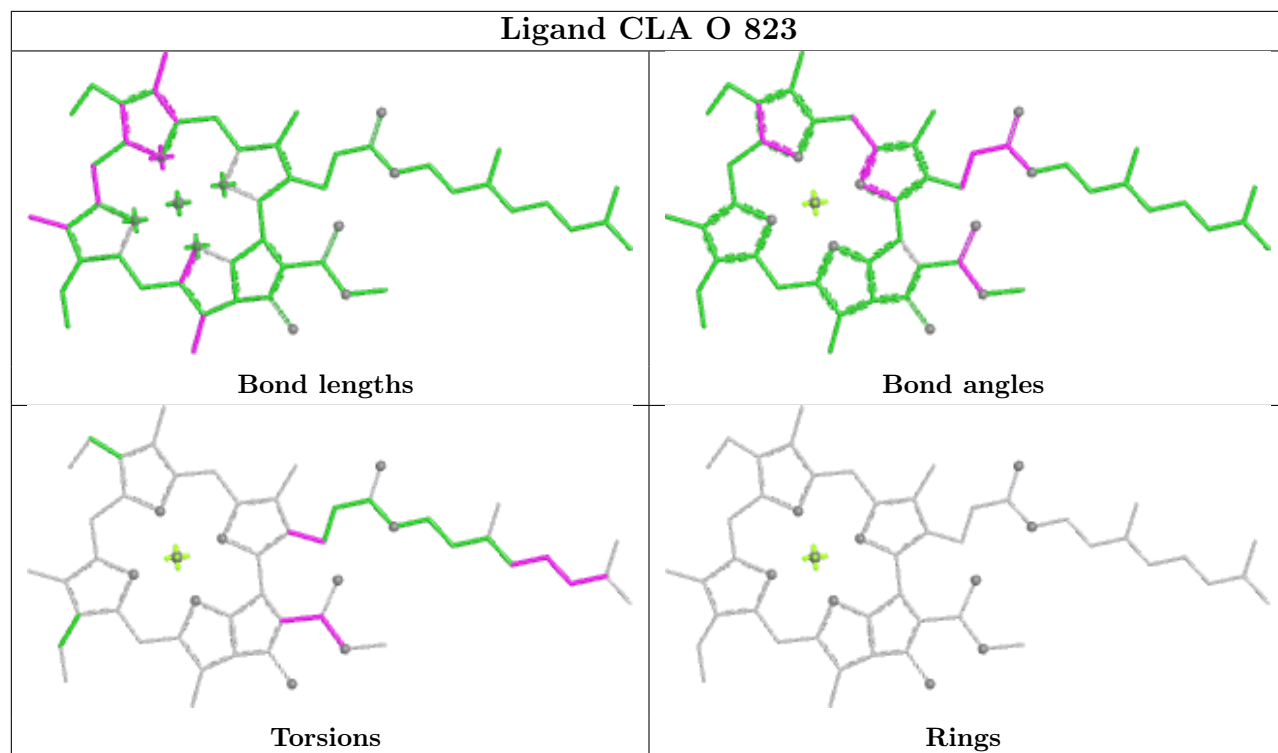




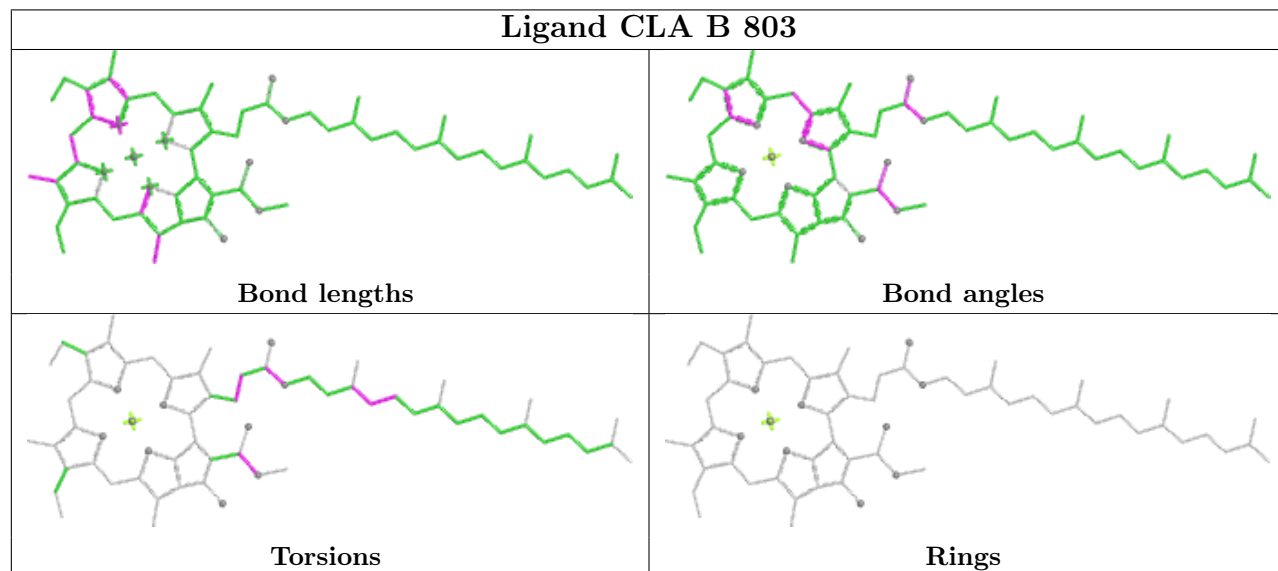


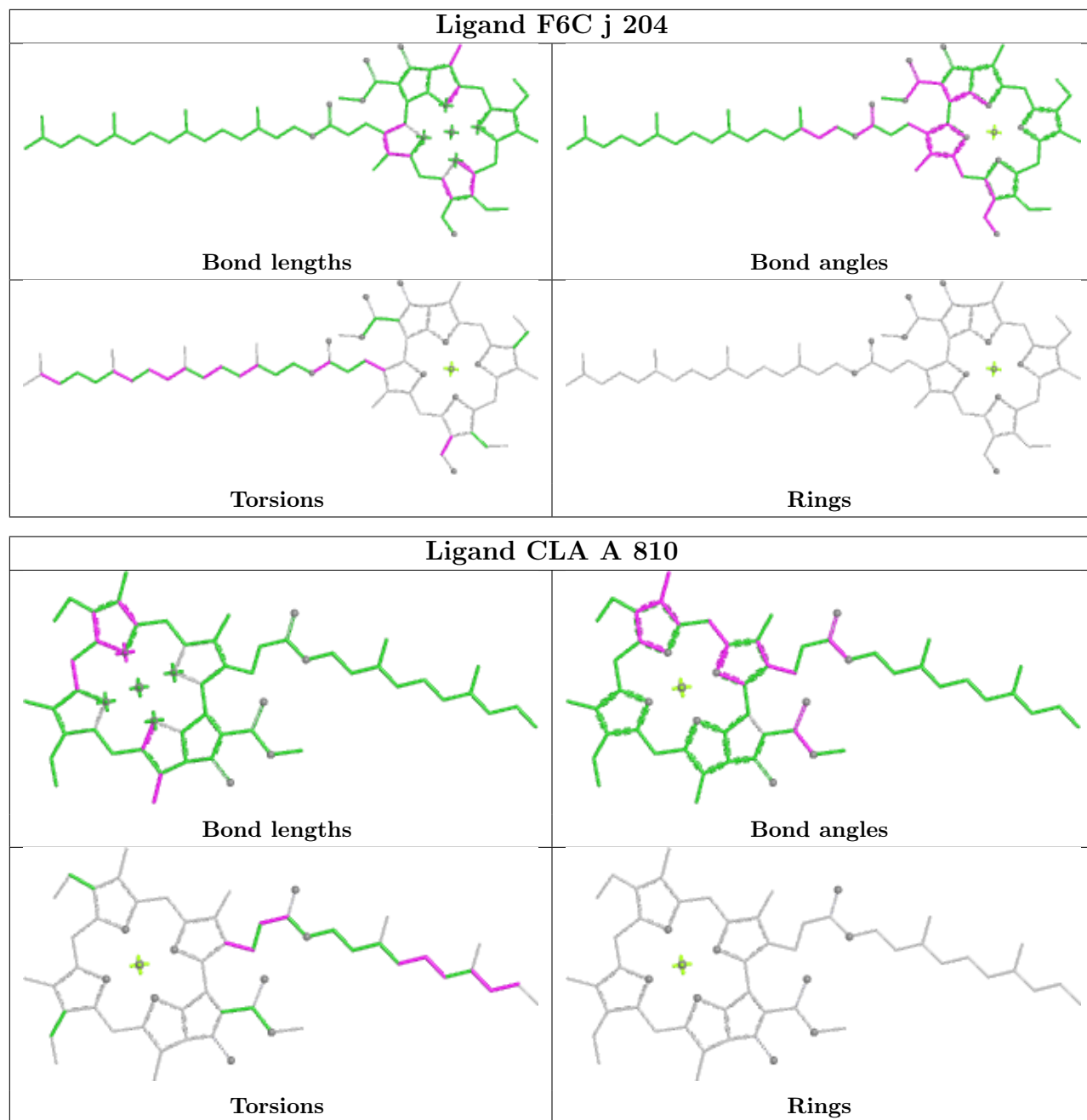


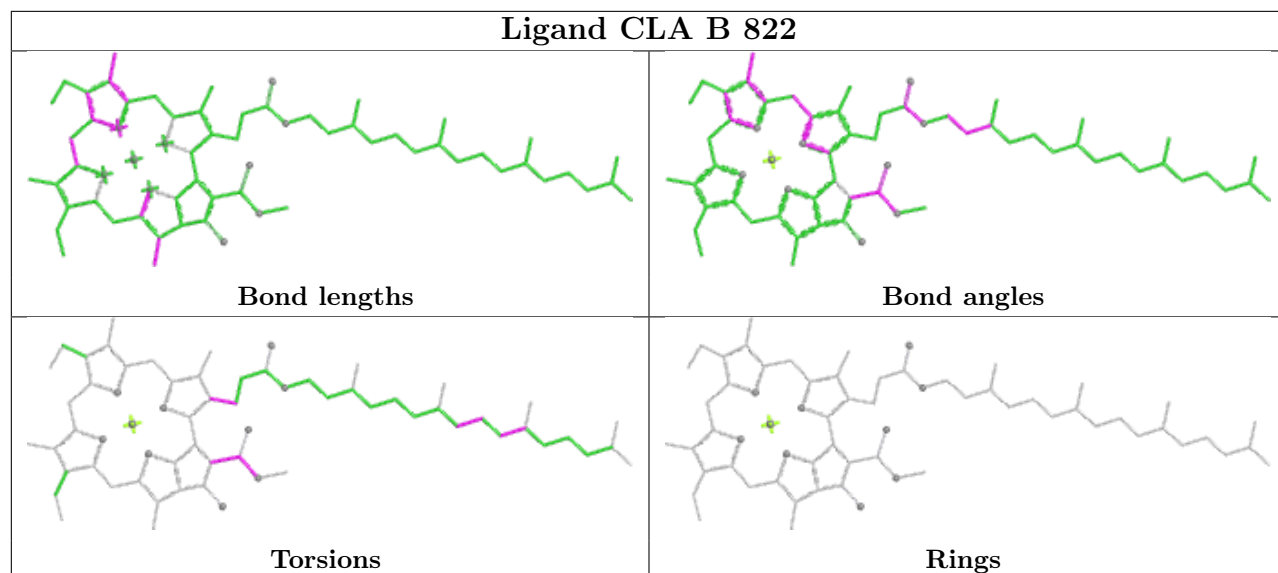
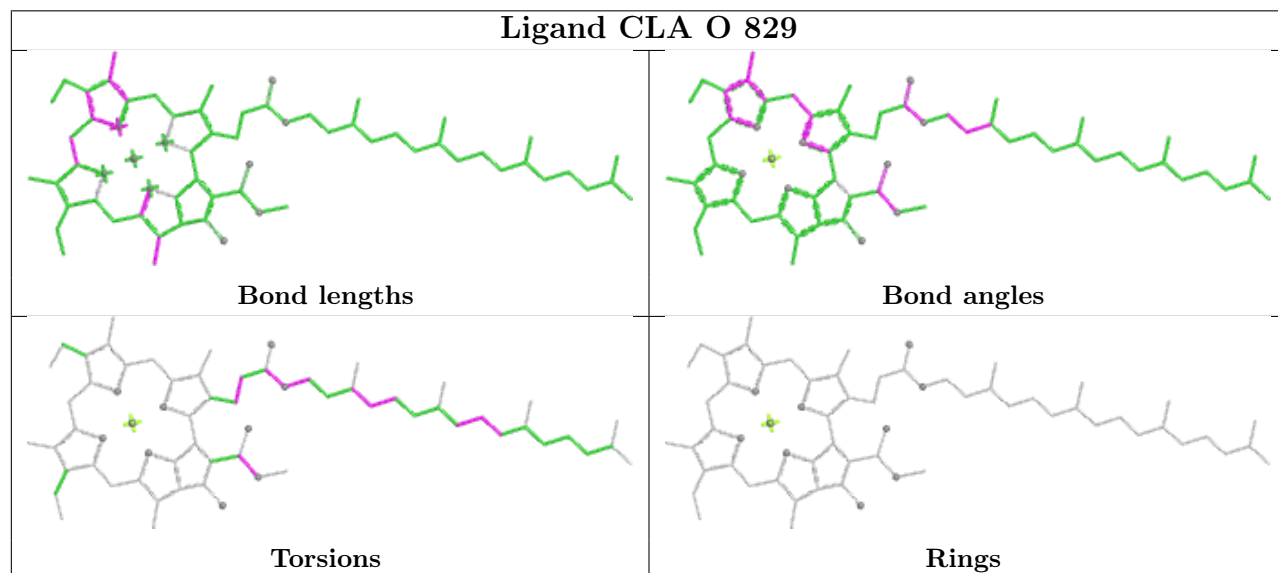
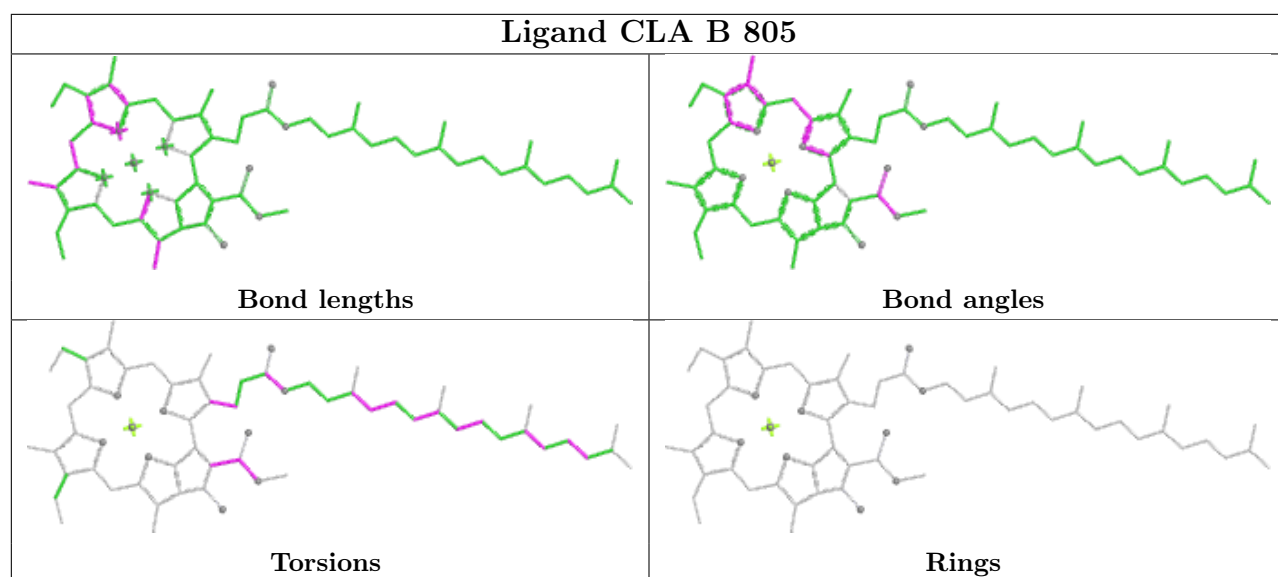
Ligand CLA O 823

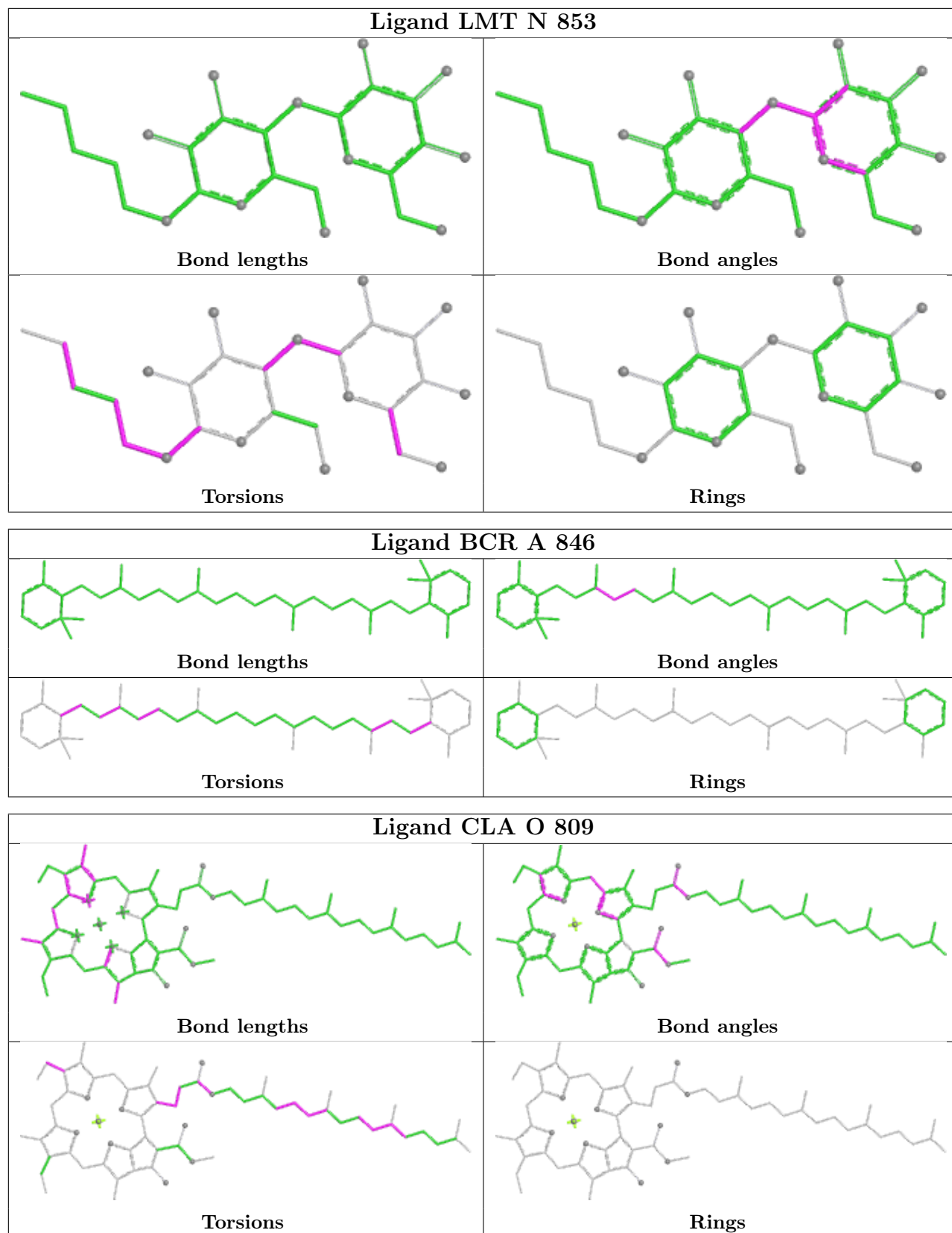


Ligand CLA B 803

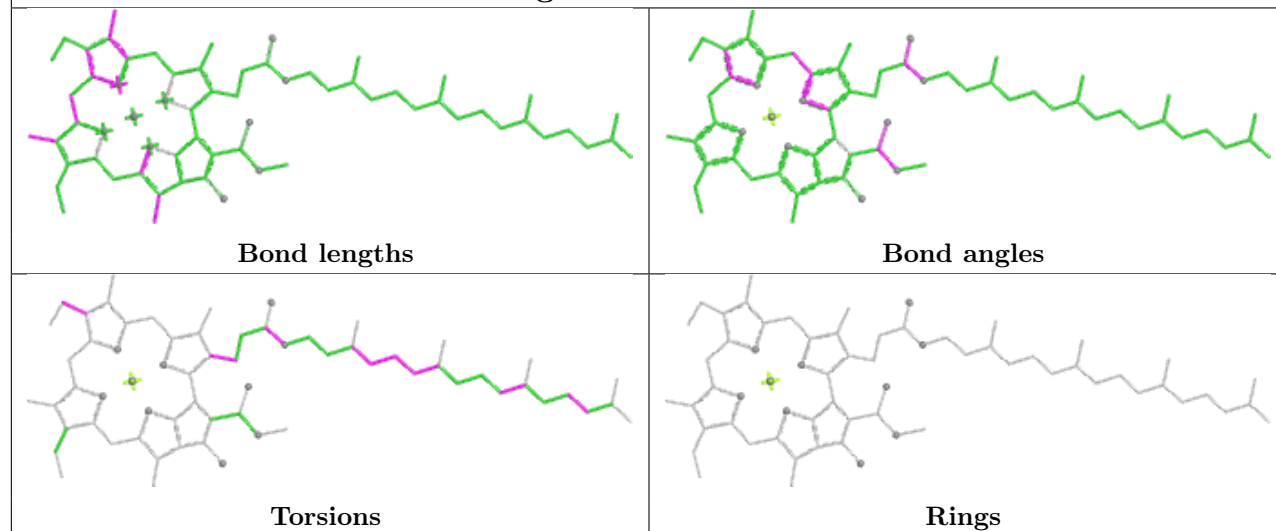




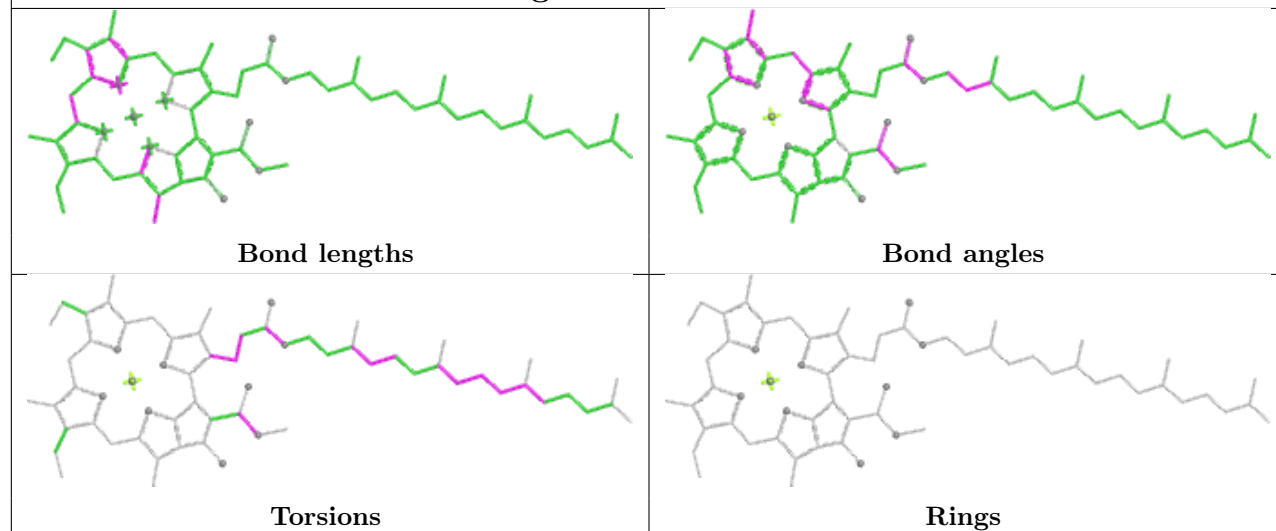




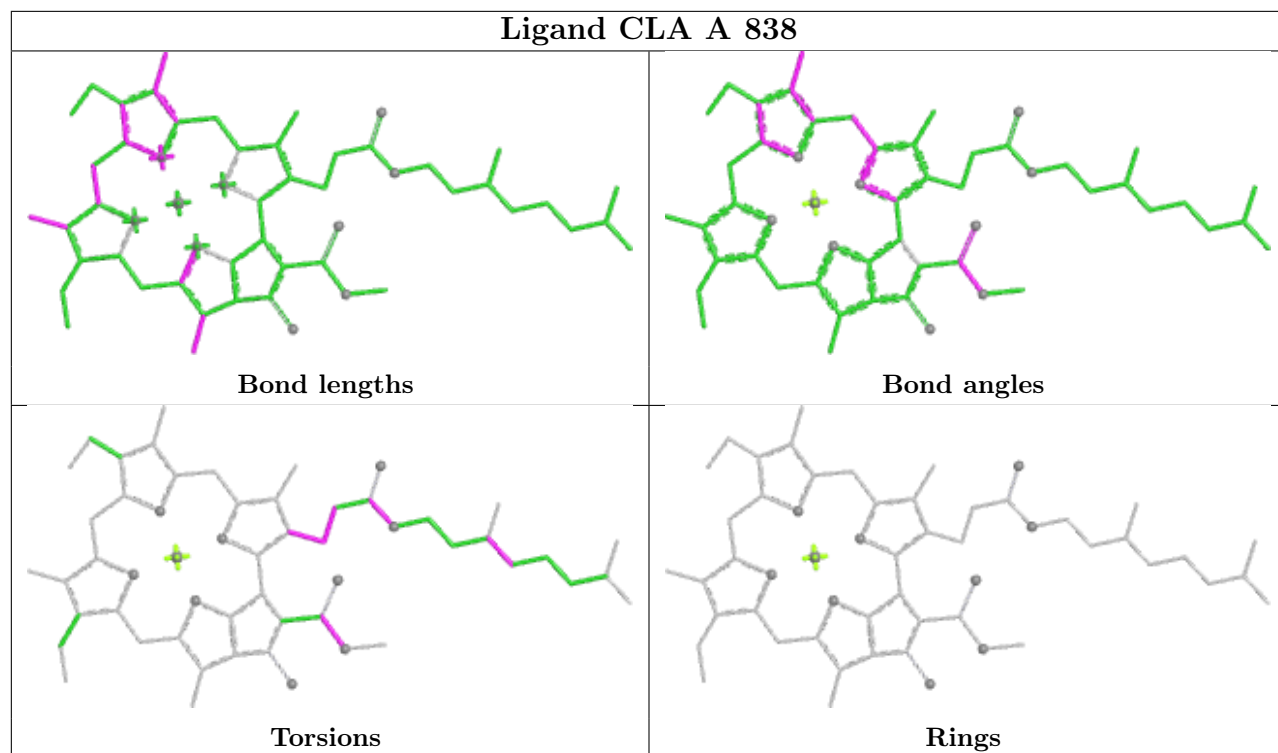
Ligand CLA a 841



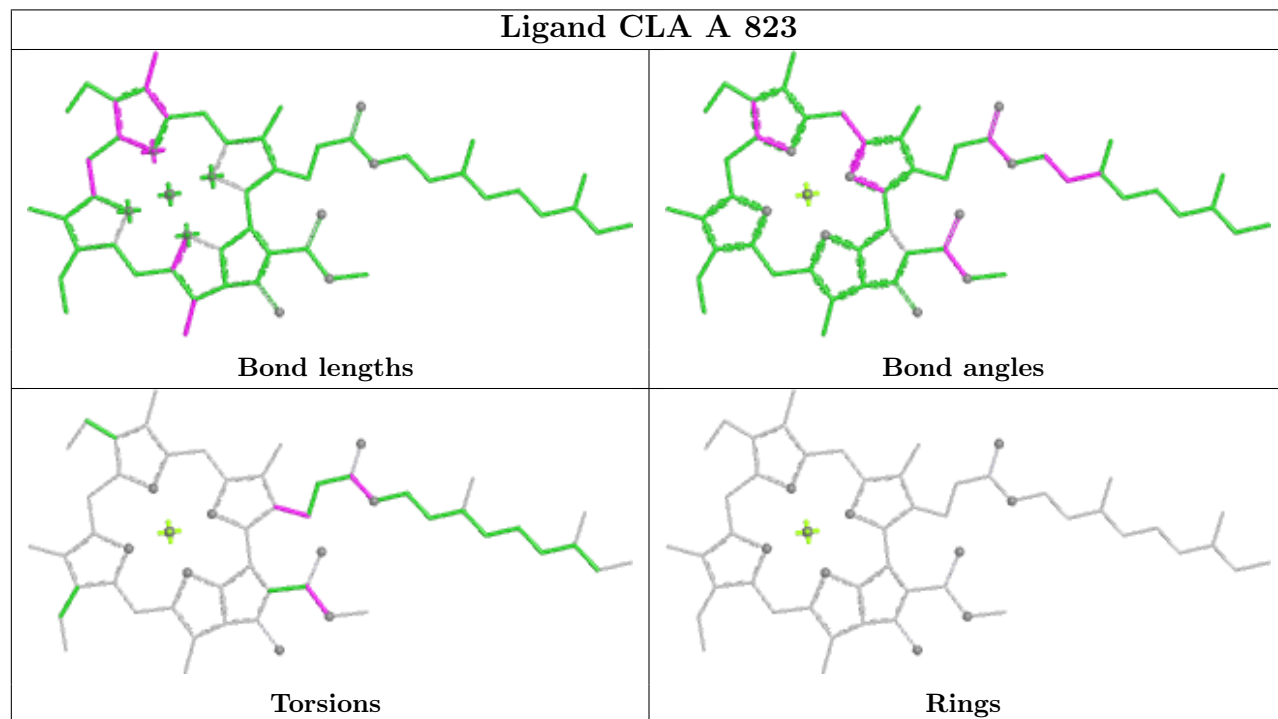
Ligand CLA O 831

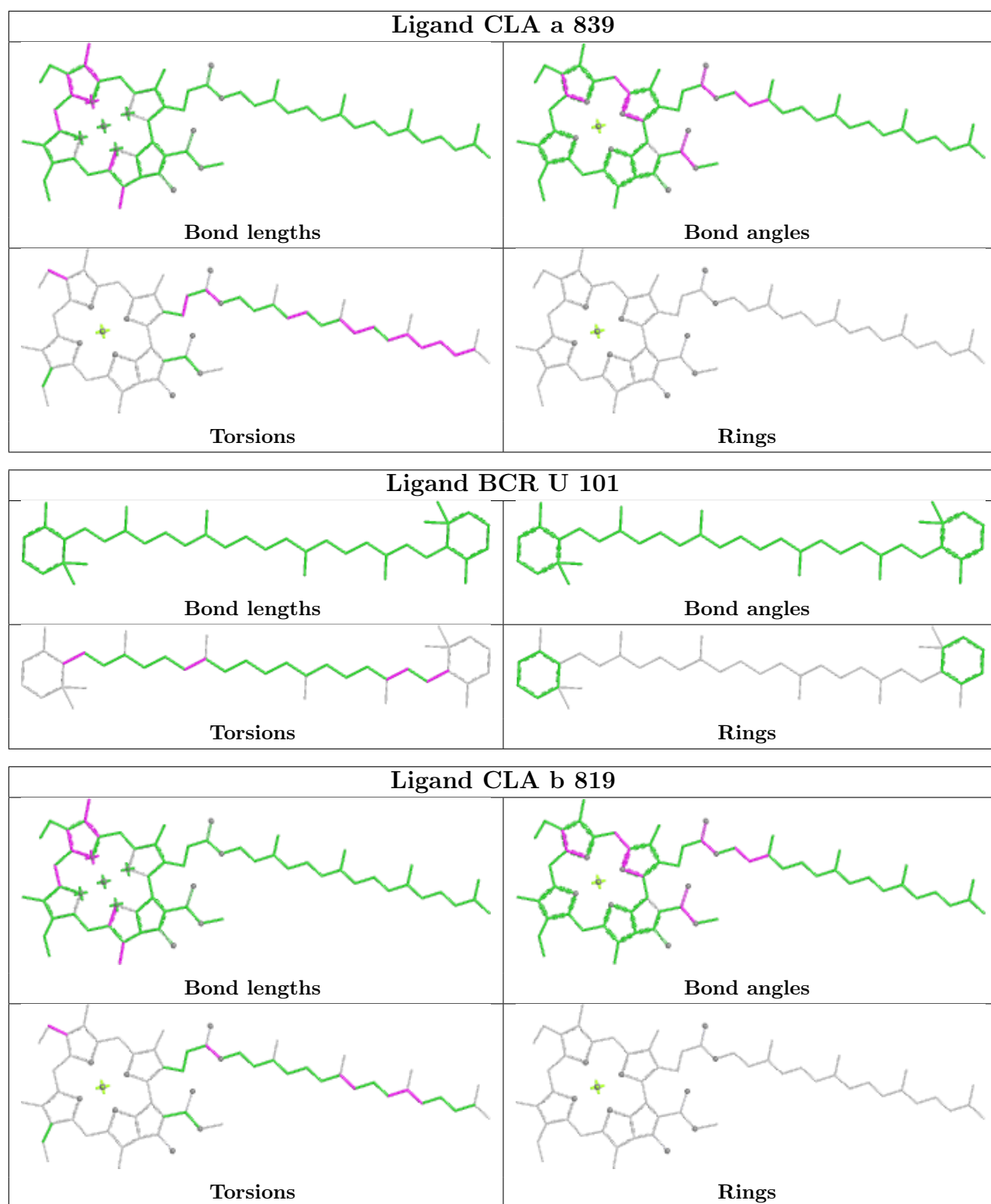


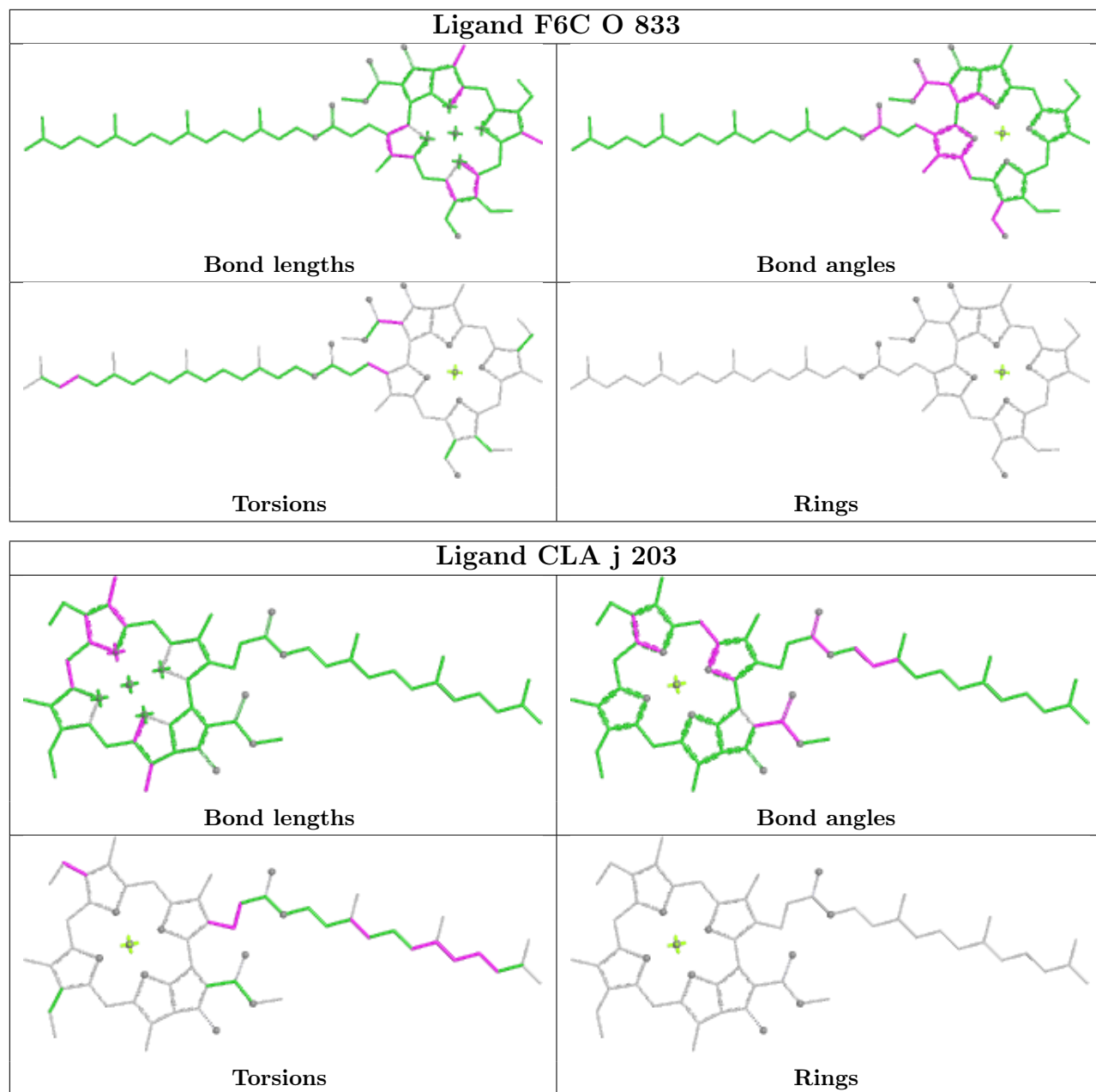
Ligand CLA A 838

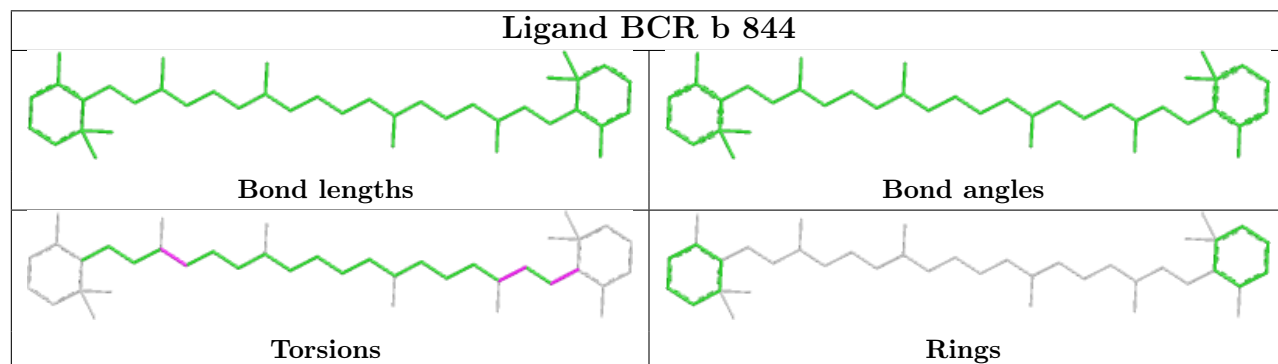
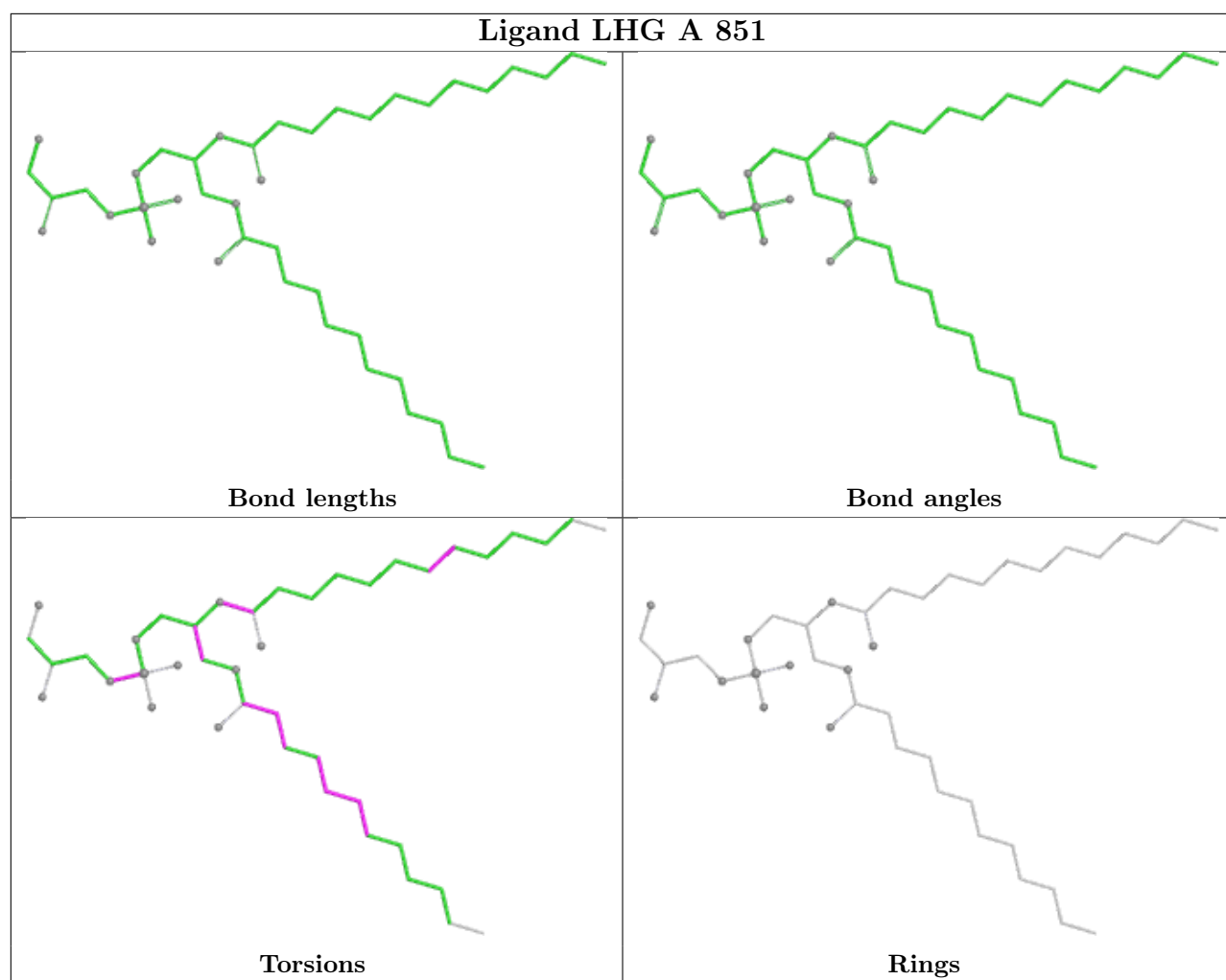


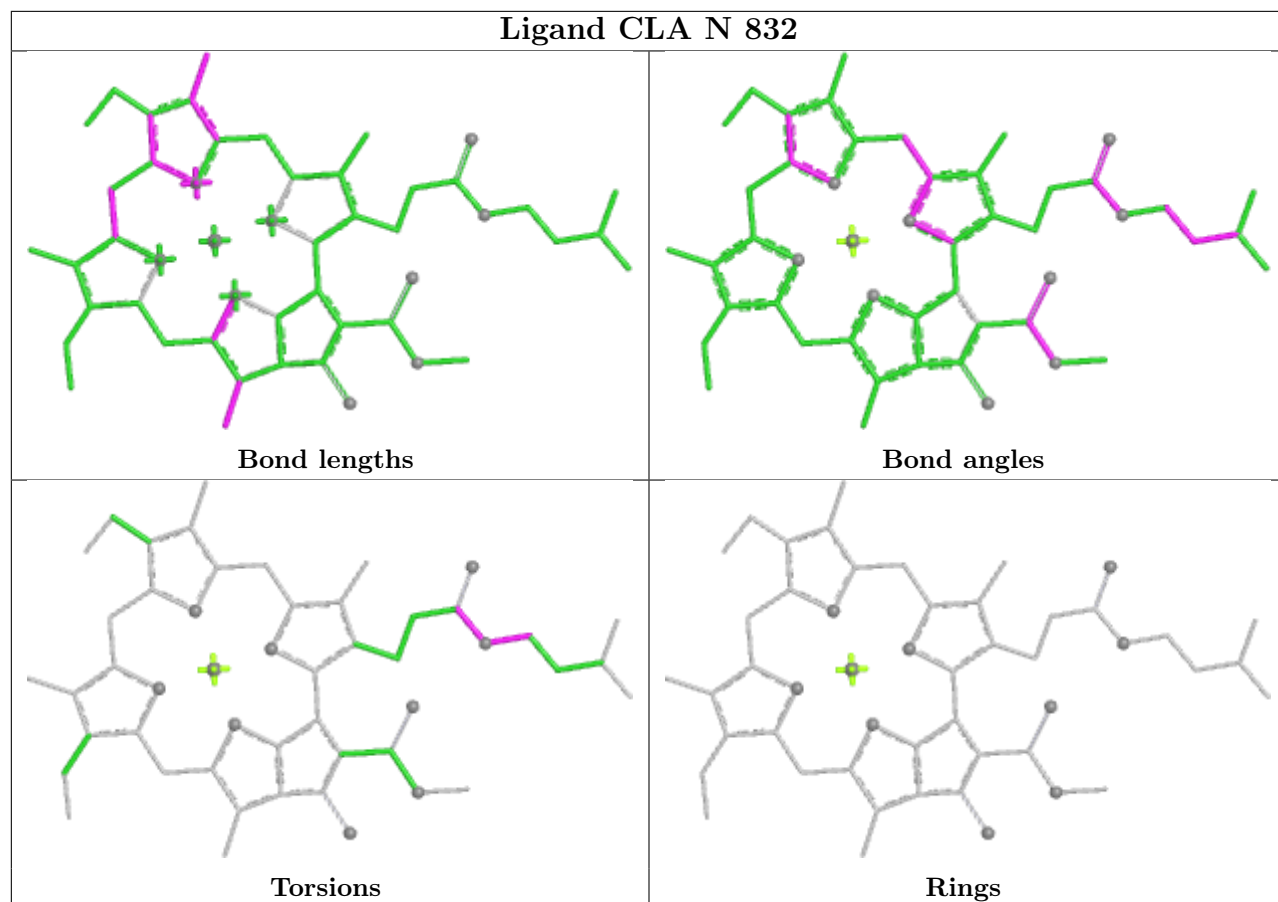
Ligand CLA A 823



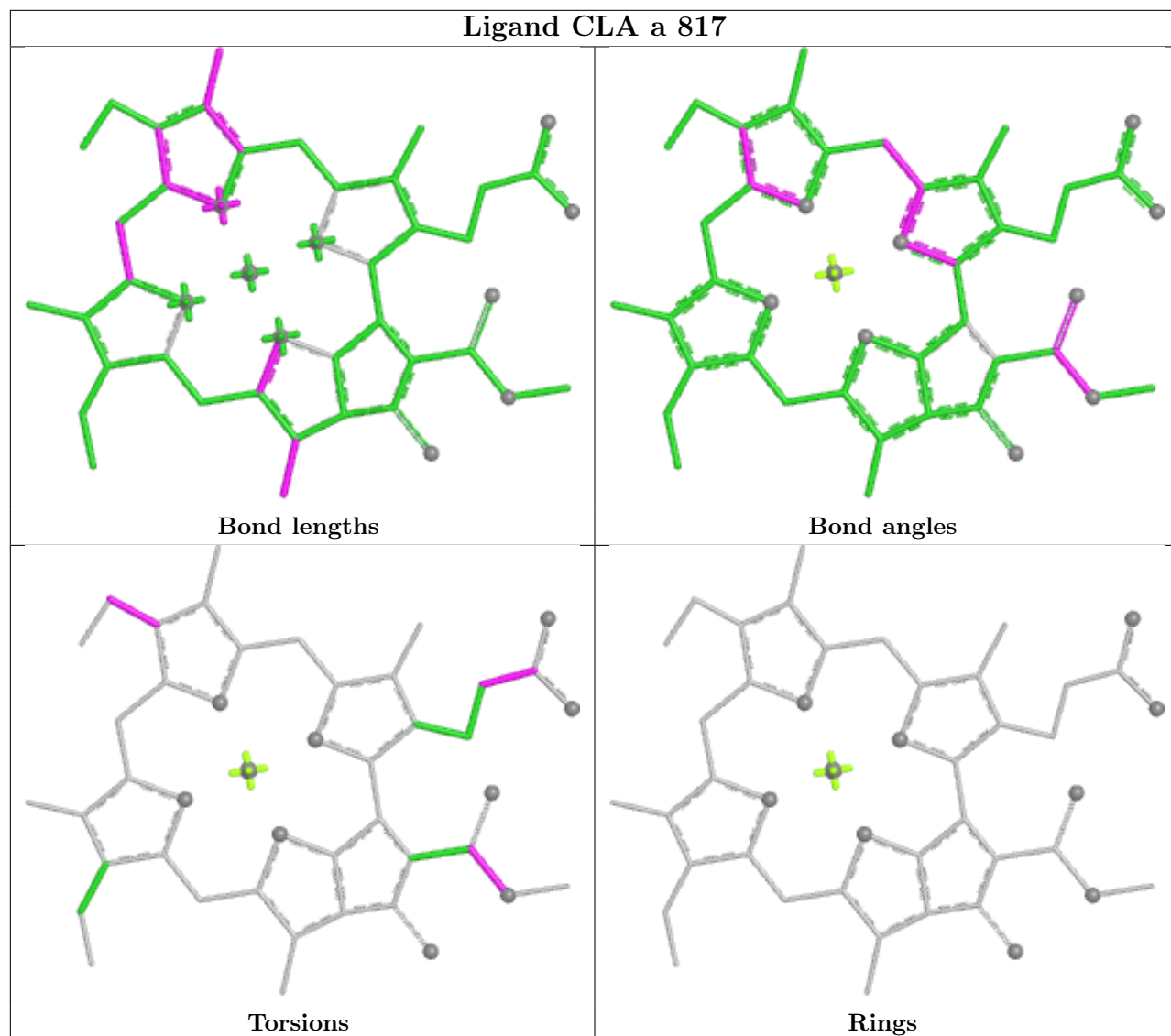




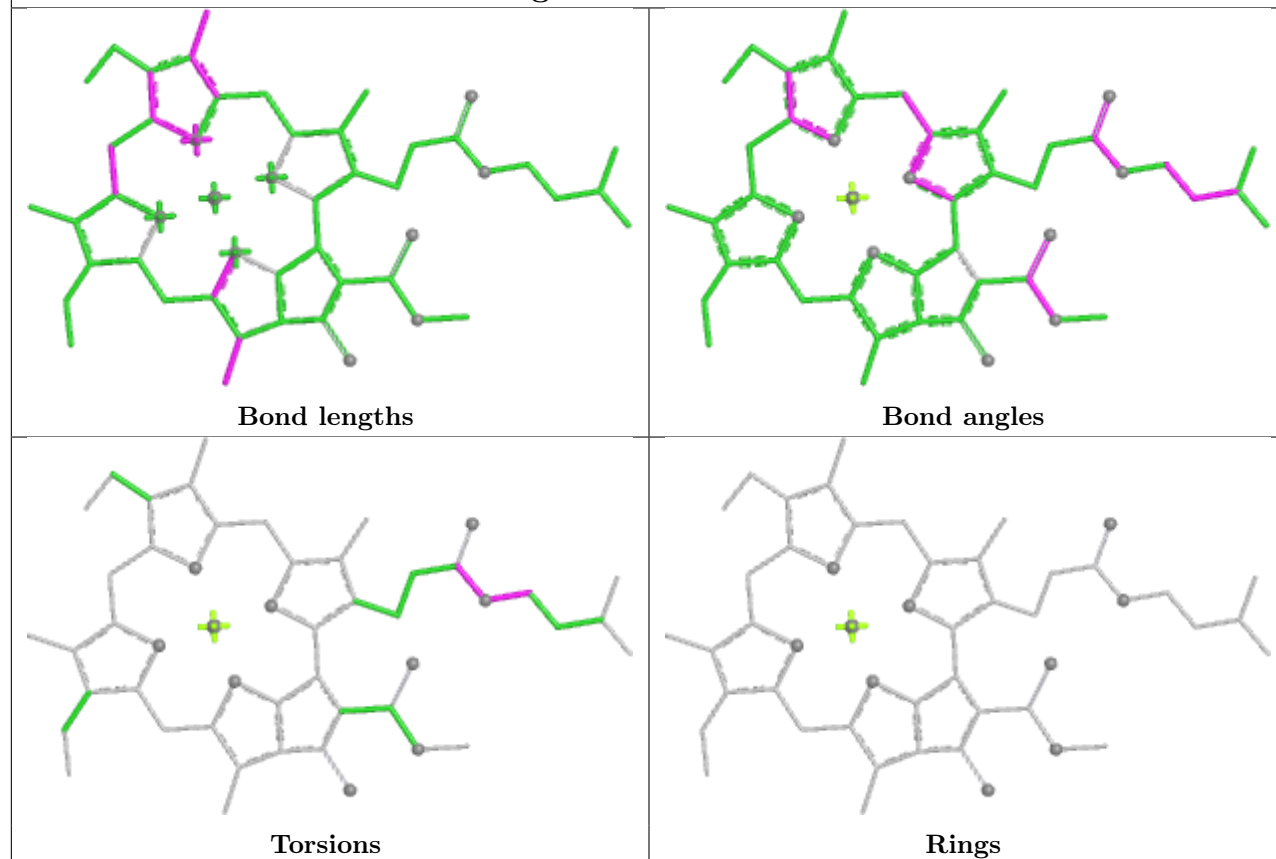




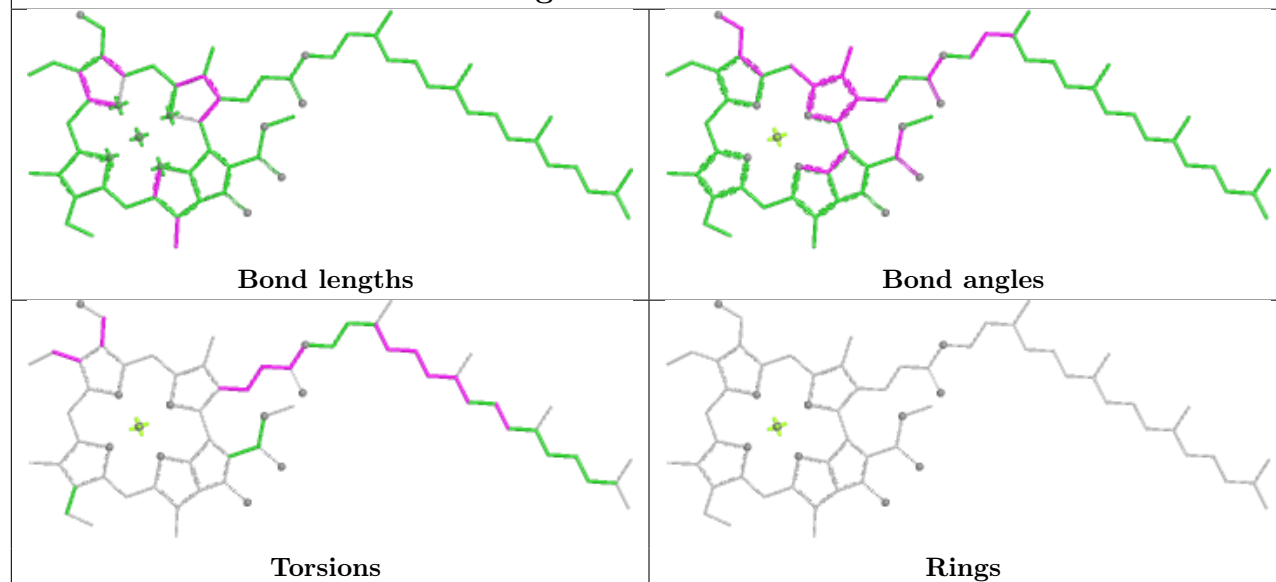
Ligand CLA a 817

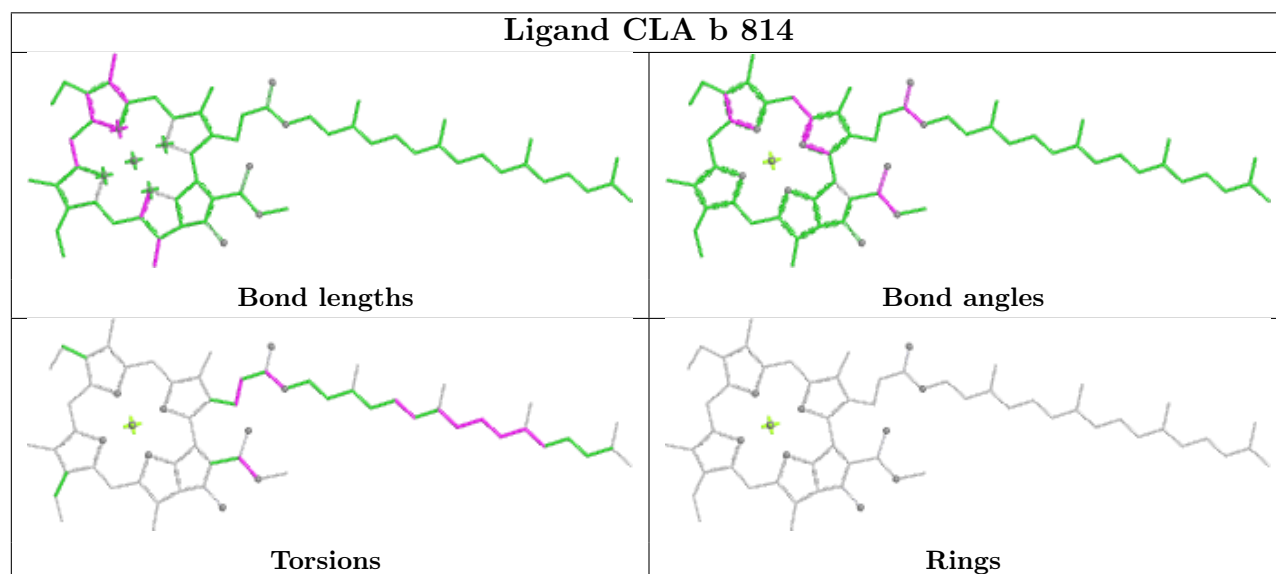
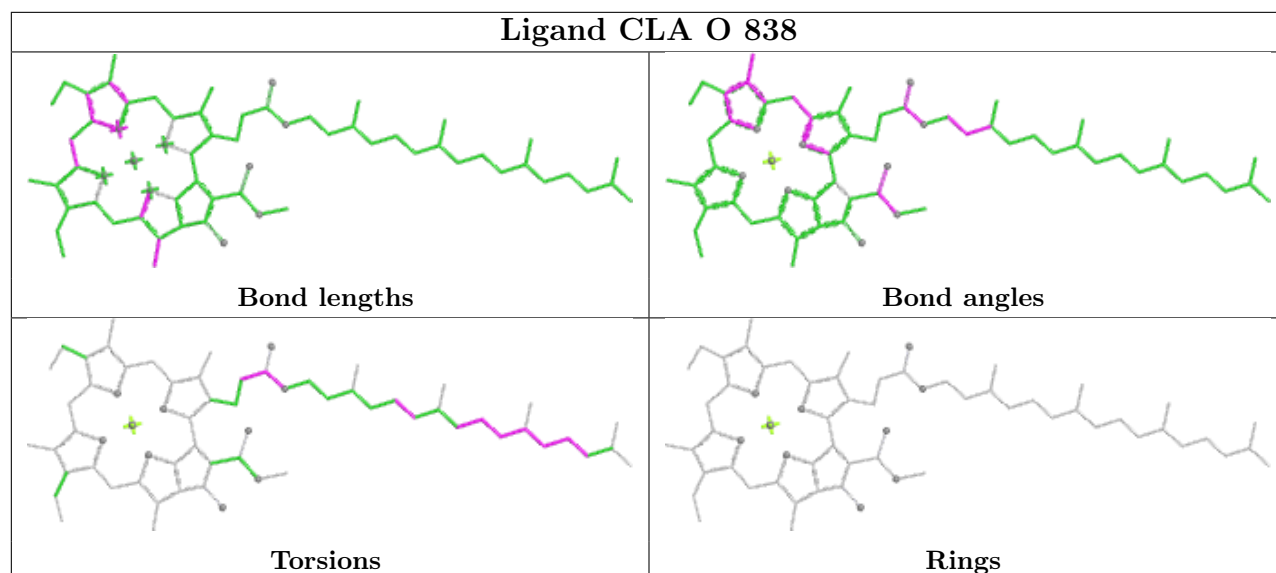
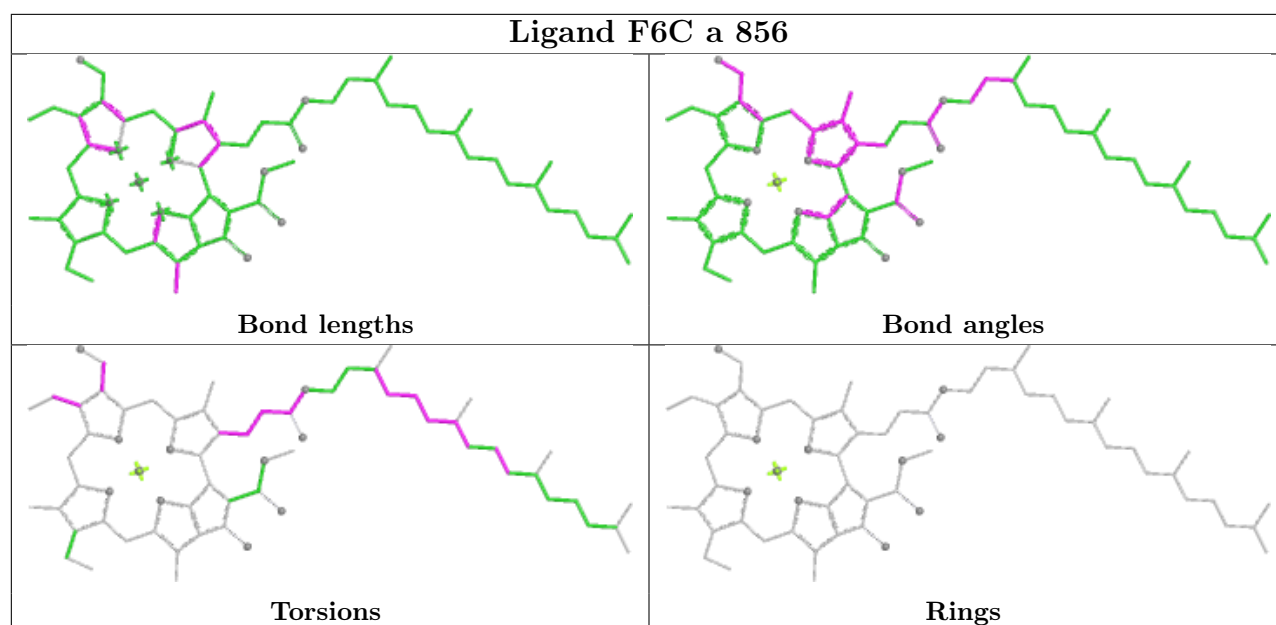


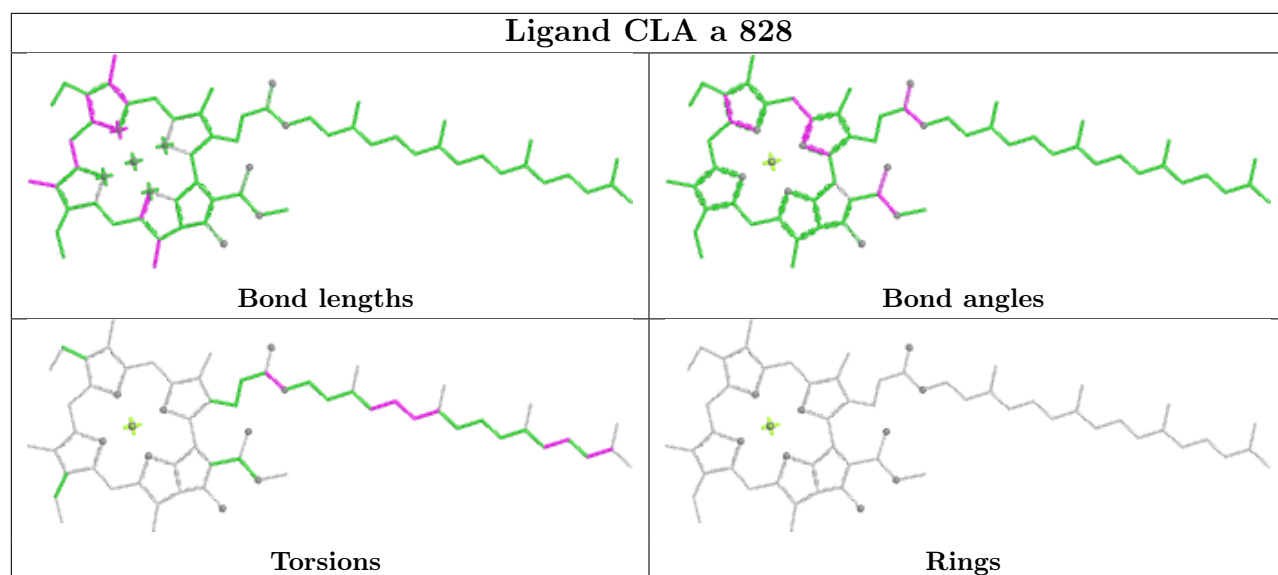
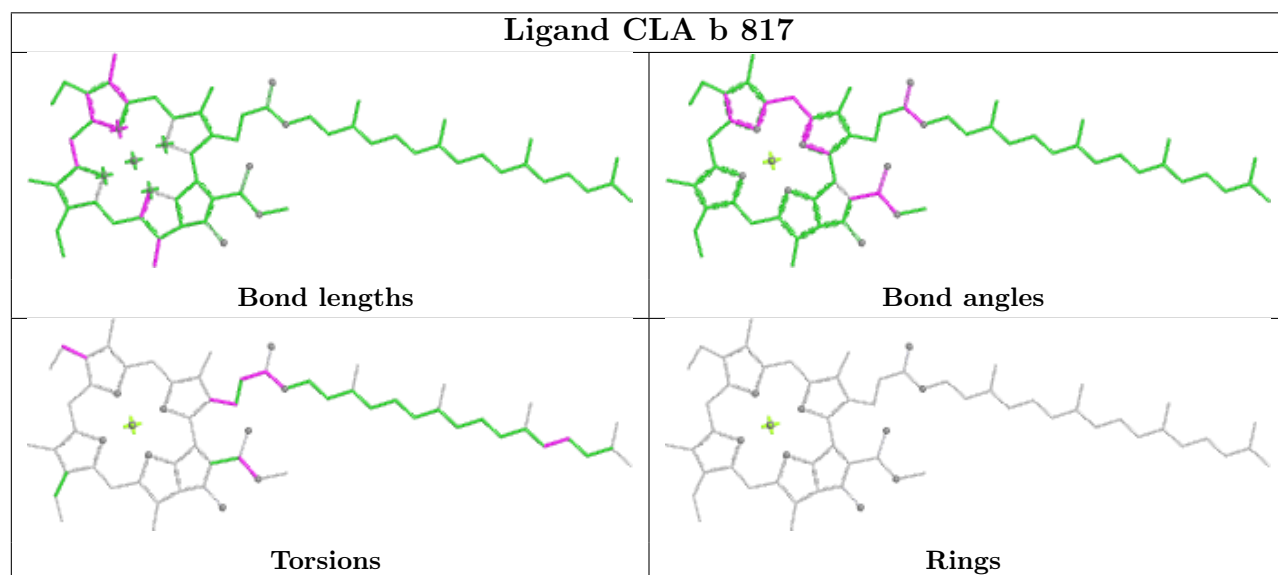
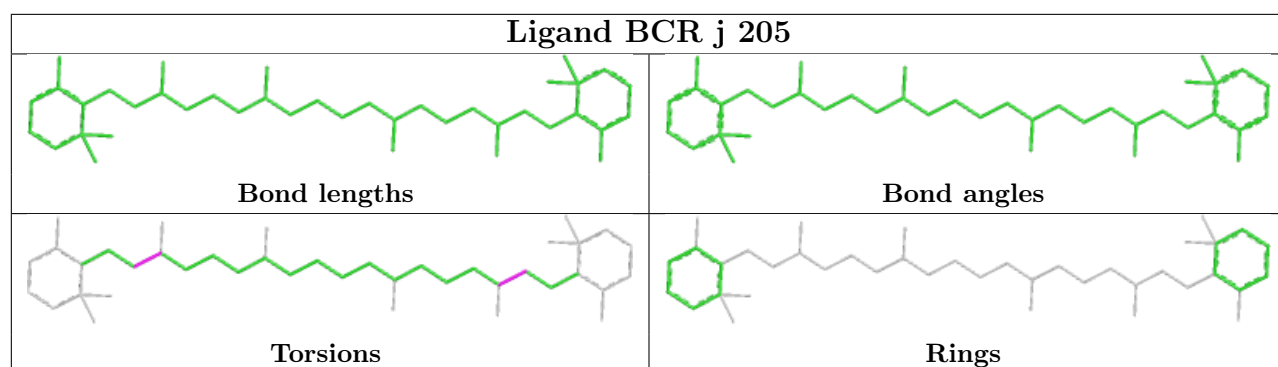
Ligand CLA A 832

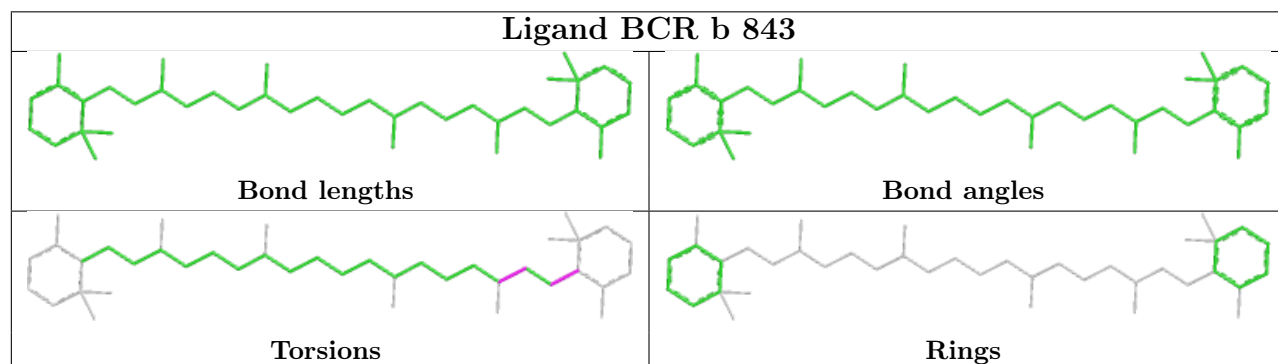
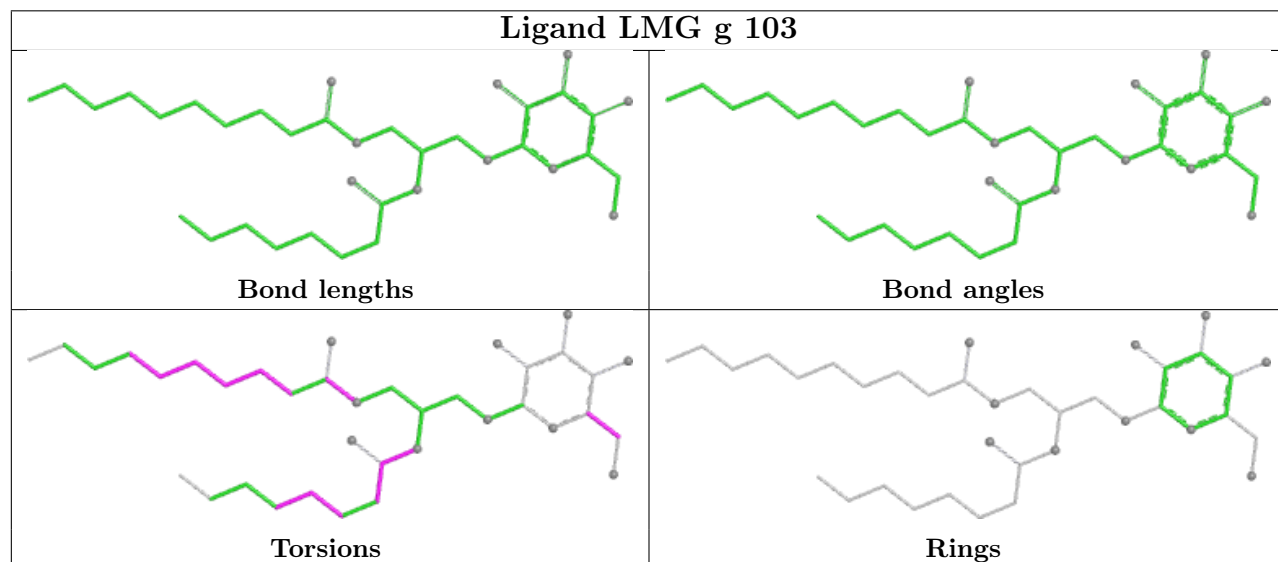
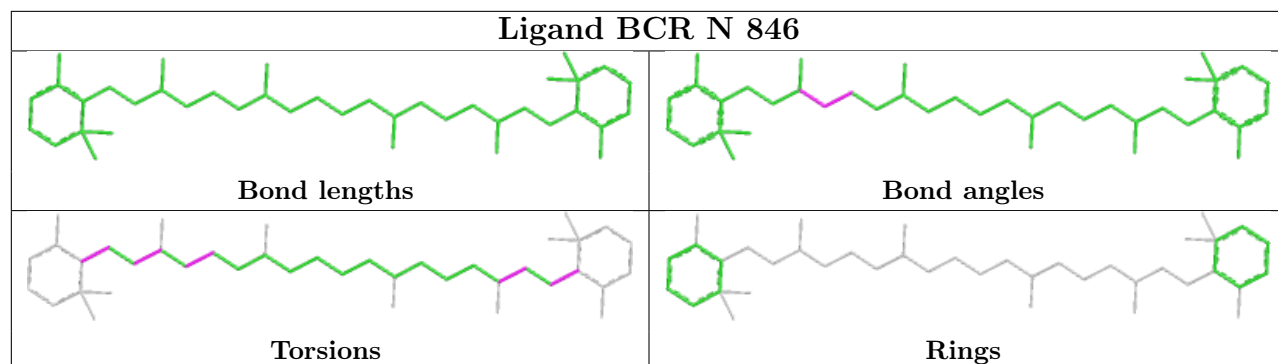


Ligand F6C A 857

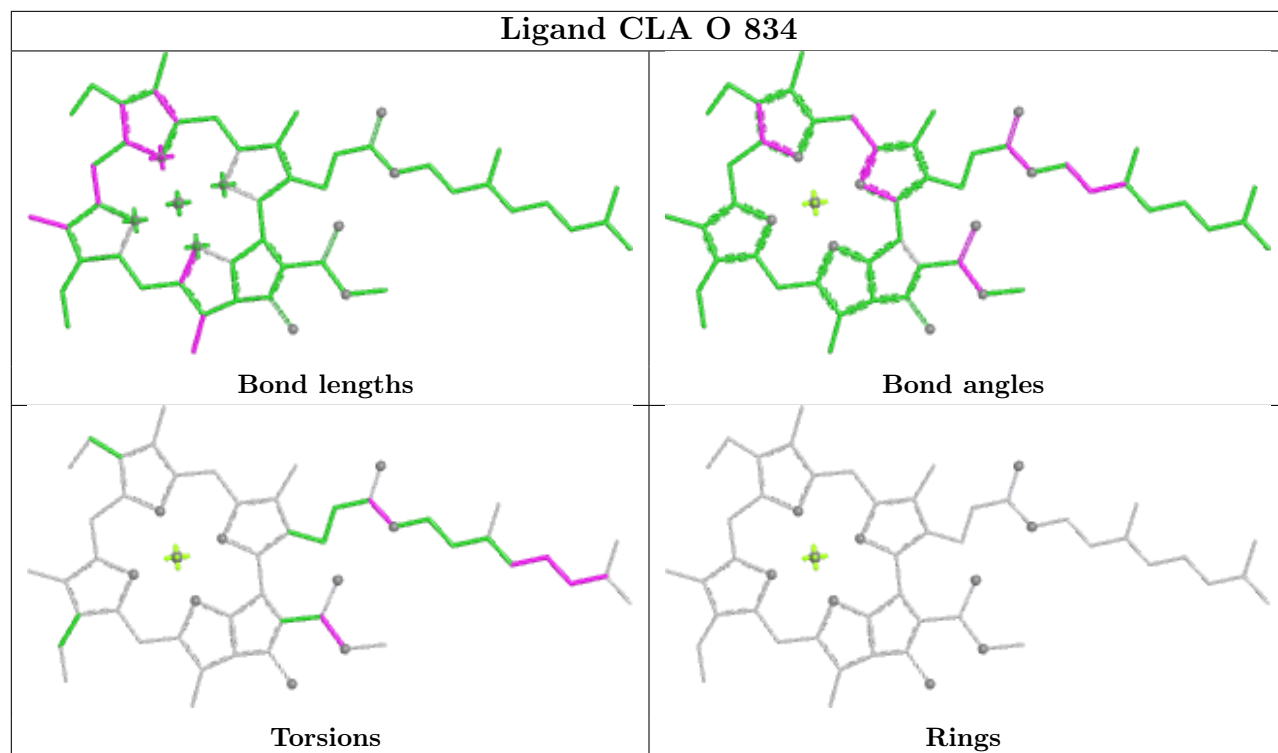




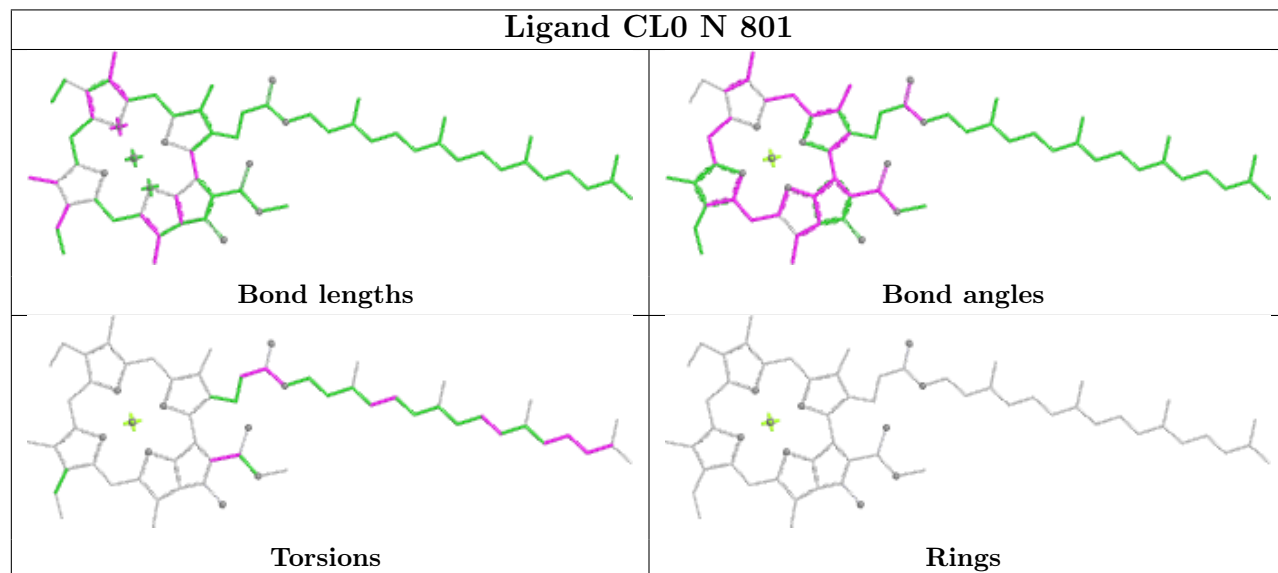


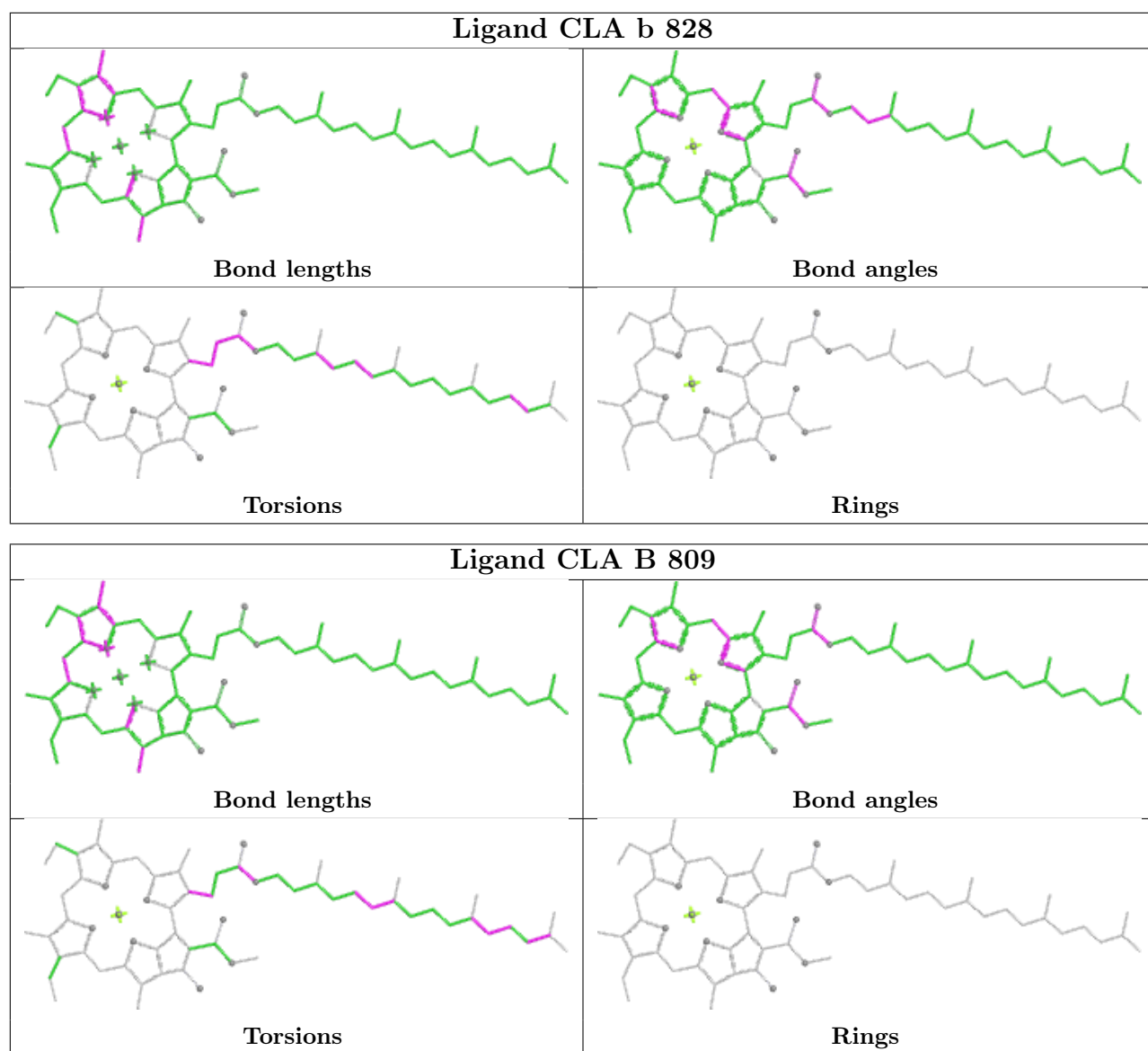


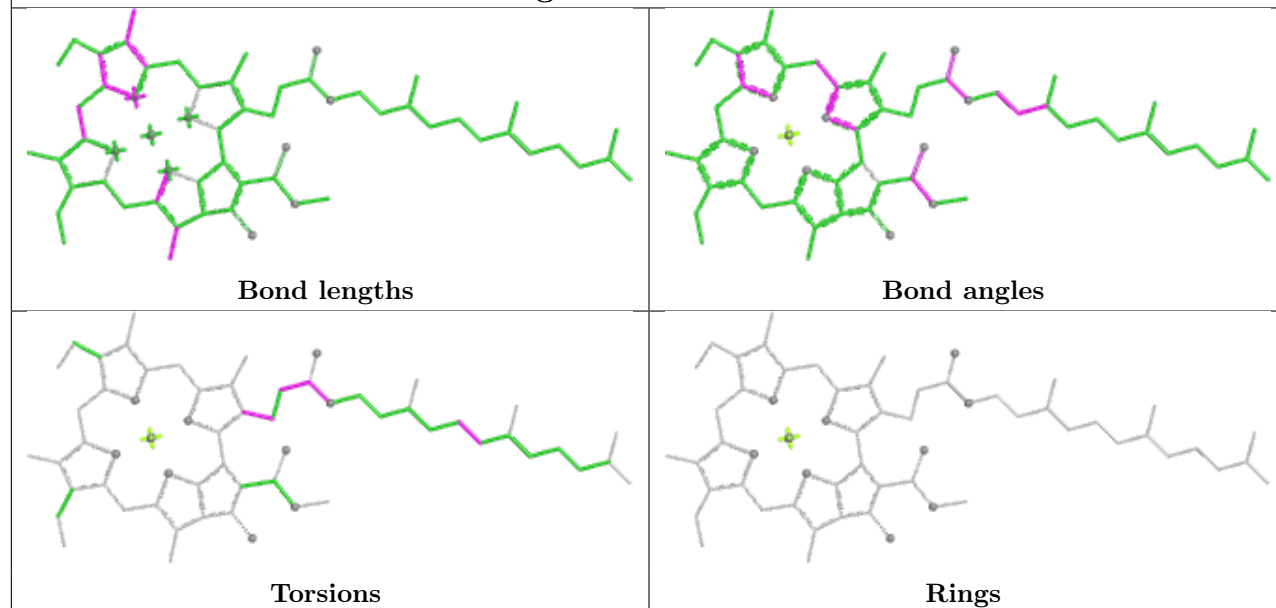
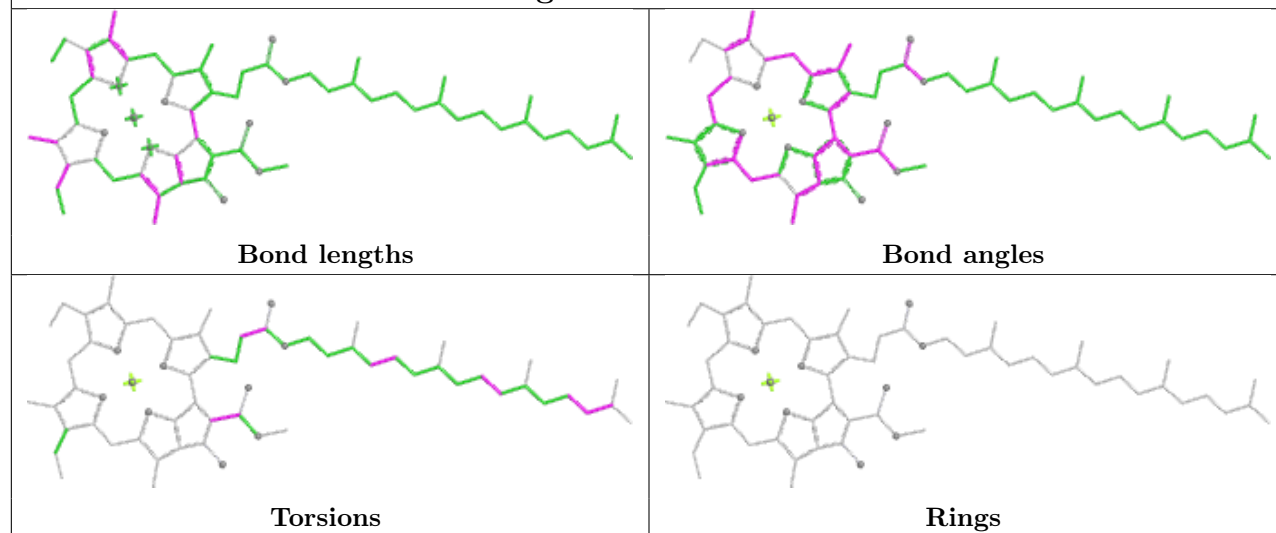
Ligand CLA O 834

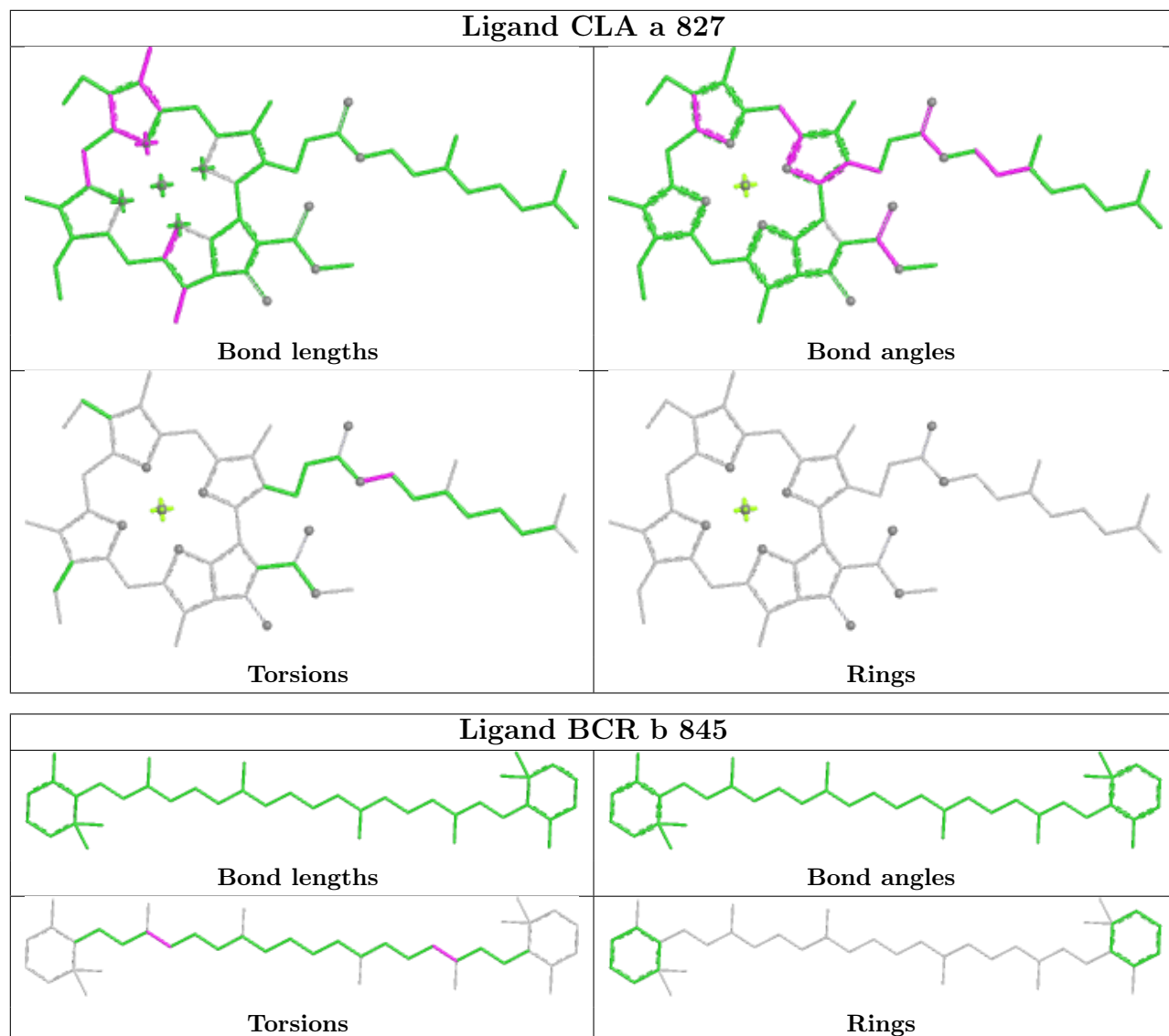


Ligand CL0 N 801

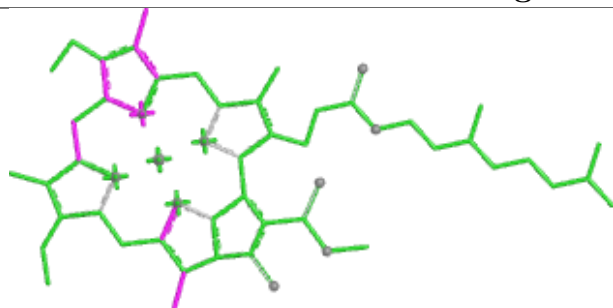




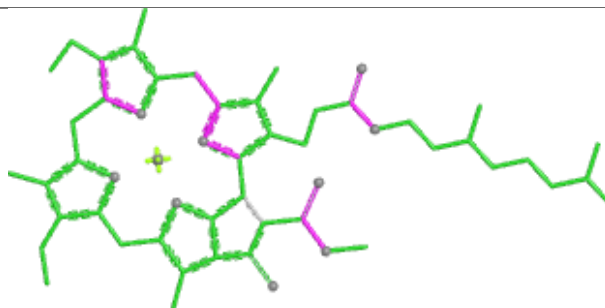
Ligand CLA a 821**Ligand CL0 A 801**



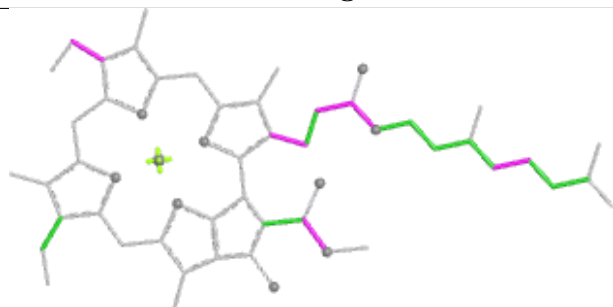
Ligand CLA B 818



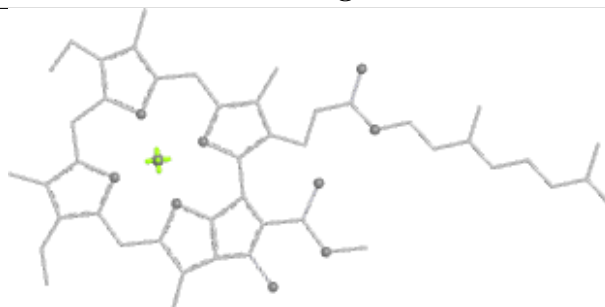
Bond lengths



Bond angles

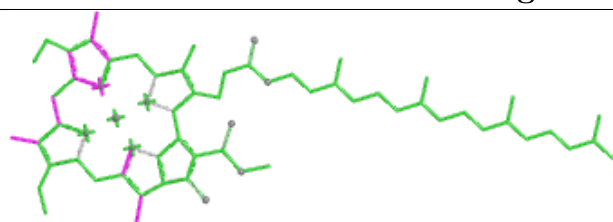


Torsions

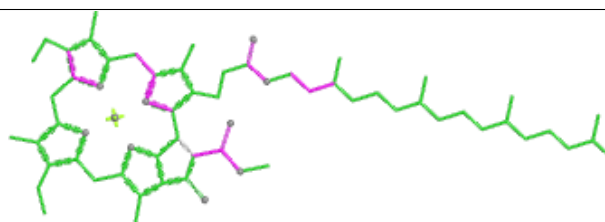


Rings

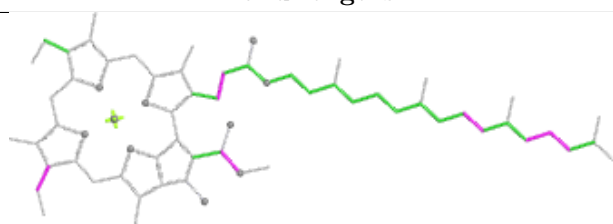
Ligand CLA b 803



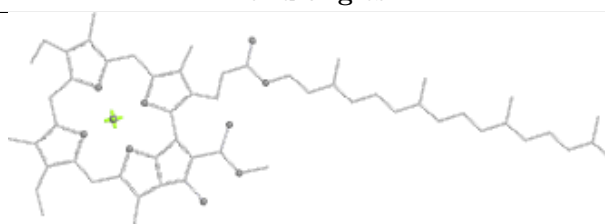
Bond lengths



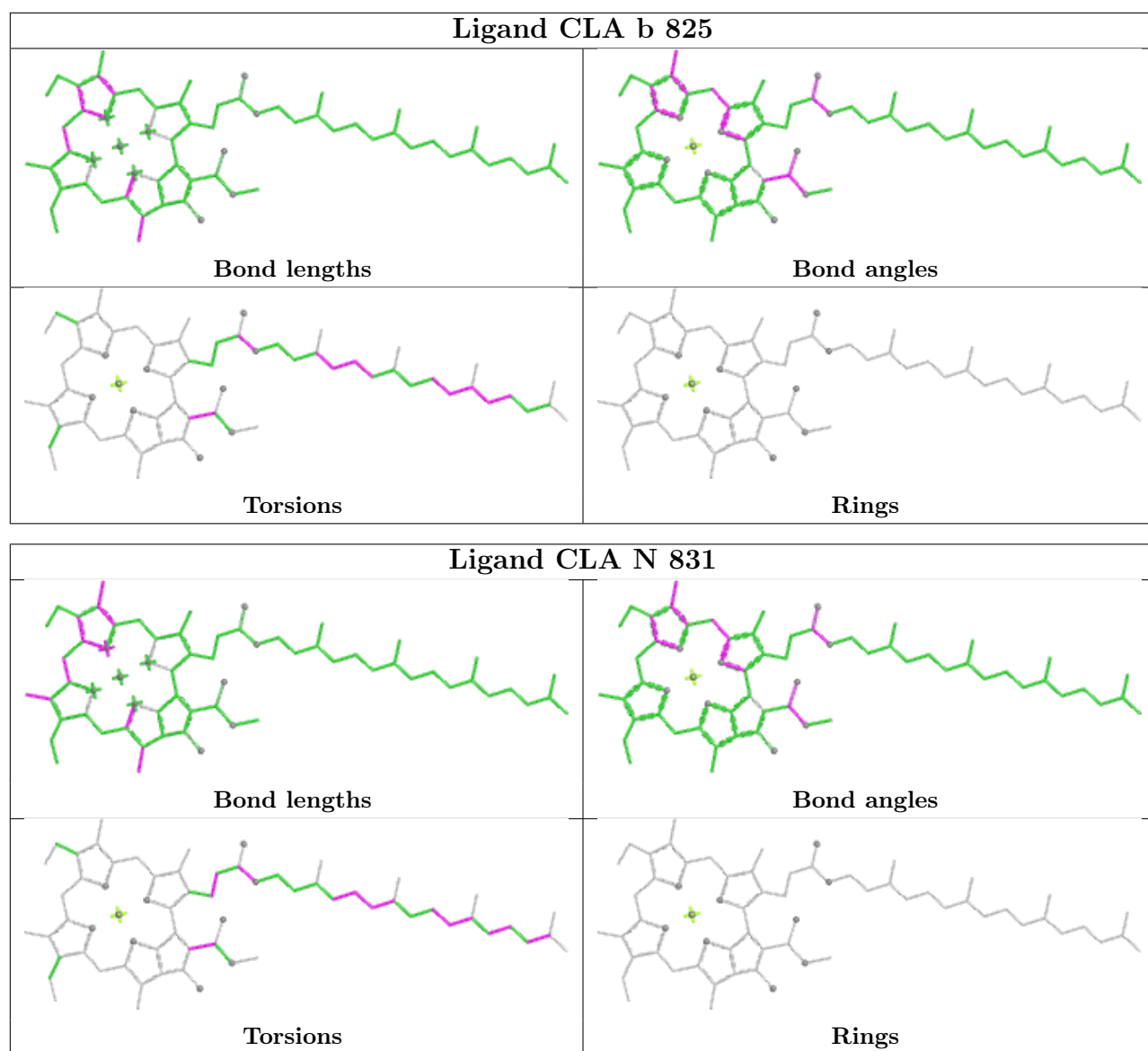
Bond angles



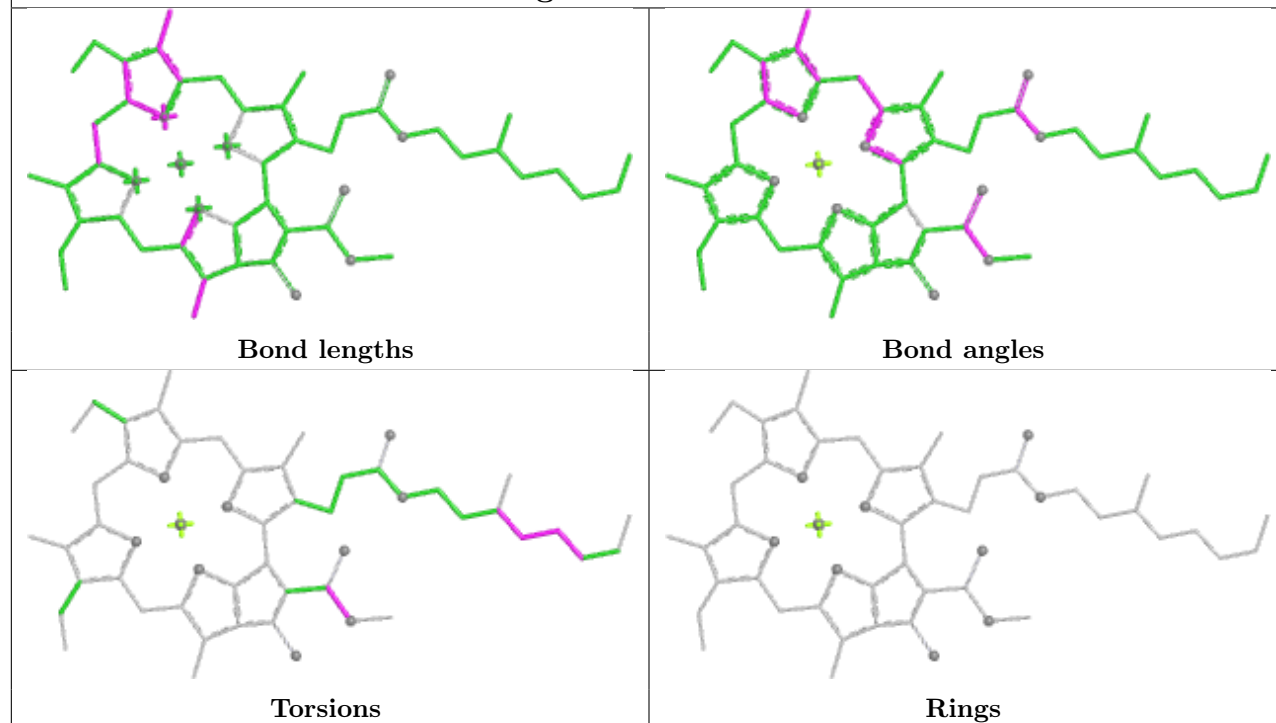
Torsions



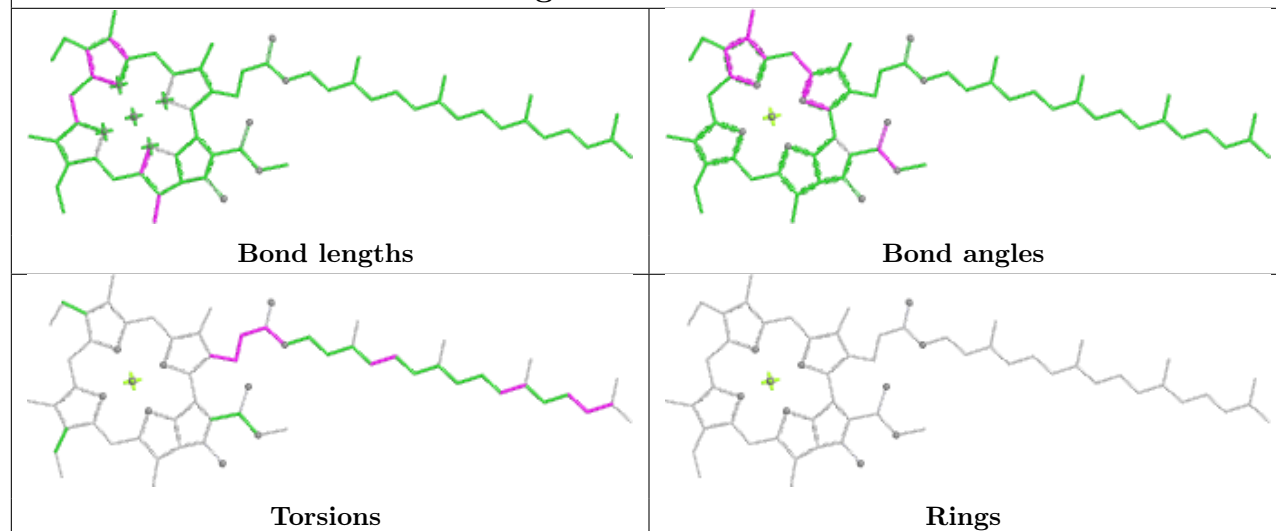
Rings

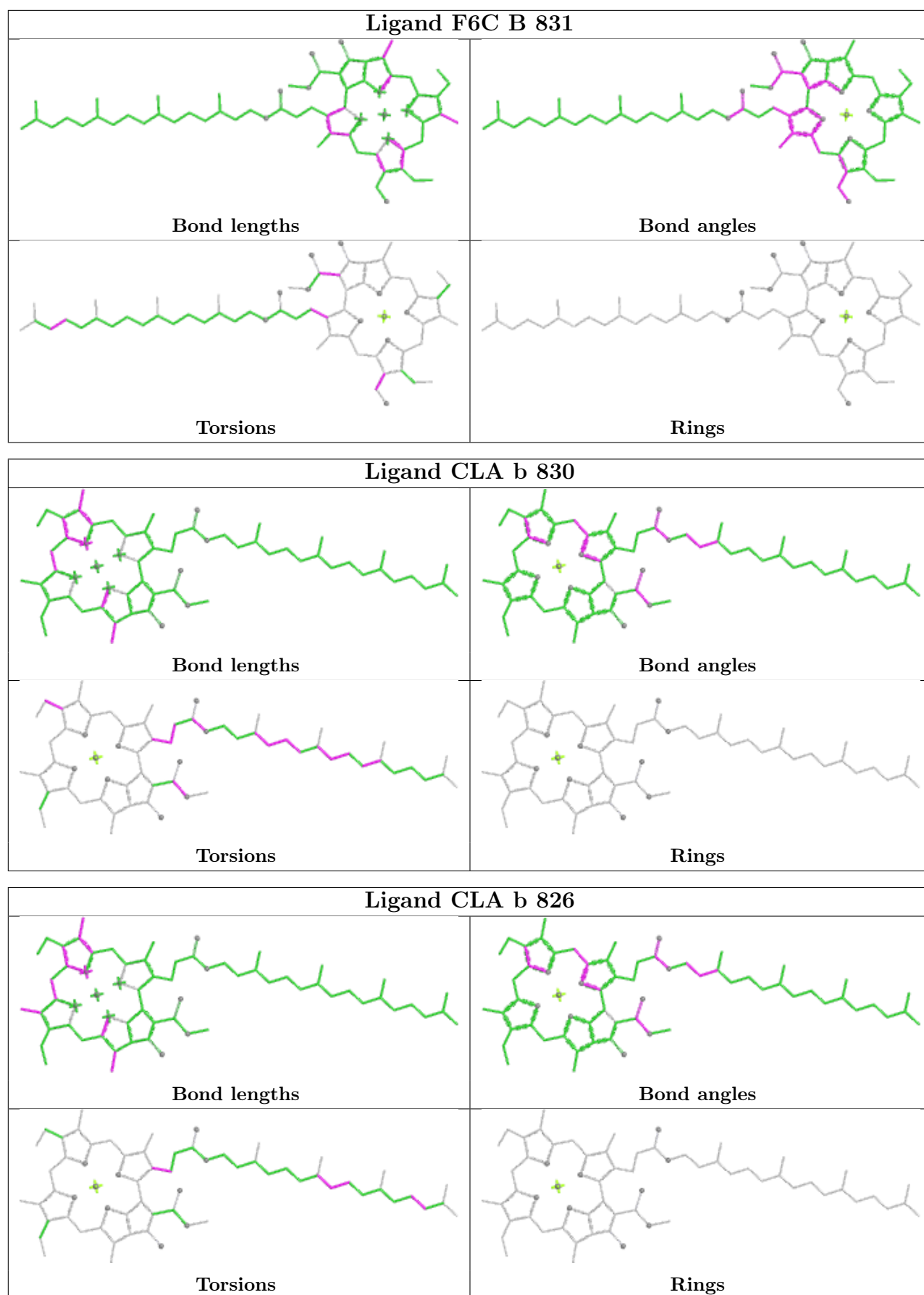


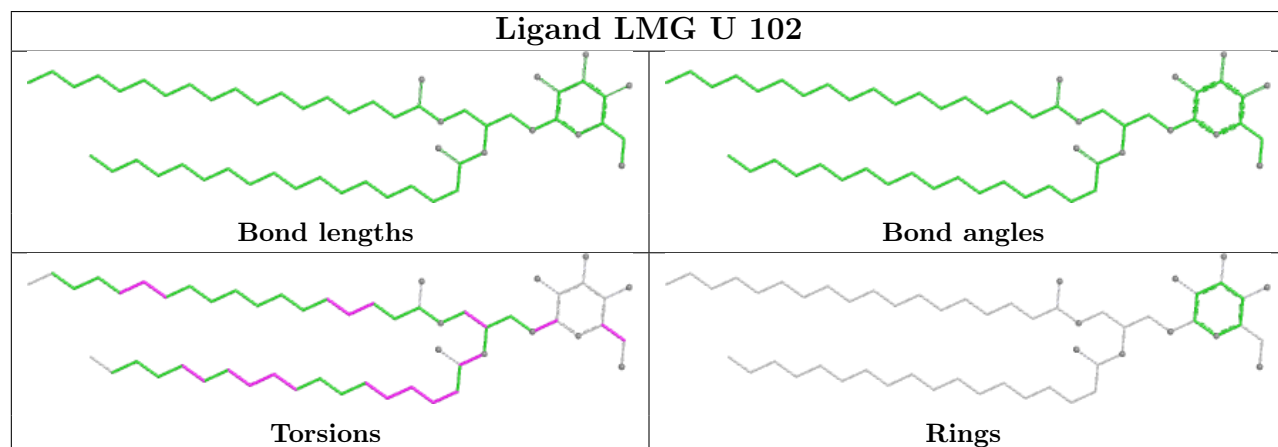
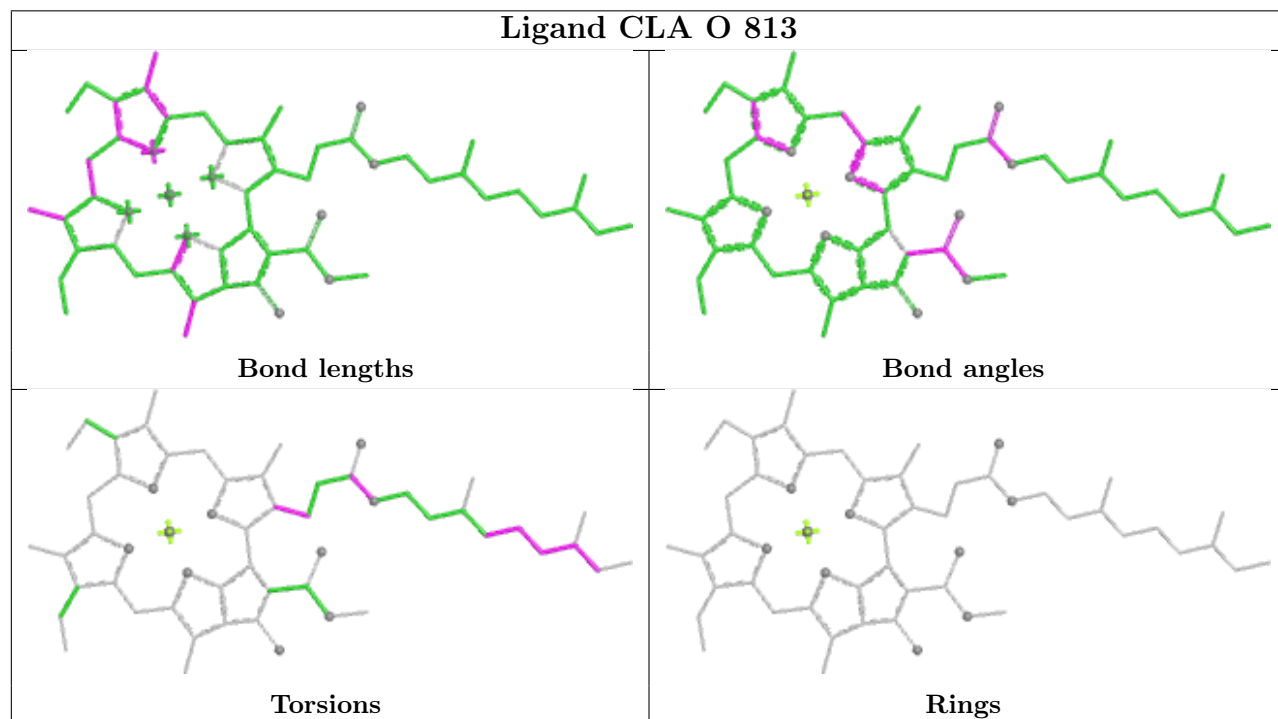
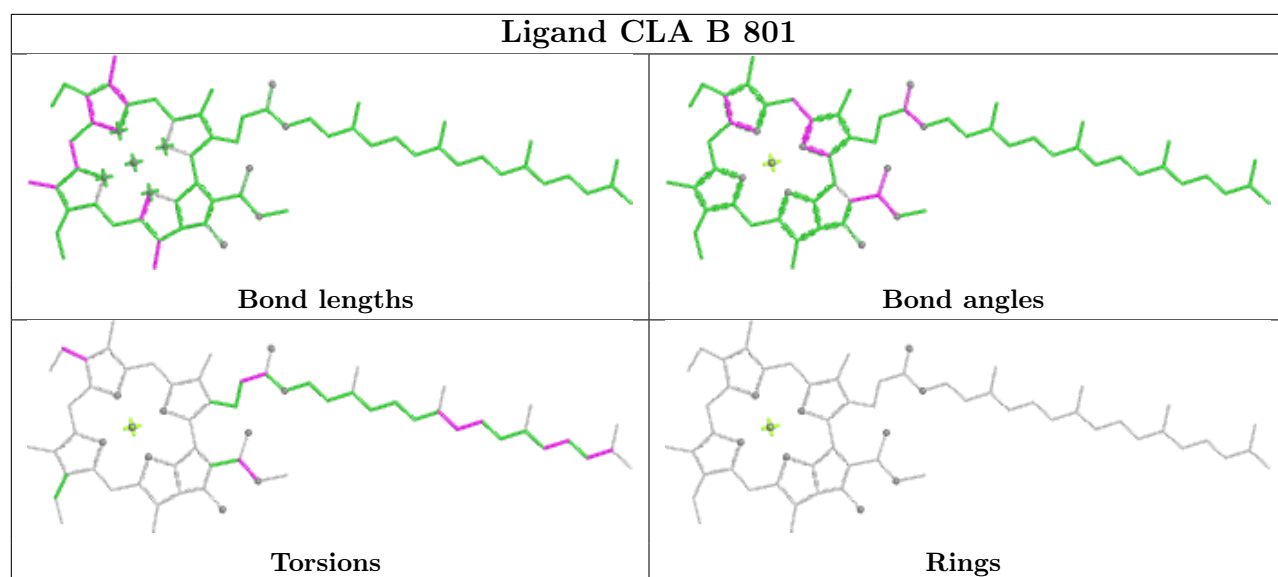
Ligand CLA a 836



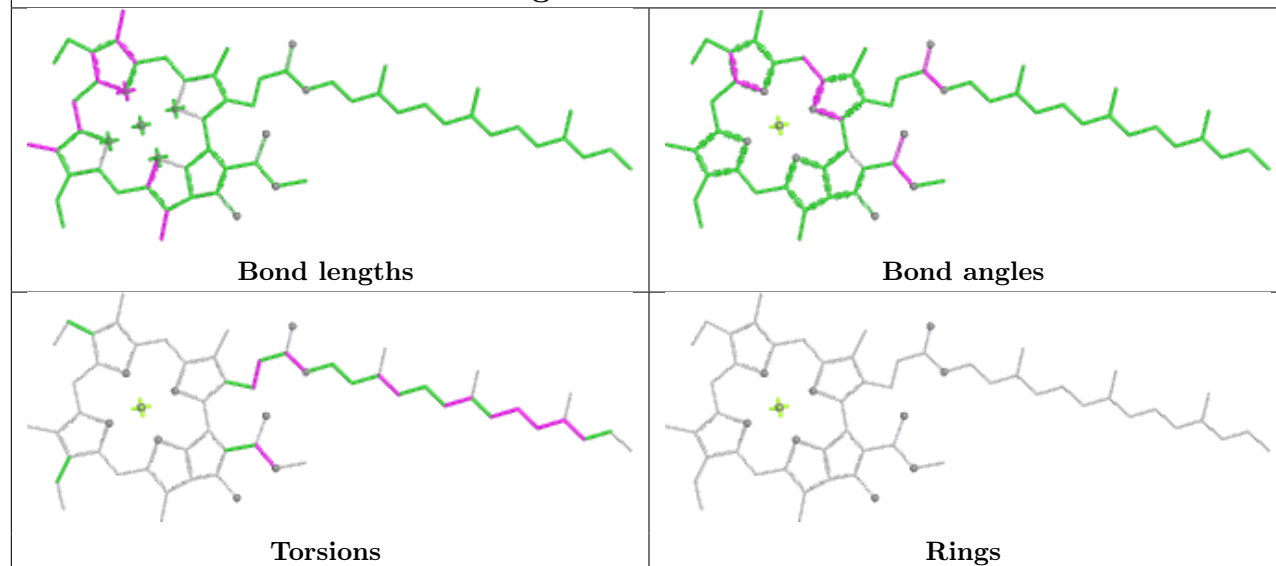
Ligand CLA b 805



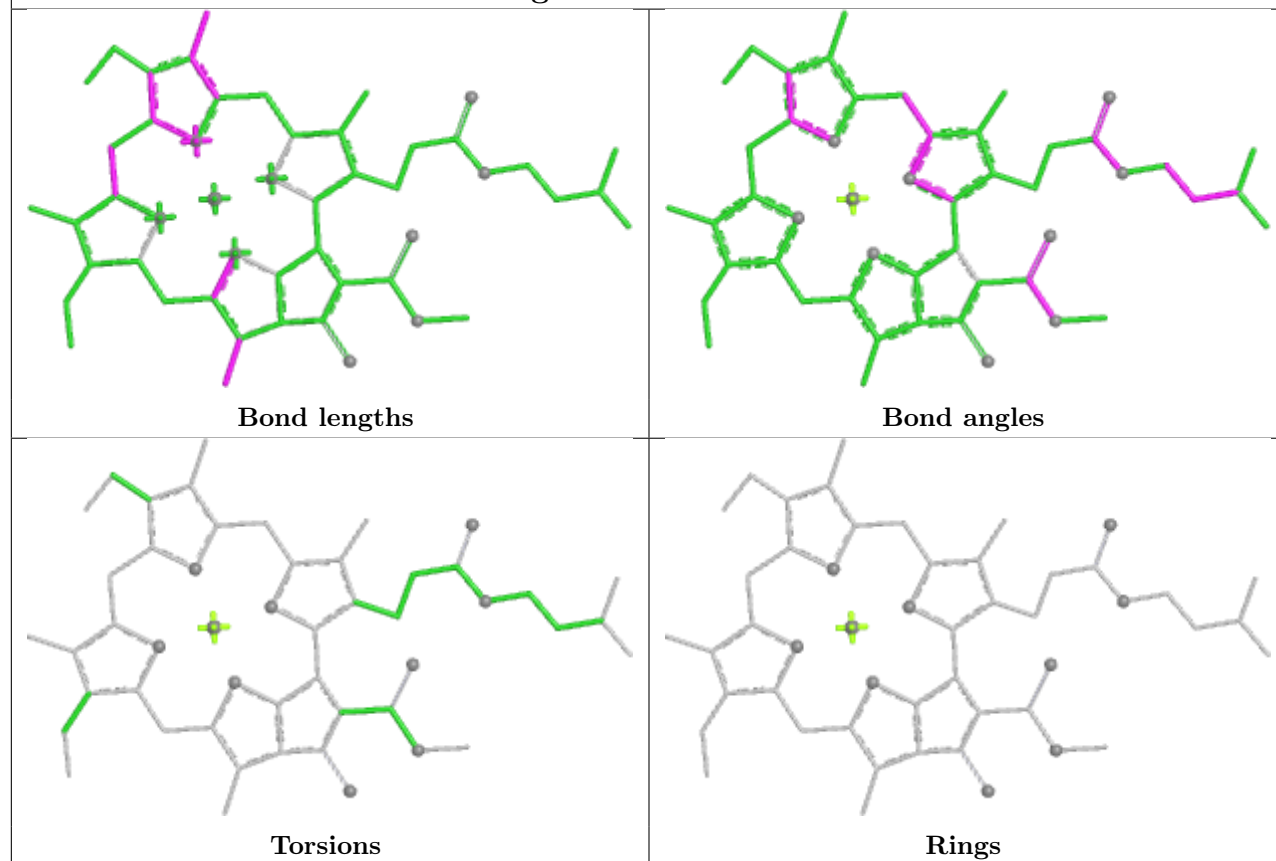


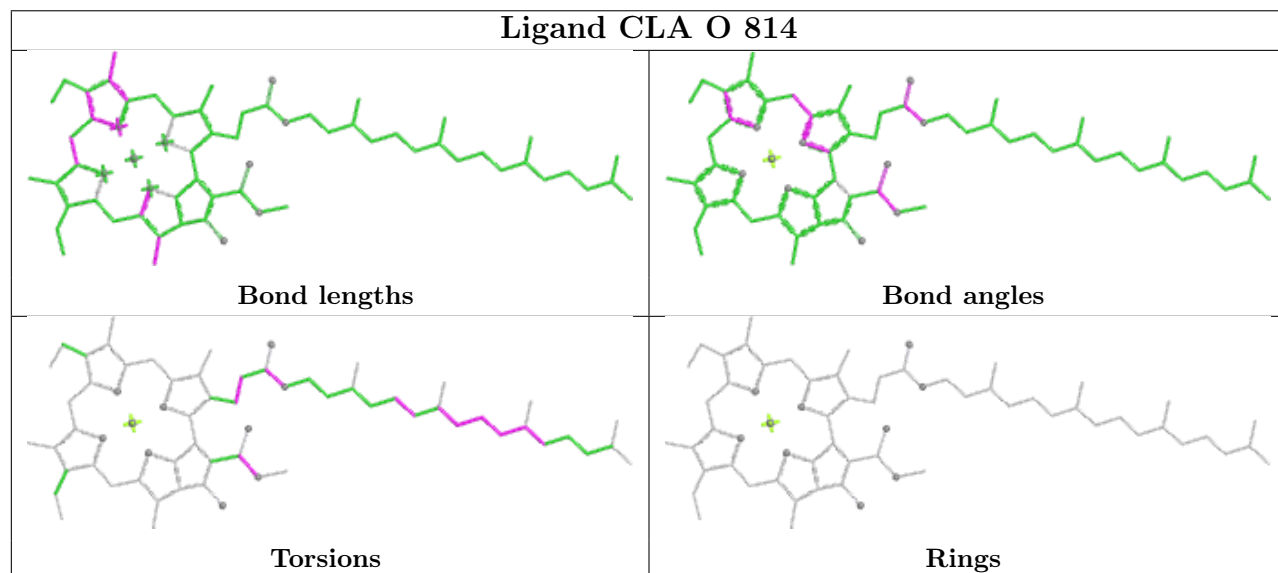
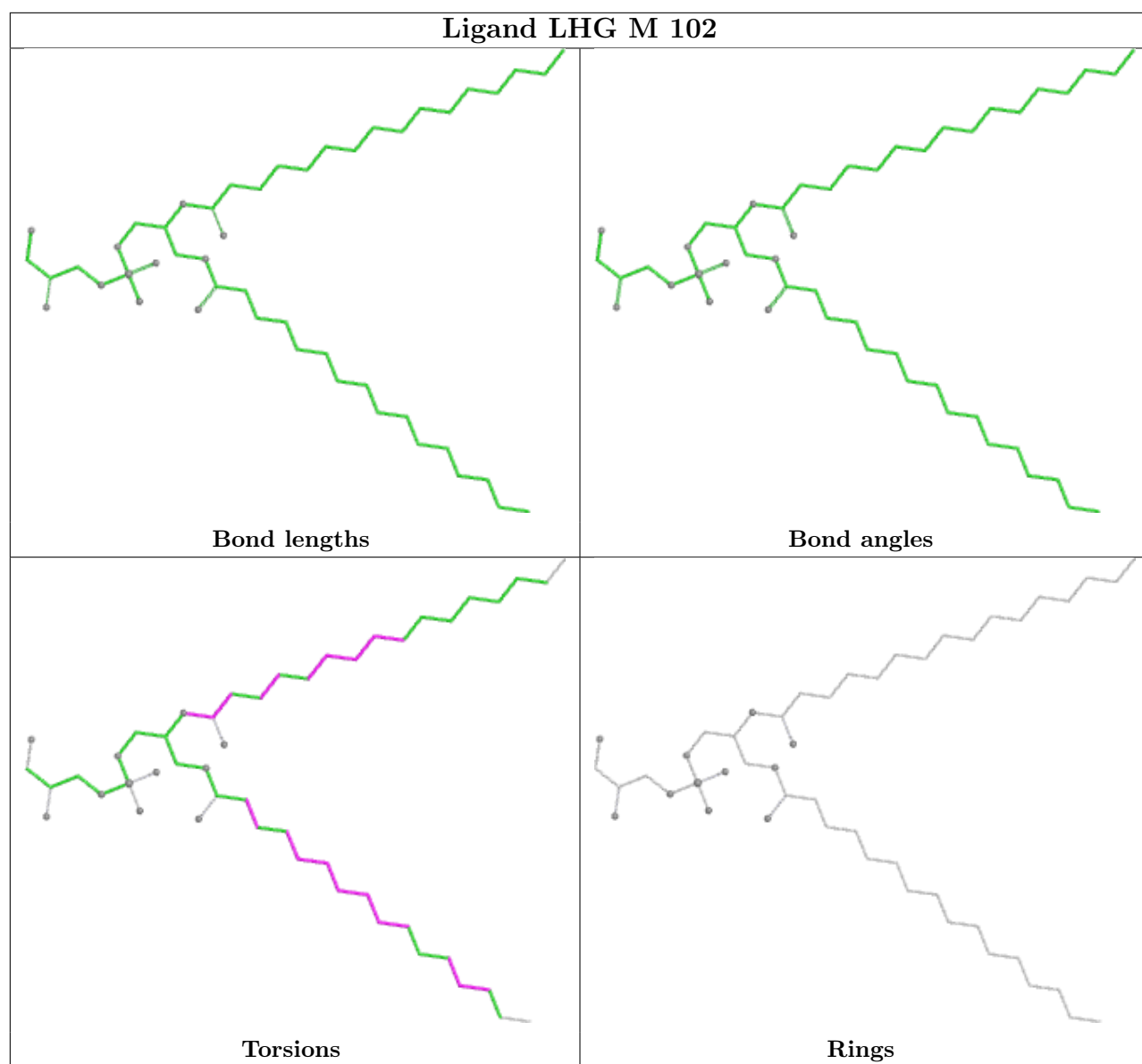


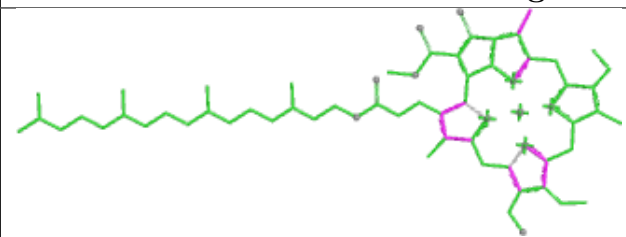
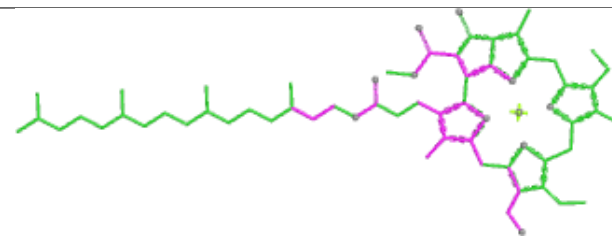
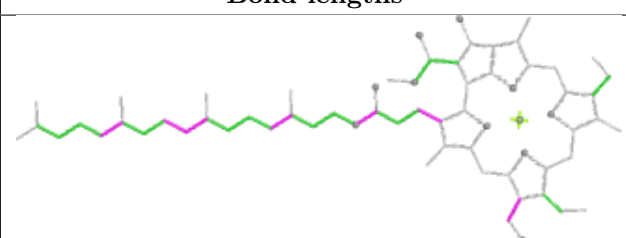
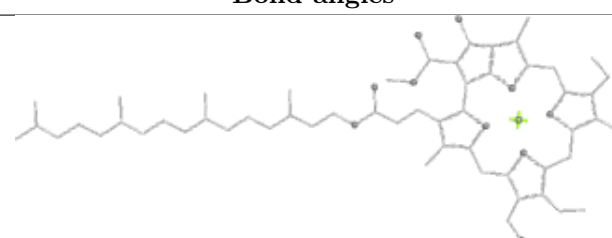
Ligand CLA B 825

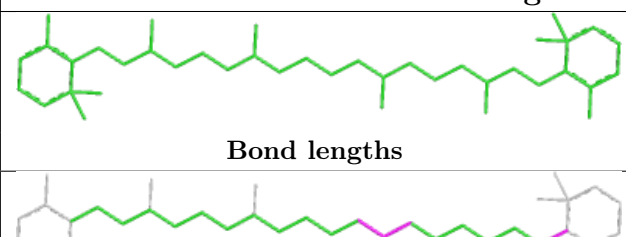
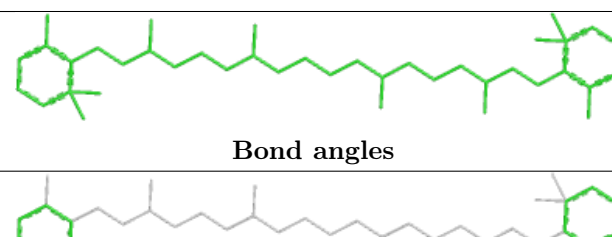
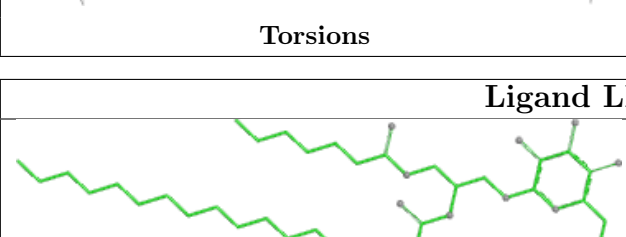


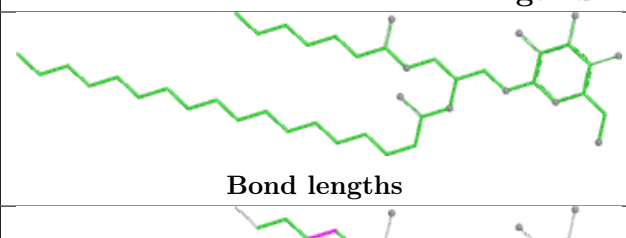
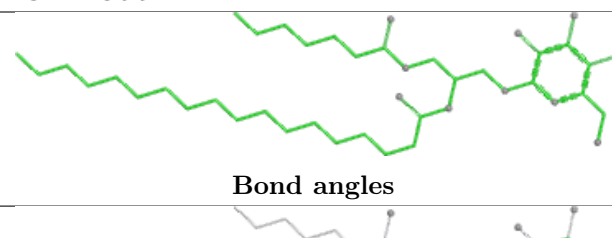
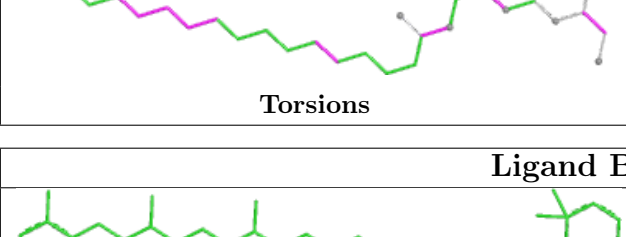
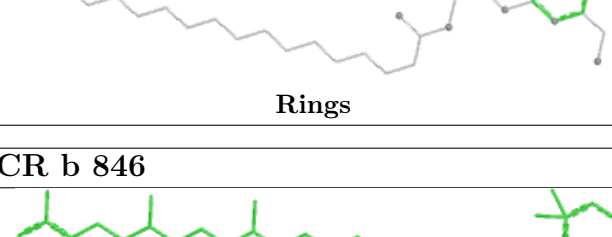
Ligand CLA N 840

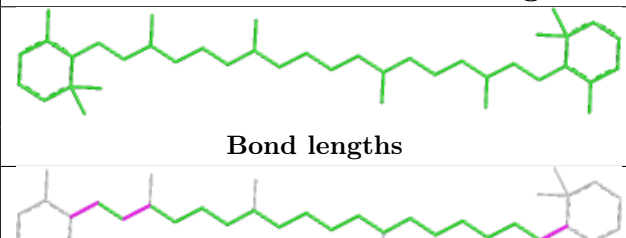
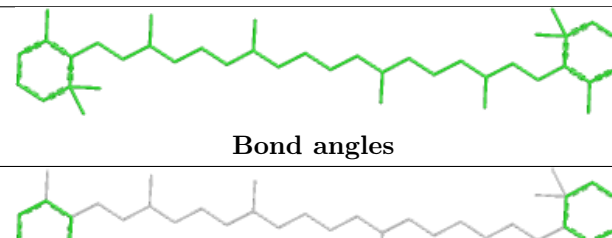


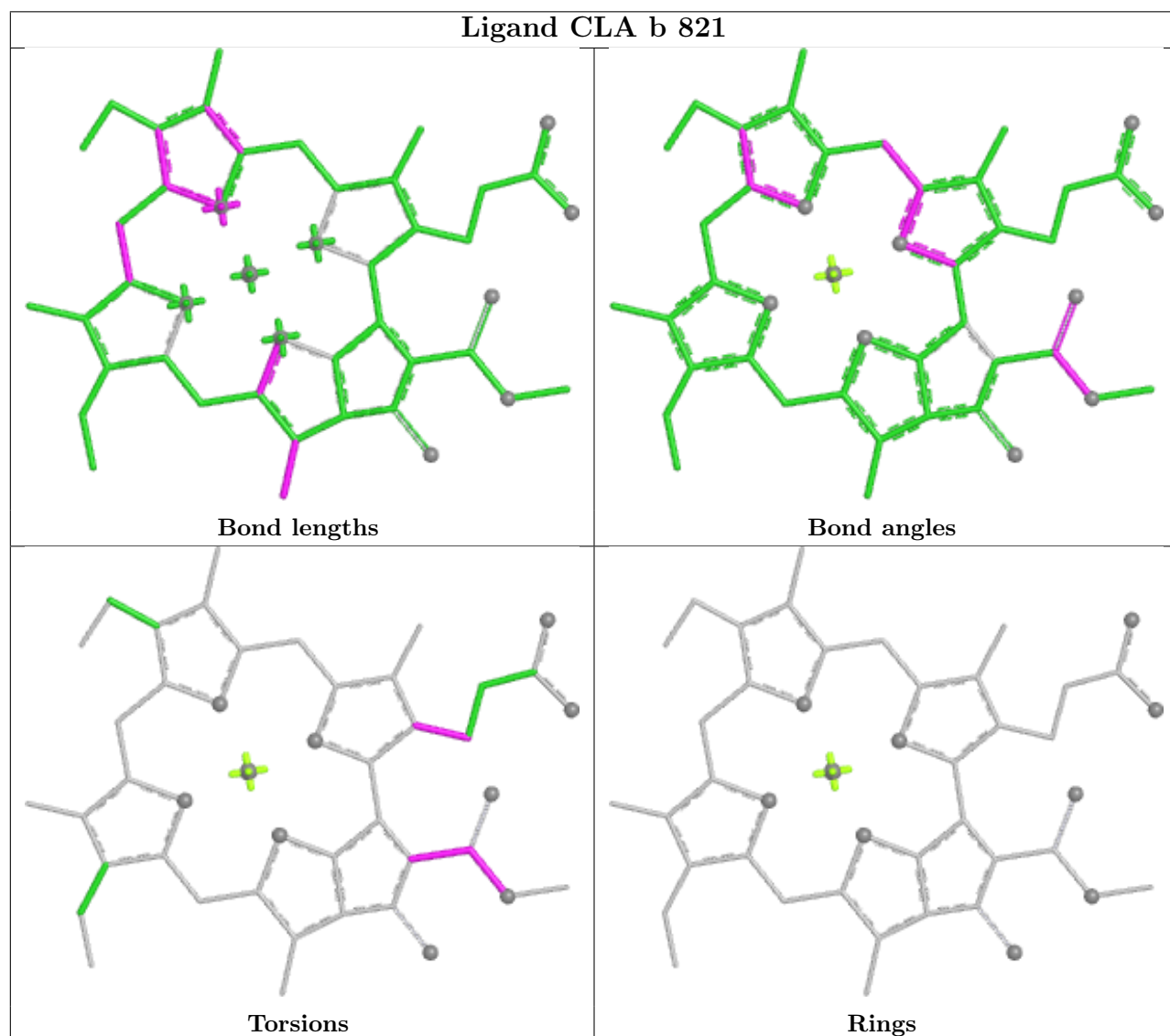
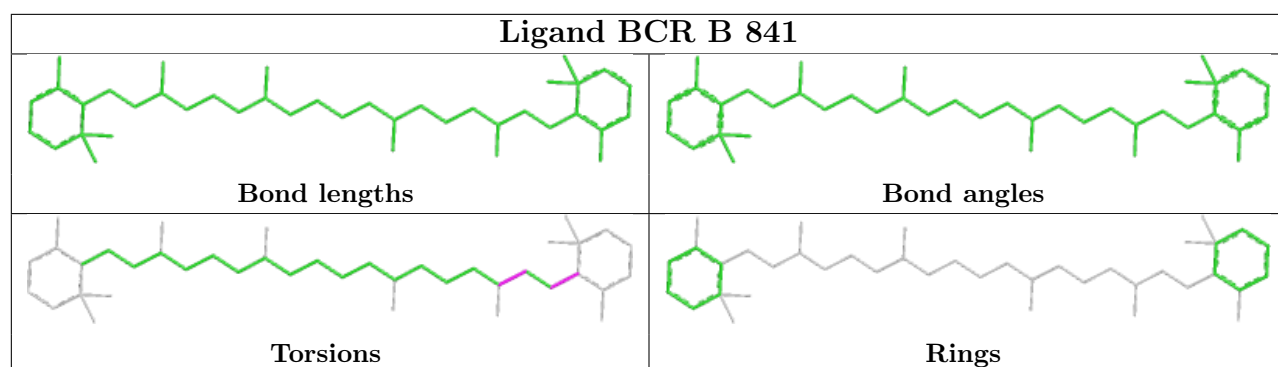


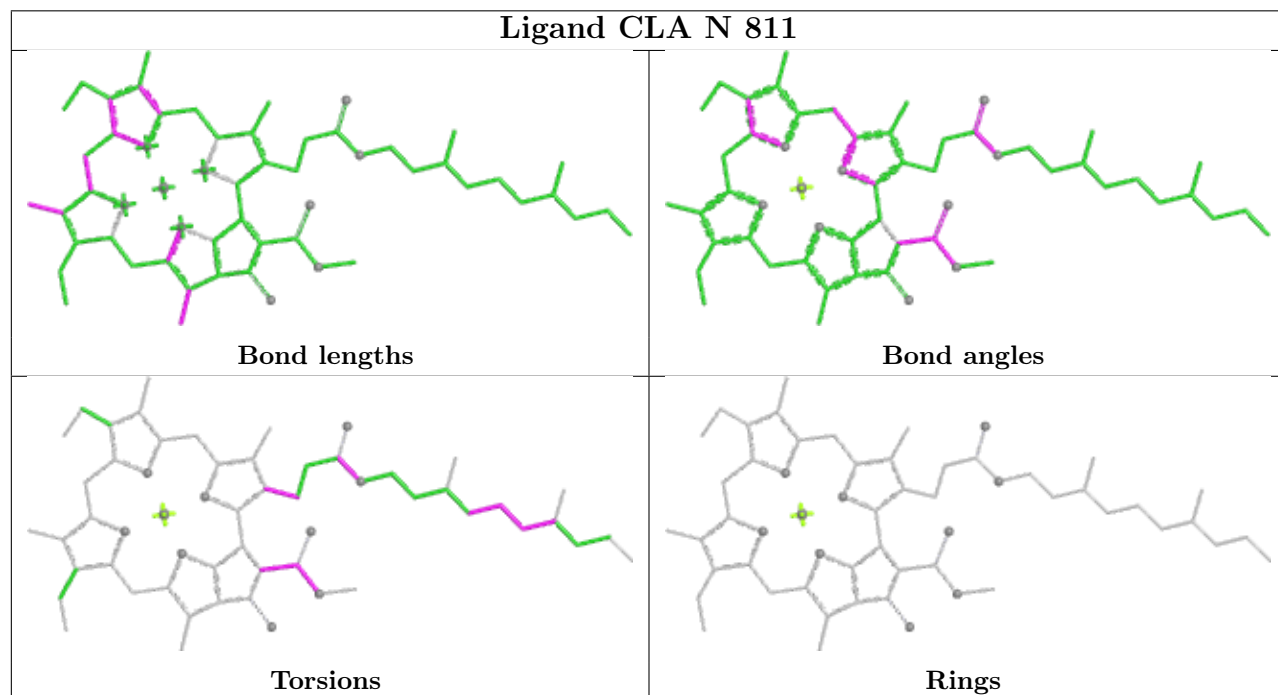
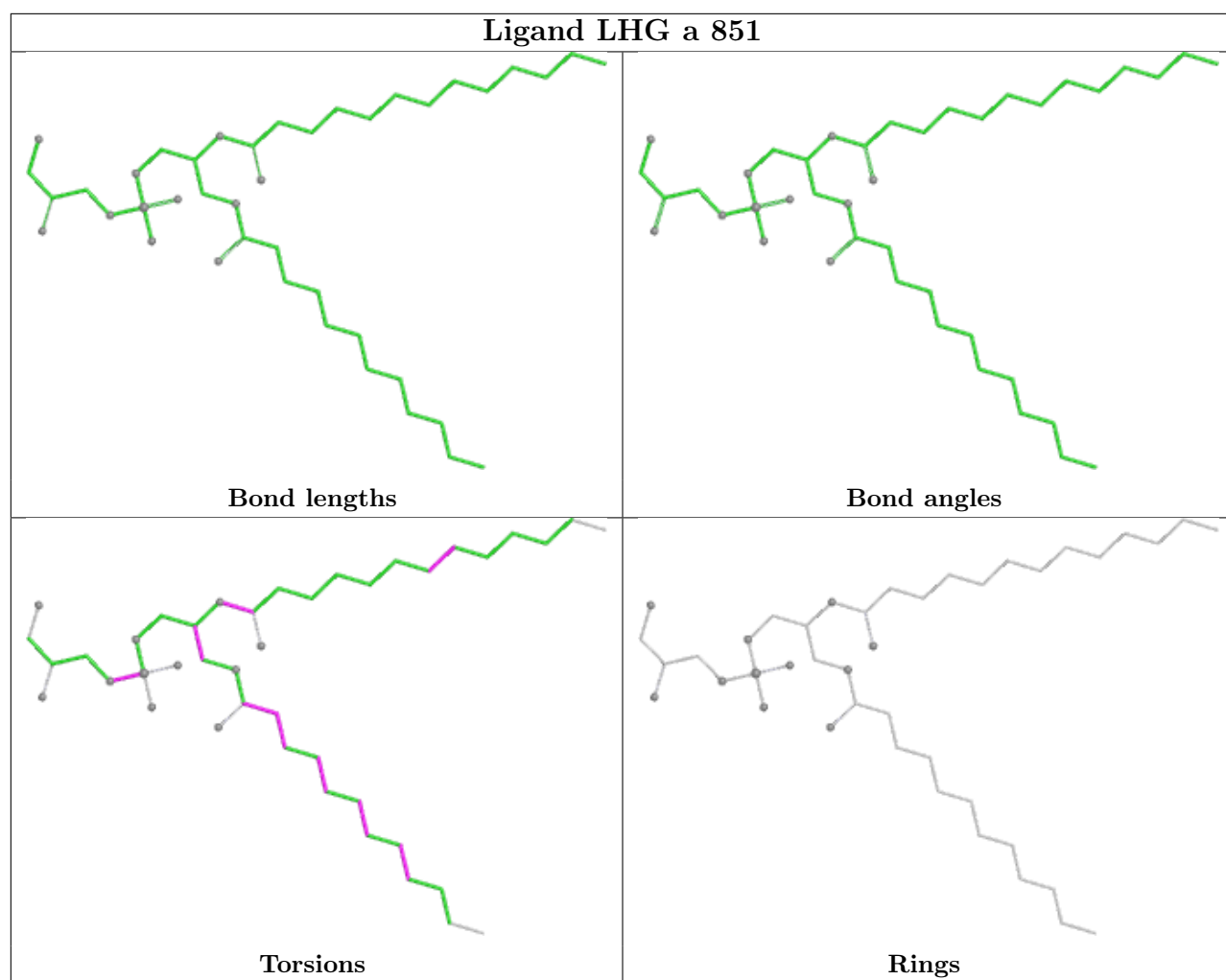
Ligand F6C L 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

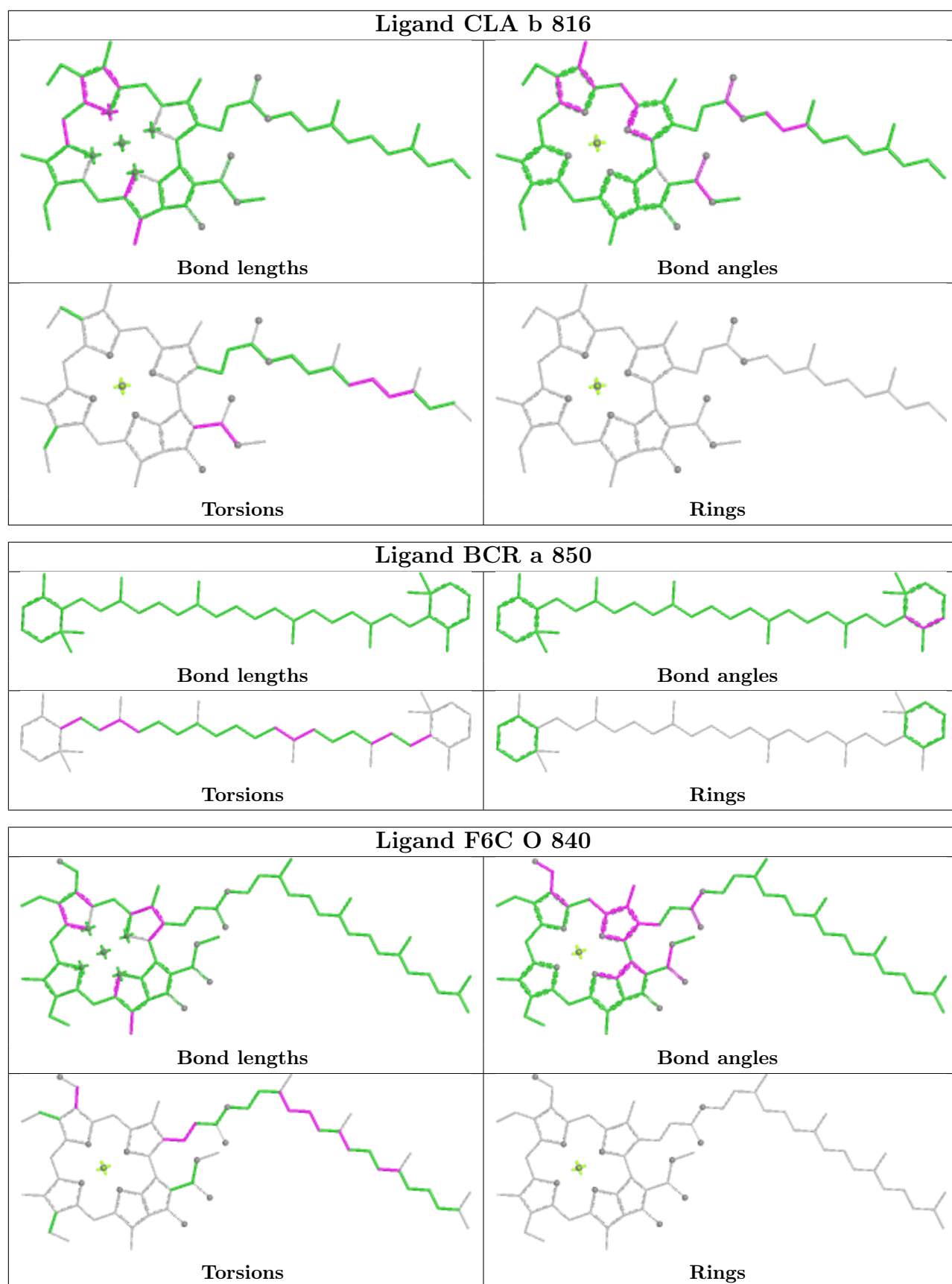
Ligand BCR a 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

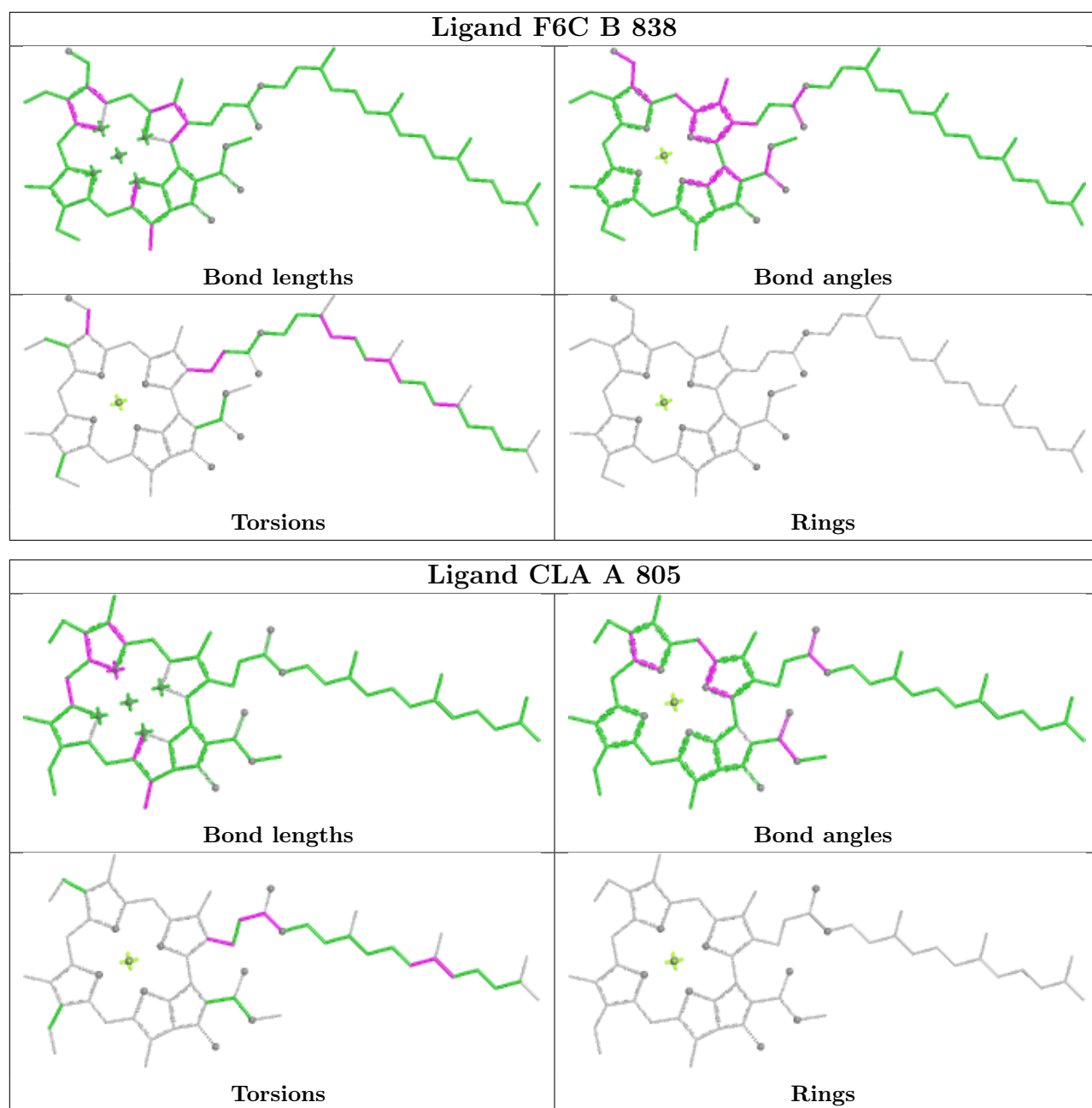
Ligand LMG A 855	
	
Bond lengths	Bond angles
	
Torsions	Rings

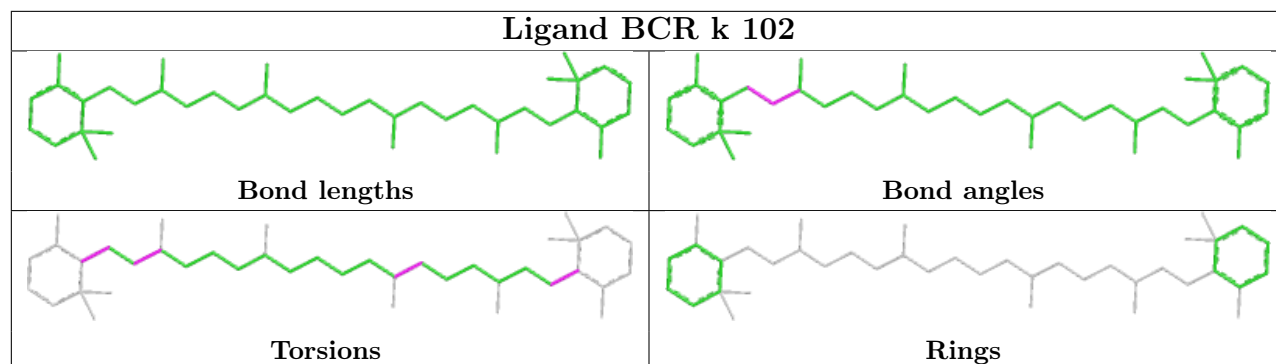
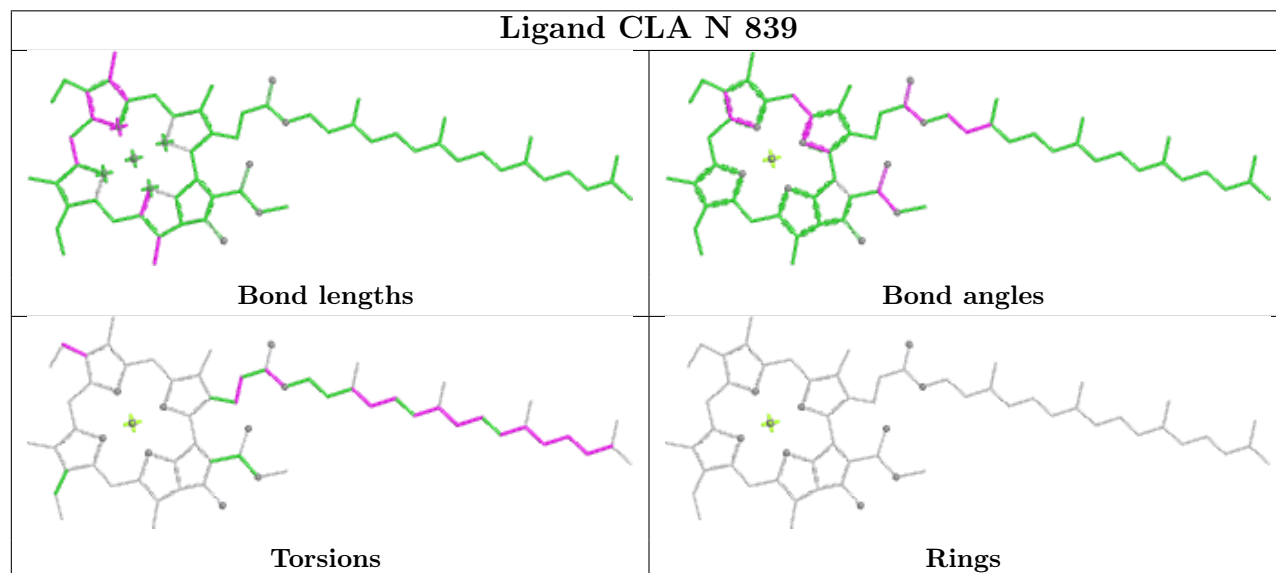
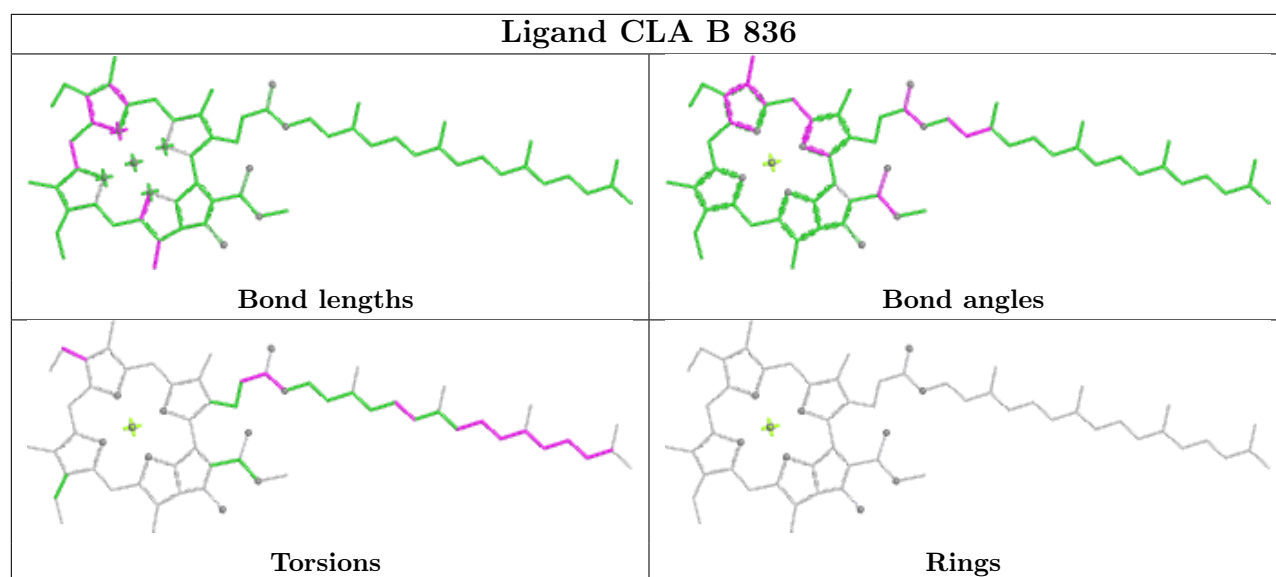
Ligand BCR b 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

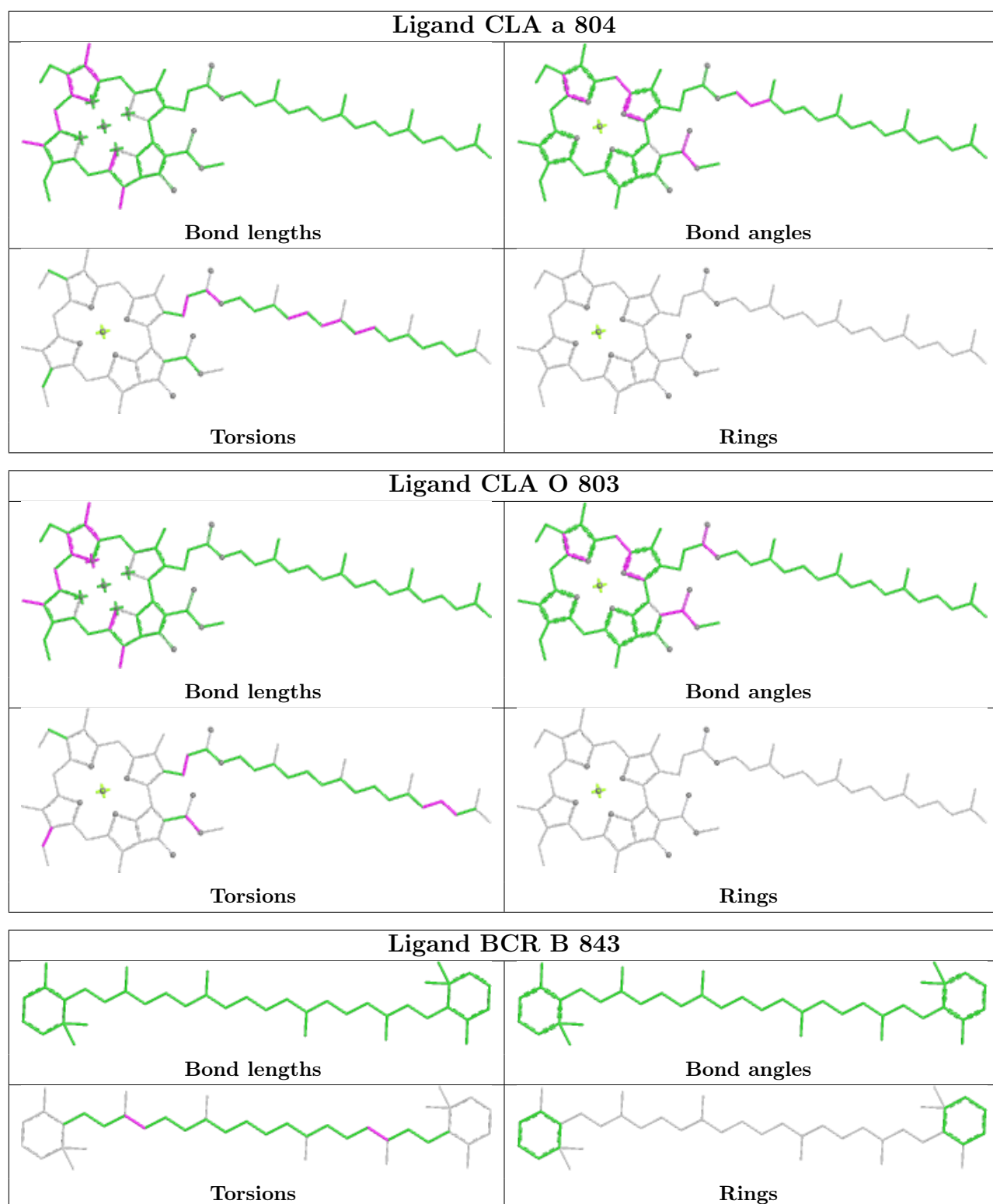


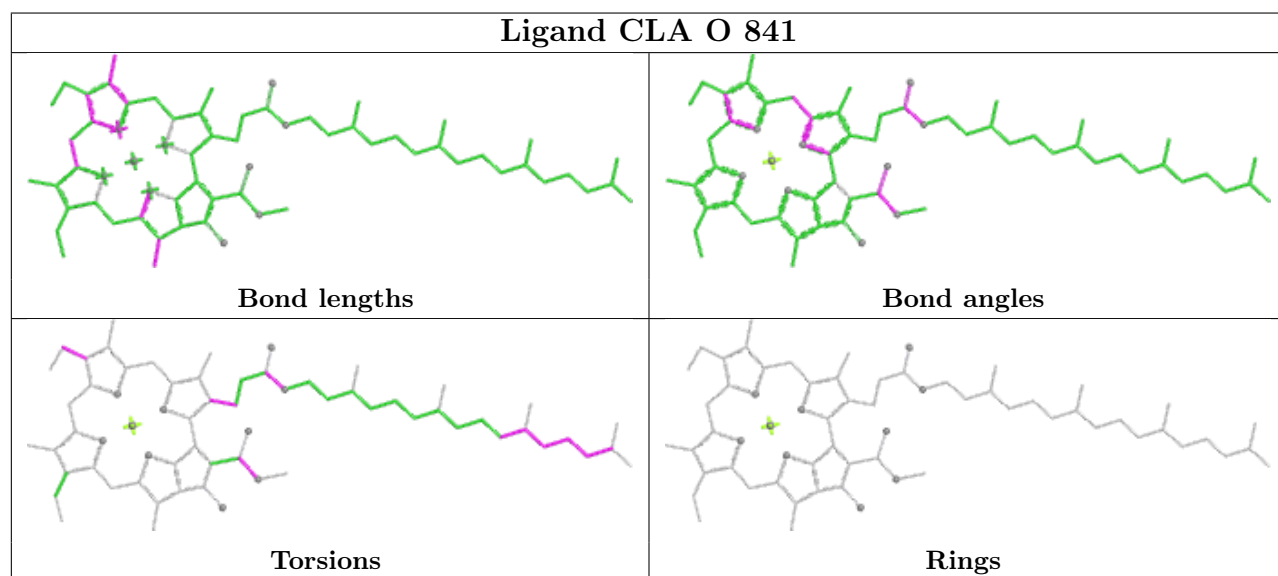
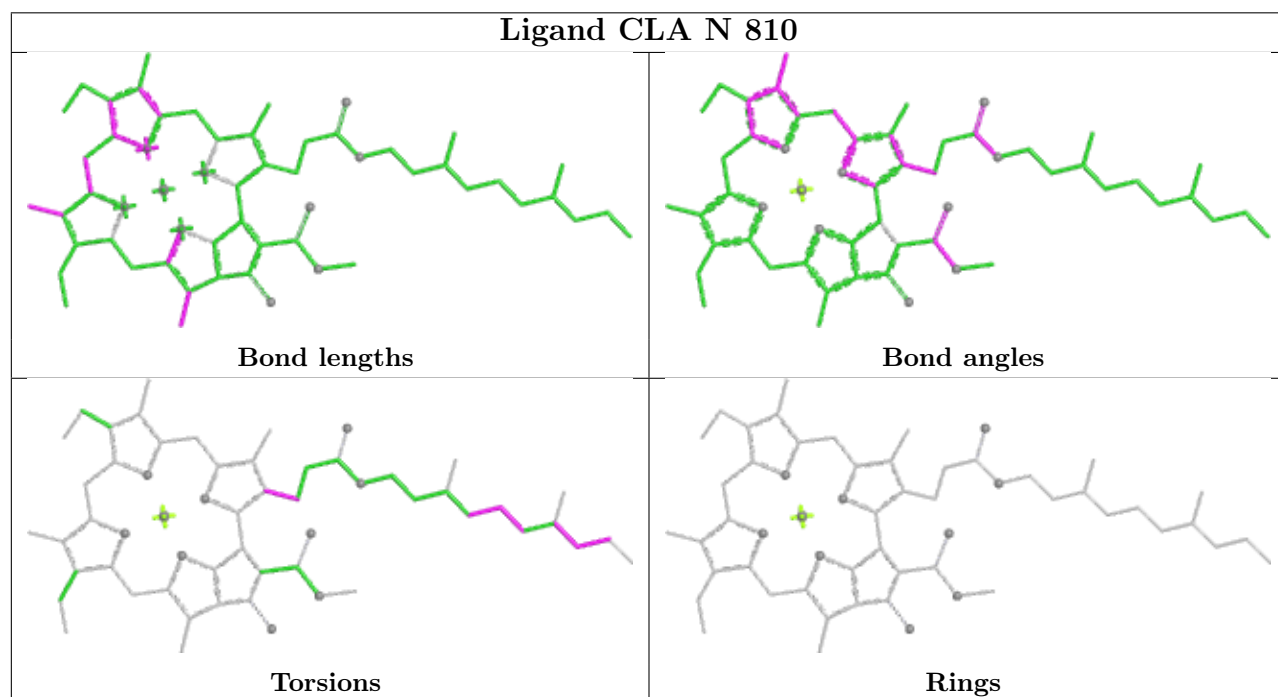
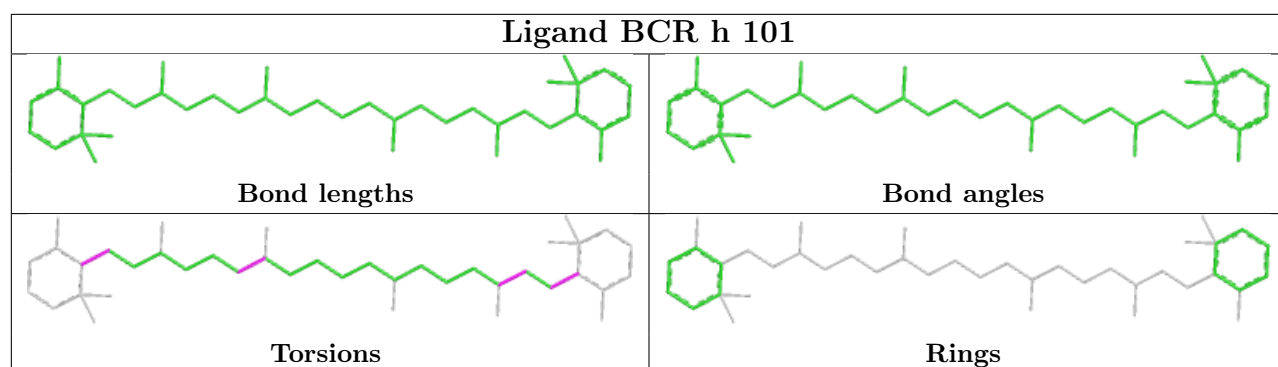




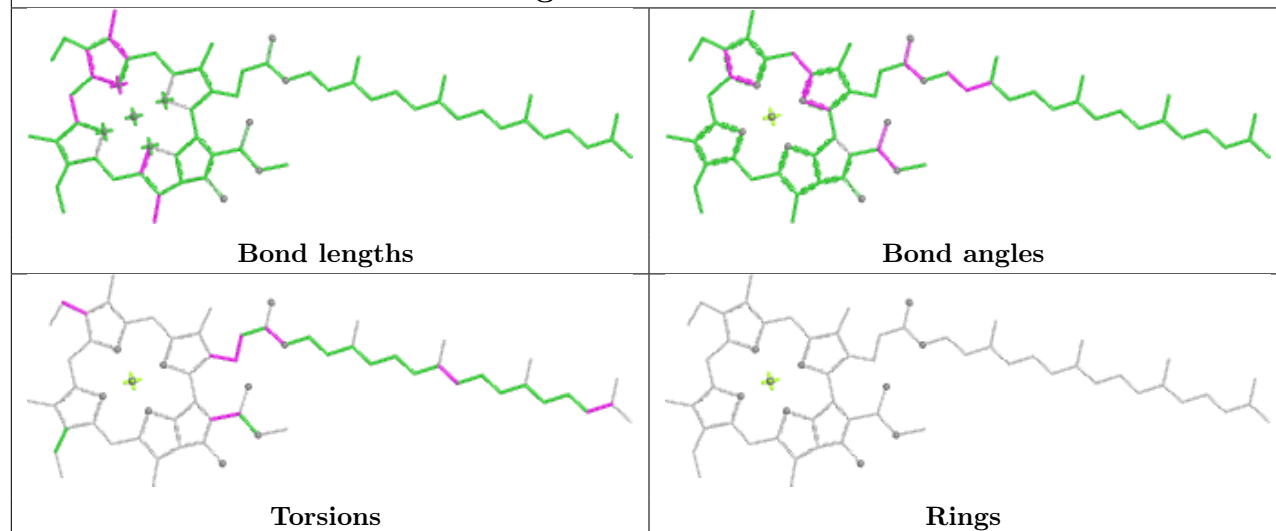




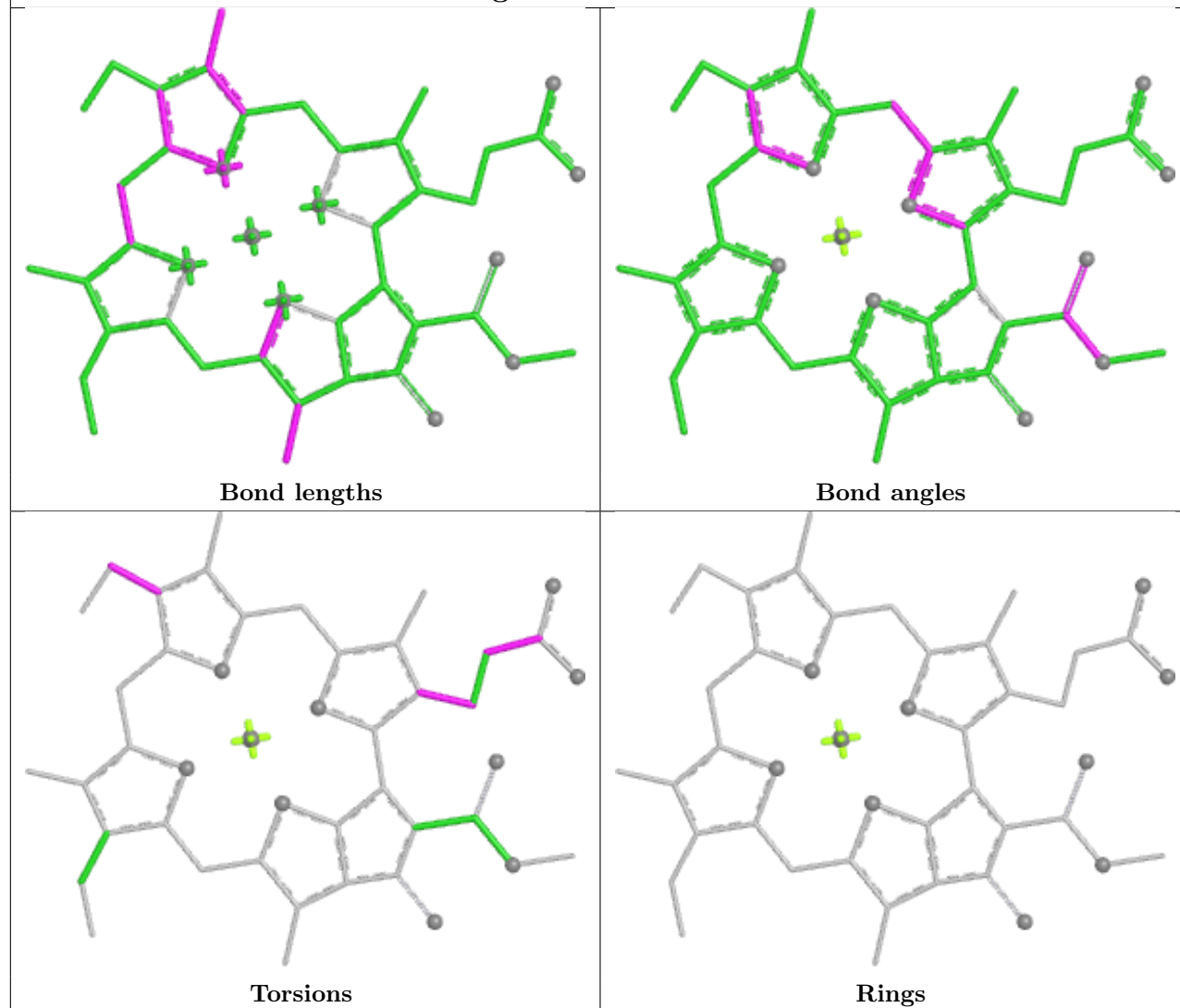


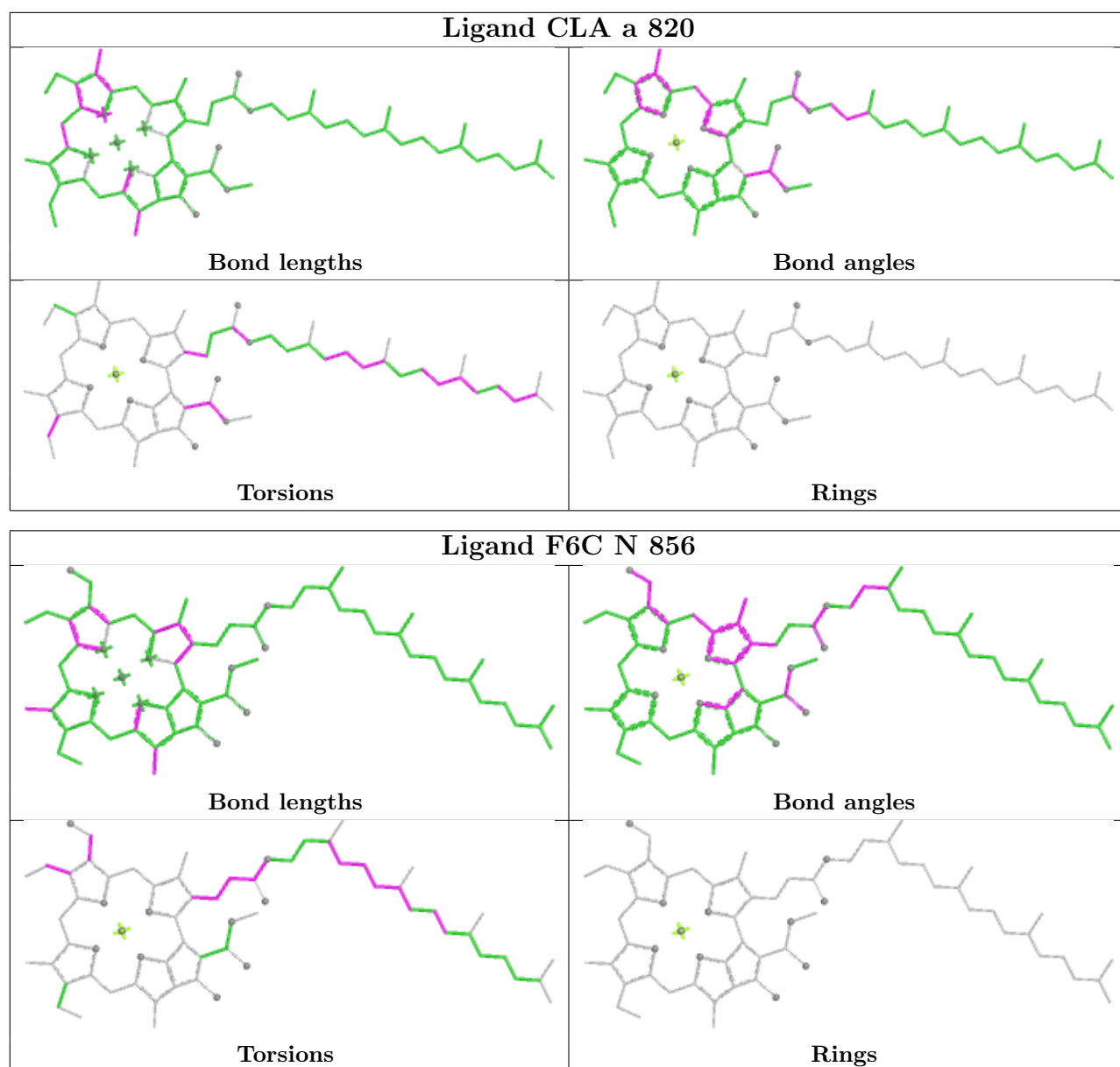


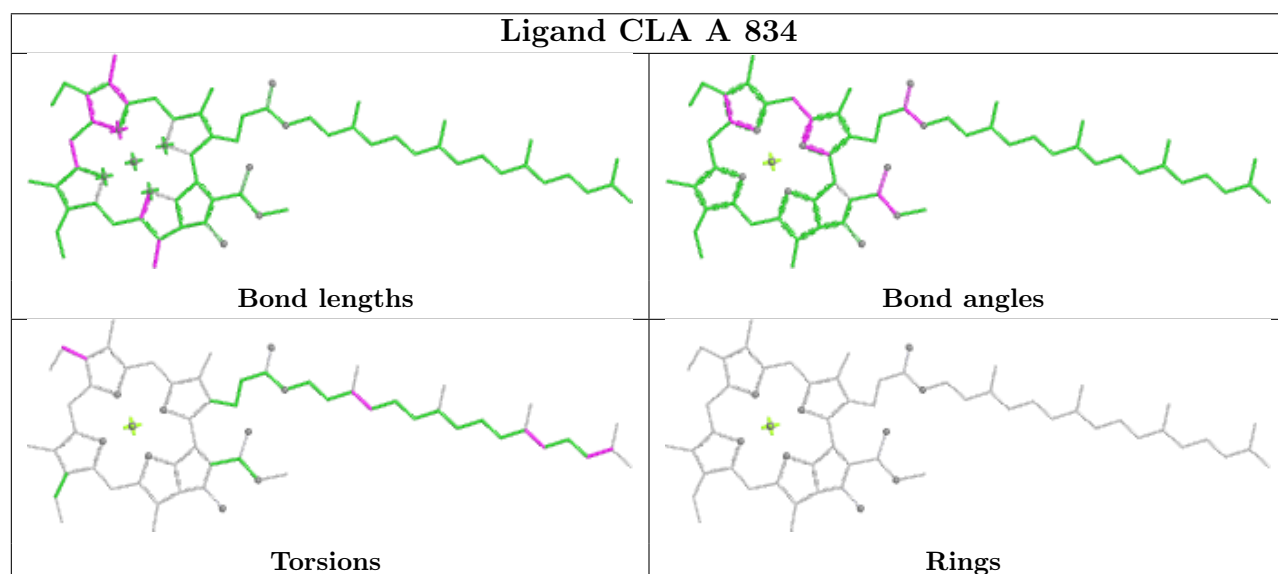
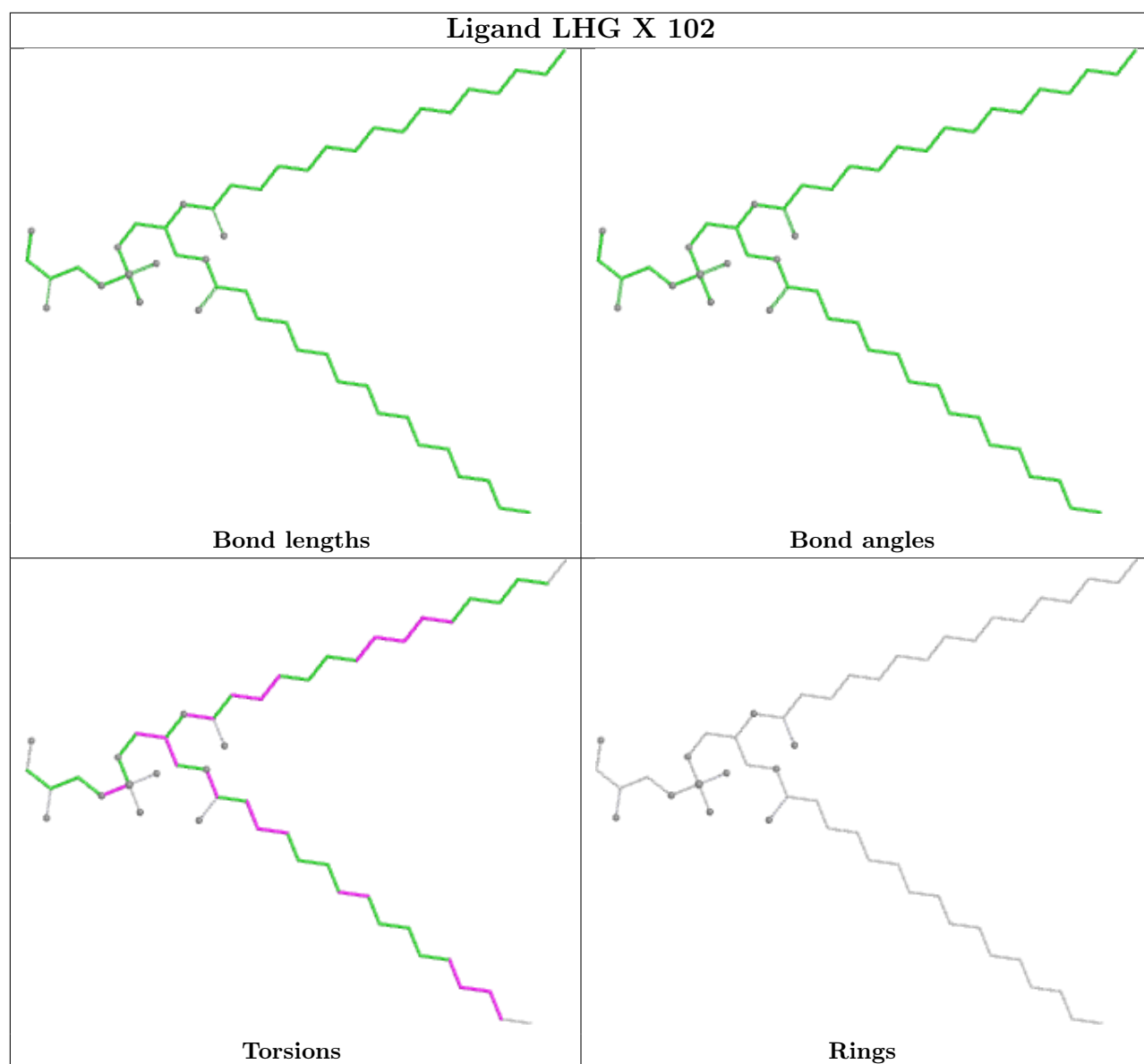
Ligand CLA a 842



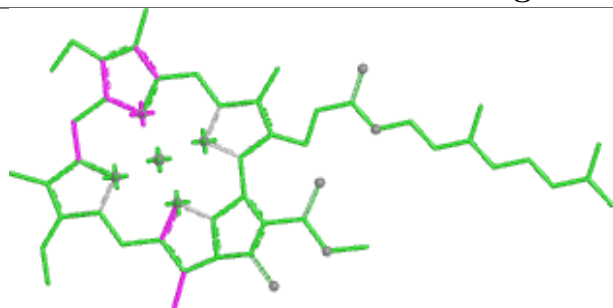
Ligand CLA B 810



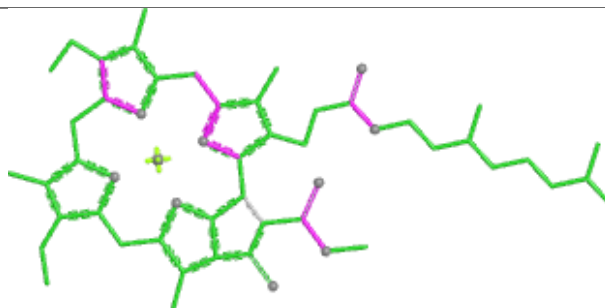




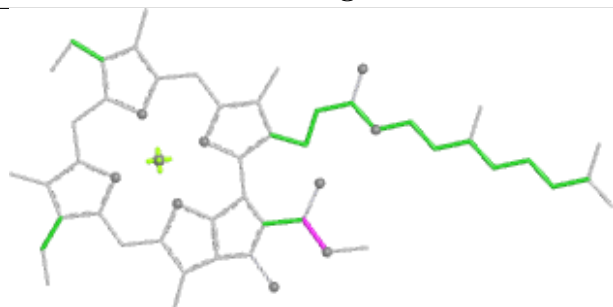
Ligand CLA X 103



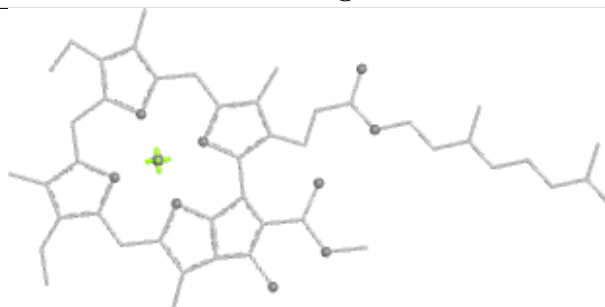
Bond lengths



Bond angles

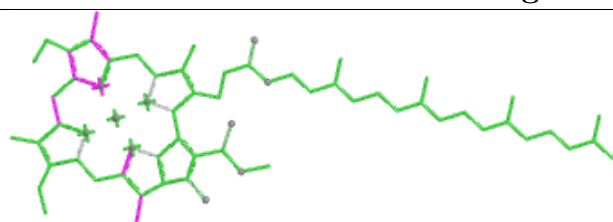


Torsions

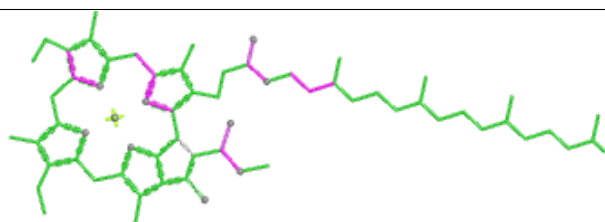


Rings

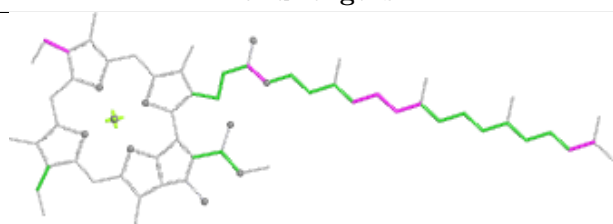
Ligand CLA f 201



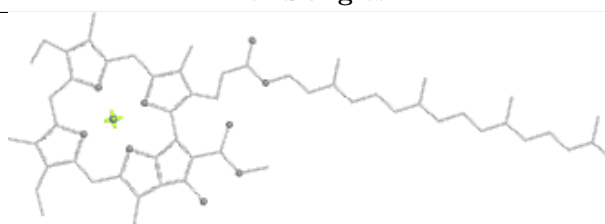
Bond lengths



Bond angles

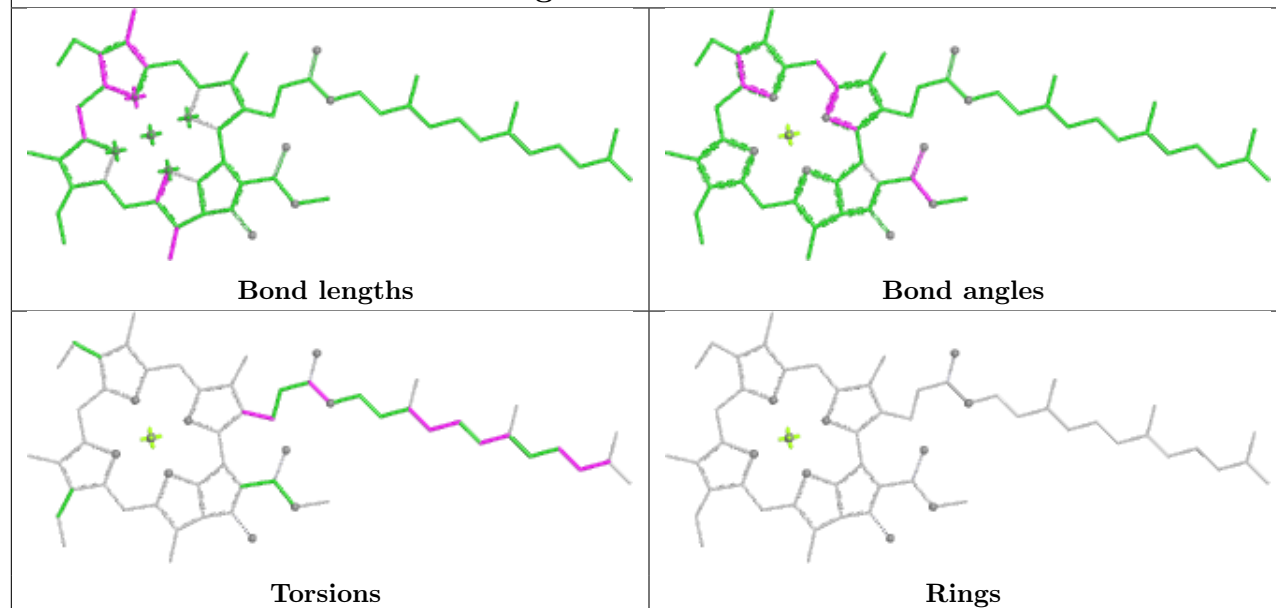


Torsions

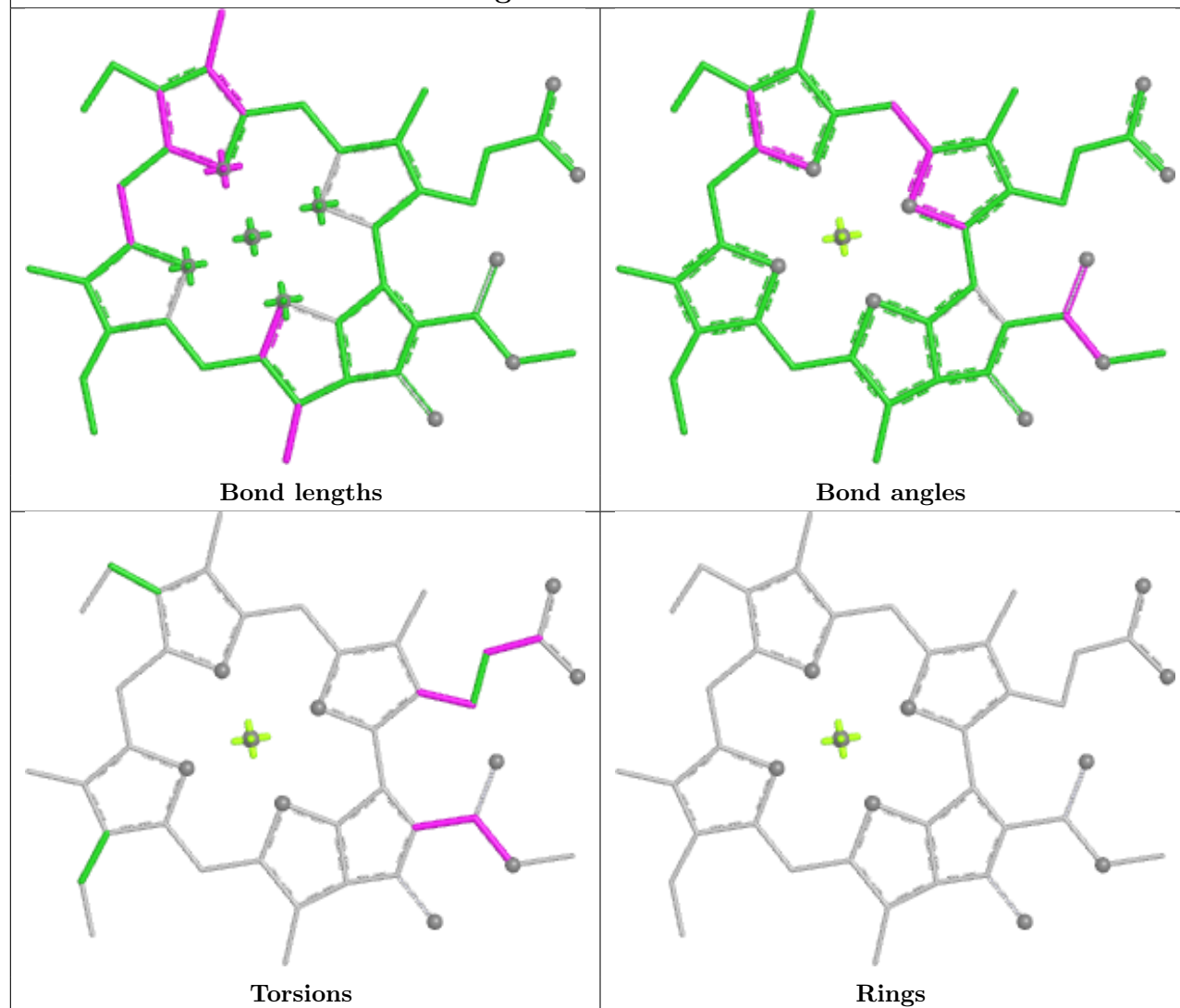


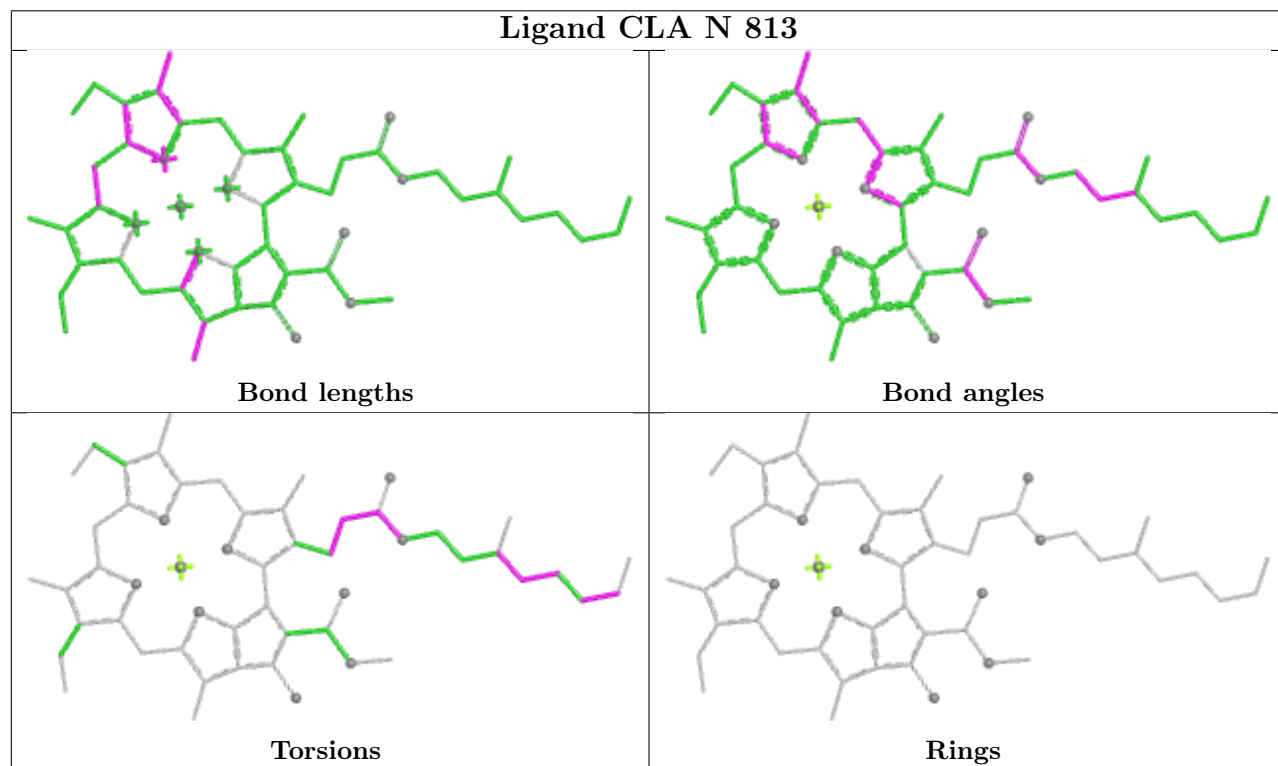
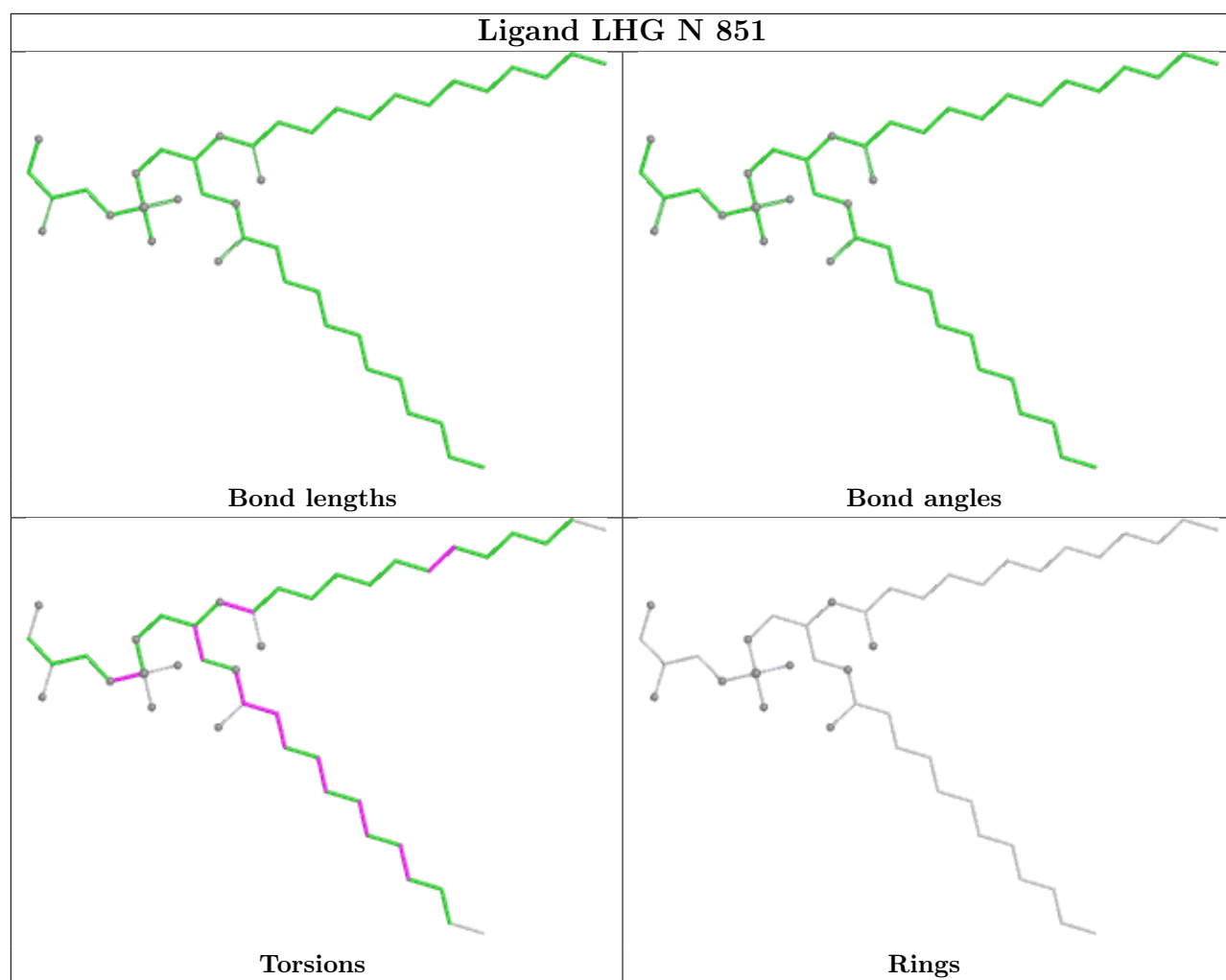
Rings

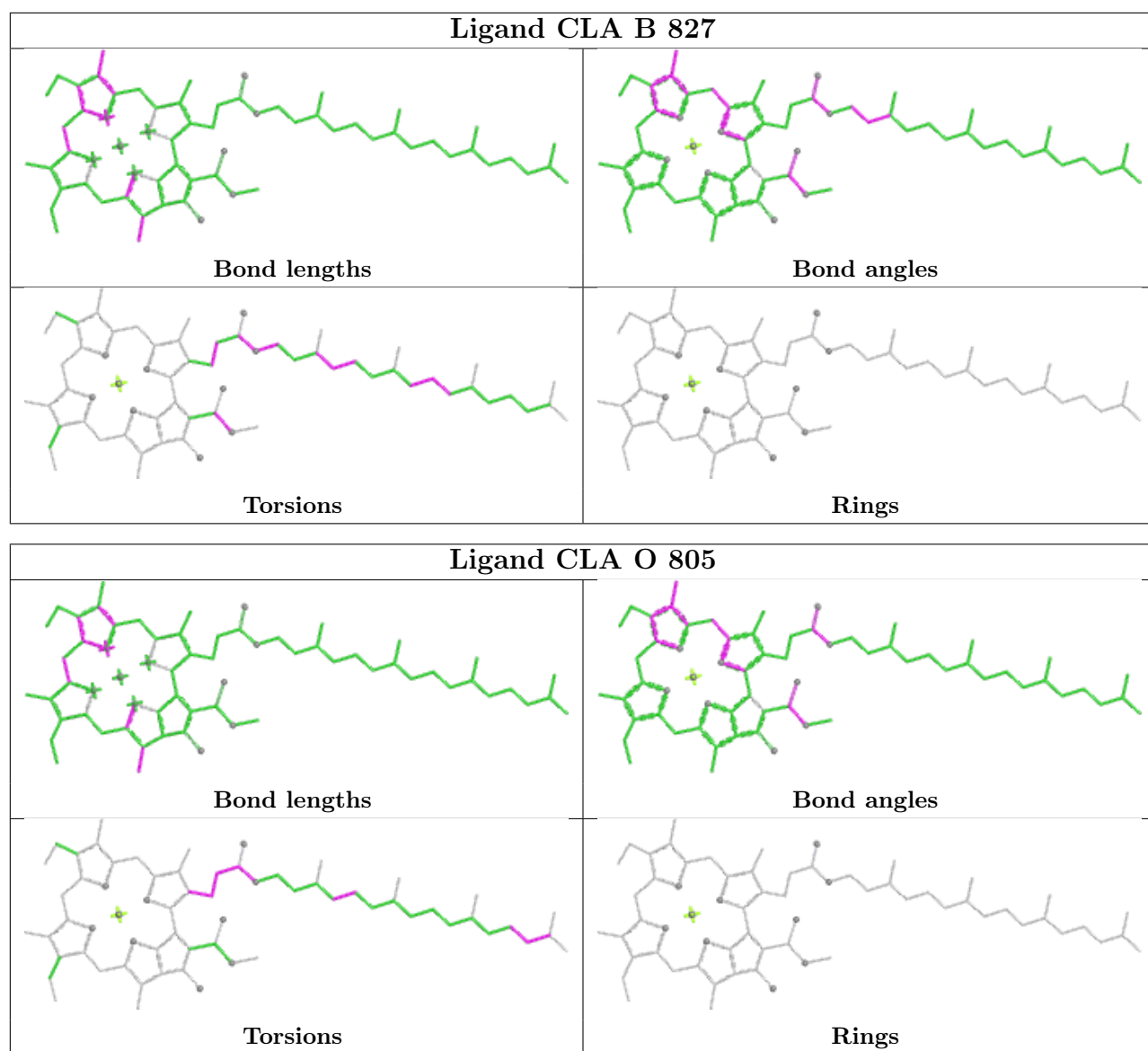
Ligand CLA b 818

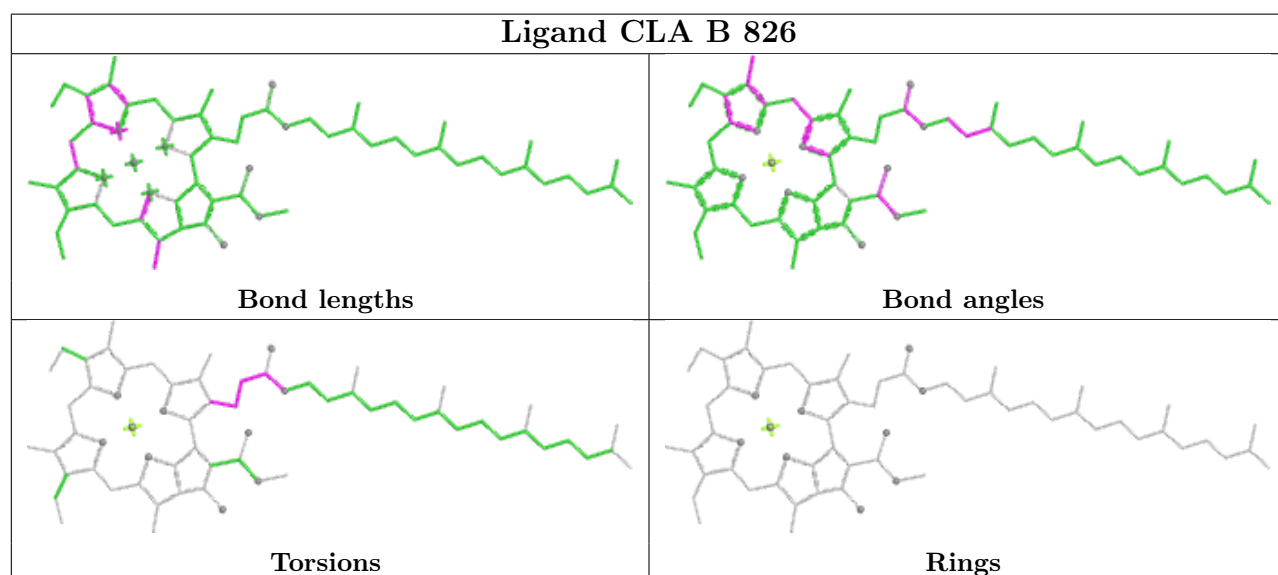
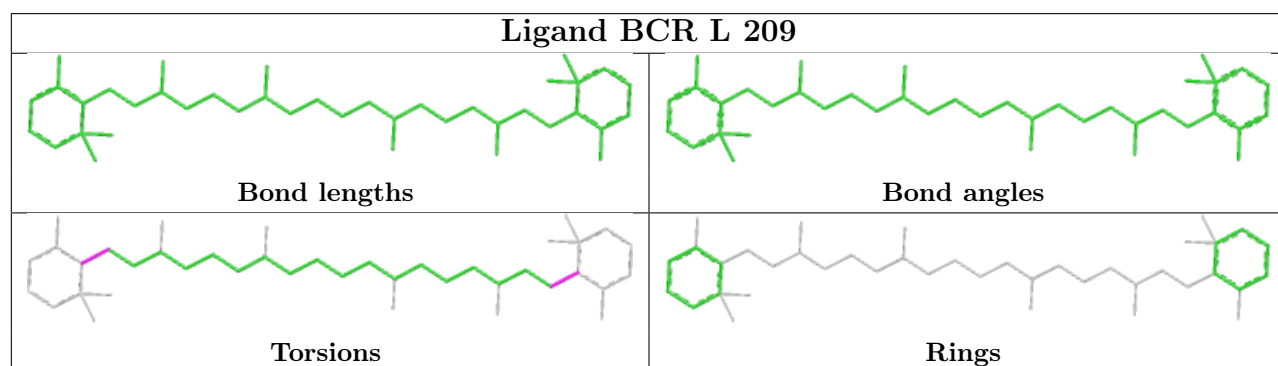
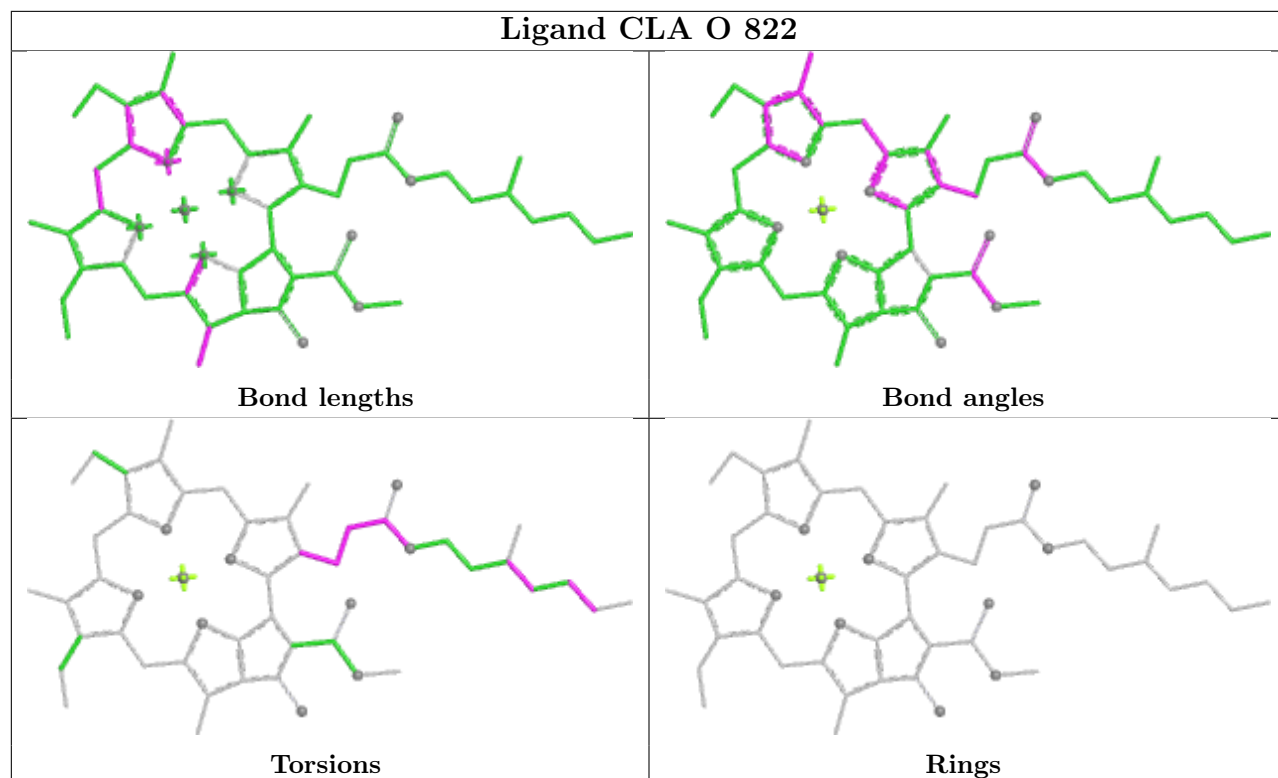


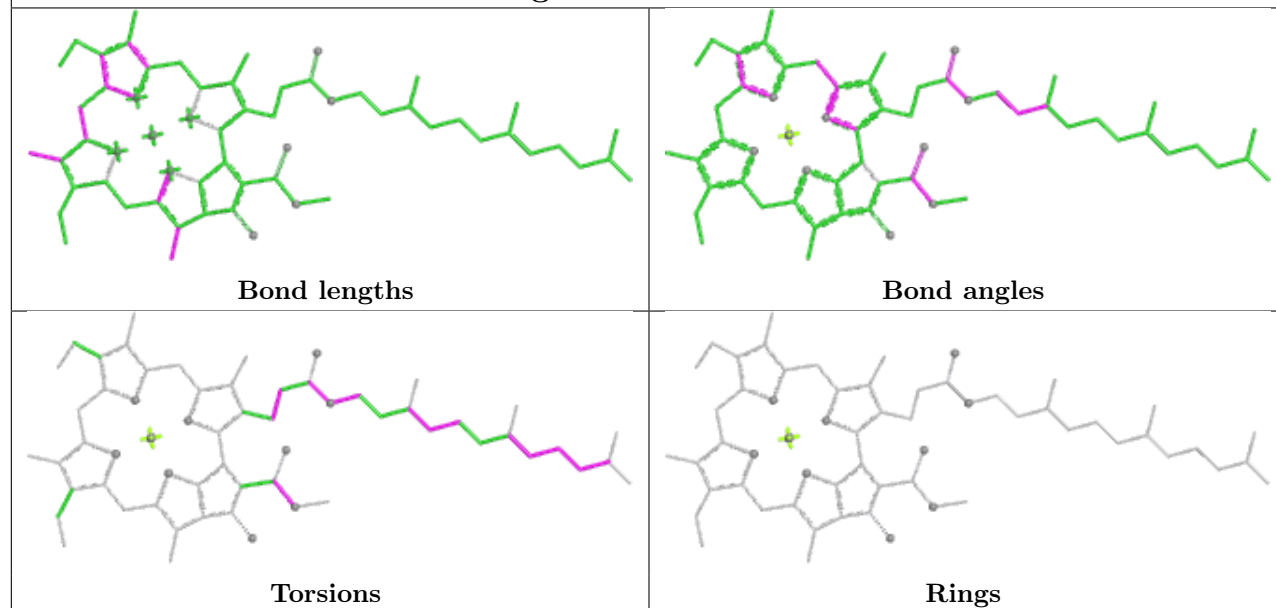
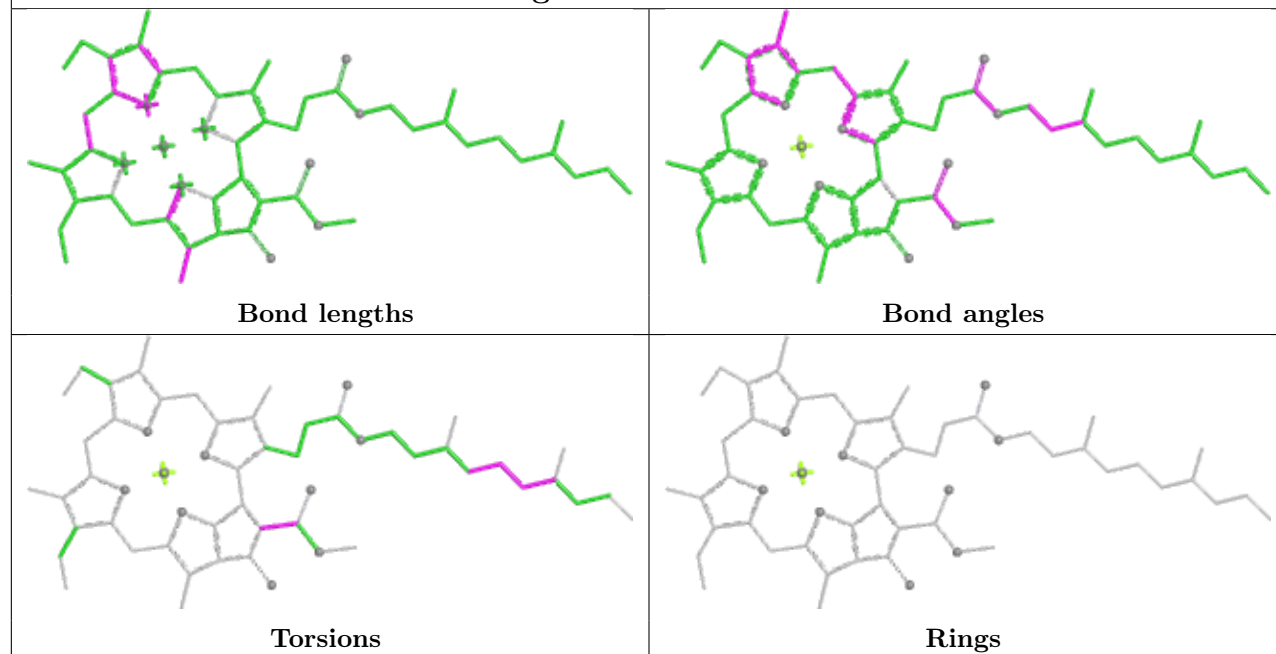
Ligand CLA b 836

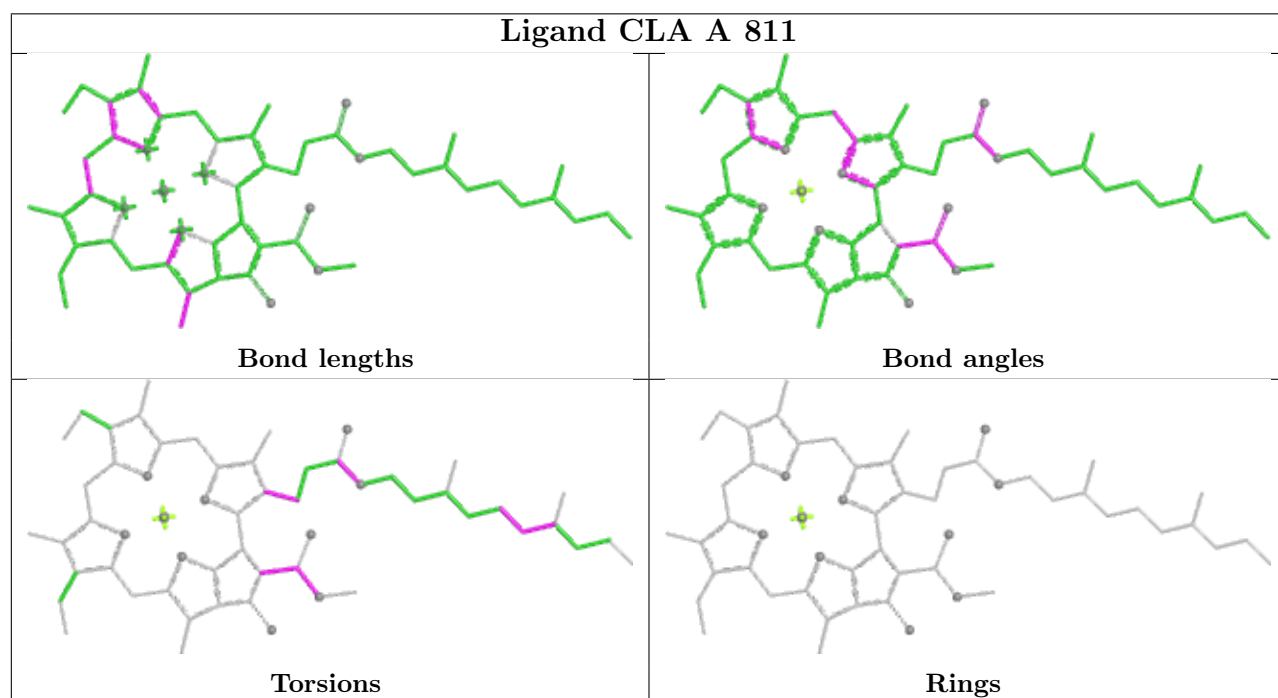
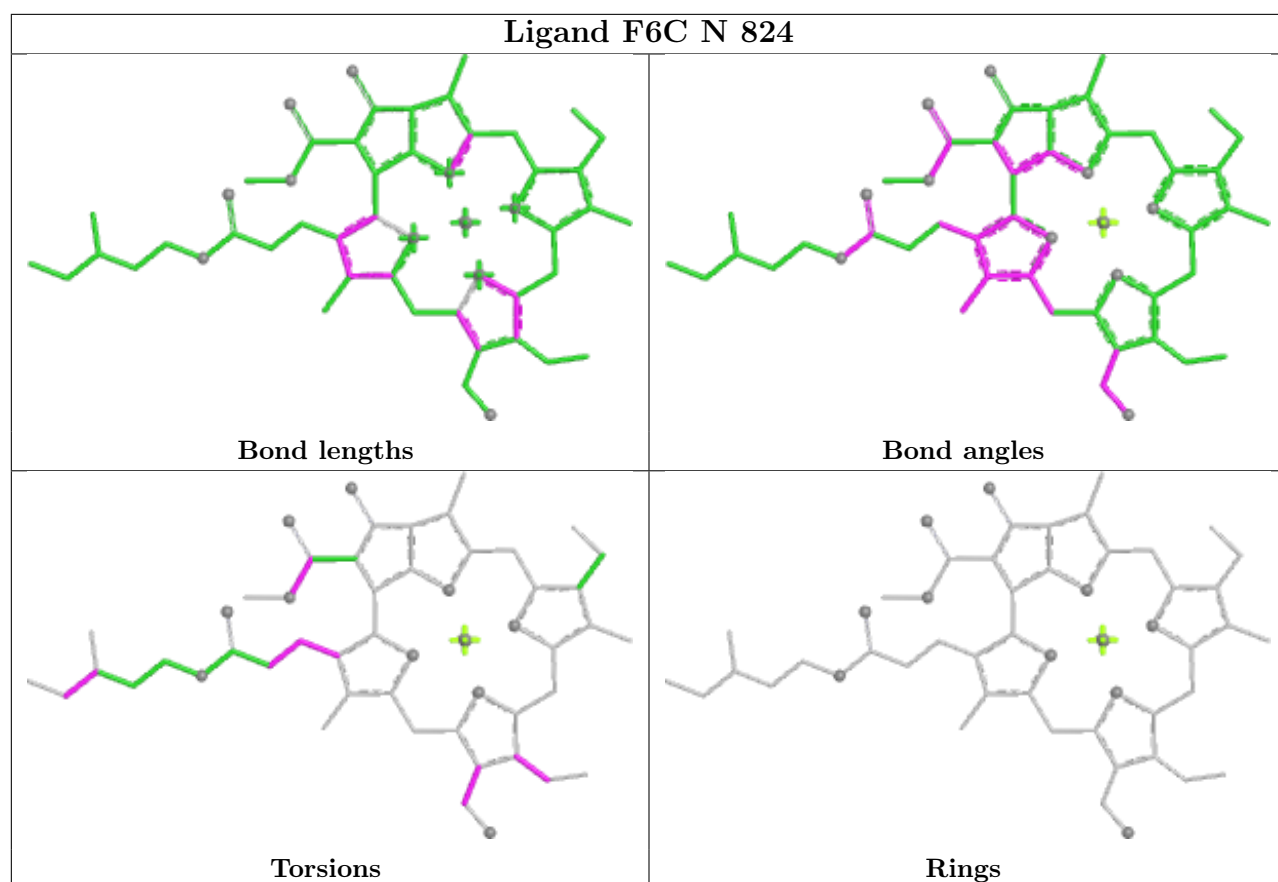


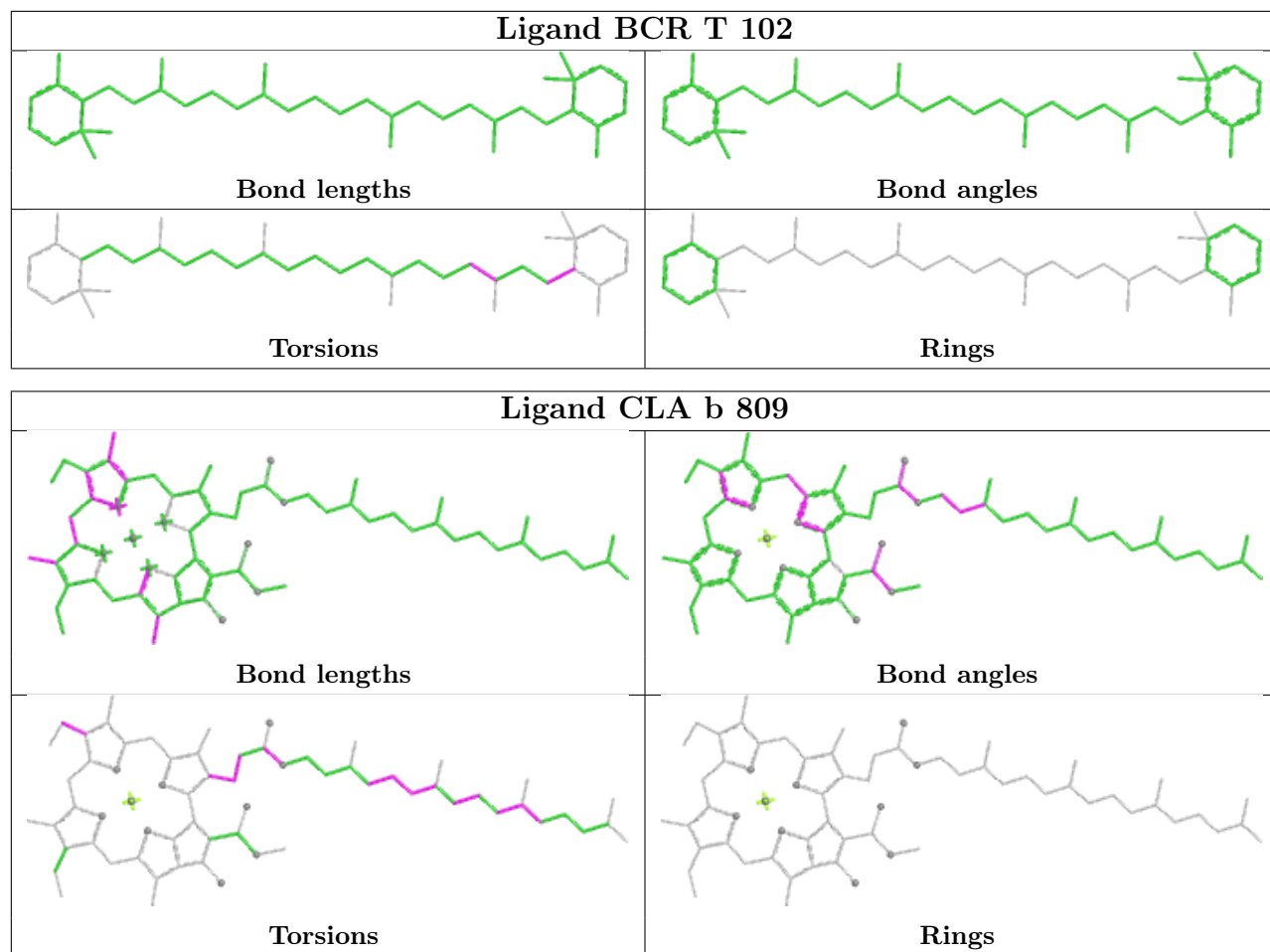


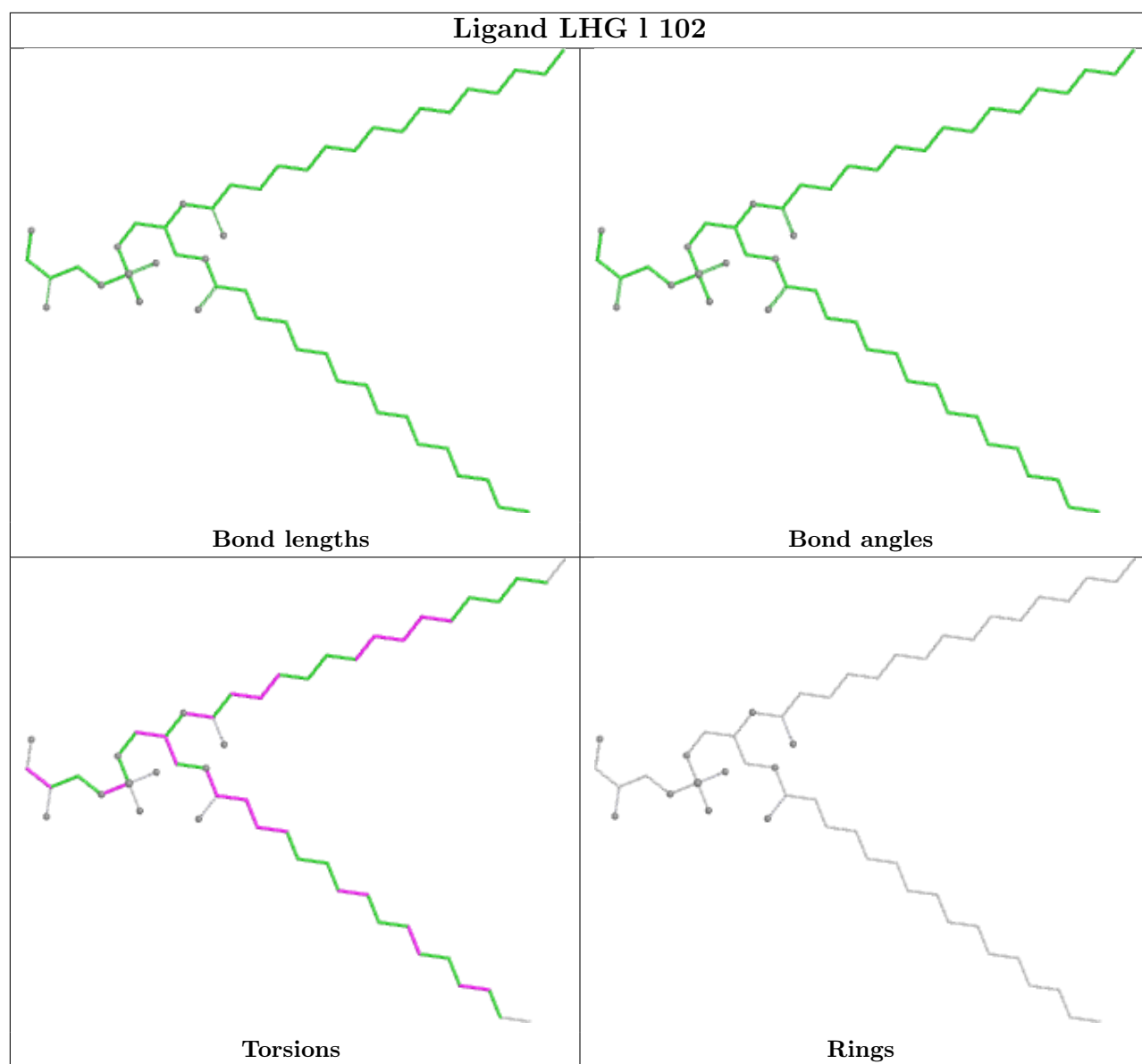




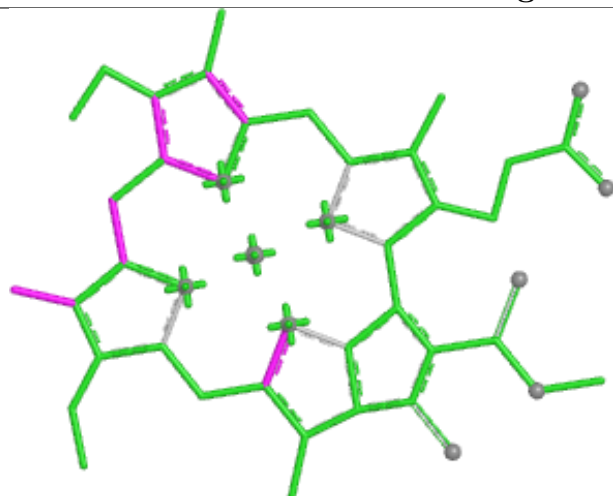
Ligand CLA A 829**Ligand CLA B 814**



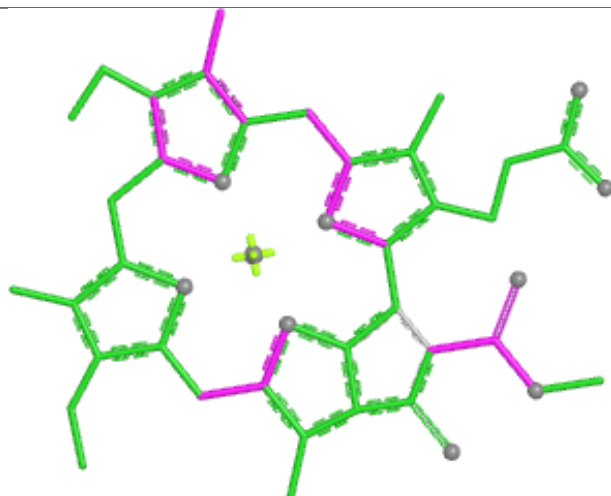




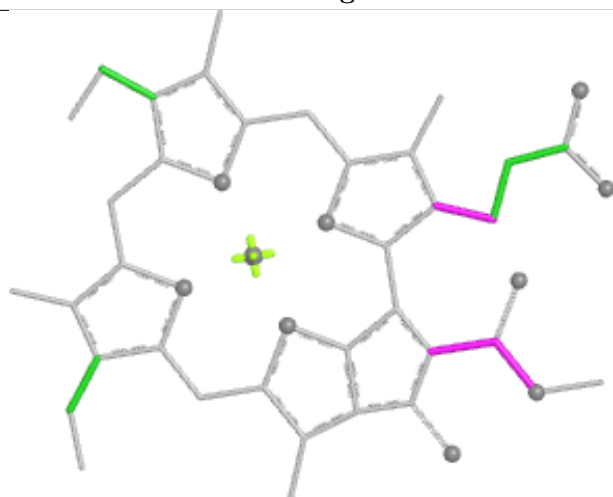
Ligand CLA b 815



Bond lengths



Bond angles

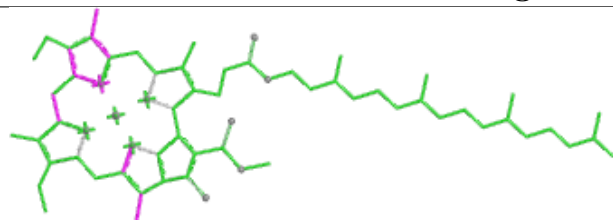


Torsions

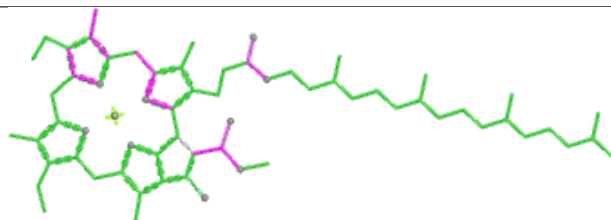


Rings

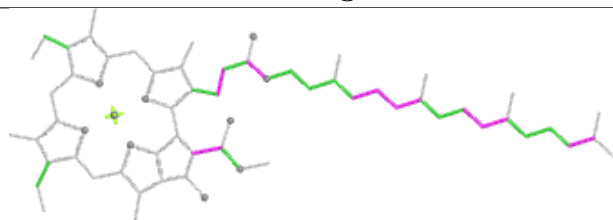
Ligand CLA A 831



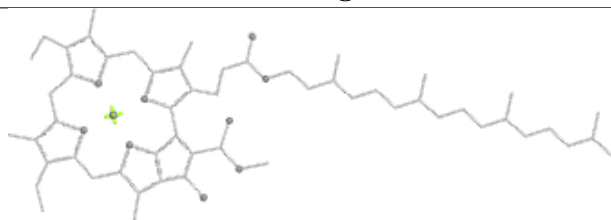
Bond lengths



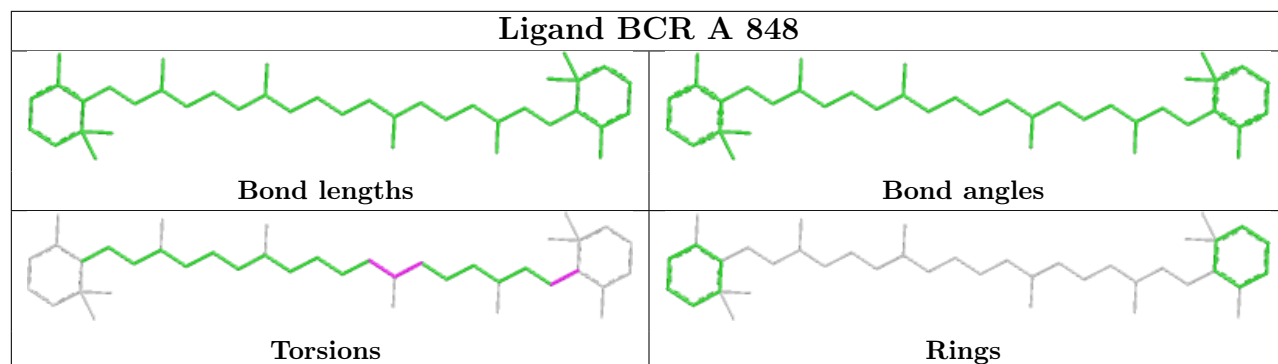
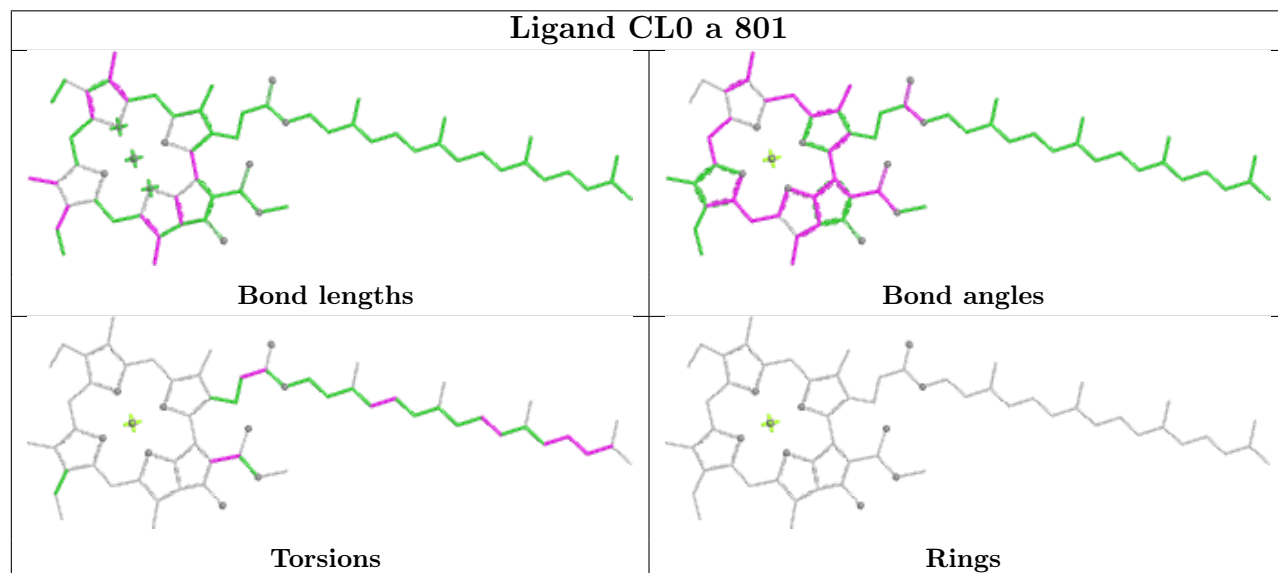
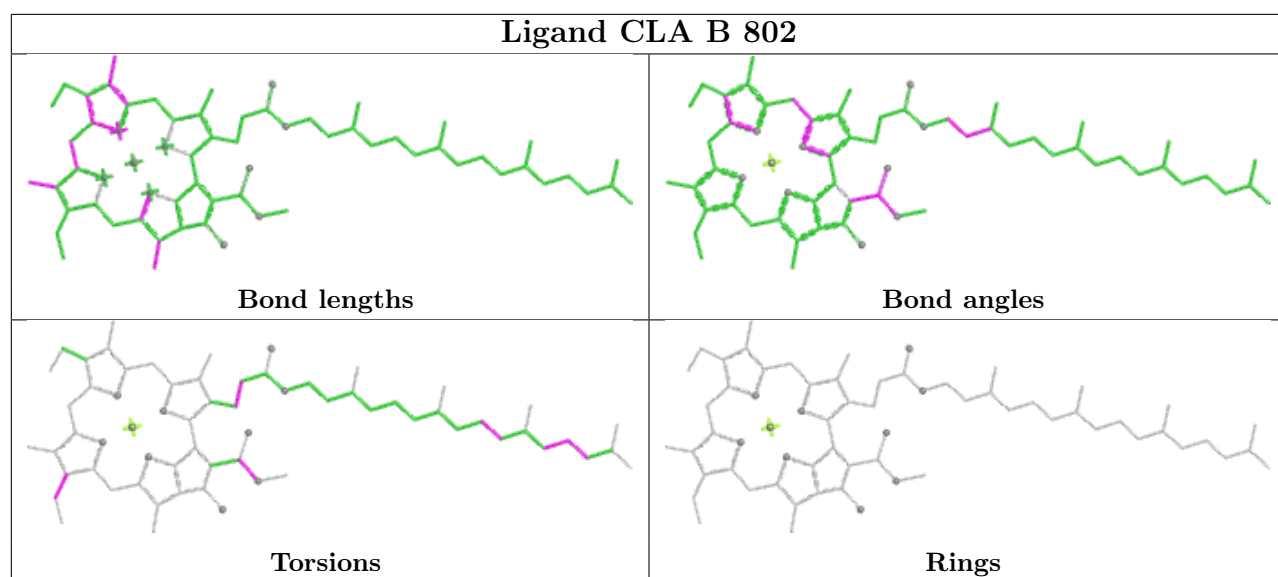
Bond angles

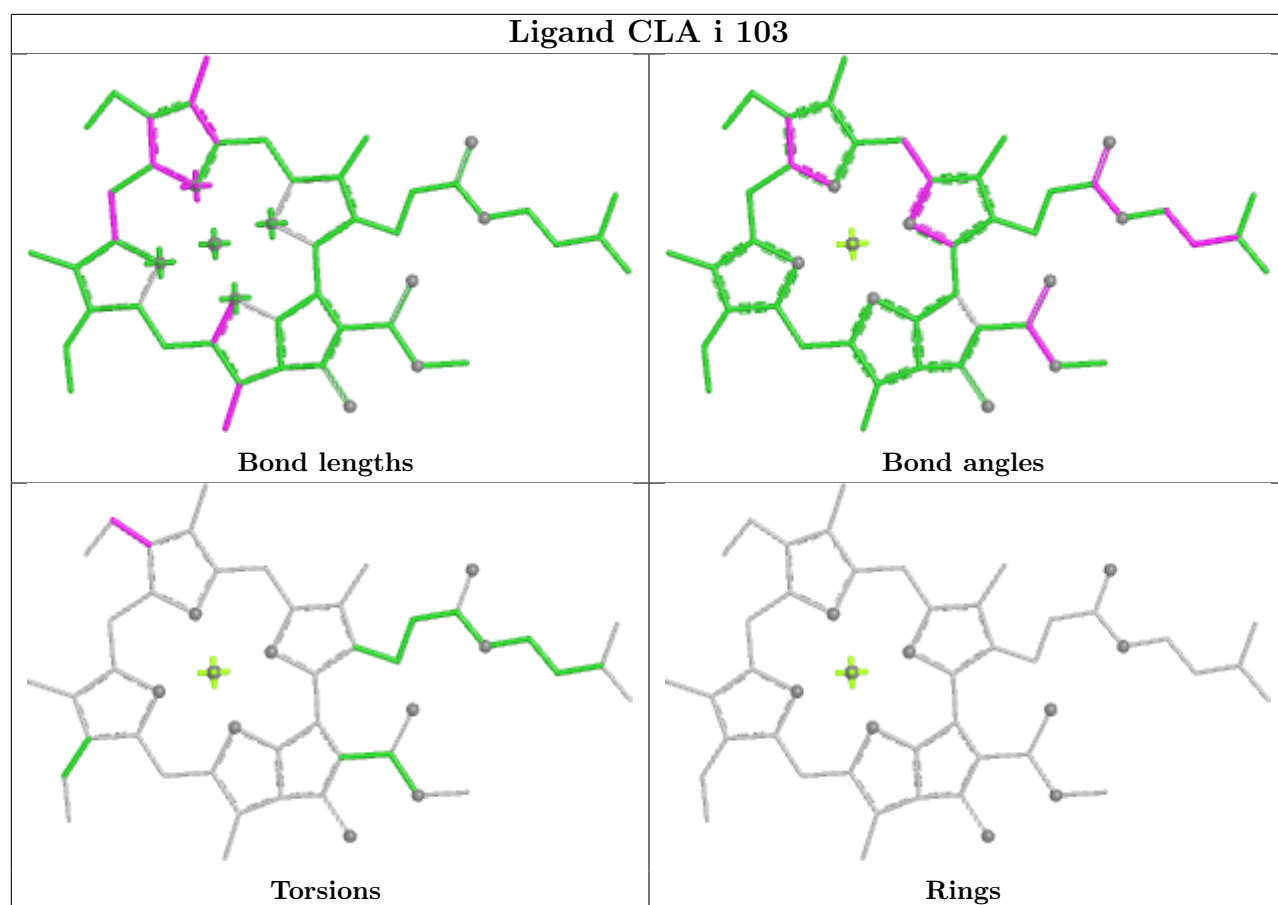


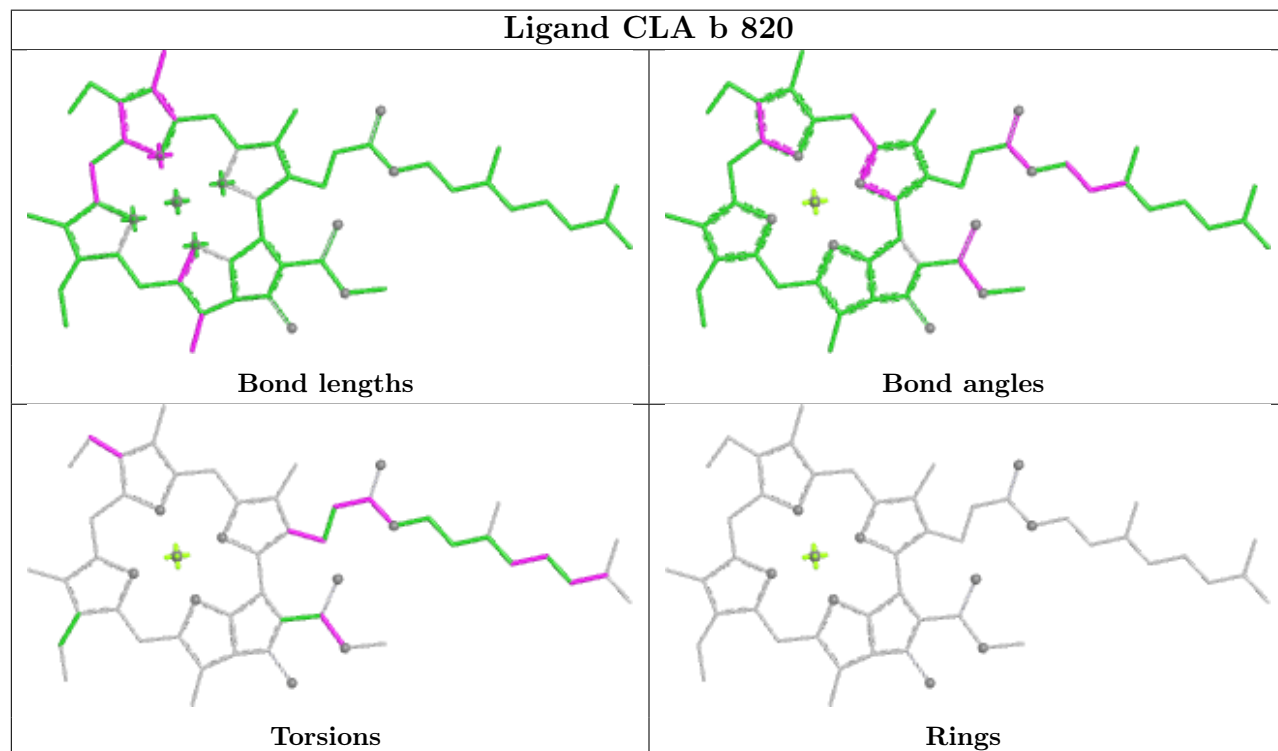
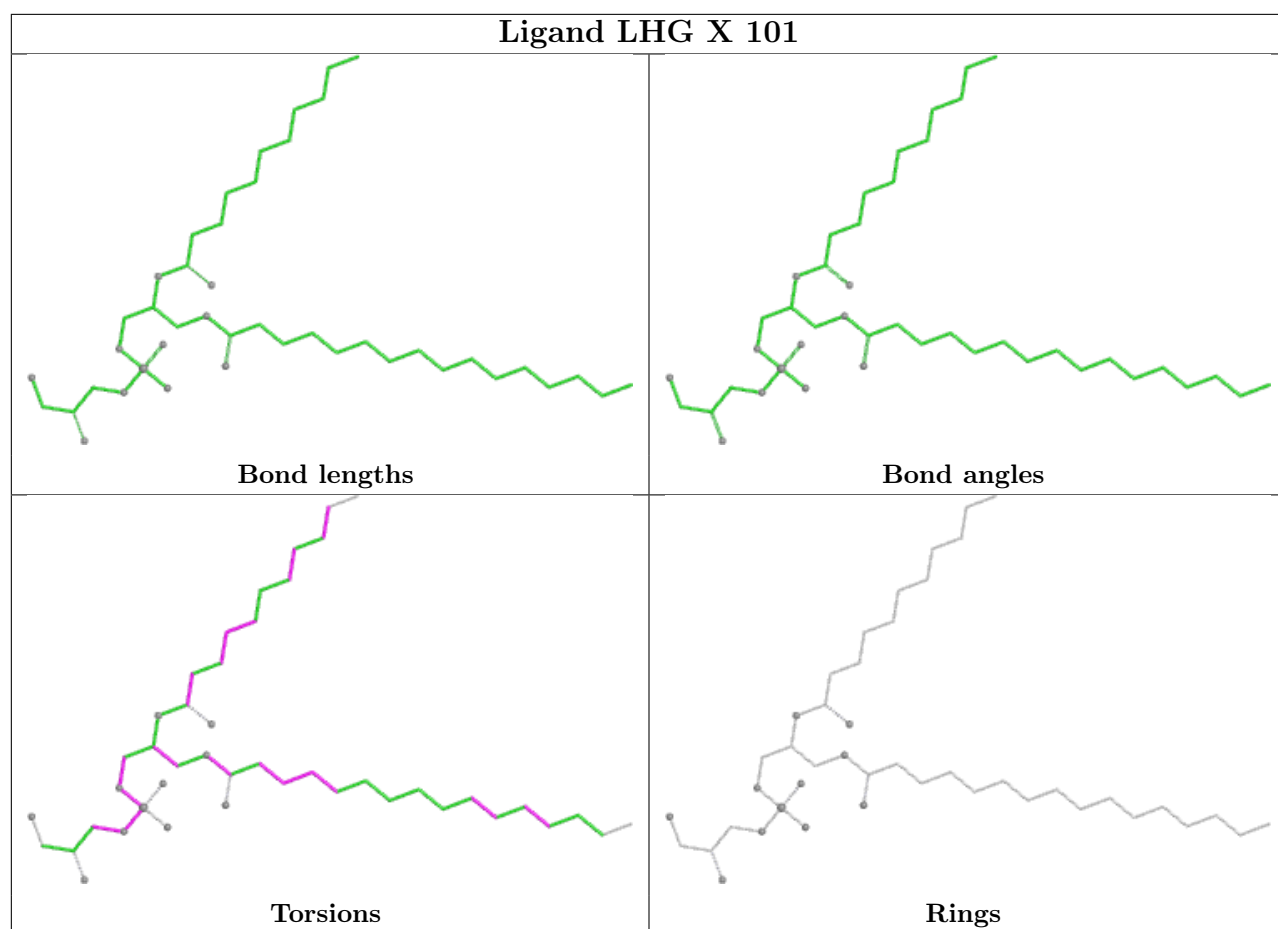
Torsions

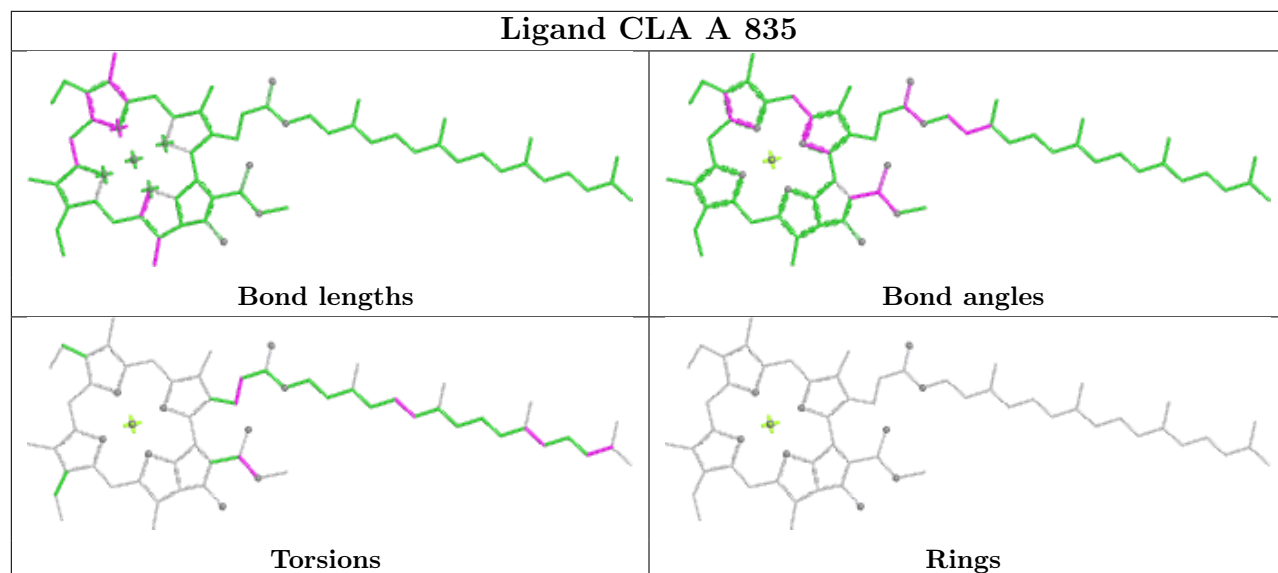
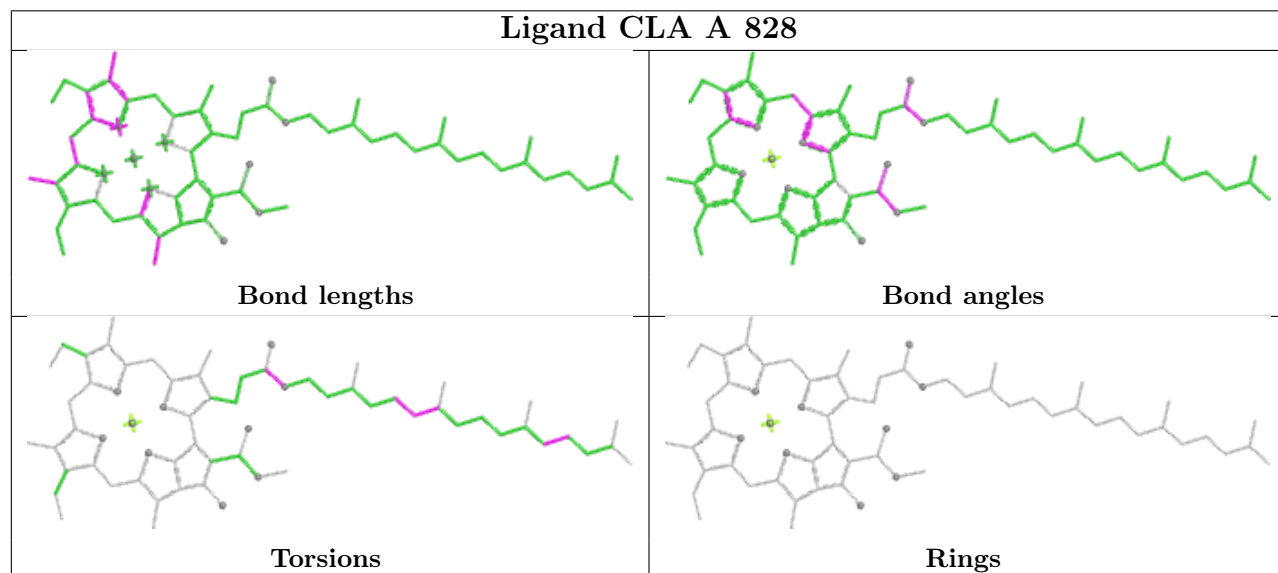
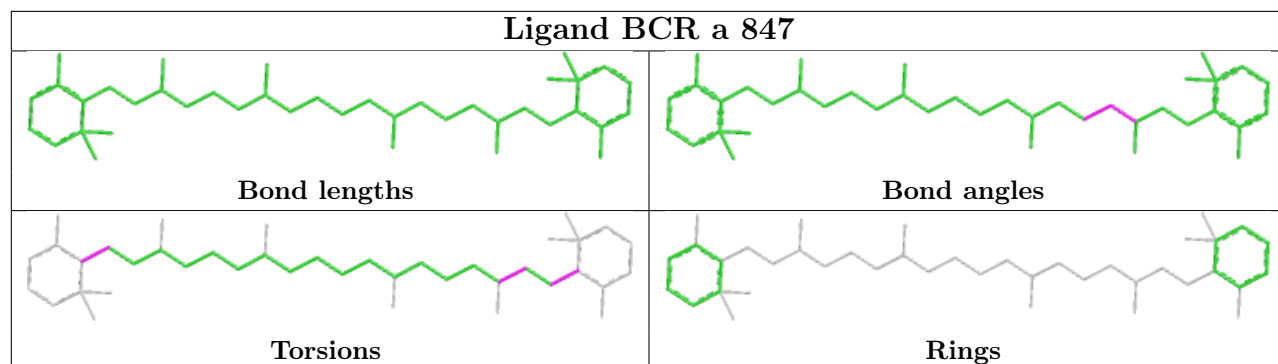


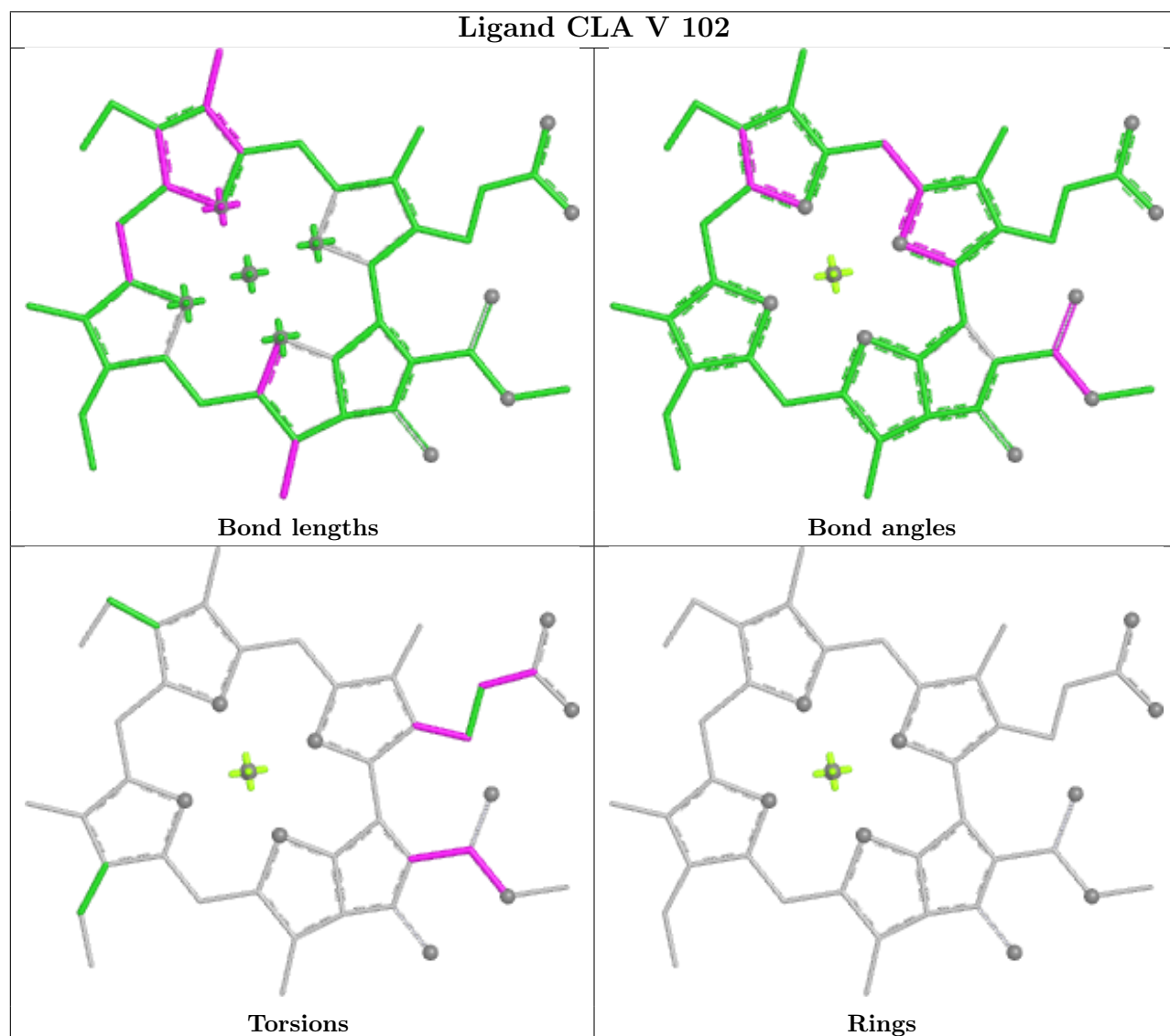
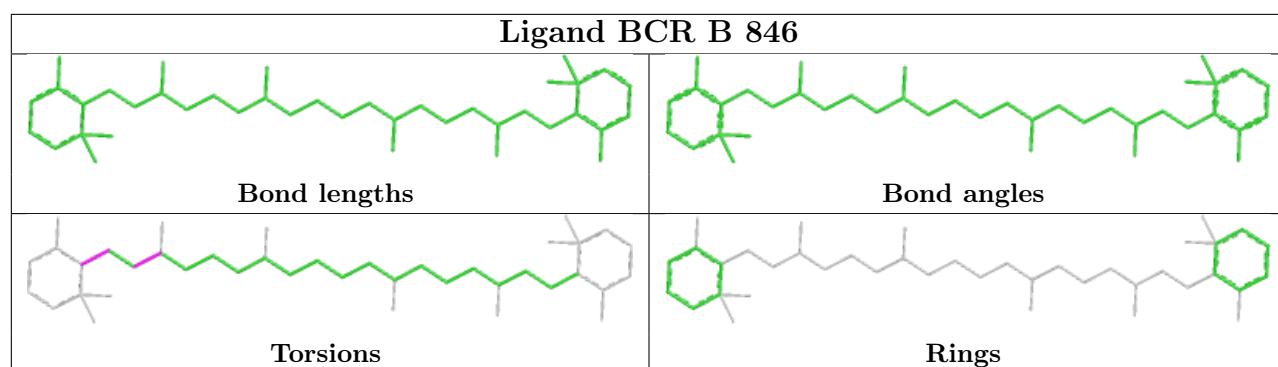
Rings

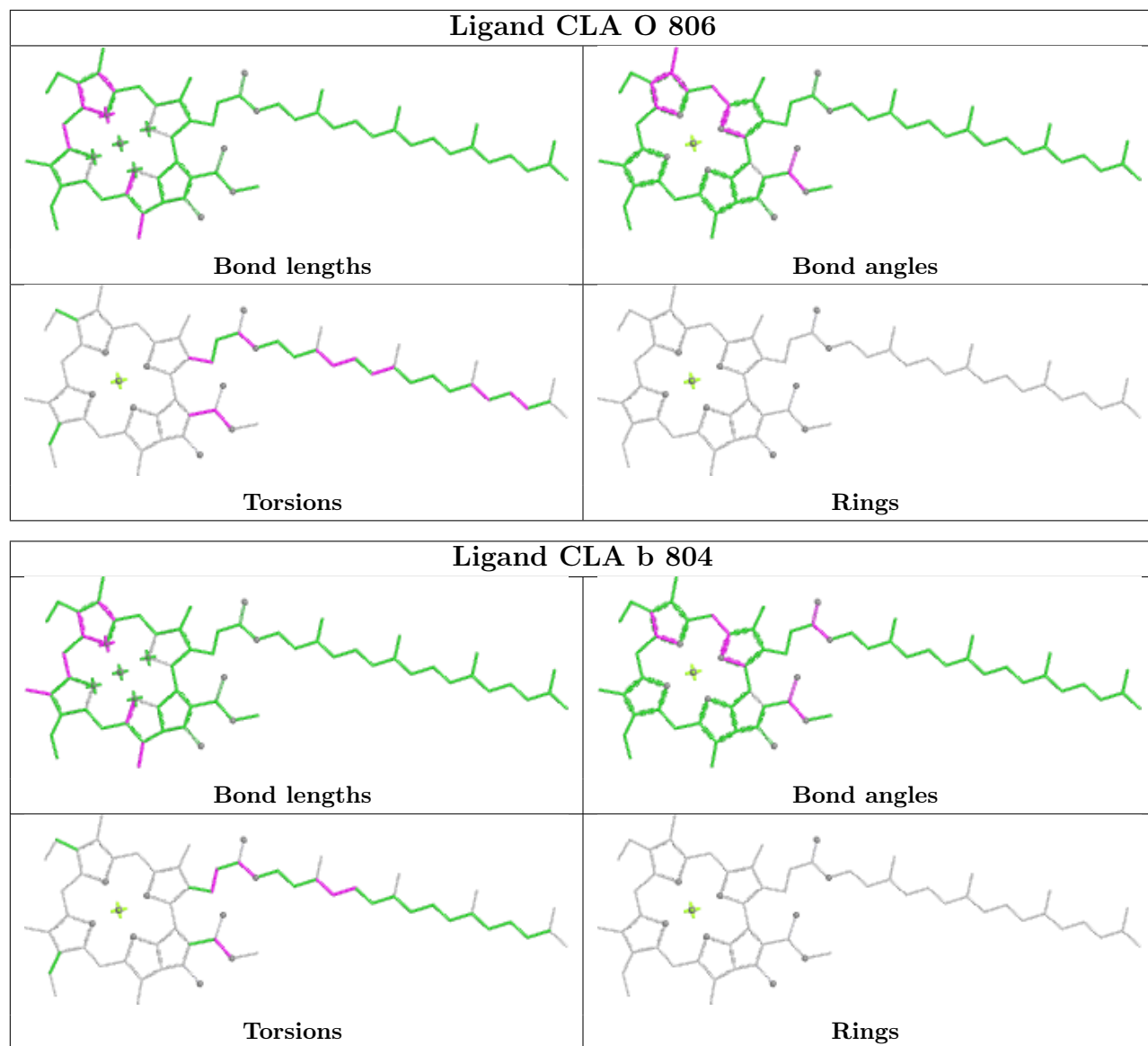




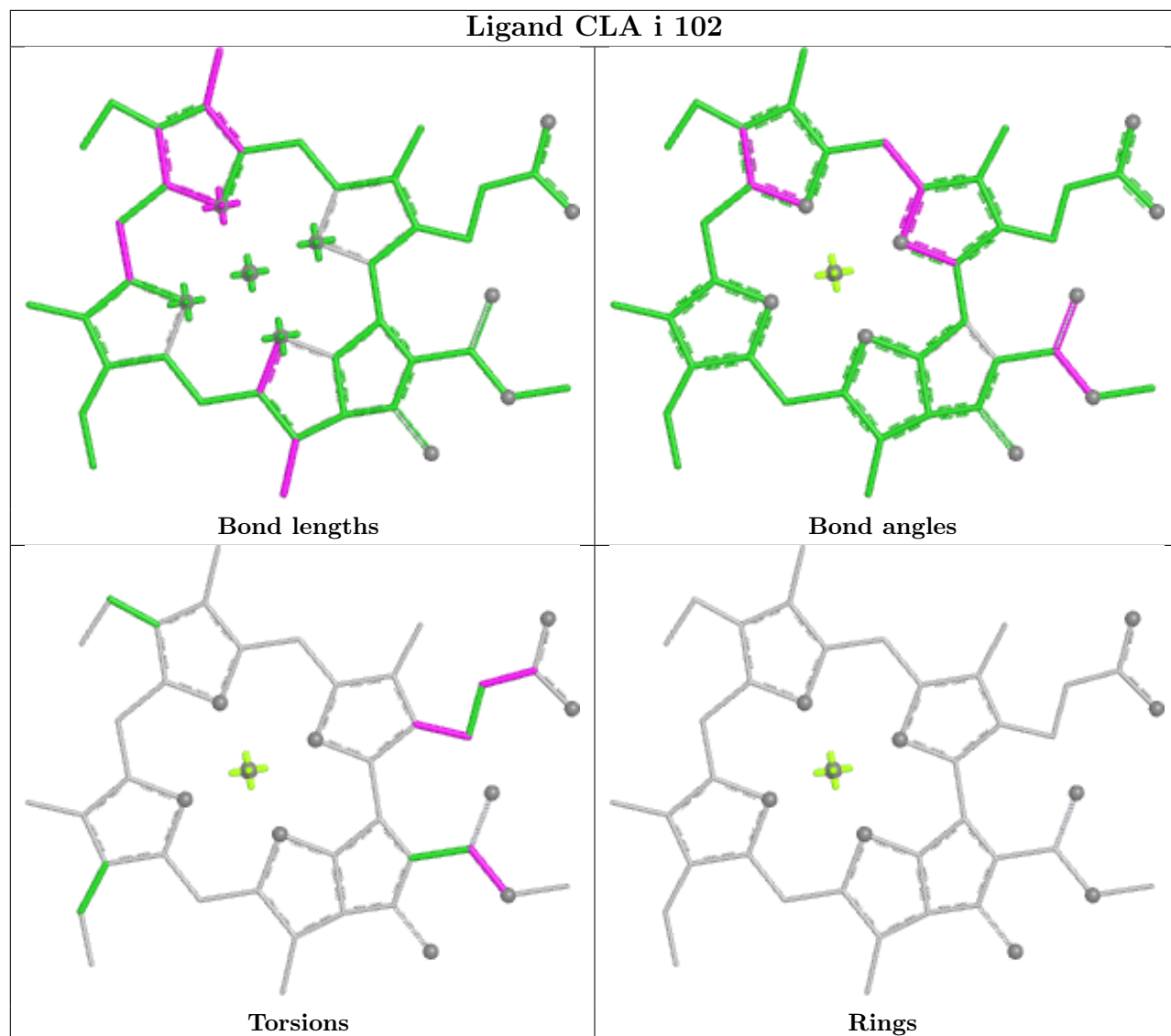


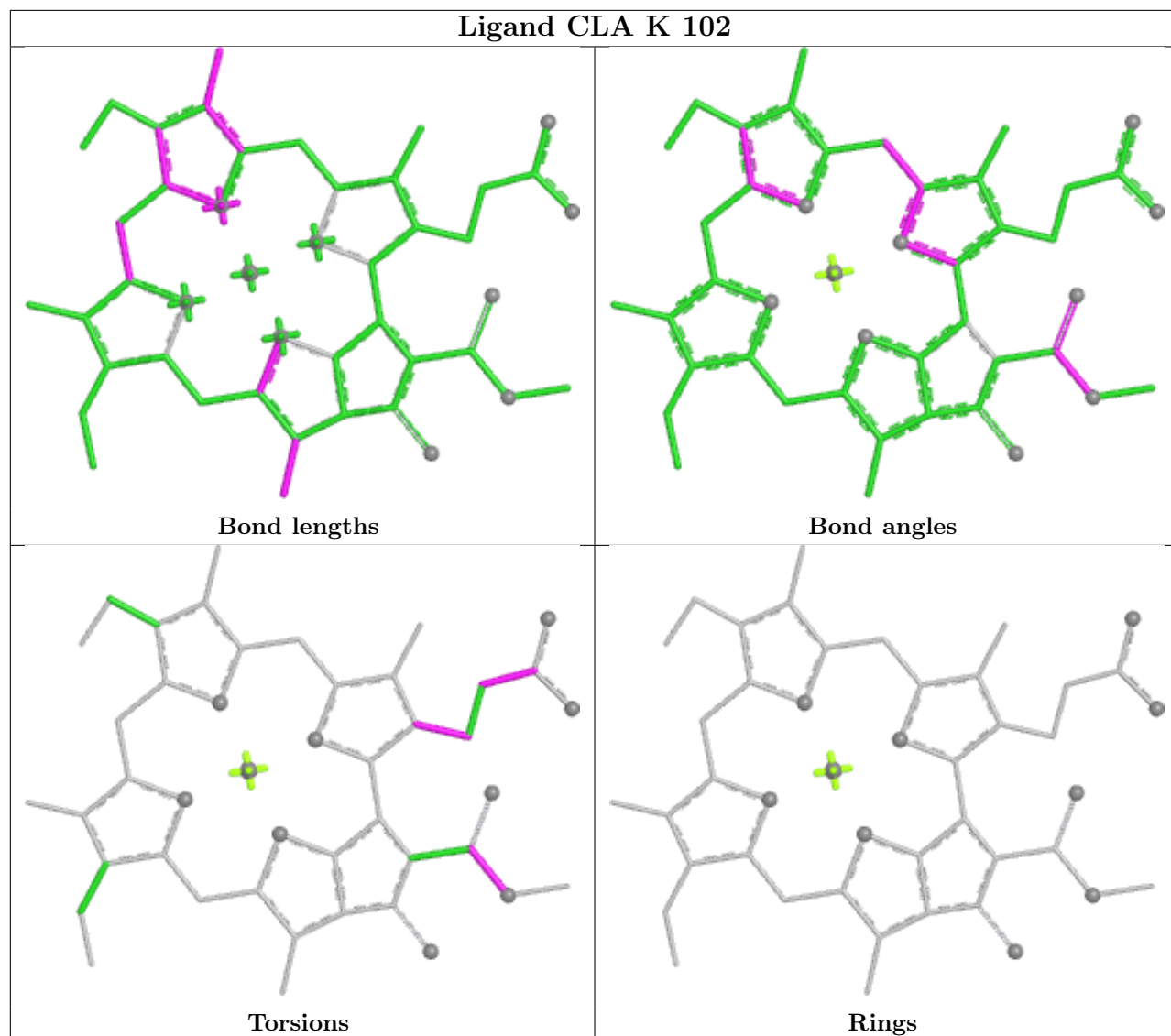


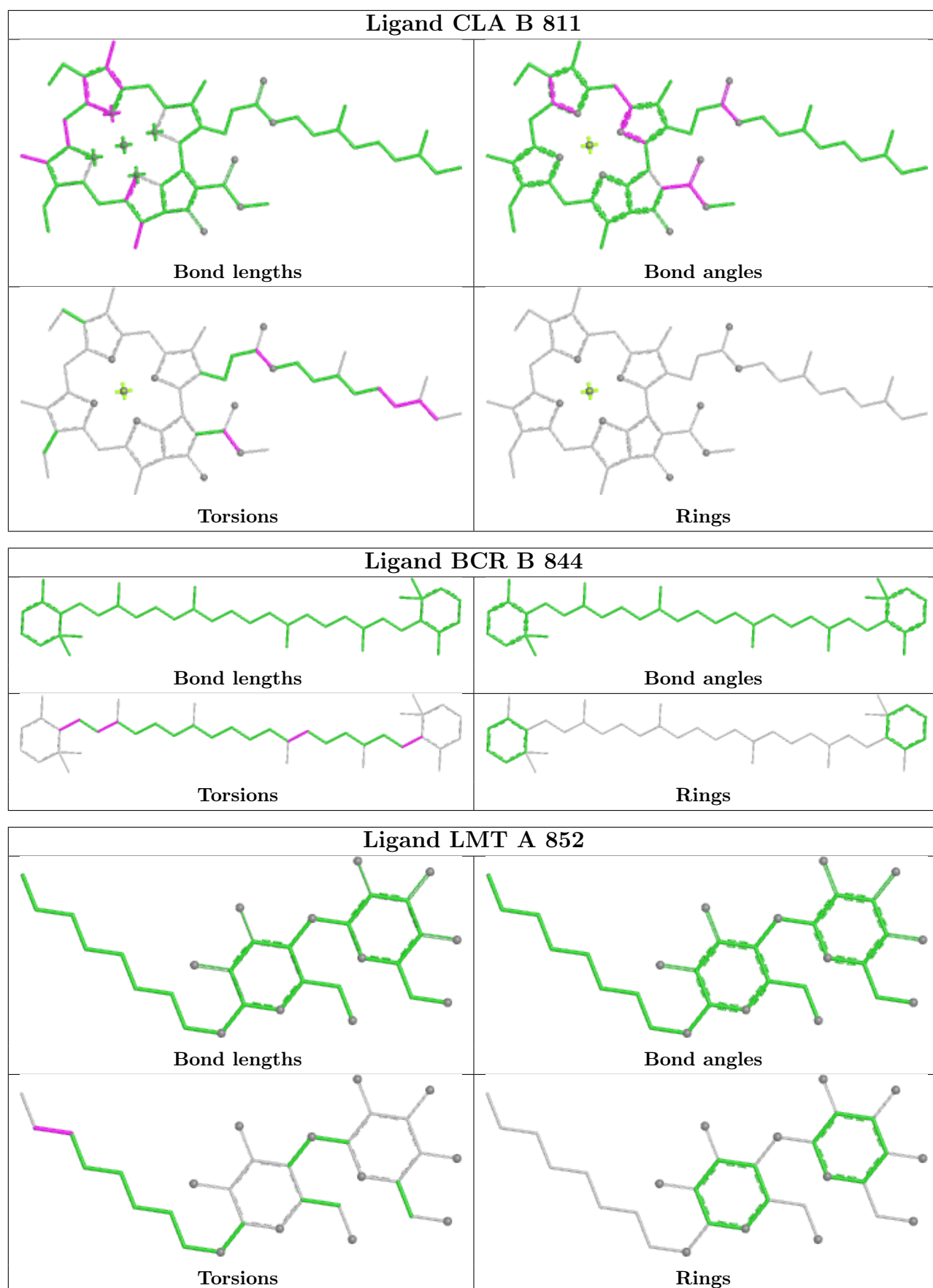




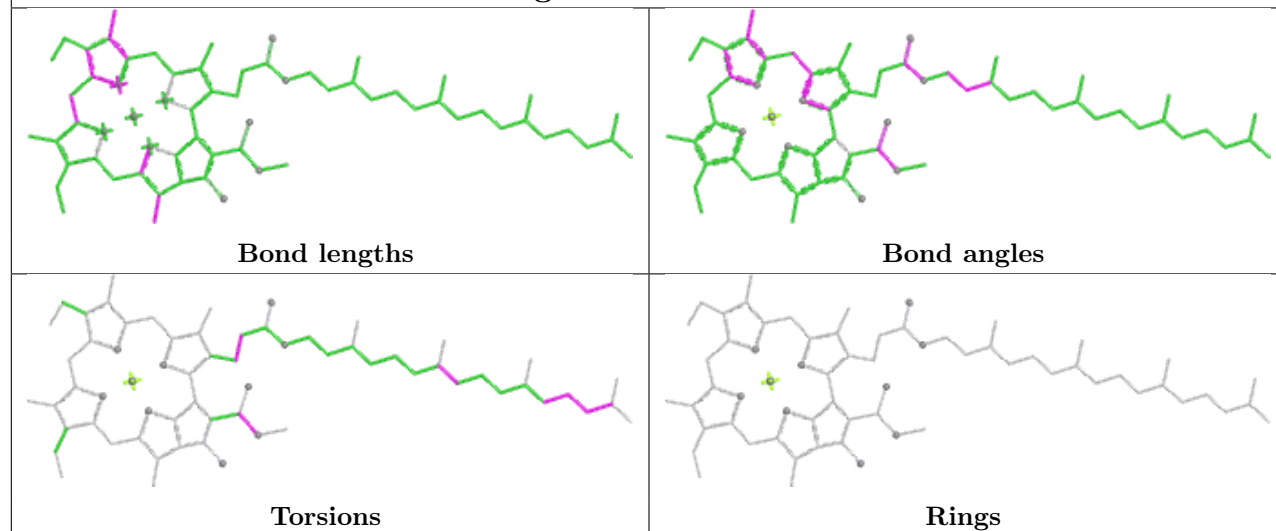
Ligand CLA i 102



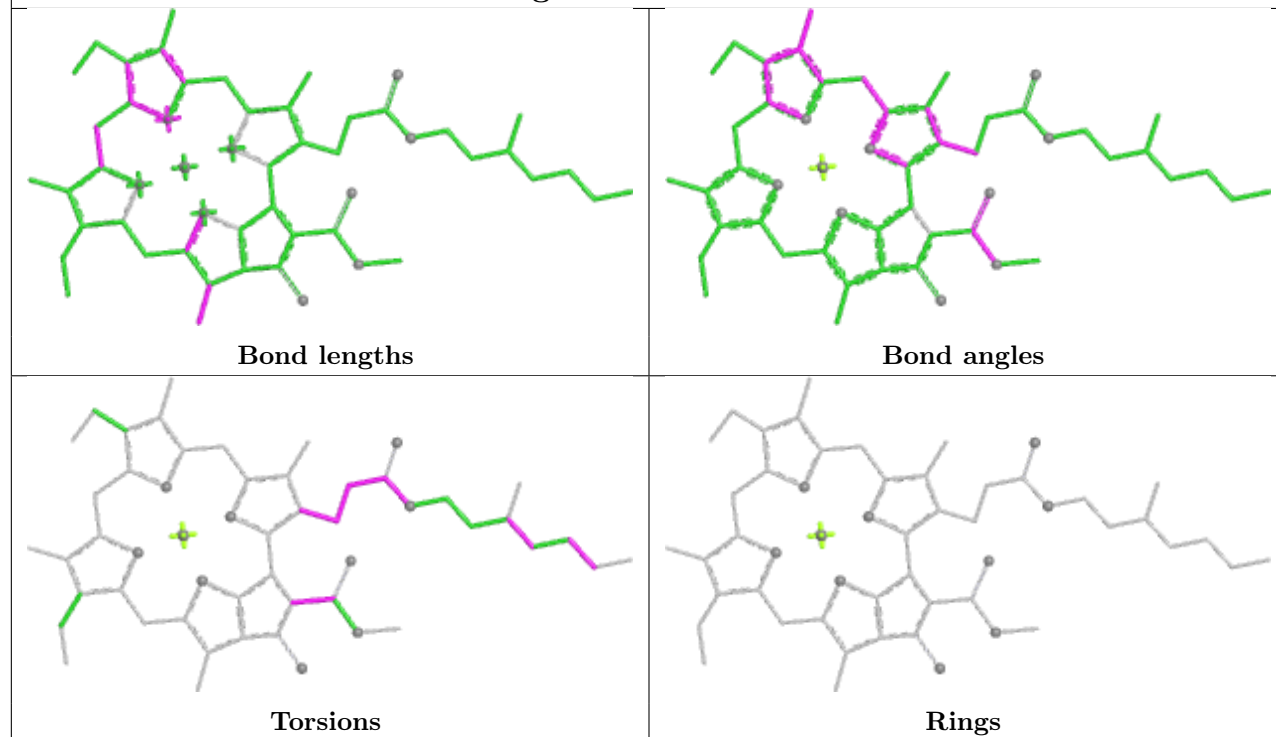




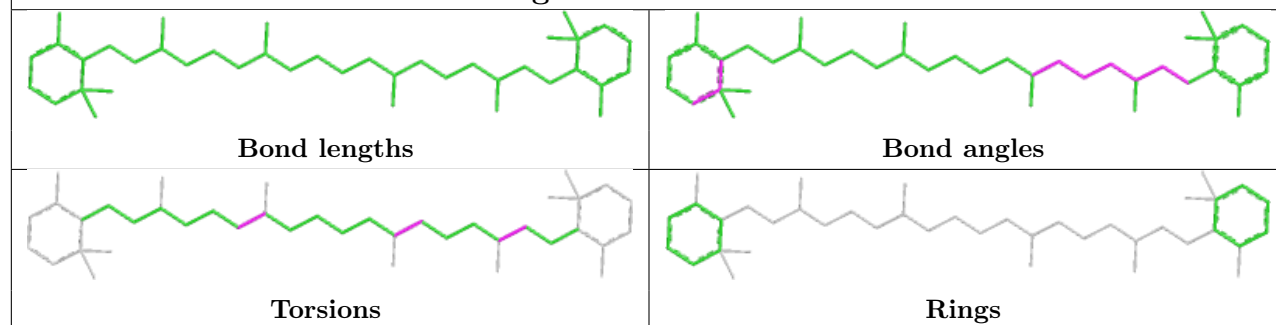
Ligand CLA L 202

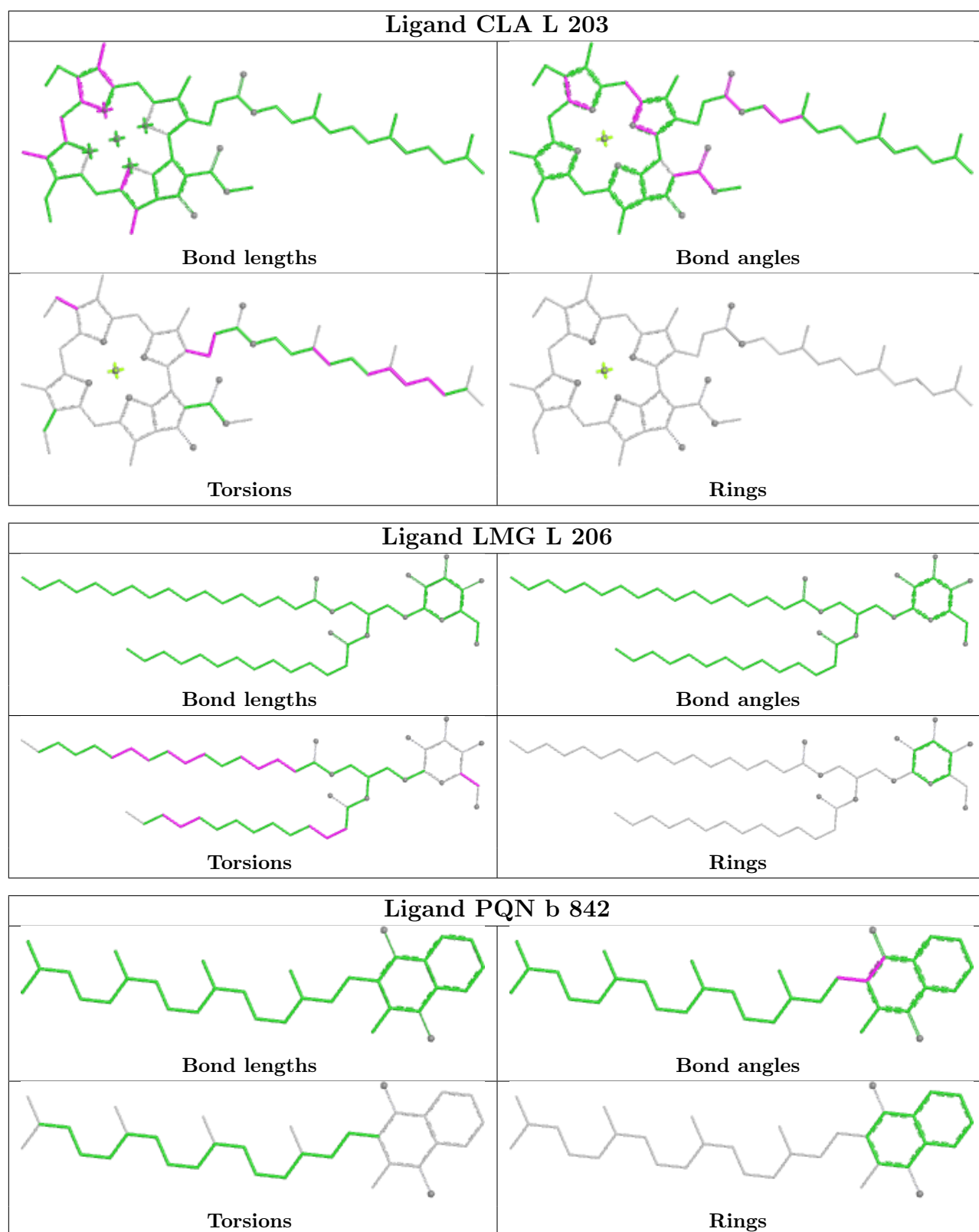


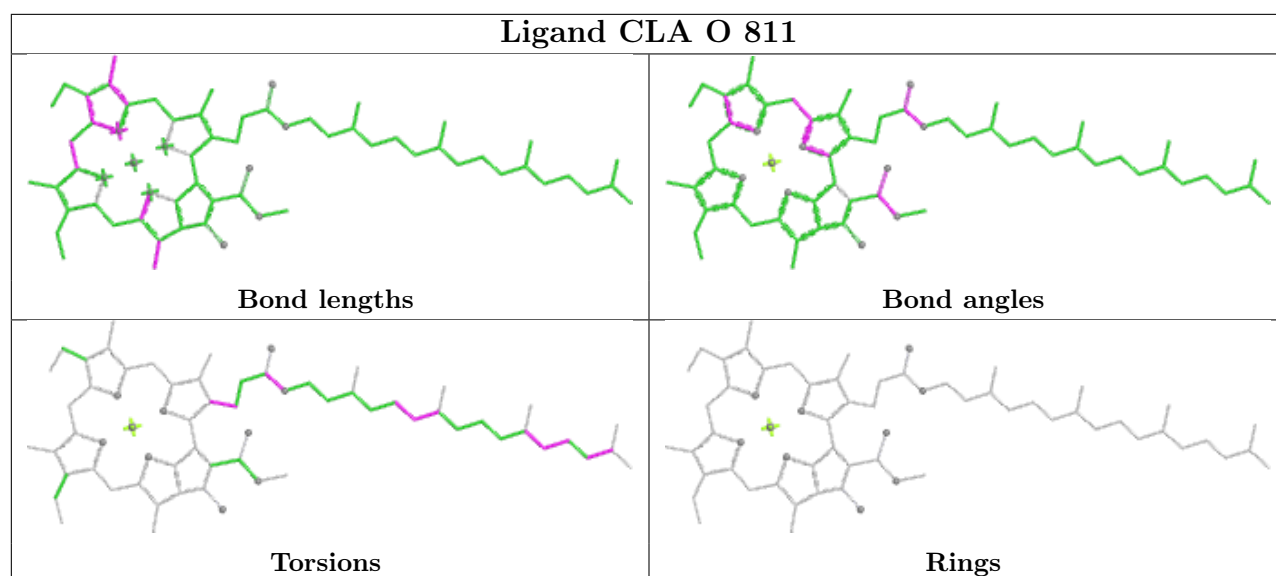
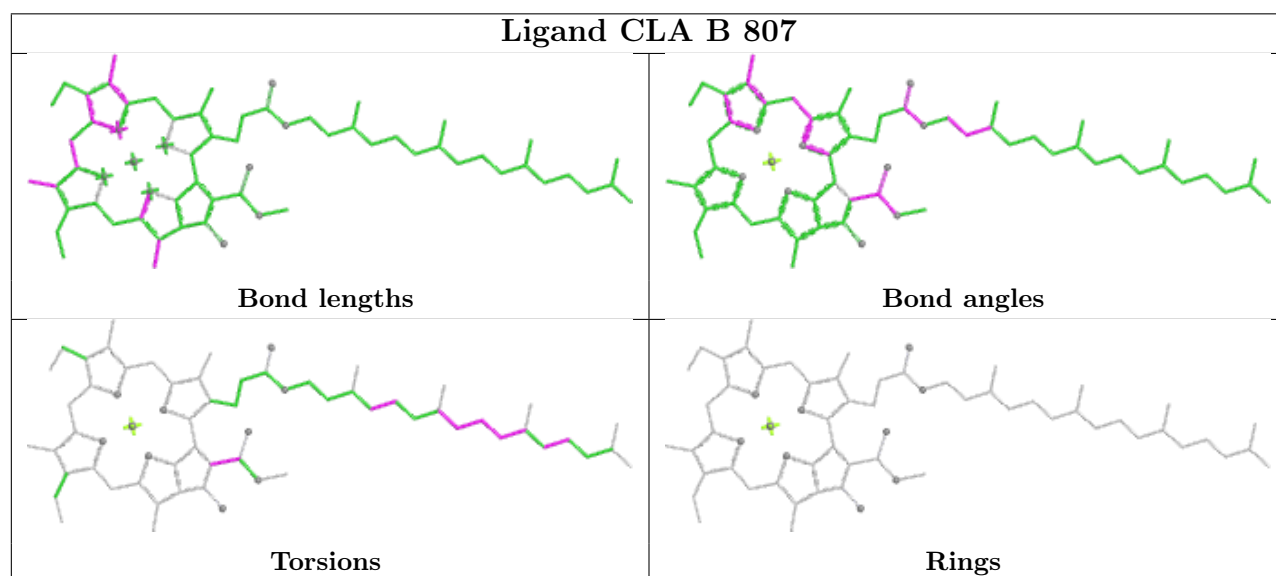
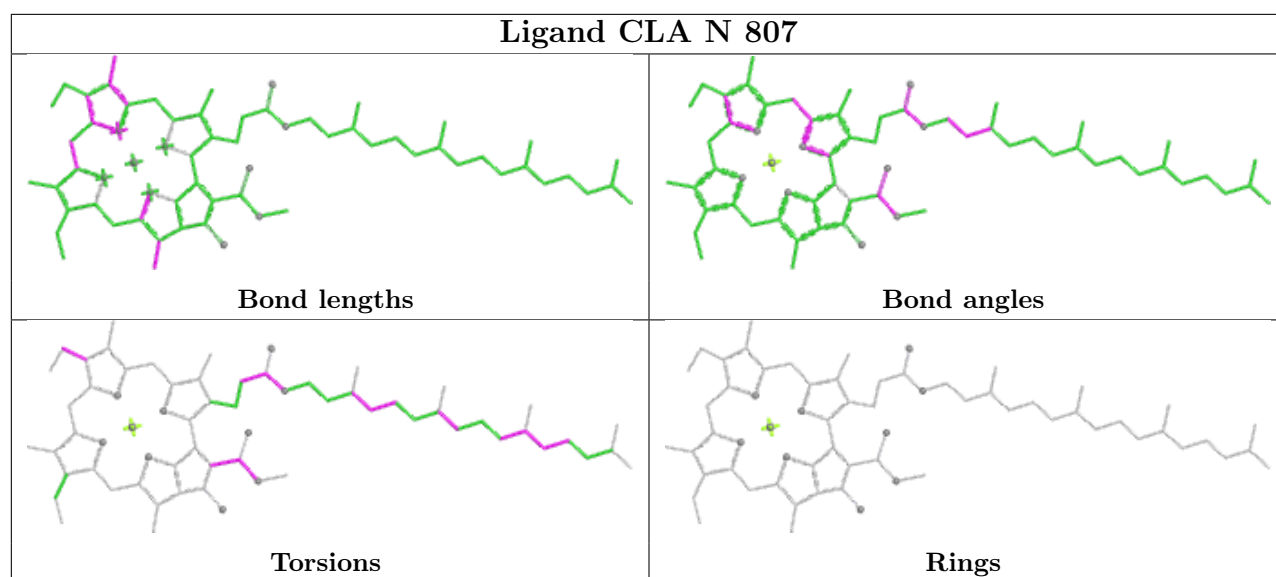
Ligand CLA B 820

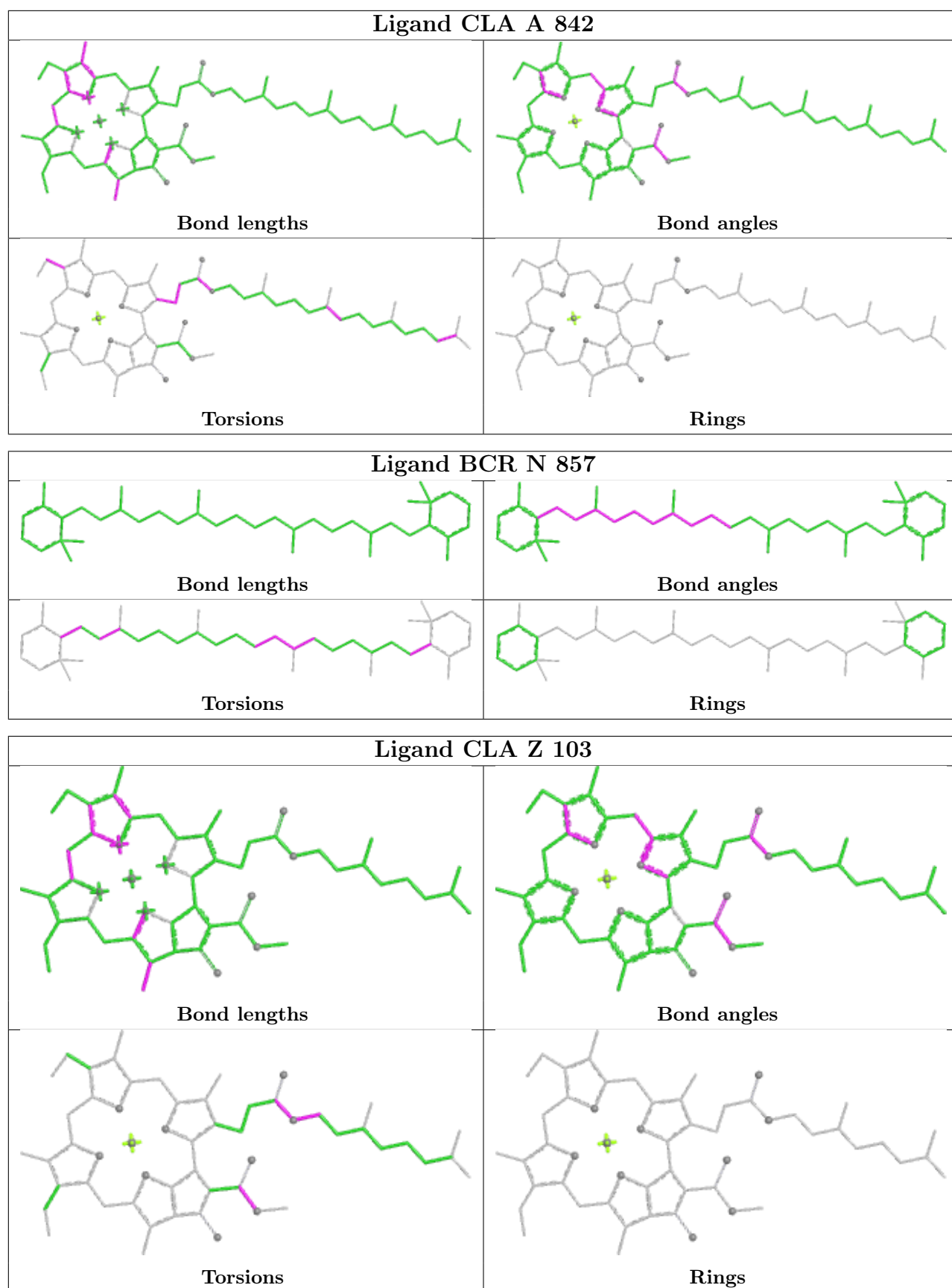


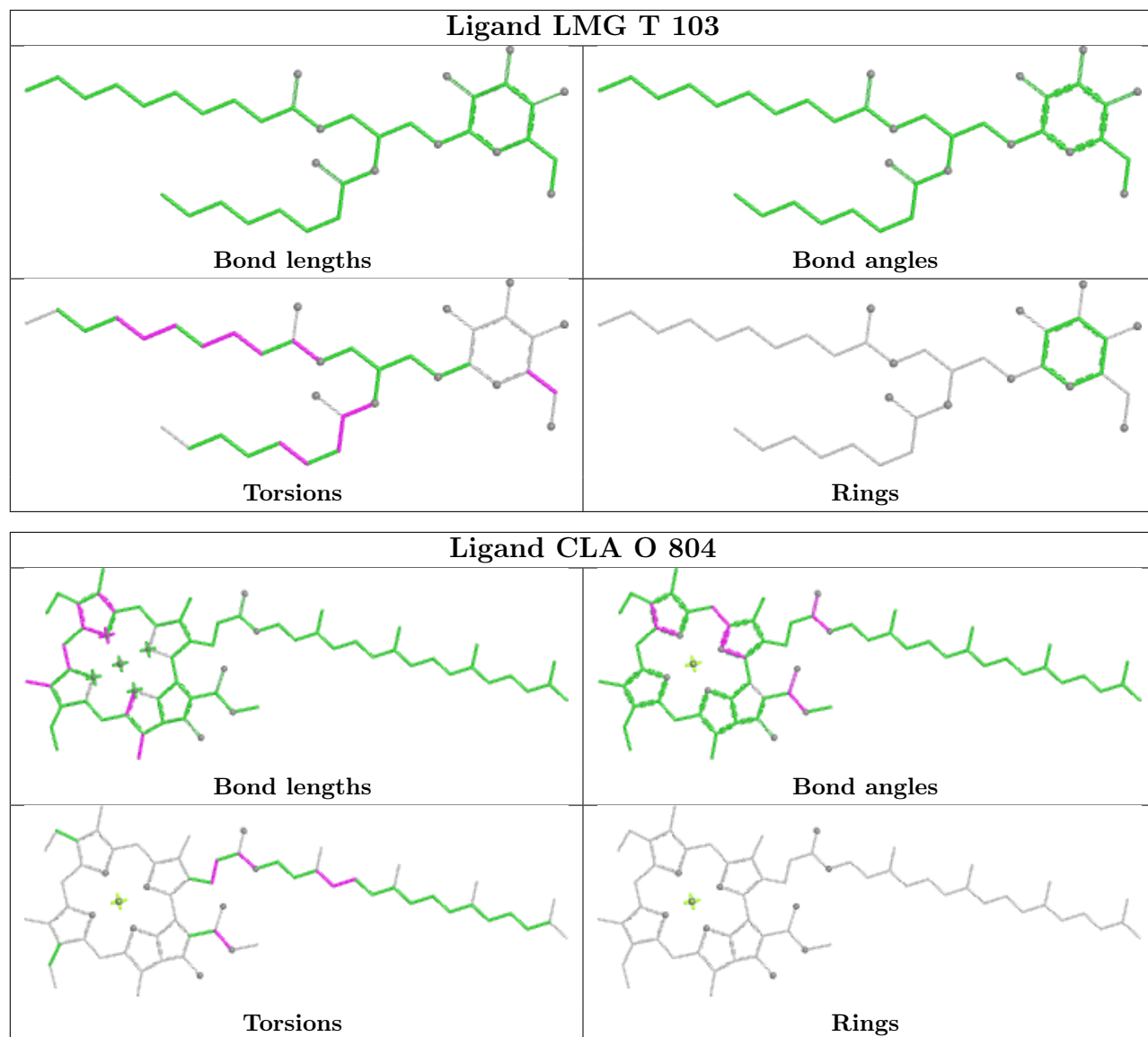
Ligand BCR F 202

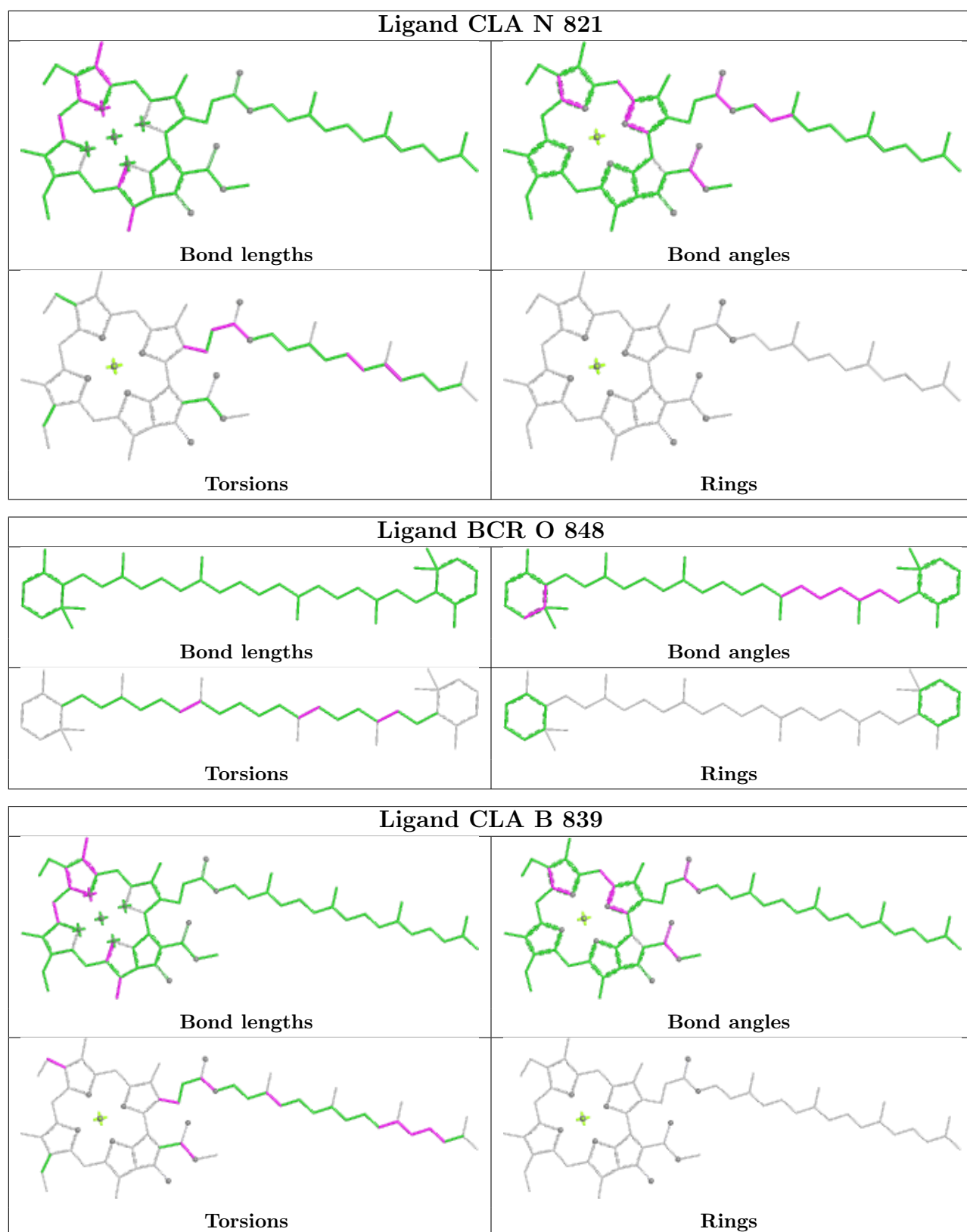


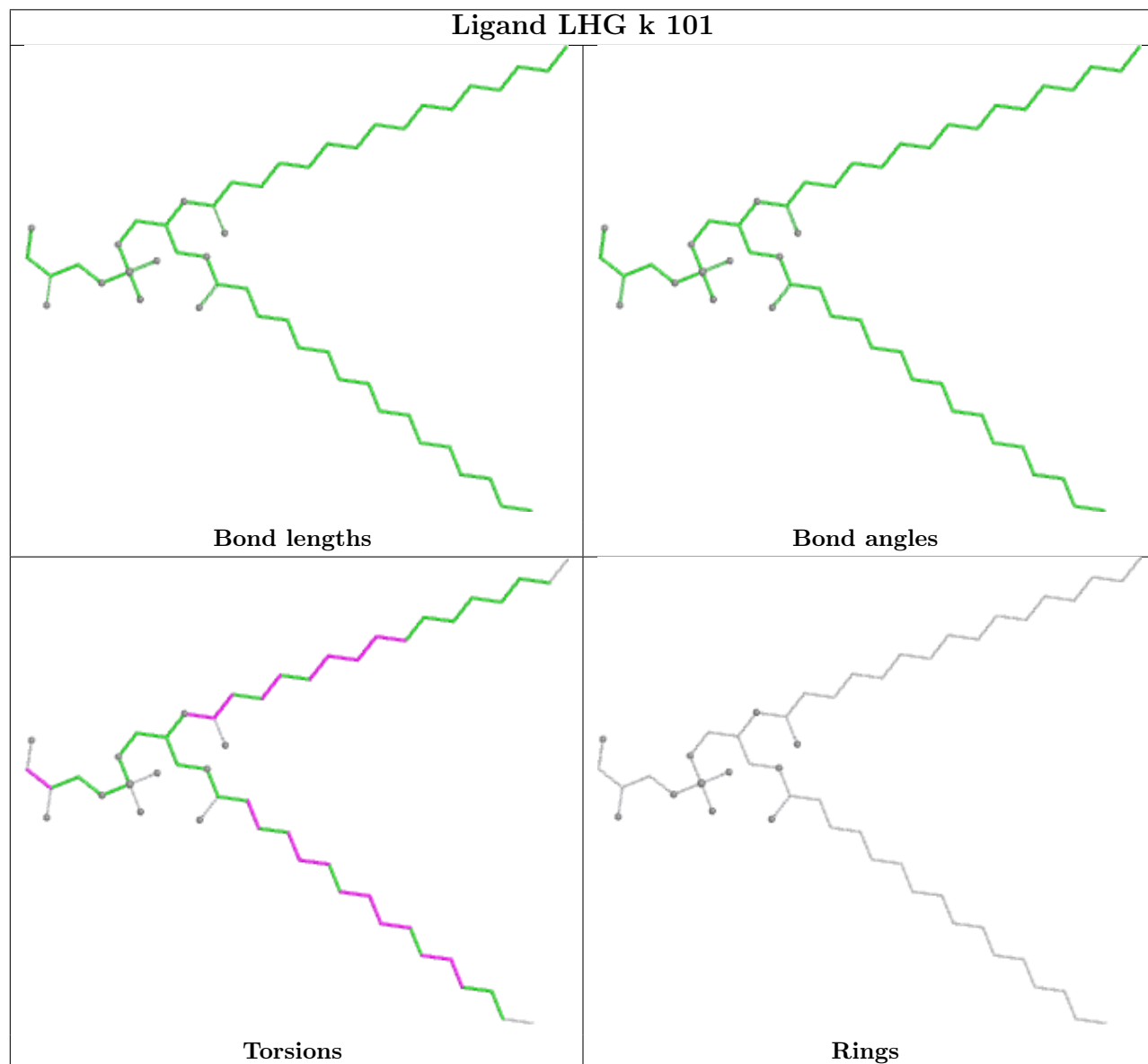
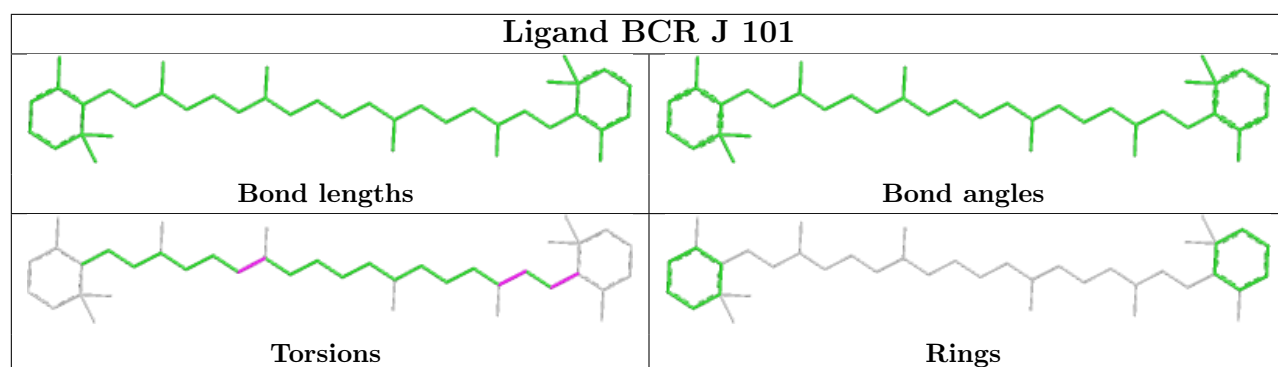




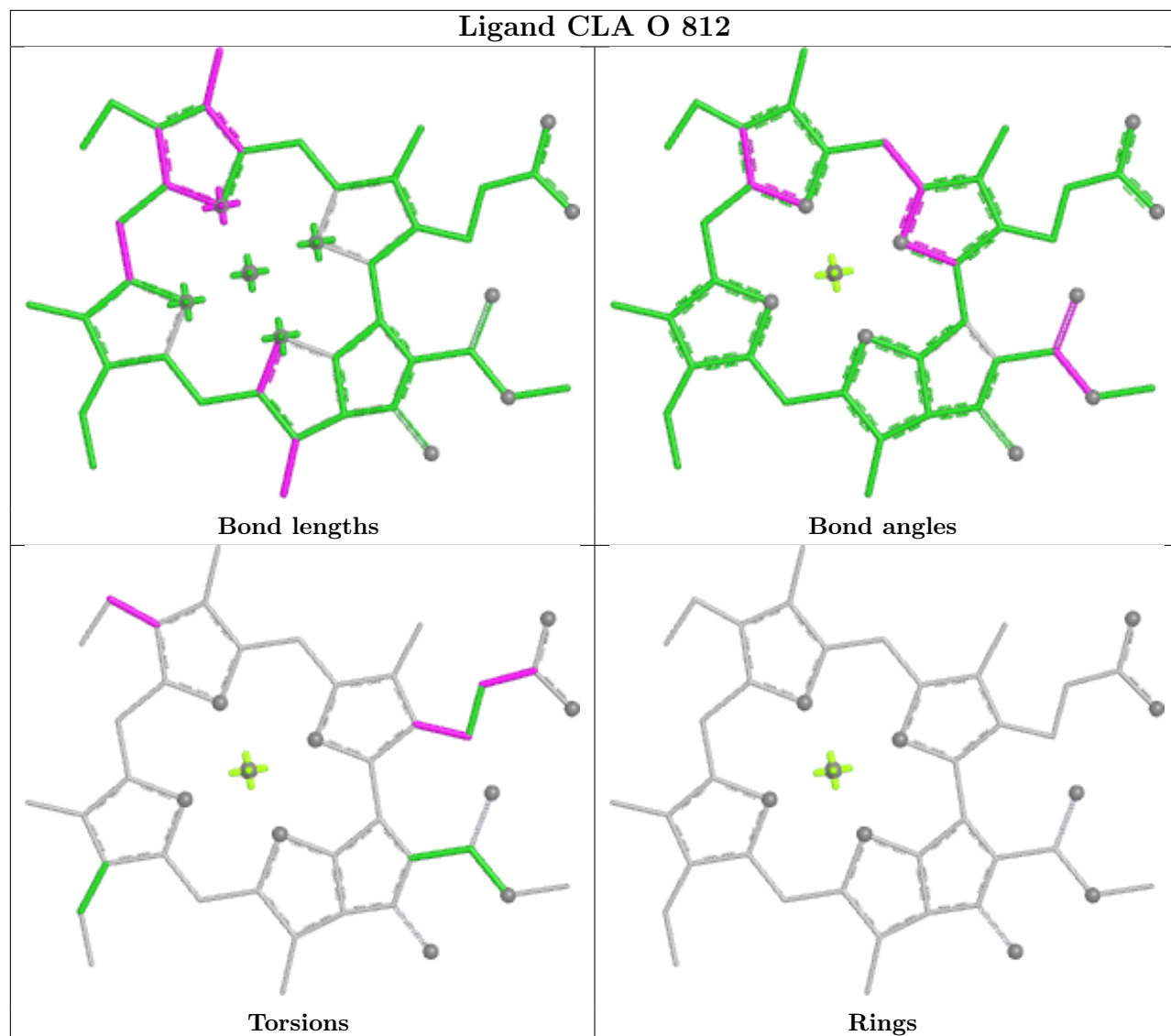




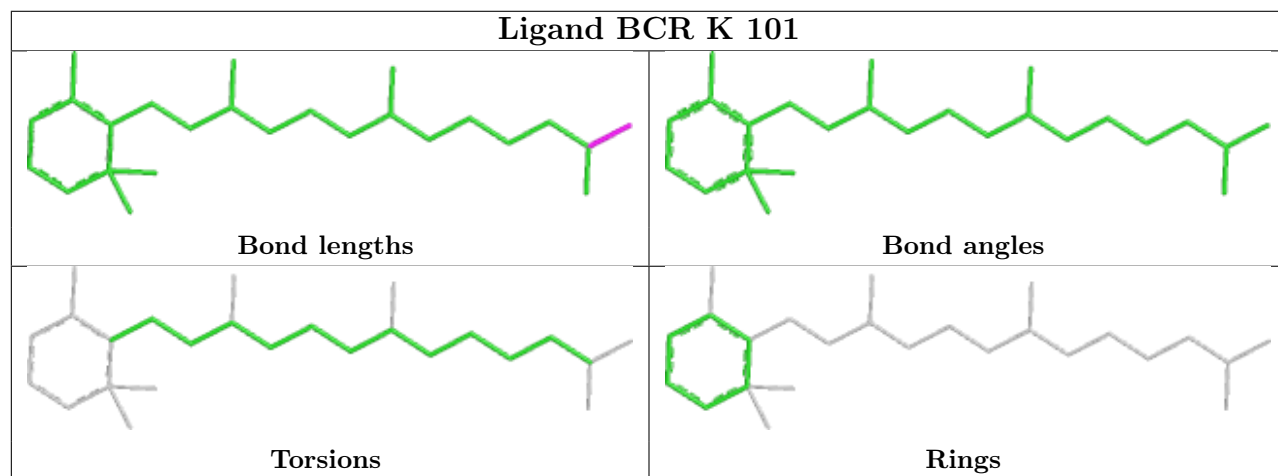


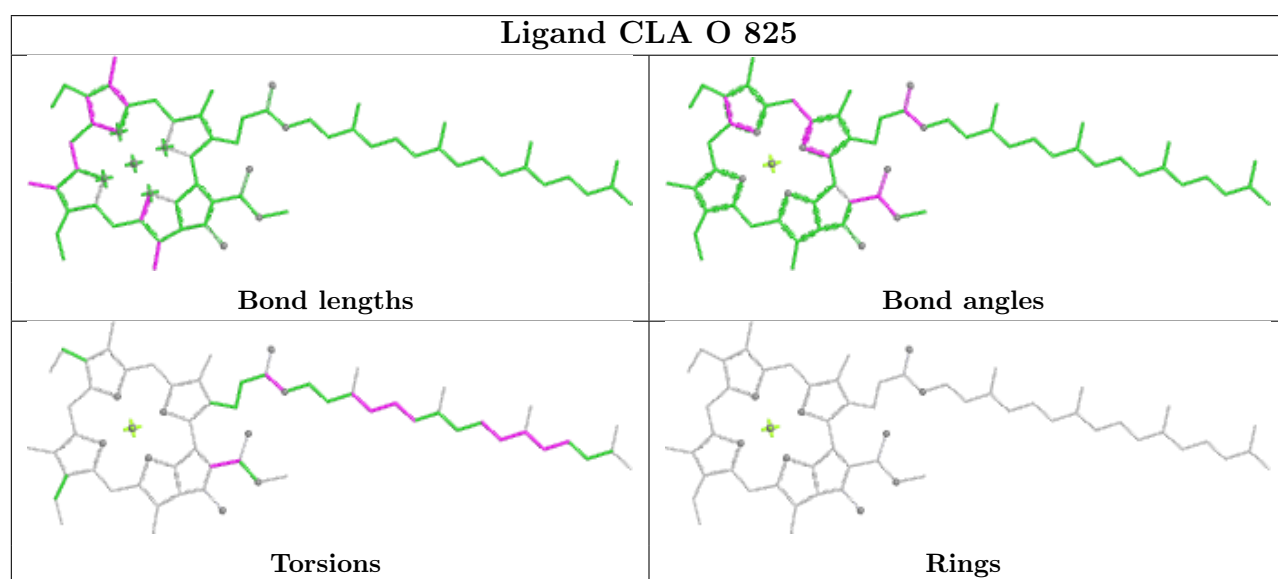
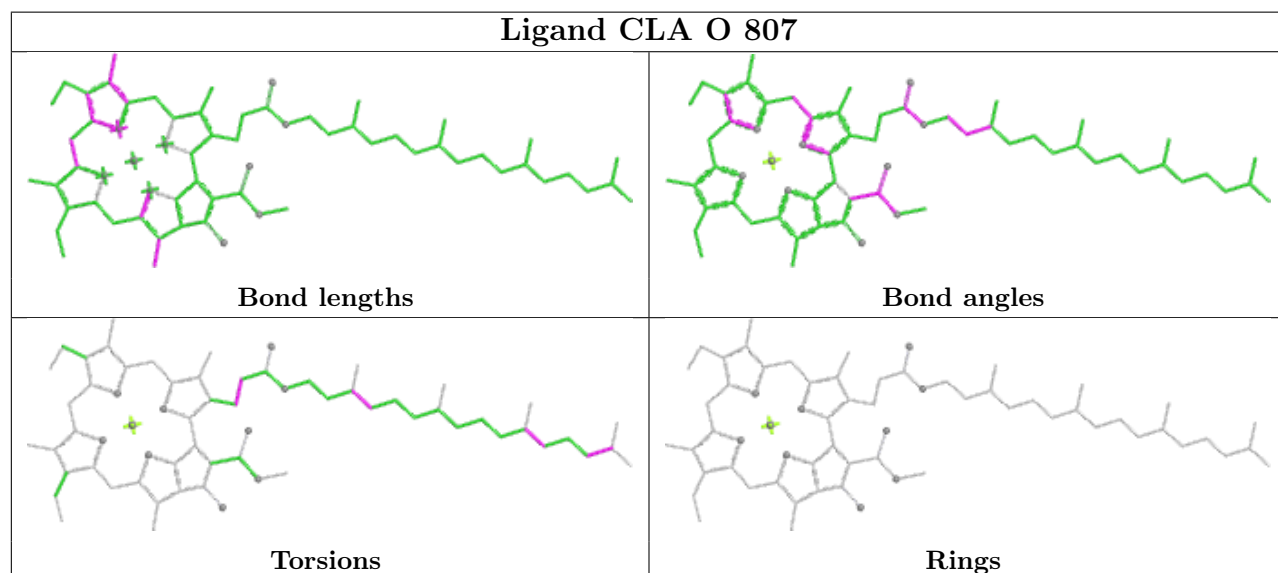
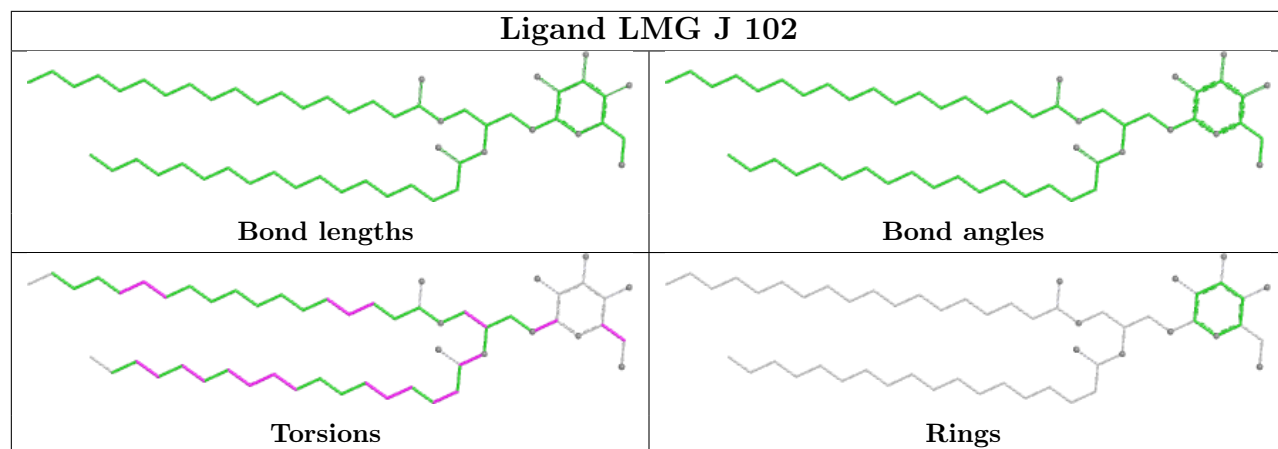


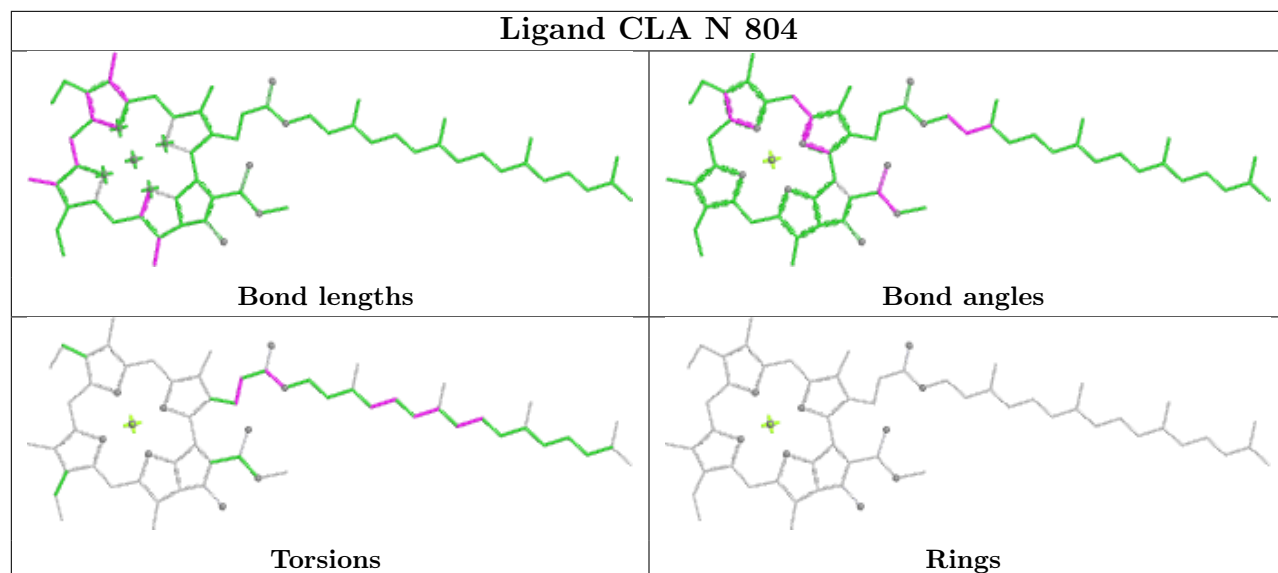
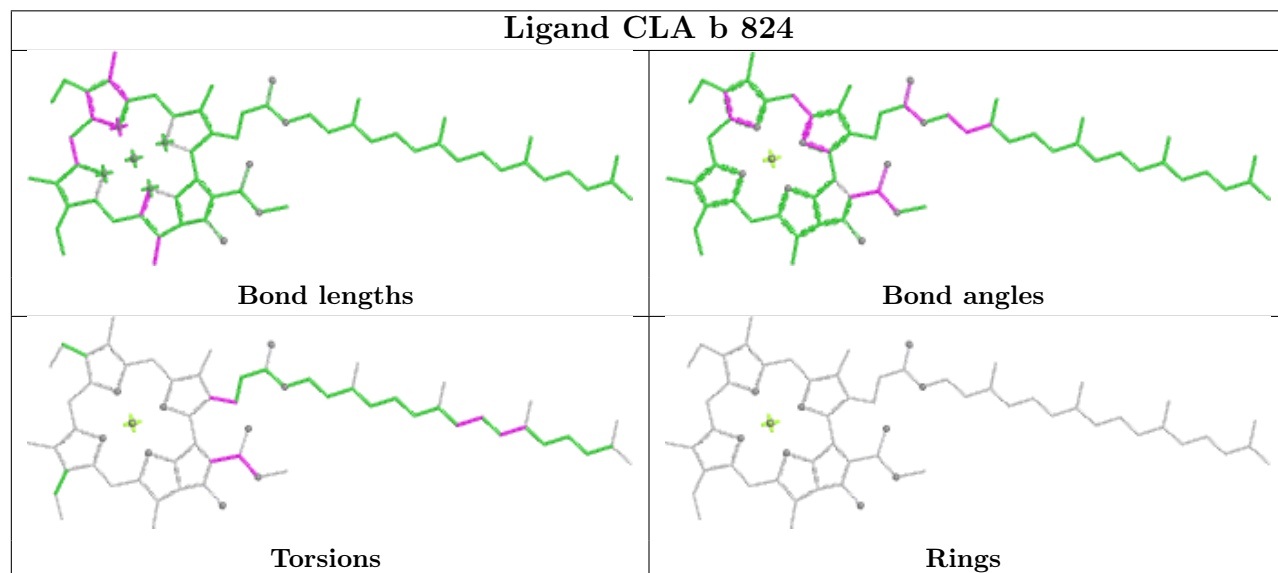
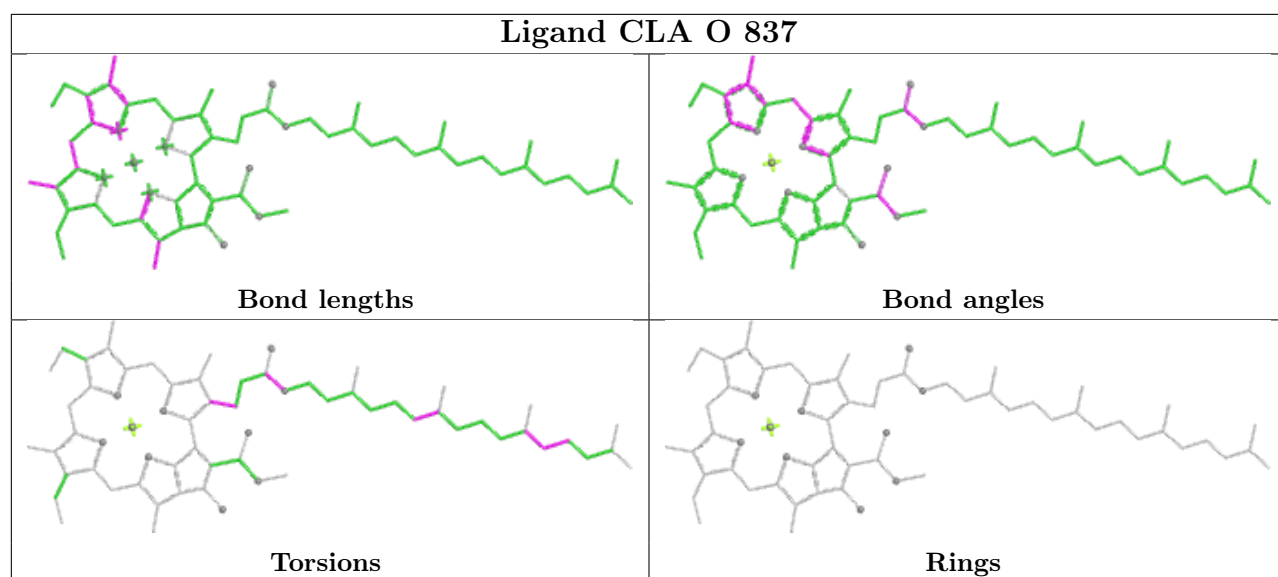
Ligand CLA O 812



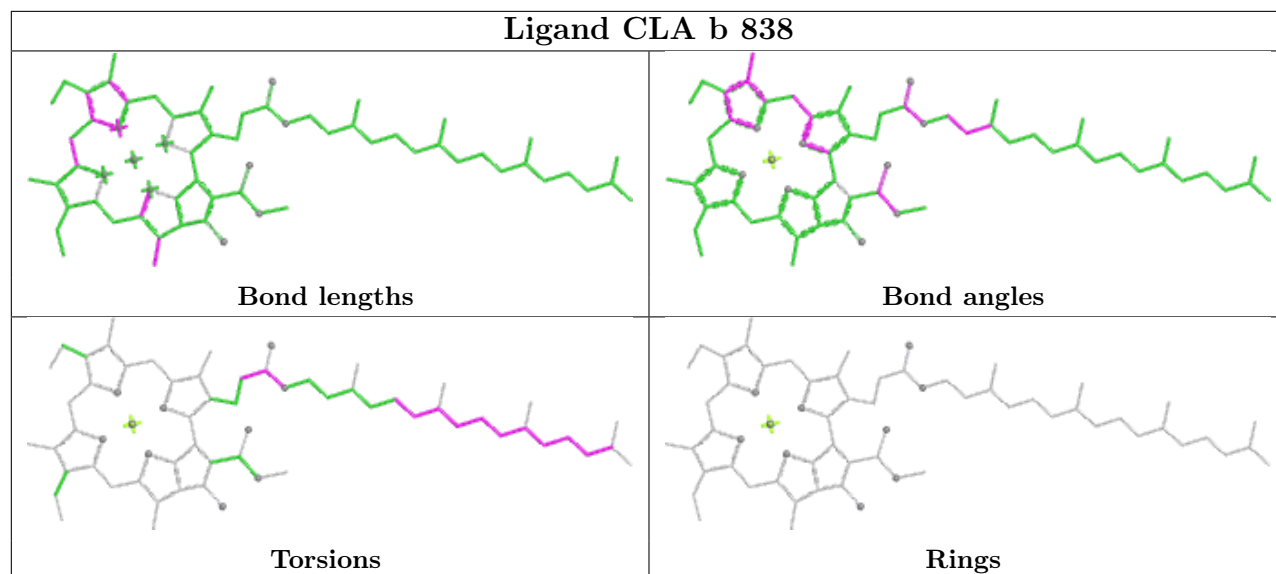
Ligand BCR K 101



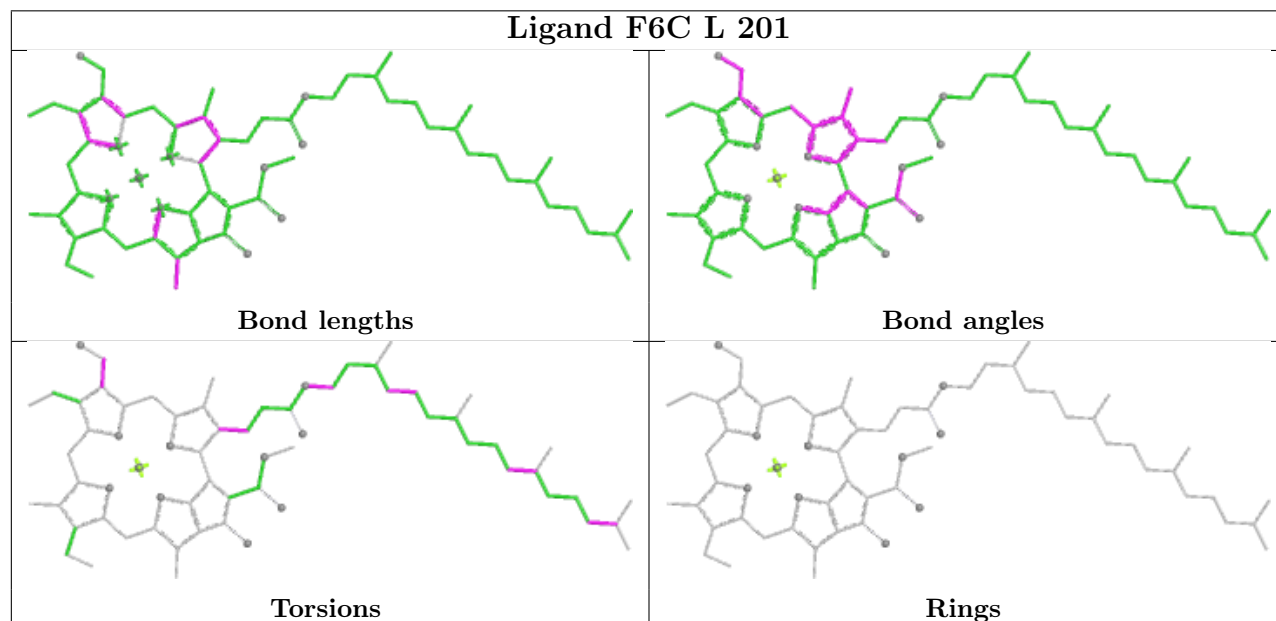




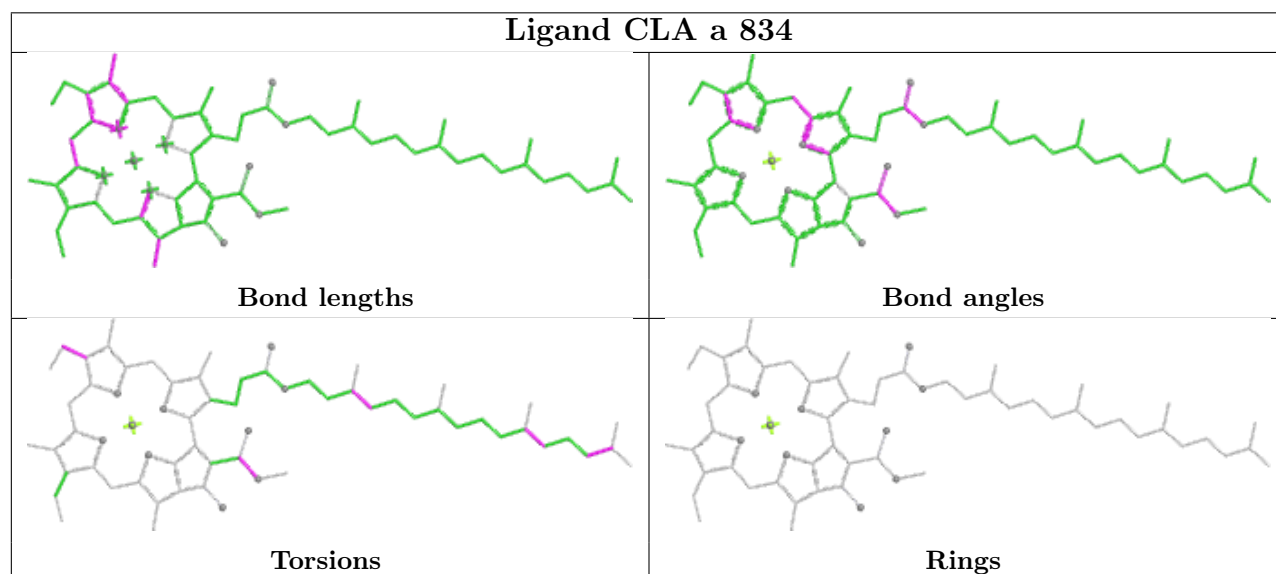
Ligand CLA b 838

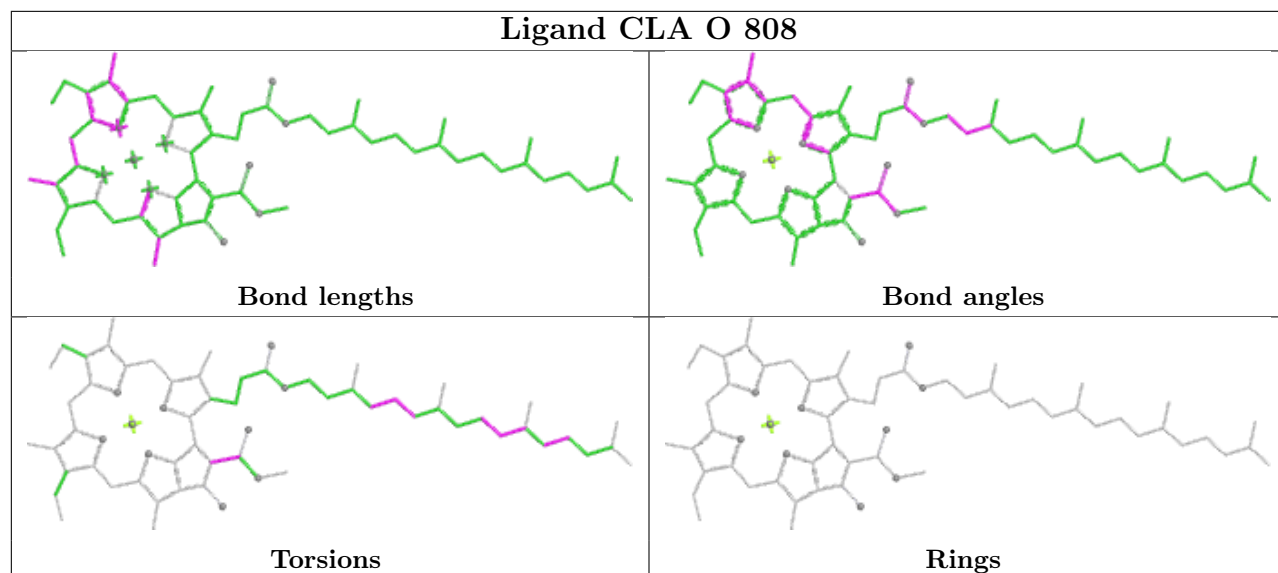
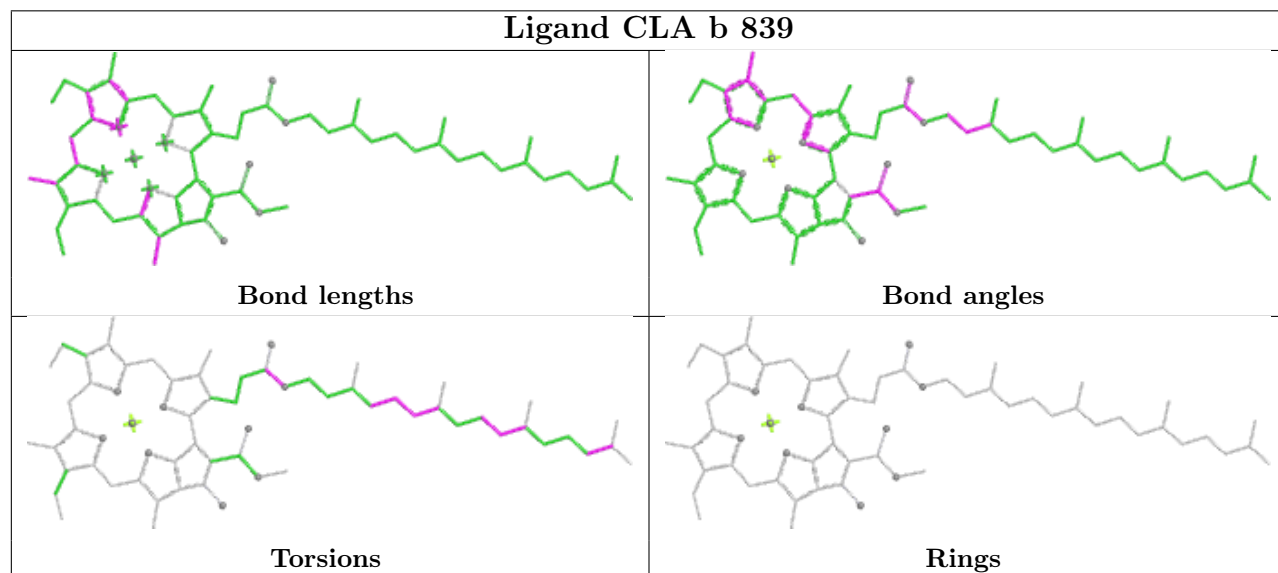
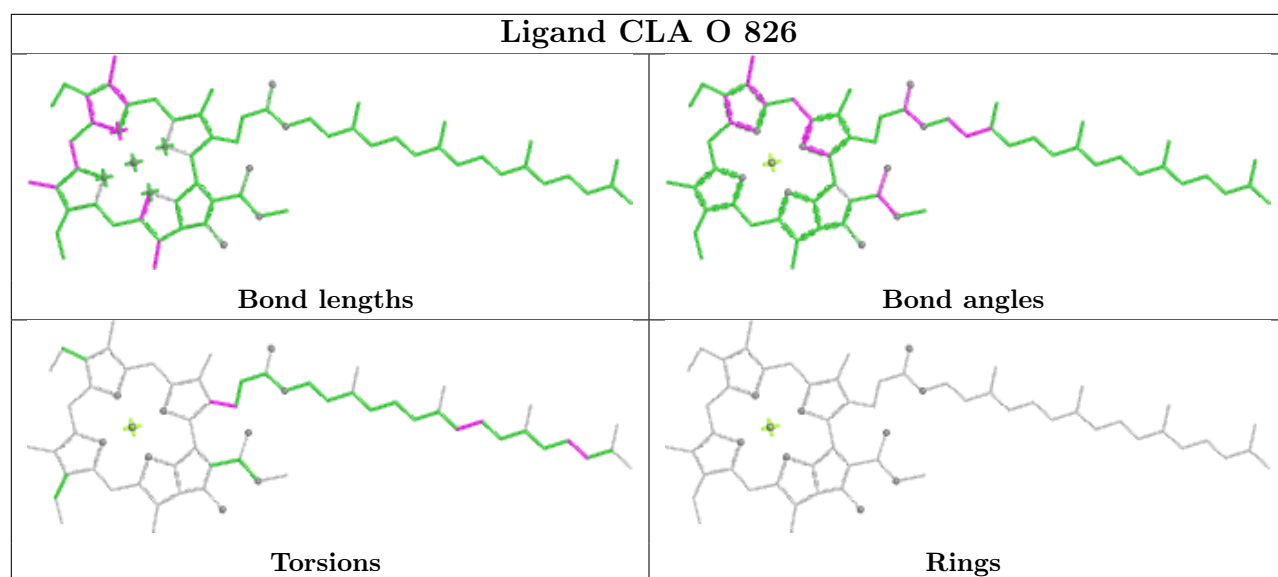


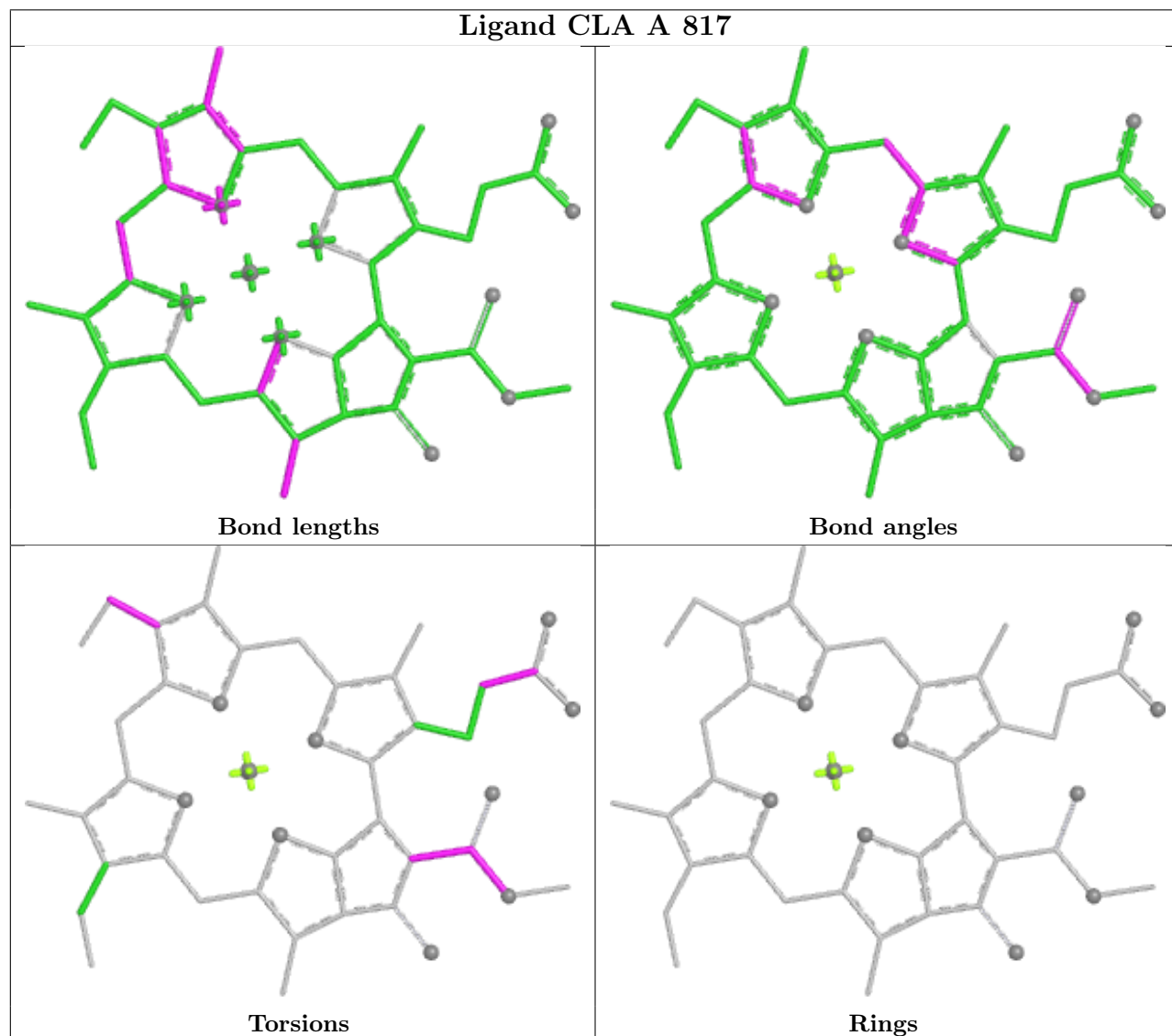
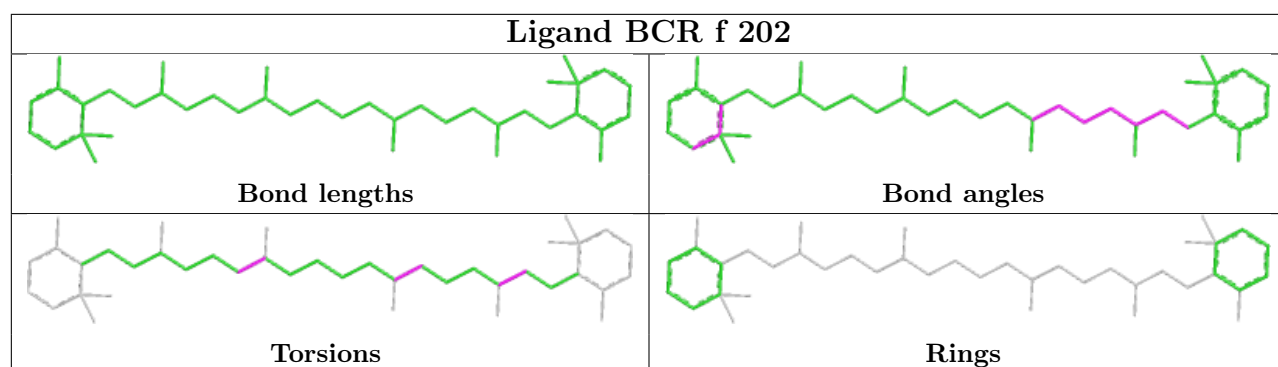
Ligand F6C L 201

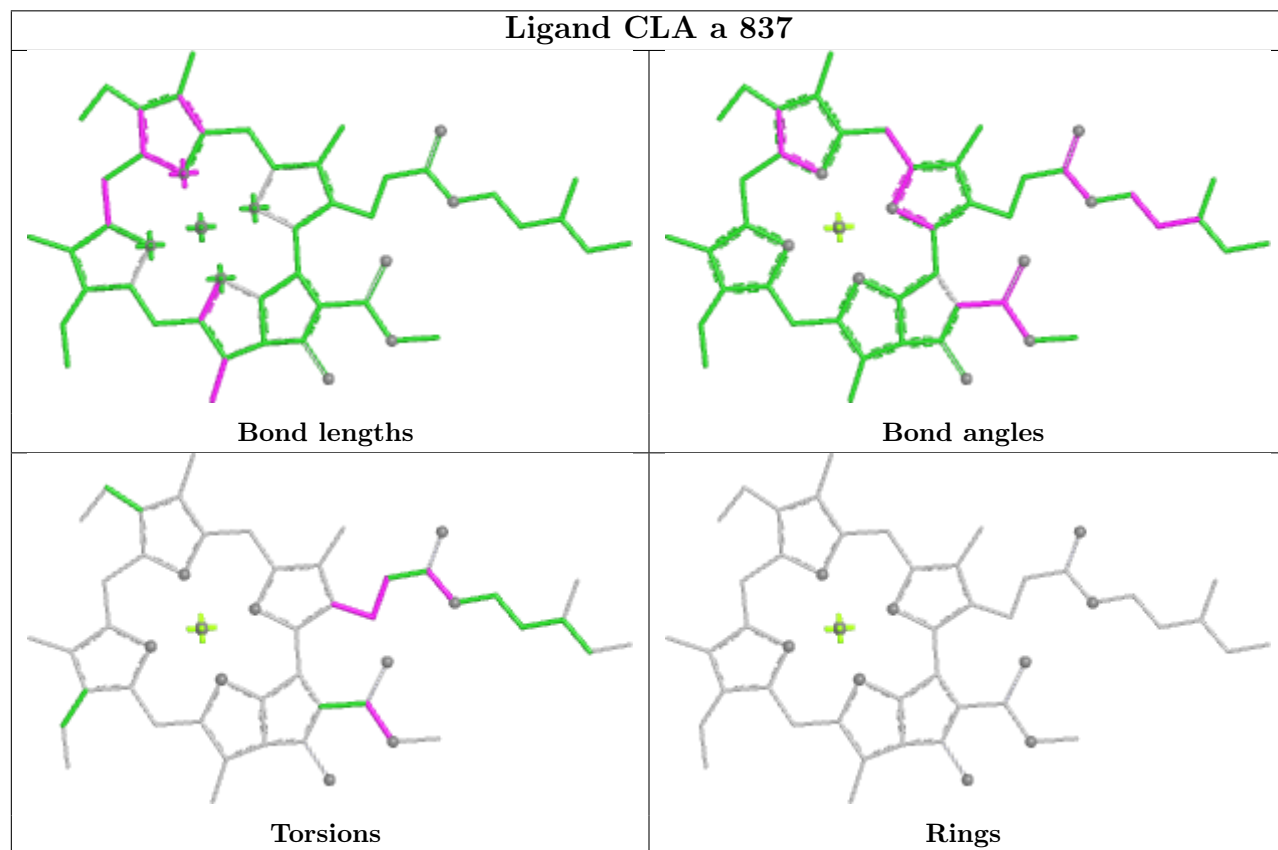
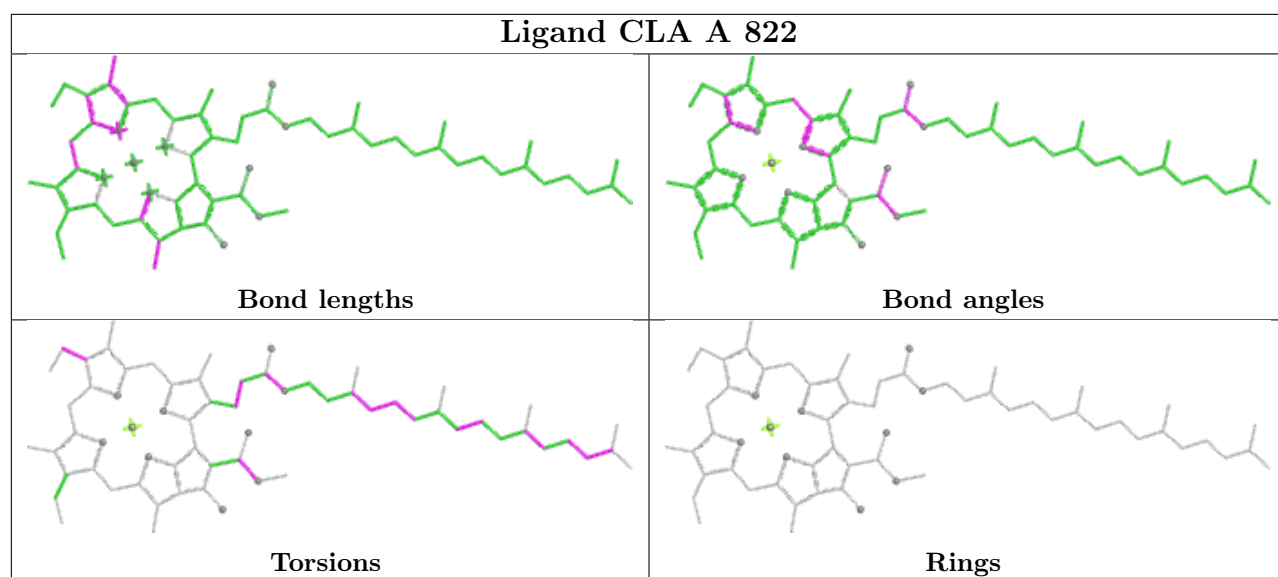


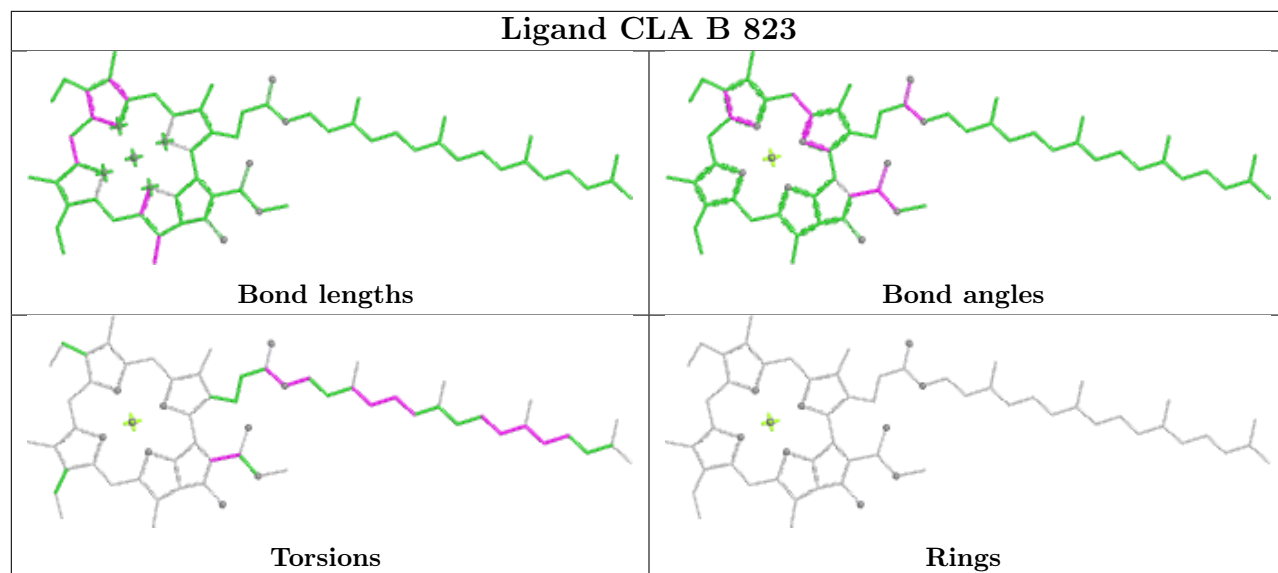
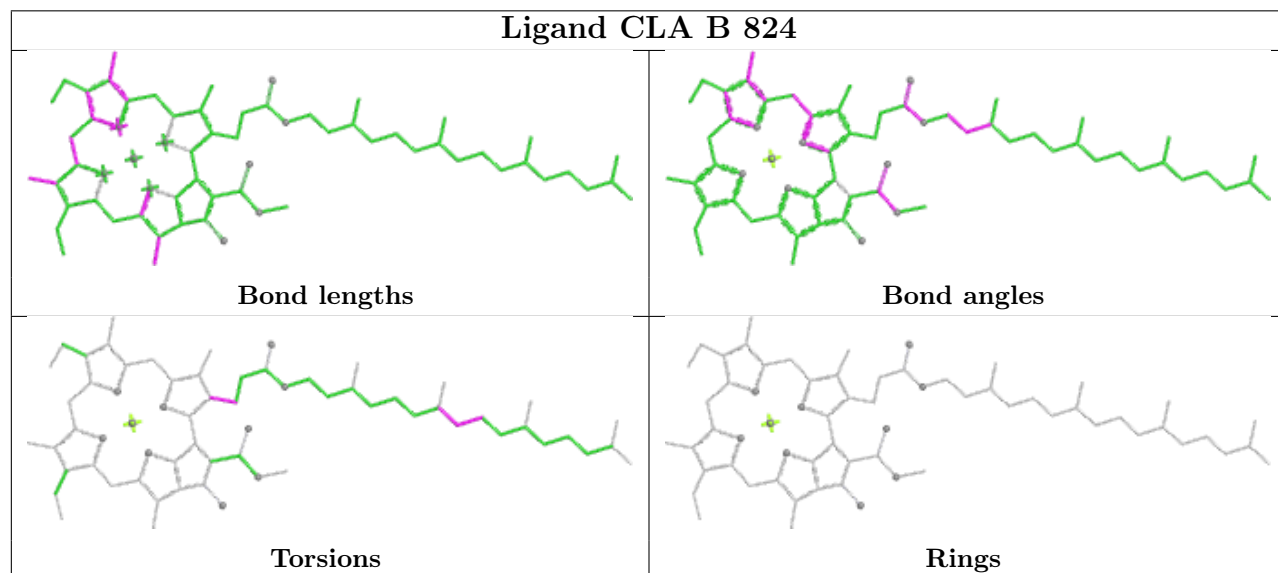
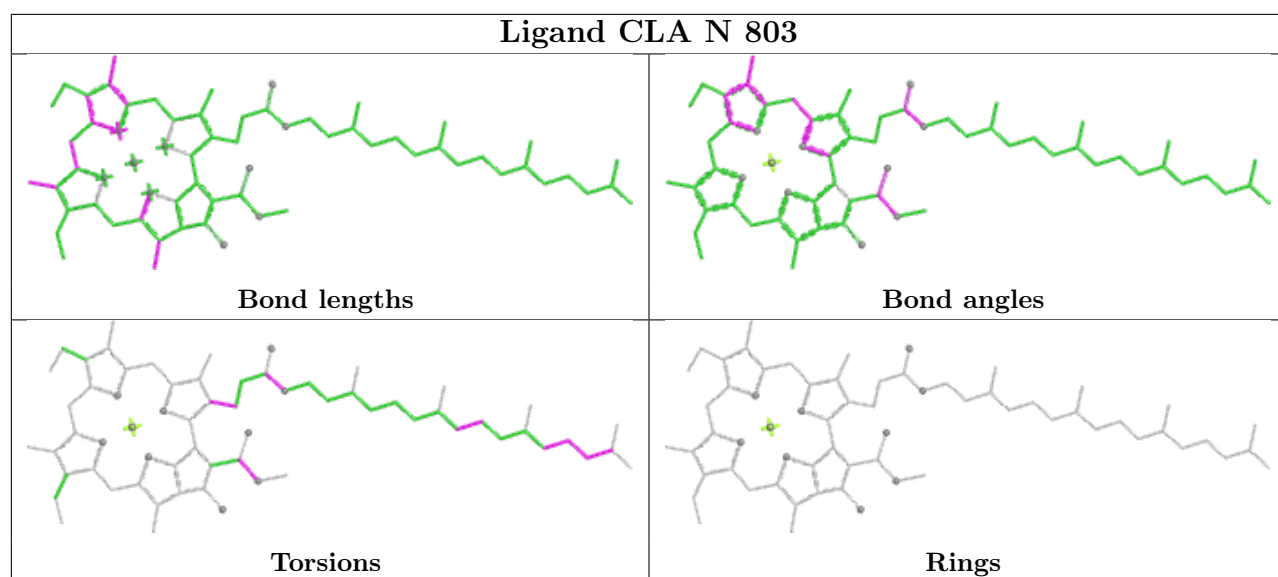
Ligand CLA a 834











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

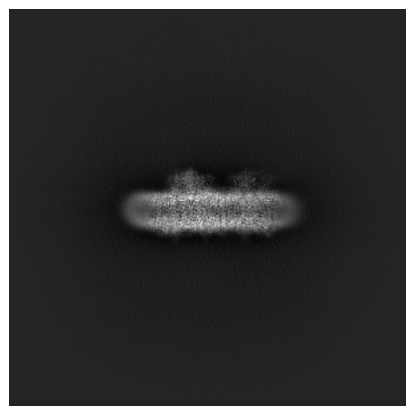
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50063. These allow visual inspection of the internal detail of the map and identification of artifacts.

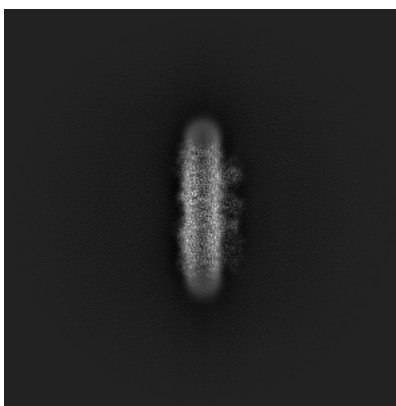
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

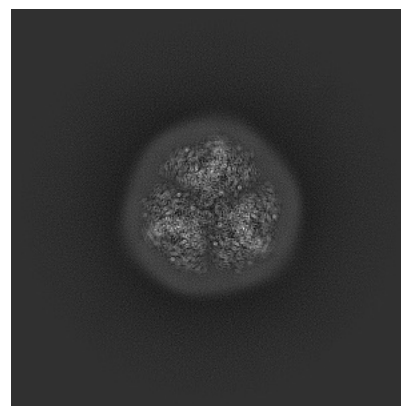
6.1.1 Primary map



X

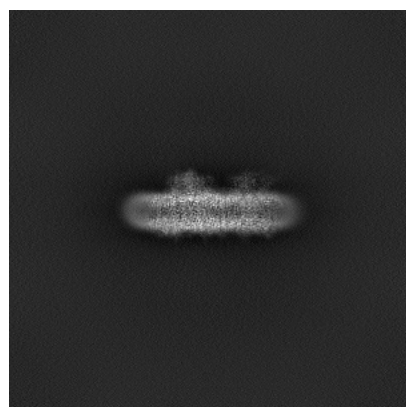


Y

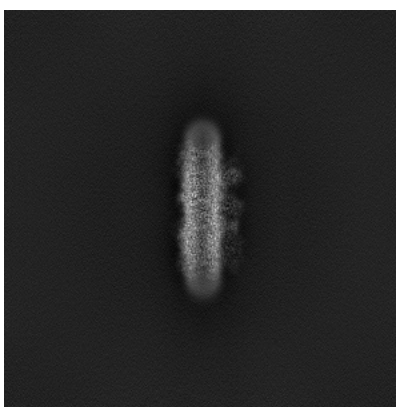


Z

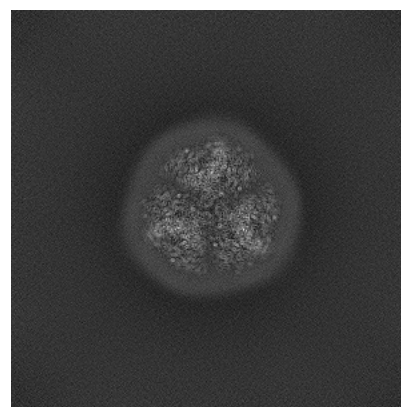
6.1.2 Raw map



X



Y

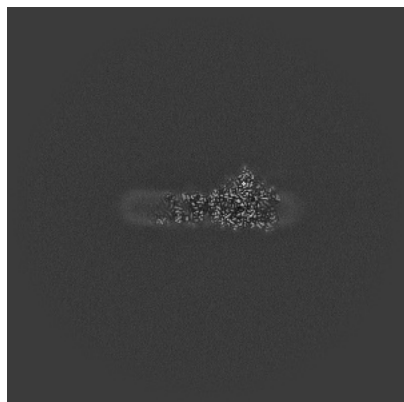


Z

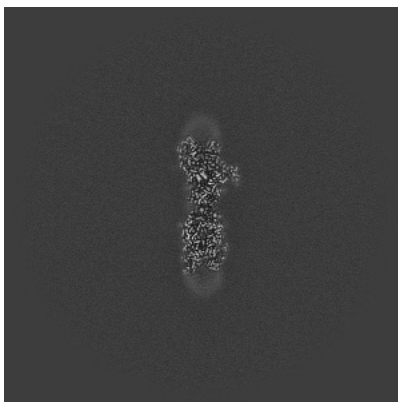
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

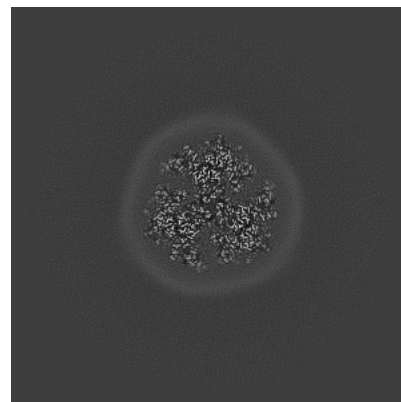
6.2.1 Primary map



X Index: 300

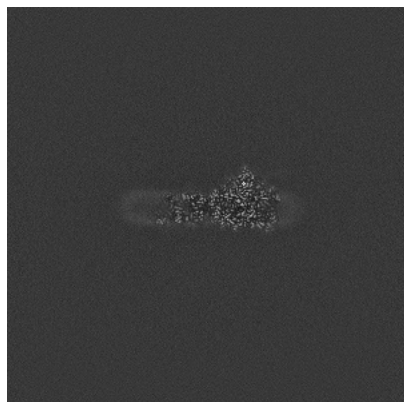


Y Index: 300

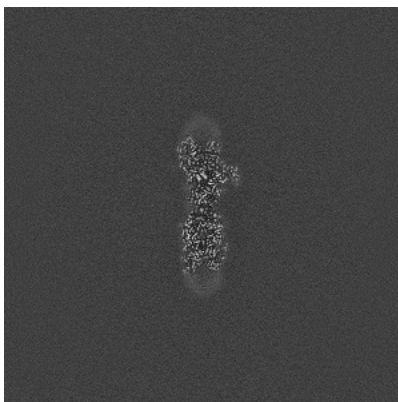


Z Index: 300

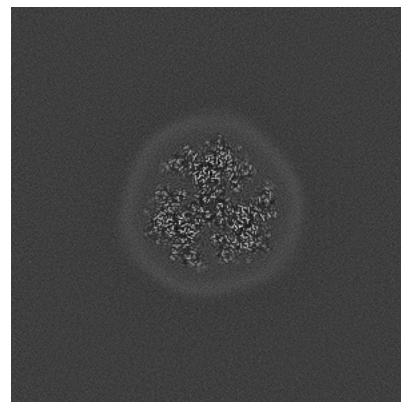
6.2.2 Raw map



X Index: 300



Y Index: 300

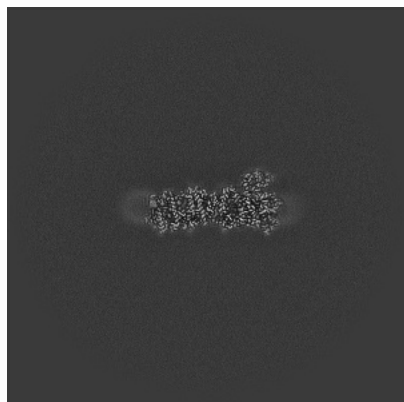


Z Index: 300

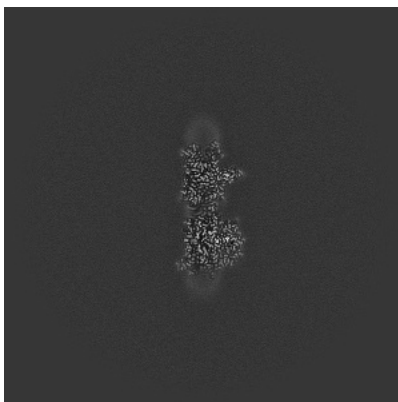
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

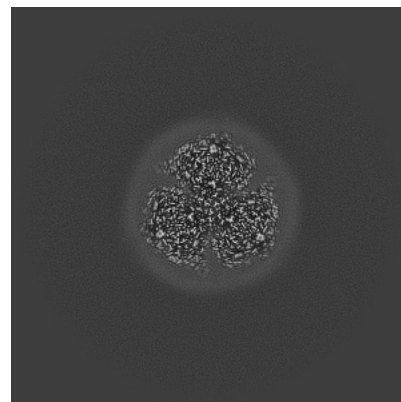
6.3.1 Primary map



X Index: 314

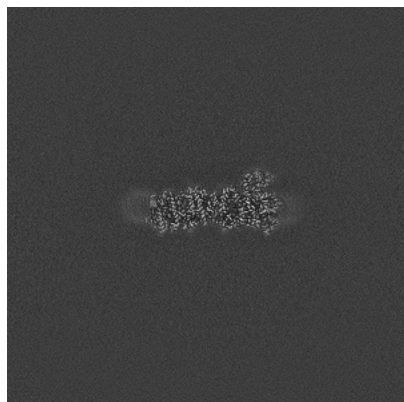


Y Index: 273

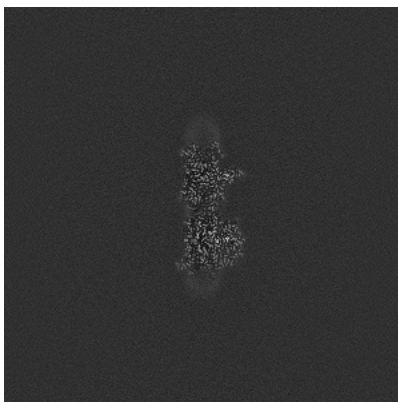


Z Index: 312

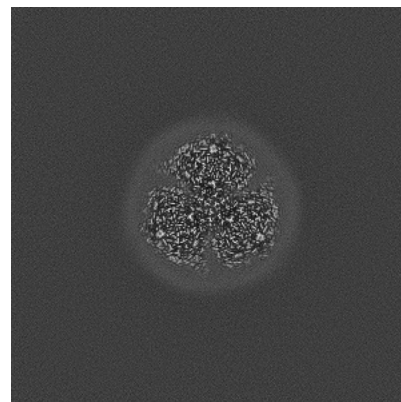
6.3.2 Raw map



X Index: 314



Y Index: 273

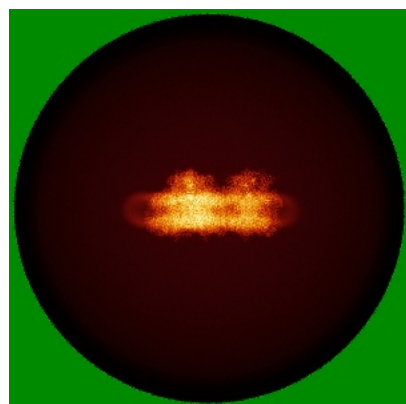


Z Index: 312

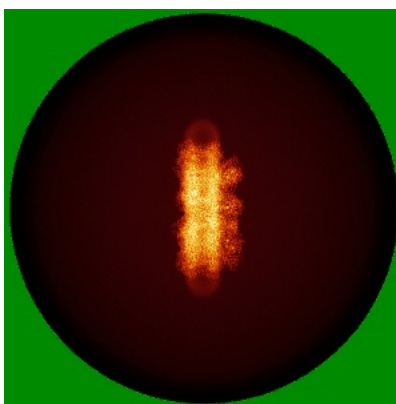
The images above show the largest variance slices of the map in three orthogonal directions.

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

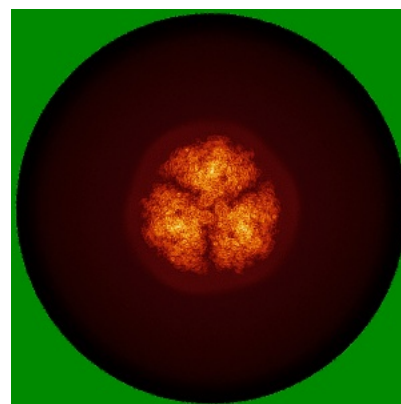
6.4.1 Primary map



X

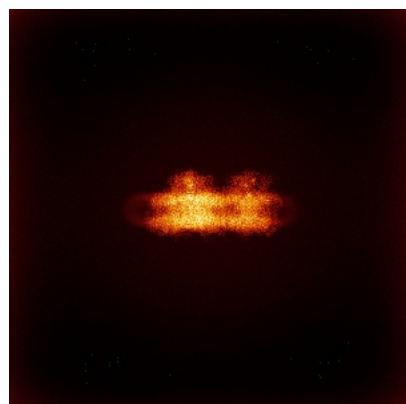


Y

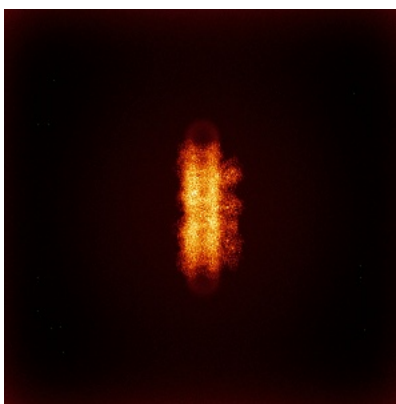


Z

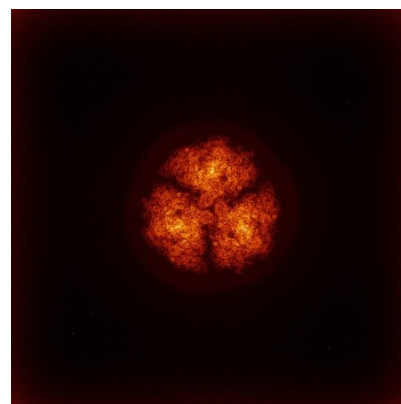
6.4.2 Raw map



X



Y

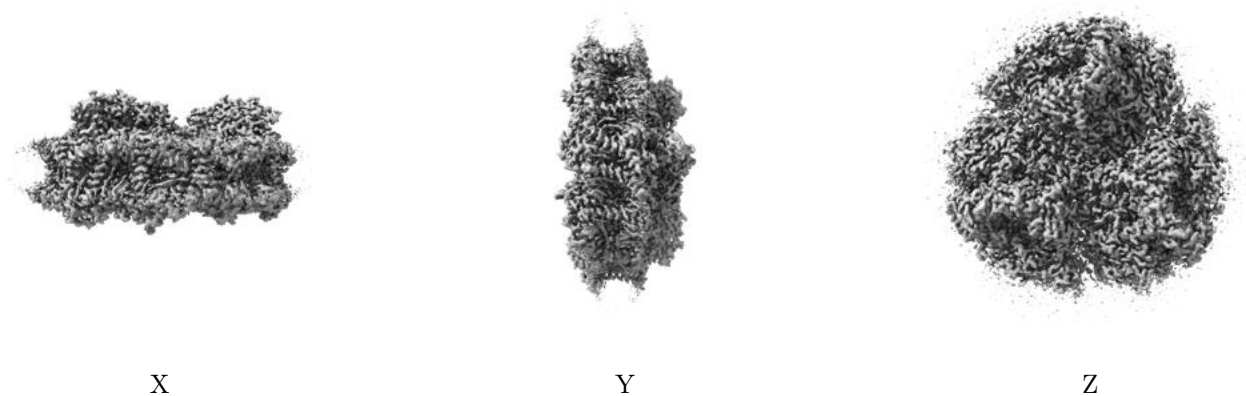


Z

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.

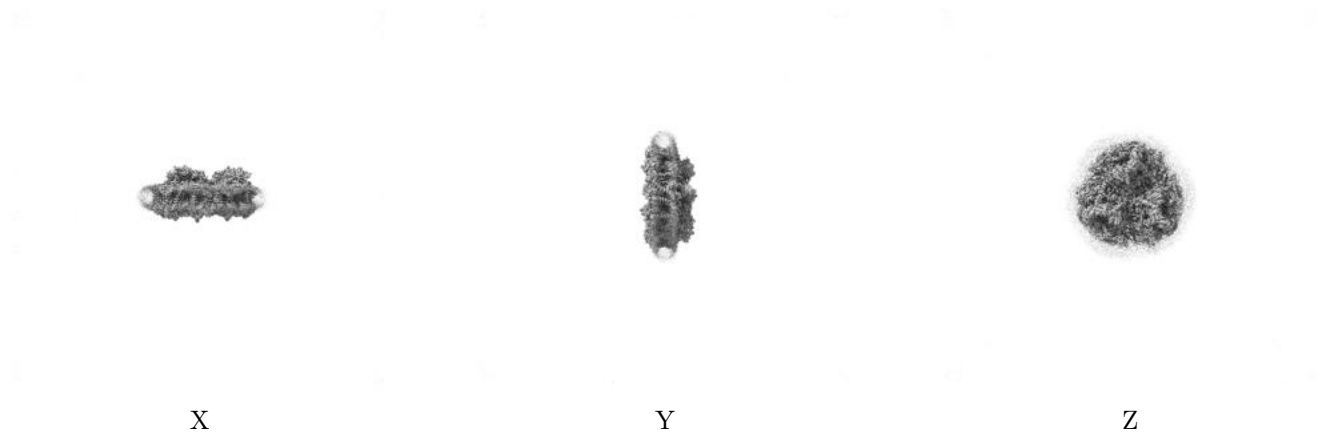
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.054. 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.

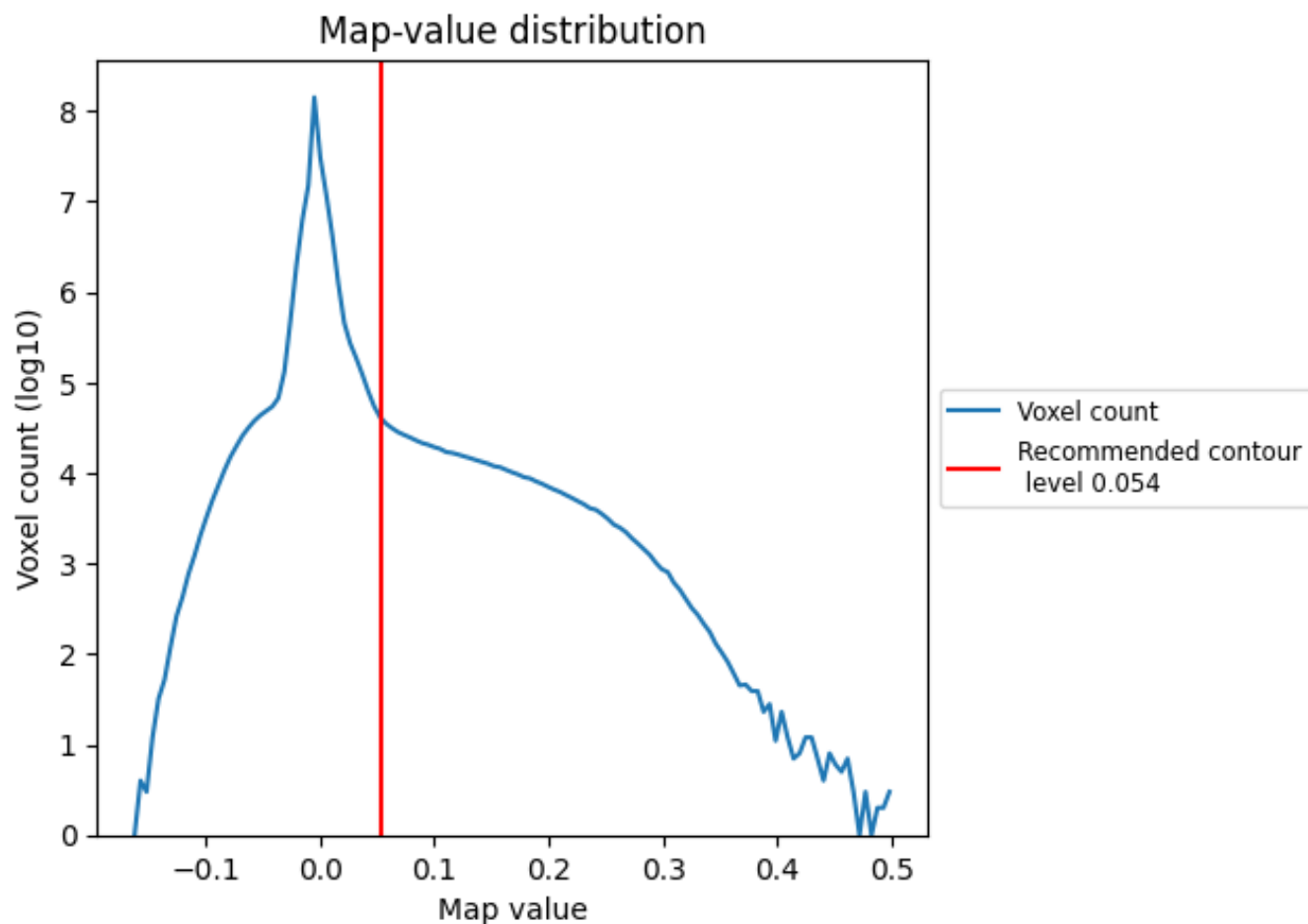
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

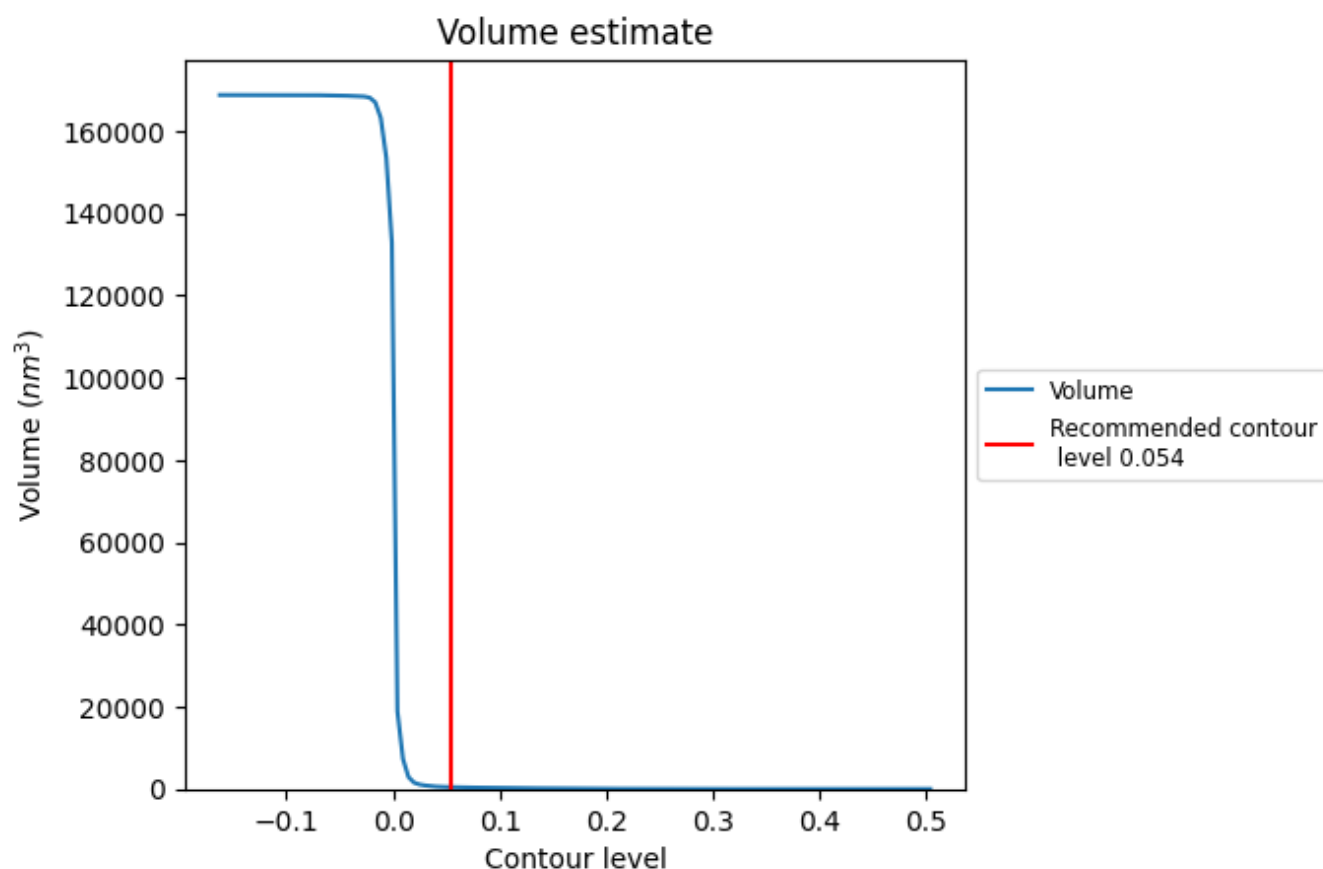
This section contains the results of statistical analysis of the map.

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.

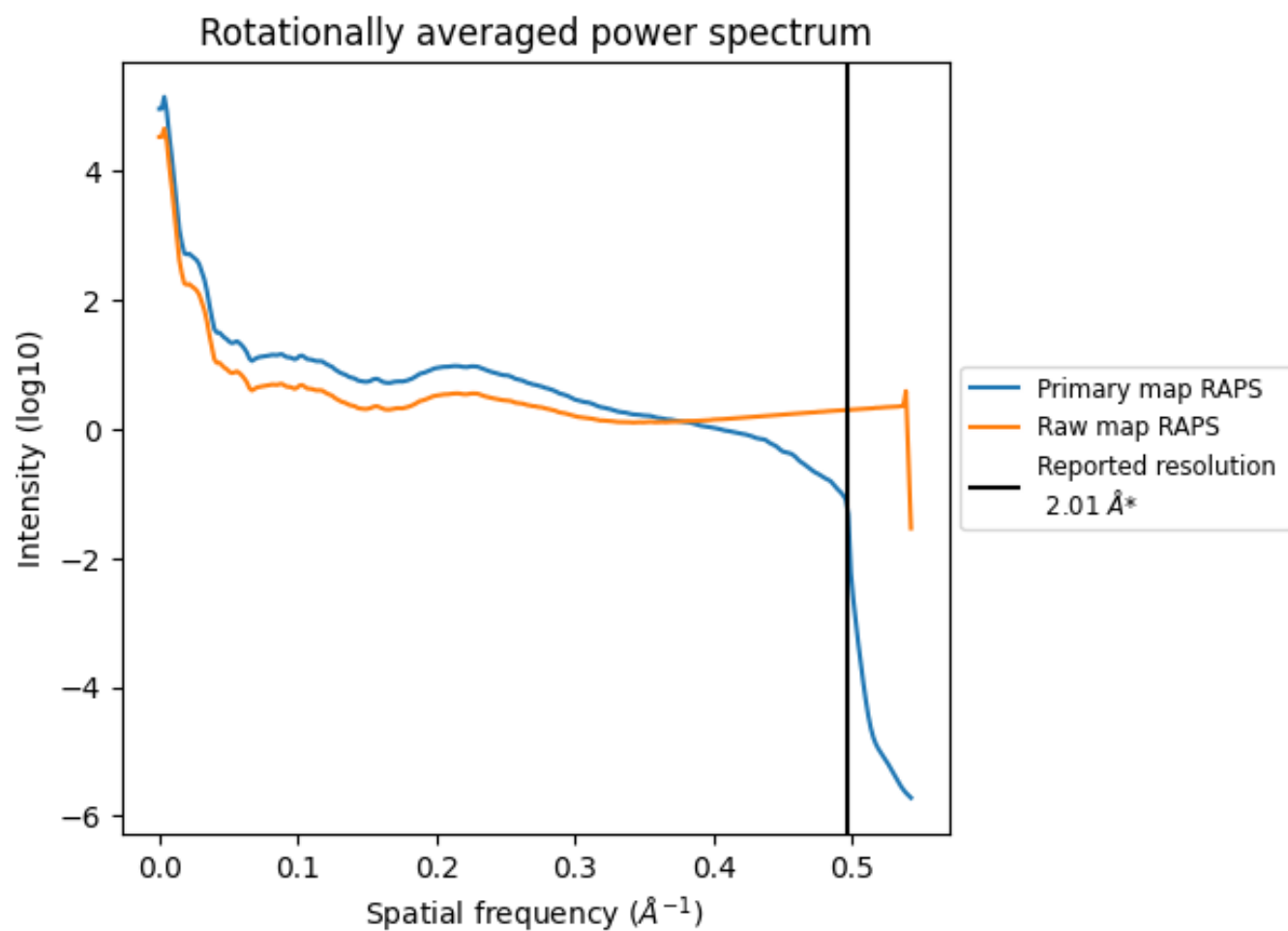
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 439 nm^3 ; this corresponds to an approximate mass of 396 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 ⓘ

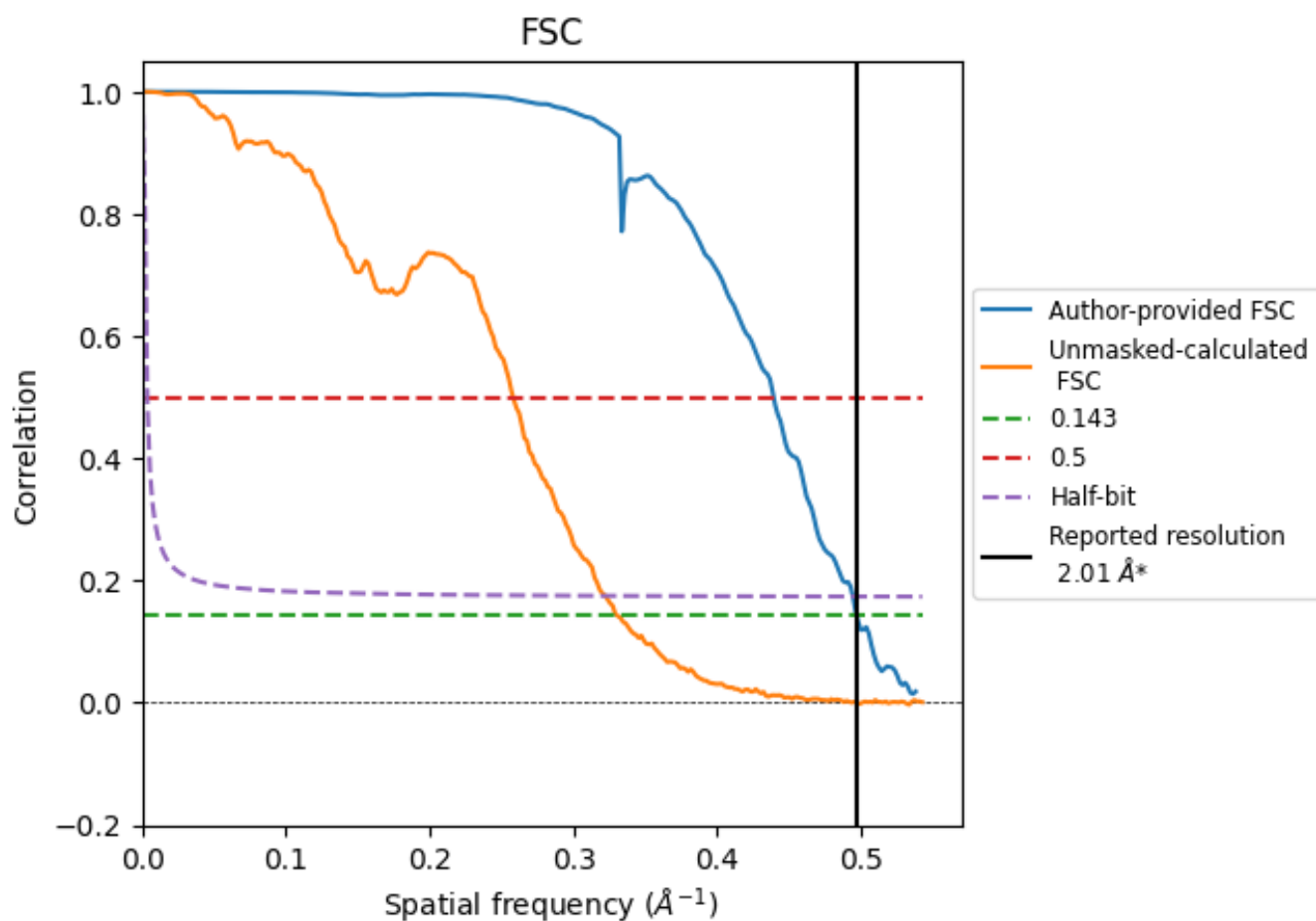


*Reported resolution corresponds to spatial frequency of 0.498 Å⁻¹

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 0.498 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

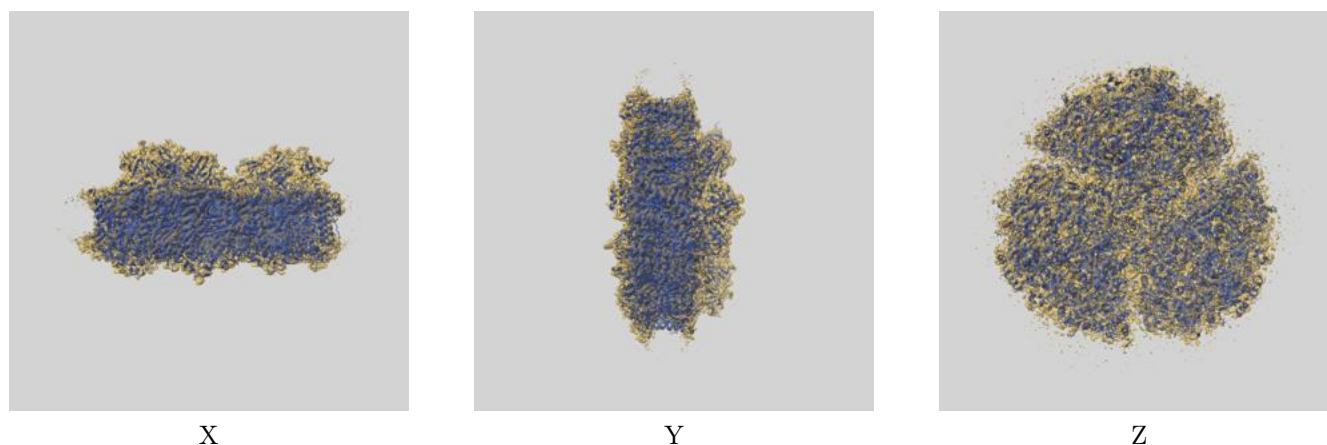
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	2.01	2.27	2.02
Unmasked-calculated*	3.03	3.87	3.10

*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 3.03 differs from the reported value 2.01 by more than 10 %

9 Map-model fit [i](#)

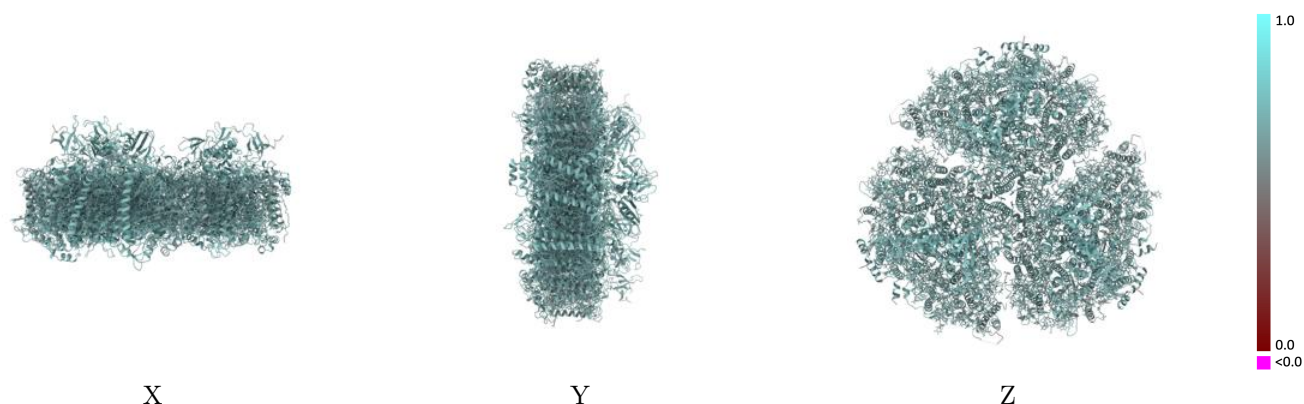
This section contains information regarding the fit between EMDB map EMD-50063 and PDB model 9EYS. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



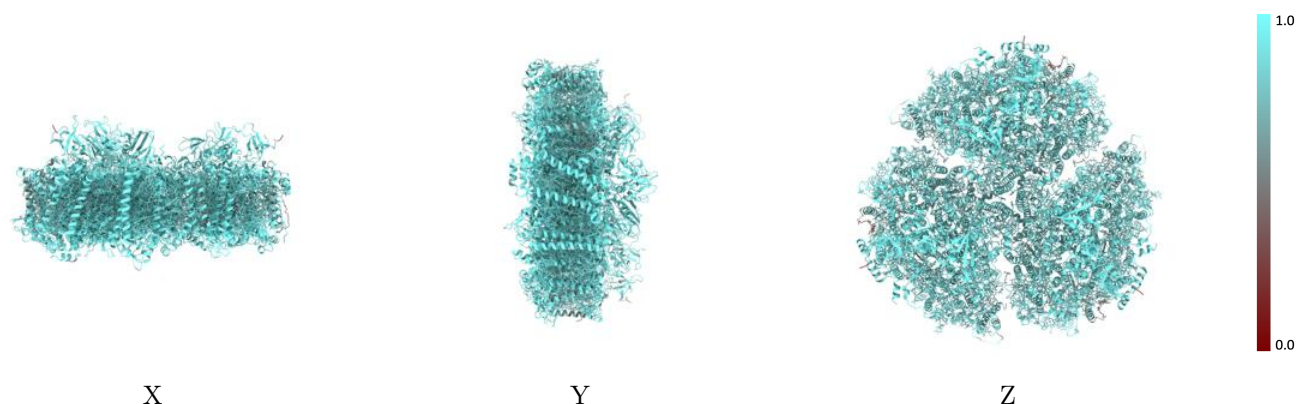
The images above show the 3D surface view of the map at the recommended contour level 0.054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



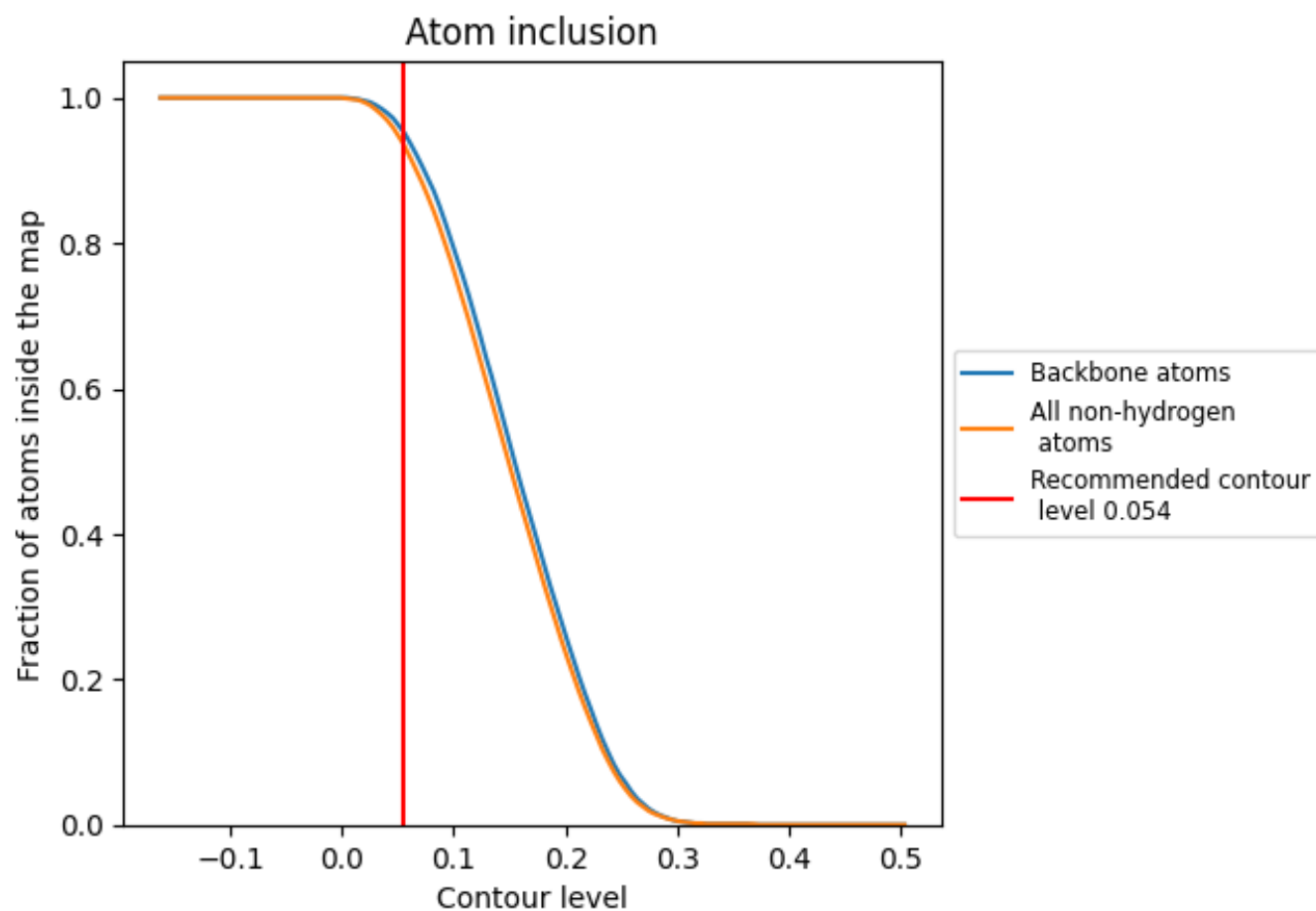
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.054).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.6720
A	 0.9470	 0.6750
B	 0.9540	 0.6780
C	 0.9900	 0.7050
D	 0.9570	 0.6740
E	 0.8950	 0.6460
F	 0.8920	 0.6430
I	 0.9590	 0.6890
J	 0.8860	 0.6330
K	 0.7630	 0.5740
L	 0.9590	 0.6910
M	 0.9230	 0.6640
N	 0.9460	 0.6760
O	 0.9530	 0.6790
P	 0.9920	 0.7070
Q	 0.9560	 0.6760
R	 0.8950	 0.6430
S	 0.8930	 0.6440
T	 0.9630	 0.6930
U	 0.8900	 0.6370
V	 0.7750	 0.5800
W	 0.9610	 0.6960
X	 0.7170	 0.5900
Y	 0.9230	 0.6650
Z	 0.7280	 0.5910
a	 0.9470	 0.6750
b	 0.9530	 0.6790
c	 0.9930	 0.7030
d	 0.9580	 0.6760
e	 0.8930	 0.6450
f	 0.9010	 0.6470
g	 0.9570	 0.6900
h	 0.8840	 0.6370
i	 0.7740	 0.5870
j	 0.9600	 0.6950



Continued on next page...

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Chain	Atom inclusion	Q-score
k	 0.9260	 0.6650
l	 0.7090	 0.5940